GyÃ¶rgy G Ferenczy

List of Publications by Year
in descending order

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92	3,015	218677	175258
papers	citations	26 h-index	52 g-index

97	97	97	3063
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The role of quantum chemistry in covalent inhibitor design. International Journal of Quantum Chemistry, 2022, 122, .	2.0	19
2	The Structure-Derived Mechanism of Box H/ACA Pseudouridine Synthase Offers a Plausible Paradigm for Programmable RNA Editing. ACS Catalysis, 2022, 12, 2756-2769.	11.2	5
3	Contribution of hydrophobic interactions to protein mechanical stability. Computational and Structural Biotechnology Journal, 2022, 20, 1946-1956.	4.1	13
4	Allosteric Molecular Switches in Metabotropic Glutamate Receptors. ChemMedChem, 2021, 16, 81-93.	3.2	12
5	Mechanistic and thermodynamic characterization of oxathiazolones as potent and selective covalent immunoproteasome inhibitors. Computational and Structural Biotechnology Journal, 2021, 19, 4486-4496.	4.1	4
6	Binding Mode Prediction and Virtual Screening Applications by Covalent Docking. Methods in Molecular Biology, 2021, 2266, 73-88.	0.9	3
7	Discovery of selective fragment-sized immunoproteasome inhibitors. European Journal of Medicinal Chemistry, 2021, 219, 113455.	5.5	9
8	WIDOCK: a reactive docking protocol for virtual screening of covalent inhibitors. Journal of Computer-Aided Molecular Design, 2021, 35, 223-244.	2.9	21
9	Fragment-Sized and Bidentate (Immuno)Proteasome Inhibitors Derived from Cysteine and Threonine Targeting Warheads. Cells, 2021, 10, 3431.	4.1	6
10	Allosteric activation of metabotropic glutamate receptor 5. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2624-2632.	3.5	7
11	Thermodynamic profiling for fragment-based lead discovery and optimization. Expert Opinion on Drug Discovery, 2020, 15, 117-129.	5.0	7
12	Affinity and Selectivity Assessment of Covalent Inhibitors by Free Energy Calculations. Journal of Chemical Information and Modeling, 2020, 60, 6579-6594.	5.4	24
13	Covalent Docking in Drug Discovery: Scope and Limitations. Current Pharmaceutical Design, 2020, 26, 5684-5699.	1.9	12
14	A detailed mechanism of the oxidative half-reaction of<scp>d</scp>-amino acid oxidase: another route for flavin oxidation. Organic and Biomolecular Chemistry, 2019, 17, 7973-7984.	2.8	14
15	Discovery of Immunoproteasome Inhibitors Using Large-Scale Covalent Virtual Screening. Molecules, 2019, 24, 2590.	3.8	11
16	Catalytic Mechanism and Covalent Inhibition of UDP-N-Acetylglucosamine Enolpyruvyl Transferase (MurA): Implications to the Design of Novel Antibacterials. Journal of Chemical Information and Modeling, 2019, 59, 5161-5173.	5.4	21
17	The role of water and protein flexibility in the structure-based virtual screening of allosteric GPCR modulators: an mGlu5 receptor case study. Journal of Computer-Aided Molecular Design, 2019, 33, 787-797.	2.9	9
18	Synthesis and Biochemical Evaluation of Lid-Open D-Amino Acid Oxidase Inhibitors. Molecules, 2019, 24, 290.	3.8	1

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19	Structure-Based Optimization Strategies for G Protein-Coupled Receptor (GPCR) Allosteric Modulators: A Case Study from Analyses of New Metabotropic Glutamate Receptor 5 (mGlu₅) X-ray Structures. Journal of Medicinal Chemistry, 2019, 62, 207-222.	6.4	67
20	Fragment-Based Approaches for Allosteric Metabotropic Glutamate Receptor (mGluR) Modulators. Current Topics in Medicinal Chemistry, 2019, 19, 1768-1781.	2.1	7
21	Discovery of isatin and 1H-indazol-3-ol derivatives as d-amino acid oxidase (DAAO) inhibitors. Bioorganic and Medicinal Chemistry, 2018, 26, 1579-1587.	3.0	10
22	Validation of tautomeric and protomeric binding modes by free energy calculations. A case study for the structure based optimization of d-amino acid oxidase inhibitors. Journal of Computer-Aided Molecular Design, 2018, 32, 331-345.	2.9	7
23	Discovery of d-amino acid oxidase inhibitors based on virtual screening against the lid-open enzyme conformation. Bioorganic and Medicinal Chemistry Letters, 2018, 28, 1693-1698.	2.2	4
24	A road map for prioritizing warheads for cysteine targeting covalent inhibitors. European Journal of Medicinal Chemistry, 2018, 160, 94-107.	5.5	80
25	Quantum chemical calculations support pseudouridine synthase reaction through a glycal intermediate and provide details of the mechanism. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	5
26	Drug discovery strategies and the preclinical development of D-amino-acid oxidase inhibitors as antipsychotic therapies. Expert Opinion on Drug Discovery, 2018, 13, 973-982.	5.0	9
27	Comparative Evaluation of Covalent Docking Tools. Journal of Chemical Information and Modeling, 2018, 58, 1441-1458.	5.4	101
28	Force generation by titin folding. Protein Science, 2017, 26, 1380-1390.	7.6	28
29	Optical Trapping Nanometry of Hypermethylated CPG-Island DNA. Biophysical Journal, 2017, 112, 512-522.	0.5	31
30	Binding thermodynamics discriminates fragments from druglike compounds: a thermodynamic description of fragment-based drug discovery. Drug Discovery Today, 2017, 22, 681-689.	6.4	16
31	Structure-based Virtual Screening Approaches in Kinase-directed Drug Discovery. Current Topics in Medicinal Chemistry, 2017, 17, 2235-2259.	2.1	63
32	Exact density functional and wave function embedding schemes based on orbital localization. Journal of Chemical Physics, 2016, 145, .	3.0	80
33	Dynamics of Transitions through the Molten-Globule State Enhance Contractility of Titin. Biophysical Journal, 2016, 110, 301a-302a.	0.5	0
34	Glossary of terms used in computational drug design, part II (IUPAC Recommendations 2015). Pure and Applied Chemistry, 2016, 88, 239-264.	1.9	12
35	Design Principles for Fragment Libraries: Maximizing the Value of Learnings from Pharma Fragment-Based Drug Discovery (FBDD) Programs for Use in Academia. Journal of Medicinal Chemistry, 2016, 59, 8189-8206.	6.4	182
36	Ensemble docking-based virtual screening yields novel spirocyclic JAK1 inhibitors. Journal of Molecular Graphics and Modelling, 2016, 70, 275-283.	2.4	9

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37	I. Discovery of a novel series of CXCR3 antagonists. Multiparametric optimization of N , N -disubstituted benzylamines. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 5418-5428.	2.2	7
38	II. Discovery of a novel series of CXCR3 antagonists with a beta amino acid core. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 5429-5437.	2.2	2
39	Mechanosensitive Structural States of Titin. Biophysical Journal, 2016, 110, 185a.	0.5	0
40	Structure-Based Consensus Scoring Scheme for Selecting Class A Aminergic GPCR Fragments. Journal of Chemical Information and Modeling, 2016, 56, 412-422.	5.4	16
41	On the enthalpic preference of fragment binding. MedChemComm, 2016, 7, 332-337.	3.4	26
42	Discovery of Subtype Selective Janus Kinase (JAK) Inhibitors by Structure-Based Virtual Screening. Journal of Chemical Information and Modeling, 2016, 56, 234-247.	5.4	23
43	A desirability function-based scoring scheme for selecting fragment-like class A aminergic GPCR ligands. Journal of Computer-Aided Molecular Design, 2015, 29, 59-66.	2.9	8
44	A QM/MM program using frozen localized orbitals and the Huzinaga equation. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	6
45	Property-based characterization of kinase-like ligand space for library design and virtual screening. MedChemComm, 2015, 6, 1898-1904.	3.4	6
46	The impact of binding thermodynamics on medicinal chemistry optimizations. Future Medicinal Chemistry, 2015, 7, 1285-1303.	2.3	8
47	Strictly Localised Molecular Orbitals in QM/MM Methods. , 2014, , 71-89.		2
48	Calculation of waveâ€functions with frozen orbitals in mixed quantum mechanics/molecular mechanics methods. Part I. Application of the Huzinaga equation. Journal of Computational Chemistry, 2013, 34, 854-861.	3.3	7
49	Calculation of waveâ€functions with frozen orbitals in mixed quantum mechanics/molecular mechanics methods. II. Application of the local basis equation. Journal of Computational Chemistry, 2013, 34, 862-869.	3.3	5
50	How Are Fragments Optimized? A Retrospective Analysis of 145 Fragment Optimizations. Journal of Medicinal Chemistry, 2013, 56, 2478-2486.	6.4	61
51	Thermodynamics of Fragment Binding. Journal of Chemical Information and Modeling, 2012, 52, 1039-1045.	5.4	64
52	Chapter 2. Thermodynamics of Ligand Binding. RSC Drug Discovery Series, 2012, , 23-79.	0.3	4
53	Enthalpic Efficiency of Ligand Binding. Journal of Chemical Information and Modeling, 2010, 50, 1536-1541.	5.4	56
54	Thermodynamics guided lead discovery and optimization. Drug Discovery Today, 2010, 15, 919-932.	6.4	122

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55	Optimization of selected molecular orbitals in group basis sets. Journal of Chemical Physics, 2009, 130, 134108.	3.0	6
56	Prolyl Oligopeptidase Inhibition byN-Acyl-pro-pyrrolidine-type Molecules. Journal of Medicinal Chemistry, 2008, 51, 7514-7522.	6.4	33
57	Toward a Consistent Treatment of Polarization in Model QM/MM Calculations. Journal of Physical Chemistry A, 2008, 112, 12151-12156.	2.5	13
58	Classical Polarization in Hybrid QM/MM Methods. Journal of Physical Chemistry A, 2006, 110, 6487-6497.	2.5	51
59	Modeling Polarization through Induced Atomic Charges. Journal of Physical Chemistry A, 2001, 105, 11470-11479.	2.5	34
60	Intra- and intermolecular interactions in crystals of polar molecules. A study by the mixed quantum mechanical/molecular mechanical SCMP-NDDO method. Journal of Computational Chemistry, 2001, 22, 1679-1690.	3.3	14
61	Fully polarizable QM/MM calculations: An application to the nonbonded iodine-oxygen interaction in dimethyl-2-iodobenzoylphosphonate. Journal of Computational Chemistry, 2000, 21, 478-482.	3.3	13
62	Electronic structure of doped fourfold coordinated amorphous semiconductors. Midgap states in amorphous carbon. Computational and Theoretical Chemistry, 1999, 463, 175-180.	1.5	3
63	Quantum mechanical study of the hydride shift step in the xylose isomerase catalytic reaction with the fragment self-consistent field method. International Journal of Quantum Chemistry, 1999, 75, 215-222.	2.0	12
64	Towards improved force fields: III. Polarization through modified atomic charges. Journal of Computational Chemistry, 1999, 20, 704-712.	3.3	35
65	Colour Polymorphism of a Bis(quinoxaline) Compound. European Journal of Organic Chemistry, 1999, 1999, 2119-2125.	2.4	13
66	Colour Polymorphism of a Bis(quinoxaline) Compound. European Journal of Organic Chemistry, 1999, 1999, 2119-2125.	2.4	2
67	Imidazo[1,2-c]quinazolines with lipid peroxidation inhibitory effect. European Journal of Medicinal Chemistry, 1998, 33, 181-187.	5.5	25
68	Theory of dopant pairs in four-fold coordinated amorphous semiconductors. Journal of Non-Crystalline Solids, 1998, 227-230, 367-371.	3.1	25
69	Valence electronic structure of selected polyorganosiloxanes; x-ray photoelectron spectroscopy and quantum chemical studies. Journal of Physics Condensed Matter, 1997, 9, 4781-4790.	1.8	7
70	Monte Carlo simulation of amorphous systems with the fragment self-consistent field method. Computational and Theoretical Chemistry, 1997, 398-399, 129-133.	1.5	3
71	Toward Improved Force Fields. 1. Multipole-Derived Atomic Charges. Journal of Physical Chemistry A, 1997, 101, 5437-5445.	2.5	43
72	Toward Improved Force Fields. 2. Effective Distributed Multipoles. Journal of Physical Chemistry A, 1997, 101, 5446-5455.	2.5	41

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73	Antioxidant Building Blocks I. The Unexpected C-Acetylation of 2,6-Di-tert-butylphenol with Isopropenyl Acetate. Collection of Czechoslovak Chemical Communications, 1996, 61, 1244-1247.	1.0	2
74	Ion beam induced chemical effects in organosilicon polymers. Nuclear Instruments & Methods in Physics Research B, 1996, 116, 299-304.	1.4	24
75	The self-consistent nonorthogonal group function approach in reduced basis frozen-core calculations. International Journal of Quantum Chemistry, 1996, 57, 361-367.	2.0	3
76	Approximate energy-evaluating schemes for a system of weakly overlapping group functions. International Journal of Quantum Chemistry, 1995, 53, 485-493.	2.0	5
77	Estimation of impurity profiles of drugs and related materials. 12. Isolation and identification of an isomeric impurity in danazol. Pharmaceutical Research, 1995, 12, 295-298.	3.5	23
78	Molecular Electrostatics. Chemical Reviews, 1995, 95, 829-847.	47.7	389
79	The neglect of diatomic differential overlap (NDDO) fragment self-consistent field method for the treatment of very large covalent systems. International Journal of Quantum Chemistry, 1994, 52, 227-236.	2.0	4
80	Quantum mechanical computations on very large molecular systems: The local self-consistent field method. Journal of Computational Chemistry, 1994, 15, 269-282.	3.3	299
81	Prediction of carcinogenicity from molecular structure; modification and reinvestigation of the method. Cancer Letters, 1994, 81, 201-207.	7.2	1
82	Transferable net atomic charges from a distributed multipole analysis for the description of electrostatic properties: a case study of saturated hydrocarbons. The Journal of Physical Chemistry, 1993, 97, 6628-6636.	2.9	74
83	Molecular wavefunctions from chemical bonds: the fragment self-consistent field theory. Computational and Theoretical Chemistry, 1992, 261, 55-62.	1.5	7
84	Protein electrostatics on personal computers. Computational and Theoretical Chemistry, 1992, 256, 113-123.	1.5	5
85	Methods for determining the reliability of semiempirical electrostatic potentials and potential derived charges. Computational and Theoretical Chemistry, 1992, 256, 249-269.	1.5	29
86	NDDO fragment self-consistent field approximation for large electronic systems. Journal of Computational Chemistry, 1992, 13, 830-837.	3.3	85
87	Charges derived from distributed multipole series. Journal of Computational Chemistry, 1991, 12, 913-917.	3.3	65
88	Semiempirical AM1 electrostatic potentials and AM1 electrostatic potential derived charges: A comparison withab initio values. Journal of Computational Chemistry, 1990, 11, 159-169.	3.3	157
89	Calculations on electrostatic properties of HY zeolite. Journal of the Chemical Society, Faraday Transactions, 1990, 86, 3461-3466.	1.7	11
90	The active site of cytochrome P-450 nifedipine oxidase: a model-building study. Journal of Molecular Graphics, 1989, 7, 206-211.	1.1	28

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91	Calculation of electrostatic potentials and fields inside zeolite cavities. Collection of Czechoslovak Chemical Communications, 1988, 53, 2308-2319.	1.0	10
92	The molecular structure of uracil: an electron diffraction study. Journal of Molecular Structure, 1986, 140, 71-77.	3.6	77