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Efpraxia Tzortzini

Molecular Biologist, M.Sc., Ph.D.

Languages

Greek (Native)
English (Full professional)
German (Limited working)
Spanish (Limited working)

Skills

- Docking (GOLD, Glide)
- Molecular Modelling
- Molecular Dynamics (MD) Simulations (Gromacs, Desmond, AMBER)
- Coarse – Grained MD Simulations
- Accurate binding free energy calculations
- VMD, PyMoL
- Data analysis and presentation
- Unix/Linux based operating systems
- Python
- SQL

Honors and Awards

- PhD scholarship from the second call of the Hellenic Foundation for Research and Innovation Scholarships to PhD Candidates. (2019-2022)
- Award performance from State Scholarships Foundation. (2010-2011)
- Entry Scholarship from State Scholarships Foundation. (2010)
- Award from Eurobank EFG program "The great moment for education" (2009-2010)

Education

PhD in Computational Chemistry (2018 – 2023)
National & Kapodistrian University of Athens, Athens, Greece
Thesis title: Study of State-dependent Allosteric Cholesterol Binding Sites in Adenosine A_{2A}, A_1 Receptors Using Coarse-Grained Molecular Dynamics Simulations in Plasma Mimetic Membranes.

MSc in Drug Discovery and Translational Biology (2015 – 2016)
University of Edinburgh, Edinburgh, UK
Thesis title: Classification of AAA+ proteins: a virtual screening approach.

Degree in Molecular Biology and Genetics (2010 – 2014)
Democritus University of Thrace, Alexandroupolis, Greece
Thesis title: Comparative detection of COL6A4P1 expression in normal and tumor samples for potential clinical use.
Thesis accomplished at the University of Liverpool under the Erasmus program.

Experience

National & Kapodistrian University of Athens, Athens, Greece
(July 2018 – now)
Working on computer-aided drug design of new allosteric antagonists for P2X7 receptor, studying the protein – lipid interactions for the A_1 & A_{2A} adenosine receptor and studying the E channel of the SARS-CoV-2 virus.

Biomedical Research Foundation of the Academy of Athens, Athens, Greece
(December 2014 - May 2015)
Study of the mechanisms by which the human interferon genes responds to virus infection.

Democritus University of Thrace, Alexandroupolis, Greece
(February 2013 – March 2014)
Familiarization with molecular biology techniques from DNA extraction and cloning to protein expression and purification.

Publications

Tzortzini E, Kolocouris A. Molecular Biophysics of Class A G Protein Coupled Receptors–Lipids Interactome at a Glance—Highlights from the A_{2A} Adenosine Receptor. Biomolecules 2023, 13(6), 957.

Tzortzini, E.; et al. Comparative Study of Receptor-, Receptor State-, and Membrane-Dependent Cholesterol Binding Sites in A_{2A} and A_1 Adenosine Receptors Using Coarse-Grained Molecular Dynamics Simulations. J. Chem. Inf. Model. 2023.

Liolios, C.; Patsis, C.; Lambrinidis, G.; *Tzortzini,E.;* et al. Investigation of Tumor Cells and Receptor-Ligand Simulation Models for the Development of PET Imaging Probes Targeting PSMA and GRPR and a Possible Crosstalk between the Two Receptors. Molecular PET Imaging Probes, Tumor cell Models and Computational Chemistry Models. Mol Pharm. 2022 Jul 4;19(7):2231-2247.

Stampelou, M.; Suchankova, A.; *Tzortzini, E.;* et al. Dual A_1/A_3 Adenosine Receptor Antagonists: Binding Kinetics and Structure-Activity Relationship Studies Using Mutagenesis and Alchemical Binding Free Energy Calculations. J Med Chem. 2022 Oct 13;65(19):13305-13327.

Toft-Bertelsen, T.L.; Jeppesen, M.G.; *Tzortzini, E.* et al. Amantadine has potential for the treatment of COVID-19 because it inhibits known and novel ion channels encoded by SARS-CoV-2. Commun Biol. 2021 Dec 1;4(1):1347.

Lagarias P., Barkan K, *Tzortzini E.*, et al. Insights to the Binding of a Selective Adenosine A_3 Receptor Antagonist Using Molecular Dynamic Simulations, MM-PBSA and MM-GBSA Free Energy Calculations, and Mutagenesis. J Chem Inf Model. 2019 Dec 23;59(12):5183-5197.