Ricardo L Mancera

List of Publications by Year
in descending order

131	4,210	109321	133252
papers	citations	35 h-index	59 g-index

136	136	136	5607
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Review: The case for studying mitochondrial function during plant cryopreservation. Plant Science, 2022, 315, 111134.	3.6	9
2	Mechanisms of Interaction of Small Hydroxylated Cryosolvents with Dehydrated Model Cell Membranes: Stabilization vs Destruction. Journal of Physical Chemistry B, 2022, 126, 197-216.	2.6	5
3	Redefining the Molecular Interplay between Dimethyl Sulfoxide, Lipid Bilayers, and Dehydration. Journal of Physical Chemistry B, 2022, 126, 2513-2529.	2.6	4
4	Novel Amylin Analogues Reduce Amyloid-Î² Cross-Seeding Aggregation and Neurotoxicity. Journal of Alzheimer's Disease, 2022, , 1-18.	2.6	2
5	Myrtaceae in Australia: Use of Cryobiotechnologies for the Conservation of a Significant Plant Family under Threat. Plants, 2022, 11, 1017.	3.5	6
6	Structure and intermolecular interactions in spheroidal high-density lipoprotein subpopulations. Journal of Structural Biology: X, 2021, 5, 100042.	1.3	5
7	Identification and characterisation of putative drug binding sites in human ATP-binding cassette B5 (ABCB5) transporter. Computational and Structural Biotechnology Journal, 2021, 19, 691-704.	4.1	5
8	Does the SARS-CoV-2 Spike Protein Receptor Binding Domain Interact Effectively with the DPP4 (CD26) Receptor? A Molecular Docking Study. International Journal of Molecular Sciences, 2021, 22, 7001.	4.1	24
9	Design and Characterization of a Cell-Penetrating Peptide Derived from the SOX2 Transcription Factor. International Journal of Molecular Sciences, 2021, 22, 9354.	4.1	4
10	Pharmacological and structure-activity relationship studies of oleoyl-lysophosphatidylinositol synthetic mimetics. Pharmacological Research, 2021, 172, 105822.	7.1	4
11	BZD9L1 sirtuin inhibitor: Identification of key molecular targets and their biological functions in HCT 116 colorectal cancer cells. Life Sciences, 2021, 284, 119747.	4.3	7
12	An automated and combinative method for the predictive ranking of candidate effector proteins of fungal plant pathogens. Scientific Reports, 2021, 11, 19731.	3.3	27
13	Assessing Plant Metabolic Rates During Cryopreservation. Cryobiology, 2021, 103, 169.	0.7	1
14	Cryostorage of Macadamia Nut Embryonic Axes Using Droplet-Vitrification. Cryobiology, 2021, 103, 163.	0.7	0
15	The unusual conformation of crossâ€strand disulfide bonds is critical to the stability of Î²â€hairpin peptides. Proteins: Structure, Function and Bioinformatics, 2020, 88, 485-502.	2.6	10
16	Molecular Dynamics Simulation of Small Molecules Interacting with Biological Membranes. ChemPhysChem, 2020, 21, 1486-1514.	2.1	37
17	The acidic tail of HMGB1 regulates its secondary structure and conformational flexibility: A circular dichroism and molecular dynamics simulation study. Computational and Structural Biotechnology Journal, 2020, 18, 1160-1172.	4.1	10
18	Revisiting the Interaction of Melittin with Phospholipid Bilayers: The Effects of Concentration and Ionic Strength. International Journal of Molecular Sciences, 2020, 21, 746.	4.1	16

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19	Characterization of Protein-Facilitated Ion-Transfer Mechanism at a Polarized Aqueous/Organic Interface. Journal of Physical Chemistry B, 2019, 123, 7436-7444.	2.6	18
20	Definition of the Minimal Contents for the Molecular Simulation of the Yeast Cytoplasm. Frontiers in Molecular Biosciences, 2019, 6, 97.	3.5	1
21	Seed storage behaviour of tropical members of the aquatic basal angiosperm genus Nymphaea L. (Nymphaeaceae). , 2019, 7, coz021.		3
22	Current issues in plant cryopreservation and importance for ex situ conservation of threatened Australian native species. Australian Journal of Botany, 2019, 67, 1.	0.6	44
23	Secondary Structural Changes in Proteins as a Result of Electroadsorption at Aqueousâ€“Organogel Interfaces. Langmuir, 2019, 35, 5821-5829.	3.5	9
24	Inhibitors of Xanthine Oxidase: Scaffold Diversity and Structureâ€Based Drug Design. ChemMedChem, 2019, 14, 714-743.	3.2	60
25	Does Sucrose Change Its Mechanism of Stabilization of Lipid Bilayers during Desiccation? Influences of Hydration and Concentration. Langmuir, 2019, 35, 15389-15400.	3.5	18
26	Influence of Bilayer Size and Number in Multi-Bilayer DOPC Simulations at Full and Low Hydration. Langmuir, 2019, 35, 2399-2411.	3.5	16
27	Current methods for the prediction of Tâ€cell epitopes. Peptide Science, 2018, 110, e24046.	1.8	12
28	Gomesin peptides prevent proliferation and lead to the cell death of devil facial tumour disease cells. Cell Death Discovery, 2018, 4, 19.	4.7	15
29	Role of the cell membrane interface in modulating production and uptake of Alzheimer's beta amyloid protein. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 1639-1651.	2.6	47
30	Studies of the benzopyran class of selective COX-2 inhibitors using 3D-QSAR and molecular docking. Archives of Pharmacal Research, 2018, 41, 1178-1189.	6.3	31
31	The Biological and Biophysical Properties of the Spider Peptide Gomesin. Molecules, 2018, 23, 1733.	3.8	15
32	Characterisation of the Structure and Oligomerisation of Islet Amyloid Polypeptides (IAPP): A Review of Molecular Dynamics Simulation Studies. Molecules, 2018, 23, 2142.	3.8	28
33	Molecular dynamics simulations of a DMSO/water mixture using the AMBER force field. Journal of Molecular Modeling, 2018, 24, 174.	1.8	11
34	Molecular Dynamics Visualization (MDV): Stereoscopic 3D Display of Biomolecular Structure and Interactions Using the Unity Game Engine. Journal of Integrative Bioinformatics, 2018, 15, .	1.5	22
35	Electrochemistry of proteins at the interface between two immiscible electrolyte solutions. Current Opinion in Electrochemistry, 2018, 12, 27-32.	4.8	26
36	Atomistic molecular dynamics simulations of bioactive engrailed 1 interference peptides (EN1-iPeps). Oncotarget, 2018, 9, 22383-22397.	1.8	9

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37	The selfâ€association of <scp>HMGB</scp>1 and its possible role in the binding to <scp>DNA</scp> and cell membrane receptors. FEBS Letters, 2017, 591, 282-294.	2.8	40
38	Computational site-directed mutagenesis studies of the role of the hydrophobic triad on substrate binding in cholesterol oxidase. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1645-1655.	2.6	4
39	Molecular Dynamics Simulation of Tau Peptides for the Investigation of Conformational Changes Induced by Specific Phosphorylation Patterns. Methods in Molecular Biology, 2017, 1523, 33-59.	0.9	6
40	Advances in understanding the fundamental aspects required for successful cryopreservation of Australian flora. In Vitro Cellular and Developmental Biology - Plant, 2017, 53, 289-298.	2.1	26
41	Monitoring of oxidative status in three native Australian species during cold acclimation and cryopreservation. Plant Cell Reports, 2017, 36, 1903-1916.	5.6	15
42	Understanding Insulin Endocrinology in Decapod Crustacea: Molecular Modelling Characterization of an Insulin-Binding Protein and Insulin-Like Peptides in the Eastern Spiny Lobster, Sagmariasus verreauxi. International Journal of Molecular Sciences, 2017, 18, 1832.	4.1	37
43	Waking up dormant tumor suppressor genes with zinc fingers, TALEs and the CRISPR/dCas9 system. Oncotarget, 2016, 7, 60535-60554.	1.8	61
44	Influence of abiotic stress preconditioning on antioxidant enzymes in shoot tips of Lomandra sonderi (Asparagaceae) prior to cryostorage. Australian Journal of Botany, 2016, 64, 260.	0.6	9
45	New arylated benzo[h]quinolines induce anti-cancer activity by oxidative stress-mediated DNA damage. Scientific Reports, 2016, 6, 38128.	3.3	54
46	The effect of physicochemical factors on the self-association of HMGB1: A surface plasmon resonance study. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2016, 1864, 1620-1629.	2.3	12
47	Optimization of proteinâ€“protein docking for predicting Fcâ€“protein interactions. Journal of Molecular Recognition, 2016, 29, 555-568.	2.1	10
48	Adsorption and Unfolding of Lysozyme at a Polarized Aqueousâ€“Organic Liquid Interface. Journal of Physical Chemistry B, 2016, 120, 3100-3112.	2.6	16
49	Optimization of surface plasmon resonance experiments: Case of high mobility group box 1 (HMGB1) interactions. Analytical Biochemistry, 2016, 499, 43-50.	2.4	7
50	Ex situ conservation of the endangered species Androcalva perlaria (Malvaceae) by micropropagation and cryopreservation. Plant Cell, Tissue and Organ Culture, 2016, 125, 341-352.	2.3	20
51	A Phosphorylationâ€Induced Turn Defines the Alzheimerâ€™s Disease AT8 Antibody Epitope on the Tau Protein. Angewandte Chemie - International Edition, 2015, 54, 6819-6823.	13.8	41
52	Evaluation of the new vacuum infiltration vitrification (viv) cryopreservation technique for native Australian plant shoot tips. Cryo-Letters, 2015, 36, 104-13.	0.3	6
53	Free Energy of Binding of Coiled-Coil Complexes with Different Electrostatic Environments: The Influence of Force Field Polarisation and Capping. Natural Products and Bioprospecting, 2014, 4, 285-295.	4.3	3
54	Development and application of site mapping methods for the design of glycosaminoglycans. Glycobiology, 2014, 24, 840-851.	2.5	24

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55	The emerging application of ultrasound in lactose crystallisation. Trends in Food Science and Technology, 2014, 38, 47-59.	15.1	43
56	Molecular dynamics simulation of the phosphorylation-induced conformational changes of a tau peptide fragment. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1907-1923.	2.6	31
57	Characterization of the Glass Transition of Water Predicted by Molecular Dynamics Simulations Using Nonpolarizable Intermolecular Potentials. Journal of Physical Chemistry B, 2014, 118, 1867-1880.	2.6	6
58	Assignment of aromaticity of the classic heterobenzenes by three aromatic criteria. Computational and Theoretical Chemistry, 2014, 1046, 20-24.	2.5	12
59	Enhanced Transdermal Peptide Delivery and Stability by Lipid Conjugation: Epidermal Permeation, Stereoselectivity and Mechanistic Insights. Pharmaceutical Research, 2014, 31, 3304-3312.	3.5	13
60	Molecular Mechanism of the Synergistic Effects of Vitrification Solutions on the Stability of Phospholipid Bilayers. Biophysical Journal, 2014, 106, 2617-2624.	0.5	20
61	Cold-induced changes affect survival after exposure to vitrification solution during cryopreservation in the south-west Australian Mediterranean climate species Lomandra sonderi (Asparagaceae). Plant Cell, Tissue and Organ Culture, 2014, 119, 347-358.	2.3	10
62	Hydrogen Bond Disruption in DNA Base Pairs from ¹⁴C Transmutation. Journal of Physical Chemistry B, 2014, 118, 10430-10435.	2.6	5
63	Molecular dynamics simulations of the interactions of DMSO, mono- and polyhydroxylated cryosolvents with a hydrated phospholipid bilayer. Biochimica Et Biophysica Acta - Biomembranes, 2013, 1828, 2041-2055.	2.6	48
64	Molecular dynamics simulations of mixed DOPCâ€“Î²-sitosterol bilayers and their interactions with DMSO. Soft Matter, 2013, 9, 2920.	2.7	27
65	The Effects of Cryosolvents on DOPCâ^Î²-Sitosterol Bilayers Determined from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2013, 117, 3362-3375.	2.6	27
66	Acclimation-induced changes in cell membrane composition and influence on cryotolerance of in vitro shoots of native plant species. Plant Cell, Tissue and Organ Culture, 2013, 114, 83-96.	2.3	22
67	AutoMap: A tool for analyzing proteinâ€“ligand recognition using multiple ligand binding modes. Journal of Molecular Graphics and Modelling, 2013, 40, 80-90.	2.4	14
68	Development of cryopreservation for Loxocarya cinerea---an endemic Australian plant species important for post-mining restoration. Cryo-Letters, 2013, 34, 508-19.	0.3	8
69	Computational analyses of the catalytic and heparin-binding sites and their interactions with glycosaminoglycans in glycoside hydrolase family 79 endo-β-d-glucuronidase (heparanase). Glycobiology, 2012, 22, 35-55.	2.5	44
70	Prediction of heparin binding sites in bone morphogenetic proteins (BMPs). Biochimica Et Biophysica Acta - Proteins and Proteomics, 2012, 1824, 1374-1381.	2.3	80
71	Free energy calculations of the interactions of câ€Junâ€based synthetic peptides with the câ€Fos protein. Biopolymers, 2012, 97, 899-909.	2.4	10
72	Molecular Dynamics Simulations of the Interactions of DMSO with DPPC and DOPC Phospholipid Membranes. Journal of Physical Chemistry B, 2012, 116, 11911-11923.	2.6	70

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73	Molecular modeling of Bt Cry1Ac (DIâ€“DII)â€“ASAL (Allium sativum lectin)â€“fusion protein and its interaction with aminopeptidase N (APN) receptor of Manduca sexta. Journal of Molecular Graphics and Modelling, 2012, 33, 61-76.	2.4	19
74	Developing Drugs from Sugars. , 2012, , 259-296.		0
75	Cryopreservation of Lomandra sonderi (Asparagaceae) shoot tips using droplet-vitrification. Cryo-Letters, 2012, 33, 259-70.	0.3	8
76	Molecular Dynamics Simulations of CXCL-8 and Its Interactions with a Receptor Peptide, Heparin Fragments, and Sulfated Linked Cyclitols. Journal of Chemical Information and Modeling, 2011, 51, 335-358.	5.4	32
77	A molecular mechanism of solvent cryoprotection in aqueous DMSO solutions. Physical Chemistry Chemical Physics, 2011, 13, 3839.	2.8	77
78	Prediction of the glass transition in aqueous solutions of simple amides by molecular dynamics simulations. Chemical Physics Letters, 2011, 501, 273-277.	2.6	18
79	Cryopreservation of threatened native Australian speciesâ€”what have we learned and where to from here?. In Vitro Cellular and Developmental Biology - Plant, 2011, 47, 17-25.	2.1	45
80	Heparin/heparan sulphate-based drugs. Drug Discovery Today, 2010, 15, 1058-1069.	6.4	98
81	Free Energy Calculations of Mutations Involving a Tightly Bound Water Molecule and Ligand Substitutions in a Ligandâ€Protein Complex. Molecular Informatics, 2010, 29, 589-600.	2.5	37
82	Can current force fields reproduce ring puckering in 2-O-sulfo-Î±-l-iduronic acid? A molecular dynamics simulation study. Carbohydrate Research, 2010, 345, 689-695.	2.3	33
83	Calculations of the Free Energy of Interaction of the c-Fosâ€“c-Jun Coiled Coil: Effects of the Solvation Model and the Inclusion of Polarization Effects. Journal of Chemical Information and Modeling, 2010, 50, 2201-2212.	5.4	15
84	Ligandâ€“Protein Cross-Docking with Water Molecules. Journal of Chemical Information and Modeling, 2010, 50, 415-421.	5.4	77
85	Free energy calculations of glycosaminoglycanâ€“protein interactions. Glycobiology, 2009, 19, 1103-1115.	2.5	56
86	Docking Study and Threeâ€Dimensional Quantitative Structureâ€Activity Relationship (3Dâ€QSAR) Analyses of Transforming Growth Factorâ€Î²2 Type I Receptor Kinase Inhibitors. QSAR and Combinatorial Science, 2009, 28, 1300-1308.	1.4	3
87	Molecular dynamics simulations of ligand-induced backbone conformational changes in the binding site of the periplasmic lysine-, arginine-, ornithine-binding protein. Journal of Computer-Aided Molecular Design, 2008, 22, 799-814.	2.9	6
88	The Structure of Glycosaminoglycans and their Interactions with Proteins. Chemical Biology and Drug Design, 2008, 72, 455-482.	3.2	820
89	New anti-tuberculosis drugs in clinical trials with novel mechanisms of action. Drug Discovery Today, 2008, 13, 1090-1098.	6.4	121
90	Ligandâ€“Protein Docking with Water Molecules. Journal of Chemical Information and Modeling, 2008, 48, 397-408.	5.4	128

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91	New Anti-Tuberculosis Drugs with Novel Mechanisms of Action. Current Medicinal Chemistry, 2008, 15, 1956-1967.	2.4	49
92	Platelet Endothelial Cell Adhesion Molecule 1 (PECAM-1) and Its Interactions with Glycosaminoglycans: 1. Molecular Modeling Studies. Biochemistry, 2008, 47, 4851-4862.	2.5	37
93	Platelet Endothelial Cell Adhesion Molecule 1 (PECAM-1) and Its Interactions with Glycosaminoglycans: 2. Biochemical Analyses. Biochemistry, 2008, 47, 4863-4875.	2.5	29
94	Computational Methods for the Prediction of the Structure and Interactions of Coiled-Coil Peptides. Current Bioinformatics, 2008, 3, 149-161.	1.5	3
95	A Comparative Structural Bioinformatics Analysis of the Insulin Receptor Family Ectodomain Based on Phylogenetic Information. PLoS ONE, 2008, 3, e3667.	2.5	45
96	Characterization of sequence and structural features of the Candida krusei enolase. In Silico Biology, 2008, 8, 449-60.	0.9	5
97	Molecular modeling of hydration in drug design. Current Opinion in Drug Discovery & Development, 2007, 10, 275-80.	1.9	29
98	Novel Structural Features of CDK Inhibition Revealed by an ab Initio Computational Method Combined with Dynamic Simulations. Journal of Medicinal Chemistry, 2006, 49, 5141-5153.	6.4	37
99	The effect of a tightly bound water molecule on scaffold diversity in the computer-aided de novo ligand design of CDK2 inhibitors. Journal of Molecular Modeling, 2006, 12, 422-431.	1.8	37
100	Comparative Analysis of the Surface Interaction Properties of the Binding Sites of CDK2, CDK4, and ERK2. ChemMedChem, 2006, 1, 366-375.	3.2	5
101	The molecular binding interactions of inhibitors and activators of phosphoenolpyruvate carboxylase. Computational and Theoretical Chemistry, 2005, 755, 151-159.	1.5	3
102	Expanded Interaction Fingerprint Method for Analyzing Ligand Binding Modes in Docking and Structure-Based Drug Design.. ChemInform, 2005, 36, no.	0.0	0
103	Including Tightly-Bound Water Molecules in de Novo Drug Design. Exemplification Through the in Silico Generation of Poly(ADP-ribose)polymerase Ligands.. ChemInform, 2005, 36, no.	0.0	0
104	Kinetics of the crystallisation of Niâ€“Zn ferrite powders prepared by the hydrothermal method. Materials Science and Technology, 2005, 21, 1059-1062.	1.6	1
105	Including Tightly-Bound Water Molecules in de Novo Drug Design. Exemplification through the in Silico Generation of Poly(ADP-ribose)polymerase Ligands. Journal of Chemical Information and Modeling, 2005, 45, 624-633.	5.4	51
106	A New Method for Estimating the Importance of Hydrophobic Groups in the Binding Site of a Protein. Journal of Medicinal Chemistry, 2005, 48, 1069-1078.	6.4	22
107	The effect of tightly bound water molecules on the structural interpretation of ligand-derived pharmacophore models. Journal of Computer-Aided Molecular Design, 2004, 18, 89-100.	2.9	34
108	Molecular modelling prediction of ligand binding site flexibility. Journal of Computer-Aided Molecular Design, 2004, 18, 235-250.	2.9	22

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109	Comparative estimation of vibrational entropy changes in proteins through normal modes analysis. Journal of Molecular Graphics and Modelling, 2004, 23, 167-174.	2.4	20
110	Ligand-protein docking using a quantum stochastic tunneling optimization method. Journal of Computational Chemistry, 2004, 25, 858-864.	3.3	24
111	The concentration effect on the â€˜hydrophobicâ€™ and â€˜hydrophilicâ€™ behaviour around DMSO in dilute aqueous DMSO solutions. A computer simulation study. Journal of Molecular Liquids, 2004, 110, 147-153.	4.9	50
112	A new explicit hydration penalty score for ligandâ€“protein interactions. Chemical Physics Letters, 2004, 399, 271-275.	2.6	4
113	Expanded Interaction Fingerprint Method for Analyzing Ligand Binding Modes in Docking and Structure-Based Drug Design. Journal of Chemical Information and Computer Sciences, 2004, 44, 1942-1951.	2.8	69
114	Assessment of Multiple Binding Modes in Ligandâ^'Protein Docking. Journal of Medicinal Chemistry, 2004, 47, 3334-3337.	6.4	44
115	Molecular dynamics simulation of dilute aqueous DMSO solutions. A temperature-dependence study of the hydrophobic and hydrophilic behaviour around DMSO. Physical Chemistry Chemical Physics, 2004, 6, 94.	2.8	60
116	Recent Advances in the Understanding of Hydrophobic and Hydrophilic Effects: A Theoretical and Computer Simulation Perspective. , 2004, , 387-396.		2
117	A new method for estimating the importance of hydrogen-bonding groups in the binding site of a protein. Journal of Computer-Aided Molecular Design, 2003, 17, 401-414.	2.9	8
118	WaterScore: a novel method for distinguishing between bound and displaceable water molecules in the crystal structure of the binding site of protein-ligand complexes. Journal of Molecular Modeling, 2003, 9, 172-182.	1.8	130
119	A new quantum stochastic tunnelling optimisation method for proteinâ€“ligand docking. Chemical Physics Letters, 2003, 369, 257-263.	2.6	18
120	De novo ligand design with explicit water molecules: an application to bacterial neuraminidase. Journal of Computer-Aided Molecular Design, 2002, 16, 479-499.	2.9	35
121	Computer simulation of the structural effect of pressure on the hydrophobic hydration of methane. Molecular Physics, 1999, 96, 109-122.	1.7	55
122	Influence of Salt on Hydrophobic Effects:â€‰ A Molecular Dynamics Study Using the Modified Hydration-Shell Hydrogen-Bond Model. Journal of Physical Chemistry B, 1999, 103, 3774-3777.	2.6	27
123	Does salt increase the magnitude of the hydrophobic effect? A computer simulation study. Chemical Physics Letters, 1998, 296, 459-465.	2.6	33
124	Thermodynamics of the hydration of non-polar substances. Biophysical Chemistry, 1998, 70, 57-63.	2.8	16
125	Computer simulation of the effect of salt on the hydrophobic effect. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 3549-3559.	1.7	32
126	The aggregation of methane in aqueous solution. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 2263-2267.	1.7	36

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127	Hydrogen-bonding behaviour in the hydrophobic hydration of simple hydrocarbons in water. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 2547.	1.7	22
128	Computer simulation studies of the hydration and aggregation of simple hydrophobic molecules. Faraday Discussions, 1996, 103, 141.	3.2	32
129	Towards an understanding of the molecular basis of hydrophobicity. Journal of Computer-Aided Molecular Design, 1996, 10, 321-326.	2.9	7
130	Further evidence for a temperature-dependent hydrophobic interaction: the aggregation of ethane in aqueous solutions. Chemical Physics Letters, 1995, 234, 296-303.	2.6	35
131	Quantitative structure-activity relationships of competitive inhibitors of phosphoenolpyruvate carboxylase. Bioorganic and Medicinal Chemistry, 1995, 3, 217-225.	3.0	4