Gyorgy M Keseru

List of Publications by Year in Descending Order

238 papers	6,604 citations	40 h-index	73 g-index
259 ext. papers	7,826 ext. citations	6.1 avg, IF	6.39 L-index

#	Paper	IF	Citations
238	Computational Medicinal Chemistry to Target GPCRs **2022**,		
237	Electrophilic warheads in covalent drug discovery: an overview.. *Expert Opinion on Drug Discovery*, **2022**, 1-10	6.2	7
236	A covalent strategy to target intrinsically disordered proteins: Discovery of novel tau aggregation inhibitors.. *European Journal of Medicinal Chemistry*, **2022**, 231, 114163	6.8	1
235	Warheads for designing covalent inhibitors and chemical probes **2022**, 47-73		0
234	The Impact of the Secondary Binding Pocket on the Pharmacology of Class A GPCRs.. *Frontiers in Pharmacology*, **2022**, 13, 847788	5.6	2
233	PharmacoSTORM nanoscale pharmacology reveals cariprazine binding on Islands of Calleja granule cells. *Nature Communications*, **2021**, 12, 6505	17.4	5
232	Natural Apocarotenoids and Their Synthetic Glycopeptide Conjugates Inhibit SARS-CoV-2 Replication. *Pharmaceuticals*, **2021**, 14,	5.2	2
231	Vinylation of β-Aminoazoles with Triethylamine: A General Strategy to Construct Azolo[1,5-]pyrimidines with a Nonsubstituted Ethylidene Fragment. *Organic Letters*, **2021**, 23, 2664-2669	6.2	6
230	Exploring protein hotspots by optimized fragment pharmacophores. *Nature Communications*, **2021**, 12, 3201	17.4	9
229	Controlling the selectivity of aminergic GPCR ligands from the extracellular vestibule. *Bioorganic Chemistry*, **2021**, 111, 104832	5.1	3
228	Fragment-Based Optimization of Dihydropyrazino-Benzimidazolones as Metabotropic Glutamate Receptor-2 Positive Allosteric Modulators against Migraine. *Journal of Medicinal Chemistry*, **2021**, 64, 8607-8620	8.3	0
227	Discovery of selective fragment-sized immunoproteasome inhibitors. *European Journal of Medicinal Chemistry*, **2021**, 219, 113455	6.8	2
226	Allosteric Molecular Switches in Metabotropic Glutamate Receptors. *ChemMedChem*, **2021**, 16, 81-93	3.7	3
225	Assessment of Tractable Cysteines for Covalent Targeting by Screening Covalent Fragments. *ChemBioChem*, **2021**, 22, 743-753	3.8	10
224	GPCRdb in 2021: integrating GPCR sequence, structure and function. *Nucleic Acids Research*, **2021**, 49, D335-D343	20.1	74
223	Novel potent (dihydro)benzofuranyl piperazines as human histamine receptor ligands - Functional characterization and modeling studies on H and H receptors. *Bioorganic and Medicinal Chemistry*, **2021**, 30, 115924	3.4	3
222	The future of covalent inhibition. *Annual Reports in Medicinal Chemistry*, **2021**, 56, 267-284	1.6	

221	Synthesis and characterization of new fluorescent boro-β-carboline dyes.. *RSC Advances*, **2021**, 11, 12802-12807	3.7	0
220	Mechanistic and thermodynamic characterization of oxathiazolones as potent and selective covalent immunoproteasome inhibitors. *Computational and Structural Biotechnology Journal*, **2021**, 19, 4486-4496	6.8	0
219	Binding Mode Prediction and Virtual Screening Applications by Covalent Docking. *Methods in Molecular Biology*, **2021**, 2266, 73-88	1.4	0
218	Continuous-Flow Synthesis of Thioureas, Enabled by Aqueous Polysulfide Solution. *Molecules*, **2021**, 26,	4.8	5
217	Fragment evolution for GPCRs: the role of secondary binding sites in optimization. *Chemical Communications*, **2021**, 57, 10516-10519	5.8	2
216	Convenient Multicomponent One-Pot Synthesis of 2-Iminothiazolines and 2-Aminothiazoles Using Elemental Sulfur Under Aqueous Conditions. *European Journal of Organic Chemistry*, **2021**, 2021, 3587-3597	3.2	4
215	WIDOCK: a reactive docking protocol for virtual screening of covalent inhibitors. *Journal of Computer-Aided Molecular Design*, **2021**, 35, 223-244	4.2	5
214	Chromatography-Free Multicomponent Synthesis of Thioureas Enabled by Aqueous Solution of Elemental Sulfur. *ChemistryOpen*, **2021**, 10, 16-27	2.3	6
213	Affinity and Selectivity Assessment of Covalent Inhibitors by Free Energy Calculations. *Journal of Chemical Information and Modeling*, **2020**, 60, 6579-6594	6.1	11
212	Benchmark Sets for Binding Hot Spot Identification in Fragment-Based Ligand Discovery. *Journal of Chemical Information and Modeling*, **2020**, 60, 6612-6623	6.1	3
211	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	5.9	9
210	Discovery of a novel kinase hinge binder fragment by dynamic undocking. *RSC Medicinal Chemistry*, **2020**, 11, 552-558	3.5	6
209	Application of Boroisoquinoline Fluorophores as Chemodosimeters for Fluoride Ion and Pd (0). *Materials*, **2020**, 13,	3.5	4
208	Comparative reactivity analysis of small-molecule thiol surrogates. *Bioorganic and Medicinal Chemistry*, **2020**, 28, 115357	3.4	16
207	Targeting an Intrinsically Disordered Protein by Covalent Modification. *Methods in Molecular Biology*, **2020**, 2141, 835-854	1.4	1
206	Covalent Docking in Drug Discovery: Scope and Limitations. *Current Pharmaceutical Design*, **2020**, 26, 5684-5699	3.3	4
205	Thermodynamic profiling for fragment-based lead discovery and optimization. *Expert Opinion on Drug Discovery*, **2020**, 15, 117-129	6.2	2
204	Discovery of dihydropyrazino-benzimidazole derivatives as metabotropic glutamate receptor-2 (mGluR2) positive allosteric modulators (PAMs). *European Journal of Medicinal Chemistry*, **2020**, 186, 111881	6.8	1

203	Controlling receptor function from the extracellular vestibule of G-protein coupled receptors. *Chemical Communications*, **2020**, 56, 14167-14170	5.8	6
202	Crystallographic and electrophilic fragment screening of the SARS-CoV-2 main protease. *Nature Communications*, **2020**, 11, 5047	17.4	188
201	An electrophilic warhead library for mapping the reactivity and accessibility of tractable cysteines in protein kinases. *European Journal of Medicinal Chemistry*, **2020**, 207, 112836	6.8	13
200	Small molecule inhibitors of RAS proteins with oncogenic mutations. *Cancer and Metastasis Reviews* , **2020**, 39, 1107-1126	9.6	8
199	Structural impact of GTP binding on downstream KRAS signaling. *Chemical Science*, **2020**, 11, 9272-9289	9.4	9
198	Allosteric activation of metabotropic glutamate receptor 5. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 2624-2632	3.6	4
197	Cysteine specific bioconjugation with benzyl isothiocyanates.. *RSC Advances*, **2020**, 10, 14928-14936	3.7	13
196	Covalent fragment libraries in drug discovery. *Drug Discovery Today*, **2020**, 25, 983-996	8.8	33
195	The role of water and protein flexibility in the structure-based virtual screening of allosteric GPCR modulators: an mGlu receptor case study. *Journal of Computer-Aided Molecular Design*, **2019**, 33, 787-797	4.2	4
194	Design and characterization of a heterocyclic electrophilic fragment library for the discovery of cysteine-targeted covalent inhibitors. *MedChemComm*, **2019**, 10, 263-267	5	24
193	Why Some Targets Benefit from beyond Rule of Five Drugs. *Journal of Medicinal Chemistry*, **2019**, 62, 10005-10025	8.3	42
192	Analysis of tractable allosteric sites in G protein-coupled receptors. *Scientific Reports*, **2019**, 9, 6180	4.9	21
191	DUckCov: a Dynamic Undocking-Based Virtual Screening Protocol for Covalent Binders. *ChemMedChem*, **2019**, 14, 1011-1021	3.7	17
190	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	3.4	2
189	Discovery of Immunoproteasome Inhibitors Using Large-Scale Covalent Virtual Screening. *Molecules*, **2019**, 24,	4.8	6
188	A novel three-component reaction between isocyanides, alcohols or thiols and elemental sulfur: a mild, catalyst-free approach towards -thiocarbamates and dithiocarbamates. *Beilstein Journal of Organic Chemistry*, **2019**, 15, 1523-1533	2.5	10
187	Structural Implications of STAT3 and STAT5 SH2 Domain Mutations. *Cancers*, **2019**, 11,	6.6	16
186	Catalytic Mechanism and Covalent Inhibition of UDP--Acetylglucosamine Enolpyruvyl Transferase (MurA): Implications to the Design of Novel Antibacterials. *Journal of Chemical Information and Modeling*, **2019**, 59, 5161-5173	6.1	6

185	Fragment-Based Approaches for Allosteric Metabotropic Glutamate Receptor (mGluR) Modulators. *Current Topics in Medicinal Chemistry*, **2019**, 19, 1768-1781	3	4
184	Covalent Inhibition of the Histamine H Receptor. *Molecules*, **2019**, 24,	4.8	2
183	Direct Targeting Options for STAT3 and STAT5 in Cancer. *Cancers*, **2019**, 11,	6.6	29
182	Structure-Based Optimization Strategies for G Protein-Coupled Receptor (GPCR) Allosteric Modulators: A Case Study from Analyses of New Metabotropic Glutamate Receptor 5 (mGlu) X-ray Structures. *Journal of Medicinal Chemistry*, **2019**, 62, 207-222	8.3	48
181	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	8.3	9
180	Pharmacologic inhibition of STAT5 in acute myeloid leukemia. *Leukemia*, **2018**, 32, 1135-1146	10.7	68
179	Discovery of isatin and 1H-indazol-3-ol derivatives as d-amino acid oxidase (DAAO) inhibitors. *Bioorganic and Medicinal Chemistry*, **2018**, 26, 1579-1587	3.4	6
178	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	4.2	7
177	When fragments link: a bibliometric perspective on the development of fragment-based drug discovery. *Drug Discovery Today*, **2018**, 23, 1596-1609	8.8	24
176	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	2.9	3
175	Expanding the medicinal chemistry synthetic toolbox. *Nature Reviews Drug Discovery*, **2018**, 17, 709-727	64.1	223
174	Binding kinetics of cariprazine and aripiprazole at the dopamine D receptor. *Scientific Reports*, **2018**, 8, 12509	4.9	16
173	Comparative Evaluation of Covalent Docking Tools. *Journal of Chemical Information and Modeling*, **2018**, 58, 1441-1458	6.1	61
172	Spiro[pyrrolidine-3,3'-oxindoles] as 5-HT receptor ligands. *Bioorganic and Medicinal Chemistry Letters*, **2018**, 28, 2418-2421	2.9	6
171	Computational Modeling of Drugs for Alzheimer Disease: Design of Serotonin 5-HT6 Antagonists. *Neuromethods*, **2018**, 419-461	0.4	
170	Emerging therapeutic targets in myeloproliferative neoplasms and peripheral T-cell leukemia and lymphomas. *Expert Opinion on Therapeutic Targets*, **2018**, 22, 45-57	6.4	12
169	Synthesis and fluorescent properties of boroisoquinolines, a new family of fluorophores.. *RSC Advances*, **2018**, 8, 38598-38605	3.7	2
168	Heterocyclic electrophiles as new MurA inhibitors. *Archiv Der Pharmazie*, **2018**, 351, e1800184	4.3	7

167	A road map for prioritizing warheads for cysteine targeting covalent inhibitors. *European Journal of Medicinal Chemistry*, **2018**, 160, 94-107	6.8	47
166	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	6.2	6
165	Fingerprint-Based Machine Learning Approach to Identify Potent and Selective 5-HTR Ligands. *Molecules*, **2018**, 23,	4.8	9
164	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, 2470-2494	8.3	18
163	Discovery of 4-amino-3-arylsulfoquinolines, a novel non-acetylenic chemotype of metabotropic glutamate 5 (mGlu) receptor negative allosteric modulators. *European Journal of Medicinal Chemistry*, **2017**, 133, 240-254	6.8	4
162	Binding thermodynamics discriminates fragments from druglike compounds: a thermodynamic description of fragment-based drug discovery. *Drug Discovery Today*, **2017**, 22, 681-689	8.8	15
161	Spiro[pyrrolidine-3,3'-oxindoles] and Their Indoline Analogues as New 5-HT6 Receptor Chemotypes. *Molecules*, **2017**, 22,	4.8	13
160	Structure-based Virtual Screening Approaches in Kinase-directed Drug Discovery. *Current Topics in Medicinal Chemistry*, **2017**, 17, 2235-2259	3	45
159	The first synthesis of isoxazolo[3,4-c]pyridine-7-ones. *Tetrahedron Letters*, **2016**, 57, 4401-4404	2	
158	Identification of 8-Hydroxyquinoline Derivatives Active Against Somatic V658F Mutant JAK1-Dependent Cells. *Archiv Der Pharmazie*, **2016**, 349, 925-933	4.3	5
157	Ensemble docking-based virtual screening yields novel spirocyclic JAK1 inhibitors. *Journal of Molecular Graphics and Modelling*, **2016**, 70, 275-283	2.8	4
156	Structure-Based Consensus Scoring Scheme for Selecting Class A Aminergic GPCR Fragments. *Journal of Chemical Information and Modeling*, **2016**, 56, 412-22	6.1	14
155	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	2.9	1
154	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, 1249-52	2.9	11
153	On the enthalpic preference of fragment binding. *MedChemComm*, **2016**, 7, 332-337	5	23
152	The first synthesis of furo[2,3- c]pyridazin-4(1 H)-one derivatives. *Tetrahedron Letters*, **2016**, 57, 64-66	2	2
151	Discovery of Subtype Selective Janus Kinase (JAK) Inhibitors by Structure-Based Virtual Screening. *Journal of Chemical Information and Modeling*, **2016**, 56, 234-47	6.1	17
150	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, 8189-206	8.3	134

149	Structure-based discovery and binding site analysis of histamine receptor ligands. *Expert Opinion on Drug Discovery*, **2016**, 11, 1165-1185	6.2	7
148	Ligand Efficiency Metrics and their Use in Fragment Optimizations. *Methods and Principles in Medicinal Chemistry*, **2016**, 75-98	0.4	1
147	Is there a link between selectivity and binding thermodynamics profiles?. *Drug Discovery Today*, **2015**, 20, 86-94	8.8	37
146	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	4.2	6
145	Cell-based and virtual fragment screening for adrenergic β2C receptor agonists. *Bioorganic and Medicinal Chemistry*, **2015**, 23, 3991-9	3.4	10
144	Property-based characterization of kinase-like ligand space for library design and virtual screening. *MedChemComm*, **2015**, 6, 1898-1904	5	4
143	The impact of binding thermodynamics on medicinal chemistry optimizations. *Future Medicinal Chemistry*, **2015**, 7, 1285-303	4.1	7
142	Dynamics and structural determinants of ligand recognition of the 5-HT6 receptor. *Journal of Computer-Aided Molecular Design*, **2015**, 29, 1137-49	4.2	5
141	Thermodynamics-Guided Optimizations in Medicinal Chemistry. *Methods and Principles in Medicinal Chemistry*, **2015**, 63-80	0.4	
140	From Molecular Understanding to Structure–Thermodynamic Relationships, the Case of Acetylcholine Binding Proteins. *Methods and Principles in Medicinal Chemistry*, **2015**, 81-105	0.4	1
139	Thermodynamics in Lead Optimization. *Methods and Principles in Medicinal Chemistry*, **2015**, 107-135	0.4	
138	Thermodynamics and Binding Kinetics in Drug Discovery. *Methods and Principles in Medicinal Chemistry*, **2015**, 313-329	0.4	
137	Thieno[2,3-b]pyridines as negative allosteric modulators of metabotropic GluR5 receptors: Lead optimization. *Bioorganic and Medicinal Chemistry Letters*, **2015**, 25, 1724-1729	2.9	13
136	Validity of ligand efficiency metrics. *ACS Medicinal Chemistry Letters*, **2014**, 5, 616-8	4.3	85
135	The role of ligand efficiency metrics in drug discovery. *Nature Reviews Drug Discovery*, **2014**, 13, 105-21	64.1	649
134	Novel histamine H4 receptor ligands and their potential therapeutic applications: an update. *Expert Opinion on Therapeutic Patents*, **2014**, 24, 1185-97	6.8	28
133	Multiple fragment docking and linking in primary and secondary pockets of dopamine receptors. *ACS Medicinal Chemistry Letters*, **2014**, 5, 1010-4	4.3	29
132	Thieno[2,3-b]pyridines as negative allosteric modulators of metabotropic GluR5 receptors: hit-to-lead optimization. *Bioorganic and Medicinal Chemistry Letters*, **2014**, 24, 3845-9	2.9	6

131	Anthropogenic reaction parameters--the missing link between chemical intuition and the available chemical space. *Chemical Society Reviews*, **2014**, 43, 5387-99	58.5	27
130	Identification of Novel Histamine H4 Ligands by Virtual Screening on Molecular Dynamics Ensembles. *Molecular Informatics*, **2014**, 33, 264-8	3.8	7
129	Design of novel multiple-acting ligands towards SERT and 5-HT2C receptors. *Bioorganic and Medicinal Chemistry Letters*, **2014**, 24, 2118-22	2.9	3
128	Virtual fragment screening on GPCRs: a case study on dopamine D3 and histamine H4 receptors. *European Journal of Medicinal Chemistry*, **2014**, 77, 38-46	6.8	45
127	The Jak2 small molecule inhibitor, G6, reduces the tumorigenic potential of T98G glioblastoma cells in vitro and in vivo. *PLoS ONE*, **2014**, 9, e105568	3.7	6
126	Structure-based ß-secretase (BACE1) inhibitors. *Current Pharmaceutical Design*, **2014**, 20, 3373-9	3.3	4
125	Positive allosteric modulators for mGluR2 receptors: a medicinal chemistry perspective. *Current Topics in Medicinal Chemistry*, **2014**, 14, 1771-88	3	11
124	ADMET Prediction Based on Protein Structures **2014**, 287-322		
123	Fragment-based lead discovery on G-protein-coupled receptors. *Expert Opinion on Drug Discovery*, **2013**, 8, 811-20	6.2	10
122	The impact of molecular dynamics sampling on the performance of virtual screening against GPCRs. *Journal of Chemical Information and Modeling*, **2013**, 53, 2990-9	6.1	47
121	Contributions of molecular properties to drug promiscuity. *Journal of Medicinal Chemistry*, **2013**, 56, 1788-95	5.9	109
120	Fragments to link. A multiple docking strategy for second site binders. *MedChemComm*, **2013**, 4, 510-514	3	5
119	How are fragments optimized? A retrospective analysis of 145 fragment optimizations. *Journal of Medicinal Chemistry*, **2013**, 56, 2478-86	8.3	52
118	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, 1402-7	2.9	8
117	Quinolinyl- and phenantridinyl-acetamides as bradykinin B1 receptor antagonists. *Bioorganic and Medicinal Chemistry Letters*, **2012**, 22, 3095-9	2.9	19
116	Discovery of cariprazine (RGH-188): a novel antipsychotic acting on dopamine D3/D2 receptors. *Bioorganic and Medicinal Chemistry Letters*, **2012**, 22, 3437-40	2.9	60
115	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, 83-9	3.5	17
114	Comparative evaluation of pK(a) prediction tools on a drug discovery dataset. *Journal of Pharmaceutical and Biomedical Analysis*, **2012**, 67-68, 63-70	3.5	32

113	Histamine H4 receptor ligands and their potential therapeutic applications: an update. *Expert Opinion on Therapeutic Patents*, **2012**, 22, 205-21	6.8	29
112	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, 858-65	5.8	6
111	Bradykinin B1 receptor antagonists: a patent update 2009 - 2012. *Expert Opinion on Therapeutic Patents*, **2012**, 22, 1443-52	6.8	9
110	Thermodynamics of fragment binding. *Journal of Chemical Information and Modeling*, **2012**, 52, 1039-45	6.1	55
109	Impact of lipophilic efficiency on compound quality. *Journal of Medicinal Chemistry*, **2012**, 55, 1252-60	8.3	126
108	Finding the sweet spot: the role of nature and nurture in medicinal chemistry. *Nature Reviews Drug Discovery*, **2012**, 11, 355-65	64.1	295
107	Chapter 2:Thermodynamics of Ligand Binding. *RSC Drug Discovery Series*, **2012**, 23-79	0.6	4
106	Discovery of novel histamine H4 and serotonin transporter ligands using the topological feature tree descriptor. *Journal of Chemical Information and Modeling*, **2012**, 52, 233-42	6.1	7
105	Multiple ligand docking by Glide: implications for virtual second-site screening. *Journal of Computer-Aided Molecular Design*, **2012**, 26, 821-34	4.2	17
104	A46, a benzothiophene-derived compound, suppresses Jak2-mediated pathologic cell growth. *Experimental Hematology*, **2012**, 40, 22-34	3.1	
103	The Jak2 inhibitor, G6, alleviates Jak2-V617F-mediated myeloproliferative neoplasia by providing significant therapeutic efficacy to the bone marrow. *Neoplasia*, **2011**, 13, 1058-68	6.4	9
102	Homology modeling and binding site assessment of the human P-glycoprotein. *Future Medicinal Chemistry*, **2011**, 3, 297-307	4.1	16
101	Virtual Screening on Homology Models. *Methods and Principles in Medicinal Chemistry*, **2011**, 381-410	0.4	3
100	Integration of virtual and high throughput screening in lead discovery settings. *Combinatorial Chemistry and High Throughput Screening*, **2011**, 14, 889-97	1.3	24
99	In silico site of metabolism prediction of cytochrome P450-mediated biotransformations. *Expert Opinion on Drug Metabolism and Toxicology*, **2011**, 7, 299-312	5.5	50
98	Cell death induced by the Jak2 inhibitor, G6, correlates with cleavage of vimentin filaments. *Biochemistry*, **2011**, 50, 7774-86	3.2	6
97	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, 4280-91	5.4	12
96	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	2.2	

95	Structure-function correlation of G6, a novel small molecule inhibitor of Jak2: indispensability of the stilbenoid core. *Journal of Biological Chemistry*, **2010**, 285, 31399-407	5.4	11
94	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	6.4	8
93	Virtual fragment docking by Glide: a validation study on 190 protein-fragment complexes. *Journal of Chemical Information and Modeling*, **2010**, 50, 1165-72	6.1	75
92	Recent developments on JAK2 inhibitors: a patent review. *Expert Opinion on Therapeutic Patents*, **2010**, 20, 471-95	6.8	32
91	LC Determination of Peroxynitrite Scavenging Activity of Phenols from Salvia spp.. *Chromatographia*, **2010**, 71, 51-59	2.1	2
90	Enthalpic efficiency of ligand binding. *Journal of Chemical Information and Modeling*, **2010**, 50, 1536-41	6.1	51
89	Site of metabolism prediction on cytochrome P450 2C9: a knowledge-based docking approach. *Journal of Computer-Aided Molecular Design*, **2010**, 24, 399-408	4.2	29
88	Thermodynamics guided lead discovery and optimization. *Drug Discovery Today*, **2010**, 15, 919-32	8.8	111
87	Hit-to-lead optimization of disubstituted oxadiazoles and tetrazoles as mGluR5 NAMs. *Bioorganic and Medicinal Chemistry Letters*, **2010**, 20, 3737-41	2.9	19
86	Carbamoyloximes as novel non-competitive mGlu5 receptor antagonists. *Bioorganic and Medicinal Chemistry Letters*, **2010**, 20, 4371-5	2.9	16
85	The influence of lead discovery strategies on the properties of drug candidates. *Nature Reviews Drug Discovery*, **2009**, 8, 203-12	64.1	466
84	Identification of a novel inhibitor of JAK2 tyrosine kinase by structure-based virtual screening. *Bioorganic and Medicinal Chemistry Letters*, **2009**, 19, 3598-601	2.9	39
83	Hit-to-lead optimization of pyrrolo[1,2-a]quinoxalines as novel cannabinoid type 1 receptor antagonists. *Bioorganic and Medicinal Chemistry Letters*, **2009**, 19, 3471-5	2.9	27
82	Histamine H4 receptor ligands and their potential therapeutic applications. *Expert Opinion on Therapeutic Patents*, **2009**, 19, 119-35	6.8	20
81	Activation mechanism of the human histamine H4 receptor--an explicit membrane molecular dynamics simulation study. *Journal of Chemical Information and Modeling*, **2008**, 48, 1199-210	6.1	34
80	Discovery of novel human histamine H4 receptor ligands by large-scale structure-based virtual screening. *Journal of Medicinal Chemistry*, **2008**, 51, 3145-53	8.3	88
79	Binding mode analysis and enrichment studies on homology models of the human histamine H4 receptor. *European Journal of Medicinal Chemistry*, **2008**, 43, 1059-70	6.8	43
78	Impact of ligand protonation on virtual screening against beta-secretase (BACE1). *Journal of Chemical Information and Modeling*, **2007**, 47, 2366-73	6.1	34

77	Selective NR1/2B N-methyl-D-aspartate receptor antagonists among indole-2-carboxamides and benzimidazole-2-carboxamides. *Journal of Medicinal Chemistry*, **2007**, 50, 901-14	8.3	35
76	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, 5340-4	2.9	15
75	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, 539-48	4.2	9
74	Application of the BD ACTOne technology for the high-throughput screening of Gs-coupled receptor antagonists. *Journal of Biomolecular Screening*, **2007**, 12, 1068-73		15
73	A high throughput luminescent assay for glycogen synthase kinase-3beta inhibitors. *Assay and Drug Development Technologies*, **2007**, 5, 75-83	2.1	98
72	Hit discovery and hit-to-lead approaches. *Drug Discovery Today*, **2006**, 11, 741-8	8.8	180
71	Ensemble docking into flexible active sites. Critical evaluation of FlexE against JNK-3 and beta-secretase. *Journal of Chemical Information and Modeling*, **2006**, 46, 1795-805	6.1	43
70	A neural network based classification scheme for cytotoxicity predictions:Validation on 30,000 compounds. *Bioorganic and Medicinal Chemistry Letters*, **2006**, 16, 1037-9	2.9	18
69	Binding mode analysis of the NADH cofactor in nitric oxide reductase: a theoretical study. *Journal of Molecular Graphics and Modelling*, **2006**, 25, 363-72	2.8	4
68	Virtual screening for beta-secretase (BACE1) inhibitors reveals the importance of protonation states at Asp32 and Asp228. *Journal of Medicinal Chemistry*, **2005**, 48, 3749-55	8.3	79
67	Comparative virtual and experimental high-throughput screening for glycogen synthase kinase-3beta inhibitors. *Journal of Medicinal Chemistry*, **2005**, 48, 7946-59	8.3	65
66	Protonation state of Asp30 exerts crucial influence over surface loop rearrangements responsible for NO release in nitrophorin 4. *FEBS Letters*, **2005**, 579, 5392-8	3.8	22
65	Functional virtual screening of estrogen receptor □modulators by FlexX-Pharm. *Computational and Theoretical Chemistry*, **2005**, 725, 239-242		3
64	Solid-phase synthesis of 6-hydroxy-2,4-diaminoquinazolines. *Tetrahedron*, **2005**, 61, 9375-9380	2.4	10
63	Identification of nitric oxide donors by biomimetic HTS application. *Combinatorial Chemistry and High Throughput Screening*, **2005**, 8, 347-52	1.3	3
62	A neural network based prediction of octanol-water partition coefficients using atomic5 fragmental descriptors. *Bioorganic and Medicinal Chemistry Letters*, **2004**, 14, 851-3	2.9	32
61	Oxamides as novel NR2B selective NMDA receptor antagonists. *Bioorganic and Medicinal Chemistry Letters*, **2004**, 14, 3953-6	2.9	37
60	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		2

59	Homology modelling and binding site mapping of the human histamine H1 receptor. *European Journal of Medicinal Chemistry*, **2004**, 39, 959-67	6.8	30
58	Solid-phase synthesis of an N-(phenylalkyl)cinnamide library via Horner-Wadsworth-Emmons reaction. *Bioorganic and Medicinal Chemistry Letters*, **2004**, 14, 1279-81	2.9	9
57	Structure / function / SAR and molecular design. *Molecular Diversity*, **2003**, 7, 1	3.1	1
56	Recent advances in the prediction of blood-brain partitioning from molecular structure. *Journal of Pharmaceutical Sciences*, **2003**, 92, 360-70	3.9	85
55	Prediction of hERG potassium channel affinity by traditional and hologram qSAR methods. *Bioorganic and Medicinal Chemistry Letters*, **2003**, 13, 2773-5	2.9	114
54	A neural network based virtual screening of cytochrome P450 3A4 inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2002**, 12, 419-21	2.9	65
53	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 ring. *Journal of Organic Chemistry*, **2002**, 67, 7255-60	4.2	18
52	Distinct behavior of mutant triosephosphate isomerase in hemolysate and in isolated form: molecular basis of enzyme deficiency. *Blood*, **2001**, 98, 3106-12	2.2	30
51	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	3.5	52
50	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	1.2	9
49	A virtual high throughput screen for high affinity cytochrome P450cam substrates. Implications for in silico prediction of drug metabolism. *Journal of Computer-Aided Molecular Design*, **2001**, 15, 649-57	4.2	36
48	Solvent and ligand effects on selective mono- and dilithiation of 1-(chlorophenyl)pyrroles and 1-(methoxyphenyl)pyrroles. *Journal of the Chemical Society, Perkin Transactions 1*, **2001**, 1039-1043		23
47	High-throughput prediction of blood-brain partitioning: a thermodynamic approach. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 120-8		62
46	Fully flexible low-mode docking: application to induced fit in HIV integrase. *Journal of the American Chemical Society*, **2001**, 123, 12708-9	16.4	91
45	Construction of a 3D model of oligopeptidase B, a potential processing enzyme in prokaryotes. *Journal of Molecular Graphics and Modelling*, **2000**, 18, 7-17, 57-8	2.8	23
44	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, 1775-7	2.9	9
43	Cytochrome P450 catalyzed nitric oxide synthesis: a theoretical study. *Journal of Biomolecular Structure and Dynamics*, **2000**, 17, 759-67	3.6	12
42	A neural network based virtual high throughput screening test for the prediction of CNS activity. *Combinatorial Chemistry and High Throughput Screening*, **2000**, 3, 535-40	1.3	18

41	Effect of a trifluoromethyl group on molecular structure: Competitive mono- and dilithiation of 1-[(trifluoromethyl)phenyl]pyrroles. *Tetrahedron*, **1999**, 55, 7881-7892	2.4	15
40	Enantiomeric recognition of Ⅱ(1-naphthyl)ethylammonium perchlorate by enantiomerically pure dimethylphenazino-18-crown-6 ligand in solid and gas phases. *Tetrahedron: Asymmetry*, **1999**, 10, 1995-2005		12
39	Metalloporphyrin catalysed biomimetic oxidation of aryl benzyl ethers. Implications for lignin peroxidase catalysis. *Tetrahedron*, **1999**, 55, 4457-4466	2.4	14
38	A semiempirical approach to hydrogen bonding networks. Application of the Cyclic Cluster Model to organic crystals. *Computational and Theoretical Chemistry*, **1999**, 463, 169-174		2
37	Inhibitors of cytochrome P450 catalyzed insecticide metabolism: A rational approach. *International Journal of Quantum Chemistry*, **1999**, 73, 123-135	2.1	13
36	Piperonyl butoxide-mediated inhibition of cytochrome P450-catalysed insecticide metabolism: a rational approach. *Pest Management Science*, **1999**, 55, 1004-1006		
35	Role of proximal His93 in nitric oxide binding to metmyoglobin. Application of continuum solvation in Monte Carlo protein simulations. *Biochemistry*, **1999**, 38, 6614-22	3.2	9
34	Chemical models of cytochrome P450 catalyzed insecticide metabolism. Application to the oxidative metabolism of carbamate insecticides. *Journal of Agricultural and Food Chemistry*, **1999**, 47, 762-9	5.7	18
33	Communication to the editor piperonyl butoxide-mediated inhibition of cytochrome P450-catalysed insecticide metabolism: A rational approach. *Pest Management Science*, **1999**, 55, 1004-1006		2
32	. *European Journal of Organic Chemistry*, **1998**, 1998, 521-524	3.2	19
31	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	16.4	16
30	Synthesis of Isoplagiochin A *Journal of Organic Chemistry*, **1997**, 62, 3666-3670	4.2	10
29	Cytochrome P-450 Catalyzed Insecticide Metabolism. Prediction of Regio- and Stereoselectivity in the Primer Metabolism of Carbofuran: A Theoretical Study. *Journal of the American Chemical Society*, **1997**, 119, 5126-5131	16.4	24
28	On the conformation of tiazofurin analogues. *Journal of Medicinal Chemistry*, **1997**, 40, 4154-9	8.3	27
27	1-(2,4,6-Tri-tert-butylphenyl)-3-methylphosphole: A Phosphole with a Significantly Flattened Phosphorus Pyramid Having Pronounced Characteristics of Aromaticity. *Journal of the American Chemical Society*, **1997**, 119, 5095-5099	16.4	84
26	Steric vs. electrostatic effects in the nucleophilic addition to a hindered cyclohexanone. *Structural Chemistry*, **1997**, 8, 257-261	1.8	3
25	Nuclear magnetic resonance and molecular modeling study on mycophenolic acid: implications for binding to inosine monophosphate dehydrogenase. *Journal of Medicinal Chemistry*, **1996**, 39, 1236-42	8.3	15
24	Theoretical studies on long-range substituent effects in the reduction of 7-norbornanones. *Journal of the Chemical Society Perkin Transactions II*, **1996**, 2231-2234		1

23	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	2.4	7
22	Molecular similarity analysis on biologically active macrocyclic bis(bibenzyls) **1996**, 9, 133-138		7
21	The biological activity of cyclic bis(bibenzyls): a rational approach. *Bioorganic and Medicinal Chemistry*, **1995**, 3, 1511-7	3.4	27
20	Molecular asymmetry of macrocyclic bis(bibenzyl)s, natural products from liverwort species. *Journal of Molecular Structure*, **1995**, 356, 143-148	3.4	6
19	Isolation and antibacterial activity of marchantin A, a cyclic bis(bibenzyl) constituent of Hungarian Marchantia polymorpha. *Planta Medica*, **1995**, 61, 387-8	3.1	31
18	The chemistry of macrocyclic bis(bibenzyls). *Natural Product Reports*, **1995**, 12, 69-75	15.1	49
17	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		
16	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	1.8	6
15	Synthesis of Garugamblin-2, a Macrocyclic Diarylheptanoid Constituent of Garuga gamblei. *Liebigs Annalen Der Chemie*, **1994**, 1994, 361-364		13
14	Designed nucleophilic attack based on molecular electrostatic potential. *Tetrahedron Letters*, **1994**, 35, 9255-9258	2	9
13	Back donation in dichloro-bis(pyridme)-cobalt(II) complexes. *Computational and Theoretical Chemistry*, **1994**, 306, 289-292		3
12	On the mechanism of the alkylation of quinoline and naphthyridine derivatives. *Journal of the Chemical Society Perkin Transactions II*, **1994**, 591-594		4
11	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		5
10	Synthesis and revised structure of garuganin III. *Journal of Organic Chemistry*, **1993**, 58, 6725-6728	4.2	25
9	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		4
8	The synthesis of garugamblin-1. *Tetrahedron*, **1993**, 49, 4893-4900	2.4	22
7	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	2.4	8
6	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		6

5	Total synthesis of plagiochins C and D, macrocyclic bis(bibenzyl) constituents of plagiochila acantophylla. *Tetrahedron*, **1992**, 48, 913-922	2.4	29
4	Biosynthesis and molecular strain. A computational study on the conformation of cyclic bis(bibenzyl) constituents of liverwort species. *Phytochemistry*, **1992**, 31, 1573-1576	4	16
3	Synthese von Plagiochin A und B, zwei macrocyclische Bis(bibenzylether) aus Plagiochila acantophylla. *Liebigs Annalen Der Chemie*, **1992**, 1992, 1239-1243		7
2	Crystallographic and electrophilic fragment screening of the SARS-CoV-2 main protease		9
1	The role of quantum chemistry in covalent inhibitor design. *International Journal of Quantum Chemistry*,	2.1	2