Artificial Intelligence in Drug Discovery and Development

Improve Your "Hit Rate" for Successful Projects

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Summary

Life Science companies have demonstrated a strong appetite for artificial intelligence solutions to support both the drug discovery and drug development processes. The percentage of those using AI soared from 44 percent in 2017 to 70 percent in 2019[1]. Overall biopharma R&D budgets have remained strong in that time, which has funded increased investment in AI. Biopharma companies are feeding their growing demand for AI by hiring specialists and by contracting with outside firms to gain the skills and solutions they need. Both approaches present challenges. Hiring requires competing for candidates during an acute global talent shortage. Contracting requires shopping in a market where the "products" change daily as startups appear, others are acquired and subsumed by more established firms, and still other competitors emerge from adjacent industries. Whether an organization chooses to build or buy, both approaches take time, so efficiencies gained need to be timely and reliable if they are going to offset investment and improve the years-long effort to bring new drugs to market.

The good news is that applying AI can be successful and worth the effort. In many cases, suitable AI solutions and partners already exist for biopharma companies seeking to support drug discovery and development. More than 125 startups related to AI have been identified for drug discovery alone. These companies raised $1.8 Billion in funding in the last decade, including at least $100 Million every year between 2015 – 2019[2]. Meanwhile, IT and business process service providers have achieved some impressive success stories in helping Life Science companies with AI initiatives. The challenges are how to find the right solution or provider, and then how to rapidly help your organization make the most of that investment in an emerging field.

With strong R&D budgets, there is a growing demand by biopharma companies for capitalizing on AI by hiring specialists.

More good news: The process of identifying, vetting, contracting with and managing specialized AI partners is nowhere near as arduous as the drug discovery and development processes themselves. ISG has identified processes and principles for effectively working with service providers, and we have helped Life Science companies apply them successfully in AI-driven engagements. Successes across the compound lifecycle include: identifying candidate molecules; safety-case processing and improving patient experience during trials. Other use cases include combining AI with robotic process automation (RPA) to form intelligent automation solutions to manage trial data and streamline reporting; and scaling AI and RPA efforts to non-scientific business processes throughout the organization.

This white paper describes some drug discovery and development AI use cases and their value, and it provides guidance to help Life Science companies evaluate potential partners and structure working relationships.

The Case for AI

AI is one of the latest and most promising avenues that biopharma companies are pursuing in their continuing efforts to improve the drug discovery and development processes. Considering the length of the compound lifecycle, challenges with success rates, the volume of data to be managed, reporting requirements and many other time-intensive tasks, even slight improvements in time or cost will yield important benefits to overall cost and the potential for finishing ahead of the competition.

Every organization's AI motivations and requirements are different, but ISG has observed several widespread trends across the Life Science sector. Based on our experience in AI, machine learning, RPA and other technologies, as well as our extensive work with Life Science companies, ISG has identified four priority areas for stakeholders to consider for AI-enabled intelligent automation:

- Optimizing drug discovery and design through the use of algorithms and advanced analytics.

- Improving the patient experience during trials through increased personalization.

- Streamlining data collection and processing, which goes beyond EDC, ePRO, wearables and more.

- Taking real-world evidence (RWE) and real-world data (RWD) mainstream.

- We've highlighted these use cases below, and there are many others.

Optimizing Drug Discovery

AI and predictive analytics are being successfully applied to evaluate molecule and compound candidates. AI-based tools have made predicting the 3D structure of a target protein more accurate and sophisticated. With predictive analytics software, developers can now simulate drug-molecule combinations using mathematical simulations.

COVID-19 Is a Catalyst

The COVID-19 outbreak has increased the urgency of many initiatives in Life Science, including companies' plans to harness AI and intelligent automation. COVID-19 has been a catalyst for the tech community too. AI startups, business process and IT service providers, and other organizations in the ecosystem have stepped up their offerings and efforts to help Life Science companies.

Over a two-month period early in the COVID-19 outbreak, Life Science firms announced more than 100 alliances for coronavirus research, many involving tech firms. Researchers in China trained AI to detect coronavirus from routine chest X-rays, without requiring additional testing. Many service providers began their own efforts. For example, TCS has applied its AI expertise to finding new molecules to target in order to combat SARS-CoV-2 and has identified more than two dozen candidates.

The Case for AI (continued)

Enabled by cloud infrastructure, AI and predictive analytics helps to evaluate molecule and compound candidates for accelerated drug discovery.

For example, in January 2020, Sumitomo Dainippon Pharma announced that by working with AI specialist Exscientia it completed the exploratory research phase for an OCD drug candidate in 12 months, a process that usually took the company 4.5 years[3]. Phase I clinical trials for the new drug have already begun. Exscientia is also working with Celgene (now BMS) to help it identify target molecules. French AI startup Iktos quickly joined the fight against COVID-19 by contracting with research center SRI International to apply AI-enabled generative modeling technology to design novel, optimized compounds. TCS is engaged in a similar project with the Council of Scientific and Industrial Research (CSIR).

AI and analytics add value to the molecule evaluation process in part because they are highly scalable, especially when they are deployed on a cloud infrastructure. Scalability makes it more practical for drug researchers to start with a wide number of compound combinations because they can be assessed relatively quickly compared to traditional methods. Even when hit rates remain low, automated discovery is a practical way to evaluate a range of options because of the speed at which it provides assessments. Use of appropriate automation reliably results in faster delivery and more accurate results.

Improving Patient Experience During Clinical Trials

One way to improve clinical trial effectiveness is to improve the patient experience. The "consumerization of healthcare" is a well-documented development that is traditionally associated with patient care, but it extends to clinical trials too. AI can contribute to mobile apps, patient portals and other technology-enabled patient touchpoints to provide a more personalized and engaging patient experience. A higher level of personal interaction increases the ability to retain patients on trial and enhances compliance. And AI enables customization at scale.

FDA Guidance on Conduct of Clinical Trials during COVID-19

"… Consider establishing and implementing policy and procedures, or revise existing policy and procedures, to describe approaches to be used to protect trial participants and manage study conduct during possible disruption of the study as a result of COVID-19 control measures at study sites. Changes to policy and procedures could address, but not be limited to, impact on the informed consent process, study visits and procedures, data collection, study monitoring, adverse event reporting, and changes in investigator(s), site staff, and/or monitor(s) secondary to travel restrictions, quarantine measures, or COVID-19 illness itself."

In light of this new guidance, AI can provide the ability to maintain requirements around patient safety and reporting, as well as rapidly implementing new processes.

The Case for AI (continued)

AI can specifically be used to anticipate patient needs and trigger an appropriate response at any point in the trial. These responses might be to send an encouragement or a reminder, deliver health management information related to the patient's condition, or provide other content. AI can support such outreach by determining the next-best recommended action for each patient to generate a customized communication. This can be done in real time by using AI to analyze patient data collected through wearable devices. There are quite a variety of consumer devices and purpose-built medical sensors being used to support clinical trials, including patches, headbands, wristbands, smart watches, cuffs, finger-worn sensors and smart clothing. Seventy percent of clinical trials will include wearables by 2025, according to a study commissioned by Intel[4].

> AI enables at-scale delivery of personalized and differentiated patient experiences to help retain patients on trial and enhance compliance.

Streamlining Data Collection and Processing

> AI and RPA in intelligent automation builds error proofing and high throughput efficiency into processes, which include logging EDC and posting data queries.

Most biopharma companies that ISG works with are already using robotic process automation in some administrative operations and now are actively trying to expand its use to get more benefits and leverage their prior investments. RPA mimics human behavior and can be applied to automate many steps related to receiving, reviewing, recording and sharing data. Integrating AI with RPA adds value by increasing the scope of use cases, because AI can conduct data analysis and quality control, not only data collection and input.

RPA is especially well suited for the well-defined processes widely used in Life Science. Clinical trials and other parts of the drug development process have several use cases where RPA has proven valuable. The Society for Clinical Data Management (SCDM) suggests in a white paper that RPA bots could log EDC and post data queries[5], and says, "You could have as many virtual robots as you need working 24 hours a day and 7 days a week to manage the study workload." Multiple ISG Life Science clients have also demonstrated that RPA increases both quality and compliance without sacrificing productivity.

AI can improve data accuracy by rapidly identifying data points that fall outside of expected ranges and flagging them as possible errors. Therefore, combining AI and RPA in intelligent automation builds error proofing and high throughput efficiency into these processes. Among the use cases SCDM suggests for AI-enabled RPA are analyzing comments captured in EDC to identify potential adverse events, extracting data from documents, and supporting compliance by ensuring required elements are included in contracts.

The Case for AI (continued)

Delivering on the Potential of RWD and RWE

The 21st Century Cures Act brought real-world data (RWD) and real-world evidence (RWE) into mainstream use in the drug development process. Biopharma companies can use AI to bring value to their RWD and RWE initiatives. Many organizations in the Life Science are actively pursuing opportunities to maximize the value of their data lakes.

AI with cloud infrastructure can process high volumes of RWD and RWE, including unstructured data about patient populations or other variables that may be useful both for clinical trials and for post-marketing applications. AI can help by improving data quality, as previously described, as well as through its ability to find correlations. There are many potential use cases related to effectiveness studies, disease progression, outcome research, safety surveillance and other areas. Organizations also are using AI with RWD and RWE to guide clinical trial design and observational studies to find new treatment approaches.

> Use of AI with RWD and RWE helps guide clinical trial design and observational studies to find new treatment approaches.

While AI has proven its value in multiple Life Science use cases, its use in the sector is far from mature. The less mature a technology is, the more important it becomes to have a strategy and realistic expectations for using it. This can be a challenge for many Life Science companies, since AI development has not historically been a part of their core business. A range of service providers are positioning to fill the void. The following sections provide guidance for planning the solution, selecting the right partner and getting the most value from the engagement.

> In the Life Science, there is no room for error when it comes to AI, and in order to make the technology work for the industry, we need highly trained, specialist data experts to meet this challenge. There is now also an abundance of data streams – such as Real World Evidence, clinical trials data, and genomic data, which could have real value in drug discovery and development, as long as we're able to analyze it. The industry must work closely with academic organizations and educators to highlight these opportunities, and attract the next generation of data scientists."
>
> – Dr. Steve Arlington, President The Pistoia Alliance[6]

Need for innovation spurs demand for Intelligent Automation

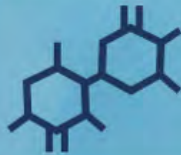## Robust AI activity in drug discovery and drug development

Life science enterprises using AI soared from **44%** in 2017 to **70%** in 2019.

125 AI startups in drug discovery have raised **$1.8 Billion** in the last decade
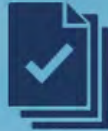
Four areas where AI has potential

1. Optimized drug discovery and design

2. Improved patient experience during trials

3. Streamlined data collection and processing

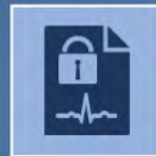**4.** Mainstream use of real-world evidence (RWE) and real-world data (RWD)

Use of AI comes with challenges

Need for fast pace of innovation

Rise of non-traditional providers

Increasing need for patient privacy, data integrity and regulatory compliance

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Achieving the true potential of AI is based on key principles

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Determine the business problem that needs to be solved

Assess the criticality of the system and potential to take risk

Make project decisions based on factors that define success

Identify stakeholders that can be champions of transformation programs

Make prudent budget decisions for execution and due diligence

Identify a service provider and structure an effective working relationship

Finding the Right Partner and then Partnering Right

Biopharma companies deciding how to invest in new technologies are required to be more sophisticated than ever. The playing field now includes non-traditional providers that are finding ways to bring their experience around the cloud, digital and big data into the Life Science space. And the lightning-fast pace of innovation can make it even more challenging to ensure adequate protection of patient privacy, data integrity and maintain regulatory compliance.

It is much easier to identify the right solution provider or other partner if you understand your strategy. A partner can be very helpful for strategy development, but you'll still need to independently assess whether the strategy is right for you. Here are some questions to investigate to help set and assess strategy, which in turn will inform the partner selection process.

- What business problem are you trying to solve?

- Can you define the right scope? Choosing the right use cases is essential. Can you get the right data, in the right format and in sufficient amounts to make AI successful?

- How would you define success?

- Who are the key stakeholders, and where might their needs conflict? Come to agreement on who "owns" AI initiatives within the organization.

- How much money and effort are you willing to invest in the solution, first for the selection, development and implementation phases, and then to run AI on an ongoing basis?

> Contracting with and managing specialized AI partners is nowhere near as arduous as the drug discovery and development processes themselves.

What is the business problem you're looking to solve?

Until you can clearly articulate this, you won't be able to drive decisions with internal stakeholders and you will run the risk of unintended scope creep once your project gets started. In addition to clearly understanding your business drivers, make sure you can state exactly where this project falls on your organization's IT roadmap. Without a cross-functional commitment to an implementation timeline, it will be difficult for you to get the most out of the investment.

How business-critical is the system or process you want to upgrade or replace?

Knowing how a new solution might impact your ability to conduct business will help you understand how much risk you can afford to take. Assess upfront whether your desired solution has to be fully operational the day you flip the switch in which case it had better be proven and fully supported or if you can afford to try something more innovative.

What are the main drivers of your business case?

Are you looking for something faster? Cheaper? More user-friendly? Many different factors contribute to your competitive position. Decide what is most important to your stakeholders in their definition of project success, and let that influence decisions around cost, features and the best path to implementation.

Finding the Right Partner and then Partnering Right (continued)

Who are your key stakeholders?

All change requires champions, but this is especially true for technology change because of how it impacts the way people conduct their work. Initiatives like these always benefit from the guidance of a steering committee, which would ideally include leadership from the relevant operational functions as well as appropriate expertise from the IT, finance, procurement and quality organizations. Also consider a test-user group selected from your target end-user community. These people can provide important input about desirable vs. superficial features and valuable feedback when it comes time to test the solution. They can also become your change ambassadors when you begin implementation.

How much resource commitment is required to launch and integrate the solution?

Remember that every unplanned change you make once your project starts is going to have a cost. Make your initial planning as robust as possible, but be sure to build room into your budget for the inevitable and unexpected changes that come up along the way.

How much time and what resources will be needed for due diligence?

Your procurement team can be a rich source of information about the marketplace. As part of due diligence, be sure to request "live" demos of capabilities (as opposed to static presentations) and request as much historical performance data as the vendor can provide. Complete a thorough reference check that includes industry peers. Document everything that leads to your final decision. Scorecards are a great way to quantify information, but also be sure to keep copies of presentations, evaluations, meeting minutes and relevant emails. This information will be invaluable should you get audited in the future.

Identifying and Evaluating Service Providers

There are several advantages to working with established outsourcing service providers to support AI efforts. The leading providers in the Life Science sector have been investing heavily to develop AI solutions and have been snapping up startups. These service providers tend to come to the market with perspective and competency in specific business processes and issues in the industry. They already have Life Science experience and are developing AI to augment it, which contrasts with AI specialists that are learning to fit their technology to specific industries' needs. Service providers are also generally well positioned to combine AI with robotic process automation, as are the leading RPA vendors.

The right match for your organization is probably out there. After the company has been identified, the next step is to structure an effective working relationship. ISG has helped more than 150 Life Science companies develop their AI, RPA and other digital strategies and conduct the service provider selection process. We have advised more than $22 Billion worth of contract awards and helped establish terms of engagement and governance process that carefully align the provider with the client's interests.

Based on this experience we present the following high-level best practices to apply to outsourcing relationships:

Start with the right contract.

Make sure vendor agreements are fit for purpose. They should be clear about deliverables and expectations and easily understood by the people who need to implement them. Then make sure they're operationalized in a way that's consistent with their original intent. What if a contract is out of date or if those initial operating ideas just don't work as needed? Consider renegotiating. It's important to keep outsourcing contracts up to date with best practices. Companies in other industries do so all the time.

Establish clear lines of accountability.

Remember that regulators will evaluate oversight effectiveness against what sponsors said they would be doing. Simplify as much as possible. Determine and clearly communicate who is in charge, who to go to with questions, who resolves conflicts, who approves deliverables and who approves changes to operating strategies.

Identifying and Evaluating
Service Providers (continued)

Document requirements and expectations.

Even if there hasn't been a lack of vendor oversight in the biopharma industry, there has been a lack of documentation. Without sufficient documentation, there is no way to prove adequate oversight has taken place.

Monitor performance.

Establish in advance what successful deliverables will look like, how often they are expected and what interim measures of success are going to be evaluated. Use metrics and key performance indicators, not raw output, to measure progress against risk plans, quality plans, project plans and customer satisfaction criteria. Use audit techniques to evaluate quality.

Communicate constantly.

Sponsor companies should not assume a vendor knows what's most critical if business drivers change, which happens more often than any of us would like. Be prepared to bring new team members up to date if needed. Proactively manage frustrations. They will not go away by ignoring them. Most importantly, ensure all project staff are trained to use these standards. Otherwise, people are likely to default to the way they've always done things.

Remain flexible.

Encourage vendors to suggest alternative ways to get the job done. Make maximum use of their experience, but also continually assess the maturity of their processes and the health of the relationship. If necessary, renegotiate critical terms in the contract to reflect newly established oversight practices.

Effective oversight begins with the realization that vendor resources are an integral part of the project delivery team. Appropriately conducted oversight is the most powerful tool a company can use to ensure the return on investment from outsourcing. The digital influence has considerably changed sourcing governance requirements and best practices in just the last few years because of the new workflows and metrics that technology enables.

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Conclusion

Artificial intelligence competency has become a new theater of competition for Life Science companies. The technology's proven ability to help with drug discovery and development has made solutions and specialists highly sought after, and new use cases are emerging all the time. Clear goals and a strategy are needed to effectively prioritize the use cases to pursue, and vendor partners are often needed to execute them. Progressing through these steps takes work but doesn't have to be daunting. Even though AI's functional capabilities and vendor community are changing over time, there are well-established principles for identifying the best use cases and partners to make programs successful in the Life Science industry.

References

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Meet the Team

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Jenn offers more than 20 years of experience in the consulting industry where she has worked with the world's leading organizations providing management, technology and outsourcing services. She has extensive experience in the life science industry and has served as both an advisor and provider of consulting services. Jenn's consulting leadership's roles include Managing Director at Alsbridge; Partner at Accenture, Global Account Leader at PwC/BearingPoint and Capgemini, where she set up its first Shared Service center. Jenn was awarded bronze Stevie® Awards in the category of Transformational Sourcing Relations Leadership at the 15th Annual Stevie Awards for Women in Business.
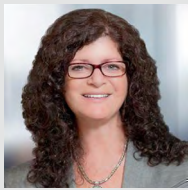
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Fran works with global and regional biopharma and contract research organizations to streamline and optimize all phases of drug development and clinical sourcing. She helps identify gaps in alignment, implement practices that deliver measurable efficiencies and increase the value of outsourced relationships for all parties. Fran provides both broad insight and specific strategic and operational expertise on clinical outsourcing, service provider selection and engagement, service integration, governance, operational excellence and utilization of metrics.

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John has been an author and editor for content at ISG Research since 2008 and is heavily involved in IT market research. He applies the skills and lessons learned to support the next wave of disruptive technologies and processes, working in telehealth and other healthcare transformation. Prior to joining ISG, John was an award-winning journalist in the technology industry.

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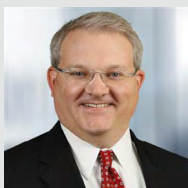
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Acknowledgements

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