

Computational chemistry approaches for understanding how structure determines properties

Katritzky, Alan R.; Slavov, Svetoslav H.; Radzvilovits, Maksim; Stoyanova-Slavova, Iva B.; Karelson, Mati Zeitschrift für Naturforschung B - a journal of chemical sciences 2009 / 6, p. 773-777

Computational study of cyclohexylhemicucurbiturils = Tsükloheksüülhemikukurbituriilide arvutuskeemiline modelleerimine

Öeren, Mario 2015 https://www.ester.ee/record=b4522693*est

DFT study of the cesium cation containing complexes relevant to the cesium cation binding by the humic acids = DFT arvutus Cs katiooni interaktsioonidest humiinhenditega orgaaniliste mudelühendite baasil

Tamp, Sven 2007 https://www.ester.ee/record=b2269605*est

Isobaric vapor-liquid equilibria of the ternary system methylbutyl ketone+1-pentanol+anisole

Kirss, Helle; Kuus, Mati; Siimer, Enn Journal of chemical and engineering data 2009 / p. 2128-2131 : ill
<https://pubs.acs.org/doi/10.1021/jc900058p>

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Reproducibility of QSAR/QSPR models in the scientific literature - perspective for regulatory use

Kahn, Iiris; Piir, Geven; Oja, Mare Scientific programme & book of abstracts : QSAR 2014 2014 / p. 109