

Ali A El-Emam

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

219
papers

2,480
citations

23
h-index

42
g-index

228
ext. papers

2,768
ext. citations

2.8
avg, IF

4.92
L-index

#	Paper	IF	Citations
219	Supramolecular Self-Assembly Mediated by Multiple Hydrogen Bonds and the Importance of C-S···N Chalcogen Bonds in β -(Adamantan-2-ylidene)hydrazide Derivatives.. <i>ACS Omega</i> , 2022 , 7, 10608-10621	3.9	0
218	Adamantane-linked isothiourea derivatives suppress the growth of experimental hepatocellular carcinoma inhibition of TLR4-MyD88-NF- κ B signaling. <i>American Journal of Cancer Research</i> , 2021 , 11, 350-369	4.4	4
217	Investigation of the electronic properties of solvents (water, benzene, methanol) using IEFPCM model, spectroscopic investigation with docking and MD simulations of a thiadiazole derivative with anti-tumor activities. <i>Journal of Molecular Liquids</i> , 2021 , 118061	6	0
216	Crystallographic and Theoretical Exploration of Weak Hydrogen Bonds in Arylmethyl β -(adamantan-1-yl)piperidine-1-carbothioimidates and Molecular Docking Analysis. <i>ACS Omega</i> , 2021 , 6, 27026-27037	3.9	0
215	Supramolecular Self-Assembly Built by Weak Hydrogen, Chalcogen, and Unorthodox Nonbonded Motifs in 4-(4-Chlorophenyl)-3-[(4-fluorobenzyl)sulfanyl]-5-(thiophen-2-yl)-4,1,2,4-triazole, a Selective COX-2 Inhibitor: Insights from X-ray and Theoretical Studies. <i>ACS Omega</i> , 2021 , 6, 6996-7007	3.9	3
214	1,3,4-Oxadiazole -Mannich Bases: Synthesis, Antimicrobial, and Anti-Proliferative Activities. <i>Molecules</i> , 2021 , 26,	4.8	8
213	Invariant and Variable Supramolecular Self-Assembly in 6-Substituted Uracil Derivatives: Insights from X-ray Structures and Quantum Chemical Study. <i>Crystal Growth and Design</i> , 2021 , 21, 3234-3250	3.5	0
212	Structural Insights of Three 2,4-Disubstituted Dihydropyrimidine-5-carbonitriles as Potential Dihydrofolate Reductase Inhibitors. <i>Molecules</i> , 2021 , 26,	4.8	1
211	Synthesis and Biological Evaluation of Thiazole-Based Derivatives as Potential Acetylcholinesterase Inhibitors. <i>ACS Omega</i> , 2021 , 6, 19202-19211	3.9	2
210	Probing the Effect of Halogen Substituents (Br, Cl, and F) on the Non-covalent Interactions in 1-(Adamantan-1-yl)-3-arylthiourea Derivatives: A Theoretical Study. <i>ACS Omega</i> , 2021 , 6, 4816-4830	3.9	2
209	Comparative MD Study of Inhibitory Activity of Opaganib and Adamantane-Isothiourea Derivatives toward COVID-19 Main Protease M.. <i>ChemistrySelect</i> , 2021 , 6, 8603-8610	1.8	3
208	Reactivity properties and adsorption behavior of a triazole derivative [DFT and MD simulation studies. <i>Journal of Molecular Liquids</i> , 2021 , 341, 117439	6	6
207	X-ray and theoretical investigation of β -(adamantan-1-yl)-1-(phenyl or 3-chlorophenyl)-3-(4-bromobenzyl)isothioureas: an exploration involving weak non-covalent interactions, chemotherapeutic activities and QM/MM binding energy. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 14, 111-124	3.6	3
206	Quantitative assessment of the nature of noncovalent interactions in β -substituted-5-(adamantan-1-yl)-1,3,4-thiadiazole-2-amines: insights from crystallographic and QTAIM analysis.. <i>RSC Advances</i> , 2020 , 10, 9840-9853	3.7	17
205	Synthesis and Structure Insights of Two Novel Broad-Spectrum Antibacterial Candidates Based on β -(Heteroaryl)methylene]adamantane-1-carbohydrazides. <i>Molecules</i> , 2020 , 25,	4.8	3
204	1,4,5,6,7,8-Hexahydroquinolines and 5,6,7,8-tetrahydronaphthalenes: A new class of antitumor agents targeting the colchicine binding site of tubulin. <i>Bioorganic Chemistry</i> , 2020 , 99, 103831	5.1	5
203	Synthesis and crystal structure of 3-(adamantan-1-yl)-4-(2-bromo-4-fluoro-phen-yl)-1,2,4-triazole-5(4)-thione. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2020 , 76, 162-166	0.7	2

202	Crystal structure of 1-(adamantan-1-yl)-3-aminothiourea, C ₁₁ H ₁₉ N ₃ S. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2020 , 235, 1115-1117	0.2	
201	DFT Study on the Electronic Properties, Spectroscopic Profile, and Biological Activity of 2-Amino-5-trifluoromethyl-1,3,4-thiadiazole with Anticancer Properties. <i>ACS Omega</i> , 2020 , 5, 30073-30087	3.7	4
200	Interplay of weak intermolecular interactions in two Schiff's bases with organic fluorine derived from 5-nitrothiophene-2-carboxaldehyde: Crystal structures, DFT calculation and in vitro evaluation of bioactivities. <i>Journal of Molecular Structure</i> , 2020 , 1221, 128883	3.4	1
199	Quantitative analysis of hydrogen and chalcogen bonds in two pyrimidine-5-carbonitrile derivatives, potential DHFR inhibitors: an integrated crystallographic and theoretical study.. <i>RSC Advances</i> , 2020 , 10, 36806-36817	3.7	3
198	Design, synthesis and biological evaluation of new series of hexahydroquinoline and fused quinoline derivatives as potent inhibitors of wild-type EGFR and mutant EGFR (L858R and T790M). <i>Bioorganic Chemistry</i> , 2020 , 105, 104274	5.1	3
197	Structural, Vibrational and UV/Vis Studies of Adamantane-Containing Triazole Thiones by Spectral, DFT and Multi-reference ab initio Methods. <i>Zeitschrift Fur Physikalische Chemie</i> , 2020 , 234, 85-106	3.1	1
196	Insights into the weak Csp ³ H⋯HCsp ³ mediated supramolecular architecture in ethyl 2-(5-bromopentanamido)-4,5,6,7-tetrahydrobenzo[b]thiophene-3-carboxylate, a probable selective COX-2 lead molecule: An integrated crystallographic and theoretical approach. <i>Journal of Molecular Structure</i> , 2020 , 1199, 127019	3.4	5
195	Spectral and quantum chemical analysis of ethyl 4-[3-(adamantan-1-yl)-4-phenyl-5-sulfanylidene-4,5-dihydro-1H-1,2,4-triazole-1-yl]methylpiperazine-1-carboxylate. <i>Journal of Theoretical and Computational Chemistry</i> , 2019 , 18, 1950029		
194	Insights into the nature of weak noncovalent interactions in 3-(4-fluorophenyl)-6-(2-fluorophenyl)-1,2,4-triazolo[3,4-b][1,3,4]thiadiazole, a potential bioactive agent: X-ray, QTAIM and molecular docking analysis. <i>Journal of Molecular Structure</i> , 2019 , 1183, 331-341	3.4	7
193	Experimental and theoretical DFT (B3LYP, X3LYP, CAM-B3LYP and M06-2X) study on electronic structure, spectral features, hydrogen bonding and solvent effects of 4-methylthiadiazole-5-carboxylic acid. <i>Molecular Simulation</i> , 2019 , 45, 1029-1043	2	15
192	Investigation of potential anti-malarial lead candidate 2-(4-fluorobenzylthio)-5-(5-bromothiophen-2-yl)-1,3,4-oxadiazole: Insights from crystal structure, DFT, QTAIM and hybrid QM/MM binding energy analysis. <i>Journal of Molecular Structure</i> , 2019 , 1175, 230-240	3.4	13
191	Theoretical and experimental spectroscopic studies, XPS analysis, dimer interaction energies and molecular docking study of 5-(adamantan-1-yl)-N-methyl-1,3,4-thiadiazol-2-amine. <i>Journal of Physics and Chemistry of Solids</i> , 2019 , 135, 109091	3.9	4
190	Crystal structure of 3,5-bis(trifluoromethyl)benzyl (Z)-N'-(adamantan-1-yl)-4-phenylpiperazine-1-carbothioimidate, C ₃₀ H ₃₃ F ₆ N ₃ S. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2019 , 234, 1009-1012	0.2	1
189	Molecular docking, Hirshfeld surface analysis and spectroscopic investigations of 1-(adamantan-1-yl)-3-(4-fluorophenyl)thiourea: A potential bioactive agent. <i>Chemical Physics Letters</i> , 2019 , 735, 136762	2.5	5
188	Crystal structures and Hirshfeld surface analysis of 2-(adamantan-1-yl)-5-(4-fluoro-phen-yl)-1,3,4-oxa-diazole and 2-(adamantan-1-yl)-5-(4-chloro-phen-yl)-1,3,4-oxa-diazole. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2019 , 75, 611-615	0.7	3
187	Crystal structure of 4-bromobenzyl (Z)-N-(adamantan-1-yl)morpholine-4-carbothioimidate, C ₂₂ H ₂₉ BrN ₂ OS. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2019 , 234, 1001-1003	0.2	3
186	Crystal structure, Hirshfeld surface analysis and DFT studies of 5-(adamantan-1-yl)-3-[(4-chlorobenzyl)sulfanyl]-4-methyl-4H-1,2,4-triazole, a potential 11βHSD1 inhibitor. <i>Scientific Reports</i> , 2019 , 9, 19745	4.9	27
185	Synthesis, Antimicrobial, and Anti-Proliferative Activities of Novel 4-(Adamantan-1-yl)-1-arylidene-3-thiosemicarbazides, 4-Arylmethyl '-(Adamantan-1-yl)piperidine-1-carbothioimidates, and Related Derivatives. <i>Molecules</i> , 2019 , 24,	4.8	9

184	Spectroscopic (FT-IR, FT-Raman, UV, ¹ H and ¹³ C NMR) insights, electronic profiling and DFT computations on ((E)-[3-(1H-imidazol-1-yl)-1-phenylpropylidene]amino)oxy)(4-nitrophenyl)methanone, an imidazole-bearing anti-Candida agent. <i>Open Chemistry</i> , 2018 , 16, 50-63	1.6	4
183	Theoretical investigations of two adamantane derivatives: A combined X-ray, DFT, QTAIM analysis and molecular docking. <i>Journal of Molecular Structure</i> , 2018 , 1159, 233-245	3.4	19
182	Probing vibrational activities, electronic properties, molecular docking and Hirshfeld surfaces analysis of 4-chlorophenyl (((1E)-3-(1H-imidazol-1-yl)-1-phenylpropylidene]amino)oxy)methanone: A promising anti-Candida agent. <i>Journal of Molecular Structure</i> , 2018 , 1159, 83-95	3.4	16
181	Synthesis, spectroscopic analyses, chemical reactivity and molecular docking study and anti-tubercular activity of pyrazine and condensed oxadiazole derivatives. <i>Journal of Molecular Structure</i> , 2018 , 1164, 459-469	3.4	14
180	Study on the structure, vibrational analysis and molecular docking of fluorophenyl derivatives using FT-IR and density functional theory computations. <i>Journal of Molecular Structure</i> , 2018 , 1164, 172-179	3.4	11
179	Experimental (FT-IR, Laser-Raman and NMR) and theoretical comparative study on 2-benzylsulfanyl-4-pentyl-6-(phenylsulfanyl)pyrimidine-5-carbonitrile, a potential bioactive agent. <i>Journal of Theoretical and Computational Chemistry</i> , 2018 , 17, 1850035	1.8	3
178	Spectral Analysis of 3-(Adamantan-1-yl)-4-Ethyl-1-[(4-Phenylpiperazin-1-yl)Methyl]-1H-1,2,4-Triazole-5(4H)-Thione. <i>Journal of Applied Spectroscopy</i> , 2018 , 85, 203-215	0.7	1
177	4-[(4-acetylphenyl)amino]-2-methylidene-4-oxobutanoic acid, a newly synthesized amide with hydrophilic and hydrophobic segments: Spectroscopic characterization and investigation of its reactive properties. <i>Journal of the Serbian Chemical Society</i> , 2018 , 83, 1-18	0.9	10
176	Crystal structure of 3,5-bis(trifluoromethyl)benzyl(Z)-N-(adamantan-1-yl)morpholine-4-carbothioimidate, C ₂₄ H ₂₈ F ₆ N ₂ O ₅ . <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2018 , 233, 607-609	0.2	3
175	A combined experimental and theoretical DFT (B3LYP, CAM-B3LYP and M06-2X) study on electronic structure, hydrogen bonding, solvent effects and spectral features of methyl 1H-indol-5-carboxylate. <i>Journal of Molecular Structure</i> , 2017 , 1137, 725-741	3.4	32
174	FT-IR and FT-Raman characterization and investigation of reactive properties of N-(3-iodo-4-methylphenyl)pyrazine-2-carboxamide by molecular dynamics simulations and DFT calculations. <i>Journal of Molecular Structure</i> , 2017 , 1136, 14-24	3.4	17
173	Vibrational Spectra of 3-(Adamantan-1-yl)-4-(2-Propen-1-yl)-1H-1,2,4-Triazole-5(4H)-Thione. <i>Journal of Applied Spectroscopy</i> , 2017 , 83, 924-930	0.7	1
172	Experimental (FT-IR, Laser-Raman and NMR) and theoretical spectroscopic analysis of 3-[(N-methylanilino)methyl]-5-(thiophen-2-yl)-1,3,4-oxadiazole-2(3H)-thione. <i>Journal of Theoretical and Computational Chemistry</i> , 2017 , 16, 1750024	1.8	2
171	First principle study of a potential bioactive molecule with tetrahydroisoquinoline, carbothiomide and adamantane scaffolds. <i>Journal of Molecular Structure</i> , 2017 , 1143, 204-216	3.4	2
170	Insight into the reactive properties of newly synthesized 1,2,4-triazole derivative by combined experimental (FT-IR and FR-Raman) and theoretical (DFT and MD) study. <i>Journal of Molecular Structure</i> , 2017 , 1141, 542-550	3.4	11
169	Synthesis, vibrational spectroscopic investigations, molecular docking, antibacterial studies and molecular dynamics study of 5-[(4-nitrophenyl)acetamido]-2-(4-tert-butylphenyl)benzoxazole. <i>Journal of Molecular Structure</i> , 2017 , 1133, 557-573	3.4	7
168	Adamantane-Isothiourea Hybrid Derivatives: Synthesis, Characterization, In Vitro Antimicrobial, and In Vivo Hypoglycemic Activities. <i>Molecules</i> , 2017 , 22,	4.8	31
167	Crystal structure of 2-[3,5-bis(trifluoromethyl)benzylsulfanyl]-5-(5-bromothiophen-2-yl)-1,3,4-oxadiazole, C ₁₅ H ₇ BrF ₆ N ₂ O ₅ . <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2017 , 232, 131-133	0.2	1

166	Vibrational spectroscopic investigations and molecular docking studies of biologically active 2-[4-(4-phenylbutanamido)phenyl]-5-ethylsulphonyl-benzoxazole. <i>Journal of Molecular Structure</i> , 2017 , 1148, 119-133	3.4	9
165	Crystal structure of 4-bromobenzyl (Z)-N ⁷ -(adamantan-1-yl)-4-phenylpiperazine-1-carbothioimide, C ₂₈ H ₃₄ BrN ₃ S. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2017 , 232, 189-191	0.2	4
164	Molecular conformational analysis, reactivity, vibrational spectral analysis and molecular dynamics and docking studies of 6-chloro-5-isopropylpyrimidine-2,4(1H,3H)-dione, a potential precursor to bioactive agent. <i>Journal of Molecular Structure</i> , 2017 , 1127, 427-436	3.4	8
163	Reactive, spectroscopic and antimicrobial assessments of 5-[(4-methylphenyl)acetamido]-2-(4-tert-butylphenyl)benzoxazole: Combined experimental and computational study. <i>Journal of Molecular Structure</i> , 2017 , 1128, 694-706	3.4	12
162	Crystal structure of (Z)-3-(adamantan-1-yl)-1-(3-chlorophenyl)-S-benzylisothiourea, C ₂₄ H ₂₇ ClN ₂ S. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2017 , 232, 453-456	0.2	2
161	Crystal structure of 3-(adamantan-1-yl)-4-(4-fluorophenyl)-1H-1,2,4-triazole-5(4H)-thione, C ₁₈ H ₂₀ FN ₃ S. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2017 , 232, 443-445	0.2	1
160	Crystal structure of 3-(adamantan-1-yl)-1-(4-bromophenyl)urea, C ₁₇ H ₂₁ BrN ₂ O. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2017 , 232, 37-39	0.2	1
159	Syntheses and crystal structures of two adamantyl-substituted 1,2,4-triazole-5-thione -Mannich bases. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2017 , 73, 1135-1139	0.7	2
158	Crystal structure of 1-(adamantan-1-yl)-3-(3-chlorophenyl)thiourea, C ₁₇ H ₂₁ ClN ₂ S. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2017 , 232, 33-35	0.2	2
157	Crystal structure of 6-(4-chlorophenyl)-3-(thiophen-2-yl)-[1,2,4]triazolo[3,4-b][1,3,4]-thiadiazole, C ₁₃ H ₇ ClN ₄ S ₂ . <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2016 , 231, 931-932	0.2	1
156	Vibrational spectroscopic studies, Fukui functions, HOMO-LUMO, NLO, NBO analysis and molecular docking study of (E)-1-(1,3-benzodioxol-5-yl)-4,4-dimethylpent-1-en-3-one, a potential precursor to bioactive agents. <i>Journal of Molecular Structure</i> , 2016 , 1123, 375-383	3.4	38
155	Structure of N ⁷ -(adamantan-2-ylidene)benzohydrazide, a potential antibacterial agent, in solution: Molecular dynamics simulations, quantum chemical calculations and Ultraviolet-Visible spectroscopy studies. <i>Journal of Chemical Sciences</i> , 2016 , 128, 1933-1942	1.8	4
154	Crystal structure of N ⁷ -(adamantan-2-ylidene)pyridine-3-carbohydrazide, C ₁₆ H ₁₉ N ₃ O. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2016 , 231, 573-575	0.2	2
153	Crystal structure of 1-(adamantan-1-yl)-3-(4-chlorophenyl)thiourea, C ₁₇ H ₂₁ ClN ₂ S. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2016 , 231, 707-709	0.2	2
152	Crystal structure of N ⁷ -[(1E)-(2,6-dichlorophenyl)-methylidene]adamantane-1-carbohydrazide, C ₁₈ H ₂₀ Cl ₂ N ₂ O. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2016 , 231, 1037-1039	0.2	2
151	Spectroscopic and electronic structure calculation of a potential antibacterial agent incorporating pyrido-dipyrimidine-dione moiety using first principles. <i>Journal of Molecular Structure</i> , 2016 , 1110, 128-137	3.4	5
150	Spectroscopic investigations and molecular docking study of 3-(1H-imidazol-1-yl)-1-phenylpropan-1-one, a potential precursor to bioactive agents. <i>Journal of Molecular Structure</i> , 2016 , 1109, 131-138	3.4	10
149	Raman, infrared and DFT studies of N ⁷ -(adamantan-2-ylidene)benzohydrazide, a potential antibacterial agent. <i>Journal of Molecular Structure</i> , 2016 , 1115, 258-266	3.4	15

148	Crystal structure of N [?] -(adamantan-2-ylidene)-isonicotinohydrazide, C ₁₆ H ₁₉ N ₃ O. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2016 , 231, 273-275	0.2	2
147	Crystal structure of 5-(adamantan-1-yl)-3-[(4-chloroanilino)methyl]-2,3-dihydro-1,3,4-oxadiazole-2-thione, C ₁₉ H ₂₂ ClN ₃ OS. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2016 , 231, 301-303	0.2	1
146	Synthesis, vibrational spectroscopic investigations, molecular docking, antibacterial and antimicrobial studies of 5-ethylsulphonyl-2-(p-aminophenyl)benzoxazole. <i>Journal of Molecular Structure</i> , 2016 , 1115, 94-104	3.4	13
145	Vibrational and structural observations and molecular docking study on 1-[3-(4-chlorophenyl)-5-[4-(propan-2-yl)phenyl]-4,5-dihydro-1H-pyrazol-1-yl]-ethanone. <i>Journal of Molecular Structure</i> , 2016 , 1112, 136-146	3.4	27
144	Crystal structure of 1-(adamantan-1-yl)-3-phenylthiourea, C ₁₇ H ₂₂ N ₂ S. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2016 , 231, 593-595	0.2	5
143	Crystal structure of 6-(2-fluorophenyl)-3-phenyl-[1,2,4]-triazolo[3,4-b][1,3,4]thiadiazole, C ₁₅ H ₉ FN ₄ S. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2016 , 231, 661-663	0.2	1
142	Conformational search, spectral analysis and electronic properties of 5-(4-Pyridinyl)-1,3,4-thiadiazol-2-amine. <i>Journal of Molecular Structure</i> , 2016 , 1108, 112-125	3.4	5
141	Crystal structure of 3-[[4-(2-methoxyphenyl)piperazin-1-yl]methyl]-5-(thiophen-2-yl)-1,3,4-oxadiazole-2(3H)-thione. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2016 , 72, 269-72	0.7	1
140	Structural and spectroscopic characterization of N [?] [(1E)-(4-fluorophenyl)methylidene]thiophene-2-carbohydrazide, a potential precursor to bioactive agents. <i>Macedonian Journal of Chemistry and Chemical Engineering</i> , 2016 , 35, 63	1.1	3
139	Crystal structure of 5-ethyl-6-[(3-methylphenyl)sulfonyl]pyrimidine-2,4(1H,3H)-dione, C ₁₃ H ₁₄ N ₂ O ₂ S. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2016 , 231, 601-603	0.2	
138	Crystal structure of 6-oxo-4-propyl-2-(propylthio)-1,6-dihydropyrimidine-5-carbonitrile, C ₁₁ H ₁₅ N ₃ OS. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2016 , 231, 583-585	0.2	2
137	Crystal structure of 3-(adamantan-1-yl)-1-[[4-benzylpiperazin-1-yl)methyl]-4-[(E)-(2,6-difluorobenzylidene)amino]-1H-1,2,4-triazole-5(4H)-thione, C ₃₁ H ₃₆ F ₂ N ₆ S. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2016 , 231, 927-929		
136	Crystal structure of 5-(adamantan-1-yl)-3-[(2-trifluoromethylanilino)methyl]-2,3-dihydro-1,3,4-oxadiazole-2-thione, C ₂₀ H ₂₂ F ₃ N ₃ OS. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2016 , 231, 815-817	0.2	1
135	Crystal structure of 1-(adamantan-1-yl)-3-(4-bromophenyl)thiourea, C ₁₇ H ₂₁ BrN ₂ S. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2016 , 231, 1033-1035	0.2	1
134	Crystal structure of 4-[(E)-(2-chloro-6-fluorobenzylidene)amino]-1,2-dihydro-2,3-dimethyl-1-phenylpyrazol-5-one, C ₁₈ H ₁₅ ClFN ₃ O. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2016 , 231, 777-780	0.2	
133	Crystal structure of N-(adamantan-1-yl)-4-phenylpiperazine-1-carbothioamide, C ₂₁ H ₂₉ N ₃ S. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2016 , 231, 991-993	0.2	4
132	Spectroscopic, quantum chemical studies, Fukui functions, in vitro antiviral activity and molecular docking of 5-chloro-N-(3-nitrophenyl)pyrazine-2-carboxamide. <i>Journal of Molecular Structure</i> , 2016 , 1119, 188-199	3.4	39
131	Spectroscopic investigations and molecular docking study of (2E)-1-(4-Chlorophenyl)-3-[4-(propan-2-yl)phenyl]prop-2-en-1-one using quantum chemical calculations. <i>Journal of Molecular Structure</i> , 2016 , 1120, 317-326	3.4	14

130	Crystal structure of 2-[(4-fluorobenzyl)sulfanyl]-4-(2-methylpropyl)-6-oxo-1,6-dihydropyrimidine-5-carbonitrile, C16H16FN3OS. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2016 , 231, 285-287	0.2	1
129	Spectroscopic investigations, NBO, HOMO-LUMO, NLO analysis and molecular docking of 5-(adamantan-1-yl)-3-anilino-methyl-2,3-dihydro-1,3,4-oxadiazole-2-thione, a potential bioactive agent. <i>Journal of Molecular Structure</i> , 2015 , 1096, 1-14	3.4	36
128	Study on molecular structure, spectroscopic behavior, NBO, and NLO analysis of 3-methylbezothiazole-2-thione. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 146, 129-41	4.4	9
127	Crystal structure of 3-(adamantan-1-yl)-4-(4-chloro-phen-yl)-1H-1,2,4-triazole-5(4H)-thione. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2015 , 71, o115-6	0.7	1
126	Crystal structure of 3-[(4-benzyl-piperazin-1-yl)methyl]-5-(thio-phen-2-yl)-2,3-dihydro-1,3,4-oxadiazole-2-thione. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2015 , 71, o175-6	0.7	1
125	Crystal structure of 3-[[4-(4-fluorophenyl)piperazin-1-yl]methyl]-5-(thiophen-2-yl)-2,3-dihydro-1,3,4-oxadiazole-2-thione, C17H17FN4OS2. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2015 , 230, 267-268	0.2	
124	Spectroscopic and electronic structure calculation of a potential chemotherapeutic agent 5-propyl-6-(p-tolylsulfanyl)pyrimidine-2,4(1H,3H)-dione using first principles. <i>Journal of Molecular Structure</i> , 2015 , 1100, 225-236	3.4	2
123	Spectroscopic investigation (FT-IR, FT-Raman), HOMO-LUMO, NBO analysis and molecular docking study of 2-[(4-chlorobenzyl)sulfanyl]-4-(2-methylpropyl)-6-[3-trifluoromethyl]-anilino]pyrimidine-5-carbonitrile,	4.4	7
122	Vibrational spectroscopic (FT-IR and FT-Raman) studies, HOMO-LUMO, NBO analysis and MEP of 6-methyl-1-(((2E)-2-methyl-3-phenyl-prop-2-en-1-yl)oxy)methyl)-1,2,3,4-tetra-hydroquinazoline-2,4-dione, a potential chemotherapeutic agent, using density functional methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 134, 316-25	4.4	14
121	Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMO-LUMO analysis and molecular docking study of 2-(Adamantan-1-yl)-5-(4-nitrophenyl)-1,3,4-oxadiazole. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 135, 973-83	4.4	31
120	Vibrational spectroscopic and molecular docking study of 2-Benzylsulfanyl-4-[(4-methylphenyl)-sulfanyl]-6-pentylpyrimidine-5-carbonitrile, a potential chemotherapeutic agent. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 137, 569-80	4.4	21
119	Crystal structure of 6-(phenylsulfanyl)-5-propylpyrimidine-2,4(1H,3H)-dione, C13H14N2O2S. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2015 , 230, 289-291	0.2	
118	Crystal structures of 4-phenyl-piperazin-1-ium 6-chloro-5-ethyl-2,4-dioxypyrimidin-1-ide and 4-phenyl-piperazin-1-ium 6-chloro-5-isopropyl-2,4-dioxypyrimidin-1-ide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2015 , 71, 956-9	0.7	0
117	Synthesis, Antimicrobial and Hypoglycemic Activities of Novel N-(1-Adamantyl)carbothioamide Derivatives. <i>Molecules</i> , 2015 , 20, 8125-43	4.8	20
116	Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMO-LUMO, NBO, MEP analysis and molecular docking study of 2-[(4-chlorobenzyl)sulfanyl]-4-(2-methylpropyl)-6-(phenylsulfanyl)-pyrimidine-5-carbonitrile, a	4.4	15
115	potential chemotherapeutic agent. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 130, 43-24	4.4	13
114	FT-IR and FT-Raman spectroscopic signatures, vibrational assignments, NBO, NLO analysis and molecular docking study of 2-[[5-(adamantan-1-yl)-4-methyl-4H-1,2,4-triazol-3-yl]sulfanyl]-N,N-dimethylethanamine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 140, 1-14	4.4	10
113	Use of vibrational spectroscopy to study 4-benzyl-3-(thiophen-2-yl)-4,5-dihydro-1H-1,2,4-triazole-5-thione: A combined theoretical and experimental approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 126, 280-90	4.4	9
	The biomolecule, 2-[(2-methoxyl)sulfanyl]-4-(2-methylpropyl)-6-oxo-1,6-dihydropyrimidine-5-carbonitrile: FT-IR, Laser-Raman spectra and DFT. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 126, 86-97	4.4	9

112	Experimental FT-IR, Laser-Raman and DFT spectroscopic analysis of a potential chemotherapeutic agent 6-(2-methylpropyl)-4-oxo-2-sulfanylidene-1,2,3,4-tetrahydropyrimidine-5-carbonitrile. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 120, 97-105	4.4	15
111	Structural and spectroscopic analysis of 3-[(4-phenylpiperazin-1-yl)methyl]-5-(thiophen-2-yl)-2,3-dihydro-1,3,4-oxadiazole-2-thione with experimental (FT-IR, Laser-Raman) techniques and ab initio calculations. <i>Journal of Molecular Structure</i> , 2014 , 123, 439-448	3.4	8
110	Molecular structure and vibrational spectra of 2-Ethoxymethyl-6-ethyl-2,3,4,5-tetrahydro-1,2,4-triazine-3,5-dione, a potential chemotherapeutic agent, by density functional methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 123, 439-448	4.4	4
109	Theoretical investigations on the molecular structure, vibrational spectra, HOMO-LUMO analyses and NBO study of 1-[(Cyclopropylmethoxy)methyl]-5-ethyl-6-(4-methylbenzyl)-1,2,3,4-tetrahydropyrimidine-2,4-dione. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 123, 449-456	4.4	21
108	Vibrational spectra, NBO analysis, HOMO-LUMO and first hyperpolarizability of 2-[(2-Methylprop-2-en-1-yl)oxy]methyl-6-phenyl-2,3,4,5-tetrahydro-1,2,4-triazine-3,5-dione, a potential chemotherapeutic agent based on density functional theory calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 123, 449-456	4.4	18
107	Structural, spectroscopic (FT-IR, FT-Raman and UV) studies, HOMO-LUMO, NBO, NLO analysis and reactivity descriptors of 2,3-Difluoroaniline and 2,4-Difluoroaniline. <i>Journal of Molecular Structure</i> , 2014 , 1074, 457-466	3.4	16
106	Spectroscopic (FT-IR, FT-Raman, and UV-visible) and quantum chemical studies on molecular geometry, Frontier molecular orbitals, NBO, NLO and thermodynamic properties of 1-acetylindole. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 133, 626-38	4.4	13
105	Vibrational spectroscopic studies (FT-IR, FT-Raman) and quantum chemical calculations on 5-(Adamantan-1-yl)-3-[(4-fluoroanilino)methyl]-2,3-dihydro-1,3,4-oxadiazole-2-thione, a potential chemotherapeutic agent. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 133, 605-18	4.4	13
104	Synthesis, antimicrobial, and anti-inflammatory activity, of novel S-substituted and N-substituted 5-(1-adamantyl)-1,2,4-triazole-3-thiols. <i>Drug Design, Development and Therapy</i> , 2014 , 8, 505-18	4.4	31
103	Unusual Sulfuric Acid-Induced Thiol Oxidation on Dehydrative Cyclization of Potassium N-(1-Adamantylcarbonyl)Dithiocarbamate at Room Temperature. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2014 , 189, 477-482	1	
102	Antimicrobial and hypoglycemic activities of novel N-Mannich bases derived from 5-(1-adamantyl)-4-substituted-1,2,4-triazoline-3-thiones. <i>International Journal of Molecular Sciences</i> , 2014 , 15, 22995-3010	6.3	10
101	Pyrimidine-5-carbonitriles II: synthesis and antimicrobial activity of novel 6-alkyl-2,4-disubstituted pyrimidine-5-carbonitriles. <i>Drug Research</i> , 2014 , 64, 31-9	1.8	13
100	Crystal structure of 2-(adamantan-1-yl)-5-(4-bromo-phen-yl)-1,3,4-oxa-diazole. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o1231-2		3
99	3-(Adamantan-1-yl)-4-ethyl-1-[[4-(2-methoxy-phen-yl)piperazin-1-yl]methyl]-1H-1,2,4-triazole-5(4H)-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o25-6		2
98	5-Propyl-6-(p-tolyl-sulfanyl)pyrimidine-2,4(1H,3H)-dione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o179-80		3
97	4-(2-Methoxy-phen-yl)piperazin-1-ium 6-chloro-5-isopropyl-2,4-dioxypyrimidin-1-ide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o245-6		3
96	3-(Adamantan-1-yl)-4-benzyl-1H-1,2,4-triazole-5(4H)-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o766-7		4
95	6-[(2-Methyl-phen-yl)sulfanyl]-5-propyl-pyrimidine-2,4(1H,3H)-dione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o768-9		1

94	FT-IR, FT-Raman, molecular structure, first order hyperpolarizability, HOMO and LUMO analysis, MEP and NBO analysis of 3-(adamantan-1-yl)-4-(prop-2-en-1-yl)-1H-1,2,4-triazole-5(4H)-thione, a potential bioactive agent. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 132, 295-304	4.4	31
93	Structural and spectroscopic characterization of a novel potential anti-inflammatory agent 3-(adamantan-1-yl)-4-ethyl-1H-1,2,4-triazole-5(4H)thione by first principle calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 124, 108-23	4.4	15
92	Vibrational spectroscopy of N'-(Adamantan-2-ylidene)thiophene-2-carbohydrazide, a potential antibacterial agent. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014 , 128, 874-9	4.4	6
91	Crystal structure of 6-chloro-5-iso-propyl-pyrimidine-2,4(1H,3H)-dione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014 , 70, o1144-5		
90	Synthesis and antimicrobial activity of novel 5-(1-adamantyl)-2-aminomethyl-4-substituted-1,2,4-triazoline-3-thiones. <i>European Journal of Medicinal Chemistry</i> , 2013 , 68, 96-102	6.8	77
89	Pyrimidine-5-carbonitriles [part III: synthesis and antimicrobial activity of novel 6-(2-substituted propyl)-2,4-disubstituted pyrimidine-5-carbonitriles. <i>Heterocyclic Communications</i> , 2013 , 19,	1.7	12
88	Synthesis of novel 2-(substituted amino)alkylthiopyrimidin-4(3H)-ones as potential antimicrobial agents. <i>Molecules</i> , 2013 , 19, 279-90	4.8	7
87	4-Benzyl-3-(thio-phen-2-yl)-4,5-di-hydro-1H-1,2,4-triazole-5-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2013 , 69, o697		
86	5-(Adamantan-1-yl)-N-methyl-1,3,4-thia-diazol-2-amine. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2013 , 69, o683		3
85	3-(Adamantan-1-yl)-4-[(E)-(2,6-di-fluoro-benzyl-idene)amino]-1-[(4-ethyl-piperazin-1-yl)meth-yl]-4,5-di-hydro-1H-1,2,4-triazole-5-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2013 , 69, o685-6		3
84	3-[(4-Phenyl-piperazin-1-yl)meth-yl]-5-(thio-phen-2-yl)-2,3-di-hydro-1,3,4-oxa-diazole-2-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2013 , 69, o684		5
83	N-(Adamantan-1-yl)-1,2,3,4-tetra-hydro-iso-quinoline-2-carbo-thio-amide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2013 , 69, o1815		2
82	3-(Adamantan-1-yl)-1-[(4-benzyl-piperazin-1-yl)meth-yl]-4-ethyl-1H-1,2,4-triazole-5(4H)-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2013 , 69, o1813-4		2
81	5-(Adamantan-1-yl)-3-[(4-fluoro-anilino)meth-yl]-2,3-di-hydro-1,3,4-oxa-diazole-2-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2013 , 69, o730		2
80	5-(Adamantan-1-yl)-3-anilinomethyl-2,3-di-hydro-1,3,4-oxa-diazole-2-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2013 , 69, o729		2
79	3-(Adamantan-1-yl)-4-methyl-1-((4-[3-(tri-fluoro-meth-yl)phen-yl]piperazin-1-yl)meth-yl)-4,5-di-hydro-1H-1,2,4-triazole-5-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2013 , 69, o695-6		
78	Structural and spectroscopic characterization of a novel potential chemotherapeutic agent 3-(1-adamantyl)-1-[(4-(2-methoxyphenyl)piperazin-1-yl)methyl]-4-methyl-1H-1,2,4-triazole-5(4H)-thione by first principle calculations. <i>Journal of Molecular Structure</i> , 2012 , 1022, 49-60	3.4	32
77	Synthesis and antimicrobial activity of N'-heteroarylidene-1-adamantylcarbohydrazides and (E)-2-(1-adamantyl)-4-acetyl-5-[5-(4-substituted phenyl-3-isoxazolyl)]-1,3,4-oxadiazolines. <i>Molecules</i> , 2012 , 17, 3475-83	4.8	15

76	2-[[2-Methyl-prop-2-en-1-yl)-oxy]meth-yl]-6-phenyl-2,3,4,5-tetra-hydro-1,2,4-triazine-3,5-dione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o347	1
75	2-[(Cyclo-hex-3-en-1-yl)meth-oxy)meth-yl]-6-phenyl-1,2,4-triazine-3,5(2H,4H)-dione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o1776-7	1
74	2-Benzyl-sulfanyl-4-[(4-methyl-phen-yl)sulfan-yl]-6-pentyl-pyrimidine-5-carbonitrile. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o2054	
73	2-(Adamantan-1-yl)-5-(4-nitro-phen-yl)-1,3,4-oxadiazole. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o795	6
72	6-(2-Methyl-prop-yl)-4-oxo-2-sulfanyl-idene-1,2,3,4-tetra-hydro-pyrimidine-5-carbonitrile. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o676-7	3
71	3-(Adamantan-1-yl)-1-[(4-ethyl-piperazin-1-yl)meth-yl]-4-[(E)-(4-hy-droxy-benzyl-idene)amino]-1H-1,2,4-triazole-5(4H)-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o657-8	6
70	3-(Adamantan-1-yl)-4-(prop-2-en-1-yl)-1H-1,2,4-triazole-5(4H)-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o656	16
69	3-(Adamantan-1-yl)-1-[(4-benzyl-piperazin-1-yl)meth-yl]-4-[(E)-(2-hy-droxy-benzyl-idene)amino]-1H-1,2,4-triazole-5(4H)-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o1766-7	2
68	6-(3,5-Dimethyl-benz-yl)-5-ethyl-1-[(3-phenyl-prop-oxy)meth-yl]-1,2,3,4-tetra-hydro-pyrimidine-2,4-dione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o316	2
67	N'-[(1E)-(2,6-Difluoro-phen-yl)methyl-idene]thio-phen-2-carbohydrazide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o315	2
66	4-Benzyl-N-methyl-piperazine-1-carbothio-amide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o712-3	
65	2-[[5-(Adamantan-1-yl)-4-methyl-4H-1,2,4-triazol-3-yl]sulfan-yl]-N,N-dimethyl-ethanamine. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o1356	3
64	5-(Adamantan-1-yl)-3-[(4-benzyl-piperazin-1-yl)meth-yl]-1,3,4-oxadiazole-2(3H)-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o2172-3	4
63	5-(Adamantan-1-yl)-3-[(2-meth-oxy-eth-yl)sulfan-yl]-4-phenyl-4H-1,2,4-triazole. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o2326	2
62	Ethyl 4-[[3-(adamantan-1-yl)-4-phenyl-5-sulfanyl-idene-4,5-dihydro-1H-1,2,4-triazol-1-yl]meth-yl]piperazine-1-carboxylate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o531	8
61	1-[(Cyclo-propyl-meth-oxy)meth-yl]-5-ethyl-6-(4-methyl-benzyl)-1,2,3,4-tetra-hydro-pyrimidine-2,4-dione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o348	
60	1-[(Cyclo-propyl-meth-oxy)meth-yl]-6-(3,4-dimeth-oxy-benzyl)-5-ethyl-1,2,3,4-tetra-hydro-pyrimidine-2,4-dione ethanol hemisolvate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o349-50	
59	3-(Adamantan-1-yl)-1-[(4-benzyl-piperazin-1-yl)meth-yl]-4-phenyl-1H-1,2,4-triazole-5(4H)-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o344	4

58	3-(Adamantan-1-yl)-4-phenyl-1-[(4-phenyl-piperazin-1-yl)meth-yl]-1H-1,2,4-triazole-5(4H)-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o345	6
57	2-Eth-oxy-methyl-6-ethyl-2,3,4,5-tetra-hydro-1,2,4-triazine-3,5-dione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o346	2
56	2-[(2-Meth-oxy-eth-yl)sulfan-yl]-4-(2-methyl-prop-yl)-6-oxo-1,6-dihydro-pyrimidine-5-carbonitrile. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o1379	3
55	3-(Adamantan-1-yl)-4-ethyl-1H-1,2,4-triazole-5(4H)-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o1347	4
54	3-[(N-Methyl-anilino)meth-yl]-5-(thio-phen-2-yl)-1,3,4-oxadiazole-2(3H)-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o1345-6	4
53	3-(1-Adamant-yl)-4-amino-1-(2-benzoyl-1-phenyl-eth-yl)-1H-1,2,4-triazol-5(4H)-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o1439-40	1
52	1-(Adamantan-1-yl)-3-(4-fluoro-phen-yl)thio-urea. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o1523	3
51	5-Meth-oxy-2-[(5-meth-oxy-1H-indol-1-yl)carbon-yl]-1H-indole. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o1775	1
50	6-Chloro-1-(((2E)-2-methyl-3-phenyl-prop-2-en-1-yl)-oxy)meth-yl)-1,2,3,4-tetra-hydro-quinazoline-2,4-dione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o1770-1	2
49	3-(Adamantan-1-yl)-4-methyl-1-[(4-phenyl-piperazin-1-yl)meth-yl]-1H-1,2,4-triazole-5(4H)-thione dichloro-methane hemisolvate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o1772-3	1
48	1-[[2,3-Dihydro-1H-inden-2-yl)-oxy]meth-yl]quinazoline-2,4(1H,3H)-dione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o1866-7	1
47	3-(Adamantan-1-yl)-4-[(E)-(2,6-difluoro-benzyl-idene)amino]-1-[(4-phenyl-piperazin-1-yl)meth-yl]-1H-1,2,4-triazole-5(4H)-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o2031	1
46	2-[(4-Chloro-benz-yl)sulfan-yl]-4-(2-methyl-prop-yl)-6-(phenyl-sulfan-yl)pyrimidine-5-carbonitrile. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o2055-6	
45	2-[(4-Chloro-benz-yl)sulfanyl]-4-(2-methyl-prop-yl)-6-[3-(trifluoro-meth-yl)anilino]-pyrimidine-5-carbonitrile. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o2059-60	
44	N'-(Adamantan-2-yl-idene)benzo-hydrazide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o2247-8	2
43	3-(Adamantan-1-yl)-4-ethyl-1-[(4-phenyl-piperazin-1-yl)meth-yl]-1H-1,2,4-triazole-5(4H)-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o2380-1	2
42	5-(Adamantan-1-yl)-3-(benzyl-sulfan-yl)-4-methyl-4H-1,2,4-triazole. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2012 , 68, o2427-8	1
41	N'-(Adamantan-2-yl-idene)thio-phen-2-carbohydrazide. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011 , 67, o3127	6

40	Synthesis of novel 6-phenyl-2,4-disubstituted pyrimidine-5-carbonitriles as potential antimicrobial agents. <i>European Journal of Medicinal Chemistry</i> , 2011 , 46, 4642-7	6.8	39
39	6-(3,5-Dimethyl-benz-yl)-5-ethyl-1-[(2-phen-oxy-eth-oxy)meth-yl]-1,2,3,4-tetra-hydro-pyrimidine-2,4-dione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011 , 67, o2839		4
38	2-Benzyl-sulfanyl-4-pentyl-6-(phenyl-sulfan-yl)pyrimidine-5-carbonitrile. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2011 , 67, o3126		1
37	Synthesis and antimicrobial activity of some novel 5-alkyl-6-substituted uracils and related derivatives. <i>Molecules</i> , 2011 , 16, 4764-74	4.8	10
36	N'-[(2-n-Butyl-4-chloro-1H-imidazol-5-yl)-methyl-idene]adamantane-1-carbo-hydrazide sesquihydrate ethanol hemi-solvate. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2010 , 66, o2131		4
35	Some Observations on the Base-Catalyzed Cyclocondensation of 2,6-Dihalobenzaldehydes, Ethyl Cyanoacetate, and Thiourea. <i>Synthetic Communications</i> , 2010 , 40, 1530-1538	1.7	9
34	Synthesis, antimicrobial, and anti-inflammatory activities of novel 5-(1-adamantyl)-4-arylideneamino-3-mercapto-1,2,4-triazoles and related derivatives. <i>Molecules</i> , 2010 , 15, 2526-50	4.8	71
33	3-(1-Adamant-yl)-1-{[4-(2-meth-oxy-phen-yl)piperazin-1-yl]meth-yl}-4-methyl-1H-1,2,4-triazole-5(4H)-thione. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2010 , 66, o1756		24
32	Synthesis, antimicrobial and antiviral testing of some new 1-adamantyl analogues. <i>Saudi Pharmaceutical Journal</i> , 2010 , 18, 123-8	4.4	22
31	Synthesis, antimicrobial and anti-inflammatory activities of novel 5-(1-adamantyl)-1,3,4-thiadiazole derivatives. <i>European Journal of Medicinal Chemistry</i> , 2010 , 45, 5006-11	6.8	137
30	Synthesis of novel uracil non-nucleoside derivatives as potential reverse transcriptase inhibitors of HIV-1. <i>Archiv Der Pharmazie</i> , 2009 , 342, 663-70	4.3	23
29	Synthesis of Diazen-1-ium-1,2-diolates Monitored by the NOtizer Apparatus: Relationship between Formation Rates, Molecular Structure and the Release of Nitric Oxide. <i>European Journal of Organic Chemistry</i> , 2007 , 2007, 616-624	3.2	18
28	Synthesis, antimicrobial, and anti-inflammatory activities of novel 2-(1-adamantyl)-5-substituted-1,3,4-oxadiazoles and 2-(1-adamantylamino)-5-substituted-1,3,4-thiadiazoles. <i>European Journal of Medicinal Chemistry</i> , 2007 , 42, 225-42	6.8	227
27	Synthesis of Novel Uracil Non-Nucleosides Analogues of 3,4-Dihydro-2-Alkylthio-6-benzyl-4-oxopyrimidines and 6-benzyl-1-ethoxymethyl-5-isopropyluracil. <i>Journal of Chemical Research</i> , 2007 , 2007, 263-267	0.6	16
26	Microwave-Assisted Dehydrosulfurization: An Efficient, Solvent-Free Synthesis of 5-(1-Adamantyl)-2-arylamino-1,2,4-triazolo[3,4-b][1,3,4]thiadiazoles. <i>Heterocycles</i> , 2007 , 71, 379	0.8	11
25	Synthesis, antimicrobial, and anti-inflammatory activities of novel 2-[3-(1-adamantyl)-4-substituted-5-thioxo-1,2,4-triazolin-1-yl] acetic acids, 2-[3-(1-adamantyl)-4-substituted-5-thioxo-1,2,4-triazolin-1-yl]propionic acids and related derivatives. <i>Journal of Chemical Research</i> , 2007 , 2007, 263-267		27
24	NO-donors, part 9 : diazeniumdiolates inhibit human platelet aggregation and induce a transient vasodilatation of porcine pulmonary arteries in accordance with the NO-releasing rates. <i>European Journal of Medicinal Chemistry</i> , 2005 , 40, 281-7	6.8	7
23	The NOtizer--a device for the convenient preparation of diazen-1-ium-1,2-diolates. <i>Methods in Enzymology</i> , 2005 , 396, 17-26	1.7	6

22	Synthesis, antimicrobial, and anti-HIV-1 activity of certain 5-(1-adamantyl)-2-substituted thio-1,3,4-oxadiazoles and 5-(1-adamantyl)-3-substituted aminomethyl-1,3,4-oxadiazoline-2-thiones. <i>Bioorganic and Medicinal Chemistry</i> , 2004 , 12, 5107-13	3.4	312
21	Determination of lisinopril in dosage forms and spiked human plasma through derivatization with 7-chloro-4-nitrobenzo-2-oxa-1,3-diazole (NBD-Cl) followed by spectrophotometry or HPLC with fluorimetric detection. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2004 , 34, 35-44	3.5	48
20	1,3,4-THIADIAZOLES. REGIOSELECTIVE O-DEMETHYLATION ON DEHYDRATIVE CYCLIZATION OF 1-(3,4,5-TRIMETHOXYBENZOYL)4-SUBSTITUTED THIOSEMICARBAZIDES WITH SULPHURIC ACID. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2004 , 179, 2509-2517	1	12
19	Synthesis of Certain 6-(Arylthio)uracils and Related Derivatives as Potential Antiviral Agents. <i>Bulletin of the Korean Chemical Society</i> , 2004 , 25, 991-996	1.2	25
18	Spectrophotometric determination of propranolol in formulations via oxidative coupling with 3-methylbenzothiazoline-2-one hydrazone. <i>Il Farmaco</i> , 2003 , 58, 1179-86		26
17	SYNTHESIS OF CERTAIN 6-(ARYLTHIO)URACILS AS POTENTIAL ANTIVIRAL AGENTS. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2001 , 174, 25-35	1	11
16	Synthesis of an AZT-HEPT hybrid and homologous AzddU derivatives. <i>Acta Chemica Scandinavica</i> , 1996 , 50, 417-21		5
15	Synthesis, antimicrobial and antiviral evaluation of certain thienopyrimidine derivatives. <i>European Journal of Medicinal Chemistry</i> , 1995 , 30, 445-449	6.8	53
14	Synthesis of 2-Alkylthio Analogues of AZT and Their Activity against HIV-1. <i>Heterocycles</i> , 1995 , 41, 2507	0.8	7
13	Nucleosides: Synthesis of Some New Naphthimidazole Ribonucleosides as Potential Antibacterial Agents. <i>Journal of the Chinese Chemical Society</i> , 1992 , 39, 257-261	1.5	1
12	Synthesis of 1-phenyl-1H-tetrazolo[4,5-d]tetrazole and 5-aryl-1-(4-bromophenyl)-1,2,4-triazolo[4,3-d]tetrazoles. <i>Journal of the Chinese Chemical Society</i> , 1991 , 38, 199-201	1.5	5
11	Percentages of the deuterium retained after para-hydroxylation of (R)(+)4-2H-phenytoin and (S)(-)4-2H-phenytoin in rat. <i>Archives of Pharmacal Research</i> , 1991 , 14, 35-40	6.1	1
10	Synthesis of certain mercapto-and aminopyrimidine derivatives as potential antimicrobial agents. <i>Archives of Pharmacal Research</i> , 1990 , 13, 142-146	6.1	2
9	Synthesis of certain uracil-6-yl or tetrazol-5-ylpyrazolin-5-one and pyrazole derivatives as potential anti-inflammatory agents. <i>Archives of Pharmacal Research</i> , 1990 , 13, 204-206	6.1	3
8	Thienobenzothiopyranones III new 4H-thieno[2,3-b][1]benzothiopyran-4-ones carrying different heterocyclic moieties of expected pharmacological interest. <i>Archives of Pharmacal Research</i> , 1990 , 13, 24-27	6.1	5
7	Triazoles and fused triazoles, III: Facile and efficient synthesis of 2,5-disubstituted-s-triazolo[3,4-b]-1,3,4-thiadiazoles. <i>Monatshefte Für Chemie</i> , 1990 , 121, 221-225	1.4	16
6	Synthesis of certain substituted pyrimidines as potential schistosomicidal agents. <i>Journal of Heterocyclic Chemistry</i> , 1989 , 26, 913-915	1.9	2
5	Synthesis of substituted arylazothioxanones as potential schistosomicidal agents. <i>Archives of Pharmacal Research</i> , 1989 , 12, 5-7	6.1	1

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2	Synthesis of certain thioxanthenes as potential schistosomicidal agents. <i>Archives of Pharmacal Research</i> , 1986 , 9, 25-28	6.1	3
1	Spectroscopic, Solvation Effects and MD Simulation of an Adamantane-Carbohydrazide Derivative, a Potential Antiviral Agent. <i>Polycyclic Aromatic Compounds</i> , 1-15	1.3	1