Hugh M O'neill

List of Publications by Year
in descending order

135 papers	5,616 citations	87723 38 h-index	95083 68 g-index
140 all docs	140 docs citations	140 times ranked	7466 citing authors

#	Article	IF	Citations
1	Structural plasticity of SARS-CoV-2 3CL Mpro active site cavity revealed by room temperature X-ray crystallography. Nature Communications, 2020, 11, 3202.	5.8	334
2	Biomimetic synthesis of calcium-deficient hydroxyapatite in a natural hydrogel. Biomaterials, 2006, 27, 4661-4670.	5.7	318
3	Palladium-bacterial cellulose membranes for fuel cells. Biosensors and Bioelectronics, 2003, 18, 917-923.	5.3	209
4	Common processes drive the thermochemical pretreatment of lignocellulosic biomass. Green Chemistry, 2014, 16, 63-68.	4.6	198
5	Comparative Structural and Computational Analysis Supports Eighteen Cellulose Synthases in the Plant Cellulose Synthesis Complex. Scientific Reports, 2016, 6, 28696.	1.6	174
6	High photo-electrochemical activity of thylakoidâ€“carbon nanotube composites for photosynthetic energy conversion. Energy and Environmental Science, 2013, 6, 1891.	15.6	173
7	Self-organized photosynthetic nanoparticle for cell-free hydrogen production. Nature Nanotechnology, 2010, 5, 73-79.	15.6	171
8	Breakdown of Cell Wall Nanostructure in Dilute Acid Pretreated Biomass. Biomacromolecules, 2010, 11, 2329-2335.	2.6	143
9	Dynamics of Protein and its Hydration Water: Neutron Scattering Studies on Fully Deuterated GFP. Biophysical Journal, 2012, 103, 1566-1575.	0.2	121
10	Effect of lignin content on changes occurring in poplar cellulose ultrastructure during dilute acid pretreatment. Biotechnology for Biofuels, 2014, 7, 150.	6.2	113
11	Mechanical formation of micro- and nano-plastic materials for environmental studies in agricultural ecosystems. Science of the Total Environment, 2019, 685, 1097-1106.	3.9	108
12	Malleability of the SARS-CoV-2 3CL Mpro Active-Site Cavity Facilitates Binding of Clinical Antivirals. Structure, 2020, 28, 1313-1320.e3.	1.6	108
13	A Structural Study of CESA1 Catalytic Domain of Arabidopsis Cellulose Synthesis Complex: Evidence for CESA Trimers. Plant Physiology, 2016, 170, 123-135.	2.3	104
14	Unusual zwitterionic catalytic site of SARSâ€“CoV-2 main protease revealed by neutron crystallography. Journal of Biological Chemistry, 2020, 295, 17365-17373.	1.6	97
15	A microbial fuel cell operating at low pH using the acidophile Acidiphilium cryptum. Biotechnology Letters, 2008, 30, 1367-1372.	1.1	95
16	Organization and Flexibility of Cyanobacterial Thylakoid Membranes Examined by Neutron Scattering. Journal of Biological Chemistry, 2013, 288, 3632-3640.	1.6	89
17	Generation of the configurational ensemble of an intrinsically disordered protein from unbiased molecular dynamics simulation. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 20446-20452.	3.3	88
18	The Shape of Native Plant Cellulose Microfibrils. Scientific Reports, 2018, 8, 13983.	1.6	86

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19	The Bio-SANS instrument at the High Flux Isotope Reactor of Oak Ridge National Laboratory. Journal of Applied Crystallography, 2014, 47, 1238-1246.	1.9	83
20	Modification of the nanostructure of lignocellulose cell walls via a non-enzymatic lignocellulose deconstruction system in brown rot wood-decay fungi. Biotechnology for Biofuels, 2017, 10, 179.	6.2	83
21	Dynamics of water bound to crystalline cellulose. Scientific Reports, 2017, 7, 11840.	1.6	82
22	Gradients in Wall Mechanics and Polysaccharides along Growing Inflorescence Stems. Plant Physiology, 2017, 175, 1593-1607.	2.3	82
23	Characterization of the Influence of the Ionic Liquid 1-Butyl-3-methylimidazolium Chloride on the Structure and Thermal Stability of Green Fluorescent Protein. Journal of Physical Chemistry B, 2010, 114, 13866-13871.	1.2	75
24	Self-similar multiscale structure of lignin revealed by neutron scattering and molecular dynamics simulation. Physical Review E, 2011, 83, 061911.	0.8	72
25	Description of Hydration Water in Protein (Green Fluorescent Protein) Solution. Journal of the American Chemical Society, 2017, 139, 1098-1105.	6.6	68
26	Secondary structure and rigidity in model proteins. Soft Matter, 2013, 9, 9548.	1.2	65
27	Effect of antimicrobial peptide on the dynamics of phosphocholine membrane: role of cholesterol and physical state of bilayer. Soft Matter, 2015, 11, 6755-6767.	1.2	62
28	Nanoscopic Dynamics of Phospholipid in Unilamellar Vesicles: Effect of Gel to Fluid Phase Transition. Journal of Physical Chemistry B, 2015, 119, 4460-4470.	1.2	58
29	Structural coarsening of aspen wood by hydrothermal pretreatment monitored by small- and wide-angle scattering of X-rays and neutrons on oriented specimens. Cellulose, 2014, 21, 1015-1024.	2.4	56
30	Enhanced Photocatalytic Hydrogen Evolution by Covalent Attachment of Plastocyanin to Photosystem I. Nano Letters, 2004, 4, 1815-1819.	4.5	55
31	Room-temperature X-ray crystallography reveals the oxidation and reactivity of cysteine residues in SARS-CoV-2 3CL M^{pro}: insights into enzyme mechanism and drug design. IUCrJ, 2020, 7, 1028-1035.	1.0	49
32	Elastic and Conformational Softness of a Globular Protein. Physical Review Letters, 2013, 110, 028104.	2.9	47
33	Comparison of changes in cellulose ultrastructure during different pretreatments of poplar. Cellulose, 2014, 21, 2419-2431.	2.4	47
34	Neutron scattering in the biological sciences: progress and prospects. Acta Crystallographica Section D: Structural Biology, 2018, 74, 1129-1168.	1.1	47
35	The effect of deuteration on the structure of bacterial cellulose. Carbohydrate Research, 2013, 374, 82-88.	1.1	45
36	Hydration Control of the Mechanical and Dynamical Properties of Cellulose. Biomacromolecules, 2014, 15, 4152-4159.	2.6	44

#	Article	IF	Citations
37	Direct Determination of Hydroxymethyl Conformations of Plant Cell Wall Cellulose Using ¹H Polarization Transfer Solid-State NMR. Biomacromolecules, 2018, 19, 1485-1497.	2.6	44
38	Revealing the Dynamics of Thylakoid Membranes in Living Cyanobacterial Cells. Scientific Reports, 2016, 6, 19627.	1.6	43
39	A resorbable calcium-deficient hydroxyapatite hydrogel composite for osseous regeneration. Cellulose, 2009, 16, 887-898.	2.4	39
40	Transient and stabilized complexes of Nsp7, Nsp8, and Nsp12 in SARS-CoV-2 replication. Biophysical Journal, 2021, 120, 3152-3165.	0.2	39
41	Cellulose-lignin composite fibres as precursors for carbon fibres. Part 1 â€“ Manufacturing and properties of precursor fibres. Carbohydrate Polymers, 2021, 252, 117133.	5.1	38
42	Morphological changes in the cellulose and lignin components of biomass occur at different stages during steam pretreatment. Cellulose, 2014, 21, 873-878.	2.4	37
43	Mean-squared atomic displacements in hydrated lysozyme, native and denatured. Journal of Biological Physics, 2010, 36, 291-297.	0.7	36
44	Protein Localization in Silica Nanospheres Derived via Biomimetic Mineralization. Advanced Functional Materials, 2010, 20, 3031-3038.	7.8	36
45	Bacterial Cellulose Ionogels as Chemosensory Supports. ACS Applied Materials & Interfaces, 2017, 9, 38042-38051.	4.0	35
46	Characterization of Solâ^'Gel-Encapsulated Proteins Using Small-Angle Neutron Scattering. ACS Applied Materials & Interfaces, 2009, 1, 2262-2268.	4.0	34
47	Insight into the Structure of Light-Harvesting Complex II and Its Stabilization in Detergent Solution. Journal of Physical Chemistry B, 2009, 113, 16377-16383.	1.2	34
48	Distinguishing Surface versus Bulk Hydroxyl Groups of Cellulose Nanocrystals Using Vibrational Sum Frequency Generation Spectroscopy. Journal of Physical Chemistry Letters, 2018, 9, 70-75.	2.1	32
49	Small Angle Neutron Scattering Shows Nanoscale PMMA Distribution in Transparent Wood Biocomposites. Nano Letters, 2021, 21, 2883-2890.	4.5	32
50	Arabinose substitution effect on xylan rigidity and self-aggregation. Cellulose, 2019, 26, 2267-2278.	2.4	31
51	Controlled incorporation of deuterium into bacterial cellulose. Cellulose, 2014, 21, 927-936.	2.4	30
52	Impact of hydration and temperature history on the structure and dynamics of lignin. Green Chemistry, 2018, 20, 1602-1611.	4.6	30
53	Nanostructural Analysis of Enzymatic and Non-enzymatic Brown Rot Fungal Deconstruction of the Lignocellulose Cell Wallâ€. Frontiers in Microbiology, 2020, 11, 1389.	1.5	30
54	SANS study of cellulose extracted from switchgrass. Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 1189-1193.	2.5	29

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55	Small Angle Neutron Scattering Reveals pH-dependent Conformational Changes in Trichoderma reesei Cellobiohydrolase I. Journal of Biological Chemistry, 2011, 286, 32801-32809.	1.6	29
56	Probing the consequences of antenna modification in cyanobacteria. Photosynthesis Research, 2013, 118, 17-24.	1.6	29
57	In Vivo Protein Dynamics on the Nanometer Length Scale and Nanosecond Time Scale. Journal of Physical Chemistry Letters, 2017, 8, 1899-1904.	2.1	29
58	Understanding Multiscale Structural Changes During Dilute Acid Pretreatment of Switchgrass and Poplar. ACS Sustainable Chemistry and Engineering, 2017, 5, 426-435.	3.2	29
59	Deconstruction of biomass enabled by local demixing of cosolvents at cellulose and lignin surfaces. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 16776-16781.	3.3	29
60	Interaction of Zinc Oxide Nanoparticles with Water: Implications for Catalytic Activity. ACS Applied Nano Materials, 2019, 2, 4257-4266.	2.4	28
61	Ammonia-salt solvent promotes cellulosic biomass deconstruction under ambient pretreatment conditions to enable rapid soluble sugar production at ultra-low enzyme loadings. Green Chemistry, 2020, 22, 204-218.	4.6	28
62	Neutron Scattering Studies of the Interplay of Amyloid Î² Peptide(1â€“40) and An Anionic Lipid 1,2-dimyristoyl-sn-glycero-3-phosphoglycerol. Scientific Reports, 2016, 6, 30983.	1.6	27
63	Dynamical Transition of Collective Motions in Dry Proteins. Physical Review Letters, 2017, 119, 048101.	2.9	27
64	Cloning and Analysis of the Genes for a Novel Electron-transferring Flavoprotein from Megasphaera elsdenii. Journal of Biological Chemistry, 1998, 273, 21015-21024.	1.6	26
65	The application and use of chemical space mapping to interpret crystallization screening results. Acta Crystallographica Section D: Biological Crystallography, 2008, 64, 1240-1249.	2.5	26
66	Role of methyl groups in dynamics and evolution of biomolecules. Journal of Biological Physics, 2012, 38, 497-505.	0.7	26
67	Tension wood structure and morphology conducive for better enzymatic digestion. Biotechnology for Biofuels, 2018, 11, 44.	6.2	26
68	Spectroscopy and Photochemistry of Spinach Photosystem I Entrapped and Stabilized in a Hybrid Organosilicate Glass. Chemistry of Materials, 2005, 17, 2654-2661.	3.2	25
69	Biochemical and structural analyses reveal that the tumor suppressor neurofibromin (NF1) forms a high-affinity dimer. Journal of Biological Chemistry, 2020, 295, 1105-1119.	1.6	25
70	Biochemical and structural analyses reveal that the tumor suppressor neurofibromin (NF1) forms a high-affinity dimer. Journal of Biological Chemistry, 2020, 295, 1105-1119.	1.6	25
71	Apparent Decoupling of the Dynamics of a Protein from the Dynamics of its Aqueous Solvent. Journal of Physical Chemistry Letters, 2012, 3, 380-385.	2.1	24
72	Coherent Neutron Scattering and Collective Dynamics in the Protein, GFP. Biophysical Journal, 2013, 105, 2182-2187.	0.2	24

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73	Protein extraction into the bicontinuous microemulsion phase of a Water/SDS/pentanol/dodecane winsor-III system: Effect on nanostructure and protein conformation. Colloids and Surfaces B: Biointerfaces, 2017, 160, 144-153.	2.5	24
74	Analysis of the solution structure of Thermosynechococcus elongatus photosystem I in n-dodecyl-Î²-d-maltoside using small-angle neutron scattering and molecular dynamics simulation. Archives of Biochemistry and Biophysics, 2014, 550-551, 50-57.	1.4	23
75	Dependence of Sum Frequency Generation (SFG) Spectral Features on the Mesoscale Arrangement of SFG-Active Crystalline Domains Interspersed in SFG-Inactive Matrix: A Case Study with Cellulose in Uniaxially Aligned Control Samples and Alkali-Treated Secondary Cell Walls of Plants. Journal of Physical Chemistry C, 2017, 121, 10249-10257.	1.5	22
76	Nanoscopic dynamics of bicontinous microemulsions: effect of membrane associated protein. Soft Matter, 2017, 13, 4871-4880.	1.2	22
77	Hemicelluloseâ€“Cellulose Composites Reveal Differences in Cellulose Organization after Dilute Acid Pretreatment. Biomacromolecules, 2019, 20, 893-903.	2.6	21
78	Excited-State Dynamics of Water-Soluble Polythiophene Derivatives: Temperature and Side-Chain Length Effects. Journal of Physical Chemistry B, 2012, 116, 14451-14460.	1.2	20
79	Deuterium incorporation in biomass cell wall components by NMR analysis. Analyst, The, 2012, 137, 1090.	1.7	19
80	Physical Insight into Switchgrass Dissolution in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate. ACS Sustainable Chemistry and Engineering, 2014, 2, 1264-1269.	3.2	19
81	Small-Angle X-ray Scattering Study of Photosystem Iâ^'Detergent Complexes:Â Implications for Membrane Protein Crystallization. Journal of Physical Chemistry B, 2007, 111, 4211-4219.	1.2	18
82	Temperature Dependence of Logarithmic-like Relaxational Dynamics of Hydrated tRNA. Journal of Physical Chemistry Letters, 2013, 4, 936-942.	2.1	18
83	Effect of D2O on Growth Properties and Chemical Structure of Annual Ryegrass (Lolium) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 5	2.4	18
84	Effect of Protein Incorporation on the Nanostructure of the Bicontinuous Microemulsion Phase of Winsor-III Systems: A Small-Angle Neutron Scattering Study. Langmuir, 2015, 31, 1901-1910.	1.6	18
85	Small-angle neutron scattering reveals the assembly of alpha-synuclein in lipid membranes. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2015, 1854, 1881-1889.	1.1	18
86	Effects of soil particles and convective transport on dispersion and aggregation of nanoplastics via small-angle neutron scattering (SANS) and ultra SANS (USANS). PLoS ONE, 2020, 15, e0235893.	1.1	18
87	Cellulose synthase interactive1- and microtubule-dependent cell wall architecture is required for acid growth in Arabidopsis hypocotyls. Journal of Experimental Botany, 2020, 71, 2982-2994.	2.4	18
88	Title is missing!. Biotechnology Letters, 2002, 24, 783-790.	1.1	17
89	Laser-induced breakdown spectroscopy used to detect palladium and silver metal dispersed in bacterial cellulose membranes. Applied Optics, 2003, 42, 6174.	2.1	17
90	Neutron Technologies for Bioenergy Research. Industrial Biotechnology, 2012, 8, 209-216.	0.5	17

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91	Folding propensity of intrinsically disordered proteins by osmotic stress. Molecular BioSystems, 2016, 12, 3695-3701.	2.9	17
92	2Hâ€“13C correlation solid-state NMR for investigating dynamics and water accessibilities of proteins and carbohydrates. Journal of Biomolecular NMR, 2017, 68, 257-270.	1.6	17
93	Combined Small-Angle Neutron Scattering, Diffusion NMR, and Molecular Dynamics Study of a Eutectogel: Illuminating the Dynamical Behavior of Glyceline Confined in Bacterial Cellulose Gels. Journal of Physical Chemistry B, 2020, 124, 7647-7658.	1.2	17
94	Supramolecular assembly of biohybrid photoconversion systems. Energy and Environmental Science, 2011, 4, 181-188.	15.6	16
95	Production of deuterated switchgrass by hydroponic cultivation. Planta, 2015, 242, 215-222.	1.6	15
96	Enhanced Dynamics of Hydrated tRNA on Nanodiamond Surfaces: A Combined Neutron Scattering and MD Simulation Study. Journal of Physical Chemistry B, 2016, 120, 10059-10068.	1.2	14
97	Conformational Dynamics in the Interaction of SARS-CoV-2 Papain-like Protease with Human Interferon-Stimulated Gene 15 Protein. Journal of Physical Chemistry Letters, 2021, 12, 5608-5615.	2.1	14
98	Bicontinuous microemulsions as a biomembrane mimetic system for melittin. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 624-632.	1.4	12
99	New Technologies are Needed to Improve the Recycling and Upcycling of Waste Plastics. ChemSusChem, 2021, 14, 3982-3984.	3.6	12
100	Solâ€“gel entrapped light harvesting antennas: immobilization and stabilization of chlorosomes for energy harvesting. Journal of Materials Chemistry, 2012, 22, 22582.	6.7	11
101	Production of Bacterial Cellulose with Controlled Deuteriumâ€“Hydrogen Substitution for Neutron Scattering Studies. Methods in Enzymology, 2015, 565, 123-146.	0.4	11
102	Incorporation of Melittin Enhances Interfacial Fluidity of Bicontinuous Microemulsions. Journal of Physical Chemistry C, 2019, 123, 11197-11206.	1.5	11
103	Influence of Chemically Disrupted Photosynthesis on Cyanobacterial Thylakoid Dynamics in Synechocystis sp. PCC 6803. Scientific Reports, 2019, 9, 5711.	1.6	10
104	Chemical and Morphological Structure of Transgenic Switchgrass Organosolv Lignin Extracted by Ethanol, Tetrahydrofuran, and Î³-Valerolactone Pretreatments. ACS Sustainable Chemistry and Engineering, 2022, 10, 9041-9052.	3.2	10
105	Localized entrapment of green fluorescent protein within nanostructured polymer films. Soft Matter, 2011, 7, 11453.	1.2	9
106	Biosynthesis and characterization of deuterated chitosan in filamentous fungus and yeast. Carbohydrate Polymers, 2021, 257, 117637.	5.1	8
107	Direct Experimental Characterization of Contributions from Self-Motion of Hydrogen and from Interatomic Motion of Heavy Atoms to Protein Anharmonicity. Journal of Physical Chemistry B, 2018, 122, 9956-9961.	1.2	7
108	Structural Insights into Low and High Recalcitrance Natural Poplar Variants Using Neutron and X-ray Scattering. ACS Sustainable Chemistry and Engineering, 2020, 8, 13838-13849.	3.2	7

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109	Structural Reorganization of Noncellulosic Polymers Observed In Situ during Dilute Acid Pretreatment by Small-Angle Neutron Scattering. ACS Sustainable Chemistry and Engineering, 2022, 10, 314-322.	3.2	7
110	Engineered zinc oxide-based nanotherapeutics boost systemic antibacterial efficacy against phloem-restricted diseases. Environmental Science: Nano, 2022, 9, 2869-2886.	2.2	7
111	Metabolic Prosthesis for Oxygenation of Ischemic Tissue. IEEE Transactions on Biomedical Engineering, 2009, 56, 528-531.	2.5	5
112	Observation of a structural gradient in Winsor-III microemulsion systems. Soft Matter, 2018, 14, 5270-5276.	1.2	5
113	Identifying Stable Fragments of Arabidopsis thaliana Cellulose Synthase Subunit 3 by Yeast Display. Biotechnology Journal, 2019, 14, e1800353.	1.8	5
114	Effect of Surface Attachment on Synthesis of Bacterial Cellulose. Applied Biochemistry and Biotechnology, 2005, 121, 0439-0450.	1.4	4
115	Characterization of Morphology and Active Agent Mobility within Hybrid Silica Solâ€“Gel Composites. Journal of Physical Chemistry C, 2012, 116, 13972-13979.	1.5	4
116	Fed-batch production of deuterated protein in Escherichia coli for neutron scattering experimentation. Methods in Enzymology, 2021, 659, 219-240.	0.4	4
117	Cloning of Electron-Transferring Flavoprotein from Megasphaera elsdenii. Biochemical Society Transactions, 1995, 23, 379S-379S.	1.6	3
118	Reentrant condensation of lysozyme: Implications for studying dynamics of lysozyme in aqueous solutions of lithium chloride. Biopolymers, 2014, 101, 624-629.	1.2	3
119	Collective Excitations in Protein as a Measure of Balance Between its Softness and Rigidity. Journal of Physical Chemistry B, 2017, 121, 923-930.	1.2	3
120	Multi-Purpose Cellulosic Ionogels. ACS Symposium Series, 2017, , 143-155.	0.5	3
121	Allelopathic effects of exogenous phenylalanine: a comparison of four monocot species. Planta, 2017, 246, 673-685.	1.6	3
122	Production of deuterated biomass by cultivation of Lemna minor (duckweed) in D2O. Planta, 2019, 249, 1465-1475.	1.6	3
123	Publisherâ€™s Note: Self-similar multiscale structure of lignin revealed by neutron scattering and molecular dynamics simulation [Phys. Rev. E83, 061911 (2011)]. Physical Review E, 2011, 84, .	0.8	2
124	Development of Bacterial Cellulose Nanocomposites. Materials Research Society Symposia Proceedings, 2011, 1312, 1.	0.1	2
125	Crystallization and preliminary X-ray diffraction analysis ofHypocrea jecorinaCel7A in two new crystal forms. Acta Crystallographica Section F, Structural Biology Communications, 2014, 70, 773-776.	0.4	2
126	Structural Studies of Deuterium-Labeled Switchgrass Biomass. ACS Symposium Series, 2019, , 17-32.	0.5	2

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127	Incorporation of Membrane Proteins Into Bicontinuous Microemulsions Through Winsorâ€III Systemâ€Based Extraction. Journal of Surfactants and Detergents, 2021, 24, 649-660.	1.0	2
128	Melittin exerts opposing effects on short- and long-range dynamics in bicontinuous microemulsions. Journal of Colloid and Interface Science, 2021, 590, 94-102.	5.0	2
129	Investigation of detergent effects on the solution structure of spinach Light Harvesting Complex II. Journal of Physics: Conference Series, 2010, 251, 012041.	0.3	1
130	Oligomerization state and pigment binding strength of the peridininâ€Chlaâ€protein. FEBS Letters, 2015, 589, 2713-2719.	1.3	1
131	Electron-transferring flavoprotein from Megasphaera elsdenii; gene organisation and structural information. Biochemical Society Transactions, 1998, 26, S214-S214.	1.6	0
132	The Nicotinamide Cofactors: Applications in Biotechnology. ACS Symposium Series, 2001, , 103-130.	0.5	0
133	Publisherâ€™s Note: Elastic and Conformational Softness of a Globular Protein [Phys. Rev. Lett.110, 028104 (2013)]. Physical Review Letters, 2013, 110, .	2.9	0
134	Investigating the structural flexibility of intrinsically disordered proteins. FASEB Journal, 2010, 24, 684.8.	0.2	0
135	Effect of Surface Attachment on Synthesis of Bacterial Cellulose. , 2005, , 439-450.		0