10th International Symposium on Computational Methods in Toxicology and Pharmacology Integrating Internet Resources

Book of abstracts

James Devillers (CTIS, France)
Athina Geronikaki (University Thessaloniki, Greece)
Organizers

CMTPI-2019
Ioannina, Greece, 23-27 June, 2019

Computational Methods in Toxicology and Pharmacology Integrating Internet Resources
(CMTPI-2019)
Ioannina, 23-27 June, 2019

Sunday 23 June

10.00-18.00 **Registration**

Monday 24 June

08.30-10.00 **Registration**
10.00-10.30 **Opening Ceremony**
J. Devillers (France) and **A. Geronikaki** (Greece)

Opening Lectures (Chairpersons: **J. Devillers** and **A. Geronikaki**)

10.30-11.00 **A. Tsantili-Kakoulidou** (Greece). Fraction Lipophilicity Index (FLI). A drug-like metric for orally administered ionizable drugs.
11.00-11.30 **A.K. Saxena** (India). ATP synthase inhibitors as anti-tubercular agents: QSAR studies in novel substituted quinolines.
11.30-12.00 **G. Gini** (Italy). Could deep learning in neural networks improve the QSAR models?

12.00-14.00 Lunch

Internet Tools and Databases (Chairpersons: **K.T. No** and **T. Puzyn**)

14.00-14.30 **V. Poroikov** (Russia). Online resource for prediction of multitarget anti-HIV agents.
14.30-15.00 **E.V. Radchenko** (Russia). Advanced neural network approach and online service for prediction and analysis of pharmacokinetic properties and toxicity of organic compounds.
15.00-15.30 **U. Maran** (Estonia). Best practices for the predictive model reporting – way towards transparency and reproducibility of *in silico* models.
15.30-15.50 **V.M. Alves** (USA). The Multi-Descriptor Read Across (MuDRA) as a novel computational approach for chemical toxicity prediction.

15.50-16.30 Coffee Break

Endocrine Targets (Chairpersons: **A. Furuhama** and **M. Vracko)**

16.30-17.00 **A. Szymoszek** (Germany). Modeling of endocrine disrupting properties for regulatory purposes.
17.00-17.30 **E. Benfenati** (Italy). *In silico* models towards aromatase inhibition of conazoles.
17.30-17.50 **H. Tzoupis** (Greece). Gonadotropin releasing hormone and GnRH receptor: Structure and drug development prospects.

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Gonadotropin releasing hormone and GnRH receptor: Structure and drug development prospects

Haralambos Tzoupis[1], Agathi Nteli[1], Marilena Androutsou[2] and Theodore Tselios[1]

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Gonadotropin Releasing Hormone (GnRH) is a key aspect in the sexual maturation and regulation of the reproductive cycle in humans. GnRH interacts through the activation of the Gonadotropin Releasing Hormone Receptors (GnRHR). Any impairments/ dysfunctions of the GnRH– GnRHR complex lead to the development of various cancer types and disorders. GnRHR is part of the rhodopsin G-protein-coupled receptor family and comprises seven trans–membrane helical domains connected via extra– and intra–cellular segments. The development of robust computational tools has provided the necessary tools for a cost-effective way to rationally design new innovative pharmaceutical molecules. *The lack of any structural data for GnRHR impedes the design of new drugs.* Our aim is to construct a model of GnRHR in order to be implemented for the rational design of altered peptide GnRH analogues. Moreover, molecular dynamics (MD) simulations have been employed for the refinement of the model and to explore the impact of the bilayer membrane in GnRHR conformation. Additionally, we have implemented the information from our model on GnRHR to design and synthesize altered peptide as potential anti-cancer agents.

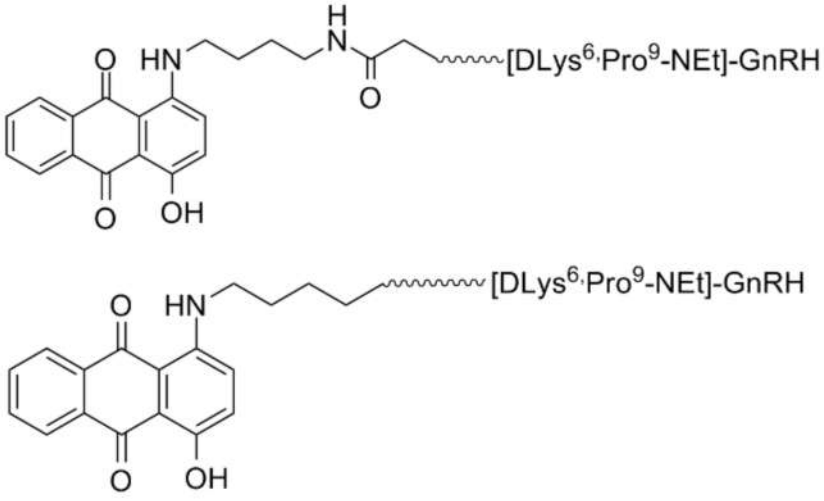

Figure: Designed anthraquinnone analogues as anti-cancer agents.