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	The Structure of Glycosaminoglycans and their Interactions with Proteins. Chemical Biology and Drug Design, 2008, 72, 455-482.	3.2	820
2	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
3	Ligandâ"Protein Docking with Water Molecules. Journal of Chemical Information and Modeling, 2008, 48, 397-408.	5.4	128
4	New anti-tuberculosis drugs in clinical trials with novel mechanisms of action. Drug Discovery Today, 2008, 13, 1090-1098.	6.4	121
5	Heparin/heparan sulphate-based drugs. Drug Discovery Today, 2010, 15, 1058-1069.	6.4	98
6	Prediction of heparin binding sites in bone morphogenetic proteins (BMPs). Biochimica Et Biophysica Acta - Proteins and Proteomics, 2012, 1824, 1374-1381.	2.3	80
7	Ligandâ"Protein Cross-Docking with Water Molecules. Journal of Chemical Information and Modeling, 2010, 50, 415-421.	5.4	77
8	A molecular mechanism of solvent cryoprotection in aqueous DMSO solutions. Physical Chemistry Chemical Physics, 2011, 13, 3839.	2.8	77
9	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
10	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
11	Waking up dormant tumor suppressor genes with zinc fingers, TALEs and the CRISPR/dCas9 system. Oncotarget, 2016, 7, 60535-60554.	1.8	61
12	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
13	Inhibitors of Xanthine Oxidase: Scaffold Diversity and Structureâ€Based Drug Design. ChemMedChem, 2019, 14, 714-743.	3.2	60
14	Free energy calculations of glycosaminoglycanâ€"protein interactions. Glycobiology, 2009, 19, 1103-1115.	2.5	56
15	Computer simulation of the structural effect of pressure on the hydrophobic hydration of methane. Molecular Physics, 1999, 96, 109-122.	1.7	55
16	New arylated benzo[h]quinolines induce anti-cancer activity by oxidative stress-mediated DNA damage. Scientific Reports, 2016, 6, 38128.	3.3	54
17	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
18	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

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19	New Anti-Tuberculosis Drugs with Novel Mechanisms of Action. Current Medicinal Chemistry, 2008, 15, 1956-1967.	2.4	49
20	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
21	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
22	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
23	A Comparative Structural Bioinformatics Analysis of the Insulin Receptor Family Ectodomain Based on Phylogenetic Information. PLoS ONE, 2008, 3, e3667.	2.5	45
24	Assessment of Multiple Binding Modes in Ligandâ^'Protein Docking. Journal of Medicinal Chemistry, 2004, 47, 3334-3337.	6.4	44
25	Computational analyses of the catalytic and heparin-binding sites and their interactions with glycosaminoglycans in glycoside hydrolase family 79 endo-l²-d-glucuronidase (heparanase). Glycobiology, 2012, 22, 35-55.	2.5	44
26	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
27	The emerging application of ultrasound in lactose crystallisation. Trends in Food Science and Technology, 2014, 38, 47-59.	15.1	43
28	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
29	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
30	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
31	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
32	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
33	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
34	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
35	Molecular Dynamics Simulation of Small Molecules Interacting with Biological Membranes. ChemPhysChem, 2020, 21, 1486-1514.	2.1	37
36	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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37	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
38	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
39	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
40	Does salt increase the magnitude of the hydrophobic effect? A computer simulation study. Chemical Physics Letters, 1998, 296, 459-465.	2.6	33
41	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
42	Computer simulation studies of the hydration and aggregation of simple hydrophobic molecules. Faraday Discussions, 1996, 103, 141.	3.2	32
43	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
44	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
45	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
46	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
47	Platelet Endothelial Cell Adhesion Molecule 1 (PECAM-1) and Its Interactions with Glycosaminoglycans: 2. Biochemical Analyses. Biochemistry, 2008, 47, 4863-4875.	2.5	29
48	Molecular modeling of hydration in drug design. Current Opinion in Drug Discovery & Development, 2007, 10, 275-80.	1.9	29
49	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
50	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
51	Molecular dynamics simulations of mixed DOPCâ€“Î²-sitosterol bilayers and their interactions with DMSO. Soft Matter, 2013, 9, 2920.	2.7	27
52	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
53	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
54	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

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55	Electrochemistry of proteins at the interface between two immiscible electrolyte solutions. Current Opinion in Electrochemistry, 2018, 12, 27-32.	4.8	26
56	Ligand-protein docking using a quantum stochastic tunneling optimization method. Journal of Computational Chemistry, 2004, 25, 858-864.	3.3	24
57	Development and application of site mapping methods for the design of glycosaminoglycans. Glycobiology, 2014, 24, 840-851.	2.5	24
58	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
59	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
60	Molecular modelling prediction of ligand binding site flexibility. Journal of Computer-Aided Molecular Design, 2004, 18, 235-250.	2.9	22
61	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
62	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
63	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
64	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
65	Molecular Mechanism of the Synergistic Effects of Vitrification Solutions on the Stability of Phospholipid Bilayers. Biophysical Journal, 2014, 106, 2617-2624.	0.5	20
66	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
67	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
68	A new quantum stochastic tunnelling optimisation method for proteinâ€“ligand docking. Chemical Physics Letters, 2003, 369, 257-263.	2.6	18
69	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
70	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
71	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
72	Thermodynamics of the hydration of non-polar substances. Biophysical Chemistry, 1998, 70, 57-63.	2.8	16

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73	Adsorption and Unfolding of Lysozyme at a Polarized Aqueousâ€“Organic Liquid Interface. Journal of Physical Chemistry B, 2016, 120, 3100-3112.	2.6	16
74	Influence of Bilayer Size and Number in Multi-Bilayer DOPC Simulations at Full and Low Hydration. Langmuir, 2019, 35, 2399-2411.	3.5	16
75	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
76	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
77	Monitoring of oxidative status in three native Australian species during cold acclimation and cryopreservation. Plant Cell Reports, 2017, 36, 1903-1916.	5.6	15
78	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
79	The Biological and Biophysical Properties of the Spider Peptide Gomesin. Molecules, 2018, 23, 1733.	3.8	15
80	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
81	Enhanced Transdermal Peptide Delivery and Stability by Lipid Conjugation: Epidermal Permeation, Stereoselectivity and Mechanistic Insights. Pharmaceutical Research, 2014, 31, 3304-3312.	3.5	13
82	Assignment of aromaticity of the classic heterobenzenes by three aromatic criteria. Computational and Theoretical Chemistry, 2014, 1046, 20-24.	2.5	12
83	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
84	Current methods for the prediction of Tâ€cell epitopes. Peptide Science, 2018, 110, e24046.	1.8	12
85	Molecular dynamics simulations of a DMSO/water mixture using the AMBER force field. Journal of Molecular Modeling, 2018, 24, 174.	1.8	11
86	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
87	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
88	Optimization of proteinâ€“protein docking for predicting Fcâ€“protein interactions. Journal of Molecular Recognition, 2016, 29, 555-568.	2.1	10
89	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
90	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

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91	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
92	Secondary Structural Changes in Proteins as a Result of Electroadsorption at Aqueousâ€“Organogel Interfaces. Langmuir, 2019, 35, 5821-5829.	3.5	9
93	Atomistic molecular dynamics simulations of bioactive engrailed 1 interference peptides (EN1-iPeps). Oncotarget, 2018, 9, 22383-22397.	1.8	9
94	Review: The case for studying mitochondrial function during plant cryopreservation. Plant Science, 2022, 315, 111134.	3.6	9
95	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
96	Cryopreservation of Lomandra sonderi (Asparagaceae) shoot tips using droplet-vitrification. Cryo-Letters, 2012, 33, 259-70.	0.3	8
97	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
98	Towards an understanding of the molecular basis of hydrophobicity. Journal of Computer-Aided Molecular Design, 1996, 10, 321-326.	2.9	7
99	Optimization of surface plasmon resonance experiments: Case of high mobility group box 1 (HMGB1) interactions. Analytical Biochemistry, 2016, 499, 43-50.	2.4	7
100	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
101	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
102	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
103	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
104	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
105	Myrtaceae in Australia: Use of Cryobiotechnologies for the Conservation of a Significant Plant Family under Threat. Plants, 2022, 11, 1017.	3.5	6
106	Comparative Analysis of the Surface Interaction Properties of the Binding Sites of CDK2, CDK4, and ERK2. ChemMedChem, 2006, 1, 366-375.	3.2	5
107	Hydrogen Bond Disruption in DNA Base Pairs from ¹⁴C Transmutation. Journal of Physical Chemistry B, 2014, 118, 10430-10435.	2.6	5
108	Structure and intermolecular interactions in spheroidal high-density lipoprotein subpopulations. Journal of Structural Biology: X, 2021, 5, 100042.	1.3	5

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109	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
110	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
111	Characterization of sequence and structural features of the Candida krusei enolase. In Silico Biology, 2008, 8, 449-60.	0.9	5
112	Quantitative structure-activity relationships of competitive inhibitors of phosphoenolpyruvate carboxylase. Bioorganic and Medicinal Chemistry, 1995, 3, 217-225.	3.0	4
113	A new explicit hydration penalty score for ligandâ€“protein interactions. Chemical Physics Letters, 2004, 399, 271-275.	2.6	4
114	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
115	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
116	Pharmacological and structure-activity relationship studies of oleoyl-lysophosphatidylinositol synthetic mimetics. Pharmacological Research, 2021, 172, 105822.	7.1	4
117	Redefining the Molecular Interplay between Dimethyl Sulfoxide, Lipid Bilayers, and Dehydration. Journal of Physical Chemistry B, 2022, 126, 2513-2529.	2.6	4
118	The molecular binding interactions of inhibitors and activators of phosphoenolpyruvate carboxylase. Computational and Theoretical Chemistry, 2005, 755, 151-159.	1.5	3
119	Computational Methods for the Prediction of the Structure and Interactions of Coiled-Coil Peptides. Current Bioinformatics, 2008, 3, 149-161.	1.5	3
120	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
121	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
122	Seed storage behaviour of tropical members of the aquatic basal angiosperm genus Nymphaea L. (Nymphaeaceae). , 2019, 7, coz021.		3
123	Recent Advances in the Understanding of Hydrophobic and Hydrophilic Effects: A Theoretical and Computer Simulation Perspective. , 2004, , 387-396.		2
124	Novel Amylin Analogues Reduce Amyloid-Î²2 Cross-Seeding Aggregation and Neurotoxicity. Journal of Alzheimer's Disease, 2022, , 1-18.	2.6	2
125	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
126	Definition of the Minimal Contents for the Molecular Simulation of the Yeast Cytoplasm. Frontiers in Molecular Biosciences, 2019, 6, 97.	3.5	1

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127	Assessing Plant Metabolic Rates During Cryopreservation. Cryobiology, 2021, 103, 169.	0.7	1
128	Expanded Interaction Fingerprint Method for Analyzing Ligand Binding Modes in Docking and Structure-Based Drug Design.. ChemInform, 2005, 36, no.	0.0	0
129	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
130	Developing Drugs from Sugars. , 2012, , 259-296.		0
131	Cryostorage of Macadamia Nut Embryonic Axes Using Droplet-Vitrification. Cryobiology, 2021, 103, 163.	0.7	0