

BIOVIA COSMOtherm 関連論文リスト (1/69)

No.	First author	Title	Year	Journal name	Link
1	Rahul Jha	In silico cocrystal screening using COSMO-RS: A rapid and efficient approach for solubility prediction and crystal engineering	2025	Journal of Molecular Liquids	link
2	M. Kiene	Maßgeschneiderte tief eutektische Systeme als zukunftsfähige Extraktionsmittel für bioaktive Naturstoffe	2025	Lebensmittelchemie	link
3	H. Präßler	Methodenoptimierung zur Gewinnung des Sesquiterpens Alismol aus Bixa orellana mittels Hochleistungs - Gegenstromverteilungschromatographie (HPCCC) und in silico COSMO - RS Berechnungen	2025	Lebensmittelchemie	link
4	Haoyang Xu	Cosolvents Screening and Data Association for the 1-Octene Hydration Reaction System	2025	Journal of Solution Chemistry	link
5	Na Deng	A novel quantitative structure–property relationship model for predicting the maximum volumetric heating capacity and the corresponding working temperature of heat pump refrigerants	2025	Chemical Engineering Science	link
6	Eva Pietropaoli	Exploring the Synergy between $\pi - \pi$ Interactions and Hydrogen-Bonding in the Formation of Type V Deep Eutectic Solvents	2025	ACS Sustainable Chemistry & Engineering	link
7	Se-Ra Jin	Development and optimization of imine-functionalized cellulose adsorbent for anionic micropollutant removal	2025	Cellulose	link

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8	Ying Zhao	Micro-mechanism and process study of green deep eutectic solvents in water/ γ -valerolactone separation	2025	Chemical Engineering and Processing - Process Intensification	link
9	Ylenia F. Rodríguez	Alkylimidazolium-based ionic liquid Mixtures: The case of [EMIM][BF ₄] + [EMIM][MeSO ₃]	2025	Journal of Molecular Liquids	link
10	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
11	Boutaina Illoussamen	Hydrophobic deep eutectic solvents as green solvents for phenolic compounds extraction from olive mill wastewater	2025	Journal of environmental chemical engineering	link
12	Mehtab Ali Darban	Computational study on amino acid base ionic liquids (AAILs) for gas separation using COSMO-RS	2025	Materials research proceedings	link
13	Ting Wu	Methodological Roadmap for Machine Learning in Deep Eutectic Solvent Research: A Framework-Driven Review and Perspective	2025	Industrial & Engineering Chemistry Research	link
14	Fedor Zhuravlev	Recent Advances in Liquid-Liquid Extraction in Flow of Radiometals for Positron Emission Tomography	2025	Automated Technologies for the Development and Production of Radiopharmaceuticals	link
15	Yuriy A. Abramov	Computational and Experimental Cocrystal Screening of Tiopronin and Dapagliflozin APIs: Development and Validation of a New Virtual Screening Model	2025	Crystal Growth & Design	link

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16	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
17	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
18	Changyue Xing	Strategies to Reduce Uncertainties from the Best Available Physicochemical Parameters Used for Modeling Novel Organophosphate Esters across Multimedia Environments	2025	Environmental Science & Technology	link
19	Juho-Pekka Laakso	Machine learning modeling of the CO ₂ solubility in ionic liquids by using σ -profile descriptors	2025	Chemical Engineering Science	link
20	Miguel Viar	Biomass-Derived Solvents and Low-GWP Refrigerants as Working Fluids for Sustainable Absorption Refrigeration	2025	ACS Sustainable Chemistry & Engineering	link
21	Zaeem Aman	Solubility Enhancement of valine using deep eutectic Solvents: COSMO-RS and experimental validation	2025	Journal of Molecular Liquids	link
22	Dingkai Hu	Quantum Chemistry-Guided Machine Learning for Accelerated Design of CO ₂ -Solubilizing Deep Eutectic Solvents	2025	ACS Sustainable Chemistry & Engineering	link
23	Damalka Balasuryia	Experimental Determination of pKa for 10 PFAS, Mono-, Di-, and Trifluoroacetic Acid by ¹⁹ F-NMR	2025	Environmental Science & Technology Letters	link
24	Yinxin Yang	Cocrystal Technology in the Screening of Pharmaceutical Solid Forms and Chiral Resolution of Drugs: a Review	2025	Crystal Research and Technology	link

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25	Gina Wycich	Desulfurizative Fluorination of N-CF(3) Thioformamides for the Efficient Synthesis of N(CF(3))(CF(2)H) Amines with Enhanced Stability	2025	Angewandte International Edition	Chemie	link
26	Souhib Bennaadja	Sustainable drug delivery innovations: Enhancing Ferulic Acid release using Deep Eutectic Solvents in dimyristoyl phosphatidylcholine (DMPC) systems	2025	Journal of Molecular Liquids		link
27	Matteo Guidetti	Discovery of Cilnidipine Cocrystals with Enhanced Dissolution by the Use of Computational Tools and Semiautomatic High-Throughput Screening	2025	Crystal Growth & Design		link
28	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
29	Prathiksha Prabhakar	Influence of functional groups on drug solubility using choline chloride-based deep eutectic solvents	2025	Journal of Molecular Modeling		link
30	Mahtab Moradi	Enantioseparation of ofloxacin using a liquid – liquid extraction system based on hydrophobic eutectic solvents	2025	Separation and Purification Technology		link
31	Adrian Racki	Recent Advances in the Modeling of Ionic Liquids Using Artificial Neural Networks	2025	Journal of Chemical Information and Modeling		link
32	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

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33	Mirjana Sulejmanović	Sustainable isolation of ginger (<i>Zingiber officinale</i>) herbal dust bioactive compounds with favorable toxicological profile employing natural deep eutectic solvents (NADES)	2025	Food Chemistry	link
34	Yichun Dong	Efficient separation of methanol, acetonitrile, and benzene ternary azeotropic mixture using ionic liquid in extractive distillation	2025	Separation and Purification Technology	link
35	Dawei Zhen	Unveiling the interaction between micelles of different surface-active ionic liquids and peptide drug HPV16E749-57	2025	Materials Today Chemistry	link
36	M.M. Alavianmehr	Multiscale characterization of ethanol – amino alcohol mixtures: thermophysical properties, hydrogen bonding, and in silico assessment for CO ₂ capture	2025	Journal of Molecular Liquids	link
37	Sebastián Ormazábal-Latorre	Methoxyphenols extraction from hydrodeoxygenation aliphatic-model phases: An in-silico and experimental study	2025	Journal of Molecular Liquids	link
38	Justin P. Edaugal	Solvent Screening for Separation Processes Using Machine Learning and High-Throughput Technologies	2025	Chem & Bio Engineering	link
39	Anja Damjanović	Design of protein-stabilizing deep eutectic solvents: a combined experimental and computational approach	2025	Journal of Molecular Liquids	link
40	Wenquan Wu	Ionic liquid-based hybrid acidic catalysts enabling phase splitting and reactive separation for methyl esterification of long-chain fatty acids	2025	Chemical Engineering Science	link

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41	Joshua W. Sin	Highly parallel optimisation of chemical reactions through automation and machine intelligence	2025	Nature Communications	link
42	Vanessa Buchweitz	Evaluation of Green and Biobased Solvent Systems for the Extraction of beta-Carotene and Lipids from <i>Rhodospiridium toruloides</i>	2025	ACS Omega	link
43	Anantha Rajmohan Muthusamy	Navigating Solid-Form Screening Using In Silico Methods Validated with Experimental Data for a Drug-like Molecule	2025	Crystal Growth & Design	link
44	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
45	Amit Kumar Halder	Applications of Predictive QSPR Modeling for Deep Eutectic Solvents	2025	Challenges and advances in computational chemistry and physics	link
46	Mengyang Qu	Machine learning-driven generation and screening of potential ionic liquids for cellulose dissolution	2025	Journal of Cheminformatics	link
47	Cassandra Johannessen	Tire-Derived Organic Chemicals in Urban Air at the Source-Sector Scale and Guidance on the Application of Polyurethane Foam Disk Passive Air Samplers	2025	ACS ES&T Air	link
48	Sojung Seo	Effect of Structural Isomerism in Imidazolium-Based Ionic Liquid on Polycarbonate Ethanolysis	2025	Industrial & Engineering Chemistry Research	link
49	Lowie Tomme	Accelerating reaction rate predictions: a machine learning approach using a novel quantum chemical property for nucleophilic aromatic substitutions	2025	Machine Learning Science and Technology	link

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50	Kimia Fereydooni	Development of a Generalizable Gradient Boosting Regression-Based Framework for Predicting the Properties of Single and Binary IL Systems	2025	ACS Applied Engineering Materials	link
51	Jingrui Xiang	Predicting thermally-stable fluids for vanadium flow battery based on conductor-like screening model for realistic solvation (COSMO-RS) theory	2025	Computational and Theoretical Chemistry	link
52	Qi Wang	Per- and polyfluoroalkyl substances (PFAS) in the marine environment: An overview and prospects	2025	Marine Pollution Bulletin	link
53	Adeeb Hayyan	Enhancing the Solubility of Dihomo - gamma - Linolenic Acid Using Natural Deep Eutectic Solvents for Human Tumors Therapy Development	2025	ChemistrySelect	link
54	Yi Hu	Investigation on the molecular interaction mechanisms of ionic liquid-organic mixed entrainers for azeotrope separation in extractive distillation	2025	Separation and Purification Technology	link
55	Yu Wang	Separation of ethanol/n-hexane azeotrope by imidazolium ionic liquids: Experimental study and mechanism analysis	2025	Separation and Purification Technology	link
56	Viktória Licul-Kucera	Determining the Temperature-Dependent Air-Water Partitioning of Ether- and Thioether-Alcohol Perfluoroalkyl and Polyfluoroalkyl Substances Using a Modified Static Headspace Method	2025	Environmental Science & Technology	link
57	Flora Esposito	Predicting Surface Tension of Organic Molecules using COSMO-RS Theory and Machine Learning	2025	Systems and Control Transactions	link

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58	Niklas Schmickler	Identification of Ti(salen) Complexes for Efficient Catalysis in Single-Electron Steps by Cyclic Voltammetry	2025	Angewandte Chemie International Edition	link
59	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
60	Ashfaq Iftakher	Design Space Exploration and Machine Learning Prediction of Hydrofluorocarbon Solubility in Ionic Liquids for Refrigerant Separation	2025	Journal of Chemical Information and Modeling	link
61	Guilherme Dallarmi Sorita	An innovative approach for the recovery of nobiletin, hesperidin, and other phytochemicals from tangerine leaves (Citrus reticulata) by-products using a solvent mixture based on natural compounds	2025	Food Chemistry	link
62	Sophia K. Nelson	Cyclosiloxane artifacts explain reported Henry's law constants for nonvolatile fluorotelomer sulfonates	2025	Journal of Hazardous Materials	link
63	Sabrina Belén Rodríguez-Reartes	Characterizing the Potential of Phosphonium-Based Ionic Liquids for CO2 Capture via Multiscale Modeling	2025	Industrial & Engineering Chemistry Research	link
64	Pan Xu	Efficient capture of DMC and CO2 in battery electrolyte VOCs with organic solvent plus ionic liquid	2025	Separation and Purification Technology	link
65	Leon Gomm	Reversible C-H Bond Activation of Unactivated Arenes by a Nickel-Silylene Complex	2025	Journal of the American Chemical Society	link
66	Timo Fockenberg	Synthesis, Characterization and Electrochemical Properties of Tri- and Tetranuclear CoIII - Oxo Complexes	2025	European Journal of Inorganic Chemistry	link

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67	Sasmit Yewale	Computational Tools for Solubility Prediction	2025	Applications of Computational Tools in Drug Design and Development	link
68	Pengpeng Yang	Theoretical and Experimental Exploration of Multicomponent Forms of Cordycepin for Sustained Release	2025	Industrial & Engineering Chemistry Research	link
69	M.M. Alavianmehr	Unraveling molecular interactions: A study of [BMIM][SCN] ionic liquid blends with 1,2-propanediol and benzyl alcohol	2025	Journal of Molecular Liquids	link
70	Perman Jorayev	Machine Learning-Driven Optimization of Continuous-Flow Photoredox Amine Synthesis	2025	Organic Process Research & Development	link
71	Wei Ge	Machine Learning in Polymer Research	2025	Advanced Materials	link
72	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
73	Chengkang Chen	Exploring the Long-Term Human Exposure to Short-, Medium-, and Long-Chain Chlorinated Paraffins under Variant Environmental Release Trends and Patterns	2025	Environmental Science & Technology	link
74	Sara Gracia-Barberán	Eco-Friendly Solvents for Bioactives: Solubilization of Hydroxycinnamic Acids in Glycerol-Derived Ethers	2025	ACS Sustainable Chemistry & Engineering	link
75	Mervé Yagmur	Towards sustainable cosmetic Ingredients: A Simplified in silico approach for selecting Innovative natural mixtures as solvents in biomass extraction	2025	Separation and Purification Technology	link

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76	Juho-Pekka Laakso	Liquid-liquid equilibrium and modelling insight: molecular interaction analysis of water + methanol + dimethyl carbonate + 1-ethyl-3-methylimidazolium methanesulfonate ternary systems	2025	Physical Chemistry Physics	Chemical	link
77	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
78	Laetitia Reinert	Toward Sustainable Biphasic Systems Using Deep Eutectic Solvents and Bio-Based Solvents for Centrifugal Partition Chromatography: An Experimental and Theoretical Study Using COSMO-RS	2025	Industrial & Engineering Chemistry Research		link
79	Jovian Lazare	pK(a) Data-Driven Insights into Multiple Linear Regression Hydrolysis QSARs: Applicability to Perfluorinated Alkyl Esters	2025	Environmental Science & Technology		link
80	Zakiah D. Nurfajrin	Accelerated Screening of Deep Eutectic Solvents for Nickel/Cobalt Extraction: Integrating Quantum Chemistry, Machine Learning, and Experimental Validation	2025	Industrial & Engineering Chemistry Research		link
81	Qian Liu	Multilevel screening and mechanism analysis of ionic liquids for separating pyridine from coal pyrolysis model oil	2025	Separation and Purification Technology		link
82	Hao Qin	Rational design of hydrophobic type V deep eutectic solvents as efficient CO ₂ absorbents	2025	Chemical Engineering Science		link

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83	Peng Liao	QSAR modeling to describe n-octanol-water partition coefficients of perfluorinated/polyfluorinated alkyl compounds	2025	Marine Pollution Bulletin	link
84	Jonathan W. Zheng	pK(a) prediction in non-aqueous solvents	2025	Journal of Computational Chemistry	link
85	S. A. Katsyuba	Revisiting Tautomerism and Rotamerism of 1,2-Dihydro-N-(2-hydroxyethyl)-4,6-dimethyl-2-oxopyrimidine (Drug Xymedon) in Aqueous and Lipophilic Media	2025	Russian Journal of General Chemistry	link
86	J. Mark Parnis	The potential for atmospheric transport of contaminants to remote lakes: An assessment using COSMO-RS solvation theory	2025	Chemosphere	link
87	Adroit T.N. Fajar	Generating eco-friendly ionic liquids with enhanced CO ₂ solubility using language models	2025	Artificial Intelligence Chemistry	link
88	Juda Baikété	Machine learning prediction of pK _a of organic acids	2025	Artificial Intelligence Chemistry	link
89	Yufeng Zeng	Integration of COSMO-RS and ANN-GA for extraction of echinacoside and acteoside from <i>Cistanche deserticola</i> using natural deep eutectic solvents	2025	Food Chemistry	link
90	Wenli Liu	Analysis of steric hindrance in the separation of ethanol-methyl acetate azeotropic mixture using deep eutectic solvents	2025	AIChE Journal	link
91	Sara Rozas	An in silico study on the carbon capture performance of menthol-based natural deep eutectic solvent	2025	Fuel	link

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92	Ashfaq Iftakher	Integrated Molecular Screening and Process Optimization To Identify Ionic Liquids for Energy-Efficient Refrigerant Separation	2025	ACS Sustainable Chemistry & Engineering	link
93	Lukas Hehn	Assessing Electronic - Structure Methods for Redox Potentials of an Iron - Sulfur Cluster	2025	International Journal of Quantum Chemistry	link
94	Maan Singh	Advancements in Computational Screening Methods for Pharmaceutical Cocrystals	2025	Cocrystals in Pharmaceutical Sciences	link
95	Eunji Lee	Effect of Hydration States on the Anti-Icing/Frosting Performance of Zwitterionic Hydrogel-Coated Surfaces	2025	Langmuir	link
96	João P. Santos	Artificial Intelligence in the Discovery of Deep Eutectic Solvents with Lubricant Applications	2025	ACS Omega	link
97	Akshat S. Mallya	Computational Design of Natural Deep Eutectic Systems Using COSMO-RS for Ice Control Applications	2025	ACS Sustainable Chemistry & Engineering	link
98	Dinis O. Abranches	Exploring the role of temperature on hydrotrophy	2025	Chemical Engineering Science	link
99	Kong Fanzhuo	Efficient cooling crystallization of phytosterol assisted by solubility and thermodynamics analysis in organic solvents	2025	Journal of Molecular Liquids	link
100	Chengna Dai	Remarkable chlorobenzene absorption by carboxylic acid based deep eutectic solvents	2025	Separation and Purification Technology	link
101	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

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102	Kai Wang	Evaluation of hexamethyldisiloxane/ethyl isobutyrate/ethanol/water solvent system for liquid-liquid chromatography	2025	Journal of Chromatography A	link
103	Barbara Bong	Reaction Equilibria in the Hydrogen Loading and Release of the LOHC System Benzyltoluene/Perhydro Benzyltoluene	2025	Chemical Engineering & Technology	link
104	Dian Jin	Predicting deep eutectic solvents for absorption of SO ₂ based on multilayer perceptron	2025	Separation and Purification Technology	link
105	Thomas Nevolianis	Multi-fidelity graph neural networks for predicting toluene/water partition coefficients	2025	Journal of Cheminformatics	link
106	Chao Sun	Comparison of deep eutectic solvents and ionic liquids effects on the separation of Isopropyl alcohol–Isopropyl acetate based on experiments and molecular simulations	2025	Journal of environmental chemical engineering	link
107	A. Marta Navarro-Cuñado	In silico characterization of Ciwujianoside E: Structural features, solvation dynamics, and eco-toxicological assessment	2025	Computational and Structural Biotechnology Journal	link
108	Jan Weinreich	Calculated solvation and ionization energies for thousands of organic molecules relevant to battery design	2025	arXiv (Cornell University)	link
109	Fritz Wortelkamp	Joint Partial Least Squares Modeling of Experimental and Computational Data for Electrolyte Prescreening in Lithium–Sulfur Batteries	2025	ChemElectroChem	link
110	Johanna Timhagen	Successes and failures predicting the solubility of solid electrolyte interphase (SEI) species	2025	Electrochimica Acta	link

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111	Jan Weinreich	Calculated solvation and ionization energies for thousands of organic molecules relevant to battery design	2025	Machine Learning Science and Technology	link
112	Arya Das	Molecular Chemical Engineering-Aided Design and Assessment of an Alternate Ligand-Solvent System for PUREX Process	2025	The Journal of Physical Chemistry B	link
113	Ruoyu Hu	Synergistic effect of hydrogen bond donors in deep eutectic solvents on separation of dimethyl carbonate/ethanol	2025	AIChE Journal	link
114	Jing Tian	Study on the dissolution and degradation patterns of cellulose in phosphonate-based ionic liquids and the construction of ternary phase diagrams	2025	International Journal of Biological Macromolecules	link
115	Yusuke Tsuchida	Hydrophobicity-Driven and Interaction-Corrected Modeling for Gold Ion-Pair Extraction Using Ammonium and Phosphonium Ionic Liquids in 1,2-Dichloroethane	2025	The Journal of Physical Chemistry B	link
116	Yue Wang	Hydrophobic Imidazole-Based Ionic Liquids for Efficient Extraction of Furfural from Wood Pulp Waste Liquor: Extraction Study and Mechanism Analysis	2025	Journal of Chemical & Engineering Data	link
117	Egis Zeneli	Guiding excipient selection for physically stable amorphous solid dispersions: A combined in-vitro in-silico approach	2025	European Journal of Pharmaceutical Sciences	link
118	Jun Wang	Synthesis and Properties of 1,3-Dimethoxyacetone: A Glycerol-Derived Solvent	2025	Industrial & Engineering Chemistry Research	link

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119	Teja Kumar Ponduri	Computational Modelling for Formulation Design	2025	Applications of Computational Tools in Drug Design and Development	link
120	Maan Singh	Cocrystal Engineering-Based Strategies for Enhancing the Permeability of Poorly Permeable APIs	2025	Crystal Growth & Design	link
121	Melba Simon	Resolution of Double Salts via Crystallization - Induced Diastereomeric Transformation (CIDT)	2025	Chemical Engineering & Technology	link
122	Shengtao Jiang	Presence, partitioning, and toxicity of lithium-ion battery-derived cyclotriphosphazenes in aquatic environment	2025	Environmental Pollution	link
123	Aginmariya Kottarathil	Huckel anion based concentrated electrolytes for lithium-sulfur batteries	2025	Physical Chemistry Chemical Physics	link
124	PPaula V.A. Pontes	COSMO-RS assisted selection of eutectic solvents for lignin dissolution and enhanced laccase activity	2025	International Journal of Biological Macromolecules	link
125	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
126	Mariam Kholany	Extraction and separation of pigments from Saccharina latissima using eutectic solvents	2025	Separation and Purification Technology	link
127	Alejandro Belinchón	Extractive distillation for separating short-chain alcohols from water using cyclic carbonates as an extractive solvent: Experimental and process simulation	2025	Separation and Purification Technology	link

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128	Shaida Panbachi	Abiraterone acetate fixed-dosed combinations with ibuprofen-based therapeutic eutectic and deep eutectic solvents	2025	International Journal of Pharmaceutics	link
129	Sergio de-la-Huerta-Sainz	Nature's tool kit: Designing biocompatible and affordable NADES for sustainable extraction of plant bioactives	2025	Deleted Journal	link
130	Yongqiang Cheng	Vapor-liquid phase equilibrium study and computational thermodynamics of mixed inorganic salt aqueous solution	2025	Chemical Engineering Science	link
131	David Asubonteng	Screening of effective ionic liquid for neodymium extraction using COSMO-RS	2025	Journal of the Indian Chemical Society	link
132	Siyi Han	Molecular Mechanism and Liquid-Liquid Equilibrium of Ionic Liquids for the Extraction Process of the Cyclohexane-Tert-Butanol Azeotropic System	2025	Journal of Chemical & Engineering Data	link
133	Adélaïde Savoy	Solvation Free Energies of Ion Dissociations in Dichloromethane: En Route to Accurate Computations	2025	The Journal of Physical Chemistry B	link
134	Nazir Fattahi	Using COSMO-RS in the designing and screening of different eutectic solvents for the extraction of carbaryl	2025	Separation and Purification Technology	link
135	Wenyu Zheng	Steady and cyclic recovery of potato protein from starch waste via tailored deep eutectic solvent system	2025	Chemical Engineering Journal	link
136	Rajat Goyal	Advancements and Applications of Herbal Cocrystals	2025	Cocrystals in Pharmaceutical Sciences	link
137	Felipe Sanchez Bragagnolo	An updated gradient PLE-SPExHPLC-PDA system for the extraction, concentration, fractionation, and analysis of valuable compounds from cocoa bean shells	2025	Food Chemistry	link

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138	Pengfei Jiao	Enhanced deep eutectic solvent extraction of phenolic compounds from hawthorn seeds with ultrasonic and resin in-situ adsorption assistance: Process optimization, component analysis, and extraction mechanism	2025	Food Chemistry	link
139	Rubén Santiago	Prediction of partition coefficients in aqueous organic systems using COSMO-RS	2025	Separation and Purification Technology	link
140	Hao Qin	Multiscale theoretical screening of deep eutectic solvents for selective separation of the R410A blend	2025	Journal of Molecular Liquids	link
141	Junxu Li	Transplacental transfer of p-phenylenediamine antioxidants: Insights from human gestational exposure and an optimized BeWo cell monolayer model	2025	Journal of Hazardous Materials	link
142	Zhongyuan Zhai	Isobaric Vapor–Liquid Equilibrium Data for the Near-Boiling System 1,2,4-Trimethylbenzene + 1,3,5-Trimethylbenzene + Dimethyl Sulfoxide or Sulfolane at 101.3 kPa	2025	Journal of Chemical & Engineering Data	link
143	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
144	Weilong Peng	Eco-friendly extraction of polysaccharides from Moringa oleifera Lam. leaves using COSMO-RS screened natural deep eutectic solvents	2025	Food Research International	link

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145	Tatsuya Oshima	Machine Learning Prediction of Au(III) Extractability of Various Organic Solvents Based on Ion Solvation in Hydrochloric Acid Media	2025	ACS Sustainable Chemistry & Engineering	link
146	Todd M. Martin	Physicochemical Property Models for Poly- and Perfluorinated Alkyl Substances and Other Chemical Classes	2025	Journal of Chemical Information and Modeling	link
147	Shumin Chen	Theoretical study on adsorption and separation of SF ₆ /N ₂ by halogenated two-dimensional imine-based covalent organic frameworks	2025	Materials Today Communications	link
148	Abubakkar Saddeeq	Advances of Ionic-Mediated Polymer Architectures for CO ₂ Gas Separation Membranes: A Comprehensive Review of Design, Progress, and Future Prospects	2025	ACS Omega	link
149	Zhao Qin	Enhanced lignocellulose biomass hydrolysis in a confined space with cellulase-containing liposomes for high-levels succinic acid production	2025	International Journal of Biological Macromolecules	link
150	Jacek Zeglinski	Toward Predicting Nucleation Difficulty of Organic Compounds Crystallized from Different Solvents	2025	Crystal Growth & Design	link
151	Mohammed K. Al-Sakkaf	Deciphering Zn(II)-Carboxylic Acid Interactions: Tailoring Oil/Water Interfaces and Surfactant Efficiency	2025	Langmuir	link
152	Ali Ebrahimpoor Gorji	MLR Data-Driven for the Prediction of Infinite Dilution Activity Coefficient of Water in Ionic Liquids (ILs) Using QSPR-Based COSMO Descriptors	2025	Journal of Chemical Information and Modeling	link

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153	B. Bernicot	Design and characterization of novel hydrophobic eutectic solvents based on metal-extracting ligands	2025	Journal of Molecular Liquids	link
154	Ayat Hussein Adhab	Development of Smart Models to Accurately Predict Dynamic Viscosity of CO ₂ -Saturated Polyethylene Glycol	2025	JOURNAL OF CHEMICAL ENGINEERING OF JAPAN	link
155	Murilo L. Alcantara	Density and viscosity of alkylammonium ionic liquids: Experimental and COSMO-RS	2025	Journal of Molecular Liquids	link
156	Shuning Jiang	Molecular interaction mechanism and process analysis of separation of cyclohexane/ethyl acetate by extractive distillation	2025	Separation and Purification Technology	link
157	Babar Saeed	Enhanced Bioethanol Separation via Thymol-Based DES-Integrated Membranes Derived from Waste PET Bottles	2025	ACS Sustainable Chemistry & Engineering	link
158	Davi Simões Lucas	Liquid-liquid extraction of n-butanol and n-butyl acetate with ionic liquid and thermodynamic modeling with COSMO-RS and NRTL	2025	Separation Science and Technology	link
159	Guanfeng Deng	Extraction of polysaccharides from Camellia oleifera leaves by dual enzymes combined with deep eutectic solvents screened by ANN and COSMO-RS	2025	International Journal of Biological Macromolecules	link
160	Francisco Paes	Integrating Solvent Effects into the Prediction of Kinetic Constants Using a COSMO-Based Equation of State	2025	Journal of Chemical Theory and Computation	link

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161	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
162	Jun Wang	Synthesis and Properties of Novel Glycerol-Derived Liquids with Dual Functional Groups: Nonsymmetric (E/Z)-Isomeric Mixtures of 1,3-Diether-2-Alkenes	2025	Chemistry - A European Journal	link
163	Pu-Fei Yang	Phase Distribution, Deposition, and Precipitation Scavenging of Atmospheric Semivolatile Organic Compounds under Steady-State Partitioning Theory	2025	Environmental Science & Technology	link
164	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
165	Xinhui Peng	Multi-scale study on the volatility of essential oil and its modulation methods	2025	Journal of Drug Delivery Science and Technology	link
166	Qi Wang	Spatiotemporal Trend of PFAS in Estuarine Sediments: Insights into Chlorinated Polyfluoroalkyl Ether Sulfonate Transformation	2025	Environmental Science & Technology	link
167	Tianwei Yan	Pigment removal from reverse-printed laminated flexible films by solvent-targeted recovery and precipitation	2025	Science Advances	link
168	Monika Nendza	Consolidated octanol/water partition coefficients: combining multiple estimates from different methods to reduce uncertainties in log KOW	2025	Environmental Sciences Europe	link

BIOVIA COSMOtherm 関連論文リスト (21/69)

169	Jun Wang	Synthesis and properties of symmetric glycerol-derived (E/Z)-1,3-diether-2-alkenes	2025	Industrial Chemistry and Materials	link
170	Rokas Elijošius	Predictive design of crystallographic chiral separation	2025	Nature Communications	link
171	María Antonieta Escobedo-Monge	Rational Design of Eco-Friendly Deep Eutectic Solvent Systems for the Recovery of High-Value Phytosterol Compounds	2025	Food and Bioprocess Technology	link
172	Harpreet Singh	Design and Structural Characteristics of Pharmaceutical Cocrystals	2025	Cocrystals in Pharmaceutical Sciences	link
173	Hua Du	Natural deep eutectic solvents combined with COSMO-RS model for efficient extraction of essential oil from Fructus Aurantii: Theoretical screening, process optimization, biological activity and mechanism	2025	Microchemical Journal	link
174	Edoardo Parascandolo	Accurate VLE Predictions via COSMO-RS-Guided Deep Learning Models: Solubility and Selectivity in Physical Solvent Systems for Carbon Capture	2025	Journal of Chemical Information and Modeling	link
175	Sonia Martel-Martín	Computational study of eco-friendly PFOA extraction via matrine-based low melting mixture	2025	Journal of Molecular Liquids	link
176	Nikhil Kumar	Multi-scale computational screening and mechanistic insights of cyclic amines as solvents for improved lignocellulosic biomass processing	2025	Green Chemistry	link
177	Weilong Peng	Efficient polyphenol extraction from Moringa oleifera Lam. leaves using natural deep eutectic solvents: COSMO-RS	2025	LWT	link

BIOVIA COSMOtherm 関連論文リスト (22/69)

		screening, ANN-GA optimization and antioxidant activity evaluation			
178	Stephan Beil	Decentralized graywater treatment by a combination of sequencing batch reactor and advanced oxidation processes for reuse in Vietnam	2025	Water Environment Research	link
179	Theaveraj Ravi	Optimization of oxidative extractive desulfurization process using high performance natural amino acid-based deep eutectic solvent as extractant: Experimental versus computational study	2025	Journal of Molecular Liquids	link
180	Hansen Wang	Application-driven design of non-aqueous electrolyte solutions through quantification of interfacial reactions in lithium metal batteries	2025	Nature Nanotechnology	link
181	Hisham S. Bamufleh	An Experimental and Theoretical Carbon Dioxide Capture - Based Investigation of Methyltrioctylammonium Trifluoromethanesulfonate Ionic Liquid	2025	International Journal of Energy Research	link
182	Florian Mast	Quaternary Ammonium Salts as Supporting Electrolytes in Cathodic Reductions: An Analysis of Their Electrochemical Stability	2025	The Journal of Physical Chemistry B	link
183	Jiahui Zhang	Molecular Insights and Process Integration for Efficient Separation of Methanol/Methyl Ethyl Ketone by Ionic Liquid Extractive Distillation	2025	ACS Sustainable Chemistry & Engineering	link
184	Thomas Nevolianis	Solvation Free Energies of Anions: From Curated Reference Data to Predictive Models	2025	PubMed	link

BIOVIA COSMOtherm 関連論文リスト (23/69)

185	Jialiang Ma	Unveiling a large fraction of hidden organosulfates in ambient organic aerosol	2025	Nature Communications	link
186	Zijun Li	Predicting hygroscopic growth of organosulfur aerosol particles using COSMOtherm	2024	Atmospheric Chemistry and Physics	link
187	Liwen Zhuang	Enhancing the solubility of carbamazepine using ionic liquids: An experiment and theoretical calculation	2024	Journal of Molecular Structure	link
188	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
189	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
190	Tong YANG	Prediction of vapor-liquid equilibrium data of uranium hexafluoride and fluoride and simulation of distillation process	2024	CIESC Journal	link
191	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
192	Sille Štěpánová	Acidity constants and protonation sites of cyclic dinucleotides determined by capillary electrophoresis, quantum chemical calculations, and NMR spectroscopy	2024	Electrophoresis	link

BIOVIA COSMOtherm 関連論文リスト (24/69)

193	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
194	Marta-Lisette Pikma	pKaH values and θ H angles of phosphanes to predict their electronic and steric parameters	2024	Dalton Transactions	link
195	Alexandre M. S. Jorge	Unravelling the molecular interactions behind the formation of PEG/PPG aqueous two-phase systems	2024	Physical Chemistry Chemical Physics	link
196	Mia Radović	Rational design of deep eutectic solvents for the stabilization of dehydrogenases: an artificial neural network prediction approach	2024	Frontiers in Chemistry	link
197	Ebert, C Dahley	Can membrane permeability of zwitterionic compounds be predicted by the solubility diffusion model?	2024	European Journal of Pharmaceutical Sciences	link
198	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
199	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
200	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
201	Zhengxing Dai	Predicting PC-SAFT parameters based on COSMO-RS	2024	AIChE Journal	link

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202	Nimra Javed	Separation of CO ₂ and TFE by using diethanolamine and diisopropylamine	2024	Separation Science and Technology	link
203	Fateme Molajafari	Computational screening for prediction of co-crystals: method comparison and experimental validation	2024	CrystEngComm	link
204	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
205	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
206	Austin N. Keller	Thermophysical property prediction of anion-functionalized ionic liquids for CO ₂ capture	2024	Journal of Molecular Liquids	link
207	Martin P. Andersson	The shape of water-how cluster formation explains the hydrophobic effect	2024	Journal of Molecular Liquids	link
208	Jing Fan	Hybrid data-driven and physics-based modeling for viscosity prediction of ionic liquids	2024	Green Energy & Environment	link
209	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
210	Zhengxing Dai	Melting points of ionic liquids: Review and evaluation	2024	Green Energy & Environment	link
211	Amal A.M. Elgharbawy	Antibacterial performance enhancement using hydrophobic deep eutectic solvents: COSMO-RS	2024	Journal of Molecular Liquids	link

BIOVIA COSMOtherm 関連論文リスト (26/69)

		prediction, experimental validation, and synergistic action with antibiotics			
212	Sebastian Steiner	Ring Opening of Diketene in Superacidic Media	2024	The Journal of Organic Chemistry	link
213	Shiyi Qin	Identifying Green Solvent Mixtures for Bioproduct Separation Using Bayesian Experimental Design	2024	ACS Sustainable Chemistry & Engineering	link
214	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
215	Changhang Zhang	Innovative formaldehyde adsorption with optimized deep eutectic solvents: An experiment and multilevel computational chemistry approach	2024	Environmental Research	link
216	Martin P. Andersson	Prediction of Surface Tension Using COSMO-RS	2024	Industrial & Engineering Chemistry Research	link
217	Nuria Aguilar	Insights into Carvone: Fatty Acid Hydrophobic NADES for Alkane Solubilization	2024	Energy & Fuels	link
218	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
219	Muhammad Irfan Khawar	Streamlining Linear Free Energy Relationships of Proteins through Dimensionality Analysis and Linear Modeling	2024	Journal of Chemical Information and Modeling	link

BIOVIA COSMOtherm 関連論文リスト (27/69)

220	Stephanie Peper	Resource-Efficient Solvent Utilization: Solvent Selection Criteria Based on Solvent Swap Characteristics	2024	ACS Sustainable Chemistry & Engineering	link
221	Palwasha Khan	Simulation-Driven Design and Synthesis of DES-PDMS Membranes for Enhanced Ethanol Pervaporation	2024	ACS Sustainable Chemistry & Engineering	link
222	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
223	Viraj De Silva	Cocrystals and Salts: The Structural Landscape of Multicomponent Solids of Chalcogenadiazoles	2024	Crystal Growth & Design	link
224	Yue Zhi	Environmental Occurrence and Biotic Concentrations of Ultrashort-Chain Perfluoroalkyl Acids: Overlooked Global Organofluorine Contaminants	2024	Environmental Science & Technology	link
225	Luis Alfonso Jiménez-Ortega	Synergistic Antioxidant Activity in Deep Eutectic Solvents: Extracting and Enhancing Natural Products	2024	ACS Food Science & Technology	link
226	Zejun Wu	Solubility prediction and interaction mechanism of FOX-7 in ten solvents by molecular and thermodynamic modeling	2024	Chemical Engineering Journal	link
227	Axel Schultheis	Crystallization - Based Separation of ϵ - Caprolactam from a Depolymerization Reaction Mixture – Fundamentals and Potential Separation Strategies	2024	Chemie Ingenieur Technik	link

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228	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
229	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
230	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
231	Federico Droghetti	Selective and Efficient Light-Driven CO ₂ Reduction to CO with a Heptacoordinated Polypyridine Iron(II) Catalyst	2024	ACS Catalysis	link
232	Ylenia F. Rodríguez	Unveiling the intermolecular forces and unique properties of [EMIM][EtSO ₄] + [EMIM][MeSO ₃]	2024	Journal of Molecular Liquids	link
233	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
234	Anastasia Komarova	O. Xylose Acetals - a New Class of Sustainable Solvents and Their Application in Enzymatic Polycondensation	2024	ChemSusChem	link
235	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

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236	Elsa Anselmi	Focus on Physico-Chemical Properties of Sulfoximines: Acidity, Basicity and Lipophilicity	2024	Chemistry - A European Journal	link
237	Ahmed Halilu	Reaching machine learning leverage to advance performance of electrocatalytic CO(2) conversion in non-aqueous deep eutectic electrolytes	2024	Scientific Reports	link
238	Daniel T. Gweme	OH Radical Oxidation of Organosulfates in the Atmospheric Aqueous Phase	2024	The Journal of Physical Chemistry A	link
239	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
240	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
241	Sérgio M Vilas-Boas	Solvent screening for the purification of monoterpenoids by countercurrent and centrifugal partition chromatography	2024	Journal of Chemical Technology & Biotechnology	link
242	Timothy M. Schwartz	Varying Lewis Acidity, Covalency, and Halide Mobility to Govern Oxidative Addition Reactivity of Ni-Group 13 Bimetallic Complexes	2024	Organometallics	link
243	Sara Rozas	In silico study on helicenes in hydrophobic natural deep eutectic solvent	2024	FlatChem	link

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244	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
245	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
246	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
247	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
248	Martin Stinglhamer	Site-selective Photoredox-Catalyzed Late-stage Benzylic Hydrogen Isotope Exchange	2024	Angewandte Chemie International Edition	link
249	Isadora Lopes de Oliveira	Selective Separation of α -Punicalagin, β -Punicalagin, and Ellagic Acid from Pomegranate Husk Aqueous Extract by an Optimized Adsorption Process Employing a (Deep) Eutectic Solvent	2024	Food and Bioprocess Technology	link
250	Ahmad S. Darwish	Enhanced furfural extraction using neoteric hydrophobic solvents for sustainable biomass recovery and bioenergy applications	2024	Bioresource Technology	link

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251	Kevin A. Spiekermann	Accurately Predicting Barrier Heights for Radical Reactions in Solution Using Deep Graph Networks	2024	The Journal of Physical Chemistry A	link
252	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
253	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
254	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
255	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
256	Fareeha Shadab	Guiding the Selection of Novel Amines for CO2 Capture Using a Molecular-Based and Multicriteria Modeling Approach	2024	Energy & Fuels	link
257	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
258	Clara Gomez-Urios	Unlocking Value from Waste: a Comparative Study of Orange Peel Extraction Methods Using Choline Chloride-Based Natural Deep Eutectic Solvents	2024	ACS Food Science & Technology	link

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259	Hussein K. Amusa	Synergistic ternary deep eutectic solvents: An archetype for sustainable and eco-conscious Li and Co recovery from spent batteries	2024	Chemical Engineering Journal	link
260	Samaneh Barani Pour	Exploring the efficiency of caprylic acid and quaternary ammonium salt-based deep eutectic solvents for separation of CO ₂ and H ₂ S from gas mixtures using molecular dynamics simulations and COSMO-RS	2024	Chemical Engineering Journal Advances	link
261	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
262	Yaru Peng	Per- and polyfluoroalkyl substances removal in water and wastewater treatment plants: overall efficiency and performance of adsorption	2024	Environmental Research Communications	link
263	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
264	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
265	Gabriel Teixeira	Designing type V deep eutectic solvents with antimalarial pharmaceutical ingredients	2024	European Journal of Pharmaceutics and Biopharmaceutics	link
266	Martin Kurfiřt	Influence of Selective Deoxyfluorination on the Molecular Structure of Type-2 N-Acetylglucosamine	2024	The Journal of Organic Chemistry	link

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267	Ville Tuppurainen		Conceptual design of furfural extraction, oxidative upgrading and product recovery: COSMO-RS-based process-level solvent screening	2024	Computers & Chemical Engineering	link
268	Andrew VanderWeide	I.	Multisite Ligand Noninnocence of (CpN3)Fe(CO)3+ with Exogenous Hydride Donors: Kinetics and Mechanism	2024	Organometallics	link
269	Kejun Hu		Tissue distribution of emerging per- and polyfluoroalkyl substances in wild fish species from Qiantang river, east China: Comparison of 6:2 Cl-PFESA with PFOS	2024	Environmental Research	link
270	Juan Wang		Unveiling Solubilization Mechanisms of Natural Deep Eutectic Solvents in Triazole Fungicides: COSMO-RS Calculations and Screening for Eco-Friendly, High-Efficiency Pesticide Systems	2024	ACS Sustainable Chemistry & Engineering	link
271	D. Hospital-Benito		Techno-economic assessment of bio-hythane upgrading processes based on ionic liquids	2024	Chemical Engineering Journal	link
272	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
273	Maarten Dobbelaere	R.	Geometric deep learning for molecular property predictions with chemical accuracy across chemical space	2024	Journal of Cheminformatics	link
274	Jie Zhang		Controlling Lignin Solubility in Nonpolar Lubricating Oil via Multiple Fatty Chains Modification Strategy	2024	ACS Sustainable Chemistry & Engineering	link

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275	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
276	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
277	Jennifer Osamede Airouyuwa	Sustainable green extraction of anthocyanins and carotenoids using deep eutectic solvents (DES): A review of recent developments	2024	Food chemistry	link
278	Huanxin Li	The dissolution behavior of 3,4-O-isopropylidene clindamycin in twelve mono-solvents: Solubility, intermolecular interactions, and apparent thermodynamics	2024	Thermochimica acta	link
279	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
280	Zhijia Miao	Discovery of perfluoroalkyl sulfonyl quaternary ammonium substances in the environment and their environmental behaviors	2024	Water Research	link
281	Widad Benmouloud	Quantitative structure - property relationship techniques for predicting carbon dioxide solubility in ionic liquids using machine learning methods	2024	International Journal of Quantum Chemistry	link

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282	Niamh Mac Fhionnlaioich	A hybrid approach to aqueous solubility prediction using COSMO-RS and machine learning	2024	Process Safety and Environmental Protection	link
283	Anthony J. Sigman - Lowery	Estimating Octanol–Water Partition Coefficients of Novel Brominated Flame Retardants by Reversed-Phase High-Performance Liquid Chromatography and Computational Models	2024	Environmental Toxicology and Chemistry	link
284	Noora Hyttinen	Machine Learning Model to Predict Saturation Vapor Pressures of Atmospheric Aerosol Constituents	2024	ACS ES&T Air	link
285	Yuanchen Zhu	Effect and mechanism of ionic liquid-polymer composite coating on enhancing hydrogen embrittlement resistance of X80 pipeline steel for hydrogen blended natural gas transportation	2024	International Journal of Hydrogen Energy	link
286	Chandrakant Mukesh	Insight into lignin oxidative depolymerization in ionic liquids and deep eutectic solvents	2024	Biomass and Bioenergy	link
287	Yurou Shao	A facile synthesis of trioctylphosphine oxide-based azole deep eutectic solvents: Efficient reversible CO ₂ capture	2024	Fuel	link
288	Kathrin Marina Eckert	Exploring pNIPAM hydrogels: Experimental study on swelling equilibria in various organic solvents and mixtures, supported by COSMO-RS analysis	2024	Fluid Phase Equilibria	link
289	Gayathri Mahavishnu	Investigation of molecular polarity and thermal stability of monoethanolamine based deep eutectic solvents	2024	Journal of Dispersion Science and Technology	link
290	Ahmad S. Darwish	High-throughput screening of 2,500 ionic liquids for sustainable furfural recovery: Bridging quantum	2024	Chemical Engineering Journal	link

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		simulations, machine learning, and experimental validation			
291	Chenjun He	Glycol-based Alkaline Deep Eutectic Solvents for “Lignin-First” Dissolution from Coconut Shells	2024	ACS Sustainable Chemistry & Engineering	link
292	Yan Liu	Temperature Evaluation Considering Gradient Distribution for MV Cable XLPE Insulation Based on Wave Velocity	2024	Symmetry	link
293	Sana Eid	Rapid and highly efficient removal of aqueous perfluorooctanoic acid using deep eutectic solvents for sustainable water remediation: An integrated experimental-modeling approach	2024	Chemical Engineering Journal	link
294	Anita Šalić	Extraction of polyphenolic compounds from ginkgo leaves using deep eutectic solvents: A potential solution for the sustainable and environmentally friendly isolation of biflavonoids	2024	Industrial Crops and Products	link
295	Tunga Salthammer	Assessment of methods for predicting physical and chemical properties of organic compounds	2024	Indoor Environments	link
296	Jian Wang	Thermodynamic properties, electrochemical properties, and interaction behaviors of quaternary ammonium salts-based deep eutectic solvents	2024	Journal of Molecular Liquids	link
297	Andrea Sánchez-Monedero	Efficient recovery of antioxidants from olive leaves through green solvent extraction and enzymatic	2024	Journal of Molecular Liquids	link

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			hydrolysis: Experimental evaluation and COSMO-RS analysis			
298	Aginmariya Kottarathil		The Role of the Anion in Concentrated Electrolytes for Lithium-Sulfur Batteries	2024	Journal of The Electrochemical Society	link
299	Christopher Burcham	L.	Pharmaceutical Digital Design: From Chemical Structure through Crystal Polymorph to Conceptual Crystallization Process	2024	Crystal Growth & Design	link
300	Amira Neni		Evaluating asphaltene dispersion with choline chloride or menthol based deep eutectic solvents: A COSMO-RS analysis	2024	Journal of Molecular Liquids	link
301	Robin Wollesen de Jonge		Natural Marine Precursors Boost Continental New Particle Formation and Production of Cloud Condensation Nuclei	2024	Environmental Science & Technology	link
302	Biting Qiao		Multimedia distribution and release characteristics of emerging PFAS in wastewater treatment plants in Tianjin, China	2024	Journal of Hazardous Materials	link
303	Kai Wang		Assessment of COSMO-RS for Predicting Liquid-Liquid Equilibrium in Systems Containing Deep Eutectic Solvents	2024	Industrial & Engineering Chemistry Research	link
304	Mantra Dheendayal		Enhanced Electron Transfer Rates Between Surface-Attached Dye Molecules with Large Pendant Moieties and Co ³⁺ /2 ⁺ Complex Redox Mediators	2024	The Journal of Physical Chemistry C	link

BIOVIA COSMOtherm 関連論文リスト (38/69)

305	Pu-Fei Yang	Temperature dependence of the rain-gas and snow-gas partition coefficients for nearly a thousand chemicals	2024	Chemosphere	link
306	Andrea Mio	Beyond the Veil: Free Energy Profiles and Partition Coefficients for Antimelanoma Drugs in Self-Assembled Nanomicelles via COSMOmic and Atomistic Molecular Dynamics Simulations	2024	Journal of chemical and engineering data/Journal of chemical & engineering data	link
307	Omri D. Abarbanel	QupKake: Integrating Machine Learning and Quantum Chemistry for Micro-pK(a) Predictions	2024	Journal of Chemical Theory and Computation	link
308	Moein Adel	A comparative simulation study of piezoelectric properties in zigzag and armchair boron nitride nanotubes: by discovering a pioneering protocol	2024	Journal of Mathematical Chemistry	link
309	Laura Marie Grimm	Fluorescent Paracyclophanes: Unveiling Ultra - Strong Binding with Cucurbit[8]uril in Aqueous Environments	2024	ChemistryEurope	link
310	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
311	Ana M. Ferreira	Valorizing banana peels by extracting rutin with hydrated organic acids	2024	Food Chemistry Advances	link
312	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

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313	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
314	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
315	Adrien Fusina	Hydrotropic and solvent strategies to enhance the solubilization of polyphenols in relation to their chemical structure	2024	Journal of Molecular Liquids	link
316	Zheng-Wang Qu	Mechanism of Alkaline Earth Metal Amide Catalyzed Hydrogenation of Challenging Alkenes and Arenes	2024	ChemSusChem	link
317	Derek M. Dalton	Utopia Point Bayesian Optimization Finds Condition-Dependent Selectivity for N-Methyl Pyrazole Condensation	2024	Journal of the American Chemical Society	link
318	Weiping Qin	Species Difference? Bovine, Trout, and Human Plasma Protein Binding of Per- and Polyfluoroalkyl Substances	2024	Environmental science & technology	link
319	Florian Mast	Choice of the Right Supporting Electrolyte in Electrochemical Reductions: A Principal Component Analysis	2024	Journal of the American Chemical Society	link
320	Bin Li	Deep eutectic solvent self-assembled reverse nanomicelles for transdermal delivery of sparingly soluble drugs	2024	Journal of nanobiotechnology	link

BIOVIA COSMOtherm 関連論文リスト (40/69)

321	Sholpan Islam	Desulfurization and Denitrogenation Using Betaine-Based Deep Eutectic Solvents	2024	Journal of chemical and engineering data/Journal of chemical & engineering data	link
322	Isabella W. Cordova	Using Molecular Conformers in COSMO-RS to Predict Drug Solubility in Mixed Solvents	2024	Industrial & engineering chemistry research	link
323	Henrik Möbitz	Nonclassical Zwitterions as a Design Principle to Reduce Lipophilicity without Impacting Permeability	2024	Journal of medicinal chemistry	link
324	Zhou Xu	Natural Deep Eutectic Solvent-Based Ultrasound-Assisted Extraction of Flavonoids from Fagopyrum tataricum Bran	2024	Separations	link
325	Sung Eun Jerng	Machine learning for CO2 capture and conversion: A review	2024	Energy and AI	link
326	Abir Boublia	Zinc chloride-assisted activation of açai 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

BIOVIA COSMOtherm 関連論文リスト (41/69)

327	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
328	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
329	Ana Casas	Machine learning screening tools for the prediction of extraction yields of pharmaceutical compounds from wastewaters	2024	Journal of water process engineering	link
330	Andrea Ebert	Can membrane permeability of zwitterionic compounds be predicted by the solubility-diffusion model?	2024	European journal of pharmaceutical sciences	link
331	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
332	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
333	Leonhard Schill	Rational solvent selection for the preparation of industrial monolithic supported liquid-phase (SLP) olefin hydroformylation catalyst	2024	Green technologies and sustainability	link
334	Jemilat Yetunde Yusuf	Eco-friendly Functionalization of MWCNTs with Deep Eutectic Solvents	2024	Inorganic chemistry communications/Inorganic	link

BIOVIA COSMOtherm 関連論文リスト (42/69)

				chemistry communications (Online)	
335	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
336	Alejandro Belinchón	A step closer to sustainable CO2 conversion: Limonene carbonate production driven by ionic liquids	2024	Journal of cleaner production	link
337	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
338	Mariana Almeida Bortholazzi	Strategies Employed to Design Biocompatible Metal Nanoparticles for Medical Science and Biotechnology Applications	2024	ACS applied materials & interfaces	link
339	Sebastian Höthker	Stereoconvergent Approach to the Enantioselective Construction of alpha-Quaternary Alcohols by Radical Epoxide Allylation	2024	Angewandte Chemie	link
340	Mood Mohan	High-Throughput Screening and Accurate Prediction of Ionic Liquid Viscosities Using Interpretable Machine Learning	2024	ACS sustainable chemistry & engineering	link
341	Luise F. Kaven	Dynamic Modeling for Synthesis of Tailored Microgels with Charged Domains	2024	Industrial & engineering chemistry research	link

BIOVIA COSMOtherm 関連論文リスト (43/69)

342	Fernanda Pelaquim	Paludetto	Prediction of Greenhouse Gas Solubility in Eutectic Solvents Using COSMO-RS	2024	International journal of thermophysics	link
343	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/ <input checked="" type="checkbox"/> The <input checked="" type="checkbox"/> Journal of chemical physics/Journal of chemical physics	link
344	Safrina Hardiningtyas	Dyah	Sustainable Synthesis of Cellulose Nanofibers from Industrial Agar Seaweed Waste Biomass Using Hydrated Deep Eutectic Solvents	2024	Waste and biomass valorization	link
345	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
346	Tadej Menegatti		Tuning Mechanical Characteristics and Permeability of Alginate Hydrogel by Polyvinyl Alcohol and Deep Eutectic Solvent Addition	2024	Bioengineering	link
347	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
348	Huanxin Li		Application of ionic liquid extractant in enhanced separation of 2-propanol-n-hexane azeotrope system	2024	Journal of physics. Condensed matter	link
349	Martin P. Andersson		The shape of water - how cluster formation explains the hydrophobic effect	2024	Journal of molecular liquids	link

BIOVIA COSMOtherm 関連論文リスト (44/69)

350	Nuria Aguilar	In silico study of therapeutic deep eutectic solvent for tetracaine liquid delivery	2024	Journal of molecular liquids	link
351	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
352	Zhihan Huang	Effect of N-o-nitrobenzylation on conformation and membrane permeability of linear peptides	2024	Bioorganic chemistry	link
353	Nikhil Kumar	Inhibition of asphaltene aggregation using deep eutectic solvents: COSMO-RS calculations and experimental validation	2024	Journal of molecular liquids	link
354	Tristan Dupeux	Molecular insights into fragrance release from SDS and SLES micelles	2024	Colloids and surfaces. A, Physicochemical and engineering aspects	link
355	Carolin Dahley	Predicting the intrinsic membrane permeability of Caco-2/MDCK cells by the solubility-diffusion model	2024	European journal of pharmaceutical sciences	link
356	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
357	Chuxin Qi	Rational screening of ionic liquids as phase transfer catalysts for aromatic O- and S-glycosidations exemplified by acetobromo-alpha-D-galactose with phenolic compound	2024	Journal of molecular liquids	link

BIOVIA COSMOtherm 関連論文リスト (45/69)

358	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
359	Wenxiu Li	Separation of Ethyl Acetate and Ethanol Azeotropic System by Acetate-Based Ionic Liquid	2024	Journal of solution chemistry	link
360	Zhijie Shang	Ionic-Liquid-Assisted Capture of Volatile Low-Carbon Alcohols in Printing Plant Exhaust Gas	2024	ACS sustainable chemistry & engineering	link
361	Mehmet Ogün Biçer	Industrial Distillation Aspects of Diketene	2024	Chimia	link
362	Judite Resende	Sustainable Phytosterol Extraction from <i>Codium tomentosum</i> Using Eutectic Solvents	2024	ACS sustainable chemistry & engineering	link
363	Fernando A. Lugo	Improved Approach for ab Initio Calculations of Rate Coefficients for Secondary Reactions in Acrylate Free-Radical Polymerization	2024	Polymers	link
364	Timothy F. M. Rodgers	Bioretention Design Modifications Increase the Simulated Capture of Hydrophobic and Hydrophilic Trace Organic Compounds	2024	Environmental science & technology	link
365	Philipp Petermeier	Integrated preservation of water activity as key to intensified chemoenzymatic synthesis of bio-based styrene derivatives	2024	Communications chemistry	link
366	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

BIOVIA COSMOtherm 関連論文リスト (46/69)

367	Tomasz Jeliński	Deep Eutectic Solvents as Agents for Improving the Solubility of Edaravone: Experimental and Theoretical Considerations	2024	Molecules/Molecules online/Molecules annual	link
368	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
369	Mohd Amirul Mukmin Abdullah	Discovering [C4C1im][BF4] as draw solution in forward osmosis	2024	Journal of advanced manufacturing and processing	link
370	Thomas Gasevic	Benchmark Study on the Calculation of ²⁰⁷ Pb NMR Chemical Shifts	2024	Inorganic chemistry	link
371	Gangqiang Yu	Hydrocarbon Extraction with Ionic Liquids	2024	Chemical reviews	link
372	Shufen Wang	Vapor–Liquid Equilibrium of Monoterpene–Sesquiterpene System Containing Resin Acid	2024	Industrial & engineering chemistry research	link
373	Rita Kol	Increasing the Dissolution Rate of Polystyrene Waste in Solvent-Based Recycling	2024	ACS sustainable chemistry & engineering	link
374	Ekta Pardhi	Nanocrystal technologies in biomedical science: From the bench to the clinic	2024	Drug discovery today	link
375	Batoul Zohra Sari-Ali	Fatima containing (methanol, or propan-1-ol, or water, or acetonitrile) and 1-ethyl-3-methylimidazolium thiocyanate ionic liquid: Measurements and modeling	2024	Journal of molecular liquids	link

BIOVIA COSMOtherm 関連論文リスト (47/69)

376	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
377	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
378	Piotr Cysewski	Intermolecular Interactions as a Measure of Dapsone Solubility in Neat Solvents and Binary Solvent Mixtures	2023	Materials	link
379	A.K.D. Celsie	Metrics for estimating vapour pressure deviation from ideality in binary mixtures	2023	SAR and QSAR in Environmental Research	link
380	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
381	Ana Pacheco	Green Solvent Selection for Emulsifiable Concentrate Agrochemical Formulations	2023	Organic Process Research & Development	link
382	Jonathan P. Antle	Building Chemical Intuition about Physicochemical Properties of C8-Per-/Polyfluoroalkyl Carboxylic Acids through Computational Means	2023	ACS ES&T Engineering	link
383	Rubén Santiago	Predicting Partition Coefficients in Organic Biphasic Systems Using COSMO-RS	2023	Industrial & Engineering Chemistry Research	link
384	Hui Tian	Feasibility Analysis for the Direct Hydration of 1-Octene in a Catalytic Distillation Process Using Residual Curve Maps	2023	Processes	link

BIOVIA COSMOtherm 関連論文リスト (48/69)

385	Cariny Polesca	Sustainable keratin recovery process using a bio-based ionic liquid aqueous solution and its techno-economic assessment	2023	Green Chemistry	link
386	Marten Lache	Water and Ethanol as Refrigerant Mixture Enabling Adsorption Cooling below 0 C	2023	Energy Technology	link
387	Noora Hyttinen	Predicting liquid–liquid phase separation in ternary organic–organic–water mixtures	2023	Physical Chemistry Chemical Physics	link
388	Mohsen Ghasemi	A Molecular Thermodynamic Model of Coacervation in Solutions of Polycations and Oppositely Charged Micelles	2023	Langmuir	link
389	Théophile Gaudin	Robust definition and prediction of dispersive Hansen solubility parameter δD with COSMO-RS	2023	Computational and Theoretical Chemistry	link
390	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
391	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
392	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

BIOVIA COSMOtherm 関連論文リスト (49/69)

393	Minghao SONG	Multi-scale simulation and study of volatile phenols removal from simulated oil by ionic liquids	2023	CIESC Journal	link
394	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
395	Nicola Piasentin	In Silico Prediction of Stratum Corneum Partition Coefficients via COSMOmic and Molecular Dynamics Simulations	2023	The Journal of Physical Chemistry B	link
396	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
397	Shiyi Qin	Capturing molecular interactions in graph neural networks: A case study in multi-component phase equilibrium	2023	Digital Discovery	link
398	Pan Xu	Biomethane purification with quaternary ammonium salts-based deep eutectic solvents: Experiment and computational thermodynamics	2023	Separation and Purification Technology	link
399	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

BIOVIA COSMOtherm 関連論文リスト (50/69)

400	Ye Tao	Exploring controls on perfluorocarboxylic acid (PFCA) gas-particle partitioning using a model with observational constraints	2023	Environmental Science: Processes & Impacts	link
401	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
402	Zehao Mi	Theoretical analysis of CO2 absorption by polyamines-TFSA type protic ionic liquids	2023	Chemical Industry and Engineering Progress	link
403	Pan Xu	Efficient purification of biogas using ionic liquid as absorbent: Molecular thermodynamics, dynamics and experiment	2023	Journal of Environmental Chemical Engineering	link
404	A. Viñas-Ospino	Using novel hydrophobic deep eutectic solvents to improve a sustainable carotenoid extraction from orange peels	2023	Food Bioscience	link
405	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
406	Vitus Besel	Atomic structures, conformers and thermodynamic properties of 32k atmospheric molecules	2023	Scientific data	link
407	Mengke Zhang	Estimation of vapor pressures of perfluoroalkyl substances (PFAS) using COSMOtherm	2023	Journal of Hazardous Materials	link

BIOVIA COSMOtherm 関連論文リスト (51/69)

408	Chunjie Liu	Designing Deep Eutectic Solvents with Crystalline Features: A New-Generation Green Crystallization-Induced Porogen	2023	ACS Sustainable Chemistry & Engineering	link
409	Kaihang Zhang	Screening ionic liquids for efficiently extracting perfluoroalkyl chemicals (PFACs) from wastewater	2023	Journal of Environmental Sciences	link
410	Noora Hyttinen	The effect of atmospherically relevant aminium salts on water uptake	2023	Atmospheric Chemistry and Physics	link
411	Rubén Santiago	Anticipating APIs solubility in natural eutectic solvents: Lidocaine and caffeine case studies	2023	Food Bioscience	link
412	Zijun Li	Saturation vapor pressure characterization of selected low-volatility organic compounds using a residence time chamber	2023	Environmental Science & Technology	link
413	Juliane Glüge	Evaluation of Physicochemical Property Data in the ECHA Database	2023	Scientific data	link
414	Zehao Mi	DFT and COSMO-RS theoretical analysis of SO ₂ absorption by polyamines type ionic liquids	2023	Journal of Hazardous Materials	link
415	Michael Diedenhofen	COSMO-RS blind prediction of distribution coefficients and aqueous pKa values from the SAMPL8 challenge	2023	ACS Sustainable Chemistry & Engineering	link
416	Satoshi Endo	Intermolecular Interactions, Solute Descriptors, and Partition Properties of Neutral Per-and Polyfluoroalkyl Substances (PFAS)	2023	Journal of Environmental Sciences	link

BIOVIA COSMOtherm 関連論文リスト (52/69)

417	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
418	Xia Li		Study on Vapor–Liquid Equilibrium and Microscopic Properties of Glycine + H ₂ O, l-Histidine + H ₂ O, and l-Tryptophan + H ₂ O	2023	Journal of Molecular Liquids	link
419	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
420	Laura Guidugli	Fronchetti	Understanding Microcystin-LR separation by hydrophobic deep eutectic solvents with COSMO simulation and experimental findings	2023	Journal of Physical and Chemical Reference Data	link
421	Pablo Sánchez	Gutiérrez-	Extraction of antibiotics identified in the EU Watch List 2020 from hospital wastewater using hydrophobic eutectic solvents and terpenoids	2022	CIESC Journal	link
422	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
423	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
424	Rubén Santiago		Assessment of bio-ionic liquids as promising solvents in industrial separation processes: Computational screening using COSMO-RS method	2022	Chemosphere	link

BIOVIA COSMOtherm 関連論文リスト (53/69)

425	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
426	Juan Wang	COSMO-RS prediction and experimental verification of deep eutectic solvents for water insoluble pesticides with high solubility	2022	Chemical Data Collections	link
427	Clinton J. Chapman	Evaluation of solvate and co-crystal screening methods for CL-20 containing energetic materials	2022	Journal of Molecular Liquids	link
428	Noora Hyttinen	Machine learning for predicting chemical potentials of multifunctional organic compounds in atmospherically relevant solutions	2022	Separation and Purification Technology	link
429	Shuai Qian	Experimental and Computational Study of the Properties of Imidazole Compounds with Branched and Cycloalkyl Substituents	2022	Foods	link
430	Mohsen Taheri	Ionic liquid screening for CO ₂ capture and H ₂ S removal from gases: The syngas purification case	2021	Molecules	link
431	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
432	Sivani Baskaran	Reliable prediction of the octanol–air partition ratio	2021	Environmental Science & Technology	link
433	Huma Warsi Khan	Design and selection of ionic liquids via COSMO for pharmaceuticals and medicine	2021	Journal of Molecular Liquids	link

BIOVIA COSMOtherm 関連論文リスト (54/69)

434	Noora Hyttinen	Gas-to-Particle Partitioning of Cyclohexene- and α -Pinene-Derived Highly Oxygenated Dimers Evaluated Using COSMOtherm	2021	Journal of Energetic Materials	link
435	Emma Lumiaro	Predicting gas-particle partitioning coefficients of atmospheric molecules with machine learning	2021	The Journal of Physical Chemistry Letters	link
436	Timothy F. M. Rodgers	Novel Bayesian method to derive final adjusted values of physicochemical properties: application to 74 compounds	2021	Liquids	link
437	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
438	Judith Warnau	COSMO-RS predictions of logP in the SAMPL7 blind challenge	2021	Molecules	link
439	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
440	Boluwatife Awonaiké	Precipitation-induced transport and phase partitioning of organophosphate esters (OPEs) in urban and rural watersheds	2021	Application of Ionic Liquids in Drug Delivery	link
441	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

BIOVIA COSMOtherm 関連論文リスト (55/69)

442	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
443	Samuel Boobier	Machine learning with physicochemical relationships: solubility prediction in organic solvents and water	2020	Environmental Science & Technology	link
444	Alina Lampic	Property estimation of per- and polyfluoroalkyl substances: A comparative assessment of estimation methods	2020	Environmental Science: Processes & Impacts	link
445	Christoph Loschen	COSMO-RS based predictions for the SAMPL6 logP challenge	2020	Journal of Computer-Aided Molecular Design	link
446	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
447	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
448	Noora Hyttinen	Thermodynamic properties of isoprene- and monoterpene-derived organosulfates estimated with COSMOtherm	2020	Scientific Reports	link
449	Noora Hyttinen	Improving Solubility and Activity Estimates of Multifunctional Atmospheric Organics by Selecting Conformers in COSMOtherm	2020	Engineering, Technology & Applied Science Research	link

BIOVIA COSMOtherm 関連論文リスト (56/69)

450	Noora Hyttinen	Estimating aqueous solubilities and activity coefficients of mono- and α, ω -dicarboxylic acids using COSMOtherm	2020	Nature communications	link
451	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
452	Benjamin Sanchez-Lengeling	A Bayesian approach to predict solubility parameters	2019	Journal of Computer-Aided Molecular Design	link
453	Varun Kundi	Predicting Octanol-Water Partition Coefficients: Are Quantum Mechanical Implicit Solvent Models Better than Empirical Fragment-Based Methods?	2019	ACS omega	link
454	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
455	Georgia Michailoudi	Solubility and Activity Coefficients of Atmospheric Surfactants in Aqueous Solution Evaluated Using COSMOtherm	2019	Atmospheric Chemistry and Physics	link
456	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
457	Vishwesh Venkatraman	Predicting ionic liquid melting points using machine learning	2018	Atmospheric Chemistry and Physics	link

BIOVIA COSMOtherm 関連論文リスト (57/69)

458	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
459	R. Santiago	Acetylene absorption by ionic liquids: A multiscale analysis based on molecular and process simulation	2018	Advanced Theory and Simulations	link
460	Theo Kurtén	Estimating the saturation vapor pressures of isoprene oxidation products and using COSMO-RS	2018	The Journal of Physical Chemistry B	link
461	Yuriy A. Abramov	Rational solvent selection for pharmaceutical impurity purge	2018	Chemical Engineering Science	link
462	Vishwesh Venkatraman	Predicting CO2 capture of ionic liquids using machine learning	2017	The Journal of Physical Chemistry A	link
463	Miranda Roesing	Solubility characteristics of poly (3-hexylthiophene)	2017	Journal of Molecular Liquids	link
464	Meysam Lotfi	Solubility of acyclovir in nontoxic and biodegradable ionic liquids: COSMO-RS prediction and experimental verification	2017	Journal of Molecular Liquids	link
465	Chen Wang	Uncertain Henry's law constants compromise equilibrium partitioning calculations of atmospheric oxidation products	2017	Journal of Computer-Aided Molecular Design	link
466	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

BIOVIA COSMOtherm 関連論文リスト (58/69)

467	Martta Toivola	Can COSMOTherm predict a salting in effect?	2017	Atmospheric Chemistry and Physics	link
468	Emad Ali	Modeling of CO2 Solubility in Selected Imidazolium-Based Ionic Liquids	2017	Crystal Growth & Design	link
469	Boluwatife Awonaike	Quantifying the equilibrium partitioning of substituted polycyclic aromatic hydrocarbons in aerosols and clouds using COSMOtherm	2017	Journal of CO2 Utilization	link
470	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
471	Andreas Klamt	Prediction of cyclohexane-water distribution coefficients with COSMO-RS on the SAMPL5 data set	2016	Journal of Molecular Liquids	link
472	Sebastian Brox	Alternative Single-Solvent Electrolytes Based on Cyanoesters for Safer Lithium-Ion Batteries	2016	Atmospheric Chemistry and Physics	link
473	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
474	Xingang Li	Ionic liquid-assisted solvent extraction for unconventional oil recovery: computational simulation and experimental tests	2016	The Journal of Physical Chemistry A	link

BIOVIA COSMOtherm 関連論文リスト (59/69)

475	Meysam Lotfi	Analysis of multiple solvation interactions of methotrexate and ammonium based ionic liquids using COSMO-RS	2016	Chemical Engineering Communications	link
476	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
477	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
478	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
479	Christoph Schütter	Toward new solvents for EDLCs: from computational screening to electrochemical validation	2015	ChemSusChem	link
480	Tamara Husch	Large-scale virtual high-throughput screening for the identification of new battery electrolyte solvents: computing infrastructure and collective properties	2015	Chemosphere	link
481	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
482	Tamara Husch	Charting the known chemical space for non-aqueous lithium-air battery electrolyte solvents	2015	Procedia Engineering	link

BIOVIA COSMOtherm 関連論文リスト (60/69)

483	W. Jeffrey Horne	Effect of branched and cycloalkyl functionalities on CO ₂ separation performance of poly (IL) membranes	2015	Fluid Phase Equilibria	link
484	Chen Wang	Calculating Equilibrium Phase Distribution during the Formation of Secondary Organic Aerosol Using COSMOtherm	2015	Science of The Total Environment	link
485	Anett Geisler	Predicting storage-lipid water partitioning of organic solutes from molecular structure	2015	Physical Chemistry Chemical Physics	link
486	Markéta Paloncýová	Amphiphilic drug-like molecules accumulate in a membrane below the head group region	2014	The Journal of Physical Chemistry C	link
487	Chen Wang	Measuring and modeling the salting-out effect in ammonium sulfate solutions	2014	Physical Chemistry Chemical Physics	link
488	W. Jeffrey Horne	Correlating fractional free volume to CO ₂ selectivity in [Rmim][Tf ₂ N] ionic liquids	2014	Atmospheric Environment	link
489	Angelika Stenzel	Prediction of partition coefficients for complex environmental contaminants: Validation of COSMOtherm, ABSOLV, and SPARC	2014	Physical Chemistry Chemical Physics	link
490	Jens Reinisch	Prediction of free energies of hydration with COSMO-RS on the SAMPL4 data set	2014	Separation and Purification Technology	link
491	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
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493	Matthew S. Shannon	Properties and Performance of Ether-Functionalized Imidazoles as Physical Solvents for CO ₂ Separations	2013	The Journal of Physical Chemistry B	link
494	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
495	Jason E. Bara	COSMOtherm as a Tool for Estimating the Thermophysical Properties of Alkylimidazoles as Solvents for CO ₂ Separations	2013	The Journal of Chemical Thermodynamics	link
496	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
497	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
498	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
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502	Shannon M. Mahurin	High CO ₂ solubility, permeability and selectivity in ionic liquids with the tetracyanoborate anion	2012	Industrial & Engineering Chemistry Research	link
503	Juan Pablo Gutiérrez	COSMO-RS-based ionic-liquid selection for extractive distillation processes	2012	Journal of Environmental Chemistry and Ecotoxicology	link
504	Judith Schenzel	Experimentally determined soil organic matter-water sorption coefficients for different classes of natural toxins and comparison with estimated numbers	2012	Journal of Chemical & Engineering Data	link
505	Jens Reinisch	Prediction of free energies of hydration with COSMO-RS on the SAMPL3 data set	2012	Journal of Environmental Chemistry and Ecotoxicology	link
506	Andreas Klamt	The COSMO and COSMO-RS solvation models	2011	Industrial & Engineering Chemistry Research	link
507	Zhanyun Wang	Using COSMOtherm to predict physicochemical properties of poly- and perfluorinated alkyl substances (PFASs)	2011	Journal of pharmaceutical sciences	link
508	Kazi Z. Sumon	Ionic liquids for CO ₂ capture using COSMO-RS: Effect of structure, properties and molecular interactions on solubility and selectivity	2011	Green chemistry	link
509	Victoria P. Sacks	Development and use of polyethylene passive samplers to detect triclosans and alkylphenols in an urban estuary	2011	RSC advances	link
510	Matthew B. Miller	Critical Assessment of CO ₂ Solubility in Volatile Solvents at 298.15 K	2011	Industrial & Engineering Chemistry Research	link

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511	Kai-Uwe Goss	Predicting equilibrium sorption of neutral organic chemicals into various polymeric sorbents with COSMO-RS	2011	Environmental Science & Technology	link
512	Jens Reinisch	Prediction of the temperature dependence of a polyether-water mixture using COSMOtherm	2011	Journal of Computer-Aided Molecular Design	link
513	Gábor Járvas	COSMO-RS based CFD model for flat surface evaporation of non-ideal liquid mixtures	2011	WIREs Computational Molecular Science	link
514	Bernd Schröder	Prediction of aqueous solubilities of solid carboxylic acids with COSMO-RS	2010	Environmental Chemistry	link
515	Sarah E. Hale	Partitioning of organochlorine pesticides from water to polyethylene passive samplers	2010	Fluid Phase Equilibria	link
516	Xianming Zhang	Assessment of chemical screening outcomes based on different partitioning property estimation methods	2010	Environmental science & technology	link
517	Andreas Klamt	Blind prediction test of free energies of hydration with COSMO-RS	2010	Journal of Chemical & Engineering Data	link
518	Guido Bronner	Hexadecane/air partitioning coefficients of multifunctional compounds: Experimental data and modeling	2010	Analytical chemistry	link
519	Bernd Schröder	Prediction of environmental parameters of polycyclic aromatic hydrocarbons with COSMO-RS	2010	Fluid phase equilibria	link
520	Espen Mariussen	Relevance of 1, 2, 5, 6, 9, 10-hexabromocyclododecane diastereomer structure on partitioning properties, column-retention and clean-up procedures	2010	International Journal of Heat and Mass Transfer	link

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521	Andreas Klamt	Some conclusions regarding the predictions of tautomeric equilibria in solution based on the SAMPL2 challenge	2010	Fluid Phase Equilibria	link
522	Sandra Roy	Predictions of thermodynamic properties of energetic materials using COSMO-RS	2010	Environmental pollution	link
523	Frank Eckert	Prediction of acidity in acetonitrile solution with COSMO-RS	2009	Environment International	link
524	Andreas Klamt	On the performance of continuum solvation methods. A comment on “Universal approaches to solvation modeling”	2009	Journal of Computer-Aided Molecular Design	link
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528	Sierra Rayne	Computational approaches may underestimate pKa values of longer-chain perfluorinated carboxylic acids: Implications for assessing environmental and biological effects	2009	Journal of Computer-Aided Molecular Design	link
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530	Hans Peter H. Arp	Ambient gas/particle partitioning. 3. Estimating partition coefficients of apolar, polar, and ionizable organic compounds by their molecular structure	2009	Journal of Computational Chemistry	link
531	Kai-Uwe Goss	Predicting Adsorption of Organic Chemicals at the Air-Water Interface	2009	Accounts of Chemical Research	link
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536	Zheng Guo	Predictions of flavonoid solubility in ionic liquids by COSMO-RS: experimental verification, structural elucidation, and solvation characterization	2007	Fluid phase equilibria	link
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539	Andreas Klamt	Prediction, fine tuning, and temperature extrapolation of a vapor liquid equilibrium using COSMOtherm	2007	Chemosphere	link
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545	Hans Grensemann	Performance of a conductor-like screening model for real solvents model in comparison to classical group contribution methods	2005	Environmental science & technology	link
546	Martin Hornig	COSMOfrag: A Novel Tool for High-Throughput ADME Property Prediction and Similarity Screening Based on Quantum Chemistry	2005	Fluid phase equilibria	link
547	Dana Constantinescu	Vapor-liquid equilibrium prediction at high pressures using activity coefficients at infinite dilution from COSMO-type methods	2005	Fluid phase equilibria	link
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549	Hiroataka Ikeda	Prediction of solubility of drugs by conductor-like screening model for real solvents	2005	Journal of computational chemistry	link
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553	Gudrun Schürer	Prediction of adsorption equilibria from physical properties of the pure components	2005	Journal of chemical information and modeling	link
554	K.N Marsh	Room temperature ionic liquids and their mixtures - a review	2004	Fluid phase equilibria	link
555	Andreas Klamt	Prediction of vapor liquid equilibria using COSMOtherm	2004	Environmental Toxicology and Chemistry	link
556	Oliver Spuhl	COSMO-RS Predictions in Chemical Engineering A Study of the Applicability to Binary VLE	2004	Chemical and Pharmaceutical Bulletin	link
557	C.-T. Wu	Liquid-liquid equilibria of room-temperature ionic liquids and butan-1-ol	2003	Fluid Phase Equilibria	link
558	Andreas Klamt	First Principles Calculations of Aqueous pKa Values for Organic and Inorganic Acids Using COSMO-RS Reveal an Inconsistency in the Slope of the pKa Scale	2003	Journal of Chemical Information and Modeling	link
559	Michael Diedenhofen	Prediction of infinite dilution activity coefficients of organic compounds in ionic liquids using COSMO-RS	2003	Fluid Phase Equilibria	link

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560	Andreas Klamt	Prediction of the mutual solubilities of hydrocarbons and water with COSMO-RS	2003	Adsorption	link
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562	Frank Eckert	Prediction of halocarbon thermodynamics with COSMO-RS	2003	Fluid phase equilibria	link
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564	Kenneth N. Marsh	Room temperature ionic liquids as replacements for conventional solvents—A review	2002	Journal of Chemical & Engineering Data	link
565	Andreas Klamt	Prediction of aqueous solubility of drugs and pesticides with COSMO-RS	2002	The Journal of Physical Chemistry A	link
566	C. Mehler	Use of COSMO-RS for the prediction of adsorption equilibria	2002	Journal of Chemical & Engineering Data	link
567	Andreas Klamt	Prediction of soil sorption coefficients with a conductor-like screening model for real solvents	2002	Fluid Phase Equilibria	link
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569	Andreas Klamt	COSMO-RS: A novel view to physiological solvation and partition questions	2001	Fluid phase equilibria	link
570	Frank Eckert	Validation of the COSMO-RS method: Six binary systems	2001	AIChE Journal	link
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572	Andreas Klamt	Refinement and parametrization of COSMO-RS	1998	Journal of Computational Chemistry	link
573	Andreas Klamt	Conductor-like screening model for real solvents: a new approach to the quantitative calculation of solvation phenomena	1995	AIChE journal	link
