

## BIOVIA COSMOtherm 関連論文リスト (1/21)

No.	First author	Title	Year	Journal name	Link
1	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	<a href="#">link</a>
2	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	<a href="#">link</a>
3	Zhengxing Dai	Predicting PC-SAFT parameters based on COSMO-RS	2024	AIChE Journal	<a href="#">link</a>
4	Nimra Javed	Separation of CO <sub>2</sub> and TFE by using diethanolamine and diisopropylamine	2024	Separation Science and Technology	<a href="#">link</a>
5	Fateme Molajafari	Computational screening for prediction of co-crystals: method comparison and experimental validation	2024	CrystEngComm	<a href="#">link</a>
6	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	<a href="#">link</a>
7	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	<a href="#">link</a>
8	Austin N. Keller	Thermophysical property prediction of anion-functionalized ionic liquids for CO <sub>2</sub> capture	2024	Journal of Molecular Liquids	<a href="#">link</a>
9	Martin P. Andersson	The shape of water-how cluster formation explains the hydrophobic effect	2024	Journal of Molecular Liquids	<a href="#">link</a>

## BIOVIA COSMOtherm 関連論文リスト (2/21)

10	Mehmet Ogün Biçer	Industrial Distillation Aspects of Diketene	2024	Chimia	<a href="#">link</a>
11	Zhijie Shang	Ionic-Liquid-Assisted Capture of Volatile Low-Carbon Alcohols in Printing Plant Exhaust Gas	2024	ACS Sustainable Chemistry & Engineering	<a href="#">link</a>
12	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	<a href="#">link</a>
13	Piotr Cysewski	Experimental and Theoretical Insights into the Intermolecular Interactions in Saturated Systems of Dapsone in Conventional and Deep Eutectic Solvents	2024	Molecules	<a href="#">link</a>
14	Jing Fan	Hybrid data-driven and physics-based modeling for viscosity prediction of ionic liquids	2024	Green Energy & Environment	<a href="#">link</a>
15	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	<a href="#">link</a>
16	Zhengxing Dai	Melting points of ionic liquids: Review and evaluation	2024	Green Energy & Environment	<a href="#">link</a>
17	Amal A.M. Elgharbawy	Antibacterial performance enhancement using hydrophobic deep eutectic solvents: COSMO-RS prediction, experimental validation, and synergistic action with antibiotics	2024	Journal of Molecular Liquids	<a href="#">link</a>
18	A. Viñas-Ospino	Using novel hydrophobic deep eutectic solvents to improve a sustainable carotenoid extraction from orange peels	2023	Food Bioscience	<a href="#">link</a>

## BIOVIA COSMOtherm 関連論文リスト (3/21)

19	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	<a href="#">link</a>
20	Vitus Besel	Atomic structures, conformers and thermodynamic properties of 32k atmospheric molecules	2023	Scientific data	<a href="#">link</a>
21	Mengke Zhang	Estimation of vapor pressures of perfluoroalkyl substances (PFAS) using COSMOtherm	2023	Journal of Hazardous Materials	<a href="#">link</a>
22	Chunjie Liu	Designing Deep Eutectic Solvents with Crystalline Features: A New-Generation Green Crystallization-Induced Porogen	2023	ACS Sustainable Chemistry & Engineering	<a href="#">link</a>
23	Kaihang Zhang	Screening ionic liquids for efficiently extracting perfluoroalkyl chemicals (PFACs) from wastewater	2023	Journal of Environmental Sciences	<a href="#">link</a>
24	Noora Hyttinen	The effect of atmospherically relevant aminium salts on water uptake	2023	Atmospheric Chemistry and Physics	<a href="#">link</a>
25	Rubén Santiago	Anticipating APIs solubility in natural eutectic solvents: Lidocaine and caffeine case studies	2023	Food Bioscience	<a href="#">link</a>
26	Zijun Li	Saturation vapor pressure characterization of selected low-volatility organic compounds using a residence time chamber	2023	Environmental Science & Technology	<a href="#">link</a>
27	Juliane Glüge	Evaluation of Physicochemical Property Data in the ECHA Database	2023	Scientific data	<a href="#">link</a>

## BIOVIA COSMOtherm 関連論文リスト (4/21)

28	Zehao Mi	DFT and COSMO-RS theoretical analysis of SO <sub>2</sub> absorption by polyamines type ionic liquids	2023	Journal of Hazardous Materials	<a href="#">link</a>
29	Michael Diedenhofen	COSMO-RS blind prediction of distribution coefficients and aqueous pKa values from the SAMPL8 challenge	2023	ACS Sustainable Chemistry & Engineering	<a href="#">link</a>
30	Satoshi Endo	Intermolecular Interactions, Solute Descriptors, and Partition Properties of Neutral Per- and Polyfluoroalkyl Substances (PFAS)	2023	Journal of Environmental Sciences	<a href="#">link</a>
31	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	<a href="#">link</a>
32	Xia Li	Study on Vapor–Liquid Equilibrium and Microscopic Properties of Glycine + H <sub>2</sub> O, l-Histidine + H <sub>2</sub> O, and l-Tryptophan + H <sub>2</sub> O	2023	Journal of Molecular Liquids	<a href="#">link</a>
33	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	<a href="#">link</a>
34	Laura Fronchetti Guidugli	Understanding Microcystin-LR separation by hydrophobic deep eutectic solvents with COSMO simulation and experimental findings	2023	Journal of Physical and Chemical Reference Data	<a href="#">link</a>
35	Pablo Gutiérrez-Sánchez	Extraction of antibiotics identified in the EU Watch List 2020 from hospital wastewater using hydrophobic eutectic solvents and terpenoids	2022	CIESC Journal	<a href="#">link</a>

## BIOVIA COSMOtherm 関連論文リスト (5/21)

36	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	<a href="#">link</a>
37	Manuela Panić	Prediction of pH value of aqueous acidic and basic deep eutectic solvent using COSMO-RS $\sigma$ Profiles' molecular descriptors	2022	Environmental Science & Technology	<a href="#">link</a>
38	Rubén Santiago	Assessment of bio-ionic liquids as promising solvents in industrial separation processes: Computational screening using COSMO-RS method	2022	Chemosphere	<a href="#">link</a>
39	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	<a href="#">link</a>
40	Juan Wang	COSMO-RS prediction and experimental verification of deep eutectic solvents for water insoluble pesticides with high solubility	2022	Chemical Data Collections	<a href="#">link</a>
41	Clinton J. Chapman	Evaluation of solvate and co-crystal screening methods for CL-20 containing energetic materials	2022	Journal of Molecular Liquids	<a href="#">link</a>
42	Noora Hyttinen	Machine learning for predicting chemical potentials of multifunctional organic compounds in atmospherically relevant solutions	2022	Separation and Purification Technology	<a href="#">link</a>
43	Shuai Qian	Experimental and Computational Study of the Properties of Imidazole Compounds with Branched and Cycloalkyl Substituents	2022	Foods	<a href="#">link</a>

## BIOVIA COSMOtherm 関連論文リスト (6/21)

44	Mohsen Taheri	Ionic liquid screening for CO <sub>2</sub> capture and H <sub>2</sub> S removal from gases: The syngas purification case	2021	Molecules	<a href="#">link</a>
45	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	<a href="#">link</a>
46	Sivani Baskaran	Reliable prediction of the octanol–air partition ratio	2021	Environmental Science & Technology	<a href="#">link</a>
47	Huma Warsi Khan	Design and selection of ionic liquids via COSMO for pharmaceuticals and medicine	2021	Journal of Molecular Liquids	<a href="#">link</a>
48	Noora Hyttinen	Gas-to-Particle Partitioning of Cyclohexene- and $\alpha$ -Pinene-Derived Highly Oxygenated Dimers Evaluated Using COSMOtherm	2021	Journal of Energetic Materials	<a href="#">link</a>
49	Emma Lumiaro	Predicting gas–particle partitioning coefficients of atmospheric molecules with machine learning	2021	The Journal of Physical Chemistry Letters	<a href="#">link</a>
50	Timothy F. M. Rodgers	Novel Bayesian method to derive final adjusted values of physicochemical properties: application to 74 compounds	2021	Liquids	<a href="#">link</a>
51	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	<a href="#">link</a>
52	Judith Warnau	COSMO-RS predictions of logP in the SAMPL7 blind challenge	2021	Molecules	<a href="#">link</a>

## BIOVIA COSMOtherm 関連論文リスト (7/21)

53	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	<a href="#">link</a>
54	Boluwatife Awonaike	Precipitation-induced transport and phase partitioning of organophosphate esters (OPEs) in urban and rural watersheds	2021	Application of Ionic Liquids in Drug Delivery	<a href="#">link</a>
55	Jort Hammer	Congener-specific partition properties of chlorinated paraffins evaluated with COSMOtherm and gas chromatographic retention indices	2021	The Journal of Physical Chemistry A	<a href="#">link</a>
56	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	<a href="#">link</a>
57	Samuel Boobier	Machine learning with physicochemical relationships: solubility prediction in organic solvents and water	2020	Environmental Science & Technology	<a href="#">link</a>
58	Alina Lampic	Property estimation of per- and polyfluoroalkyl substances: A comparative assessment of estimation methods	2020	Environmental Science: Processes & Impacts	<a href="#">link</a>
59	Christoph Loschen	COSMO-RS based predictions for the SAMPL6 logP challenge	2020	Journal of Computer-Aided Molecular Design	<a href="#">link</a>
60	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	<a href="#">link</a>

## BIOVIA COSMOtherm 関連論文リスト (8/21)

61	Elenitsa Boli	Ionic liquids as entrainers for the separation of azeotropic mixtures: Experimental measurements and COSMO-RS predictions	2020	Environmental Science: Water Research & Technology	<a href="#">link</a>
62	Noora Hyttinen	Thermodynamic properties of isoprene- and monoterpene-derived organosulfates estimated with COSMOtherm	2020	Scientific Reports	<a href="#">link</a>
63	Noora Hyttinen	Improving Solubility and Activity Estimates of Multifunctional Atmospheric Organics by Selecting Conformers in COSMOtherm	2020	Engineering, Technology & Applied Science Research	<a href="#">link</a>
64	Noora Hyttinen	Estimating aqueous solubilities and activity coefficients of mono- and $\alpha, \omega$ -dicarboxylic acids using COSMOtherm	2020	Nature communications	<a href="#">link</a>
65	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	<a href="#">link</a>
66	Benjamin Sanchez-Lengeling	A Bayesian approach to predict solubility parameters	2019	Journal of Computer-Aided Molecular Design	<a href="#">link</a>
67	Varun Kundi	Predicting Octanol-Water Partition Coefficients: Are Quantum Mechanical Implicit Solvent Models Better than Empirical Fragment-Based Methods?	2019	ACS omega	<a href="#">link</a>



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68	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	<a href="#">link</a>
69	Georgia Michailoudi	Solubility and Activity Coefficients of Atmospheric Surfactants in Aqueous Solution Evaluated Using COSMOtherm	2019	Atmospheric Chemistry and Physics	<a href="#">link</a>
70	Mohamed Taha	Molecular design of mass-separating agents for separation of cyclic ethers and acetonitrile from water	2019	The Journal of Physical Chemistry A	<a href="#">link</a>
71	Vishwesh Venkatraman	Predicting ionic liquid melting points using machine learning	2018	Atmospheric Chemistry and Physics	<a href="#">link</a>
72	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	<a href="#">link</a>
73	R. Santiago	Acetylene absorption by ionic liquids: A multiscale analysis based on molecular and process simulation	2018	Advanced Theory and Simulations	<a href="#">link</a>
74	Theo Kurtén	Estimating the saturation vapor pressures of isoprene oxidation products and using COSMO-RS	2018	The Journal of Physical Chemistry B	<a href="#">link</a>
75	Yuriy A. Abramov	Rational solvent selection for pharmaceutical impurity purge	2018	Chemical Engineering Science	<a href="#">link</a>
76	Vishwesh Venkatraman	Predicting CO <sub>2</sub> capture of ionic liquids using machine learning	2017	The Journal of Physical Chemistry A	<a href="#">link</a>
77	Miranda Roesing	Solubility characteristics of poly (3-hexylthiophene)	2017	Journal of Molecular Liquids	<a href="#">link</a>

## BIOVIA COSMOtherm 関連論文リスト (10/21)

78	Meysam Lotfi	Solubility of acyclovir in nontoxic and biodegradable ionic liquids: COSMO-RS prediction and experimental verification	2017	Journal of Molecular Liquids	<a href="#">link</a>
79	Chen Wang	Uncertain Henry's law constants compromise equilibrium partitioning calculations of atmospheric oxidation products	2017	Journal of Computer-Aided Molecular Design	<a href="#">link</a>
80	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	<a href="#">link</a>
81	Martta Toivola	Can COSMOtherm predict a salting in effect?	2017	Atmospheric Chemistry and Physics	<a href="#">link</a>
82	Emad Ali	Modeling of CO <sub>2</sub> Solubility in Selected Imidazolium-Based Ionic Liquids	2017	Crystal Growth & Design	<a href="#">link</a>
83	Boluwatife Awonaiké	Quantifying the equilibrium partitioning of substituted polycyclic aromatic hydrocarbons in aerosols and clouds using COSMOtherm	2017	Journal of CO <sub>2</sub> Utilization	<a href="#">link</a>
84	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	<a href="#">link</a>
85	Andreas Klamt	Prediction of cyclohexane-water distribution coefficients with COSMO-RS on the SAMPL5 data set	2016	Journal of Molecular Liquids	<a href="#">link</a>

## BIOVIA COSMOtherm 関連論文リスト (11/21)

86	Sebastian Brox	Alternative Single-Solvent Electrolytes Based on Cyanoesters for Safer Lithium-Ion Batteries	2016	Atmospheric Chemistry and Physics	<a href="#">link</a>
87	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	<a href="#">link</a>
88	Xingang Li	Ionic liquid-assisted solvent extraction for unconventional oil recovery: computational simulation and experimental tests	2016	The Journal of Physical Chemistry A	<a href="#">link</a>
89	Meysam Lotfi	Analysis of multiple solvation interactions of methotrexate and ammonium based ionic liquids using COSMO-RS	2016	Chemical Engineering Communications	<a href="#">link</a>
90	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	<a href="#">link</a>
91	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	<a href="#">link</a>
92	Yongsheng Zhao	A quantitative prediction of the viscosity of ionic liquids using $S$ $\sigma$ -profile molecular descriptors	2015	Journal of Computer-Aided Molecular Design	<a href="#">link</a>
93	Christoph Schütter	Toward new solvents for EDLCs: from computational screening to electrochemical validation	2015	ChemSusChem	<a href="#">link</a>

## BIOVIA COSMOtherm 関連論文リスト (12/21)

94	Tamara Husch	Large-scale virtual high-throughput screening for the identification of new battery electrolyte solvents: computing infrastructure and collective properties	2015	Chemosphere	<a href="#">link</a>
95	J. Mark Parnis	Temperature dependence of Henry's law constants and KOA for simple and heteroatom-substituted PAHs by COSMO-RS	2015	Energy & Fuels	<a href="#">link</a>
96	Tamara Husch	Charting the known chemical space for non-aqueous lithium-air battery electrolyte solvents	2015	Procedia Engineering	<a href="#">link</a>
97	W. Jeffrey Horne	Effect of branched and cycloalkyl functionalities on CO <sub>2</sub> separation performance of poly (IL) membranes	2015	Fluid Phase Equilibria	<a href="#">link</a>
98	Chen Wang	Calculating Equilibrium Phase Distribution during the Formation of Secondary Organic Aerosol Using COSMOtherm	2015	Science of The Total Environment	<a href="#">link</a>
99	Anett Geisler	Predicting storage-lipid water partitioning of organic solutes from molecular structure	2015	Physical Chemistry Chemical Physics	<a href="#">link</a>
100	Markéta Paloncýová	Amphiphilic drug-like molecules accumulate in a membrane below the head group region	2014	The Journal of Physical Chemistry C	<a href="#">link</a>
101	Chen Wang	Measuring and modeling the salting-out effect in ammonium sulfate solutions	2014	Physical Chemistry Chemical Physics	<a href="#">link</a>
102	W. Jeffrey Horne	Correlating fractional free volume to CO <sub>2</sub> selectivity in [Rmim][Tf <sub>2</sub> N] ionic liquids	2014	Atmospheric Environment	<a href="#">link</a>

## BIOVIA COSMOtherm 関連論文リスト (13/21)

103	Angelika Stenzel	Prediction of partition coefficients for complex environmental contaminants: Validation of COSMOtherm, ABSOLV, and SPARC	2014	Physical Chemistry Chemical Physics	<a href="#">link</a>
104	Jens Reinisch	Prediction of free energies of hydration with COSMO-RS on the SAMPL4 data set	2014	Separation and Purification Technology	<a href="#">link</a>
105	Vasu Neela	Addition of malodorants to lighter gas—The phase equilibrium properties of mixtures of lighter gas and selected substances	2014	Environmental Science & Technology	<a href="#">link</a>
106	Juliane Glüge	Calculation of physicochemical properties for short-and medium-chain chlorinated paraffins	2013	Environmental Science & Technology	<a href="#">link</a>
107	Matthew S. Shannon	Properties and Performance of Ether-Functionalized Imidazoles as Physical Solvents for CO <sub>2</sub> Separations	2013	The Journal of Physical Chemistry B	<a href="#">link</a>
108	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	<a href="#">link</a>
109	Jason E. Bara	COSMOtherm as a Tool for Estimating the Thermophysical Properties of Alkylimidazoles as Solvents for CO <sub>2</sub> Separations	2013	The Journal of Chemical Thermodynamics	<a href="#">link</a>
110	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	<a href="#">link</a>

## BIOVIA COSMOtherm 関連論文リスト (14/21)

111	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	<a href="#">link</a>
112	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	<a href="#">link</a>
113	Matthew S. Shannon	Free volume as the basis of gas solubility and selectivity in imidazolium-based ionic liquids	2012	Journal of Physical and Chemical Reference Data	<a href="#">link</a>
114	Yuriy A. Abramov	Rational cofomer or solvent selection for pharmaceutical cocrystallization or desolvation	2012	Energy & Fuels	<a href="#">link</a>
115	Laurianne Moity	Panorama of sustainable solvents using the COSMO-RS approach	2012	RSC Advances	<a href="#">link</a>
116	Shannon M. Mahurin	High CO <sub>2</sub> solubility, permeability and selectivity in ionic liquids with the tetracyanoborate anion	2012	Industrial & Engineering Chemistry Research	<a href="#">link</a>
117	Juan Pablo Gutiérrez	COSMO-RS-based ionic-liquid selection for extractive distillation processes	2012	Journal of Environmental Chemistry and Ecotoxicology	<a href="#">link</a>
118	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	<a href="#">link</a>
119	Jens Reinisch	Prediction of free energies of hydration with COSMO-RS on the SAMPL3 data set	2012	Journal of Environmental Chemistry and Ecotoxicology	<a href="#">link</a>
120	Andreas Klamt	The COSMO and COSMO-RS solvation models	2011	Industrial & Engineering Chemistry Research	<a href="#">link</a>

## BIOVIA COSMOtherm 関連論文リスト (15/21)

121	Zhanyun Wang	Using COSMOtherm to predict physicochemical properties of poly-and perfluorinated alkyl substances (PFASs)	2011	Journal of pharmaceutical sciences	<a href="#">link</a>
122	Kazi Z. Sumon	Ionic liquids for CO2 capture using COSMO-RS: Effect of structure, properties and molecular interactions on solubility and selectivity	2011	Green chemistry	<a href="#">link</a>
123	Victoria P. Sacks	Development and use of polyethylene passive samplers to detect triclosans and alkylphenols in an urban estuary	2011	RSC advances	<a href="#">link</a>
124	Matthew B. Miller	Critical Assessment of CO2 Solubility in Volatile Solvents at 298.15 K	2011	Industrial & Engineering Chemistry Research	<a href="#">link</a>
125	Kai-Uwe Goss	Predicting equilibrium sorption of neutral organic chemicals into various polymeric sorbents with COSMO-RS	2011	Environmental Science & Technology	<a href="#">link</a>
126	Jens Reinisch	Prediction of the temperature dependence of a polyether-water mixture using COSMOtherm	2011	Journal of Computer-Aided Molecular Design	<a href="#">link</a>
127	Gábor Járvas	COSMO-RS based CFD model for flat surface evaporation of non-ideal liquid mixtures	2011	WIREs Computational Molecular Science	<a href="#">link</a>
128	Bernd Schröder	Prediction of aqueous solubilities of solid carboxylic acids with COSMO-RS	2010	Environmental Chemistry	<a href="#">link</a>
129	Sarah E. Hale	Partitioning of organochlorine pesticides from water to polyethylene passive samplers	2010	Fluid Phase Equilibria	<a href="#">link</a>
130	Xianming Zhang	Assessment of chemical screening outcomes based on different partitioning property estimation methods	2010	Environmental science & technology	<a href="#">link</a>

## BIOVIA COSMOtherm 関連論文リスト (16/21)

131	Andreas Klamt	Blind prediction test of free energies of hydration with COSMO-RS	2010	Journal of Chemical & Engineering Data	<a href="#">link</a>
132	Guido Bronner	Hexadecane/air partitioning coefficients of multifunctional compounds: Experimental data and modeling	2010	Analytical chemistry	<a href="#">link</a>
133	Bernd Schröder	Prediction of environmental parameters of polycyclic aromatic hydrocarbons with COSMO-RS	2010	Fluid phase equilibria	<a href="#">link</a>
134	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	<a href="#">link</a>
135	Andreas Klamt	Some conclusions regarding the predictions of tautomeric equilibria in solution based on the SAMPL2 challenge	2010	Fluid Phase Equilibria	<a href="#">link</a>
136	Sandra Roy	Predictions of thermodynamic properties of energetic materials using COSMO-RS	2010	Environmental pollution	<a href="#">link</a>
137	Frank Eckert	Prediction of acidity in acetonitrile solution with COSMO-RS	2009	Environment International	<a href="#">link</a>
138	Andreas Klamt	On the performance of continuum solvation methods. A comment on “Universal approaches to solvation modeling”	2009	Journal of Computer-Aided Molecular Design	<a href="#">link</a>
139	Andreas Klamt	Prediction of the free energy of hydration of a challenging set of pesticide-like compounds	2009	Fluid phase equilibria	<a href="#">link</a>
140	M. Buggert	COSMO-RS calculations of partition coefficients: different tools for conformation search	2009	Chemosphere	<a href="#">link</a>



## BIOVIA COSMOtherm 関連論文リスト (17/21)

141	Matthew B. Miller	Solubility of CO <sub>2</sub> in CO <sub>2</sub> -philic oligomers; COSMOtherm predictions and experimental results	2009	Journal of Chromatography A	<a href="#">link</a>
142	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	<a href="#">link</a>
143	Andreas Klamt	Prediction of partition coefficients and activity coefficients of two branched compounds using COSMOtherm	2009	Procedia Computer Science	<a href="#">link</a>
144	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	<a href="#">link</a>
145	Kai-Uwe Goss	Predicting Adsorption of Organic Chemicals at the Air-Water Interface	2009	Accounts of Chemical Research	<a href="#">link</a>
146	Carsten Wittekindt	Screening the partition behavior of a large number of chemicals with a quantum-chemical software	2009	The Journal of Physical Chemistry B	<a href="#">link</a>
147	Kai-Uwe Goss	Partition behavior of hexachlorocyclohexane isomers	2008	WIREs Computational Molecular Science	<a href="#">link</a>
148	Christian Niederer	Effect of ortho-chlorine substitution on the partition behavior of chlorophenols	2008	Fluid Phase Equilibria	<a href="#">link</a>
149	Satoshi Endo	Evaluating coal tar-water partitioning coefficient estimation methods and solute-solvent molecular interactions in tar phase	2008	Journal of Environmental Science and Health, Part A	<a href="#">link</a>

## BIOVIA COSMOtherm 関連論文リスト (18/21)

150	Zheng Guo	Predictions of flavonoid solubility in ionic liquids by COSMO-RS: experimental verification, structural elucidation, and solvation characterization	2007	Fluid phase equilibria	<a href="#">link</a>
151	Zhigang Lei	COSMO-RS modeling on the extraction of stimulant drugs from urine sample by the double actions of supercritical carbon dioxide and ionic liquid	2007	Environmental science & technology	<a href="#">link</a>
152	Christian Niederer	Quantum chemical modeling of humic acid/air equilibrium partitioning of organic vapors	2007	The Journal of Physical Chemistry A	<a href="#">link</a>
153	Andreas Klamt	Prediction, fine tuning, and temperature extrapolation of a vapor liquid equilibrium using COSMOtherm	2007	Chemosphere	<a href="#">link</a>
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