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1	Wei Ge	Machine Learning in Polymer Research	2025	Advanced Materials	link
2	Shengchao Xu	Physicochemical Properties and Molecular Interactions of Long-Chain 1-Alkanols and N-Dodecyl-2-pyrrolidone: Density, Viscosity, Thermodynamics, Spectroscopy, and Theoretical Calculations	2025	Journal of Chemical & Engineering Data	link
3	Linkun Miao	Photolytic and Thermal Reactions of [C(6)H(4)(PPh(2))(2)(mu-N(2))] and Its Lewis Acid Adducts: N-N Bond Cleavage and Liberation of N(2)	2025	Journal of the American Chemical Society	link
4	Peng Liao	QSAR modeling to describe n-octanol-water partition coefficients of perfluorinated/polyfluorinated alkyl compounds	2025	Marine Pollution Bulletin	link
5	Eunji Lee	Effect of Hydration States on the Anti-Icing/Frosting Performance of Zwitterionic Hydrogel-Coated Surfaces	2025	Langmuir	link
6	Vanessa Buchweitz	Evaluation of Green and Biobased Solvent Systems for the Extraction of beta-Carotene and Lipids from Rhodosporidium toruloides	2025	ACS Omega	link
7	Siwen Zhang	Microwave-assisted extraction of luteolin from peanut shells using natural deep eutectic solvents and its molecular mechanism	2025	Industrial Crops and Products	link
8	Xinyu Wu	Nano structural regulation of lignin and evaluation of its ultraviolet light absorption properties through quantum chemistry calculations	2025	International Journal of Biological Macromolecules	link

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9	Kong Fanzhuo	Efficient cooling crystallization of phytosterol assisted by solubility and thermodynamics analysis in organic solvents	2025	Journal of Molecular Liquids	link
10	Mahtab Moradi	Enantioseparation of ofloxacin using a liquid–liquid extraction system based on hydrophobic eutectic solvents	2025	Separation and Purification Technology	link
11	Qian Liu	Multilevel screening and mechanism analysis of ionic liquids for separating pyridine from coal pyrolysis model oil	2025	Separation and Purification Technology	link
12	Zaeem Aman	Solubility Enhancement of valine using deep eutectic Solvents: COSMO-RS and experimental validation	2025	Journal of Molecular Liquids	link
13	Dian Jin	An integrated ML model for the prediction of the melting points, phase diagrams, and eutectic points of the Type III and V deep eutectic solvents	2025	Chemical Engineering Science	link
14	Juho-Pekka Laakso	Machine learning modeling of the CO2 solubility in ionic liquids by using σ-profile descriptors	2025	Chemical Engineering Science	link
15	Shaida Panbachi	Abiraterone acetate fixed-dosed combinations with ibuprofen-based therapeutic eutectic and deep eutectic solvents	2025	International Journal of Pharmaceutics	link
16	Shirui Sun	Towards sustainable recovery of tetrahydrofuran, ethyl acetate, and methanol from waste effluent via thermal coupled extractive distillation and multi-objective optimization	2025	Process Safety and Environmental Protection	link

17	Jonathan W. Zheng	pK(a) prediction in non-aqueous solvents	2025	Journal of Computational Chemistry	link
18	Martina Bagović Kolić	Rational design of natural deep eutectic solvents contributes to desirable shift of ciprofloxacin in Biopharmaceutics classification system	2025	Journal of Molecular Liquids	link
19	Yanjiang He	The importance of process simulation to aid molecular screening of ionic liquid for acidic gas removal in natural gas	2025	Separation and Purification Technology	link
20	Yuxuan Zheng	A cross-linked sulfonated polyimide membrane with regulated acid-base interaction and high-performance for vanadium redox flow battery	2025	Journal of Membrane Science	link
21	Yichun Dong	Efficient separation of methanol, acetonitrile, and benzene ternary azeotropic mixture using ionic liquid in extractive distillation	2025	Separation and Purification Technology	link
22	Sergio de-la-Huerta-Sainz	Nature's tool kit: Designing biocompatible and affordable NADES for sustainable extraction of plant bioactives	2025	Deleted Journal	link
23	Gilles Van Eygen	CFD modelling and experimental analysis of aromatic amine extraction in a flat sheet supported liquid membrane contactor	2025	Journal of Water Process Engineering	link
24	Chengna Dai	Remarkable chlorobenzene absorption by carboxylic acid based deep eutectic solvents	2025	Separation and Purification Technology	link
25	Théophile Gaudin	Driving the future of cosmetics, fragrances and foods with COSMO-RS.Part 2–From theory to practice	2025	Current Opinion in Colloid & Interface Science	link

26	Murilo L. Alcantara	Density and viscosity of alkylammonium ionic liquids: Experimental and COSMO-RS	2025	Journal of Molecular Liquids	link
27	Théophile Gaudin	Driving the future of cosmetics, fragrances, and foods with COSMO-RS. Part 1—Bibliometric analysis and introductory framework	2025	Current Opinion in Colloid & Interface Science	link
28	Mariam Kholany	Extraction and separation of pigments from Saccharina latissima using eutectic solvents	2025	Separation and Purification Technology	link
29	Mirjana Sulejmanović	Sustainable isolation of ginger (Zingiber officinale) herbal dust bioactive compounds with favorable toxicological profile employing natural deep eutectic solvents (NADES)	2025	Food Chemistry	link
30	Yu Wang	Separation of ethanol/n-hexane azeotrope by imidazolium ionic liquids: Experimental study and mechanism analysis	2025	Separation and Purification Technology	link
31	Gaomiao Zhang	Heat-integrated extractive distillation for separating tetrahydrofuran/methanol/water with ionic liquid-based mixed entrainer: Molecular mechanism and process integration	2025	Separation and Purification Technology	link
32	Shuning Jiang	Molecular interaction mechanism and process analysis of separation of cyclohexane/ethyl acetate by extractive distillation	2025	Separation and Purification Technology	link
33	Shengchao Xu	In-situ formation of hydrophobic deep eutectic solvents to separate lactic acid: Lactam as hydrogen bond acceptor and lactic acid as hydrogen bond donor	2025	Separation and Purification Technology	link

34	Dian Jin	Predicting deep eutectic solvents for absorption of SO2 based on multilayer perceptron	2025	Separation and Purification Technology	link
35	Zijun Li	Predicting hygroscopic growth of organosulfur aerosol particles using COSMOtherm	2024	Atmospheric Chemistry and Physics	link
36	Liwen Zhuang	Enhancing the solubility of carbamazepine using ionic liquids: An experiment and theoretical calculation	2024	Journal of Molecular Structure	link
37	Huma Warsi Khan	Ionic liquid-based dispersive liquid–liquid microextraction of succinic acid from aqueous streams: COSMO-RS screening and experimental verification	2024	Environmental Technology	link
38	Nimra Javed	Ionic liquids based azeotropic separation of refrigerants R410A (R32+ R125) and R508B (R23+ R116) through hybrid extractive distillation	2024	Separation Science and Technology	link
39	Tong YANG	Prediction of vapor-liquid equilibrium data of uranium hexafluoride and fluoride and simulation of distillation process	2024	CIESC Journal	link
40	Jean-Baptiste Chagnoleau	Using COSMO-RS to design organic biphasic systems containing deep eutectic solvents for the separation of natural compounds	2024	Journal of Molecular Liquids	link
41	Sille Štěpánová	Acidity constants and protonation sites of cyclic dinucleotides determined by capillary electrophoresis, quantum chemical calculations, and NMR spectroscopy	2024	Electrophoresis	link

42	Luis A. Gallo-García	Liquid-liquid equilibrium of the 1-butyl-3-methylimidazolium-based ionic liquids+ sodium citrate+ water systems at 298.15 K	2024	Journal of Molecular Liquids	link
43	Marta-Lisette Pikma	pKaH values and θH angles of phosphanes to predict their electronic and steric parameters	2024	Dalton Transactions	link
44	Alexandre M. S. Jorge	Unravelling the molecular interactions behind the formation of PEG/PPG aqueous two-phase systems	2024	Physical Chemistry Chemical Physics	link
45	Mia Radović	Rational design of deep eutectic solvents for the stabilization of dehydrogenases: an artificial neural network prediction approach	2024	Frontiers in Chemistry	link
46	Ebert, C Dahley	Can membrane permeability of zwitterionic compounds be predicted by the solubility diffusion model?	2024	European Journal of Pharmaceutical Sciences	link
47	J. Mark Parnis	Oil sands process-affected water composition effect on Henry's law constants for polycyclic aromatic compounds: Theory and experiment	2024	Chemosphere	link
48	Filip Šebesta	Determination of Amino Acids' pKa: Importance of Cavity Scaling within Implicit Solvation Models and Choice of DFT Functionals	2024	The Journal of Physical Chemistry B	link
49	Yong Deng	Ultrasound-Assisted Accelerated Penetration Extraction of Polyphenols from Pomegranate Peels: Enhanced Mass Transfer by Calcium Ion Precipitation and Utilization of Fick’s Law	2024	Food and Bioprocess Technology	link
50	Zhengxing Dai	Predicting PC-SAFT parameters based on COSMO-RS	2024	AIChE Journal	link

51	Nimra Javed	Separation of CO2 and TFE by using diethanolamine and diisopropylamine	2024	Separation Science and Technology	link
52	Fateme Molajafari	Computational screening for prediction of co-crystals: method comparison and experimental validation	2024	CrystEngComm	link
53	Zuzana Osifová	What are the minimal folding seeds in proteins? Experimental and theoretical assessment of secondary structure propensities of small peptide fragments	2024	Chemical Science	link
54	Ainul MAGHFIRAH	L-Leucine Propyl Ester–Fatty Acid-Based Pseudo-Protic Ionic Liquids: Synthesis, Extraction Ability, and Ecotoxicity Prediction by Machine Learning	2024	Solvent Extraction Research and Development, Japan	link
55	Austin N. Keller	Thermophysical property prediction of anion-functionalized ionic liquids for CO2 capture	2024	Journal of Molecular Liquids	link
56	Martin P. Andersson	The shape of water-how cluster formation explains the hydrophobic effect	2024	Journal of Molecular Liquids	link
57	Jing Fan	Hybrid data-driven and physics-based modeling for viscosity prediction of ionic liquids	2024	Green Energy & Environment	link
58	Mehdi Akbari	Optimization of solid-state fermentation conditions to improve phenolic content in corn bran, followed by extraction of bioactive compounds using natural deep eutectic solvents	2024	Innovative Food Science & Emerging Technologies	link
59	Zhengxing Dai	Melting points of ionic liquids: Review and evaluation	2024	Green Energy & Environment	link
60	Amal A.M. Elgharbawy	Antibacterial performance enhancement using hydrophobic deep eutectic solvents: COSMO-RS	2024	Journal of Molecular Liquids	link

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61	Sebastian Steiner	Ring Opening of Diketene in Superacidic Media	2024	The Journal of Organic Chemistry	link
62	Shiyi Qin	Identifying Green Solvent Mixtures for Bioproduct Separation Using Bayesian Experimental Design	2024	ACS Sustainable Chemistry & Engineering	link
63	Mohammad Bagheri	Elucidating the Interaction Interplay Between the Gabapentin an Anticonvulsant Drug and 2-Hydroxyethylammonium Octanoate-Based Surface-Active Ionic Liquids	2024	International Journal of Thermophysics	link
64	Changhang Zhang	Innovative formaldehyde adsorption with optimized deep eutectic solvents: An experiment and multilevel computational chemistry approach	2024	Environmental Research	link
65	Martin P. Andersson	Prediction of Surface Tension Using COSMO-RS	2024	Industrial & Engineering Chemistry Research	link
66	Nuria Aguilar	Insights into Carvone: Fatty Acid Hydrophobic NADES for Alkane Solubilization	2024	Energy & Fuels	link
67	Martina Iulini	Application of PBK models for long-chain PFAS to short-chain PFAS: a proposal for toxicokinetic evaluation and in vitro to in vivo extrapolation	2024	2021 IEEE International Conference on Bioinformatics and Biomedicine (BIBM)	link
68	Muhammad Irfan Khawar	Streamlining Linear Free Energy Relationships of Proteins through Dimensionality Analysis and Linear Modeling	2024	Journal of Chemical Information and Modeling	link

69	Stephanie Peper	Resource-Efficient Solvent Utilization: Solvent Selection Criteria Based on Solvent Swap Characteristics	2024	ACS Sustainable Chemistry & Engineering	link
70	Palwasha Khan	Simulation-Driven Design and Synthesis of DES-PDMS Membranes for Enhanced Ethanol Pervaporation	2024	ACS Sustainable Chemistry & Engineering	link
71	Karla R. Sanchez-Lievanos	Synthesis and Evaluation of Cationic Porphyrin-Based Organic Nanocages for the Removal of 38 PFAS from Water: Experimental, Theoretical, and Eco-toxicological Insights	2024	ACS ES&T Engineering	link
72	Viraj De Silva	Cocrystals and Salts: The Structural Landscape of Multicomponent Solids of Chalcogenadiazoles	2024	Crystal Growth & Design	link
73	Yue Zhi	Environmental Occurrence and Biotic Concentrations of Ultrashort-Chain Perfluoroalkyl Acids: Overlooked Global Organofluorine Contaminants	2024	Environmental Science & Technology	link
74	Luis Alfonso Jiménez-Ortega	Synergistic Antioxidant Activity in Deep Eutectic Solvents: Extracting and Enhancing Natural Products	2024	ACS Food Science & Technology	link
75	Zejun Wu	Solubility prediction and interaction mechanism of FOX-7 in ten solvents by molecular and thermodynamic modeling	2024	Chemical Engineering Journal	link
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77	Honghua Zuo	Silylium-Ion-Promoted (3 + 2) Annulation of Allenylsilanes with Internal Alkynes Involving a Pentadienyl-to-Allyl Cation Electrocyclization	2024	Journal of the American Chemical Society	link
78	Estela Mayoral	Dissipative Particle Dynamics Using Conductor-Like Screening Model for Real Solvents-Based Interaction Parameters for Classical Simulations of Dibenzothiophene Adsorption on Molybdenum Disulfide Nanoparticles	2024	ACS Omega	link
79	Junaid Afridi	Extraction of rare earth elements from ion adsorption clay using bio-based ionic liquid via COSMO-RS: computational and experimental validation	2024	Journal of Rare Earths	link
80	Federico Droghetti	Selective and Efficient Light-Driven CO2 Reduction to CO with a Heptacoordinated Polypyridine Iron(II) Catalyst	2024	ACS Catalysis	link
81	Ylenia F. Rodríguez	Unveiling the intermolecular forces and unique properties of [EMIM][EtSO4] + [EMIM][MeSO3]	2024	Journal of Molecular Liquids	link
82	Dedong Wu	Discovery of the most stable form of an adenosine receptor antagonist through virtual polymorph screening and targeted crystallization	2024	Journal of Pharmaceutical Sciences	link
83	Anastasia O. Komarova	Xylose Acetals - a New Class of Sustainable Solvents and Their Application in Enzymatic Polycondensation	2024	ChemSusChem	link
84	Xudong Zhang	Screening deep eutectic solvents as green solvents for efficient extraction of carbazole from model crude anthracene oil	2024	Journal of Molecular Liquids	link

85	Elsa Anselmi	Focus on Physico-Chemical Properties of Sulfoximines: Acidity, Basicity and Lipophilicity	2024	Chemistry - A European Journal	link
86	Ahmed Halilu	Reaching machine learning leverage to advance performance of electrocatalytic CO(2) conversion in non-aqueous deep eutectic electrolytes	2024	Scientific Reports	link
87	Daniel T. Gweme	OH Radical Oxidation of Organosulfates in the Atmospheric Aqueous Phase	2024	The Journal of Physical Chemistry A	link
88	Amrita Das	Design and investigation of novel iridoid-based peptide conjugates for targeting EGFR and its mutants L858R and T790M/L858R/C797S: an in silico study	2024	Molecular Diversity	link
89	Monique M. Strieder	Screening and Characterization of 1,8-Cineole-Based Solvents as an Alternative to Hexane for Obtaining Nonpolar Compounds from Plant-Based Milk Coproducts	2024	ACS Sustainable Chemistry & Engineering	link
90	Sérgio M Vilas-Boas	Solvent screening for the purification of monoterpenoids by countercurrent and centrifugal partition chromatography	2024	Journal of Chemical Technology & Biotechnology	link
91	Timothy M. Schwartz	Varying Lewis Acidity, Covalency, and Halide Mobility to Govern Oxidative Addition Reactivity of Ni–Group 13 Bimetallic Complexes	2024	Organometallics	link
92	Sara Rozas	In silico study on helicenes in hydrophobic natural deep eutectic solvent	2024	FlatChem	link

93	Lei Tian	Optimization of solvent cooling crystallization process for separating phenanthrene from 9-fluorenone by COSMO-RS and solubility calculation approach	2024	Journal of Molecular Liquids	link
94	Hassane Lgaz	How does the integration of amino acids enhance the bonding ability of triazine-based inhibitors with iron surfaces: Insights from SCC-DFTB, COSMO-RS and molecular dynamics simulations	2024	Journal of Molecular Liquids	link
95	Boris M. Popović	Solubility and extractability enhancement of the main food flavonoids by using choline chloride-based natural deep eutectic solvents	2024	Journal of Molecular Liquids	link
96	Yang Liu	Prediction of organic sulfur solubility in mixed solvent using feature-based transfer learning and a hybrid Henry's law constant calculation method	2024	Green Chemical Engineering	link
97	Martin Stinglhamer	Site-selective Photoredox-Catalyzed Late-stage Benzylic Hydrogen Isotope Exchange	2024	Angewandte Chemie International Edition	link
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100	Kevin A. Spiekermann	Accurately Predicting Barrier Heights for Radical Reactions in Solution Using Deep Graph Networks	2024	The Journal of Physical Chemistry A	link
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102	Juraj Velcicky	Discovery and In Vivo Exploration of 1,3,4-Oxadiazole and alpha-Fluoroacrylate Containing IL-17 Inhibitors	2024	Journal of Medicinal Chemistry	link
103	Ozce Durak	In Silico-Directed Design and Experimental Validation of an IL/UiO-66 Nanocomposite with Exceptional CO2 Selectivity across a Wide Pressure Range	2024	ACS Applied Nano Materials	link
104	Elisa Hernández	Dissociation role on the catalytic activity of organic halides in CO2 conversion to cyclic carbonates: Experimental and computational study	2024	Journal of CO2 Utilization	link
105	Fareeha Shadab	Guiding the Selection of Novel Amines for CO2 Capture Using a Molecular-Based and Multicriteria Modeling Approach	2024	Energy & Fuels	link
106	Zhiyuan Wang	Novel 1,3-Dimethylimidazolium Dimethyl Phosphate Ionic Liquid for Efficient Separation of the 1,3,5-Trioxane/Water Azeotropic System by Extractive Distillation: Molecular Insights and Process Enhancement	2024	ACS Sustainable Chemistry & Engineering	link
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109	Samaneh Barani Pour	Exploring the efficiency of caprylic acid and quaternary ammonium salt-based deep eutectic solvents for separation of CO2 and H2S from gas mixtures using molecular dynamics simulations and COSMO-RS	2024	Chemical Engineering Journal Advances	link
110	Luz Alonso-Dasques	Application of terpenoids for the remediation of environmental water polluted with bisphenol A and its analogs using an in silico approach	2024	The Science of The Total Environment	link
111	Yaru Peng	Per-and polyfluoroalkyl substances removal in water and wastewater treatment plants: overall efficiency and performance of adsorption	2024	Environmental Research Communications	link
112	Clara Gomez-Urios	Natural deep eutectic solvents: A paradigm of stability and permeability in the design of new ingredients	2024	Journal of Molecular Liquids	link
113	Okorie Ekwe Agwu	Carbon capture using ionic liquids: An explicit data driven model for carbon (IV) Oxide solubility estimation	2024	Journal of Cleaner Production	link
114	Gabriel Teixeira	Designing type V deep eutectic solvents with antimalarial pharmaceutical ingredients	2024	European Journal of Pharmaceutics and Biopharmaceutics	link
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116	Ville Tuppurainen	Conceptual design of furfural extraction, oxidative upgrading and product recovery: COSMO-RS-based process-level solvent screening	2024	Computers & Chemical Engineering	link
117	Andrew I. VanderWeide	Multisite Ligand Noninnocence of (CpN3)Fe(CO)3+ with Exogenous Hydride Donors: Kinetics and Mechanism	2024	Organometallics	link
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122	Maarten R. Dobbelaere	Geometric deep learning for molecular property predictions with chemical accuracy across chemical space	2024	Journal of Cheminformatics	link
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124	Jiayi Xu	Differential uptake and translocation of perfluoroalkyl substances by vegetable roots and leaves: Insight into critical influencing factors	2024	The Science of The Total Environment	link
125	Ke Li	Green and efficient method to acquire high-value phycobiliprotein from microalgal biomass involving deep eutectic solvent-based ultrasound-assisted extraction	2024	Food chemistry	link
126	Jennifer Osamede Airouyuwa	Sustainable green extraction of anthocyanins and carotenoids using deep eutectic solvents (DES): A review of recent developments	2024	Food chemistry	link
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128	Qi Jin	Bioaccumulation of legacy and emerging per- and polyfluoroalkyl substances in hydroponic lettuce and risk assessment for human exposure	2024	Journal of Environmental Sciences	link
129	Zhijia Miao	Discovery of perfluoroalkyl sulfonyl quaternary ammonium substances in the environment and their environmental behaviors	2024	Water Research	link
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151	Biting Qiao	Multimedia distribution and release characteristics of emerging PFAS in wastewater treatment plants in Tianjin, China	2024	Journal of Hazardous Materials	link
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156	Omri D. Abarbanel	QupKake: Integrating Machine Learning and Quantum Chemistry for Micro-pK(a) Predictions	2024	Journal of Chemical Theory and Computation	link
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159	Joaquín Meruane-Anich	Sustainable synthesis and extraction of 5-methyl-N-phenyl-2-pyrrolidone produced via reductive amination of levulinic acid	2024	Separation and Purification Technology	link
160	Ana M. Ferreira	Valorizing banana peels by extracting rutin with hydrated organic acids	2024	Food Chemistry Advances	link
161	Hua Du	Natural deep eutectic solvent-ultrasound for the extraction of flavonoids from Fructus aurantii: Theoretical screening, experimental and mechanism	2024	Arabian Journal of Chemistry	link

162	Adriana Viñas-Ospino	Comparison of green solvents for the revalorization of orange by-products: Carotenoid extraction and in vitro antioxidant activity	2024	Food Chemistry	link
163	Shiling Feng	Extraction and identification of polyphenol from Camellia oleifera leaves using tailor-made deep eutectic solvents based on COSMO-RS design	2024	Food chemistry	link
164	Adrien Fusina	Hydrotropic and solvent strategies to enhance the solubilization of polyphenols in relation to their chemical structure	2024	Journal of Molecular Liquids	link
165	Zheng-Wang Qu	Mechanism of Alkaline Earth Metal Amide Catalyzed Hydrogenation of Challenging Alkenes and Arenes	2024	ChemSusChem	link
166	Derek M. Dalton	Utopia Point Bayesian Optimization Finds Condition-Dependent Selectivity for N-Methyl Pyrazole Condensation	2024	Journal of the American Chemical Society	link
167	Weiping Qin	Species Difference? Bovine, Trout, and Human Plasma Protein Binding of Per- and Polyfluoroalkyl Substances	2024	Environmental science & technology	link
168	Florian Mast	Choice of the Right Supporting Electrolyte in Electrochemical Reductions: A Principal Component Analysis	2024	Journal of the American Chemical Society	link
169	Bin Li	Deep eutectic solvent self-assembled reverse nanomicelles for transdermal delivery of sparingly soluble drugs	2024	Journal of nanobiotechnology	link

170	Sholpan Islam	Desulfurization and Denitrogenation Using Betaine-Based Deep Eutectic Solvents	2024	Journal of chemical and engineering data/Journal of chemical & engineering data	link
171	Isabella W. Cordova	Using Molecular Conformers in COSMO-RS to Predict Drug Solubility in Mixed Solvents	2024	Industrial & engineering chemistry research	link
172	Henrik Möbitz	Nonclassical Zwitterions as a Design Principle to Reduce Lipophilicity without Impacting Permeability	2024	Journal of medicinal chemistry	link
173	Zhou Xu	Natural Deep Eutectic Solvent-Based Ultrasound-Assisted Extraction of Flavonoids from Fagopyrum tataricum Bran	2024	Separations	link
174	Sung Eun Jerng	Machine learning for CO2 capture and conversion: A review	2024	Energy and AI	link
175	Abir Boublia	Zinc chloride-assisted activation of açaí biomass for herbicide removal: Insights from adsorption and molecular modeling	2024	Process safety and environmental protection/Transactions of the Institution of Chemical Engineers. Part B, Process safety and environmental protection/Chemical engineering research and design/Chemical engineering research & design	link

176	Raphaël Lebeuf	Glycidyl methyl ether: A safer alternative to ethylene oxide for designing ethoxy-free non-ionic surfactants	2024	Colloids and surfaces. A, Physicochemical and engineering aspects	link
177	Xiaojun Zhou	QSPR modeling for the prediction of partitioning of VOCs and SVOCs to indoor fabrics: Integrating environmental factors	2024	Journal of hazardous materials	link
178	Ana Casas	Machine learning screening tools for the prediction of extraction yields of pharmaceutical compounds from wastewaters	2024	Journal of water process engineering	link
179	Andrea Ebert	Can membrane permeability of zwitterionic compounds be predicted by the solubility-diffusion model?	2024	European journal of pharmaceutical sciences	link
180	Pengyu Chen	Hepatotoxicity and lipid metabolism disorders of 8:2 polyfluoroalkyl phosphate diester in zebrafish: In vivo and in silico evidence	2024	Journal of hazardous materials	link
181	Francisco Heras	Energy and economic analysis of alternatives for the valorization of hydrogen rich stream produced in the aqueous phase reforming of pyrolysis bio-oil aqueous fraction	2024	Bioresource technology	link
182	Leonhard Schill	Rational solvent selection for the preparation of industrial monolithic supported liquid-phase (SLP) olefin hydroformylation catalyst	2024	Green technologies and sustainability	link
183	Jemilat Yetunde Yusuf	Eco-friendly Functionalization of MWCNTs with Deep Eutectic Solvents	2024	Inorganic chemistry communications/Inorganic	link

				chemistry communications (Online)	
184	Francisco Paes	Predicting solvation energies of free radicals and their mixtures: A robust approach coupling the Peng-Robinson and COSMO-RS models	2024	Journal of molecular liquids	link
185	Alejandro Belinchón	A step closer to sustainable CO2 conversion: Limonene carbonate production driven by ionic liquids	2024	Journal of cleaner production	link
186	Junzhong Wang	Screening of Green and Environmentally Friendly Deep Eutectic Solvents and Study on Molecular Mechanism and Process for Separation of Isopropanol and Cyclohexane	2024	ACS sustainable chemistry & engineering	link
187	Mariana Bortholazzi Almeida	Strategies Employed to Design Biocompatible Metal Nanoparticles for Medical Science and Biotechnology Applications	2024	ACS applied materials & interfaces	link
188	Sebastian Höthker	Stereoconvergent Approach to the Enantioselective Construction of alpha-Quaternary Alcohols by Radical Epoxide Allylation	2024	Angewandte Chemie	link
189	Mood Mohan	High-Throughput Screening and Accurate Prediction of Ionic Liquid Viscosities Using Interpretable Machine Learning	2024	ACS sustainable chemistry & engineering	link
190	Luise F. Kaven	Dynamic Modeling for Synthesis of Tailored Microgels with Charged Domains	2024	Industrial & engineering chemistry research	link

191	Fernanda Paludetto Pelaquim	Prediction of Greenhouse Gas Solubility in Eutectic Solvents Using COSMO-RS	2024	International journal of thermophysics	link
192	Mehrangiz Torkzadeh	Multiscale modeling of CO2 capture in dicationic ionic liquids: Evaluating the influence of hydroxyl groups using DFT-IR, COSMO-RS, and MD simulation methods	2024	Journal of chemical physics online/☒The ☒Journal of chemical physics/Journal of chemical physics	link
193	Safrina Dyah Hardiningtyas	Sustainable Synthesis of Cellulose Nanofibers from Industrial Agar Seaweed Waste Biomass Using Hydrated Deep Eutectic Solvents	2024	Waste and biomass valorization	link
194	Zixin Chen	Prediction of Electrical Conductivity of Ionic Liquids: From COSMO-RS Derived QSPR Evaluation to Boosting Machine Learning	2024	ACS sustainable chemistry & engineering	link
195	Tadej Menegatti	Tuning Mechanical Characteristics and Permeability of Alginate Hydrogel by Polyvinyl Alcohol and Deep Eutectic Solvent Addition	2024	Bioengineering	link
196	Piotr Cysewski	Experimental and Theoretical Insights into the Intermolecular Interactions in Saturated Systems of Dapsone in Conventional and Deep Eutectic Solvents	2024	Molecules/Molecules online/Molecules annual	link
197	Huanxin Li	Application of ionic liquid extractant in enhanced separation of 2-propanol-n-hexane azeotrope system	2024	Journal of physics. Condensed matter	link
198	Martin P. Andersson	The shape of water - how cluster formation explains the hydrophobic effect	2024	Journal of molecular liquids	link

199	Nuria Aguilar	In silico study of therapeutic deep eutectic solvent for tetracaine liquid delivery	2024	Journal of molecular liquids	link
200	Cassandra Johannessen	Targeted screening of passive samplers as an “Early Warning” of novel contaminants in the Great Lakes Basin	2024	Journal of Great Lakes research	link
201	Zhihan Huang	Effect of N-o-nitrobenzylation on conformation and membrane permeability of linear peptides	2024	Bioorganic chemistry	link
202	Nikhil Kumar	Inhibition of asphaltene aggregation using deep eutectic solvents: COSMO-RS calculations and experimental validation	2024	Journal of molecular liquids	link
203	Tristan Dupeux	Molecular insights into fragrance release from SDS and SLES micelles	2024	Colloids and surfaces. A, Physicochemical and engineering aspects	link
204	Carolin Dahley	Predicting the intrinsic membrane permeability of Caco-2/MDCK cells by the solubility-diffusion model	2024	European journal of pharmaceutical sciences	link
205	Lu Qi	Exploration of different water content on the performance of reactive-extractive distillation for separating the ternary azeotropic mixture	2024	Separation and Purification Technology	link
206	Chuxin Qi	Rational screening of ionic liquids as phase transfer catalysts for aromatic O- and S-glycosidations examplified by acetobromo-alpha-D-galactose with phenolic compound	2024	Journal of molecular liquids	link

207	Yongqiang Cheng	Ionic liquid-assisted extractive distillation for separating of ethyl acetate/isopropanol from chemical wastewater: Molecular insights and process intensification	2024	Separation and purification technology	link
208	Wenxiu Li	Separation of Ethyl Acetate and Ethanol Azeotropic System by Acetate-Based Ionic Liquid	2024	Journal of solution chemistry	link
209	Zhijie Shang	Ionic-Liquid-Assisted Capture of Volatile Low-Carbon Alcohols in Printing Plant Exhaust Gas	2024	ACS sustainable chemistry & engineering	link
210	Mehmet Ogün Biçer	Industrial Distillation Aspects of Diketene	2024	Chimia	link
211	Judite Resende	Sustainable Phytosterol Extraction from Codium tomentosum Using Eutectic Solvents	2024	ACS sustainable chemistry & engineering	link
212	Fernando A. Lugo	Improved Approach for ab Initio Calculations of Rate Coefficients for Secondary Reactions in Acrylate Free-Radical Polymerization	2024	Polymers	link
213	Timothy F. M. Rodgers	Bioretention Design Modifications Increase the Simulated Capture of Hydrophobic and Hydrophilic Trace Organic Compounds	2024	Environmental science & technology	link
214	Philipp Petermeier	Integrated preservation of water activity as key to intensified chemoenzymatic synthesis of bio-based styrene derivatives	2024	Communications chemistry	link
215	Bhavik A. Mehta	Integrated Filtration and Washing Modeling: Optimization of Impurity Rejection for Filtration and Washing of Active Pharmaceutical Ingredients	2024	Organic process research & development	link

216	Tomasz Jeliński	Deep Eutectic Solvents as Agents for Improving the Solubility of Edaravone: Experimental and Theoretical Considerations	2024	Molecules/Molecules online/Molecules annual	link
217	Molly E. Murray	Exploring the binding interactions of NOP receptor with designed natural phytochemical-neuropeptide conjugates: an in silico and SPR study	2024	Applied biological chemistry	link
218	Mohd Amirul Mukmin Abdullah	Discovering [C4C1im][BF4] as draw solution in forward osmosis	2024	Journal of advanced manufacturing and processing	link
219	Thomas Gasevic	Benchmark Study on the Calculation of 207Pb NMR Chemical Shifts	2024	Inorganic chemistry	link
220	Gangqiang Yu	Hydrocarbon Extraction with Ionic Liquids	2024	Chemical reviews	link
221	Shufen Wang	Vapor–Liquid Equilibrium of Monoterpene-Sesquiterpene System Containing Resin Acid	2024	Industrial & engineering chemistry research	link
222	Rita Kol	Increasing the Dissolution Rate of Polystyrene Waste in Solvent-Based Recycling	2024	ACS sustainable chemistry & engineering	link
223	Ekta Pardhi	Nanocrystal technologies in biomedical science: From the bench to the clinic	2024	Drug discovery today	link
224	Batoul Fatima Zohra Sari-Ali	Isothermal vapor–liquid equilibria of binary mixtures containing (methanol, or propan-1-ol, or water, or acetonitrile) and 1-ethyl-3-methylimidazolium thiocynate ionic liquid: Measurements and modeling	2024	Journal of molecular liquids	link

225	Jingwen Shi	Improving the sublimation stability of ligustrazine with gallic acid by forming pharmaceutical cocrystal based on the Etter's rules	2024	Journal of Solid State Chemistry	link
226	Laura Fronchetti Guidugli	Fundamental insight on how carbon chain length affects per-and polyfluoroalkyl substances adsorption onto hydrophobic deep eutectic solvents	2024	Journal of molecular liquids	link
227	Piotr Cysewski	Intermolecular Interactions as a Measure of Dapsone Solubility in Neat Solvents and Binary Solvent Mixtures	2023	Materials	link
228	A.K.D. Celsie	Metrics for estimating vapour pressure deviation from ideality in binary mixtures	2023	SAR and QSAR in Environmental Research	link
229	Juliane Glüge	How error-prone bioaccumulation experiments affect the risk assessment of hydrophobic chemicals and what could be improved	2023	Integrated Environmental Assessment and Management	link
230	Ana Pacheco	Green Solvent Selection for Emulsifiable Concentrate Agrochemical Formulations	2023	Organic Process Research & Development	link
231	Jonathan P. Antle	Building Chemical Intuition about Physicochemical Properties of C8-Per-/Polyfluoroalkyl Carboxylic Acids through Computational Means	2023	ACS ES&T Engineering	link
232	Rubén Santiago	Predicting Partition Coefficients in Organic Biphasic Systems Using COSMO-RS	2023	Industrial & Engineering Chemistry Research	link
233	Hui Tian	Feasibility Analysis for the Direct Hydration of 1-Octene in a Catalytic Distillation Process Using Residual Curve Maps	2023	Processes	link

234	Cariny Polesca	Sustainable keratin recovery process using a bio-based ionic liquid aqueous solution and its techno-economic assessment	2023	Green Chemistry	link
235	Marten Lache	Water and Ethanol as Refrigerant Mixture Enabling Adsorption Cooling below 0 C	2023	Energy Technology	link
236	Noora Hyttinen	Predicting liquid–liquid phase separation in ternary organic–organic–water mixtures	2023	Physical Chemistry Chemical Physics	link
237	Mohsen Ghasemi	A Molecular Thermodynamic Model of Coacervation in Solutions of Polycations and Oppositely Charged Micelles	2023	Langmuir	link
238	Théophile Gaudin	Robust definition and prediction of dispersive Hansen solubility parameter δD with COSMO-RS	2023	Computational and Theoretical Chemistry	link
239	Elvira Rudin	Per- and polyfluoroalkyl substances (PFASs) registered under REACH—What can we learn from the submitted data and how important will mobility be in PFASs hazard assessment?	2023	Science of the Total Environment	link
240	Hongwei Kang	Extractive distillation for separation of isopropanol-n-propanol-water ternary system: Mechanism analysis and process design	2023	Chemical Engineering Research and Design	link
241	Leonardo M. de Souza Mesquita	Combining eutectic solvents and pressurized liquid extraction coupled in-line with solid-phase extraction to recover, purify and stabilize anthocyanins from Brazilian berry waste	2023	Green Chemistry	link

242	Minghao SONG	Multi-scale simulation and study of volatile phenols removal from simulated oil by ionic liquids	2023	CIESC Journal	link
243	Huma Warsi Khan	Ionic liquid-based dispersive liquid–liquid microextraction of succinic acid from aqueous streams: COSMO-RS screening and experimental verification	2023	Environmental Technology	link
244	Nicola Piasentin	In Silico Prediction of Stratum Corneum Partition Coefficients via COSMOmic and Molecular Dynamics Simulations	2023	The Journal of Physical Chemistry B	link
245	Jenny Oh	The atmospheric fate of 1,2-dibromo-4-(1,2-dibromoethyl)cyclohexane (TBECH): spatial patterns, seasonal variability, and deposition to Canadian coastal regions	2023	Atmospheric Chemistry and Physics	link
246	Shiyi Qin	Capturing molecular interactions in graph neural networks: A case study in multi-component phase equilibrium	2023	Digital Discovery	link
247	Pan Xu	Biomethane purification with quaternary ammonium salts-based deep eutectic solvents: Experiment and computational thermodynamics	2023	Separation and Purification Technology	link
248	Youqi Li	Measurement and prediction of isothermal vapor–liquid equilibrium of α-pinene + camphene/longifolene + abietic acid + palustric acid + neoabietic acid system	2023	Chinese Journal of Chemical Engineering	link

249	Ye Tao	Exploring controls on perfluorocarboxylic acid (PFCA) gas–particle partitioning using a model with observational constraints	2023	Environmental Science: Processes & Impacts	link
250	Sadra Kashef Ol Gheta	Predicting absolute aqueous solubility by applying a machine learning model for an artificially liquid-state as proxy for the solid-state	2023	Journal of Computer-Aided Molecular Design	link
251	Zehao Mi	Theoretical analysis of CO2 absorption by polyamines-TFSA type protic ionic liquids	2023	Chemical Industry and Engineering Progress	link
252	Pan Xu	Efficient purification of biogas using ionic liquid as absorbent: Molecular thermodynamics, dynamics and experiment	2023	Journal of Environmental Chemical Engineering	link
253	A. Viñas-Ospino	Using novel hydrophobic deep eutectic solvents to improve a sustainable carotenoid extraction from orange peels	2023	Food Bioscience	link
254	Satoshi Endo	Experimental Determination of Air/Water Partition Coefficients for 21 Per-and Polyfluoroalkyl Substances Reveals Variable Performance of Property Prediction Models	2023	Environmental Science & Technology	link
255	Vitus Besel	Atomic structures, conformers and thermodynamic properties of 32k atmospheric molecules	2023	Scientific data	link
256	Mengke Zhang	Estimation of vapor pressures of perfluoroalkyl substances (PFAS) using COSMOtherm	2023	Journal of Hazardous Materials	link

257	Chunjie Liu	Designing Deep Eutectic Solvents with Crystalline Features: A New-Generation Green Crystallization-Induced Porogen	2023	ACS Sustainable Chemistry & Engineering	link
258	Kaihang Zhang	Screening ionic liquids for efficiently extracting perfluoroalkyl chemicals (PFACs) from wastewater	2023	Journal of Environmental Sciences	link
259	Noora Hyttinen	The effect of atmospherically relevant aminium salts on water uptake	2023	Atmospheric Chemistry and Physics	link
260	Rubén Santiago	Anticipating APIs solubility in natural eutectic solvents: Lidocaine and caffeine case studies	2023	Food Bioscience	link
261	Zijun Li	Saturation vapor pressure characterization of selected low-volatility organic compounds using a residence time chamber	2023	Environmental Science & Technology	link
262	Juliane Glüge	Evaluation of Physicochemical Property Data in the ECHA Database	2023	Scientific data	link
263	Zehao Mi	DFT and COSMO-RS theoretical analysis of SO2 absorption by polyamines type ionic liquids	2023	Journal of Hazardous Materials	link
264	Michael Diedenhofen	COSMO-RS blind prediction of distribution coefficients and aqueous pKa values from the SAMPL8 challenge	2023	ACS Sustainable Chemistry & Engineering	link
265	Satoshi Endo	Intermolecular Interactions, Solute Descriptors, and Partition Properties of Neutral Per-and Polyfluoroalkyl Substances (PFAS)	2023	Journal of Environmental Sciences	link

266	Alena K.D. Celsie	COSMO-RS solute partition ratios for solvent mixtures of unknown composition: Henry's law constants as descriptors for mixture sigma profiles	2023	Atmospheric Chemistry and Physics	link
267	Xia Li	Study on Vapor–Liquid Equilibrium and Microscopic Properties of Glycine + H2O, l-Histidine + H2O, and l-Tryptophan + H2O	2023	Journal of Molecular Liquids	link
268	Anju Kumari	Separation of Iso-Nicotinic acid from aqueous solution using ionic liquids: Screening using COSMO-RS and equilibrium studies	2023	Atmospheric Chemistry and Physics	link
269	Laura Fronchetti Guidugli	Understanding Microcystin-LR separation by hydrophobic deep eutectic solvents with COSMO simulation and experimental findings	2023	Journal of Physical and Chemical Reference Data	link
270	Pablo Gutiérrez-Sánchez	Extraction of antibiotics identified in the EU Watch List 2020 from hospital wastewater using hydrophobic eutectic solvents and terpenoids	2022	CIESC Journal	link
271	Clara Gómez-Urios	Sustainable development and storage stability of orange by-products extract using natural deep eutectic solvents	2022	Journal of Computer-Aided Molecular Design	link
272	Manuela Panić	Prediction of pH value of aqueous acidic and basic deep eutectic solvent using COSMO-RS σ Profiles' molecular descriptors	2022	Environmental Science & Technology	link
273	Rubén Santiago	Assessment of bio-ionic liquids as promising solvents in industrial separation processes: Computational screening using COSMO-RS method	2022	Chemosphere	link

274	Jort Hammer	Volatility and nonspecific van der Waals interaction properties of per-and polyfluoroalkyl substances (PFAS): Evaluation using hexadecane/air partition coefficients	2022	Journal of Chemical & Engineering Data	link
275	Juan Wang	COSMO-RS prediction and experimental verification of deep eutectic solvents for water insoluble pesticides with high solubility	2022	Chemical Data Collections	link
276	Clinton J. Chapman	Evaluation of solvate and co-crystal screening methods for CL-20 containing energetic materials	2022	Journal of Molecular Liquids	link
277	Noora Hyttinen	Machine learning for predicting chemical potentials of multifunctional organic compounds in atmospherically relevant solutions	2022	Separation and Purification Technology	link
278	Shuai Qian	Experimental and Computational Study of the Properties of Imidazole Compounds with Branched and Cycloalkyl Substituents	2022	Foods	link
279	Mohsen Taheri	Ionic liquid screening for CO2 capture and H2S removal from gases: The syngas purification case	2021	Molecules	link
280	Manuela Panić	Cosmotherm as an effective tool for selection of deep eutectic solvents based ready-to-use extracts from Graševina grape pomace	2021	Fluid Phase Equilibria	link
281	Sivani Baskaran	Reliable prediction of the octanol–air partition ratio	2021	Environmental Science & Technology	link
282	Huma Warsi Khan	Design and selection of ionic liquids via COSMO for pharmaceuticals and medicine	2021	Journal of Molecular Liquids	link

283	Noora Hyttinen	Gas-to-Particle Partitioning of Cyclohexene- and α-Pinene-Derived Highly Oxygenated Dimers Evaluated Using COSMOtherm	2021	Journal of Energetic Materials	link
284	Emma Lumiaro	Predicting gas–particle partitioning coefficients of atmospheric molecules with machine learning	2021	The Journal of Physical Chemistry Letters	link
285	Timothy F. M. Rodgers	Novel Bayesian method to derive final adjusted values of physicochemical properties: application to 74 compounds	2021	Liquids	link
286	Satoshi Endo	Refinement and extension of COSMO-RS-trained fragment contribution models for predicting the partition properties of C10-20 chlorinated paraffin congeners	2021	Chemical Engineering Science	link
287	Judith Warnau	COSMO-RS predictions of logP in the SAMPL7 blind challenge	2021	Molecules	link
288	Rubén Santiago	Extending the ability of cyclic carbonates for extracting BTEX to challenging low aromatic content naphtha: the designer solvent role at process scale	2021	Environmental Toxicology and Chemistry	link
289	Boluwatife Awonaike	Precipitation-induced transport and phase partitioning of organophosphate esters (OPEs) in urban and rural watersheds	2021	Application of Ionic Liquids in Drug Delivery	link
290	Jort Hammer	Congener-specific partition properties of chlorinated paraffins evaluated with COSMOtherm and gas chromatographic retention indices	2021	The Journal of Physical Chemistry A	link

291	K. Zaher	In-silico Study of the Developed Hydroxychloroquine-based ACE2 Inhibitor Molecules Against COVID-19: Molecular Modeling and Docking	2021	Atmospheric Chemistry and Physics	link
292	Samuel Boobier	Machine learning with physicochemical relationships: solubility prediction in organic solvents and water	2020	Environmental Science & Technology	link
293	Alina Lampic	Property estimation of per- and polyfluoroalkyl substances: A comparative assessment of estimation methods	2020	Environmental Science: Processes & Impacts	link
294	Christoph Loschen	COSMO-RS based predictions for the SAMPL6 logP challenge	2020	Journal of Computer-Aided Molecular Design	link
295	Kyle McGaughy	Liquid–Liquid Extraction of Furfural from Water by Hydrophobic Deep Eutectic Solvents: Improvement of Density Function Theory Modeling with Experimental Validations	2020	Computers & Chemical Engineering	link
296	Elenitsa Boli	Ionic liquids as entrainers for the separation of azeotropic mixtures: Experimental measurements and COSMO-RS predictions	2020	Environmental Science: Water Research & Technology	link
297	Noora Hyttinen	Thermodynamic properties of isoprene- and monoterpene-derived organosulfates estimated with COSMOtherm	2020	Scientific Reports	link
298	Noora Hyttinen	Improving Solubility and Activity Estimates of Multifunctional Atmospheric Organics by Selecting Conformers in COSMOtherm	2020	Engineering, Technology & Applied Science Research	link

299	Noora Hyttinen	Estimating aqueous solubilities and activity coefficients of mono- and α,ω-dicarboxylic acids using COSMOtherm	2020	Nature communications	link
300	Mingyuan Hu	Vapor–Liquid Equilibrium Measurements of Cyclohexene-Isophorone and Cyclohexanol-Isophorone Binary Systems and Predictions for Cyclohexene-Cyclohexanol-Isophorone Ternary System	2020	Environmental toxicology and chemistry	link
301	Benjamin Sanchez-Lengeling	A Bayesian approach to predict solubility parameters	2019	Journal of Computer-Aided Molecular Design	link
302	Varun Kundi	Predicting Octanol-Water Partition Coefficients: Are Quantum Mechanical Implicit Solvent Models Better than Empirical Fragment-Based Methods?	2019	ACS omega	link
303	Mattia Turchi	An evaluation of in-silico methods for predicting solute partition in multiphase complex fluids - A case study of octanol/water partition coefficient	2019	Chemical Engineering Science	link
304	Georgia Michailoudi	Solubility and Activity Coefficients of Atmospheric Surfactants in Aqueous Solution Evaluated Using COSMOtherm	2019	Atmospheric Chemistry and Physics	link
305	Mohamed Taha	Molecular design of mass-separating agents for separation of cyclic ethers and acetonitrile from water	2019	The Journal of Physical Chemistry A	link
306	Vishwesh Venkatraman	Predicting ionic liquid melting points using machine learning	2018	Atmospheric Chemistry and Physics	link

307	Philipp Pracht	High accuracy quantum-chemistry-based calculation and blind prediction of macroscopic pKa values in the context of the SAMPL6 challenge	2018	Journal of Chemical & Engineering Data	link
308	R. Santiago	Acetylene absorption by ionic liquids: A multiscale analysis based on molecular and process simulation	2018	Advanced Theory and Simulations	link
309	Theo Kurtén	Estimating the saturation vapor pressures of isoprene oxidation products and using COSMO-RS	2018	The Journal of Physical Chemistry B	link
310	Yuriy A. Abramov	Rational solvent selection for pharmaceutical impurity purge	2018	Chemical Engineering Science	link
311	Vishwesh Venkatraman	Predicting CO2 capture of ionic liquids using machine learning	2017	The Journal of Physical Chemistry A	link
312	Miranda Roesing	Solubility characteristics of poly (3-hexylthiophene)	2017	Journal of Molecular Liquids	link
313	Meysam Lotfi	Solubility of acyclovir in nontoxic and biodegradable ionic liquids: COSMO-RS prediction and experimental verification	2017	Journal of Molecular Liquids	link
314	Chen Wang	Uncertain Henry's law constants compromise equilibrium partitioning calculations of atmospheric oxidation products	2017	Journal of Computer-Aided Molecular Design	link
315	Johannes A. H. Schwöbel	High-Throughput Screening of Working Fluids for the Organic Rankine Cycle (ORC) Based on Conductor-like Screening Model for Realistic Solvation (COSMO-RS) and Thermodynamic Process Simulations	2017	Separation and Purification Technology	link

316	Martta Toivola	Can COSMOTherm predict a salting in effect?	2017	Atmospheric Chemistry and Physics	link
317	Emad Ali	Modeling of CO2 Solubility in Selected Imidazolium-Based Ionic Liquids	2017	Crystal Growth & Design	link
318	Boluwatife Awonaike	Quantifying the equilibrium partitioning of substituted polycyclic aromatic hydrocarbons in aerosols and clouds using COSMOtherm	2017	Journal of CO2 Utilization	link
319	Mattia Turchi	Multi-scale modelling of solute partition equilibria of micelle-water and microemulsion-water systems using molecular dynamics and COSMOtherm	2017	Journal of Polymer Science, Part B	link
320	Andreas Klamt	Prediction of cyclohexane-water distribution coefficients with COSMO-RS on the SAMPL5 data set	2016	Journal of Molecular Liquids	link
321	Sebastian Brox	Alternative Single-Solvent Electrolytes Based on Cyanoesters for Safer Lithium-Ion Batteries	2016	Atmospheric Chemistry and Physics	link
322	Joseph O. Okeme	Polydimethylsiloxane-air partition ratios for semi-volatile organic compounds by GC-based measurement and COSMO-RS estimation: Rapid measurements and accurate modelling	2016	Industrial & Engineering Chemistry Research	link
323	Xingang Li	Ionic liquid-assisted solvent extraction for unconventional oil recovery: computational simulation and experimental tests	2016	The Journal of Physical Chemistry A	link

324	Meysam Lotfi	Analysis of multiple solvation interactions of methotrexate and ammonium based ionic liquids using COSMO-RS	2016	Chemical Engineering Communications	link
325	Huihong Liu	Interpretation and prediction of the vapor–liquid equilibrium of formaldehyde-water-methanol ternary system by the conductor-like screening model for real solvents	2016	Environmental Science: Processes & Impacts	link
326	Melissa Ines Gomis	A modeling assessment of the physicochemical properties and environmental fate of emerging and novel per-and polyfluoroalkyl substances	2015	Computer Aided Chemical Engineering	link
327	Yongsheng Zhao	A quantitative prediction of the viscosity of ionic liquids using S σ-profile molecular descriptors	2015	Journal of Computer-Aided Molecular Design	link
328	Christoph Schütter	Toward new solvents for EDLCs: from computational screening to electrochemical validation	2015	ChemSusChem	link
329	Tamara Husch	Large-scale virtual high-throughput screening for the identification of new battery electrolyte solvents: computing infrastructure and collective properties	2015	Chemosphere	link
330	J. Mark Parnis	Temperature dependence of Henry's law constants and KOA for simple and heteroatom-substituted PAHs by COSMO-RS	2015	Energy & Fuels	link
331	Tamara Husch	Charting the known chemical space for non-aqueous lithium-air battery electrolyte solvents	2015	Procedia Engineering	link

332	W. Jeffrey Horne	Effect of branched and cycloalkyl functionalities on CO2 separation performance of poly (IL) membranes	2015	Fluid Phase Equilibria	link
333	Chen Wang	Calculating Equilibrium Phase Distribution during the Formation of Secondary Organic Aerosol Using COSMOtherm	2015	Science of The Total Environment	link
334	Anett Geisler	Predicting storage-lipid water partitioning of organic solutes from molecular structure	2015	Physical Chemistry Chemical Physics	link
335	Markéta Paloncýová	Amphiphilic drug-like molecules accumulate in a membrane below the head group region	2014	The Journal of Physical Chemistry C	link
336	Chen Wang	Measuring and modeling the salting-out effect in ammonium sulfate solutions	2014	Physical Chemistry Chemical Physics	link
337	W. Jeffrey Horne	Correlating fractional free volume to CO2 selectivity in [Rmim][Tf2N] ionic liquids	2014	Atmospheric Environment	link
338	Angelika Stenzel	Prediction of partition coefficients for complex environmental contaminants: Validation of COSMOtherm, ABSOLV, and SPARC	2014	Physical Chemistry Chemical Physics	link
339	Jens Reinisch	Prediction of free energies of hydration with COSMO-RS on the SAMPL4 data set	2014	Separation and Purification Technology	link
340	Vasu Neela	Addition of malodorants to lighter gas–The phase equilibrium properties of mixtures of lighter gas and selected substances	2014	Environmental Science & Technology	link
341	Juliane Glüge	Calculation of physicochemical properties for short-and medium-chain chlorinated paraffins	2013	Environmental Science & Technology	link

342	Matthew S. Shannon	Properties and Performance of Ether-Functionalized Imidazoles as Physical Solvents for CO2 Separations	2013	The Journal of Physical Chemistry B	link
343	Patrick C. Hillesheim	Effect of alkyl and aryl substitutions on 1, 2, 4-triazolium-based ionic liquids for carbon dioxide separation and capture	2013	Environmental Science & Technology	link
344	Jason E. Bara	COSMOTherm as a Tool for Estimating the Thermophysical Properties of Alkylimidazoles as Solvents for CO2 Separations	2013	The Journal of Chemical Thermodynamics	link
345	S. I. Mustapha	Improvement of carbon dioxide absorption technology using conductor-like screening model for real solvents (COSMO-RS) method	2013	Environmental Toxicology and Chemistry	link
346	Andreas M. Buser	Comparing the performance of computational estimation methods for physicochemical properties of dimethylsiloxanes and selected siloxanols	2013	Journal of Computer-Aided Molecular Design	link
347	A. Y. Zakari	Computational study of environmental fate of ionic liquids using conductor-like screening model for real solvents (COSMO-RS) method	2013	Chemical Engineering Research and Design	link
348	Matthew S. Shannon	Free volume as the basis of gas solubility and selectivity in imidazolium-based ionic liquids	2012	Journal of Physical and Chemical Reference Data	link
349	Yuriy A. Abramov	Rational coformer or solvent selection for pharmaceutical cocrystallization or desolvation	2012	Energy & Fuels	link
350	Laurianne Moity	Panorama of sustainable solvents using the COSMO-RS approach	2012	RSC Advances	link

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