# Structure activity investigations of 5-substituted 3-methylisoxazole[5,4-d]1,2,3-triazin-4-one derivatives.

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The series of 5-substituted 3-methylisoxazole[5,4-d]1,2,3-triazin-4-one derivatives was obtained by diazotization of 5-amino-3-methylisoxazol-4- carboxylic acid hydrazide. The immunological activity of these compounds was investigated experimentally in several in vitro and in vivo assays in mice and human models. In the next step, quantum-chemical investigations were performed using density functional theory with the B3LYP hybrid exchange-correlation energy functional and 6-31G(d,p) basis set. The Polarizable Continuum (SCRF/PCM) solvent model was also taken into account in order to show solvent influence on electron density and electrostatic potential around the exemplary molecules. Correlations between molecular structure and biological properties were found using a stepwise selection of scales for the multiple linear regression (MLR).

Słowa kluczowe

5-substituted 3-methylisoxazole[5, 4-d]1, molecule, 3-triazin-4-one, DFT, Immunological activity, Molecular properties, SCRF/PCM

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