Sumera Zaib

List of Publications by Year
in descending order

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103	1,763	304743	377865
papers	citations	22 h-index	34 g-index

107	107	107	1874
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	CRISPR-Cas9 Genome Engineering: Trends in Medicine and Health. Mini-Reviews in Medicinal Chemistry, 2022, 22, 410-421.	2.4	10
2	Histone Modifications and their Role in Epigenetics of Cancer. Current Medicinal Chemistry, 2022, 29, 2399-2411.	2.4	21
3	Role of Mitochondrial Membrane Potential and Lactate Dehydrogenase A in Apoptosis. Anti-Cancer Agents in Medicinal Chemistry, 2022, 22, 2048-2062.	1.7	50
4	New acetylphenol-based acyl thioureas broaden the scope of drug candidates for urease inhibition: synthesis, in vitro screening and in silico analysis. International Journal of Biological Macromolecules, 2022, 198, 157-167.	7.5	17
5	Discovery of urease inhibitory effect of sulfamate derivatives: Biological and computational studies. Bioorganic Chemistry, 2022, 119, 105545.	4.1	12
6	Inhibition of Aldose Reductase by Ginsenoside Derivatives via a Specific Structure Activity Relationship with Kinetics Mechanism and Molecular Docking Study. Molecules, 2022, 27, 2134.	3.8	8
7	Antiproliferative and Proapoptotic Effect of Daucus carota in Cervical Cancer Cells: An In Vitro Approach. ChemistrySelect, 2022, 7, .	1.5	1
8	Nanomedicines Targeting Heat Shock Protein 90 Gene Expression in the Therapy of Breast Cancer. ChemistrySelect, 2022, 7, .	1.5	2
9	An efficient numerical simulation and mathematical modeling for the prevention of tuberculosis. International Journal of Biomathematics, 2022, 15, .	2.9	9
10	Isolation and Characterization of a Flavonoid and a Neolignan from Silybum marianum : Inâ€vitro Cytotoxic Evaluation. ChemistrySelect, 2022, 7, .	1.5	0
11	Evaluation of indole-picolinamide hybrid molecules as carbonic anhydrase-II inhibitors: Biological and computational studies. Journal of Molecular Structure, 2022, , 133048.	3.6	0
12	Investigation of solid state architectures in tetrazolyl tryptophol stabilized by crucial aromatic interactions and hydrogen bonding: Experimental and theoretical analysis. Journal of Molecular Structure, 2022, 1262, 133079.	3.6	6
13	Rational Design of Antiâ€Epileptic Peptides to Inhibit MAPK/MKPâ€2 Interactions for Epilepsy Therapeutics**. ChemistrySelect, 2022, 7, .	1.5	0
14	Fabrication and Evaluation of Voriconazole Loaded Transethosomal Gel for Enhanced Antifungal and Antileishmanial Activity. Molecules, 2022, 27, 3347.	3.8	9
15	Synthesis, characterization, alkaline phosphatase inhibition assay and molecular modeling studies of 1-benzylidene-2-(4-tert- butylthiazol-2-yl) hydrazines. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6140-6153.	3.5	11
16	Structure-based virtual screening of dipeptidyl peptidase 4 inhibitors and their in vitro analysis. Computational Biology and Chemistry, 2021, 91, 107326.	2.3	7
17	Anticancer evaluation of a manganese complex on HeLa and MCF-7 cancer cells: design, deterministic solvothermal synthesis approach, Hirshfeld analysis, DNA binding, intracellular reactive oxygen species production, electrochemical characterization and density functional theory. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1068-1081.	3.5	6
18	Utilization of the common functional groups in bioactive molecules: Exploring dual inhibitory potential and computational analysis of keto esters against Î±-glucosidase and carbonic anhydrase-II enzymes. International Journal of Biological Macromolecules, 2021, 167, 233-244.	7.5	30

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19	Antiproliferative and Pro-Apoptotic Effects of Thiazolo[3,2â€“b][1,2,4]triazoles in Breast and Cervical Cancer Cells. Anti-Cancer Agents in Medicinal Chemistry, 2021, 21, 2181-2191.	1.7	3
20	Triorganotin (IV) carboxylates as potential anticancer agents: Their synthesis, physiochemical characterization, and cytotoxic activity against HeLa and MCFâ€7 cancer cells. Applied Organometallic Chemistry, 2021, 35, e6165.	3.5	8
21	Rhodanine-3-acetamide derivatives as aldose and aldehyde reductase inhibitors to treat diabetic complications: synthesis, biological evaluation, molecular docking and simulation studies. BMC Chemistry, 2021, 15, 28.	3.8	11
22	New Hybrid Scaffolds Based on Carbazole-Chalcones as Potent Anticancer Agents. Anti-Cancer Agents in Medicinal Chemistry, 2021, 21, 1082-1091.	1.7	3
23	Inhibition of Angiotensin-I Converting Enzyme by Ginsenosides: Structureâ€“Activity Relationships and Inhibitory Mechanism. Journal of Agricultural and Food Chemistry, 2021, 69, 6073-6086.	5.2	10
24	Design of a novel multiple epitope-based vaccine: An immunoinformatics approach to combat SARS-CoV-2 strains. Journal of Infection and Public Health, 2021, 14, 938-946.	4.1	31
25	Indane-1,3-diones: As Potential and Selective Î±-glucosidase Inhibitors, their Synthesis, in vitro and in silico Studies. Medicinal Chemistry, 2021, 17, 887-902.	1.5	4
26	Machine Intelligence Techniques for the Identification and Diagnosis of COVID-19. Current Medicinal Chemistry, 2021, 28, 5268-5283.	2.4	2
27	Potent Inhibitors of Cholinesterases: A Biochemical and In Silico Approach. Molecules, 2021, 26, 656.	3.8	19
28	Alkynoates as Versatile and Powerful Chemical Tools for the Rapid Assembly of Diverse Heterocycles under Transition-Metal Catalysis: Recent Developments and Challenges. Topics in Current Chemistry, 2021, 379, 3.	5.8	16
29	Synthesis of Chalcones as Potential Î± â€Glucosidase Inhibitors, Inâ€Vitro and Inâ€Silico Studies. ChemistrySelect, 2021, 6, 9933-9940.	1.5	1
30	Preventive and Therapeutic Features of Combination Therapy for HIV. Frontiers in Clinical Drug Research - HIV, 2021, , 175-202.	0.0	0
31	Hybrid Quinoline-Thiosemicarbazone Therapeutics as a New Treatment Opportunity for Alzheimerâ€™s Diseaseâ€'Synthesis, In Vitro Cholinesterase Inhibitory Potential and Computational Modeling Analysis. Molecules, 2021, 26, 6573.	3.8	24
32	Fabrication and Biological Assessment of Antidiabetic Î±-Mangostin Loaded Nanosponges: In Vitro, In Vivo, and In Silico Studies. Molecules, 2021, 26, 6633.	3.8	9
33	Green Strategies for Sustainable Câ€“H Bond Functionalizations. Current Organic Chemistry, 2021, 25, 2909-2911.	1.6	0
34	Preparation, Characterization, and Pharmacological Investigation of Withaferin-A Loaded Nanosponges for Cancer Therapy; In Vitro, In Vivo and Molecular Docking Studies. Molecules, 2021, 26, 6990.	3.8	16
35	Synthesis and antitumor activities of novel Mannich base derivatives derived from natural flavonoids. , 2021, , .		5
36	Synthesis, characterization, and anticancer activity of Schiff bases. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3246-3259.	3.5	68

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37	Synthesis, characterization, in vitro tissue-nonspecific alkaline phosphatase (TNAP) and intestinal alkaline phosphatase (IAP) inhibition studies and computational evaluation of novel thiazole derivatives. Bioorganic Chemistry, 2020, 102, 104088.	4.1	17
38	Evaluation of sulfonate and sulfamate derivatives possessing benzofuran or benzothiophene nucleus as inhibitors of nucleotide pyrophosphatases/phosphodiesterases and anticancer agents. Bioorganic Chemistry, 2020, 104, 104305.	4.1	9
39	Synthetic and medicinal chemistry of phthalazines: Recent developments, opportunities and challenges. Bioorganic Chemistry, 2020, 105, 104425.	4.1	18
40	New frontiers in the transition-metal-free synthesis of heterocycles from alkynoates: an overview and current status. Organic Chemistry Frontiers, 2020, 7, 3734-3791.	4.5	43
41	Mechanistic insight of DACH1 receptor in the development of carcinoma insurgence through MD simulation studies. Journal of Biomolecular Structure and Dynamics, 2020, , 1-10.	3.5	3
42	Bisthioureas of pimelic acid and 4-methylsalicylic acid derivatives as selective inhibitors of tissue-nonspecific alkaline phosphatase (TNAP) and intestinal alkaline phosphatase (IAP): Synthesis and molecular docking studies. Bioorganic Chemistry, 2020, 101, 103996.	4.1	9
43	Synthesis, biological evaluation, and docking studies of new pyrazole-based thiourea and sulfonamide derivatives as inhibitors of nucleotide pyrophosphatase/phosphodiesterase. Bioorganic Chemistry, 2020, 99, 103783.	4.1	20
44	Recent advances with alkaline phosphatase isoenzymes and their inhibitors. Archiv Der Pharmazie, 2020, 353, e2000011.	4.1	48
45	Poncirin, an orally active flavonoid exerts antidiabetic complications and improves glucose uptake activating PI3K/Akt signaling pathway in insulin resistant C2C12 cells with anti-glycation capacities. Bioorganic Chemistry, 2020, 102, 104061.	4.1	14
46	Sesquiterpene Coumarins from Ferula narthex 15-LOX, Î±-Glucosidase Inhibition and Molecular Docking Studies. Revista Brasileira De Farmacognosia, 2020, 30, 12-17.	1.4	2
47	Exploiting oxadiazole-sulfonamide hybrids as new structural leads to combat diabetic complications via aldose reductase inhibition. Bioorganic Chemistry, 2020, 99, 103852.	4.1	10
48	An efficient synthetic approach toward a sporadic heterocyclic scaffold: 1,3-Oxathiol-2-ylidenes; alkaline phosphatase inhibition and molecular docking studies. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127238.	2.2	7
49	Recent Advances in the Sustainable Synthesis of Quinazolines Using Earth-Abundant First Row Transition Metals. Current Organic Chemistry, 2020, 24, 1775-1792.	1.6	5
50	Highly Potent and Selective Ectonucleoside Triphosphate Diphosphohydrolase (ENTPDase1, 2, 3 and 8) Inhibitors Having 2-substituted-7- trifluoromethyl-thiadiazolopyrimidones Scaffold. Medicinal Chemistry, 2020, 16, 689-702.	1.5	4
51	15-LOX Inhibitors: Biochemical Evaluation of Flurbiprofen and its Derivatives. Life and Science, 2020, 1, 6.	0.1	6
52	Sulfonate and sulfamate derivatives possessing benzofuran or benzothiophene nucleus as potent carbonic anhydrase II/IX/XII inhibitors. Bioorganic and Medicinal Chemistry, 2019, 27, 3889-3901.	3.0	10
53	Design, synthesis and biological evaluation of trinary benzocoumarin-thiazoles-azomethines derivatives as effective and selective inhibitors of alkaline phosphatase. Bioorganic Chemistry, 2019, 91, 103137.	4.1	18
54	Synthesis, biological evaluation, and docking studies of new raloxifene sulfonate or sulfamate derivatives as inhibitors of nucleotide pyrophosphatase/phosphodiesterase. European Journal of Medicinal Chemistry, 2019, 181, 111560.	5.5	24

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55	Synthesis of 2â€Arylâ€12 H â€benzothiazolo[2,3â€•b]quinazolinâ€12â€•ones and Their Activity Against Monoamine Oxidases. ChemistrySelect, 2019, 4, 11071-11076.	1.5	3
56	Synthesis and Inhibitory Activity towards Monoamine Oxidase A and B of 8â€Functionalized 3â€Fluoroâ€2â€•methylâ€benzo[4,5]thiazolo[3,2â€•a]pyrimidinâ€4â€•ones. ChemistrySelect, 2019, 4, 7284-7291.	1.5	4
57	Investigation of potent inhibitors of cholinesterase based on thiourea and pyrazoline derivatives: Synthesis, inhibition assay and molecular modeling studies. Bioorganic Chemistry, 2019, 90, 103036.	4.1	19
58	Synthesis, biological evaluation, and molecular docking study of sulfonate derivatives as nucleotide pyrophosphatase/phosphodiesterase (NPP) inhibitors. Bioorganic and Medicinal Chemistry, 2019, 27, 2741-2752.	3.0	17
59	Didymin, a dietary citrus flavonoid exhibits anti-diabetic complications and promotes glucose uptake through the activation of PI3K/Akt signaling pathway in insulin-resistant HepG2 cells. Chemico-Biological Interactions, 2019, 305, 180-194.	4.0	44
60	Investigation of new quinoline derivatives as promising inhibitors of NTPDases: Synthesis, SAR analysis and molecular docking studies. Bioorganic Chemistry, 2019, 87, 218-226.	4.1	17
61	Probing the high potency of pyrazolyl pyrimidinetriones and thioxopyrimidinediones as selective and efficient non-nucleotide inhibitors of recombinant human ectonucleotidases. Bioorganic Chemistry, 2019, 88, 102893.	4.1	11
62	Synthesis, X-ray crystal and monoamine oxidase inhibitory activity of 4,6-dihydrobenzo[c]pyrano[2,3-e][1,2]thiazine 5,5-dioxides: In vitro studies and docking analysis. European Journal of Pharmaceutical Sciences, 2019, 131, 9-22.	4.0	14
63	Synthesis of 2â€Alkynylâ€•and2â€Aminoâ€12 H â€benzothiazolo[2,3â€•b]quinazolinâ€12â€•ones and Their Inhibitory Potential against Monoamine Oxidase A and B. ChemistrySelect, 2019, 4, 13760-13767.	1.5	3
64	Antidiabetic activities of chloroform fraction of Anthocleista vogelii Planch root bark in rats with diet- and alloxan-induced obesity-diabetes. Journal of Ethnopharmacology, 2019, 229, 293-302.	4.1	25
65	Synthesis and in vitro urease inhibitory activity of benzohydrazide derivatives, in silico and kinetic studies. Bioorganic Chemistry, 2019, 82, 163-177.	4.1	22
66	Cytotoxicity, Pro-apoptotic Activity and in silico Studies of Dithiocarbamates and their Structure Based Design and SAR Studies. Medicinal Chemistry, 2019, 15, 892-902.	1.5	7
67	Carbonic Anhydrase Inhibitory Potential of 1,2,4-triazole-3-thione Derivatives of Flurbiprofen, Ibuprofen and 4-tert-butylbenzoic Hydrazide: Design, Synthesis, Characterization, Biochemical Evaluation, Molecular Docking and Dynamic Simulation Studies. Medicinal Chemistry, 2019, 15, 298-310.	1.5	7
68	Cytotoxicity Potential of Nelsonia canescens (Lam.) Spreng Extracts against Cervical Cancer Cell Lines. Saudi Journal of Biomedical Research, 2019, 04, 439-443.	0.2	1
69	Synthesis, molecular modelling and biological evaluation of tetrasubstituted thiazoles towards cholinesterase enzymes and cytotoxicity studies. Bioorganic Chemistry, 2018, 78, 141-148.	4.1	21
70	Synthesis, characterization, monoamine oxidase inhibition, molecular docking and dynamic simulations of novel 2,1-benzothiazine-2,2-dioxide derivatives. Bioorganic Chemistry, 2018, 80, 498-510.	4.1	15
71	A new entry into the portfolio of Î±-glucosidase inhibitors as potent therapeutics for type 2 diabetes: Design, bioevaluation and one-pot multi-component synthesis of diamine-bridged coumarinyl oxadiazole conjugates. Bioorganic Chemistry, 2018, 77, 190-202.	4.1	48
72	A domino reaction of 3-chlorochromones with aminoheterocycles. Synthesis of pyrazolopyridines and benzofuropyridines and their optical and ecto-5â€²-nucleotidase inhibitory effects. Organic and Biomolecular Chemistry, 2018, 16, 717-732.	2.8	28

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73	Synthesis, crystal structure, molecular docking studies and bio-evaluation of some N ⁴-benzyl-substituted isatin- 3-thiosemicarbazones as urease and glycation inhibitors. Heterocyclic Communications, 2018, 24, 51-58.	1.2	20
74	Pd(II)-based heteroleptic complexes with N-(acyl)-Nâ€², Nâ€²-(disubstituted)thioureas and phosphine ligands: Synthesis, characterization and cytotoxic studies against lung squamous, breast adenocarcinoma and Leishmania tropica. Inorganica Chimica Acta, 2018, 479, 189-196.	2.4	16
75	Solution-phase microwave assisted parallel synthesis, biological evaluation and in silico docking studies of 2-chlorobenzoyl thioureas derivatives. Journal of Molecular Structure, 2018, 1164, 354-362.	3.6	11
76	Synthesis, monoamine oxidase inhibition activity and molecular docking studies of novel 4-hydroxy-Nâ€²-[benzylidene or 1-phenylethylidene]-2-H/methyl/benzyl-1,2-benzothiazine-3-carbohydrazide 1,1-dioxides. European Journal of Medicinal Chemistry, 2018, 143, 1373-1386.	5.5	26
77	Modification of Bischler-MÃ¶hlau indole derivatives through palladium catalyzed Suzuki reaction as effective cholinesterase inhibitors, their kinetic and molecular docking studies. Bioorganic Chemistry, 2018, 76, 166-176.	4.1	8
78	Carbonic anhydrase inhibition of Schiff base derivative of imino-methyl-naphthalen-2-ol: Synthesis, structure elucidation, molecular docking, dynamic simulation and density functional theory calculations. Journal of Molecular Structure, 2018, 1156, 193-200.	3.6	20
79	Synthesis of Novel Benzothiazolo[3,2â€•a]pyridimidinâ€4â€•ones with Potential Cytotoxic and Proâ€Apoptotic Potential. ChemistrySelect, 2018, 3, 12213-12218.	1.5	2
80	Identification of New Chromenone Derivatives as Cholinesterase Inhibitors and Molecular Docking Studies. Medicinal Chemistry, 2018, 14, 809-817.	1.5	1
81	Quinolinic Carboxylic Acid Derivatives as Potential Multi-target Compounds for Neurodegeneration: Monoamine Oxidase and Cholinesterase Inhibition. Medicinal Chemistry, 2018, 14, 74-85.	1.5	15
82	Dithallium(III)-Containing 30-Tungsto-4-phosphate, [Tl₂Na₂(H₂O)₂(P₂W₁₅O₅₆)₂]¹⁶⁻: Synthesis, Structural Characterization, and Biological Studies. Inorganic Chemistry, 2018, 57, 7168-7179.	4.6	13
83	Synthesis and in vitro Bio-activity Evaluation of N4-benzyl Substituted 5-Chloroisatin-3-thiosemicarbazones as Urease and Glycation Inhibitors. Acta Chimica Slovenica, 2018, 65, 108-118.	0.6	23
84	Antidiabetic potential of methanol extracts from leaves of Piper umbellatum L. and Persea americana Mill.. Asian Pacific Journal of Tropical Biomedicine, 2018, 8, 160.	1.2	9
85	In vitro Antiobesity Activities and In vivo Anti-Lipolytic Effect of Alstonia boonei Stem Bark Fraction. Proceedings for Annual Meeting of the Japanese Pharmacological Society, 2018, WCP2018, PO4-8-3.	0.0	0
86	Synthesis, X-ray molecular structure, biological evaluation and molecular docking studies of some N 4 -benzyl substituted 5-nitroisatin-3-thiosemicarbazones. Bioorganic and Medicinal Chemistry, 2017, 25, 1022-1029.	3.0	11
87	Pyrazolobenzothiazine-based carbothioamides as new structural leads for the inhibition of monoamine oxidases: design, synthesis, in vitro bioevaluation and molecular docking studies. MedChemComm, 2017, 8, 452-464.	3.4	18
88	New prospects for the development of selective inhibitors of Î± -glucosidase based on coumarin-iminothiazolidinone hybrids: Synthesis, in-vitro biological screening and molecular docking analysis. Journal of the Taiwan Institute of Chemical Engineers, 2017, 81, 119-133.	5.3	26
89	Exploration of aroyl/heteroaroyl iminothiazolines featuring 2,4,5-trichlorophenyl moiety as a new class of potent, selective, and in vitro efficacious glucosidase inhibitors. Bioorganic Chemistry, 2017, 74, 134-144.	4.1	18
90	A multi-target therapeutic potential of Prunus domestica gum stabilized nanoparticles exhibited prospective anticancer, antibacterial, urease-inhibition, anti-inflammatory and analgesic properties.. BMC Complementary and Alternative Medicine, 2017, 17, 276.	3.7	53

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91	Symmetrical aryl linked bis-iminothiazolidinones as new chemical entities for the inhibition of monoamine oxidases: Synthesis, in vitro biological evaluation and molecular modelling analysis. Bioorganic Chemistry, 2017, 70, 17-26.	4.1	17
92	Synthesis, Characterization and Biological Activities of Creatinine Amides and Creatinine Schiff Bases. Medicinal Chemistry, 2017, 13, 196-203.	1.5	4
93	Unraveling the Alkaline Phosphatase Inhibition, Anticancer, and Antileishmanial Potential of Coumarinâ€"Triazolothiadiazine Hybrids: Design, Synthesis, and Molecular Docking Analysis. Archiv Der Pharmazie, 2016, 349, 553-565.	4.1	29
94	Solution-phase microwave assisted parallel synthesis, biological evaluation and in silico docking studies of N,Nâ€²-disubstituted thioureas derived from 3-chlorobenzoic acid. Bioorganic and Medicinal Chemistry, 2016, 24, 4452-4463.	3.0	31
95	Synthesis, biological evaluation and docking studies of some novel isatin-3-hydrazonothiazolines. RSC Advances, 2016, 6, 60826-60844.	3.6	18
96	Exploiting the potential of aryl acetamide derived Zn(<scp>ii</scp>) complexes in medicinal chemistry: synthesis, structural analysis, assessment of biological profile and molecular docking studies. New Journal of Chemistry, 2016, 40, 7084-7094.	2.8	20
97	Exploration of a library of triazolothiadiazole and triazolothiadiazine compounds as a highly potent and selective family of cholinesterase and monoamine oxidase inhibitors: design, synthesis, X-ray diffraction analysis and molecular docking studies. RSC Advances, 2015, 5, 21249-21267.	3.6	45
98	Synthesis, characterization and urease inhibition, in vitro anticancer and antileishmanial studies of Ni(II) complexes with N,N,Nâ€²-trisubstituted thioureas. Journal of Biological Inorganic Chemistry, 2015, 20, 541-554.	2.6	45
99	Synthesis, crystal structure and biological evaluation of some novel 1,2,4-triazolo[3,4-b]-1,3,4-thiadiazoles and 1,2,4-triazolo[3,4-b]-1,3,4-thiadiazines. European Journal of Medicinal Chemistry, 2014, 78, 167-177.	5.5	86
100	Active compounds from a diverse library of triazolothiadiazole and triazolothiadiazine scaffolds: Synthesis, crystal structure determination, cytotoxicity, cholinesterase inhibitory activity, and binding mode analysis. Bioorganic and Medicinal Chemistry, 2014, 22, 6163-6173.	3.0	54
101	Synthesis, molecular docking studies, and in vitro screening of sulfanilamide-thiourea hybrids as antimicrobial and urease inhibitors. Medicinal Chemistry Research, 2013, 22, 3653-3662.	2.4	46
102	Synthesis, urease inhibition, antioxidant and antibacterial studies of some 4-amino-5-aryl-3H-1,2,4-triazole-3-thiones and their 3,6-disubstituted 1,2,4-triazolo[3,4-b]1,3,4-thiadiazole derivatives. Journal of the Brazilian Chemical Society, 2012, 23, 854-860.	0.6	71
103	Centroidâ‹¯centroid and hydrogen bond interactions as robust supramolecular units for crystal engineering: X-ray crystallographic, computational and urease inhibitory investigations of 1,2,4-triazolo[3,4-a]phthalazines. CrystEngComm, 0, , .	2.6	5