

Supporting information for

**Ultrasound assisted multicomponent reactions: a green method
for the synthesis of highly functionalized selenopyridines using
reusable polyethylene glycol as reaction medium†**

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General Experimental Information

All the reagents were purchased from commercial sources and used without further purification. All the reactions were monitored by TLC on Merck GF 254 with detection by UV light and/or using iodine vapor chamber for visualization. IR spectra were recorded on a Shimadzu Affinity 1, FTIR spectrophotometer. ¹H and ¹³C NMR was recorded on a Bruker Avance II 400 and Jeol 500 MHz spectrometer in DMSO-d₆ or DMSO-d₆+CDCl₃ using TMS as internal reference. CHN analyses were carried out either on in an Elementar Vario EL III or Perkin-Elmer 2400 II elemental analyzers. Zeiotech water bath was used for ultrasonication reactions. Melting points were recorded using SRS EZ- Melt automated melting point apparatus by capillary methods and uncorrected.

General procedure for the synthesis of 2-amino-4-aryl/alkyl-6-(phenylselanyl)pyridine-3,5-dicarbonitrile (4a-4k** and **5a-5b**):** A mixture of aldehyde (1.0 mmol), malononitrile (2.0 mmol) and benzeneselenol (1.0 mmol) in 2.0 ml PEG-400 was taken in a 10 ml vial and was placed in an ultrasonic bath filled with water. This mixture was then irradiated at room temperature for appropriate time as mentioned in the Table 1. The progress of the reaction was monitored by TLC. After completion of the reaction, it was removed from the ultrasonic bath and 2.0 ml ethanol was added followed by stirring to obtain the solid precipitate. The precipitate was then filtered off and washed with ethanol and dried under reduced pressure. The isolated solid was pure enough for further characterization. (In some cases where, solid precipitates were not observed after addition of ethanol it was kept as such for 1-2 days in ethanolic solution for slow evaporation to get the precipitates, Eg., **4g** and **4h**).

X-ray Analysis and Structure Refinement.

Data were collected on a Bruker SMART CCD4 X-ray diffraction instrument using graphite-monochromated Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$) at 100 K. The crystal was solved by direct methods using the *SIR92* program¹ and refined using full-matrix least squares on F^2 (*SHELX97*).² The structure was expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed at geometrically idealized positions. Table 3 contains the final refinement parameters for **4b**. All of these software packages were the integrated *WINGX* software package. CCDC 1004592 contains the supplementary crystallographic data for this paper. Copies of this information can be obtained free of charge upon application to CCDC, 12 Union Road, Cambridge CB21EZ, U.K. (fax □44-1223/336-033; e-mail deposit@ccdc.cam.ac.uk).

2-amino-4-phenyl-6-(phenylselanyl)pyridine-3,5-dicarbonitrile (4a): White solid; Yield:

76%, m.p. 220-222 °C; IR (KBr): 3471, 3346, 3210, 3062, 2221, 2210, 1623, 1607, 1532, 1261, 833, 748 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆ + CDCl₃) δ (ppm): 7.81 (bs, 2H, -NH₂), 7.69-7.66 (m, 2H, Ar-H), 7.60-7.52 (m, 6H, Ar-H), 7.48-7.42 (m, 2H, Ar-H); ¹³C NMR (100 MHz, DMSO-*d*₆ + CDCl₃) δ (ppm): 165.0, 159.6, 157.9, 135.5, 133.8, 130.3, 129.4, 129.1, 128.7, 128.3, 125.9, 115.7, 114.9, 96.3, 87.5; Anal. calcd. for C₁₉H₁₂N₄Se: C, 60.81; H, 3.22; N, 14.93 %. Found: C, 60.84; H, 3.25; N, 14.95 %.

2-amino-4-(4-methoxyphenyl)-6-(phenylselanyl)pyridine-3,5-dicarbonitrile (4b): White

solid; Yield: 82%, m.p. 247-249 °C; IR (KBr): 3443, 3331, 3225, 3090, 2982, 2845, 2228, 2212, 1638, 1606, 1544, 1419, 1288, 1259, 1189, 1018, 835, 810, 746 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆ + CDCl₃) δ (ppm): 7.71 (bs, 2H, -NH₂), 7.69-7.65 (m, 2H, Ar-H), 7.50 (d, *J* = 8.8 Hz, 2H, Ar-H), 7.47-7.41 (m, 3H, Ar-H), 7.11 (d, *J* = 8.8 Hz, 2H, Ar-H), 3.86 (s, 3H, -OCH₃); ¹³C NMR (100 MHz, DMSO-*d*₆ + CDCl₃) δ (ppm): 165.1, 160.8, 159.7, 157.5, 135.5, 130.1, 129.3, 128.9, 126.0, 125.6, 115.9, 115.2, 114.0, 96.3, 87.3, 55.2; Anal. calcd. for C₂₀H₁₄N₄OSe: C, 59.27; H, 3.48; N, 13.82 %. Found: C, 59.31; H, 3.51; N, 13.86 %.

2-amino-4-(3-phenoxyphenyl)-6-(phenylselanyl)pyridine-3,5-dicarbonitrile (4c): White

solid; Yield: 84%, m.p. 242-244 °C; IR (KBr): 3435, 3328, 3216, 3061, 2225, 2213, 1627, 1583, 1544, 1517, 1485, 1439, 1312, 1264, 1243, 1225, 1022, 952, 859, 745 cm⁻¹; ¹H NMR (500 MHz, DMSO-*d*₆) δ (ppm): 7.85 (bs, 2H, -NH₂), 7.65-7.63 (m, 2H, Ar-H), 7.58 (t, *J* = 8.0 Hz, 1H, Ar-H), 7.47-7.37 (m, 5H, Ar-H), 7.31-7.29 (m, 1H, Ar-H), 7.22-7.15 (m, 3H, Ar-H), 7.08-7.06 (m, 2H, Ar-H); ¹³C NMR (125 MHz, DMSO-*d*₆) δ (ppm): 164.9, 159.5, 157.1, 156.5, 156.0, 135.5, 130.7, 130.2, 129.6, 129.2, 125.9, 123.9, 123.5, 118.8, 118.6, 116.0, 115.0, 96.3, 87.6; Anal. calcd. for C₂₅H₁₆N₄OSe: C, 64.24; H, 3.45; N, 11.99 %. Found: C, 64.26; H, 3.48; N, 12.03 %.

2-amino-4-(4-bromophenyl)-6-(phenylselanyl)pyridine-3,5-dicarbonitrile (4d): Brown

solid; Yield: 71%, m.p. 238-240 °C; IR (KBr): 3437, 3368, 3233, 3081, 2227, 1638, 1552, 1251, 751 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆ + CDCl₃) δ (ppm): 7.81 (bs, 2H, -NH₂), 7.69-7.66 (m, 2H, Ar-H), 7.60-7.52 (m, 6H, Ar-H), 7.48-7.42 (m, 2H, Ar-H); ¹³C NMR (100 MHz, DMSO-*d*₆ + CDCl₃) δ (ppm): 165.0, 159.6, 157.9, 135.5, 133.8, 130.3, 129.4, 129.1, 128.7, 128.3, 125.9, 115.7, 114.9, 96.3, 87.5; Anal. calcd. for C₁₉H₁₂N₄BrSe: C, 57.71; H, 3.22; N, 14.93 %. Found: C, 57.74; H, 3.25; N, 14.95 %.

S3

(ppm): 7.96 (s, 2H, -NH₂), 7.76 (d, *J* = 8.4 Hz, 2H, Ar-H), 7.67-7.65 (m, 2H, Ar-H), 7.48 (d, *J* = 8.4 Hz, 2H, Ar-H), 7.46-7.41 (m, 3H, Ar-H); ¹³C NMR (100 MHz, DMSO-*d*₆ + CDCl₃) δ (ppm): 165.3, 159.5, 156.5, 135.5, 132.8, 131.7, 130.3, 129.3, 128.9, 125.8, 124.2, 115.4, 114.7, 96.1, 87.2; Anal. calcd. For C₁₉H₁₁BrN₄Se: C, 50.24; H, 2.44; N, 12.34 %. Found: C, 50.27; H, 2.46; N, 12.38 %.

2-amino-4-(4-cyanophenyl)-6-(phenylselanyl)pyridine-3,5-dicarbonitrile (4e): Yellow

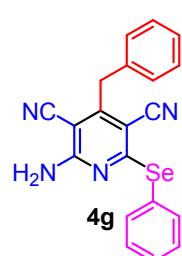
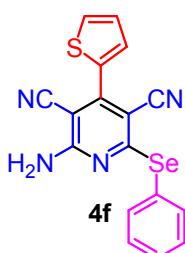
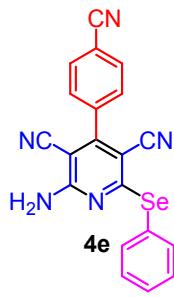
solid; Yield: 85%, m.p. 272-274 °C; IR (KBr): 3396, 3317, 3224, 3086, 2239, 2217, 1640, 1545, 1522, 1462, 1440, 1316, 1254, 1019, 998, 839, 743, 694, 665, 586 cm⁻¹; ¹H NMR (500 MHz, DMSO-*d*₆) δ (ppm): 8.07 (dd, *J* = 6.6, 1.8 Hz, 2H, Ar-H), 7.97 (bs, 2H, -NH₂), 7.78 (dd, *J* = 6.6, 1.8 Hz, 2H, Ar-H), 7.67-7.65 (m, 2H, Ar-H), 7.47-7.44 (m, 3H, Ar-H); ¹³C NMR (125 MHz, DMSO-*d*₆) δ (ppm): 165.4, 159.8, 157.0, 138.9, 135.9, 133.1, 130.1, 130.0, 129.7, 126.2, 118.6, 116.0, 115.1, 113.5, 96.5, 87.8; Anal. calcd. for C₂₀H₁₁N₅Se: C, 60.01; H, 2.77; N, 17.50 %. Found: C, 60.04; H, 2.80; N, 17.54 %.

2-amino-6-(phenylselanyl)-4-(thiophen-2-yl)pyridine-3,5-dicarbonitrile (4f): Brown solid;

Yield: 87%, m.p. 201-203 °C; IR (KBr): 3482, 3364, 3207, 3093, 3060, 2223, 2199, 1617, 1545, 1517, 1507, 1430, 1312, 1241, 1021, 982, 850, 771, 718, 681, 670 cm⁻¹; ¹H NMR (500 MHz, DMSO-*d*₆) δ (ppm): 7.95 (dd, *J* = 5.0, 1.3 Hz, 1H, Ar-H), 7.87 (bs, 2H, -NH₂), 7.67-7.65 (m, 2H, Ar-H), 7.57 (dd, 5.0, 1.3 Hz, 1H, Ar-H), 7.47-7.41 (m, 3H, Ar-H), 7.28 (dd, 5.0, 3.7 Hz, 1H, Ar-H); ¹³C NMR (125 MHz, DMSO-*d*₆) δ (ppm): 165.6, 159.8, 150.4, 135.6, 132.6, 131.4, 130.9, 129.6, 129.2, 128.0, 125.9, 116.0, 115.2, 96.1, 87.3; Anal. calcd. for C₁₇H₁₀N₄SSe: C, 53.55; H, 2.64; N, 14.69 %. Found: C, 53.58; H, 2.68; N, 14.73 %.

2-amino-4-benzyl-6-(phenylselanyl)pyridine-3,5-dicarbonitrile (4g): White solid; Yield:

67%, m.p. 197-199 °C; IR (KBr): 3471, 3357, 3221, 3089, 2967, 2845, 2226, 2189, 1623, 1521, 1351, 1247, 1019, 913, 726, 668 cm⁻¹; ¹H NMR (500 MHz, DMSO-*d*₆) δ (ppm): 7.88 (bs, 2H, -NH₂), 7.71-7.62 (m, 2H, Ar-H), 7.42-7.41 (m, 3H, Ar-H), 7.34-7.29 (m, 5H, Ar-H), 4.11 (s, 2H, -CH₂-); ¹³C NMR (125



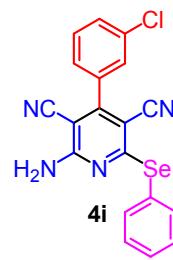
MHz, DMSO-*d*₆) δ (ppm): 165.1, 159.7, 158.0, 136.0, 135.4, 129.3, 128.9, 128.6, 128.3, 127.0, 125.9, 115.6, 114.8, 96.9, 87.9, 38.4; Anal. calcd. for C₂₀H₁₄N₄Se: C, 61.70; H, 3.62; N, 14.39 %. Found: C, 61.73; H, 3.66; N, 14.44%.

2-amino-6-(phenylselanyl)-4-p-tolylpyridine-3,5-dicarbonitrile (4h): Yellow solid; Yield:



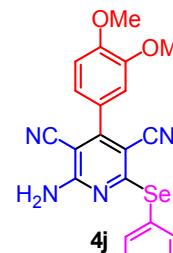
68%, m.p. 214-216 °C; IR (KBr): 3467, 3359, 3218, 3071, 2933, 2829, 2219, 1636, 1552, 1465, 1252, 1191, 1007, 841, 762 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆ + CDCl₃) δ (ppm): 7.65 (bs, 2H, -NH₂), 7.61-7.57 (m, 2H, Ar-H), 7.50-7.46 (m, 3H, Ar-H), 7.42 (d, *J* = 8.1 Hz, 2H, Ar-H), 7.37 (d, *J* = 8.1 Hz, 2H, Ar-H), 2.43 (s, 3H, -CH₃); ¹³C NMR (100 MHz, DMSO-*d*₆ + CDCl₃) δ (ppm): 166.3; 159.7, 158.3, 140.2, 134.7, 130.9, 129.4, 129.2, 129.1, 128.2, 127.3, 115.2, 115.0, 93.4, 86.9, 21.0; Anal. calcd. for C₂₀H₁₄N₄Se: C, 61.70; H, 3.62; N, 14.39 %. Found: C, 61.74; H, 3.65; N, 14.44 %.

2-amino-4-(3-chlorophenyl)-6-(phenylselanyl)pyridine-3,5-dicarbonitrile (4i): Yellow



solid; Yield: 81%, m.p. 258-260 °C; IR (KBr): 3441, 3338, 3229, 3067, 2223, 1641, 1538, 1467, 1323, 1256, 1038, 759, 721 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆ + CDCl₃) δ (ppm): 7.74 (bs, 2H, -NH₂), 7.63-7.56 (m, 5H, Ar-H), 7.50-7.47 (m, 4H, Ar-H); ¹³C NMR (100 MHz, DMSO-*d*₆ + CDCl₃) δ (ppm): 166.4, 159.5, 156.7, 135.7, 134.7, 133.5, 130.5, 130.2, 129.5, 129.2, 128.1, 127.1, 127.0, 114.8, 114.6, 93.3, 87.0; Anal. calcd. for C₁₉H₁₁ClN₄Se: C, 55.70; H, 2.71; N, 13.67 %. Found: C, 55.74; H, 2.75; N, 13.72%.

2-amino-4-(3,4-dimethoxyphenyl)-6-(phenylselanyl)pyridine-3,5-dicarbonitrile (4j):



White solid; Yield: 86%, m.p. 232-234°C; IR (KBr): 3438, 3328, 3219, 3088, 2978, 2837, 2826, 2221, 2218, 1640, 1617, 1538, 1423, 1276, 1249, 1191, 1027, 838, 827, 752 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆ + CDCl₃) δ (ppm): 7.61 (bs, 2H, -NH₂), 7.60-7.56 (m, 2H, Ar-H), 7.50-7.47 (m, 3H, Ar-H), 7.15 (s, 1H, Ar-H), 7.13-7.11 (bs, 2H, Ar-H), 3.88 (s, 3H, -OCH₃), 3.84 (s, 3H, -OCH₃); ¹³C NMR (100 MHz, DMSO-*d*₆ + CDCl₃) δ (ppm): 166.3, 159.8, 158.0, 150.4, 148.3, 134.7, 129.4, 129.2, 127.3, 125.7, 121.5, 115.4, 115.3, 112.1, 111.3, 93.4, 86.9, 55.6, 55.5; Anal. calcd. for C₂₁H₁₆N₄O₂Se: C, 57.94; H, 3.70; N, 12.87 %. Found: C, 57.98; H, 3.73; N, 12.92%.

2-amino-4-(3,4-dichlorophenyl)-6-(phenylselanyl)pyridine-3,5-dicarbonitrile (4k): White

solid; Yield: 78%, m.p. 197-199 °C; IR (KBr): 3438, 3324, 3217, 3059, 2221, 1652, 1529, 1451, 1329, 1242, 1153, 1033, 762, 718 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆ + CDCl₃) δ (ppm): 7.78 (bs, 2H, -NH₂), 7.75 (s, 1H, Ar-H), 7.73-7.72 (m, 1H, Ar-H), 7.59-7.55 (m, 3H, Ar-H), 7.51-7.47 (m, 3H, Ar-H); ¹³C NMR (100 MHz, DMSO-*d*₆ + CDCl₃) δ (ppm): 166.8, 159.5, 155.4, 134.7, 133.9, 133.7, 132.1, 130.8, 130.1, 129.3, 129.0, 128.1, 127.0, 114.6, 114.5, 93.2, 86.7; Anal. calcd. for C₁₉H₁₀N₄Se: C, 51.38; H, 2.27; N, 12.61 %. Found: C, 51.41; H, 2.31; N, 12.66 %.

2-amino-4-(2,6-dichlorophenyl)-6-(phenylselanyl)-1,4-dihydropyridine-3,5-

dicarbonitrile (5a): White solid; Yield: 87%, m.p. 282-284 °C; IR (KBr): 3457, 3362, 3241,

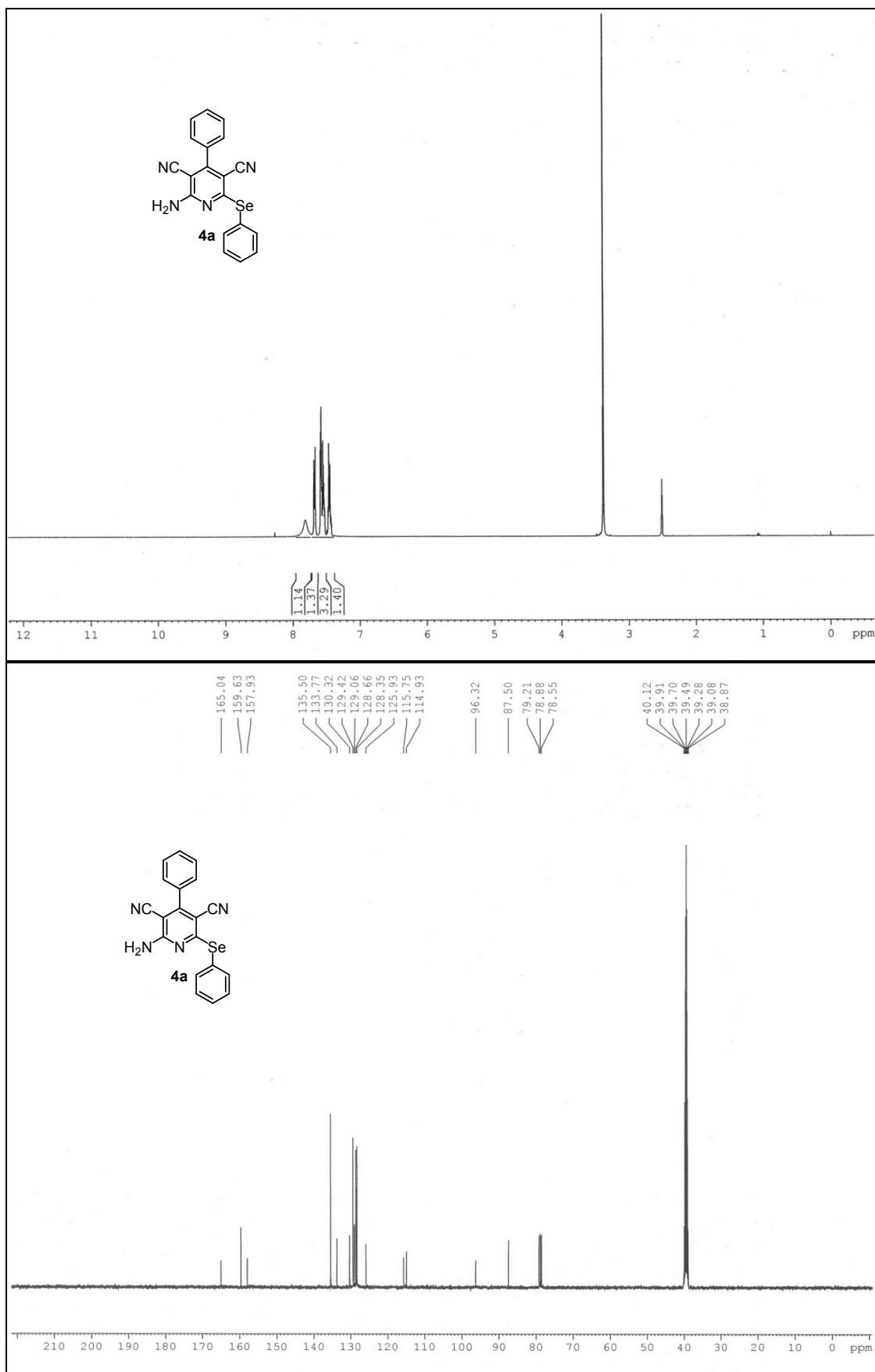
3077, 2962, 2870, 2224, 2183, 1652, 1614, 1507, 1437, 1248, 1107, 1009, 752, 746, 685, 557 cm⁻¹; ¹H NMR (500 MHz, DMSO-*d*₆) δ (ppm): 9.21 (s, 1H, -NH-), 7.61-7.59 (m, 2H, Ar-H), 7.51-7.49 (m, 2H, Ar-H), 7.42-7.41(m, 3H, Ar-H), 7.35-7.33 (m, 1H, Ar-H), 5.97 (s, 2H, -NH₂), 5.59 (s, 1H, -CH-); ¹³C NMR (125 MHz, DMSO-*d*₆) δ (ppm): 151.4, 138.8, 135.3, 132.7, 130.2, 129.9, 128.7, 126.9, 119.9, 118.3, 89.2, 52.2, 38.0; Anal. calcd. for C₁₉H₁₂Cl₂N₄Se: C, 51.14; H, 2.71; N, 12.56 %. Found: C, 51.17; H, 2.75; N, 12.60 %.

2-amino-4-(2,6-dimethoxyphenyl)-6-(phenylselanyl)-1,4-dihydropyridine-3,5-

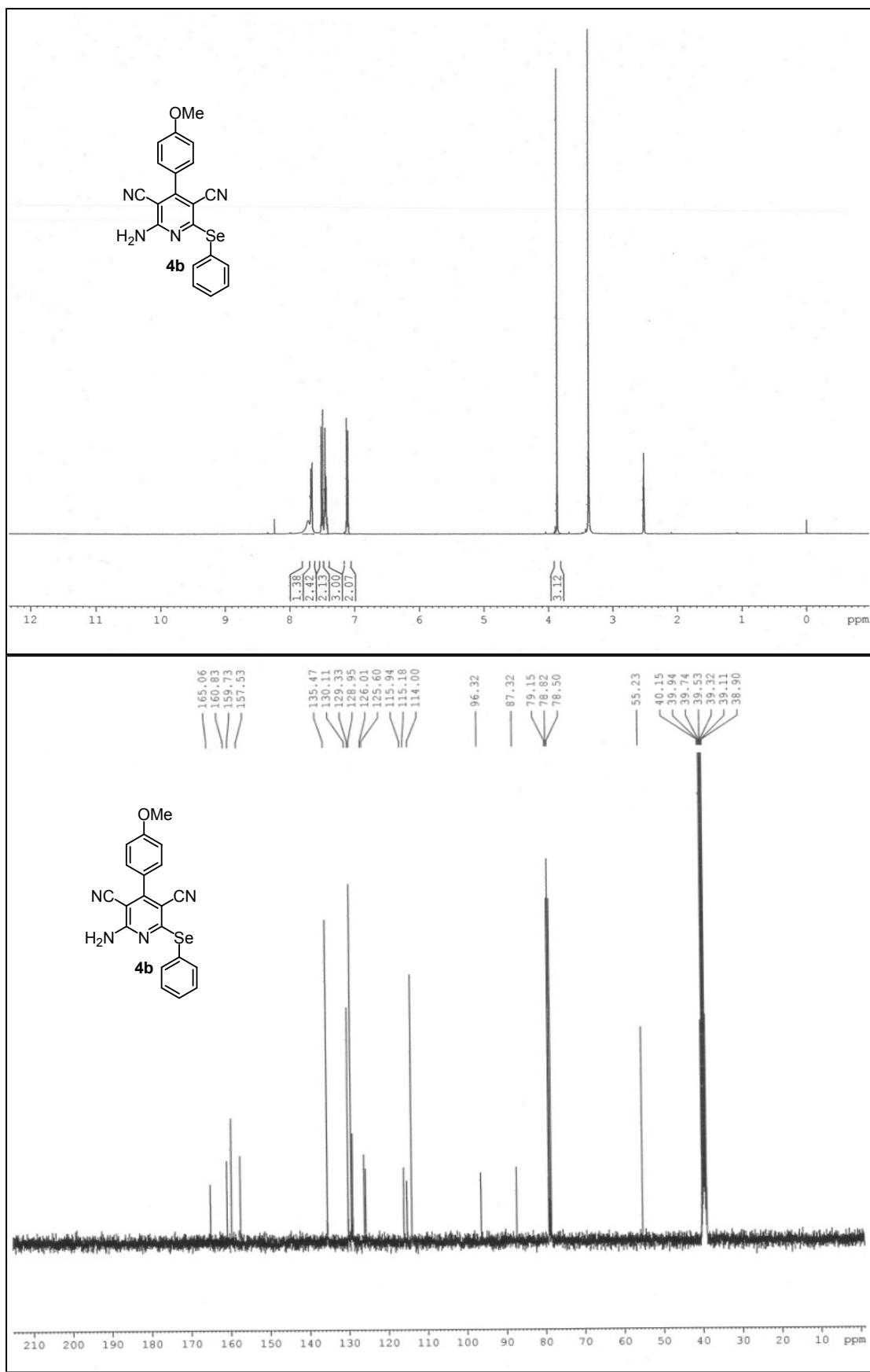
dicarbonitrile (5b): White solid; Yield: 90%, m.p. 224-226 °C; IR (KBr): 3437, 3337, 3228,

3072, 3018, 2978, 2937, 2883, 2732, 2217, 2192, 1662, 1651, 1607, 1487, 1340, 1238, 1107, 1041, 773, 749, 662, 561 cm⁻¹; (400 MHz, DMSO-*d*₆ + CDCl₃) δ (ppm): 8.99 (s, 1H, -NH-), 7.46-7.43 (m, 4H, Ar-H), 7.38-7.34 (m, 1H, Ar-H), 7.23 (t, *J* = 8.4 Hz, 1H, Ar-H), 6.68 (d, *J* = 8.4, 2H, Ar-H), 5.62 (s, 2H, -NH₂), 5.08 (s, 1H, -CH-), 3.74 (s, 6H, -OCH₃); ¹³C NMR (125 MHz, DMSO-*d*₆ + CDCl₃) δ (ppm): 158.4, 151.5, 140.4, 131.2, 129.6, 129.3, 128.9, 127.8, 120.9, 118.5, 118.4, 104.7, 91.5, 56.1, 53.6, 31.3; Anal. calcd. for C₂₁H₁₈N₄O₂Se: C, 57.67; H, 4.15; N, 12.81 %. Found: C, 57.69; H, 4.19; N, 12.86 %.

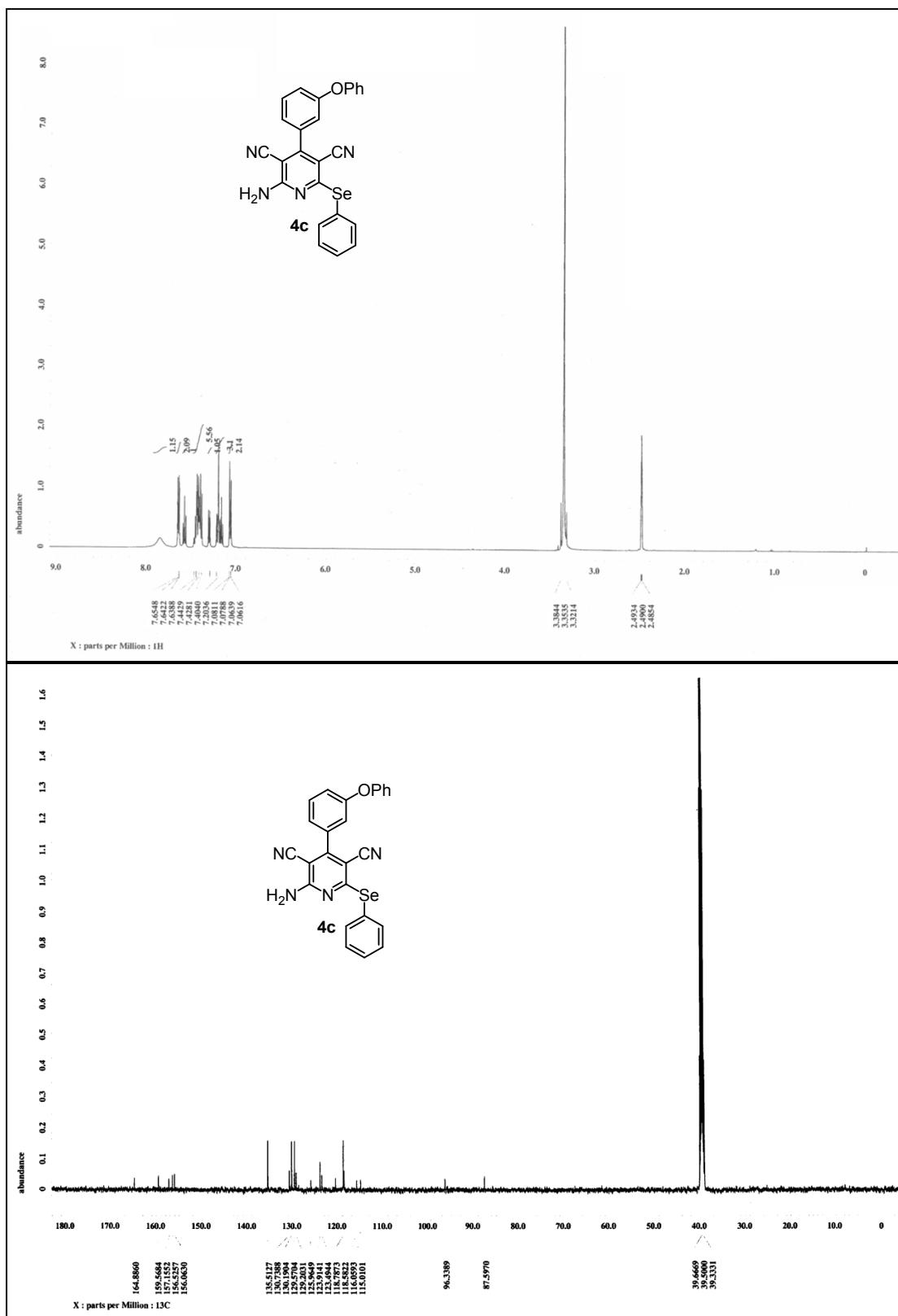
¹H and ¹³C NMR spectra of 4a



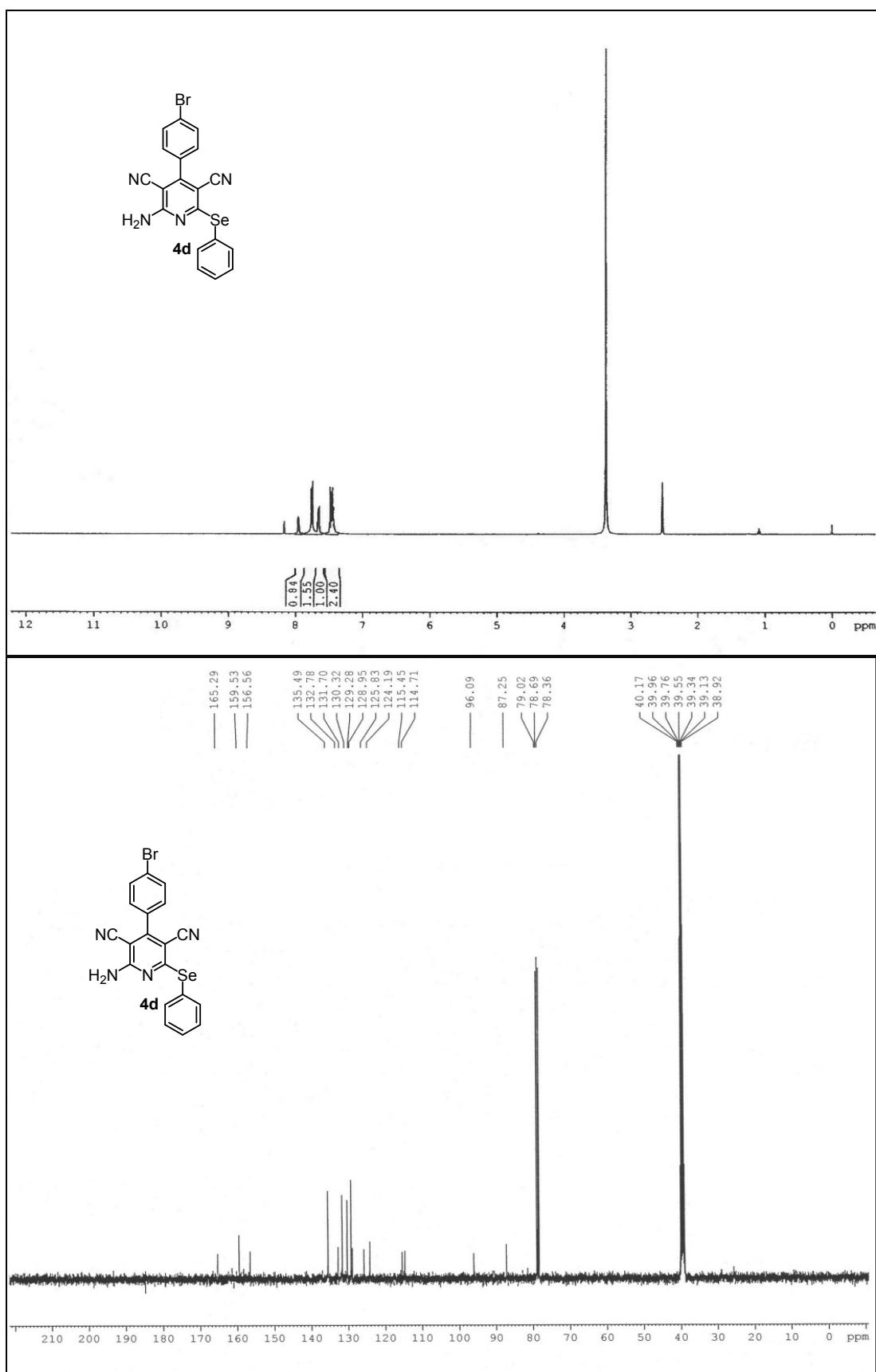
¹H and ¹³C NMR spectra of 4b



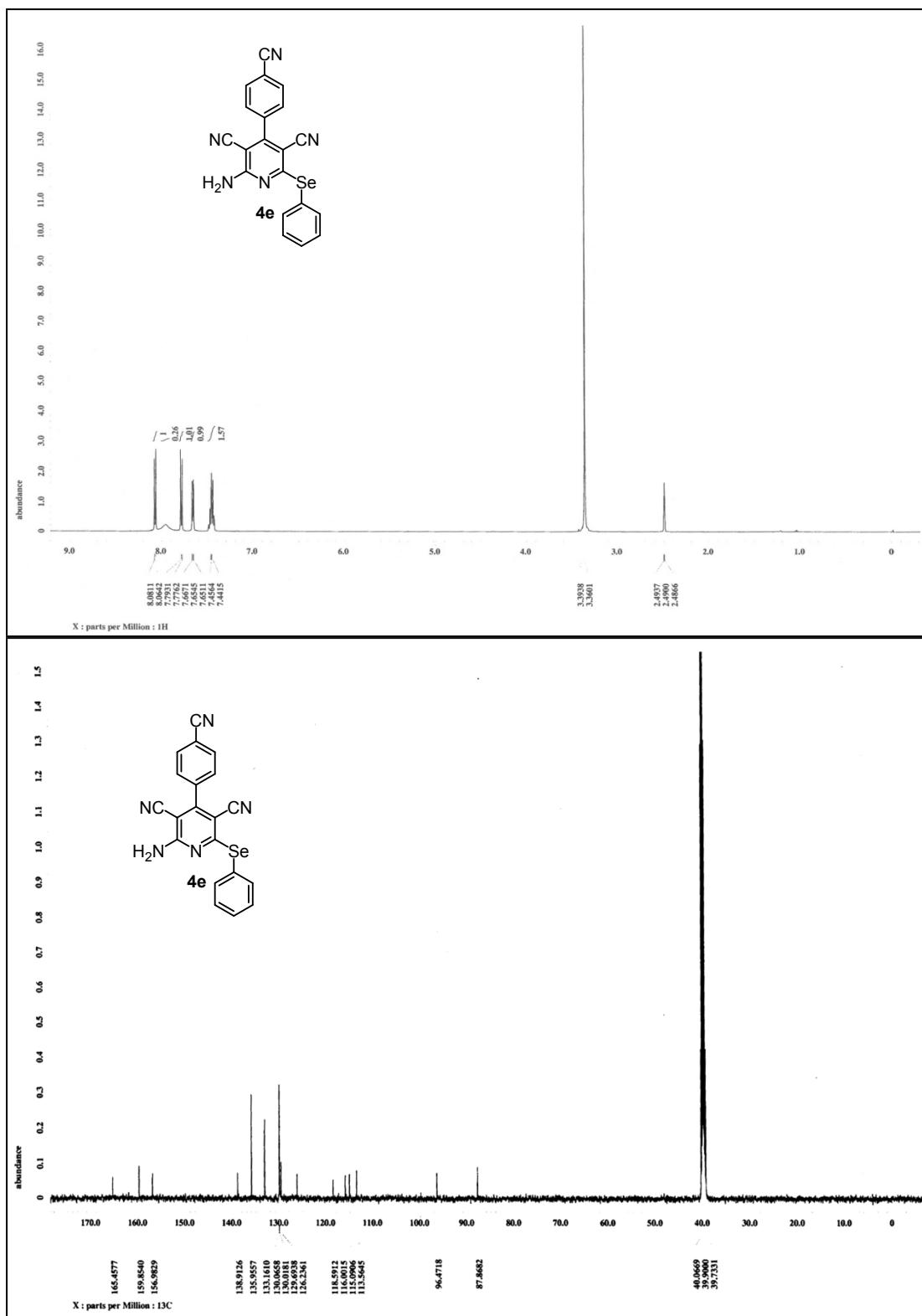
¹H and ¹³C NMR spectra of 4c



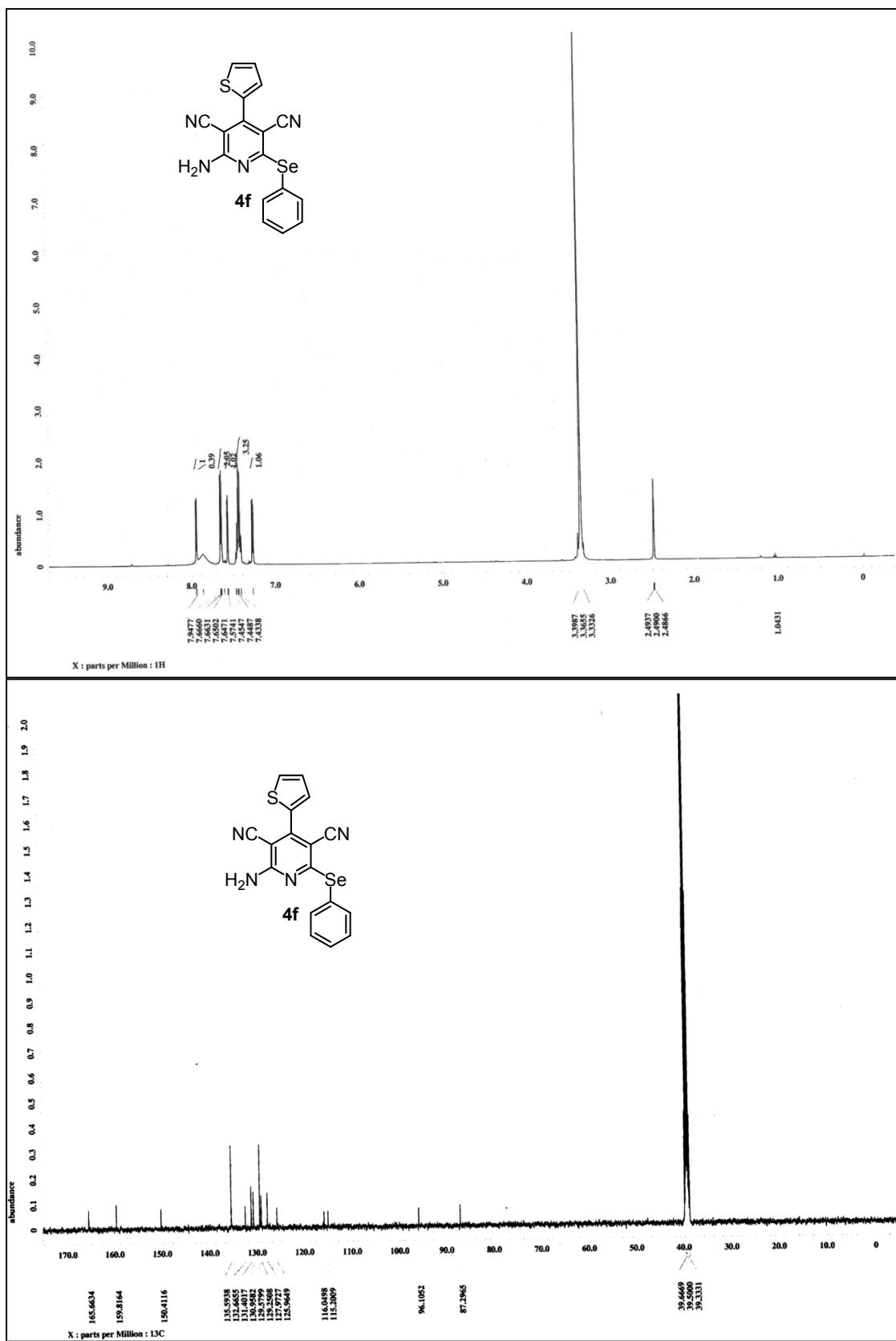
¹H and ¹³C NMR spectra of 4d



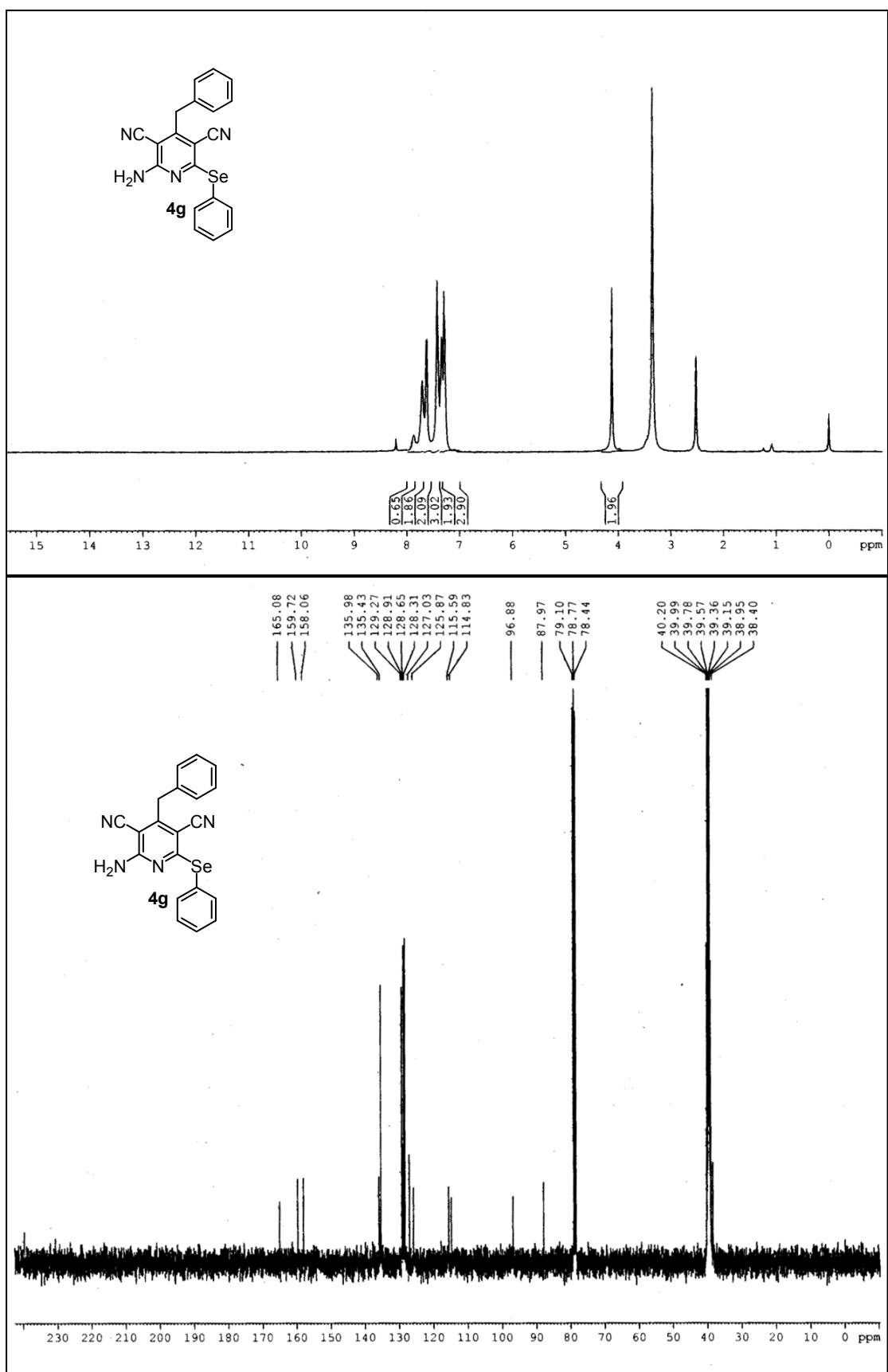
¹H and ¹³C NMR spectra of 4e



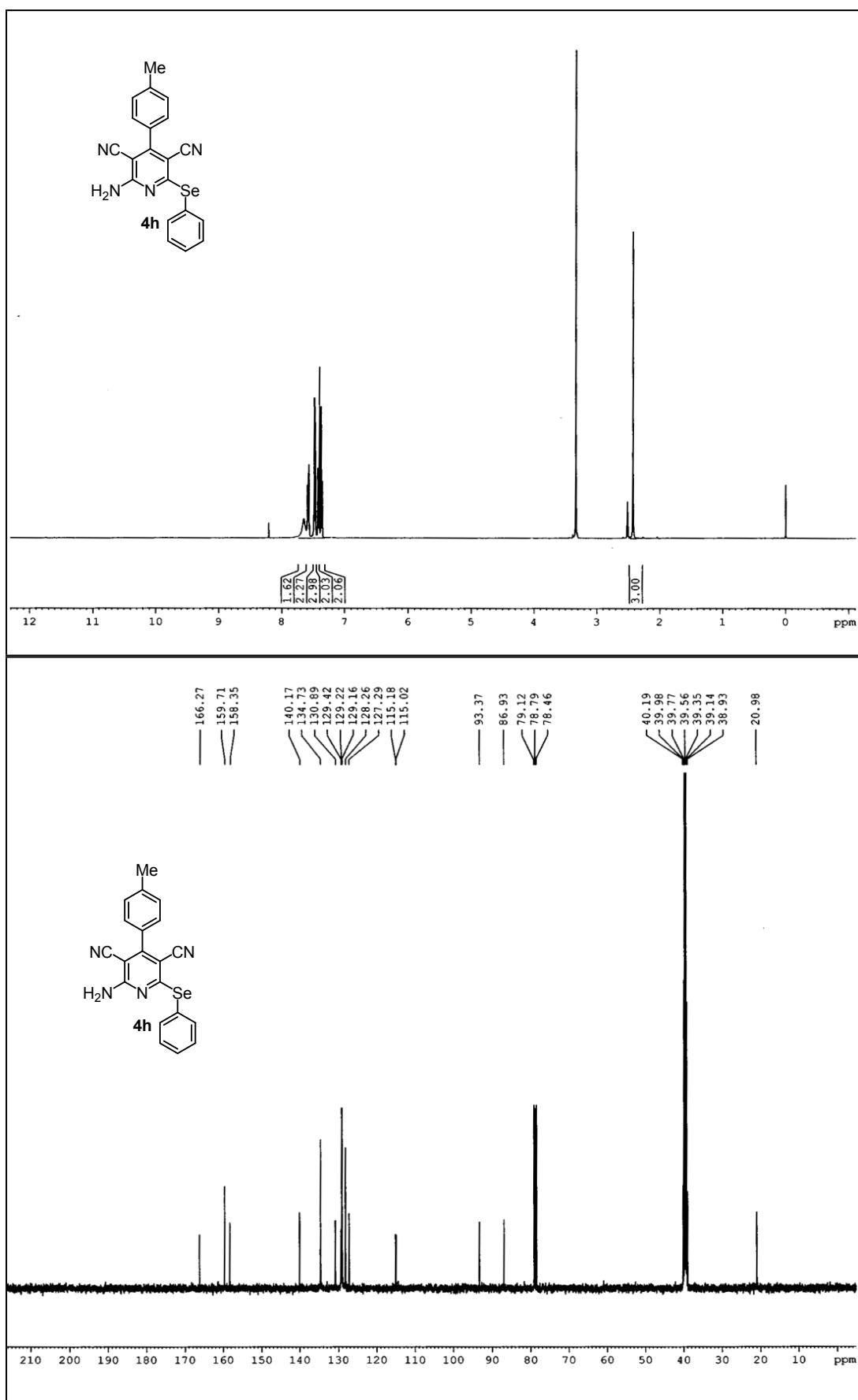
¹H and ¹³C NMR spectra of 4f



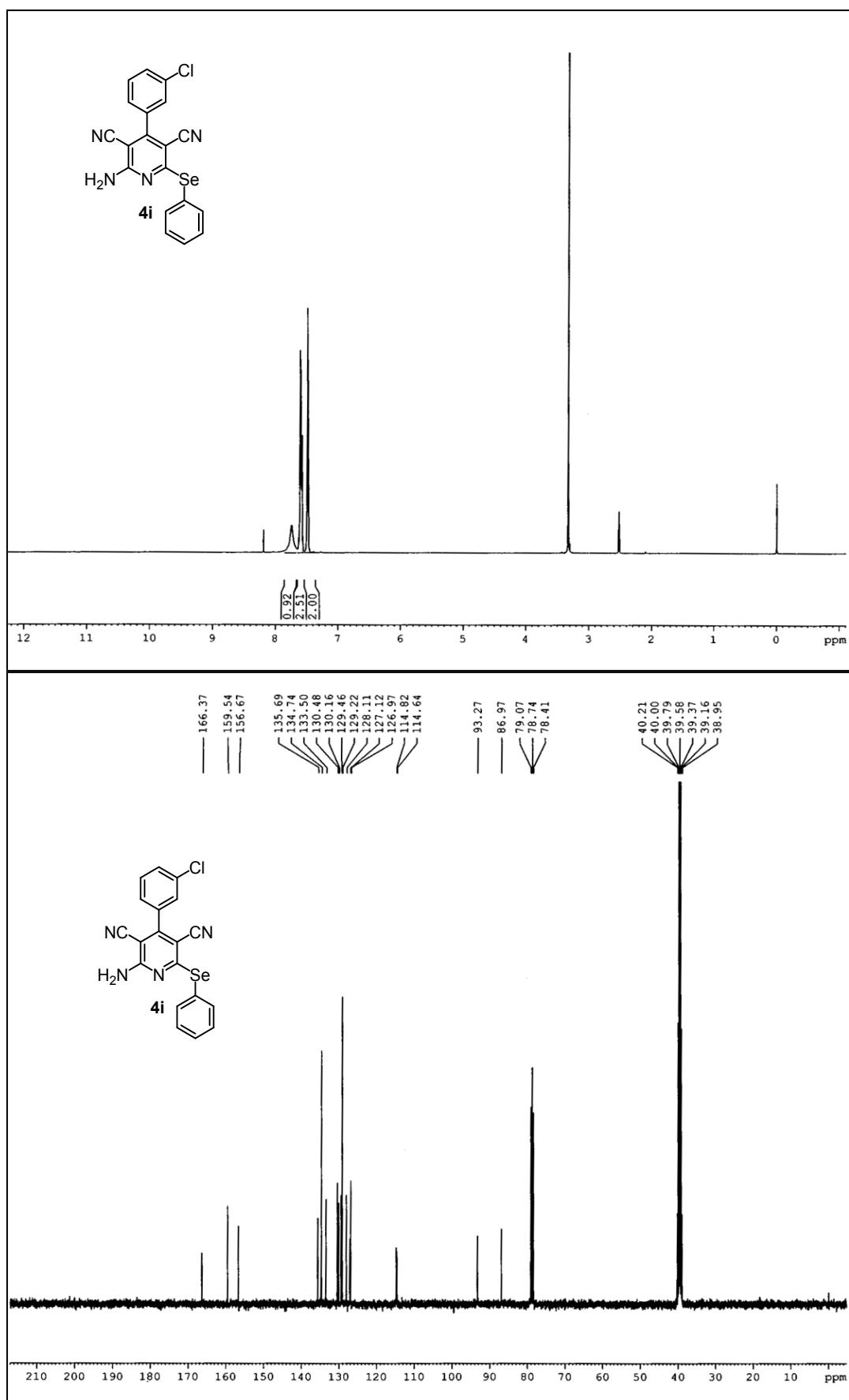
¹H and ¹³C NMR spectra of 4g



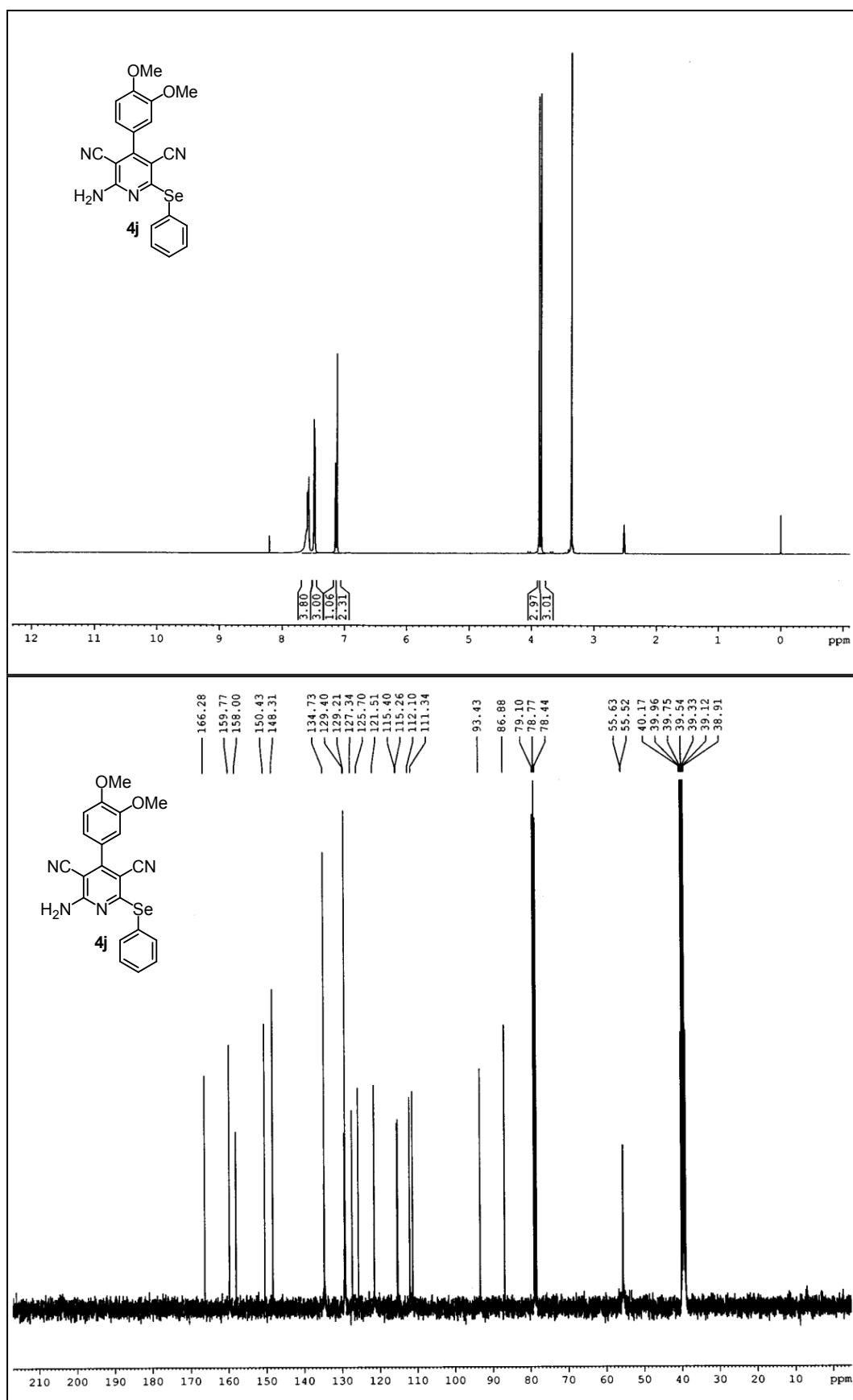
¹H and ¹³C NMR spectra of 4h



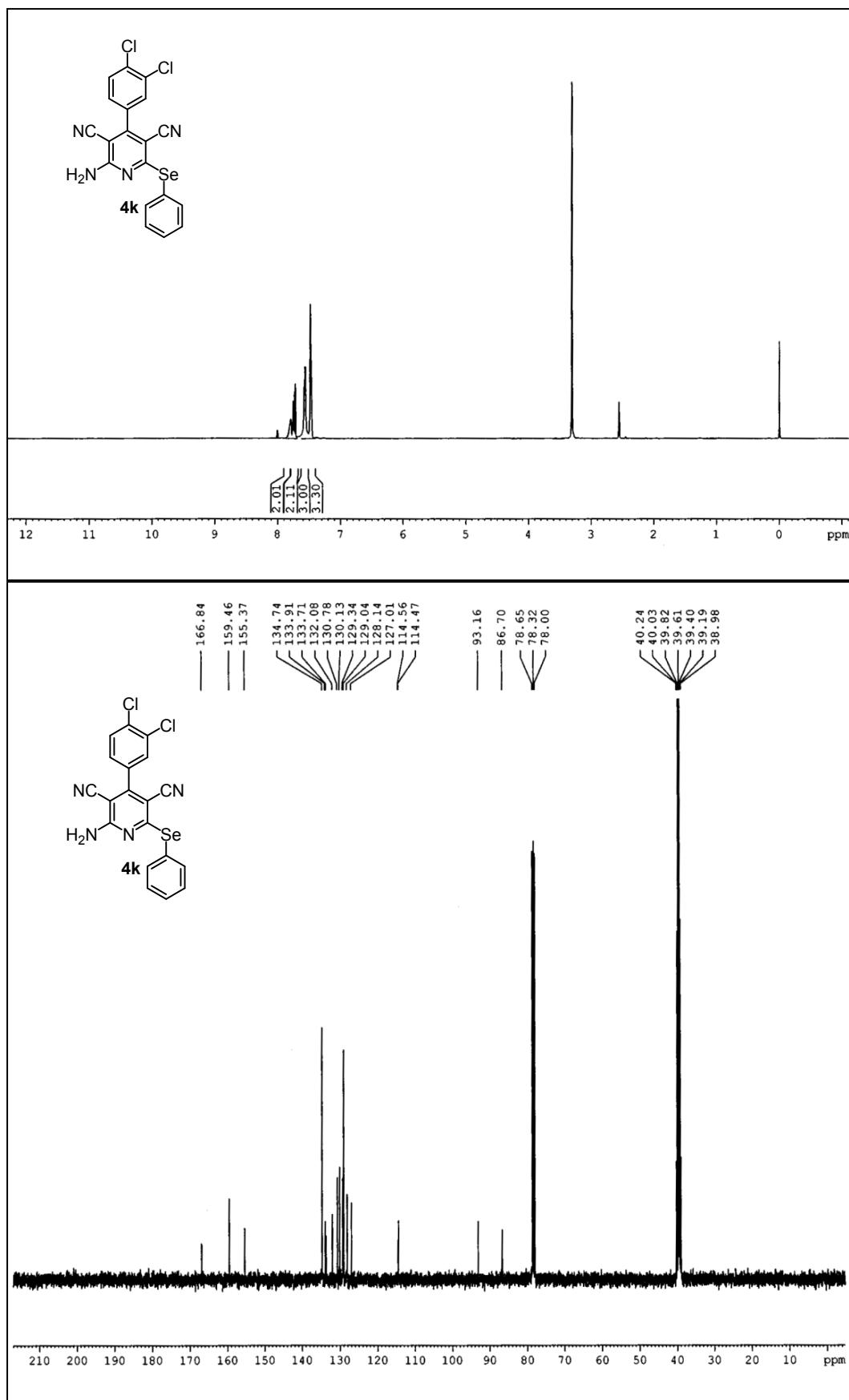
¹H and ¹³C NMR spectra of 4i



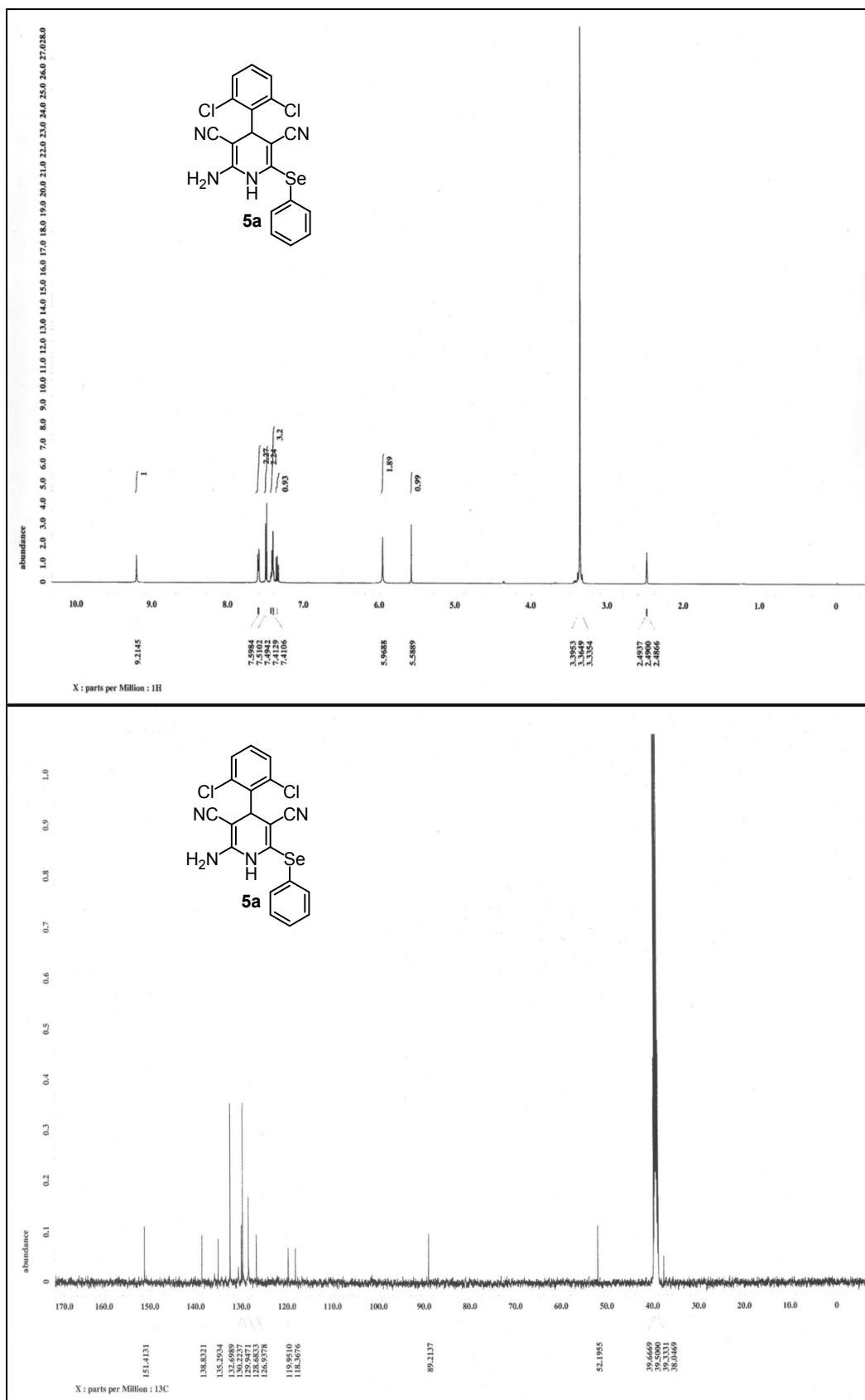
¹H and ¹³C NMR spectra of 4j



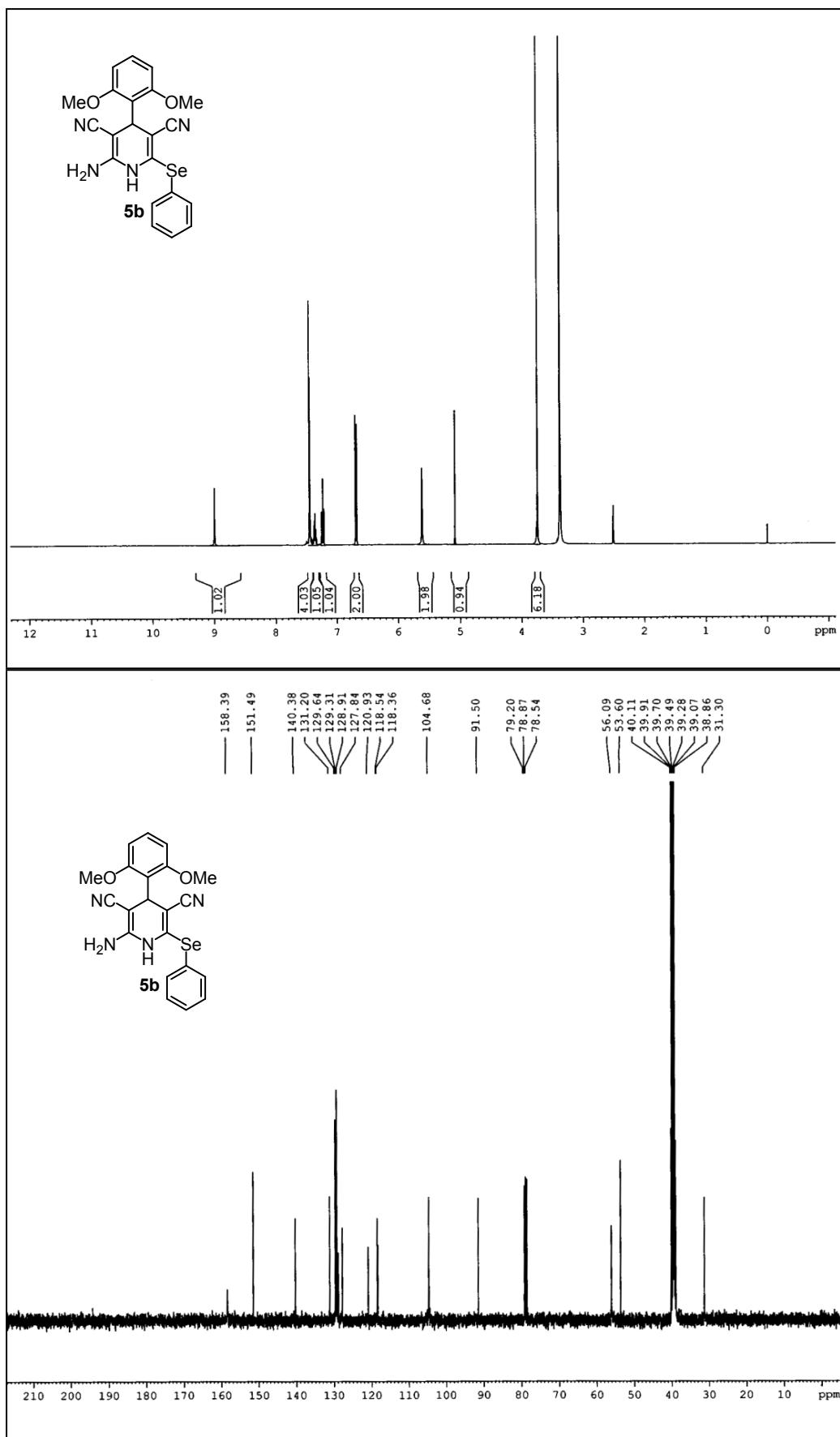
¹H and ¹³C NMR spectra of 4k



¹H and ¹³C NMR spectra of 5a



¹H and ¹³C NMR spectra of 5b



Crystallographic Informations

Table 3. Crystallographic Data for compound **4b**

Identification code	4b
empirical formula	C ₂₀ H ₁₄ N ₄ OSe
fw	405.31
cryst color	Yellow
cryst size (mm)	0.29×0.20×0.15
cryst syst	Monoclinic
space group	P21/n
a (Å)	7.9301(5)
b (Å)	18.6114(12)
c (Å)	11.7983(8)
α (deg)	90.00
β (deg)	96.431(2)
γ (deg)	90.00
V (Å ³)	1730.4(2)
Dcalcd (mg m ⁻³)	1.556
Z	4
μ(Mo-Kα) (mm ⁻¹)	2.187
F(000)	816
2θ range	2.79 - 25.49
reflns measd	3230
indep refln	2728 [R(int) = 0.0491]
reflns obsd [I > 2σ(I)]	3230
no. of param	243
final R1, wR2 (obsd data)	R1 = 0.0320, wR2 = 0.0743
GOF (obsd data)	1.037
CCDC no.	1004592

Table 4. Hydrogen bonds distances and angles for the compounds **4b** (Å, °)

D–H···A	D–H/ Å	H···A/ Å	D···A/ Å	D–H···A/ (°)
N4–H1N4···N3	0.82(2)	2.26(2)	3.056(3)	162(2)
N4–H2N4···O1	0.84(4)	2.45(3)	3.146(3)	141(3)
C19–H19···N1	0.93(0)	2.49(0)	3.342(3)	153(0)
C20–H20A···N3	0.96(0)	2.46(0)	3.344(3)	154(0)

Table 5. Bond distances (in Å) and bond angles (in °) of **4b**.

Bond distances (Å)					
C1–C2	1.382(4)	C1–C6	1.390(3)	C14–C15	1.393(3)
C1–Se1	1.913(2)	C2–C3	1.390(4)	C15–C16	1.379(3)
C3–C4	1.377(4)	C4–C5	1.391(4)	C17–O1	1.367(3)
C5–C6	1.377(3)	C7–N1	1.325(3)	C18–C19	1.380(3)
C7–C8	1.402(3)	C7–Se1	1.909(2)	C14–C19	1.396(3)
C8–C9	1.406(3)	C8–C12	1.438(3)	C16–C17	1.390(3)

C9–C10	1.395(3)	C9–C14	1.477(3)	C17–C18	1.381(3)
C10–C11	1.420(3)	C10–C13	1.430(3)	C20–O1	1.436(3)
C11–N4	1.341(3)	C11–N1	1.344(3)	C13–N3	1.147(3)
C12–N2	1.145(3)				
Bond angles (°)					
C1–C2–C3	119.5(2)	C2–C1–Se1	117.62(19)	N1–C7–C8	124.4(2)
C2–C1–C6	120.4(2)	C17–O1–C20	115.84(19)	C8–C7–Se1	117.68(17)
C6–C1–Se1	121.63(19)	C3–C4–C5	119.2(2)	C7–C8–C12	119.1(2)
C4–C3–C2	120.6(2)	C5–C6–C1	119.3(2)	C10–C9–C8	116.7(2)
C6–C5–C4	120.9(2)	N1–C7–Se1	117.82(18)	C8–C9–C14	123.0(2)
C9–C10–C13	121.8(2)	C7–C8–C9	118.8(2)	C11–C10–C13	117.9(2)
N4–C11–N1	116.3(2)	C9–C8–C12	122.1(2)	N4–C11–C10	121.8(2)
N1–C11–C10	121.9(2)	C10–C9–C14	120.3(2)	N2–C12–C8	177.5(3)
N3–C13–C10	175.8(3)	C9–C10–C11	120.3(2)	C15–C14–C19	118.1(2)
C15–C14–C9	122.5(2)	C19–C14–C9	119.4(2)	C19–C18–C17	119.8(2)
C16–C15–C14	121.0(2)	C15–C16–C17	119.9(2)	C7–N1–C11	117.7(2)
O1–C17–C18	123.9(2)	O1–C17–C16	116.2(2)	C7–Se1–C1	101.56(10)
C18–C17–C16	119.9(2)	C18–C19–C14	121.2(2)		

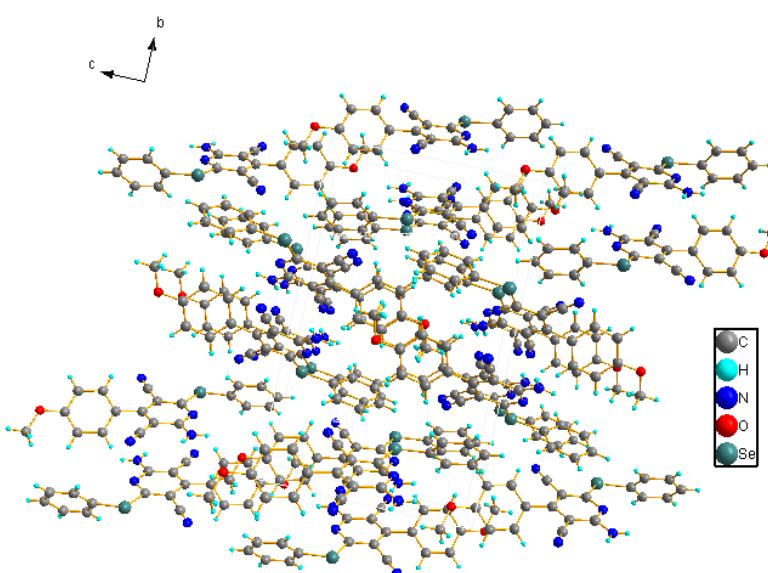


Fig 4. The 2D layer structure of **4b**

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