

# Mohamed Reda Aouad

## List of Publications by Year in descending order

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73  
papers

1,476  
citations

304368

22  
h-index

377514

34  
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78  
all docs

78  
docs citations

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times ranked

1163  
citing authors

#	ARTICLE	IF	CITATIONS
1	Discovery of triaromatic flexible agents bearing 1,2,3-Triazole with selective and potent anti-breast cancer activity and CDK9 inhibition supported by molecular dynamics. <i>Journal of Molecular Structure</i> , 2022, 1249, 131568.	1.8	18
2	Synthesis, DFT Molecular Geometry and Anticancer Activity of Symmetrical 2,2- $\alpha$ -(2-Oxo-1H-benzo[d]imidazole-1,3(2H)-diyl) Diacetate and Its Arylideneacetohydrazide Derivatives. <i>Materials</i> , 2022, 15, 2544.	1.3	4
3	Exploring the Antiparasitic Activity of Tris-1,3,4-Thiadiazoles against <i>Toxoplasma gondii</i> -Infected Mice. <i>Molecules</i> , 2022, 27, 2246.	1.7	7
4	Synthesis, Characterization and Nanoformulation of Novel Sulfonamide-1,2,3-triazole Molecular Conjugates as Potent Antiparasitic Agents. <i>International Journal of Molecular Sciences</i> , 2022, 23, 4241.	1.8	10
5	Targeting the interplay between MMP-2, CA II and VEGFR-2 via new sulfonamide-tethered isomeric triazole hybrids; Microwave-assisted synthesis, computational studies and evaluation. <i>Bioorganic Chemistry</i> , 2022, 124, 105816.	2.0	10
6	Dicationic Bis-Pyridinium Hydrazone-Based Amphiphiles Encompassing Fluorinated Counteranions: Synthesis, Characterization, TGA-DSC, and DFT Investigations. <i>Molecules</i> , 2022, 27, 2492.	1.7	4
7	Novel Hybrid 1,2,4- and 1,2,3-Triazoles Targeting Mycobacterium Tuberculosis Enoyl Acyl Carrier Protein Reductase (InhA): Design, Synthesis, and Molecular Docking. <i>International Journal of Molecular Sciences</i> , 2022, 23, 4706.	1.8	12
8	Tailoring of some novel bis-hydrazone metal chelates, spectral based characterization and DFT calculations for pharmaceutical applications and in-silico treatments for verification. <i>Journal of Molecular Structure</i> , 2022, 1264, 133263.	1.8	36
9	Design, Synthesis and Molecular Docking of Novel Acetophenone-1,2,3-Triazoles Containing Compounds as Potent Enoyl-Acyl Carrier Protein Reductase (InhA) Inhibitors. <i>Pharmaceuticals</i> , 2022, 15, 799.	1.7	6
10	Novel 1,2,3-Triazole-sulphadiazine-ZnO Hybrids as Potent Antimicrobial Agents against Carbapenem Resistant Bacteria. <i>Antibiotics</i> , 2022, 11, 916.	1.5	6
11	Design, click conventional and microwave syntheses, DNA binding, docking and anticancer studies of benzotriazole-1,2,3-triazole molecular hybrids with different pharmacophores. <i>Journal of Molecular Structure</i> , 2021, 1225, 129192.	1.8	30
12	Design and Synthesis of Novel Imidazole Derivatives Possessing Triazole Pharmacophore with Potent Anticancer Activity, and In Silico ADMET with GSK-3 $\beta$ Molecular Docking Investigations. <i>International Journal of Molecular Sciences</i> , 2021, 22, 1162.	1.8	17
13	Design, synthesis, DNA binding, modeling, anticancer studies and DFT calculations of Schiff bases tethering benzothiazole-1,2,3-triazole conjugates. <i>Journal of Molecular Structure</i> , 2021, 1225, 129148.	1.8	52
14	Microwave versus conventional synthesis, anticancer, DNA binding and docking studies of some 1,2,3-triazoles carrying benzothiazole. <i>Arabian Journal of Chemistry</i> , 2021, 14, 102997.	2.3	5
15	Novel 1,2,3-Triazole Derivatives as Potential Inhibitors against Covid-19 Main Protease: Synthesis, Characterization, Molecular Docking and DFT Studies. <i>ChemistrySelect</i> , 2021, 6, 3468-3486.	0.7	23
16	Design of molecular hybrids of phthalimide-triazole agents with potent selective MCF-7/HepG2 cytotoxicity: Synthesis, EGFR inhibitory effect, and metabolic stability. <i>Bioorganic Chemistry</i> , 2021, 111, 104835.	2.0	34
17	Halting Tumor Progression via Novel Non-Hydroxamate Triazole-Based Mannich Bases MMP-2/9 Inhibitors; Design, Microwave-Assisted Synthesis, and Biological Evaluation. <i>International Journal of Molecular Sciences</i> , 2021, 22, 10324.	1.8	16
18	New 1,2,3-Triazole Scaffold Schiff Bases as Potential Anti-COVID-19: Design, Synthesis, DFT-Molecular Docking, and Cytotoxicity Aspects. <i>Vaccines</i> , 2021, 9, 1012.	2.1	23

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19	Novel Dipyridinium Lipophile-Based Ionic Liquids Tethering Hydrazone Linkage: Design, Synthesis and Antitumorogenic Study. <i>International Journal of Molecular Sciences</i> , 2021, 22, 10487.	1.8	7
20	Anti-COVID-19 activity of some benzofused 1,2,3-triazolesulfonamide hybrids using in silico and in vitro analyses. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2021, 217, 104421.	1.8	16
21	Design, Synthesis, Molecular Modeling, Anticancer Studies, and Density Functional Theory Calculations of 4-(1,2,4-Triazol-3-ylsulfanylmethyl)-1,2,3-triazole Derivatives. <i>ACS Omega</i> , 2021, 6, 301-316.	1.6	53
22	Introducing of acyclonucleoside analogues tethered 1,2,4-triazole as anticancer agents with dual epidermal growth factor receptor kinase and microtubule inhibitors. <i>Bioorganic Chemistry</i> , 2020, 94, 103446.	2.0	22
23	Synthesis, Characterization, DNA Binding, Docking, and Anticancer Studies of Novel Bis(1,2,3-triazoles) Phthalonitrile. <i>ChemistrySelect</i> , 2020, 5, 11347-11353.	0.7	17
24	Novel scaffold hopping of potent benzothiazole and isatin analogues linked to 1,2,3-triazole fragment that mimic quinazoline epidermal growth factor receptor inhibitors: Synthesis, antitumor and mechanistic analyses. <i>Bioorganic Chemistry</i> , 2020, 103, 104133.	2.0	53
25	Synthesis, Characterization, DNA Binding, Anticancer, and Molecular Docking Studies of Novel Imidazolium-Based Ionic Liquids with Fluorinated Phenylacetamide Tethers. <i>ACS Omega</i> , 2020, 5, 4807-4815.	1.6	39
26	Novel Fluorinated Imidazolium Ionic Liquids: Eco-friendly, Facile and Efficient Construction, Characterization, in vitro Anticancer Activity, Toxicity and in silico Analysis. <i>Asian Journal of Chemistry</i> , 2020, 32, 690-696.	0.1	5
27	Microwave and conventional synthesis of ester based dicationic pyridinium ionic liquids carrying hydrazone linkage: DNA binding, anticancer and docking studies. <i>Journal of Molecular Structure</i> , 2020, 1207, 127756.	1.8	21
28	Green microwave versus conventional synthesis, crystal structure of 1-(4-(Benzothiazol-2-yl)piperazin-1-yl)-2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethenone and HS-Analysis. <i>Journal of Taibah University for Science</i> , 2020, 14, 549-556.	1.1	1
29	A Profile of the In Vitro Anti-Tumor Activity and In Silico ADME Predictions of Novel Benzothiazole Amide-Functionalized Imidazolium Ionic Liquids. <i>International Journal of Molecular Sciences</i> , 2019, 20, 2865.	1.8	28
30	Crystal structure of (E)-4-((2-fluoro-3-(trifluoromethyl)benzylidene)amino)-3-methyl-1H-1,2,4-triazole-5-thione, C <sub>11</sub> H <sub>8</sub> F <sub>4</sub> N <sub>4</sub> S. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2019, 234, 343-344.	0.1	1
31	Crystal structure of 5-(4-fluorophenyl)-4-methyl-2,4-dihydro-3H-1,2,4-triazole-3-thione, C <sub>9</sub> H <sub>8</sub> FN <sub>3</sub> S. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2019, 234, 345-346.	0.1	0
32	Synthesis, Characterization, and Antimicrobial Screening of Novel 1,2,4-Triazoles, 1,3,4-Thiadiazoles, and 1,3,4-Oxadiazoles Bearing the Indole Moiety. <i>Organic Preparations and Procedures International</i> , 2019, 51, 270-286.	0.6	7
33	Novel pyridinium based ionic liquids with amide tethers: Microwave assisted synthesis, molecular docking and anticancer studies. <i>Journal of Molecular Liquids</i> , 2019, 285, 790-802.	2.3	20
34	Design, click synthesis, anticancer screening and docking studies of novel benzothiazole-1,2,3-triazoles appended with some bioactive benzofused heterocycles. <i>Journal of Molecular Structure</i> , 2019, 1188, 153-164.	1.8	52
35	A novel dicationic ionic liquids encompassing pyridinium hydrazone-phenoxy conjugates as antimicrobial agents targeting diverse high resistant microbial strains. <i>Journal of Molecular Liquids</i> , 2019, 284, 431-444.	2.3	27
36	Crystal structure of 1-nonylpyridazin-1-ium iodide, C <sub>13</sub> H <sub>23</sub> N <sub>2</sub> I. <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2019, 234, 857-859.	0.1	1

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37	Hydrophobic pocket docking, double-proton prototropic tautomerism in contradiction to single-proton transfer in thione $\rightleftharpoons$ thiol Schiff base with triazole-thione moiety: Green synthesis, XRD and DFT-analysis. <i>Journal of Molecular Structure</i> , 2019, 1180, 455-461.	1.8	30
38	Action of Thioglycosides of 1,2,4-Triazoles and Imidazoles on the Oxidative Stress and Glycosidases in Mice with Molecular Docking. <i>Letters in Drug Design and Discovery</i> , 2019, 16, 696-710.	0.4	0
39	Crystal structure of the coordination polymer $\left[ \text{catena-poly} \left[ \text{chlorido-}\lambda_4\text{-2-}((3,5\text{-dimethyl-1H-pyrazol-1-yl)methyl)amino-3\text{-hydroxybutanoato-}\lambda^{\text{p}}\text{-4-Cu}^{\text{II}}\right] \right]_n \cdot 11\text{H}_2\text{O} \cdot 16\text{Cl} \cdot 2\text{Cu} \cdot 3\text{O}$ . <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2018, 233, 493-494.	0.1	0
40	Microwave-assisted synthesis of novel imidazolium, pyridinium and pyridazinium-based ionic liquids and/or salts and prediction of physico-chemical properties for their toxicity and antibacterial activity. <i>Journal of Molecular Liquids</i> , 2018, 249, 747-753.	2.3	48
41	Novel amphiphilic pyridinium ionic liquids-supported Schiff bases: ultrasound assisted synthesis, molecular docking and anticancer evaluation. <i>Chemistry Central Journal</i> , 2018, 12, 118.	2.6	12
42	Crystal structure of 4-phenyl-3-((4-phenyl-1H-1,2,3-triazol-1-yl)methyl)-1H-1,2,4-triazole-5(4H)-thione, $\text{C}_{17}\text{H}_{14}\text{N}_6\text{S}$ . <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2018, 233, 697-698.	0.1	0
43	Design, synthesis, ADME prediction and pharmacological evaluation of novel benzimidazole-1,2,3-triazole-sulfonamide hybrids as antimicrobial and antiproliferative agents. <i>Chemistry Central Journal</i> , 2018, 12, 110.	2.6	49
44	Design, Synthesis and Anticancer Screening of Novel Benzothiazole-Piperazine-1,2,3-Triazole Hybrids. <i>Molecules</i> , 2018, 23, 2788.	1.7	46
45	Single proton intramigration in novel 4-phenyl-3-((4-phenyl-1H-1,2,3-triazol-1-yl)methyl)-1H-1,2,4-triazole-5(4H)-thione: XRD-crystal interactions, physicochemical, thermal, Hirshfeld surface, DFT realization of thiol/thione tautomerism. <i>Journal of Molecular Liquids</i> , 2018, 264, 621-630.	2.3	43
46	Identification of new pyridinium ionic liquids tagged with Schiff bases: Design, synthesis, in silico ADMET predictions and biological evaluations. <i>Journal of Molecular Liquids</i> , 2018, 264, 367-374.	2.3	20
47	Crystal structure of 1-heptylpyridazin-1-ium iodide, $\text{C}_{11}\text{H}_{19}\text{N}_2\text{I}$ . <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2018, 233, 739-741.	0.1	1
48	Microwave-Assisted Synthesis of Some Potential Bioactive Imidazolium-Based Room-Temperature Ionic Liquids. <i>Molecules</i> , 2018, 23, 1727.	1.7	21
49	Crystal structure of 4-(dimethylamino)-1-(prop-2-yn-1-yl)pyridin-1-ium perchlorate, $\text{C}_{10}\text{H}_{13}\text{ClN}_2\text{O}_4$ . <i>Zeitschrift Fur Kristallographie - New Crystal Structures</i> , 2018, 233, 897-898.	0.1	0
50	Design, synthesis, in-silico and in-vitro evaluation of di-cationic pyridinium ionic liquids as potential anticancer scaffolds. <i>Journal of Molecular Liquids</i> , 2018, 265, 428-441.	2.3	24
51	Click Synthesis and Antimicrobial Screening of Novel Isatin-1,2,3-Triazoles with Piperidine, Morpholine, or Piperazine Moieties. <i>Organic Preparations and Procedures International</i> , 2017, 49, 216-227.	0.6	27
52	Green ultrasound-assisted three-component click synthesis of novel 1H-1,2,3-triazole carrying benzothiazoles and fluorinated-1,2,4-triazole conjugates and their antimicrobial evaluation. <i>Acta Pharmaceutica</i> , 2017, 67, 309-324.	0.9	23
53	Design, synthesis, in silico and in vitro antimicrobial screenings of novel 1,2,4-triazoles carrying 1,2,3-triazole scaffold with lipophilic side chain tether. <i>Chemistry Central Journal</i> , 2017, 11, 117.	2.6	49
54	Click 1,4-regioselective synthesis, characterization, and antimicrobial screening of novel 1,2,3-triazoles tethering fluorinated 1,2,4-triazole and lipophilic side chain. <i>Research on Chemical Intermediates</i> , 2017, 43, 995-1011.	1.3	23

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55	Green Ultrasound versus Conventional Synthesis and Characterization of Specific Task Pyridinium Ionic Liquid Hydrazones Tethering Fluorinated Counter Anions: Novel Inhibitors of Fungal Ergosterol Biosynthesis. <i>Molecules</i> , 2017, 22, 1532.	1.7	15
56	Synthesis and crystal structure of a new pyridinium bromide salt: 4-methyl-1-(3-phenoxypropyl)pyridinium bromide. <i>Acta Crystallographica Section E: Crystallographic Communications</i> , 2017, 73, 1831-1834.	0.2	2
57	An Eco-Friendly Ultrasound-Assisted Synthesis of Novel Fluorinated Pyridinium Salts-Based Hydrazones and Antimicrobial and Antitumor Screening. <i>International Journal of Molecular Sciences</i> , 2016, 17, 766.	1.8	27
58	Preparation of Novel 3-Fluorophenyl Triazolothiadiazoles and of Triazolothiadiazines. <i>Organic Preparations and Procedures International</i> , 2016, 48, 355-370.	0.6	9
59	Liquid-liquid extraction of metal ions, DFT and TD-DFT analysis of some 1,2,4-triazole Schiff Bases with high selectivity for Pb(II) and Fe(II). <i>Journal of Molecular Structure</i> , 2016, 1113, 99-107.	1.8	24
60	Synthesis of Novel 2,5-Disubstituted-1,3,4-thiadiazoles Clubbed 1,2,4-Triazole, 1,3,4-Thiadiazole, 1,3,4-Oxadiazole and/or Schiff Base as Potential Antimicrobial and Antiproliferative Agents. <i>Molecules</i> , 2015, 20, 16048-16067.	1.7	70
61	Efficient Eco-Friendly Solvent-Free Click Synthesis and Antimicrobial Evaluation of New Fluorinated 1,2,3-Triazoles and their Conversion into Schiff Bases. <i>Journal of the Brazilian Chemical Society</i> , 2015, , .	0.6	8
62	Synthesis and characterization of some novel 1,2,4-triazoles, 1,3,4-thiadiazoles and Schiff bases incorporating imidazole moiety as potential antimicrobial agents. <i>Acta Pharmaceutica</i> , 2015, 65, 117-132.	0.9	19
63	Synthesis, characterization, and POM analysis of novel bioactive imidazolium-based ionic liquids. <i>Medicinal Chemistry Research</i> , 2015, 24, 1387-1395.	1.1	35
64	ew pyridinium-based ionic liquids: An eco-friendly ultrasound-assisted synthesis, characterization and biological activity. <i>South African Journal of Chemistry</i> , 2015, , .	0.3	1
65	Synthesis, Characterization and Antimicrobial Evaluation of Some New Schiff, Mannich and Acetylenic Mannich Bases Incorporating a 1,2,4-Triazole Nucleus. <i>Molecules</i> , 2014, 19, 18897-18910.	1.7	18
66	New Eco-Friendly 1-Alkyl-3-(4-phenoxybutyl) Imidazolium-Based Ionic Liquids Derivatives: A Green Ultrasound-Assisted Synthesis, Characterization, Antibacterial Activity and POM Analyses. <i>Molecules</i> , 2014, 19, 11741-11759.	1.7	28
67	Weight Loss, Electrochemical, Quantum Chemical Calculation, and Molecular Dynamics Simulation Studies on 2-(Benzylthio)-1,4,5-triphenyl-1H-imidazole as an Inhibitor for Carbon Steel Corrosion in Hydrochloric Acid. <i>Industrial &amp; Engineering Chemistry Research</i> , 2013, 52, 14315-14327.	1.8	71
68	Synthesis of Bis-Acyclonucleoside Analogues Bearing Benzothenyl-1,2,4-Triazol-3-yl-Disulfide under Conventional and Microwave Methods. <i>Nucleosides, Nucleotides and Nucleic Acids</i> , 2013, 32, 28-41.	0.4	4
69	Synthesis, Characterization and Evaluation of Antimicrobial Activity of Some Novel 1,2,4-Triazoles and 1,3,4-Thiadiazoles Bearing Imidazole Nuclues. <i>Heterocycles</i> , 2012, 85, 1141.	0.4	6
70	Synthesis and Characterization of a New Five and Six Membered Selenoheterocyclic Compounds Homologues of Ebselen. <i>Organic Chemistry International</i> , 2011, 2011, 1-7.	1.0	5
71	Revisit to the Reaction of O-Phenylene Diamine with Thiosemicarbazide to Give Benzimidazole-2-Thione Rather than Benzotriazine-2-Thione and its Glycosylation. <i>Nucleosides, Nucleotides and Nucleic Acids</i> , 2010, 29, 698-706.	0.4	7
72	Regioselectivity in the glycosylation of 5-(3-chlorobenzo[b]thien-2-yl)-4H-1,2,4-triazole-3-thiol. <i>Carbohydrate Research</i> , 2009, 344, 725-733.	1.1	16

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73	Regioselectivity of the reactions of 4,5-diphenylimidazole-2-thione with 1-chloro-2,3-epoxypropane and 1-bromo-2-propene, efficient precursors for imidazo[2,1-b]thiazine and thiazole. Effect of microwave and solid support. Journal of Heterocyclic Chemistry, 2008, 45, 1321-1327.	1.4	12