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	Thermodynamics for processes in finite time. Accounts of Chemical Research, 1984, 17, 266-271.	15.6	258
2	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
3	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
4	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
5	Maximum work from a finite reservoir by sequential Carnot cycles. American Journal of Physics, 1981, 49, 681-685.	0.7	114
6	Energetics and dynamics of large Van der Waals molecules. Faraday Discussions of the Chemical Society, 1982, 73, 153.	2.2	112
7	Electronic structure of the Creutz-Taube ion. Journal of the American Chemical Society, 1987, 109, 1666-1671.	13.7	95
8	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
9	Biochemical functional predictions for protein structures of unknown or uncertain function. Computational and Structural Biotechnology Journal, 2015, 13, 182-191.	4.1	77
10	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
11	Identification of Functional Subclasses in the DJ-1 Superfamily Proteins. PLoS Computational Biology, 2007, 3, e15.	3.2	64
12	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
13	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
14	Selective prediction of interaction sites in protein structures with THEMATICS. BMC Bioinformatics, 2007, 8, 119.	2.6	51
15	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
16	pH-Dependent Interdomain Tethers of CD1b Regulate Its Antigen Capture. Immunity, 2008, 28, 774-786.	14.3	47
17	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
18	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

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19	Highâ€performance prediction of functional residues in proteins with machine learning and computed input features. Biopolymers, 2011, 95, 390-400.	2.4	44
20	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
21	Thermodynamics in finite time: A chemically driven engine. Journal of Chemical Physics, 1980, 72, 5118-5124.	3.0	41
22	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
23	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
24	Thermodynamics in finite time: Processes with temperatureâ€dependent chemical reactions. Journal of Chemical Physics, 1980, 73, 5838-5843.	3.0	37
25	POOL server: machine learning application for functional site prediction in proteins. Bioinformatics, 2012, 28, 2078-2079.	4.1	37
26	Two-dimensional potential surfaces for bridged mixed-valence dimers. The Journal of Physical Chemistry, 1984, 88, 5919-5923.	2.9	33
27	Enhanced performance in prediction of protein active sites with THEMATICS and support vector machines. Protein Science, 2008, 17, 333-341.	7.6	33
28	A Model for Enzymeâ^'Substrate Interaction in Alanine Racemase. Journal of the American Chemical Society, 2001, 123, 2830-2834.	13.7	32
29	A Tale of Two Isomerases: Compact versus Extended Active Sites in Ketosteroid Isomerase and Phosphoglucose Isomerase. Biochemistry, 2011, 50, 9283-9295.	2.5	32
30	Adiabatic potentials for a bridged three-site electron-transfer system. Chemical Physics Letters, 1982, 93, 421-424.	2.6	31
31	Prediction of active sites for protein structures from computed chemical properties. Bioinformatics, 2005, 21, i258-i265.	4.1	31
32	Protein structure to function: insights from computation. Cellular and Molecular Life Sciences, 2004, 61, 387-392.	5.4	29
33	Hexaammineruthenium(II,III) and pentaamminedinitrogenruthenium(II). A Hartree-Fock-Slater study. Journal of the American Chemical Society, 1981, 103, 1656-1659.	13.7	27
34	Future directions in protein function prediction. Molecular Biology Reports, 2002, 29, 329-335.	2.3	27
35	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
36	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

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37	A model for the intervalence transfer band profile of bridged mixed-valence dimers. Chemical Physics Letters, 1984, 112, 507-512.	2.6	24
38	Prediction of distal residue participation in enzyme catalysis. Protein Science, 2015, 24, 762-778.	7.6	23
39	Intramolecular electron transfer: Simple theory of purely electronic effects. Molecular Physics, 1976, 32, 1233-1245.	1.7	22
40	Tri-arginine exosite patch of caspase-6 recruits substrates for hydrolysis. Journal of Biological Chemistry, 2019, 294, 71-88.	3.4	21
41	The electronic structure of the creutz-taube ion: A hartree-fock-slater study. Chemical Physics Letters, 1984, 109, 50-55.	2.6	20
42	Theory of Electroabsorption Spectroscopy in Pyrazine-Bridged Ru Dimers. Journal of the American Chemical Society, 1999, 121, 2594-2596.	13.7	20
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	20
44	A treatment of vibrational relaxation without the rotating wave approximation. Chemical Physics, 1976, 16, 49-59.	1.9	18
45	FUNCTIONAL CLASSIFICATION OF PROTEIN 3D STRUCTURES FROM PREDICTED LOCAL INTERACTION SITES. Journal of Bioinformatics and Computational Biology, 2010, 08, 1-15.	0.8	18
46	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
47	Prediction of Active Site and Distal Residues in E. coli DNA Polymerase III alpha Polymerase Activity. Biochemistry, 2018, 57, 1063-1072.	2.5	16
48	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
49	Protein function annotation with Structurally Aligned Local Sites of Activity (SALSAs). BMC Bioinformatics, 2013, 14, S13.	2.6	15
50	Intramolecular electron transfer in simple model systems: A propagator study. Journal of Chemical Physics, 1977, 66, 938-946.	3.0	14
51	An electronic mechanism for electron pairing in antiferromagnetic bridged mixedâ€valence systems. Journal of Chemical Physics, 1992, 96, 3255-3261.	3.0	14
52	Comment on the Calculation of Absorption Line Shapes for Mixed-Valence Dimers. The Journal of Physical Chemistry, 1994, 98, 11230-11232.	2.9	12
53	Theory of the Stark Effect spectral lineshape for a delocalized mixed-valence complex. Inorganic Chemistry Communication, 1998, 1, 137-140.	3.9	12
54	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

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55	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
56	ACTIVE SITE PREDICTION FOR COMPARATIVE MODEL STRUCTURES WITH THEMATICS. Journal of Bioinformatics and Computational Biology, 2005, 03, 127-143.	0.8	10
57	Design and evaluation of xanthine based adenosine receptor antagonists: Potential hypoxia targeted immunotherapies. Bioorganic and Medicinal Chemistry, 2013, 21, 7453-7464.	3.0	10
58	Local structure based method for prediction of the biochemical function of proteins: Applications to glycoside hydrolases. Methods, 2016, 93, 51-63.	3.8	9
59	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
60	Through-bridge electron transfer: A propagator study of a simple three-site model. Chemical Physics Letters, 1982, 88, 538-542.	2.6	8
61	Third-order nonlinear optical properties of finite bridged polymers. Chemical Physics Letters, 1993, 205, 85-90.	2.6	8
62	Functional classification of protein structures by local structure matching in graph representation. Protein Science, 2018, 27, 1125-1135.	7.6	8
63	Amino acid interactions that facilitate enzyme catalysis. Journal of Chemical Physics, 2021, 154, 195101.	3.0	8
64	Electron transfer in fixed-nuclei systems: A comparison of propagator descriptions. Journal of Chemical Physics, 1979, 71, 2244.	3.0	7
65	A Hubbard model for the second hyperpolarizability in alternating polymers. Chemical Physics Letters, 1998, 291, 325-332.	2.6	7
66	Physicochemical Methods for Prediction of Functional Information for Proteins. Israel Journal of Chemistry, 2004, 44, 299-308.	2.3	7
67	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
68	Electron donor-acceptor couples. International Reviews in Physical Chemistry, 1995, 14, 1-14.	2.3	6
69	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
70	Functional Characterization of Structural Genomics Proteins in the Crotonase Superfamily. ACS Chemical Biology, 2022, 17, 395-403.	3.4	6
71	Bridged Mixed-Valence Systems. Advances in Chemistry Series, 1989, , 225-235.	0.6	5
72	Potential energy surfaces for a mixed-valence dimer in an applied electric field. Theoretica Chimica Acta, 1995, 90, 331-339.	0.8	5

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73	Fluorinated Adenosine A2A Receptor Antagonists Inspired by Preladenant as Potential Cancer Immunotherapeutics. International Journal of Medicinal Chemistry, 2017, 2017, 1-8.	2.2	5
74	Analysis of electrostatic coupling throughout the laboratory evolution of a designed retroaldolase. Protein Science, 2021, 30, 1617-1627.	7.6	5
75	Probing remote residues important for catalysis in Escherichia coli ornithine transcarbamoylase. PLoS ONE, 2020, 15, e0228487.	2.5	4
76	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
77	High Conservation of Amino Acids with Anomalous Protonation Behavior. Current Bioinformatics, 2010, 5, 134-140.	1.5	3
78	Reintegrating Biology Through the Nexus of Energy, Information, and Matter. Integrative and Comparative Biology, 2022, 61, 2082-2094.	2.0	3
79	Electrostatic fingerprints of catalytically active amino acids in enzymes. Protein Science, 2022, 31, e4291.	7.6	3
80	Enzyme active sites: Identification and prediction of function using computational chemistry. Current Opinion in Structural Biology, 2022, 74, 102384.	5.7	3
81	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
82	A hybrid hubbard model for discrete and periodic backbonded complexes. Chemical Physics Letters, 1990, 165, 208-212.	2.6	2
83	Identifying Functional Sites Based on Prediction of Charged Group Behavior. Current Protocols in Bioinformatics, 2004, 6, Unit 8.6.	25.8	2
84	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
85	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
86	Adapting Undergraduate Research to Remote Work to Increase Engagement. The Biophysicist, 2021, 2, 28-32.	0.3	2
87	Best Practices to Diversify Chemistry Faculty. Journal of Chemical Education, 2022, 99, 435-443.	2.3	2
88	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
89	Models for the spectra of bridged mixed-valence dimers. International Journal of Quantum Chemistry, 1985, 28, 393-401.	2.0	1
90	American Indian Science and Engineering Society (AISES): Building a Successful Model for Diversity and Inclusion. ACS Symposium Series, 2014, , 255-264.	0.5	1

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91	A Practical Synthesis of Glycinamide Ribonucleotide. Heterocycles, 2018, 97, 776.	0.7	1
92	Introducing a Practice-Oriented Approach in the Physical Chemistry Instructional Laboratory. Journal of Chemical Education, 1999, 76, 601.	2.3	0
93	Identification, Characterization and Drug Discovery for Novel Target Sites for SARSâ€CoVâ€2 Proteins. FASEB Journal, 2021, 35, .	0.5	0
94	Site Prediction for Computer Aided Functional Annotation of Structural Genomics Proteins. FASEB Journal, 2008, 22, 798.9.	0.5	0
95	Electrostatic Properties for Protein Functional Site Prediction. , 2011, , 183-196.		0
96	Identification of critical residues in DNA polymerase III alpha through protein engineering. FASEB Journal, 2011, 25, 880.4.	0.5	0
97	Successful computational prediction of residues important for function in DNA polymerase III alpha subunit. FASEB Journal, 2012, 26, 739.1.	0.5	0
98	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
99	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
100	Computational prediction and validation of putative ketosteroid isomerase (KSI) structural genomics proteins. FASEB Journal, 2013, 27, 811.5.	0.5	0
101	Mixed Valency Oligomers: Model Pathways for the Control of Their Properties. , 1991, , 335-340.		0
102	Functional Characterization of Structural Genomics Proteins in the Crotonase Superfamily. FASEB Journal, 2015, 29, 573.18.	0.5	0
103	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
104	Understanding How Distal Residues Play a Role in Parkin Activity. FASEB Journal, 2018, 32, 654.7.	0.5	0
105	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
106	Electrostatic interactions in natural enzymes: What can we learn for enzyme design?. FASEB Journal, 2018, 32, 655.26.	0.5	0
107	Thinking Outside the Informatics Box: Computed Chemical Properties for Protein Function Annotation. FASEB Journal, 2019, 33, 473.5.	0.5	0
108	Computed chemical properties for predicting protein function. Biophysical Journal, 2022, 121, 132a.	0.5	0

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109	Stereoselective Synthesis of Î²-Glycinamide Ribonucleotide. Molecules, 2022, 27, 2528.	3.8	0
110	Electrostatic Fingerprints of Catalytically Active Amino Acids in Enzymes. FASEB Journal, 2022, 36, .	0.5	0