Alya A Arabi

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Effects of external electric fields on double proton transfer kinetics in the formic acid dimer. Physical Chemistry Chemical Physics, 2011, 13, 13738.	1.3	121
2	The bioisosteric similarity of the tetrazole and carboxylate anions: Clues from the topologies of the electrostatic potential and of the electron density. European Journal of Medicinal Chemistry, 2010, 45, 1868-1872.	2.6	65
3	Electron-density descriptors as predictors in quantitative structure–activity/property relationships and drug design. Future Medicinal Chemistry, 2011, 3, 969-994.	1.1	53
4	Atomic Partitioning of the Dissociation Energy of the Pâ^'O(H) Bond in Hydrogen Phosphate Anion (HPO ₄ ²⁻):  Disentangling the Effect of Mg ²⁺ . Journal of Physical Chemistry A, 2007, 111, 8864-8872.	1.1	43
5	Effects of Intense Electric Fields on the Double Proton Transfer in the Watson–Crick Guanine–Cytosine Base Pair. Journal of Physical Chemistry B, 2018, 122, 8631-8641.	1.2	38
6	Distribution of heavy metals in the coastal area of Abu Dhabi in the United Arab Emirates. Marine Pollution Bulletin, 2015, 97, 494-498.	2.3	35
7	Where is Electronic Energy Stored in Adenosine Triphosphate?. Journal of Physical Chemistry A, 2009, 113, 3360-3368.	1.1	32
8	The influence of base pair tautomerism on single point mutations in aqueous DNA. Interface Focus, 2020, 10, 20190120.	1.5	29
9	Nonempirical density-functional theory for van der Waals interactions. Canadian Journal of Chemistry, 2010, 88, 1057-1062.	0.6	27
10	Artificial intelligence in drug design: algorithms, applications, challenges and ethics. Future Drug Discovery, 2021, 3, .	0.8	21
11	Routes to drug design via bioisosterism of carboxyl and sulfonamide groups. Future Medicinal Chemistry, 2017, 9, 2167-2180.	1.1	19
12	Assessment of the PW86+PBE+XDM density functional on van der Waals complexes at non-equilibrium geometries. Journal of Chemical Physics, 2012, 137, 014104.	1.2	14
13	Regional effects of streptozotocin-induced diabetes on shortening and calcium transport in epicardial and endocardial myocytes from rat left ventricle. Physiological Reports, 2016, 4, e13034.	0.7	14
14	Adenine–thymine tautomerization under the influence of strong homogeneous electric fields. Physical Chemistry Chemical Physics, 2018, 20, 12406-12412.	1.3	11
15	Diastereoselective Additions of Allylmagnesium Reagents to α-Substituted Ketones When Stereochemical Models Cannot Be Used. Journal of Organic Chemistry, 2021, 86, 7203-7217.	1.7	11
16	The influence of external electric fields on proton transfer tautomerism in the guanine–cytosine base pair. Physical Chemistry Chemical Physics, 2021, 23, 6252-6265.	1.3	10
17	Electrostatic potentials and average electron densities of bioisosteres in methylsquarate and acetic acid. Future Medicinal Chemistry, 2016, 8, 361-371.	1.1	8
18	Method Development for Selective and Nontargeted Identification of Nitro Compounds in Diesel Particulate Matter. Energy & Fuels, 2017, 31, 11615-11626.	2.5	6

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19	Atomic and molecular properties of nonclassical bioisosteric replacements of the carboxylic acid group. Future Medicinal Chemistry, 2020, 12, 1111-1120.	1.1	4
20	Distribution of heavy metals around the Barakah nuclear power plant in the United Arab Emirates. Environmental Science and Pollution Research, 2017, 24, 19835-19851.	2.7	3
21	Rare Earth Elements Around the Barakah Nuclear Power Plant, UAE. Natural Resources Research, 2020, 29, 4149-4160.	2.2	3
22	Radiological baseline around the Barakah Nuclear Power Plant, UAE. Arabian Journal of Chemistry, 2021, 14, 103125.	2.3	3
23	Evaluating dispersion forces for optimization of van der Waals complexes using a non-empirical functional. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2016, 374, 20160145.	1.6	1
24	Binding energies of van der Waals complexes at non-equilibrium geometries. Chemical Physics, 2020, 529, 110545.	0.9	1