Antonio Macchiarulo

List of Publications by Year
in descending order

161 papers	7,422 citations	101496 36 h-index	62565 80 g-index
170 all docs	170 docs citations	170 times ranked	10413 citing authors

#	Article	IF	Citations
1	TGR5-Mediated Bile Acid Sensing Controls Glucose Homeostasis. Cell Metabolism, 2009, 10, 167-177.	7.2	1,465
2	Aryl hydrocarbon receptor control of a disease tolerance defence pathway. Nature, 2014, 511, 184-190.	13.7	574
3	Family-wide chemical profiling and structural analysis of PARP and tankyrase inhibitors. Nature Biotechnology, 2012, 30, 283-288.	9.4	410
4	Novel Potent and Selective Bile Acid Derivatives as TGR5 Agonists: Biological Screening, Structureâ"Activity Relationships, and Molecular Modeling Studies. Journal of Medicinal Chemistry, 2008, 51, 1831-1841.	2.9	259
5	A Relay Pathway between Arginine and Tryptophan Metabolism Confers Immunosuppressive Properties on Dendritic Cells. Immunity, 2017, 46, 233-244.	6.6	241
6	Discovery of 6Î±-Ethyl-23(S)-methylcholic Acid (S-EMCA, INT-777) as a Potent and Selective Agonist for the TGR5 Receptor, a Novel Target for Diabesity. Journal of Medicinal Chemistry, 2009, 52, 7958-7961.	2.9	220
7	Glucocorticoid-Induced Leucine Zipper Inhibits the Raf-Extracellular Signal-Regulated Kinase Pathway by Binding to Raf-1. Molecular and Cellular Biology, 2002, 22, 7929-7941.	1.1	161
8	Glucocorticoid-induced leucine zipper (GILZ)/NF-ÂB interaction: role of GILZ homo-dimerization and C-terminal domain. Nucleic Acids Research, 2006, 35, 517-528.	6.5	126
9	Highlights at the gate of tryptophan catabolism: a review on the mechanisms of activation and regulation of indoleamine 2,3-dioxygenase (IDO), a novel target in cancer disease. Amino Acids, 2009, 37, 219-229.	1.2	114
10	1,4-Benzothiazine and 1,4-Benzoxazine imidazole derivatives with antifungal activity: A docking study. Bioorganic and Medicinal Chemistry, 2002, 10, 3415-3423.	1.4	101
11	Nongenomic Actions of Bile Acids. Synthesis and Preliminary Characterization of 23- and 6,23-Alkyl-Substituted Bile Acid Derivatives as Selective Modulators for the G-Protein Coupled Receptor TGR5. Journal of Medicinal Chemistry, 2007, 50, 4265-4268.	2.9	97
12	Modeling of Poly(ADP-ribose)polymerase (PARP) Inhibitors. Docking of Ligands and Quantitative Structureâ"Activity Relationship Analysis. Journal of Medicinal Chemistry, 2001, 44, 3786-3794.	2.9	93
13	Ligand selectivity and competition between enzymes in silico. Nature Biotechnology, 2004, 22, 1039-1045.	9.4	80
14	Poly(ADP-ribose) Catabolism Triggers AMP-dependent Mitochondrial Energy Failure. Journal of Biological Chemistry, 2009, 284, 17668-17676.	1.6	80
15	Genotyping of an Italian papillary thyroid carcinoma cohort revealed high prevalence of BRAF mutations, absence of RAS mutations and allowed the detection of a new mutation of BRAF oncoprotein (BRAFV599Ins). Clinical Endocrinology, 2006, 64, 105-109.	1.2	77
16	Indoleamine 2,3-Dioxygenase 1 (IDO1) Is Up-Regulated in Thyroid Carcinoma and Drives the Development of an Immunosuppressant Tumor Microenvironment. Journal of Clinical Endocrinology and Metabolism, 2014, 99, E832-E840.	1.8	73
17	<scp>PARP</scp> inhibitors: polypharmacology versus selective inhibition. FEBS Journal, 2013, 280, 3563-3575.	2.2	70
18	Targeting glucocorticoid side effects: selective glucocorticoid receptor modulator or glucocorticoidâ€induced leucine zipper? A perspective. FASEB Journal, 2014, 28, 5055-5070.	0.2	68

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19	Synthesis, docking studies and anti-inflammatory activity of 4,5,6,7-tetrahydro-2H-indazole derivatives. Bioorganic and Medicinal Chemistry, 2007, 15, 3463-3473.	1.4	63
20	Rat brain guanosine binding site. Bioorganic and Medicinal Chemistry, 2003, 11, 5417-5425.	1.4	61
21	Positive allosteric modulation of indoleamine 2,3-dioxygenase 1 restrains neuroinflammation. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 3848-3857.	3.3	58
22	QSAR and Molecular Modeling Studies of Baclofen Analogues as GABABAgonists. Insights into the Role of the Aromatic Moiety in GABABBinding and Activation. Journal of Medicinal Chemistry, 2001, 44, 1827-1832.	2.9	57
23	Biochemical and molecular characterization of the novel BRAFV599Ins mutation detected in a classic papillary thyroid carcinoma. Oncogene, 2006, 25, 4235-4240.	2.6	56
24	Indoleamine 2,3â€dioxygenase 1 (IDO1): an upâ€toâ€date overview of an eclectic immunoregulatory enzyme. FEBS Journal, 2022, 289, 6099-6118.	2.2	56
25	Identification by Virtual Screening and In Vitro Testing of Human DOPA Decarboxylase Inhibitors. PLoS ONE, 2012, 7, e31610.	1.1	56
26	Docking studies on PARP-1 inhibitors: insights into the role of a binding pocket water molecule. Bioorganic and Medicinal Chemistry, 2005, 13, 1151-1157.	1.4	54
27	Design, Synthesis, and Microbiological Evaluation of NewCandida albicansCYP51 Inhibitors. Journal of Medicinal Chemistry, 2005, 48, 7658-7666.	2.9	51
28	Distinct roles of immunoreceptor tyrosineâ€based motifs in immunosuppressive indoleamine 2,3â€dioxygenase 1. Journal of Cellular and Molecular Medicine, 2017, 21, 165-176.	1.6	51
29	Discovery of 3Î±,7Î±,11Î²-Trihydroxy-6Î±-ethyl-5Î²-cholan-24-oic Acid (TC-100), a Novel Bile Acid as Potent and Highly Selective FXR Agonist for Enterohepatic Disorders. Journal of Medicinal Chemistry, 2016, 59, 9201-9214.	2.9	50
30	Targeting Wnt-driven cancers: Discovery of novel tankyrase inhibitors. European Journal of Medicinal Chemistry, 2017, 142, 506-522.	2.6	47
31	4,5-Diarylisoxazol-3-carboxylic acids: A new class of leukotriene biosynthesis inhibitors potentially targeting 5-lipoxygenase-activating protein (FLAP). European Journal of Medicinal Chemistry, 2016, 113, 1-10.	2.6	45
32	Beyond Bile Acids: Targeting Farnesoid X Receptor (FXR) with Natural and Synthetic Ligands. Current Topics in Medicinal Chemistry, 2014, 14, 2129-2142.	1.0	44
33	Patented TGR5 modulators: a review (2006 â€“ present). Expert Opinion on Therapeutic Patents, 2012, 22, 1399-1414.	2.4	43
34	Ligand Binding and Functional Selectivity of <scp>l</scp>-Tryptophan Metabolites at the Mouse Aryl Hydrocarbon Receptor (mAhR). Journal of Chemical Information and Modeling, 2014, 54, 3373-3383.	2.5	42
35	Novel Polymorphisms of Nuclear Receptor SHP Associated with Functional and Structural Changes. Journal of Biological Chemistry, 2010, 285, 24871-24881.	1.6	40
36	Adamantyl-Substituted Retinoid-Derived Molecules That Interact with the Orphan Nuclear Receptor Small Heterodimer Partner: Effects of Replacing the 1-Adamantyl or Hydroxyl Group on Inhibition of Cancer Cell Growth, Induction of Cancer Cell Apoptosis, and Inhibition of Src Homology 2 Domain-Containing Protein Tyrosine Phosphatase-2 Activity. Journal of Medicinal Chemistry, 2008, 51, 5650-5662.	2.9	38

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37	Extending SAR of bile acids as FXR ligands: Discovery of 23-N-(carbocinnamyloxy)-3Î±,7Î±-dihydroxy-6Î±-ethyl-24-nor-5Î²-cholan-23-amine. Bioorganic and Medicinal Chemistry, 2011, 19, 2650-2658.	1.4	38
38	Targeting the MDM2/MDM4 Interaction Interface as a Promising Approach for p53 Reactivation Therapy. Cancer Research, 2015, 75, 4560-4572.	0.4	38
39	Pyrazole[3,4-e][1,4]thiazepin-7-one derivatives as a novel class of Farnesoid X Receptor (FXR) agonists. Bioorganic and Medicinal Chemistry, 2012, 20, 3429-3445.	1.4	37
40	AhR-Mediated, Non-Genomic Modulation of IDO1 Function. Frontiers in Immunology, 2014, 5, 497.	2.2	37
41	Exploring the other side of biologically relevant chemical space: Insights into carboxylic, sulfonic and phosphonic acid bioisosteric relationships. Journal of Molecular Graphics and Modelling, 2007, 26, 728-739.	1.3	36
42	Sâ€Tritylâ€(R)â€cysteine, a powerful chiral selector for the analytical and preparative ligandâ€exchange chromatography of amino acids. Journal of Separation Science, 2008, 31, 696-704.	1.3	36
43	Probing the Binding Site of Bile Acids in TGR5. ACS Medicinal Chemistry Letters, 2013, 4, 1158-1162.	1.3	36
44	Spiro[2.2]pentane as a Dissymmetric Scaffold for Conformationally Constrained Analogues of Glutamic Acid:Â Focus on Racemic 1-Aminospiro[2.2]pentyl-1,4-dicarboxylic Acids. Journal of Organic Chemistry, 2002, 67, 5497-5507.	1.7	35
45	Molecular Dynamics Simulation of the Ligand Binding Domain of Farnesoid X Receptor. Insights into Helix-12 Stability and Coactivator Peptide Stabilization in Response to Agonist Binding. Journal of Medicinal Chemistry, 2005, 48, 3251-3259.	2.9	35
46	Targeting Aryl hydrocarbon receptor for next-generation immunotherapies: Selective modulators (SAhRMs) versus rapidly metabolized ligands (RMAhRLs). European Journal of Medicinal Chemistry, 2020, 185, 111842.	2.6	35
47	Pharmacophore Models of Group I and Group II Metabotropic Glutamate Receptor Agonists. Analysis of Conformational, Steric, and Topological Parameters Affecting Potency and Selectivity. Journal of Medicinal Chemistry, 1999, 42, 2816-2827.	2.9	34
48	Avicholic Acid: A Lead Compound from Birds on the Route to Potent TGR5 Modulators. ACS Medicinal Chemistry Letters, 2012, 3, 273-277.	1.3	33
49	Advances in indoleamine 2,3-dioxygenase 1 medicinal chemistry. MedChemComm, 2017, 8, 1378-1392.	3.5	33
50	Bile Acid Derivatives as Ligands of the Farnesoid X Receptor: Molecular Determinants for Bile Acid Binding and Receptor Modulation. Current Topics in Medicinal Chemistry, 2014, 14, 2159-2174.	1.0	33
51	Modeling of Amino-Terminal Domains of Group I Metabotropic Glutamate Receptors:Â Structural Motifs Affecting Ligand Selectivity. Journal of Medicinal Chemistry, 1999, 42, 5390-5401.	2.9	32
52	Very-long-chain fatty acid sphingomyelin in nuclear lipid microdomains of hepatocytes and hepatoma cells: can the exchange from C24:0 to C16:0 affect signal proteins and vitamin D receptor?. Molecular Biology of the Cell, 2015, 26, 2418-2425.	0.9	32
53	From Polypharmacology to Target Specificity: The Case of PARP Inhibitors. Current Topics in Medicinal Chemistry, 2013, 13, 2939-2954.	1.0	32
54	Dynamic ligand-exchange chiral stationary phase from S-benzyl-(R)-cysteine. Chirality, 2006, 18, 509-518.	1.3	31

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55	Molecular docking and spatial coarse graining simulations as tools to investigate substrate recognition, enhancer binding and conformational transitions in indoleamine-2,3-dioxygenase (IDO). Biochimica Et Biophysica Acta - Proteins and Proteomics, 2007, 1774, 1058-1068.	1.1	31
56	Bulky 1,4-benzoxazine derivatives with antifungal activity. Bioorganic and Medicinal Chemistry, 2009, 17, 3838-3846.	1.4	31
57	Design, Synthesis, Crystallographic Studies, and Preliminary Biological Appraisal of New Substituted Triazolo[4,3-b]pyridazin-8-amine Derivatives as Tankyrase Inhibitors. Journal of Medicinal Chemistry, 2014, 57, 2807-2812.	2.9	31
58	Modulation of the Kynurine Pathway of Tryptophan Metabolism in Search for Neuroprotective Agents. Focus on Kynurenine-3-Hydroxylase. Advances in Experimental Medicine and Biology, 2003, 527, 621-628.	0.8	31
59	3-hydroxy-L-kynurenamine is an immunomodulatory biogenic amine. Nature Communications, 2021, 12, 4447.	5.8	30
60	Design, synthesis and preliminary evaluation of novel 3â€²-Substituted carboxycyclopropylglycines as antagonists at group 2 metabotropic glutamate receptors. Bioorganic and Medicinal Chemistry Letters, 2001, 11, 3179-3182.	1.0	29
61	Is Antagonism ofE/Z-Guggulsterone at the Farnesoid X Receptor Mediated by a Noncanonical Binding Site? A Molecular Modeling Study. Journal of Medicinal Chemistry, 2005, 48, 6948-6955.	2.9	29
62	Pharmacophore model for bile acids recognition by the FPR receptor. Journal of Computer-Aided Molecular Design, 2006, 20, 295-303.	1.3	29
63	The effect of the copper(II) salt anion in the Chiral Ligand-Exchange Chromatography of amino acids. Analytica Chimica Acta, 2009, 638, 225-233.	2.6	29
64	Sequence Variants in Kynurenine Aminotransferaseâ€…II (KATâ€…II) Orthologs Determine Different Potencies of the Inhibitor Sâ€ESBA. ChemMedChem, 2008, 3, 1199-1202.	1.6	28
65	Targeting the Conformational Transitions of MDM2 and MDMX: Insights into Dissimilarities and Similarities of p53 Recognition. Journal of Chemical Information and Modeling, 2008, 48, 1999-2009.	2.5	28
66	Design, synthesis and biological evaluation of novel bicyclo[1.1.1]pentane-based Ï‰-acidic amino acids as glutamate receptors ligands. Bioorganic and Medicinal Chemistry, 2009, 17, 242-250.	1.4	28
67	Computational studies in enantioselective liquid chromatography: Forty years of evolution in docking- and molecular dynamics-based simulations. TrAC - Trends in Analytical Chemistry, 2020, 122, 115703.	5.8	28
68	Concepts and Molecular Aspects in the Polypharmacology of PARPâ€1 Inhibitors. ChemMedChem, 2016, 11, 1219-1226.	1.6	27
69	Insights into the molecular function of the inactivating mutations of B-Raf involving the DFG motif. Biochimica Et Biophysica Acta - Molecular Cell Research, 2009, 1793, 1634-1645.	1.9	26
70	Puzzling over MDM4â€“p53 network. International Journal of Biochemistry and Cell Biology, 2010, 42, 1080-1083.	1.2	26
71	Unveiling hidden features of orphan nuclear receptors: The case of the small heterodimer partner (SHP). Journal of Molecular Graphics and Modelling, 2006, 24, 362-372.	1.3	25
72	Cysteine-based chiral selectors for the ligand-exchange separation of amino acidsâ˜†. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2008, 875, 108-117.	1.2	25

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73	Preclinical discovery and development of fingolimod for the treatment of multiple sclerosis. Expert Opinion on Drug Discovery, 2019, 14, 1199-1212.	2.5	25
74	Exploiting Chemical Toolboxes for the Expedited Generation of Tetracyclic Quinolines as a Novel Class of PXR Agonists. ACS Medicinal Chemistry Letters, 2019, 10, 677-681.	1.3	25
75	Synthesis and Preliminary Biological Evaluation of 2â€²-Substituted 2-(3â€²-Carboxybicyclo[1.1.1]pentyl)glycine Derivatives as Groupâ€…I Selective Metabotropic Glutamate Receptor Ligands. ChemMedChem, 2006, 1, 358-365.	1.6	24
76	Integrating multicomponent flow synthesis and computational approaches for the generation of a tetrahydroquinoline compound based library. MedChemComm, 2016, 7, 439-446.	3.5	24
77	Class IA PI3Ks regulate subcellular and functional dynamics of IDO1. EMBO Reports, 2020, 21, e49756.	2.0	24
78	Laboratory-Scale Preparative Enantioseparations of Pharmaceutically Relevant Compounds on Commercially Available Chiral Stationary Phases for HPLC. Current Medicinal Chemistry, 2017, 24, 796-817.	1.2	24
79	Towards new neuroprotective agents: design and synthesis of 4H-thieno[2,3-c] isoquinolin-5-one derivatives as potent PARP-1 inhibitors. Il Farmaco, 2003, 58, 851-858.	0.9	23
80	Binding mode of 6ECDCA, a potent bile acid agonist of the farnesoid X receptor (FXR). Bioorganic and Medicinal Chemistry Letters, 2003, 13, 1865-1868.	1.0	23
81	Novel ketoconazole analogues based on the replacement of 2,4-dichlorophenyl group with 1,4-benzothiazine moiety: Design, synthesis, and microbiological evaluation. Bioorganic and Medicinal Chemistry, 2006, 14, 5196-5203.	1.4	23
82	Molecular Field Analysis and 3D-Quantitative Structureâ^'Activity Relationship Study (MFA 3D-QSAR) Unveil Novel Features of Bile Acid Recognition at TGR5. Journal of Chemical Information and Modeling, 2008, 48, 1792-1801.	2.5	23
83	Derived chromatographic indices as effective tools to study the self-aggregation process of bile acids. Journal of Pharmaceutical and Biomedical Analysis, 2009, 50, 613-621.	1.4	23
84	Scaffold hopping approach on the route to selective tankyrase inhibitors. European Journal of Medicinal Chemistry, 2014, 87, 611-623.	2.6	20
85	Binding Mode and Structureâ€“Activity Relationships of ITE as an Aryl Hydrocarbon Receptor (AhR) Agonist. ChemMedChem, 2018, 13, 270-279.	1.6	20
86	QSAR Study of Anticonvulsant Negative Allosteric Modulators of the AMPA Receptor. Journal of Medicinal Chemistry, 2004, 47, 1860-1863.	2.9	19
87	Chiral mobile phase in ligand-exchange chromatography of amino acids: Exploring the copper(II) salt anion effect with a computational approach. Journal of Chromatography A, 2012, 1269, 316-324.	1.8	18
88	Synthesis, Molecular Modeling Studies, and Preliminary Pharmacological Characterization of All Possible 2-(2â€˜-Sulfonocyclopropyl)glycine Stereoisomers as Conformationally ConstrainedL-Homocysteic Acid Analogs. Journal of Medicinal Chemistry, 2007, 50, 4630-4641.	2.9	17
89	Computational studies for the elucidation of the enantiomer elution order of amino acids in chiral ligand-exchange chromatography. Journal of Chromatography A, 2010, 1217, 7523-7527.	1.8	17
90	Discovery and characterization of novel potent PARP-1 inhibitors endowed with neuroprotective properties: From TIQ-A to HYDAMTIQ. MedChemComm, 2011, 2, 559.	3.5	17

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91	Divergent and stereoselective synthesis of dafachronic acids. Tetrahedron, 2011, 67, 1924-1929.	1.0	17
92	Signal Transducer and Activator of Transcription 1 Plays a Pivotal Role in RET/PTC3 Oncogene-induced Expression of Indoleamine 2,3-Dioxygenase 1. Journal of Biological Chemistry, 2017, 292, 1785-1797.	1.6	17
93	Fragment-based approach to identify IDO1 inhibitor building blocks. European Journal of Medicinal Chemistry, 2017, 141, 169-177.	2.6	17
94	Evaluation of the enantiomeric selectivity in the chiral ligand-exchange chromatography of amino acids by a computational model. Journal of Chromatography A, 2004, 1033, 363-367.	1.8	16
95	Homology model of the multidrug transporter LmrA from Lactococcus lactis. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 5823-5826.	1.0	16
96	(S)-(â€“)-Î±,Î±-Di(2-naphthyl)-2-pyrrolidinemethanol, a useful tool to study the recognition mechanism in chiral ligand-exchange chromatography. Journal of Separation Science, 2007, 30, 21-27.	1.3	16
97	Exploring the effect of PARP-1 flexibility in docking studies. Journal of Molecular Graphics and Modelling, 2013, 45, 192-201.	1.3	16
98	Expanding the horizon of chemotherapeutic targets: From MDM2 to MDMX (MDM4). MedChemComm, 2011, 2, 455.	3.5	15
99	Investigating the allosteric reverse signalling of PARP inhibitors with microsecond molecular dynamic simulations and fluorescence anisotropy. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2014, 1844, 1765-1772.	1.1	15
100	Exploring the enantiorecognition mechanism of Cinchona alkaloidâ€based zwitterionic chiral stationary phases and the basic transâ€paroxetine enantiomers. Journal of Separation Science, 2018, 41, 1199-1207.	1.3	15
101	Phenolic Acids from Lycium barbarum Leaves: In Vitro and In Silico Studies of the Inhibitory Activity against Porcine Pancreatic Î±-Amylase. Processes, 2020, 8, 1388.	1.3	15
102	Insights into Phenylalanine Derivatives Recognition of VLA-4 Integrin:â€‰ From a Pharmacophoric Study to 3D-QSAR and Molecular Docking Analyses. Journal of Chemical Information and Computer Sciences, 2004, 44, 1829-1839.	2.8	14
103	Descriptive structureâ€“separation relationship studies in chiral ligandâ€exchange chromatography. Journal of Separation Science, 2008, 31, 2395-2403.	1.3	14
104	Mapping Human Metabolic Pathways in the Small Molecule Chemical Space. Journal of Chemical Information and Modeling, 2009, 49, 2272-2289.	2.5	14
105	Synthesis, physicochemical properties, and biological activity of bile acids 3-glucuronides: Novel insights into bile acid signalling and detoxification. European Journal of Medicinal Chemistry, 2018, 144, 349-358.	2.6	14
106	D-leucine microparticles as an excipient to improve the aerosolization performances of dry powders for inhalation. European Journal of Pharmaceutical Sciences, 2019, 130, 54-64.	1.9	14
107	A novel mutation of indoleamine 2,3-dioxygenase 1 causes a rapid proteasomal degradation and compromises protein function. Journal of Autoimmunity, 2020, 115, 102509.	3.0	14
108	Oxime and Oxime Ether Derivatives of 1,4-Benzothiazine Related to Oxiconazole. ChemMedChem, 2007, 2, 1208-1213.	1.6	13

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109	Protective Effects of Commiphora erythraea Resin Constituents Against Cellular Oxidative Damage. Molecules, 2011, 16, 10357-10369.	1.7	13
110	The Janus-faced nature of IDO1 in infectious diseases: challenges and therapeutic opportunities. Future Medicinal Chemistry, 2016, 8, 39-54.	1.1	13
111	Homology model of the closed, functionally active, form of the amino terminal domain of mGluR1. Bioorganic and Medicinal Chemistry, 2001, 9, 847-852.	1.4	12
112	Binding modes of noncompetitive AMPA antagonists: a computational approach. Il Farmaco, 2003, 58, 107-113.	0.9	12
113	The role of electrostatic interaction in the molecular recognition of selective agonists to metabotropic glutamate receptors. Proteins: Structure, Function and Bioinformatics, 2003, 50, 609-619.	1.5	12
114	Targeting the conformational transitions of MDM2 and MDMX: Insights into key residues affecting p53 recognition. Proteins: Structure, Function and Bioinformatics, 2009, 77, 524-535.	1.5	12
115	Charting the Chemical Space of Target Sites: Insights into the Binding Modes of Amine and Amidine Groups. Journal of Chemical Information and Modeling, 2009, 49, 900-912.	2.5	12
116	MDM2/MDMX inhibitor peptide: WO2008106507. Expert Opinion on Therapeutic Patents, 2009, 19, 721-726.	2.4	12
117	Chiral ligand-exchange separation and resolution of extremely rigid glutamate analogs: 1-aminospiro[2.2]pentyl-1,4-dicarboxylic acids. Analytical and Bioanalytical Chemistry, 2010, 397, 1997-2011.	1.9	12
118	Molecular Interaction Fields and 3D-QSAR Studies of p53â^'MDM2 Inhibitors Suggest Additional Features of Ligandâ^'Target Interaction. Journal of Chemical Information and Modeling, 2010, 50, 1451-1465.	2.5	12
119	Metabotropic glutamate receptors: structure and new subtype-selective ligands. Il Farmaco, 2001, 56, 91-94.	0.9	11
120	Fitting the complexity of GPCRs modulation into simple hypotheses of ligand design. Journal of Molecular Graphics and Modelling, 2012, 38, 70-81.	1.3	11
121	From Molecular Docking to 3Dâ€Quantitative Structureâ€Activity Relationships (3Dâ€QSAR): Insights into the Binding Mode of 5â€Lipoxygenase Inhibitors. Molecular Informatics, 2012, 31, 123-134.	1.4	11
122	Docking Studies and Molecular Dynamic Simulations Reveal Different Features of IDO1 Structure. Molecular Informatics, 2016, 35, 449-459.	1.4	11
123	New Insights from Crystallographic Data: Diversity of Structural Motifs and Molecular Recognition Properties between Groups of IDO1 Structures. ChemMedChem, 2020, 15, 891-899.	1.6	11
124	Taxifolin and gastro-adhesive microparticles containing taxifolin promotes gastric healing in vivo, inhibits Helicobacter pylori in vitro and proton pump reversibly in silico. Chemico-Biological Interactions, 2021, 339, 109445.	1.7	11
125	Choline Kinase Active Site Provides Features for Designing Versatile Inhibitors. Current Topics in Medicinal Chemistry, 2015, 14, 2684-2693.	1.0	11
126	Metabotropic glutamate receptors: a structural view point. Pharmaceutica Acta Helvetiae, 2000, 74, 231-237.	1.2	10

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127	Quantum mechanics/molecular mechanics (QM/MM) modeling of the irreversible transamination of l-kynurenine to kynurenic acid: The round dance of kynurenine aminotransferase II. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2009, 1794, 1802-1812.	1.1	10
128	Computational modelling of the binding of arachidonic acid to the human monooxygenase CYP2J2. Journal of Molecular Modeling, 2016, 22, 279.	0.8	10
129	Elucidation of the Chromatographic Enantiomer Elution Order Through Computational Studies. Mini-Reviews in Medicinal Chemistry, 2018, 18, 88-97.	1.1	10
130	Structure of metalâ€“carbenoid intermediates derived from the dirhodium(II)tetracarboxylate mediated decomposition of Î±-diazocarbonyl compounds: a DFT study. Computational and Theoretical Chemistry, 2002, 581, 111-115.	1.5	9
131	Conformational properties of cholic acid, a lead compound at the crossroads of bile acid inspired drug discovery. MedChemComm, 2014, 5, 750-757.	3.5	9
132	Synthesis and biological evaluation of C(5)-substituted derivatives of leukotriene biosynthesis inhibitor BRP-7. European Journal of Medicinal Chemistry, 2016, 122, 510-519.	2.6	9
133	Discovery of Novel 5-Lipoxygenase-Activating Protein (FLAP) Inhibitors by Exploiting a Multistep Virtual Screening Protocol. Journal of Chemical Information and Modeling, 2020, 60, 1737-1748.	2.5	9
134	The Stone Guest: How Does pH Affect Binding Properties of PDâ€1/PDâ€L1 Inhibitors?. ChemMedChem, 2021, 16, 568-577.	1.6	9
135	Insights into the binding mode and mechanism of action of some atypical retinoids as ligands of the small heterodimer partner (SHP). Journal of Computer-Aided Molecular Design, 2010, 24, 943-956.	1.3	8
136	Alternative strategies for targeting mouse double minute 2 activity with small molecules: novel patents on the horizon?. Expert Opinion on Therapeutic Patents, 2011, 21, 287-294.	2.4	8
137	Pharmacophoreâ€Based Virtual Screening to Discover New Active Compounds for Human Choline Kinase Î±1. Molecular Informatics, 2015, 34, 458-466.	1.4	8
138	Binding properties of different categories of IDO1 inhibitors: a microscale thermophoresis study. Future Medicinal Chemistry, 2017, 9, 1327-1338.	1.1	8
139	Enantioselective HPLC Analysis to Assist the Chemical Exploration of Chiral Imidazolines. Molecules, 2020, 25, 640.	1.7	8
140	Molecular dynamics simulation of the ligand binding domain of mGluR1 in response to agonist and antagonist binding. Journal of Computer-Aided Molecular Design, 2002, 16, 779-784.	1.3	7
141	Optimized one-pot derivatization and enantioseparation of cysteine: Application to the study of a dietary supplement. Journal of Pharmaceutical and Biomedical Analysis, 2020, 180, 113066.	1.4	7
142	Fragment based drug design and diversity-oriented synthesis of carboxylic acid isosteres. Bioorganic and Medicinal Chemistry, 2020, 28, 115731.	1.4	7
143	Metabotropic glutamate receptors: targets for therapy of cerebral ischaemia. Expert Opinion on Therapeutic Targets, 2001, 5, 669-683.	1.5	6
144	Synthesis and Quantitative Structure-Property Relationships of Side Chain-Modified Hyodeoxycholic Acid Derivatives. Molecules, 2013, 18, 10497-10513.	1.7	6

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145	Opportunities and challenges in drug discovery targeting metabotropic glutamate receptor 4. Expert Opinion on Drug Discovery, 2018, 13, 411-423.	2.5	6
146	Tracking Hidden Binding Pockets Along the Molecular Recognition Path of <scp>l</scp>â€Trp to Indoleamine 2,3â€Dioxygenase 1. ChemMedChem, 2019, 14, 2084-2092.	1.6	6
147	Critical Assessment of a Structure-Based Screening Campaign for IDO1 Inhibitors: Tips and Pitfalls. International Journal of Molecular Sciences, 2022, 23, 3981.	1.8	6
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