



AI IN BIG PHARMA AND GUIDELINES FOR SUCCESS – ADD-ON ANALYSIS ON A PREVIOUS STUDY AND ITS COMMENTARY

REFLECTION AND ANALYSIS DOCUMENT

BASED ON:

“THE UPSIDE OF BEING A DIGITAL PHARMA PLAYER” (SCHUHMACHER, A.; GATTO, A.; HINDER, M.; KUSS, M. AND GASSMANN, O., DRUG DISCOVERY TODAY, 2020 – ORIGINAL STUDY)

“DEEP DIVE INTO BIG PHARMA AI PRODUCTIVITY: ONE STUDY SHAKING THE PHARMACEUTICAL INDUSTRY” (ZHAVORONKOV, A., FORBES, 2020 – COMMENTARY)

ZURICH, AUGUST 2020



(DISCLAIMERS)

This document has been created by Zereon Associates GmbH ("ZA") as a reflection, analysis and further development of 1) a recent, top industry experts' study / paper on the use and application of AI by large global Pharma industry players, and 2) a commentary issued on such paper by a recognized industry player (specific references and authorship on the previous Title Page above). This document, with the ultimate aim to hopefully add some value and perhaps some additional insight to both pieces of work, is distributed for free and with "open source" spirit with no further counter-obligations whatsoever by the reader, except citation, document change protection and no occultation of our authorship, as described below. The document has been created voluntarily and is offered for divulgation, public reference and ZA's general promotion purposes only, without any gainful commercial payment involved in cash or in kind by any party. After-the-fact advisory business by the author to future and current Clients derived from later discussions might be possible if interested parties so request.

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The Author & Acknowledgements



I. INTRODUCTION: THE PREVIOUS STUDIES (1)

- This document by Zereon Associates GmbH intends to be a reflection, quantitative analysis and further development of two authoritative studies, as follows below.
- In the words of Dr. Alex Zhavoronkov, recognized expert in healthcare & biotech AI, Insilico Medicine Founder & CEO, and Forbes collaborator:

“Some (...) pharmaceutical companies managed to demonstrate very impressive results (**in AI since 2013-14**)”.

“However, it was **not possible to get a comprehensive overview** and comparison of the **major pharmaceutical companies (in AI) (...) until now**”.

“On June 15th (2020), one article (...) quietly went online in a reputable peer-reviewed journal (...)”

Upon a closer look it turned out to be (...) a comprehensive research study with **a head-to-head comparison of the pharmaceutical companies** by their efforts in **AI in research and development**”.

“The authors of the study certainly deserve to be referred to as industry experts in the pharmaceutical AI R&D as they did a **gargantuan amount of work** to compile the three relatively simple figures in the study and **at the moment no other study like that exists**”.

“The upside of being a digital pharma player” (Schuhmacher, A.; Gatto, A.; Hinder, M.; Kuss, M. and Gassmann, O., Drug Discovery Today, 2020)



I. INTRODUCTION: THE PREVIOUS STUDIES (2)



- Dr. Zhavoronkov, on top of the above quotes and in his own “**Deep Dive Into Big Pharma AI Productivity: One Study Shaking The Pharmaceutical Industry**” (Forbes 2020), reflects profound commentary and interviews with the original paper authors, expanding on global Pharma AI “state of the art”.



- The present document attempts to serve as quantitative **add-on analysis** to both works, and maybe **offer some more interesting insight and benchmark to industry players and/or interested parties**.



- To do so, we 1) review some additional literature, 2) take part of the data published in the studies referred, 3) add more stats, regressions, etc. and 4) generate conclusions on the analysis.



- Part of the analysis and conclusions might overlap with the published work – but we hope we have been able to provide a **new, complementary perspective** and obtain **relevant and useful findings**, nonetheless.



- In the next pages we offer an Executive Summary, and then details of our analysis. As Annexes, we show some additional information on AI funding and technological companies active in AI Life Sciences R&D.



II. EXECUTIVE SUMMARY (1)

N. of AI-based scientific Publications for the 21 global Pharma companies studied:

In general explained away (80%+) simply by the N. of AI-related activities implemented.

(under the model used - statistically significant no-intercept linear regression and R² analysis).

Interestingly, however, N. of AI-external activities taken alone seem to be an even better predictor (85%+) of total N. of AI-based Publications than the total N. of AI activities.

(“external activities”: sum of joint ventures, alliances, acquisitions, cooperation with startups and other companies, etc.).

Companies can expect to get ca. 2.54 Publications per each AI-activity developed, on average

- but differences do exist b/w higher and lower apparent “AI Productivity” companies.

A closer analysis of regressions and R² shows that:

Drug Discovery Publications might be best pursued by a mix of preferentially AI External with some selective Internal initiatives.

Whereas Drug Development and Other AI could be done mostly externally.

Two clusters of companies, according to Publication Productivity Ratios (N. of AI-based Publications per each AI-related activity):

Higher Productivity Companies (10)

3.4-7.0 AI publications per each AI activity; group average = 4.4

67% of their total AI activities are External, vs. 33% Internal.

8 of 10 companies have more External activities than Internal.

7 of 10 companies are US/UK headquartered.

Lower Productivity Companies (11)

0.0-2.5 AI publications per each AI activity; group average = 1.5

53% of their total AI activities are Internal, vs. 47% External.

8 of 11 companies have more Internal or at least an equal number of activities than External.

Almost equally US/UK and non-US/UK headquartered (6 vs. 5).

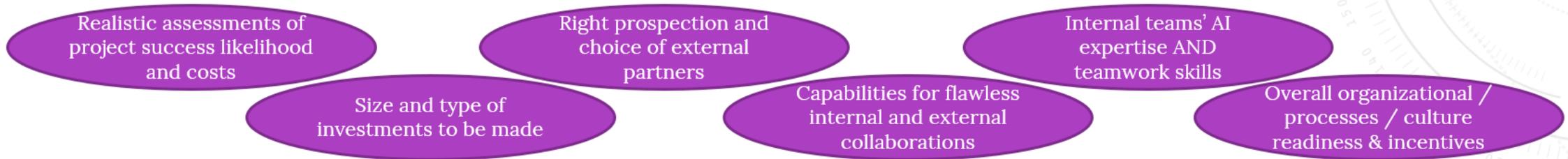


II. EXECUTIVE SUMMARY (2)

Where to go ? Depends on Company strategy, business plans and objectives, etc., but three AI decision-making areas may be of interest:



Influencing factors to consider regarding External / Internal activities to undertake in those areas could be:



Our study concludes that **more successful Companies mostly liaise with External ones** – those may have **more immediate or superior AI technical firepower or data**, especially for Drug Development/Other AI. For Drug Discovery, preferentially External with selective Internal AI may work best.

Regarding specific companies' AI success, we would suggest the following guidelines / best practices (details in the document):



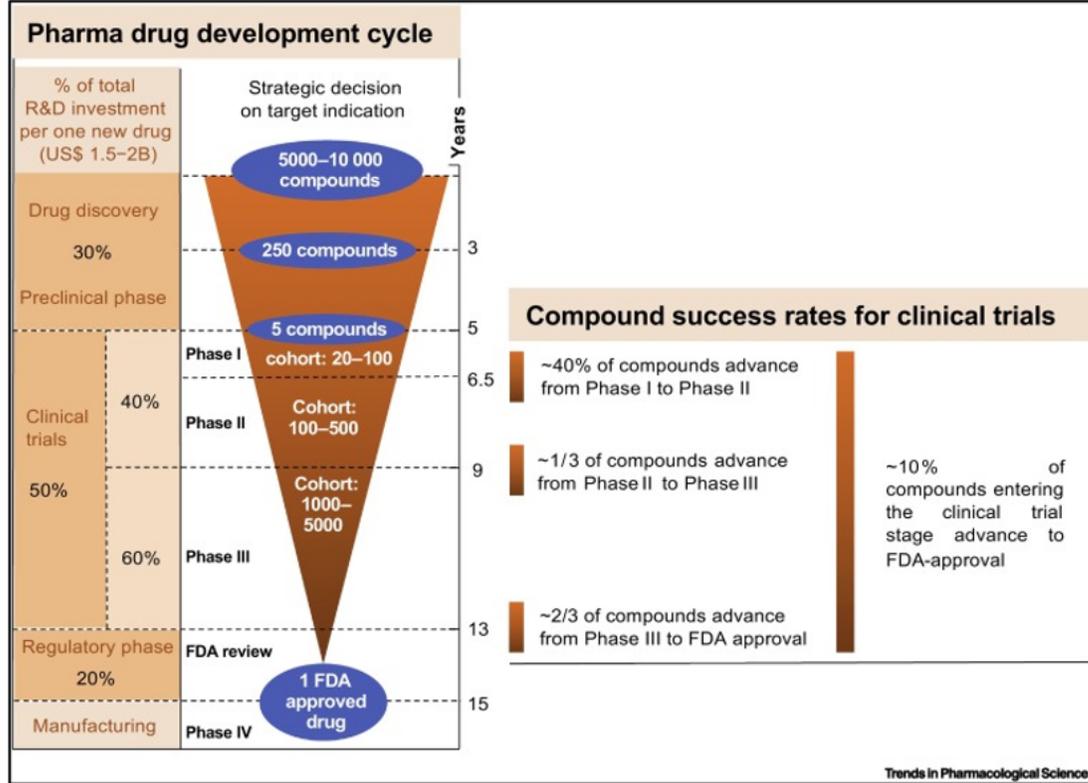
The most successful Companies are not waiting to leverage on External efforts for improved AI results. Those companies are, at the same time, transforming themselves quickly.

Such transformation requires add-ons to classic Pharma industry practices, new profiles / capabilities, and new ways of working. Companies will need to put agile change plans and initiatives in place, facilitated by internal and external experts to help with the journey.

The prize may not just be the delivery of an astounding economic value and a superior competitive position, but an opportunity to improve/save more people's lives – or even indeed win Nobel prizes and change the world itself.

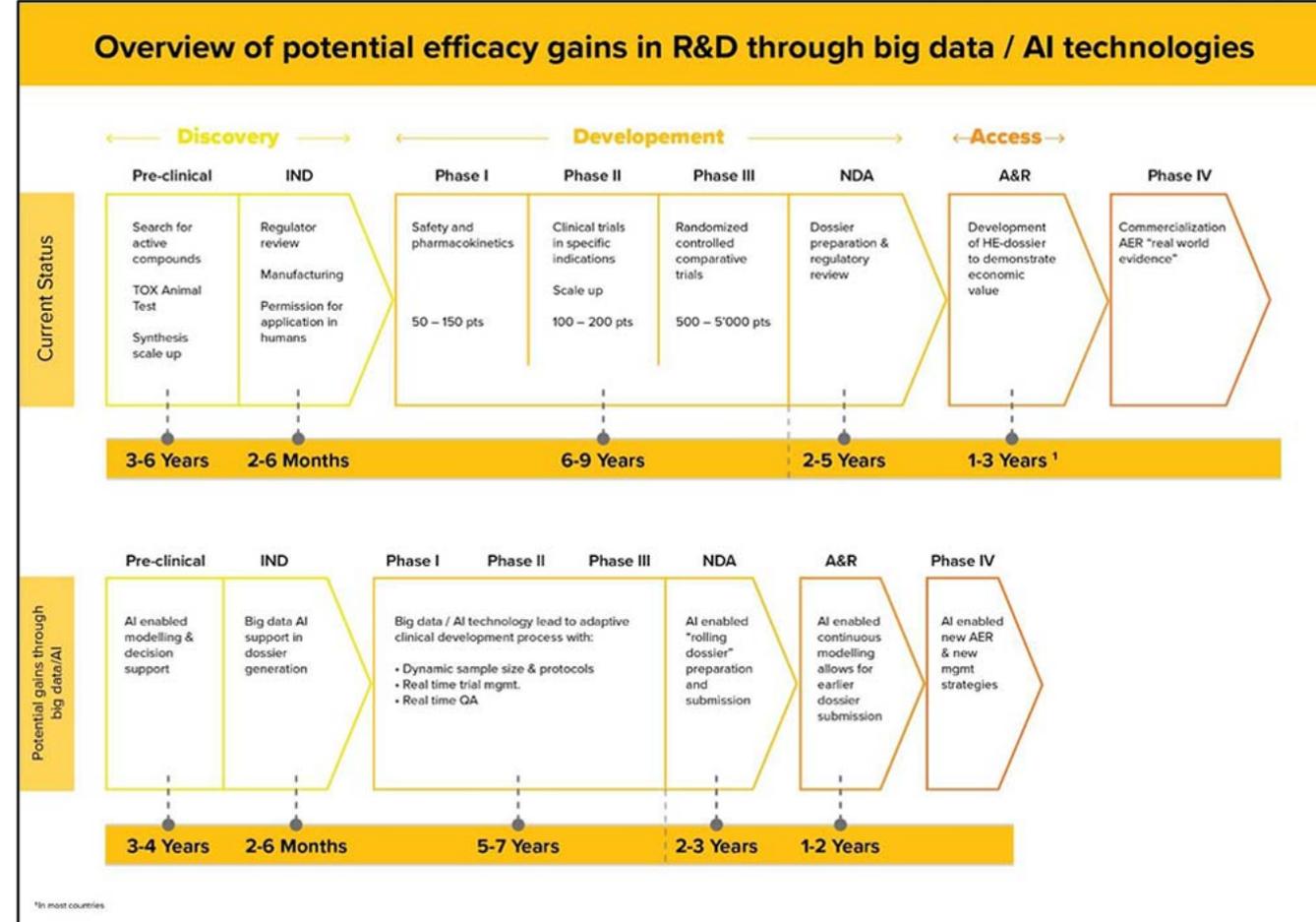


III.CONTEXT: SOME PRIOR OVERALL INDUSTRY INFORMATION



Sources: "Artificial Intelligence for Clinical Trial Design"; Trends in Pharmacological Sciences; Harrer, S., Shah, P., Antony, B., Hu, J.; Aug. 2019.

"The Impact of Digitalization and AI on Research and Development in the Biopharmaceutical Industry"; Innoplexus (blog), Jul. 2020.



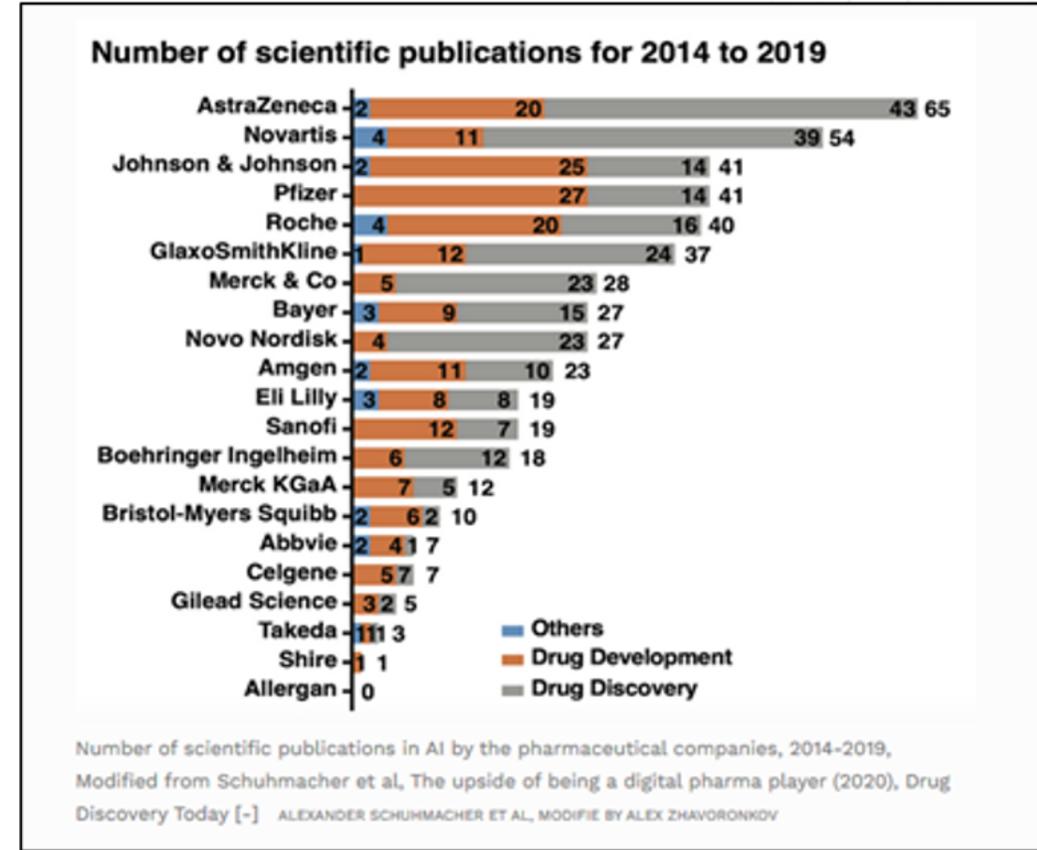
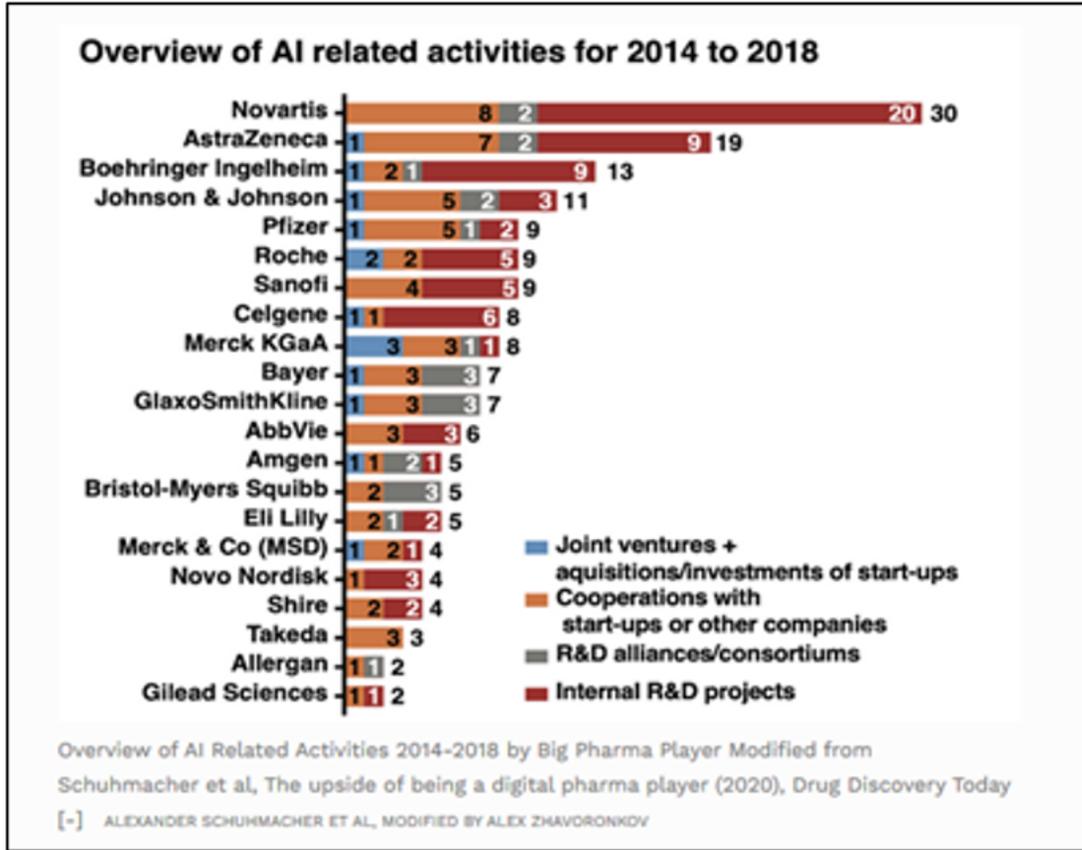
"It takes up to 15 years and an average R&D of 1.5-2 bill. USD to bring a drug to market. In the US, only one of 10 compounds entering trials advances to FDA approval. High trial failure rates are one major cause."

AI may shorten the whole cycle (and related cost) by 2-4 years - and is already helping discover, distribute and sell new compounds, realize trials, etc.

Global Pharma companies deploy different AI activities, which if successful are normally reflected on AI-related scientific Publications (see next slide).



IV. BASIC PHARMA COMPANIES' DATA USED (1)



- These data pieces, in themselves, are already excellent findings on AI in the Pharma industry, as a whole and as per individual company.
- We proceed on from there to a) see if there is relevant correlation, or not, between N. of AI-related activities implemented 2014-18, and N. of AI-based scientific publications 2014-19, b) drill down by type of activity (external / internal) and type of publication, c) analyze apparent Productivity (Ratio of Publications' per each Activity) and d) see if there is some pattern / basic clusterization among companies.
- We will be mostly using no-intercept simple linear regression models, which reveal to be statistically significant in all cases. Other models such as logarithmic, multiple linear regressions, etc. could be applicable, but data shape generally indicates appropriateness of model overall.

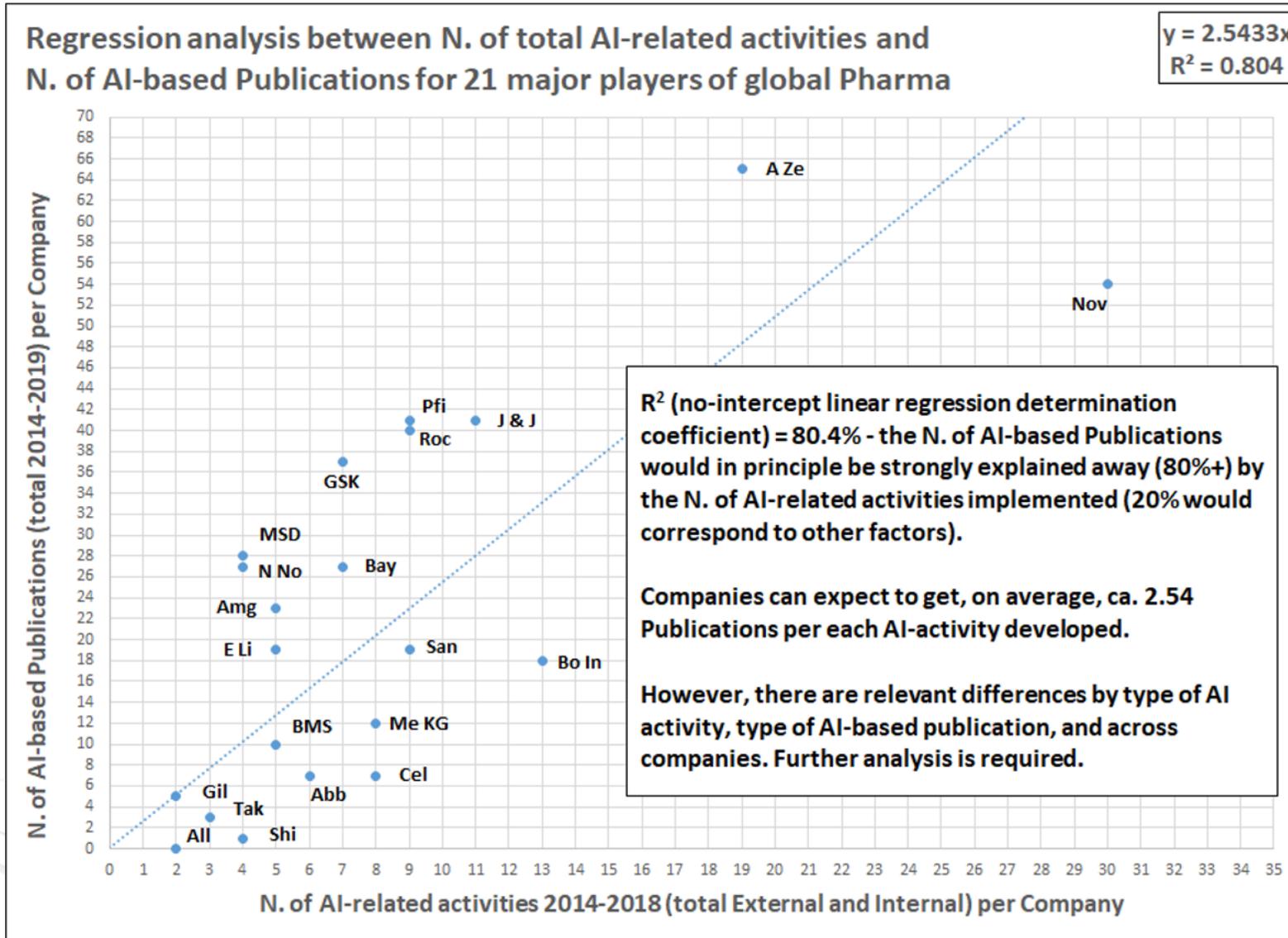


IV. BASIC PHARMA COMPANIES' DATA USED (2)

TABULATED DATA:

	Startups' Acq/JVs	Cooperation startup or Cny	R&D Alliances	External Activities	Internal Activities	E>I	AI-related activ. 2014-18	Drug Discovery	Drug Developm.	Other	AI-based Publi- cations 2014-19	Apparent Productivity Ratio
Astra Zeneca	1	7	2	10	9	1	19	43	20	2	65	3.4
Novartis	0	8	2	10	20	-10	30	39	11	4	54	1.8
Pfizer	1	5	1	7	2	5	9	14	27	0	41	4.6
Johnson & Johnson	1	5	2	8	3	5	11	14	25	2	41	3.7
Roche	2	2	0	4	5	-1	9	16	20	4	40	4.4
GlaxoSmithKline	1	3	3	7	0	7	7	24	12	1	37	5.3
Merck & Co (MSD)	1	2	0	3	1	2	4	23	5	0	28	7.0
Novo Nordisk	0	1	0	1	3	-2	4	23	4	0	27	6.8
Bayer	1	3	3	7	0	7	7	15	9	3	27	3.9
Amgen	1	1	2	4	1	3	5	10	11	2	23	4.6
Eli Lilly	0	2	1	3	2	1	5	8	8	3	19	3.8
Sanofi	0	4	0	4	5	-1	9	7	12	0	19	2.1
Bohringer Ingelheim	1	2	1	4	9	-5	13	12	6	0	18	1.4
Merck KGaA	3	3	1	7	1	6	8	5	7	0	12	1.5
Bristol-Myers Squibb	0	2	3	5	0	5	5	2	6	2	10	2.0
AbbVie	0	3	0	3	3	0	6	1	4	2	7	1.2
Celgene	1	1	0	2	6	-4	8	2	5	0	7	0.9
Gilead Sciences	0	1	0	1	1	0	2	2	3	0	5	2.5
Takeda	0	3	0	3	0	3	3	1	1	1	3	1.0
Shire	0	2	0	2	2	0	4	0	1	0	1	0.3
Allergan	0	1	0	1	1	0	2	0	0	0	0	0.0
TOTAL / AVERAGE	14	61	21	96	74	22	170	261	197	26	484	2.8

V. GENERAL REGRESSION ANALYSIS: N. OF TOTAL AI-RELATED ACTIVITIES VS. N. OF AI-BASED PUBLICATIONS

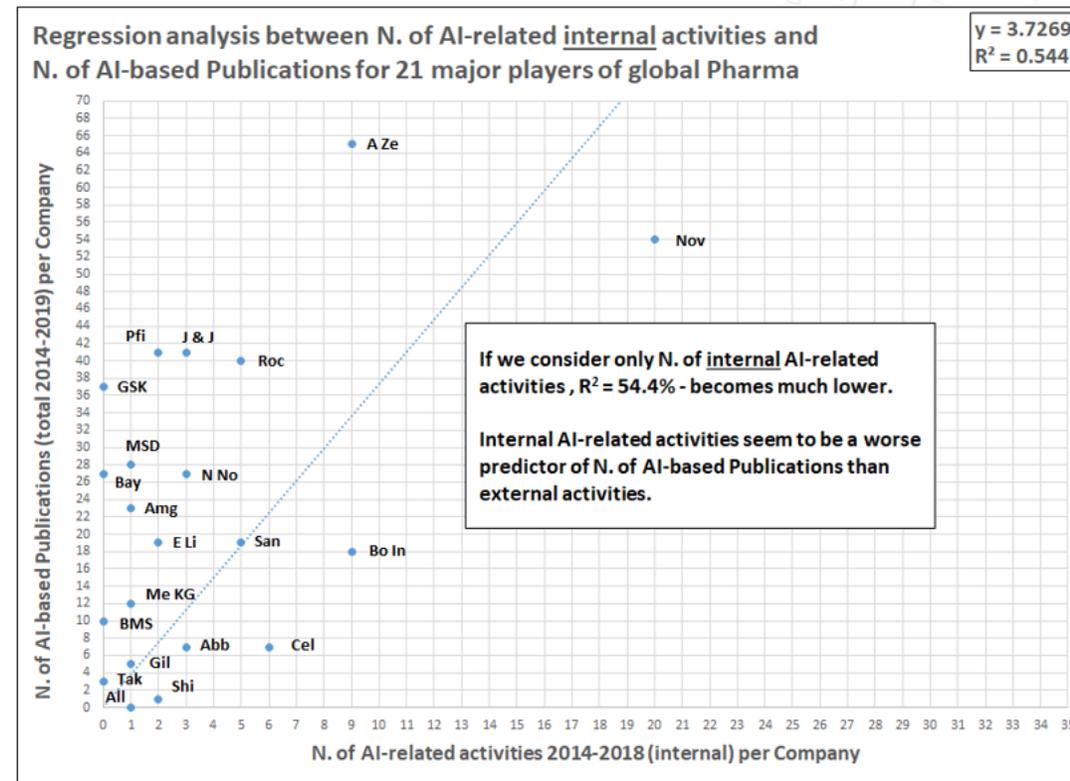
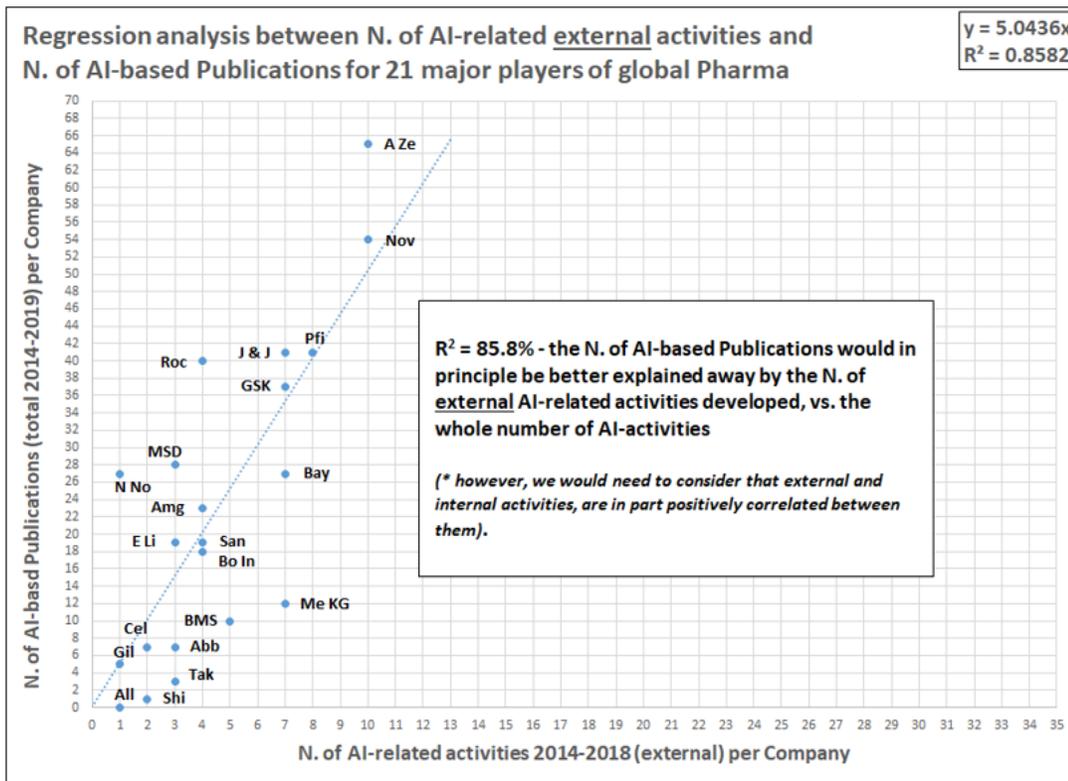


Even if some companies may be capitalizing previous years or different investment levels, expecting Publications later, etc., **intense, positive linear Correlation seems to be there**, and fits with the intuitive idea of, starting with zero, more AI-based Publications are obtained as more AI activities are put in place.

However, **the effects differ by individual company** - companies above and below the line seem to produce more or less Publications each for the same effort.

It is also **worth checking the type of activity** (external / internal), **and the type of publication** (AI in drug discovery, AI in drug development, other AI).

VI. DIFFERENTIATION EXTERNAL VS. INTERNAL AI ACTIVITIES



(We define “external activities” as the sum of JVs/Acquisitions of Startups, Cooperation with Startups or other Companies, and Participation in R&D Alliances)

N. of AI-external activities taken alone seem to be a better predictor of total N. of AI-based Publications than the total N. of AI activities. Internal activities alone are less accurate predictors of total Publications generated.

This fits overall with the conclusions of the main study and its commentaries.

VII. ANALYSIS OF IMPACT ON AI-BASED DRUG DISCOVERY, DRUG DEVELOPMENT AND OTHER PUBLICATIONS



<i>(Apparent strength of relationship - Determination Coefficients of No-Intercept Linear Regressions)</i>	TOTAL OF AI-BASED PUBLICATIONS	IN DRUG DISCOVERY	IN DRUG DEVELOPMENT	IN OTHER AI
N. OF EXTERNAL AND INTERNAL AI ACTIVITIES	80.4%	77.0%	62.0%	54.7%
<i>(Expected N. of Publications per Activity)</i>	2.54	1.48	0.93	0.13
<i>N. OF EXTERNAL ACTIVITIES ALONE</i>	85.8%	73.4%	78.6%	56.7%
<i>N. OF INTERNAL ACTIVITIES ALONE</i>	54.4%	59.0%	33.6%	38.2%

(* All figures statistically significant at the 95% confidence level)

Out of 2.54 AI-based Publications on average expected per AI activity developed (apparent Productivity Ratio), in principle **we could expect 1.48 AI-based Drug Discovery Publications, 0.93 Drug Development ones, and 0.13 Others** (but obviously, this depends on specific activity developed, company, etc.).

N. of AI-based Drug Discovery Publications is in principle **best predicted by the N. of total AI activities** (external and internal) – ($R^2= 77.0\%$), even if N. of External activities alone apparently also works well ($R^2= 73.4\%$).

However, **N. of AI-based Drug Development and Other Publications** is in principle **best predicted by the N. of external AI activities alone** – ($R^2= 78.6\%/56.7\%$), vs. total N. of activities. Internal activities taken alone even seem to be weak predictors.

According to all this, **AI Drug Discovery Publications might be best pursued by a combination of predominantly External with some selected Internal initiatives**, whereas **Drug Development and Other AI could even be done mostly externally**.

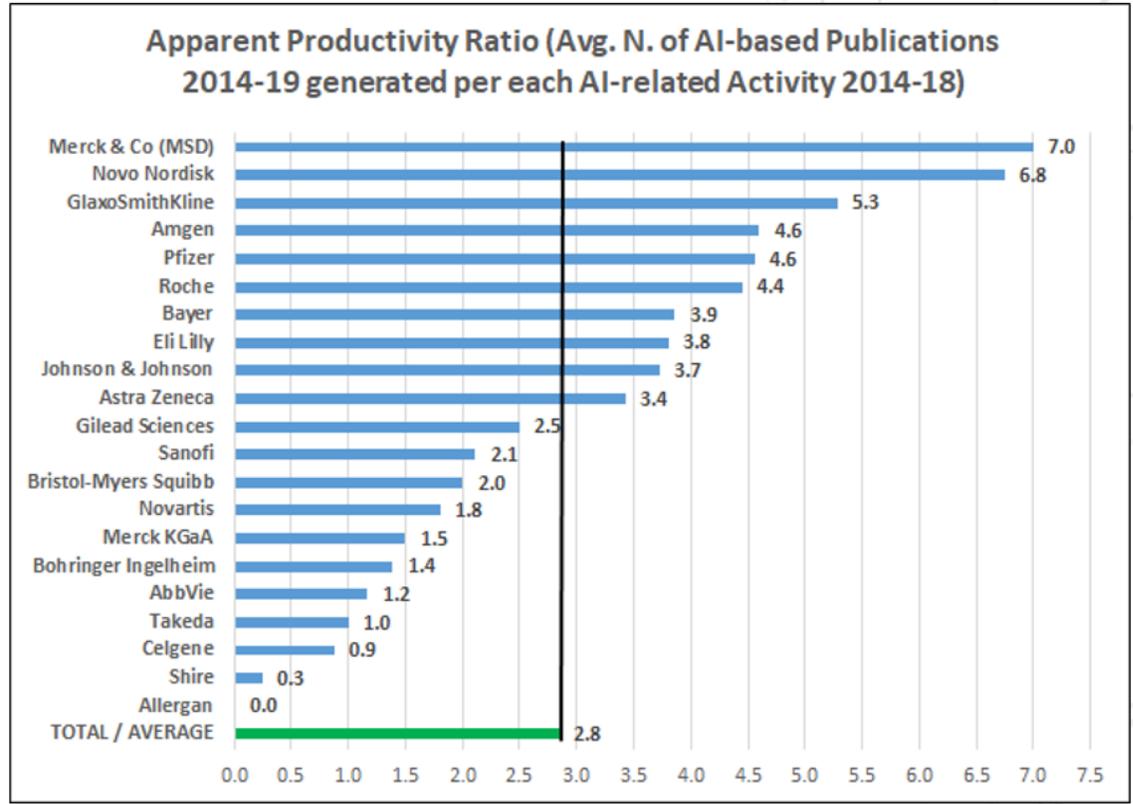
VIII. APPARENT PUBLICATION PRODUCTIVITY AND COMPANY CLUSTERS (1)



Higher apparent AI Productivity Companies

Lower apparent AI Productivity Companies

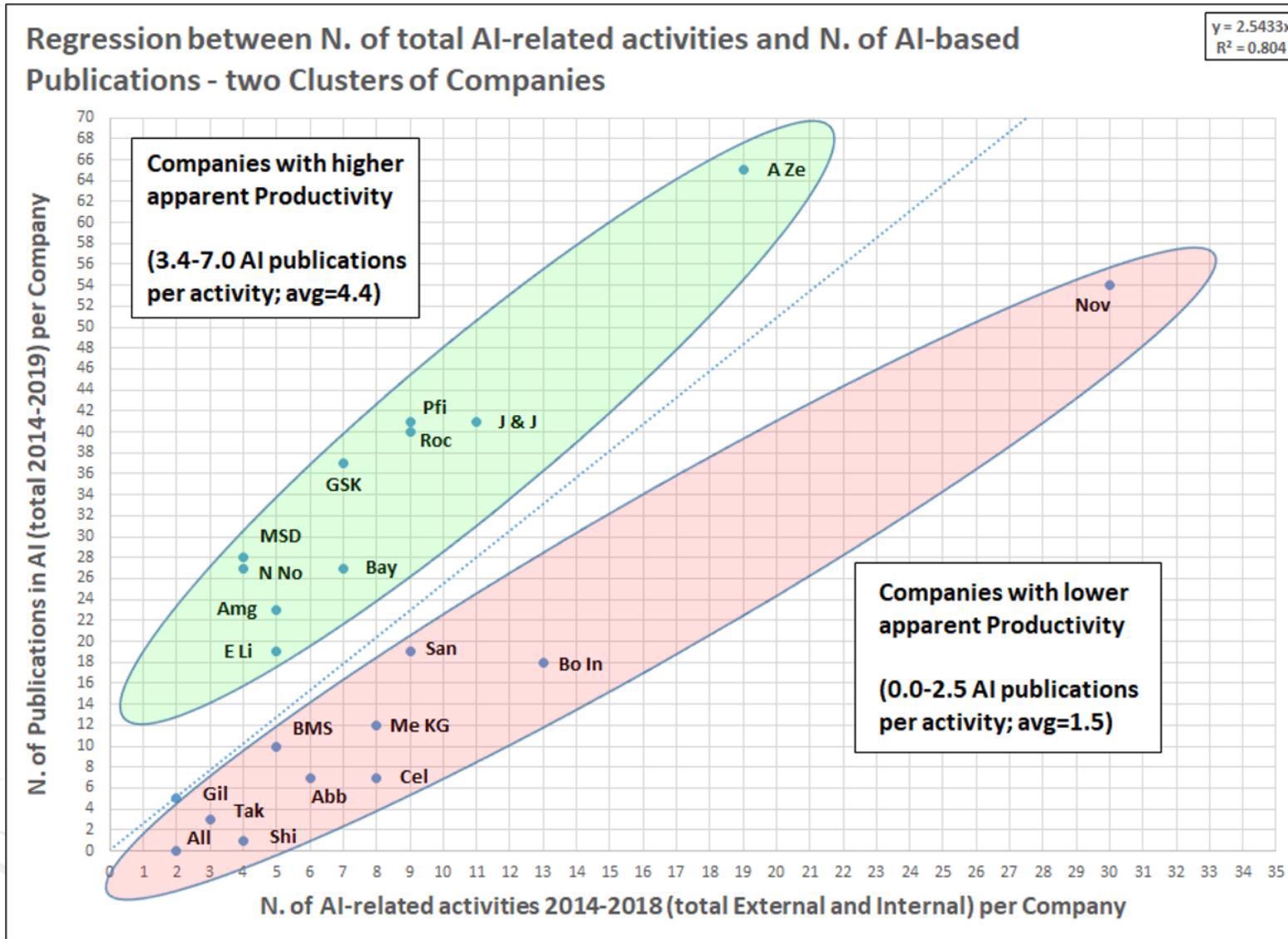
	AI-related activ. 2014-18	AI-based Publications 2014-19	Apparent Productivity Ratio	
Merck & Co (MSD)	4	28	7.0	4.4
Novo Nordisk	4	27	6.8	
GlaxoSmithKline	7	37	5.3	
Amgen	5	23	4.6	
Pfizer	9	41	4.6	
Roche	9	40	4.4	
Bayer	7	27	3.9	
Eli Lilly	5	19	3.8	
Johnson & Johnson	11	41	3.7	
Astra Zeneca	19	65	3.4	
Gilead Sciences	2	5	2.5	1.5
Sanofi	9	19	2.1	
Bristol-Myers Squibb	5	10	2.0	
Novartis	30	54	1.8	
Merck KGaA	8	12	1.5	
Bohringer Ingelheim	13	18	1.4	
AbbVie	6	7	1.2	
Takeda	3	3	1.0	
Celgene	8	7	0.9	
Shire	4	1	0.3	
Allergan	2	0	0.0	
TOTAL / AVERAGE	170	484	2.8	



Looking into comparative apparent **Publication Productivity Ratios** (defined as avg. N. of AI-based Publications 2014-19 generated per each AI-related Activity 2014-18), **differences across companies seem to exist.**

We intend to find out if the **companies cluster themselves according to these ratios** in some way, and if there is some **“common denominator” in the companies inside** each of those possible clusters.

VIII. APPARENT PUBLICATION PRODUCTIVITY AND COMPANY CLUSTERS (2)

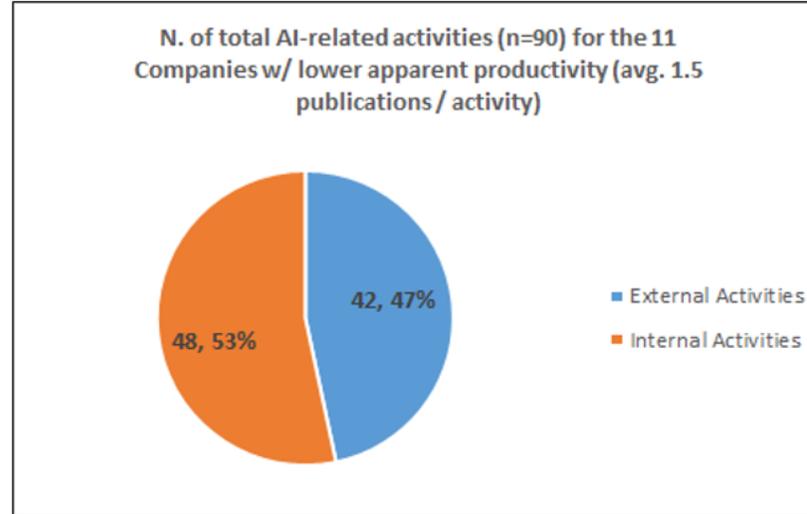
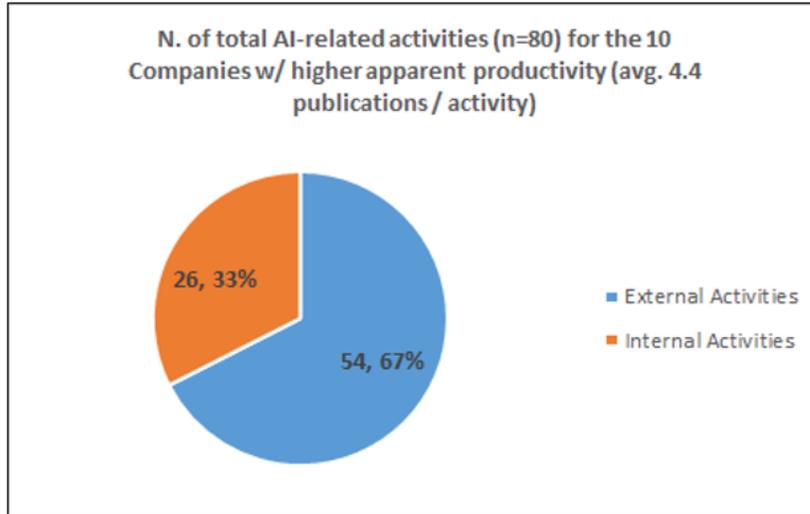


Choosing the no-intercept linear regression line as a very simple yet quite distinct way of separating companies, reveals that **there could basically be two company clusters as per Productivity Ratio.**

(* Other, more sophisticated Machine Learning clustering techniques such as k-means, support vector machines, etc. could be used – but the results might be similar, with the exception perhaps of Astra Zeneca and Novartis).

With these two basic clusters, **Publications would follow two Productivity patterns** (higher vs. lower) – and possibly **there can be differences in internal vs. external approach chosen, and other factors.**

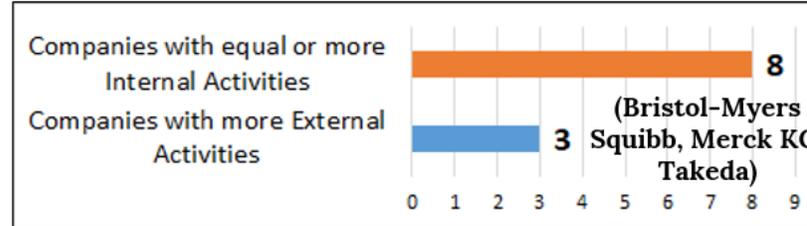
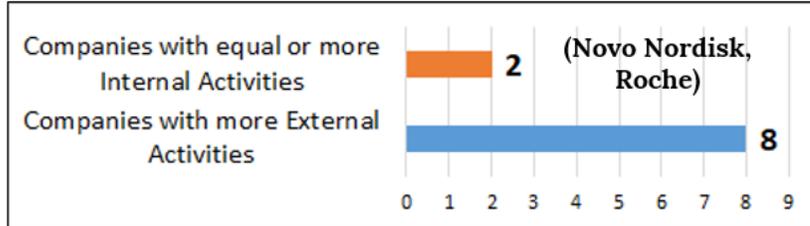
IX. HIGHER/LOWER APPARENT PRODUCTIVITY COMPANIES' CHARACTERIZATION (1)



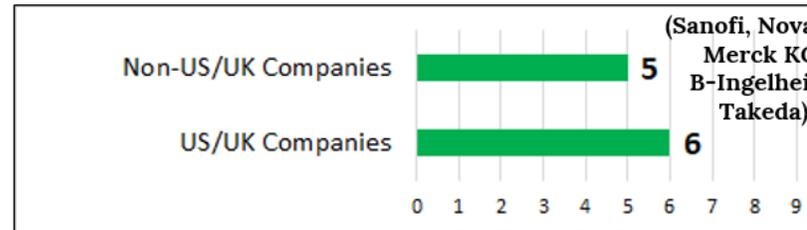
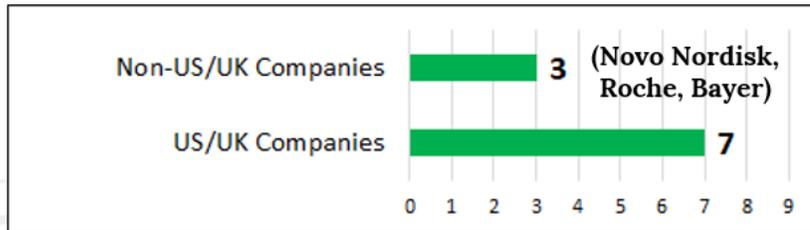
67% of the total AI activities by the companies with the higher Publication Productivity Ratios are External, and 33% Internal.

8 of 10 companies have more External activities than Internal.

Most companies in the first group (7 of 10) are US/UK headquartered.



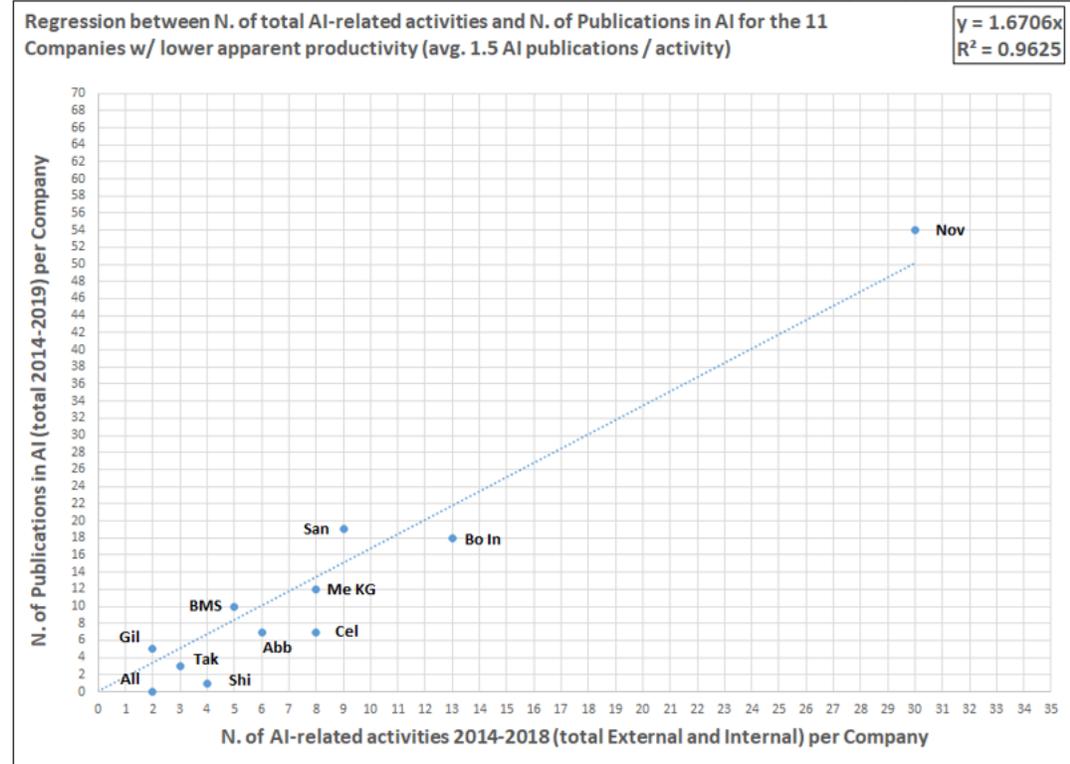
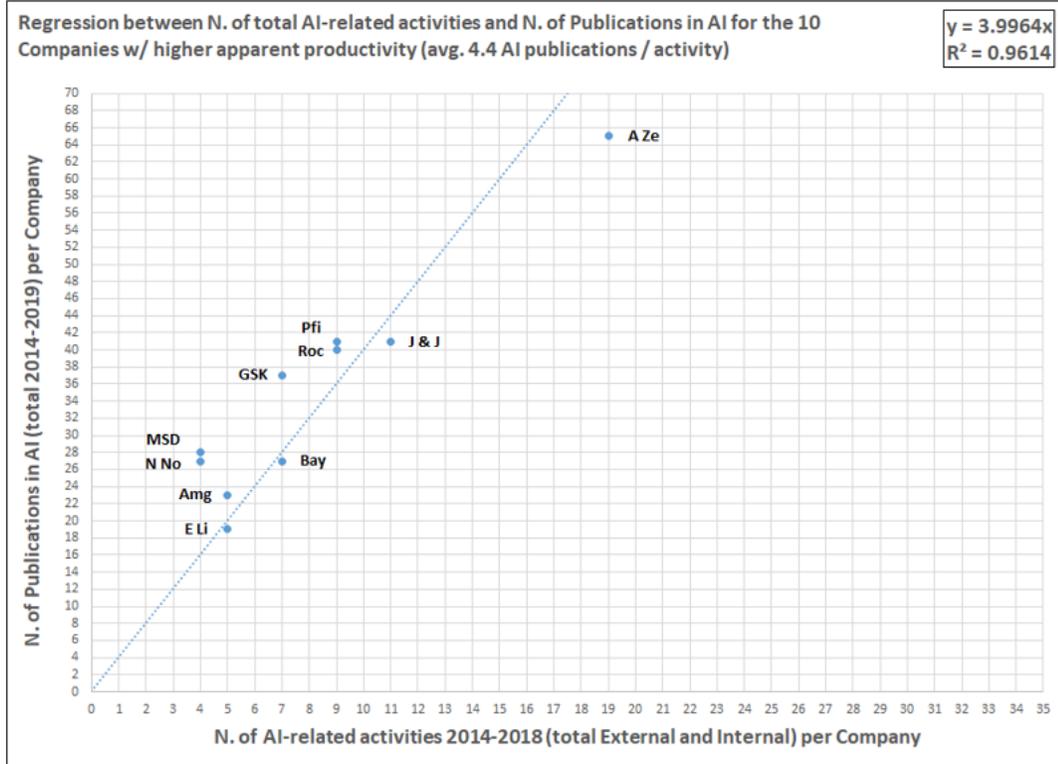
As opposed to the above, 53% of total AI activities by companies with the lower Publication Productivity Ratios are Internal, vs. 47% External.



8 of 11 companies have more Internal activities, or at least equal, than External.

Companies in the second group are almost equally US/UK and non-US/UK headquartered.

IX. HIGHER/LOWER APPARENT PRODUCTIVITY COMPANIES' CHARACTERIZATION (2)



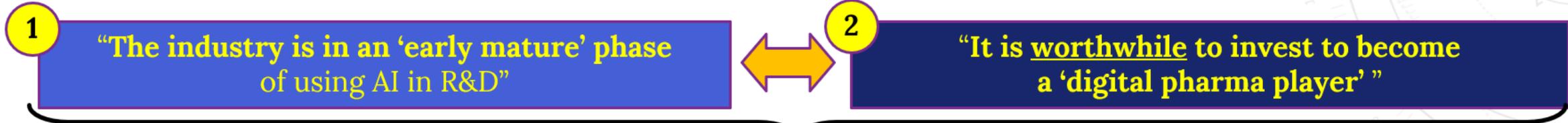
The clusterization made appears to have a very high degree of robustness if we separate higher and lower Productivity companies ($R^2 = 96.14\%$ and 96.25% , higher than the unclustered 80.4%), in itself and on top of the respective different nature of activities (External vs. Internal) and to a lesser extent, company origin (UK/US vs. non-UK/US).

Higher Productivity companies may possibly expect ca. 4 AI-related Publications per each AI activity, vs. ca. 1.7 for lower Productivity ones.

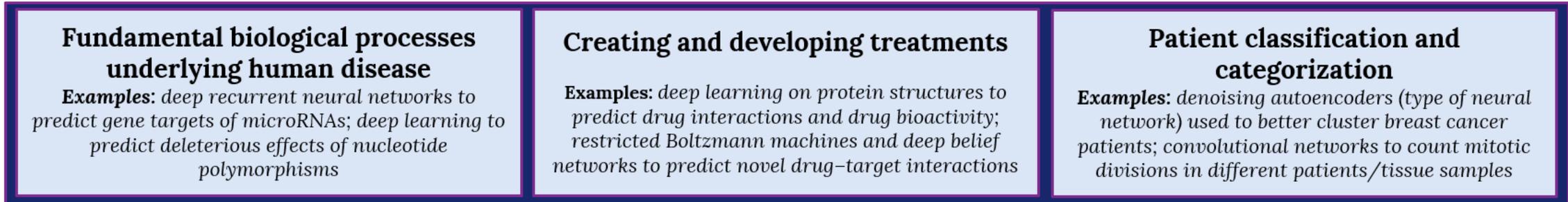
X. POSSIBLE DECISION-MAKING AREAS FOR COMPANIES AND FACTORS TO CONSIDER



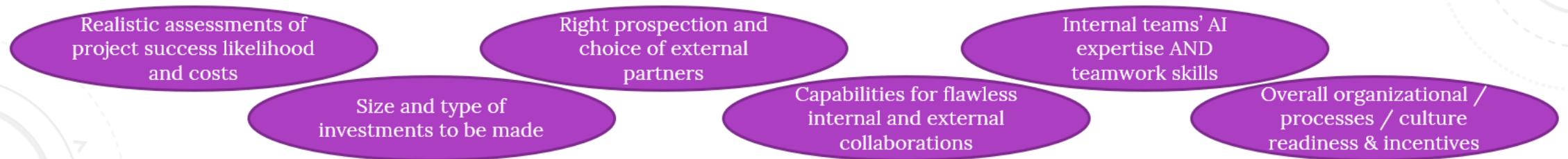
Schuhmacher et al. (2020) very clearly put it forward, after their very exhaustive research comprising analysis of annual company reports, investor relations information, patent applications, and scientific publications, about the 21 Pharma ‘blue chip’ companies referred for the years 2014 to 2019:



Where to go ? Depends on Company strategy, business plans and objectives, etc., but three AI decision-making areas may be of interest:
(Source: “Opportunities and obstacles for deep learning in biology and medicine”; Ching, T. et al. (crowdsourced paper); The Royal Society; April 2018).



However, as we have seen and as far as AI Publications go, Companies have had different outcomes, for different reasons. Influencing factors to consider regarding External / Internal activities to undertake in those areas could be:



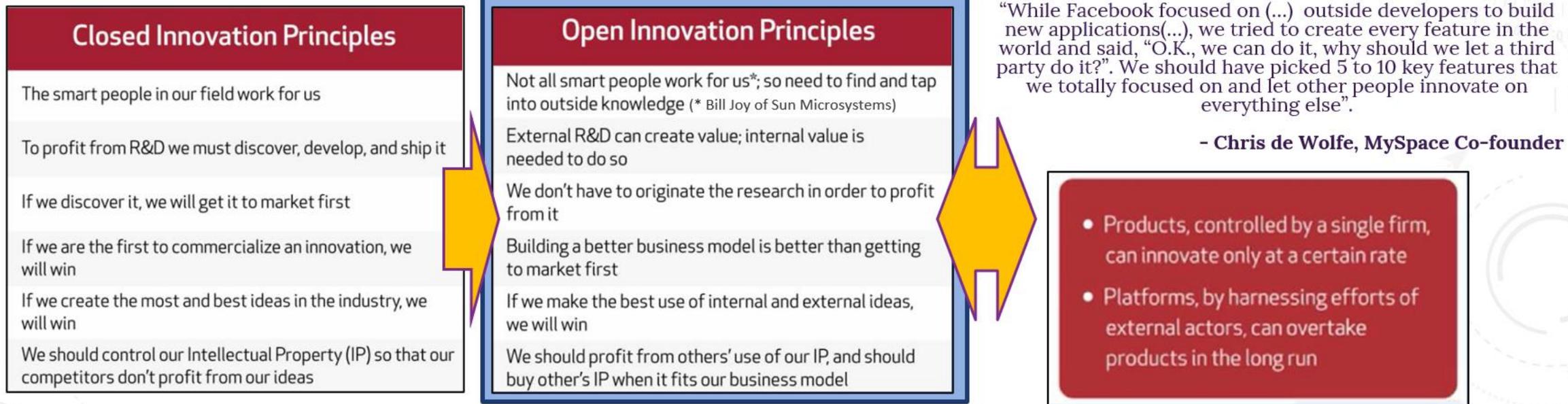
XI. PROPOSED GUIDELINES FOR SUCCESS, BEST PRACTICES AND CONCLUSIONS (1)



Our study concludes that **more successful Companies mostly liaise with External ones** - those may have **more immediate or superior AI technical firepower or data sets**, especially for Drug Development/Other AI.

For Drug Discovery, preferentially External with selective Internal AI may work best.

This fits with other ideas and approaches on modern R&D / innovation :

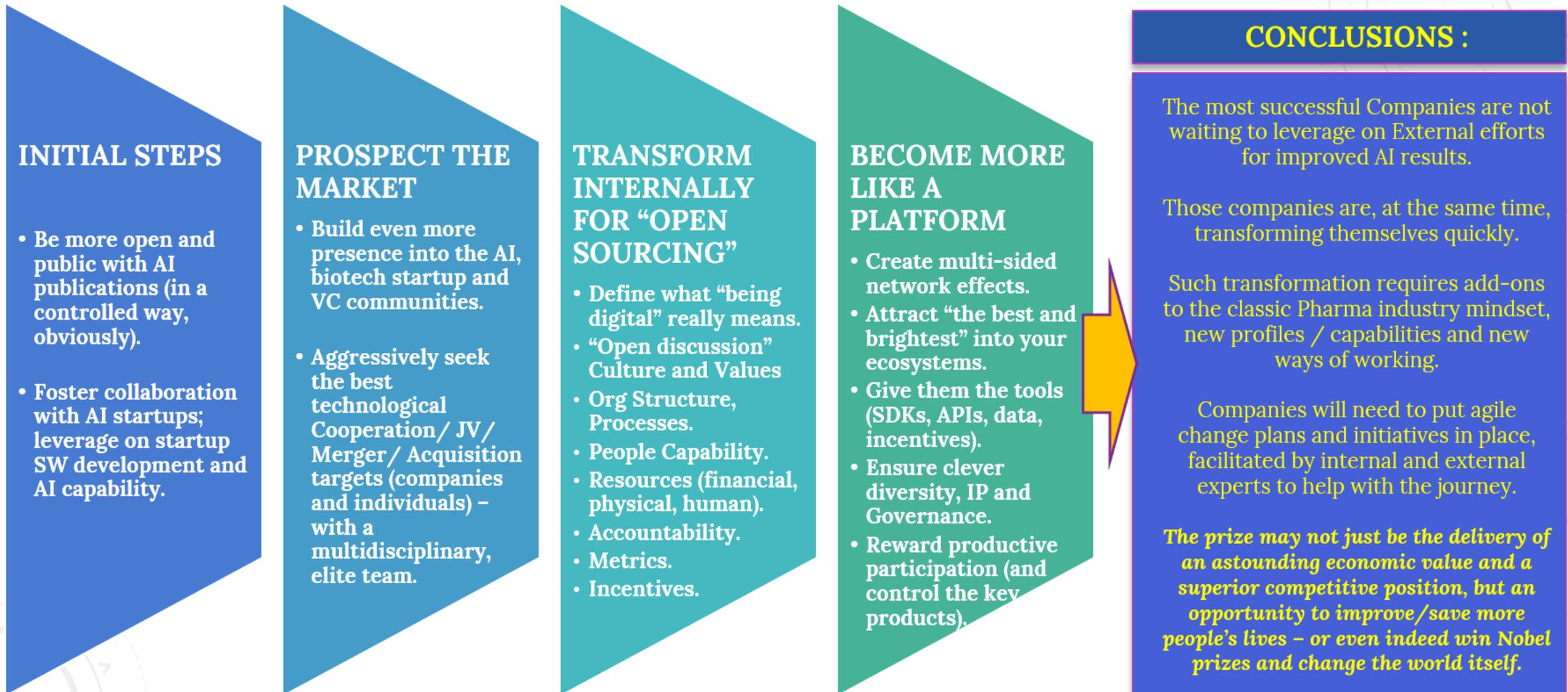


(Source: “Digital Transformation: Platform Strategies for Success”; Parker, G. et al. (Executive Education Course); MIT Sloan–Emeritus Institute; April 2019).

XI. PROPOSED GUIDELINES FOR SUCCESS, BEST PRACTICES AND CONCLUSIONS (2)



For all of the above, and regarding specific companies' AI success, we would suggest the following guidelines / best practices:



ANNEXE 1: 50 BEST-FUNDED AI COMPANIES IN HEALTHCARE



Exhibit 2.2 – Since 2010, \$8.5 billion of VC funding has been invested in the 50 best-funded AI companies in healthcare

	Company	Headquarters	Total raised \$ million		Company	Headquarters	Total raised \$ million
1	Ping An Medical and Healthcare Mgmt	China	1,150	27	Singlera Genomics	China	80
2	Babylon Health	UK	635	28	Viz	US	79
3	Indigo Agriculture	US	621	29	VoxelCloud	US	79
4	Zymergen	US	592	30	Healthy.io	Israel	78
5	Change Healthcare	US	557	31	Sight Diagnostics	Israel	77
6	Tempus	US	520	32	Saama	US	76
7	Recursion Pharmaceuticals	US	249	33	PathAI	US	75
8	Accolade	US	240	34	Infervision	China	74
9	iCarbonX	China	200	35	AIcure	US	69
10	insitro	US	200	36	Olive (Robotic Process Automation)	US	68
11	Synthego	US	162	37	Healx	UK	68
12	GoForward	US	158	38	Frontier Medicines	US	67
13	LinkDoc	China	151	39	XtalPi	US	66
14	Sophia Genetics	Switzerland	140	40	Lark Technologies	US	64
15	Beta Bionics	US	132	41	TeraRecon	US	62
16	OrCam	Israel	130	42	InSilico Medicine	US	61
17	Blackthorn Therapeutics	US	130	43	Evidation Health	US	61
18	Verana Health	US	119	44	ImagenTechnologies	US	60
19	Augmedix	US	116	45	Mindstrong Health	US	60
20	Clarify Health Solutions	US	108	46	Nuritas	Ireland	60
21	Finch Therapeutics	US	105	47	Paige.ai	US	59
22	MeMed Diagnostics	Israel	101	48	Atomwise	US	58
23	AI Therapeutics	US	98	49	K Health	US	56
24	caresyntax	US	91	50	GNS Healthcare	US	56
25	HealthTap	US	88				
26	Helian Health	China	84				

Total funding reported

Top 50

\$8,490 million

Top 10

\$4,964 million (58%)

Source: PitchBook Data, Inc., <http://pitchbook.com/research-process> – cited in “Transforming Healthcare with AI – The impact on the workforce and organisations”; EIT Health–McKinsey; March 2020.



ANNEXE 2: 30+ TECH COMPANIES IN AI LIFE SCIENCE R&D

Arterys	Medical Imaging Cloud AI – The AI assistant for radiologists
Asimov	Programmes living cells with genetic circuits
Atomwise	Artificial Intelligence for drug discovery
BenevolentAI	Artificial Intelligence for scientific innovation
Berg	Therapeutic discovery using its unique AI-based Interrogative Biology® platform
Biovia	Collaborative, knowledge-driven innovation and predictive analytics
BioXel	AI and Big Data technologies to power the next wave of medicines
Cyclica Inc	Harnesses biophysics, bioinformatics and artificial intelligence (AI) to help pharmaceutical companies navigate the drug discovery pipeline by assessing the safety and efficacy of drugs
Deep 6 AI	Artificial Intelligence and natural language processing to medical records to find more patients for clinical trials
Deep Genomics	Geneticists, molecular biologists and chemists are supported by its biologically-accurate artificial intelligence technology
Digital Reasoning Syntheses	Reads and combines data from all sources, including human language to build a comprehensive picture of individual patients, revealing insights that aid clinicians' care decisions
Exscientia	AI-driven systems to automate drug design
Genpact Cora	An artificial-intelligence (AI)-based platform for digital transformation
Google DeepMind	Delivers tools that clinicians can use to make sense of the huge inflows of information which overwhelms them
Healx	To transform the lives of rare disease patients by intelligently matching drug treatments
IBM Watson	Machine learning capabilities to find unique connections between recorded symptoms and other clinical data, such as timing and dosing of medicine
Infosys Mana	A platform that brings machine learning together with the deep knowledge of an organisation, to drive automation and innovation
Insilico Medicine	Artificial Intelligence for drug discovery and ageing research
InveniAI	To extend the human experience in the use of artificial intelligence over the discovery process

Knowledgegent	Enabling advanced and agile analytics, the digital enterprise and robotics
Microsoft Hanover	AI for precision medicine
Nference	AI to tackle the challenge of synthesising the world's biomedical knowledge
nQ Medical	Supports diagnosis of neurodegenerative disease years earlier than current gold standard tools
Palantir Technologies	Analysing real-world data for differentiated biomedical insight requires dealing with tremendous scale and complexity, as well as potential privacy concerns
Phenomic AI	State-of-the-art deep learning-based algorithms for analysing cell and tissue phenotypes in microscopy data
Precision Digital Health	Accelerates the adoption of digital health for researchers by providing a real-world evidence solution
QuantumBlack	In its raw form, data can be stubbornly unyielding. We use it to seek out the incisive insights and clear-cut response
Recursion Pharmaceuticals	Discovering transformative new treatments by leveraging the speed of automation with the intelligence of computers
Salesforce Einstein	A layer within the Salesforce platform that infuses Artificial Intelligence features and capabilities across all Salesforce Clouds. Einstein takes care of the data prep and modelling
Sema4	To revolutionise clinical diagnostics by combining comprehensive screening and diagnostic testing, predictive modelling, cutting-edge technologies and open-access data
Syntel SyntBots	Transform your business with intelligent automation
Transformative AI	Using cutting-edge artificial intelligence and novel analysis techniques to transform the treatment of serious medical conditions by collecting and translating clinical data into real-time, predictive assessments that guide the actions of patients and healthcare providers
twoXAR	Improving health on a global scale by building a profit-generating business utilising Artificial Intelligence
Viyasa	Enterprise scale deep learning platform, with consideration for Big Data scale data handling and provision to a range of deep learning approaches
WCG	Delivers transformational solutions that stimulate growth, foster compliance and maximise efficiency for those who perform clinical trials
Welth	Application of behavioural economics through scalable technology to achieve better adherence, engagement and health
Wipro HOLMES	AI and automation
Zebra Medical Vision	Provides radiologists with the tools they need to make the next leap in patient care
...and many more!	

Source: “Artificial Intelligence & Biopharma R&D IT”; The Prisme Forum; Drug Discovery World; Spring issue 2018.

THE AUTHOR & ACKNOWLEDGEMENTS



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THANK YOU !

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