Eamonn F Healy

List of Publications by Year
in descending order

46 papers	14,474 citations	471061 17 h-index	253896 43 g-index
46 all docs	46 docs citations	46 times ranked	9221 citing authors

#	Article	IF	Citations
1	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.	6.6	13,340
2	Location of transition states in reaction mechanisms. Journal of the Chemical Society, Faraday Transactions 2, 1984, 80, 227.	1.1	266
3	Revised MNDO parameters for silicon. Organometallics, 1986, 5, 375-379.	1.1	79
4	Why life exists. Organometallics, 1982, 1, 1705-1708.	1.1	71
5	Comments on a comparison of AM1 with the recently developed PM3 method. Journal of Computational Chemistry, 1990, 11, 541-542.	1.5	70
6	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.	6.6	65
7	Ab initio study of the chair cope rearrangement of 1,5-hexadiene. Chemical Physics Letters, 1987, 141, 521-524.	1.2	59
8	Ground states of molecules. 73. MNDO calculations for compounds containing germanium. Organometallics, 1987, 6, 186-189.	1.1	52
9	Ground states of molecules. 68. MNDO study of the Claisen rearrangement. Journal of the American Chemical Society, 1984, 106, 7127-7131.	6.6	51
10	Ground states of molecules. 64.MNDO Calculations for compounds containing bromine. Journal of Computational Chemistry, 1983, 4, 542-551.	1.5	49
11	Ground states of molecules. 67.MNDO Calculations for compounds containing iodine. Journal of Computational Chemistry, 1984, 5, 358-362.	1.5	42
12	An evaluation of AM1 calculated vibrational frequencies. Computational and Theoretical Chemistry, 1993, 281, 141-156.	1.5	39
13	A docking study of l-chicoric acid with HIV-1 integrase. Journal of Molecular Graphics and Modelling, 2009, 27, 584-589.	1.3	36
14	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.	6.6	23
15	AM1 parameters for tin. Organometallics, 1991, 10, 431-435.	1.1	20
16	Bonding in clusters. Part 3. Protonation of nido-pentaborane(9), nido-hexaborane(10), and closo-hexaborate(6)(2â€“). Journal of the Chemical Society Dalton Transactions, 1981, , 2515-2522.	1.1	19
17	A high level ab initio study of corner-protonated cyclopropane. Journal of the Chemical Society Chemical Communications, 1987, , 943.	2.0	18
18	A model for COVID-19-induced dysregulation of ACE2 shedding by ADAM17. Biochemical and Biophysical Research Communications, 2021, 573, 158-163.	1.0	16

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19	Tyrosine kinase inhibition: Ligand binding and conformational change in câ€Kit and câ€Abl. FEBS Letters, 2009, 583, 2899-2906.	1.3	12
20	Acetylenic inhibitors of ADAM10 and ADAM17: In silico analysis of potency and selectivity. Journal of Molecular Graphics and Modelling, 2010, 29, 436-442.	1.3	12
21	The effect of desolvation on nucleophilic halogenase activity. Computational and Theoretical Chemistry, 2011, 964, 91-93.	1.1	12
22	A Model for Small Heat Shock Protein Inhibition of Polyglutamine Aggregation. Cell Biochemistry and Biophysics, 2014, 69, 275-281.	0.9	12
23	Cruciaromaticity in organometallic compounds. Pure and Applied Chemistry, 1986, 58, 67-74.	0.9	10
24	A study of the aluminum hydride reduction of unsaturated cyclic epoxides. Tetrahedron Letters, 1994, 35, 6647-6648.	0.7	10
25	Tips and Tools for Teaching Organic Synthesis Online. Journal of Chemical Education, 2020, 97, 3163-3167.	1.1	10
26	A model for gain of function in superoxide dismutase. Biochemistry and Biophysics Reports, 2020, 21, 100728.	0.7	9
27	A dramatic heavy-atom effect in the quenching of dichlorosubstituted lucigenin fluorescence. Chemical Physics Letters, 2010, 485, 258-261.	1.2	8
28	A mechanism of action for small heat shock proteins. Biochemical and Biophysical Research Communications, 2012, 417, 268-273.	1.0	7
29	Heisenbergâ€™s chemical legacy: resonance and the chemical bond. Foundations of Chemistry, 2011, 13, 39-49.	0.4	6
30	An in silico study of the effect of SOD1 electrostatic loop dynamics on amyloidâ€like filament formation. European Biophysics Journal, 2016, 45, 853-859.	1.2	6
31	A prion-like mechanism for the propagated misfolding of SOD1 from in silico modeling of solvated near-native conformers. PLoS ONE, 2017, 12, e0177284.	1.1	6
32	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.	1.0	6
33	A model for non-obligate oligomer formation in protein aggregration. Biochemical and Biophysical Research Communications, 2015, 465, 523-527.	1.0	5
34	Should Organic Chemistry Be Taught as Science?. Journal of Chemical Education, 2019, 96, 2069-2071.	1.1	5
35	A model for heterooligomer formation in the heat shock response of Escherichia coli. Biochemical and Biophysical Research Communications, 2012, 420, 639-643.	1.0	4
36	An immunomodulatory role for the Mycobacterium tuberculosis Acr protein in the formation of the tuberculous granuloma. FEBS Letters, 2021, 595, 284-293.	1.3	4

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37	A mechanism for propagated SOD1 misfolding from frustration analysis of a G85R mutant protein assembly. Biochemical and Biophysical Research Communications, 2016, 478, 1634-1639.	1.0	3
38	A unified mechanism for plant polyketide biosynthesis derived from in silico modeling. Biochemical and Biophysical Research Communications, 2018, 497, 1123-1128.	1.0	3
39	Visualizing the molecular wave function in ï f-coordinated complexes. Computational and Theoretical Chemistry, 2018, 1125, 128-132.	1.1	3
40	Peptide conformational analysis using the TRIPOS force field. International Journal of Quantum Chemistry, 1992, 44, 543-548.	1.0	2
41	In Defense of a Heuristic Interpretation of Quantum Mechanics. Journal of Chemical Education, 2010, 87, 559-563.	1.1	2
42	Comparison of single point ab initio energies calculated using 3-21G and AM1 geometries. Journal of the Chemical Society Chemical Communications, 1989, , 1452.	2.0	1
43	Michael J. S. Dewar: A Model Iconoclast. ACS Symposium Series, 2013, , 139-153.	0.5	1
44	Reply to Comment on â€œShould Organic Chemistry Be Taught as Science?â€• Journal of Chemical Education, 2020, 97, 1215-1215.	1.1	0
45	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.	1.5	0
46	Organic chemistry as representation. Foundations of Chemistry, 2021, 23, 59-68.	0.4	0