

# 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  
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394  
all docs

394  
docs citations

394  
times ranked

7505  
citing authors

#	ARTICLE	IF	CITATIONS
1	Exploring the concerted mechanistic pathway for HIV-1 PRα€"substrate revealed by umbrella sampling simulation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 1736-1747.	3.5	6
2	Mechanistic insight on the inhibition of D, D-carboxypeptidase from <i>&lt; i&gt;Mycobacterium tuberculosis&lt;/i&gt;</i> by <i>&lt; i&gt;Î²&lt;/i&gt;-lactam antibiotics: an ÖNIOM acylation study</i> . <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 7645-7655.	3.5	1
3	Experimental measurement of kinetic parameters using quantum plasmonic sensing. <i>Journal of Applied Physics</i> , 2022, 131, 084402.	2.5	4
4	Measuring kinetic parameters using quantum plasmonic sensing. <i>Physical Review A</i> , 2022, 105, .	2.5	3
5	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
6	Synthesis, Crystal structure, photoluminescence properties and quantum mechanics studies of two schiff bases of 2-amino-p-cresol. <i>Journal of Molecular Structure</i> , 2022, 1262, 133046.	3.6	4
7	3-Br-Bromoacetylcoumarin, a Crucial Key for Facial Synthesis of Biological Active Compounds. <i>ChemistrySelect</i> , 2022, 7, .	1.5	3
8	Active targeting of CD4 <sup>+</sup> T lymphocytes by PEI-capped, peptide-functionalized gold nanoparticles. <i>Nanotechnology</i> , 2022, 33, 405101.	2.6	2
9	Organic Base-Mediated Carboxylation of (Hetero)aromatic Compounds Using Supercritical Carbon Dioxide (scCO <sub>2</sub> ). <i>Synthesis</i> , 2022, 54, 4827-4833.	2.3	3
10	Drug repurposing and computational modeling for discovery of inhibitors of the main protease (M <sup>pro</sup> ) of SARS-CoV-2. <i>RSC Advances</i> , 2021, 11, 23450-23458.	3.6	15
11	Crystal, spectroscopic and quantum mechanics studies of Schiff bases derived from 4-nitrocinnamaldehyde. <i>Scientific Reports</i> , 2021, 11, 8151.	3.3	23
12	Alterations in neurotransmitter levels and transcription factor expression following intranasal buprenorphine administration. <i>Biomedicine and Pharmacotherapy</i> , 2021, 138, 111515.	5.6	2
13	Potential of brain mast cells for therapeutic application in the immune response to bacterial and viral infections. <i>Brain Research</i> , 2021, 1767, 147524.	2.2	0
14	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
15	Trends in NMR Structural Elucidation Of Polycyclic Cages, Namely: Adamantane, Pentacycloundecane and Trishomocubane. <i>South African Journal of Chemistry</i> , 2021, 75, .	0.6	0
16	Purification and characterization of Î±-amylase from <i>&lt; i&gt;Paenibacillus&lt;/i&gt;</i> sp. D9 and <i>&lt; i&gt;Escherichia coli&lt;/i&gt;</i> recombinants. <i>Biocatalysis and Biotransformation</i> , 2020, 38, 24-34.	2.0	4
17	Mass spectrometric investigations into the brain delivery of abacavir, stavudine and didanosine in a rodent model. <i>Xenobiotica</i> , 2020, 50, 570-579.	1.1	2
18	Serendipitous discovery of new pentacycloundecane molecules. <i>Journal of Molecular Structure</i> , 2020, 1204, 127497.	3.6	4

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19	The development of a sub/supercritical fluid chromatography based purification method for peptides. Journal of Pharmaceutical and Biomedical Analysis, 2020, 190, 113539.	2.8	10
20	Evaluating the Performance of a Non-Bonded Cu <sup>2+</sup> Model Including Jahn-Teller Effect into the Binding of Tyrosinase Inhibitors. International Journal of Molecular Sciences, 2020, 21, 4783.	4.1	14
21	Microwave-assisted synthesis of <i>&lt; i&gt;meso&lt;/i&gt;-carboxyalkyl-BODIPYs and an application to fluorescence imaging</i> . Organic and Biomolecular Chemistry, 2020, 18, 7876-7883.	2.8	6
22	Sub/supercritical fluid chromatography employing water-rich modifier enables the purification of biosynthesized human insulin. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2020, 1155, 122126.	2.3	25
23	A novel and more efficient biosynthesis approach for human insulin production in <i>Escherichia coli</i> (E.) Tj ETQq1 1 0.784314 rgBT /Overexpression	3.8	56
24	A 2018–2019 patent review of metallo beta-lactamase inhibitors. Expert Opinion on Therapeutic Patents, 2020, 30, 541-555.	5.0	19
25	Mass Spectrometric Imaging of the Brain Demonstrates the Regional Displacement of 6-Monoacetylmorphine by Naloxone. ACS Omega, 2020, 5, 12596-12602.	3.5	4
26	Improved Synthesis and Isolation of Bedaquiline. ACS Omega, 2020, 5, 3607-3611.	3.5	12
27	Microwave-Accelerated N-Acylation of Sulfoximines with Aldehydes under Catalyst-Free Conditions. Synthesis, 2020, 52, 1279-1286.	2.3	7
28	Concerted hydrolysis mechanism of HIV-1 natural substrate against subtypes B and C-SA PR: insight through molecular dynamics and hybrid QM/MM studies. Physical Chemistry Chemical Physics, 2020, 22, 2530-2539.	2.8	10
29	From Recognition to Reaction Mechanism: An Overview on the Interactions between HIV-1 Protease and its Natural Targets. Current Medicinal Chemistry, 2020, 27, 2514-2549.	2.4	9
30	Structure and Function of L,D- and D,D-Transpeptidase Family Enzymes from <i>Mycobacterium tuberculosis</i> . Current Medicinal Chemistry, 2020, 27, 3250-3267.	2.4	13
31	In Silico Modelling in the Development of Novel Radiolabelled Peptide Probes. Current Medicinal Chemistry, 2020, 27, 7048-7063.	2.4	7
32	Development of a paper-based microfluidic device for the quantification of ammonia in industrial wastewater. Water S A, 2020, 46, .	0.4	3
33	Correction to “Improved Synthesis and Isolation of Bedaquiline”. ACS Omega, 2020, 5, 24154-24154.	3.5	0
34	Kinetic and thermodynamic characterisation of HIV-protease inhibitors against E35D/S mutant in the South African HIV-1 subtype C protease. Journal of Enzyme Inhibition and Medicinal Chemistry, 2019, 34, 1451-1456.	5.2	4
35	Theoretical Model for HIV-1 PR That Accounts for Substrate Recognition and Preferential Cleavage of Natural Substrates. Journal of Physical Chemistry B, 2019, 123, 6389-6400.	2.6	5
36	Fabrication and application of a gold nanoparticle-based colorimetric device for the determination of NaCl in seawater and estuarine water. Journal of Nanoparticle Research, 2019, 21, 1.	1.9	11

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37	Zidovudine and Lamivudine as Potential Agents to Combat HIV-Associated Neurocognitive Disorder. Assay and Drug Development Technologies, 2019, 17, 322-329.	1.2	3
38	Investigating time dependent brain distribution of nevirapine via mass spectrometric imaging. Journal of Molecular Histology, 2019, 50, 593-599.	2.2	5
39	Identification of potent L,D-transpeptidase 5 inhibitors for <i>Mycobacterium tuberculosis</i> as potential anti-TB leads: virtual screening and molecular dynamics simulations. Journal of Molecular Modeling, 2019, 25, 328.	1.8	13
40	<math>\text{N}</math>-Trifluoromethylthiolated Sulfonimidamides and Sulfoximines: Anti-microbial, Anti-mycobacterial, and Cytotoxic Activity. ACS Medicinal Chemistry Letters, 2019, 10, 1457-1461.	2.8	31
41	Optimized Procedure for Recovering HIV-1 Protease (C-SA) from Inclusion Bodies. Protein Journal, 2019, 38, 30-36.	1.6	2
42	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. Rapid Communications in Mass Spectrometry, 2019, 33, 1643-1651.	1.5	23
43	Rilpivirine as a potential candidate for the treatment of HIV-associated neurocognitive disorders (HAND). Journal of Molecular Histology, 2019, 50, 295-303.	2.2	9
44	Optimization of CIEL*a*b*/Yxy colour system for colorimetric devices fabricated with gold nanoparticles. Journal of Molecular Structure, 2019, 1191, 271-277.	3.6	6
45	The Driving Force for the Acylation of $\beta$ -Lactam Antibiotics by L,D-Transpeptidase 2: Quantum Mechanics/Molecular Mechanics (QM/MM) Study. ChemPhysChem, 2019, 20, 1126-1134.	2.1	13
46	Brain penetration of ketamine: Intranasal delivery VS parenteral routes of administration. Journal of Psychiatric Research, 2019, 112, 7-11.	3.1	13
47	Crystal structure of (E)-2-(4-cyanophenyl)ethenesulfonyl fluoride, C9H6FNO2S. Zeitschrift Fur Kristallographie - New Crystal Structures, 2019, 234, 441-442.	0.3	0
48	Mass Spectrometry Imaging Demonstrates the Regional Brain Distribution Patterns of Three First-Line Antiretroviral Drugs. ACS Omega, 2019, 4, 21169-21177.	3.5	18
49	Inhibition mechanism of L,D-transpeptidase 5 in presence of the $\beta$ -lactams using ONIOM method. Journal of Molecular Graphics and Modelling, 2019, 87, 204-210.	2.4	12
50	Unraveling the concerted catalytic mechanism of the human immunodeficiency virus type 1 (HIV-1) protease: a hybrid QM/MM study. Structural Chemistry, 2019, 30, 409-417.	2.0	15
51	N-Vanine-2-(3,5-dimethyl-1,1-dioxido-2H-1,2,6-thiadiazin-4-yl)Benzamide: Synthesis, X-ray Structure and Hirshfeld Surface Analysis. Journal of Chemical Crystallography, 2019, 49, 65-71.	1.1	0
52	Time-dependent regional brain distribution of methadone and naltrexone in the treatment of opioid addiction. Addiction Biology, 2019, 24, 438-446.	2.6	13
53	Development and Evaluation of Peptide-Functionalized Gold Nanoparticles for HIV Integrase Inhibition. International Journal of Peptide Research and Therapeutics, 2019, 25, 311-322.	1.9	12
54	The South African Journal of Chemistry 1918-2018: A Celebration. South African Journal of Chemistry, 2019, 72, 201-206.	0.6	0

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55	Crystal structure of 2-(bis(3,5-dimethylphenyl) ((methyldiphenylsilyl)oxy)methyl) pyrrolidine, C <sub>34</sub> H <sub>39</sub> NOSi. Zeitschrift Fur Kristallographie - New Crystal Structures, 2019, 234, 413-415.	0.3	0
56	A Computational Study of the Mechanism of Formation of the Penta-Cyclo Undecane (PCU) Cage Lactam., 2019, , 511-514.		0
57	An insight to the molecular interactions of the FDA approved HIV-PR drugs against L38L <sup>N</sup> L PR mutant. Journal of Computer-Aided Molecular Design, 2018, 32, 459-471.	2.9	11
58	An unexpected re-arrangement of the antibiotic carbapenem core to new 1,4-diazepin-5-one scaffolds. RSC Advances, 2018, 8, 190-193.	3.6	1
59	Bedaquiline has potential for targeting tuberculosis reservoirs in the central nervous system. RSC Advances, 2018, 8, 11902-11907.	3.6	19
60	Clofazimine protects against Mycobacterium tuberculosis dissemination in the central nervous system following aerosol challenge in a murine model. International Journal of Antimicrobial Agents, 2018, 51, 77-81.	2.5	12
61	<sc>DFT</sc> study of the acid-catalyzed esterification reaction mechanism of methanol with carboxylic acid and its halide derivatives. International Journal of Quantum Chemistry, 2018, 118, e25497.	2.0	41
62	The downfall of TBA-354 – a possible explanation for its neurotoxicity <i>via</i> mass spectrometric imaging. Xenobiotica, 2018, 48, 938-944.	1.1	19
63	Synthesis of novel 1,2,4-thiadiazinane 1,1-dioxides <i>via</i> three component SuFEx type reaction. RSC Advances, 2018, 8, 37503-37507.	3.6	10
64	Inhibition of <i>Mycobacterium tuberculosis</i> L,D-transpeptidase 5 by Carbapenems: MD and QM/MM Mechanistic Studies. ChemistrySelect, 2018, 3, 13603-13612.	1.5	6
65	Crystal structure of (E)-2-(4-bromophenyl)ethenesulfonyl fluoride (C <sub>8</sub> H <sub>6</sub> BrFO <sub>2</sub> S). Zeitschrift Fur Kristallographie - New Crystal Structures, 2018, 233, 793-794.	0.3	1
66	The catalytic role of water in the binding site of L,D-transpeptidase 2 within acylation mechanism: A QM/MM (ONIOM) modelling. Tuberculosis, 2018, 113, 222-230.	1.9	13
67	Molecular insight on the non-covalent interactions between carbapenems and L,D-transpeptidase 2 from Mycobacterium tuberculosis: ONIOM study. Journal of Computer-Aided Molecular Design, 2018, 32, 687-701.	2.9	10
68	A DFT mechanistic study of the ODH of n-hexane over isolated H <sub>3</sub> VO <sub>4</sub> . Molecular Catalysis, 2018, 452, 83-92.	2.0	4
69	Enhanced brain penetration of pretomanid by intranasal administration of an oil-in-water nanoemulsion. Nanomedicine, 2018, 13, 997-1008.	3.3	23
70	Introduction and Importance of Synthetic Organic Dyes. , 2018, , 1-7.		6
71	Exploring the flap dynamics of the South African HIV subtype C protease in presence of FDA-approved inhibitors: MD study. Chemical Biology and Drug Design, 2018, 92, 1899-1913.	3.2	3
72	The Dyes Based on Several Chromophores. , 2018, , 223-243.		0

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73	Synthesis, Characterization and Biocompatibility of a Multifunctional Gold Nanoparticle System for the Delivery of Single-Stranded RNA to Lymphocytes. <i>South African Journal of Chemistry</i> , 2018, 71, 1-14.	0.6	6
74	Fast and efficient detection of tuberculosis antigens using liposome encapsulated secretory proteins of <i>Mycobacterium tuberculosis</i> . <i>Journal of Microbiology, Immunology and Infection</i> , 2017, 50, 189-198.	3.1	12
75	A Synthesis of “Dual Warhead” $\beta^2$ -Aryl Ethenesulfonyl Fluorides and One-Pot Reaction to $\beta^2$ -Sultams. <i>Organic Letters</i> , 2017, 19, 480-483.	4.6	91
76	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
77	Microwave-Assisted Synthesis of Antimicrobial Peptides. <i>Methods in Molecular Biology</i> , 2017, 1548, 51-59.	0.9	6
78	Crystal structure of 5-acetyl-3-(3-fluoro-4-morpholinophenyl)oxazolidin-2-one, C15H17FN2O4. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2017, 232, 427-428.	0.3	0
79	Differential flap dynamics in $\alpha$ -transpeptidase2 from <i>mycobacterium tuberculosis</i> revealed by molecular dynamics. <i>Molecular BioSystems</i> , 2017, 13, 1223-1234.	2.9	36
80	Lansoprazole sulfide, pharmacokinetics of this promising anti-tuberculous agent. <i>Biomedical Chromatography</i> , 2017, 31, e4035.	1.7	18
81	I36T $\rightarrow$ T mutation in South African subtype C (C-SA) HIV-1 protease significantly alters protease-drug interactions. <i>Biological Chemistry</i> , 2017, 398, 1109-1117.	2.5	10
82	Post heroin dose tissue distribution of 6-monoacetylmorphine (6-MAM) with MALDI imaging. <i>Journal of Molecular Histology</i> , 2017, 48, 285-292.	2.2	11
83	Crystal structure of 4,10,16,22-tetrahydroxy-6,12,18,24-tetramethoxy-2,8,14,20-tetraethylphenylresorcin[4]arene ethyl acetate (1/1), C <sub>68</sub> H <sub>72</sub> O <sub>10</sub> . <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2017, 232, 305-307.	0.3	0
84	Synthesis, in vitro evaluation, and $^{68}$ Ga $\rightarrow$ radiolabeling of CDP1 toward PET/CT imaging of bacterial infection. <i>Chemical Biology and Drug Design</i> , 2017, 90, 572-579.	3.2	10
85	Synthetic approaches to radiochemical probes for imaging of bacterial infections. <i>European Journal of Medicinal Chemistry</i> , 2017, 133, 287-308.	5.5	19
86	Sulfonimidamide in medizinischer Chemie und Agrochemie. <i>Angewandte Chemie</i> , 2017, 129, 4160-4170.	2.0	34
87	Sulfonimidamides in Medicinal and Agricultural Chemistry. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 4100-4109.	13.8	145
88	The role of nanotechnology in the treatment of viral infections. <i>Therapeutic Advances in Infectious Disease</i> , 2017, 4, 105-131.	1.8	233
89	Crystal structure of (S)-benzyl 3-(benzylcarba-moyl)-3,4-dihydroisoquinoline-2(1H)-carboxylate, C <sub>25</sub> H <sub>24</sub> N <sub>2</sub> O <sub>3</sub> . <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2017, 232, 425-426.	0.3	0
90	Crystal structure of methyl 1-(2-(fluorosulfonyl)ethyl)-2-oxocyclopentanecarboxylate, C <sub>9</sub> H <sub>13</sub> FO <sub>5</sub> S. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2017, 232, 697-698.	0.3	0

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91	Metabolic Imaging of Infection. <i>Journal of Nuclear Medicine</i> , 2017, 58, 1727-1732.	5.0	40
92	Investigation of the binding free energies of FDA approved drugs against subtype B and C-SA HIV PR: ONIOM approach. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 76, 77-85.	2.4	12
93	Evaluation of a Flexible NOTA-RGD Kit Solution Using Gallium-68 from Different 68Ge/68Ga-Generators: Pharmacokinetics and Biodistribution in Nonhuman Primates and Demonstration of Solitary Pulmonary Nodule Imaging in Humans. <i>Molecular Imaging and Biology</i> , 2017, 19, 469-482.	2.6	13
94	Computational model for the acylation step of the $\beta$ -lactam ring: Potential application for l,d-transpeptidase 2 in mycobacterium tuberculosis. <i>Journal of Molecular Structure</i> , 2017, 1128, 94-102.	3.6	41
95	Crystal structure of <i>i&gt;tert&lt;/i&gt;-butyl (phenylsulfinyl)carbamate, C&lt;sub&gt;11&lt;/sub&gt;H&lt;sub&gt;15&lt;/sub&gt;NO&lt;sub&gt;3&lt;/sub&gt;S. Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2017, 232, 577-578.	0.3	2
96	Crystal structure of 5,11,17,23-tetra(tert-butyl)-25,26,27,28-tetrahexoxycalix[4]arene, C<sub>68</sub>H<sub>104</sub>O<sub>4</sub>. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2017, 232, 397-402.	0.3	0
97	Potential inhibition of HIV-1 encapsidation by oligoribonucleotide&ndash;dendrimer nanoparticle complexes. <i>International Journal of Nanomedicine</i> , 2017, Volume 12, 317-325.	6.7	14
98	Preclinical Assessment of a 68Ga-DOTA-Functionalized Depsipeptide as a Radiodiagnostic Infection Imaging Agent. <i>Molecules</i> , 2017, 22, 1403.	3.8	21
99	Structure-Activity Relationship of Arg10-Teixobactin: A Recently Discovered Antimicrobial Peptide. <i>Proceedings (mdpi)</i> , 2017, 1, .	0.2	0
100	Synthesis, Crystal Structure and DFT Studies of 1,3-Dimethyl-5-propionylpyrimidine-2,4,6(1H,3H,5H)-trione. <i>Crystals</i> , 2017, 7, 31.	2.2	6
101	Density functional theory studies of the uncatalysed gas-phase oxidative dehydrogenation conversion of n-hexane to hexenes. <i>Computational and Theoretical Chemistry</i> , 2017, 1114, 153-164.	2.5	10
102	Artificial Intelligence vs. Statistical Modeling and Optimization of Continuous Bead Milling Process for Bacterial Cell Lysis. <i>Frontiers in Microbiology</i> , 2016, 7, 1852.	3.5	9
103	<i>In vitro</i> evaluation of metal chelators as potential metallo- $\beta$ -lactamase inhibitors. <i>Journal of Applied Microbiology</i> , 2016, 120, 860-867.	3.1	38
104	Development and validation of a liquid chromatography-tandem mass spectrometry (LC-MS/MS) method for the quantification of tigecycline in rat brain tissues. <i>Biomedical Chromatography</i> , 2016, 30, 837-845.	1.7	15
105	Crystal structure of 2-ethyl-1- <i>tert</i> -butyl 3-oxo-2-[phenyl( <i>tert</i> -butoxycarbonylamino)methyl]-1,2-pyrrolidinedicarboxylate, C<sub>24</sub>H<sub>34</sub>N<sub>2</sub>O<sub>7</sub>. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2016, 231, 725-727.	0.3	0
106	Lysine Scanning of Arg<sub>10</sub> Teixobactin: Deciphering the Role of Hydrophobic and Hydrophilic Residues. <i>ACS Omega</i> , 2016, 1, 1262-1265.	3.5	51
107	A Facile Synthesis of NODASA-Functionalized Peptide. <i>Synlett</i> , 2016, 27, 1685-1688.	1.8	7
108	Crystal structure of 2-(ethoxycarbonyl)-2-(2-nitro-1-phenylethyl)-3-oxopyrrolidinium chloride, C<sub>15</sub>H<sub>19</sub>N<sub>2</sub>O<sub>5</sub>Cl. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2016, 231, 43-45.	0.3	0

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109	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
110	Diverse supramolecular arrangement of substituted oxopyrrolidine analogues influenced by weak intermolecular interactions ( $\text{CH}_2\text{O}/\text{CH}_2\text{C}(=\text{O})/\text{H}_2\text{O}$ ). <i>Journal of Molecular Structure</i> , 2016, 1122, 37-47.	3.6	1
111	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
112	Re-evaluation of the N-terminal substitution and the D-residues of teixobactin. <i>RSC Advances</i> , 2016, 6, 73827-73829.	3.6	34
113	Enantioselective Organocatalyzed Transformations of $\beta^2$ -Ketoesters. <i>Chemical Reviews</i> , 2016, 116, 9375-9437.	47.7	105
114	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
115	Intracellular localization of gold nanoparticles with targeted delivery in MT-4 lymphocytes. <i>Advances in Natural Sciences: Nanoscience and Nanotechnology</i> , 2016, 7, 045013.	1.5	12
116	Crystal structure of butyl 2-(3,5-dimethyl-1,1-dioxido-2H-1,2,6-thiadiazin-4-yl)benzoate, C <sub>16</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub> S. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2016, 231, 373-374.	0.3	0
117	MALDI MSI and LC-MS/MS: Towards preclinical determination of the neurotoxic potential of fluoroquinolones. <i>Drug Testing and Analysis</i> , 2016, 8, 832-838.	2.6	17
118	Neuroprotective potential of Linezolid: a quantitative and distribution study via mass spectrometry. <i>Journal of Molecular Histology</i> , 2016, 47, 429-435.	2.2	6
119	Oxyma-T, expanding the arsenal of coupling reagents. <i>Tetrahedron Letters</i> , 2016, 57, 3523-3525.	1.4	5
120	Binding Free Energy Calculations of Nine FDA-approved Protease Inhibitors Against HIV-1 Subtype C I36T <sup>†</sup> T <sup>‡</sup> Containing 100 Amino Acids Per Monomer. <i>Chemical Biology and Drug Design</i> , 2016, 87, 487-498.	3.2	23
121	Small molecule distribution in rat lung: a comparison of various cryoprotectants as inflation media and their applicability to MSI. <i>Journal of Molecular Histology</i> , 2016, 47, 213-219.	2.2	8
122	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
123	On-Water Synthesis of Biaryl Sulfonyl Fluorides. <i>Journal of Organic Chemistry</i> , 2016, 81, 2618-2623.	3.2	49
124	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
125	An Efficient Protecting-Group-Free Synthesis of Vinyllic Sulfoximines via Horner-Wadsworth-Emmons Reaction. <i>Synlett</i> , 2016, 27, 1423-1427.	1.8	9
126	Highly chemoselective ligation of thiol- and amino-peptides on a bromomaleimide core. <i>Chemical Communications</i> , 2016, 52, 2334-2337.	4.1	9

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127	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
128	Tissue distribution of pretomanid in rat brain via mass spectrometry imaging. <i>Xenobiotica</i> , 2016, 46, 247-252.	1.1	23
129	2-Methyltetrahydrofuran and cyclopentyl methyl ether for green solid-phase peptide synthesis. <i>Amino Acids</i> , 2016, 48, 419-426.	2.7	69
130	Rapid and widespread distribution of doxycycline in rat brain: a mass spectrometric imaging study. <i>Xenobiotica</i> , 2016, 46, 385-392.	1.1	8
131	Targeting the cell wall of <i>Mycobacterium tuberculosis</i> : a molecular modeling investigation of the interaction of imipenem and meropenem with <i>L</i> - <i>D</i> -transpeptidase 2. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016, 34, 304-317.	3.5	18
132	In vitro investigation of the antimicrobial activity of a series of lipophilic phenols and naphthols. <i>South African Journal of Chemistry</i> , 2016, 69, .	0.6	5
133	Stereoselective synthesis towards unnatural proline based amino acids. <i>Arkivoc</i> , 2016, 2016, 134-144.	0.5	5
134	Organocatalyzed Mannich reactions on minocycline: Towards novel tetracycline antibiotics. <i>South African Journal of Chemistry</i> , 2016, 69, .	0.6	2
135	Advances in the Discovery and Development of Peptide Therapeutics. , 2015, , .		1
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259	Methyl 1-cyclohexyl-6,7-dimethoxy-3,4-dihydroisoquinoline-3-carboxylate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011, 67, o883-o883.	0.2	1
260	( <i>S</i> )-2-Benzyl-N-(2,6-diisopropylphenyl)-1,2,3,4-tetrahydroisoquinoline-3-carboxamide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011, 67, o1106-o1106.	0.2	1
261	( <i>S</i> )-N-Benzyl-2-methyl-1,2,3,4-tetrahydroisoquinoline-3-carboxamide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011, 67, o67-o67.	0.2	6
262	3-Benzyl-5,7-dimethoxychroman-4-ol. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011, 67, o703-o703.	0.2	2
263	Benzyl 5-hydroxy-4-oxapentacyclo[5.4.1.0 <sub>2,6</sub> .0 <sub>3,10</sub> .0 <sub>8,11</sub> ]dodecane-3-carboxylate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011, 67, o877-o877.	0.2	0
264	6,7-Dimethoxy-3-methoxycarbonyl-1-(2-methoxyphenyl)-3,4-dihydroisoquinoline 2-oxide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011, 67, o1352-o1352.	0.2	0
265	(1 <i>S,3S</i> )-Methyl 2-benzyl-6,7-dimethoxy-1-phenyl-1,2,3,4-tetrahydroisoquinoline-3-carboxylate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011, 67, o1403-o1403.	0.2	5
266	N-(Adamantan-1-yl)-2-chloroacetamide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011, 67, o1444-o1444.	0.2	0
267	(1 <i>S,3S</i> )-Methyl 6,7-dimethoxy-1-phenyl-1,2,3,4-tetrahydroisoquinoline-3-carboxylate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011, 67, o1501-o1501.	0.2	0
268	Ethyl 6-methyl-2-sulfanylidene-4-[4-(trifluoromethyl)phenyl]-1,2,3,4-tetrahydropyrimidine-5-carboxylate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011, 67, o1559-o1560.	0.2	2
269	2-[(1 <i>R,3S</i> )-6,7-Dimethoxy-1-phenyl-1,2,3,4-tetrahydroisoquinolin-3-yl]-4-phenyl-1,3-thiazole. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011, 67, o2722-o2722.	0.2	2
270	Ethyl 4-(1,3-benzodioxol-5-yl)-6-methyl-2-sulfanylidene-1,2,3,4-tetrahydropyrimidine-5-carboxylate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011, 67, o3069-o3070.	0.2	2

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271	(S)-Methyl 3-(3,4-dimethoxyphenyl)-2-[2-(diphenylphosphanyl)benzamido]propanoate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011, 67, o3285-o3285.	0.2	1
272	(1R,3S)-N-Benzhydryl-2-benzyl-6,7-dimethoxy-1-phenyl-1,2,3,4-tetrahydroisoquinoline-3-carbothioamide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011, 67, o3441-o3441.	0.2	1
273	<math>\text{<} \text{i} \text{>} \text{N} \text{<} \text{i} \text{>} \text{-Benzyl-5-(dimethylamino)naphthalene-1-sulfonamide. } \text{Acta Crystallographica Section E: Structure Reports Online}, 2011, 67, o2458-o2459.	0.2	3
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275	Iridium-catalyzed asymmetric hydrogenation of olefins using TiQ phosphine-oxazoline ligands. <i>Tetrahedron: Asymmetry</i> , 2010, 21, 2295-2301.	1.8	21
276	Peptide Functionalised Gold Nanoparticles: Effect of Loading on Aggregation and Proteolysis. <i>International Journal of Peptide Research and Therapeutics</i> , 2010, 16, 291-295.	1.9	2
277	NMR elucidation of novel SQ109 derivatives. <i>Structural Chemistry</i> , 2010, 21, 1203-1209.	2.0	2
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284	Synthesis of tetrahydroisoquinoline (TiQ)-oxazoline ligands and their application in enantioselective Henry reactions. <i>Tetrahedron: Asymmetry</i> , 2010, 21, 846-852.	1.8	25
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286	In vitro ADMET and physicochemical investigations of poly-N-methylated peptides designed to inhibit A <sup>12</sup> aggregation. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 5896-5902.	3.0	37
287	Design and study of peptide-based inhibitors of amylin cytotoxicity. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2010, 20, 1360-1362.	2.2	29
288	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

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290	(1R,3S)-Methyl 6,7-dimethoxy-1-(4-methoxyphenyl)-1,2,3,4-tetrahydroisoquinoline-3-carboxylate. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o3105-o3105.	0.2	2	
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292	tert-ButylN-[(11-exo-benzyloxycarbonyl-8-oxopentacyclo[5.4.0.02,6.03,10.05,9]undecane-11-endo-yloxy)carbonylmethyl]carbamate. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o2607-o2608.	0.2	2	
293	N,Nâ€“-[(8-endo,11-endo-Dihydroxypentacyclo[5.4.0.02,6.03,10.05,9]undecane-8,11-diyl)bis(methylenecarbonyl)]di-L-phenylalanine. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o2537-o2538.	0.2	2	
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301	Ethyl 4-(4-hydroxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate monohydrate. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o2502-o2502.	0.2	3	
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303	2-(4-Chloro-3-nitrophenyl)-4-(4-chlorophenyl)-1,3-thiazole. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o2611-o2612.	0.2	2	
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320	(S)-(+)2-Formylamino-3-methylbutanoic acid. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o3912-o3912.	0.2	0
321	<i>&lt;math&gt;\text{&lt;i&gt;exo&lt;/i&gt;-8,&lt;i&gt;exo&lt;/i&gt;-11-Divinylpentacyclo[5.4.0.0&lt;sup&gt;2,6&lt;/sup&gt;.0&lt;sup&gt;3,10&lt;/sup&gt;.0&lt;sup&gt;5,6&lt;/sup&gt;]undecane-&lt;i&gt;endo&lt;/i&gt;-8,&lt;i&gt;exo&lt;/i&gt;-8&lt;/math&gt;</i> . Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o3977-o3977.	0.2	0
322	<i>&lt;math&gt;\text{&lt;i&gt;exo&lt;/i&gt;-8,&lt;i&gt;exo&lt;/i&gt;-11-Diallylpentacyclo[5.4.0.0&lt;sup&gt;2,6&lt;/sup&gt;.0&lt;sup&gt;3,10&lt;/sup&gt;.0&lt;sup&gt;5,9&lt;/sup&gt;]undecane-&lt;i&gt;endo&lt;/i&gt;-8,&lt;i&gt;exo&lt;/i&gt;-8&lt;/math&gt;</i> . Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o4797-o4797.	0.2	0
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