Johan Wouters

List of Publications by Year in descending order

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301 papers	7,972 citations	50276 46 h-index	85541 71 g-index
317 all docs	317 docs citations	317 times ranked	10512 citing authors

#	Article	IF	Citations
1	Reversal of tumoral immune resistance by inhibition of tryptophan 2,3-dioxygenase. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 2497-2502.	7.1	498
2	Differential Scanning Calorimetry in Life Science: Thermodynamics, Stability, Molecular Recognition and Application in Drug Design. Current Medicinal Chemistry, 2005, 12, 2011-2020.	2.4	288
3	Structural Aspects of Monoamine Oxidase and its Reversible Inhibition. Current Medicinal Chemistry, 1998, 5, 137-162.	2.4	155
4	Tryptophan 2,3-Dioxygenase (TDO) Inhibitors. 3-(2-(Pyridyl)ethenyl)indoles as Potential Anticancer Immunomodulators. Journal of Medicinal Chemistry, 2011, 54, 5320-5334.	6.4	151
5	Crystal Structure of the Human Monoacylglycerol Lipase, a Key Actor in Endocannabinoid Signaling. ChemBioChem, 2010, 11, 218-227.	2.6	149
6	The endoxylanases from family 11: computer analysis of protein sequences reveals important structural and phylogenetic relationships. Journal of Biotechnology, 2002, 95, 109-131.	3.8	134
7	A primordial RNA modification enzyme: the case of tRNA (m1A) methyltransferase. Nucleic Acids Research, 2004, 32, 465-476.	14.5	113
8	Supramolecular Wiring of Benzoâ€1,3â€chalcogenazoles through Programmed Chalcogen Bonding Interactions. Chemistry - A European Journal, 2016, 22, 5665-5675.	3.3	105
9	Substituted 2-Thioxoimidazolidin-4-ones and Imidazolidine-2,4-diones as Fatty Acid Amide Hydrolase Inhibitors Templates. Journal of Medicinal Chemistry, 2006, 49, 417-425.	6.4	103
10	Structural basis for recognition of histone H3K36me3 nucleosome by human de novo DNA methyltransferases 3A and 3B. Journal of Structural Biology, 2016, 194, 357-367.	2.8	103
11	A Review on the Monoacylglycerol Lipase: At the Interface Between Fat and Endocannabinoid Signalling. Current Medicinal Chemistry, 2010, 17, 2588-2607.	2.4	102
12	Pharmaceutical salts and cocrystals involving amino acids: A brief structural overview of the state-of-art. European Journal of Medicinal Chemistry, 2014, 74, 411-426.	5.5	95
13	Copperâ€Catalysed Domino Silylative Aldol Reaction Leading to Stereocontrolled Chiral Quaternary Carbons. Chemistry - A European Journal, 2010, 16, 10980-10983.	3.3	89
14	Cationâ€ï€ (Na⁺â€Trp) interactions in the crystal structure of tetragonal lysozyme. Protein Science, 1998, 7, 2472-2475.	7.6	88
15	A rapid and efficient microwave-assisted synthesis of hydantoins and thiohydantoins. Tetrahedron, 2003, 59, 1301-1307.	1.9	87
16	Comparing the crystallization and polymorphic behaviour of saturated and unsaturated monoglycerides. Food Research International, 2009, 42, 1415-1425.	6.2	85
17	Synthesis and evaluation of Î²-carboline derivatives as potential monoamine oxidase inhibitors. Bioorganic and Medicinal Chemistry, 2011, 19, 134-144.	3.0	83
18	Assessing the Potential of Zwitterionic NHCÂ·CS₂ Adducts for Probing the Stereoelectronic Parameters of Nâ€Heterocyclic Carbenes. European Journal of Inorganic Chemistry, 2009, 2009, 1882-1891.	2.0	79

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19	Advances in Pharmaceutical Co-crystal Screening: Effective Co-crystal Screening through Structural Resemblance. Crystal Growth and Design, 2012, 12, 475-484.	3.0	77
20	Novel Trisubstituted Harmine Derivatives with Original in Vitro Anticancer Activity. Journal of Medicinal Chemistry, 2012, 55, 6489-6501.	6.4	75
21	Determination of physical changes of inulin related to sorption isotherms: An X-ray diffraction, modulated differential scanning calorimetry and environmental scanning electron microscopy study. Carbohydrate Polymers, 2006, 63, 210-217.	10.2	74
22	Catalytic Mechanism of Escherichia coli Isopentenyl Diphosphate Isomerase Involves Cys-67, Glu-116, and Tyr-104 as Suggested by Crystal Structures of Complexes with Transition State Analogues and Irreversible Inhibitors. Journal of Biological Chemistry, 2003, 278, 11903-11908.	3.4	72
23	A reversible monoamine oxidase a inhibitor, befloxatone: structural approach of its mechanism of action. Bioorganic and Medicinal Chemistry, 1999, 7, 1683-1693.	3.0	71
24	Analysis of Conserved Active Site Residues in Monoamine Oxidase A and B and Their Three-dimensional Molecular Modeling. Journal of Biological Chemistry, 2002, 277, 17209-17216.	3.4	70
25	Engineering Solidâ€State Molecular Switches: Nâ€Salicylidene Nâ€Heterocycle Derivatives. European Journal of Organic Chemistry, 2010, 2010, 621-637.	2.4	70
26	Transmembrane (TMEM) protein family members: Poorly characterized even if essential for the metastatic process. Seminars in Cancer Biology, 2020, 60, 96-106.	9.6	67
27	Pushing the Lewis Acidity Boundaries of Boron Compounds With Nonâ€Planar Triarylboranes Derived from Triptycenes. Angewandte Chemie - International Edition, 2019, 58, 16889-16893.	13.8	66
28	Combining piracetam and lithium salts: ionic co-crystals and co-drugs?. Chemical Communications, 2012, 48, 8219.	4.1	65
29	3,6-Disubstituted Coumarins as Mechanism-Based Inhibitors of Thrombin and Factor Xa. Journal of Medicinal Chemistry, 2005, 48, 7592-7603.	6.4	61
30	Synthesis and Catalytic Evaluation of Rutheniumâ€"Arene Complexes Generated Using Imidazol(in)ium-2-carboxylates and Dithiocarboxylates. Organometallics, 2009, 28, 4056-4064.	2.3	61
31	Cobalt(II) Complexes of Nitrileâ€Functionalized Ionic Liquids. Chemistry - A European Journal, 2010, 16, 1849-1858.	3.3	59
32	Indanesulfonamides as Carbonic Anhydrase Inhibitors. Toward Structure-Based Design of Selective Inhibitors of the Tumor-Associated Isozyme CA IX. Journal of Medicinal Chemistry, 2006, 49, 2743-2749.	6.4	58
33	Discovery and preliminary SARs of keto-indoles as novel indoleamine 2,3-dioxygenase (IDO) inhibitors. European Journal of Medicinal Chemistry, 2011, 46, 3058-3065.	5.5	57
34	Cocrystal Formation between Chiral Compounds: How Cocrystals Differ from Salts. Crystal Growth and Design, 2014, 14, 3996-4004.	3.0	57
35	A reversible monoamine oxidase inhibitor, toloxatone: Structural and electronic properties. European Journal of Medicinal Chemistry, 1992, 27, 939-948.	5.5	55
36	Substituted 5,5â€˜-Diphenyl-2-thioxoimidazolidin-4-one as CB1Cannabinoid Receptor Ligands:Â Synthesis and Pharmacological Evaluation. Journal of Medicinal Chemistry, 2005, 48, 2509-2517.	6.4	54

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37	Disulfiram is an Inhibitor of Human Purified Monoacylglycerol Lipase, the Enzyme Regulating 2-Arachidonoylglycerol Signaling. ChemBioChem, 2007, 8, 1293-1297.	2.6	54
38	Halogenâ€Bond Effects on the Thermoâ€•and Photochromic Behaviour of Anilâ€Based Molecular Coâ€crystals. Chemistry - A European Journal, 2017, 23, 5317-5329.	3.3	52
39	Coumarinic derivatives as mechanism-based inhibitors of Î±-chymotrypsin and human leukocyte elastase. Bioorganic and Medicinal Chemistry, 2000, 8, 1489-1501.	3.0	51
40	Unprecedented Copper(I) Bifluoride Complexes: Synthesis, Characterization and Reactivity. Chemistry - A European Journal, 2012, 18, 793-798.	3.3	51
41	Walking Down the Chalcogenic Group of the Periodic Table: From Singlet to Triplet Organic Emitters. Chemistry - A European Journal, 2015, 21, 15377-15387.	3.3	51
42	Polymorphic and Isomorphic Cocrystals of a N-Salicylidene-3-aminopyridine with Dicarboxylic Acids: Tuning of Solid-State Photo- and Thermochromism. Journal of Physical Chemistry C, 2016, 120, 10001-10008.	3.1	51
43	A reversible monoamine oxidase inhibitor, toloxatone: spectrophotometric and molecular orbital studies of the interaction with flavin adenine dinucleotide (FAD). European Journal of Medicinal Chemistry, 1994, 29, 269-277.	5.5	50
44	Structure and X-ray conformation of pseudodesmins A and B, two new cyclic lipodepsipeptides from Pseudomonas bacteria. Tetrahedron, 2009, 65, 4173-4181.	1.9	50
45	Polymorphism, Fluorescence, and Optoelectronic Properties of a Borazine Derivative. Chemistry - A European Journal, 2013, 19, 7771-7779.	3.3	49
46	Crystal structure of a coldâ€adapted classâ€ƒC Î²â€lactamase. FEBS Journal, 2008, 275, 1687-1697.	4.7	48
47	Sequential Acid/Base-Catalyzed Polycyclization of Tryptamine Derivatives. A Rapid Access to BÃ¼chi's KetoneÂ§. Organic Letters, 2005, 7, 5245-5248.	4.6	47
48	Structural Insights into Human 5-Lipoxygenase Inhibition:Â Combined Ligand-Based and Target-Based Approach. Journal of Medicinal Chemistry, 2006, 49, 186-195.	6.4	47
49	Exploration of the Pharmacophore of 3-Alkyl-5-Arylimidazolidinediones as New CB1Cannabinoid Receptor Ligands and Potential Antagonists: Synthesis, Lipophilicity, Affinity, and Molecular Modeling. Journal of Medicinal Chemistry, 2002, 45, 1748-1756.	6.4	46
50	Synthesis and Activity of 1,3,5-Triphenylimidazolidine-2,4-diones and 1,3,5-Triphenyl-2-thioxoimidazolidin-4-ones: Characterization of New CB1Cannabinoid Receptor Inverse Agonists/Antagonists. Journal of Medicinal Chemistry, 2006, 49, 872-882.	6.4	46
51	A harmine-derived beta-carboline displays anti-cancer effects in vitro by targeting protein synthesis. European Journal of Pharmacology, 2017, 805, 25-35.	3.5	46
52	Controlled Generation of 9â€Boratriptycene by Lewis Adduct Dissociation: Accessing a Nonâ€Planar Triarylborane. Angewandte Chemie - International Edition, 2020, 59, 12402-12406.	13.8	46
53	On the influence of using a zwitterionic coformer for cocrystallization: structural focus on naproxenâ€“proline cocrystals. CrystEngComm, 2013, 15, 3341.	2.6	44
54	Opening Pandoraâ€™s Box: Chirality, Polymorphism, and Stoichiometric Diversity in Flurbiprofen/Proline Cocrystals. Crystal Growth and Design, 2018, 18, 954-961.	3.0	44

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55	Species Distribution and Coordination of Uranyl Chloro Complexes in Acetonitrile. Inorganic Chemistry, 2008, 47, 2987-2993.	4.0	43
56	Palladium-Nanoparticle-Catalyzed 1,7-Palladium Migration Involving Câ€“H Activation, Followed by Intramolecular Amination: Regioselective Synthesis of N1-Arylbenzotriazoles and an Evaluation of Their Inhibitory Activity toward Indoleamine 2,3-Dioxygenase. Journal of Organic Chemistry, 2014, 79, 6366-6371.	3.2	43
57	Structure and Mechanism of Action of Isopentenylpyrophosphate-Dimethylallylpyrophosphate Isomerase. Journal of the American Chemical Society, 2003, 125, 3198-3199.	13.7	42
58	Microhydration of Protonated Glycine:â€‰ An ab initio Family Tree. Journal of Physical Chemistry B, 2008, 112, 2430-2438.	2.6	42
59	An allosteric heteroditopic receptor for neutral guests and contact ion pairs with a remarkable selectivity for ammonium fluoride salts. Organic and Biomolecular Chemistry, 2010, 8, 4607.	2.8	42
60	First crystal structure of an endo-inulinase, INU2, from Aspergillus ficuum: Discovery of an extra-pocket in the catalytic domain responsible for its endo-activity. Biochimie, 2012, 94, 2423-2430.	2.6	42
61	Towards the understanding of the absorption spectra of NAD(P)H/NAD(P)+ as a common indicator of dehydrogenase enzymatic activity. Chemical Physics Letters, 2007, 450, 119-122.	2.6	41
62	Synthesis, evaluation and structure-activity relationship of new 3-carboxamide coumarins as FXIIa inhibitors. European Journal of Medicinal Chemistry, 2016, 110, 181-194.	5.5	41
63	Versatile Self-Adapting Boronic Acids for H-Bond Recognition: From Discrete to Polymeric Supramolecules. Journal of the American Chemical Society, 2017, 139, 2710-2727.	13.7	41
64	Electrostatically-driven assembly of MWCNTs with a europium complex. Chemical Communications, 2011, 47, 1625-1627.	4.1	40
65	Preference of Cd(II) and Zn(II) for the Two Metal Sites inBacillus cereusÎ²-Lactamase II:Â A Perturbed Angular Correlation of Î³-rays Spectroscopic Studyâ€. Biochemistry, 1999, 38, 16500-16506.	2.5	39
66	Indol-2-yl ethanones as novel indoleamine 2,3-dioxygenase (IDO) inhibitors. Bioorganic and Medicinal Chemistry, 2011, 19, 1550-1561.	3.0	39
67	Anti-alcohol abuse drug disulfiram inhibits human PHGDH via disruption of its active tetrameric form through a specific cysteine oxidation. Scientific Reports, 2019, 9, 4737.	3.3	39
68	Crystal structures of low-melting ionic transition-metal complexes with N-alkylimidazole ligands. CrystEngComm, 2012, 14, 4902.	2.6	37
69	Synthesis, Structural Reassignment, and Biological Activity of Type B MAO Inhibitors Based on the 5H-Indeno[1,2-c]pyridazin-5-one Core. Journal of Medicinal Chemistry, 2006, 49, 3743-3747.	6.4	35
70	Mechanism-Based Thrombin Inhibitors:â€‰ Design, Synthesis, and Molecular Docking of a New Selective 2-Oxo-2H-1-benzopyran Derivative. Journal of Medicinal Chemistry, 2007, 50, 3645-3650.	6.4	34
71	â€œMagicâ€•Surface Clustering of Borazines Driven by Repulsive Intermolecular Forces. Angewandte Chemie - International Edition, 2013, 52, 7410-7414.	13.8	34
72	Synthesis and Bioactivity of Î²-Substituted Fosmidomycin Analogues Targeting 1-Deoxy-<scp>d</scp>-xylulose-5-phosphate Reductoisomerase. Journal of Medicinal Chemistry, 2015, 58, 2988-3001.	6.4	34

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73	Structural insights into the acidophilic pH adaptation of a novel endo-1,4-Î²-xylanase from Scytalidium acidophilum. Biochimie, 2010, 92, 1407-1415.	2.6	33
74	Synthesis and Organocatalytic Applications of Imidazol(in)iumâ€2â€thiocarboxylates. European Journal of Organic Chemistry, 2011, 2011, 7083-7091.	2.4	33
75	Thiosemicarbazide, a fragment with promising indolamine-2,3-dioxygenase (IDO) inhibition properties. European Journal of Medicinal Chemistry, 2014, 82, 96-105.	5.5	33
76	Taming the Lewis Superacidity of Nonâ€Planar Boranes: Cåˆ’H Bond Activation and Nonâ€Classical Binding Modes at Boron. Angewandte Chemie - International Edition, 2022, 61, .	13.8	33
77	Crystallization behavior of milk fat obtained from linseed-fed cows. Journal of Dairy Science, 2010, 93, 495-505.	3.4	32
78	Reversible inhibition of type B monoamine oxidase. Theoretical study of model diazo heterocylic compound. European Journal of Medicinal Chemistry, 1997, 32, 721-730.	5.5	31
79	Crystallographic analysis of family 11 endo-Î²-1,4-xylanase Xyl1 fromStreptomycessp. S38. Acta Crystallographica Section D: Biological Crystallography, 2001, 57, 1813-1819.	2.5	31
80	Structural insight into cocrystallization with zwitterionic co-formers: cocrystals of S-naproxen. CrystEngComm, 2014, 16, 8185.	2.6	31
81	Ionic co-crystals of racetams: solid-state properties enhancement of neutral active pharmaceutical ingredients via addition of Mg2+ and Ca2+ chlorides. CrystEngComm, 2014, 16, 5887.	2.6	31
82	A reversible monoamine oxidase inhibitor, Toloxatone: comparison of its physicochemical properties with those of other inhibitors including Brofaromine, Harmine, R40519 and Moclobemide. European Journal of Medicinal Chemistry, 1995, 30, 823-837.	5.5	30
83	Crystal Structure of BRL 42715, C6-(N1-Methyl-1,2,3-triazolylmethylene)penem, in Complex withEnterobactercloacae908R Î²-Lactamase:Â Evidence for a Stereoselective Mechanism from Docking Studies. Journal of the American Chemical Society, 2005, 127, 3262-3263.	13.7	30
84	A theoretical investigation of the hydrated glycine cation energetics and structures. Chemical Physics Letters, 2007, 445, 57-61.	2.6	29
85	Investigation of mechanism-based thrombin inhibitors: Implications of a highly conserved water molecule for the binding of coumarins within the S pocket. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 2017-2021.	2.2	28
86	Supramolecular Assistance for the Selective Demethylation of Calixarene-Based Receptors. Journal of Organic Chemistry, 2015, 80, 5084-5091.	3.2	28
87	Copper(<scp>ii</scp>) complexes with tridentate halogen-substituted Schiff base ligands: synthesis, crystal structures and investigating the effect of halogenation, leaving groups and ligand flexibility on antiproliferative activities. Dalton Transactions, 2021, 50, 3990-4007.	3.3	28
88	Mechanistic Insight into the Staudinger Reaction Catalyzed by Nâ€Heterocyclic Carbenes. Chemistry - A European Journal, 2013, 19, 9668-9676.	3.3	27
89	Versatile Access to Benzhydryl-Phenylureas through an Unexpected Rearrangement during Microwave-Enhanced Synthesis of Hydantoins. Organic Letters, 2003, 5, 3599-3602.	4.6	26
90	Structure of Thermus thermophilus type 2 isopentenyl diphosphate isomerase inferred from crystallography and molecular dynamics. Biochemical and Biophysical Research Communications, 2005, 338, 1515-1518.	2.1	26

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91	Estimation of sucrose crystallization kinetics from batch crystallizer data. Journal of Crystal Growth, 2008, 310, 798-803.	1.5	26
92	Indoleamine 2,3-dioxygenase inhibitory activity of derivatives of marine alkaloid tsitsikammamine A. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 47-54.	2.2	26
93	Small Molecule Crystallography in Drug Design. Current Pharmaceutical Design, 2001, 7, 529-545.	1.9	25
94	Expedient, Direct Synthesis of (L)Pt(0)(1,6-diene) Complexes from H2PtCl6. Organometallics, 2007, 26, 5731-5734.	2.3	25
95	Exploration of the Binding Mode of Indanesulfonamides as Selective Inhibitors of Human Carbonic Anhydrase Typeâ€…VII by Targeting Lysâ€‰91. ChemMedChem, 2007, 2, 1273-1280.	3.2	25
96	Effect of TAG composition on the crystallization behaviour of model fat blends with the same saturated fat content. Food Research International, 2010, 43, 2057-2067.	6.2	25
97	Synthesis, biological evaluation and molecular modeling studies of quinolonyl diketo acid derivatives: New structural insight into the HIV-1 integrase inhibition. European Journal of Medicinal Chemistry, 2011, 46, 1749-1756.	5.5	25
98	Solid-State Investigation of Polymorphism and Tautomerism of Phenylthiazole-thione: A Combined Crystallographic, Calorimetric, and Theoretical Survey. Crystal Growth and Design, 2015, 15, 2461-2473.	3.0	25
99	Assessing Density Functional Theory Approaches for Predicting the Structure and Relative Energy of Salicylideneaniline Molecular Switches in the Solid State. Journal of Physical Chemistry C, 2017, 121, 6898-6908.	3.1	25
100	Playing with Isomerism: Cocrystallization of Isomeric N-Salicylideneaminopyridines with Perfluorinated Compounds as Halogen Bond Donors and Its Impact on Photochromism. Crystal Growth and Design, 2018, 18, 6833-6842.	3.0	25
101	Pushing the Lewis Acidity Boundaries of Boron Compounds With Nonâ€Planar Triarylboranes Derived from Triptycenes. Angewandte Chemie, 2019, 131, 17045-17049.	2.0	25
102	Controlled Generation of 9â€Boratriptycene by Lewis Adduct Dissociation: Accessing a Nonâ€Planar Triarylborane. Angewandte Chemie, 2020, 132, 12502-12506.	2.0	25
103	Protecting role of cosolvents in protein denaturation by SDS: a structural study. BMC Structural Biology, 2008, 8, 29.	2.3	24
104	Acidâ€“base modulation of a versatile heteroditopic calix[6]arene based receptor. Organic and Biomolecular Chemistry, 2011, 9, 6373.	2.8	24
105	Chiral Resolution of Mandelic Acid through Preferential Cocrystallization with Nefiracetam. Crystal Growth and Design, 2020, 20, 7979-7988.	3.0	24
106	Crystal structure of the C67A mutant of isopentenyl diphosphate isomerase complexed with a mechanism-based irreversible inhibitor. Proteins: Structure, Function and Bioinformatics, 2003, 54, 216-221.	2.6	23
107	1-Benzhydryl-3-phenylurea and 1-Benzhydryl-3-phenylthiourea Derivatives:â€‰ New Templates among the CB1 Cannabinoid Receptor Inverse Agonists. Journal of Medicinal Chemistry, 2005, 48, 7486-7490.	6.4	23
108	Exploring polymorphism and stoichiometric diversity in naproxen/proline cocrystals. CrystEngComm, 2018, 20, 7308-7321.	2.6	23

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109	Isosterism among analogues of torasemide: conformational, electronic and lipophilicity properties. European Journal of Medicinal Chemistry, 2000, 35, 923-929.	5.5	22
110	Inhibition studies of DNA methyltransferases by maleimide derivatives of RG108 as non-nucleoside inhibitors. Future Medicinal Chemistry, 2017, 9, 1465-1481.	2.3	22
111	Refined structure ofPyrococcus furiosusornithine carbamoyltransferase at 1.87â€…A. Acta Crystallographica Section D: Biological Crystallography, 2003, 59, 2140-2149.	2.5	21
112	Indanesulfonamides as carbonic anhydrase inhibitors and anticonvulsant agents: Structureâ€“activity relationship and pharmacological evaluation. European Journal of Medicinal Chemistry, 2008, 43, 2853-2860.	5.5	21
113	Modeling the Microhydration of Protonated Alanine. Journal of Physical Chemistry B, 2008, 112, 9896-9902.	2.6	21
114	Crystal Structure of Type 2 Isopentenyl Diphosphate Isomerase fromThermus thermophilusin Complex with Inorganic Pyrophosphateâ€. Biochemistry, 2008, 47, 9051-9053.	2.5	21
115	Xylanase XYL1p from Scytalidium acidophilum: Site-directed mutagenesis and acidophilic adaptation. Bioresource Technology, 2009, 100, 6465-6471.	9.6	21
116	Design, synthesis and biological evaluation of a sulfonylcyanoguanidine as thromboxane A2 receptor antagonist and thromboxane synthase inhibitor. Journal of Pharmacy and Pharmacology, 2010, 53, 669-680.	2.4	21
117	Pyrazolo[4,3-c]isoquinolines as potential inhibitors of NF-ÎºB activation. Biochemical Pharmacology, 2010, 79, 1462-1472.	4.4	21
118	On the fractional crystallization of palm olein: Solid solutions and eutectic solidification. Food Research International, 2010, 43, 972-981.	6.2	21
119	Novel pharmaceutical compositions through co-crystallization of racetams and Li+ salts. CrystEngComm, 2013, 15, 8898.	2.6	21
120	Synthesis of Tertiary Enamides by Ag₂CO₃-Promoted Pd-Catalyzed Alkenylation of Acyclic Secondary Amides. Organic Letters, 2016, 18, 4844-4847.	4.6	21
121	Ab initio investigation of the hydration of deprotonated amino acids. Journal of the American Society for Mass Spectrometry, 2009, 20, 632-638.	2.8	20
122	Alpha-Heteroatom Derivatized Analogues of 3-(Acetylhydroxyamino)propyl Phosphonic Acid (FR900098) as Antimalarials. Journal of Medicinal Chemistry, 2013, 56, 376-380.	6.4	20
123	1-(2-Hydroxybenzoyl)-thiosemicarbazides are promising antimicrobial agents targeting d-alanine-d-alanine ligase in bacterio. European Journal of Medicinal Chemistry, 2018, 159, 324-338.	5.5	20
124	Pharmacomodulations of the benzoyl-thiosemicarbazide scaffold reveal antimicrobial agents targeting d-alanyl-d-alanine ligase in bacterio. European Journal of Medicinal Chemistry, 2020, 200, 112444.	5.5	20
125	Use of theoretical descriptors to characterize cation-? binding sites in (macro)molecules. Journal of Computational Chemistry, 2000, 21, 847-855.	3.3	19
126	Purification, Cloning, and Three-Dimensional Structure Prediction of Micrococcus luteus FAD-Containing Tyramine Oxidase. Biochemical and Biophysical Research Communications, 2000, 268, 293-297.	2.1	19

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127	Topology Prediction ofBrucella AbortusOmp2b and Omp2a Porins After Critical Assessment of Transmembrane Î² Strands Prediction by Several Secondary Structure Prediction Methods. Journal of Biomolecular Structure and Dynamics, 2000, 17, 747-757.	3.5	19
128	3D-QSAR, design, synthesis and characterization of trisubstituted harmine derivatives with inÂvitro antiproliferative properties. European Journal of Medicinal Chemistry, 2015, 94, 45-55.	5.5	19
129	Peculiar Case of Levetiracetam and Etiracetam Î±-Ketoglutaric Acid Cocrystals: Obtaining a Stable Conglomerate of Etiracetam. Crystal Growth and Design, 2016, 16, 5273-5282.	3.0	19
130	Targeting the Serine Pathway: A Promising Approach against Tuberculosis?. Pharmaceuticals, 2019, 12, 66.	3.8	19
131	Design, Synthesis, and Anticonvulsant Activity of 1-(Pyrid-3-ylsulfonamido)-2-nitroethylenes. Journal of Medicinal Chemistry, 1998, 41, 3239-3244.	6.4	18
132	Monoamine oxidase A inhibitory potency and flavin perturbation are influenced by different aspects of pirlindole inhibitor structure. Biochemical Pharmacology, 2003, 65, 1867-1874.	4.4	18
133	Conformation-controlled networking of H-bonded assemblies on surfaces. Chemical Communications, 2009, , 3525.	4.1	18
134	Analysis of the Interactions Taking Place in the Recognition Site of a Bimetallic Mg(II)â^'Zn(II) Enzyme, Isopentenyl Diphosphate Isomerase. A Parallel Quantum-Chemical and Polarizable Molecular Mechanics Study. Journal of Physical Chemistry B, 2010, 114, 4884-4895.	2.6	18
135	Structural Study of Prolinium/Fumaric Acid Zwitterionic Cocrystals: Focus on Hydrogen-Bonding Pattern Involving Zwitterionic (Ionic) Heterosynthons. Crystal Growth and Design, 2013, 13, 2373-2389.	3.0	18
136	A Structural Analysis of Spiropyran and Spirooxazine Compounds and Their Polymorphs. Crystals, 2017, 7, 84.	2.2	18
137	Chiral Resolution of RS-Oxiracetam upon Cocrystallization with Pharmaceutically Acceptable Inorganic Salts. Crystal Growth and Design, 2020, 20, 2602-2607.	3.0	18
138	Rational approaches towards reversible inhibition of type B monoamine oxidase. Design and evaluation of a novel 5H-Indeno[1,2-c]pyridazin-5-one derivative. Bioorganic and Medicinal Chemistry Letters, 2003, 13, 69-73.	2.2	17
139	Targeting an Aromatic Hotspot in Plasmodium falciparum 1â€Deoxyâ€<scp>d</scp>â€xyluloseâ€5â€phosphate Reductoisomerase with Î²â€Arylpropyl Analogues of Fosmidomycin. ChemMedChem, 2016, 11, 2024-2036.	3.2	17
140	Acidochromic spiropyranâ€“merocyanine stabilisation in the solid state. CrystEngComm, 2018, 20, 3318-3327.	2.6	17
141	Halogen-bonded cocrystals ofN-salicylidene Schiff bases and iodoperfluorinated benzenes: hydroxyl oxygen as a halogen bond acceptor. CrystEngComm, 2018, 20, 5332-5339.	2.6	17
142	Isopentenyl Diphosphate Isomerase. Mechanism-Based Inhibition by Diene Analogues of Isopentenyl Diphosphate and Dimethylallyl Diphosphate. Journal of the American Chemical Society, 2005, 127, 17433-17438.	13.7	16
143	New R/S-3,4-dihydro-2,2-dimethyl-6-halo-4-(phenylaminothiocarbonylamino)-2H-1-benzopyrans structurally related to (Â±)-cromakalim as tissue-selective pancreatic Î²-cell KATP channel openers. Bioorganic and Medicinal Chemistry, 2008, 16, 5704-5719.	3.0	16
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