

AI/ML-driven Annotation for 3D Cellular Imaging

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AI/ML in 3D Cellular Imaging

<https://www.nobelprize.org>

The Nobel Prize in Chemistry 2017



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Jacques Dubochet
Prize share: 1/3



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Joachim Frank
Prize share: 1/3



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Richard Henderson
Prize share: 1/3

The Nobel Prize in Chemistry 2017 was awarded to Jacques Dubochet, Joachim Frank and Richard Henderson "for developing cryo-electron microscopy for the high-resolution structure determination of biomolecules in solution".

Nobel Prize in Chemistry 2024



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David Baker
Prize share: 1/2



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Demis Hassabis
Prize share: 1/4

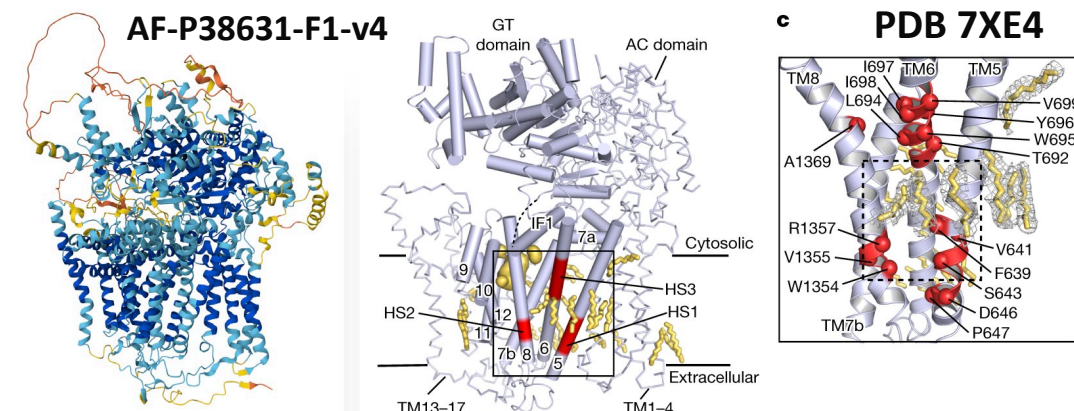


© Nobel Prize Outreach. Photo: Clément Mocin
John Jumper
Prize share: 1/4

The Nobel Prize in Chemistry 2024 was divided, one half awarded to David Baker "for computational protein design", the other half jointly to Demis Hassabis and John Jumper "for protein structure prediction"

- Rapid advances in both computational and experimental tools have led to an explosion of high-resolution structure data.

Fungal beta-1,3 glucan synthase – the target for echinocandins



- **What's still missing** - how do these proteins behave in their native cellular environment?

RCSB **PDB**
PROTEIN DATA BANK



234,136 Structures from the PDB

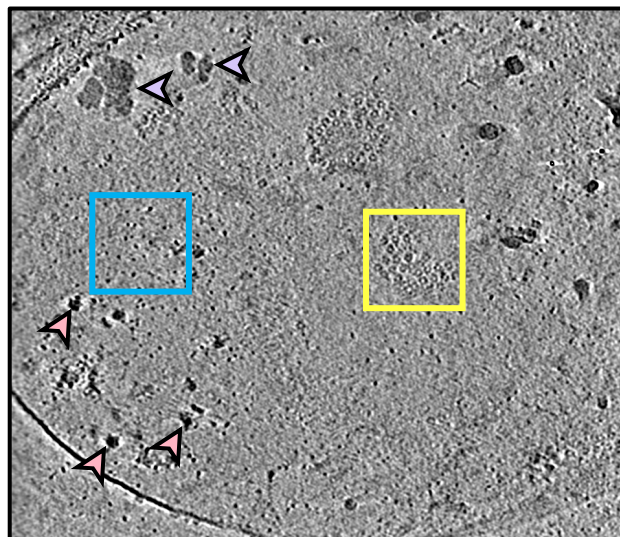


1,068,577 Computed Structure Models (CSM)

<https://www.rcsb.org>

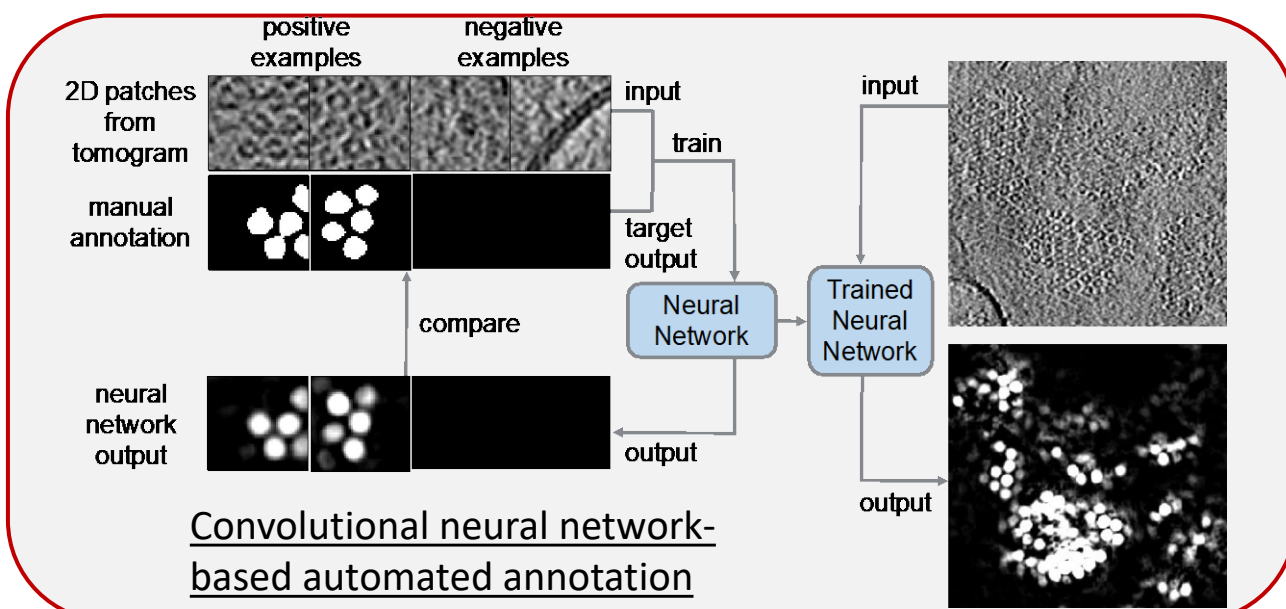
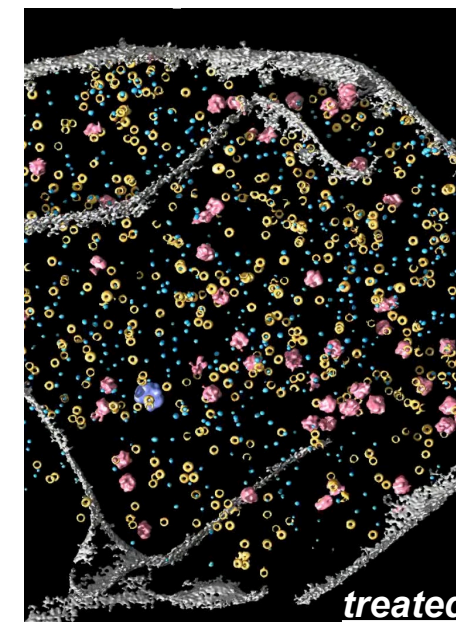
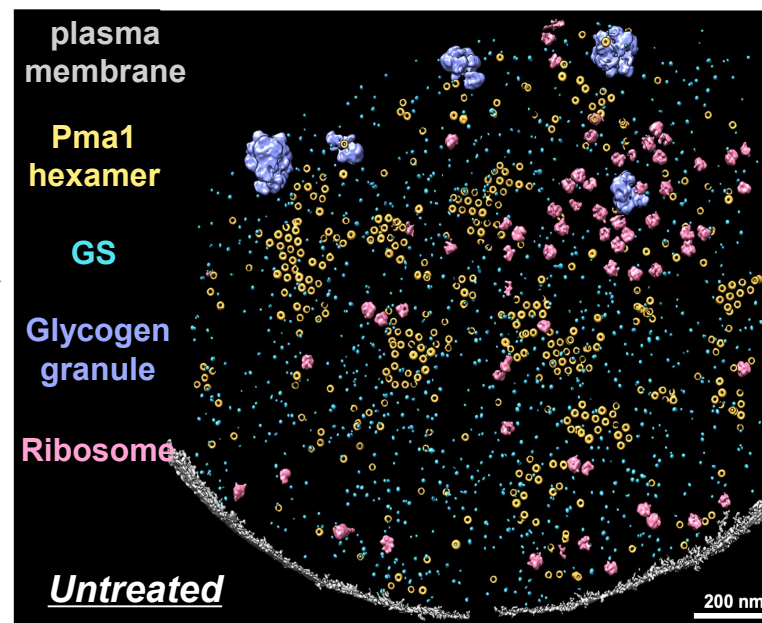
AI/ML in 3D Cellular Imaging

A tomogram of the fungal plasma membrane with GS present as in a native membrane embedded from



Annotation

- > Noisy input
- > Polymorphism
- > Validation benchmarks



Context-dependent 3D Analysis

- Infer spatial and temporal patterns from discrete, static 3D data
- Overcome intrinsic variabilities to detect condition-specific differences
- Build annotated 3D atlas for Integrative biology
- Scale analysis with growing data volume