



Artificial Intelligence Applied to Medicinal Chemistry and Structural Biology

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Message from the Guest Editor

The usage of artificial intelligence (AI) has been increasing in several sectors of society. Particularly in drug design endeavors, it has been successfully applied in several areas. Moreover, in structural biology research, AI has been used in fields such as molecular simulations, protein engineering, and quantum enzymology. It is well known that in medicinal chemistry and structural biology, an important task is the analysis and processing of the multivariable chemical and biological spaces that are organized in huge databases. To celebrate the success story and the advances on the applications of AI in Medicinal Chemistry and Structural Biology, I invite fellow scientists to submit original papers or reviews, which will be published as a Special Issue on “Artificial Intelligence Applied to Medicinal Chemistry and Structural Biology”.

We look forward to your contribution.





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Editor-in-Chief

Prof. Dr. Amélia Pilar Rauter

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Message from the Editor-in-Chief

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