

## Ring Transformation of Chromone-3-Carboxamide under Nucleophilic Conditions

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**Chromeno[4,3-*c*]pyrazol-4(1*H*)-one (**6**):** IR (KBr)  $\nu/\text{cm}^{-1}$  3217 (NH), 3054 (CH<sub>arom</sub>), 1735 (OC=O) and 1603 (C=N); <sup>1</sup>H NMR (200 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  7.61 (t, 1H, *J* 7.6 Hz, H-8), 7.79 (d, 1H, *J* 8.2 Hz, H-6), 7.93 (t, 1H, *J* 7.6 Hz, H-7), 8.16 (d, 1H, *J* 8.2 Hz, H-9), 9.12 (s, 1H, H-3), 13.23 ppm (bs, 1H, NH exchangeable with D<sub>2</sub>O).

**1-Phenylchromeno[4,3-*c*]pyrazol-4(1*H*)-one (**7**):** IR (KBr)  $\nu/\text{cm}^{-1}$  3117 (CH<sub>arom</sub>), 1751 (OC=O), 1614 (C=N), 1526 (C=C).

**Chromeno[3,4-*d*]isoxazol-4(4*H*)-one (**10**):** IR (KBr)  $\nu/\text{cm}^{-1}$  3037 (CH<sub>arom</sub>), 1728 (OC=O), 1621 (C=N), 1591 (C=C); <sup>1</sup>H NMR (300 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  7.37-7.56 (m, 2H, Ar-H), 7.65 (d, 1H, *J* 6.6 Hz, Ar-H), 7.87 7.65 (d, 1H, *J* 6.9 Hz, Ar-H), 8.88 (s, 1H, H-3<sub>isoxazole</sub>).

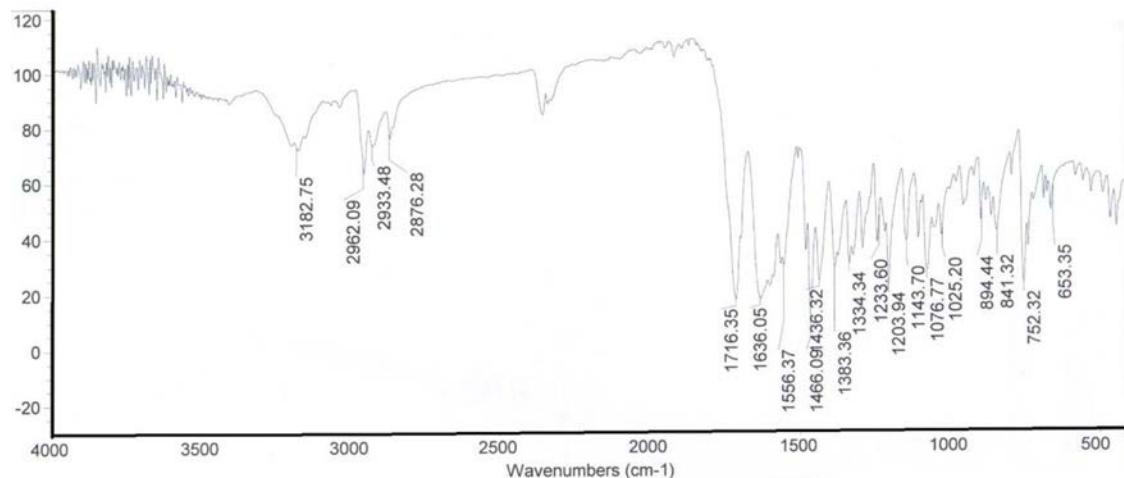
**3-(1,3-Benzothiazol-2-yl)-4-hydroxycoumarin (**17**):** obtained after cooling as yellow crystals, recrystallized

from ethanol; mp 281-282 °C (279-282 °C);<sup>1</sup> yield (0.32 g, 36%); IR (KBr)  $\nu/\text{cm}^{-1}$  3334 (OH), 3064 (CH<sub>arom</sub>), 1667 (OC=O), 1618 (C=N), 1604 (C=C); <sup>1</sup>H NMR (300 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  6.86 (d, 1H, Ar-H), 7.00 (t, 1H, Ar-H), 7.27-7.44 (m, 2H, Ar-H), 7.58-7.63 (m, 2H, Ar-H), 7.94 (d, 1H, H-8), 8.13 (d, 1H, *J* 6.6 Hz, Ar-H), 9.01 (bs, 1H, OH exchangeable with D<sub>2</sub>O).

**4-Hydroxy-3-[(1*E*)-3-oxo-3-phenylprop-1-en-1-yl]-2*H*-chromen-2-one (**21**):** IR (KBr)  $\nu/\text{cm}^{-1}$  3081 (CH<sub>arom</sub>), 1714 (OC=O), 1654 (C=O), 1607 (C=C); <sup>1</sup>H NMR (200 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  8.11-8.49 (m, 7H, Ar-H), 8.62 (d, 1H, *J* 8.6 Hz, Ar-H), 8.73 (d, 1H, *J* 8.0 Hz, Ar-H), 8.97 (d, 1H, *J* 15.2 Hz, CH<sub>olefinic</sub>), 9.50 (d, 1H, *J* 14.8 Hz, CH<sub>olefinic</sub>), 12.97 (bs, 1H, OH exchangeable with D<sub>2</sub>O).

## Reference

- Djudjic, R.; Trkovnik, M.; *Monatsh. Chem.* **1991**, 122, 77.



**Figure S1.** IR spectrum of compound 2.

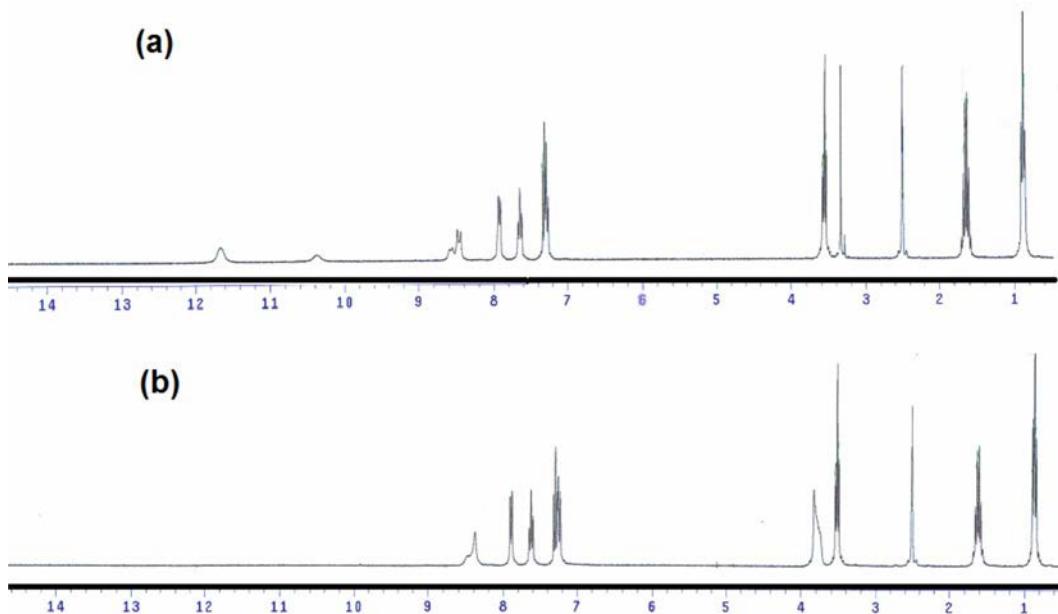


Figure S2. <sup>1</sup>H NMR spectrum of compound 2 in DMSO-*d*<sub>6</sub> (a) and DMSO-D<sub>2</sub>O (b).

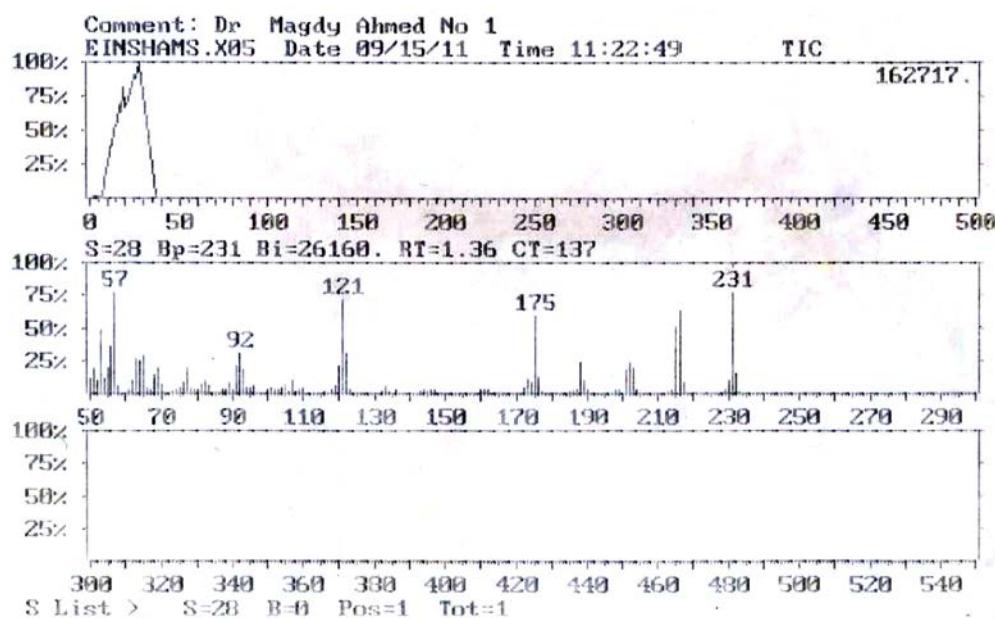
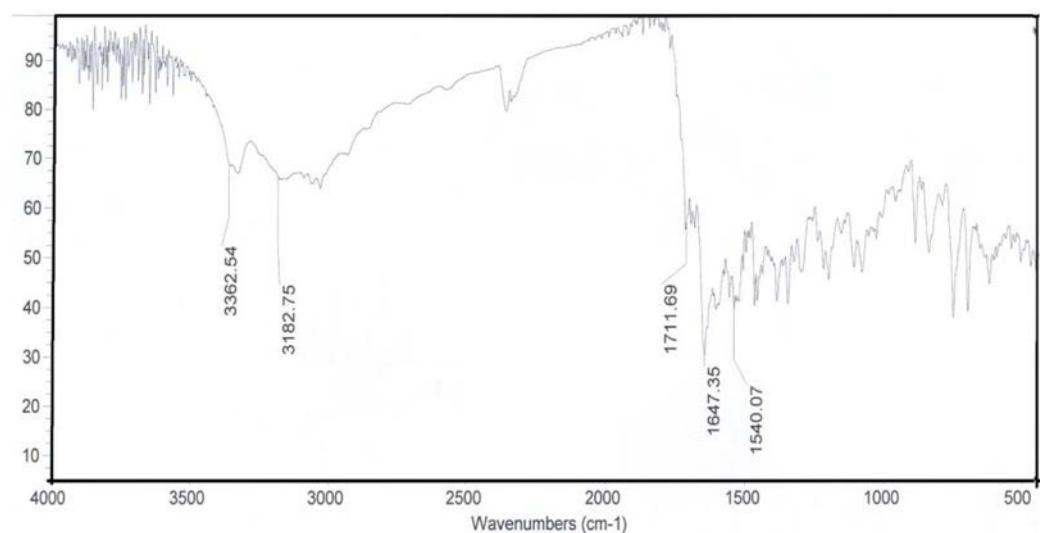
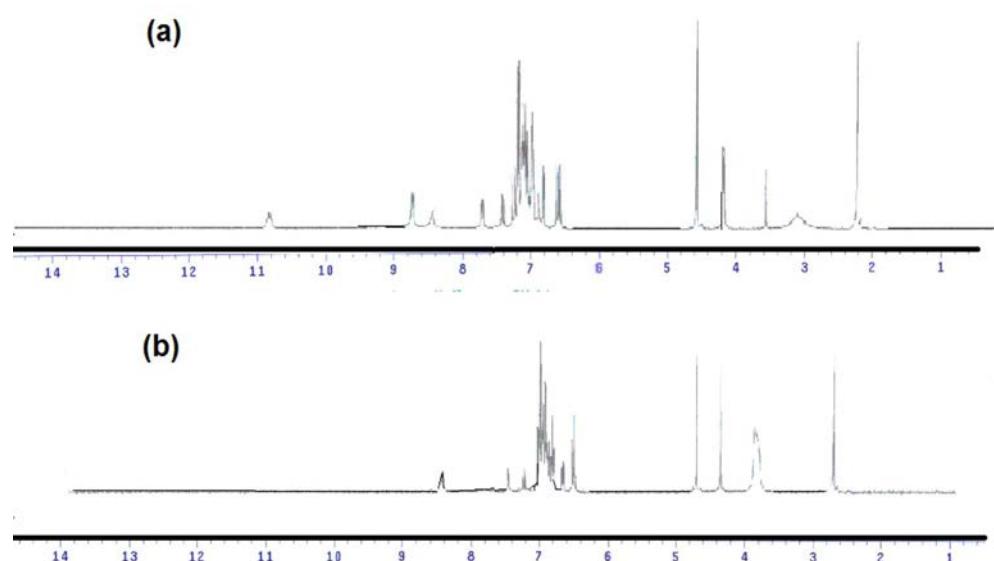


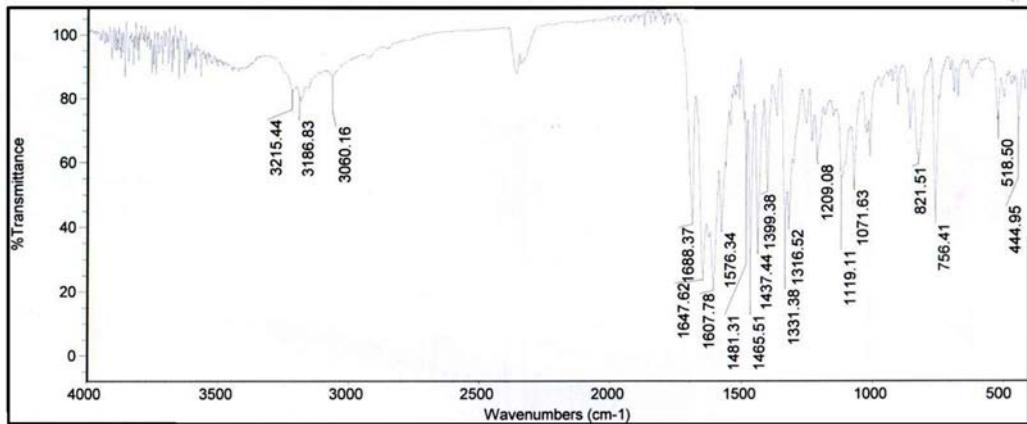
Figure S3. Mass spectrum of compound 2.



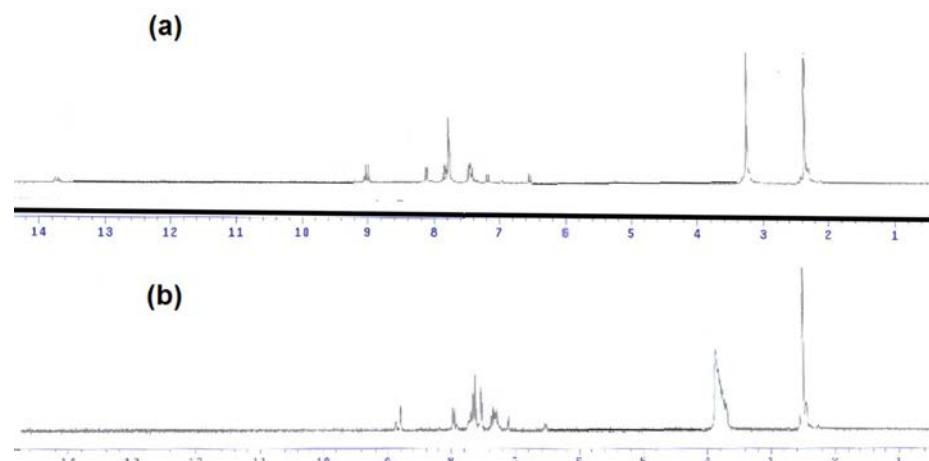
**Figure S4.** IR spectrum of compound 3.



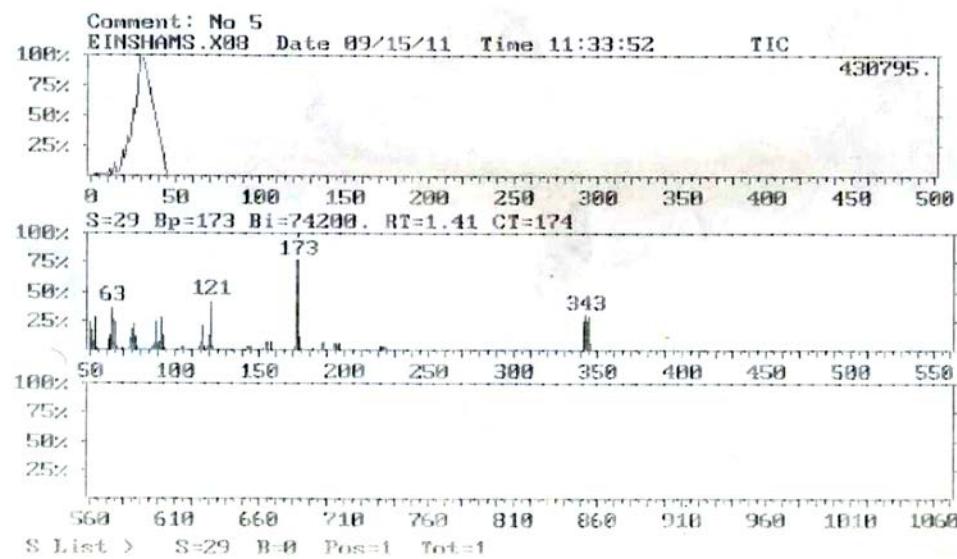
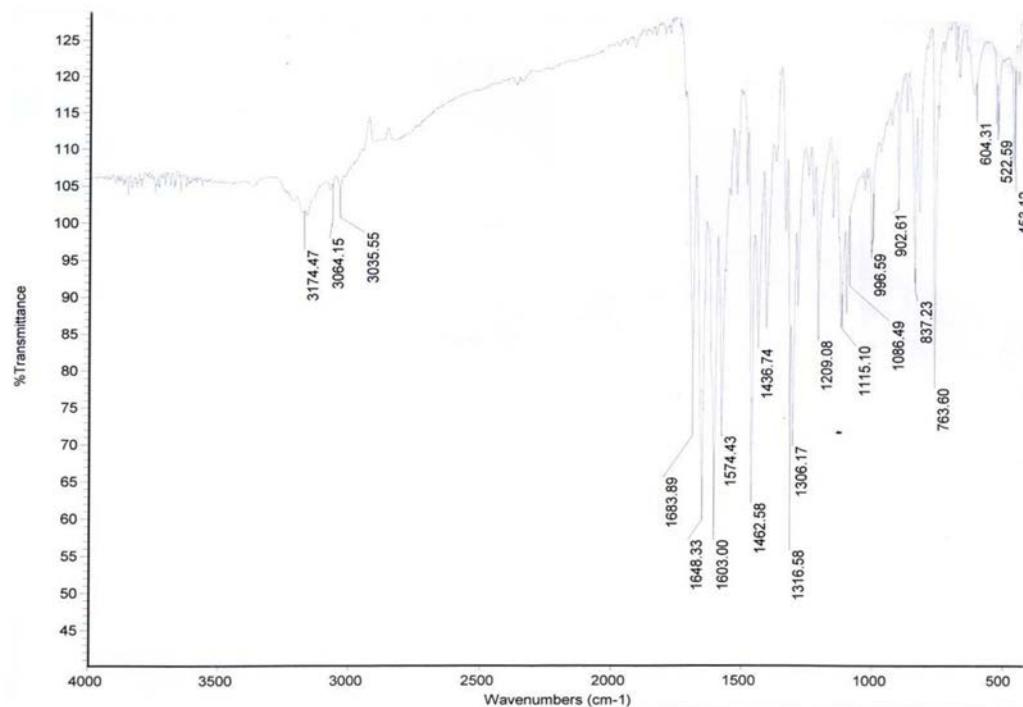
**Figure S5.** <sup>1</sup>H NMR spectra of compound 3 in DMSO-*d*<sub>6</sub> (a) and DMSO-D<sub>2</sub>O (b).

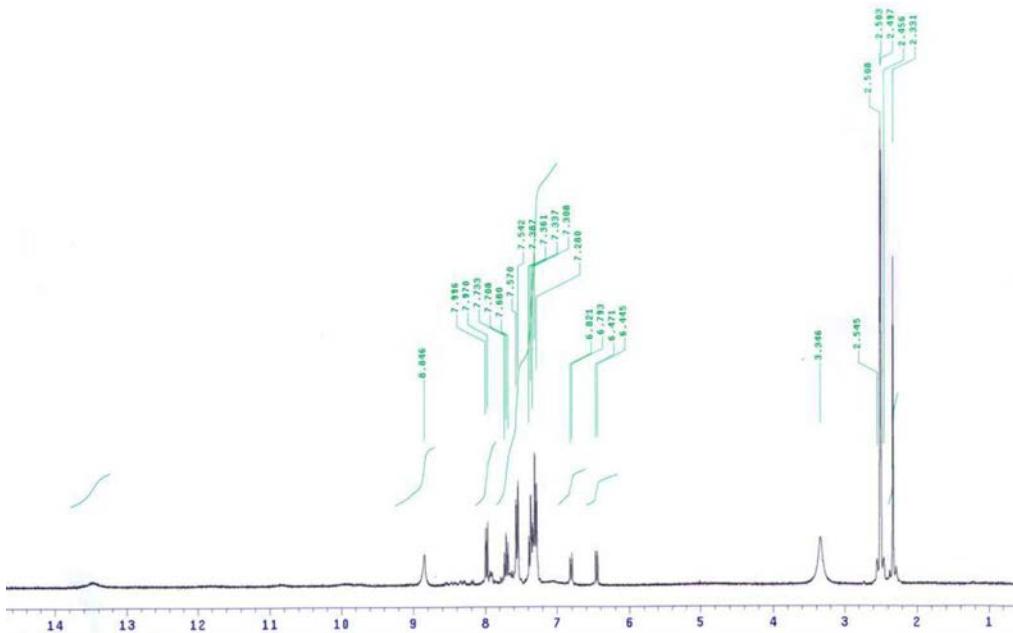


**Figure S6.** IR spectrum of compound **4**.

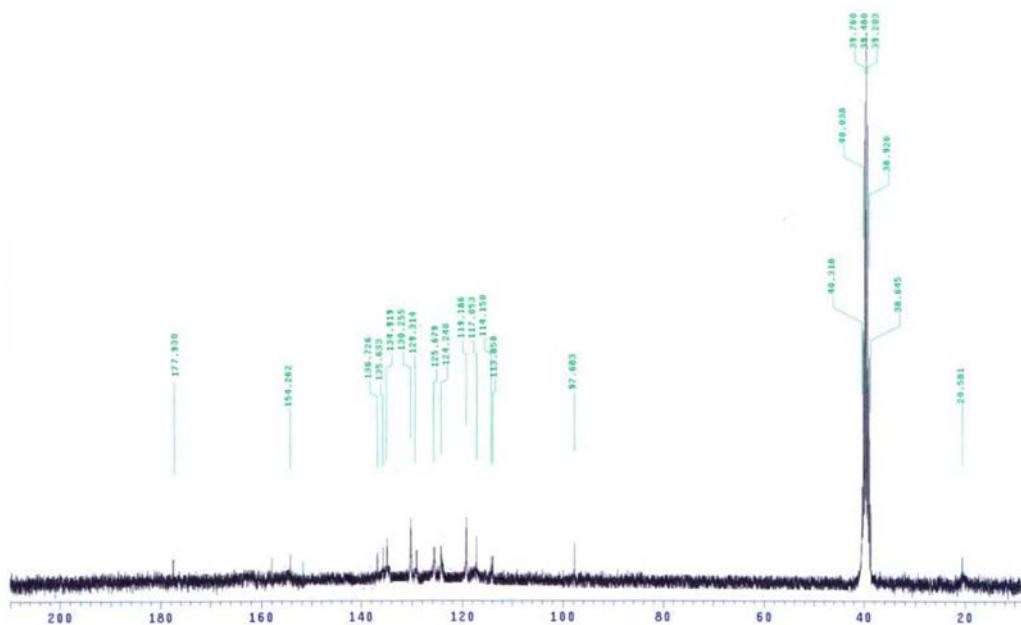


**Figure S7.**  $^1\text{H}$  NMR spectrum of compound **4** in  $\text{DMSO}-d_6$  (a) and  $\text{DMSO-D}_2\text{O}$  (b).

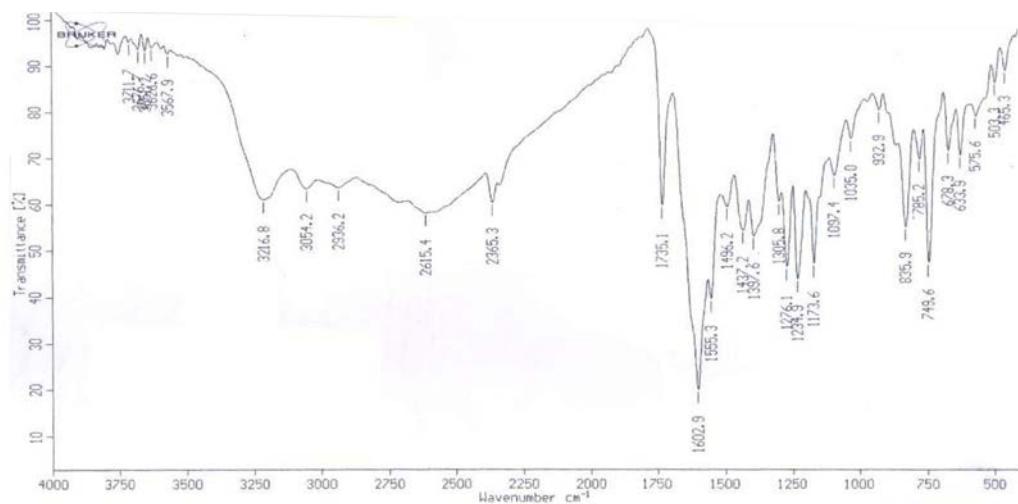
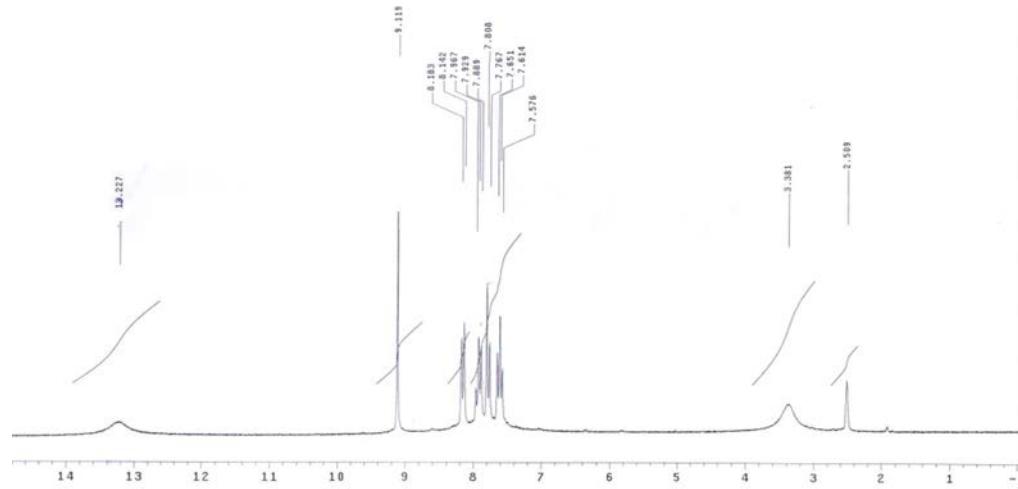
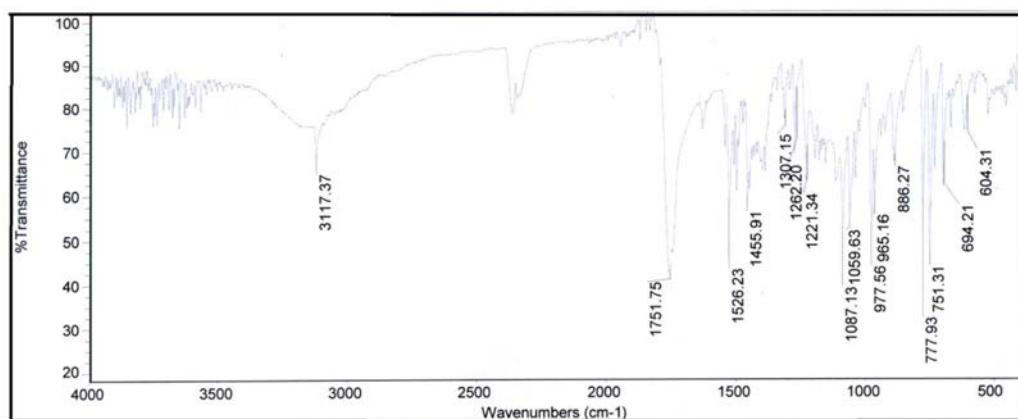
**Figure S8.** Mass spectrum of compound 4.**Figure S9.** IR spectrum of compound 5.

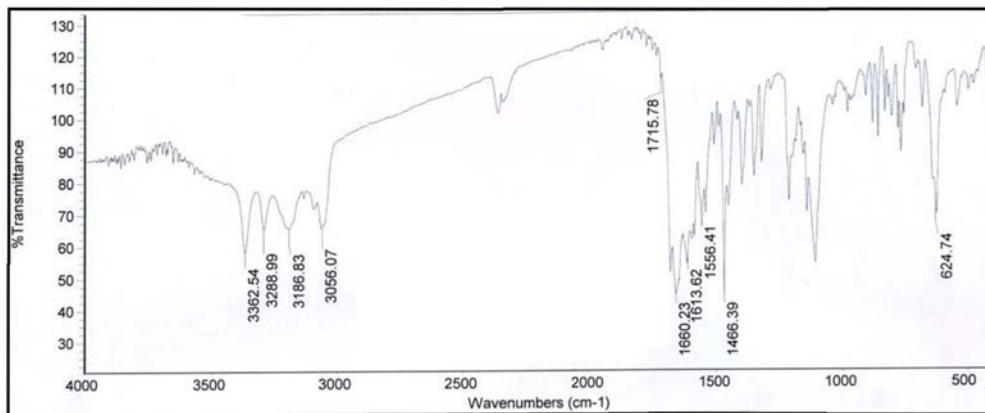


**Figure S10.**  $^1\text{H}$  NMR spectrum of compound **5** in  $\text{DMSO}-d_6$ .

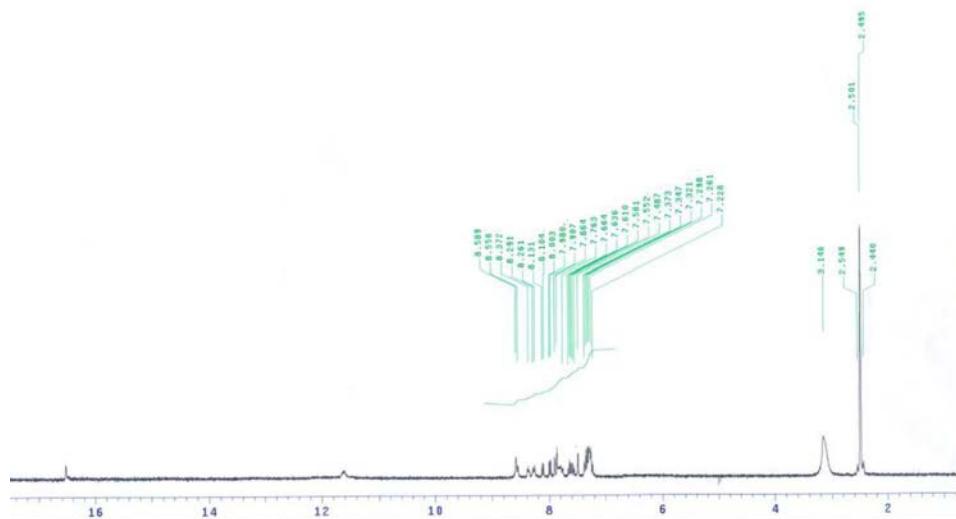


**Figure S11.**  $^{13}\text{C}$  NMR spectrum of compound **5** in  $\text{DMSO}-d_6$ .

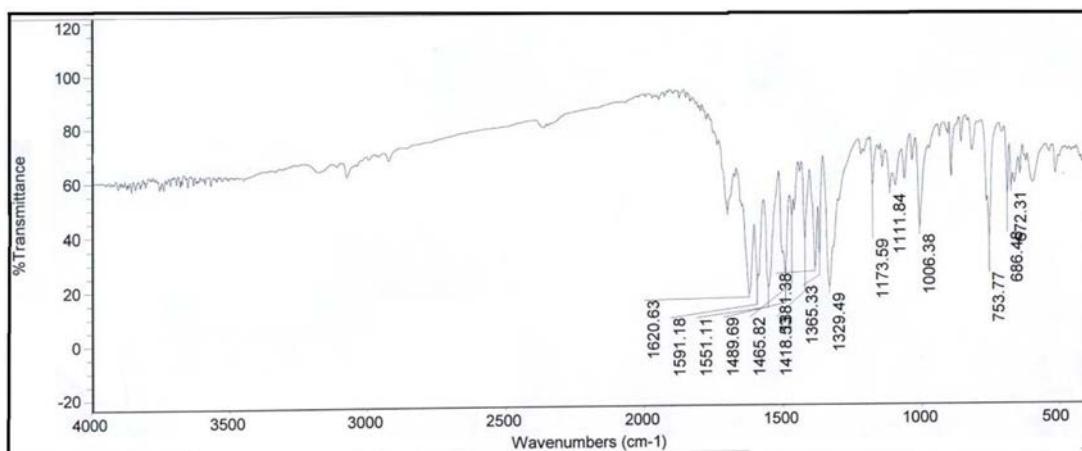
**Figure S12.** IR spectrum of compound 6.**Figure S13.**  $^1\text{H}$  NMR spectrum of compound 6 in  $\text{DMSO}-d_6$ .**Figure S14.** IR spectrum of compound 7.



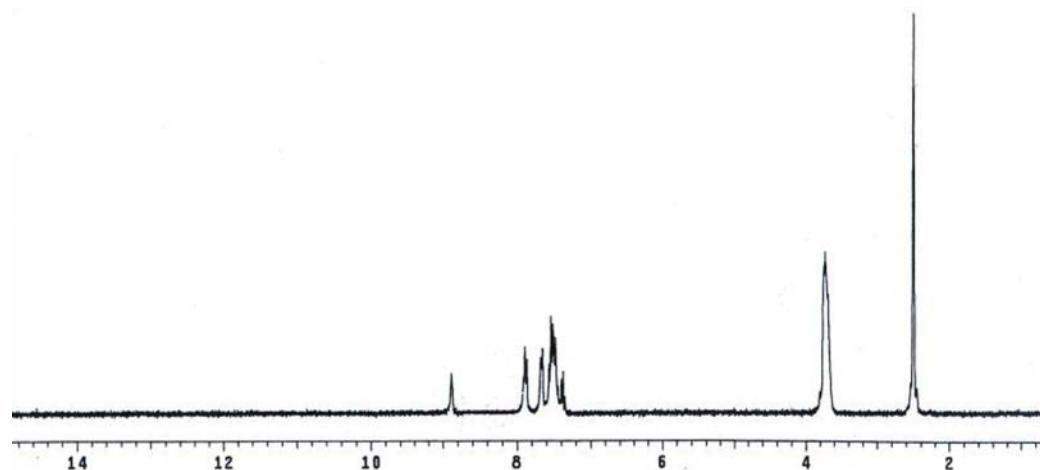
**Figure S15.** IR spectrum of compound **9**.



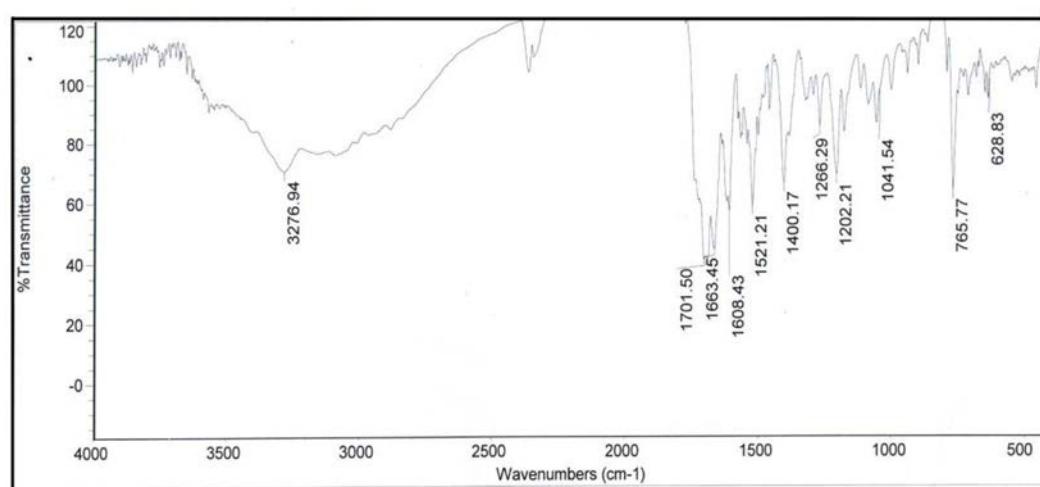
**Figure S16.** <sup>1</sup>H NMR spectrum of compound **9** in DMSO-*d*<sub>6</sub>.



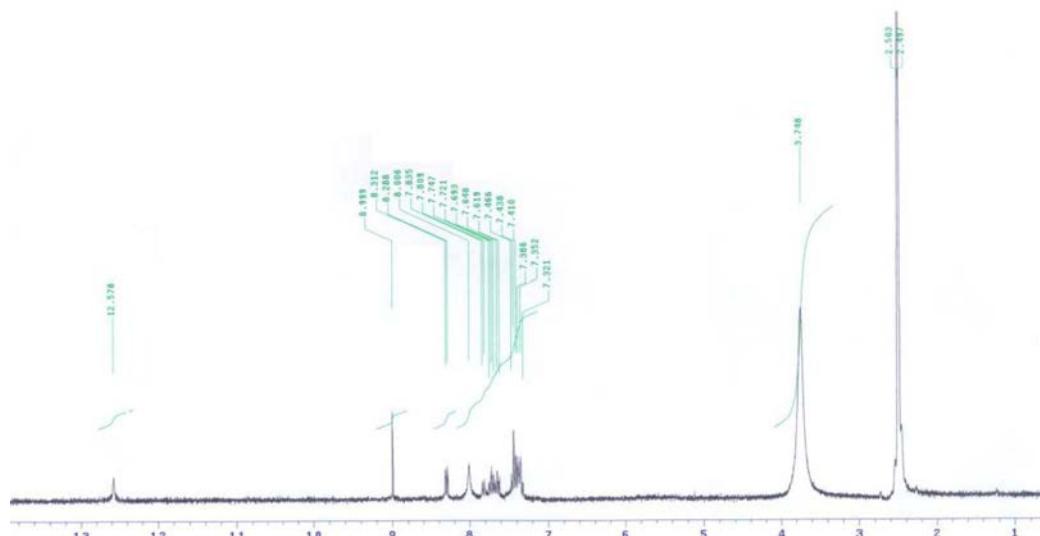
**Figure S17.** IR spectrum of compound **10**.



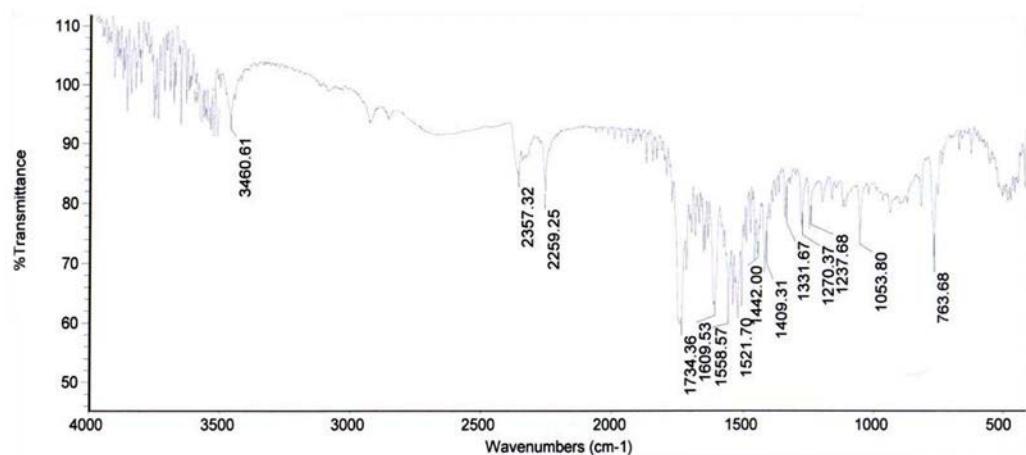
**Figure S18.**  $^1\text{H}$  NMR spectrum of compound **10** in  $\text{DMSO}-d_6$ .



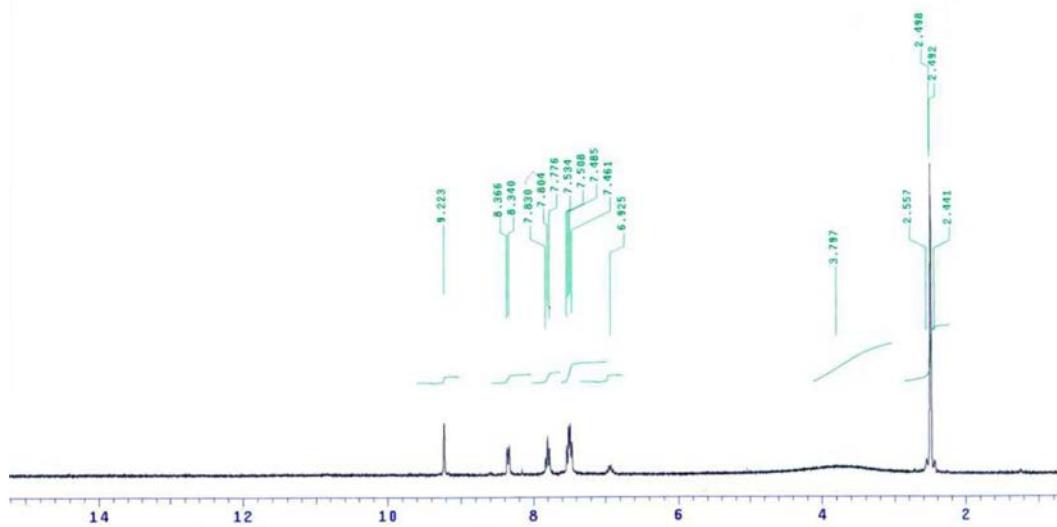
**Figure S19.** IR spectrum of compound **11**.



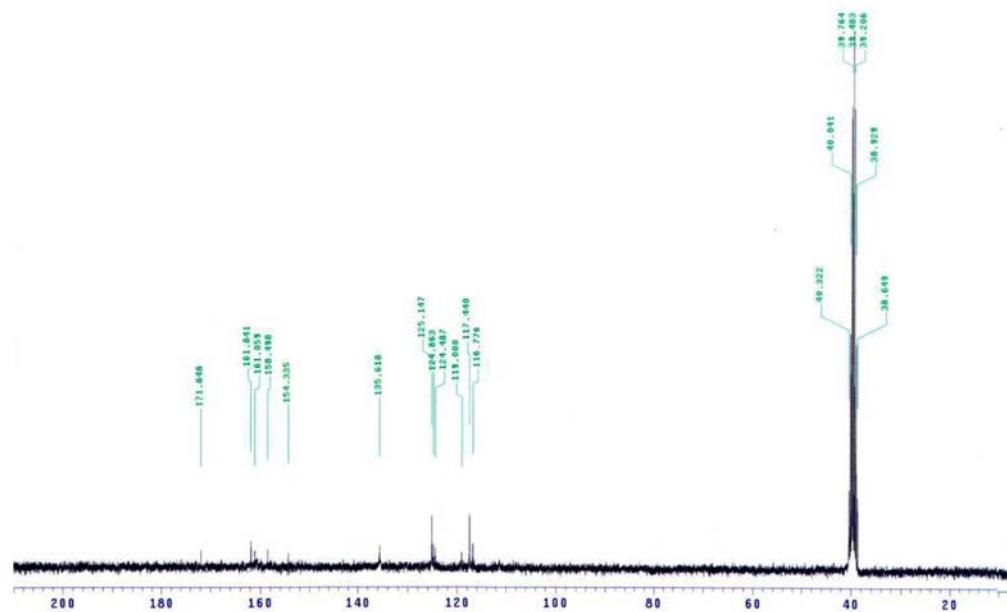
**Figure S20.**  $^1\text{H}$  NMR spectrum of compound **11** in  $\text{DMSO}-d_6$ .



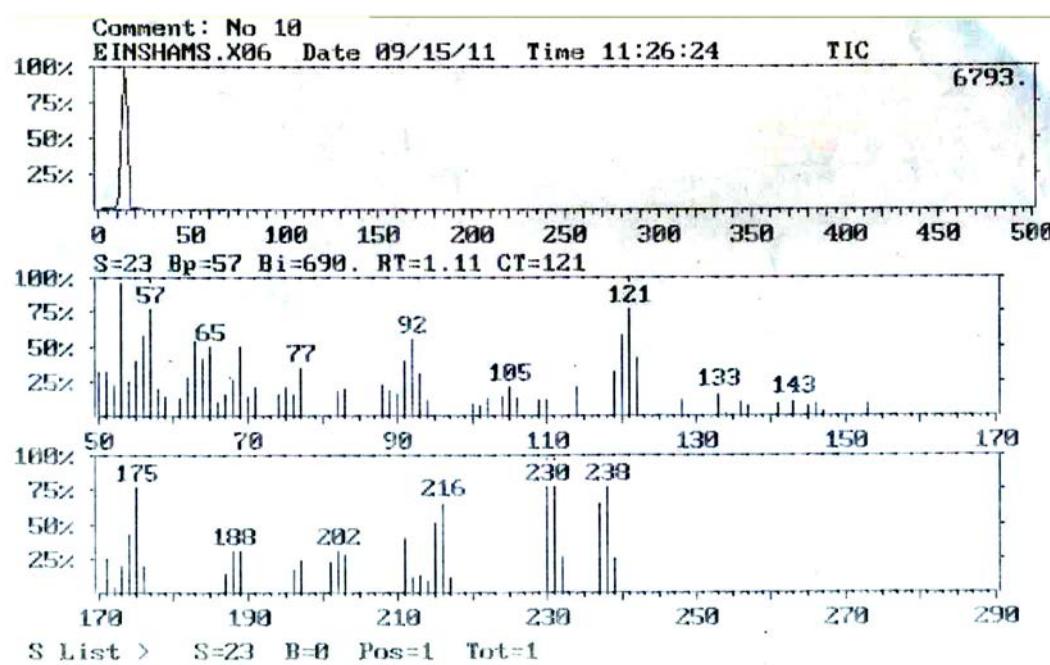
**Figure S21.** IR spectrum of compound **12**.



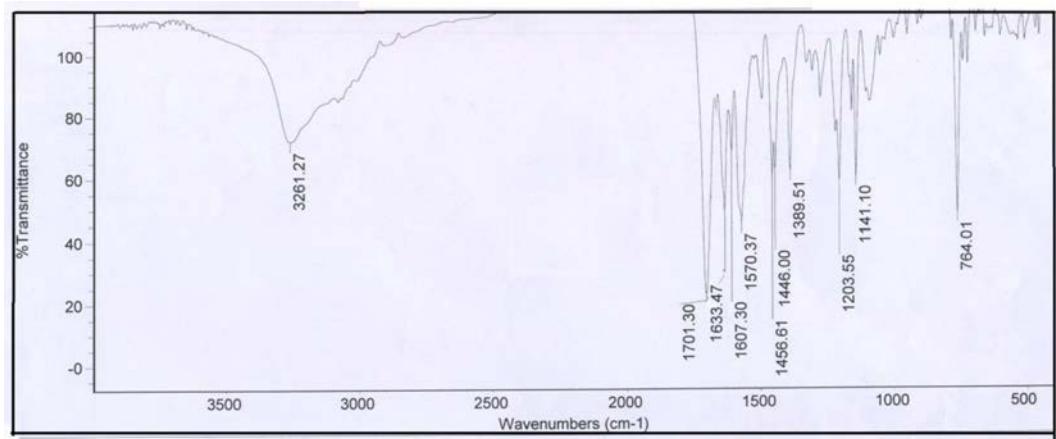
**Figure S22.** <sup>1</sup>H NMR spectrum of compound **12** in DMSO-*d*<sub>6</sub>.



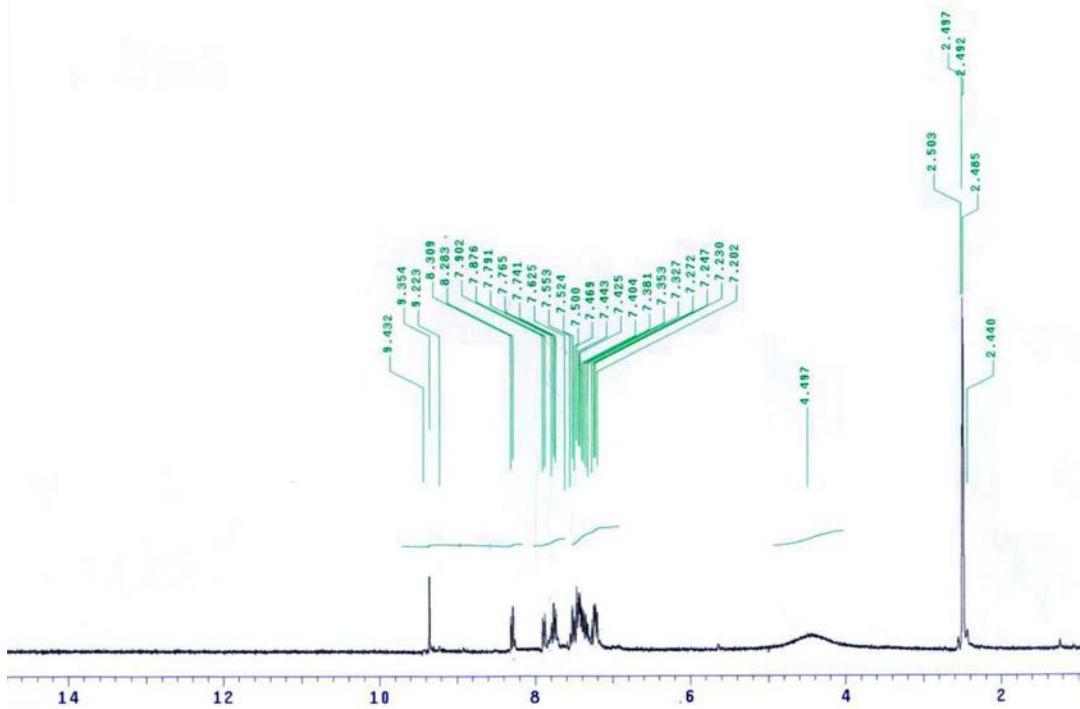
**Figure S23.**  $^{13}\text{C}$  NMR spectrum of compound **12** in  $\text{DMSO}-d_6$ .



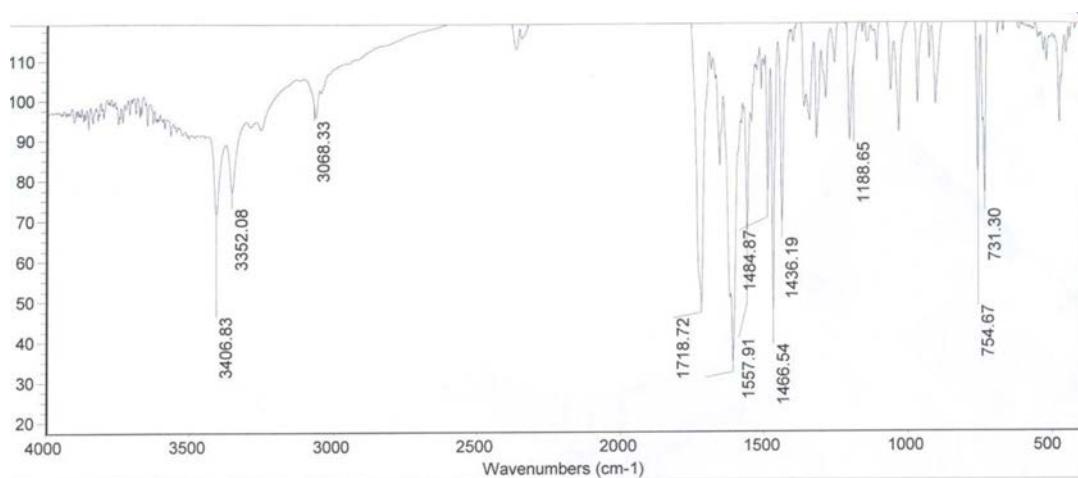
**Figure S24.** Mass spectrum of compound **12**.



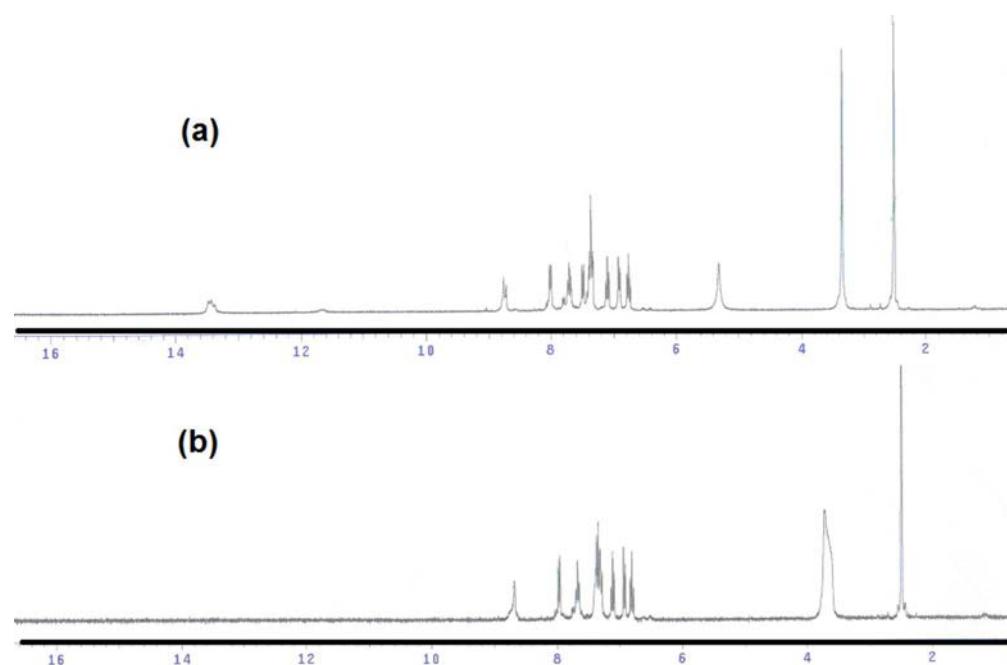
**Figure S25.** IR spectrum of compound **13**.



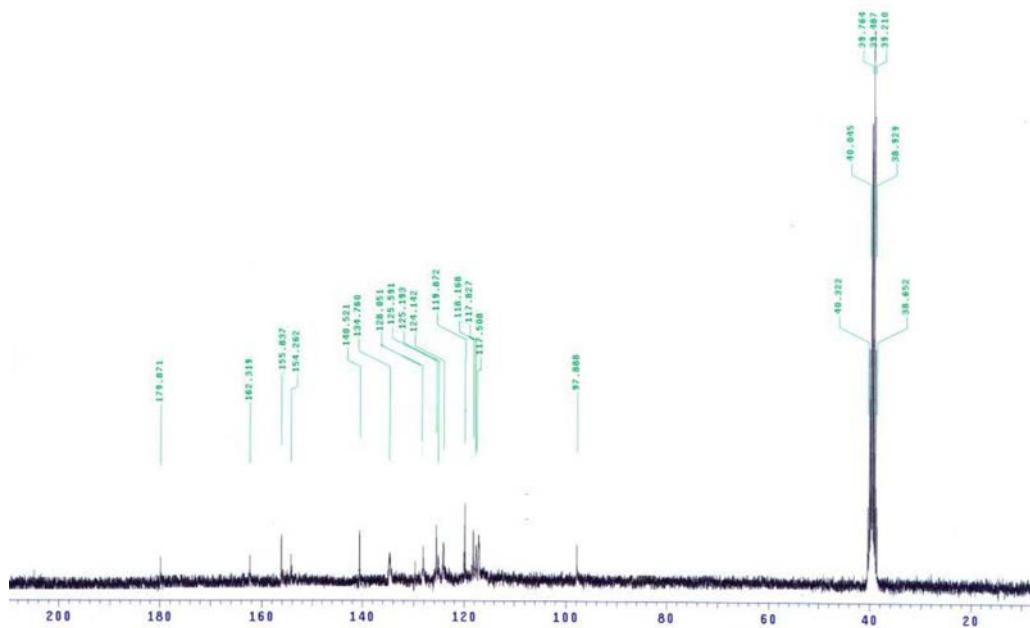
**Figure S26.** <sup>1</sup>H NMR spectrum of compound **13** in DMSO-*d*<sub>6</sub>.



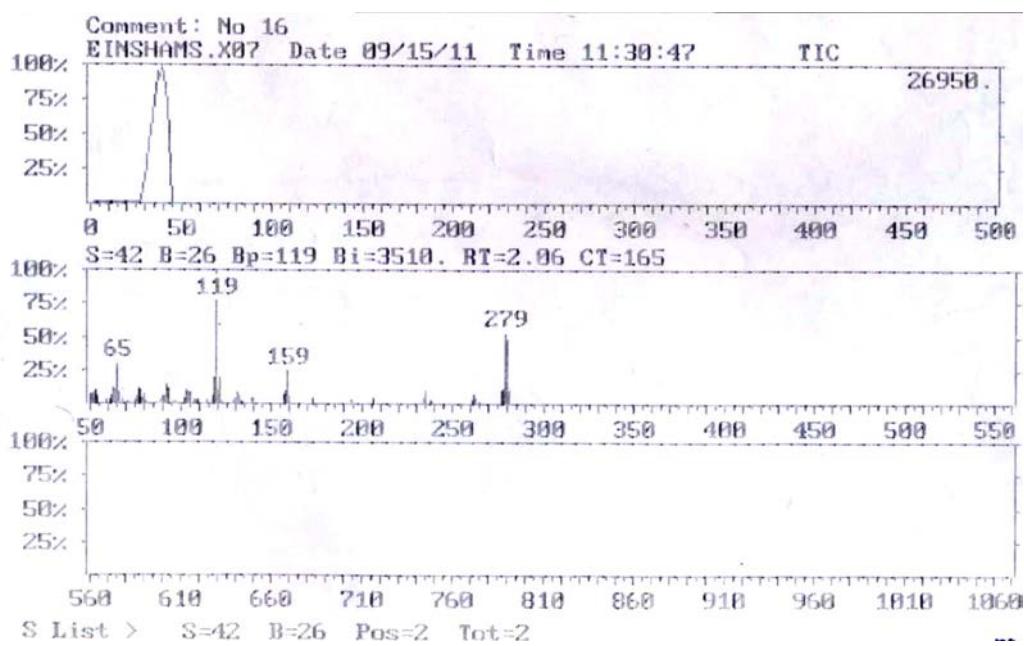
**Figure S27.** IR spectrum of compound **14**.



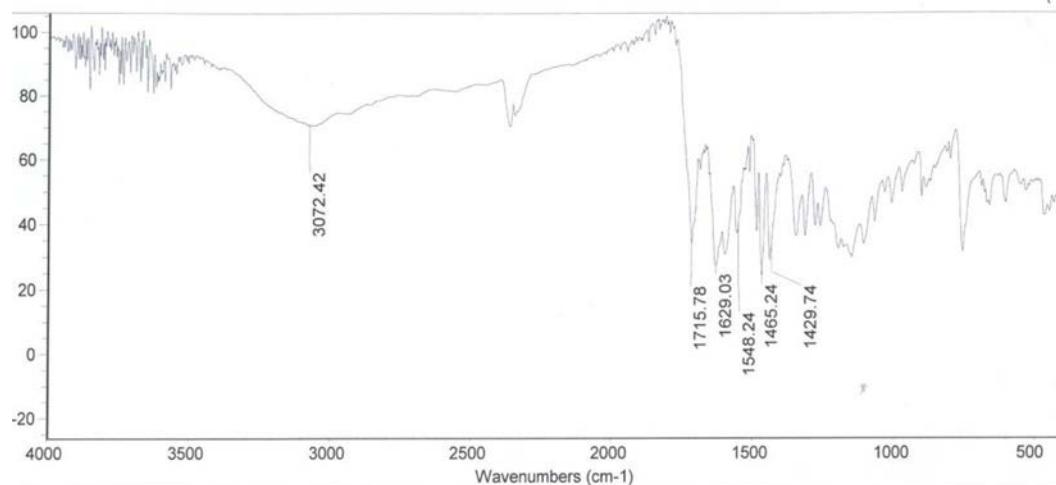
**Figure S28.** <sup>1</sup>H NMR spectra of compound **14** in DMSO-*d*<sub>6</sub> (a) and DMSO-D<sub>2</sub>O (b).



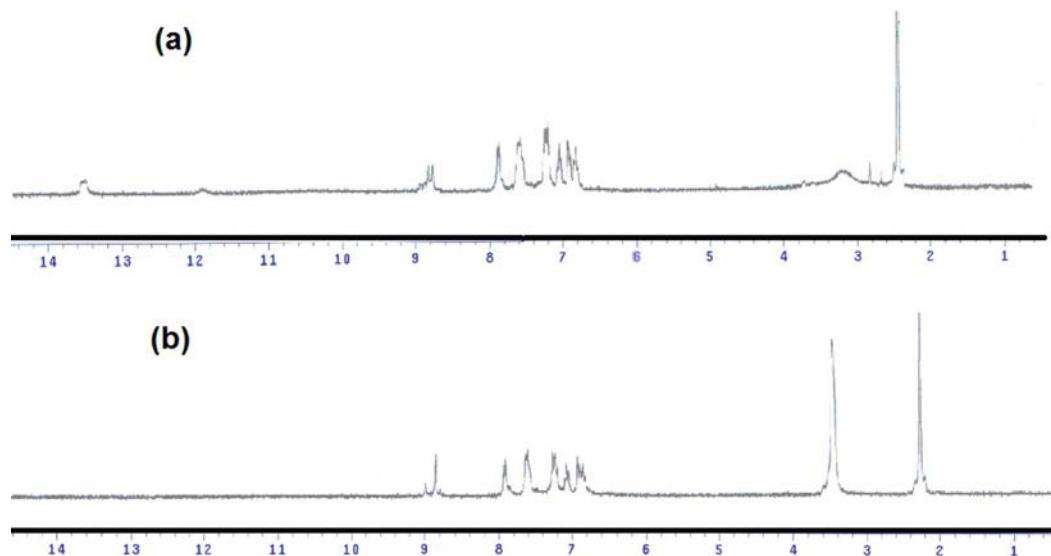
**Figure S29.**  $^{13}\text{C}$  NMR spectrum of compound **14** in  $\text{DMSO}-d_6$ .



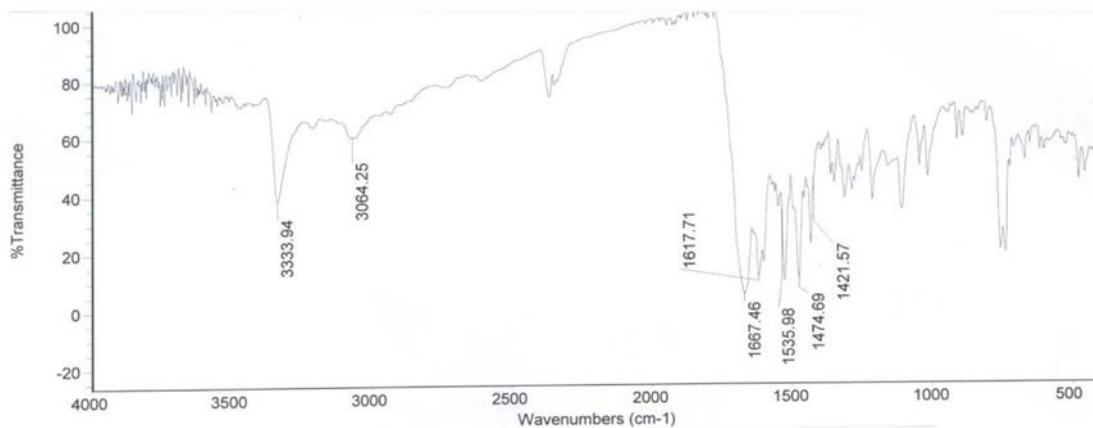
**Figure S30.** Mass spectrum of compound **14**.



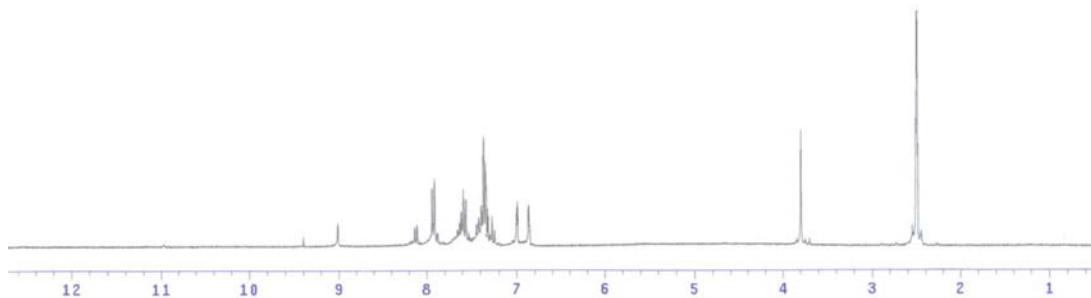
**Figure S31.** IR spectrum of compound **15**.



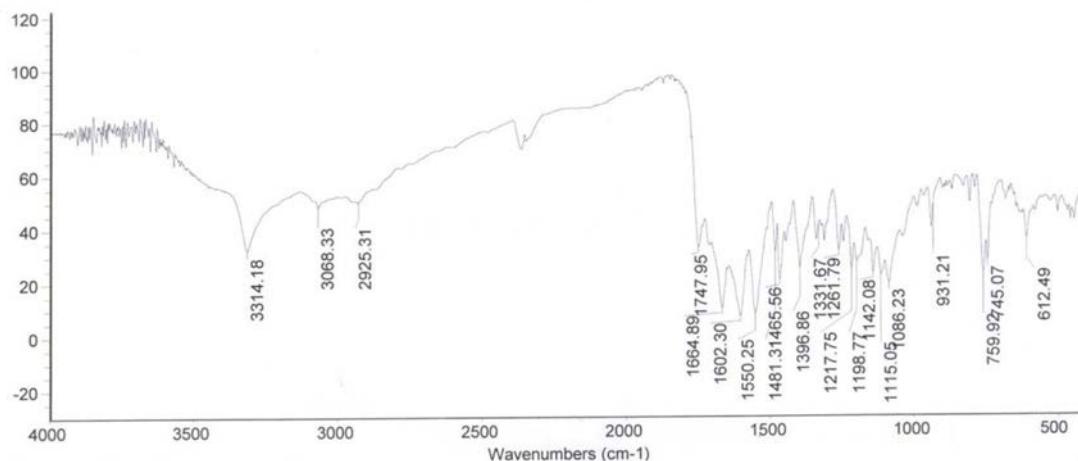
**Figure S32.** <sup>1</sup>H NMR spectra of compound **15** in DMSO-*d*<sub>6</sub> (a) and DMSO-D<sub>2</sub>O (b).



**Figure S33.** IR spectrum of compound **17**.



**Figure S34.** <sup>1</sup>H NMR spectra of compound **17** in DMSO-*d*<sub>6</sub>.



**Figure S35.** IR spectrum of compound **18**.

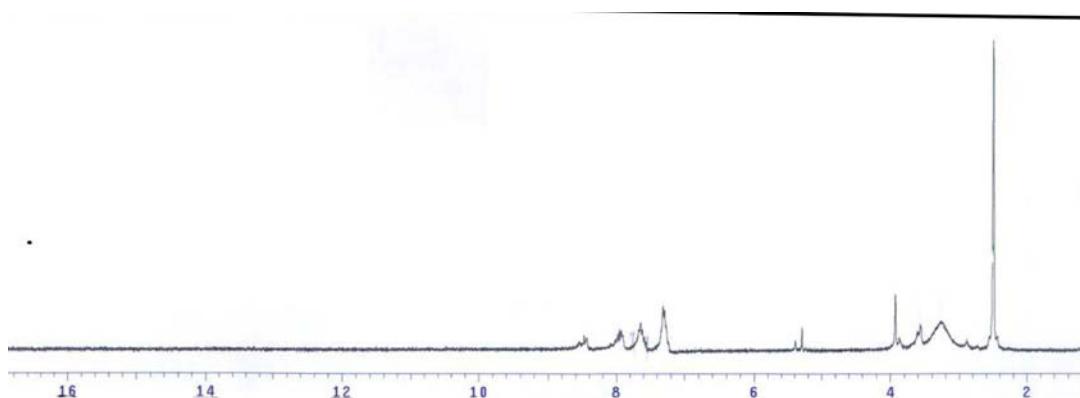


Figure S36.  $^1\text{H}$  NMR spectra of compound **18** in  $\text{DMSO}-d_6$ .

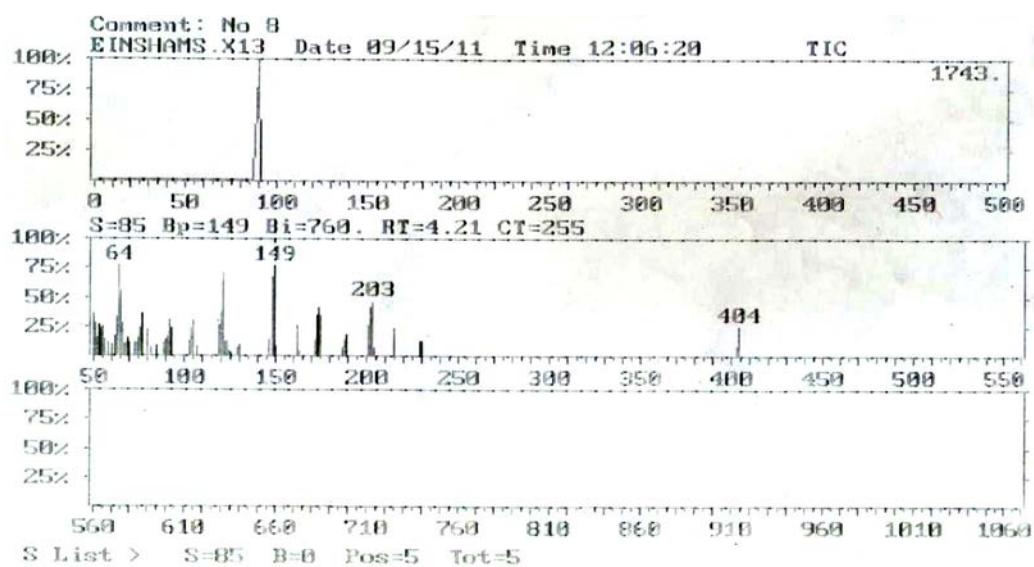


Figure S37. Mass spectrum of compound **18**.

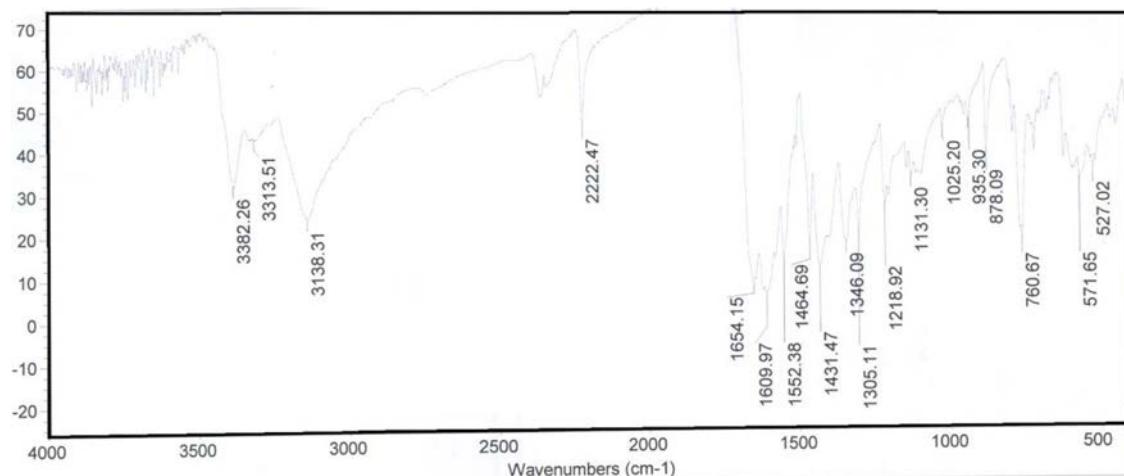
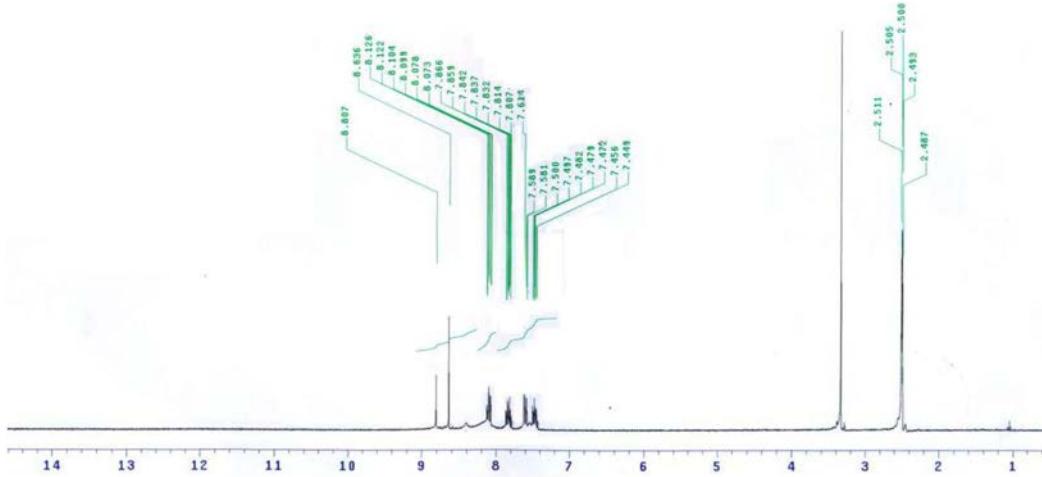
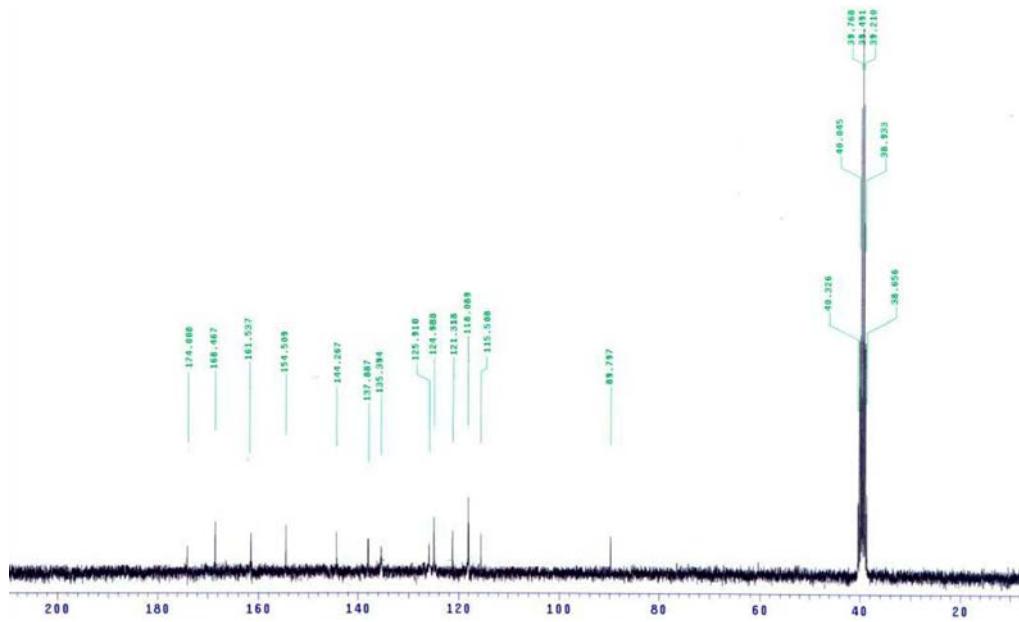


Figure S38. IR spectrum of compound **19**.



**Figure S39.**  $^1\text{H}$  NMR spectrum of compound **19** in  $\text{DMSO}-d_6$ .



**Figure S40.**  $^{13}\text{C}$  NMR spectrum of compound **19** in  $\text{DMSO}-d_6$ .

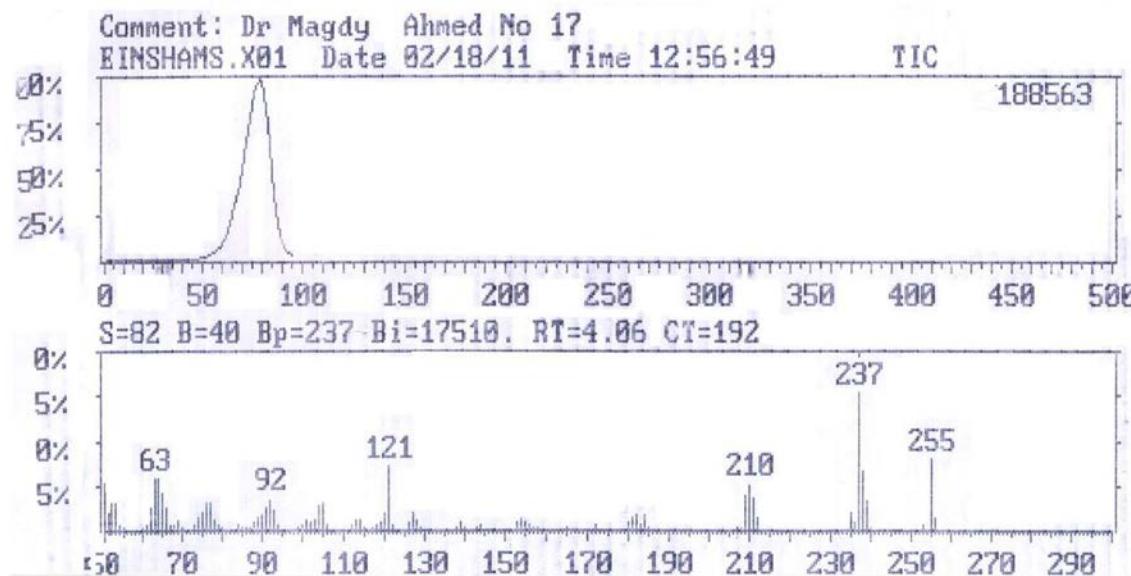


Figure S41. Mass spectrum of compound 19.

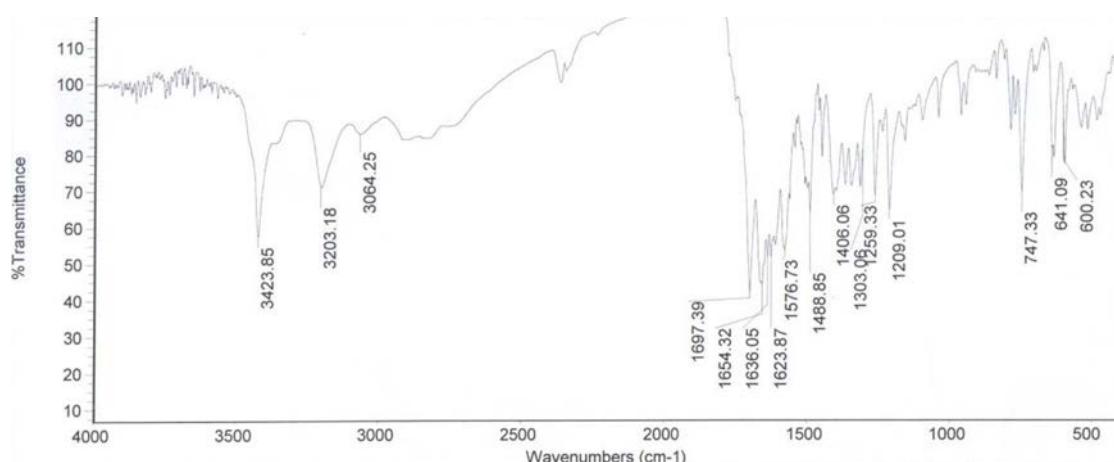
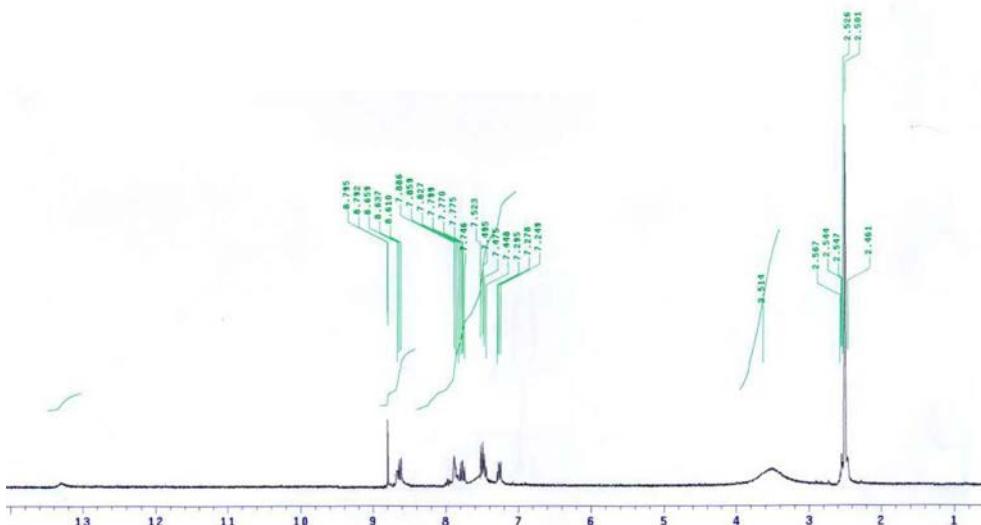
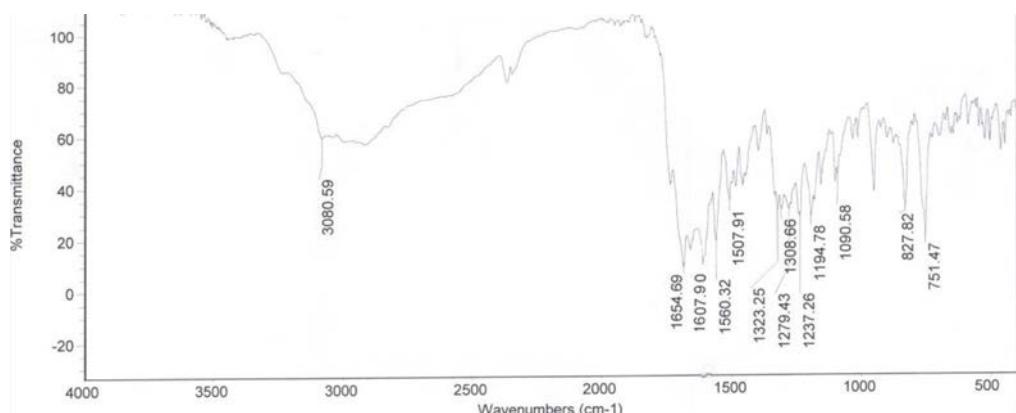


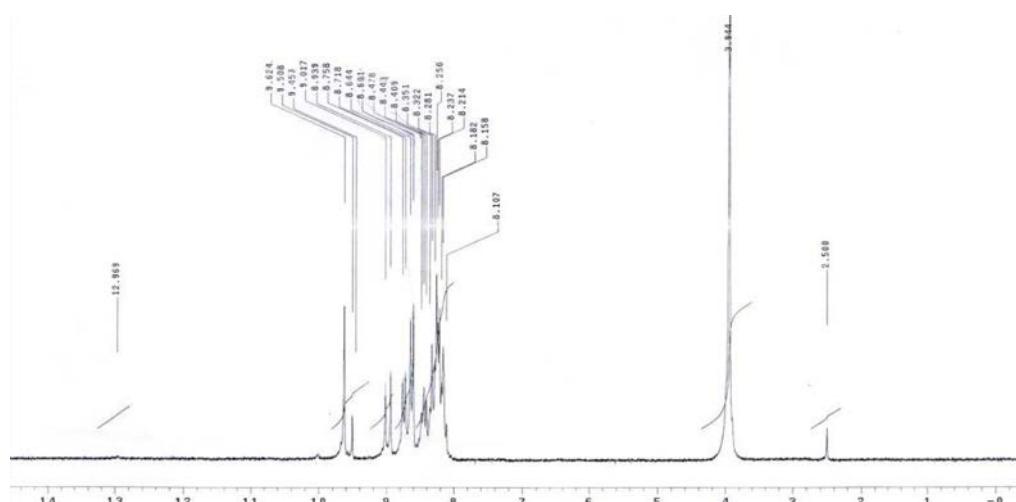
Figure S42. IR spectrum of compound 20.



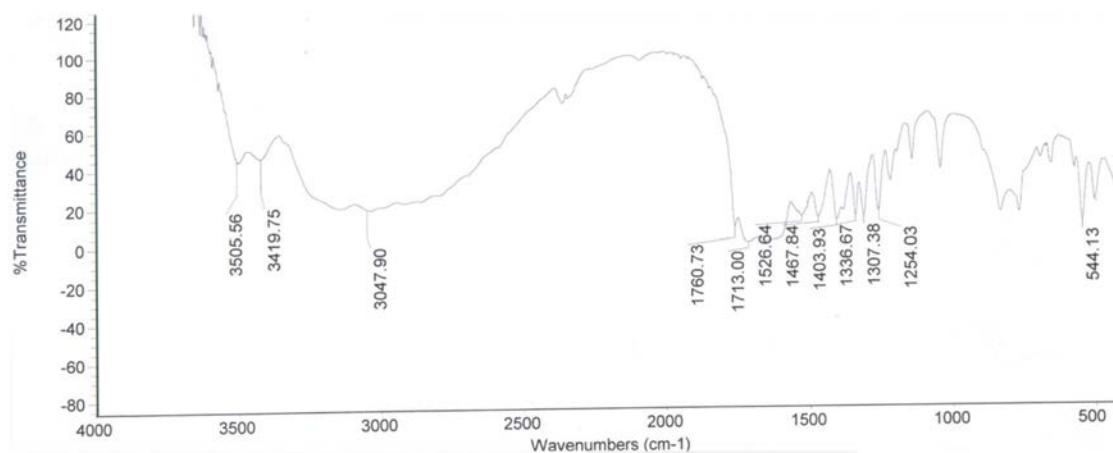
**Figure S43.**  $^1\text{H}$  NMR spectrum of compound **20** in  $\text{DMSO}-d_6$ .



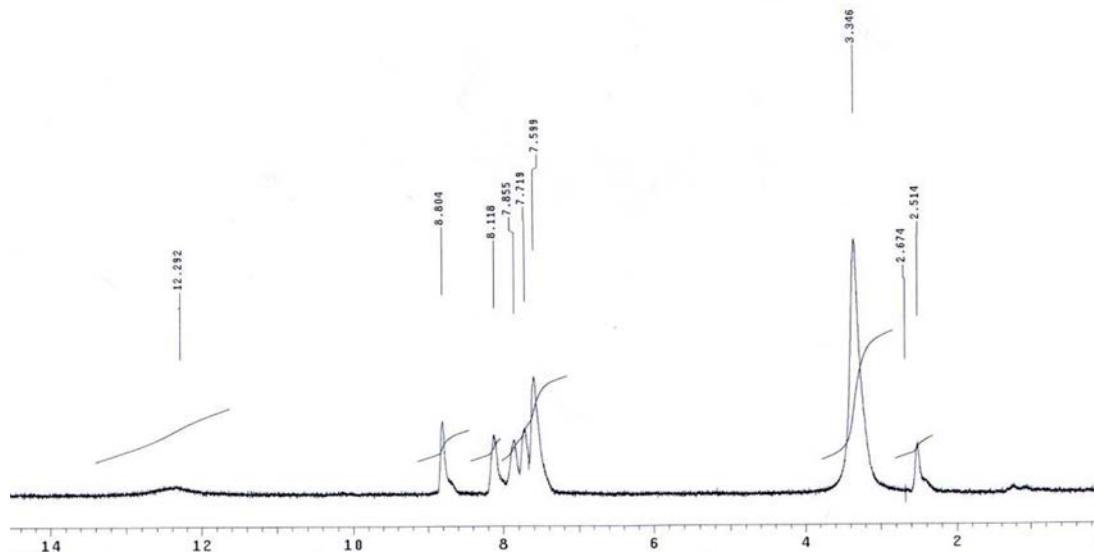
**Figure S44.** IR spectrum of compound **21**.



**Figure S45.**  $^1\text{H}$  NMR spectrum of compound **21** in  $\text{DMSO}-d_6$ .



**Figure S46.** IR spectrum of compound **22**.



**Figure S47.** <sup>1</sup>H NMR spectrum of compound **22** in DMSO-*d*<sub>6</sub>.

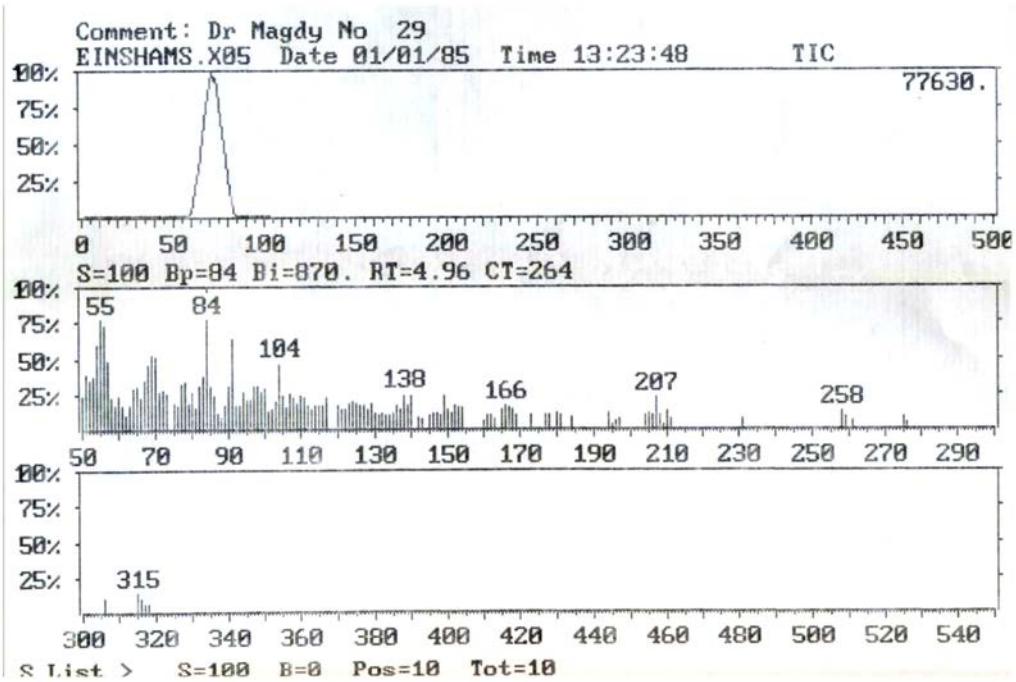


Figure S48. Mass spectrum of compound 22.