

## SUPPLEMENTARY MATERIAL

### New Hepatoprotective Isoflavone Glucosides from *Pueraria lobata* (Willd.) Ohwi

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#### Abstract

Two new isoflavone glucosides, 3'-methoxyneopuerarin A (**1**) and 3'-methoxyneopuerarin B (**2**), together with nine known isoflavone including puerarin (**3**), neopuerarin A (**4**), neopuerarin B (**5**), daidzin (**6**), daidzein (**7**), 3'-methoxypuerarin (**8**), puerarin xyloside (**9**), mirificin (**10**), 3'-hydroxypuerarin (**11**) were isolated from the water extraction of the dried roots of *Pueraria lobata* (Willd.) Ohwi. Their structures were elucidated by the means of spectroscopic and chromatographic analysis methods. All compounds were evaluated for their hepatoprotective activity on HepG2 cells. All of them showed statistically significant hepatoprotective effect.

**Keywords:** *Pueraria lobata* (Willd.) Ohwi, isoflavone, hepatoprotective effect

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Figure S1. Key 2D NMR correlations of compounds 1, 2.

## Figure S1

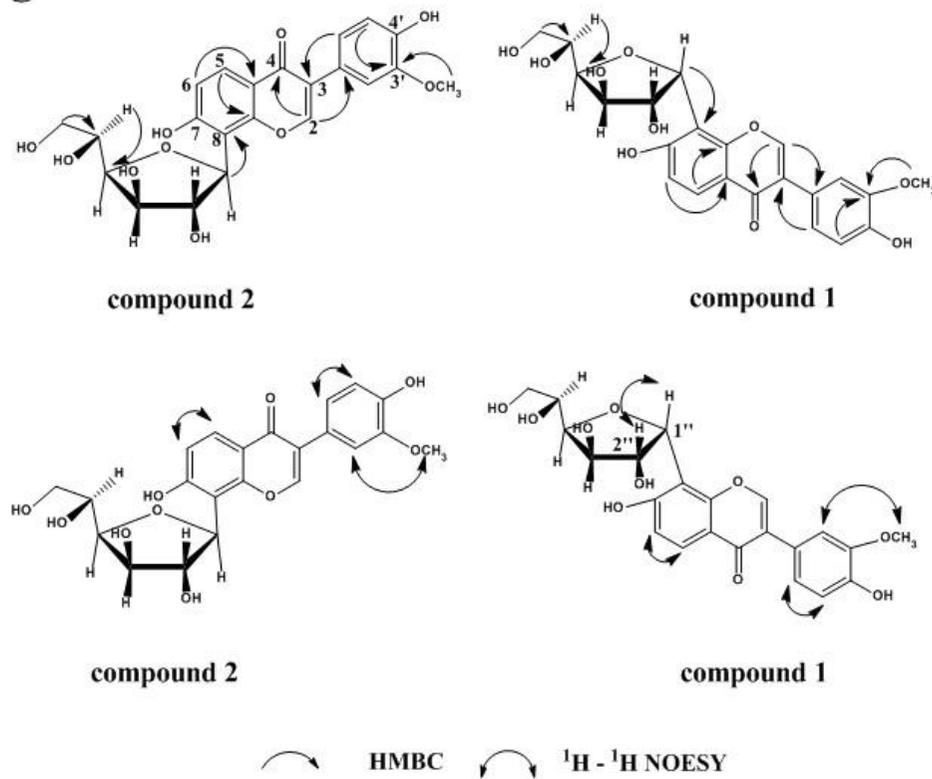
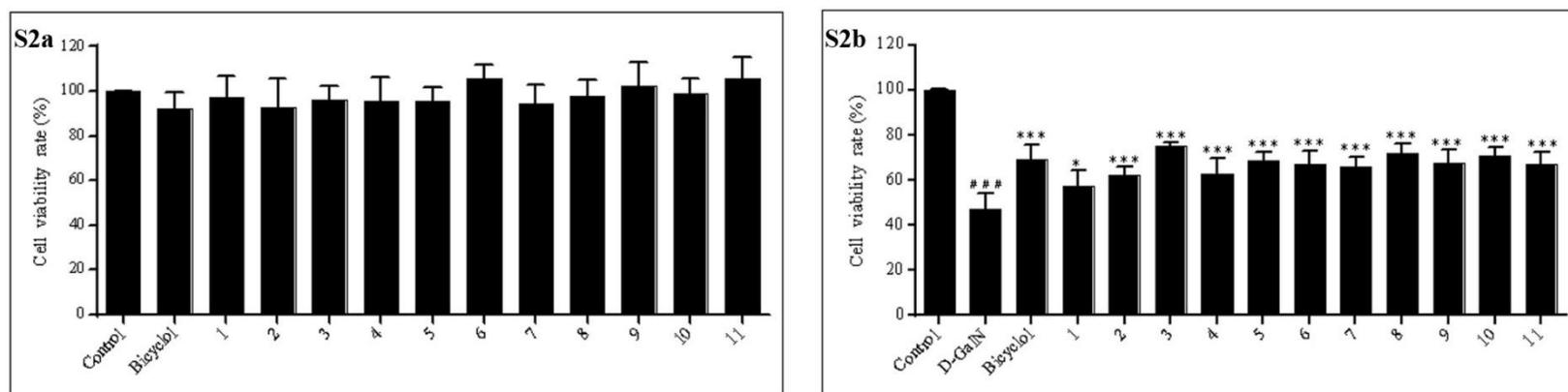


Figure S1 Key 2D NMR correlations of compounds 1-2

**Figure S2.** Cell viability (S2a) and hepatoprotective effects (S2b) of compounds **1-11**.

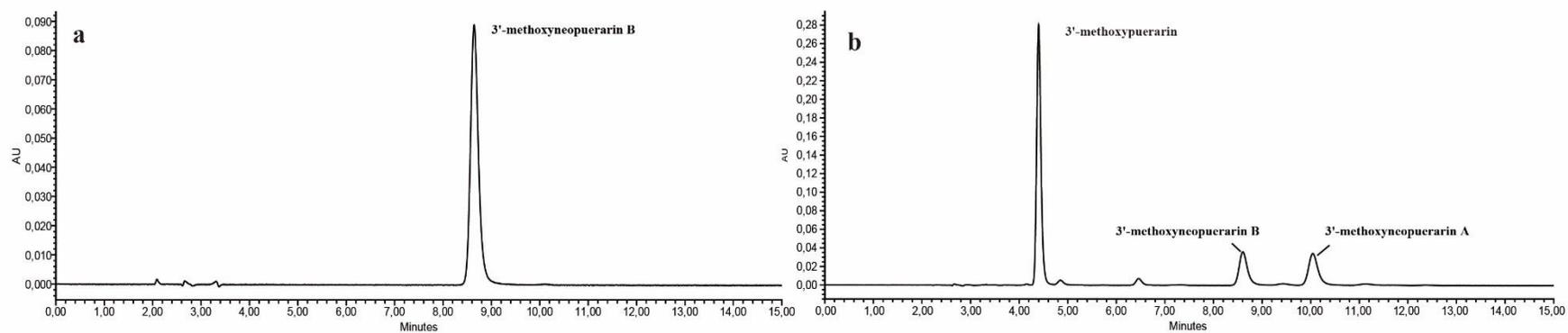
**Figure S2**



**Figure S2** Hepatoprotective effects of compounds **1-11** (10  $\mu$ M) against D-GalN-induced toxicity in HepG2 cells (S2b) and the toxicity in HepG2 cells (S2a). Results are expressed as the mean  $\pm$  SD (n = 4). Bicyclol was used as positive control (10  $\mu$ M). Compared with D-GalN group, \*\*\*p < 0.001,\*p < 0.05; Compared with control,### p < 0.001.

**Figure S3** HPLC chromatogram of 3'-methoxyneopuerarin B (a) and acid-hydrolyzed 3'-methoxyneopuerarin B (b).

### Figure. S3



**Figure S3. HPLC chromatogram of 3'-methoxyneopuerarin B (a) and acid-hydrolyzed 3'-methoxyneopuerarin B (b).**

Figure S4 HR-ESIMS of 1

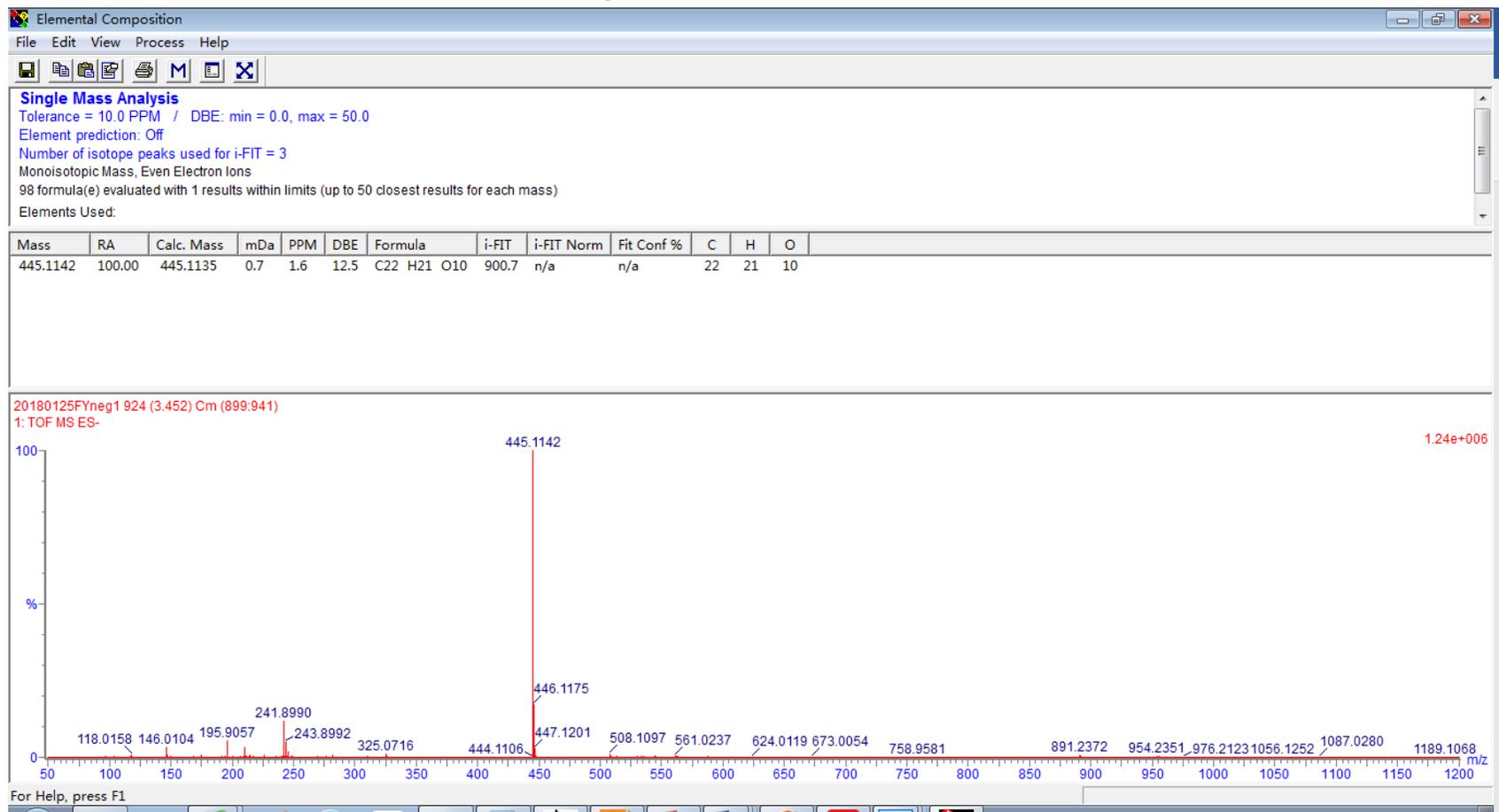
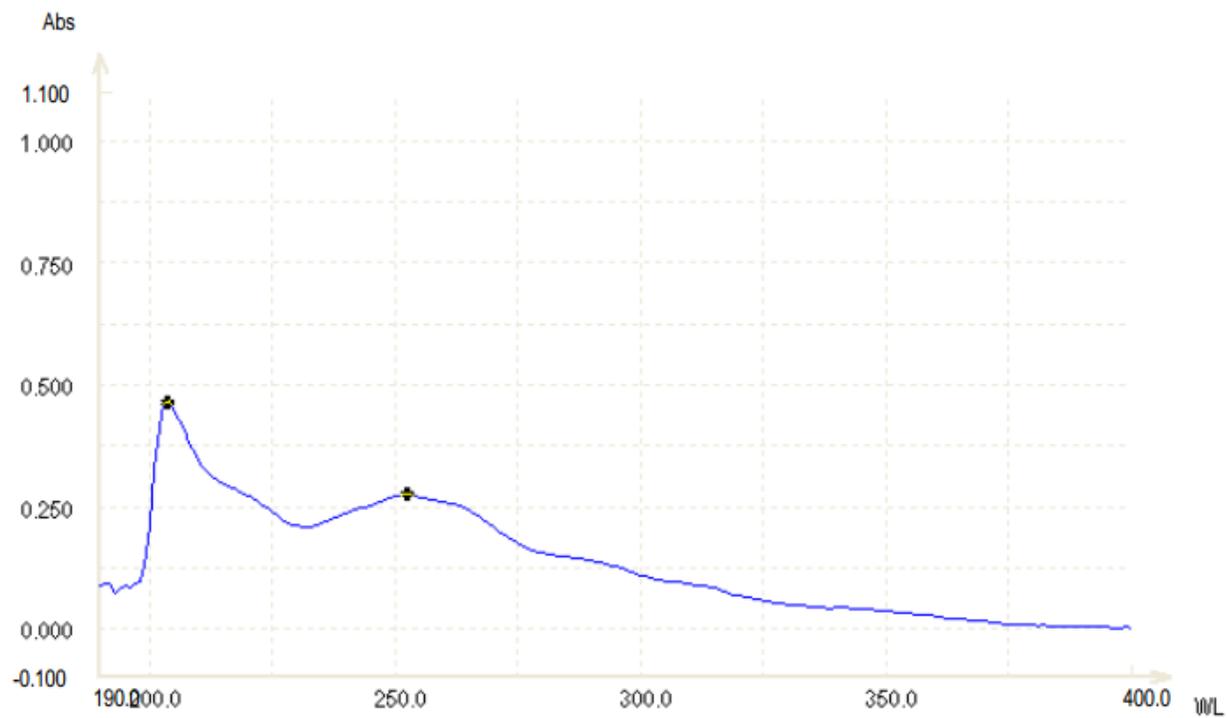


Figure S5 UV of 1 (MeOH)

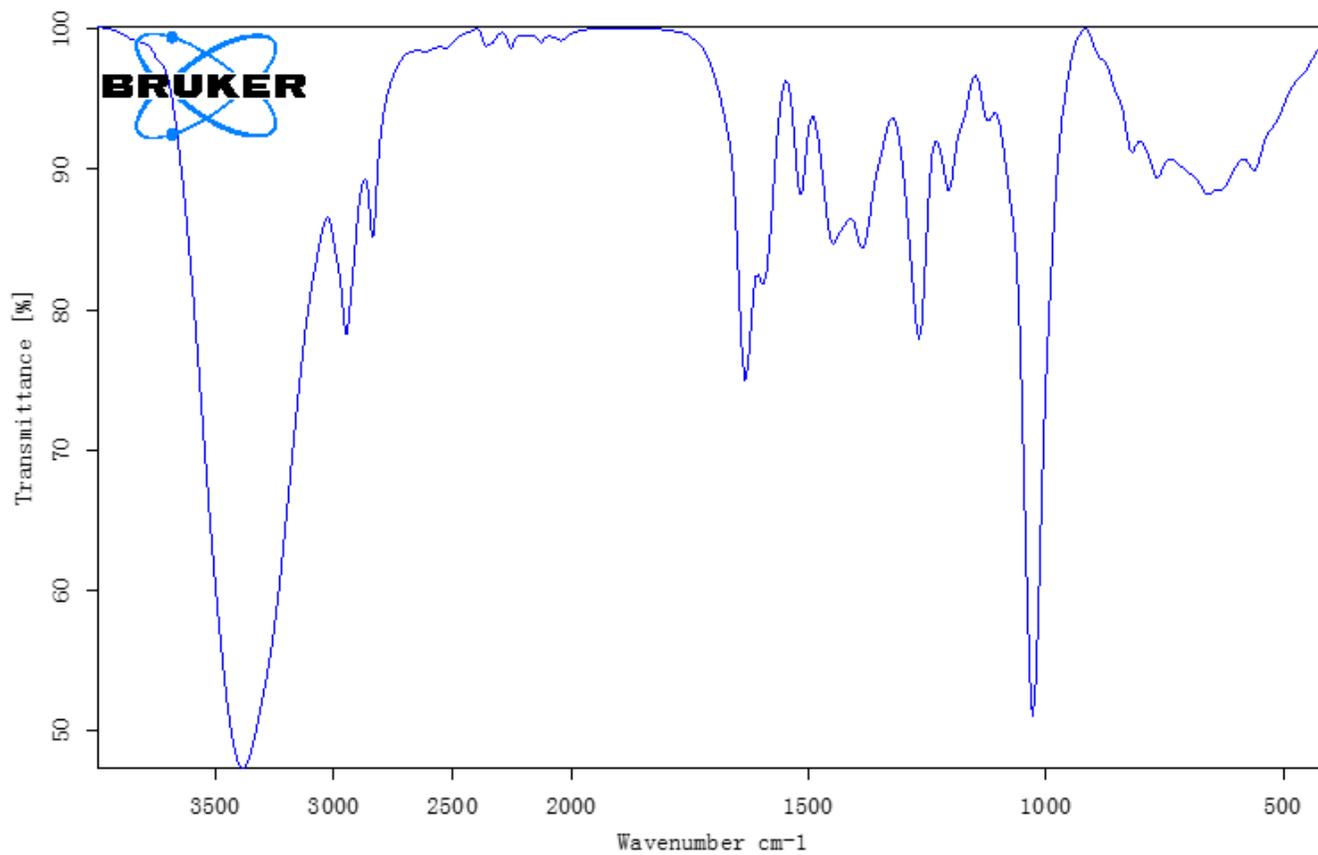


peak:

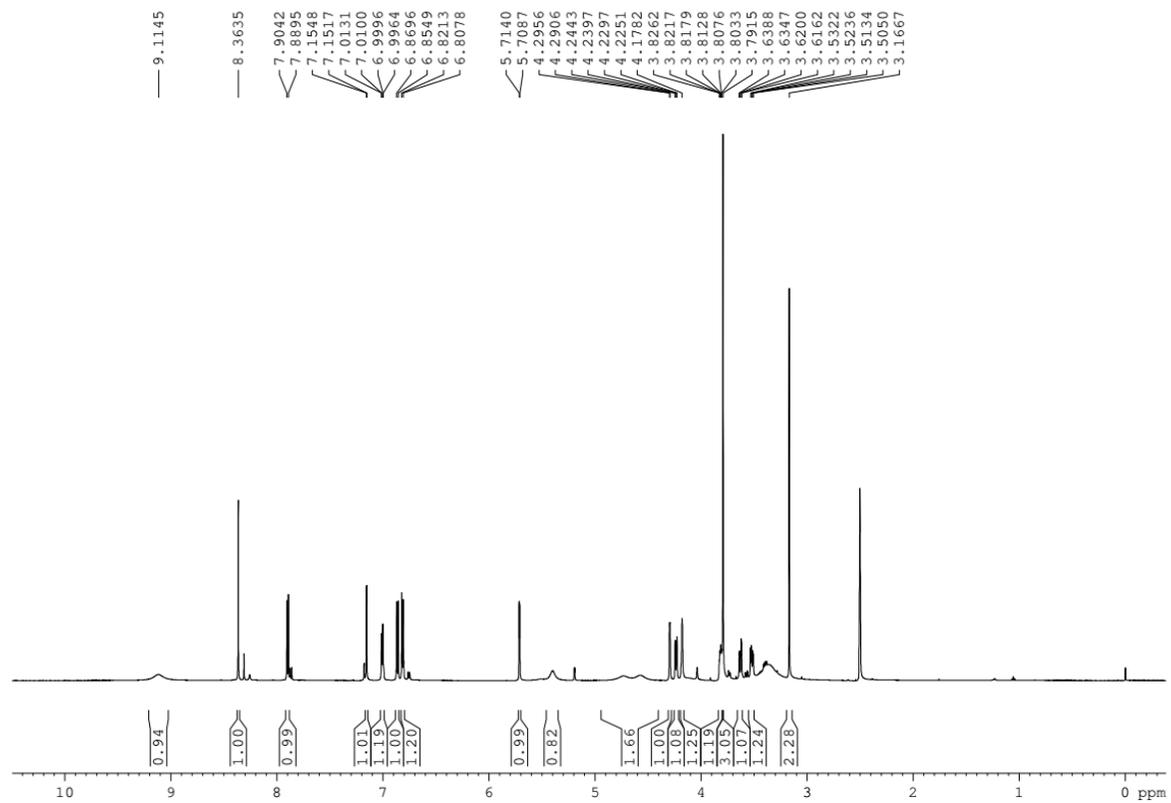
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WL02=252.0 Abs=0.275

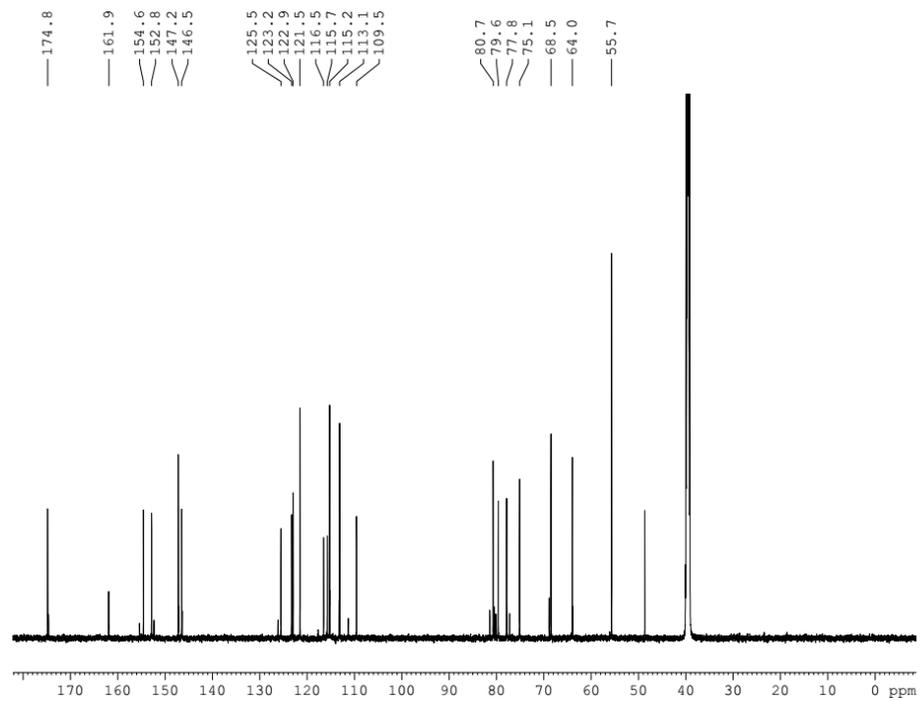
Figure S6 IR of 1



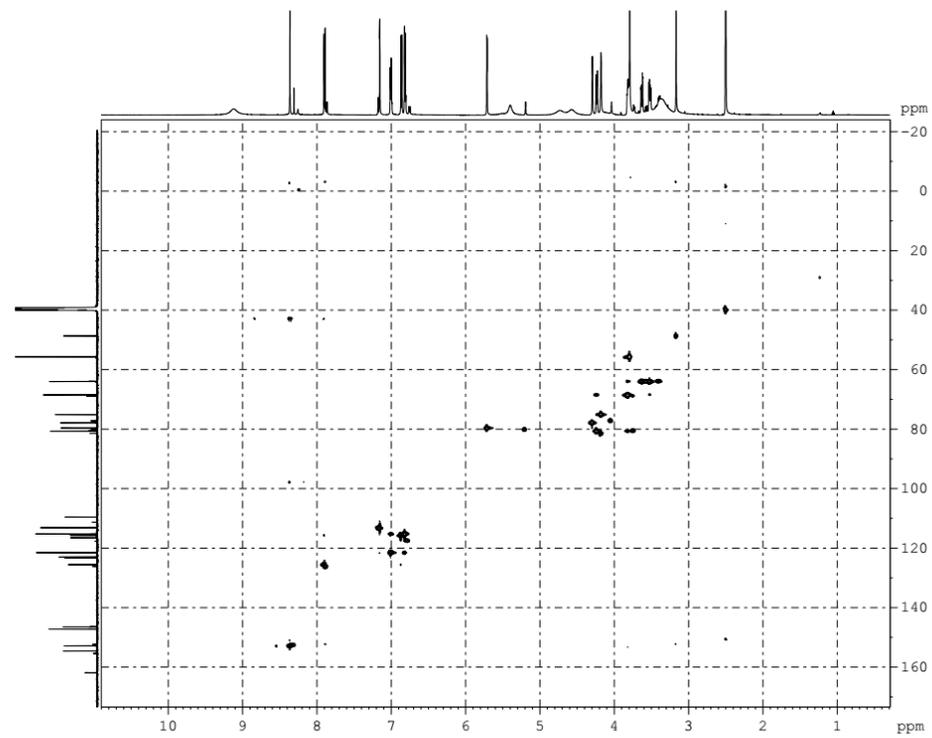
**Figure S7**  $^1\text{H-NMR}$  Spectrum of **1** in DMSO (600MHz)



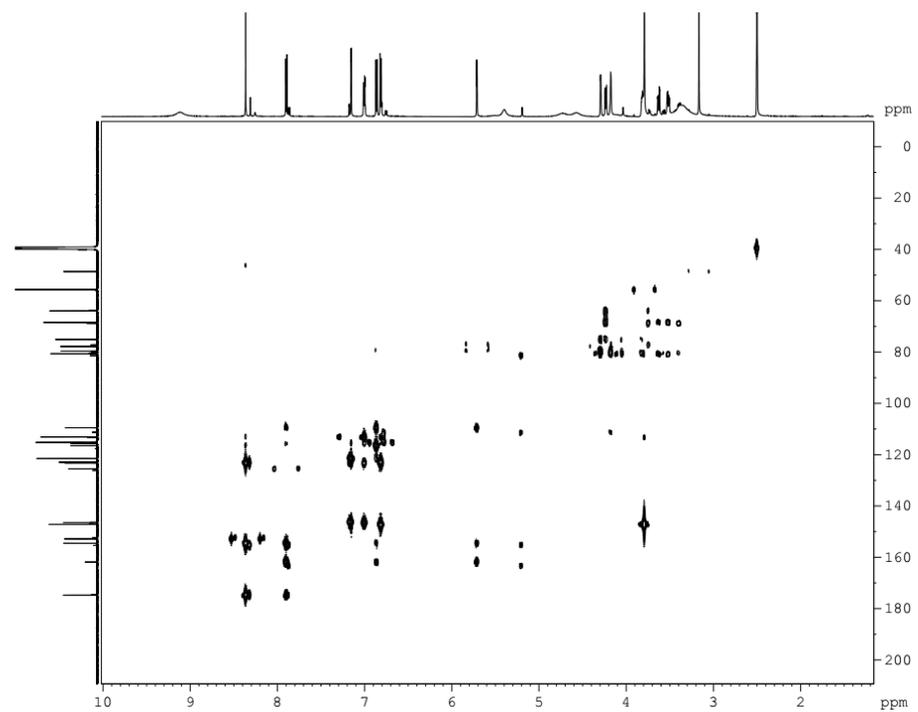
**Figure S8**  $^{13}\text{C}$ -NMR Spectrum of **1** in DMSO (150MHz)



**Figure S9** HSQC Spectrum of **1** in DMSO



**Figure S10** HMBC Spectrum of **1** in DMSO



**Figure S11** NOESY Spectrum of **1** in DMSO

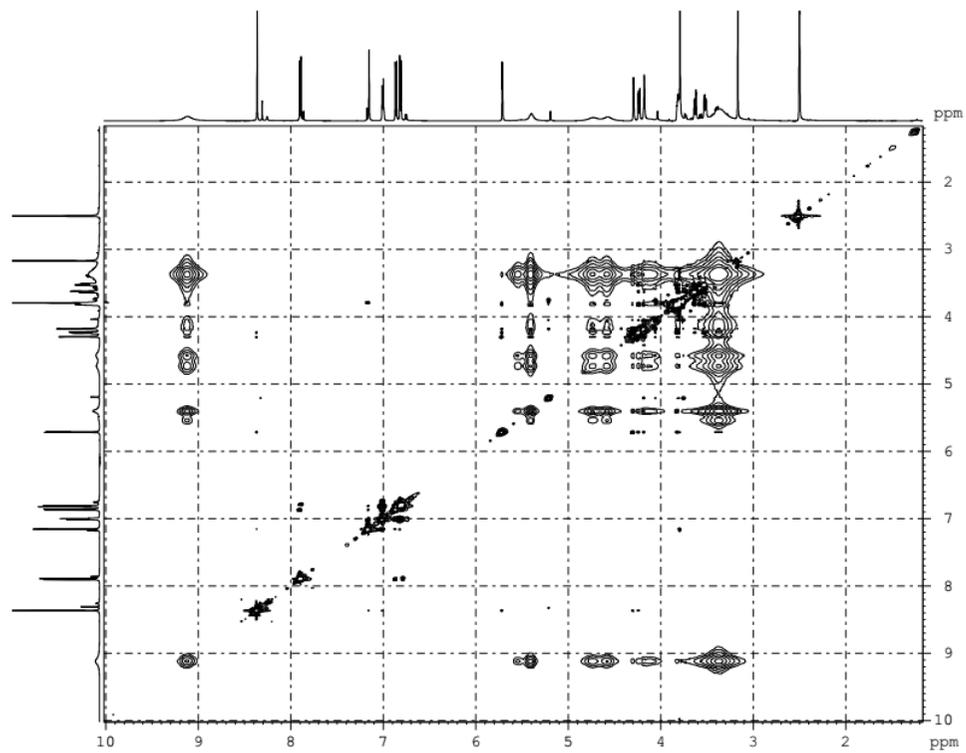


Figure S12 HR-ESIMS of 2

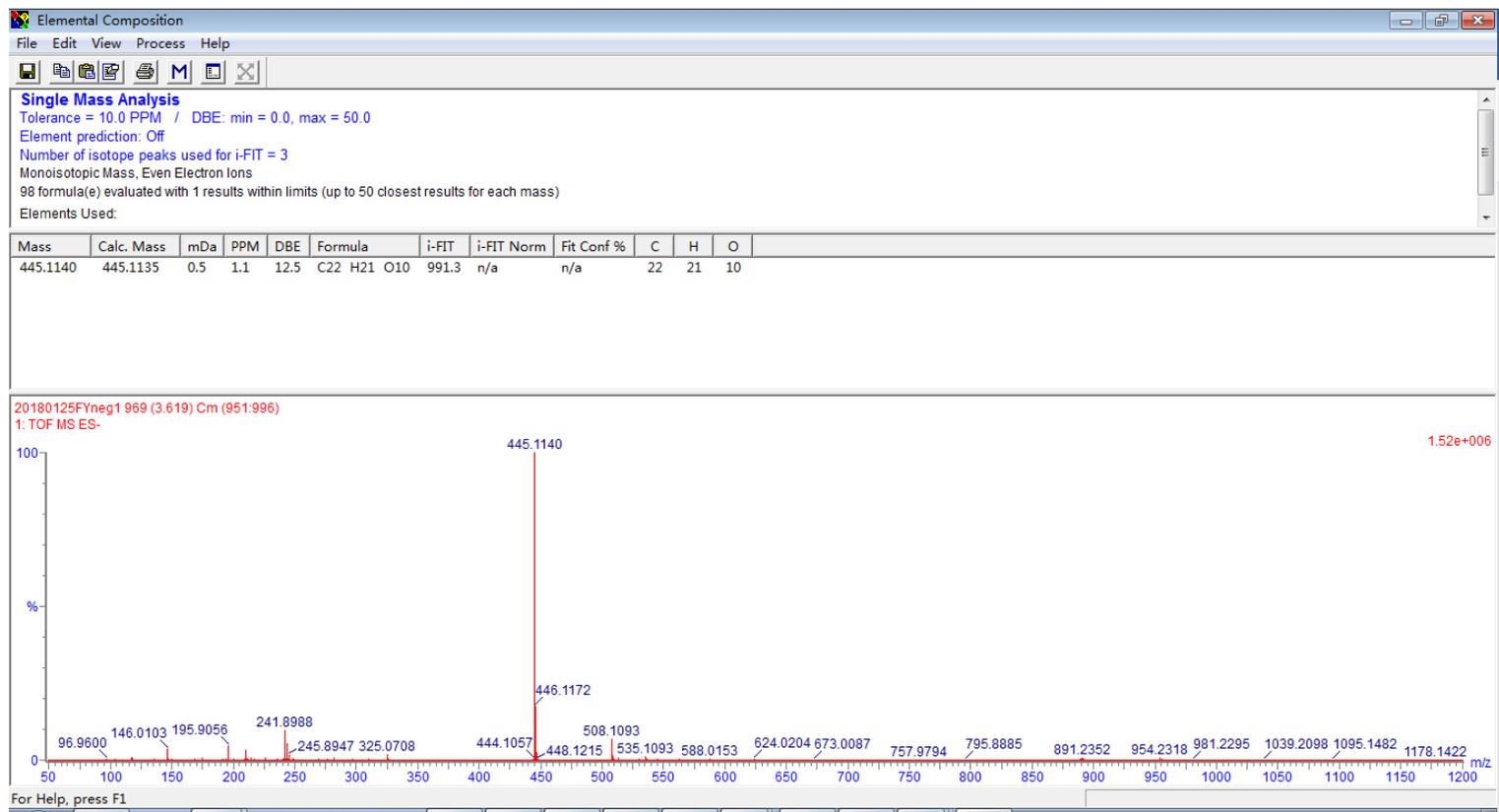
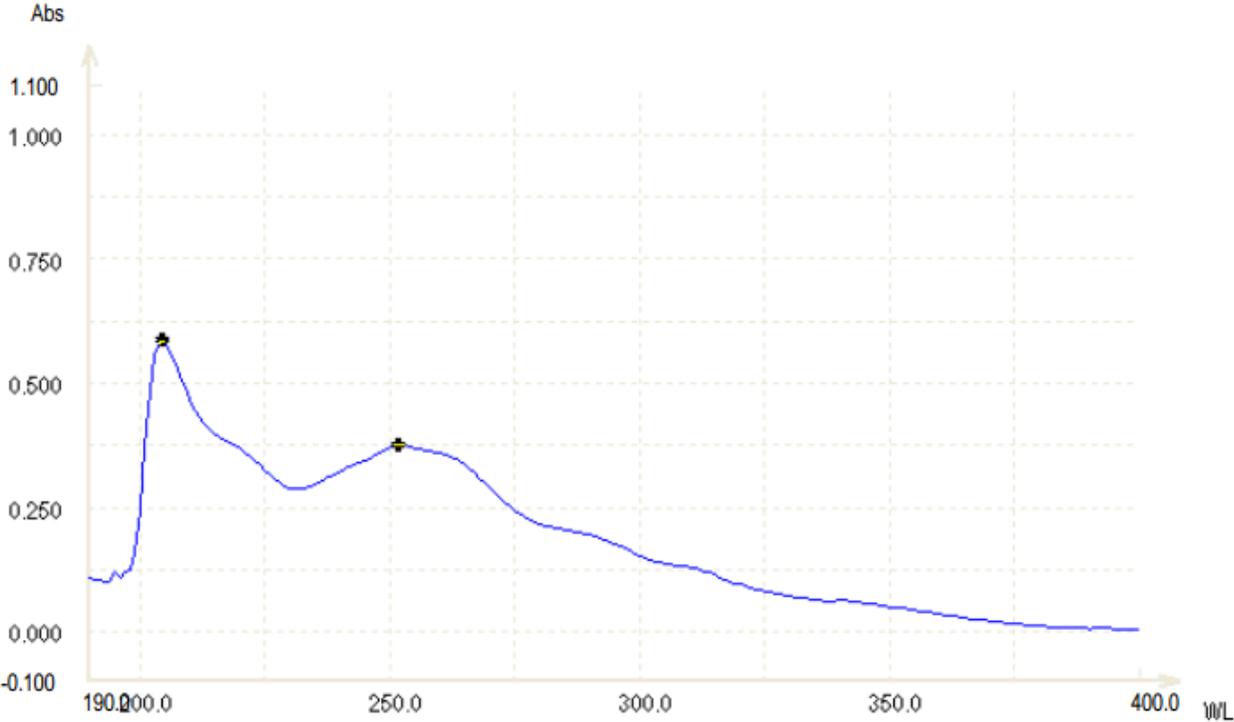
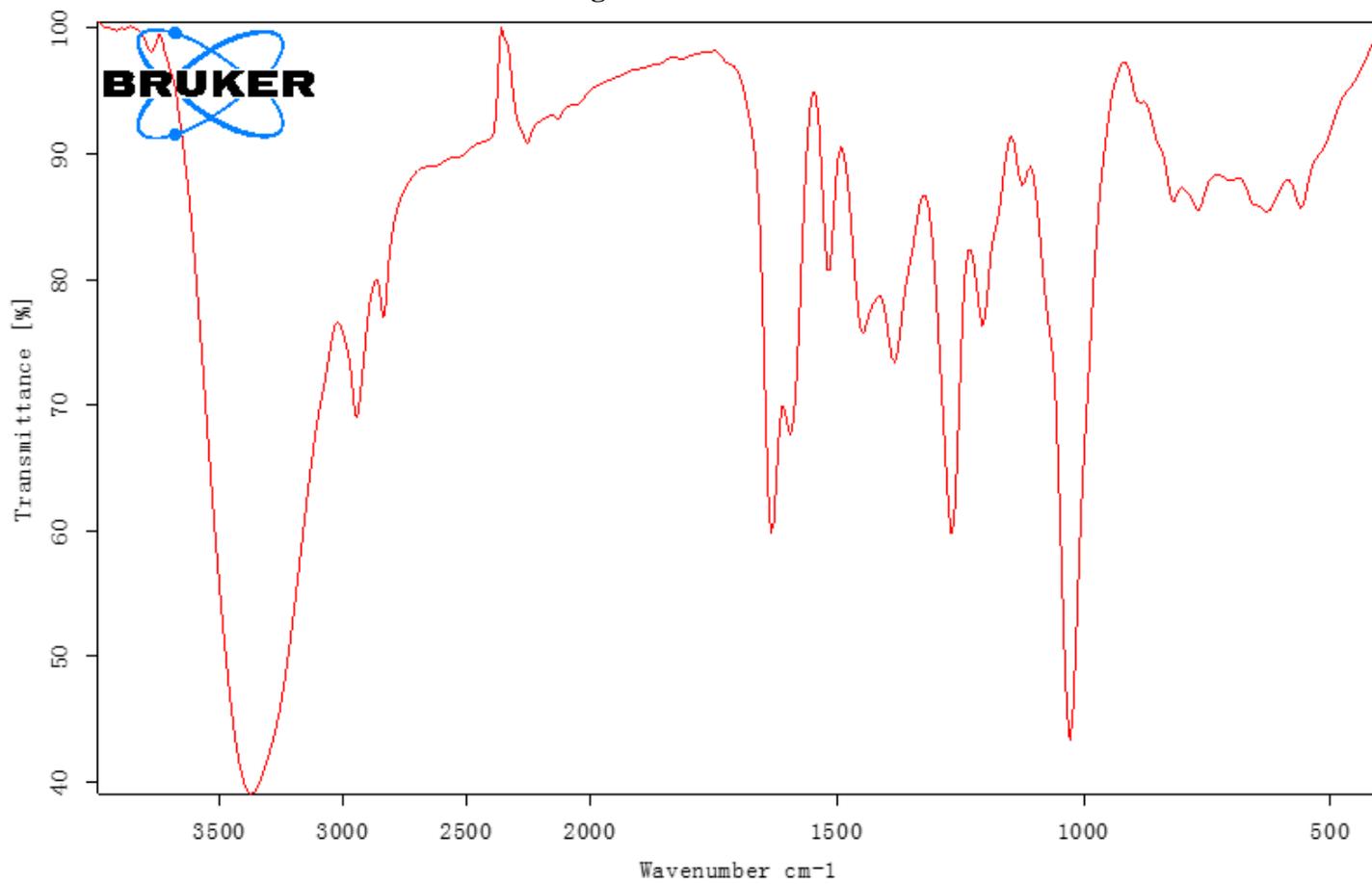


Figure S13 UV of 2 (MeOH)

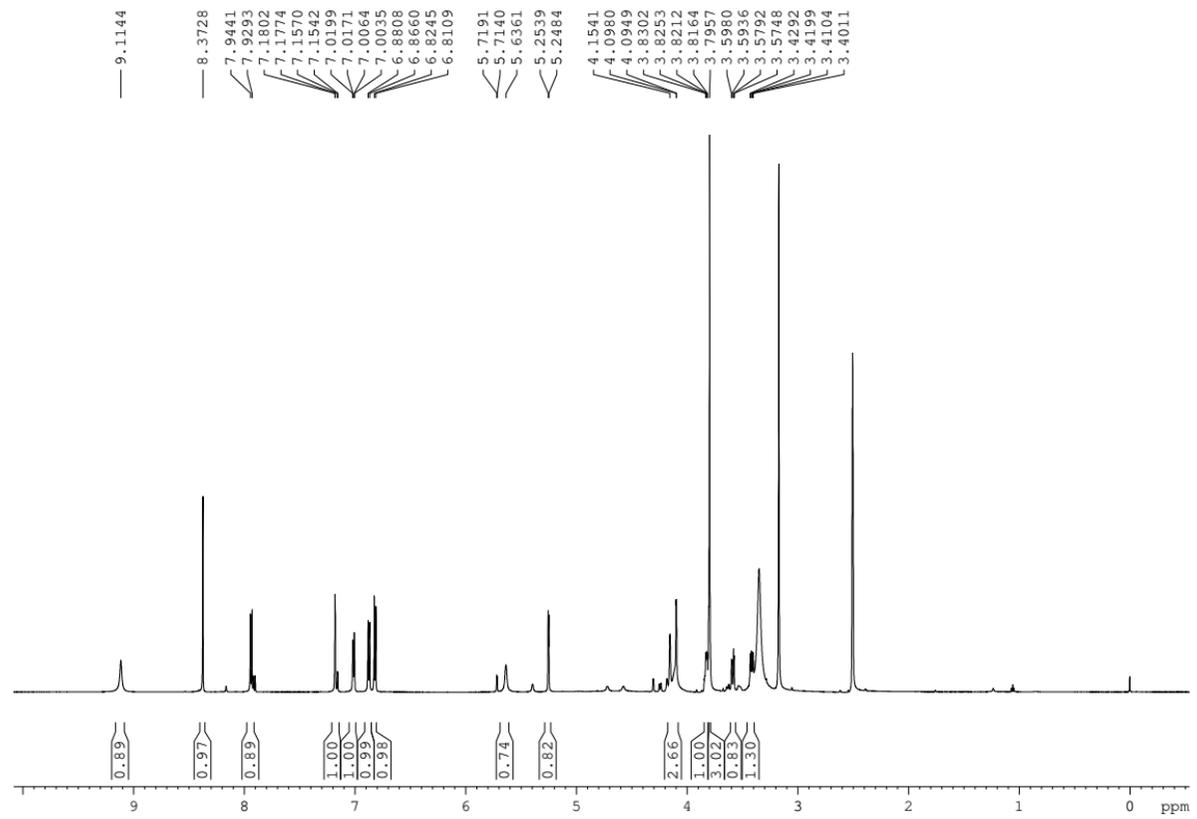


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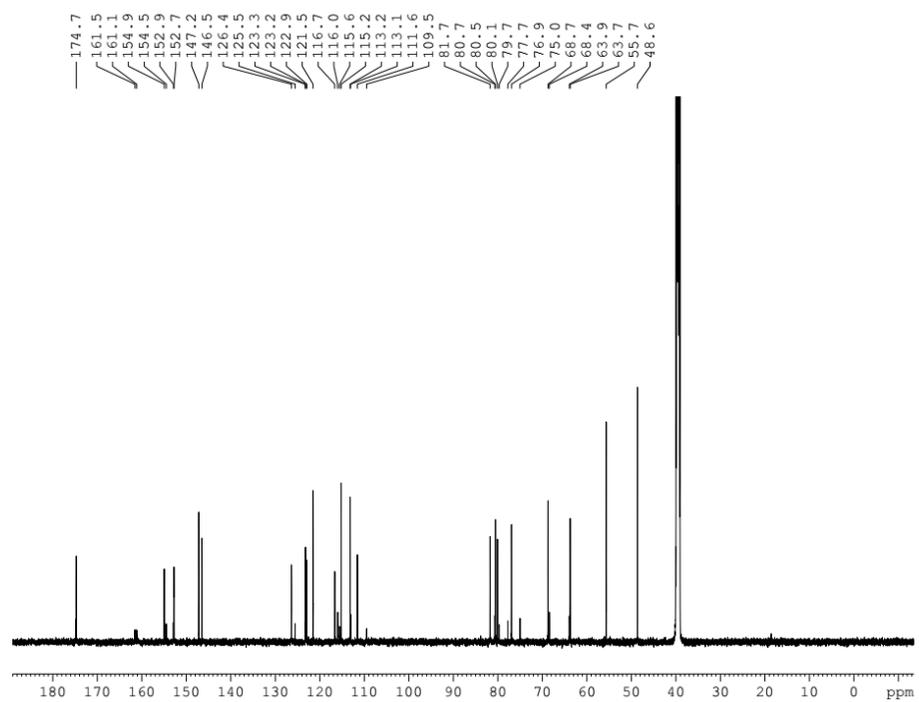
Figure S14 IR of 2



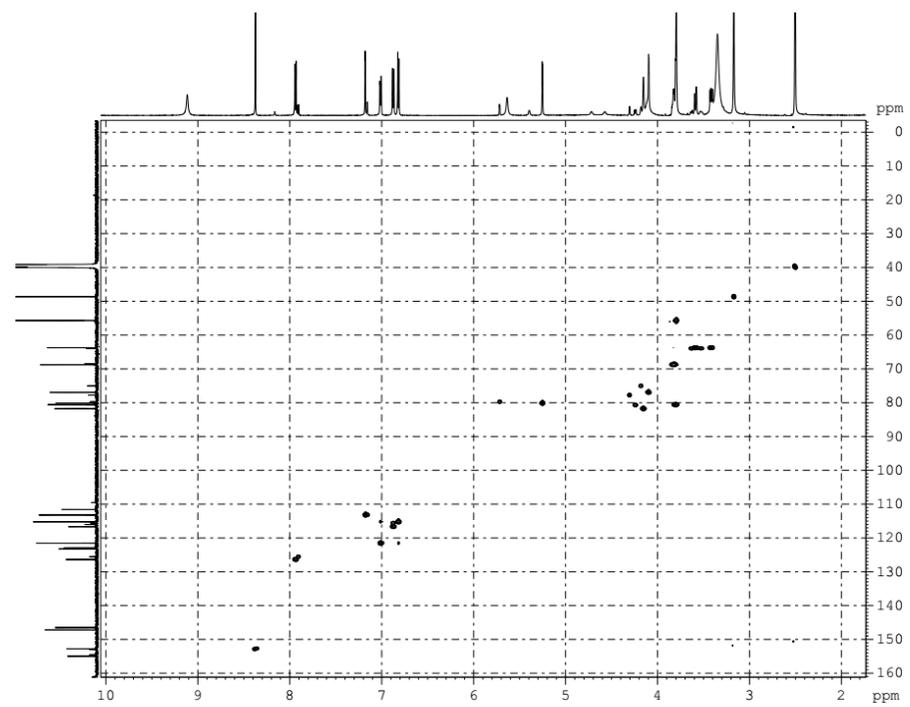
**Figure S15**  $^1\text{H-NMR}$  Spectrum of **2** in DMSO (600MHz)



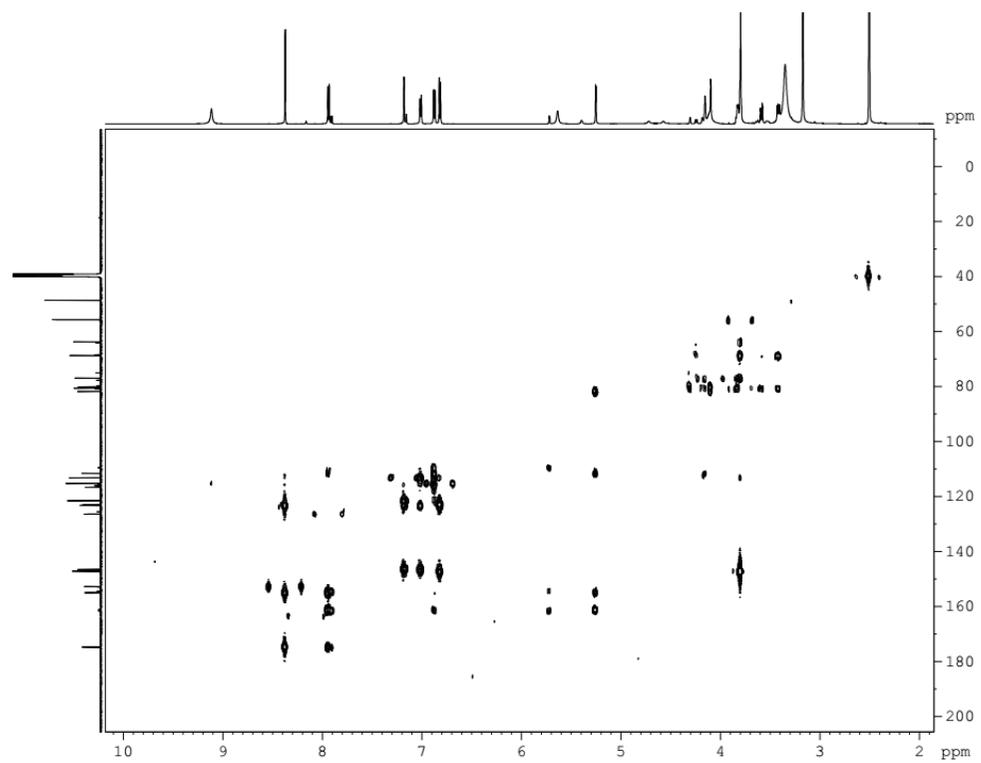
**Figure S16**  $^{13}\text{C}$ -NMR Spectrum of **2** in DMSO (150MHz)



**Figure S17** HSQC Spectrum of **2** in DMSO



**Figure S18** HMBC Spectrum of **2** in DMSO



**Figure S19** NOESY Spectrum of **2** in DMSO

