

Antonio Macchiarulo

List of Publications by Year in descending order

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161
papers

7,422
citations

101543

36
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62596

80
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170
all docs

170
docs citations

170
times ranked

10413
citing authors

#	ARTICLE	IF	CITATIONS
1	Indoleamine 2,3-dioxygenase 1 (IDO1): an update overview of an eclectic immunoregulatory enzyme. <i>FEBS Journal</i> , 2022, 289, 6099-6118.	4.7	56
2	Biological Evaluation of New Thienopyridinium and Thienopyrimidinium Derivatives as Human Choline Kinase Inhibitors. <i>Pharmaceutics</i> , 2022, 14, 715.	4.5	2
3	Critical Assessment of a Structure-Based Screening Campaign for IDO1 Inhibitors: Tips and Pitfalls. <i>International Journal of Molecular Sciences</i> , 2022, 23, 3981.	4.1	6
4	The Stone Guest: How Does pH Affect Binding Properties of PD-1/PD-L1 Inhibitors?. <i>ChemMedChem</i> , 2021, 16, 568-577.	3.2	9
5	Taxifolin and gastro-adhesive microparticles containing taxifolin promotes gastric healing in vivo, inhibits <i>Helicobacter pylori</i> in vitro and proton pump reversibly in silico. <i>Chemico-Biological Interactions</i> , 2021, 339, 109445.	4.0	11
6	3-hydroxy-L-tryptophan is an immunomodulatory biogenic amine. <i>Nature Communications</i> , 2021, 12, 4447.	12.8	30
7	One Key and Multiple Locks: Substrate Binding in Structures of Tryptophan Dioxygenases and Hydroxylases. <i>ChemMedChem</i> , 2021, 16, 2732-2743.	3.2	3
8	Targeting Aryl hydrocarbon receptor for next-generation immunotherapies: Selective modulators (SAhRMs) versus rapidly metabolized ligands (RMAhRLs). <i>European Journal of Medicinal Chemistry</i> , 2020, 185, 111842.	5.5	35
9	Computational studies in enantioselective liquid chromatography: Forty years of evolution in docking- and molecular dynamics-based simulations. <i>TrAC - Trends in Analytical Chemistry</i> , 2020, 122, 115703.	11.4	28
10	Optimized one-pot derivatization and enantioseparation of cysteine: Application to the study of a dietary supplement. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2020, 180, 113066.	2.8	7
11	Laboratory-Scale Semipreparative Enantioresolution of Phenylethanolic-Azole Heme Oxygenase-1 Inhibitors. <i>Chromatographia</i> , 2020, 83, 1509-1515.	1.3	2
12	Synthesis, biological evaluation, in silico modeling and crystallization of novel small monocationic molecules with potent antiproliferative activity by dual mechanism. <i>European Journal of Medicinal Chemistry</i> , 2020, 207, 112797.	5.5	4
13	Fragment based drug design and diversity-oriented synthesis of carboxylic acid isosteres. <i>Bioorganic and Medicinal Chemistry</i> , 2020, 28, 115731.	3.0	7
14	Phenolic Acids from <i>Lycium barbarum</i> Leaves: In Vitro and In Silico Studies of the Inhibitory Activity against Porcine Pancreatic α -Amylase. <i>Processes</i> , 2020, 8, 1388.	2.8	15
15	New Insights from Crystallographic Data: Diversity of Structural Motifs and Molecular Recognition Properties between Groups of IDO1 Structures. <i>ChemMedChem</i> , 2020, 15, 891-899.	3.2	11
16	A novel mutation of indoleamine 2,3-dioxygenase 1 causes a rapid proteasomal degradation and compromises protein function. <i>Journal of Autoimmunity</i> , 2020, 115, 102509.	6.5	14
17	Positive allosteric modulation of indoleamine 2,3-dioxygenase 1 restrains neuroinflammation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 3848-3857.	7.1	58
18	Discovery of Novel 5-Lipoxygenase-Activating Protein (FLAP) Inhibitors by Exploiting a Multistep Virtual Screening Protocol. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1737-1748.	5.4	9

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19	Enantioselective HPLC Analysis to Assist the Chemical Exploration of Chiral Imidazolines. <i>Molecules</i> , 2020, 25, 640.	3.8	8
20	Class IA PI3Ks regulate subcellular and functional dynamics of IDO1. <i>EMBO Reports</i> , 2020, 21, e49756.	4.5	24
21	Preclinical discovery and development of fingolimod for the treatment of multiple sclerosis. <i>Expert Opinion on Drug Discovery</i> , 2019, 14, 1199-1212.	5.0	25
22	D-leucine microparticles as an excipient to improve the aerosolization performances of dry powders for inhalation. <i>European Journal of Pharmaceutical Sciences</i> , 2019, 130, 54-64.	4.0	14
23	Tracking Hidden Binding Pockets Along the Molecular Recognition Path of α -Trp to Indoleamine 2,3-Dioxygenase 1. <i>ChemMedChem</i> , 2019, 14, 2084-2092.	3.2	6
24	Exploiting Chemical Toolboxes for the Expedited Generation of Tetracyclic Quinolines as a Novel Class of PXR Agonists. <i>ACS Medicinal Chemistry Letters</i> , 2019, 10, 677-681.	2.8	25
25	Opportunities and challenges in drug discovery targeting metabotropic glutamate receptor 4. <i>Expert Opinion on Drug Discovery</i> , 2018, 13, 411-423.	5.0	6
26	Binding Mode and Structure-Activity Relationships of ITE as an Aryl Hydrocarbon Receptor (AhR) Agonist. <i>ChemMedChem</i> , 2018, 13, 270-279.	3.2	20
27	Synthesis, physicochemical properties, and biological activity of bile acids 3-glucuronides: Novel insights into bile acid signalling and detoxification. <i>European Journal of Medicinal Chemistry</i> , 2018, 144, 349-358.	5.5	14
28	Exploring the enantiorecognition mechanism of Cinchona alkaloid-based zwitterionic chiral stationary phases and the basic trans-paroxetine enantiomers. <i>Journal of Separation Science</i> , 2018, 41, 1199-1207.	2.5	15
29	Microscale Thermophoresis and Docking Studies Suggest Lapachol and Auraptene are Ligands of IDO1. <i>Natural Product Communications</i> , 2018, 13, 1934578X1801300.	0.5	0
30	Lead optimization-hit expansion of new asymmetrical pyridinium/quinolinium compounds as choline kinase \pm 1 inhibitors. <i>Future Medicinal Chemistry</i> , 2018, 10, 1769-1786.	2.3	4
31	Elucidation of the Chromatographic Enantiomer Elution Order Through Computational Studies. <i>Mini-Reviews in Medicinal Chemistry</i> , 2018, 18, 88-97.	2.4	10
32	A Relay Pathway between Arginine and Tryptophan Metabolism Confers Immunosuppressive Properties on Dendritic Cells. <i>Immunity</i> , 2017, 46, 233-244.	14.3	241
33	Advances in indoleamine 2,3-dioxygenase 1 medicinal chemistry. <i>MedChemComm</i> , 2017, 8, 1378-1392.	3.4	33
34	Signal Transducer and Activator of Transcription 1 Plays a Pivotal Role in RET/PTC3 Oncogene-induced Expression of Indoleamine 2,3-Dioxygenase 1. <i>Journal of Biological Chemistry</i> , 2017, 292, 1785-1797.	3.4	17
35	Fragment-based approach to identify IDO1 inhibitor building blocks. <i>European Journal of Medicinal Chemistry</i> , 2017, 141, 169-177.	5.5	17
36	Targeting Wnt-driven cancers: Discovery of novel tankyrase inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2017, 142, 506-522.	5.5	47

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37	Immunotherapy – a pursuit race to tomorrow's medicines. <i>Future Medicinal Chemistry</i> , 2017, 9, 1297-1299.	2.3	3
38	Binding properties of different categories of IDO1 inhibitors: a microscale thermophoresis study. <i>Future Medicinal Chemistry</i> , 2017, 9, 1327-1338.	2.3	8
39	Distinct roles of immunoreceptor tyrosine-based motifs in immunosuppressive indoleamine 2,3-dioxygenase 1. <i>Journal of Cellular and Molecular Medicine</i> , 2017, 21, 165-176.	3.6	51
40	Laboratory-Scale Preparative Enantioseparations of Pharmaceutically Relevant Compounds on Commercially Available Chiral Stationary Phases for HPLC. <i>Current Medicinal Chemistry</i> , 2017, 24, 796-817.	2.4	24
41	Discovery of 3 β ,7 β ,11 β -Trihydroxy-6 α -ethyl-5 α -cholan-24-oic Acid (TC-100), a Novel Bile Acid as Potent and Highly Selective FXR Agonist for Enterohepatic Disorders. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 9201-9214.	6.4	50
42	Synthesis and biological evaluation of C(5)-substituted derivatives of leukotriene biosynthesis inhibitor BRP-7. <i>European Journal of Medicinal Chemistry</i> , 2016, 122, 510-519.	5.5	9
43	Docking Studies and Molecular Dynamic Simulations Reveal Different Features of IDO1 Structure. <i>Molecular Informatics</i> , 2016, 35, 449-459.	2.5	11
44	Computational modelling of the binding of arachidonic acid to the human monooxygenase CYP2J2. <i>Journal of Molecular Modeling</i> , 2016, 22, 279.	1.8	10
45	Concepts and Molecular Aspects in the Polypharmacology of PARP Inhibitors. <i>ChemMedChem</i> , 2016, 11, 1219-1226.	3.2	27
46	Integrating multicomponent flow synthesis and computational approaches for the generation of a tetrahydroquinoline compound based library. <i>MedChemComm</i> , 2016, 7, 439-446.	3.4	24
47	4,5-Diarylisoaxazol-3-carboxylic acids: A new class of leukotriene biosynthesis inhibitors potentially targeting 5-lipoxygenase-activating protein (FLAP). <i>European Journal of Medicinal Chemistry</i> , 2016, 113, 1-10.	5.5	45
48	The Janus-faced nature of IDO1 in infectious diseases: challenges and therapeutic opportunities. <i>Future Medicinal Chemistry</i> , 2016, 8, 39-54.	2.3	13
49	- Mechanistic Aspects of Chiral Recognition on Protein-Based Stationary Phases. , 2016, 49, 46-79.		2
50	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?. <i>Molecular Biology of the Cell</i> , 2015, 26, 2418-2425.	2.1	32
51	Pharmacophore-Based Virtual Screening to Discover New Active Compounds for Human Choline Kinase β 1. <i>Molecular Informatics</i> , 2015, 34, 458-466.	2.5	8
52	Targeting the MDM2/MDM4 Interaction Interface as a Promising Approach for p53 Reactivation Therapy. <i>Cancer Research</i> , 2015, 75, 4560-4572.	0.9	38
53	Choline Kinase Active Site Provides Features for Designing Versatile Inhibitors. <i>Current Topics in Medicinal Chemistry</i> , 2015, 14, 2684-2693.	2.1	11
54	Beyond Bile Acids: Targeting Farnesoid X Receptor (FXR) with Natural and Synthetic Ligands. <i>Current Topics in Medicinal Chemistry</i> , 2014, 14, 2129-2142.	2.1	44

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55	Ligand Binding and Functional Selectivity of α -Tryptophan Metabolites at the Mouse Aryl Hydrocarbon Receptor (mAHR). <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 3373-3383.	5.4	42
56	AhR-Mediated, Non-Genomic Modulation of IDO1 Function. <i>Frontiers in Immunology</i> , 2014, 5, 497.	4.8	37
57	Indoleamine 2,3-Dioxygenase 1 (IDO1) Is Up-Regulated in Thyroid Carcinoma and Drives the Development of an Immunosuppressant Tumor Microenvironment. <i>Journal of Clinical Endocrinology and Metabolism</i> , 2014, 99, E832-E840.	3.6	73
58	Conformational properties of cholic acid, a lead compound at the crossroads of bile acid inspired drug discovery. <i>MedChemComm</i> , 2014, 5, 750-757.	3.4	9
59	Investigating the allosteric reverse signalling of PARP inhibitors with microsecond molecular dynamic simulations and fluorescence anisotropy. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2014, 1844, 1765-1772.	2.3	15
60	Design, Synthesis, Crystallographic Studies, and Preliminary Biological Appraisal of New Substituted Triazolo[4,3- <i>b</i>]pyridazin-8-amine Derivatives as Tankyrase Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 2807-2812.	6.4	31
61	Scaffold hopping approach on the route to selective tankyrase inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2014, 87, 611-623.	5.5	20
62	Targeting glucocorticoid side effects: selective glucocorticoid receptor modulator or glucocorticoid-induced leucine zipper? A perspective. <i>FASEB Journal</i> , 2014, 28, 5055-5070.	0.5	68
63	Aryl hydrocarbon receptor control of a disease tolerance defence pathway. <i>Nature</i> , 2014, 511, 184-190.	27.8	574
64	Bile Acid Derivatives as Ligands of the Farnesoid X Receptor: Molecular Determinants for Bile Acid Binding and Receptor Modulation. <i>Current Topics in Medicinal Chemistry</i> , 2014, 14, 2159-2174.	2.1	33
65	α -PARP inhibitors: polypharmacology versus selective inhibition. <i>FEBS Journal</i> , 2013, 280, 3563-3575.	4.7	70
66	Navigations of chemical space to further the understanding of polypharmacology in human nuclear receptors. <i>MedChemComm</i> , 2013, 4, 216-227.	3.4	0
67	Exploring the effect of PARP-1 flexibility in docking studies. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 45, 192-201.	2.4	16
68	Probing the Binding Site of Bile Acids in TGR5. <i>ACS Medicinal Chemistry Letters</i> , 2013, 4, 1158-1162.	2.8	36
69	Synthesis and Quantitative Structure-Property Relationships of Side Chain-Modified Hyodeoxycholic Acid Derivatives. <i>Molecules</i> , 2013, 18, 10497-10513.	3.8	6
70	From Polypharmacology to Target Specificity: The Case of PARP Inhibitors. <i>Current Topics in Medicinal Chemistry</i> , 2013, 13, 2939-2954.	2.1	32
71	Family-wide chemical profiling and structural analysis of PARP and tankyrase inhibitors. <i>Nature Biotechnology</i> , 2012, 30, 283-288.	17.5	410
72	Chiral mobile phase in ligand-exchange chromatography of amino acids: Exploring the copper(II) salt anion effect with a computational approach. <i>Journal of Chromatography A</i> , 2012, 1269, 316-324.	3.7	18

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73	Patented TGR5 modulators: a review (2006 – present). Expert Opinion on Therapeutic Patents, 2012, 22, 1399-1414.	5.0	43
74	Chapter 10. TGR5 Agonists in Development. RSC Drug Discovery Series, 2012, , 270-305.	0.3	1
75	Fitting the complexity of GPCRs modulation into simple hypotheses of ligand design. Journal of Molecular Graphics and Modelling, 2012, 38, 70-81.	2.4	11
76	From Molecular Docking to 3D–Quantitative Structure–Activity Relationships (3D–QSAR): Insights into the Binding Mode of 5–Lipoxygenase Inhibitors. Molecular Informatics, 2012, 31, 123-134.	2.5	11
77	Avicholic Acid: A Lead Compound from Birds on the Route to Potent TGR5 Modulators. ACS Medicinal Chemistry Letters, 2012, 3, 273-277.	2.8	33
78	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.	3.0	37
79	Identification by Virtual Screening and In Vitro Testing of Human DOPA Decarboxylase Inhibitors. PLoS ONE, 2012, 7, e31610.	2.5	56
80	Expanding the horizon of chemotherapeutic targets: From MDM2 to MDMX (MDM4). MedChemComm, 2011, 2, 455.	3.4	15
81	Discovery and characterization of novel potent PARP-1 inhibitors endowed with neuroprotective properties: From TIQ-A to HYDAMTIQ. MedChemComm, 2011, 2, 559.	3.4	17
82	Protective Effects of Commiphora erythraea Resin Constituents Against Cellular Oxidative Damage. Molecules, 2011, 16, 10357-10369.	3.8	13
83	Extending SAR of bile acids as FXR ligands: Discovery of 23-N-(carbocinnamyloxy)-3 β ,7 β -dihydroxy-6 β -ethyl-24-nor-5 β -cholan-23-amine. Bioorganic and Medicinal Chemistry, 2011, 19, 2650-2658.	3.0	38
84	Divergent and stereoselective synthesis of dafachronic acids. Tetrahedron, 2011, 67, 1924-1929.	1.9	17
85	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.	5.0	8
86	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.	3.7	12
87	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.	2.9	8
88	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.	3.7	17
89	Novel Polymorphisms of Nuclear Receptor SHP Associated with Functional and Structural Changes. Journal of Biological Chemistry, 2010, 285, 24871-24881.	3.4	40
90	Puzzling over MDM4–p53 network. International Journal of Biochemistry and Cell Biology, 2010, 42, 1080-1083.	2.8	26

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91	Molecular Interaction Fields and 3D-QSAR Studies of p53 ^{WT} MDM2 Inhibitors Suggest Additional Features of Ligand ^{WT} Target Interaction. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 1451-1465.	5.4	12
92	Poly(ADP-ribose) Catabolism Triggers AMP-dependent Mitochondrial Energy Failure. <i>Journal of Biological Chemistry</i> , 2009, 284, 17668-17676.	3.4	80
93	Insights into the molecular function of the inactivating mutations of B-Raf involving the DFG motif. <i>Biochimica Et Biophysica Acta - Molecular Cell Research</i> , 2009, 1793, 1634-1645.	4.1	26
94	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. <i>Amino Acids</i> , 2009, 37, 219-229.	2.7	114
95	Derived chromatographic indices as effective tools to study the self-aggregation process of bile acids. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2009, 50, 613-621.	2.8	23
96	Targeting the conformational transitions of MDM2 and MDMX: Insights into key residues affecting p53 recognition. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 77, 524-535.	2.6	12
97	Quantum mechanics/molecular mechanics (QM/MM) modeling of the irreversible transamination of l-kynurenine to kynurenic acid: The round dance of kynurenine aminotransferase II. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2009, 1794, 1802-1812.	2.3	10
98	Design, synthesis and biological evaluation of novel bicyclo[1.1.1]pentane-based D-tryptophan acidic amino acids as glutamate receptors ligands. <i>Bioorganic and Medicinal Chemistry</i> , 2009, 17, 242-250.	3.0	28
99	Bulky 1,4-benzoxazine derivatives with antifungal activity. <i>Bioorganic and Medicinal Chemistry</i> , 2009, 17, 3838-3846.	3.0	31
100	The effect of the copper(II) salt anion in the Chiral Ligand-Exchange Chromatography of amino acids. <i>Analytica Chimica Acta</i> , 2009, 638, 225-233.	5.4	29
101	Charting the Chemical Space of Target Sites: Insights into the Binding Modes of Amine and Amidine Groups. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 900-912.	5.4	12
102	Discovery of 6 β -Ethyl-23(S)-methylcholic Acid (S-EMCA, INT-777) as a Potent and Selective Agonist for the TGR5 Receptor, a Novel Target for Diabesity. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 7958-7961.	6.4	220
103	TGR5-Mediated Bile Acid Sensing Controls Glucose Homeostasis. <i>Cell Metabolism</i> , 2009, 10, 167-177.	16.2	1,465
104	MDM2/MDMX inhibitor peptide: WO2008106507. <i>Expert Opinion on Therapeutic Patents</i> , 2009, 19, 721-726.	5.0	12
105	Mapping Human Metabolic Pathways in the Small Molecule Chemical Space. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 2272-2289.	5.4	14
106	(S)-Trityl-L-cysteine, a powerful chiral selector for the analytical and preparative ligand-exchange chromatography of amino acids. <i>Journal of Separation Science</i> , 2008, 31, 696-704.	2.5	36
107	Descriptive structure-separation relationship studies in chiral ligand-exchange chromatography. <i>Journal of Separation Science</i> , 2008, 31, 2395-2403.	2.5	14
108	Sequence Variants in Kynurenine Aminotransferase II (KAT II) Orthologs Determine Different Potencies of the Inhibitor S-ESBA. <i>ChemMedChem</i> , 2008, 3, 1199-1202.	3.2	28

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109	Cysteine-based chiral selectors for the ligand-exchange separation of amino acids†. <i>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences</i> , 2008, 875, 108-117.	2.3	25
110	Novel Potent and Selective Bile Acid Derivatives as TGR5 Agonists: Biological Screening, Structure-Activity Relationships, and Molecular Modeling Studies. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 1831-1841.	6.4	259
111	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. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 5650-5662.	6.4	38
112	Targeting the Conformational Transitions of MDM2 and MDMX: Insights into Dissimilarities and Similarities of p53 Recognition. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 1999-2009.	5.4	28
113	Molecular Field Analysis and 3D-Quantitative Structure-Activity Relationship Study (MFA 3D-QSAR) Unveil Novel Features of Bile Acid Recognition at TGR5. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 1792-1801.	5.4	23
114	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. <i>Journal of Medicinal Chemistry</i> , 2007, 50, 4265-4268.	6.4	97
115	Synthesis, Molecular Modeling Studies, and Preliminary Pharmacological Characterization of All Possible 2-(2-Sulfonocyclopropyl)glycine Stereoisomers as Conformationally Constrained L-Homocysteic Acid Analogs. <i>Journal of Medicinal Chemistry</i> , 2007, 50, 4630-4641.	6.4	17
116	Oxime and Oxime Ether Derivatives of 1,4-Benzothiazine Related to Oxiconazole. <i>ChemMedChem</i> , 2007, 2, 1208-1213.	3.2	13
117	(S)-(-)-1,1-Di(2-naphthyl)-2-pyrrolidinemethanol, a useful tool to study the recognition mechanism in chiral ligand-exchange chromatography. <i>Journal of Separation Science</i> , 2007, 30, 21-27.	2.5	16
118	Synthesis, docking studies and anti-inflammatory activity of 4,5,6,7-tetrahydro-2H-indazole derivatives. <i>Bioorganic and Medicinal Chemistry</i> , 2007, 15, 3463-3473.	3.0	63
119	Molecular docking and spatial coarse graining simulations as tools to investigate substrate recognition, enhancer binding and conformational transitions in indoleamine-2,3-dioxygenase (IDO). <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2007, 1774, 1058-1068.	2.3	31
120	Exploring the other side of biologically relevant chemical space: Insights into carboxylic, sulfonic and phosphonic acid bioisosteric relationships. <i>Journal of Molecular Graphics and Modelling</i> , 2007, 26, 728-739.	2.4	36
121	Glucocorticoid-induced leucine zipper (GILZ)/NF- κ B interaction: role of GILZ homo-dimerization and C-terminal domain. <i>Nucleic Acids Research</i> , 2006, 35, 517-528.	14.5	126
122	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). <i>Clinical Endocrinology</i> , 2006, 64, 105-109.	2.4	77
123	Biochemical and molecular characterization of the novel BRAFV599Ins mutation detected in a classic papillary thyroid carcinoma. <i>Oncogene</i> , 2006, 25, 4235-4240.	5.9	56
124	Novel ketoconazole analogues based on the replacement of 2,4-dichlorophenyl group with 1,4-benzothiazine moiety: Design, synthesis, and microbiological evaluation. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 5196-5203.	3.0	23
125	Unveiling hidden features of orphan nuclear receptors: The case of the small heterodimer partner (SHP). <i>Journal of Molecular Graphics and Modelling</i> , 2006, 24, 362-372.	2.4	25
126	Pharmacophore model for bile acids recognition by the FPR receptor. <i>Journal of Computer-Aided Molecular Design</i> , 2006, 20, 295-303.	2.9	29

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127	Dynamic ligand-exchange chiral stationary phase from S-benzyl-(R)-cysteine. <i>Chirality</i> , 2006, 18, 509-518.	2.6	31
128	Synthesis and Preliminary Biological Evaluation of 2-Substituted 2-(3-Carboxybicyclo[1.1.1]pentyl)glycine Derivatives as Group I Selective Metabotropic Glutamate Receptor Ligands. <i>ChemMedChem</i> , 2006, 1, 358-365.	3.2	24
129	Docking studies on PARP-1 inhibitors: insights into the role of a binding pocket water molecule. <i>Bioorganic and Medicinal Chemistry</i> , 2005, 13, 1151-1157.	3.0	54
130	Design, Synthesis, and Microbiological Evaluation of New <i>Candida albicans</i> CYP51 Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 7658-7666.	6.4	51
131	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. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 3251-3259.	6.4	35
132	Is Antagonism of E/Z-Guggulsterone at the Farnesoid X Receptor Mediated by a Noncanonical Binding Site? A Molecular Modeling Study. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 6948-6955.	6.4	29
133	Ligand selectivity and competition between enzymes in silico. <i>Nature Biotechnology</i> , 2004, 22, 1039-1045.	17.5	80
134	QSAR Study of Anticonvulsant Negative Allosteric Modulators of the AMPA Receptor. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 1860-1863.	6.4	19
135	Towards New Neuroprotective Agents: Design and Synthesis of 4H-Thieno[2,3-c]isoquinolin-5-one Derivatives as Potent PARP-1 Inhibitors. <i>ChemInform</i> , 2004, 35, no.	0.0	1
136	Insights into Phenylalanine Derivatives Recognition of VLA-4 Integrin: From a Pharmacophoric Study to 3D-QSAR and Molecular Docking Analyses. <i>ChemInform</i> , 2004, 35, no.	0.0	0
137	Evaluation of the enantiomeric selectivity in the chiral ligand-exchange chromatography of amino acids by a computational model. <i>Journal of Chromatography A</i> , 2004, 1033, 363-367.	3.7	16
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