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	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
2	Biological Evaluation of New Thienopyridinium and Thienopyrimidinium Derivatives as Human Choline Kinase Inhibitors. Pharmaceutics, 2022, 14, 715.	2.0	2
3	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
4	The Stone Guest: How Does pH Affect Binding Properties of PDâ€1/PDâ€L1 Inhibitors?. ChemMedChem, 2021, 16, 568-577.	1.6	9
5	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
6	3-hydroxy-L-kynurenamine is an immunomodulatory biogenic amine. Nature Communications, 2021, 12, 4447.	5.8	30
7	One Key and Multiple Locks: Substrate Binding in Structures of Tryptophan Dioxygenases and Hydroxylases. ChemMedChem, 2021, 16, 2732-2743.	1.6	3
8	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
9	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
10	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
11	Laboratory-Scale Semipreparative Enantioresolution of Phenylethanolic-Azole Heme Oxygenase-1 Inhibitors. Chromatographia, 2020, 83, 1509-1515.	0.7	2
12	Synthesis, biological evaluation, in silico modeling and crystallization of novel small monocationic molecules with potent antiproliferative activity by dual mechanism. European Journal of Medicinal Chemistry, 2020, 207, 112797.	2.6	4
13	Fragment based drug design and diversity-oriented synthesis of carboxylic acid isosteres. Bioorganic and Medicinal Chemistry, 2020, 28, 115731.	1.4	7
14	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
15	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
16	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
17	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
18	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

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19	Enantioselective HPLC Analysis to Assist the Chemical Exploration of Chiral Imidazolines. Molecules, 2020, 25, 640.	1.7	8
20	Class IA PI3Ks regulate subcellular and functional dynamics of IDO1. EMBO Reports, 2020, 21, e49756.	2.0	24
21	Preclinical discovery and development of fingolimod for the treatment of multiple sclerosis. Expert Opinion on Drug Discovery, 2019, 14, 1199-1212.	2.5	25
22	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
23	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
24	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
25	Opportunities and challenges in drug discovery targeting metabotropic glutamate receptor 4. Expert Opinion on Drug Discovery, 2018, 13, 411-423.	2.5	6
26	Binding Mode and Structureâ€“Activity Relationships of ITE as an Aryl Hydrocarbon Receptor (AhR) Agonist. ChemMedChem, 2018, 13, 270-279.	1.6	20
27	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
28	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
29	Microscale Thermophoresis and Docking Studies Suggest Lapachol and Auraptene are Ligands of IDO1. Natural Product Communications, 2018, 13, 1934578X1801300.	0.2	0
30	Lead optimization-hit expansion of new asymmetrical pyridinium/quinolinium compounds as choline kinase Î±1 inhibitors. Future Medicinal Chemistry, 2018, 10, 1769-1786.	1.1	4
31	Elucidation of the Chromatographic Enantiomer Elution Order Through Computational Studies. Mini-Reviews in Medicinal Chemistry, 2018, 18, 88-97.	1.1	10
32	A Relay Pathway between Arginine and Tryptophan Metabolism Confers Immunosuppressive Properties on Dendritic Cells. Immunity, 2017, 46, 233-244.	6.6	241
33	Advances in indoleamine 2,3-dioxygenase 1 medicinal chemistry. MedChemComm, 2017, 8, 1378-1392.	3.5	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. Journal of Biological Chemistry, 2017, 292, 1785-1797.	1.6	17
35	Fragment-based approach to identify IDO1 inhibitor building blocks. European Journal of Medicinal Chemistry, 2017, 141, 169-177.	2.6	17
36	Targeting Wnt-driven cancers: Discovery of novel tankyrase inhibitors. European Journal of Medicinal Chemistry, 2017, 142, 506-522.	2.6	47

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37	Immunotherapyâ€¦ a pursuit race to tomorrow's medicines. Future Medicinal Chemistry, 2017, 9, 1297-1299.	1.1	3
38	Binding properties of different categories of IDO1 inhibitors: a microscale thermophoresis study. Future Medicinal Chemistry, 2017, 9, 1327-1338.	1.1	8
39	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
40	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
41	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
42	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
43	Docking Studies and Molecular Dynamic Simulations Reveal Different Features of IDO1 Structure. Molecular Informatics, 2016, 35, 449-459.	1.4	11
44	Computational modelling of the binding of arachidonic acid to the human monooxygenase CYP2J2. Journal of Molecular Modeling, 2016, 22, 279.	0.8	10
45	Concepts and Molecular Aspects in the Polypharmacology of PARPâ€1 Inhibitors. ChemMedChem, 2016, 11, 1219-1226.	1.6	27
46	Integrating multicomponent flow synthesis and computational approaches for the generation of a tetrahydroquinoline compound based library. MedChemComm, 2016, 7, 439-446.	3.5	24
47	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
48	The Janus-faced nature of IDO1 in infectious diseases: challenges and therapeutic opportunities. Future Medicinal Chemistry, 2016, 8, 39-54.	1.1	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?. Molecular Biology of the Cell, 2015, 26, 2418-2425.	0.9	32
51	Pharmacophoreâ€Based Virtual Screening to Discover New Active Compounds for Human Choline Kinase Î±1. Molecular Informatics, 2015, 34, 458-466.	1.4	8
52	Targeting the MDM2/MDM4 Interaction Interface as a Promising Approach for p53 Reactivation Therapy. Cancer Research, 2015, 75, 4560-4572.	0.4	38
53	Choline Kinase Active Site Provides Features for Designing Versatile Inhibitors. Current Topics in Medicinal Chemistry, 2015, 14, 2684-2693.	1.0	11
54	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

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55	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
56	AhR-Mediated, Non-Genomic Modulation of IDO1 Function. Frontiers in Immunology, 2014, 5, 497.	2.2	37
57	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
58	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
59	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
60	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
61	Scaffold hopping approach on the route to selective tankyrase inhibitors. European Journal of Medicinal Chemistry, 2014, 87, 611-623.	2.6	20
62	Targeting glucocorticoid side effects: selective glucocorticoid receptor modulator or glucocorticoidâ€induced leucine zipper? A perspective. FASEB Journal, 2014, 28, 5055-5070.	0.2	68
63	Aryl hydrocarbon receptor control of a disease tolerance defence pathway. Nature, 2014, 511, 184-190.	13.7	574
64	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
65	<scp>PARP</scp> inhibitors: polypharmacology versus selective inhibition. FEBS Journal, 2013, 280, 3563-3575.	2.2	70
66	Navigations of chemical space to further the understanding of polypharmacology in human nuclear receptors. MedChemComm, 2013, 4, 216-227.	3.5	0
67	Exploring the effect of PARP-1 flexibility in docking studies. Journal of Molecular Graphics and Modelling, 2013, 45, 192-201.	1.3	16
68	Probing the Binding Site of Bile Acids in TGR5. ACS Medicinal Chemistry Letters, 2013, 4, 1158-1162.	1.3	36
69	Synthesis and Quantitative Structure-Property Relationships of Side Chain-Modified Hyodeoxycholic Acid Derivatives. Molecules, 2013, 18, 10497-10513.	1.7	6
70	From Polypharmacology to Target Specificity: The Case of PARP Inhibitors. Current Topics in Medicinal Chemistry, 2013, 13, 2939-2954.	1.0	32
71	Family-wide chemical profiling and structural analysis of PARP and tankyrase inhibitors. Nature Biotechnology, 2012, 30, 283-288.	9.4	410
72	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

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73	Patented TGR5 modulators: a review (2006 â€“ present). Expert Opinion on Therapeutic Patents, 2012, 22, 1399-1414.	2.4	43
74	Chapter 10. TGR5 Agonists in Development. RSC Drug Discovery Series, 2012, , 270-305.	0.2	1
75	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
76	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
77	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
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.	1.4	37
79	Identification by Virtual Screening and In Vitro Testing of Human DOPA Decarboxylase Inhibitors. PLoS ONE, 2012, 7, e31610.	1.1	56
80	Expanding the horizon of chemotherapeutic targets: From MDM2 to MDMX (MDM4). MedChemComm, 2011, 2, 455.	3.5	15
81	Discovery and characterization of novel potent PARP-1 inhibitors endowed with neuroprotective properties: From TIQ-A to HYDAMTIQ. MedChemComm, 2011, 2, 559.	3.5	17
82	Protective Effects of Commiphora erythraea Resin Constituents Against Cellular Oxidative Damage. Molecules, 2011, 16, 10357-10369.	1.7	13
83	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
84	Divergent and stereoselective synthesis of dafachronic acids. Tetrahedron, 2011, 67, 1924-1929.	1.0	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.	2.4	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.	1.9	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.	1.3	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.	1.8	17
89	Novel Polymorphisms of Nuclear Receptor SHP Associated with Functional and Structural Changes. Journal of Biological Chemistry, 2010, 285, 24871-24881.	1.6	40
90	Puzzling over MDM4â€“p53 network. International Journal of Biochemistry and Cell Biology, 2010, 42, 1080-1083.	1.2	26

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91	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
92	Poly(ADP-ribose) Catabolism Triggers AMP-dependent Mitochondrial Energy Failure. Journal of Biological Chemistry, 2009, 284, 17668-17676.	1.6	80
93	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
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. Amino Acids, 2009, 37, 219-229.	1.2	114
95	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
96	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
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. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2009, 1794, 1802-1812.	1.1	10
98	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
99	Bulky 1,4-benzoxazine derivatives with antifungal activity. Bioorganic and Medicinal Chemistry, 2009, 17, 3838-3846.	1.4	31
100	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
101	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
102	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
103	TGR5-Mediated Bile Acid Sensing Controls Glucose Homeostasis. Cell Metabolism, 2009, 10, 167-177.	7.2	1,465
104	MDM2/MDMX inhibitor peptide: WO2008106507. Expert Opinion on Therapeutic Patents, 2009, 19, 721-726.	2.4	12
105	Mapping Human Metabolic Pathways in the Small Molecule Chemical Space. Journal of Chemical Information and Modeling, 2009, 49, 2272-2289.	2.5	14
106	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
107	Descriptive structureâ€“separation relationship studies in chiral ligandâ€exchange chromatography. Journal of Separation Science, 2008, 31, 2395-2403.	1.3	14
108	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

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109	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
110	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
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. Journal of Medicinal Chemistry, 2008, 51, 5659-5662.	2.9	38
112	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
113	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
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. Journal of Medicinal Chemistry, 2007, 50, 4265-4268.	2.9	97
115	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
116	Oxime and Oxime Ether Derivatives of 1,4-Benzothiazine Related to Oxiconazole. ChemMedChem, 2007, 2, 1208-1213.	1.6	13
117	(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
118	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
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). Biochimica Et Biophysica Acta - Proteins and Proteomics, 2007, 1774, 1058-1068.	1.1	31
120	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
121	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
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). Clinical Endocrinology, 2006, 64, 105-109.	1.2	77
123	Biochemical and molecular characterization of the novel BRAFV599Ins mutation detected in a classic papillary thyroid carcinoma. Oncogene, 2006, 25, 4235-4240.	2.6	56
124	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
125	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
126	Pharmacophore model for bile acids recognition by the FPR receptor. Journal of Computer-Aided Molecular Design, 2006, 20, 295-303.	1.3	29

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127	Dynamic ligand-exchange chiral stationary phase from S-benzyl-(R)-cysteine. Chirality, 2006, 18, 509-518.	1.3	31
128	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
129	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
130	Design, Synthesis, and Microbiological Evaluation of NewCandida albicansCYP51 Inhibitors. Journal of Medicinal Chemistry, 2005, 48, 7658-7666.	2.9	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. Journal of Medicinal Chemistry, 2005, 48, 3251-3259.	2.9	35
132	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
133	Ligand selectivity and competition between enzymes in silico. Nature Biotechnology, 2004, 22, 1039-1045.	9.4	80
134	QSAR Study of Anticonvulsant Negative Allosteric Modulators of the AMPA Receptor. Journal of Medicinal Chemistry, 2004, 47, 1860-1863.	2.9	19
135	Towards New Neuroprotective Agents: Design and Synthesis of 4H-Thieno[2,3-c]isoquinolin-5-one Derivatives as Potent PARP-1 Inhibitors.. ChemInform, 2004, 35, no.	0.1	1
136	Insights into Phenylalanine Derivatives Recognition of VLA-4 Integrin: From a Pharmacophoric Study to 3D-QSAR and Molecular Docking Analyses.. ChemInform, 2004, 35, no.	0.1	0
137	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
138	Homology model of the multidrug transporter LmrA from Lactococcus lactis. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 5823-5826.	1.0	16
139	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
140	Binding modes of noncompetitive AMPA antagonists: a computational approach. Il Farmaco, 2003, 58, 107-113.	0.9	12
141	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
142	Rat brain guanosine binding site. Bioorganic and Medicinal Chemistry, 2003, 11, 5417-5425.	1.4	61
143	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
144	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

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145	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
146	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
147	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
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