

SUPPLEMENTARY INFORMATION

A redox active organodiselenide as an efficacious catalyst for synthesis of oxygen containing heterocyclic compounds

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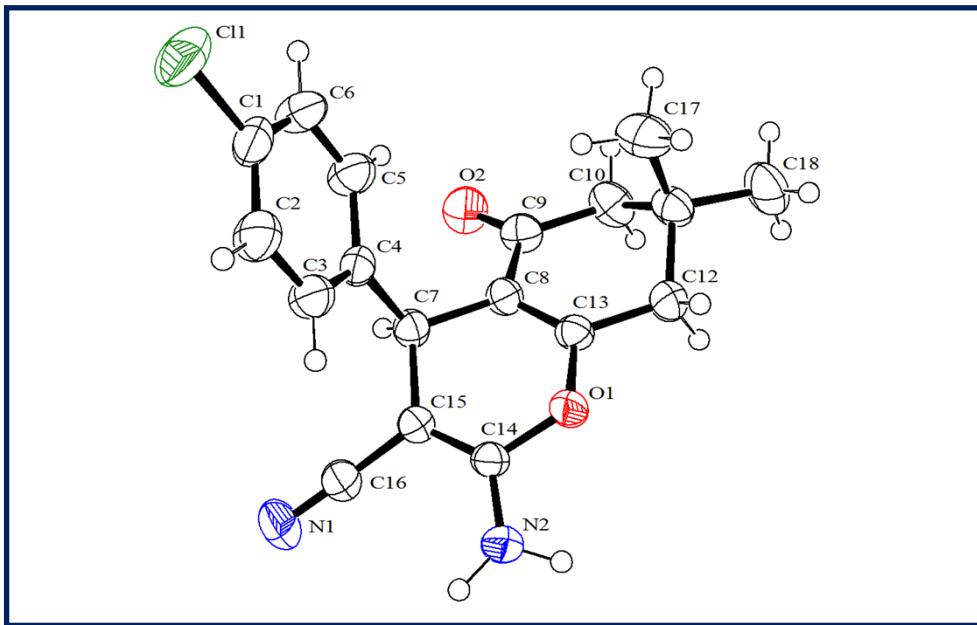
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1. X Ray Crystallography Data for the compound 4a



X-ray crystallography data for compound **4a** (CCDC NO. 2249462)

Datablock: shelx

Bond precision: C-C = 0.0045 Å Wavelength=1.54184

Cell: a=9.4113(1) b=16.8257(1) c=10.9139(1)

alpha=90

beta=112.124(1)

gamma=90

Temperature: 298 K

	Calculated	Reported
Volume	1600.99(3)	1600.99(3)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C18 H17 Cl N2 O2	?
Sum formula	C18 H17 Cl N2 O2	C18 H17 Cl N2 O2
Mr	328.79	328.79
Dx, g cm ⁻³	1.364	1.364
Z	4	4
Mu (mm ⁻¹)	2.204	2.204
F000	688.0	688.0
F000'	691.31	
h,k,lmax	11,21,13	11,21,13
Nref	3398	3363
Tmin, Tmax	0.876, 0.896	0.683, 1.000
Tmin'	0.802	

Correction method= # Reported T Limits: Tmin=0.683 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.990 Theta (max)= 77.336

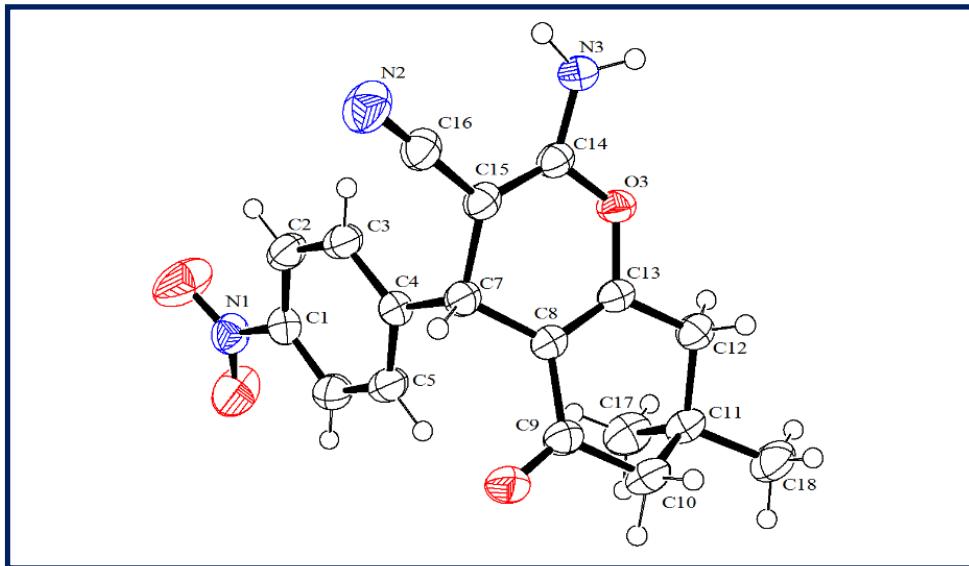
R(reflections)= 0.0655(2879)

wR2 (reflections)=
0.2959(3363)

S = 1.085

Npar= 218

2. X Ray Crystallography Data for the compound 4c



X-ray crystallography data for compound 4c (CCDC NO. 2249461)

Datablock: shelx

Bond precision:	C-C = 0.0029 Å	Wavelength=1.54184	
Cell:	a=15.8444 (1)	b=6.5350 (1)	c=16.2557 (1)
	alpha=90	beta=98.636 (1)	gamma=90
Temperature:	298 K		

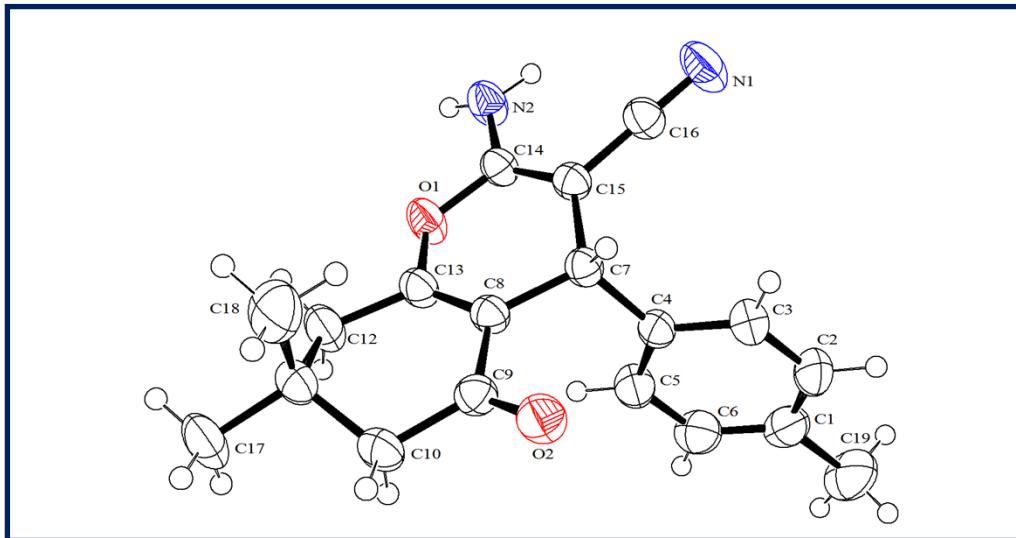
	Calculated	Reported
Volume	1664.08 (3)	1664.08 (3)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C19 H20 N2 O2	?
Sum formula	C19 H20 N2 O2	C19 H20 N2 O2
Mr	308.37	308.37
Dx, g cm ⁻³	1.231	1.231
Z	4	4
μ (mm ⁻¹)	0.643	0.643
F000	656.0	656.0
F000'	657.91	
h,k,lmax	20,8,20	19,8,20
Nref	3518	3468
Tmin, Tmax	0.938, 0.968	0.520, 1.000
Tmin'	0.938	

Correction method= # Reported T Limits: Tmin=0.520 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.986 Theta (max)= 77.073

R(reflections)= 0.0658 (3067)	wR2(reflections)= 0.2688 (3468)
S = 1.150	Npar= 220

3. X Ray Crystallography Data for the compound 4i



X-ray crystallography data for compound **4i** (CCDC NO. 2249463)

Datablock: shelx

Bond precision: C-C = 0.0020 Å Wavelength=1.54184

Cell: a=9.5870(1) b=16.5558(1) c=10.7117(1)
 alpha=90 beta=111.072(1) gamma=90

Temperature: 298 K

	Calculated	Reported
Volume	1586.48(3)	1586.47(3)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C18 H17 N3 O4	?
Sum formula	C18 H17 N3 O4	C18 H17 N3 O4
Mr	339.35	339.34
Dx, g cm ⁻³	1.421	1.421
Z	4	4
Mu (mm ⁻¹)	0.848	0.848
F000	712.0	712.0
F000'	714.33	
h, k, lmax	12, 20, 13	12, 20, 13
Nref	3347	3288
Tmin, Tmax	0.919, 0.958	0.712, 1.000
Tmin'	0.919	

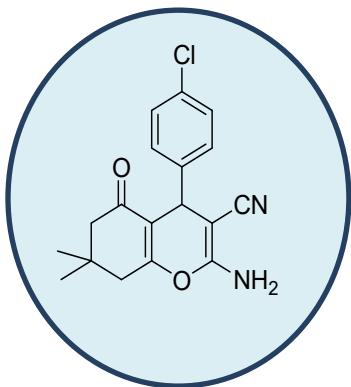
Correction method= # Reported T Limits: Tmin=0.712 Tmax=1.000
 AbsCorr = MULTI-SCAN

Data completeness= 0.982 Theta(max) = 76.864

R(reflections)= 0.0395(2904)	wR2(reflections)= 0.1347(3288)
S = 1.147	Npar= 237

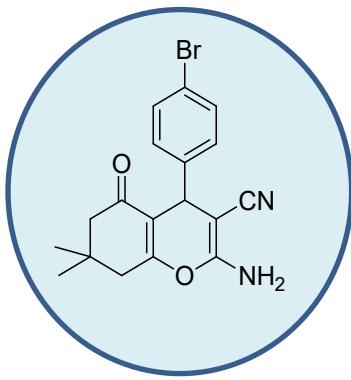
SPECTRAL DATA OF THE SYNTHESIZED COMPOUNDS

2-amino-4-(4-chlorophenyl)-5,6,7,8-tetrahydro-7,7-dimethyl-5-oxo-4H-chromene-3-carbonitrile, 4a



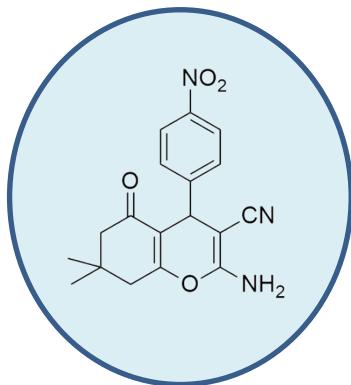
Off white solid, m.p. 213-215 °C,
 IR (KBr): ν 3381, 3185, 2953, 2187, 1672, 1633, 1495, 1240 cm⁻¹.
¹H NMR (400 MHz, DMSO-d₆): δ 7.32 (d, J = 7.9 Hz, 2H), 7.15 (d, J = 8.0 Hz, 2H), 7.01 (s, 2H), 4.17 (s, 1H), 2.49 (s, 2H), 2.23 (d, J = 16.1 Hz, 1H), 2.07 (d, J = 16.0 Hz, 1H), 1.01 (s, 3H), 0.92 (s, 3H) ppm. ¹³C NMR (100 MHz, DMSO-d₆): δ 196.40, 163.22, 158.93, 144.13, 131.61, 129.54, 128.75, 120.02, 112.73, 58.29, 50.37, 35.53, 32.22, 28.72, 27.26 ppm.

2-amino-4-(4-bromophenyl)-5,6,7,8-tetrahydro-7,7-dimethyl-5-oxo-4H-chromene-3-carbonitrile, 4b



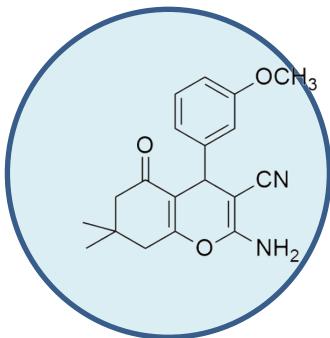
White solid, m.p. 203-205 °C,
 IR (KBr): ν 3379, 3283, 3192, 2965, 2194, 1676, 1607, 1489, 1258 cm⁻¹. ¹H NMR (400 MHz, DMSO-d₆): δ 7.33 (d, J = 7.5 Hz, 2H), 7.16 (d, J = 7.5 Hz, 2H), 7.03 (s, 2H), 4.18 (s, 1H), 2.49 (s, 2H), 2.23 (d, J = 16.0 Hz, 1H), 2.08 (d, J = 16.0 Hz, 1H), 1.01 (s, 3H), 0.93 (s, 3H) ppm. ¹³C NMR (100 MHz, DMSO-d₆): δ 196.24, 163.13, 158.94, 144.16, 131.59, 129.56, 128.75, 120.01, 112.76, 58.26, 50.38, 35.55, 32.23, 28.74, 27.29 ppm.

2-amino-4-(4-nitrophenyl)-5,6,7,8-tetrahydro-7,7-dimethyl-5-oxo-4H-chromene-3-carbonitrile, 4c



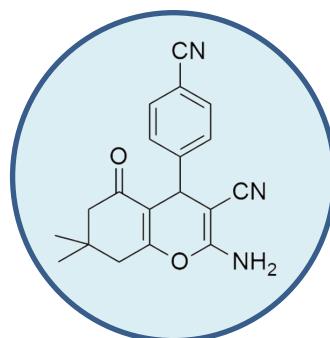
White solid, m.p. 178-179 °C,
 IR (KBr): ν 3391, 3317, 3215, 2964, 2191, 1673, 1607, 1484, 1257 cm⁻¹. ¹H NMR (400 MHz, DMSO-d₆): δ 8.15 (d, J = 6.9 Hz, 2H), 7.43 (d, J = 6.9 Hz, 2H), 7.15 (s, 2H), 4.35 (s, 1H), 2.52 (s, 2H), 2.25 (d, J = 15.8 Hz, 1H), 2.09 (d, J = 15.9 Hz, 1H), 1.02 (s, 3H), 0.94 (s, 3H) ppm. ¹³C NMR (100 MHz, DMSO-d₆): δ 196.27, 163.63, 159.03, 152.72, 146.71, 129.06, 124.12, 119.78, 112.16, 57.48, 50.31, 36.10, 32.25, 28.68, 27.37 ppm

2-amino-4-(3-methoxyphenyl)-5,6,7,8-tetrahydro-7,7-dimethyl-5-oxo-4H-chromene-3-carbonitrile, 4d



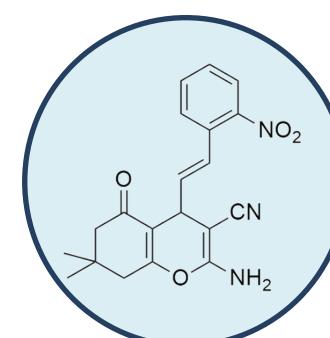
White solid, m.p. 210-211 °C,
 IR (KBr): ν 3381, 3192, 2188, 1689, 1604, 1098 cm⁻¹. ¹H NMR (400 MHz, DMSO-d₆): δ 7.19 (t, J = 7.6 Hz, 1H), 6.97 (s, 2H), 6.72 (dd, J = 14.9, 7.9 Hz, 2H), 6.64 (s, 1H), 4.13 (s, 1H), 3.69 (s, 3H), 2.50 (s, 2H), 2.25 (d, J = 16.1 Hz, 1H), 2.10 (d, J = 16.1 Hz, 1H), 1.02 (s, 3H), 0.95 (s, 3H). ¹³C NMR (100 MHz, DMSO-d₆): δ 196.22, 163.10, 159.66, 146.74, 129.92, 120.14, 119.78, 113.68, 113.03, 111.91, 55.36, 50.41, 35.89, 32.22, 28.87, 27.17 ppm.

2-amino-4-(4-cyanophenyl)-5,6,7,8-tetrahydro-7,7-dimethyl-5-oxo-4H-chromene-3-carbonitrile, 4e



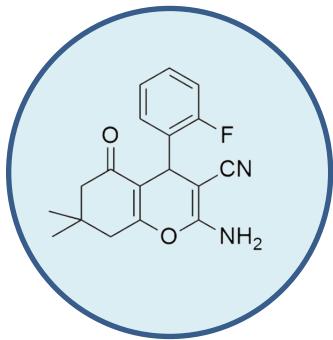
Off white solid, m.p. 224-225 °C °C,
 IR (KBr): ν 3398, 3324, 3213, 2964, 2227, 1686, 1658, 1605, 1215, 859 cm⁻¹. ¹H NMR (400 MHz, DMSO-d₆): δ 7.75 (d, J = 7.5 Hz, 2H), 7.34 (d, J = 7.6 Hz, 2H), 7.11 (s, 1H), 4.27 (s, 1H), 2.50 – 2.44 (m, 2H), 2.24 (d, J = 16.0 Hz, 1H), 2.09 (d, J = 16.0 Hz, 1H), 1.02 (s, 3H), 0.93 (s, 3H) ppm. ¹³C NMR (100 MHz, DMSO-d₆): δ 196.27, 163.59, 158.99, 150.66, 132.86, 128.79, 119.80, 119.22, 112.18, 109.88, 57.59, 50.31, 36.24, 32.26, 28.66, 27.38 ppm.

2-amino-7,7-dimethyl-4-(2-nitrostyryl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile, 4f



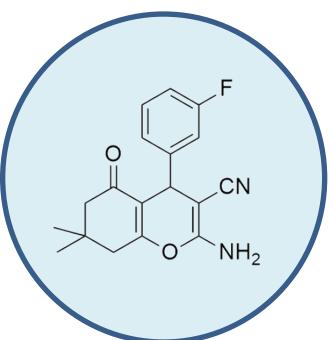
White solid, m.p. 185-187 °C,
 IR (KBr): ν 3388, 3293, 3025, 2956, 2187, 1681, 1658, 1604, 1377, 1243 cm⁻¹. ¹H NMR (400 MHz, DMSO-d₆): 7.89 (d, J = 7.8 Hz, 2H), 7.58 (ddd, J = 47.8, 14.1, 7.0 Hz, 1H), 7.10 (s, 2H), 6.65 (d, J = 15.6 Hz, 1H), 6.24 (dd, J = 15.5, 6.6 Hz, 1H), 3.86 (d, J = 6.2 Hz, 2H), 2.49-2.16 (m, 4H), 1.02 (s, 3H), 0.99 (s, 3H) ppm. ¹³C NMR (100 MHz, DMSO-d₆): δ 196.40, 163.28, 159.91, 148.14, 137.11, 133.72, 131.29, 128.99, 128.42, 124.63, 124.03, 120.11, 111.96, 54.88, 50.46, 33.17, 32.22, 28.79, 27.21 ppm.

2-amino-4-(2-fluorophenyl)-5,6,7,8-tetrahydro-7,7-dimethyl-5-oxo-4H-chromene-3-carbonitrile, 4g



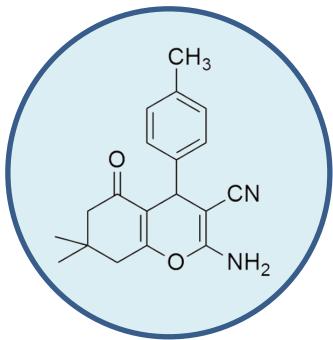
White solid, m.p. 213-215 °C,
IR (KBr): ν 3471, 3324, 3015, 2961, 2870, 2198, 1653, 1607, 1470, 1368, 1249 cm⁻¹. ¹H NMR (400 MHz, DMSO-d₆): δ 7.29 – 7.06 (m, 4H), 6.98 (s, 2H), 4.44 (s, 1H), 2.49 (q, J = 17.7 Hz, 1H), 2.24 (d, J = 16.1 Hz, 1H), 2.06 (d, J = 16.1 Hz, 1H), 1.02 (s, 3H), 0.93 (s, 3H) ppm. ¹³C NMR (100 MHz, DMSO-d₆): δ 196.30, 163.71, 159.23, 158.77, 131.62, 131.46, 130.08, 129.14, 129.05, 124.90, 111.80, 56.56, 50.32, 32.20, 30.28, 28.90, 26.97 ppm.

2-amino-4-(3-fluorophenyl)-5,6,7,8-tetrahydro-7,7-dimethyl-5-oxo-4H-chromene-3-carbonitrile, 4h



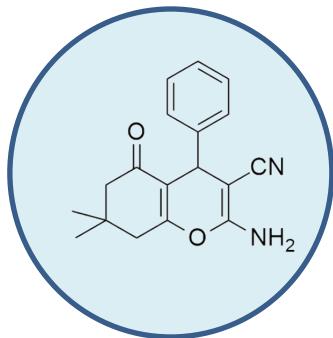
White solid, m.p. 211-212 °C,
IR (KBr): ν 3473, 3327, 3009, 2970, 2868, 2195, 1652, 1609, 1473, 1366, 1247 cm⁻¹. ¹H NMR (400 MHz, DMSO-d₆): δ 7.32 (d, J = 5.7 Hz, 1H), 6.97 (dd, J = 27.8, 10.9 Hz, 4H), 4.22 (s, 1H), 2.51 (s, 2H), 2.24 (d, J = 15.8 Hz, 1H), 2.11 (d, J = 15.9 Hz, 1H), 1.02 (s, 3H), 0.94 (s, 3H) ppm. ¹³C NMR (100 MHz, DMSO-d₆): δ 196.26, 163.32, 158.99, 148.10, 130.79, 130.70, 123.68, 119.98, 114.01, 113.73, 112.63, 58.21, 50.39, 35.77, 32.23, 28.69, 27.32 ppm.

2-amino-7,7-dimethyl-5-oxo-4-(*p*-tolyl)-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile, 4i



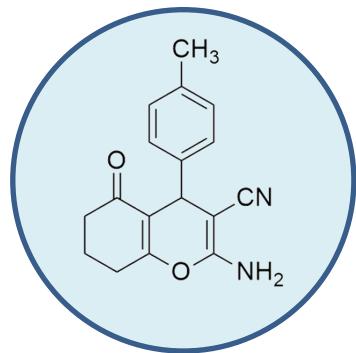
Off white solid, m.p. 215-217 °C,
IR (KBr): ν 3424, 3328, 3025, 2953, 2197, 1675, 1637, 1511, 1249 cm⁻¹. ¹H NMR (400 MHz, DMSO-d₆): δ 7.08 – 6.98 (m, 4H), 6.91 (s, 2H), 4.10 (s, 1H), 2.23 (d, J = 9.4 Hz, 4H), 2.06 (d, J = 16.1 Hz, 1H), 1.01 (s, 3H), 0.92 (s, 3H) ppm. ¹³C NMR (100 MHz, DMSO-d₆): δ 196.36, 162.90, 158.89, 142.19, 136.18, 129.36, 127.49, 120.23, 113.28, 58.99, 50.42, 35.59, 32.21, 28.84, 27.16, 21.00 ppm.

2-amino-7,7-dimethyl-5-oxo-4-phenyl-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile, 4j



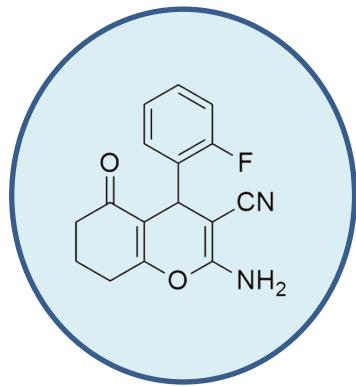
Off white solid, m.p. 225-227 °C,
 IR (KBr): ν 3398, 3326, 3211, 3026, 2963, 2201, 1686, 1602, 1247 cm⁻¹. ¹H NMR (400 MHz, DMSO-d₆): δ 7.27-7.14 (m, 5H), 6.08 (s, 2H), 4.16 (s, 1H), 2.51 (s, 2H), 2.23 (d, 1H, *J* = 16 Hz), 2.12 (d, 1H, *J* = 16 Hz), 1.03 (s, 3H), 0.95 (s, 3H) ppm. ¹³C NMR (100 MHz, DMSO-d₆): δ 196.33, 163.07, 158.94, 145.14, 128.82, 127.57, 127.08, 120.19, 113.16, 58.83, 50.42, 36.00, 32.24, 28.83, 27.22 ppm.

2-amino-5-oxo-4-(*p*-tolyl)-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile, 5a



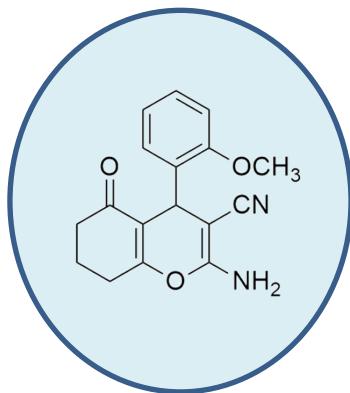
White solid, m.p. 211-213 °C,
 IR (KBr): ν 3411, 3334, 3217, 2195, 1680, 1661, 1604, 1363 cm⁻¹.
¹H NMR (400 MHz, DMSO-d₆): δ 7.02 (d, 2H, *J* = 8 Hz), 6.99 (d, 2H, *J* = 8 Hz), 6.86 (s, 2H), 4.10 (s, 1H), 2.57-2.27 (m, 4H), 2.21 (s, 3H), 1.92-1.85 (m, 2H) ppm. ¹³C NMR (100 MHz, DMSO-d₆): δ 196.44, 164.78, 158.87, 142.23, 136.10, 129.33, 127.46, 120.21, 114.38, 58.91, 36.78, 35.45, 26.88, 20.99, 20.24 ppm.

2-amino-4-(2-fluorophenyl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile, 5b



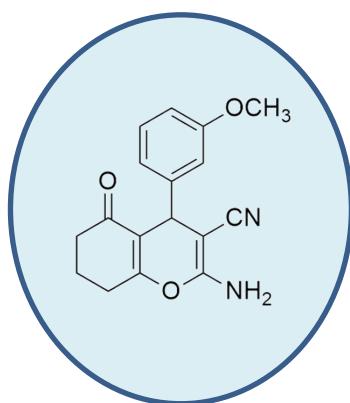
White solid, m.p. 214-216 °C,
 IR (KBr): ν 3329, 3255, 3183, 2957, 2191, 1653, 1607, 1472, 1369 cm⁻¹. ¹H NMR (400 MHz, DMSO-d₆): δ 7.21 – 7.02 (m, 4H), 6.94 (s, 2H), 4.43 (s, 1H), 2.58 (t, *J* = 5.4 Hz, 2H), 2.24 (dt, *J* = 12.0, 5.9 Hz, 2H), 1.91 (dd, *J* = 12.3, 6.4 Hz, 2H) ppm. ¹³C NMR (100 MHz, DMSO-d₆): δ 196.38, 165.60, 160.47, 159.13, 129.90, 128.93, 124.97, 119.92, 115.91, 112.88, 57.32, 36.69, 29.90, 26.89, 20.27 ppm.

2-amino-4-(2-methoxyphenyl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile, 5c



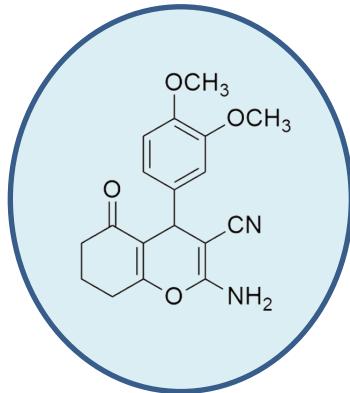
White solid, m.p. 208-210 °C,
 IR (KBr): ν 3382, 3325, 3190, 2962, 2187, 1685, 1606, 1099 cm⁻¹.
¹H NMR (400 MHz, DMSO-d₆): δ 7.12 (t, J = 7.4 Hz, 1H), 6.93 (t, J = 6.6 Hz, 2H), 6.81 (t, J = 7.2 Hz, 1H), 6.72 (s, 2H), 4.50 (s, 1H), 3.73 (s, 3H), 2.53 (d, J = 29.9 Hz, 2H), 2.33 – 2.09 (m, 2H), 2.04 – 1.69 (m, 2H) ppm. ¹³C NMR (100 MHz, DMSO-d₆): δ 196.37, 165.57, 159.36, 157.25, 132.92, 128.52, 128.20, 120.96, 120.24, 113.53, 112.11, 58.16, 56.15, 36.85, 30.08, 26.93, 20.37 ppm.

2-amino-4-(3-methoxyphenyl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile, 5d



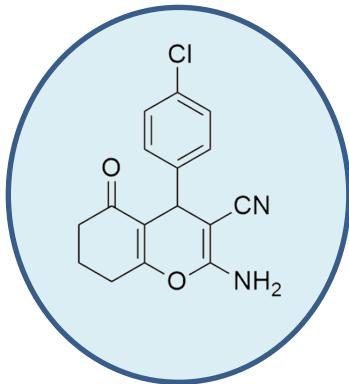
White solid, m.p. 210-212 °C,
 IR (KBr): ν 3392, 3315, 3214, 2959, 2197, 1677, 1604, 1487, 1259 cm⁻¹. ¹H NMR (400 MHz, DMSO-d₆): δ 7.17 (t, J = 7.7 Hz, 1H), 6.91 (s, 2H), 6.80 – 6.58 (m, 3H), 4.12 (s, 1H), 3.68 (s, 3H), 2.59 – 2.57 (m, 4H), 1.93-1.87 (m, 2H) ppm. ¹³C NMR (100 MHz, DMSO-d₆): δ 196.47, 165.06, 159.65, 158.95, 146.73, 129.93, 119.71, 114.10, 113.74, 111.85, 58.63, 55.37, 36.77, 35.73, 26.88, 20.24 ppm.

2-amino-4-(3,4-dimethoxyphenyl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile, 5e



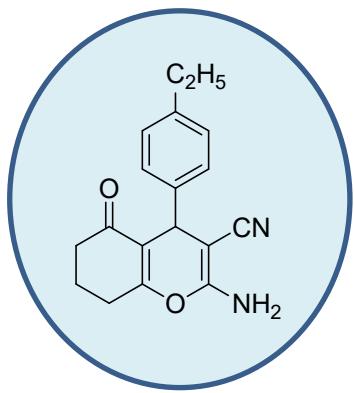
White solid, m.p. 214-217 °C,
 IR (KBr): ν 3388, 3316, 3215, 2960, 2198, 1677, 1603, 1489, 1254 cm⁻¹. ¹H NMR (400 MHz, DMSO-d₆): δ 6.96 – 6.75 (m, 3H), 6.68 (s, 1H), 6.61 (d, J = 7.9 Hz, 1H), 3.68 (s, 6H), 2.57 (s, 2H), 2.24 (s, 2H), 1.99 – 1.78 (m, 2H) ppm. ¹³C NMR (100 MHz, DMSO-d₆): δ 196.55, 164.77, 158.85, 148.89, 148.01, 137.78, 120.29, 119.43, 114.34, 112.39, 111.65, 58.91, 55.96, 36.83, 35.28, 26.90, 20.28 ppm.

2-amino-4-(4-chlorophenyl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile, 5f



White solid, m.p. 221-223 °C,
 IR (KBr): ν 3416, 3338, 3215, 2190, 1682, 1649, 1600, 1519, 1367 cm⁻¹. ¹H NMR (400 MHz, DMSO-d₆): δ 7.30 (d, *J* = 7.7 Hz, 2H), 7.14 (d, *J* = 7.8 Hz, 2H), 6.96 (s, 2H), 4.16 (s, 1H), 2.57 (s, 2H), 2.30 – 2.15 (m, 2H), 1.90 (dd, *J* = 11.2, 5.7 Hz, 2H) ppm. ¹³C NMR (100 MHz, DMSO-d₆): δ 196.50, 165.18, 158.90, 144.18, 131.57, 129.51, 128.73, 113.79, 58.27, 36.73, 35.43, 26.90, 20.18 ppm.

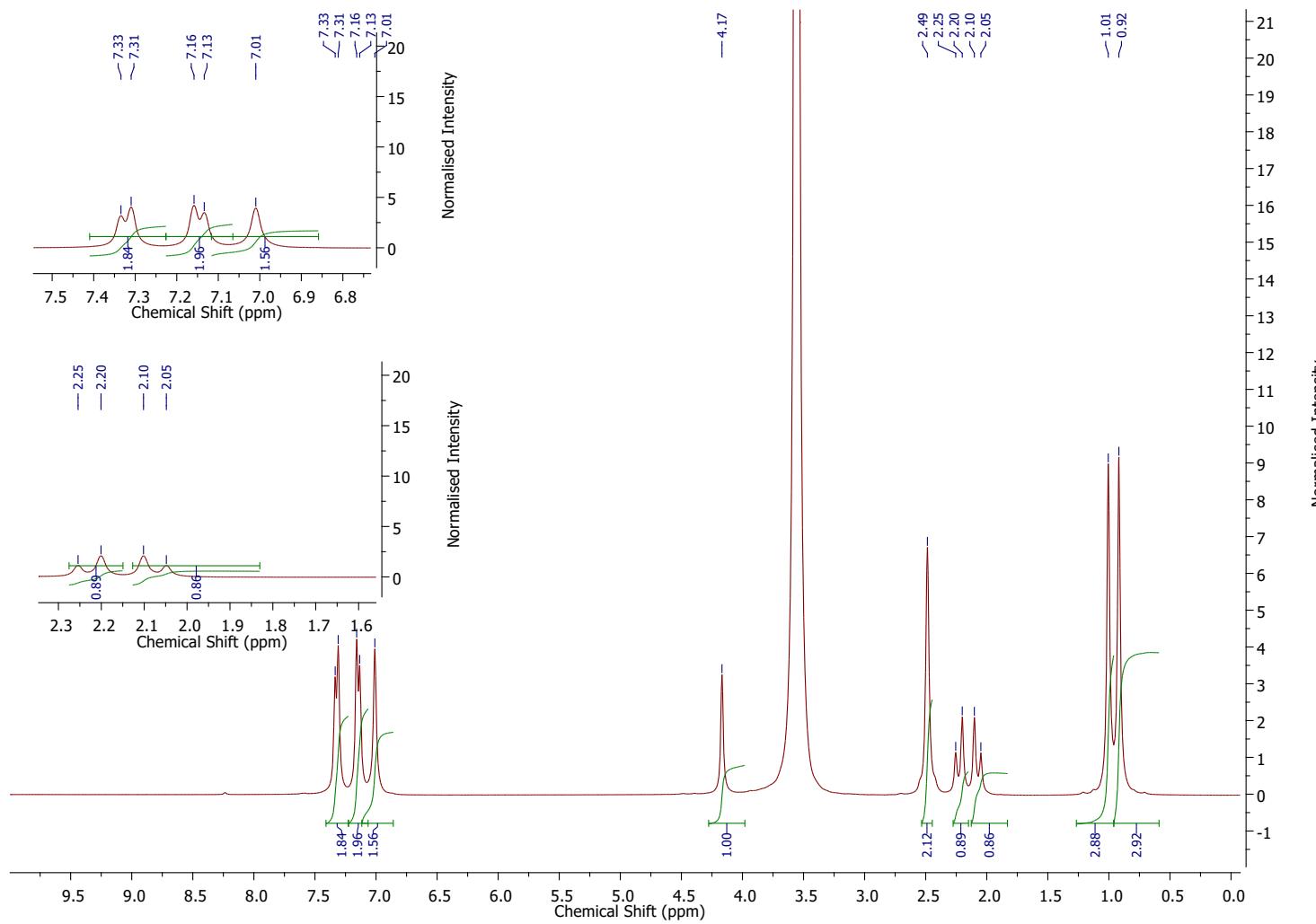
2-amino-4-(2-ethylphenyl)-5-oxo-5,6,7,8-tetrahydro-4H-chromene-3-carbonitrile, 5g



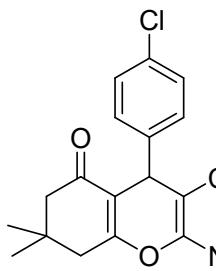
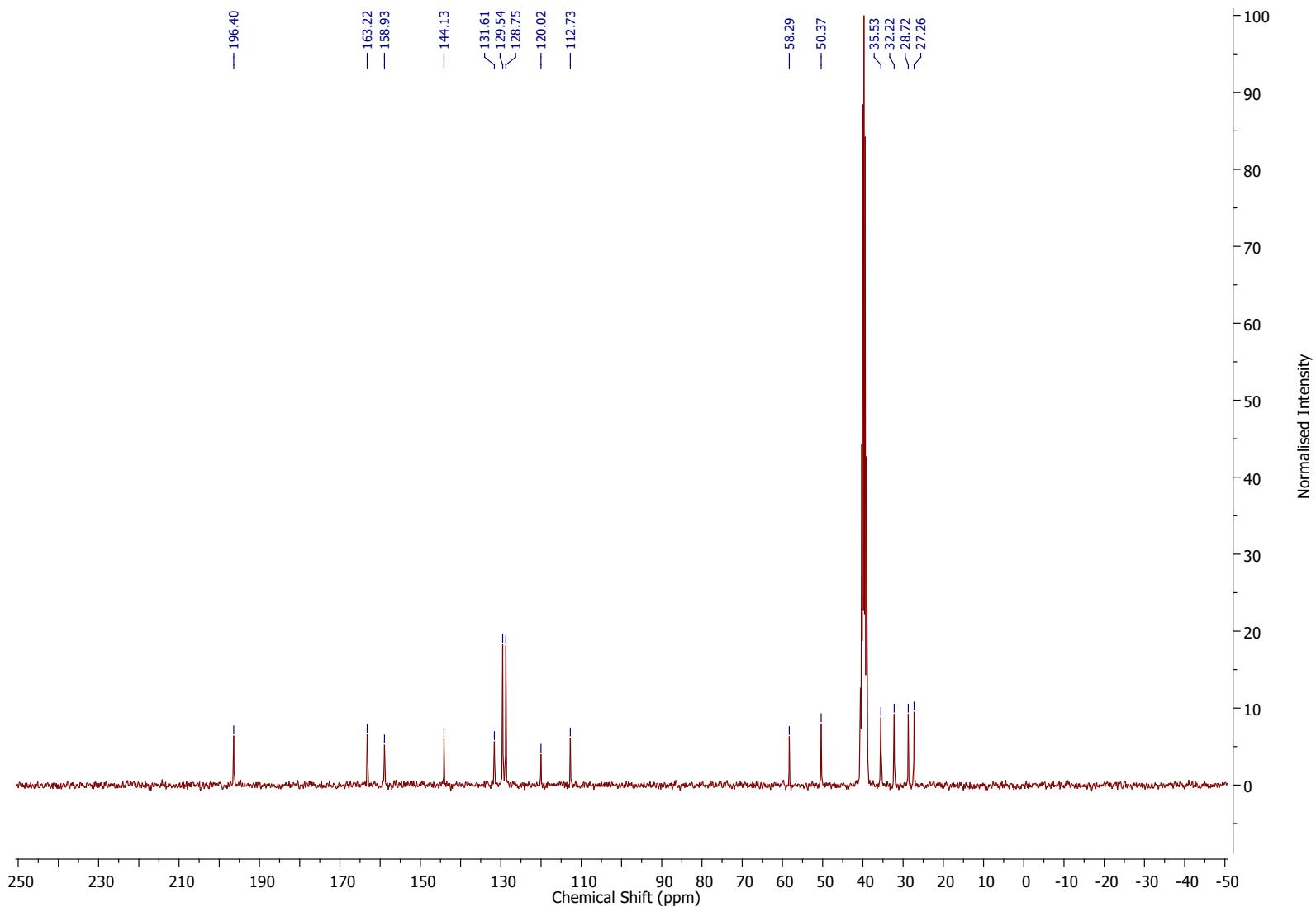
White solid, m.p. 213-215 °C,
 IR (KBr): ν 3328, 3254, 3182, 2955, 2190, 1650, 1606, 1470, 1368 cm⁻¹. ¹H NMR (400 MHz, DMSO-d₆): δ 7.08 (d, *J* = 8 Hz, 2H), 7.01 (d, *J* = 8 Hz, 2H), 6.87 (s, 4H), 4.11 (s, 1H), 2.57-2.47 (m, 2H), 2.27-2.21 (m, 2H), 1.93-1.84 (m, 2H), 1.93-1.44 (m, 3H), 1.12 (t, *J* = 7.5 Hz, 2H) ppm. ¹³C NMR (100 MHz, DMSO-d₆): δ 196.48, 164.86, 158.89, 142.44, 128.17, 127.46, 120.25, 114.37, 58.91, 36.78, 35.45, 28.16, 26.88, 20.23, 15.93 ppm.

¹H & ¹³C NMR SPECTRA OF THE SYNTHESIZED COMPOUNDS

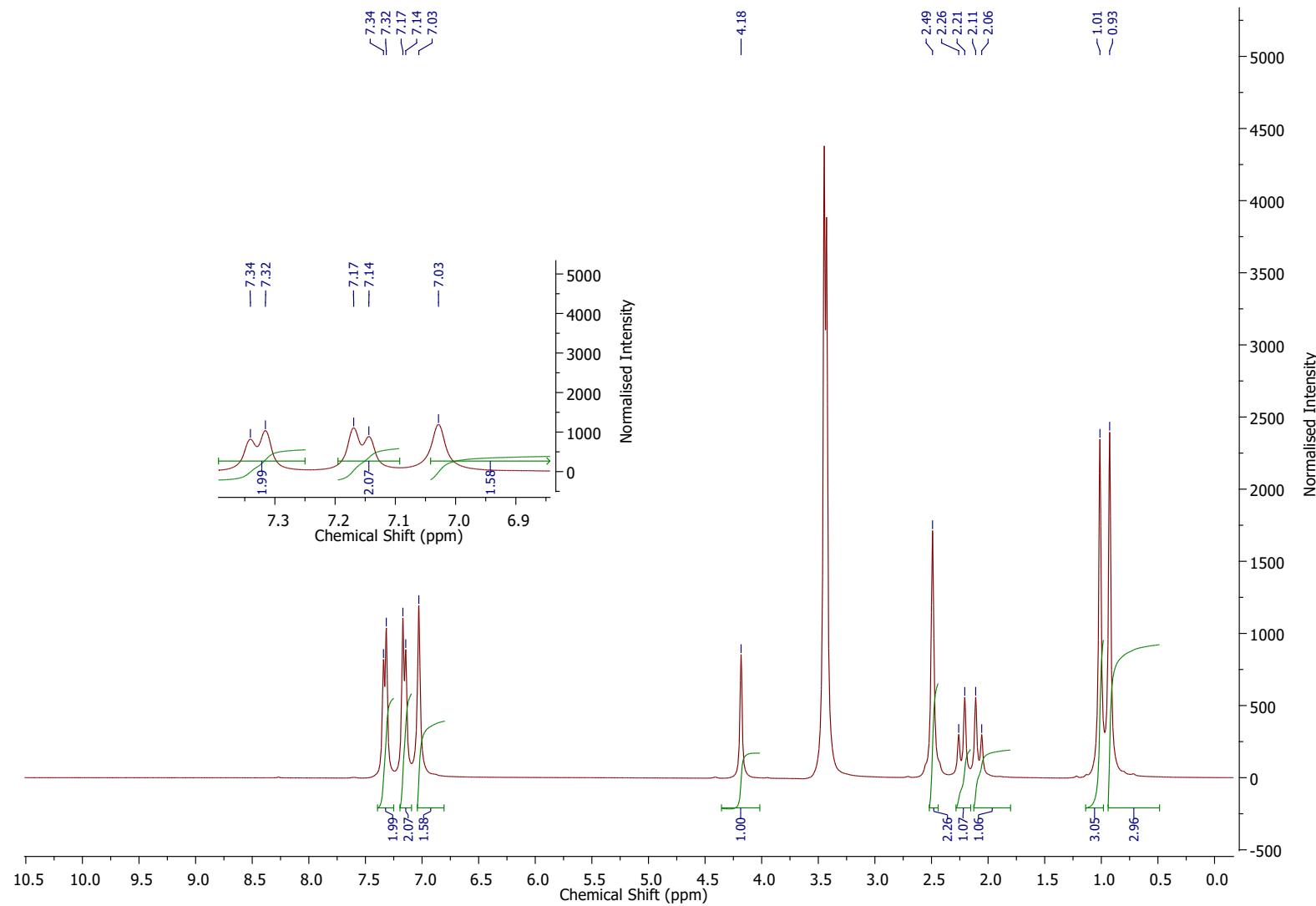
¹H NMR Spectrum of 4a



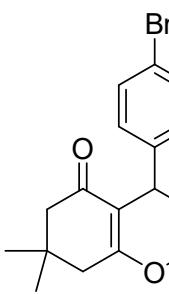
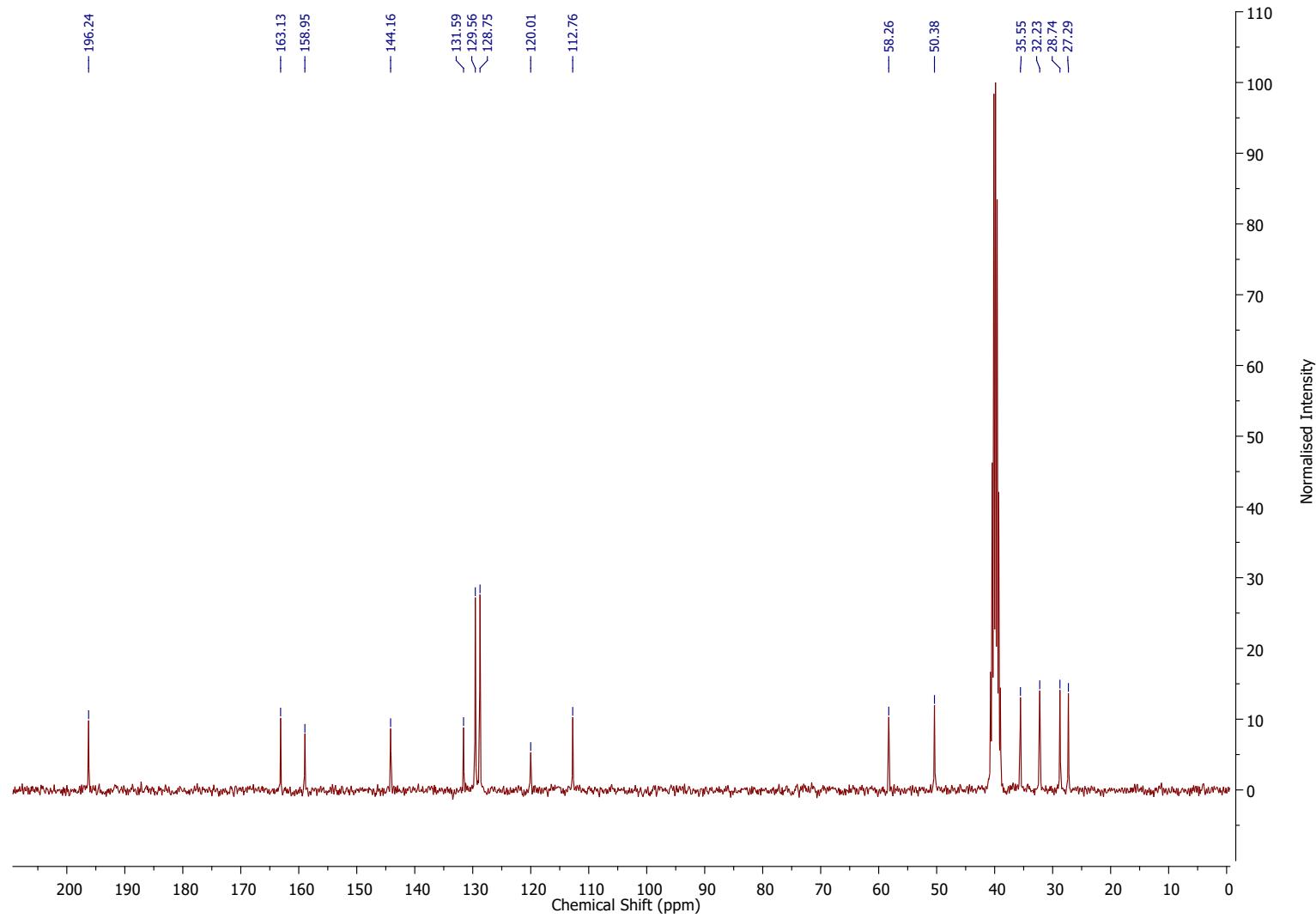
¹³C NMR Spectrum of 4a



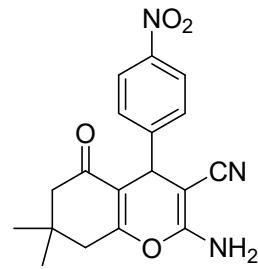
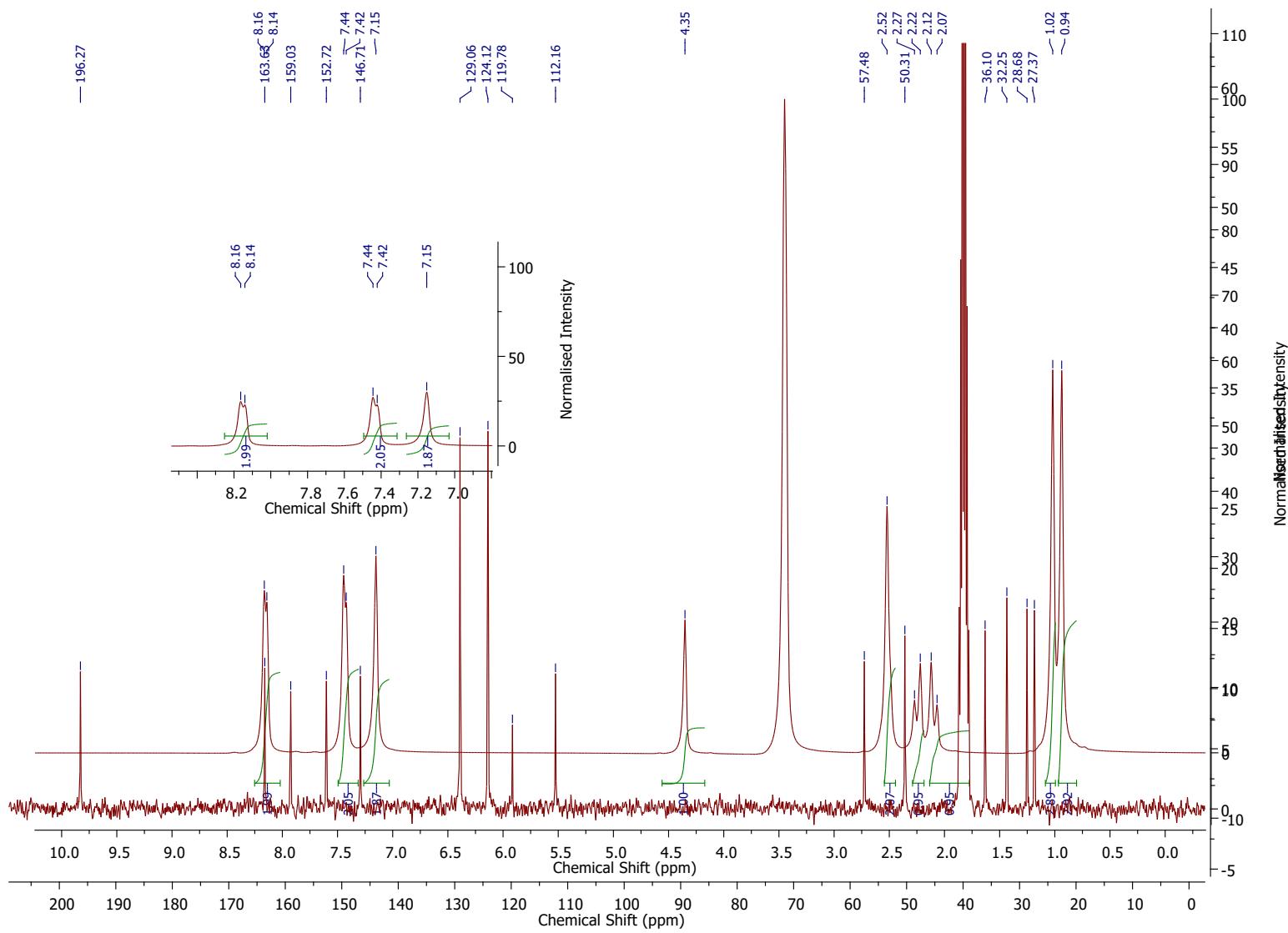
¹H NMR Spectrum of 4b



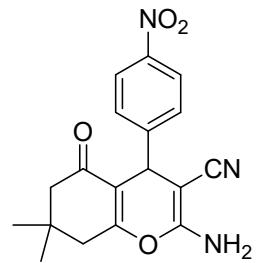
¹³C NMR Spectrum of 4b



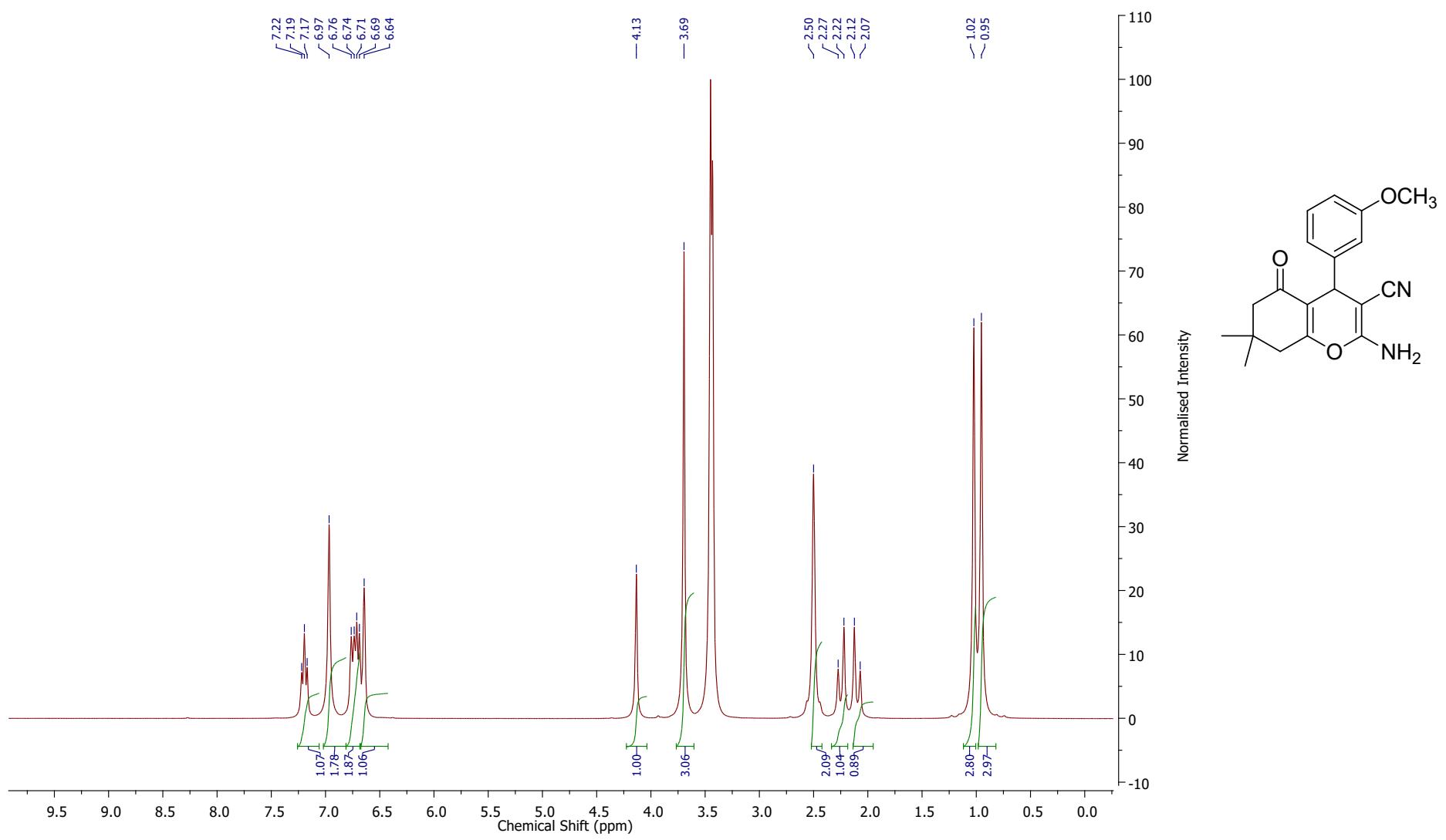
¹H NMR Spectrum of 4c



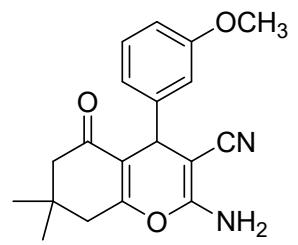
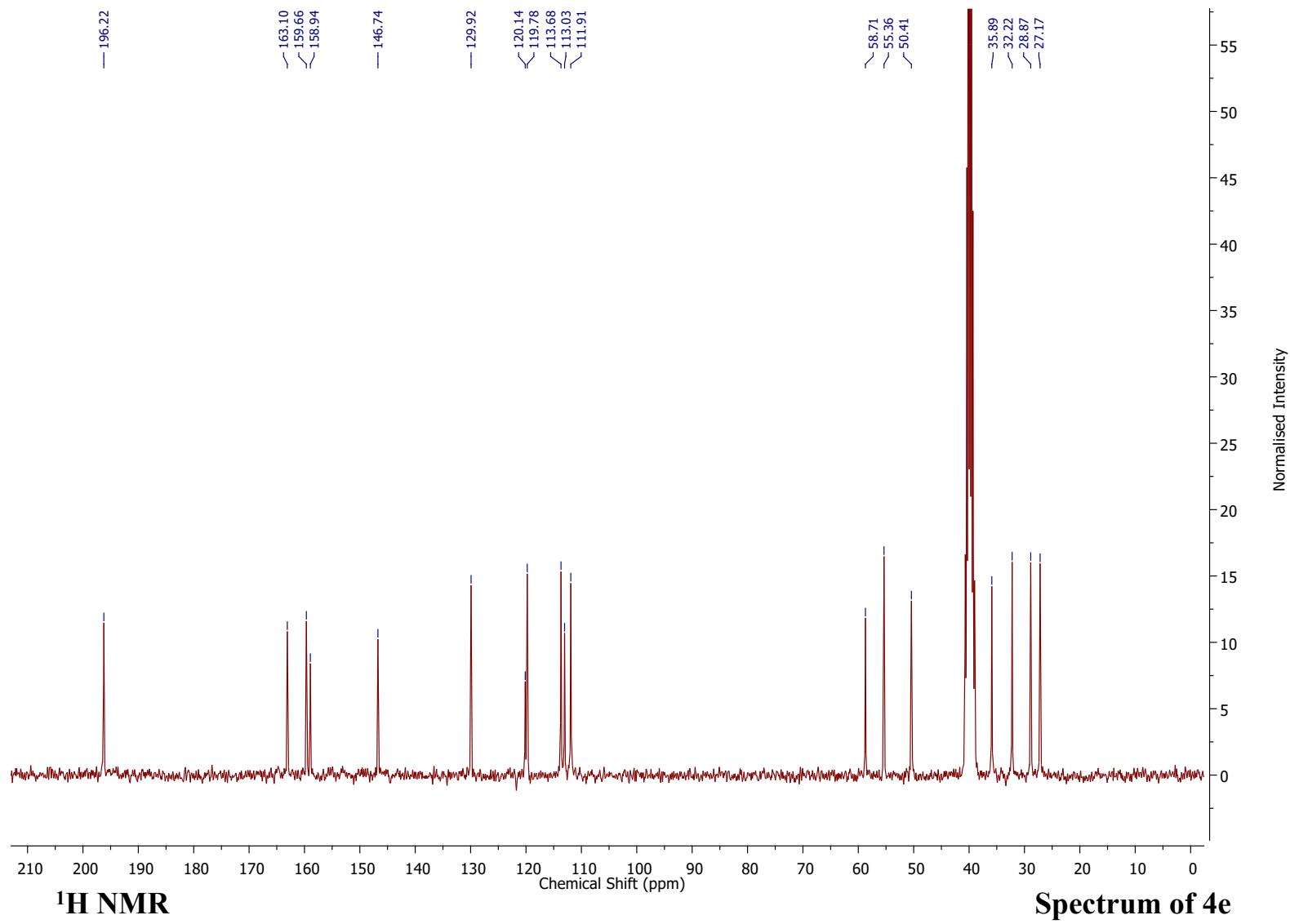
¹³C NMR Spectrum of 4c

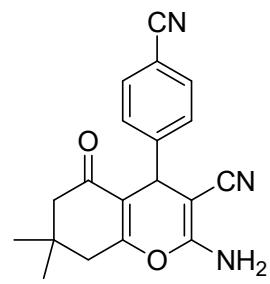
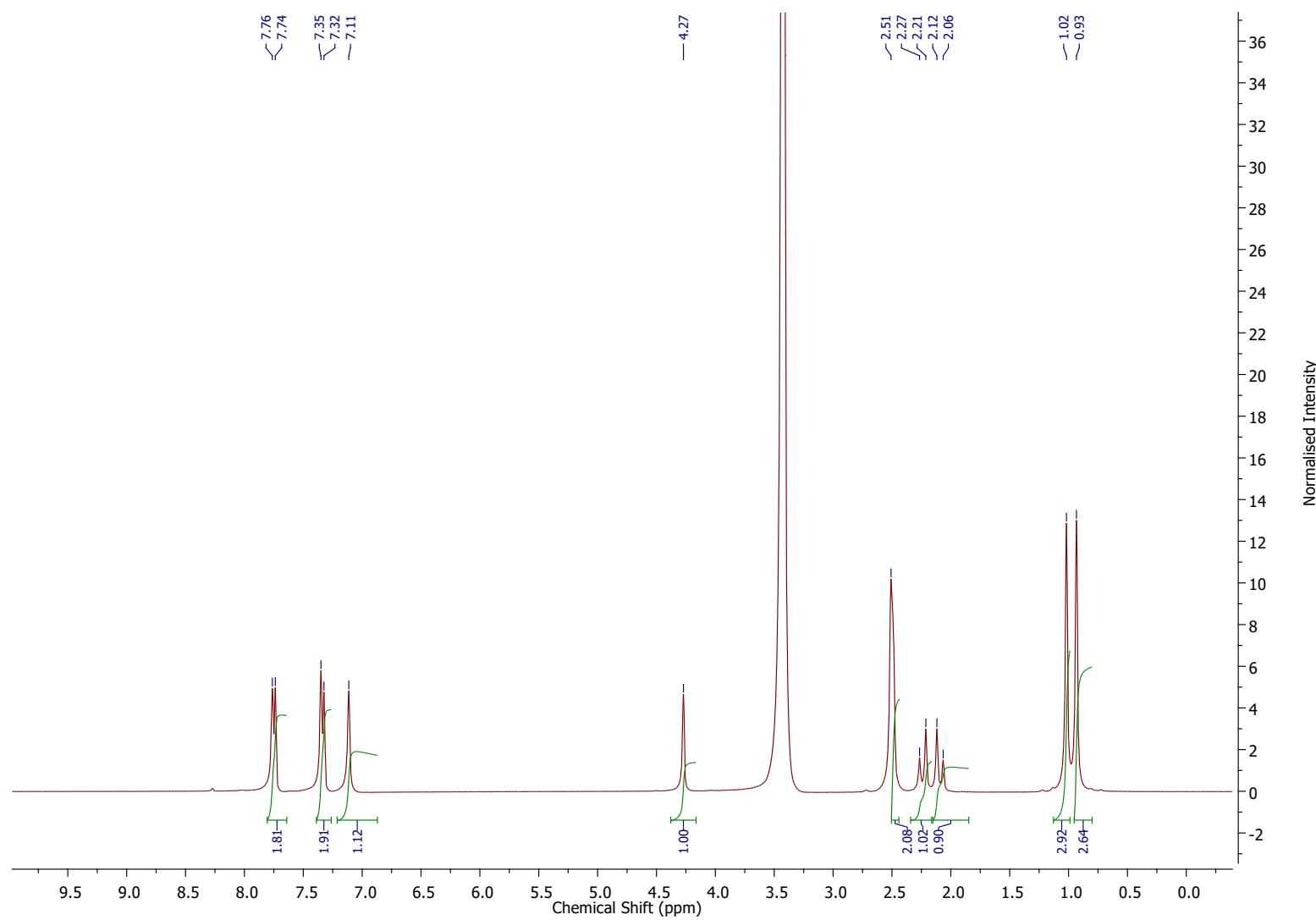


^1H NMR Spectrum of 4d

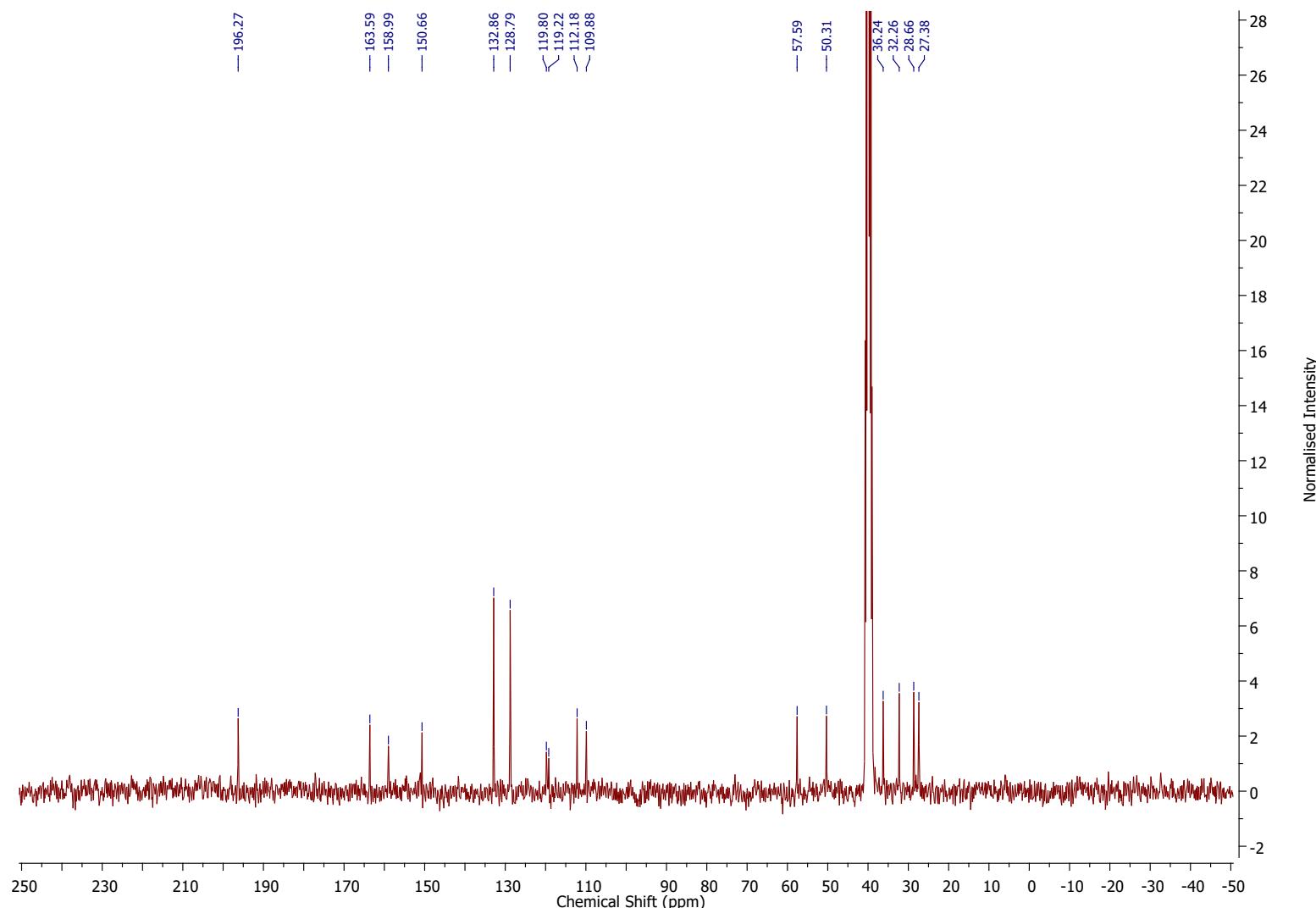


^{13}C NMR Spectrum of 4d

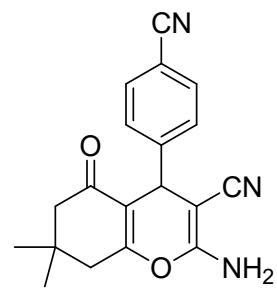


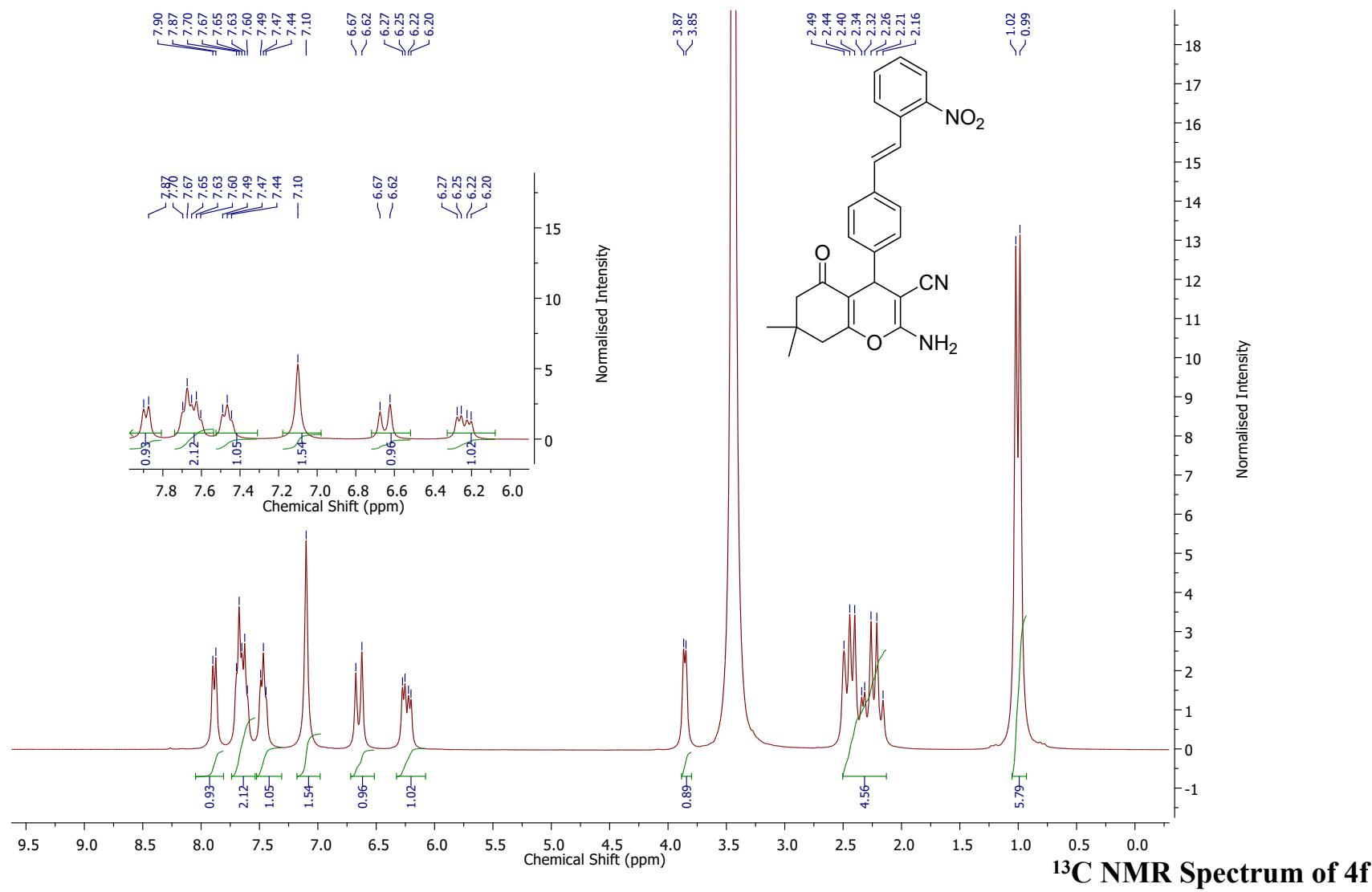


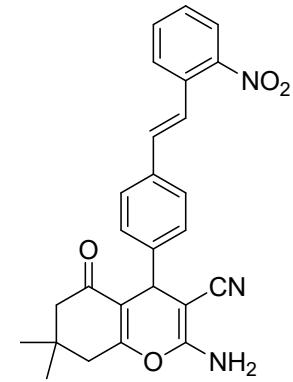
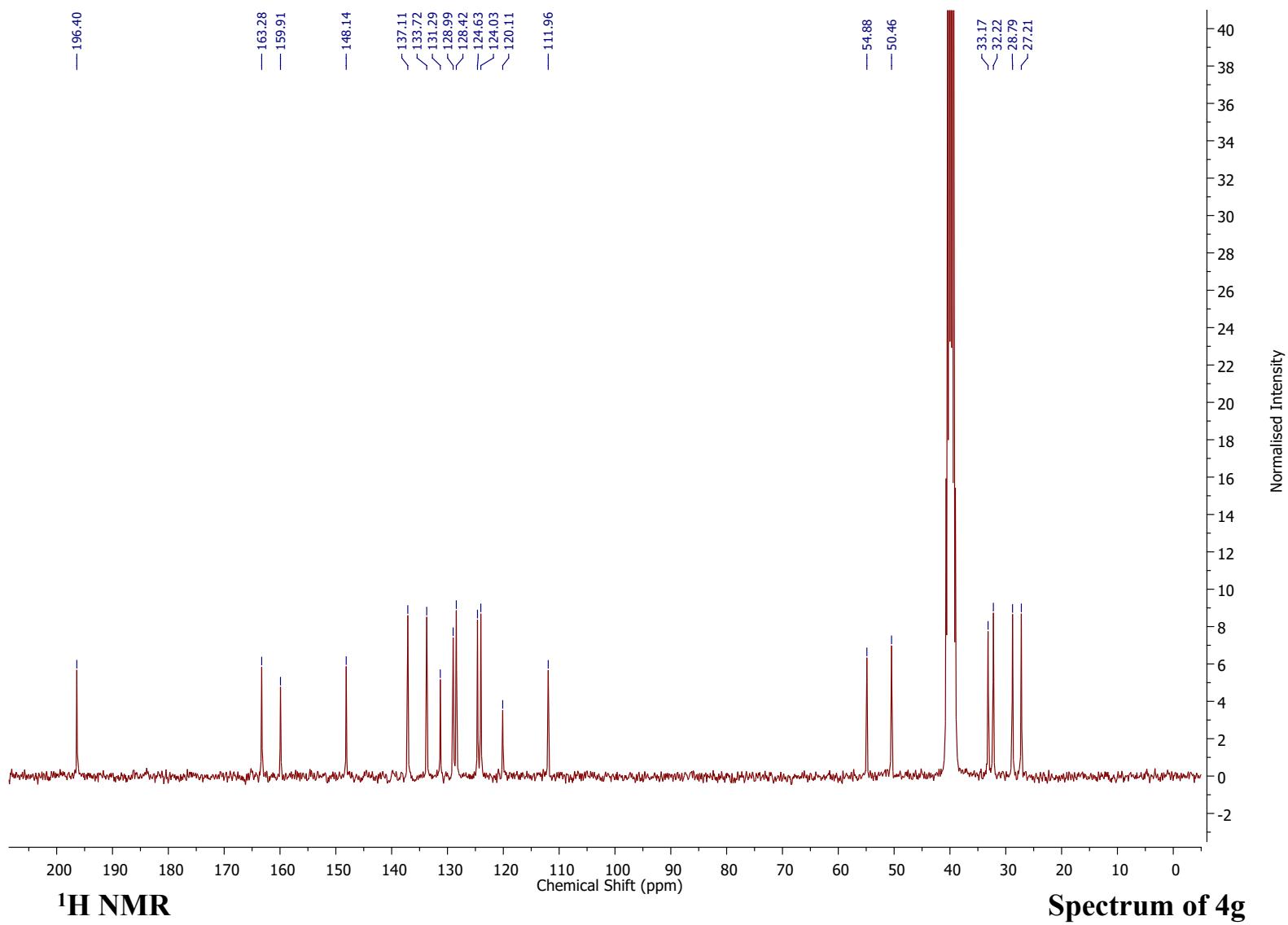
¹³C NMR Spectrum of 4e

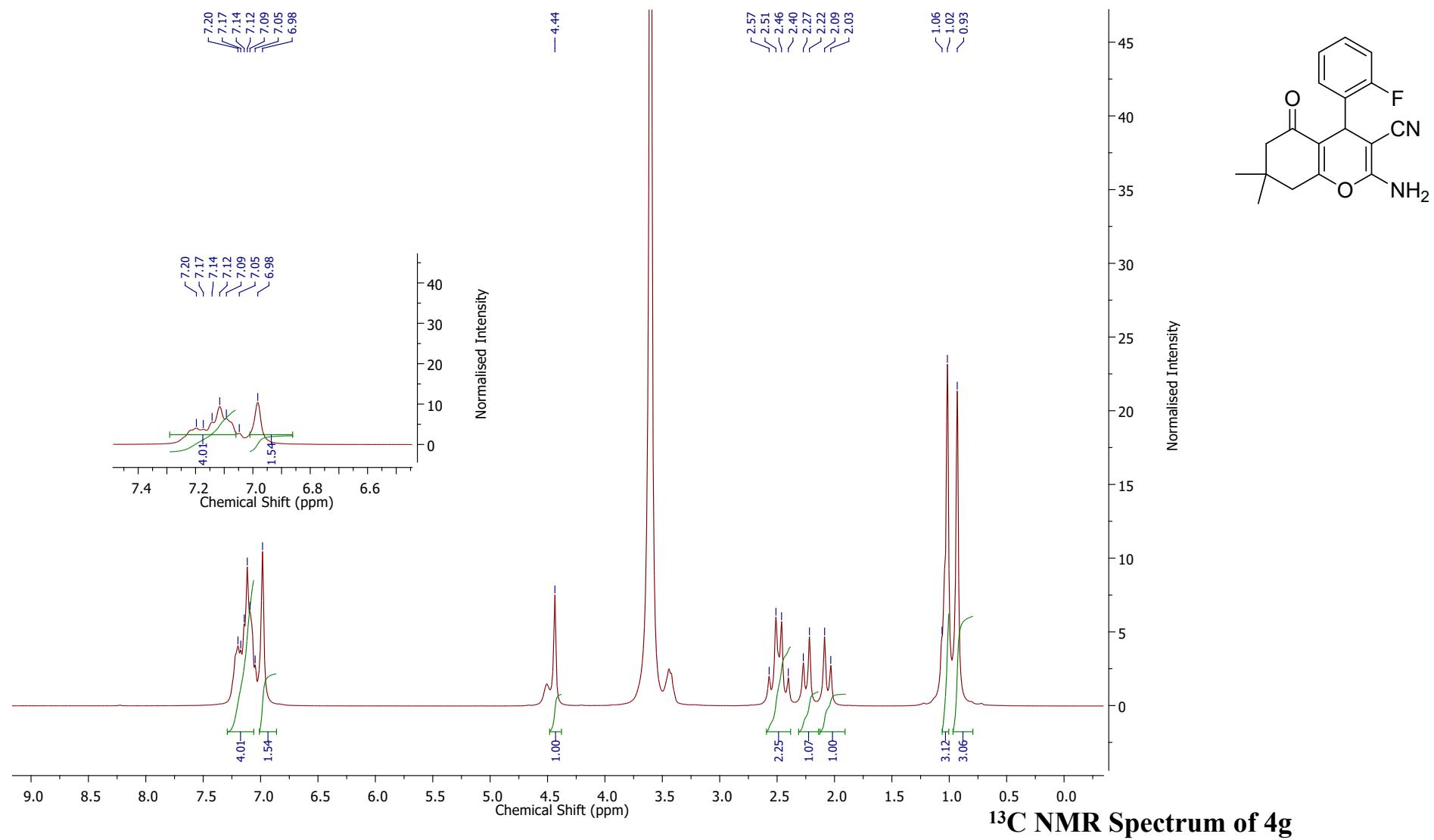


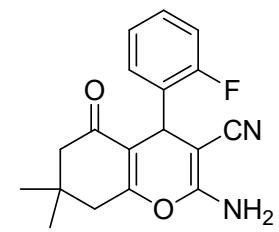
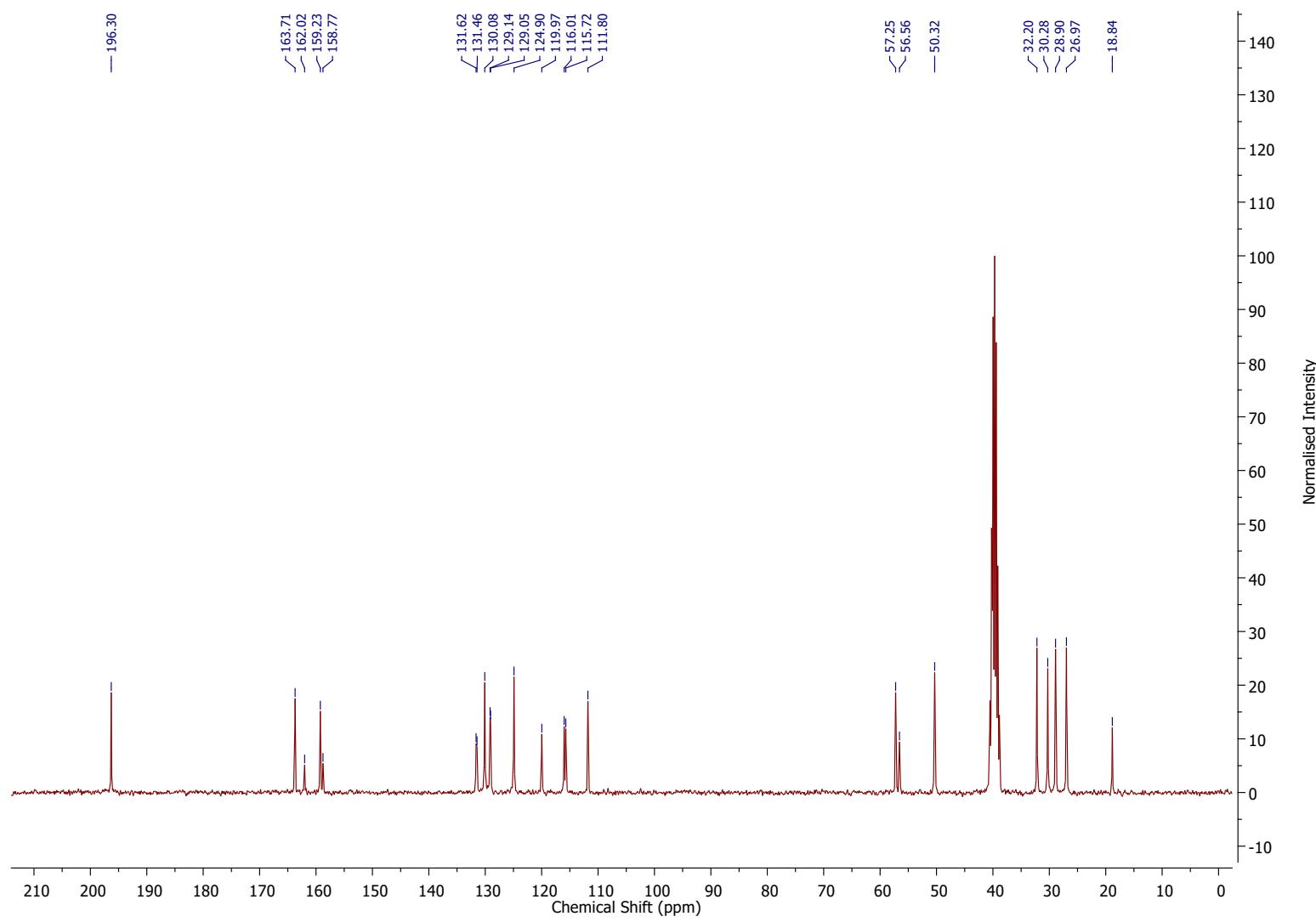
¹H NMR Spectrum of 4f

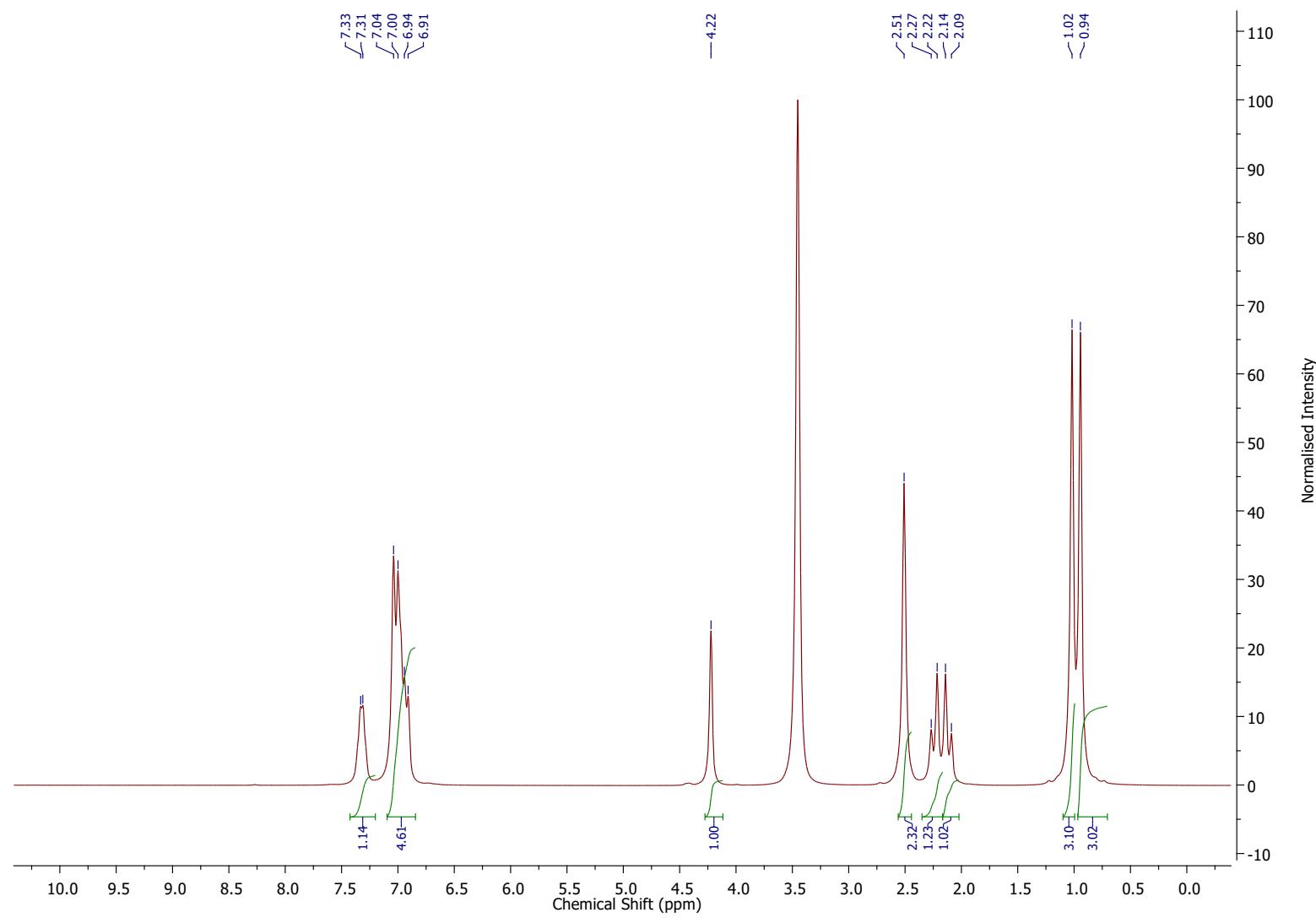




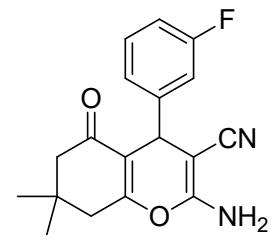


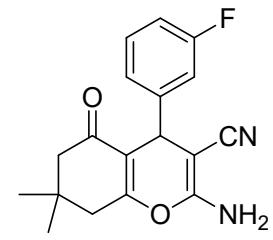
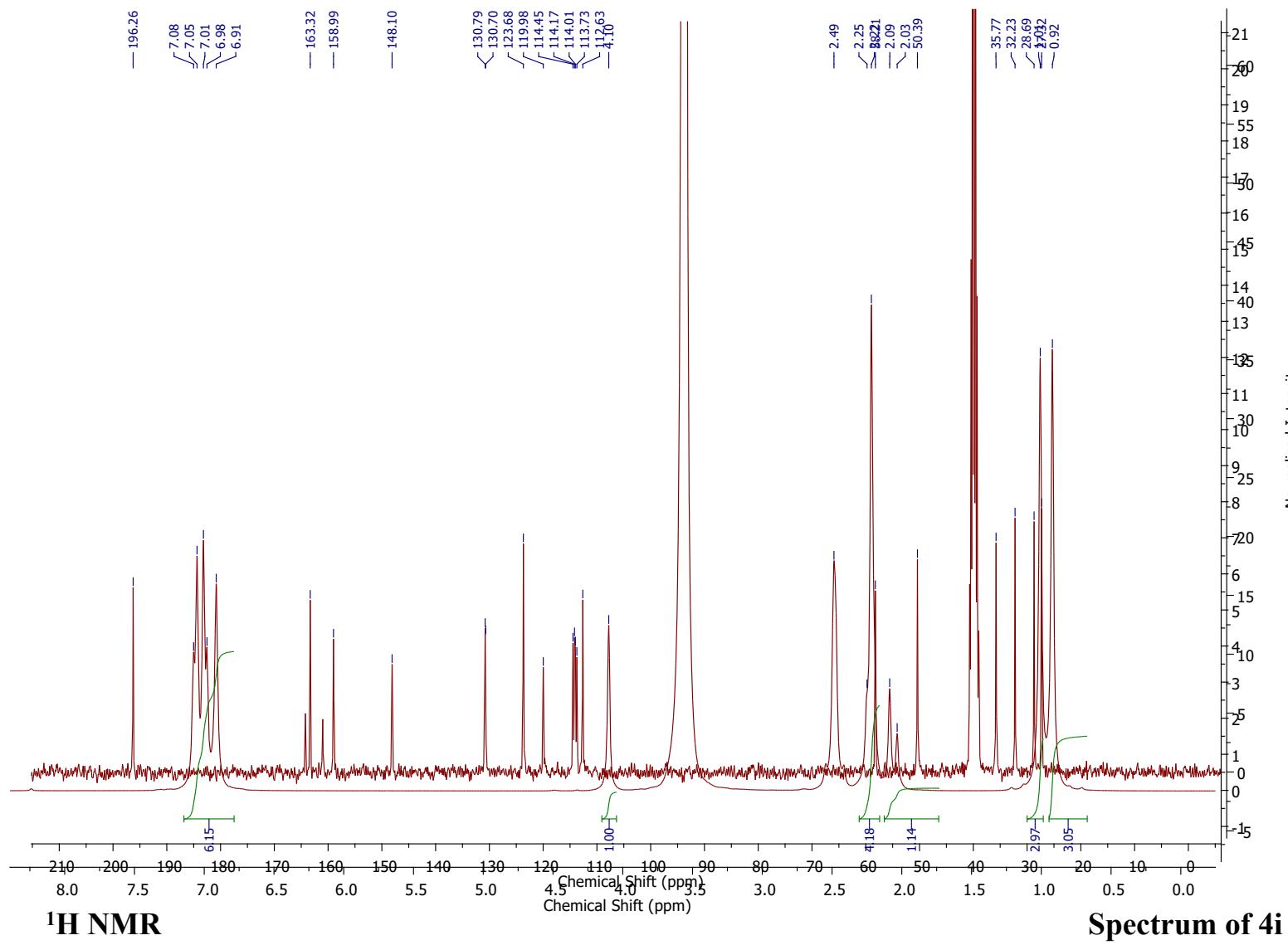


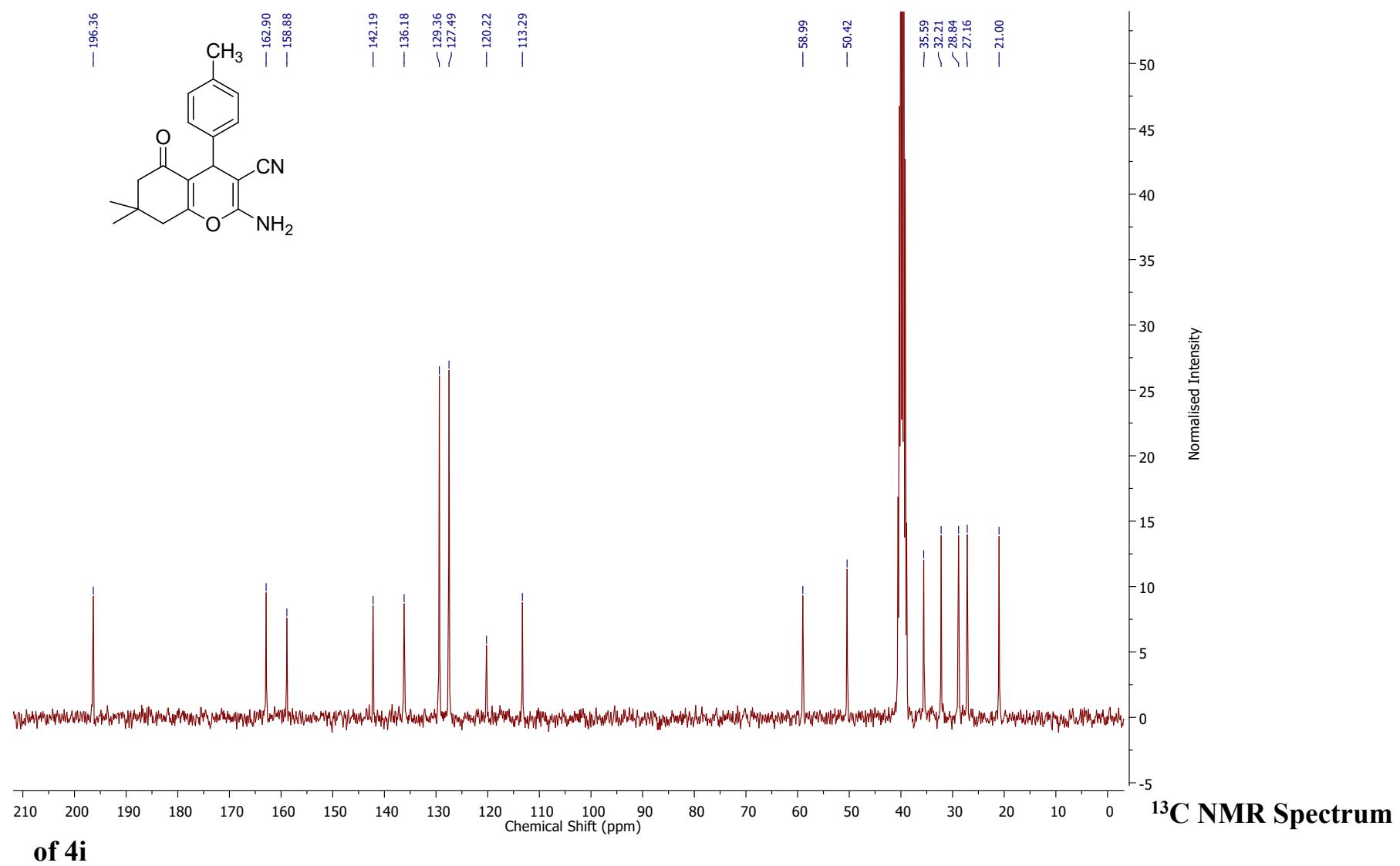


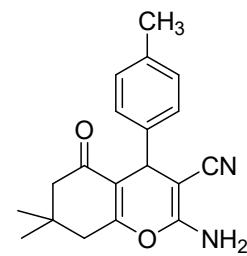


^{13}C NMR Spectrum of **4h**

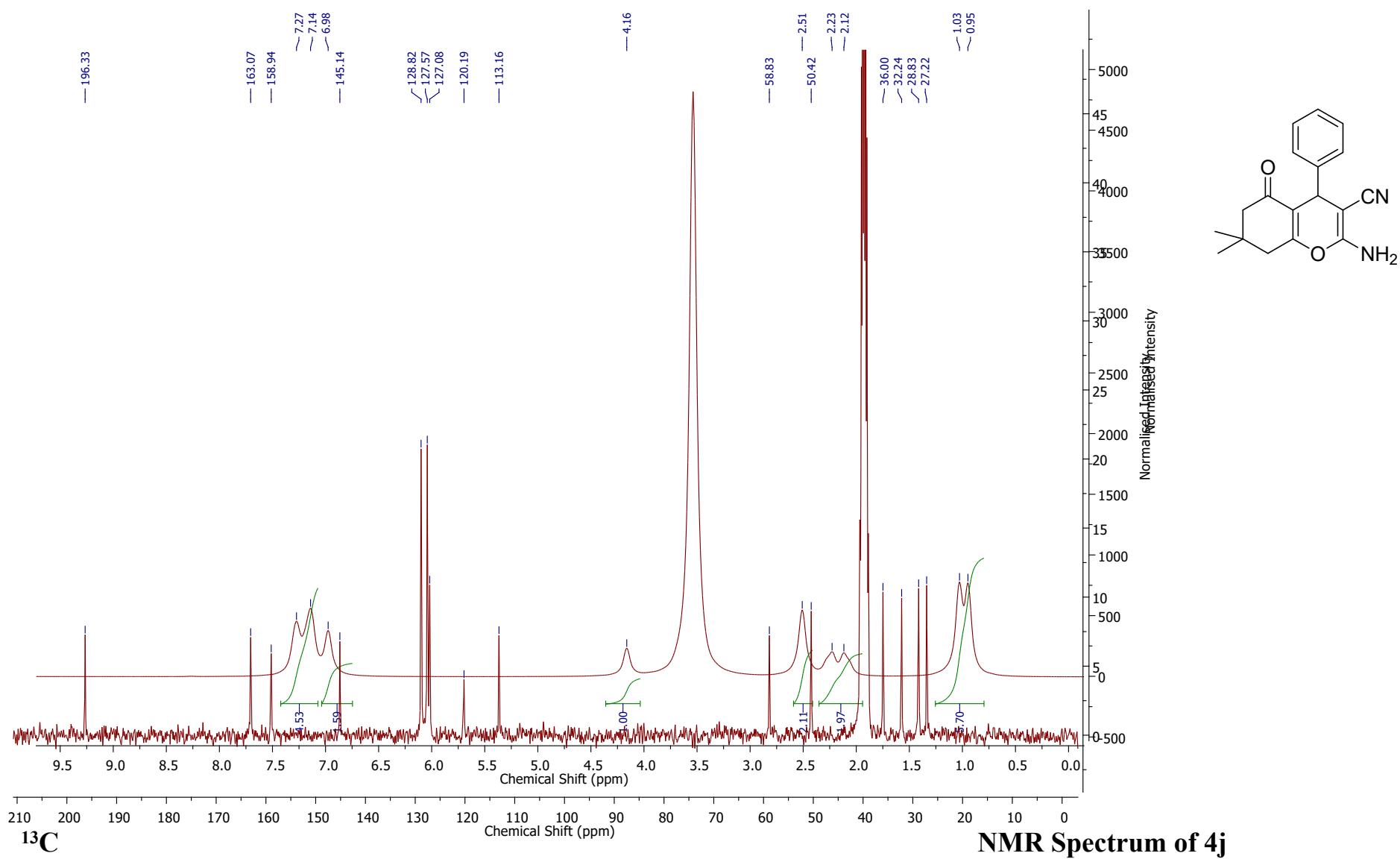


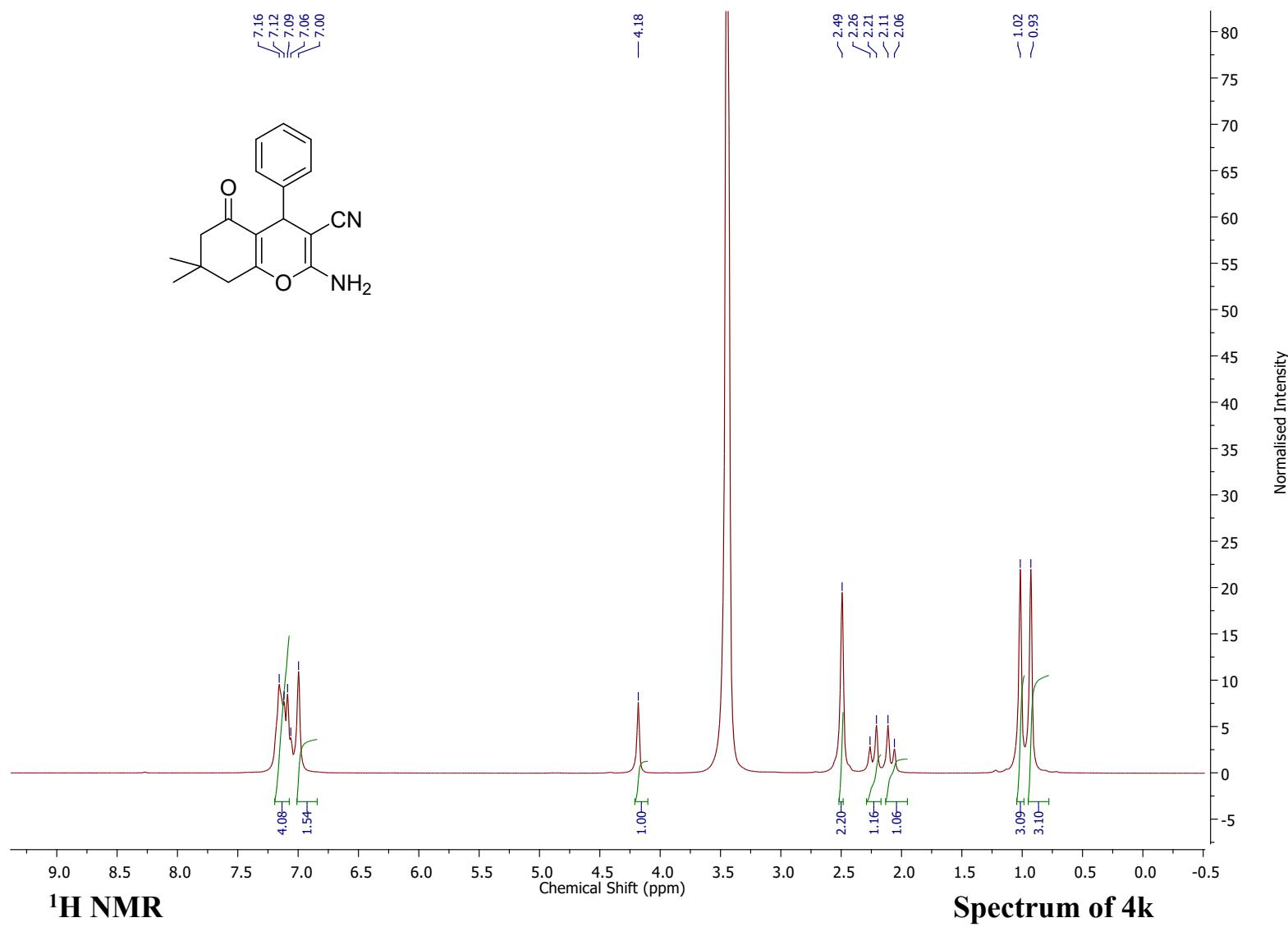


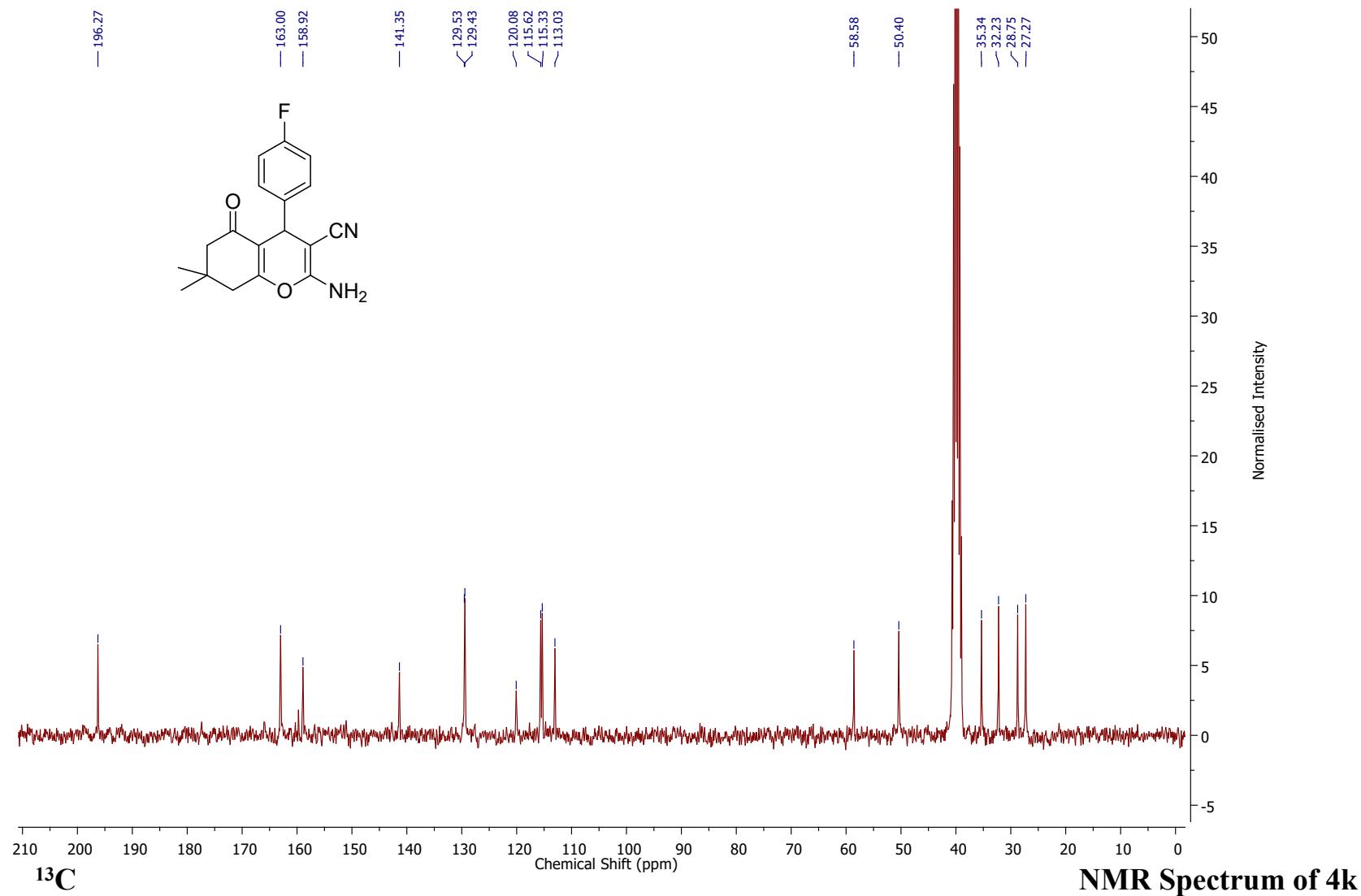


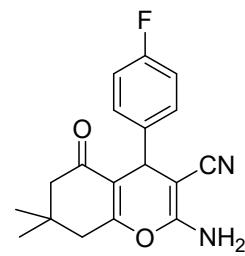


^1H NMR Spectrum of 4j

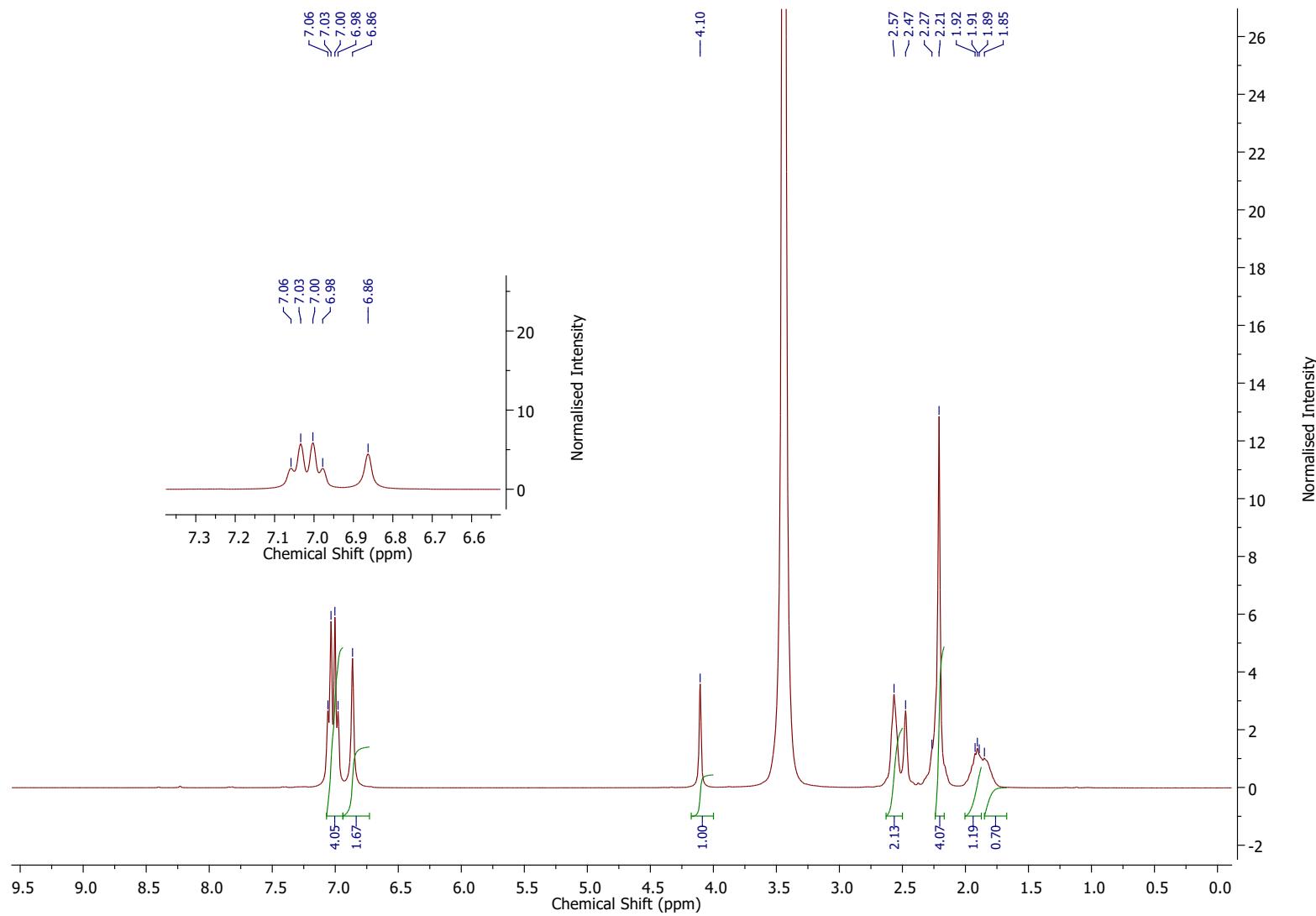




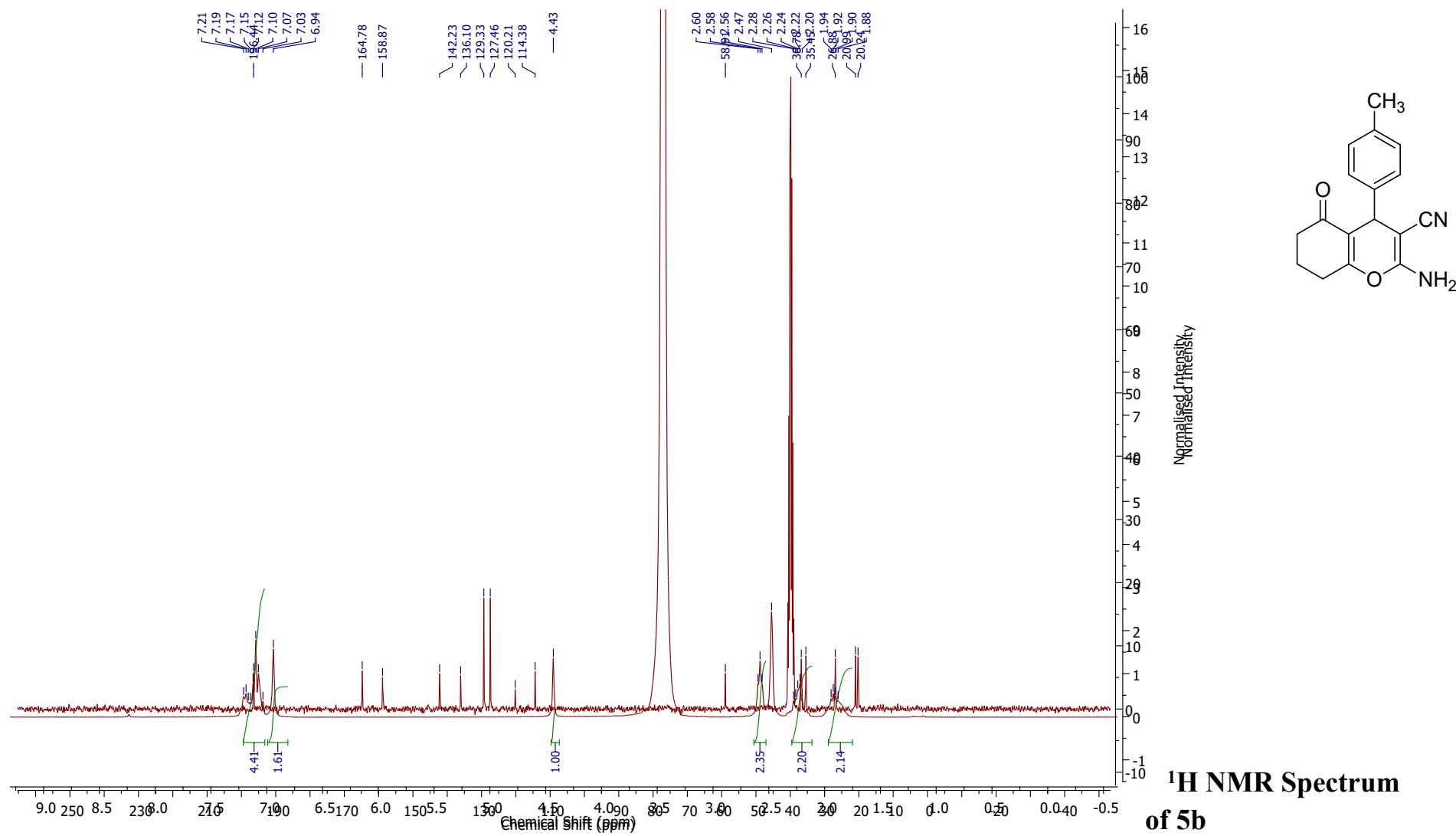


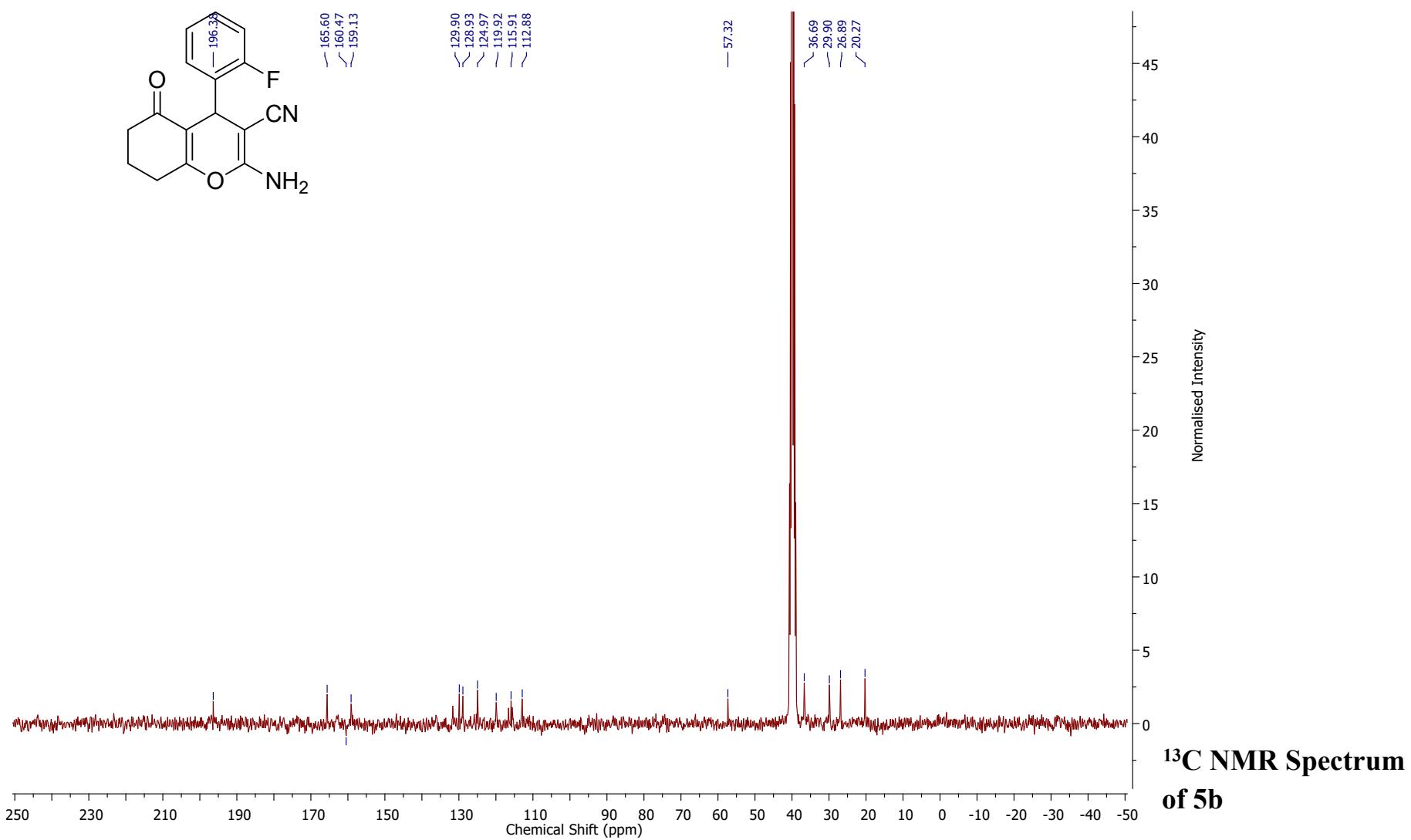


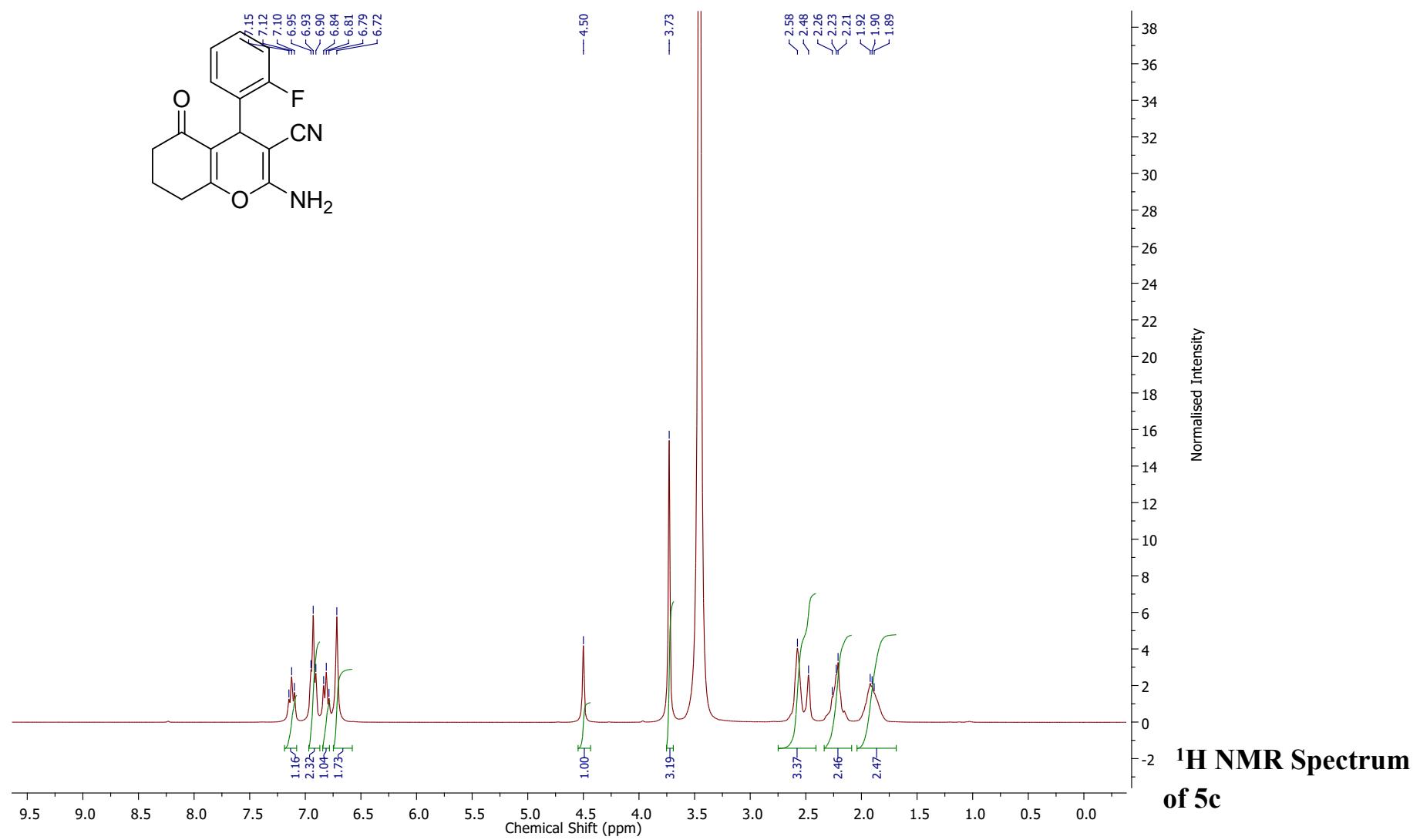
¹H NMR Spectrum of 5a

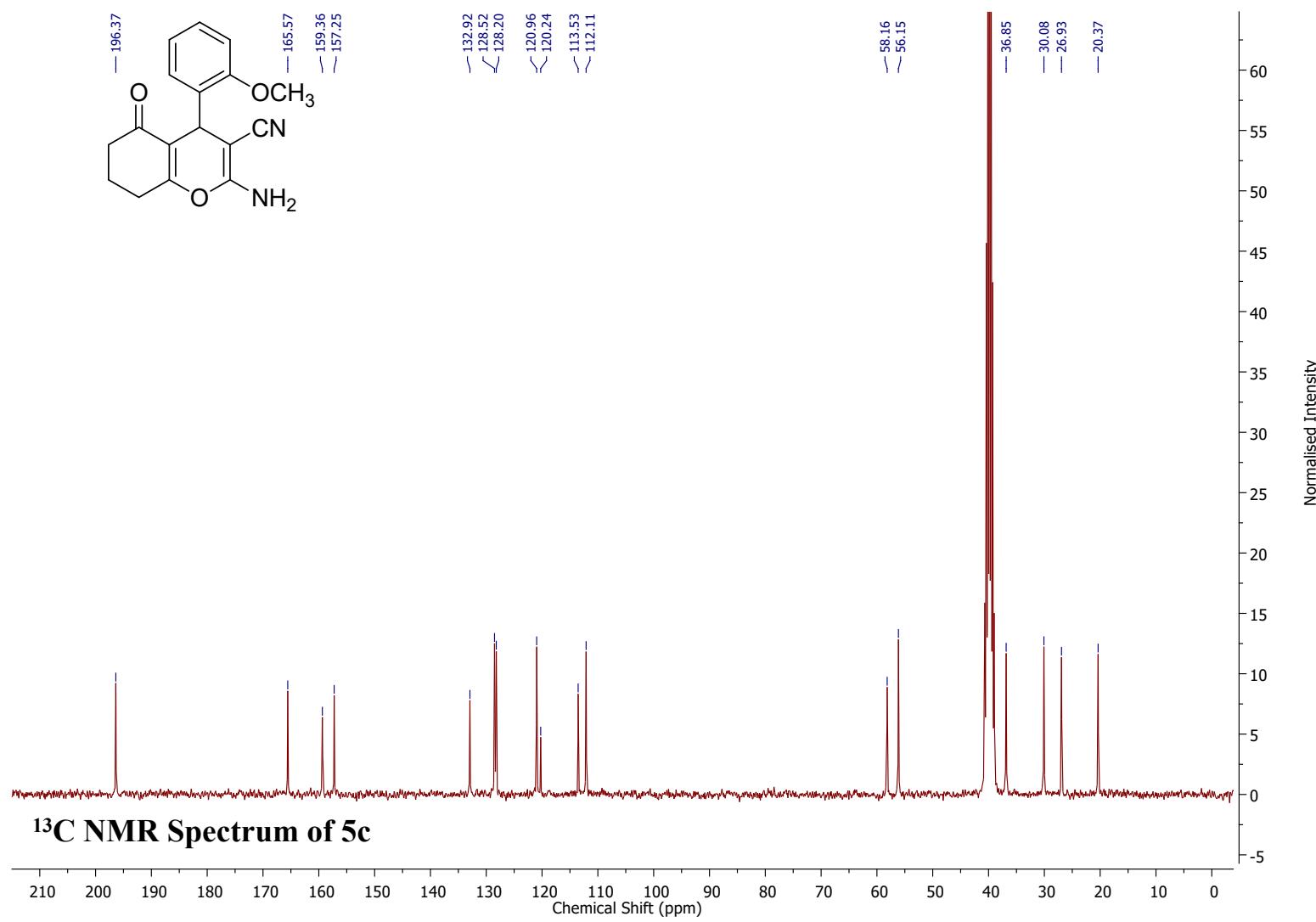


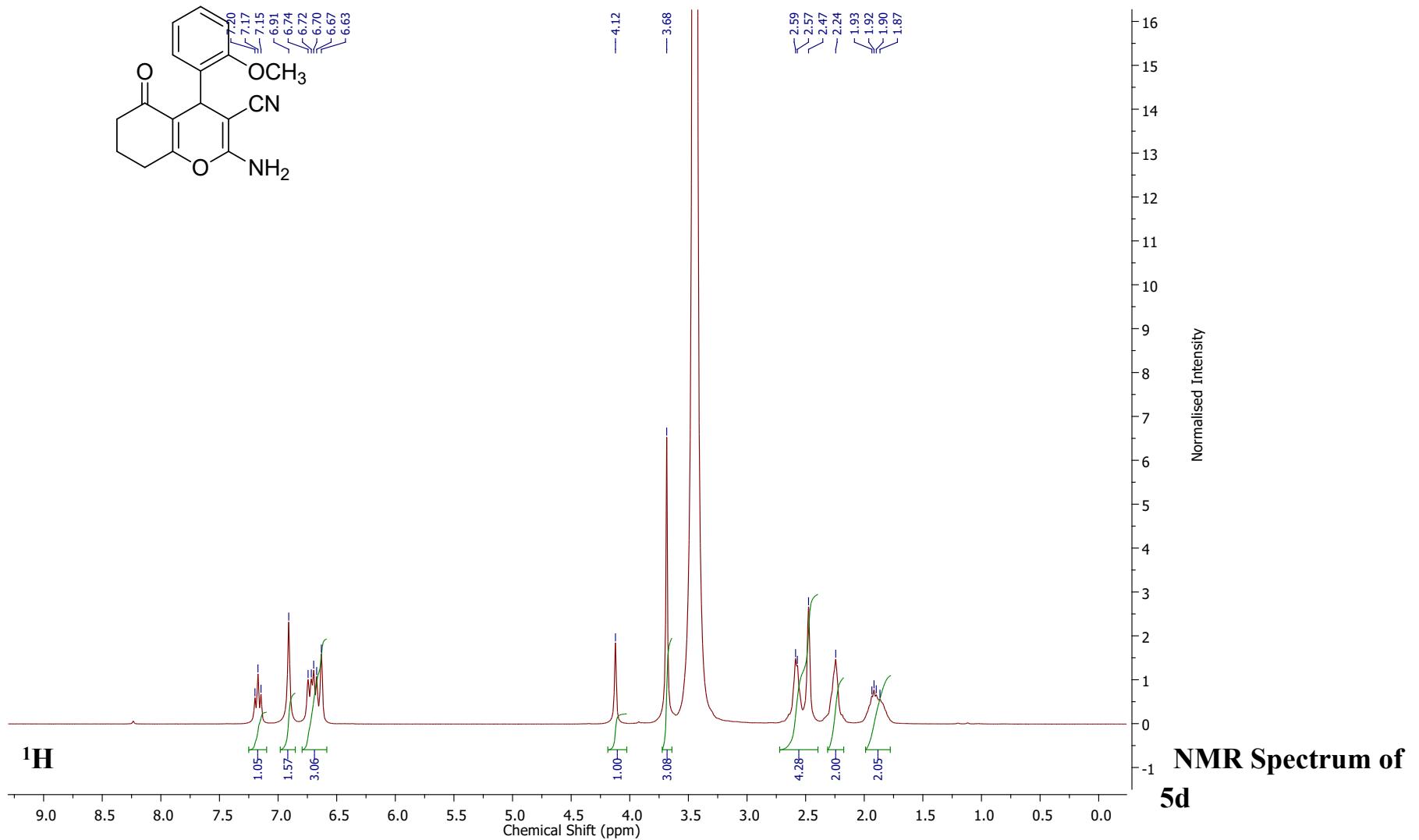
^{13}C NMR Spectrum of 5a

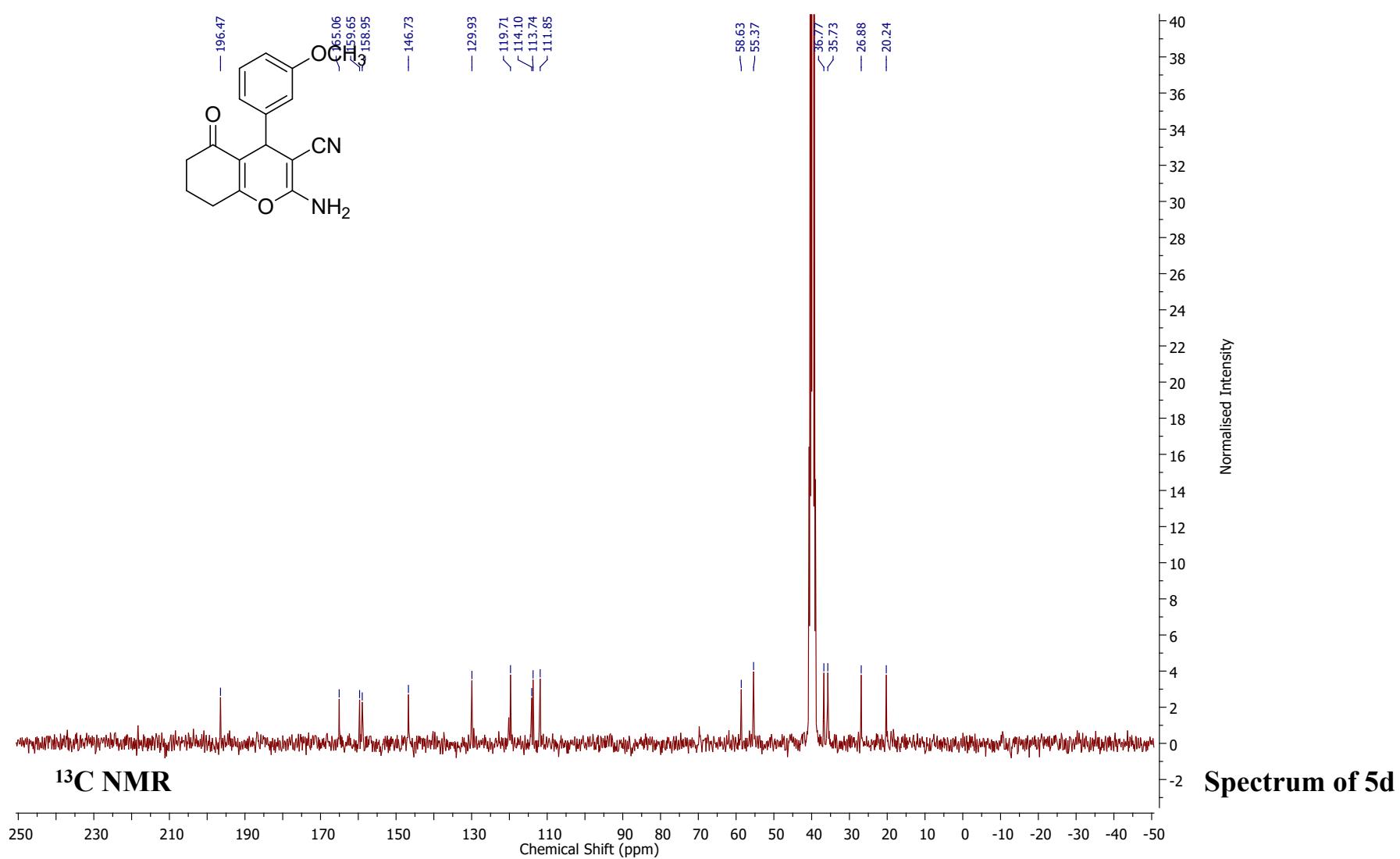


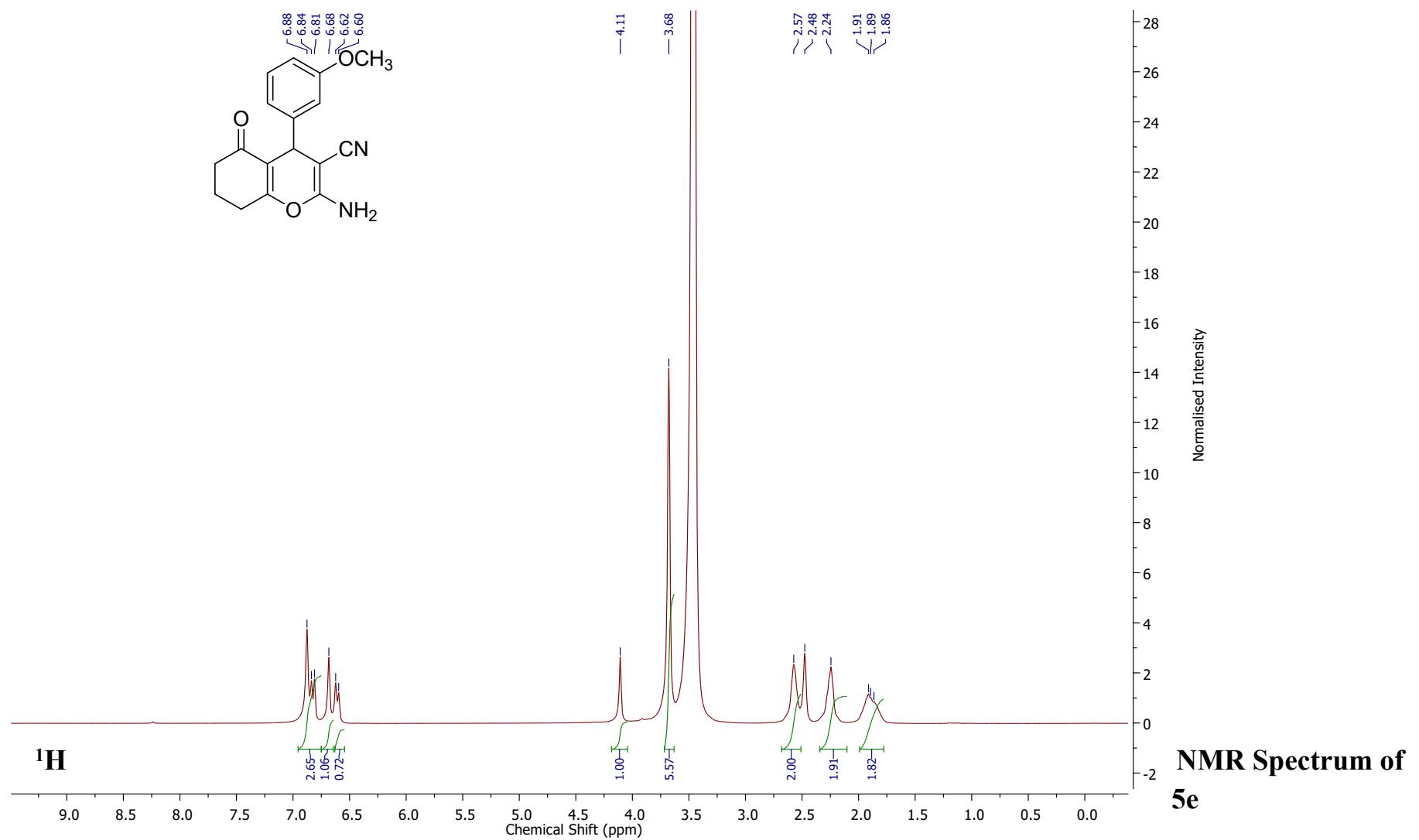


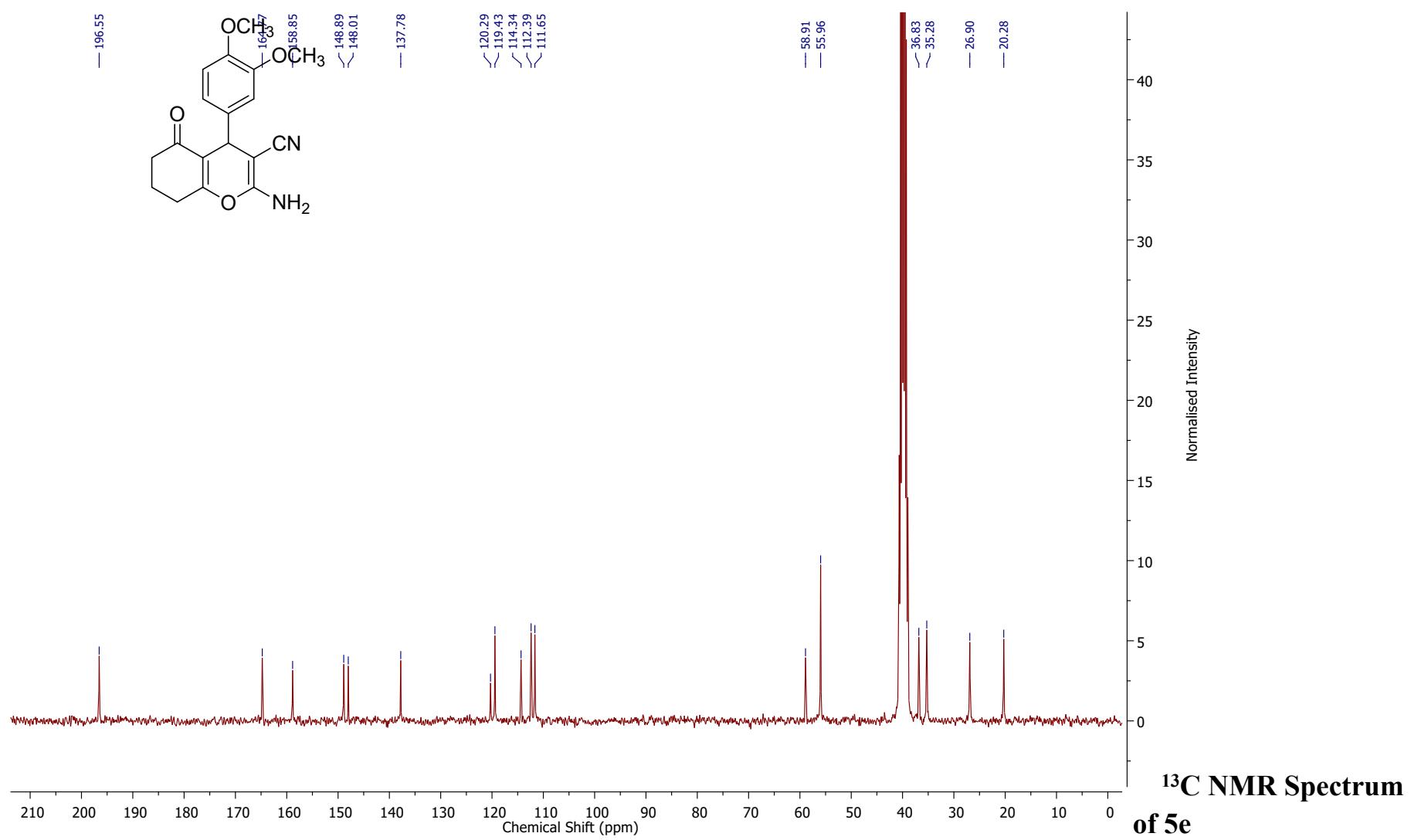


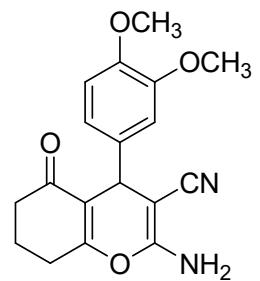












^1H NMR Spectrum of 5f

