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 ligand efficiency metrics in drug discovery. Nature Reviews Drug Discovery, 2014, 13, 105-121.	46.4	849
2	The influence of lead discovery strategies on the properties of drug candidates. Nature Reviews Drug Discovery, 2009, 8, 203-212.	46.4	543
3	Expanding the medicinal chemistry synthetic toolbox. Nature Reviews Drug Discovery, 2018, 17, 709-727.	46.4	391
4	Crystallographic and electrophilic fragment screening of the SARS-CoV-2 main protease. Nature Communications, 2020, 11, 5047.	12.8	376
5	Finding the sweet spot: the role of nature and nurture in medicinal chemistry. Nature Reviews Drug Discovery, 2012, 11, 355-365.	46.4	334
6	GPCRdb in 2021: integrating GPCR sequence, structure and function. Nucleic Acids Research, 2021, 49, D335-D343.	14.5	254
7	Hit discovery and hit-to-lead approaches. Drug Discovery Today, 2006, 11, 741-748.	6.4	212
8	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
9	Impact of Lipophilic Efficiency on Compound Quality. Journal of Medicinal Chemistry, 2012, 55, 1252-1260.	6.4	148
10	Contributions of Molecular Properties to Drug Promiscuity. Journal of Medicinal Chemistry, 2013, 56, 1789-1795.	6.4	144
11	Prediction of hERG potassium channel affinity by traditional and hologram qSAR methods. Bioorganic and Medicinal Chemistry Letters, 2003, 13, 2773-2775.	2.2	126
12	Thermodynamics guided lead discovery and optimization. Drug Discovery Today, 2010, 15, 919-932.	6.4	122
13	Validity of Ligand Efficiency Metrics. ACS Medicinal Chemistry Letters, 2014, 5, 616-618.	2.8	112
14	Pharmacologic inhibition of STAT5 in acute myeloid leukemia. Leukemia, 2018, 32, 1135-1146.	7.2	112
15	A High Throughput Luminescent Assay for Glycogen Synthase Kinase-3Î² Inhibitors. Assay and Drug Development Technologies, 2007, 5, 75-84.	1.2	107
16	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
17	Comparative Evaluation of Covalent Docking Tools. Journal of Chemical Information and Modeling, 2018, 58, 1441-1458.	5.4	101
18	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

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19	Recent Advances in the Prediction of Bloodâ€“Brain Partitioning from Molecular Structure. Journal of Pharmaceutical Sciences, 2003, 92, 360-370.	3.3	98
20	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
21	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
22	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
23	A road map for prioritizing warheads for cysteine targeting covalent inhibitors. European Journal of Medicinal Chemistry, 2018, 160, 94-107.	5.5	80
24	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
25	Why Some Targets Benefit from beyond Rule of Five Drugs. Journal of Medicinal Chemistry, 2019, 62, 10005-10025.	6.4	75
26	Comparative Virtual and Experimental High-Throughput Screening for Glycogen Synthase Kinase-3Î² Inhibitors. Journal of Medicinal Chemistry, 2005, 48, 7946-7959.	6.4	72
27	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
28	A neural network based virtual screening of cytochrome P450 3A4 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2002, 12, 419-421.	2.2	69
29	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
30	Direct Targeting Options for STAT3 and STAT5 in Cancer. Cancers, 2019, 11, 1930.	3.7	65
31	Covalent fragment libraries in drug discovery. Drug Discovery Today, 2020, 25, 983-996.	6.4	65
32	Thermodynamics of Fragment Binding. Journal of Chemical Information and Modeling, 2012, 52, 1039-1045.	5.4	64
33	Structure-based Virtual Screening Approaches in Kinase-directed Drug Discovery. Current Topics in Medicinal Chemistry, 2017, 17, 2235-2259.	2.1	63
34	How Are Fragments Optimized? A Retrospective Analysis of 145 Fragment Optimizations. Journal of Medicinal Chemistry, 2013, 56, 2478-2486.	6.4	61
35	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
36	Enthalpic Efficiency of Ligand Binding. Journal of Chemical Information and Modeling, 2010, 50, 1536-1541.	5.4	56

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37	The chemistry of macrocyclic bis(bibenzyls). Natural Product Reports, 1995, 12, 69-75.	10.3	53
38	In silicosite of metabolism prediction of cytochrome P450-mediated biotransformations. Expert Opinion on Drug Metabolism and Toxicology, 2011, 7, 299-312.	3.3	52
39	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
40	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
41	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
42	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
43	Structural Implications of STAT3 and STAT5 SH2 Domain Mutations. Cancers, 2019, 11, 1757.	3.7	45
44	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
45	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
46	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
47	A virtual high throughput screen for high affinity cytochrome P450cam substrates. Implications for in silico prediction of drug metabolism. , 2001, 15, 649-657.		42
48	Oxamides as novel NR2B selective NMDA receptor antagonists. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 3953-3956.	2.2	42
49	Isolation and Antibacterial Activity of Marchantin A, a Cyclic Bis(bibenzyl) Constituent of HungarianMarchantia polymorpha. Planta Medica, 1995, 61, 387-388.	1.3	41
50	Is there a link between selectivity and binding thermodynamics profiles?. Drug Discovery Today, 2015, 20, 86-94.	6.4	41
51	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
52	Impact of Ligand Protonation on Virtual Screening against Î²-Secretase (BACE1). Journal of Chemical Information and Modeling, 2007, 47, 2366-2373.	5.4	37
53	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
54	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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55	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
56	When fragments link: a bibliometric perspective on the development of fragment-based drug discovery. Drug Discovery Today, 2018, 23, 1596-1609.	6.4	36
57	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
58	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
59	Total synthesis of plagiochins C and D, macrocyclic bis(bibenzyl) constituents of plagiochila acantophylla. Tetrahedron, 1992, 48, 913-922.	1.9	34
60	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
61	Recent developments on JAK2 inhibitors: a patent review. Expert Opinion on Therapeutic Patents, 2010, 20, 471-495.	5.0	34
62	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
63	Homology modelling and binding site mapping of the human histamine H1 receptor. European Journal of Medicinal Chemistry, 2004, 39, 959-967.	5.5	33
64	Novel histamine H4receptor ligands and their potential therapeutic applications: an update. Expert Opinion on Therapeutic Patents, 2014, 24, 1185-1197.	5.0	33
65	Histamine H4 receptor ligands and their potential therapeutic applications: an update. Expert Opinion on Therapeutic Patents, 2012, 22, 205-221.	5.0	32
66	Analysis of tractable allosteric sites in G protein-coupled receptors. Scientific Reports, 2019, 9, 6180.	3.3	31
67	Multiple Fragment Docking and Linking in Primary and Secondary Pockets of Dopamine Receptors. ACS Medicinal Chemistry Letters, 2014, 5, 1010-1014.	2.8	30
68	The biological activity of cyclic bis(bibenzyls): a rational approach. Bioorganic and Medicinal Chemistry, 1995, 3, 1511-1517.	3.0	29
69	On the Conformation of Tiazofurin Analogues. Journal of Medicinal Chemistry, 1997, 40, 4154-4159.	6.4	29
70	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
71	Binding kinetics of cariprazine and aripiprazole at the dopamine D3 receptor. Scientific Reports, 2018, 8, 12509.	3.3	29
72	Electrophilic warheads in covalent drug discovery: an overview. Expert Opinion on Drug Discovery, 2022, 17, 413-422.	5.0	29

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73	Synthesis and revised structure of garuganin III. Journal of Organic Chemistry, 1993, 58, 6725-6728.	3.2	28
74	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
75	Exploring protein hotspots by optimized fragment pharmacophores. Nature Communications, 2021, 12, 3201.	12.8	28
76	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
77	Multiple ligand docking by Glide: implications for virtual second-site screening. Journal of Computer-Aided Molecular Design, 2012, 26, 821-834.	2.9	26
78	On the enthalpic preference of fragment binding. MedChemComm, 2016, 7, 332-337.	3.4	26
79	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
80	Comparative reactivity analysis of small-molecule thiol surrogates. Bioorganic and Medicinal Chemistry, 2020, 28, 115357.	3.0	26
81	The synthesis of garugamblin-1. Tetrahedron, 1993, 49, 4893-4900.	1.9	25
82	Structural impact of GTP binding on downstream KRAS signaling. Chemical Science, 2020, 11, 9272-9289.	7.4	25
83	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
84	Affinity and Selectivity Assessment of Covalent Inhibitors by Free Energy Calculations. Journal of Chemical Information and Modeling, 2020, 60, 6579-6594.	5.4	24
85	PharmacoSTORM nanoscale pharmacology reveals cariprazine binding on Islands of Calleja granule cells. Nature Communications, 2021, 12, 6505.	12.8	24
86	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
87	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
88	Histamine H4 receptor ligands and their potential therapeutic applications. Expert Opinion on Therapeutic Patents, 2009, 19, 119-135.	5.0	22
89	Heterocyclic electrophiles as new MurA inhibitors. Archiv Der Pharmazie, 2018, 351, e1800184.	4.1	22
90	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

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91	Carbamoyloximes as novel non-competitive mGlu5 receptor antagonists. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 4371-4375.	2.2	21
92	Quinolinyl- and phenantridinyl-acetamides as bradykinin B1 receptor antagonists. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 3095-3099.	2.2	21
93	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
94	Cysteine specific bioconjugation with benzyl isothiocyanates. RSC Advances, 2020, 10, 14928-14936.	3.6	21
95	WIDOCK: a reactive docking protocol for virtual screening of covalent inhibitors. Journal of Computer-Aided Molecular Design, 2021, 35, 223-244.	2.9	21
96	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
97	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
98	Hit-to-lead optimization of disubstituted oxadiazoles and tetrazoles as mGluR5 NAMs. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 3737-3741.	2.2	20
99	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
100	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
101	Fingerprint-Based Machine Learning Approach to Identify Potent and Selective 5-HT2BR Ligands. Molecules, 2018, 23, 1137.	3.8	19
102	Assessment of Tractable Cysteines for Covalent Targeting by Screening Covalent Fragments. ChemBioChem, 2021, 22, 743-753.	2.6	19
103	The role of quantum chemistry in covalent inhibitor design. International Journal of Quantum Chemistry, 2022, 122, .	2.0	19
104	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
105	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
106	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
107	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
108	DUckCov: a Dynamic Undockingâ€Based Virtual Screening Protocol for Covalent Binders. ChemMedChem, 2019, 14, 1011-1021.	3.2	18

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109	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
110	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
111	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
112	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
113	Homology modeling and binding site assessment of the human P-glycoprotein. Future Medicinal Chemistry, 2011, 3, 297-307.	2.3	17
114	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
115	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
116	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
117	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
118	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
119	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
120	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
121	Spiro[pyrrolidine-3,3â€²-oxindoles] and Their Indoline Analogues as New 5-HT6 Receptor Chemotypes. Molecules, 2017, 22, 2221.	3.8	15
122	Small molecule inhibitors of RAS proteins with oncogenic mutations. Cancer and Metastasis Reviews, 2020, 39, 1107-1126.	5.9	15
123	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
124	Synthesis of Garugamblinâ€², a Macrocyclic Diarylheptanoid Constituent of Garuga gamblei. Liebigs Annalen Der Chemie, 1994, 1994, 361-364.	0.8	14
125	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
126	Metalloporphyrin catalysed biomimetic oxidation of aryl benzyl ethers. Implications for lignin peroxidase catalysis. Tetrahedron, 1999, 55, 4457-4466.	1.9	14

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127	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
128	Inhibitors of cytochrome P450 catalyzed insecticide metabolism: A rational approach. International Journal of Quantum Chemistry, 1999, 73, 123-135.	2.0	13
129	Cytochrome P450 Catalyzed Nitric Oxide Synthesis: A Theoretical Study. Journal of Biomolecular Structure and Dynamics, 2000, 17, 759-767.	3.5	13
130	Synthesis of Isoplagiochin Aâ€. Journal of Organic Chemistry, 1997, 62, 3666-3670.	3.2	12
131	Structure-based discovery and binding site analysis of histamine receptor ligands. Expert Opinion on Drug Discovery, 2016, 11, 1165-1185.	5.0	12
132	Allosteric Molecular Switches in Metabotropic Glutamate Receptors. ChemMedChem, 2021, 16, 81-93.	3.2	12
133	Covalent Docking in Drug Discovery: Scope and Limitations. Current Pharmaceutical Design, 2020, 26, 5684-5699.	1.9	12
134	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
135	Structure-Function Correlation of G6, a Novel Small Molecule Inhibitor of Jak2. Journal of Biological Chemistry, 2010, 285, 31399-31407.	3.4	11
136	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
137	Cell-based and virtual fragment screening for adrenergic Î±2C receptor agonists. Bioorganic and Medicinal Chemistry, 2015, 23, 3991-3999.	3.0	11
138	Spiro[pyrrolidine-3,3â€²-oxindoles] as 5-HT 7 receptor ligands. Bioorganic and Medicinal Chemistry Letters, 2018, 28, 2418-2421.	2.2	11
139	Discovery of Immunoproteasome Inhibitors Using Large-Scale Covalent Virtual Screening. Molecules, 2019, 24, 2590.	3.8	11
140	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
141	Controlling receptor function from the extracellular vestibule of G-protein coupled receptors. Chemical Communications, 2020, 56, 14167-14170.	4.1	11
142	Positive Allosteric Modulators for mGluR2 Receptors: A Medicinal Chemistry Perspective. Current Topics in Medicinal Chemistry, 2014, 14, 1771-1788.	2.1	11
143	Designed nucleophilic attack based on molecular electrostatic potential. Tetrahedron Letters, 1994, 35, 9255-9258.	1.4	10
144	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

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145	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
146	Solid-phase synthesis of 6-hydroxy-2,4-diaminoquinazolines. Tetrahedron, 2005, 61, 9375-9380.	1.9	10
147	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
148	Fragment-based lead discovery on G-protein-coupled receptors. Expert Opinion on Drug Discovery, 2013, 8, 811-820.	5.0	10
149	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
150	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
151	Discovery of a novel kinase hinge binder fragment by dynamic undocking. RSC Medicinal Chemistry, 2020, 11, 552-558.	3.9	10
152	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
153	Chromatographyâ€Free Multicomponent Synthesis of Thioureas Enabled by Aqueous Solution of Elemental Sulfur. ChemistryOpen, 2021, 10, 16-27.	1.9	10
154	The Impact of the Secondary Binding Pocket on the Pharmacology of Class A GPCRs. Frontiers in Pharmacology, 2022, 13, 847788.	3.5	10
155	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
156	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
157	Bradykinin B1 receptor antagonists: a patent update 2009 â€“ 2012. Expert Opinion on Therapeutic Patents, 2012, 22, 1443-1452.	5.0	9
158	Ensemble docking-based virtual screening yields novel spirocyclic JAK1 inhibitors. Journal of Molecular Graphics and Modelling, 2016, 70, 275-283.	2.4	9
159	What is the future for fragment-based drug discovery?. Future Medicinal Chemistry, 2017, 9, 1457-1460.	2.3	9
160	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
161	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
162	Continuous-Flow Synthesis of Thioureas, Enabled by Aqueous Polysulfide Solution. Molecules, 2021, 26, 303.	3.8	9

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163	Discovery of selective fragment-sized immunoproteasome inhibitors. European Journal of Medicinal Chemistry, 2021, 219, 113455.	5.5	9
164	Synthese von Plagiochin A und B, zwei macrocyclische Bis(bibenzylether) ausPlagiochila acantophylla. Liebigs Annalen Der Chemie, 1992, 1992, 1239-1243.	0.8	8
165	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
166	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
167	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
168	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
169	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
170	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
171	The impact of binding thermodynamics on medicinal chemistry optimizations. Future Medicinal Chemistry, 2015, 7, 1285-1303.	2.3	8
172	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
173	Bromo-Cyclobutenaminones as New Covalent UDP-N-Acetylglucosamine Enolpyruvyl Transferase (MurA) Inhibitors. Pharmaceuticals, 2020, 13, 362.	3.8	8
174	Synthesis and characterization of new fluorescent boro-Î²-carboline dyes. RSC Advances, 2021, 11, 12802-12807.	3.6	8
175	Controlling the selectivity of aminergic GPCR ligands from the extracellular vestibule. Bioorganic Chemistry, 2021, 111, 104832.	4.1	8
176	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
177	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
178	Molecular similarity analysis on biologically active macrocyclic bis(bibenzyls). Journal of Molecular Recognition, 1996, 9, 133-138.	2.1	7
179	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
180	Identification of Novel Histamine H4 Ligands by Virtual Screening on Molecular Dynamics Ensembles. Molecular Informatics, 2014, 33, 264-268.	2.5	7

#	Article	IF	Citations
181	Identification of 8â€Hydroxyquinoline Derivatives Active Against Somatic V658F Mutant JAK1â€Dependent Cells. Archiv Der Pharmazie, 2016, 349, 925-933.	4.1	7
182	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
183	Allosteric activation of metabotropic glutamate receptor 5. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2624-2632.	3.5	7
184	Thermodynamic profiling for fragment-based lead discovery and optimization. Expert Opinion on Drug Discovery, 2020, 15, 117-129.	5.0	7
185	Targeting STAT3 and STAT5 in Cancer. Cancers, 2020, 12, 2002.	3.7	7
186	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
187	Fragment-Based Approaches for Allosteric Metabotropic Glutamate Receptor (mGluR) Modulators. Current Topics in Medicinal Chemistry, 2019, 19, 1768-1781.	2.1	7
188	Natural Apocarotenoids and Their Synthetic Glycopeptide Conjugates Inhibit SARS-CoV-2 Replication. Pharmaceuticals, 2021, 14, 1111.	3.8	7
189	Molecular asymmetry of macrocyclic bis(bibenzyl)s, natural products from liverwort species. Journal of Molecular Structure, 1995, 356, 143-148.	3.6	6
190	Cell Death Induced by the Jak2 Inhibitor, G6, Correlates with Cleavage of Vimentin Filaments. Biochemistry, 2011, 50, 7774-7786.	2.5	6
191	Fragments to link. A multiple docking strategy for second site binders. MedChemComm, 2013, 4, 510-514.	3.4	6
192	Property-based characterization of kinase-like ligand space for library design and virtual screening. MedChemComm, 2015, 6, 1898-1904.	3.4	6
193	Synthesis and fluorescent properties of boroisoquinolines, a new family of fluorophores. RSC Advances, 2018, 8, 38598-38605.	3.6	6
194	Application of Boroisoquinoline Fluorophores as Chemodosimeters for Fluoride Ion and Pd (0). Materials, 2020, 13, 199.	2.9	6
195	Fragment-Sized and Bidentate (Immuno)Proteasome Inhibitors Derived from Cysteine and Threonine Targeting Warheads. Cells, 2021, 10, 3431.	4.1	6
196	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
197	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
198	Steric vs. electrostatic effects in the nucleophilic addition to a hindered cyclohexanone. Structural Chemistry, 1997, 8, 257-261.	2.0	5

#	Article	IF	Citations
199	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
200	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
201	The first synthesis of furo[2,3- c]pyridazin-4(1 H)-one derivatives. Tetrahedron Letters, 2016, 57, 64-66.	1.4	5
202	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
203	Covalent Inhibition of the Histamine H3 Receptor. Molecules, 2019, 24, 4541.	3.8	5
204	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
205	Fragment evolution for GPCRs: the role of secondary binding sites in optimization. Chemical Communications, 2021, 57, 10516-10519.	4.1	5
206	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
207	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
208	Functional virtual screening of estrogen receptor Î± modulators by FlexX-Pharm. Computational and Theoretical Chemistry, 2005, 725, 239-242.	1.5	4
209	Chapter 2. Thermodynamics of Ligand Binding. RSC Drug Discovery Series, 2012, , 23-79.	0.3	4
210	Design of novel multiple-acting ligands towards SERT and 5-HT2C receptors. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 2118-2122.	2.2	4
211	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
212	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
213	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
214	Structure-Based β-Secretase (BACE1) Inhibitors. Current Pharmaceutical Design, 2014, 20, 3373-3379.	1.9	4
215	Back donation in dichloro-bis(pyridme)-cobalt(II) complexes. Computational and Theoretical Chemistry, 1994, 306, 289-292.	1.5	3
216	Identification of Nitric Oxide Donors by Biomimetic HTS Application. Combinatorial Chemistry and High Throughput Screening, 2005, 8, 347-352.	1.1	3

#	Article	IF	Citations
217	Breakthroughs in Medicinal Chemistry: New Targets and Mechanisms, New Drugs, New Hopes. Molecules, 2017, 22, 743.	3.8	3
218	Binding Mode Prediction and Virtual Screening Applications by Covalent Docking. Methods in Molecular Biology, 2021, 2266, 73-88.	0.9	3
219	Consensus Virtual Screening Identified [1,2,4]Triazolo[1,5â€•b]isoquinolines As MELK Inhibitor Chemotypes. ChemMedChem, 2021, , .	3.2	3
220	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
221	Computational Medicinal Chemistry to Target GPCRs. , 2022, , 84-114.		3
222	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
223	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
224	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
225	LC Determination of Peroxynitrite Scavenging Activity of Phenols from Salvia spp.. Chromatographia, 2010, 71, 51-59.	1.3	2
226	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
227	Warheads for designing covalent inhibitors and chemical probes. , 2022, , 47-73.		2
228	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
229	Piperonyl butoxide-mediated inhibition of cytochrome P450-catalysed insecticide metabolism: a rational approach. Pest Management Science, 1999, 55, 1004-1006.	0.4	1
230	Structure / function / SAR and molecular design. Molecular Diversity, 2003, 7, 1.	3.9	1
231	Special issue in flow chemistry. Molecular Diversity, 2011, 15, 603-604.	3.9	1
232	The first synthesis of isoxazolo[3,4-c]pyridine-7-ones. Tetrahedron Letters, 2016, 57, 4401-4404.	1.4	1
233	Synthesis and Biochemical Evaluation of Lid-Open D-Amino Acid Oxidase Inhibitors. Molecules, 2019, 24, 290.	3.8	1
234	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

#	Article	IF	Citations
235	Targeting an Intrinsically Disordered Protein by Covalent Modification. Methods in Molecular Biology, 2020, 2141, 835-854.	0.9	1
236	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
237	A46, a benzothiophene-derived compound, suppresses Jak2-mediated pathologic cell growth. Experimental Hematology, 2012, 40, 22-34.	0.4	0
238	The future of covalent inhibition. Annual Reports in Medicinal Chemistry, 2021, 56, 267-284.	0.9	0
239	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
240	ADMET Prediction Based on Protein Structures. , 2014, , 287-322.		0
241	Computational Modeling of Drugs for Alzheimerâ€™s Disease: Design of Serotonin 5-HT6 Antagonists. Neuromethods, 2018, , 419-461.	0.3	0
242	Maximizing the integration of virtual and experimental screening in hit discovery. Expert Opinion on Drug Discovery, 0, , 1-12.	5.0	0