

S Murugavel

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Computer Aided Drug Design of 1,2,3-Triazole Fused Bioactive Derivative Targeting Glucosamine-6-Phosphate Synthase (GlmS) â€“ XRD, Computational Crystallography, and Molecular Simulation Approach. Polycyclic Aromatic Compounds, 2023, 43, 3223-3239.	2.6	1
2	Crystal structure, quantum computational, molecular docking and in vitro anti-proliferative investigations of 1Hâ€“imidazoleâ€“2â€“thione analogues derivative. Journal of Molecular Structure, 2022, 1250, 131833.	3.6	2
3	Synthesis, crystal structure elucidation, <sc>DFT</sc> analysis, drugâ€“likeness and <sc>ADMET</sc> evaluation and molecular docking studies of triazole derivatives: Binary inhibition of spike protein and <sc>ACE2</sc> receptor protein of <sc>COVID</sc>â€“19. Journal of the Chinese Chemical Society, 2022, 69, 884-900.	1.4	6
4	Optimized Structure, in Silico interaction and Molecular Docking Analysis of Two Benzimidazole-2-Thione Derivatives. Material Science Research India, 2022, 19, 01-16.	0.7	0
5	Synthesis, X-ray crystal structure, DFT, Hirshfeld surfaces, energy frameworks, and molecular docking analysis of a bicyclic ortho-aminocarbonitrile derivative. European Journal of Chemistry, 2022, 13, 135-144.	0.6	0
6	Synthesis of novel thiophene fused pyrazoline-thiocyanatoethanone derivative: Spectral, DFT, pharmacological, docking and in vitro antibacterial studies. Journal of Molecular Structure, 2021, 1229, 129487.	3.6	5
7	Synthesis, spectral, crystal structure, drugâ€“likeness, in silico, and in vitro biological screening of halogen [Cl, Br] substituted <sc>i>N</i>-phenylbenzo</sc> [<sc>i>g</i>] indazole derivatives as antimicrobial agents. Journal of Heterocyclic Chemistry, 2021, 58, 841-863.	2.6	2
8	Crystallographic Structure and in Silico Molecular Docking Analysis of 2-Cyclohexylidene-Hydrazine-Carbothioamide. Crystallography Reports, 2021, 66, 1306-1310.	0.6	0
9	Synthesis, structural, DFT investigations and antibacterial activity assessment of pyrazolineâ€“thiocyanatoethanone derivatives as thymidylate kinase inhibitors. Journal of the Chinese Chemical Society, 2020, 67, 1100-1112.	1.4	8
10	Synthesis, structural, spectral and antibacterial activity of 3,3a,4,5-tetrahydro-2H-benzo[g]indazole fused carbothioamide derivatives as antibacterial agents. Journal of Molecular Structure, 2020, 1222, 128961.	3.6	11
11	Synthesis, Structural Commentary, Supramolecular Architecture and Molecular Docking Investigations of a Novel Thiophene-Fused 1,2,3,4-Tetrahydroisoquinoline Derivative as a Potent Anti-Cancer Agent. Journal of Structural Chemistry, 2019, 60, 1143-1149.	1.0	0
12	Synthesis, computational quantum chemical study, in silico ADMET and molecular docking analysis, in vitro biological evaluation of a novel sulfur heterocyclic thiophene derivative containing 1,2,3-triazole and pyridine moieties as a potential human topoisomerase IIIâ€“ inhibiting anticancer agent. Computational Biology and Chemistry, 2019, 79, 73-82.	2.3	38
13	Structural correlation and computational quantum chemical explorations of two 1,2,3-triazolyl-methoxypyridine derivatives as CYP51 antifungal inhibitors. Structural Chemistry, 2019, 30, 2225-2243.	2.0	2
14	Synthesis, crystal structure analysis, spectral investigations (NMR, FT-IR, UV), DFT calculations, ADMET studies, molecular docking and anticancer activity of 2-(1-benzyl-5-methyl-1H-1,2,3-triazol-4-yl)-4-(2-chlorophenyl)-6-methoxypyridine â€“ A novel potent human topoisomerase IIIâ€“ inhibitor. Journal of Molecular Structure, 2019, 1176, 729-742.	3.6	50
15	Structure investigation, spectral characterization, electronic properties, and antimicrobial and molecular docking studies of 3â€“(1â€“benzylâ€“5â€“methylâ€“1H-1,2,3-triazoleâ€“4â€“carbonyl)â€“1â€“(2â€“methylâ€“4â€“phenylâ€“1H-1,2,3-triazol-4-yl)â€“5H-spiro[acridine-9,5'-indazole] derivative. Journal of the Chinese Chemical Society, 2019, 66, 205-217.	1.4	6
16	Crystal Structure, Spectral, Electronic, NLO Studies, and Bioactivity of 3â€“(1-Benzyl-5-Methyl-1H-1,2,3-Triazole-4-Carbonyl)-4â€“(4-Bromophenyl)-1â€“(2-Methyl-2H-Spiro [Acenaphthylene-1,2â€“Pyrrolidine]-2-One. Brazilian Journal of Physics, 2019, 49, 28-43.	1.4	4
17	A Green and Efficient Synthesis of Bioactive 1, 2, 3 â€“Triazolylâ€“Pyridine/Cyanopyridine Hybrids <i>via</i> Oneâ€“Pot Multicomponent Grinding Protocol. ChemistrySelect, 2018, 3, 10388-10393.	1.5	7
18	A Smart and Efficient Oneâ€“Pot Green Synthesis of Novel 1, 2, 3â€“Triazolyl Pyrazolineâ€“Indazolylâ€“Carbothioamide Hybrids under Solventâ€“Free Grinding Strategy at Room Temperature. ChemistrySelect, 2018, 3, 10091-10095.	1.5	2

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19	Molecular Structure, Spectral, Electronic and Thermodynamic, First Order Hyperpolarizability, NBO and Molecular Docking Studies of Novel Acenaphthylene Pyrrolidine Derivative. <i>ChemistrySelect</i> , 2018, 3, 11552-11564.	1.5	0
20	Synthesis, characterization, pharmacological, molecular modeling and antimicrobial activity evaluation of novel isomer quinoline derivatives. <i>Structural Chemistry</i> , 2018, 29, 1677-1695.	2.0	8
21	Crystal structure and molecular docking studies of 1,2,4,5-tetraaryl substituted imidazoles. <i>Heterocyclic Communications</i> , 2018, 24, 205-210.	1.2	0
22	Water mediated one-pot synthesis and biological evaluation of 1,2,3-triazolyl-1,4-dihydropyridine hybrids. <i>Research on Chemical Intermediates</i> , 2017, 43, 187-202.	2.7	7
23	Synthesis, structural elucidation, antioxidant, CT-DNA binding and molecular docking studies of novel chloroquinoline derivatives: Promising antioxidant and anti-diabetic agents. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2017, 173, 216-230.	3.8	28
24	Synthesis, crystal structure analysis, spectral (NMR, FT-IR, FT-Raman and UV-Vis) investigations, molecular docking studies, antimicrobial studies and quantum chemical calculations of a novel 4-chloro-8-methoxyquinoline-2(1H)-one: An effective antimicrobial agent and an inhibition of DNA gyrase and lanosterol-14 α -demethylase enzymes. <i>Journal of Molecular Structure</i> , 2017, 1131, 51-72.	3.6	19
25	Synthesis of a novel methyl(2E)-2-([N-(2-formylphenyl)(4-methylbenzene)sulfonamido]methyl)-3-(2-methoxyphenyl)prop-2-enoate: Molecular structure, spectral, antimicrobial, molecular docking and DFT computational approaches. <i>Journal of Molecular Structure</i> , 2017, 1127, 457-475.	3.6	10
26	Synthesis, crystal structure investigation, spectroscopic characterizations and DFT computations on a novel 1-(2-chloro-4-phenylquinolin-3-yl)ethanone. <i>Journal of Molecular Structure</i> , 2016, 1122, 134-145.	3.6	9
27	Sequential change in one-pot, three-component protocol: A stepping stone in heterocyclic synthesis. <i>Synthetic Communications</i> , 2016, 46, 942-948.	2.1	13
28	Synthesis, crystal structure analysis, spectral investigations, DFT computations, Biological activities and molecular docking of methyl(2E)-2-([N-(2-formylphenyl)(4-methylbenzene)sulfonamido]methyl)-3-(4-fluorophenyl)prop-2-enoate, a potential bioactive agent. <i>Journal of Molecular Structure</i> , 2016, 1108, 150-167.	3.6	25
29	Synthesis, growth, spectral, optical and thermal properties of a novel metal-organic family single crystal: Bis (thiocyanato) cobalt(II) di thiourea. <i>Optik</i> , 2016, 127, 4964-4969.	2.9	4
30	Experimental and computational approaches of a novel methyl (2E)-2-([N-(2-formylphenyl)(4-methylbenzene)sulfonamido]methyl)-3-(4-chlorophenyl)prop-2-enoate: A potential antimicrobial agent and an inhibition of penicillin-binding protein. <i>Journal of Molecular Structure</i> , 2016, 1115, 33-54.	3.6	18
31	Experimental and Theoretical Studies of 4-(1-benzyl-5-methyl-1H-1,2,3-triazol-4-yl)-6-(2,4-dichlorophenyl)pyrimidin-2-amine: A Potential Antibacterial Agent. <i>Journal of the Chinese Chemical Society</i> , 2015, 62, 974-983.	1.4	1
32	Synthesis, Crystal Structure and DFT Studies of 4-(1-Benzyl-5-methyl-1H-1,2,3-triazol-4-yl)-6-(o-tolyl)pyrimidin-2-amine. <i>Asian Journal of Chemistry</i> , 2015, 27, 974-978.	0.3	0
33	Crystal structure of [(2S,3R)-3-hydroxy-3-phenylbutan-2-yl]pyrrolidinium chloride. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2015, 71, o758-o758.	0.5	0
34	SYNTHESIS, CRYSTAL STRUCTURE, DFT AND ANTIBACTERIAL ACTIVITY STUDIES OF (E)-2-BENZYL-3-(FURAN-3-YL)-6,7-DIMETHOXY-4-(2-PHENYL-1H-INDEN-1-YLIDENE)-1,2,3,4-Tetrahydroisoquinoline. <i>Journal of the Chilean Chemical Society</i> , 2015, 60, 3015-3020.	1.5	15
35	Crystal structure of (E)-N-(3,3-diphenylallylidene)-9-ethyl-9H-carbazol-3-amine. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2015, 71, 418-420.	0.5	1
36	Crystal structure of (E)-N-[(2-chloro-6-methoxyquinolin-3-yl)methylidene]-9-ethyl-9H-carbazol-3-amine. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2015, 71, 421-423.	0.5	0

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37	Crystal structure of (Z)-3-(4-methoxybenzylidene)-2,3-dihydrobenzo[b][1,4]thiazepin-4(5H)-one. Acta Crystallographica Section E: Crystallographic Communications, 2015, 71, o21-o22.	0.5	0
38	Crystal structure of methyl 2-[2,4-bis(4-fluorophenyl)-3-azabicyclo[3.3.1]nonan-9-ylidene]hydrazinecarboxylate. Acta Crystallographica Section E: Structure Reports Online, 2014, 70, 145-147.	0.2	1
39	Crystal structure of methyl 6-methoxy-11-(4-methoxyphenyl)-16-methyl-14-phenyl-8,12-dioxo-14,15-diazatetracyclo[8.7.0.0.2,7.0.13,17]heptadeca-2(7),3,5,13(17)-tetraene-1,11-dicarboxylate. Acta Crystallographica Section E: Structure Reports Online, 2014, 70, 127-129.	0.2	0
40	An eco-friendly and water mediated product selective synthesis of 2-aminopyrimidines and their in vitro anti-bacterial evaluation. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 4999-5007.	2.2	18
41	CRYSTAL STRUCTURE AND DFT STUDIES OF 4-(1-BENZYL-5-METHYL-1H-1,2,3-TRIAZOL-4-YL)-6-(3-(4-METHOXYBENZYLIDENE)-2,3-DIHYDRO-1,5-BENZOTHAIAZEPIN-4(5H)-ONE). Acta Crystallographica Section E: Structure Reports Online, 2013, 69, o562-o563.	0.2	3
42	(Z)-3-(2,4-Dichlorobenzyl)-1,5-benzothiazepin-4(5H)-one. Acta Crystallographica Section E: Structure Reports Online, 2013, 69, o564-o564.	0.2	1
43	(Z)-3-(3,4-Dimethoxybenzylidene)-2,3-dihydro-1,5-benzothiazepin-4(5H)-one. Acta Crystallographica Section E: Structure Reports Online, 2013, 69, o562-o563.	0.2	3
44	(E)-3-(2-(4-methoxybenzyl)-1,5-benzothiazepin-4(5H)-one)-1,5-benzothiazepin-4(5H)-one. Acta Crystallographica Section E: Structure Reports Online, 2013, 69, o493-o494.	0.2	0
45	3-(4-Methoxybenzyl)-1,5-benzothiazepin-4(5H)-one. Acta Crystallographica Section E: Structure Reports Online, 2013, 69, o693-o693.	0.2	0
46	(Z)-3-(3,4-Dimethoxybenzyl)-1,5-benzothiazepin-4(5H)-one. Acta Crystallographica Section E: Structure Reports Online, 2013, 69, o708-o708.	0.2	0
47	1-methyl-4-(4-methylphenyl)dispiro[1-benzopyran-3(4H),3-pyrrolidine-2-indoline]-2,2-dione. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o11-o11.	0.2	0
48	Methyl (2E)-2-[(2,4-dioxo-1,3-thiazolidin-3-yl)methyl]-3-phenylprop-2-enoate. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o328-o329.	0.2	0
49	Methyl (2Z)-2-[[N-(2-formylphenyl)-4-methylbenzenesulfonamido]methyl]-3-(naphthalen-1-yl)prop-2-enoate. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o330-o331.	0.2	3
50	(E)-3-(2-Chlorophenyl)-2-[(2-formylphenoxy)methyl]prop-2-enenitrile. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o934-o934.	0.2	0
51	(E)-2-[(2-Formylphenoxy)methyl]-3-(4-methylphenyl)prop-2-enenitrile. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o28-o28.	0.2	1
52	(Z)-3-(4-Chlorophenyl)-2-[[N-(2-formylphenyl)-4-methylbenzenesulfonamido]methyl]prop-2-enenitrile. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o56-o57.	0.2	1
53	Methyl (Z)-2-[(2,4-dioxothiazolidin-3-yl)methyl]-3-(2-methylphenyl)prop-2-enoate. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o156-o157.	0.2	2
54	Methyl (2Z)-2-[[N-[2-(hydroxymethyl)phenyl]-4-methylbenzenesulfonamido]methyl]-3-phenylprop-2-enoate. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o418-o419.	0.2	0

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73	(E)-N-(Anthracen-9-ylmethylidene)-4-nitroaniline. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o2577-o2577.	0.2	0
74	(Z)-Methyl 2-[(4-bromo-2-formylphenoxy)methyl]-3-o-tolylacrylate. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o2690-o2690.	0.2	2
75	(Z)-Methyl 2-bromomethyl-3-(2-chlorophenyl)acrylate. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o2812-o2812.	0.2	1
76	Methyl (Z)-2-[[N-(2-formylphenyl)-4-methylbenzenesulfonamido]methyl]-3-phenylprop-2-enoate. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o3511-o3511.	0.2	4
77	1,6-Dimethyl-4-phenylspiro[1-benzopyran-3(4H),3-pyrrolidine-2,3-indoline]-2,2-dione. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o3516-o3517.	0.2	0
78	2-[[4-(Diethylamino)phenyl]iminomethyl]-4,6-diiodophenol. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o3089-o3089.	0.2	0
79	Piperazinedium dioxamate. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o1004-o1004.	0.2	4
80	Aminoguanidinium hydrogen succinate. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o454-o454.	0.2	3
81	4-(3-Ethoxy-4-hydroxystyryl)-1-methylpyridinium tosylate monohydrate. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o71-o71.	0.2	3
82	3-[2-(9-Ethyl-9H-carbazol-3-yl)-6-methyl-3-quinolyl]propan-1-ol. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o139-o140.	0.2	4
83	Aminoguanidinium hydrogen fumarate. Acta Crystallographica Section E: Structure Reports Online, 2009, 65, o548-o548.	0.2	2
84	2,3,4,9-Tetrahydro-1H-carbazole. Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o2433-o2433.	0.2	6
85	9-Ethyl-2,3-dihydro-9H-carbazol-4(1H)-one. Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o1681-o1681.	0.2	1
86	(E)-1,5-Di-2-thienylpenta-1,4-dien-3-one. Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o1807-o1807.	0.2	0
87	(Z)-3-(4-Fluorophenyl)-1-[4-(methylsulfonyl)phenyl]-2-tosylprop-2-en-1-one. Acta Crystallographica Section E: Structure Reports Online, 2008, 64, o2194-o2194.	0.2	0
88	Methyl (2-hydroxy-1,3-dioxindan-2-yl)-1,3-dioxindane-2-spiro-3-pyrrolizidine-1-carboxylate. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o3610-o3610.	0.2	0
89	Methyl (3-hydroxy-2-oxo-2,3-dihydro-1H-indol-3-yl)-2-oxo-2,3-dihydro-1H-indole-3-spiro-3-pyrrolizidine-1-carboxylate. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o3625-o3626.		0
90	3-(4-Methyl-1,3-thiazol-5-yl)-1-[1-(4-methyl-1,3-thiazol-5-yl)-2-oxo-2,3,5,6,7,7a-octahydro-1H-indole-3-spiro-3-pyrrolizidine-1-carboxylate. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o4106-o4107.	0.2	5

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91	6-[(4-Bromophenyl)iminomethyl]-1,3-dimethyl-7-(2-methylpropenyl)-1,2,3,4-tetrahydro-7H-pyrrolo[2,3-d]pyrimidine-2,4-dione, Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o4108-o4108.	0.2	1
92	(2E)-3-(2-Chlorophenyl)-1-[1 ² -(2-chlorophenyl)indoline-3-spiro-3 ² -perhydropyrrolo[1,2-a]indol-2 ² -yl]prop-2-en-1-one. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o4851-o4851.	0.2	0
93	Ethyl 3-phenyl-4-[(Z)-3-phenylacryloyl] 5-(3,4,5-trimethoxyphenyl)pyrrolidine-2-carboxylate. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o4873-o4873.	0.2	0
94	Synthesis, quantum chemical, and molecular modeling investigations of 1,2,3-triazole fused dicarboxylate bioorganic derivative as angiotensin ² -converting enzyme inhibitor. Journal of the Chinese Chemical Society, 0, , .	1.4	0
95	Quantum, Hirshfeld surface, crystal voids, energy framework and molecular docking analysis of two halogen-containing benzimidazole-2-thione structures. Molecular Crystals and Liquid Crystals, 0, , 1-15.	0.9	2