2016 YILI TÜBİTAK BİLİM TEŞVİK ÖDÜLÜ ALAN **DOÇ. DR. SERDAR DURDAĞI** (BAHÇEŞEHİR ÜNİVERSİTESİ) İLAÇ SALINIMI VE BİYOLOJİK AKTİF BİLEŞİKLER DERSİNİN MİSAFİR ÖĞRETİM ÜYESİ OLARAK 14 KASIM 2016 PAZARTESİ GÜNÜ 10.30-12.00 ARASI SEMİNER VERMEK ÜZERE GELECEKTİR.

SEMİNERE KATILMAK İSTİYENLERE DUYURULUR:

TARİH: **28 KASIM 2016**

SAAT **10.30-12.00**

SINIF: **B2D13**

KONU:

**Virtual Screening of Small Molecules Databases: Combination of Molecular Modeling and Experimental Studies**

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In this talk, examples of structure-based and ligand-based screening of small molecules databases for different targets will be highlighted. Filtered structures based on predicted binding energy results using high throughput virtual screening (HTVS) techniques are used in more sophisticated molecular simulations approaches (i.e., Glide/SP, Glide/XP, Induced Fit Docking- IFD, and Quantum Mechanics Polarized Ligand Docking- QPLD). Potent high binding affinity compounds that are predicted by molecular simulations are then tested by long molecular dynamics (MD) simulations. The molecular mechanism analysis, Free Energy Perturbation calculations using long multiple MD simulations for the identified compounds which show high predicted binding affinity against specific target structures, as well as structure-based pharmacophore development (E-pharmacophore) studies (Figure 1) will be summarized.1-9



**Figure 1.** E-pharmacophore modeling resulted 6-sited AAADRR hypothesis as top-scored hypothesis for both known PARP-1 inhibitors CHEMBL2322618 and olaparib.