**SUPPLEMENTARY MATERIAL**

# Persicaline, a new antioxidant sulphur-containing imidazoline alkaloid from *Salvadora persica* roots

Mohamed F. Abd El Halim[a], Wael M Abdel-Mageed[a,b,*], Omer A. Basudan[a] and Ali A. El-Gamal[a,c,*]

[a]*Pharmacognosy Department, King Saud University, College of Pharmacy, , P.O. Box 2457, Riyadh 11451, Saudi Arabia e-mails:* wabdelmageed@ksu.edu.sa, & *aelgamal00@yahoo.com*

[b] *Pharmacognosy Department, Assiut University, Faculty of Pharmacy, , Assiut P.O. Box 71526, Egypt*

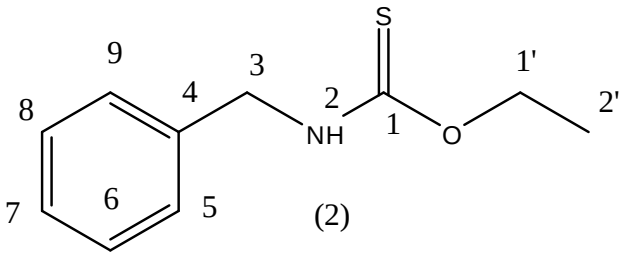
[c]*Pharmacognosy Department, Mansoura University, Faculty of Pharmacy, , Mansoura P.O. Box 35516, Egypt*

## Abstract

*Salvadora persica* L. is a popular chewing stick commonly known as 'miswak'. During our ongoing research activities on the chemical constituents of *Salvadora persica* roots, a new sulphur-containing imidazoline alkaloid 1,3-Dibenzyl-4-(1,2,3,4-tetrahydroxy-butyl)-1,3-dihydro-imidazole-2-thione, persicaline, (**1**) along with five known compounds (**2-6**) are identified. Compounds (**2-3**) were reported for the first time from the family *Salvadoraeceae*. The structure of the new compound was established by extensive spectroscopic data and HR-MS. The antioxidant activities of the fractions and isolates were evaluated using different *in vitro* methods such as DPPH, superoxide anion and nitric oxide radicals scavenging assays. Compound (**1**) showed a promising antioxidant activity with $IC_{50}$ 0.1, 0.08 and 0.09 µM in the three assays respectively comparable to ascorbic acid.

**Keywords:** *Salvadora persica*; *Persicaline*; Imidazoline Alkaloids; Sulphur-containing compounds; Radical Scavenging Activity.

**Content**




(2)

Benzyl-thiocarbamic acid *O*-ethyl ester

**Table S1** $^{1}H$ (500 MHz) of compound **2** and $^{13}C$ (125 MHz) NMR spectral data of compounds **2** in $CDCl_3$

| **Position** | **$H^{1}$ NMR data** **$\delta_H$ (ppm) (*J* in Hz)** | **$C^{13}$ NMR data** **$\delta_C$ (ppm)** |
|---|---|---|
| **1** | - | 190 (*Z*)<br>190.73 (*E*) |
| **2** | 6.5 br. (*Z*)<br>6.9 br. **(*E*)** | - |
| **3** | 4.46 (2H, d, *J* = 5.8 Hz, $CH_2$, *Z*)<br>4.78 (2H, d, *J* = 5.7 Hz, $CH_2$, *E*) | 47.27 (*Z*)<br>49.31 (*E*) |
| **4** | - | 136.63<br>136.96 |
| **5** | 7.36 (1H, d, *J*= 7.5Hz) | 128.92 |
| **6** | 7.33(1H, d, *J*= 7.5Hz) | 127.98 |
| **7** | 7.31(1H, m) | 127.79 |
| **8** | 7.33(1H, d, *J*= 7.5Hz) | 127.98 |
| **9** | 7.36 (1H, d, *J*= 7.5Hz) | 128.92 |
| **1'** | 4.58 (2H, q, *J* = 7.2 Hz, *Z*)<br>4.53 (2H, q, *J* = 7.2 Hz, *E*), | 66.69(*Z*)<br>68.17 (*E*) |
| **2'** | 1.37 (3H, t, *J* = 7.2 Hz, *Z*)<br>1.33 (3H, t, *J* = 7.2 Hz, *E*) | 14.32 (*Z*)<br>14.38 (*E*) |

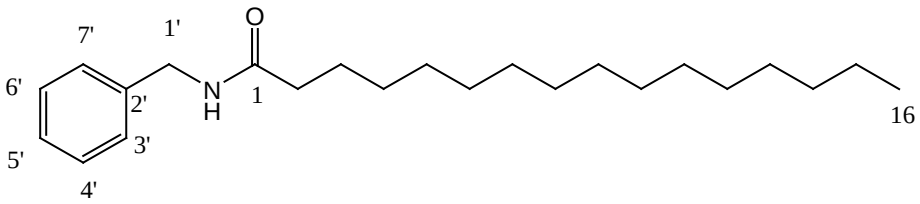



**Table S2** $^{1}H$ (500 MHz) of compound **2** and $^{13}C$ (125 MHz) NMR spectral data of compounds **3** in $CDCl_3$

| **Position** | **$H^{1}$ NMR data** $\delta_H$ **(ppm) (*J* in Hz)** | **$C^{13}$ NMR data** $\delta_C$ **(ppm)** |
|---|---|---|
| 1 | - | 173.0 |
| 2 | 2.20 (t) | 36.88 |
| 3 | 1.65 (m) | 22.72 to 31.95 |
| 4 | 1.16-1.29 | 22.72 to 31.95 |
| 5 | 1.16-1.29 | 22.72 to 31.95 |
| 6 | 1.16-1.29 | 22.72 to 31.95 |
| 7 | 1.16-1.29 | 22.72 to 31.95 |
| 8 | 1.16-1.29 | 22.72 to 31.95 |
| 9 | 1.16-1.29 | 22.72 to 31.95 |
| 10 | 1.16-1.29 | 22.72 to 31.95 |
| 11 | 1.16-1.29 | 22.72 to 31.95 |
| 12 | 1.16-1.29 | 22.72 to 31.95 |
| 13 | 1.16-1.29 | 22.72 to 31.95 |
| 14 | 1.16-1.29 | 22.72 to 31.95 |
| 15 | 1.16-1.29 | 22.72 |
| 16 | 0.88 | 14.16. |
| 1' | 4.45 (d) | 43.62 |
| 2' | - | 138.40 |
| 3' | 7.17 (1H, d, *J*= 8.0 Hz) | 127.9 |
| 4' | 7.33(1H, m, overlapped) | 128.8 |
| 5' | 7.33(1H, m, overlapped) | 127.55 |
| 6' | 7.33(1H, m, overlapped) | 128.8 |
| 7' | 7.17 (1H, d, *J*= 8.0 Hz) | 127.9 |

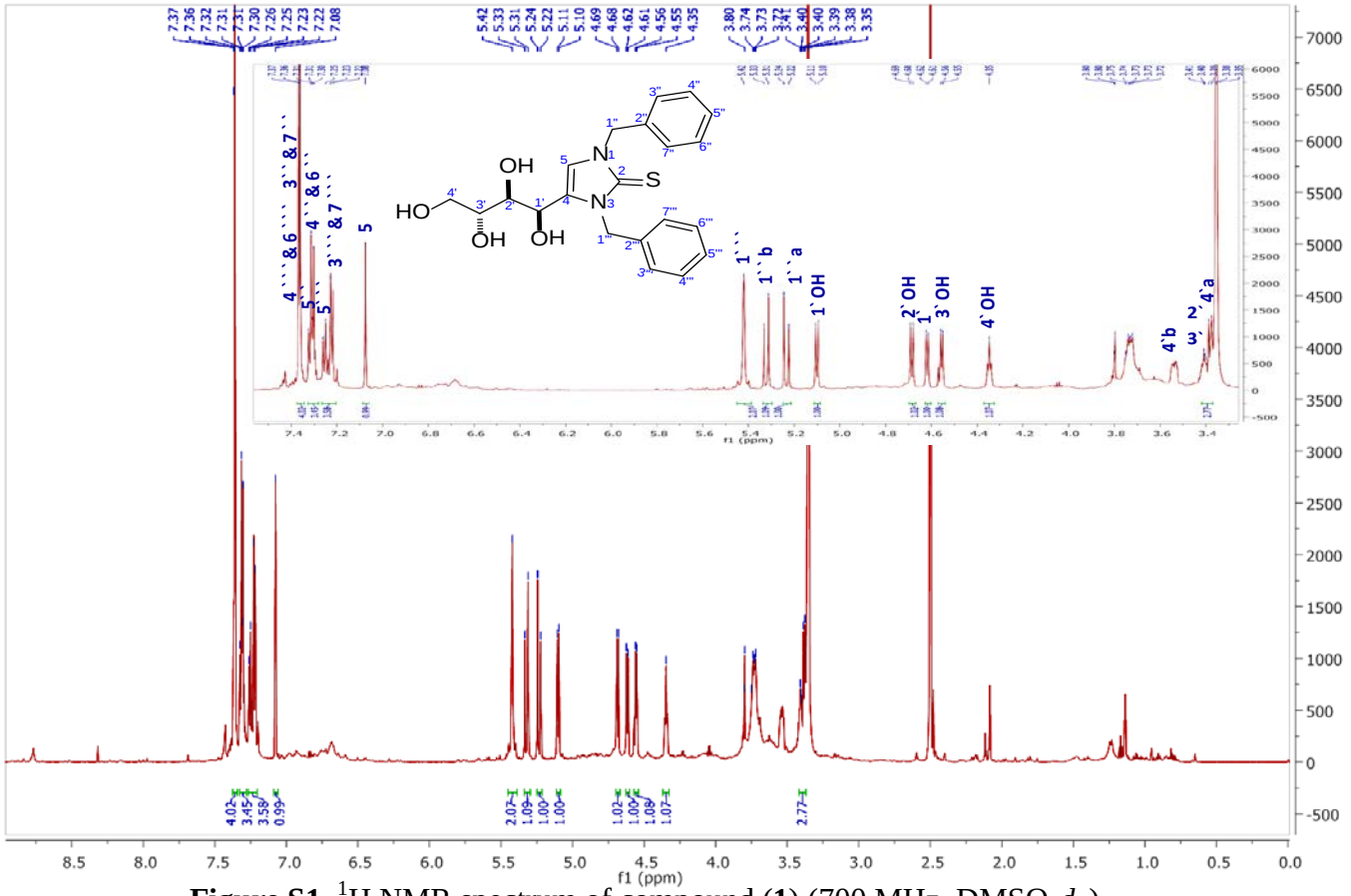


**Figure S1.** $^{1}$H NMR spectrum of compound (**1**) (700 MHz, DMSO-$d_6$)

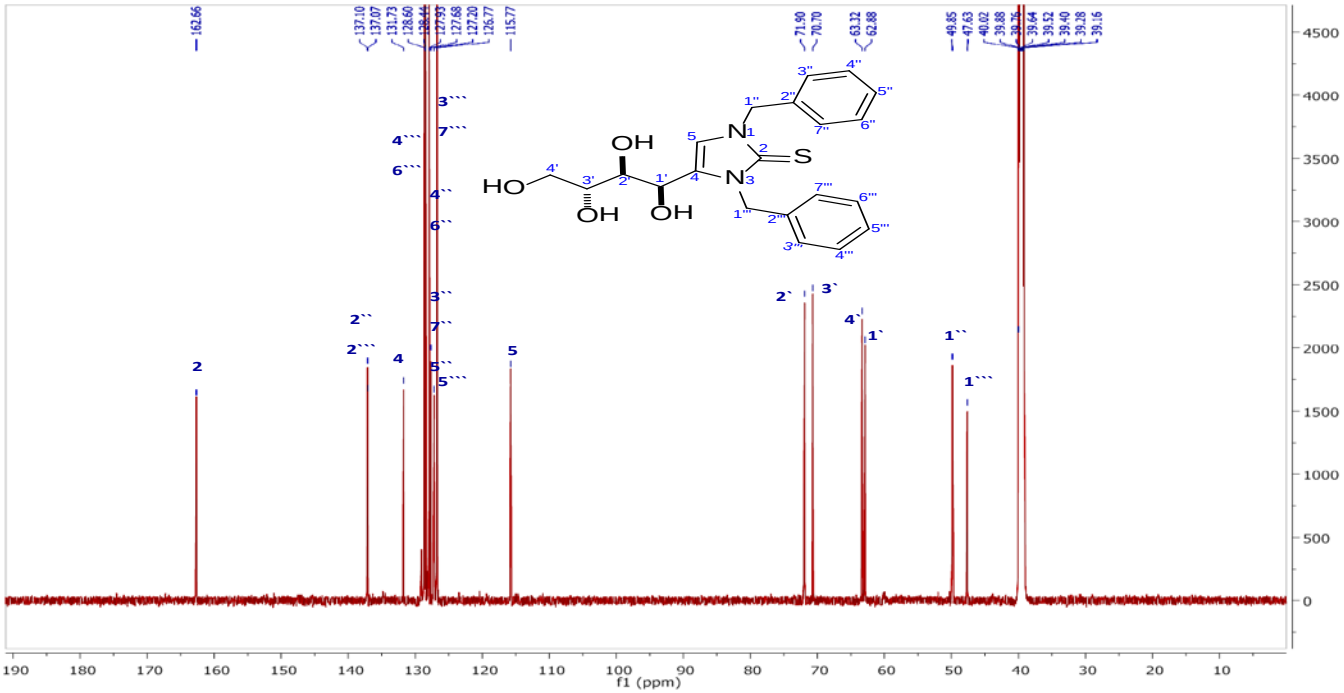


**Figure S2.** $^{13}$C NMR spectrum of compound (**1**) (175 MHz, DMSO-$d_6$)

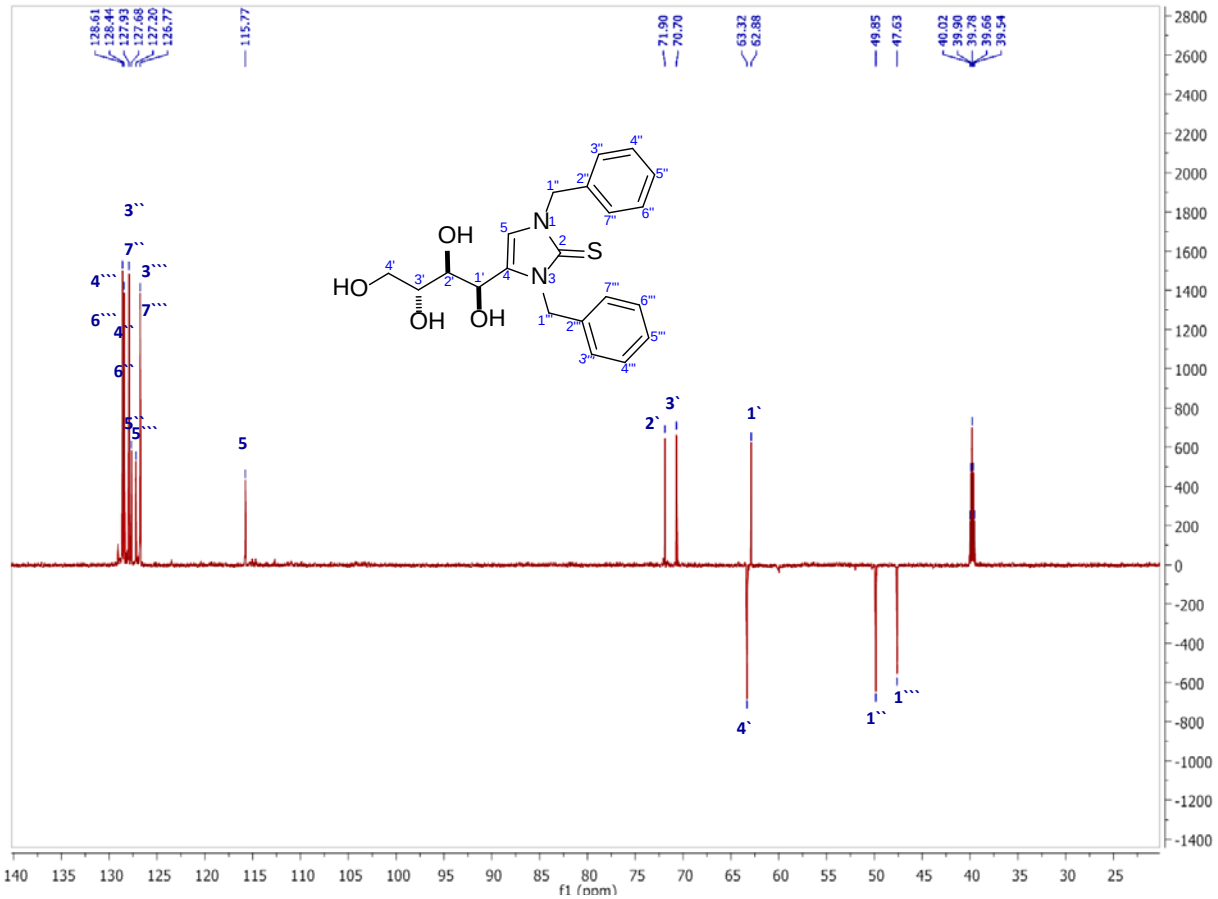


**Figure S3.** DEPT 135 spectrum of compound (**1**) (175 MHz, DMSO-$d_6$)

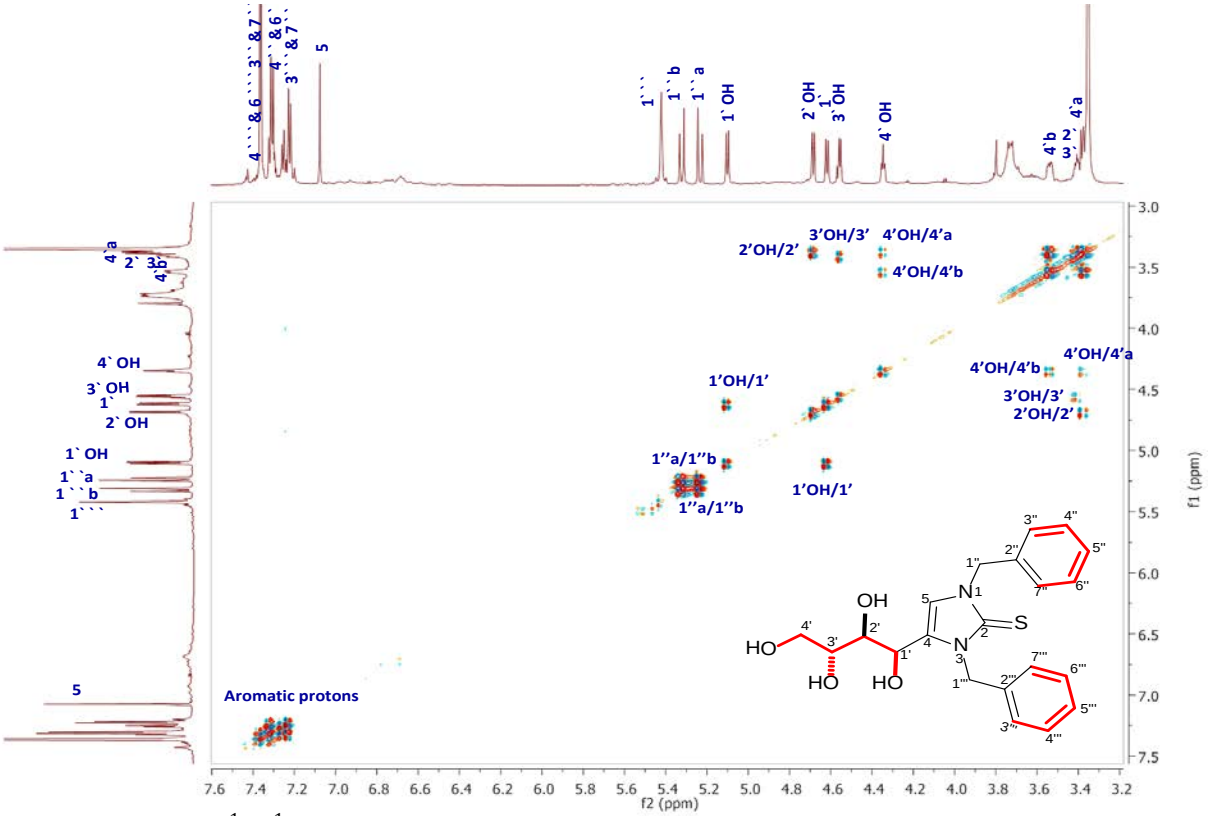



**Figure S4.** $^{1}$H-$^{1}$H COSY spectrum of compound (**1**) (700 MHz, DMSO-$d_6$)

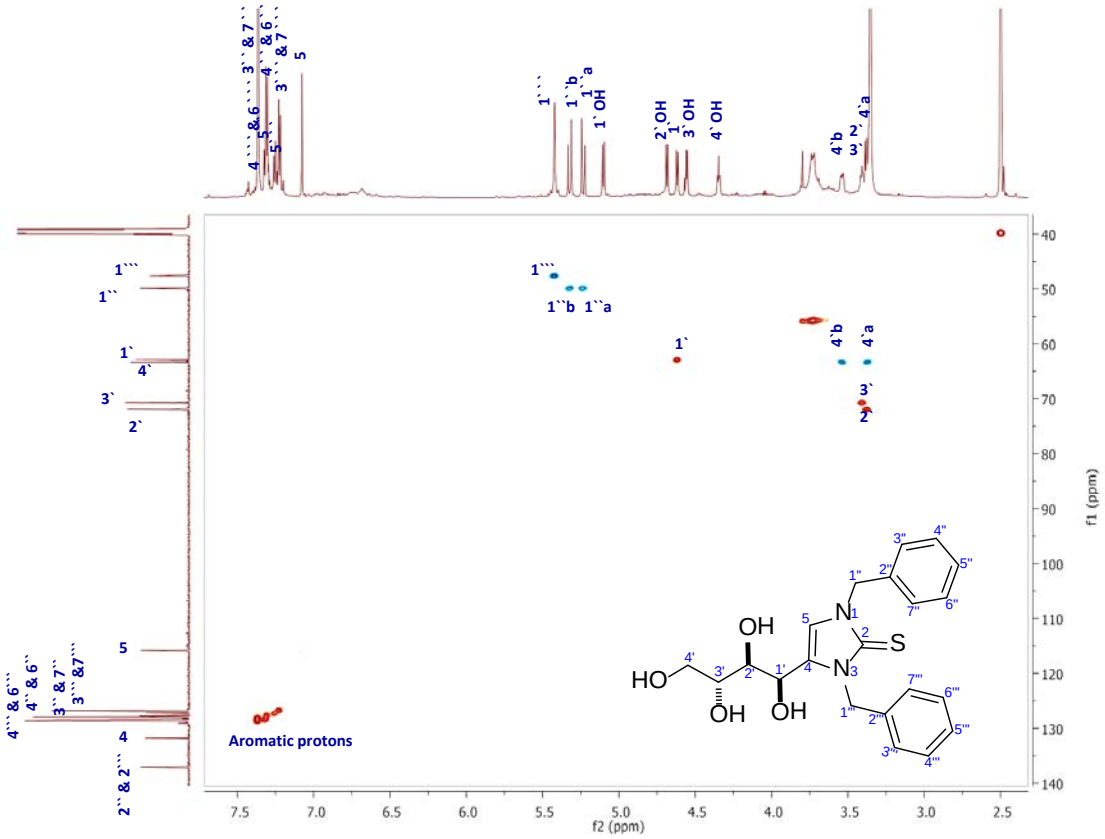



**Figure S5.** $^{1}$H-$^{13}$C HSQC spectrum of compound (**1**) (700 MHz, DMSO-$d_6$)

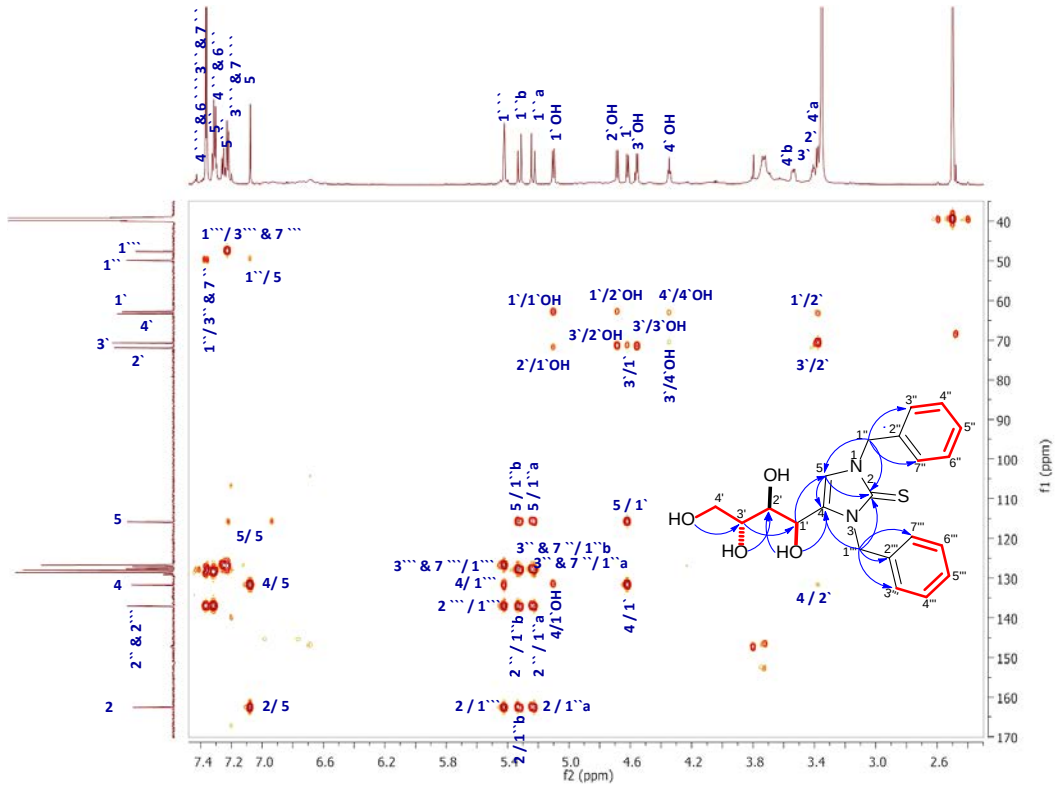



**Figure S6.** $^{1}$H-$^{13}$C HMBC spectrum of compound (**1**) (700 MHz, DMSO-$d_6$)

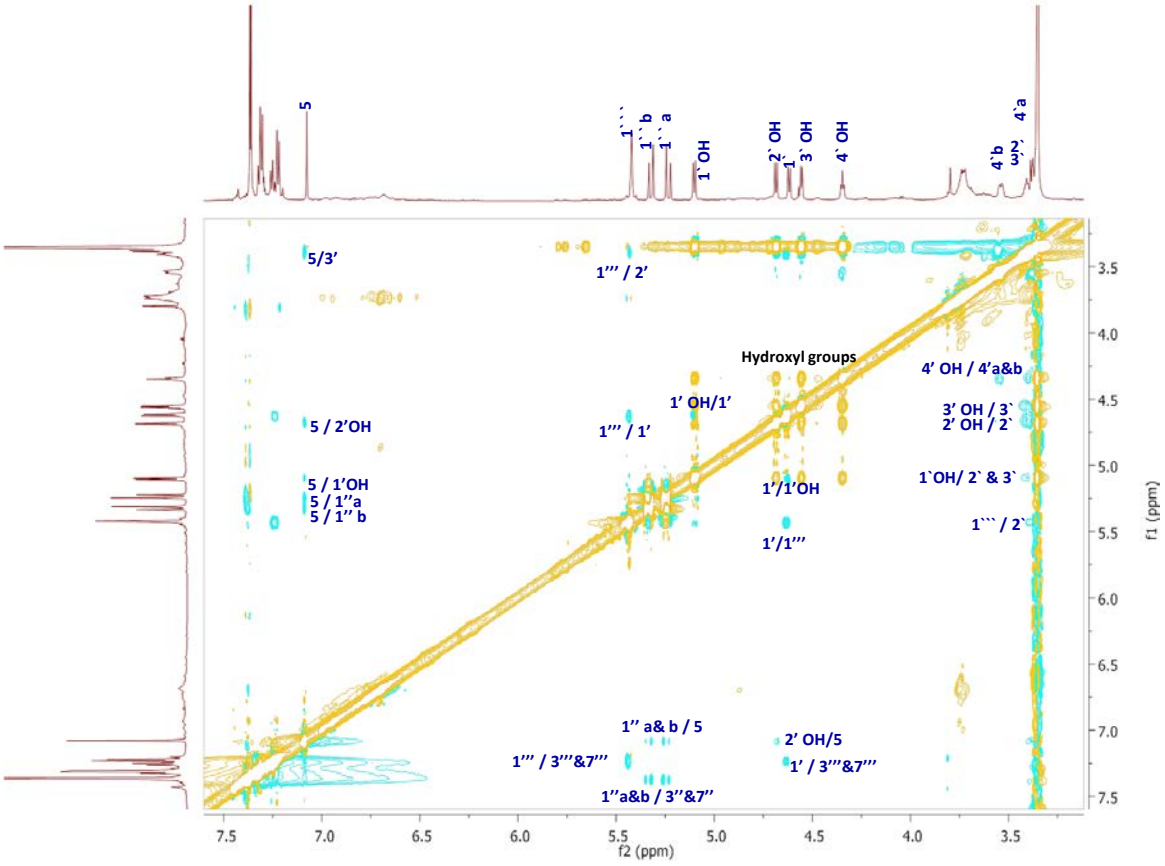



**Figure S7.** $^{1}$H-$^{1}$H NOESY spectrum of compound (**1**) (700 MHz, DMSO-$d_6$)

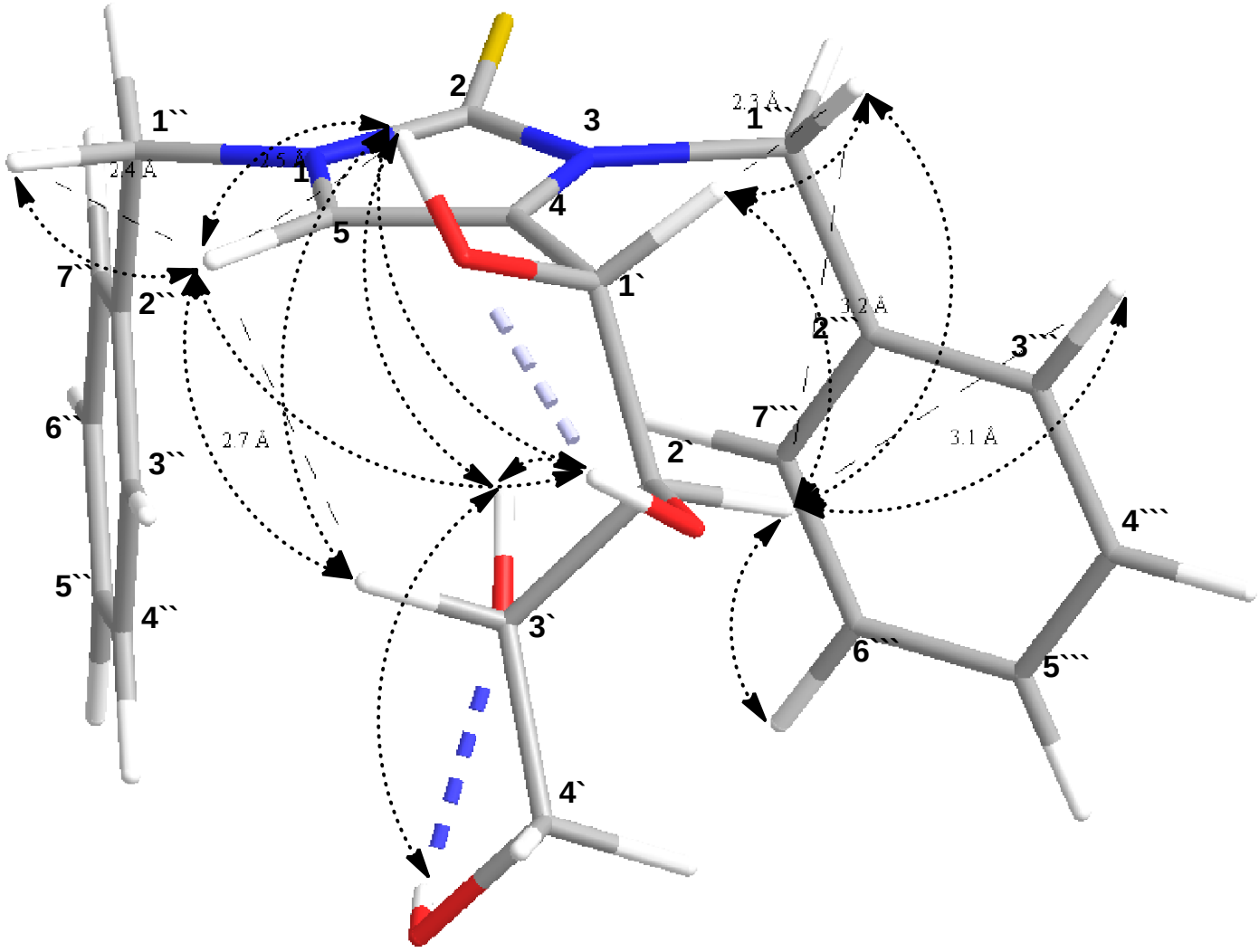



**Figure S8.** Key NOESY (→, black) correlations and global energy minimum of **1**.