

# Patricia Amara

## List of Publications by Year in descending order

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37  
papers

2,477  
citations

331670

21  
h-index

330143

37  
g-index

37  
all docs

37  
docs citations

37  
times ranked

2020  
citing authors

#	ARTICLE	IF	CITATIONS
1	A Generalized Hybrid Orbital (GHO) Method for the Treatment of Boundary Atoms in Combined QM/MM Calculations. <i>Journal of Physical Chemistry A</i> , 1998, 102, 4714-4721.	2.5	481
2	Gas access to the active site of Ni-Fe hydrogenases probed by X-ray crystallography and molecular dynamics. <i>Nature Structural Biology</i> , 1997, 4, 523-526.	9.7	325
3	X-ray crystallographic and computational studies of the O <sub>2</sub> -tolerant [NiFe]-hydrogenase 1 from <i>Escherichia coli</i> . <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 5305-5310.	7.1	194
4	A Hybrid Density Functional Theory/Molecular Mechanics Study of Nickel~Iron Hydrogenase: Investigation of the Active Site Redox States. <i>Journal of the American Chemical Society</i> , 1999, 121, 4468-4477.	13.7	142
5	(IscS~U) <sub>2</sub> Complex Structures Provide Insights into Fe <sub>2</sub> S <sub>2</sub> Biogenesis and Transfer. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 5439-5442.	13.8	123
6	X-ray Structure of the [FeFe]-Hydrogenase Maturase HydE from <i>Thermotoga maritima</i> . <i>Journal of Biological Chemistry</i> , 2008, 283, 18861-18872.	3.4	119
7	Global energy minimum searches using an approximate solution of the imaginary time Schroedinger equation. <i>The Journal of Physical Chemistry</i> , 1993, 97, 6715-6721.	2.9	115
8	The generalized hybrid orbital method for combined quantum mechanical/molecular mechanical calculations: formulation and tests of the analytical derivatives. <i>Theoretical Chemistry Accounts</i> , 2000, 104, 336-343.	1.4	110
9	Evaluation of an ab initio quantum mechanical/molecular mechanical hybrid-potential link-atom method. <i>Theoretical Chemistry Accounts</i> , 2003, 109, 43-52.	1.4	109
10	Unexpected electron transfer mechanism upon AdoMet cleavage in radical SAM proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 14867-14871.	7.1	84
11	Crystal Structure of Tryptophan Lyase (NosL): Evidence for Radical Formation at the Amino Group of Tryptophan. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 11840-11844.	13.8	81
12	Carbon~sulfur bond-forming reaction catalysed by the radical SAM enzyme HydE. <i>Nature Chemistry</i> , 2016, 8, 491-500.	13.6	72
13	Fine-tuning of a radical-based reaction by radical <i>S</i> -adenosyl-L-methionine tryptophan lyase. <i>Science</i> , 2016, 351, 1320-1323.	12.6	53
14	Is There a Covalent Intermediate in the Viral Neuraminidase Reaction? A Hybrid Potential Free-Energy Study. <i>Journal of the American Chemical Society</i> , 1999, 121, 9693-9702.	13.7	49
15	An Artificial Oxygenase Built from Scratch: Substrate Binding Site Identified Using a Docking Approach. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 3922-3925.	13.8	42
16	Folding model proteins using kinetic and thermodynamic annealing of the classical density distribution. <i>The Journal of Physical Chemistry</i> , 1995, 99, 14840-14853.	2.9	41
17	Crystal Structure of HydG from <i>Carboxydotherrmus hydrogenoformans</i> : A Trifunctional [FeFe]-Hydrogenase Maturase. <i>ChemBioChem</i> , 2015, 16, 397-402.	2.6	41
18	The Structural Plasticity of the Proximal [4Fe3S] Cluster is Responsible for the O <sub>2</sub> Tolerance of Membrane-Bound [NiFe] Hydrogenases. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 2002-2006.	13.8	31

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19	The structure of the periplasmic nickel-binding protein NikA provides insights for artificial metalloenzyme design. <i>Journal of Biological Inorganic Chemistry</i> , 2012, 17, 817-829.	2.6	27
20	Simulated annealing using coarse grained classical dynamics: Smoluchowski dynamics in the Gaussian density approximation. <i>Journal of Chemical Physics</i> , 1995, 103, 1574-1581.	3.0	25
21	Further Characterization of the [FeFe]-Hydrogenase Maturase HydG. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 1121-1127.	2.0	23
22	Structural Basis for Enantioselectivity in the Transfer Hydrogenation of a Ketone Catalyzed by an Artificial Metalloenzyme. <i>European Journal of Inorganic Chemistry</i> , 2013, 2013, 3596-3600.	2.0	23
23	The Crystal Structure of Fe <sub>4</sub> S <sub>4</sub> Quinolate Synthase Unravels an Enzymatic Dehydration Mechanism That Uses Tyrosine and a Hydrolase-Type Triad. <i>Journal of the American Chemical Society</i> , 2014, 136, 5253-5256.	13.7	23
24	1,2-Diol Dehydration by the Radical SAM Enzyme AprD4: A Matter of Proton Circulation and Substrate Flexibility. <i>Journal of the American Chemical Society</i> , 2018, 140, 1365-1371.	13.7	19
25	Crystal Structure of the Transcription Regulator RsrR Reveals a [2Fe-2S] Cluster Coordinated by Cys, Glu, and His Residues. <i>Journal of the American Chemical Society</i> , 2019, 141, 2367-2375.	13.7	18
26	Energy minimization using the classical density distribution: Application to sodium chloride clusters. <i>Physical Review B</i> , 1996, 53, 13857-13863.	3.2	15
27	An unexpected P-cluster like intermediate <i>en route</i> to the nitrogenase FeMo-co. <i>Chemical Science</i> , 2021, 12, 5269-5274.	7.4	15
28	Crystal Structures of Quinolate Synthase in Complex with a Substrate Analogue, the Condensation Intermediate, and Substrate-Derived Product. <i>Journal of the American Chemical Society</i> , 2016, 138, 11802-11809.	13.7	14
29	Radical S-Adenosyl-methionine Tryptophan Lyase (NosL): How the Protein Controls the Carboxyl Radical $\text{CO}_2$ Migration. <i>Journal of the American Chemical Society</i> , 2018, 140, 16661-16668.	13.7	12
30	Radical SAM Enzymes and Metallocofactor Assembly: A Structural Point of View. <i>ACS Bio &amp; Med Chem Au</i> , 2022, 2, 36-52.	3.7	12
31	Electron and Proton Transfers Modulate DNA Binding by the Transcription Regulator RsrR. <i>Journal of the American Chemical Society</i> , 2020, 142, 5104-5116.	13.7	11
32	Electronic states of the O <sub>2</sub> -tolerant [NiFe] hydrogenase proximal cluster. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, E2538.	7.1	9
33	Crystallographic Trapping of Reaction Intermediates in Quinolinic Acid Synthesis by NadA. <i>ACS Chemical Biology</i> , 2018, 13, 1209-1217.	3.4	9
34	L-tyrosine-bound ThiH structure reveals C-C bond break differences within radical SAM aromatic amino acid lyases. <i>Nature Communications</i> , 2022, 13, 2284.	12.8	7
35	Crystallographic evidence for unexpected selective tyrosine hydroxylations in an aerated achiral Ru-papain conjugate. <i>Metallomics</i> , 2018, 10, 1452-1459.	2.4	1
36	Transient Formation of a Second Active Site Cavity during Quinolinic Acid Synthesis by NadA. <i>ACS Chemical Biology</i> , 2021, 16, 2423-2433.	3.4	1

#	ARTICLE	IF	CITATIONS
37	Global minimization on rugged energy landscapes. DIMACS Series in Discrete Mathematics and Theoretical Computer Science, 1995, , 1-13.	0.0	1