Gyorgy M Keseru

List of Publications by Year
in descending order

242 papers	8,868 citations	61984 43 h-index	56724 83 g-index
259 all docs	259 docs citations	259 times ranked	11056 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	Warheads for designing covalent inhibitors and chemical probes. , 2022, , 47-73.		2
3	Computational Medicinal Chemistry to Target GPCRs. , 2022, , 84-114.		3
4	Electrophilic warheads in covalent drug discovery: an overview. Expert Opinion on Drug Discovery, 2022, 17, 413-422.	5.0	29
5	A covalent strategy to target intrinsically disordered proteins: Discovery of novel tau aggregation inhibitors. European Journal of Medicinal Chemistry, 2022, 231, 114163.	5.5	8
6	The Impact of the Secondary Binding Pocket on the Pharmacology of Class A GPCRs. Frontiers in Pharmacology, 2022, 13, 847788.	3.5	10
7	Designed Peptide Inhibitors of STEP Phosphataseâ€“GluA2 AMPA Receptor Interaction Enhance the Cognitive Performance in Rats. Journal of Medicinal Chemistry, 2022, 65, 217-233.	6.4	3
8	A stepwise one-pot synthesis of aliphatic thiols and their derivatives from acrylamides and sulfur. Organic and Biomolecular Chemistry, 2022, 20, 4361-4368.	2.8	2
9	Allosteric Molecular Switches in Metabotropic Glutamate Receptors. ChemMedChem, 2021, 16, 81-93.	3.2	12
10	Assessment of Tractable Cysteines for Covalent Targeting by Screening Covalent Fragments. ChemBioChem, 2021, 22, 743-753.	2.6	19
11	GPCRdb in 2021: integrating GPCR sequence, structure and function. Nucleic Acids Research, 2021, 49, D335-D343.	14.5	254
12	Novel potent (dihydro)benzofuranyl piperazines as human histamine receptor ligands â€“ Functional characterization and modeling studies on H3 and H4 receptors. Bioorganic and Medicinal Chemistry, 2021, 30, 115924.	3.0	5
13	The future of covalent inhibition. Annual Reports in Medicinal Chemistry, 2021, 56, 267-284.	0.9	0
14	Synthesis and characterization of new fluorescent boro-Î²-carboline dyes. RSC Advances, 2021, 11, 12802-12807.	3.6	8
15	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
16	Binding Mode Prediction and Virtual Screening Applications by Covalent Docking. Methods in Molecular Biology, 2021, 2266, 73-88.	0.9	3
17	Continuous-Flow Synthesis of Thioureas, Enabled by Aqueous Polysulfide Solution. Molecules, 2021, 26, 303.	3.8	9
18	Fragment evolution for GPCRs: the role of secondary binding sites in optimization. Chemical Communications, 2021, 57, 10516-10519.	4.1	5

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19	Vinylation of Î±-Aminoazoles with Triethylamine: A General Strategy to Construct Azolo[1,5-a]pyrimidines with a Nonsubstituted Ethylidene Fragment. Organic Letters, 2021, 23, 2664-2669.	4.6	16
20	Exploring protein hotspots by optimized fragment pharmacophores. Nature Communications, 2021, 12, 3201.	12.8	28
21	Controlling the selectivity of aminergic GPCR ligands from the extracellular vestibule. Bioorganic Chemistry, 2021, 111, 104832.	4.1	8
22	Fragment-Based Optimization of Dihydropyrazino-Benzimidazolones as Metabotropic Glutamate Receptor-2 Positive Allosteric Modulators against Migraine. Journal of Medicinal Chemistry, 2021, 64, 8607-8620.	6.4	1
23	Discovery of selective fragment-sized immunoproteasome inhibitors. European Journal of Medicinal Chemistry, 2021, 219, 113455.	5.5	9
24	Convenient Multicomponent Oneâ€Pot Synthesis of 2â€Iminothiazolines and 2â€Aminothiazoles Using Elemental Sulfur Under Aqueous Conditions. European Journal of Organic Chemistry, 2021, 2021, 3587-3597.	2.4	10
25	WIDOCK: a reactive docking protocol for virtual screening of covalent inhibitors. Journal of Computer-Aided Molecular Design, 2021, 35, 223-244.	2.9	21
26	Chromatographyâ€Free Multicomponent Synthesis of Thioureas Enabled by Aqueous Solution of Elemental Sulfur. ChemistryOpen, 2021, 10, 16-27.	1.9	10
27	Consensus Virtual Screening Identified [1,2,4]Triazolo[1,5â€b]isoquinolines As MELK Inhibitor Chemotypes. ChemMedChem, 2021, , .	3.2	3
28	Natural Apocarotenoids and Their Synthetic Glycopeptide Conjugates Inhibit SARS-CoV-2 Replication. Pharmaceuticals, 2021, 14, 1111.	3.8	7
29	PharmacoSTORM nanoscale pharmacology reveals cariprazine binding on Islands of Calleja granule cells. Nature Communications, 2021, 12, 6505.	12.8	24
30	Fragment-Sized and Bidentate (Immuno)Proteasome Inhibitors Derived from Cysteine and Threonine Targeting Warheads. Cells, 2021, 10, 3431.	4.1	6
31	Allosteric activation of metabotropic glutamate receptor 5. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2624-2632.	3.5	7
32	Thermodynamic profiling for fragment-based lead discovery and optimization. Expert Opinion on Drug Discovery, 2020, 15, 117-129.	5.0	7
33	Discovery of dihydropyrazino-benzimidazole derivatives as metabotropic glutamate receptor-2 (mGluR2) positive allosteric modulators (PAMs). European Journal of Medicinal Chemistry, 2020, 186, 111881.	5.5	4
34	Controlling receptor function from the extracellular vestibule of G-protein coupled receptors. Chemical Communications, 2020, 56, 14167-14170.	4.1	11
35	Crystallographic and electrophilic fragment screening of the SARS-CoV-2 main protease. Nature Communications, 2020, 11, 5047.	12.8	376
36	An electrophilic warhead library for mapping the reactivity and accessibility of tractable cysteines in protein kinases. European Journal of Medicinal Chemistry, 2020, 207, 112836.	5.5	28

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37	Small molecule inhibitors of RAS proteins with oncogenic mutations. Cancer and Metastasis Reviews, 2020, 39, 1107-1126.	5.9	15
38	Targeting STAT3 and STAT5 in Cancer. Cancers, 2020, 12, 2002.	3.7	7
39	Structural impact of GTP binding on downstream KRAS signaling. Chemical Science, 2020, 11, 9272-9289.	7.4	25
40	Affinity and Selectivity Assessment of Covalent Inhibitors by Free Energy Calculations. Journal of Chemical Information and Modeling, 2020, 60, 6579-6594.	5.4	24
41	Benchmark Sets for Binding Hot Spot Identification in Fragment-Based Ligand Discovery. Journal of Chemical Information and Modeling, 2020, 60, 6612-6623.	5.4	10
42	Bromo-Cyclobutenaminones as New Covalent UDP-N-Acetylglucosamine Enolpyruvyl Transferase (MurA) Inhibitors. Pharmaceuticals, 2020, 13, 362.	3.8	8
43	The European Research Network on Signal Transduction (ERNEST): Toward a Multidimensional Holistic Understanding of G Protein-Coupled Receptor Signaling. ACS Pharmacology and Translational Science, 2020, 3, 361-370.	4.9	15
44	Discovery of a novel kinase hinge binder fragment by dynamic undocking. RSC Medicinal Chemistry, 2020, 11, 552-558.	3.9	10
45	Application of Boroisoquinoline Fluorophores as Chemodosimeters for Fluoride Ion and Pd (0). Materials, 2020, 13, 199.	2.9	6
46	Comparative reactivity analysis of small-molecule thiol surrogates. Bioorganic and Medicinal Chemistry, 2020, 28, 115357.	3.0	26
47	Cysteine specific bioconjugation with benzyl isothiocyanates. RSC Advances, 2020, 10, 14928-14936.	3.6	21
48	Covalent fragment libraries in drug discovery. Drug Discovery Today, 2020, 25, 983-996.	6.4	65
49	Covalent Docking in Drug Discovery: Scope and Limitations. Current Pharmaceutical Design, 2020, 26, 5684-5699.	1.9	12
50	Targeting an Intrinsically Disordered Protein by Covalent Modification. Methods in Molecular Biology, 2020, 2141, 835-854.	0.9	1
51	Discovery of Immunoproteasome Inhibitors Using Large-Scale Covalent Virtual Screening. Molecules, 2019, 24, 2590.	3.8	11
52	A novel three-component reaction between isocyanides, alcohols or thiols and elemental sulfur: a mild, catalyst-free approach towards O-thiocarbamates and dithiocarbamates. Beilstein Journal of Organic Chemistry, 2019, 15, 1523-1533.	2.2	20
53	Structural Implications of STAT3 and STAT5 SH2 Domain Mutations. Cancers, 2019, 11, 1757.	3.7	45
54	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

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55	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
56	Design and characterization of a heterocyclic electrophilic fragment library for the discovery of cysteine-targeted covalent inhibitors. MedChemComm, 2019, 10, 263-267.	3.4	50
57	Why Some Targets Benefit from beyond Rule of Five Drugs. Journal of Medicinal Chemistry, 2019, 62, 10005-10025.	6.4	75
58	Analysis of tractable allosteric sites in G protein-coupled receptors. Scientific Reports, 2019, 9, 6180.	3.3	31
59	DUckCov: a Dynamic Undockingâ€Based Virtual Screening Protocol for Covalent Binders. ChemMedChem, 2019, 14, 1011-1021.	3.2	18
60	Synthesis and Biochemical Evaluation of Lid-Open D-Amino Acid Oxidase Inhibitors. Molecules, 2019, 24, 290.	3.8	1
61	The impact of binding site waters on the activity/selectivity trade-off of Janus kinase 2 (JAK2) inhibitors. Bioorganic and Medicinal Chemistry, 2019, 27, 1497-1508.	3.0	5
62	Covalent Inhibition of the Histamine H3 Receptor. Molecules, 2019, 24, 4541.	3.8	5
63	Direct Targeting Options for STAT3 and STAT5 in Cancer. Cancers, 2019, 11, 1930.	3.7	65
64	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
65	Fragment Based Optimization of Metabotropic Glutamate Receptor 2 (mGluR2) Positive Allosteric Modulators in the Absence of Structural Information. Journal of Medicinal Chemistry, 2019, 62, 234-246.	6.4	11
66	Fragment-Based Approaches for Allosteric Metabotropic Glutamate Receptor (mGluR) Modulators. Current Topics in Medicinal Chemistry, 2019, 19, 1768-1781.	2.1	7
67	Pharmacologic inhibition of STAT5 in acute myeloid leukemia. Leukemia, 2018, 32, 1135-1146.	7.2	112
68	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
69	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
70	When fragments link: a bibliometric perspective on the development of fragment-based drug discovery. Drug Discovery Today, 2018, 23, 1596-1609.	6.4	36
71	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
72	Emerging therapeutic targets in myeloproliferative neoplasms and peripheral T-cell leukemia and lymphomas. Expert Opinion on Therapeutic Targets, 2018, 22, 45-57.	3.4	19

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73	Synthesis and fluorescent properties of boroisoquinolines, a new family of fluorophores. RSC Advances, 2018, 8, 38598-38605.	3.6	6
74	Heterocyclic electrophiles as new MurA inhibitors. Archiv Der Pharmazie, 2018, 351, e1800184.	4.1	22
75	A road map for prioritizing warheads for cysteine targeting covalent inhibitors. European Journal of Medicinal Chemistry, 2018, 160, 94-107.	5.5	80
76	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
77	Fingerprint-Based Machine Learning Approach to Identify Potent and Selective 5-HT2BR Ligands. Molecules, 2018, 23, 1137.	3.8	19
78	Expanding the medicinal chemistry synthetic toolbox. Nature Reviews Drug Discovery, 2018, 17, 709-727.	46.4	391
79	Binding kinetics of cariprazine and aripiprazole at the dopamine D3 receptor. Scientific Reports, 2018, 8, 12509.	3.3	29
80	Comparative Evaluation of Covalent Docking Tools. Journal of Chemical Information and Modeling, 2018, 58, 1441-1458.	5.4	101
81	Spiro[pyrrolidine-3,3â€²-oxindoles] as 5-HT 7 receptor ligands. Bioorganic and Medicinal Chemistry Letters, 2018, 28, 2418-2421.	2.2	11
82	Computational Modeling of Drugs for Alzheimerâ€™s Disease: Design of Serotonin 5-HT6 Antagonists. Neuromethods, 2018, , 419-461.	0.3	0
83	Discovery and Preclinical Characterization of 3-((4-(4-Chlorophenyl)-7-fluoroquinoline-3-yl)sulfonyl)benzonitrile, a Novel Non-acetylenic Metabotropic Glutamate Receptor 5 (mGluR5) Negative Allosteric Modulator for Psychiatric Indications. Journal of Medicinal Chemistry, 2017, 60, 2470-2484.	6.4	26
84	Discovery of 4-amino-3-arylsulfoquinolines, a novel non-acetylenic chemotype of metabotropic glutamate 5 (mGlu 5) receptor negative allosteric modulators. European Journal of Medicinal Chemistry, 2017, 133, 240-254.	5.5	8
85	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
86	What is the future for fragment-based drug discovery?. Future Medicinal Chemistry, 2017, 9, 1457-1460.	2.3	9
87	Breakthroughs in Medicinal Chemistry: New Targets and Mechanisms, New Drugs, New Hopes. Molecules, 2017, 22, 743.	3.8	3
88	Spiro[pyrrolidine-3,3â€²-oxindoles] and Their Indoline Analogues as New 5-HT6 Receptor Chemotypes. Molecules, 2017, 22, 2221.	3.8	15
89	Structure-based Virtual Screening Approaches in Kinase-directed Drug Discovery. Current Topics in Medicinal Chemistry, 2017, 17, 2235-2259.	2.1	63
90	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

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91	Structure-based discovery and binding site analysis of histamine receptor ligands. Expert Opinion on Drug Discovery, 2016, 11, 1165-1185.	5.0	12
92	The first synthesis of isoxazolo[3,4-c]pyridine-7-ones. Tetrahedron Letters, 2016, 57, 4401-4404.	1.4	1
93	Identification of 8â€Hydroxyquinoline Derivatives Active Against Somatic V658F Mutant JAK1â€Dependent Cells. Archiv Der Pharmazie, 2016, 349, 925-933.	4.1	7
94	Ensemble docking-based virtual screening yields novel spirocyclic JAK1 inhibitors. Journal of Molecular Graphics and Modelling, 2016, 70, 275-283.	2.4	9
95	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
96	The influence of 5-HT 2A activity on a 5-HT 2C specific in vivo assay used for early identification of multiple acting SERT and 5-HT 2C receptor ligands. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 914-920.	2.2	2
97	4-Aryl-3-arylsulfonyl-quinolines as negative allosteric modulators of metabotropic GluR5 receptors: From HTS hit to development candidate. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 1249-1252.	2.2	16
98	On the enthalpic preference of fragment binding. MedChemComm, 2016, 7, 332-337.	3.4	26
99	The first synthesis of furo[2,3- c]pyridazin-4(1 H)-one derivatives. Tetrahedron Letters, 2016, 57, 64-66.	1.4	5
100	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
101	Thieno[2,3- b]pyridines as negative allosteric modulators of metabotropic GluR5 receptors: Lead optimization. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 1724-1729.	2.2	14
102	Is there a link between selectivity and binding thermodynamics profiles?. Drug Discovery Today, 2015, 20, 86-94.	6.4	41
103	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
104	Cell-based and virtual fragment screening for adrenergic Î±2C receptor agonists. Bioorganic and Medicinal Chemistry, 2015, 23, 3991-3999.	3.0	11
105	Property-based characterization of kinase-like ligand space for library design and virtual screening. MedChemComm, 2015, 6, 1898-1904.	3.4	6
106	The impact of binding thermodynamics on medicinal chemistry optimizations. Future Medicinal Chemistry, 2015, 7, 1285-1303.	2.3	8
107	Dynamics and structural determinants of ligand recognition of the 5-HT6 receptor. Journal of Computer-Aided Molecular Design, 2015, 29, 1137-1149.	2.9	5
108	Identification of Novel Histamine H4 Ligands by Virtual Screening on Molecular Dynamics Ensembles. Molecular Informatics, 2014, 33, 264-268.	2.5	7

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109	Design of novel multiple-acting ligands towards SERT and 5-HT2C receptors. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 2118-2122.	2.2	4
110	Virtual fragment screening on GPCRs: A case study on dopamine D3 and histamine H4 receptors. European Journal of Medicinal Chemistry, 2014, 77, 38-46.	5.5	49
111	Validity of Ligand Efficiency Metrics. ACS Medicinal Chemistry Letters, 2014, 5, 616-618.	2.8	112
112	The role of ligand efficiency metrics in drug discovery. Nature Reviews Drug Discovery, 2014, 13, 105-121.	46.4	849
113	Novel histamine H4receptor ligands and their potential therapeutic applications: an update. Expert Opinion on Therapeutic Patents, 2014, 24, 1185-1197.	5.0	33
114	Multiple Fragment Docking and Linking in Primary and Secondary Pockets of Dopamine Receptors. ACS Medicinal Chemistry Letters, 2014, 5, 1010-1014.	2.8	30
115	Thieno[2,3-b]pyridines as negative allosteric modulators of metabotropic GluR5 receptors: Hit-to-lead optimization. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 3845-3849.	2.2	8
116	Anthropogenic reaction parameters â€“ the missing link between chemical intuition and the available chemical space. Chemical Society Reviews, 2014, 43, 5387-5399.	38.1	34
117	The Jak2 Small Molecule Inhibitor, G6, Reduces the Tumorigenic Potential of T98G Glioblastoma Cells In Vitro and In Vivo. PLoS ONE, 2014, 9, e105568.	2.5	7
118	Structure-Based β-Secretase (BACE1) Inhibitors. Current Pharmaceutical Design, 2014, 20, 3373-3379.	1.9	4
119	Positive Allosteric Modulators for mGluR2 Receptors: A Medicinal Chemistry Perspective. Current Topics in Medicinal Chemistry, 2014, 14, 1771-1788.	2.1	11
120	ADMET Prediction Based on Protein Structures. , 2014, , 287-322.		0
121	Fragment-based lead discovery on G-protein-coupled receptors. Expert Opinion on Drug Discovery, 2013, 8, 811-820.	5.0	10
122	The Impact of Molecular Dynamics Sampling on the Performance of Virtual Screening against GPCRs. Journal of Chemical Information and Modeling, 2013, 53, 2990-2999.	5.4	52
123	Contributions of Molecular Properties to Drug Promiscuity. Journal of Medicinal Chemistry, 2013, 56, 1789-1795.	6.4	144
124	Fragments to link. A multiple docking strategy for second site binders. MedChemComm, 2013, 4, 510-514.	3.4	6
125	How Are Fragments Optimized? A Retrospective Analysis of 145 Fragment Optimizations. Journal of Medicinal Chemistry, 2013, 56, 2478-2486.	6.4	61
126	Comparative evaluation of pKa prediction tools on a drug discovery dataset. Journal of Pharmaceutical and Biomedical Analysis, 2012, 67-68, 63-70.	2.8	38

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127	Histamine H4 receptor ligands and their potential therapeutic applications: an update. Expert Opinion on Therapeutic Patents, 2012, 22, 205-221.	5.0	32
128	The Small Molecule Inhibitor G6 Significantly Reduces Bone Marrow Fibrosis and the Mutant Burden in a Mouse Model of Jak2-Mediated Myelofibrosis. American Journal of Pathology, 2012, 181, 858-865.	3.8	7
129	Bradykinin B1 receptor antagonists: a patent update 2009 â€“ 2012. Expert Opinion on Therapeutic Patents, 2012, 22, 1443-1452.	5.0	9
130	Thermodynamics of Fragment Binding. Journal of Chemical Information and Modeling, 2012, 52, 1039-1045.	5.4	64
131	Impact of Lipophilic Efficiency on Compound Quality. Journal of Medicinal Chemistry, 2012, 55, 1252-1260.	6.4	148
132	Finding the sweet spot: the role of nature and nurture in medicinal chemistry. Nature Reviews Drug Discovery, 2012, 11, 355-365.	46.4	334
133	Chapter 2. Thermodynamics of Ligand Binding. RSC Drug Discovery Series, 2012, , 23-79.	0.3	4
134	Discovery of Novel Histamine H4 and Serotonin Transporter Ligands Using the Topological Feature Tree Descriptor. Journal of Chemical Information and Modeling, 2012, 52, 233-242.	5.4	8
135	Multiple ligand docking by Glide: implications for virtual second-site screening. Journal of Computer-Aided Molecular Design, 2012, 26, 821-834.	2.9	26
136	A46, a benzothiophene-derived compound, suppresses Jak2-mediated pathologic cell growth. Experimental Hematology, 2012, 40, 22-34.	0.4	0
137	Identification of novel SAR properties of the Jak2 small molecule inhibitor G6: Significance of the para-hydroxyl orientation. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 1402-1407.	2.2	8
138	Quinolinyl- and phenantridinyl-acetamides as bradykinin B1 receptor antagonists. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 3095-3099.	2.2	21
139	Discovery of cariprazine (RGH-188): A novel antipsychotic acting on dopamine D3/D2 receptors. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 3437-3440.	2.2	75
140	Antioxidant activity-guided phytochemical investigation of Artemisia gmelinii Webb. ex Stechm.: Isolation and spectroscopic challenges of 3,5-O-dicaffeoyl (epi?) quinic acid and its ethyl ester. Journal of Pharmaceutical and Biomedical Analysis, 2012, 59, 83-89.	2.8	18
141	Cell Death Induced by the Jak2 Inhibitor, G6, Correlates with Cleavage of Vimentin Filaments. Biochemistry, 2011, 50, 7774-7786.	2.5	6
142	The Jak2 Inhibitor, G6, Alleviates Jak2-V617Fâ€“Mediated Myeloproliferative Neoplasia by Providing Significant Therapeutic Efficacy to the Bone Marrow. Neoplasia, 2011, 13, 1058-1068.	5.3	11
143	Homology modeling and binding site assessment of the human P-glycoprotein. Future Medicinal Chemistry, 2011, 3, 297-307.	2.3	17
144	Integration of Virtual and High Throughput Screening in Lead Discovery Settings. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 889-897.	1.1	37

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145	In silicosite of metabolism prediction of cytochrome P450-mediated biotransformations. Expert Opinion on Drug Metabolism and Toxicology, 2011, 7, 299-312.	3.3	52
146	Special issue in flow chemistry. Molecular Diversity, 2011, 15, 603-604.	3.9	1
147	The Stilbenoid Tyrosine Kinase Inhibitor, G6, Suppresses Jak2-V617F-mediated Human Pathological Cell Growth in Vitro and in Vivo. Journal of Biological Chemistry, 2011, 286, 4280-4291.	3.4	15
148	The Jak2 Kinase Inhibitor, G6, Reduces the Mutant Burden and Reverses Marrow Fibrosis in a Mouse Model of Jak2-V617F Mediated PMF,. Blood, 2011, 118, 3858-3858.	1.4	0
149	LC Determination of Peroxynitrite Scavenging Activity of Phenols from Salvia spp.. Chromatographia, 2010, 71, 51-59.	1.3	2
150	Enthalpic Efficiency of Ligand Binding. Journal of Chemical Information and Modeling, 2010, 50, 1536-1541.	5.4	56
151	Site of metabolism prediction on cytochrome P450 2C9: a knowledge-based docking approach. Journal of Computer-Aided Molecular Design, 2010, 24, 399-408.	2.9	35
152	Thermodynamics guided lead discovery and optimization. Drug Discovery Today, 2010, 15, 919-932.	6.4	122
153	Hit-to-lead optimization of disubstituted oxadiazoles and tetrazoles as mGluR5 NAMs. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 3737-3741.	2.2	20
154	Carbamoyloximes as novel non-competitive mGlu5 receptor antagonists. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 4371-4375.	2.2	21
155	Structure-Function Correlation of G6, a Novel Small Molecule Inhibitor of Jak2. Journal of Biological Chemistry, 2010, 285, 31399-31407.	3.4	11
156	Molecular Dynamics Simulation at High Sodium Chloride Concentration: Toward the Inactive Conformation of the Human Adenosine A2A Receptor. Journal of Physical Chemistry Letters, 2010, 1, 1008-1013.	4.6	8
157	Virtual Fragment Docking by Glide: a Validation Study on 190 Proteinâ^'Fragment Complexes. Journal of Chemical Information and Modeling, 2010, 50, 1165-1172.	5.4	102
158	Recent developments on JAK2 inhibitors: a patent review. Expert Opinion on Therapeutic Patents, 2010, 20, 471-495.	5.0	34
159	The influence of lead discovery strategies on the properties of drug candidates. Nature Reviews Drug Discovery, 2009, 8, 203-212.	46.4	543
160	Identification of a novel inhibitor of JAK2 tyrosine kinase by structure-based virtual screening. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 3598-3601.	2.2	43
161	Hit-to-lead optimization of pyrrolo[1,2-a]quinoxalines as novel cannabinoid type 1 receptor antagonists. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 3471-3475.	2.2	35
162	Histamine H4 receptor ligands and their potential therapeutic applications. Expert Opinion on Therapeutic Patents, 2009, 19, 119-135.	5.0	22

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163	Binding mode analysis and enrichment studies on homology models of the human histamine H4 receptor. European Journal of Medicinal Chemistry, 2008, 43, 1059-1070.	5.5	43
164	Activation Mechanism of the Human Histamine H4 Receptor - An Explicit Membrane Molecular Dynamics Simulation Study. Journal of Chemical Information and Modeling, 2008, 48, 1199-1210.	5.4	37
165	Discovery of Novel Human Histamine H4 Receptor Ligands by Large-Scale Structure-Based Virtual Screening. Journal of Medicinal Chemistry, 2008, 51, 3145-3153.	6.4	97
166	Application of the BD ACTOneâ„¢ Technology for the High-Throughput Screening of Gs-Coupled Receptor Antagonists. Journal of Biomolecular Screening, 2007, 12, 1068-1073.	2.6	16
167	A High Throughput Luminescent Assay for Glycogen Synthase Kinase-3Î² Inhibitors. Assay and Drug Development Technologies, 2007, 5, 75-84.	1.2	107
168	Impact of Ligand Protonation on Virtual Screening against Î²-Secretase (BACE1). Journal of Chemical Information and Modeling, 2007, 47, 2366-2373.	5.4	37
169	Selective NR1/2BN-Methyl-d-aspartate Receptor Antagonists among Indole-2-carboxamides and Benzimidazole-2-carboxamides. Journal of Medicinal Chemistry, 2007, 50, 901-914.	6.4	43
170	Novel sulfonamides having dual dopamine D2 and D3 receptor affinity show in vivo antipsychotic efficacy with beneficial cognitive and EPS profile. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 5340-5344.	2.2	17
171	Effective virtual screening protocol for CYP2C9 ligands using a screening site constructed from flurbiprofen and S-warfarin pockets. Journal of Computer-Aided Molecular Design, 2007, 21, 539-548.	2.9	10
172	Ensemble Docking into Flexible Active Sites. Critical Evaluation of FlexE against JNK-3 and Î²-Secretaseâ€. Journal of Chemical Information and Modeling, 2006, 46, 1795-1805.	5.4	48
173	A neural network based classification scheme for cytotoxicity predictions:Validation on 30,000 compounds. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 1037-1039.	2.2	18
174	Binding mode analysis of the NADH cofactor in nitric oxide reductase: A theoretical study. Journal of Molecular Graphics and Modelling, 2006, 25, 363-372.	2.4	5
175	Hit discovery and hit-to-lead approaches. Drug Discovery Today, 2006, 11, 741-748.	6.4	212
176	Functional virtual screening of estrogen receptor Î± modulators by FlexX-Pharm. Computational and Theoretical Chemistry, 2005, 725, 239-242.	1.5	4
177	Solid-phase synthesis of 6-hydroxy-2,4-diaminoquinazolines. Tetrahedron, 2005, 61, 9375-9380.	1.9	10
178	Identification of Nitric Oxide Donors by Biomimetic HTS Application. Combinatorial Chemistry and High Throughput Screening, 2005, 8, 347-352.	1.1	3
179	Virtual Screening for Î²-Secretase (BACE1) Inhibitors Reveals the Importance of Protonation States at Asp32 and Asp228. Journal of Medicinal Chemistry, 2005, 48, 3749-3755.	6.4	85
180	Comparative Virtual and Experimental High-Throughput Screening for Glycogen Synthase Kinase-3Î² Inhibitors. Journal of Medicinal Chemistry, 2005, 48, 7946-7959.	6.4	72

#	Article	IF	Citations
181	Protonation state of Asp30 exerts crucial influence over surface loop rearrangements responsible for NO release in nitrophorin 4. FEBS Letters, 2005, 579, 5392-5398.	2.8	22
182	A neural network based prediction of octanolâ€“water partition coefficients using atomic5 fragmental descriptors. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 851-853.	2.2	36
183	Oxamides as novel NR2B selective NMDA receptor antagonists. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 3953-3956.	2.2	42
184	Optimization of virtual screening protocols: FlexX based virtual screening for COX-2 inhibitors reveals the importance of tailoring screen parameters. Computational and Theoretical Chemistry, 2004, 676, 1-5.	1.5	2
185	Homology modelling and binding site mapping of the human histamine H1 receptor. European Journal of Medicinal Chemistry, 2004, 39, 959-967.	5.5	33
186	Solid-phase synthesis of an N -(phenylalkyl)cinnamide library via Hornerâ€“Wadsworthâ€“Emmons reaction. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 1279-1281.	2.2	9
187	Structure / function / SAR and molecular design. Molecular Diversity, 2003, 7, 1.	3.9	1
188	Recent Advances in the Prediction of Bloodâ€“Brain Partitioning from Molecular Structure. Journal of Pharmaceutical Sciences, 2003, 92, 360-370.	3.3	98
189	Prediction of hERG potassium channel affinity by traditional and hologram qSAR methods. Bioorganic and Medicinal Chemistry Letters, 2003, 13, 2773-2775.	2.2	126
190	Synthesis of Vinca Alkaloids and Related Compounds. 100. Stereoselective Oxidation Reactions of Compounds with the Aspidospermane and Quebrachamine Ring System. First Synthesis of Some Alkaloids Containing the Epoxy Ring1a. Journal of Organic Chemistry, 2002, 67, 7255-7260.	3.2	20
191	A neural network based virtual screening of cytochrome P450 3A4 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2002, 12, 419-421.	2.2	69
192	Solvent and ligand effects on selective mono- and dilithiation of 1-(chlorophenyl)pyrroles and 1-(methoxyphenyl)pyrrolesâ€Šâ€. Journal of the Chemical Society, Perkin Transactions 1, 2001, , 1039-1043.	1.3	29
193	High-Throughput Prediction of Bloodâ^'Brain Partitioning:â€‰ A Thermodynamic Approach. Journal of Chemical Information and Computer Sciences, 2001, 41, 120-128.	2.8	70
194	Fully Flexible Low-Mode Docking:â€‰ Application to Induced Fit in HIV Integrase. Journal of the American Chemical Society, 2001, 123, 12708-12709.	13.7	100
195	Distinct behavior of mutant triosephosphate isomerase in hemolysate and in isolated form: molecular basis of enzyme deficiency. Blood, 2001, 98, 3106-3112.	1.4	34
196	Hessian-free low-mode conformational search for large-scale protein loop optimization: application to c-jun N-terminal kinase JNK3. Journal of Computational Chemistry, 2001, 22, 21-30.	3.3	58
197	Unusually large reactivity differences in the transformation of cyclopropane lactones to 1-aminocyclopropane-1-phosphonic acids and their carboxylic acid analogues. Heteroatom Chemistry, 2001, 12, 90-96.	0.7	10
198	A virtual high throughput screen for high affinity cytochrome P450cam substrates. Implications for in silico prediction of drug metabolism. , 2001, 15, 649-657.		42

#	Article	IF	Citations
199	Construction of a 3D model of oligopeptidase B, a potential processing enzyme in prokaryotes. Journal of Molecular Graphics and Modelling, 2000, 18, 7-17.	2.4	26
200	Metalloporphyrin catalyzed oxidation of n-hydroxyguanidines: a biomimetic model for the H2O2-dependent activity of nitric oxide synthase. Bioorganic and Medicinal Chemistry Letters, 2000, 10, 1775-1777.	2.2	11
201	Cytochrome P450 Catalyzed Nitric Oxide Synthesis: A Theoretical Study. Journal of Biomolecular Structure and Dynamics, 2000, 17, 759-767.	3.5	13
202	A Neural Network Based Virtual High Throughput Screening Test for the Prediction of CNS Activity. Combinatorial Chemistry and High Throughput Screening, 2000, 3, 535-540.	1.1	18
203	Effect of a trifluoromethyl group on molecular structure: Competitive mono- and dilithiation of 1-[(trifluoromethyl)phenyl]pyrroles. Tetrahedron, 1999, 55, 7881-7892.	1.9	18
204	Enantiomeric recognition of Î±-(1-naphthyl)ethylammonium perchlorate by enantiomerically pure dimethylphenazino-18-crown-6 ligand in solid and gas phases. Tetrahedron: Asymmetry, 1999, 10, 1995-2005.	1.8	14
205	Metalloporphyrin catalysed biomimetic oxidation of aryl benzyl ethers. Implications for lignin peroxidase catalysis. Tetrahedron, 1999, 55, 4457-4466.	1.9	14
206	A semiempirical approach to hydrogen bonding networks. Application of the Cyclic Cluster Model to organic crystals. Computational and Theoretical Chemistry, 1999, 463, 169-174.	1.5	4
207	Inhibitors of cytochrome P450 catalyzed insecticide metabolism: A rational approach. International Journal of Quantum Chemistry, 1999, 73, 123-135.	2.0	13
208	Piperonyl butoxide-mediated inhibition of cytochrome P450-catalysed insecticide metabolism: a rational approach. Pest Management Science, 1999, 55, 1004-1006.	0.4	1
209	Role of Proximal His93 in Nitric Oxide Binding to Metmyoglobin. Application of Continuum Solvation in Monte Carlo Protein Simulations. Biochemistry, 1999, 38, 6614-6622.	2.5	9
210	Chemical Models of Cytochrome P450 Catalyzed Insecticide Metabolism. Application to the Oxidative Metabolism of Carbamate Insecticides. Journal of Agricultural and Food Chemistry, 1999, 47, 762-769.	5.2	20
211	Communication to the editor piperonyl butoxide-mediated inhibition of cytochrome P450-catalysed insecticide metabolism: A rational approach. Pest Management Science, 1999, 55, 1004-1006.	0.4	3
212	Synthesis of Acerogenin C and (+)-Acerogenin A, Two Macrocyclic Diarylheptanoid Constituents ofAcer nikoense. European Journal of Organic Chemistry, 1998, 1998, 521-524.	2.4	21
213	Stereoelectronic Control on the Coordination of Substrates to Globin Proteins. The Role of Proximal His93 on the NO Release from Myoglobin. Journal of the American Chemical Society, 1998, 120, 7991-7992.	13.7	17
214	Synthesis of Isoplagiochin Aâ€. Journal of Organic Chemistry, 1997, 62, 3666-3670.	3.2	12
215	Cytochrome P-450 Catalyzed Insecticide Metabolism. Prediction of Regio- and Stereoselectivity in the Primer Metabolism of Carbofuran:Â A Theoretical Study. Journal of the American Chemical Society, 1997, 119, 5126-5131.	13.7	24
216	On the Conformation of Tiazofurin Analogues. Journal of Medicinal Chemistry, 1997, 40, 4154-4159.	6.4	29

#	Article	IF	Citations
217	1-(2,4,6-Tri-tert-butylphenyl)-3-methylphosphole:Â A Phosphole with a Significantly Flattened Phosphorus Pyramid Having Pronounced Characteristics of Aromaticity. Journal of the American Chemical Society, 1997, 119, 5095-5099.	13.7	95
218	Steric vs. electrostatic effects in the nucleophilic addition to a hindered cyclohexanone. Structural Chemistry, 1997, 8, 257-261.	2.0	5
219	Nuclear Magnetic Resonance and Molecular Modeling Study on Mycophenolic Acid:Â Implications for Binding to Inosine Monophosphate Dehydrogenase. Journal of Medicinal Chemistry, 1996, 39, 1236-1242.	6.4	17
220	Theoretical studies on long-range substituent effects in the reduction of 7-norbornanones. Journal of the Chemical Society Perkin Transactions II, 1996, , 2231-2234.	0.9	2
221	On the anomalous behaviour of certain 1-(4-methoxyphenyl)azetidin-2-ones towards cerium(IV) ammonium nitrate (CAN). Structure-reactivity studies. Tetrahedron, 1996, 52, 771-782.	1.9	10
222	Molecular similarity analysis on biologically active macrocyclic bis(bibenzyls). Journal of Molecular Recognition, 1996, 9, 133-138.	2.1	7
223	The biological activity of cyclic bis(bibenzyls): a rational approach. Bioorganic and Medicinal Chemistry, 1995, 3, 1511-1517.	3.0	29
224	Molecular asymmetry of macrocyclic bis(bibenzyl)s, natural products from liverwort species. Journal of Molecular Structure, 1995, 356, 143-148.	3.6	6
225	Isolation and Antibacterial Activity of Marchantin A, a Cyclic Bis(bibenzyl) Constituent of HungarianMarchantia polymorpha. Planta Medica, 1995, 61, 387-388.	1.3	41
226	The chemistry of macrocyclic bis(bibenzyls). Natural Product Reports, 1995, 12, 69-75.	10.3	53
227	Conformation of 6H,12H,18H-tribenzo[b,f,j][1,5,9]trithiacyclododecin revisited. Journal of the Chemical Society Perkin Transactions II, 1995, , 935-938.	0.9	0
228	Pyridine-type complexes of transition-metal halides. III: Structural and thermal relationships among the cobalt(II) complexes with halide ions and 2-, 3-, and 4-Methylpyridine, the crystal structure of dibromotetrakis (3-methylpyridine)cobalt(II). Structural Chemistry, 1994, 5, 123-128.	2.0	8
229	Synthesis of Garugamblinâ€2, a Macrocyclic Diarylheptanoid Constituent of Garuga gamblei. Liebigs Annalen Der Chemie, 1994, 1994, 361-364.	0.8	14
230	Designed nucleophilic attack based on molecular electrostatic potential. Tetrahedron Letters, 1994, 35, 9255-9258.	1.4	10
231	Back donation in dichloro-bis(pyridme)-cobalt(II) complexes. Computational and Theoretical Chemistry, 1994, 306, 289-292.	1.5	3
232	On the mechanism of the alkylation of quinoline and naphthyridine derivatives. Journal of the Chemical Society Perkin Transactions II, 1994, , 591-594.	0.9	5
233	Crystal structure and conformation of pakyonol, a macrocyclic bis(bibenzyl) constituent of Mannia fragrans. Journal of the Chemical Society Perkin Transactions II, 1994, , 595-597.	0.9	5
234	The synthesis of garugamblin-1. Tetrahedron, 1993, 49, 4893-4900.	1.9	25

#	Article	IF	Citations
235	On the anomalous behaviour of (3RS,4RS)-[(2RS)-3-acetylthiazolidin-2-yl]-1-(4-methoxyphenyl)azetidin-2-ones towards cerium(IV) ammonium nitrate (CAN). An unprecedented oxidative ring transformation.. Tetrahedron, 1993, 49, 7803-7822.	1.9	15
236	Prediction of antibacterial activity of some diarylheptanoids isolated from Garuga species by molecular mechanics and molecular orbital calculations. Computational and Theoretical Chemistry, 1993, 286, 259-265.	1.5	7
237	Synthesis and revised structure of garuganin III. Journal of Organic Chemistry, 1993, 58, 6725-6728.	3.2	28
238	Determination of the preferred conformation of a macrocyclic bis(bibenzyl) by nuclear magnetic resonance spectroscopy and molecular mechanics calculations. Journal of the Chemical Society Perkin Transactions II, 1993, , 563-566.	0.9	4
239	Total synthesis of plagiochins C and D, macrocyclic bis(bibenzyl) constituents of plagiochila acantophylla. Tetrahedron, 1992, 48, 913-922.	1.9	34
240	Biosynthesis and molecular strain. A computational study on the conformation of cyclic bis(bibenzyl) constituents of liverwort species. Phytochemistry, 1992, 31, 1573-1576.	2.9	18
241	Synthese von Plagiochin A und B, zwei macrocyclische Bis(bibenzylether) ausPlagiochila acantophylla. Liebigs Annalen Der Chemie, 1992, 1992, 1239-1243.	0.8	8
242	Maximizing the integration of virtual and experimental screening in hit discovery. Expert Opinion on Drug Discovery, 0, , 1-12.	5.0	0