

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

Boroznjak, Roman; Lomaka, Andre; Sõritski, Vitali; Reut, Jekaterina Tartu Ülikooli ASTRA projekt PER ASPERA : Funktsionaalsed materjalid ja tehnoloogiad : [7-8 märts 2017, Tartu : teesid] 2017 / [1] p. : ill <http://fmdtk.ut.ee/teesid/>

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

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

Karelson, Mati; Dobchev, Dimitar; Tamm, Tarmo; Tulp, Indrek; Jänes, Jaak; Tamm, Kaido; Lomaka, Andre; Savchenko, Deniss; Karelson, Gunnar Arkivoc 2008 / XVI, p. 38-60 : ill <https://www.arkat-usa.org/get-file/26925/>

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)]

Katritzky, Alan R.; Jain, Ritu; **Lomaka, Andre; Petrukhin, Ruslan; Karelson, Mati**; Visser, Ann E.; Rodgers, Robin D. Journal of chemical information and modeling 2005 / 2, p. 533-534 <https://pubs.acs.org/doi/10.1021/ci049691z>

In silico approach to finding new scaffolds for LRRK2 inhibition

Kahn, Iiris; Lomaka, Andre; Karelson, Mati European Pharma Summit : Berlin, Germany, May 5-8, 2015 : abstracts 2015 / [1] p

Linearization of moment tensor potentials

Lomaka, Andre; Tamm, Toomas 10th Congress of the International Society of Theoretical Chemical Physics, Tromsø, 11-17 July 2019 : ISTCP-X : book of abstracts 2019 / Poster: P1-61 <http://istcp-2019.org/assets/pdf/BookOfAbstracts.pdf>

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

Lomaka, Andre; Tamm, Toomas The Journal of chemical physics 2020 / art. 164115, 8 p. : ill <https://doi.org/10.1063/5.0007473> [Journal metrics at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

QSAR study of pharmacological permeabilities

Karelson, Mati; Karelson, Gunnar; Tamm, Tarmo; Tulp, Indrek; Jänes, Jaak; Tamm, Kaido; Lomaka, Andre; Savtšenko, Deniss; Dobchev, Dimitar Arkivoc 2009 / 2, p. 218-238 : ill <https://citeseerx.ist.psu.edu/document?repid=rep1&type=pdf&doi=04010557f978e40f8e33b61f9570340690f7940e>

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

Kahn, Iiris; Lomaka, Andre; Karelson, Mati Molecular informatics 2014 / p. 269-275 : ill <https://doi.org/10.1002/minf.201300057> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Using a private desktop grid system for accelerating drug discovery

Kovacs, Jozsef; Kacsuk, Peter; **Lomaka, Andre** Future generation computer systems 2011 / p. 657-666 : ill