

# Biomodeling *Biotech*

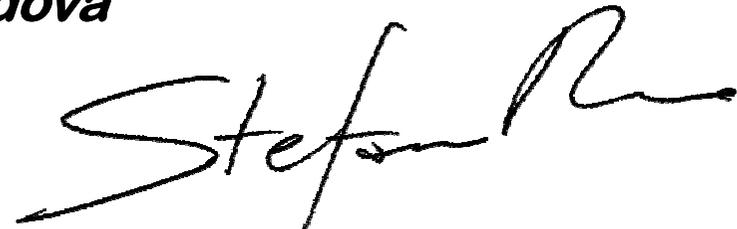
**by Stefano Moro**

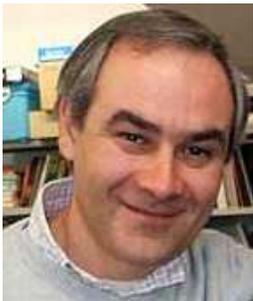
***Molecular Modeling Section (MMS)***

***Department of Pharmaceutical and Pharmacological Sciences***

***University of Padova***

**©2019**





# How do we organize? <http://mms.ds.farim.unipd.it>



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## MMS

### Molecular Modeling Section

Department of Pharmaceutical and Pharmacological Sciences, University of Padova  
Via Marzolo 5, 35131 Padova (Italy) - phone: +39 049 8275704, fax: +39 049 8275366

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Projects

Publications

@learning

MMStools

MMS\_Intranet



April 01, 2016

MMS launches MMSYouTube channel. [more...](#)

October 01, 2015

MMS launches the DockBench tool. [more...](#)

January 24, 2014

MMS launches the Supervised Molecular Dynamics

### MMS: Events

November 16-17, 2017

5th CD DD Meeting in Milan... [more](#)

### MMS: Latest Hot Publication

Salmasso et al. "Exploring Protein-Peptide Recognition Pathways Using a Supervised Molecular Dynamics Approach." *Structure* (2017) [more...](#)

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Chimica Farmaceutica 2 (CTF)

Progettazione e Sviluppo di un  
Farmaco (CTF)

Biomodeling (BTF)

Cheminformatica (ISF)

Tossicologia Computazionale  
(Master REACH, Sp...

Master, PhD and Adv...

updates

A GPU Grant [more...](#)

**MMS:**

November 16-17, 2017

5<sup>th</sup> CDDD Meeting in Milan... [more](#)

**MMS: Latest Hot Publication**

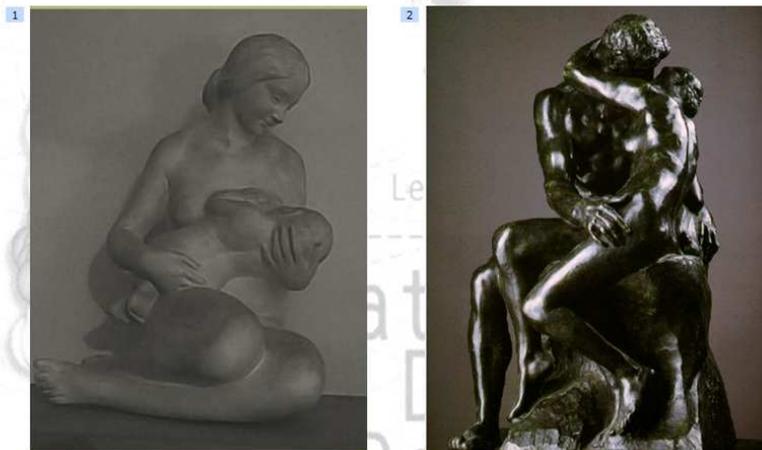
Salmaso et al. "Exploring Protein-Peptide Recognition Pathways Using a Supervised Molecular Dynamics Approach." *Structure* (2017) [more...](#)

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*S. MORO – Biomodeling Biotech*

# Main focus of our *Biomodeling course* *Biotech*



Understanding the logic of recognition!



validation and analysis. It will cover the background of different structural data. In addition, participants will learn how to critically assess the quality of different techniques, thus enabling the analysis of protein structure data for different purposes: a) Tools and resources for drug discovery; b) Homology modeling; c) Tools and resources for drug discovery

Introduction to Computational Structural Biology

Protein-protein interaction: the magic role of molecular surfaces

Protein-protein interaction: molecular docking

Protein-protein interaction: stability and potential energy of the system.

Protein-protein interaction: the role of the time.

MMSLAB:

@sertiamoci:

Useful free computational structural biology software:

1. Chimera (UCSF)
2. Pymol (DeLano Scientific LLC)
3. VMD (UIUC)



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**MMS@Lab... broadening perspectives.**



<b>Select your PDB:</b>	<a href="#">MS</a>
<b>Project Aims:</b>	<a href="#">MS</a>
<b>Download Chimera:</b>	<a href="#">MS</a>
<b>Tutorials:</b>	<a href="#">Veronica and Mattia's Tutorial</a> <a href="#">MS</a> <a href="#">Official Chimera's Tutorial</a> <a href="#">MS</a> <a href="#">UCSF Chimera Video Tutorials</a> <a href="#">MS</a> <a href="#">PDB Video Tutorial</a> <a href="#">MS</a>

This project was possible thanks to the irreplaceable contributions of [Veronica Salmaso](#) and [Mattia Sturlese](#). We warmly thank UCSF Resource for Biocomputing, Visualization, and Informatics for giving access to [Chimera](#).



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# http://mms.dsfarm.unipd.it



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## MMS

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Cerca

Here is when you can find Stefano in the lab:

### Where is Stefano?

Oggi ◀ ▶ maggio 2019 Stampa Settimana Mese Agenda

dom	lun	mar	mer	gio	ven	sab
28	29	30	1 mag	2	3	4
	9:30AM Lezione CFTI	9:30AM Lezione CFTI		9:30AM Lezione CFTI	9AM Giorgio Modena	
-5	6	7	8	9	10	11
	9:30AM Lezione Bion 4:30PM Incontro Stu	2:30PM Informale di	4:30PM Incontro Stu		11:30AM Teleconferen	
12	13	14	15	16	17	18
19	20	21	22	23	24	25
		1PM Semianrio dott	2PM Lezione Trieste	9AM Lezione Trieste		
26	27	28	29	30	31	1 giu
	Workshop "Quality					

Supervised Molecular Dynamics (SuMD) Simulations." JCOM (2016) [more...](#)

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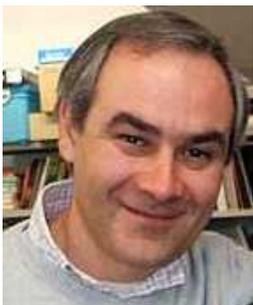
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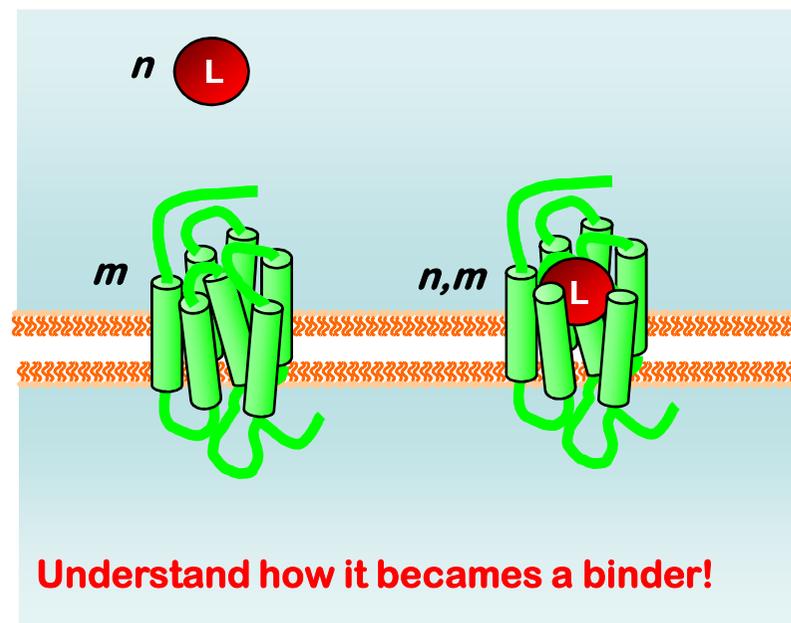
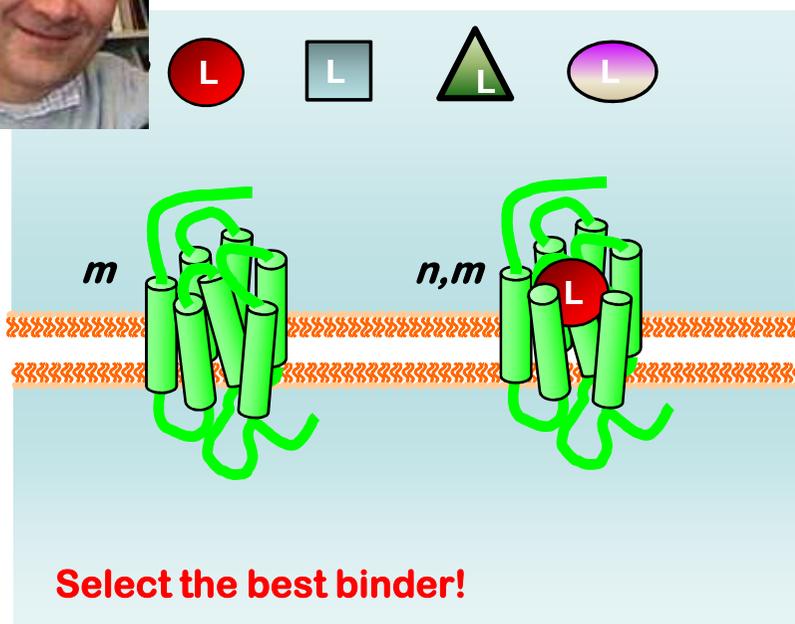
# Main focus of our *Biomodeling course* *Biotech*



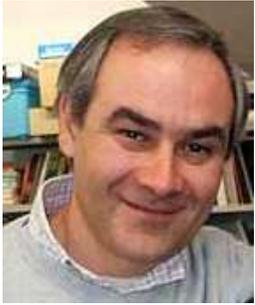
**Understanding the logic of recognition!**



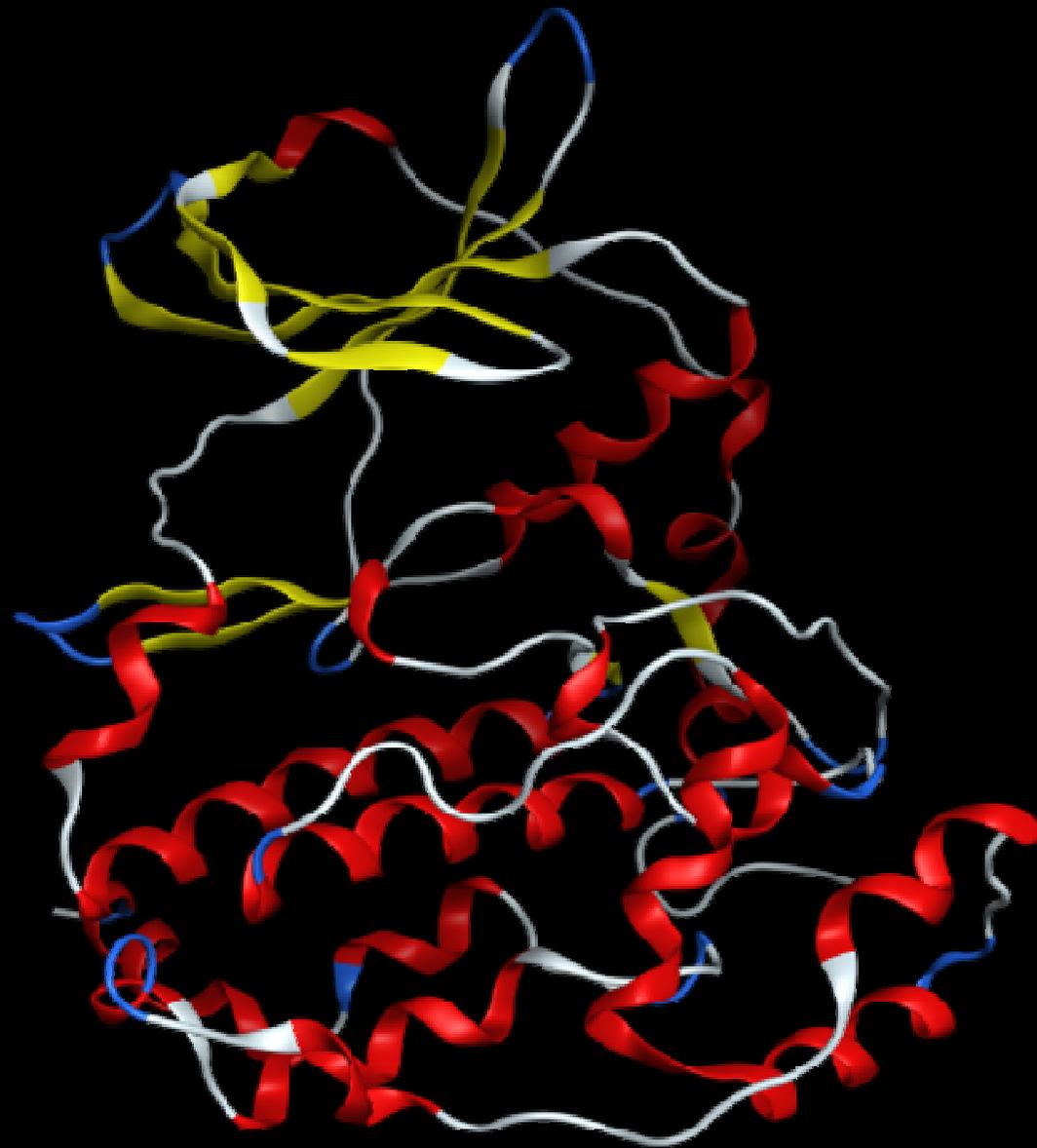
# From a molecular point of view, of course!

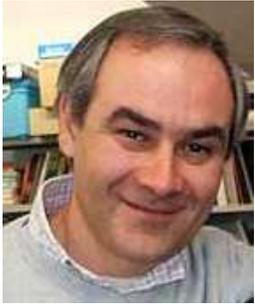


**MMStools**



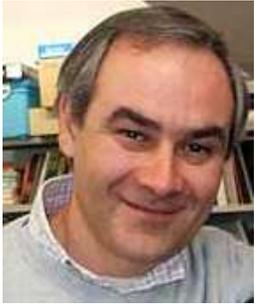
**I would like to start with this provocation...  
answer to this simple question: what is it?**





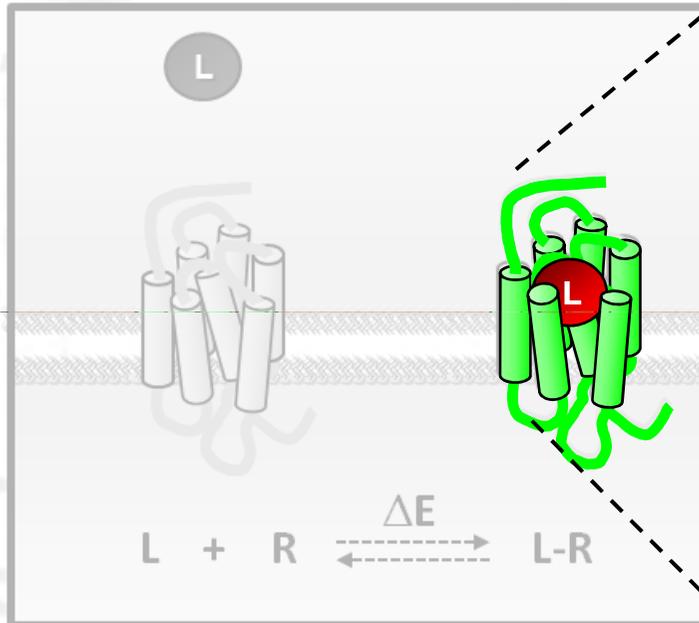
**I would like to start with this provocation...  
answer to this simple question: what is it?**





# Why we consider the 3D structures are exciting?

Single event

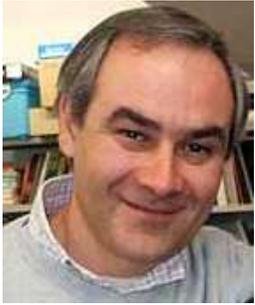


*closed system, T constant.*

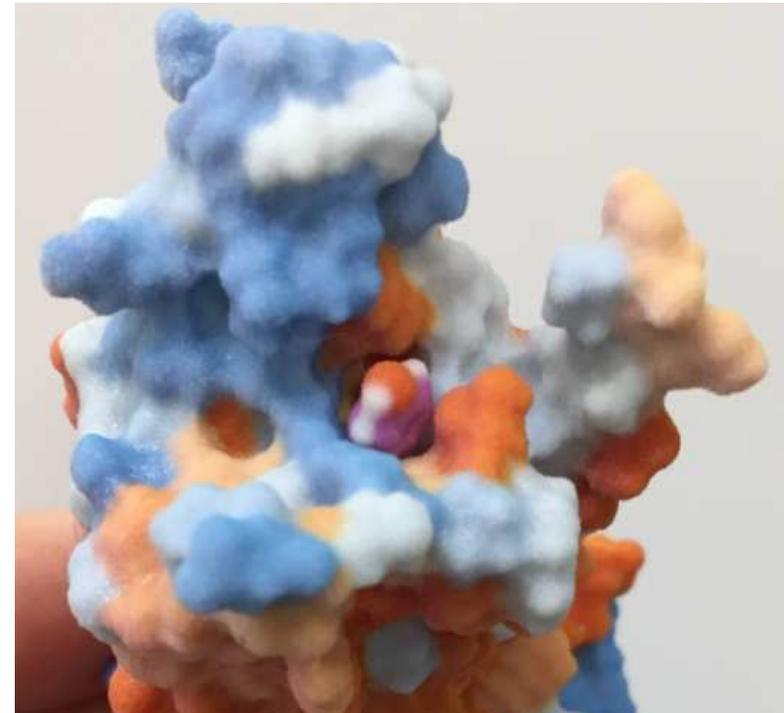


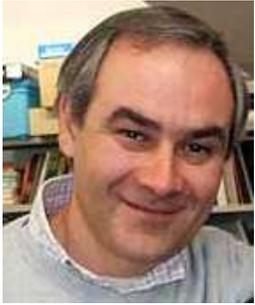
The natural link with a ligand-receptor recognition process.

MMS Lab (2015): 3D printed model of the human A2A adenosine receptor co-crystallized with its antagonist ZM 241385 (PDB entry: 4EIY)

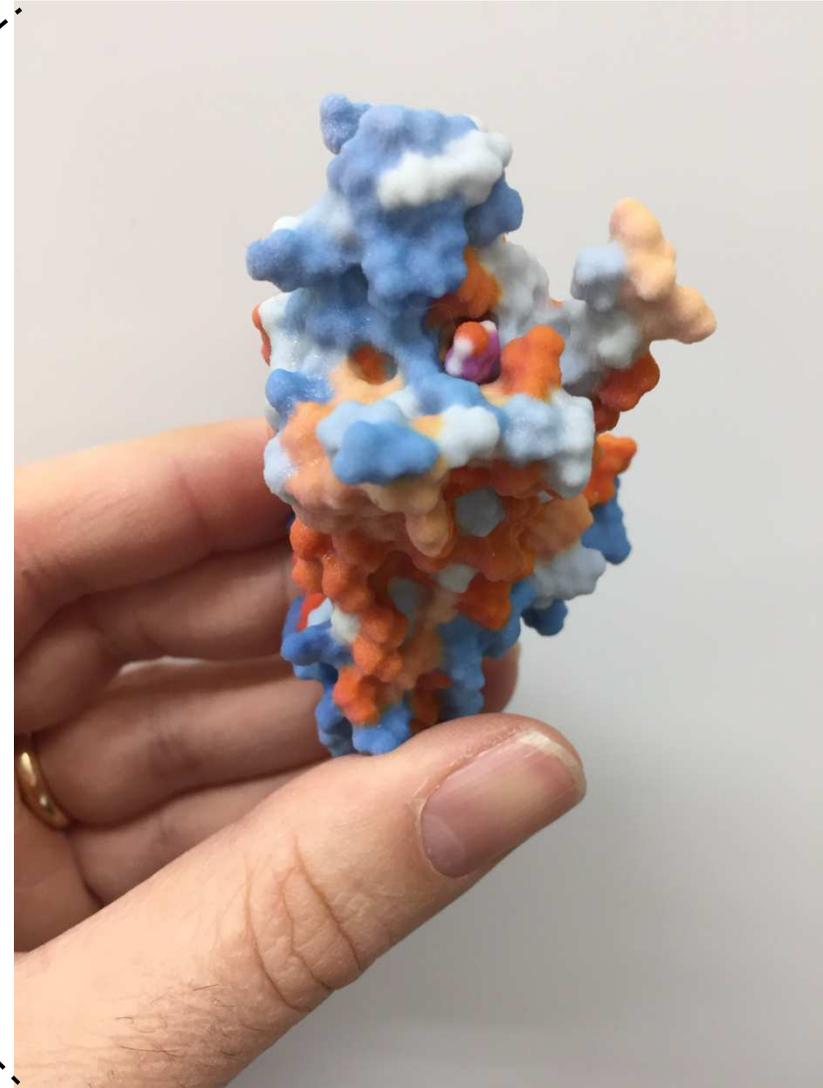
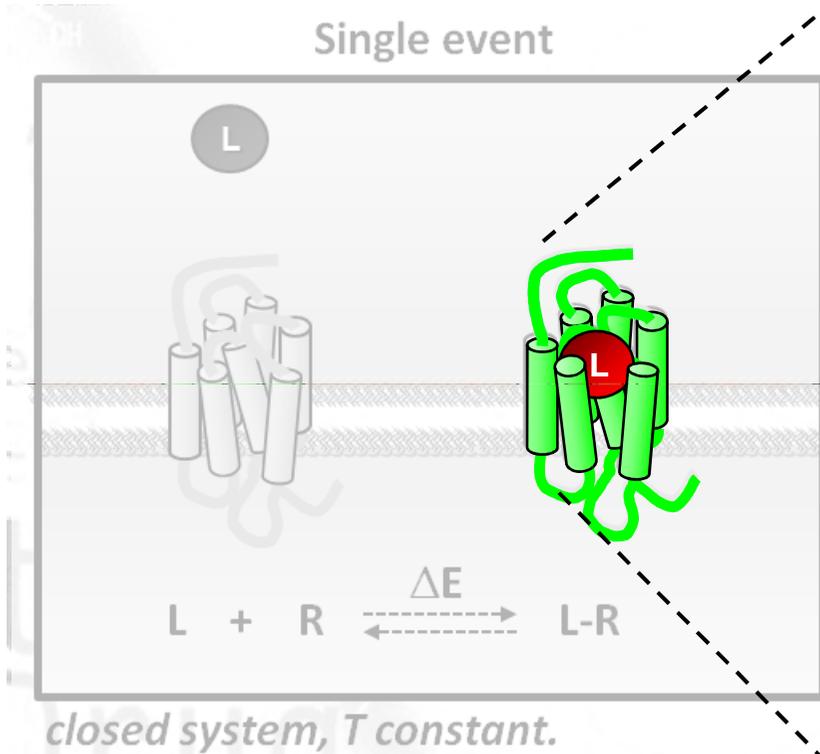


# How is it possible to create a realisting protein (molecule) 3D printing?

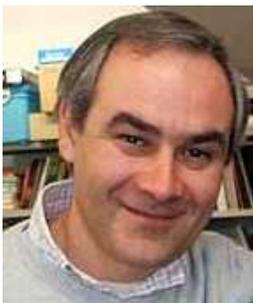




# But why we consider the 3D structures exciting... but no so exciting?

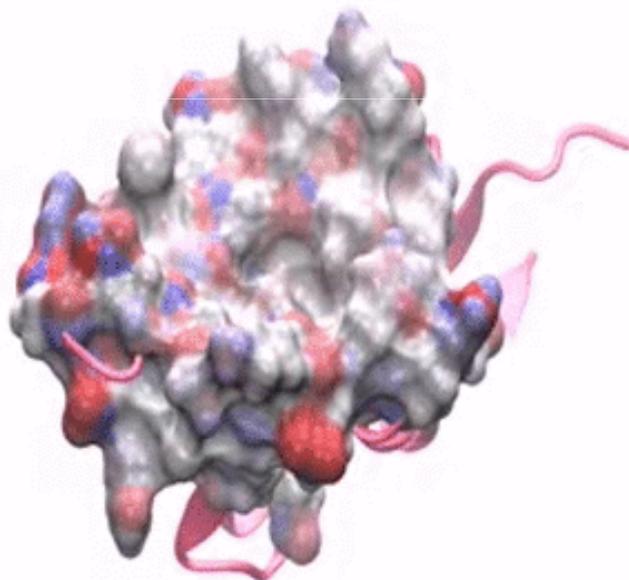
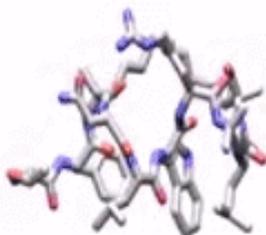


MMS Lab (2015): 3D printed model of the human A2A adenosine receptor co-crystallized with its antagonist ZM 241385 (PDB entry: 4EIY)



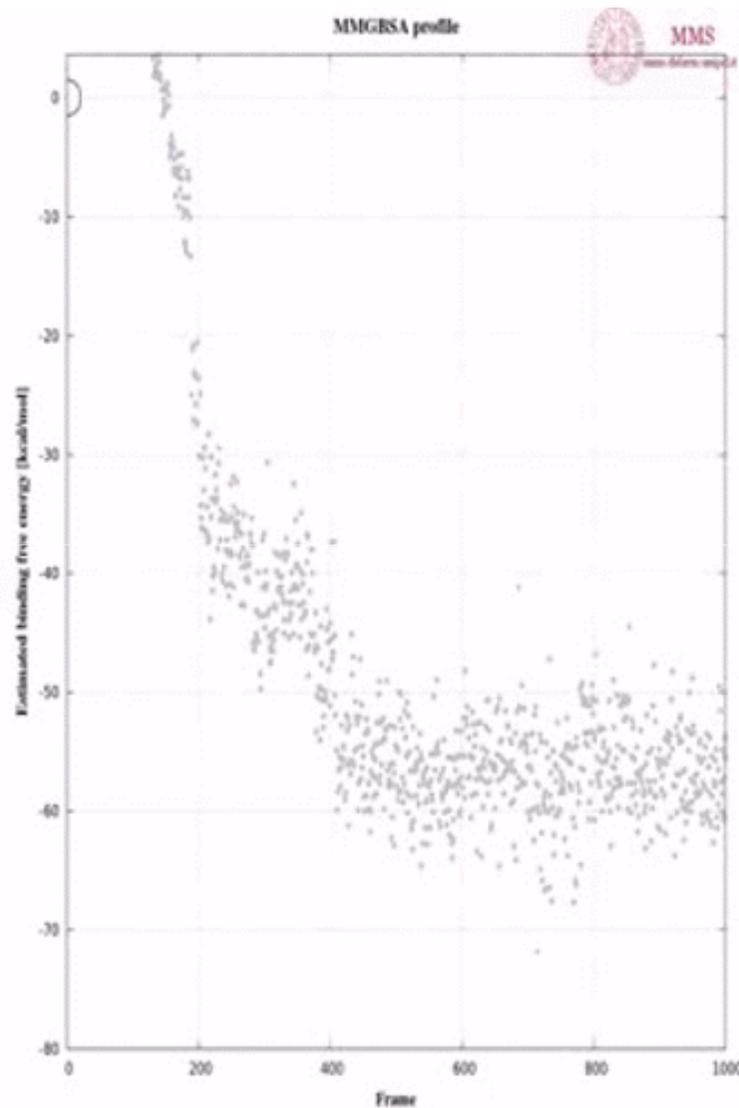
# We miss the essence of the life...

SuMD simulation time: 0.01 ns



Stapled p53 Peptide Bound to Mdm2; PDB-ID: 3V3B

MMGBSA profile



Salmaso V., Sturlese M.; Cuzzolin A.; Moro S. Structure 25, 655-662 (2017)

... incontrarsi... riconoscersi... scegliersi...



**M. Sturlese**

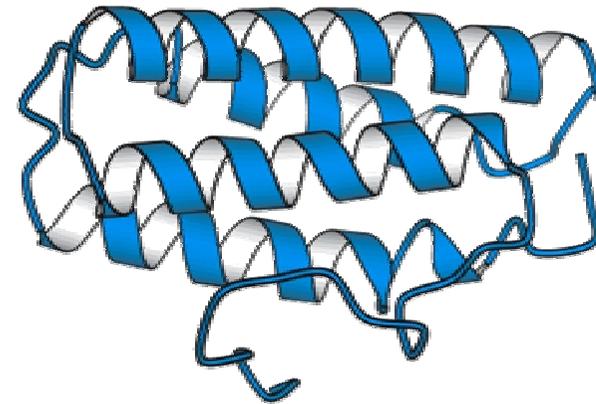
**V. Salmaso**

**A. Cuzzolin**

Salmaso V., Sturlese M.; Cuzzolin A.; Moro S. Structure 25, 655-662 (2017)



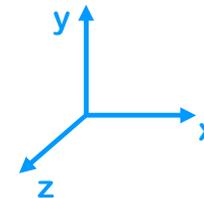
I would like to start from here... Silvio!!!

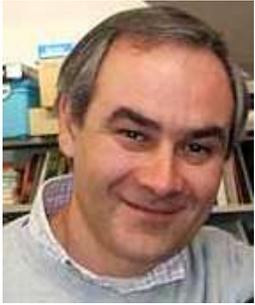


**1D**

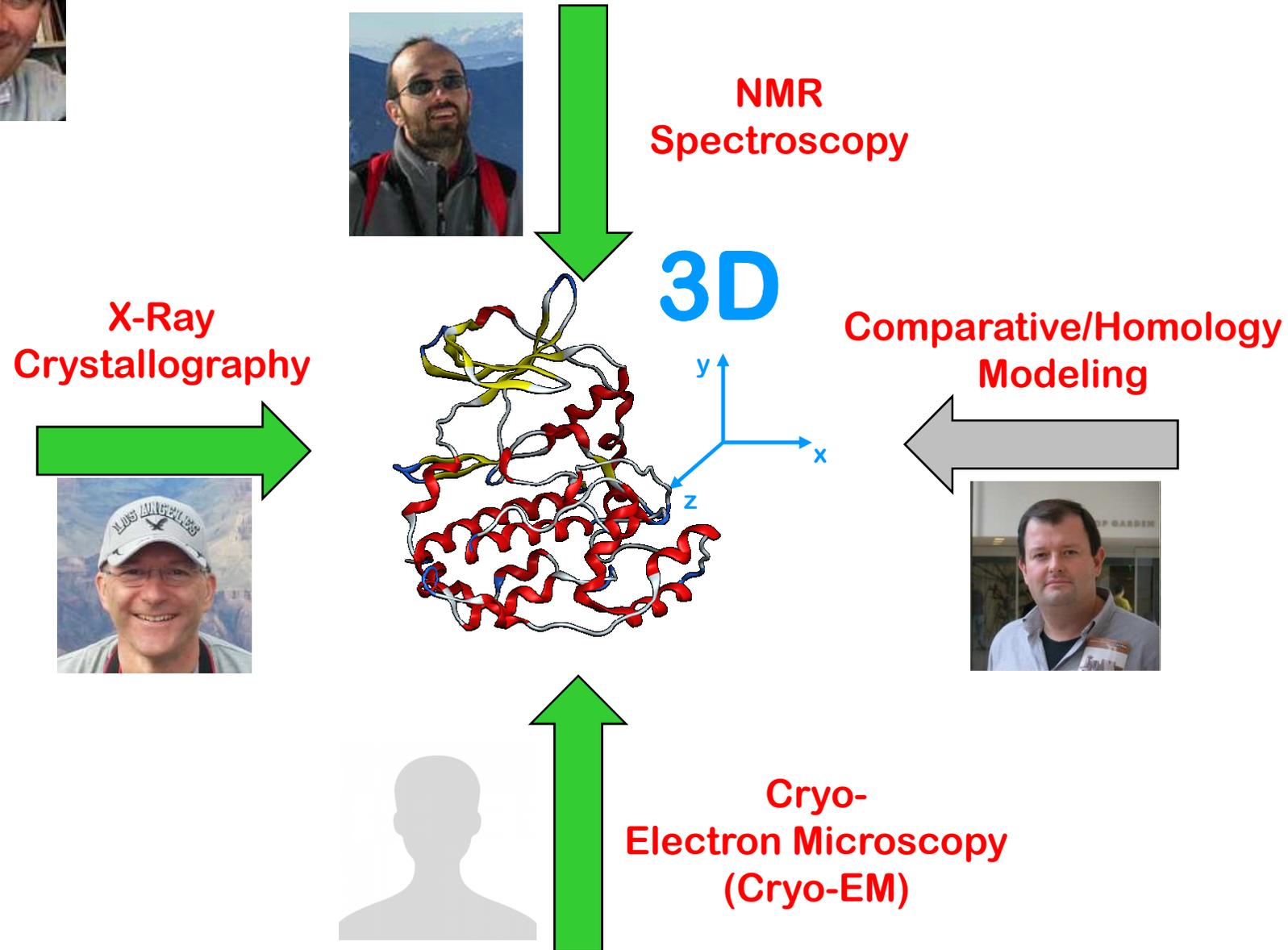


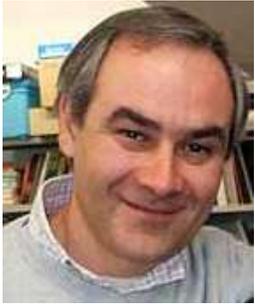
**3D**



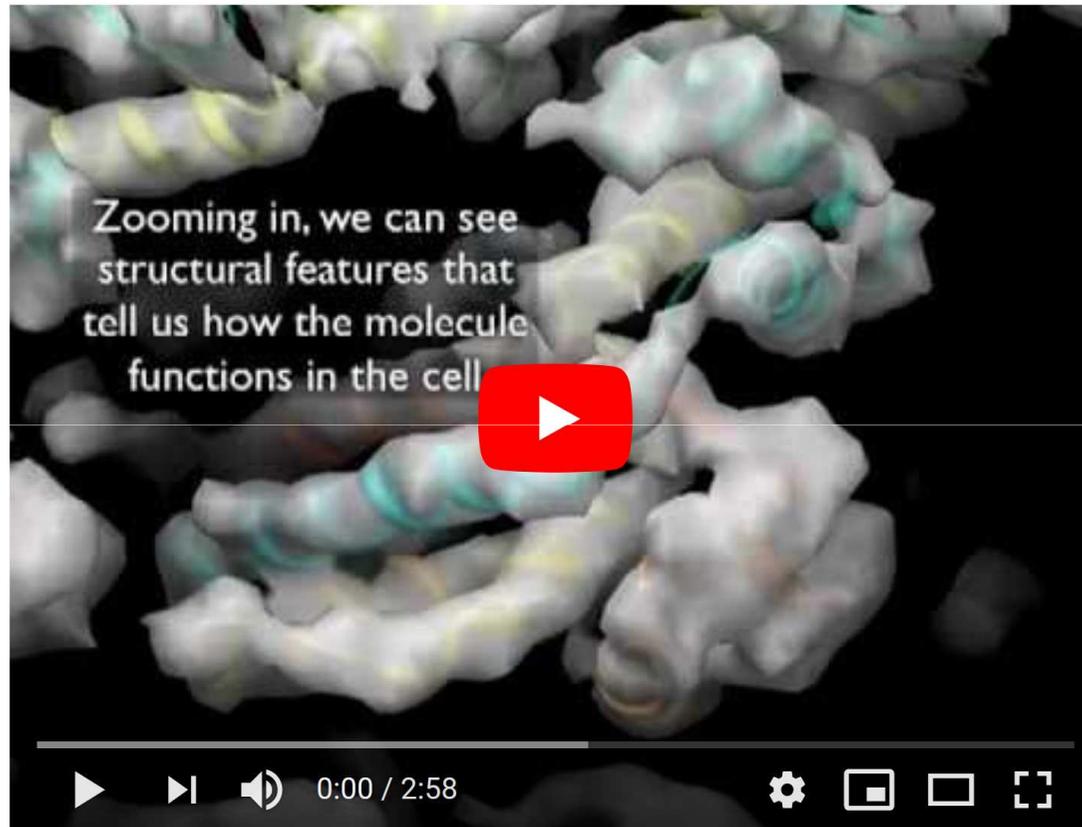


# We love Silvio but, ptacmatically, we prefer...





# Cryo-EM: the future of structural biochemistry is today!



A 3 minute introduction to CryoEM

credits: <https://www.youtube.com/watch?v=BJKkC0W-6Qk>

