

Three-component one-pot synthesis of novel pyrido[2,3-d]pyrimidine indole substituted derivatives and DFT analysis

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Pyridopyrimidines are heterocyclic aromatic compounds known by their antibacterial and medicinal properties. In this work, a series of pyrido[2,3-d]pyrimidine indole derivatives were synthesized by three-component one pot cyclocondensation Michael reaction between 2,6-diaminopyrimidin-4(3H)-one, 3-(2-cyanoacetyl)indole and aromatic aldehydes in boiling acetic acid as solvent. The compounds differ with respect to the substituents of the aromatic aldehyde which are comprised by -C₆H₅, -4-ClC₆H₄, -4-NO₂C₆H₄, -3,4-OCH₂OC₆H₃, -3-OCH₃, 4-OH, 5-NO₂C₆H₂, and -3,4,5-tri-H₃COC₆H₂, respectively. The compounds were synthesized with reasonable yields. They were characterized by IR, mass, and NMR spectrometry. The protocol employed offers the convenient advantages of a one-step synthesis, considerable savings of solvents, and easy isolation of reaction products. In addition, DFT and TD-DFT quantum chemical calculations were used to characterize the geometry and electronic structure of the compounds. © 2017 Elsevier B.V.

Indole

One-step synthesis

Pyrido[2,3-d]pyrimidine

Three-component reaction

Addition reactions

Aldehydes

Aromatization

Chemical compounds

Electronic structure

Polycyclic aromatic hydrocarbons

Quantum chemistry

Heterocyclic aromatic compounds

Indole

Indole derivatives

Michael reactions

One step synthesis

Pyrido[2,3-d]pyrimidine

Quantum chemical calculations

Three component reactions

Aromatic compounds