UNITED STATES
SECURITIES AND EXCHANGE COMMISSION
WASHINGTON, DC 20549

FORM 10-Q

(Mark One)

☒ **QUARTERLY REPORT PURSUANT TO SECTION 13 OR 15(d) OF THE SECURITIES EXCHANGE ACT OF 1934**

For the quarterly period ended March 31, 2022

OR

☐ **TRANSITION REPORT PURSUANT TO SECTION 13 OR 15(d) OF THE SECURITIES EXCHANGE ACT OF 1934**

For the transition period from to

Commission File Number: 001-39206

Schrodinger, Inc.

(Exact Name of Registrant as Specified in its Charter)

Delaware	**95-4284541**
(State or other jurisdiction of incorporation or organization)	**(I.R.S. Employer Identification No.)**
1540 Broadway, 24th Floor New York, NY	**10036**
(Address of principal executive offices)	**(Zip Code)**

Registrant's telephone number, including area code: (212) 295-5800

Securities registered pursuant to Section 12(b) of the Act:

Title of each class	Trading Symbol(s)	Name of each exchange on which registered
Common stock, par value $0.01 per share	SDGR	The Nasdaq Stock Market LLC

Indicate by check mark whether the registrant (1) has filed all reports required to be filed by Section 13 or 15(d) of the Securities Exchange Act of 1934 during the preceding 12 months (or for such shorter period that the registrant was required to file such reports), and (2) has been subject to such filing requirements for the past 90 days. Yes ☒ No ☐

Indicate by check mark whether the registrant has submitted electronically every Interactive Data File required to be submitted pursuant to Rule 405 of Regulation S-T (§232.405 of this chapter) during the preceding 12 months (or for such shorter period that the registrant was required to submit such files). Yes ☒ No ☐

Indicate by check mark whether the registrant is a large accelerated filer, an accelerated filer, a non-accelerated filer, smaller reporting company, or an emerging growth company. See the definitions of "large accelerated filer," "accelerated filer," "smaller reporting company," and "emerging growth company" in Rule 12b-2 of the Exchange Act.

Large accelerated filer	☒	Accelerated filer	☐
Non-accelerated filer	☐	Smaller reporting company	☐
Emerging growth company	☐		

If an emerging growth company, indicate by check mark if the registrant has elected not to use the extended transition period for complying with any new or revised financial accounting standards provided pursuant to Section 13(a) of the Exchange Act. ☐

Indicate by check mark whether the registrant is a shell company (as defined in Rule 12b-2 of the Exchange Act). Yes ☐ No ☒

As of April 19, 2022, the registrant had 61,973,968 shares of common stock, $0.01 par value per share, and 9,164,193 shares of limited common stock, $0.01 par value per share, outstanding.

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CAUTIONARY NOTE REGARDING FORWARD-LOOKING STATEMENTS

This Quarterly Report on Form 10-Q, or this Quarterly Report, contains forward-looking statements within the meaning of the U.S. Private Securities Litigation Reform Act and Section 21E of the Securities Exchange Act of 1934, as amended, that involve substantial risks and uncertainties. All statements, other than statements of historical fact, contained in this Quarterly Report, including statements regarding our strategy, future operations, future financial position, future revenue, projected costs, prospects, plans and objectives of management, are forward-looking statements. The words “aim,” “anticipate,” “believe,” “contemplate,” “continue,” “could,” “estimate,” “expect,” “goal,” “intend,” “may,” “might,” “plan,” “potential,” “predict,” “project,” “should,” “target,” “will,” “would” or the negative of these words or other similar expressions are intended to identify forward-looking statements, although not all forward-looking statements contain these identifying words.

The forward-looking statements in this Quarterly Report include, among other things, statements about:

- the potential advantages of our physics-based computational platform;
- our strategic plans to accelerate the growth of our software business;
- our research and development efforts for our internal drug discovery programs and our computational platform;
- the initiation, timing, progress, and results of our internal drug discovery programs or the drug discovery programs of our collaborators;
- our plans to submit investigational new drug applications to the U.S. Food and Drug Administration for our internal drug discovery programs;
- our plans to discover and develop product candidates and to maximize their commercial potential by advancing such product candidates ourselves or in collaboration with others;
- our plans to leverage the synergies between our businesses;
- the timing of, the ability to submit applications for and the ability to obtain and maintain regulatory approvals for any product candidates we or one of our collaborators may develop;
- our drug discovery collaborations and our estimates or expectations regarding any milestone or other payments we may receive from such collaborations, including pursuant to our collaboration with Bristol-Myers Squibb Company;
- our expectations regarding our ability to fund our operating expenses and capital expenditure requirements with our cash, cash equivalents, and marketable securities;
- the potential advantages of our drug discovery programs;
- the rate and degree of market acceptance of our software solutions;
- the potential continued impact of the COVID-19 pandemic on our business, operations, liquidity and prospects;
- the rate and degree of market acceptance and clinical utility of our products;
- our estimates regarding the potential market opportunity for our software solutions and any product candidate we or any of our collaborators may in the future develop;
- our marketing capabilities and strategy;
- our intellectual property position;
- our ability to identify technologies with significant commercial potential that are consistent with our commercial objectives;
- our expectations related to the use of our cash, cash equivalents, and marketable securities;
- our expectations related to the key drivers of our performance;
- the impact of government laws and regulations;
- our competitive position and expectations regarding developments and projections relating to our competitors and any competing products, technologies, or therapies that are or become available;
- our ability to maintain and establish collaborations or obtain additional funding; and
- our reliance on key personnel and our ability to identify, recruit, and retain skilled personnel.

We may not actually achieve the plans, intentions, or expectations disclosed in our forward-looking statements, and you should not place undue reliance on our forward-looking statements. Actual results or events could differ materially from the plans, intentions, and expectations disclosed in the forward-looking statements we make. We have included important factors in the cautionary statements included in this Quarterly Report, particularly in "Risk Factor Summary" below and Part II, Item 1A. "Risk Factors", that we believe could cause actual results or events to differ materially from the forward-looking statements that we make. Moreover, we operate in a competitive and rapidly changing environment. New risks and uncertainties emerge from time to time, and it is not possible for us to predict all risks and uncertainties that could have an impact on the forward-looking statements contained in this Quarterly Report. Our forward-looking statements do not reflect the potential impact of any future acquisitions, mergers, dispositions, collaborations, joint ventures, or investments we may make or enter into.

You should read this Quarterly Report and the documents that we file with the Securities and Exchange Commission, or the SEC, with the understanding that our actual future results may be materially different from what we expect. The forward-looking statements contained in this Quarterly Report are made as of the date of this Quarterly Report, and we do not assume any obligation to update any forward-looking statements, whether as a result of new information, future events or otherwise, except as required by applicable law.

In addition, statements that "we believe" and similar statements reflect our beliefs and opinions on the relevant subject. These statements are based upon information available to us as of the date of this Quarterly Report, and while we believe such information forms a reasonable basis for such statements, such information may be limited or incomplete. Our statements should not be read to indicate that we have conducted an exhaustive inquiry into, or review of, all potentially available relevant information. These statements are inherently uncertain and investors are cautioned not to unduly rely upon these statements.

Unless the context otherwise requires, we use the terms "company," "we," "us" and "our" in this Quarterly Report to refer to Schrödinger, Inc. and its consolidated subsidiaries.

RISK FACTOR SUMMARY

Our business is subject to a number of risks of which you should be aware before making an investment decision. Below we summarize what we believe are the principal risk factors but these risks are not the only ones we face, and you should carefully review and consider the full discussion of our risk factors in the section titled “Risk Factors”, together with the other information in this Quarterly Report.

- We have a history of significant operating losses, and we expect to incur losses over the next several years.
- If we are unable to increase sales of our software, or if we and our current and future collaborators are unable to successfully develop and commercialize drug products, our revenues may be insufficient for us to achieve or maintain profitability.
- Our quarterly and annual results may fluctuate significantly, which could adversely impact the value of our common stock.
- If our existing customers do not renew their licenses, do not buy additional solutions from us, or renew at lower prices, our business and operating results will suffer.
- A significant portion of our revenues are generated by sales to life sciences industry customers, and factors that adversely affect this industry could also adversely affect our software sales.
- The markets in which we participate are highly competitive, and if we do not compete effectively, our business and operating results could be adversely affected.
- We may never realize a return on our investment of resources and cash in our drug discovery collaborations.
- Although we believe that our computational platform has the potential to identify more promising molecules than traditional methods and to accelerate drug discovery, our focus on using our platform technology to discover and design molecules with therapeutic potential may not result in the discovery and development of commercially viable products for us or our collaborators.
- We may not be successful in our efforts to identify, discover or develop product candidates and may fail to capitalize on programs, collaborations, or product candidates that may present a greater commercial opportunity or for which there is a greater likelihood of success.
- As a company, we do not have any experience in clinical development and have not advanced any product candidate into clinical development.
- Conducting successful clinical trials requires the enrollment of a sufficient number of patients, and suitable patients may be difficult to identify and recruit.
- A widespread outbreak of an illness or other health issue, such as the COVID-19 pandemic, could negatively affect various aspects of our business and make it more difficult to meet our obligations to our customers, and could result in reduced demand from our customers as well as delays in our drug discovery and development programs.
- If we fail to comply with our obligations under our existing license agreements with Columbia University, under any of our other intellectual property licenses, or under any future intellectual property licenses, or otherwise experience disruptions to our business relationships with our current or any future licensors, we could lose intellectual property rights that are important to our business.
- If we are unable to obtain, maintain, enforce, and protect patent protection for our technology and product candidates or if the scope of the patent protection obtained is not sufficiently broad, our competitors could develop and commercialize technology and products similar or identical to ours, and our ability to successfully develop and commercialize our technology and product candidates may be adversely affected.
- Our internal information technology systems, or those of our third-party vendors, contractors, or consultants, may fail or suffer security breaches, loss or leakage of data, and other disruptions, which could result in a material disruption of our services, compromise sensitive information related to our business, or prevent us from accessing critical information, potentially exposing us to liability or otherwise adversely affecting our business.
- Our future success depends on our ability to retain key executives and to attract, retain, and motivate qualified personnel.
- We are pursuing multiple business strategies and expect to expand our development and regulatory capabilities, and as a result, we may encounter difficulties in managing our multiple business units and our growth, which could disrupt our operations.

- Our executive officers, directors, and principal stockholders, if they choose to act together, have the ability to influence all matters submitted to stockholders for approval.
- Our actual operating results may differ significantly from our guidance.

PART I—FINANCIAL INFORMATION

Item 1. Financial Statements.

SCHRÖDINGER, INC. AND SUBSIDIARIES

Condensed Consolidated Balance Sheets (Unaudited)

(in thousands, except for share and per share amounts)

Assets	March 31, 2022	December 31, 2021
Current assets:		
Cash and cash equivalents	$ 117,257	$ 120,267
Restricted cash	3,500	3,000
Marketable securities	408,275	456,212
Accounts receivable, net of allowance for doubtful accounts of $127 and $108	29,321	31,744
Unbilled and other receivables, net for allowance for unbilled receivables of $40 and $30	16,273	8,807
Prepaid expenses	11,542	5,030
Total current assets	586,168	625,060
Property and equipment, net	11,120	10,025
Equity investments	37,002	43,167
Goodwill	4,791	—
Intangible assets, net	986	—
Right of use assets	78,136	75,384
Other assets	1,334	2,851
Total assets	$ 719,537	$ 756,487
Liabilities and Stockholders' Equity		
Current liabilities:		
Accounts payable	$ 9,766	$ 8,079
Accrued payroll, taxes, and benefits	10,951	18,405
Deferred revenue	53,771	55,368
Lease liabilities	4,151	2,042
Other accrued liabilities	6,893	7,317
Total current liabilities	85,532	91,211
Deferred revenue, long-term	24,582	30,064
Lease liabilities, long-term	77,353	77,827
Other liabilities, long-term	1,400	300
Total liabilities	188,867	199,402
Commitments and contingencies (Note 6)		
Stockholders' equity:		
Preferred stock, $0.01 par value. Authorized 10,000,000 shares; zero shares issued and outstanding at March 31, 2022 and December 31, 2021	—	—
Common stock, $0.01 par value. Authorized 500,000,000 shares; 61,972,400 and 61,834,515 shares issued and outstanding at March 31, 2022 and December 31, 2021, respectively	620	618
Limited common stock, $0.01 par value. Authorized 100,000,000 shares; 9,164,193 shares issued and outstanding at March 31, 2022 and December 31, 2021	92	92
Additional paid-in capital	797,004	786,964
Accumulated deficit	(264,392)	(229,952)
Accumulated other comprehensive loss	(2,657)	(651)
Total stockholders' equity of Schrödinger stockholders	530,667	557,071
Noncontrolling interest	3	14
Total stockholders' equity	530,670	557,085
Total liabilities and stockholders' equity	$ 719,537	$ 756,487

See accompanying notes to unaudited condensed consolidated financial statements.

SCHRÖDINGER, INC. AND SUBSIDIARIES

Condensed Consolidated Statements of Operations (Unaudited)

(in thousands, except for share and per share amounts)

	Three Months Ended March 31,	
	2022	2021
Revenues:		
Software products and services	$ 33,081	$ 26,340
Drug discovery	15,582	5,787
Total revenues	48,663	32,127
Cost of revenues:		
Software products and services	7,511	5,906
Drug discovery	13,169	10,057
Total cost of revenues	20,680	15,963
Gross profit	27,983	16,164
Operating expenses:		
Research and development	27,822	21,448
Sales and marketing	6,671	5,239
General and administrative	22,133	13,389
Total operating expenses	56,626	40,076
Loss from operations	(28,643)	(23,912)
Other (expense) income:		
Loss on equity investments	—	(1,781)
Change in fair value	(6,164)	24,824
Interest income	328	420
Total other (expense) income	(5,836)	23,463
Loss before income taxes	(34,479)	(449)
Income tax (benefit) expense	(28)	74
Net loss	(34,451)	(523)
Net loss attributable to noncontrolling interest	(11)	(494)
Net loss attributable to Schrödinger common and limited common stockholders	$ (34,440)	$ (29)
Net loss per share attributable to Schrödinger common and limited common stockholders, basic and diluted:	$ (0.48)	$ (0.00)
Weighted average shares used to compute net loss per share attributable to Schrödinger common and limited common stockholders, basic and diluted:	71,050,432	70,071,625

See accompanying notes to unaudited condensed consolidated financial statements.

SCHRÖDINGER, INC. AND SUBSIDIARIES

Condensed Consolidated Statements of Comprehensive Loss (Unaudited)

(in thousands)

	Three Months Ended March 31,	
	2022	2021
Net loss attributable to Schrödinger common and limited common stockholders	$ (34,440)	$ (29)
Changes in market value of investments, net of tax:		
Unrealized loss on marketable securities	(2,006)	(240)
Comprehensive loss	$ (36,446)	$ (269)

See accompanying notes to unaudited condensed consolidated financial statements.

SCHRÖDINGER, INC. AND SUBSIDIARIES

Condensed Consolidated Statements of Stockholders' Equity (Unaudited)

(in thousands, except for share amounts)

	Common stock		Limited common stock		Additional paid-in capital	Accumulated deficit	Accumulated other comprehensive income (loss)	Non controlling interest	Total stockholders' equity
	Shares	Amount	Shares	Amount					
Balance at December 31, 2021	61,834,515	$ 618	9,164,193	$ 92	$ 786,964	$ (229,952)	$ (651)	$ 14	$ 557,085
Change in unrealized loss on marketable securities	—	—	—	—	—	—	(2,006)	—	(2,006)
Issuances of common stock upon stock option exercise	137,885	2	—	—	906	—	—	—	908
Stock-based compensation	—	—	—	—	9,134	—	—	—	9,134
Net loss	—	—	—	—	—	(34,440)	—	(11)	(34,451)
Balance at March 31, 2022	61,972,400	$ 620	9,164,193	$ 92	$ 797,004	$ (264,392)	$ (2,657)	$ 3	$ 530,670
Balance at December 31, 2020	60,713,534	$ 607	9,164,193	$ 92	$ 752,558	$ (129,559)	$ 317	$ 4	$ 624,019
Change in unrealized loss on marketable securities	—	—	—	—	—	—	(240)	—	(240)
Issuances of common stock upon stock option exercise	587,141	6	—	—	3,650	—	—	—	3,656
Stock-based compensation	—	—	—	—	4,366	—	—	—	4,366
Contributions by non-controlling interest	—	—	—	—		—	—	498	498
Net loss	—	—	—	—	—	(29)	—	(494)	(523)
Balance at March 31, 2021	61,300,675	$ 613	9,164,193	$ 92	$ 760,574	$ (129,588)	$ 77	$ 8	$ 631,776

See accompanying notes to unaudited condensed consolidated financial statements.

SCHRÖDINGER, INC. AND SUBSIDIARIES

Condensed Consolidated Statements of Cash Flows (Unaudited)

(in thousands)

	Three Months Ended March 31,	
	2022	**2021**
Cash flows from operating activities:		
Net loss	$ (34,451)	$ (523)
Adjustments to reconcile net loss to net cash used in operating activities:		
Loss on equity investments	—	1,781
Noncash revenue from equity investments	—	(5)
Fair value adjustments	6,164	(24,824)
Depreciation and amortization	969	887
Stock-based compensation	9,134	4,366
Noncash research and development expenses	—	498
Noncash investment amortization	1,504	1,955
(Gain) loss on disposal of property and equipment	(4)	19
Decrease (increase) in assets, net of acquisition:		
Accounts receivable, net	2,935	20,153
Unbilled and other receivables	(7,390)	(3,065)
Reduction in the carrying amount of right of use assets	1,221	1,264
Prepaid expenses and other assets	(7,725)	(3,549)
Increase (decrease) in liabilities, net of acquisition:		
Accounts payable	1,328	(1,230)
Accrued payroll, taxes, and benefits	(7,454)	(1,655)
Deferred revenue	(7,079)	(8,447)
Lease liabilities	489	(1,352)
Other accrued liabilities	637	2,806
Net cash used in operating activities	(39,722)	(10,921)
Cash flows from investing activities:		
Purchases of property and equipment	(1,696)	(513)
Distribution from equity investment	—	40
Proceeds from sale of equity investments	—	15,735
Acquisition, net of acquired cash	(6,427)	—
Purchases of marketable securities	(55,068)	(143,671)
Proceeds from maturity of marketable securities	99,495	66,500
Net cash provided by (used in) investing activities	36,304	(61,909)
Cash flows from financing activities:		
Issuances of common stock upon stock option exercises	908	3,656
Net cash provided by financing activities	908	3,656
Net decrease in cash and cash equivalents and restricted cash	(2,510)	(69,174)
Cash and cash equivalents and restricted cash, beginning of period	123,267	202,796
Cash and cash equivalents and restricted cash, end of period	$ 120,757	$ 133,622
Supplemental disclosure of cash flow and noncash information		
Cash paid for income taxes	$ 37	$ 119
Supplemental disclosure of non-cash investing and financing activities		
Purchases of property and equipment in accounts payable	317	52
Purchases of property and equipment in accrued liabilities	343	—
Acquisition of right to use assets, contingency resolution	1,513	—
Acquisition of right of use assets	1,146	—
Acquisition of lease liabilities	1,146	—

See accompanying notes to unaudited condensed consolidated financial statements.

SCHRÖDINGER, INC. AND SUBSIDIARIES

Notes to Condensed Consolidated Financial Statements (Unaudited)

For the three months ended March 31, 2022 and 2021

(in thousands, except for share and per share amounts)

(1) Description of Business

Schrödinger, Inc. (the "Company") has developed a differentiated, physics-based software platform that enables discovery of high-quality, novel molecules for drug development and materials applications more rapidly and at a lower cost, compared to traditional methods. The Company sells its software to biopharmaceutical and industrial companies, academic institutions, and government laboratories. The Company also applies its computational platform to a broad pipeline of drug discovery and development programs in collaboration with biopharmaceutical companies. In addition, the Company uses its platform to advance a pipeline of internal drug discovery programs.

(2) Significant Accounting Policies

(a) Recently Issued Accounting Pronouncements

In October 2021, the Financial Accounting Standards Board issued Accounting Standards Update ("ASU") No. 2021-08, *Business Combinations* (Topic 805) – *Accounting for Contract Assets and Contract Liabilities from Contracts with Customers*, which requires the measurement and recognition of contract assets and contract liabilities acquired in a business combination in accordance with Accounting Standards Codification ("ASC") 606, *Revenue from Contracts with Customers* (Topic 606). This update replaces the existing guidance requiring contract assets and contract liabilities to be measured and recognized at fair value. The standard is effective on a prospective basis for annual periods beginning after December 15, 2022, including interim periods within the fiscal year, with early adoption permitted. The Company early adopted this new standard effective January 1, 2022 with no material impact on its unaudited condensed consolidated financial statements.

(b) Basis of Presentation and Use of Estimates

The accompanying unaudited condensed consolidated financial statements and the related interim disclosures have been prepared in accordance with U.S. generally accepted accounting principles ("U.S. GAAP") and pursuant to the rules and regulations of the Securities and Exchange Commission ("SEC") for the interim financial information. These unaudited condensed consolidated financial statements include all adjustments necessary, consisting of only normal recurring adjustments, to fairly state the financial position and the results of the Company's operations and cash flows for interim periods in accordance with U.S. GAAP. Certain information and footnote disclosures normally included in financial statements prepared in accordance with GAAP have been condensed or omitted as permitted by the SEC's rules and regulations for interim reporting. Interim period results are not necessarily indicative of results of operations or cash flows for a full year or any subsequent interim period. The accompanying unaudited condensed consolidated financial statements should be read in conjunction with the audited consolidated financial statements and notes included in the Company's Annual Report on Form 10-K for the year ended December 31, 2021, which was filed with the SEC on February 24, 2022.

The preparation of financial statements in conformity with U.S. GAAP requires management to make estimates and assumptions that affect the reported amounts of assets and liabilities, disclosure of contingent assets and liabilities at the date of the consolidated financial statements, and the reported amounts of revenues and expenses during the reporting period. Significant estimates include the assumptions used in the allocation of revenue, estimates regarding the progress of completing performance obligations under collaboration agreements, and the valuation of stock-based compensation. Actual results could differ from those estimates, and such differences may be material to the unaudited condensed consolidated financial statements.

(c) Principles of Consolidation

The Company's unaudited condensed consolidated financial statements include the accounts of Schrödinger, Inc., its wholly owned subsidiaries, and its variable interest entity. All intercompany balances and transactions have been eliminated in consolidation. The functional currency for foreign entities is the United States dollar. The Company accounts for investments over which it has significant influence, but not a controlling financial interest, using the equity method.

(d) Restricted Cash

Restricted cash consists of letters of credit held with the Company's financial institution related to facility leases and is classified as current in the Company's balance sheets based on the maturity of the underlying letters of credit.

(e) Concentrations

Financial instruments that potentially subject the Company to concentrations of credit risk consist primarily of trade receivables.

The Company does not require customers to provide collateral to support accounts receivable. If deemed necessary, credit reviews of significant new customers may be performed prior to extending credit. The determination of a customer's ability to pay requires judgment, and failure to collect from a customer can adversely affect revenue, cash flows, and results of operations.

As of March 31, 2022, two customers accounted for 34% and 12% of total accounts receivable, respectively. As of December 31, 2021, three customers accounted for 17%, 15%, and 11% of total accounts receivable, respectively. One customer accounted for 15% of total revenues during the three months ended March 31, 2022 and no customers accounted for more than 10% of total revenues during the three months ended March 31, 2021.

(f) Income Taxes

The Company records deferred tax assets and liabilities for the expected future tax consequences of temporary differences between the financial statement carrying amounts and the tax basis of the assets and liabilities. Deferred tax assets are reduced by a valuation allowance when it is estimated to become more likely than not that a portion of the deferred tax assets will not be realized. Accordingly, the Company currently maintains a full valuation allowance against existing net deferred tax assets.

The Company recognizes the effect of income tax positions only if such positions are deemed "more likely than not" capable of being sustained. Interest and penalties accrued on unrecognized tax benefits are included within income tax expense in the unaudited condensed consolidated financial statements.

(g) Equity Investments

In the normal course of business, the Company has entered, and may continue to enter, into collaboration agreements with companies to perform drug design services for such companies in exchange for equity ownership stakes in such companies. If it is determined that the Company has control over the investee, the investee is consolidated in the financial statements. If the investee is consolidated with the Company and less than 100% of the equity is owned by the Company, the Company will present non-controlling interest to represent the portion of the investee owned by other investors. If it is determined that the Company does not have control over the investee, the Company evaluates the investment for the ability to exercise significant influence.

Equity investments over which the Company has significant influence may be accounted for under equity method accounting in accordance with ASC Topic 323, *Equity Method and Joint Ventures*. If it is determined that the Company does not have significant influence over the investee, and there is no readily determinable fair value for the investment, the equity investment may be accounted for at cost minus impairment in accordance with ASC Topic 321, *Equity Securities.*

For further information regarding the Company's equity investments, see Note 5, Fair Value Measurements, Note 10, Noncontrolling Interest, and Note 12, Equity Investments.

(h) Net Loss per Share Attributable to Common and Limited Common Stockholders

The outstanding equity of the Company consists of common stock and limited common stock. Under the Company's certificate of incorporation, the rights of the holders of common stock and limited common stock are identical, except with respect to voting and conversion. Holders of limited common stock are precluded from voting such shares in any election of directors or on the removal of directors. Limited common stock may be converted into common stock at any time at the option of the stockholder.

Undistributed earnings allocated to the participating securities are subtracted from net income in determining net (loss) income attributable to common and limited common stockholders. Basic net (loss) income per share is computed by dividing net (loss) income attributable to common and limited common stockholders by the weighted-average number of shares of common and limited common stock outstanding during the period.

For the calculation of diluted net income, net income attributable to common and limited common stockholders for basic net income is adjusted by the effect of dilutive securities, including awards under the Company's equity compensation plans. Diluted net income per share attributable to common and limited common stockholders is computed by dividing the resulting net income attributable to common and limited common stockholders by the weighted-average number of fully diluted shares of common and limited common stock outstanding.

(3) Revenue Recognition

Revenue is recognized upon transfer of control of promised products or services to customers in an amount that reflects the consideration to which the Company expects to be entitled in exchange for promised goods or services. The Company's performance obligations are satisfied either over time or at a point in time.

The following table illustrates the timing of the Company's revenue recognition:

	Three Months Ended March 31,	
	2022	2021
Software products and services – point in time	44.8%	54.0%
Software products and services – over time	23.2	28.0
Drug Discovery – point in time	19.0	-
Drug Discovery – over time	13.0	18.0

(a) Software Products and Services

The Company enters into contracts that can include various combinations of licenses, products and services, some of which are distinct and are accounted for as separate performance obligations. For contracts with multiple performance obligations, the Company allocates the transaction price of the contract to each performance obligation on a relative standalone selling price ("SSP") basis. Revenue is recognized net of any sale and value-added taxes collected from customers and subsequently remitted to governmental authorities.

The Company's software business derives revenue from five sources: (i) on-premise software license fees, (ii) hosted software subscription fees, (iii) software maintenance fees, (iv) professional services fees, and (v) contributions.

On-premise software. The Company's on-premise software license arrangements grant customers the right to use its software on their own in-house servers or their own cloud instances for a specified term, typically for one year. The Company recognizes revenue for on-premise software license fees upfront, either upon delivery of the license or the effective date of the agreement, whichever is later. In instances where the timing of delivery differs from the timing of invoicing, the Company considers whether a significant financing component exists. *The Company has elected the practical expedient to not assess for significant financing where the term is less than one year. The Company's updates and upgrades are not integral to maintaining the utility of the software licenses. Payments typically are received upfront or annually.*

Hosted software. Hosted software revenue consists primarily of fees to provide the Company's customers with hosted licenses, which allows these customers to access the Company's cloud-based software solution on their own hardware without taking control of licenses. Hosted software is recognized ratably over the term of the arrangement.

Software maintenance. Software maintenance includes technical support, updates, and upgrades related to our on-premise software licenses. Software maintenance revenue is considered to be a separate performance obligation and is recognized ratably over the term of the arrangement.

Professional services. Professional services, such as training, technical setup, installation or assisting customers with modeling and structural biology services, where the Company uses its software to perform tasks such as virtual screening and homology modeling on behalf of the Company's customers, generally are not related to the core functionality of the Company's software and are recognized as revenue when resources are consumed. The Company has historically estimated project status with relative accuracy, although a number of internal and external factors can affect such estimates, including labor rates, utilization and efficiency variances. Payments for services are due in advance or upon consumption of resources.

Software contribution revenue. Software contribution revenue consists of funds received under a non-reciprocal agreement with Gates Ventures, LLC. The agreement is an unconditional non-exchange contribution without restrictions. Revenue was recognized upon

execution of the agreement and on the first anniversary of the agreement when invoiced in accordance with ASC Topic 958, *Not-for-Profit Entities* as the agreement is not an exchange transaction.

The agreement with Gates Ventures, LLC covers the period from June 23, 2020 through June 22, 2023 for total consideration of up to $3,000. The Company received $1,000 in connection with its entry into the agreement in the second quarter of 2020, and $1,000 in the second quarter of 2021 on the first anniversary of its entry into the agreement. The Company is also entitled to receive an additional $1,000 payment on or around the second anniversary of the agreement, subject to the Company providing certain progress reports to the Trustees of Columbia University in the City of New York. As of March 31, 2022, the Company had no deferred revenue balance related to this agreement.

The following table presents the revenue recognized from the sources of software products and services revenue:

	Three Months Ended March 31,	
	2022	2021
On-premise software	$ 21,686	$ 17,355
Hosted software	3,255	2,600
Software maintenance	4,726	4,105
Professional services	3,414	2,280
Total software revenue	$ 33,081	$ 26,340

(b) Drug Discovery

Drug discovery services. Revenue from drug discovery and collaboration services contracts is recognized either over time, typically by using costs incurred or hours expended to measure progress, or at a point in time based on the achievement of milestones. Payments for services are generally due upon achieving milestones stated in a contract, upfront at the start of a contract, or upon consumption of resources. Services may at times include variable consideration and milestone payments. The Company has estimated the amount of consideration that is variable using the most likely amount method. The Company evaluates milestones on a case-by-case basis, including whether there are factors outside the Company's control that could result in a significant reversal of revenue, and the likelihood and magnitude of a potential reversal. If achievement of a milestone is not considered probable, the Company constrains (reduces) variable consideration to exclude the milestone payment until it is probable to be achieved.

As of March 31, 2022, milestones not yet achieved that were determined to be probable of achievement totaled $5,500, of which $3,500 was recognized as revenue for the three months ended March 31, 2022 and $2,000 was recognized as revenue during the three months ended December 31, 2021. As of March 31, 2021, milestones not yet achieved that were determined to be probable of achievement totaled $2,500, of which $2,213 was recognized as revenue for the three months ended March 31, 2021.

Drug discovery contribution revenue. Drug discovery contribution revenue consists of funds received under an agreement with Bill and Melinda Gates Foundation on a cost reimbursement basis, to perform services aimed at accelerating drug discovery in women's health, which began in November 2021. Revenue is recognized as conditions are met in accordance with ASC Topic 958, *Not-for-Profit Entities.* As of March 31, 2022, there was a $788 deferred revenue balance related to this agreement.

The following table presents the revenue recognized from the sources of drug discovery revenue:

	Three Months Ended March 31,	
	2022	2021
Drug discovery services revenue from contracts with customers	$ 15,241	$ 5,787
Drug discovery contribution	341	—
Total drug discovery revenue	$ 15,582	$ 5,787

(c) Collaboration and License Agreement

On November 22, 2020, the Company entered into an exclusive, worldwide collaboration and license agreement with Bristol-Myers Squibb Company ("BMS"), pursuant to which the Company and BMS have agreed to collaborate in the discovery, research and preclinical development of new small molecule compounds for disease indications in oncology, neurology, and immunology therapeutics areas. The Company will be responsible, at its own cost and expense, for the discovery of small molecule compounds directed to five specified biological targets pursuant to a mutually agreed research plan for each such target. The initial targets included HIF-2 alpha and SOS1/KRAS, which were two of the Company's internal programs. In November 2021, the Company and BMS mutually agreed to replace the HIF-2 alpha target with another precision oncology target. Following the replacement election, all rights

to the HIF-2 alpha target program reverted to the Company. Once a development candidate meeting specified criteria for a target under the agreement has been identified by the Company, BMS will be solely responsible for the further development, manufacturing and commercialization of such development candidate at its own cost and expense.

Under the terms of the agreement, BMS paid the Company an initial upfront fee payment of $55,000. The Company also is entitled to receive up to $2,700,000 in total milestone payments across all potential targets, consisting of: a) up to $585,000 in milestone payments per oncology target, including $360,000 in the aggregate for the achievement of certain specified research, development, and regulatory milestones and $225,000 in the aggregate for the achievement of certain specified commercial milestones; and b) up to $482,000 in milestone payments per neurology and immunology target, including $257,000 in the aggregate for the achievement of certain specified research, development, and regulatory milestones and $225,000 in the aggregate for the achievement of certain specified commercial milestones.

The Company is also entitled to a tiered percentage royalty on annual net sales ranging from mid-single digits to low-double digits, subject to certain specified reductions. Royalties are payable by BMS on a licensed product-by-licensed product and country-by-country basis until the later of the expiration of the last valid claim covering the licensed product in such country, expiration of all applicable regulatory exclusivities in such country for such licensed product and the tenth anniversary of the first commercial sale of such licensed product in such country.

The Company assessed the collaboration and license agreement in accordance with ASC 606, and concluded that BMS is a customer based on the agreement structure. At inception, the Company identified one performance obligation for each of the five programs under the agreement, which includes research activities for each program and a license grant for the underlying intellectual property. The Company determined that the license grant for intellectual property is not separable from the research activities, as the research activities are expected to significantly modify or enhance the license grant over the period of service, and therefore are not distinct in the context of the contract.

The Company determined that the transaction price at the onset of the agreement is $55,000. Additional consideration to be paid to the Company upon the achievement of future milestone payments were excluded from the transaction price as they represent milestone payments that are not considered probable as of the inception date such that there is not a significant risk of revenue reversal.

The Company has allocated the transaction price of $55,000 to each performance obligation based on the SSP of each performance obligation at inception, which was determined based on each performance obligation’s estimated SSP. The Company determined the estimated SSP at contract inception of the research activities based on internal estimates of the costs to perform the services, inclusive of a reasonable profit margin. Significant inputs used to determine the total costs to perform the research activities included the length of time required, the internal hours expected to be incurred on the services and the number and costs of various studies that will be performed to complete the research plan.

Revenue associated with the research activities is recognized on a proportional performance basis over the period of service for research activities, using input-based measurements of total costs of research incurred to estimate the proportion performed. Progress towards completion is remeasured at the end of each reporting period.

During the three months ended March 31, 2022 the Company recognized $4,000 associated with the agreement based on the research activities performed. As of March 31, 2022, there was $36,263 of deferred revenue related to the agreement, which was classified as either current or non-current in the condensed consolidated balance sheet based on the period the services are expected to be performed.

(d) Significant Judgments

Significant judgments and estimates are required under ASC Topic 606. Due to the complexity of certain contracts, the actual revenue recognition treatment required under Topic 606 for the Company’s arrangements may be dependent on contract-specific terms and may vary in some instances.

The Company’s contracts with customers often include promises to transfer multiple software products and services, including training, professional services, technical support services, and rights to unspecified updates. Determining whether licenses and services are distinct performance obligations that should be accounted for separately, or are not distinct and therefore should be accounted for together, requires significant judgment. In some arrangements, such as most of the Company’s term-based software license arrangements, the Company has concluded that the licenses and associated services are distinct from each other. In other arrangements, including collaboration services arrangements, the licenses and certain services may not be distinct from each other. The Company’s time-based software arrangements may include multiple software licenses and a right to updates or upgrades to the licensed software

products, and technical support. The Company has concluded that such promised goods and services are separate distinct performance obligations.

The Company is required to estimate the total consideration expected to be received from contracts with customers, including any variable consideration. Once the estimated transaction price is established, amounts are allocated to the performance obligations that have been identified. The transaction price is allocated to each separate performance obligation on a relative SSP basis.

Judgment is required to determine the SSP for each distinct performance obligation. The Company rarely licenses or sells products on a standalone basis, so the Company is required to estimate the range of SSPs for each performance obligation. In instances where the SSP is not directly observable because the Company does not sell the license, product, or service separately, the Company determines the SSP using information that includes historical discounting practices, market conditions, cost-plus analysis, and other observable inputs. The Company typically has more than one SSP for individual performance obligations due to the stratification of those items by classes of customers and circumstances. In these instances, the Company may use information such as the size and geographic region of the customer in determining the SSP. Professional service revenue is recognized as costs and hours are incurred, and judgment is required in estimating both the project status and the costs incurred or hours expended.

If a group of agreements are so closely related to each other that they are, in effect, part of a single arrangement, such agreements are deemed to be one arrangement for revenue recognition purposes. The Company exercises significant judgment to evaluate the relevant facts and circumstances in determining whether the separate agreements should be accounted for separately or as, in substance, a single arrangement. The Company's judgments about whether a group of contracts comprises a single arrangement can affect the allocation of consideration to the distinct performance obligations, which could have an effect on results of operations for the periods involved.

Judgment is required to determine the total costs to perform research activities, which include the length of time required, the internal hours expected to be incurred on the services, and the number and costs of various studies that may be performed by third-parties to complete the research plan.

Generally, the Company has not experienced significant returns or refunds to customers.

The Company's estimates related to revenue recognition require significant judgment and a change in these estimates could have an effect on the Company's results of operations during the periods involved.

(e) Contract Balances

The timing of revenue recognition may differ from the timing of invoicing to customers and these timing differences result in receivables, contract assets, or contract liabilities (deferred revenue) on the condensed consolidated balance sheets. The Company records a contract asset when revenue is recognized prior to invoicing. A deferred revenue liability is recorded when revenue is expected to be recognized subsequent to invoicing. For the Company's time-based software agreements, customers are generally invoiced at the beginning of the arrangement for the entire term, though when the term spans multiple years the customers may be invoiced on an annual basis. For certain drug discovery agreements where the milestones are deemed probable in a period prior to when the milestone is achieved, the Company records a contract asset for the full value of the milestone.

Contract assets are included in unbilled and other receivables within the condensed consolidated balance sheets and are transferred to receivables when the Company invoices the customer.

Contract balances were as follows:

	As of March 31, 2022	As of December 31, 2021
Contract assets	$ 14,765	$ 8,271
Deferred revenue, short-term:		
Software products and services	32,074	32,945
Drug discovery	21,697	22,423
Deferred revenue, long-term:		
Software products and services	3,633	3,938
Drug discovery	20,949	26,126

For the three months ended March 31, 2022 and 2021, respectively, the Company recognized $25,542 and $19,024 of revenue that was included in deferred revenue at December 31, 2021 and December 31, 2020, respectively. All other deferred revenue activity is due to the timing of invoices in relation to the timing of revenue, as described above. The Company expects to recognize as revenue approximately 69% of its March 31, 2022 deferred revenue balance in the next 12 months and the remainder thereafter. Additionally, contracted but unsatisfied performance obligations that had not yet been billed to the customer or included in deferred revenue were $23,927 as of March 31, 2022.

Payment terms and conditions vary by contract type, although terms typically require payment within 30 to 60 days. In instances where the timing of revenue recognition differs from that of invoicing, the Company has determined that its contracts generally do not include a significant financing component. The primary purpose of invoicing terms is to provide customers with simplified and predictable ways of purchasing the Company's products and services, not to facilitate financing arrangements.

(f) Deferred Sales Commissions

The Company has applied the practical expedient for sales commission expense, as any material compensation paid to sales representatives to obtain a contract relates to a period of one year or less. Therefore, the Company has not capitalized any costs related to sales commissions.

(4) Business Acquisition

On January 14, 2022, the Company used cash on hand to acquire all outstanding shares of XTAL BioStructures, Inc. ("XTAL"), a company that provides structural biology services, including biophysical methods, protein production and purification, and X-ray crystallography. The transaction qualified as a business combination for accounting purposes, which involves application of the acquisition method described in ASC Topic 805 *Business Combinations*. The cash purchase price was approximately $7,429 which included $6,427 in upfront purchase price, net of cash acquired. The acquisition of XTAL enables the Company to pursue scientific advancements in the field of structural biology, augment its ability to produce high quality target structures for its drug discovery programs, and expand its offerings to include an advanced and differentiated service that provides customers access to protein structures that have been computationally validated and are ready for structure-based virtual screening and lead optimization, giving rise to expected benefits supporting the amount of acquired goodwill.

The following table summarizes the provisional fair values of the assets acquired and liabilities assumed by the Company as of the January 14, 2022 acquisition date. The amounts recorded for unbilled revenue recorded in other current assets and deferred revenue recorded in current liabilities are preliminary and open for the finalization of the adoption of ASC 606. The Company has elected to use both practical expedients provided by ASU No. 2021-08 for the valuation of contract assets and contract liabilities from contracts with customers, with no material impact to the unaudited condensed consolidated financial statements.

Cash	$	1,002
Accounts receivable		588
Other current assets		95
Property, plant and equipment		297
Intangible assets		1,100
Goodwill		4,791
Total assets acquired		7,873
Current liabilities		209
Deferred tax liability		235
Total liabilities assumed		444
Net assets acquired	$	7,429

The following table summarizes the provisional purchase price allocation to the identifiable intangible assets and their estimated useful lives as of the January 14, 2022 acquisition date:

	Amount	Useful Life (years)
Backlog	$ 270	1
Customer relationships	710	5
Tradename/Trademark	120	1
	$ 1,100	

The results of operations for XTAL beginning as of the January 14, 2022 acquisition date are included in these unaudited condensed consolidated financial statements. For the three months ended March 31, 2022, the amount of revenues and net income of XTAL were not material to the unaudited condensed consolidated financial statements taken as a whole. Because the pro forma results of operations of the Company for the periods presented in this report would not be materially different as a result of the acquisition, such information is not presented. The costs incurred to acquire XTAL were not material and have been fully expensed and are included in general and administrative expenses in the unaudited condensed consolidated statements of operations.

(5) Fair Value Measurements

Various inputs are used in determining the fair value of the Company's financial assets and liabilities. These inputs are summarized into the following three broad categories:

Level 1 – quoted prices in active markets for identical securities

Level 2 – other significant observable inputs, including quoted prices for similar securities, interest rates, credit risk, etc.

Level 3 – significant unobservable inputs, including the Company's own assumptions in determining fair value

The inputs or methodology used for valuing securities are not necessarily an indication of the risk associated with investing in those securities. Marketable securities, which consist primarily of corporate and U.S. government agency bonds, are classified as available for sale and fair value does not differ significantly from carrying value as of March 31, 2022 and December 31, 2021. The following table presents information about the Company's assets and liabilities measured at fair value as of March 31, 2022:

	Level 1	Level 2	Level 3	Total
Assets:				
Marketable securities	$ —	$ 408,275	$ —	$ 408,275
Equity investments	33,524	—	1,759	35,283
Total	$ 33,524	$ 408,275	$ 1,759	$ 443,558

The following table presents information about the Company's assets and liabilities measured at fair value as of December 31, 2021:

	Level 1	Level 2	Level 3	Total
Assets:				
Marketable securities	$ —	$ 456,212	$ —	$ 456,212
Equity investments	39,561	—	1,887	41,448
Total	$ 39,561	$ 456,212	$ 1,887	$ 497,660

Fair value of the Company's investments in Nimbus Therapeutics, LLC ("Nimbus"), ShouTi Inc. ("ShouTi"), and Eonix, LLC ("Eonix"), classified as Level 3 in the fair value hierarchy, was determined under the hypothetical liquidated book value method ("HLBV method"), as further described in Note 12, Equity Investments. Significant unobservable inputs used under the HLBV method include

Nimbus', ShouTi's, and Eonix's annual financial statements and the Company's respective liquidation priorities. The following table sets forth changes in fair value of the Company's Level 3 investments:

	Amount
As of December 31, 2020	$ —
Cash contributions	2,000
Unrealized loss	(113)
As of December 31, 2021	1,887
Unrealized loss	(128)
As of March 31, 2022	$ 1,759

Unrealized gains and losses arising from changes in fair value of the Company's equity investments are classified within change in fair value in the condensed consolidated statements of operations. During the three months ended March 31, 2022 and the year ended December 31, 2021 there were no transfers between Level 1, Level 2 and Level 3 investments. See Note 12, Equity Investments, for further information.

(6) Commitments and Contingencies

(a) Leases

The Company leases office space under operating leases that expire at various dates through 2037. The Company has elected the package of practical expedients under the transition guidance of ASC Topic 842, *Leases*, to exclude short-term leases from the balance sheet and to combine lease and non-lease components.

Upon inception of a lease, the Company determines if an arrangement is a lease, if it includes options to extend or terminate the lease, and if it is reasonably certain that the Company will exercise the options. Lease cost, representing lease payments over the term of the lease and any capitalizable direct costs less any incentives received, is recognized on a straight-line basis over the lease term as lease expense.

In determining the present value of lease payments, the Company uses its incremental borrowing rate based on the information available at the lease commencement date if the rate implicit in the lease is not readily determinable. Upon execution of a new lease, the Company performs an analysis to determine its incremental borrowing rate using its current borrowing rate, adjusted for various factors including level of collateralization and lease term. As of March 31, 2022, the remaining weighted average lease term was 15 years.

During the three months ended March 31, 2022, right-of-use ("ROU") assets increased by $1,146 due to the accounting commencement of two new leases and by $2,828 due to a contingency resolution associated with the Company's New York office lease. There were no lease costs or incentives associated with acquiring the leases.

On November 1, 2021, the Company entered into an office lease agreement for 16,727 square feet of office space located at One Main Street, Cambridge, Massachusetts. Under the terms of the agreement, the Company will pay base rent of approximately $135 per month with a 3% annual rental escalation. The Company estimates that the lease commencement date will occur during the three months ending June 30, 2022 and continue to the end of the lease, which is 10 years after commencement.

On March 8, 2022, the Company entered into an office lease agreement for 15,045 square feet of office space located at 9868 Scranton Road, San Diego, California. Under the terms of the agreement, the Company will pay base rent of approximately $103 per month for the first year of the lease. Beginning the second year of the lease, the Company will pay base rent of approximately $61 per month with a 3% annual rental escalation. The Company estimates that the lease commencement date will occur during the three months ending March 31, 2023 and continue to the end of the lease, which is 8 years after commencement.

Variable and short-term lease costs were immaterial for the three months ended March 31, 2022. Additional details of the Company's operating leases are presented in the following table:

	Three Months Ended March 31,	
	2022	2021
Operating lease costs	$ 2,460	$ 1,470
Cash paid for operating leases	549	1,396

Maturities of operating lease liabilities as of March 31, 2022 under noncancelable operating leases were as follows:

Year ending December 31:		
Remainder of 2022	$	1,850
2023		8,960
2024		9,605
2025		9,236
2026		8,754
Thereafter		93,655
Total future minimum lease payments		132,060
Less: imputed interest		(50,556)
Present value of future minimum lease payments		81,504
Less: current portion of operating leases payments		(4,151)
Lease liabilities, long-term	$	77,353

(b) Legal Matters

From time to time, the Company may become involved in routine litigation arising in the ordinary course of business. While the results of such litigation cannot be predicted with certainty, management believes that the final outcome of such matters is not likely to have a material adverse effect on the Company's financial position or results of operations or cash flows.

(7) Income Taxes

The Company estimates an annual effective income tax rate based on projected results for the year and applies this rate to income before taxes to calculate income tax expense. Any refinements made due to subsequent information that affects the estimated annual effective income tax rate are reflected as adjustments in the current period.

For the three months ended March 31, 2022 and 2021, the Company's income tax (benefit) expense was $(28) and $74, respectively. For the three months ended March 31, 2022, the difference between the effective rate and the statutory rate was primarily attributed to the change in the valuation allowance against net deferred tax assets.

The Company recognizes the effect of income tax positions only if those positions are "more likely than not" capable of being sustained. As of March 31, 2022, the Company had $2,095 of unrecognized tax benefits. Interest and penalties accrued on unrecognized tax benefits are recorded as tax expense within the unaudited condensed consolidated financial statements. The Company does not expect a significant increase or decrease to the total amounts of unrecognized tax benefits within the next twelve months.

The Company and its subsidiaries file U.S. federal income tax returns and various state, local and foreign income tax returns. At March 31, 2022, the Company's statutes of limitations are open for all federal and state years filed after the year ended December 31, 2016 and 2015, respectively. Net operating loss ("NOL") and credit carryforwards from all years are subject to examination and adjustments for the three years following the year in which the carryforwards are utilized. The Company is not currently under Internal Revenue Service or state examination.

Pursuant to Internal Revenue Code Sections 382 and 383, the utilization of NOLs and other tax attributes may be substantially limited due to cumulative changes in ownership greater than 50% that may have occurred or could occur during applicable testing periods. The Company has performed an analysis through March 31, 2021 and determined that such an ownership change has occurred. There was no material impact to the financial statements due to this ownership change.

(8) Stockholders' Equity

(a) Common Stock

As of March 31, 2022, the Company had authorized 500,000,000 shares of common stock with a par value of $0.01 per share. Holders of common stock are entitled to one vote per share, to receive dividends, if and when declared by the board of directors, and upon liquidation or dissolution, to receive a portion of the assets available for distributions to stockholders, subject to preferential amounts owed to holders of the Company's preferred stock, if any.

Common stockholders have no preemptive or other subscription rights and there are no redemption or sinking fund provisions with respect to such shares. The rights, preferences and privileges of holders of the common stock are subject to and may be adversely affected by the right of the holders of shares of any series of preferred stock that the Company may designate and issue in the future.

(b) Limited Common Stock

As of March 31, 2022, the Company had authorized 100,000,000 shares of limited common stock with a par value of $0.01 per share. Holders of limited common stock are entitled to one vote per share, however, the holders of limited common stock shall not be entitled to vote such shares in any election of directors or on the removal of directors. Holders of limited common stock are entitled to receive dividends, if and when declared by the board of directors, and upon liquidation or dissolution, to receive a portion of the assets available for distributions to stockholders, subject to preferential amounts owed to holders of the Company's preferred stock, if any. Holders of the Company's limited common stock have the right to convert each share of limited common stock into one share of the Company's common stock.

Limited common stockholders have no preemptive or other subscription rights and there are no redemption or sinking fund provisions with respect to such shares. The rights, preferences and privileges of holders of the limited common stock are subject to and may be adversely affected by the right of the holders of shares of any series of preferred stock that the Company may designate and issue in the future.

(c) Preferred Stock

As of March 31, 2022, the Company had authorized 10,000,000 shares of undesignated preferred stock with a par value of $0.01 per share. The Company's board of directors has the discretion to determine the rights, preferences, privileges, and restrictions, including voting rights, dividend rights, conversion rights, redemption privileges, and liquidation preferences, of each series of preferred stock.

(9) Stock-Based Compensation

Stock Incentive Plans

As of March 31, 2022, the Company's stock incentive plans included the 2010 Stock Plan (the "2010 Plan"), the 2020 Equity Incentive Plan (the "2020 Plan"), and the 2021 Inducement Equity Incentive Plan (the "2021 Plan") (together, the "Plans"). The 2020 Plan provides for the award of incentive stock options, nonstatutory stock options, stock appreciation rights, restricted stock awards, restricted stock units, and other stock-based awards to employees, directors, consultants or advisors.

The 2021 Plan provides for the award of incentive stock options, nonstatutory stock options, stock appreciation rights, restricted stock awards, restricted stock units, and other stock-based awards to persons who were not previously an employee or director of the Company or who are commencing employment with the Company following a bona fide period of non-employment, in either case, as an inducement material to such person's entry into employment with the Company and in accordance with the requirements of the Nasdaq Stock Market Rule 5635(c)(4). Neither consultants nor advisors are eligible to participate in the 2021 Plan.

The 2010 Plan provided for the granting of incentive stock options and nonstatutory stock options to employees, directors, consultants or advisors. As of the effective date of the 2020 Plan, no further awards will be made under the 2010 Plan. Any options or awards outstanding under the 2010 Plan remain outstanding and effective. Shares of common stock subject to outstanding awards granted under the 2010 Plan that expire, terminate, or are otherwise surrendered, cancelled, forfeited, or repurchased by the Company are available for issuance under the 2020 Plan.

As of March 31, 2022 and December 31, 2021, there were 354,595 and 2,283,037 shares available for grant under the Plans. The following table presents classification of stock-based compensation expense within the unaudited condensed consolidated statements of operations:

	Three Months Ended March 31,	
	2022	2021
Cost of sales	$ 1,288	$ 657
Research and development	2,582	1,228
Sales and marketing	524	218
General and administrative	4,740	2,263
Total stock-based compensation	$ 9,134	$ 4,366

Restricted Stock Units

Each restricted stock unit ("RSU") represents the right to receive one share of the Company's common stock upon vesting. The fair value of RSUs granted by the Company was calculated based upon the Company's closing stock price on the date of the grant, and the stock-based compensation expense is recognized over the vesting period. RSUs generally vest over four years with 25% of the grants vesting at the end of the first year and the remaining vesting annually over the following three years.

The weighted average grant date fair value for each RSU granted during the three months ended March 31, 2022 was $27.76. There was no intrinsic value of RSUs settled during the three months ended March 31, 2022.

As of March 31, 2022, there was $1,299 of unrecognized compensation cost related to RSUs granted under the Plans, which is expected to be recognized over a weighted average period of 3.87 years. No RSUs vested during the three months ended March 31, 2022.

Stock Options

Stock options must be granted at an exercise price not less than 100% of the fair market value per share at the grant date. The board of directors or compensation committee determines the exercise price of the Company's stock options based on the closing price of the common stock as reported on the Nasdaq Global Select Market on the day of the grant. The maximum contractual term of options granted under the Plans is typically 10 years, options generally vest over four years with 25% of the shares underlying the option vesting at the end of the first year and the remaining vesting monthly over the following three years.

During the three months ended March 31, 2022 and 2021, 137,885 and 587,141 options under the Plans were exercised for total proceeds of $908 and $3,656, respectively.

The fair value of each option award is determined on the date of grant using the Black Scholes Merton option-pricing model. The calculation of fair value includes several assumptions that require management's judgment. The expected terms of options granted to employees during 2021 and 2020 were calculated using an average of historical exercises. Estimated volatility for the three months ended March 31, 2022 and 2021 incorporates a calculated volatility derived from the historical closing prices of shares of common stock of similar entities whose share prices were publicly available for the expected term of the option. The risk-free interest rate is based on the U.S. Treasury constant maturities in effect at the time of grant for the expected term of the option. The Company accounts for forfeitures as they occur, as such, the Company does not estimate forfeitures at the time of grant.

Following are the weighted average valuation assumptions used for option awards during the periods presented:

	Three Months Ended March 31,	
	2022	2021
Valuation assumptions		
Expected dividend yield	—%	—%
Expected volatility	56%	59%
Expected term (years)	4.74	4.67
Risk-free interest rate	1.77%	0.67%

The weighted average grant date fair value per share of options granted during the three months ended March 31, 2022 and 2021 was $13.52 and $49.30, respectively. The intrinsic value of options exercised during the three months ended March 31, 2022 and 2021 was $3,309 and $43,077, respectively.

As of March 31, 2022, there was $109,764 of unrecognized compensation cost related to unvested stock options granted under the Plans, which is expected to be recognized over a weighted average period of 3.09 years. The fair value of shares vested during the three months ended March 31, 2022 and 2021 was $19,545 and $9,462, respectively.

(10) Noncontrolling Interest

The Company reviews each legal entity formed by parties related to the Company to determine whether or not the Company has a variable interest in the entity and whether or not the entity would meet the definition of a variable interest entity ("VIE") in accordance with ASC Topic 810, *Consolidation*. If the entity is a VIE, the Company assesses whether or not the Company is the primary beneficiary of that VIE based on a number of factors, including (i) which party has the power to direct the activities that most significantly affect the VIE's economic performance, (ii) the parties' contractual rights and responsibilities pursuant to any contractual agreements and (iii) which party has the obligation to absorb losses or the right to receive benefits from the VIE. If the Company determines it is the primary beneficiary of a VIE, the Company consolidates the financial statements of the VIE into the Company's consolidated financial statements at the time that determination is made. The Company evaluates whether it continues to be the primary beneficiary of any consolidated

VIEs on a quarterly basis. If the Company were to determine that it is no longer the primary beneficiary of a consolidated VIE, or no longer has a variable interest in the VIE, it would deconsolidate the VIE in the period that the determination is made.

If the Company determines it is the primary beneficiary of a VIE that meets the definition of a business, the Company measures the assets, liabilities and noncontrolling interests of the newly consolidated entity at fair value in accordance with ASC Topic 805, *Business Combinations* at the date the reporting entity first becomes the primary beneficiary.

In October 2018, Faxian Therapeutics, LLC (“Faxian”) was formed in the United States. In April 2019, upon consummation of the joint venture, the Company and WuXi AppTech ("WuXi"), each received a 50% equity interest in the entity in exchange for their contributions to the entity. The Company determined that Faxian was a VIE and concluded that it is the primary beneficiary of the VIE. As such, the Company has consolidated Faxian's results into the unaudited condensed consolidated financial statements, and eliminated WuXi's ownership as a non-controlling interest.

(11) Net Loss per Share Attributable to Common and Limited Common Stockholders

The following table presents the calculation of basic and diluted net loss per share attributable to common and limited common stockholders for the periods presented (in thousands, except for share and per share data):

	Three Months Ended March 31,	
	2022	2021
Numerator:		
Net loss attributable to Schrödinger common and limited common stockholders	$ (34,440)	$ (29)
Denominator:		
Weighted average shares used to compute net loss per share attributable to Schrödinger common and limited common stockholders, basic and diluted:	71,050,432	70,071,625
Net loss per share attributable to Schrödinger common and limited common stockholders, basic and diluted:	$ (0.48)	$ (0.00)

Since the Company was in a loss position for the three months ended March 31, 2022 and 2021, basic net loss per share is the same as diluted net loss per share as the inclusion of all potential common shares and limited common shares outstanding would have been anti-dilutive. Potentially dilutive securities that were not included in the diluted per share calculations because they would be anti-dilutive were as follows:

	Three Months Ended March 31,	
	2022	2021
Shares subject to outstanding common stock options and RSUs	10,613,602	7,962,984

(12) Equity Investments

(a) Nimbus

The Company provides collaboration services for Nimbus under the terms of a master services agreement executed on May 18, 2010, as amended. Collaboration agreements are separate from the transaction that resulted in equity ownership and related fees are paid in cash to the Company. As Nimbus is a limited liability company and the Company is not a passive investor due to its collaboration with Nimbus on a number of drug discovery targets, the Company's management determined that it has significant influence over the entity and therefore accounts for the investment as an equity method investment.

The Company has concluded that the carrying value of its equity investment in Nimbus should reflect its contractual rights to substantive profits. The Company further determined that the HLBV method for valuing contractual rights to substantive profits provides the best representation of its financial position in Nimbus.

The HLBV method is a balance sheet-oriented approach to equity method accounting. Under the HLBV method, the Company determines its share of earnings or losses by comparing its claim on the book value at the beginning and end of each reporting period. This claim is calculated as the amount that the Company would receive (or be obligated to pay) if the investee were to liquidate all of

its assets at recorded amounts, determined as of the balance sheet date in accordance with U.S. GAAP, and distribute the resulting cash to creditors and investors in accordance with their respective priorities.

The carrying value of the Nimbus investment was zero as of March 31, 2022 and December 31, 2021. The Company has no obligation to fund Nimbus losses in excess of its initial investment. For the three months ended March 31, 2022 and March 31, 2021, the Company reported no gain or loss on the Nimbus investment.

(b) Morphic

The Company accounts for its investment in Morphic Holding, Inc. ("Morphic") at fair value based on the share price of Morphic's common stock at the measurement date.

For the three months ended March 31, 2022, the Company reported a loss of $6,037 on the Morphic investment. For the three months ended March 31, 2021, the Company reported a gain of $24,824 on the Morphic investment. As of March 31, 2022 and December 31, 2021, the carrying value of the Company's investment in Morphic was $33,524 and $39,561, respectively.

(c) Ravenna

In connection with the merger of Petra Pharma Corporation ("Petra") and a third party, the Company received 2,676,191 shares of common stock of Ravenna Pharmaceuticals, Inc. ("Ravenna"). The Company concluded that its equity investment in Ravenna should be valued as a non-marketable equity security as the Company does not exercise significant influence over Ravenna. As of each of March 31, 2022 and December 31, 2021, the carrying value of the Company's investment in Ravenna was $19.

(d) Ajax

In May 2021, the Company purchased 631,377 shares of Series B preferred stock of Ajax Therapeutics, Inc. ("Ajax") for $1,700 in cash. The Company has concluded that its equity investment in Ajax should be valued as a non-marketable equity security as the Company does not exercise significant influence over Ajax. As of each of March 31, 2022 and December 31, 2021, the carrying value of the Company's investment in Ajax was $1,700.

(e) ShouTi

In July 2021, the Company purchased 494,035 shares of Series B preferred stock of ShouTi for $2,000 in cash. As ShouTi is structured as a company limited by shares, incorporated under the laws of the Cayman Islands and the Company is not a passive investor due to its collaboration with ShouTi on a number of drug discovery targets, the Company's management determined that it has significant influence over the entity and therefore accounts for the investment as an equity method investment.

The Company has determined that the HLBV method for valuing contractual rights to substantive profits provides the best representation of its financial position in ShouTi. The carrying value of ShouTi was $1,759 and $1,887 as of March 31, 2022 and December 31, 2021, respectively. The Company has no obligation to fund ShouTi losses in excess of its initial investment. For the three months ended March 31, 2022 and 2021 the Company recorded losses of $128 and zero on the ShouTi investment, respectively.

(f) Eonix

On March 31, 2022, the Company received 4,000,000 membership interest units of Eonix in exchange for material science collaboration services under the terms of a master services agreement executed on March 31, 2022. As Eonix is a limited liability company and the Company is not a passive investor due to its collaboration with Eonix on a number of material science targets, the Company's management determined that it has significant influence over the entity and therefore accounts for the investment as an equity method investment.

The Company has determined that the HLBV method for valuing contractual rights to substantive profits provides the best representation of its financial position in Eonix. The carrying value of Eonix was zero as of March 31, 2022. For the three months ended March 31, 2022 the Company recorded no gain or loss on the Eonix investment.

(13) Related Party Transactions

(a) Board Member

For the three months ended March 31, 2022 and 2021, the Company paid consulting fees of $100 and $95, respectively, to a member of its board of directors.

(b) Bill and Melinda Gates Foundation

For the three months ended March 31, 2022 and 2021, the Bill & Melinda Gates Foundation, an entity under common control with Bill and Melinda Gates Foundation Trust, a stockholder of the Company, issued a grant under which it agreed to pay the Company directly for certain licenses and services provided to a specified group of third-party organizations. Revenue recognized for services provided by the Company under this grant were $200 and $730 for the three months ended March 31, 2022 and 2021, respectively. As of March 31, 2022 and December 31, 2021, the Company had net receivables of $8 and $165, respectively, due from the Bill & Melinda Gates Foundation.

For the three months ended March 31, 2022 and December 31, 2021, the Company recognized $341 and $111, respectively, in drug discovery contribution revenue related to funds received under an agreement with the Bill & Melinda Gates Foundation, aimed at accelerating drug discovery in women's health. As of March 31, 2022 and December 31, 2021, the Company had no receivables due under this agreement from the Bill & Melinda Gates Foundation.

The Company received $1,000 in contribution revenue in connection with its entry into an agreement with Gates Ventures, LLC in the second quarter of 2020, and $1,000 in contribution revenue in the second quarter of 2021 on the first anniversary of its entry into the agreement. Gates Ventures, LLC is an entity under control of William H. Gates III, who may be deemed to be the beneficial owner of more than 5% of the Company's voting securities. As of March 31, 2022 and December 31, 2021, the Company had no net receivables due from Gates Ventures, LLC.

(c) ShouTi

During the year ended December 31, 2021, the Company entered into multiple software agreements with ShouTi and its subsidiary for approximately $650. The Company recognized revenue of approximately $77 in the aggregate related to these agreements during the three months ended March 31, 2022.

(14) Segment Reporting

The Company has determined that its chief executive officer ("CEO") is its chief operating decision maker ("CODM"). The Company's CEO evaluates the financial performance of the Company based on two reportable segments: Software and Drug Discovery. The Software segment is focused on licensing the Company's software to transform molecular discovery. The Drug Discovery segment is focused on building a portfolio of preclinical and clinical drug programs, internally and through collaborations.

The CODM reviews segment performance and allocates resources based upon segment revenue and segment gross profit of the Software and Drug Discovery reportable segments. Segment gross profit is derived by deducting operational expenditures, with the exception of research and development, sales and marketing, and general and administrative activities from U.S. GAAP revenue. Operational expenditures are expenditures made that are directly attributable to the reportable segment. These expenditures are allocated to the segments based on headcount. The reportable segment expenditures include compensation, supplies, and services from contract research organizations.

Certain cost items are not allocated to the Company's reportable segments. These cost items primarily consist of compensation and general operational expenses associated with the Company's research and development, sales and marketing, and general and administrative. These costs are incurred by both segments and due to the integrated nature of the Company's Software and Drug Discovery segments, any allocation methodology would be arbitrary and provide no meaningful analysis.

All segment revenue is earned in the United States and there are no intersegment revenues. Additionally, the Company reports assets on a consolidated basis and does not allocate assets to its reportable segments for purposes of assessing segment performance or allocating resources. Presented below is financial information with respect to the Company's reportable segments for the periods presented:

	Three Months Ended March 31,	
	2022	2021
Segment revenues:		
Software	$ 33,081	$ 26,340
Drug discovery	15,582	5,787
Total segment revenues	$ 48,663	$ 32,127
Segment gross profit:		
Software	$ 25,570	$ 20,434
Drug discovery	2,413	(4,270)
Total segment gross profit	27,983	16,164
Unallocated:		
Research and development	(27,822)	(21,448)
Sales and marketing	(6,671)	(5,239)
General and administrative	(22,133)	(13,389)
Loss on equity investments	—	(1,781)
Change in fair value	(6,164)	24,824
Interest income	328	420
Income tax benefit (expense)	28	(74)
Consolidated net loss	$ (34,451)	$ (523)

The following table sets forth revenues by geographic area for the three months ended March 31, 2022 and 2021:

	Three Months Ended March 31,	
	2022	2021
United States	$ 30,275	$ 16,905
Europe	12,645	10,545
Japan	1,557	1,535
Rest of World	4,186	3,142
	$ 48,663	$ 32,127

(15) Subsequent Events

In April 2022, the Company entered into an agreement with the third party who previously acquired a collaborator in which the Company held an equity stake pursuant to which the Company agreed to terminate its rights to receive potential earnouts under the acquisition agreement in consideration for approximately $11,800 in cash.

Item 2. Management's Discussion and Analysis of Financial Condition and Results of Operations.

You should read the following discussion and analysis of our financial condition and results of operations together with our unaudited condensed consolidated financial statements and related notes appearing elsewhere in this Quarterly Report. Some of the information contained in this discussion and analysis or set forth elsewhere in this Quarterly Report, including information with respect to our plans and strategy for our business and related financing, includes forward-looking statements that involve risks and uncertainties. As a result of many factors, including those factors set forth in Part II, Item 1A. "Risk Factors" of this Quarterly Report, our actual results could differ materially from the results described in or implied by the forward-looking statements contained in the following discussion and analysis. For further information regarding our forward-looking statements, see "Cautionary Note Regarding Forward-Looking Statements" in this Quarterly Report.

Overview

We are transforming the way therapeutics and materials are discovered. Our differentiated, physics-based software platform enables discovery of high-quality, novel molecules for drug development and materials applications more rapidly and at a lower cost, compared to traditional methods. Our software platform is used by biopharmaceutical and industrial companies, academic institutions, and government laboratories around the world. Our multidisciplinary drug discovery team also leverages our software platform to advance collaborative drug discovery and development programs and our own pipeline of novel therapeutics to address unmet medical needs.

Since our founding, we have been primarily focused on developing our computational platform, which is capable of predicting critical properties of molecules with a high degree of accuracy, as well as advancing drug discovery programs both with our collaborators and internally. We have devoted substantially all of our resources to introducing new capabilities and refining our software, conducting research and development activities, recruiting skilled personnel, and providing general and administrative support for these operations.

We are using our computational platform for both collaborative and internal drug discovery programs. Over the last decade, we have entered into a number of collaborations with biopharmaceutical companies that have provided us with significant income and have the potential to produce additional milestone payments, option fees, and future royalties. Furthermore, in mid-2018, we launched a pipeline of internal, wholly-owned programs. We continue to advance multiple internal programs through investigational new drug, or IND, -enabling studies. We expect to submit an IND application to the U.S. Food and Drug Administration, or FDA, for our MALT1 program in the first half of 2022, and subject to receiving regulatory clearance, we expect to initiate a Phase 1 clinical trial of our MALT1 inhibitor, which we refer to as SGR-1505, in patients with relapsed and resistant lymphoma in the second half of 2022. We also plan to submit IND applications to the FDA for our CDC7 program in early 2023 and our WEE1 program in 2023, subject to favorable data from IND-enabling studies. In addition, we plan to initiate a Phase 1 clinical trial of our CDC7 inhibitor in 2023, subject to receipt of regulatory clearance.

We have funded our operations to date principally from the sale of our equity securities, including our initial public offering and our follow-on public offering, and to a lesser extent, from sales of our software solutions and from upfront payments, research funding and milestone payments from our drug discovery collaborations, and from distributions on account of, or proceeds from the sale of, our equity stakes in our collaborators.

We currently conduct our operations through two reportable segments: software and drug discovery. The software segment is focused on selling our software to transform drug discovery across the life sciences industry, as well as to customers in materials science industries. The drug discovery segment is focused on generating revenue from a diverse portfolio of preclinical and clinical programs, internally and through collaborations, that have advanced to various stages of discovery and development.

Our software segment generates revenue from software product licenses, hosted software subscriptions, software maintenance, professional services, and contributions. The revenue we generate through our software solutions from each of our customers varies largely depending on the number of software licenses our customers purchase from us. The licenses that our customers purchase from us provide them the ability to perform a certain number of calculations used in the design of molecules for drug discovery or materials science. We deliver our software through either (i) a product license that permits our customers to install the software solution directly on their own in-house hardware and use it for a specified term, or (ii) a subscription that allows our customers to access our cloud-based software solution on their own hardware without taking control of licenses.

We currently generate drug discovery revenue from our collaborations, including upfront payments, research funding payments and discovery and development milestones. In the future, we may also derive drug discovery revenue from our collaborations from option fees, the achievement of commercial milestones, and royalties on commercial drug sales. In addition to revenue from our collaborations, we may also derive drug discovery revenue from collaborating on or out-licensing our internal drug discovery programs

when we believe it will help maximize the commercial potential of the program. In November 2020, we entered into an exclusive, worldwide collaboration and license agreement with Bristol-Myers Squibb Company, or BMS, pursuant to which we and BMS agreed to collaborate in the discovery, research and development of small molecule compounds for biological targets in the oncology, neurology and immunology therapeutic areas. The initial collaboration targets included HIF-2 alpha and SOS1/KRAS, which were two of our internal pipeline programs. In November 2021, we and BMS mutually agreed to replace the HIF-2 alpha target with another precision oncology target. Following the replacement election, all rights to the HIF-2 alpha target program reverted to us. Under the terms of the agreement, we received an upfront payment of $55.0 million, and we are eligible to receive up to $2.7 billion in total milestone payments across all potential targets, as well as a tiered percentage royalty on net sales of each product commercialized by BMS ranging from mid-single digits to low-double digits, subject to certain specified reductions. See “Collaboration and License Agreement” in Note 3 to our unaudited condensed consolidated financial statements for additional information relating to this agreement.

In August 2021, we entered into a global discovery, development and commercialization collaboration with Zai Lab Limited focused on a novel program in oncology targeting DNA damage response. Under the terms of the agreement, we are entitled to receive an upfront payment to help fund our share of research costs, and if we elect to co-fund clinical development of a product candidate under the collaboration, we will be entitled to receive 50% of any profits from the commercialization of an approved therapeutic in the United States. We are also eligible to receive up to approximately $338 million in preclinical, clinical, regulatory and sales-based milestone payments from Zai Lab Limited for any product candidate developed under the collaboration, and we are entitled to receive tiered royalties on net sales outside the United States.

Furthermore, in January 2022, we acquired XTAL BioStructures, Inc., or XTAL, a company that provides structural biology services, including biophysical methods, protein production and purification, and X-ray crystallography, which we believe will expand our future offerings to include an advanced and differentiated service that provides customers access to protein structures that have been computationally validated and are ready for structure-based virtual screening and lead optimization. See “Business Acquisition” in Note 4 to our unaudited condensed consolidated financial statements for additional information relating to this acquisition.

We generated revenue of $48.7 million and $32.1 million during the three months ended March 31, 2022 and 2021, respectively, representing year-over-year growth of 51%. Our net loss attributable to Schrödinger common stockholders and limited common stockholders was $34.4 million and $0.0 million for the three months ended March 31, 2022 and 2021, respectively.

Business Impact of COVID-19 Pandemic

In order to safeguard the health of our employees in light of the COVID-19 pandemic, in early March 2020 we implemented a company-wide work-from-home policy. Beginning in June 2020, we began limited re-openings of certain of our offices in the United States and abroad. We have continued to phase-in the re-opening of our offices as our management and federal, state, or local authorities advise, and we may take further actions that alter our operations as may be required by federal, state, or local authorities, or which we determine are in our best interests.

We did not see material impacts to our business from the COVID-19 pandemic during the three months ended March 31, 2022 and the fiscal year ended December 31, 2021. While we do not expect the COVID-19 pandemic to have future material impacts on our business, the full extent of the future impact will depend on many factors outside of our control, including, without limitation, the extent, trajectory and duration of the COVID-19 pandemic, the development, availability and distribution of effective treatments and vaccines, the imposition of protective public safety measures, the emergence of new strains and variants of COVID-19 and the effectiveness of vaccines against such strains and variants, and the impact of the COVID-19 pandemic on the global economy. For instance, with respect to our software business, some of our customers may experience increasing budgetary pressures as a result of downturns or uncertainty in their respective businesses, which may cause them to delay or reduce purchases. In addition, due to the restrictions related to COVID-19 that remain in certain geographic regions, our sales force has limited in-person interactions, and their ability to attend events that promote and expand knowledge of our company and platform, including industry conferences and events, has been hampered. Relative to our and our collaborators’ drug discovery programs, the COVID-19 pandemic has resulted in and may in the future result in disruptions in current and future IND-enabling studies and clinical trials, manufacturing disruptions, trial site disruptions and impact the ability to obtain necessary institutional review board, institutional biosafety committee, or other necessary site approvals. These disruptions have caused and may in the future cause delays in certain of our and our collaborators’ drug discovery programs. For example, our contract manufacturing organizations, or CMOs, and our contract research organizations, or CROs, have experienced reductions in the capacity to undertake research-scale production and delays in executing some preclinical studies, including our IND-enabling studies for our CDC7 program. We now expect to submit the IND application to the FDA for our CDC7 program in early 2023 and to initiate a Phase 1 clinical trial in 2023. In addition, the recent resurgence of COVID-19 in certain cities in China, and related subsequent lockdowns, have also reduced the capacity of a number of CROs that we work with in those affected areas. We, together with our CMOs and CROs, are closely monitoring the impact of the COVID-19 pandemic on these operations, and we are actively

working to add supplemental or substitute capacity to minimize the impact of these reduced operations. Furthermore, if our collaborators experience similar delays with their drug discovery and development programs, that could cause additional delays in our achievement of milestones and related revenue. While there remains uncertainty about the extent of the effect of the COVID-19 pandemic, we do not envision a long-term impact from the COVID-19 pandemic on our ability to execute on our strategy.

Management is actively monitoring the COVID-19 pandemic and its possible effects on our financial condition, liquidity, operations, customers, contractors, and workforce. For additional information on risks posed by the COVID-19 pandemic, please see Part II, Item 1A.“Risk Factors –A widespread outbreak of an illness or other health issue, such as the COVID-19 pandemic, could negatively affect various aspects of our business and make it more difficult to meet our obligations to our customers, and could result in reduced demand from our customers as well as delays in our drug discovery and development programs,” included elsewhere in this Quarterly Report.

In response to the COVID-19 pandemic, we have joined a multi-company philanthropic effort to discover and develop novel small-molecule antiviral therapeutics to address COVID-19. The intent of the alliance, which to date also includes Takeda Pharmaceutical Company Limited, Novartis AG, Alphabet, Inc., Gilead Sciences, Inc., and WuXi AppTec, Inc., is to make any discoveries from this alliance available to the public. There is no expectation that this effort will generate revenue for any of the companies involved in the alliance, including us.

Components of Results of Operations

Software Products and Services Revenue

Our software business generates revenue from five sources: (i) on-premise software license fees, (ii) hosted software subscription fees, (iii) software maintenance fees, (iv) professional services fees, and (v) contributions.

On-premise software. Our on-premise software license arrangements grant customers the right to use our software on their own in-house servers or their own cloud instances for a specified term, typically for one year. We recognize revenue for on-premise software license fees upfront, either upon delivery of the license or the effective date of the agreement, whichever is later.

Hosted software. Hosted software revenue consists primarily of fees to provide our customers with hosted licenses, which allows these customers to access our cloud-based software solution on their own hardware without taking control of the licenses, and is recognized ratably over the term of the arrangement, which is typically one year. When a customer enters into a hosted arrangement for which revenue is recognized over time, the amount paid upfront that is not recognized in the current period is included in deferred revenue in our statement of financial position until the period in which it is recognized.

Software maintenance. Software maintenance includes technical support, updates, and upgrades related to our on-premise software licenses. Software maintenance revenue is recognized ratably over the term of the arrangement. Software maintenance activities are performed in connection with the use of our on-premise software, and may fluctuate from period to period.

Professional services. Professional services, such as training, technical setup, installation or assisting customers with modeling and structural biology services, where we use our software to perform tasks such as virtual screening and homology modeling on behalf of our customers, generally are not related to the core functionality of our software and are recognized as revenue when resources are consumed. Since each professional services agreement represents a unique, ad hoc engagement, professional services revenue may fluctuate from period to period.

Software contribution revenue. Software contribution revenue consists of funds received under a non-reciprocal agreement with Gates Ventures, LLC entered into June 2020. The agreement is an unconditional non-exchange contribution without restrictions. Revenue was recognized upon execution of the agreement and on the first anniversary of the agreement when invoiced, in accordance with Accounting Standard Codification, or ASC Topic 958, *Not-for-Profit Entities* as the agreement is not an exchange transaction. Additional revenue is expected to be recognized on the second anniversary of the agreement.

Drug Discovery Revenue

Drug discovery services. We currently generate drug discovery revenue from discovery collaboration arrangements, including research funding payments and discovery and development milestones. We expect our drug discovery revenue to trend higher over time as collaboration arrangements advance and we receive additional revenue from research funding payments, the achievement of discovery, development, and commercial milestones, option fees, and royalties on commercial drug sales. The majority of our current collaborations are in the discovery stage. Milestone payments typically increase in magnitude as a program advances. In addition to

revenue from our collaborations, we may also derive drug discovery revenue from entering into collaborations or out-licensing our internal drug discovery programs when we believe it will help maximize the commercial potential of the program. For example, in November 2020, we entered into an exclusive, worldwide collaboration and license agreement with BMS, pursuant to which we received an upfront payment of $55.0 million from BMS, of which approximately $4.0 million was included in our drug discovery revenue for the three months ended March 31, 2022. However, we expect that our revenue will fluctuate from period to period due to the inherently uncertain nature of the timing of milestone achievement and our dependence on the program decisions of our collaborators.

Drug discovery contribution revenue. Contribution revenue consists of funds received under an agreement with the Bill and Melinda Gates Foundation on a cost reimbursement basis, to perform services aimed at accelerating drug discovery in women's health. Revenue is recognized as conditions are met in accordance with ASC Topic 958, *Not-for-Profit Entities*.

Cost of Revenues

Software products and services. Cost of revenues for software includes personnel-related expenses (comprised of salaries, benefits, and stock-based compensation) for employees directly involved in the delivery of software solutions, maintenance and professional services, royalties paid for products sold and services performed using third-party licensed software functionality, and allocated overhead (facilities and information technology support) costs. Pursuant to various third-party arrangements, we license technology that is used in our software. These arrangements require us to pay royalties based on sales volume.

Drug discovery. Costs of revenue for drug discovery includes personnel-related expenses and costs of third-party contract research organizations, or CROs, that support discovery activities in our collaborations, royalties paid for services performed using third-party licensed software functionality, and allocated compute capacity and overhead costs. While we have incurred costs associated with discovery efforts since late 2017, we have recognized and expect to continue to recognize revenues in the future if and when milestones are achieved. Generally, drug discovery costs of revenue for collaborations are incurred in advance of the revenue milestone achievement.

We expect our drug discovery costs of revenue to trend higher over time as our discovery collaborations advance.

Gross Profit and Gross Margin

Gross profit represents revenue less cost of revenues. Gross margin is gross profit expressed as a percentage of revenue. Our software products and services gross margin may fluctuate from period to period as our revenue fluctuates, and as a result of changes in sales mix between on-premise and hosted software solutions. For example, the cost of royalties due for sales of our hosted software arrangements are recognized upfront, whereas the associated revenue is recognized over the term of the underlying agreement. Currently, gross margin is not meaningful for measuring the operating results of our drug discovery business.

Research and Development Expense

Research and development expense accounts for a significant portion of our operating expenses. We recognize research and development expense as incurred. Research and development expense consists of internal drug discovery and development program costs and costs incurred for continuous development of the technology and science that supports our computational platform, primarily:

- personnel-related expenses, including salaries, benefits, bonuses, and stock-based compensation for employees engaged in research and development functions;
- expenses incurred under agreements with third-party CROs and consultants involved in our internal discovery and development programs; and
- allocated compute capacity on our internal discovery and development programs and overhead (facilities and information technology support) costs.

We expect our research and development expense to increase substantially in absolute dollars for the foreseeable future as we continue to invest in activities related to discovery and development of our internal drug discovery programs, in advancing our platform, and as we incur expenses associated with hiring additional personnel directly involved in such efforts. At this time, we do not know, nor can we reasonably estimate, the nature, timing, or costs of the efforts that will be necessary to complete the development of any of our internal drug discovery programs. Since our internal drug discovery efforts are in the early stages, currently we do not track research and development expense on a program-by-program basis.

Sales and Marketing Expense

Sales and marketing expense consists primarily of personnel-related costs for our sales and marketing staff and application scientists supporting our sales efforts, including salaries, benefits, bonuses, and stock-based compensation. Other sales and marketing costs include promotional events that promote and expand knowledge of our company and platform, including industry conferences and events and our annual user group meetings in the United States and Europe, advertising, and allocated overhead costs. Due to the inherent scientific complexity of our software solutions, a high level of scientific expertise is needed to support our sales and marketing efforts. We plan to make focused investments in sales and marketing over the foreseeable future to foster the growth of our business as we aim to expand software sales to existing customers and increase our customer base.

General and Administrative Expense

General and administrative expense consists of personnel-related expenses associated with our executive, legal, finance, human resources, information technology, and other administrative functions, including salaries, benefits, bonuses, and stock-based compensation. General and administrative expense also includes professional fees for external legal, accounting and other consulting services, allocated overhead costs, and other general operating expenses.

We expect to increase the size of our general and administrative staff to support the anticipated growth of our business. We expect to continue to incur additional expenses as a result of operating as a public company, including costs to comply with the rules and regulations applicable to companies listed on a U.S. securities exchange and costs related to compliance and reporting obligations pursuant to the rules and regulations of the Securities and Exchange Commission, or SEC. In addition, as a public company, we expect to continue to incur increased expenses such as insurance and professional services. As a result, we expect the dollar amount of our general and administrative expense to increase for the foreseeable future.

Loss on Equity Investments

Loss on equity investments consists of realized gains in the form of cash distributions received from our equity investments offset by realized losses on the sale of equity.

Change in Fair Value

Fair value gains and losses consist of adjustments to the fair value of our equity investments, including Nimbus Therapeutics, Inc., or Nimbus, ShouTi Inc., or ShouTi, Eonix, LLC, or Eonix, and Morphic Holding, Inc., or Morphic. We remeasure our investments at each period end.

We expect that fair value gains and losses will fluctuate significantly in future periods.

Interest Income

Interest income consists of interest earned on our cash equivalents and marketable securities.

Income Tax (Benefit) Expense

Income tax (benefit) expense consists of U.S. federal and state income taxes and income taxes in certain foreign jurisdictions in which we conduct business. We maintain a full valuation allowance on our federal and state deferred tax assets as we have concluded that it is not more likely than not that the deferred tax assets will be realized.

Results of Operations

Comparison of the three months ended March 31, 2022 and 2021

The following table summarizes our unaudited results of operations data for the three months ended March 31, 2022 and 2021:

	Three Months Ended March 31,		Change	
	2022	2021	$	%
	(in thousands)			
Revenues:				
Software products and services	$ 33,081	$ 26,340	$ 6,741	26%
Drug discovery	15,582	5,787	9,795	169%
Total revenues	48,663	32,127	16,536	51%
Cost of revenues:				
Software products and services	7,511	5,906	1,605	27%
Drug discovery	13,169	10,057	3,112	31%
Total cost of revenues	20,680	15,963	4,717	30%
Gross profit	27,983	16,164	11,819	73%
Operating expenses:				
Research and development	27,822	21,448	6,374	30%
Sales and marketing	6,671	5,239	1,432	27%
General and administrative	22,133	13,389	8,744	65%
Total operating expenses	56,626	40,076	16,550	41%
Loss from operations	(28,643)	(23,912)	(4,731)	20%
Other (expense) income:				
Loss on equity investments	—	(1,781)	1,781	N/M
Change in fair value	(6,164)	24,824	(30,988)	N/M
Interest income	328	420	(92)	N/M
Total other (expense) income	(5,836)	23,463	(29,299)	N/M
Loss before income taxes	(34,479)	(449)	(34,030)	N/M
Income tax (benefit) expense	(28)	74	(102)	N/M
Net loss	(34,451)	(523)	(33,928)	N/M
Net loss attributable to noncontrolling interest	(11)	(494)	483	N/M
Net loss attributable to Schrödinger common and limited common stockholders	$ (34,440)	$ (29)	$ (34,411)	N/M

N/M – not meaningful

Revenues

	Three Months Ended March 31,		Change	
	2022	2021	$	%
	(in thousands)			
Revenues:				
Software				
On-premise software	$ 21,686	$ 17,355	$ 4,331	25%
Hosted software	3,255	2,600	655	25%
Software maintenance	4,726	4,105	621	15%
Professional services	3,414	2,280	1,134	50%
Total software products and services	33,081	26,340	6,741	26%
Drug discovery				
Drug discovery services	15,241	5,787	9,454	163%
Drug discovery contribution	341	—	341	-
Total drug discovery	15,582	5,787	9,795	169%
Total revenues	$ 48,663	$ 32,127	$ 16,536	51%

On-premise software. The increase in revenues for on-premise software for the three months ended March 31, 2022 as compared to the three months ended March 31, 2021 was primarily attributable to increased sales from existing and new customers, growth in multi-year agreements, and timing of revenue for customer renewals.

Hosted software. The increase in revenues for hosted software for the three months ended March 31, 2022 as compared to the three months ended March 31, 2021 was primarily due to growth in new customers purchasing hosted software subscriptions, as well as increased spend from existing hosted customers, for which revenue is recognized ratably over time.

Software maintenance. The increase in revenues for software maintenance for the three months ended March 31, 2022 as compared to the three months ended March 31, 2021 was primarily due to the increase in on-premise software sales in current and previous years. Software maintenance revenue is recognized over time.

Professional services. The increase in revenues from professional services for the three months ended March 31, 2022 as compared to the three months ended March 31, 2021 was primarily due to the addition of XTAL, revenue subsequent to the acquisition, and the timing of technology and modeling service projects.

Software contribution revenue. There was no contribution revenue for the three months ended March 31, 2022 and 2021 from the agreement with Gates Ventures, LLC, which began in June 2020.

Drug discovery services. The increase in revenues for drug discovery services for the three months ended March 31, 2022 as compared to the three months ended March 31, 2021 was primarily due to the timing and amount of collaboration milestones achieved, the progress of existing and new collaborations accomplished during the period, as well as research funding received during the three months ended March 31, 2022. We expect that our revenue will fluctuate from period to period due to the inherently uncertain nature of the timing of milestone achievement and our dependence on the program decisions of our collaborators.

Drug discovery contribution revenue. Contribution revenue for the three months ended March 31, 2022 was due to services performed under an agreement with the Bill and Melinda Gates Foundation, aimed at accelerating drug discovery in women's health, which began in November 2021.

Cost of Revenues

	Three Months Ended March 31,		Change	
	2022	2021	$	%
	(in thousands)			
Cost of revenues:				
Software products and services	$ 7,511	$ 5,906	$ 1,605	27%
Gross margin	77%	78%		
Drug discovery	13,169	10,057	3,112	31%

Software products and services. The increase in cost of revenues for software products and services during the three months ended March 31, 2022 compared to the three months ended March 31, 2021 was attributable to increases of approximately $0.9 million in personnel-related expense, approximately $0.4 million in royalty expense due to higher sales levels, and approximately $0.3 million in other expenses.

Software products and services gross margin. The decrease in software gross margin during the three months ended March 31, 2022 compared to the three months ended March 31, 2021 reflects our investment to support the rollout of large-scale deployments of our platform, as well as an increase in royalty fees.

Drug discovery. The increase in cost of revenues for drug discovery during the three months ended March 31, 2022 compared to the three months ended March 31, 2021 was attributable to increases of approximately $1.6 million in third-party CRO costs associated with the expansion and progression of collaboration drug discovery programs, including the BMS collaboration, approximately $1.4 million in personnel-related expense, and approximately $0.1 million in other expenses.

Research and Development Expense

	Three Months Ended March 31,		Change	
	2022	2021	$	%
	(in thousands)			
Research and development	$ 27,822	$ 21,448	$ 6,374	30%

The increase in research and development expense during the three months ended March 31, 2022 compared to the three months ended March 31, 2021 was attributable to increases of approximately $4.5 million in personnel-related expense, approximately $1.0 million in CRO costs associated with the expansion and progression of internal drug discovery programs, approximately $0.8 million in cloud computing expenses, and approximately $0.1 million in other expenses.

Sales and Marketing Expense

	Three Months Ended March 31,		Change	
	2022	2021	$	%
	(in thousands)			
Sales and marketing	$ 6,671	$ 5,239	$ 1,432	27%

The increase in sales and marketing expense during the three months ended March 31, 2022 compared to the three months ended March 31, 2021 was attributable to increases of approximately $0.8 million in personnel-related expense, approximately $0.2 million in travel and entertainment expenses, approximately $0.1 million in cloud computing expenses, and approximately $0.3 million in other expenses.

General and Administrative Expense

	Three Months Ended March 31,		Change	
	2022	2021	$	%
	(in thousands)			
General and administrative	$ 22,133	$ 13,389	$ 8,744	65%

The increase in general and administrative expense during the three months ended March 31, 2022 compared to the three months ended March 31, 2021 was attributable to increases of approximately $5.5 million in personnel-related expense, approximately $1.1 million related to a one-time non-recurring state and local tax item, approximately $0.7 million related to professional services, and approximately $1.4 million of other expenses, primarily reflecting costs necessary to build and maintain a public company infrastructure.

Loss on Equity Investments

	Three Months Ended March 31,		
	2022	2021	Change
	(in thousands)		
Loss on equity investments	$ -	$ (1,781)	$ 1,781

The loss on equity investments during the three months ended March 31, 2021 was primarily due to the realized loss on the disposal of our equity stake in Relay Therapeutics, Inc., or Relay.

Change in Fair Value

	Three Months Ended March 31,		
	2022	2021	Change
	(in thousands)		
Change in fair value	$ (6,164)	$ 24,824	$ (30,988)

The change in fair value during the three months ended March 31, 2022 was primarily due to a loss on our investment in Morphic. The change in fair value during the three months ended March 31, 2021 was due to a gain on our investment in Morphic of $24.8.

Interest Income

	Three Months Ended March 31,		
	2022	2021	Change
	(in thousands)		
Interest income	$ 328	$ 420	$ (92)

Interest income decreased during the three months ended March 31, 2022 compared to the three months ended March 31, 2021 primarily due to lower bond investment balances.

Income Tax (Benefit) Expense

	Three Months Ended March 31,		
	2022	2021	Change
	(in thousands)		
Income tax (benefit) expense	$ (28)	$ 74	$ (102)

The income tax benefit during the three months ended March 31, 2022 was due to the release of the valuations allowance due to the acquisition of XTAL. During the three months ended March 31, 2021, due to the full valuation allowance on our U.S. federal and state tax assets, income tax expense primarily represented our income tax obligations in certain foreign jurisdictions in which we conduct business.

Critical Accounting Estimates

Detailed information about our critical accounting estimates is set forth in Part II, Item 7 of our Annual Report on Form 10-K for the year ended December 31, 2021. There were no material changes to our critical accounting estimates during the three months ended March 31, 2022.

Liquidity, Capital Resources and Funding Requirements

We have a history of significant operating losses and have incurred negative cash flows from operations from inception through the three months ended March 31, 2022. As of March 31, 2022, we had an accumulated deficit of $264.4 million.

We have funded our operations to date principally from the sale our equity securities, including our initial public offering and our follow-on public offering, and to a lesser extent, from sales of our software solutions and from upfront payments, research funding and milestone payments from our drug discovery collaborations, and from distributions on account of, or proceeds from the sale of, our equity stakes in our collaborators. Our operating cash flows are impacted by the magnitude and timing of our software sales and by the magnitude and timing of our drug discovery milestone achievements and research funding fees.

As of March 31, 2022, we had cash, cash equivalents and marketable securities of $529.0 million.

On March 4, 2021, we filed a universal shelf registration statement on Form S-3 which allows us to offer and sell an indeterminate number of shares of common stock, preferred stock, depositary shares or warrants, or an indeterminate principal amount of debt securities, from time to time pursuant to one or more offerings at prices and terms to be determined at the time of the sale. As of March 31, 2022, no securities had been sold under the Form S-3.

We believe our existing cash, cash equivalents and marketable securities will be sufficient to fund our operating expenses and capital expenditure requirements through at least the next 24 months. Our future capital requirements will depend on many factors, including the growth of our software revenue, the timing and extent of spending to support research and development efforts, the continued expansion of software sales and marketing activities, the timing and receipt of milestone payments from our collaborations, as well as spending to support, advance, and broaden our internal programs. Furthermore, our capital requirements will also change depending on the timing and receipt of any distributions we may receive from our equity stakes in our drug discovery collaborators and partners. The potential for these distributions, and the amounts which we may be entitled to receive, are difficult to predict due to the inherent uncertainty of the events which may trigger such distributions.

We plan to utilize the existing cash, cash equivalents and marketable securities on hand primarily to fund our software and drug discovery activities. With respect to our internal programs, as part of our strategy we may choose to enter into collaborations or pursue out-licensing arrangements when we believe it will help maximize the commercial value of any such program.

We may be required to seek additional equity or debt financing. In the event that we require additional financing, we may not be able to raise such financing on terms acceptable to us or at all. If we are unable to raise additional capital or generate cash flows necessary to maintain or expand our operations and invest in our platform, we may not be able to compete successfully, which would harm our business, operations and financial condition. In addition, we may seek additional capital due to favorable market conditions or strategic considerations, even if we believe we have sufficient funds for our current or future operating plans.

Our contractual obligations as of March 31, 2022 include operating lease obligations of $132.1 million, consisting of our continuing rent obligations through December 2037, primarily for our principal offices located in New York, New York and Portland, Oregon, which expire in December 2037 and September 2026, respectively. In addition, see Note 6, “Commitments and Contingencies” to our unaudited condensed consolidated financial statements for information relating to executed leases that have not yet commenced.

In December 2020, we entered into a five-year agreement with a third-party cloud provider for compute power. The agreement contains a minimum payment obligation, which totals $60 million over the five years after the date we entered into the agreement. There is no annual commitment.

We enter into agreements in the normal course of business with CRO vendors for research and preclinical studies, professional consultants for expert advice, and other vendors for various products and services. These contracts do not contain any minimum purchase commitments and are cancelable at any time by us, generally upon 30 days prior written notice, and therefore we believe that our non-cancelable obligations under these agreements are not material. We have also agreed to pay volume-based royalties to third-parties for use of software functionality under various licensing and related agreements.

Cash Flows

The following table presents a summary of our cash flows for the periods shown:

	Three Months Ended March 31,	
	2022	2021
	(in thousands)	
Net cash used in operating activities	$ (39,722)	$ (10,921)
Net cash provided by (used in) investing activities	36,304	(61,909)
Net cash provided by financing activities	908	3,656
Net decrease in cash and cash equivalents and restricted cash	$ (2,510)	$ (69,174)

Operating activities

During the three months ended March 31, 2022, operating activities used approximately $39.7 million of cash, primarily due to a net loss of $34.5 million, including a $6.2 million non-cash loss from changes in fair value and $11.6 million of non-cash operating expenses included in net loss, including depreciation and amortization and stock-based compensation costs. Changes in our operating assets and liabilities used cash of approximately $23.0 million.

During the three months ended March 31, 2021, operating activities used approximately $10.9 million of cash, primarily due to a $24.8 million non-cash gain from changes in fair value, partially offset by $7.7 million of non-cash operating expenses included in net loss, including depreciation and stock-based compensation costs, $1.8 million of non-cash loss on equity investments, and approximately $0.5 million due to net loss. Changes in our operating assets and liabilities provided cash of approximately $4.9 million.

Investing activities

During the three months ended March 31, 2022, investing activities provided approximately $36.3 million of cash, consisting of $44.4 million provided by marketable securities maturities, net of purchases, $1.7 million used for purchases of property and equipment and $6.4 million used to acquire XTAL, net of cash acquired.

During the three months ended March 31, 2021, investing activities used approximately $61.9 million of cash, consisting of $77.2 million used for purchases of marketable securities, net of maturities, and $0.7 million used for purchases of property and equipment, partially offset by $15.8 million provided by the sale of our equity stake in Relay.

Financing activities

During the three months ended March 31, 2022, financing activities provided approximately $0.9 million of cash attributable to proceeds received upon stock option exercises.

During the three months ended March 31, 2021, financing activities provided approximately $3.7 million of cash attributable to proceeds received upon stock option exercises.

Item 3. Quantitative and Qualitative Disclosures About Market Risk.

There have been no material changes in our reported market risks or risk management policies since the filing of our Annual Report on Form 10-K for the fiscal year ended December 31, 2021, which was filed with the Securities and Exchange Commission on February 24, 2022.

Item 4. Controls and Procedures.

Evaluation of Disclosure Controls and Procedures

Our management, with the participation of our principal executive officer and principal financial officer, has evaluated the effectiveness of our disclosure controls and procedures (as defined in Rules 13a-15(e) and 15d-15(e) under the Securities Exchange Act of 1934, as amended, or the Exchange Act), as of March 31, 2022. The term “disclosure controls and procedures,” means controls and other procedures of a company that are designed to ensure that information required to be disclosed by a company in the reports that it files or submits under the Exchange Act is recorded, processed, summarized and reported, within the time periods specified in the Securities and Exchange Commission’s rules and forms. Disclosure controls and procedures include, without limitation, controls and procedures designed to ensure that information required to be disclosed by a company in the reports that it files or submits under the Exchange Act is accumulated and communicated to the company’s management, including its principal executive and principal financial officers, or persons performing similar functions, as appropriate to allow timely decisions regarding required disclosure. Management recognizes that any controls and procedures, no matter how well designed and operated, can provide only reasonable assurance of achieving their objectives and management necessarily applies its judgment in evaluating the cost-benefit relationship of possible controls and procedures. Based on such evaluation of our disclosure controls and procedures as of March 31, 2022, our principal executive officer and principal financial officer have concluded that as of such date, our disclosure controls and procedures were effective at the reasonable assurance level.

Changes in Internal Control Over Financial Reporting

There has been no change in our internal control over financial reporting (as defined in Rules 13a-15(f) and 15d-15(f) under the Exchange Act) that occurred during the period covered by this report that has materially affected, or is reasonably likely to materially affect, our internal control over financial reporting.

PART II—OTHER INFORMATION

Item 1. Legal Proceedings.

We are not currently subject to any material legal proceedings.

Item 1A. Risk Factors.

You should carefully consider the risks and uncertainties described below together with all of the other information contained in this Quarterly Report and our other public filings with the SEC. The risks described below are not the only risks facing our company. The occurrence of any of the following risks, or of additional risks and uncertainties not presently known to us or that we currently believe to be immaterial, could cause our business, prospects, operating results, and financial condition to suffer materially.

Risks Related to Our Financial Position and Need for Additional Capital

We have a history of significant operating losses, and we expect to incur losses over the next several years.

We have a history of significant operating losses. Our net loss attributable to Schrödinger common stockholders and limited common stockholders for the three months ended March 31, 2022 and 2021 was $34.4 million and $0.0 million, respectively. Our net losses for the years ended December 31, 2021 and 2020 were $101.2 million and $26.6 million, respectively. As of March 31, 2022, we had an accumulated deficit of $264.4 million.

We anticipate that our operating expenses will increase substantially in the foreseeable future as we continue to invest in our internal drug discovery programs, sales and marketing infrastructure, and our computational platform. We are still in the early stages of development of our own drug discovery programs. We continue to advance multiple internal programs through investigational new drug, or IND, -enabling studies, and we expect to submit an IND application to the U.S. Food and Drug Administration, or FDA, for our MALT1 program in the first half of 2022, and subject to receiving regulatory clearance, we expect to initiate a Phase 1 clinical trial of our MALT1 inhibitor, which we refer to as SGR-1505, in patients with relapsed and resistant lymphoma in the second half of 2022. We also plan to submit IND applications to the FDA for our CDC7 program in early 2023 and our WEE1 program in 2023, subject to favorable data from IND-enabling studies. In addition, we plan to initiate a Phase 1 clinical trial of our CDC7 inhibitor in 2023, subject to receipt of regulatory clearance. We have no drug products licensed for commercial sale and have not generated any revenue from our own drug product sales to date. We expect to continue to incur significant expenses and operating losses over the next several years. Our operating expenses and net income or loss may fluctuate significantly from quarter to quarter and year to year. We anticipate that our expenses will increase substantially as we:

- continue to invest in and develop our computational platform and software solutions;
- continue our research and development efforts for our internal drug discovery programs;
- conduct preclinical studies and initiate and conduct clinical trials for any of our product candidates;
- maintain, expand, enforce, defend, and protect our intellectual property;
- hire additional software engineers, programmers, sales and marketing, and other personnel to support our software business;
- hire additional clinical, quality control, and other scientific personnel; and
- add operational, financial, and management information systems and personnel to support our operations as a public company.

If we are unable to increase sales of our software, or if we and our current and future collaborators are unable to successfully develop and commercialize drug products, our revenues may be insufficient for us to achieve or maintain profitability.

To achieve and maintain profitability, we must succeed in significantly increasing our software sales, or we and our current or future collaborators must succeed in developing, and eventually commercializing, a drug product or drug products that generate significant revenue. We currently generate revenues primarily from the sales of our software solutions and expect to continue to derive most of our revenue from sales of our software until such time as our or our collaborators' drug development and commercialization efforts are successful, if ever. As such, increasing sales of our software to existing customers and successfully marketing our software to new customers are critical to our success. Demand for our software solutions may be affected by a number of factors, including continued market acceptance by the biopharmaceutical industry, market adoption of our software solutions beyond the biopharmaceutical industry including for material science applications, the ability of our platform to identify more promising molecules and accelerate and lower the costs of discovery as compared to traditional methods, timing of development and release of new offerings

by our competitors, technological change, and the rate of growth in our target markets. If we are unable to continue to meet the demands of our customers, our business operations, financial results, and growth prospects will be adversely affected.

Achieving success in drug development will require us or our current or future collaborators to be effective in a range of challenging activities, including completing preclinical testing and clinical trials of product candidates, obtaining regulatory approval for these product candidates and manufacturing, marketing, and selling any products for which we or they may obtain regulatory approval. We and most of our current drug discovery collaborators are only in the preliminary stages of most of these activities. We and they may never succeed in these activities and, even if we do, we may never generate revenues that are significant enough to achieve and sustain profitability, or even if our collaborators do, we may not receive option fees, milestone payments, or royalties from them that are significant enough for us to achieve and sustain profitability. Because of the intense competition in the market for our software solutions and the numerous risks and uncertainties associated with biopharmaceutical product development, we are unable to accurately predict when, or if, we will be able to achieve or sustain profitability.

Even if we achieve profitability, we may not be able to sustain or increase profitability on a quarterly or annual basis. Our failure to become and remain profitable would depress the value of our company and could impair our ability to raise capital, expand our business, maintain our research and development efforts, increase sales of our software, develop a pipeline of product candidates, enter into collaborations, or even continue our operations. A decline in the value of our company could also cause our stockholders to lose all or part of their investment.

In addition, although we have experienced revenue growth in recent periods, we may not be able to sustain revenue growth consistent with our recent history or at all. Our total revenues increased by 51% from $32.1 million in the three months ended March 31, 2021 to $48.7 million in the three months ended March 31, 2022, and increased by 28% from $108.1 million in the fiscal year ended December 31, 2020 to $137.9 million in the fiscal year ended December 31, 2021. You should not consider our revenue growth in recent periods as indicative of our future performance. As we grow our business, our revenue growth rates may slow in future periods.

Our quarterly and annual results may fluctuate significantly, which could adversely impact the value of our common stock.

Our results of operations, including our revenues, gross margin, profitability, and cash flows, have historically varied from period to period, and we expect that they will continue to do so. As a result, period-to-period comparisons of our operating results may not be meaningful, and our quarterly and annual results should not be relied upon as an indication of future performance. Our quarterly and annual financial results may fluctuate as a result of a variety of factors, many of which are outside of our control. Factors that may cause fluctuations in our quarterly and annual financial results include, without limitation, those listed elsewhere in this “Risk Factors” section and those listed below:

- customer renewal rates and the timing and terms of customer renewals, including the seasonality of customer renewals of our on-premise software arrangements, for which revenue historically has been recognized at a single point in time in the first and fourth quarter of each fiscal year;
- our ability to attract new customers for our software;
- the addition or loss of large customers, including through acquisitions or consolidations of such customers;
- the amount and timing of operating expenses related to the maintenance and expansion of our business, operations, and infrastructure;
- network outages or security breaches;
- general economic, industry, and market conditions, including within the life sciences industry;
- our ability to collect receivables from our customers;
- the amount of software purchased by our customers, including the mix of on-premise and hosted software sold during a period;
- variations in the timing of the sales of our software, which may be difficult to predict;
- changes in the pricing of our solutions and in our pricing policies or those of our competitors;
- the timing and success of the introduction of new software solutions by us or our competitors or any other change in the competitive dynamics of our industry, including consolidation among competitors, customers, or strategic collaborators;
- changes in the fair value of or receipt of distributions or proceeds on account of the equity interests we hold in our drug discovery collaborators, such as Morphic Holding, Inc.;

- the success of our drug discovery collaborators in developing and commercializing drug products for which we are entitled to receive milestone payments or royalties and the timing of receipt of such payments, if any, such as under our collaboration agreement with Bristol-Myers Squibb Company, or BMS; and
- the timing of expenses related to our drug discovery programs, the development or acquisition of technologies or businesses and potential future charges for impairment of goodwill from acquired companies.

In addition, because we recognize revenues from our hosted software solutions ratably over the life of the contract, a significant upturn or downturn in sales of our hosted software solutions may not be reflected immediately in our operating results. As a result of these factors, we believe that period-to-period comparisons of our operating results are not a good indication of our future performance and that our interim financial results are not necessarily indicative of results for a full year or for any subsequent interim period.

We may require additional capital to fund our operations. If we are unable to raise additional capital on terms acceptable to us or at all or generate cash flows necessary to maintain or expand our operations, we may not be able to compete successfully, which would harm our business, operations, and financial condition.

We expect to devote substantial financial resources to our ongoing and planned activities, including the development of drug discovery programs and continued investment in our computational platform. We expect our expenses to increase substantially in connection with our ongoing and planned activities, particularly as we advance our internal drug discovery programs, initiate or progress preclinical and IND-enabling studies, submit IND applications, initiate and progress clinical trials and invest in the further development of our platform. In addition, if we determine to complete clinical development and seek regulatory approval on our own, we expect to incur significant additional expenses. Furthermore, we incur additional costs associated with operating as a public company, as compared to when we were a private company.

Our current drug discovery collaborators, from whom we are entitled to receive milestone payments upon achievement of various development, regulatory, and commercial milestones as well as royalties on commercial sales, if any, under the collaboration agreements that we have entered into with them, face numerous risks in the development of drugs, including the conduct of preclinical and clinical testing, obtaining regulatory approval, and achieving product sales. In addition, the amounts we are entitled to receive upon the achievement of such milestones tend to be smaller for near-term development milestones and increase if and as a collaborative product candidate advances through regulatory development to commercialization and will vary depending on the level of commercial success achieved, if any. We do not anticipate receiving significant milestone payments from many of our drug discovery collaborators for several years, if at all, and our drug discovery collaborators may never achieve milestones that result in significant cash payments to us. Accordingly, we may need to obtain substantial additional capital to fund our continuing operations.

As of March 31, 2022, we had cash, cash equivalents, restricted cash, and marketable securities of $529.0 million. We believe that our existing cash, cash equivalents, and marketable securities will be sufficient to fund our operating expenses and capital expenditure requirements through at least the next 24 months. However, we have based this estimate on assumptions that may prove to be wrong, and our operating plans may change as a result of many factors currently unknown to us. As a result, we could deplete our capital resources sooner than we currently expect.

Our future capital requirements will depend on many factors, including:

- the growth of our software revenue;
- the timing and extent of spending to support research and development efforts;
- the continued expansion of software sales and marketing activities;
- the timing and receipt of payments from our collaborations as well as spending to support, advance, and broaden our internal drug discovery programs; and
- the timing and receipt of any distributions or proceeds we may receive from our equity stakes in our drug discovery collaborators and partners.

In the event that we require additional financing, we may not be able to raise such financing on terms acceptable to us or at all. In addition, we may seek additional capital due to favorable market conditions or strategic considerations, even if we believe we have sufficient funds for our current or future operating plans. If we are unable to raise additional capital on terms acceptable to us or at all or generate cash flows necessary to maintain or expand our operations and invest in our computational platform, we may not be able to compete successfully, which would harm our business, operations, and financial condition.

Raising additional capital may cause dilution to our stockholders, restrict our operations, or require us to relinquish rights to our technologies or drug programs.

To the extent that we raise additional capital through the sale of equity or convertible debt securities, our stockholders' ownership interests will be diluted, and the terms of these securities may include liquidation or other preferences that adversely affect our stockholders' rights as common stockholders. Debt financing and preferred equity financing, if available, may involve agreements that include covenants limiting or restricting our ability to take specific actions, such as incurring additional debt, selling or licensing our assets, making product acquisitions, making capital expenditures, or declaring dividends.

If we raise additional funds through collaborations, strategic alliances or marketing, distribution, or licensing arrangements with third parties, we may have to relinquish valuable rights to our technologies, future revenue streams, research programs, or product candidates or grant licenses on terms that may not be favorable to us or agree to exploit a drug development target exclusively for one of our collaborators when we may prefer to pursue the drug development target for ourselves.

If our estimates or judgments relating to our critical accounting policies prove to be incorrect or financial reporting standards or interpretations change, our results of operations could be adversely affected.

The preparation of financial statements in conformity with generally accepted accounting principles in the United States, or U.S. GAAP, requires management to make estimates and assumptions that affect the amounts reported in the consolidated financial statements and accompanying notes. We base our estimates on historical experience, known trends and events, and various other factors that we believe to be reasonable under the circumstances, as provided in Part II, Item 7. "Management's Discussion and Analysis of Financial Condition and Results of Operations—Critical Accounting Policies and Significant Judgments and Critical Accounting Estimates" of our Annual Report on Form 10-K for the year ended December 31, 2021. The results of these estimates form the basis for making judgments about the carrying values of assets and liabilities that are not readily apparent from other sources. Significant assumptions and estimates used in preparing our unaudited condensed consolidated financial statements include determining the allocation of the transaction price and measurement of progress, including (1) the constraint on variable consideration, (2) the allocation of the transaction price to the performance obligations using their standalone selling price basis, and (3) the appropriate input or output based method to recognize collaboration revenue and the extent of progress to date, and the expected stock price volatility and the calculation of expected term of the award estimates used in the calculation of stock-based compensation.

Our results of operations may be adversely affected if our assumptions change or if actual circumstances differ from those in our assumptions, which could cause our results of operations to fall below the expectations of securities analysts and investors, resulting in a decline in the trading price of our common stock.

Additionally, we regularly monitor our compliance with applicable financial reporting standards and review new pronouncements and drafts thereof that are relevant to us. As a result of new standards, changes to existing standards and changes in their interpretation, we might be required to change our accounting policies, alter our operational policies, and implement new or enhance existing systems so that they reflect new or amended financial reporting standards, or we may be required to restate our published financial statements. Such changes to existing standards or changes in their interpretation may have an adverse effect on our reputation, business, financial position, and profit.

Risks Related to Our Software

If our existing customers do not renew their licenses, do not buy additional solutions from us, or renew at lower prices, our business and operating results will suffer.

We expect to continue to derive a significant portion of our software revenues from renewal of existing license agreements. As a result, maintaining the renewal rate of our existing customers and selling additional software solutions to them is critical to our future operating results. Factors that may affect the renewal rate for our customers and our ability to sell additional solutions to them include:

- the price, performance, and functionality of our software solutions;
- the availability, price, performance, and functionality of competing software solutions;
- the effectiveness of our professional services;
- our ability to develop or acquire complementary software solutions, applications, and services;
- the success of competitive products or technologies;
- the stability, performance, and security of our technological infrastructure; and
- the business environment of our customers.

We deliver our software through either (i) a product license that permits our customers to install the software solution directly on their own in-house hardware and use it for a specified term, or (ii) a subscription that allows our customers to access the cloud-based software solution on their own hardware without taking control of the licenses. Our customers have no obligation to renew their product licenses or subscriptions for our software solutions after the license term expires, which is typically after one year, and many of our contracts may be terminated or reduced in scope either immediately or upon notice. In addition, our customers may negotiate terms less advantageous to us upon renewal, which may reduce our revenues from these customers. Factors that are not within our control may contribute to a reduction in our software revenues. For instance, our customers may reduce the number of their employees who are engaged in research and who would have use of our software, which would result in a corresponding reduction in the number of user licenses needed for some of our solutions and thus a lower aggregate renewal fee. The loss, reduction in scope, or delay of a large contract, or the loss or delay of multiple contracts, could materially adversely affect our business.

Our future operating results also depend, in part, on our ability to sell new software solutions and licenses to our existing customers. For example, the willingness of existing customers to license our software will depend on our ability to scale and adapt our existing software solutions to meet the performance and other requirements of our customers, which we may not do successfully. If our customers fail to renew their agreements, renew their agreements upon less favorable terms or at lower fee levels, or fail to purchase new software solutions and licenses from us, our revenues may decline and our future revenues may be constrained.

Our software sales cycle can vary and be long and unpredictable.

The timing of sales of our software solutions is difficult to forecast because of the length and unpredictability of our sales cycle. We sell our solutions primarily to biopharmaceutical companies, and our sales cycles can be as long as nine to twelve months or longer. Further, the length of time that potential customers devote to their testing and evaluation, contract negotiation, and budgeting processes varies significantly, depending on the size of the organization and the nature of their needs. In addition, we might devote substantial time and effort to a particular unsuccessful sales effort, and as a result, we could lose other sales opportunities or incur expenses that are not offset by an increase in revenue, which could harm our business.

A significant portion of our revenues are generated by sales to life sciences industry customers, and factors that adversely affect this industry could also adversely affect our software sales.

A significant portion of our current software sales are to customers in the life sciences industry, in particular the biopharmaceutical industry. Demand for our software solutions could be affected by factors that adversely affect the life sciences industry. The life sciences industry is highly regulated and competitive and has experienced periods of considerable consolidation. Consolidation among our customers could cause us to lose customers, decrease the available market for our solutions, and adversely affect our business. In addition, changes in regulations that make investment in the life sciences industry less attractive or drug development more expensive could adversely impact the demand for our software solutions. For these reasons and others, selling software to life sciences companies can be competitive, expensive, and time consuming, often requiring significant upfront time and expense without any assurance that we will successfully complete a software sale. Accordingly, our operating results and our ability to efficiently provide our solutions to life sciences companies and to grow or maintain our customer base could be adversely affected as a result of factors that affect the life sciences industry generally.

We also intend to continue leveraging our solutions for broad application to industrial challenges in molecule design, including in the fields of aerospace, energy, semiconductors, and electronic displays. However, we believe the materials science industry is in the very early stages of recognizing the potential of computational methods for molecular discovery, and there can be no assurance that the industry will adopt computational methods such as our platform. Any factor adversely affecting our ability to market our software solutions to customers outside of the life sciences industry, including in these new fields, could increase our dependence on the life sciences industry and adversely affect the growth rate of our revenues, operating results, and business.

The markets in which we participate are competitive, and if we do not compete effectively, our business and operating results could be adversely affected.

The overall market for molecular discovery and design software is global, rapidly evolving, competitive, and subject to changing technology and shifting customer focus. Our software solutions face competition from commercial competitors in the business of selling or providing simulation and modeling software to biopharmaceutical companies. These competitors include BIOVIA, a brand of Dassault Systèmes SE, or BIOVIA, Chemical Computing Group (US) Inc., Cresset Biomolecular Discovery Limited, OpenEye Scientific Software, Inc., Optibrium Limited, Cyrus Biotechnology, Inc., Molsoft LLC, Insilico Medicine, Inc., Iktos, XtalPi Inc., and Simulations Plus, Inc.

We also have competitors in materials science, such as BIOVIA and Materials Design, Inc., and in enterprise software for the life sciences, such as BIOVIA, Certara USA, Inc., ChemAxon, PerkinElmer, Inc., and Dotmatics, Inc. In some cases, these competitors are well-established providers of these solutions and have long-standing relationships with many of our current and potential customers, including large biopharmaceutical companies. In addition, there are academic consortia that develop physics-based simulation programs for life sciences and materials applications. In life sciences, the most prominent academic simulation packages include AMBER, CHARMm, GROMACS, GROMOS, OpenMM, and OpenFF. These packages are primarily maintained and developed by graduate students and post-doctoral researchers, often without the intent for commercialization.

We also face competition from solutions that biopharmaceutical companies develop internally and from smaller companies that offer products and services directed at more specific markets than we target, enabling these smaller competitors to focus a greater proportion of their efforts and resources on these markets, as well as a large number of companies that have been founded with the goal of applying machine learning technologies to drug discovery.

Many of our competitors are able to devote greater resources to the development, promotion, and sale of their software solutions and services. It is possible that our focus on internal drug discovery will result in loss of management focus and resources relating to our software business, thereby resulting in decreasing revenues from our software business. Furthermore, third parties with greater available resources and the ability to initiate or withstand substantial price competition could acquire our current or potential competitors. Our competitors may also establish cooperative relationships among themselves or with third parties that may further enhance their product offerings or resources. If our competitors' products, services, or technologies become more accepted than our solutions, if our competitors are successful in bringing their products or services to market earlier than ours, if our competitors are able to respond more quickly and effectively to new or changing opportunities, technologies, or customer requirements, or if their products or services are more technologically capable than ours, then our software revenues could be adversely affected.

We may be required to decrease our prices or modify our pricing practices in order to attract new customers or retain existing customers due to increased competition. Pricing pressures and increased competition could result in reduced sales, reduced margins, losses, or a failure to maintain or improve our competitive market position, any of which could adversely affect our business.

We have invested and expect to continue to invest in research and development efforts that further enhance our computational platform. Such investments may affect our operating results, and, if the return on these investments is lower or develops more slowly than we expect, our revenue and operating results may suffer.

We have invested and expect to continue to invest in research and development efforts that further enhance our computational platform, often in response to our customers' requirements. These investments may involve significant time, risks, and uncertainties, including the risk that the expenses associated with these investments may affect our margins and operating results and that such investments may not generate sufficient revenues to offset liabilities assumed and expenses associated with these new investments. The software industry changes rapidly as a result of technological and product developments, which may render our solutions less desirable. We believe that we must continue to invest a significant amount of time and resources in our platform and software solutions to maintain and improve our competitive position. If we do not achieve the benefits anticipated from these investments, if the achievement of these benefits is delayed, or if a slowdown in general computing power impacts the rate at which we expect our physics-based simulations to increase in power and domain applicability, our revenue and operating results may be adversely affected.

If we are unable to collect receivables from our customers, our operating results may be adversely affected.

While the majority of our current customers are well-established, large companies and universities, we also provide software solutions to smaller companies. Our financial success depends upon the creditworthiness and ultimate collection of amounts due from our customers, including our smaller customers with fewer financial resources. If we are not able to collect amounts due from our customers, we may be required to write-off significant accounts receivable and recognize bad debt expenses, which could materially and adversely affect our operating results.

Defects or disruptions in our solutions could result in diminishing demand for our solutions, a reduction in our revenues, and subject us to substantial liability.

Our software business and the level of customer acceptance of our software depend upon the continuous, effective, and reliable operation of our software and related tools and functions. Our software solutions are inherently complex and may contain defects or errors. Errors may result from our own technology or from the interface of our software solutions with legacy systems and data, which we did not develop. The risk of errors is particularly significant when a new software solution is first introduced or when new versions or enhancements of existing software solutions are released. We have from time to time found defects in our software, and new errors in our existing software may be detected in the future. Any errors, defects, disruptions, or other performance problems with our software

could hurt our reputation and may damage our customers' businesses. If that occurs, our customers may delay or withhold payment to us, cancel their agreements with us, elect not to renew, make service credit claims, warranty claims, or other claims against us, and we could lose future sales. The occurrence of any of these events could result in diminishing demand for our software, a reduction of our revenues, an increase in collection cycles for accounts receivable, require us to increase our warranty provisions, or incur the expense of litigation or substantial liability.

We rely upon third-party providers of cloud-based infrastructure to host our software solutions. Any disruption in the operations of these third-party providers, limitations on capacity, or interference with our use could adversely affect our business, financial condition, and results of operations.

We outsource substantially all of the infrastructure relating to our hosted software solutions to third-party hosting services. Customers of our hosted software solutions need to be able to access our computational platform at any time, without interruption or degradation of performance, and we provide them with service-level commitments with respect to uptime. Our hosted software solutions depend on protecting the virtual cloud infrastructure hosted by third-party hosting services by maintaining its configuration, architecture, features, and interconnection specifications, as well as the information stored in these virtual data centers, which is transmitted by third-party internet service providers. Any limitation on the capacity of our third-party hosting services could impede our ability to onboard new customers or expand the usage of our existing customers, which could adversely affect our business, financial condition, and results of operations. In addition, any incident affecting our third-party hosting services' infrastructure that may be caused by cyber-attacks, natural disasters, fire, flood, severe storm, earthquake, power loss, telecommunications failures, terrorist or other attacks, and other similar events beyond our control could negatively affect our cloud-based solutions. A prolonged service disruption affecting our cloud-based solutions for any of the foregoing reasons would negatively impact our ability to serve our customers and could damage our reputation with current and potential customers, expose us to liability, cause us to lose customers, or otherwise harm our business. We may also incur significant costs for using alternative equipment or taking other actions in preparation for, or in reaction to, events that damage the third-party hosting services we use.

In the event that our service agreements with our third-party hosting services are terminated, or there is a lapse of service, elimination of services or features that we utilize, interruption of internet service provider connectivity, or damage to such facilities, we could experience interruptions in access to our platform as well as significant delays and additional expense in arranging or creating new facilities and services and/or re-architecting our hosted software solutions for deployment on a different cloud infrastructure service provider, which could adversely affect our business, financial condition, and results of operations.

If our security measures are breached or unauthorized access to customer data is otherwise obtained, our solutions may be perceived as not being secure, customers may reduce the use of or stop using our solutions, and we may incur significant liabilities.

Our solutions involve the collection, analysis, and storage of our customers' proprietary information and sensitive proprietary data related to the discovery efforts of our customers. As a result, unauthorized access or security breaches, as a result of third-party action, employee error, malfeasance, or otherwise could result in the loss of information, litigation, indemnity obligations, damage to our reputation, and other liability. Because the techniques used to obtain unauthorized access or sabotage systems change frequently and generally are not identified until they are launched against a target, we may be unable to anticipate these techniques or to implement adequate preventative measures. In addition, if our employees fail to adhere to practices we have established to maintain a firewall between our internal drug discovery team and our teams that work with software customers, or if the technical solutions we have adopted to maintain the firewall malfunction, our customers and collaborators may lose confidence in our ability to maintain the confidentiality of their intellectual property, we may have trouble attracting new customers and collaborators, we may be subject to breach of contract claims by our customers and collaborators, and we may suffer reputational and other harm as a result. Any or all of these issues could adversely affect our ability to attract new customers, cause existing customers to elect to not renew their licenses, result in reputational damage or subject us to third-party lawsuits or other action or liability, which could adversely affect our operating results. Our insurance may not be adequate to cover losses associated with such events, and in any case, such insurance may not cover all of the types of costs, expenses, and losses we could incur to respond to and remediate a security breach.

Any failure to offer high-quality technical support services could adversely affect our relationships with our customers and our operating results.

Our customers depend on our support organization to resolve technical issues relating to our solutions, as our software requires expert usage to fully exploit its capabilities. Certain of our customers also rely on us to troubleshoot problems with the performance of the software, introduce new features requested for specific customer projects, inform them about the best way to set up and analyze various types of simulations and illustrate our techniques for drug discovery using examples from publicly available data sets. We may be unable to respond quickly enough to accommodate short-term increases in customer demand for these support services. Increased customer demand for our services, without corresponding revenues, could increase costs and adversely affect our operating results. In

addition, our sales process is highly dependent on the reputation of our solutions and business and on positive recommendations from our existing customers. Any failure to offer high-quality technical support, or a market perception that we do not offer high-quality support, could adversely affect our reputation, our ability to sell our solutions to existing and prospective customers and our business and operating results.

Our solutions utilize third-party open-source software, and any failure to comply with the terms of one or more of these open-source software licenses could adversely affect our business or our ability to sell our software solutions, subject us to litigation, or create potential liability.

Our solutions include software licensed by third parties under any one or more open-source licenses, including the GNU General Public License, the GNU Lesser General Public License, the Affero General Public License, the BSD License, the MIT License, the Apache License, and others, and we expect to continue to incorporate open-source software in our solutions in the future. Moreover, we cannot ensure that we have effectively monitored our use of open-source software or that we are in compliance with the terms of the applicable open-source licenses or our current policies and procedures. There have been claims against companies that use open-source software in their products and services asserting that the use of such open-source software infringes the claimants' intellectual property rights. As a result, we and our customers could be subject to suits by third parties claiming that what we believe to be licensed open-source software infringes such third parties' intellectual property rights, and we may be required to indemnify our customers against such claims. Additionally, if an author or other third party that distributes such open-source software were to allege that we had not complied with the conditions of one or more of these licenses, we or our customers could be required to incur significant legal expenses defending against such allegations and could be subject to significant damages, enjoined from the sale of our solutions that contain the open-source software and required to comply with onerous conditions or restrictions on these solutions, which could disrupt the distribution and sale of these solutions. Litigation could be costly for us to defend, have a negative effect on our business, financial condition, and results of operations, or require us to devote additional research and development resources to change our solutions.

Use of open-source software may entail greater risks than use of third-party commercial software, as open-source licensors generally do not provide warranties or other contractual protections regarding infringement claims or the quality of the code, including with respect to security vulnerabilities. In addition, certain open-source licenses require that source code for software programs that interact with such open-source software be made available to the public at no cost and that any modifications or derivative works to such open-source software continue to be licensed under the same terms as the open-source software license. The terms of various open-source licenses have not been interpreted by courts in the relevant jurisdictions, and there is a risk that such licenses could be construed in a manner that imposes unanticipated conditions or restrictions on our ability to market our solutions. By the terms of certain open-source licenses, we could be required to release the source code of our proprietary software, and to make our proprietary software available under open-source licenses, if we combine our proprietary software with open-source software in a certain manner. In the event that portions of our proprietary software are determined to be subject to an open-source license, we could be required to publicly release the affected portions of our source code, re-engineer all or a portion of our solutions, or otherwise be limited in the licensing of our solutions, each of which could reduce or eliminate the value of our solutions. Disclosing our proprietary source code could allow our competitors to create similar products with lower development effort and time and ultimately could result in a loss of sales. Any of these events could create liability for us and damage our reputation, which could have a material adverse effect on our revenue, business, results of operations, and financial condition and the market price of our shares.

Risks Related to Drug Discovery

We may never realize a return on our investment of resources and cash in our drug discovery collaborations.

We use our computational platform to provide drug discovery services to collaborators who are engaged in drug discovery and development. These collaborators include start-up companies, pre-commercial biotechnology companies, and large-scale pharmaceutical companies. When we engage in drug discovery with these collaborators, we typically provide access to our platform and platform experts who assist the drug discovery collaborator in identifying molecules that have activity against one or more specified protein targets. We historically have not received significant initial cash consideration for these services, except for the upfront payment of $55.0 million we received from BMS upon entry into our collaboration agreement with BMS. However, we have received equity consideration in certain of our collaborators and/or the right to receive option fees, cash milestone payments upon the achievement of specified development, regulatory, and commercial sales milestones for the drug discovery targets, and potential royalties. From time to time, we have also made additional equity investments in our drug discovery collaborators.

We may never realize return on our investment of resources and cash in our drug discovery collaborations. Clinical drug development involves a lengthy and expensive process, with an uncertain outcome. Our drug discovery collaborators may incur

additional costs or experience delays in completing, or ultimately be unable to complete, the development and commercialization of any product candidates. In addition, our ability to realize return from our drug discovery collaborations is subject to the following risks:

- drug discovery collaborators have significant discretion in determining the amount and timing of efforts and resources that they will apply to our collaborations and may not perform their obligations as expected;
- drug discovery collaborators may not pursue development or commercialization of any product candidates for which we are entitled to option fees, milestone payments, or royalties or may elect not to continue or renew development or commercialization programs based on results of clinical trials or other studies, changes in the collaborator's strategic focus or available funding, or external factors, such as an acquisition, that divert resources or create competing priorities;
- drug discovery collaborators may delay clinical trials for which we are entitled to milestone payments;
- we may not have access to, or may be restricted from disclosing, certain information regarding our collaborators' product candidates being developed or commercialized and, consequently, may have limited ability to inform our stockholders about the status of, and likelihood of achieving, milestone payments or royalties under such collaborations;
- drug discovery collaborators could independently develop, or develop with third parties, products that compete directly or indirectly with any product candidates and products for which we are entitled to milestone payments or royalties if the collaborator believes that the competitive products are more likely to be successfully developed or can be commercialized under terms that are more economically attractive;
- product candidates discovered in drug discovery collaborations with us may be viewed by our collaborators as competitive with their own product candidates or products, which may cause our collaborators to cease to devote resources to the commercialization of any such product candidates;
- existing drug discovery collaborators and potential future drug discovery collaborators may begin to perceive us to be a competitor more generally, particularly as we advance our internal drug discovery programs, and therefore may be unwilling to continue existing collaborations with us or to enter into new collaborations with us;
- a drug discovery collaborator may fail to comply with applicable regulatory requirements regarding the development, manufacture, distribution, or marketing of a product candidate or product, which may impact our ability to receive milestone payments;
- disagreements with drug discovery collaborators, including disagreements over intellectual property or proprietary rights, contract interpretation, or the preferred course of development, might cause delays or terminations of the research, development, or commercialization of product candidates for which we are eligible to receive milestone payments, or might result in litigation or arbitration;
- drug discovery collaborators may not properly obtain, maintain, enforce, defend or protect our intellectual property or proprietary rights or may use our proprietary information in such a way as to potentially lead to disputes or legal proceedings that could jeopardize or invalidate our or their intellectual property or proprietary information or expose us and them to potential litigation;
- drug discovery collaborators may infringe, misappropriate, or otherwise violate the intellectual property or proprietary rights of third parties, which may expose us to litigation and potential liability;
- drug discovery collaborators could suffer from operational delays as a result of global health impacts, such as the COVID-19 pandemic; and
- drug discovery collaborations may be terminated prior to our receipt of any significant value from the collaboration.

Our drug discovery collaborations may not lead to development or commercialization of product candidates that results in our receipt of option fees, milestone payments, or royalties in a timely manner, or at all. If any drug discovery collaborations that we enter into do not result in the successful development and commercialization of drug products that result in option fees, milestone payments, or royalties to us, we may not receive return on the resources we have invested in the drug discovery collaboration. Moreover, even if a drug discovery collaboration initially leads to the achievement of milestones that result in payments to us, it may not continue to do so.

We also rely on collaborators for the development and potential commercialization of product candidates we discover internally when we believe it will help maximize the commercial value of the product candidate. For example, under our collaboration agreement with BMS, after mutual agreement on the targets(s) of interest, our drug discovery group will be responsible for the discovery of development candidates. Once a development candidate meeting specified criteria for a target has been identified, BMS will be solely responsible for the development, manufacturing and commercialization of such development candidate. Even if we successfully identify

one or more development candidates for BMS to develop and commercialize under our collaboration agreement, BMS may not achieve the research, development, regulatory and sales milestones for those development candidates that result in additional payments to us.

We may never realize a return on our equity investments in our drug discovery collaborators.

We may never realize a return on our equity investments in our drug discovery collaborators. None of the drug discovery collaborators in which we hold equity generate revenue from commercial sales of drug products. They are therefore dependent on the availability of capital on favorable terms to continue their operations. In addition, if the drug discovery collaborators in which we hold equity raise additional capital, our ownership interest in and degree of control over these drug discovery collaborators will be diluted, unless we have sufficient resources and choose to invest in them further or successfully negotiate contractual anti-dilution protections for our equity investment. The financial success of our equity investment in any collaborator will likely be dependent on a liquidity event, such as a public offering, acquisition, or other favorable market event reflecting appreciation in the value of the equity we hold. The capital markets for public offerings and acquisitions are dynamic, and the likelihood of liquidity events for the companies in which we hold equity interests could significantly worsen. Further, valuations of privately held companies are inherently complex due to the lack of readily available market data. If we determine that any of our investments in such companies have experienced a decline in value, we may be required to record an impairment, which could negatively impact our financial results. The fair value of our equity interests in public companies, such as Morphic, may fluctuate significantly in future periods since we determine the fair value of such equity interests based on the market value of such companies' common stock as of a given reporting date. All of the equity we hold in our drug discovery collaborators is subject to a risk of partial or total loss of our investment.

Our drug discovery collaborators have significant discretion in determining when to make announcements, if any, about the status of our collaborations, including about clinical developments and timelines for advancing collaborative programs, and the price of our common stock may decline as a result of announcements of unexpected results or developments.

Our drug discovery collaborators have significant discretion in determining when to make announcements about the status of our collaborations, including about preclinical and clinical developments and timelines for advancing the collaborative programs. While as a general matter we intend to periodically report on the status of our collaborations, our drug discovery collaborators, and in particular, our privately-held collaborators, may wish to report such information more or less frequently than we intend to or may not wish to report such information at all. The price of our common stock may decline as a result of the public announcement of unexpected results or developments in our collaborations, or as a result of our collaborators withholding such information.

Although we believe that our computational platform has the potential to identify more promising molecules than traditional methods and to accelerate drug discovery, our focus on using our platform technology to discover and design molecules with therapeutic potential may not result in the discovery and development of commercially viable products for us or our collaborators.

Our scientific approach focuses on using our platform technology to conduct "computational assays" that leverage our deep understanding of physics-based modeling and theoretical chemistry to design molecules and predict their key properties without conducting time-consuming and expensive physical experiments. Our computational platform underpins our software solutions, our drug discovery collaborations and our own internal drug discovery programs.

While the results of certain of our drug discovery collaborators suggest that our platform is capable of accelerating drug discovery and identifying high quality product candidates, these results do not assure future success for our drug discovery collaborators or for us with our internal drug discovery programs.

Even if we or our drug discovery collaborators are able to develop product candidates that demonstrate potential in preclinical studies, we or they may not succeed in demonstrating safety and efficacy of product candidates in human clinical trials. For example, in collaboration with us, Nimbus Therapeutics, LLC, or Nimbus, was able to identify a unique series of acetyl-CoA carboxylase, or ACC, allosteric protein-protein interaction inhibitors with favorable pharmaceutical properties that inhibit the activity of the ACC enzyme. Nimbus achieved proof of concept in a Phase 1b clinical trial of its ACC inhibitor, firsocostat, and later sold the program to Gilead Sciences, Inc., or Gilead Sciences, in a transaction valued at approximately $1.2 billion, comprised of an upfront payment and earn outs. Of this amount, $601.3 million has been paid to Nimbus to date, and we received a total of $46.0 million in cash distributions in 2016 and 2017. In December 2019, Gilead Sciences announced topline results from its Phase 2 clinical trial which included firsocostat, both as a monotherapy and in combination with other investigational therapies for advanced fibrosis due to nonalcoholic steatohepatitis, in which the primary endpoint was not met. Moreover, preclinical and clinical data are often susceptible to varying interpretations and analyses, and many companies that have believed their product candidates performed satisfactorily in preclinical studies and clinical trials have nonetheless failed to obtain marketing approval of their product candidates.

We may not be successful in our efforts to identify, discover or develop product candidates and may fail to capitalize on programs, collaborations, or product candidates that may present a greater commercial opportunity or for which there is a greater likelihood of success.

Research programs to identify new product candidates require substantial technical, financial, and human resources. As an organization, we have selected our first development candidates, which are for our MALT1 and CDC7 inhibitor programs, and advanced the programs into IND-enabling studies. We have not yet advanced any other programs into IND-enabling studies, and we may fail to identify potential product candidates for clinical development. Similarly, a key element of our business plan is to expand the use of our computational platform through an increase in software sales and drug discovery collaborations. A failure to demonstrate the utility of our platform by successfully using it ourselves to discover internal product candidates could harm our business prospects.

Because we have limited resources, we focus our research programs on protein targets where we believe our computational assays are a good substitute for experimental assays, where we believe it is theoretically possible to discover a molecule with properties that are required for the molecule to become a drug and where we believe there is a meaningful commercial opportunity, among other factors. The focus of our initial internal drug discovery programs was in the area of oncology, and we have only recently begun expanding into other therapeutic areas, including neurology and immunology. We may forego or delay pursuit of opportunities with certain programs, collaborations, or product candidates or for indications that later prove to have greater commercial potential. However, the development of any product candidate we pursue may ultimately prove to be unsuccessful or less successful than another potential product candidate that we might have chosen to pursue on a more aggressive basis with our capital resources. If we do not accurately evaluate the commercial potential for a particular product candidate, we may relinquish valuable rights to that product candidate through strategic collaboration, partnership, licensing, or other arrangements in cases in which it would have been more advantageous for us to retain sole development and commercialization rights to such product candidate. Alternatively, we may allocate internal resources to a product candidate in a therapeutic area in which it would have been more advantageous to enter into a collaboration.

Our research programs may show initial promise in identifying potential product candidates internally or with collaborators, yet fail to yield product candidates for clinical development for a number of reasons, including:

- our research methodology or that of any collaborator may be unsuccessful in identifying potential product candidates that are successful in clinical development;
- potential product candidates may be shown to have harmful side effects or may have other characteristics that may make the product candidates unmarketable or unlikely to receive marketing approval;
- our current or future collaborators may change their development profiles for potential product candidates or abandon a therapeutic area; or
- new competitive developments may render our product candidates obsolete or noncompetitive.

If any of these events occur, we may be forced to abandon our development efforts for a program or programs, which would have a material adverse effect on our business.

We rely on contract research organizations to synthesize any molecules with therapeutic potential that we discover. If such organizations do not meet our supply requirements, or if such organizations do not otherwise perform satisfactorily, development of any product candidate we may develop may be delayed.

We rely and expect to continue to rely on third parties to synthesize any molecules with therapeutic potential that we discover. Reliance on third parties may expose us to different risks than if we were to synthesize molecules ourselves. Our reliance on these third parties will reduce our control over these activities but will not relieve us of our responsibilities. If these third parties do not successfully carry out their contractual duties, meet expected deadlines, or synthesize molecules in accordance with regulatory requirements, if there are disagreements between us and such parties or if such parties are unable to expand capacities, we may not be able to fulfill, or may be delayed in producing sufficient product candidates to meet, our supply requirements, and we may not be able to complete, or may be delayed in completing, the necessary preclinical studies to enable us to progress viable product candidates for IND, submissions and we will not be able to, or may be delayed in our efforts to, successfully develop and commercialize such product candidates. These facilities may also be affected by natural disasters, such as floods or fire, or geopolitical developments or public health pandemics, such as COVID-19, or such facilities could face production issues, such as contamination or regulatory concerns following a regulatory inspection of such facility. In such instances, we may need to locate an appropriate replacement third-party facility and establish a contractual relationship, which may not be readily available or on acceptable terms, which would cause additional delay and increased expense, and may have a material adverse effect on our business.

We or any third party may also encounter shortages in the raw materials or active pharmaceutical ingredient, or API, necessary to synthesize any molecule we may discover in the quantities needed for preclinical studies or clinical trials, as a result of capacity constraints or delays or disruptions in the market for the raw materials or API. Even if raw materials or API are available, we may be unable to obtain sufficient quantities at an acceptable cost or quality. The failure by us or the third parties to obtain the raw materials or API necessary to synthesize sufficient quantities of any molecule we may discover could delay, prevent, or impair our development efforts and may have a material adverse effect on our business.

If we are not able to establish or maintain collaborations to develop and commercialize any of the product candidates we discover internally, we may have to alter our development and commercialization plans for those product candidates and our business could be adversely affected.

We expect to rely on future collaborators for the development and potential commercialization of product candidates we discover internally when we believe it will help maximize the commercial value of the product candidate. We face significant competition in seeking appropriate collaborators for these activities, and a number of more established companies may also be pursuing such collaborations. These established companies may have a competitive advantage over us due to their size, financial resources, and greater clinical development and commercialization expertise. Whether we reach a definitive agreement for such collaborations will depend, among other things, upon our assessment of the collaborator's resources and expertise, the terms and conditions of the proposed collaboration, and the proposed collaborator's evaluation of a number of factors. Those factors may include the design or results of preclinical studies and clinical trials, the likelihood of approval by the FDA or similar regulatory authorities outside the United States, the potential market for the subject product candidate, the costs and complexities of manufacturing and delivering such product candidate to patients, the potential of competing products, the existence of uncertainty with respect to our ownership of technology, which can exist if there is a challenge to such ownership without regard to the merits of the challenge, and industry and market conditions generally. The collaborator may also consider alternative product candidates or technologies for similar indications that may be available to collaborate on and whether such a collaboration could be more attractive than the one with us for our product candidate. Collaborations are complex and time-consuming to negotiate and document. In addition, there have been a significant number of recent business combinations among large biopharmaceutical companies that have resulted in a reduced number of potential future collaborators.

If we are unable to reach agreements with suitable collaborators on a timely basis, on acceptable terms or at all, we may have to curtail the development of a product candidate, reduce or delay its development program or one or more of our other development programs, or increase our expenditures and undertake development or commercialization activities at our own expense. If we elect to fund and undertake development or commercialization activities on our own, we may need to obtain additional expertise and additional capital, which may not be available to us on acceptable terms or at all. If we fail to enter into collaborations and do not have sufficient funds or expertise to undertake the necessary development and commercialization activities, we may not be able to further develop any product candidates or bring them to market.

As a company, we do not have any experience in clinical development and have not advanced any product candidates into clinical development.

We only began conducting our own internal drug discovery efforts in mid-2018. We have selected our first development candidates, which are for our MALT1 and CDC7 inhibitor programs, and advanced the programs into IND-enabling studies. As a company, we do not have any experience in clinical development and have not advanced any product candidates into clinical development. We expect to submit an investigational new drug, or IND, application to the FDA, for our MALT1 program in the first half of 2022, and subject to receiving regulatory clearance, we expect to initiate our first clinical trial in the second half of 2022. We also plan to submit IND applications to the FDA for our CDC7 program in early 2023 and our WEE1 program in 2023, subject to favorable data from IND-enabling studies. In addition, we plan to initiate a Phase 1 clinical trial of our CDC7 inhibitor in 2023, subject to receipt of regulatory clearance. Our lack of experience in conducting clinical development activities may adversely impact the likelihood that we will be successful in advancing our programs. Further, any predictions you make about the future success or viability of our internal drug discovery programs may not be as accurate as they could be if we had a history of conducting clinical trials and developing our own product candidates.

In addition, as our internal drug discovery business grows, we may encounter unforeseen expenses, difficulties, complications, delays, and other known and unknown factors. Our internal drug discovery business may need to transition to a business capable of supporting clinical development activities. We may not be successful in such a transition.

Conducting successful clinical trials requires the enrollment of a sufficient number of patients, and suitable patients may be difficult to identify and recruit.

Conducting successful clinical trials requires the enrollment of a sufficient number of patients, and suitable patients may be difficult to identify and recruit. Identifying and qualifying patients to participate in future clinical trials for any other product candidate we develop is critical to our success. Patient enrollment in clinical trials and completion of patient participation and follow-up depends on many factors, including the severity of disease; size of the patient population; the nature of the trial protocol; the attractiveness of, or the discomforts and risks associated with, the treatments received by enrolled subjects; the availability of clinical trial investigators with appropriate competencies and experience; support staff; the number of ongoing clinical trials in the same indication that compete for the same patients; proximity of patients to clinical sites; availability of trial sites; ability to comply with the eligibility and exclusion criteria for participation in the clinical trial; ability to obtain and maintain patient consents; patient compliance; the ability to monitor patients during and after treatment; and the impact of the ongoing COVID-19 pandemic. For example, patients may be discouraged from enrolling in our clinical trials if the trial protocol requires them to undergo extensive post-treatment procedures or follow-up to assess the safety and effectiveness of our product candidates. Patients may also not participate in our clinical trials if they choose to participate in contemporaneous clinical trials of competitive products.

Our inability to locate and enroll a sufficient number of patients for our clinical trials would result in significant delays, could require us to abandon one or more clinical trials altogether and could delay or prevent our receipt of necessary regulatory approvals. Enrollment delays in our clinical trials may result in increased development costs for our product candidates, which would cause the value of our company to decline and limit our ability to obtain additional financing.

We plan to rely on third parties to conduct our clinical trials, and those third parties may not perform satisfactorily, including failing to meet deadlines for the completion of such trials, which may prevent or delay our ability to seek or obtain marketing approval for or commercialize our product candidates or otherwise harm our business.

We plan to rely on third-party clinical research organizations, in addition to other third parties such as research collaboratives, clinical data management organizations, medical institutions and clinical investigators, to conduct our future clinical trials. These contract research organizations and other third parties will play a significant role in the conduct and timing of these trials and subsequent collection and analysis of data. These third-party arrangements might terminate for a variety of reasons, including a failure to perform by the third parties. If we need to enter into alternative arrangements, our product development activities might be delayed.

Our reliance on third parties for research and development activities reduces our control over these activities but does not relieve us of our responsibilities. For example, we are responsible for ensuring that each of our studies is conducted in accordance with the applicable protocol, and legal, regulatory and scientific standards, and our reliance on third parties does not relieve us of our responsibility to comply with any such standards. We and these third parties are required to comply with current good clinical practices, or cGCP, which are regulations and guidelines enforced by the FDA for all of our products in clinical development. Regulatory authorities in Europe and other jurisdictions have similar requirements. Regulatory authorities enforce these cGCPs through periodic inspections of trial sponsors, principal investigators and trial sites. If we or any of these third parties fail to comply with applicable cGCPs, the clinical data generated in our clinical trials may be deemed unreliable and the FDA or comparable foreign regulatory authorities may require us to perform additional clinical trials before approving our marketing applications. We cannot assure you a given regulatory authority will determine that any of our clinical trials comply with cGCP regulations. We also are required to register ongoing clinical trials and post the results of completed clinical trials on a U.S. government-sponsored database, clinicaltrials.gov, within certain timeframes. Failure to do so can result in fines, adverse publicity and civil and criminal sanctions.

Furthermore, third parties on whom we rely may also have relationships with other entities, some of which may be our competitors. In addition, these third parties are not our employees, and except for remedies available to us under our agreements with such third parties, we cannot control whether or not they devote sufficient time and resources to our on-going clinical, nonclinical and preclinical programs. If these third parties do not successfully carry out their contractual duties or obligations or meet expected deadlines, if they need to be replaced or if the quality or accuracy of the clinical data they obtain is compromised, our clinical trials may be extended, delayed or terminated and we may not be able to obtain, or may be delayed in obtaining, marketing approvals for our product candidates and will not be able to, or may be delayed in our efforts to, successfully commercialize our medicines.

If we and any current or future collaborators are unable to successfully complete clinical development, obtain regulatory approval for, or commercialize any product candidates, or experience delays in doing so, our business may be materially harmed.

We are early in our development efforts. Our most advanced development candidates are in IND-enabling studies, and we have not advanced any product candidate into clinical development. Our ability to generate product revenues, which we do not expect will occur for many years, if ever, will depend heavily on the successful development and eventual commercialization of our product

candidates. The success of our and any current or future collaborators' development and commercialization programs will depend on several factors, including the following:

- successful completion of necessary preclinical studies to enable the initiation of clinical trials;
- successful enrollment of patients in, and the completion of, the clinical trials;
- acceptance by the FDA or other regulatory agencies of regulatory filings for any product candidates we and our current or future collaborators may develop;
- expanding and maintaining a workforce of experienced scientists and others to continue to develop any product candidates;
- obtaining and maintaining intellectual property protection and regulatory exclusivity for any product candidates we and our current or future collaborators may develop;
- making arrangements with third-party manufacturers for, or establishing, clinical and commercial manufacturing capabilities;
- establishing sales, marketing, and distribution capabilities for drug products and successfully launching commercial sales, if and when approved;
- acceptance of any product candidates we and our current or future collaborators may develop, if and when approved, by patients, the medical community, and third-party payors;
- effectively competing with other therapies;
- obtaining and maintaining coverage, adequate pricing, and adequate reimbursement from third-party payors, including government payors;
- patients' willingness to pay out-of-pocket in the absence of coverage and/or adequate reimbursement from third-party payors;
- ongoing or future restrictions resulting from the COVID-19 pandemic and its collateral consequences may result in internal and external operational delays and limitations; and
- maintaining a continued acceptable safety profile following receipt of any regulatory approvals.

Many of these factors are beyond our control, including clinical outcomes, the regulatory review process, potential threats to our intellectual property rights, and the manufacturing, marketing, and sales efforts of any current or future collaborator. Clinical drug development involves a lengthy and expensive process, with an uncertain outcome. If we or our current or future collaborators are unable to develop, receive marketing approval for, and successfully commercialize any product candidates, or if we or they experience delays as a result of any of these factors or otherwise, we may need to spend significant additional time and resources, which would adversely affect our business, prospects, financial condition, and results of operations.

We face substantial competition, which may result in others discovering, developing or commercializing products before or more successfully than we do, thus rendering our products non-competitive, obsolete or reducing the size of our market.

We face competition with respect to our and our collaborators' product candidates from biopharmaceutical and biotechnology companies. The biotechnology and pharmaceutical industries are characterized by rapidly advancing technologies, intense competition and a strong emphasis on proprietary and novel products and product candidates. Our competitors have developed, are developing or may develop products, product candidates and processes competitive with our product candidates. Any product candidates that we successfully develop and commercialize, internally or with our collaborators, will compete with existing therapies and new therapies that may become available in the future.

In particular, there is intense competition in the fields of oncology we are pursuing. We have competitors both in the United States and internationally, including major multinational pharmaceutical companies, established biotechnology companies, specialty pharmaceutical companies, emerging and start-up companies, universities and other research institutions. We also compete with these organizations to recruit management, scientists and clinical development personnel, which could negatively affect our level of expertise and our ability to execute our business plan. We will also face competition in establishing clinical trial sites, enrolling subjects for clinical trials and in identifying new product candidates.

Large pharmaceutical and biotechnology companies, in particular, have extensive experience in clinical testing, obtaining regulatory approvals, recruiting patients and manufacturing biotechnology products. These companies also have significantly greater research and marketing capabilities than we do and may also have products that have been approved or are in late stages of development,

and collaborative arrangements in our target markets with leading companies and research institutions. Established pharmaceutical and biotechnology companies may also invest heavily to accelerate discovery and development of novel compounds or to in-license novel compounds that could make the product candidates that we develop obsolete. Our commercial opportunity could be reduced or eliminated if our competitors develop and commercialize products that are safer, more effective, have fewer or less severe side effects, are more convenient or are less expensive than our products. Smaller or early-stage companies may also prove to be significant competitors, particularly through collaborative arrangements with large and established companies, as well as in acquiring technologies complementary to, or necessary for, our programs. As a result of all of these factors, our competitors may succeed in obtaining approval from the FDA or other comparable foreign regulatory authorities or in discovering, developing and commercializing products in our field before we do.

Risks Related to Our Operations

Doing business internationally creates operational and financial risks for our business.

For the three months ended March 31, 2022 and the year ended December 31, 2021, sales to customers outside of the United States accounted for approximately 38% and 34% of our total revenues, respectively. Operating in international markets requires significant resources and management attention and subjects us to regulatory, economic, and political risks that are different from those in the United States. We have limited operating experience in some international markets, and we cannot assure you that our expansion efforts into other international markets will be successful. Our experience in the United States and other international markets in which we already have a presence may not be relevant to our ability to expand in other markets. Our international expansion efforts may not be successful in creating further demand for our solutions outside of the United States or in effectively selling our solutions in the international markets we enter. In addition, we face risks in doing business internationally that could adversely affect our business, including:

- the need to localize and adapt our solutions for specific countries, including translation into foreign languages;
- data privacy laws which require that customer data be stored and processed in a designated territory or handled in a manner that differs significantly from how we typically handle customer data;
- difficulties in staffing and managing foreign operations, including employee laws and regulations;
- different pricing environments, longer sales cycles, and longer accounts receivable payment cycles and collections issues;
- new and different sources of competition;
- weaker protection for intellectual property and other legal rights than in the United States and practical difficulties in enforcing intellectual property and other rights outside of the United States;
- laws and business practices favoring local competitors;
- compliance challenges related to the complexity of multiple, conflicting, and changing governmental laws and regulations, including employment, tax, reimbursement and pricing, privacy and data protection, and anti-bribery laws and regulations;
- increased financial accounting and reporting burdens and complexities;
- restrictions on the transfer of funds;
- changes in diplomatic and trade relationships, including new tariffs, trade protection measures, import or export licensing requirements, trade embargoes, and other trade barriers;
- changes in social, political, and economic conditions or in laws, regulations, and policies governing foreign trade, manufacturing, development, and investment both domestically as well as in the other countries and jurisdictions;
- adverse tax consequences, including the potential for required withholding taxes;
- global health pandemics, such as COVID-19; and
- unstable regional, economic and political conditions.

Our international agreements may provide for payment denominated in local currencies and our local operating costs are denominated in local currencies. Therefore, fluctuations in the value of the U.S. dollar and foreign currencies may impact our operating results when translated into U.S. dollars. We do not currently engage in currency hedging activities to limit the risk of exchange rate fluctuations.

Furthermore, with respect to our drug discovery programs, the current conflict involving Russia and Ukraine may impact the ability of our CROs in the region to produce materials we require to conduct certain of our preclinical studies. If the conflict were to be prolonged or worsened, and if we are unable to obtain alternative sources for such materials that we require, the ability for us to timely execute and complete certain of our preclinical studies may be adversely impacted.

Additionally, we could face heightened risks as a result of the recent withdrawal of the United Kingdom from the European Union, commonly referred to as Brexit. Since the regulatory framework for pharmaceutical products in the United Kingdom covering quality, safety and efficacy of pharmaceutical products, clinical trials, marketing authorization, commercial sales and distribution of pharmaceutical products is derived from European Union directives and regulations, the consequences of Brexit and the future regulatory regime that applies to products and the approval of product candidates in the United Kingdom remains unclear.

A widespread outbreak of an illness or other health issue, such as the COVID-19 pandemic, could negatively affect various aspects of our business and make it more difficult to meet our obligations to our customers, and could result in reduced demand from our customers as well as delays in our drug discovery and development programs.

Our business and operations could be adversely affected by health epidemics, including the ongoing COVID-19 pandemic, impacting the markets and industries in which we and our customers and collaborators operate.

In early March 2020, we implemented a work-from-home policy for all of our employees. Beginning in June 2020, we began limited re-openings of certain of our offices in the United States and abroad. We have continued to phase-in the re-opening of our offices as our management and federal, state, or local authorities advise, and we may take further actions that alter our operations as may be required by federal, state, or local authorities, or which we determine are in our best interests. While most of our operations can be performed remotely, there is no guarantee that we will continue to be as effective while working remotely because our team is dispersed, many employees may have additional personal needs to attend to (such as looking after children as a result of school closures or family who become sick), and employees may become sick themselves and be unable to work. Decreased effectiveness of our team could adversely affect our results due to our inability to meet in person with potential or current customers and collaborators, or other decreases in productivity that could seriously harm our business.

The full extent of the future impact will depend on many factors outside of our control, including, without limitation, the extent, trajectory and duration of the pandemic, the development, availability and distribution of effective treatments and vaccines, the imposition of protective public safety measures, the emergence of new strains and variants of COVID-19 and the effectiveness of vaccines against such strains and variants, and the impact of the pandemic on the global economy. For instance, if certain of our customers experience downturns or uncertainty in their own business operations and revenue because of the economic effects resulting from the spread of COVID-19, they may decrease their spending, which may result in decreased software revenue. Furthermore, as a result of the restrictions related to COVID-19 that remain in certain geographic areas, our sales force has limited in-person interactions, and their ability to attend events that promote and expand knowledge of our company and platform, including industry conferences and events has been hampered.

In addition, as a result of the COVID-19 pandemic, we may experience delays in the progress of certain of our and our collaborators' drug discovery and development programs, particularly those that are in preclinical studies and clinical trials or that are preparing to enter clinical trials. Relative to our and our collaborators' drug discovery programs, the COVID-19 pandemic has resulted in and may in the future result in disruptions in current and future IND-enabling studies and clinical trials, manufacturing disruptions, trial site disruptions and impact the ability to obtain necessary institutional review board, institutional biosafety committee, or other necessary site approvals. These disruptions have caused and may in the future cause delays in certain of our and our collaborators' drug discovery programs. For example, our contract manufacturing organizations, or CMOs, and our contract research organizations, or CROs, have experienced reductions in the capacity to undertake research-scale production and have experienced delays in executing preclinical studies, including our IND-enabling studies for our CDC7 program. We now expect to submit the IND application to the FDA for our CDC7 program in early 2023 and to initiate a Phase 1 clinical trial in 2023. In addition, the recent resurgence of COVID-19 in certain cities in China, and related subsequent lockdowns, have also reduced the capacity of a number of CROs that we work with in those affected areas. These reductions and delays may persist in the future, and we, together with our CMOs and CROs, are closely monitoring the impact of the COVID-19 pandemic on these operations, and we are actively working to add supplemental or substitute capacity to minimize the impact of these reduced operations. Furthermore, if our collaborators experience similar delays with their drug discovery and development programs, that could cause additional delays in our achievement of milestones and related revenue.

Inadequate funding or disruptions at the FDA and other agencies may also slow the time necessary for new product candidates to be reviewed and/or approved by necessary government agencies, which would adversely affect our business. For example, over the last several years the U.S. government has shut down several times and certain regulatory agencies, such as the FDA and the SEC, have had to furlough critical FDA, SEC and other government employees and stop critical activities. If a prolonged government shutdown occurs,

it could significantly impact the ability of the FDA to timely review and process our regulatory submissions, which could have a material adverse effect on our business. Further, future government shutdowns could impact our ability to access the public markets and obtain necessary capital in order to properly capitalize and continue our operations.

The global impact of COVID-19 continues to rapidly evolve, and we will continue to monitor the situation closely. The ultimate impact of the COVID-19 pandemic or a similar health epidemic is highly uncertain and subject to change. We do not yet know the full extent of potential delays or impacts on our business, operations, or the global economy as a whole. While the spread of COVID-19 may eventually be contained or mitigated, there is no guarantee that a future outbreak of this or any other widespread epidemics will not occur, or that the global economy will recover, either of which could seriously harm our business.

If we fail to manage our technical operations infrastructure, our existing customers, and our internal drug discovery team, may experience service outages, and our new customers may experience delays in the deployment of our solutions.

We have experienced significant growth in the number of users and data that our operations infrastructure supports. We seek to maintain sufficient excess capacity in our operations infrastructure to meet the needs of all of our customers and to support our internal drug discovery programs. We also seek to maintain excess capacity to facilitate the rapid provision of new customer deployments and the expansion of existing customer deployments. In addition, we need to properly manage our technological operations infrastructure in order to support version control, changes in hardware and software parameters and the evolution of our solutions. However, the provision of new hosting infrastructure requires adequate lead-time. We have experienced, and may in the future experience, website disruptions, outages, and other performance problems. These types of problems may be caused by a variety of factors, including infrastructure changes, human or software errors, viruses, security attacks, fraud, spikes in usage, and denial of service issues. In some instances, we may not be able to identify the cause or causes of these performance problems within an acceptable period of time. If we do not accurately predict our infrastructure requirements, our existing customers may experience service outages that may subject us to financial penalties, financial liabilities, and customer losses. If our operations infrastructure fails to keep pace with increased sales and usage, customers and our internal drug discovery team may experience delays in the deployment of our solutions as we seek to obtain additional capacity, which could adversely affect our reputation and adversely affect our revenues.

Changes in tax laws or in their implementation or interpretation could adversely affect our business and financial condition.

Changes in tax law may adversely affect our business or financial condition. The Tax Cuts and Jobs Act, or the 2017 Tax Act, as amended by the Coronavirus Aid, Relief, and Economic Security Act, or CARES Act, significantly revises the Internal Revenue Code of 1986, as amended, or the Code. The 2017 Tax Act, among other things, contains significant changes to corporate taxation, including a reduction of the corporate tax rate from a top marginal rate of 35% to a flat rate of 21%, the limitation of the tax deduction for net interest expense to 30% of adjusted taxable income (except for certain small businesses), the limitation of the deduction for net operating losses, or NOLs, to 80% of current-year taxable income and elimination of NOL carrybacks, in each case, for losses arising in taxable years beginning after December 31, 2017 (though any such NOLs may be carried forward indefinitely and such NOLs arising in taxable years beginning before January 1, 2021 are generally eligible to be carried back up to five years), the imposition of a one-time taxation of offshore earnings at reduced rates regardless of whether they are repatriated, the elimination of U.S. tax on foreign earnings (subject to certain important exceptions), the allowance of immediate deductions for certain new investments instead of deductions for depreciation expense over time, and the modification or repeal of many business deductions and credits.

In addition to the CARES Act, as part of Congress's response to the COVID-19 pandemic, economic relief legislation has been enacted in 2020 and 2021 containing tax provisions. Regulatory guidance under the 2017 Tax Act and such additional legislation is and continues to be forthcoming, and such guidance could ultimately increase or lessen the impact of these laws on our business and financial condition. Also, as a result of the changes in the U.S. presidential administration and control of the U.S. Senate in 2021, additional tax legislation may be enacted; any such additional legislation could have an impact on our company. In addition, it is uncertain if and to what extent various states will conform to the 2017 Tax Act and additional tax legislation.

Our ability to use our NOLs and research and development tax credit carryforwards to offset future taxable income may be subject to certain limitations.

As of December 31, 2021, we had federal NOLs of approximately $283.3 million and state NOLs of approximately $148.1 million, which, if not utilized, generally begin to expire in 2022. As of December 31, 2021, we also had federal research and development tax credit carryforwards of approximately $15.5 million and state research and development tax credit carryforwards of approximately $1.0 million. Unused credits began to expire in 2021 and generally expire over time if they remain unused. These NOLs and research and development tax credit carryforwards could expire unused and be unavailable to offset future income tax liabilities.

In addition, under Section 382 of the Code, and corresponding provisions of state law, a corporation that undergoes an "ownership change," generally defined as a greater than 50 percentage point change (by value) in its equity ownership by certain stockholders over a three-year period, is subject to limitations on its ability to utilize its pre-change NOLs and research and development tax credit carryforwards to offset future taxable income. We have performed an analysis through March 31, 2021 and determined that such an ownership change has occurred. As a result of such ownership change or future ownership changes, our ability to use our NOLs and research and development tax credit carryforwards may be materially limited.

There is also a risk that due to regulatory changes, such as suspension of the use of NOLs, or other unforeseen reasons, our existing NOLs could expire or otherwise become unavailable to offset future income tax liabilities. As described above in "Changes in tax laws or in their implementation or interpretation could adversely affect our business and financial condition," the 2017 Tax Act as amended by the CARES Act, includes changes to U.S. federal tax rates and rules governing NOL carryforwards that may significantly impact our ability to utilize NOLs to offset taxable income in the future. In addition, state NOLs generated in one state cannot be used to offset income generated in another state. For these reasons, we may be unable to use a material portion of our NOLs and other tax attributes.

Our international operations subject us to potentially adverse tax consequences.

We report our taxable income in various jurisdictions worldwide based upon our business operations in those jurisdictions. These jurisdictions include Germany, Japan, India and South Korea. The international nature and organization of our business activities are subject to complex transfer pricing regulations administered by taxing authorities in various jurisdictions. The relevant taxing authorities may disagree with our determinations as to the income and expenses attributable to specific jurisdictions. If such a disagreement were to occur, and our position were not sustained, we could be required to pay additional taxes, interest, and penalties, which could result in one-time tax charges, higher effective tax rates, reduced cash flows, and lower overall profitability of our operations.

Taxing authorities may successfully assert that we should have collected or in the future should collect sales and use, value added, or similar taxes, and we could be subject to tax liabilities with respect to past or future sales, which could adversely affect our results of operations.

We do not collect sales and use, value added, and similar taxes in all jurisdictions in which we have sales, based on our belief that such taxes are not applicable or that we are not required to collect such taxes with respect to the jurisdiction. Sales and use, value added, and similar tax laws and rates vary greatly by jurisdiction. Certain jurisdictions in which we do not collect such taxes may assert that such taxes are applicable, which could result in tax assessments, penalties, and interest, and we may be required to collect such taxes in the future. Such tax assessments, penalties, and interest or future requirements may adversely affect our results of operations.

Unanticipated changes in our effective tax rate could harm our future results.

We are subject to income taxes in the United States and various foreign jurisdictions, and our domestic and international tax liabilities are subject to the allocation of expenses in differing jurisdictions. Forecasting our estimated annual effective tax rate is complex and subject to uncertainty, and there may be material differences between our forecasted and actual tax rates. Our effective tax rate could be adversely affected by changes in the mix of earnings and losses in countries with differing statutory tax rates, certain non-deductible expenses as a result of acquisitions, the valuation of deferred tax assets and liabilities, and changes in federal, state, or international tax laws and accounting principles. Increases in our effective tax rate would reduce our profitability or in some cases increase our losses.

In addition, we may be subject to income tax audits by many tax jurisdictions throughout the world. Although we believe our income tax liabilities are reasonably estimated and accounted for in accordance with applicable laws and principles, an adverse resolution of one or more uncertain tax positions in any period could have a material impact on the results of operations for that period.

We have recently acquired, and we may again in the future acquire, companies or technologies, which could divert our management's attention, result in additional dilution to our stockholders, and otherwise disrupt our operations and adversely affect our operating results.

We have recently acquired, and we may again in the future seek to acquire or invest in, businesses, solutions, or technologies that we believe could complement or expand our solutions, enhance our technical capabilities, or otherwise offer growth opportunities. For example, in January 2022, we acquired XTAL, a company that provides structural biology services, including biophysical methods, protein production and purification, and X-ray crystallography, which will augment our ability to produce high quality target structures for our drug discovery programs. The pursuit of potential acquisitions may divert the attention of management and cause us to incur various expenses in identifying, investigating, and pursuing suitable acquisitions, whether or not they are consummated.

In addition, other than our acquisition of XTAL, we have limited experience in acquiring other businesses. If we acquire additional businesses, we may not be able to integrate the acquired personnel, operations, and technologies successfully, effectively manage the combined business following the acquisition or preserve the operational synergies between our business units that we believe currently exist. We cannot assure you that following any acquisition we would achieve the expected synergies to justify the transaction, due to a number of factors, including:

- inability to integrate or benefit from acquired technologies or services in a profitable manner;
- unanticipated costs or liabilities associated with the acquisition;
- incurrence of acquisition-related costs;
- difficulty integrating the accounting systems, operations, and personnel of the acquired business;
- difficulties and additional expenses associated with supporting legacy products and hosting infrastructure of the acquired business;
- difficulty converting the customers of the acquired business onto our solutions and contract terms, including disparities in the revenues, licensing, support, or professional services model of the acquired company;
- diversion of management's attention from other business concerns;
- adverse effects to our existing business relationships with business partners and customers as a result of the acquisition;
- the potential loss of key employees;
- use of resources that are needed in other parts of our business; and
- use of substantial portions of our available cash to consummate the acquisition.

In addition, a significant portion of the purchase price of companies we acquire may be allocated to acquired goodwill and other intangible assets, which must be assessed for impairment at least annually. In the future, if our acquisitions do not yield expected returns, we may be required to take charges to our operating results based on this impairment assessment process, which could adversely affect our results of operations.

Acquisitions could also result in dilutive issuances of equity securities or the incurrence of debt, which could adversely affect our operating results. In addition, if an acquired business fails to meet our expectations, our operating results, business, and financial position may suffer.

Our operations may be interrupted by the occurrence of a natural disaster or other catastrophic event at our primary facilities.

Our operations are primarily conducted at our facilities in New York, New York and Portland, Oregon and our internal hosting facility located in Clifton, New Jersey. The occurrence of natural disasters or other catastrophic events could disrupt our operations. Any natural disaster or catastrophic event in our facilities or the areas in which they are located could have a significant negative impact on our operations.

Risks Related to Our Intellectual Property

If we fail to comply with our obligations under our existing license agreements with Columbia University, under any of our other intellectual property licenses, or under any future intellectual property licenses, or otherwise experience disruptions to our business relationships with our current or any future licensors, we could lose intellectual property rights that are important to our business.

We are party to a number of license agreements pursuant to which we have been granted exclusive and non-exclusive worldwide licenses to certain patents, software code, and software programs to, among other things, reproduce, use, execute, copy, operate, sublicense, and distribute the licensed technology in connection with the marketing and sale of our software solutions and to develop improvements thereto. In particular, the technology that we license from Columbia University pursuant to our license agreements with them are used in and incorporated into a number of our software solutions which we market and license to our customers. For further information regarding our license agreements with Columbia University, see "Item 1. Business—License Agreements with Columbia University" in our Annual Report on Form 10-K for the fiscal year ended December 31, 2021. Our license agreements with Columbia University and other licensors impose, and we expect that future licenses will impose, specified royalty and other obligations on us.

In spite of our best efforts, our current or any future licensors might conclude that we have materially breached our license agreements with them and might therefore terminate the license agreements, thereby delaying our ability to market and sell our existing

software solutions and develop and commercialize new software solutions that utilize technology covered by these license agreements. If these in-licenses are terminated, or if the underlying intellectual property fails to provide the intended exclusivity, competitors could market, products and technologies similar to ours. This could have a material adverse effect on our competitive position, business, financial condition, results of operations, and prospects.

Disputes may arise regarding intellectual property subject to a licensing agreement, including:

- the scope of rights granted under the license agreement and other interpretation related issues;
- the extent to which our technology and processes infringe on intellectual property of the licensor that is not subject to the licensing agreement;
- the sublicensing of patent and other rights under any collaborative development relationships;
- the inventorship and ownership of inventions and know-how resulting from the joint creation or use of intellectual property by our current or future licensors and us and our collaborators; and
- the priority of invention of patented technology.

In addition, license agreements are complex, and certain provisions in such agreements may be susceptible to multiple interpretations. The resolution of any contract interpretation disagreement that may arise could narrow what we believe to be the scope of our rights to the relevant intellectual property or technology, or increase what we believe to be our financial or other obligations under the relevant agreement. For example, our counterparties have in the past and may in the future dispute the amounts owed to them pursuant to payment obligations. If disputes over intellectual property that we have licensed prevent or impair our ability to maintain our current licensing arrangements on commercially acceptable terms, we may experience delays in the development and commercialization of new software solutions and in our ability to market and sell existing software solutions, which could have a material adverse effect on our business, financial condition, results of operations, and prospects.

Our obligations under our existing or future drug discovery collaboration agreements may limit our intellectual property rights that are important to our business. Further, if we fail to comply with our obligations under our existing or future collaboration agreements, or otherwise experience disruptions to our business relationships with our prior, current, or future collaborators, we could lose intellectual property rights that are important to our business.

We are party to collaboration agreements with biopharmaceutical companies, pursuant to which we provide drug discovery services but have no ownership rights, or only co-ownership rights, to certain intellectual property generated through the collaborations. We are also party to a collaboration agreement with BMS for the development and potential commercialization of product candidates we discover internally, which also provides for co-ownership rights to certain intellectual property generated through the collaboration in certain scenarios. We may enter into additional collaboration agreements in the future, pursuant to which we may have no ownership rights, or only co-ownership rights, to certain intellectual property generated through the future collaborations. If we are unable to obtain ownership or license of such intellectual property generated through our prior, current, or future collaborations and overlapping with, or related to, our own proprietary technology or product candidates, then our business, financial condition, results of operations, and prospects could be materially harmed.

Our existing collaboration agreements contain certain exclusivity obligations that require us to design compounds exclusively for our collaborators with respect to certain specific targets over a specified time period. Our future collaboration agreements may grant similar exclusivity rights to future collaborators with respect to target(s) that are the subject of such collaborations. Existing or future collaboration agreements may also impose diligence obligations on us. For example, existing or future collaboration agreements may impose restrictions on us from pursuing the drug development targets for ourselves or for our other current or future collaborators, thereby removing our ability to develop and commercialize, or to jointly develop and commercialize with other current or future collaborators, product candidates, and technology related to the drug development targets. Under our collaboration with BMS, for example, we are prohibited from developing and commercializing product candidates anywhere in the world that are directed at the targets specified under the agreement, until the earlier of such target ceasing to be included under the agreement or the expiration of the last to expire royalty term for the program related to the target. In spite of our best efforts, our prior, current, or future collaborators might conclude that we have materially breached our collaboration agreements. If these collaboration agreements are terminated, or if the underlying intellectual property, to the extent we have ownership or license of, fails to provide the intended exclusivity, competitors would have the freedom to seek regulatory approval of, and to market, products and technology identical to ours. This could have a material adverse effect on our competitive position, business, financial condition, results of operations, and prospects.

Disputes may arise regarding intellectual property subject to a collaboration agreement, including:

- the scope of ownership or license granted under the collaboration agreement and other interpretation related issues;
- the extent to which our technology and product candidates infringe on intellectual property that generated through the collaboration to of which we do not have ownership or license under the collaboration agreement;
- the assignment or sublicense of intellectual property rights and other rights under the collaboration agreement;
- our diligence obligations under the collaboration agreement and what activities satisfy those diligence obligations; and
- the inventorship and ownership of inventions and know-how resulting from the joint creation or use of intellectual property by us and our current or future collaborators.

In addition, collaboration agreements are complex, and certain provisions in such agreements may be susceptible to multiple interpretations. The resolution of any contract interpretation disagreement that may arise could narrow what we believe to be the scope of our rights to the relevant intellectual property, or increase what we believe to be our obligations under the relevant agreements, either of which could have a material adverse effect on our business, financial condition, results of operations, and prospects. Moreover, if disputes over intellectual property that we have owned, co-owned, or in-licensed under the collaboration agreements prevent or impair our ability to maintain our current collaboration arrangements on commercially acceptable terms, we may be unable to successfully develop and commercialize the affected technology or product candidates, which could have a material adverse effect on our business, financial condition, results of operations, and prospects.

If we are unable to obtain, maintain, enforce, and protect patent protection for our technology and product candidates or if the scope of the patent protection obtained is not sufficiently broad, our competitors could develop and commercialize technology and products similar or identical to ours, and our ability to successfully develop and commercialize our technology and product candidates may be adversely affected.

Our success depends in large part on our ability to obtain and maintain protection of the intellectual property we may own solely and jointly with others or may license from others, particularly patents, in the United States and other countries with respect to any proprietary technology and product candidates we develop. We seek to protect our proprietary position by filing patent applications in the United States and abroad related to our technology and any product candidates we may develop that are important to our business and by in-licensing intellectual property related to our technology and product candidates. If we are unable to obtain or maintain patent protection with respect to any proprietary technology or product candidate, our business, financial condition, results of operations, and prospects could be materially harmed.

The patent prosecution process is expensive, time-consuming, and complex, and we may not be able to file, prosecute, maintain, defend, or license all necessary or desirable patent applications at a reasonable cost or in a timely manner. It is also possible that we will fail to identify patentable aspects of our research and development output before it is too late to obtain patent protection. Moreover, in some circumstances, we may not have the right to control the preparation, filing, and prosecution of patent applications, or to maintain, enforce, and defend the patents, covering technology that we co-own with third parties or license from third parties. Therefore, these co-owned and in-licensed patents and applications may not be prepared, filed, prosecuted, maintained, defended, and enforced in a manner consistent with the best interests of our business.

The patent position of software and biopharmaceutical companies generally is highly uncertain, involves complex legal and factual questions, and has in recent years been the subject of much litigation. In addition, the scope of patent protection outside of the United States is uncertain and laws of non-U.S. countries may not protect our rights to the same extent as the laws of the United States or vice versa. With respect to both owned and in-licensed patent rights, we cannot predict whether the patent applications we, our collaborators, and our licensor are currently pursuing will issue as patents in any particular jurisdiction or whether the claims of any issued patents will provide sufficient protection from competitors. Further, we may not be aware of all third-party intellectual property rights or prior art potentially relating to our computational platform, technology, and any product candidates we may develop. In addition, publications of discoveries in the scientific literature often lag behind the actual discoveries, and patent applications in the United States and other jurisdictions are typically not published until 18 months after filing of the priority application, or in some cases not published at all. Therefore, neither we nor our collaborators, or our licensor can know with certainty whether either we, our collaborators, or our licensor were the first to make the inventions claimed in the patents and patent applications we own or in-license now or in the future, or that either we, our collaborators, or our licensor were the first to file for patent protection of such inventions. As a result, the issuance, scope, validity, enforceability, and commercial value of our owned, co-owned, and in-licensed patent rights are highly uncertain. Moreover, our owned, co-owned, and in-licensed pending and future patent applications may not result in patents being issued that protect our technology and product candidates, in whole or in part, or that effectively prevent others from commercializing competitive technologies and products. Changes in either the patent laws or interpretation of the patent laws in the United States and other countries may diminish

the value of our owned, co-owned, or in-licensed current or future patents and our ability to obtain, protect, maintain, defend, and enforce our patent rights, narrow the scope of our patent protection and, more generally, could affect the value of, or narrow the scope of, our patent rights. For example, recent Supreme Court decisions have served to curtail the scope of subject matter eligible for patent protection in the United States, and many software patents have since been invalidated on the basis that they are directed to abstract ideas.

In order to pursue protection based on our pending provisional patent applications, we will need to file Patent Cooperation Treaty applications, non-U.S. applications, and/or U.S. non-provisional patent applications prior to applicable deadlines. Even then, as highlighted above, patents may never issue from our patent applications, or the scope of any patent may not be sufficient to provide a competitive advantage.

Moreover, we, our collaborators, or our licensor may be subject to a third-party preissuance submission of prior art to the U.S. Patent and Trademark Office, or USPTO, or become involved in opposition, derivation, revocation, reexamination, *inter partes* review, post-grant review or interference proceedings challenging our patent rights or the patent rights of others. An adverse determination in any such submission, proceeding or litigation could reduce the scope of, or invalidate, our patent rights or allow third parties to commercialize our technology or product candidates and compete directly with us, without payment to us. If the breadth or strength of protection provided by our owned, co-owned, or in-licensed current or future patents and patent applications is threatened, regardless of the outcome, it could dissuade companies from collaborating with us to license, develop, or commercialize current or future technology or product candidates.

Additionally, the coverage claimed in a patent application can be significantly reduced before the patent is issued, and its scope can be reinterpreted after issuance. Even if our owned, co-owned, and in-licensed current and future patent applications issue as patents, they may not issue in a form that will provide us with any meaningful protection, prevent competitors from competing with us, or otherwise provide us with any competitive advantage. The issuance of a patent is not conclusive as to its inventorship, scope, validity, or enforceability, and our owned and in-licensed patents may be challenged in the courts or patent offices in the United States and abroad. Such challenges may result in loss of exclusivity or in patent claims being narrowed, invalidated, or held unenforceable, in whole or in part, which could limit our ability to stop others from using or commercializing similar or identical technology and products, or limit the duration of the patent protection of our technology and product candidates. Such proceedings also may result in substantial cost and require significant time from our management and employees, even if the eventual outcome is favorable to us. In particular, given the amount of time required for the development, testing, and regulatory review of new product candidates, patents protecting such candidates might expire before or shortly after such candidates are commercialized. Furthermore, our competitors may be able to circumvent our owned, co-owned, or in-licensed current or future patents by developing similar or alternative technologies or products in a non-infringing manner. As a result, our owned, co-owned, and in-licensed current or future patent portfolio may not provide us with sufficient rights to exclude others from commercializing technology and products similar or identical to any of our technology and product candidates.

Changes to patent laws in the United States and other jurisdictions could diminish the value of patents in general, thereby impairing our ability to protect our products.

Changes in either the patent laws or interpretation of patent laws in the United States, including patent reform legislation such as the Leahy-Smith America Invents Act, or the Leahy-Smith Act, could increase the uncertainties and costs surrounding the prosecution of our owned and in-licensed patent applications and the maintenance, enforcement or defense of our owned and in-licensed issued patents. The Leahy-Smith Act includes a number of significant changes to United States patent law. These changes include provisions that affect the way patent applications are prosecuted, redefine prior art, provide more efficient and cost-effective avenues for competitors to challenge the validity of patents, and enable third-party submission of prior art to the USPTO during patent prosecution and additional procedures to attack the validity of a patent at USPTO-administered post-grant proceedings, including post-grant review, *inter partes* review, and derivation proceedings. Assuming that other requirements for patentability are met, prior to March 2013, in the United States, the first to invent the claimed invention was entitled to the patent, while outside the United States, the first to file a patent application was entitled to the patent. After March 2013, under the Leahy-Smith Act, the United States transitioned to a first-to-file system in which, assuming that the other statutory requirements for patentability are met, the first inventor to file a patent application will be entitled to the patent on an invention regardless of whether a third party was the first to invent the claimed invention. As such, the Leahy-Smith Act and its implementation could increase the uncertainties and costs surrounding the prosecution of our patent applications and the enforcement or defense of our issued patents, all of which could have a material adverse effect on our business, financial condition, results of operations and prospects.

In addition, the patent positions of companies in the development and commercialization of software, biologics and pharmaceuticals are particularly uncertain. Recent U.S. Supreme Court rulings have narrowed the scope of patent protection available in certain circumstances and weakened the rights of patent owners in certain situations. This combination of events has created uncertainty with respect to the validity and enforceability of patents once obtained. Depending on future actions by the U.S. Congress,

the federal courts, and the USPTO, the laws and regulations governing patents could change in unpredictable ways that could have a material adverse effect on our patent rights and our ability to protect, defend and enforce our patent rights in the future.

A number of recent cases decided by the U.S. Supreme Court have involved questions of when claims reciting abstract ideas, laws of nature, natural phenomena and/or natural products are eligible for a patent, regardless of whether the claimed subject matter is otherwise novel and inventive. These cases include Association for Molecular Pathology v. Myriad Genetics, Inc., 569 U.S. 12-398 (2013) or Myriad; Alice Corp. v. CLS Bank International, 573 U.S. 13-298 (2014); and Mayo Collaborative Services v. Prometheus Laboratories, Inc., or Prometheus, 566 U.S. 10-1150 (2012). In response to these cases, federal courts have held numerous patents invalid as claiming subject matter ineligible for patent protection. Moreover, the USPTO has issued guidance to the examining corps on how to apply these cases during examination. The full impact of these decisions is not yet known.

In addition to increasing uncertainty with regard to our ability to obtain future patents, this combination of events has created uncertainty with respect to the value of patents, once obtained. Depending on these and other decisions by Congress, the federal courts and the USPTO, the laws and regulations governing patents could change or be interpreted in unpredictable ways that would weaken our ability to obtain new patents or to enforce any patents that may issue to us in the future. In addition, these events may adversely affect our ability to defend any patents that may issue in procedures in the USPTO or in courts.

We, our prior, existing, or future collaborators, and our existing or future licensors, may become involved in lawsuits to protect or enforce our patent or other intellectual property rights, which could be expensive, time-consuming and unsuccessful.

Competitors and other third parties may infringe, misappropriate, or otherwise violate our, our prior, current and future collaborators', or our current and future licensors' issued patents or other intellectual property. As a result, we, our prior, current, or future collaborators, or our current or future licensor may need to file infringement, misappropriation, or other intellectual property related claims, which can be expensive and time-consuming. Any claims we assert against perceived infringers could provoke such parties to assert counterclaims against us alleging that we infringe, misappropriate, or otherwise violate their intellectual property. In addition, in a patent infringement proceeding, such parties could assert that the patents we, our collaborators, or our licensors have asserted are invalid or unenforceable. In patent litigation in the United States, defenses alleging invalidity or unenforceability are commonplace. Grounds for a validity challenge could be an alleged failure to meet any of several statutory requirements, including lack of novelty, obviousness, or non-enablement. Grounds for an unenforceability assertion could be an allegation that someone connected with prosecution of the patent withheld relevant information from the USPTO, or made a misleading statement, during prosecution. Third parties may institute such claims before administrative bodies in the United States or abroad, even outside the context of litigation. Such mechanisms include re-examination, post-grant review, *inter partes* review, interference proceedings, derivation proceedings, and equivalent proceedings in non-U.S. jurisdictions (e.g., opposition proceedings). The outcome following legal assertions of invalidity and unenforceability is unpredictable.

An adverse result in any such proceeding could put one or more of our owned, co-owned, or in-licensed current or future patents at risk of being invalidated or interpreted narrowly and could put any of our owned, co-owned, or in-licensed current or future patent applications at risk of not yielding an issued patent. A court may also refuse to stop the third party from using the technology at issue in a proceeding on the grounds that our owned, co-owned, or in-licensed current or future patents do not cover such technology. Furthermore, because of the substantial amount of discovery required in connection with intellectual property litigation, there is a risk that some of our confidential information or trade secrets could be compromised by disclosure during this type of litigation. Any of the foregoing could allow such third parties to develop and commercialize competing technologies and products in a non-infringing manner and have a material adverse impact on our business, financial condition, results of operations, and prospects.

Interference or derivation proceedings provoked by third parties, or brought by us or by our collaborators or licensor, or declared by the USPTO may be necessary to determine the priority of inventions with respect to our patents or patent applications. An unfavorable outcome could require us to cease using the related technology or to attempt to license rights to it from the prevailing party. Our business could be harmed if the prevailing party does not offer us a license on commercially reasonable terms or at all, or if a non-exclusive license is offered and our competitors gain access to the same technology. Our defense of litigation or interference or derivation proceedings may fail and, even if successful, may result in substantial costs and distract our management and other employees. In addition, the uncertainties associated with litigation could have a material adverse effect on our ability to raise the funds necessary to conduct clinical trials, continue our research programs, license necessary technology from third parties, or enter into development collaborations that would help us bring any product candidates to market.

Third parties may initiate legal proceedings alleging that we are infringing, misappropriating or otherwise violating their intellectual property rights, the outcome of which would be uncertain and could have a material adverse effect on the success of our business.

Our commercial success depends upon our ability and the ability of our collaborators and licensor to develop, manufacture, market and sell any product candidates we may develop and for our collaborators, licensor, customers and partners to use our proprietary technologies without infringing, misappropriating or otherwise violating the intellectual property and proprietary rights of third parties. There is considerable patent and other intellectual property litigation in the software, pharmaceutical, and biotechnology industries. We may become party to, or threatened with, adversarial proceedings or litigation regarding intellectual property rights with respect to our technology and product candidates, including interference proceedings, post grant review, *inter partes* review, and derivation proceedings before the USPTO and similar proceedings in non-U.S. jurisdictions such as oppositions before the European Patent Office. Numerous U.S. and non-U.S. issued patents and pending patent applications, which are owned by third parties, exist in the fields in which we are pursuing development candidates. As the biotechnology and pharmaceutical industries expand and more patents are issued, the risk increases that our technologies or product candidates that we may identify may be subject to claims of infringement of the patent rights of third parties.

The legal threshold for initiating litigation or contested proceedings is low, so that even lawsuits or proceedings with a low probability of success might be initiated and require significant resources to defend. Litigation and contested proceedings can also be expensive and time-consuming, and our adversaries in these proceedings may have the ability to dedicate substantially greater resources to prosecuting these legal actions than we can. The risks of being involved in such litigation and proceedings may increase if and as any product candidates near commercialization and as we gain the greater visibility associated with being a public company. Third parties may assert infringement claims against us based on existing patents or patents that may be granted in the future, regardless of merit. We may not be aware of all such intellectual property rights potentially relating to our technology and product candidates and their uses, or we may incorrectly conclude that third-party intellectual property is invalid or that our activities and product candidates do not infringe such intellectual property. Thus, we do not know with certainty that our technology and product candidates, or our development and commercialization thereof, do not and will not infringe, misappropriate or otherwise violate any third party's intellectual property.

Third parties may assert that we are employing their proprietary technology without authorization. There may be third-party patents or patent applications with claims to materials, formulations or methods, such as methods of manufacture or methods for treatment, related to the discovery, use or manufacture of the product candidates that we may identify or related to our technologies. Because patent applications can take many years to issue, there may be currently pending patent applications which may later result in issued patents that the product candidates that we may identify may infringe. In addition, third parties may obtain patents in the future and claim that use of our technologies infringes upon these patents. Moreover, as noted above, there may be existing patents that we are not aware of or that we have incorrectly concluded are invalid or not infringed by our activities. If any third-party patents were held by a court of competent jurisdiction to cover, for example, the manufacturing process of the product candidates that we may identify, any molecules formed during the manufacturing process or any final product itself, the holders of any such patents may be able to block our ability to commercialize such product candidate unless we obtained a license under the applicable patents, or until such patents expire.

Parties making claims against us may obtain injunctive or other equitable relief, which could effectively block our ability to further develop and commercialize the product candidates that we may identify. Defense of these claims, regardless of their merit, would involve substantial litigation expense and would be a substantial diversion of employee resources from our business. In the event of a successful claim of infringement against us, we may have to pay substantial damages, including treble damages and attorneys' fees for willful infringement, pay royalties, redesign our infringing products, be forced to indemnify our customers, licensor, or collaborators or obtain one or more licenses from third parties, which may be impossible or require substantial time and monetary expenditure.

We may choose to take a license or, if we are found to infringe, misappropriate or otherwise violate a third party's intellectual property rights, we could also be required to obtain a license from such third party to continue developing, manufacturing and marketing our technology and product candidates. However, we may not be able to obtain any required license on commercially reasonable terms or at all. Even if we were able to obtain a license, it could be non-exclusive, thereby giving our competitors and other third parties access to the same technologies licensed to us and could require us to make substantial licensing and royalty payments. We could be forced, including by court order, to cease developing, manufacturing and commercializing the infringing technology or product. A finding of infringement could prevent us from commercializing any product candidates or force us to cease some of our business operations, which could materially harm our business. In addition, we may be forced to redesign any product candidates, seek new regulatory approvals and indemnify third parties pursuant to contractual agreements. Claims that we have misappropriated the confidential information or trade secrets of third parties could have a similar material adverse effect on our business, financial condition, results of operations and prospects.

We may be subject to claims by third parties asserting that our employees, consultants, or contractors have wrongfully used or disclosed confidential information of third parties, or we have wrongfully used or disclosed alleged trade secrets of their current or former employers or claims asserting we have misappropriated their intellectual property, or claiming ownership of what we regard as our own intellectual property.

Certain of our employees, consultants, and contractors were previously employed at universities or other software or biopharmaceutical companies, including our competitors or potential competitors. Although we try to ensure that our employees, consultants and contractors do not use the proprietary information or know-how of others in their work for us, we may be subject to claims that these individuals or we have used or disclosed intellectual property, including trade secrets or other proprietary information, of any such individual's current or former employer. Litigation may be necessary to defend against these claims.

In addition, while it is our policy to require that our employees, consultants and contractors who may be involved in the development of intellectual property to execute agreements assigning such intellectual property to us, we may be unsuccessful in executing such an agreement with each party who in fact develops intellectual property that we regard as our own. Our intellectual property assignment agreements with them may not be self-executing or may be breached, and we may be forced to bring claims against third parties, or defend claims they may bring against us, to determine the ownership of what we regard as our intellectual property. Such claims could have a material adverse effect on our business, financial condition, results of operations, and prospects.

If we fail in prosecuting or defending any such claims, in addition to paying monetary damages, we may lose valuable intellectual property rights or personnel, which could have a material adverse effect on our competitive business position and prospects. Such intellectual property rights could be awarded to a third party, and we could be required to obtain a license from such third party to commercialize our technology or products, which license may not be available on commercially reasonable terms, or at all, or such license may be non-exclusive. Even if we are successful in prosecuting or defending against such claims, litigation could result in substantial costs and be a distraction to our management and employees.

If we are unable to protect the confidentiality of our trade secrets, our business and competitive position may be harmed.

In addition to seeking patents for any product candidates and technology, we also rely on trade secrets and confidentiality agreements to protect our unpatented know-how, technology, and other proprietary information, to maintain our competitive position. We seek to protect our trade secrets and other proprietary technology, in part, by entering into non-disclosure and confidentiality agreements with parties who have access to them, such as our employees, corporate collaborators, outside scientific collaborators, contract research organizations, contract manufacturers, consultants, advisors, collaborators, and other third parties. We also enter into confidentiality and invention or patent assignment agreements with our employees and consultants, but we cannot guarantee that we have entered into such agreements with each party that may have or has had access to our trade secrets or proprietary technology. Despite these efforts, any of these parties may breach the agreements and disclose our proprietary information, including our trade secrets, and we may not be able to obtain adequate remedies for such breaches. Detecting the disclosure or misappropriation of a trade secret and enforcing a claim that a party illegally disclosed or misappropriated a trade secret is difficult, expensive, and time-consuming, and the outcome is unpredictable. In addition, some courts inside and outside of the United States are less willing or unwilling to protect trade secrets. If any of our trade secrets were to be lawfully obtained or independently developed by a competitor or other third party, we would have no right to prevent them, or those to whom they communicate it, from using that technology or information to compete with us. If any of our trade secrets were to be disclosed to or independently developed by a competitor or other third party, our competitive position may be materially and adversely harmed.

Risks Related to Regulatory and Other Legal Compliance Matters

Even if we complete the necessary preclinical studies and clinical trials, the regulatory approval process is expensive, time consuming and uncertain and may prevent us from obtaining approvals for the commercialization of some or all of our product candidates. As a result, we cannot predict when or if, and in which territories, we will obtain marketing approval to commercialize a product candidate.

The research, testing, manufacturing, labeling, approval, selling, marketing, promotion and distribution of products are subject to extensive regulation by the FDA and comparable foreign regulatory authorities. We are not permitted to market our product candidates in the United States or in other countries until we receive approval of an NDA from the FDA or marketing approval from applicable regulatory authorities outside the United States. Our product candidates are in various stages of development and are subject to the risks of failure inherent in development. We have not submitted an application for or received marketing approval for any of our product candidates in the United States or in any other jurisdiction. We have no experience as a company in filing and supporting the applications necessary to gain marketing approvals and expect to rely on third-party CROs to assist us in this process.

The process of obtaining marketing approvals, both in the United States and abroad, is lengthy, expensive and uncertain. It may take many years, if approval is obtained at all, and can vary substantially based upon a variety of factors, including the type, complexity and novelty of the product candidates involved. Securing marketing approval requires the submission of extensive preclinical and clinical

data and supporting information, including manufacturing information, to regulatory authorities for each therapeutic indication to establish the product candidate's safety and efficacy. The FDA or other regulatory authorities may determine that our product candidates are not safe and effective, only moderately effective or have undesirable or unintended side effects, toxicities or other characteristics that preclude our obtaining marketing approval or prevent or limit commercial use.

In addition, changes in marketing approval policies during the development period, changes in or the enactment or promulgation of additional statutes, regulations or guidance or changes in regulatory review for each submitted product application, may cause delays in the approval or rejection of an application. Regulatory authorities have substantial discretion in the approval process and varying interpretations of the data obtained from preclinical and clinical testing could delay, limit or prevent marketing approval of a product candidate. Any marketing approval we ultimately obtain may be limited or subject to restrictions or post-approval commitments that render the approved product not commercially viable.

In order to market and sell our products in the European Union and other foreign jurisdictions, we must obtain separate marketing approvals and comply with numerous and varying regulatory requirements. The approval procedure varies among countries and can involve additional testing. The time required to obtain approval may differ substantially from that required to obtain FDA approval. The marketing approval process outside the United States generally includes all of the risks associated with obtaining FDA approval. We may not obtain approvals from regulatory authorities outside the United States on a timely basis, if at all. Approval by the FDA does not ensure approval by regulatory authorities in other countries or jurisdictions, and approval by one regulatory authority outside the United States does not ensure approval by regulatory authorities in other countries or jurisdictions or by the FDA. We may file for marketing approvals but not receive necessary approvals to commercialize our products in any market.

We may seek certain designations for our product candidates, including Breakthrough Therapy, Fast Track and Priority Review designations in the United States, and PRIME Designation in the European Union, but we might not receive such designations, and even if we do, such designations may not lead to a faster development or regulatory review or approval process.

We may seek certain designations for one or more of our product candidates that could expedite review and approval by the FDA. A Breakthrough Therapy product is defined as a product that is intended, alone or in combination with one or more other products, to treat a serious condition, and preliminary clinical evidence indicates that the product may demonstrate substantial improvement over existing therapies on one or more clinically significant endpoints, such as substantial treatment effects observed early in clinical development. For products that have been designated as Breakthrough Therapies, interaction and communication between the FDA and the sponsor of the trial can help to identify the most efficient path for clinical development while minimizing the number of patients placed in ineffective control regimens.

The FDA may also designate a product for Fast Track review if it is intended, whether alone or in combination with one or more other products, for the treatment of a serious or life threatening disease or condition, and it demonstrates the potential to address unmet medical needs for such a disease or condition. For Fast Track products, sponsors may have greater interactions with the FDA and the FDA may initiate review of sections of a Fast Track product's application before the application is complete. This rolling review may be available if the FDA determines, after preliminary evaluation of clinical data submitted by the sponsor, that a Fast Track product may be effective.

We may also seek a priority review designation for one or more of our product candidates. If the FDA determines that a product candidate offers major advances in treatment or provides a treatment where no adequate therapy exists, the FDA may designate the product candidate for priority review. A priority review designation means that the goal for the FDA to review an application is six months, rather than the standard review period of ten months.

These designations are within the discretion of the FDA. Accordingly, even if we believe that one of our product candidates meets the criteria for these designations, the FDA may disagree and instead determine not to make such designation. Further, even if we receive a designation, the receipt of such designation for a product candidate may not result in a faster development or regulatory review or approval process compared to products considered for approval under conventional FDA procedures and does not assure ultimate approval by the FDA. In addition, even if one or more of our product candidates qualifies for these designations, the FDA may later decide that the product candidates no longer meet the conditions for qualification or decide that the time period for FDA review or approval will not be shortened.

In the EU, we may seek PRIME designation for our product candidates in the future. PRIME is a voluntary program aimed at enhancing the EMA's role to reinforce scientific and regulatory support in order to optimize development and enable accelerated assessment of new medicines that are of major public health interest with the potential to address unmet medical needs. The program focuses on medicines that target conditions for which there exists no satisfactory method of treatment in the EU or even if such a method exists, it may offer a major therapeutic advantage over existing treatments. PRIME is limited to medicines under development and not authorized in the EU and the applicant intends to apply for an initial marketing authorization application through the centralized procedure. To be accepted for PRIME, a product candidate must meet the eligibility criteria in respect of its major public health interest and therapeutic innovation based on information that is capable of substantiating the claims. The benefits of a PRIME designation include the appointment of a CHMP rapporteur to provide continued support and help to build knowledge ahead of a marketing authorization application, early dialogue and scientific advice at key development milestones, and the potential to qualify products for accelerated review, meaning reduction in the review time for an opinion on approvability to be issued earlier in the application process. PRIME enables an applicant to request parallel EMA scientific advice and health technology assessment advice to facilitate timely market access. Even if we receive PRIME designation for any of our product candidates, the designation may not result in a materially

faster development process, review or approval compared to conventional EMA procedures. Further, obtaining PRIME designation does not assure or increase the likelihood of EMA's grant of a marketing authorization.

Compliance with global privacy and data security requirements could result in additional costs and liabilities to us or inhibit our ability to collect and process data globally, and the failure to comply with such requirements could subject us to significant fines and penalties, which may have a material adverse effect on our business, financial condition, or results of operations.

The regulatory framework for the collection, use, safeguarding, sharing, transfer, and other processing of information worldwide is rapidly evolving and is likely to remain uncertain for the foreseeable future. Globally, virtually every jurisdiction in which we operate has established its own data security and privacy frameworks with which we must comply. For example, the collection, use, disclosure, transfer, or other processing of personal data regarding individuals in the European Union, including personal health data and employee data, is subject to the European Union General Data Protection Regulation, or the GDPR, which took effect across all member states of the European Economic Area, or EEA, in May 2018. The GDPR is wide-ranging in scope and imposes numerous requirements on companies that process personal data, including requirements relating to processing health and other sensitive data, obtaining consent of the individuals to whom the personal data relates, providing information to individuals regarding data processing activities, implementing safeguards to protect the security and confidentiality of personal data, providing notification of data breaches, and taking certain measures when engaging third-party processors. The GDPR would increase our obligations with respect to any clinical trials conducted in the EEA by expanding the definition of personal data to include coded data and requiring changes to informed consent practices and more detailed notices for clinical trial subjects and investigators. In addition, the GDPR also imposes strict rules on the transfer of personal data to countries outside the European Union, including the United States and, as a result, increases the scrutiny that such rules should apply to transfers of personal data from any clinical trial sites located in the EEA to the United States. The GDPR also permits data protection authorities to require destruction of improperly gathered or used personal information and/or impose substantial fines for violations of the GDPR, which can be up to four percent of global revenues or 20 million Euros, whichever is greater, and confers a private right of action on data subjects and consumer associations to lodge complaints with supervisory authorities, seek judicial remedies, and obtain compensation for damages resulting from violations of the GDPR. In addition, the GDPR provides that European Union member states may make their own further laws and regulations limiting the processing of personal data, including genetic, biometric, or health data.

Given the breadth and depth of changes in data protection obligations, preparing for and complying with the GDPR's requirements is rigorous and time intensive and requires significant resources and a review of our technologies, systems and practices, as well as those of any third-party collaborators, service providers, contractors, or consultants that process or transfer personal data collected in the European Union. The GDPR and other changes in laws or regulations associated with the enhanced protection of certain types of sensitive data, such as healthcare data or other personal information, could require us to change our business practices and put in place additional compliance mechanisms, may interrupt or delay our development, regulatory and commercialization activities and increase our cost of doing business, and could lead to government enforcement actions, private litigation, and significant fines and penalties against us, and could have a material adverse effect on our business, financial condition, or results of operations.

Similar privacy and data security requirements are either in place or underway in the United States. There are a broad variety of data protection laws that may be applicable to our activities, and a range of enforcement agencies at both the state and federal levels that can review companies for privacy and data security concerns. The Federal Trade Commission and state Attorneys General all are aggressive in reviewing privacy and data security protections for consumers. New laws also are being considered at both the state and federal levels. For example, the California Consumer Privacy Act, or CCPA, which went into effect on January 1, 2020, is creating similar risks and obligations as those created by GDPR. Because of this, we may need to engage in additional activities (e.g., data mapping) to identify the personal information we are collecting and the purposes for which such information is collected. In addition, we will need to ensure that our policies recognize the rights granted to consumers (as that phrase is broadly defined in the CCPA and can include business contact information), including granting consumers the right to opt-out of the sale of their personal information. Many other states are considering similar legislation. A broad range of legislative measures also have been introduced at the federal level. Accordingly, failure to comply with current and any future federal and state laws regarding privacy and security of personal information could expose us to fines and penalties. We also face a threat of consumer class actions related to these laws and the overall protection of personal data. Even if we are not determined to have violated these laws, investigations into these issues typically require the expenditure of significant resources and generate negative publicity, which could harm our reputation and our business.

We, and the collaborators who use our computational platform, may be subject to applicable anti-kickback, fraud and abuse, false claims, transparency, health information privacy and security, and other healthcare laws and regulations. Failure to comply with such laws and regulations, may result in substantial penalties.

We, and the collaborators who use our computational platform, may be subject to broadly applicable healthcare laws and regulations that may constrain the business or financial arrangements and relationships through which we market, sell, and distribute our software solutions and any products for which we obtain marketing approval. Such healthcare laws and regulations include, but are not limited to, the federal health care Anti-Kickback Statute; federal civil and criminal false claims laws, such as the federal False Claims Act; the federal Health Insurance Portability and Accountability Act of 1996, or HIPAA; the Federal Food, Drug, and Cosmetic Act;

the federal Physician Payments Sunshine Act; and analogous state and foreign laws and regulations, such as state anti-kickback and false claims laws and transparency laws.

Efforts to ensure that our business arrangements with third parties will comply with applicable healthcare laws and regulations will involve substantial costs. It is possible that governmental authorities will conclude that our business practices may not comply with current or future statutes, regulations, or case law involving applicable fraud and abuse or other healthcare laws and regulations. Violations of applicable healthcare laws and regulations may result in significant civil, criminal, and administrative penalties, damages, disgorgement, fines, imprisonment, exclusion of products from government funded healthcare programs, such as Medicare and Medicaid, additional reporting requirements, and/or oversight if a corporate integrity agreement or similar agreement is executed to resolve allegations of non-compliance with these laws and the curtailment or restructuring of operations. In addition, violations may also result in reputational harm, diminished profits, and future earnings.

We are subject to anti-corruption laws, as well as export control laws, customs laws, sanctions laws, and other laws governing our operations. If we fail to comply with these laws, we could be subject to civil or criminal penalties, other remedial measures, and legal expenses, be precluded from developing, manufacturing, and selling certain products outside the United States or be required to develop and implement costly compliance programs, which could adversely affect our business, results of operations and financial condition.

Our operations are subject to anti-corruption laws, including the U.K. Bribery Act 2010, or Bribery Act, the U.S. Foreign Corrupt Practices Act, or FCPA, and other anti-corruption laws that apply in countries where we do business and may do business in the future. The Bribery Act, FCPA, and these other laws generally prohibit us, our officers, and our employees and intermediaries from bribing, being bribed, or making other prohibited payments to government officials or other persons to obtain or retain business or gain some other business advantage. Compliance with the FCPA, in particular, is expensive and difficult, particularly in countries in which corruption is a recognized problem. In addition, the FCPA presents particular challenges in the biopharmaceutical industry, because, in many countries, hospitals are operated by the government, and doctors and other hospital employees are considered foreign officials. Certain payments to hospitals in connection with clinical trials and other work have been deemed to be improper payments to government officials and have led to FCPA enforcement actions.

We may in the future operate in jurisdictions that pose a high risk of potential Bribery Act or FCPA violations, and we may participate in collaborations and relationships with third parties whose actions could potentially subject us to liability under the Bribery Act, FCPA, or local anti-corruption laws. In addition, we cannot predict the nature, scope or effect of future regulatory requirements to which our international operations might be subject or the manner in which existing laws might be administered or interpreted. If we further expand our operations outside of the United States, we will need to dedicate additional resources to comply with numerous laws and regulations in each jurisdiction in which we plan to operate.

We are also subject to other laws and regulations governing our international operations, including regulations administered by the governments of the United Kingdom and the United States, and authorities in the European Union, including applicable export control regulations, economic sanctions on countries and persons, customs requirements, and currency exchange regulations, collectively referred to as the Trade Control laws. In addition, various laws, regulations, and executive orders also restrict the use and dissemination outside of the United States, or the sharing with certain non-U.S. nationals, of information classified for national security purposes, as well as certain products and technical data relating to those products. If we expand our presence outside of the United States, it will require us to dedicate additional resources to comply with these laws, and these laws may preclude us from developing, manufacturing, or selling certain products and product candidates outside of the United States, which could limit our growth potential and increase our development costs.

There is no assurance that we will be completely effective in ensuring our compliance with all applicable anti-corruption laws, including the Bribery Act, the FCPA, or other legal requirements, including Trade Control laws. If we are not in compliance with the Bribery Act, the FCPA, and other anti-corruption laws or Trade Control laws, we may be subject to criminal and civil penalties, disgorgement and other sanctions and remedial measures, and legal expenses, which could have an adverse impact on our business, financial condition, results of operations, and liquidity. The U.S. Securities and Exchange Commission, or SEC, also may suspend or bar issuers from trading securities on U.S. exchanges for violations of the FCPA's accounting provisions. Any investigation of any potential violations of the Bribery Act, the FCPA, other anti-corruption laws or Trade Control laws by the United Kingdom, U.S., or other authorities could also have an adverse impact on our reputation, our business, results of operations, and financial condition.

Our employees, independent contractors, consultants, and vendors may engage in misconduct or other improper activities, including non-compliance with regulatory standards and requirements and insider trading laws, which could cause significant liability for us and harm our reputation.

We are exposed to the risk of fraud or other misconduct by our employees, independent contractors, consultants, and vendors. Misconduct by these partners could include intentional failures to comply with FDA regulations or similar regulations of comparable foreign regulatory authorities, provide accurate information to the FDA or comparable foreign regulatory authorities, comply with manufacturing standards, comply with federal and state healthcare fraud and abuse laws and regulations and similar laws and regulations established and enforced by comparable foreign regulatory authorities, report financial information or data accurately, or disclose unauthorized activities to us. Employee misconduct could also involve the improper use of information obtained in the course of clinical trials, which could result in regulatory sanctions and serious harm to our reputation. This could include violations of HIPAA, other U.S. federal and state law, and requirements of non-U.S. jurisdictions, including the European Union Data Protection Directive. We are also exposed to risks in connection with any insider trading violations by employees or others affiliated with us. It is not always possible to identify and deter employee misconduct, and the precautions we take to detect and prevent this activity may not be effective in controlling unknown or unmanaged risks or losses or in protecting us from governmental investigations or other actions or lawsuits stemming from a failure to be in compliance with such laws, standards, regulations, guidance, or codes of conduct. Furthermore, our employees may, from time to time, bring lawsuits against us for employment issues, including injury, discrimination, wage and hour disputes, sexual harassment, hostile work environment, or other employment issues. If any such actions are instituted against us, and we are not successful in defending ourselves or asserting our rights, those actions could have a significant impact on our business and results of operations, including the imposition of significant fines or other sanctions.

Our internal information technology systems, or those of our third-party vendors, contractors, or consultants, may fail or suffer security breaches, loss or leakage of data, and other disruptions, which could result in a material disruption of our services, compromise sensitive information related to our business, or prevent us from accessing critical information, potentially exposing us to liability or otherwise adversely affecting our business.

We are increasingly dependent upon information technology systems, infrastructure, and data to operate our business. In the ordinary course of business, we collect, store, and transmit confidential information (including but not limited to intellectual property, proprietary business information, and personal information). It is critical that we do so in a secure manner to maintain the confidentiality and integrity of such confidential information. We also have outsourced elements of our operations to third parties, and as a result we manage a number of third-party vendors and other contractors and consultants who have access to our confidential information.

Despite the implementation of security measures, given the size and complexity of our internal information technology systems and those of our third-party vendors and other contractors and consultants, and the increasing amounts of confidential information that they maintain, our information technology systems are potentially vulnerable to breakdown or other damage or interruption from service interruptions, system malfunction, natural disasters, terrorism, war, and telecommunication and electrical failures, as well as security breaches from inadvertent or intentional actions by our employees, third-party vendors, contractors, consultants, business partners, and/or other third parties, or from cyber-attacks by malicious third parties (including the deployment of harmful malware, ransomware, denial-of-service attacks, social engineering, and other means to affect service reliability and threaten the confidentiality, integrity, and availability of information), which may compromise our system infrastructure, or that of our third-party vendors and other contractors and consultants or lead to data leakage. The risk of a security breach or disruption, particularly through cyber-attacks or cyber intrusion, including by computer hackers, foreign governments, and cyber terrorists, has generally increased as the number, intensity, and sophistication of attempted attacks and intrusions from around the world have increased. We may not be able to anticipate all types of security threats, and we may not be able to implement preventive measures effective against all such security threats. For example, third parties have in the past and may in the future illegally pirate our software and make that software publicly available on peer-to-peer file sharing networks or otherwise. The techniques used by cyber criminals change frequently, may not be recognized until launched, and can originate from a wide variety of sources, including outside groups such as external service providers, organized crime affiliates, terrorist organizations, or hostile foreign governments or agencies. To the extent that any disruption or security breach were to result in a loss of, or damage to, our data or applications, or those of our third-party vendors and other contractors and consultants, or inappropriate disclosure of confidential or proprietary information, we could incur liability and reputational damage and the further development and commercialization of our software could be delayed. The costs related to significant security breaches or disruptions could be material and exceed the limits of the cybersecurity insurance we maintain against such risks. If the information technology systems of our third-party vendors and other contractors and consultants become subject to disruptions or security breaches, we may have insufficient recourse against such third parties and we may have to expend significant resources to mitigate the impact of such an event, and to develop and implement protections to prevent future events of this nature from occurring.

While we have not experienced any significant system failure, accident, or security breach to date, and believe that our data protection efforts and our investment in information technology reduce the likelihood of such incidents in the future, we cannot assure you that our data protection efforts and our investment in information technology will prevent significant breakdowns, data leakages,

breaches in our systems, or those of our third-party vendors and other contractors and consultants, or other cyber incidents that could have a material adverse effect upon our reputation, business, operations, or financial condition. For example, if such an event were to occur and cause interruptions in our operations, or those of our third-party vendors and other contractors and consultants, it could result in a material disruption of our programs and the development of our services and technologies could be delayed. Furthermore, significant disruptions of our internal information technology systems or those of our third-party vendors and other contractors and consultants, or security breaches could result in the loss, misappropriation, and/or unauthorized access, use, or disclosure of, or the prevention of access to, confidential information (including trade secrets or other intellectual property, proprietary business information, and personal information), which could result in financial, legal, business, and reputational harm to us. For example, any such event that leads to unauthorized access, use, or disclosure of personal information, including personal information regarding our customers or employees, could harm our reputation directly, compel us to comply with federal and/or state breach notification laws and foreign law equivalents, subject us to mandatory corrective action, and otherwise subject us to liability under laws and regulations that protect the privacy and security of personal information, which could result in significant legal and financial exposure and reputational damages that could potentially have an adverse effect on our business. Further, sophisticated cyber attackers (including foreign adversaries engaged in industrial espionage) are skilled at adapting to existing security technology and developing new methods of gaining access to organizations' sensitive business data, which could result in the loss of sensitive information, including trade secrets. Additionally, actual, potential, or anticipated attacks may cause us to incur increasing costs, including costs to deploy additional personnel and protection technologies, train employees, and engage third-party experts and consultants.

Risks Related to Employee Matters and Managing Growth

Our future success depends on our ability to retain key executives and to attract, retain, and motivate qualified personnel.

We are highly dependent on the research and development, clinical, financial, operational, scientific, software engineering, and other business expertise of our executive officers, as well as the other principal members of our management, scientific, clinical, and software engineering teams. Although we have entered into employment agreements with our executive officers, each of them may terminate their employment with us at any time. We do not maintain "key person" insurance for any of our executives or other employees.

The loss of the services of our executive officers or other key employees could impede the achievement of our development and sales goals in our software business and the achievement of our research, development, and commercialization objectives in our drug discovery business. In either case, the loss of the services of our executive officers or other key employees could seriously harm our ability to successfully implement our business strategy. Furthermore, replacing executive officers and key employees may be difficult and may take an extended period of time because of the limited number of individuals with the breadth of skills and experience required to successfully develop, gain regulatory approval of, and commercialize products in the life sciences industry.

Recruiting and retaining qualified scientific, clinical, manufacturing, accounting, legal, and sales and marketing personnel, as well as software engineers and computational chemists, will also be critical to our success. In the technology industry, there is substantial and continuous competition for engineers with high levels of expertise in designing, developing, and managing software and related services, as well as competition for sales executives, data scientists, and operations personnel. Competition to hire these individuals is intense, and we may be unable to hire, train, retain, or motivate these key personnel on acceptable terms given the competition among numerous biopharmaceutical and technology companies for similar personnel. We also experience competition for the hiring of scientific and clinical personnel from universities and research institutions. In addition, we rely on consultants and advisors to assist us in formulating our research and development and commercialization strategy and advancing our computational platform. Our consultants and advisors may be employed by employers other than us and may have commitments under consulting or advisory contracts with other entities that may limit their availability to us. If we are unable to continue to attract and retain high quality personnel, our ability to pursue our growth strategy will be limited and our business would be adversely affected.

We are pursuing multiple business strategies and expect to expand our development and regulatory capabilities, and as a result, we may encounter difficulties in managing our multiple business units and our growth, which could disrupt our operations.

Currently, we are pursuing multiple business strategies simultaneously, including activities in research and development, software sales, and collaborative and internal drug discovery. We believe pursuing these multiple business strategies offers financial and operational synergies, but these diversified operations place increased demands on our limited resources. Furthermore, we have recently experienced, and we expect to continue to experience, significant growth in the number of our employees and the scope of our operations, particularly in the areas of drug development, clinical and regulatory affairs. To manage our multiple business units and our ongoing and anticipated future growth, we must continue to implement and improve our managerial, operational and financial systems, expand our facilities, and continue to recruit and train additional qualified personnel. Due to our limited financial resources and our management team's limited attention and limited experience in managing a company with such ongoing and anticipated growth, we may not be able to effectively manage our multiple business units and the expansion of our operations or recruit and train additional qualified personnel.

The expansion of our operations has led to and may continue to lead to significant costs and may divert our management and business development resources. In addition, in order to meet our obligations as a public company and to support our anticipated long-term growth, we will need to increase our general and administrative capabilities. Our management, personnel, and systems may not be adequate to support this future growth. Any inability to manage our multiple business units and growth could delay the execution of our business plans or disrupt our operations and the synergies we believe currently exist between our business units. In addition, adverse developments in one of these business units may disrupt these synergies.

Risks Related to Ownership of Our Common Stock

An active trading market for our common stock may not be sustained.

Our shares of common stock began trading on the Nasdaq Global Select Market on February 6, 2020. Prior to February 6, 2020, there was no public market for our common stock, and we cannot assure you that an active trading market for our shares will be sustained. As a result, it may be difficult for our stockholders to sell their shares without depressing the market price of our common stock, or at all.

Our executive officers, directors, and principal stockholders, if they choose to act together, have the ability to influence all matters submitted to stockholders for approval.

As of April 19, 2022, our executive officers and directors and our stockholders who beneficially owned more than 5% of our outstanding common stock, in the aggregate, beneficially owned shares representing approximately 21.4% of our common stock and all of our limited common stock, or, if the holder of our limited common stock exercised its right to convert each share of its limited common stock for one share of our common stock, approximately 31.5% of our common stock. As a result, if these stockholders were to choose to act together, they would be able to influence all matters submitted to our stockholders for approval, as well as our management and affairs. For example, these persons, if they choose to act together, would influence the election of directors and approval of any merger, consolidation, or sale of all or substantially all of our assets.

This concentration of ownership control may:

- delay, defer, or prevent a change in control;
- entrench our management and board of directors; or
- delay or prevent a merger, consolidation, takeover, or other business combination involving us that other stockholders may desire.

This concentration of ownership may also adversely affect the market price of our common stock.

The price of our common stock is volatile and fluctuates substantially, which could result in substantial losses for our stockholders.

Our stock price has been, and is likely to continue to be volatile. Since our initial public offering in February 2020 and through April 19, 2022, the intraday price of our common stock has fluctuated from a low of $23.14 to a high of $117.00. As a result of volatility, our stockholders may not be able to sell their common stock at or above the price paid for the shares. The market price for our common stock may be influenced by many factors, including:

- our investment in, and the success of, our software solutions;
- the success of our research and development efforts for our internal drug discovery programs;
- initiation and progress of preclinical studies and clinical trials for any product candidates that we may develop;
- results of or developments in preclinical studies and clinical trials of any product candidates we may develop or those of our competitors or potential collaborators;
- the success of our drug discovery collaborators and any milestone or other payments we receive from such collaborators;
- the success of competitive products or technologies;
- regulatory or legal developments in the United States and other countries;
- the recruitment or departure of key personnel;
- variations in our financial results or the financial results of companies that are perceived to be similar to us;

- guidance or announcements by us with respect to our anticipated financial or operational performance;
- sales of common stock by us, our executive officers, directors or principal stockholders, or others, or the anticipation of such sales;
- market conditions in the biopharmaceutical sector;
- general economic, industry, and market conditions;
- the societal and economic impact of public health epidemics, such as the ongoing COVID-19 pandemic; and
- the other factors described in this "Risk Factors" section.

In the past, following periods of volatility in the market price of a company's securities, securities class-action litigation has often been instituted against that company. Any lawsuit to which we are a party, with or without merit, may result in an unfavorable judgment. We also may decide to settle lawsuits on unfavorable terms. Any such negative outcome could result in payments of substantial damages or fines, damage to our reputation, or adverse changes to our offerings or business practices. Such litigation may also cause us to incur other substantial costs to defend such claims and divert management's attention and resources.

Our actual operating results may differ significantly from our guidance.

We have released, and may in the future release, guidance in our annual or quarterly earnings conference calls, annual or quarterly earnings releases, or otherwise, regarding our future performance that represents our management's estimates as of the date of such guidance. Our guidance, which includes forward-looking statements, is based on projections prepared by our management. Neither our registered public accountants nor any other independent expert or outside party compiles or examines the projections. Accordingly, no such person expresses any opinion or any other form of assurance with respect to the projections.

Projections are based upon a number of assumptions and estimates that, while presented with numerical specificity, are inherently subject to significant business, economic, and competitive uncertainties and contingencies, many of which are beyond our control and are based upon specific assumptions with respect to future business decisions, some of which will change. The principal reason that we have released, and would continue to release, guidance is to provide a basis for our management to discuss our business outlook with analysts and investors. We do not accept any responsibility for any projections or reports published by any such third parties.

Guidance is necessarily speculative in nature, and it can be expected that some or all of the assumptions underlying any guidance furnished by us will not materialize or will vary significantly from actual results. Accordingly, our guidance is only an estimate of what management believes is realizable as of the date of release. Actual results may vary from our guidance and the variations may be material.

We and our collaborators may not achieve projected discovery and development milestones and other anticipated key events in the time frames that we or they announce, which could have an adverse impact on our business and could cause our stock price to decline.

From time to time, we expect that we will make public statements regarding the expected timing of certain milestones and key events, such as the commencement and completion of preclinical and IND-enabling studies in our internal drug discovery programs as well developments and milestones under our collaborations. Morphic has also made public statements regarding its expectations for the development of programs under collaboration with us and they and other collaborators may in the future make additional statements about their goals and expectations for collaborations with us. The actual timing of these events can vary dramatically due to a number of factors such as delays or failures in our or our current and future collaborators' drug discovery and development programs, including as a result of COVID-19, the amount of time, effort, and resources committed by us and our current and future collaborators, and the numerous uncertainties inherent in the development of drugs. As a result, there can be no assurance that our or our current and future collaborators' programs will advance or be completed in the time frames we or they announce or expect. If we or any collaborators fail to achieve one or more of these milestones or other key events as planned, our business could be materially adversely affected and the price of our common stock could decline.

If securities analysts do not publish or cease publishing research or reports or publish misleading, inaccurate or unfavorable research about our business or if they publish negative evaluations of our stock, the price and trading volume of our stock could decline.

The market price and trading volume for our common stock relies, in part, on the research and reports that industry or financial analysts publish about us or our business. We do not have control over these analysts. There can be no assurance that existing analysts will continue to cover us or that new analysts will begin to cover us. There is also no assurance that any covering analyst will provide favorable coverage. Although we have obtained analyst coverage, if one or more of the analysts covering our business downgrade their

evaluations of our stock or publish inaccurate or unfavorable research about our business, or provides more favorable relative recommendations about our competitors, the price of our stock could decline. If one or more of these analysts cease to cover our stock, we could lose visibility in the market for our stock, which in turn could cause our stock price and trading volume to decline.

We have broad discretion in the use of our cash, cash equivalents, and marketable securities and may not use them effectively.

Our management will have broad discretion in the application of our cash, cash equivalents, and marketable securities and could use such funds in ways that do not improve our results of operations or enhance the value of our common stock or in ways that our stockholders may not agree with. The failure by our management to apply these funds effectively could harm our business, financial condition, results of operations, and prospects and could cause the price of our common stock to decline.

Because we do not anticipate paying any cash dividends on our common stock in the foreseeable future, capital appreciation, if any, will be the sole source of gain for our stockholders.

We have never declared or paid cash dividends on our common stock. We currently intend to retain all of our future earnings to fund the development and expansion of our business. Any determination to pay dividends in the future will be at the discretion of our board of directors. As a result, capital appreciation of our common stock, if any, will be the sole source of gain for our stockholders for the foreseeable future.

Sales of a substantial number of shares of our common stock in the public market could cause the market price of our common stock to drop significantly, even if our business is doing well.

Sales of a substantial number of shares of our common stock in the public market, or the perception in the market that the holders of a large number of shares intend to sell shares, could reduce the market price of our common stock, impair our ability to raise capital through the sale of additional equity securities, and make it more difficult for our stockholders to sell their common stock at a time and price that they deem appropriate. As of April 19, 2022, we had outstanding 61,973,968 shares of common stock and 9,164,193 shares of limited common stock. All of our outstanding shares of common stock, including shares of common stock issuable upon the conversion of shares of our limited common stock, are available for sale in the public market, subject only to the restrictions of Rule 144 under the Securities Act in the case of our affiliates. In addition, certain of our executive officers, directors and affiliated stockholders have entered or may enter into Rule 10b5-1 plans providing for sales of shares of our common stock from time to time. Under a Rule 10b5-1 plan, a broker executes trades pursuant to parameters established by the executive officer, director or affiliated stockholder when entering into the plan, without further direction from the executive officer, director or affiliated stockholder. A Rule 10b5-1 plan may be amended or terminated in some circumstances. Our executive officers, directors and affiliated stockholders also may buy or sell additional shares outside of a Rule 10b5-1 plan when they are not in possession of material, nonpublic information.

We have also filed a universal shelf registration statement on Form S-3 which allows us to offer and sell an indeterminate number of shares of common stock, preferred stock, depositary shares or warrants, or an indeterminate principal amount of debt securities, from time to time pursuant to one or more offerings at prices and terms to be determined at the time of the sale. Moreover, certain holders of our common stock and our limited common stock have rights, subject to specified conditions, to include their shares in registration statements that we may file for ourselves or other stockholders and may require us to file Form S-3 registration statements covering their shares.

We also have filed registration statements on Forms S-8 to register shares of common stock that we may issue under our equity compensation plans. Shares registered under such registration statements are available for sale in the public market upon issuance, subject to volume limitations applicable to affiliates, vesting arrangements and exercise of options.

We have incurred and will continue to incur increased costs as a result of operating as a public company, and our management has devoted and will continue to be required to devote substantial time to new compliance initiatives and corporate governance practices.

As a public company, we have incurred and will continue to incur significant legal, accounting, and other expenses that we did not incur as a private company, which we expect to further increase now that we are no longer an emerging growth company. The Exchange Act, Sarbanes-Oxley Act of 2002, the Dodd-Frank Wall Street Reform and Consumer Protection Act, the listing requirements of Nasdaq, and other applicable securities rules and regulations impose various requirements on public companies, including establishment and maintenance of effective disclosure and financial controls and corporate governance practices. Our management and other personnel devote and will need to continue to devote a substantial amount of time and resources to these compliance initiatives, potentially at the expense of other business concerns, which could harm our business, financial condition, results of operations, and prospects. Moreover, these rules and regulations will increase our legal and financial compliance costs, and will make some activities more time-consuming and costly compared to when we were a private company.

We are evaluating these rules and regulations, and cannot predict or estimate the amount of additional costs we may incur or the timing of such costs. These rules and regulations are often subject to varying interpretations, in many cases due to their lack of specificity, and, as a result, their application in practice may evolve over time as new guidance is provided by regulatory and governing bodies. This could result in continuing uncertainty regarding compliance matters and higher costs necessitated by ongoing revisions to disclosure and governance practices.

As a result of becoming a public company, we are obligated to develop and maintain proper and effective internal control over financial reporting. Any failure to maintain the adequacy of these internal controls may adversely affect investor confidence in our company and, as a result, the value of our common stock.

Pursuant to Section 404 of the Sarbanes-Oxley Act, we are required to furnish a report by our management on our internal control over financial reporting on an annual basis. This assessment will need to include disclosure of any material weaknesses identified by our management in our internal control over financial reporting. Pursuant to Section 404, we are also required to have our independent registered public accounting firm issue an opinion on the effectiveness of our internal control over financial reporting on an annual basis.

During our evaluation of our internal control, if we identify one or more material weaknesses in our internal control over financial reporting, we will be unable to assert that our internal control over financial reporting is effective. In addition, if we have an unremediated material weakness, we would receive an adverse opinion regarding our internal control over financial reporting from our independent registered public accounting firm. We cannot assure you that there will not be material weaknesses or significant deficiencies in our internal control over financial reporting in the future. Any failure to maintain internal control over financial reporting could severely inhibit our ability to accurately report our financial condition, or results of operations. If we are unable to conclude that our internal control over financial reporting is effective, or if our independent registered public accounting firm determines we have a material weakness in our internal control over financial reporting, we could lose investor confidence in the accuracy and completeness of our financial reports, the market price of shares of our common stock could decline, and we could be subject to sanctions or investigations by Nasdaq, the SEC, or other regulatory authorities. Failure to remedy any material weakness in our internal control over financial reporting, or to implement or maintain other effective control systems required of public companies, could also restrict our future access to the capital markets.

Our disclosure controls and procedures may not prevent or detect all errors or acts of fraud.

As a public company, we are subject to certain reporting requirements of the Exchange Act. Our disclosure controls and procedures are designed to reasonably assure that information required to be disclosed by us in reports we file or submit under the Exchange Act is accumulated and communicated to management, recorded, processed, summarized, and reported within the time periods specified in the rules and forms of the SEC. We believe that any disclosure controls and procedures or internal controls and procedures, no matter how well conceived and operated, can provide only reasonable, not absolute, assurance that the objectives of the control system are met. These inherent limitations include the realities that judgments in decision-making can be faulty, and that breakdowns can occur because of simple error or mistake. Additionally, controls can be circumvented by the individual acts of some persons, by collusion of two or more people or by an unauthorized override of the controls. Accordingly, because of the inherent limitations in our control system, misstatements or insufficient disclosures due to error or fraud may occur and not be detected.

Provisions in our corporate charter documents and under Delaware law could make an acquisition of our company, which may be beneficial to our stockholders, more difficult and may prevent attempts by our stockholders to replace or remove our current directors and members of management.

Provisions in our certificate of incorporation and our bylaws may discourage, delay, or prevent a merger, acquisition, or other change in control of our company that stockholders may consider favorable, including transactions in which stockholders might otherwise receive a premium for their shares. These provisions could also limit the price that investors might be willing to pay in the future for shares of our common stock, thereby depressing the market price of our common stock. In addition, because our board of directors is responsible for appointing the members of our management team, these provisions may frustrate or prevent any attempts by our stockholders to replace or remove our current management by making it more difficult for stockholders to replace members of our board of directors. Among other things, these provisions:

- establish a classified board of directors such that only one of three classes of directors is elected each year;
- allow the authorized number of our directors to be changed only by resolution of our board of directors;
- limit the manner in which stockholders can remove directors from our board of directors;
- establish advance notice requirements for stockholder proposals that can be acted on at stockholder meetings and nominations to our board of directors;

- require that stockholder actions must be effected at a duly called stockholder meeting and prohibit actions by our stockholders by written consent;
- limit who may call stockholder meetings to the board of directors or to the secretary at the request of the holders of at least 25% of the outstanding shares of our common stock and limited common stock; and
- authorize our board of directors to issue preferred stock without stockholder approval, which could be used to institute a "poison pill" that would work to dilute the stock ownership of a potential hostile acquirer, effectively preventing acquisitions that have not been approved by our board of directors.

Moreover, because we are incorporated in Delaware, we are governed by the provisions of Section 203 of the Delaware General Corporation Law, or the DGCL, which prohibits a person who owns in excess of 15% of our outstanding voting stock from merging or combining with us for a period of three years after the date of the transaction in which the person acquired in excess of 15% of our outstanding voting stock, unless the merger or combination is approved in a prescribed manner.

Our certificate of incorporation designates the state courts in the State of Delaware as the sole and exclusive forum for certain types of actions and proceedings that may be initiated by our stockholders, which could discourage lawsuits against the company and our directors, officers, and employees.

Our certificate of incorporation provides that, unless we consent in writing to the selection of an alternative forum, the Court of Chancery of the State of Delaware (or, if the Court of Chancery of the State of Delaware does not have jurisdiction, the federal district court for the District of Delaware) will be the sole and exclusive forum for: (1) any derivative action or proceeding brought on our behalf, (2) any action asserting a claim of breach of a fiduciary duty owed by any of our directors, officers, employees or stockholders to our company or our stockholders, (3) any action asserting a claim arising pursuant to any provision of the DGCL or as to which the DGCL confers jurisdiction on the Court of Chancery of the State of Delaware or (4) any action asserting a claim arising pursuant to any provision of our certificate of incorporation or bylaws (in each case, as they may be amended from time to time) or governed by the internal affairs doctrine. These choice of forum provisions will not apply to suits brought to enforce a duty or liability created by the Securities Act of 1933, as amended, the Exchange Act or any other claim for which federal courts have exclusive jurisdiction.

This exclusive forum provision may limit the ability of our stockholders to bring a claim in a judicial forum that such stockholders find favorable for disputes with us or our directors, officers, or employees, which may discourage such lawsuits against us and our directors, officers, and employees. Alternatively, if a court were to find the choice of forum provision contained in our certificate of incorporation to be inapplicable or unenforceable in an action, we may incur additional costs associated with resolving such action in other jurisdictions, which could materially adversely affect our business, financial condition, and operating results.

Item 2. Unregistered Sales of Equity Securities and Use of Proceeds.

Unregistered Sales of Equity Securities

None.

Use of Proceeds

On February 5, 2020, our registration statement on Form S-1, as amended (File No. 333-235890) was declared effective by the SEC in connection with our initial public offering of common stock, pursuant to which we issued and sold on February 10, 2020, 13,664,704 shares of our common stock at a public offering price of $17.00 per share, including 1,782,352 additional shares of common stock issued upon the full exercise by the underwriters of their option to purchase additional shares, for total gross proceeds of $232.3 million. On February 10, 2020, we received net proceeds of $209.6 million, after deducting $16.3 million in underwriting discounts and commissions and $6.4 million in estimated offering expenses borne by us.

There has been no material change in the planned use of proceeds from our initial public offering from that described in the final prospectus related to the offering, dated February 5, 2020, as filed with the SEC on February 6, 2020.

Item 3. Defaults Upon Senior Securities.

Not applicable.

Item 4. Mine Safety Disclosures.

Not applicable.

Item 5. Other Information.

None.

Item 6. Exhibits.

Exhibit Number	Description	Form	File No.	Exhibit	Filing Date	Filed Herewith
10.1	Form of Stock Option Agreement and Form of Restricted Stock Unit Agreement for U.S. Participants under the 2020 Equity Incentive Plan	10-K	001-39206	10.5	2/24/2022	
10.2	Form of Restricted Stock Unit Agreement for Non-U.S. Participants under the 2020 Equity Incentive Plan	10-K	001-39206	10.6	2/24/2022	
10.3	Third Amended and Restated Director Compensation Policy					X
10.4	Transition, Separation and Release of Claims Agreement, dated as of February 28, 2022, by and between Schrödinger, Inc. and Joel Lebowitz	8-K	001-39206	10.1	3/2/2022	
10.5	Consulting Agreement, dated as of February 28, 2022, by and between Schrödinger, Inc. and Joel Lebowitz	8-K	001-39206	10.2	3/2/2022	
31.1	Certification of Principal Executive Officer Pursuant to Rules 13a-14(a) and 15d-14(a) under the Securities Exchange Act of 1934, as Adopted Pursuant to Section 302 of the Sarbanes-Oxley Act of 2002.					X
31.2	Certification of Principal Financial Officer Pursuant to Rules 13a-14(a) and 15d-14(a) under the Securities Exchange Act of 1934, as Adopted Pursuant to Section 302 of the Sarbanes-Oxley Act of 2002.					X
32.1*	Certification of Principal Executive Officer Pursuant to 18 U.S.C. Section 1350, as Adopted Pursuant to Section 906 of the Sarbanes-Oxley Act of 2002.					X
32.2*	Certification of Principal Financial Officer Pursuant to 18 U.S.C. Section 1350, as Adopted Pursuant to Section 906 of the Sarbanes-Oxley Act of 2002.					X
101.INS	Inline XBRL Instance Document – the instance document does not appear in the Interactive Data File because its XBRL tags are embedded within the Inline XBRL document.					X
101.SCH	Inline XBRL Taxonomy Extension Schema Document					X
101.CAL	Inline XBRL Taxonomy Extension Calculation Linkbase Document					X
101.DEF	Inline XBRL Taxonomy Extension Definition Linkbase Document					X
101.LAB	Inline XBRL Taxonomy Extension Label Linkbase Document					X
101.PRE	Inline XBRL Taxonomy Extension Presentation Linkbase Document					X
104	The cover page for the Company's Quarterly Report on Form 10-Q has been formatted in Inline XBRL and contained in Exhibit 101					X

* The certifications attached as Exhibits 32.1 and 32.2 that accompany this Quarterly Report, are deemed furnished and not filed with the Securities and Exchange Commission and are not to be incorporated by reference into any filing of Schrödinger, Inc. under the Securities Act of 1933, as amended, or the Securities Exchange Act of 1934, as amended, whether made before or after the date of this Quarterly Report, irrespective of any general incorporation language contained in such filing.

SIGNATURES

Pursuant to the requirements of the Securities Exchange Act of 1934, the registrant has duly caused this report to be signed on its behalf by the undersigned thereunto duly authorized.

Schrödinger, Inc.

Date: May 4, 2022

By: /s/ Ramy Farid, Ph.D.
President and Chief Executive Officer
(*Principal Executive Officer*)

Date: May 4, 2022

By: /s/ Jenny Herman
Senior Vice President, Finance and Corporate Controller
(*Principal Financial Officer and Principal Accounting Officer*)

EXHIBIT 10.3

Schrödinger, Inc.

Third Amended and Restated Director Compensation Policy

Adopted on March 15, 2022

Effective as of January 1, 2022, the non-employee directors of Schrödinger, Inc. (the "Company") shall receive the following compensation for their service as members of the Board of Directors (the "Board") of the Company.

Director Compensation

Our goal is to provide compensation for our non-employee directors in a manner that enables us to attract and retain outstanding director candidates and reflects the substantial time commitment necessary to oversee the Company's affairs. We also seek to align the interests of our directors and our stockholders and we have chosen to do so by compensating our non-employee directors with a mix of cash and equity-based compensation.

Cash Compensation

The fees that will be paid to our non-employee directors for service on the Board, and for service on each committee of the Board on which the director is then a member, and the fees that will be paid to the chairperson of the Board, if one is then appointed, and the chairperson of each committee of the Board will be as follows:

	1 **Base**	**2** **Incremental–Board Chair or Committee Chair**	**3** **Incremental – Non-Chair Committee Members**
Board of Directors	$45,000	$35,000 (Non-Executive Chair)	—
Audit Committee	—	$20,000	$10,000
Compensation Committee	—	$15,000	$7,500
Nominating and Corporate Governance Committee	—	$10,000	$5,000
Drug Discovery Committee	—	$10,000	$5,000

The foregoing fees will be payable in arrears in four equal quarterly installments on the last day of each quarter, provided that the amount of such payment will be prorated for any portion of such quarter that the director is not serving on our Board, on such committee or in such position.

Equity Compensation

Initial Grants. Upon initial election to our Board, each non-employee director will be granted, automatically and without the need for any further action by the Board, an initial equity award of an option to purchase a number of shares of our common stock having an aggregate value of $380,000 as of the grant date, determined using a Black-Scholes valuation model. The initial award shall have a term of ten years from the date of grant of the award, and shall vest and become exercisable as to 33.3333% of the shares underlying such award on each of the first, second and third anniversaries of the date of grant of the award, subject the director's continued service as a director, employee or consultant through each applicable vesting date. The vesting shall accelerate as to 100% of the shares upon a Change in Control of the Company (as defined in the Company's Executive Severance and Change in Control Benefits Plan). The exercise price shall be the closing price of our common stock on the date of grant.

Annual Grants. Beginning in calendar year 2022, each non-employee director who is serving as a member of our Board will be granted, automatically and without the need for any further action by the Board, an equity award on the date of our annual meeting of stockholders for such year of an option to purchase a number of shares of our common stock having an aggregate value of $190,000 as of the date of such annual meeting of stockholders, as determined using a Black-Scholes valuation model; provided, however, that for a non-employee director who was initially elected to the Board within the 12 months preceding the annual meeting of stockholders, the number of shares subject to such option shall be pro-rated on a monthly basis for time in service. The annual award shall have a term of ten years from the date of the award, and shall vest on the twelve-month anniversary of the date of grant of the award (or, if earlier, the date of the next annual meeting of stockholders following the date of grant of the award), subject to the director's continued service as a director, employee or consultant through the applicable vesting date. The vesting shall accelerate as to 100% of the shares upon a Change in Control of the Company. The exercise price shall be the closing price of our common stock on the date of grant.

The initial awards and the annual awards shall be subject to the terms and conditions of our 2020 Equity Incentive Plan, or any successor plan, and the terms of the option agreements entered into with each director in connection with such awards.

Expenses

Upon presentation of documentation of such expenses reasonably satisfactory to the Company, each non-employee director shall be reimbursed for his or her reasonable out-of-pocket business expenses incurred in connection with attending meetings of the Board and committees thereof or in connection with other business related to the Board, and each non-employee director shall also be reimbursed for his or her reasonable out-of-pocket business expenses authorized by the Board or a committee of the Board that are incurred in connection with attendance at various conferences or meetings with management of the Company, in accordance with the Company's travel policy, as it may be in effect from time to time.

EXHIBIT 31.1

**CERTIFICATION OF PRINCIPAL EXECUTIVE OFFICER
PURSUANT TO RULES 13a-14(a) AND 15d-14(a) UNDER THE SECURITIES
EXCHANGE ACT OF 1934, AS ADOPTED PURSUANT TO SECTION 302 OF THE SARBANES-OXLEY ACT OF 2002**

I, Ramy Farid, certify that:

1. I have reviewed this Quarterly Report on Form 10-Q of Schrödinger, Inc.;
2. Based on my knowledge, this report does not contain any untrue statement of a material fact or omit to state a material fact necessary to make the statements made, in light of the circumstances under which such statements were made, not misleading with respect to the period covered by this report;
3. Based on my knowledge, the financial statements, and other financial information included in this report, fairly present in all material respects the financial condition, results of operations and cash flows of the registrant as of, and for, the periods presented in this report;
4. The registrant's other certifying officer(s) and I are responsible for establishing and maintaining disclosure controls and procedures (as defined in Exchange Act Rules 13a-15(e) and 15d-15(e)) and internal control over financial reporting (as defined in Exchange Act Rules 13a-15(f) and 15d-15(f)) for the registrant and have:
    a. Designed such disclosure controls and procedures, or caused such disclosure controls and procedures to be designed under our supervision, to ensure that material information relating to the registrant, including its consolidated subsidiaries, is made known to us by others within those entities, particularly during the period in which this report is being prepared;
    b. Designed such internal control over financial reporting, or caused such internal control over financial reporting to be designed under our supervision, to provide reasonable assurance regarding the reliability of financial reporting and the preparation of financial statements for external purposes in accordance with generally accepted accounting principles;
    c. Evaluated the effectiveness of the registrant's disclosure controls and procedures and presented in this report our conclusions about the effectiveness of the disclosure controls and procedures, as of the end of the period covered by this report based on such evaluation; and
    d. Disclosed in this report any change in the registrant's internal control over financial reporting that occurred during the registrant's most recent fiscal quarter (the registrant's fourth fiscal quarter in the case of an annual report) that has materially affected, or is reasonably likely to materially affect, the registrant's internal control over financial reporting; and
5. The registrant's other certifying officer(s) and I have disclosed, based on our most recent evaluation of internal control over financial reporting, to the registrant's auditors and the audit committee of the registrant's board of directors (or persons performing the equivalent functions):
    a. All significant deficiencies and material weaknesses in the design or operation of internal control over financial reporting which are reasonably likely to adversely affect the registrant's ability to record, process, summarize and report financial information; and

b. Any fraud, whether or not material, that involves management or other employees who have a significant role in the registrant's internal control over financial reporting.

Date: May 4, 2022

/s/ Ramy Farid

Ramy Farid
President and Chief Executive Officer (Principal Executive Officer)

EXHIBIT 31.2

CERTIFICATION OF PRINCIPAL FINANCIAL OFFICER
PURSUANT TO RULES 13a-14(a) AND 15d-14(a) UNDER THE SECURITIES
EXCHANGE ACT OF 1934, AS ADOPTED PURSUANT TO SECTION 302 OF THE SARBANES-OXLEY ACT OF 2002

I, Jenny Herman, certify that:

1. I have reviewed this Quarterly Report on Form 10-Q of Schrödinger, Inc.;

2. Based on my knowledge, this report does not contain any untrue statement of a material fact or omit to state a material fact necessary to make the statements made, in light of the circumstances under which such statements were made, not misleading with respect to the period covered by this report;

3. Based on my knowledge, the financial statements, and other financial information included in this report, fairly present in all material respects the financial condition, results of operations and cash flows of the registrant as of, and for, the periods presented in this report;

4. The registrant's other certifying officer(s) and I are responsible for establishing and maintaining disclosure controls and procedures (as defined in Exchange Act Rules 13a-15(e) and 15d-15(e)) and internal control over financial reporting (as defined in Exchange Act Rules 13a-15(f) and 15d-15(f)) for the registrant and have:

    a. Designed such disclosure controls and procedures, or caused such disclosure controls and procedures to be designed under our supervision, to ensure that material information relating to the registrant, including its consolidated subsidiaries, is made known to us by others within those entities, particularly during the period in which this report is being prepared;

    b. Designed such internal control over financial reporting, or caused such internal control over financial reporting to be designed under our supervision, to provide reasonable assurance regarding the reliability of financial reporting and the preparation of financial statements for external purposes in accordance with generally accepted accounting principles;

    c. Evaluated the effectiveness of the registrant's disclosure controls and procedures and presented in this report our conclusions about the effectiveness of the disclosure controls and procedures, as of the end of the period covered by this report based on such evaluation; and

    d. Disclosed in this report any change in the registrant's internal control over financial reporting that occurred during the registrant's most recent fiscal quarter (the registrant's fourth fiscal quarter in the case of an annual report) that has materially affected, or is reasonably likely to materially affect, the registrant's internal control over financial reporting; and

5. The registrant's other certifying officer(s) and I have disclosed, based on our most recent evaluation of internal control over financial reporting, to the registrant's auditors and the audit committee of the registrant's board of directors (or persons performing the equivalent functions):

    a. All significant deficiencies and material weaknesses in the design or operation of internal control over financial reporting which are reasonably likely to adversely affect the registrant's ability to record, process, summarize and report financial information; and

b. Any fraud, whether or not material, that involves management or other employees who have a significant role in the registrant's internal control over financial reporting.

Date: May 4, 2022

/s/ Jenny Herman

Jenny Herman
Senior Vice President, Finance and Corporate Controller (Principal Financial Officer and Principal Accounting Officer)

Exhibit 32.1

CERTIFICATION OF PRINCIPAL EXECUTIVE OFFICER PURSUANT TO 18 U.S.C. SECTION 1350, AS ADOPTED PURSUANT TO SECTION 906 OF THE SARBANES-OXLEY ACT OF 2002

Pursuant to 18 U.S.C. Section 1350, as adopted pursuant to Section 906 of the Sarbanes-Oxley Act of 2002, the undersigned officer of Schrödinger, Inc. (the "Company") hereby certifies, to his knowledge, that:

(1) the accompanying Quarterly Report on Form 10-Q of the Company for the fiscal quarter ended March 31, 2022 (the "Report") fully complies with the requirements of Section 13(a) or Section 15(d), as applicable, of the Securities Exchange Act of 1934, as amended; and

(2) the information contained in the Report fairly presents, in all material respects, the financial condition and results of operations of the Company.

Date: May 4, 2022

/s/ Ramy Farid

Ramy Farid
President and Chief Executive Officer (Principal Executive Officer)

Exhibit 32.2

CERTIFICATION OF PRINCIPAL FINANCIAL OFFICER PURSUANT TO
18 U.S.C. SECTION 1350, AS ADOPTED PURSUANT TO
SECTION 906 OF THE SARBANES-OXLEY ACT OF 2002

Pursuant to 18 U.S.C. Section 1350, as adopted pursuant to Section 906 of the Sarbanes-Oxley Act of 2002, the undersigned officer of Schrödinger, Inc. (the "Company") hereby certifies, to her knowledge, that:

(1) the accompanying Quarterly Report on Form 10-Q of the Company for the fiscal quarter ended March 31, 2022 (the "Report") fully complies with the requirements of Section 13(a) or Section 15(d), as applicable, of the Securities Exchange Act of 1934, as amended; and

(2) the information contained in the Report fairly presents, in all material respects, the financial condition and results of operations of the Company.

Date: May 4, 2022

/s/ Jenny Herman

Jenny Herman
Senior Vice President, Finance and Corporate Controller (Principal Financial Officer and Principal Accounting Officer)