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640	Theoretical investigation of phenol adsorption on functionalized graphene using DFT calculations for effective removal of organic contaminants from wastewater. <b>2021</b> , 324, 114777	11
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562	Excited-state dynamics of [Mn(im)(CO)(phen)]: PhotoCORM, catalyst, luminescent probe?. <b>2021</b> , 154, 154102	2
561	Gas-to-Particle Partitioning of Cyclohexene- and $\beta$ -Pinene-Derived Highly Oxygenated Dimers Evaluated Using COSMO. <b>2021</b> , 125, 3726-3738	5
560	Vapor Pressure and Physicochemical Properties of {LiBr + IL-Based Additive + Water} Mixtures: Experimental Data and COSMO-RS Predictions. <b>2021</b> , 50, 473-502	4
559	Application of Quantum Chemistry Insights to the Prediction of Phase Equilibria in Associating Systems. <b>2021</b> , 60, 5992-6005	2
558	Dependence of Copolymer Composition in Radical Polymerization on Solution Properties: a Quantitative Thermodynamic Interpretation. <b>2021</b> , 60, 10566-10583	1
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551	Ionic liquid-based deep eutectic solvents as novel solvent-cum-catalyst media for thermal dehydrogenation of chemical hydrides. <b>2021</b> , 46, 15773-15779	3
550	Separation of low molecular weight alcohols from water with deep eutectic solvents: Liquid-liquid equilibria and process simulations. <b>2021</b> , 533, 112949	7
549	COSMO-SAC-supported evaluation of natural deep eutectic solvents for the extraction of tea polyphenols and process optimization. <b>2021</b> , 328, 115406	10
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547	Palladium-Catalyzed Regioselective and Stereospecific Ring-Opening Suzuki-Miyaura Arylative Cross-Coupling of 2-Arylazetidines with Arylboronic Acids. <b>2021</b> , 363, 2796-2805	3
546	Phase equilibria modeling of biorefinery-related systems: a systematic review. <b>2021</b> ,	
545	VaporLiquid Equilibrium. <b>2021</b> , 7-135	
544	Docking Paradigm in Drug Design. <b>2021</b> , 21, 507-546	7
543	Machine learning of free energies in chemical compound space using ensemble representations: Reaching experimental uncertainty for solvation. <b>2021</b> , 154, 134113	9
542	Entropy-Entropy Compensation between the Protein, Ligand, and Solvent Degrees of Freedom Fine-Tunes Affinity in Ligand Binding to Galectin-3C. <b>2021</b> , 1, 484-500	5
541	Isolation of sesquiterpenoids from <i>Matricaria chamomilla</i> by means of solvent-assisted flavor evaporation and centrifugal partition chromatography. <b>2021</b> , 413, 4387-4396	0
540	Synthesis and Characterization of Macrocyclic Ionic Liquids for CO <sub>2</sub> Separation. <b>2021</b> , 60, 8218-8226	1
539	Hydrogen Bond Acceptor Propensity of Different Fluorine Atom Types: An Analysis of Experimentally and Computationally Derived Parameters. <b>2021</b> , 27, 8764-8773	6
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537	Titanocene-Catalyzed [2+2] Cycloaddition of Bisenones and Comparison with Photoredox Catalysis and Established Methods. <b>2021</b> , 60, 14339-14344	4
536	Supervised Machine Learning-Based Classification of Li <sup>+</sup> Battery Electrolytes. <b>2021</b> , 4, 1156-1162	1
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534	Densities, speeds of sound and molar heat capacities of multicomponent liquid mixtures containing 1-methylpiperidine, pyrrolidin-2-one and cycloalkanones at varying temperatures. <b>2021</b> , 156, 106389	1
533	Synthesis and Biological Evaluation of Phosphoester and Phosphorothioate Prodrugs of STING Agonist 3',3'-c-Di(2'F,2'dAMP). <b>2021</b> , 64, 7596-7616	4
532	Influences of composition and temperature on the behaviors of a binary mixture containing methanol and 1-ethylimidazole. <b>2021</b> , 330, 115503	1
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530	Characterization of Thorium-Pyrazinoic acid complexation and its decorporation efficacy in human cells and blood. <b>2021</b> , 271, 129547	3
529	Learning to Model G-Quadruplexes: Current Methods and Perspectives. <b>2021</b> , 50, 209-243	8
528	A Novel Integrated Workflow for Isolation Solvent Selection Using Prediction and Modeling. <b>2021</b> , 25, 1143-1159	4
527	Multidimensional Lewis Acidity: A Consistent Data Set of Chloride, Hydride, Methide, Water and Ammonia Affinities for 183 p-Block Element Lewis Acids. <b>2021</b> , 22, 935-943	16
526	Molecular dynamic simulations and quantum chemical calculations of adsorption process using amino-functionalized silica. <b>2021</b> , 330, 115544	19
525	Photoluminescence of Fully Inorganic Colloidal Gold Nanocluster and Their Manipulation Using Surface Charge Effects. <b>2021</b> , 33, e2101549	4
524	Improved prediction of solvation free energies by machine-learning polarizable continuum solvation model. <b>2021</b> , 12, 3584	11
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518	A Computational Protocol Combining DFT and Cheminformatics for Prediction of pH-Dependent Redox Potentials. <b>2021</b> , 26,	2
517	Process simulation coupled with LCA for the evaluation of liquid - liquid extraction processes of phenol from aqueous streams. <b>2021</b> , 41, 102077	6

516	The Representation of Cross Second Virial Coefficients by Multifluid Mixture Models and Other Equations of State. <b>2021</b> , 60, 9286-9295	2
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512	Ionic liquid-based in situ product removal design exemplified for an acetone-butanol-ethanol fermentation. <b>2021</b> , 37, e3183	2
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466	Influence of force field used in carbon nanostructure reconstruction on simulated phenol adsorption isotherms in aqueous medium. <b>2021</b> , 344, 117548	1
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