Supplementary Material

One-pot, three component approach to synthesis of multipart fused heterocyclic compounds: Synthesis of fused pyran-2-ones

Bahador Karami,* Khalil Eskandari, and Saeed Khodabakhshi

Department of Chemistry, Yasouj University, Yasouj, Zip Code 75918-74831, P. O. Box: 353, Iran
E-mail: The karami@mail.yu.ac.ir

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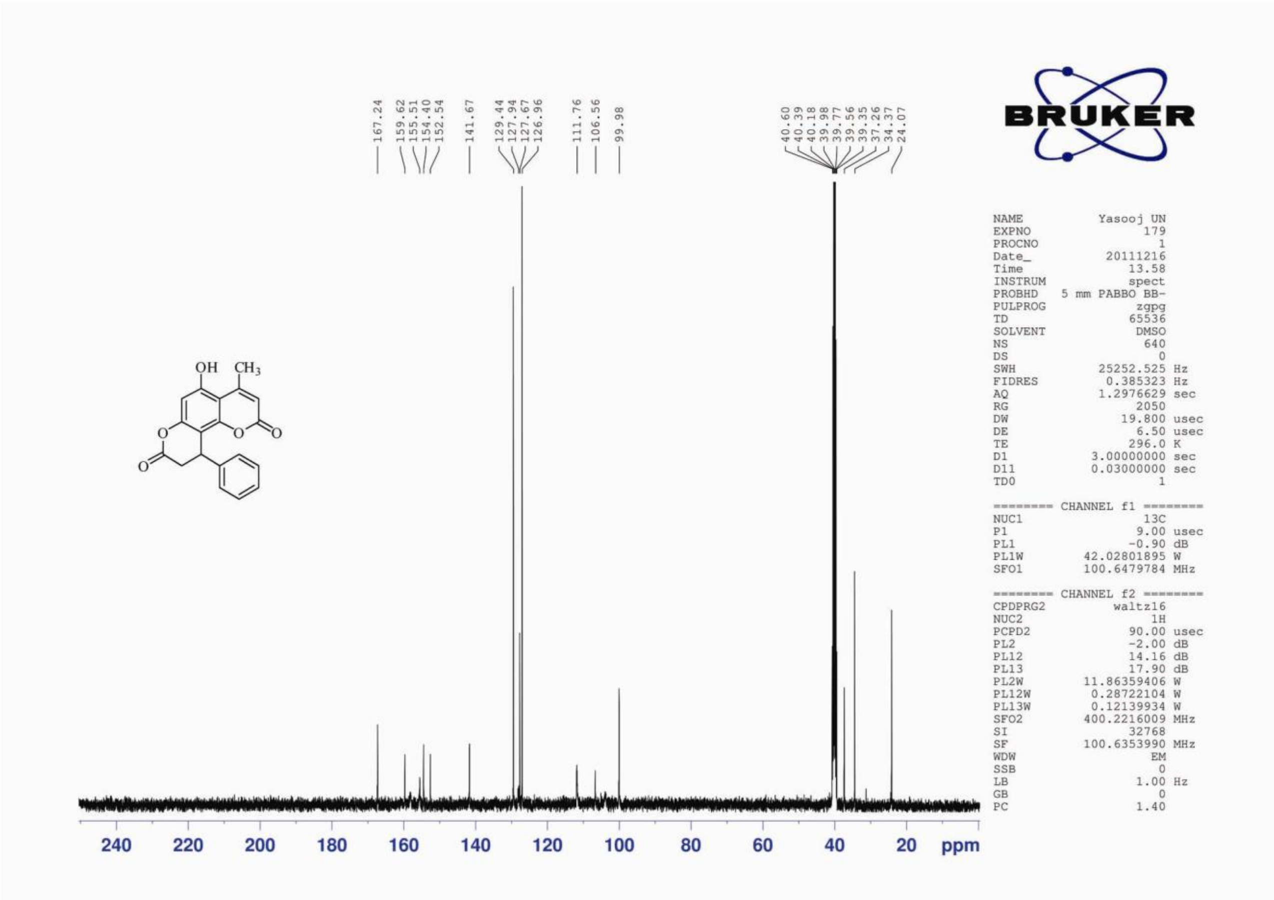
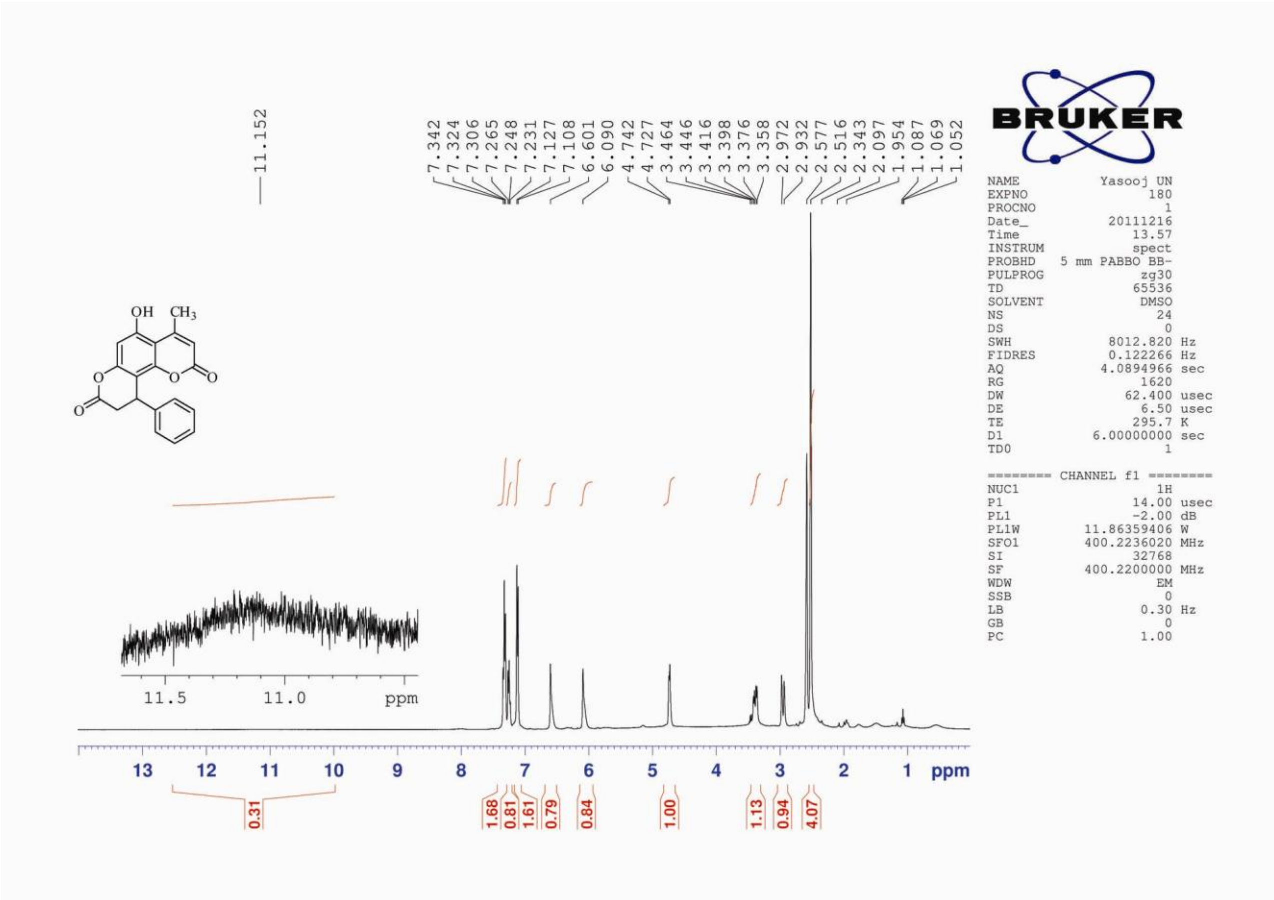
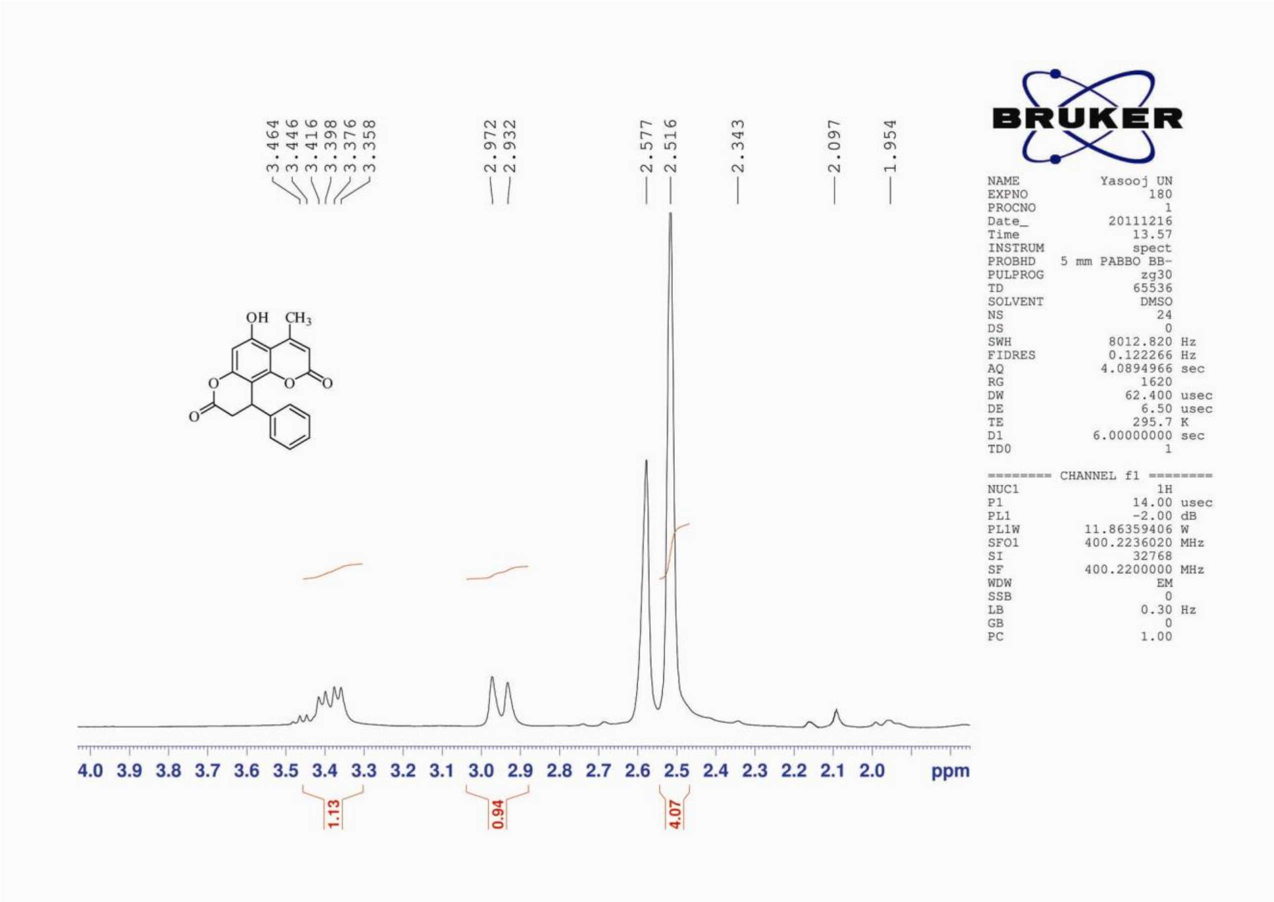


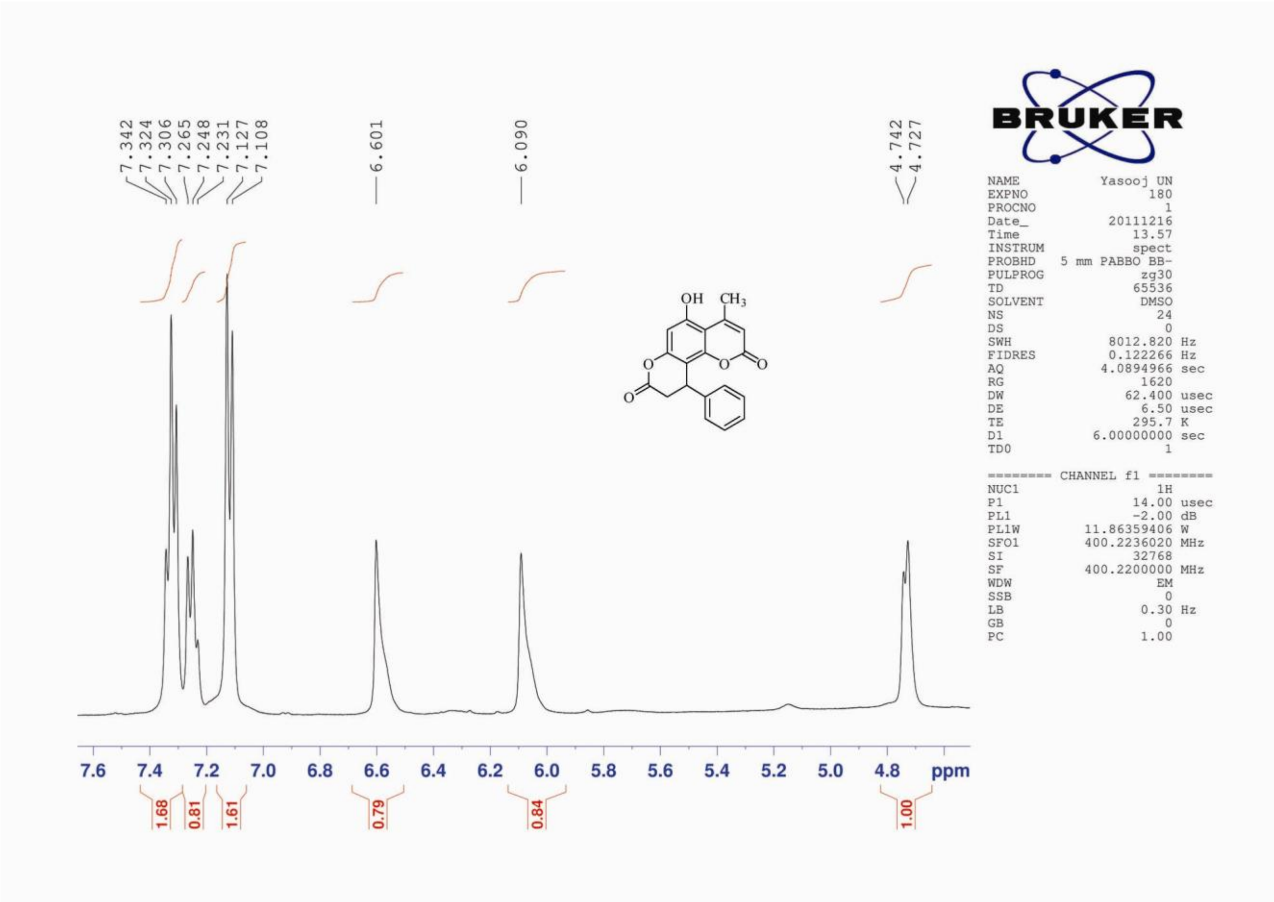
^{13}C NMR spectrum of compound **8a**



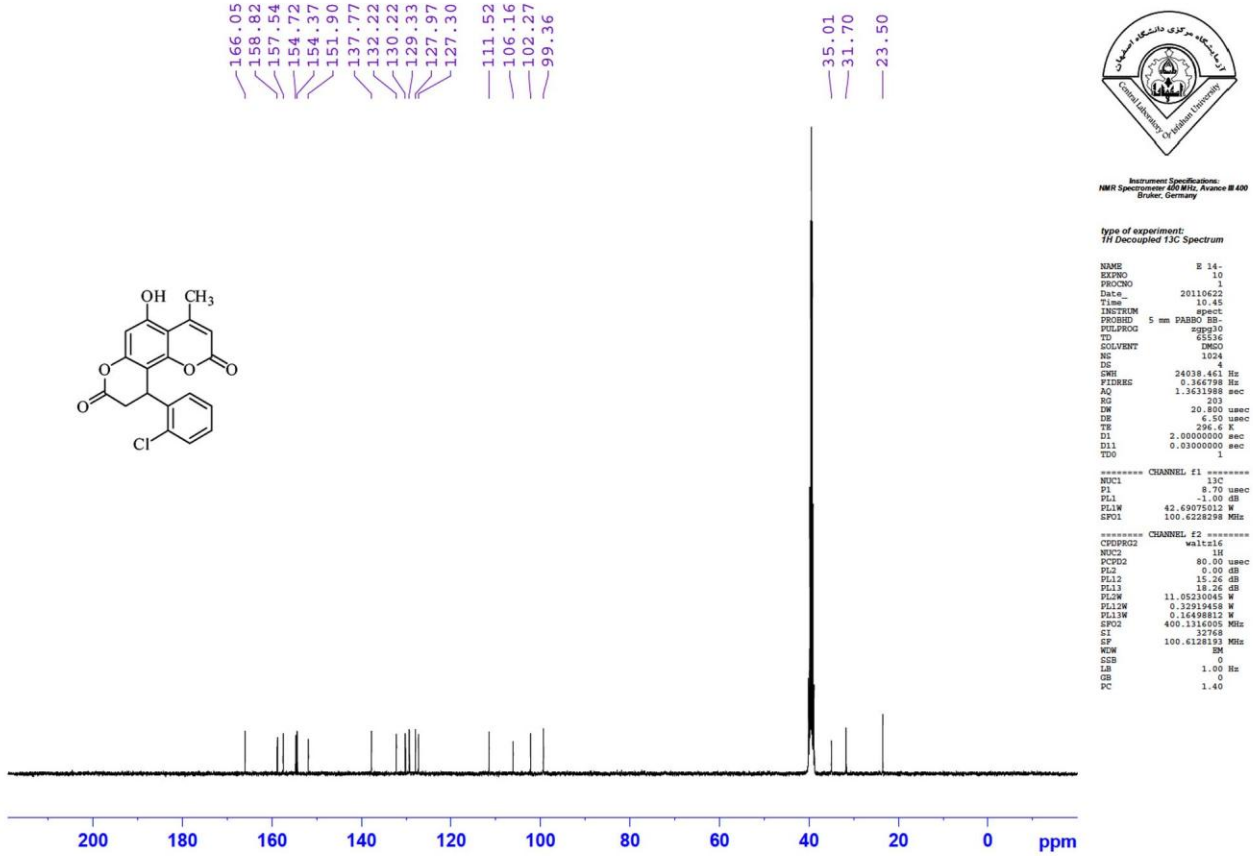
^{1}H NMR spectrum of compound **8a**



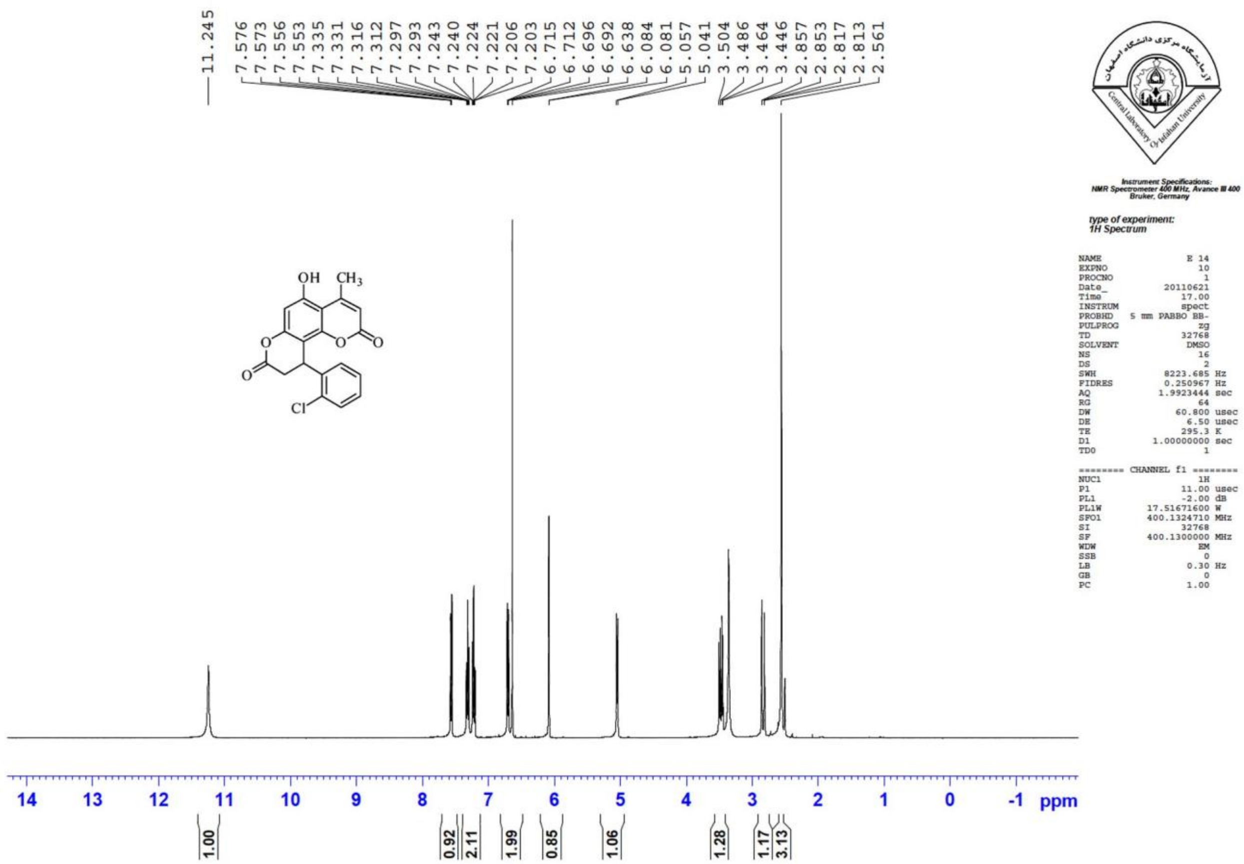
^{1}H NMR (expanded) spectrum of compound **8a**



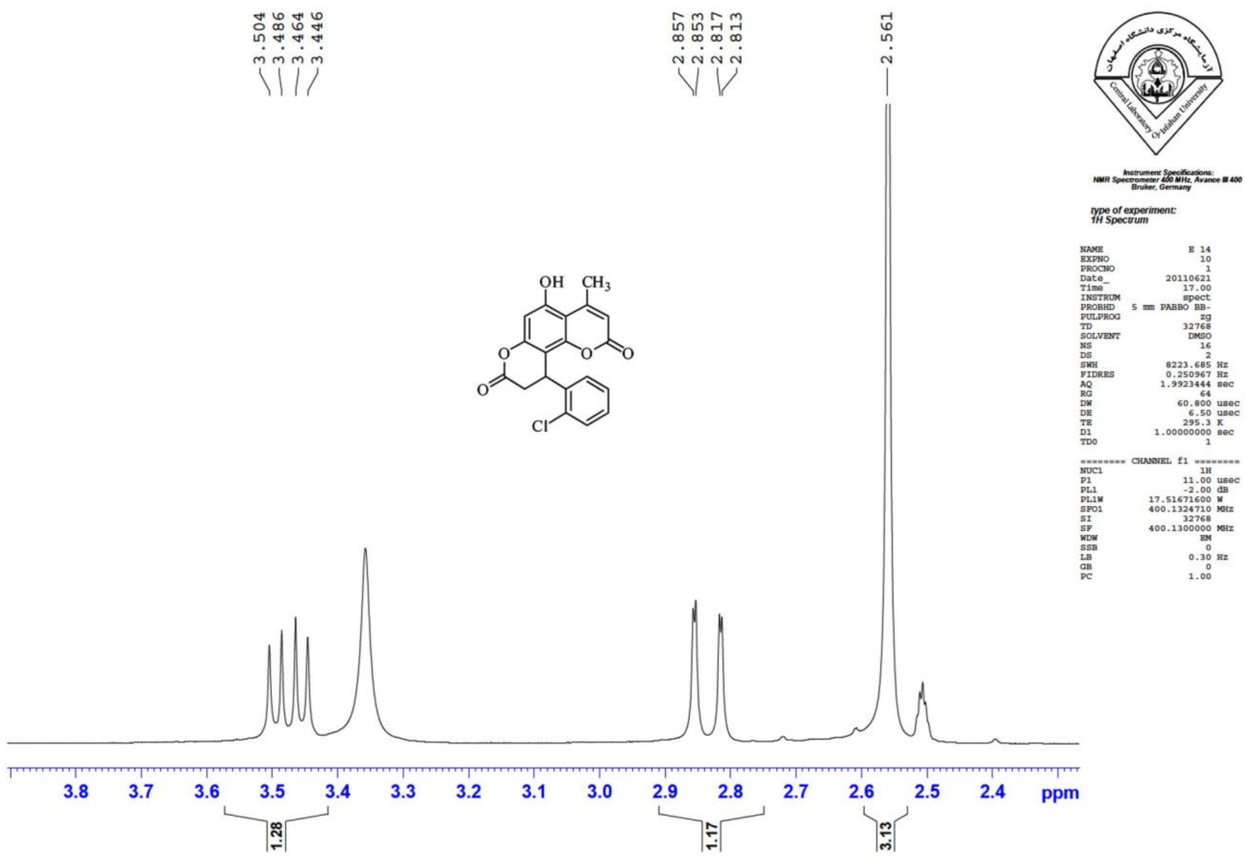
^{1}H NMR (expanded) spectrum of compound **8a**



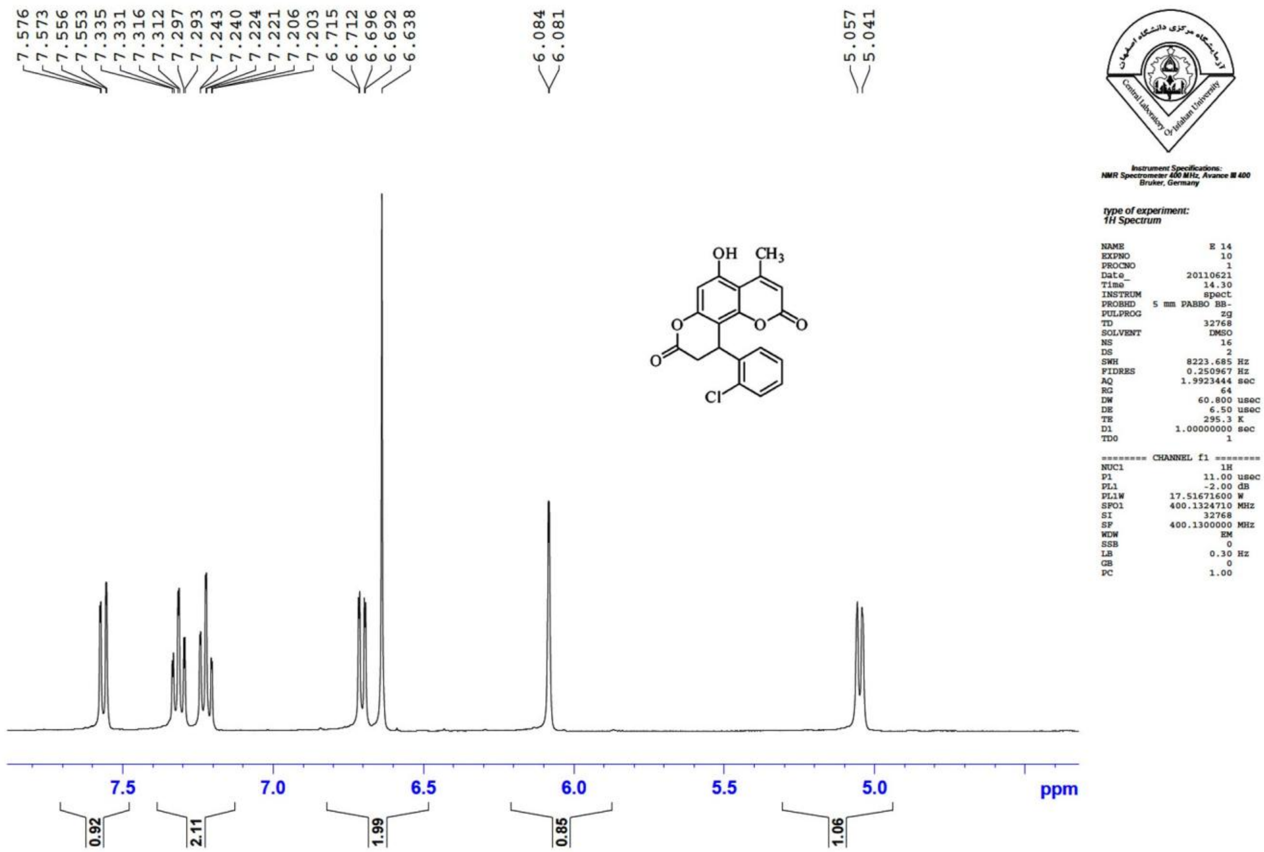
^{13}C NMR spectrum of compound **8b**



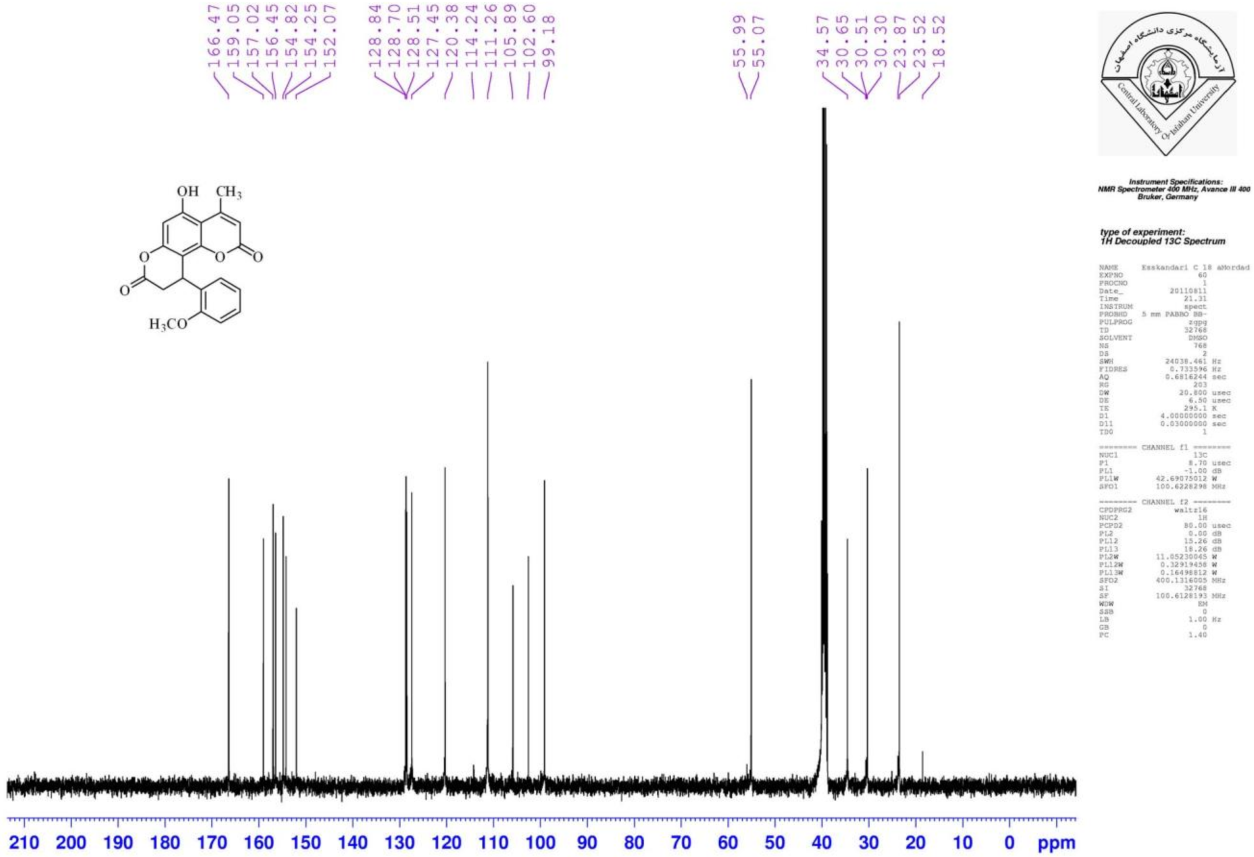
^{1}H NMR spectrum of compound **8b**



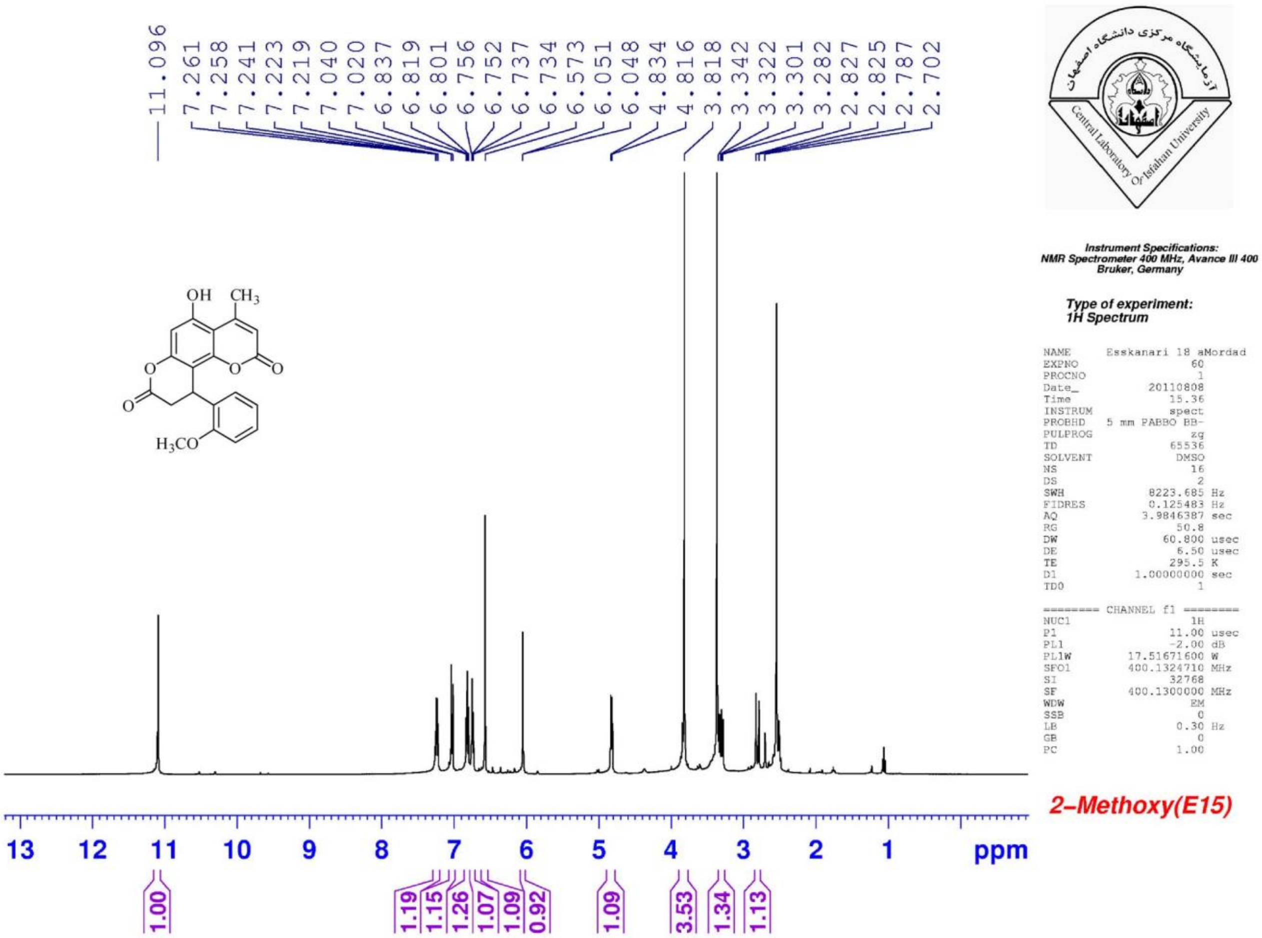
[1]H NMR (expanded) spectrum of compound **8b**



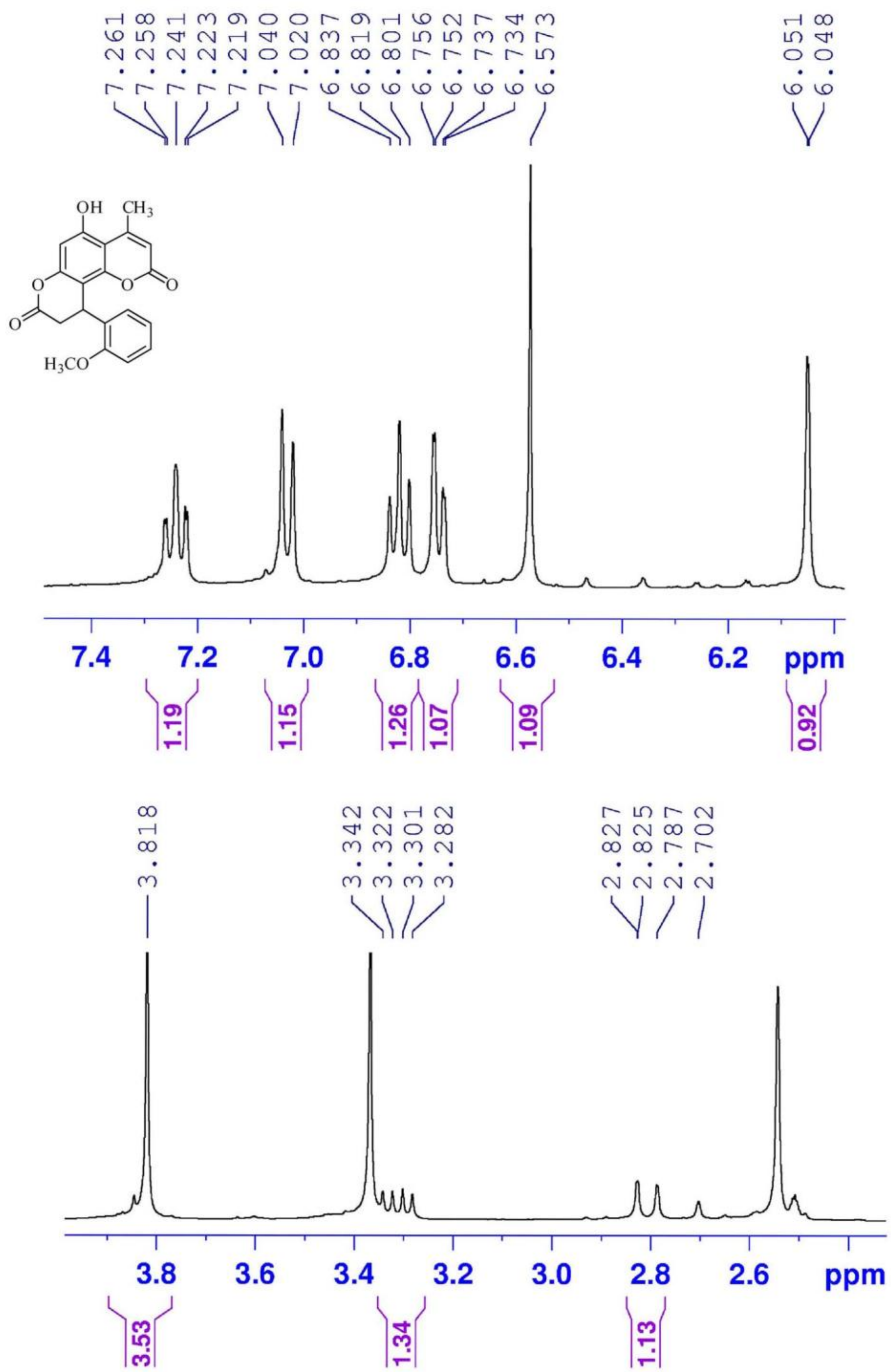
[1]H NMR (expanded) spectrum of compound **8b**



^{13}C NMR spectrum of compound **8c**



[1]H NMR spectrum of compound **8c**



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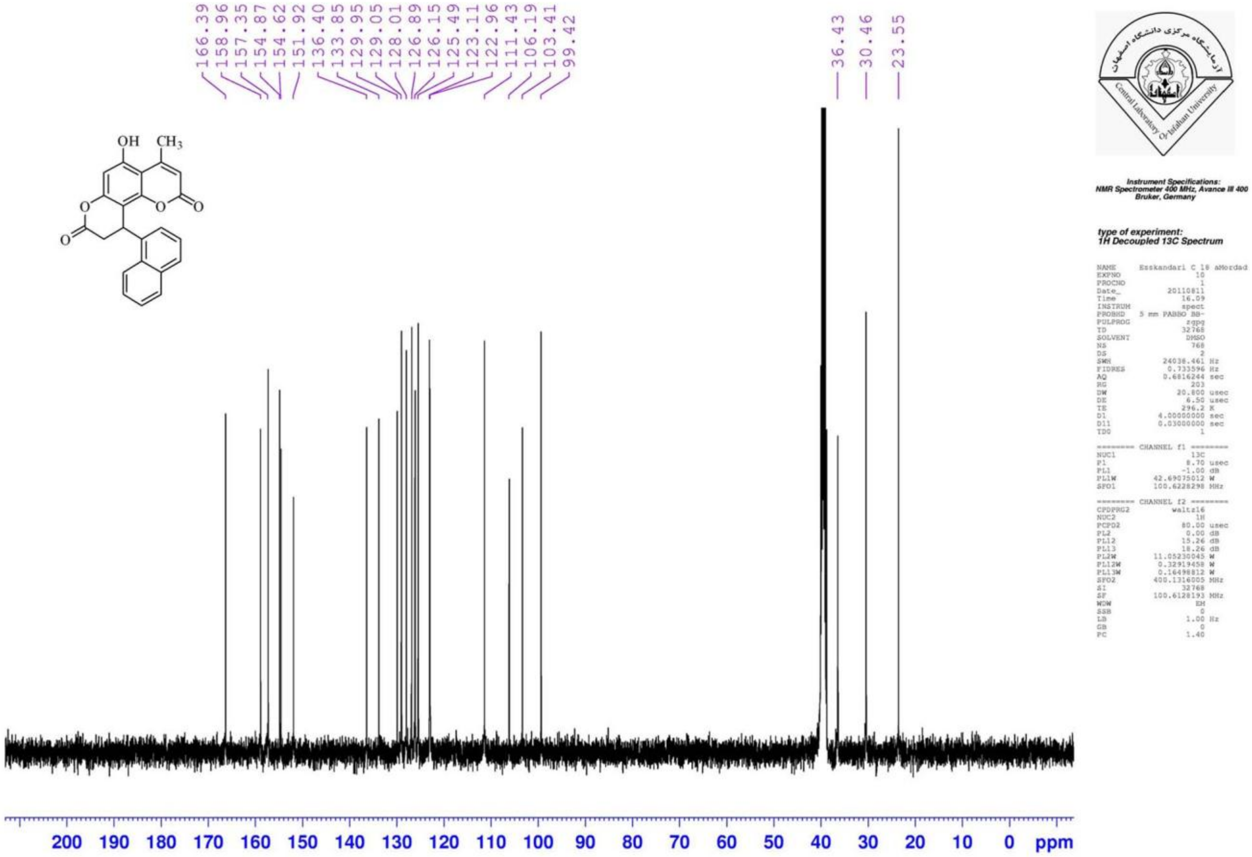

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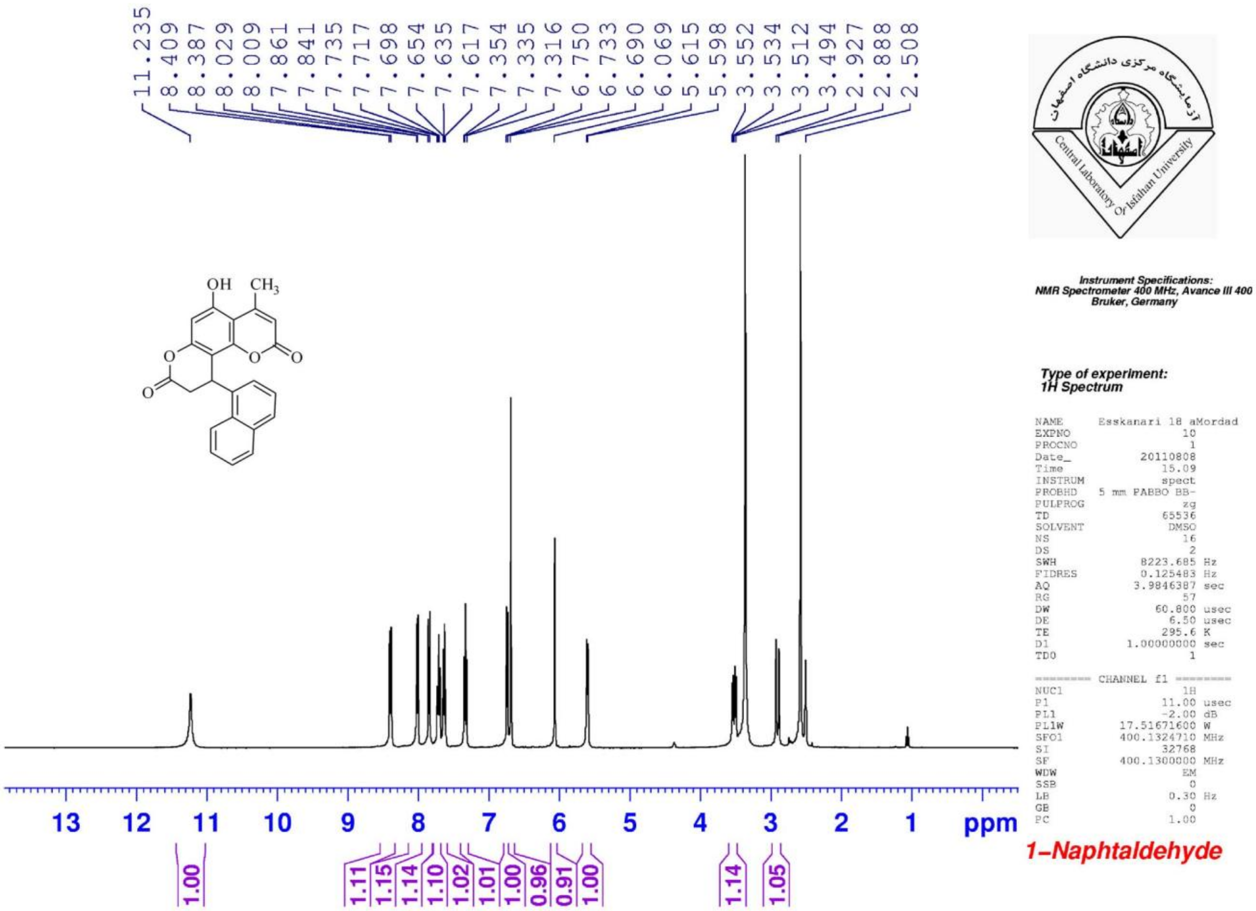
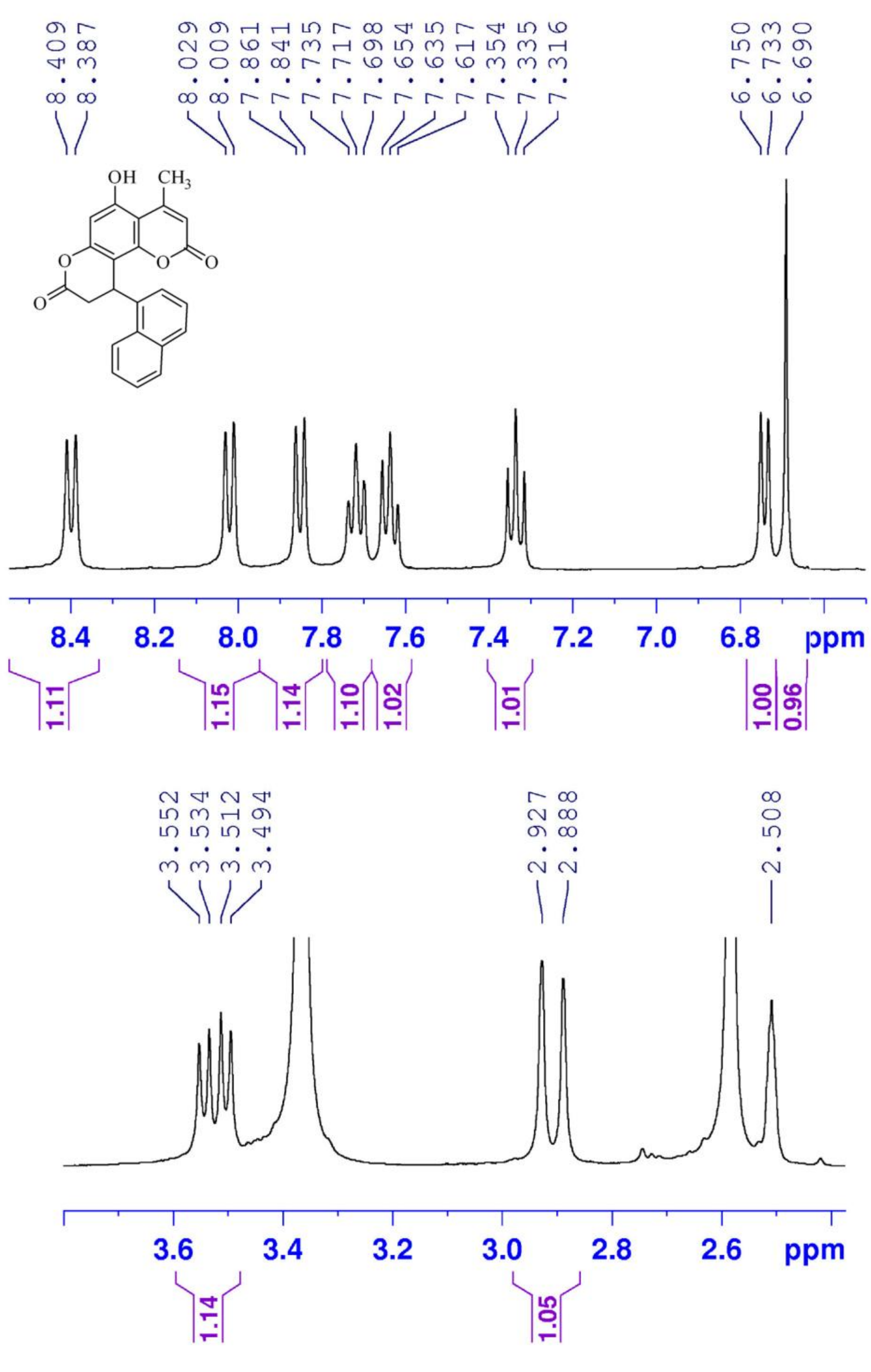
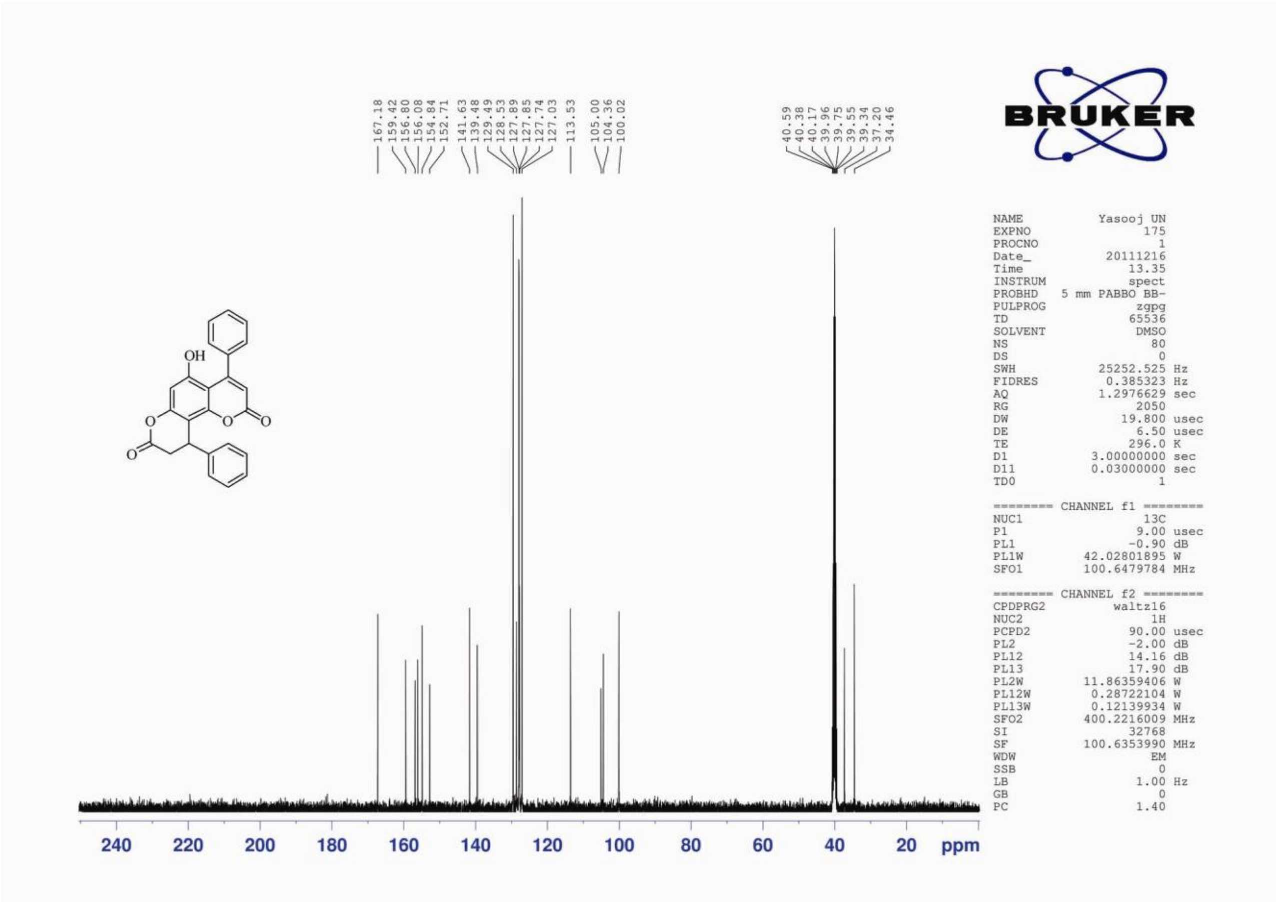


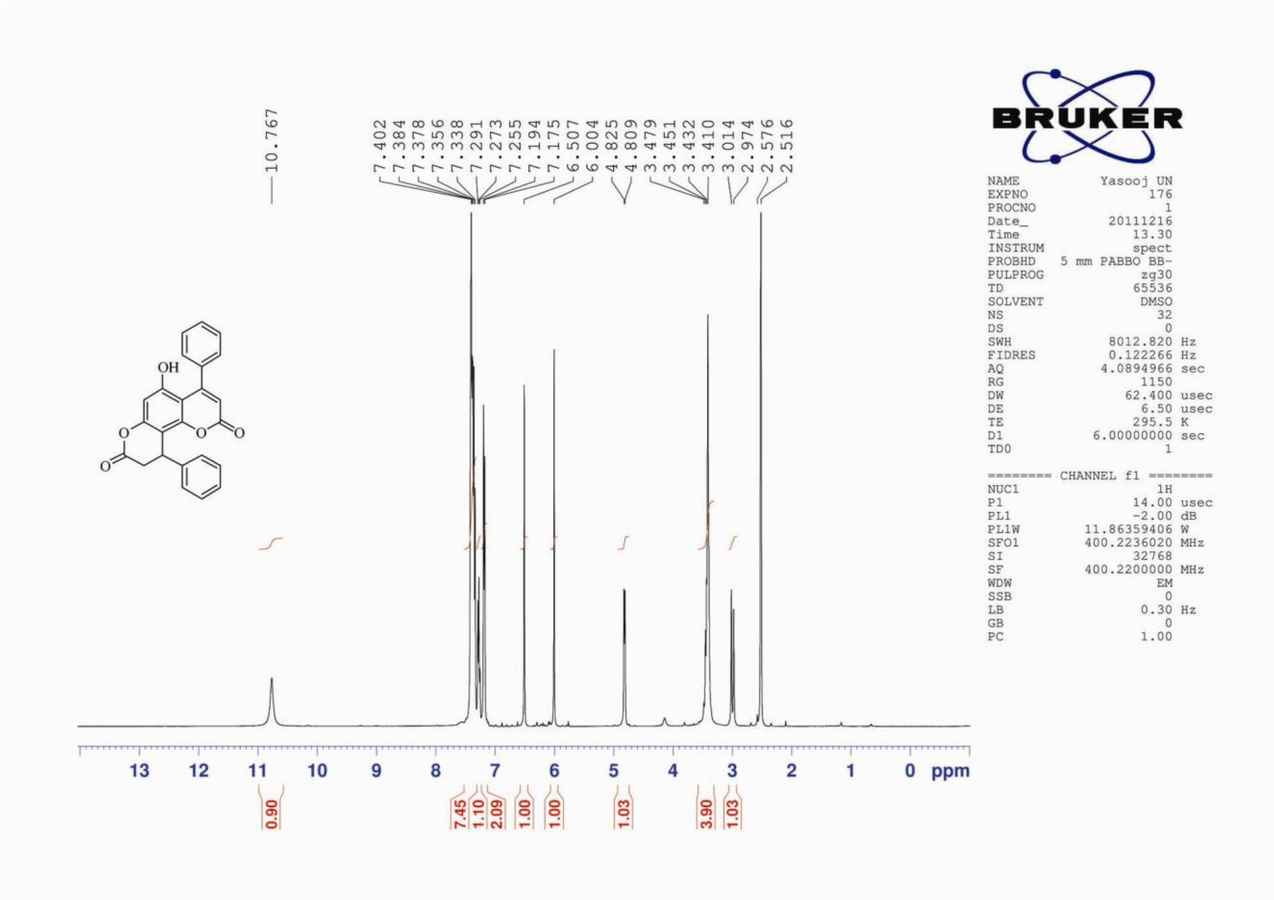
[1]H NMR spectrum of compound **8d**



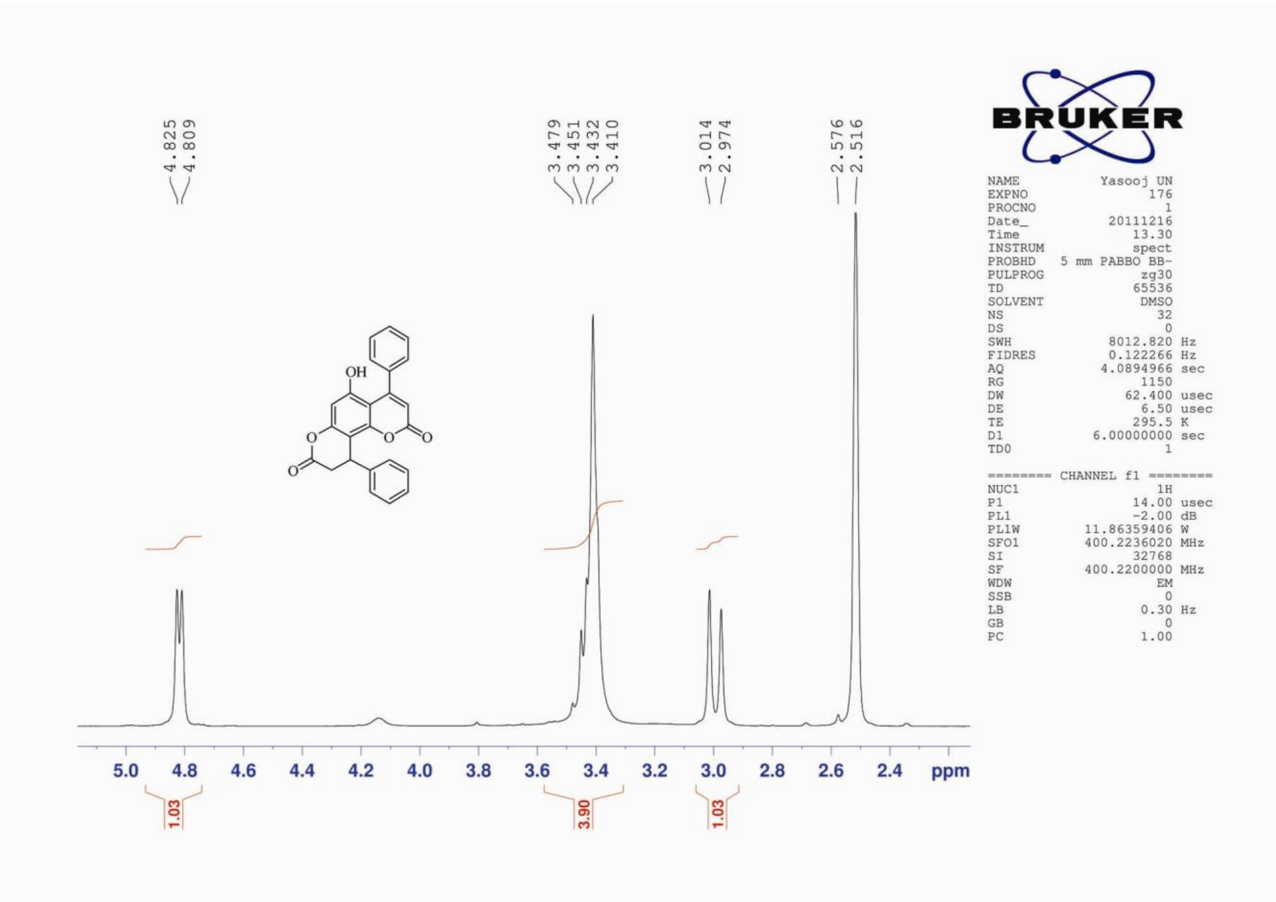
^{1}H NMR (expanded) spectrum of compound **8d**



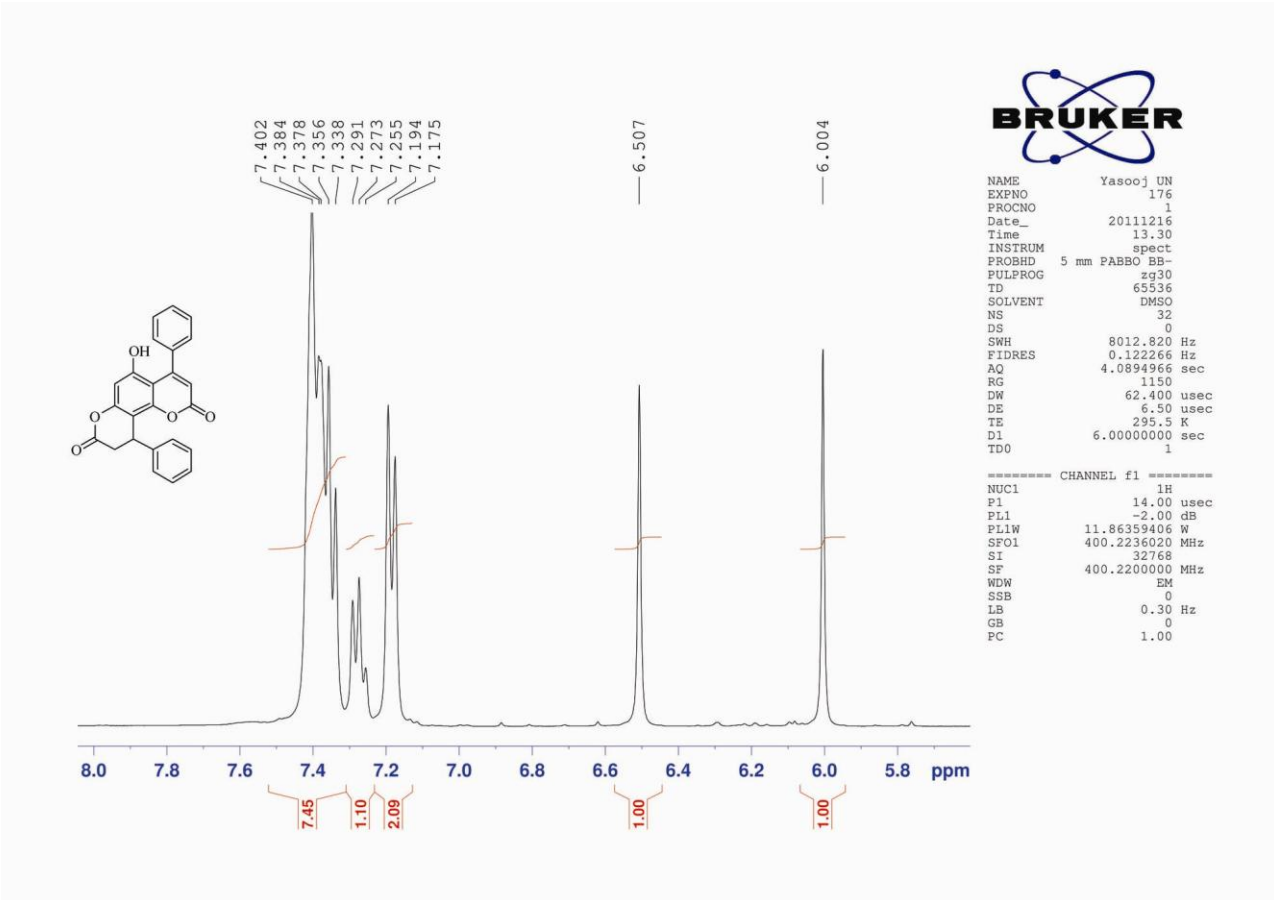
^{13}C NMR spectrum of compound **8e**



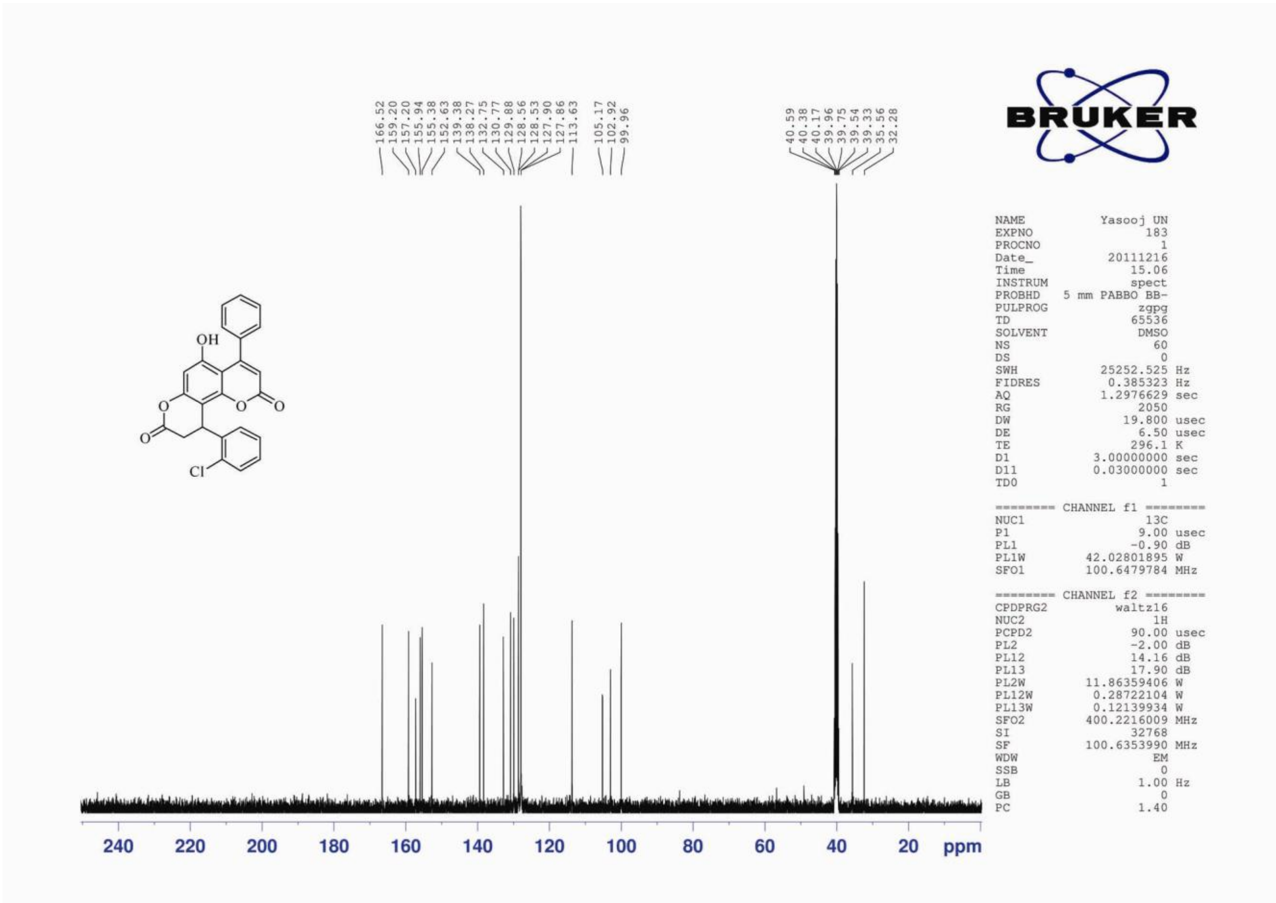
^{1}H NMR spectrum of compound **8e**



[1]H NMR (expanded) spectrum of compound **8e**



^{1}H NMR (expanded) spectrum of compound **8e**



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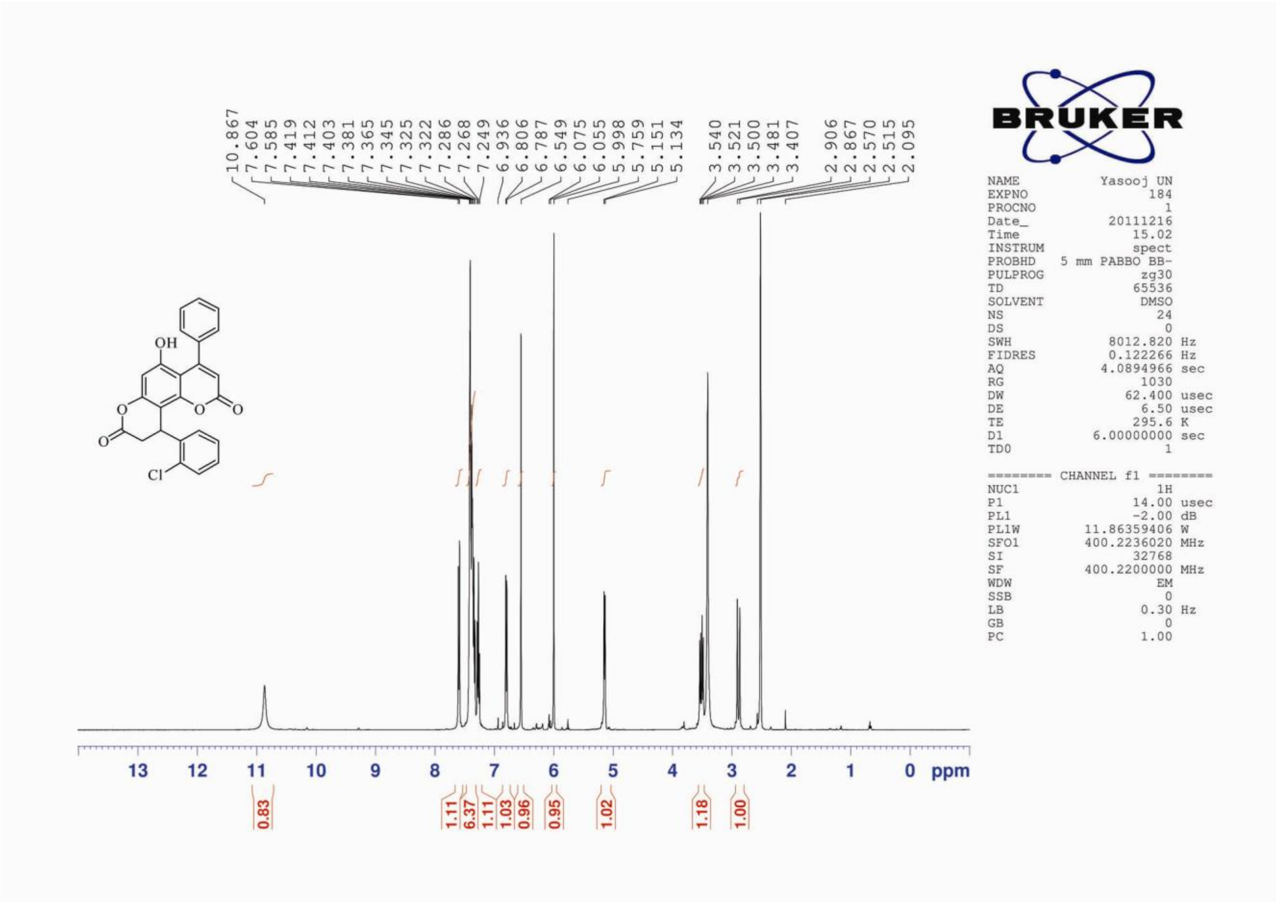
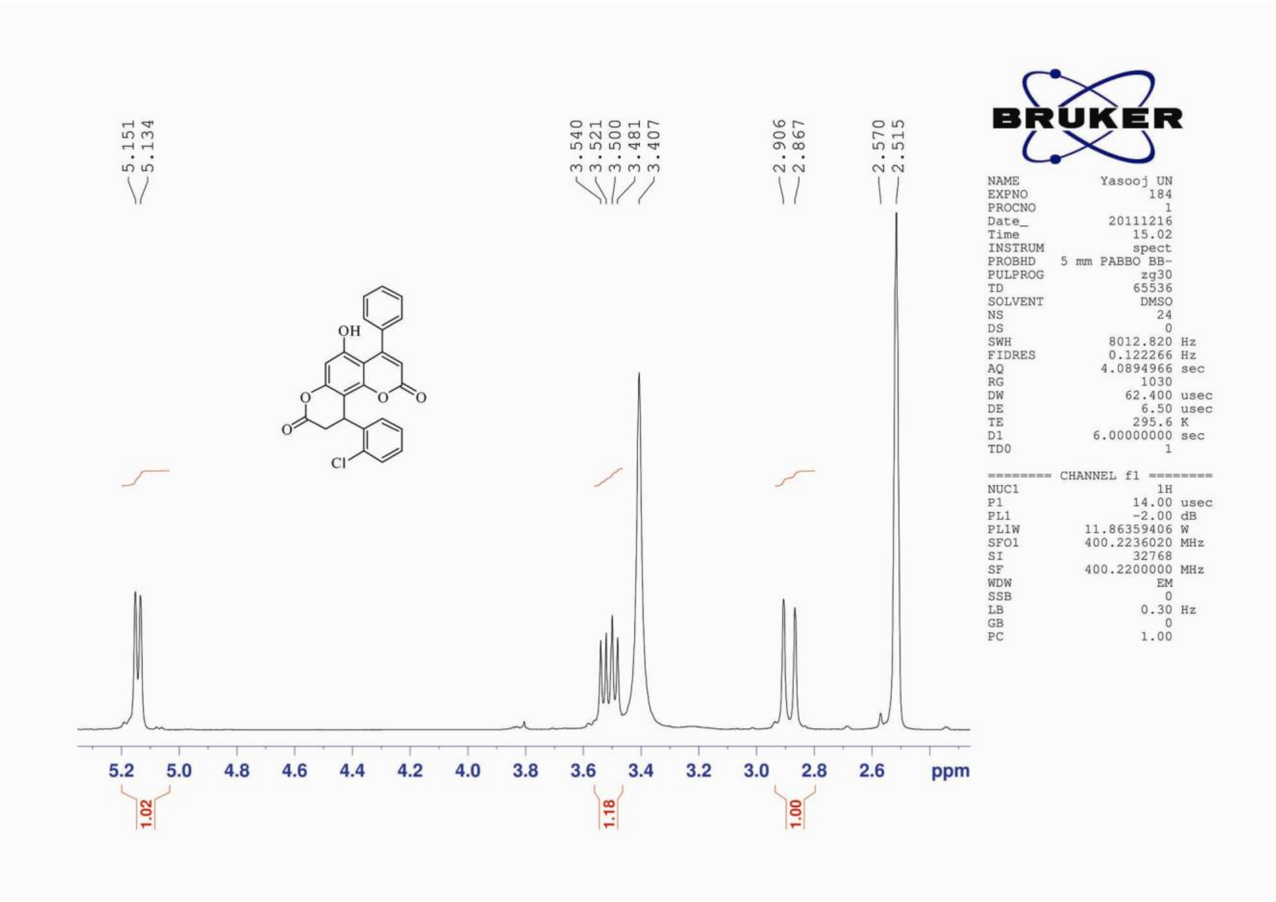
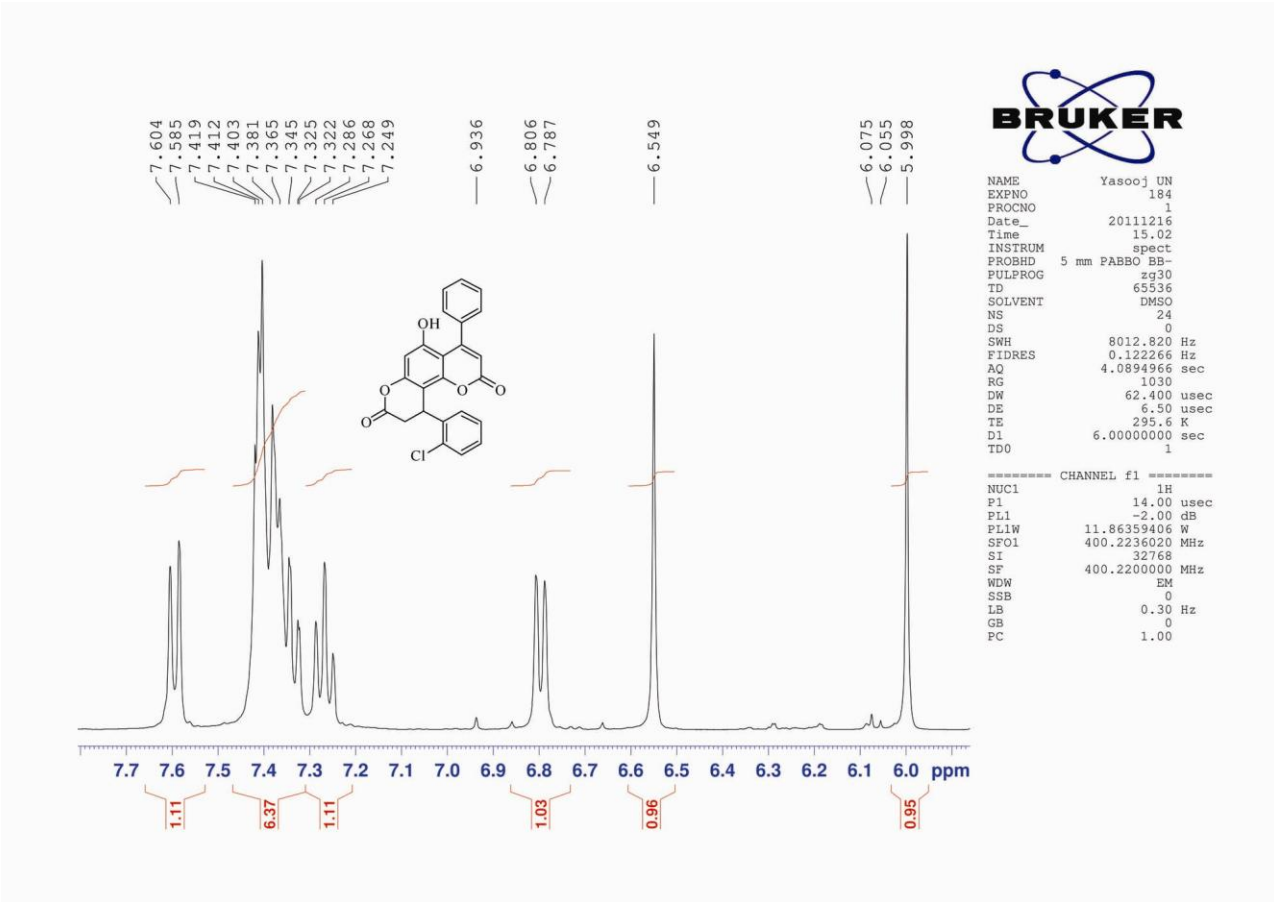


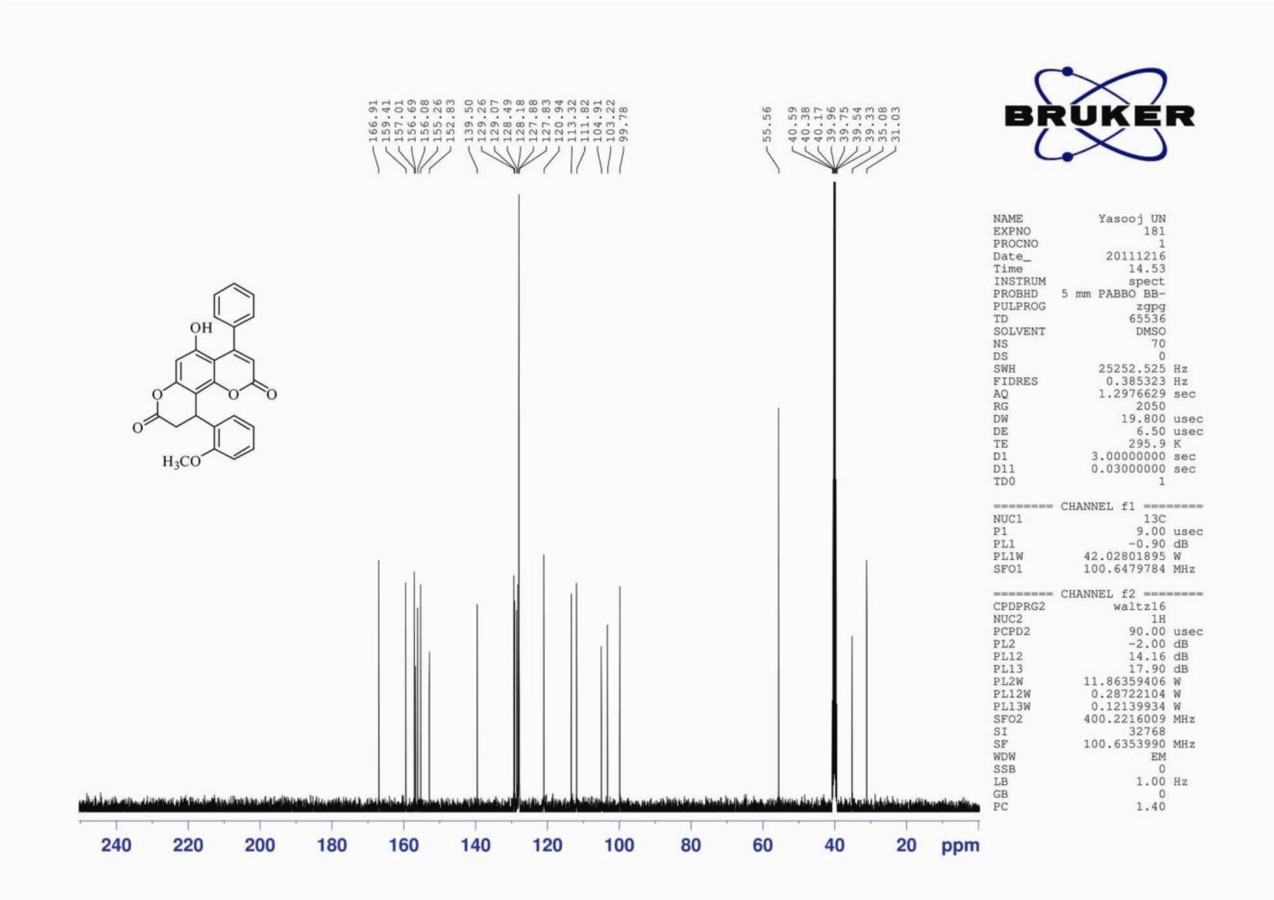
^{1}H NMR spectrum of compound **8f**



^{1}H NMR (expanded) spectrum of compound **8f**



^{1}H NMR (expanded) spectrum of compound **8f**



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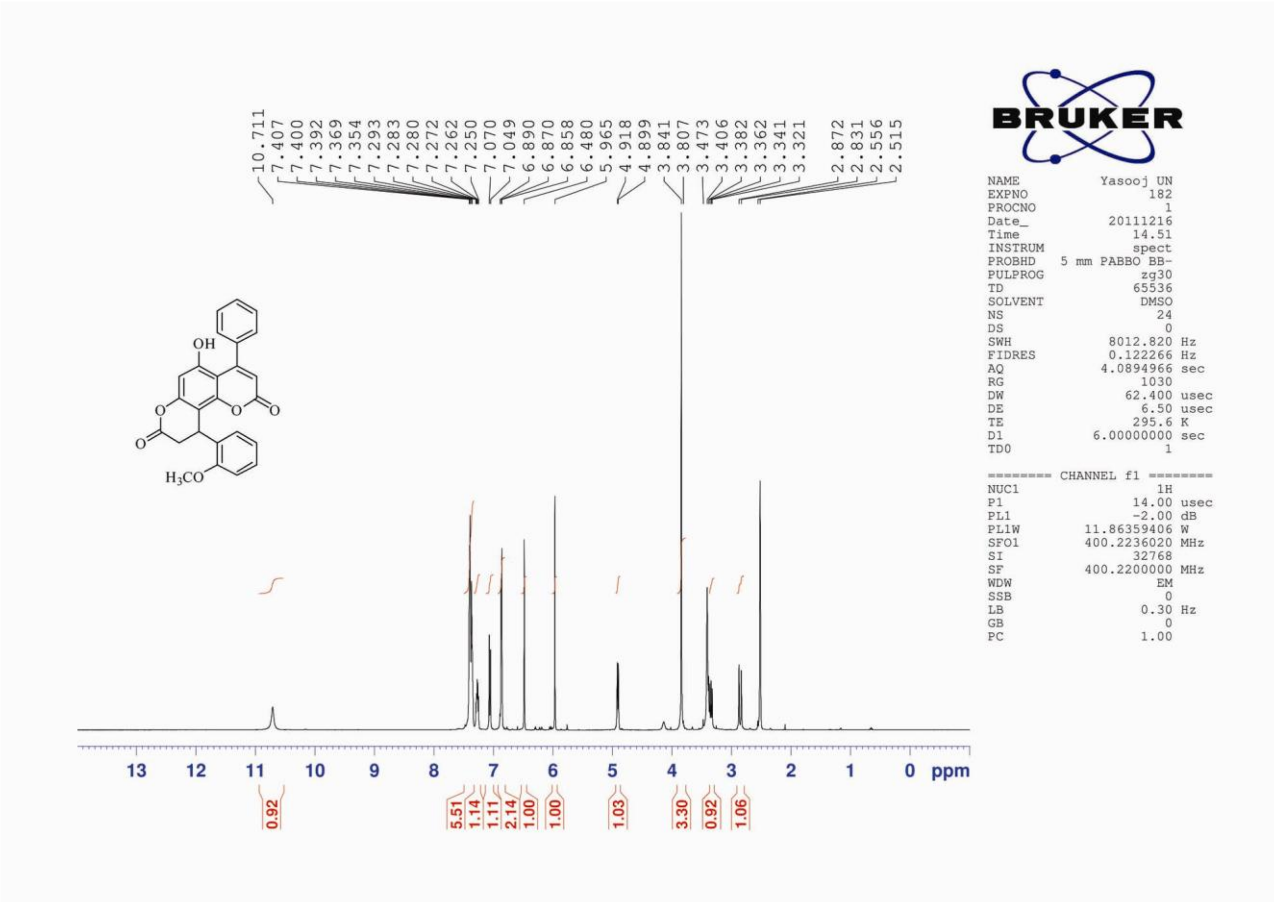
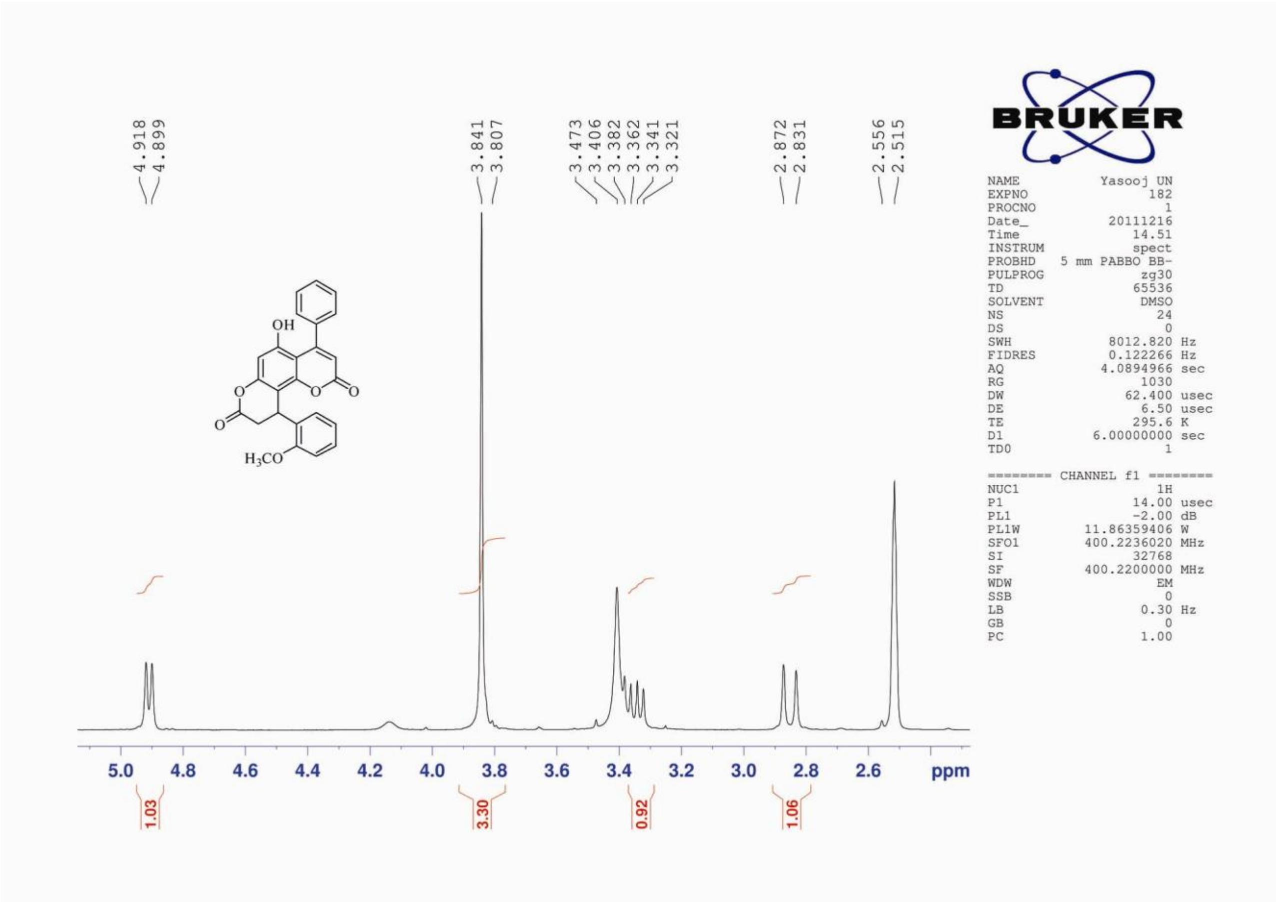
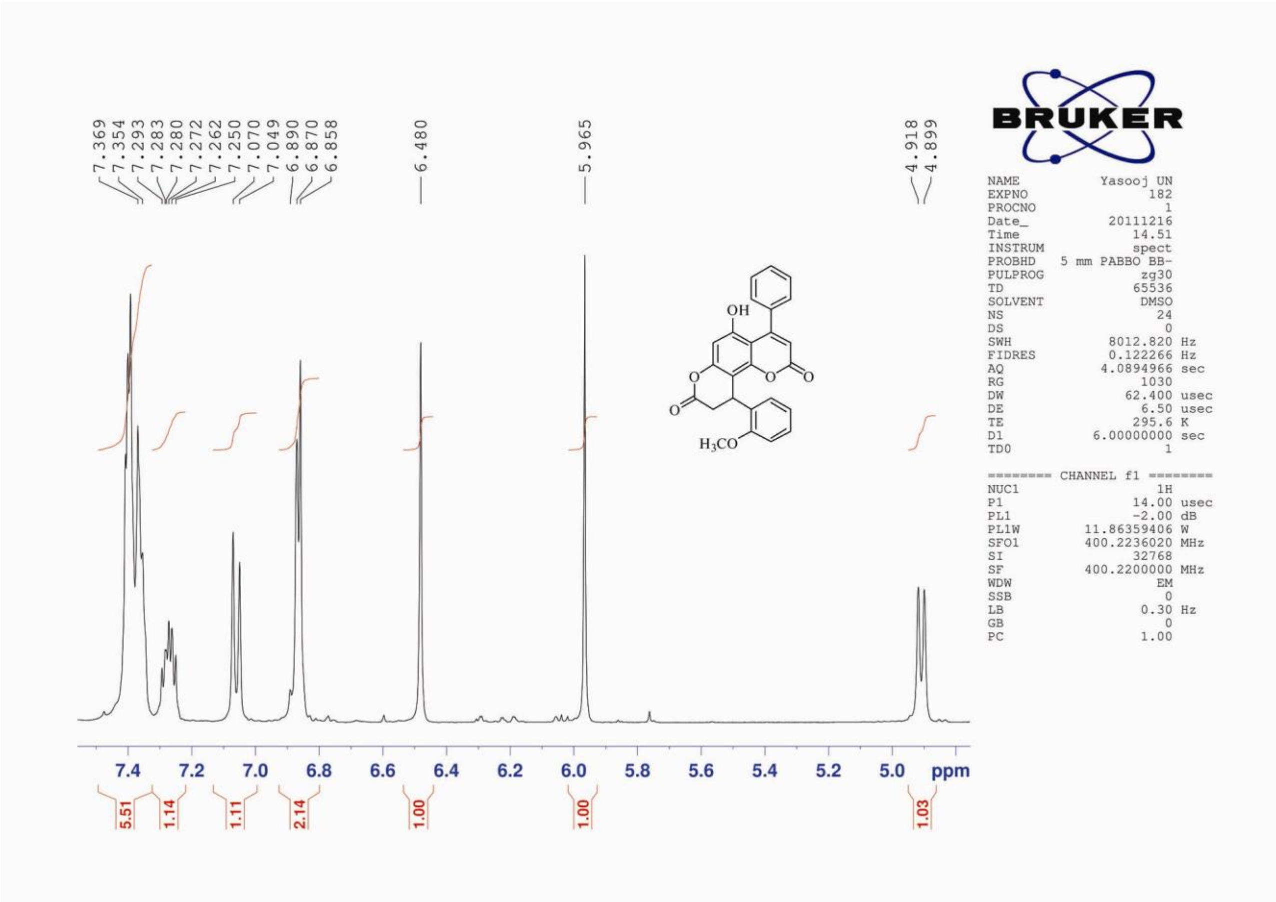


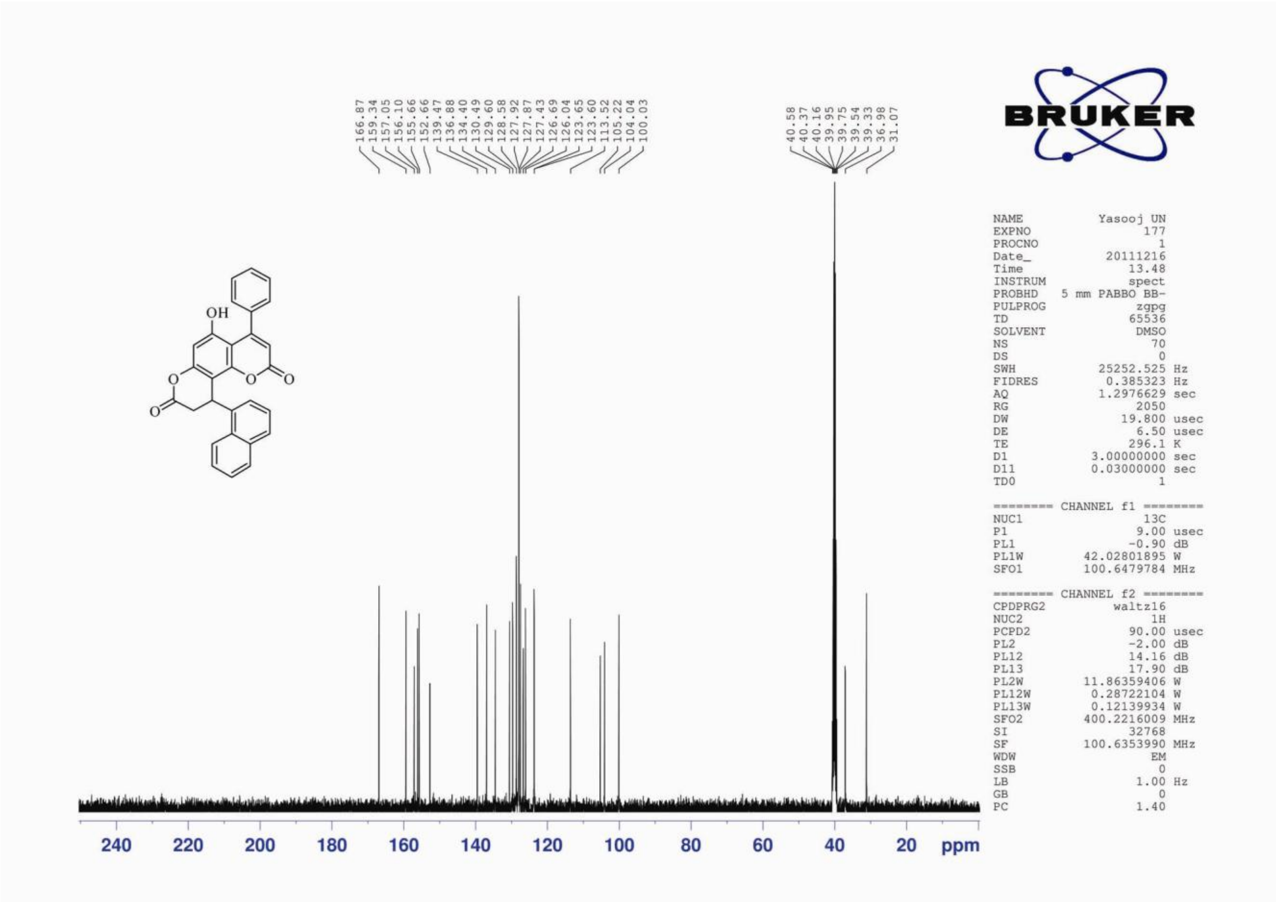
[1]H NMR spectrum of compound **8g**



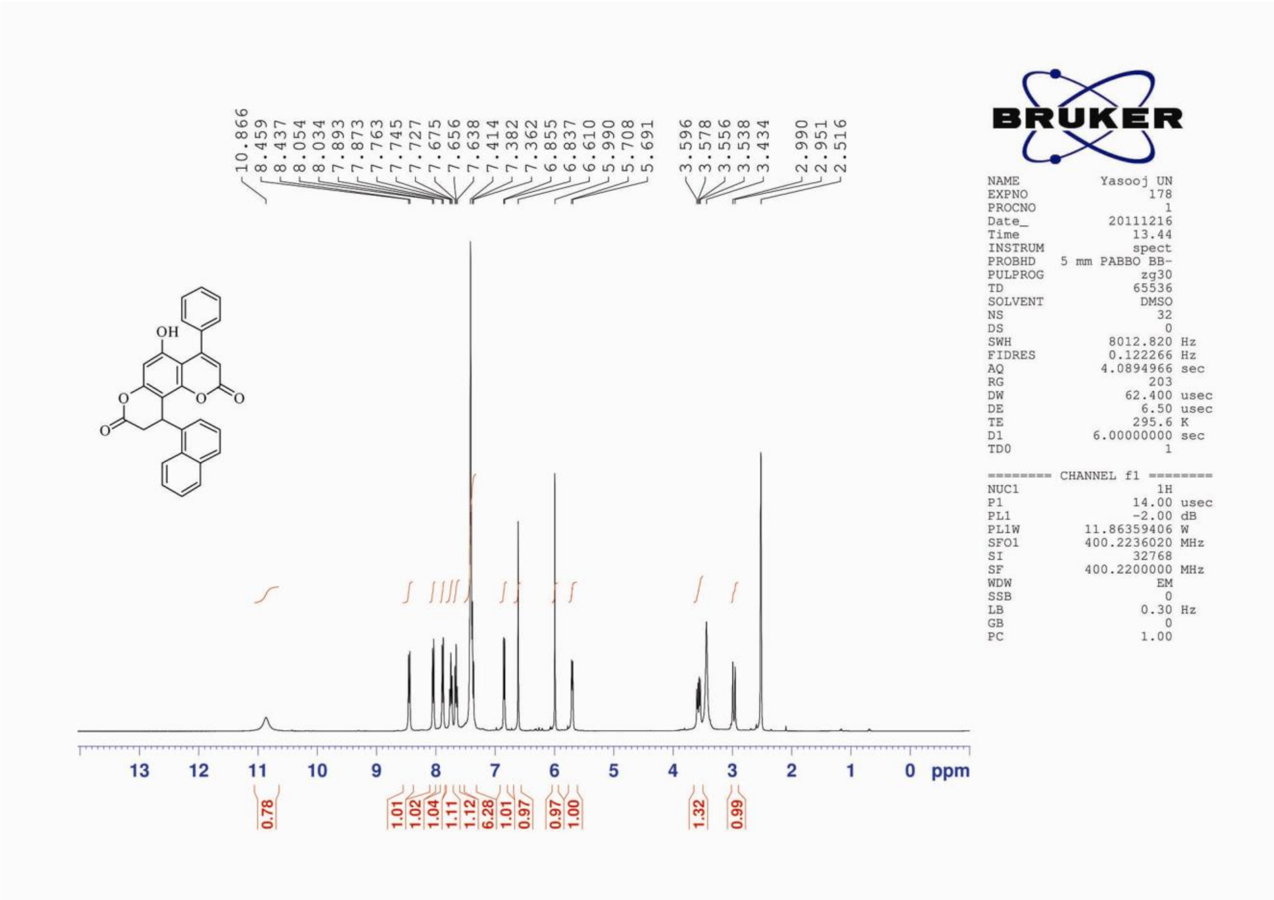
^{1}H NMR (expanded) spectrum of compound **8g**



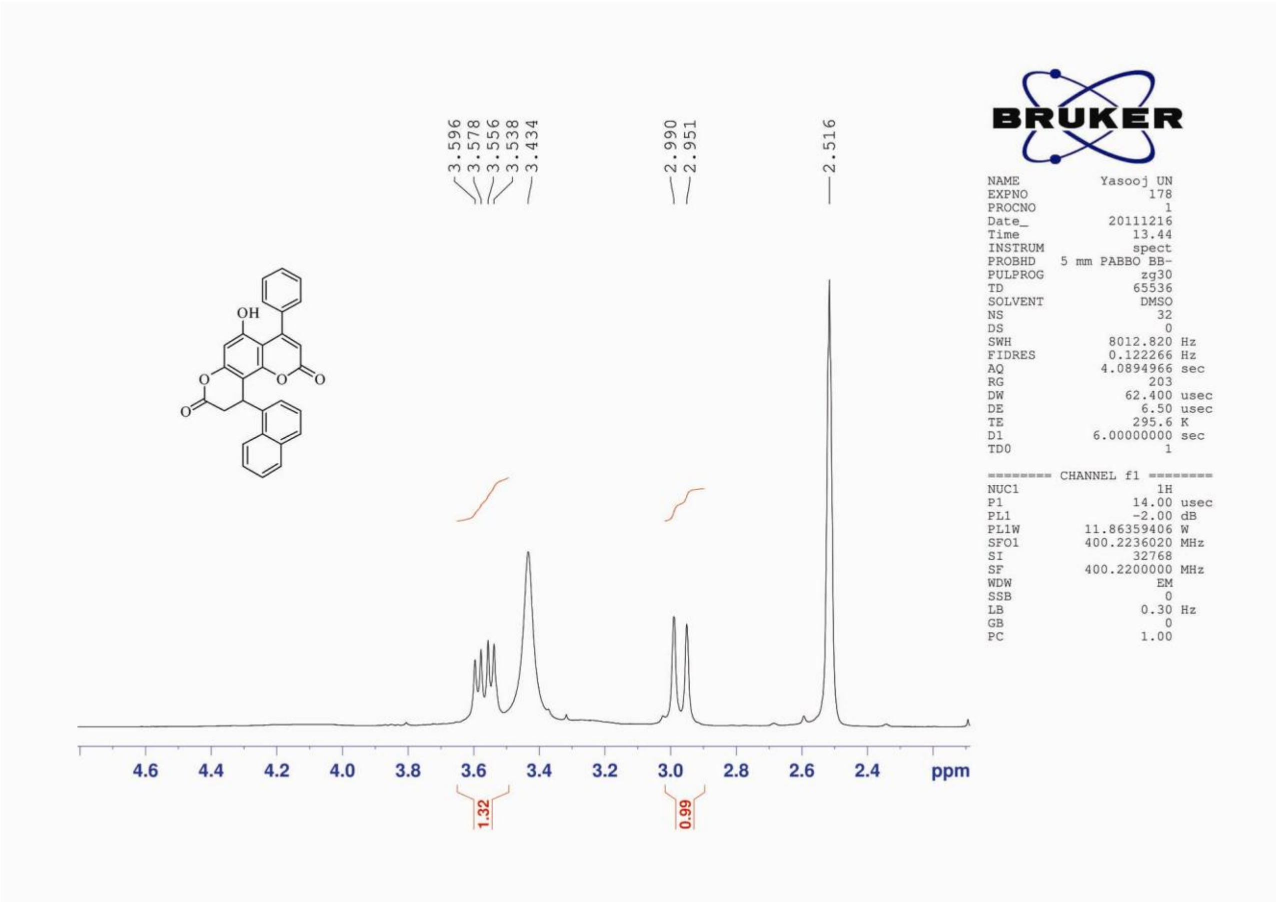
^{1}H NMR (expanded) spectrum of compound **8g**



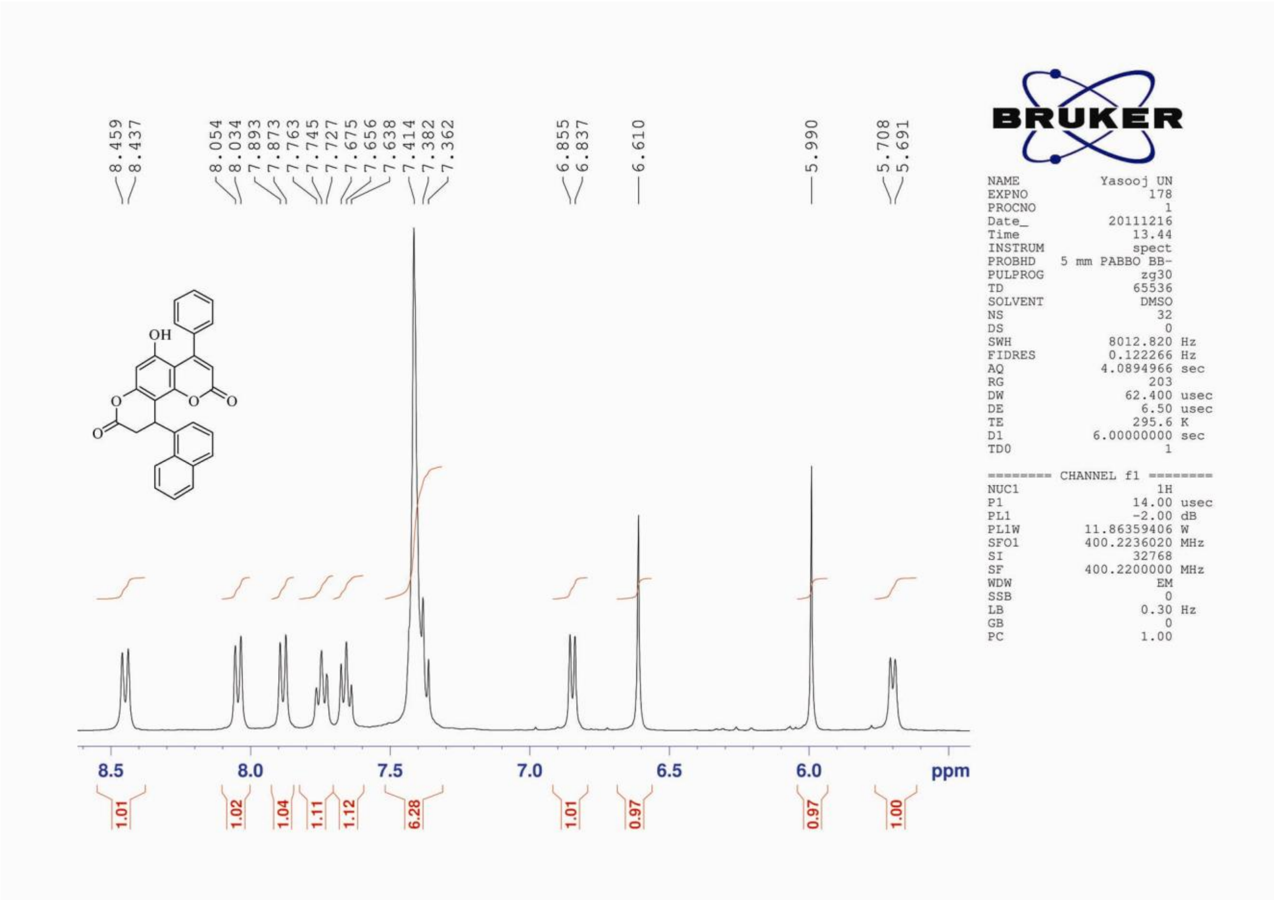
^{13}C NMR spectrum of compound **8h**



^{1}H NMR spectrum of compound **8h**



^{1}H NMR (expanded) spectrum of compound **8h**



^{1}H NMR (expanded) spectrum of compound **8h**

2. Representative spectral data

5-hydroxy-4-methyl-10-phenyl-9,10-dihydropyrano[2,3-h]chromene-2,8-dione (8a). white solids, m.p: 333 °C (decomposed); yield 0.28 g, 88%; IR (KBr) (ν_{max}, cm^{-1}): 3255, 1782, 1694, 1628, 1605, 1382, 1337, 1125, 1094, 847, 736, 700. ^{1}H NMR (400.13 MHz, DMSO-d_6) δ_H 2.51 (s, 3H, CH_3), 2.95 (d, *J*= 16 Hz, 1H, CH), 3.38 (dd, $^2J_{HH}$ = 16.0 Hz, $^3J_{HH}$ = 7.2 Hz, 1H, CH), 4.73 (d, $^3J_{HH}$ = 6.0 Hz, 1H, CH), 6.09 (s, 1H, CH), 6.60 (s, 1H, CH), 7.11 (d, $^3J_{HH}$ = 7.6 Hz, 2H, aromatic CH), 7.24 (t, $^3J_{HH}$ = 6.8 Hz, 1H, aromatic CH), 7.32 (t, $^3J_{HH}$ = 7.2 Hz, 2H, aromatic CH), 11.15 (s, 1H, OH). ^{13}CNMR (100.62 MHz, DMSO-d_6) δ_C 24.07, 34.37, 37.26, 99.98, 106.56, 111.76, 126.96, 127.67, 127.94, 129.44, 141.67, 152.54, 154.40, 155.51, 159.62, 167.24. Anal. Calcd for $C_{19}H_{14}O_5$ (322.31): C, 70.80; H, 4.38. Found: C, 70.68; H, 4.55.

5-hydroxy-4-methyl-10-(2-chlorophenyl)-9,10-dihydropyrano[2,3-h]chromene-2,8-dione (8b). white solids, m.p: 328 °C (decomposed); yield 0.33 g, 92%; IR (KBr) (ν_{max}, cm^{-1}): 3219, 1797, 1680, 1625, 1605, 1136, 1097, 852 and 548. ^{1}H NMR (400.13 MHz, DMSO-d_6) δ_H 2.56 (s, 3H, CH_3), 2.83 (dd, $^2J_{HH}$ = 16 Hz, $^3J_{HH}$ = 1.6 Hz, 1H, CH), 3.47 (dd, $^2J_{HH}$ = 16 Hz, $^3J_{HH}$ = 7.2 Hz, 1H, CH), 5.05 (d, $^3J_{HH}$ = 6.4 Hz, 1H, CH), 6.08 (s, 1H, CH), 6.63 (s, 1H, CH), 6.70 (dd, $^3J_{HH}$ = 7.8 Hz, $^4J_{HH}$ = 1.2 Hz, 1H, aromatic CH), 7.22 (m, 1H, aromatic CH), 7.31 (m, 1H, aromatic CH), 7.56 (q, $^3J_{HH}$ = 8.0 Hz, $^4J_{HH}$ = 1.2 Hz, aromatic CH), 11.24 (s, 1H, OH). ^{13}CNMR (100.62 MHz, DMSO-d_6) δ_C 23.50, 31.70, 35.01, 99.36, 102.27, 106.16, 111.52, 127.30, 127.97, 129.33, 130.22, 132.22, 137.77, 151.90, 154.37, 154.72, 157.54, 158.82, 166.05. Anal. Calcd for $C_{19}H_{13}ClO_5$ (356.76): C, 63.97; H, 3.67. Found: C, 64.08; H, 3.75.

5-hydroxy-4-methyl-10-(2-methoxyphenyl)-9,10-dihydropyrano[2,3-h]chromene-2,8-dione (8c). white solids, m.p: 337 °C (decomposed); yield 0.315 g, 90%; IR (KBr) (ν_{max}, cm^{-1}): 3271, 1778, 1688, 1628, 1605, 1133, 1095, 851, 547. ^{1}H NMR (400.13 MHz, DMSO-d_6) δ_H 2.54 (s, 3H, CH_3), 2.80 (dd, $^2J_{HH}$ = 15.2 Hz, $^3J_{HH}$ = 0.8 Hz, 1H, CH), 3.31 (dd, $^2J_{HH}$ = 16.2 Hz, $^3J_{HH}$ = 8 Hz, 1H, CH), 3.81 (s, 3H, CH_3) 4.82 (d, $^3J_{HH}$ = 7.2 Hz, 1H, CH), 6.05 (s, 1H, CH), 6.57 (s, 1H, CH), 6.74 (dd, $^3J_{HH}$ = 7.4 Hz, $^4J_{HH}$ = 1.6 Hz, 1H, aromatic CH), 6.81 (t, 1H, aromatic CH), 7.03 (d, $^3J_{HH}$ = 8 Hz, 1H, aromatic CH), 7.24 (m, 1H, aromatic CH), 11.09 (s, 1H, OH). ^{13}CNMR (100.62 MHz, DMSO-d_6) δ_C 23.52, 30.30, 34.57, 55.07, 99.18, 102.60, 105.89, 111.26, 120.38, 127.45, 128.51, 128.70, 152.07, 154.25, 154.82, 156.45, 157.02, 159.05, 166.47. Anal. Calcd for $C_{20}H_{16}O_6$ (352.34): C, 68.18; H, 4.58. Found: C, 68.26; H, 4.62.

5-hydroxy-4-methyl-10-(naphthalen-1-yl)-9,10-dihydropyrano[2,3-h]chromene-2,8-dione (8d). white solids, m.p: 350 °C (decomposed); yield 0.325 g, 88%; IR (KBr) (ν_{max}, cm^{-1}): 3226, 1784, 1678, 1624, 1606, 1170, 1134, 1097, 853, 781, 551. ^{1}H NMR (400.13 MHz, DMSO-d_6) δ_H 2.59 (s, 3H, CH_3), 2.90 (d, $^3J_{HH}$ = 15.6 Hz, 1H, CH), 3.52 (dd, $^2J_{HH}$ = 16 Hz, $^3J_{HH}$ = 7.2 Hz, 1H, CH), 5.60 (d, $^3J_{HH}$ = 6.8 Hz, 1H, CH), 6.06 (s, 1H, CH), 6.69 (s, 1H, CH), 6.74 (d, $^3J_{HH}$ = 6.8 Hz, 1H, aromatic CH), 7.33 (t, $^3J_{HH}$ = 7.6 Hz, 1H, aromatic CH), 7.63 (t, $^3J_{HH}$ = 7.6 Hz, 1H, aromatic CH), 7.71 (t, $^3J_{HH}$ = 7.6 Hz, 1H, aromatic CH), 7.85 (d, $^3J_{HH}$ = 8 Hz, 1H, aromatic CH), 8.02 (d, $^3J_{HH}$ = 8 Hz, 1H, aromatic CH), 8.39 (d, $^3J_{HH}$ = 8.8 Hz, 1H, aromatic CH), 11.23 (s, 1H, OH). ^{13}CNMR (100.62 MHz, DMSO-d_6) δ_C 23.55, 30.46, 36.43, 99.42, 103.41, 106.19, 111.43, 122.96, 123.11, 125.49, 126.15, 126.89, 128.01, 129.05, 129.95, 133.85, 136.40, 151.92, 154.62, 154.87, 157.35, 158.96, 166.39. Anal. Calcd for $C_{23}H_{16}O_5$ (372.37): C, 74.19; H, 4.33. Found: C, 74.19; H, 4.32.

5-hydroxy-4-phenyl-10-phenyl-9,10-dihydropyrano[2,3-h]chromene-2,8-dione (8e). pale yellow solids, m.p: 276-277 °C; yield 0.32 g, 85%; IR (KBr) (ν_{max}, cm^{-1}): 3330, 1789, 1732, 1691, 1624, 1601, 1437, 1375, 1332, 1172, 1126, 1090, 767, 699, 611. ^{1}H NMR (400.13 MHz, DMSO-d_6) δ_H 2.99 (d, $^3J_{HH}$ = 16.0 Hz, 1H, CH), 3.44 (m, 1H, CH), 4.81 (d, $^3J_{HH}$ = 6.4 Hz, 1H, CH), 6.00 (s, 1H, CH), 6.50 (s, 1H, CH), 7.18 (d, $^3J_{HH}$ = 7.6 Hz, 2H, aromatic CH), 7.27 (t, $^3J_{HH}$ = 7.2 Hz, 1H, aromatic CH), 7.33-7.40 (m, 7H, aromatic CH), 10.76 (s, 1H, OH). ^{13}CNMR (100.62 MHz, DMSO-d_6) δ_C 34.46, 37.20, 100.02, 104.36, 105.00, 113.53, 127.03, 127.74, 127.85, 127.89, 128.53, 129.49, 139.48, 141.63, 152.71, 154.84, 156.08, 156.80, 159.42, 167.18. Anal. Calcd for $C_{24}H_{16}O_5$ (384.38): C, 74.99; H, 4.20. Found: C, 74.75; H, 4.36.

5-hydroxy-4-phenyl-10-(2-chlorophenyl)-9,10-dihydropyrano[2,3-h]chromene-2,8-dione (8f). pale yellow solids, m.p: 298-300 °C; yield 0.37 g, 90%; IR (KBr) (ν_{max}, cm^{-1}): 3353, 3067, 1778, 1734, 1692, 1621, 1603, 1434, 1375, 1349, 1179, 1136, 1120, 1090, 764, 738, 705, 464. ^{1}H NMR (400.13 MHz, DMSO-d_6) δ_H 2.88 (d, $^3J_{HH}$ = 15.6 Hz, 1H, CH), 3.51 (dd, $^2J_{HH}$ = 16.0 Hz, $^3J_{HH}$ = 7.6 Hz, 1H, CH), 5.14 (d, $^3J_{HH}$ = 6.8 Hz, 1H, CH), 5.99 (s, 1H, CH), 6.54 (s, 1H, CH), 6.79 (d, $^3J_{HH}$ = 7.6 Hz, 1H, CH), 7.26 (t, $^3J_{HH}$ = 7.6 Hz, 1H, aromatic CH), 7.32-7.41 (m, 6H, aromatic CH), 7.59 (d, $^3J_{HH}$ = 7.6 Hz, 1H, aromatic CH), 10.86 (s, 1H, OH). ^{13}CNMR (100.62 MHz, DMSO-d_6) δ_C 32.28, 35.56, 99.96, 102.92, 105.17, 113.63, 127.86, 127.90, 128.53, 128.56, 129.88, 130.77, 132.75, 138.27, 139.38, 152.63, 155.38, 155.94, 157.20, 159.20, 166.52. Anal. Calcd for $C_{24}H_{15}ClO_5$ (418.83): C, 68.82; H, 3.61. Found: C, 68.76; H, 3.68.

5-hydroxy-4-phenyl-10-(2-methoxyphenyl)-9,10-dihydropyrano[2,3-h]chromene-2,8-dione (8g). yellow solids, m.p: 288-290 °C; yield 0.35 g, 86%; IR (KBr) (ν_{max}, cm^{-1}): 3310, 3065, 2839, 1780, 1733, 1697, 1623, 1600, 1493, 1372, 1349, 1245, 1184, 1130, 1101, 1090, 1023, 887, 845, 756, 733, 700, 613. ^{1}H NMR (400.13 MHz, DMSO-d_6) δ_H 2.85 (d, $^3J_{HH}$ = 16.4 Hz, 1H, CH), 3.35 (dd, $^2J_{HH}$ = 16.4 Hz, $^3J_{HH}$ = 8.0 Hz, 1H, CH), 3.84 (s, 3H, OCH_3), 4.90 (d, $^3J_{HH}$ = 7.6 Hz, 1H, CH), 5.96 (s, 1H, CH), 6.48 (s, 1H, CH), 6.86 (d, $^3J_{HH}$ = 4.8 Hz, 2H, aromatic CH), 7.06 (d, $^3J_{HH}$ = 8.4 Hz, 1H, aromatic CH), 7.25-7.29 (m, 1H, aromatic CH), 7.35-7.43 (m, 5H, aromatic CH), 10.71 (s, 1H, OH). ^{13}CNMR (100.62 MHz, DMSO-d_6) δ_C 31.03, 35.08, 55.56, 99.78, 103.22, 104.91, 111.82, 113.32, 120.94, 127.83, 127.88, 128.18, 128.49, 129.07, 129.26, 139.50, 152.83, 155.26, 156.08, 156.69, 157.01, 159.41, 166.91. Anal. Calcd for $C_{25}H_{18}O_6$ (414.41): C, 72.46; H, 4.38. Found: C, 72.33; H, 4.45.

5-hydroxy-4-phenyl-10-(naphthalen-1-yl)-9,10-dihydropyrano[2,3-h]chromene-2,8-dione (8h). orange solids, m.p: 285-286 °C; yield 0.36 g, 84%; IR (KBr) (ν_{max}, cm^{-1}): 3337, 3062, 1783, 1732, 1697, 1622, 1603, 1437, 1357, 1240, 1166, 1129, 1090, 1014, 889, 855, 776, 703, 615, 593, 458. ^{1}H NMR (400.13 MHz, DMSO-d_6) δ_H 2.97 (d, $^3J_{HH}$ = 15.6 Hz, 1H, CH), 3.56 (dd, $^2J_{HH}$ = 16.0 Hz, $^3J_{HH}$ = 7.2 Hz, 1H, CH), 5.70 (d, $^3J_{HH}$ = 6.8 Hz, 1H, CH), 5.99 (s, 1H, CH), 6.61 (s, 1H, CH), 6.84 (d, $^3J_{HH}$ = 7.2 Hz, 1H, aromatic CH), 7.36-7.41 (m, 6H, aromatic CH), 7.65 (t, $^3J_{HH}$ = 7.6 Hz, 1H, aromatic CH), 7.74 (t, $^3J_{HH}$ = 7.2 Hz, 1H, aromatic CH), 7.88 (d, $^3J_{HH}$ = 8.0 Hz, 1H, aromatic CH), 8.04 (d, $^3J_{HH}$ = 8.0 Hz, 1H, aromatic CH), 8.44 (d, $^3J_{HH}$ = 8.8 Hz, 1H, aromatic CH), 10.86 (s, 1H, OH). ^{13}CNMR (100.62 MHz, DMSO-d_6) δ_C 31.07, 36.98, 100.03, 104.04, 105.22, 113.52, 123.60, 123.65, 126.04, 126.69, 127.43, 127.87, 127.92, 128.58, 129.60, 130.49, 134.40, 136.88, 139.47, 152.66, 155.66, 156.10, 157.05, 159.34, 166.87. Anal. Calcd for $C_{28}H_{18}O_5$ (434.44): C, 77.41; H, 4.18. Found: C, 77.37; H, 4.23.