Supplementary Materials

Investigation of PDE5/PDE6 and PDE5/PDE11 Selective Potent Tadalafil-like PDE5 Inhibitors Using Combination of Molecular Modeling Approaches, Molecular Fingerprint-Based Virtual Screening Protocols and Structure-based Pharmacophore Development

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Figure S1. Aminoacid sequence alignments of PDE6 andPDE11 over PDE5 catalytic site residues. Alignment procedure was achieved with Blosum62 matrix via MOE software.

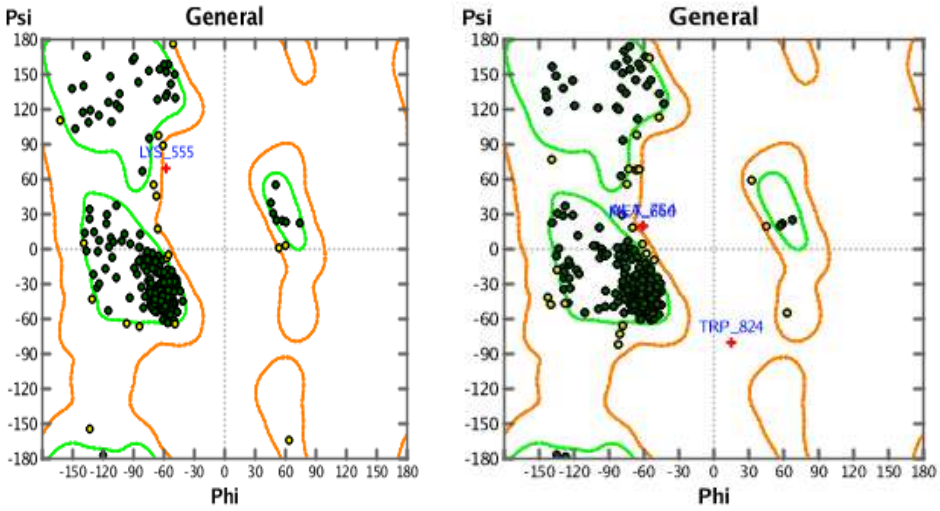

Figure S2. Ramachandran plots of the homology models of PDE6 and PDE11.

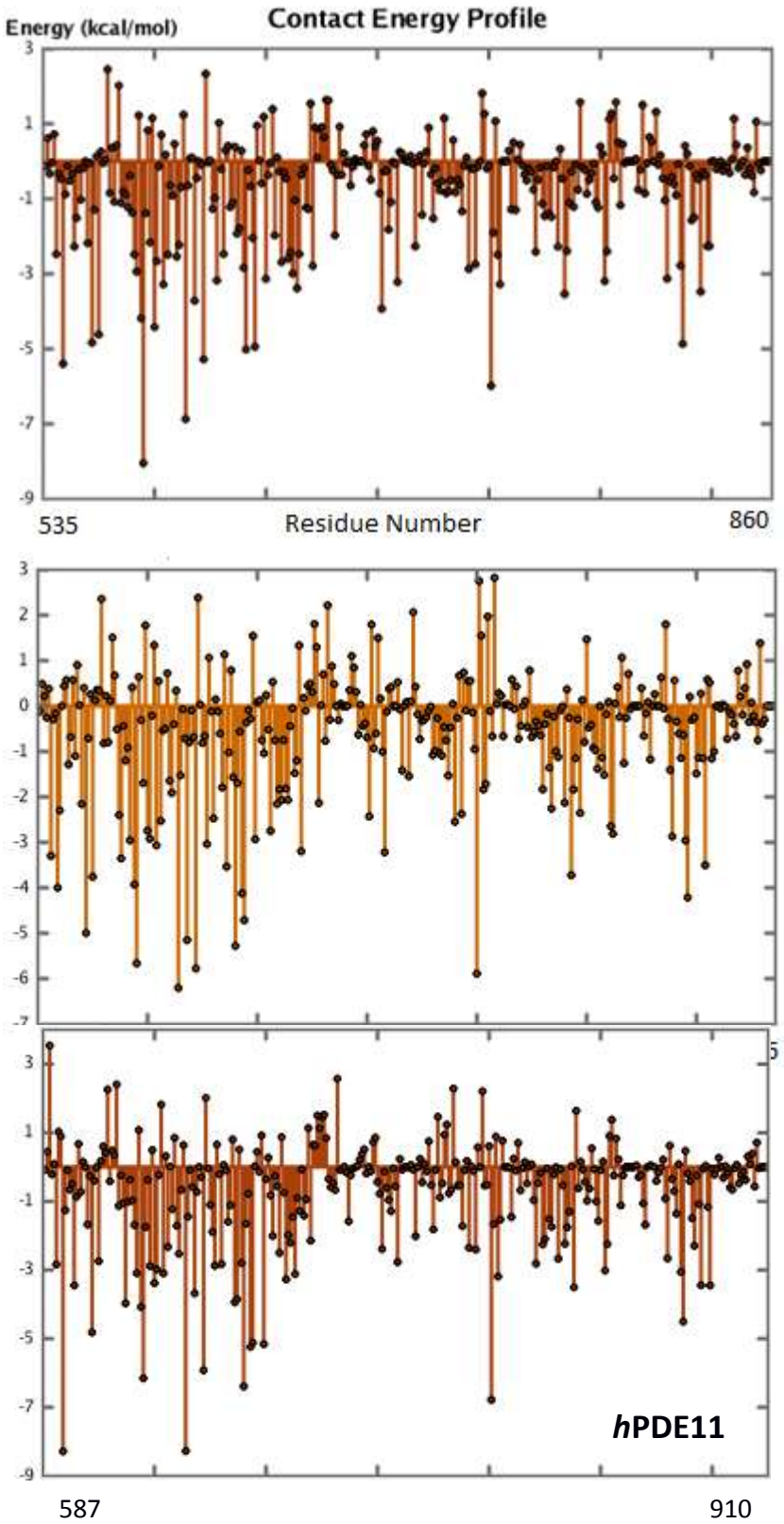

Figure S3. Contact Energy Profiles of the catalytic side residues that correspond to PDE5, PDE6 and PDE11. The x axis and y axis represent the aminoacid residues numbering and atom-atom contact pair energies in kcal/molunit, respectively.

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	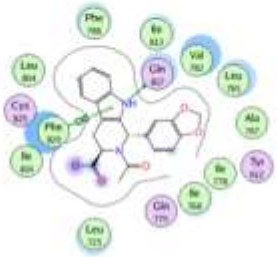	
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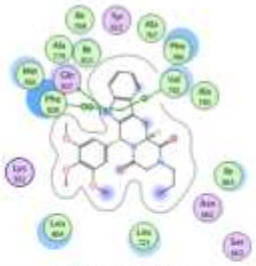		
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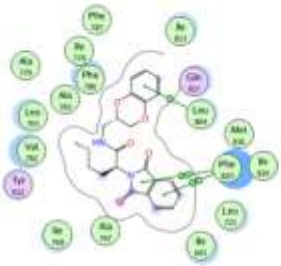	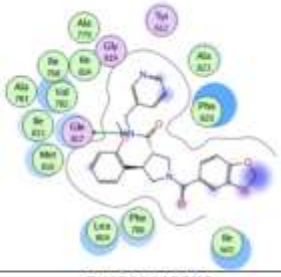	
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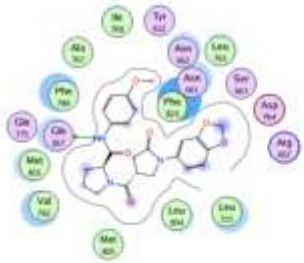		

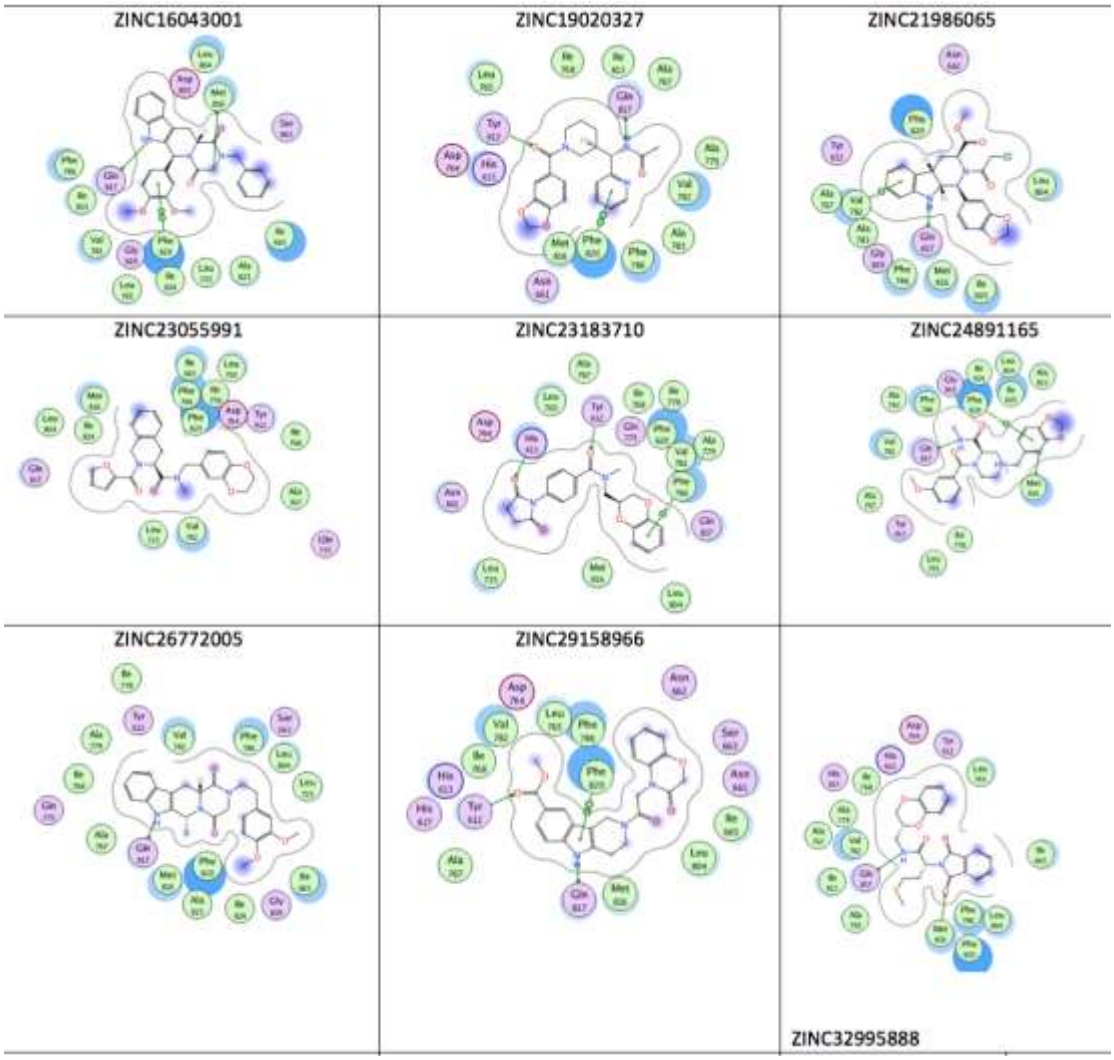

Figure S4. 2D protein-ligand interaction diagrams of the selected compounds (Table 1) with the catalytic site residues of PDE5.