

Polishchuk Pavel

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Structural, physicochemical and stereochemical interpretation of QSAR models based on simplex representation of molecular structure

Polishchuk Pavel¹, Mokshyna Elena², Kosinskaya Anna², Muats A.³, Kulinsky M.², Tinkov Oleg⁴, Ognichenko L.², Khristova Tetiana², Artemenko Anatoliy², Kuz'min V.²⁵

¹ Palacký University Olomouc,

² A.V. Bogatsky Physico-Chemical Institute of the NAS of Ukraine,

³ Odessa National University,

⁴ T.G. Shevchenko State University of Pridnestrovie, Tiraspol,

⁵ Odessa Polytechnic National University

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