

## Accepted Manuscript

Experimental and theoretical elucidation of structural and antioxidant properties of vanillylmandelic acid and its carboxylate anion

Dušan Dimić, Dejan Milenković, Jelica Ilić, Biljana Šmit, Ana Amić, Zoran Marković, Jasmina Dimitrić Marković



PII: S1386-1425(18)30181-1  
DOI: doi:[10.1016/j.saa.2018.02.063](https://doi.org/10.1016/j.saa.2018.02.063)  
Reference: SAA 15867

To appear in: *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*

Received date: 29 November 2017

Revised date: 29 January 2018

Accepted date: 24 February 2018

Please cite this article as: Dušan Dimić, Dejan Milenković, Jelica Ilić, Biljana Šmit, Ana Amić, Zoran Marković, Jasmina Dimitrić Marković, Experimental and theoretical elucidation of structural and antioxidant properties of vanillylmandelic acid and its carboxylate anion. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Saa(2017), doi:[10.1016/j.saa.2018.02.063](https://doi.org/10.1016/j.saa.2018.02.063)

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.

# Experimental and theoretical elucidation of structural and antioxidant properties of vanillylmandelic acid and its carboxylate anion

Dušan Dimić<sup>a</sup>, Dejan Milenković<sup>b</sup>, Jelica Ilić<sup>a</sup>, Biljana Šmit<sup>c</sup>, Ana Amić<sup>d</sup>,  
Zoran Marković<sup>e</sup>, Jasmina Dimitrić Marković<sup>a\*</sup>

<sup>a</sup>*Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16, 11000  
Belgrade, Serbia*

<sup>b</sup>*Bioengineering Research and Development Center, Prvoslava Stojanovića 6, 34000  
Kragujevac, Serbia*

<sup>c</sup>*Faculty of Science, University of Kragujevac, Radoja Domanovića 12, 34000 Kragujevac,  
Serbia*

<sup>d</sup>*Department of Chemistry, Josip Juraj Strossmayer University of Osijek, Cara Hadrijana 8a,  
31000 Osijek, Croatia*

<sup>e</sup>*Department for Chemical-Technological Sciences, State University of Novi Pazar, Vuka  
Karadžića bb, 3600 Novi Pazar, Serbia*

## Abstract

Vanillylmandelic acid (VMA), an important metabolite of catecholamines that is routinely screened as tumor marker, was investigated by the various spectroscopic techniques (IR, Raman, UV-Vis, antioxidant decolorization assay and NMR). Structures optimized by the employment of five common functionals (M05-2X, M06-2X, B3LYP, CAM-B3LYP, B3LYP-D3) were compared with the crystallographic data. The M05-2X functional reproduced the most reliable experimental bond lengths and angles (correlation coefficient >0.999). The importance of intramolecular hydrogen bonds for structural stability was discussed and quantified by the NBO analysis. The most prominent bands in vibrational spectrum were analyzed and compared to the experimental data. The positions of the carbon and hydrogen atoms in NMR spectra were well reproduced. The differences in UV-Vis spectrum were investigated by adding the explicit solvent and by performing NBO and QTAIM analyses. The discrepancy in the two spectra of about 50 nm could be explained by the solvent effect on carboxyl group. The most probable antioxidant activity mechanism was discussed for VMA and its carboxylate anion. The Molecular Docking study with the C -

Download English Version:

<https://daneshyari.com/en/article/7669209>

Download Persian Version:

<https://daneshyari.com/article/7669209>

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