

# Top 100 AI Leaders

## in Drug Discovery and Advanced Healthcare



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# Introduction

Over the last several years, the pharmaceutical and healthcare organizations have developed a strong interest toward applying artificial intelligence (AI) in various areas, ranging from medical image analysis and elaboration of electronic health records (EHRs), to more basic research like building disease ontologies, preclinical drug discovery, and clinical trials. The demand for the ML/AI technologies, as well as for ML/AI talent, is growing in pharmaceutical and healthcare industries and driving the formation of a new interdisciplinary industry ('data-driven healthcare').

Consequently, there is a growing number of AI-driven startups and emerging companies offering technology solutions for drug discovery and healthcare.

Another important source of advanced expertise in AI for drug discovery and healthcare comes from top technology corporations (Google, Microsoft, Tencent, etc), which are increasingly focusing on applying their technological resources for tackling health-related challenges, or providing technology platforms on a rent bases for conducting research analytics by life science professionals.

Some of the leading pharmaceutical giants, like GSK, AstraZeneca, Pfizer and Novartis, are already making steps towards aligning their internal research workflows and development strategies to start embracing AI-driven digital transformation at scale. However, the pharmaceutical industry at large is still lagging behind in adopting AI, compared to more traditional consumer industries -- finance, retail etc.

The above three main forces are driving the growth in the AI implementation in pharmaceutical and advanced healthcare research, but the overall success depends strongly on the availability of highly skilled interdisciplinary leaders, able to innovate, organize and guide in this direction.

The current report summarizes the TOP 100 most innovative and entrepreneurial AI leaders, who has been contributing largely towards data-driven transformation of the pharmaceutical and healthcare industries.

# Top-100 AI Leaders in Drug Discovery and Advanced Healthcare Report Methodology

The list of 100 artificial intelligence (AI) leaders in drug discovery and advanced healthcare is based on the assessment of the cumulative impact (CI) that a person contributed to the advancement of the AI technologies in the area of pharmaceutical research (basic biology research, drug discovery and development, drug repurposing etc), and healthcare research (diagnostics, medical data management, therapy prescription etc).

The CI is measured as a total sum of inputs from 3 highly overlapping categories:

**Science and Tech Innovators** – reflects scientific and technical contributions to the development of AI technology in the context of its application for life science tasks

**Business Leaders** – reflects entrepreneurship, business leadership and industry ecosystem development contributions to the advancement of AI technology in life sciences

**AI Thought Leaders** – reflects contribution to the science and technology communication efforts in the area of AI application for life sciences and healthcare (books, conference talks, events, educational initiatives etc)

To be nominated for the TOP 100 AI Leaders list, it was set to be a prerequisite for a candidate to have interdisciplinary technical skills and/or business/entrepreneurship/decision making skills in both of the following areas:

1. AI/ML/Statistics/Data Science/Computer Science
2. Drug Discovery/Drug Development/Drug Trials/Healthcare/Diagnostics

Another prerequisite for the inclusion in the TOP 100 AI Leaders list was the availability of an outstanding achievement in either AI, or Life Sciences **in the context of applying AI for solving Life Science tasks**, including:

- Notable innovation, technological breakthrough, considerable advancement of the tech state-of-the-art
- Notable impact on research (very high level of citations etc)
- Notable organizational or entrepreneurship achievements (founding or C-level leadership of startups or mature companies with high level of investment/market cap, impactful non-for-profit organizations, or academic institutions)
- Notable thought leadership achievements (impactful books, articles, public activity etc)

# Top-100 AI Leaders in Drug Discovery and Advanced Healthcare Report Methodology

The initial large pool of candidates (around 500) for the TOP AI Leaders list has been selected from multiple sources including:

Top pharmaceutical and healthcare AI conference program lists

Google Scholar

Databases

Google News and PR-distribution services

Companies websites

And based on the analysis of the descriptive criteria (personal page descriptions, biographies, LinkedIn and Bloomberg pages, public awards, article titles, news and PRs, and other text resources) and formal numerical metrics (number of research citations in Google Scholar, RG score in ResearchGate, number of books/talks and articles, social media activity etc).

The initial pool of around 500 top candidates has been shortlisted down to the top 100 list following an iterative approach, starting with the obvious differentiating parameters (top tech or business achievements or highest number of citations) and gradually specifying additional parameters for the final rating.

## The rating calculation model

Is a first-order homogeneous polynomial which calculates person's assessment variables and their relative impact weights (coefficients). The weights of each variable have been logically designed to underline major contributions and impact (innovations, business achievements, research citations etc) and only augment them with less important, yet valuable, contributions (conference talks, social media activity etc).

# Top-100 AI Leaders in Drug Discovery and Advanced Healthcare

- |                        |                        |                      |                        |
|------------------------|------------------------|----------------------|------------------------|
| 1. Abraham Heifets     | 26. Dan Riskin         | 51. John Baldoni     | 76. Peter Szolovits    |
| 2. Alan Aspuru-Guzik   | 27. Daniel Rubin       | 52. John Fox         | 77. Peter V. Henstock  |
| 3. Alex Aliper         | 28. Daphne Koller      | 53. Keith Dreyer     | 78. Philippe Marc      |
| 4. Alex Zhavoronkov    | 29. David B. Fogel     | 54. Ken Mulvany      | 79. Pierre Baldi       |
| 5. Alexander A Morgan  | 30. David Haussler     | 55. Kim Branson      | 80. Regina Barzilay    |
| 6. Alfonso Valencia    | 31. David Whewell      | 56. Kwabena Boahen   | 81. Robert Tibshirani  |
| 7. Alice Zhang         | 32. Edward Shortliffe  | 57. Lawrence Hunter  | 82. Ronald M. Summers  |
| 8. Andrea De Souza     | 33. Eric Topol         | 58. Leila Pirhaji    | 83. Ross D. King       |
| 9. Andreas Persidis    | 34. Eric Xing          | 59. Leo Celi         | 84. Russ Altman        |
| 10. Andrew A. Radin    | 35. Etzard Stolte      | 60. Maja Pantic      | 85. Sebastien Lefebvre |
| 11. Andrew Beck        | 36. Gabriel Musso      | 61. Manolis Kellis   | 86. Sepp Hochreiter    |
| 12. Andrew Ng          | 37. Gary Bryce Fogel   | 62. Mark Depristo    | 87. Shameer Khader     |
| 13. Anne E. Carpenter  | 38. Guido Lanza        | 63. Mark Gerstein    | 88. Slava Akmaev       |
| 14. Atul Butte         | 39. Hugo Ceulemans     | 64. Maryellen Giger  | 89. Stephen Muggleton  |
| 15. Babak Alipanahi    | 40. Ian Pepper         | 65. Milind Kamkolkar | 90. Steven Salzberg    |
| 16. Badhri Srinivasan  | 41. Igor Jurisica      | 66. Mustafa Suleyman | 91. Suchi Saria        |
| 17. Björn Schuller     | 42. Isaac Kohane       | 67. Neel S Madhukar  | 92. Ted Slater         |
| 18. Blake Borgeson     | 43. Izhar Wallach      | 68. Nigam Shah       | 93. Thomas Fuchs       |
| 19. Bram van Ginneken  | 44. Jackie Hunter      | 69. Niven R Narain   | 94. Tom Chittenden     |
| 20. Brandon Allgood    | 45. Jaime Carbonell    | 70. Noor Shaker      | 95. Tommi S. Jaakkola  |
| 21. Brendan Frey       | 46. Jake Chen          | 71. Nora Khaldi      | 96. Vijay Pande        |
| 22. Carole Goble       | 47. James Weatherall   | 72. Olaf Ronneberger | 97. Wang Jun           |
| 23. Christian Guttmann | 48. Jean-Philippe Vert | 73. Olga Troyanskaya | 98. Wei Fan            |
| 24. Christopher Bouton | 49. Jianlin Cheng      | 74. Olivier Elemento | 99. Yefeng Zheng       |
| 25. Cory Kidd          | 50. Jimeng Sun         | 75. Pablo Cingolani  | 100. Yoshua Bengio     |

# Top-100 AI Leaders in Drug Discovery and Advanced Healthcare

## Academia

Academia has traditionally been a cradle of innovative thought in the theoretical and practical aspects of machine learning, deep learning and artificial intelligence systems in the context of their application for drug discovery and biomedical research. Participants in this category are characterized by:

- High number of peer-reviewed publications
- High level of citation (high h-index and i10-index, RG score in ResearchGate – if applicable)
- Leadership in a particular area of theoretical or engineering aspect of ML/AI for drug discovery
- Availability of a notable theoretical breakthrough, technical invention, or widely adopted commercial model

NAME	COMPANY	POSITION	COUNTRY	CITY
Alan Aspuru-Guzik	University of Toronto	Professor of Chemistry and Computer Science	Canada	Toronto
Alfonso Valencia	Barcelona Supercomputing Centre	Director Life Science Department	Spain	Madrid
Anne E. Carpenter	Broad Institute of Harvard and MIT	Imaging Platform Director, Advisor at Recursion Pharmaceuticals	USA	Cambridge
Atul Butte	Bakar Computational Health Sciences Institute, UCSF	Director	USA	San Francisco
Björn Schuller	Imperial College London	Professor of Artificial Intelligence	UK	London
Bram van Ginneken	Radboudumc	Professor	Netherlands	Nijmegen
Carole Goble	UK Head of Node, ELIXIR, University of Manchester,	Professor	UK	Manchester
Daniel Rubin	Stanford University	Associate Professor	USA	Stanford
David Haussler	UC Santa Cruz, Genomics Institute	Scientific Director	USA	Santa Cruz, CA
Edward Shortliffe	Arizona State University, College of Health Solutions, IBM Watson Health,	Adjunct Professor of Biomedical Informatics	USA	New York City
Eric Topol	Scripps Research Institute	Founder, Director, Professor	USA	La Jolla
Igor Jurisica	University of Toronto	Full Professor	Canada	Toronto

NAME	COMPANY	POSITION	COUNTRY	CITY
Isaac Kohane	Harvard Medical School, Children's Hospital	Professor and Chair, Founding Director	USA	Boston
Jaime Carbonell	Carnegie Mellon University	Professor	USA	Pittsburg
Jake Chen	University of Alabama at Birmingham	Chief Bioinformatics Officer	USA	Birmingham, AL
Jianlin Cheng	University of Missouri	Professor	USA	Columbia, MO
Jimeng Sun	Georgia Tech	Associate Professor	USA	Atlanta
John Fox	University of Oxford	Professor	UK	Oxford
Keith Dreyer	American College Of Radiology (ACR)	ACR Data Science Institute Chief Science Officer	USA	Boston
Kwabena Boahen	Stanford University	Professor of Bioengineering and Electrical Engineering	USA	Stanford
Lawrence Hunter	University of Colorado School of Medicine	Professor of Computational Biology	USA	Denver
Leo Celi	MIT, Harvard Medical School	Associate Professor, Principal Research Scientist	USA	Boston
Maja Pantic	Imperial College London	Professor of Affective and Behavioural Computing	UK	London
Manolis Kellis	MIT	Professor	USA	Boston

NAME	COMPANY	POSITION	COUNTRY	CITY
Mark Gerstein	Yale University	Co-Director Center for Biomedical Data Science	USA	New Haven, CT
Maryellen Giger	University of Chicago	Professor, Department of Radiology	USA	Chicago
Nigam Shah	Stanford University	Associate Professor of Medicine (Biomedical Informatics)	USA	San Francisco
Olga Troyanskaya	Princeton University	Professor	USA	New York City
Olivier Elemento	Weill Cornell Medicine	Director, Laboratory of Cancer Systems Biology, Englander Institute for Precision Medicine Institute for Computational Biomed	USA	New York
Peter Szolovits	MIT	Professor	USA	Boston
Pierre Baldi	University of California	Professor	USA	Orange County, CA
Regina Barzilay	MIT EECS, member MLPDS	Professor	USA	Cambridge
Robert Tibshirani	Stanford University	Professor of Biomedical Data Sciences	USA	San Francisco

NAME	COMPANY	POSITION	COUNTRY	CITY
Ronald M. Summers	National Institutes of Health	Senior Investigator	USA	Washington
Ross D. King	University of Manchester	Professor of Computer Science	UK	Manchester
Russ Altman	Stanford University	Professor	USA	Menlo Park, CA
Sepp Hochreiter	Institute for Machine Learning at the Johannes Kepler University	Director	Austria	Linz
Stephen Muggleton	Imperial College London	Head of the Computational Bioinformatics Laboratory	UK	London
Steven Salzberg	McKusick-Nathans Institute of Genetic Medicine, Johns Hopkins School of Medicine, Forbes	Professor, Blogger, Director	USA	Baltimore
Suchi Saria	Johns Hopkins University	Director of Hopkins Machine Learning and Healthcare Lab	USA	New York
Thomas Fuchs	Memorial Sloan Kettering Cancer Center	Director of Computational Pathology	USA	New York
Tommi S. Jaakkola	MIT EECS, member MLPDS, Journal of Machine Learning Research	Professor, Editor	USA	Cambridge
Yoshua Bengio	Université de Montréal	Full professor, Advisor at Recursion Pharmaceuticals	Canada	Montreal

# Top-100 AI Leaders in Drug Discovery and Advanced Healthcare

## AI Companies

The interest of pharma and biotech organizations towards ML/AI has been growing over the last several years and it created a substantial demand for advanced AI-driven solutions for drug discovery and healthcare. As a consequence, the number of new companies (startups) offering such solutions is steadily growing.

Participants in this category are, primarily, founders or top leaders of some of the most active and impacting emerging AI companies working in life sciences. They are characterized by the following peculiar qualities:

- Outstanding business leadership in the area of introducing AI for drug discovery/biotech/healthcare
- High level of interdisciplinary expertise in both hi-tech and life sciences
- Publicly active position, thought leadership activity

NAME	COMPANY	POSITION	COUNTRY	CITY
Abraham Heifets	Atomwise	CEO, co-founder	USA	San Francisco
Alex Aliper	Insilico Medicine	President	USA	Rockville
Alex Zhavoronkov	Insilico Medicine	CEO, co-founder	USA	Baltimore
Alice Zhang	Verge Genomics	CEO, Co-founder	USA	San Francisco
Andreas Persidis	Biovista	Co-founder and CEO	USA	Charlottesville
Andrew A. Radin	TwoXAR	CEO, co-founder	USA	San Francisco
Andrew Beck	PathAI	CEO, Co-founder	USA	Boston
Blake Borgeson	Recursion Pharmaceuticals	Co-founded, Scientific Advisor	USA	Salt Lake City
Brandon Allgood	Numerate	co-founder and CTO	USA	San Francisco
Brendan Frey	Deep Genomics	CEO	Canada	Toronto

NAME	COMPANY	POSITION	COUNTRY	CITY
Christopher Bouton	Vyasa	CEO	USA	Boston
Cory Kidd	Catalia Health	CEO, Co-founder	USA	San Francisco
Dan Riskin	Verantos	CEO	USA	Palo Alto
Daphne Koller	Insitro	Founder and CEO	USA	San Francisco
David B. Fogel	Trials.ai, Natural Selection, Inc.	Advisor/Chief Science Officer	USA	San Diego
Eric Xing	Petuum Inc./ Carnegie Mellon University	CEO, co-founder, Chief Scientist, Professor	USA	Pittsburgh
Gabriel Musso	BioSymetrics	Chief Scientific Officer	Canada	Etobicoke
Gary Bryce Fogel	Natural Selection, BioSystems Journal	CEO, Editor-in-chief	USA	San Diego
Guido Lanza	Numerate	President & CEO	USA	San Francisco
Izhar Wallach	Atomwise	CTO, co-founder	USA	San Francisco

NAME	COMPANY	POSITION	COUNTRY	CITY
Jackie Hunter	BenefvolentBio	CEO	UK	Stevenage
Ken Mulvany	BenefvolentAI	Chairman and Founder	UK	London
Leila Pirhaji	ReviveMed	Founder and CEO	USA	Boston
Neel S Madhukar	OneThree Biotech	CEO	USA	New York
Niven R Narain	BERG Health	Co-Founder, President & CEO	USA	Boston
Noor Shaker	GTN	CEO, Co-founder	UK	London
Nora Khaldi	Nuritas	Founder & Chief Scientific Officer	Ireland	Dublin
Slava Akmaev	BERG Health	Senior Vice President and Chief Analytics Officer	USA	Boston
Tom Chittenden	WuXi NextCode, Advanced Artificial Intelligence Research Laboratory	Vice President, Statistical Sciences and Founding Director,	USA	Medford
Wang Jun	iCarbonX	CEO, co-founder	China	Shenzhen

# Top-100 AI Leaders in Drug Discovery and Advanced Healthcare

## Pharma Corporations

While there is a surge of life science startups, emerging biotechs and AI-focused vendors, large pharmaceutical corporations remain the key driver of the pharmaceutical industry and innovative drugs market. It is the success (or failure) in adopting the ML/AI technologies by pharma corporations, that will largely shape the dynamics of the progress in the area of pharmaceutical AI.

Leaders in this category include top pharmaceutical executives, who embraced the importance of shaping a data-driven strategy with AI, and have immense decision-making influence on this process in their organizations.

The typical features of participants in this list include:

- C-level executive role, or leading research role in largest pharmaceutical companies
- Strong background in digital technologies, cheminformatics/bioinformatics
- Strong technology leadership ability
- Knowledge of ML/AI (either career major, or as an additional training)

NAME	COMPANY	POSITION	COUNTRY	CITY
Andrea De Souza	Eli Lilly	Senior Director	USA	New York
Badhri Srinivasan	Novartis	Head, Global Development Operations	Switzerland	Basel
David Whewell	Merck	Former Director of Architecture and Software Innovation	Switzerland	Lausanne Area
Etzard Stolte	Roche	Global Head of Knowledge Management PTD	Switzerland	Basel
Hugo Ceulemans	Janssen Pharmaceutical	Scientific Director Discovery Data Sciences	Belgium	Bertem
Ian Pepper	Novartis	CTO, Head Strategy and Integration Architecture	Ireland	Dublin
James Weatherall	AstraZeneca	Head, Advanced Analytics Centre, Biometrics & Information Sciences, Global Medicines Development	UK	Stockport
John Baldoni	GSK	Sr. vice president of Platform Technology and Science	UK	Brentford

NAME	COMPANY	POSITION	COUNTRY	CITY
Kim Branson	Genentech	Head of A.I (ECDi)	USA	San Francisco
Milind Kamkolkar	Sanofi	Chief Data Officer	USA	New York
Pablo Cingolani	AstraZeneca	Principal Scientist, Bioinformatics & AI	USA	Boston
Peter V. Henstock	Pfizer	Senior Data Scientist, AI/ML	USA	Medford
Philippe Marc	Novartis Institutes for Biomedical Research	Global Head of Integrated Data Sciences	Switzerland	Basel
Sebastien Lefebvre	Alexion Pharmaceuticals	Senior Director, Data Analytics & Decision Support	USA	Boston
Shameer Khader	AstraZeneca	Senior Director (Advanced Analytics, Data Science, Bioinformatics)	USA	New York

# Top-100 AI Leaders in Drug Discovery and Advanced Healthcare

## Tech Corporations

Largest technology corporations have developed the strongest capabilities in the ML/AI tech, and required infrastructures, available on the planet. Now they are increasingly attempting to shift a focus on healthcare and even basic pharmaceutical research and drug discovery, hoping to leverage the unmatched AI expertise in a “foreign”, but very promising for them market.

Top AI-leaders in this category are typically from deeply technological backgrounds (Computer Science, Artificial Intelligence, Data Science, Engineering, Statistics/Math), with some acquired level of expertise in life sciences.

Characteristics are:

- Top level research or business leadership position at large technology corporations
- Involvement in the application of ML/AI tech for pharmaceutical/healthcare tasks

NAME	COMPANY	POSITION	COUNTRY	CITY
Andrew Ng	Landing AI (recently worked at Baidu), Stanford University	CEO, Co-founder, Professor	USA	Palo Alto
Jean-Philippe Vert	Google	Senior Staff Research Scientist at Google Brain	France	Paris
Mark Depristo	Google	Head of Deep Learning for Genetics and Genomics	USA	Los Altos, CA
Mustafa Suleyman	Google Deepmind	Co-Founder	UK	London
Olaf Ronneberger	Google Deepmind	Senior Research Scientist	UK	London
Wei Fan	Tencent	Head of Medical AI Lab	USA	Sunnyvale
Yefeng Zheng	Tencent	R&D Director of Medical AI	China	Shenzhen City

# Top-100 AI Leaders in Drug Discovery and Advanced Healthcare

## Others

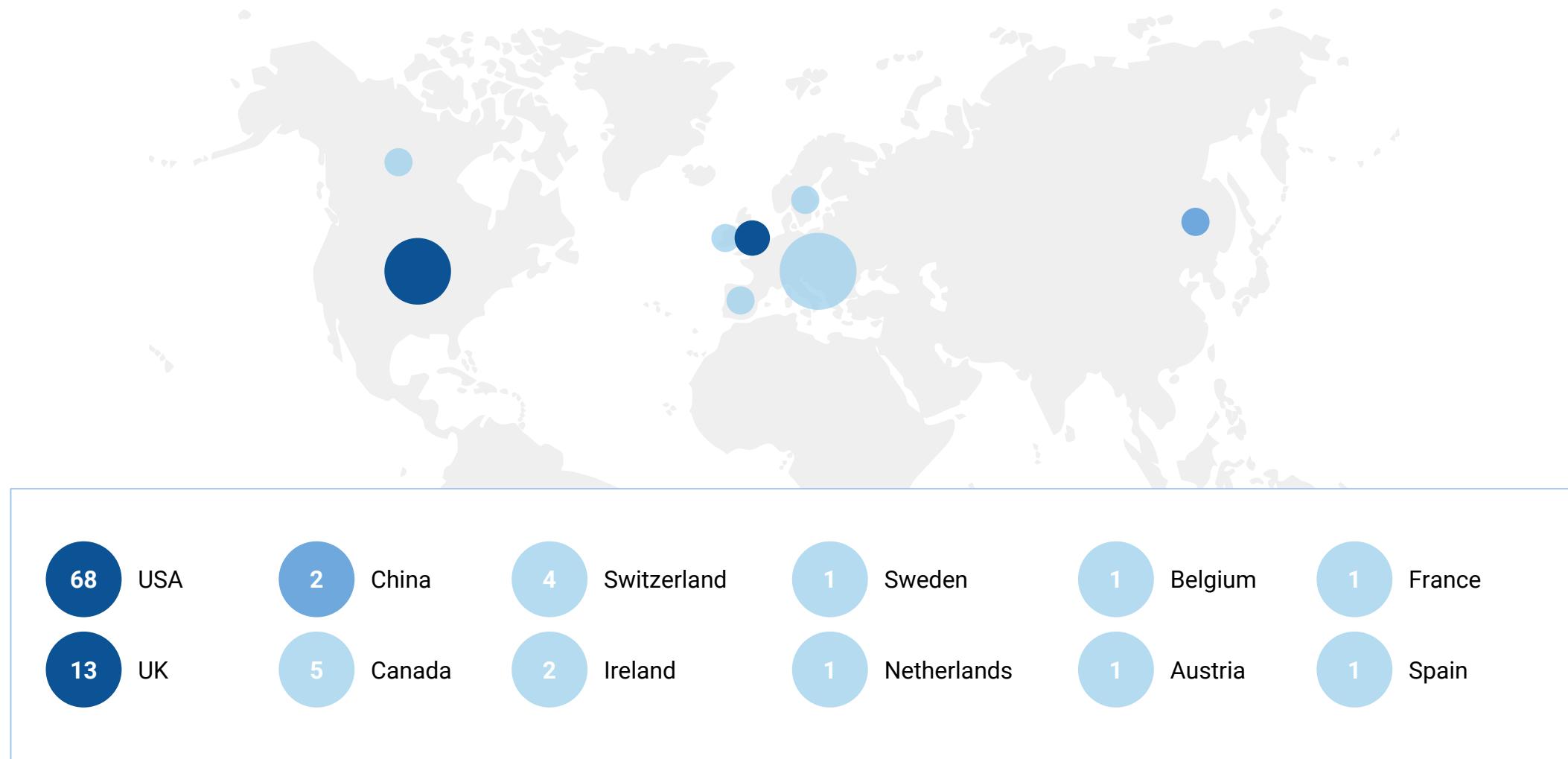
This category summarizes top AI leaders from various uncategorized organizations, helping advance this technology in the pharmaceutical research or healthcare. Peculiar features include:

- Leadership research or business roles in the organization
- Substantial technical expertise in either AI/ML or life sciences (with mandatory acquired minor expertise in the other of the two subjects)
- Notable leadership or research contributions to the advancement of AI in pharmaceutical industry or healthcare

NAME	COMPANY	POSITION	COUNTRY	CITY
Alexander A Morgan	Khosla Ventures	Principal	USA	San Francisco
Babak Alipanahi	23andMe	Senior Scientist, AI + Computational Biology	USA	San Francisco
Christian Guttmann	Tieto Sweden AB, Nordic Artificial Intelligence Institute	VP, Global Head of Artificial Intelligence & Data Science, Executive Founding Director	Sweden	Stockholm
Ted Slater	Cray	Global Head, Scientific AI & Analytics	USA	Saginaw, MI
Vijay Pande	Andreessen Horowitz	General partner	USA	San Francisco
Babak Alipanahi	23andMe	Senior Scientist, AI + Computational Biology	USA	San Francisco

# Top-100 AI Experts in Drug Discovery

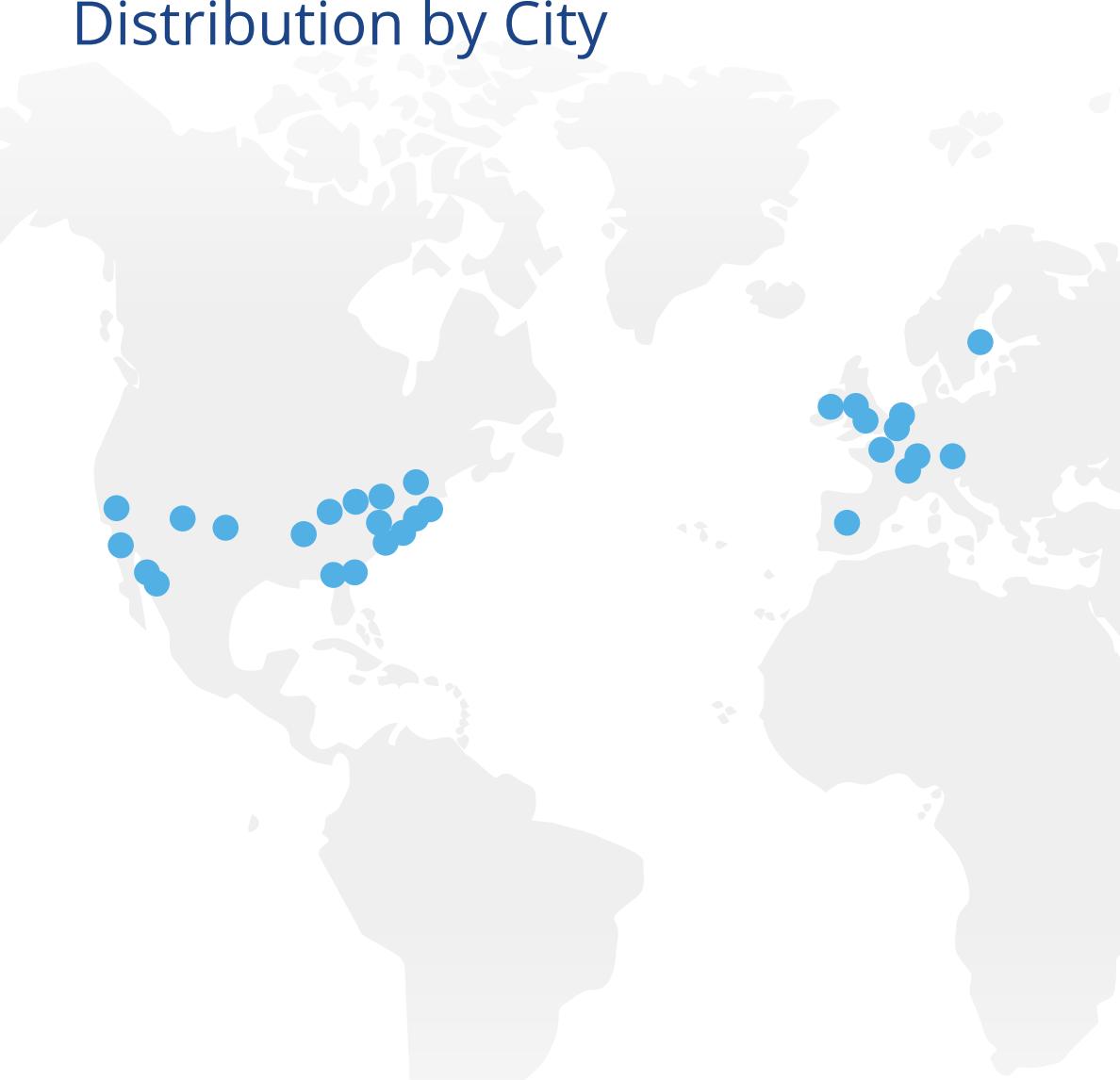
## Distribution by Countries



This diagram illustrates location of the top AI leaders in pharma and healthcare across the globe. USA and Great Britain remain home for the largest number of top experts. However, it should be noted that China has a potential to substantially alter this statistics in the coming years due to reverse migration of top AI experts from the USA.

# Top-100 AI Experts in Drug Discovery

## Distribution by City

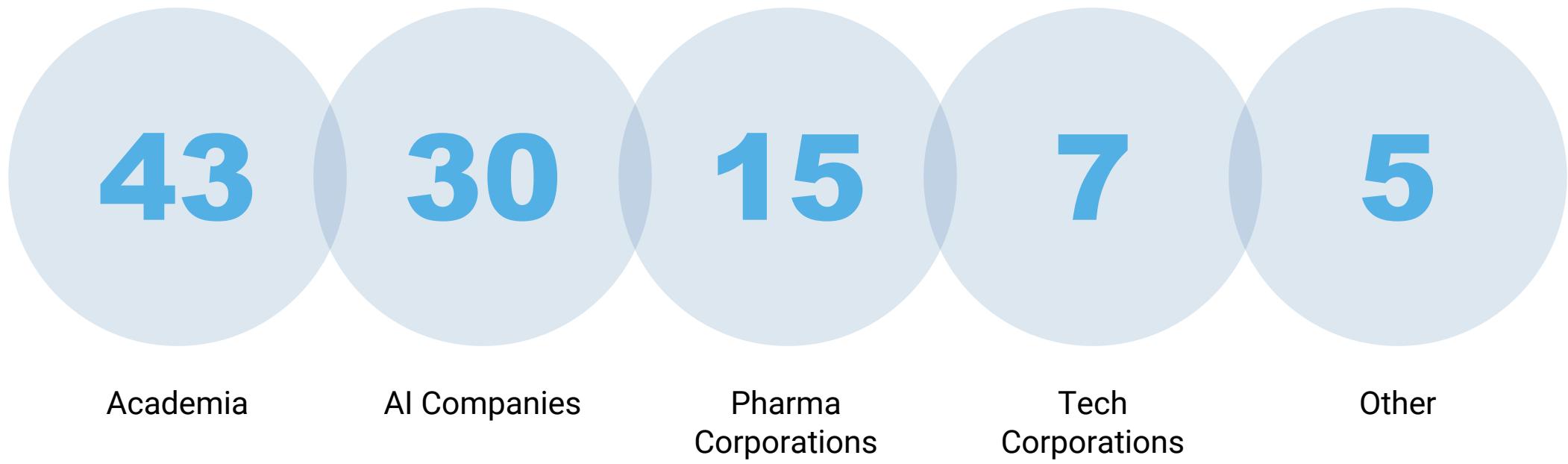


This map shows that most of the top AI experts in pharma and healthcare reside in American and European cities, with Boston, San Francisco, New York and London being among the most attractive cities for this kind of experts.

15	San Francisco	1	Pittsburg
12	Boston	1	Paris
7	New York	1	Oxford
7	London	1	Orange County, CA
3	Toronto	1	Nijmegen
3	Cambridge	1	New Haven, CT
3	Basel	1	Montreal
2	Stanford	1	Menlo Park, CA
2	San Diego	1	Madrid
2	Palo Alto	1	Los Altos, CA
2	New York City	1	Linz
2	Medford	1	Lausanne Area
2	Manchester	1	La Jolla
2	Dublin	1	Etobicoke
1	Sunnyvale	1	Denver
1	Stockport	1	Columbia, MO
1	Stockholm	1	Chicago
1	Stevenage	1	Charlottesville
1	Shenzhen City	1	Birmingham, AL
1	Santa Cruz, CA	1	Bertem
1	Salt Lake City	1	Baltimore
1	Saginaw, MI	1	Atlanta
1	Pittsburgh		

# Top-100 AI Experts in Drug Discovery

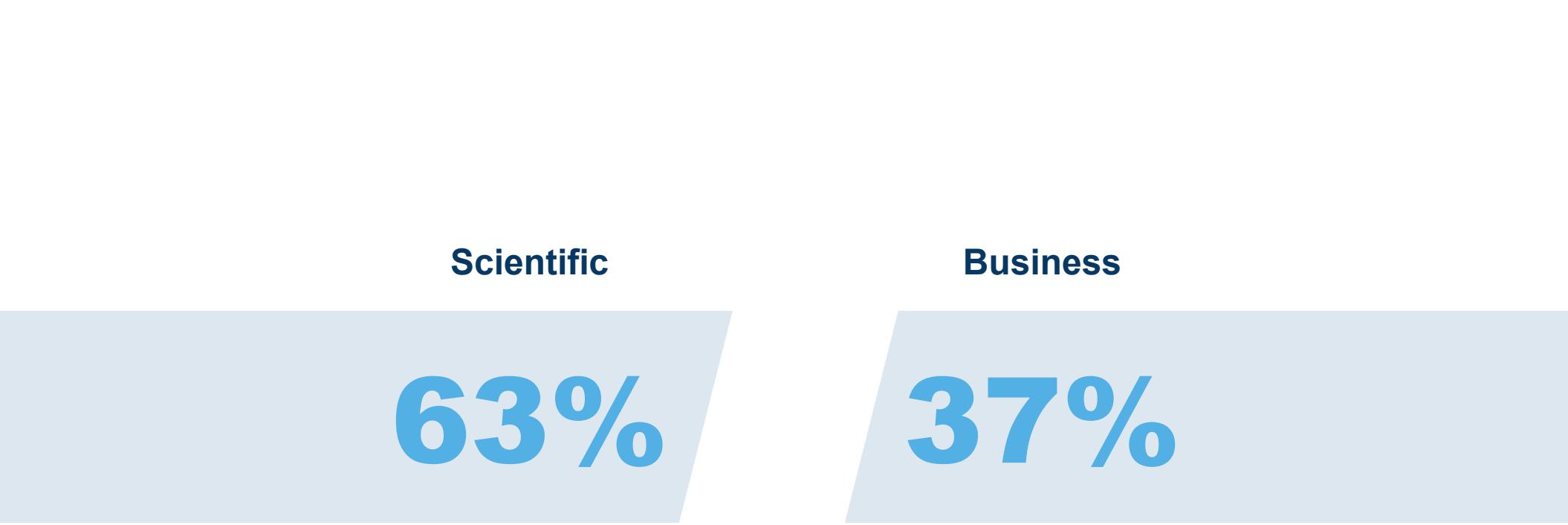
## Distribution by Organization Type



Academia has traditionally been home to the most of the top research minds in the area of pharmaceutical and healthcare AI, which is in accordance with the current statistics. A major part of top AI experts also involved in entrepreneurship and run their own AI companies. The remaining list of top experts is distributed between pharma corporations, technology corporations, and various uncategorized companies.

# Top-100 AI Experts in Drug Discovery

## Distribution by Role in the Organization



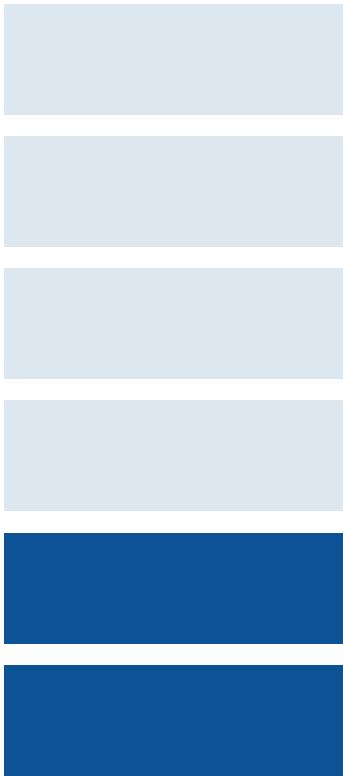
Top 100 AI leaders list includes experts who have multifold types of contributions towards advancing AI in pharma and healthcare. Research vs business/entrepreneurship roles are roughly distributed as 2 : 1.

# Top-100 AI Experts in Drug Discovery

## Distribution by Primary Activity

Business Roles

**17%**



AI Research/Technology

**46%**



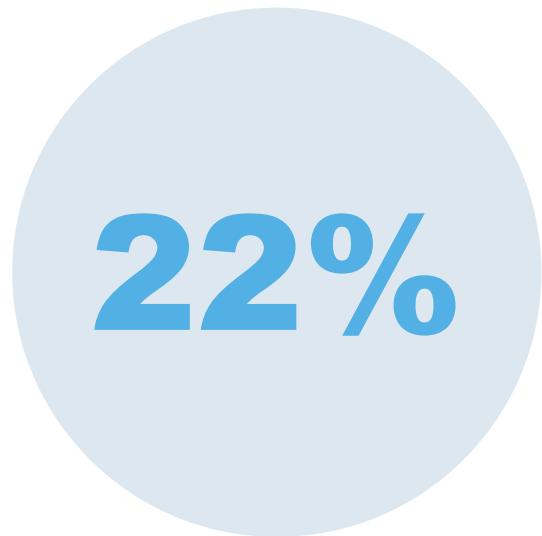
Life Sciences  
Research/Technology

**37%**



# Top-100 AI Experts in Drug Discovery

## Distribution by the Impact on the Industry



Business Leaders



Science and tech innovators



Thought Leaders

This diagram characterizes the types of impact that top AI leaders are making on the industry to advance ML/AI technologies in pharma or healthcare. The majority of effort is spent on the innovation and research, as well as thought leadership and education, while only 1% of the effort is dedicated to entrepreneurship and organizational activities.

# Introduction

Over the last several years, the pharmaceutical and healthcare organizations have developed a strong interest toward applying artificial intelligence (AI) in various areas, ranging from medical image analysis and elaboration of electronic health records (EHRs), to more basic research like building disease ontologies, preclinical drug discovery, and clinical trials. The demand for the ML/AI technologies, as well as for ML/AI talent, is growing in pharmaceutical and healthcare industries and driving the formation of a new interdisciplinary field -- data-driven drug discovery/healthcare.

Consequently, there is a growing number of AI-driven startups and emerging companies offering technology solutions for drug discovery and healthcare ([ref1](#), [ref2](#)). In most cases, AI-driven startups are born within the cradle of academic institutions, where early concepts and prototypes are developed and validated -- prior to getting funded by venture capitalists.

Another important source of advanced AI expertise for drug discovery and healthcare comes from largest technology corporations (Google, Microsoft, Tencent, etc), which are increasingly focusing on applying their technological resources for tackling health-related challenges, or providing technology platforms on project-based or rent-based conditions for conducting research analytics by life science professionals.

Some of the leading pharmaceutical giants, like GSK, AstraZeneca, and Novartis, are already making steps towards aligning their internal research workflows, hiring ML/AI/Data Science talent, and shaping development strategies to start embracing AI-driven digital transformation at scale ([ref1](#), [ref2](#) [ref3](#)). However, the pharmaceutical industry at large is still lagging behind in adopting AI, compared to more traditional consumer industries -- finance, retail etc.

The above three main trends are driving the growth in the AI implementation in pharmaceutical and advanced healthcare research, but the overall success depends strongly on the presence of highly skilled interdisciplinary leaders, able to innovate, organize and guide in this direction.

# The existing challenge of hiring top ML/AI talent in pharmaceutical setting

It comes as no surprise that talent acquisition and team building appears to be among the most challenging parts in the whole strategy of AI adoption by pharmaceutical companies and drug discovery organizations. All the complexity, in this case, arises from the fact that drug discovery and healthcare are the complex areas of knowledge requiring years of theoretical training and practical experience to understand how to model them in the ML/AI-driven fashion. In other words, it is not possible to efficiently apply ML/AI skills for this kind of tasks without certain level of domain expertise to understand data semantics, proper features and general ontologies. This is, indeed, very different from “traditional” AI tasks, like the image processing, where the object of modelling is easily understandable without deep expertise (images are simply matrices of pixels with color attributes). In contrast, to comprehend datasets from, say, gene expression studies in the context of identifying novel biological modulators, or genetic polymorphism in the context of studying various types of pathogenesis in species, requires a deep knowledge in biology, genetics etc.

In the same time, the ML/AI in itself is a complex multidisciplinary domain of knowledge, requiring strong foundations in Statistics and Probability Theory, Calculus and Linear Algebra, Data Analytics and specialized topics like Graph Theory, advanced programming skills, and hands-on experience in developing, training and deploying ML models in distributed environments (clouds).

In addition to the above technical and research “hard” skills, a number of “soft” skills is usually sought to complement a portrait of an “ideal candidate” for leadership roles to adopt AI in pharmaceutical organizations. They include leadership, project/product management experience, executive experience, or experience running industrial grade projects.

The above unique set of requirements explains well substantial scarcity of highly skilled talent in this area, and in the same time, it conditions highest “price tags” for specialist of this kind: we predict that AI specialists with substantial domain expertise in Life Sciences will become some of the most highly paid employees in the world within several years.

More practically, pharma organizations will be attempting to solve the need of “dual” expertise in ML/AI and Life Sciences by creating highly interdisciplinary teams bringing together experts from ML/AI and Life Sciences and making them communicate and collaborate closely. Yet, even this scenario requires a leader, or a group of leaders, with strong foundations in both areas to create an integral vision of a project and make sure both “camps” collaborate efficiently.

# The goal of the report

In order to understand how to build efficient interdisciplinary teams able to deliver meaningful milestones on the road to the AI-driven transformation of drug discovery and healthcare organizations, it is crucial to analyze the existing examples of accomplished leaders in this area, their backgrounds, technical skill-sets, strengths, competencies, roles in the organizations, and types of impact they have on the industry in general.

The current report summarizes the TOP 100 most innovative and entrepreneurial AI leaders, who has been contributing largely towards data-driven transformation of the pharmaceutical and healthcare industries. It has a goal of providing a “bird's view” on the global leadership scene in the area of adopting ML/AI-driven methods in drug discovery and healthcare to serve as a benchmark tool for shaping successful talent acquisition strategies.

# Report Methodology

The list of 100 artificial intelligence (AI) leaders in drug discovery and advanced healthcare is based on the assessment of the cumulative impact (CI) that a person contributed to the advancement of the AI technologies in the area of pharmaceutical research (basic biology research, drug discovery and development, drug repurposing etc), and healthcare research (diagnostics, medical data management, therapy prescription etc).

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Another prerequisite for the inclusion in the TOP 100 AI Leaders list was the availability of an outstanding achievement in either AI, or Life Sciences **in the context of applying AI for solving Life Science tasks**, including:

- Notable innovation, technological breakthrough, considerable advancement of the tech state-of-the-art
- Notable impact on research (very high level of citations etc)
- Notable organizational or entrepreneurship achievements (founding or C-level leadership of startups or mature companies with high level of investment/market cap, impactful non-for-profit organizations, or academic institutions)
- Notable thought leadership achievements (impactful books, articles, public activity etc)

# Report Methodology

The initial large pool of candidates (around 500) for the TOP AI Leaders list has been selected from multiple sources including:

Top pharmaceutical and healthcare AI conference program lists

Google Scholar

Databases

Google News and PR-distribution services

Companies websites

And based on the analysis of the descriptive criteria (personal page descriptions, biographies, LinkedIn and Bloomberg pages, public awards, article titles, news and PRs, and other text resources) and formal numerical metrics (number of research citations in Google Scholar, RG score in ResearchGate, number of books/talks and articles, social media activity etc).

The initial pool of around 500 top candidates has been shortlisted down to the top 100 list following an iterative approach, starting with the obvious differentiating parameters (top tech or business achievements or highest number of citations) and gradually specifying additional parameters for the final rating.

## The rating calculation model

Is a first-order homogeneous polynomial which calculates person's assessment variables and their relative impact weights (coefficients). The weights of each variable have been logically designed to underline major contributions and impact (innovations, business achievements, research citations etc) and only augment them with less important, yet valuable, contributions (conference talks, social media activity etc).

# Key report observations

## Where do TOP-100 AI leaders reside?

It might come as no surprise that the USA and UK still remain home for the largest number of top AI experts in pharmaceutical and healthcare R&D sectors with 68% and 31% of list TOP 100 list participants residing there, respectively (see [Distribution by Countries](#)). Being major innovation hubs, San Francisco, Boston, New York and London are topping the list of cities with the largest numbers of TOP 100 AI leaders working there.

A particular attention should be given to China. While formally it has a small count of participants from the TOP 100 AI leaders list (only 2), the real potential of this country in data-driven pharmaceutical and healthcare research is among the biggest. The currently underrepresented position of China is explained by a relatively recent explosion of the AI talent in this country, while the list of TOP 100 AI leaders has an emphasis of the historical achievements (USA and UK historically were home to many pioneering advances in the field) and currently recognized leadership positions (rather, than potential for the future). Secondly, all Chinese experts working in Western offices of Chinese companies and residing in USA or UK were associated with those countries to increase their score.

We predict, that this statistics may substantially change over the coming years in favor of China, firstly -- due to a strong government support for AI-driven healthcare and pharma initiatives, secondly -- due to relatively lower bureaucratic and regulatory barriers for "controversial" research, and thirdly -- due to an emerging trend for a "reverse migration" of Chinese top experts from Western countries back to China.

# Key report observations

## Where do TOP-100 AI leaders work?

It was found that the majority of the TOP 100 list participants work in academia (43%), which is predictable -- academia has traditionally been a cradle of the innovative thought not only in drug discovery, but also in the theoretical and practical aspects of ML/DL/AI in the context of the application for drug discovery and biomedical research. The impact of AI leaders in this category is usually characterized by:

- High number of peer-reviewed publications
- High level of citation (high h-index and i10-index, RG score in ResearchGate -- if applicable)
- Pioneering roles in a particular area of theoretical or engineering aspect of ML/AI for drug discovery
- Availability of a notable theoretical breakthrough, technical invention, or widely adopted commercial model

Founders and top research executives of the AI-driven drug discovery startups constitute the second largest group (30%) of leaders in the TOP 100 list. The abundance of the emerging companies in this area is a consequence of an increasing demand for the AI-driven solutions from the side of pharmaceutical companies. Those AI leaders who advance the industry thought their entrepreneurial ambitions are usually characterized by the following set of demonstrated abilities:

- Outstanding business leadership in the area of introducing AI for drug discovery/biotech/healthcare
- High level of interdisciplinary expertise in both hi-tech and life sciences to realize an integral vision of their projects
- Publicly active position, thought leadership activity

# Key report observations

15% of the AI-leaders in the TOP 100 list work in the largest pharmaceutical companies, which reflects a somewhat slow change in the perception of “big pharma” regarding ML/AI-related opportunities. However, we expect substantial expansion of this category in the nearest time – as pharma becomes more striving for AI-talent and leadership. Leaders in this category includes top pharmaceutical executives, who possess substantial influence on the fate of adopting ML/AI-driven strategy in their organizations, and already made practical steps towards this vision. Typical features of the participants in this group include:

- C-level executive role, or leading research role in some of the largest pharmaceutical companies
- Strong background in digital technologies, cheminformatics/bioinformatics
- Strong technology leadership ability
- Knowledge of ML/AI (either career major, or as an additional training)

The rest of the leaders in the TOP 100 list are from the world’s largest non-pharma technology corporations, like Google, and Tencent (7%), and companies in various uncategorised industries (5%).

Particular attention should be given to the segment “Technology Corporations” as these companies have already developed the strongest capabilities in the ML/AI available on the planet, with best-in-class IT-infrastructures. Now they are increasingly attempting to shift their focus to healthcare, drug discovery and even basic pharmaceutical research, hoping to leverage the unmatched AI expertise in a “foreign”, but very promising for them market. At this moment, technology giants are not able to enter the medicines R&D market on a meaningful scale, but things are changing rapidly. We expect, that large technology corporations might, at some point in time, substantially increase the competition pressure on the currently dominating pharma and biotech organizations. In this case, the ML/AI technologies serve as a sort of “democratizing” factor, allowing a non-pharma corporation enter pharmaceutical R&D market.

# Key report observations

The AI leaders in this category typically possess deep technological backgrounds (Computer Science, Artificial Intelligence, Data Science, Engineering, Statistics/Math), with some acquired level of expertise in life sciences. They are characterized by:

- Top level research or business leadership position at large technology corporations
- Involvement in the application of ML/AI technologies for solving pharmaceutical/healthcare tasks, leading life science-oriented projects

## What kind of roles do the TOP 100 AI leaders have?

The TOP 100 AI leaders list includes experts who have various types of contributions towards advancing AI in pharma and healthcare. 63% of all participants are primarily involved in research-related activities, while only 37% are directly involved in entrepreneurship and executive management (including research leadership) (see **Distribution by Role in the Organization**).

Going in more details, 16.8% are focusing primarily on a general business/management aspect, 46.5% are more involved in dealing with ML/AI research/technology aspect (both science and business), and 36.8% are more involved with Life Science side of things (both science and business) – see **Distribution by Primary Activity**.

All the participants of the TOP 100 AI Leaders list have enormous impact on the advancement of ML/AI innovations in the pharmaceutical industry and healthcare, which is illustratively divided into the three main types (see **Distribution by the Impact on the Industry**).

# Key report observations

## AI Science and Tech Innovators

**40%**

of the participants have directly contributed to scientific innovations and advancing technology.

## AI Thought Leaders

**38%**

contributed largely as thought leaders in the field, shaping the ideas and opportunities in an easy-to-understand messages for a wider audience of non-tech experts and decision-makers (investors, budgeting organizations, CEOs etc).

## AI Business Leaders

**22%**

are distinguished for their input in building novel companies, establishing non-profit organizations, and facilitating multidisciplinary industrial collaborations.

Concluding the review of the TOP 100 list, it becomes obvious that successful AI-leaders in pharmaceutical/healthcare fields originate from a variety of quite different backgrounds and fields of specialization, and they have a wide range of possible roles to play in the projects, ranging from purely scientific ones, to entrepreneurship and general management. It suggests that any successful AI talent acquisition strategy, aimed at a organization-wide AI adoption, has to include a wide range of different roles and departments, and not be limited to only hiring highly-specific staff to augment R&D or IT departments.

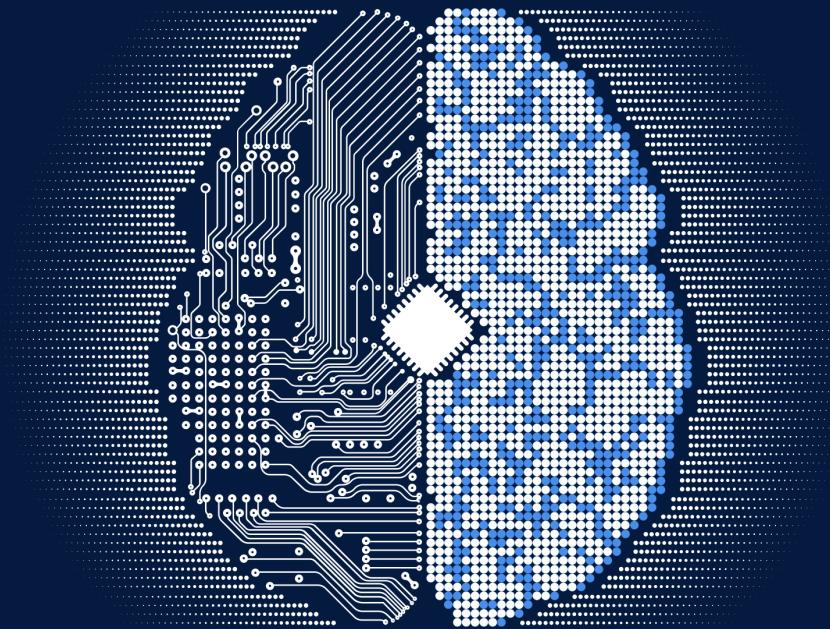
# The coming race for AI talent

Considering a rapidly increasing realization that AI-based technologies are an transformative opportunity for the pharmaceutical organizations, it is easy to predict the coming frantic race for the AI talent, especially, with experience in Life Sciences -- demand for this type of expertise will be growing to far outpace supply for years to come.

An additional constraint in the AI talent acquisition strategy will be conditioned by the growing external competition for the available talent -- as large technology giants, like Google, Microsoft, Tencent, and Amazon are increasingly focusing on the Life Sciences and healthcare. Hence, pharmaceutical giants will be competing for the available talent not only with closest pharma competitors, but also with a growing pool of pharmaceutical AI-startups, and increasingly -- with global technology corporations.

To gain momentum and set themselves for a long-term AI-driven growth, pharmaceutical corporations will have to focus on the most efficient talent acquisition strategies:

- 1. Focus on collaboration with academia:** Closer and more flexible types of collaboration with academia, since academic institutions are not only a cradle of innovation in the AI, but also the main source of scientific talent. Engaging with talented PhD-level specialists early in their career is a crucial aspect to set them for work in pharmaceutical industry, rather than letting them drift away towards careers in technology corporations. This strategy should be wisely balanced to avoid a "brain-drain" from academia -- a harmful phenomenon, with far-reaching negative implications for both science and educational process.
- 2. M&A Strategy:** Setting focus on the merger and acquisition (M&A) activity is an important component of AI-talent acquisition work. The growing wave of AI-driven drug discovery and healthcare startups are yielding highly skilled teams with strong understanding in both ML/AI and Life Sciences. We anticipate that the most successful startups in this area will soon become lucrative targets for M&A by pharmaceutical and technology corporations.
- 3. Increasing intrapreneurship culture:** Creating intrapreneurship programs and business incubators will have to become an important element of an AI-talent acquisition strategy by pharmaceutical corporations. Companies like Google are well-known for outstanding conditions for internal innovators and intrapreneurs. Pharmaceutical companies, being notoriously conservative, will have to embrace a more agile strategies regarding internal innovation and intrapreneurship.



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