

## **SUPPLEMENTARY MATERIAL**

### **Class I histone deacetylase inhibition by aryl butenoic acid derivatives: *in silico* and *in vitro* studies**

Gamze BORA<sup>1</sup>\*, Suat SARI<sup>2</sup>, Gülce TAŞKOR<sup>3</sup>, Sevim DALKARA<sup>2</sup>, Hayat ERDEM-YURTER<sup>1</sup>

1 Department of Medical Biology, Faculty of Medicine, Hacettepe University, Ankara, Turkey.

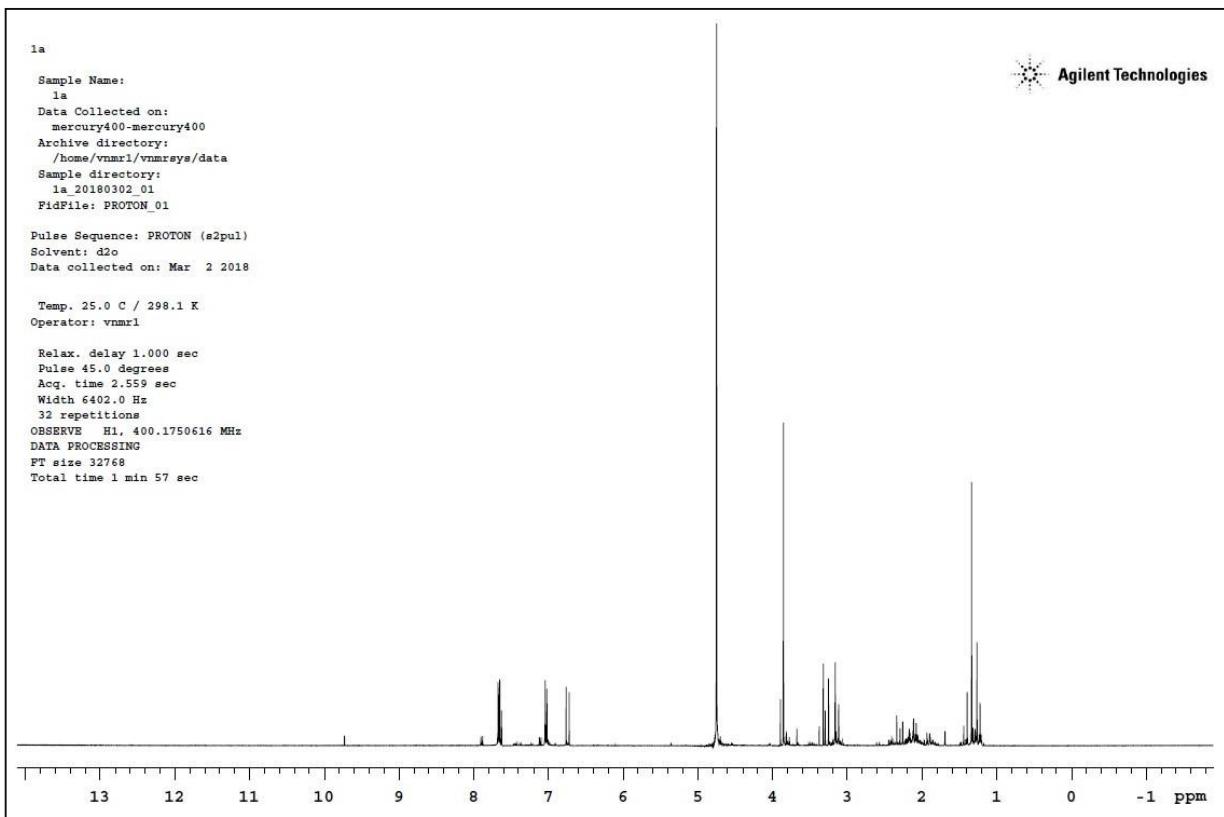
2 Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Hacettepe University, Ankara, Turkey.

3 Department of Basic Pharmaceutical Sciences, Faculty of Pharmacy, Hacettepe University, Ankara, Turkey.

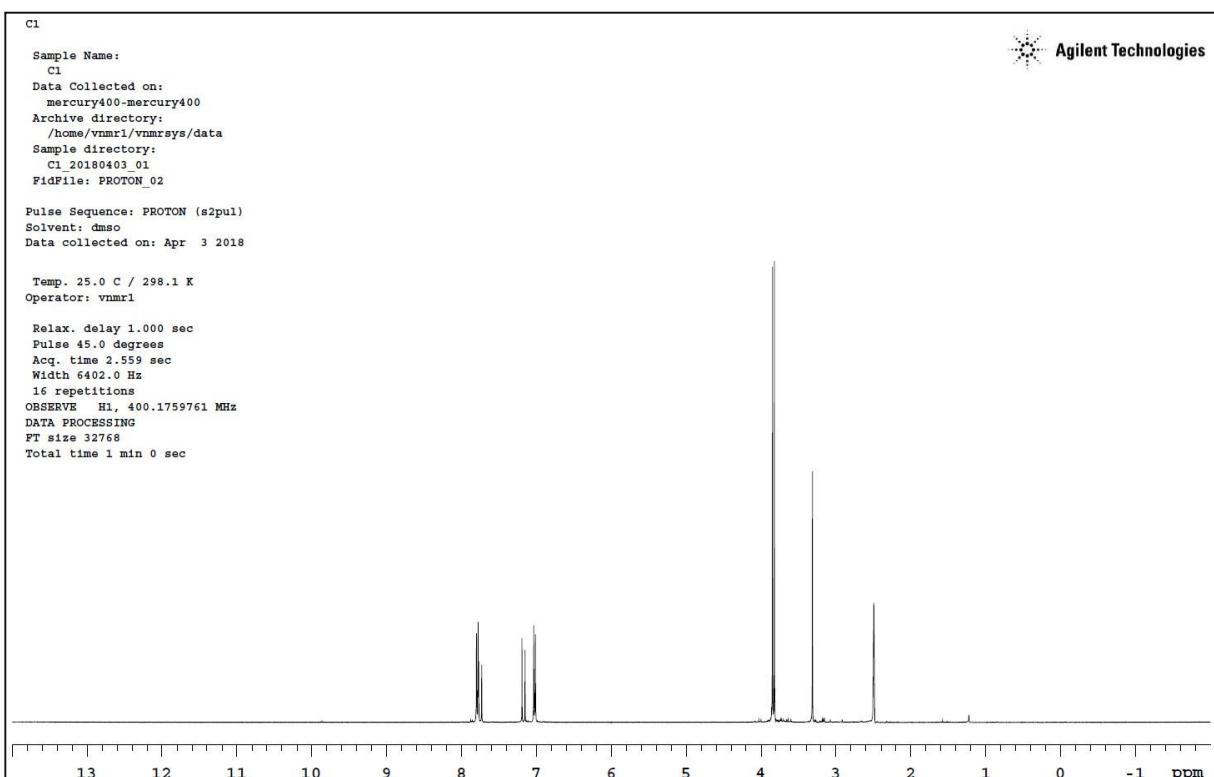
\* Corresponding Author. E-mail: gamzeb@hacettepe.edu.tr (G.B); Tel. +90-312-305 25 41; Fax. +90-312-309 60 60.

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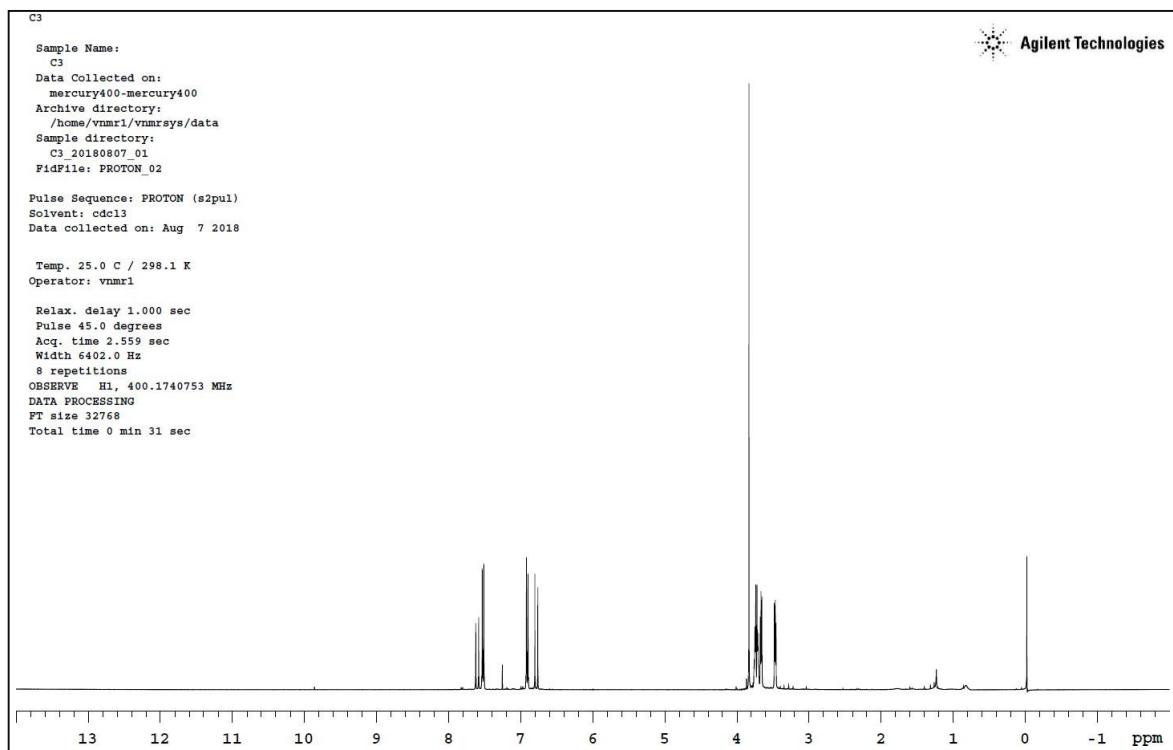
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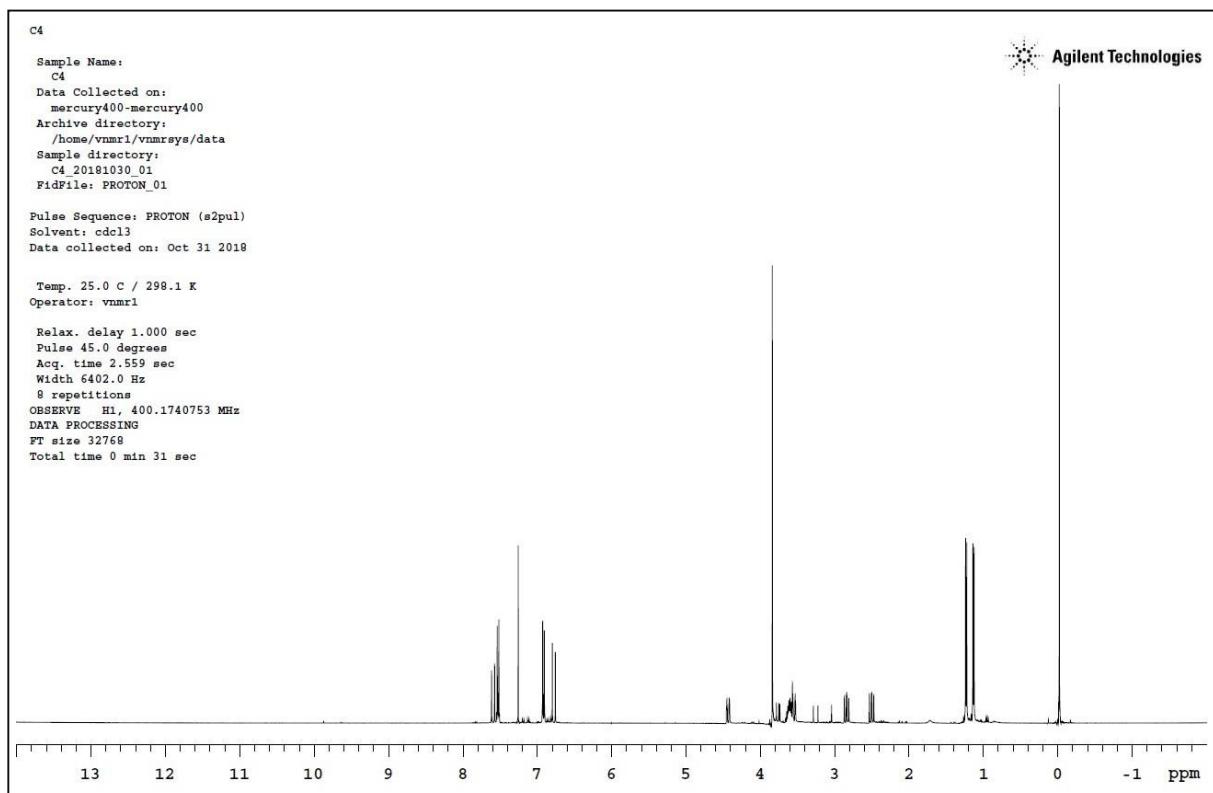
**Figure S1.**  $^1\text{H}$ -NMR spectrum of potassium 4-(4-methoxyphenyl)-2-oxobut-3-enoate (1a)



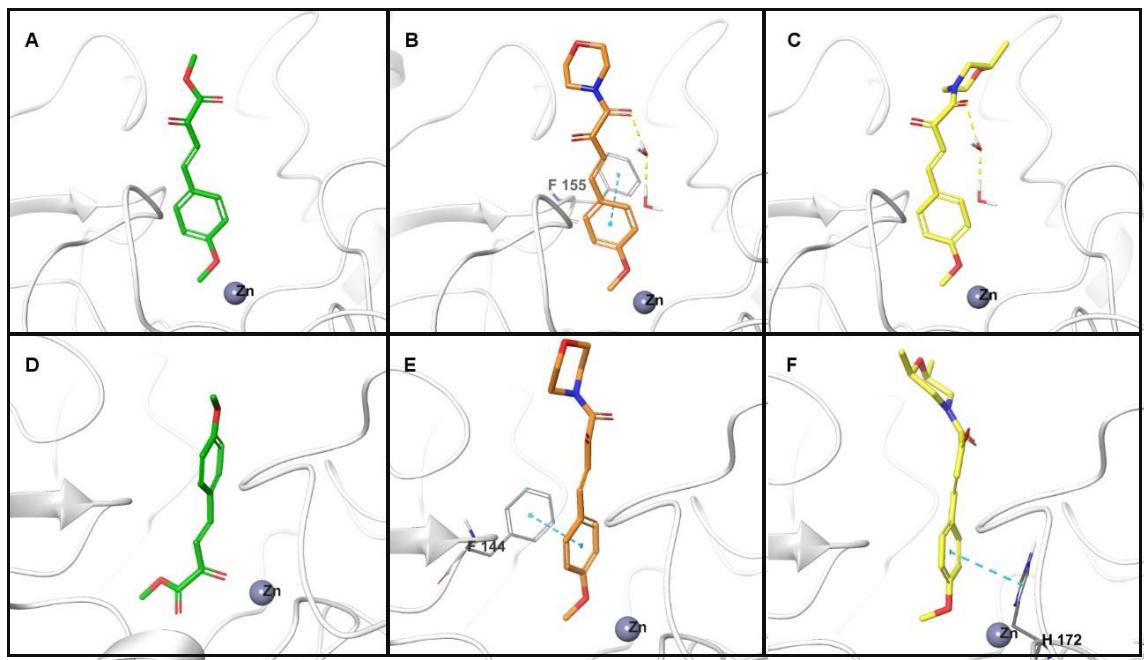
**Figure S2.**  $^1\text{H}$ -NMR spectrum of (E)-methyl 4-(4-methoxyphenyl)-2-oxobut-3-enoate (C1)



**Figure S3.**  $^1\text{H}$ -NMR spectrum of (*E*)-4-(4-methoxyphenyl)-1-morpholinobut-3-ene-1,2-dione (C3)



**Figure S4.**  $^1\text{H}$ -NMR spectrum of (*E*)-1-(2,6-dimethylmorpholino)-4-(4-methoxyphenyl)but-3-ene-1,2-dione (C4)



**Figure S5.** Docking poses of **C1** (green), **C3** (orange), and **C4** (yellow) in the catalytic site of HDAC2 (A, B, and C, respectively) and HDAC3 (D, E, and F, respectively).