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## Ligand efficiency: a useful metric for lead selection

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4 <sup>23</sup>	Structure-based optimization of free fatty acid receptor 1 agonists bearing thiazole scaffold. <b>2018</b> , 77, 429-435		13
4 <sup>22</sup>	Binding-Site Compatible Fragment Growing Applied to the Design of $\beta$ Adrenergic Receptor Ligands. <i>Journal of Medicinal Chemistry</i> , <b>2018</b> , 61, 1118-1129	8.3	28
4 <sup>21</sup>	Identification of highly potent and orally available free fatty acid receptor 1 agonists bearing isoxazole scaffold. <b>2018</b> , 26, 703-711		6
4 <sup>20</sup>	When fragments link: a bibliometric perspective on the development of fragment-based drug discovery. <i>Drug Discovery Today</i> , <b>2018</b> , 23, 1596-1609	8.8	24
4 <sup>19</sup>	Discovery of benzimidazole-based <i>Leishmania mexicana</i> cysteine protease CPB2.8 $\mu$ TE inhibitors as potential therapeutics for leishmaniasis. <b>2018</b> , 92, 1585-1596		15
4 <sup>18</sup>	Lipophilic Efficiency as an Important Metric in Drug Design. <i>Journal of Medicinal Chemistry</i> , <b>2018</b> , 61, 6401-6420	8.3	111
4 <sup>17</sup>	New fluorescence-based high-throughput screening assay for small molecule inhibitors of tyrosyl-DNA phosphodiesterase 2 (TDP2). <b>2018</b> , 118, 67-79		11
4 <sup>16</sup>	Molecular Insights into hERG Potassium Channel Blockade by Lubeluzole. <b>2018</b> , 45, 2233-2245		10
4 <sup>15</sup>	Insights into the structural/conformational requirements of cytotoxic oxadiazoles as potential chemotherapeutic target binding agents. <b>2018</b> , 1164, 9-22		7
4 <sup>14</sup>	Exploration of Novel Human Tyrosinase Inhibitors by Molecular Modeling, Docking and Simulation Studies. <b>2018</b> , 10, 68-80		49
4 <sup>13</sup>	Fragment-based virtual screening approach and molecular dynamics simulation studies for identification of BACE1 inhibitor leads. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2018</b> , 36, 1878-1892	3.6	18
4 <sup>12</sup>	Fragment-to-Lead Medicinal Chemistry Publications in 2016. <i>Journal of Medicinal Chemistry</i> , <b>2018</b> , 61, 1774-1784	8.3	27
4 <sup>11</sup>	Molecular modeling studies of pseudouridine isoxazolidinyl nucleoside analogues as potential inhibitors of the pseudouridine 5'-monophosphate glycosidase. <b>2018</b> , 91, 519-525		10
4 <sup>10</sup>	Structure based virtual screening of the Ebola virus trimeric glycoprotein using consensus scoring. <b>2018</b> , 72, 170-180		29
4 <sup>09</sup>	Structure-Based Design of 6-Chloro-4-aminoquinazoline-2-carboxamide Derivatives as Potent and Selective p21-Activated Kinase 4 (PAK4) Inhibitors. <i>Journal of Medicinal Chemistry</i> , <b>2018</b> , 61, 265-285	8.3	28
4 <sup>08</sup>	Design and synthesis of a potent, highly selective, orally bioavailable, retinoic acid receptor alpha agonist. <b>2018</b> , 26, 798-814		8
4 <sup>07</sup>	Causes and Significance of Increased Compound Potency in Cellular or Physiological Contexts. <i>Journal of Medicinal Chemistry</i> , <b>2018</b> , 61, 1767-1773	8.3	19

406	Fragment-Based Drug Discovery of Phosphodiesterase Inhibitors. <i>Journal of Medicinal Chemistry</i> , <b>2018</b> , 61, 1415-1424	8.3	14
405	Biophysical screening in fragment-based drug design: a brief overview. <b>2018</b> , 11,		9
404	GCDB: a glaucomatous chemogenomics database for in silico drug discovery. <b>2018</b> , 2018,		1
403	An Application of Fit Quality to Screen MDM2/p53 Protein-Protein Interaction Inhibitors. <i>Molecules</i> , <b>2018</b> , 23,	4.8	1
402	In silico identification and experimental validation of hits active against KPC-2 $\beta$ -lactamase. <b>2018</b> , 13, e0203241		5
401	Discovery of Potent, Efficient, and Selective Inhibitors of Phosphoinositide 3-Kinase through a Deconstruction and Regrowth Approach. <i>Journal of Medicinal Chemistry</i> , <b>2018</b> , 61, 11061-11073	8.3	9
400	Case report on recovery from Japanese encephalitis virus infection by complementary use of phytolacca-mother tincture and in silico analysis. <b>2018</b> , 14, 22-28		0
399	Hit-to-Lead: Hit Validation and Assessment. <b>2018</b> , 610, 265-309		8
398	3,5-Disubstituted-indole-7-carboxamides as IKK inhibitors: Optimization of Oral Activity via the C3 Substituent. <i>ACS Medicinal Chemistry Letters</i> , <b>2018</b> , 9, 1164-1169	4.3	4
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395	A Molecular Hybridization Approach for the Design of Potent, Highly Selective, and Brain-Penetrant N-Myristoyltransferase Inhibitors. <i>Journal of Medicinal Chemistry</i> , <b>2018</b> , 61, 8374-8389	8.3	29
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393	Synthesis and profiling of a 3-aminopyridin-2-one-based kinase targeted fragment library: Identification of 3-amino-5-(pyridin-4-yl)pyridin-2(1H)-one scaffold for monopolar spindle 1 (MPS1) and Aurora kinases inhibition. <b>2018</b> , 26, 3021-3029		6
392	Cheminformatic Insight into the Differences between Terrestrial and Marine Originated Natural Products. <i>Journal of Chemical Information and Modeling</i> , <b>2018</b> , 58, 1182-1193	6.1	32
391	'Tethering' fragment-based drug discovery to identify inhibitors of the essential respiratory membrane protein type II NADH dehydrogenase. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2018</b> , 28, 2239-2243	2.9	8
390	Hot Spot-Based Design of Small-Molecule Inhibitors for Protein-Protein Interactions. <b>2018</b> , 53-71		0
389	Applications of NMR Spectroscopy in FBDD. <b>2018</b> , 2211-2231		2

388	Targeting Protein-Protein Interactions by Small Molecules. <b>2018</b> ,		5
387	Design of Novel Dual-Target Hits Against Malaria and Tuberculosis Using Computational Docking. <b>2018</b> , 419-442		
386	Design, synthesis, and biological evaluation of novel oxadiazole- and thiazole-based histamine HR ligands. <b>2018</b> , 26, 4034-4046		14
385	LeadOp+R: Structure-Based Lead Optimization With Synthetic Accessibility. <b>2018</b> , 9, 96		2
384	Lead-like Drugs: A Perspective. <i>Journal of Medicinal Chemistry</i> , <b>2018</b> , 61, 10375-10384	8.3	29
383	NMR-Fragment Based Virtual Screening: A Brief Overview. <i>Molecules</i> , <b>2018</b> , 23,	4.8	28
382	VSpine, an Integrated Resource for Virtual Screening and Hit Selection: Applications to Protein Tyrosine Phosphatase Inhibition. <i>Molecules</i> , <b>2018</b> , 23,	4.8	8
381	New aziridine-based inhibitors of cathepsin L-like cysteine proteases with selectivity for the Leishmania cysteine protease LmCPB2.8. <b>2018</b> , 156, 587-597		7
380	Structure-Activity Relationships and Docking Studies of Hydroxychavicol and Its Analogs as Xanthine Oxidase Inhibitors. <b>2018</b> , 66, 741-747		8
379	Evolution of In Silico Strategies for Protein-Protein Interaction Drug Discovery. <i>Molecules</i> , <b>2018</b> , 23,	4.8	50
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374	Overview of the Development of Glutaminase Inhibitors: Achievements and Future Directions. <i>Journal of Medicinal Chemistry</i> , <b>2019</b> , 62, 1096-1115	8.3	50
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369	Using Physicochemical Measurements to Influence Better Compound Design. <b>2019</b> , 24, 791-801		11
368	A Receptor Model With Binding Affinity, Activation Efficacy, and Signal Amplification Parameters for Complex Fractional Response Versus Occupancy Data. <b>2019</b> , 10, 605		14
367	Computational Screening of Potential Inhibitors of $\beta$ -N-Acetyl-D-Hesosaminidases Using Combined Core-Fragment Growth and Pharmacophore Restraints. <b>2019</b> , 189, 1262-1273		0
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364	Synthesis and structure activity relationship of 1, 3-benzo-thiazine-2-thiones as selective HDAC8 inhibitors. <b>2019</b> , 184, 111756		12
363	Shortcuts to schistosomiasis drug discovery: The state-of-the-art. <b>2019</b> , 139-180		2
362	Discovery and Pharmacophore Mapping of a Low-Nanomolar Inhibitor of P. falciparum Growth. <b>2019</b> , 14, 1982-1994		4
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345	Exploring the Chemical Space of Cytochrome P450 Inhibitors Using Integrated Physicochemical Parameters, Drug Efficiency Metrics and Decision Tree Models. <b>2019</b> , 7, 26		3
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336	In Silico Target Druggability Assessment: From Structural to Systemic Approaches. <b>2019</b> , 1953, 63-88		4
335	Properties of FDA-approved small molecule protein kinase inhibitors. <i>Pharmacological Research</i> , <b>2019</b> , 144, 19-50	10.2	247

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328	Accelerated drug discovery by rapid candidate drug identification. <i>Drug Discovery Today</i> , <b>2019</b> , 24, 1237-1241	8.2	14
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326	Targeting ERK1/2 protein-serine/threonine kinases in human cancers. <i>Pharmacological Research</i> , <b>2019</b> , 142, 151-168	10.2	100
325	Structure-based design, synthesis and biological evaluation of a novel series of isoquinolone and pyrazolo[4,3-c]pyridine inhibitors of fascin 1 as potential anti-metastatic agents. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2019</b> , 29, 1023-1029	2.9	19
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323	The discovery of quinoline-3-carboxamides as hematopoietic prostaglandin D synthase (H-PGDS) inhibitors. <b>2019</b> , 27, 1456-1478		12
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320	Concepts and Core Principles of Fragment-Based Drug Design. <i>Molecules</i> , <b>2019</b> , 24,	4.8	45
319	Small-Molecule Intervention At The Dimerization Interface Of Survivin By Novel Rigidized Scaffolds. <b>2019</b> , 13, 4247-4263		3
318	Benford's law in medicinal chemistry: Implications for drug design. <b>2019</b> , 11, 2247-2253		4
317	Medicines discovery for auditory disorders: Challenges for industry. <b>2019</b> , 146, 3652		8



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312	Fragment-to-Lead Medicinal Chemistry Publications in 2017. <i>Journal of Medicinal Chemistry</i> , <b>2019</b> , 62, 3857-3872	8.3	27
311	NMR screening and studies of target-ligand interactions. <b>2019</b> , 88, 59-98		6
310	Synthesis and Biological Investigation of Phenothiazine-Based Benzhydroxamic Acids as Selective Histone Deacetylase 6 Inhibitors. <i>Journal of Medicinal Chemistry</i> , <b>2019</b> , 62, 1138-1166	8.3	52
309	Computer-aided design, synthesis and biological characterization of novel inhibitors for PKMYT1. <b>2019</b> , 161, 479-492		11
308	Fragment-Based Drug Discovery: Advancing Fragments in the Absence of Crystal Structures. <b>2019</b> , 26, 9-15		53
307	Discovery of potent HIV-1 non-nucleoside reverse transcriptase inhibitors by exploring the structure-activity relationship of solvent-exposed regions I. <b>2019</b> , 93, 430-437		8
306	Structure-based exploration and pharmacological evaluation of N-substituted piperidin-4-yl-methanamine CXCR4 chemokine receptor antagonists. <b>2019</b> , 162, 631-649		8
305	Applications of Metabolic Phenotyping in Pharmaceutical Research and Development. <b>2019</b> , 407-447		1
304	Discovery of potent azaindazole leucine-rich repeat kinase 2 (LRRK2) inhibitors possessing a key intramolecular hydrogen bond - Part 2. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2019</b> , 29, 674-680	2.9	3
303	Interaction between 1-pyrenesulfonic acid and albumin: Moving inside the protein. <b>2019</b> , 208, 243-254		10
302	In silico screening of a novel scaffold for fructose-1,6-bisphosphatase (FBPase) inhibitors. <b>2019</b> , 86, 142-148		4
301	The Drug Discovery Process. <b>2019</b> , 323-371		
300	NAOMInext - Synthetically feasible fragment growing in a structure-based design context. <b>2019</b> , 163, 747-762		4
299	Advances in Lead Generation. <i>Bioorganic and Medicinal Chemistry Letters</i> , <b>2019</b> , 29, 517-524	2.9	18

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297	Virtual screening in drug-likeness and structure/activity relationship of pyridazine derivatives as Anti-Alzheimer drugs. <b>2019</b> , 31, 595-601		17
296	Designing of benzothiazole derivatives as promising EGFR tyrosine kinase inhibitors: a pharmacoinformatics study. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2020</b> , 38, 1365-1374	3.6	5
295	Development of ERK1/2 inhibitors as a therapeutic strategy for tumour with MAPK upstream target mutations. <b>2020</b> , 28, 154-165		7
294	Flexible Fragment Growing Boosts Potency of Quorum-Sensing Inhibitors against <i>Pseudomonas aeruginosa</i> Virulence. <b>2020</b> , 15, 188-194		13
293	Citral Inhibition of Human Salivary Aldehyde Dehydrogenase. <b>2020</b> , 78, 31-42		5
292	Development of a Web-Based Laboratory Class to Reduce the Challenges in Teaching Fragment-Based Drug Design. <b>2020</b> , 97, 427-436		9
291	Fragment-to-Lead Medicinal Chemistry Publications in 2018. <i>Journal of Medicinal Chemistry</i> , <b>2020</b> , 63, 4430-4444	8.3	37
290	Computational screening of promising beta-secretase 1 inhibitors through multi-step molecular docking and molecular dynamics simulations - Pharmacoinformatics approach. <b>2020</b> , 1205, 127660		11
289	Properties of FDA-approved small molecule protein kinase inhibitors: A 2020 update. <i>Pharmacological Research</i> , <b>2020</b> , 152, 104609	10.2	244
288	Identifying Ortholog Selective Fragment Molecules for Bacterial Glutaredoxins by NMR and Affinity Enhancement by Modification with an Acrylamide Warhead. <i>Molecules</i> , <b>2019</b> , 25,	4.8	3
287	Virtual screening identification and chemical optimization of substituted 2-arylbenzimidazoles as new non-zinc-binding MMP-2 inhibitors. <b>2020</b> , 28, 115257		2
286	Fluorescent ligands: Bringing light to emerging GPCR paradigms. <b>2020</b> , 177, 978-991		26
285	. <b>2020</b> ,		0
284	Setup and Validation of a Reliable Docking Protocol for the Development of Neuroprotective Agents by Targeting the Sigma-1 Receptor (S1R). <i>International Journal of Molecular Sciences</i> , <b>2020</b> , 21,	6.3	2
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282	Solution structure of the Hop TPR2A domain and investigation of target druggability by NMR, biochemical and in silico approaches. <b>2020</b> , 10, 16000		4
281	Alkaloids from as Potential Inhibitors of SARS-CoV-2 Viral Proteins: An Study. <b>2020</b> , 2020, 5324560		30

280	Design and Synthesis of a Highly Selective and -Capable Inhibitor of the Second Bromodomain of the Bromodomain and Extra Terminal Domain Family of Proteins. <i>Journal of Medicinal Chemistry</i> , <b>2020</b> , 63, 9070-9092	8.3	21
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278	Pharmacokinetics (ADME). <b>2020</b> , 133-224		
277	Current Challenges and Opportunities in Designing Protein-Protein Interaction Targeted Drugs. <b>2020</b> , 13, 11-25		10
276	Fragment-to-Lead Medicinal Chemistry Publications in 2019. <i>Journal of Medicinal Chemistry</i> , <b>2020</b> , 63, 15494-15507	8.3	18
275	Understanding binding between donepezil and human ferritin: molecular docking and molecular dynamics simulation approach. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2020</b> , 1-9	3.6	2
274	Discovery of Novel and Highly Selective Cyclopropane ALK Inhibitors through a Fragment-Assisted, Structure-Based Drug Design. <b>2020</b> , 5, 31984-32001		2
273	Highly Potent and Selective -Aryl Oxamic Acid-Based Inhibitors for Protein Tyrosine Phosphatase B. <i>Journal of Medicinal Chemistry</i> , <b>2020</b> , 63, 9212-9227	8.3	9
272	Chemical Biology Toolsets for Drug Discovery and Target Identification. <b>2020</b> ,		1
271	The Optimization of a Novel, Weak Bromo and Extra Terminal Domain (BET) Bromodomain Fragment Ligand to a Potent and Selective Second Bromodomain (BD2) Inhibitor. <i>Journal of Medicinal Chemistry</i> , <b>2020</b> , 63, 9093-9126	8.3	23
270	Identification of high-affinity inhibitors of SARS-CoV-2 main protease: Towards the development of effective COVID-19 therapy. <b>2020</b> , 288, 198102		43
269	Design, Synthesis, and Pharmacological Characterization of a Neutral, Non-Prodrug Thrombin Inhibitor with Good Oral Pharmacokinetics. <i>Journal of Medicinal Chemistry</i> , <b>2020</b> , 63, 12574-12594	8.3	6
268	InstaDock: A single-click graphical user interface for molecular docking-based virtual high-throughput screening. <b>2021</b> , 22,		37
267	Optimization of kinetic stabilizers of tetrameric transthyretin: A prospective ligand efficiency-guided approach. <b>2020</b> , 28, 115794		3
266	Discovery of IPN60090, a Clinical Stage Selective Glutaminase-1 (GLS-1) Inhibitor with Excellent Pharmacokinetic and Physicochemical Properties. <i>Journal of Medicinal Chemistry</i> , <b>2020</b> , 63, 12957-12977	8.3	14
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