Thierry Langer

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4905297/publications.pdf

Version: 2024-02-01

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	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
2	Why Drugs Fail - A Study on Side Effects in New Chemical Entities. Current Pharmaceutical Design, 2005, 11, 3545-3559.	0.9	383
3	Recognizing Pitfalls in Virtual Screening: A Critical Review. Journal of Chemical Information and Modeling, 2012, 52, 867-881.	2.5	358
4	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
5	Molecule-pharmacophore superpositioning and pattern matching in computational drug design. Drug Discovery Today, 2008, 13, 23-29.	3.2	287
6	Efficient overlay of small organic molecules using 3D pharmacophores. Journal of Computer-Aided Molecular Design, 2007, 20, 773-788.	1.3	265
7	Acetylcholinesterase Inhibitory Activity of Scopolin and Scopoletin Discovered by Virtual Screening of Natural Products. Journal of Medicinal Chemistry, 2004, 47, 6248-6254.	2.9	193
8	A compact review of molecular property prediction with graph neural networks. Drug Discovery Today: Technologies, 2020, 37, 1-12.	4.0	182
9	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
10	Comparative Analysis of Protein-Bound Ligand Conformations with Respect to Catalyst's Conformational Space Subsampling Algorithms. Journal of Chemical Information and Modeling, 2005, 45, 422-430.	2.5	148
11	Recent Advances in Docking and Scoring. Current Computer-Aided Drug Design, 2005, 1, 93-102.	0.8	146
12	In silicoTarget Fishing for Rationalized Ligand Discovery Exemplified on Constituents ofRuta graveolens. Planta Medica, 2009, 75, 195-204.	0.7	131
13	Virtual Screening An Effective Tool for Lead Structure Discovery. Current Pharmaceutical Design, 2001, 7, 509-527.	0.9	127
14	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
15	Discovery of High-Affinity Ligands of Ïƒ1Receptor, ERG2, and Emopamil Binding Protein by Pharmacophore Modeling and Virtual Screening. Journal of Medicinal Chemistry, 2005, 48, 4754-4764.	2.9	117
16	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
17	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
18	5-Arylidene-2,4-thiazolidinediones as inhibitors of protein tyrosine phosphatases. Bioorganic and Medicinal Chemistry, 2007, 15, 5137-5149.	1.4	104

#	Article	IF	Citations
19	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
20	GBPM: GRID-based pharmacophore model: concept and application studies to protein-protein recognition. Bioinformatics, 2006, 22, 1449-1455.	1.8	102
21	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
22	Virtual screening for the discovery of bioactive natural products. , 2008, 65, 211-249.		94
23	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, 4275-4284.	2.9	92
24	Non-Peptide Angiotensin II Receptor Antagonists:Â Chemical Feature Based Pharmacophore Identification. Journal of Medicinal Chemistry, 2003, 46, 716-726.	2.9	92
25	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
26	Strategies for Efficient Lead Structure Discovery from Natural Products. Current Medicinal Chemistry, 2006, 13, 1491-1507.	1.2	89
27	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, 2692-2704.	2.9	86
28	The Identification of Ligand Features Essential for PXR Activation by Pharmacophore Modeling. Journal of Chemical Information and Modeling, 2005, 45, 431-439.	2.5	85
29	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
30	Recent advancements on the use of 2-methyltetrahydrofuran in organometallic chemistry. Monatshefte FÃ¼r Chemie, 2017, 148, 37-48.	0.9	84
31	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
32	5-Arylidene-2-phenylimino-4-thiazolidinones as PTP1B and LMW-PTP inhibitors. Bioorganic and Medicinal Chemistry, 2009, 17, 1928-1937.	1.4	79
33	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
34	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
35	Enhancing Drug Discovery Through In Silico Screening: Strategies to Increase True Positives Retrieval Rates. Current Medicinal Chemistry, 2008, 15, 2040-2053.	1.2	76
36	Pharmacophore definition and 3D searches. Drug Discovery Today: Technologies, 2004, 1, 203-207.	4.0	75

#	Article	IF	Citations
37	Novel Potent and Selective Central 5-HT3Receptor Ligands Provided with Different Intrinsic Efficacy. 1. Mapping the Central 5-HT3Receptor Binding Site by Arylpiperazine Derivatives. Journal of Medicinal Chemistry, 1998, 41, 728-741.	2.9	73
38	Comparative enzymology of 11Î²-hydroxysteroid dehydrogenase type 1 from six species. Journal of Molecular Endocrinology, 2005, 35, 89-101.	1.1	71
39	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
40	Chemoselective Schwartz Reagent Mediated Reduction of Isocyanates to Formamides. Organic Letters, 2016, 18, 2750-2753.	2.4	70
41	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
42	Mapping and Fitting the Peripheral Benzodiazepine Receptor Binding Site by Carboxamide Derivatives. Comparison of Different Approaches to Quantitative Ligandâ^'Receptor Interaction Modeling. Journal of Medicinal Chemistry, 2001, 44, 1134-1150.	2.9	68
43	Why is 11Î²-hydroxysteroid dehydrogenase type 1 facing the endoplasmic reticulum lumen?. Molecular and Cellular Endocrinology, 2006, 248, 15-23.	1.6	68
44	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
45	Combining Ethnopharmacology and Virtual Screening for Lead Structure Discovery:â€‰ COX-Inhibitors as Application Example. Journal of Chemical Information and Computer Sciences, 2004, 44, 480-488.	2.8	67
46	Pharmacophore Identification, in Silico Screening, and Virtual Library Design for Inhibitors of the Human Factor Xa. Journal of Chemical Information and Modeling, 2005, 45, 146-159.	2.5	67
47	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, 6516-6521.	2.9	66
48	Pharmacophore modeling and parallel screening for PPAR ligands. Journal of Computer-Aided Molecular Design, 2007, 21, 575-590.	1.3	65
49	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
50	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
51	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
52	Lead Identification for Modulators of Multidrug Resistance based onin silico Screening with a Pharmacophoric Feature Model. Archiv Der Pharmazie, 2004, 337, 317-327.	2.1	61
53	Impact of Scoring Functions on Enrichment in Docking-Based Virtual Screening:â€‰ An Application Study on Renin Inhibitorsâ€. Journal of Chemical Information and Computer Sciences, 2004, 44, 1123-1129.	2.8	60
54	Influenza Virus Neuraminidase Inhibitors:â€‰ 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, 1849-1856.	2.8	59

#	Article	IF	Citations
55	Common Hits Approach: Combining Pharmacophore Modeling and Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2017, 57, 365-385.	2.5	59
56	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
57	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
58	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
59	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
60	Pharmacophore modelling: applications in drug discovery. Expert Opinion on Drug Discovery, 2006, 1, 261-267.	2.5	54
61	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
62	Discovering COX-Inhibiting Constituents ofMorusRoot Bark: Activity-Guided versus Computer-Aided Methods. Planta Medica, 2005, 71, 399-405.	0.7	52
63	Parallel Screening and Activity Profiling with HIV Protease Inhibitor Pharmacophore Models. Journal of Chemical Information and Modeling, 2007, 47, 563-571.	2.5	52
64	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
65	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
66	Molecular Docking and 3D-Pharmacophore Modeling to Study the Interactions of Chalcone Derivatives with Estrogen Receptor Alpha. Pharmaceuticals, 2017, 10, 81.	1.7	52
67	Pharmacophores in Drug Research. Molecular Informatics, 2010, 29, 470-475.	1.4	51
68	Fluoxetine Inhibits Enterovirus Replication by Targeting the Viral 2C Protein in a Stereospecific Manner. ACS Infectious Diseases, 2019, 5, 1609-1623.	1.8	50
69	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-HT1AReceptors. Journal of Medicinal Chemistry, 2002, 45, 4128-4139.	2.9	47
70	Chemoselective Addition of Halomethyllithiums to Functionalized Isatins:A Straightforward Access to Spiroâ€Epoxyoxindoles. Advanced Synthesis and Catalysis, 2016, 358, 172-177.	2.1	47
71	Morphinans and isoquinolines: Acetylcholinesterase inhibition, pharmacophore modeling, and interaction with opioid receptors. Bioorganic and Medicinal Chemistry, 2010, 18, 5071-5080.	1.4	46
72	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

#	Article	IF	Citations
73	Azinyl and Diazinyl Hydrazones Derived from ArylN-Heteroaryl Ketones:Â Synthesis and Antiproliferative Activityâ€,â€¡. Journal of Medicinal Chemistry, 1997, 40, 4420-4425.	2.9	44
74	Pharmacophore Modeling, Docking, and Principal Component Analysis Based Clustering:Â Combined Computer-Assisted Approaches To Identify New Inhibitors of the Human Rhinovirus Coat ProteinÂ§. Journal of Medicinal Chemistry, 2005, 48, 6250-6260.	2.9	44
75	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
76	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
77	Highly efficient synthesis of functionalized Î±-oxyketones via Weinreb amides homologation with Î±-oxygenated organolithiums. Chemical Communications, 2016, 52, 7584-7587.	2.2	44
78	Thiazolyl and benzothiazolyl hydrazones derived from Î±-(N)-acetylpyridines and diazines: synthesis, antiproliferative activity and CoMFA studies. European Journal of Medicinal Chemistry, 1997, 32, 397-408.	2.6	43
79	Development and Validation of an In Silico P450 Profiler Based on Pharmacophore Models. Current Drug Discovery Technologies, 2006, 3, 1-48.	0.6	43
80	Conformational Sampling of Small Molecules With iCon: Performance Assessment in Comparison With OMEGA. Frontiers in Chemistry, 2018, 6, 229.	1.8	43
81	Applications of the Pharmacophore Concept in Natural Product inspired Drug Design. Molecular Informatics, 2020, 39, e2000059.	1.4	42
82	Chemical Function Based Pharmacophore Generation of Endothelin-A Selective Receptor Antagonists. Journal of Medicinal Chemistry, 2004, 47, 2750-2760.	2.9	38
83	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
84	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
85	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
86	Discovery of Novel CB₂ Receptor Ligands by a Pharmacophore-Based Virtual Screening Workflow. Journal of Medicinal Chemistry, 2009, 52, 369-378.	2.9	37
87	External Action of Di- and Polyamines on Maxi Calcium-Activated Potassium Channels: An Electrophysiological and Molecular Modeling Study. Biophysical Journal, 1998, 74, 722-730.	0.2	36
88	Virtual combinatorial chemistry and in silico screening: Efficient tools for lead structure discovery?. Pure and Applied Chemistry, 2004, 76, 991-996.	0.9	36
89	A Competitive Enzyme Immunoassay for the Pyrrolizidine Alkaloids of the Senecionine Type*. Planta Medica, 1996, 62, 267-271.	0.7	35
90	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

#	Article	IF	Citations
91	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
92	Integrated in Silico Tools for Exploiting the Natural Productsâ€™ Bioactivity. Planta Medica, 2006, 72, 671-678.	0.7	32
93	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
94	Antivirals against the Chikungunya Virus. Viruses, 2021, 13, 1307.	1.5	32
95	Accessing biological actions of Ganoderma secondary metabolites by in silico profiling. Phytochemistry, 2015, 114, 114-124.	1.4	31
96	In vitro opioid activity profiles of 6-amino acid substituted derivatives of 14-O-methyloxymorphone. European Journal of Pharmacology, 2004, 483, 301-308.	1.7	30
97	Design, synthesis, and SAR analysis of novel selective Ïƒ1 ligands. Bioorganic and Medicinal Chemistry, 2007, 15, 771-783.	1.4	30
98	Human Rhinovirus 3C Protease:Â Generation of Pharmacophore Models for Peptidic and Nonpeptidic Inhibitors and Their Application in Virtual Screening. Journal of Chemical Information and Modeling, 2005, 45, 716-724.	2.5	29
99	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
100	A Computational Approach to Identify Potential Novel Inhibitors against the Coronavirus SARSâ€CoVâ€². Molecular Informatics, 2020, 39, e2000090.	1.4	28
101	Conserved Ca2+-antagonist-binding properties and putative folding structure of a recombinant high-affinity dihydropyridine-binding domain. Biochemical Journal, 2000, 347, 829.	1.7	27
102	DNA Minor Groove Pharmacophores Describing Sequence Specific Properties. Journal of Chemical Information and Modeling, 2007, 47, 1580-1589.	2.5	27
103	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
104	Chemical feature-based pharmacophores and virtual library screening for discovery of new leads. Current Opinion in Drug Discovery & Development, 2003, 6, 370-6.	1.9	27
105	Thienoquinolines as Novel Disruptors of the PKCÎµ/RACK2 Proteinâ€“Protein Interaction. Journal of Medicinal Chemistry, 2014, 57, 3235-3246.	2.9	26
106	Discovery of Mycobacterium tuberculosis InhA Inhibitors by Binding Sites Comparison and Ligands Prediction. Journal of Medicinal Chemistry, 2016, 59, 11069-11078.	2.9	26
107	Evaluating the stability of pharmacophore features using molecular dynamics simulations. Biochemical and Biophysical Research Communications, 2016, 470, 685-689.	1.0	26
108	Heterocyclic Analogues of Modafinil as Novel, Atypical Dopamine Transporter Inhibitors. Journal of Medicinal Chemistry, 2017, 60, 9330-9348.	2.9	26

#	Article	IF	Citations
109	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.	0.5	25
110	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
111	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
112	Application of the In Combo Screening Approach For the Discovery of Non-Alkaloid Acetylcholinesterase Inhibitors from Cichorium intybus. Current Drug Discovery Technologies, 2005, 2, 185-193.	0.6	24
113	Hit finding: towards â€˜smarterâ€™ approaches. Current Opinion in Pharmacology, 2009, 9, 589-593.	1.7	24
114	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
115	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
116	Variability in chemical constituents in Petasites hybridus from Austria. Biochemical Systematics and Ecology, 2000, 28, 421-432.	0.6	23
117	Predicting Drug Metabolism Induction In Silico. Current Topics in Medicinal Chemistry, 2006, 6, 1627-1640.	1.0	23
118	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
119	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
120	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
121	Structureâ€“Activity Relationships of Novel Thiazole-Based Modafinil Analogues Acting at Monoamine Transporters. Journal of Medicinal Chemistry, 2020, 63, 391-417.	2.9	23
122	Chemoselective Homologationâ€“Deoxygenation Strategy Enabling the Direct Conversion of Carbonyls into (n+1)-Halomethyl-Alkanes. Organic Letters, 2020, 22, 7629-7634.	2.4	23
123	On the Use of Chemical Function-Based Alignments as Input for 3D-QSAR. Journal of Chemical Information and Computer Sciences, 1998, 38, 325-330.	2.8	22
124	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
125	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, 950-957.	2.9	20
126	Molecular structure and dynamics of some potent 5-HT 3 receptor antagonists. Insight into the interaction with the receptor. Bioorganic and Medicinal Chemistry, 1996, 4, 1255-1269.	1.4	20

#	Article	IF	Citations
127	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
128	DockingVersus 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.	1.5	19
129	Reinstatement of synaptic plasticity in the aging brain through specific dopamine transporter inhibition. Molecular Psychiatry, 2021, 26, 7076-7090.	4.1	19
130	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
131	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
132	Building a model of interaction at the NK-2 receptors: Polycondensed heterocycles containing the pyrimidoindole skeleton. European Journal of Medicinal Chemistry, 1998, 32, 973-985.	2.6	16
133	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
134	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
135	On the Bioisosteric Potential of Diazines:Â Diazine Analogues of the Combined Thromboxane A2Receptor Antagonist and Synthetase Inhibitor Ridogrelâ€. Journal of Medicinal Chemistry, 1996, 39, 4058-4064.	2.9	15
136	Comparing pharmacophore models derived from crystal structures and from molecular dynamics simulations. Monatshefte FÃ¼r Chemie, 2016, 147, 553-563.	0.9	15
137	R-Modafinil exerts weak effects on spatial memory acquisition and dentate gyrus synaptic plasticity. PLoS ONE, 2017, 12, e0179675.	1.1	15
138	GRAIL: GRids of phArmacophore Interaction fieLds. Journal of Chemical Theory and Computation, 2018, 14, 4958-4970.	2.3	15
139	Novel Class of Chikungunya Virus Small Molecule Inhibitors That Targets the Viral Capping Machinery. Antimicrobial Agents and Chemotherapy, 2020, 64, .	1.4	15
140	In silico screening with benzofurane- and benzopyrane-type MDR-modulators. Il Farmaco, 2003, 58, 185-191.	0.9	14
141	Sequenceâ€Specific Positions of Water Molecules at the Interface between DNA and Minor Groove Binders. ChemPhysChem, 2008, 9, 2766-2771.	1.0	14
142	A Combination of Pharmacophore and Dockingâ€based Virtual Screening to Discover new Tyrosinase Inhibitors. Molecular Informatics, 2020, 39, e1900054.	1.4	14
143	Improved Lipophilicity and Aqueous Solubility Prediction with Composite Graph Neural Networks. Molecules, 2021, 26, 6185.	1.7	14
144	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

#	Article	IF	Citations
145	Aryl Diazinyl Ketoximes: Synthesis and Configurational Assignment. Heterocycles, 1996, 43, 151.	0.4	13
146	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
147	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
148	Pyridazines. LXVIII. Convenient Synthesis of Phenyl (6â€Substituted 3â€Pyridazinyl) Ketones via the Oxidative Decyanation Route. Journal of Heterocyclic Chemistry, 1993, 30, 1685-1689.	1.4	12
149	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
150	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
151	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
152	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
153	Update on PET Tracer Development for Muscarinic Acetylcholine Receptors. Pharmaceuticals, 2021, 14, 530.	1.7	11
154	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
155	3D Quantitative Structureâ€“Property Relationships. , 2008, , 587-604.		10
156	Pharmacophore-based Virtual Screening in Drug Discovery. , 2008, , 76-119.		10
157	Molecular Mingling: Multimodal Predictions of Ligand Promiscuity in Pentameric Ligand-Gated Ion Channels. Frontiers in Molecular Biosciences, 2022, 9, .	1.6	10
158	Improving Small Molecule pKa Prediction Using Transfer Learning With Graph Neural Networks. Frontiers in Chemistry, 2022, 10, .	1.8	10
159	Efficient Large-Scale Preparation of Phenyl 3-Pyridazinyl Ketone1. Synthetic Communications, 1994, 24, 773-778.	1.1	9
160	Long chain diamines inhibit growth of C6 glioma cells according to their hydrophobicity. An in vitro and molecular modeling study. Naunyn-Schmiedeberg's Archives of Pharmacology, 2000, 361, 235-246.	1.4	9
161	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
162	Pharmacophores for medicinal chemists: a personal view. Future Medicinal Chemistry, 2011, 3, 901-904.	1.1	9

#	Article	IF	Citations
163	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
164	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
165	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
166	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
167	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
168	Identification of repurposing therapeutics toward SARS-CoV-2 main protease by virtual screening. PLoS ONE, 2022, 17, e0269563.	1.1	9
169	New Principal Components Derived Parameters Describing Molecular Diversity of Heteroaromatic Residues. QSAR and Combinatorial Science, 1998, 17, 211-223.	1.4	8
170	Chemical function based pharmacophore models as suitable filters for virtual 3D-database screening. Computational and Theoretical Chemistry, 2000, 503, 59-72.	1.5	8
171	QPHAR: quantitative pharmacophore activity relationship: method and validation. Journal of Cheminformatics, 2021, 13, 57.	2.8	8
172	Rational Drug Design Paradigms: The Odyssey for Designing Better Drugs. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 238-256.	0.6	8
173	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
174	Synthetic Building Blocks Containing the 1,2-Diazine Moiety: N- and O-Protected 3-(4-Pyridazinyl)isoserines. Heterocycles, 1996, 43, 1057.	0.4	7
175	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
176	Inhibitors of prolyl endopeptidase: Characterization of the pharmacophoric pattern using conformational analysis and 3D-QSAR. Journal of Computer-Aided Molecular Design, 1993, 7, 253-262.	1.3	6
177	Pharmacophore-Based Screening for the Successful Identification of Bio-Active Natural Products. Chimia, 2007, 61, 350-354.	0.3	6
178	Fragment pharmacophore-based in silico screening: a powerful approach for efficient lead discovery. MedChemComm, 2016, 7, 506-511.	3.5	6
179	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
180	Pyridazines LXXVIII On the reactivity of 4â€methoxyâ€[(4â€pyridazinyl)methylidene]aniline in ester enolateâ€imine condensation reactions. Journal of Heterocyclic Chemistry, 1996, 33, 1731-1735.	1.4	5

#	Article	IF	Citations
181	Acylation of a novel quinoxalinyl substituted pyrazole derivative. synthesis, quantum chemistry calculations, and x-ray structure analysis. Journal of Heterocyclic Chemistry, 1998, 35, 113-115.	1.4	5
182	Pharmacy Practice and Education in Austria. Pharmacy (Basel, Switzerland), 2018, 6, 55.	0.6	5
183	SAR-Guided Scoring Function and Mutational Validation Reveal the Binding Mode of CGS-8216 at the Î±1+Î²2â€“ Benzodiazepine Site. Journal of Chemical Information and Modeling, 2018, 58, 1682-1696.	2.5	5
184	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
185	Computational Identification of Novel Kir6 Channel Inhibitors. Frontiers in Pharmacology, 2019, 10, 549.	1.6	5
186	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
187	Cognitive profiling and proteomic analysis of the modafinil analogue S-CE-123 in experienced aged rats. Scientific Reports, 2021, 11, 23962.	1.6	5
188	Novel diazinyl 3â€pyridyl ketones: Efficient synthesis and complete assignment of ¹H and ¹³C NMR spectra. Journal of Heterocyclic Chemistry, 1997, 34, 17-19.	1.4	4
189	Molecular similarity characterization using CoMFA. Journal of Computer - Aided Molecular Design, 1998, 12/14, 215-231.	1.0	4
190	Potential of Pyrazolooxadiazinone Derivatives as Serine Protease Inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2001, 16, 15-34.	0.5	4
191	LigandScout: 3-D Pharmacophores Derived from Protein-Bound Lingands and Their Use as Virtual Screening Filters.. ChemInform, 2005, 36, no.	0.1	4
192	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
193	In Silico Screening. , 2008, , 210-227.		4
194	The use of the Comins-Meyers Amide in Synthetic Chemistry: An Overview. Natural Product Communications, 2016, 11, 1934578X1601101.	0.2	4
195	In Silico Identification of Potential Druggable Binding Sites on CIN85 SH3 Domain. International Journal of Molecular Sciences, 2021, 22, 534.	1.8	4
196	Putative Dynamics of Vasopressin in its V1a Receptor Binding Site. Receptors and Channels, 2003, 9, 93-106.	1.1	4
197	Design, Synthesis, and Biological Evaluation of 4,4â€™-Difluorobenzhydrol Carbamates as Selective M1 Antagonists. Pharmaceuticals, 2022, 15, 248.	1.7	4
198	Synthesis, Biological Evaluation, and Docking Studies of Antagonistic Hydroxylated Arecaidine Esters Targeting mAChRs. Molecules, 2022, 27, 3173.	1.7	4

#	Article	IF	Citations
199	Alkylation of nonâ€electron rich nitrogen heterocycles by alkyl orthoformates: Quantum chemistry calculations. Journal of Heterocyclic Chemistry, 1996, 33, 1413-1415.	1.4	3
200	Molecular Similarity Determination of Heteroaromatic Ring Fragments Using GRID and Multivariate Data Analysis. QSAR and Combinatorial Science, 1996, 15, 469-474.	1.4	3
201	Use of 3D Pharmacophore Models in 3D Database Searching. , 2003, , .		3
202	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
203	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
204	Pharmacophore Models Derived from Molecular Dynamics Simulations of Protein-Ligand Complexes: A Case Study. Natural Product Communications, 2016, 11, 1934578X1601101.	0.2	2
205	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
206	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
207	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
208	Molecular Similarity Determination of Heteroaromatics Using CoMFA and Multivariate Data Analysis. QSAR and Combinatorial Science, 1994, 13, 402-405.	1.4	1
209	MolekÃ¼lsonden zur Erforschung von IonenkanÃlen: Der Weg von Ionen durch die Zellmembran. Biologie in Unserer Zeit, 2002, 32, 102-109.	0.3	1
210	N-(3,4-Dichlorobenzyl)azolesâ€"Investigations Regarding Synthesis, NMR-Spectroscopy and Affinity Towards Sisma-1 and Sigma-2 Receptors. Scientia Pharmaceutica, 2004, 72, 197-211.	0.7	1
211	The Use of Dynamic Pharmacophore in Computer-Aided Hit Discovery: A Case Study. Methods in Molecular Biology, 2018, 1824, 317-333.	0.4	1
212	Greedy 3-Point Search (G3PS)â€"A Novel Algorithm for Pharmacophore Alignment. Molecules, 2021, 26, 7201.	1.7	1
213	3D-QSAR STUDY OF NEW ACETYL-COA:CHOLESTEROL O-ACYL TRANSFERASE (ACAT) INHIBITORS. Scientia Pharmaceutica, 2000, 68, 65-73.	0.7	0
214	Molecular Similarity Characterization Using CoMFA. , 1998, , 215-231.		0
215	In silico Screening with Benzofuran- and Benzopyran-Type MDR-Modulators.. ChemInform, 2003, 34, no.	0.1	0
216	Combining Ethnopharmacology and Virtual Screening for Lead Structure Discovery: COX-Inhibitors as Application Example.. ChemInform, 2004, 35, no.	0.1	0

#	Article	IF	Citations
217	Influenza Virus Neuraminidase Inhibitors: Generation and Comparison of Structure-Based and Common Feature Pharmacophore Hypotheses and Their Application in Virtual Screening.. ChemInform, 2004, 35, no.	0.1	0
218	Pharmacophore Identification, in Silico Screening, and Virtual Library Design for Inhibitors of the Human Factor Xa.. ChemInform, 2005, 36, no.	0.1	0
219	Comparative Analysis of Protein-Bound Ligand Conformations with Respect to Catalystâ€²s Conformational Space Subsampling Algorithms.. ChemInform, 2005, 36, no.	0.1	0
220	The Identification of Ligand Features Essential for PXR Activation by Pharmacophore Modeling.. ChemInform, 2005, 36, no.	0.1	0
221	Human Rhinovirus 3C Protease: Generation of Pharmacophore Models for Peptidic and Nonpeptidic Inhibitors and Their Application in Virtual Screening.. ChemInform, 2005, 36, no.	0.1	0
222	In silicoTarget Fishing for Rationalized Ligand Discovery Exemplified on Constituents ofRuta graveolensL.. Planta Medica, 2009, 75, 293-293.	0.7	0
223	EFMCâ€ASMC Kongress in Wien. Nachrichten Aus Der Chemie, 2018, 66, 563-563.	0.0	0
224	Consecutive and Selective Double Methylene Insertion of Lithium Carbenoids to Isothiocyanates: A Direct Assembly of Fourâ€membered Sulfurâ€Containing Cycles. Angewandte Chemie, 0, , .	1.6	0
225	Chemical Function Based Alignment Generation for 3D QSAR of Highly Flexible Platelet Aggregation Inhibitors. , 2000, , 318-320.		0