Karoly Heberger

List of Publications by Year
in descending order

169 papers	7,508 citations	76326 40 h-index	62596 80 g-index
181 all docs	181 docs citations	181 times ranked	7931 citing authors

#	Article	IF	Citations
1	Factor analysis, sparse PCA, and Sum of Ranking Differences-based improvements of the Promethee-GAIA multicriteria decision support technique. PLoS ONE, 2022, 17, e0264277.	2.5	4
2	Extended continuous similarity indices: theory and application for QSAR descriptor selection. Journal of Computer-Aided Molecular Design, 2022, 36, 157-173.	2.9	7
3	Multiobject Optimization of National Football League Drafts: Comparison of Teams and Experts. Applied Sciences (Switzerland), 2022, 12, 6303.	2.5	0
4	Molecular Dynamics Simulations and Diversity Selection by Extended Continuous Similarity Indices. Journal of Chemical Information and Modeling, 2022, 62, 3415-3425.	5.4	9
5	Multicriteria decision making for evergreen problems in food science by sum of ranking differences. Food Chemistry, 2021, 344, 128617.	8.2	16
6	Effect of Dataset Size and Train/Test Split Ratios in QSAR/QSPR Multiclass Classification. Molecules, 2021, 26, 1111.	3.8	106
7	Differential Consistency Analysis: Which Similarity Measures can be Applied in Drug Discovery?. Molecular Informatics, 2021, 40, e2060017.	2.5	12
8	Extended similarity indices: the benefits of comparing more than two objects simultaneously. Part 2: speed, consistency, diversity selection. Journal of Cheminformatics, 2021, 13, 33.	6.1	24
9	Extended similarity indices: the benefits of comparing more than two objects simultaneously. Part 1: Theory and characteristicsâ€. Journal of Cheminformatics, 2021, 13, 32.	6.1	25
10	How to predict choice using eye-movements data?. Food Research International, 2021, 143, 110309.	6.2	5
11	Machine learning models for classification tasks related to drug safety. Molecular Diversity, 2021, 25, 1409-1424.	3.9	24
12	Extended many-item similarity indices for sets of nucleotide and protein sequences. Computational and Structural Biotechnology Journal, 2021, 19, 3628-3639.	4.1	10
13	Comprehensive Classification and Regression Modeling of Wine Samples Using 1H NMR Spectra. Foods, 2021, 10, 64.	4.3	5
14	Comprehensible Visualization of Multidimensional Data: Sum of Ranking Differences-Based Parallel Coordinates. Mathematics, 2021, 9, 3203.	2.2	2
15	Elemental composition of Russula cyanoxantha along an urbanization gradient in Cluj-Napoca (Romania). Chemosphere, 2020, 238, 124566.	8.2	19
16	Apportionment and districting by Sum of Ranking Differences. PLoS ONE, 2020, 15, e0229209.	2.5	9
17	Reagent-free total protein quantification of intact extracellular vesicles by attenuated total reflection Fourier transform infrared (ATR-FTIR) spectroscopy. Analytical and Bioanalytical Chemistry, 2020, 412, 4619-4628.	3.7	24
18	Estimating Nanoscale Surface Roughness of Polyethylene Terephthalate Fibers. ACS Omega, 2020, 5, 3670-3677.	3.5	9

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19	Comparison of Data Fusion Methods as Consensus Scores for Ensemble Docking. Molecules, 2019, 24, 2690.	3.8	14
20	Data on elemental composition of Russula cyanoxantha along an urbanization gradient in Cluj-Napoca (Romania). Data in Brief, 2019, 27, 104572.	1.0	0
21	Which insect species can best be proposed for human consumption?. Innovative Food Science and Emerging Technologies, 2019, 52, 358-367.	5.6	29
22	Comparison of validation variants by sum of ranking differences and <scp>ANOVA</scp>. Journal of Chemometrics, 2019, 33, e3104.	1.3	19
23	Intercorrelation Limits in Molecular Descriptor Preselection for QSAR/QSPR. Molecular Informatics, 2019, 38, e1800154.	2.5	34
24	Column Characterization and Selection Systems in Reversed-Phase High-Performance Liquid Chromatography. Chemical Reviews, 2019, 119, 3674-3729.	47.7	191
25	Multi-Level Comparison of Machine Learning Classifiers and Their Performance Metrics. Molecules, 2019, 24, 2811.	3.8	61
26	Is soft independent modeling of class analogies a reasonable choice for supervised pattern recognition?. RSC Advances, 2018, 8, 10-21.	3.6	30
27	Ranking and similarity of conventional, microwave and ultrasound element sequential extraction methods. Chemosphere, 2018, 198, 103-110.	8.2	6
28	Binary similarity measures for fingerprint analysis of qualitative metabolomic profiles. Metabolomics, 2018, 14, 29.	3.0	17
29	Life beyond the Tanimoto coefficient: similarity measures for interaction fingerprints. Journal of Cheminformatics, 2018, 10, 48.	6.1	77
30	Modelling methods and cross-validation variants in QSAR: a multi-level analysis[$]. SAR and QSAR in Environmental Research, 2018, 29, 661-674.	2.2	32
31	Elemental composition of wild growing Agaricus campestris mushroom in urban and peri-urban regions of Transylvania (Romania). Journal of Food Composition and Analysis, 2018, 72, 15-21.	3.9	12
32	Development and comparison of regression models for the determination of quality parameters in margarine spread samples using NIR spectroscopy. Analytical Methods, 2018, 10, 3089-3099.	2.7	7
33	Which just-about-right feature should be changed if evaluations deviate? A case study using sum of ranking differences. Chemometrics and Intelligent Laboratory Systems, 2017, 161, 130-135.	3.5	10
34	How to compare separation selectivity of high-performance liquid chromatographic columns properly?. Journal of Chromatography A, 2017, 1488, 45-56.	3.7	16
35	Chemical Data Formats, Fingerprints, and Other Molecular Descriptions for Database Analysis and Searching. , 2017, , 329-378.		27
36	Which Performance Parameters Are Best Suited to Assess the Predictive Ability of Models?. Challenges and Advances in Computational Chemistry and Physics, 2017, , 89-104.	0.6	4

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37	Multivariate assessment of lipophilicity scalesâ€"computational and reversed phase thin-layer chromatographic indices. Journal of Pharmaceutical and Biomedical Analysis, 2016, 127, 81-93.	2.8	54
38	Anomalous temperature dependence of gas chromatographic retention indices of polar compounds on non-polar stationary phases. Journal of Chromatography A, 2016, 1445, 126-134.	3.7	9
39	Quantitative determination and classification of energy drinks using near-infrared spectroscopy. Analytical and Bioanalytical Chemistry, 2016, 408, 6403-6411.	3.7	20
40	Comparison of classification methods with â€œn-classâ€•receiver operating characteristic curves: A case study of energy drinks. Chemometrics and Intelligent Laboratory Systems, 2016, 151, 34-43.	3.5	11
41	‹sup›1‹/sup›Hâ€NMR and isotopic fingerprinting of olive oil and its unsaponifiable fraction: Geographical origin of virgin olive oils by pattern recognition. European Journal of Lipid Science and Technology, 2015, 117, 1991-2006.	1.5	22
42	Generalized Pairwise Correlation and method comparison: Impact assessment for JAR attributes on overall liking. Food Quality and Preference, 2015, 43, 88-96.	4.6	23
43	Why is Tanimoto index an appropriate choice for fingerprint-based similarity calculations?. Journal of Cheminformatics, 2015, 7, 20.	6.1	775
44	Chromatographic and computational assessment of lipophilicity using sum of ranking differences and generalized pair-correlation. Journal of Chromatography A, 2015, 1380, 130-138.	3.7	45
45	Sum of ranking differences (SRD) to ensemble multivariate calibration model merits for tuning parameter selection and comparing calibration methods. Analytica Chimica Acta, 2015, 869, 21-33.	5.4	39
46	Quantitative determination of coenzyme Q10 from dietary supplements by FT-NIR spectroscopy and statistical analysis. Analytical and Bioanalytical Chemistry, 2015, 407, 2887-2898.	3.7	25
47	Towards better understanding of lipophilicity: Assessment of in silico and chromatographic logP measures for pharmaceutically important compounds by nonparametric rankings. Journal of Pharmaceutical and Biomedical Analysis, 2015, 115, 183-191.	2.8	47
48	Comparison of antioxidant capacity assays with chemometric methods. Analytical Methods, 2015, 7, 4216-4224.	2.7	23
49	Consistency of QSAR models: Correct split of training and test sets, ranking of models and performance parameters. SAR and QSAR in Environmental Research, 2015, 26, 683-700.	2.2	85
50	Sum of ranking differences to rank stationary phases used in packed column supercritical fluid chromatography. Journal of Chromatography A, 2015, 1409, 241-250.	3.7	26
51	Best conditions for biodegradation of diesel oil by chemometric tools. Brazilian Journal of Microbiology, 2014, 45, 117-126.	2.0	8
52	Classification and unscrambling a classâ€insideâ€class situation by object target rotation: Hungarian silver coins of the ÃrpÃ¡d Dynasty, ‹scp›ad‹/scp› 997â€"1301. Journal of Chemometrics, 2014, 28, 287-292.	1.3	6
53	Evaluation of single-cell gel electrophoresis data: Combination of variance analysis with sum of ranking differences. Mutation Research - Genetic Toxicology and Environmental Mutagenesis, 2014, 771, 15-22.	1.7	21
54	Sorption, solubility, and mass changes of hydroxyapatiteâ€containing composites in artificial saliva, food simulating solutions, tea, and coffee. Journal of Applied Polymer Science, 2014, 131, .	2.6	6

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55	Similarity and grouping of perlite and zeolite abrasive fillers: A replacement test. Journal of Applied Polymer Science, 2013, 127, 3839-3847.	2.6	8
56	Classification of Hungarian medieval silver coins using x-ray fluorescent spectroscopy and multivariate data analysis. Heritage Science, 2013, 1, .	2.3	10
57	Method and model comparison by sum of ranking differences in cases of repeated observations (ties). Chemometrics and Intelligent Laboratory Systems, 2013, 127, 139-146.	3.5	127
58	Estimation of influential points in any data set from coefficient of determination and its leave-one-out cross-validated counterpart. Journal of Computer-Aided Molecular Design, 2013, 27, 837-844.	2.9	22
59	Characterization of Hybrid Materials by Means of Inverse Gas Chromatography and Chemometrics. Journal of Pharmaceutical Sciences, 2013, 102, 1524-1531.	3.3	10
60	Comparison of comet assay parameters for estimation of genotoxicity by sum of ranking differences. Analytical and Bioanalytical Chemistry, 2013, 405, 4879-4885.	3.7	34
61	Comparison of multianalyte proficiency test results by sum of ranking differences, principal component analysis, and hierarchical cluster analysis. Analytical and Bioanalytical Chemistry, 2013, 405, 8363-8375.	3.7	12
62	Synergism Between Constituents of Multicomponent Catalysts Designed for Ethanol Steam Reforming Using Partial Least Squares Regression and Artificial Neural Networks. Combinatorial Chemistry and High Throughput Screening, 2012, 15, 105-113.	1.1	5
63	Ranking and similarity for quantitative structureâ€“retention relationship models in predicting Lee retention indices of polycyclic aromatic hydrocarbons. Analytica Chimica Acta, 2012, 716, 92-100.	5.4	37
64	Discrimination of mineral waters by electronic tongue, sensory evaluation and chemical analysis. Food Chemistry, 2012, 135, 2947-2953.	8.2	63
65	Quantitative Structureâ€“Retention Relationships. , 2012, , 451-475.		1
66	Effectiveness of in-needle extraction device for liquid samples. Analytica Chimica Acta, 2012, 751, 182-188.	5.4	10
67	Sum of ranking differences for method discrimination and its validation: comparison of ranks with random numbers. Journal of Chemometrics, 2011, 25, 151-158.	1.3	184
68	Conferentia Chemometrica 2009, SiÃ³fok, Hotel Magistern, 27-30 September 2009. Journal of Chemometrics, 2010, 24, 95-95.	1.3	0
69	Sum of ranking differences compares methods or models fairly. TrAC - Trends in Analytical Chemistry, 2010, 29, 101-109.	11.4	237
70	Comparison of physicochemical and gas chromatographic polarity measures for simple organic compounds. Journal of Chromatography A, 2010, 1217, 2895-2902.	3.7	24
71	Role of Hansen solubility parameters in solid phase extraction. Journal of Chromatography A, 2010, 1217, 5564-5570.	3.7	23
72	Multivariate analysis of NMR fingerprint of the unsaponifiable fraction of virgin olive oils for authentication purposes. Food Chemistry, 2010, 118, 956-965.	8.2	120

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73	Virgin Olive Oil Authentication by Multivariate Analyses of ¹H NMR Fingerprints and Î´¹³C and Î´²H Data. Journal of Agricultural and Food Chemistry, 2010, 58, 5586-5596.	5.2	94
74	Ranking of QSAR Models to Predict Minimal Inhibitory Concentrations Toward Mycobacterium tuberculosis for a Set of Fluoroquinolones. Acta Chimica Slovenica, 2010, 57, 586-90.	0.6	15
75	4th International Symposium on Computer Applications and Chemometrics in Analytical Chemistry Glashotel, BalatonalmÃ¡di, Hungary, September 1-4, 2008. Journal of Chemometrics, 2009, 23, 153-153.	1.3	0
76	Botanical and Geographical Characterization of Green Coffee (Coffea arabica and Coffea canephora): Chemometric Evaluation of Phenolic and Methylxanthine Contents. Journal of Agricultural and Food Chemistry, 2009, 57, 4224-4235.	5.2	168
77	Mass spectrometric and linear discriminant analysis of N-glycans of human serum alpha-1-acid glycoprotein in cancer patients and healthy individuals. Journal of Proteomics, 2008, 71, 186-197.	2.4	64
78	Cluster and principal component analysis for KovÃ¡tsâ€™ retention indices on apolar and polar stationary phases in gas chromatography. Journal of Chromatography A, 2008, 1177, 175-182.	3.7	16
79	Prediction of retention indices for identification of fatty acid methyl esters. Journal of Chromatography A, 2008, 1198-1199, 188-195.	3.7	27
80	Chemoinformaticsâ€”multivariate mathematicalâ€“statistical methods for data evaluation. , 2008, , 141-169.		22
81	Metabolomics Applied to Exhaled Breath Condensate in Childhood Asthma. American Journal of Respiratory and Critical Care Medicine, 2007, 175, 986-990.	5.6	224
82	Wavelength Selection for Multivariate Calibration Using Tikhonov Regularization. Applied Spectroscopy, 2007, 61, 85-95.	2.2	40
83	The inherent accuracy of 1H NMR spectroscopy to quantify plasma lipoproteins is subclass dependent. Atherosclerosis, 2007, 190, 352-358.	0.8	51
84	Classification of Gilthead Sea Bream (Sparus aurata) from ¹H NMR Lipid Profiling Combined with Principal Component and Linear Discriminant Analysis. Journal of Agricultural and Food Chemistry, 2007, 55, 9963-9968.	5.2	54
85	Conferentia Chemometrica 2005. Chemometrics and Intelligent Laboratory Systems, 2007, 87, 1-2.	3.5	0
86	Quantitative structureâ€“(chromatographic) retention relationships. Journal of Chromatography A, 2007, 1158, 273-305.	3.7	350
87	Supervised pattern recognition in food analysis. Journal of Chromatography A, 2007, 1158, 196-214.	3.7	815
88	Predictive performance of â€œhighly complexâ€•artificial neural networks. Applied Catalysis A: General, 2007, 324, 90-93.	4.3	19
89	Selection of solubility parameters for characterization of pharmaceutical excipients. Journal of Chromatography A, 2007, 1171, 90-97.	3.7	43
90	Prediction of Tumoricidal Activity and Accumulation of Photosensitizers in Photodynamic Therapy Using Multiple Linear Regression and Artificial Neural NetworksÂ¶. Photochemistry and Photobiology, 2007, 75, 471-478.	2.5	0

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91	Aqueous salting-out effect of inorganic cations and anions on non-electrolytes. Chemosphere, 2006, 65, 802-810.	8.2	127
92	Inverse gas chromatographic and chemometric tools for determination of interactions between the components of polymeric composition. Analytica Chimica Acta, 2006, 559, 221-226.	5.4	10
93	Evaluation of chemometric techniques to select orthogonal chromatographic systems. Journal of Pharmaceutical and Biomedical Analysis, 2006, 41, 141-151.	2.8	31
94	Newly synthesized tetraoxa-diaza crown ether derivatives versus commercialized crown ethers in the separation of positional isomers with capillary electrophoresis. Journal of Pharmaceutical and Biomedical Analysis, 2006, 41, 1164-1170.	2.8	6
95	Classification and replacement test of HPLC systems using principal component analysis. Analytica Chimica Acta, 2005, 536, 71-81.	5.4	38
96	Selection of orthogonal chromatographic systems based on parametric and non-parametric statistical tests. Analytica Chimica Acta, 2005, 539, 1-10.	5.4	31
97	Temperature dependence of solvation heat capacities by gas chromatography. Analytica Chimica Acta, 2005, 549, 134-139.	5.4	8
98	Classification of olive oils using high throughput flow 1H NMR fingerprinting with principal component analysis, linear discriminant analysis and probabilistic neural networks. Analytica Chimica Acta, 2005, 552, 13-24.	5.4	149
99	Principal component analysis of polymerâ€“solvent and fillerâ€“solvent interactions by inverse gas chromatography. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2005, 260, 29-37.	4.7	23
100	Solvation enthalpies and heat capacities ofn-alkanes in four polymer phases by capillary gas chromatography. Journal of Separation Science, 2005, 28, 506-512.	2.5	8
101	Comparison of Ridge Regression, Partial Least-Squares, Pairwise Correlation, Forward- and Best Subset Selection Methods for Prediction of Retention Indices for Aliphatic Alcohols.. ChemInform, 2005, 36, no.	0.0	1
102	Determination of the geographical origin of green coffee by principal component analysis of carbon, nitrogen and boron stable isotope ratios. Rapid Communications in Mass Spectrometry, 2005, 19, 2111-2115.	1.5	65
103	Comparison of Ridge Regression, Partial Least-Squares, Pairwise Correlation, Forward- and Best Subset Selection Methods for Prediction of Retention Indices for Aliphatic Alcohols. Journal of Chemical Information and Modeling, 2005, 45, 339-346.	5.4	39
104	Effect of Film Thickness on the Retention Index of Nitro and Cyano Compounds. Interpretation of the Logarithmic Equation. Journal of Chromatographic Science, 2004, 42, 288-292.	1.4	4
105	Prediction of anti-HIV-1 Activity of a Series of Tetrapyrrole Molecules.. ChemInform, 2004, 35, no.	0.0	0
106	Chemometrics in Hungary (the last 10 years). Chemometrics and Intelligent Laboratory Systems, 2004, 72, 115-122.	3.5	3
107	Quantitative structureâ€“retention relationships XIV. Chemometrics and Intelligent Laboratory Systems, 2004, 72, 173-184.	3.5	39
108	Prediction of ozone concentration in ambient air using multivariate methods. Chemosphere, 2004, 57, 889-896.	8.2	57

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109	Quantitative Structure â€“ Antioxidant Activity Relationships of Flavonoid Compounds. Molecules, 2004, 9, 1079-1088.	3.8	104
110	Minimum in the temperature dependence of the KovÃ¡ts retention indices of nitroalkanes and alkanenitriles on an apolar phase. Journal of Chromatography A, 2003, 985, 11-19.	3.7	26
111	Principal Component and Linear Discriminant Analyses of Free Amino Acids and Biogenic Amines in Hungarian Wines. Journal of Agricultural and Food Chemistry, 2003, 51, 8055-8060.	5.2	104
112	Prediction of Anti-HIV-1 Activity of a Series of Tetrapyrrole Molecules. Journal of Chemical Information and Computer Sciences, 2003, 43, 1829-1836.	2.8	29
113	Variable selection using pair-correlation method. Environmental applications. SAR and QSAR in Environmental Research, 2002, 13, 541-554.	2.2	21
114	Principal Component Analysis of Biogenic Amines and Polyphenols in Hungarian Wines. Journal of Agricultural and Food Chemistry, 2002, 50, 3768-3774.	5.2	69
115	MECHGEN:â€‰ Computer Aided Generation and Reduction of Reaction Mechanisms. Journal of Chemical Information and Computer Sciences, 2002, 42, 208-214.	2.8	19
116	Generalization of pair correlation method (PCM) for non-parametric variable selection. Journal of Chemometrics, 2002, 16, 436-443.	1.3	41
117	Differentiation of vegetable oils by mass spectrometry combined with statistical analysis. Rapid Communications in Mass Spectrometry, 2002, 16, 2291-2297.	1.5	73
118	Temperature dependence of KovÃ¡ts indices in gas chromatography revisited. Journal of Chromatography A, 2002, 973, 135-142.	3.7	36
119	Comparative analysis of different plant oils by high-performance liquid chromatographyâ€“atmospheric pressure chemical ionization mass spectrometry. Journal of Chromatography A, 2002, 976, 255-263.	3.7	121
120	Prediction of Tumoricidal Activity and Accumulation of Photosensitizers in Photodynamic Therapy Using Multiple Linear Regression and Artificial Neural NetworksÂ¶. Photochemistry and Photobiology, 2002, 75, 471.	2.5	12
121	Conditional Fisher's exact test as a selection criterion for pair-correlation method. Type I and Type II errors. Chemometrics and Intelligent Laboratory Systems, 2001, 57, 1-14.	3.5	32
122	Correlation between retention indices and quantum-chemical descriptors of ketones and aldehydes on stationary phases of different polarity. Analytica Chimica Acta, 2001, 428, 73-82.	5.4	52
123	Benzene, toluene, ethyl benzene and xylenes in ambient air and Pinus sylvestris L. needles: a comparative study between Belgium, Hungary and Latvia. Atmospheric Environment, 2001, 35, 6327-6335.	4.1	37
124	Estimation of Molar Heat Capacities in Solution from Gas Chromatographic Data. Journal of Chromatographic Science, 2001, 39, 113-120.	1.4	16
125	Principal Component Analysis of Polarity and Interaction Parameters in Inverse Gas Chromatography. Journal of Chromatographic Science, 2001, 39, 375-384.	1.4	18
126	Separation of polar and enthalpy effects in radical addition reactions using polar (?) and radical (?ï¿½) sigma scales. Journal of Physical Organic Chemistry, 2000, 13, 151-156.	1.9	7

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127	Partial least squares modeling of retention data of oxo compounds in gas chromatography. Chromatographia, 2000, 51, 595-600.	1.3	24
128	Enthalpies of Solution and Excess Enthalpies of Oxo Compounds by Capillary Gas Chromatography. Journal of Chromatographic Science, 1999, 37, 11-16.	1.4	23
129	Evaluation of polarity indicators and stationary phases by principal component analysis in gasâ€“liquid chromatography. Chemometrics and Intelligent Laboratory Systems, 1999, 47, 41-49.	3.5	53
130	Quantitative structureâ€“retention relationships. Chemometrics and Intelligent Laboratory Systems, 1999, 47, 205-217.	3.5	22
131	Thermodynamic significance of boiling point correlations for alkylbenzenes in gas chromatography. Journal of Chromatography A, 1999, 845, 13-20.	3.7	20
132	Principal component analysis of KovÃ¡ts indices for carbonyl compounds in capillary gas chromatography. Journal of Chromatography A, 1999, 845, 21-31.	3.7	63
133	Influence of extraction parameters and medium on efficiency of solid-phase microextraction sampling in analysis of aliphatic aldehydes. Journal of Chromatography A, 1999, 845, 337-347.	3.7	26
134	Principal component analysis of measured quantities during degradation of hydroperoxides in oxidized vegetable oils. Lipids, 1999, 34, 83-92.	1.7	26
135	Comparison of chemometric methods for prediction of rate constants and activation energies of radical addition reactions. Journal of Chemometrics, 1999, 13, 473-489.	1.3	26
136	Computer modeling of formation of soot precursors in the oxidation of methane. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1998, 102, 257-261.	0.9	1
137	Assessment of Nucleophilicity and Electrophilicity of Radicals, and of Polar and Enthalpy Effects on Radical Addition Reactions1. Journal of Organic Chemistry, 1998, 63, 8646-8653.	3.2	83
138	Identification of Volatile Compounds in Sunflower Oil by Headspace SPME and Ion-Trap GC/MS. Journal of High Resolution Chromatography, 1998, 21, 368-370.	1.4	32
139	Determination of heats of vaporization and gibbs free energies of alkylbenzenes on GC stationary phases of different polarity. Chromatographia, 1998, 48, 89-94.	1.3	20
140	Quantitative Analysis of aliphatic aldehydes by headspace SPME sampling and ion-trap GC-MS. Chromatographia, 1998, 48, 127-132.	1.3	18
141	Thermodynamic properties of alkylbenzenes from retention-boiling point correlations in gas chromatography. Chromatographia, 1997, 44, 179-186.	1.3	23
142	Separation of polar and enthalpic effects on radical addition reactions using principal component analysis. Journal of the Chemical Society Perkin Transactions II, 1995, , 91-96.	0.9	15
143	Linear free energy relationships in radical reactions. II. hydrogen abstraction from substituted toluenes byTert-Butyl,Tert-Butoxyl andTert-Butylperoxyl radicals. Journal of Physical Organic Chemistry, 1994, 7, 244-250.	1.9	15
144	Principal component analysis of data on the catalytic oxidation of toluene. Applied Catalysis A: General, 1994, 119, L7-L12.	4.3	11

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145	Oxidative decarboxylation of cyclohexane monocarboxylic acid III. Initiated oxidation. Reaction Kinetics and Catalysis Letters, 1994, 53, 385-390.	0.6	0
146	Oxidative decarboxylation of cyclohexane monocarboxylic acid as a degenerate branching chain reaction. I. kinetics. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1994, 98, 75-81.	0.9	7
147	Oxidative decarboxylation of cyclohexane monocarboxylic acid as a degenerate branching chain reaction II. Mechanism. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1994, 98, 1303-1307.	0.9	4
148	Rate constants for the addition of the 2-cyano-2-propyl radical to alkenes in solution. International Journal of Chemical Kinetics, 1993, 25, 249-263.	1.6	87
149	Rate constants for the addition of the 2-hydroxy-2-propyl radical to alkenes in solution. International Journal of Chemical Kinetics, 1993, 25, 913-920.	1.6	49
150	Reactivity of HO₂^{Â·} Radicals in Alcohols. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1992, 96, 175-179.	0.9	6
151	Addition of Benzyl Radicals to Alkenes: The Role of Radical Deformation in the Transition State. Angewandte Chemie International Edition in English, 1992, 31, 635-636.	4.4	47
152	Die Addition von Benzylradikalen an Alkene: Zur Rolle von Radikaldeformationen im Ãœbergangszustand. Angewandte Chemie, 1992, 104, 651-653.	2.0	22
153	Discrimination between linear and non-linear models describing retention data of alkylbenzenes in gas-chromatography. Chromatographia, 1990, 29, 375-384.	1.3	39
154	Identification of C5H8isomers through reactions of singlet methylene, CH2(Ã£1A1), with unsaturated hydrocarbons using capillary gas chromatography-mass spectrometry. Analyst, The, 1990, 115, 725-729.	3.5	3
155	Limitations of evaluation methods for inhibited oxidation of hydrocarbons in the liquid phase. Expressions based on oxygen consumption. Reaction Kinetics and Catalysis Letters, 1989, 39, 115-122.	0.6	1
156	Limitations of evaluation methods for inhibited oxidation based on chemiluminescence. Reaction Kinetics and Catalysis Letters, 1989, 38, 51-56.	0.6	2
157	Linear free energy relationships for peroxy radical-phenol reactions. Influence of thepara-substituent, theortho-di-tert-butyl groups and the peroxy radical. International Journal of Chemical Kinetics, 1989, 21, 1181-1193.	1.6	6
158	Empirical correlations between gas-chromatographic retention data and physical or topological properties of solute molecules. Analytica Chimica Acta, 1989, 223, 161-174.	5.4	35
159	The reaction of CH₂(XÌ„³B₁) with C₆H₆. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1989, 93, 80-87.	0.9	10
160	Empirical correlation equations describing retention data of hydrocarbons on dinonylphatalate and polyethyleneglycol 4000. Chromatographia, 1988, 25, 725-730.	1.3	31
161	On the errors of Arrhenius parameters and estimated rate constant values. International Journal of Chemical Kinetics, 1987, 19, 171-181.	1.6	68
162	Limitations of evaluation methods for inhibited oxidation processes in the liquid phase. Journal of the Chemical Society Faraday Transactions I, 1986, 82, 2621.	1.0	3

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163	Thermodynamic consistency test for binary VLE data. Fluid Phase Equilibria, 1986, 27, 405-425.	2.5	8
164	On the interaction of hydroperoxide and inhibitor molecules. International Journal of Chemical Kinetics, 1985, 17, 271-275.	1.6	0
165	Rate Coefficients of Elementary Steps in the Inhibited Oxidation of Ethylbenzene, II. Interaction between Hydroperoxide and Alcohol Molecules. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1984, 88, 63-65.	0.9	5
166	Rate Coefficients of Elementary Steps in the Inhibited Oxidation of Ethylbenzene, I. Interaction between Peroxy Radicals and Inhibitor Molecules. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1983, 87, 606-609.	0.9	7
167	Some aspects of modeling hydrocarbon oxidation. Proceedings of the Combustion Institute, 1981, 18, 1321-1331.	0.3	1
168	Injection Flow NMR as a Tool for the High Throughput Screening of Oils. Special Publication - Royal Society of Chemistry, 0, , 124-130.	0.0	2
169	Comparison of Descriptor- and Fingerprint Sets in Machine Learning Models for ADME-Tox Targets. Frontiers in Chemistry, 0, 10, .	3.6	21