

Antonio Gustavo Gonzalez

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139
papers

6,113
citations

42
h-index

74
g-index

146
ext. papers

6,719
ext. citations

5.2
avg. IF

5.54
L-index

#	Paper	IF	Citations
139	Electrohydrodynamics and dielectrophoresis in microsystems: scaling laws. <i>Journal Physics D: Applied Physics</i> , 2003 , 36, 2584-2597	3	493
138	The Correlation Coefficient: An Overview. <i>Critical Reviews in Analytical Chemistry</i> , 2006 , 36, 41-59	5.2	393
137	A practical guide to analytical method validation, including measurement uncertainty and accuracy profiles. <i>TrAC - Trends in Analytical Chemistry</i> , 2007 , 26, 227-238	14.6	378
136	Fluid flow induced by nonuniform ac electric fields in electrolytes on microelectrodes. III. Observation of streamlines and numerical simulation. <i>Physical Review E</i> , 2002 , 66, 026305	2.4	285
135	Intra-laboratory testing of method accuracy from recovery assays. <i>Talanta</i> , 1999 , 48, 729-36	6.2	264
134	Electrothermally induced fluid flow on microelectrodes. <i>Journal of Electrostatics</i> , 2001 , 53, 71-87	1.7	218
133	Differentiation of tea (<i>Camellia sinensis</i>) varieties and their geographical origin according to their metal content. <i>Journal of Agricultural and Food Chemistry</i> , 2001 , 49, 4775-9	5.7	197
132	Pumping of liquids with ac voltages applied to asymmetric pairs of microelectrodes. <i>Physical Review E</i> , 2003 , 67, 056302	2.4	179
131	HPLC determination of catechins and caffeine in tea. Differentiation of green, black and instant teas. <i>Analyst, The</i> , 2000 , 125, 421-5	5	133
130	Electrothermal flows generated by alternating and rotating electric fields in microsystems. <i>Journal of Fluid Mechanics</i> , 2006 , 564, 415	3.7	127
129	Pumping of liquids with traveling-wave electroosmosis. <i>Journal of Applied Physics</i> , 2005 , 97, 084906	2.5	127
128	HPLC analysis of tocopherols and triglycerides in coffee and their use as authentication parameters. <i>Food Chemistry</i> , 2001 , 73, 93-101	8.5	103
127	Fatty acid profiles as discriminant parameters for coffee varieties differentiation. <i>Talanta</i> , 2001 , 54, 291-7	6.2	96
126	Multi-element analysis of tea beverages by inductively coupled plasma atomic emission spectrometry. <i>Food Chemistry</i> , 2002 , 76, 483-489	8.5	90
125	Study of catechin and xanthine tea profiles as geographical tracers. <i>Journal of Agricultural and Food Chemistry</i> , 2002 , 50, 1833-9	5.7	89
124	Electric field induced fluid flow on microelectrodes: the effect of illumination. <i>Journal Physics D: Applied Physics</i> , 2000 , 33, L13-L17	3	89
123	Pattern recognition procedures for differentiation of Green, Black and Oolong teas according to their metal content from inductively coupled plasma atomic emission spectrometry. <i>Talanta</i> , 2001 , 53, 1249-57	6.2	79

122	Discrimination between arabica and robusta green coffee varieties according to their chemical composition. <i>Talanta</i> , 1998 , 46, 1259-64	6.2	71
121	Multivariate characterisation of beers according to their mineral content. <i>Talanta</i> , 2002 , 57, 45-52	6.2	70
120	Mineral content and electrical conductivity of the honeys produced in Northwest Morocco and their contribution to the characterisation of unifloral honeys. <i>Journal of the Science of Food and Agriculture</i> , 2003 , 83, 637-643	4.3	69
119	Estimation of the uncertainty of indirect measurements from the propagation of distributions by using the Monte-Carlo method: An overview. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2005 , 79, 115-122	3.8	69
118	Characterisation of Moroccan unifloral honeys using multivariate analysis. <i>European Food Research and Technology</i> , 2003 , 218, 88-95	3.4	67
117	Intra-laboratory assessment of method accuracy (trueness and precision) by using validation standards. <i>Talanta</i> , 2010 , 82, 1995-8	6.2	65
116	Characterization of arabica and robusta roasted coffee varieties and mixture resolution according to their metal content. <i>Food Chemistry</i> , 1999 , 66, 365-370	8.5	63
115	Simultaneous determination of caffeine and non-steroidal anti-inflammatory drugs in pharmaceutical formulations and blood plasma by reversed-phase HPLC from linear gradient elution. <i>Talanta</i> , 1999 , 49, 453-459	6.2	60
114	Determination of Al, Ba, Ca, Cu, Fe, K, Mg, Mn, Na, Sr and Zn in red wine samples by inductively coupled plasma optical emission spectroscopy: Evaluation of preliminary sample treatments. <i>Microchemical Journal</i> , 2008 , 88, 56-61	4.8	58
113	Differentiation of two Canary DO red wines according to their metal content from inductively coupled plasma optical emission spectrometry and graphite furnace atomic absorption spectrometry by using Probabilistic Neural Networks. <i>Talanta</i> , 2007 , 72, 263-8	6.2	57
112	Differentiation of sparkling wines (cava and champagne) according to their mineral content. <i>Talanta</i> , 2004 , 63, 377-82	6.2	57
111	Multivariate characterization of wine vinegars from the south of Spain according to their metallic content. <i>Talanta</i> , 1997 , 45, 379-86	6.2	54
110	Characterization of green coffee varieties according to their metal content. <i>Analytica Chimica Acta</i> , 1998 , 358, 177-183	6.6	54
109	Optimization and validation of headspace sorptive extraction for the analysis of volatile compounds in wine vinegars. <i>Journal of Chromatography A</i> , 2008 , 1204, 93-103	4.5	52
108	Evaluation of measurement uncertainty in analytical assays by means of Monte-Carlo simulation. <i>Talanta</i> , 2004 , 64, 415-22	6.2	50
107	Authentication of green coffee varieties according to their sterolic profile. <i>Analytica Chimica Acta</i> , 1998 , 370, 131-139	6.6	48
106	Two level factorial experimental designs based on multiple linear regression models: a tutorial digest illustrated by case studies. <i>Analytica Chimica Acta</i> , 1998 , 360, 227-241	6.6	47
105	Differentiation of two Andalusian DO wines according to their metal content from ICP-OES by using supervised pattern recognition methods. <i>Microchemical Journal</i> , 2007 , 87, 72-76	4.8	47

104	The effect of size on trace metal levels in raft cultivated mussels (<i>Mytilus galloprovincialis</i>). <i>Science of the Total Environment</i> , 2004 , 318, 115-24	10.2	47
103	Study of mineral profile of Montilla-Moriles fino wines using inductively coupled plasma atomic emission spectrometry methods. <i>Journal of Food Composition and Analysis</i> , 2007 , 20, 391-395	4.1	45
102	Ion chromatographic determination of some organic acids, chloride and phosphate in coffee and tea. <i>Talanta</i> , 2003 , 61, 95-101	6.2	44
101	Nonlinear electrohydrodynamics of free surfaces. <i>IEEE Transactions on Dielectrics and Electrical Insulation</i> , 1998 , 5, 334-343	2.3	44
100	Ion-exclusion chromatographic determination of organic acids in vinegars. <i>Journal of Chromatography A</i> , 1998 , 822, 45-51	4.5	43
99	Solvent effects on the dissociation of aliphatic carboxylic acids in water-N,N-dimethylformamide mixtures: Correlation between acidity constants and solvatochromic parameters. <i>Journal of Solution Chemistry</i> , 1994 , 23, 1101-1109	1.8	43
98	Differentiation of Spanish brandies according to their metal content. <i>Talanta</i> , 2001 , 54, 53-9	6.2	42
97	Cylindrospermopsin determination in water by LC-MS/MS: optimization and validation of the method and application to real samples. <i>Environmental Toxicology and Chemistry</i> , 2012 , 31, 2233-8	3.8	39
96	Accuracy profiles from uncertainty measurements. <i>Talanta</i> , 2006 , 70, 896-901	6.2	38
95	Flow reversal in traveling-wave electrokinetics: an analysis of forces due to ionic concentration gradients. <i>Langmuir</i> , 2009 , 25, 4988-97	4	37
94	Classification of tea samples by their chemical composition using discriminant analysis. <i>Talanta</i> , 1996 , 43, 415-9	6.2	37
93	Estimation of pH and autoprotolysis constants in mixtures of aliphatic amides with water: Medium effect on the 4-aminoazobenzene system. <i>Talanta</i> , 1993 , 40, 479-84	6.2	36
92	A linear analysis of the effect of Faradaic currents on traveling-wave electroosmosis. <i>Journal of Colloid and Interface Science</i> , 2007 , 309, 323-31	9.3	35
91	Optimisation of a pressurised liquid extraction method for haloanisoles in cork stoppers. <i>Analytica Chimica Acta</i> , 2005 , 540, 17-24	6.6	32
90	Non-linear QSAR modeling by using multilayer perceptron feedforward neural networks trained by back-propagation. <i>Talanta</i> , 2002 , 56, 79-90	6.2	32
89	Authentication and differentiation of irish whiskeys by higher-alcohol congener analysis. <i>Analytica Chimica Acta</i> , 1999 , 381, 257-264	6.6	32
88	Practical digest for evaluating the uncertainty of analytical assays from validation data according to the LGC/VAM protocol. <i>Talanta</i> , 2005 , 65, 1022-30	6.2	31
87	Determination of the arabica/robusta composition of roasted coffee according to their sterolic content. <i>Analyst, The</i> , 1999 , 124, 999-1002	5	30

86	Improving the quality of African robustas: QTLs for yield- and quality-related traits in Coffea canephora. <i>Tree Genetics and Genomes</i> , 2011 , 7, 781-798	2.1	29
85	Application of pattern recognition to the discrimination of roasted coffees. <i>Analytica Chimica Acta</i> , 1996 , 320, 191-197	6.6	29
84	Effect of the combined action of Faradaic currents and mobility differences in ac electro-osmosis. <i>Physical Review E</i> , 2010 , 81, 016320	2.4	27
83	Uncertainty evaluation from Monte-Carlo simulations by using Crystal-Ball software. <i>Accreditation and Quality Assurance</i> , 2005 , 10, 149-154	0.7	27
82	Potentiometric titrations in acetonitrile-water mixtures: evaluation of aqueous ionisation constant of ketoprofen. <i>Talanta</i> , 2002 , 56, 769-75	6.2	27
81	Optimization of pharmaceutical formulations based on response-surface experimental designs. <i>International Journal of Pharmaceutics</i> , 1993 , 97, 149-159	6.5	26
80	Classification of aniseed drinks by means of cluster, linear discriminant analysis and soft independent modelling of class analogy based on their Zn, B, Fe, Mg, Ca, Na and Si content. <i>Talanta</i> , 2005 , 66, 1350-4	6.2	25
79	Supervised pattern recognition procedures for discrimination of whiskeys from gas chromatography/mass spectrometry congener analysis. <i>Journal of Agricultural and Food Chemistry</i> , 2006 , 54, 1982-9	5.7	25
78	Interspecific variation of metal concentrations in three bivalve mollusks from Galicia. <i>Archives of Environmental Contamination and Toxicology</i> , 2004 , 47, 341-51	3.2	25
77	DESCRIPTIVE SENSORY ANALYSIS OF WINE VINEGAR: TASTING PROCEDURE AND RELIABILITY OF NEW ATTRIBUTES. <i>Journal of Sensory Studies</i> , 2010 , 25, 216-230	2.2	24
76	Solubility prediction of caffeine in aqueous N,N-dimethylformamide mixtures using the Extended Hildebrand Solubility Approach. <i>International Journal of Pharmaceutics</i> , 1997 , 156, 239-244	6.5	24
75	HPLC determination of 2-furaldehyde and 5-hydroxymethyl-2-furaldehyde in alcoholic beverages. <i>Microchemical Journal</i> , 2006 , 82, 22-28	4.8	24
74	Development and optimization of a method for the determination of Cylindrospermopsin from strains of Aphanizomenon cultures: intra-laboratory assessment of its accuracy by using validation standards. <i>Talanta</i> , 2012 , 100, 356-63	6.2	23
73	Some observations on fitting a straight line to data. <i>Microchemical Journal</i> , 1989 , 40, 216-225	4.8	23
72	Differentiation between microcystin contaminated and uncontaminated fish by determination of unconjugated MCs using an ELISA anti-Adda test based on receiver-operating characteristic curves threshold values: application to Tinca tinca from natural ponds. <i>Environmental Toxicology</i> , 2011 , 26, 45-56	4.2	22
71	Correction factors for the glass electrode revisited. <i>Talanta</i> , 1992 , 39, 91	6.2	22
70	Use and misuse of supervised pattern recognition methods for interpreting compositional data. <i>Journal of Chromatography A</i> , 2007 , 1158, 215-25	4.5	21
69	Ionization constants of water insoluble arylpropionic acids in aqueous N,N-dimethylformamide mixtures from potentiometric pH-titrations. <i>Analytica Chimica Acta</i> , 1997 , 356, 253-258	6.6	20

68	The correlation coefficient attacks again. <i>Accreditation and Quality Assurance</i> , 2006 , 11, 256-258	0.7	19
67	Performing procrustes discriminant analysis with HOLMES. <i>Talanta</i> , 1999 , 49, 189-97	6.2	19
66	Solvent effects on the dissociation of aliphatic carboxylic acids in water/N,N -dimethylformamide mixtures. <i>Analytica Chimica Acta</i> , 1990 , 228, 301-306	6.6	19
65	Determination of Zn, B, Fe, Mg, Ca, Na and Si in anisette samples by inductively coupled plasma atomic emission spectrometry. <i>Talanta</i> , 2004 , 63, 297-302	6.2	18
64	Adaptation of linear discriminant analysis to second level-pattern recognition classification. <i>Analytica Chimica Acta</i> , 1998 , 363, 89-95	6.6	17
63	Repeated red wine consumption and changes on plasma antioxidant capacity and endogenous antioxidants (uric acid and protein thiol groups). <i>Journal of Agricultural and Food Chemistry</i> , 2007 , 55, 9713-8	5.7	17
62	Determination of Phosphate in Cola Beverages Using Nonsuppressed Ion Chromatography: An Experiment Introducing Ion Chromatography for Quantitative Analysis. <i>Journal of Chemical Education</i> , 1996 , 73, 1174	2.4	17
61	Kamlet-Taft solvatochromic parameters of aqueous binary mixtures of tert-butyl alcohol and ethyleneglycol. <i>Journal of Solution Chemistry</i> , 1996 , 25, 289-293	1.8	17
60	Determination of vanadium in mussels by electrothermal atomic absorption spectrometry without chemical modifiers. <i>Analytical and Bioanalytical Chemistry</i> , 2004 , 379, 72-6	4.4	16
59	Computational program for evaluating and optimizing response-surface curves based on uniform shell designs. <i>Talanta</i> , 1999 , 49, 433-9	6.2	16
58	Korteweg-de Vries-Burgers equation for surface waves in nonideal conducting liquids. <i>Physical Review E</i> , 1994 , 49, 2935-2940	2.4	16
57	Spectrophotometric determination of total procyanidins in wine vinegars. <i>Talanta</i> , 1997 , 44, 119-23	6.2	15
56	Holmes, a program for performing Procrustes Transformations. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2001 , 57, 133-137	3.8	15
55	holmes: a program for target factor analysis. <i>Analytica Chimica Acta</i> , 1994 , 295, 119-125	6.6	15
54	Pumping of electrolytes using travelling-wave electro-osmosis: a weakly nonlinear analysis. <i>Microfluidics and Nanofluidics</i> , 2008 , 5, 507-515	2.8	14
53	Supercritical carbon dioxide extraction of lipids from Eucalyptus globulus wood. <i>Journal of Proteomics</i> , 2000 , 43, 345-51		14
52	Inorganic indicators of the origin of edible salts marketed in Spain from a chemometric approach. <i>Journal of Food Protection</i> , 1998 , 61, 891-5	2.5	14
51	Advantages of target factor analysis against multiple linear regression methods for testing model equations in linear free energy relationships. <i>Analytica Chimica Acta</i> , 1995 , 312, 295-306	6.6	14

50	Acid-base behaviour of some substituted azo dyes in aqueous N,N-dimethylformamide mixtures. <i>Analytica Chimica Acta</i> , 1991 , 246, 429-434	6.6	13
49	Determination of trigonelline in green and roasted coffee from single column ionic chromatography. <i>Fresenius Journal of Analytical Chemistry</i> , 1997 , 357, 357-358		12
48	Evaluation of acidity constants in dioxane-water mixtures by spectrophotometric and potentiometric pH titrations. <i>Analytica Chimica Acta</i> , 1991 , 251, 321-325	6.6	12
47	Estimation of dietary intake and target hazard quotients for metals by consumption of wines from the Canary Islands. <i>Food and Chemical Toxicology</i> , 2017 , 108, 10-18	4.7	11
46	The assessment of electronic balances for accuracy of mass measurements in the analytical laboratory. <i>Accreditation and Quality Assurance</i> , 2007 , 12, 21-29	0.7	11
45	Computational program for validating analytical methods. <i>Fresenius Journal of Analytical Chemistry</i> , 1993 , 346, 885-887		11
44	Metallic contaminants in Andalusian vinegars. <i>Molecular Nutrition and Food Research</i> , 1988 , 32, 743-8		11
43	Mineral profile of fino-wines using inductively coupled plasma optical emission spectrometry methods. <i>Food Chemistry</i> , 2012 , 135, 309-313	8.5	10
42	Enzymatic-spectrophotometric determination of sucrose in coffee beans. <i>Talanta</i> , 2005 , 67, 760-6	6.2	10
41	Study of the mineral profile of Catalanian Brut Cava using atomic spectrometric methods. <i>European Food Research and Technology</i> , 2004 , 218, 448-451	3.4	10
40	Evaluation of solvent effects on the dissociation of aliphatic carboxylic acids in aqueous N,N-dimethylformamide mixtures according to the scaled particle theory. <i>Journal of Physical Organic Chemistry</i> , 1991 , 4, 87-95	2.1	10
39	Metallic profiles of Sherry brandies. <i>Sciences Des Aliments</i> , 2000 , 20, 433-440		10
38	Differentiation of mangoes (<i>Mangifera indica</i> L.) conventional and organically cultivated according to their mineral content by using support vector machines. <i>Talanta</i> , 2012 , 97, 325-30	6.2	9
37	Interfacial electrohydrodynamic instability: The Kath and Hburg model revisited. <i>Physics of Fluids A, Fluid Dynamics</i> , 1992 , 4, 1307-1309		9
36	An iterative algorithm for consistent and unbiased estimation of linear regression parameters when there are errors in both the x and y variables. <i>Computers & Chemistry</i> , 1992 , 16, 25-27		8
35	Supercritical-carbon-dioxide extraction of lipids from a contaminated soil. <i>Journal of Chromatography A</i> , 1999 , 845, 365-371	4.5	7
34	Holmes: a program for target factor analysis. <i>Analytica Chimica Acta</i> , 1994 , 297, 473	6.6	7
33	Computational program for evaluating and optimizing response-surface curves based on central composite designs. <i>Analytica Chimica Acta</i> , 1994 , 298, 65-73	6.6	7

32	The Use of Catechins and Purine Alkaloids as Descriptors for the Differentiation of Tea Beverages. <i>Mikrochimica Acta</i> , 2003 , 142, 79-84	5.8	6
31	Determination of β -adrenoceptor blocking agents in tablets using reversed-phase high-performance liquid chromatography. <i>International Journal of Pharmaceutics</i> , 1995 , 123, 149-151	6.5	6
30	Solubility of theophylline in aqueous N,N-dimethylformamide mixtures. <i>International Journal of Pharmaceutics</i> , 1994 , 108, 149-154	6.5	6
29	Application of the extended Hildebrand solubility parameter treatment for optimizing reversed-phase high-performance liquid chromatography determination of pharmaceuticals. <i>International Journal of Pharmaceutics</i> , 1993 , 93, 183-188	6.5	6
28	Metallic profiles of Sherry wines using inductively coupled plasma atomic emission spectrometry methods (ICP-AES). <i>Sciences Des Aliments</i> , 2007 , 27, 83-92		6
27	Simultaneous determination of organic acids and sweeteners in soft drinks by ion-exclusion HPLC. <i>Journal of Separation Science</i> , 2001 , 24, 879-884	3.4	5
26	Hydrophobicity of β -adrenoceptor blocking agents: Study of correlations between retention in reversed-phase HPLC systems and octanol-water partition constants. <i>International Journal of Pharmaceutics</i> , 1995 , 120, 215-220	6.5	5
25	Statistical assessment of a new criterion for selecting the number of factors in factor analysis. <i>Analytica Chimica Acta</i> , 1995 , 314, 251-252	6.6	5
24	Resolution of acid strength in non-aqueous acid-base titrations. <i>Analytica Chimica Acta</i> , 1993 , 281, 179-183		5
23	Solvent effects on the dissociation of bromopyridinium ions in N,N-dimethylformamide mixtures by electrochemical measurements. <i>Analytica Chimica Acta</i> , 1989 , 224, 109-117	6.6	5
22	AC electrokinetic pumping of liquids using arrays of microelectrodes 2005 ,		4
21	Estimation of the uncertainty of mass measurements from in-house calibrated analytical balances. <i>Accreditation and Quality Assurance</i> , 2005 , 10, 386-391	0.7	4
20	Comment on "Theoretical Model of Electrode Polarization and AC Electroosmotic Fluid Flow in Planar Electrode Arrays" <i>Journal of Colloid and Interface Science</i> , 2001 , 243, 265-266	9.3	4
19	Practical digest for the evaluation of acidity constants of drugs by reversed-phase high performance liquid chromatography. <i>International Journal of Pharmaceutics</i> , 1993 , 91, R1-R5	6.5	4
18	Determination of phosphorous oxoanions in pharmaceuticals using non-suppressed ion chromatography. <i>Analisis - European Journal of Analytical Chemistry</i> , 1999 , 27, 97-100		4
17	Classification of Spanish Red Wines Using Artificial Neural Networks with Enological Parameters and Mineral Content. <i>American Journal of Enology and Viticulture</i> , 2018 , 69, 167-175	2.2	3
16	A multiple hollow fibre liquid-phase microextraction method for the determination of halogenated solvent residues in olive oil. <i>Analytical and Bioanalytical Chemistry</i> , 2014 , 406, 1567-71	4.4	3
15	Computational method for evaluating and optimizing response surface curves based on mixture designs. <i>Analytica Chimica Acta</i> , 1994 , 293, 205-210	6.6	3

14	Spectrophotometric determination of acidity constants of compounds with unsuitable absorption features. <i>International Journal of Pharmaceutics</i> , 1991 , 72, 193-197	6.5	3
13	Computational method for unbiased evaluation of equivalence volumes and ionization constants from potentiometric acid-base titrations. <i>Analytica Chimica Acta</i> , 1992 , 257, 29-33	6.6	3
12	Determination of microcystins in biological samples from freshwater fish. <i>International Journal of Environmental Analytical Chemistry</i> , 2010 , 90, 1000-1013	1.8	2
11	The feasibility and accuracy of nonaqueous acid-base titrations. <i>Microchemical Journal</i> , 1991 , 44, 243-248	4.8	2
10	Drug solubility prediction by using solvatochromic parameters. <i>International Journal of Pharmaceutics</i> , 1991 , 75, R13-R16	6.5	2
9	Validation of a simple method for the determination of glyphosate and aminomethylphosphonic acid in human urine by UPLC-MS/MS. <i>Microchemical Journal</i> , 2021 , 170, 106760	4.8	2
8	A Practical Way to ISO/GUM Measurement Uncertainty for Analytical Assays Including In-House Validation Data 2018 ,		1
7	Gradient Scouting in Reversed-Phase HPLC Revisited. <i>Journal of Chemical Education</i> , 2011 , 88, 74-76	2.4	1
6	Manipulation of Bio-Particles in Microelectrode Structures by Means of Non-Uniform AC Electric Fields 2002 , 165		1
5	NEUTIT: a computer program for evaluating equivalence volumes and ionization constants in polar non-aqueous or partially aqueous media. <i>Analytica Chimica Acta</i> , 1994 , 298, 203-207	6.6	1
4	Evaluation of acidity constants for sparingly soluble compounds from fluorescence measurements. <i>International Journal of Pharmaceutics</i> , 1991 , 67, R1-R4	6.5	1
3	Evaluation of ionization constants of drugs in aqueous organic mixtures from reversed phase high-performance liquid chromatography. <i>International Journal of Pharmaceutics</i> , 1992 , 84, R1-R4	6.5	1
2	Manipulation of bio-particles by means of nonuniform AC electric fields 2005 , 5839, 138		
1	A computational method for approximate evaluation of ionization constants from potentiometric data. <i>Talanta</i> , 1988 , 35, 249-52	6.2	