AI for Public Good
Drug Discovery

Advocacy Efforts and a Further Call to Action

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GPAI | THE GLOBAL PARTNERSHIP ON ARTIFICIAL INTELLIGENCE

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Co-Leads:
Alice H. Oh*, KAIST School of Computing
Yoshua Bengio*, Mila

The report was written by: **Allison Cohen**†, AI for Humanity, Mila; and **Elliot Layne**†, School of Computer Science, McGill University, and Mila, under the supervision of the following GPAI Expert: **Yoshua Bengio***, Mila.

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* Expert of GPAI's Responsible AI Working Group
** Observer at GPAI's Responsible AI Working Group
† Invited Specialist
‡ Contracted Parties by the CofEs to contribute to projects

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Introduction

This document presents an update on the progress made by the AI for Public Good Drug Discovery Project Advisory Group following the publication of the 2021 GPAI report, Artificial Intelligence for Public Good Drug Discovery: Recommendations for Policy Development. Our previous report presents a series of policy recommendations, with the aim of effectively leveraging AI for the purpose of combating global public health challenges, including the rise of antimicrobial resistance (AMR) and the threat of future pandemics. These recommendations were centered on three broad themes:

1. Government leadership on incentivizing or pursuing tasks related to these significant public health threats that are not sufficiently addressed by private industry.
2. Emboldening the uptake of AI throughout the drug research and development process.
3. Accelerating progress through promotion of Open Science and Open Data practices wherever feasible.

Following the publication of our report, the focus of the Project Advisory Group turned to advocating for and supporting the implementation of our recommendations. This update document will summarize our progress along two separate approaches. The group has pursued extensive engagement with relevant stakeholders in both the public and private sectors, to spread awareness of our recommendations, encourage their uptake, and receive further feedback on how to maximize the effectiveness of our efforts. A summary of the results of these engagements makes up the first component of this report. Second, we outline a call to action for the broader AI community, to make a more direct impact on critical public health challenges. We outline a possible avenue, via a novel international initiative, tasked with deploying AI-enabling expertise and resources to impactful points of intervention throughout ongoing antibiotic R&D projects.

Feedback from Stakeholder Engagement Efforts

The Project Advisory Group's 2022 work included a series of engagements with stakeholders from a variety of domains, on topics surrounding the use of AI for public good drug discovery. The feedback and perspectives from these engagements has been detailed below, grouped by domain of origin. Together, these findings present a picture of the level of concern with regards to public health issues related to drug R&D held by various stakeholders, as well as the amount of interest in leveraging AI/ML towards potential solutions, and various concerns held on potential roadblocks to be overcome.

Sector	Feedback
Public Sector	• There exists global interest in tackling severe public health threats that are not being researched within large pharmaceutical companies, namely the public health threat of Antimicrobial Resistance (AMR); in fact, AMR is on the list of the top 3 priorities among G7 countries

Sector	Feedback
	• It was the finance ministers of G7 countries that committed to bolstering drug R&D in this domain, suggesting a willingness to provide financial support • There is agreement among G7 countries that public health priorities should be managed collaboratively at the global level • In order to stimulate innovative developments in the domain of drug discovery, the federal government needs to design a series of incentive structures that can be categorized as “push” and “pull” incentives in order to ensure a strong pipeline from early stage research to late stage deployment • The UK is consistently cited as having “advanced” capabilities in AMR relative to the other countries of the G7 • Innovative policy making in this domain should engage smaller companies, which can often be more innovative than large pharmaceutical companies • In Canada, policy makers are attune to AI’s potential in the domains of predictive analytics, surveillance and drug development
Private Sector	• The usefulness of existing open data resources are limited by virtue of time lags and datasets that are inappropriate for many use cases or are of poor quality; this makes the creation of in-house datasets critical for the prospect of establishing a drug R&D company • Creating biotech companies and other small and medium enterprises in the drug discovery industry is challenging due to the large, up-front capital expenditure that is required; rendering government investment in this domain vital • Venture Capital firms are not necessarily the right investors in the domain of drug discovery because their short term time horizons are incompatible with the time it takes to complete the drug R&D lifecycle • AI can help to speed up the drug discovery process, which may present new funding opportunities among funders looking for a quicker Return on Investment

Sector	Feedback
International Health Organizations	• International health agencies often act conservatively without having the freedom and flexibility to innovate; thus, navigating the bureaucracy of the institution itself is critical using strategic points of intervention • There is a gap in data-driven interventions • It is challenging to coordinate between donors; thus, the program must focus on ways of successfully coordinating between funders • Innovation is disproportionate when comparing the Global North and the Global South, with the Global South often contributing to datasets in an extractive process that does not result in a sharing of benefits • Global agreements on data governance programming must be established since each population will likely have a unique approach to how they'd like their data governed, protected and compensated • Data protection should not be overly restrictive so as to promote as much data sharing as possible
Venture Capital Organizations	• Investment is dictated by the potential for Return on Investment as defined by the donor • Donors of different types have varying time horizons in terms of when they'd expect to see Return on Investment • Greater amounts of innovation can be derived from the demand-side, rather than the supply-side of the market; meaning, if the drug discovery ecosystem is predicated on consumer demand rather than available supply, there will be greater innovation in the domain

Moonshot Project

Society is experiencing a significant market failure in the domain of drug R&D that is preventing meaningful investment in high priority research areas. Specifically, the market failure being exhibited is one in which critical drugs are not sufficiently profitable to justify pharmaceutical investment. If this problem is not addressed, market dynamics will continue to guide drug R&D, to the detriment of human well-being in the long term. The associated risks are broad and severe in nature, as have been articulated in the previously mentioned 2021 GPAI report.

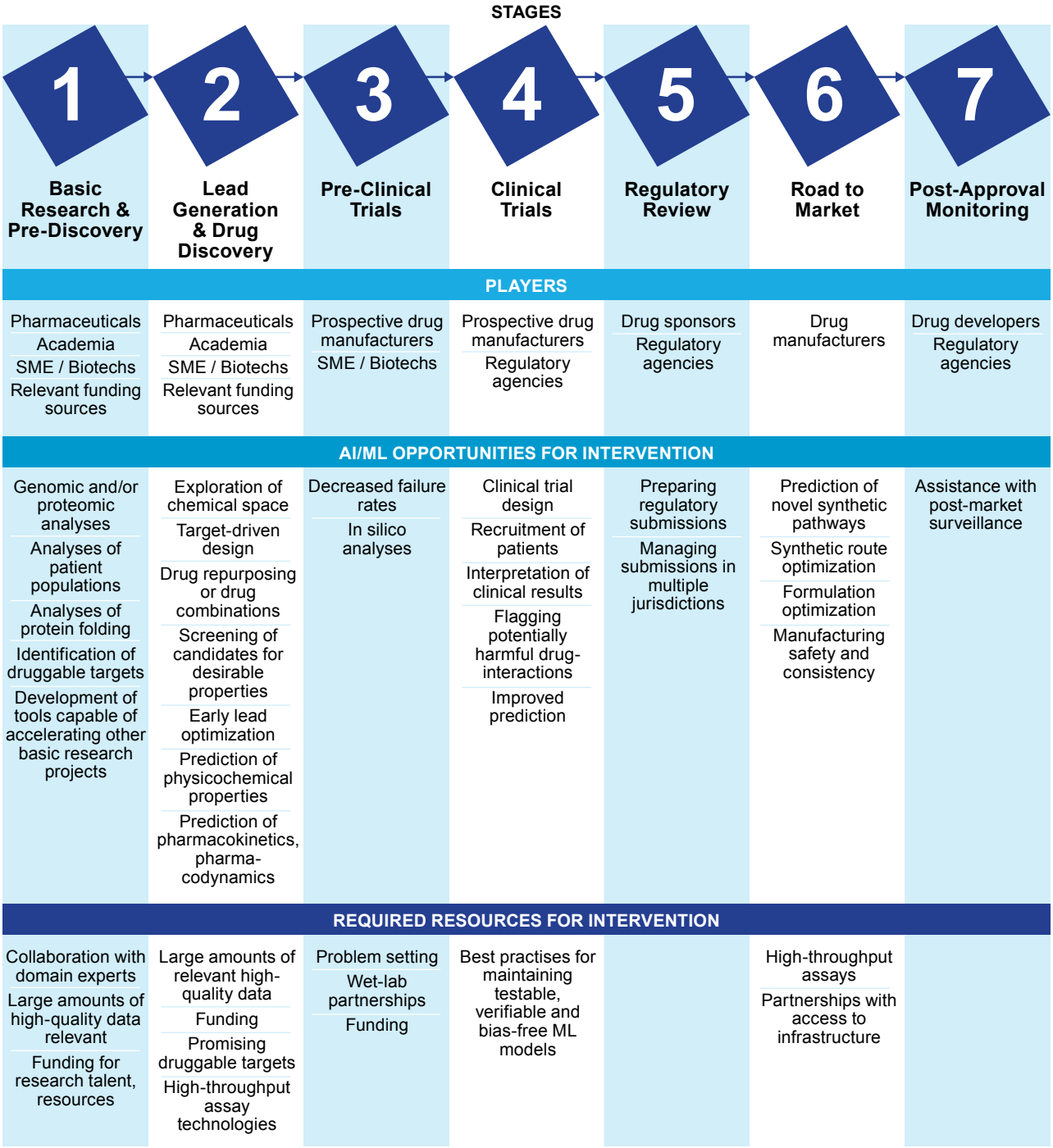
Fortunately, there already exists global health programming that is designed to direct research efforts in those domains currently neglected by pharmaceutical companies. These organizations include AMR Action Fund, Drugs for Neglected Diseases initiative (DNDi), Global Antibiotic Research and Development Partnership (GARDP), Rapidly Emerging Antiviral Drug Development Initiative (READDI) and AI-driven Structure-enabled Antiviral Platform (ASAP). However, in many cases, these institutions lack the technical resources or competencies that are needed to realize the productivity gains associated with next generation AI-driven drug discovery. Specifically, today's global health initiatives are often not leveraging industry-grade data science and/or AI/ML expertise, which represents a missed opportunity to advance, improve, and hasten research efforts.

The capabilities of AI/ML create significant opportunities for drug developers working to tackle neglected diseases, including antimicrobial resistance (AMR) and rare/orphan diseases. The chemical space containing potentially useful drugs is far too vast and complex to be fully explored by wet-lab research alone - AI can aid researchers in more efficiently navigating under-explored chemical areas of opportunity. Additionally, these technologies allow drug developers to conduct their work in ways that change the economics of drug development, rendering medication more affordable and accessible. This reduction in cost can be accomplished by increasing the speed of research, and reducing the failure rate of drug candidates. AI tools can also be re-usable, allowing investments in research directed towards antibiotic development to produce methods useful for the pursuit of other categories of drugs.

The moonshot project seeks to embolden global health initiatives by facilitating partnerships with entities that have appropriate AI and data science expertise. It recommends ways of connecting global health initiatives with academia, small and medium enterprises (SMEs), and pharmaceutical companies throughout the drug discovery and development pipeline; generating a federated approach to drug development that will encourage the use and adoption of AI.

One of the innovations of this proposal is the recommendation to incentivize the concepts of Open Science and Open Data among stakeholders in the drug development pipeline. Furthermore, it is recommended that this policy apply to research that is both successful as well as unsuccessful, with the goal of allowing AI innovation to beget future AI innovation. With access to shared datasets, algorithms, and other scientific methods, the future projects will be able to build on existing scientific progress without having to shoulder the full cost. While this approach is designed to stimulate research in neglected areas of drug development, it can *also* help with drug R&D that is otherwise profitable (from an industry/market perspective). Additionally, data sets and scientific methodologies can also be used *across* scientific domains further enabling widespread productivity growth.

Points of AI Intervention throughout the Pharmaceutical Research and Development Process



Summary of possible points of AI intervention within ongoing antibiotic and drug discovery initiatives - see the full details here

Next Steps: A Two-Pronged Approach

The Drug Discovery team's goal is to create a strong, collaborative healthcare effort that provides global health institutions with streamlined access to AI talent and resources and does so in ways that facilitate an increasingly robust drug discovery research ecosystem. To build this ecosystem, we will be:

- Determining strategic applications of AI / data science within the drug development pipeline (detailed above);
- Locating appropriate AI service providers;
- Defining the incentive structures that will be necessary to solicit interest among AI service providers along with securing and managing funding.

The Drug Discovery Project Team will be taking a two-pronged approach to the aforementioned steps. To begin, efforts will center on fostering national interest and strategic points of intervention within Canada. This work will allow us to develop our understanding of the barriers and opportunities that are affecting drug developers, policy makers and other stakeholders in this domain. Furthermore, it will facilitate our learnings on the best practices needed to conduct engagement efforts among federal policy makers on a global scale. Finally, we hope that this approach will cement Canada's engagement in the moonshot programming, which will help to elicit support from other G7 countries.

Simultaneously, we plan on engaging global stakeholders from the public and private sector along with academia to discuss their involvement in the moonshot project pipeline. It will be critical to the success of this program to ensure that the moonshot project incorporates the unique perspectives and considerations affecting a number of stakeholders outside of the Canadian context. Once we have sufficient international support to suggest significant future reach and impact, we will be able to design a foundational version of the initiative, and seek to establish a pilot project with an appropriate international health institution.

Possible Funding Model

It is envisioned that this project will be made possible through collaborative investments at the global level. This financing would be used to "push" and "pull" stakeholder engagement in the global health R&D ecosystem. These financial incentives may come in the form of subsidies, grants, tax credits, advance market commitments, procurement, or other reward mechanisms along the drug discovery and development pipeline.

We are investigating what a BARDA-type program might look like in the Canadian context and determining whether this strategy is the right approach for a global funding model. If so, governments around the world would create an entity to fund drug discovery innovation and coordinate their funding programs to favor international collaboration, open science, and data sharing. They would do so in ways that focus on the achievement of addressing priority areas for global health and prosperity.