

Hendrik G. Kruger

List of Publications by Year in descending order

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358
papers

6,835
citations

94433

37
h-index

102487

66
g-index

394
all docs

394
docs citations

394
times ranked

7505
citing authors

#	ARTICLE	IF	CITATIONS
1	Bis- and Trisindolylmethanes (BIMs and TIMs). <i>Chemical Reviews</i> , 2010, 110, 2250-2293.	47.7	513
2	Therapeutic peptides. <i>Future Medicinal Chemistry</i> , 2012, 4, 1527-1531.	2.3	261
3	The role of nanotechnology in the treatment of viral infections. <i>Therapeutic Advances in Infectious Disease</i> , 2017, 4, 105-131.	1.8	233
4	Current trends in computer aided drug design and a highlight of drugs discovered via computational techniques: A review. <i>European Journal of Medicinal Chemistry</i> , 2021, 224, 113705.	5.5	229
5	Antimicrobial Peptides: Their Role as Infection-Selective Tracers for Molecular Imaging. <i>BioMed Research International</i> , 2014, 2014, 1-15.	1.9	151
6	Sulfonimidamides in Medicinal and Agricultural Chemistry. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 4100-4109.	13.8	145
7	Design of Ionic Liquid 3-Methyl-1-sulfonic Acid Imidazolium Nitrate as Reagent for the Nitration of Aromatic Compounds by <i>in Situ</i> Generation of NO ₂ in Acidic Media. <i>Journal of Organic Chemistry</i> , 2012, 77, 3640-3645.	3.2	128
8	Nanotechnology and the Treatment of HIV Infection. <i>Viruses</i> , 2012, 4, 488-520.	3.3	106
9	Synthesis of pyranopyrazoles using isonicotinic acid as a dual and biological organocatalyst. <i>RSC Advances</i> , 2013, 3, 25681.	3.6	106
10	Enantioselective Organocatalyzed Transformations of β -Ketoesters. <i>Chemical Reviews</i> , 2016, 116, 9375-9437.	47.7	105
11	Integrated Approach to Structure-Based Enzymatic Drug Design: Molecular Modeling, Spectroscopy, and Experimental Bioactivity. <i>Chemical Reviews</i> , 2014, 114, 493-537.	47.7	100
12	A Synthesis of α -Dual Warhead β -Aryl Ethenesulfonyl Fluorides and One-Pot Reaction to β -Sultams. <i>Organic Letters</i> , 2017, 19, 480-483.	4.6	91
13	Green Solid-Phase Peptide Synthesis 2. 2-Methyltetrahydrofuran and Ethyl Acetate for Solid-Phase Peptide Synthesis under Green Conditions. <i>ACS Sustainable Chemistry and Engineering</i> , 2016, 4, 6809-6814.	6.7	85
14	Synthesis and Biological Evaluation of a Teixobactin Analogue. <i>Organic Letters</i> , 2015, 17, 6182-6185.	4.6	77
15	Tandem Knoevenagel-Michael-cyclocondensation reactions of malononitrile, various aldehydes and dimedone using acetic acid functionalized ionic liquid. <i>New Journal of Chemistry</i> , 2014, 38, 2342.	2.8	75
16	Preclinical Evaluation of ⁶⁸ Ga-Labeled 1,4,7-Triazacyclononane-1,4,7-Triacetic Acid-Ubiquitin as a Radioligand for PET Infection Imaging. <i>Journal of Nuclear Medicine</i> , 2014, 55, 308-314.	5.0	75
17	Advances in the application of N ₂ O ₄ /NO ₂ in organic reactions. <i>Tetrahedron</i> , 2010, 66, 9077-9106.	1.9	74
18	Polycyclic Cage Structures as Lipophilic Scaffolds for Neuroactive Drugs. <i>ChemMedChem</i> , 2012, 7, 375-384.	3.2	70

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19	Tandem Knoevenagel–Michael cyclocondensation reaction of malononitrile, various aldehydes and 2-naphthol over acetic acid functionalized ionic liquid. <i>Chemical Engineering Journal</i> , 2014, 248, 122-127.	12.7	69
20	Peptide synthesis beyond DMF: THF and ACN as excellent and friendlier alternatives. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 2393-2398.	2.8	69
21	2-Methyltetrahydrofuran and cyclopentyl methyl ether for green solid-phase peptide synthesis. <i>Amino Acids</i> , 2016, 48, 419-426.	2.7	69
22	Short AntiMicrobial Peptides (SAMPs) as a class of extraordinary promising therapeutic agents. <i>Journal of Peptide Science</i> , 2016, 22, 438-451.	1.4	64
23	The effect of N-methylation of amino acids (Ac-X-OMe) on solubility and conformation: a DFT study. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 9993-10006.	2.8	55
24	Structural and functional features of enzymes of <i>Mycobacterium tuberculosis</i> peptidoglycan biosynthesis as targets for drug development. <i>Tuberculosis</i> , 2015, 95, 95-111.	1.9	54
25	Green Solid-Phase Peptide Synthesis (GSPPS) 3. Green Solvents for Fmoc Removal in Peptide Chemistry. <i>Organic Process Research and Development</i> , 2017, 21, 365-369.	2.7	52
26	Anticancer activity of ruthenium(II) arene complexes bearing 1,2,3,4-tetrahydroisoquinoline amino alcohol ligands. <i>European Journal of Medicinal Chemistry</i> , 2013, 66, 407-414.	5.5	51
27	NOTA: a potent metallo- β -lactamase inhibitor. <i>Journal of Antimicrobial Chemotherapy</i> , 2015, 70, 1594-1596.	3.0	51
28	Lysine Scanning of Arg ₁₀ –Teixobactin: Deciphering the Role of Hydrophobic and Hydrophilic Residues. <i>ACS Omega</i> , 2016, 1, 1262-1265.	3.5	51
29	Peptide synthesis, characterization and ⁶⁸ Ga-radiolabeling of NOTA-conjugated ubiquitin fragments for prospective infection imaging with PET/CT. <i>Nuclear Medicine and Biology</i> , 2014, 41, 390-400.	0.6	50
30	On-Water Synthesis of Biaryl Sulfonyl Fluorides. <i>Journal of Organic Chemistry</i> , 2016, 81, 2618-2623.	3.2	49
31	Composite ceramic-metal coatings by means of combined electrophoretic deposition and galvanic methods. <i>Journal of Materials Science</i> , 2004, 39, 839-844.	3.7	42
32	Computational model for the acylation step of the β -lactam ring: Potential application for l,d-transpeptidase 2 in <i>mycobacterium tuberculosis</i> . <i>Journal of Molecular Structure</i> , 2017, 1128, 94-102.	3.6	41
33	DFT study of the acid-catalyzed esterification reaction mechanism of methanol with carboxylic acid and its halide derivatives. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25497.	2.0	41
34	Metabolic Imaging of Infection. <i>Journal of Nuclear Medicine</i> , 2017, 58, 1727-1732.	5.0	40
35	Synthesis and evaluation of SQ109 analogues as potential anti-tuberculosis candidates. <i>European Journal of Medicinal Chemistry</i> , 2010, 45, 2075-2079.	5.5	39
36	Mechanistic investigation of the uncatalyzed esterification reaction of acetic acid and acid halides with methanol: a DFT study. <i>Journal of Molecular Modeling</i> , 2016, 22, 235.	1.8	39

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37	Synthesis and structural studies of pentacycloundecane-based HIV-1 PR inhibitors: A hybrid 2D NMR and docking/QM/MM/MD approach. <i>European Journal of Medicinal Chemistry</i> , 2011, 46, 3976-3985.	5.5	38
38	<i>In vitro</i> evaluation of metal chelators as potential metallo- β -lactamase inhibitors. <i>Journal of Applied Microbiology</i> , 2016, 120, 860-867.	3.1	38
39	Synthesis of chiral pentacyclo-undecane ligands and their use in the enantioselective alkylation of benzaldehyde with diethylzinc. <i>Tetrahedron: Asymmetry</i> , 2004, 15, 2661-2666.	1.8	37
40	In vitro ADMET and physicochemical investigations of poly-N-methylated peptides designed to inhibit A β aggregation. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 5896-5902.	3.0	37
41	Differential flap dynamics in <i>l</i> , <i>d</i> -transpeptidase2 from mycobacterium tuberculosis revealed by molecular dynamics. <i>Molecular BioSystems</i> , 2017, 13, 1223-1234.	2.9	36
42	Ab initio mechanistic study of the protection of alcohols and amines with anhydrides. <i>Computational and Theoretical Chemistry</i> , 2002, 577, 281-285.	1.5	34
43	Pentacyclo-undecane derived cyclic tetra-amines: Synthesis and evaluation as potent anti-tuberculosis agents. <i>European Journal of Medicinal Chemistry</i> , 2009, 44, 4297-4305.	5.5	34
44	FriedlÄnder Annulation in the Synthesis of Azaheterocyclic Compounds. <i>Advances in Heterocyclic Chemistry</i> , 2011, 102, 139-227.	1.7	34
45	Synthesis of tetrahydropyridines by one-pot multicomponent reaction using nano-sphere silica sulfuric acid. <i>Journal of the Iranian Chemical Society</i> , 2015, 12, 855-861.	2.2	34
46	Re-evaluation of the N-terminal substitution and the D-residues of teixobactin. <i>RSC Advances</i> , 2016, 6, 73827-73829.	3.6	34
47	Sulfonimidamide in medizinischer Chemie und Agrochemie. <i>Angewandte Chemie</i> , 2017, 129, 4160-4170.	2.0	34
48	Synthesis and Screening of C ¹ -Substituted Tetrahydroisoquinoline Derivatives for Asymmetric Transfer Hydrogenation Reactions. <i>European Journal of Organic Chemistry</i> , 2010, 2010, 972-980.	2.4	33
49	Novel Approach to Sodium Hydroxide Separation: Synergistic Pseudo-Hydroxide Extraction by a Fluorinated Alcohol and Cage-Functionalized Crown Ethers. <i>Journal of the American Chemical Society</i> , 2001, 123, 12099-12100.	13.7	32
50	Pentacycloundecane-based inhibitors of wild-type C-South African HIV-protease. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2011, 21, 2274-2277.	2.2	32
51	Comparison of the Molecular Dynamics and Calculated Binding Free Energies for Nine FDA-Approved HIV-1 PR Drugs Against Subtype B and C Δ 8.9 HIV PR. <i>Chemical Biology and Drug Design</i> , 2013, 81, 208-218.	3.2	32
52	Application of silica vanadic acid as a heterogeneous, selective and highly reusable catalyst for oxidation of sulfides at room temperature. <i>Journal of Molecular Catalysis A</i> , 2013, 370, 80-86.	4.8	31
53	<i>N</i> -Trifluoromethylthiolated Sulfonimidamides and Sulfoximines: Anti-microbial, Anti-mycobacterial, and Cytotoxic Activity. <i>ACS Medicinal Chemistry Letters</i> , 2019, 10, 1457-1461.	2.8	31
54	Novel tetrahydroisoquinoline based organocatalysts for asymmetric Diels-Alder reactions: insight into the catalytic mode using ROESY NMR and DFT studies. <i>Tetrahedron: Asymmetry</i> , 2010, 21, 2859-2867.	1.8	30

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55	Synthesis and transport studies of a new class of cage-annulated chiral macrocycles. <i>Tetrahedron: Asymmetry</i> , 2003, 14, 1553-1557.	1.8	29
56	Design and study of peptide-based inhibitors of amylin cytotoxicity. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2010, 20, 1360-1362.	2.2	29
57	Synthesis of 8,11-dihydroxy-pentacyclo[5.4.0.02,6.03,10.05,9]Undecane-8,11-lactam. <i>Tetrahedron</i> , 1993, 49, 9573-9580.	1.9	28
58	Conformational analysis of small peptides of the type Ac-X-NHMe, where X=Gly, Ala, Aib and Cage. <i>Computational and Theoretical Chemistry</i> , 2005, 731, 127-137.	1.5	28
59	A new and facile access to the 2-(indol-3-yl)-3-nitriloquinolines based on Friedländer annulations. <i>Tetrahedron</i> , 2012, 68, 6059-6064.	1.9	28
60	Novel polycyclic cage TM -1,2-diamines as potential anti-tuberculosis agents. <i>European Journal of Medicinal Chemistry</i> , 2012, 54, 1-9.	5.5	28
61	Oxyma-B, an excellent racemization suppressor for peptide synthesis. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 8379-8385.	2.8	28
62	Synthesis, ⁶⁸ Ga-Radiolabeling, and Preliminary <i>In Vivo</i> Assessment of a Depsipeptide-Derived Compound as a Potential PET/CT Infection Imaging Agent. <i>BioMed Research International</i> , 2015, 2015, 1-12.	1.9	28
63	Evidence for the presence of clofazimine and its distribution in the healthy mouse brain. <i>Journal of Molecular Histology</i> , 2015, 46, 439-442.	2.2	27
64	Cu(OAc) ₂ -Catalysed Oxidative Dual ¹ H/ ¹⁵ N Activation of Terminal Alkynes and <i>N</i> -Deprotected Sulfonimidamides: An Easy Access to <i>N</i> -Alkynylated Sulfonimidamides. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 2861-2867.	2.4	27
65	Synthesis of β -lactams from pentacyclo[5.4.0.02,6.03,10.05,9]Undecane-8,11-dione. <i>Tetrahedron</i> , 1994, 50, 10783-10790.	1.9	26
66	Synthesis of tetrahydroisoquinoline-diamine ligands and their application in asymmetric transfer hydrogenation. <i>Tetrahedron: Asymmetry</i> , 2010, 21, 679-687.	1.8	26
67	Total synthesis of a depsidomycin analogue by convergent solid-phase peptide synthesis and macrolactonization strategy for antitubercular activity. <i>Journal of Peptide Science</i> , 2011, 17, 683-689.	1.4	26
68	Synthesis of tetrahydroisoquinoline (TIQ)-oxazoline ligands and their application in enantioselective Henry reactions. <i>Tetrahedron: Asymmetry</i> , 2010, 21, 846-852.	1.8	25
69	Visualization of Time-Dependent Distribution of Rifampicin in Rat Brain Using MALDI MSI and Quantitative LCMS/MS. <i>Assay and Drug Development Technologies</i> , 2015, 13, 277-284.	1.2	25
70	Sub/supercritical fluid chromatography employing water-rich modifier enables the purification of biosynthesized human insulin. <i>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences</i> , 2020, 1155, 122126.	2.3	25
71	Enantioselective synthesis of amino acids from pentacyclo[5.4.0.02,6.03,10.05,9]undecane-8,11-dione. <i>Tetrahedron</i> , 2001, 57, 1601-1607.	1.9	24
72	Pore formation in phospholipid bilayers by amphiphilic cavitands. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 4498.	2.8	24

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73	Synthesis of arylidenepyruvic amide derivatives via Ugi-four component condensation. <i>Tetrahedron Letters</i> , 2012, 53, 3546-3549.	1.4	23
74	Cu(OAc) ₂ promoted Chan–Evans–Lam C–N cross coupling reactions on the N- and N ² -nitrogen atoms of sulfonimidamides with aryl boronic acids. <i>Tetrahedron</i> , 2014, 70, 5428-5433.	1.9	23
75	Dynamics of the thumb-finger regions in a GH11 xylanase <i>Bacillus circulans</i> : comparison between the Michaelis and covalent intermediate. <i>RSC Advances</i> , 2015, 5, 82381-82394.	3.6	23
76	Binding Free Energy Calculations of Nine FDA-approved Protease Inhibitors Against HIV-1 Subtype C I36T†T Containing 100 Amino Acids Per Monomer. <i>Chemical Biology and Drug Design</i> , 2016, 87, 487-498.	3.2	23
77	A comparative modeling and molecular docking study on <i>Mycobacterium tuberculosis</i> targets involved in peptidoglycan biosynthesis. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016, 34, 2399-2417.	3.5	23
78	Tissue distribution of pretomanid in rat brain via mass spectrometry imaging. <i>Xenobiotica</i> , 2016, 46, 247-252.	1.1	23
79	Enhanced brain penetration of pretomanid by intranasal administration of an oil-in-water nanoemulsion. <i>Nanomedicine</i> , 2018, 13, 997-1008.	3.3	23
80	Spatial distribution of elvitegravir and tenofovir in rat brain tissue: Application of matrix-assisted laser desorption/ionization mass spectrometry imaging and liquid chromatography/tandem mass spectrometry. <i>Rapid Communications in Mass Spectrometry</i> , 2019, 33, 1643-1651.	1.5	23
81	Crystal, spectroscopic and quantum mechanics studies of Schiff bases derived from 4-nitrocinnamaldehyde. <i>Scientific Reports</i> , 2021, 11, 8151.	3.3	23
82	Tetrahydroisoquinoline-Based <i>N</i> -Oxides as Chiral Organocatalysts for the Asymmetric Allylation of Aldehydes. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 6923-6932.	2.4	22
83	Pentacycloundecane derived hydroxy acid peptides: A new class of irreversible non-scissile ether bridged type isoster as potential HIV-1 wild type C-SA protease inhibitors. <i>Bioorganic Chemistry</i> , 2012, 40, 19-29.	4.1	22
84	Immobilized Coupling Reagents: Synthesis of Amides/Peptides. <i>ACS Combinatorial Science</i> , 2014, 16, 579-601.	3.8	22
85	EDC·HCl and Potassium Salts of Oxyma and Oxyma-B as Superior Coupling Cocktails for Peptide Synthesis. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 3116-3120.	2.4	22
86	Purification and characterization of naturally occurring HIV-1 (South African subtype C) protease mutants from inclusion bodies. <i>Protein Expression and Purification</i> , 2016, 122, 90-96.	1.3	22
87	Pathogenesis of COVID-19 described through the lens of an undersulfated and degraded epithelial and endothelial glycocalyx. <i>FASEB Journal</i> , 2022, 36, e22052.	0.5	22
88	A theoretical study of pentacyclo-undecane cage peptides of the type [Ac-X-Y-NHMe]. <i>Journal of Peptide Science</i> , 2006, 12, 92-105.	1.4	21
89	Iridium-catalyzed asymmetric hydrogenation of olefins using TIQ phosphine-oxazoline ligands. <i>Tetrahedron: Asymmetry</i> , 2010, 21, 2295-2301.	1.8	21
90	Determination of the antitubercular drug PA-824 in rat plasma, lung and brain tissues by liquid chromatography tandem mass spectrometry: Application to a pharmacokinetic study. <i>Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences</i> , 2015, 988, 187-194.	2.3	21

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91	Preclinical Assessment of a ⁶⁸ Ga-DOTA-Functionalized Depsipeptide as a Radiodiagnostic Infection Imaging Agent. <i>Molecules</i> , 2017, 22, 1403.	3.8	21
92	Trishomocubane Amino Acid as a Turn scaffold. <i>Chemical Biology and Drug Design</i> , 2008, 71, 125-130.	3.2	20
93	Silica-bonded vanadic acid [SiO ₂ -VO(OH) ₂] as a heterogeneous and recyclable catalyst for thiocyanation of organic compounds in aqueous media at room temperature. <i>Catalysis Communications</i> , 2012, 26, 34-38.	3.3	19
94	Synthesis, 2D-NMR and molecular modelling studies of pentacycloundecane lactam-peptides and peptoids as potential HIV-1 wild type C-SA protease inhibitors. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2013, 28, 78-88.	5.2	19
95	A critical survey of average distances between catalytic carboxyl groups in glycoside hydrolases. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 1747-1755.	2.6	19
96	Simulating the inhibition reaction of <i>Mycobacterium tuberculosis</i> -transpeptidase 2 by carbapenems. <i>Chemical Communications</i> , 2015, 51, 12560-12562.	4.1	19
97	Synthetic approaches to radiochemical probes for imaging of bacterial infections. <i>European Journal of Medicinal Chemistry</i> , 2017, 133, 287-308.	5.5	19
98	Bedaquiline has potential for targeting tuberculosis reservoirs in the central nervous system. <i>RSC Advances</i> , 2018, 8, 11902-11907.	3.6	19
99	The downfall of TBA-354 – a possible explanation for its neurotoxicity via mass spectrometric imaging. <i>Xenobiotica</i> , 2018, 48, 938-944.	1.1	19
100	A 2018–2019 patent review of metallo beta-lactamase inhibitors. <i>Expert Opinion on Therapeutic Patents</i> , 2020, 30, 541-555.	5.0	19
101	Computational study of the conformational preferences of the (R)-8-amino-pentacyclo[5.4.0.0 ^{2,6} .0 ^{3,10} .0 ^{5,9}] undecane-8-carboxylic acid mono-peptide. <i>Journal of Peptide Science</i> , 2004, 10, 274-284.	1.4	18
102	Targeting the cell wall of <i>Mycobacterium tuberculosis</i> : a molecular modeling investigation of the interaction of imipenem and meropenem with L,D-transpeptidase 2. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016, 34, 304-317.	3.5	18
103	Lansoprazole-sulfide, pharmacokinetics of this promising anti-tuberculous agent. <i>Biomedical Chromatography</i> , 2017, 31, e4035.	1.7	18
104	Mass Spectrometry Imaging Demonstrates the Regional Brain Distribution Patterns of Three First-Line Antiretroviral Drugs. <i>ACS Omega</i> , 2019, 4, 21169-21177.	3.5	18
105	Synthesis of chiral pentacyclo-undecane macrocycles and their use in enantioselective Michael addition reactions. <i>Tetrahedron: Asymmetry</i> , 2004, 15, 3775-3781.	1.8	17
106	Regioselective protection of hydantoins – essential for hydantoin based anti-epileptic drugs. <i>Structural Chemistry</i> , 2006, 17, 121-125.	2.0	17
107	Analysis of the conformational profile of trishomocubane amino acid dipeptide. <i>Biopolymers</i> , 2006, 81, 339-349.	2.4	17
108	NMR assignments of a di-pentacyclo-undecane cyclic ether. <i>Magnetic Resonance in Chemistry</i> , 2006, 44, 1058-1062.	1.9	17

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109	Microwave assisted SPPS of amylin and its toxicity of the pure product to RIN β 5F cells. <i>Biopolymers</i> , 2010, 94, 323-330.	2.4	17
110	Crystal structure and potent antifungal activity of synthetic homoisoflavanone analogues. <i>Journal of Pharmacy Research</i> , 2013, 6, 1-5.	0.4	17
111	Microreactors for peptide synthesis: looking through the eyes of twenty first century !!! <i>Amino Acids</i> , 2014, 46, 2091-2104.	2.7	17
112	MALDI MSI and LC \AA MS/MS: Towards preclinical determination of the neurotoxic potential of fluoroquinolones. <i>Drug Testing and Analysis</i> , 2016, 8, 832-838.	2.6	17
113	Chemical speciation of copper(ii) diaminediamide derivative of pentacycloundecane \AA a potential anti-inflammatory agent. <i>Dalton Transactions</i> , 2007, , 1140-1149.	3.3	16
114	Microwave \AA Assisted Synthesis of Guanidine Organocatalysts Bearing a Tetrahydroisoquinoline Framework and Their Evaluation in Michael Addition Reactions. <i>European Journal of Organic Chemistry</i> , 2012, 2012, 3331-3337.	2.4	16
115	Synthesis and molecular modelling studies of novel carbapeptide analogs for inhibition of HIV-1 protease. <i>European Journal of Medicinal Chemistry</i> , 2012, 53, 13-21.	5.5	16
116	Base-catalyzed cyclization of Ugi-adducts to substituted indolyl based β -lactams. <i>Monatshefte F\AAur Chemie</i> , 2014, 145, 1947-1952.	1.8	16
117	A novel and more efficient biosynthesis approach for human insulin production in <i>Escherichia coli</i> (E. Tj ETQq1 1 0.784314 r β BT /Ove	3.0	16
118	Complete NMR Elucidation of Two N-Protected Trishomocubane Hydantoins and the Ethyl Ester of the Corresponding Amino Acid. <i>Structural Chemistry</i> , 2005, 16, 129-134.	2.0	15
119	Experimental and computational studies of the regioselective protection of hydantoins using anhydride. <i>Computational and Theoretical Chemistry</i> , 2006, 771, 165-170.	1.5	15
120	Synthesis, screening and computational investigation of pentacycloundecane-peptoids as potent CSA-HIV PR inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2012, 57, 459-467.	5.5	15
121	Pentacycloundecane \AA diol \AA Based HIV \AA 1 Protease Inhibitors: Biological Screening, 2 \AA ... \AA NMR, and Molecular Simulation Studies. <i>ChemMedChem</i> , 2012, 7, 1009-1019.	3.2	15
122	Molecular Modeling of <i>T.Ârangeli</i> , <i>T.Âbrucei gambiense</i> , and <i>T.Âevansi</i> Sialidases in Complex with the DANA Inhibitor. <i>Chemical Biology and Drug Design</i> , 2012, 80, 114-120.	3.2	15
123	Catalytic asymmetric carbon \AA carbon bond forming reactions catalyzed by tetrahydroisoquinoline (TIQ) N,N \AA 2-dioxide ligands. <i>Tetrahedron: Asymmetry</i> , 2013, 24, 191-195.	1.8	15
124	Development and validation of a liquid chromatography \AA tandem mass spectrometry (LC \AA MS/MS) method for the quantification of tigecycline in rat brain tissues. <i>Biomedical Chromatography</i> , 2016, 30, 837-845.	1.7	15
125	An improved and efficient strategy for the total synthesis of a colistin-like peptide. <i>Tetrahedron Letters</i> , 2016, 57, 1885-1888.	1.4	15
126	Unraveling the concerted catalytic mechanism of the human immunodeficiency virus type 1 (HIV-1) protease: a hybrid QM/MM study. <i>Structural Chemistry</i> , 2019, 30, 409-417.	2.0	15

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127	Drug repurposing and computational modeling for discovery of inhibitors of the main protease (M ^{pro}) of SARS-CoV-2. RSC Advances, 2021, 11, 23450-23458.	3.6	15
128	Interconversions between β -Lactam and β -Lactone Derivatives Initiated by Unique Transannular Interactions of the Rigid Cyclohexane Boat Structure in Pentacycloundecane. Journal of Organic Chemistry, 2004, 69, 4863-4866.	3.2	14
129	Synthesis and NMR elucidation of pentacyclo-undecane diamine derivatives as potential anti-tuberculosis drugs. Structural Chemistry, 2008, 19, 719-726.	2.0	14
130	Proline N-oxides: modulators of the 3D conformation of linear peptides through α -NO-turns. Organic and Biomolecular Chemistry, 2014, 12, 4479.	2.8	14
131	A sensitive WST-8-based bioassay for PEGylated granulocyte colony stimulating factor using the NFS-60 cell line. Pharmaceutical Biology, 2015, 53, 849-854.	2.9	14
132	Potential inhibition of HIV-1 encapsidation by oligoribonucleotide–dendrimer nanoparticle complexes. International Journal of Nanomedicine, 2017, Volume 12, 317-325.	6.7	14
133	Evaluating the Performance of a Non-Bonded Cu ²⁺ Model Including Jahn-Teller Effect into the Binding of Tyrosinase Inhibitors. International Journal of Molecular Sciences, 2020, 21, 4783.	4.1	14
134	Synthesis of 4-oxahexacyclo[5.4.1.0 ^{2,6} .0 ^{3,10} .0 ^{5,9} .0 ^{8,11}]dodecane-3-carboxylic acid. Tetrahedron, 1993, 49, 6527-6532.	1.9	13
135	Complete NMR elucidation of a novel trishomocubane hydantoin and its mono- and bis-t-Boc protected derivatives. Magnetic Resonance in Chemistry, 2004, 42, 617-623.	1.9	13
136	Simulated annealing study of the pentacyclo-undecane cage amino acid tripeptides of the type [Ac-X-Y-Z-NHMe]. Computational and Theoretical Chemistry, 2006, 759, 145-157.	1.5	13
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