

Tentative Outline

Special/Thematic Issue for the journal "Current Pharmaceutical Design - CPD"

Tentative Title: Artificial intelligence in the Drug Discovery pipeline – Are we on the right track or just the fast track?

Guest Editor: Dakshinamurthy Sivakumar & Sangwook Wu

Scope of the Thematic Issue:

Artificial intelligence concepts are widely used in computer-aided drug design to expedite the drug discovery process by reducing time and cost. But there are many questions to be answered, including the usage of voluminous and right data, effective model building and reproducibility, and reusability. This issue welcomes the articles which support the AI-based methods that support the drug designing process and the pros and cons associated with it.

Keywords: drug design, voluminous, reproducibility, reusability, Artificial intelligence

Sub-topics:

- Unsolved problems and solutions using AI approaches
- Virtual screening using large databases – by applying AI methods
- Deep learning for targeted drug design
- Machine learning-based free energy calculations
- Lead optimization and property predictions using traditional methods and ML models
- Developing meaningful chemical fragmented using AI methods
- Comparison of selectivity and specificity in drug design using AI and traditional methods.
- Tracking the critical interacting water molecules using ML models and novel methods
- Developing effective models using optimal datasets
- Classical methods are still the best and not outdated
- Hybrid of traditional and machine learning methods in drug design
- Conventional drug discovery methods and its improvisation with and without AI approaches.

Tentative titles of the articles:

- A systematic review on conventional drug discovery methods with and without AI methods
- Conventional drug discovery methods and their improvisation with and without AI approaches.
- Selectivity and specificity in drug design using AI and traditional methods
- Review on machine learning approaches for SARS CoV2 research
- Artificial intelligence approaches for rational drug design and discovery
- Role of critical interacting water molecules using different theoretical methods
- Drug discovery methods – pre and post-AI era
- Accelerated drug discovery process by AI-assisted large scale screening
- Lead optimization and property predictions using traditional methods
- Hybrid of traditional and machine learning methods in drug design

Schedule:

- ✧ Complete Thematic issue submission deadline: **September 2022**

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