

The computational approach for rational monomer selection in molecularly imprinted polymer synthesis [Online resource]

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A computational approach to study functional monomer-protein molecular interactions to optimize protein molecular imprinting

Boroznjak, Roman; Reut, Jekaterina; Tretjakov, Aleksei; Lomaka, Andre; Öpik, Andres; Sõritski, Vitali Journal of molecular recognition 2017 / art. e2635, p. 1-9 : ill <https://doi.org/10.1002/jmr.2635>

Correlation of blood-brain penetration and human serum albumin binding with theoretical descriptions

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Correlation of the melting points of potential ionic liquids (Imidazolium Bromides and Benzimidazolium Bromides) using CODESSA program [J.Chem.Inf.Comput.Sci. 42, 225-231 (2002)]

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In silico approach to finding new scaffolds for LRRK2 inhibition

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Linearization of moment tensor potentials

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Linearization of moment tensor potentials for multicomponent systems with a preliminary assessment for short-range interaction energy in water dimer and trimer

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[Journal metrics at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

QSAR study of pharmacological permeabilities

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Topological fingerprints as an aid in finding structural patterns for LRRK2 inhibition

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Using a private desktop grid system for accelerating drug discovery

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