

## Tentative Outline

### Special Thematic Issue for the journal : *Current Drug Targets*

#### Title of the Thematic Issue: Medicinal Chemistry Studies of Hybrid Compounds

Guest Editors: Dr. Luciana Scotti and Dr. Marcus T. Scotti

- **Scope of the Thematic Issue:**

Hybrid compounds are formed by two pharmacophores group membership. Despite being formed by two pharmacophore groups, the hybrid drug may offer greater efficacy and adherence to treatment. The hybrid molecules can often exhibit two or more activities acting as multi-target drug. This began to be possible thanks to new methodologies in various areas of medicinal chemistry, that comprise synthesis, natural products, semi-synthesis, evaluation of biological activities, and / or theoretical approaches the ligand-based, structure-based approaches, SAR, QSAR, docking and several cheminformatics methods.

Several free ligand databases are widely available today. Virtual structure-based screening has become prominent in drug discovery. Using homology of peptides, crystallographic or modeled protein structures, molecular docking is often employed to screen compound libraries and to predict the conformation of a protein-ligand complex and calculate its affinity energy. Targeting these interactions with small molecule inhibitors as well as searches for new targets is of increased interest for therapeutic purposes of diseases.

This special issue will be dedicated to all hybrid chemicals (drugs, organic compounds, nanoparticles), including (but limited to) multiple mechanisms of action.

**Keywords:** hybrid compounds, drug, disease, medicinal chemistry, target, inhibitors.

#### Schedule:

- ✧ Authors submission deadline: 15<sup>th</sup> November, 2021.
- ✧ Tentative submission of revised manuscript: 30<sup>th</sup> January, 2022.
- ✧ Submission of issue: 15<sup>th</sup> February 2022.

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