Theoretical prediction of the environmental impact of pesticides

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Language Spanish

Description:

Proyecto asignado a través de la Red Española de Supercomputación (RES [2]).

The project will develop a large database of quantum chemical calculation of pesticide that will be central part of an expert system to predict the environmental impact of pesticides based exclusively in Quantum Chemistry calculations.

The ultimate goal is to develop and validate new computational tools to predict the impact of pesticides and their degradation products, providing new predictive decision-making tools in environmental policy.

Web:

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Links

[1] https://www.uam.es/uam/inicio [2] https://www.res.es/