

Research Article

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Estimation of Bond Free Energy with Gmx_Mmpbsa in Ndm-1 Complexes

Published On: October 18, 2024 | Pages: 067 - 072

Author(s): Eduvan Valencia* and Mauricio Galvis

We report the values obtained for the binding free energies (G_{bind}) of the complexes: NDM-1-M25 (43.80 kcal/mol), NDM-1-M26 (12.71 kcal/mol), NDM-1-M35 (19.92 kcal/mol), NDM-1-M37 (2.46 kcal/mol) and the reference system NDM-1-Meropenem (-10.09 kcal/mol). These results are based on previous absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties ...

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Pulsed galvanostatic electrodeposition of tellurium nanostructures on stainless steel from copper anode slimes plating bath: Effect of pulse parameters

Published On: June 24, 2024 | Pages: 058 - 066

Author(s): Mazyar Abolfathi, Taher Yousefi*, Mohammad Hassan Mallah, Abbas Rashidi and Hamid Reza Moazami

The electrochemical behavior of Te in alkaline media was determined by cyclic voltammetry and linear sweep voltammetry measurements. It indicated that TeO_3^{2-} ion was first reduced to Te(s), then to Te^{2+} ion. For the first time, the pulsed electrodeposition of tellurium on stainless steel has been studied in an alkaline bath and the effect of duty cycle, frequency, an ...

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A efficient, regioselective and solvent free synthesis of 5,9-dihydropyrimido[4,5-e][1,2,4]triazolo[1,5-a]pyrimidine-6,8(4H,7H)-diones derivatives in presence nanocatalyst sulfuric acid grafted with silica-3-aminotriazol

Published On: April 24, 2024 | Pages: 032 - 043

Author(s): Arezoo Pourkazemi*, Bahador Karami and Mahnaz Farahi

In this research, SO₃H-functionalized Silica grafted 3-amino triazol has been prepared and identified through FT-IR, XRD, EDX, Fe-SEM, and TGA spectra. 3-chloropropyltriethoxysilane was first reacted with silica nanoparticles and then treated with 3-amino-1H-1,2,4-triazoles and grafted finally with chlorosulfonic acid to prepare SiO₂@(CH₂)₃-AT/SO₃H (SNPS-AT/SO₃H). Aft ...

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Interaction of 6-Bromo- and 6-Chloro-Ubiquinone derivatives with mitochondrial electron transfer system

Published On: April 06, 2024 | Pages: 024 - 031

Author(s): Chang-An Yu*, Xiao-long Li, Lian-Quan Gu and Linda Yu

To understand the reaction mechanism of quinone-mediated electron transfer, a series of ubiquinone (Q)-derivatives with a bromine or chlorine atom at the 6-position and a different alkyl side chains at the 5-position of the benzoquinone ring were synthesized and characterized. The chemical properties and electron transfer activities were compared with the native ubiqu ...

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Intrinsic defects in non-irradiated silicon carbide crystals

Published On: March 12, 2024 | Pages: 004 - 019

Author(s): Evgeniy N Mokhov*, Pavel G Baranov and Olga P Kazarova

A comprehensive study of the intrinsic defects in sublimation-grown SiC crystals, depending on the growth conditions and thermal annealing is carried out. Complexes of the intrinsic defects including carbon vacancy (VC) and impurities atoms are found in the Si-rich SiC crystals grown by physical vapor transport at low temperatures below 2200 °C. Similar defects are al ...

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Review Article

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On population-space description of chemical reactivity

Published On: May 31, 2024 | Pages: 047 - 057

Author(s): Roman F Nalewajski*

The electron-population degrees-of-freedom of donor-acceptor systems are reexamined and alternative simple models of charge-transfer reactivity are discussed in the substrate and atomic resolutions. The in situ differential descriptors of the polarized subsystems are emphasized and alternative energy profiles in interactions between hard and soft acidic and basic reac ...

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Case Report

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Scope of a short & obese patient for thymoma surgery with the risk of difficulty in weaning from general anaesthesia

Published On: March 26, 2024 | Pages: 020 - 023

Author(s): Krishna Prasad T*, Ajit Kumar Kayal, Kavin Adhithya and Balu Sankar

Obese patients had more difficulty with tracheal intubation and a higher incidence of post-extubation stridor. Obesity is such a ubiquitous issue in our culture, and it is a significant risk factor for many diseases, thus it is not surprising that many obese patients are treated in ICU. The objective of this article is to explore challenges for short, obese patients (...

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Enhancing future technologies: Sol-Gel synthesis of $\text{Sr}_{0.6}\text{Ag}_{0.4}\text{MnO}_3$ manganite perovskite

Published On: May 04, 2024 | Pages: 044 - 046

Author(s): Faouzia Tayari*, Kais Iben Nassar and Majdi Benamara

The research successfully produced $\text{Sr}_{0.6}\text{Ag}_{0.4}\text{MnO}_3$, a silver strontium manganite with the desired perovskite crystal structure, using the sol-gel technique. Extensive analysis revealed its notable characteristics, indicating potential uses across various fields. X-ray diffraction showed the compound's tetragonal structure at room temperature, affirming its stability. M ...

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The transformative role of Computational Fluid Dynamics (CFD) in chemical engineering

Published On: March 12, 2024 | Pages: 001 - 003

Author(s): Bibhab Kumar Lodh*

Chemical engineering is a discipline intrinsically linked to fluid behavior. From reaction kinetics to reactor design, understanding how fluids flow, mix, and transfer heat is paramount. Traditionally, this relied heavily on experimentation, a time-consuming and resource-intensive process. The emergence of Computational Fluid Dynamics (CFD) has revolutionized the field ...

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Conceptual Study of Enzymatic Organic Reactions in the Bacteriophage Therapy

Published On: November 26, 2024 | Pages: 073 - 079

Author(s): Topwe Milongwe Mwene-Mbeja*

In order to neutralize bacteria, bacteriophages hydrolyze chemical constituents of the bacterial cellular membrane, such as phospholipids, glycolipids as well as glycoproteins before reaching the bacterial cytoplasm, an intracellular environment containing water, salts, and a diversity of organic compounds notably ribonucleic acid (RNA) along with deoxyribonucleic aci ...

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