The CCAIM Experience:

Leveraging AI for Drug Discovery and Structural Biology

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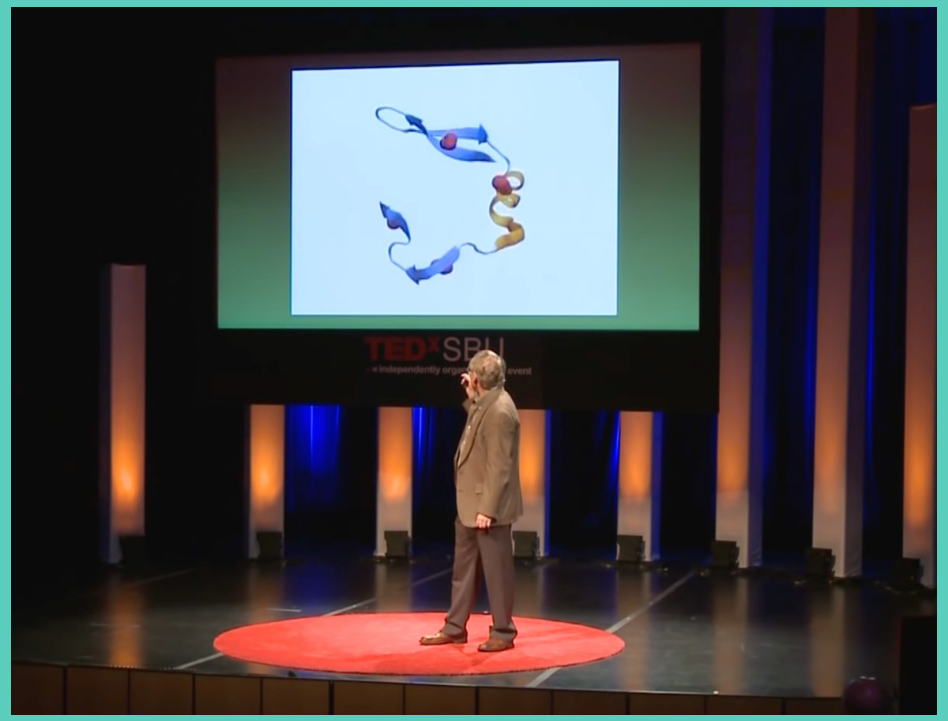
But first…a little me me

BSc Biochemistry **- Imperial College London**

MSc Bioinformatics and Theoretical Systems Biology **– Imperial College London**

How it all started



www.youtube.com/watch?v=zm-3kovWpNQ

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NEWS | 30 November 2020

‘It will change everything’: DeepMind’s AI makes gigantic leap in solving protein structures

Google’s deep-learning program for determining the 3D shapes of proteins stands to transform biology, say scientists.

CASP/DEEPMIND/VTAGLIABRACCIDTOMCHICK,UT SOUTHWESTE

A DeepMind model of a protein from the Legionnaire's disease bacteria (Casp-14)

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Why CCAIM?

- Focus on interdisciplinary research and supervision
- Access to both computational and experimental laboratories
- Heavy emphasis on collaborations with industry
- Plus: all the usual benefits

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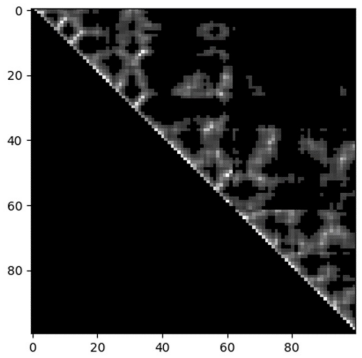
Representations of proteins for ML models

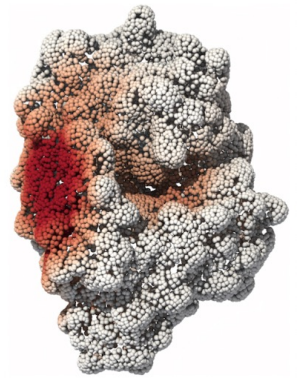
Distance matrix (CNNs)



Graph based

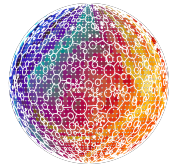
(Jamasb et al, 2020)

Surface based



(Sverrisson et al, 2020)

Graphein



graphein.ai

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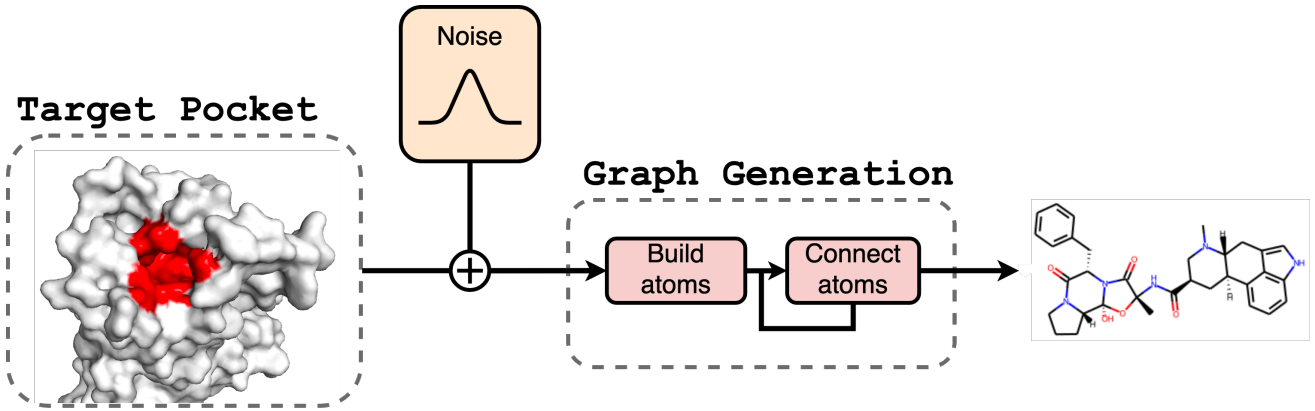
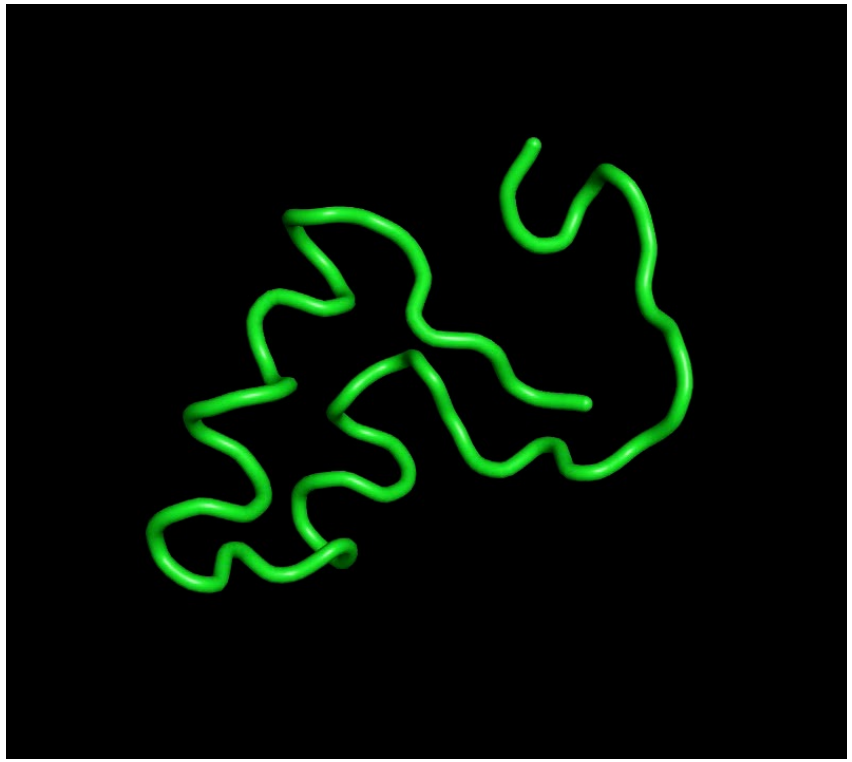
A little sample





Thank you!

Feel free to contact me!

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