

Quantum-chemical study with application of the PCM model on correlation between biological activity and molecular structure of 5-amino-3-methylisoxazole-4-carboxylic acid hydrazide Schiff base derivatives.

Autorzy

Aneta Jezierska
Jarosław Panek
Stanisław Ryng
Michał Zimecki
Adam Fedorowicz
Aleksander Koll

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Streszczenie

Theoretical calculations on 5-amino-3-methylisoxazole-4-carboxylic acid hydrazide Schiff base derivatives using Polarizable Continuum Model in order to account for water solvation effects are presented. The compounds studied exhibit biological (immuno-suppressing or immunostimulating) activity, measured experimentally in various assays. The quantum chemical DFT calculations are used to obtain electronic descriptors of molecular structure. These descriptors, together with other physicochemical parameters, are used to derive quantitative relationships between the structure and the biological activity.