Eamonn F Healy

List of Publications by Year in Descending Order

45 papers	12,995 citations	16 h-index	46 g-index
46 ext. papers	13,316 ext. citations	4 avg, IF	5.6 L-index

#	Paper	IF	Citations
45	How tetraspanin-mediated cell entry of SARS-CoV-2 can dysregulate the shedding of the ACE2 receptor by ADAM17.. *Biochemical and Biophysical Research Communications*, **2022**, 593, 52-56	3.4	1
44	Organic chemistry as representation. *Foundations of Chemistry*, **2021**, 23, 59-68	0.7	
43	An immunomodulatory role for the Mycobacterium tuberculosis Acr protein in the formation of the tuberculous granuloma. *FEBS Letters*, **2021**, 595, 284-293	3.8	2
42	A model for COVID-19-induced dysregulation of ACE2 shedding by ADAM17. *Biochemical and Biophysical Research Communications*, **2021**, 573, 158-163	3.4	5
41	Reply to Comment on "Should Organic Chemistry Be Taught as Science?" *Journal of Chemical Education*, **2020**, 97, 1215-1215	2.4	
40	Protein dynamics of [Cu-Zn] superoxide dismutase (SOD1): How protein motions at the global and local levels impact the reactivity of SOD1. *Journal of Inorganic Biochemistry*, **2020**, 210, 111161	4.2	
39	A model for gain of function in superoxide dismutase. *Biochemistry and Biophysics Reports*, **2020**, 21, 100728	2.2	7
38	Tips and Tools for Teaching Organic Synthesis Online. *Journal of Chemical Education*, **2020**, 97, 3163-3167	2.4	3
37	Should Organic Chemistry Be Taught as Science?. *Journal of Chemical Education*, **2019**, 96, 2069-2071	2.4	4
36	A unified mechanism for plant polyketide biosynthesis derived from in silico modeling. *Biochemical and Biophysical Research Communications*, **2018**, 497, 1123-1128	3.4	3
35	Visualizing the molecular wave function in coordinated complexes. *Computational and Theoretical Chemistry*, **2018**, 1125, 128-132	2	2
34	A prion-like mechanism for the propagated misfolding of SOD1 from in silico modeling of solvated near-native conformers. *PLoS ONE*, **2017**, 12, e0177284	3.7	4
33	A mechanism for propagated SOD1 misfolding from frustration analysis of a G85R mutant protein assembly. *Biochemical and Biophysical Research Communications*, **2016**, 478, 1634-9	3.4	1
32	An in silico study of the effect of SOD1 electrostatic loop dynamics on amyloid-like filament formation. *European Biophysics Journal*, **2016**, 45, 853-859	1.9	5
31	A model for non-obligate oligomer formation in protein aggregration. *Biochemical and Biophysical Research Communications*, **2015**, 465, 523-7	3.4	5
30	A model for small heat shock protein inhibition of polyglutamine aggregation. *Cell Biochemistry and Biophysics*, **2014**, 69, 275-81	3.2	10
29	Michael J. S. Dewar: A Model Iconoclast. *ACS Symposium Series*, **2013**, 139-153	0.4	1

28	A mechanism of action for small heat shock proteins. *Biochemical and Biophysical Research Communications*, **2012**, 417, 268-73	3.4	7
27	A model for heterooligomer formation in the heat shock response of Escherichia coli. *Biochemical and Biophysical Research Communications*, **2012**, 420, 639-43	3.4	4
26	Heisenberg□ chemical legacy: resonance and the chemical bond. *Foundations of Chemistry*, **2011**, 13, 39-49	0.7	4
25	The effect of desolvation on nucleophilic halogenase activity. *Computational and Theoretical Chemistry*, **2011**, 964, 91-93	2	11
24	In Defense of a Heuristic Interpretation of Quantum Mechanics. *Journal of Chemical Education*, **2010**, 87, 559-563	2.4	1
23	Acetylenic inhibitors of ADAM10 and ADAM17: in silico analysis of potency and selectivity. *Journal of Molecular Graphics and Modelling*, **2010**, 29, 436-42	2.8	11
22	A dramatic heavy-atom effect in the quenching of dichlorosubstituted lucigenin fluorescence. *Chemical Physics Letters*, **2010**, 485, 258-261	2.5	6
21	Tyrosine kinase inhibition: Ligand binding and conformational change in c-Kit and c-Abl. *FEBS Letters*, **2009**, 583, 2899-906	3.8	11
20	A docking study of L-chicoric acid with HIV-1 integrase. *Journal of Molecular Graphics and Modelling*, **2009**, 27, 584-9	2.8	30
19	A study of the aluminum hydride reduction of unsaturated cyclic epoxides. *Tetrahedron Letters*, **1994**, 35, 6647-6648	2	8
18	Development and use of quantum mechanical molecular models. 76. AM1: a new general purpose quantum mechanical molecular model. [Erratum to document cited in CA103(2):11627f]. *Journal of the American Chemical Society*, **1993**, 115, 5348-5348	16.4	59
17	An evaluation of AM1 calculated vibrational frequencies. *Computational and Theoretical Chemistry*, **1993**, 281, 141-156		36
16	Peptide conformational analysis using the TRIPOS force field. *International Journal of Quantum Chemistry*, **1992**, 44, 543-548	2.1	1
15	AM1 parameters for tin. *Organometallics*, **1991**, 10, 431-435	3.8	17
14	Comments on a comparison of AM1 with the recently developed PM3 method. *Journal of Computational Chemistry*, **1990**, 11, 541-542	3.5	57
13	A high level ab initio study of corner-protonated cyclopropane. *Journal of the Chemical Society Chemical Communications*, **1987**, 943		15
12	An unusually large secondary deuterium isotope effect. Thermal trans-cis isomerization of trans-1-phenylcyclohexene. *Journal of the American Chemical Society*, **1987**, 109, 6869-6870	16.4	18
11	Ground states of molecules. 73. MNDO calculations for compounds containing germanium. *Organometallics*, **1987**, 6, 186-189	3.8	46

10	Ab initio study of the chair cope rearrangement of 1,5-hexadiene. *Chemical Physics Letters*, **1987**, 141, 521-524	2.5	55
9	Cruciaromaticity in organometallic compounds. *Pure and Applied Chemistry*, **1986**, 58, 67-74	2.1	9
8	Revised MNDO parameters for silicon. *Organometallics*, **1986**, 5, 375-379	3.8	76
7	Development and use of quantum mechanical molecular models. 76. AM1: a new general purpose quantum mechanical molecular model. *Journal of the American Chemical Society*, **1985**, 107, 3902-3909	16.4	12010
6	Ground states of molecules. 67.MNDO Calculations for compounds containing iodine. *Journal of Computational Chemistry*, **1984**, 5, 358-362	3.5	40
5	Location of transition states in reaction mechanisms. *Journal of the Chemical Society, Faraday Transactions 2*, **1984**, 80, 227		237
4	Ground states of molecules. 68. MNDO study of the Claisen rearrangement. *Journal of the American Chemical Society*, **1984**, 106, 7127-7131	16.4	45
3	Ground states of molecules. 64.MNDO Calculations for compounds containing bromine. *Journal of Computational Chemistry*, **1983**, 4, 542-551	3.5	47
2	Why life exists. *Organometallics*, **1982**, 1, 1705-1708	3.8	64
1	Bonding in clusters. Part 3. Protonation of nido-pentaborane(9), nido-hexaborane(10), and closo-hexaborate(6)(2−). *Journal of the Chemical Society Dalton Transactions*, **1981**, 2515-2522		16