

Accepted Manuscript

A rapid synthesis of 2-((2-amino-4,6-dimethylpyrimidine-5yl)diazenyl)benzoic acid:
Experimental, DFT study and DNA cleavage activity

Çiğdem Karabacak Atay, Fatih Duman, Merve Gökalp, Tahir Tiliki, Sevgi Ozdemir
Kart



PII: S0022-2860(18)30733-6

DOI: [10.1016/j.molstruc.2018.06.032](https://doi.org/10.1016/j.molstruc.2018.06.032)

Reference: MOLSTR 25319

To appear in: *Journal of Molecular Structure*

Received Date: 14 March 2018

Revised Date: 8 June 2018

Accepted Date: 8 June 2018

Please cite this article as: Çğ. Karabacak Atay, F. Duman, M. Gökalp, T. Tiliki, S. Ozdemir Kart, A rapid synthesis of 2-((2-amino-4,6-dimethylpyrimidine-5yl)diazenyl)benzoic acid: Experimental, DFT study and DNA cleavage activity, *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.06.032.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

A rapid synthesis of 2-((2-amino-4,6-dimethylpyrimidine-5yl)diazenyl)benzoic acid:**Experimental, DFT study and DNA cleavage activity**

Çiğdem KARABACAK ATAY¹, Fatih DUMAN², Merve GÖKALP³, Tahir TİLKI^{3*}, Sevgi OZDEMIR KART⁴

¹*Mehmet Akif Ersoy University, Education Faculty, Elementary Education Department, 15030, Burdur, Turkey*

²*Erciyes University, Faculty of Science, Biology Department, 38039, Kayseri, Turkey*

³*Süleyman Demirel University, Faculty of Science & Arts, Chemistry Department, 32260, Isparta, Turkey*

⁴*Pamukkale University, Art and Science Faculty, Department of Physics, 20020, Denizli, Turkey*

tahirtilki@sdu.edu.tr

Abstract

The newly synthesized 2-((2-amino-4,6-dimethylpyrimidine-5yl)diazenyl)benzoic acid has been prepared by diazotization of anthranilic acid and coupling with 2-amino-4,6-dimethylpyrimidine. Its structure has been characterized by spectroscopic measurements (¹H-NMR spectra, FT-IR spectra, mass spectra and UV-visible spectra) and thermal analysis technique. The DNA cleavage activity of compound is evaluated by agarose gel electrophoresis with a series of concentrations. Our measurements show that neither a disruptive effect created by 2-((2-amino-4,6-dimethylpyrimidine-5yl)diazenyl)benzoic acid on pBR 322 DNA are observed, nor the dependence of the concentration on the activity of newly synthesized chemical on pBR 322 plasmid DNA such as cleavage or break DNA double helix structure. Moreover, computational chemistry method based on Density Functional Theory (DFT) employing B3LYP level with 6-31G(d) basis set has been used to study geometry and spectroscopic properties such as FT-IR and UV-vis spectra of the titled compound considered in this work. The computations of the chemical shifts for ¹H-NMR of the title compound have been carried out via Gauge-Invariant Atomic Orbital (GIAO) method utilizing the same basis set. It is observed that DFT results are compatible with the experimental results.

Download English Version:

<https://daneshyari.com/en/article/7807033>

Download Persian Version:

<https://daneshyari.com/article/7807033>

[Daneshyari.com](https://daneshyari.com)