Gyorgy M Keseru

List of Publications by Citations

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	The role of ligand efficiency metrics in drug discovery. *Nature Reviews Drug Discovery*, **2014**, 13, 105-21	64.1	649
237	The influence of lead discovery strategies on the properties of drug candidates. *Nature Reviews Drug Discovery*, **2009**, 8, 203-12	64.1	466
236	Finding the sweet spot: the role of nature and nurture in medicinal chemistry. *Nature Reviews Drug Discovery*, **2012**, 11, 355-65	64.1	295
235	Expanding the medicinal chemistry synthetic toolbox. *Nature Reviews Drug Discovery*, **2018**, 17, 709-727	64.1	223
234	Crystallographic and electrophilic fragment screening of the SARS-CoV-2 main protease. *Nature Communications*, **2020**, 11, 5047	17.4	188
233	Hit discovery and hit-to-lead approaches. *Drug Discovery Today*, **2006**, 11, 741-8	8.8	180
232	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
231	Impact of lipophilic efficiency on compound quality. *Journal of Medicinal Chemistry*, **2012**, 55, 1252-60	8.3	126
230	Prediction of hERG potassium channel affinity by traditional and hologram qSAR methods. *Bioorganic and Medicinal Chemistry Letters*, **2003**, 13, 2773-5	2.9	114
229	Thermodynamics guided lead discovery and optimization. *Drug Discovery Today*, **2010**, 15, 919-32	8.8	111
228	Contributions of molecular properties to drug promiscuity. *Journal of Medicinal Chemistry*, **2013**, 56, 1789-95	8.3	109
227	A high throughput luminescent assay for glycogen synthase kinase-3beta inhibitors. *Assay and Drug Development Technologies*, **2007**, 5, 75-83	2.1	98
226	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
225	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
224	Validity of ligand efficiency metrics. *ACS Medicinal Chemistry Letters*, **2014**, 5, 616-8	4.3	85
223	Recent advances in the prediction of blood-brain partitioning from molecular structure. *Journal of Pharmaceutical Sciences*, **2003**, 92, 360-70	3.9	85
222	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

221	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
220	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
219	GPCRdb in 2021: integrating GPCR sequence, structure and function. *Nucleic Acids Research*, **2021**, 49, D335-D343	20.1	74
218	Pharmacologic inhibition of STAT5 in acute myeloid leukemia. *Leukemia*, **2018**, 32, 1135-1146	10.7	68
217	Comparative virtual and experimental high-throughput screening for glycogen synthase kinase-3beta inhibitors. *Journal of Medicinal Chemistry*, **2005**, 48, 7946-59	8.3	65
216	A neural network based virtual screening of cytochrome P450 3A4 inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2002**, 12, 419-21	2.9	65
215	High-throughput prediction of blood-brain partitioning: a thermodynamic approach. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 120-8		62
214	Comparative Evaluation of Covalent Docking Tools. *Journal of Chemical Information and Modeling*, **2018**, 58, 1441-1458	6.1	61
213	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
212	Thermodynamics of fragment binding. *Journal of Chemical Information and Modeling*, **2012**, 52, 1039-45	6.1	55
211	How are fragments optimized? A retrospective analysis of 145 fragment optimizations. *Journal of Medicinal Chemistry*, **2013**, 56, 2478-86	8.3	52
210	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
209	Enthalpic efficiency of ligand binding. *Journal of Chemical Information and Modeling*, **2010**, 50, 1536-41	6.1	51
208	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
207	The chemistry of macrocyclic bis(bibenzyls). *Natural Product Reports*, **1995**, 12, 69-75	15.1	49
206	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
205	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
204	A road map for prioritizing warheads for cysteine targeting covalent inhibitors. *European Journal of Medicinal Chemistry*, **2018**, 160, 94-107	6.8	47

203	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
202	Structure-based Virtual Screening Approaches in Kinase-directed Drug Discovery. *Current Topics in Medicinal Chemistry*, **2017**, 17, 2235-2259	3	45
201	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
200	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
199	Why Some Targets Benefit from beyond Rule of Five Drugs. *Journal of Medicinal Chemistry*, **2019**, 62, 10005-10025	8.3	42
198	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
197	Is there a link between selectivity and binding thermodynamics profiles?. *Drug Discovery Today*, **2015**, 20, 86-94	8.8	37
196	Oxamides as novel NR2B selective NMDA receptor antagonists. *Bioorganic and Medicinal Chemistry Letters*, **2004**, 14, 3953-6	2.9	37
195	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
194	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
193	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
192	Impact of ligand protonation on virtual screening against beta-secretase (BACE1). *Journal of Chemical Information and Modeling*, **2007**, 47, 2366-73	6.1	34
191	Covalent fragment libraries in drug discovery. *Drug Discovery Today*, **2020**, 25, 983-996	8.8	33
190	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
189	Recent developments on JAK2 inhibitors: a patent review. *Expert Opinion on Therapeutic Patents*, **2010**, 20, 471-95	6.8	32
188	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
187	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
186	Homology modelling and binding site mapping of the human histamine H1 receptor. *European Journal of Medicinal Chemistry*, **2004**, 39, 959-67	6.8	30

185	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
184	Multiple fragment docking and linking in primary and secondary pockets of dopamine receptors. *ACS Medicinal Chemistry Letters*, **2014**, 5, 1010-4	4.3	29
183	Histamine H4 receptor ligands and their potential therapeutic applications: an update. *Expert Opinion on Therapeutic Patents*, **2012**, 22, 205-21	6.8	29
182	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
181	Total synthesis of plagiochins C and D, macrocyclic bis(bibenzyl) constituents of plagiochila acantophylla. *Tetrahedron*, **1992**, 48, 913-922	2.4	29
180	Direct Targeting Options for STAT3 and STAT5 in Cancer. *Cancers*, **2019**, 11,	6.6	29
179	Novel histamine H4 receptor ligands and their potential therapeutic applications: an update. *Expert Opinion on Therapeutic Patents*, **2014**, 24, 1185-97	6.8	28
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177	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
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174	Synthesis and revised structure of garuganin III. *Journal of Organic Chemistry*, **1993**, 58, 6725-6728	4.2	25
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169	On the enthalpic preference of fragment binding. *MedChemComm*, **2016**, 7, 332-337	5	23
168	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

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166	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
165	The synthesis of garugamblin-1. *Tetrahedron*, **1993**, 49, 4893-4900	2.4	22
164	Analysis of tractable allosteric sites in G protein-coupled receptors. *Scientific Reports*, **2019**, 9, 6180	4.9	21
163	Histamine H4 receptor ligands and their potential therapeutic applications. *Expert Opinion on Therapeutic Patents*, **2009**, 19, 119-35	6.8	20
162	Quinolinyl- and phenantridinyl-acetamides as bradykinin B1 receptor antagonists. *Bioorganic and Medicinal Chemistry Letters*, **2012**, 22, 3095-9	2.9	19
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158	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
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148	Structural Implications of STAT3 and STAT5 SH2 Domain Mutations. *Cancers*, **2019**, 11,	6.6	16
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146	Carbamoyloximes as novel non-competitive mGlu5 receptor antagonists. *Bioorganic and Medicinal Chemistry Letters*, **2010**, 20, 4371-5	2.9	16
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144	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
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139	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
138	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
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133	Synthesis of Garugamblin-2, a Macrocyclic Diarylheptanoid Constituent of Garuga gamblei. *Liebigs Annalen Der Chemie*, **1994**, 1994, 361-364		13
132	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

131	Cysteine specific bioconjugation with benzyl isothiocyanates.. *RSC Advances*, **2020**, 10, 14928-14936	3.7	13
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115	Bradykinin B1 receptor antagonists: a patent update 2009 - 2012. *Expert Opinion on Therapeutic Patents*, **2012**, 22, 1443-52	6.8	9
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112	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
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91	Electrophilic warheads in covalent drug discovery: an overview.. *Expert Opinion on Drug Discovery*, **2022**, 1-10	6.2	7
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88	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
87	Discovery of a novel kinase hinge binder fragment by dynamic undocking. *RSC Medicinal Chemistry*, **2020**, 11, 552-558	3.5	6
86	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
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84	Discovery of Immunoproteasome Inhibitors Using Large-Scale Covalent Virtual Screening. *Molecules*, **2019**, 24,	4.8	6
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81	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
80	Cell death induced by the Jak2 inhibitor, G6, correlates with cleavage of vimentin filaments. *Biochemistry*, **2011**, 50, 7774-86	3.2	6
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