Gabriele Cruciani

List of Publications by Year
in descending order

239 papers	11,552 citations	32410 55 h-index	40945 97 g-index
269 all docs	269 docs citations	269 times ranked	12029 citing authors

#	Article	IF	Citations
1	<scp>Endoplasmic reticulum</scp> stress and <scp>NFâ€kB</scp> activation in <scp>SARSâ€CoV</scp>â€2 infected cells and their response to antiviral therapy. IUBMB Life, 2022, 74, 93-100.	1.5	26
2	Role of cardiolipins, mitochondria, and autophagy in the differentiation process activated by all-trans retinoic acid in acute promyelocytic leukemia. Cell Death and Disease, 2022, 13, 30.	2.7	3
3	Pharmacophore-Based Discovery of Substrates of a Novel Drug/Proton-Antiporter in the Human Brain Endothelial hCMEC/D3 Cell Line. Pharmaceutics, 2022, 14, 255.	2.0	6
4	FragExplorer: GRID-Based Fragment Growing and Replacement. Journal of Chemical Information and Modeling, 2022, 62, 1224-1235.	2.5	4
5	Lipid metabolism analysis in liver of different chicken genotypes and impact on nutritionally relevant polyunsaturated fatty acids of meat. Scientific Reports, 2022, 12, 1888.	1.6	19
6	Getting Insights into Structural and Energetic Properties of Reciprocal Peptideâ€“Protein Interactions. Journal of Chemical Information and Modeling, 2022, 62, 1113-1125.	2.5	8
7	Mapping the Lipids of Skin Sebaceous Glands and Hair Follicles by High Spatial Resolution MALDI Imaging Mass Spectrometry. Pharmaceuticals, 2022, 15, 411.	1.7	3
8	Resistance to PI3KÎ´ inhibitors in marginal zone lymphoma can be reverted by targeting the IL-6/PDGFRA axis. Haematologica, 2022, 107, 2685-2697.	1.7	10
9	Melatonin modulates Nrf2 activity to protect porcine preâ€pubertal Sertoli cells from the abnormal H₂O₂ generation and reductive stress effects of cadmium. Journal of Pineal Research, 2022, 73, .	3.4	18
10	Discovery of novel SARS-CoV-2 inhibitors targeting the main protease Mpro by virtual screenings and hit optimization. Antiviral Research, 2022, 204, 105350.	1.9	11
11	Evidence of two metamorphic cycles preserved in garnet from felsic granulite in the southern Variscan belt of Corsica, France. Lithos, 2021, 380-381, 105919.	0.6	6
12	Effects of MTX-23, a Novel PROTAC of Androgen Receptor Splice Variant-7 and Androgen Receptor, on CRPC Resistant to Second-Line Antiandrogen Therapy. Molecular Cancer Therapeutics, 2021, 20, 490-499.	1.9	55
13	Targeting Nsp9 as an anti-SARS-CoV-2 strategy. New Journal of Chemistry, 2021, 45, 522-525.	1.4	9
14	Binding of Androgen- and Estrogen-Like Flavonoids to Their Cognate (Non)Nuclear Receptors: A Comparison by Computational Prediction. Molecules, 2021, 26, 1613.	1.7	20
15	SARS-CoV-2 Survival on Surfaces and the Effect of UV-C Light. Viruses, 2021, 13, 408.	1.5	77
16	Enhanced triacylglycerol catabolism by carboxylesterase 1 promotes aggressive colorectal carcinoma. Journal of Clinical Investigation, 2021, 131, .	3.9	25
17	Metamorphic evolution and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>P</mml:mi></mml:math>â€“<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>T</mml:mi></mml:math> path of the Posada Valley amphibolites: new insights on the Variscan high pressure metamorphism in NE Sardinia, Italy. Comptes Rendus - Geoscience, 2021, 353, 227-246.	0.4	2
18	Combining machine learning and quantum mechanics yields more <scp>chemically aware</scp> molecular descriptors for medicinal chemistry applications. Journal of Computational Chemistry, 2021, 42, 2068-2078.	1.5	6

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19	SARS-CoV2 infection impairs the metabolism and redox function of cellular glutathione. Redox Biology, 2021, 45, 102041.	3.9	58
20	Indomethacin-based PROTACs as pan-coronavirus antiviral agents. European Journal of Medicinal Chemistry, 2021, 226, 113814.	2.6	46
21	Effect of a UV-C Automatic Last-Generation Mobile Robotic System on Multi-Drug Resistant Pathogens. International Journal of Environmental Research and Public Health, 2021, 18, 13019.	1.2	4
22	Vitamin E: metabolism and molecular aspects. , 2020, , 487-518.		5
23	A novel small-molecule inhibitor of the human papillomavirus E6-p53 interaction that reactivates p53 function and blocks cancer cells growth. Cancer Letters, 2020, 470, 115-125.	3.2	39
24	A Novel Lipidomics-Based Approach to Evaluating the Risk of Clinical Hepatotoxicity Potential of Drugs in 3D Human Microtissues. Chemical Research in Toxicology, 2020, 33, 258-270.	1.7	10
25	LipostarMSI: Comprehensive, Vendor-Neutral Software for Visualization, Data Analysis, and Automated Molecular Identification in Mass Spectrometry Imaging. Journal of the American Society for Mass Spectrometry, 2020, 31, 155-163.	1.2	57
26	Understanding the Metabolism of Proteolysis Targeting Chimeras (PROTACs): The Next Step toward Pharmaceutical Applications. Journal of Medicinal Chemistry, 2020, 63, 11615-11638.	2.9	69
27	Garnet-Rich Veins in an Ultrabasic Amphibolite from NE Sardinia, Italy: An Example of Vein Mineralogical Re-Equilibration during the Exhumation of a Granulite Terrane. Geosciences (Switzerland), 2020, 10, 344.	1.0	4
28	Virtual screening identifies broad-spectrum Î²-lactamase inhibitors with activity on clinically relevant serine- and metallo-carbapenemases. Scientific Reports, 2020, 10, 12763.	1.6	25
29	A liquid chromatography-high resolution mass spectrometry method for the determination of thirty-three per- and polyfluoroalkyl substances in animal liver. Journal of Chromatography A, 2020, 1628, 461442.	1.8	17
30	Geology of the Montigiu Nieddu metamorphic basement, NE Sardinia (Italy). Journal of Maps, 2020, 16, 543-551.	1.0	3
31	Use of Phenotypically Poor Metabolizer Individual Donor Human Liver Microsomes To Identify Selective Substrates of UGT2B10. Drug Metabolism and Disposition, 2020, 48, 176-186.	1.7	6
32	Synthetic Peptide Libraries: From Random Mixtures to In Vivo Testing. Current Medicinal Chemistry, 2020, 27, 997-1016.	1.2	9
33	Bisphenol A binding promiscuity: A virtual journey through the universe of proteins. ALTEX: Alternatives To Animal Experimentation, 2020, 37, 85-94.	0.9	3
34	Non animal methodologies (NAMs): Research, testing, assessment and applications â€“ ecopa Symposium 2019. ALTEX: Alternatives To Animal Experimentation, 2020, 37, 317-320.	0.9	0
35	Subspace discriminant index to expedite exploration of multi-class omics data. Chemometrics and Intelligent Laboratory Systems, 2020, 206, 104160.	1.8	3
36	How computational chemistry develops: a tribute to Peter Goodford. Journal of Computer-Aided Molecular Design, 2019, 33, 699-703.	1.3	0

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37	Role of mitochondria and cardiolipins in growth inhibition of breast cancer cells by retinoic acid. Journal of Experimental and Clinical Cancer Research, 2019, 38, 436.	3.5	11
38	Redox lipidomics and adductomics - Advanced analytical strategies to study oxidized lipids and lipid-protein adducts. Free Radical Biology and Medicine, 2019, 144, 1-5.	1.3	9
39	A computational study toward the â€œpersonalizedâ€•activity of alternariol â€“ Does it matter for safe food at individual level?. Food and Chemical Toxicology, 2019, 130, 199-206.	1.8	10
40	A comparative study of the antimicrobial and antioxidant activities of Inonotus hispidus fruit and their mycelia extracts. International Journal of Food Properties, 2019, 22, 768-783.	1.3	34
41	Interaction of Mycotoxin Alternariol with Serum Albumin. International Journal of Molecular Sciences, 2019, 20, 2352.	1.8	39
42	Computational solutions in redox lipidomics â€“ Current strategies and future perspectives. Free Radical Biology and Medicine, 2019, 144, 110-123.	1.3	36
43	Nutritional and lipidomics biomarkers of docosahexaenoic acid-based multivitamin therapy in pediatric NASH. Scientific Reports, 2019, 9, 2045.	1.6	51
44	Discovering New Casein Kinase 1d Inhibitors with an Innovative Molecular Dynamics Enabled Virtual Screening Workflow. ACS Medicinal Chemistry Letters, 2019, 10, 487-492.	1.3	10
45	Garnet zoning in kyaniteâ€bearing eclogite from Golfo Aranci: New data on the early prograde Pâ€“T evolution in NE Sardinia, Italy. Geological Journal, 2019, 54, 190-205.	0.6	8
46	Abstract A127: Secretion of IL16 is associated with resistance to ibrutinib in pre-clinical models of lymphoma. , 2019, , .		3
47	Secreted Factors Determine Resistance to Idelalisib in Marginal Zone Lymphoma Models of Resistance. Blood, 2019, 134, 2569-2569.	0.6	3
48	Anticlockwise pressureâ€“temperature paths record Variscan upperâ€plate exhumation: Example from micaschists of the Porto Vecchio region, Corsica. Journal of Metamorphic Geology, 2018, 36, 55-77.	1.6	38
49	Metavolcanics from Capo Malfatano, SW Sardinia, Italy: New insight on the age and nature of Ordovician volcanism in the Variscan foreland zone. Geological Journal, 2018, 53, 1573-1585.	0.6	10
50	From Experiments to a Fast Easy-to-Use Computational Methodology to Predict Human Aldehyde Oxidase Selectivity and Metabolic Reactions. Journal of Medicinal Chemistry, 2018, 61, 360-371.	2.9	29
51	Quantitative structureâ€property relationship modeling of small organic molecules for solar cells applications. Journal of Chemometrics, 2018, 32, e2957.	0.7	5
52	On the Mechanism of Action of Anti-Inflammatory Activity of Hypericin: An In Silico Study Pointing to the Relevance of Janus Kinases Inhibition. Molecules, 2018, 23, 3058.	1.7	20
53	Physical Activity Modulates the Overexpression of the Inflammatory miRâ€146aâ€5p in Obese Patients. IUBMB Life, 2018, 70, 1012-1022.	1.5	26
54	Delving into the Polar Lipidome by Optimized Chromatographic Separation, High-Resolution Mass Spectrometry, and Comprehensive Identification with Lipostar: Microalgae as Case Study. Analytical Chemistry, 2018, 90, 12230-12238.	3.2	17

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55	Vitamin E metabolism and its putative role as fat-soluble antioxidant in the redox-lipidomics era. Free Radical Biology and Medicine, 2018, 120, S128.	1.3	0
56	Electrostatic recognition in substrate binding to serine proteases. Journal of Molecular Recognition, 2018, 31, e2727.	1.1	13
57	Overview of the Biological Activities of a Methanol Extract from Wild Red Belt Conk, Fomitopsis pinicola (Agaricomycetes), Fruiting Bodies from Central Italy. International Journal of Medicinal Mushrooms, 2018, 20, 1047-1063.	0.9	8
58	Determination of tocopherols and their metabolites by liquid-chromatography coupled with tandem mass spectrometry in human plasma and serum. Talanta, 2017, 170, 552-561.	2.9	38
59	Lipostar, a Comprehensive Platform-Neutral Cheminformatics Tool for Lipidomics. Analytical Chemistry, 2017, 89, 6257-6264.	3.2	76
60	Improved Potency of Indole-Based NorA Efflux Pump Inhibitors: From Serendipity toward Rational Design and Development. Journal of Medicinal Chemistry, 2017, 60, 517-523.	2.9	33
61	Use of the Distribution Coefficient in Brain Polar Lipids for the Assessment of Drug-Induced Phospholipidosis Risk. Chemical Research in Toxicology, 2017, 30, 1145-1156.	1.7	7
62	Structureâ€“metabolism relationships in human- AOX: Chemical insights from a large database of aza-aromatic and amide compounds. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E3178-E3187.	3.3	51
63	Side-Chain Modified Ergosterol and Stigmasterol Derivatives as Liver X Receptor Agonists. Journal of Medicinal Chemistry, 2017, 60, 6548-6562.	2.9	21
64	ADME-Space: a new tool for medicinal chemists to explore ADME properties. Scientific Reports, 2017, 7, 6359.	1.6	58
65	Vitamin E: Emerging aspects and new directions. Free Radical Biology and Medicine, 2017, 102, 16-36.	1.3	320
66	Computational and biological profile of boronic acids for the detection of bacterial serine- and metallo-Î²-lactamases. Scientific Reports, 2017, 7, 17716.	1.6	35
67	Detecting similar binding pockets to enable systems polypharmacology. PLoS Computational Biology, 2017, 13, e1005522.	1.5	35
68	Diagnostic application of lipidomics fingerprints to bladder carcinoma. Translational Cancer Research, 2017, 6, 1197-1206.	0.4	3
69	Sequence Protein Identification by Randomized Sequence Database and Transcriptome Mass Spectrometry (SPIDER-TMS): From Manual to Automatic Application of a â€˜de Novo Sequencingâ€™ Approach. European Journal of Mass Spectrometry, 2016, 22, 193-198.	0.5	2
70	Multiclass method for the determination of 62 antibiotics in milk. Journal of Mass Spectrometry, 2016, 51, 792-804.	0.7	39
71	Comparing Drug Images and Repurposing Drugs with BioGPS and FLAPdock: The Thymidylate Synthase Case. ChemMedChem, 2016, 11, 1653-1666.	1.6	21
72	Metabolism study and biological evaluation of bosentan derivatives. European Journal of Medicinal Chemistry, 2016, 121, 658-670.	2.6	13

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73	Indole Based Weapons to Fight Antibiotic Resistance: A Structureâ€“Activity Relationship Study. Journal of Medicinal Chemistry, 2016, 59, 867-891.	2.9	64
74	Effects of different routes of application on ethylenediurea persistence in tobacco leaves. Environmental Pollution, 2016, 212, 559-564.	3.7	14
75	Analytical strategies to assess the functional metabolome of vitamin E. Journal of Pharmaceutical and Biomedical Analysis, 2016, 124, 399-412.	1.4	38
76	Cyto- and enzyme toxicities of ionic liquids modelled on the basis of VolSurf+ descriptors and their principal properties. SAR and QSAR in Environmental Research, 2016, 27, 221-244.	1.0	19
77	Screening and confirmatory method for multiclass determination of 62 antibiotics in meat. Journal of Chromatography A, 2016, 1429, 175-188.	1.8	43
78	Decoding the Structural Basis For Carbapenem Hydrolysis By Class A Î²-lactamases: Fishing For A Pharmacophore. Current Drug Targets, 2016, 17, 983-1005.	1.0	27
79	Pharmacophoreâ€based discovery of inhibitors of a novel drug/proton antiporter in human brain endothelial hCMEC/D3 cell line. British Journal of Pharmacology, 2015, 172, 4888-4904.	2.7	28
80	Discovery of Novel, Potent, and Specific Cellâ€Death Inducers in the Jurkat Acute Lymphoblastic Leukemia Cell Line. ChemMedChem, 2015, 10, 1700-1706.	1.6	0
81	BioGPS: Navigating biological space to predict polypharmacology, off-targeting, and selectivity. Proteins: Structure, Function and Bioinformatics, 2015, 83, 517-532.	1.5	68
82	Quantitative structureâ€“property relationship modeling of ruthenium sensitizers for solar cells applications: novel tools for designing promising candidates. RSC Advances, 2015, 5, 23865-23873.	1.7	14
83	Re-equilibration history and Pâ€“T path of eclogites from Variscan Sardinia, Italy: a case study from the medium-grade metamorphic complex. International Journal of Earth Sciences, 2015, 104, 797-814.	0.9	22
84	Molecular modelling approach to evaluate poisoning of topoisomerase I by alternariol derivatives. Food Chemistry, 2015, 189, 93-101.	4.2	25
85	A Broad Anti-influenza Hybrid Small Molecule That Potently Disrupts the Interaction of Polymerase Acidic Proteinâ€“Basic Protein 1 (PA-PB1) Subunits. Journal of Medicinal Chemistry, 2015, 58, 3830-3842.	2.9	81
86	A Pipeline To Enhance Ligand Virtual Screening: Integrating Molecular Dynamics and Fingerprints for Ligand and Proteins. Journal of Chemical Information and Modeling, 2015, 55, 2256-2274.	2.5	65
87	Expanding the chemical space of human serine racemase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 4297-4303.	1.0	22
88	Nature and age of pre-Variscan eclogite protoliths from the Low- to Medium-Grade Metamorphic Complex of northâ€“central Sardinia (Italy) and comparisons with coeval Sardinian eclogites in the northern Gondwana context. Journal of the Geological Society, 2015, 172, 792-807.	0.9	16
89	Zn-Al-rich chlorite in interleaved phyllosilicate grains from the low-temperature metamorphic Ordovician terrane of Iglesiente, south-west Sardinia, Italy. Mineralogy and Petrology, 2015, 109, 713-718.	0.4	1
90	BioGPS Descriptors for Rational Engineering of Enzyme Promiscuity and Structure Based Bioinformatic Analysis. PLoS ONE, 2014, 9, e109354.	1.1	18

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91	Some considerations on the predictions of pharmacokinetic alterations in subjects with liver disease. Expert Opinion on Drug Metabolism and Toxicology, 2014, 10, 1397-1408.	1.5	15
92	Metabolism of JWH-015, JWH-098, JWH-251, and JWH-307 in silico and in vitro: a pilot study for the detection of unknown synthetic cannabinoids metabolites. Analytical and Bioanalytical Chemistry, 2014, 406, 3621-3636.	1.9	29
93	BioGPS: The Music for the Chemoâ€•and Bioinformatics Walzer. Molecular Informatics, 2014, 33, 446-453.	1.4	11
94	LC/MS lipid profiling from human serum: a new method for global lipid extraction. Analytical and Bioanalytical Chemistry, 2014, 406, 7937-7948.	1.9	115
95	Optimization of Small-Molecule Inhibitors of Influenza Virus Polymerase: From Thiophene-3-Carboxamide to Polyamido Scaffolds. Journal of Medicinal Chemistry, 2014, 57, 4337-4350.	2.9	59
96	Flavin Monooxygenase Metabolism: Why Medicinal Chemists Should Matter. Journal of Medicinal Chemistry, 2014, 57, 6183-6196.	2.9	39
97	Anatectic amphibole and restitic garnet in Variscan migmatite from NE Sardinia, Italy: insights into partial melting from mineral trace elements. European Journal of Mineralogy, 2014, 26, 381-395.	0.4	20
98	Targeting Cystalysin, a Virulence Factor of Treponema denticolaâ€Supported Periodontitis. ChemMedChem, 2014, 9, 1501-1511.	1.6	26
99	Long-chain metabolites of Î±-tocopherol occur in human serum and inhibit macrophage foam cell formation in vitro. Free Radical Biology and Medicine, 2014, 68, 43-51.	1.3	54
100	Geothermobarometry on anatectic melts â€“ a high-pressure Variscan migmatite from northeast Sardinia. International Geology Review, 2013, 55, 1490-1505.	1.1	24
101	Structural Investigation of Cycloheptathiophene-3-carboxamide Derivatives Targeting Influenza Virus Polymerase Assembly. Journal of Medicinal Chemistry, 2013, 56, 10118-10131.	2.9	51
102	Metabolites: structure determination and prediction. Drug Discovery Today: Technologies, 2013, 10, e145-e146.	4.0	5
103	Exposition and reactivity optimization to predict sites of metabolism in chemicals. Drug Discovery Today: Technologies, 2013, 10, e155-e165.	4.0	40
104	Pressureâ€“temperature and deformational evolution of high-pressure metapelites from Variscan NE Sardinia, Italy. Lithos, 2013, 175-176, 272-284.	0.6	37
105	Molecular interaction fields in drug discovery: recent advances and future perspectives. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 594-613.	6.2	36
106	Modeling Phospholipidosis Induction: Reliability and Warnings. Journal of Chemical Information and Modeling, 2013, 53, 1436-1446.	2.5	46
107	Isozyme-Specific Ligands for O-acetylserine sulfhydrylase, a Novel Antibiotic Target. PLoS ONE, 2013, 8, e77558.	1.1	43
108	Disrupting Proteinâ€“Protein Interfaces Using GRID Molecular Interaction Fields. , 2013, , 61-82.		1

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109	Inhibitor of Ovarian Cancer Cells Growth by Virtual Screening: A New Thiazole Derivative Targeting Human Thymidylate Synthase. Journal of Medicinal Chemistry, 2012, 55, 10272-10276.	2.9	20
110	Human Cytomegalovirus Inhibitor AL18 Also Possesses Activity against Influenza A and B Viruses. Antimicrobial Agents and Chemotherapy, 2012, 56, 6009-6013.	1.4	38
111	Absolute configuration and biological profile of two thiazinooxadiazol-3-ones with L-type calcium channel activity: a study of the structural effects. Organic and Biomolecular Chemistry, 2012, 10, 8994.	1.5	9
112	1,4-Dihydropyridine Scaffold in Medicinal Chemistry, The Story So Far And Perspectives (Part 2): Action in Other Targets and Antitargets. Current Medicinal Chemistry, 2012, 19, 4306-4323.	1.2	104
113	Ligand Promiscuity between the Efflux Pumps Human P-Glycoprotein and S. aureus NorA. ACS Medicinal Chemistry Letters, 2012, 3, 248-251.	1.3	20
114	GRID-Based Three-Dimensional Pharmacophores II: PharmBench, a Benchmark Data Set for Evaluating Pharmacophore Elucidation Methods. Journal of Chemical Information and Modeling, 2012, 52, 2599-2608.	2.5	36
115	Early stage evolution of the mafic-ultramafic belt at La Melada, Sierra de San Luis, Argentina: Pâ€“T constraints from metapyroxenite pseudosection modelling. Journal of South American Earth Sciences, 2012, 37, 1-12.	0.6	7
116	GRID-Based Three-Dimensional Pharmacophores I: FLAPpharm, a Novel Approach for Pharmacophore Elucidation. Journal of Chemical Information and Modeling, 2012, 52, 2587-2598.	2.5	76
117	BDDCS Class Prediction for New Molecular Entities. Molecular Pharmaceutics, 2012, 9, 570-580.	2.3	78
118	Small molecule inhibitors of influenza A and B viruses that act by disrupting subunit interactions of the viral polymerase. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 6247-6252.	3.3	114
119	Improving the prediction of the brain disposition for orally administered drugs using BDDCS. Advanced Drug Delivery Reviews, 2012, 64, 95-109.	6.6	65
120	Discovery of Novel Inhibitors of the NorA Multidrug Transporter of Staphylococcus aureus. Journal of Medicinal Chemistry, 2011, 54, 354-365.	2.9	67
121	1,4-Dihydropyridine Scaffold in Medicinal Chemistry, The Story so Far And Perspectives (Part 1): Action in Ion Channels and GPCRs. Current Medicinal Chemistry, 2011, 18, 4901-4922.	1.2	86
122	Pâ€“T evolution of eclogite-facies metabasite from NE Sardinia, Italy: Insights into the prograde evolution of Variscan eclogites. Lithos, 2011, 121, 135-150.	0.6	33
123	A Novel Approach for Predicting P-Glycoprotein (ABCB1) Inhibition Using Molecular Interaction Fields. Journal of Medicinal Chemistry, 2011, 54, 1740-1751.	2.9	141
124	Mineral re-equilibration and P-T path of metagabbros, Sierra de San Luis, Argentina: insights into the exhumation of a mafic-ultramafic belt. European Journal of Mineralogy, 2011, 23, 590-607.	0.4	5
125	Computational approaches to identifying and characterizing protein binding sites for ligand design. Journal of Molecular Recognition, 2010, 23, 209-219.	1.1	172
126	Molecular fields in drug discovery: getting old or reaching maturity?. Drug Discovery Today, 2010, 15, 23-32.	3.2	67

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127	Transporterâ€Mediated Efflux Influences CNS Side Effects: ABCB1, from Antitarget to Target. Molecular Informatics, 2010, 29, 16-26.	1.4	35
128	Ligand-based virtual screening and ADME-tox guided approach to identify triazolo-quinoxalines as folate cycle inhibitors. Bioorganic and Medicinal Chemistry, 2010, 18, 7773-7785.	1.4	20
129	Extending pKa prediction accuracy: High-throughput pKa measurements to understand pKa modulation of new chemical series. European Journal of Medicinal Chemistry, 2010, 45, 4270-4279.	2.6	107
130	Metabasite from the Variscan belt in NE Sardinia, Italy: within-plate OIB-like melts with very high Sr and low Nd isotope ratios. European Journal of Mineralogy, 2010, 22, 509-523.	0.4	20
131	Homodimeric Enzymes as Drug Targets. Current Medicinal Chemistry, 2010, 17, 826-846.	1.2	45
132	Grid-derived structure-based 3D pharmacophores and their performance compared to docking. Drug Discovery Today: Technologies, 2010, 7, e213-e219.	4.0	15
133	High-Throughput Virtual Screening of Proteins Using GRID Molecular Interaction Fields. Journal of Chemical Information and Modeling, 2010, 50, 155-169.	2.5	75
134	On the catalytic role of the active site residue E121 of E. coli l-aspartate oxidase. Biochimie, 2010, 92, 1335-1342.	1.3	13
135	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
136	The challenges ofin silicocontributions to drug metabolism in lead optimization. Expert Opinion on Drug Metabolism and Toxicology, 2010, 6, 851-861.	1.5	29
137	Ligands of Diltiazem Binding Site: An Overview of Some Chemotypes. Mini-Reviews in Medicinal Chemistry, 2009, 9, 1379-1388.	1.1	1
138	In silico pK_a Prediction and ADME Profiling. Chemistry and Biodiversity, 2009, 6, 1812-1821.	1.0	70
139	Predicting protein pK_a by environment similarity. Proteins: Structure, Function and Bioinformatics, 2009, 76, 484-495.	1.5	20
140	Stereoselective Behavior of the Functional Diltiazem Analogue 1-[(4-Chlorophenyl)sulfonyl]-2-(2-thienyl)pyrrolidine, a New L-Type Calcium Channel Blocker. Journal of Medicinal Chemistry, 2009, 52, 6637-6648.	2.9	10
141	L-Type Calcium Channel Blockers: From Diltiazem to 1,2,4-Oxadiazol-5-ones via Thiazinooxadiazol-3-one Derivatives. Journal of Medicinal Chemistry, 2009, 52, 2352-2362.	2.9	29
142	Tautomer Enumeration and Stability Prediction for Virtual Screening on Large Chemical Databases. Journal of Chemical Information and Modeling, 2009, 49, 68-75.	2.5	119
143	Integrating Crystallography into Early Metabolism Studies. NATO Science for Peace and Security Series A: Chemistry and Biology, 2009, , 63-77.	0.5	0
144	Petrogenesis of Alâ€“silicate-bearing trondhjemitic migmatites from NE Sardinia, Italy. Lithos, 2008, 102, 554-574.	0.6	40

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145	Amphibole-bearing migmatites from the Variscan Belt of NE Sardinia, Italy: Partial melting of mid-Ordovician igneous sources. Lithos, 2008, 105, 208-224.	0.6	39
146	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
147	Discovery of Novel and Cardioselective Diltiazem-like Calcium Channel Blockers via Virtual Screening. Journal of Medicinal Chemistry, 2008, 51, 5552-5565.	2.9	27
148	Interaction of DDSDEEN peptide with N-CAM protein. Possible mechanism enhancing neuronal differentiation. Peptides, 2008, 29, 2232-2242.	1.2	0
149	New and Original pK_a Prediction Method Using Grid Molecular Interaction Fields. Journal of Chemical Information and Modeling, 2007, 47, 2172-2181.	2.5	277
150	A Common Reference Framework for Analyzing/Comparing Proteins and Ligands. Fingerprints for Ligands And Proteins (FLAP):â€‰ Theory and Application. Journal of Chemical Information and Modeling, 2007, 47, 279-294.	2.5	410
151	Calcium Channel Antagonists Discovered by a Multidisciplinary Approach. Journal of Medicinal Chemistry, 2006, 49, 5206-5216.	2.9	61
152	Predictive models for hERG potassium channel blockers. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 3637-3642.	1.0	98
153	Layered amphibolite sequence in NE Sardinia, Italy: remnant of a pre-Variscan mafic silicic layered intrusion?. Contributions To Mineralogy and Petrology, 2005, 149, 164-180.	1.2	20
154	MetaSite:Â Understanding Metabolism in Human Cytochromes from the Perspective of the Chemist. Journal of Medicinal Chemistry, 2005, 48, 6970-6979.	2.9	466
155	Predicting Human Serum Albumin Affinity of Interleukin-8 (CXCL8) Inhibitors by 3D-QSPR Approach. Journal of Medicinal Chemistry, 2005, 48, 2469-2479.	2.9	35
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