Thierry Langer

List of Publications by Year
in descending order

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225 papers	11,177 citations	26567 56 h-index	37111 96 g-index
261 all docs	261 docs citations	261 times ranked	10448 citing authors

#	Article	IF	Citations
1	Tricyclic antipsychotics and antidepressants can inhibit Î±5â€containing GABA_A receptors by two distinct mechanisms. British Journal of Pharmacology, 2022, 179, 3675-3692.	2.7	7
2	Design, Synthesis, and Biological Evaluation of 4,4â€™-Difluorobenzhydrol Carbamates as Selective M1 Antagonists. Pharmaceuticals, 2022, 15, 248.	1.7	4
3	Molecular Mingling: Multimodal Predictions of Ligand Promiscuity in Pentameric Ligand-Gated Ion Channels. Frontiers in Molecular Biosciences, 2022, 9, .	1.6	10
4	Synthesis, Biological Evaluation, and Docking Studies of Antagonistic Hydroxylated Arecaidine Esters Targeting mAChRs. Molecules, 2022, 27, 3173.	1.7	4
5	Improving Small Molecule pKa Prediction Using Transfer Learning With Graph Neural Networks. Frontiers in Chemistry, 2022, 10, .	1.8	10
6	A Novel and Selective Dopamine Transporter Inhibitor, (S)-MK-26, Promotes Hippocampal Synaptic Plasticity and Restores Effort-Related Motivational Dysfunctions. Biomolecules, 2022, 12, 881.	1.8	14
7	Identification of repurposing therapeutics toward SARS-CoV-2 main protease by virtual screening. PLoS ONE, 2022, 17, e0269563.	1.1	9
8	In Silico Identification of Potential Druggable Binding Sites on CIN85 SH3 Domain. International Journal of Molecular Sciences, 2021, 22, 534.	1.8	4
9	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.	1.4	9
10	Update on PET Tracer Development for Muscarinic Acetylcholine Receptors. Pharmaceuticals, 2021, 14, 530.	1.7	11
11	Reinstatement of synaptic plasticity in the aging brain through specific dopamine transporter inhibition. Molecular Psychiatry, 2021, 26, 7076-7090.	4.1	19
12	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, 7714.	1.8	11
13	Antivirals against the Chikungunya Virus. Viruses, 2021, 13, 1307.	1.5	32
14	QPHAR: quantitative pharmacophore activity relationship: method and validation. Journal of Cheminformatics, 2021, 13, 57.	2.8	8
15	In vitro and in silico studies of holothurin A on androgen receptor in prostate cancer. Journal of Biomolecular Structure and Dynamics, 2021, , 1-9.	2.0	5
16	Consecutive and Selective Double Methylene Insertion of Lithium Carbenoids to Isothiocyanates: A Direct Assembly of Fourâ€Membered Sulfurâ€Containing Cycles. Angewandte Chemie - International Edition, 2021, 60, 24854-24858.	7.2	20
17	Improved Lipophilicity and Aqueous Solubility Prediction with Composite Graph Neural Networks. Molecules, 2021, 26, 6185.	1.7	14
18	Greedy 3-Point Search (G3PS)â€”A Novel Algorithm for Pharmacophore Alignment. Molecules, 2021, 26, 7201.	1.7	1

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19	Cognitive profiling and proteomic analysis of the modafinil analogue S-CE-123 in experienced aged rats. Scientific Reports, 2021, 11, 23962.	1.6	5
20	A Combination of Pharmacophore and Dockingâ€based Virtual Screening to Discover new Tyrosinase Inhibitors. Molecular Informatics, 2020, 39, e1900054.	1.4	14
21	Multiple Virtual Screening Strategies for the Discovery of Novel Compounds Active Against Dengue Virus: A Hit Identification Study. Scientia Pharmaceutica, 2020, 88, 2.	0.7	24
22	Structureâ€“Activity Relationships of Novel Thiazole-Based Modafinil Analogues Acting at Monoamine Transporters. Journal of Medicinal Chemistry, 2020, 63, 391-417.	2.9	23
23	A Computational Approach to Identify Potential Novel Inhibitors against the Coronavirus SARSâ€CoVâ€2. Molecular Informatics, 2020, 39, e2000090.	1.4	28
24	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, 4485.	1.7	9
25	Methylation of Methyl 4-Hydroxy-2-thioxo-1,2-dihydroquinoline-3-carboxylate: Synthetic, Crystallographic, and Molecular Docking Studies. Molecules, 2020, 25, 4238.	1.7	2
26	Chemoselective Homologationâ€“Deoxygenation Strategy Enabling the Direct Conversion of Carbonyls into (n+1)-Halomethyl-Alkanes. Organic Letters, 2020, 22, 7629-7634.	2.4	23
27	A compact review of molecular property prediction with graph neural networks. Drug Discovery Today: Technologies, 2020, 37, 1-12.	4.0	182
28	Novel Class of Chikungunya Virus Small Molecule Inhibitors That Targets the Viral Capping Machinery. Antimicrobial Agents and Chemotherapy, 2020, 64, .	1.4	15
29	Identification of 2-(4-(Phenylsulfonyl)piperazine-1-yl)pyrimidine Analogues as Novel Inhibitors of Chikungunya Virus. ACS Medicinal Chemistry Letters, 2020, 11, 906-912.	1.3	16
30	Applications of the Pharmacophore Concept in Natural Product inspired Drug Design. Molecular Informatics, 2020, 39, e2000059.	1.4	42
31	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.	1.7	9
32	A-ring and E-ring modifications of the cytotoxic alkaloid Luotonin A: Synthesis, computational and biological studies. Bioorganic and Medicinal Chemistry, 2020, 28, 115443.	1.4	3
33	Crystal structure, Hirshfeld analysis and a molecular 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-oxadiazol-3-yl]methyl}-2H-1,2,6-thiadiazine-4-carboxylate. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 12-17.	0.2	2
34	Fluoxetine Inhibits Enterovirus Replication by Targeting the Viral 2C Protein in a Stereospecific Manner. ACS Infectious Diseases, 2019, 5, 1609-1623.	1.8	50
35	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.	1.0	5
36	The Novel Atypical Dopamine Uptake Inhibitor (S)-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.	1.6	35

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37	Computational Identification of Novel Kir6 Channel Inhibitors. Frontiers in Pharmacology, 2019, 10, 549.	1.6	5
38	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.	1.4	11
39	Cytotoxicity Of Chalcone Of Eugenia aquea 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, Volume 12, 33-43.	1.6	7
40	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.	1.0	2
41	LigandScout Remote: A New User-Friendly Interface for HPC and Cloud Resources. Journal of Chemical Information and Modeling, 2019, 59, 31-37.	2.5	6
42	A Straightforward Homologation of Carbon Dioxide with Magnesium Carbenoids en Route to Î±â€Halocarboxylic Acids. Advanced Synthesis and Catalysis, 2019, 361, 1001-1006.	2.1	9
43	Modular and Chemoselective Strategy for the Direct Access to Î±-Fluoroepoxides and Aziridines via the Addition of Fluoroiodomethyllithium to Carbonyl-Like Compounds. Organic Letters, 2019, 21, 584-588.	2.4	65
44	Discovery of Potent Inhibitors for the Large Neutral Amino Acid Transporter 1 (LAT1) by Structure-Based Methods. International Journal of Molecular Sciences, 2019, 20, 27.	1.8	38
45	Sustainable Asymmetric Organolithium Chemistry: Enantioâ€•and Chemoselective Acylations through Recycling of Solvent, Sparteine, and Weinreb â€œAmineâ€• ChemSusChem, 2019, 12, 1147-1154.	3.6	23
46	Telescoped, Divergent, Chemoselective C1 and C1â€C1 Homologation of Imine Surrogates: Access to Quaternary Chloroâ€•and Halomethylâ€Trifluoromethyl Aziridines. Angewandte Chemie - International Edition, 2019, 58, 2479-2484.	7.2	64
47	Design, Synthesis, and Pharmacological Evaluation of Novel Î²2/3 Subunit-Selective Î³-Aminobutyric Acid Type A (GABA_A) Receptor Modulators. Journal of Medicinal Chemistry, 2019, 62, 317-341.	2.9	9
48	The Pharmacophore Concept and Its Applications in Computer-Aided Drug Design. Progress in the Chemistry of Organic Natural Products, 2019, 110, 99-141.	0.8	38
49	A daily single dose of a novel modafinil analogue CE-123 improves memory acquisition and memory retrieval. Behavioural Brain Research, 2018, 343, 83-94.	1.2	25
50	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.	2.5	3
51	GRAIL: GRids of phArmacophore Interaction fieLds. Journal of Chemical Theory and Computation, 2018, 14, 4958-4970.	2.3	15
52	The Use of Dynamic Pharmacophore in Computer-Aided Hit Discovery: A Case Study. Methods in Molecular Biology, 2018, 1824, 317-333.	0.4	1
53	In Silico Workflow for the Discovery of Natural Products Activating the G Protein-Coupled Bile Acid Receptor 1. Frontiers in Chemistry, 2018, 6, 242.	1.8	16
54	Pharmacy Practice and Education in Austria. Pharmacy (Basel, Switzerland), 2018, 6, 55.	0.6	5

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55	SAR-Guided Scoring Function and Mutational Validation Reveal the Binding Mode of CGS-8216 at the Î±1+/Î³2â€“ Benzodiazepine Site. Journal of Chemical Information and Modeling, 2018, 58, 1682-1696.	2.5	5
56	The Mu.Ta.Lig. Chemotheca: A Community-Populated Molecular Database for Multi-Target Ligands Identification and Compound-Repurposing. Frontiers in Chemistry, 2018, 6, 130.	1.8	13
57	Conformational Sampling of Small Molecules With iCon: Performance Assessment in Comparison With OMEGA. Frontiers in Chemistry, 2018, 6, 229.	1.8	43
58	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.	2.5	27
59	Homologation of halostannanes with carbenoids: a convenient and straightforward one-step access to Î±-functionalized organotin reagents. Chemical Communications, 2018, 54, 10112-10115.	2.2	18
60	EFMCâ€ASMC Kongress in Wien. Nachrichten Aus Der Chemie, 2018, 66, 563-563.	0.0	0
61	Common Hits Approach: Combining Pharmacophore Modeling and Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2017, 57, 365-385.	2.5	59
62	A Molecular Dynamicsâ€“Shared Pharmacophore Approach to Boost Earlyâ€Enrichment Virtual Screening: A Case Study on Peroxisome Proliferatorâ€Activated Receptorâ€…Î±. ChemMedChem, 2017, 12, 1399-1407.	1.6	23
63	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.	1.2	11
64	Recent advancements on the use of 2-methyltetrahydrofuran in organometallic chemistry. Monatshefte FÃ¼r Chemie, 2017, 148, 37-48.	0.9	84
65	Efficient Access to Allâ€Carbon Quaternary and Tertiary Î±â€Functionalized Homoallylâ€type Aldehydes from Ketones. Angewandte Chemie, 2017, 129, 12851-12856.	1.6	23
66	Heterocyclic Analogues of Modafinil as Novel, Atypical Dopamine Transporter Inhibitors. Journal of Medicinal Chemistry, 2017, 60, 9330-9348.	2.9	26
67	Exploiting a â€œBeastâ€•in Carbenoid Chemistry: Development of a Straightforward Direct Nucleophilic Fluoromethylation Strategy. Journal of the American Chemical Society, 2017, 139, 13648-13651.	6.6	104
68	Efficient Access to Allâ€Carbon Quaternary and Tertiary Î±â€Functionalized Homoallylâ€type Aldehydes from Ketones. Angewandte Chemie - International Edition, 2017, 56, 12677-12682.	7.2	71
69	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.	2.2	52
70	Molecular Docking and 3D-Pharmacophore Modeling to Study the Interactions of Chalcone Derivatives with Estrogen Receptor Alpha. Pharmaceuticals, 2017, 10, 81.	1.7	52
71	A Novel Dopamine Transporter Inhibitor CE-123 Improves Cognitive Flexibility and Maintains Impulsivity in Healthy Male Rats. Frontiers in Behavioral Neuroscience, 2017, 11, 222.	1.0	24
72	R-Modafinil exerts weak effects on spatial memory acquisition and dentate gyrus synaptic plasticity. PLoS ONE, 2017, 12, e0179675.	1.1	15

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73	Pharmacophore Models Derived from Molecular Dynamics Simulations of Protein-Ligand Complexes: A Case Study. Natural Product Communications, 2016, 11, 1934578X1601101.	0.2	2
74	The use of the Comins-Meyers Amide in Synthetic Chemistry: An Overview. Natural Product Communications, 2016, 11, 1934578X1601101.	0.2	4
75	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, 127-137.	1.2	11
76	Chemoselective Addition of Halomethyllithiums to Functionalized Isatins:A Straightforward Access to Spiroâ€Epoxyoxindoles. Advanced Synthesis and Catalysis, 2016, 358, 172-177.	2.1	47
77	Discovery of Mycobacterium tuberculosis InhA Inhibitors by Binding Sites Comparison and Ligands Prediction. Journal of Medicinal Chemistry, 2016, 59, 11069-11078.	2.9	26
78	Chemoselective Schwartz Reagent Mediated Reduction of Isocyanates to Formamides. Organic Letters, 2016, 18, 2750-2753.	2.4	70
79	Highly efficient synthesis of functionalized Î±-oxyketones via Weinreb amides homologation with Î±-oxygenated organolithiums. Chemical Communications, 2016, 52, 7584-7587.	2.2	44
80	Fragment pharmacophore-based in silico screening: a powerful approach for efficient lead discovery. MedChemComm, 2016, 7, 506-511.	3.5	6
81	Evaluating the stability of pharmacophore features using molecular dynamics simulations. Biochemical and Biophysical Research Communications, 2016, 470, 685-689.	1.0	26
82	Comparing pharmacophore models derived from crystal structures and from molecular dynamics simulations. Monatshefte FÃ¼r Chemie, 2016, 147, 553-563.	0.9	15
83	A heterocyclic compound CE-103 inhibits dopamine reuptake and modulates dopamine transporter and dopamine D1-D3 containing receptor complexes. Neuropharmacology, 2016, 102, 186-196.	2.0	13
84	Identification of the putative binding pocket of valerenic acid on GABA A receptors using docking studies and siteâ€directed mutagenesis. British Journal of Pharmacology, 2015, 172, 5403-5413.	2.7	28
85	A Robust, Ecoâ€Friendly Access to Secondary Thioamides through the Addition of Organolithium Reagents to Isothiocyanates in Cyclopentyl Methyl Ether (CPME). Chemistry - A European Journal, 2015, 21, 18966-18970.	1.7	38
86	Design, Virtual Screening, and Synthesis of Antagonists of Î±_{IIb}Î²₃ as Antiplatelet Agents. Journal of Medicinal Chemistry, 2015, 58, 7681-7694.	2.9	22
87	Accessing biological actions of Ganoderma secondary metabolites by in silico profiling. Phytochemistry, 2015, 114, 114-124.	1.4	31
88	Rational Drug Design Paradigms: The Odyssey for Designing Better Drugs. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 238-256.	0.6	8
89	Thienoquinolines as Novel Disruptors of the PKCÎµ/RACK2 Proteinâ€“Protein Interaction. Journal of Medicinal Chemistry, 2014, 57, 3235-3246.	2.9	26
90	Recognizing Pitfalls in Virtual Screening: A Critical Review. Journal of Chemical Information and Modeling, 2012, 52, 867-881.	2.5	358

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91	Barbituric acid derivative BAS 02104951 inhibits PKCÂ, PKCÂ, PKCÂ/RACK2 interaction, Elk-1 phosphorylation in HeLa and PKCÂ and Â translocation in PC3 cells following TPA-induction. Journal of Biochemistry, 2011, 149, 331-336.	0.9	9
92	Identification of chemically diverse, novel inhibitors of 17Î²-hydroxysteroid dehydrogenase type 3 and 5 by pharmacophore-based virtual screening. Journal of Steroid Biochemistry and Molecular Biology, 2011, 125, 148-161.	1.2	33
93	Pharmacophores for medicinal chemists: a personal view. Future Medicinal Chemistry, 2011, 3, 901-904.	1.1	9
94	Applications of Integrated Data Mining Methods to Exploring Natural Product Space for Acetylcholinesterase Inhibitors. Combinatorial Chemistry and High Throughput Screening, 2010, 13, 54-66.	0.6	18
95	The UV-filter benzophenone-1 inhibits 17Î²-hydroxysteroid dehydrogenase type 3: Virtual screening as a strategy to identify potential endocrine disrupting chemicals. Biochemical Pharmacology, 2010, 79, 1189-1199.	2.0	78
96	Pharmacophores in Drug Research. Molecular Informatics, 2010, 29, 470-475.	1.4	51
97	Synthesis, semipreparative HPLC separation, biological evaluation, and 3D-QSAR of hydrazothiazole derivatives as human monoamine oxidase B inhibitors. Bioorganic and Medicinal Chemistry, 2010, 18, 5063-5070.	1.4	44
98	Morphinans and isoquinolines: Acetylcholinesterase inhibition, pharmacophore modeling, and interaction with opioid receptors. Bioorganic and Medicinal Chemistry, 2010, 18, 5071-5080.	1.4	46
99	Epidermis-Type Lipoxygenase 3 Regulates Adipocyte Differentiation and Peroxisome Proliferator-Activated Receptor Î³ Activity. Molecular and Cellular Biology, 2010, 30, 4077-4091.	1.1	45
100	In silicoTarget Fishing for Rationalized Ligand Discovery Exemplified on Constituents ofRuta graveolensL.. Planta Medica, 2009, 75, 293-293.	0.7	0
101	In silicoTarget Fishing for Rationalized Ligand Discovery Exemplified on Constituents ofRuta graveolens. Planta Medica, 2009, 75, 195-204.	0.7	131
102	Structureâ€Based Optimization of Benzoic Acids as Inhibitors of Protein Tyrosine Phosphatase 1B and Low Molecular Weight Protein Tyrosine Phosphatase. ChemMedChem, 2009, 4, 957-962.	1.6	32
103	5-Arylidene-2-phenylimino-4-thiazolidinones as PTP1B and LMW-PTP inhibitors. Bioorganic and Medicinal Chemistry, 2009, 17, 1928-1937.	1.4	79
104	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, 2658-2672.	1.4	44
105	Hydrogen-Bonding Patterns of Minor Groove-Binderâ"DNA Complexes Reveal Criteria for Discovery of New Scaffolds. Journal of Chemical Information and Modeling, 2009, 49, 1063-1069.	2.5	11
106	Hit finding: towards â€˜smarterâ€™ approaches. Current Opinion in Pharmacology, 2009, 9, 589-593.	1.7	24
107	Discovery of Novel CB₂ Receptor Ligands by a Pharmacophore-Based Virtual Screening Workflow. Journal of Medicinal Chemistry, 2009, 52, 369-378.	2.9	37
108	Evaluation of the performance of 3D virtual screening protocols: RMSD comparisons, enrichment assessments, and decoy selectionâ€"What can we learn from earlier mistakes?. Journal of Computer-Aided Molecular Design, 2008, 22, 213-228.	1.3	330

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109	Sequenceâ€Specific Positions of Water Molecules at the Interface between DNA and Minor Groove Binders. ChemPhysChem, 2008, 9, 2766-2771.	1.0	14
110	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, 5840-5852.	1.4	58
111	Molecule-pharmacophore superpositioning and pattern matching in computational drug design. Drug Discovery Today, 2008, 13, 23-29.	3.2	287
112	Virtual screening for the discovery of bioactive natural products. , 2008, 65, 211-249.		94
113	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, 6303-6317.	2.9	65
114	3D Quantitative Structureâ€“Property Relationships. , 2008, , 587-604.		10
115	Structure-Based Virtual Screening for the Discovery of Natural Inhibitors for Human Rhinovirus Coat Protein. Journal of Medicinal Chemistry, 2008, 51, 842-851.	2.9	83
116	Discovery of Nonsteroidal 17Î²-Hydroxysteroid Dehydrogenase 1 Inhibitors by Pharmacophore-Based Screening of Virtual Compound Libraries. Journal of Medicinal Chemistry, 2008, 51, 4188-4199.	2.9	55
117	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, 7021-7040.	2.9	91
118	Discovery of Novel Cathepsin S Inhibitors by Pharmacophore-Based Virtual High-Throughput Screening. Journal of Chemical Information and Modeling, 2008, 48, 1693-1705.	2.5	25
119	In Silico Screening. , 2008, , 210-227.		4
120	Enhancing Drug Discovery Through In Silico Screening: Strategies to Increase True Positives Retrieval Rates. Current Medicinal Chemistry, 2008, 15, 2040-2053.	1.2	76
121	Pharmacophore-based Virtual Screening in Drug Discovery. , 2008, , 76-119.		10
122	Pharmacophore-Based Screening for the Successful Identification of Bio-Active Natural Products. Chimia, 2007, 61, 350-354.	0.3	6
123	Parallel Screening and Activity Profiling with HIV Protease Inhibitor Pharmacophore Models. Journal of Chemical Information and Modeling, 2007, 47, 563-571.	2.5	52
124	Fast and Efficient in Silico 3D Screening:â€‰ Toward Maximum Computational Efficiency of Pharmacophore-Based and Shape-Based Approaches. Journal of Chemical Information and Modeling, 2007, 47, 2182-2196.	2.5	69
125	DNA Minor Groove Pharmacophores Describing Sequence Specific Properties. Journal of Chemical Information and Modeling, 2007, 47, 1580-1589.	2.5	27
126	Design, synthesis, and SAR analysis of novel selective Ïƒ1 ligands. Bioorganic and Medicinal Chemistry, 2007, 15, 771-783.	1.4	30

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127	5-Arylidene-2,4-thiazolidinediones as inhibitors of protein tyrosine phosphatases. Bioorganic and Medicinal Chemistry, 2007, 15, 5137-5149.	1.4	104
128	Evaluation of in vitro aldose redutase inhibitory activity of 5-arylidene-2,4-thiazolidinediones. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 3886-3893.	1.0	54
129	High-throughput structure-based pharmacophore modelling as a basis for successful parallel virtual screening. Journal of Computer-Aided Molecular Design, 2007, 20, 703-715.	1.3	52
130	Efficient overlay of small organic molecules using 3D pharmacophores. Journal of Computer-Aided Molecular Design, 2007, 20, 773-788.	1.3	265
131	Generation of a homology model of the human histamine H3 receptor for ligand docking and pharmacophore-based screening. Journal of Computer-Aided Molecular Design, 2007, 21, 437-453.	1.3	68
132	Pharmacophore modeling and parallel screening for PPAR ligands. Journal of Computer-Aided Molecular Design, 2007, 21, 575-590.	1.3	65
133	Structure-Based Pharmacophore Design and Virtual Screening for Novel Angiotensin Converting Enzyme 2 Inhibitors. Journal of Chemical Information and Modeling, 2006, 46, 708-716.	2.5	84
134	Pharmacophore modelling: applications in drug discovery. Expert Opinion on Drug Discovery, 2006, 1, 261-267.	2.5	54
135	Parallel Screening:â€‰ A Novel Concept in Pharmacophore Modeling and Virtual Screening. Journal of Chemical Information and Modeling, 2006, 46, 2146-2157.	2.5	123
136	Pharmacophore Modeling and in Silico Screening for New P450 19 (Aromatase) Inhibitorsâ€. Journal of Chemical Information and Modeling, 2006, 46, 1301-1311.	2.5	101
137	Taspine:â€‰ Bioactivity-Guided Isolation and Molecular Ligandâ^'Target Insight of a Potent Acetylcholinesterase Inhibitor from Magnolia x soulangiana. Journal of Natural Products, 2006, 69, 1341-1346.	1.5	57
138	Comparative Performance Assessment of the Conformational Model Generators Omega and Catalyst:Â A Large-Scale Survey on the Retrieval of Protein-Bound Ligand Conformations. Journal of Chemical Information and Modeling, 2006, 46, 1848-1861.	2.5	159
139	Influence of the Conditions in Pharmacophore Generation, Scoring, and 3D Database Search for Chemical Feature-Based Pharmacophore Models:Â One Application Study of ETA- and ETB-Selective Antagonists. Journal of Chemical Information and Modeling, 2006, 46, 1439-1455.	2.5	4
140	Why is 11Î²-hydroxysteroid dehydrogenase type 1 facing the endoplasmic reticulum lumen?. Molecular and Cellular Endocrinology, 2006, 248, 15-23.	1.6	68
141	Further Studies on Imidazo[4,5-b]pyridine AT1Angiotensin 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, 6451-6464.	2.9	78
142	The Discovery of New 11Î²-Hydroxysteroid Dehydrogenase Type 1 Inhibitors by Common Feature Pharmacophore Modeling and Virtual Screening. Journal of Medicinal Chemistry, 2006, 49, 3454-3466.	2.9	114
143	Integrated in Silico Tools for Exploiting the Natural Productsâ€™ Bioactivity. Planta Medica, 2006, 72, 671-678.	0.7	32
144	Predicting Drug Metabolism Induction In Silico. Current Topics in Medicinal Chemistry, 2006, 6, 1627-1640.	1.0	23

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145	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, 1411-1428.	1.2	58
146	Strategies for Efficient Lead Structure Discovery from Natural Products. Current Medicinal Chemistry, 2006, 13, 1491-1507.	1.2	89
147	Development and Validation of an In Silico P450 Profiler Based on Pharmacophore Models. Current Drug Discovery Technologies, 2006, 3, 1-48.	0.6	43
148	GBPM: GRID-based pharmacophore model: concept and application studies to protein-protein recognition. Bioinformatics, 2006, 22, 1449-1455.	1.8	102
149	Why Drugs Fail - A Study on Side Effects in New Chemical Entities. Current Pharmaceutical Design, 2005, 11, 3545-3559.	0.9	383
150	Structureâ€“activity relationships and molecular modelling of 5-arylidene-2,4-thiazolidinediones active as aldose reductase inhibitors. Bioorganic and Medicinal Chemistry, 2005, 13, 2809-2823.	1.4	107
151	LigandScout:Â 3-D Pharmacophores Derived from Protein-Bound Ligands and Their Use as Virtual Screening Filters. Journal of Chemical Information and Modeling, 2005, 45, 160-169.	2.5	1,576
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