Glenn E M Maguire

List of Publications by Year
in descending order

229	4,082	172457	138484
papers	citations	29 h-index	58 g-index

244	244	244	4404
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Exploring the concerted mechanistic pathway for HIV-1 PRâ€"substrate revealed by umbrella sampling simulation. Journal of Biomolecular Structure and Dynamics, 2022, 40, 1736-1747.	3.5	6
2	Mechanistic insight on the inhibition of D, D-carboxypeptidase from Mycobacterium tuberculosis by Î²-lactam antibiotics: an ONIOM acylation study. Journal of Biomolecular Structure and Dynamics, 2022, 40, 7645-7655.	3.5	1
3	Experimental measurement of kinetic parameters using quantum plasmonic sensing. Journal of Applied Physics, 2022, 131, 084402.	2.5	4
4	Measuring kinetic parameters using quantum plasmonic sensing. Physical Review A, 2022, 105, .	2.5	3
5	Synthesis, Crystal structure, photoluminescence properties and quantum mechanics studies of two schiff bases of 2-amino-p-cresol. Journal of Molecular Structure, 2022, 1262, 133046.	3.6	4
6	Crystal, spectroscopic and quantum mechanics studies of Schiff bases derived from 4-nitrocinnamaldehyde. Scientific Reports, 2021, 11, 8151.	3.3	23
7	Current trends in computer aided drug design and a highlight of drugs discovered via computational techniques: A review. European Journal of Medicinal Chemistry, 2021, 224, 113705.	5.5	229
8	Serendipitous discovery of new pentacycloundecane molecules. Journal of Molecular Structure, 2020, 1204, 127497.	3.6	4
9	Microwave-assisted synthesis of meso-carboxyalkyl-BODIPYs and an application to fluorescence imaging. Organic and Biomolecular Chemistry, 2020, 18, 7876-7883.	2.8	6
10	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
11	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
12	Structure and Function of L,D- and D,D-Transpeptidase Family Enzymes from Mycobacterium tuberculosis. Current Medicinal Chemistry, 2020, 27, 3250-3267.	2.4	13
13	Kinetic and thermodynamic characterisation of HIV-protease inhibitors against E35Dâ†'Gâ†'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
14	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
15	Identification of potent L,D-transpeptidase 5 inhibitors for Mycobacterium tuberculosis as potential anti-TB leads: virtual screening and molecular dynamics simulations. Journal of Molecular Modeling, 2019, 25, 328.	1.8	13
16	Optimized Procedure for Recovering HIV-1 Protease (C-SA) from Inclusion Bodies. Protein Journal, 2019, 38, 30-36.	1.6	2
17	The Driving Force for the Acylation of Î² â€Lactam Antibiotics by L,Dâ€Transpeptidase 2: Quantum Mechanics/Molecular Mechanics (QM/MM) Study. ChemPhysChem, 2019, 20, 1126-1134.	2.1	13
18	Inhibition mechanism of L,D-transpeptidase 5 in presence of the Î²-lactams using ONIOM method. Journal of Molecular Graphics and Modelling, 2019, 87, 204-210.	2.4	12

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19	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
20	N-Valine-2-(3,5-dimethy-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
21	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
22	Structural Characterization and Thermal Properties of the Anti-malarial Drug: Lumefantrine. South African Journal of Chemistry, 2019, 72, 253-262.	0.6	3
23	An insight to the molecular interactions of the FDA approved HIVÂPR drugs against L38Lâ†'Nâ†'L PR mutant. Journal of Computer-Aided Molecular Design, 2018, 32, 459-471.	2.9	11
24	<scp>DFT</scp> study of the acidâ€catalyzed esterification reaction mechanism of methanol with carboxylic acid and its halide derivatives. International Journal of Quantum Chemistry, 2018, 118, e25497.	2.0	41
25	The Heterogeneous Aminohydroxylation Reaction Using Hydrotalcite-Like Catalysts Containing Osmium. Catalysts, 2018, 8, 547.	3.5	0
26	Crystal structure of methyl (1-phenylethyl)carbamate, C₁₀H₁₃NO₂. Zeitschrift Fur Kristallographie - New Crystal Structures, 2018, 233, 561-563.	0.3	0
27	Inhibition of Mycobacterium tuberculosis L,Dâ€Transpeptidase 5â€‰by Carbapenems: MD and QM/MM Mechanistic Studies. ChemistrySelect, 2018, 3, 13603-13612.	1.5	6
28	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
29	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
30	Exploring the flap dynamics of the South African HIV subtype C protease in presence of FDAâ€approved inhibitors: MD study. Chemical Biology and Drug Design, 2018, 92, 1899-1913.	3.2	3
31	The Current Status of Heterogeneous Palladium Catalysed Heck and Suzuki Cross-Coupling Reactions. Molecules, 2018, 23, 1676.	3.8	123
32	Synthesis, Characterization and Biocompatibility of a Multifunctional Gold Nanoparticle System for the Delivery of Single-Stranded RNA to Lymphocytes. South African Journal of Chemistry, 2018, 71, 1-14.	0.6	6
33	Differential flap dynamics in <scp>l</scp>,<scp>d</scp>-transpeptidase2 from mycobacterium tuberculosis revealed by molecular dynamics. Molecular BioSystems, 2017, 13, 1223-1234.	2.9	36
34	Lansoprazoleâ€sulfide, pharmacokinetics of this promising antiâ€tuberculous agent. Biomedical Chromatography, 2017, 31, e4035.	1.7	18
35	I36Tâ†'T mutation in South African subtype C (C-SA) HIV-1 protease significantly alters protease-drug interactions. Biological Chemistry, 2017, 398, 1109-1117.	2.5	10
36	Crystal structure of 4,10,16,22-tetrahydroxy-6,12,18,24-tetramethoxy-2,8,14,20-tetraethylphenylresorcin[4]arene â€" ethyl acetate (1/1), C₆₈H₇₂O₁₀. Zeitschrift Fur Kristallographie - New Crystal Structures, 2017, 232, 305-307.	0.3	0

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37	PdCuCeOâ€“TPAB: a new catalytic system for quasi-heterogeneous Suzukiâ€“Miyaura cross-coupling reactions under ligand-free conditions in water. New Journal of Chemistry, 2017, 41, 13560-13566.	2.8	13
38	Pd0.09Ce0.91O2-Î´: A sustainable ionic solid-solution precatalyst for heterogeneous, ligand free Heck coupling reactions. Molecular Catalysis, 2017, 443, 60-68.	2.0	8
39	The role of nanotechnology in the treatment of viral infections. Therapeutic Advances in Infectious Disease, 2017, 4, 105-131.	1.8	233
40	Investigation of the binding free energies of FDA approved drugs against subtype B and C-SA HIV PR: ONIOM approach. Journal of Molecular Graphics and Modelling, 2017, 76, 77-85.	2.4	12
41	Computational model for the acylation step of the Î²-lactam ring: Potential application for l,d-transpeptidase 2 in mycobacterium tuberculosis. Journal of Molecular Structure, 2017, 1128, 94-102.	3.6	41
42	Crystal structure of 5,11,17,23-tetra(tert-butyl)-25,26,27,28-tetrahexoxycalix[4]arene, C68H104O4. Zeitschrift Fur Kristallographie - New Crystal Structures, 2017, 232, 397-402.	0.3	0
43	Potential inhibition of HIV-1 encapsidation by oligoribonucleotide–dendrimer nanoparticle complexes. International Journal of Nanomedicine, 2017, Volume 12, 317-325.	6.7	14
44	Pdo.o2Ceo.98O2: a copper- and ligand-free quasi-heterogeneous catalyst for aquacatalytic Sonogashira cross-coupling reaction. Journal of the South African Institute of Mining and Metallurgy, 2017, 117, 955-962.	0.5	4
45	Development and validation of a liquid chromatographyâ€tandem mass spectrometry (LCâ€MS/MS) method for the quantification of tigecycline in rat brain tissues. Biomedical Chromatography, 2016, 30, 837-845.	1.7	15
46	Crystal structure of 2-(ethoxycarbonyl)-2-(2-nitro-1-phenylethyl)-3-oxopyrrolidinium chloride, C15H19N2O5Cl. Zeitschrift Fur Kristallographie - New Crystal Structures, 2016, 231, 43-45.	0.3	0
47	Mechanistic investigation of the uncatalyzed esterification reaction of acetic acid and acid halides with methanol: a DFT study. Journal of Molecular Modeling, 2016, 22, 235.	1.8	39
48	Enantioselective Organocatalyzed Transformations of Î²-Ketoesters. Chemical Reviews, 2016, 116, 9375-9437.	47.7	105
49	Intracellular localization of gold nanoparticles with targeted delivery in MT-4 lymphocytes. Advances in Natural Sciences: Nanoscience and Nanotechnology, 2016, 7, 045013.	1.5	12
50	Crystal structure of butyl 2-(3,5-dimethyl-1,1-dioxido-2H-1,2,6-thiadiazin-4-yl)benzoate, C16H20N2O4S. Zeitschrift Fur Kristallographie - New Crystal Structures, 2016, 231, 373-374.	0.3	0
51	Crystal structure of N-phenyl-2-(pyridin-4-ylcarbonyl)hydrazinecarboxamide with Zâ€² = 4, C13H12N4O2. Zeitschrift Fur Kristallographie - New Crystal Structures, 2016, 231, 649-652.	0.3	0
52	Physicochemical characterization and decomposition kinetics of (S)-4-[1-(2,3-dimethylphenyl)ethyl]-3H-imidazole HCl/S-enantiomer of medetomidineHCl. Journal of Thermal Analysis and Calorimetry, 2016, 124, 269-278.	3.6	1
53	Binding Free Energy Calculations of Nine FDAâ€approved Protease Inhibitors Against HIVâ€1 Subtype C I36Tâ†'T Containing 100 Amino Acids Per Monomer. Chemical Biology and Drug Design, 2016, 87, 487-498.	3.2	23
54	Clathrate tetraldehyde cavitand: single-crystal structure and NMR study. Supramolecular Chemistry, 2016, 28, 329-334.	1.2	0

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55	Purification and characterization of naturally occurring HIV-1 (South African subtype C) protease mutants from inclusion bodies. Protein Expression and Purification, 2016, 122, 90-96.	1.3	22
56	A comparative modeling and molecular docking study onMycobacterium tuberculosistargets involved in peptidoglycan biosynthesis. Journal of Biomolecular Structure and Dynamics, 2016, 34, 2399-2417.	3.5	23
57	Rapid and widespread distribution of doxycycline in rat brain: a mass spectrometric imaging study. Xenobiotica, 2016, 46, 385-392.	1.1	8
58	Targeting the cell wall ofMycobacterium tuberculosis: a molecular modeling investigation of the interaction of imipenem and meropenem withL,D-transpeptidase 2. Journal of Biomolecular Structure and Dynamics, 2016, 34, 304-317.	3.5	18
59	Crystal structure of 1-[2-[(2-chloro-3-thienyl)methoxy]-2-(2,4-dichlorophenyl) ethyl]-1H-imidazole, C16H13Cl3N2OS. Zeitschrift Fur Kristallographie - New Crystal Structures, 2015, 230, 5-6.	0.3	0
60	Crystal structure of bis(dicyclohexylammonium) 4-(2-carboxylatophenyl)-3,5-dimethyl-1,2,6-thiadiazin-2-ide 1,1-dioxide methanol monosolvate, C37H62N4O5S. Zeitschrift Fur Kristallographie - New Crystal Structures, 2015, 230, 53-55.	0.3	0
61	Crystal structure of potassium 4-(2-carboxyphenyl)-3,5-dimethyl-1,2,6- thiadiazin-2-ide 1,1-dioxide monohydrate, C12H13KN2O5S. Zeitschrift Fur Kristallographie - New Crystal Structures, 2015, 230, 211-212.	0.3	0
62	Hydrogen bonded co-crystallised layered isopropanol-pyrogallol[4]arenes. Supramolecular Chemistry, 2015, 27, 545-551.	1.2	0
63	Synthesis and NMR elucidation of novel octa-amino acid resorcin[4]arenes derivatives. South African Journal of Chemistry, 2015, 68, .	0.6	0
64	Synthesis and structural elucidation of a novel polymorph of alcaftadine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 142, 311-319.	3.9	5
65	Structural and functional features of enzymes of Mycobacterium tuberculosis peptidoglycan biosynthesis as targets for drug development. Tuberculosis, 2015, 95, 95-111.	1.9	54
66	Tetramethoxy resorcin[4]arene-tetraester derivatives. Journal of Thermal Analysis and Calorimetry, 2015, 120, 653-665.	3.6	2
67	Isolation, characterization and x-ray structure determination of the schiff base ligand: 5-methyl-2-phenyl-4-[phenyl-(4-phenyl-thiazol-2-ylamino)-methylene]-2,4-dihydro-pyrazol-3-one. South African Journal of Chemistry, 2015, 68, .	0.6	4
68	Visualization of Time-Dependent Distribution of Rifampicin in Rat Brain Using MALDI MSI and Quantitative LCMS/MS. Assay and Drug Development Technologies, 2015, 13, 277-284.	1.2	25
69	Simulating the inhibition reaction of Mycobacterium tuberculosis<scp>l</scp>,<scp>d</scp>-transpeptidase 2 by carbapenems. Chemical Communications, 2015, 51, 12560-12562.	4.1	19
70	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. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2015, 988, 187-194.	2.3	21
71	Pentacycloundecane lactam vs lactone norstatine type protease HIV inhibitors: binding energy calculations and DFT study. Journal of Biomedical Science, 2015, 22, 15.	7.0	13
72	The effect of N-methylation of amino acids (Ac-X-OMe) on solubility and conformation: a DFT study. Organic and Biomolecular Chemistry, 2015, 13, 9993-10006.	2.8	55

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73	Crystal structure of 2-(2,4-dioxopentan-3-yl)benzoic acid, C12H12O4. Zeitschrift Fur Kristallographie - New Crystal Structures, 2014, 229, 323-324.	0.3	0
74	Crystal structure of 2-methyl-(2,4-dioxopentan-3-yl)benzoate, C13H14O4. Zeitschrift Fur Kristallographie - New Crystal Structures, 2014, 229, 325-326.	0.3	0
75	Crystal structure of N-butyl-2-(3,5-dimethyl-1,1-dioxido-2H-1,2,6- thiadiazin-4-yl)benzamide, C16H21N3O3S. Zeitschrift Fur Kristallographie - New Crystal Structures, 2014, 229, .	0.3	0
76	Crystal structure of 2-(3-chloro-phenyl)-5-methyl-4-[1-(4-p-tolyl-thiazol-) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 627 Td (2-ylamino)-ethylid Crystal Structures, 2014, 229, 319-320.	0.3	0
77	Integrated Approach to Structure-Based Enzymatic Drug Design: Molecular Modeling, Spectroscopy, and Experimental Bioactivity. Chemical Reviews, 2014, 114, 493-537.	47.7	100
78	The Impact of Active Site Mutations of South African <scp>HIV PR</scp> on Drug Resistance: Insight from Molecular Dynamics Simulations, Binding Free Energy and Perâ€Residue Footprints. Chemical Biology and Drug Design, 2014, 83, 472-481.	3.2	13
79	Organocatalytic Mannich Reactions on a Carbapenem Core â€“ Synthesis of Mannich Bases and Bicyclic Diazanonanes. European Journal of Organic Chemistry, 2014, 2014, 2253-2260.	2.4	11
80	Proline N-oxides: modulators of the 3D conformation of linear peptides through â€œNO-turnsâ€• Organic and Biomolecular Chemistry, 2014, 12, 4479.	2.8	14
81	l-Proline organocatalyzed Michael synthesis of monobactam and carbapenem Î²-lactam cores. Tetrahedron: Asymmetry, 2014, 25, 969-973.	1.8	5
82	Synthesis and NMR elucidation of novel amino acid cavitand derivatives. Tetrahedron, 2014, 70, 7057-7066.	1.9	3
83	Preparation of Enantiomerically Pure C₄â€Symmetric Tetramethoxyresorcarenes by Using the (â€“)â€(S)â€1â€Phenylethyl Isocyanate Chiral Auxiliary. European Journal of Organic Chemistry, 2014, 2014, 4600-4609.	2.4	11
84	Crystal structure of 5-methyl-2-phenyl-4-[1-(4-p-tolyl-thiazol-2-ylamino)-ethylidene]-2,4-dihydropyrazol-3-one, C22H20N4OS. Zeitschrift Fur Kristallographie - New Crystal Structures, 2014, 229, 313-314.	0.3	0
85	Crystal structure of N-(2,6-diisopropylphenyl)-1,2,3,4-tetrahydroisoquinoline-3-carboxamide, C22H28N2O. Zeitschrift Fur Kristallographie - New Crystal Structures, 2014, 229, 1-2.	0.3	0
86	Crystal structure of 2-isopropyl-(3,5-dimethyl-1,1-dioxo-2H-1,2,6- thiadiazine-4-yl)-benzoate, C15H18N2O4S. Zeitschrift Fur Kristallographie - New Crystal Structures, 2014, 229, .	0.3	0
87	Crystal structure of 1,21,23,25-tetrapentyl-2,20:3,19-dimetheno-1H,21H,23H,25H-bis[1,3]dioxocino[5,4-i:5',4'-i']benzo[1,2-d:5,4-d']-bis- [1,3]benzodioxocin-7,11,15,28-tetrol], C56H72O14. Zeitschrift Fur Kristallographie - New Crystal Structures, 2014, 229, 479-481.	0.3	0
88	Novel PCU cage diol peptides as potential targets against wild-type CSA HIV-1 protease: synthesis, biological screening and molecular modelling studies. Medicinal Chemistry Research, 2013, 22, 3918-3933.	2.4	4
89	Synthesis and NMR elucidation of pentacycloundecane-derived hydroxy acid peptides as potential anti-HIV-1 agents. Structural Chemistry, 2013, 24, 1461-1471.	2.0	3
90	Synthesis of novel N-alkyl-2-(3,5-dimethyl-1,1-dioxido-2H-1,2,6-thiadiazin-4-yl)benzamides as potential antimicrobial agents. Journal of Pharmacy Research, 2013, 6, 355-360.	0.4	2

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91	Investigation and folding pattern of l-ido and d-gluco peptides by EASY ROESY NMR and X-ray. RSC Advances, 2013, 3, 23355.	3.6	0
92	Linear and cyclic glycopeptide as HIV protease inhibitors. European Journal of Medicinal Chemistry, 2013, 60, 144-154.	5.5	9
93	Bisthiourea: thermal and structural investigation. Journal of Thermal Analysis and Calorimetry, 2013, 111, 597-603.	3.6	6
94	Anticancer activity of ruthenium(II) arene complexes bearing 1,2,3,4-tetrahydroisoquinoline amino alcohol ligands. European Journal of Medicinal Chemistry, 2013, 66, 407-414.	5.5	51
95	Synthesis, 2D-NMR and molecular modelling studies of pentacycloundecane lactam-peptides and peptoids as potential HIV-1 wild type C-SA protease inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2013, 28, 78-88.	5.2	19
96	Comparison of the Molecular Dynamics and Calculated Binding Free Energies for Nine FDAâ€Approved HIVâ€1 PR Drugs Against Subtype B and Câ€SA HIV PR. Chemical Biology and Drug Design, 2013, 81, 208-218.	3.2	32
97	Catalytic asymmetric carbonâ€“carbon bond forming reactions catalyzed by tetrahydroisoquinoline (TIQ) N,Nâ€²-dioxide ligands. Tetrahedron: Asymmetry, 2013, 24, 191-195.	1.8	15
98	{2-[(1,3-Benzothiazol-2-yl)methoxy]-5-fluorophenyl}(4-chlorophenyl)methanone. Acta Crystallographica Section E: Structure Reports Online, 2013, 69, o1007-o1008.	0.2	1
99	Crystal structure of 5-methyl-4-[1-(5-methyl-4-phenyl-thiazol-2-ylamino)-ethylidene]-2-p-tolyl-2,4-dihydro-pyrazol-3-one, C23H22N4OS. Zeitschrift Fur Kristallographie - New Crystal Structures, 2013, 228, 457-458.	0.3	0
100	Crystal structure of 2-(3-chloro-phenyl)-5-methyl-4-[1-(5-methyl-4-ptolyl-) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 387 Td (thiazol-2-ylimino New Crystal Structures, 2013, 228, 471-472.	0.3	0
101	Crystal structure of bis(tert.-butylaminium) 4-(2-carboxylatophenyl)-3,5-dimethyl-4H-1,2,6-thiadiazin-4-ide 1,1-dioxide , C20H34N4O4S. Zeitschrift Fur Kristallographie - New Crystal Structures, 2013, 228, 469-470.	0.3	0
102	[2-(1,3-Benzothiazol-2-ylmethoxy)-5-bromophenyl](4-chlorophenyl)methanone. Acta Crystallographica Section E: Structure Reports Online, 2013, 69, o70-o70.	0.2	4
103	Crystal structure of (S)-tert-butyl 3-carbamothioyl-3,4-dihydroisoquinoline- 2(1H)-carboxylate, C63H86N8O9S4. Zeitschrift Fur Kristallographie - New Crystal Structures, 2013, 228, 449-450.	0.3	0
104	Crystal structure of (S)-benzyl-3-{(4-bromophenyl)carbamoyl}-3,4-dihydroisoquinoline-2(1H)-carboxylate, C24H21BrN2O3. Zeitschrift Fur Kristallographie - New Crystal Structures, 2013, 228, 437-439.	0.3	0
105	A Review of Cyanoacetyl Indoles (CAIs): Versatile Starting Materials in Organic Synthesis.. Current Organic Synthesis, 2013, 10, 737-750.	1.3	10
106	Crystal structure of (S)-N-benzyl-1,2,3,4-tetrahydroisoquinoline-3-carboxamide, C17H20N2O2. Zeitschrift Fur Kristallographie - New Crystal Structures, 2013, 228, 401-402.	0.3	0
107	Nanotechnology and the Treatment of HIV Infection. Viruses, 2012, 4, 488-520.	3.3	106
108	(S)-Benzyl 3-phenylcarbamoyl-1,2,3,4-tetrahydroisoquinoline-2-carboxylate. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o883-o883.	0.2	1

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109	(2-(Benzo[d]thiazol-2yl-methoxy)-5-chlorophenyl)(phenyl)methanone. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o3125-o3125.	0.2	4
110	6,12,18,24-Tetramethoxy-4,10,16,22-tetrakis[(methoxycarbonyl)methoxy]-2,8,14,20-tetrakis(2-phenylethyl)resorcin[4]arene. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o97-o98.	0.2	2
111	(S)-4-Phenyl-2-(1,2,3,4-tetrahydroisoquinolin-3-yl)-1,3-thiazole. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o176-o176.	0.2	0
112	(S)-Methyl 2-benzamido-3-(3,4-dimethoxyphenyl)propanoate. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o177-o177.	0.2	1
113	Ethyl 2-(3,5-dimethyl-1,1-dioxo-2H-1Î»⁶,2,6-thiadiazin-4-yl)benzoate. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o2160-o2160.	0.2	3
114	(S)-4-tert-Butyl-2-(1,2,3,4-tetrahydroisoquinolin-3-yl)-1,3-thiazole. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o2487-o2487.	0.2	0
115	2-(3,5-Dimethyl-1,1-dioxo-2H-1Î»6,2,6-thiadiazin-4-yl)benzoic acid. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o2859-o2859.	0.2	2
116	Methyl 2-(2,3,5-trimethyl-1,1-dioxo-2H-1Î»6,2,6-thiadiazin-4-yl)benzoate. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o3360-o3360.	0.2	1
117	Asymmetric conjugate addition of thioglycolate to a range of chalcones using tetrahydroisoquinoline (TIQ) N,Nâ€²-dioxide ligands. Tetrahedron: Asymmetry, 2012, 23, 616-622.	1.8	8
118	Interaction of Î²-Amyloid Interactions with Peptide Functionalized Gold Nanoparticles. Journal of Nanoscience and Nanotechnology, 2012, 12, 2179-2184.	0.9	8
119	Novel polycyclic â€˜cageâ€™-1,2-diamines as potential anti-tuberculosis agents. European Journal of Medicinal Chemistry, 2012, 54, 1-9.	5.5	28
120	Synthesis, screening and computational investigation of pentacycloundecane-peptoids as potent CSA-HIV PR inhibitors. European Journal of Medicinal Chemistry, 2012, 57, 459-467.	5.5	15
121	Synthesis and NMR elucidation of novel tetrapeptides. Journal of Peptide Science, 2012, 18, 114-121.	1.4	3
122	Microwaveâ€Assisted Synthesis of Guanidine Organocatalysts Bearing a Tetrahydroisoquinoline Framework and Their Evaluation in Michael Addition Reactions. European Journal of Organic Chemistry, 2012, 2012, 3331-3337.	2.4	16
123	Pentacycloundecaneâ€diolâ€Based HIVâ€1 Protease Inhibitors: Biological Screening, 2<scp>Dâ€…</scp>NMR, and Molecular Simulation Studies. ChemMedChem, 2012, 7, 1009-1019.	3.2	15
124	Inside Cover: Pentacycloundecane-diol-Based HIV-1 Protease Inhibitors: Biological Screening, 2Dâ€…NMR, and Molecular Simulation Studies (ChemMedChem 6/2012). ChemMedChem, 2012, 7, 938-938.	3.2	0
125	Synthesis and molecular modelling studies of novel carbapeptide analogs for inhibition of HIV-1 protease. European Journal of Medicinal Chemistry, 2012, 53, 13-21.	5.5	16
126	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. Bioorganic Chemistry, 2012, 40, 19-29.	4.1	22

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127	Molecular Modeling of T.Ârangeli, T.Âbrucei gambiense, and T.Âevansi Sialidases in Complex with the DANA Inhibitor. Chemical Biology and Drug Design, 2012, 80, 114-120.	3.2	15
128	endo-11-(Dibenzylamino)tetracyclo[5.4.0.03,10.05,9]undecane-8-one. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o619-o619.	0.2	0
129	Enzymatic Activation of a Peptide Functionalised Gold Nanoparticle System for Prodrug Delivery. Journal of Nanoscience and Nanotechnology, 2011, 11, 3075-3083.	0.9	6
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143	(S)-2-Benzyl-N-(2,6-diisopropylphenyl)-1,2,3,4-tetrahydroisoquinoline-3-carboxamide. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o1106-o1106.	0.2	1
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