# Special Issue

# QSAR Approaches in Contemporary Molecular Engineering

## Message from the Guest Editors

This Special Issue is focused on application of cutting-edge QSAR approaches in molecular engineering from the following aspects:

- Prediction and modeling of antibacterial, antifungal, and antiviral activity;
- Prediction and modeling of anticancer activity;
- Prediction and modeling of antioxidant activity;
- Prediction and modeling of anti-inflammatory activity;
- Molecular docking;
- Molecular dynamics;
- Pharmacophore design;
- Modeling of drug–drug interactions;
- QSAR-guided design of nanomaterials and biomaterials;
- Hybrid approaches combining QSAR with molecular descriptors;
- Predictive modeling for natural product derivatives;
- Application of artificial intelligence in QSAR processes.

## Guest Editors

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## Deadline for manuscript submissions

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