Peter Ertl

List of Publications by Year
in descending order

84 papers	8,900 citations	182225 30 h-index	66518 82 g-index
100 all docs	100 docs citations	100 times ranked	11798 citing authors

#	Article	IF	Citations
1	Magic Rings: Navigation in the Ring Chemical Space Guided by the Bioactive Rings. Journal of Chemical Information and Modeling, 2022, 62, 2164-2170.	2.5	16
2	Substituents of life: The most common substituent patterns present in natural products. Bioorganic and Medicinal Chemistry, 2022, 54, 116562.	1.4	7
3	Ring replacement recommender: Ring modifications for improving biological activity. European Journal of Medicinal Chemistry, 2022, 238, 114483.	2.6	3
4	CAVIAR: a method for automatic cavity detection, description and decomposition into subcavities. Journal of Computer-Aided Molecular Design, 2021, 35, 737-750.	1.3	12
5	NP Navigator: A New Look at the Natural Product Chemical Space. Molecular Informatics, 2021, 40, e2100068.	1.4	16
6	The Most Common Functional Groups in Bioactive Molecules and How Their Popularity Has Evolved over Time. Journal of Medicinal Chemistry, 2020, 63, 8408-8418.	2.9	163
7	Artificial intelligence in chemistry and drug design. Journal of Computer-Aided Molecular Design, 2020, 34, 709-715.	1.3	79
8	Identification of Bioisosteric Substituents by a Deep Neural Network. Journal of Chemical Information and Modeling, 2020, 60, 3369-3375.	2.5	5
9	Cheminformatics Analysis of Natural Product Scaffolds: Comparison of Scaffolds Produced by Animals, Plants, Fungi and Bacteria. Molecular Informatics, 2020, 39, e2000017.	1.4	16
10	Craig plot 2.0: an interactive navigation in the substituent bioisosteric space. Journal of Cheminformatics, 2020, 12, 8.	2.8	17
11	Structure-Based and Property-Driven Optimization of N-Aryl Imidazoles toward Potent and Selective Oral RORÎ³t Inhibitors. Journal of Medicinal Chemistry, 2019, 62, 10816-10832.	2.9	15
12	5,5- and 5,6-Membered Spirocyclic Indolinone Hit-Finding Libraries. ACS Combinatorial Science, 2019, 21, 528-536.	3.8	1
13	A Systematic Cheminformatics Analysis of Functional Groups Occurring in Natural Products. Journal of Natural Products, 2019, 82, 1258-1263.	1.5	142
14	Natural product drug delivery: A special challenge?. Progress in Medicinal Chemistry, 2019, 58, 157-187.	4.1	13
15	Reducing the Concepts of Data Science and Machine Learning to Tools for the Bench Chemist. Chimia, 2019, 73, 1001-1005.	0.3	1
16	Chiral Cliffs: Investigating the Influence of Chirality on Binding Affinity. ChemMedChem, 2018, 13, 1315-1324.	1.6	22
17	Construction of a 3D-shaped, natural product like fragment library by fragmentation and diversification of natural products. Bioorganic and Medicinal Chemistry, 2017, 25, 921-925.	1.4	35
18	An algorithm to identify functional groups in organic molecules. Journal of Cheminformatics, 2017, 9, 36.	2.8	75

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19	Evaluation of a Semi-Automated Workflow for Fragment Growing. Journal of Chemical Information and Modeling, 2015, 55, 180-193.	2.5	5
20	Unique Macrocycles in the Taiwan Traditional Chinese Medicine Database. Planta Medica, 2015, 81, 459-466.	0.7	6
21	Wikipedia Chemical Structure Explorer: substructure and similarity searching of molecules from Wikipedia. Journal of Cheminformatics, 2015, 7, 10.	2.8	29
22	Visualization of chemical space for medicinal chemists. Journal of Cheminformatics, 2014, 6, O4.	2.8	3
23	Intuitive Ordering of Scaffolds and Scaffold Similarity Searching Using Scaffold Keys. Journal of Chemical Information and Modeling, 2014, 54, 1617-1622.	2.5	43
24	JSME: a free molecule editor in JavaScript. Journal of Cheminformatics, 2013, 5, 24.	2.8	204
25	Database of bioactive ring systems with calculated properties and its use in bioisosteric design and scaffold hopping. Bioorganic and Medicinal Chemistry, 2012, 20, 5436-5442.	1.4	19
26	IADE: a system for intelligent automatic design of bioisosteric analogs. Journal of Computer-Aided Molecular Design, 2012, 26, 1207-1215.	1.3	18
27	Natural product-likeness score revisited: an open-source, open-data implementation. BMC Bioinformatics, 2012, 13, 106.	1.2	63
28	The Molecule Cloud - compact visualization of large collections of molecules. Journal of Cheminformatics, 2012, 4, 12.	2.8	42
29	Gazing into the crystal ball; the future of computer-aided drug design. Journal of Computer-Aided Molecular Design, 2012, 26, 77-79.	1.3	3
30	The graphical representation of ADME-related molecule properties for medicinal chemists. Drug Discovery Today, 2011, 16, 65-72.	3.2	141
31	Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information. Journal of Computer-Aided Molecular Design, 2011, 25, 533-554.	1.3	453
32	The Scaffold Tree: An Efficient Navigation in the Scaffold Universe. Methods in Molecular Biology, 2010, 672, 245-260.	0.4	21
33	Bioisosteric Replacement and Scaffold Hopping in Lead Generation and Optimization. Molecular Informatics, 2010, 29, 366-385.	1.4	181
34	Molecular structure input on the web. Journal of Cheminformatics, 2010, 2, 1.	2.8	92
35	Compound Set Enrichment: A Novel Approach to Analysis of Primary HTS Data. Journal of Chemical Information and Modeling, 2010, 50, 2067-2078.	2.5	48
36	Computational Analysis of Structureâ€“Activity Relationships. Progress in Medicinal Chemistry, 2010, 49, 113-160.	4.1	20

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37	Estimation of synthetic accessibility score of drug-like molecules based on molecular complexity and fragment contributions. Journal of Cheminformatics, 2009, 1, 8.	2.8	786
38	Natural product-likeness score and its applications in the drug discovery process. Chemistry Central Journal, 2008, 2, .	2.6	2
39	Cheminformatics analysis of natural products: Lessons from nature inspiring the design of new drugs. , 2008, 66, 217-235.		31
40	Natural Product-likeness Score and Its Application for Prioritization of Compound Libraries. Journal of Chemical Information and Modeling, 2008, 48, 68-74.	2.5	271
41	Designing Drugs on the Internet? Free Web Tools and Services Supporting Medicinal Chemistry. Current Topics in Medicinal Chemistry, 2007, 7, 1491-1501.	1.0	24
42	Cheminformatic Analysis of Natural Products and their Chemical Space. Chimia, 2007, 61, 355-360.	0.3	109
43	The Scaffold Tree â˜' Visualization of the Scaffold Universe by Hierarchical Scaffold Classification. Journal of Chemical Information and Modeling, 2007, 47, 47-58.	2.5	322
44	Clustering and Rule-Based Classifications of Chemical Structures Evaluated in the Biological Activity Space. Journal of Chemical Information and Modeling, 2007, 47, 325-336.	2.5	50
45	Estimation of pKa for Druglike Compounds Using Semiempirical and Information-Based Descriptors. Journal of Chemical Information and Modeling, 2007, 47, 450-459.	2.5	70
46	In silico identification of bioisosteric functional groups. Current Opinion in Drug Discovery & Development, 2007, 10, 281-8.	1.9	7
47	Quest for the Rings. In Silico Exploration of Ring Universe To Identify Novel Bioactive Heteroaromatic Scaffolds. Journal of Medicinal Chemistry, 2006, 49, 4568-4573.	2.9	221
48	Applications of Self-Organizing Neural Networks in Virtual Screening and Diversity Selection. Journal of Chemical Information and Modeling, 2006, 46, 2319-2323.	2.5	35
49	Identification and Classification of GPCR Ligands Using Self-Organizing Neural Networks. QSAR and Combinatorial Science, 2005, 24, 270-276.	1.5	20
50	Virtual Computational Chemistry Laboratory â€“ Design and Description. Journal of Computer-Aided Molecular Design, 2005, 19, 453-463.	1.3	1,250
51	Charting biologically relevant chemical space: A structural classification of natural products (SCONP). Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 17272-17277.	3.3	534
52	Computational Chemistry at Novartis. Chimia, 2005, 59, 545-549.	0.3	7
53	Web-based cheminformatics tools deployed via corporate Intranets. Drug Discovery Today Biosilico, 2004, 2, 201-207.	0.7	24
54	ToxizitÃtsvorhersage im Intranet. Nachrichten Aus Der Chemie, 2004, 52, 162-164.	0.0	2

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55	Cheminformatics Analysis of Organic Substituents: Identification of the Most Common Substituents, Calculation of Substituent Properties, and Automatic Identification of Drug-Like Bioisosteric Groups.. ChemInform, 2003, 34, no.	0.1	2
56	Cheminformatics Analysis of Organic Substituents:â€‰ Identification of the Most Common Substituents, Calculation of Substituent Properties, and Automatic Identification of Drug-like Bioisosteric Groups. Journal of Chemical Information and Computer Sciences, 2003, 43, 374-380.	2.8	253
57	Diastereomeric ecdysteroids with a cyclic hemiacetal in the side chain produced by cytochrome P450 in hormonally resistant insect cells. Archives of Biochemistry and Biophysics, 2002, 400, 180-187.	1.4	11
58	Stereoselectivity of 1,3-Dipolar Cycloadditions of d-Erythrose and d-Threose Derived Nitrones with Methyl Acrylate. Synlett, 2001, 2001, 1862-1865.	1.0	14
59	Synthesis of 8-substituted 5H,9H-6-oxa-7-aza-benzocyclononene-10,11-dione-11-O-methyloximes, a new [1,2]-oxazonine ring system. Tetrahedron Letters, 2000, 41, 1381-1384.	0.7	4
60	Fast Calculation of Molecular Polar Surface Area as a Sum of Fragment-Based Contributions and Its Application to the Prediction of Drug Transport Properties. Journal of Medicinal Chemistry, 2000, 43, 3714-3717.	2.9	2,413
61	World Wide Web-based system for the calculation of substituent parameters and substituent similarity searches. Journal of Molecular Graphics and Modelling, 1998, 16, 11-13.	1.3	28
62	WWW-based chemical information system. Computational and Theoretical Chemistry, 1997, 419, 113-120.	1.5	33
63	Simple Quantum Chemical Parameters as an Alternative to the Hammett Sigma Constants in QSAR Studies. QSAR and Combinatorial Science, 1997, 16, 377-382.	1.4	48
64	Synthesis of Spiroisoxazolines by 1,3-Dipolar Cycloaddition. Molecules, 1997, 2, 57-61.	1.7	11
65	Complexation of phthalides and substituted 3-benzylidene phthalides with Cr(CO)6. Journal of Organometallic Chemistry, 1994, 464, 65-69.	0.8	6
66	Synthesis of Ferrocenyl-Substituted Heterocycles: The Beneficial Effect of the Microwave Irradiation. Collection of Czechoslovak Chemical Communications, 1994, 59, 175-185.	1.0	26
67	Regio- and Stereoselective Reduction of 3,5-Disubstituted 3a,6a-Dihydro-4H-pyrrolo[3,4-d]isoxazole-4,6(5H)-diones with Sodium Borohydride. Liebigs Annalen Der Chemie, 1993, 1993, 1047-1050.	0.8	9
68	Concepts of sterically hindered resonance and buttressing effect: gas-phase acidities of methyl-substituted benzoic acids and basicities of their methyl esters. Journal of the American Chemical Society, 1993, 115, 12071-12078.	6.6	62
69	C2H4B2N2: a prediction of ring and chain [boron-nitrogen-carbon] compounds. Journal of the American Chemical Society, 1992, 114, 10955-10956.	6.6	15
70	Electron distribution on an intramolecular hydrogen bond: A semiempirical AM1 study. Structural Chemistry, 1992, 3, 301-305.	1.0	7
71	Preparation and stereoselectivity of 1,3-dipolar cycloaddition of C-glycosyl nitrones to N-arylmaleimides. Monatshefte FÃ¼r Chemie, 1992, 123, 999-1013.	0.9	18
72	Regio- and stereo-selective synthesis of carbohydrate isoxazolidines by 1,3-dipolar cycloaddition of nitrones to 5,6-di-deoxy-1,2- O -isopropylidene-l±- d - xylo -hex-5-enofuranose. Carbohydrate Research, 1992, 226, 49-56.	1.1	15

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73	Regio- and stereoselectivity in the 1,3-dipolar cycloaddition of C,N-diarylnitrones to 3,3-methylene-5,5-dimethyl-2-pyrrolidinone. Monatshefte FÃ¼r Chemie, 1991, 122, 977-985.	0.9	14
74	Energies of excited states calculated with MNDO and AM1. Monatshefte FÃ¼r Chemie, 1991, 122, 1015-1018.	0.9	5
75	Regioselectivity in the 1,3-dipolar cycloaddition of nitrile oxides to 3,3-methylene-5,5-dimethyl-2-pyrrolidinone. Monatshefte FÃ¼r Chemie, 1991, 122, 821-828.	0.9	16
76	MNDO CI study of the photoisomerization about polar double bonds. International Journal of Quantum Chemistry, 1990, 38, 231-238.	1.0	5
77	MNDO and AM1 study of molecular geometries in excited states. Collection of Czechoslovak Chemical Communications, 1990, 55, 1399-1403.	1.0	8
78	Influence of solvent polarity on the dual fluorescence of p-N,N-dimethylaminobenzonitrile: An AM1 theoretical study. Collection of Czechoslovak Chemical Communications, 1990, 55, 1891-1895.	1.0	2
79	MNDO CI study of the photoisomerization of pentadieniminium. Collection of Czechoslovak Chemical Communications, 1990, 55, 2874-2879.	1.0	2
80	Calculation of energies of excited states with MNDO CI method. Collection of Czechoslovak Chemical Communications, 1989, 54, 1433-1436.	1.0	4
81	MNDO CI study of vertical excitation energies. Computational and Theoretical Chemistry, 1988, 165, 1-8.	1.5	19
82	MNDO study of the E-Z isomerization mechanism of H2C=NR molecules (R = H, CH3, NH2, OH, F). Collection of Czechoslovak Chemical Communications, 1988, 53, 2986-2994.	1.0	4
83	A quantum-chemical study of structure of H3O+ in electronically excited states. Collection of Czechoslovak Chemical Communications, 1986, 51, 738-745.	1.0	3
84	Quantum-chemical study of photochemical E-Z isomerization of methanimine and its fluoro derivatives. Collection of Czechoslovak Chemical Communications, 1985, 50, 1283-1290.	1.0	0