



# Structural Chemistry

Computational and Experimental Studies of Chemical and Biological Systems

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## Volume 33, issue 4, August 2022

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Istvan Hargittai

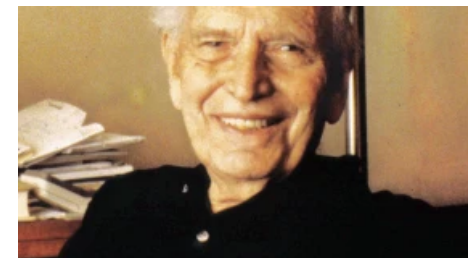
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## Paradigms and paradoxes: complementarity in chemical structures—a tribute to Erwin Chargaff

Istvan Hargittai

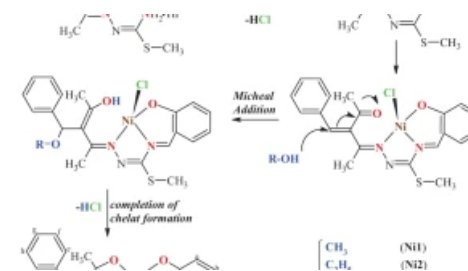
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## Synthesis of the nickel(II) complexes bearing tetradentate thiosemicarbazone through Michael addition of n-alcohols. Experimental, theoretical characterization and antioxidant properties

Tuncay Karakurt, Büşra Kaya ... Bahri Ülküseven

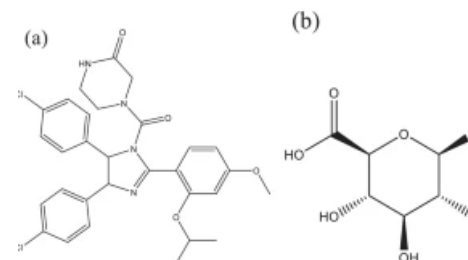
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## Computational investigation of pyrrolidin derivatives as novel GPX4/MDM2–p53 inhibitors using 2D/3D-QSAR, ADME/toxicity, molecular docking, molecular dynamics simulations, and MM-GBSA free energy

Kamal Tabti, Soukayna Baammi ... Tahar Lakhlifi

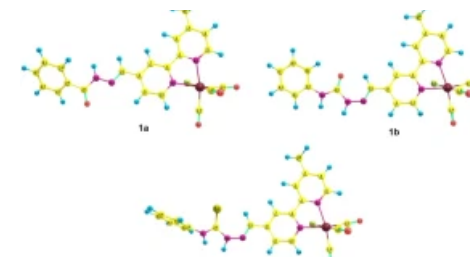
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## Structural behavior of rhenium complexes in fluoride sensing: a spectroscopic and computational study

Murugesan Velayudham, Arumugam Ramdass ... Seenivasan Rajagopal

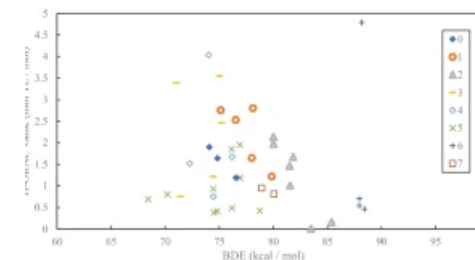
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## Structure–antioxidant activity (oxygen radical absorbance capacity) relationships of phenolic compounds

Shuhei Sakurai, Yuta Kawakami ... Hiroaki Gotoh

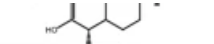
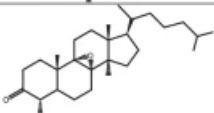
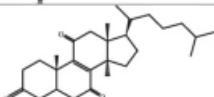
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## 3D-QSAR, ADME-Tox, and molecular docking of semisynthetic triterpene derivatives as antibacterial and insecticide agents

Ossama Daoui, Nouredine Mazoir ... Samir Chtita

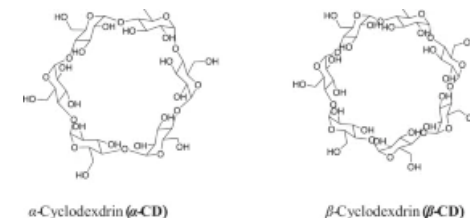
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	20.6	4.686
	23.18	4.635

## Reversible coloring/decoring reactions of thermochromic leuco dyes controlled by a macrocyclic compound developer

Sanguansak Sriphalang, Audchara Saenkham ... Datchanee Pattavarakorn

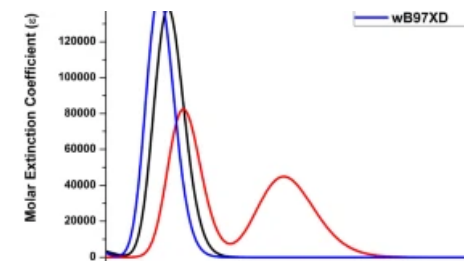
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Anbarasan Ponnusamy Munusamy, Arunkumar Ammasi & Mohd Shkir

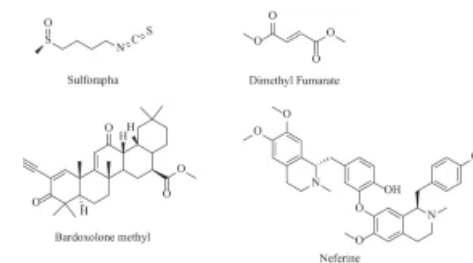
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## QSAR study, molecular docking, and ADMET prediction of vinyl sulfone-containing Nrf2 activator derivatives for treating Parkinson disease

Jian-Bo Tong, Jie Wang ... Xing Zhang

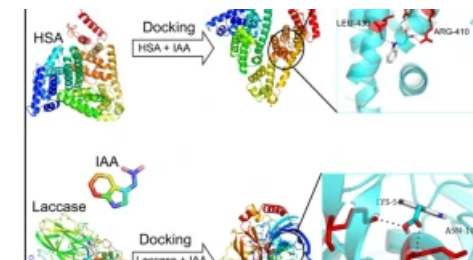
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Sana Daneshamouz, Shaghayegh Saadati & Amira Abdelrasoul

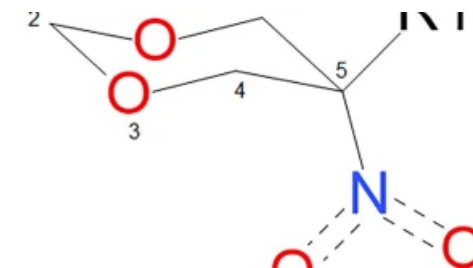
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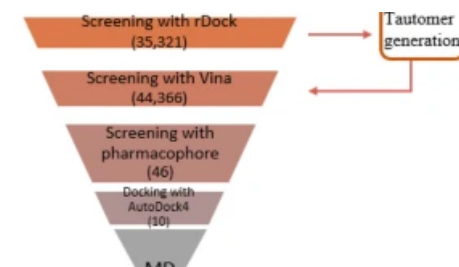
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## *In silico* discovery of potential azole-containing mPGES-1 inhibitors by virtual screening, pharmacophore modeling and molecular dynamics simulations

Lalehan Ozalp, İlkay Küçükgülzel & Ayşe Ogan

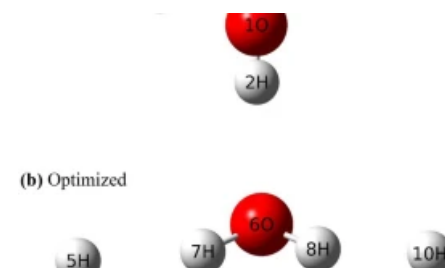
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## Acid-based analogs of certain water tetramers: an examination of some crystal structures in the literature

Hiroko Ajiki, Ivan Bernal & Lou Massa

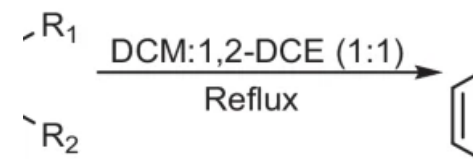
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## Synthesis, computational analyses, antibacterial and antibiofilm properties of nicotinamide derivatives

Ayşe Hümeysra Taşkın Kafa, Gamze Tüzün ... Hilmi Ataseven

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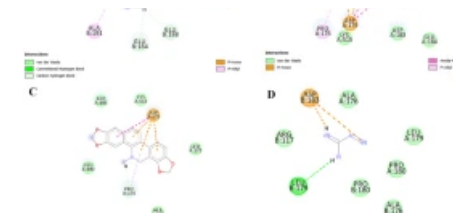
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## between some alkaloids and human serum albumin

Morteza Sadeghi, Mehran Miroliaei ... Mohammad Moradi

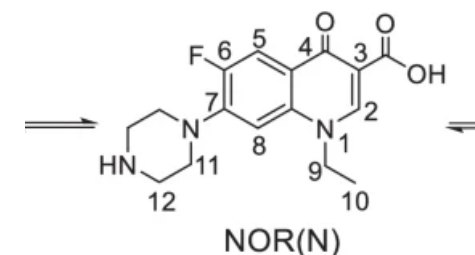
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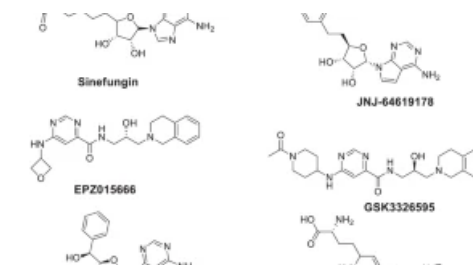
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## Structural insight into PRMT5 inhibitors through amalgamating pharmacophore-based virtual screening, ADME toxicity, and binding energy studies to identify new inhibitors by molecular docking

Revanth Bathula, Goverdhan Lanka ... Sarita Rajender Potlapally

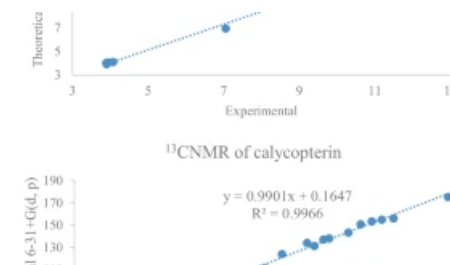
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Arjang Jalezadeh, Zohreh Mirjafary ... Hamid Saeidian

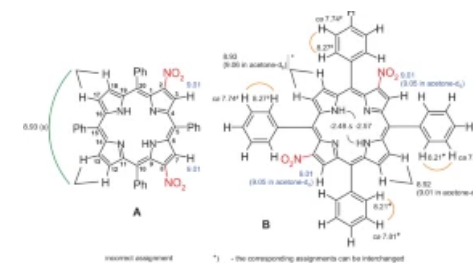
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Agnieszka Mikus & Stanisław Ostrowski

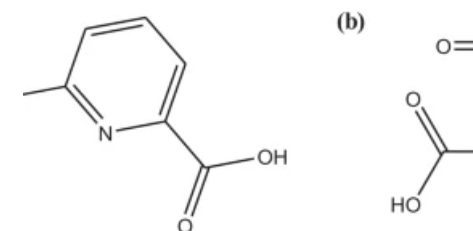
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Adedibu C. Tella, Adetola C. Oladipo ... Richard I. Walton

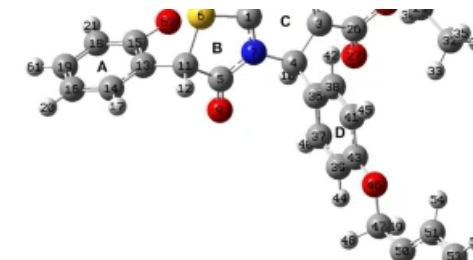
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Jamelah S. Al-Otaibi, Renyer Alves Costa ... Y. Shyma Mary

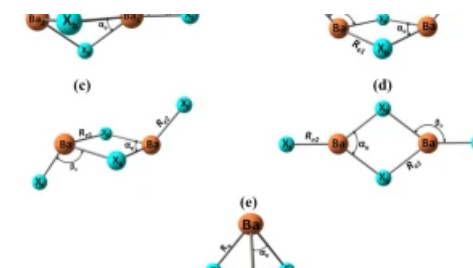
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Fortunatus Jacob

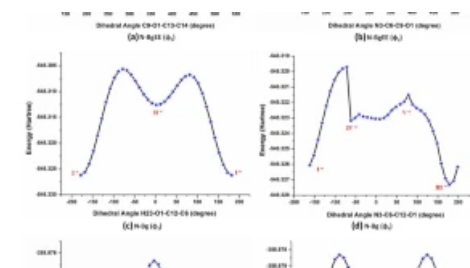
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Thirunavukkarasu Manickavelu, Balaji Govindrajan ... Ahmad Irfan

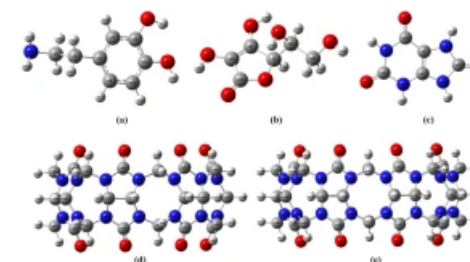
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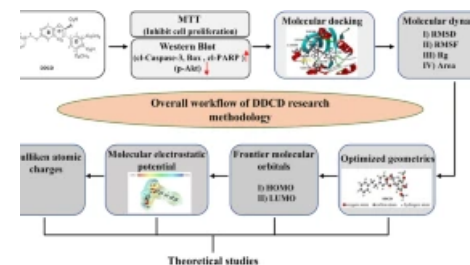
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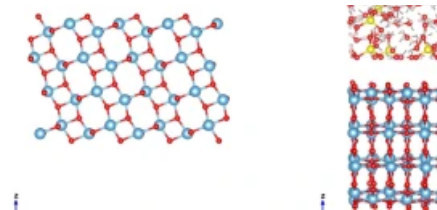
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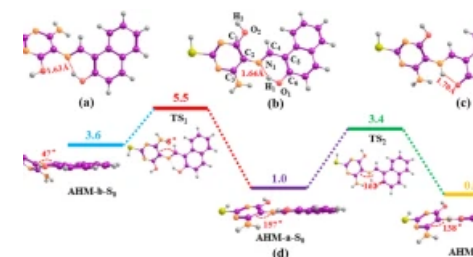
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## Theoretical investigation and reconsideration of intramolecular proton-transfer-induced the twisted charge-transfer for the fluorescent sensor to detect the aluminum ion

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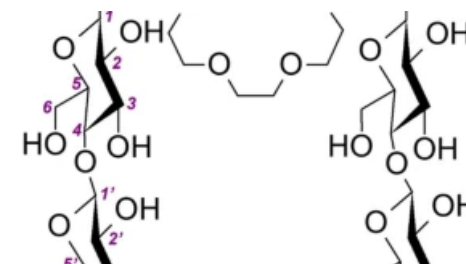
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