

# Halima Mouhib

## List of Publications by Year in descending order

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38  
papers

584  
citations

567281

15  
h-index

642732

23  
g-index

38  
all docs

38  
docs citations

38  
times ranked

568  
citing authors

#	ARTICLE	IF	CITATIONS
1	Structural insight from intermolecular interactions and energy framework analyses of 2-substituted 6,7,8,9-tetrahydro-11 <i>H</i> -pyrido[2,1- <i>b</i> ]quinazolin-11-ones. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2021, 77, 416-426.	1.1	2
2	Large Amplitude Motions in Fruit Flavors: The Case of Alkyl Butyrates. <i>ChemPhysChem</i> , 2020, 21, 20-25.	2.1	3
3	The first microsolvation step for furans: New experiments and benchmarking strategies. <i>Journal of Chemical Physics</i> , 2020, 152, 164303.	3.0	28
4	The hydrophobic effect characterises the thermodynamic signature of amyloid fibril growth. <i>PLoS Computational Biology</i> , 2020, 16, e1007767.	3.2	29
5	The heavy atom structures and <sup>33</sup> S quadrupole coupling constants of 2-thiophenecarboxaldehyde: insights from microwave spectroscopy. <i>Molecular Physics</i> , 2020, 118, e1728406.	1.7	12
6	Quantifying soft degrees of freedom in volatile organic compounds: insight from quantum chemistry and focused single molecule experiments. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 27850-27860.	2.8	2
7	Copper-Chalcogen Bonds in Olfaction: Accurate ab Initio Characterization of CuSH and CuOH. <i>Journal of Physical Chemistry A</i> , 2019, 123, 1177-1185.	2.5	0
8	Challenging the Molecular Parameters of Vetiver: Can 4,5-Dimethyl-3-(3-methylbutyl)-4-phenylcyclopent-2-en-1-one Mimic Zizanonones? <i>European Journal of Organic Chemistry</i> , 2019, 2019, 2643-2652.		
9	The furan microsolvation blind challenge for quantum chemical methods: First steps. <i>Journal of Chemical Physics</i> , 2018, 148, 014301.	3.0	44
10	Highlights from the Faraday Discussion 296: quantum effects in small molecular systems, 10 <sup>th</sup> September 2018, Edinburgh, United Kingdom. <i>Chemical Communications</i> , 2018, 54, 13620-13625.	4.1	0
11	Molecules in confinement in clusters, quantum solvents and matrices: general discussion. <i>Faraday Discussions</i> , 2018, 212, 569-601.	3.2	4
12	Competing Dispersive Interactions: From Small Energy Differences to Large Structural Effects in Methyl Jasmonate and Zingerone. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 5906-5914.	4.6	18
13	Communication through the furan ring: the conformational effect on the internal rotation of 5-methyl furfural studied by microwave spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 25577-25582.	2.8	14
14	Methyl Internal Rotation in the Microwave Spectrum of <i>o</i> -Methyl Anisole. <i>ChemPhysChem</i> , 2017, 18, 1855-1859.	2.1	35
15	Molecular structure and ring tunneling of phenyl formate as observed by microwave spectroscopy and quantum chemistry. <i>Journal of Molecular Spectroscopy</i> , 2017, 337, 59-64.	1.2	14
16	Favored Conformations of Carbonyl Compounds: A Structural Study of <i>n</i> -Octanal. <i>ChemPhysChem</i> , 2017, 18, 2631-2636.	2.1	9
17	Laboratory microwave, millimeter wave and far-infrared spectra of dimethyl sulfide. <i>Astronomy and Astrophysics</i> , 2016, 589, A127.	5.1	17
18	Mechanical Unfolding of an Autotransporter Passenger Protein Reveals the Secretion Starting Point and Processive Transport Intermediates. <i>ACS Nano</i> , 2016, 10, 5710-5719.	14.6	21

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19	Conformational dimorphism in <i>o</i> -nitrobenzoic acid: alternative ways to avoid the O...O clash. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2016, 72, 566-571.	0.5	5
20	Conformational analysis of tert-butyl acetate using a combination of microwave spectroscopy and quantum chemical calculations. <i>Journal of Molecular Spectroscopy</i> , 2016, 322, 38-42.	1.2	9
21	Charge density of the biologically active molecule (2-oxo-1,3-benzoxazol-3(2H-yl)acetic acid. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2016, 72, 142-150.	1.1	4
22	Conformational ensemble of human Î±-synuclein physiological form predicted by molecular simulations. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 5702-5706.	2.8	32
23	The microwave spectrum of allyl acetone. <i>Journal of Molecular Spectroscopy</i> , 2015, 312, 46-50.	1.2	10
24	From Cats and Blackcurrants: Structure and Dynamics of the Sulfur-Containing Cassis Odorant Cat Ketone. <i>Chemistry and Biodiversity</i> , 2014, 11, 1554-1566.	2.1	6
25	Understanding the structure and dynamic of odorants in the gas phase using a combination of microwave spectroscopy and quantum chemical calculations. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2014, 47, 143001.	1.5	9
26	Quantum-Chemical Ab Initio Calculations on Ala-(C <sub>5</sub> H <sub>5</sub> Al) and Galabenzene (C <sub>5</sub> H <sub>5</sub> Ga). <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2014, 69, 349-359.	1.5	5
27	The Conformation of Pentanoates in the Solid and in the Gas Phase. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2014, 69, 303-312.	1.5	6
28	Sulfur-Containing Flavors: Gas Phase Structures of Dihydro-2-methyl-3-thiophenone. <i>Journal of Physical Chemistry A</i> , 2013, 117, 6652-6656.	2.5	10
29	Conformational Landscape of Diisopropyl Ketone: Quantum Chemical Calculations Validated by Microwave Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2013, 117, 311-314.	2.5	6
30	A touch of lavender: gas-phase structure and dynamics of the monoterpene linalool validated by microwave spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 10012.	2.8	29
31	Efficient Macrocyclization by a Novel Oxy-Cope Reaction: Synthesis and Olfactory Properties of New Macrocyclic Musks. <i>Chemistry - A European Journal</i> , 2012, 18, 7010-7015.	3.3	28
32	Conformational Analysis of Green Apple Flavour: The Gas-Phase Structure of Ethyl Valerate Validated by Microwave Spectroscopy. <i>ChemPhysChem</i> , 2012, 13, 1297-1301.	2.1	28
33	Structural Studies on Ethyl Isovalerate by Microwave Spectroscopy and Quantum Chemical Calculations. <i>Journal of Physical Chemistry A</i> , 2011, 115, 118-122.	2.5	26
34	The Conformation of Odorants in Different States of Aggregation: A Joint Venture in Microwave Spectroscopy and X-ray Diffraction. <i>ChemPhysChem</i> , 2011, 12, 761-764.	2.1	21
35	Cassis Odor through Microwave Eyes: Olfactory Properties and Gas-Phase Structures of all the Cassyrane Stereoisomers and its Dihydro Derivatives. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 5576-5580.	13.8	35
36	Two conformers of ethyl pivalate studied by microwave spectroscopy. <i>Journal of Molecular Spectroscopy</i> , 2010, 261, 59-62.	1.2	17

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37	The microwave spectrum of allyl acetate. <i>Molecular Physics</i> , 2010, 108, 763-770.	1.7	37
38	Impact of pathogenic mutations of the GLUT1 glucose transporter on channel dynamics using ConsDYN enhanced sampling. <i>F1000Research</i> , 0, 8, 322.	1.6	0