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# Applying machine learning and artificial intelligence to the development of a pharmaceutical tablet

Edward Yost

Genentech, Small Molecule Pharmaceuticals

Chair – Bay Area Discussion Group (BADG) of the  
American Association of Pharmaceutical Scientists (AAPS)



# **American Association of Pharmaceutical Scientists - Bay Area Discussion Group**

*A meeting place for pharmaceutical scientists*

**Connect**

**Collaborate**

**Advance**

## 2020 BADG Executive Committee

Chair: Edward Yost

Chair-Elect: Jing Ling

Co-Secretary: Robert Jones

Co-Secretary: Christine Bowman

Treasurer: Rajiv Nayar



A wide-angle photograph of the Golden Gate Bridge in San Francisco, showing its iconic orange-red structure spanning the blue water of the bay. The city skyline is visible in the background under a clear sky.

# AAPS - Bay Area Discussion Group

*A meeting place for pharmaceutical scientists*

## 2019 BADG Events Presenters

Developing oral peptides

Dennis H. Leung (Genentech)

Delivering oral peptides

Radhika Korupolu (Rani Therapeutics/Incube Labs)

Advanced engineering of DNA and proteins

Sridhar Govindarajan (ATUM)

Long acting delivery of biologics to the eye

Karthik Rajagopal (Genentech)

Solid-state in small molecule drug dev

Paroma Chakravarty (Genentech)

Robotic manufacturing of personalized drug delivery

Fred Parietti (Multiply Labs)

Deep learning in healthcare

Beau Norgeot (UCSF)

ML to accelerate materials dev

Julia Ling (Citrine Informatics)

AI/ML in biopharma

Norman Packard (Daptics Inc)

# AAPS - Bay Area Discussion Group

*A meeting place for pharmaceutical scientists*

Connect with BADG on our social media platforms

**aaps-badg.org**



AAPS Bay Area Discussion Group



@aapsbadg



Group: AAPS - Bay Area Discussion Group  
Page: @BADG.AAPS



@bayareadiscussiongroup



Bay Area Discussion Group (an AAPS Discussion Group)

# Presentation References

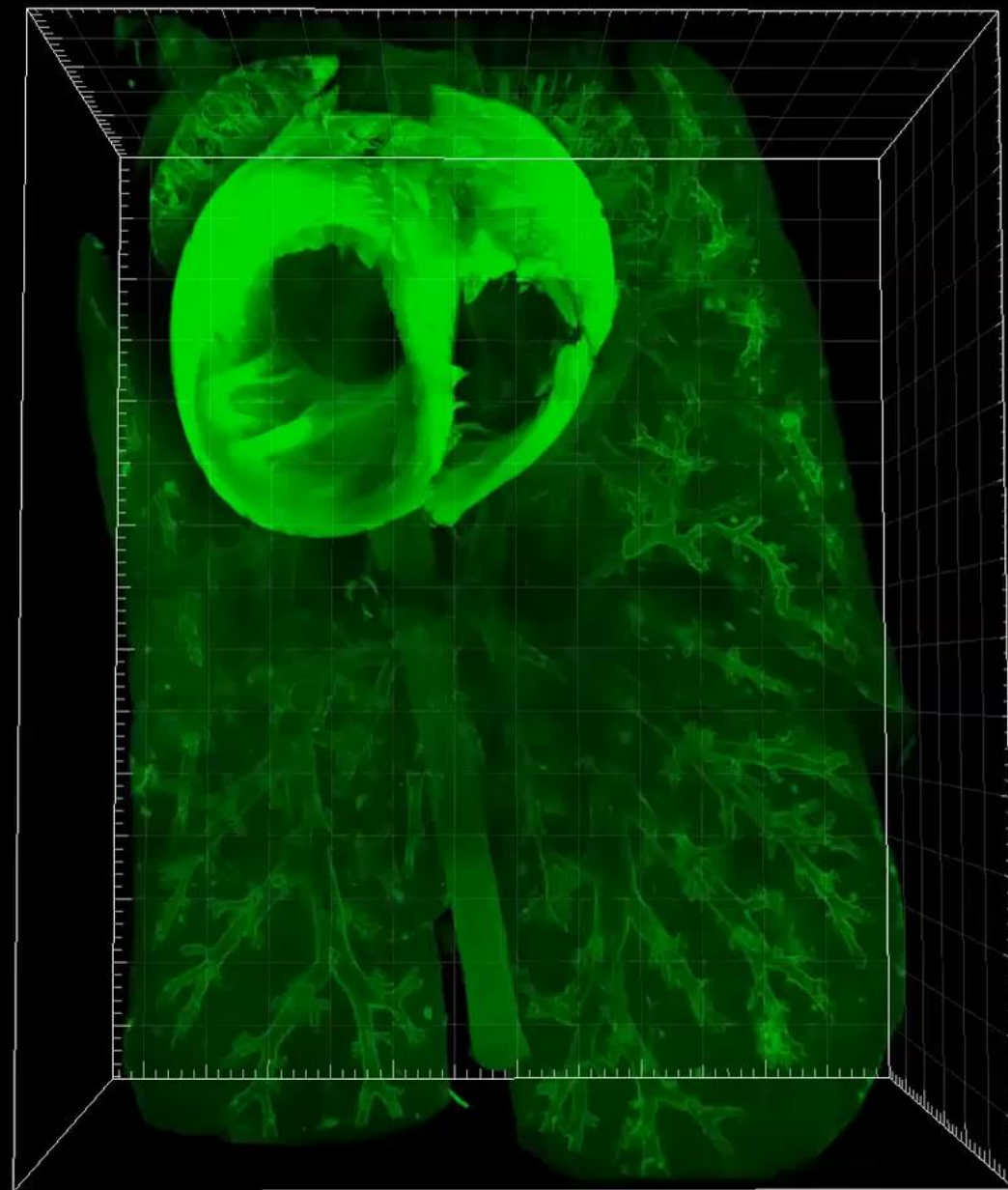
- Yost E et al., Journal of Pharmaceutical Sciences, 2019; 108(5):1818-1830
- Zhang, S. et al., 2018. Cambridge University Press, 24(S1), 1400-1401.  
<https://doi.org/10.1017/S1431927618007481>
- Pan et al., 2019, Cell 179, 1661–1676
- Ma et al, Journal of Pharmaceutical Sciences, 2020;  
<https://doi.org/10.1016/j.xphs.2020.01.014>
- Bi et al, CA: A Cancer Journal for Clinicians 69(2):127-157

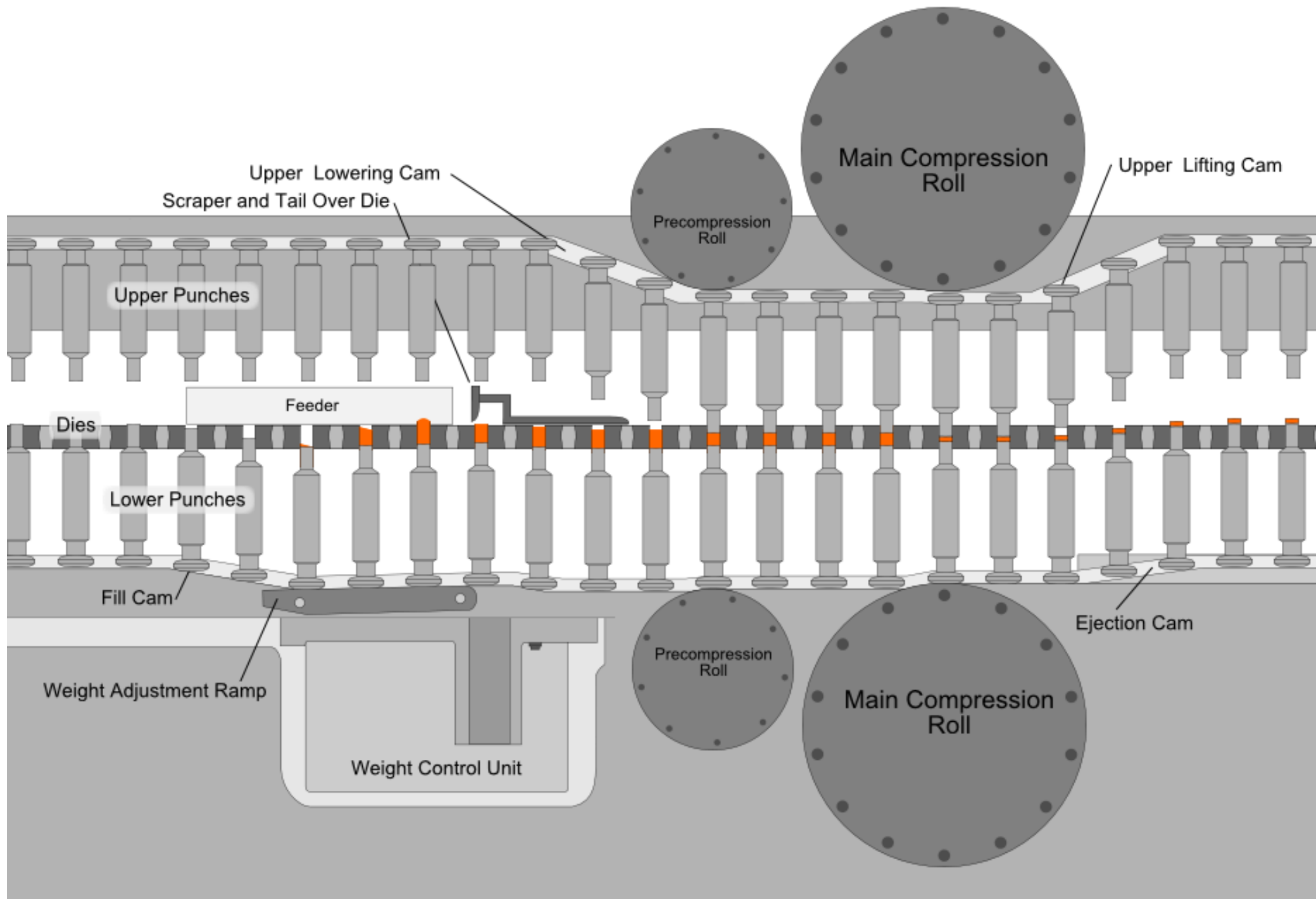


# Scientific understanding supported with technology











See New Warnings

# Motrin<sup>®</sup> IB

for Tablets USP, 200 mg  
(NSAID)

**Ibuprofen Tablets USP, 200 mg**  
**Pain / Fever Reducer (NSAID)**

**Ibuprofen Tablets (NSAID)**  
Pain Reliever / Fever Reducer (NSAID)



**2**  
**Coated Caplets\*\***  
1 POUCH OF 2 CAPLETS  
shaped Tablets

1 POUCH OF 2 CAPSULE-SHAPED TABLETS



**Lil' Drug Store**

LOT  
EXP

2025/2528

**Motrin IB**  
Ibuprofen Tablets USP, 200 mg

**ibuprofen Tablets USP 200 mg**  
Nattive Kieffer / Fever Reducer (NSAID)  
2 Coated Caplets

**DO NOT USE IF POUCH IS TORN**

caplet)

- **Noninflammatory drug**
- **Pain relief**

muscular aches and  
temporal

... socially in people... and pains... minor... reduce... shock...

medical ... the allergic ... pain ... fever ... red ...

... help right  
... stomach  
... edine

ing problems

Stomach

...NSAIDs, ...

NSAIDs

Aspirin  
If you  
allergic reaction  
ask a doctor

the stomach before

...each  
...you have



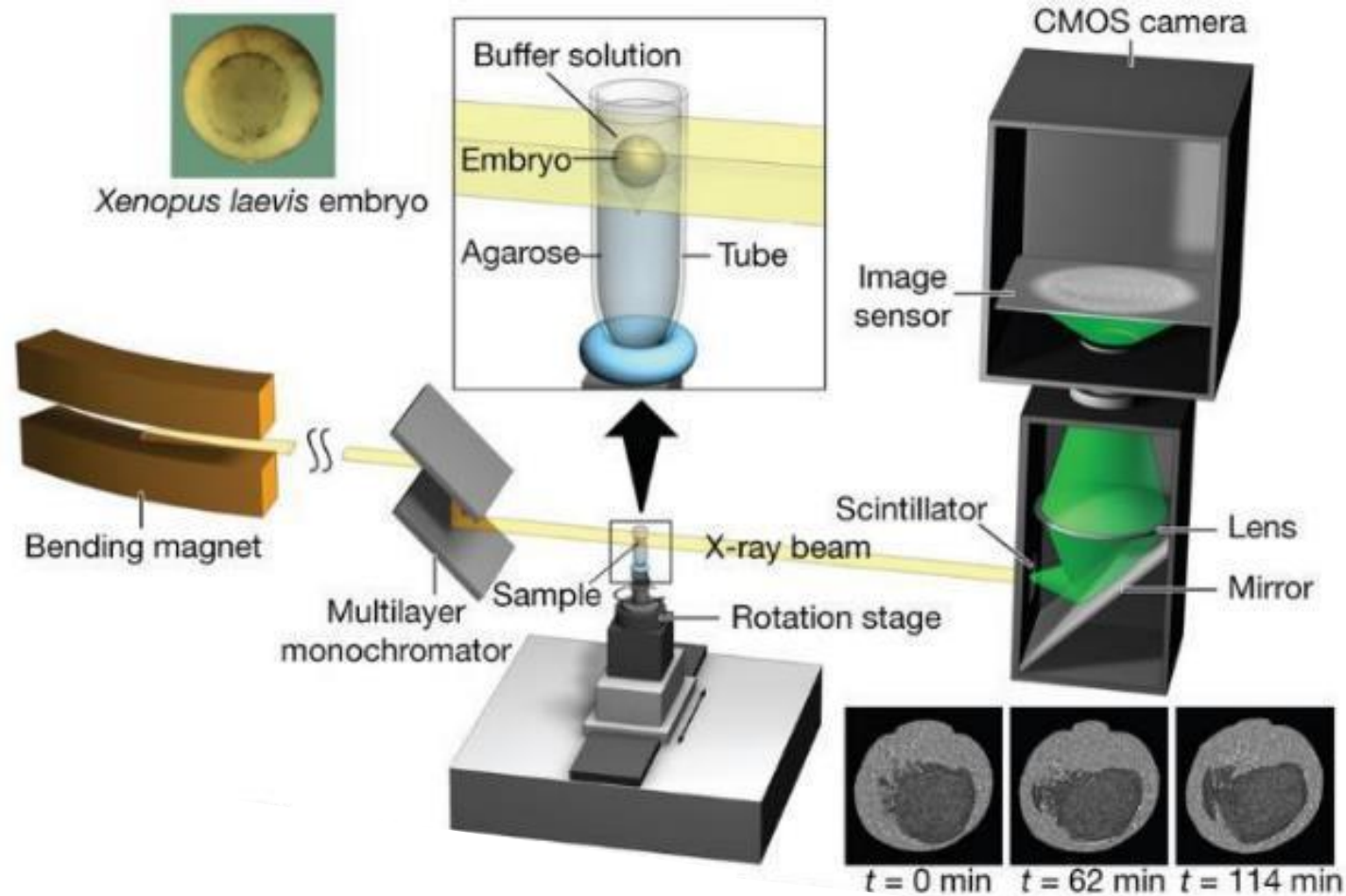
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# MECHANISTIC UNDERSTANDING TO IMPROVE PRODUCT KNOWLEDGE



# MicroCT, NanoCT, and X-ray Microscopy

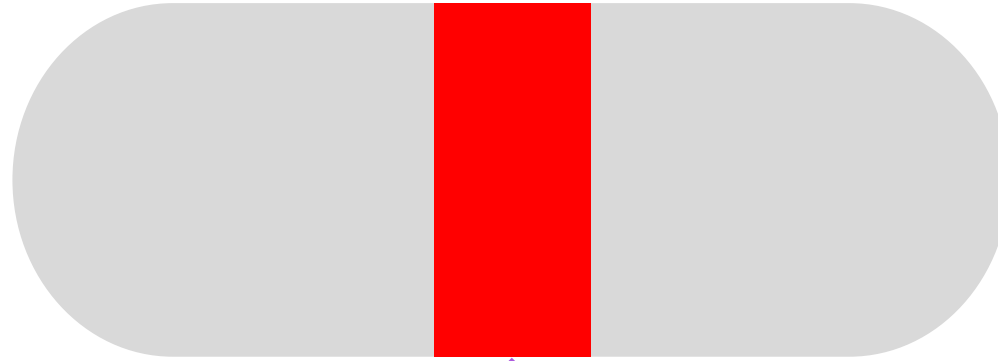
0.3-30  $\mu\text{m}$  resolution



DigiM Solution



**analyzed tablet shape**



region of X $\mu$ CT  
analysis

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# CAN WE QUANTIFY INTERNAL DEFECTS?

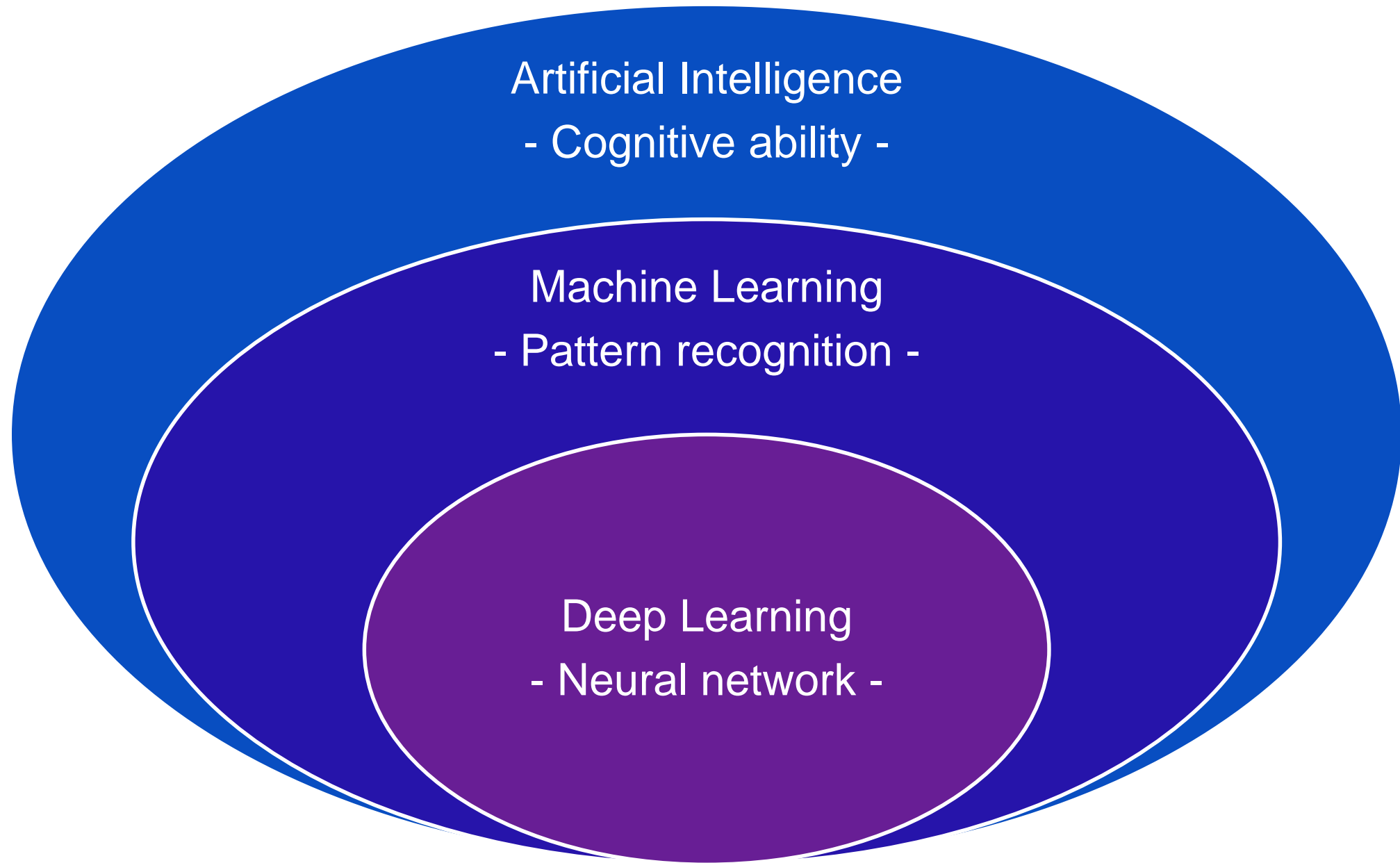
Artificial Intelligence  
- Cognitive ability -





Artificial Intelligence  
- Cognitive ability -

Machine Learning  
- Pattern recognition -



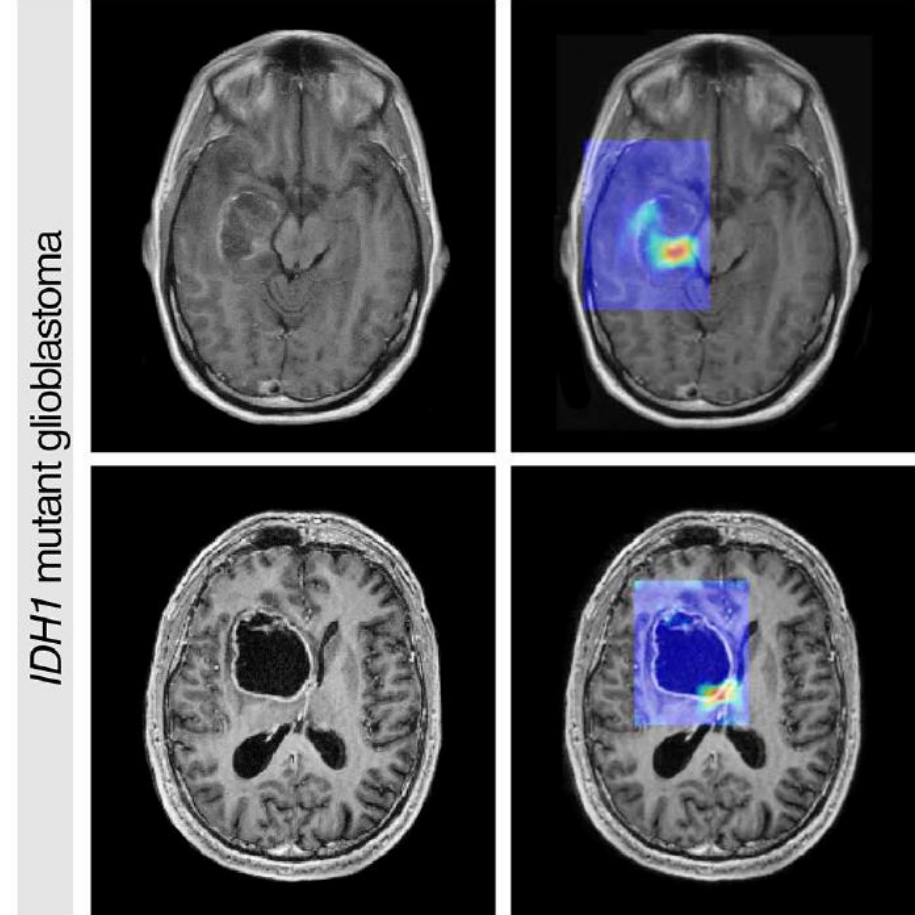
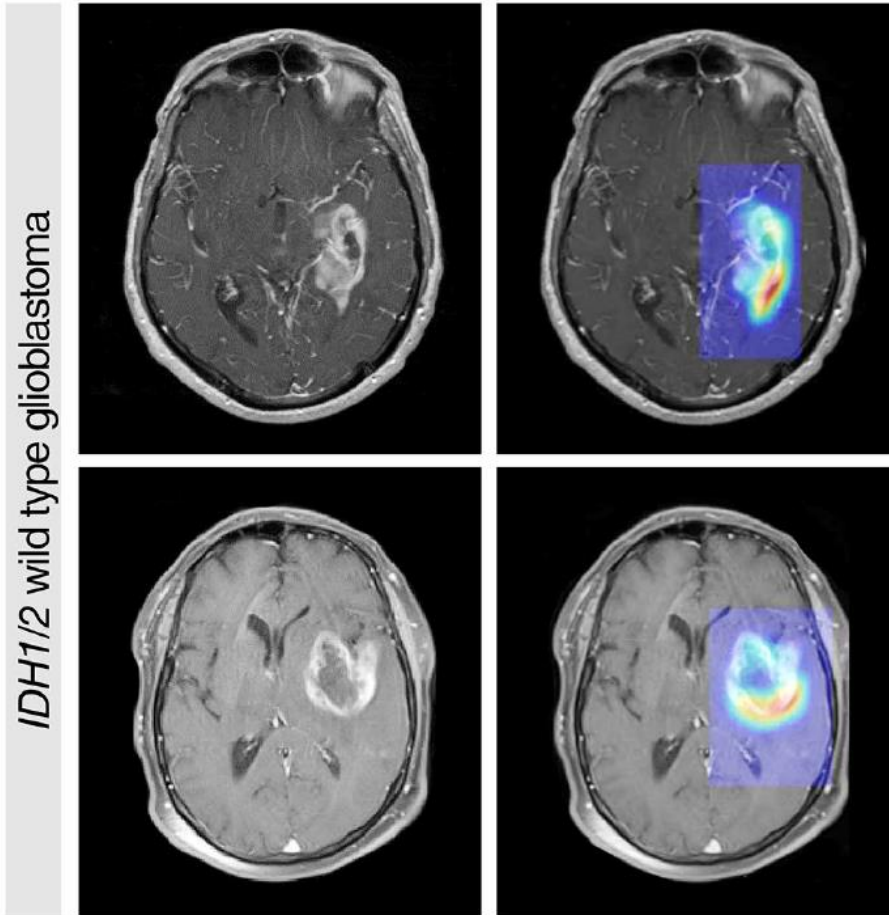
# AI applied to drug development

“AI in drug discovery to find new targets”  
– Hal Barron, GSK





# Computational pathology



Bi et al, CA: A Cancer Journal for Clinicians 69(2):127-157



# Focus on less routine tasks





# Watch out for the hype





# Bay Area AI Startups in Drug Discovery

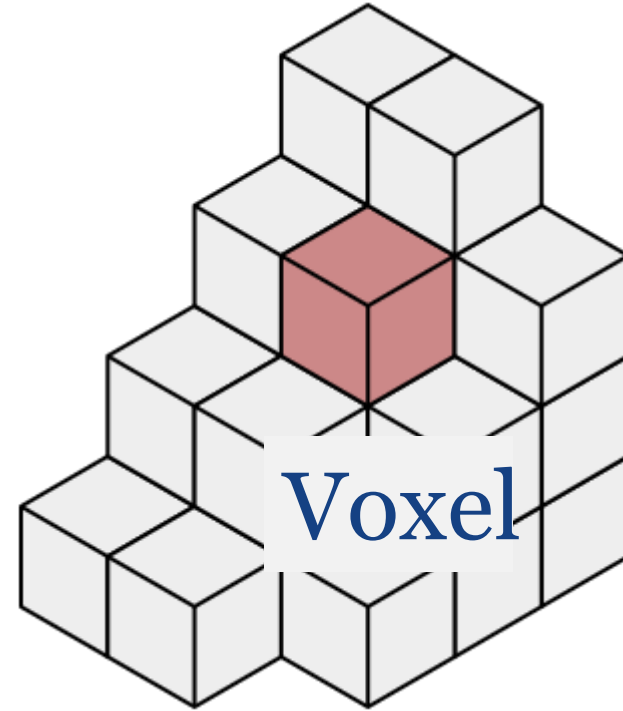
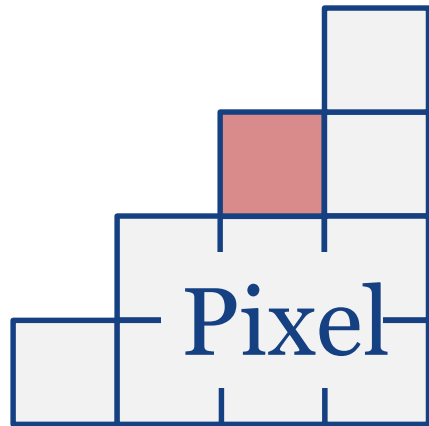
Athelas  
Atomwise  
Auransa  
Berkeley Lights  
BioAge Labs  
Biotrillion  
BlackThorn Therapeutics  
Brite Health  
Data2Discovery  
Datavant  
Emerald Cloud Lab  
Engine Biosciences

Genesis Therapeutics  
Gritstone Oncology  
Insitro  
Kyndi  
Medable  
Mendel.ai  
Notable  
NuMedii  
Numerate  
OccamzRazor  
Researchably

Spring Discovery  
Strateos  
Syntekabio  
TeselaGen  
ThoughtSpot  
TwoXAR  
uBiome  
Unnatural Products  
Verge Genomics  
VERISIM Life  
X-37

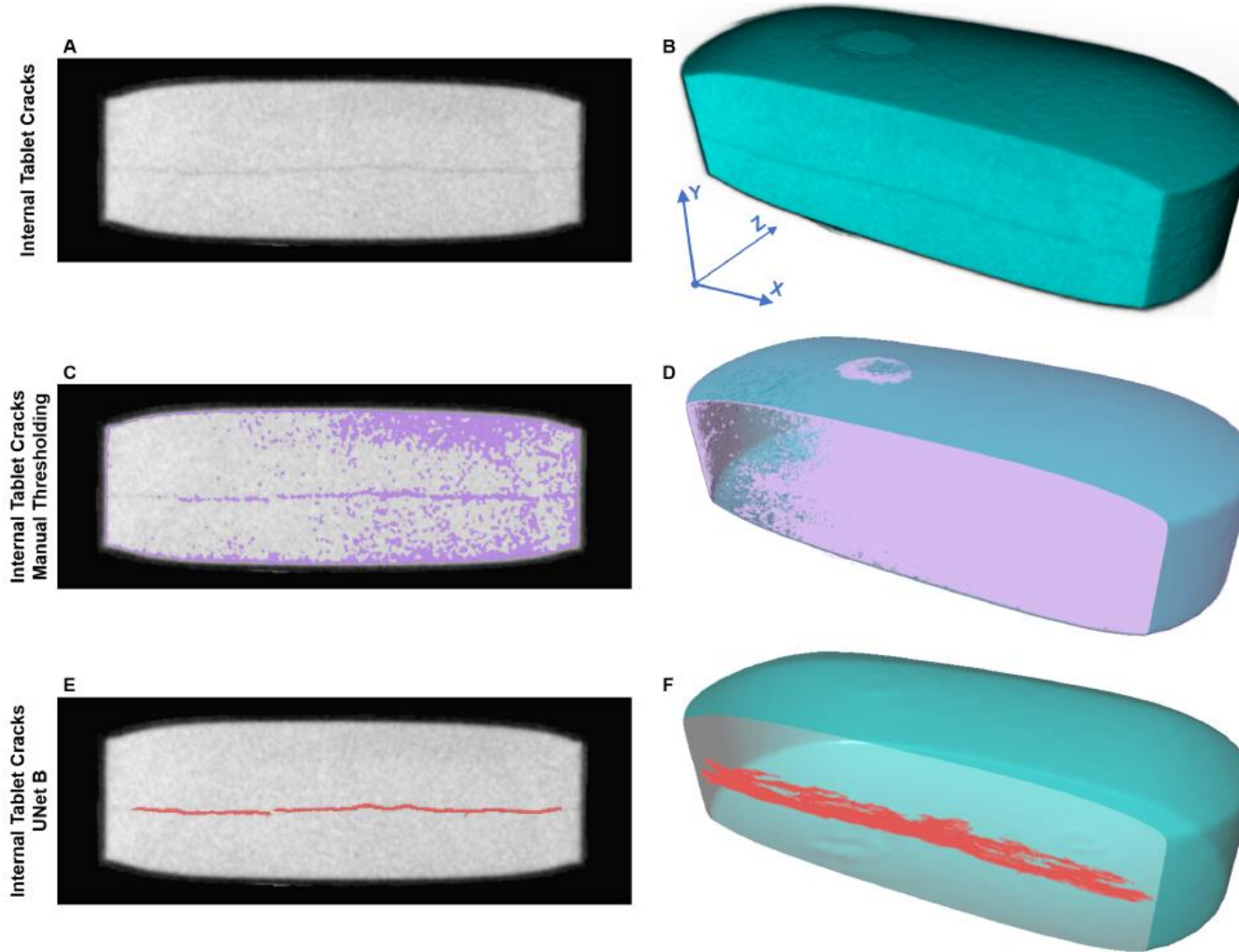
<https://blog.benchsci.com/startups-using-artificial-intelligence-in-drug-discovery>

# Digital images are data rich



# Convolutional neural network-based deep learning analysis

Internal Tablet Cracks



Manual Threshold

CNN

Ma et al, J Pharm Sci, 2020;  
<https://doi.org/10.1016/j.xphs.2020.01.014>

# Technology supplements scientific understanding and innovation



# Acknowledgments

## Genentech

**Ajit Narang**

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## Roche

**Stefanie Peter**

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**Shawn Zhang (DigiM Solutions)**

**Pascal Chalus (Lonza)**

# THANK YOU

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