SUPPLEMENTARY INFORMATION FOR

A Nano-organo catalyzed route towards the efficient synthesis of benzo[b]pyran derivatives under Ultrasonic irradiation.

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General procedure for the preparation of the catalyst

Preparation of the Fe_3O_4 NPs

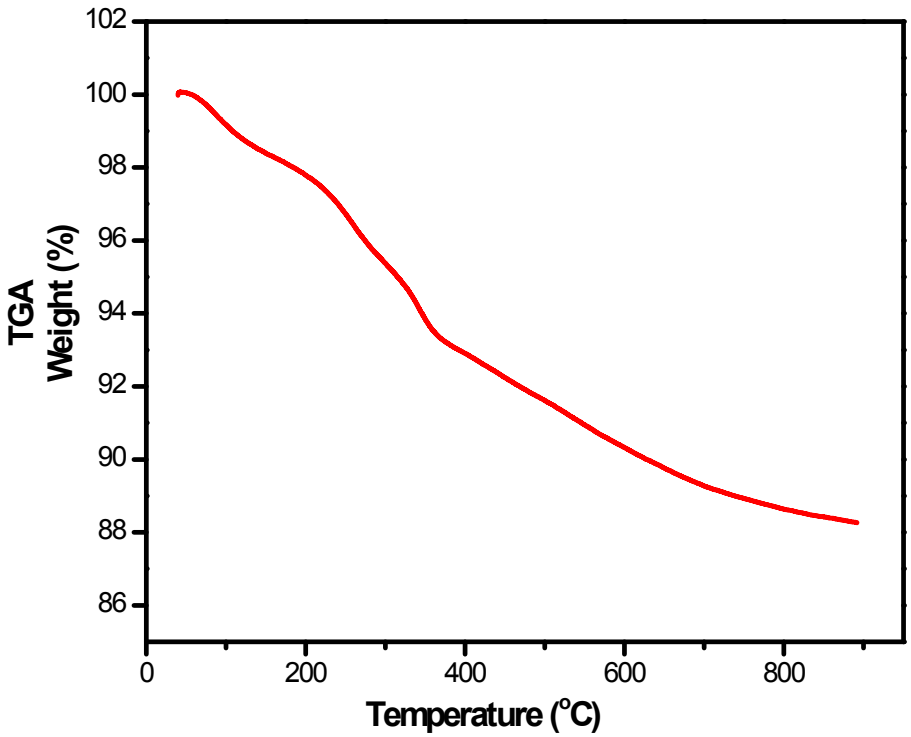
Fe (II) and Fe (III) salts in the ratio of 1:2 was dissolved in 100ml millipore water, 1.5 M NaOH was then added dropwise and stirred vigorously for about 2 hours. The pH of the solution was adjusted in the range of 11-12. The resultant black precipitate was then isolated using an ordinary magnet and rinsed several times with millipore water.

Preparation of the Fe_2O_3@ SiO_2 NPs

The prepared Fe_3O_4 NP was calcined at temperature > 500 ^oC to convert it completely into Fe_2O_3 NP. 2g of the magnetic nanoparticle was dispersed in methanol and ultrasonicated for 15 minutes. 10 ml of tetraethylorthosilicate (TEOS) was then added and further ultrasonicated for 2 hours at 50 ^oC. The coated nanoparticle was retrieved using a magnet and washed with methanol, diethyl ether then finally dried at 60 ^oC under vacuum.

Preparation of the Fe_2O_3@SiO_2@VB_1 NPs

To a suspension of Fe_2O_3@SiO_2 NPs (1g) in methanol, 1.5 ml of trimethylamine was added and ultrasonicated for 30 minutes. An aqueous solution of thiamine hydrochloride (0.6g) was then added to the mixture which was further ultrasonicated for 3 hours at 50 ^oC. The solid thus obtained was washed with millipore water, diethyl ether and dried under vacuum at 60 ^oC which were then acidified with dil HCl at 0 ^oC to obtain Fe_2O_3@SiO_2@VB_1 NPs.



Thermogravimetric analysis (TGA) curve of the prepared

Fe_2O_3@SiO_2@$VitB_1$-Nps.

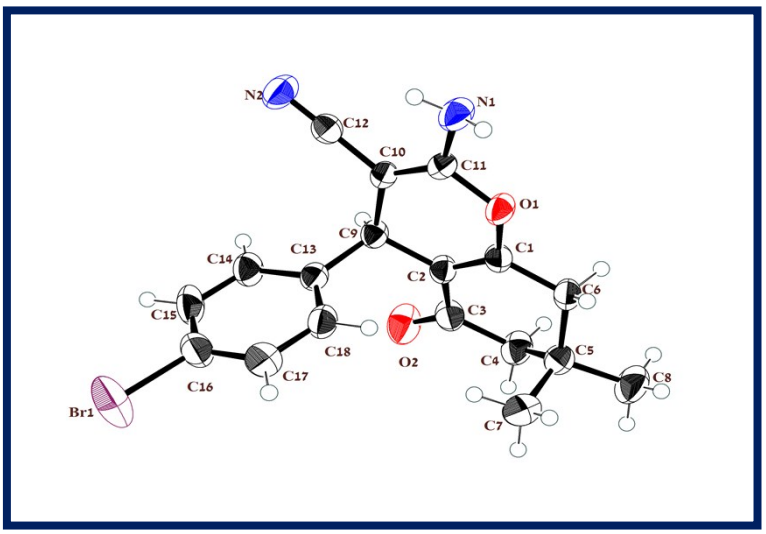


Table I.1. X-ray crystallography data for compound.**7b (CCDC NO 1477443)**

Empirical formula	$C_{18}H_{17}BrN_2O_2$
Formula weight	373.25
Crystal system	triclinic
Space group	P1
a(Å)	8.1438(7)
b(Å)	9.3009(7)
c(Å)	13.9430(13)
α(⁰)	76.176(7)
β(⁰)	88.325(7)
γ(⁰)	78.354(7)
Volume (Å)	1004.21(15)
ρ (calculated) (g cm-3)	1.2343
T(K)	293.1(5)
Absorption coefficient (mm-1)	2.055
Total reflection collected	7833
Independent reflection	4519
Refine parameter	210
θ range (⁰)	6.16 to 57.44
Final R Indexes [1>=2σ(I)]	R_1 = 0.0595
Final R indexes [all data]	R_1 = 0.1026
Goodness-of-fit on F2	1.007

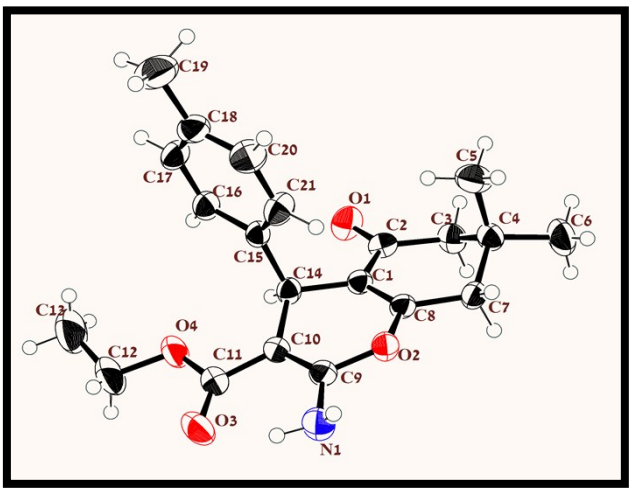


Table I.2. X-ray crystallography data for compound **10a (CCDC NO1477627)**

Empirical formula	$C_{21}H_{25}NO_4$
Formula weight	355.44
Crystal system	monoclinic
Space group	P2
a(Å)	14.2687(10)
b(Å)	8.0116(7)
c(Å)	16.7510(11)
$\alpha(^0)$	90
$\beta(^0)$	96.487(6)
$\gamma(^0)$	90
Volume (Å)	1902.6(2)
ρ (calculated) (g cm-3)	1.2407
T(K)	294.12(18)
Absorption coefficient (mm-1)	0.085
Total reflection collected	8690
Independent reflection	4379
Refine parameter	239
θ range (°)	6.46 to 57.58
Final R Indexes [1>=2σ(I)]	0.0607
Final R indexes [all data]	0.0822
Goodness-of-fit on F2	1.027

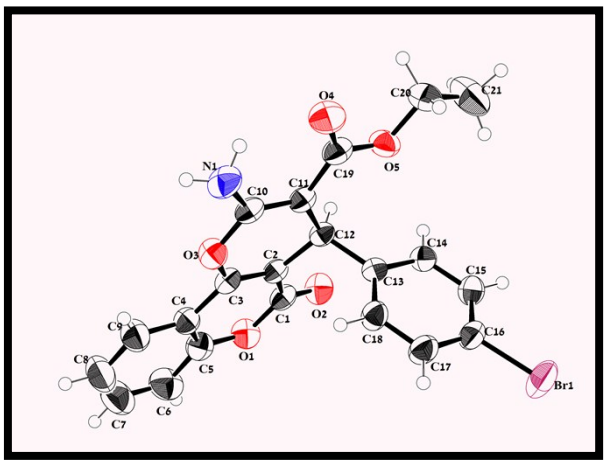
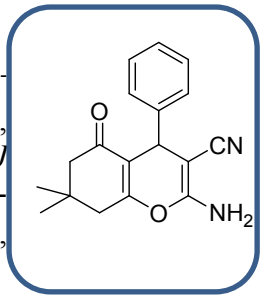


Table I.3. X-ray crystallography data for compound **11d (CCDC NO1477628)**

Empirical formula	$C_{21}H_{16}BrNO_5$
Formula weight	442.27
Crystal system	triclinic
Space group	P1
a(Å)	8.6633(7)
b(Å)	10.4989(11)
c(Å)	10.9588(10)
α(⁰)	99.683(8)
β(⁰)	100.554(7)
γ(⁰)	92.904(7)
Volume (Å)	962.52(15)
ρ (calculated) (g cm-3)	1.5259
T(K)	294.3(3)
Absorption coefficient (mm-1)	2.168
Total reflection collected	7088
Independent reflection	4309
Refine parameter	262
θ range (°)	6.46 to 57.28
Final R Indexes [1>=2σ(I)]	R_1 = 0.0450
Final R indexes [all data]	R_1 = 0.0762
Goodness-of-fit on F2	1.023

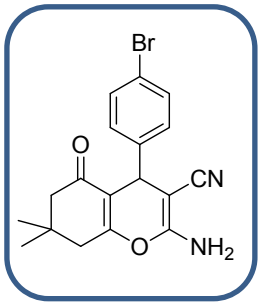
SPECTRAL DATA

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



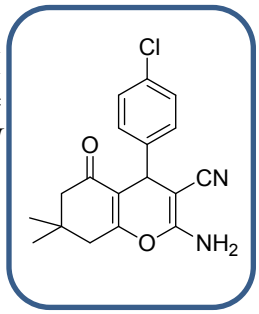
Off white solid, m.p. 224-226 ^{o}C.
IR (KBr): ν 3397, 3325, 3213, 3028, 2961, 2200, 1680, 1605, 1249 cm^{-1}.^{1}H NMR (400 MHz, DMSO-d$_6$): δ 7.29-7.11 (m, 5H), 7.01 (s, 2H), 4.15 (s, 1H), 2.56-2.46 (m, 2H), 2.24 (d, 1H, J = 16 Hz), 2.09 (d, 1H, J = 16 Hz), 1.03 (s, 3H), 0.94 (s, 3H) ppm. ^{13}C NMR (100 MHz, DMSO-d$_6$): δ 195.6, 162.4, 158.4, 144.7, 128.2, 127.1, 126.5, 119.6, 112.6, 58.2, 49.9, 35.5, 31.7, 28.3, 26.7 ppm. ESI-MS: *m/z* 294 [M]$^{+}$

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



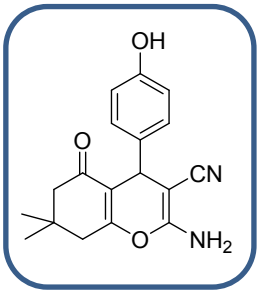
White solid, m.p. 202-204 ^{o}C.
IR (KBr): ν 3393, 3319, 3212, 2963, 2191, 1678, 1605, 1486, 1252 cm^{-1}. ^{1}H NMR (400 MHz, DMSO-d$_6$): δ 7.47 (d, 2H, J = 8.8 Hz), 7.11-7.09 (m, 4H,), 4.17 (s, 1H), 2.55 -2.45 (m, 2H), 2.24 (d, 1H, J = 16 Hz), 2.09 (d, 1H, J = 16 Hz), 1.02 (s, 3H), 0.94 (s, 3H) ppm.^{13}C NMR (100 MHz, DMSO-d$_6$): δ 195.6, 162.5, 158.4, 144.1, 131.1, 129.4, 119.5, 112.2, 57.6, 55.9, 49.8, 35.1, 31.7, 28.2, 26.8 ppm. ESI-MS: *m/z* 372 [M]$^{+}$, 374 [M+2] $^{+}$.

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



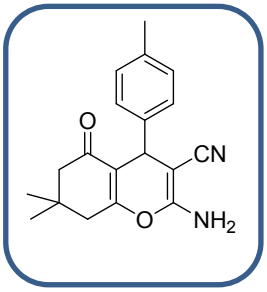
Off white solid, m.p. 214-216 ^{o}C.
IR (KBr): ν 3380, 3183, 2958, 2188, 1675, 1635, 1491, 1246 cm^{-1}. ^{1}H NMR (400 MHz, DMSO-d$_6$): δ 7.34 (d, 2H, J = 7.2 Hz), 7.16 (d, 2H, J = 7.2 Hz), 7.07 (s, 2H), 4.18 (s, 1H), 2.66 -2.45 (m, 2H), 2.24 (d, 1H, J =15.6 Hz), 2.09 (d, 1H, J = 16 Hz), 1.05 (s, 3H), 0.95 (s, 3H) ppm. ^{13}C NMR (100 MHz, DMSO-d$_6$): δ 195.6, 162.5, 158.4, 143.7, 131.0, 129.0, 128.2, 119.5, 112.2, 57.6, 49.8, 35.0, 31.7, 28.2, 26.8 ppm.
ESI-MS: *m/z* 328 [M]$^{+}$, 330 [M+2]$^{+}$.

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



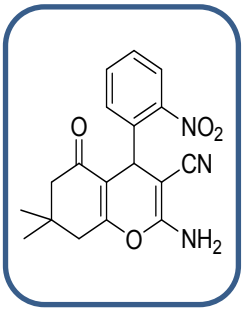
White solid, m.p. 211-213 ^{o}C.
IR (KBr): ν 3420, 3287, 3163, 2965, 2191, 1679, 1658, 1510, 1246 cm^{-1}. ^{1}H NMR (400 MHz, DMSO-d$_6$): δ 9.25 (s, 1H) 6.92-6.90 (m, 4H), 6.64 (d, 2H, J = 8.8 Hz), 4.05 (s, 1H), 2.53-2.42 (m, 2H), 2.23 (d, 1H, J = 15.6 Hz), 2.08 (d, 1H, J = 16 Hz), 1.02 (s, 3H), 0.93 (s, 3H) ppm.^{13}C NMR (100 MHz, DMSO-d$_6$): δ 195.6, 161.9, 158.3, 155.9, 135.1, 128.1, 119.8, 114.9, 113.1, 58.7, 49.9, 34.6, 31.7, 28.3, 26.7 ppm. ESI-MS: *m/z* 310 [M]$^{+}$.

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



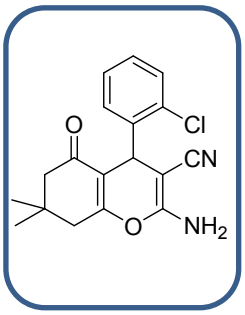
Off white solid, m.p. 214-216 °C.
IR (KBr): ν 3426, 3330, 3023, 2957, 2191, 1672, 1639, 1510, 1248 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$+DMSO-d_6): δ 7.04-6.99 (m, 4H), 5.71 (s, 2H), 4.22 (s, 1H), 2.22 (s, 3H), 2.19-2.07 (m, 4H), 1.04 (s, 3H), 0.96 (s, 3H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$+DMSO-d_6): δ 195.5, 161.3, 157.8, 140.5, 135.7, 128.5, 126.8, 119.1, 113.3, 60.5, 50.1, 40.1, 34.7, 31.6, 28.4, 27.0, 20.5 ppm. ESI-MS: *m/z* 308 $[M]^+$

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



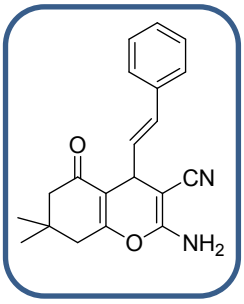
White yellowish solid, m.p. 220-222 °C.
IR (KBr): ν 3471, 3333, 3036, 2959, 2194, 1667, 1597, 1523, 1470, 1254 cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6): δ 7.56 (d, 1H, *J* = 7.2 Hz), 7.40 (t, 1H, *J* = 7.6 Hz), 7.17 (t, 1H, *J* = 8.8 Hz), 7.10 (d, 1H, J = 7.2 Hz), 6.97 (s, 2H), 4.67 (s, 1H), 2.30-2.18 (m, 2H), 1.96 (d, 1H, *J* = 17.2 Hz), 1.76 (d, 1H, *J* =16 Hz), 0.75 (s, 3H), 0.62 (s. 3H) ppm.^{13}C NMR (100 MHz, DMSO-d_6): δ 195.7, 162.6, 159.1, 148.9, 138.9, 133.3, 130.2, 127.8, 123.6, 119.0, 112.2, 56.2, 49.4, 31.8, 29.8, 28.2, 26.6 ppm. ESI-MS: *m/z* 339 $[M]^+$

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



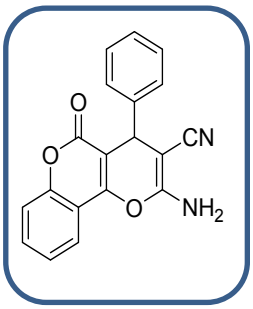
White solid, m.p. 214-216 °C.
IR (KBr): ν 3473, 3328, 3010, 2960, 2874, 2197, 1658, 1605, 1469, 1366, 1250 cm^{-1}.^1H NMR (400 MHz, DMSO-d_6): δ 7.36 (d, 1H, *J* = 7.6 Hz), 7.27 (t, 1H, *J* = 7.2 Hz), 7.21-7.15 (m, 2H), 7.05 (s, 2H), 4.68 (s, 1H), 2.57-2.45 (m, 2H), 2.24 (d, 1H, *J* = 16 Hz), 2.07 (d, 1H, *J* = 16 Hz), 1.03 (s, 3H), 0.97 (s, 3H) ppm.^{13}C NMR (100 MHz, DMSO-d_6): δ 195.5, 163.1, 158.6, 141.5, 132.0, 129.9, 129.4, 128.1, 127.4, 119.2, 111.7, 56.7, 49.8, 32.7, 31.7, 28.3, 26.8 ppm. ESI-MS: *m/z* 328 $[M]^+$, 330 $[M+2]^+$.

2-amino-5,6,7,8-tetrahydro-7,7-dimethyl-5-oxo-4-styryl-4*H*-chromene-3-carbonitrile. (7j)



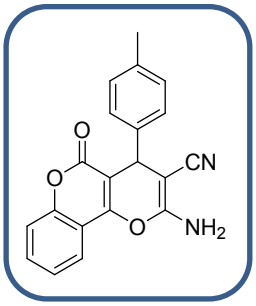
White solid, m.p. 180-182 °C.
IR (KBr): ν 3386, 3297, 3023, 2959, 2184, 1680, 1655, 1608, 1376, 1245 cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6): δ 7.37 (d, 2H, *J* = 7.6 Hz), 7.29 (t, 2H, *J* = 7.6 Hz), 7.22-7.19 (m, 1H), 7.08 (s, 2H), 6.35 (d, 1H, *J* = 16 Hz), 6.06 (dd, 1H, *J* = 16 Hz, 8Hz), 3.80 (d, 1H, *J* = 8Hz), 2.48 - 2.37 (m, 2H), 2.27 (d, 1H, *J* = 16 Hz), 2.20 (d, 1H, *J* = 16 Hz), 1.02 (s, 3H), 0.99 (s, 3H) ppm.^{13}C NMR (100 MHz, DMSO-d_6): δ 195.8, 162.4, 159.2, 136.4, 131.0, 129.2, 128.5, 127.3, 126.1, 119.8, 111.8, 55.1, 50.0, 32.7, 31.7, 28.1, 26.8 ppm. ESI-MS: m/z 320 $[M]^+$.

2-amino-5-oxo-4-phenyl-4,5-dihydropyrano[3,2-*c*]chromene-3-carbonitrile. (8a)



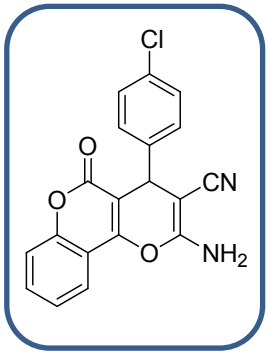
White solid, m.p. 255-257 °C.
IR (KBr): *ν* 3378, 3285, 3180, 2198, 1709, 1675, 1606, 1381, 1273, 1171 cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6): δ 7.89 (d, 1H, *J* = 7.2 Hz), 7.71 (t, 1H, *J* = 8.8 Hz), 7.51-7.44 (m, 2H), 7.41 (s, 2H), 7.33-7.21 (m, 5H), 4.44 (s, 1H) ppm.^{13}C NMR (100 MHz, DMSO-d_6): δ 159.4, 157.9, 153.3, 152.0, 143.2, 132.8, 128.4, 127.5, 127.0, 124.6, 122.4, 119.2, 116.5, 112.9, 103.9, 57.9, 36.9 ppm. ESI-MS: *m/z* 316 $[M]^+$.

2-amino-5-oxo-4-(*p*-tolyl)-4,5-dihydropyrano[3,2-*c*]chromene-3-carbonitrile. (8b)



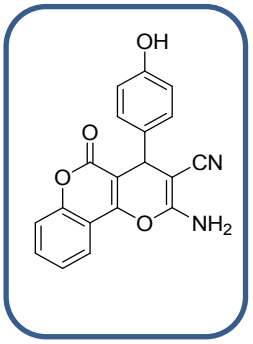
White solid, m.p. 250-252 °C.
IR (KBr): *ν* 3390, 3313, 3194, 3042, 2919, 2195, 1715, 1677, 1638, 1611, 1608, 1377 cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6): δ 7.88 (d, 1H, *J* = 7.2 Hz), 7.72-7.68 (m, 1H), 7.50-7.44 (m, 4H), 7.38 (s, 2H), 7.13-7.09 (m, 4H), 4.39 (s, 1H), 2.25 (s, 3H) ppm.^{13}C NMR (100 MHz, DMSO-d_6): δ 159.4 157.8, 153.3, 152.0, 140.3, 136.2, 132.8, 129.0, 127.4, 124.6, 122.4, 119.2, 116.5, 112.9, 104.0, 58.0, 36.5, 20.5 ppm. ESI-MS: *m/z* 330 $[M]^+$.

2-amino-4-(4-chlorophenyl)-4,5-dihydro-5-oxopyrano[3,2-*c*]chromene-3-carbonitrile. (8c)



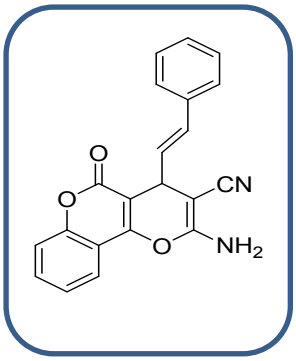
White solid, m.p. 261-263 °C.
IR (KBr): *ν* 3382, 3311, 3291, 3189, 3050, 2192, 1712, 1679, 1638, 1610, 1377 cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6): δ 7.89 (d, 1H, *J* = 8.4 Hz), 7.71 (t, 1H, *J* = 8.8 Hz), 7.51-7.45 (m, 4H), 7.36 (d, 2H, *J* = 7.6 Hz), 7.30 (d, 2H, *J* = 7.6 Hz), 4.48 (s, 1H) ppm.^{13}C NMR (100 MHz, DMSO-d_6): δ 159.4, 157.9, 153.5, 152.1, 142.2, 132.9, 131.6, 129.6, 128.3, 124.6, 122.4, 119.0, 116.5, 112.8, 103.4, 57.4, 36.3 ppm. ESI-MS: m/z 350 $[M]^+$, 352 $[M+2]^+$.

2-amino-4,5-dihydro-4-(4-hydroxyphenyl)-5-oxopyrano[3,2-*c*]chromene-3-carbonitrile. (8d)



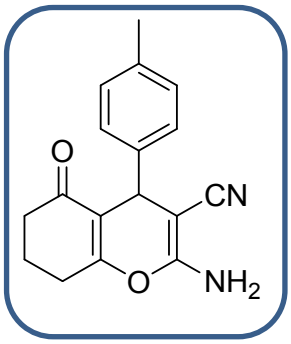
White solid, m.p. 260-262 °C.
IR (KBr): *ν* 3505, 3408, 3287, 3184, 2197, 1696, 1674, 1610, 1513, 1460, 1381 cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6): δ 9.36 (s, 1H), 7.88 (d, 1H, *J* = 7.2 Hz), 7.70 (t, 1H, *J* = 8 Hz), 7.50-7.44 (m, 2H), 7.34 (s, 2H), 7.03 (d, 2H, *J* = 8.4 Hz), 6.67 (d, 1H, *J* = 7.2 Hz), 4.32 (s, 1H) ppm.^{13}C NMR (100 MHz, DMSO-d_6): δ 159.5, 157.8, 156.4, 152.9, 151.9, 133.6, 132.7, 128.6, 124.5, 122.3, 119.5, 116.4, 115.1, 112.9, 104.4, 58.3, 36.0 ppm. ESI-MS: *m/z* 332$[M]^+$.

2-amino-4,5-dihydro-5-oxo-4-styrylpyrano[3,2-*c*]chromene-3-carbonitrile. (8e)



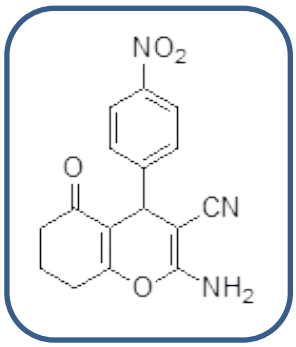
Yellow solid, m.p. 198-200 °C.
IR (KBr): ν 3320, 3200, 3021, 2190, 1712, 1675, 1606, 1495, 1376 cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6): δ 7.84 (d, 1H, J = 7.6 Hz), 7.70 (t, 1H, J = 7.2 Hz), 7.48-7.41 (m, 6H), 7.30 (t, 2H, J = 7.6 Hz), 7.23- 7.20 (m, 1H), 6.53 (d, 1H, J = 16Hz), 6.22 (dd, 1H, J = 16 Hz, 8 Hz), 4.03 (d, 1H, J = 8 Hz) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ 159.6, 158.5, 153.2, 152.0, 136.2, 132.8, 130.4, 129.6, 128.5, 127.5, 126.3, 124.5, 122.2, 119.4, 116.5, 113.0, 103.0, 55.1, 34.4 ppm. ESI-MS: *m/z* 342$[M]^+$.

2-amino-5,6,7,8-tetrahydro-5-oxo-4-*p*-tolyl-4*H*-chromene-3-carbonitrile. (9b)



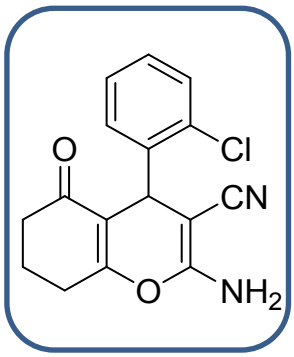
White solid, m.p. 210-212 °C.
IR (KBr): ν 3410, 3333, 3219, 2197, 1684, 1660, 1605, 1368 cm^{-1}.
^1H NMR (400 MHz, DMSO-d_6): δ 7.06 (d, 2H, J = 8.8 Hz), 7.01 (d, 2H, J = 7.2 Hz), 6.96 (s, 2H), 4.11 (s, 1H), 2.63-2.58 (m, 2H), 2.31-2.25 (m, 2H), 2.23 (s, 3H), 1.94-1.86 (m, 2H) ppm.^{13}C NMR (100 MHz, DMSO-d_6): δ 195.8, 164.2, 158.3, 141.8, 135.5, 128.8, 127.0, 119.7, 113.8, 58.2, 36.2, 34.9, 26.4, 20.5, 19.7 ppm. ESI-MS: *m/z* 280 $[M]^+$.

2-amino-5,6,7,8-tetrahydro-4-(4-nitrophenyl)-5-oxo-4*H*-chromene-3-carbonitrile. (9c)



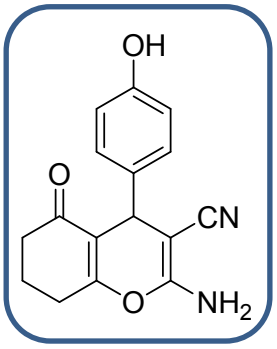
Yellow solid, m.p. 220-222 °C.
IR (KBr): ν 3415, 3336, 3218, 2195, 1681, 1652, 1602, 1518, 1364 cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6): δ 8.14 (d, 2H, J = 8.4 Hz), 7.44 (d, 2H, J = 8.4 Hz), 7.18 (s, 2H), 4.34 (s, 1H), 2.63-2.30 (m, 2H), 2.29-2.19 (m, 2H), 1.95-1.91 (m, 2H) ppm.^{13}C NMR (100 MHz, DMSO-d_6): δ 195.8, 165.0, 158.4, 152.2, 146.1, 128.5, 123.6, 119.3, 112.6, 58.8, 36.1, 35.5, 26.4, 19.6 ppm. ESI-MS: *m/z* 311$[M]^+$.

2-amino-4-(2-chlorophenyl)-5,6,7,8-tetrahydro-5-oxo-4*H*-chromene-3-carbonitrile. (9d)



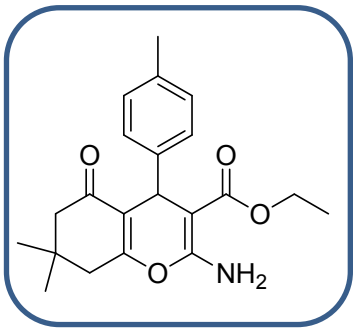
White solid, m.p. 213-215 °C,
IR (KBr): ν 3328, 3254, 3182, 2955, 2190, 1650, 1606, 1470, 1368 cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6): δ 7.34 (d, 1H, J = 8.8 Hz), 7.26- 7.16 (m, 3H), 7.02 (s, 2H), 4.68 (s, 1H), 2.65-2.58 (m, 2H), 2.28-2.17 (m, 2H), 1.95-1.88 (m, 2H) ppm.^{13}C NMR (100 MHz, DMSO-d_6): δ 195.6, 165.0, 158.4, 141.7, 132.0, 129.7, 129.2, 128.0, 127.4, 119.2, 112.8, 56.7, 36.2, 32.6, 26.4, 19.7 ppm. ESI-MS: *m/z* 300 $[M]^+$, 302 $[M+2]^+$.

2-amino-5,6,7,8-tetrahydro-4-(4-hydroxyphenyl)-5-oxo-4*H*-chromene-3-carbonitrile. (9e)



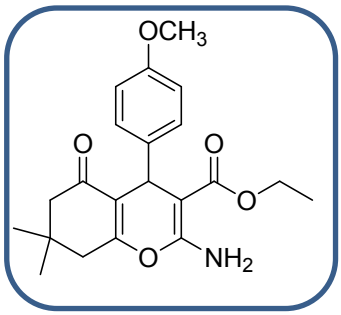
White solid, m.p. 240-242 °C,
IR (KBr): ν 3380, 3194, 2817, 2199, 1674, 1646, 1604, 1512, 1374 cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6): δ 9.25 (s, 1H), 6.92-6.90 (m, 4H), 6.63 (d, 2H, J = 8.4 Hz), 4.05 (s, 1H), 2.65-2.57 (m, 2H), 2.25-2.22 (m, 2H), 1.93-1.83 (m, 2H) ppm.^{13}C NMR (100 MHz, DMSO-d_6): δ 195.8, 163.9, 158.3, 155.9, 135.1, 128.0, 119.9, 114.9, 114.2, 58.8, 36.3, 34.4, 26.3, 19.7 ppm. ESI-MS: *m/z* 282 $[M]^+$.

Ethyl-2-amino-7,7-dimethyl-5-oxo-4-(*p*-tolyl)-5,6,7,8-tetrahydro-4*H*-chromene-3-carboxylate. (10a)



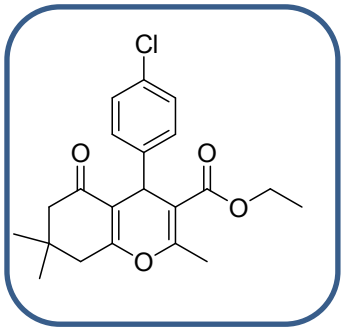
White solid, m.p. 151-153 °C.
IR (KBr): ν 3408, 3293, 2980, 1689, 1668, 1623, 1523, 1472, 1366 cm^{-1}.^1H NMR (400 MHz, DMSO-d_6): δ 7.52 (s, 2H), 7.02-6.98 (m, 4H), 4.45 (s, 1H), 3.97-3.90 (m, 2H), 2.56-2.42 (m, 2H), 2.25 (d,1 H, *J* = 16.8 Hz), 2.20 (s, 3H), 2.04 (d, 1H, *J* = 16 Hz), 1.10 (t, 3H, *J* = 8 Hz), 1.03 (s, 3H), 0.88 (s, 3H) ppm.^{13}C NMR (100 MHz, DMSO-d_6): δ 195.7, 167.9, 161.9, 159.0, 143.3, 134.6, 128.2, 127.5, 115.6, 77.9, 58.7, 49.9, 32.7, 31.8, 28.6, 26.3, 20.5, 14.1 ppm. ESI-MS: *m/z* 355 $[M]^+$.

Ethyl-2-amino-4-(4-methoxyphenyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4*H*-chromene-3-carboxylate. (10b)



White solid, m.p. 140-142 °C.
IR (KBr): ν 3412, 3304, 2959, 2837, 1670, 1625, 1527, 1445, 1367 cm^{-1}.^1H NMR (400 MHz, DMSO-d_6): δ 7.51 (s, 2H), 7.02 (d, 2H, *J* = 8.4 Hz), 6.75 (d, 2H, *J* = 8.4 Hz), 4.43 (s, 1H), 3.96-3.90 (m, 2H), 3.66 (s, 3H), 2.53 (d, 1H, *J* = 16 Hz), 2.43 (d, 1H, *J* = 18 Hz), 2.24 (d, 1H, *J* = 17.2 Hz), 2.04 (d, 1H, *J* = 15.6 Hz), 1.09 (t, 3H, *J* = 8 Hz) 1.02 (s, 3H), 0.89 (s, 3H) ppm.^{13}C NMR (100 MHz, DMSO-d_6): δ 195.8, 168.0, 161.8, 159.0, 157.2, 138.4, 128.5, 115.7, 113.0, 78.0, 58.7, 54.8, 49.9, 32.2, 31.8, 28.6, 26.4, 14.1 ppm. ESI-MS: *m/z* 371 $[M]^+$.

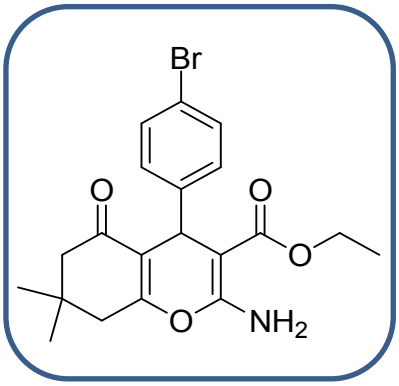
Ethyl-4-(4-chlorophenyl)-2,7,7-trimethyl-5-oxo-5,6,7,8-tetrahydro-4*H*-chromene-3-carboxylate. (10c)



White solid, m.p. 150-152 °C.
IR (KBr): ν 3479, 3331, 2975, 2880, 1687, 1658, 1621, 1526, 1489, 1369 cm^{-1}.^1H NMR (400 MHz, DMSO-d_6): δ 7.60 (s, 2H), 7.26 (d, 2H, *J* = 8.4 Hz), 7.14 (d, 2H, *J* = 8.4 Hz), 4.47 (s, 1H), 3.94 (q, 2H, *J* = 7.2 Hz), 2.55 (d, 1H, *J* = 16.8 Hz), 2.45 (d, 1H, *J* = 16Hz), 2.26 (d, 1H, *J* = 16 Hz), 2.07 (d, 1H, *J* = 16 Hz), 1.08 (t, 3H, *J* = 8Hz) 1.03 (s, 3H), 0.88 (s, 3H) ppm.^{13}C NMR (100 MHz, DMSO-d_6): δ 195.8, 167.7, 162.2, 159.0, 145.3, 130.2, 129.5, 127.6, 115.0, 77.2, 58.8,

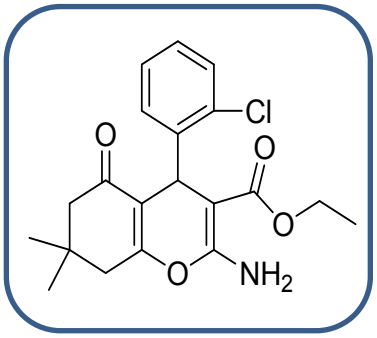
49.8, 32.9, 31.8, 28.5, 26.4, 14.1 ppm. ESI-MS: *m/z* 374 $[M]^+$, 376 $[M+2]^+$.

Ethyl-4-(4-bromophenyl)-2,7,7-trimethyl-5-oxo-5,6,7,8-tetrahydro-4*H*-chromene-3-carboxylate. (10d)



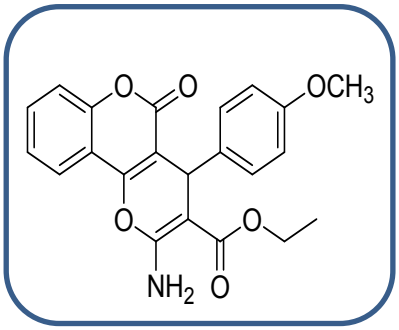
White solid, m.p. 156-158 °C.
IR (KBr): ν 3474, 3333, 2973, 2880, 1688, 1658, 1621, 1525, 1370 cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6): δ 7.59 (s, 2H), 7.39 (d, 2H, *J* = 8.8 Hz), 7.08 (d, 2H, *J* = 8.8 Hz), 4.45 (s, 1H), 3.94 (q, 2H, *J* = 7.2 Hz), 2.55 (d, 1H, *J* = 16.8 Hz), 2.45 (d, 1H, *J* = 17.2 Hz), 2.26 (d, 1H, *J* = 15.6 Hz), 2.05 (d, 1H, *J* = 16 Hz), 1.08 (t, 3H, *J* = 7.2 Hz), 1.03 (s, 3H), 0.88 (s, 3H) ppm.^{13}C NMR (100 MHz, DMSO-d_6): δ 195.8, 167.7, 162.2, 159.0, 145.7, 130.5, 129.9, 118.7, 114.9, 77.1, 58.8, 49.8, 33.0, 31.8, 28.5, 26.4, 14.1 ppm. ESI-MS: m/z 419$[M]^+$, 421 $[M+2]^+$.

Ethyl-4-(2-chlorophenyl)-2,7,7-trimethyl-5-oxo-5,6,7,8-tetrahydro-4*H*-chromene-3-carboxylate. (10e)



White solid, m.p. 166-168 °C.
IR (KBr): ν 3418, 3306, 2957, 1670, 1615, 1516, 1474, 1365 cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6): δ 7.64 (s, 2H), 7.24 - 7.08 (m, 4H), 4.82 (s, 1H), 3.89 (q, 2H, *J* = 7.6 Hz), 2.56 (d, 1H, *J* = 16.8 Hz), 2.40 (d, 1H, *J* = 18.4 Hz), 2.24 (d, 1H, *J* = 16 Hz), 2.01 (d, 1H, *J* = 15.6Hz), 1.03-1.00 (m, 6H) 0.89 (s, 3H) ppm.^{13}C NMR (100 MHz, DMSO-d_6): δ 195.5, 168.0, 162.2, 159.2, 142.7, 132.5, 131.8, 129.2, 127.3, 126.3, 113.8, 76.2, 58.6, 49.9, 32.1, 31.6, 28.6, 26.3, 14.1 ppm. ESI-MS: m/z 375 $[M]^+$, 377 $[M+2]^+$.

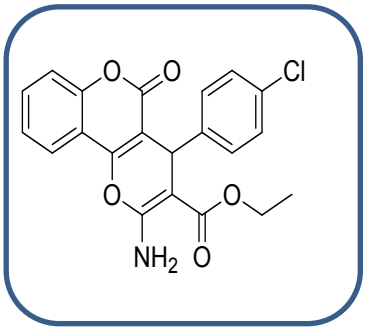
Ethyl-2-amino-4-(4-methoxyphenyl)-5-oxo-4,5-dihydropyrano[3,2-*c*]chromene-3-carboxylate. (11b)



White solid, m.p. 164-166 °C.
IR (KBr): ν 3396, 3285, 2953, 2199, 1686, 1651, 1612, 1533, 1493, 1377 cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6): δ 7.95 (d, 1H, *J* = 8 Hz), 7.79 (s, 2H), 7.68 (t, 1H, *J* = 8 Hz), 7.49-7.42 (m, 2H), 7.12 (d, 2H, *J* = 8 Hz), 6.78 (d, 2H, J = 8 Hz), 4.63 (s, 1H), 3.99-3.97 (m, 2H), 3.66 (s, 3H), 1.11 (t, 3H, *J* = 8 Hz) ppm.
^{13}C NMR (100 MHz, DMSO-d_6): δ 167.5, 159.8, 158.4, 157.7, 152.8, 151.9, 137.0, 132.5, 128.8, 124.5, 122.3, 116.4, 113.3, 113.1, 107.0, 77.2, 58.9, 54.8, 34.2, 14.1 ppm. ESI-MS: m/z 393$[M]^+$.

Ethyl-2-amino-4-(4-chlorophenyl)-5-oxo-4,5-dihydropyrano[3,2-*c*]chromene-3-carboxylate. (11c)

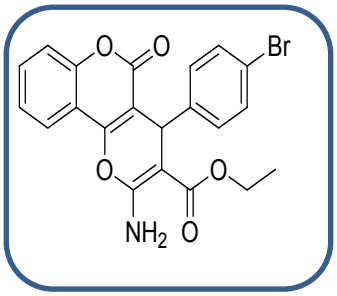
White solid, m.p. 190-192 ^{o}C.



IR (KBr): ν 3419, 3297, 2913, 1715, 1692, 1651, 1610, 1519, 1489, 1375 cm^{-1}. ^{1}H NMR (400 MHz, DMSO-d$_6$): δ 7.71 (d, 1H, *J* = 7.2 Hz), 7.63 (s, 2H), 7.50 (t, 1H, *J* = 8 Hz), 7.26-7.19 (m, 2H), 7.05- 6.99 (m, 4H), 4.42 (s, 1H), 3.74 (q, 2H, *J* = 7.2 Hz), 0.85 (t, 3H, *J* = 8 Hz) ppm.^{13}C NMR (100 MHz, DMSO-d$_6$): δ 167.3, 159.8, 158.4, 153.1, 152.0, 143.9, 132.7, 130.8, 129.9, 127.8, 124.5, 122.4, 116.4, 113.0, 106.2, 76.5, 59.0, 34.8, 14.1 ppm. ESI-MS: m/z 397 [M]$^{+}$, 399 [M+ 2]$^{+}$.

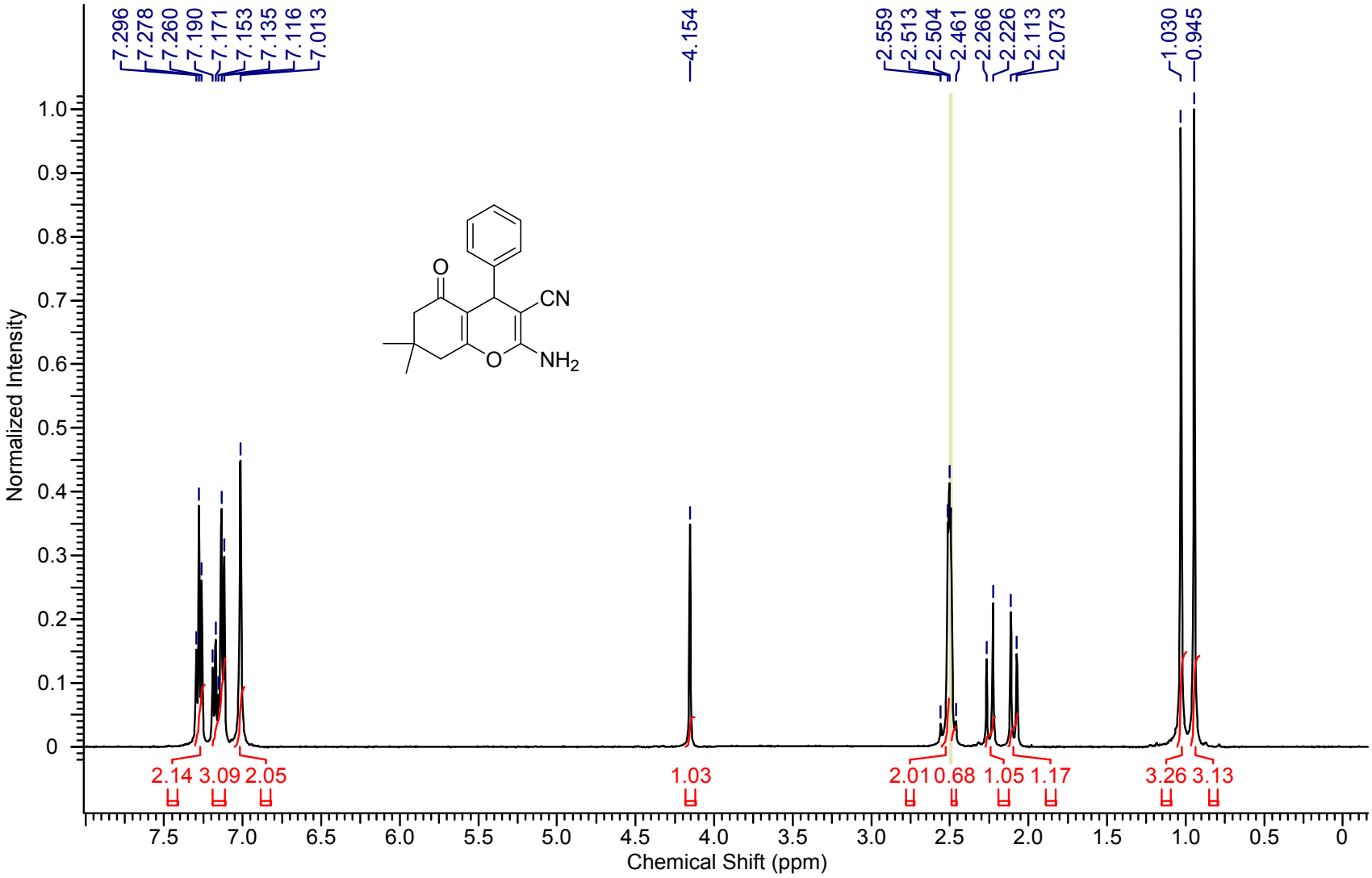
Ethyl-2-amino-4-(4-bromophenyl)-5-oxo-4,5-dihydropyrano[3,2-*c*]chromene-3-carboxylate. (11d)

White solid, m.p. 194-196 ^{o}C.

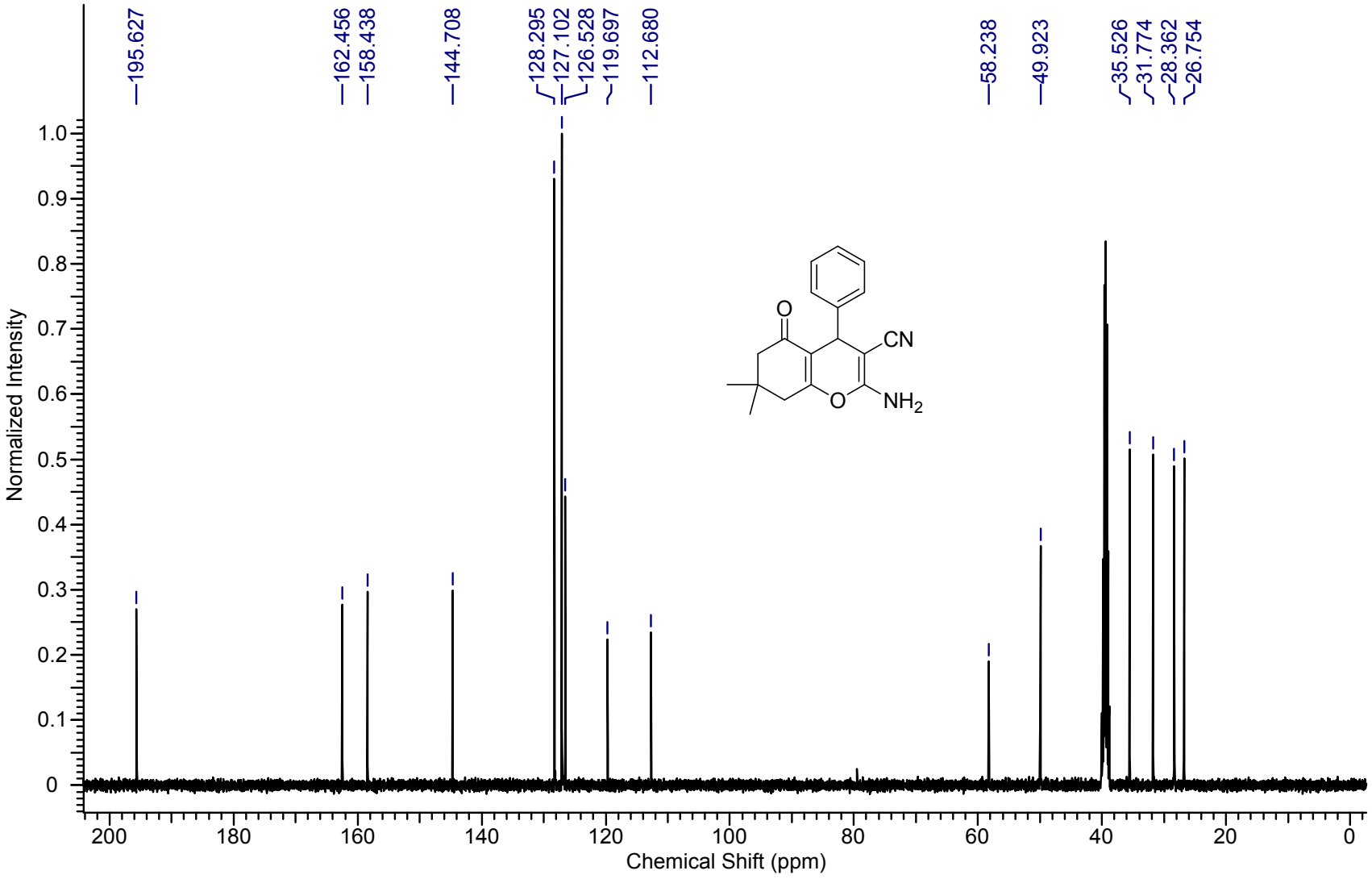


IR (KBr): ν 3421, 3295, 2982, 1716, 1651, 1610, 1535, 1519, 1491, 1375 cm^{-1}. ^{1}H NMR (400 MHz, DMSO-d$_6$): δ 7.95 (d, 1H, *J* = 8 Hz), 7.87 (s, 2H), 7.68 (t, 1H, *J* = 7.2 Hz), 7.49-7.40 (m, 4H), 7.19- 6.17 (m, 2H), 4.65 (s, 1H), 3.98 (q, 2H, *J* = 7.2 Hz), 1.09 (t, 3H, *J* = 7.2 Hz) ppm.^{13}C NMR (100 MHz, DMSO-d$_6$): δ 167.3, 159.8, 158.4, 153.2, 152.0, 144.3, 132.7, 130.7, 130.2, 124.6, 122.4, 119.3, 116.5, 113.0, 106.1, 76.4, 59.0, 34.8, 14.1 ppm. ESI-MS: m/z 441 [M]$^{+}$, 443 [M+2]$^{+}$

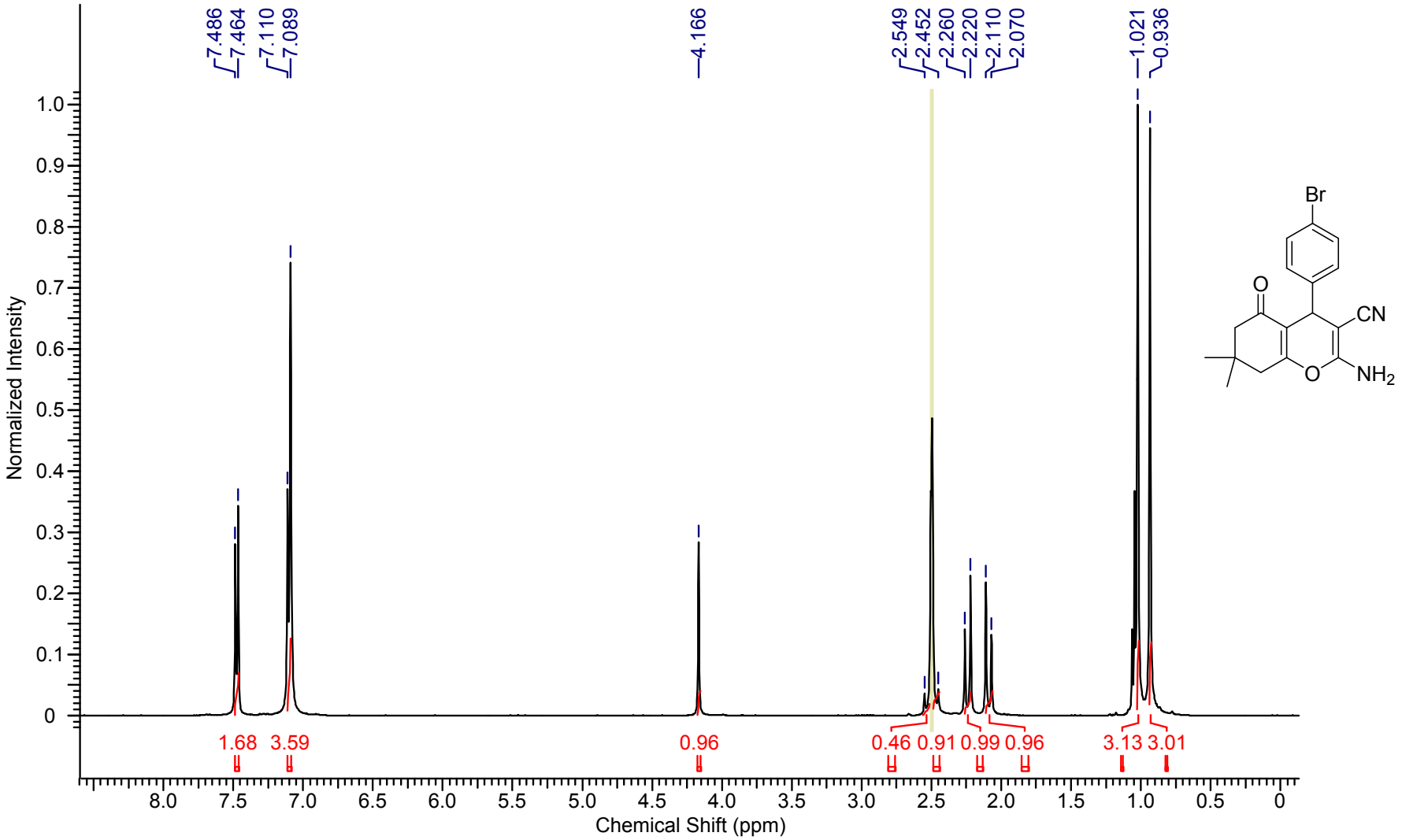
^{1}H NMR of 7a


7.296
7.278
7.260
7.190
7.171
7.153
7.135
7.116
7.013
4.154
2.559
2.513
2.504
2.461
2.266
2.226
2.113
2.073
1.030
0.945
O
CN
O
NH2
Normalized Intensity
Chemical Shift (ppm)
2.14 3.09 2.05
1.03
2.01 0.68 1.05 1.17
3.26 3.13

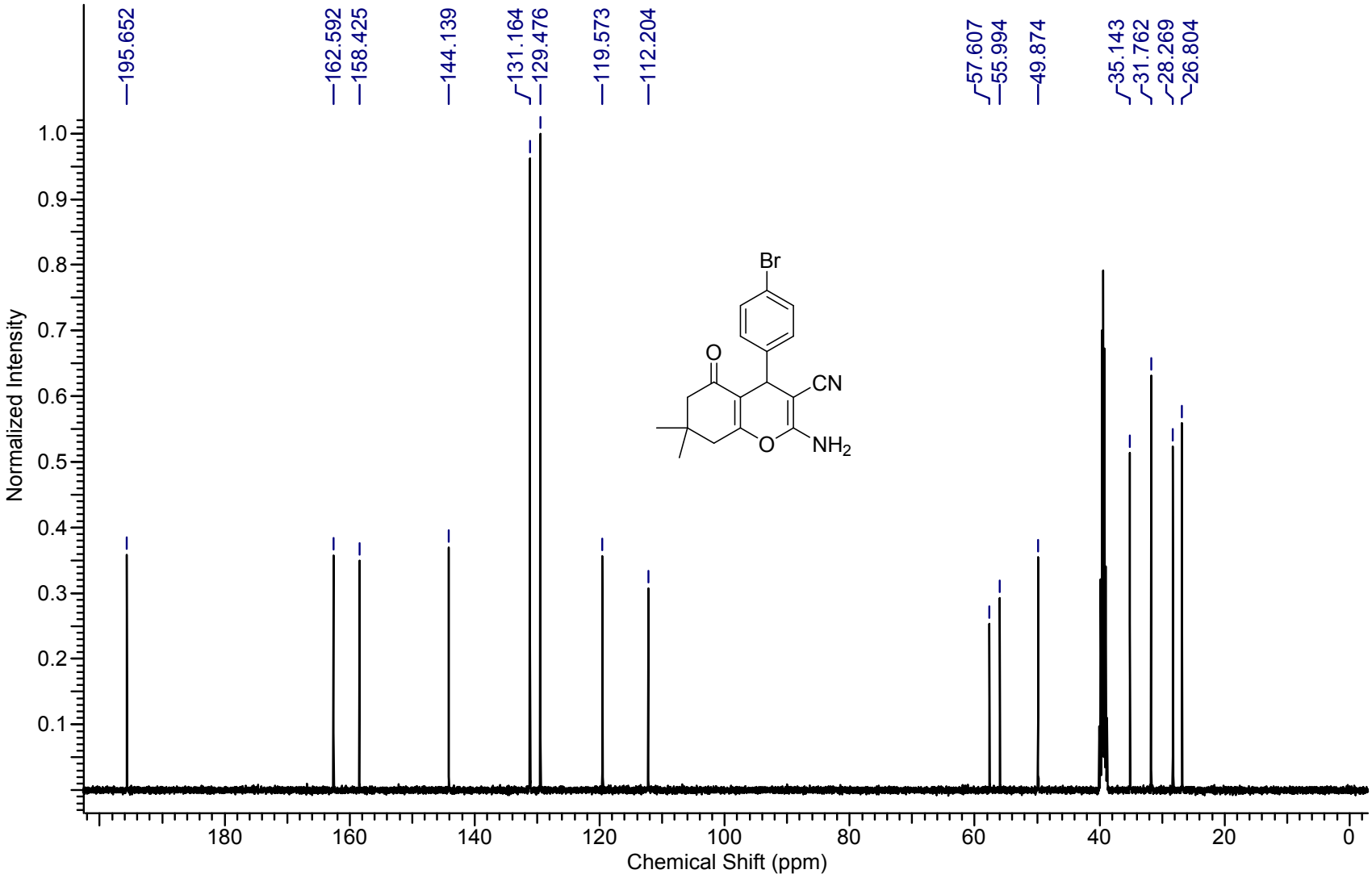
^{13}C NMR of 7a


195.627
162.456
158.438
144.708
128.295
127.102
126.528
119.697
112.680
58.238
49.923
35.526
31.774
28.362
26.754
Normalized Intensity
Chemical Shift (ppm)
O
CN
O
NH2

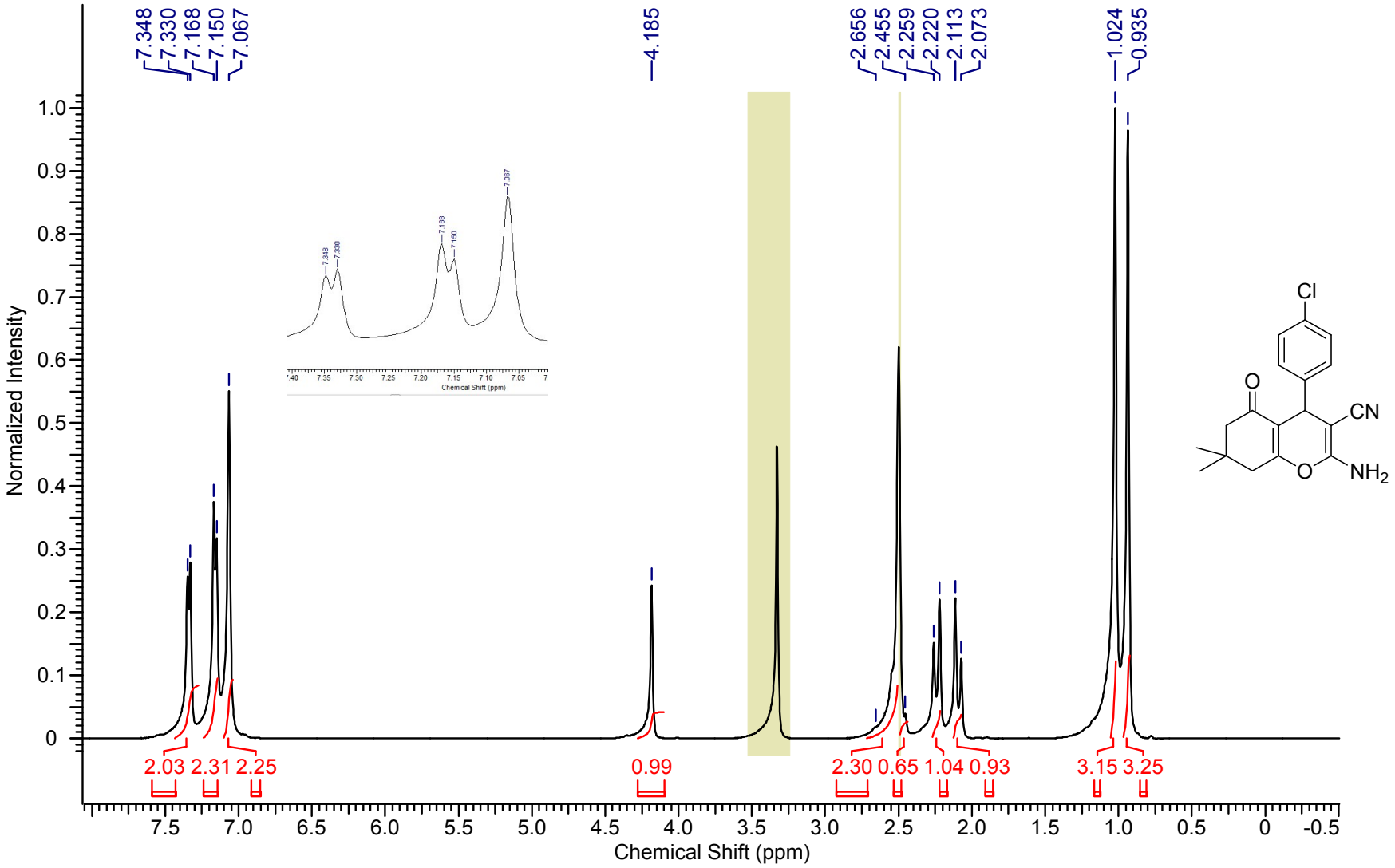
^{1}H NMR of 7b


7.486
7.464
7.110
7.089
4.166
2.549
2.452
2.260
2.220
2.110
2.070
1.021
0.936
Normalized Intensity
Chemical Shift (ppm)
1.68
3.59
0.96
0.46
0.91
0.99
0.96
3.13
3.01
Br
O
CN
O
NH2

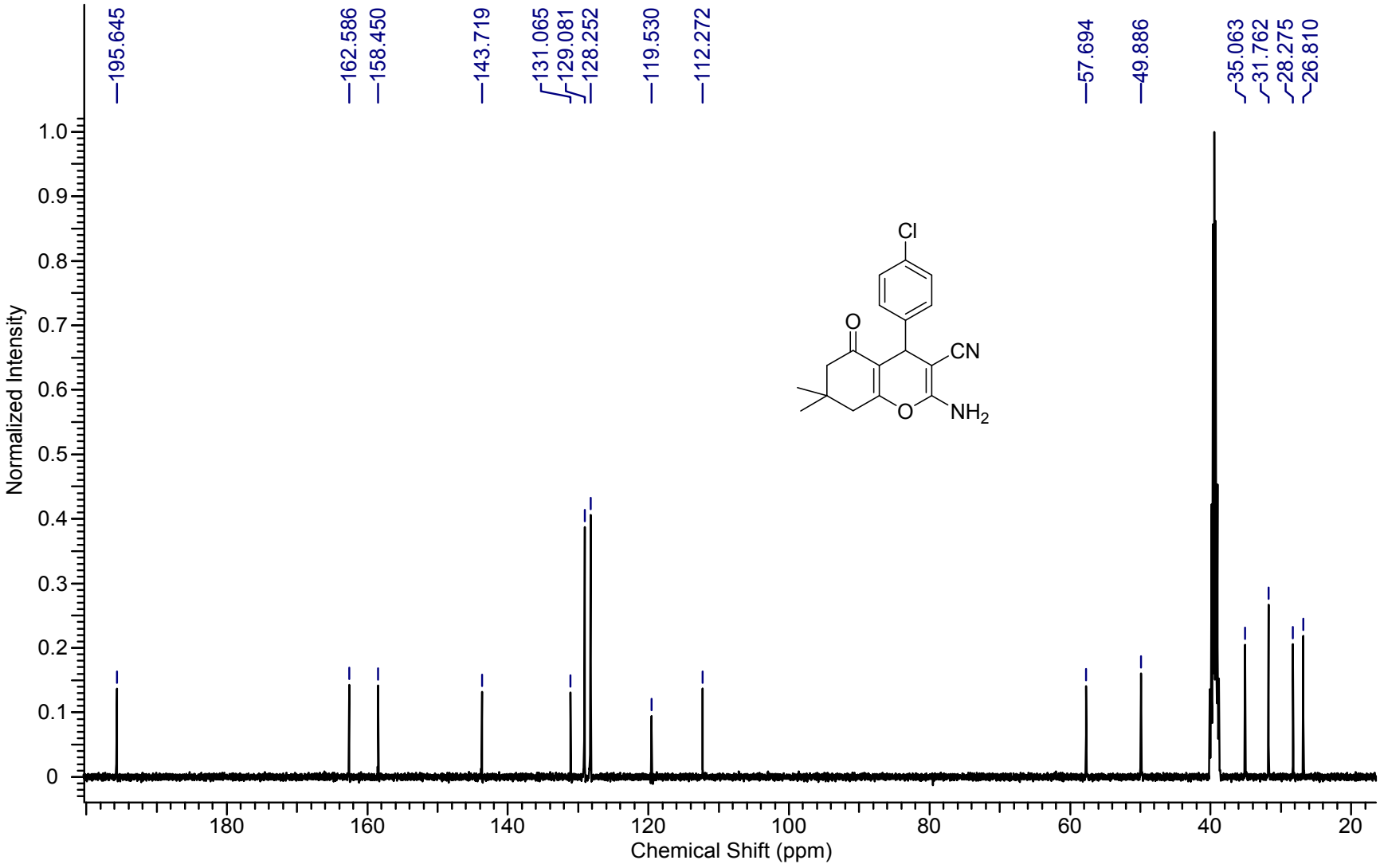
^{13}C NMR of 7b


195.652
162.592
158.425
144.139
131.164
129.476
119.573
112.204
57.607
55.994
49.874
35.143
31.762
28.269
26.804
Br
O
CN
O
NH2
Normalized Intensity
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

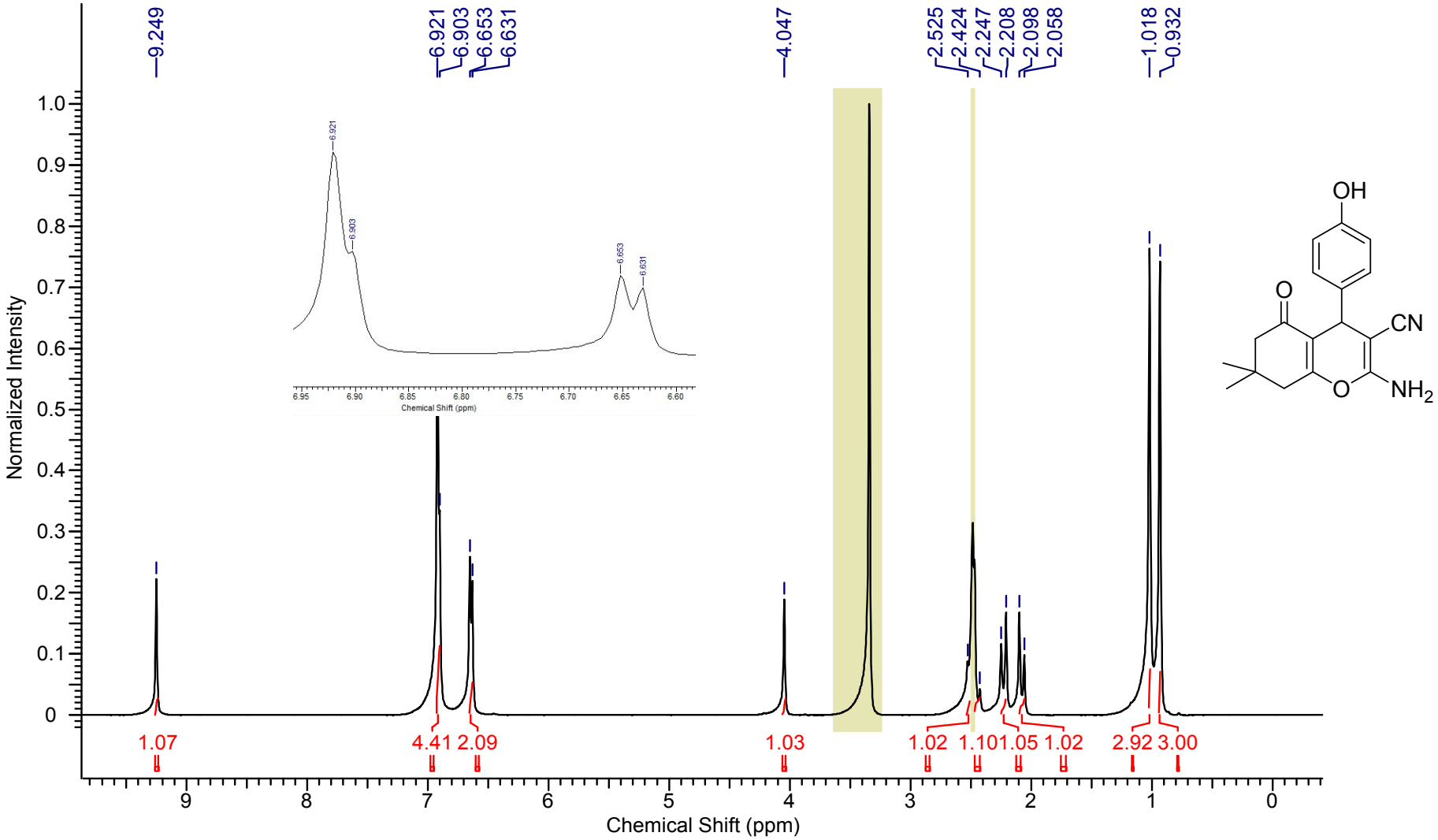
^{1}H NMR of 7c


7.348
7.330
7.168
7.150
7.067
4.185
2.656
2.455
2.259
2.220
2.113
2.073
1.024
0.935
Normalized Intensity
Chemical Shift (ppm)
2.03 2.31 2.25
0.99
2.30 0.65 1.04 0.93
3.15 3.25
Cl
O
CN
O
NH2

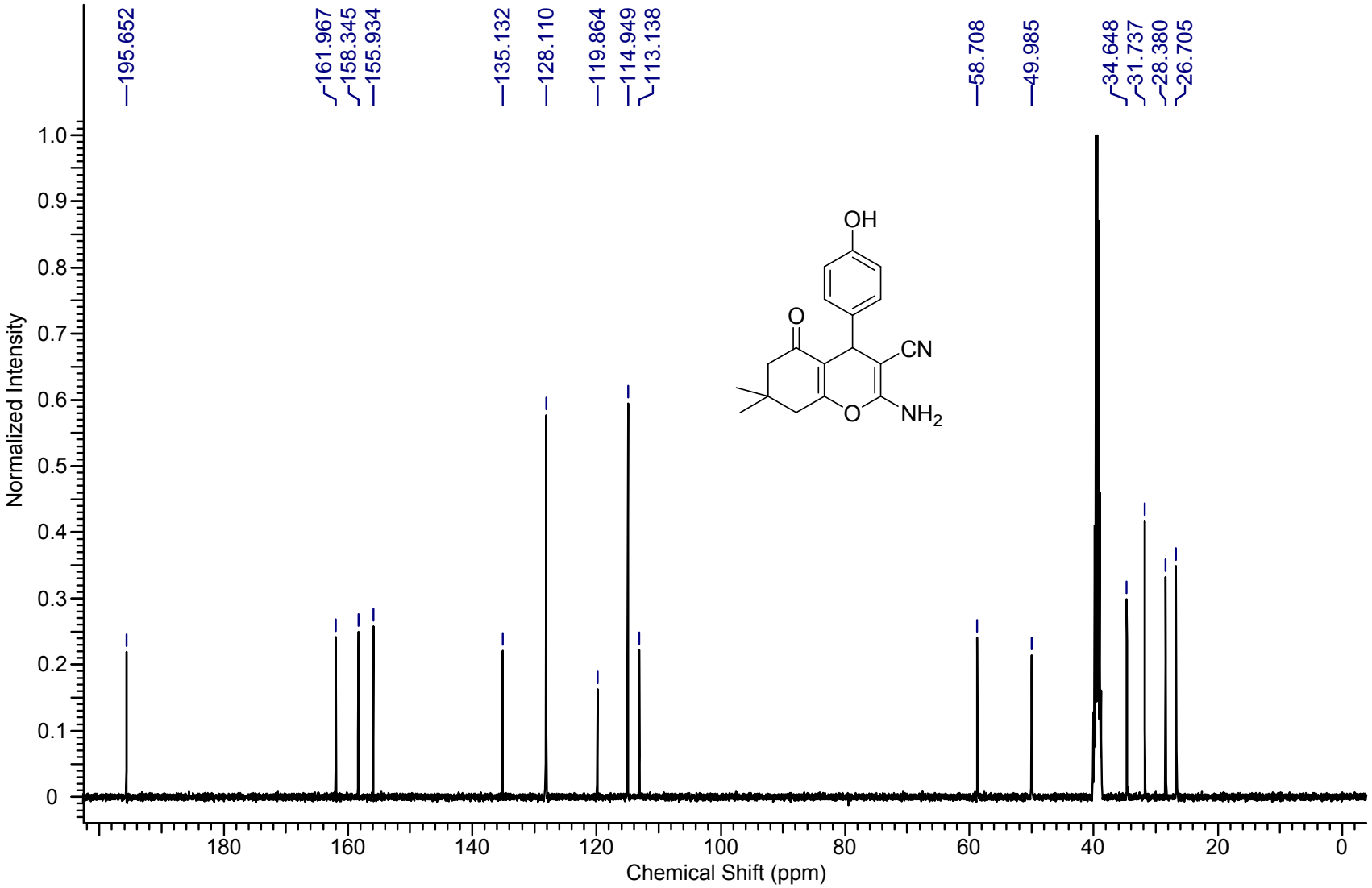
^{13}C NMR of 7c


195.645
162.586
158.450
143.719
131.065
129.081
128.252
119.530
112.272
57.694
49.886
35.063
31.762
28.275
26.810
Cl
O
CN
O
NH2
Normalized Intensity
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
180
160
140
120
100
80
60
40
20
Chemical Shift (ppm)

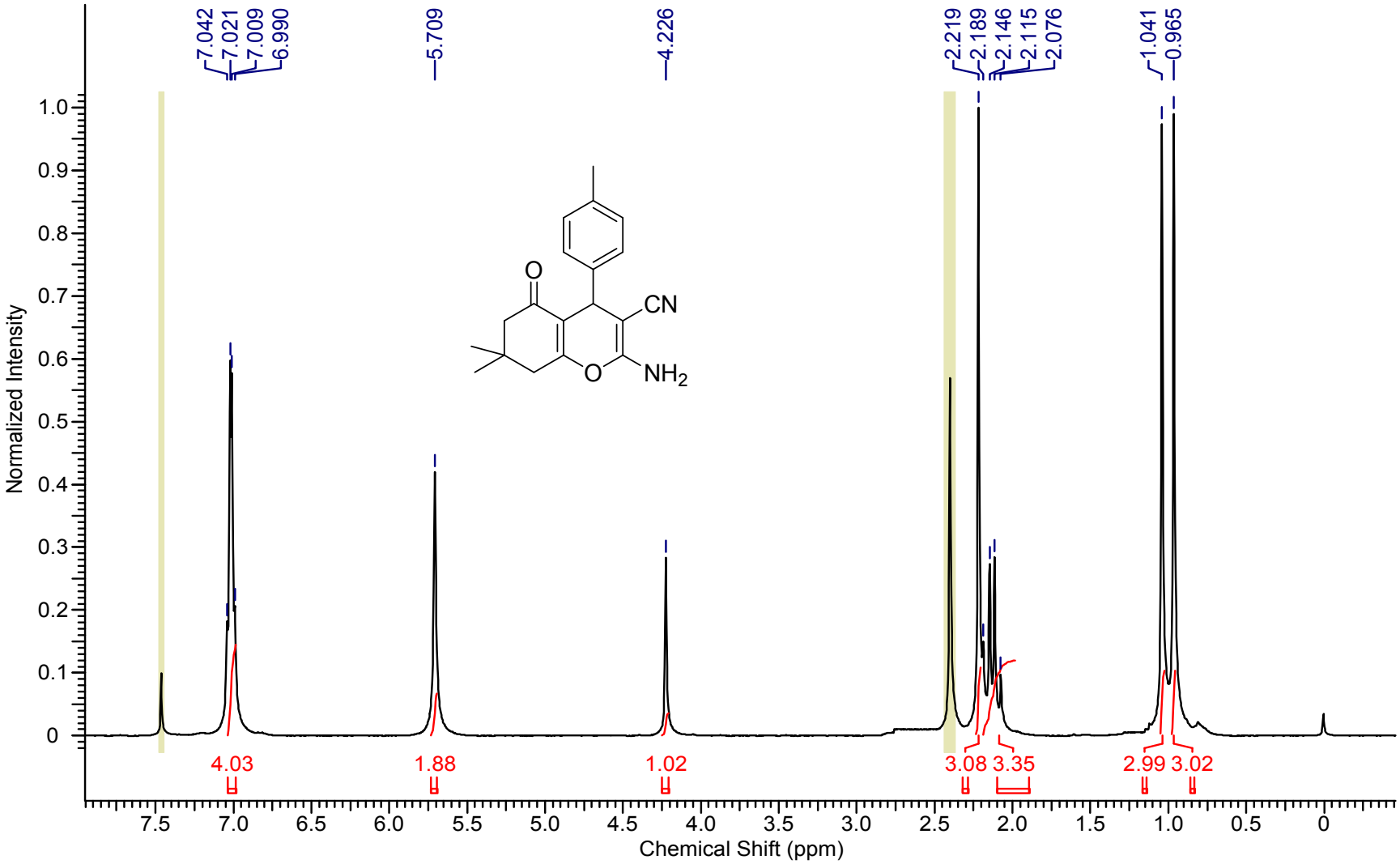
^{1}H NMR of 7e


9.249
6.921
6.903
6.653
6.631
4.047
2.525
2.424
2.247
2.208
2.098
2.058
1.018
0.932
Normalized Intensity
Chemical Shift (ppm)
1.07
4.41
2.09
1.03
1.02
1.10
1.05
1.02
2.92
3.00
OH
O
CN
O
NH2

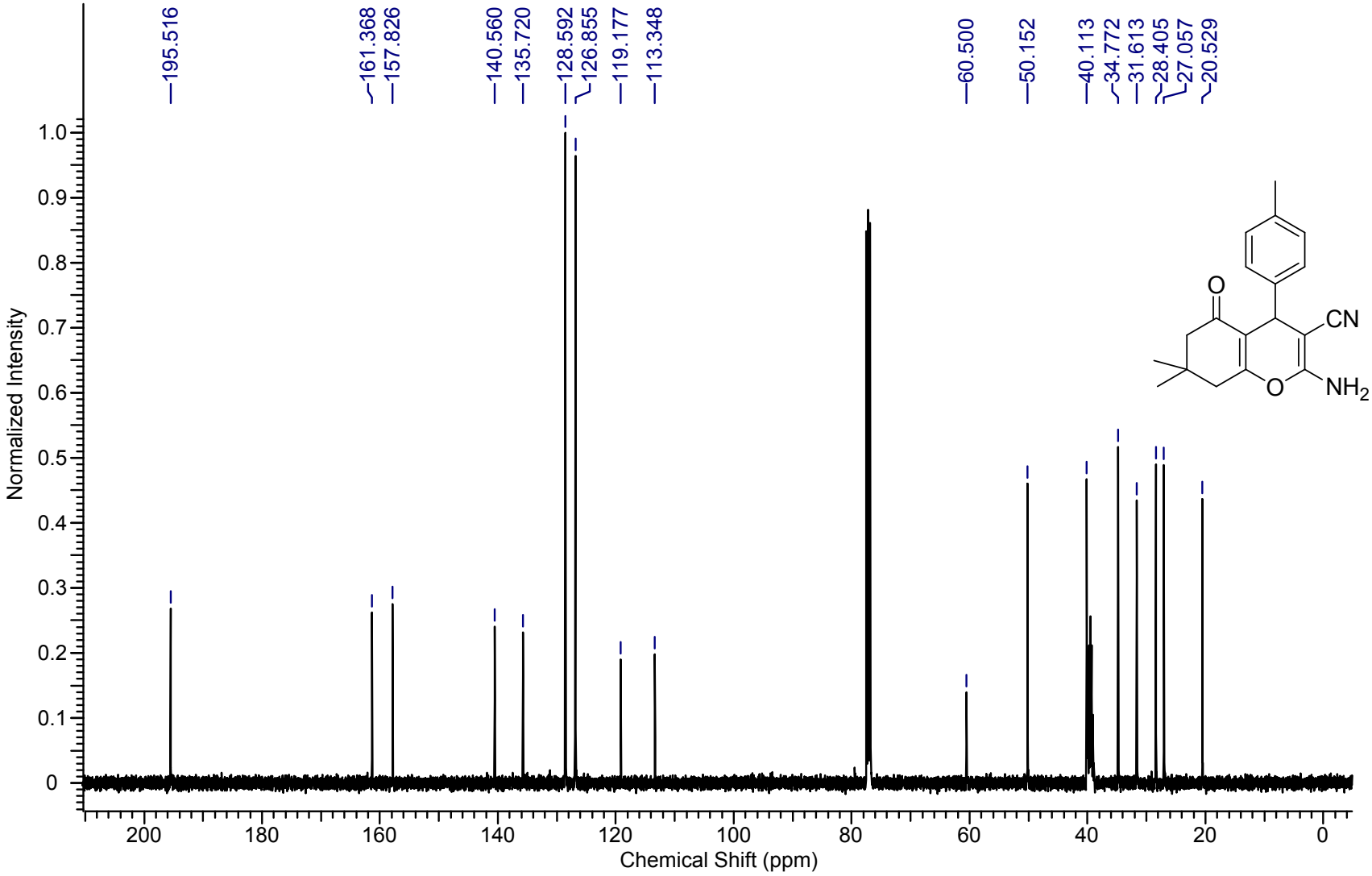
^{13}C NMR of 7e


195.652
161.967
158.345
155.934
135.132
128.110
119.864
114.949
113.138
58.708
49.985
34.648
31.737
28.380
26.705
OH
O
CN
O
NH2
Normalized Intensity
Chemical Shift (ppm)

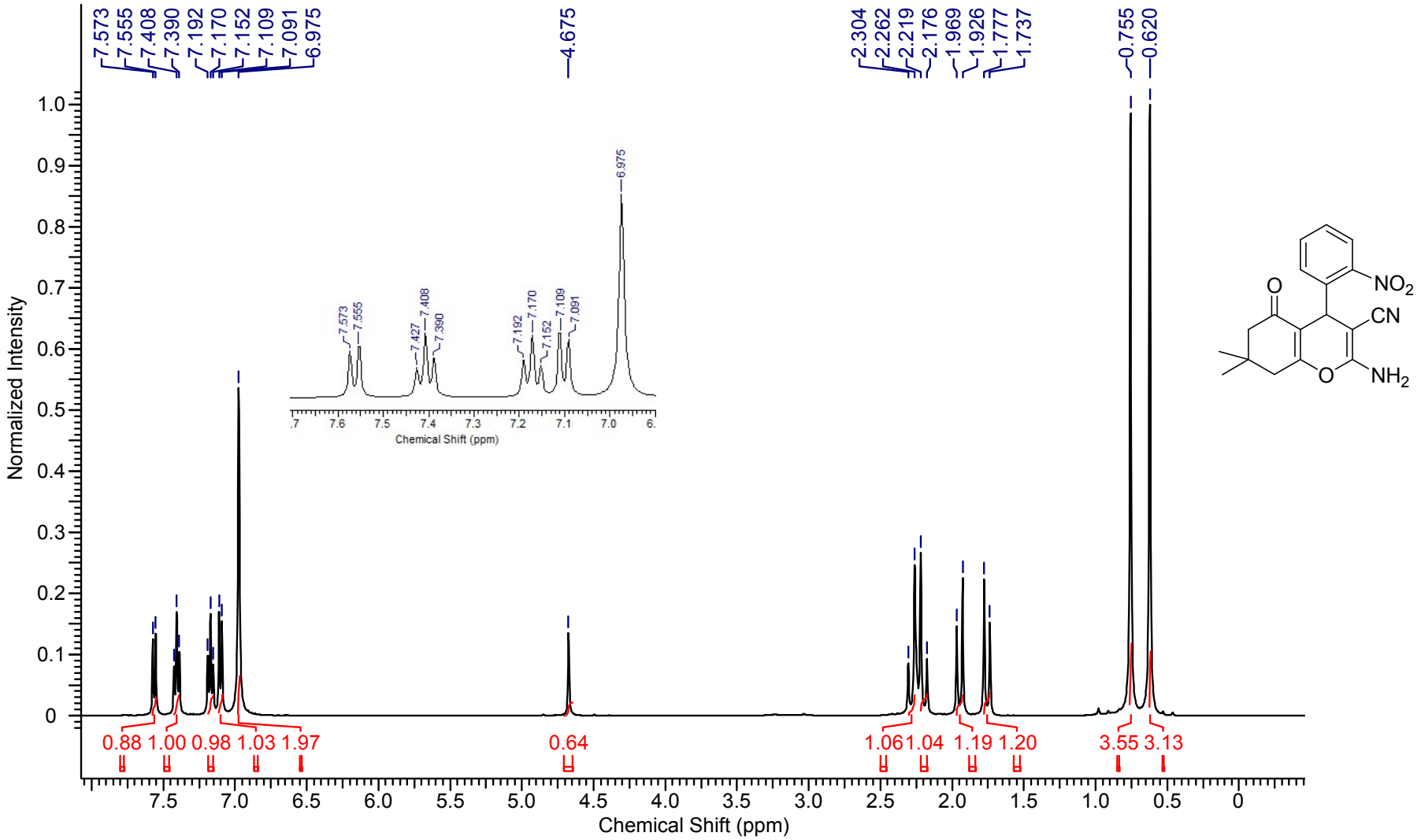
^{1}H NMR of 7f ($CDCl_3$+$DMSOd_6$)



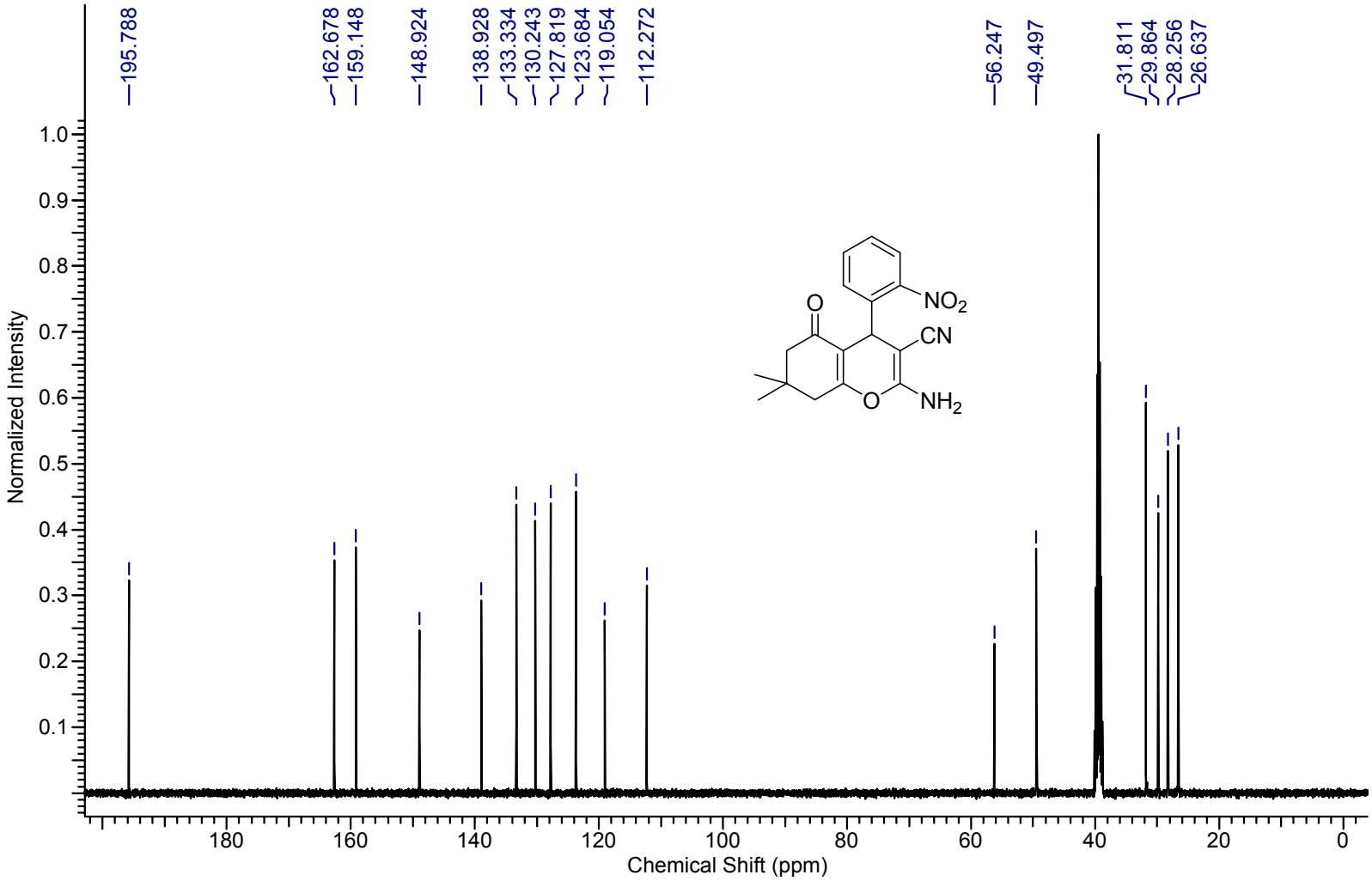
^{13}C NMR of 7f ($CDCl_3$+$DMSOd_6$)



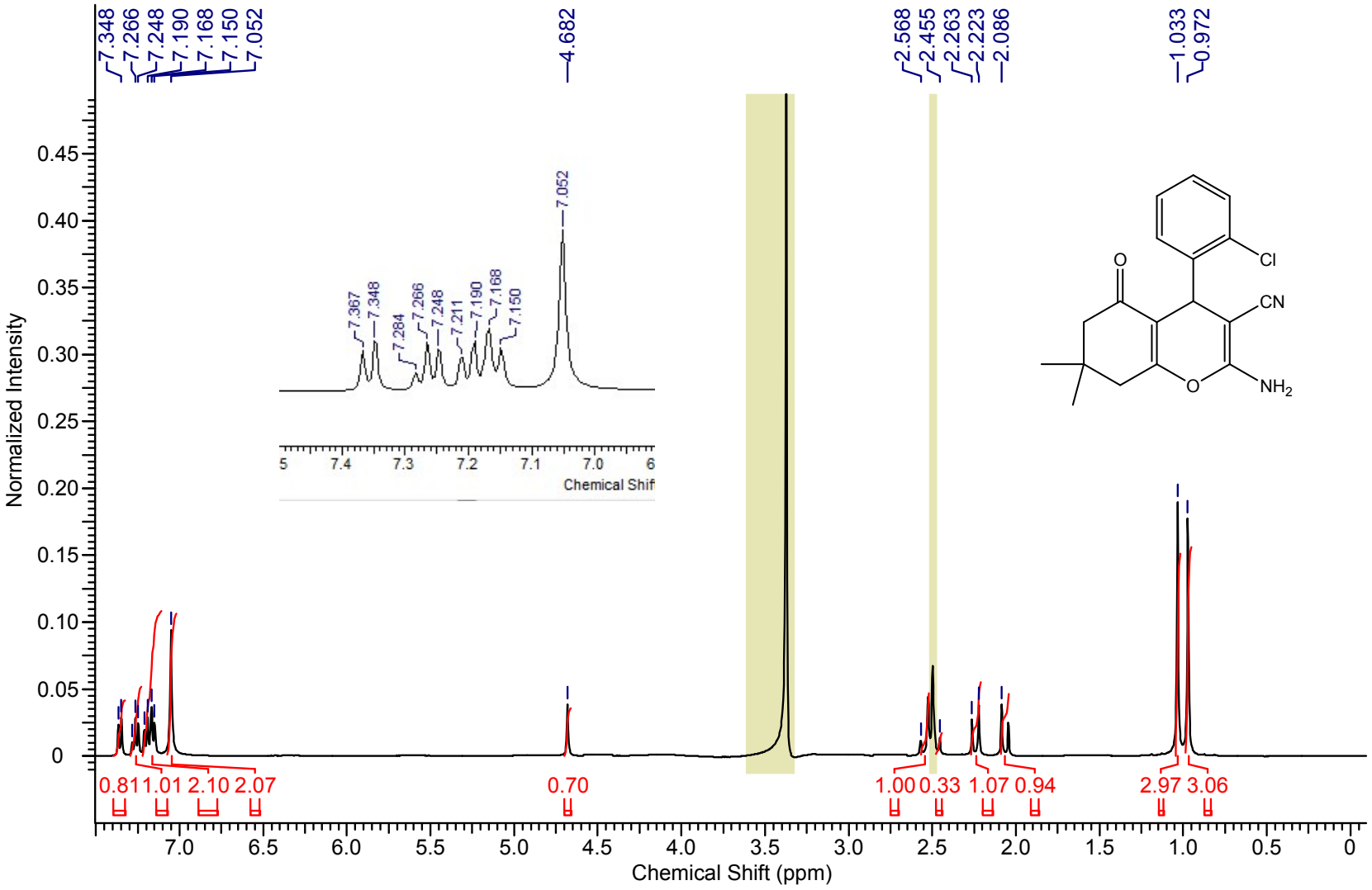
^{1}H NMR of 7g


7.573
7.555
7.408
7.390
7.192
7.170
7.152
7.109
7.091
6.975
4.675
2.304
2.262
2.219
2.176
1.969
1.926
1.777
1.737
0.755
0.620
Normalized Intensity
Chemical Shift (ppm)
0.88 1.00 0.98 1.03 1.97
0.64
1.06 1.04 1.19 1.20
3.55 3.13
NO2
CN
NH2
O
O

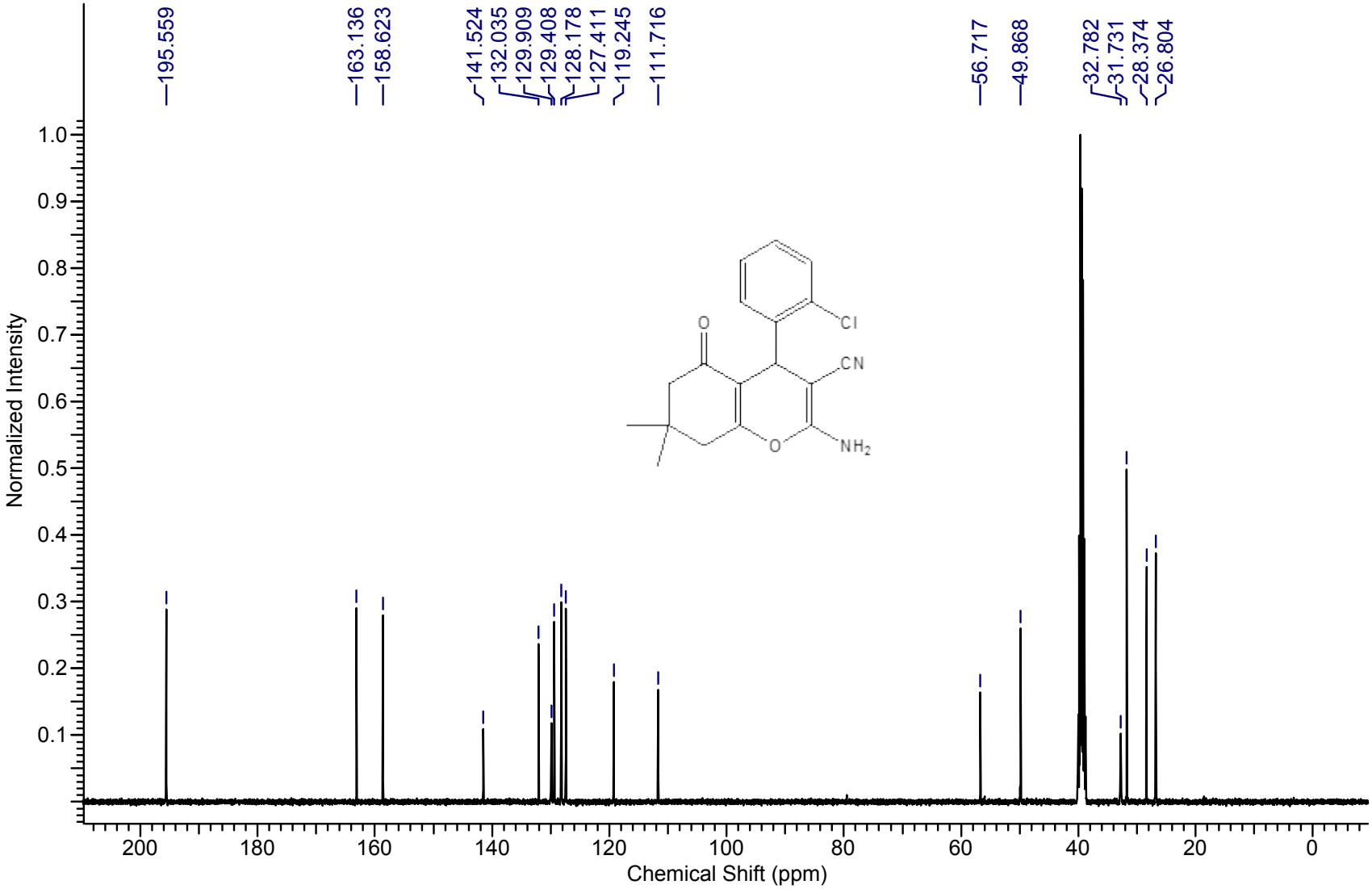
^{13}C NMR of 7g


195.788
162.678
159.148
148.924
138.928
133.334
130.243
127.819
123.684
119.054
112.272
56.247
49.497
31.811
29.864
28.256
26.637
Normalized Intensity
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)
O
NO2
CN
O
NH2

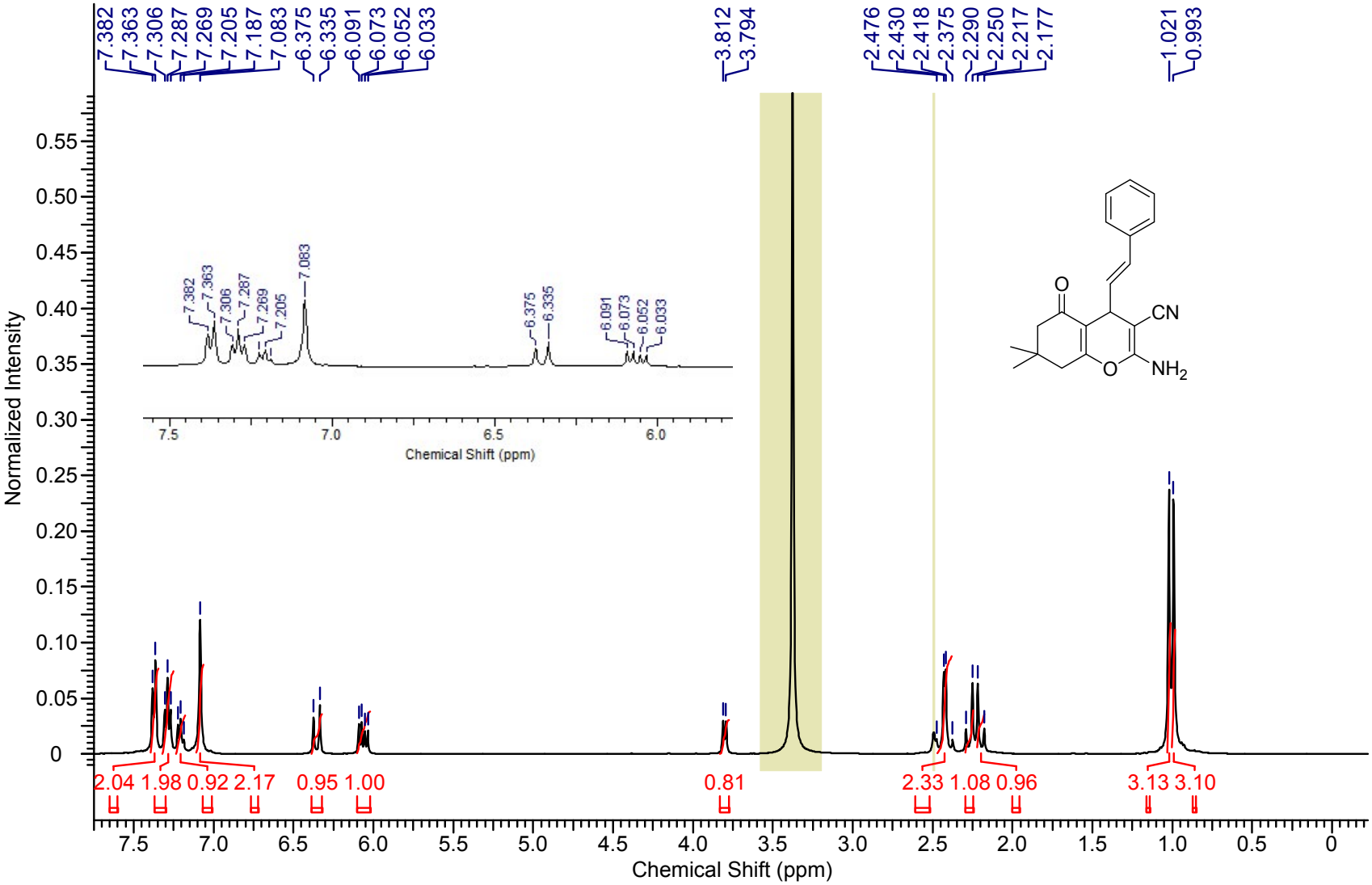
^{1}H NMR of 7h


7.348
7.266
7.248
7.190
7.168
7.150
7.052
4.682
2.568
2.455
2.263
2.223
2.086
1.033
0.972
Normalized Intensity
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0
0.81 1.01 2.10 2.07
0.70
1.00 0.33 1.07 0.94
2.97 3.06
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0
Chemical Shift (ppm)
7.367
7.348
7.284
7.266
7.248
7.211
7.190
7.168
7.150
7.052
5 7.4 7.3 7.2 7.1 7.0 6
Chemical Shif
O
Cl
CN
O
NH2

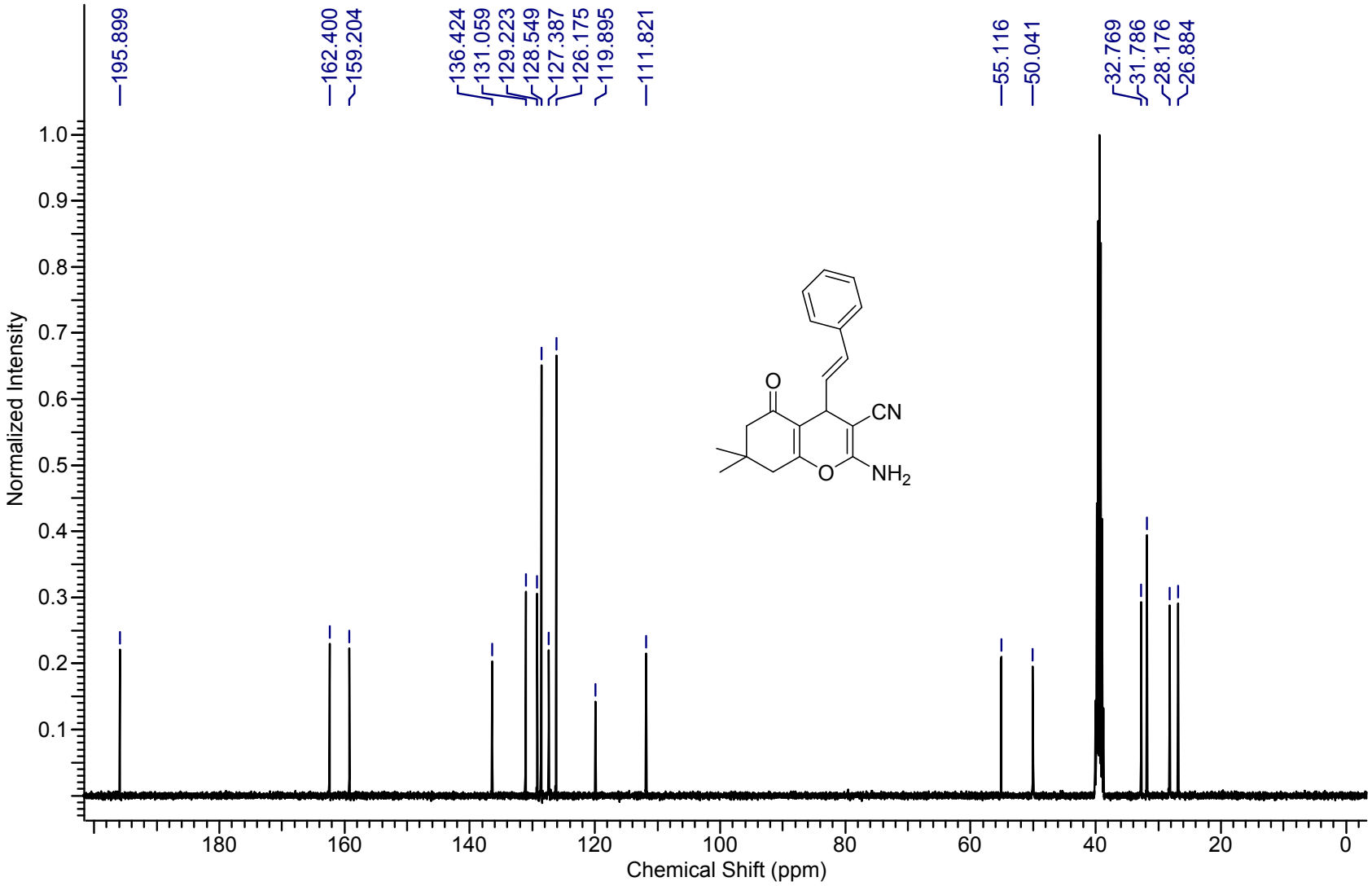
^{13}C NMR of 7h


195.559
163.136
158.623
141.524
132.035
129.909
129.408
128.178
127.411
119.245
111.716
56.717
49.868
32.782
31.731
28.374
26.804
Normalized Intensity
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
200
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)
O
Cl
CN
O
NH2

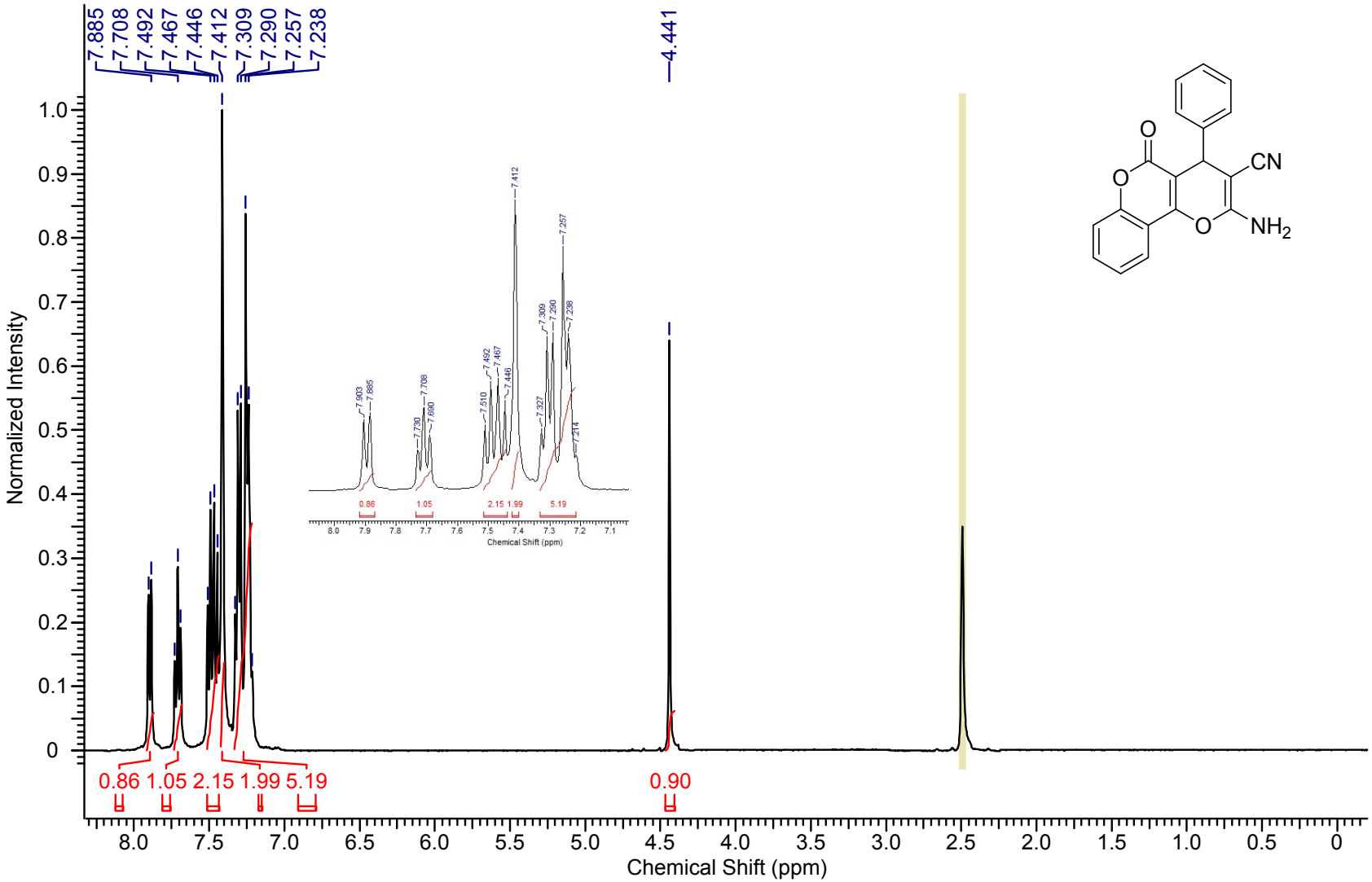
^{1}H NMR of 7j


7.382
7.363
7.306
7.287
7.269
7.205
7.187
7.083
6.375
6.335
6.091
6.073
6.052
6.033
3.812
3.794
2.476
2.430
2.418
2.375
2.290
2.250
2.217
2.177
1.021
0.993
Normalized Intensity
Chemical Shift (ppm)
O
CN
O
NH2
2.04 1.98 0.92 2.17 0.95 1.00 0.81 2.33 1.08 0.96 3.13 3.10

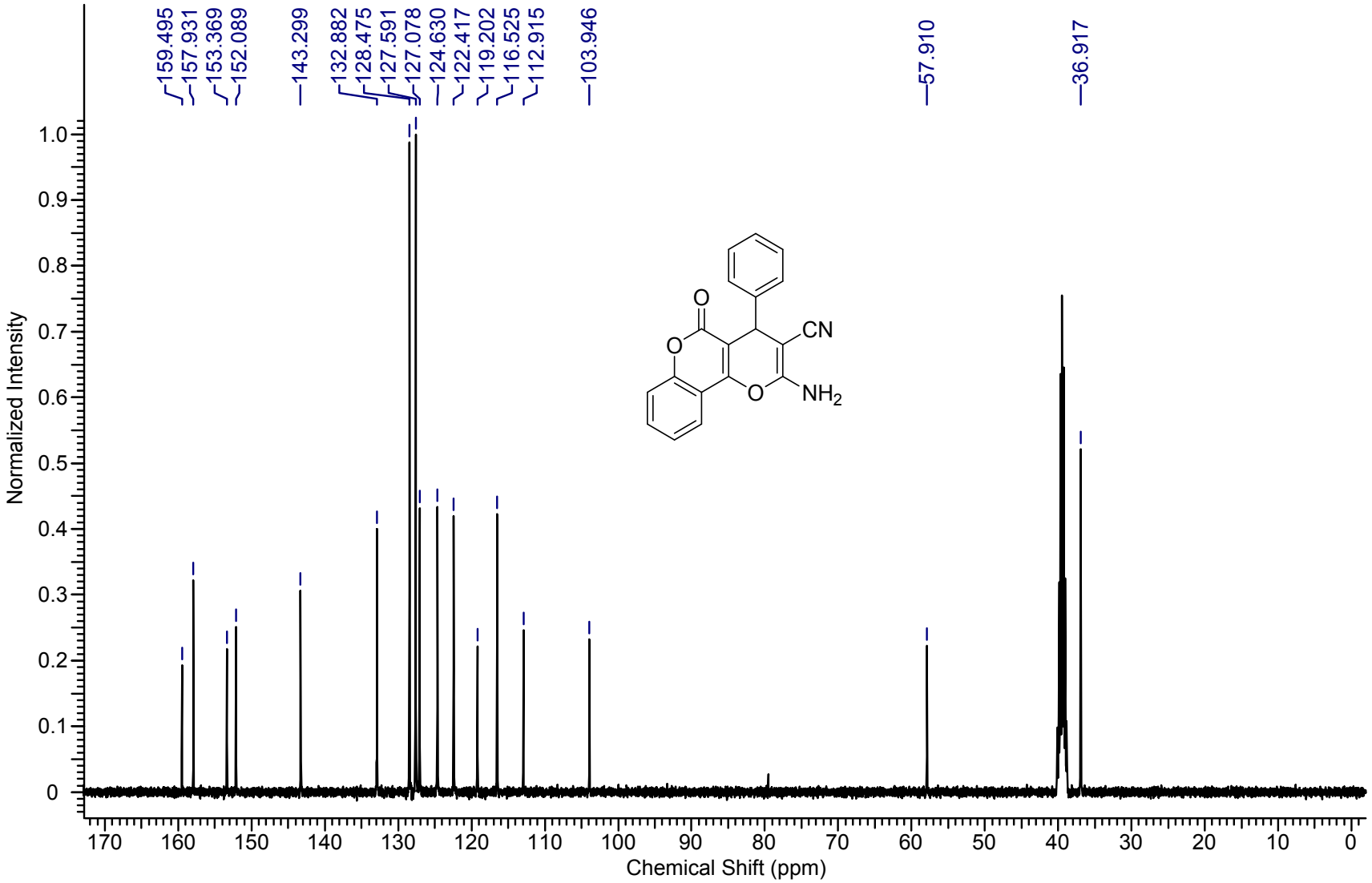
^{13}C NMR of 7j


195.899
162.400
159.204
136.424
131.059
129.223
128.549
127.387
126.175
119.895
111.821
55.116
50.041
32.769
31.786
28.176
26.884
Normalized Intensity
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)
O
CN
O
NH2

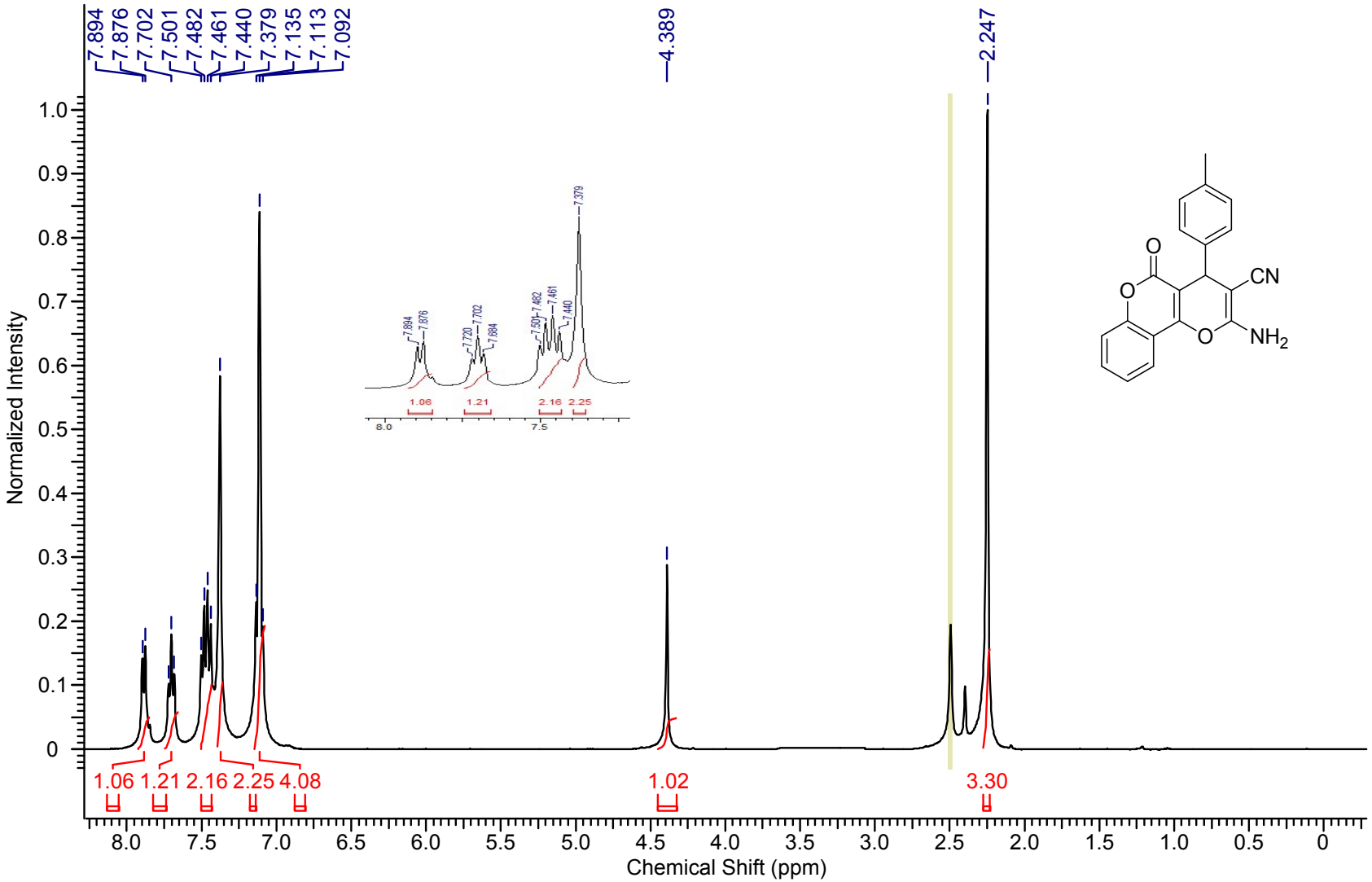
^{1}H NMR of 8a


7.885
7.708
7.492
7.467
7.446
7.412
7.309
7.290
7.257
7.238
4.441
Normalized Intensity
0.86 1.05 2.15 1.99 5.19
0.90
Chemical Shift (ppm)
O
O
O
CN
NH2

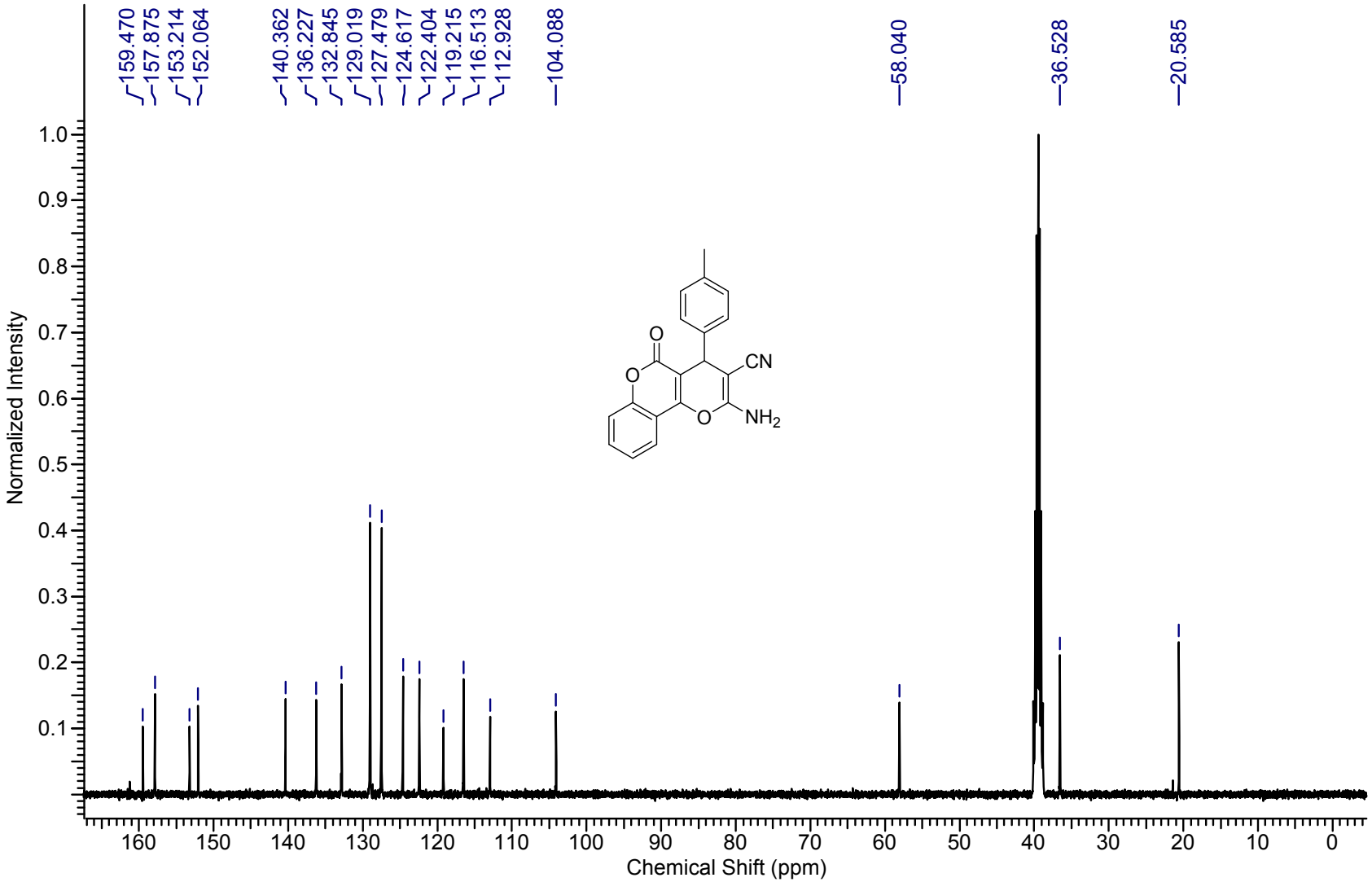
^{13}C NMR of 8a


159.495
157.931
153.369
152.089
143.299
132.882
128.475
127.591
127.078
124.630
122.417
119.202
116.525
112.915
103.946
57.910
36.917
Normalized Intensity
Chemical Shift (ppm)
O
O
O
CN
NH2

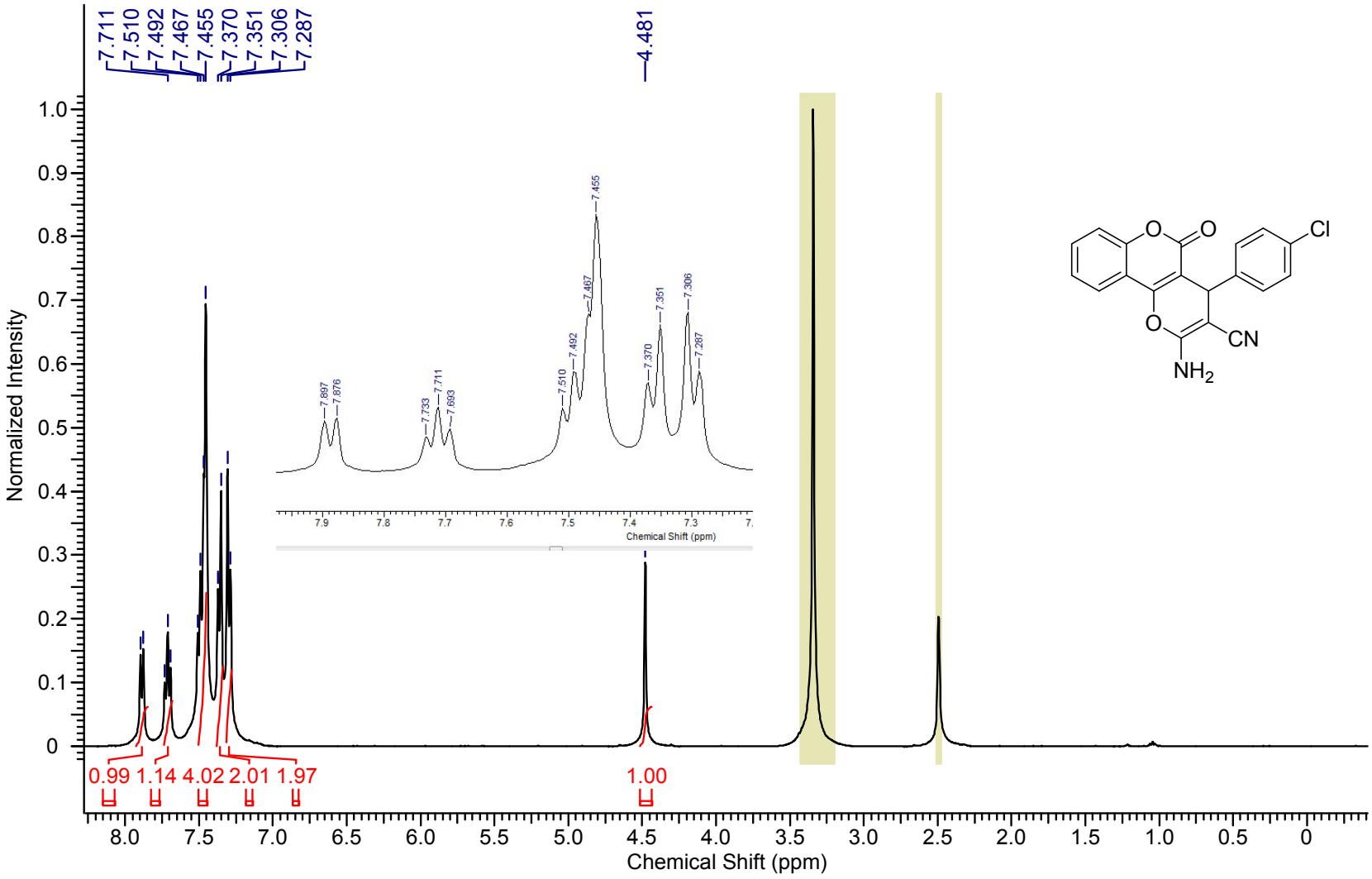
^{1}H NMR of 8b


7.894
7.876
7.702
7.501
7.482
7.461
7.440
7.379
7.135
7.113
7.092
4.389
2.247
Normalized Intensity
1.06 1.21 2.16 2.25 4.08
1.02
3.30
Chemical Shift (ppm)
O
O
O
CN
NH2

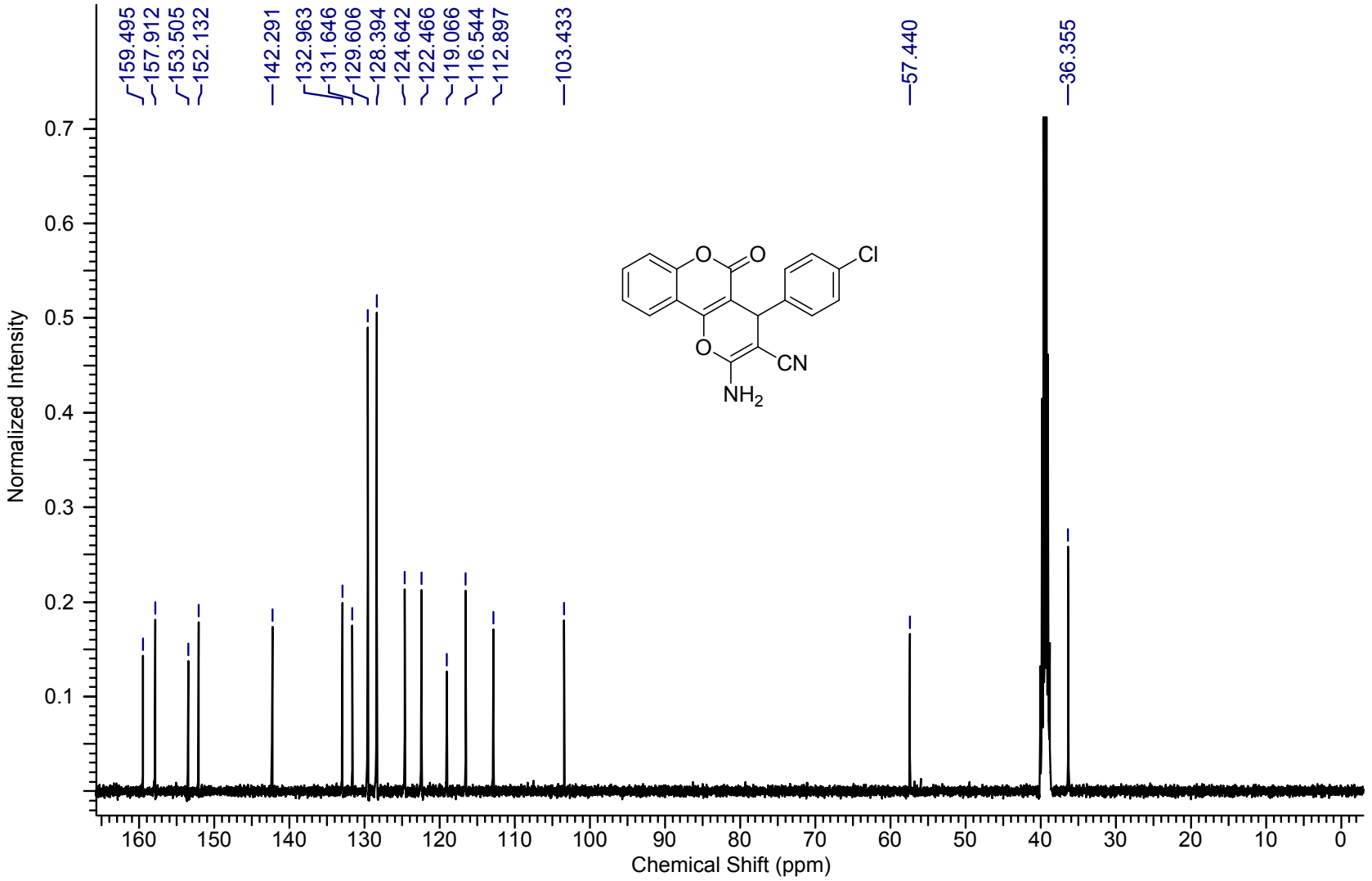
^{13}C NMR of 8b


159.470
157.875
153.214
152.064
140.362
136.227
132.845
129.019
127.479
124.617
122.404
119.215
116.513
112.928
104.088
58.040
36.528
20.585
Normalized Intensity
Chemical Shift (ppm)
CN
NH2
O
O
O

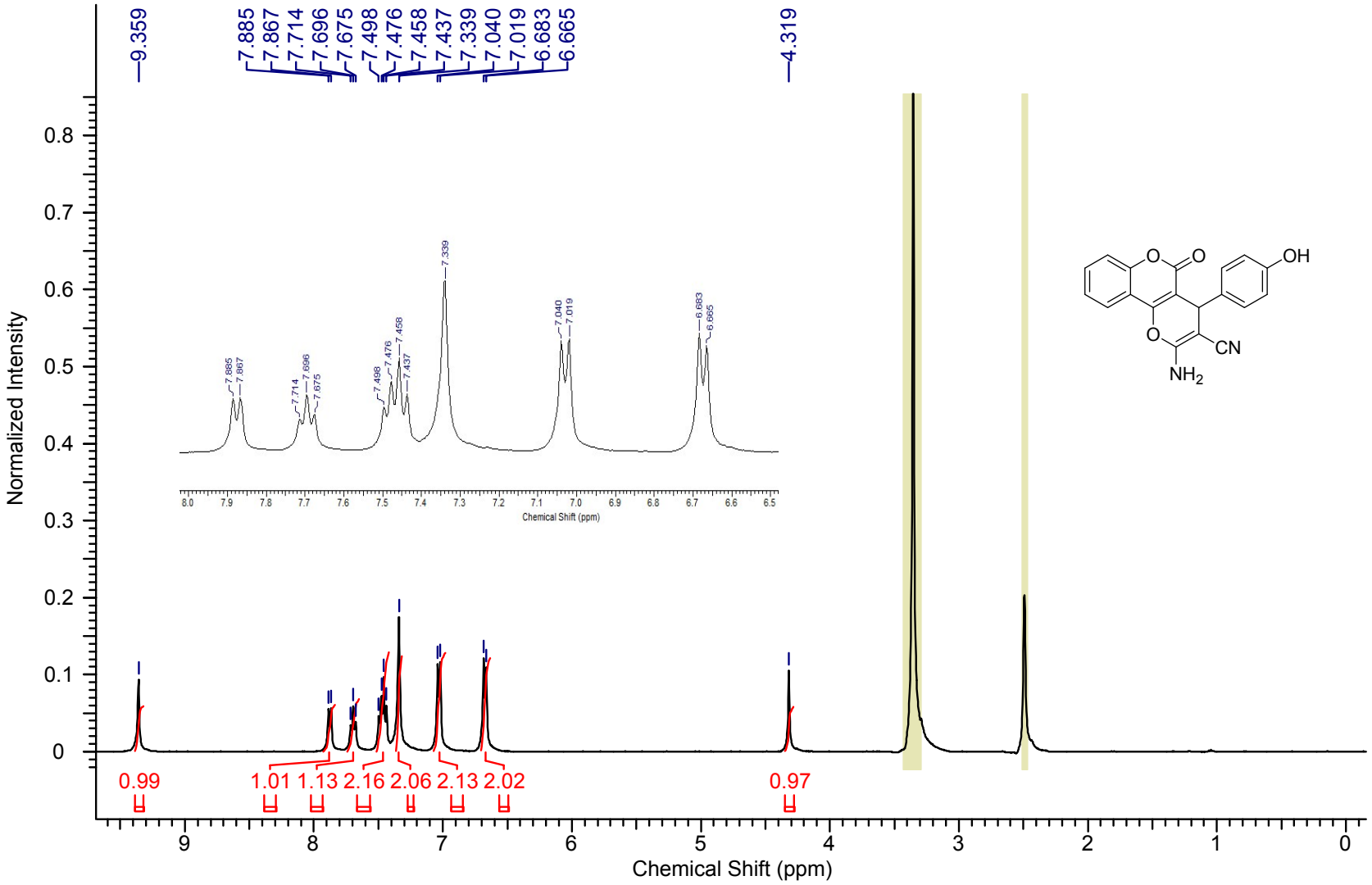
^{1}H NMR of 8c


7.711
7.510
7.492
7.467
7.455
7.370
7.351
7.306
7.287
4.481
Normalized Intensity
0.99 1.14 4.02 2.01 1.97
1.00
Chemical Shift (ppm)
7.897
7.876
7.733
7.711
7.693
7.510
7.492
7.467
7.455
7.370
7.351
7.306
7.287
Chemical Shift (ppm)
O
O
Cl
O
CN
NH2

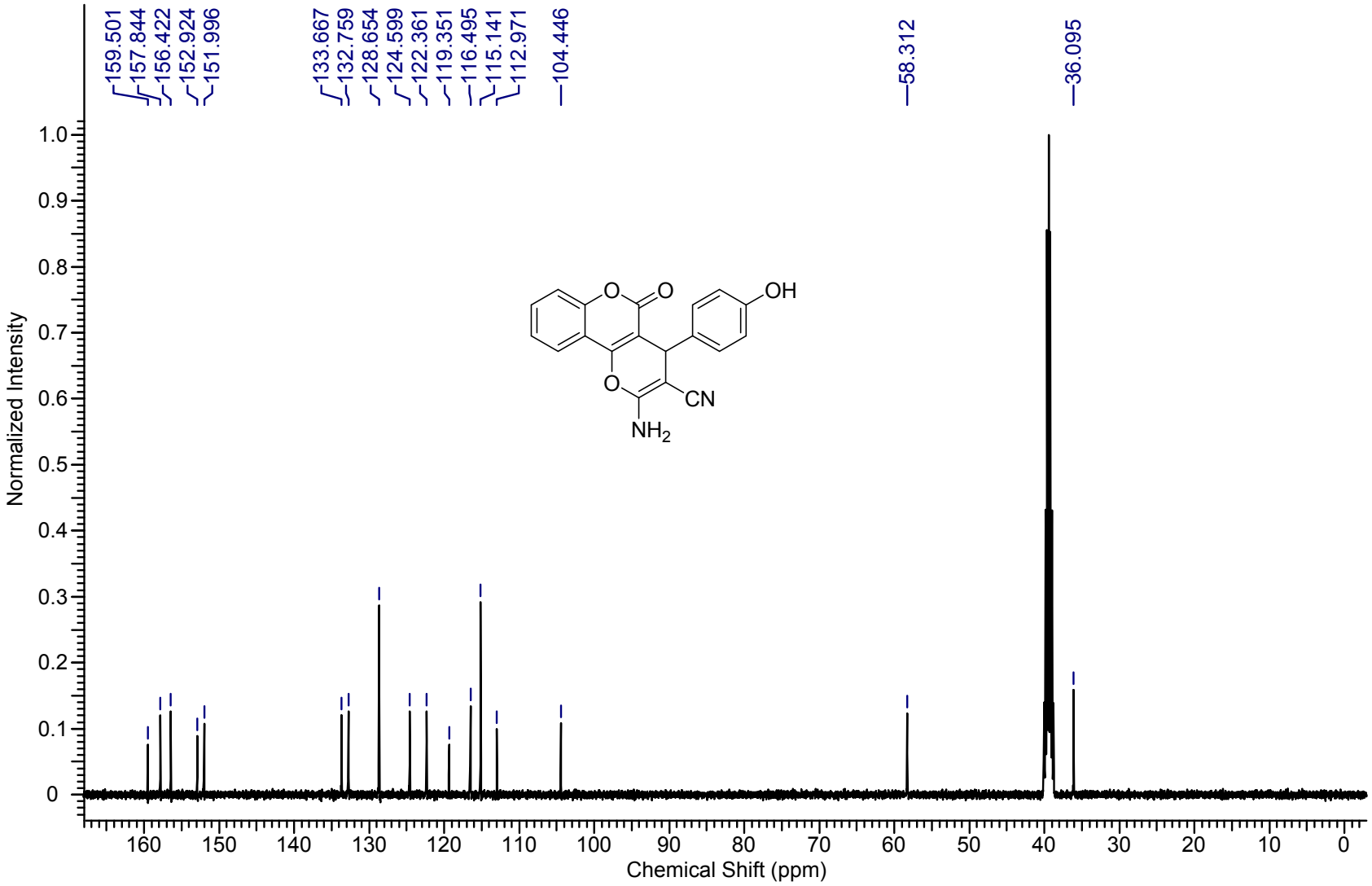
^{13}C NMR of 8c


159.495
157.912
153.505
152.132
142.291
132.963
131.646
129.606
128.394
124.642
122.466
119.066
116.544
112.897
103.433
57.440
36.355
Normalized Intensity
0.7
0.6
0.5
0.4
0.3
0.2
0.1
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)
O
O
Cl
O
CN
NH2

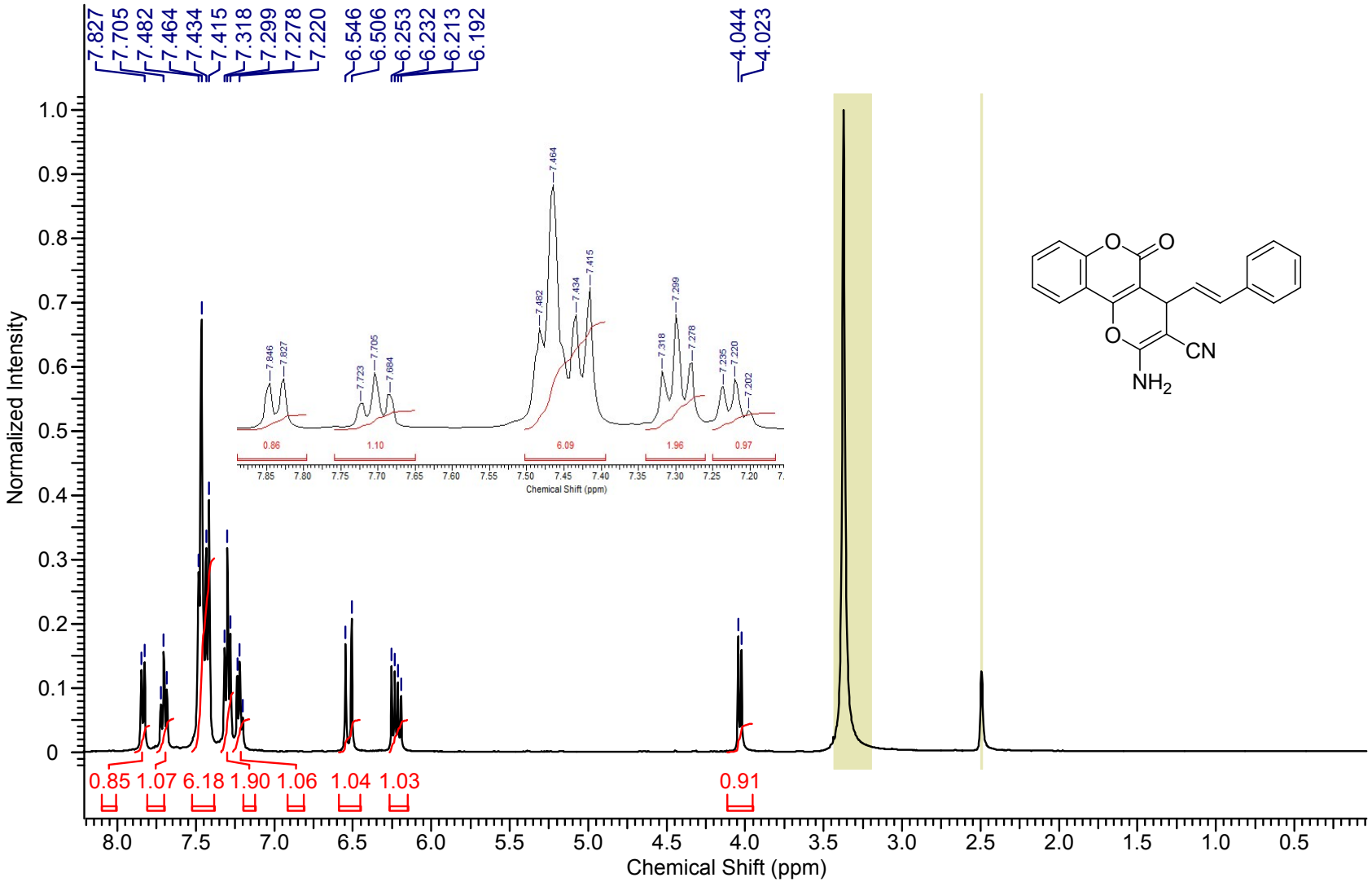
^{1}H NMR of 8d


9.359
7.885
7.867
7.714
7.696
7.675
7.498
7.476
7.458
7.437
7.339
7.040
7.019
6.683
6.665
4.319
Normalized Intensity
Chemical Shift (ppm)
0.99
1.01
1.13
2.16
2.06
2.13
2.02
0.97
OH
CN
NH2

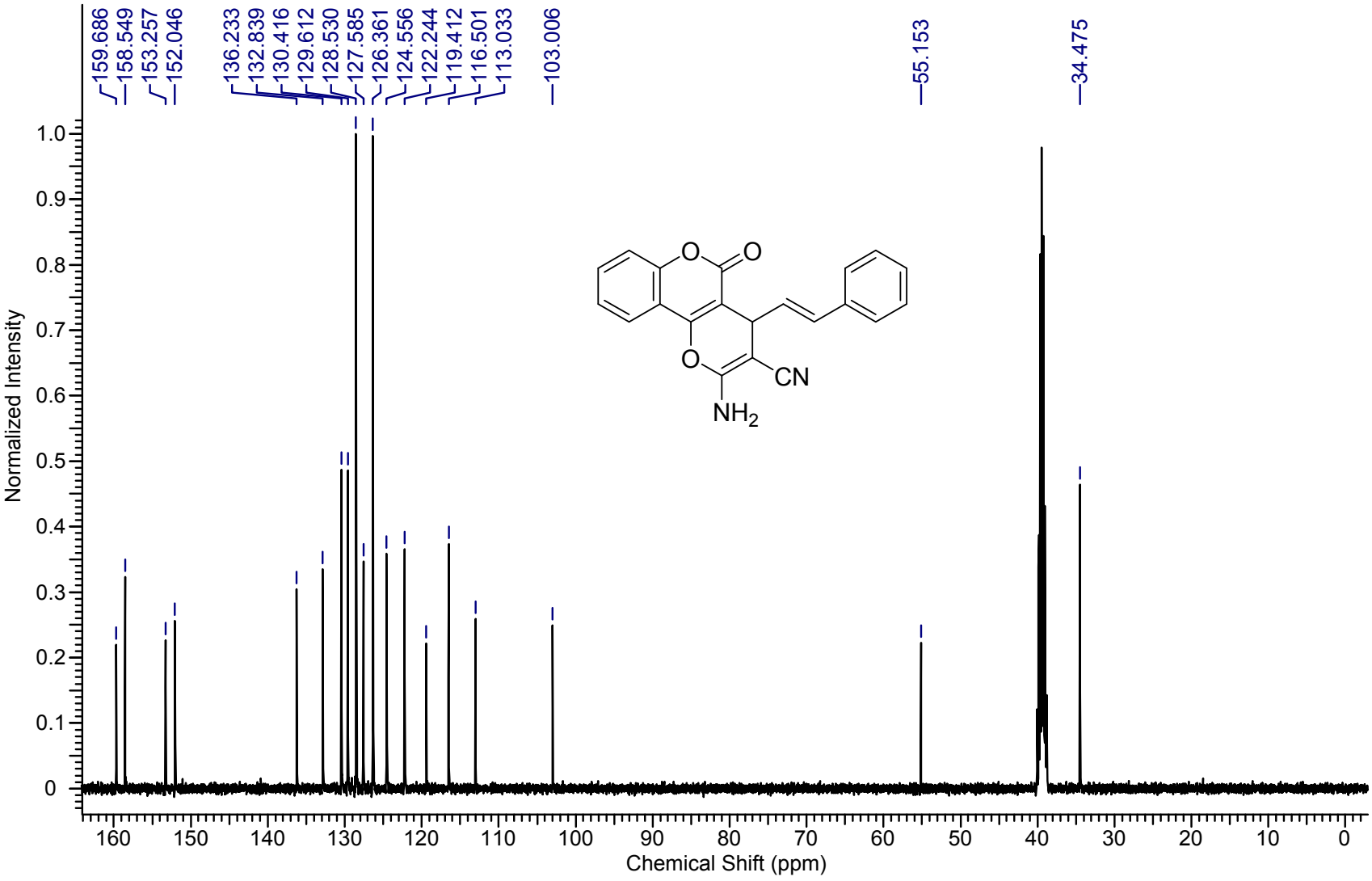
^{13}C NMR of 8d


159.501
157.844
156.422
152.924
151.996
133.667
132.759
128.654
124.599
122.361
119.351
116.495
115.141
112.971
104.446
58.312
36.095
Normalized Intensity
Chemical Shift (ppm)
OH
O
O
O
CN
NH2

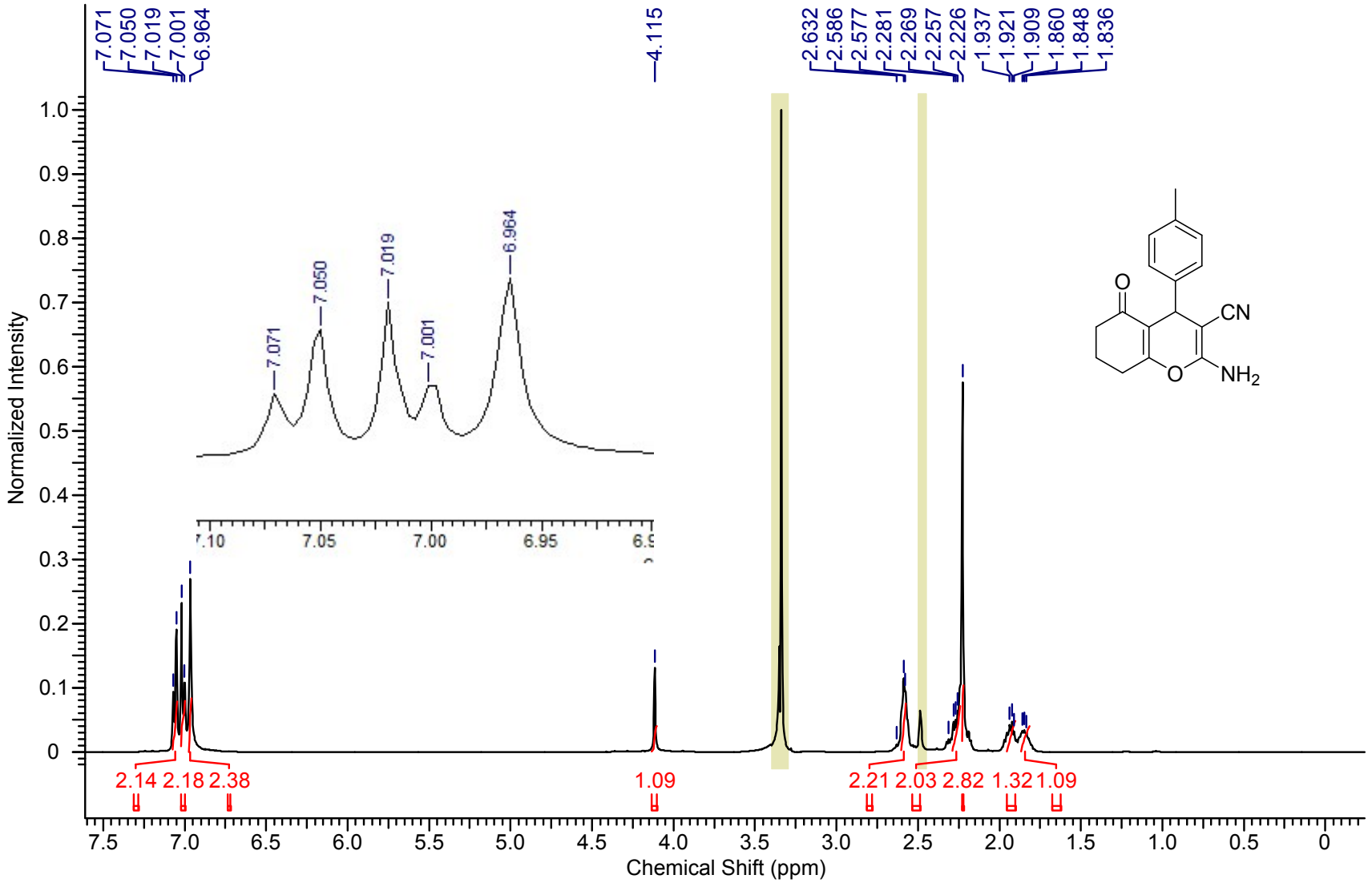
^{1}H NMR of 8e


7.827
7.705
7.482
7.464
7.434
7.415
7.318
7.299
7.278
7.220
6.546
6.506
6.253
6.232
6.213
6.192
4.044
4.023
Normalized Intensity
0.85 1.07 6.18 1.90 1.06 1.04 1.03
0.91
Chemical Shift (ppm)
0.86
1.10
6.09
1.96
0.97
O
O
O
CN
NH2

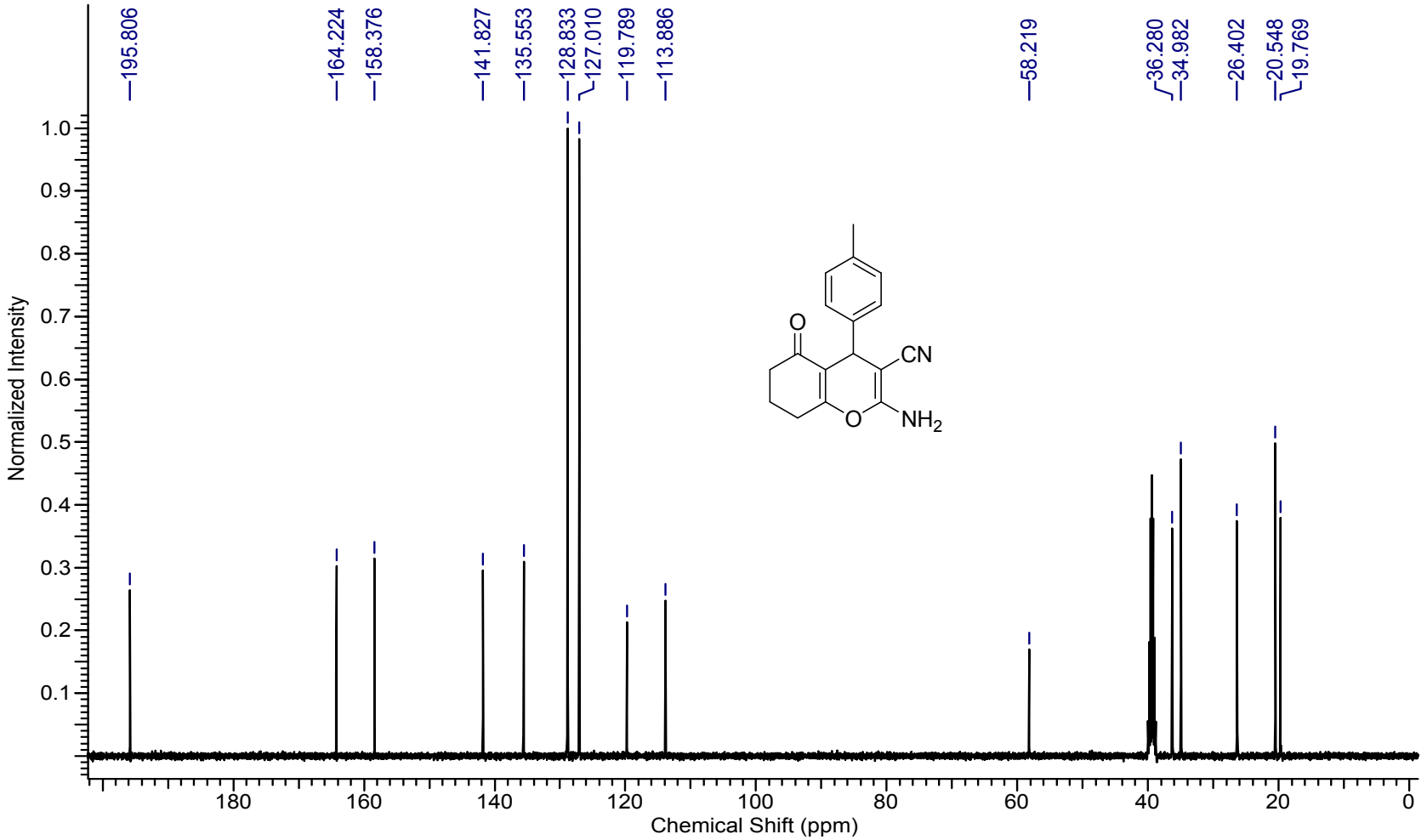
^{13}C NMR of 8e


159.686
158.549
153.257
152.046
136.233
132.839
130.416
129.612
128.530
127.585
126.361
124.556
122.244
119.412
116.501
113.033
103.006
55.153
34.475
Normalized Intensity
Chemical Shift (ppm)
O
O
O
CN
NH2

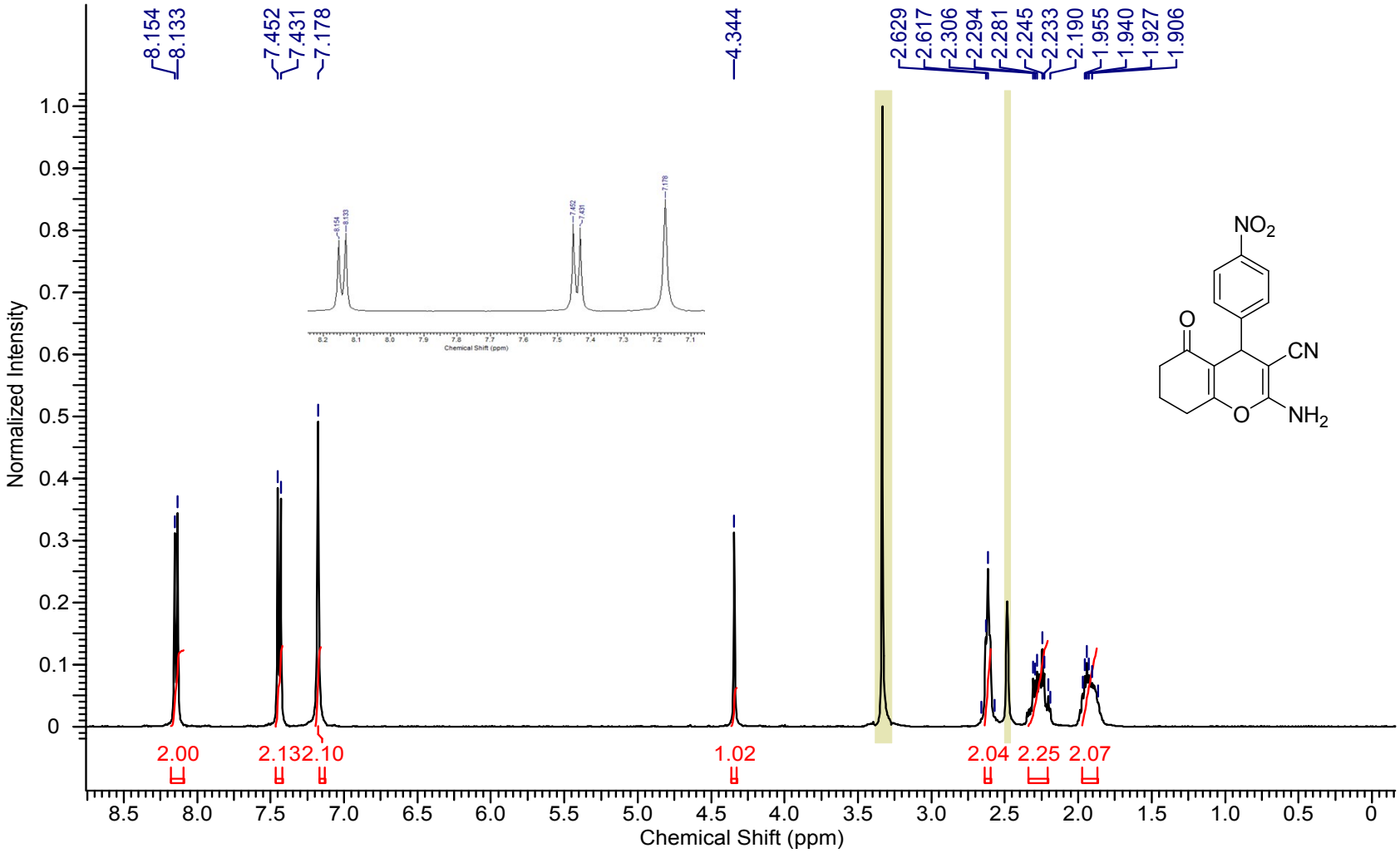
^{1}H NMR of 9b


7.071
7.050
7.019
7.001
6.964
4.115
2.632
2.586
2.577
2.281
2.269
2.257
2.226
1.937
1.921
1.909
1.860
1.848
1.836
Normalized Intensity
Chemical Shift (ppm)
2.14 2.18 2.38
1.09
2.21 2.03 2.82 1.32 1.09
O
CN
O
NH2

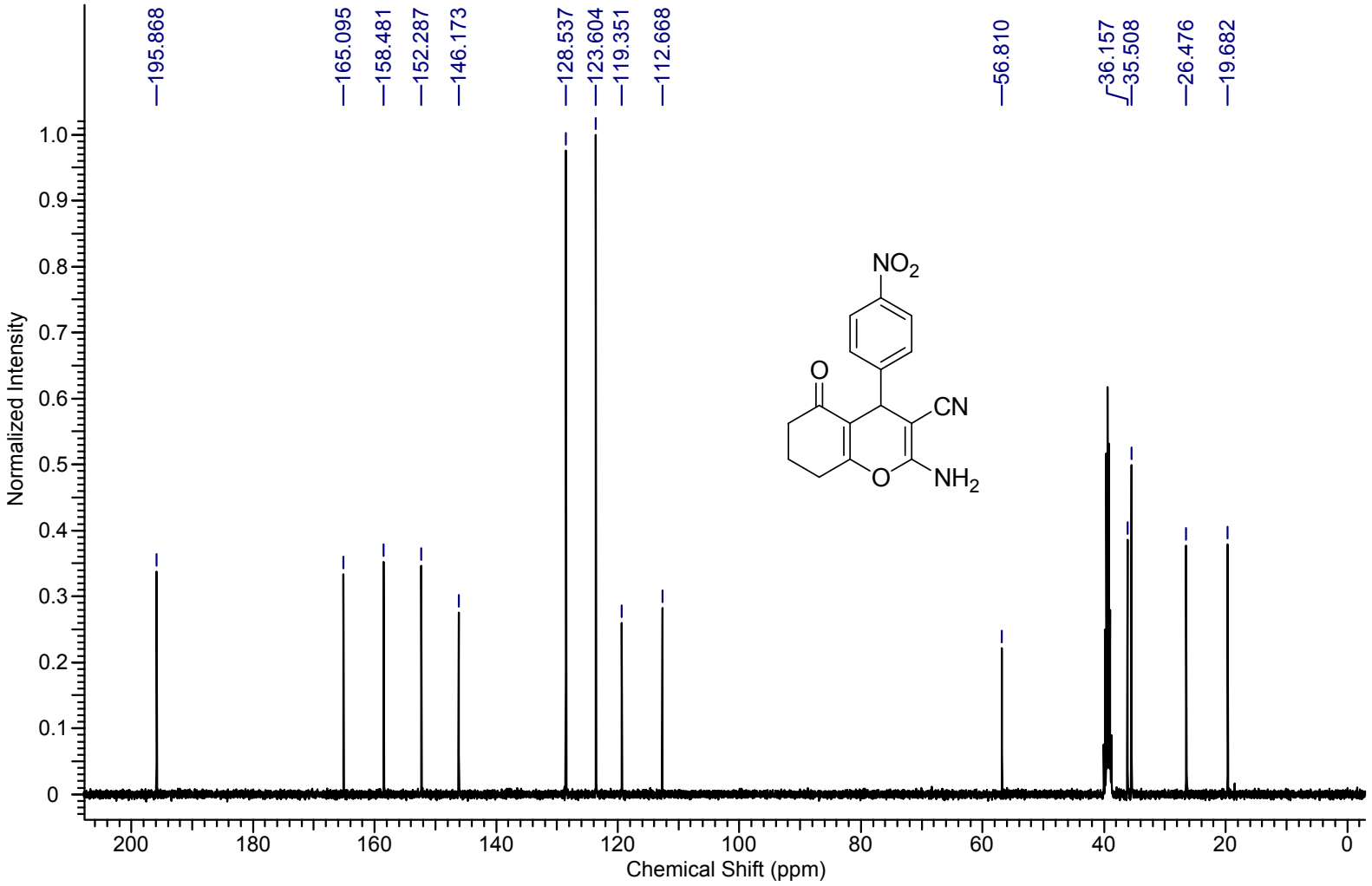
^{13}C NMR of 9b


195.806
164.224
158.376
141.827
135.553
128.833
127.010
119.789
113.886
58.219
36.280
34.982
26.402
20.548
19.769
Normalized Intensity
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)
O
CN
O
NH2

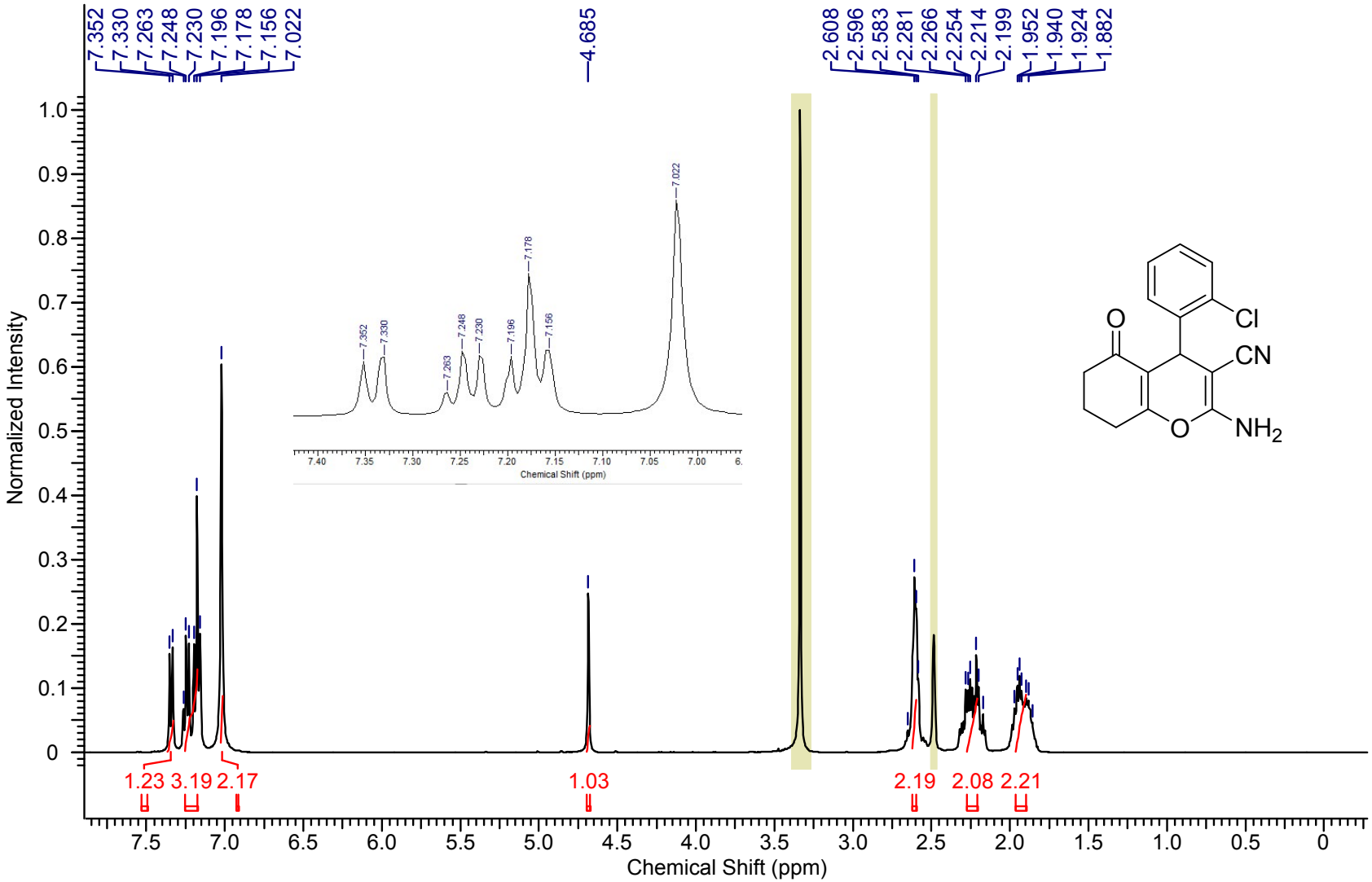
^{1}H NMR of 9c


8.154
8.133
7.452
7.431
7.178
4.344
2.629
2.617
2.306
2.294
2.281
2.245
2.233
2.190
1.955
1.940
1.927
1.906
Normalized Intensity
Chemical Shift (ppm)
2.00
2.13
2.10
1.02
2.04
2.25
2.07
NO2
O
CN
O
NH2

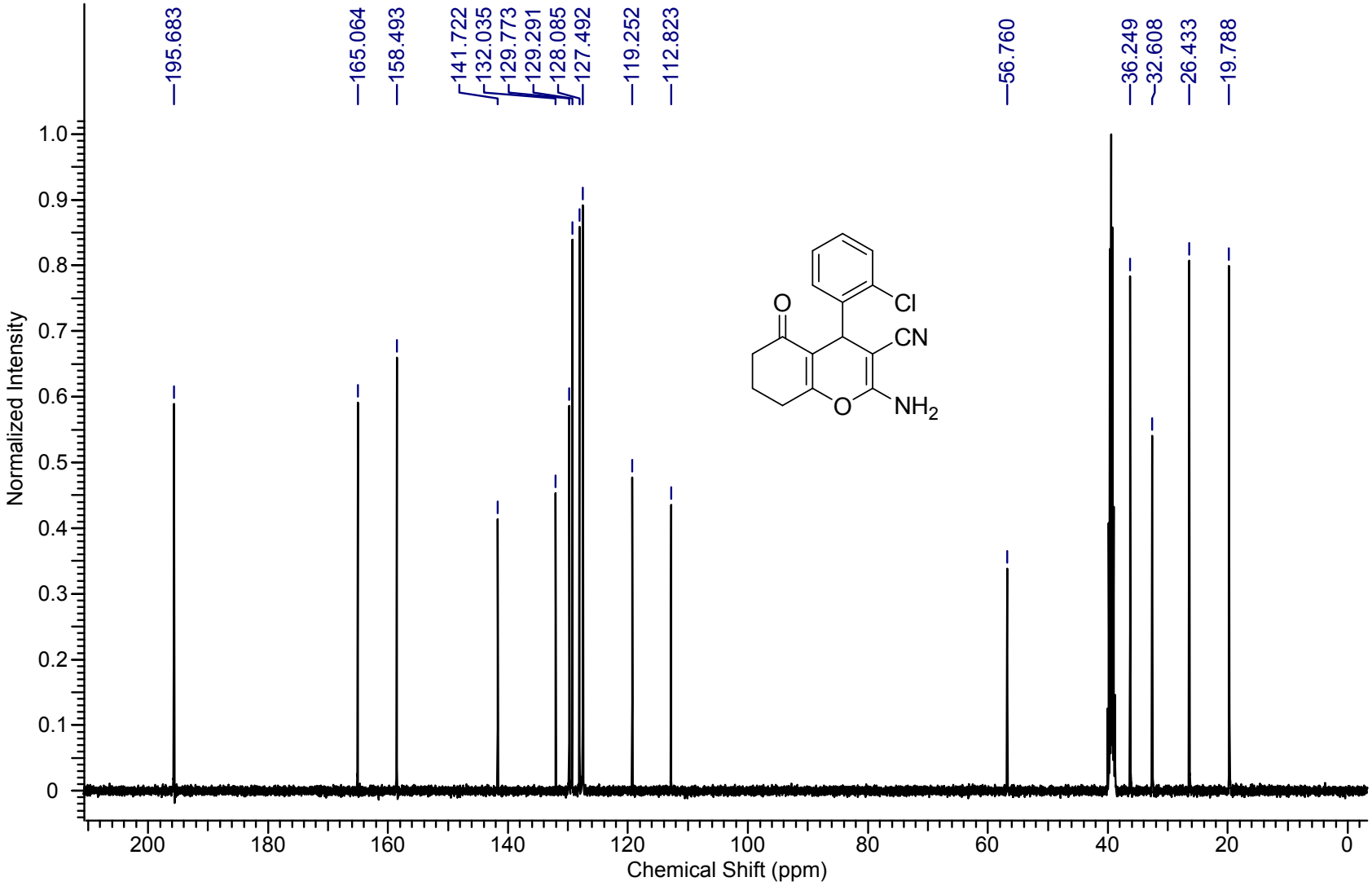
^{13}C NMR of 9c


195.868
165.095
158.481
152.287
146.173
128.537
123.604
119.351
112.668
56.810
36.157
35.508
26.476
19.682
Normalized Intensity
Chemical Shift (ppm)
NO2
O
CN
O
NH2

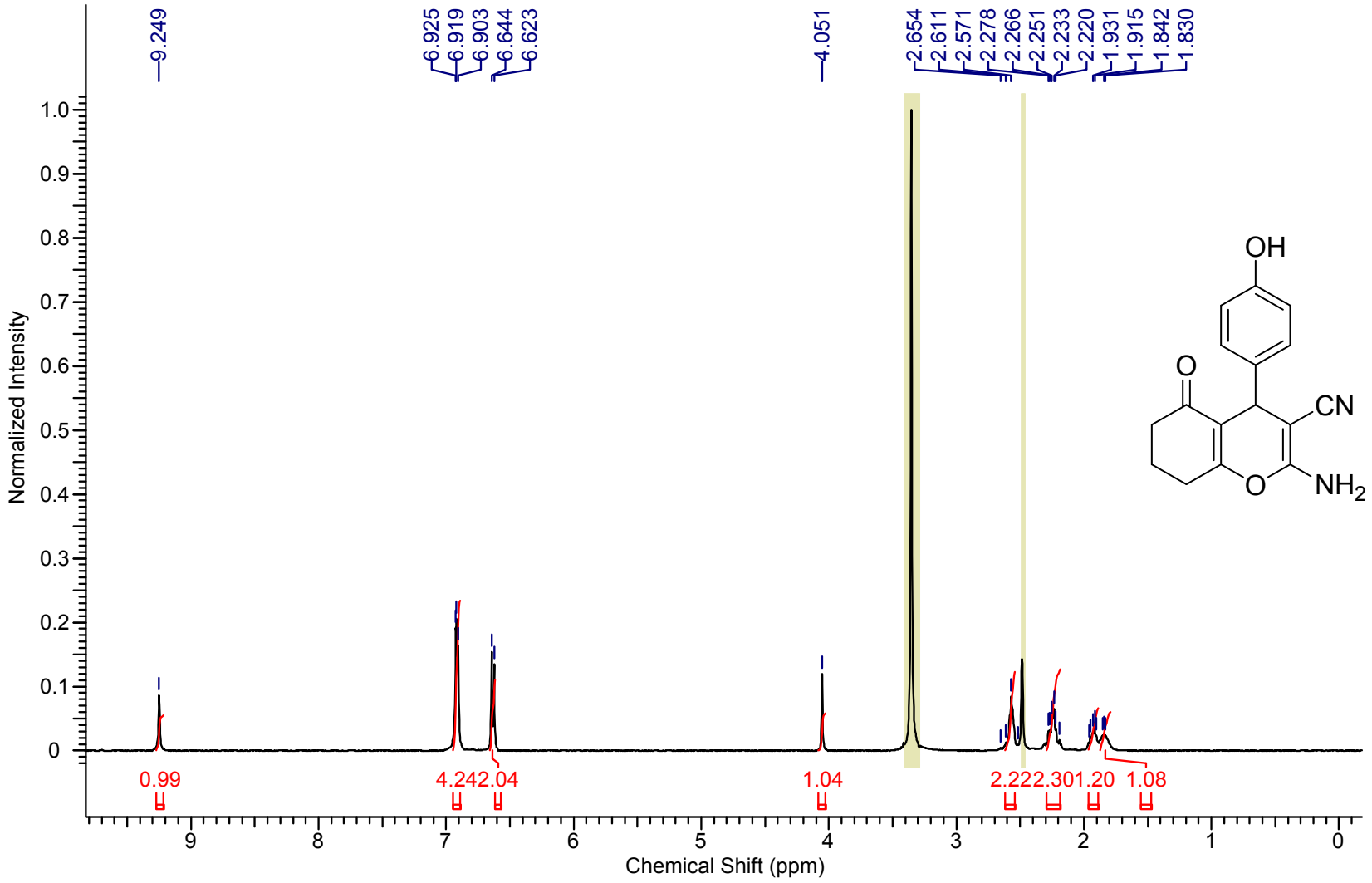
^{1}H NMR of 9d


7.352
7.330
7.263
7.248
7.230
7.196
7.178
7.156
7.022
4.685
2.608
2.596
2.583
2.281
2.266
2.254
2.214
2.199
1.952
1.940
1.924
1.882
Normalized Intensity
Chemical Shift (ppm)
1.23 3.19 2.17
1.03
2.19 2.08 2.21
O
Cl
CN
O
NH2

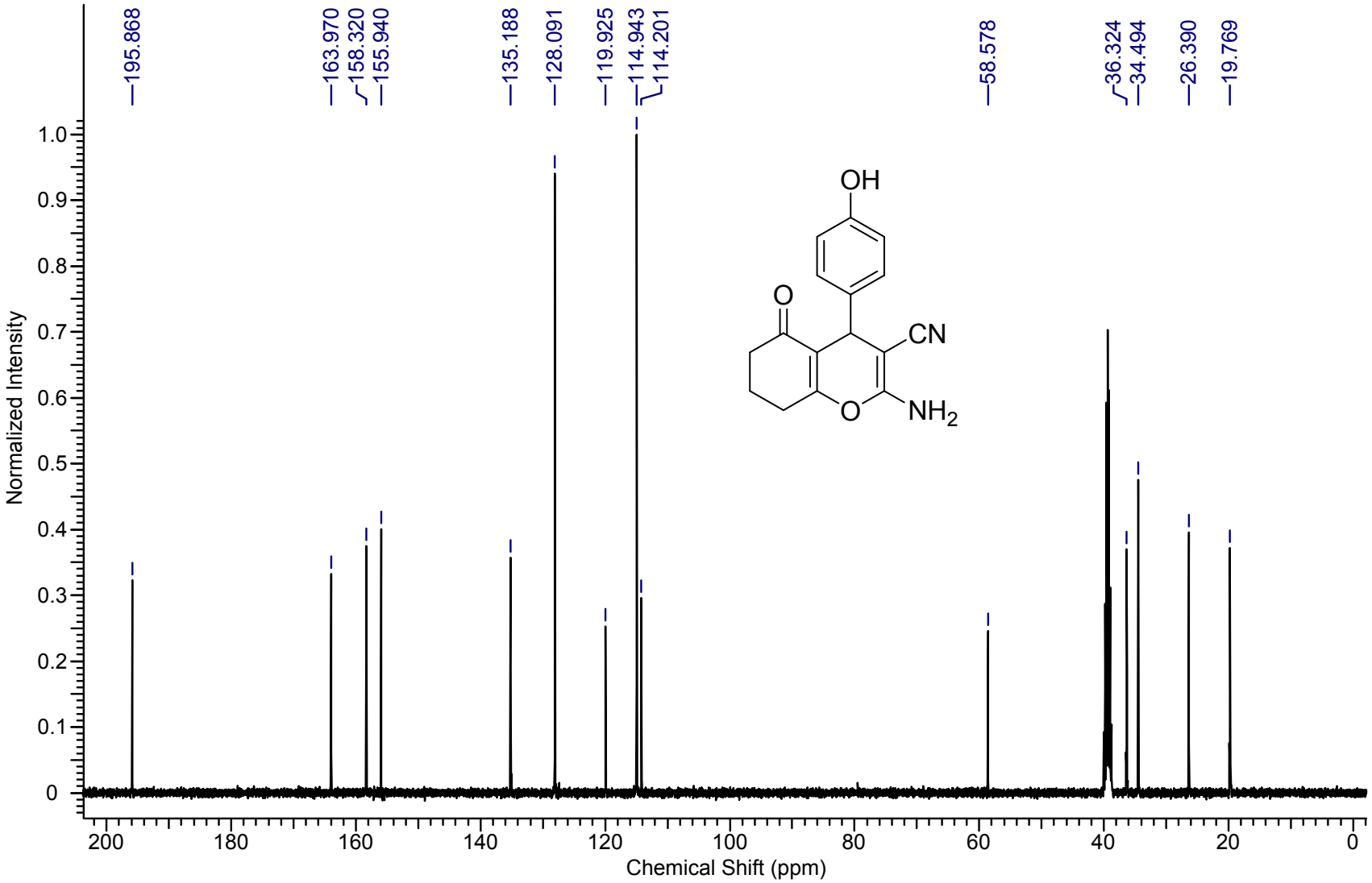
^{13}C NMR of 9d


195.683
165.064
158.493
141.722
132.035
129.773
129.291
128.085
127.492
119.252
112.823
56.760
36.249
32.608
26.433
19.788
Normalized Intensity
Chemical Shift (ppm)
O
Cl
CN
O
NH2

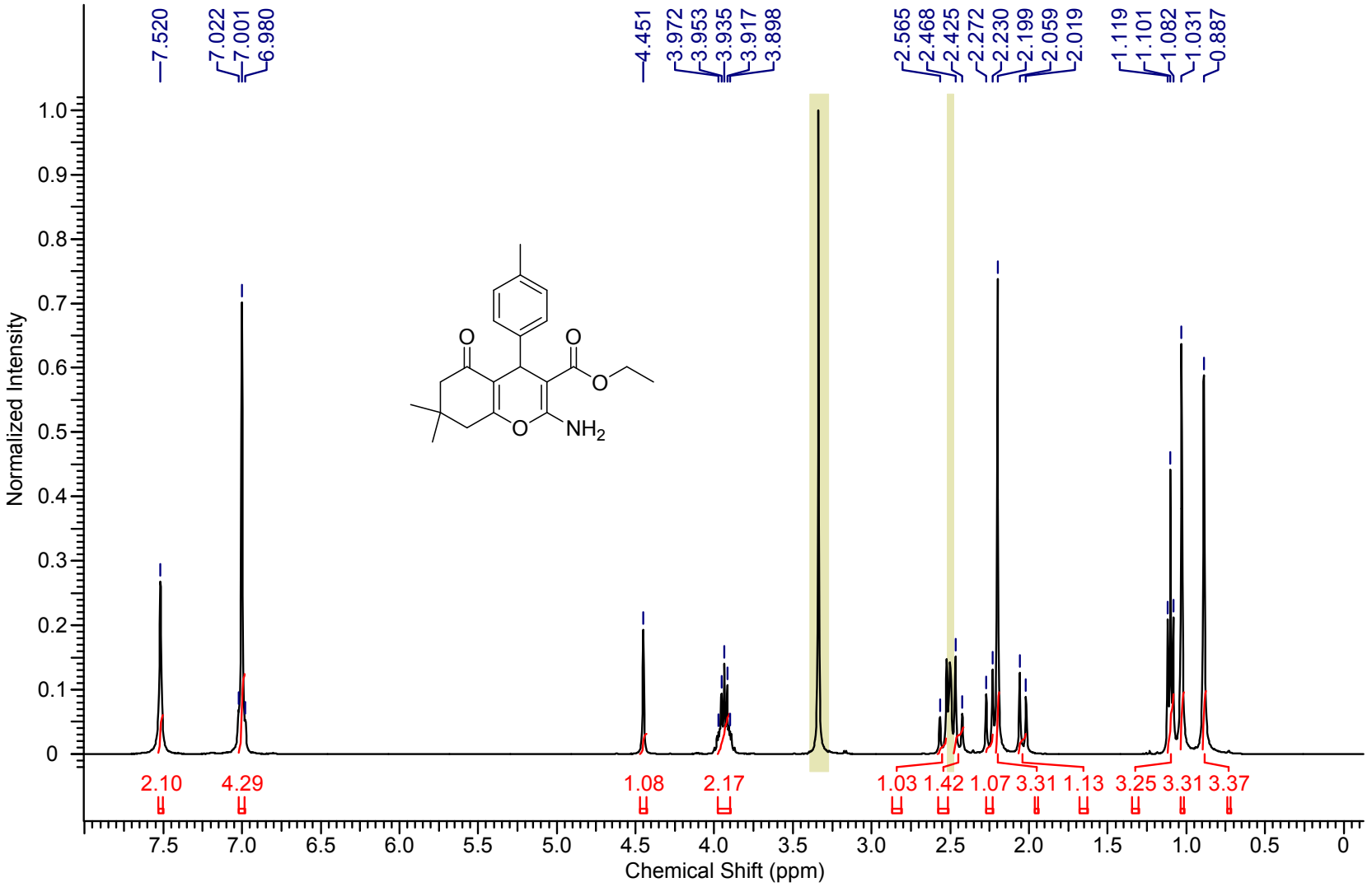
^{1}H NMR of 9e


9.249
6.925
6.919
6.903
6.644
6.623
4.051
2.654
2.611
2.571
2.278
2.266
2.251
2.233
2.220
1.931
1.915
1.842
1.830
Normalized Intensity
Chemical Shift (ppm)
0.99
4.24
2.04
1.04
2.22
2.30
1.20
1.08
OH
O
CN
O
NH2

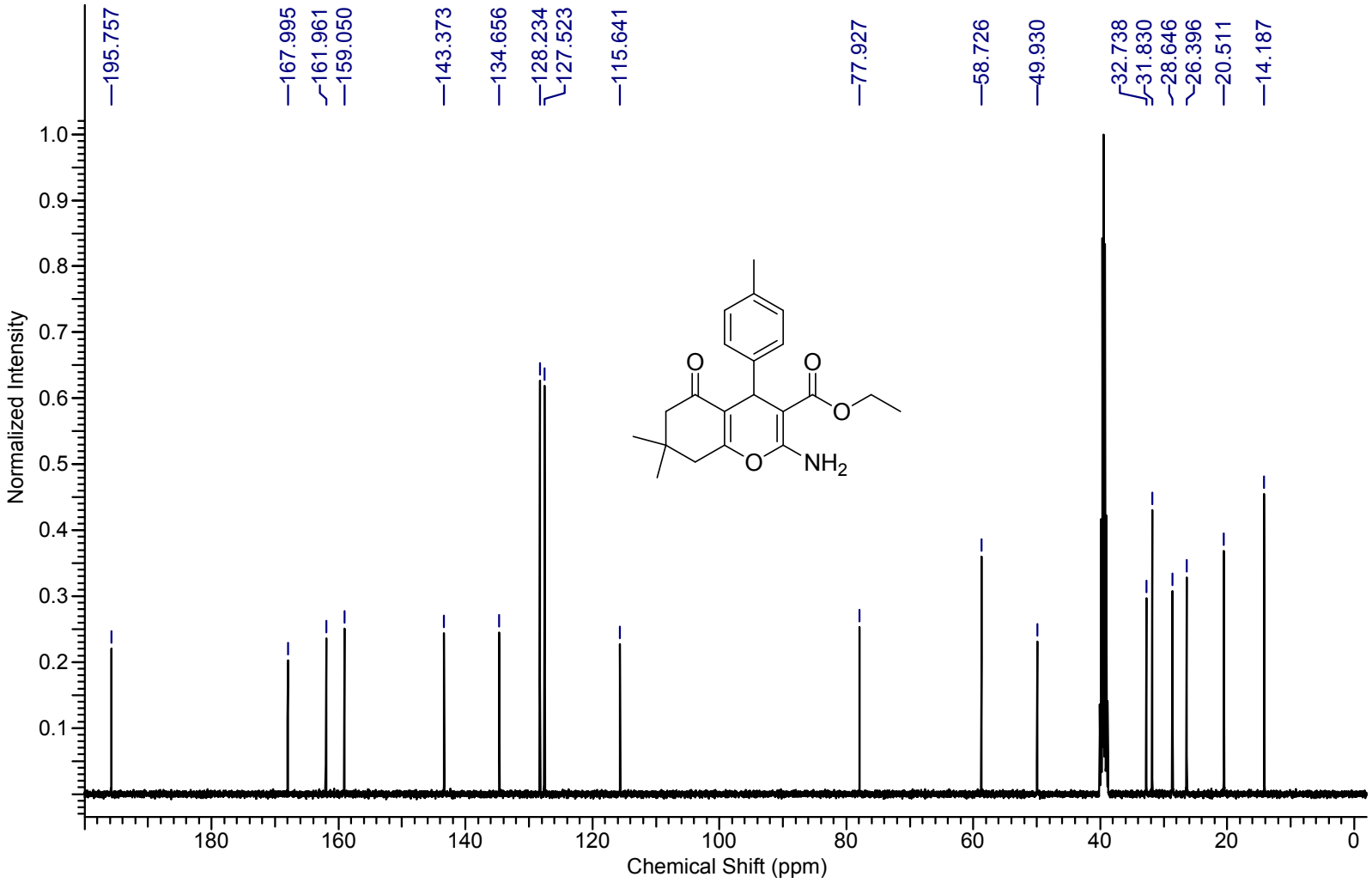
^{13}C NMR of 9e


195.868
163.970
158.320
155.940
135.188
128.091
119.925
114.943
114.201
58.578
36.324
34.494
26.390
19.769
OH
O
CN
O
NH2
Normalized Intensity
Chemical Shift (ppm)

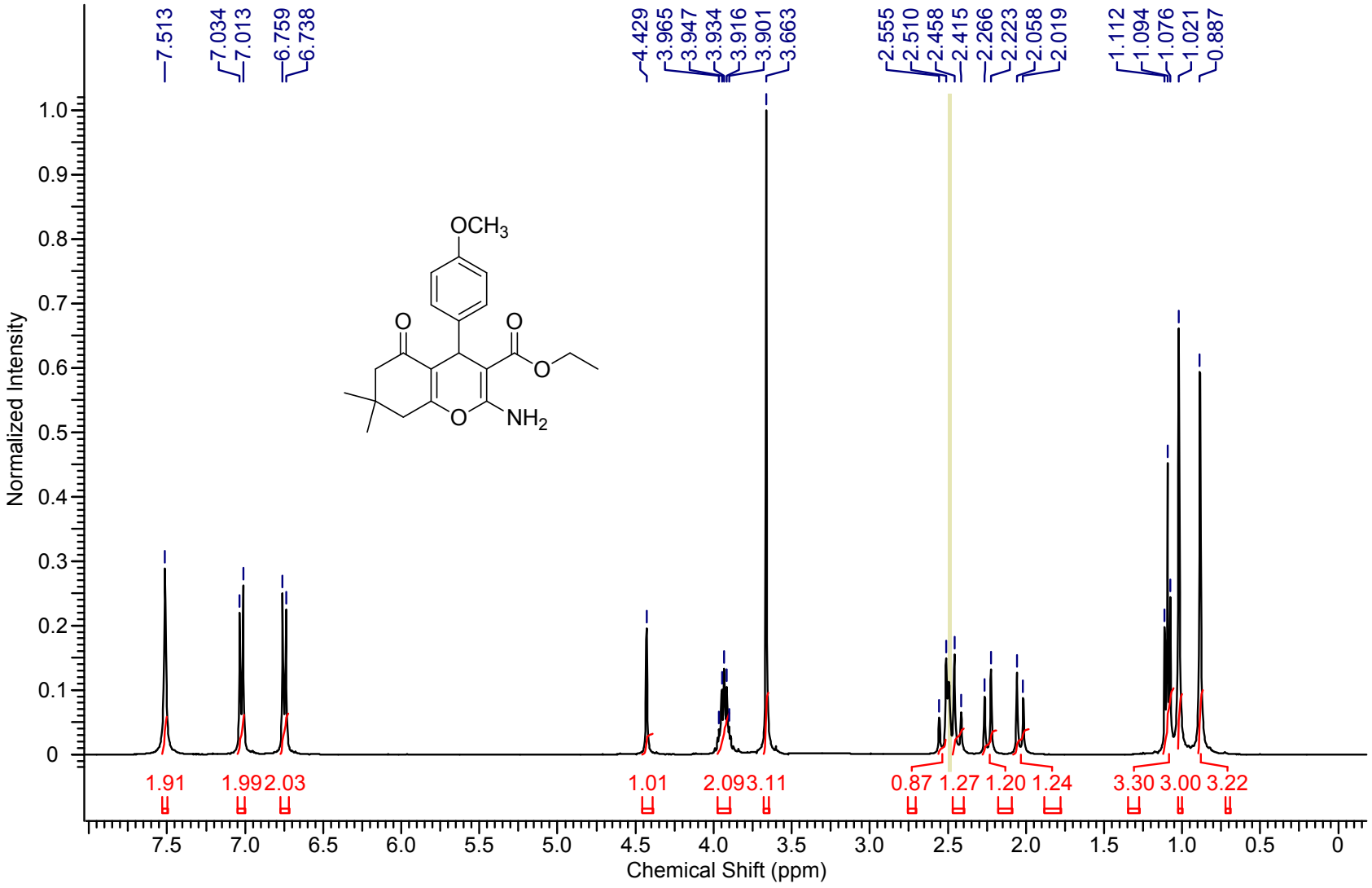
^{1}H NMR of 10a


7.520
7.022
7.001
6.980
4.451
3.972
3.953
3.935
3.917
3.898
2.565
2.468
2.425
2.272
2.230
2.199
2.059
2.019
1.119
1.101
1.082
1.031
0.887
Normalized Intensity
Chemical Shift (ppm)
2.10
4.29
1.08
2.17
1.03
1.42
1.07
3.31
1.13
3.25
3.31
3.37
O
O
O
O
NH2

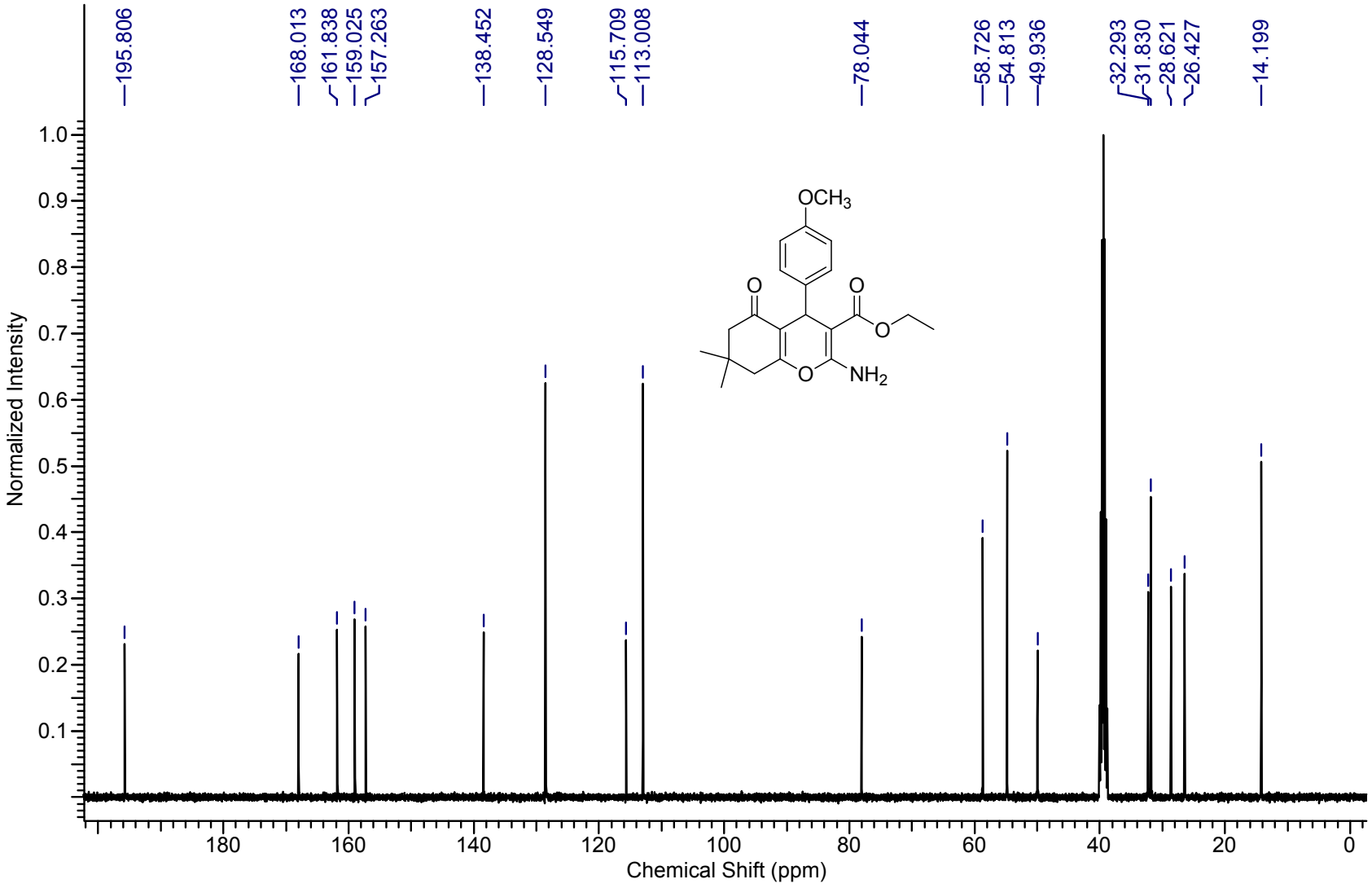
^{13}C NMR of 10a



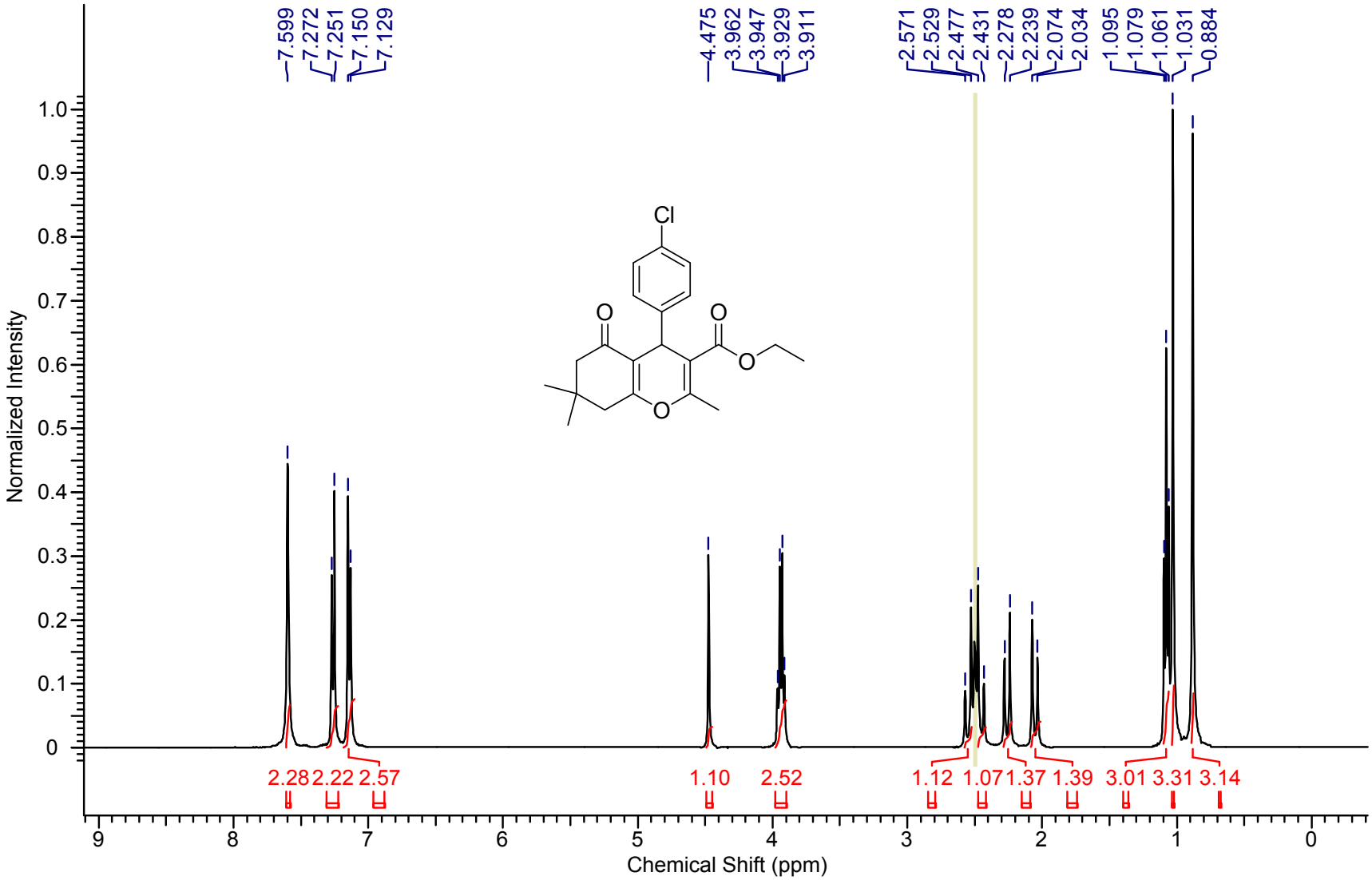
^{1}H NMR of 10b


7.513
7.034
7.013
6.759
6.738
4.429
3.965
3.947
3.934
3.916
3.901
3.663
2.555
2.510
2.458
2.415
2.266
2.223
2.058
2.019
1.112
1.094
1.076
1.021
0.887
OCH3
O
O
O
O
NH2
Normalized Intensity
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
1.91
1.99
2.03
1.01
2.09
3.11
0.87
1.27
1.20
1.24
3.30
3.00
3.22
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

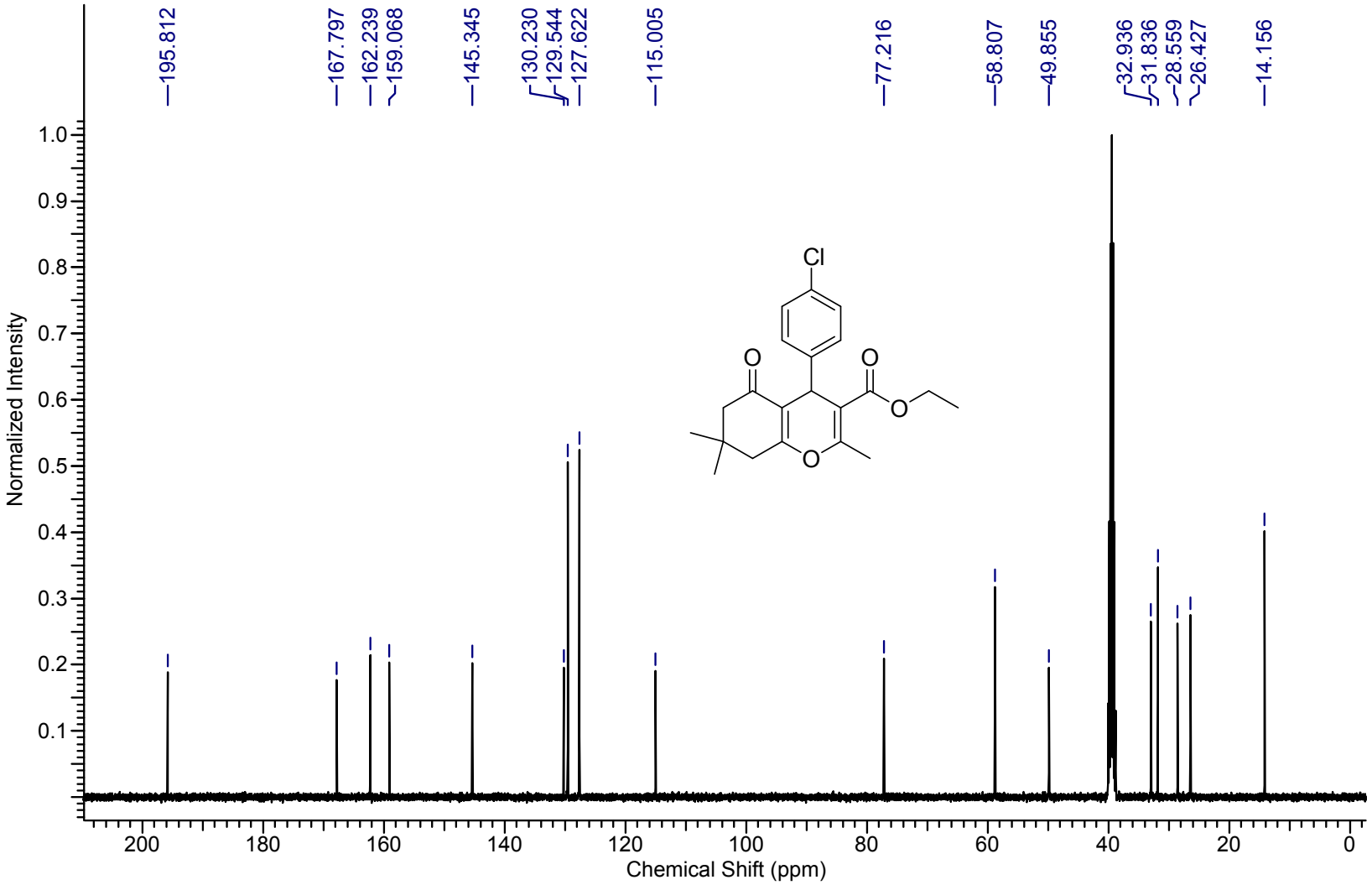
^{13}C NMR of 10b



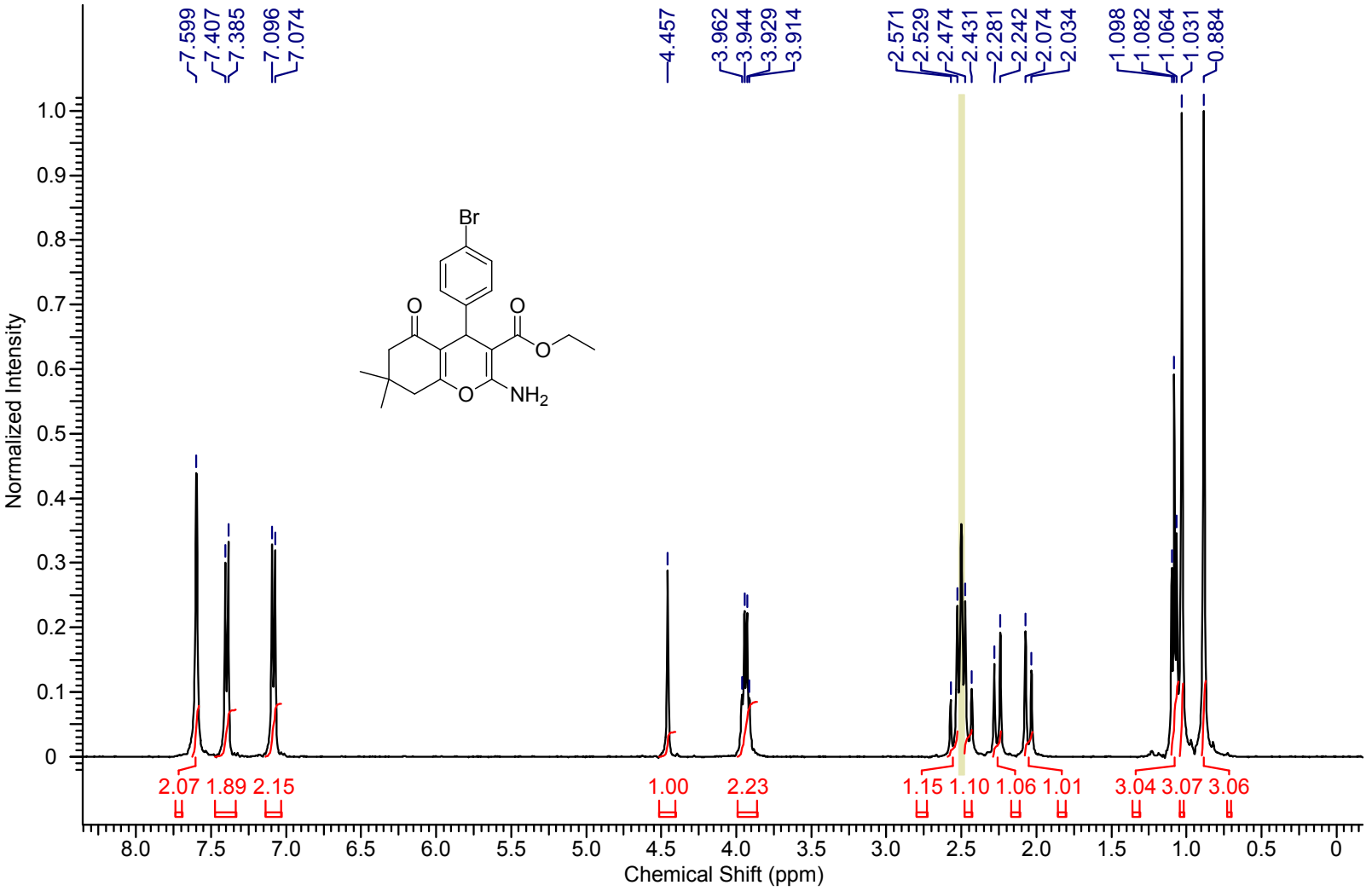
^{1}H NMR of 10c


7.599
7.272
7.251
7.150
7.129
4.475
3.962
3.947
3.929
3.911
2.571
2.529
2.477
2.431
2.278
2.239
2.074
2.034
1.095
1.079
1.061
1.031
0.884
Cl
O
O
O
O
Normalized Intensity
Chemical Shift (ppm)
2.28
2.22
2.57
1.10
2.52
1.12
1.07
1.37
1.39
3.01
3.31
3.14

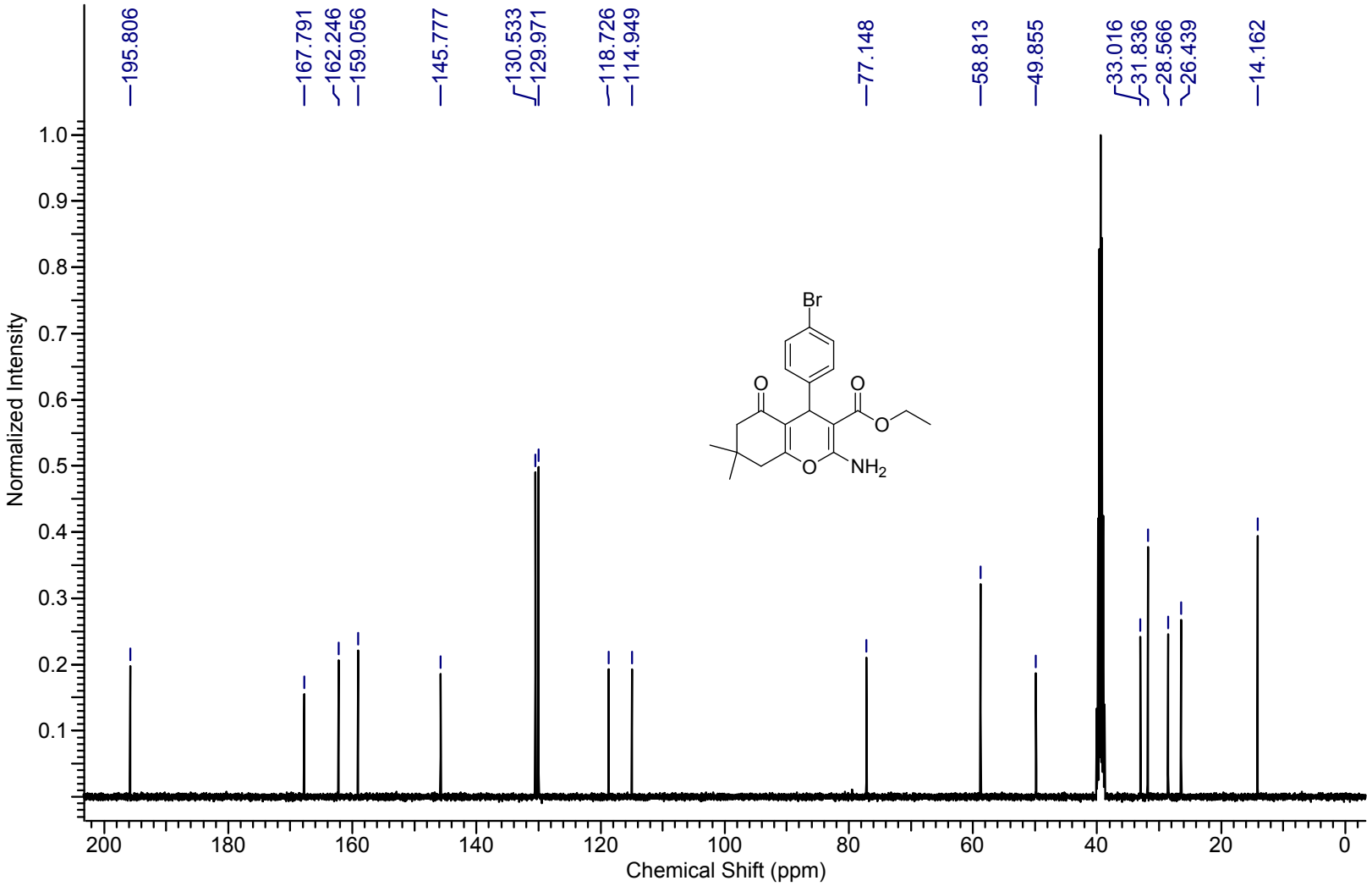
^{13}C NMR of 10c



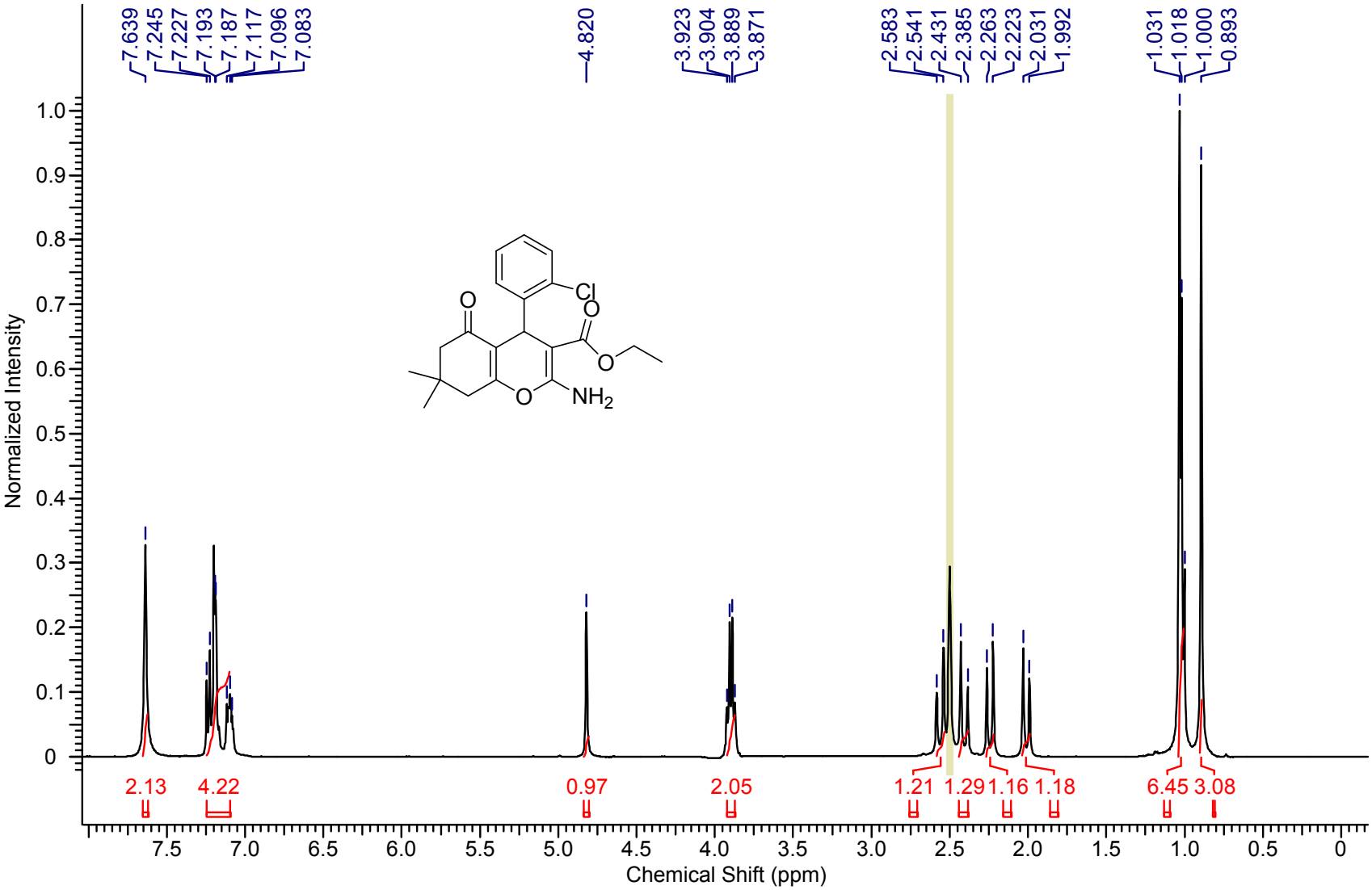
^{1}H NMR of 10d


7.599
7.407
7.385
7.096
7.074
4.457
3.962
3.944
3.929
3.914
2.571
2.529
2.474
2.431
2.281
2.242
2.074
2.034
1.098
1.082
1.064
1.031
0.884
Br
O
O
O
O
NH2
Normalized Intensity
Chemical Shift (ppm)
2.07 1.89 2.15
1.00 2.23
1.15 1.10 1.06 1.01
3.04 3.07 3.06

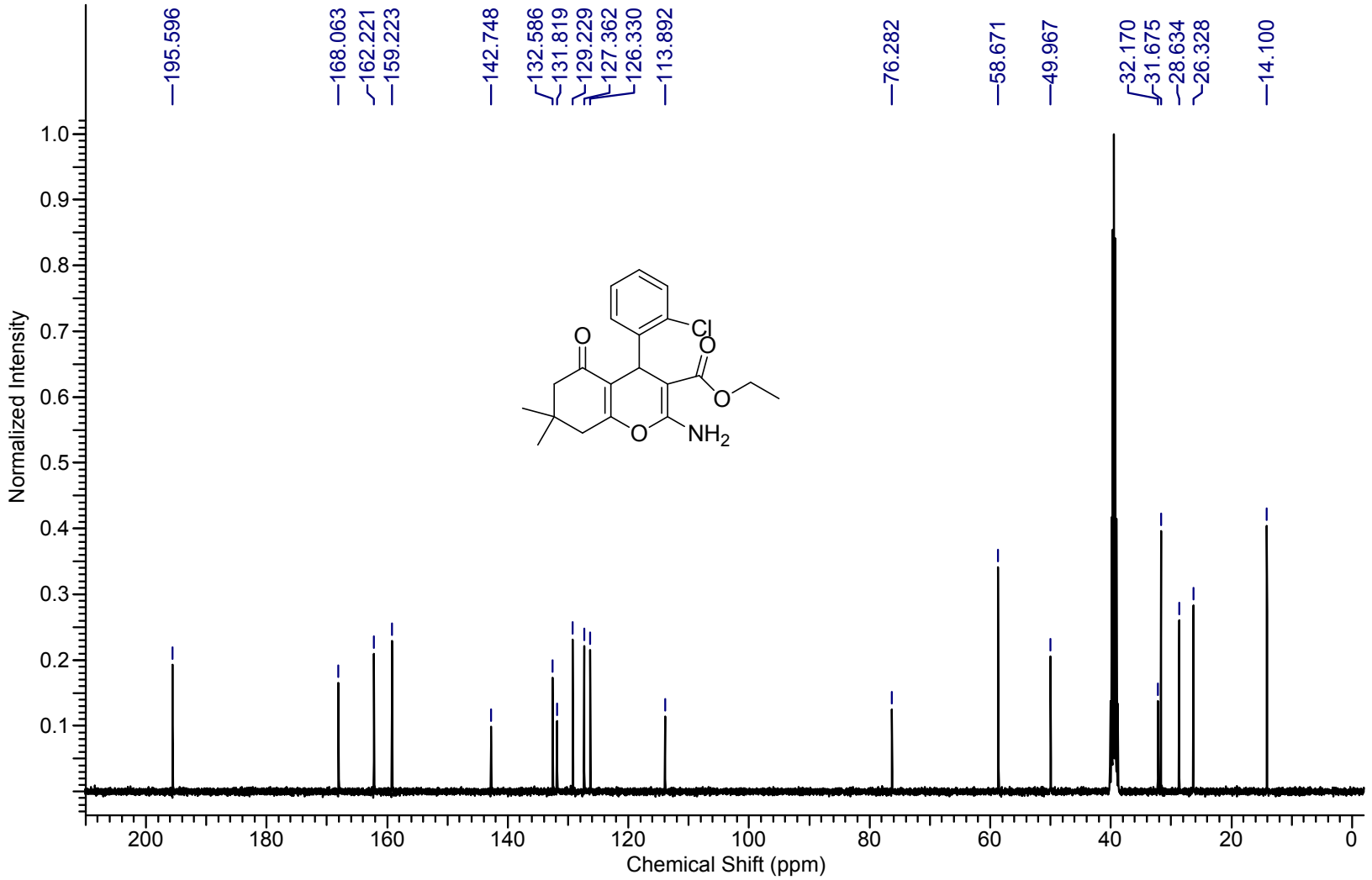
^{13}C NMR of 10d



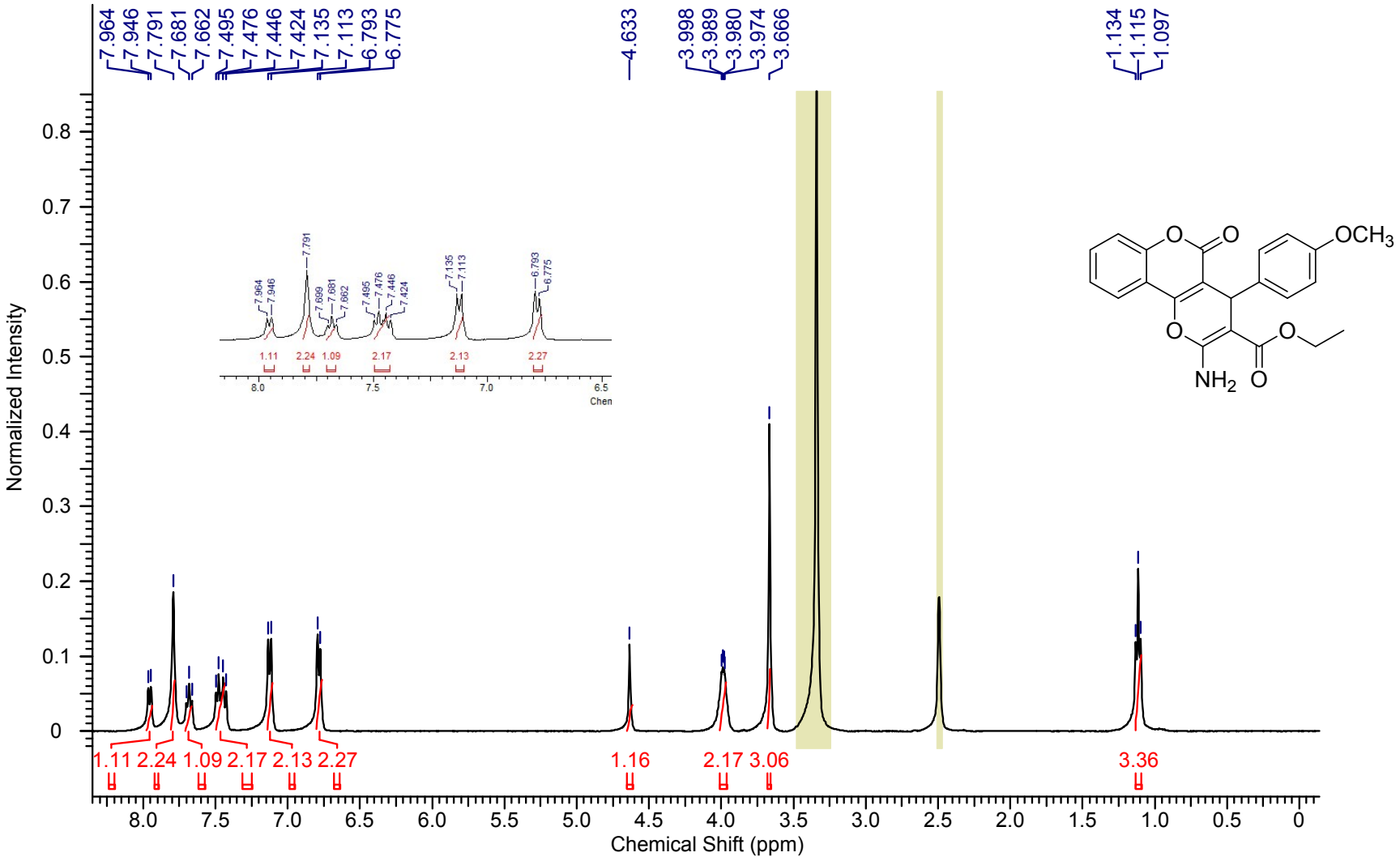
^{1}H NMR of 10e


7.639
7.245
7.227
7.193
7.187
7.117
7.096
7.083
4.820
3.923
3.904
3.889
3.871
2.583
2.541
2.431
2.385
2.263
2.223
2.031
1.992
1.031
1.018
1.000
0.893
Cl
O
O
O
O
NH2
Normalized Intensity
Chemical Shift (ppm)
2.13
4.22
0.97
2.05
1.21
1.29
1.16
1.18
6.45
3.08

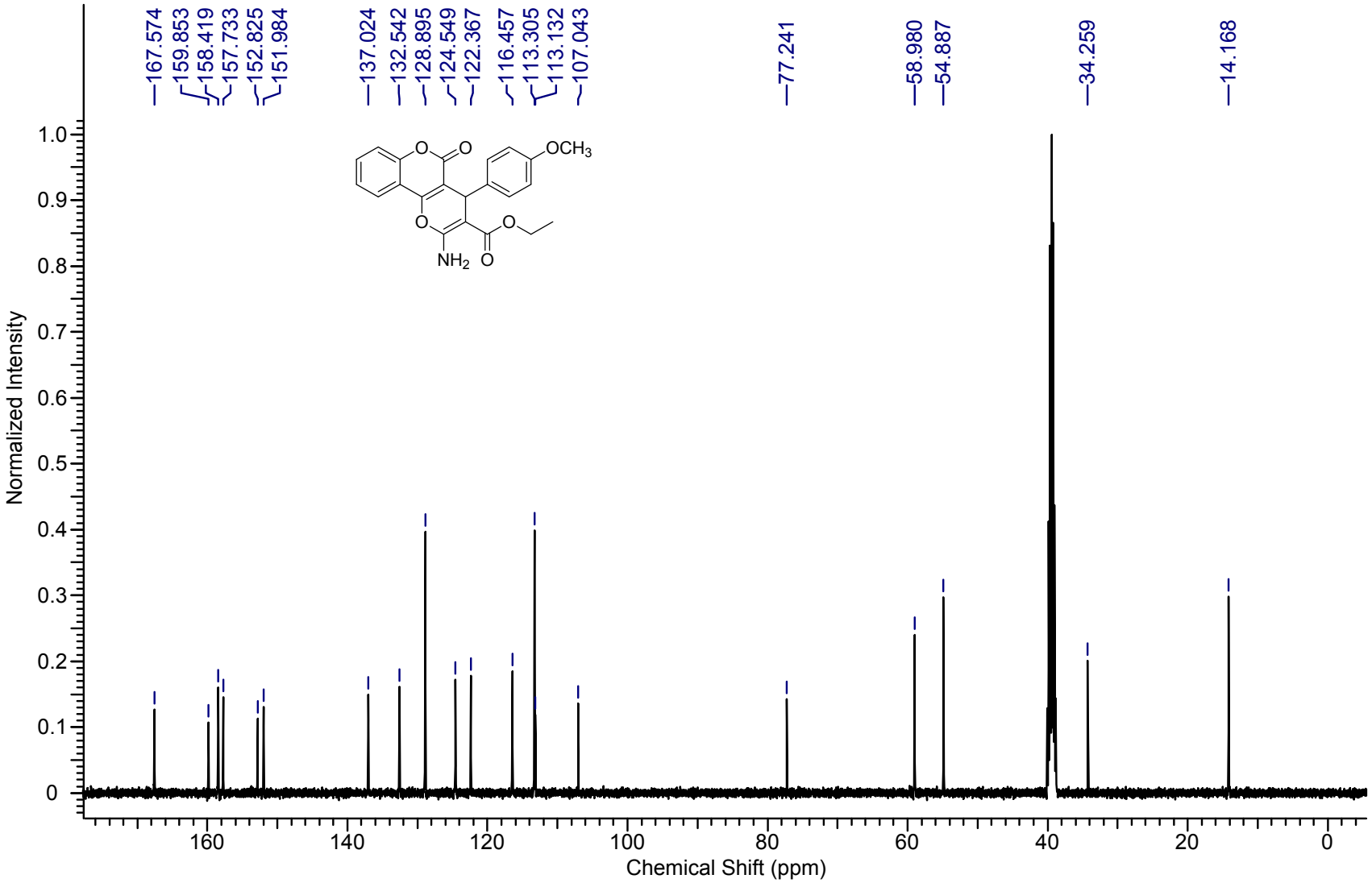
^{13}C NMR of 10e



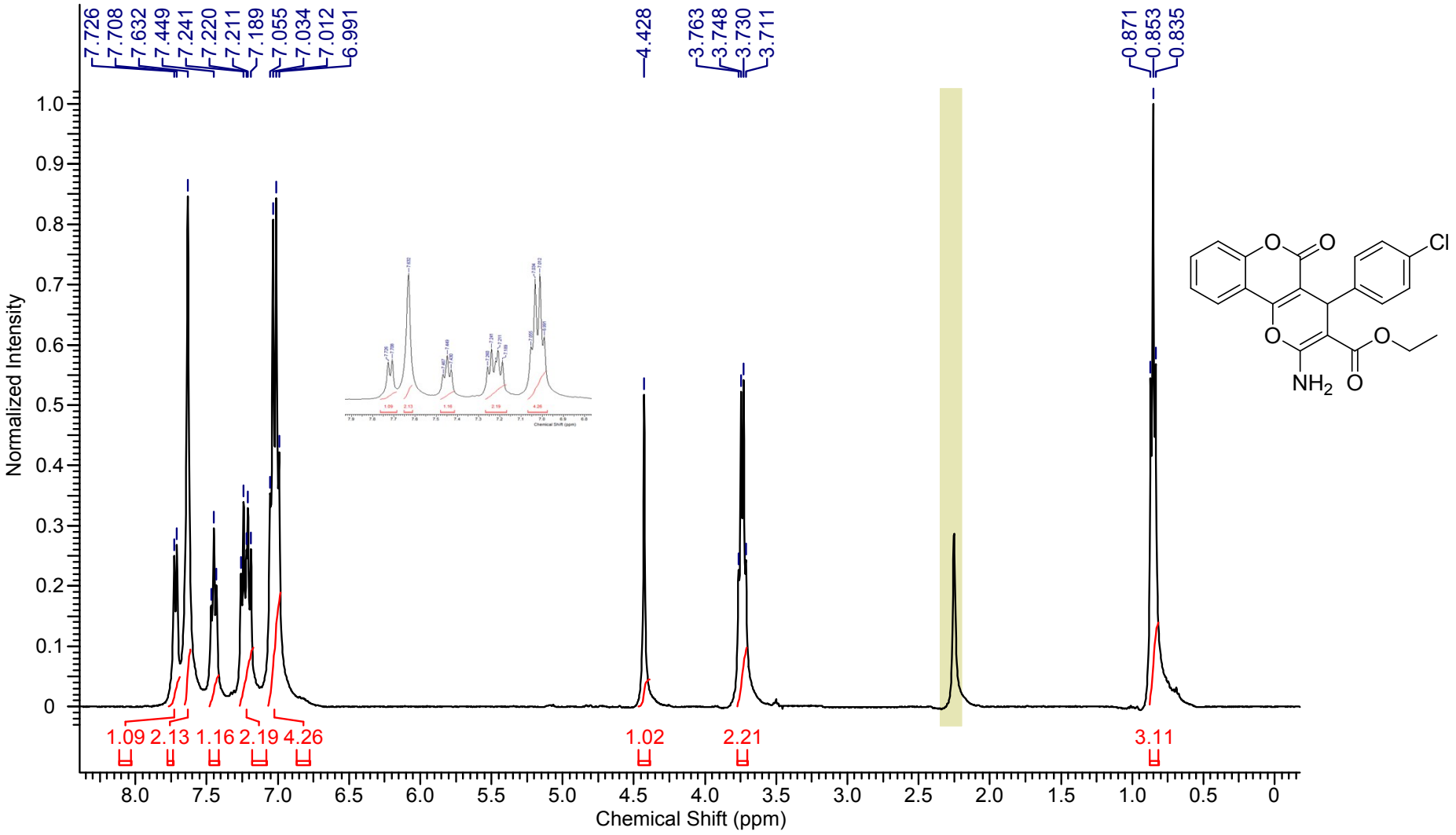
^{1}H NMR of 11b


7.964
7.946
7.791
7.681
7.662
7.495
7.476
7.446
7.424
7.135
7.113
6.793
6.775
4.633
3.998
3.989
3.980
3.974
3.666
1.134
1.115
1.097
Normalized Intensity
1.11 2.24 1.09 2.17 2.13 2.27
1.16
2.17 3.06
3.36
Chemical Shift (ppm)
OCH3
NH2

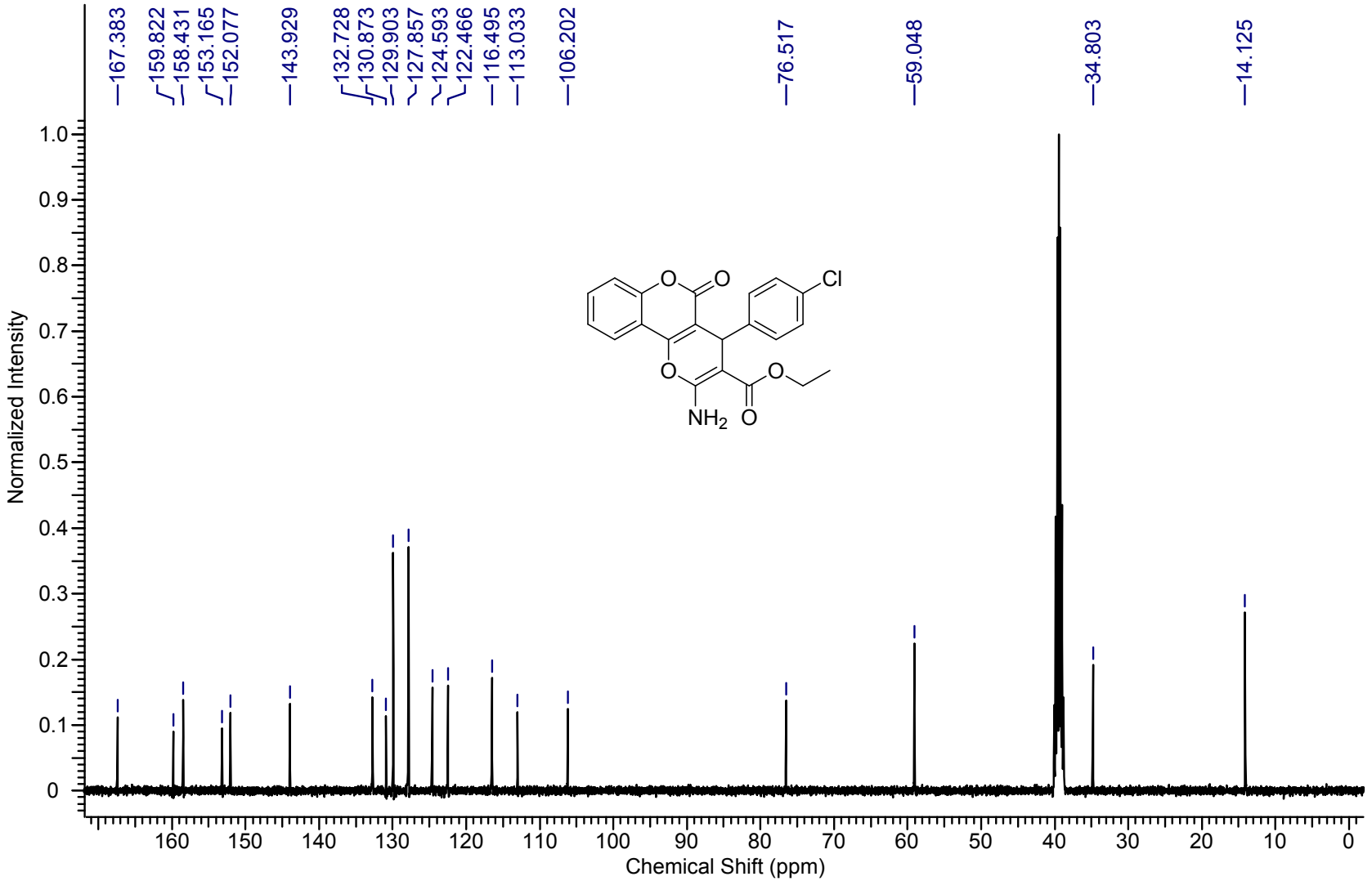
^{13}C NMR of 11b



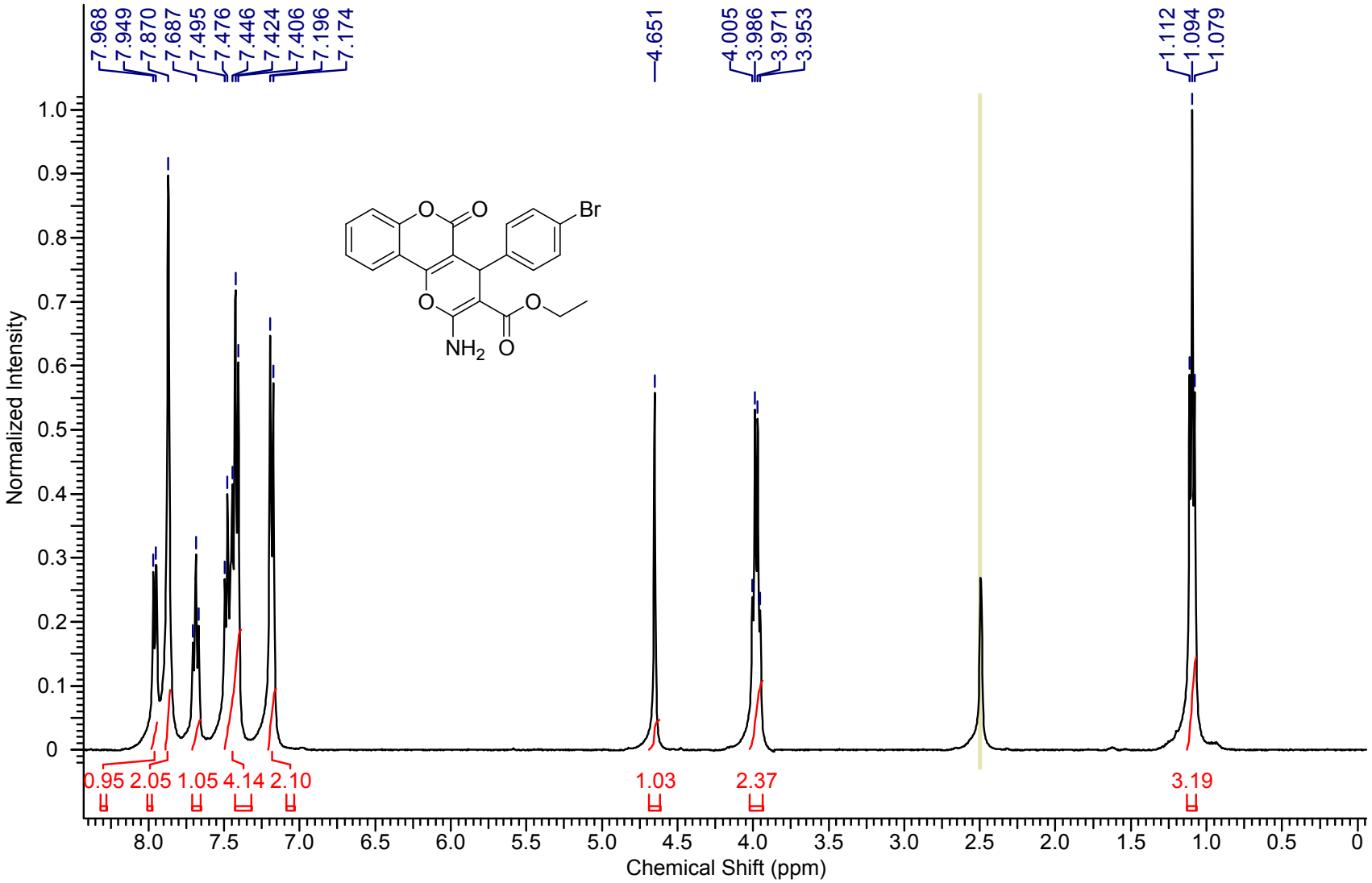
^{1}H NMR of 11c


7.726
7.708
7.632
7.449
7.241
7.220
7.211
7.189
7.055
7.034
7.012
6.991
4.428
3.763
3.748
3.730
3.711
0.871
0.853
0.835
Normalized Intensity
1.09 2.13 1.16 2.19 4.26
1.02
2.21
3.11
Chemical Shift (ppm)
Cl
O
O
O
O
NH2
O

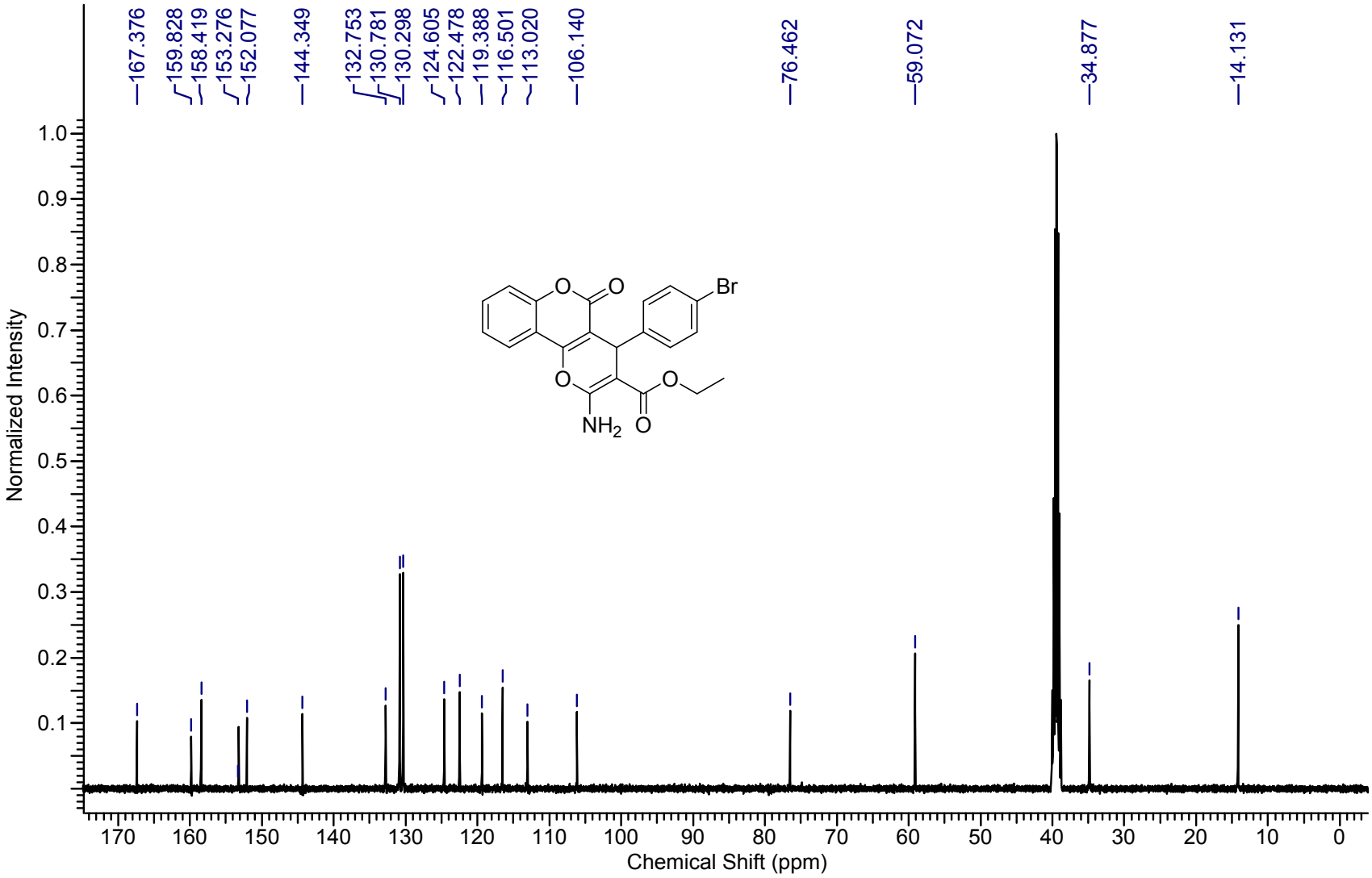
^{13}C NMR of 11c



^{1}H NMR of 11d


7.968
7.949
7.870
7.687
7.495
7.476
7.446
7.424
7.406
7.196
7.174
4.651
4.005
3.986
3.971
3.953
1.112
1.094
1.079
Br
O
O
O
O
O
NH2
O
Normalized Intensity
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0.95
2.05
1.05
4.14
2.10
1.03
2.37
3.19
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)

^{13}C NMR of 11d



Standard Orientation for IS_1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.328882	-1.481502	-0.055717
2	6	0	-1.473785	-0.353204	-0.056978
3	6	0	-2.077394	0.919956	0.022962
4	6	0	-3.456794	1.047588	0.100917
5	6	0	-4.298874	-0.075821	0.105545
6	6	0	-3.706841	-1.344556	0.021922
7	1	0	-1.897127	-2.474574	-0.121977
8	1	0	-1.470349	1.812517	0.020512
9	1	0	-3.889553	2.041569	0.157625
10	1	0	-4.331310	-2.232342	0.015576
11	6	0	-0.043961	-0.606629	-0.146134
12	6	0	1.057191	0.201391	-0.183501
13	6	0	1.047280	1.628098	-0.136965
14	6	0	2.405224	-0.475766	-0.283033
15	7	0	1.025786	2.791625	-0.098200
16	8	0	3.412587	0.408724	-0.279941
17	8	0	2.566832	-1.682441	-0.296644
18	6	0	4.770143	-0.110412	-0.331031
19	6	0	5.306664	-0.356302	1.068093
20	1	0	5.263880	0.555203	1.668108
21	1	0	4.740264	-1.141888	1.572469
22	1	0	6.350380	-0.677794	1.005925
23	1	0	5.334220	0.670306	-0.842901
24	1	0	4.772403	-1.022031	-0.929488
25	1	0	0.226308	-1.659209	-0.195195
26	6	0	-5.792987	0.077673	0.229644
27	1	0	-6.322701	-0.743350	-0.259042
28	1	0	-6.096620	0.079677	1.282594
29	1	0	-6.137562	1.017189	-0.208473

Rotational constants (GHZ): 1.5404945 0.2090121 0.1881950
Standard basis: 6-31+G(d,p) (6D, 7F)
There are 369 symmetry adapted basis functions of A symmetry.

Standard Orientation for IS_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.431670	1.535414	-0.817561
2	6	0	-0.401815	1.102897	0.515147
3	6	0	0.490813	1.689413	1.422444
4	6	0	1.353283	2.708884	0.997023

5	6	0	1.323106	3.141701	-0.335594
6	6	0	0.430722	2.554866	-1.242932
7	1	0	0.513862	1.358948	2.439832
8	1	0	2.034861	3.156834	1.689616
9	1	0	0.407758	2.885067	-2.260390
10	6	0	-1.350357	-0.016798	0.982077
11	6	0	-2.644613	0.027000	0.148613
12	6	0	-0.664464	-1.382857	0.794029
13	6	0	-0.351157	-1.559578	-0.706729
14	6	0	0.618169	-1.397966	1.652097
15	6	0	1.020842	-1.174461	-1.290713
16	6	0	1.985738	-1.013730	1.057762
17	6	0	2.140591	-1.629538	-0.341672
18	1	0	1.159470	-1.668130	-2.229907
19	1	0	2.765755	-1.400541	1.679800
20	6	0	-2.735819	-0.687999	-1.000992
21	8	0	-2.826247	-1.347924	-2.066507
22	8	0	-1.241032	-2.013668	-1.471861
23	8	0	0.541810	-1.716266	2.867148
24	6	0	-3.728064	0.805563	0.577438
25	7	0	-4.613395	1.443095	0.929867
26	6	0	2.074670	-3.162290	-0.209881
27	6	0	3.501893	-1.212978	-0.929155
28	1	0	4.286452	-1.546194	-0.282334
29	1	0	3.541187	-0.147389	-1.017735
30	1	0	3.623987	-1.655970	-1.895458
31	1	0	1.126848	-3.444795	0.198438
32	1	0	2.194645	-3.608768	-1.174867
33	1	0	2.856789	-3.498475	0.438369
34	1	0	-1.319556	-2.165009	1.116740
35	1	0	1.057858	-0.114754	-1.434389
36	1	0	2.061891	0.052478	1.009367
37	1	0	-1.586890	0.124219	2.016132
38	1	0	-1.112996	1.087280	-1.510350
39	6	0	2.270681	4.262513	-0.802887
40	1	0	1.793148	5.211035	-0.671734
41	1	0	3.170421	4.233069	-0.224490
42	1	0	2.506748	4.121962	-1.837035

Rotational constants (GHZ): 0.3048446 0.2745180 0.1996884

Standard basis: 6-31+G(d,p) (6D, 7F)

There are 532 symmetry adapted basis functions of A symmetry

Standard Orientation for IS_3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.294889	0.335537	-0.760460
2	6	0	1.706033	-0.130377	0.422814
3	6	0	2.276962	-1.208652	1.112219

4	6	0	3.436743	-1.820952	0.618334
5	6	0	4.025534	-1.355050	-0.564968
6	6	0	3.454579	-0.276808	-1.254385
7	1	0	1.827397	-1.564393	2.015641
8	1	0	3.872748	-2.644206	1.144701
9	1	0	3.904107	0.078907	-2.157860
10	6	0	0.431563	0.542791	0.965237
11	6	0	0.423869	2.028542	0.560163
12	6	0	-0.808258	-0.156159	0.377133
13	6	0	-1.345132	0.284245	-0.790701
14	6	0	-1.436620	-1.351005	1.112397
15	6	0	-2.588310	-0.402114	-1.402496
16	6	0	-2.673015	-2.030484	0.510914
17	6	0	-3.474501	-0.986719	-0.283885
18	1	0	-3.150967	0.318609	-1.958257
19	1	0	-3.281322	-2.432728	1.293894
20	6	0	-0.144632	2.409166	-0.609823
21	8	0	-0.672319	2.763143	-1.695990
22	8	0	-0.751597	1.397584	-1.463796
23	8	0	-0.943689	-1.765432	2.193561
24	6	0	1.005451	2.988245	1.402557
25	7	0	1.480730	3.768138	2.092145
26	6	0	-3.922503	0.145537	0.658834
27	6	0	-4.713581	-1.657072	-0.905650
28	1	0	-5.327448	-2.062342	-0.128637
29	1	0	-4.402464	-2.443437	-1.561127
30	1	0	-5.271711	-0.931182	-1.459211
31	1	0	-3.061668	0.611335	1.091130
32	1	0	-4.480243	0.871244	0.104633
33	1	0	-4.536861	-0.259279	1.435767
34	1	0	-2.273813	-1.190593	-2.053877
35	1	0	-2.366025	-2.820864	-0.141691
36	1	0	0.412827	0.463916	2.032202
37	1	0	1.858988	1.158876	-1.286803
38	6	0	5.299998	-2.028069	-1.107569
39	1	0	6.161441	-1.542364	-0.699004
40	1	0	5.305572	-3.060349	-0.826179
41	1	0	5.318482	-1.949144	-2.174438
42	1	0	-1.427723	1.875063	-1.950085

Rotational constants (GHZ): 0.3669839 0.1942557 0.1628345

Standard basis: 6-31+G(d,p) (6D, 7F)

There are 532 symmetry adapted basis functions of A symmetry.

Standard Orientation for IS_4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.703164	1.686464	-0.937759
2	6	0	-0.966346	1.480349	0.246869
3	6	0	-0.828749	2.535558	1.116982

4	6	0	-1.355763	3.753651	0.938928
5	6	0	-2.137625	3.969909	-0.226477
6	6	0	-2.335191	2.968172	-1.152532
7	1	0	-0.247250	2.346354	1.969918
8	1	0	-1.182412	4.579761	1.675856
9	1	0	-2.957454	3.167794	-2.059328
10	6	0	-0.224795	0.056703	0.737035
11	6	0	-0.910627	-1.191017	0.077771
12	6	0	1.300034	0.016008	0.361573
13	6	0	1.811497	0.266657	-0.933504
14	6	0	2.212978	-0.261207	1.517473
15	6	0	3.386108	0.391207	-1.128458
16	6	0	3.750426	-0.012205	1.341958
17	6	0	4.204229	-0.414490	-0.072083
18	1	0	3.677647	0.048734	-2.121641
19	1	0	4.309884	-0.606674	2.032356
20	6	0	-0.264410	-1.827151	-1.007885
21	8	0	1.056174	0.441464	-1.978252
22	8	0	1.717597	-0.658252	2.614042
23	6	0	-2.253290	-1.624742	0.582662
24	6	0	4.055136	-1.932530	-0.269257
25	6	0	5.668420	-0.033459	-0.222977
26	1	0	6.245254	-0.537205	0.511430
27	1	0	5.753499	1.027430	-0.083110
28	1	0	6.011107	-0.288166	-1.196372
29	1	0	3.029767	-2.217332	-0.178283
30	1	0	4.412166	-2.199845	-1.239723
31	1	0	4.630199	-2.438521	0.478215
32	1	0	3.628705	1.412324	-1.012831
33	1	0	3.952442	1.022990	1.499999
34	1	0	-0.326370	0.020797	1.835508
35	1	0	-1.771090	0.913280	-1.630067
36	1	0	1.435722	0.704469	-2.830906
37	7	0	0.351209	-2.433148	-2.042124
38	1	0	-0.290927	-2.729102	-2.879537
39	8	0	-2.779085	-1.145183	1.651993
40	8	0	-2.948531	-2.544808	-0.073464
41	6	0	-4.101484	-3.103378	0.442266
42	6	0	-4.513571	-4.273258	-0.425389
43	1	0	-4.865449	-2.393270	0.438970
44	1	0	-3.886389	-3.421456	1.465004
45	1	0	-5.414166	-4.688676	-0.035697
46	1	0	-4.655439	-3.919534	-1.405621
47	1	0	-3.754243	-5.032611	-0.414091
48	6	0	-2.765467	5.319889	-0.447265
49	1	0	-2.087892	6.073163	-0.113260
50	1	0	-2.971818	5.441150	-1.482747
51	1	0	-3.673273	5.373662	0.116681

Rotational constants (GHZ): 0.2135412 0.1571881
0.1098676

Standard basis: 6-31+G(d,p) (6D, 7F)

There are 619 symmetry adapted basis functions of A symmetry.

Standard Orientation for IS_5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.330921	1.810771	-1.258437
2	6	0	0.081599	1.322824	-0.858971
3	6	0	0.322843	1.004056	0.677715
4	6	0	-0.794479	1.712850	1.442811
5	6	0	-0.896650	3.096918	0.847919
6	1	0	-1.991837	1.006974	-1.009239
7	1	0	1.285603	1.366772	1.033611
8	1	0	-1.313045	3.806516	1.536097
9	6	0	-3.202255	3.163055	-0.275681
10	6	0	-1.675950	3.103213	-0.459683
11	6	0	-1.208231	4.378918	-1.203161
12	8	0	0.987072	1.140761	-1.713838
13	8	0	-1.481226	1.256669	2.389706
14	1	0	-1.426503	2.049529	-2.298274
15	1	0	0.112023	3.376123	0.614269
16	1	0	-1.440814	5.242275	-0.615848
17	1	0	-0.150770	4.330480	-1.364076
18	1	0	-3.456729	4.040844	0.283138
19	1	0	-3.533050	2.295449	0.247518
20	1	0	-3.677446	3.205820	-1.236040
21	1	0	-1.707155	4.448752	-2.149959
22	6	0	-1.842734	-1.595114	1.495889
23	6	0	-0.946149	-1.265856	0.446037
24	6	0	-1.232936	-1.653239	-0.851455
25	6	0	-2.391684	-2.395242	-1.118263
26	6	0	-3.253343	-2.770521	-0.085131
27	6	0	-2.989368	-2.355236	1.229223
28	1	0	-1.654737	-1.257859	2.499897
29	1	0	-0.569043	-1.377474	-1.644906
30	1	0	-2.610921	-2.692311	-2.123369
31	1	0	-3.658556	-2.630280	2.025982
32	6	0	0.373005	-0.531590	0.771970
33	6	0	1.486677	-0.764045	-0.278949
34	6	0	1.411805	-2.137696	-0.956683
35	6	0	2.883958	-0.591799	0.433706
36	7	0	1.356717	-3.148242	-1.455278
37	8	0	3.979908	-1.154225	-0.046646
38	8	0	2.969093	0.090330	1.509808
39	6	0	5.267718	-0.807998	0.435149
40	6	0	5.807735	0.365357	-0.408910
41	1	0	5.871363	0.064832	-1.437848
42	1	0	5.143346	1.197788	-0.324469
43	1	0	6.779790	0.641685	-0.060475
44	1	0	5.917357	-1.654298	0.334193
45	1	0	5.206521	-0.519714	1.460417
46	1	0	0.635324	-0.896489	1.754713
47	6	0	-4.514191	-3.618465	-0.376701
48	1	0	-4.254975	-4.660403	-0.328851
49	1	0	-5.270599	-3.415301	0.357715

50	1	0	-4.885669	-3.386842	-1.346412
51	1	0	1.376040	-0.040424	-1.023438

Rotational constants (GHZ): 0.2431581 0.1714028 0.1217261
Standard basis: 6-31+G(d,p) (6D, 7F)
There are 619 symmetry adapted basis functions of A symmetry.

Standard Orientation for IS_6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.834581	1.049578	-0.698714
2	6	0	-0.960782	1.049228	0.446014
3	6	0	-0.984020	2.192435	1.298854
4	6	0	-1.833148	3.277128	1.034150
5	6	0	-2.702065	3.240394	-0.041486
6	6	0	-2.715175	2.149866	-0.906659
7	1	0	-0.336866	2.232628	2.154589
8	1	0	-1.817183	4.119454	1.659374
9	1	0	-3.381792	2.144997	-1.723040
10	6	0	-0.004024	-0.140182	0.867471
11	6	0	-0.462423	-1.505343	0.286851
12	6	0	1.497082	0.085236	0.448874
13	6	0	1.899522	0.759196	-0.686218
14	6	0	2.569470	-0.515730	1.400072
15	6	0	3.443107	1.029633	-0.916104
16	6	0	4.052856	-0.212498	1.192614
17	6	0	4.347825	-0.079611	-0.297950
18	1	0	3.642954	1.083819	-1.974989
19	1	0	4.641611	-1.008888	1.595894
20	6	0	-0.349587	-1.541397	-1.233147
21	8	0	0.933684	1.253475	-1.639096
22	8	0	2.209267	-1.231599	2.370081
23	6	0	-1.912521	-1.782116	0.711166
24	6	0	4.123553	-1.442731	-0.993465
25	6	0	5.825383	0.314041	-0.465861
26	1	0	6.447434	-0.428420	-0.016449
27	1	0	5.997026	1.247691	0.008683
28	1	0	6.062692	0.388629	-1.496609
29	1	0	3.108832	-1.745472	-0.885687
30	1	0	4.358760	-1.364592	-2.028668
31	1	0	4.754562	-2.181369	-0.545194
32	1	0	3.693013	1.952205	-0.456706
33	1	0	4.290980	0.691008	1.694650
34	1	0	-0.012590	-0.183738	1.954748
35	1	0	-1.837320	0.230659	-1.391490
36	1	0	1.362859	1.295360	-2.501222
37	7	0	-0.264773	-1.568491	-2.375504
38	8	0	-2.282546	-1.503554	1.854509

39	8	0	-2.695382	-2.287683	-0.152383
40	6	0	-4.007819	-2.723796	0.260222
41	6	0	-4.702561	-3.435512	-0.918259
42	1	0	-4.592431	-1.879415	0.527207
43	1	0	-3.943003	-3.387534	1.106031
44	1	0	-5.688883	-3.743833	-0.637311
45	1	0	-4.779358	-2.759380	-1.737741
46	1	0	-4.147456	-4.287395	-1.209695
47	1	0	0.224216	-2.268773	0.668261
48	6	0	-3.625977	4.398484	-0.244997
49	1	0	-3.145837	5.280373	0.124002
50	1	0	-3.829076	4.494813	-1.284111
51	1	0	-4.524607	4.213677	0.298546

Rotational constants (GHZ): 0.2709428 0.1460954 0.1161549

Standard basis: 6-31+G(d,p) (6D, 7F)

There are 619 symmetry adapted basis functions of A symmetry.

Standard Orientation for A

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.043130	-0.741264	-0.019062
2	6	0	0.693958	-1.215291	-1.238546
3	6	0	-1.592423	-0.550600	-0.944796
4	6	0	-1.329853	-0.049434	0.293829
5	6	0	0.119562	0.239162	0.707663
6	6	0	-2.479074	0.224112	1.277909
7	6	0	-3.047592	-0.851467	-1.378972
8	6	0	-3.918033	-0.086070	0.849927
9	6	0	-3.895504	-1.249611	-0.154693
10	6	0	-3.279151	-2.495593	0.510149
11	6	0	-5.335057	-1.566962	-0.603942
12	1	0	-2.279121	-2.275407	0.821568
13	1	0	-5.921909	-1.843668	0.246888
14	1	0	-3.864491	-2.773258	1.361215
15	1	0	-5.763910	-0.702642	-1.066571
16	1	0	-3.263943	-3.303381	-0.191498
17	1	0	-5.319349	-2.375425	-1.304519
18	8	0	-0.528888	-0.808855	-1.878550
19	8	0	-2.241808	0.694780	2.420004
20	1	0	-4.349390	0.778116	0.388810
21	1	0	-4.498708	-0.358880	1.705962
22	1	0	-3.044805	-1.657605	-2.082594
23	1	0	-3.470715	0.019935	-1.834233
24	6	0	0.501292	1.679802	0.316578
25	6	0	1.039892	1.932266	-0.952181
26	6	0	0.314938	2.734537	1.221337
27	6	0	1.399796	3.236452	-1.315105
28	1	0	1.177016	1.127335	-1.644616
29	6	0	0.676984	4.040207	0.858179

30	1	0	-0.101713	2.543356	2.188241
31	6	0	1.220074	4.290537	-0.410201
32	1	0	1.811932	3.426841	-2.284652
33	1	0	0.538695	4.845773	1.548536
34	1	0	0.223538	0.117435	1.766307
35	6	0	2.366674	-1.182907	0.634326
36	6	0	3.978003	-2.854658	0.892538
37	6	0	4.947650	-3.788442	0.146056
38	8	0	3.246150	-2.075287	-0.055820
39	8	0	2.676775	-0.755821	1.776905
40	1	0	4.533699	-2.204651	1.535710
41	1	0	3.297639	-3.438403	1.477595
42	1	0	5.496900	-4.372130	0.854292
43	1	0	4.393148	-4.437696	-0.498013
44	1	0	5.627570	-3.202997	-0.437149
45	7	0	1.505062	-2.075607	-1.861746
46	1	0	1.259649	-2.429741	-2.763864
47	1	0	2.357220	-2.364723	-1.425276
48	6	0	1.619840	5.723083	-0.810802
49	1	0	1.918329	6.267484	0.060538
50	1	0	2.433999	5.685808	-1.504159
51	1	0	0.784823	6.212072	-1.267775

Rotational constants (GHZ): 0.2054545 0.1715098 0.1137810

Standard basis: 6-31+G(d,p) (6D, 7F)

There are 619 symmetry adapted basis functions of A symmetry.

Standard Orientation for B

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.278392	0.245304	-0.776183
2	6	0	1.674120	-0.199206	0.407535
3	6	0	2.231481	-1.269852	1.119567
4	6	0	3.393116	-1.895984	0.647883
5	6	0	3.997390	-1.451470	-0.535833
6	6	0	3.440027	-0.380827	-1.247866
7	1	0	1.770106	-1.609247	2.023361
8	1	0	3.818675	-2.713443	1.191537
9	1	0	3.901404	-0.041431	-2.151659
10	6	0	0.397603	0.488856	0.925874
11	6	0	0.392172	1.958795	0.496848
12	6	0	-0.837019	-0.199119	0.334536
13	6	0	-1.354713	0.235291	-0.846692
14	6	0	-1.485452	-1.377000	1.079502
15	6	0	-2.601683	-0.448908	-1.456197
16	6	0	-2.723914	-2.049514	0.477275
17	6	0	-3.504846	-1.006766	-0.337610
18	1	0	-3.151850	0.269073	-2.027789
19	1	0	-3.343647	-2.433903	1.260267
20	6	0	-0.168176	2.313651	-0.684418

21	8	0	-0.755836	1.333722	-1.557638
22	8	0	-1.006402	-1.782957	2.170043
23	6	0	0.964826	2.934325	1.324089
24	6	0	-3.946600	0.143865	0.585699
25	6	0	-4.746976	-1.670113	-0.961055
26	1	0	-5.372619	-2.056934	-0.183984
27	1	0	-4.440180	-2.469296	-1.602991
28	1	0	-5.291167	-0.945004	-1.529363
29	1	0	-3.083684	0.604555	1.019334
30	1	0	-4.490138	0.869027	0.016835
31	1	0	-4.572911	-0.242521	1.362448
32	1	0	-2.290450	-1.251149	-2.092156
33	1	0	-2.421193	-2.852278	-0.162124
34	1	0	0.369037	0.425033	1.993587
35	1	0	1.852834	1.062764	-1.319836
36	8	0	-0.171897	3.566121	-1.037528
37	1	0	-0.565350	3.828095	-1.873090
38	7	0	1.433363	3.732483	2.000926
39	6	0	5.273915	-2.139524	-1.054163
40	1	0	5.270691	-3.167490	-0.757220
41	1	0	5.304462	-2.076795	-2.121885
42	1	0	6.133528	-1.652349	-0.643521

Rotational constants (GHZ): 0.3517217 0.1975243 0.1585231

Standard basis: 6-31+G(d,p) (6D, 7F)

There are 532 symmetry adapted basis functions of A symmetry.