Mary Jo Ondrechen

List of Publications by Year
in descending order

110 papers	2,860 citations	172457 29 h-index	182427 51 g-index
115 all docs	115 docs citations	115 times ranked	1923 citing authors

#	Article	IF	Citations
1	Reintegrating Biology Through the Nexus of Energy, Information, and Matter. Integrative and Comparative Biology, 2022, 61, 2082-2094.	2.0	3
2	Best Practices to Diversify Chemistry Faculty. Journal of Chemical Education, 2022, 99, 435-443.	2.3	2
3	â€œHow Do We Do This at a Distance?!â€•A Descriptive Study of Remote Undergraduate Research Programs during COVID-19. CBE Life Sciences Education, 2022, 21, ar1.	2.3	17
4	Synthesis and Characterization of 5-(2-Fluoro-4-[¹¹C]methoxyphenyl)-2,2-dimethyl-3,4-dihydro-2H-pyrano[2,3-b]pyridine-7-carboxamide as a PET Imaging Ligand for Metabotropic Glutamate Receptor 2. Journal of Medicinal Chemistry, 2022, 65, 2593-2609.	6.4	2
5	Functional Characterization of Structural Genomics Proteins in the Crotonase Superfamily. ACS Chemical Biology, 2022, 17, 395-403.	3.4	6
6	Computed chemical properties for predicting protein function. Biophysical Journal, 2022, 121, 132a.	0.5	0
7	Electrostatic fingerprints of catalytically active amino acids in enzymes. Protein Science, 2022, 31, e4291.	7.6	3
8	Stereoselective Synthesis of Î²-Glycinamide Ribonucleotide. Molecules, 2022, 27, 2528.	3.8	0
9	Electrostatic Fingerprints of Catalytically Active Amino Acids in Enzymes. FASEB Journal, 2022, 36, .	0.5	0
10	Enzyme active sites: Identification and prediction of function using computational chemistry. Current Opinion in Structural Biology, 2022, 74, 102384.	5.7	3
11	Design, Synthesis, and Characterization of [¹⁸F]mG2P026 as a High-Contrast PET Imaging Ligand for Metabotropic Glutamate Receptor 2. Journal of Medicinal Chemistry, 2022, 65, 9939-9954.	6.4	3
12	Amino acid interactions that facilitate enzyme catalysis. Journal of Chemical Physics, 2021, 154, 195101.	3.0	8
13	Identification, Characterization and Drug Discovery for Novel Target Sites for SARSâ€CoVâ€2 Proteins. FASEB Journal, 2021, 35, .	0.5	0
14	Analysis of electrostatic coupling throughout the laboratory evolution of a designed retroaldolase. Protein Science, 2021, 30, 1617-1627.	7.6	5
15	Adapting Undergraduate Research to Remote Work to Increase Engagement. The Biophysicist, 2021, 2, 28-32.	0.3	2
16	Design, Synthesis, and Characterization of Benzimidazole Derivatives as Positron Emission Tomography Imaging Ligands for Metabotropic Glutamate Receptor 2. Journal of Medicinal Chemistry, 2020, 63, 12060-12072.	6.4	9
17	Probing remote residues important for catalysis in Escherichia coli ornithine transcarbamoylase. PLoS ONE, 2020, 15, e0228487.	2.5	4
18	Synthesis of benzoylbenzamide derivatives of 17Î±-E-vinyl estradiol and evaluation as ligands for the estrogen receptor-Î± ligand binding domain. Steroids, 2019, 144, 15-20.	1.8	2

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19	Tri-arginine exosite patch of caspase-6 recruits substrates for hydrolysis. Journal of Biological Chemistry, 2019, 294, 71-88.	3.4	21
20	Thinking Outside the Informatics Box: Computed Chemical Properties for Protein Function Annotation. FASEB Journal, 2019, 33, 473.5.	0.5	0
21	In Vitro and in Vivo Evaluation of ¹¹C-Labeled Azetidinecarboxylates for Imaging Monoacylglycerol Lipase by PET Imaging Studies. Journal of Medicinal Chemistry, 2018, 61, 2278-2291.	6.4	41
22	Functional classification of protein structures by local structure matching in graph representation. Protein Science, 2018, 27, 1125-1135.	7.6	8
23	Prediction of Active Site and Distal Residues in E. coli DNA Polymerase III alpha Polymerase Activity. Biochemistry, 2018, 57, 1063-1072.	2.5	16
24	A Practical Synthesis of Glycinamide Ribonucleotide. Heterocycles, 2018, 97, 776.	0.7	1
25	Probing the role of distal residues in DinB and Pol Kappa in the extension step of DNA damage bypass. FASEB Journal, 2018, 32, 646.3.	0.5	0
26	Understanding How Distal Residues Play a Role in Parkin Activity. FASEB Journal, 2018, 32, 654.7.	0.5	0
27	Functional assignment of Structural Genomics proteins through computed chemical properties, graph representation of active sites, and biochemical validation. FASEB Journal, 2018, 32, lb94.	0.5	0
28	Electrostatic interactions in natural enzymes: What can we learn for enzyme design?. FASEB Journal, 2018, 32, 655.26.	0.5	0
29	Fluorinated Adenosine A2A Receptor Antagonists Inspired by Preladenant as Potential Cancer Immunotherapeutics. International Journal of Medicinal Chemistry, 2017, 2017, 1-8.	2.2	5
30	Local structure based method for prediction of the biochemical function of proteins: Applications to glycoside hydrolases. Methods, 2016, 93, 51-63.	3.8	9
31	Prediction of distal residue participation in enzyme catalysis. Protein Science, 2015, 24, 762-778.	7.6	23
32	Synthesis and evaluation of 2-halogenated-1,1-bis(4-hydroxyphenyl)-2-(3-hydroxyphenyl)-ethylenes as potential estrogen receptor-targeted radiodiagnostic and radiotherapeutic agents. Steroids, 2015, 96, 50-62.	1.8	2
33	Biochemical functional predictions for protein structures of unknown or uncertain function. Computational and Structural Biotechnology Journal, 2015, 13, 182-191.	4.1	77
34	Functional Characterization of Structural Genomics Proteins in the Crotonase Superfamily. FASEB Journal, 2015, 29, 573.18.	0.5	0
35	American Indian Science and Engineering Society (AISES): Building a Successful Model for Diversity and Inclusion. ACS Symposium Series, 2014, , 255-264.	0.5	1
36	Protein function annotation with Structurally Aligned Local Sites of Activity (SALSAs). BMC Bioinformatics, 2013, 14, S13.	2.6	15

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37	The human Aurora kinase inhibitor danusertib is a lead compound for anti-trypanosomal drug discovery via target repurposing. European Journal of Medicinal Chemistry, 2013, 62, 777-784.	5.5	44
38	Design and evaluation of xanthine based adenosine receptor antagonists: Potential hypoxia targeted immunotherapies. Bioorganic and Medicinal Chemistry, 2013, 21, 7453-7464.	3.0	10
39	Using the Structurally Aligned Local Sites of Activity (SALSAs) computational method to determine biochemical function of structural genomics proteins. FASEB Journal, 2013, 27, 811.4.	0.5	0
40	Successful computational prediction of active site and distal residues essential for function in DNA polymerase III alpha subunit. FASEB Journal, 2013, 27, 541.3.	0.5	0
41	Computational prediction and validation of putative ketosteroid isomerase (KSI) structural genomics proteins. FASEB Journal, 2013, 27, 811.5.	0.5	0
42	POOL server: machine learning application for functional site prediction in proteins. Bioinformatics, 2012, 28, 2078-2079.	4.1	37
43	Effects of nonâ€catalytic, distal amino acid residues on activity of E. coli DinB (DNA polymerase) Tj ETQq1 1 0.784314 rgBT /Ov	2.2	26
44	Successful computational prediction of residues important for function in DNA polymerase III alpha subunit. FASEB Journal, 2012, 26, 739.1.	0.5	0
45	Evidence of the Participation of Remote Residues in the Catalytic Activity of Co-Type Nitrile Hydratase from Pseudomonas putida. Biochemistry, 2011, 50, 4923-4935.	2.5	48
46	A Tale of Two Isomerases: Compact versus Extended Active Sites in Ketosteroid Isomerase and Phosphoglucose Isomerase. Biochemistry, 2011, 50, 9283-9295.	2.5	32
47	Pharmacological Validation of Trypanosoma brucei Phosphodiesterases B1 and B2 as Druggable Targets for African Sleeping Sickness. Journal of Medicinal Chemistry, 2011, 54, 8188-8194.	6.4	46
48	Crystal structure of a metalâ€dependent phosphoesterase (YP_910028.1) from Bifidobacterium adolescentis: Computational prediction and experimental validation of phosphoesterase activity. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2146-2160.	2.6	11
49	Highâ€performance prediction of functional residues in proteins with machine learning and computed input features. Biopolymers, 2011, 95, 390-400.	2.4	44
50	Electrostatic Properties for Protein Functional Site Prediction. , 2011, , 183-196.		0
51	Identification of critical residues in DNA polymerase III alpha through protein engineering. FASEB Journal, 2011, 25, 880.4.	0.5	0
52	FUNCTIONAL CLASSIFICATION OF PROTEIN 3D STRUCTURES FROM PREDICTED LOCAL INTERACTION SITES. Journal of Bioinformatics and Computational Biology, 2010, 08, 1-15.	0.8	18
53	High Conservation of Amino Acids with Anomalous Protonation Behavior. Current Bioinformatics, 2010, 5, 134-140.	1.5	3
54	Partial Order Optimum Likelihood (POOL): Maximum Likelihood Prediction of Protein Active Site Residues Using 3D Structure and Sequence Properties. PLoS Computational Biology, 2009, 5, e1000266.	3.2	65

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55	Prediction of interaction sites from apo 3D structures when the holo conformation is different. Proteins: Structure, Function and Bioinformatics, 2008, 72, 980-992.	2.6	11
56	Enhanced performance in prediction of protein active sites with THEMATICS and support vector machines. Protein Science, 2008, 17, 333-341.	7.6	33
57	pH-Dependent Interdomain Tethers of CD1b Regulate Its Antigen Capture. Immunity, 2008, 28, 774-786.	14.3	47
58	Site Prediction for Computer Aided Functional Annotation of Structural Genomics Proteins. FASEB Journal, 2008, 22, 798.9.	0.5	0
59	Identification of Functional Subclasses in the DJ-1 Superfamily Proteins. PLoS Computational Biology, 2007, 3, e15.	3.2	64
60	Selective prediction of interaction sites in protein structures with THEMATICS. BMC Bioinformatics, 2007, 8, 119.	2.6	51
61	Statistical criteria for the identification of protein active sites using theoretical microscopic titration curves. Proteins: Structure, Function and Bioinformatics, 2005, 59, 183-195.	2.6	59
62	ACTIVE SITE PREDICTION FOR COMPARATIVE MODEL STRUCTURES WITH THEMATICS. Journal of Bioinformatics and Computational Biology, 2005, 03, 127-143.	0.8	10
63	Prediction of active sites for protein structures from computed chemical properties. Bioinformatics, 2005, 21, i258-i265.	4.1	31
64	Identifying Functional Sites Based on Prediction of Charged Group Behavior. Current Protocols in Bioinformatics, 2004, 6, Unit 8.6.	25.8	2
65	Protein structure to function: insights from computation. Cellular and Molecular Life Sciences, 2004, 61, 387-392.	5.4	29
66	Physicochemical Methods for Prediction of Functional Information for Proteins. Israel Journal of Chemistry, 2004, 44, 299-308.	2.3	7
67	Future directions in protein function prediction. Molecular Biology Reports, 2002, 29, 329-335.	2.3	27
68	A Model for Enzymeâ˜Substrate Interaction in Alanine Racemase. Journal of the American Chemical Society, 2001, 123, 2830-2834.	13.7	32
69	Numerical Aspects of the Calculation of Second Hyperpolarizabilities Using the Finite Field Method Coupled with a Simple Lanczos Algorithm. Journal of Computational Chemistry, 2001, 22, 468-474.	3.3	3
70	THEMATICS: A simple computational predictor of enzyme function from structure. Proceedings of the National Academy of Sciences of the United States of America, 2001, 98, 12473-12478.	7.1	214
71	Introducing a Practice-Oriented Approach in the Physical Chemistry Instructional Laboratory. Journal of Chemical Education, 1999, 76, 601.	2.3	0
72	Theory of Electroabsorption Spectroscopy in Pyrazine-Bridged Ru Dimers. Journal of the American Chemical Society, 1999, 121, 2594-2596.	13.7	20

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73	A Hubbard model for the second hyperpolarizability in alternating polymers. Chemical Physics Letters, 1998, 291, 325-332.	2.6	7
74	Theory of the Stark Effect spectral lineshape for a delocalized mixed-valence complex. Inorganic Chemistry Communication, 1998, 1, 137-140.	3.9	12
75	Theory of the Stark Effect in protein systems containing an electron donorâ€“acceptor couple. Journal of Inorganic Biochemistry, 1998, 70, 245-252.	3.5	6
76	Role of vibronic coupling and correlation effects on the optical properties of mixed-valent and monovalent dimer compounds: the Creutz-Taube ion and its monovalent analogs. The Journal of Physical Chemistry, 1995, 99, 10484-10491.	2.9	58
77	Potential energy surfaces for a mixed-valence dimer in an applied electric field. Theoretica Chimica Acta, 1995, 90, 331-339.	0.8	5
78	Electron donor-acceptor couples. International Reviews in Physical Chemistry, 1995, 14, 1-14.	2.3	6
79	Comment on the Calculation of Absorption Line Shapes for Mixed-Valence Dimers. The Journal of Physical Chemistry, 1994, 98, 11230-11232.	2.9	12
80	The electronic structure of pentaammine(pyrazine) ruthenium(II) and (III): the metal-ligand ï€ conjugation and its implications in electron delocalization. Inorganica Chimica Acta, 1994, 226, 43-51.	2.4	25
81	Third-order nonlinear optical properties of finite bridged polymers. Chemical Physics Letters, 1993, 205, 85-90.	2.6	8
82	An electronic mechanism for electron pairing in antiferromagnetic bridged mixedâ€valence systems. Journal of Chemical Physics, 1992, 96, 3255-3261.	3.0	14
83	Mixed Valency Oligomers: Model Pathways for the Control of Their Properties. , 1991, , 335-340.		0
84	A hybrid hubbard model for discrete and periodic backbonded complexes. Chemical Physics Letters, 1990, 165, 208-212.	2.6	2
85	Bridged Mixed-Valence Systems. Advances in Chemistry Series, 1989, , 225-235.	0.6	5
86	Nonadiabatic quantum mechanical treatment of the absorption lineshape of bridged mixed-valence dimers. The Journal of Physical Chemistry, 1989, 93, 3030-3034.	2.9	39
87	A model for the optical absorption spectrum of (.mu.-pyrazine) decaamminediruthenium(5+): What hath Creutz and Taube wrought?. Journal of the American Chemical Society, 1987, 109, 1672-1676.	13.7	90
88	Electronic structure of the Creutz-Taube ion. Journal of the American Chemical Society, 1987, 109, 1666-1671.	13.7	95
89	An analysis of the absorption and fluorescence spectra of trimethylamine. Determination of the ~A-~X origin and the ground state inversion barrier. Journal of the American Chemical Society, 1986, 108, 3907-3912.	13.7	26
90	Creutz-Taube ion: a model for the EPR g tensor which includes the bridging ligand. Journal of the American Chemical Society, 1986, 108, 1712-1713.	13.7	15

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91	Line shape of the intervalence transfer band in bridged mixed-valence dimers: the delocalized case. Journal of the American Chemical Society, 1985, 107, 6161-6167.	13.7	44
92	Models for the spectra of bridged mixed-valence dimers. International Journal of Quantum Chemistry, 1985, 28, 393-401.	2.0	1
93	The electronic structure of the creutz-taube ion: A hartree-fock-slater study. Chemical Physics Letters, 1984, 109, 50-55.	2.6	20
94	A model for the intervalence transfer band profile of bridged mixed-valence dimers. Chemical Physics Letters, 1984, 112, 507-512.	2.6	24
95	Thermodynamics for processes in finite time. Accounts of Chemical Research, 1984, 17, 266-271.	15.6	258
96	Two-dimensional potential surfaces for bridged mixed-valence dimers. The Journal of Physical Chemistry, 1984, 88, 5919-5923.	2.9	33
97	The generalized Carnot cycle: A working fluid operating in finite time between finite heat sources and sinks. Journal of Chemical Physics, 1983, 78, 4721-4727.	3.0	121
98	Energetics and dynamics of large Van der Waals molecules. Faraday Discussions of the Chemical Society, 1982, 73, 153.	2.2	112
99	Adiabatic potentials for a bridged three-site electron-transfer system. Chemical Physics Letters, 1982, 93, 421-424.	2.6	31
100	Through-bridge electron transfer: A propagator study of a simple three-site model. Chemical Physics Letters, 1982, 88, 538-542.	2.6	8
101	Model calculations of potential surfaces of van der Waals complexes containing large aromatic molecules. Journal of the American Chemical Society, 1981, 103, 6586-6592.	13.7	182
102	Hexaammineruthenium(II,III) and pentaamminedinitrogenruthenium(II). A Hartree-Fock-Slater study. Journal of the American Chemical Society, 1981, 103, 1656-1659.	13.7	27
103	Maximum work from a finite reservoir by sequential Carnot cycles. American Journal of Physics, 1981, 49, 681-685.	0.7	114
104	Thermodynamics in finite time: Processes with temperatureâ€dependent chemical reactions. Journal of Chemical Physics, 1980, 73, 5838-5843.	3.0	37
105	Thermodynamics in finite time: A chemically driven engine. Journal of Chemical Physics, 1980, 72, 5118-5124.	3.0	41
106	Electron transfer in fixed-nuclei systems: A comparison of propagator descriptions. Journal of Chemical Physics, 1979, 71, 2244.	3.0	7
107	Intramolecular electron transfer in simple model systems: A propagator study. Journal of Chemical Physics, 1977, 66, 938-946.	3.0	14
108	Effect of basis function overlap on intramolecular electron transfer amplitudes: some results for a two-site hubbard model. Chemical Physics Letters, 1977, 51, 573-577.	2.6	6

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109	A treatment of vibrational relaxation without the rotating wave approximation. Chemical Physics, 1976, 16, 49-59.	1.9	18
110	Intramolecular electron transfer: Simple theory of purely electronic effects. Molecular Physics, 1976, 32, 1233-1245.	1.7	22