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On The Frontline of AI-Driven Transformation of Drug Discovery

The pharmaceutical AI sector is “heating up”

The pharmaceutical AI ecosystem is currently a rapidly expanding sector of the pharmaceutical industry. Deep Pharma Intelligence, we have profiled **240 actively developing AI-driven biotech startups**, adding some 40 companies since our 2019 edition, **90+ big pharma and contract research organizations**, and **35 R&D centers** actively involved in the discovery and implementation of various AI technologies.

A steady growth in the “AI for Drug Discovery sector” can be observed in terms of substantially increased amount of venture capital pouring into the AI-driven biotech startups (**around $1.9B in 2020 alone**, so far), the increasing number of research partnerships between leading pharma organizations and AI-biotechs, and AI-technology vendors, a continuing pipeline of industry developments, research breakthroughs, and proof of concept studies, as well as exploding attention of leading media and consulting companies to the topic of AI in pharma and healthcare.

Bayer appears to be leading the pack of big pharma companies focused on developing the data-driven “AI-first” strategy of the pharmaceutical innovation.

AI Partnerships and Programs at Bayer

Bayer is among leaders in the "artificial intelligence race", exploring opportunities through multiple external collaborations, investments, joint projects and internal R&D programs focused on the adoption of machine learning (ML) and deep learning (DL) for drug design, diagnostics, pharmacovigilance, and crop protection research.

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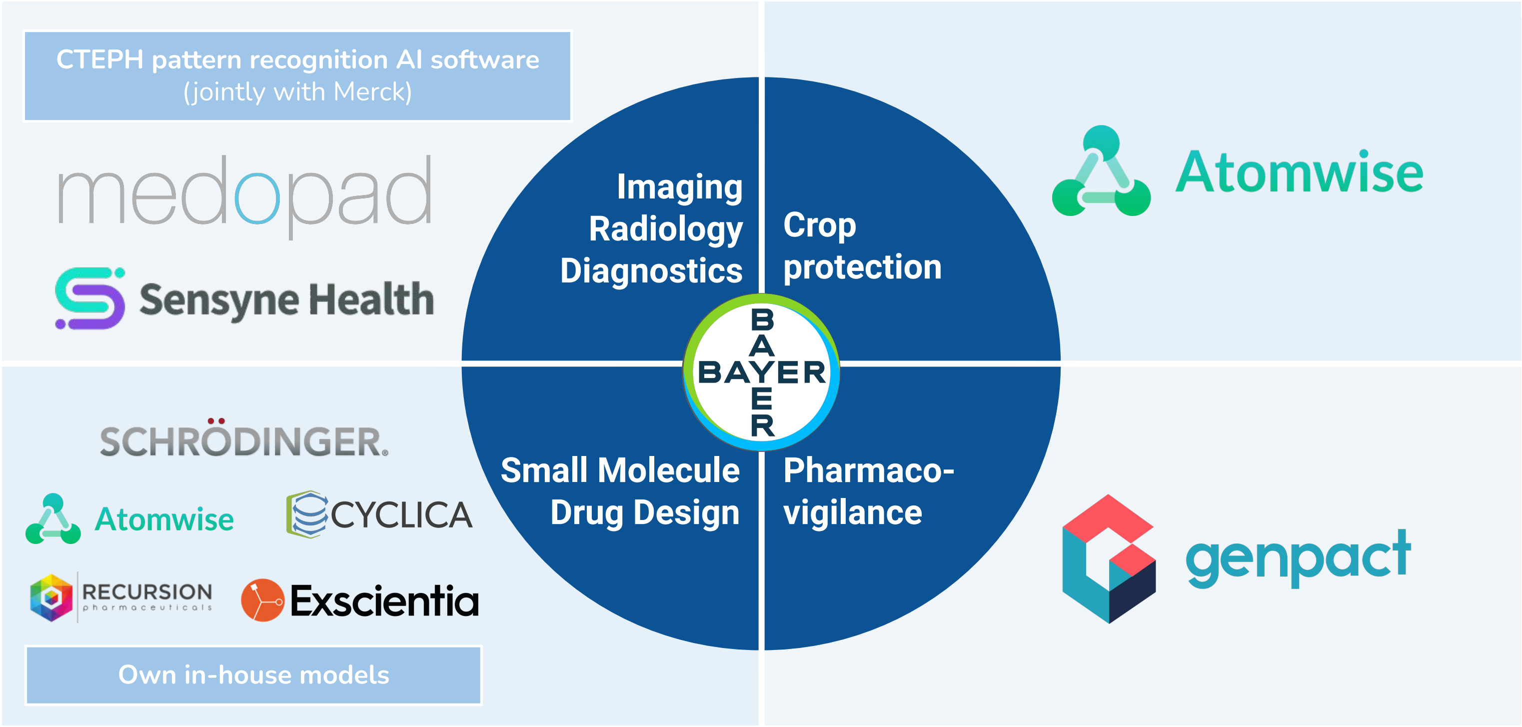

Pharma AI Deals Structure 2020

AI Companies	Pharma Corporations	Pharma Corporations	AI Companies
Exscientia, Atomwise, turbine, CYCLICA	BAYER	BAYER	SYSTEMS ONCOLOGY, RECURSION pharmaceuticals, SCHRÖDINGER, BERKELEY LIGHTS
saama, BERKELEY LIGHTS, XtalPi, Biovista	Pfizer	Pfizer	Atomwise, CytoReason, Insilico Medicine 英科智能
BERG, Alibaba Group, Tencent 腾讯	AstraZeneca	AstraZeneca	BenevolentAI, ProteinQure
FOUNDATION MEDICINE, RECURSION pharmaceuticals, Insilico Medicine 英科智能, WAVE	Takeda	gsk	Exscientia, CloudPharmaceuticals, Insilico Medicine 英科智能, CytoReason
BioSymetrics, RESONANT, DATAVANT	Janssen	NOVARTIS	Biovista, BenevolentAI, A2A PHARMA, DYNO THERAPEUTICS
ReverieLabs, Genialis, Exscientia	Roche	Boehringer Ingelheim	Insilico Medicine 英科智能, BERG, NANNA THERAPEUTICS
Atomwise, IKTOS, CYCLICA	MERCK	SANOFI	Researchably, Exscientia, BERG
sirenas, Concerto HealthAI	Bristol-Myers Squibb	abbvie	药明康德 WuXi AppTec, Atomwise
BERKELEY LIGHTS, e-therapeutics	novo nordisk	AMGEN	GeneTech, GNS HEALTHCARE
turbine	Johnson & Johnson	Celgene	Exscientia
	evotec	astellas	Biovista
CYCLICA	AUM BIOSCIENCES	VIVA	SCHRÖDINGER
Genialis	OncXerna	ImmunoPrecise	EVQLV
CYCLICA	YUHAN	almirall	IKTOS
Atomwise	HANSOH PHARMA	GC	Atomwise

Notable Bayer's AI-related Business Activity

September 2020: Recursion Pharmaceuticals raises $239M in series D funding round. This includes $50 million from **Bayer**'s investment arm **Leaps.** Recursion has also entered drug discovery R&D partnership with Bayer -- up to $100M.

January 2020: Bayer taps **Exscientia** for a 3-year $266 million agreement to leverage AI to accelerate the discovery of small molecules candidates programs for oncology and cardiovascular diseases.

January 2020: Bayer partners with **Schrödinger** for a 5-year agreement to work on a new virtual platform for small molecules design, which will be able to design and screen synthetically feasible compounds

January 2020: Bayer exercises right to enter into follow-on research and collaboration option agreement with **Atomwise** to continue crop protection development programs using AI-driven screening platform.

July 2019: Bayer and **Sensyne Health** are collaborating to develop treatments for cardiovascular disease. Sensyne has a unique partnership with the NHS to leverage its electronic patient record data while protecting patient privacy. The partners also established the "LifeHub" project, focused on AI-enabled radiology and imaging.

November 2018: Genpact partnered with Bayer to apply AI to pharmacovigilance. Genpact's technology automatically extracts adverse event data from source documents.

September 2017: Bayer taps **Berkeley Lights** for the innovation and acceleration of cell line development, antibody discovery, and research using Berkeley Lights' AI-enabled Beacon platform to automate biological workflows and gain efficiencies in its drug development process.

Participation in the AI-focused consortia and projects

Machine Learning Ledger Orchestration for Drug Discovery (MELLODDY):

Bayer is a member of the MELLODDY project, aimed at developing a new paradigm of working with data from various parties and edge devices in a secure format -- via federated learning architecture. This allows utilizing common knowledge from diverse datasets without compromising know-hows, commercial secrets, and IP rights.
(MELLODDY | IMI Innovative Medicines Initiative)

Machine Learning for Pharmaceutical Discovery and Synthesis Consortium (MLDPS):

Bayer is a member of MLDPS, a global effort, jointly with MIT, to develop software for automating small molecule discovery and synthesis.
(Applying machine learning to challenges in the pharmaceutical industry)

Alliance of Artificial Intelligence in Healthcare (AAIH):

Bayer is a member of AAIH, the global advocacy organization dedicated to the discovery, development and delivery of better solutions to improve patient lives.
(Current members)

Bayer’s AI-related investments and initiatives

Bayers’ Investment Arm	Accelerator Program (G4A)	LifeHub UK
Bayer joins $25M investment in data-driven digital health startup Medopad, an artificial intelligence startup using data from provider databases and patient devices for remote disease monitoring, raised $25 million in a Series B funding round led by Bayer's life sciences innovation arm. Recursion Pharma nets $239M, plus an AI research contract with Bayer Bayer took the lead role in the artificial intelligence company’s series D round, bestowing $50 million through its equity investment arm Leaps. The brought the round to a total of $239M. Recursion also entered in drug discovery collaboration with Bayer for up to $100M.	G4A is a global program within Bayer that “supports startups and companies that are developing innovative solutions in health and care, focused on AI and digital tech. Cyclica, Agamon In 2018 AI-driven startup Cyclica joined Bayer G4A as one of six finalists selected from over 1800 applicants globally. The company develops AI-based first-in-class-proteome screening technology, among other drug design tools. Later Bayer partnered with Cyclica to apply its AI technology for polypharmacology drug design. Agamon is another company in G4A, building AI-based clinical data intelligence platform.	In 2019 Bayer launches LifeHub UK focused on Artificial Intelligence to optimize data-driven drug discovery and disease diagnosis. Sensyne Health The first LifeHub UK’s project focused on the development of AI-enabled radiology solutions using Sensyne Health’s proprietary clinical AI technology platform to identify digital solutions for automated image evaluation. The project will analyse research from three million anonymised, ethically sourced NHS patient records and imaging data provided through Sensyne Health’s partnerships with NHS trusts, developing digital solutions to help radiologists improve the quality of the diagnosis.

Bayer's in-house AI program

Bayer's *in silico* ADMET platform: a journey of machine learning over the past two decades

Bayer has been developing its *in silico* absorption, distribution, metabolism, and excretion (ADMET) platform for around 20 years. The platform includes various components of AI, including statistical, machine learning, and deep learning modules.

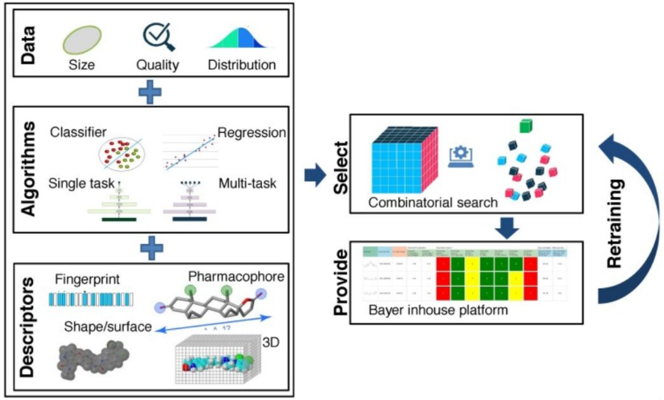

Image credit: ScienceDirect

Artificial intelligence software for CTEPH pattern recognition (Bayer, Merck)

In 2018 FDA granted Breakthrough Device Designation to the Artificial Intelligence Software for Chronic Thromboembolic Pulmonary Hypertension (CTEPH) Pattern Recognition, which Bayer developed jointly with MSD (Merck & Co., Inc.,)

Image credit: HealthImaging

Conclusions

The segment of the pharmaceutical AI is growing, stimulated by the mounting numbers of proof-of-concept research and practical use cases, suggesting that AI technology has matured enough to become a game changer.

Most of the big pharma companies and CRO organizations are now actively exploring ways to apply AI tech into their R&D and business workflows. Bayer is taking the lead in the overall race, in terms of the number of AI-related partnerships and programs. The company is active in R&D collaborations with AI startups (milestone based), venture capital investment via its investment arm, and grant programs to tap into the AI and digital tech innovations ecosystem (e.g. Bayer G4A).

The company is also developing in-house programs involving AI research -- in the areas of diagnostics and preclinical drug discovery.

However, most of the programs are still in the discovery/proof-of-concept stage, and will take time for a company-wide adoption and commercial validation to meet global KPIs.

Considering well-balanced and diverse strategy for AI and digital tech onboarding, and a strong leadership team, including high-profile data scientists and researchers, we believe Bayer can cement its leadership position in the AI race and become among the first companies to transition to a data-centric AI-first R&D business model within the foreseeable future.

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E-mail: info@deep-pharma.tech	Website: deep-pharma.tech