

Special Issue

Pesticide Molecular Modeling: From Properties to Toxicology

Message from the Guest Editor

This Special Issue aims to bring together contributions in this field. Topics for this Special Issue will include the development of new in silico approaches for pesticide discovery, as well as applications of established methods, such as molecular docking, molecular dynamics, pharmacophore modeling, homology modeling, and/or hybrid QM/MM or QM/QM^{*} simulations. Submissions focused on determining key pesticide properties through quantum mechanics methods are also welcome.

Guest Editor

Prof. Dr. Jean-Yves Le Questel

Laboratoire CEISAM, UMR CNRS 6230, Université de Nantes, F-44000 Nantes, France

Deadline for manuscript submissions

closed (24 June 2025)



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MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
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Prof. Dr. José L. Quiles
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Avda. Conocimiento s/n, 18100 Armilla, Granada, Spain

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