Thierry Langer

List of Publications by Year in Descending Order

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	Design, Synthesis, and Biological Evaluation of 4,4RDifluorobenzhydrol Carbamates as Selective M Antagonists.. *Pharmaceuticals*, **2022**, 15,	5.2	2
222	Synthesis, Biological Evaluation, and Docking Studies of Antagonistic Hydroxylated Arecaidine Esters Targeting mAChRs. *Molecules*, **2022**, 27, 3173	4.8	0
221	Improved Lipophilicity and Aqueous Solubility Prediction with Composite Graph Neural Networks. *Molecules*, **2021**, 26,	4.8	5
220	Structural Insights into the Mechanisms of Action of Functionally Distinct Classes of Chikungunya Virus Nonstructural Protein 1 Inhibitors. *Antimicrobial Agents and Chemotherapy*, **2021**, 65, e0256620	5.9	4
219	Update on PET Tracer Development for Muscarinic Acetylcholine Receptors. *Pharmaceuticals*, **2021**, 14,	5.2	2
218	In Silico Identification of Potential Druggable Binding Sites on CIN85 SH3 Domain. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	2
217	Support Vector Machine as a Supervised Learning for the Prioritization of Novel Potential SARS-CoV-2 Main Protease Inhibitors. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	2
216	Antivirals against the Chikungunya Virus. *Viruses*, **2021**, 13,	6.2	6
215	QPHAR: quantitative pharmacophore activity relationship: method and validation. *Journal of Cheminformatics*, **2021**, 13, 57	8.6	1
214	and studies of holothurin A on androgen receptor in prostate cancer. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-9	3.6	2
213	Consecutive and Selective Double Methylene Insertion of Lithium Carbenoids to Isothiocyanates: A Direct Assembly of Four-Membered Sulfur-Containing Cycles. *Angewandte Chemie - International Edition*, **2021**, 60, 24854-24858	16.4	3
212	Cognitive profiling and proteomic analysis of the modafinil analogue S-CE-123 in experienced aged rats.. *Scientific Reports*, **2021**, 11, 23962	4.9	1
211	Novel Class of Chikungunya Virus Small Molecule Inhibitors That Targets the Viral Capping Machinery. *Antimicrobial Agents and Chemotherapy*, **2020**, 64,	5.9	8
210	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
209	Applications of the Pharmacophore Concept in Natural Product inspired Drug Design. *Molecular Informatics*, **2020**, 39, e2000059	3.8	13
208	Differences in Hypothalamic Lipid Profiles of Young and Aged Male Rats With Impaired and Unimpaired Spatial Cognitive Abilities and Memory. *Frontiers in Aging Neuroscience*, **2020**, 12, 204	5.3	5
207	Crystal structure, Hirshfeld analysis and a mol-ecular docking study of a new inhibitor of the Hepatitis B virus (HBV): ethyl 5-methyl-1,1-dioxo-2-{[5-(pentan-3-yl)-1,2,4-oxa-diazol-3-yl]meth-yl}-2-1,2,6-thia-diazine-4-carboxyl-ate. *Acta Crystallographica Section E: Crystallographic Communications*, **2020**, 76, 12-17	0.7	1

206	A Combination of Pharmacophore and Docking-based Virtual Screening to Discover new Tyrosinase Inhibitors. *Molecular Informatics*, **2020**, 39, e1900054	3.8	7
205	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
204	Structure-Activity Relationships of Novel Thiazole-Based Modafinil Analogues Acting at Monoamine Transporters. *Journal of Medicinal Chemistry*, **2020**, 63, 391-417	8.3	9
203	A Computational Approach to Identify Potential Novel Inhibitors against the Coronavirus SARS-CoV-2. *Molecular Informatics*, **2020**, 39, e2000090	3.8	21
202	A Novel Series of [1,2,4]Triazolo[4,3-a]Pyridine Sulfonamides as Potential Antimalarial Agents: In Silico Studies, Synthesis and In Vitro Evaluation. *Molecules*, **2020**, 25,	4.8	3
201	Methylation of Methyl 4-Hydroxy-2-thioxo-1,2-dihydroquinoline-3-carboxylate: Synthetic, Crystallographic, and Molecular Docking Studies. *Molecules*, **2020**, 25,	4.8	1
200	Chemoselective Homologation-Deoxygenation Strategy Enabling the Direct Conversion of Carbonyls into ()-Halomethyl-Alkanes. *Organic Letters*, **2020**, 22, 7629-7634	6.2	12
199	A compact review of molecular property prediction with graph neural networks.. *Drug Discovery Today: Technologies*, **2020**, 37, 1-12	7.1	37
198	A-ring and E-ring modifications of the cytotoxic alkaloid Luotonin A: Synthesis, computational and biological studies. *Bioorganic and Medicinal Chemistry*, **2020**, 28, 115443	3.4	1
197	Computational Identification of Novel Kir6 Channel Inhibitors. *Frontiers in Pharmacology*, **2019**, 10, 549	5.6	2
196	Fluoxetine Inhibits Enterovirus Replication by Targeting the Viral 2C Protein in a Stereospecific Manner. *ACS Infectious Diseases*, **2019**, 5, 1609-1623	5.5	37
195	Synthesis, X-ray Crystal Structure, Hirshfeld Surface Analysis, and Molecular Docking Study of Novel Hepatitis B (HBV) Inhibitor: 8-Fluoro-5-(4-fluorobenzyl)-3-(2-methoxybenzyl)-3,5-dihydro-4H-pyrimido[5,4-b]indol-4-one. *Crystals*, **2019**, 9, 379	2.3	4
194	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
193	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
192	Synthesis, X-ray crystal structure, Hirshfeld surface analysis, and molecular docking study of novel inhibitor of hepatitis B: methyl 4-fluoro-3-(morpholinosulfonyl)benzo[b]thiophene-2-carboxylate. *Heliyon*, **2019**, 5, e02738	3.6	7
191	Cytotoxicity Of Chalcone Of Burm F. Leaves Against T47D Breast Cancer Cell Lines And Its Prediction As An Estrogen Receptor Antagonist Based On Pharmacophore-Molecular Dynamics Simulation. *Advances and Applications in Bioinformatics and Chemistry*, **2019**, 12, 33-43	1.5	2
190	Synthesis, Single Crystal X-Ray Analysis, Prediction and Study of Pharmacological Activity of 4-(1H-Benzo[d]imidazol-2-yl)-1-Phenyl-1H-1,2,3-triazol-5-Amine and Its Solvates. *Crystals*, **2019**, 9, 644	2.3	1
189	LigandScout Remote: A New User-Friendly Interface for HPC and Cloud Resources. *Journal of Chemical Information and Modeling*, **2019**, 59, 31-37	6.1	3

188	A Straightforward Homologation of Carbon Dioxide with Magnesium Carbenoids en Route to -Halocarboxylic Acids. *Advanced Synthesis and Catalysis*, **2019**, 361, 1001-1006	5.6	7
187	Modular and Chemoselective Strategy for the Direct Access to -Fluoroepoxides and Aziridines via the Addition of Fluoroiodomethyllithium to Carbonyl-Like Compounds. *Organic Letters*, **2019**, 21, 584-588	6.2	43
186	Sustainable Asymmetric Organolithium Chemistry: Enantio- and Chemoselective Acylations through Recycling of Solvent, Sparteine, and Weinreb "Amine". *ChemSusChem*, **2019**, 12, 1147-1154	8.3	11
185	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
184	Design, Synthesis, and Pharmacological Evaluation of Novel 2/3 Subunit-Selective -Aminobutyric Acid Type A (GABA) Receptor Modulators. *Journal of Medicinal Chemistry*, **2019**, 62, 317-341	8.3	6
183	A daily single dose of a novel modafinil analogue CE-123 improves memory acquisition and memory retrieval. *Behavioural Brain Research*, **2018**, 343, 83-94	3.4	13
182	GRAIL: GRids of phArmacophore Interaction fieLds. *Journal of Chemical Theory and Computation*, **2018**, 14, 4958-4970	6.4	12
181	The Use of Dynamic Pharmacophore in Computer-Aided Hit Discovery: A Case Study. *Methods in Molecular Biology*, **2018**, 1824, 317-333	1.4	1
180	Workflow for the Discovery of Natural Products Activating the G Protein-Coupled Bile Acid Receptor 1. *Frontiers in Chemistry*, **2018**, 6, 242	5	13
179	Pharmacy Practice and Education in Austria. *Pharmacy (Basel, Switzerland)*, **2018**, 6,	2	3
178	SAR-Guided Scoring Function and Mutational Validation Reveal the Binding Mode of CGS-8216 at the +/- Benzodiazepine Site. *Journal of Chemical Information and Modeling*, **2018**, 58, 1682-1696	6.1	3
177	The Mu.Ta.Lig. Chemotheca: A Community-Populated Molecular Database for Multi-Target Ligands Identification and Compound-Repurposing. *Frontiers in Chemistry*, **2018**, 6, 130	5	6
176	Conformational Sampling of Small Molecules With iCon: Performance Assessment in Comparison With OMEGA. *Frontiers in Chemistry*, **2018**, 6, 229	5	22
175	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
174	Homologation of halostannanes with carbenoids: a convenient and straightforward one-step access to -Functionalized organotin reagents. *Chemical Communications*, **2018**, 54, 10112-10115	5.8	13
173	Discovery of Potent Inhibitors for the Large Neutral Amino Acid Transporter 1 (LAT1) by Structure-Based Methods. *International Journal of Molecular Sciences*, **2018**, 20,	6.3	21
172	Pharmacophore-based discovery of 2-(phenylamino)aceto-hydrazides as potent eosinophil peroxidase (EPO) inhibitors. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2018**, 33, 1529-1536	5.6	0
171	Common Hits Approach: Combining Pharmacophore Modeling and Molecular Dynamics Simulations. *Journal of Chemical Information and Modeling*, **2017**, 57, 365-385	6.1	47

170	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
169	A novel heterocyclic compound improves working memory in the radial arm maze and modulates the dopamine receptor D1R in frontal cortex of the Sprague-Dawley rat. *Behavioural Brain Research* , **2017**, 332, 308-315	3.4	5
168	3D Pharmacophore Modeling Techniques in Computer-Aided Molecular Design Using LigandScout **2017**, 279-309		8
167	Recent advancements on the use of 2-methyltetrahydrofuran in organometallic chemistry. *Monatshefte F Chemie*, **2017**, 148, 37-48	1.4	55
166	Efficient Access to All-Carbon Quaternary and Tertiary Functionalized Homoallyl-type Aldehydes from Ketones. *Angewandte Chemie*, **2017**, 129, 12851-12856	3.6	18
165	Heterocyclic Analogues of Modafinil as Novel, Atypical Dopamine Transporter Inhibitors. *Journal of Medicinal Chemistry*, **2017**, 60, 9330-9348	8.3	10
164	R-Modafinil exerts weak effects on spatial memory acquisition and dentate gyrus synaptic plasticity. *PLoS ONE*, **2017**, 12, e0179675	3.7	7
163	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
162	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
161	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
160	Molecular Docking and 3D-Pharmacophore Modeling to Study the Interactions of Chalcone Derivatives with Estrogen Receptor Alpha. *Pharmaceuticals*, **2017**, 10,	5.2	30
159	A Novel Dopamine Transporter Inhibitor CE-123 Improves Cognitive Flexibility and Maintains Impulsivity in Healthy Male Rats. *Frontiers in Behavioral Neuroscience*, **2017**, 11, 222	3.5	12
158	Pharmacophore Models Derived from Molecular Dynamics Simulations of Protein-Ligand Complexes: A Case Study. *Natural Product Communications*, **2016**, 11, 1934578X1601101	0.9	2
157	Fragment pharmacophore-based in silico screening: a powerful approach for efficient lead discovery. *MedChemComm*, **2016**, 7, 506-511	5	4
156	Evaluating the stability of pharmacophore features using molecular dynamics simulations. *Biochemical and Biophysical Research Communications*, **2016**, 470, 685-689	3.4	23
155	Comparing pharmacophore models derived from crystal structures and from molecular dynamics simulations. *Monatshefte F Chemie*, **2016**, 147, 553-563	1.4	13
154	A heterocyclic compound CE-103 inhibits dopamine reuptake and modulates dopamine transporter and dopamine D1-D3 containing receptor complexes. *Neuropharmacology*, **2016**, 102, 186-96	5.5	12
153	The use of the Comins-Meyers Amide in Synthetic Chemistry: An Overview. *Natural Product Communications*, **2016**, 11, 1934578X1601101	0.9	2

152	A novel heterocyclic compound targeting the dopamine transporter improves performance in the radial arm maze and modulates dopamine receptors D1-D3. *Behavioural Brain Research*, **2016**, 312, 127-37	3.4	6
151	Chemoselective Addition of Halomethyllithiums to Functionalized Isatins:A Straightforward Access to Spiro-Epoxyoxindoles. *Advanced Synthesis and Catalysis*, **2016**, 358, 172-177	5.6	40
150	Discovery of Mycobacterium tuberculosis InhA Inhibitors by Binding Sites Comparison and Ligands Prediction. *Journal of Medicinal Chemistry*, **2016**, 59, 11069-11078	8.3	21
149	Chemoselective Schwartz Reagent Mediated Reduction of Isocyanates to Formamides. *Organic Letters*, **2016**, 18, 2750-3	6.2	52
148	Highly efficient synthesis of functionalized -oxyketones via Weinreb amides homologation with -oxygenated organolithiums. *Chemical Communications*, **2016**, 52, 7584-7	5.8	35
147	Design, Virtual Screening, and Synthesis of Antagonists of b3 as Antiplatelet Agents. *Journal of Medicinal Chemistry*, **2015**, 58, 7681-94	8.3	18
146	Accessing biological actions of Ganoderma secondary metabolites by in silico profiling. *Phytochemistry*, **2015**, 114, 114-24	4	23
145	Identification of the putative binding pocket of valerenic acid on GABAA receptors using docking studies and site-directed mutagenesis. *British Journal of Pharmacology*, **2015**, 172, 5403-13	8.6	21
144	A Robust, Eco-Friendly Access to Secondary Thioamides through the Addition of Organolithium Reagents to Isothiocyanates in Cyclopentyl Methyl Ether (CPME). *Chemistry - A European Journal*, **2015**, 21, 18966-70	4.8	34
143	Rational drug design paradigms: the odyssey for designing better drugs. *Combinatorial Chemistry and High Throughput Screening*, **2015**, 18, 238-56	1.3	8
142	Thienoquinolines as novel disruptors of the PKC/RACK2 protein-protein interaction. *Journal of Medicinal Chemistry*, **2014**, 57, 3235-46	8.3	20
141	Data Mining Using Ligand Profiling and Target Fishing. *Methods and Principles in Medicinal Chemistry*, **2013**, 257-270	0.4	2
140	Computational methods for drug target profiling and polypharmacology **2013**, 178-188		1
139	Recognizing pitfalls in virtual screening: a critical review. *Journal of Chemical Information and Modeling*, **2012**, 52, 867-81	6.1	295
138	Selective Optimization of Side Activities (SOSA): A Promising way for Drug Discovery **2012**, 227-243		9
137	Pharmacophore Models for Virtual Screening. *Methods and Principles in Medicinal Chemistry*, **2011**, 115-152	4	5
136	Identification of chemically diverse, novel inhibitors of 17-hydroxysteroid dehydrogenase type 3 and 5 by pharmacophore-based virtual screening. *Journal of Steroid Biochemistry and Molecular Biology*, **2011**, 125, 148-61	5.1	30
135	Barbituric acid derivative BAS 02104951 inhibits PKC-PKC-PKC/RACK2 interaction, Elk-1 phosphorylation in HeLa and PKC-and -translocation in PC3 cells following TPA-induction. *Journal of Biochemistry*, **2011**, 149, 331-6	3.1	7

134	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
133	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
132	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
131	Pharmacophores in Drug Research. *Molecular Informatics*, **2010**, 29, 470-5	3.8	43
130	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
129	Morphinans and isoquinolines: acetylcholinesterase inhibition, pharmacophore modeling, and interaction with opioid receptors. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 5071-80	3.4	40
128	In silico target fishing for rationalized ligand discovery exemplified on constituents of Ruta graveolens. *Planta Medica*, **2009**, 75, 195-204	3.1	111
127	Structure-based optimization of benzoic acids as inhibitors of protein tyrosine phosphatase 1B and low molecular weight protein tyrosine phosphatase. *ChemMedChem*, **2009**, 4, 957-62	3.7	27
126	5-Arylidene-2-phenylimino-4-thiazolidinones as PTP1B and LMW-PTP inhibitors. *Bioorganic and Medicinal Chemistry*, **2009**, 17, 1928-37	3.4	66
125	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
124	Hydrogen-bonding patterns of minor groove-binder-DNA complexes reveal criteria for discovery of new scaffolds. *Journal of Chemical Information and Modeling*, **2009**, 49, 1063-9	6.1	11
123	Hit finding: towards Smarter approaches. *Current Opinion in Pharmacology*, **2009**, 9, 589-93	5.1	21
122	Discovery of novel CB2 receptor ligands by a pharmacophore-based virtual screening workflow. *Journal of Medicinal Chemistry*, **2009**, 52, 369-78	8.3	30
121	Molecule-pharmacophore superpositioning and pattern matching in computational drug design. *Drug Discovery Today*, **2008**, 13, 23-9	8.8	249
120	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
119	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
118	3D Quantitative Structure Property Relationships **2008**, 587-604		9
117	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

116	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
115	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
114	Discovery of novel cathepsin S inhibitors by pharmacophore-based virtual high-throughput screening. *Journal of Chemical Information and Modeling*, **2008**, 48, 1693-705	6.1	23
113	In Silico Screening **2008**, 210-227		1
112	Why Drugs Fail A Study on Side Effects in New Chemical Entities. *Methods and Principles in Medicinal Chemistry*, **2008**, 1-22	0.4	2
111	Ligand Features Essential for Cytochrome P450 Induction. *Methods and Principles in Medicinal Chemistry*, **2008**, 317-339	0.4	
110	Enhancing drug discovery through in silico screening: strategies to increase true positives retrieval rates. *Current Medicinal Chemistry*, **2008**, 15, 2040-53	4.3	72
109	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
108	Sequence-specific positions of water molecules at the interface between DNA and minor groove binders. *ChemPhysChem*, **2008**, 9, 2766-71	3.2	13
107	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
106	Chapter 3:Pharmacophore-based Virtual Screening in Drug Discovery **2008**, 76-119		9
105	Parallel screening and activity profiling with HIV protease inhibitor pharmacophore models. *Journal of Chemical Information and Modeling*, **2007**, 47, 563-71	6.1	44
104	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
103	DNA minor groove pharmacophores describing sequence specific properties. *Journal of Chemical Information and Modeling*, **2007**, 47, 1580-9	6.1	21
102	Design, synthesis, and SAR analysis of novel selective sigma1 ligands. *Bioorganic and Medicinal Chemistry*, **2007**, 15, 771-83	3.4	26
101	5-Arylidene-2,4-thiazolidinediones as inhibitors of protein tyrosine phosphatases. *Bioorganic and Medicinal Chemistry*, **2007**, 15, 5137-49	3.4	93
100	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
99	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

98	Pharmacophore modeling and parallel screening for PPAR ligands. *Journal of Computer-Aided Molecular Design*, **2007**, 21, 575-90	4.2	58
97	Pharmacophore-Based Screening for the Successful Identification of Bio-Active Natural Products. *Chimia*, **2007**, 61, 350-354	1.3	6
96	High-throughput structure-based pharmacophore modelling as a basis for successful parallel virtual screening. *Journal of Computer-Aided Molecular Design*, **2006**, 20, 703-15	4.2	47
95	Efficient overlay of small organic molecules using 3D pharmacophores. *Journal of Computer-Aided Molecular Design*, **2006**, 20, 773-88	4.2	211
94	Integrated in silico tools for exploiting the natural productsR bioactivity. *Planta Medica*, **2006**, 72, 671-8	3.1	25
93	Predicting drug metabolism induction in silico. *Current Topics in Medicinal Chemistry*, **2006**, 6, 1627-40	3	20
92	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
91	Strategies for efficient lead structure discovery from natural products. *Current Medicinal Chemistry*, **2006**, 13, 1491-507	4.3	77
90	Development and validation of an in silico P450 profiler based on pharmacophore models. *Current Drug Discovery Technologies*, **2006**, 3, 1-48	1.5	39
89	Are You Sure You Have a Good Model?. *Methods and Principles in Medicinal Chemistry*, **2006**, 325-364	0.4	13
88	GBPM: GRID-based pharmacophore model: concept and application studies to protein-protein recognition. *Bioinformatics*, **2006**, 22, 1449-55	7.2	93
87	Application of Structure-Based Alignment Methods for 3D QSAR Analyses. *Methods and Principles in Medicinal Chemistry*, **2006**, 223-249	0.4	1
86	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
85	Pharmacophore modelling: applications in drug discovery. *Expert Opinion on Drug Discovery*, **2006**, 1, 261-7	6.2	40
84	Parallel screening: a novel concept in pharmacophore modeling and virtual screening. *Journal of Chemical Information and Modeling*, **2006**, 46, 2146-57	6.1	107
83	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
82	Taspine: bioactivity-guided isolation and molecular ligand-target insight of a potent acetylcholinesterase inhibitor from Magnolia x soulangiana. *Journal of Natural Products*, **2006**, 69, 1341-6	4.9	46
81	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

80	Influence of the conditions in pharmacophore generation, scoring, and 3D database search for chemical feature-based pharmacophore models: one application study of ETA- and ETB-selective antagonists. *Journal of Chemical Information and Modeling*, **2006**, 46, 1439-55	6.1	3
79	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
78	Application of Pharmacophore Models in Medicinal Chemistry. *Methods and Principles in Medicinal Chemistry*, **2006**, 251-282	0.4	1
77	Pharmacophores from Macromolecular Complexes with LigandScout. *Methods and Principles in Medicinal Chemistry*, **2006**, 131-150	0.4	20
76	GRID-based Pharmacophore Models: Concept and Application Examples. *Methods and Principles in Medicinal Chemistry*, **2006**, 151-170	0.4	3
75	Alignment-Free Pharmacophore Patterns A Correlation-Vector Approach. *Methods and Principles in Medicinal Chemistry*, **2006**, 49-79	0.4	12
74	Pharmacophore Model Generation Software Tools. *Methods and Principles in Medicinal Chemistry*, **2006**, 15-47	0.4	12
73	Pharmacophores for Human ADME/Tox-Related Proteins. *Methods and Principles in Medicinal Chemistry*, **2006**, 299-324	0.4	4
72	Application of Pharmacophore Fingerprints to Structure-Based Design and Data Mining. *Methods and Principles in Medicinal Chemistry*, **2006**, 193-206	0.4	6
71	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
70	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
69	Comparative analysis of protein-bound ligand conformations with respect to catalyst conformational space subsampling algorithms. *Journal of Chemical Information and Modeling*, **2005**, 45, 422-30	6.1	125
68	Comparative enzymology of 11beta-hydroxysteroid dehydrogenase type 1 from six species. *Journal of Molecular Endocrinology*, **2005**, 35, 89-101	4.5	63
67	Human rhinovirus 3C protease: generation of pharmacophore models for peptidic and nonpeptidic inhibitors and their application in virtual screening. *Journal of Chemical Information and Modeling*, **2005**, 45, 716-24	6.1	27
66	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
65	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
64	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
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