



## **“Discovery of novel Arp2/3 inhibitors: Synthesis, in silico design and in vitro analysis”**

**Greece-Turkey bilateral collaboration project**

**3<sup>rd</sup> Project Meeting  
17-18 March 2015**

**Biomedical Research Foundation, Academy of Athens  
Athens, Greece**

### **Tuesday 17 March**

11:00 – 11:30 The synthesized small Arp2/3 inhibitors with their in vitro and in silico results.  
Dr Levent Çavas

11:30 – 12:00 Presentation of overall progress on synthetic strategies for the optimization of the known Arp2/3 inhibitors CK-666 and CK-869 and the carbazole-oxazolone library.  
Dr Mustafa Yavuz Ergün

*12:00 – 12:10 Coffee break*

12:10 – 13:00 Guest Lecture: 3D Quantitative structure-activity relationships employed for the optimization of CK-666  
Dr. Eleni Vrontaki & Dimitra Petropoulou

*13:00 – 14:00 Lunch*

14:00 – 14:30 Optimization of CK-666 using Free Energy Perturbation calculations  
Dr. Evi Gkeka

14:30 – 15:00 Presentation of overall progress of the project from the Greek team  
Zoe Cournia

15:00 – 15:30 *Coffee Break*

15:30 – 17:00 Discussion on structure-activity relationships of CK-666

18:00 *Visit to the Athens Science Festival*  
<http://www.athens-science-festival.gr>

21:00 *Dinner*

### **Wednesday 18 March**

10:00 – 10:30 Optimization of CK-869 using Free Energy Perturbation calculations  
Theodora Tafari

10:30 – 11:00 Effect of CK-666 and CK-869 on the structure and dynamics of the Arp2/3 studied with MD simulations  
Dr. Spyros Vicatos

11:00 – 13:00 Discussion on the structure-activity relationships of the CK-666/CK-869 analogs and further synthetic strategies for the production of optimized analogs.

13:00 – 14:00 Lunch

End of Project Meeting

