Thierry Langer

List of Publications by Citations

223 papers	8,839 citations	51 h-index	87 g-index
261 ext. papers	9,919 ext. citations	4.7 avg, IF	6.12 L-index

#	Paper	IF	Citations
223	LigandScout: 3-D pharmacophores derived from protein-bound ligands and their use as virtual screening filters. *Journal of Chemical Information and Modeling*, **2005**, 45, 160-9	6.1	1255
222	Why drugs fail--a study on side effects in new chemical entities. *Current Pharmaceutical Design*, **2005**, 11, 3545-59	3.3	329
221	Recognizing pitfalls in virtual screening: a critical review. *Journal of Chemical Information and Modeling*, **2012**, 52, 867-81	6.1	295
220	Evaluation of the performance of 3D virtual screening protocols: RMSD comparisons, enrichment assessments, and decoy selection--what can we learn from earlier mistakes?. *Journal of Computer-Aided Molecular Design*, **2008**, 22, 213-28	4.2	278
219	Molecule-pharmacophore superpositioning and pattern matching in computational drug design. *Drug Discovery Today*, **2008**, 13, 23-9	8.8	249
218	Efficient overlay of small organic molecules using 3D pharmacophores. *Journal of Computer-Aided Molecular Design*, **2006**, 20, 773-88	4.2	211
217	Acetylcholinesterase inhibitory activity of scopolin and scopoletin discovered by virtual screening of natural products. *Journal of Medicinal Chemistry*, **2004**, 47, 6248-54	8.3	167
216	Comparative performance assessment of the conformational model generators omega and catalyst: a large-scale survey on the retrieval of protein-bound ligand conformations. *Journal of Chemical Information and Modeling*, **2006**, 46, 1848-61	6.1	151
215	Comparative analysis of protein-bound ligand conformations with respect to catalystÂ conformational space subsampling algorithms. *Journal of Chemical Information and Modeling*, **2005**, 45, 422-30	6.1	125
214	Recent Advances in Docking and Scoring. *Current Computer-Aided Drug Design*, **2005**, 1, 93-102	1.4	115
213	In silico target fishing for rationalized ligand discovery exemplified on constituents of Ruta graveolens. *Planta Medica*, **2009**, 75, 195-204	3.1	111
212	Parallel screening: a novel concept in pharmacophore modeling and virtual screening. *Journal of Chemical Information and Modeling*, **2006**, 46, 2146-57	6.1	107
211	The discovery of new 11beta-hydroxysteroid dehydrogenase type 1 inhibitors by common feature pharmacophore modeling and virtual screening. *Journal of Medicinal Chemistry*, **2006**, 49, 3454-66	8.3	107
210	Discovery of high-affinity ligands of sigma1 receptor, ERG2, and emopamil binding protein by pharmacophore modeling and virtual screening. *Journal of Medicinal Chemistry*, **2005**, 48, 4754-64	8.3	104
209	5-Arylidene-2,4-thiazolidinediones as inhibitors of protein tyrosine phosphatases. *Bioorganic and Medicinal Chemistry*, **2007**, 15, 5137-49	3.4	93
208	GBPM: GRID-based pharmacophore model: concept and application studies to protein-protein recognition. *Bioinformatics*, **2006**, 22, 1449-55	7.2	93
207	Structure-activity relationships and molecular modelling of 5-arylidene-2,4-thiazolidinediones active as aldose reductase inhibitors. *Bioorganic and Medicinal Chemistry*, **2005**, 13, 2809-23	3.4	92

206	Virtual screening: an effective tool for lead structure discovery?. *Current Pharmaceutical Design*, **2001**, 7, 509-27	3.3	90
205	Molecular basis of peripheral vs central benzodiazepine receptor selectivity in a new class of peripheral benzodiazepine receptor ligands related to alpidem. *Journal of Medicinal Chemistry*, **1996**, 39, 4275-84	8.3	85
204	Non-peptide angiotensin II receptor antagonists: chemical feature based pharmacophore identification. *Journal of Medicinal Chemistry*, **2003**, 46, 716-26	8.3	84
203	Pharmacophore modeling and in silico screening for new P450 19 (aromatase) inhibitors. *Journal of Chemical Information and Modeling*, **2006**, 46, 1301-11	6.1	83
202	The Protein Data Bank (PDB), its related services and software tools as key components for in silico guided drug discovery. *Journal of Medicinal Chemistry*, **2008**, 51, 7021-40	8.3	81
201	Exploiting a "Beast" in Carbenoid Chemistry: Development of a Straightforward Direct Nucleophilic Fluoromethylation Strategy. *Journal of the American Chemical Society*, **2017**, 139, 13648-13651	16.4	79
200	Novel, potent, and selective 5-HT3 receptor antagonists based on the arylpiperazine skeleton: synthesis, structure, biological activity, and comparative molecular field analysis studies. *Journal of Medicinal Chemistry*, **1995**, 38, 2692-704	8.3	79
199	Strategies for efficient lead structure discovery from natural products. *Current Medicinal Chemistry*, **2006**, 13, 1491-507	4.3	77
198	Structure-based pharmacophore design and virtual screening for novel angiotensin converting enzyme 2 inhibitors. *Journal of Chemical Information and Modeling*, **2006**, 46, 708-16	6.1	75
197	The identification of ligand features essential for PXR activation by pharmacophore modeling. *Journal of Chemical Information and Modeling*, **2005**, 45, 431-9	6.1	73
196	Enhancing drug discovery through in silico screening: strategies to increase true positives retrieval rates. *Current Medicinal Chemistry*, **2008**, 15, 2040-53	4.3	72
195	Novel potent and selective central 5-HT3 receptor ligands provided with different intrinsic efficacy. 1. Mapping the central 5-HT3 receptor binding site by arylpiperazine derivatives. *Journal of Medicinal Chemistry*, **1998**, 41, 728-41	8.3	71
194	Virtual screening for the discovery of bioactive natural products. *Progress in Drug Research Fortschritte Der Arzneimittelforschung Progres Des Recherches Pharmaceutiques*, **2008**, 65, 211, 213-49		70
193	Structure-based virtual screening for the discovery of natural inhibitors for human rhinovirus coat protein. *Journal of Medicinal Chemistry*, **2008**, 51, 842-51	8.3	70
192	Further studies on imidazo[4,5-b]pyridine AT1 angiotensin II receptor antagonists. Effects of the transformation of the 4-phenylquinoline backbone into 4-phenylisoquinolinone or 1-phenylindene scaffolds. *Journal of Medicinal Chemistry*, **2006**, 49, 6451-64	8.3	70
191	5-Arylidene-2-phenylimino-4-thiazolidinones as PTP1B and LMW-PTP inhibitors. *Bioorganic and Medicinal Chemistry*, **2009**, 17, 1928-37	3.4	66
190	Fast and efficient in silico 3D screening: toward maximum computational efficiency of pharmacophore-based and shape-based approaches. *Journal of Chemical Information and Modeling*, **2007**, 47, 2182-96	6.1	64
189	Generation of a homology model of the human histamine H(3) receptor for ligand docking and pharmacophore-based screening. *Journal of Computer-Aided Molecular Design*, **2007**, 21, 437-53	4.2	63

188	Comparative enzymology of 11beta-hydroxysteroid dehydrogenase type 1 from six species. *Journal of Molecular Endocrinology*, **2005**, 35, 89-101	4.5	63
187	Synthesis and pharmacological evaluation of 1H-imidazoles as ligands for the estrogen receptor and cytotoxic inhibitors of the cyclooxygenase. *Journal of Medicinal Chemistry*, **2005**, 48, 6516-21	8.3	62
186	The UV-filter benzophenone-1 inhibits 17beta-hydroxysteroid dehydrogenase type 3: Virtual screening as a strategy to identify potential endocrine disrupting chemicals. *Biochemical Pharmacology*, **2010**, 79, 1189-99	6	61
185	Why is 11beta-hydroxysteroid dehydrogenase type 1 facing the endoplasmic reticulum lumen? Physiological relevance of the membrane topology of 11beta-HSD1. *Molecular and Cellular Endocrinology*, **2006**, 248, 15-23	4.4	61
184	Mapping and fitting the peripheral benzodiazepine receptor binding site by carboxamide derivatives. Comparison of different approaches to quantitative ligand-receptor interaction modeling. *Journal of Medicinal Chemistry*, **2001**, 44, 1134-50	8.3	61
183	Discovery of novel PPAR ligands by a virtual screening approach based on pharmacophore modeling, 3D shape, and electrostatic similarity screening. *Journal of Medicinal Chemistry*, **2008**, 51, 6303-17	8.3	60
182	Pharmacophore definition and 3D searches. *Drug Discovery Today: Technologies*, **2004**, 1, 203-7	7.1	59
181	Pharmacophore modeling and parallel screening for PPAR ligands. *Journal of Computer-Aided Molecular Design*, **2007**, 21, 575-90	4.2	58
180	Pharmacophore identification, in silico screening, and virtual library design for inhibitors of the human factor Xa. *Journal of Chemical Information and Modeling*, **2005**, 45, 146-59	6.1	57
179	Impact of scoring functions on enrichment in docking-based virtual screening: an application study on renin inhibitors. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 1123-9		56
178	Recent advancements on the use of 2-methyltetrahydrofuran in organometallic chemistry. *Monatshefte F□ Chemie*, **2017**, 148, 37-48	1.4	55
177	Lead identification for modulators of multidrug resistance based on in silico screening with a pharmacophoric feature model. *Archiv Der Pharmazie*, **2004**, 337, 317-27	4.3	55
176	Synthesis, biological evaluation and 3D-QSAR of 1,3,5-trisubstituted-4,5-dihydro-(1H)-pyrazole derivatives as potent and highly selective monoamine oxidase A inhibitors. *Current Medicinal Chemistry*, **2006**, 13, 1411-28	4.3	54
175	Influenza virus neuraminidase inhibitors: generation and comparison of structure-based and common feature pharmacophore hypotheses and their application in virtual screening. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 1849-56		54
174	Combining ethnopharmacology and virtual screening for lead structure discovery: COX-inhibitors as application example. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 480-8		53
173	Chemoselective Schwartz Reagent Mediated Reduction of Isocyanates to Formamides. *Organic Letters*, **2016**, 18, 2750-3	6.2	52
172	Discovery of nonsteroidal 17beta-hydroxysteroid dehydrogenase 1 inhibitors by pharmacophore-based screening of virtual compound libraries. *Journal of Medicinal Chemistry*, **2008** , 51, 4188-99	8.3	51
171	Efficient Access to All-Carbon Quaternary and Tertiary □Functionalized Homoallyl-type Aldehydes from Ketones. *Angewandte Chemie - International Edition*, **2017**, 56, 12677-12682	16.4	50

170	Synthesis, induced-fit docking investigations, and in vitro aldose reductase inhibitory activity of non-carboxylic acid containing 2,4-thiazolidinedione derivatives. *Bioorganic and Medicinal Chemistry* , **2008**, 16, 5840-52	3.4	49
169	Common Hits Approach: Combining Pharmacophore Modeling and Molecular Dynamics Simulations. *Journal of Chemical Information and Modeling*, **2017**, 57, 365-385	6.1	47
168	Evaluation of in vitro aldose redutase inhibitory activity of 5-arylidene-2,4-thiazolidinediones. *Bioorganic and Medicinal Chemistry Letters*, **2007**, 17, 3886-93	2.9	47
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162	Modular and Chemoselective Strategy for the Direct Access to α-Fluoroepoxides and Aziridines via the Addition of Fluoroiodomethyllithium to Carbonyl-Like Compounds. *Organic Letters*, **2019**, 21, 584-588	6.2	43
161	Thiazolyl and benzothiazolyl hydrazones derived from α-(N)-acetylpyridines and diazines: synthesis, antiproliferative activity and CoMFA studies. *European Journal of Medicinal Chemistry*, **1997**, 32, 397-408	6.8	42
160	Synthesis and molecular modeling of new 1-aryl-3-[4-arylpiperazin-1-yl]-1-propane derivatives with high affinity at the serotonin transporter and at 5-HT(1A) receptors. *Journal of Medicinal Chemistry*, **2002**, 45, 4128-39	8.3	42
159	Epidermis-type lipoxygenase 3 regulates adipocyte differentiation and peroxisome proliferator-activated receptor gamma activity. *Molecular and Cellular Biology*, **2010**, 30, 4077-91	4.8	41
158	Synthesis, semipreparative HPLC separation, biological evaluation, and 3D-QSAR of hydrazothiazole derivatives as human monoamine oxidase B inhibitors. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 5063-70	3.4	41
157	Azinyl and diazinyl hydrazones derived from aryl N-heteroaryl ketones: synthesis and antiproliferative activity. *Journal of Medicinal Chemistry*, **1997**, 40, 4420-5	8.3	41
156	Morphinans and isoquinolines: acetylcholinesterase inhibition, pharmacophore modeling, and interaction with opioid receptors. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 5071-80	3.4	40
155	Pharmacophore modelling: applications in drug discovery. *Expert Opinion on Drug Discovery*, **2006**, 1, 261-7	6.2	40
154	Pharmacophore modeling, docking, and principal component analysis based clustering: combined computer-assisted approaches to identify new inhibitors of the human rhinovirus coat protein. *Journal of Medicinal Chemistry*, **2005**, 48, 6250-60	8.3	40
153	Chemoselective Addition of Halomethyllithiums to Functionalized Isatins:A Straightforward Access to Spiro-Epoxyoxindoles. *Advanced Synthesis and Catalysis*, **2016**, 358, 172-177	5.6	40

152	Evidence and isolation of tetrahedral intermediates formed upon the addition of lithium carbenoids to Weinreb amides and N-acylpyrroles. *Chemical Communications*, **2017**, 53, 9498-9501	5.8	39
151	Development and validation of an in silico P450 profiler based on pharmacophore models. *Current Drug Discovery Technologies*, **2006**, 3, 1-48	1.5	39
150	Fluoxetine Inhibits Enterovirus Replication by Targeting the Viral 2C Protein in a Stereospecific Manner. *ACS Infectious Diseases*, **2019**, 5, 1609-1623	5.5	37
149	Chemical function based pharmacophore generation of endothelin-A selective receptor antagonists. *Journal of Medicinal Chemistry*, **2004**, 47, 2750-60	8.3	37
148	A compact review of molecular property prediction with graph neural networks.. *Drug Discovery Today: Technologies*, **2020**, 37, 1-12	7.1	37
147	Telescoped, Divergent, Chemoselective C1 and C1-C1 Homologation of Imine Surrogates: Access to Quaternary Chloro- and Halomethyl-Trifluoromethyl Aziridines. *Angewandte Chemie - International Edition*, **2019**, 58, 2479-2484	16.4	37
146	Synthesis, activity and molecular modeling of a new series of chromones as low molecular weight protein tyrosine phosphatase inhibitors. *Bioorganic and Medicinal Chemistry*, **2009**, 17, 2658-72	3.4	35
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143	External action of di- and polyamines on maxi calcium-activated potassium channels: an electrophysiological and molecular modeling study. *Biophysical Journal*, **1998**, 74, 722-30	2.9	34
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141	Virtual combinatorial chemistry and in silico screening: Efficient tools for lead structure discovery?. *Pure and Applied Chemistry*, **2004**, 76, 991-996	2.1	33
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122	Variability in chemical constituents in Petasites hybridus from Austria. *Biochemical Systematics and Ecology*, **2000**, 28, 421-432	1.4	21
121	A Computational Approach to Identify Potential Novel Inhibitors against the Coronavirus SARS-CoV-2. *Molecular Informatics*, **2020**, 39, e2000090	3.8	21
120	Discovery of Mycobacterium tuberculosis InhA Inhibitors by Binding Sites Comparison and Ligands Prediction. *Journal of Medicinal Chemistry*, **2016**, 59, 11069-11078	8.3	21
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115	Docking Versus Pharmacophore Model Generation: A Comparison of High-Throughput Virtual Screening Strategies for the Search of Human Rhinovirus Coat Protein Inhibitors. *QSAR and Combinatorial Science*, **2005**, 24, 470-479		19
114	Computer-aided molecular modeling, synthesis, and biological evaluation of 8-(benzyloxy)-2-phenylpyrazolo[4,3-c]quinoline as a novel benzodiazepine receptor agonist ligand. *Journal of Medicinal Chemistry*, **1995**, 38, 950-7	8.3	19
113	Efficient Access to All-Carbon Quaternary and Tertiary □Functionalized Homoallyl-type Aldehydes from Ketones. *Angewandte Chemie*, **2017**, 129, 12851-12856	3.6	18
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111	The Novel Atypical Dopamine Uptake Inhibitor -CE-123 Partially Reverses the Effort-Related Effects of the Dopamine Depleting Agent Tetrabenazine and Increases Progressive Ratio Responding. *Frontiers in Pharmacology*, **2019**, 10, 682	5.6	18
110	Molecular structure and dynamics of some potent 5-HT3 receptor antagonists. Insight into the interaction with the receptor. *Bioorganic and Medicinal Chemistry*, **1996**, 4, 1255-69	3.4	18
109	On the Use of Chemical Function-Based Alignments as Input for 3D-QSAR. *Journal of Chemical Information and Computer Sciences*, **1998**, 38, 325-330		17
108	The Pharmacophore Concept and Its Applications in Computer-Aided Drug Design. *Progress in the Chemistry of Organic Natural Products*, **2019**, 110, 99-141	1.9	17
107	A Molecular Dynamics-Shared Pharmacophore Approach to Boost Early-Enrichment Virtual Screening: A Case Study on Peroxisome Proliferator-Activated Receptor □*ChemMedChem*, **2017**, 12, 1399-1407	3.7	16
106	Binding investigation and preliminary optimisation of the 3-amino-1,2,4-triazin-5(2H)-one core for the development of new Fyn inhibitors. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2018**, 33, 956-961	5.6	16
105	Applications of integrated data mining methods to exploring natural product space for acetylcholinesterase inhibitors. *Combinatorial Chemistry and High Throughput Screening*, **2010**, 13, 54-66	1.3	16
104	A 3D QSAR study of monoamino oxidase-B inhibitors using the chemical function based pharmacophore generation approach. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2001**, 16, 199-215		15
103	Applications of the Pharmacophore Concept in Natural Product inspired Drug Design. *Molecular Informatics*, **2020**, 39, e2000059	3.8	13
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94	Identification of 2-(4-(Phenylsulfonyl)piperazine-1-yl)pyrimidine Analogues as Novel Inhibitors of Chikungunya Virus. *ACS Medicinal Chemistry Letters*, **2020**, 11, 906-912	4.3	12
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84	Multiple Virtual Screening Strategies for the Discovery of Novel Compounds Active Against Dengue Virus: A Hit Identification Study. *Scientia Pharmaceutica*, **2020**, 88, 2	4.3	11
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82	Heterocyclic Analogues of Modafinil as Novel, Atypical Dopamine Transporter Inhibitors. *Journal of Medicinal Chemistry*, **2017**, 60, 9330-9348	8.3	10
81	Selective Optimization of Side Activities (SOSA): A Promising way for Drug Discovery **2012**, 227-243		9

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79	Pyridazines. LXVIII. Convenient Synthesis of Phenyl (6-Substituted 3-Pyridazinyl) Ketones via the Oxidative Decyanation Route. *Journal of Heterocyclic Chemistry*, **1993**, 30, 1685-1689	1.9	9
78	Chapter 3:Pharmacophore-based Virtual Screening in Drug Discovery **2008**, 76-119		9
77	Structure-Activity Relationships of Novel Thiazole-Based Modafinil Analogues Acting at Monoamine Transporters. *Journal of Medicinal Chemistry*, **2020**, 63, 391-417	8.3	9
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75	Novel Class of Chikungunya Virus Small Molecule Inhibitors That Targets the Viral Capping Machinery. *Antimicrobial Agents and Chemotherapy*, **2020**, 64,	5.9	8
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