Peter Ertl

List of Publications by Citations

86 papers	6,750 citations	28 h-index	82 g-index
100 ext. papers	7,729 ext. citations	5 avg, IF	6.04 L-index

#	Paper	IF	Citations
86	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, 3714-7	8.3	1960
85	Virtual computational chemistry laboratory--design and description. *Journal of Computer-Aided Molecular Design*, **2005**, 19, 453-63	4.2	1061
84	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, 17272-7	11.5	489
83	Estimation of synthetic accessibility score of drug-like molecules based on molecular complexity and fragment contributions. *Journal of Cheminformatics*, **2009**, 1, 8	8.6	370
82	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, 533-54	4.2	311
81	The scaffold tree--visualization of the scaffold universe by hierarchical scaffold classification. *Journal of Chemical Information and Modeling*, **2007**, 47, 47-58	6.1	288
80	Cheminformatics analysis of organic substituents: 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, 374-80		212
79	Natural product-likeness score and its application for prioritization of compound libraries. *Journal of Chemical Information and Modeling*, **2008**, 48, 68-74	6.1	205
78	Quest for the rings. In silico exploration of ring universe to identify novel bioactive heteroaromatic scaffolds. *Journal of Medicinal Chemistry*, **2006**, 49, 4568-73	8.3	198
77	JSME: a free molecule editor in JavaScript. *Journal of Cheminformatics*, **2013**, 5, 24	8.6	149
76	Bioisosteric Replacement and Scaffold Hopping in Lead Generation and Optimization. *Molecular Informatics*, **2010**, 29, 366-85	3.8	129
75	The graphical representation of ADME-related molecule properties for medicinal chemists. *Drug Discovery Today*, **2011**, 16, 65-72	8.8	94
74	Cheminformatic Analysis of Natural Products and their Chemical Space. *Chimia*, **2007**, 61, 355-360	1.3	93
73	Molecular structure input on the web. *Journal of Cheminformatics*, **2010**, 2, 1	8.6	83
72	Estimation of pKa for druglike compounds using semiempirical and information-based descriptors. *Journal of Chemical Information and Modeling*, **2007**, 47, 450-9	6.1	59
71	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	16.4	49
70	A Systematic Cheminformatics Analysis of Functional Groups Occurring in Natural Products. *Journal of Natural Products*, **2019**, 82, 1258-1263	4.9	48

69	Natural product-likeness score revisited: an open-source, open-data implementation. *BMC Bioinformatics*, **2012**, 13, 106	3.6	48
68	The Most Common Functional Groups in Bioactive Molecules and How Their Popularity Has Evolved over Time. *Journal of Medicinal Chemistry*, **2020**, 63, 8408-8418	8.3	47
67	Clustering and rule-based classifications of chemical structures evaluated in the biological activity space. *Journal of Chemical Information and Modeling*, **2007**, 47, 325-36	6.1	44
66	Compound set enrichment: a novel approach to analysis of primary HTS data. *Journal of Chemical Information and Modeling*, **2010**, 50, 2067-78	6.1	43
65	An algorithm to identify functional groups in organic molecules. *Journal of Cheminformatics*, **2017**, 9, 36	8.6	41
64	Simple Quantum Chemical Parameters as an Alternative to the Hammett Sigma Constants in QSAR Studies. *QSAR and Combinatorial Science*, **1997**, 16, 377-382		38
63	Intuitive ordering of scaffolds and scaffold similarity searching using scaffold keys. *Journal of Chemical Information and Modeling*, **2014**, 54, 1617-22	6.1	36
62	WWW-based chemical information system. *Computational and Theoretical Chemistry*, **1997**, 419, 113-120		31
61	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	3.4	30
60	Applications of self-organizing neural networks in virtual screening and diversity selection. *Journal of Chemical Information and Modeling*, **2006**, 46, 2319-23	6.1	30
59	The Molecule Cloud - compact visualization of large collections of molecules. *Journal of Cheminformatics*, **2012**, 4, 12	8.6	28
58	Polar Surface Area. *Methods and Principles in Medicinal Chemistry*, **2007**, 111-126	0.4	25
57	Wikipedia Chemical Structure Explorer: substructure and similarity searching of molecules from Wikipedia. *Journal of Cheminformatics*, **2015**, 7, 10	8.6	24
56	World Wide Web-based system for the calculation of substituent parameters and substituent similarity searches. *Journal of Molecular Graphics and Modelling*, **1998**, 16, 11-3, 36	2.8	24
55	Cheminformatics analysis of natural products: lessons from nature inspiring the design of new drugs. *Progress in Drug Research Fortschritte Der Arzneimittelforschung Progres Des Recherches Pharmaceutiques*, **2008**, 66, 217, 219-35		22
54	Designing drugs on the internet? Free web tools and services supporting medicinal chemistry. *Current Topics in Medicinal Chemistry*, **2007**, 7, 1491-501	3	22
53	Synthesis of Ferrocenyl-Substituted Heterocycles: The Beneficial Effect of the Microwave Irradiation. *Collection of Czechoslovak Chemical Communications*, **1994**, 59, 175-185		22
52	Web-based cheminformatics tools deployed via corporate Intranets. *Drug Discovery Today Biosilico*, **2004**, 2, 201-207		21

51	MNDO CI study of vertical excitation energies. *Computational and Theoretical Chemistry*, **1988**, 165, 1-8		19
50	The scaffold tree: an efficient navigation in the scaffold universe. *Methods in Molecular Biology*, **2011**, 672, 245-60	1.4	18
49	IADE: a system for intelligent automatic design of bioisosteric analogs. *Journal of Computer-Aided Molecular Design*, **2012**, 26, 1207-15	4.2	16
48	Preparation and stereoselectivity of 1,3-dipolar cycloaddition of C-glycosyl nitrones to N-arylmaleimides. *Monatshefte F□ Chemie*, **1992**, 123, 999-1013	1.4	16
47	Database of bioactive ring systems with calculated properties and its use in bioisosteric design and scaffold hopping. *Bioorganic and Medicinal Chemistry*, **2012**, 20, 5436-42	3.4	15
46	Chiral Cliffs: Investigating the Influence of Chirality on Binding Affinity. *ChemMedChem*, **2018**, 13, 1315-1324	3.7	14
45	Computational analysis of structure-activity relationships. *Progress in Medicinal Chemistry*, **2010**, 49, 113-60	7.9	14
44	Identification and Classification of GPCR Ligands Using Self-Organizing Neural Networks. *QSAR and Combinatorial Science*, **2005**, 24, 270-276		14
43	Stereoselectivity of 1,3-Dipolar Cycloadditions of d-Erythrose and d-Threose Derived Nitrones with Methyl Acrylate. *Synlett*, **2001**, 2001, 1862-1865	2.2	14
42	Regioselectivity in the 1,3-dipolar cycloaddition of nitrile oxides to 3,3-methylene-5,5-dimethyl-2-pyrrolidinone. *Monatshefte F□ Chemie*, **1991**, 122, 821-828	1.4	13
41	Regio- and stereo-selective synthesis of carbohydrate isoxazolidines by 1,3-dipolar cycloaddition of nitrones to 5,6-dideoxy-1,2-O-isopropylidene- alpha-D-xylo-hex-5-enofuranose. *Carbohydrate Research*, **1992**, 226, 49-56	2.9	13
40	Regio- and stereoselectivity in the 1,3-dipolar cycloaddition of C,N-diarylnitrones to 3,3-methylene-5,5-dimethyl-2-pyrrolidinone. *Monatshefte F□ Chemie*, **1991**, 122, 977-985	1.4	12
39	C2H4B2N2: a prediction of ring and chain [boron-nitrogen-carbon] compounds. *Journal of the American Chemical Society*, **1992**, 114, 10955-10956	16.4	12
38	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, 180-7	4.1	11
37	Natural product drug delivery: A special challenge?. *Progress in Medicinal Chemistry*, **2019**, 58, 157-187	7.3	10
36	Synthesis of Spiroisoxazolines by 1,3-Dipolar Cycloaddition. *Molecules*, **1997**, 2, 57-61	4.8	9
35	NP Navigator: A New Look at the Natural Product Chemical Space. *Molecular Informatics*, **2021**, 40, e2100068	3.8	9
34	Cheminformatics Analysis of Natural Product Scaffolds: Comparison of Scaffolds Produced by Animals, Plants, Fungi and Bacteria. *Molecular Informatics*, **2020**, 39, e2000017	3.8	8

33	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		8
32	MNDO and AM1 study of molecular geometries in excited states. *Collection of Czechoslovak Chemical Communications*, **1990**, 55, 1399-1403		7
31	Structure-Based and Property-Driven Optimization of -Aryl Imidazoles toward Potent and Selective Oral RORγ Inhibitors. *Journal of Medicinal Chemistry*, **2019**, 62, 10816-10832	8.3	6
30	Electron distribution on an intramolecular hydrogen bond: A semiempirical AM1 study. *Structural Chemistry*, **1992**, 3, 301-305	1.8	6
29	In silico identification of bioisosteric functional groups. *Current Opinion in Drug Discovery & Development*, **2007**, 10, 281-8		6
28	Craig plot 2.0: an interactive navigation in the substituent bioisosteric space. *Journal of Cheminformatics*, **2020**, 12, 8	8.6	5
27	Energies of excited states calculated with MNDO and AM1. *Monatshefte Für Chemie*, **1991**, 122, 1015-1018	1.4	5
26	Unique macrocycles in the Taiwan traditional Chinese medicine database. *Planta Medica*, **2015**, 81, 459-66	3.1	4
25	Evaluation of a semi-automated workflow for fragment growing. *Journal of Chemical Information and Modeling*, **2015**, 55, 180-93	6.1	4
24	Complexation of phthalides and substituted 3-benzylidene phthalides with Cr(CO)6. *Journal of Organometallic Chemistry*, **1994**, 464, 65-69	2.3	4
23	MNDO CI study of the photoisomerization about polar double bonds. *International Journal of Quantum Chemistry*, **1990**, 38, 231-238	2.1	4
22	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		4
21	Calculation of energies of excited states with MNDO CI method. *Collection of Czechoslovak Chemical Communications*, **1989**, 54, 1433-1436		4
20	Gazing into the crystal ball; the future of computer-aided drug design. *Journal of Computer-Aided Molecular Design*, **2012**, 26, 77-9	4.2	3
19	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	2	3
18	A quantum-chemical study of structure of H3O+ in electronically excited states. *Collection of Czechoslovak Chemical Communications*, **1986**, 51, 738-745		3
17	Computational Chemistry at Novartis. *Chimia*, **2005**, 59, 545-549	1.3	3
16	Identification of Bioisosteric Substituents by a Deep Neural Network. *Journal of Chemical Information and Modeling*, **2020**, 60, 3369-3375	6.1	2

15	Visualization of chemical space for medicinal chemists. *Journal of Cheminformatics*, **2014**, 6, O4	8.6	2
14	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		2
13	Toxizitätsvorhersage im Intranet. *Nachrichten Aus Der Chemie*, **2004**, 52, 162-164	0.1	2
12	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		2
11	MNDO CI study of the photoisomerization of pentadieniminium. *Collection of Czechoslovak Chemical Communications*, **1990**, 55, 2874-2879		2
10	Magic Rings: Navigation in the Ring Chemical Space Guided by the Bioactive Rings. *Journal of Chemical Information and Modeling*, **2021**,	6.1	2
9	5,5- and 5,6-Membered Spirocyclic Indolinone Hit-Finding Libraries. *ACS Combinatorial Science*, **2019**, 21, 528-536	3.9	1
8	Physicochemical Properties **2012**, 129-139		1
7	Cheminformatics Analysis of Natural Product Scaffolds: Comparison of Scaffolds Produced by Animals, Plants, Fungi and Bacteria		1
6	Reducing the Concepts of Data Science and Machine Learning to Tools for the Bench Chemist. *Chimia*, **2019**, 73, 1001-1005	1.3	1
5	Web-Based Calculation of Molecular Properties1336-1348		1
4	Substituents of life: The most common substituent patterns present in natural products.. *Bioorganic and Medicinal Chemistry*, **2021**, 54, 116562	3.4	0
3	CAVIAR: a method for automatic cavity detection, description and decomposition into subcavities. *Journal of Computer-Aided Molecular Design*, **2021**, 35, 737-750	4.2	0
2	Ring replacement recommender: Ring modifications for improving biological activity. *European Journal of Medicinal Chemistry*, **2022**, 238, 114483	6.8	0
1	World Wide Web-Based Calculation of Substituent Parameters for QSAR Studies **2000**, 267-268		