

NBO Bibliography 2019

2249 publications – Revised and compiled by Ariel Andrea on Aug. 9, 2021

Aarjane, M.; Slassi, S.; Tazi, B.; Maouloua, M.; Amine, A.

Novel series of acridone-1,2,3-triazole derivatives: microwave-assisted synthesis, DFT study and antibacterial activities

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Aayisha, S.; Devi, T. S. R.; Janani, S.; Muthu, S.; Raja, M.; Sevvanthi, S.

DFT, molecular docking and experimental FT-IR, FT-Raman, NMR inquisitions on "4-chloro-N-(4,5-dihydro-1H-imidazol-2-yl)-6-methoxy-2-methylpyrimidin-5 -amine": Alpha-2-imidazoline receptor agonist antihypertensive agent

Journal of Molecular Structure, (1186): 468-481 2019. 10.1016/j.molstruc.2019.03.056

Aayisha, S.; Devi, T. S. R.; Janani, S.; Muthu, S.; Raja, M.; Sevvanthi, S.; Raajaraman, B. R.

Vibrational and computational analysis for molecular structure properties of N-(2-(trifluoromethyl)phenyl)acetamide: Density functional theory approach

Spectroscopy Letters, (52): 563-576 2019. 10.1080/00387010.2019.1678175

Abbaz, T.; Bendjeddou, A.; Villemin, D.

MOLECULAR STRUCTURE, MULLIKEN AND HOMO-LUMO ANALYSIS OF 1,2,4-TRIAZOLO 3,4-B -1,3,4-THIADIAZINE BENZENESULFONAMIDE DERIVATIVES BASED ON DFT CALCULATIONS

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Synthesis, Structural Characterization, Thermal Behaviour and Antimicrobial Activity of Copper, Cadmium and Zinc Chelates of Traizole-thiole Ligand in Comparison with Theoretical Molecular Orbital Calculations

Egyptian Journal of Chemistry, (62): 145-163 2019. 10.21608/ejchem.2019.16723.2015

Abd El-Mageed, H. R.; Taha, M.

Exploring the intermolecular interaction of serine and threonine dipeptides with gold nanoclusters and nanoparticles of different shapes and sizes by quantum mechanics and molecular simulations

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Abdel-Kader, N. S.; Abdel-Latif, S. A.; El-Ansary, A. L.; Sayed, A. G.

Combined experimental, DFT theoretical calculations and biological activity of sulfaclozine azo dye with 1-hydroxy-2-naphthoic acid and its complexes with some metal ions

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Abdeveiszadeh, Z.; Shakerzadeh, E.; Noorizadeh, S.

Computational screening of carbon monoxide (CO) adsorption over neutral and charged Al-7 clusters

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Abedi, M.; Levi, G.; Zederkof, D. B.; Henriksen, N. E.; Papai, M.; Moller, K. B.

Excited-state solvation structure of transition metal complexes from molecular dynamics simulations and assessment of partial atomic charge methods

Physical Chemistry Chemical Physics, (21): 4082-4095 2019. 10.1039/c8cp06567e

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