

Special Issue

Studies of Protein–Ligand Interactions in the Evaluation of the Biological Activity of Compounds

Message from the Guest Editor

The interactions of drugs and environmental contaminants with proteins have a significant influence on the pharmacokinetic activity of compounds, for example, the transport across biological barriers in humans and animals, the availability of free (unbound) compounds, and the binding to receptors and enzymes. We welcome submissions of original research papers and reviews focused on (but not limited to) the following:

- Experimental (in vivo, ex vivo, in vitro) or in silico (e.g., by molecular docking or dynamic simulation methods) studies of protein–ligand interactions with a focus on the therapeutic activity of compounds;
- Experimental and computational investigations of protein–ligand interactions leading to compound toxicity or interactions with drugs;
- Studies of protein–ligand interactions influencing the ADME properties of compounds;
- Novel methodologies of quantitative and qualitative studies of protein–ligand interactions;
- Simplified/surrogate/theoretical models of enzymes or receptors to be used in experimental or computational studies of protein–ligand interactions.

Guest Editor

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Message from the Editor-in-Chief

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Editor-in-Chief

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