

**CM1406****Epigenetic Chemical Biology – Action CM1406****Computational Methods in Drug Design****Student Training Meeting****22 – 24 March 2018****Kadir Has University – Istanbul**

Time	Speaker	Title	Chair
<b>22<sup>nd</sup> of March - Thursday</b>			
09:00 – 09:30	Registration		
09:30 – 9:45	Kemal Yelekçi	Welcome	
9:45 – 11:30	A.Ganesan	Epigenetic targets	Kemal Yelekçi
11:30 -12:00	Coffee break		
12:00 – 12:45	Sheraz Gul	The properties of a lead and clinical candidate compound	
13:00 – 14:00	Lunch		
14:00 – 14:45	Katarina Nikolić	Computer-aided design of multitarget ligands	Katarina Nikolić
14:45 – 15:30	Maija Lahtela	Virtual screening of sirtuin modulators	
15:30 – 16:00	Coffee break		
16:00 – 16:45	Kemal Yelekçi	In silico modeling of histon deacetyase enzyme and design of novel inhibitors	Katarina Nikolić
Free evening			
<b>23<sup>th</sup> of March– Friday</b>			
09:30 – 12:00	Abdullahi I. Uba	Case Study: Practical application how to design selective and potent HDAC inhibitors	Maija Lahtela
12:00 – 14:00	Lunch		
14:00 – 14:45	Demet Akten Akdoğan	Discovery of high affinity ligands for $\alpha$ -2-adrenergic receptor through pharmacophore-based high-throughput virtual screening and docking	Maija Lahtela

14:45- 15:15	Sheraz Gul	<i>In-vitro</i> aspects of ADME and lead optimization.	
15:15 – 17:15	Akram Alian	Application of crystallography to proteins ?	Maija Lahtela
19:00	Farewell Dinner		
<b>24<sup>th</sup> March Saturday</b>			
09:00 – 12:00	Teodora Djicic	Homology modeling and application to dopamine transporter (DAT)	
12:00- 14:00	Lunch		
14:00- 15:00	Discussions and Final Remarks (A.Ganesan and Kemal Yelekçi)		