## **Table of contents**

Γuesday 07 March 2017		
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## Conference on Atomistic Simulations of Biomolecules: towards a Quantitative Understanding of Life Machinery | (smr 2828)

## Tuesday 07 March 2017

Session 4 - LB (Euler Lecture Hall) (09:00-14:00)

## AGGREGATES AND MOLECULAR SWITCHES

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time	title	presenter
09:00	Introduction - Chair: Alessandro LAIO	
09:05	Caffeine self-association in Aqueous solution: from the supramolecular to atomic scale clustering	TAVAGNACCO, Letizia
09:45	Stability of Biopolymers in Aqueous Solution. GMPC Approach	ASATRYAN, Arevik
10:25	On the development of a Novel Bio-Molecular NanoSwitch: A Theoretical Investigation	ELEL SAYED EL HABASHY, Hadeer
10:55	Coffee break	
11:25	Interaction of antimicrobial peptides with POPC lipid structures modeled by molecular dynamics simulations	BALATTI, Galo E.
11:55	Role of the subunit interactions in the conformational transitions in adult human hemoglobin: an explicit solvent molecular dynamics study	YUSUFF, Olaniyi Kamil
12:25	Lunch break	