Charles H Reynolds

List of Publications by Year
in descending order

56	3,928	186265 28	155660 55
papers	citations	h-index	g-index

56	56	56	5372
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The role of ligand efficiency metrics in drug discovery. Nature Reviews Drug Discovery, 2014, 13, 105-121.	46.4	849
2	An improved set of mndo parameters for sulfur. Journal of Computational Chemistry, 1986, 7, 140-143.	3.3	250
3	Ligand Binding Efficiency: Trends, Physical Basis, and Implications. Journal of Medicinal Chemistry, 2008, 51, 2432-2438.	6.4	250
4	Performance of Similarity Measures in 2D Fragment-Based Similarity Searching:â€‰ Comparison of Structural Descriptors and Similarity Coefficients. Journal of Chemical Information and Computer Sciences, 2002, 42, 1407-1414.	2.8	189
5	Ligand efficiency and fragment-based drug discovery. Drug Discovery Today, 2009, 14, 278-283.	6.4	173
6	Gadolinium-Loaded Nanoparticles:â€‰ New Contrast Agents for Magnetic Resonance Imaging. Journal of the American Chemical Society, 2000, 122, 8940-8945.	13.7	153
7	The role of molecular size in ligand efficiency. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 4258-4261.	2.2	153
8	2-Amino-3,4-dihydroquinazolines as Inhibitors of BACE-1 (Î²-Site APP Cleaving Enzyme):â€‰ Use of Structure Based Design to Convert a Micromolar Hit into a Nanomolar Lead. Journal of Medicinal Chemistry, 2007, 50, 4261-4264.	6.4	146
9	Thermodynamics of Ligand Binding and Efficiency. ACS Medicinal Chemistry Letters, 2011, 2, 433-437.	2.8	141
10	Validity of Ligand Efficiency Metrics. ACS Medicinal Chemistry Letters, 2014, 5, 616-618.	2.8	112
11	Free Energy Perturbation Study of Octanol/Water Partition Coefficients:â€‰ Comparison with Continuum GB/SA Calculations. Journal of Physical Chemistry B, 1999, 103, 714-726.	2.6	100
12	Discovery of 2-[3,5-Dichloro-4-(5-isopropyl-6-oxo-1,6-dihydropyridazin-3-yloxy)phenyl]-3,5-dioxo-2,3,4,5-tetrahydro[1,2,4]triazine-6-carbonitrile (MGL-3196), a Highly Selective Thyroid Hormone Receptor Î² Agonist in Clinical Trials for the Treatment of Dyslipidemia. Journal of Medicinal Chemistry, 2014, 57, 3912-3923.	6.4	94
13	Assigning the Protonation States of the Key Aspartates in Î²-Secretase Using QM/MM X-ray Structure Refinement. Journal of Chemical Theory and Computation, 2006, 2, 1057-1069.	5.3	89
14	A two-state homology model of the hERG K+ channel: application to ligand binding. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 1737-1741.	2.2	87
15	Modeling the Protonation States of the Catalytic Aspartates in Î²-Secretase. Journal of Medicinal Chemistry, 2004, 47, 5159-5166.	6.4	73
16	Theoretical Study of the Structure and Rotational Flexibility of Diacylhydrazines:Â Implications for the Structure of Nonsteroidal Ecdysone Agonists and Azapeptides. Journal of the American Chemical Society, 1996, 118, 9395-9401.	13.7	69
17	Nonpeptide Urotensin-II Receptor Antagonists: A New Ligand Class Based on Piperazino-Phthalimide and Piperazino-Isoindolinone Subunits. Journal of Medicinal Chemistry, 2009, 52, 7432-7445.	6.4	69
18	GB/SA water model for the Merck molecular force field (MMFF). Journal of Molecular Graphics and Modelling, 2000, 18, 273-282.	2.4	59

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19	Calculation of the Binding Affinity of Î²-Secretase Inhibitors Using the Linear Interaction Energy Method. Journal of Medicinal Chemistry, 2003, 46, 2074-2082.	6.4	58
20	Designing Diverse and Focused Combinatorial Libraries of Synthetic Polymers. ACS Combinatorial Science, 1999, 1, 297-306.	3.3	57
21	Lead Discovery Using Stochastic Cluster Analysis (SCA):â€‰ A New Method for Clustering Structurally Similar Compounds. Journal of Chemical Information and Computer Sciences, 1998, 38, 305-312.	2.8	50
22	Ground states of molecules. 64. .pi.-Complexes as intermediates in reactions. Biomimetic cyclization. Journal of the American Chemical Society, 1984, 106, 1744-1750.	13.7	49
23	Equilibria for the adsorption of antibiotics onto neutral polymeric sorbents: Experimental and modeling studies. Biotechnology and Bioengineering, 1995, 47, 215-226.	3.3	47
24	An AM1 theoretical study of the structure and electronic properties of porphyrin. Journal of Organic Chemistry, 1988, 53, 6061-6064.	3.2	43
25	Structure and relative stability of halogenated carbocations: the C2H4X+ and C4H8X+ (X = fluoro,) Tj ETQq1 1 0.784314 rgBT /Overlo	13.7	42
26	Proteinâ€“Ligand Cocrystal Structures: We Can Do Better. ACS Medicinal Chemistry Letters, 2014, 5, 727-729.	2.8	38
27	Conformational Analysis of the Eight-Membered Ring of the Oxidized Cysteinyl-Cysteine Unit Implicated in Nicotinic Acetylcholine Receptor Ligand Recognition. Journal of the American Chemical Society, 2001, 123, 12664-12669.	13.7	36
28	Ground states of molecules. 61. Relative stabilities of o-, m-, and p-benzyne. Journal of the American Chemical Society, 1983, 105, 3162-3167.	13.7	35
29	Estimating Lipophilicity Using the GB/SA Continuum Solvation Model: A Direct Method for Computing Partition Coefficients. Journal of Chemical Information and Computer Sciences, 1995, 35, 738-742.	2.8	29
30	Macrocyclic BACE inhibitors: Optimization of a micromolar hit to nanomolar leads. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 3158-3160.	2.2	28
31	Ligand efficiency metrics: why all the fuss?. Future Medicinal Chemistry, 2015, 7, 1363-1365.	2.3	27
32	Diversity and Coverage of Structural Sublibraries Selected Using the SAGE and SCA Algorithms. Journal of Chemical Information and Computer Sciences, 2001, 41, 1470-1477.	2.8	23
33	Linear interaction energy models for Î²-secretase (BACE) inhibitors: Role of van der Waals, electrostatic, and continuum-solvation terms. Journal of Molecular Graphics and Modelling, 2006, 24, 475-484.	2.4	23
34	Methyl chloride-formic acid van der Waals complex: a model for carbon as a hydrogen bond donor. Journal of the American Chemical Society, 1990, 112, 7903-7908.	13.7	22
35	Group Additivity in Ligand Binding Affinity: An Alternative Approach to Ligand Efficiency. Journal of Chemical Information and Modeling, 2017, 57, 3086-3093.	5.4	22
36	GB/SA-Based Continuum Solvation Model for Octanol. Journal of Physical Chemistry B, 1997, 101, 10479-10487.	2.6	21

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37	Modeling the reactivity of acrylic acid and acrylate anion with biological nucleophiles. Toxicology Letters, 1989, 47, 241-247.	0.8	20
38	Potent nonpeptide vasopressin receptor antagonists based on oxazino- and thiazinobenzodiazepine templates. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 2747-2752.	2.2	19
39	Modeling the binding affinities of Î²-secretase inhibitors: application to subsite specificity. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 4843-4846.	2.2	18
40	Quantum Mechanical Pairwise Decomposition Analysis of Protein Kinase B Inhibitors: Validating a New Tool for Guiding Drug Design. Journal of Chemical Information and Modeling, 2010, 50, 651-661.	5.4	17
41	Ground states of molecules. 68. The C4H7+ potential surface. Journal of the American Chemical Society, 1984, 106, 6388-6392.	13.7	16
42	An ab initio investigation of the double proton shift in azophenine. Journal of the American Chemical Society, 1989, 111, 3466-3468.	13.7	16
43	Semiempirical MO methods: the middle ground in molecular modeling. Computational and Theoretical Chemistry, 1997, 401, 267-277.	1.5	15
44	Hit Triage Using Efficiency Indices after Screening of Compound Libraries in Drug Discovery. Current Topics in Medicinal Chemistry, 2009, 9, 1718-1724.	2.1	14
45	Tritium migration in tritiated anisole. Journal of the American Chemical Society, 1982, 104, 3244-3246.	13.7	13
46	Chemical Information Based Scaling of Molecular Descriptors:â€‰A Universal Chemical Scale for Library Design and Analysis. Journal of Chemical Information and Computer Sciences, 2002, 42, 879-884.	2.8	13
47	Thermal reorganizations of 1,2:3,4-dibenzotropilidene (5H-dibenzo[a,c]cycloheptene), 7,7'-bi(1,2:3,4-dibenzotropyl) [5,5'-bi(5H-dibenzo[a,c]cycloheptenyl)], and the 1,2:3,4-dibenzotropyl (dibenzo[a,c]cycloheptenyl) free radical. Journal of Organic Chemistry, 1984, 49, 4029-4032.	3.2	10
48	A MINDO/3 study of the ethylene dication. Computational and Theoretical Chemistry, 1986, 136, 209-214.	1.5	9
49	Modelling of shape/size selective separations: AM1 rotational barriers for some substituted benzenes. Computational and Theoretical Chemistry, 1988, 163, 79-88.	1.5	9
50	Improved AMBERâˆ— torsional parameters for the Nâ€“N rotational barrier in diacylhydrazines. Journal of Molecular Graphics and Modelling, 1999, 17, 315-324.	2.4	9
51	Defining Privileged Reagents Using Subsimilarity Comparison. Journal of Chemical Information and Computer Sciences, 2004, 44, 1810-1815.	2.8	9
52	A quantum mechanical approach to ligand binding â€” Calculation of ligandâ€“protein binding affinities for stromelysin-1 (MMP-3) inhibitors. Canadian Journal of Chemistry, 2009, 87, 1480-1484.	1.1	6
53	Hydride affinities of halogen substituted carbocations: the C2H4X+ (X = F, Cl or Br) cations. Computational and Theoretical Chemistry, 1992, 259, 257-263.	1.5	5
54	Combined Molecular Orbital and Group Additivity Approach for Modeling Thermochemical Properties: Application to Hydrazides. Journal of Chemical Information and Computer Sciences, 1994, 34, 671-675.	2.8	2

#	Article	IF	Citations
55	Fragment and protein simulation methods in fragment based drug design. Drug Development Research, 2011, 72, 130-137.	2.9	2
56	In This Issue, Volume 9, Issue 2. ACS Medicinal Chemistry Letters, 2018, 9, 65-65.	2.8	0