

Clara RÃ fols

List of Publications by Year in descending order

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papers

4,706
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87888

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63
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118
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118
docs citations

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times ranked

4270
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#	ARTICLE	IF	CITATIONS
1	Molecular characteristics of several drugs evaluated from solvent/water partition measurements: Solvation parameters and intramolecular hydrogen bond indicator. <i>European Journal of Pharmaceutical Sciences</i> , 2022, 168, 106066.	4.0	7
2	Synthesis and Characterization of a New Norfloxacin/Resorcinol Cocrystal with Enhanced Solubility and Dissolution Profile. <i>Pharmaceutics</i> , 2022, 14, 49.	4.5	16
3	Evaluation of the Interactions between Human Serum Albumin (HSA) and Non-Steroidal Anti-Inflammatory (NSAIDs) Drugs by Multiwavelength Molecular Fluorescence, Structural and Computational Analysis. <i>Pharmaceutics</i> , 2021, 14, 214.	3.8	18
4	A Novel, Extremely Bioavailable Cocrystal of Pterostilbene. <i>Crystal Growth and Design</i> , 2021, 21, 2315-2323.	3.0	22
5	Equations for the Correlation and Prediction of Partition Coefficients of Neutral Molecules and Ionic Species in the Water-Isopropanol Solvent System. <i>Journal of Solution Chemistry</i> , 2021, 50, 458-472.	1.2	9
6	Ionizable Drug Self-Associations and the Solubility Dependence on pH: Detection of Aggregates in Saturated Solutions Using Mass Spectrometry (ESI-Q-TOF-MS/MS). <i>Molecular Pharmaceutics</i> , 2021, 18, 2311-2321.	4.6	9
7	Prediction of the n-octanol/water partition coefficients in the SAMPL6 blind challenge from MST continuum solvation calculations. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 443-451.	2.9	11
8	Capillary electrophoresis for drug analysis and physicochemical characterization. <i>Handbook of Analytical Separations</i> , 2020, , 633-666.	0.8	5
9	Potentiometric CheqSol and standardized shake-flask solubility methods are complimentary tools in physicochemical profiling. <i>European Journal of Pharmaceutical Sciences</i> , 2020, 148, 105305.	4.0	2
10	Ionic equilibria in aqueous organic solvent mixtures. Speciation of hydrofluoric acid in several ethanol/water solutions. <i>Journal of Electroanalytical Chemistry</i> , 2019, 848, 113318.	3.8	0
11	Molecular interactions between warfarin and human (HSA) or bovine (BSA) serum albumin evaluated by isothermal titration calorimetry (ITC), fluorescence spectrometry (FS) and frontal analysis capillary electrophoresis (FA/CE). <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2018, 150, 452-459.	2.8	72
12	Effect of vinylpyrrolidone polymers on the solubility and supersaturation of drugs; a study using the Cheqsol method. <i>European Journal of Pharmaceutical Sciences</i> , 2018, 117, 227-235.	4.0	18
13	Dissolution rate of ciprofloxacin and its cocrystal with resorcinol. <i>ADMET and DMPK</i> , 2018, 6, 61.	2.1	7
14	Evaluation of the interactions between human serum albumin (HSA) and warfarin or diflunisal by using molecular fluorescence using two approaches. <i>ADMET and DMPK</i> , 2018, 6, 47.	2.1	5
15	Critical comparison of shake-flask, potentiometric and chromatographic methods for lipophilicity evaluation ($\log P_{o/w}$) of neutral, acidic, basic, amphoteric, and zwitterionic drugs. <i>European Journal of Pharmaceutical Sciences</i> , 2018, 122, 331-340.	4.0	21
16	Poly(2-Ethyl-2-Oxazoline) as an Alternative to Poly(Vinylpyrrolidone) in Solid Dispersions for Solubility and Dissolution Rate Enhancement of Drugs. <i>Journal of Pharmaceutical Sciences</i> , 2018, 107, 2428-2438.	3.3	24
17	Lipophilicity of amphoteric and zwitterionic compounds: A comparative study of determination methods. <i>Talanta</i> , 2017, 162, 293-299.	5.5	20
18	Solubility-pH profiles of a free base and its salt: sibutramine as a case study. <i>ADMET and DMPK</i> , 2017, 5, 253-256.	2.1	2

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19	Equilibrium solubility measurement of ionizable drugs – consensus recommendations for improving data quality. <i>ADMET and DMPK</i> , 2016, 4, 117.	2.1	78
20	The Ca ²⁺ -EDTA chelation as standard reaction to validate Isothermal Titration Calorimeter measurements (ITC). <i>Talanta</i> , 2016, 154, 354-359.	5.5	22
21	Phenothiazines solution complexity – Determination of pKa and solubility-pH profiles exhibiting sub-micellar aggregation at 25 and 37°C. <i>European Journal of Pharmaceutical Sciences</i> , 2016, 93, 163-176.	4.0	15
22	Binding thermodynamics of paromomycin, neomycin, neomycin-dinucleotide and diPNA conjugates to bacterial and human rRNA. <i>Journal of Molecular Recognition</i> , 2016, 29, 142-150.	2.1	3
23	Setup and validation of shake-flask procedures for the determination of partition coefficients (logD) from low drug amounts. <i>European Journal of Pharmaceutical Sciences</i> , 2015, 76, 181-191.	4.0	139
24	Molecular Details of INH-C ₁₀ Binding to wt KatG and Its S315T Mutant. <i>Molecular Pharmaceutics</i> , 2015, 12, 898-909.	4.6	12
25	Molecular interactions between some non-steroidal anti-inflammatory drugs (NSAIDs) and bovine (BSA) or human (HSA) serum albumin estimated by means of isothermal titration calorimetry (ITC) and frontal analysis capillary electrophoresis (FA/CE). <i>Talanta</i> , 2014, 130, 241-250.	5.5	59
26	Evaluation of log Po/w values of drugs from some molecular structure calculation softwares. <i>ADMET and DMPK</i> , 2014, 2, .	2.1	17
27	Evaluation of the suitability of chromatographic systems to predict human skin permeation of neutral compounds. <i>European Journal of Pharmaceutical Sciences</i> , 2013, 50, 557-568.	4.0	26
28	The contribution of the hydrogen bond acidity on the lipophilicity of drugs estimated from chromatographic measurements. <i>European Journal of Pharmaceutical Sciences</i> , 2013, 48, 484-493.	4.0	16
29	Determination of acidity constants by the capillary electrophoresis internal standard method. IV. Polyprotic compounds. <i>Journal of Chromatography A</i> , 2013, 1279, 108-116.	3.7	29
30	Solubility-pH profiles of some acidic, basic and amphoteric drugs. <i>European Journal of Pharmaceutical Sciences</i> , 2013, 48, 291-300.	4.0	54
31	Temperature variation effects on the determination of acidity constants through the internal standard capillary electrophoresis method. <i>Electrophoresis</i> , 2013, 34, 1203-1211.	2.4	15
32	Acidity and Hydrophobicity of Several New Potential Antitubercular Drugs: Isoniazid and Benzimidazole Derivatives. <i>Journal of Chemical & Engineering Data</i> , 2012, 57, 330-338.	1.9	43
33	Modeling Nonspecific Toxicity of Organic Compounds to the Fathead Minnow Fish by Means of Chromatographic Systems. <i>Analytical Chemistry</i> , 2012, 84, 3446-3452.	6.5	21
34	Performance of chromatographic systems to model soil-water sorption. <i>Journal of Chromatography A</i> , 2012, 1252, 136-145.	3.7	13
35	Extension of the liquid chromatography/quantitative structure-property relationship method to assess the lipophilicity of neutral, acidic, basic and amphoteric drugs. <i>Journal of Chromatography A</i> , 2012, 1240, 113-122.	3.7	22
36	Chromatographic Hydrophobicity Index (CHI). <i>Advances in Chromatography</i> , 2012, 50, 377-414.	1.0	6

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37	Isothermal titration calorimetry of Ni(II) binding to histidine and to N-2-aminoethylglycine. <i>Talanta</i> , 2011, 84, 347-354.	5.5	6
38	Lipophilicity assessment of basic drugs (logPo/w determination) by a chromatographic method. <i>Journal of Chromatography A</i> , 2011, 1218, 6356-6368.	3.7	29
39	Simultaneous effect of pH, temperature and mobile phase composition in the chromatographic retention of ionizable compounds. <i>Journal of Chromatography A</i> , 2011, 1218, 4995-5009.	3.7	26
40	A fast high throughput method for the determination of acidity constants by capillary electrophoresis. 3. Basic internal standards. <i>Journal of Chromatography A</i> , 2011, 1218, 3928-3934.	3.7	34
41	Fast high-throughput method for the determination of acidity constants by capillary electrophoresis. II. Acidic internal standards. <i>Journal of Chromatography A</i> , 2010, 1217, 8340-8345.	3.7	37
42	Solute-solvent interactions in micellar electrokinetic chromatography: VII. Characterization of sodium cholate-sodium deoxycholate mixed-micellar systems. <i>Journal of Chromatography A</i> , 2010, 1217, 1701-1708.	3.7	8
43	Determination of the hydrophobicity of organic compounds measured as logPo/w through a new chromatographic method. <i>Journal of Chromatography A</i> , 2010, 1217, 3026-3037.	3.7	33
44	Estimation of Biological Properties by Means of Chromatographic Systems: Evaluation of the Factors That Contribute to the Variance of Biological-Chromatographic Correlations. <i>Analytical Chemistry</i> , 2010, 82, 10236-10245.	6.5	16
45	Acid-Base Dissociation Constants of <i>o</i> -Phthalic Acid in Acetonitrile/Water Mixtures over the (15 to 50) °C Temperature Range and Related Thermodynamic Quantities. <i>Journal of Chemical & Engineering Data</i> , 2010, 55, 85-91.	1.9	12
46	A Fast Method for pK_a Determination by Capillary Electrophoresis. <i>Chemistry and Biodiversity</i> , 2009, 6, 1822-1827.	2.1	17
47	Kinetic and Thermodynamic Solubility Values of Some Bioactive Compounds. <i>Chemistry and Biodiversity</i> , 2009, 6, 1789-1795.	2.1	6
48	Enthalpies and constants of dissociation of several neutral and cationic acids in aqueous and methanol/water solutions at various temperatures. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2009, 49, 923-930.	2.8	15
49	Fast high-throughput method for the determination of acidity constants by capillary electrophoresis. <i>Journal of Chromatography A</i> , 2009, 1216, 3646-3651.	3.7	39
50	Prediction of retention in reversed-phase liquid chromatography by means of the polarity parameter model. <i>Journal of Chromatography A</i> , 2009, 1216, 5214-5227.	3.7	22
51	Erratum to "Solute-solvent interactions in micellar electrokinetic chromatography. III. Characterization of the selectivity of micellar electrokinetic chromatography systems" [J. Chromatogr. A 942 (2002) 237-248]. <i>Journal of Chromatography A</i> , 2009, 1216, 6877-6879.	3.7	7
52	Chromatographic hydrophobicity index: pH profile for polyprotic compounds. <i>Journal of Chromatography A</i> , 2009, 1216, 7798-7805.	3.7	8
53	Acidity of Several Anilinium Derivatives in Pure Tetrahydrofuran. <i>Journal of Solution Chemistry</i> , 2008, 37, 689-700.	1.2	18
54	Effect of temperature on the chromatographic retention of ionizable compounds. III. Modeling retention of pharmaceuticals as a function of eluent pH and column temperature in RPLC. <i>Journal of Separation Science</i> , 2008, 31, 969-980.	2.5	14

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55	Critical evaluation of buffering solutions for p <i>K</i> _a determination by capillary electrophoresis. <i>Electrophoresis</i> , 2008, 29, 2841-2851.	2.4	54
56	Characterization of the acidity of residual silanol groups in immobilized artificial membranes. <i>Journal of Chromatography A</i> , 2008, 1182, 233-236.	3.7	7
57	Potentiometric determination of aqueous dissociation constants of flavonols sparingly soluble in water. <i>Talanta</i> , 2008, 74, 1008-1013.	5.5	54
58	Acidity of several polyprotic acids, amiodarone and quetiapine hemifumarate in pure methanol. <i>Talanta</i> , 2007, 73, 115-120.	5.5	13
59	Static Dielectric Constants of Acetonitrile/Water Mixtures at Different Temperatures and Debye-Hückel Parameters for Activity Coefficients. <i>Journal of Chemical & Engineering Data</i> , 2007, 52, 1103-1107.	1.9	139
60	Conversion Parameter between pH Scales (and) in Acetonitrile/Water Mixtures at Various Compositions and Temperatures. <i>Analytical Chemistry</i> , 2007, 79, 3180-3187.	6.5	74
61	Henry's Law constants or air to water partition coefficients for 1,3,5-triazines by an LFER method. <i>Journal of Environmental Monitoring</i> , 2007, 9, 234-239.	2.1	16
62	Interaction of Antioxidant Biobased Epicatechin Conjugates with Biomembrane Models. <i>Journal of Agricultural and Food Chemistry</i> , 2007, 55, 2901-2905.	5.2	9
63	Physicochemical Properties of a New Multicomponent Cosolvent System for the p <i>K</i> _a Determination of Poorly Soluble Pharmaceutical Compounds. <i>Helvetica Chimica Acta</i> , 2007, 90, 1538-1553.	1.6	21
64	Determination of flavonoid aglycones in several food samples by mixed micellar electrokinetic chromatography. <i>Journal of Separation Science</i> , 2007, 30, 2493-2500.	2.5	28
65	Determination of the chromatographic hydrophobicity index for ionisable solutes. <i>Journal of Chromatography A</i> , 2007, 1173, 110-119.	3.7	18
66	Acid-Base Equilibria in Nonpolar Media. Absolute p <i>K</i> _a Scale of Bases in Tetrahydrofuran. <i>Journal of Organic Chemistry</i> , 2006, 71, 9062-9067.	3.2	76
67	Chromatographic Estimation of Drug Disposition Properties by Means of Immobilized Artificial Membranes (IAM) and C18 Columns. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 4861-4870.	6.4	92
68	Modeling Retention and Selectivity as a Function of pH and Column Temperature in Liquid Chromatography. <i>Analytical Chemistry</i> , 2006, 78, 5858-5867.	6.5	23
69	Background electrolytes in 50% methanol/water for the determination of acidity constants of basic drugs by capillary zone electrophoresis. <i>Journal of Chromatography A</i> , 2006, 1123, 113-120.	3.7	27
70	Analysis of prominent flavonoid aglycones by high-performance liquid chromatography using a monolithic type column. <i>Journal of Chromatography A</i> , 2006, 1131, 51-57.	3.7	51
71	Acidity constants in methanol/water mixtures of polycarboxylic acids used in drug salt preparations. <i>European Journal of Pharmaceutical Sciences</i> , 2006, 28, 118-127.	4.0	39
72	Correlation of the toxicity of organic compounds to tadpoles using the Abraham model. <i>Science of the Total Environment</i> , 2006, 371, 99-109.	8.0	47

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73	Selectivity of single, mixed, and modified pseudostationary phases in electrokinetic chromatography. <i>Electrophoresis</i> , 2006, 27, 1900-1914.	2.4	51
74	Effect of temperature on the chromatographic retention of ionizable compounds. <i>Journal of Chromatography A</i> , 2005, 1077, 159-169.	3.7	30
75	Critical micelle concentration of surfactants in aqueous buffered and unbuffered systems. <i>Analytica Chimica Acta</i> , 2005, 548, 95-100.	5.4	317
76	Critical validation of a new simpler approach to estimate aqueous pKa of drugs sparingly soluble in water. <i>Analytica Chimica Acta</i> , 2005, 550, 210-221.	5.4	34
77	Characterization of immobilized artificial membrane (IAM) and XTerra columns by means of chromatographic models. <i>Journal of Chromatography A</i> , 2005, 1081, 163-173.	3.7	29
78	Determination of dissociation constants of flavonoids by capillary electrophoresis. <i>Electrophoresis</i> , 2005, 26, 1886-1895.	2.4	194
79	Hydrophobic and cation exchange mechanisms in the retention of basic compounds in a polymeric column. <i>Journal of Chromatography A</i> , 2004, 1028, 139-148.	3.7	13
80	Effect of temperature on the chromatographic retention of ionizable compounds. <i>Journal of Chromatography A</i> , 2004, 1042, 23-36.	3.7	47
81	Mixed micellar electrokinetic capillary chromatography separation of depolymerized grape procyanidins. <i>Electrophoresis</i> , 2003, 24, 707-713.	2.4	17
82	Micellar electrokinetic chromatography estimation of size and composition of procyanidins after thiolysis with cysteine. <i>Electrophoresis</i> , 2003, 24, 1404-1410.	2.4	21
83	A potentially simpler approach to measure aqueous pKa of insoluble basic drugs containing amino groups. <i>Journal of Pharmaceutical Sciences</i> , 2003, 92, 1473-1481.	3.3	44
84	Effect of temperature on pH measurements and acid-base equilibria in methanol-water mixtures. <i>Journal of Chromatography A</i> , 2003, 1002, 41-53.	3.7	59
85	Characterization of the Solvation Properties of Sodium-Dodecyl Sulfate Micelles in Buffered and Unbuffered Aqueous Phases by Solvatochromic Indicators. <i>Langmuir</i> , 2003, 19, 55-62.	3.5	36
86	Characterization of the Solvation Properties of Surfactants by Solvatochromic Indicators. <i>Langmuir</i> , 2003, 19, 6685-6692.	3.5	26
87	Solute-Solvent Interactions in Micellar Electrokinetic Chromatography. 6. Optimization of the Selectivity of Lithium Dodecyl Sulfate-Lithium Perfluorooctanesulfonate Mixed Micellar Buffers. <i>Analytical Chemistry</i> , 2002, 74, 4447-4455.	6.5	20
88	Solute-solvent interactions in micellar electrokinetic chromatography: IV. Characterization of electroosmotic flow and micellar markers. <i>Electrophoresis</i> , 2002, 23, 56.	2.4	45
89	Chiral separation of benzoporphyrin derivative mono- and diacids by laser induced fluorescence-capillary electrophoresis. <i>Electrophoresis</i> , 2002, 23, 93.	2.4	18
90	Solute-solvent interactions in micellar electrokinetic chromatography: V. Factors that produce peak splitting. <i>Electrophoresis</i> , 2002, 23, 2408-2416.	2.4	18

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91	Chromatographic Determination of Aqueous Dissociation Constants of Some Water-Insoluble Nonsteroidal Antiinflammatory Drugs. <i>Journal of Pharmaceutical Sciences</i> , 2002, 91, 991-999.	3.3	40
92	Solute-solvent interactions in micellar electrokinetic chromatography. <i>Journal of Chromatography A</i> , 2002, 942, 237-248.	3.7	85
93	Solute-solvent interactions in micellar electrokinetic chromatography. <i>Journal of Chromatography A</i> , 2001, 907, 257-265.	3.7	33
94	Solute-solvent interactions in micellar electrokinetic chromatography. <i>Journal of Chromatography A</i> , 1999, 845, 217-226.	3.7	63
95	Solute-solvent and solvent-solvent interactions in binary solvent mixtures. Part 7. Comparison of the enhancement of the water structure in alcohol-water mixtures measured by solvatochromic indicators. <i>Journal of Physical Organic Chemistry</i> , 1998, 11, 185-192.	1.9	199
96	Hydrogen bonding. Part 41.1 Factors that influence the distribution of solutes between water and hexadecylpyridinium chloride micelles. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1997, , 19-24.	0.9	51
97	Solute-solvent and solvent-solvent interactions in binary solvent mixtures. Part 6. A quantitative measurement of the enhancement of the water structure in 2-methylpropan-2-ol-water and propan-2-ol-water mixtures by solvatochromic indicators. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1997, , 1341-1348.	0.9	97
98	Solute-solvent and solvent-solvent interactions in binary solvent mixtures. Part 5. Preferential solvation of solvatochromic indicators in mixtures of propan-2-ol with hexane, benzene, ethanol and methanol. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1997, , 243-248.	0.9	50
99	Determination of sulphonated azo dyes in water and wastewater. <i>TrAC - Trends in Analytical Chemistry</i> , 1997, 16, 405-419.	11.4	83
100	Ionic equilibria in aqueous organic solvent mixtures The equilibria of HF in an ethanol + water mixture used for cleaning up semiconductors. <i>Journal of Electroanalytical Chemistry</i> , 1997, 433, 77-83.	3.8	10
101	Determination of mono- and disulphonated azo dyes by liquid chromatography-atmospheric pressure ionization mass spectrometry. <i>Journal of Chromatography A</i> , 1997, 777, 177-192.	3.7	104
102	A comparison between different approaches to estimate the aqueous pKa values of several non-steroidal anti-inflammatory drugs. <i>Analytica Chimica Acta</i> , 1997, 338, 127-134.	5.4	62
103	Ionic equilibria in aqueous organic solvent mixtures the dissociation constants of acids and salts in tetrahydrofuran/water mixtures. <i>Analytica Chimica Acta</i> , 1997, 340, 133-141.	5.4	31
104	Autoprotolysis in aqueous organic solvent mixtures. Water/dipolar protophilic solvent binary systems. <i>Analytica Chimica Acta</i> , 1997, 349, 367-376.	5.4	13
105	Dissociation constants of several non-steroidal anti-inflammatory drugs in isopropyl alcohol/water mixtures. <i>Analytica Chimica Acta</i> , 1997, 350, 249-255.	5.4	31
106	Solute-solvent and solvent-solvent interactions in binary solvent mixtures. Part 3. The ET(30) polarity of binary mixtures of hydroxylic solvents. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1996, , 1497-1503.	0.9	85
107	Autoprotolysis in aqueous organic solvent mixtures. Water/alcohol binary systems. <i>Analytica Chimica Acta</i> , 1996, 335, 291-302.	5.4	26
108	Linear free energy relationship analysis of microemulsion electrokinetic chromatographic determination of lipophilicity. <i>Journal of Chromatography A</i> , 1996, 752, 243-249.	3.7	102

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109	Variation of acidity constants and pH values of some organic acids in water-2-propanol mixtures with solvent composition. Effect of preferential solvation. <i>Analytica Chimica Acta</i> , 1995, 302, 109-119.	5.4	52
110	Autoprotolysis in aqueous organic solvent mixtures. Water-amide and water-amine binary systems. <i>Analytica Chimica Acta</i> , 1995, 302, 355-363.	5.4	8
111	Solute-solvent and solvent-solvent interactions in binary solvent mixtures. Part 1. A comparison of several preferential solvation models for describing ET(30) polarity of bipolar hydrogen bond acceptor-cosolvent mixtures. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1995, , 1607-1615.	0.9	195
112	Hydrogen bonding. Part 40. Factors that influence the distribution of solutes between water and sodium dodecylsulfate micelles. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1995, , 887.	0.9	93
113	Factors that influence tadpole narcosis. An LFER analysis. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1995, , 1843.	0.9	86
114	Interpretation of Hydroxylic Solvent Effects Based on Correlations with Solvent Parameters. Reaction of Et ₃ N with Etl. <i>Collection of Czechoslovak Chemical Communications</i> , 1994, 59, 898-904.	1.0	10
115	Standardization of potentiometric cells in propan-2-ol-water. <i>Analytica Chimica Acta</i> , 1993, 280, 75-83.	5.4	6
116	Autoprotolysis in aqueous organic solvent mixtures. <i>Analytical Chemistry</i> , 1993, 65, 2294-2299.	6.5	39
117	Ionic equilibria in neutral amphiprotic solvents: relationships between electrolyte pK values and solvent polarity and composition for several binary isopropyl alcohol mixtures. <i>Analytical Chemistry</i> , 1990, 62, 102-107.	6.5	20
118	Ionic equilibria in neutral amphiprotic solvents: Structural effects on dissociation constants of several substituted phenols and mercaptopyrimidines in isopropyl alcohol. <i>Talanta</i> , 1989, 36, 1227-1231.	5.5	20