Khaleel I Assaf

List of Publications by Year
in descending order

91 papers	4,177 citations	196777 29 h-index	129628 63 g-index
100 all docs	100 docs citations	100 times ranked	3927 citing authors

#	Article	IF	Citations
1	A molecular dynamics study of the complexation of tryptophan, phenylalanine and tyrosine amino acids with cucurbit[7]uril. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2022, 102, 159-168.	0.9	5
2	Benzimidazoleâ€“Piperazineâ€“Coumarin/Cucurbit[7]uril Supramolecular Photoinduced Electron Transfer Fluorochromes for Detection of Carnosol by Stimuli-Responsive Dye Displacement and p<i>K</i>_a Tuning. ACS Omega, 2022, 7, 2356-2363.	1.6	2
3	Binding affinity of aniline-substituted dodecaborates to cyclodextrins. Chemical Communications, 2022, 58, 2363-2366.	2.2	6
4	Supramolecular Catalysis of a Catalysis-Resistant Dielsâ€“Alder Reaction: Almost Theoretical Acceleration of Cyclopentadiene Dimerization inside Cucurbit[7]uril. ACS Catalysis, 2022, 12, 2261-2269.	5.5	21
5	Preparation, characterization, and biological activity study of thymoquinone-cucurbit[7]uril inclusion complex. RSC Advances, 2022, 12, 1982-1988.	1.7	5
6	Cinnamaldehydeâ€“cucurbituril complex: investigation of loading efficiency and its role in enhancing cinnamaldehyde <i>in vitro</i> anti-tumor activity. RSC Advances, 2022, 12, 7540-7549.	1.7	14
7	Boron clusters as broadband membrane carriers. Nature, 2022, 603, 637-642.	13.7	62
8	Binary and Ternary Complexes of Cucurbit[8]uril with Tryptophan, Phenylalanine, and Tyrosine: A Computational Study. ACS Omega, 2022, 7, 10729-10737.	1.6	7
9	Cucurbit[7]uril recognition of glucosamine anomers in water. Journal of Molecular Liquids, 2022, 358, 119178.	2.3	5
10	<i>In situ</i> activation of green sorbents for CO₂ capture upon end group backbiting. Physical Chemistry Chemical Physics, 2022, 24, 12293-12299.	1.3	4
11	CS₂/CO₂Utilization Using Mukaiyama Reagent as a (Thio)carbonylating Promoter: A Proof-of-Concept Study. ACS Omega, 2022, 7, 22511-22521.	1.6	4
12	Hostâ€“guest complexation between cucurbit[7]uril and doxepin induced supramolecular assembly. Organic and Biomolecular Chemistry, 2022, 20, 5796-5802.	1.5	1
13	Interfacial Behavior of Modified Nicotinic Acid as Conventional/Gemini Surfactants. Langmuir, 2022, 38, 8524-8533.	1.6	1
14	Investigation of spectroscopic properties and molecular dynamics simulations of the interaction of mebendazole with Î²-cyclodextrin. Journal of the Iranian Chemical Society, 2021, 18, 75-86.	1.2	4
15	Chemisorption of CO₂ by diamine-tetraamido macrocyclic motifs: a theoretical study. Organic and Biomolecular Chemistry, 2021, 19, 3873-3881.	1.5	5
16	Activation of Î²-diketones for CO₂capture and utilization. Reaction Chemistry and Engineering, 2021, 6, 2364-2375.	1.9	4
17	Template-free synthesis of hybrid silica nanoparticle with functionalized mesostructure for efficient methylene blue removal. Materials and Design, 2021, 201, 109494.	3.3	20
18	Enhanced adsorption of CO2 on cellulose and chitosan surface by H2O Co-adsorption. Computational and Theoretical Chemistry, 2021, 1204, 113413.	1.1	2

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19	Cross-linked, porous imidazolium-based poly(ionic liquid)s for CO₂ capture and utilisation. New Journal of Chemistry, 2021, 45, 16452-16460.	1.4	23
20	Mechanistic insights on CO₂ utilization using sustainable catalysis. New Journal of Chemistry, 2021, 45, 22280-22288.	1.4	11
21	CO₂ activation through Câ€“N, Câ€“O and Câ€“C bond formation. Physical Chemistry Chemical Physics, 2020, 22, 1306-1312.	1.3	18
22	Hostâ€“Guest Chemistry Meets Electrocatalysis: Cucurbit[6]uril on a Au Surface as a Hybrid System in CO₂ Reduction. ACS Catalysis, 2020, 10, 751-761.	5.5	43
23	CO₂ coupling with epoxides catalysed by using one-pot synthesised, <i>in situ</i> activated zinc ascorbate under ambient conditions. Dalton Transactions, 2020, 49, 7673-7679.	1.6	10
24	Hostâ€Guest Complexation Affects Peryleneâ€Based Dye Aggregation. ChemistrySelect, 2020, 5, 5850-5854.	0.7	8
25	Faceâ€Fusion of Icosahedral Boron Hydride Increases Affinity to Î³â€Cyclodextrin: closo , closo â€[B 21 H 18] â^' as an Anion with Very Low Free Energy of Dehydration. ChemPhysChem, 2020, 21, 971-976.	1.0	14
26	New Metrics of Green Sorbents for CO₂ Capturing. Advanced Sustainable Systems, 2020, 4, 1900121.	2.7	13
27	Encapsulation of ionic liquids inside cucurbiturils. Organic and Biomolecular Chemistry, 2020, 18, 2120-2128.	1.5	4
28	Morphological and Interaction Characteristics of Surfaceâ€Active Ionic Liquids and Palmitic Acid in Mixed Monolayers. ChemPhysChem, 2020, 21, 1858-1865.	1.0	8
29	The eternal battle to combat global warming: (thio)urea as a CO₂wet scrubbing agent. Physical Chemistry Chemical Physics, 2020, 22, 11829-11837.	1.3	13
30	Biomaterials for CO₂ Harvesting: From Regulatory Functions to Wet Scrubbing Applications. ACS Omega, 2019, 4, 11532-11539.	1.6	18
31	High-Affinity Binding of Metallacarborane Cobalt Bis(dicarbollide) Anions to Cyclodextrins and Application to Membrane Translocation. Journal of Organic Chemistry, 2019, 84, 11790-11798.	1.7	58
32	A Selective Cucurbit[8]urilâ€Peptide Beacon Ensemble for the Ratiometric Fluorescence Detection of Peptides. Chemistry - A European Journal, 2019, 25, 13088-13093.	1.7	18
33	Applications of Cucurbiturils in Medicinal Chemistry and Chemical Biology. Frontiers in Chemistry, 2019, 7, 619.	1.8	118
34	A catecholamine neurotransmitter: epinephrine as a CO₂ wet scrubbing agent. Chemical Communications, 2019, 55, 3449-3452.	2.2	18
35	Cucurbit[7]urilâ€Threaded Poly(3,4â€ethylenedioxythiophene): A Novel Processable Conjugated Polyrotaxane. European Journal of Organic Chemistry, 2019, 2019, 3442-3450.	1.2	11
36	Ratiometric DNA sensing with a hostâ€“guest FRET pair. Chemical Communications, 2019, 55, 671-674.	2.2	39

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37	Selective Detection of Nitroexplosives Using Molecular Recognition within Self-Assembled Plasmonic Nanojunctions. Journal of Physical Chemistry C, 2019, 123, 15769-15776.	1.5	31
38	Versatile, one-pot introduction of nonahalogenated 2-ammonio-decaborate ions as boron cluster scaffolds into organic molecules; hostâ€“guest complexation with Î³-cyclodextrin. Chemical Communications, 2019, 55, 13669-13672.	2.2	11
39	Preferential binding of unsaturated hydrocarbons in aryl-bisimidazoliumÂ·cucurbit[8]uril complexes furbishes evidence for small-molecule ï€â€“ï€ interactions. Chemical Science, 2019, 10, 10240-10246.	3.7	12
40	Orthogonal Molecular Recognition of Chaotropic and Hydrophobic Guests Enables Supramolecular Architectures. ChemNanoMat, 2019, 5, 124-129.	1.5	12
41	Synthesis, Crystal Structure, Spectroscopic and Computational Studies of 2-{1-[2-(1,3-Dimethyl-4-nitro-1H-pyrazol-5-yl)hydrazono]ethyl}pyridine. Heterocycles, 2019, 98, 224.	0.4	1
42	Cucurbituril Properties and the Thermodynamic Basis of Hostâ€“Guest Binding. Monographs in Supramolecular Chemistry, 2019, , 54-85.	0.2	3
43	An efficient atom-economical chemoselective CO₂ cycloaddition using lanthanum oxide/tetrabutyl ammonium bromide. Sustainable Energy and Fuels, 2018, 2, 1342-1349.	2.5	29
44	Supramolecular assemblies through hostâ€“guest complexation between cucurbiturils and an amphiphilic guest molecule. Chemical Communications, 2018, 54, 1734-1737.	2.2	35
45	Inedible saccharides: a platform for CO₂ capturing. Chemical Science, 2018, 9, 1088-1100.	3.7	39
46	The chaotropic effect as an orthogonal assembly motif for multi-responsive dodecaborate-cucurbituril supramolecular networks. Chemical Communications, 2018, 54, 2098-2101.	2.2	62
47	Structural Effects on Guest Binding in Cucurbit[8]urilâ€Perylenemonoimide Hostâ€Guest Complexes. ChemistrySelect, 2018, 3, 4699-4704.	0.7	11
48	A green sorbent for CO₂ capture: Î±-cyclodextrin-based carbonate in DMSO solution. RSC Advances, 2018, 8, 37757-37764.	1.7	17
49	Cucurbit[7]uril Inclusion Complexes with Benzimidazole Derivatives: A Computational Study. Journal of Solution Chemistry, 2018, 47, 1768-1778.	0.6	3
50	Precise supramolecular control of surface coverage densities on polymer micro- and nanoparticles. Chemical Science, 2018, 9, 8575-8581.	3.7	17
51	A Supramolecular Approach for Enhanced Antibacterial Activity and Extended Shelf-life of Fluoroquinolone Drugs with Cucurbit[7]uril. Scientific Reports, 2018, 8, 13925.	1.6	48
52	The Chaotropic Effect as an Assembly Motif in Chemistry. Angewandte Chemie - International Edition, 2018, 57, 13968-13981.	7.2	231
53	Der chaotrope Effekt als Aufbaumotiv in der Chemie. Angewandte Chemie, 2018, 130, 14164-14177.	1.6	42
54	Hostâ€“Guest Chemistry of Carboranes: Synthesis of Carboxylate Derivatives and Their Binding to Cyclodextrins. Chemistry - A European Journal, 2018, 24, 12970-12975.	1.7	24

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55	Hierarchical hostâ€“guest assemblies formed on dodecaborate-coated gold nanoparticles. Chemical Communications, 2017, 53, 4616-4619.	2.2	40
56	Binary twinned-icosahedral [B₂₁H₁₈]^{â^'} interacts with cyclodextrins as a precedent for its complexation with other organic motifs. Physical Chemistry Chemical Physics, 2017, 19, 11748-11752.	1.3	26
57	Gold nanoparticle aggregation enables colorimetric sensing assays for enzymatic decarboxylation. Analytical Methods, 2017, 9, 2784-2787.	1.3	14
58	New insights into the chemistry of ionic alkylorganic carbonates: a computational study. Physical Chemistry Chemical Physics, 2017, 19, 15403-15411.	1.3	11
59	Polyrotaxanes based on PEG-amine with cucurbit[7]uril, Î±-cyclodextrin and its tris-O-methylated derivative. European Polymer Journal, 2017, 93, 323-333.	2.6	15
60	Bis-tris propane in DMSO as a wet scrubbing agent: carbamic acid as a sequestered CO₂ species. New Journal of Chemistry, 2017, 41, 11941-11947.	1.4	24
61	Intracavity folding of a perylene dye affords a high-affinity complex with cucurbit[8]uril. Chemical Communications, 2017, 53, 9242-9245.	2.2	18
62	Chemisorption of CO₂by chitosan oligosaccharide/DMSO: organic carbamatoâ€“carbonato bond formation. Green Chemistry, 2017, 19, 4305-4314.	4.6	42
63	HYDROPHOBE Challenge: A Joint Experimental and Computational Study on the Hostâ€“Guest Binding of Hydrocarbons to Cucurbiturils, Allowing Explicit Evaluation of Guest Hydration Free-Energy Contributions. Journal of Physical Chemistry B, 2017, 121, 11144-11162.	1.2	62
64	Pentaerythritol-Based Molecular Sorbent for CO₂ Capturing: A Highly Efficient Wet Scrubbing Agent Showing Proton Shuttling Phenomenon. Energy & Fuels, 2017, 31, 8407-8414.	2.5	22
65	Tuning protonation states of tripelennamine antihistamines by cucurbit[7]uril. Journal of Physical Organic Chemistry, 2016, 29, 101-106.	0.9	22
66	Chitin-acetate/DMSO as a supramolecular green CO₂-phile. RSC Advances, 2016, 6, 22090-22093.	1.7	32
67	Cucurbit[7]uril-based fluorene polyrotaxanes. European Polymer Journal, 2016, 83, 256-264.	2.6	10
68	Nanomolar Binding of Steroids to Cucurbit[<i>n</i>]urils: Selectivity and Applications. Journal of the American Chemical Society, 2016, 138, 13022-13029.	6.6	143
69	High-affinity hostâ€“guest chemistry of large-ring cyclodextrins. Organic and Biomolecular Chemistry, 2016, 14, 7702-7706.	1.5	80
70	An investigation of carbon dioxide capture by chitin acetate/DMSO binary system. Carbohydrate Polymers, 2016, 152, 163-169.	5.1	36
71	Inclusion of neutral guests by water-soluble macrocyclic hosts â€“ a comparative thermodynamic investigation with cyclodextrins, calixarenes and cucurbiturils. Supramolecular Chemistry, 2016, 28, 384-395.	1.5	45
72	Dodecaborate-Functionalized Anchor Dyes for Cyclodextrin-Based Indicator Displacement Applications. Organic Letters, 2016, 18, 932-935.	2.4	65

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73	Photophysical properties of neutral and dissociated forms of rosmarinic acid. Journal of Luminescence, 2016, 175, 50-56.	1.5	24
74	Water Structure Recovery in Chaotropic Anion Recognition: Highâ€Affinity Binding of Dodecaborate Clusters to Î³â€Cyclodextrin. Angewandte Chemie - International Edition, 2015, 54, 6852-6856.	7.2	214
75	Molecular dynamics simulation of a cucurbituril based molecular switch triggered by pH changes. Computational and Theoretical Chemistry, 2015, 1066, 104-112.	1.1	16
76	Molecular dynamics of nor-Seco-cucurbit[10]uril complexes. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2015, 82, 323-333.	0.9	17
77	RÃ¼cktitelbild: Water Structure Recovery in Chaotropic Anion Recognition: High-Affinity Binding of Dodecaborate Clusters to Î³-Cyclodextrin (Angew. Chem. 23/2015). Angewandte Chemie, 2015, 127, 7046-7046.	1.6	1
78	Coulomb Repulsion in Short Polypeptides. Journal of Physical Chemistry B, 2015, 119, 33-43.	1.2	17
79	Triple Emission from <i>p</i>â€Dimethylaminobenzonitrileâ€"Cucurbit[8]uril Triggers the Elusive Excimer Emission. Chemistry - A European Journal, 2015, 21, 691-696.	1.7	44
80	Cucurbiturils: from synthesis to high-affinity binding and catalysis. Chemical Society Reviews, 2015, 44, 394-418.	18.7	1,100
81	Molecular dynamics simulation study of the structural features and inclusion capacities of cucurbit[6]uril derivatives in aqueous solutions. Supramolecular Chemistry, 2015, 27, 80-89.	1.5	13
82	Investigation of isomeric flavanol structures in black tea thearubigins using ultraperformance liquid chromatography coupled to hybrid quadrupole/ion mobility/time of flight mass spectrometry. Journal of Mass Spectrometry, 2014, 49, 1086-1095.	0.7	29
83	Cucurbiturils as fluorophilic receptors. Supramolecular Chemistry, 2014, 26, 657-669.	1.5	45
84	Chemistry inside molecular containers in the gas phase. Nature Chemistry, 2013, 5, 376-382.	6.6	144
85	Halogen Bonding inside a Molecular Container. Journal of the American Chemical Society, 2012, 134, 19935-19941.	6.6	119
86	Deep Inside Cucurbiturils: Physical Properties and Volumes of their Inner Cavity Determine the Hydrophobic Driving Force for Hostâ€"Guest Complexation. Israel Journal of Chemistry, 2011, 51, 559-577.	1.0	319
87	Molecular Dynamics of Methyl Viologen-Cucurbit[<i>n</i>]uril Complexes in Aqueous Solution. Journal of Chemical Theory and Computation, 2010, 6, 984-992.	2.3	45
88	Complexation of N-methyl-4-(p-methyl benzoyl)-pyridinium methyl cation and its neutral analogue by cucurbit[7]uril and Î²-cyclodextrin: a computational study. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2009, 64, 357-365.	1.6	13
89	Template-Free Synthesis of Hybrid Silica Nanoparticle With Functionalized Mesostructure for Efficient Methylene Blue Removal. SSRN Electronic Journal, 0, , .	0.4	0
90	1 Host-guest Chemistry Meets Electrocatalysis: Cucurbit[6]uril on a Au Surface as Hybrid System in CO2 Reduction. , 0, , .		0

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91	Host-guest Chemistry Meets Electrocatalysis: Cucurbit[6]uril on a Au Surface as Hybrid System in CO_2 Reduction. , 0, , .		0