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Conference on Atomistic Simulations of Biomolecules: towards a Quantitative Understanding of Life Machinery | (smr 2828)

Monday 06 March 2017

Session 3 - LB (Euler Lecture Hall) (14:00-17:15)

QM/MM, CATALYSIS

time	title	presenter
14:00	Introduction - Chair: Meher PRAKASH	
14:05	Moving domain QM/MM methods for interactions of human estrogen receptor alpha with endocrine disruptive chemicals	OMOLLOH, George Ochieng
14:45	An overview of environmentally persistent free radicals (EPFRs)	KIRURI, Lucy
15:25	Coffee break	
15:55	The Catalytic Mechanism of Pfk-2: first computational approximation	CABALLERO, Julio
16:35	Insights into N-glycosylation machinery	VERLI, Hugo