Patricia Amara

List of Publications by Year
in descending order

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	Radical SAM Enzymes and Metallocofactor Assembly: A Structural Point of View. ACS Bio & Med Chem Au, 2022, 2, 36-52.	3.7	12
2	L-tyrosine-bound ThiH structure reveals Câ€“C bond break differences within radical SAM aromatic amino acid lyases. Nature Communications, 2022, 13, 2284.	12.8	7
3	An unexpected P-cluster like intermediate en route to the nitrogenase FeMo-co. Chemical Science, 2021, 12, 5269-5274.	7.4	15
4	Transient Formation of a Second Active Site Cavity during Quinolinic Acid Synthesis by NadA. ACS Chemical Biology, 2021, 16, 2423-2433.	3.4	1
5	Electron and Proton Transfers Modulate DNA Binding by the Transcription Regulator RsrR. Journal of the American Chemical Society, 2020, 142, 5104-5116.	13.7	11
6	Crystal Structure of the Transcription Regulator RsrR Reveals a [2Feâ€“2S] Cluster Coordinated by Cys, Glu, and His Residues. Journal of the American Chemical Society, 2019, 141, 2367-2375.	13.7	18
7	Crystallographic Trapping of Reaction Intermediates in Quinolinic Acid Synthesis by NadA. ACS Chemical Biology, 2018, 13, 1209-1217.	3.4	9
8	1,2-Diol Dehydration by the Radical SAM Enzyme AprD4: A Matter of Proton Circulation and Substrate Flexibility. Journal of the American Chemical Society, 2018, 140, 1365-1371.	13.7	19
9	Radical S-Adenosyl-<scp>l</scp>-methionine Tryptophan Lyase (NosL): How the Protein Controls the Carboxyl Radical â€¢CO₂^{â€“} Migration. Journal of the American Chemical Society, 2018, 140, 16661-16668.	13.7	12
10	Crystallographic evidence for unexpected selective tyrosine hydroxylations in an aerated achiral Ruâ€“papain conjugate. Metallomics, 2018, 10, 1452-1459.	2.4	1
11	Carbonâ€“sulfur bond-forming reaction catalysed by the radical SAM enzyme HydE. Nature Chemistry, 2016, 8, 491-500.	13.6	72
12	Crystal Structures of Quinolinate Synthase in Complex with a Substrate Analogue, the Condensation Intermediate, and Substrate-Derived Product. Journal of the American Chemical Society, 2016, 138, 11802-11809.	13.7	14
13	Fine-tuning of a radical-based reaction by radical S -adenosyl-L-methionine tryptophan lyase. Science, 2016, 351, 1320-1323.	12.6	53
14	Crystal Structure of HydG from Carboxydothermus hydrogenoformans: A Trifunctional [FeFe]â€Hydrogenase Maturase. ChemBioChem, 2015, 16, 397-402.	2.6	41
15	Crystal Structure of Tryptophan Lyase (NosL): Evidence for Radical Formation at the Amino Group of Tryptophan. Angewandte Chemie - International Edition, 2014, 53, 11840-11844.	13.8	81
16	The Crystal Structure of Fe₄S₄ Quinolinate Synthase Unravels an Enzymatic Dehydration Mechanism That Uses Tyrosine and a Hydrolase-Type Triad. Journal of the American Chemical Society, 2014, 136, 5253-5256.	13.7	23
17	Electronic states of the O ₂ -tolerant [NiFe] hydrogenase proximal cluster. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, E2538.	7.1	9
18	An Artificial Oxygenase Built from Scratch: Substrate Binding Site Identified Using a Docking Approach. Angewandte Chemie - International Edition, 2013, 52, 3922-3925.	13.8	42

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19	Structural Basis for Enantioselectivity in the Transfer Hydrogenation of a Ketone Catalyzed by an Artificial Metalloenzyme. European Journal of Inorganic Chemistry, 2013, 2013, 3596-3600.	2.0	23
20	The Structural Plasticity of the Proximal [4Fe3S] Cluster is Responsible for the O₂ Tolerance of Membraneâ€Bound [NiFe] Hydrogenases. Angewandte Chemie - International Edition, 2013, 52, 2002-2006.	13.8	31
21	X-ray crystallographic and computational studies of the O ₂ -tolerant [NiFe]-hydrogenase 1 from Escherichia coli. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 5305-5310.	7.1	194
22	(IscSâ€IscU)₂ Complex Structures Provide Insights into Fe₂S₂ Biogenesis and Transfer. Angewandte Chemie - International Edition, 2012, 51, 5439-5442.	13.8	123
23	The structure of the periplasmic nickel-binding protein NikA provides insights for artificial metalloenzyme design. Journal of Biological Inorganic Chemistry, 2012, 17, 817-829.	2.6	27
24	Further Characterization of the [FeFe]â€Hydrogenase Maturase HydG. European Journal of Inorganic Chemistry, 2011, 2011, 1121-1127.	2.0	23
25	Unexpected electron transfer mechanism upon AdoMet cleavage in radical SAM proteins. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 14867-14871.	7.1	84
26	X-ray Structure of the [FeFe]-Hydrogenase Maturase HydE from Thermotoga maritima. Journal of Biological Chemistry, 2008, 283, 18861-18872.	3.4	119
27	Evaluation of an ab initio quantum mechanical/molecular mechanical hybrid-potential link-atom method. Theoretical Chemistry Accounts, 2003, 109, 43-52.	1.4	109
28	The generalized hybrid orbital method for combined quantum mechanical/molecular mechanical calculations: formulation and tests of the analytical derivatives. Theoretical Chemistry Accounts, 2000, 104, 336-343.	1.4	110
29	Is There a Covalent Intermediate in the Viral Neuraminidase Reaction? A Hybrid Potential Free-Energy Study. Journal of the American Chemical Society, 1999, 121, 9693-9702.	13.7	49
30	A Hybrid Density Functional Theory/Molecular Mechanics Study of Nickelâ˜Iron Hydrogenase:â€‰ Investigation of the Active Site Redox States. Journal of the American Chemical Society, 1999, 121, 4468-4477.	13.7	142
31	A Generalized Hybrid Orbital (GHO) Method for the Treatment of Boundary Atoms in Combined QM/MM Calculations. Journal of Physical Chemistry A, 1998, 102, 4714-4721.	2.5	481
32	Gas access to the active site of Ni-Fe hydrogenases probed by X-ray crystallography and molecular dynamics. Nature Structural Biology, 1997, 4, 523-526.	9.7	325
33	Energy minimization using the classical density distribution: Application to sodium chloride clusters. Physical Review B, 1996, 53, 13857-13863.	3.2	15
34	Simulated annealing using coarse grained classical dynamics: Smoluchowski dynamics in the Gaussian density approximation. Journal of Chemical Physics, 1995, 103, 1574-1581.	3.0	25
35	Folding model proteins using kinetic and thermodynamic annealing of the classical density distribution. The Journal of Physical Chemistry, 1995, 99, 14840-14853.	2.9	41
36	Global minimization on rugged energy landscapes. DIMACS Series in Discrete Mathematics and Theoretical Computer Science, 1995, , 1-13.	0.0	1

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37	Global energy minimum searches using an approximate solution of the imaginary time Schroedinger equation. The Journal of Physical Chemistry, 1993, 97, 6715-6721.	2.9	115