CECAM Discussion-Meeting

"Modelling bio-molecular interactions: A multi-scale approach joining theory and experiment"

Université Paris-Est Marne-La-Vallée
Laboratoire de Modélisation et Simulation Multi Echelle
Equipe de Chimie Théorique

Thursday, 18.05.2017

09:00h	**Welcome & Coffee**
09:30h - 10:05h	**Ulli Englert** Bio-molecular interactions: Experimental input from chemical crystallography
10:05h - 10:40h	**Antonia Mey** Predicting Ligand Protein Interactions with Alchemical Free Energy Methods on Blinded Datasets
	Discussion and coffee break
11:20h - 11:55h	**Paolo Carloni** Multiscale simulations in molecular medicine: recent advances from Jülich
11:55h - 14:00h	***LUNCH***
14:00h - 14:35h	**Domenica Dibenedetto** Learn about learning, from a computational neuroscientific perspective
14:35h - 15:10h	**Dulce Papy-Garcia** Tau protein and heparan sulfates interaction in Alzheimer's disease
	Discussion and coffee break
15:50h - 16:25h	**Eric Ruelland** Biomolecular interactions in situation: The example of phytohormones
16:25h - 17:00h	**Xioajing Cong** Molecular dynamics simulations of GPCR-ligand interactions and GPCR activation
17:00h – 17:30h	***Discussion***

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Friday, 19.05.2017

09:30h - 10:05h	**Majdi Hochlaf** On the role of small S-nitrosothiols (RSNOs) as light-sensitive NO-donors for delivery in biological media
10:05h – 10:40h	**Gwenaëlle André-Leroux** OH1 from Orf virus: a new tyrosine phosphatase that displays distinct structural features and triple substrate specificity
	Discussion and coffee break
11:20h - 11:55h	**Isabelle Demachy** Photoswitching mechanism of the Fluorescent protein Padron
11:55h - 14:00h	***LUNCH***
14:00h - 14:35h	**Maximilien Levesque** Free energy of solvation of molecules of any size in few minutes by molecular density functional theory
14:35h – 15:10h	**Lucie Delemotte** A multiscale computational approach to explore the complex dynamics of an ion channel voltage sensor domain
15:10h – 15:55h	***Discussion***
~ 16:00h	*Closing remarks*