SUPPORTING INFORMATION

Construction of 2*H*-1,4-selenazin-3(4*H*)-one framework via cyclization of pyrazole derivatives bearing chloroacetamide and selenocyanate fragments

Tatiana A. Kudryavtseva, Ekaterina N. Kudryavtseva and Boris V. Lichitsky*

N.D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Leninsky Pr. 47, Moscow 119991, Russian Federation

1. General procedures 2
2. Copies of NMR and HRMS spectra for compounds **3** 5
3. Copies of NMR and HRMS spectra for compound **4** 23
4. Copies of NMR and HRMS spectra for compound **5** 56
5. Copies of NMR and HRMS spectra for compound **6** 58
6. Copies of NMR and HRMS spectra for compounds **7** 88
7. Copies of NMR and HRMS spectra for compound **8** 91
8. Copies of NMR and HRMS spectra for compound **9** 94
9. Copies of NMR and HRMS spectra for compound **10** 96
10. Copies of NMR and HRMS spectra for compound **11** 99
11. Copies of NMR and HRMS spectra for compound **14** 102
12. Copies of NMR and HRMS spectra for compound **15** 105
13. Copies of NMR and HRMS spectra for compound **17** 108
14. Copies of NMR and HRMS spectra for compound **19** 114
15. Copies of NMR and HRMS spectra for compound **20** 116
16. Copies of NMR and HRMS spectra for compound **21** 119
17. X-ray crystallographic data and refinement details 122

General Procedure for the Synthesis of Compounds 3a-k and 13

A mixture of 5-aminopyrazole (4 mmol) and corresponding acylating agent (6 mmol) was stirred at room temperature in DMF (8 mL) for 3 h. Then, water (40 mL) was added. For compounds 3a-c,f-i,k the precipitated product was filtered off, washed with water (3 × 30 mL) and air dried. For compounds 3d,e,j and 13 the target product was obtained by extraction with ethyl acetate (3 × 20 mL) and washed with water (3 × 20 mL). Evaporation of the solvent afforded amides 3d,e,j and 13 which were used further without additional purification.

Synthesis of 2-chloro-*N*-(1-(2-chloroacetyl)-3-methyl-1*H*-pyrazol-5-yl)acetamide 5

A mixture of 3-methyl-1*H*-pyrazol-5-amine (4 mmol, 0.39 g) and chloroacetyl chloride (12 mmol, 1.36 g) was stirred at room temperature in DMF (8 mL) for 3 h. Then, water (40 mL) was added. The precipitated product 5 was filtered off, washed with water (3 × 30 mL) and air dried.

Synthesis of 2-chloro-*N*-(3-methyl-1*H*-pyrazol-5-yl)acetamide 3l

A solution of amide **5** (2 mmol, 0.50 g) in MeOH (10 mL) was refluxed for 3 h. Then, evaporation of the solvent afforded pure target product 3l.

Synthesis of 2-bromo-2-methyl-*N*-(3-methyl-1-phenyl-1*H*-pyrazol-5-yl)propanamide 9

A mixture of 5-aminopyrazole **1a** (4 mmol, 0.69 g) and 2-bromo-2-methylpropanoyl bromide (6 mmol, 1.38 g) was stirred at room temperature in MeCN (8 mL) for 24 h. Then, water (40 mL) and NaHCO3 (24 mmol, 2.00 g) were added and the reaction mixture was stirred at room temperature for 8 h. Then, the precipitated product Na was filtered off, washed with water (3 × 30 mL) and air dried.

General Procedure for the Synthesis of selenocyanates 4, 10 and 14

A mixture of malononitrile (3 mmol, 0.20 g), SeO_2 (6 mmol, 0.67 g) in DMF (2 mL) was stirred at room temperature for 0.25 h. Then, corresponding amide 3, 9 or 13 (2 mmol) was added to the mixture and the resulted solution was stirred for 2 h. After this, 20 mL of water was added and the obtained mixture was stirred for 2 h. The precipitated product was filtered off, washed with water (3 × 20 mL) and air dried.

General Procedure for the Synthesis of pyrazolo[4,3-*b*][1,4]selenazin-6(5*H*)-ones 6

A mixture of corresponding selenocyanate **4** (0.4 mmol) and sodium cyanoborohydride (4 mmol, 0.25 g) in MeOH (10 mL) was stirred at room temperature for 48 h. Then, the solvent was evaporated and the residue was stirred in water (5 mL) for 1 h (in the case of compound 4f conc. HCl (0.1 mL) was added

to the water). The precipitated product was filtered off, washed with water (3 × 20 mL) and air dried.

Synthesis of compound 7

A mixture of selenocyanate **4g** (0.4 mmol, 0.16 g) and sodium cyanoborohydride (4 mmol, 0.25 g) in MeOH (10 mL) was stirred at room temperature for 48 h. Then, the reaction mixture was evaporated and the residue was stirred in water (5 mL) for 1 h. The precipitated diselenide was filtered off, washed with water (3 × 20 mL) and air dried.

Synthesis of compound 11

A mixture of selenocyanate **10** (0.4 mmol, 0.17 g) and sodium cyanoborohydride (4 mmol, 0.25 g) in MeOH (10 mL) was stirred at room temperature for 48 h. Then, the reaction mixture was evaporated and the residue was stirred in water (5 mL) for 1 h. The precipitated diselenide was filtered off, washed with water (3 × 20 mL) and air dried.

Synthesis of compound 15

A mixture of selenocyanate **14** (0.4 mmol, 0.15 g) and sodium cyanoborohydride (4 mmol, 0.25 g) in MeOH (10 mL) was stirred at room temperature for 48 h. Then, the reaction mixture was evaporated and the residue was stirred in water (5 mL) for 1 h. The precipitated diselenide was filtered off, washed with water (3 × 20 mL) and air dried.

Synthesis of selenoether 17a

A mixture of selenocyanate **10** (0.4 mmol, 0.15 g), iodomethane (4 mmol, 0.57 g) and sodium cyanoborohydride (4 mmol, 0.25 g) in MeOH (10 mL) was stirred at room temperature for 48 h. Then, the reaction mixture was evaporated and the residue was stirred in water (5 mL) for 1 h. The precipitated product was filtered off, washed with water (3 × 20 mL) and air dried.

Synthesis of selenoether 17b

A mixture of selenocyanate **10** (0.4 mmol, 0.15 g), chloroacetonitrile (4 mmol, 0.30 g) and sodium cyanoborohydride (4 mmol, 0.25 g) in MeOH (10 mL) was stirred at room temperature for 48 h. Then, the reaction mixture was evaporated and the residue was stirred in water (5 mL) for 1 h. The precipitated product was filtered off, washed with water (3 × 20 mL) and air dried.

Synthesis of compound 19

A mixture of oxalate of aminothiophene **18** (4 mmol, 0.97 g) and chloroacetyl chloride (6 mmol, 0.68 g) in DMF (8 mL) was stirred at room temperature for 3 h.

Then, water (40 mL) was added. The precipitated product Na was filtered off, washed with water (3 × 30 mL) and air dried.

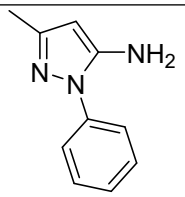
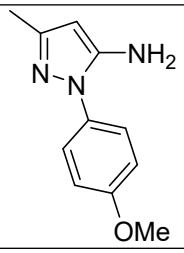
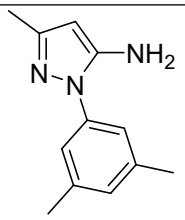
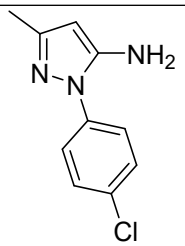
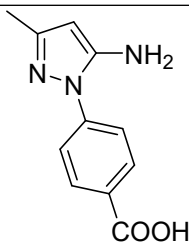
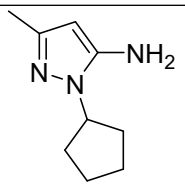
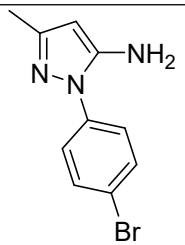
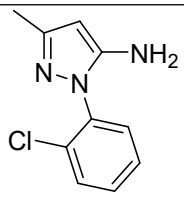
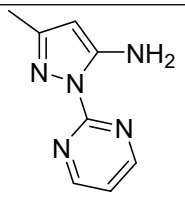
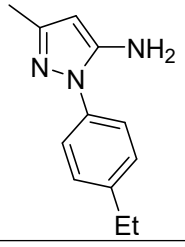
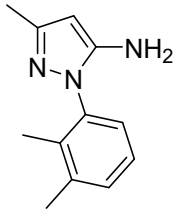
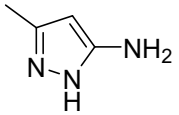
Synthesis of compound 20

A mixture of malononitrile (3 mmol, 0.20 g) and SeO_2 (6 mmol, 0.67 g) in DMF (2 mL) was stirred at room temperature for 0.25 h. Then, chloroacetamide 19 (2 mmol, 0.46 g) was added to the mixture and the resulted solution was stirred for 2 h. After this, 20 mL of water was added and the obtained mixture was stirred for 2 h. The precipitated product was filtered off, washed with water (3 × 20 ml) and air dried.

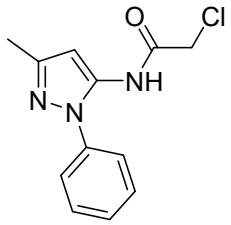
Synthesis of compound 21

A mixture of selenocyanate **20** (0.4 mmol, 0.13 g) and sodium cyanoborohydride (4 mmol, 0.25 g) in MeOH (10 mL) was stirred at room temperature for 48 h. Then, the reaction mixture was evaporated and the residue was stirred in water (5 mL) for 1 h. The precipitated product was filtered off, washed with water (3 × 20 mL) and air dried.

Table 1. Structures of the starting 5-aminopyrazoles

1a		**1e**		**1i**	
1b		**1f**		**1j**	
1c		**1g**		**1k**	
1d		**1h**		**1l**	

NMR and HRMS spectra for compounds 3



2-Chloro-N-(3-methyl-1-phenyl-1H-pyrazol-5-yl)acetamide, ***3a***

White powder, m.p. 166-168°C, yield 75% (0.75 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.26 (s, 1H), 7.52 – 7.45 (m, 4H), 7.40 – 7.34 (m, 1H), 6.26 (s, 1H), 4.23 (s, 2H), 2.21 (s, 3H). ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 165.32, 148.10, 138.48, 135.47, 129.21, 127.23, 123.47, 102.13, 42.64, 13.77. HRMS (ESI-TOF): m/z $[M+H]^+$: calcd for $[C_{12}H_{13}ClN_3O]^+$: 250.0742; found: 250.0745.

Figure-1: ^{1}H NMR spectrum (300 MHz) of **3a** in DMSO-d_6

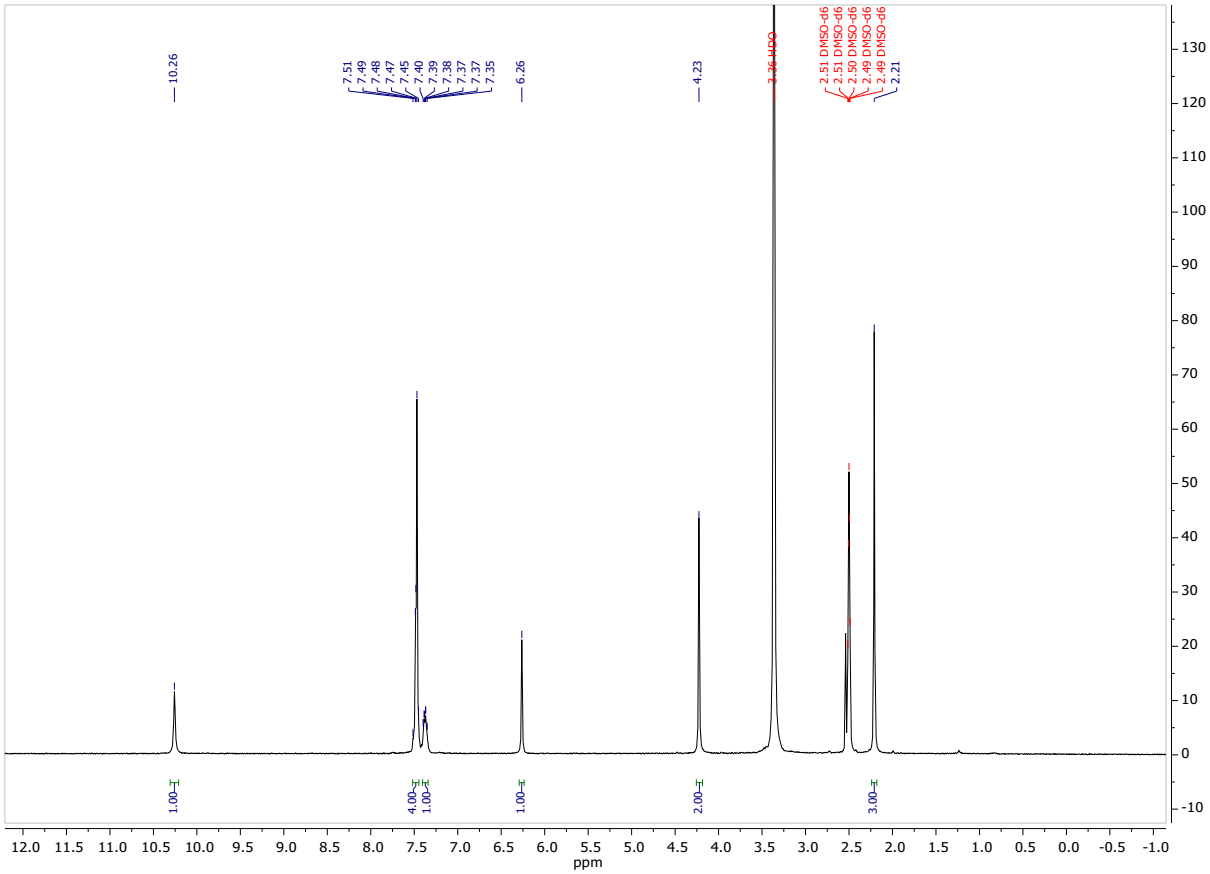


Figure-2: ^{13}C NMR spectrum (76 MHz) of **3a** in DMSO-d_6

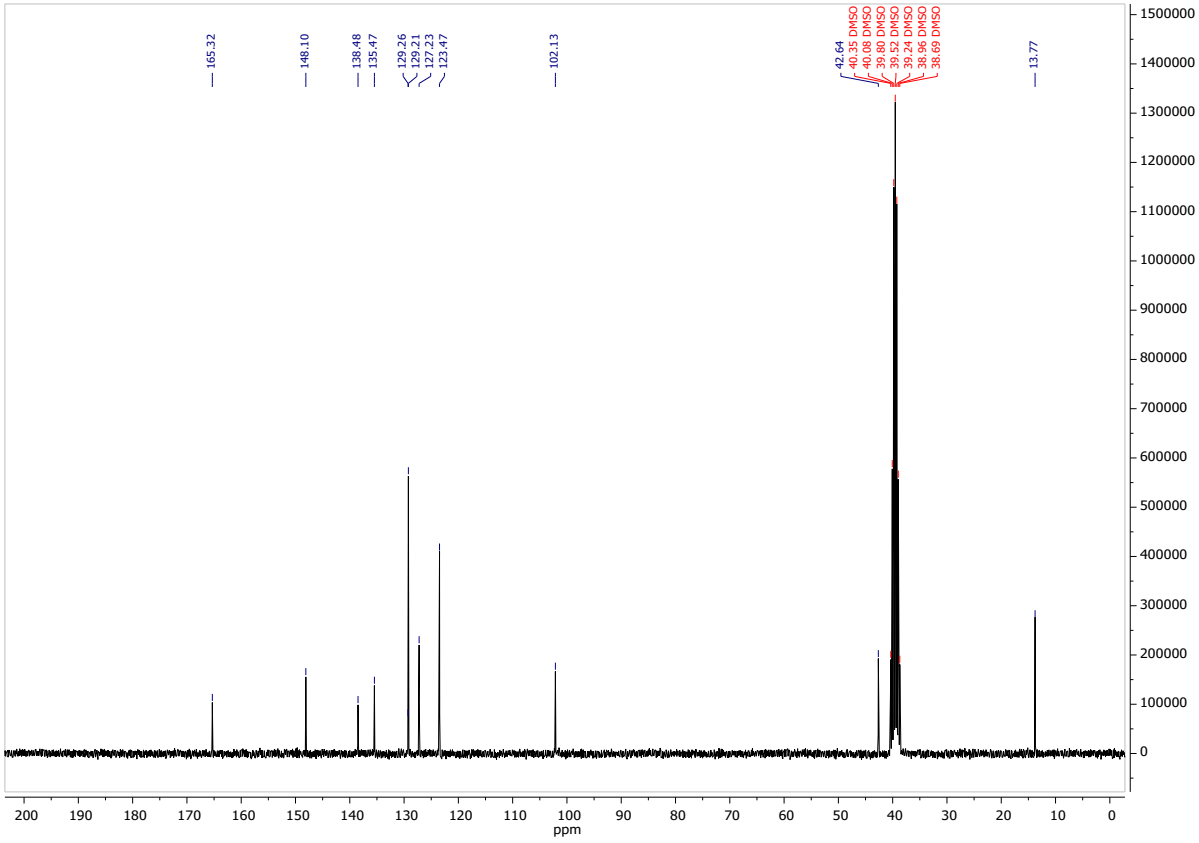
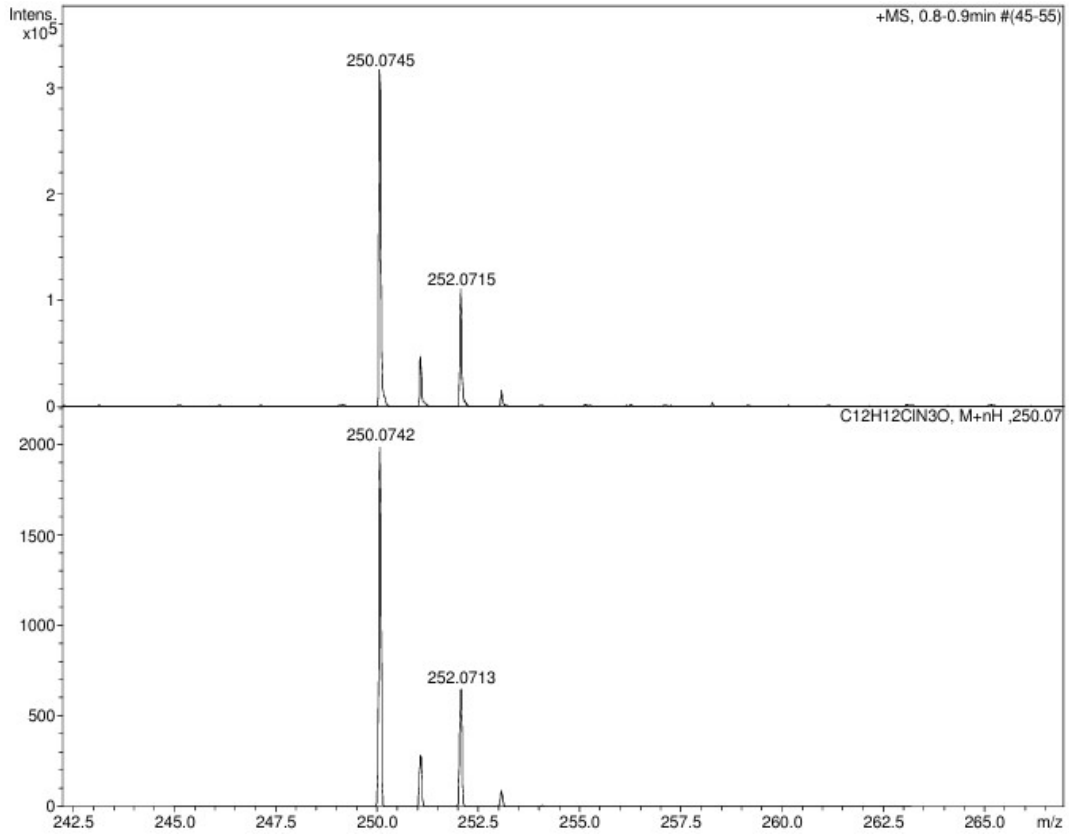
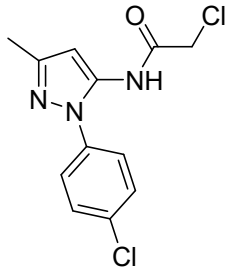


Figure-3: HRMS spectrum of compound **3a**





2-Chloro-N-(1-(4-chlorophenyl)-3-methyl-1H-pyrazol-5-yl)acetamide, ***3b***

White powder, m.p. 168-170°C, yield 89% (1 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.59 (s, 1H), 7.85 – 7.77 (m, 4H), 6.57 (s, 1H), 4.53 (s, 2H), 2.50 (s, 3H). ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 164.92, 148.13, 136.99, 135.31, 131.13, 128.81, 124.74, 101.88, 42.28, 13.38. HRMS (ESI-TOF): m/z $[M+H]^+$: calcd for $[C_{12}H_{12}Cl_2N_3O]^+$: 284.0352; found: 284.0356.

Figure-4: ^{1}H NMR spectrum (300 MHz) of **3b** in DMSO-d_6

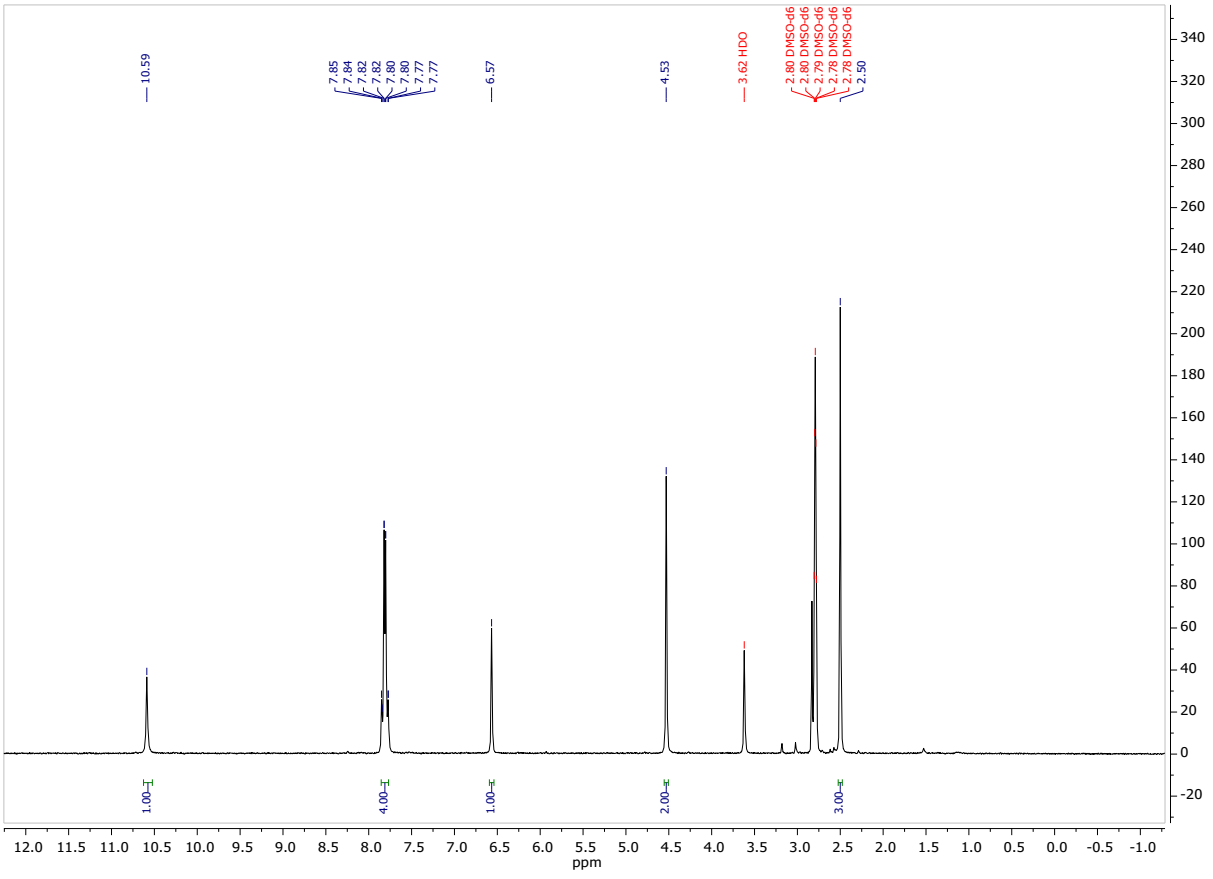


Figure-5: ^{13}C NMR spectrum (76 MHz) of **3b** in DMSO-d_6

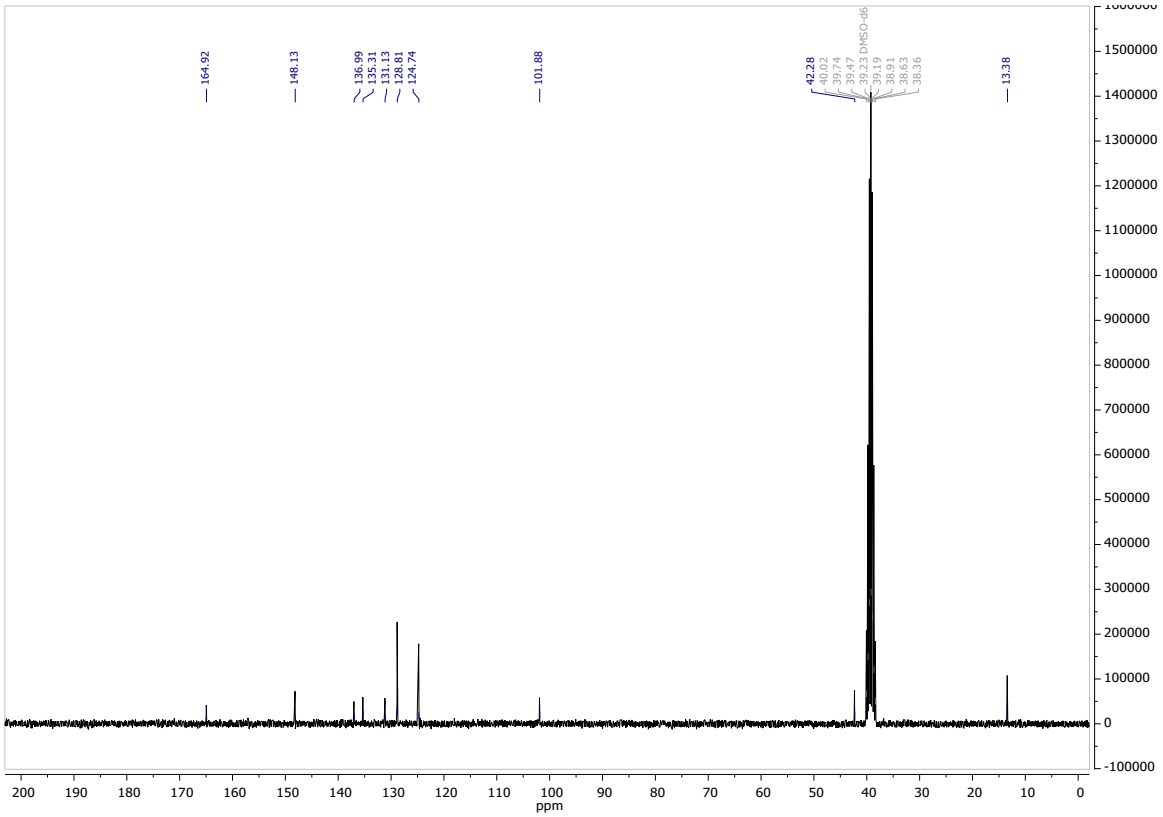
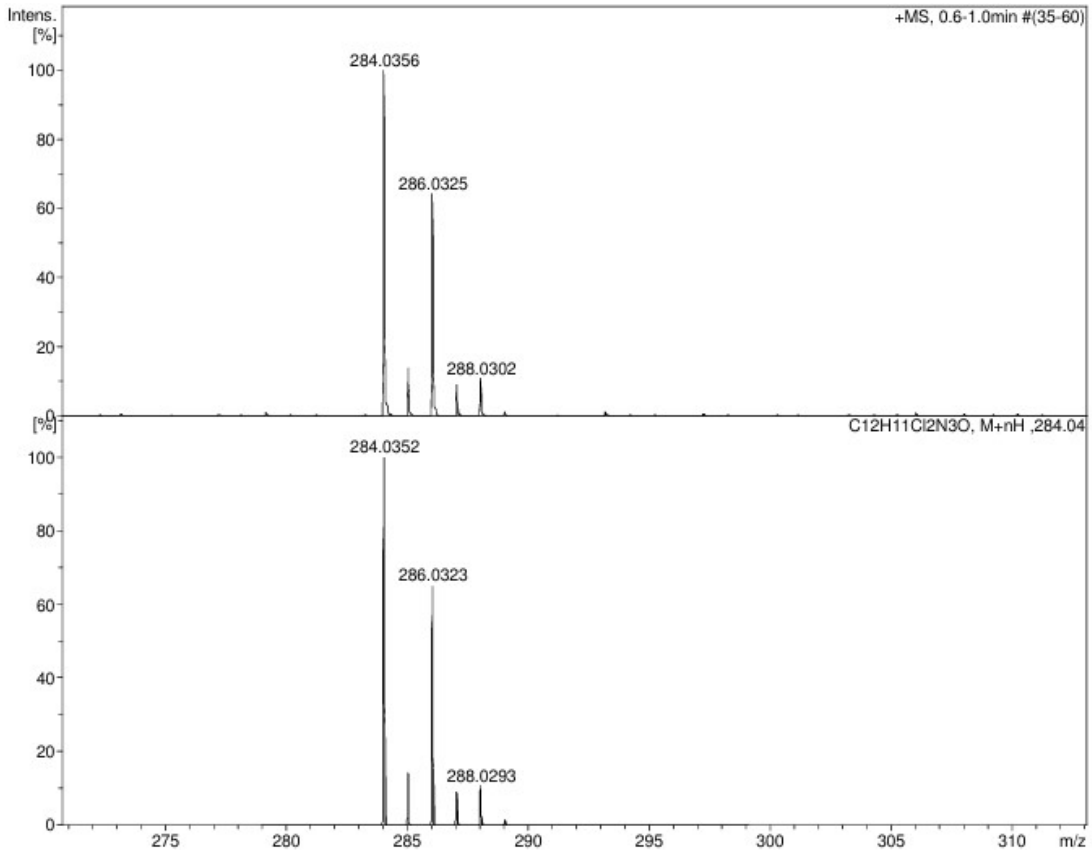
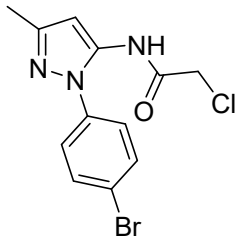


Figure-6: HRMS spectrum of compound **3b**





N-(1-(4-bromophenyl)-3-methyl-1H-pyrazol-5-yl)-2-chloroacetamide, ***3c***

White powder, m.p. 180-182°C, yield 94% (1.23 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.30 (s, 1H), 7.67 (d, J = 8.8 Hz, 2H), 7.44 (d, J = 8.7 Hz, 2H), 6.28 (s, 1H), 4.24 (s, 2H), 2.21 (s, 3H). ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 165.34, 148.57, 137.76, 135.66, 132.11, 125.36, 119.86, 102.36, 42.65, 13.75. HRMS (ESI-TOF): m/z [M+H]$^+$: calcd for [$C_{12}H_{12}BrClN_3O$]$^+$: 329.9826; found: 329.9825.

Figure-7: ^{1}H NMR spectrum (300 MHz) of **3c** in DMSO-d_6

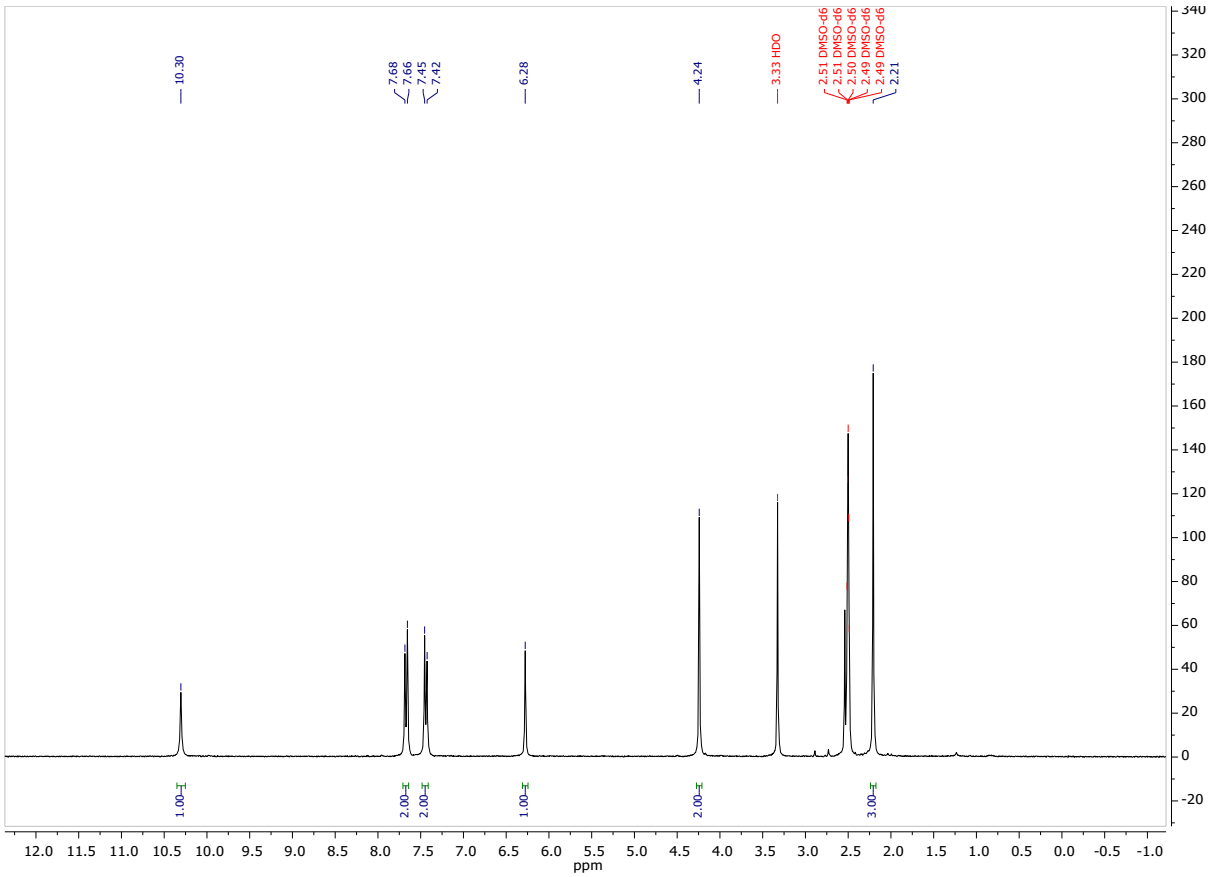


Figure-8: ^{13}C NMR spectrum (76 MHz) of **3c** in DMSO-d_6

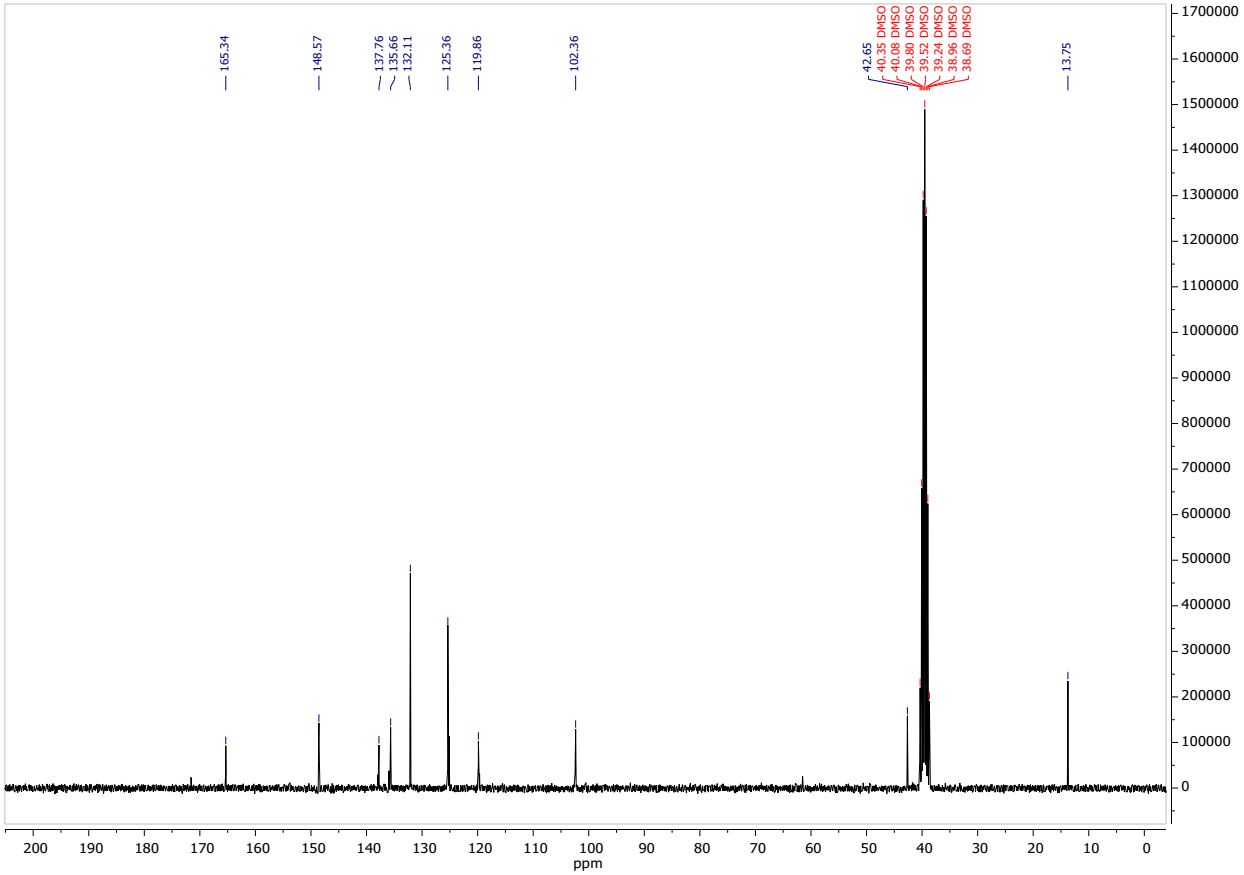
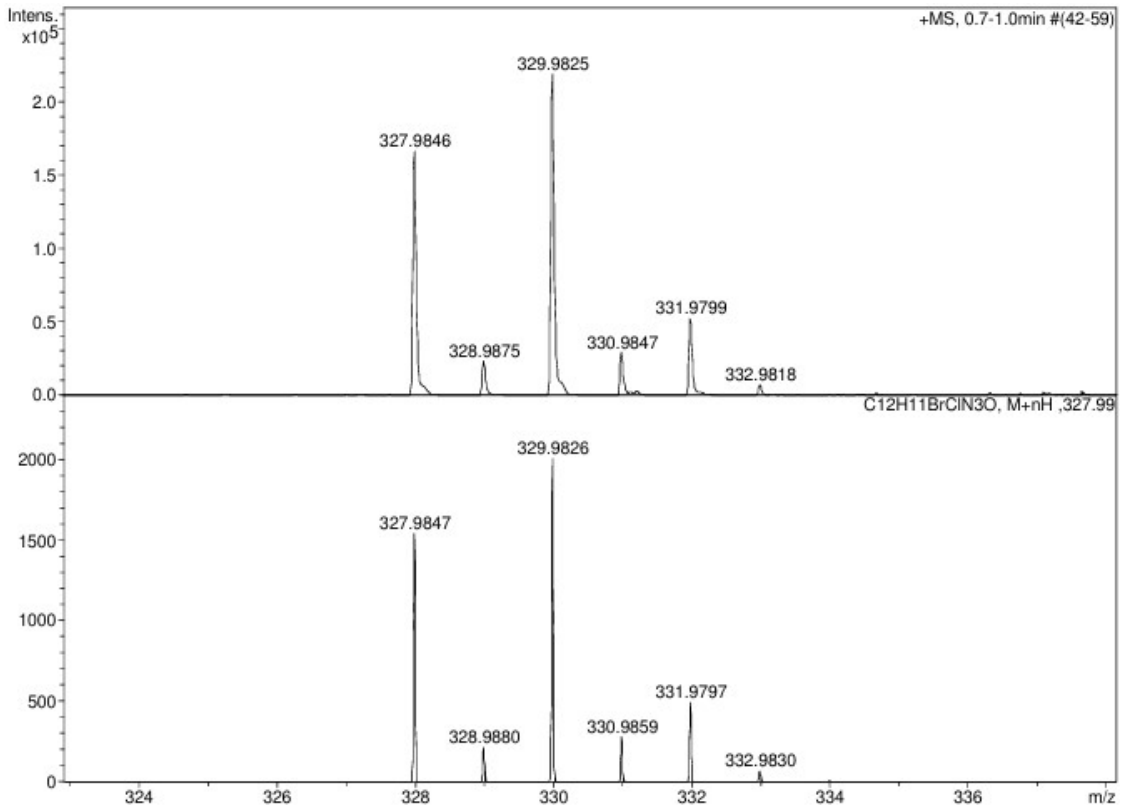
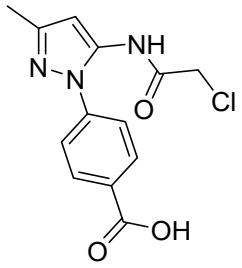


Figure-9: HRMS spectrum of compound **3c**





4-(5-(2-Chloroacetamido)-3-methyl-1H-pyrazol-1-yl)benzoic acid, ***3f***

White powder, m.p. 231-233°C, yield 85% (0.89 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 13.04 (brs, s, 1H), 10.39 (s, 1H), 8.03 (d, J = 8.6 Hz, 2H), 7.63 (d, J = 8.4 Hz, 2H), 6.30 (s, 1H), 4.27 (s, 2H), 2.23 (s, 3H). ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.71, 165.35, 149.03, 141.96, 135.82, 130.44, 128.86, 122.64, 102.97, 42.70, 13.77. HRMS (ESI-TOF): m/z [M+H]$^+$: calcd for [$C_{13}H_{13}ClN_3O_3$]$^+$: 294.0640; found: 294.0633.

Figure-10: ^{1}H NMR spectrum (300 MHz) of **3f** in DMSO-d_6

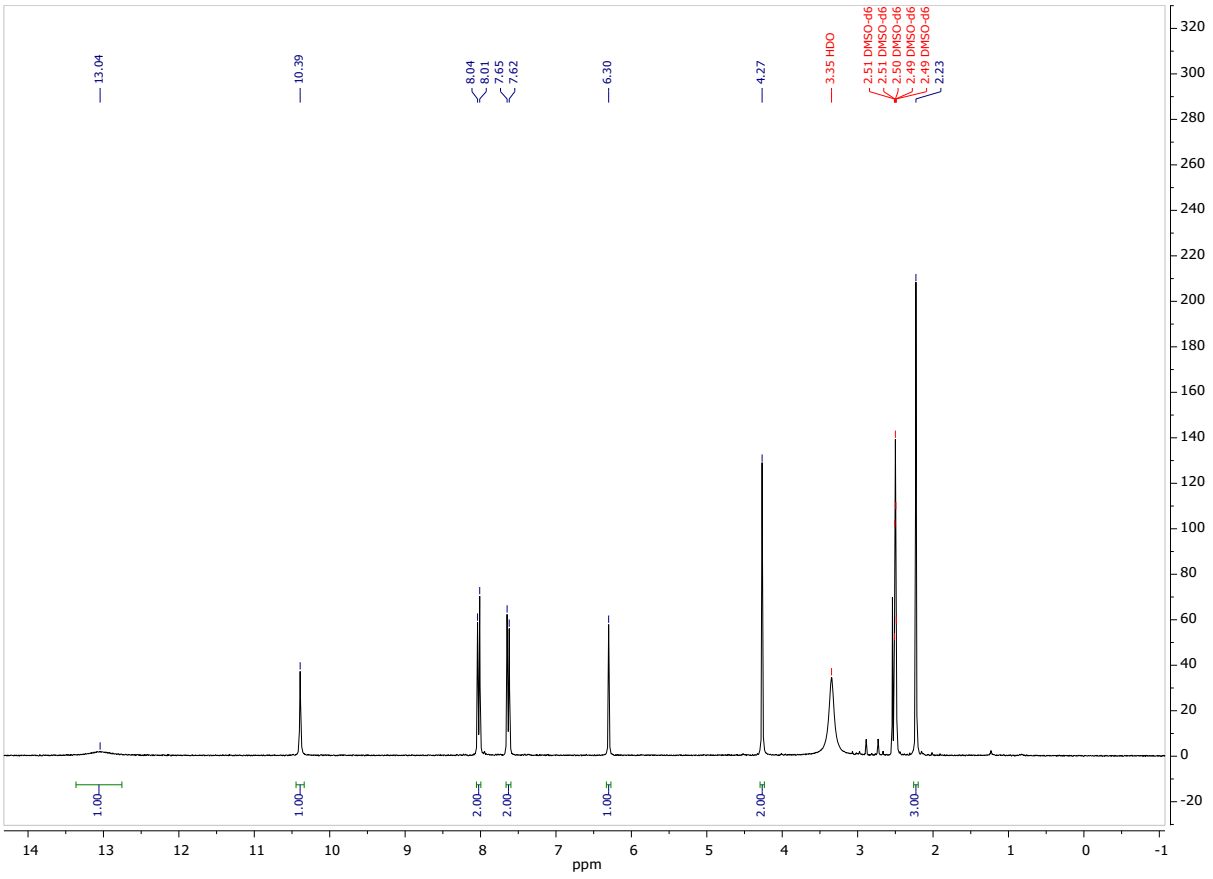


Figure-11: ^{13}C NMR spectrum (76 MHz) of **3f** in DMSO-d_6

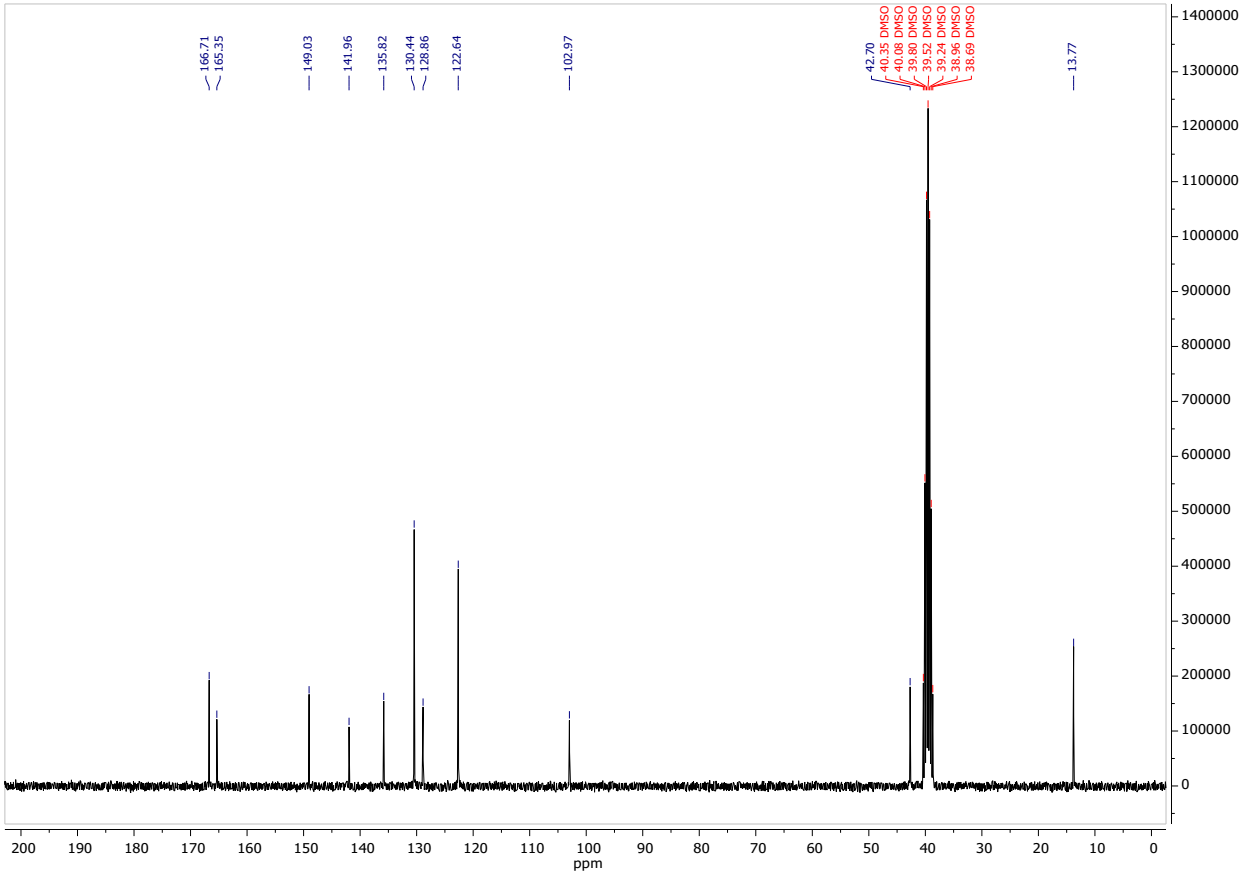
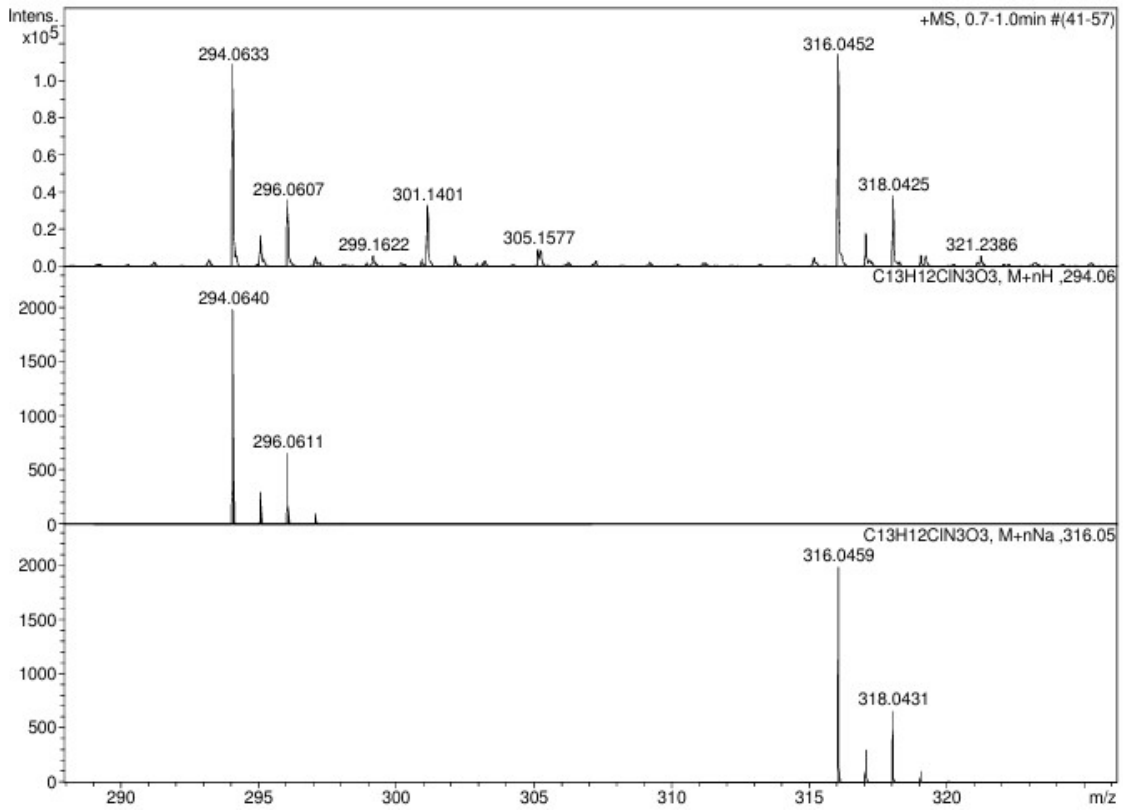
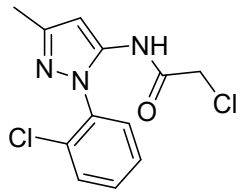


Figure-12: HRMS spectrum of compound **3f**





2-Chloro-N-(1-(2-chlorophenyl)-3-methyl-1H-pyrazol-5-yl)acetamide, ***3g***

White powder, m.p. 147-149°C, yield 79% (0.89 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.16 (s, 1H), 7.68 – 7.63 (m, 1H), 7.57 – 7.44 (m, 3H), 6.34 (s, 1H), 4.16 (s, 2H), 2.19 (s, 3H). ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 164.27, 148.36, 137.54, 135.59, 131.27, 130.82, 130.28, 130.14, 128.02, 98.45, 42.50, 13.75. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{12}H_{12}Cl_2N_3O$]$^{+}$: 284.0352; found: 284.0354.

Figure-13: ^{1}H NMR spectrum (300 MHz) of **3g** in DMSO-d_6

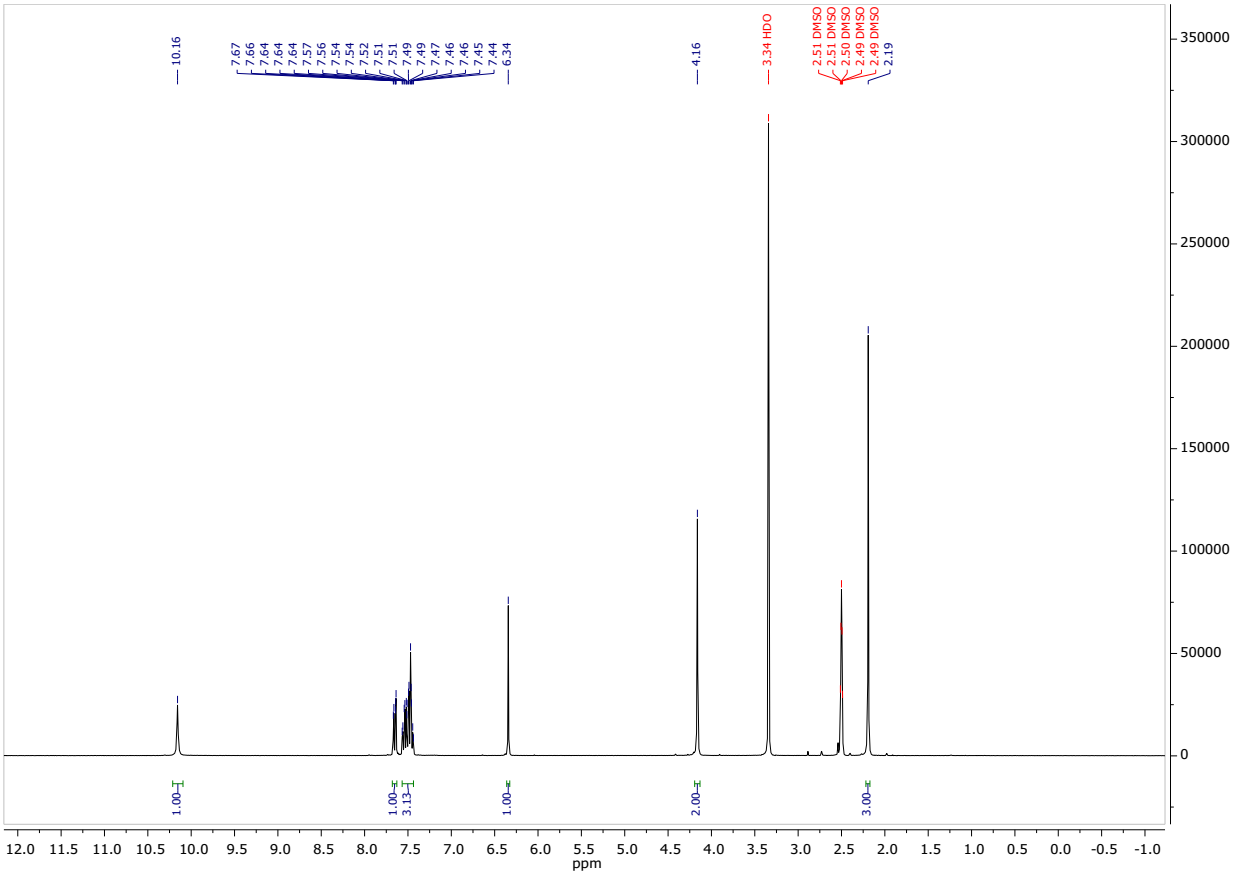


Figure-14: ^{13}C NMR spectrum (76 MHz) of **3g** in DMSO-d_6

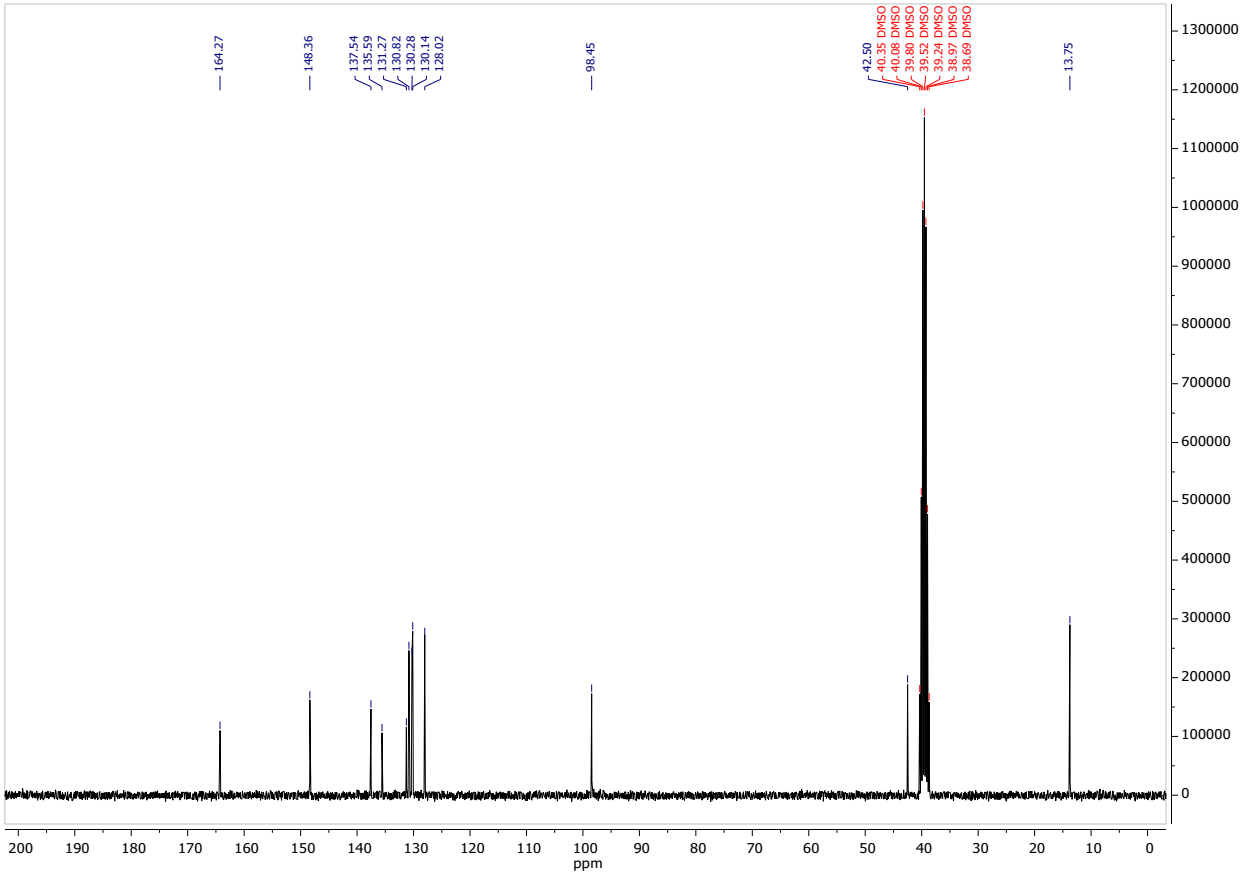
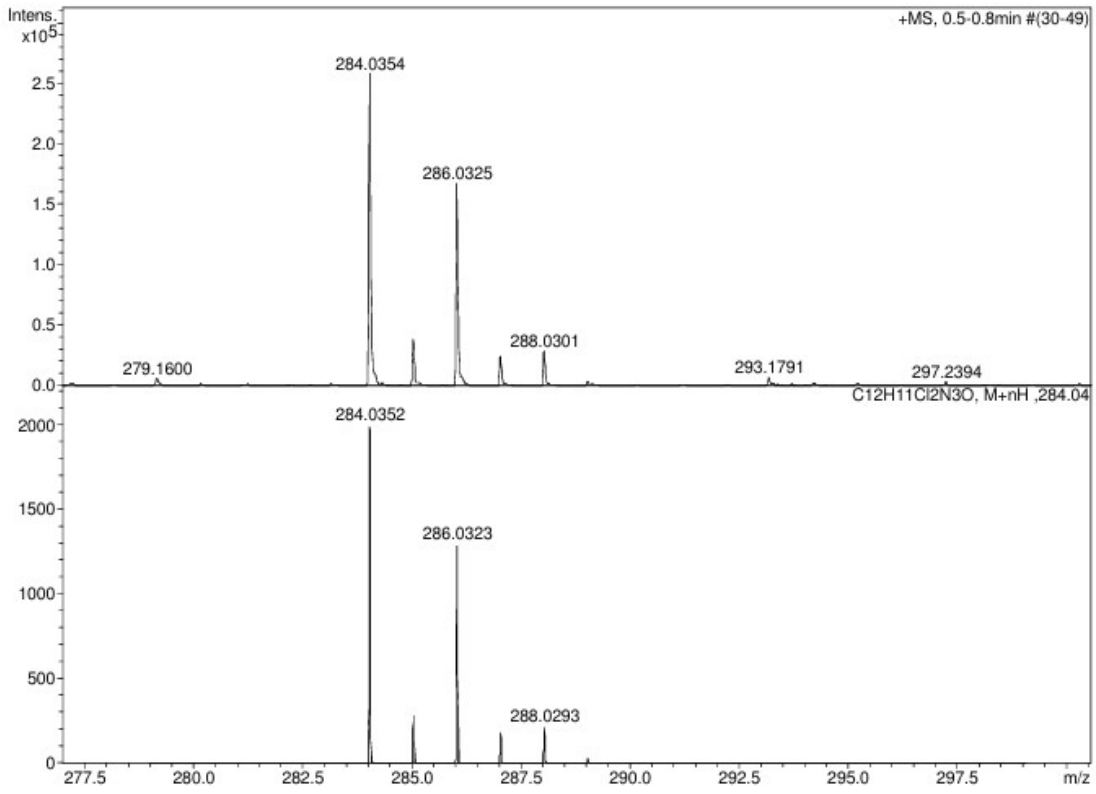
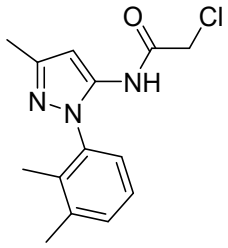


Figure-15: HRMS spectrum of compound **3g**





2-Chloro-N-(1-(2,3-dimethylphenyl)-3-methyl-1H-pyrazol-5-yl)acetamide, ***3h***

White powder, m.p. 177-179°C, yield 83% (0.92 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 9.93 (s, 1H), 7.30 (d, J = 7.4 Hz, 1H), 7.23 – 7.17 (m, 1H), 7.03 (d, J = 7.7 Hz, 1H), 6.30 (s, 1H), 4.15 (s, 2H), 2.30 (s, 3H), 2.19 (s, 3H), 1.85 (s, 3H). ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 164.52, 147.39, 137.89, 137.11, 136.94, 134.52, 130.36, 125.81, 125.52, 98.46, 42.55, 19.90, 13.93, 13.76. HRMS (ESI-TOF): m/z [M+H]$^+$: calcd for [$C_{14}H_{17}ClN_3O$]$^+$: 278.1055; found: 278.1055.

Figure-16: ^{1}H NMR spectrum (300 MHz) of **3h** in DMSO-d_6

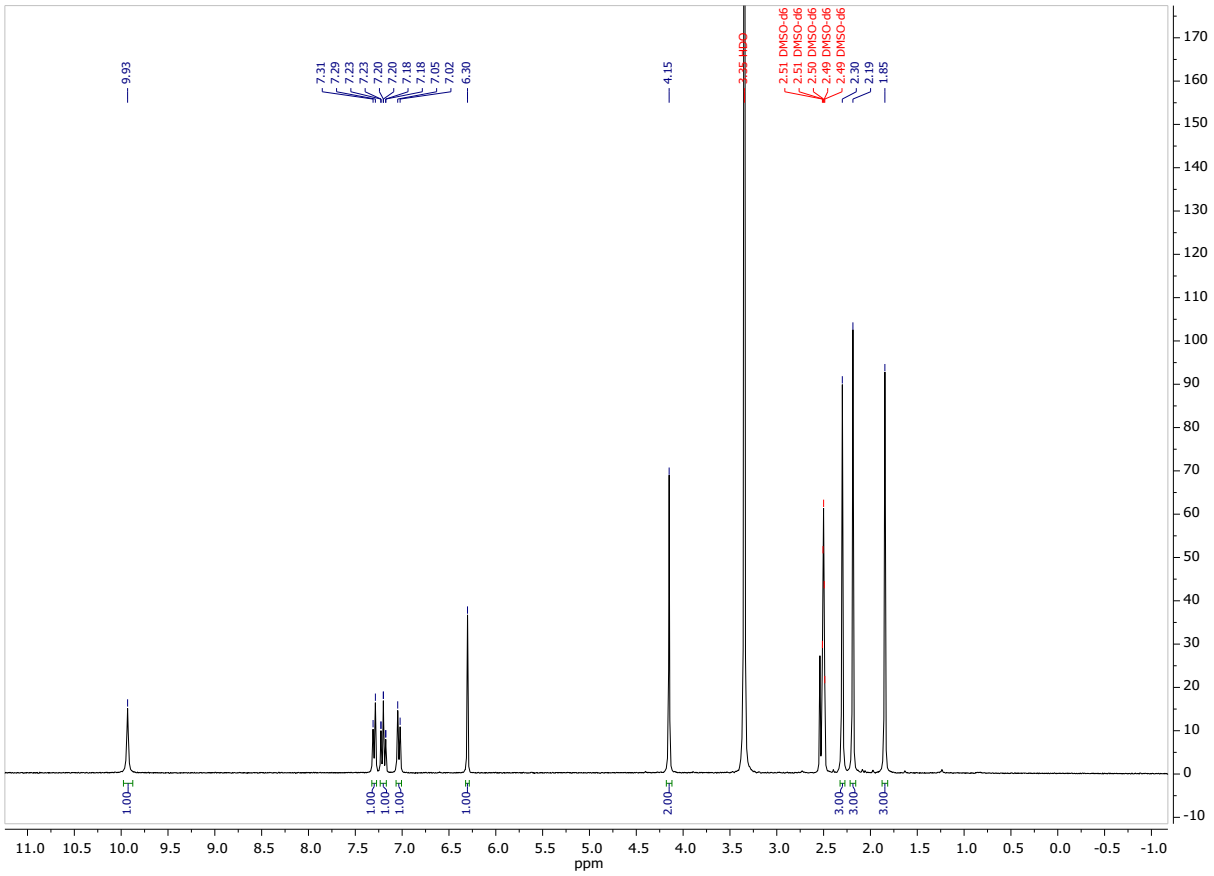


Figure-17: ^{13}C NMR spectrum (76 MHz) of **3h** in DMSO-d_6

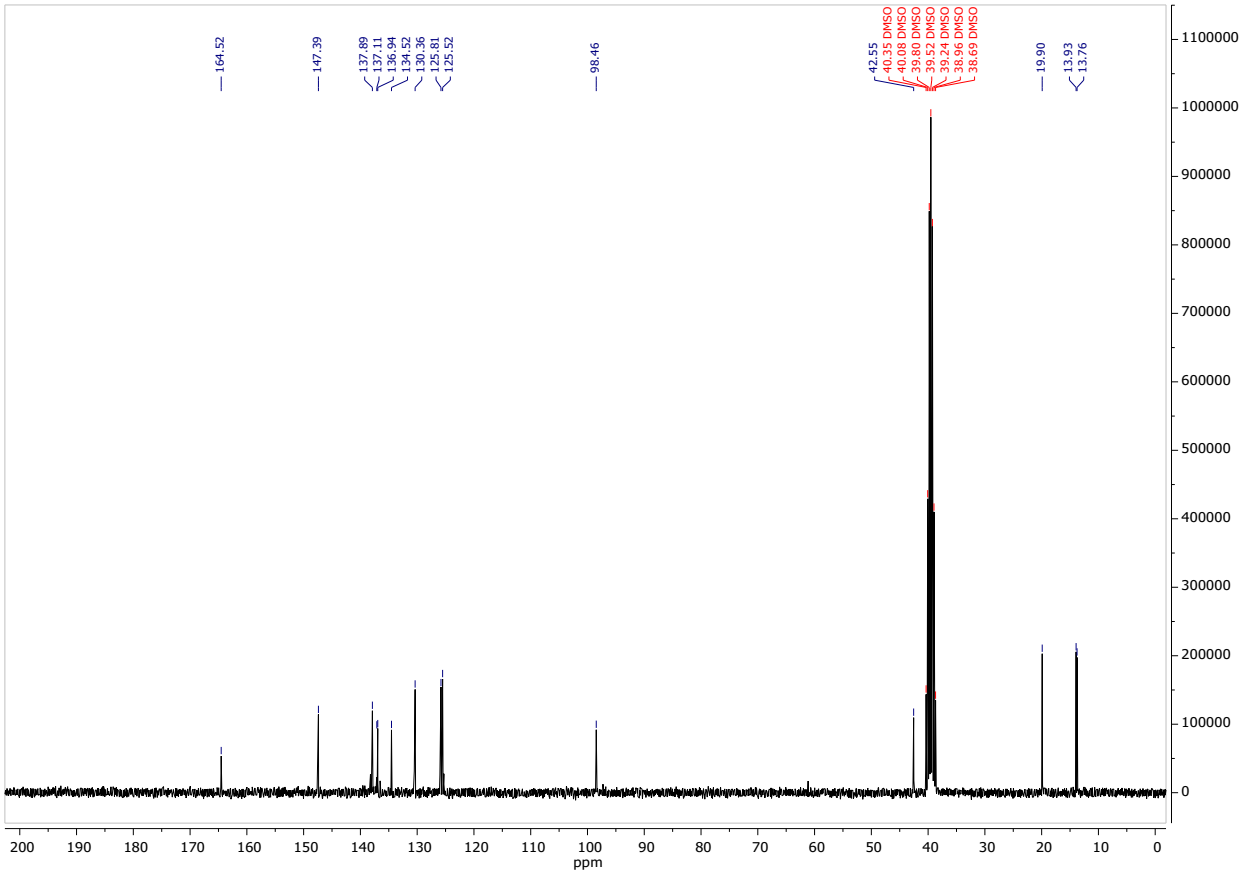
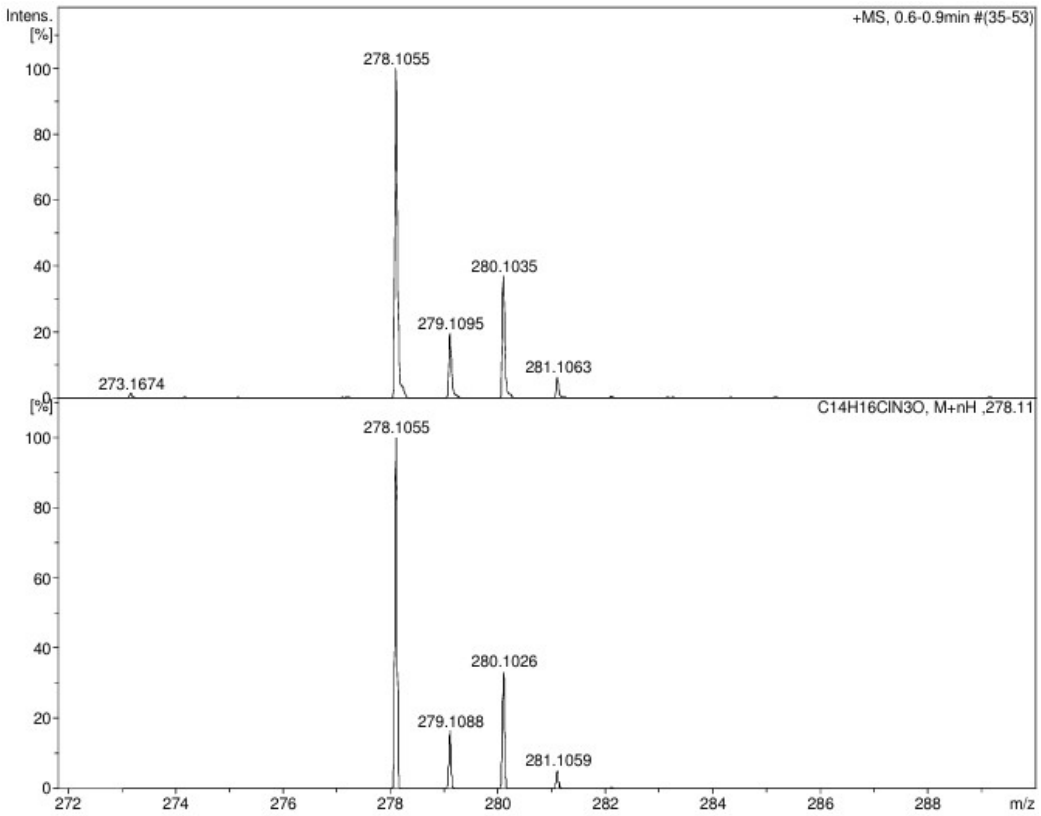
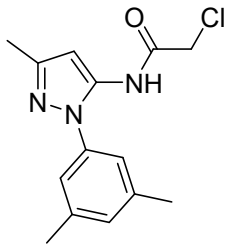


Figure-18: HRMS spectrum of compound **3h**





2-Chloro-N-(1-(3,5-dimethylphenyl)-3-methyl-1H-pyrazol-5-yl)acetamide, ***3i***

Grey powder, m.p. 124-126°C, yield 92% (1.1 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.21 (s, 1H), 7.09 (s, 2H), 7.01 (s, 1H), 6.24 (s, 1H), 4.22 (s, 2H), 2.31 (s, 6H), 2.20 (s, 3H). ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 165.17, 147.72, 138.39, 138.27, 135.27, 128.49, 121.05, 101.92, 42.60, 20.82, 13.71. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{14}H_{17}ClN_3O$]$^{+}$: 278.1055; found: 278.1055.

Figure-19: ^{1}H NMR spectrum (300 MHz) of **3i** in DMSO-d_6

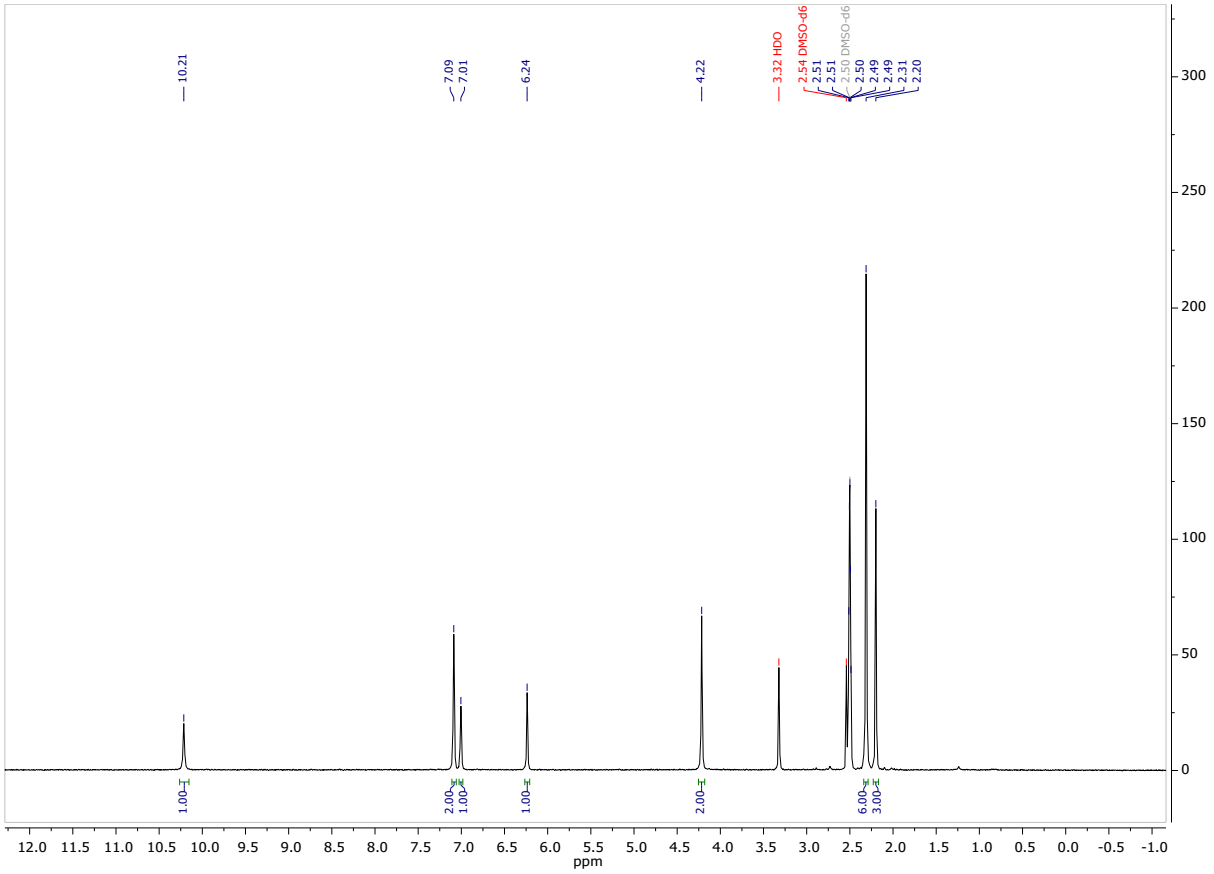


Figure-20: ^{13}C NMR spectrum (76 MHz) of **3i** in DMSO-d_6

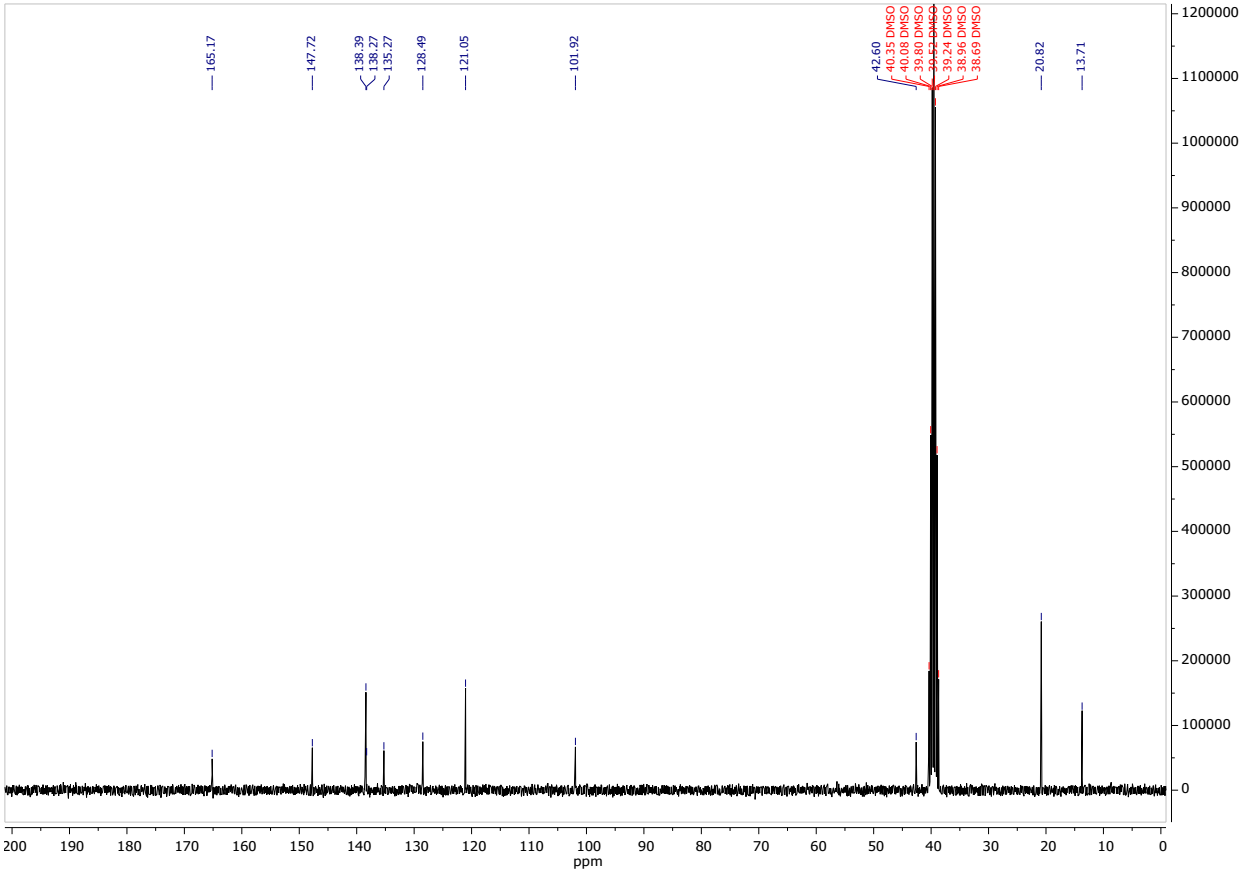
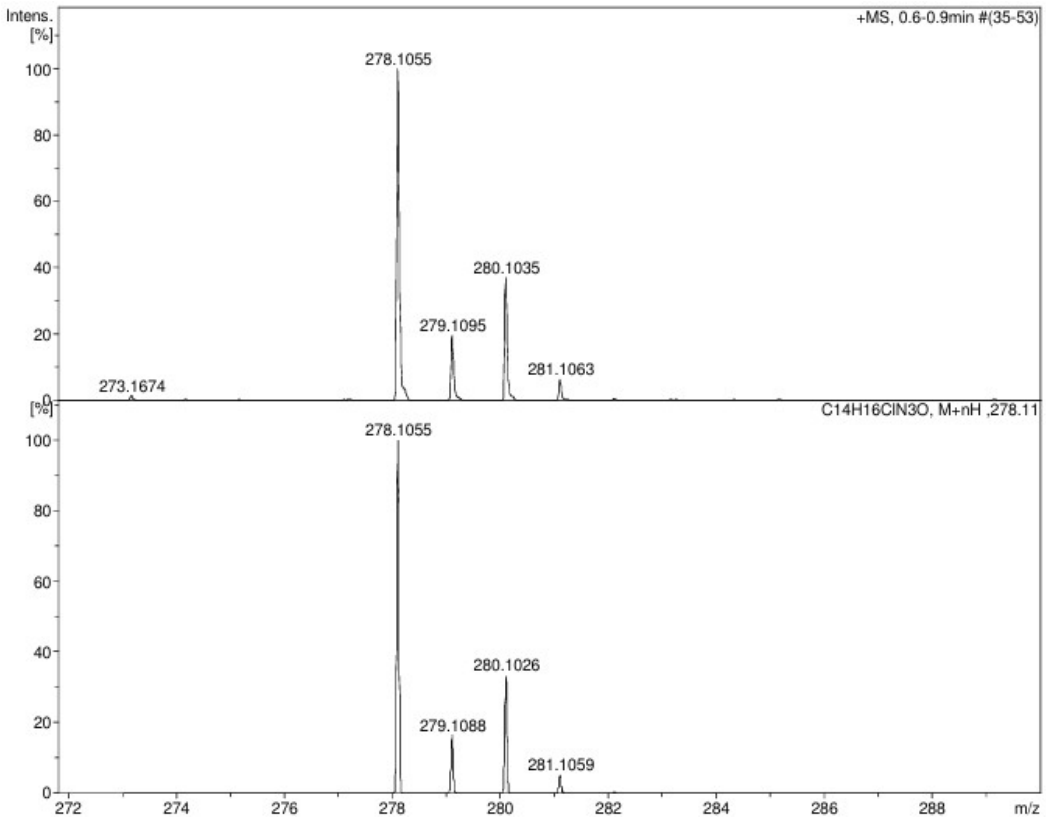
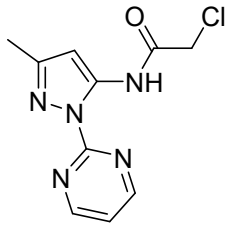


Figure-21: HRMS spectrum of compound **3i**





2-chloro-N-(3-methyl-1-(pyrimidin-2-yl)-1H-pyrazol-5-yl)acetamide, ***3k***

White powder, m.p. 202-204°C, yield 82% (0.82 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 12.28 (s, 1H), 8.89 (d, J = 4.9 Hz, 2H), 7.46 (t, J = 4.9 Hz, 1H), 6.69 (s, 1H), 4.53 (s, 2H), 2.24 (s, 3H). HRMS (ESI-TOF): m/z $[M+H]^+$: calcd for $[C_{10}H_{11}ClN_5O]^+$: 252.0647; found: 252.0648.

Figure-22: ^{1}H NMR spectrum (300 MHz) of **3k** in DMSO-d_6

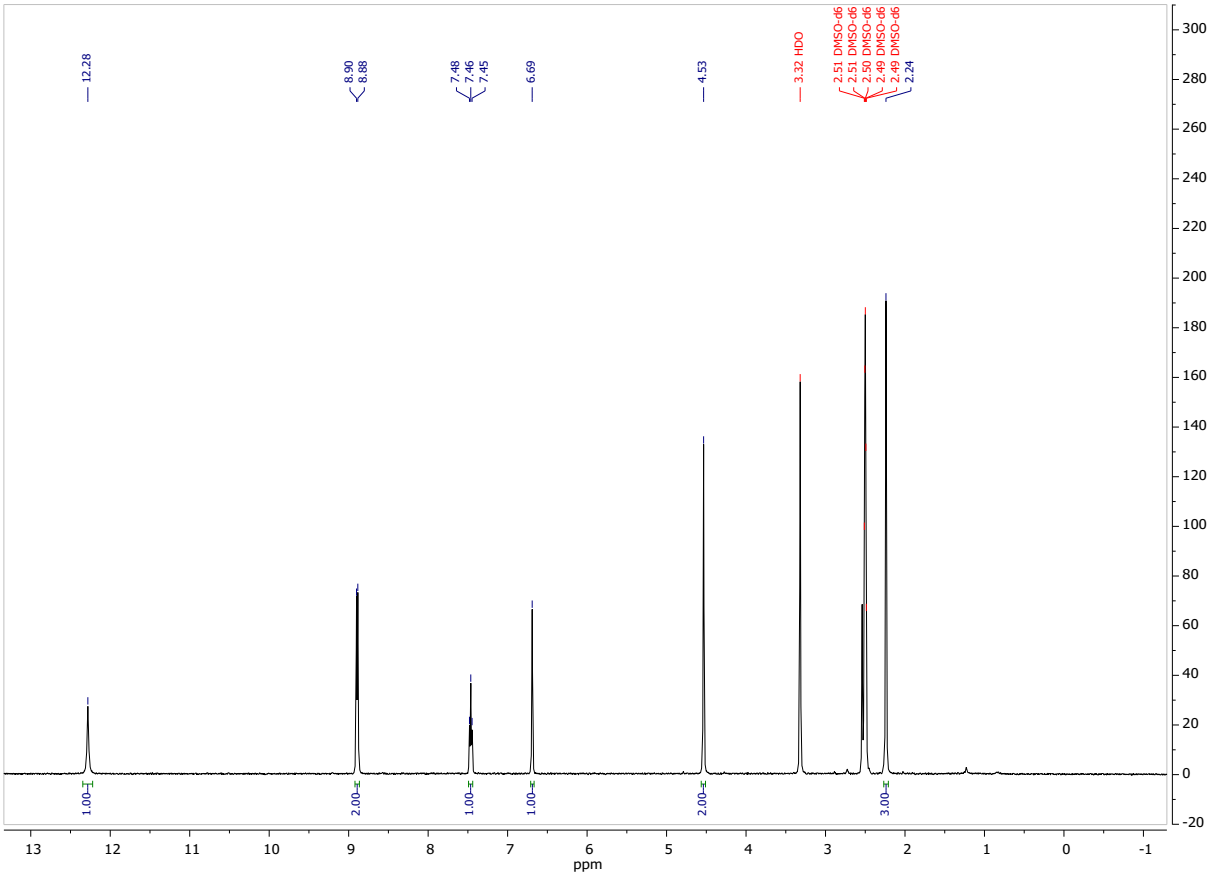
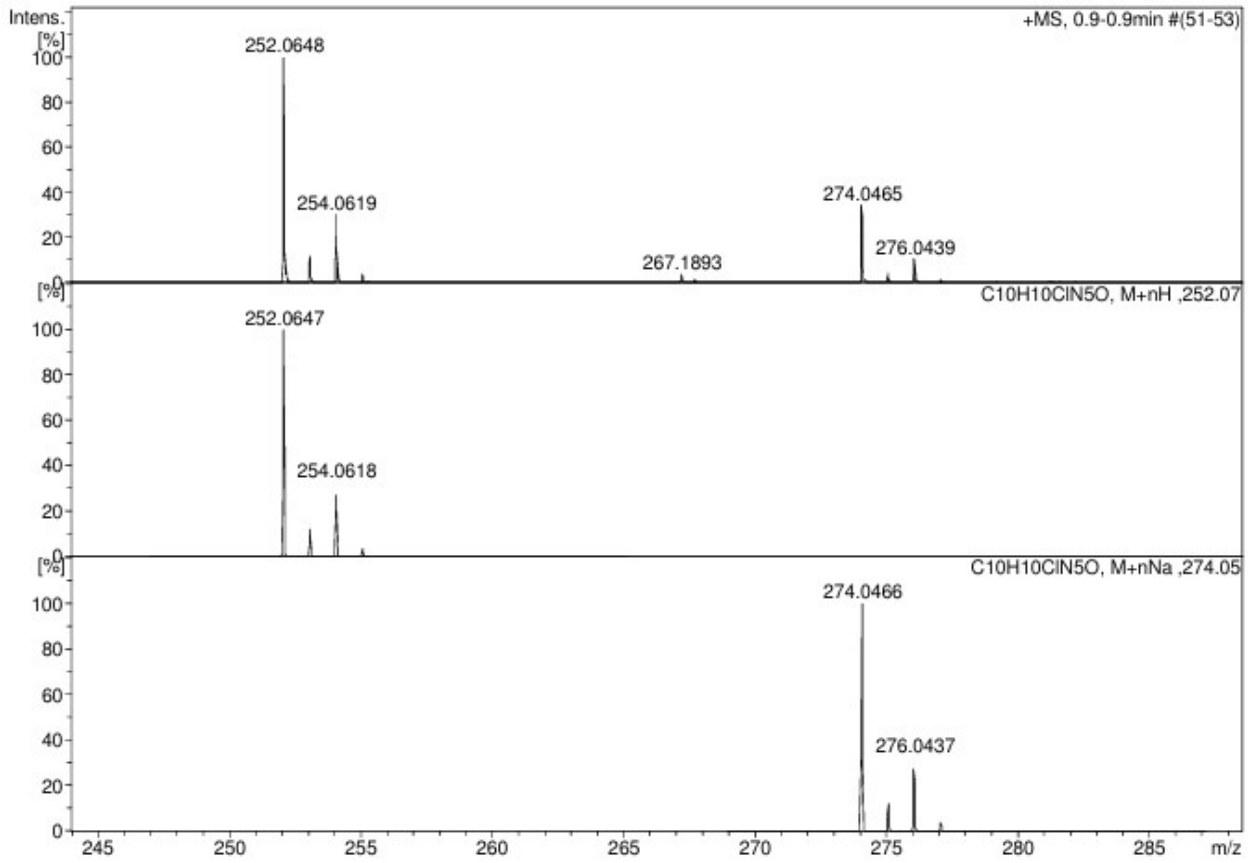
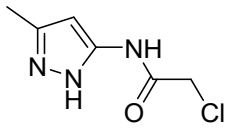


Figure-23: HRMS spectrum of compound **3k**





2-Chloro-N-(3-methyl-1H-pyrazol-5-yl)acetamide, ***3l***

White powder, m.p. 184-186°C, yield 53% (0.18g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 12.07 (s, 1H), 10.60 (s, 1H), 6.26 (s, 1H), 4.20 (s, 2H), 2.19 (s, 3H). ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 163.91, 146.13, 139.42, 95.63, 43.03, 10.80. HRMS (ESI-TOF): m/z $[M+H]^+$: calcd for $[C_6H_9ClN_3O]^+$: 174.0429; found: 174.0423.

Figure-24: ^{1}H NMR spectrum (300 MHz) of **3l** in DMSO-d_6

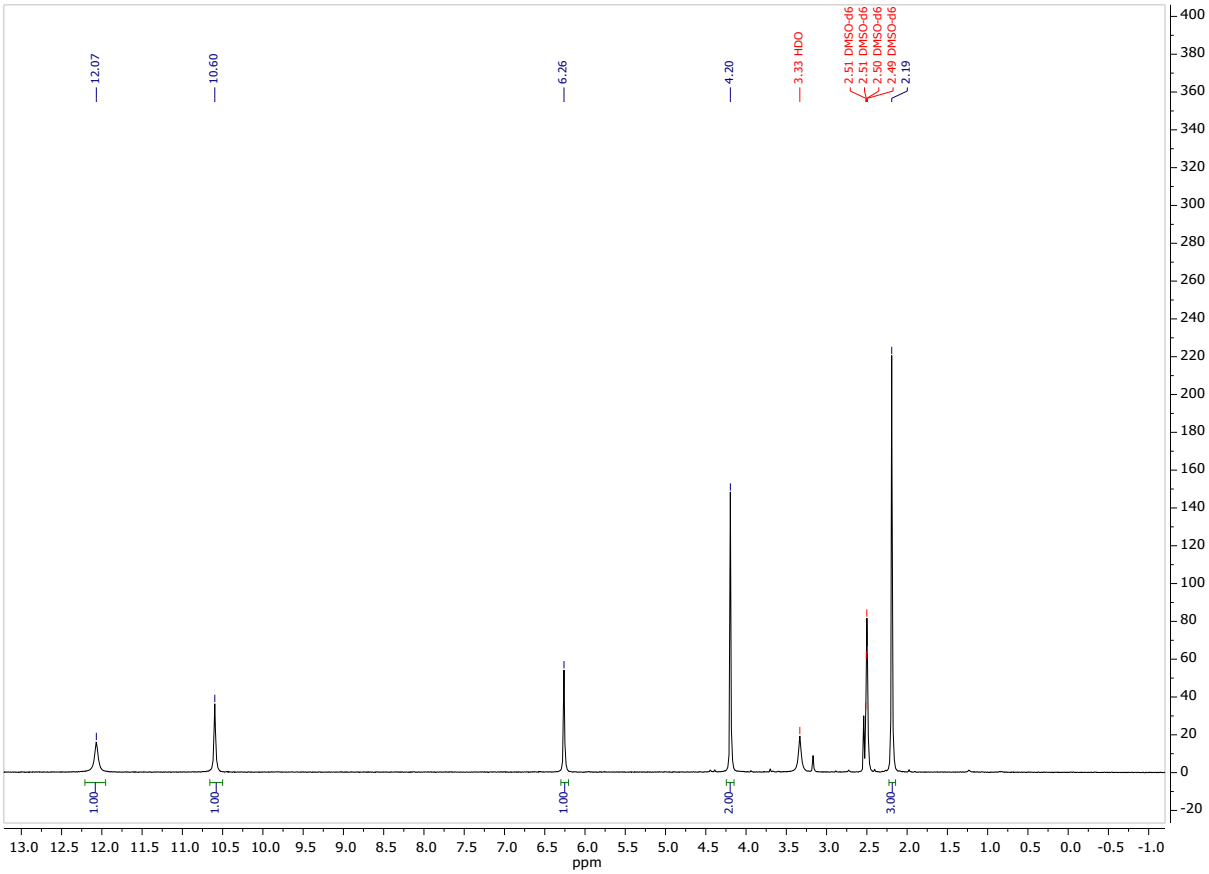


Figure-25: ^{13}C NMR spectrum (76 MHz) of **3l** in DMSO-d_6

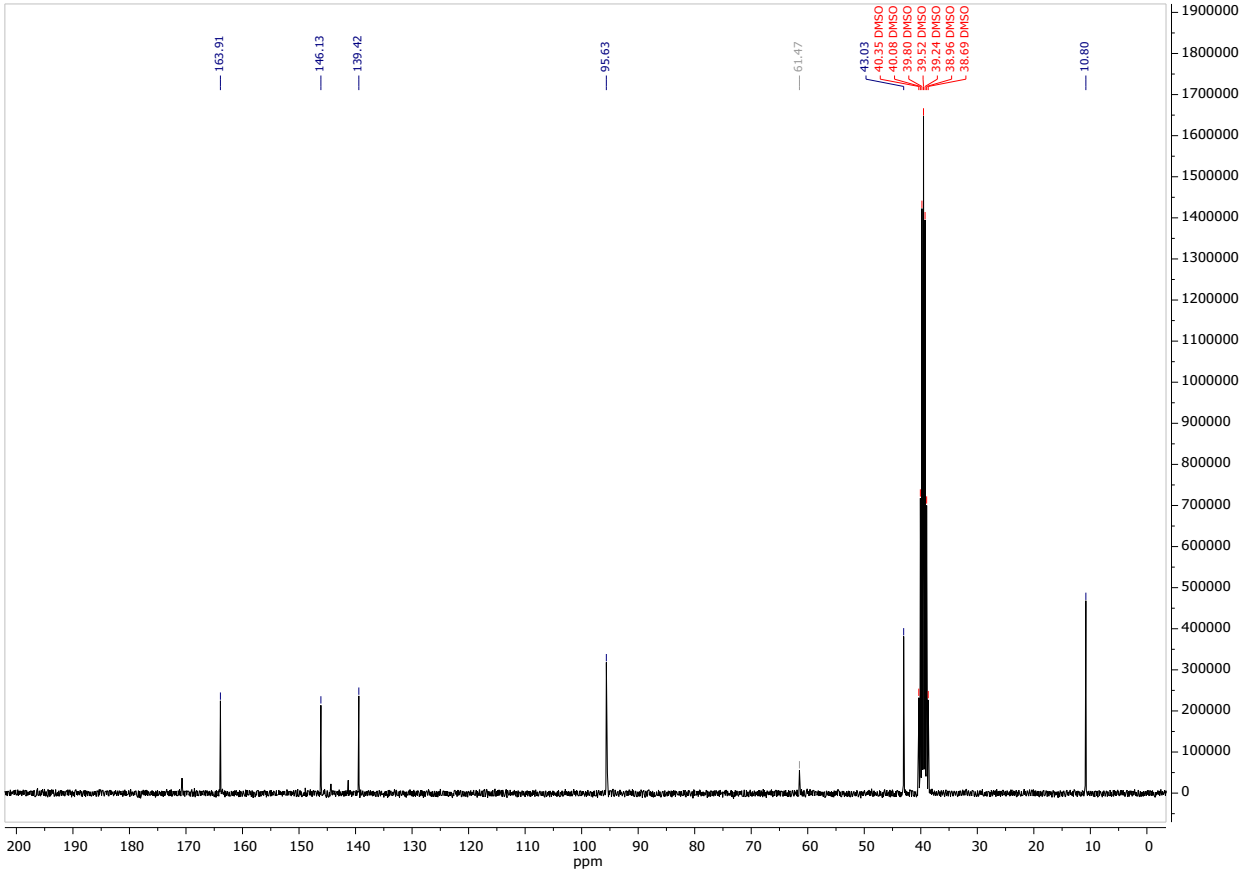
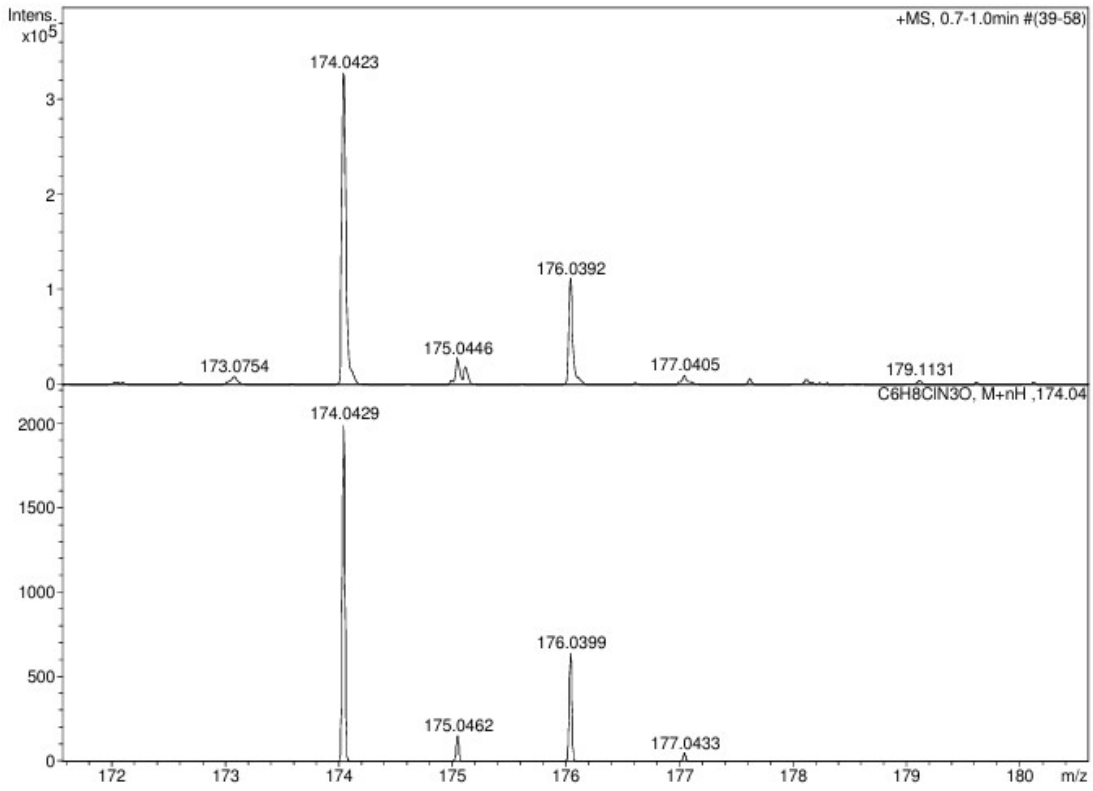
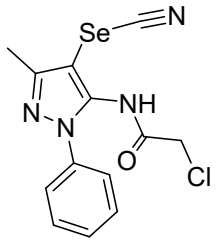


Figure-26: HRMS spectrum of compound **3l**



NMR and HRMS spectra for compounds 4



2-Chloro-N-(3-methyl-1-phenyl-4-selenocyanato-1H-pyrazol-5-yl)acetamide, ***4a***

Grey powder, m.p. 172-174°C, yield 85% (0.60 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.75 (s, 1H), 7.56 – 7.48 (m, 4H), 7.46 – 7.40 (m, 1H), 4.31 (s, 2H), 2.35 (s, 3H). ^{77}Se NMR (57 MHz, DMSO) δ 160.07. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.36, 150.78, 138.00, 137.91, 129.36, 128.11, 123.39, 103.32, 94.62, 42.29, 13.10. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{13}H_{12}ClN_4OSe$]$^{+}$: 354.9857; found: 354.9859.

Figure-27: ^{1}H NMR spectrum (300 MHz) of **4a** in DMSO-d_6

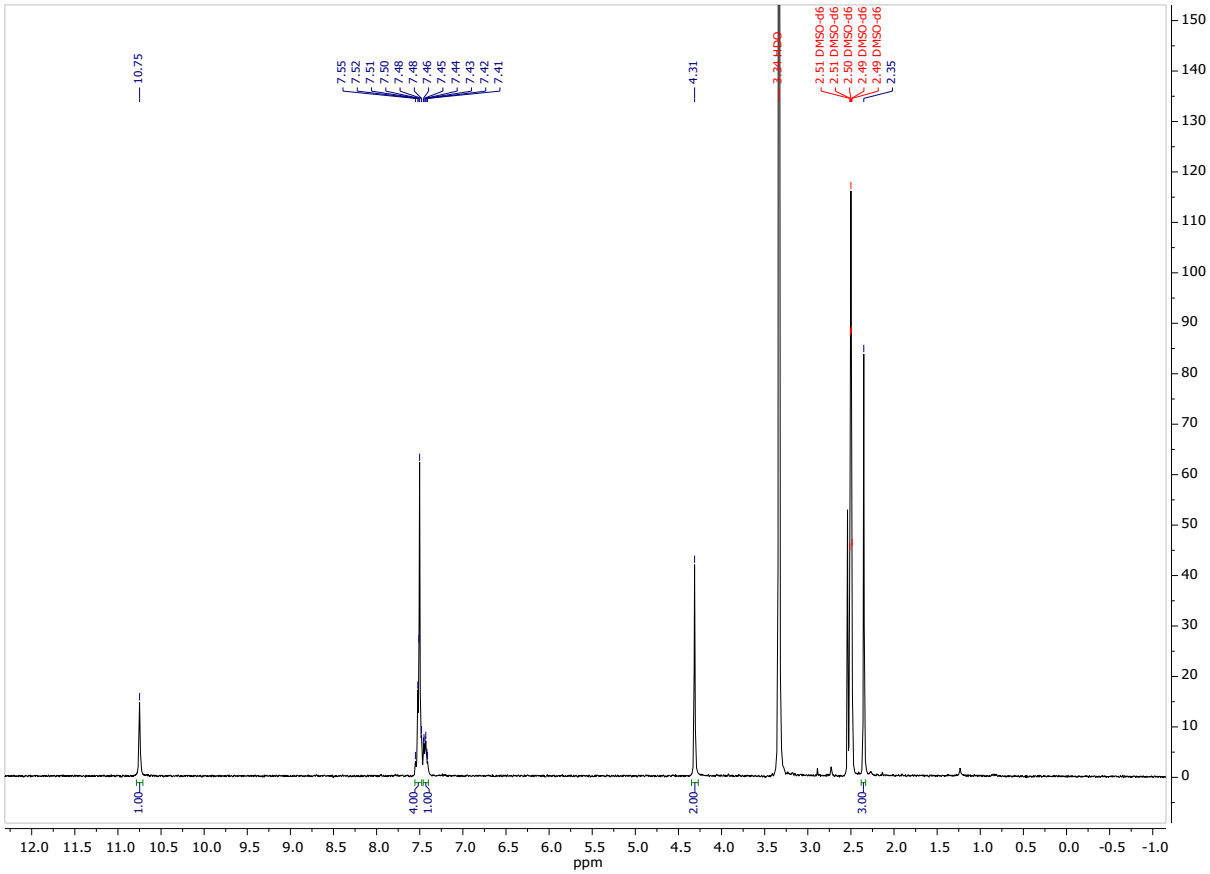


Figure-28: ^{77}Se NMR spectrum (57 MHz) of **4a** in DMSO-d_6

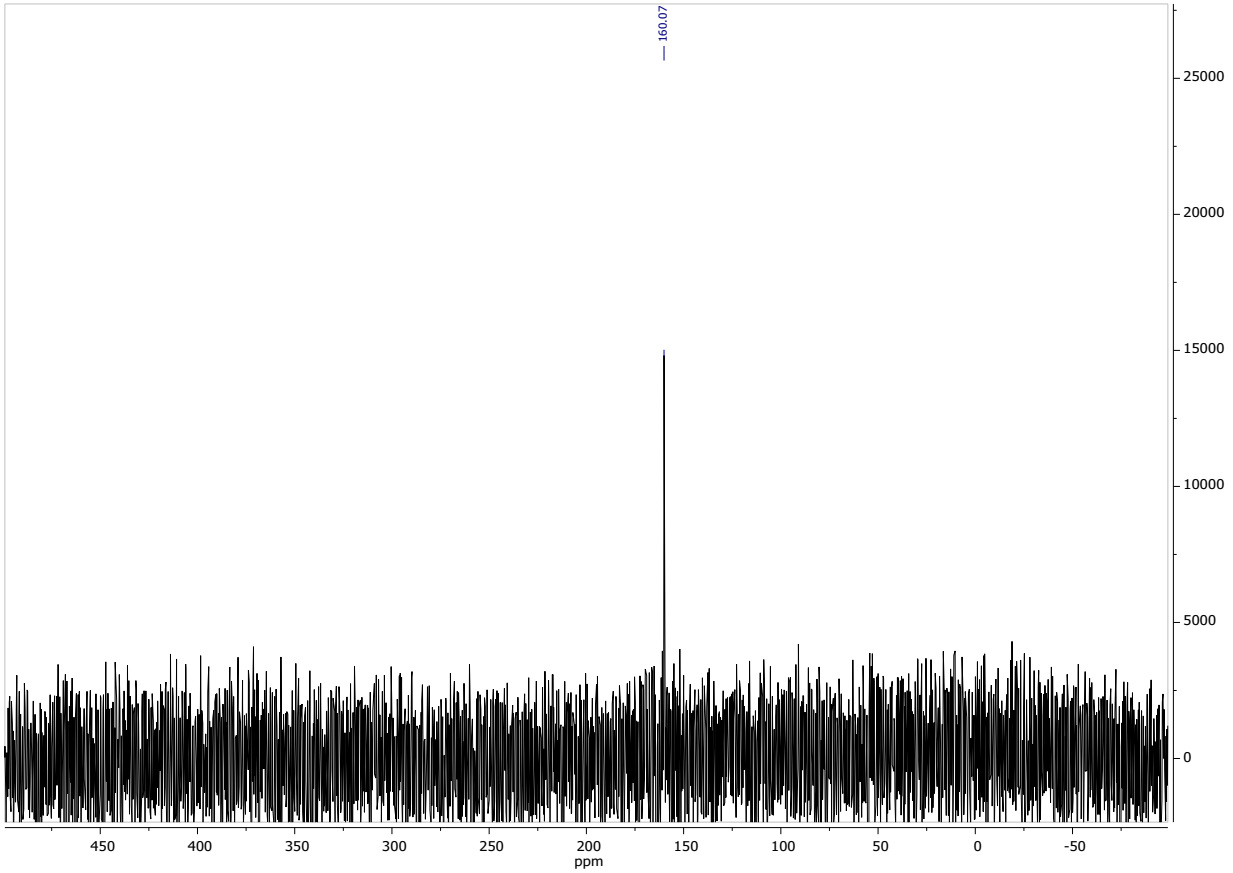


Figure-29: ^{13}C NMR spectrum (76 MHz) of **4a** in DMSO-d_6

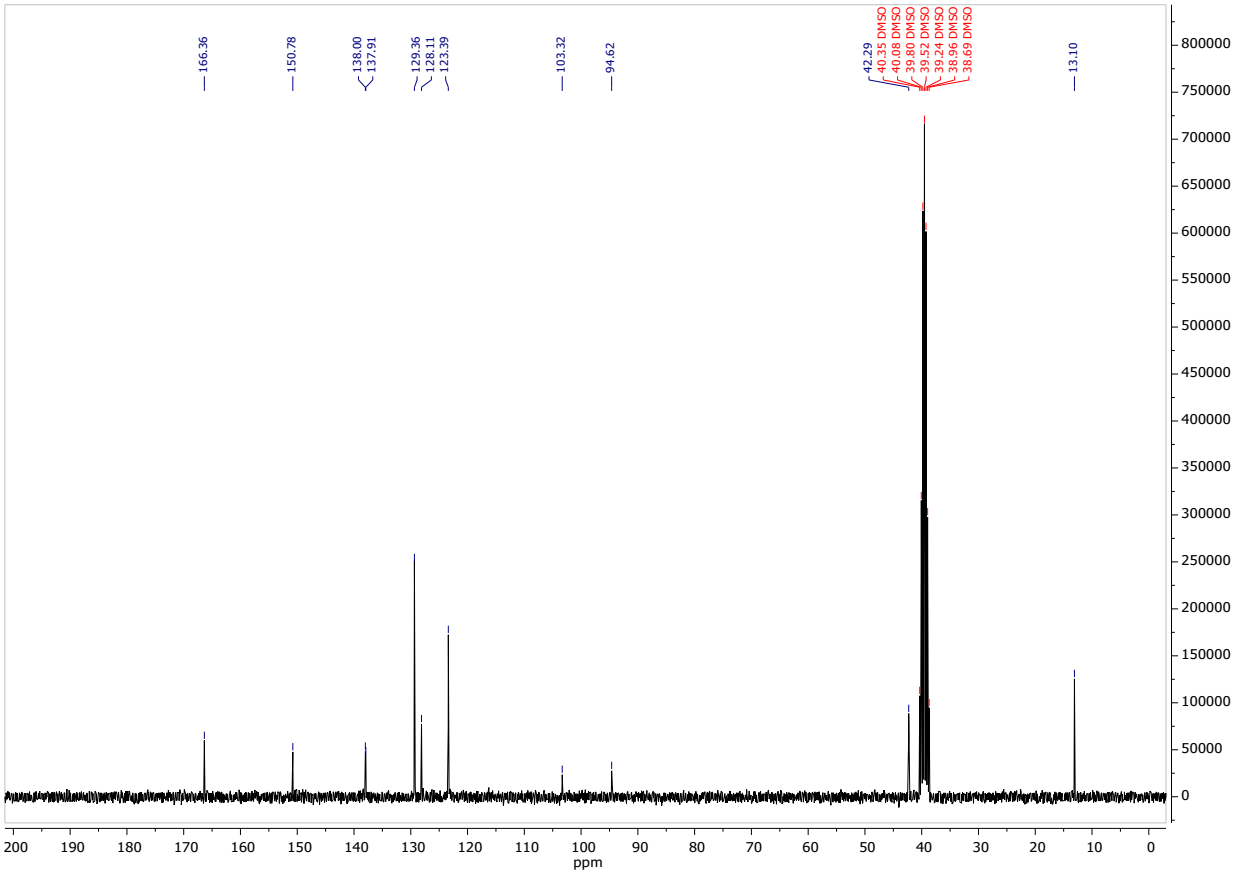
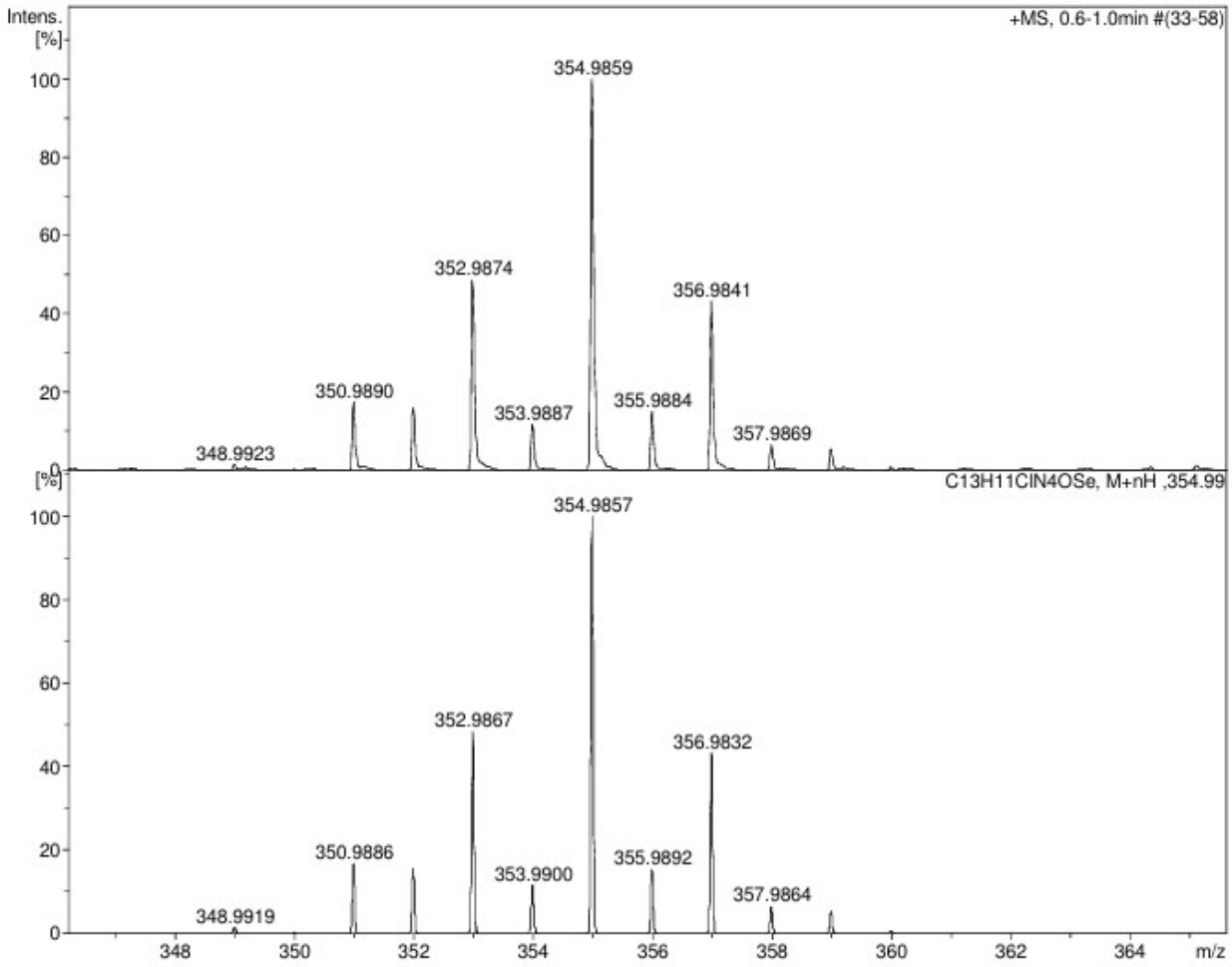
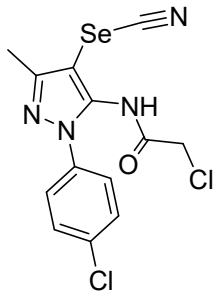


Figure-30: HRMS spectrum of compound **4a**





2-Chloro-N-(1-(4-chlorophenyl)-3-methyl-4-selenocyanato-1H-pyrazol-5-yl)acetamide, ***4b***

White powder, m.p. 191-193°C, yield 83% (0.64 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.77 (s, 1H), 7.61 – 7.51 (m, 4H), 4.33 (s, 2H), 2.35 (s, 3H). ^{77}Se NMR (57 MHz, DMSO) δ 161.08. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.29, 151.07, 138.06, 136.84, 132.41, 129.34, 125.02, 103.33, 94.88, 42.31, 13.08. HRMS (ESI-TOF): m/z $[M+H]^+$: calcd for $[C_{13}H_{11}Cl_2N_4OSe]^+$: 388.9465; found: 388.9473.

Figure-31: ^{1}H NMR spectrum (300 MHz) of **4b** in DMSO-d_6

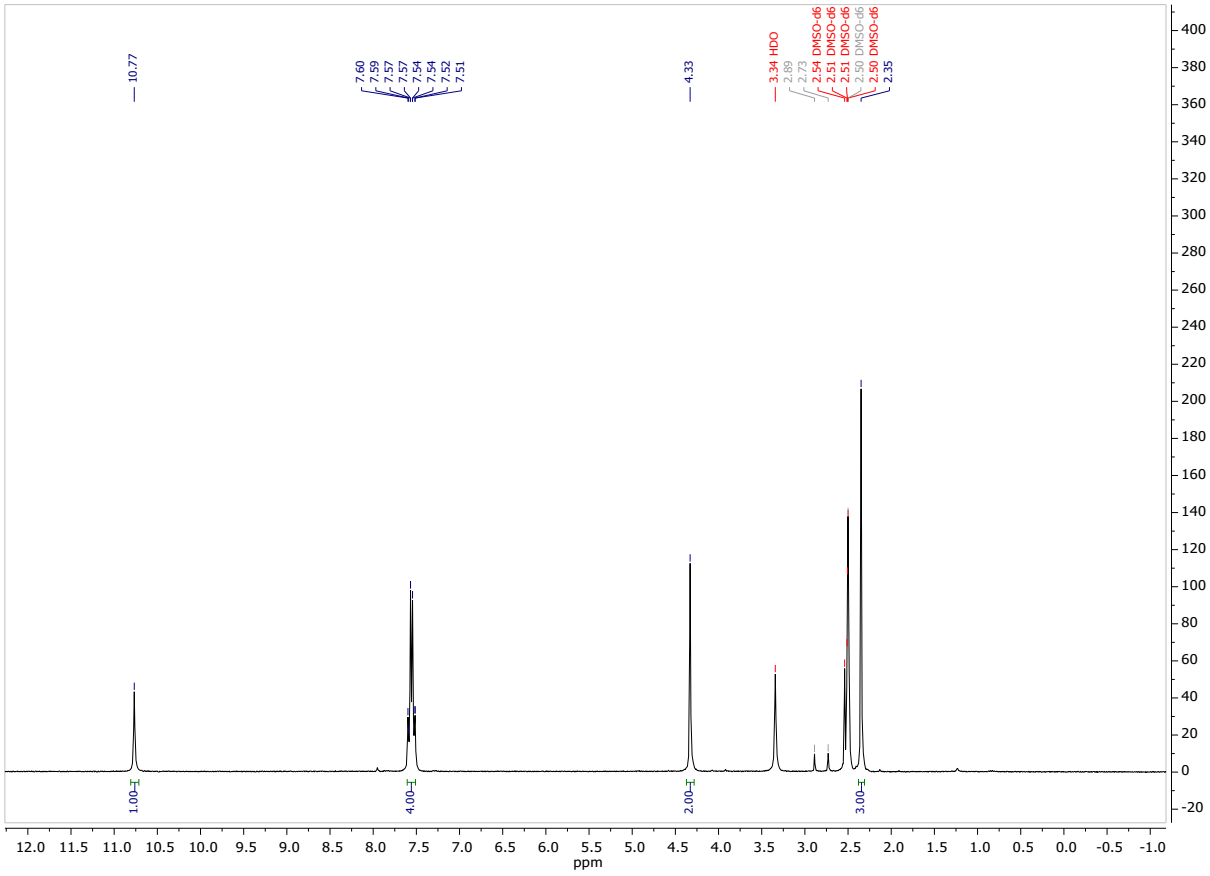


Figure-32: ^{77}Se NMR spectrum (57 MHz) of **4b** in DMSO-d_6

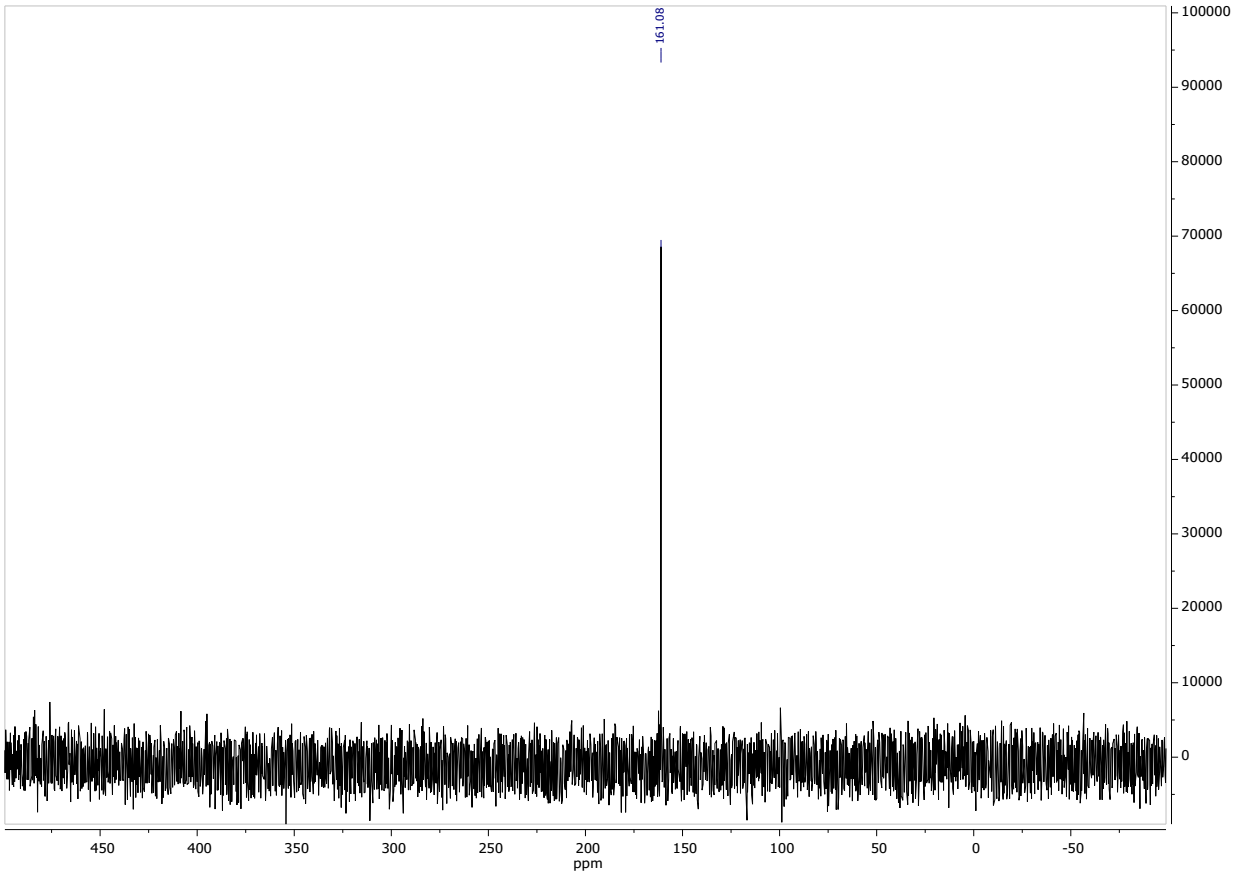


Figure-33: ^{13}C NMR spectrum (76 MHz) of **4b** in DMSO-d_6

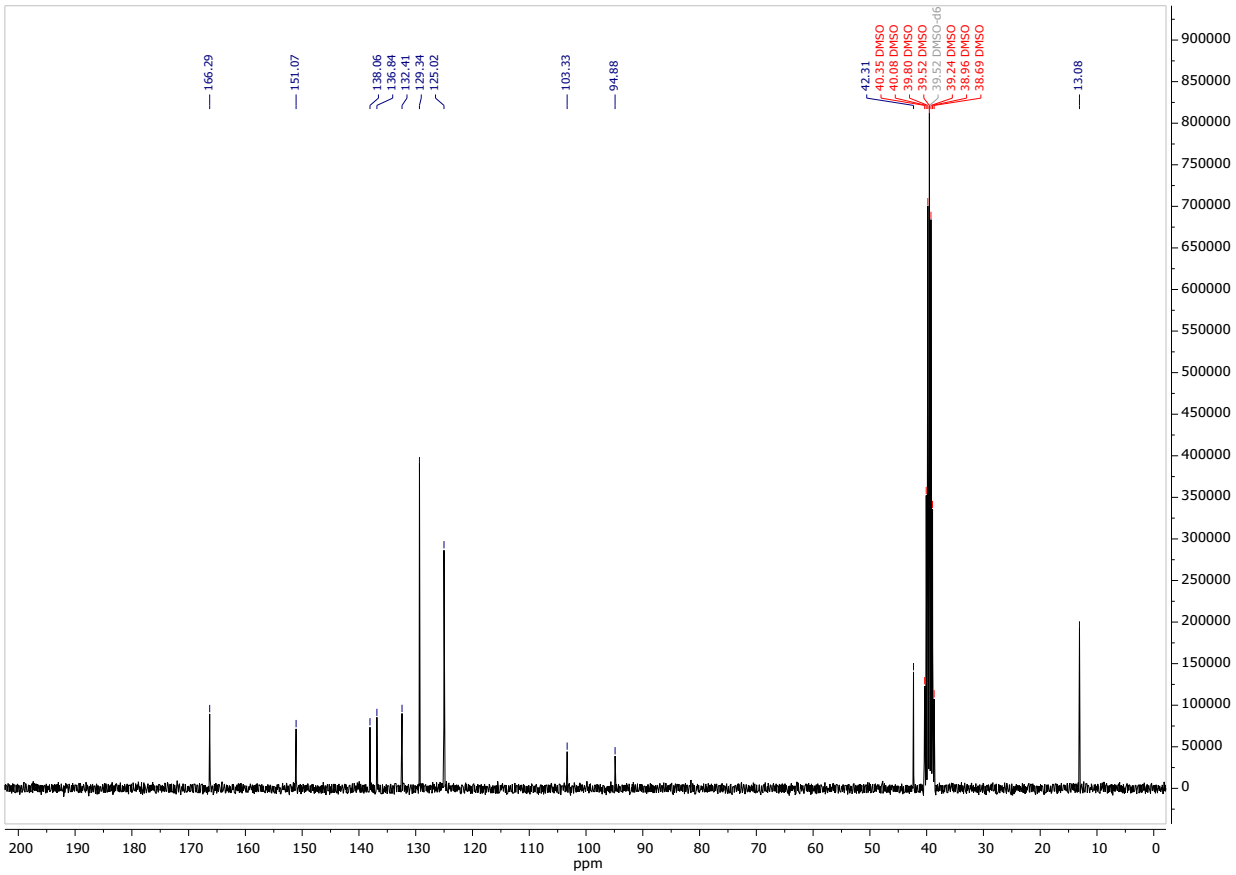
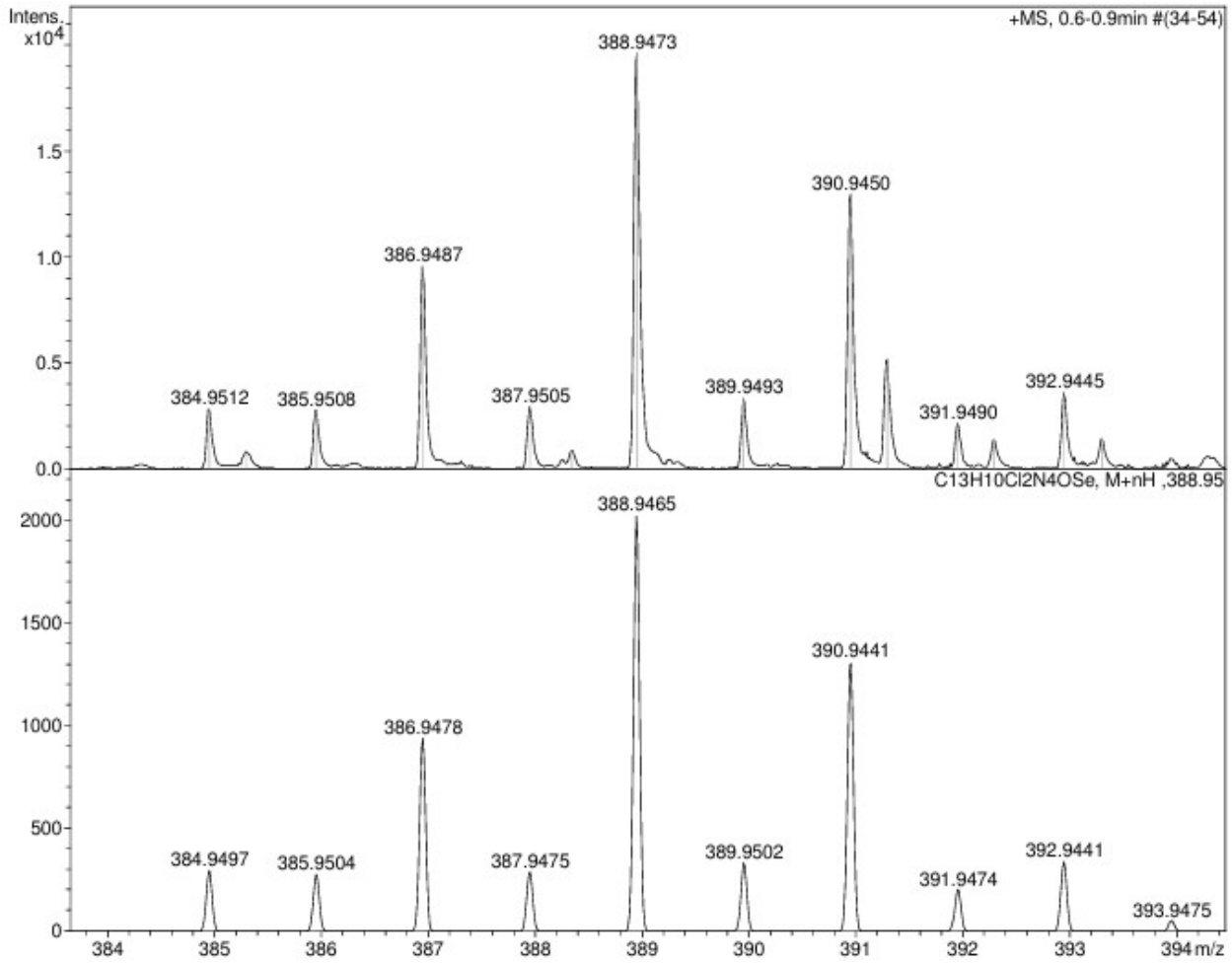
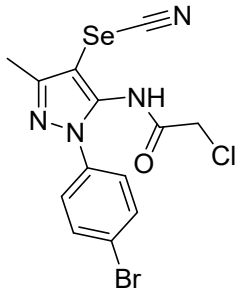


Figure-34: HRMS spectrum of compound **4b**





N-(1-(4-bromophenyl)-3-methyl-4-selenocyanato-1H-pyrazol-5-yl)-2-chloroacetamide, ***4c***

Grey powder, m.p. 169-171°C, yield 96% (0.83 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.78 (s, 1H), 7.71 (d, J = 8.5 Hz, 2H), 7.46 (d, J = 8.6 Hz, 2H), 4.33 (s, 2H), 2.34 (s, 3H). ^{77}Se NMR (57 MHz, DMSO) δ 161.08. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.37, 151.19, 138.10, 137.30, 132.34, 125.32, 120.90, 103.39, 95.00, 42.36, 13.14. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{13}H_{11}BrClN_4OSe$]$^{+}$: 432,8959; found: 432,8959.

Figure-35: ^{1}H NMR spectrum (300 MHz) of **4c** in DMSO-d_6

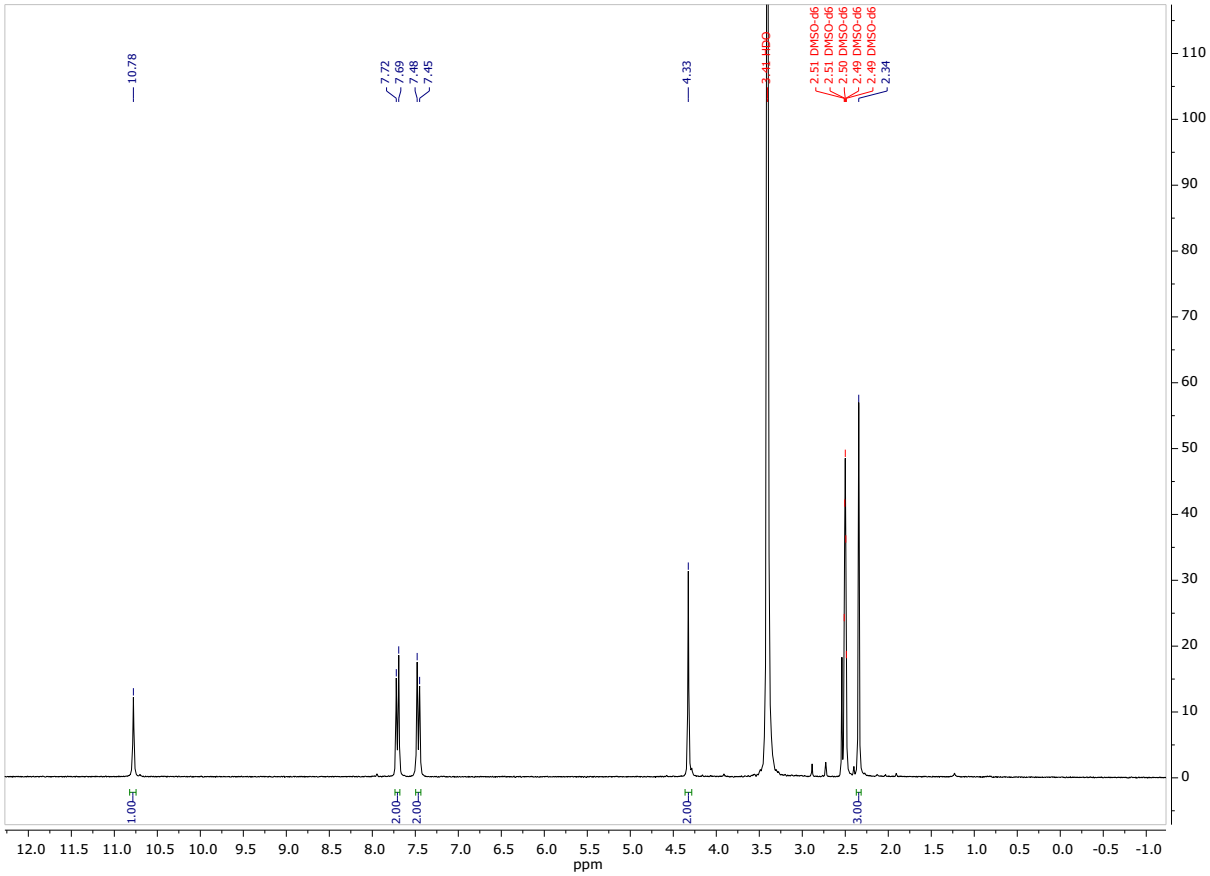


Figure-36: ^{77}Se NMR spectrum (57 MHz) of **4c** in DMSO-d_6

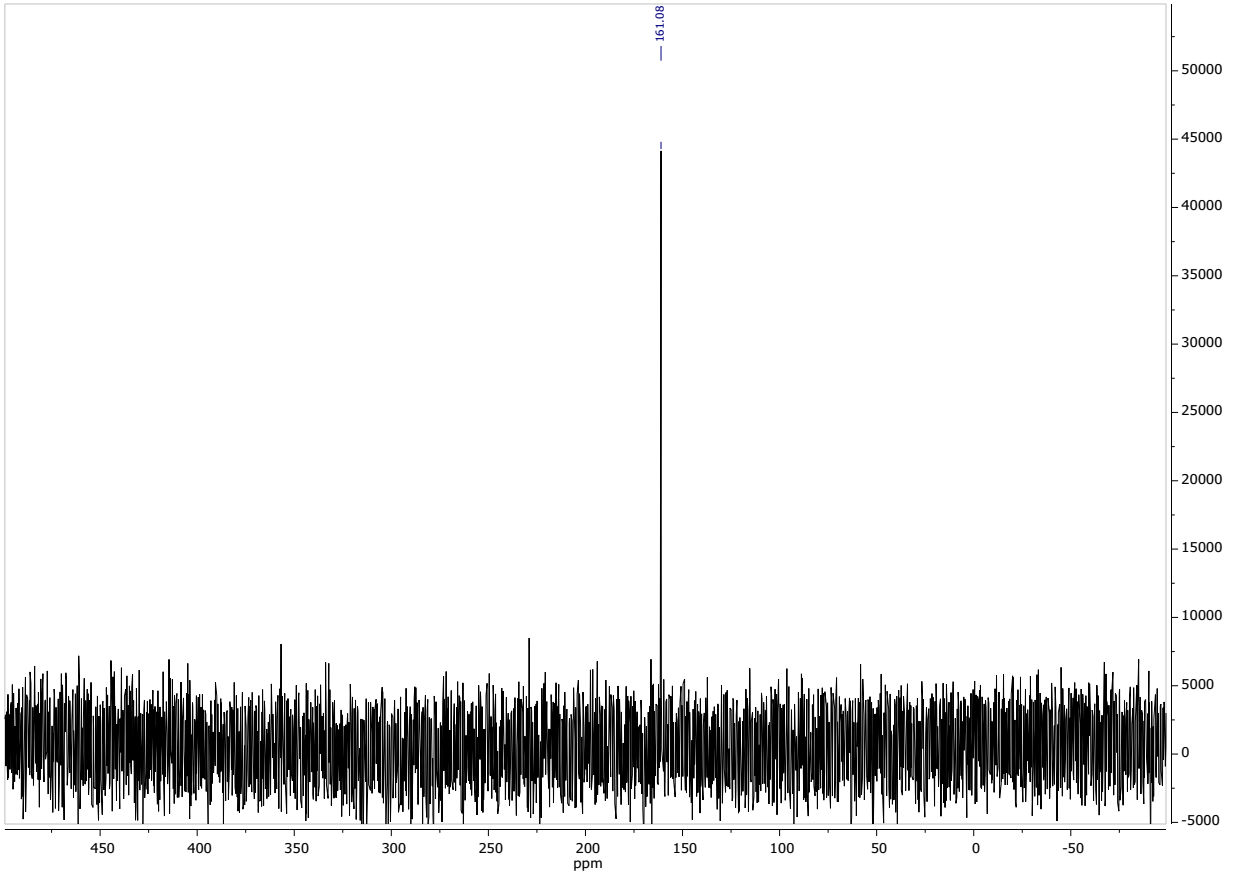


Figure-37: ^{13}C NMR spectrum (76 MHz) of **4c** in DMSO-d_6

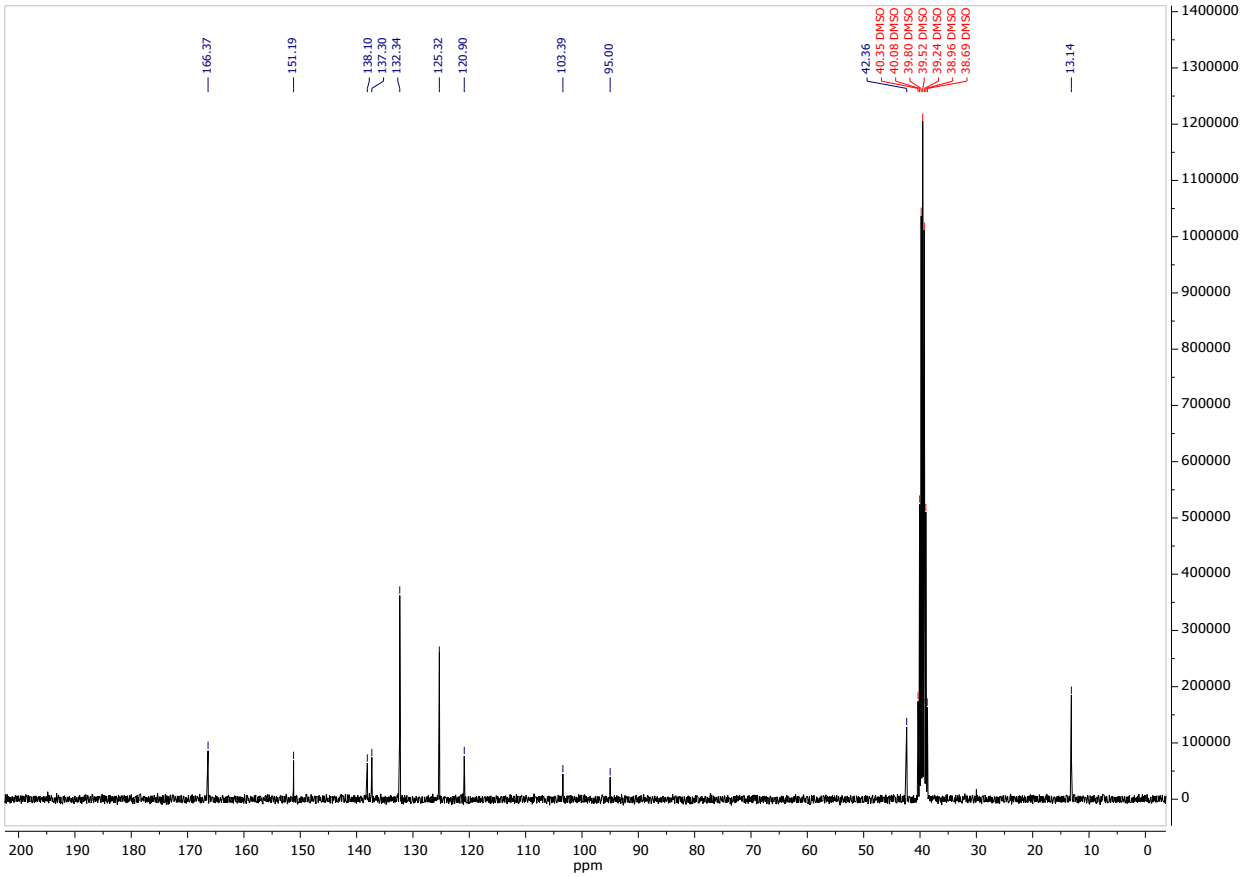
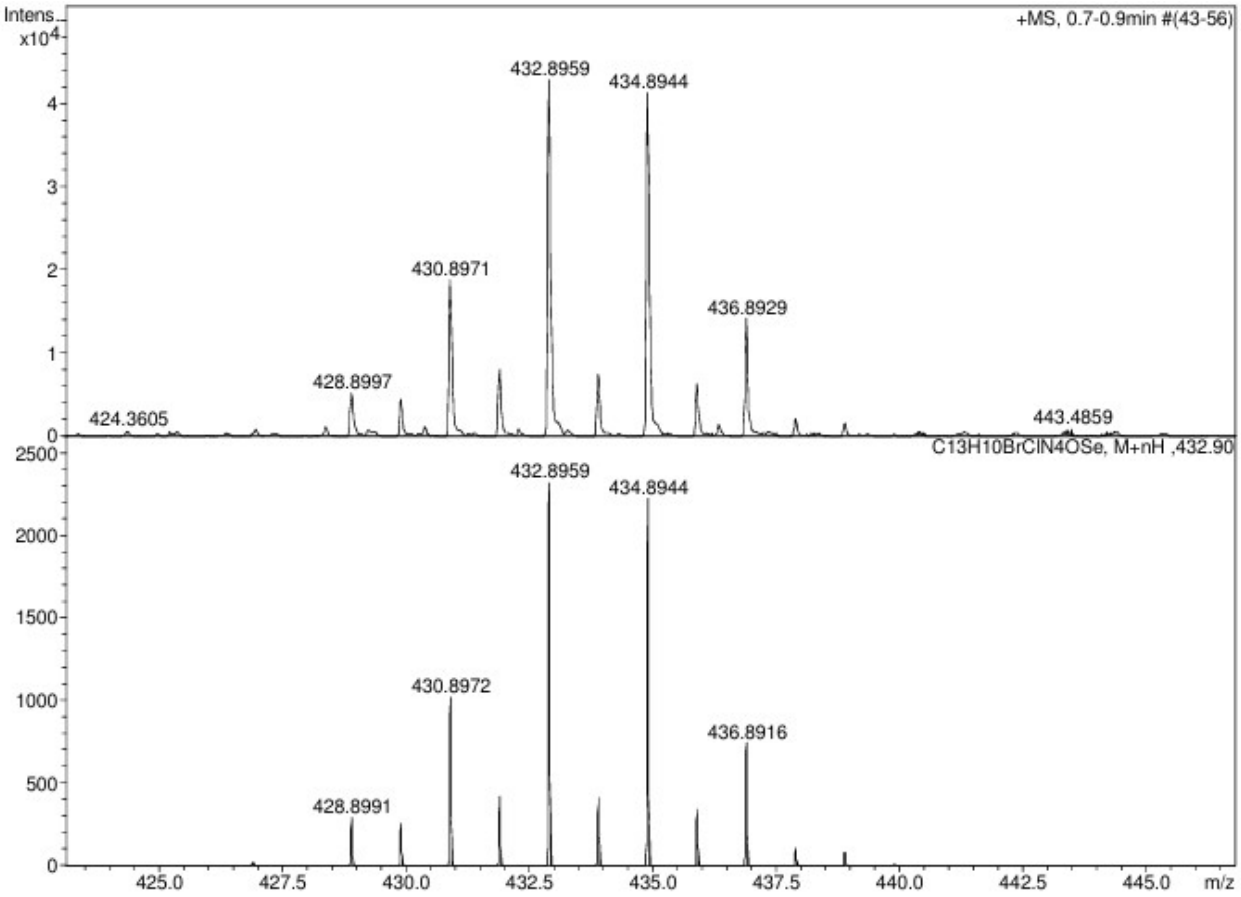
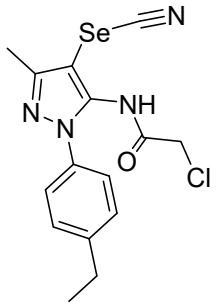


Figure-38: HRMS spectrum of compound **4c**





2-Chloro-N-(1-(4-ethylphenyl)-3-methyl-4-selenocyanato-1H-pyrazol-5-yl)acetamide, ***4d***

White powder, m.p. 142-144°C, yield 85% (0.65 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.72 (s, 1H), 7.46 – 7.28 (m, 4H), 4.32 (s, 2H), 2.66 (q, J = 7.6 Hz, 2H), 2.34 (s, 3H), 1.21 (t, J = 7.6 Hz, 3H). ^{77}Se NMR (57 MHz, DMSO) δ 160.21. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.38, 150.55, 143.85, 137.76, 135.78, 128.58, 123.36, 103.28, 94.28, 42.28, 27.71, 15.43, 13.08. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{15}H_{16}ClN_4OSe$]$^{+}$: 383.0170; found: 383.0167.

Figure-39: ^{1}H NMR spectrum (300 MHz) of **4d** in DMSO-d_6

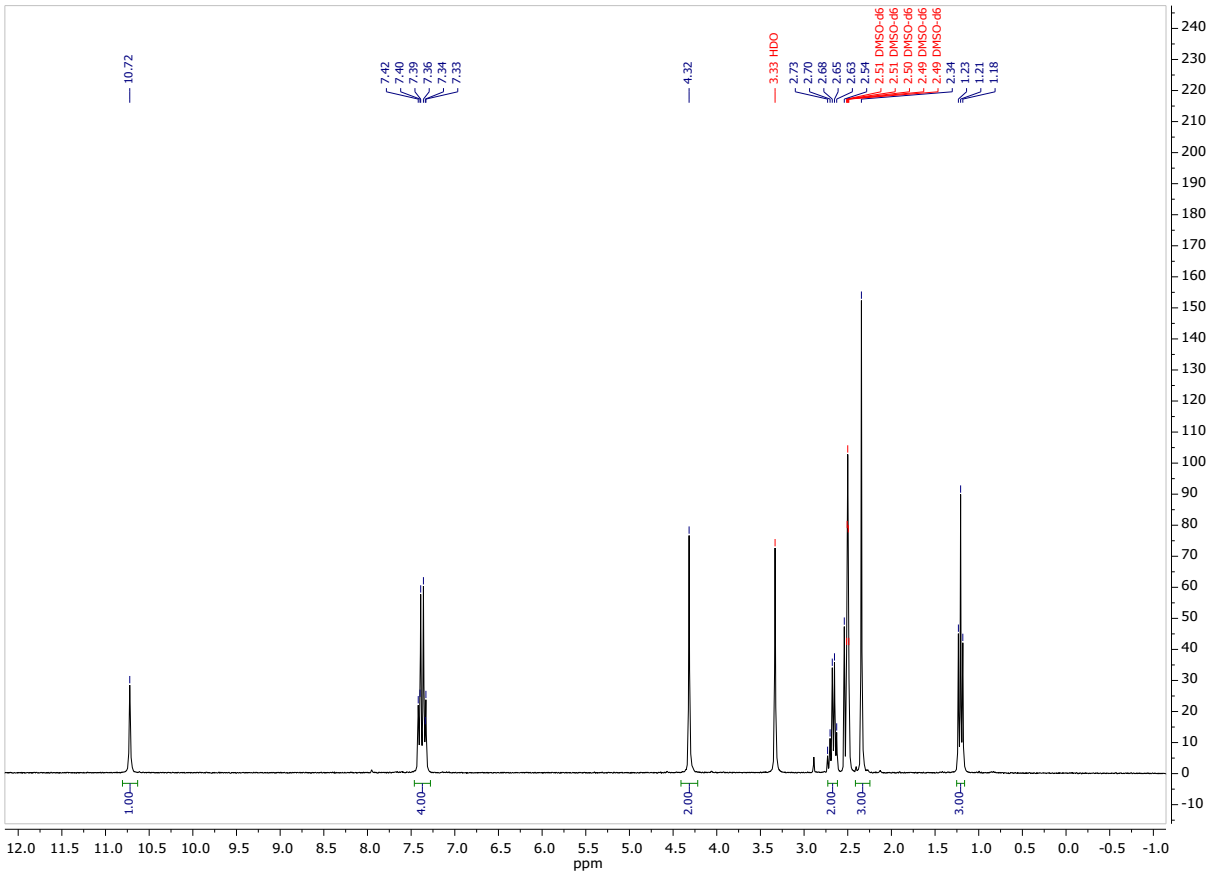


Figure-40: ^{77}Se NMR spectrum (57 MHz) of **4d** in DMSO-d_6

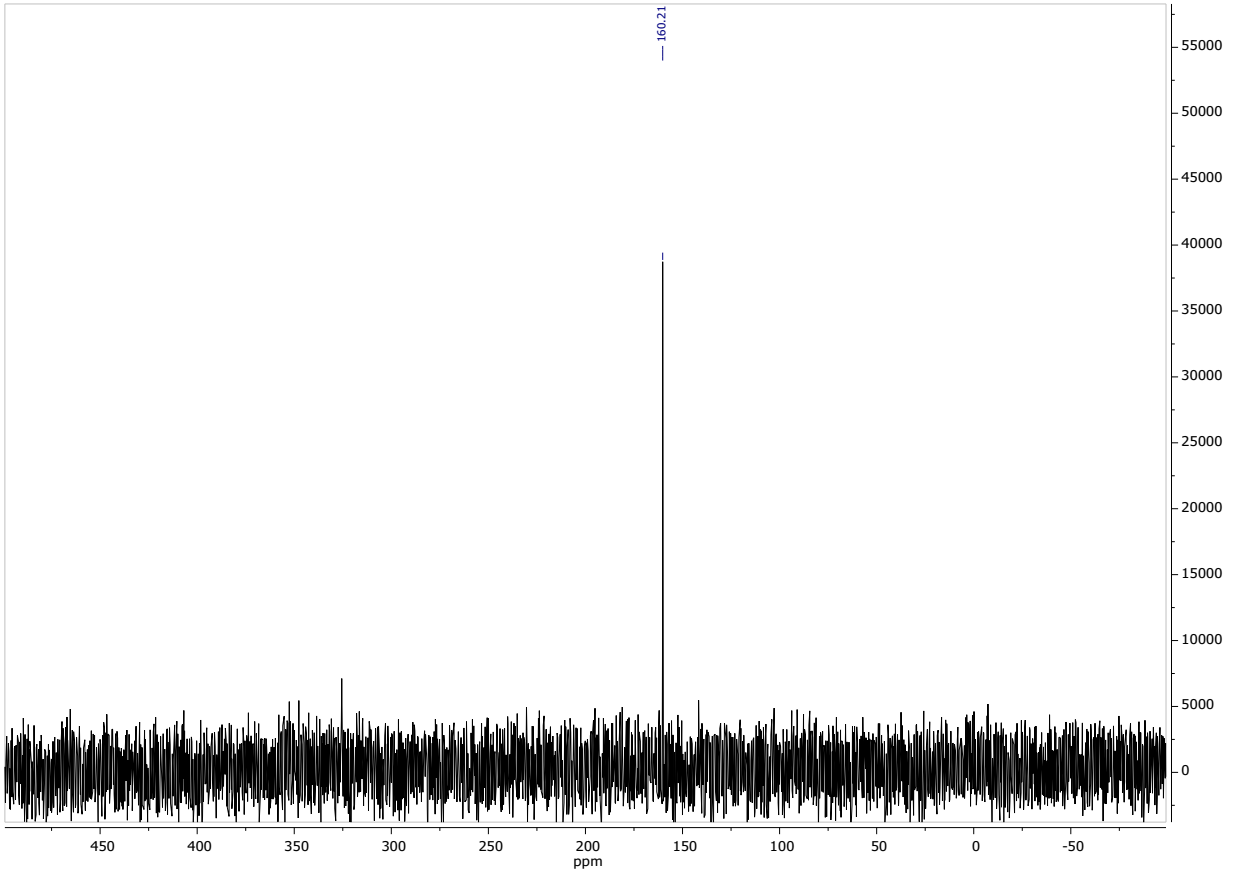


Figure-41: ^{13}C NMR spectrum (76 MHz) of **4d** in DMSO-d_6

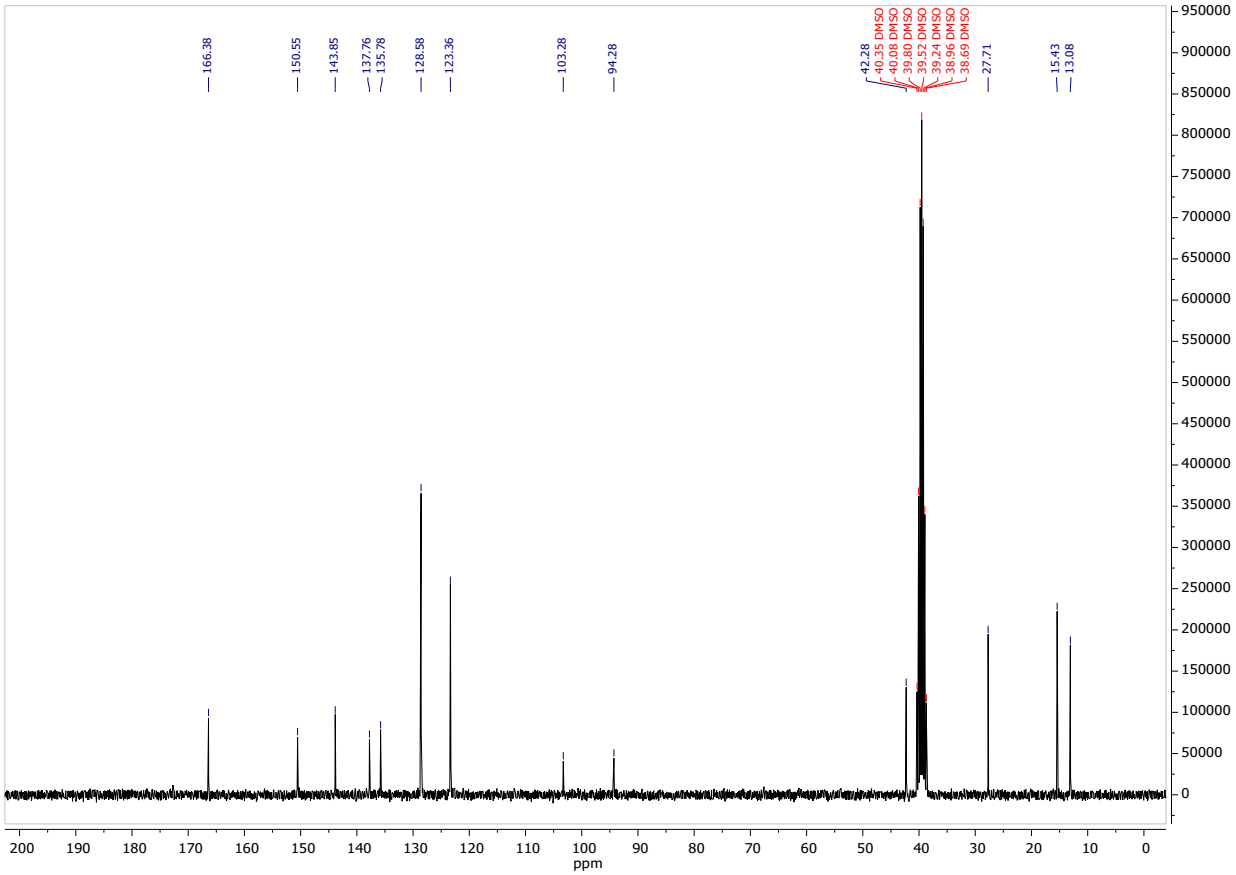
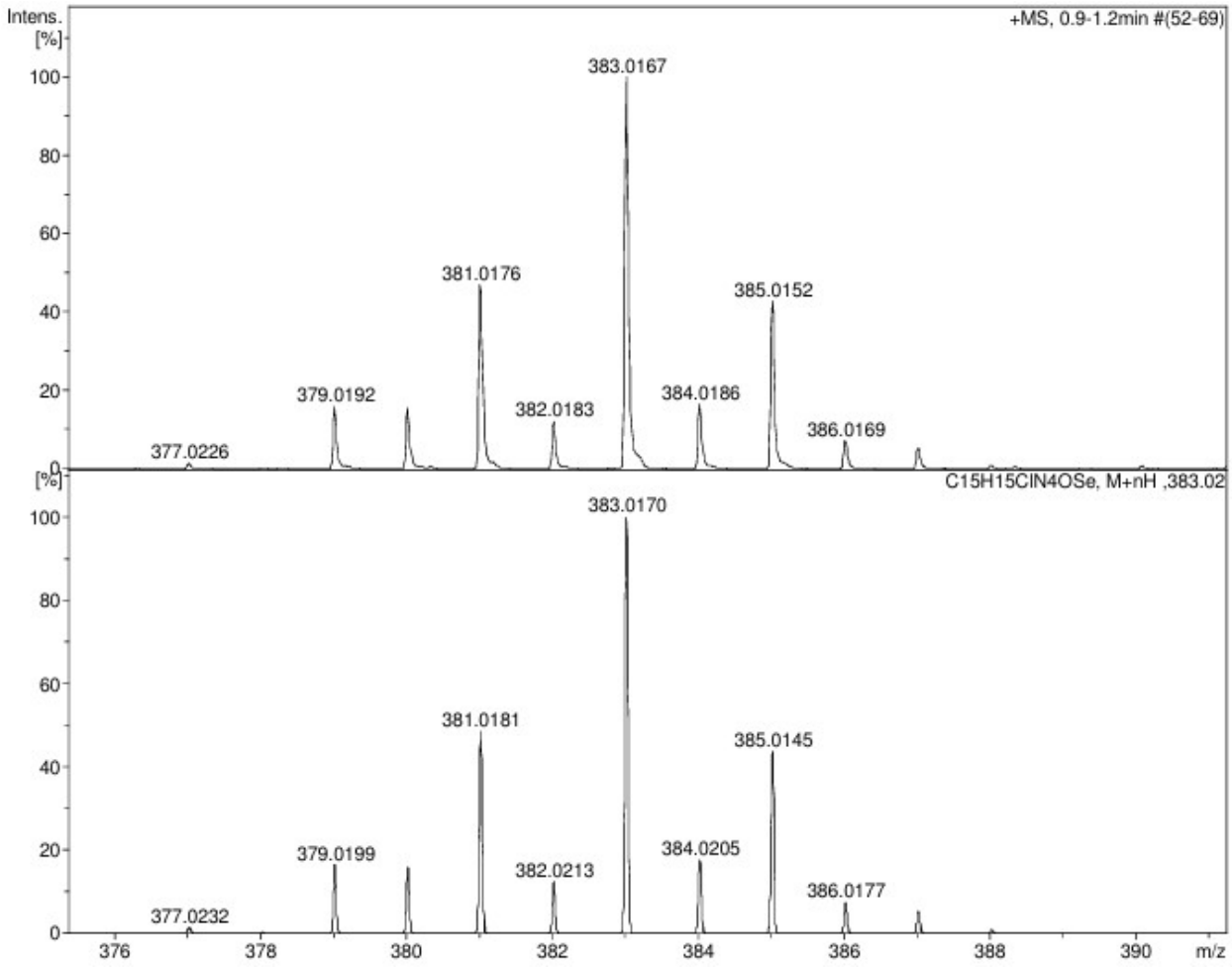
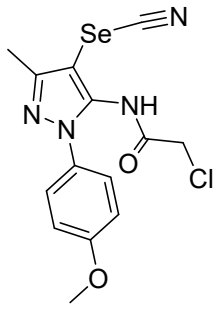


Figure-42: HRMS spectrum of compound **4d**





2-Chloro-N-(1-(4-methoxyphenyl)-3-methyl-4-selenocyanato-1H-pyrazol-5-yl)acetamide, ***4e***

Grey powder, m.p. 177-179°C, yield 64% (0.49 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.66 (s, 1H), 7.39 (d, J = 8.8 Hz, 2H), 7.05 (d, J = 8.9 Hz, 2H), 4.29 (s, 2H), 3.80 (s, 3H), 2.33 (s, 3H). ^{77}Se NMR (57 MHz, DMSO) δ 159.32. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.41, 158.92, 150.39, 137.90, 131.04, 125.17, 114.41, 103.34, 93.87, 55.53, 42.28, 13.09. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{14}H_{14}ClN_4O_2Se$]$^{+}$: 384.9963; found: 384.9959.

Figure-43: ^{1}H NMR spectrum (300 MHz) of **4e** in DMSO-d_6

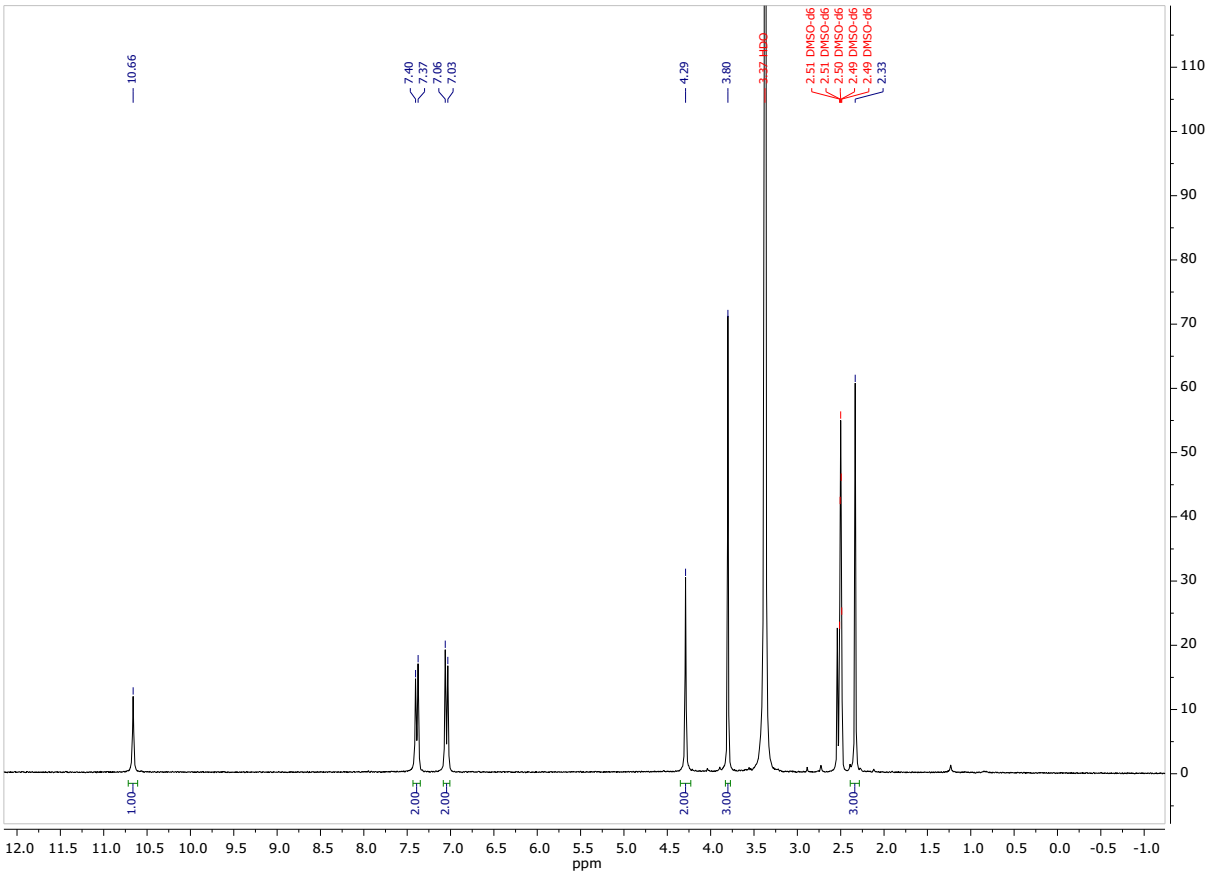


Figure-44: ^{77}Se NMR spectrum (57 MHz) of **4e** in DMSO-d_6

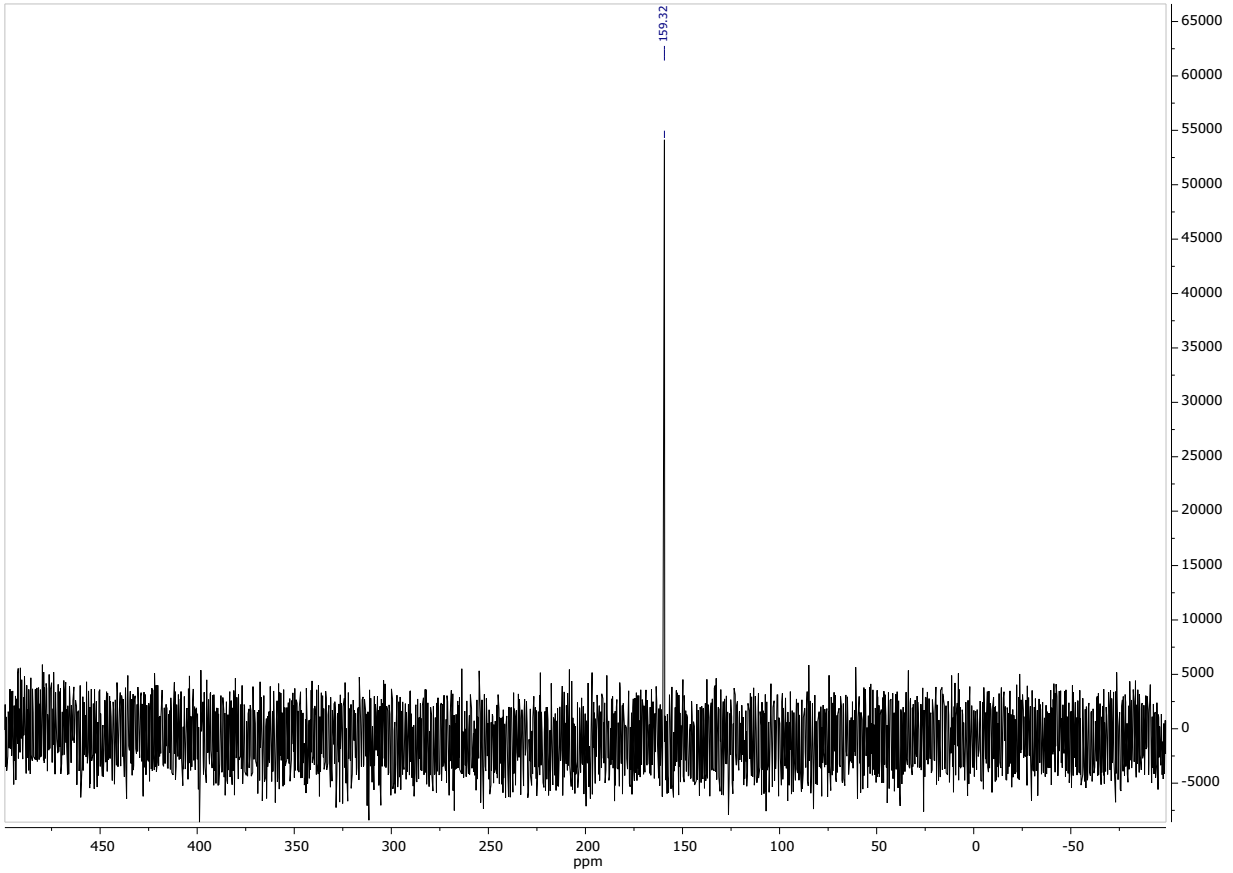


Figure-45: ^{13}C NMR spectrum (76 MHz) of **4e** in DMSO-d_6

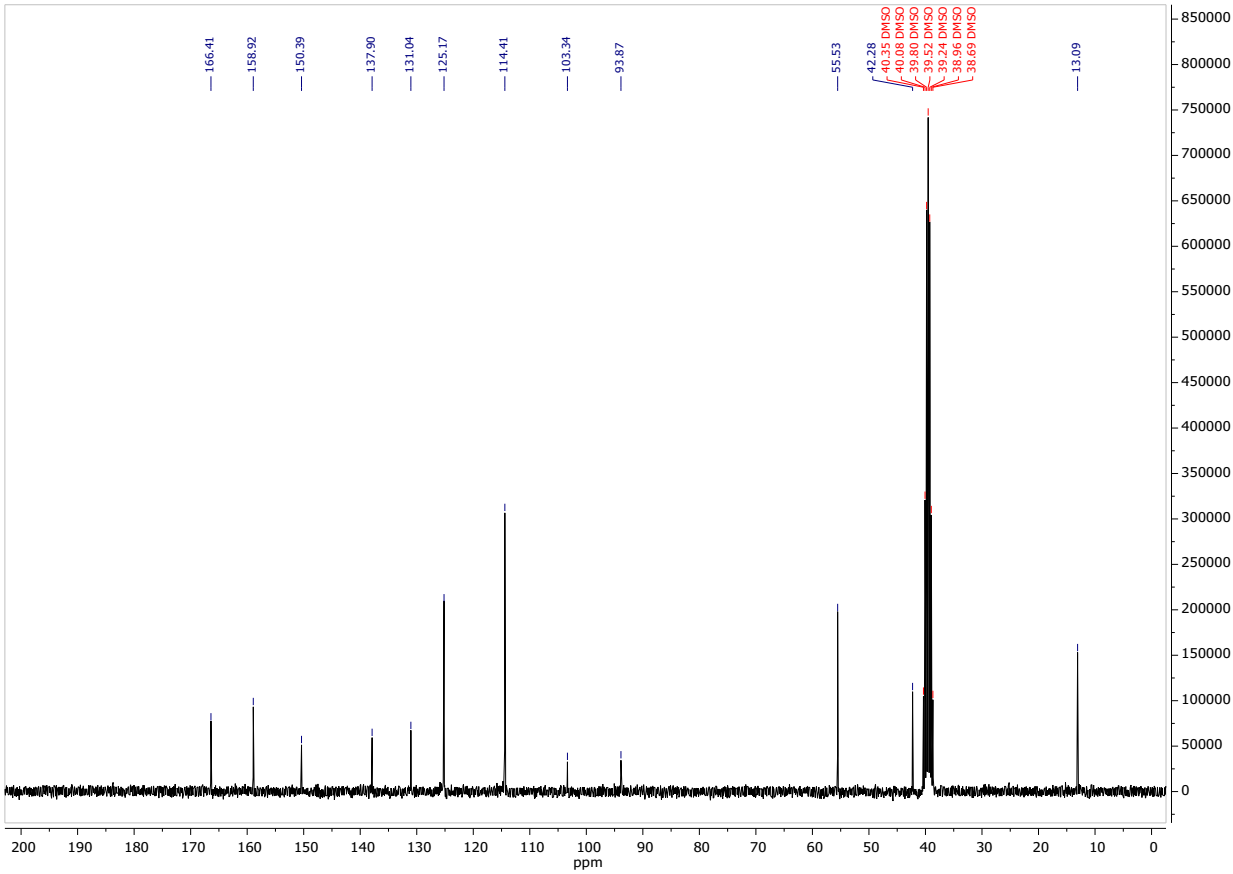
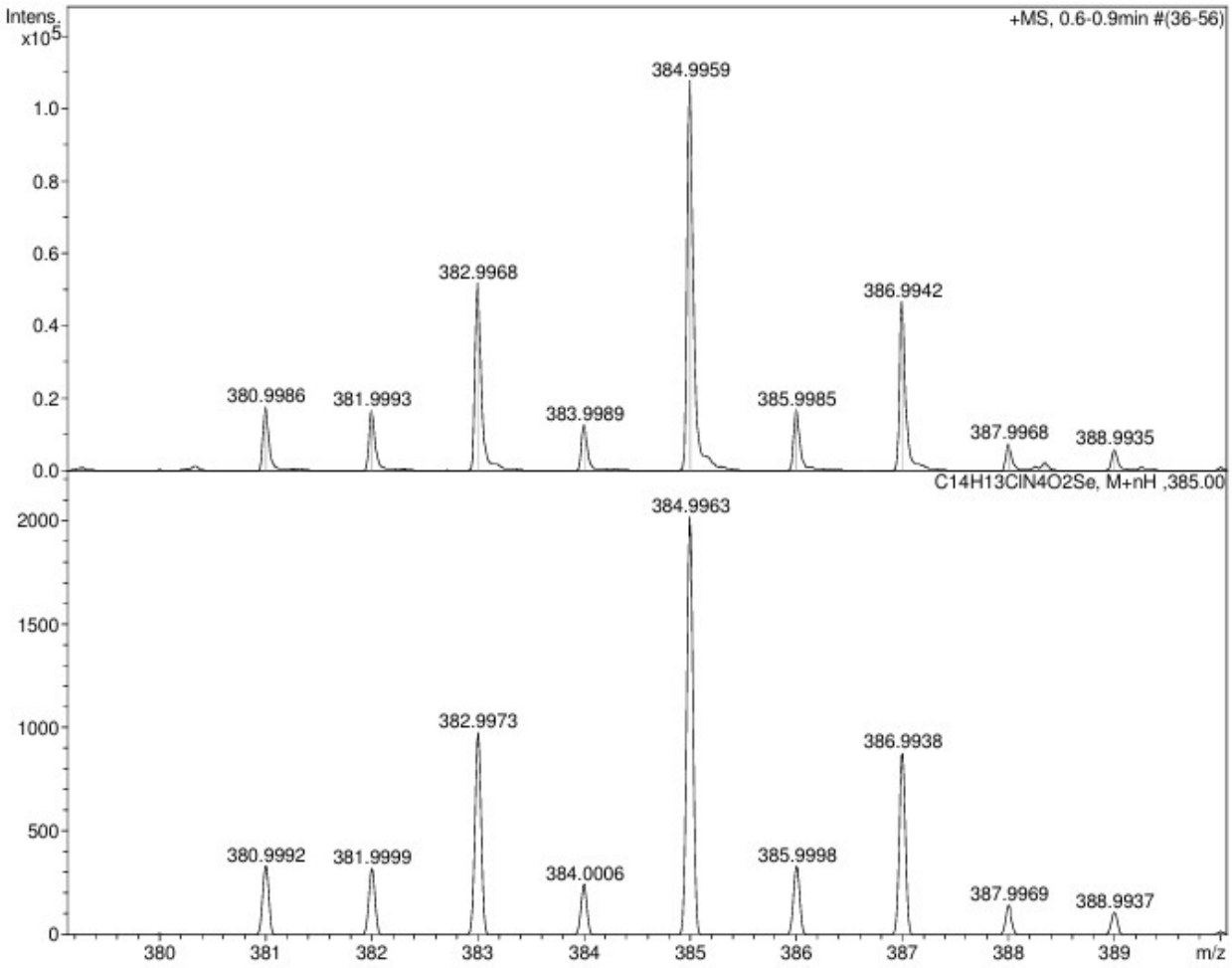
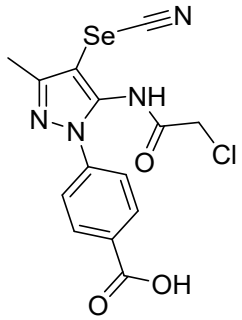


Figure-46: HRMS spectrum of compound **4e**





4-(5-(2-Chloroacetamido)-3-methyl-4-selenocyanato-1H-pyrazol-1-yl)benzoic acid, ***4f***

Grey powder, m.p. 279-281°C, yield 77% (0.62 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 13.14 (brs, s, 1H), 10.87 (s, 1H), 8.05 (d, J = 8.3 Hz, 2H), 7.66 (d, J = 8.3 Hz, 2H), 4.36 (s, 2H), 2.36 (s, 3H). ^{77}Se NMR (57 MHz, DMSO) δ 161.74. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.56, 166.32, 151.47, 141.38, 138.22, 130.56, 129.82, 122.79, 103.37, 95.58, 42.40, 13.15. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{14}H_{12}ClN_4O_3Se$]$^{+}$: 398.9756; found: 398.9755.

Figure-47: ^{1}H NMR spectrum (300 MHz) of **4f** in DMSO-d_6

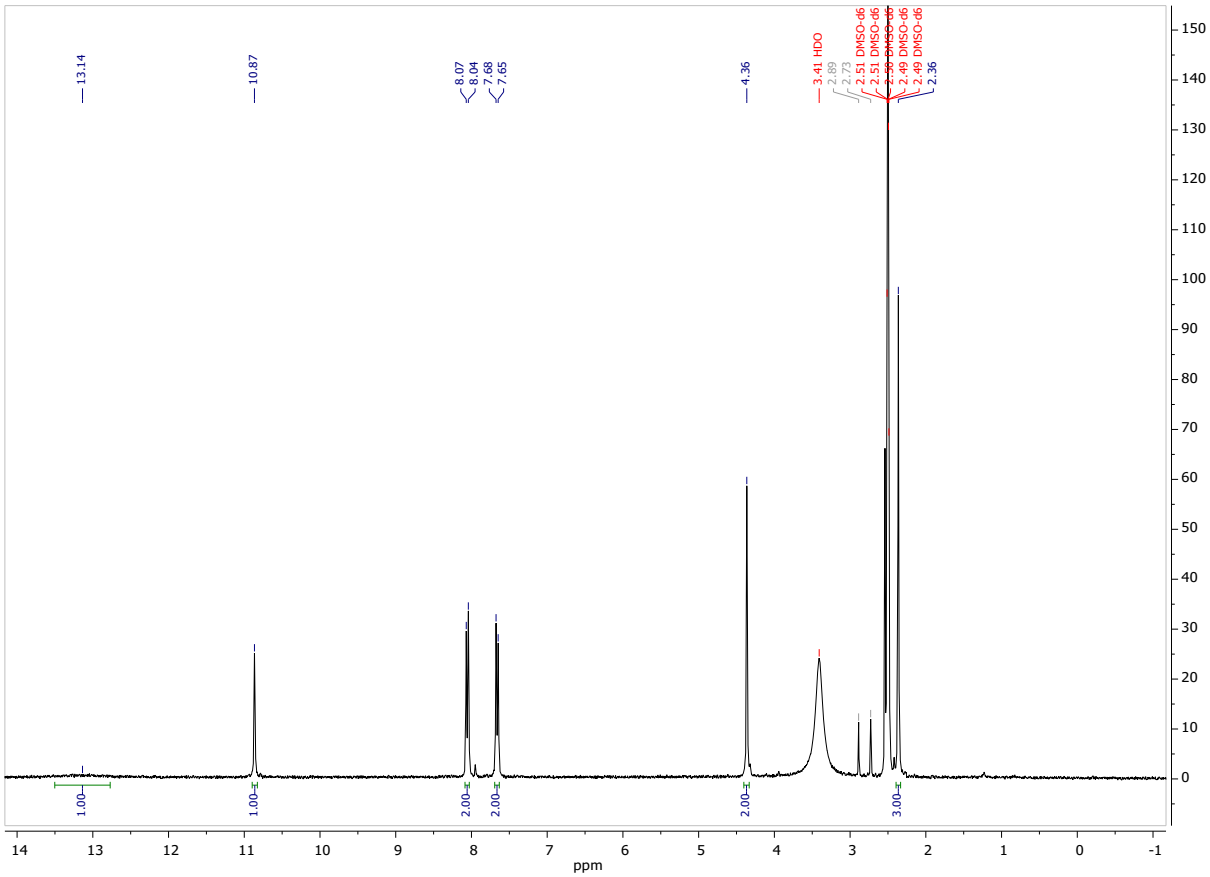


Figure-48: ^{77}Se NMR spectrum (57 MHz) of **4f** in DMSO-d_6

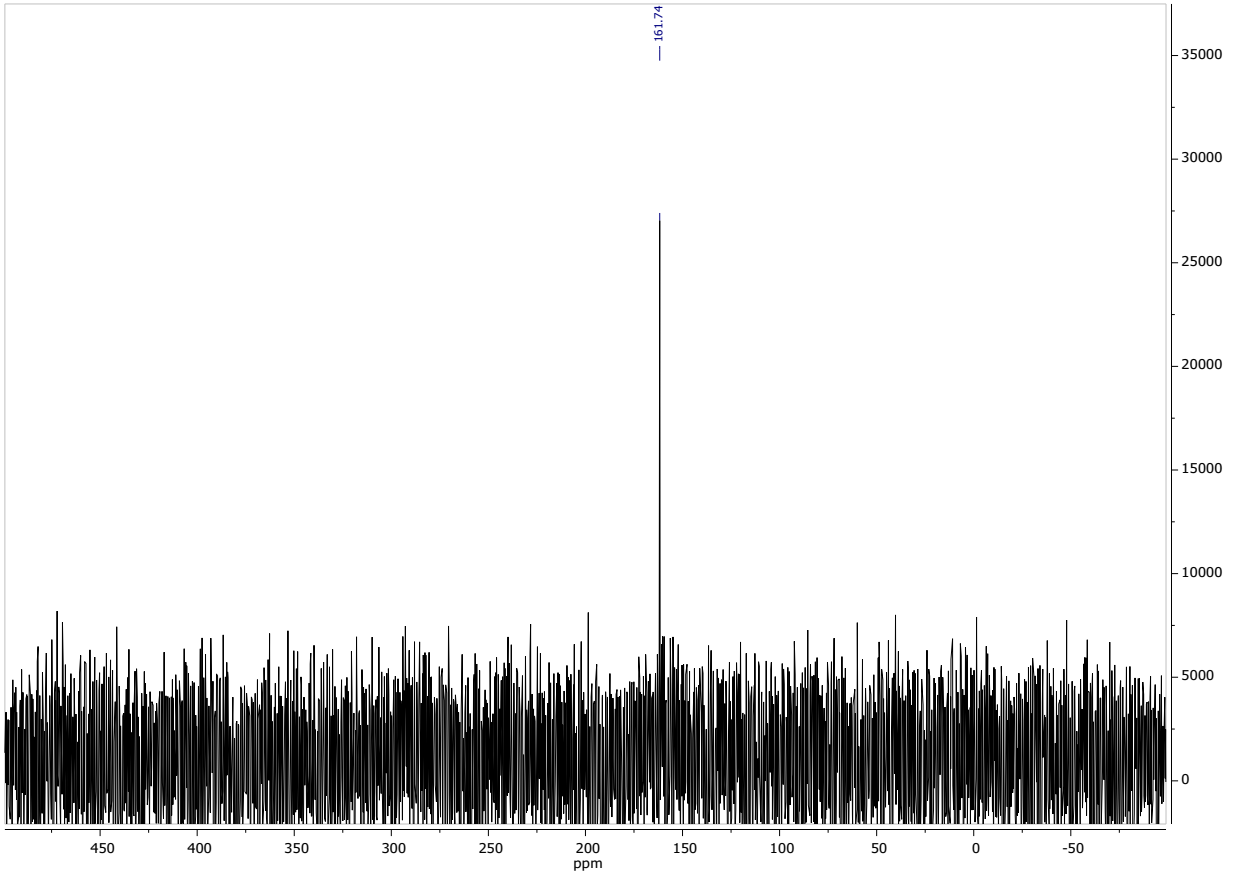


Figure-49: ^{13}C NMR spectrum (76 MHz) of **4f** in DMSO-d_6

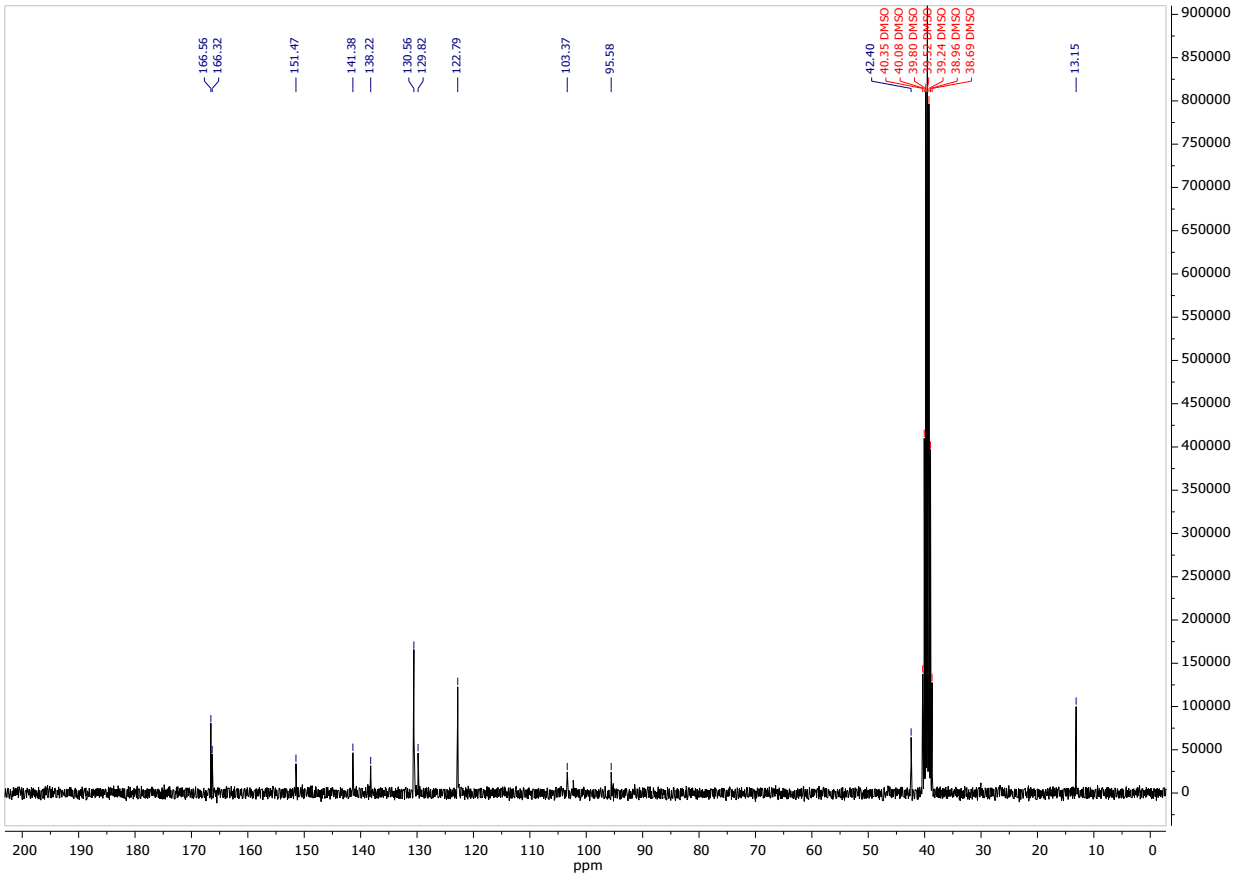
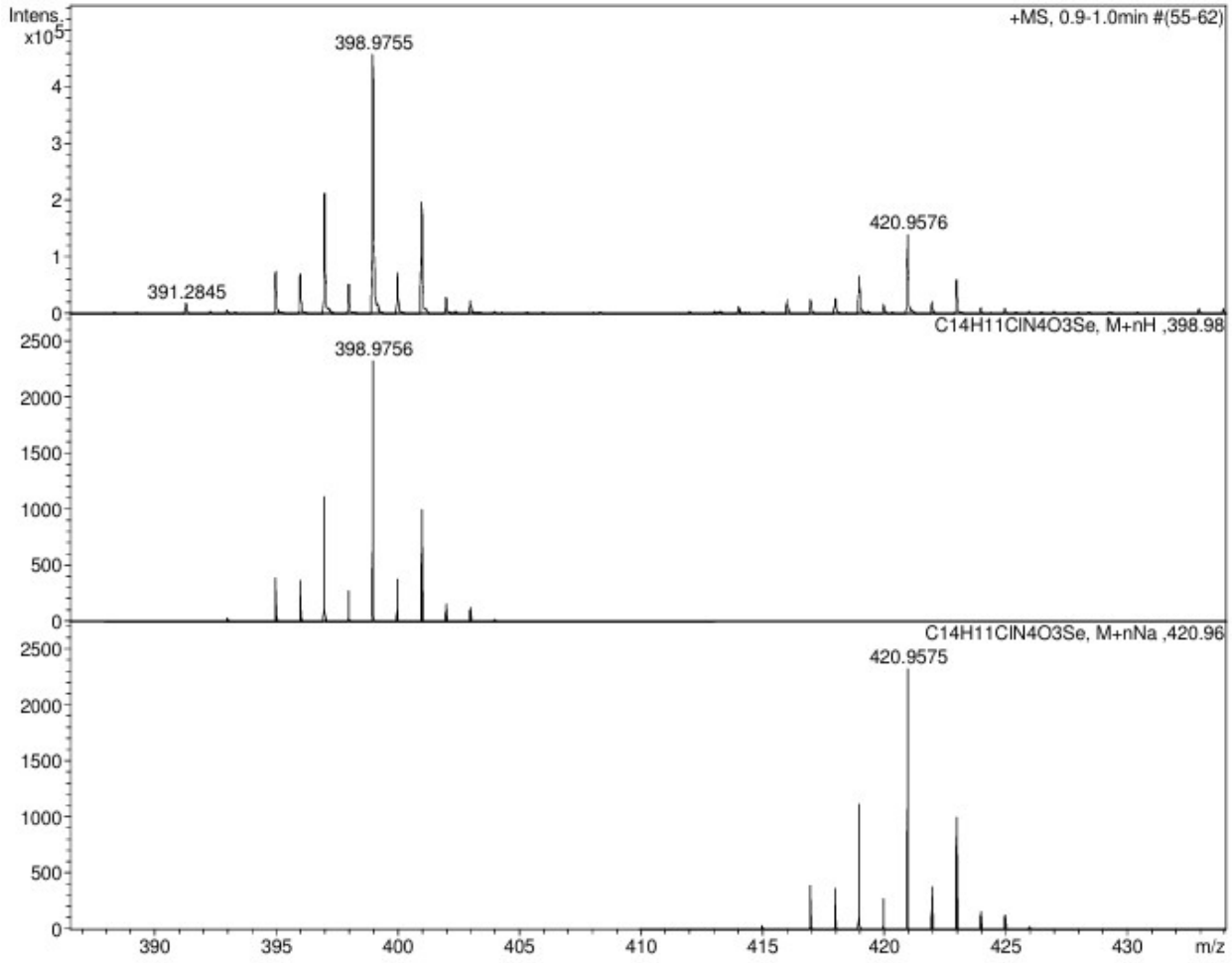
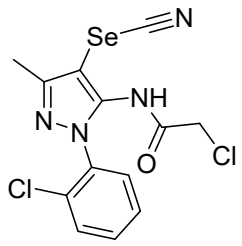


Figure-50: HRMS spectrum of compound **4f**





2-Chloro-N-(1-(2-chlorophenyl)-3-methyl-4-selenocyanato-1H-pyrazol-5-yl)acetamide, ***4g***

Grey powder, m.p. 124-126°C, yield 89% (0.69 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.76 (s, 1H), 7.69 – 7.64 (m, 1H), 7.59 – 7.48 (m, 3H), 4.20 (s, 2H), 2.33 (s, 3H). ^{77}Se NMR (57 MHz, DMSO) δ 164.62. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.14, 150.84, 139.26, 135.19, 131.38, 130.56, 130.22, 129.97, 128.21, 103.87, 103.59, 42.16, 13.20. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{13}H_{11}Cl_2N_4OSe$]$^{+}$: 388.9465; found: 388.9460.

Figure-51: ^{1}H NMR spectrum (300 MHz) of **4g** in DMSO-d_6

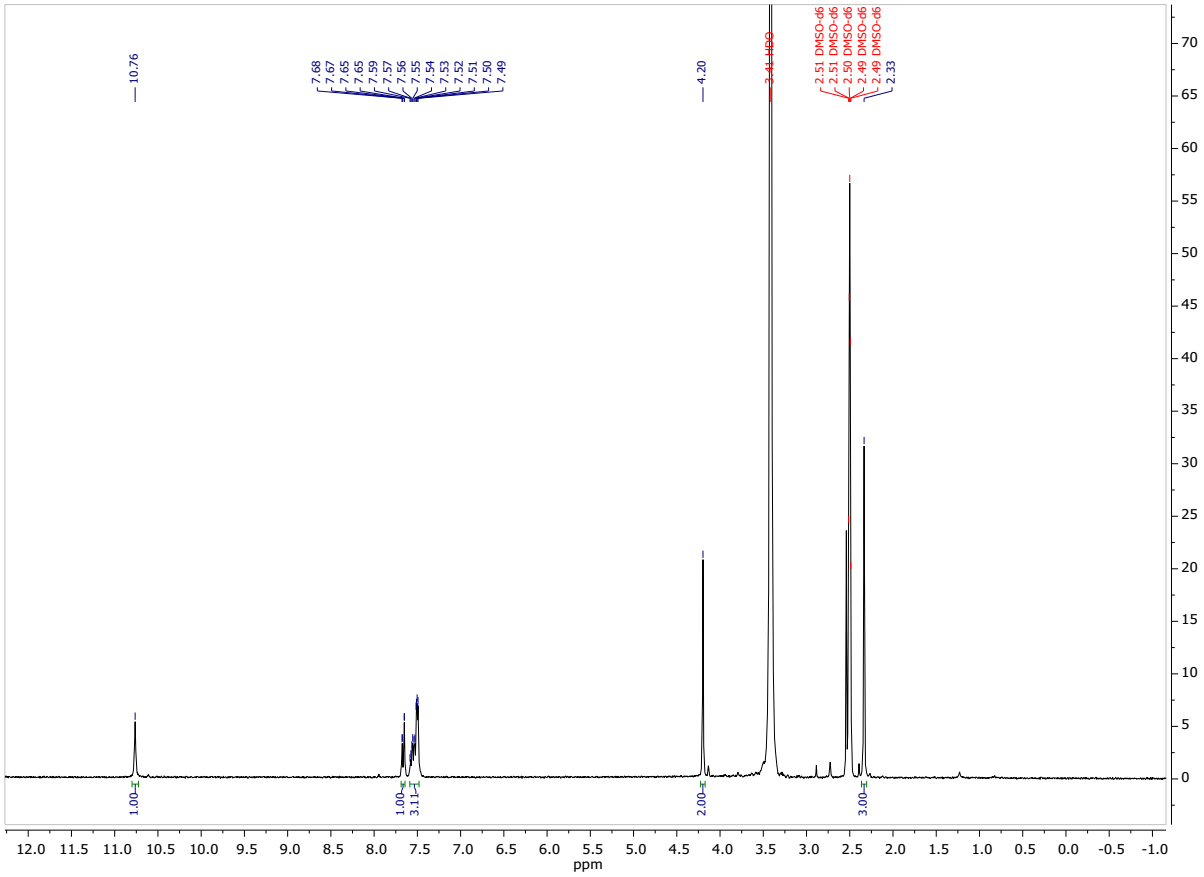


Figure-52: ^{77}Se NMR spectrum (57 MHz) of **4g** in DMSO-d_6

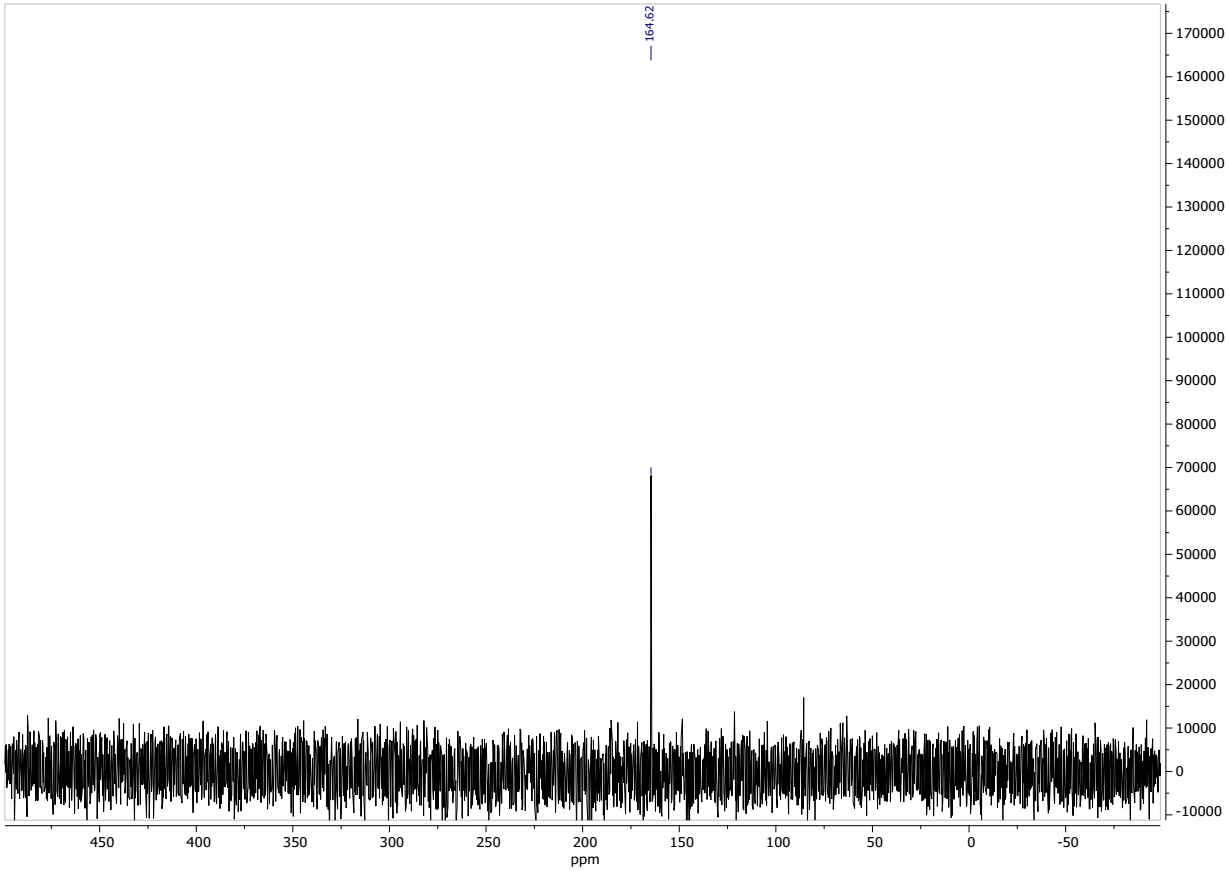


Figure-53: ^{13}C NMR spectrum (76 MHz) of **4g** in DMSO-d_6

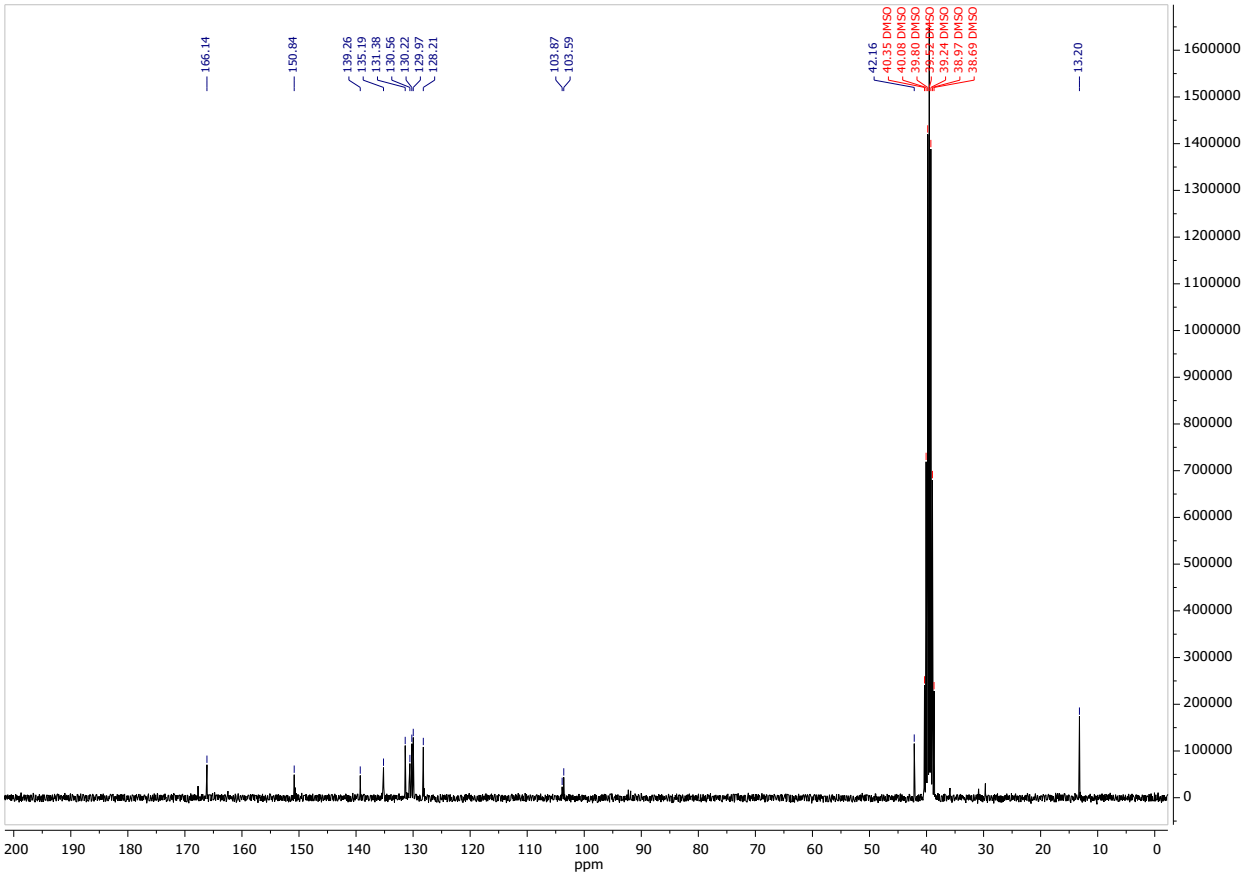
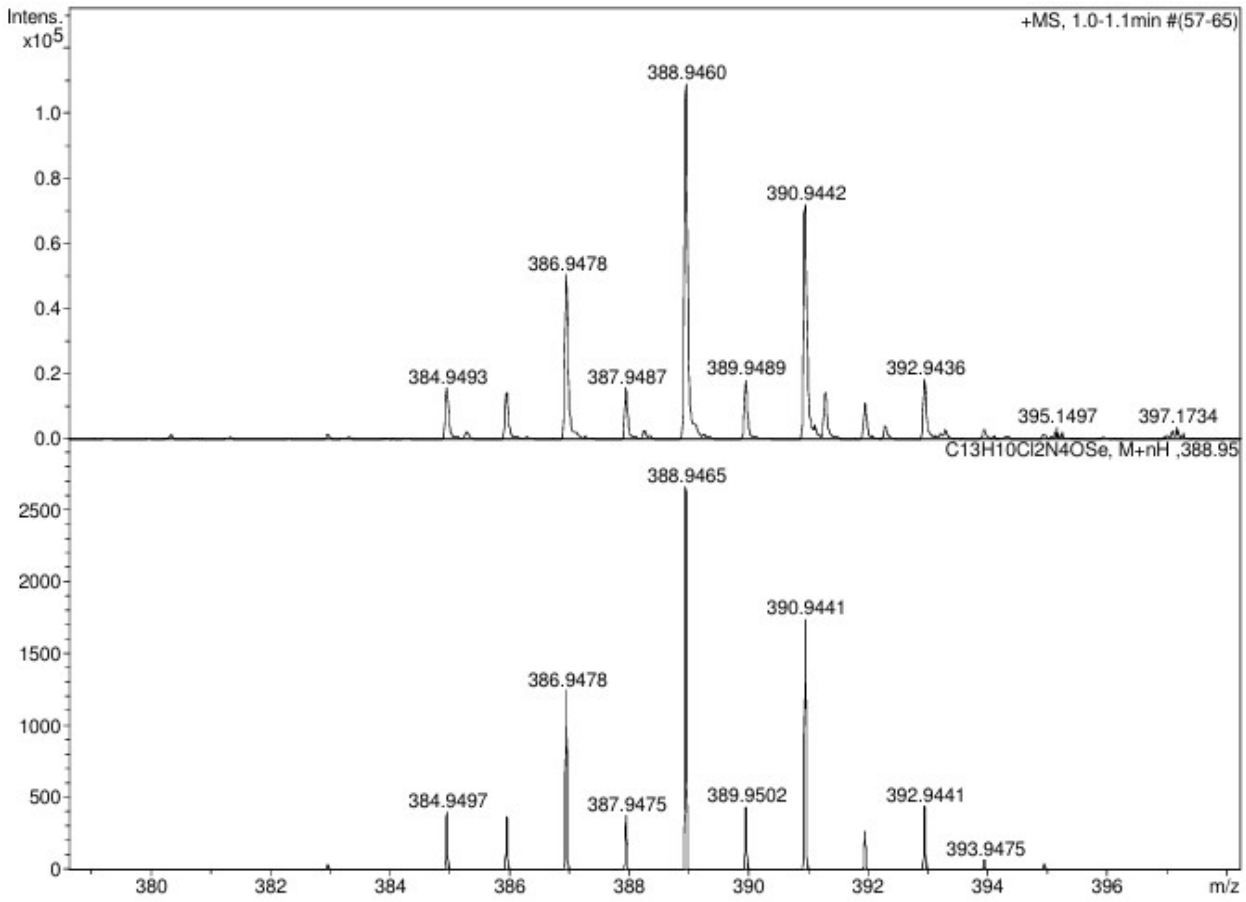
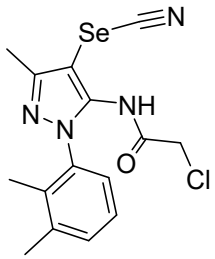


Figure-54: HRMS spectrum of compound **4g**





2-Chloro-N-(1-(2,3-dimethylphenyl)-3-methyl-4-selenocyanato-1H-pyrazol-5-yl)acetamide, ***4h***

Gray powder, m.p. 179-181°C, yield 80% (0.61 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.56 (s, 1H), 7.32 (d, J = 7.5 Hz, 1H), 7.21 (t, J = 7.7 Hz, 1H), 7.04 (d, J = 7.8 Hz, 1H), 4.18 (s, 2H), 2.33 (s, 3H), 2.29 (s, 3H), 1.84 (s, 3H). ^{77}Se NMR (57 MHz, DMSO) δ 161.10. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.20, 150.12, 138.90, 138.06, 136.72, 133.95, 130.76, 125.88, 125.06, 103.47, 91.93, 42.09, 19.85, 13.95, 13.13. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{15}H_{16}ClN_4OSe$]$^{+}$: 383.0170; found: 383.0159.

Figure-55: ^{1}H NMR spectrum (300 MHz) of **4h** in DMSO-d_6

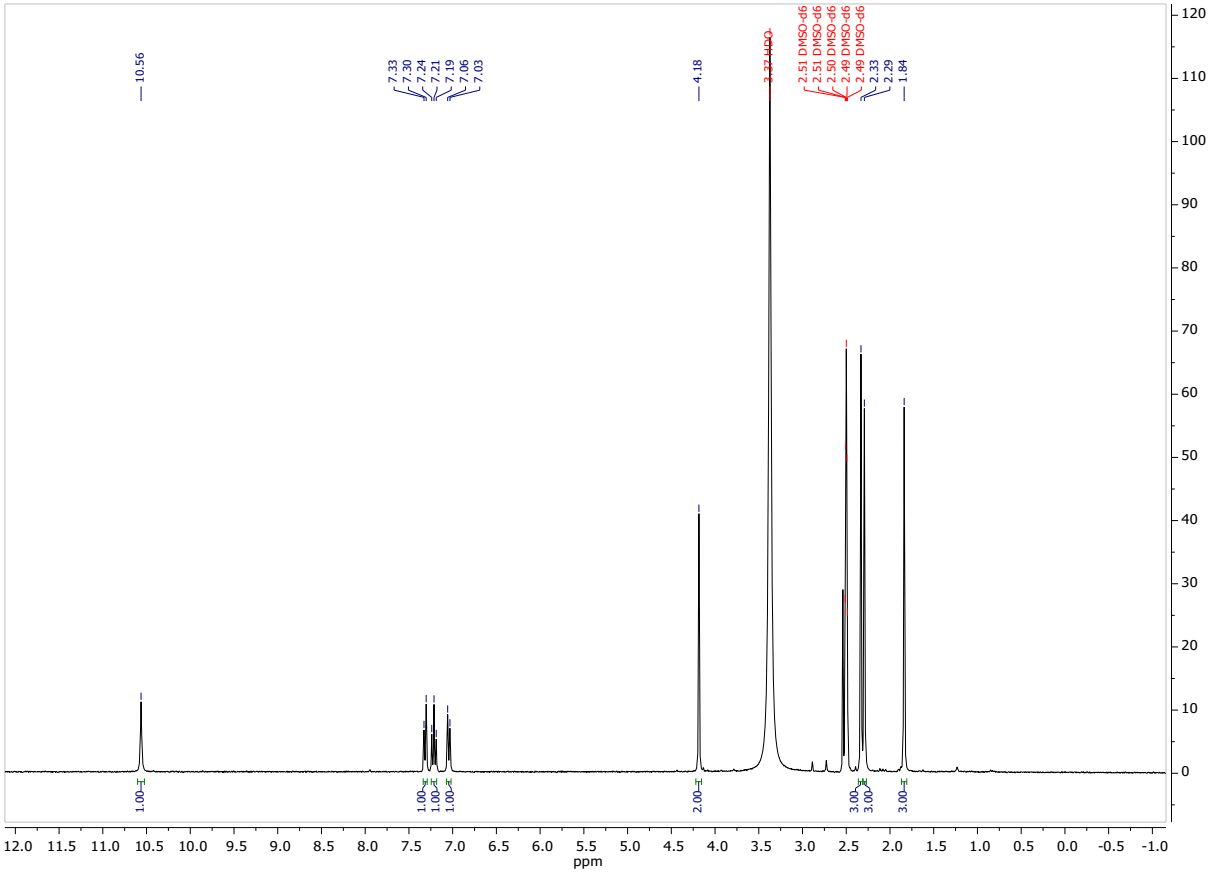


Figure-56: ^{77}Se NMR spectrum (57 MHz) of **4h** in DMSO-d_6

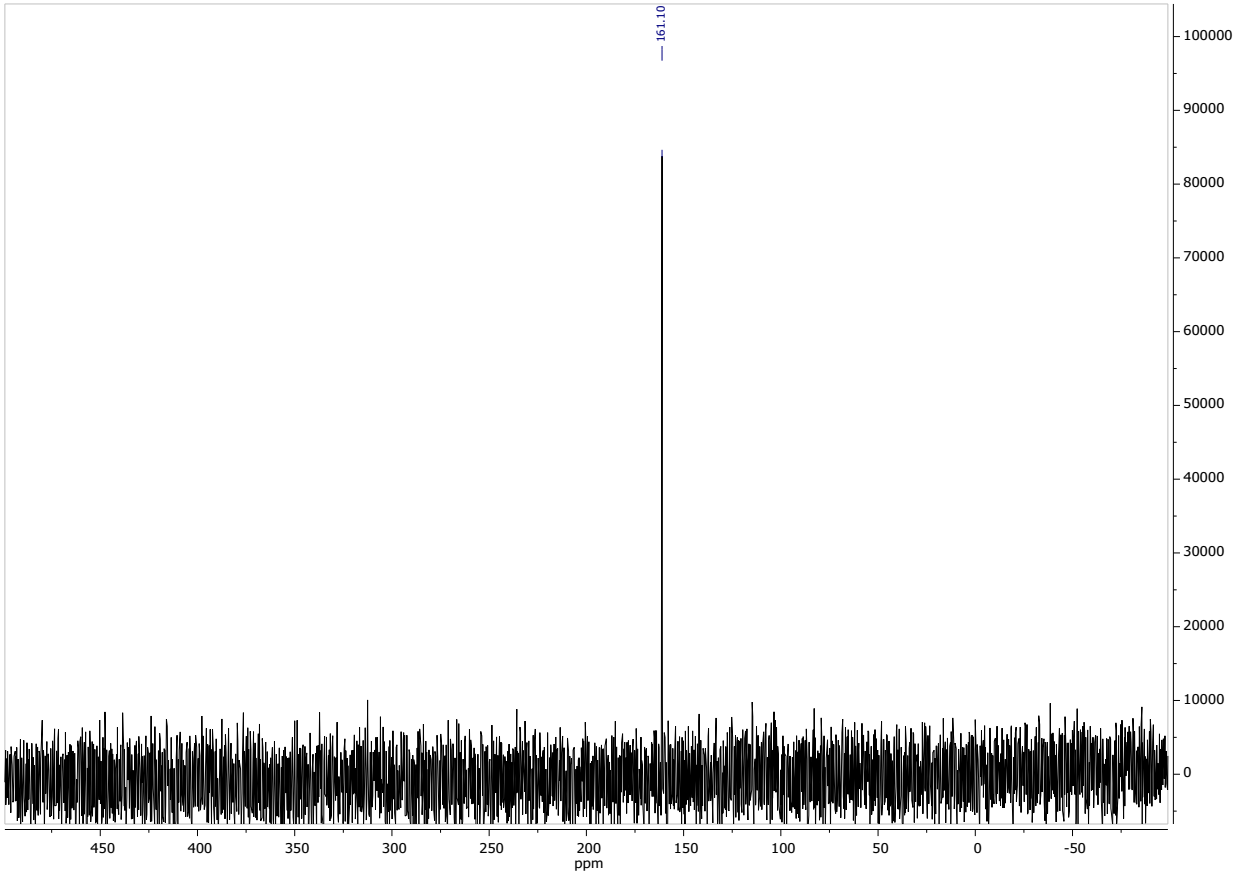


Figure-57: ^{13}C NMR spectrum (76 MHz) of **4h** in DMSO-d_6

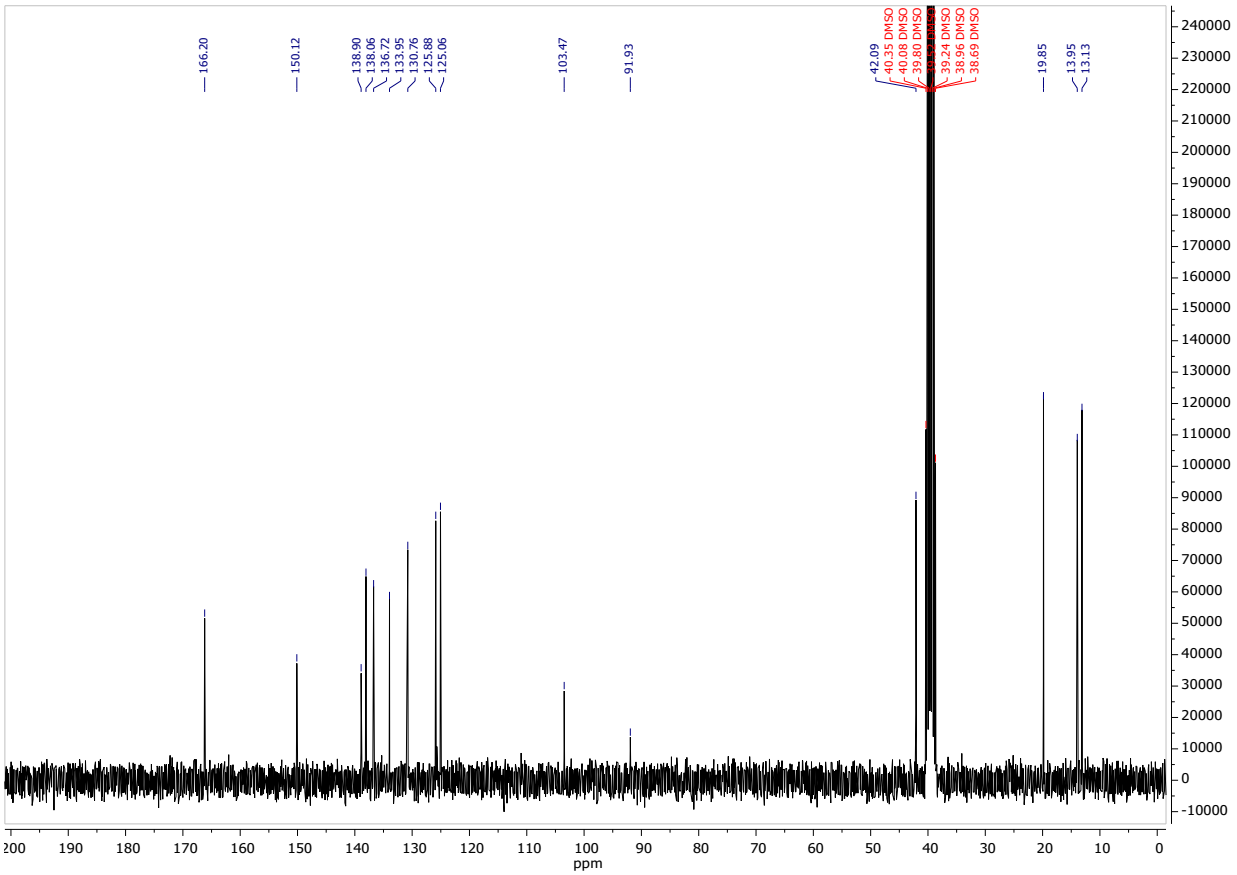
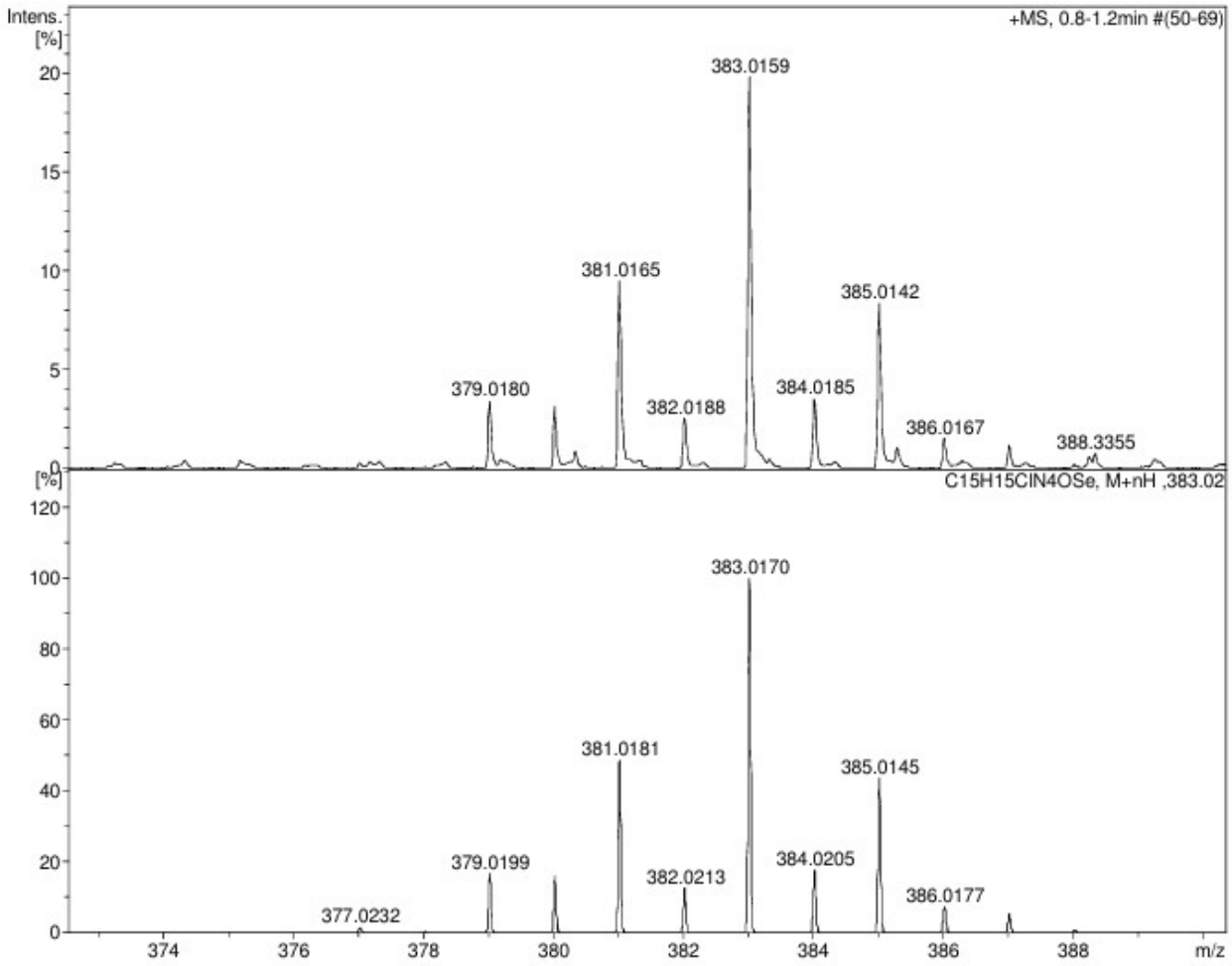
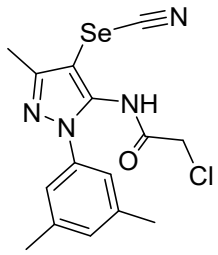


Figure-58: HRMS spectrum of compound **4h**





2-Chloro-N-(1-(3,5-dimethylphenyl)-3-methyl-4-selenocyanato-1H-pyrazol-5-yl)acetamide, ***4i***

White powder, m.p. 179-181°C, yield 91% (0.69 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.73 (s, 1H), 7.11 (s, 2H), 7.06 (s, 1H), 4.30 (s, 2H), 2.34 (s, 3H), 2.32 (s, 6H). ^{77}Se NMR (57 MHz, DMSO) δ 160.20. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.28, 150.50, 138.66, 137.82, 137.72, 129.37, 120.92, 103.30, 94.42, 42.22, 20.77, 13.05. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{15}H_{16}ClN_4OSe$]$^{+}$: 383.0170; found: 383.0174.

Figure-59: ^{1}H NMR spectrum (300 MHz) of **4i** in DMSO-d_6

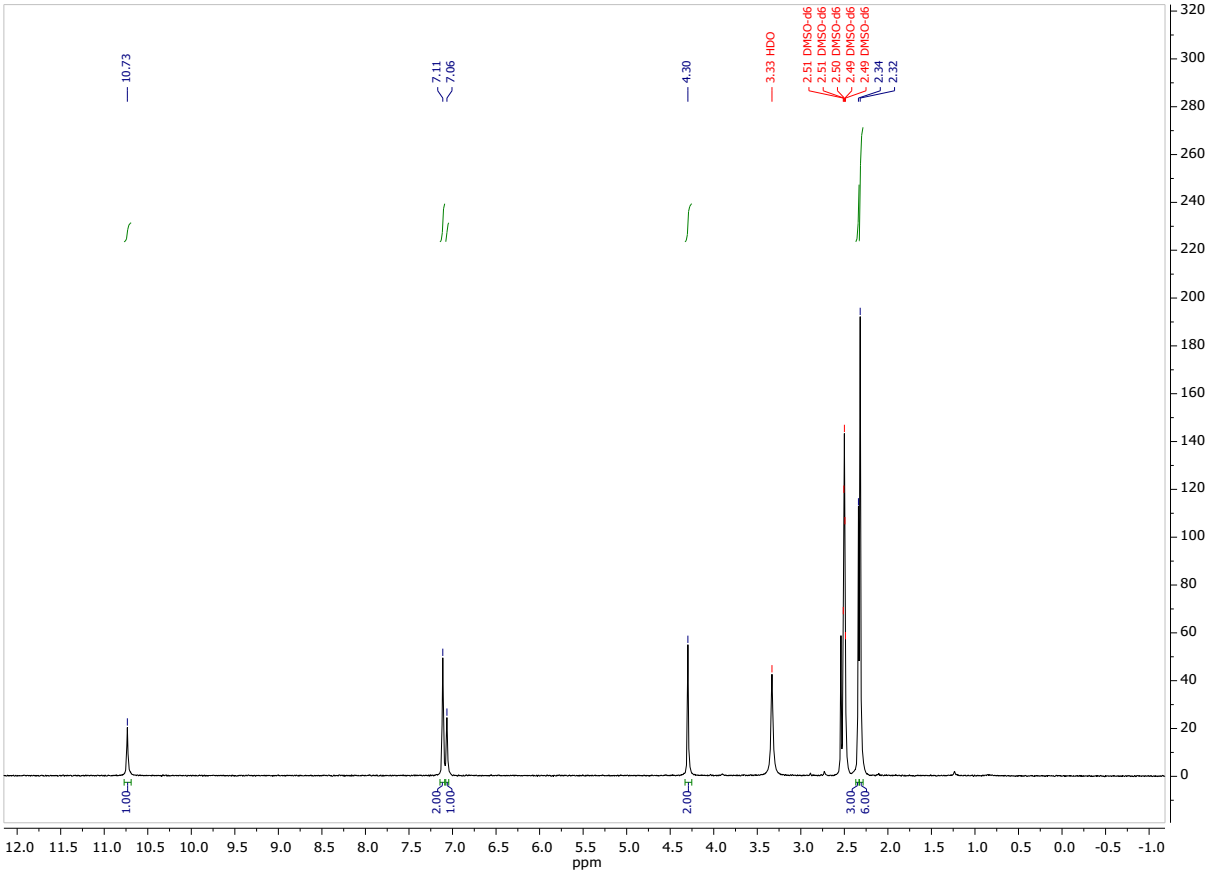


Figure-60: ^{77}Se NMR spectrum (57 MHz) of **4i** in DMSO-d_6

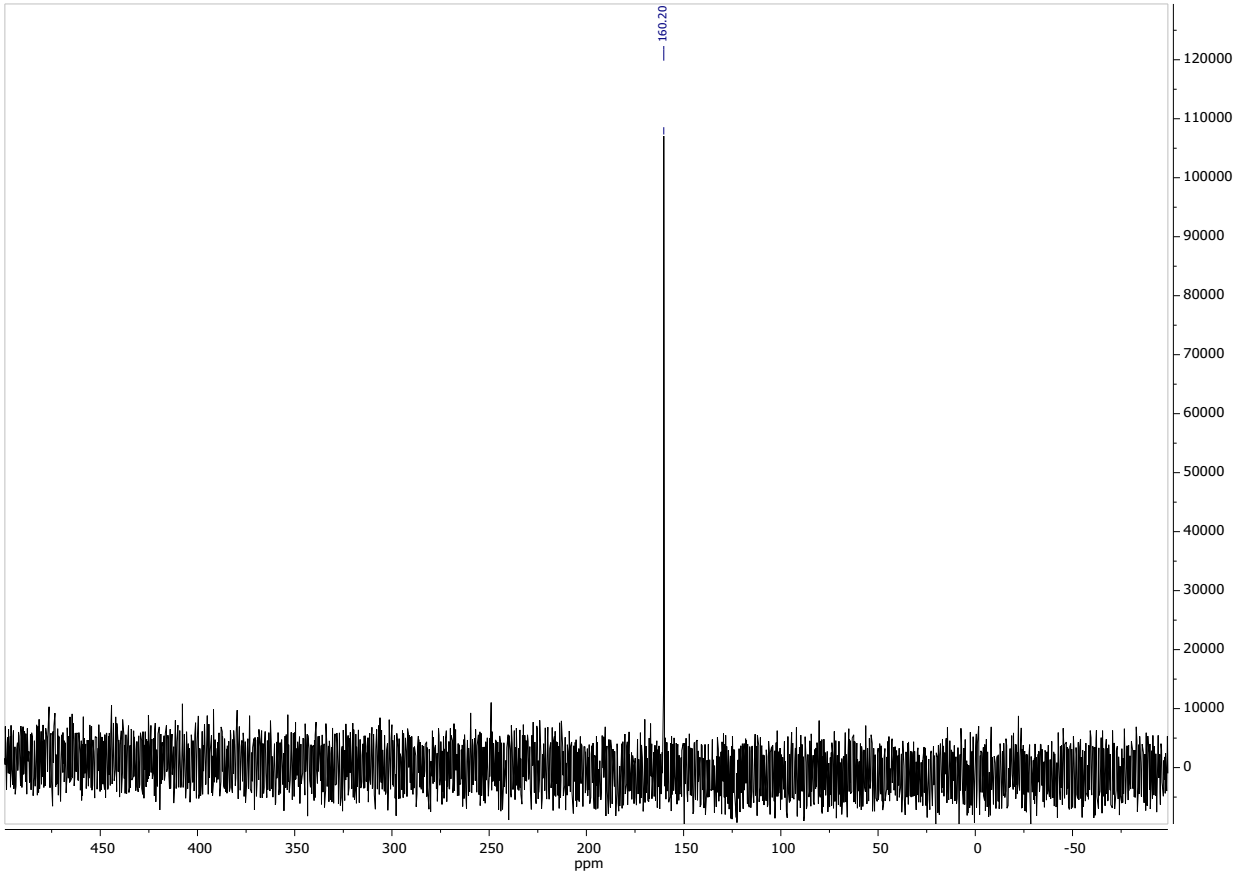


Figure-61: ^{13}C NMR spectrum (76 MHz) of **4i** in DMSO-d_6

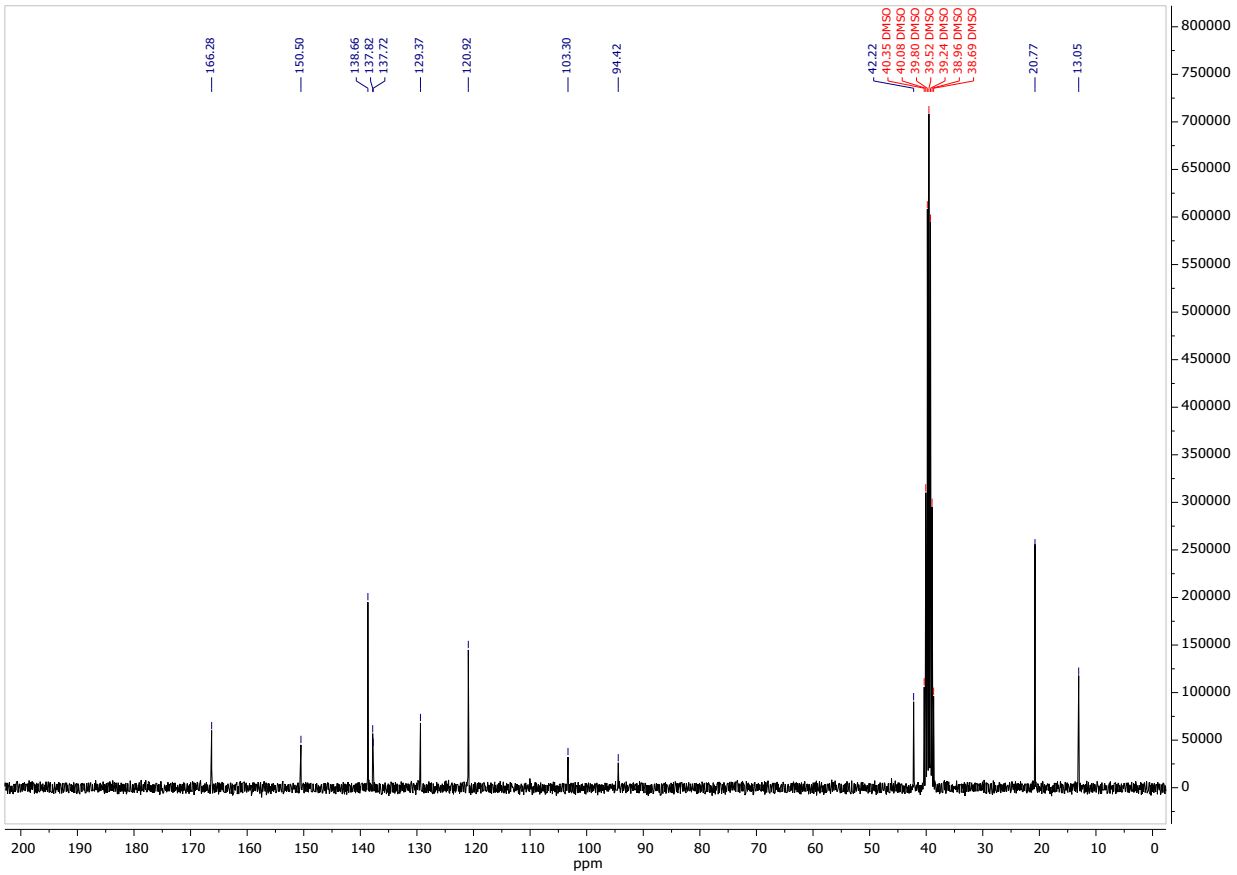
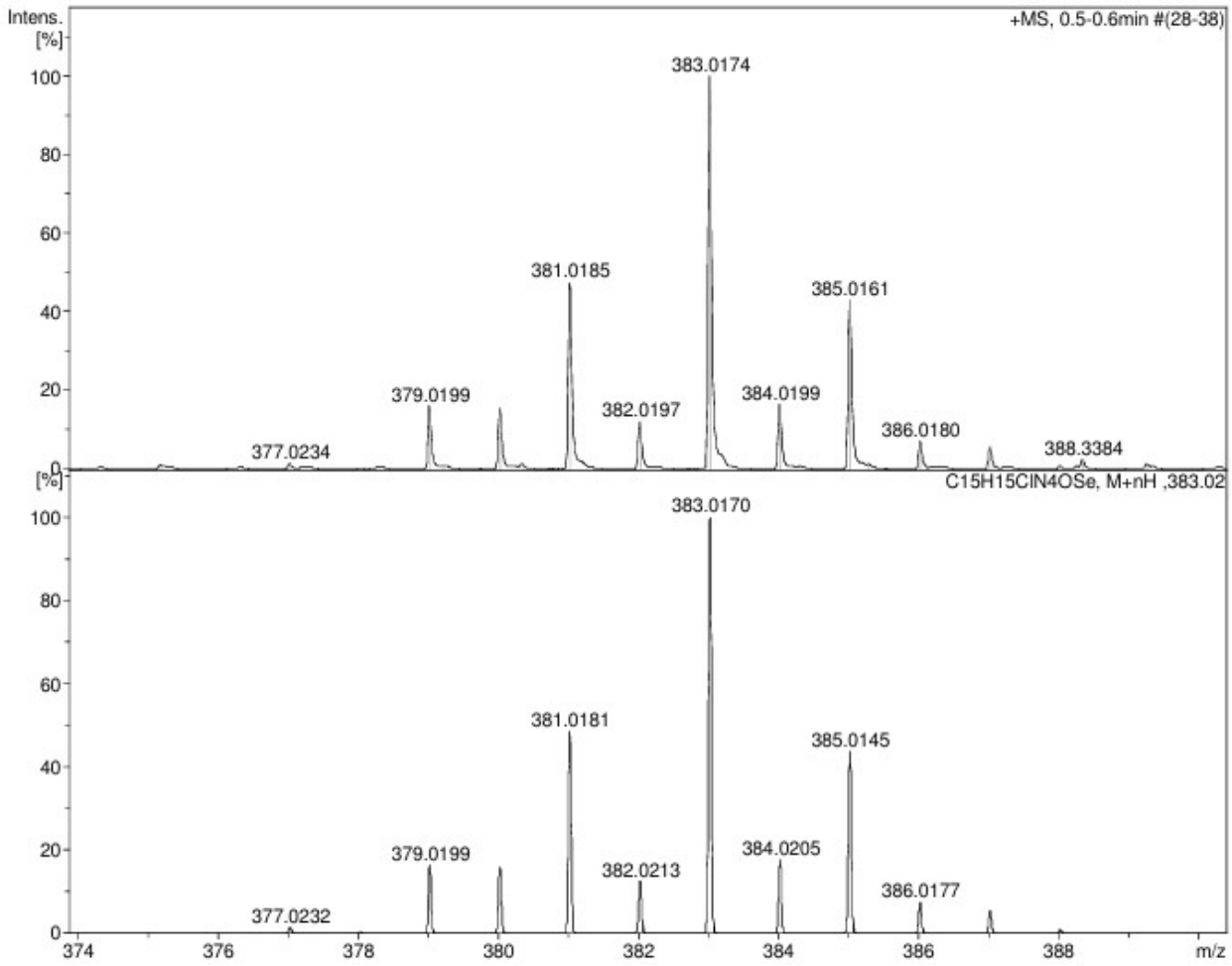
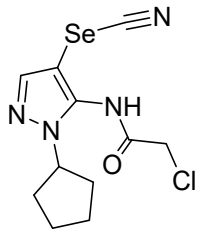


Figure-62: HRMS spectrum of compound **4i**





2-Chloro-N-(1-cyclopentyl-4-selenocyanato-1H-pyrazol-5-yl)acetamide, ***4j***

White powder, m.p. 167-169°C, yield 86% (0.57 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.63 (s, 1H), 7.72 (s, 1H), 4.70 – 4.60 (m, 1H), 4.41 (s, 2H), 2.06 – 1.94 (m, 2H), 1.89 – 1.75 (m, 4H), 1.66 – 1.54 (m, 2H). ^{77}Se NMR (57 MHz, DMSO) δ 170.04. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.48, 141.82, 136.86, 104.21, 90.72, 58.61, 42.48, 32.25, 24.21. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{11}H_{14}ClN_4OSe$]$^{+}$: 333.0013; found: 333.0016.

Figure-63: ^{1}H NMR spectrum (300 MHz) of **4j** in DMSO-d_6

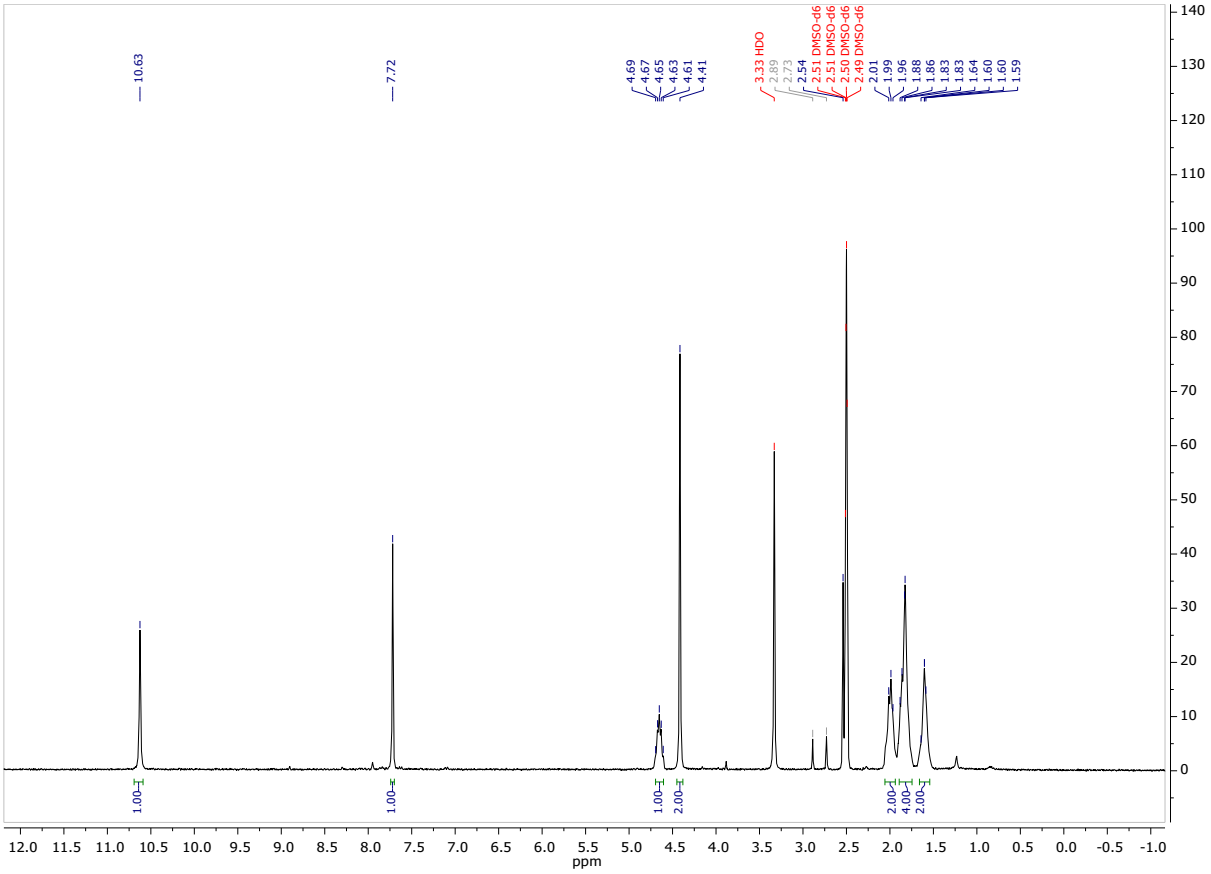


Figure-64: ^{77}Se NMR spectrum (57 MHz) of **4j** in DMSO-d_6

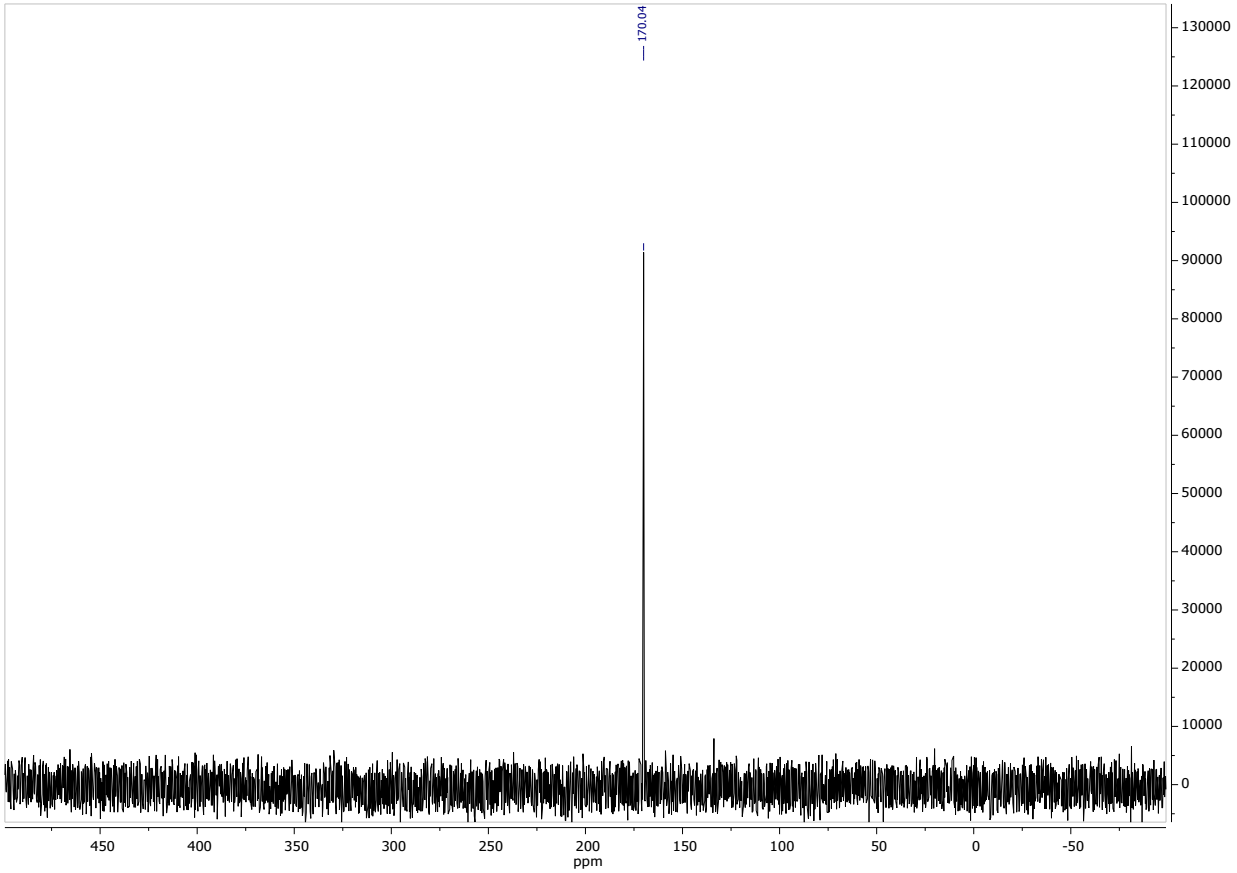


Figure-65: ^{13}C NMR spectrum (76 MHz) of **4j** in DMSO-d_6

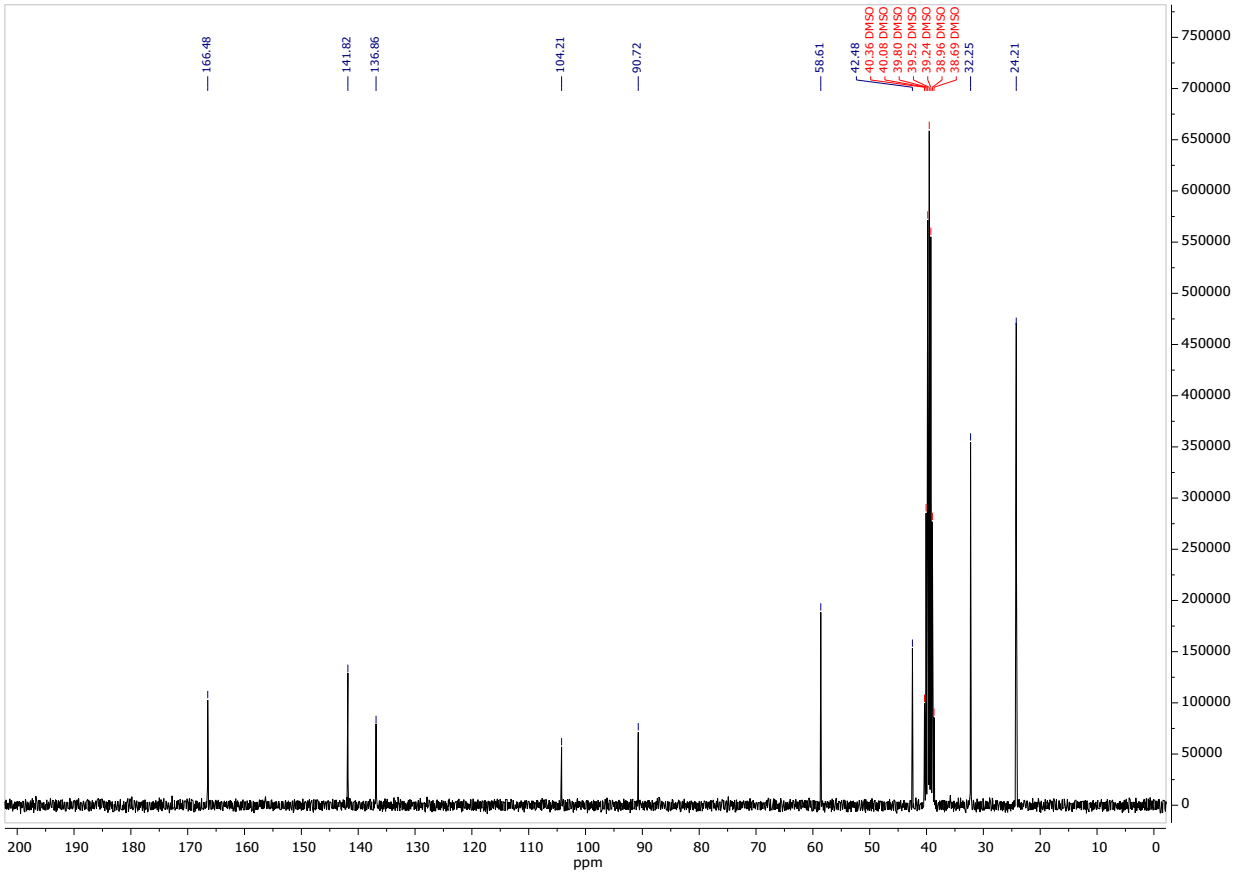
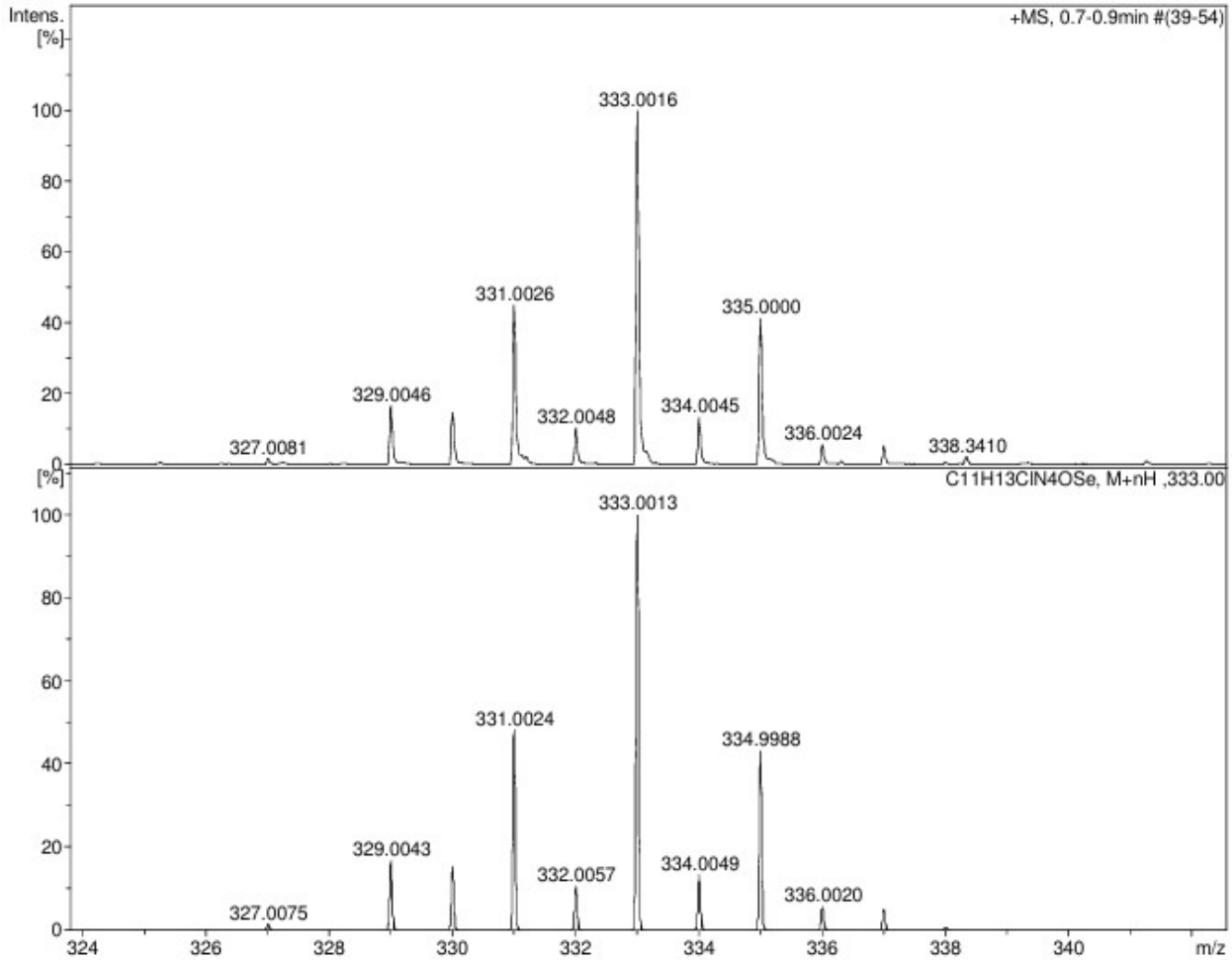
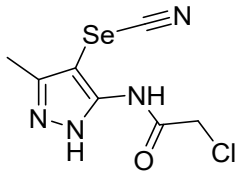


Figure-66: HRMS spectrum of compound **4j**





2-Chloro-N-(3-methyl-4-selenocyanato-1H-pyrazol-5-yl)acetamide, ***4l***

White powder, m.p. 221-223°C, yield 65% (0.36 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.78 (s, 1H), 4.30 (s, 2H), 2.32 (s, 3H). ^{77}Se NMR (57 MHz, DMSO) δ 157.67. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.44, 145.87, 143.11, 103.83, 88.00, 42.45, 10.85. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_7H_8ClN_4OSe$]$^{+}$: 278.9544; found: 278.9545.

Figure-67: ^{1}H NMR spectrum (300 MHz) of **4l** in DMSO-d_6

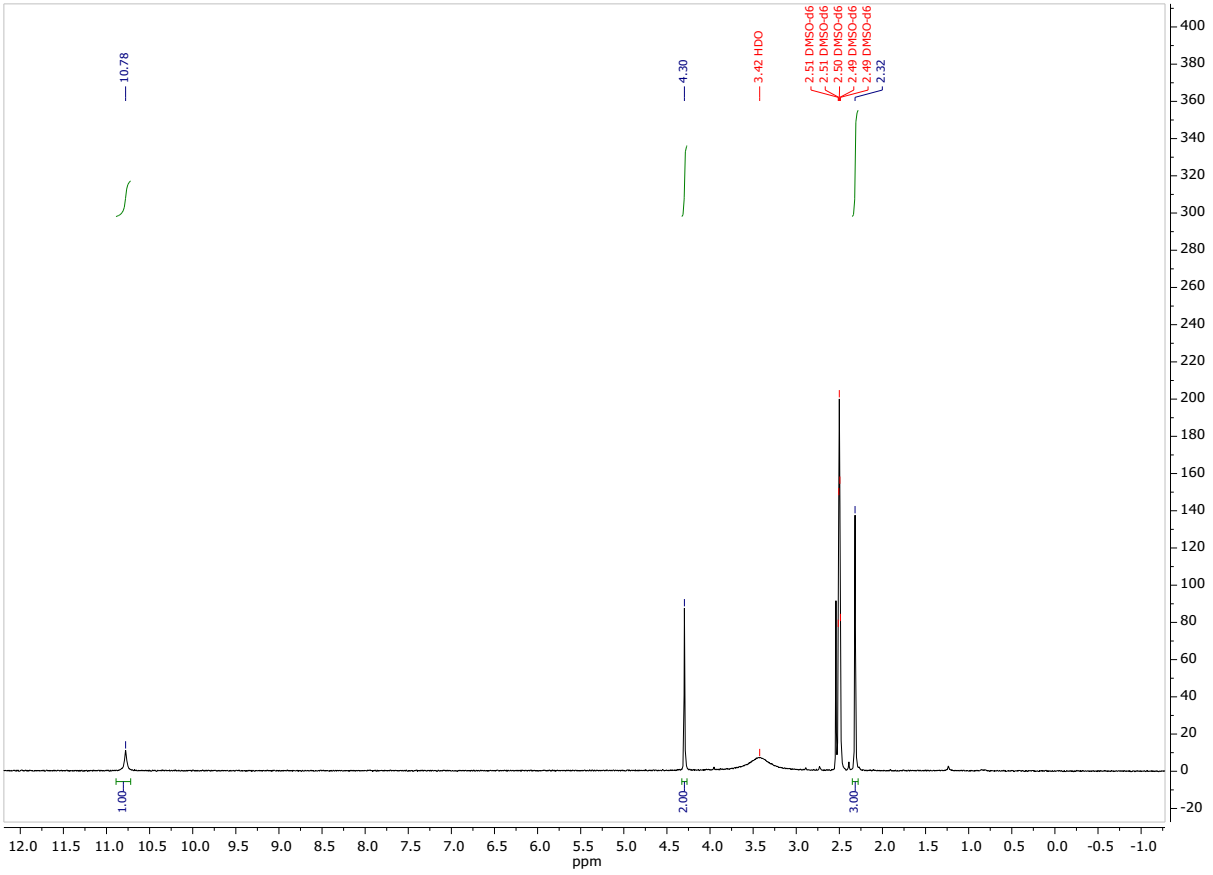


Figure-68: ^{77}Se NMR spectrum (57 MHz) of **4l** in DMSO-d_6

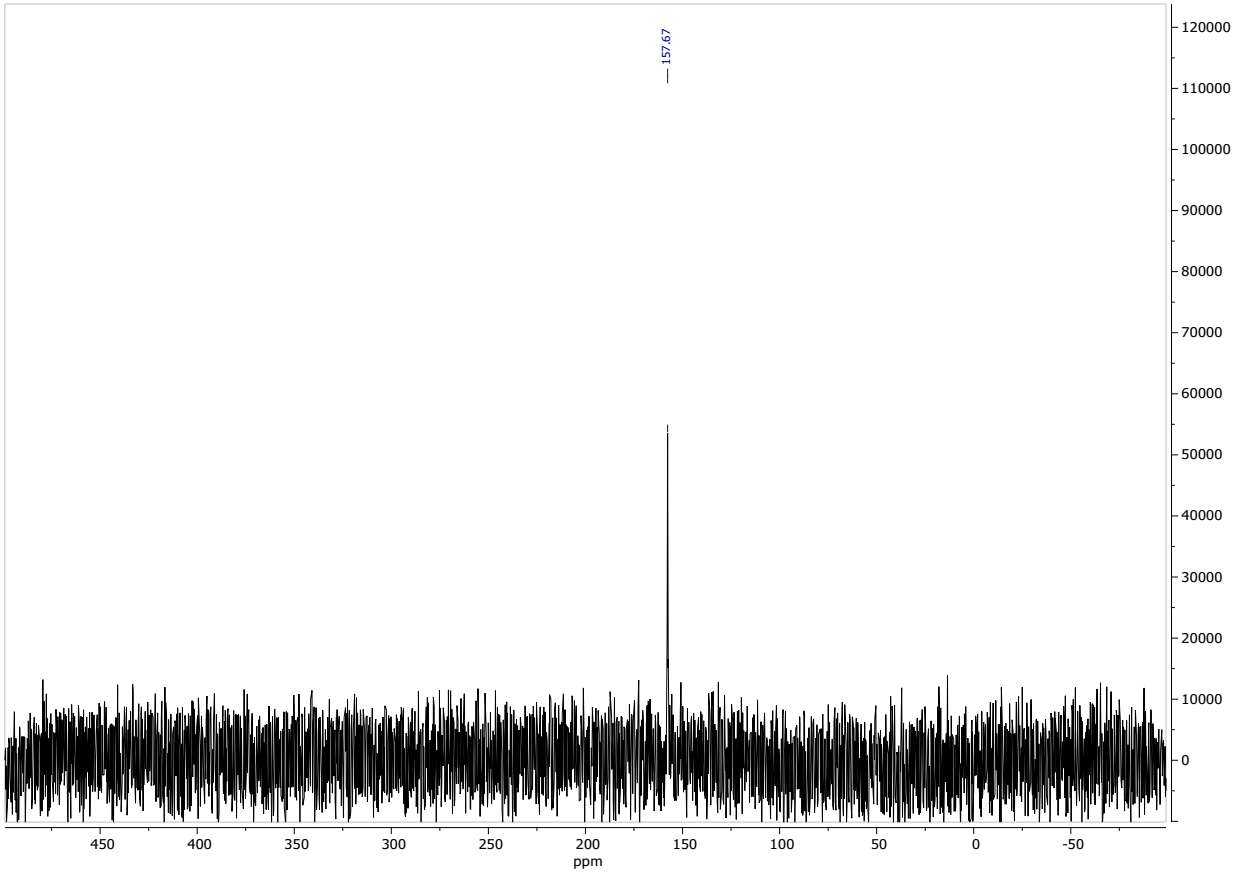


Figure-69: ^{13}C NMR spectrum (76 MHz) of **4l** in DMSO-d_6

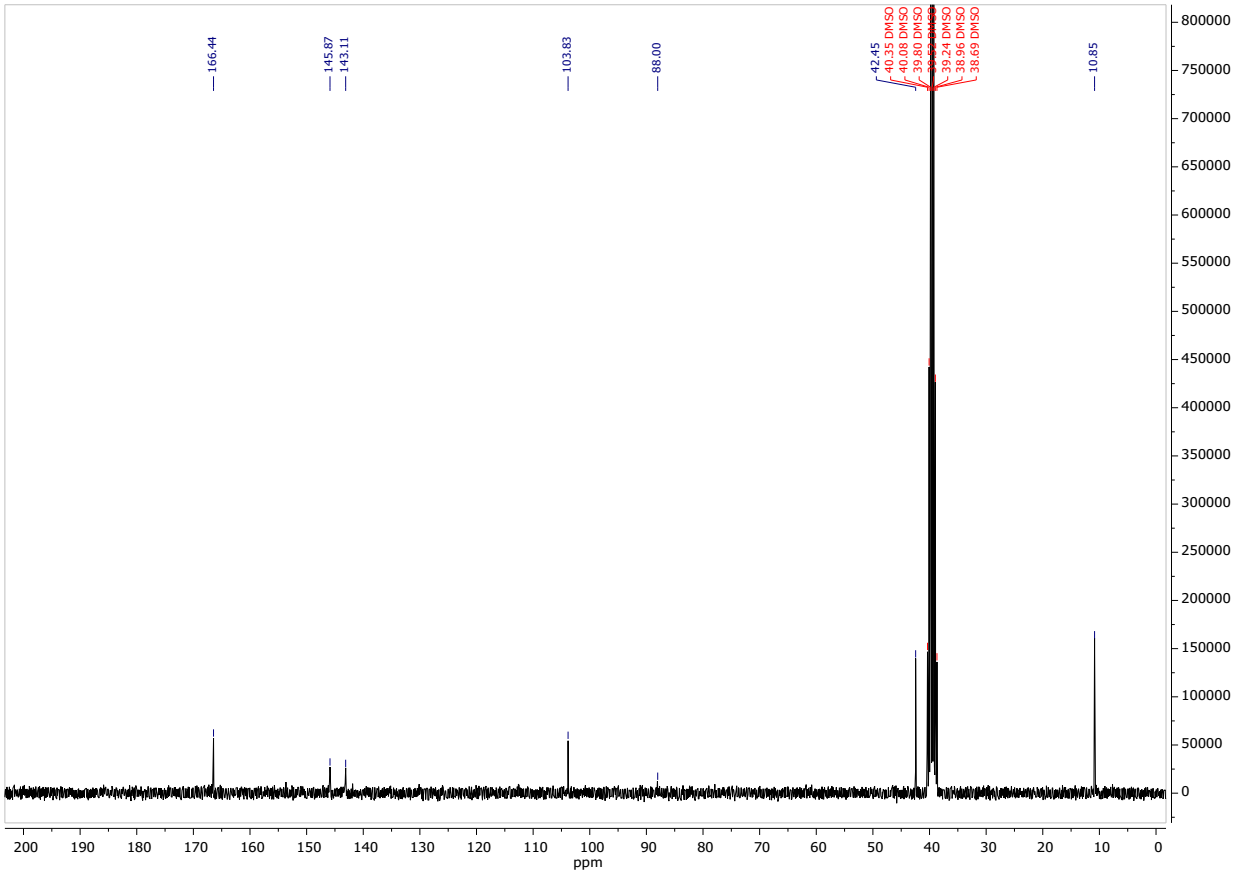
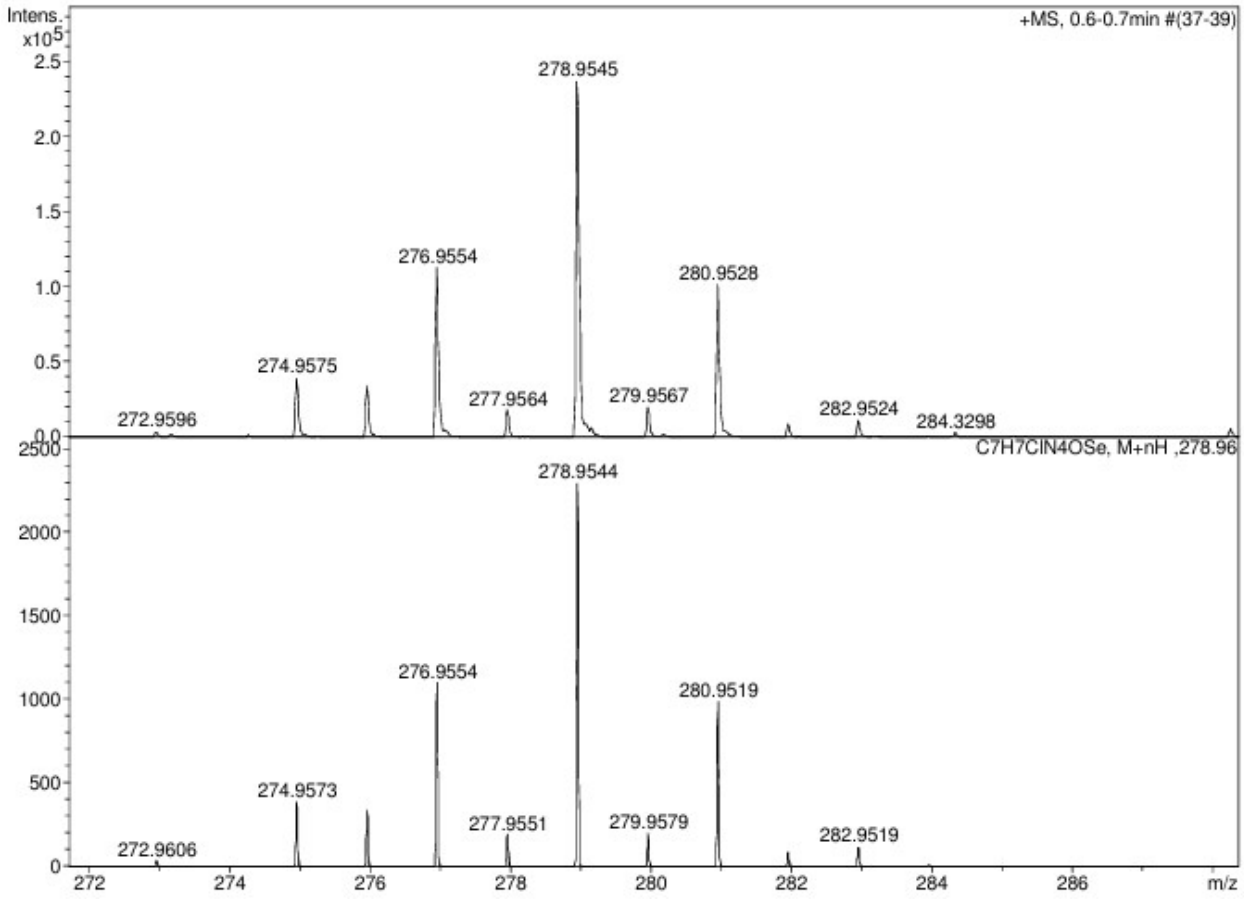
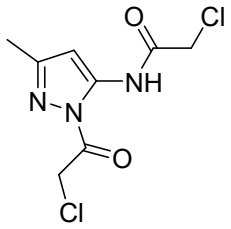


Figure-70: HRMS spectrum of compound **4l**



NMR and HRMS spectra for compound 5



2-Chloro-N-(1-(2-chloroacetyl)-3-methyl-1H-pyrazol-5-yl)acetamide, ***5***

White powder, m.p. 153-155°C, yield 53% (0.53 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 11.21 (s, 1H), 6.77 (s, 1H), 5.04 (s, 2H), 4.28 (s, 2H), 2.53 (s, 3H). ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 165.91, 165.20, 149.26, 144.42, 104.07, 43.87, 42.88, 14.08. HRMS (ESI-TOF): m/z $[M+H]^+$: calcd for $[C_8H_{10}Cl_2N_3O_2]^+$: 271.9964; found: 271.9971.

Figure-71: ^{1}H NMR spectrum (300 MHz) of **5** in DMSO-d_6

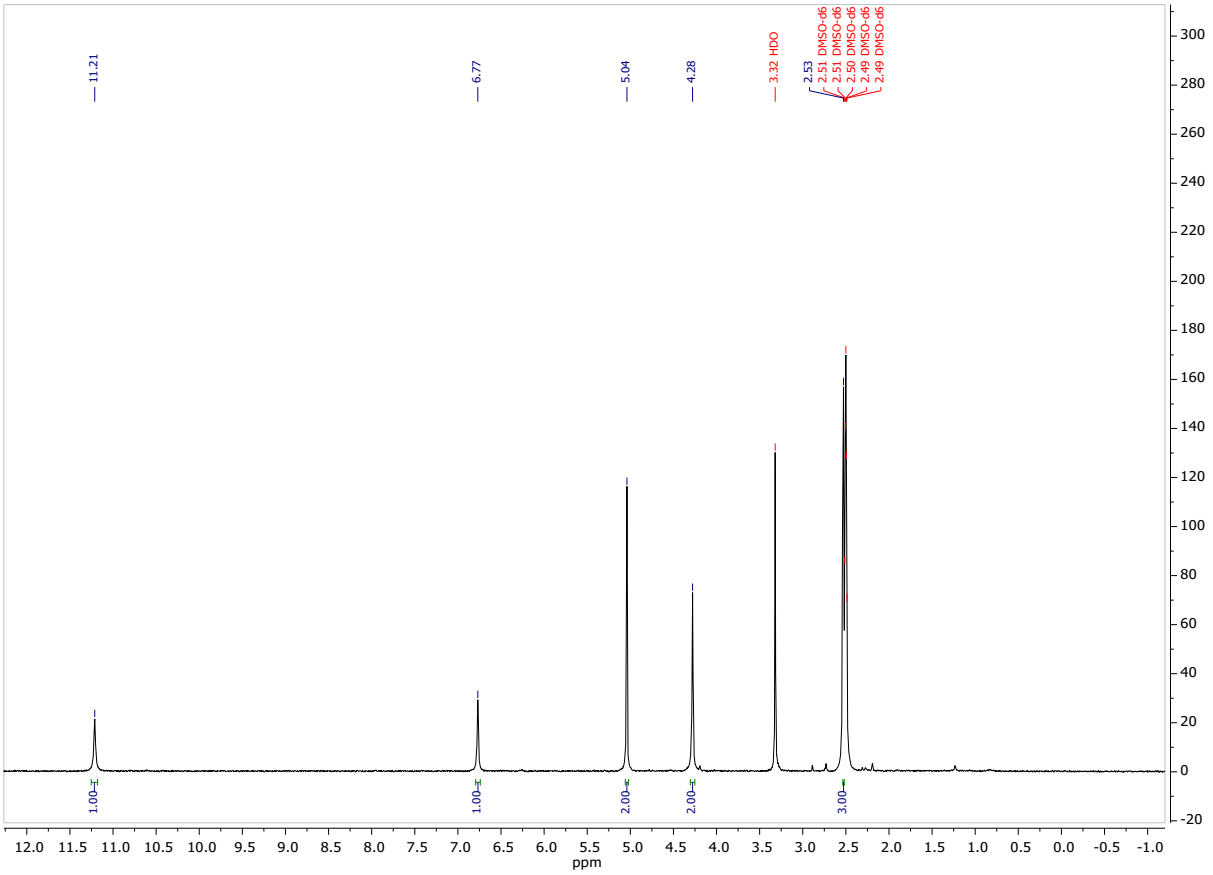


Figure-72: ^{13}C NMR spectrum (76 MHz) of **5** in DMSO-d_6

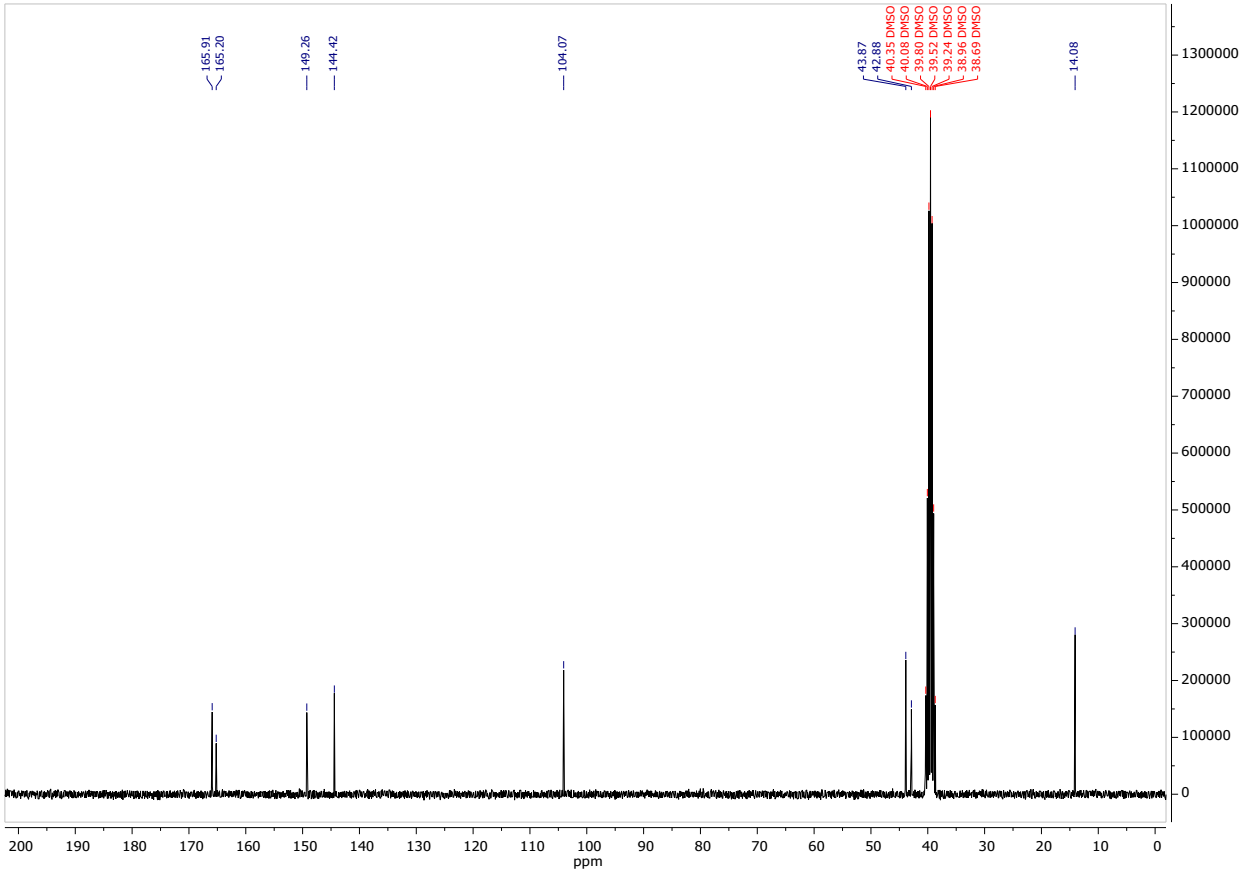
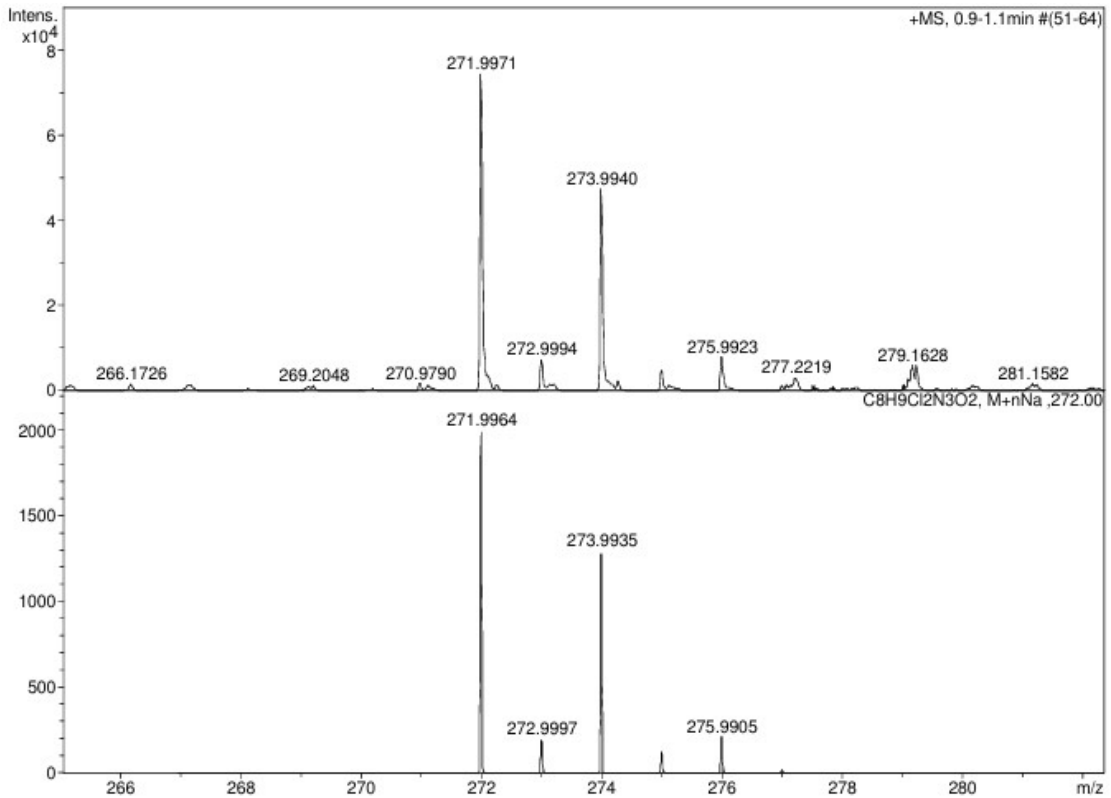
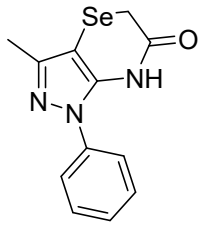


Figure-73: HRMS spectrum of compound **5**



NMR and HRMS spectra for compound 6



3-Methyl-1-phenyl-1,7-dihydropyrazolo[4,3-b][1,4]selenazin-6(5H)-one, ***6a***

Pale yellow powder, m.p. 124-126°C, yield 77% (0.09 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.56 (s, 1H), 7.55 – 7.46 (m, 4H), 7.39 – 7.32 (m, 1H), 3.41 (s, 2H), 2.15 (s, 3H). ^{77}Se NMR (57 MHz, DMSO) δ 86.21. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.30, 145.99, 138.71, 138.18, 129.20, 127.01, 122.64, 89.15, 22.45, 12.96. HRMS (ESI-TOF): m/z $[M+H]^+$: calcd for $[C_{12}H_{12}N_3OSe]^+$: 294.0140; found: 294.0145.

Figure-74: ^{1}H NMR spectrum (300 MHz) of **6a** in DMSO-d_6

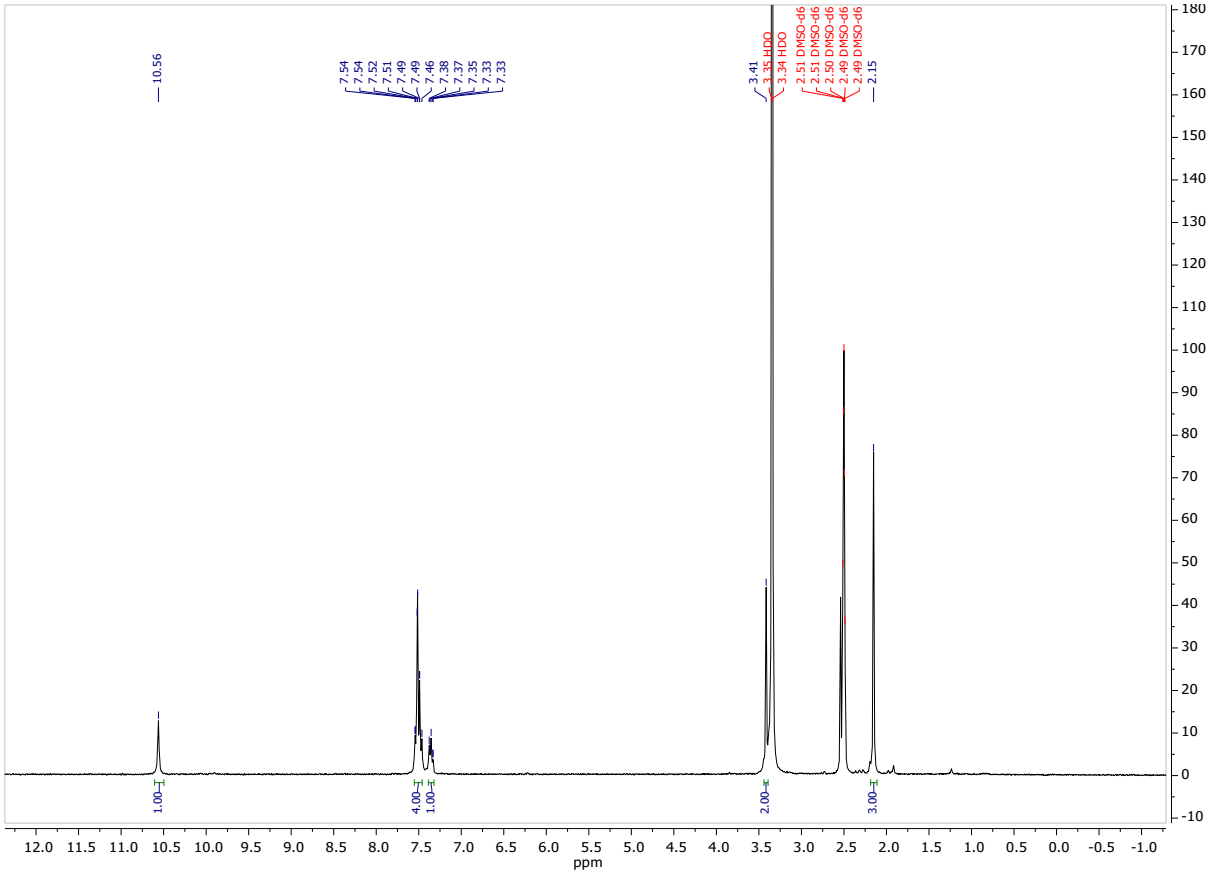


Figure-75: ^{77}Se NMR spectrum (57 MHz) of **6a** in DMSO-d_6

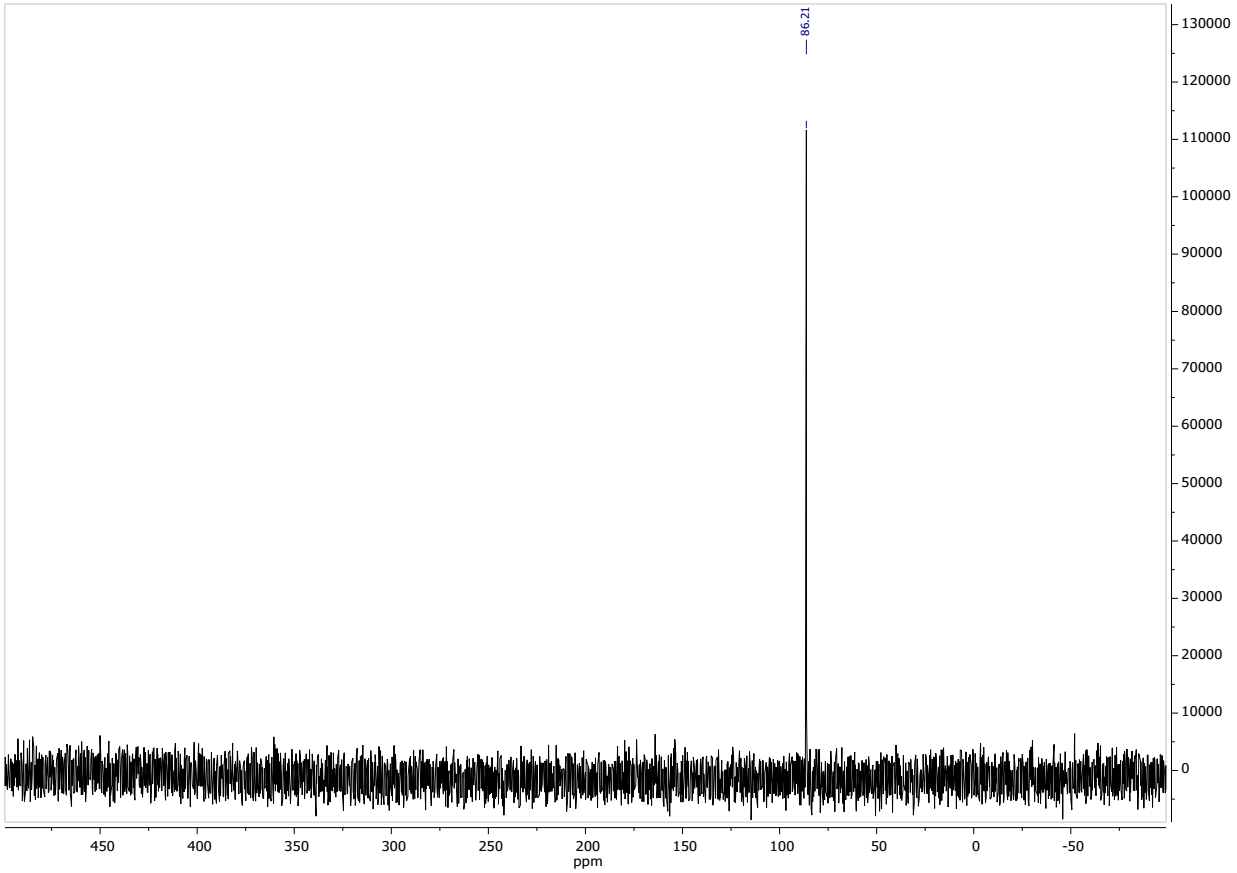


Figure-76: ^{13}C NMR spectrum (76 MHz) of **6a** in DMSO-d_6

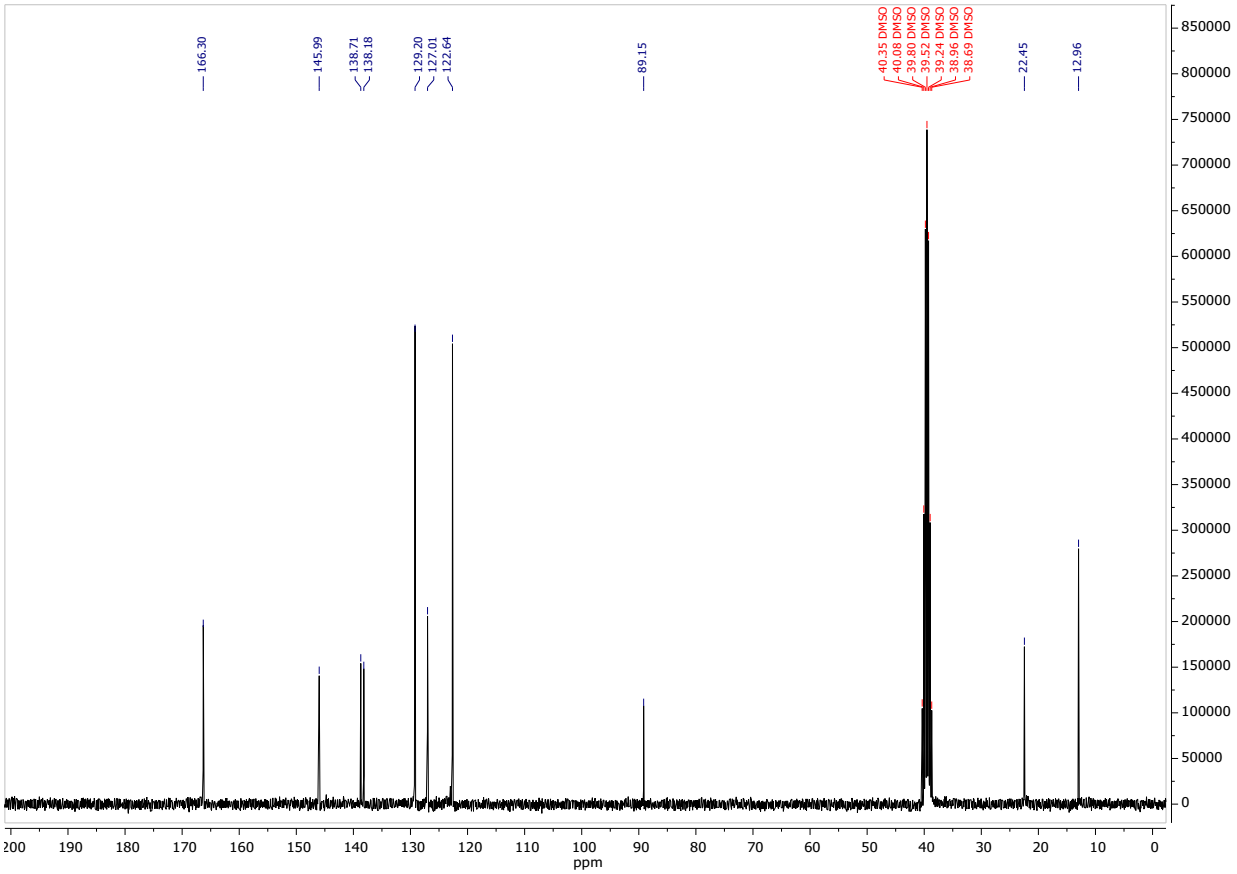
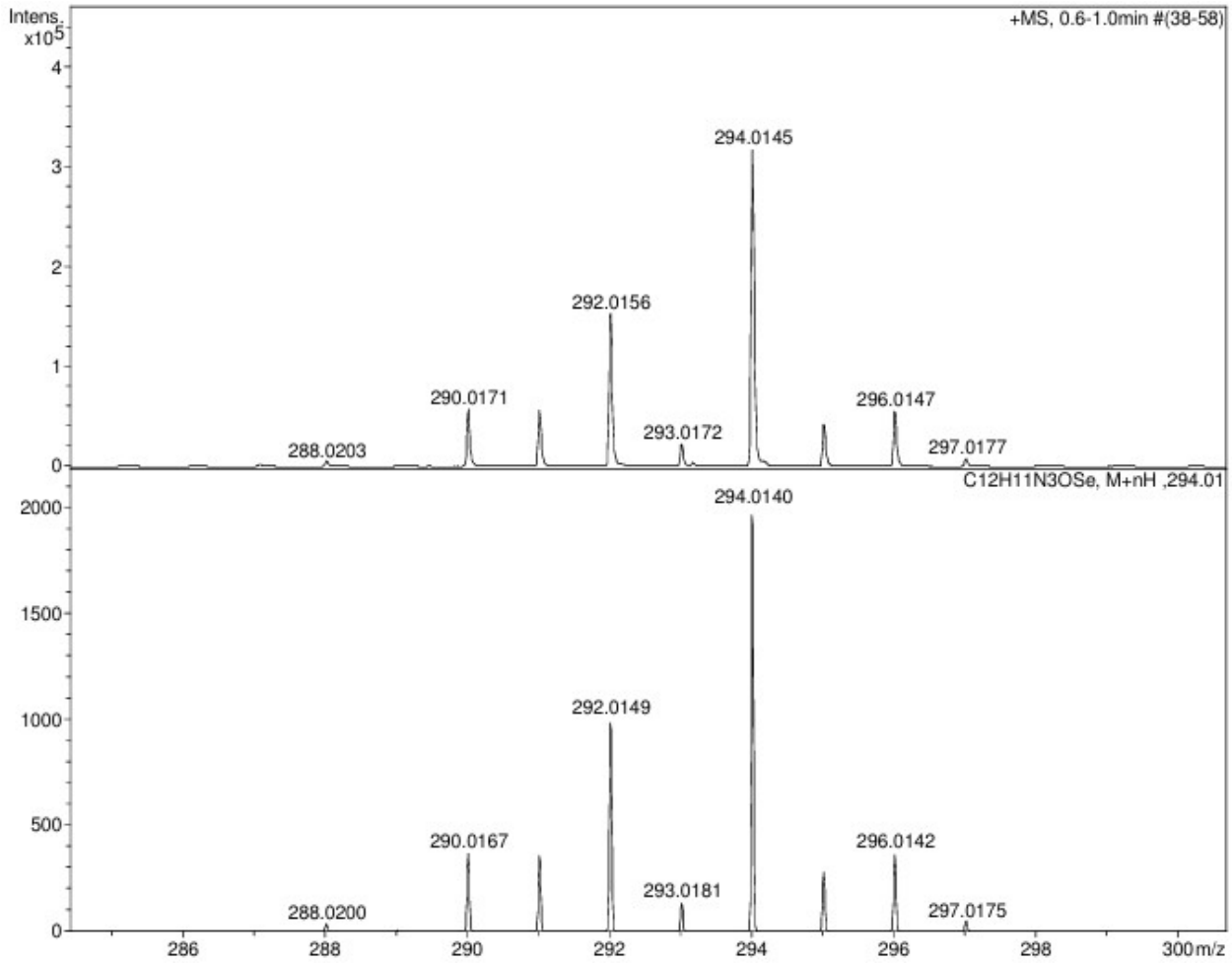
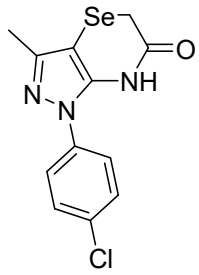


Figure-77: HRMS spectrum of compound **6a**





1-(4-Chlorophenyl)-3-methyl-1,7-dihydropyrazolo[4,3-b][1,4]selenazin-6(5H)-one, ***6b***

White powder, m.p. 118-120^{o}C, yield 87% (0.11 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.61 (s, 1H), 7.55 (s, 4H), 3.42 (s, 2H), 2.15 (s, 3H). ^{77}Se NMR (57 MHz, DMSO) δ 87.48. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.24, 146.34, 138.76, 136.94, 131.19, 129.13, 124.29, 89.38, 22.34, 12.93. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{12}H_{11}ClN_3OSe$]$^{+}$: 327.9748; found: 327.9744.

Figure-78: ^{1}H NMR spectrum (300 MHz) of **6b** in DMSO-d_6

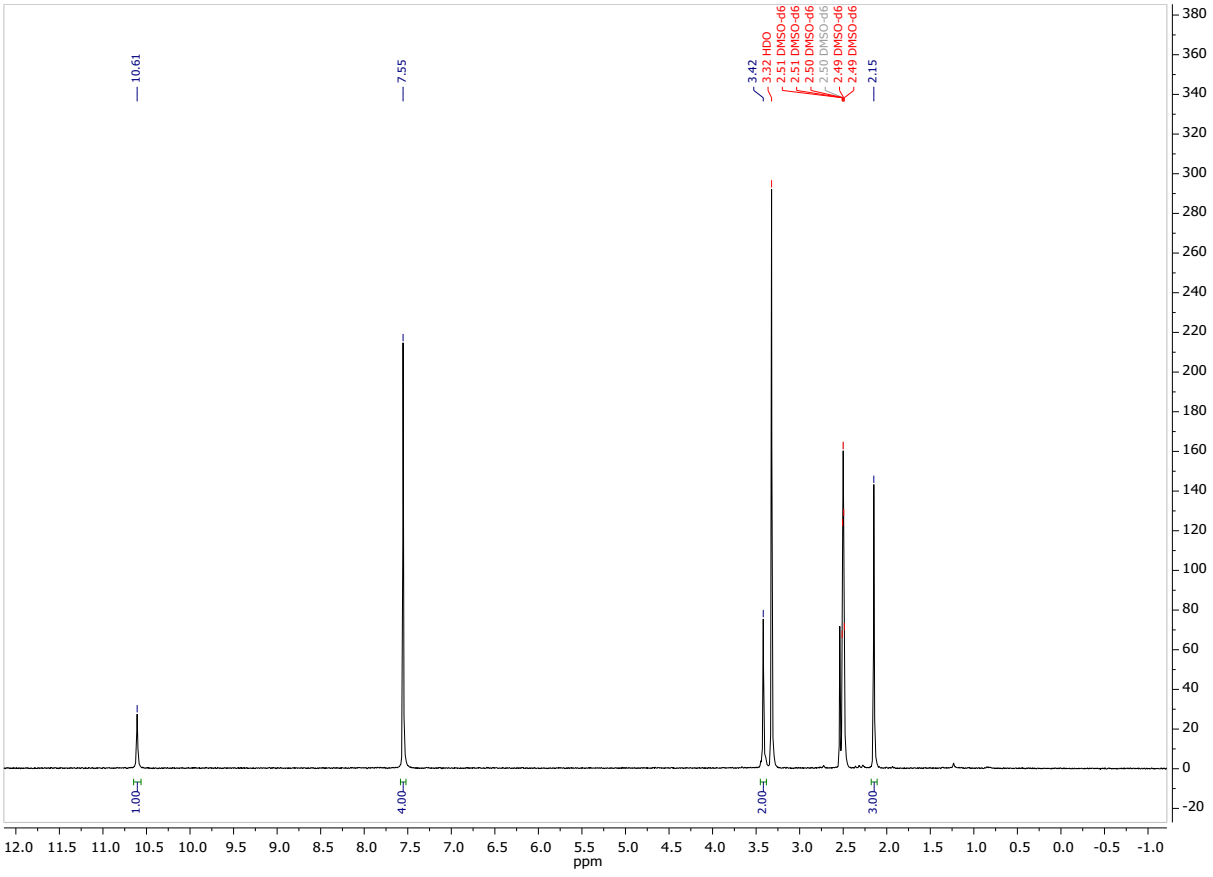


Figure-79: ^{77}Se NMR spectrum (57 MHz) of **6b** in DMSO-d_6

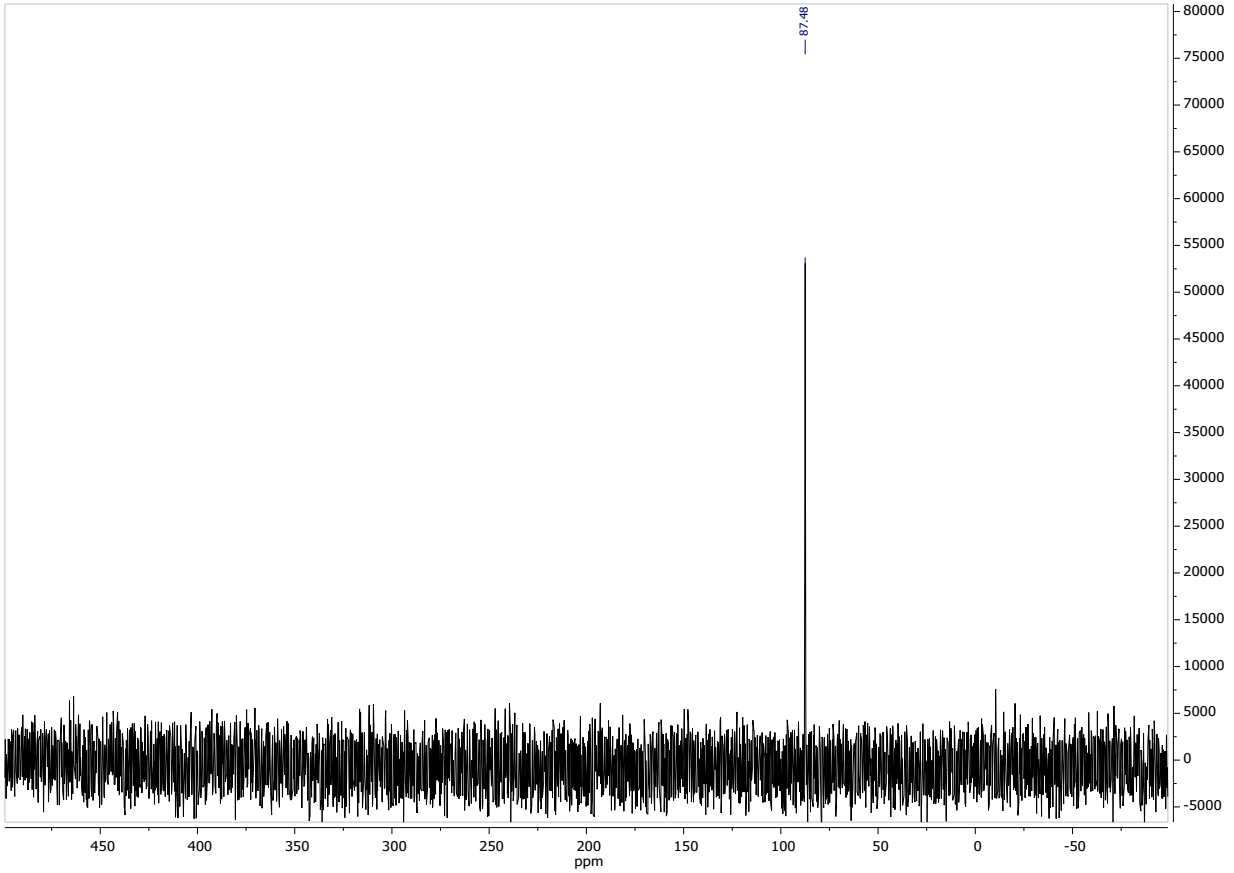


Figure-80: ^{13}C NMR spectrum (76 MHz) of **6b** in DMSO-d_6

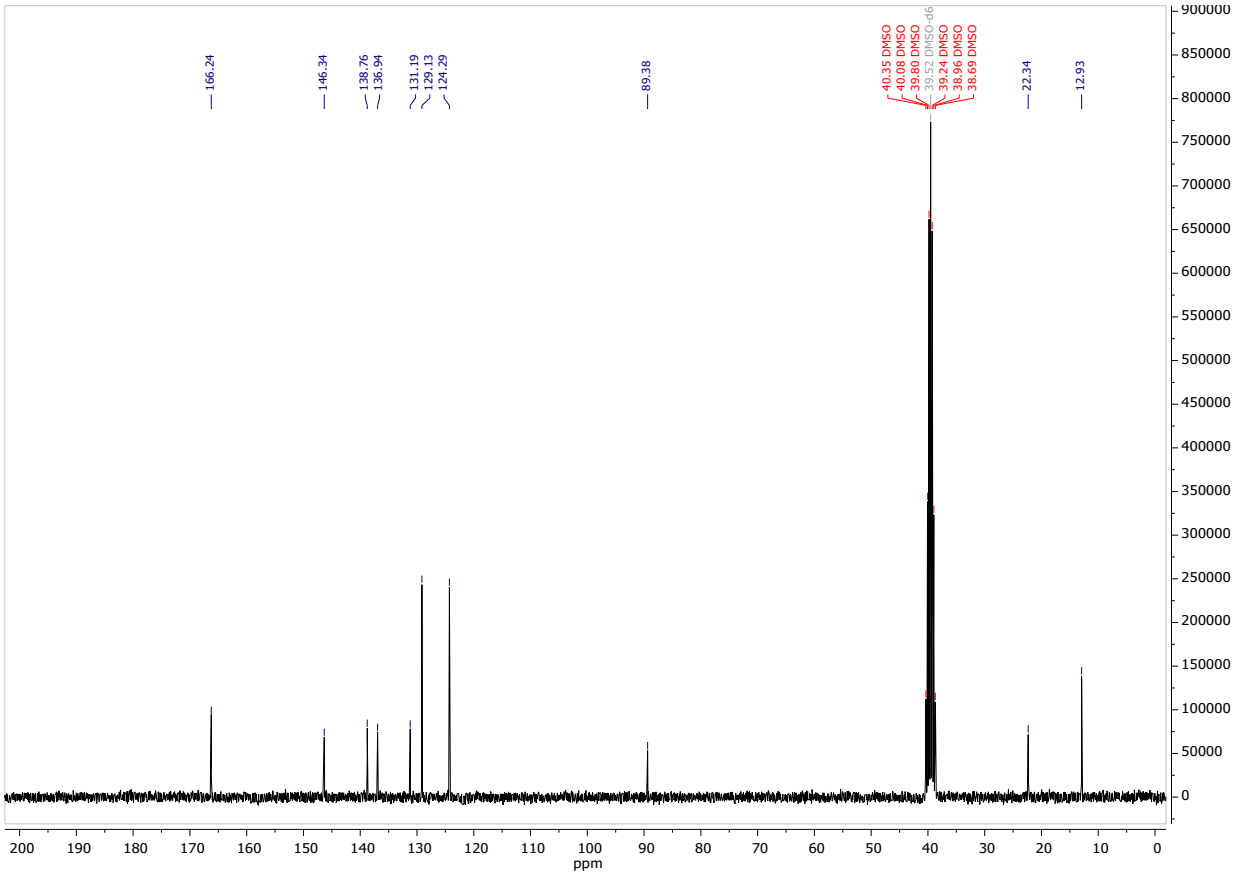
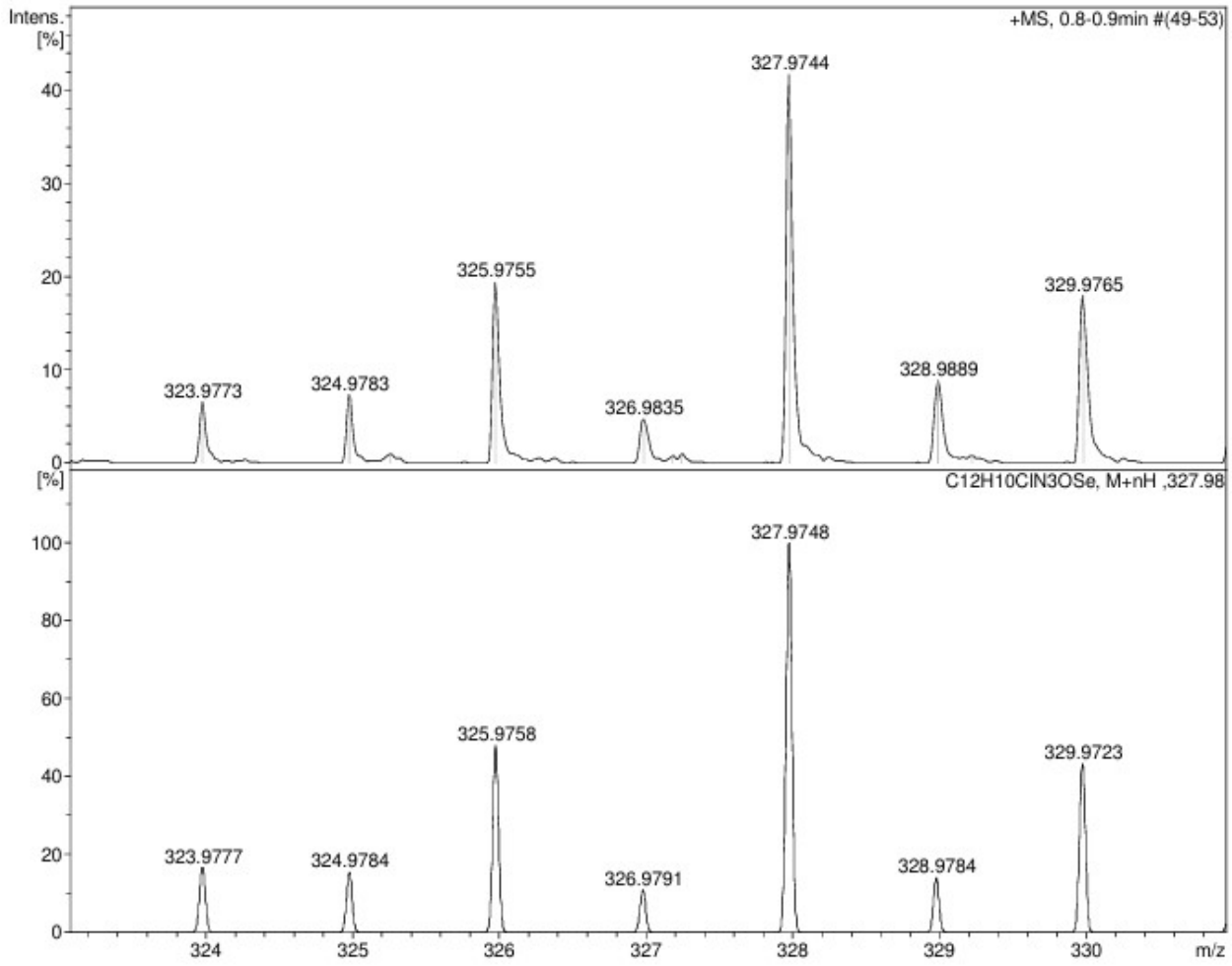
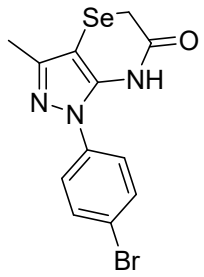


Figure-81: HRMS spectrum of compound **6b**





1-(4-Bromophenyl)-3-methyl-1,7-dihydropyrazolo[4,3-b][1,4]selenazin-6(5H)-one, ***6c***

White powder, m.p. 127-129°C, yield 78% (0.12 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.60 (s, 1H), 7.68 (d, J = 8.8 Hz, 2H), 7.48 (d, J = 8.8 Hz, 2H), 3.40 (s, 2H), 2.14 (s, 3H). ^{77}Se NMR (57 MHz, DMSO) δ 88.03. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.42, 146.59, 138.85, 137.43, 132.22, 124.74, 119.74, 89.61, 22.45, 13.05. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{12}H_{11}BrN_3OSe$]$^{+}$: 371.9242; found: 371.9241.

Figure-82: ^{1}H NMR spectrum (300 MHz) of **6c** in DMSO-d_6

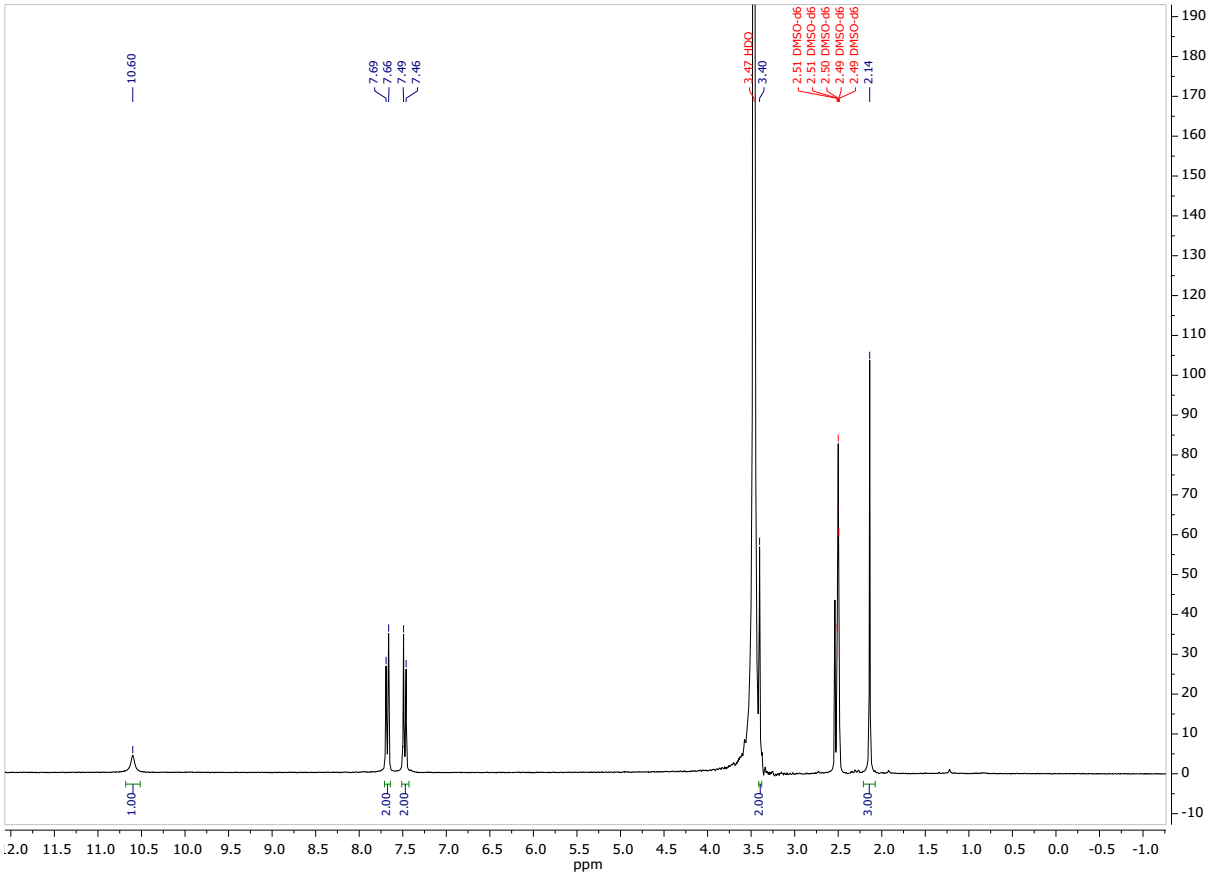


Figure-73: ^{77}Se NMR spectrum (57 MHz) of **6c** in DMSO-d_6

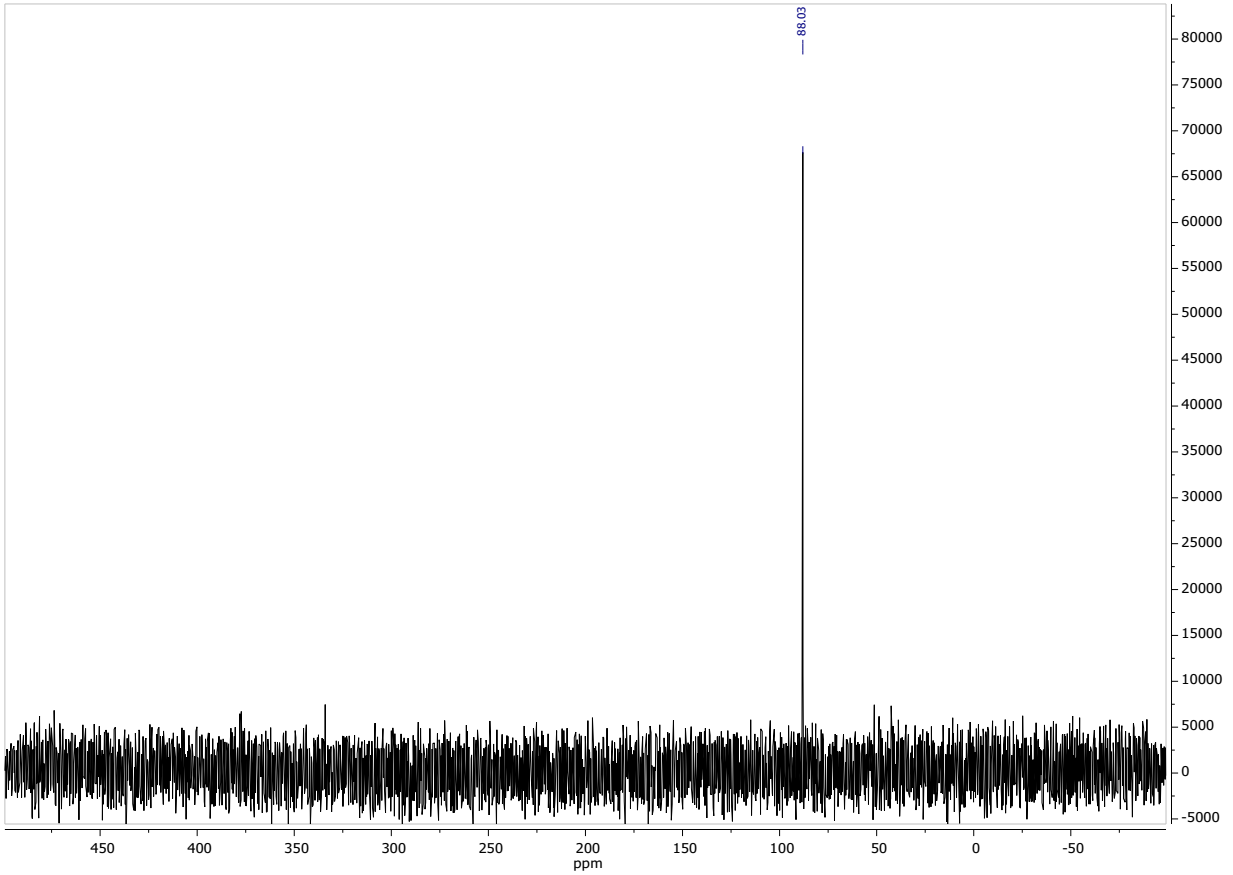


Figure-84: ^{13}C NMR spectrum (76 MHz) of **6c** in DMSO-d_6

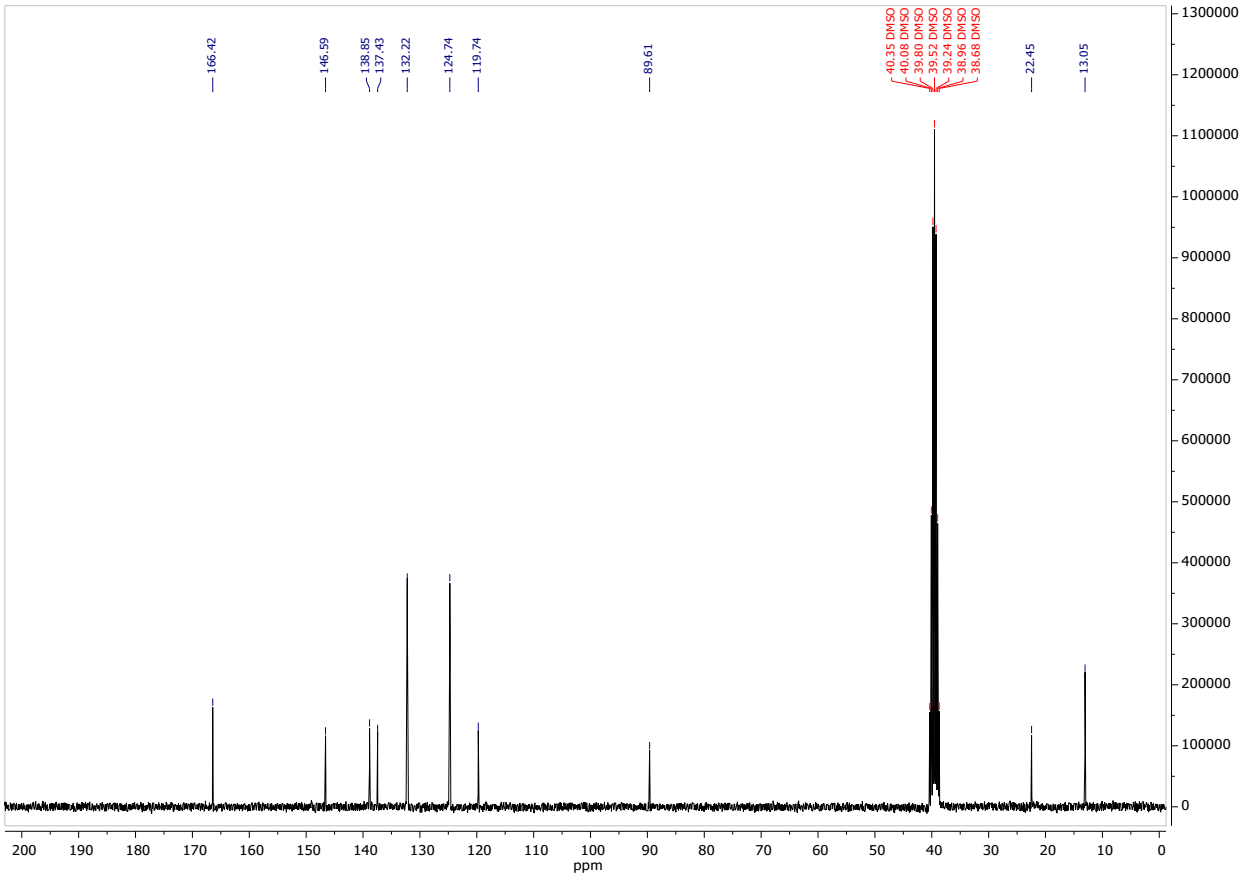
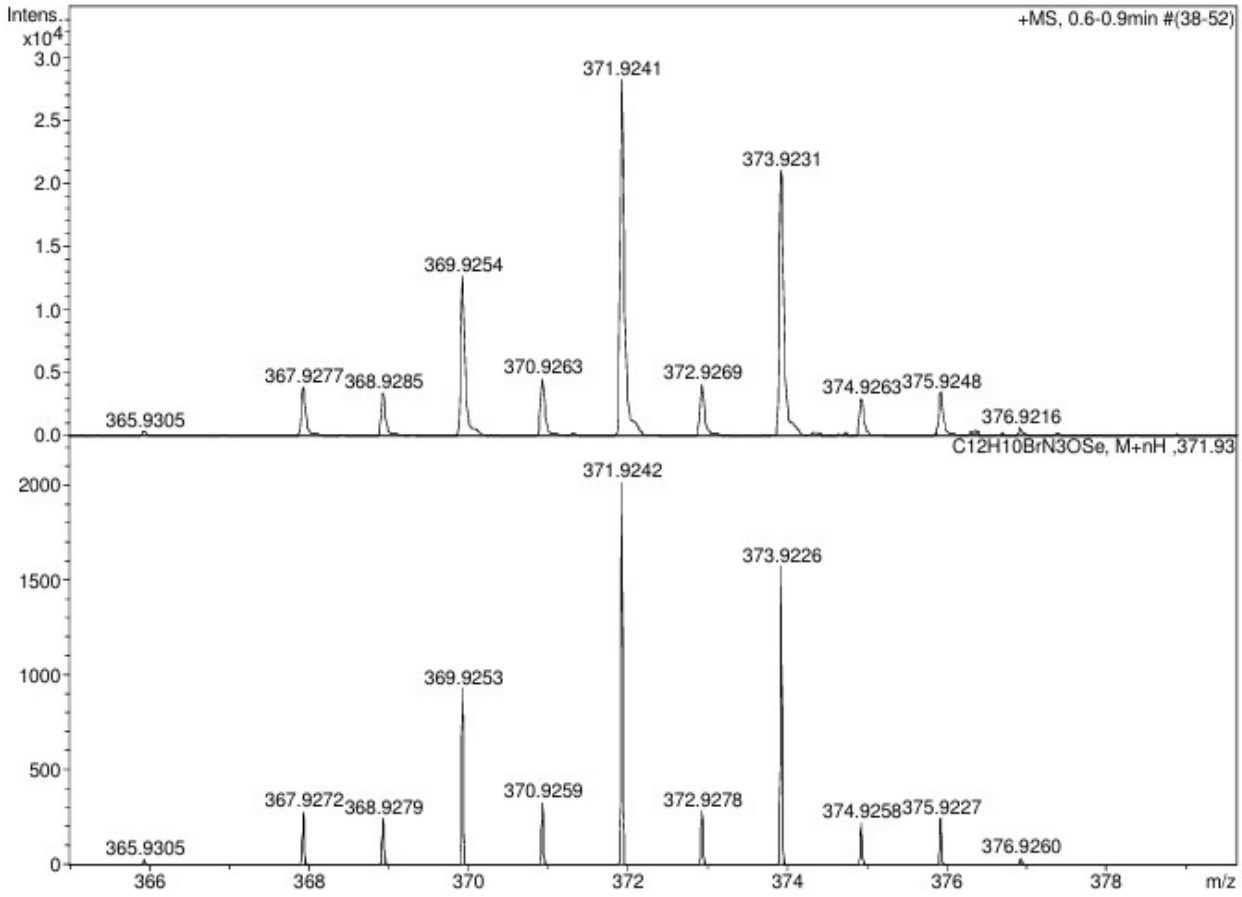
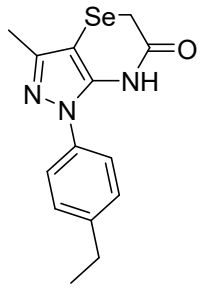


Figure-85: HRMS spectrum of compound **6c**





1-(4-Ethylphenyl)-3-methyl-1,7-dihydropyrazolo[4,3-b][1,4]selenazin-6(5H)-one, ***6d***

White powder, m.p. 100-102°C, yield 81% (0.10 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.49 (s, 1H), 7.43 (d, J = 8.4 Hz, 2H), 7.32 (d, J = 8.4 Hz, 2H), 3.40 (s, 2H), 2.65 (q, J = 7.6 Hz, 2H), 2.14 (s, 3H), 1.21 (t, J = 7.6 Hz, 3H). ^{77}Se NMR (57 MHz, DMSO) δ 85.78. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.26, 145.66, 142.69, 138.64, 135.99, 128.42, 122.68, 88.77, 27.73, 22.43, 15.60, 12.93. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{14}H_{16}N_3OSe$]$^{+}$: 322.0453; found: 322.0458.

Figure-86: ^{1}H NMR spectrum (300 MHz) of **6d** in DMSO-d_6

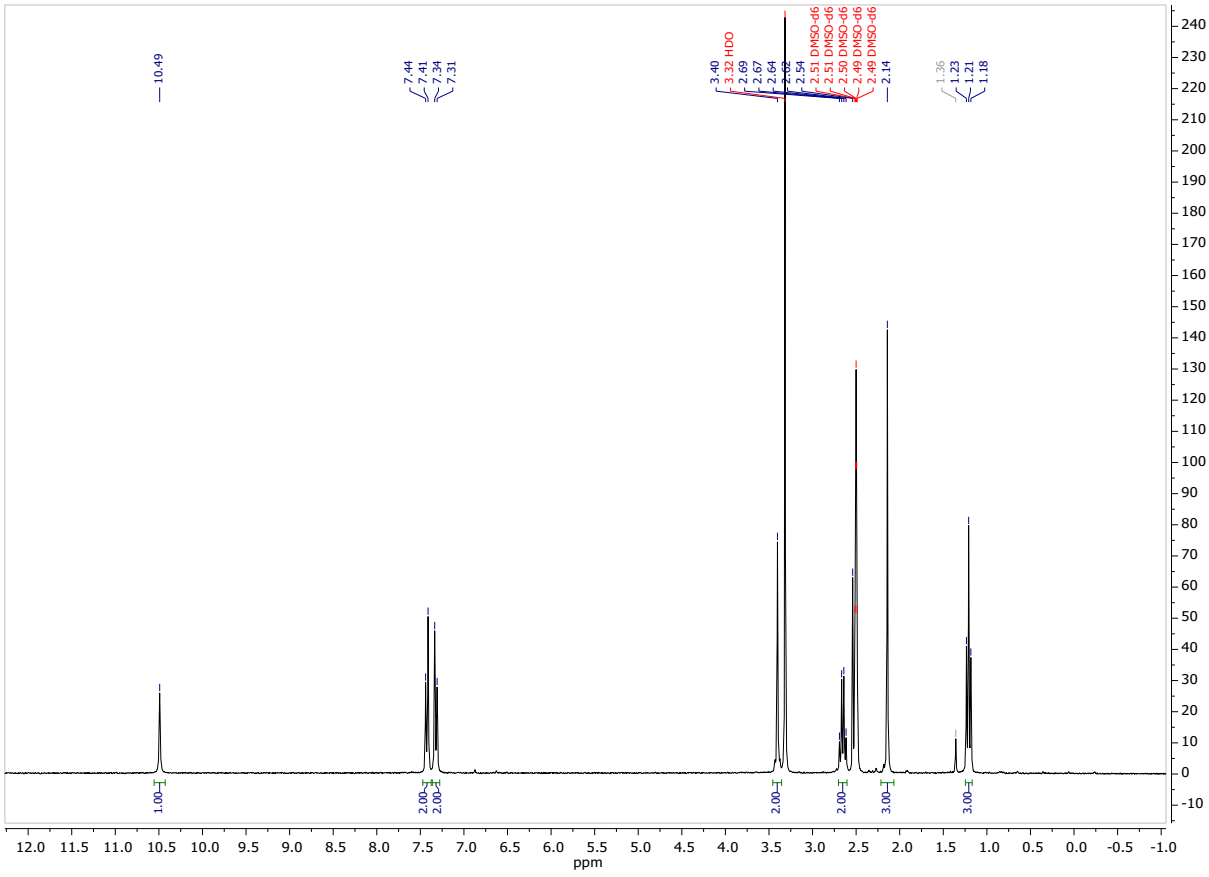


Figure-87: ^{77}Se NMR spectrum (57 MHz) of **6d** in DMSO-d_6

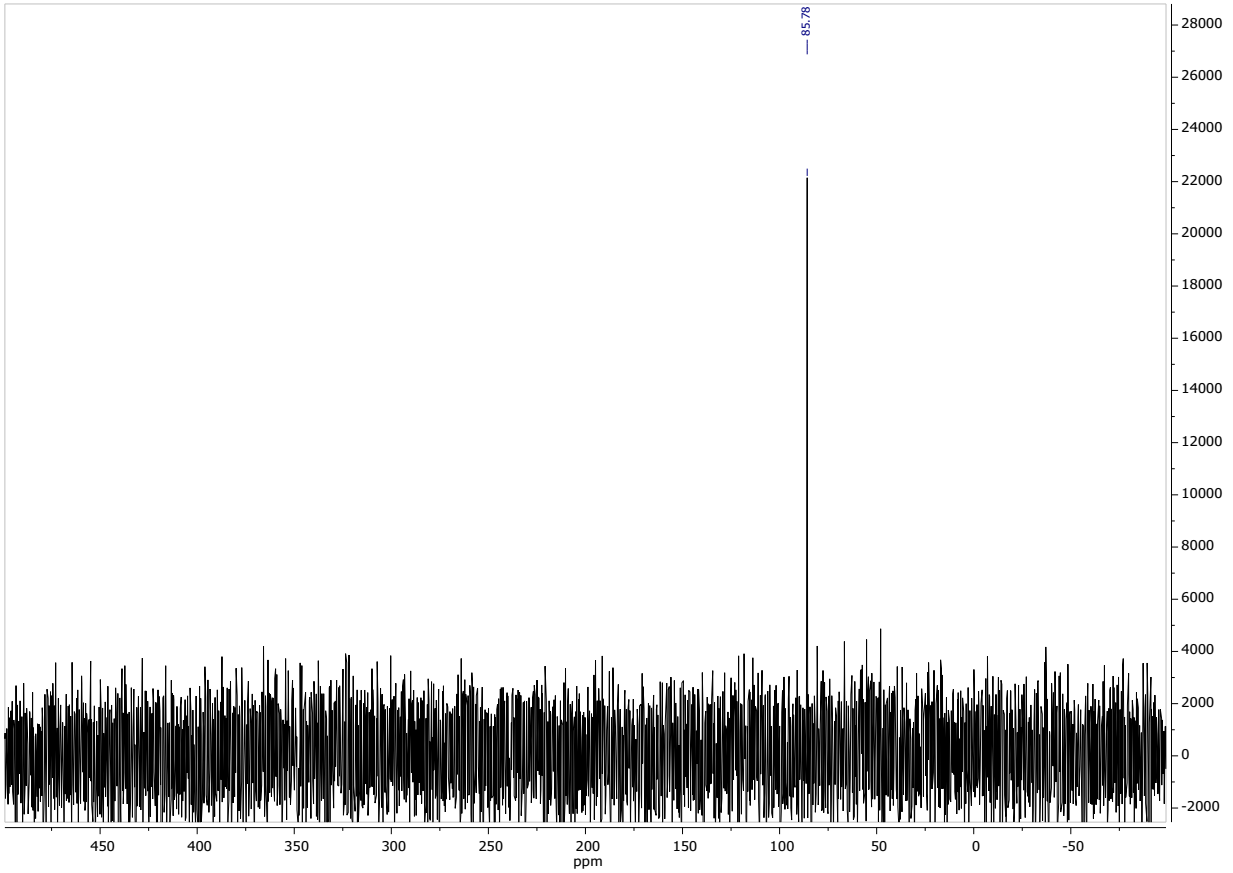


Figure-88: ^{13}C NMR spectrum (76 MHz) of **6d** in DMSO-d_6

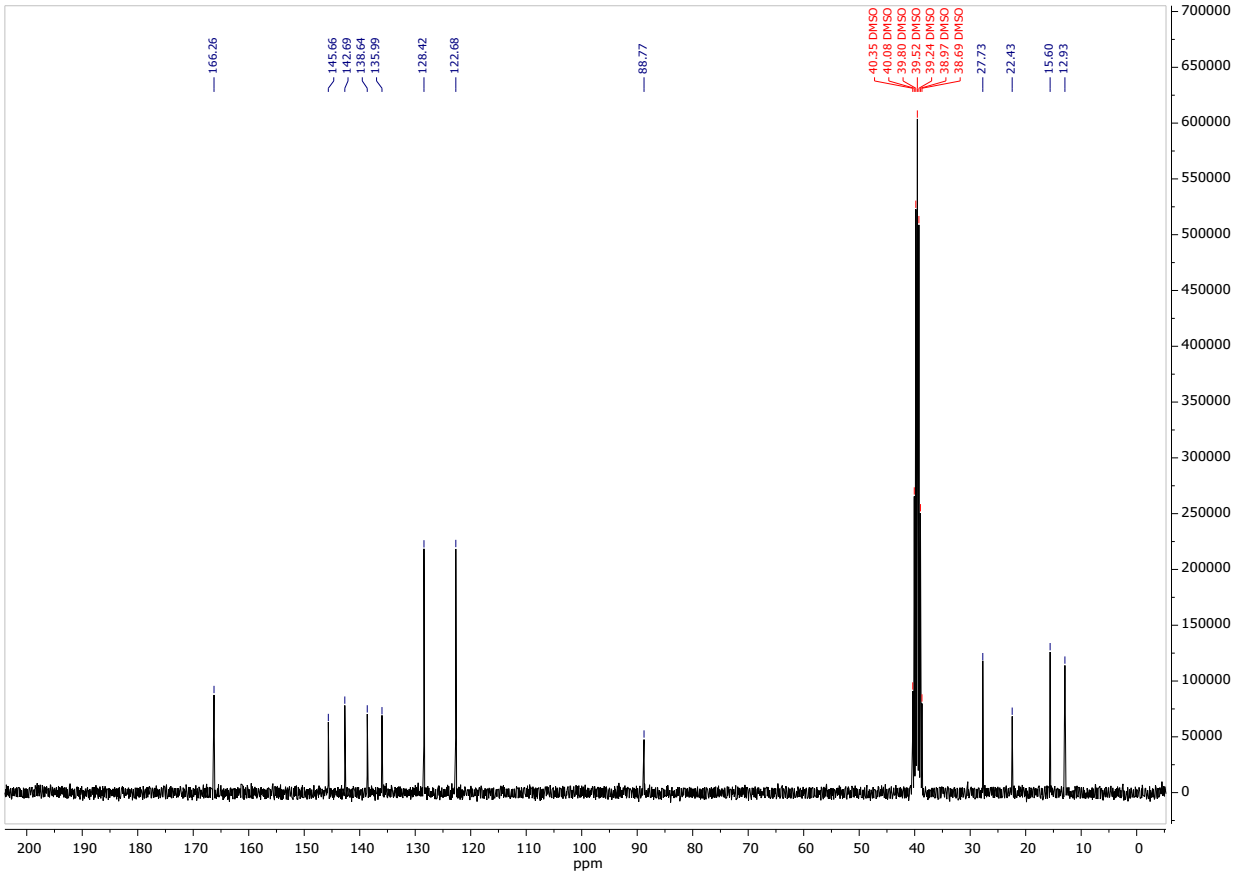
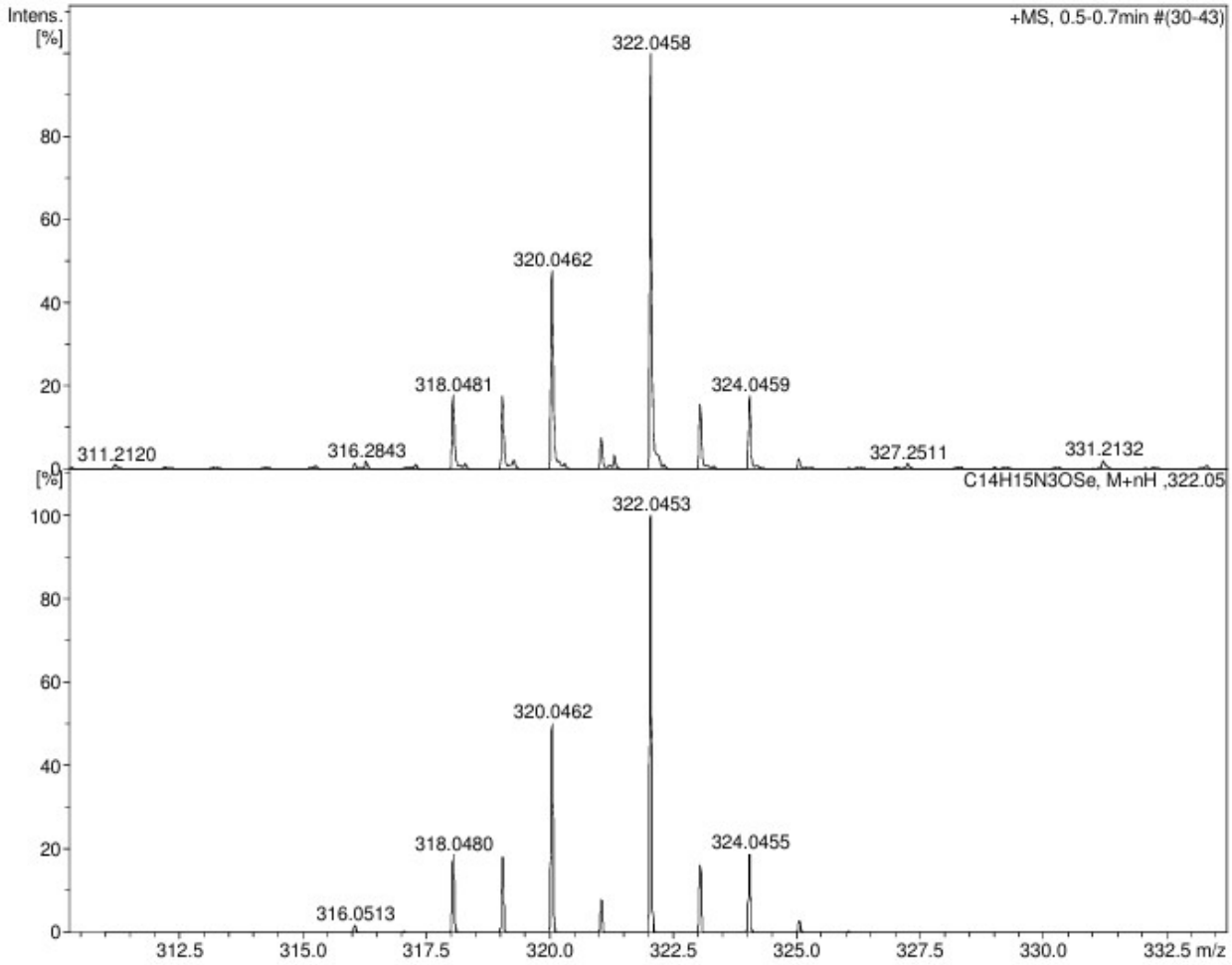
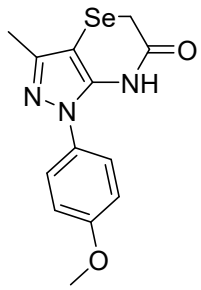


Figure-89: HRMS spectrum of compound **6d**





1-(4-Methoxyphenyl)-3-methyl-1,7-dihydropyrazolo[4,3-b][1,4]selenazin-6(5H)-one, ***6e***

Grey powder, m.p. 159-158°C, yield 72% (0.09 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.46 (s, 1H), 7.41 (d, J = 8.6 Hz, 2H), 7.03 (d, J = 8.6 Hz, 2H), 3.80 (s, 3H), 3.39 (s, 2H), 2.13 (s, 3H). ^{77}Se NMR (57 MHz, DMSO) δ 85.41. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.31, 158.24, 145.32, 138.74, 131.29, 124.61, 114.25, 88.08, 55.45, 22.38, 12.90. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{13}H_{14}N_3O_2Se$]$^{+}$: 324.0246; found: 324.0247.

Figure-90: ^{1}H NMR spectrum (300 MHz) of **6e** in DMSO-d_6

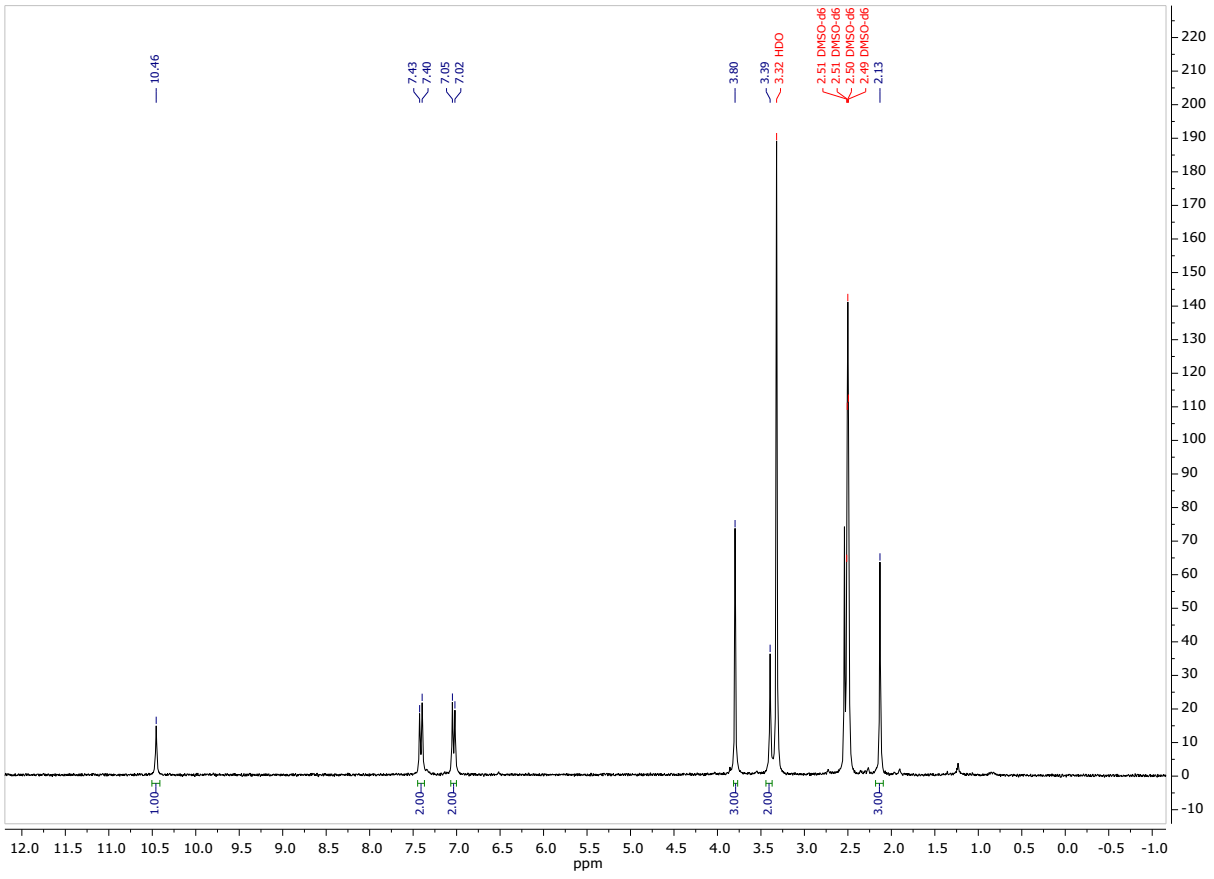


Figure-91: ^{77}Se NMR spectrum (57 MHz) of **6e** in DMSO-d_6

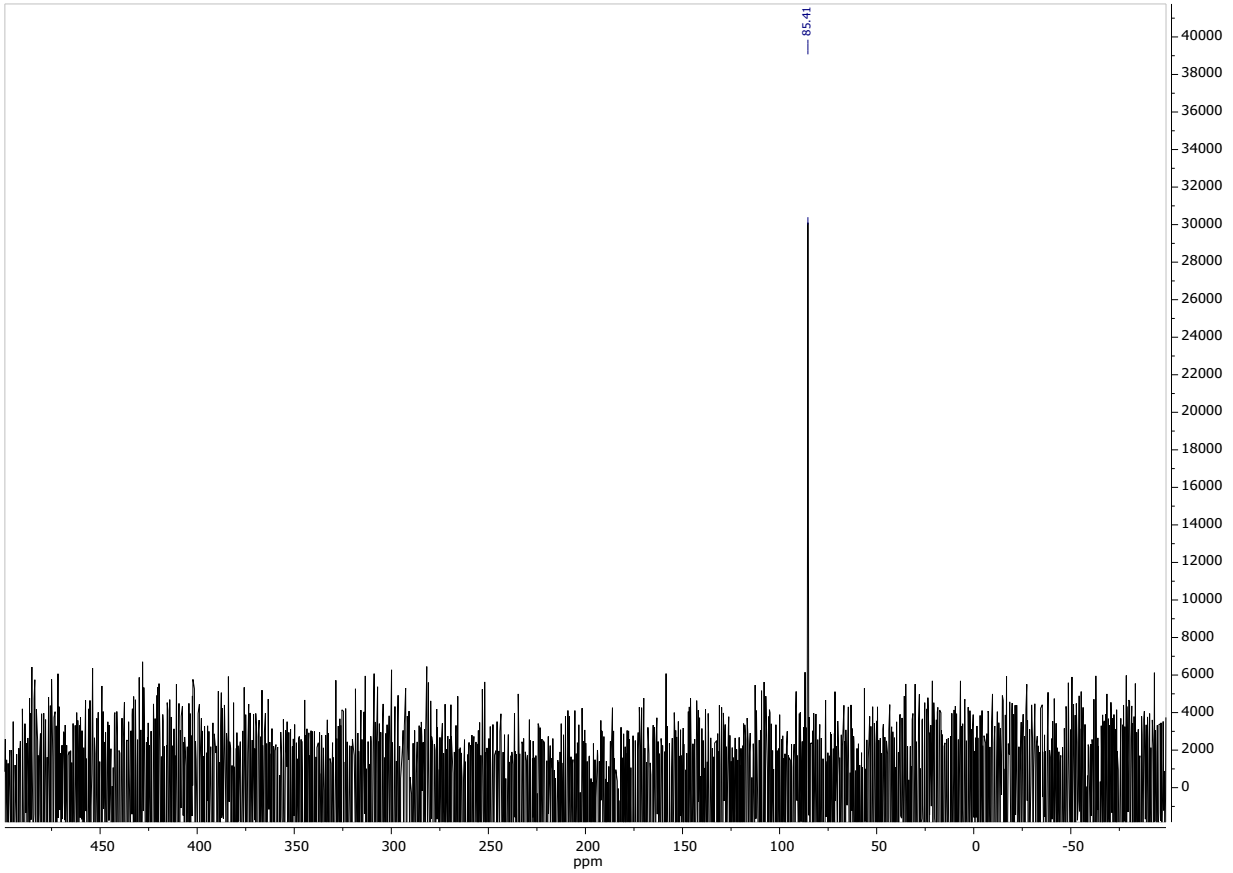


Figure-92: ^{13}C NMR spectrum (76 MHz) of **6e** in DMSO-d_6

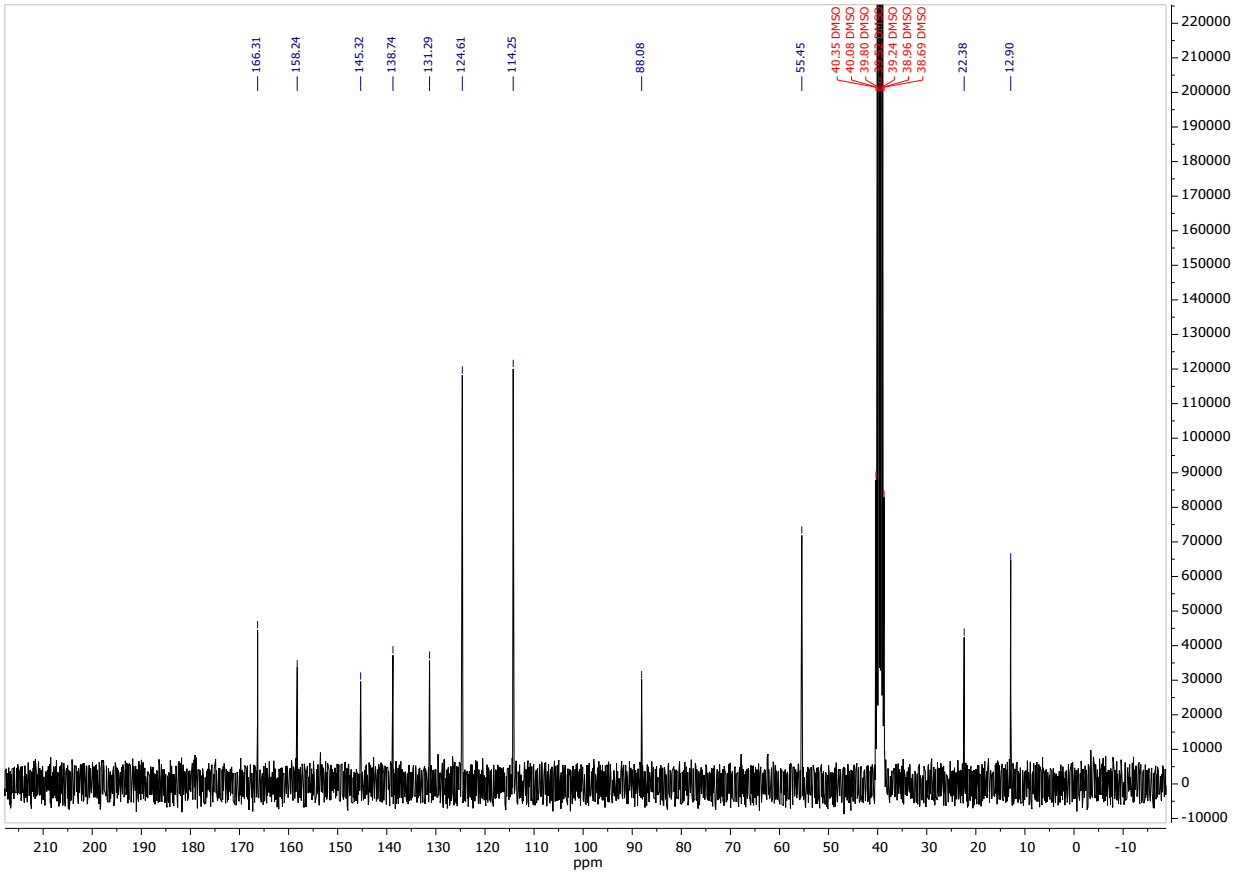
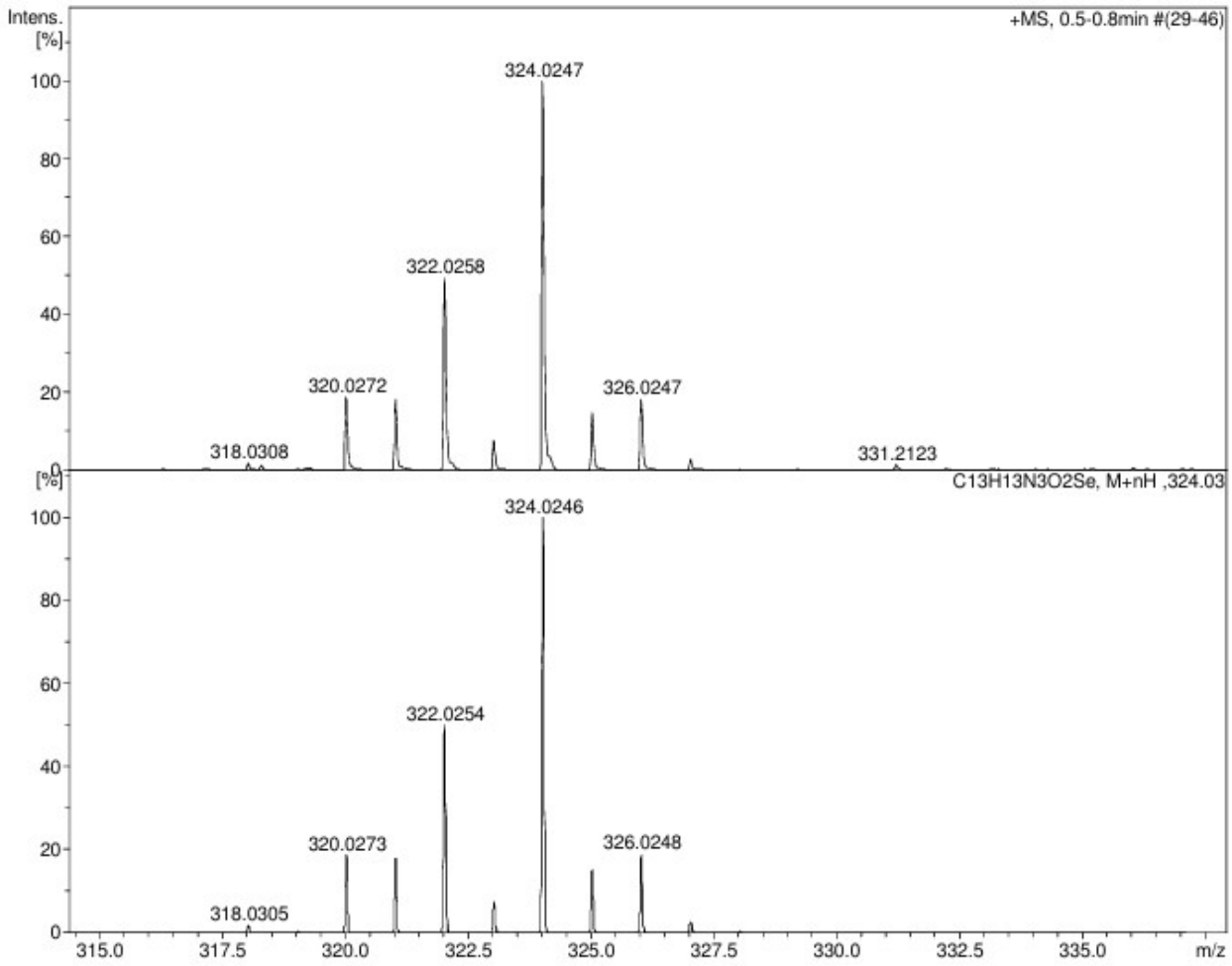
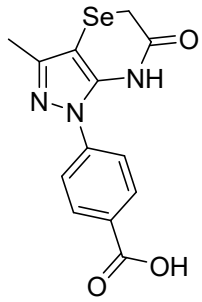


Figure-93: HRMS spectrum of compound **6e**





4-(3-Methyl-6-oxo-6,7-dihydropyrazolo[4,3-b][1,4]selenazin-1(5H)-yl)benzoic acid, ***6f***

Orange powder, m.p. 291-293 ^{o}C, yield 75% (0.10 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.69 (s, 1H), 8.04 (d, J = 8.6 Hz, 2H), 7.67 (d, J = 8.6 Hz, 2H), 3.44 (s, 2H), 2.17 (s, 3H). ^{77}Se NMR (57 MHz, DMSO) δ 88.35. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.79, 166.25, 147.00, 141.49, 138.87, 130.53, 128.68, 121.83, 90.43, 22.46, 13.03. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{13}H_{12}N_3O_3Se$]$^{+}$: 338.0039; found: 338.0043.

Figure-94: ^{1}H NMR spectrum (300 MHz) of **6f** in DMSO-d_6

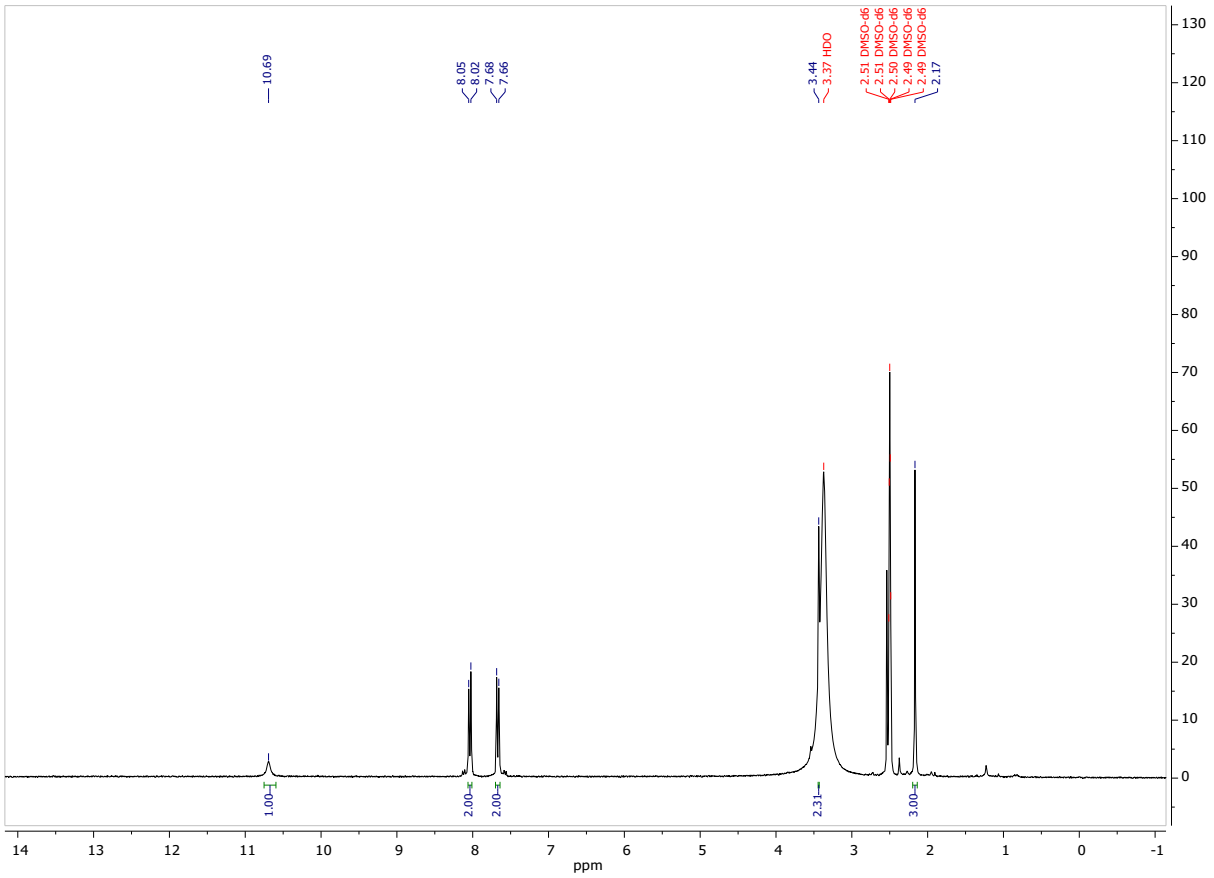


Figure-95: ^{77}Se NMR spectrum (57 MHz) of **6f** in DMSO-d_6

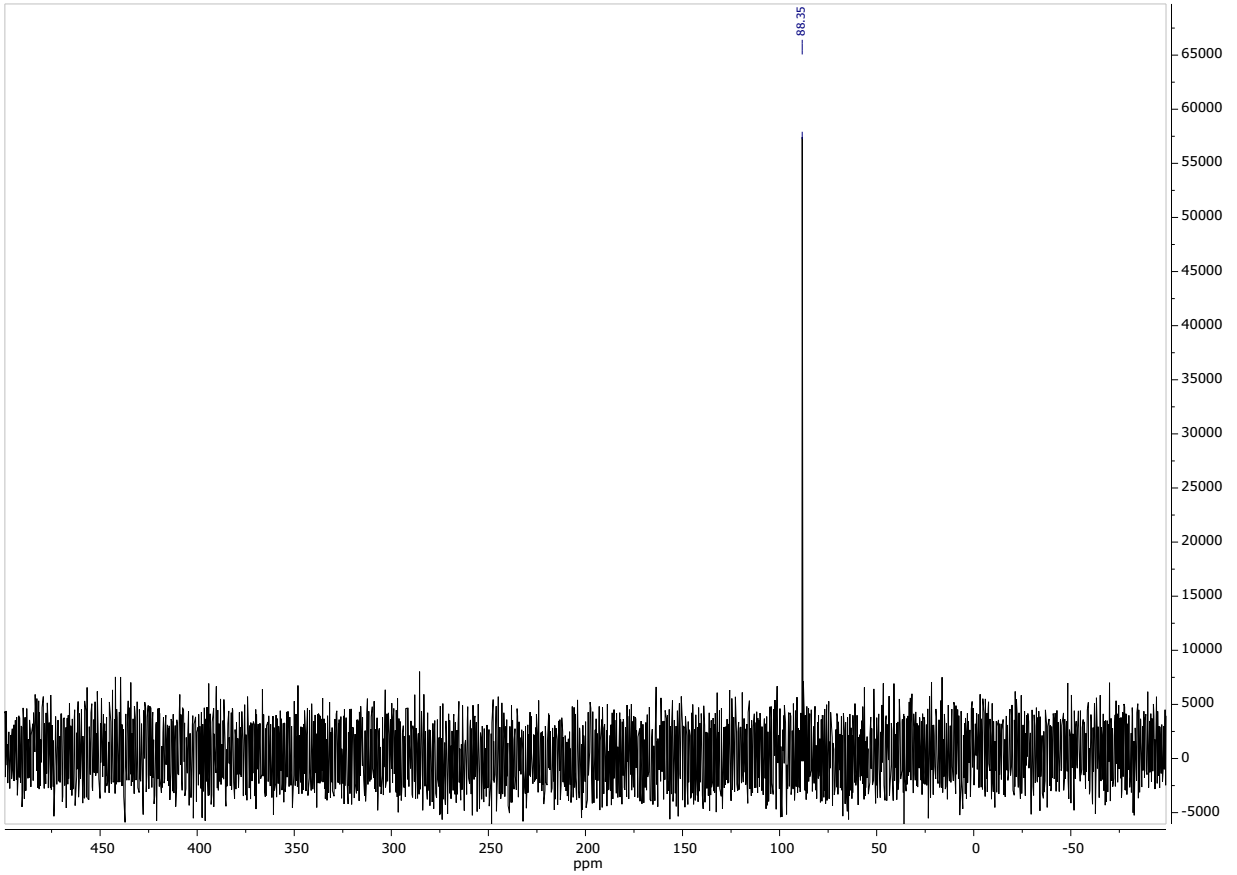


Figure-96: ^{13}C NMR spectrum (76 MHz) of **6f** in DMSO-d_6

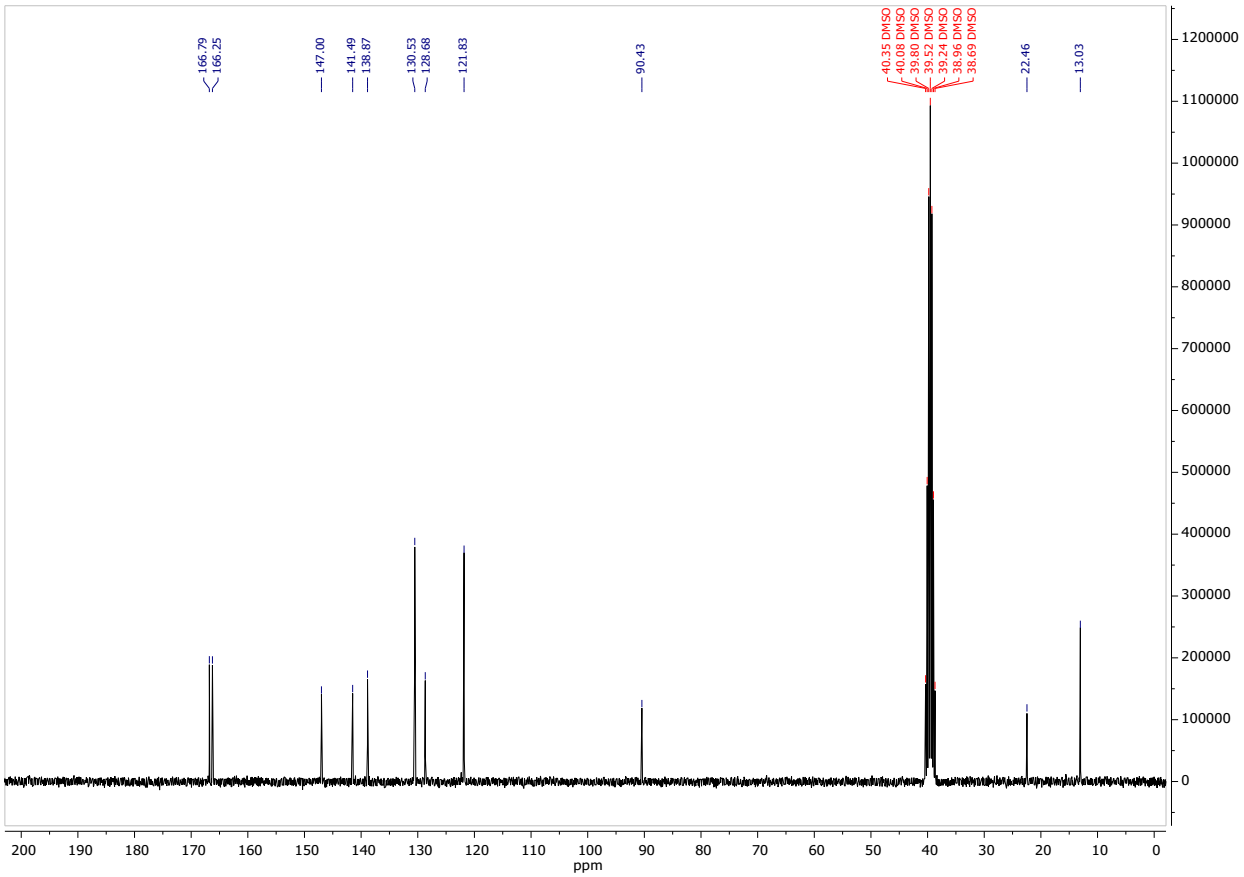
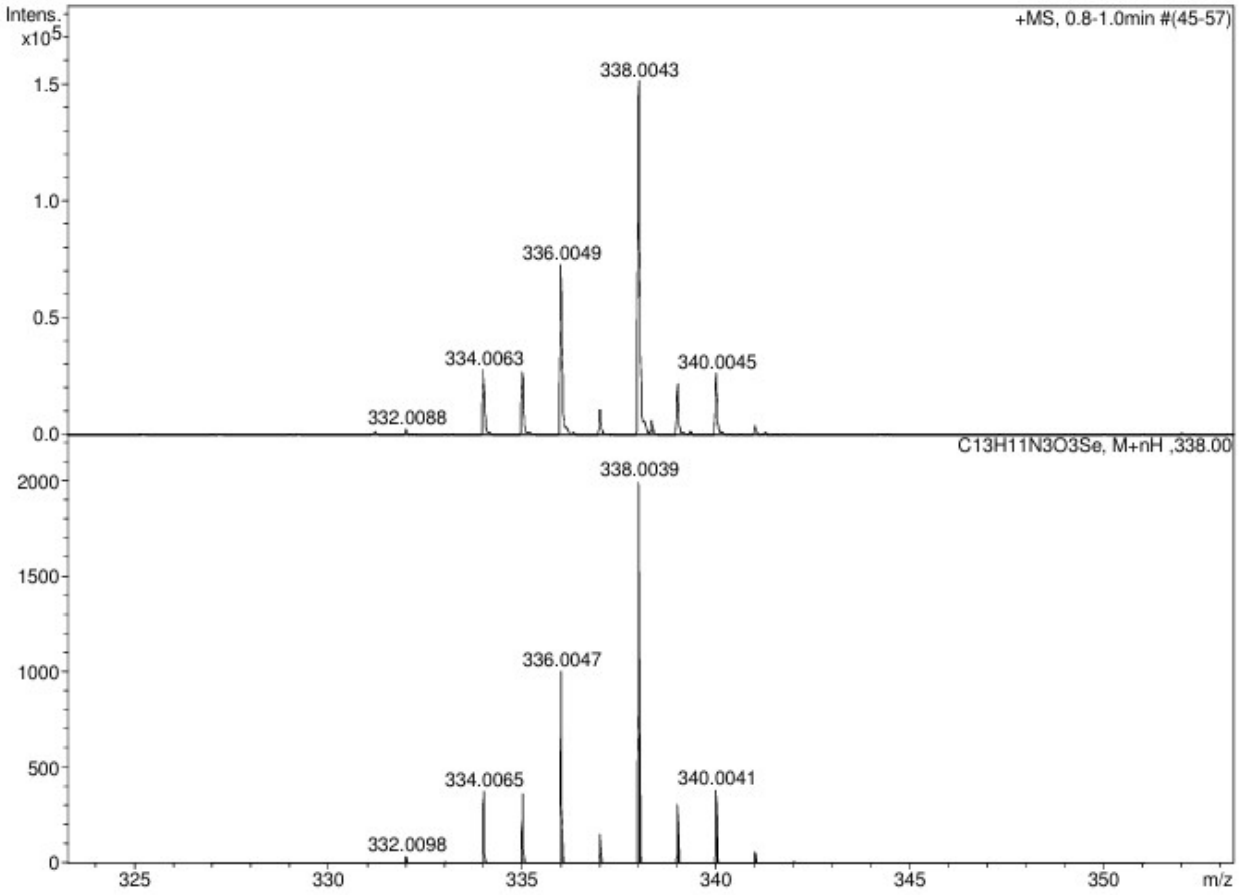
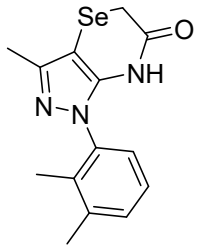


Figure-97: HRMS spectrum of compound **6f**





1-(2,3-Dimethylphenyl)-3-methyl-1,7-dihydropyrazolo[4,3-b][1,4]selenazin-6(5H)-one, ***6h***

Grey powder, m.p. 185-187°C, yield 74% (0.09 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.37 (s, 1H), 7.28 (d, J = 7.6 Hz, 1H), 7.19 (t, J = 7.7 Hz, 1H), 7.06 (d, J = 7.6 Hz, 1H), 3.37 (s, 2H), 2.29 (s, 3H), 2.13 (s, 3H), 1.88 (s, 3H). ^{77}Se NMR (57 MHz, DMSO) δ 81.90. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.29, 145.16, 140.27, 137.88, 136.76, 134.34, 130.29, 125.77, 125.36, 85.65, 22.26, 19.89, 14.06, 12.97. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{14}H_{16}N_3OSe$]$^{+}$: 322.0453; found: 322.0452.

Figure-98: ^{1}H NMR spectrum (300 MHz) of **6h** in DMSO-d_6

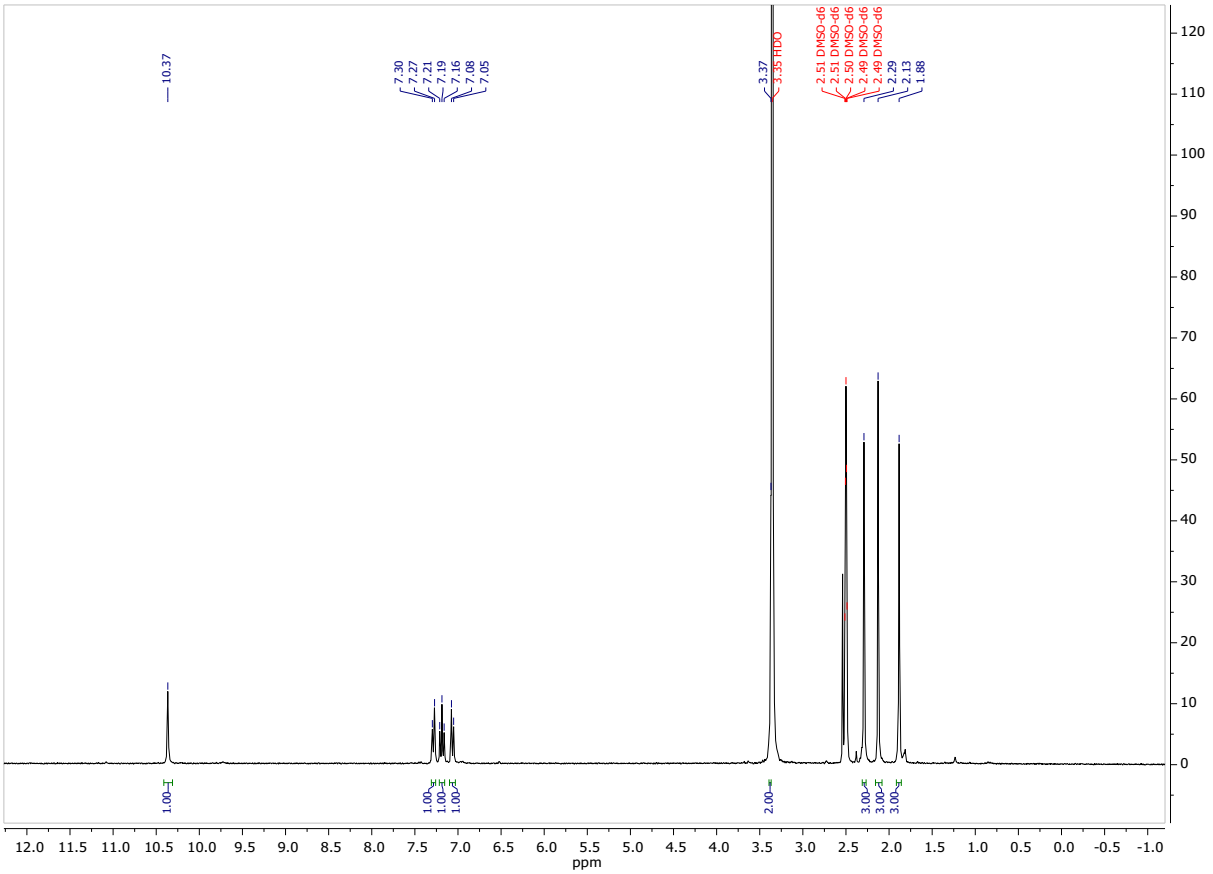


Figure-99: ^{77}Se NMR spectrum (57 MHz) of **6h** in DMSO-d_6

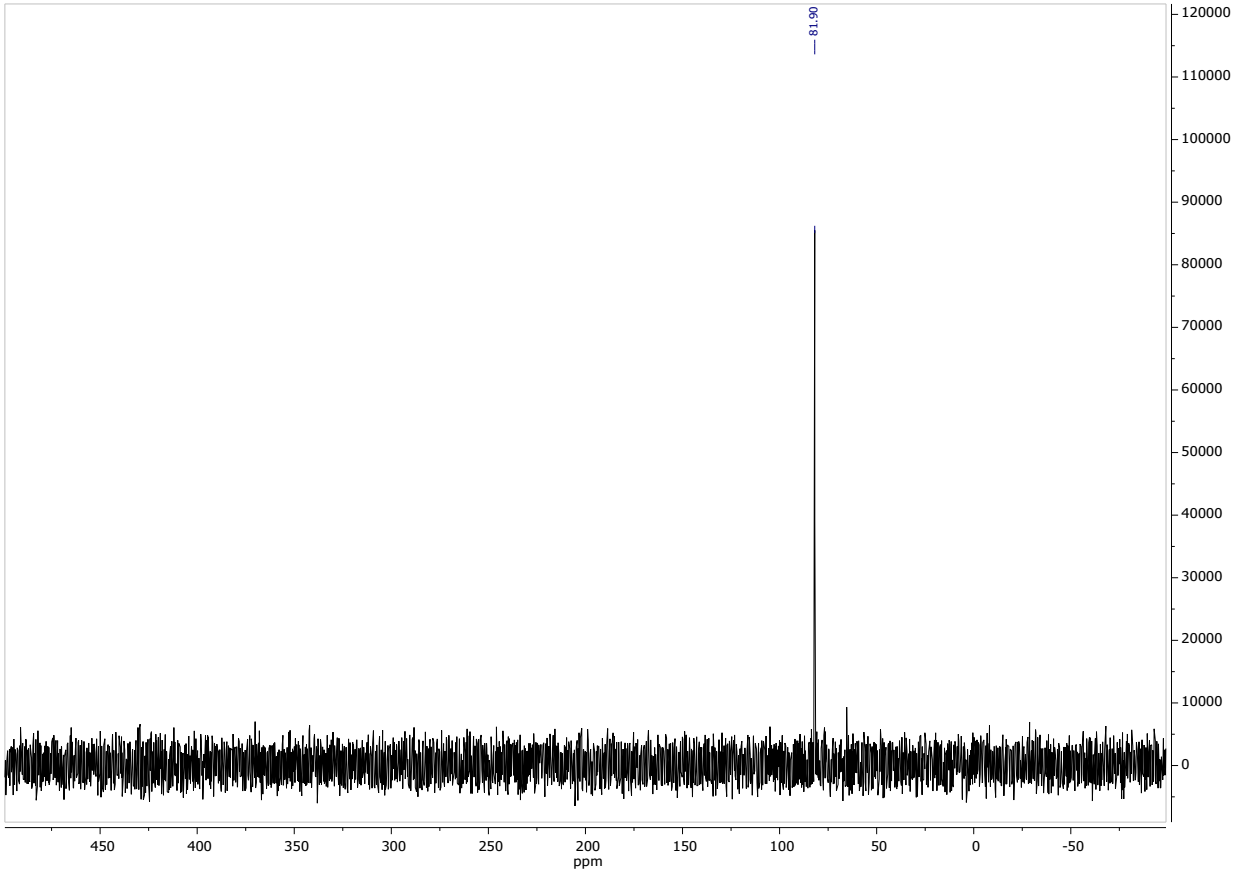


Figure-100: ^{13}C NMR spectrum (76 MHz) of **6h** in DMSO-d_6

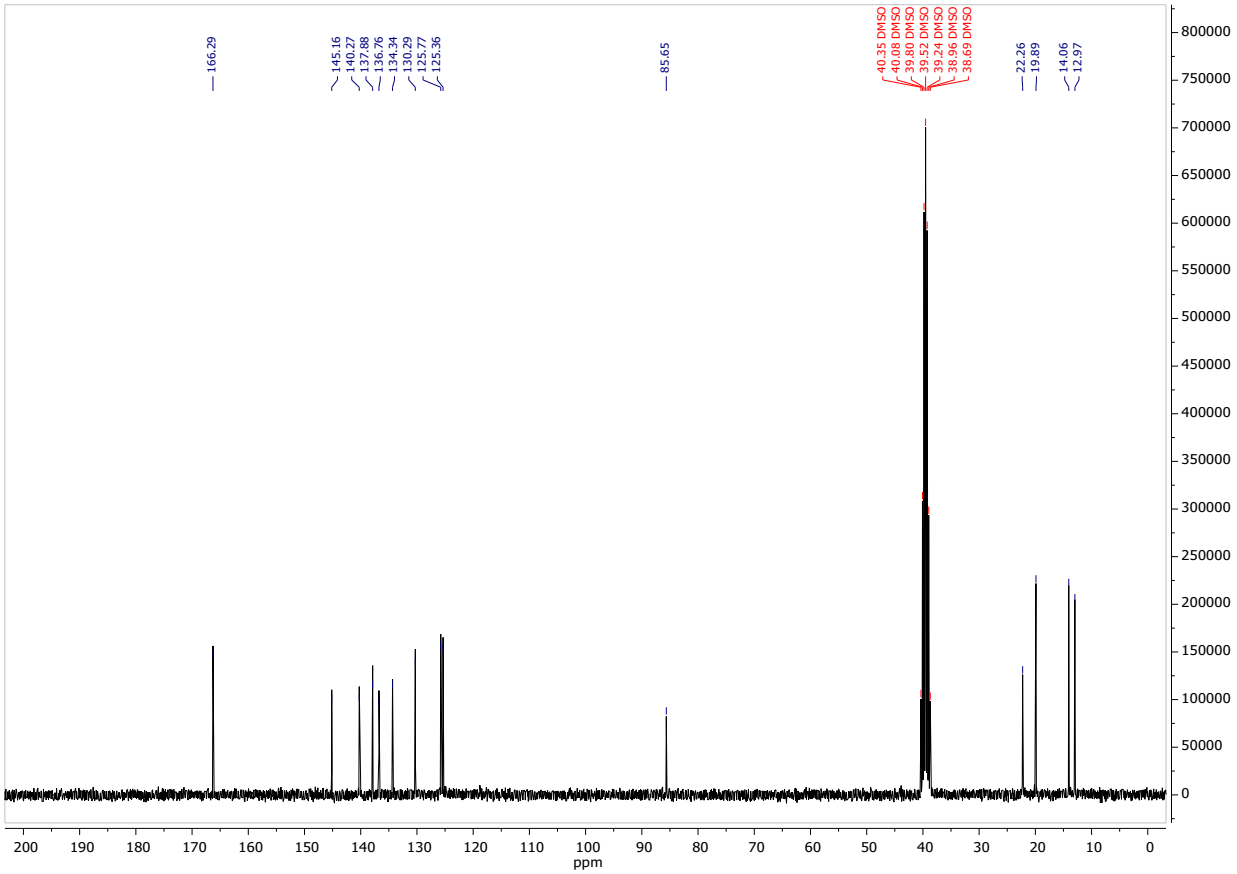
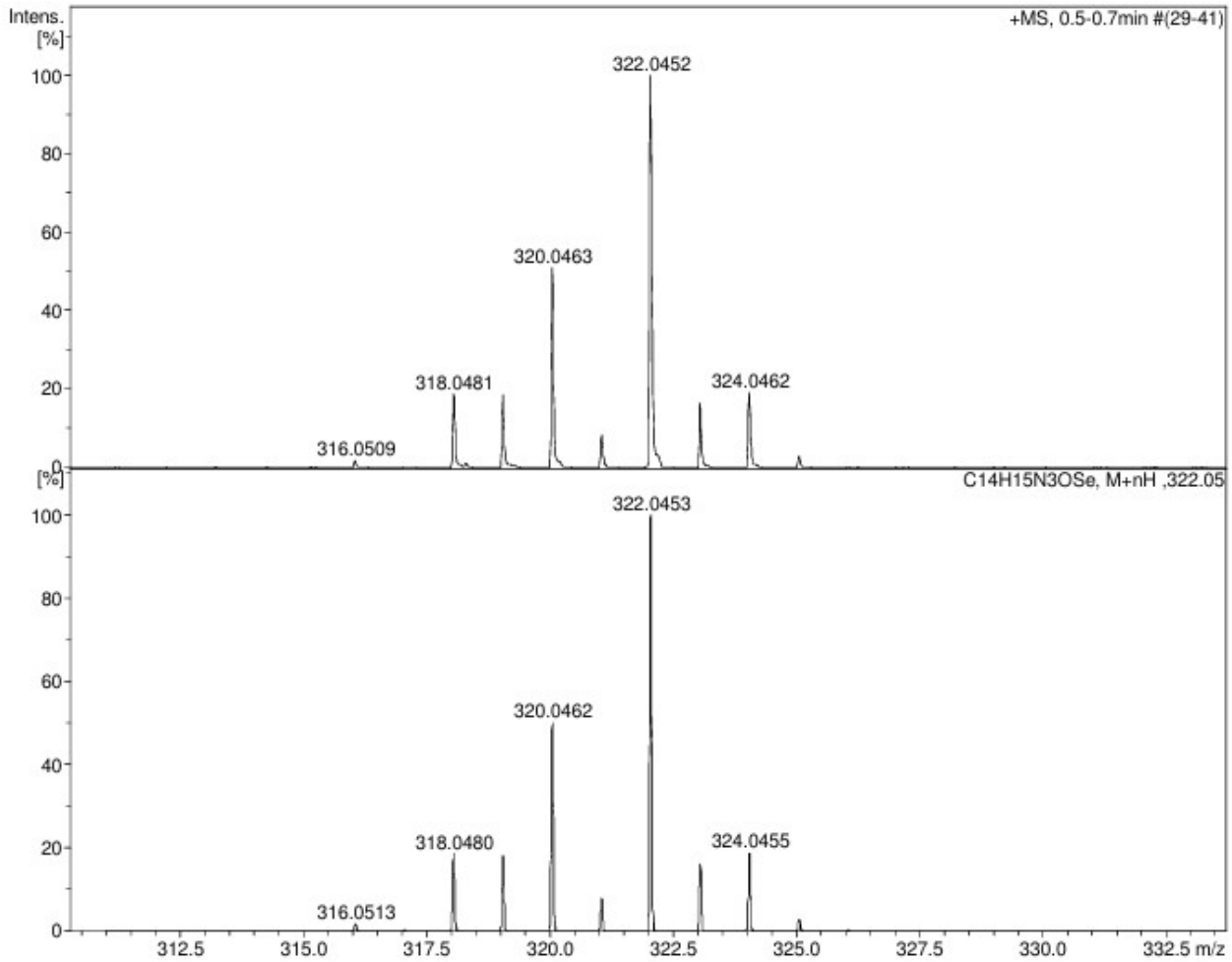
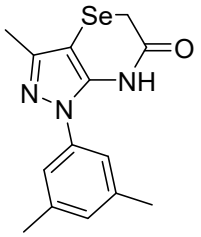


Figure-101: HRMS spectrum of compound **6h**





1-(3,5-Dimethylphenyl)-3-methyl-1,7-dihydropyrazolo[4,3-b][1,4]selenazin-6(5H)-one, ***6i***

Pale yellow powder, m.p. 181-183°C, yield 88% (0.11 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.52 (s, 1H), 7.14 (s, 2H), 6.99 (s, 1H), 3.40 (s, 2H), 2.32 (s, 6H), 2.14 (s, 3H). ^{77}Se NMR (57 MHz, DMSO) δ 84.59. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.29, 145.69, 138.58, 138.40, 137.99, 128.40, 120.31, 88.77, 22.41, 20.89, 12.92. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{14}H_{16}N_3OSe$]$^{+}$: 322.0453; found: 322.0464.

Figure-102: ^{1}H NMR spectrum (300 MHz) of **6i** in DMSO-d_6

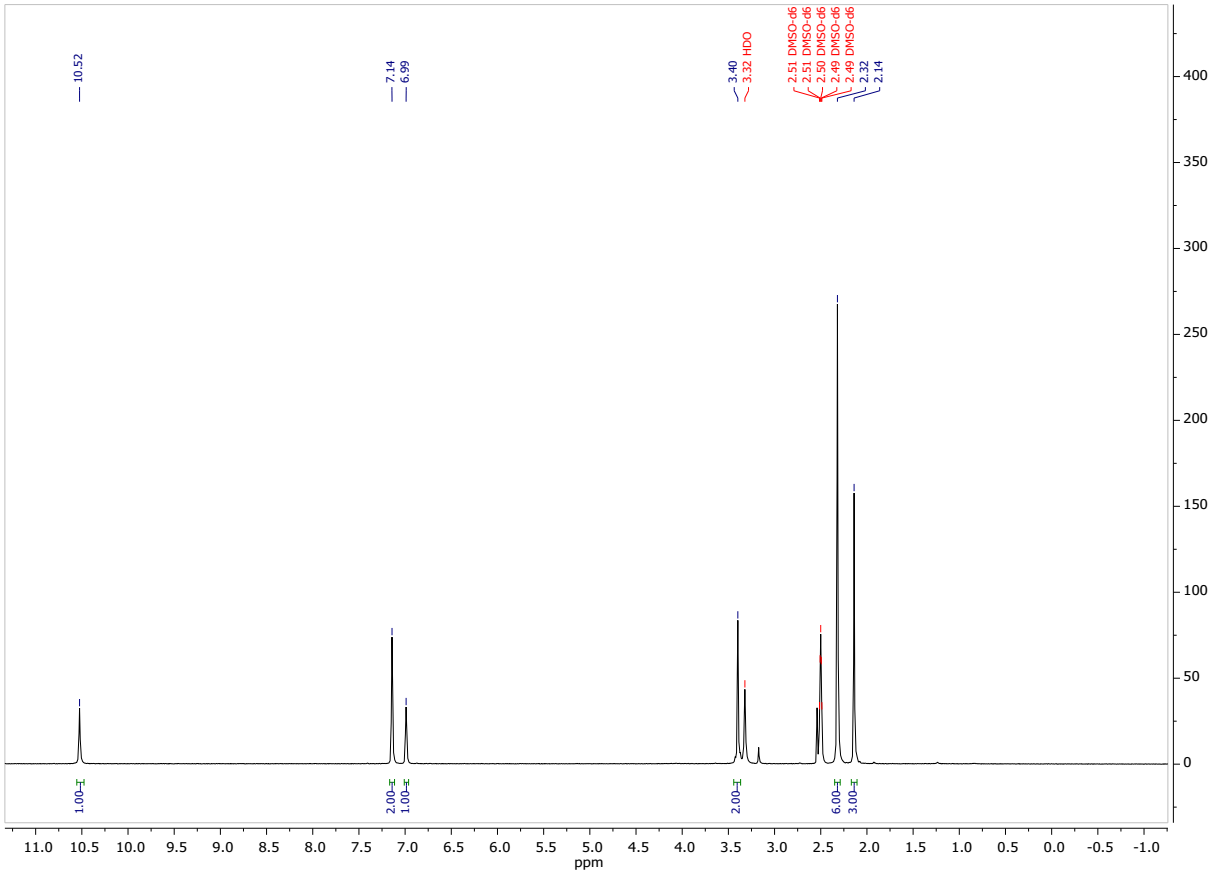


Figure-103: ^{77}Se NMR spectrum (57 MHz) of **6i** in DMSO-d_6

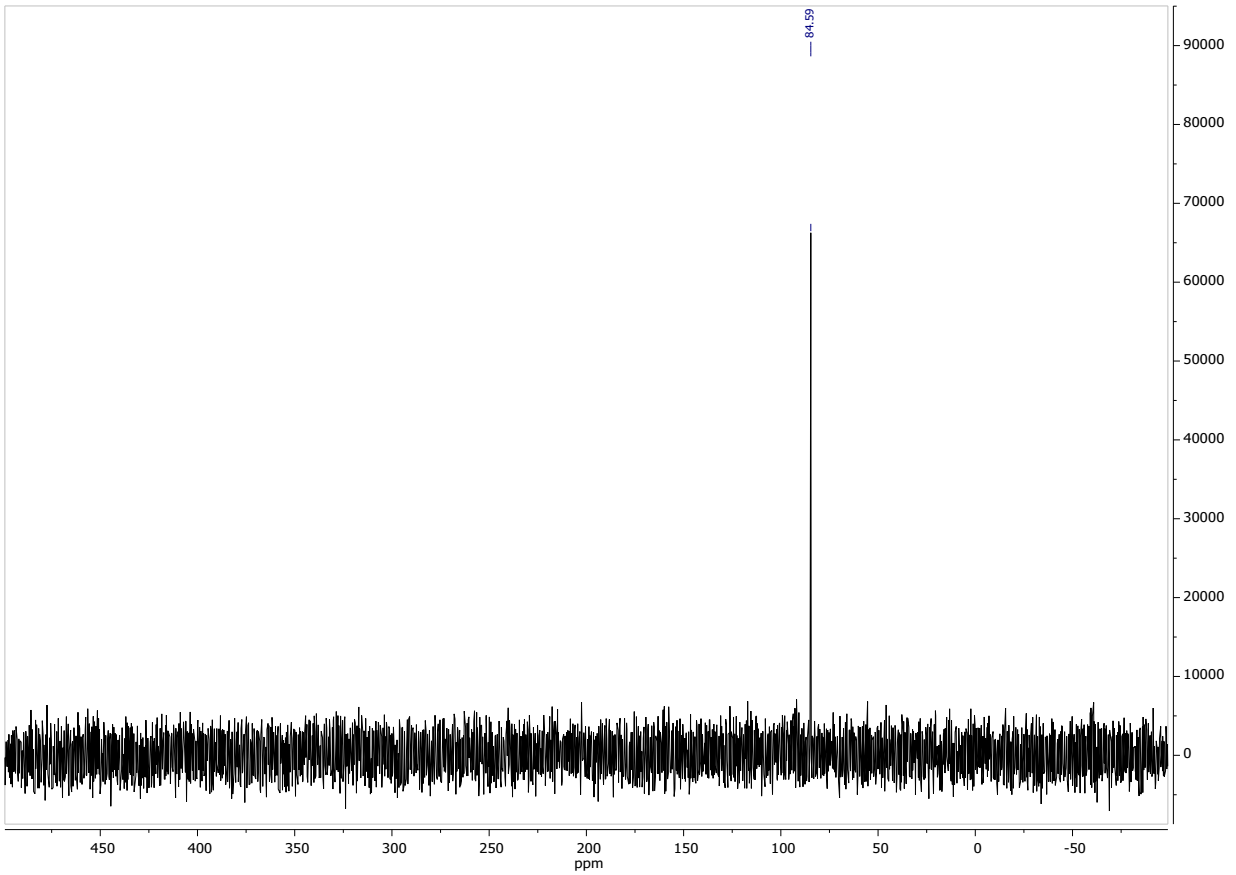


Figure-104: ^{13}C NMR spectrum (76 MHz) of **6i** in DMSO-d_6

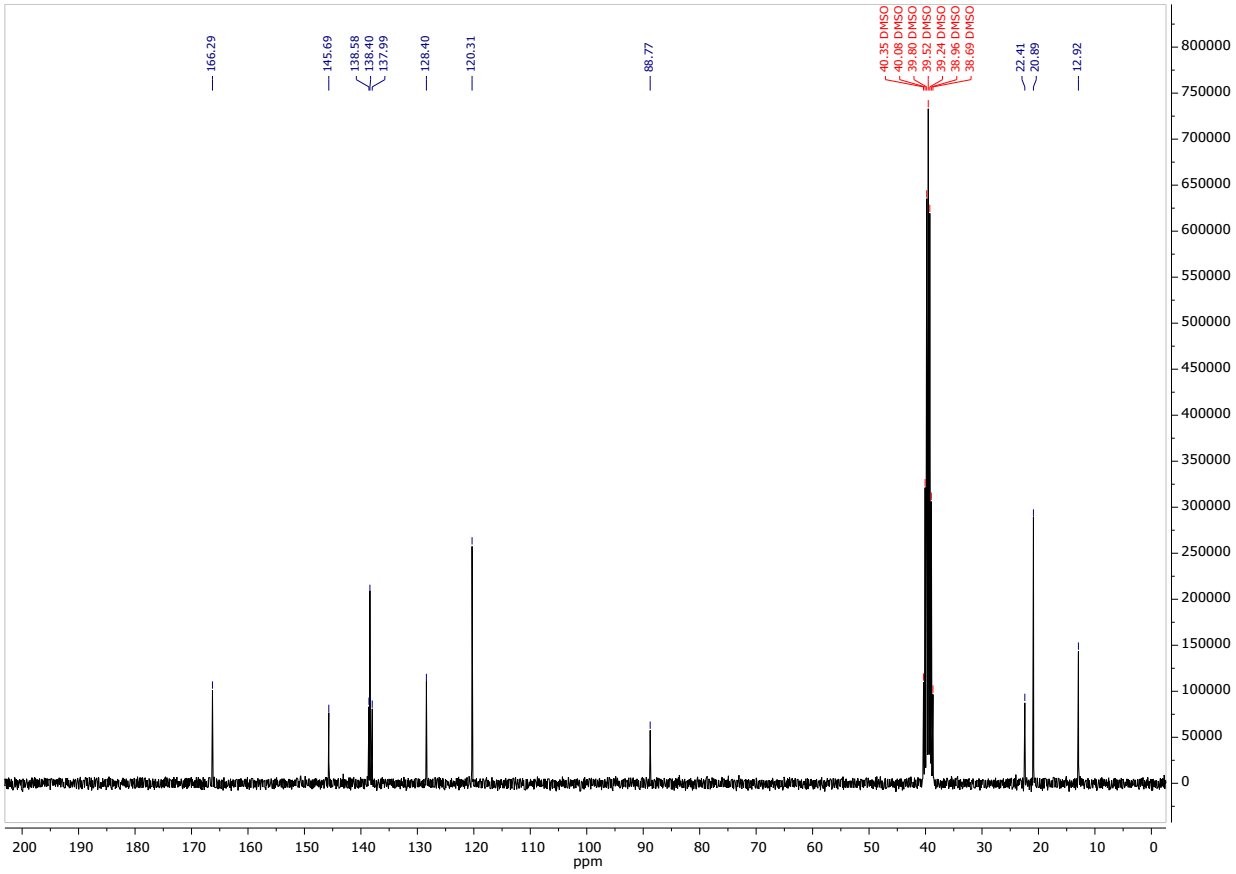
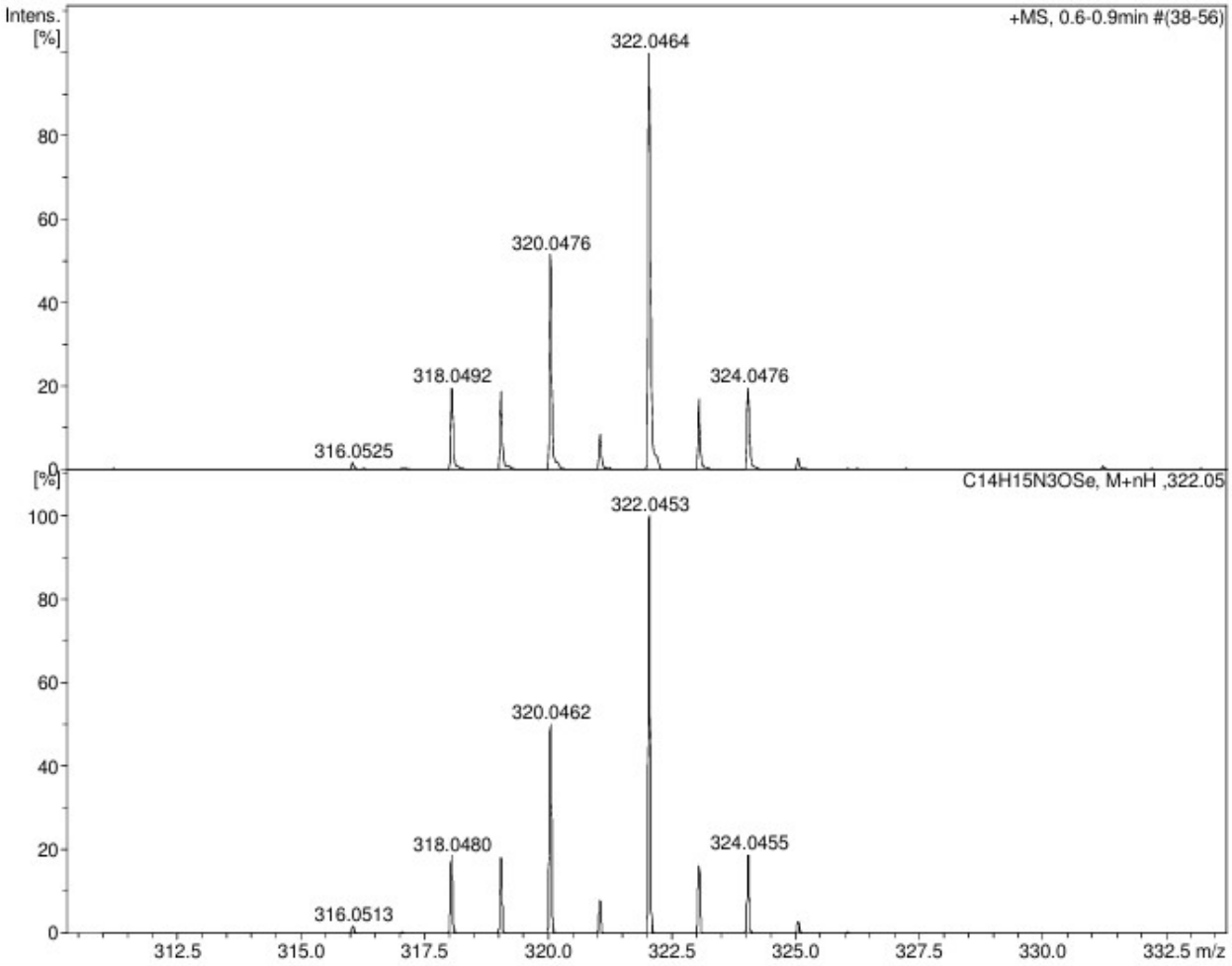
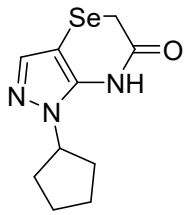


Figure-105: HRMS spectrum of compound **6i**





1-Cyclopentyl-1,7-dihydropyrazolo[4,3-b][1,4]selenazin-6(5H)-one, ***6j***

White powder, m.p. 185-187°C, yield 80% (0.09 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.72 (s, 1H), 7.30 (s, 1H), 4.74 – 4.65 (m, 1H), 3.32 (s, 2H), 2.00 – 1.92 (m, 2H), 1.87 – 1.76 (m, 4H), 1.61 – 1.54 (m, 2H). ^{77}Se NMR (57 MHz, DMSO) δ 91.74. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.38, 138.54, 136.17, 84.46, 57.70, 31.98, 24.17, 21.90. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{10}H_{14}N_3OSe$]$^{+}$: 272.0297; found: 272.0307.

Figure-106: ^{1}H NMR spectrum (300 MHz) of **6j** in DMSO-d_6

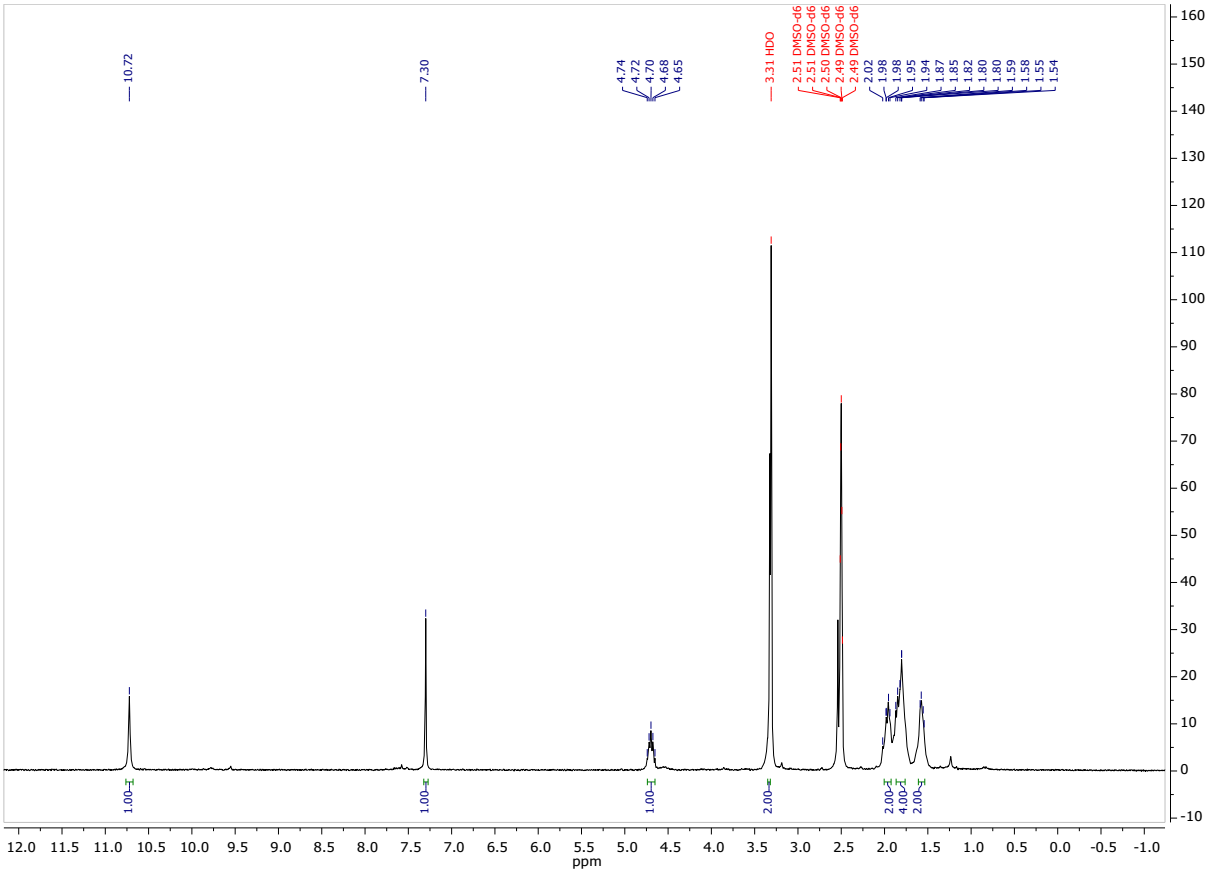


Figure-107: ^{77}Se NMR spectrum (57 MHz) of **6j** in DMSO-d_6

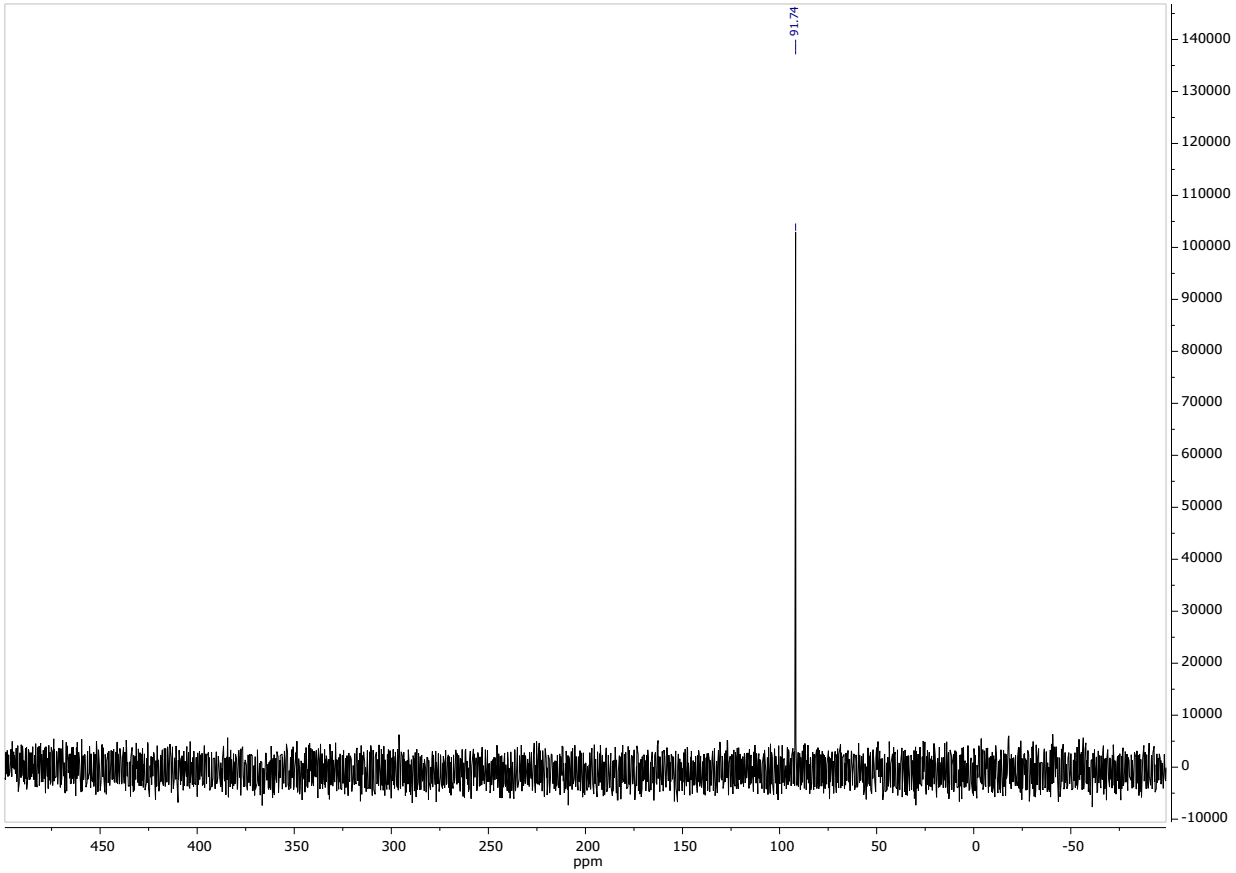


Figure-108: ^{13}C NMR spectrum (76 MHz) of **6j** in DMSO-d_6

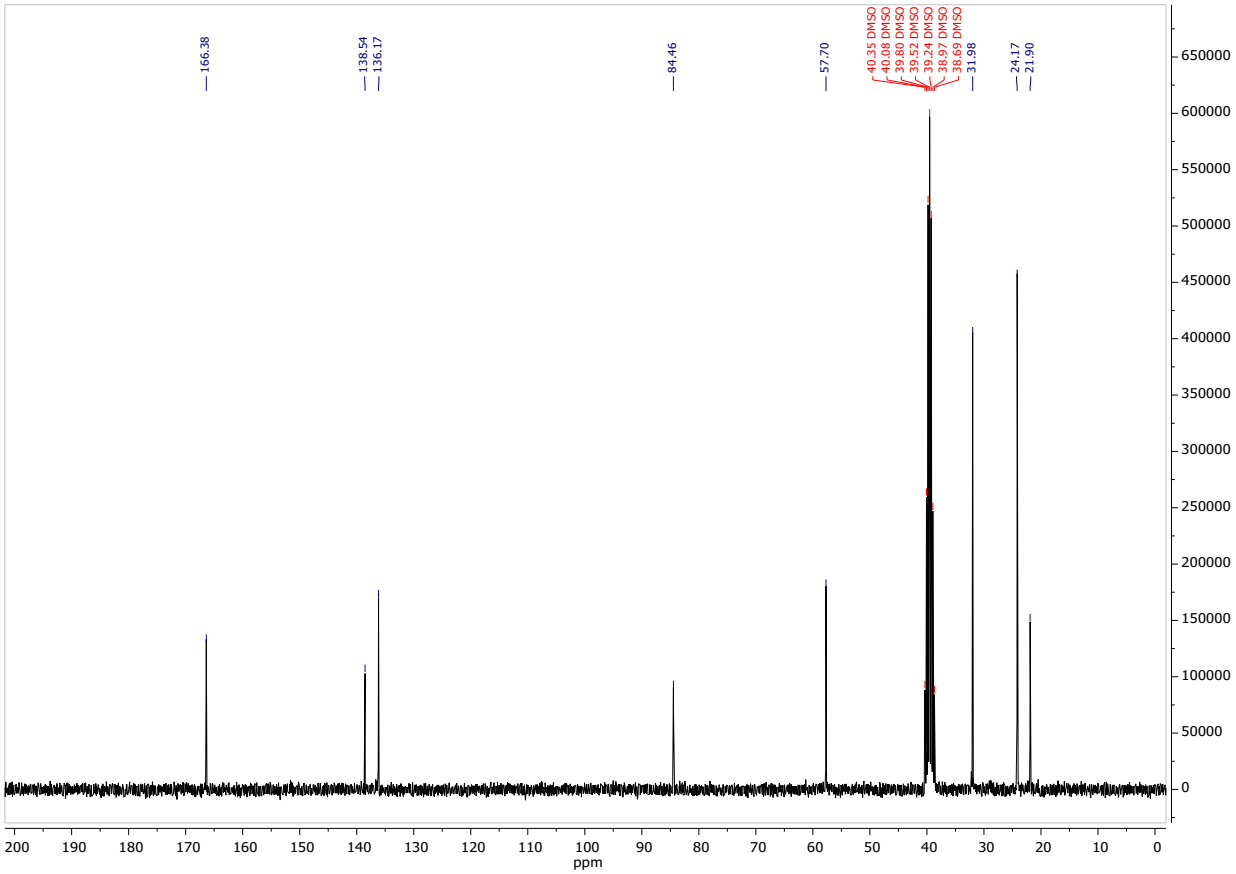
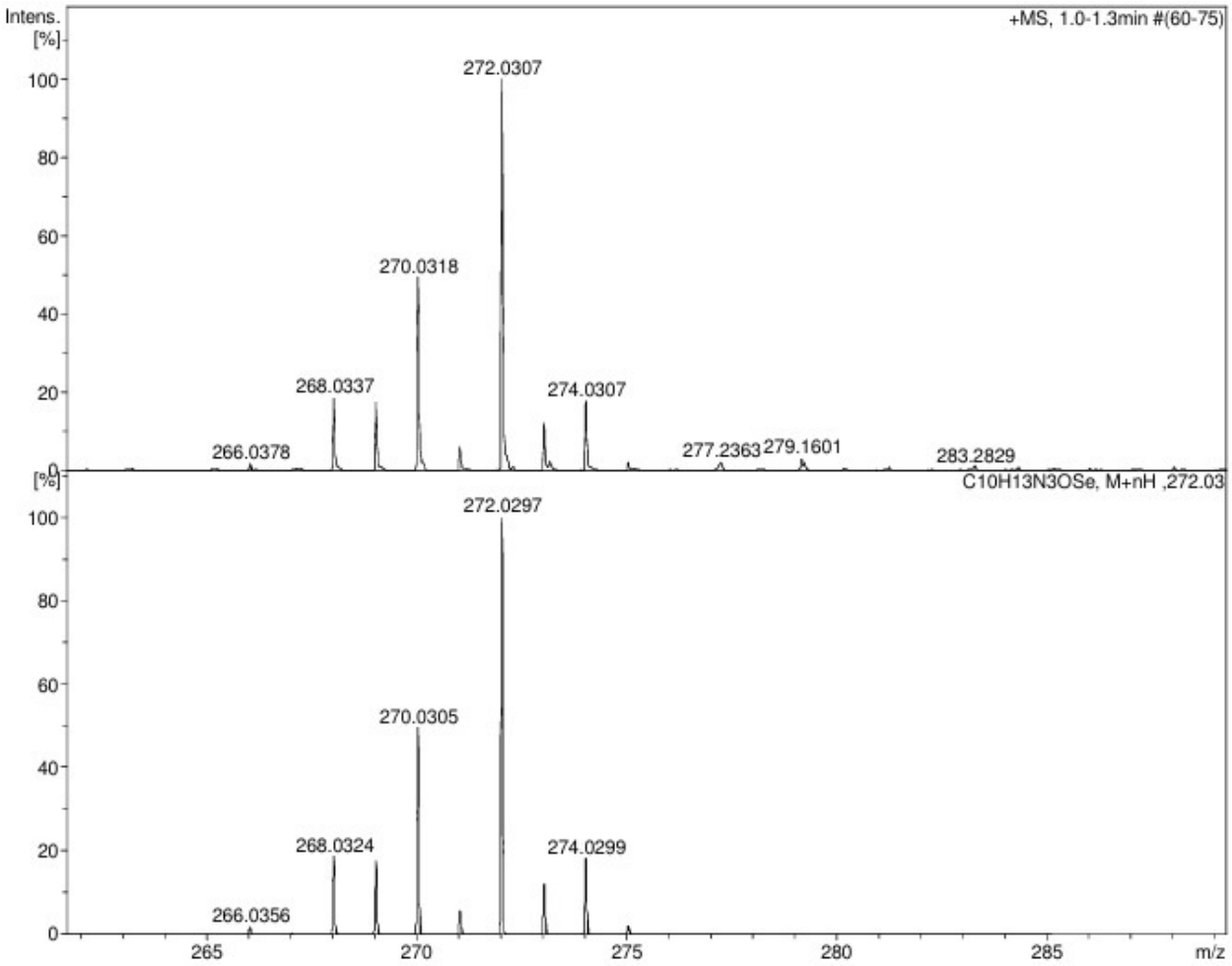
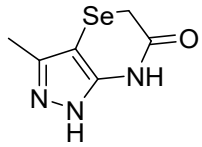


Figure-109: HRMS spectrum of compound **6j**





3-Methyl-1,7-dihydropyrazolo[4,3-b][1,4]selenazin-6(5H)-one, ***6l***

Pale yellow powder, m.p. 255-257°C, yield 62% (0.05 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 12.22 (s, 1H), 10.39 (s, 1H), 3.28 (s, 2H), 2.13 (s, 3H). ^{77}Se NMR (57 MHz, DMSO) δ 72.89. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 166.06, 149.21, 135.86, 85.03, 21.60, 10.19. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_6H_8N_3OSe$]$^{+}$: 217.9827; found: 217.9826.

Figure-110: ^{1}H NMR spectrum (300 MHz) of **6l** in DMSO-d_6

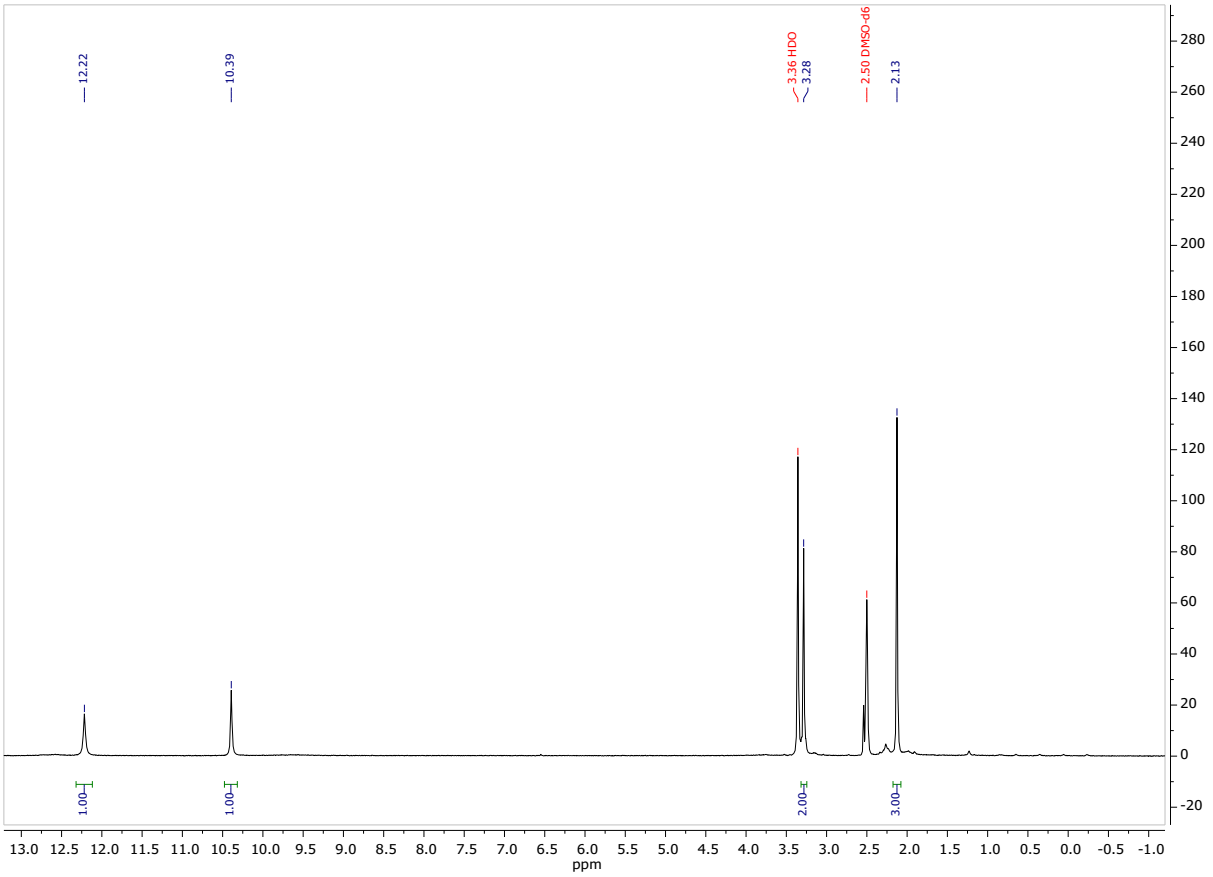


Figure-111: ^{77}Se NMR spectrum (57 MHz) of **6l** in DMSO-d_6

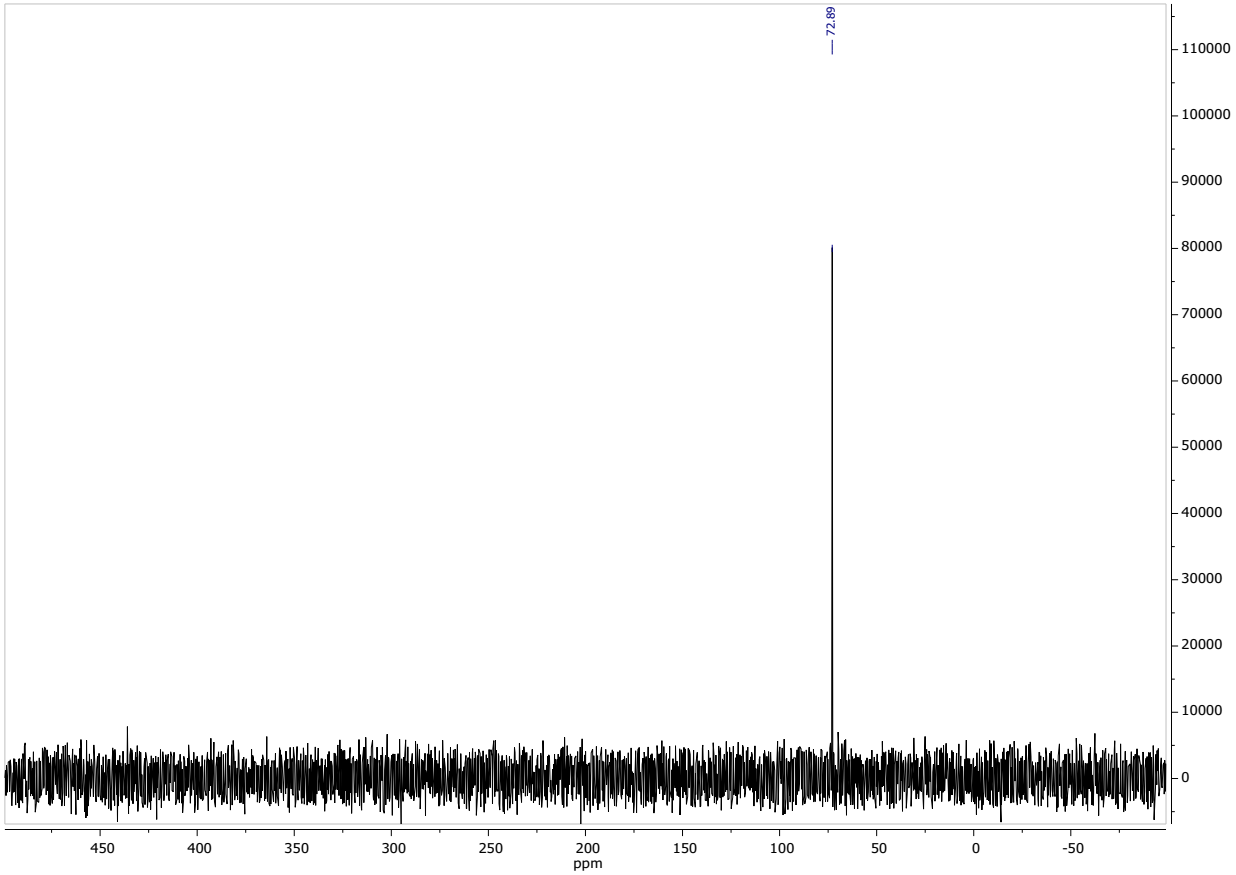


Figure-112: ^{13}C NMR spectrum (76 MHz) of **6l** in DMSO-d_6

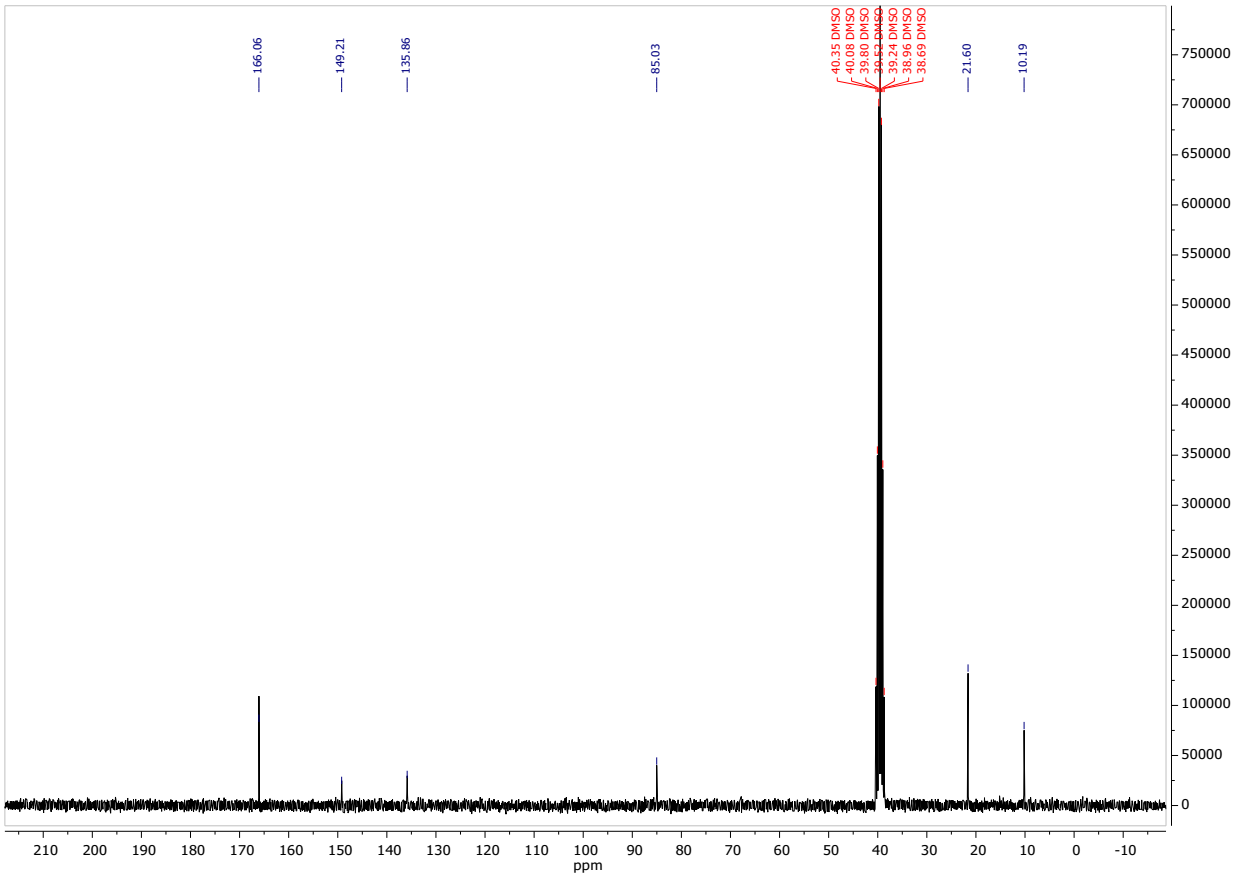
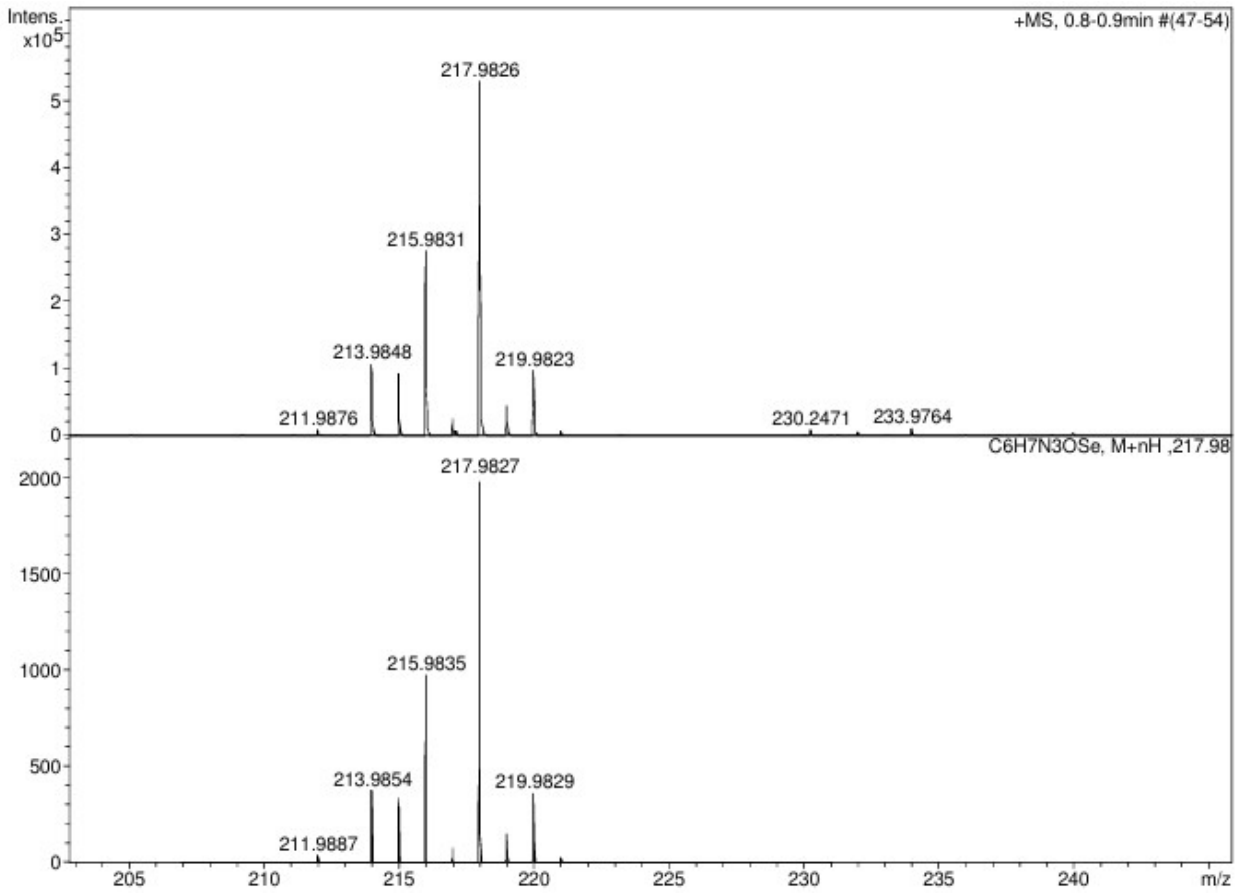
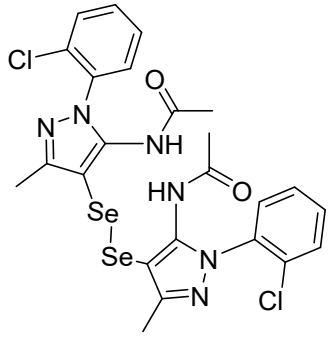


Figure-113: HRMS spectrum of compound **6l**



NMR and HRMS spectra of compound 7



*N,N'-(diselanediylbis(1-(2-chlorophenyl)-3-methyl-1H-pyrazole-4,5-diyl))diacetamide, **7***

Yellow powder, m.p. 147-149°C, yield 66% (0.17 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 9.90 (s, 2H), 7.67 – 7.60 (m, 2H), 7.53 – 7.46 (m, 4H), 7.40 – 7.35 (m, 2H), 2.11 (s, 6H), 1.85 (s, 6H). ^{77}Se NMR (57 MHz, DMSO) δ 327.22. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 169.12, 152.08, 140.81, 135.98, 130.77, 130.44, 130.06, 129.56, 127.84, 99.81, 22.37, 13.03. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{24}H_{23}Cl_2N_6O_2Se_2$]$^{+}$: 656.9590; found: 656.9588.

Figure-114: ^{1}H NMR spectrum (300 MHz) of **7** in DMSO-d_6

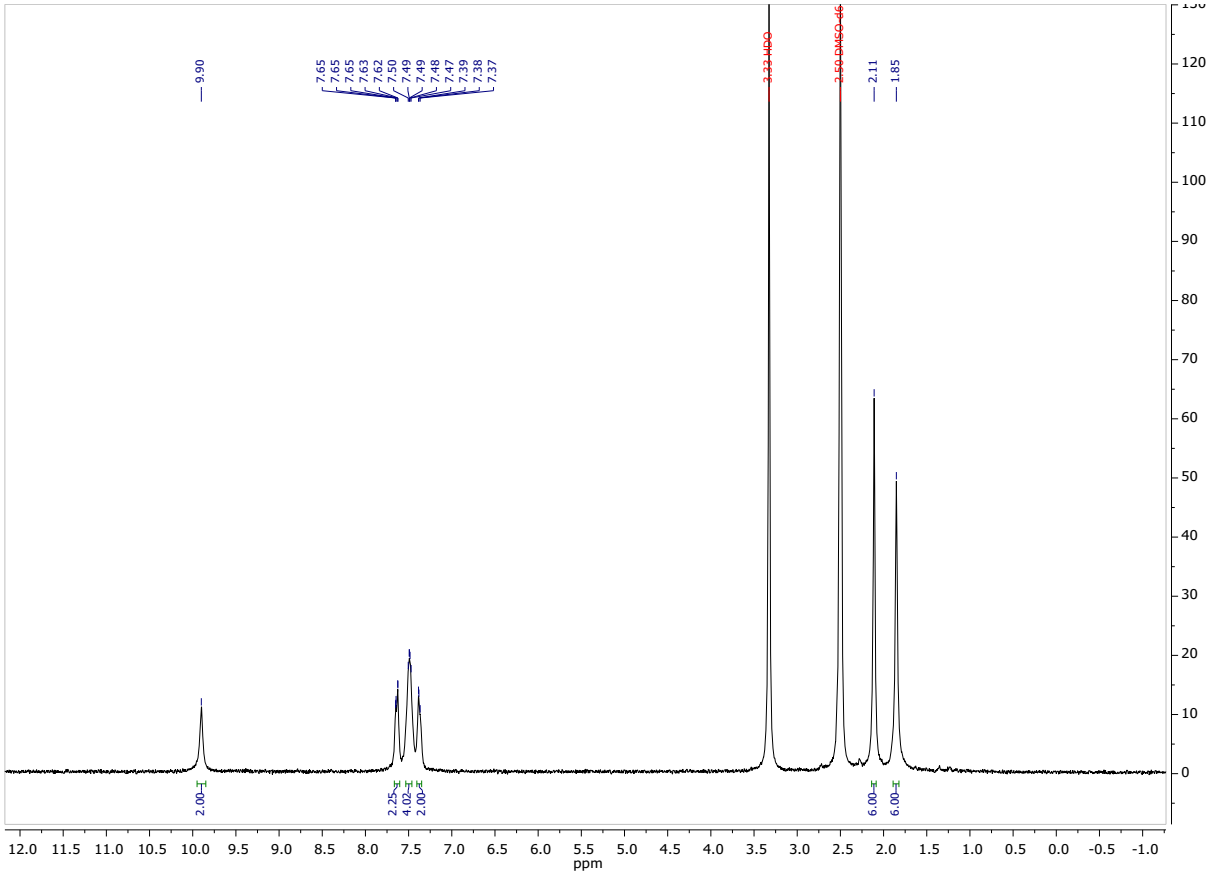


Figure-115: ^{77}Se NMR spectrum (57 MHz) of **7** in DMSO-d_6

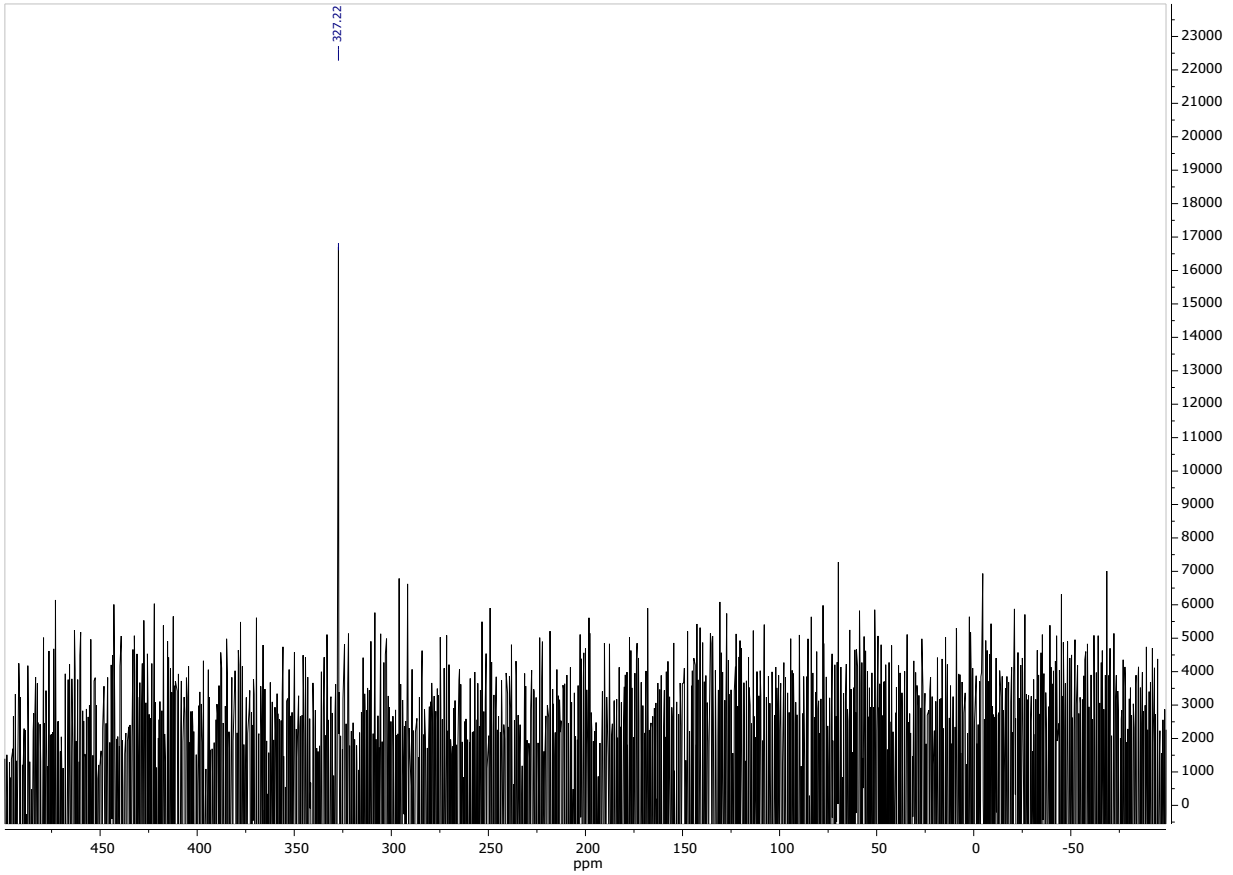


Figure-116: ^{13}C NMR spectrum (76 MHz) of **7** in DMSO-d_6

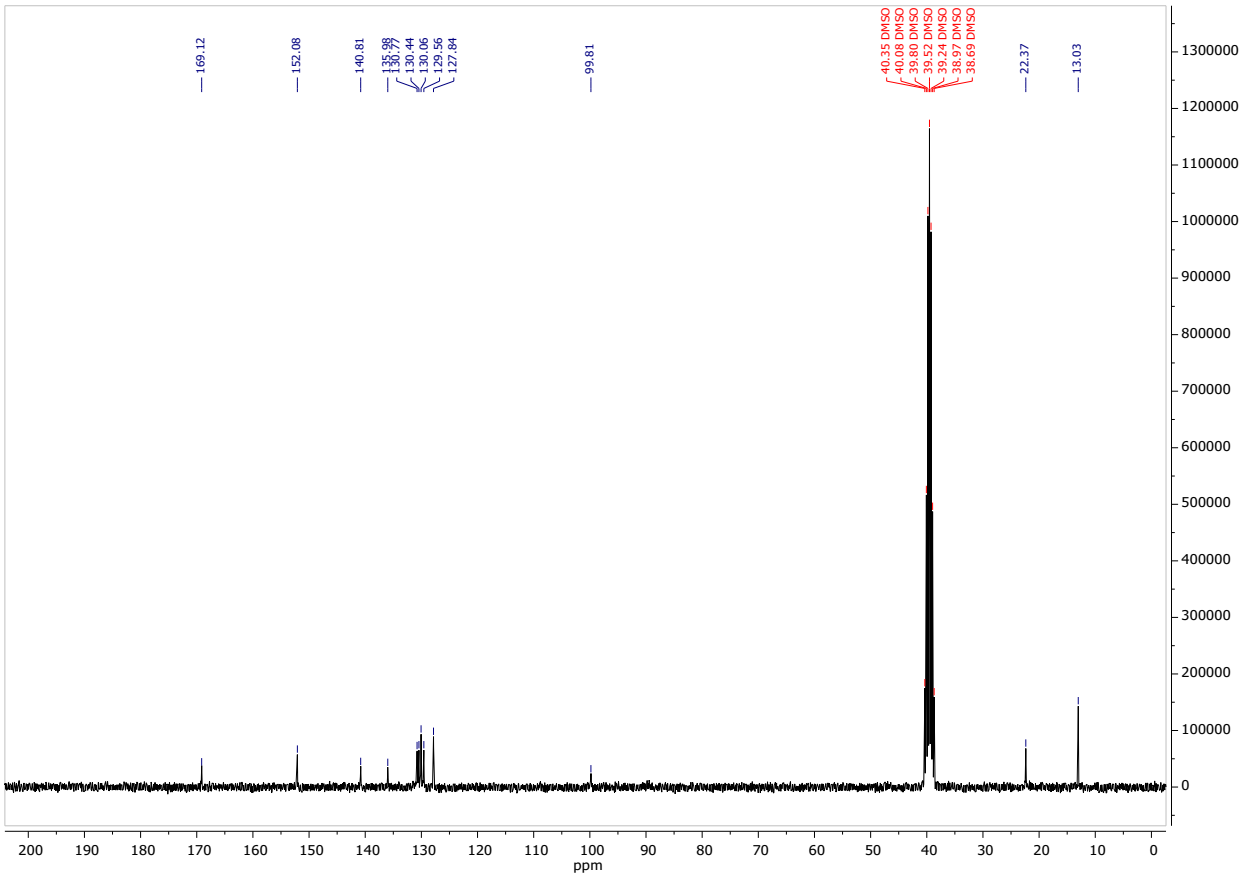
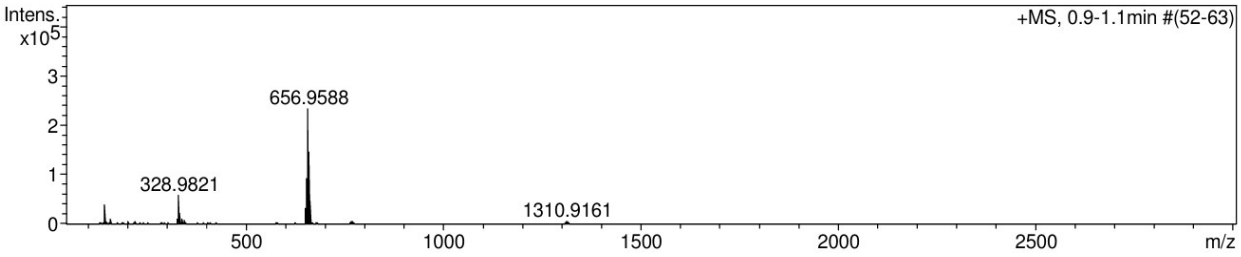
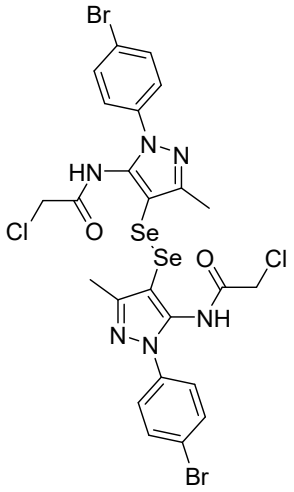


Figure-117: HRMS spectrum of compound **7**



NMR and HRMS spectra of compound 8



N,N'-(diselanediylbis(1-(4-bromophenyl)-3-methyl-1H-pyrazole-4,5-diyl))bis(2-chloroacetamide), ***8***

Yellow powder, m.p. 217-219°C, yield 63% (0.20 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.37 (s, 2H), 7.68 (d, J = 8.8 Hz, 4H), 7.44 (d, J = 8.8 Hz, 4H), 4.21 (s, 4H), 2.13 (s, 6H). ^{77}Se NMR (57 MHz, DMSO) δ 328.64. ^{13}C{^{1}H} NMR (75 MHz, DMSO-d_6) δ 166.25, 152.34, 138.21, 137.56, 132.21, 124.86, 120.42, 102.44, 42.24, 12.98. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{24}H_{21}Br_2Cl_2N_6O_2Se_2$]$^{+}$: 814.7766; found: 814.7774.

Figure-118: ^{1}H NMR spectrum (300 MHz) of **8** in DMSO-d_6

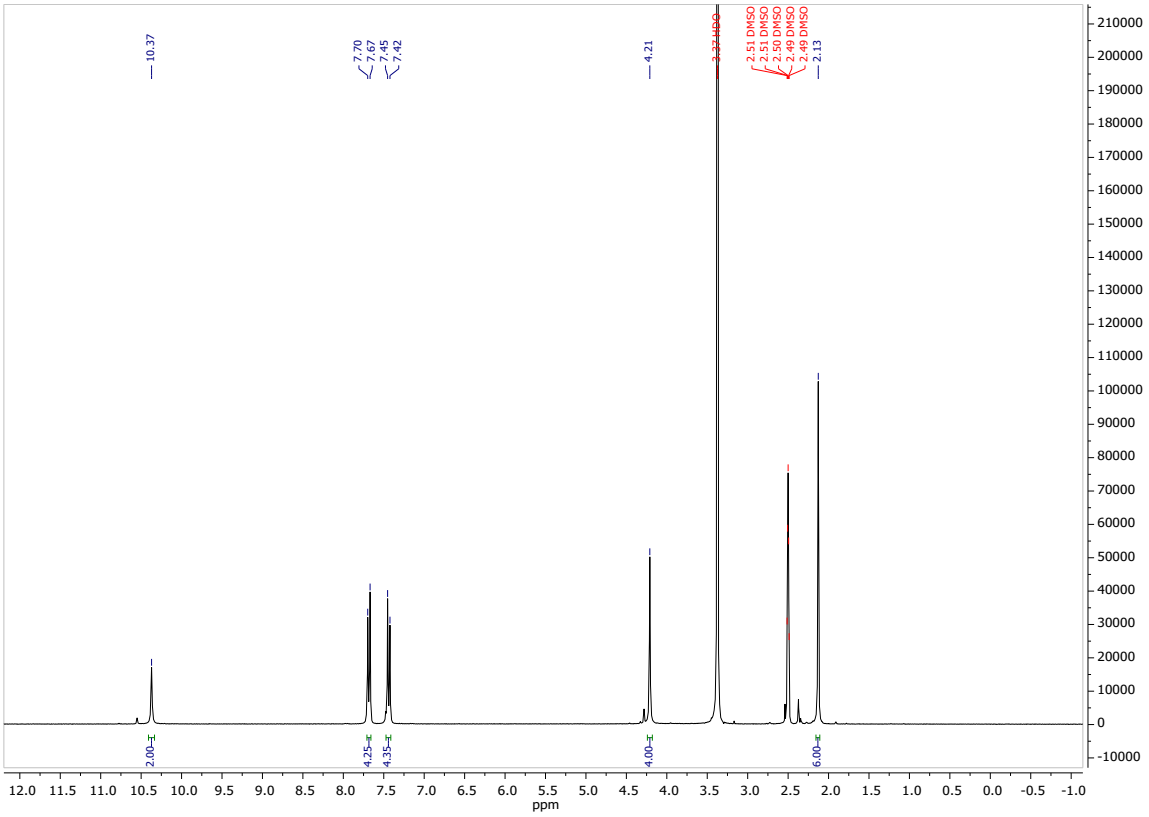


Figure-119: ^{77}Se NMR spectrum (57 MHz) of **8** in DMSO-d_6

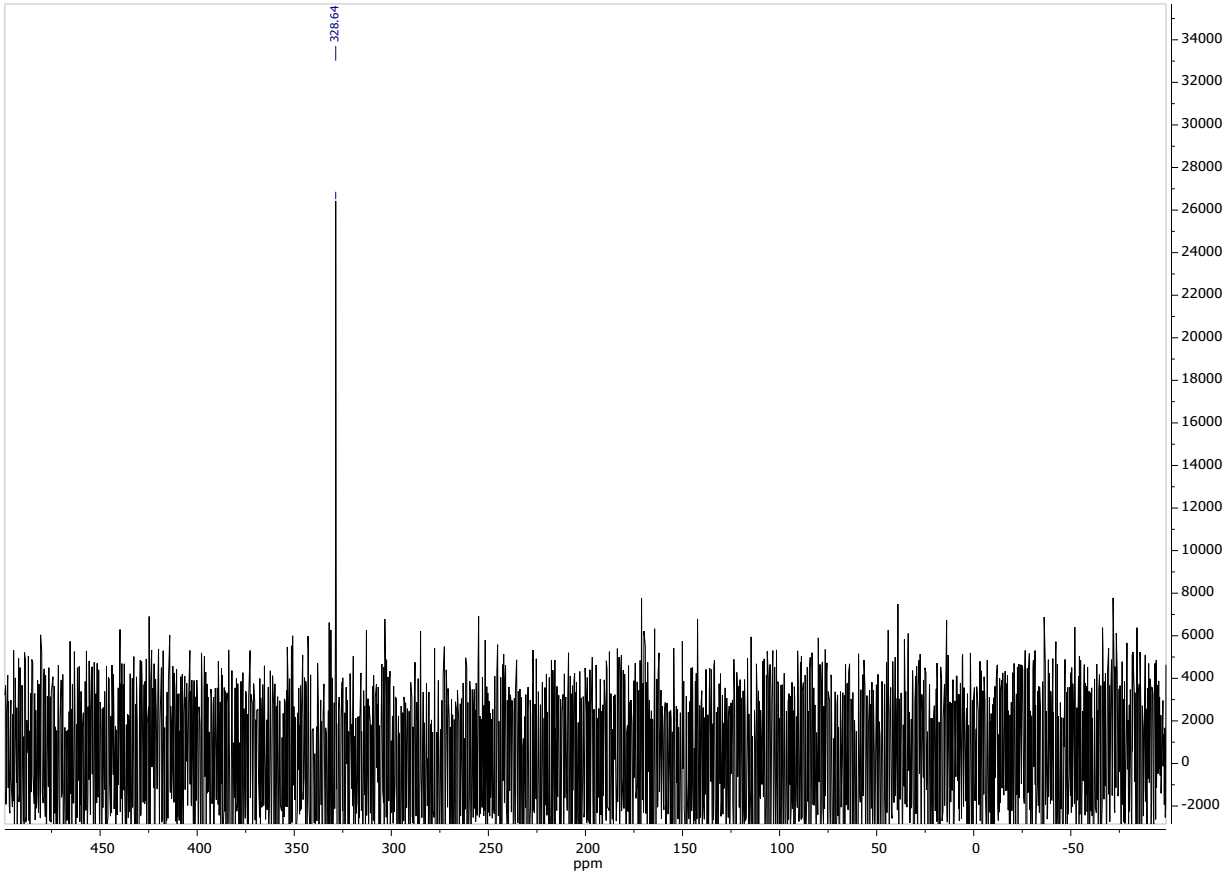


Figure-120: ^{13}C NMR spectrum (76 MHz) of **8** in DMSO-d_6

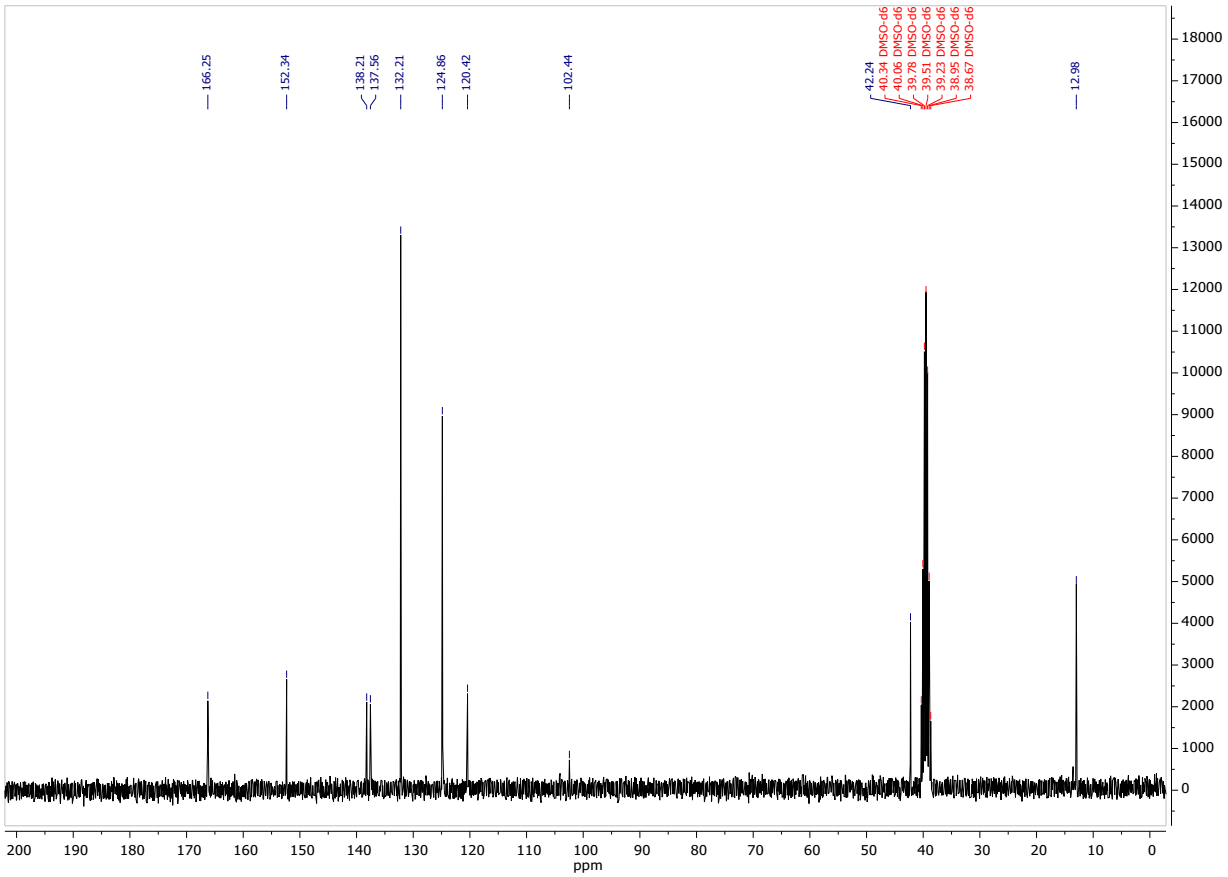
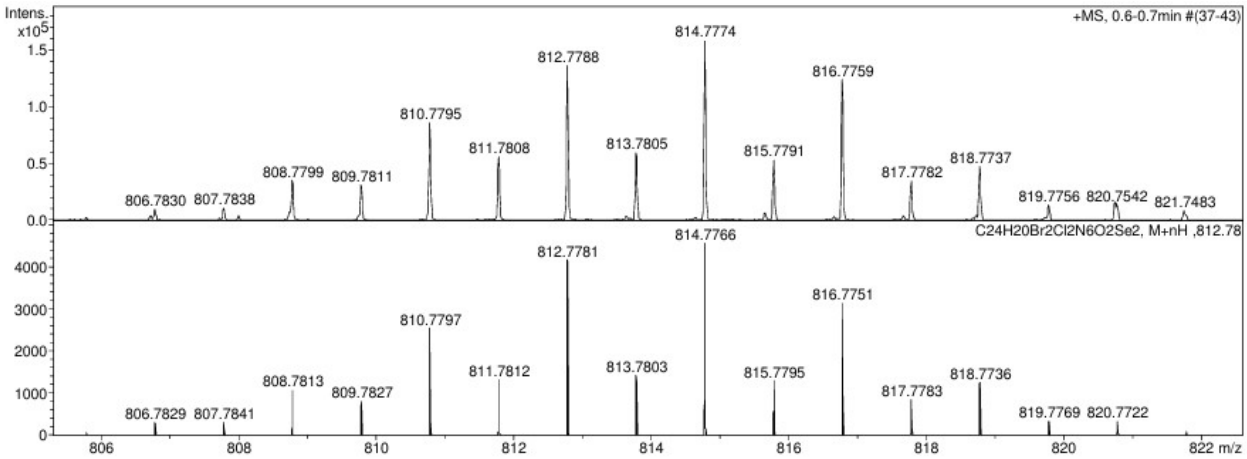
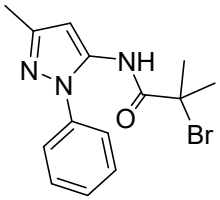


Figure-121: HRMS spectrum of compound **8**



NMR and HRMS spectra of compound 9



2-Bromo-2-methyl-N-(3-methyl-1-phenyl-1H-pyrazol-5-yl)propanamide, **9**

White powder, m.p. 118-120°C, yield 76% (0.98 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 9.98 (s, 1H), 7.51 – 7.42 (m, 4H), 7.36 – 7.30 (m, 1H), 6.16 (s, 1H), 2.23 (s, 3H), 1.87 (s, 6H). ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 170.27, 147.94, 138.64, 135.60, 128.94, 126.98, 123.08, 104.06, 59.37, 30.71, 13.83. HRMS (ESI-TOF): m/z $[M+H]^+$: calcd for $[C_{14}H_{17}BrN_3O]^+$: 322.0550; found: 322.0546.

Figure-122: ^{1}H NMR spectrum (300 MHz) of **9** in DMSO-d_6

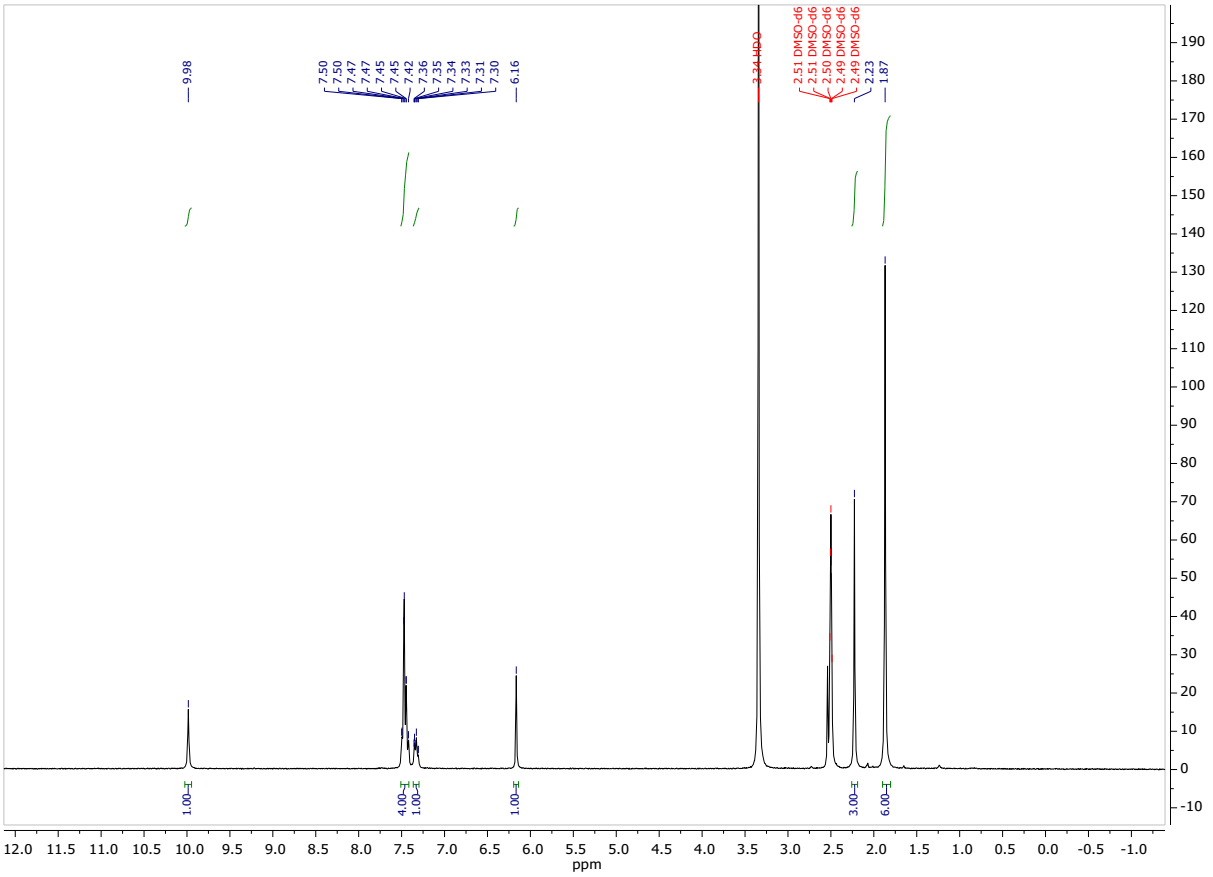


Figure-123: ^{13}C NMR spectrum (76 MHz) of **9** in DMSO-d_6

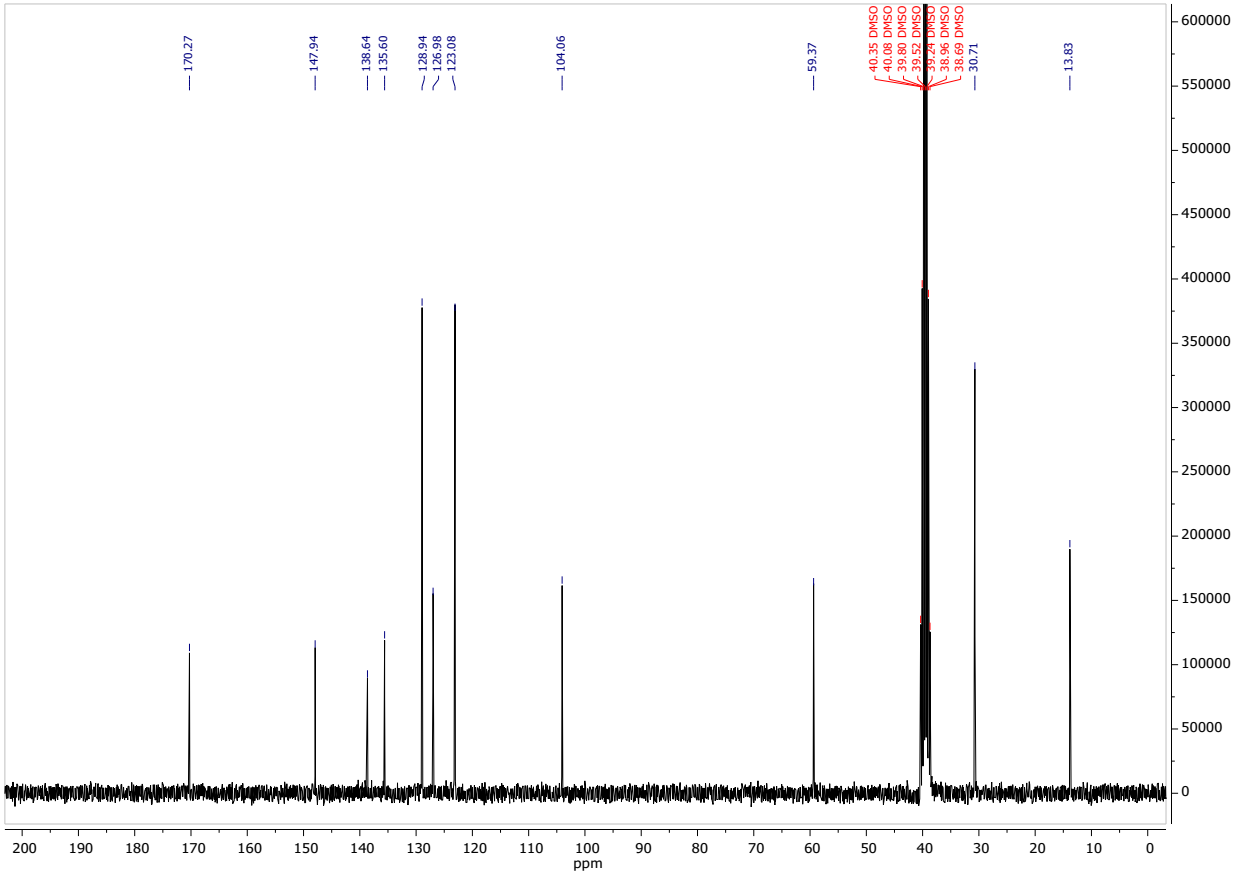
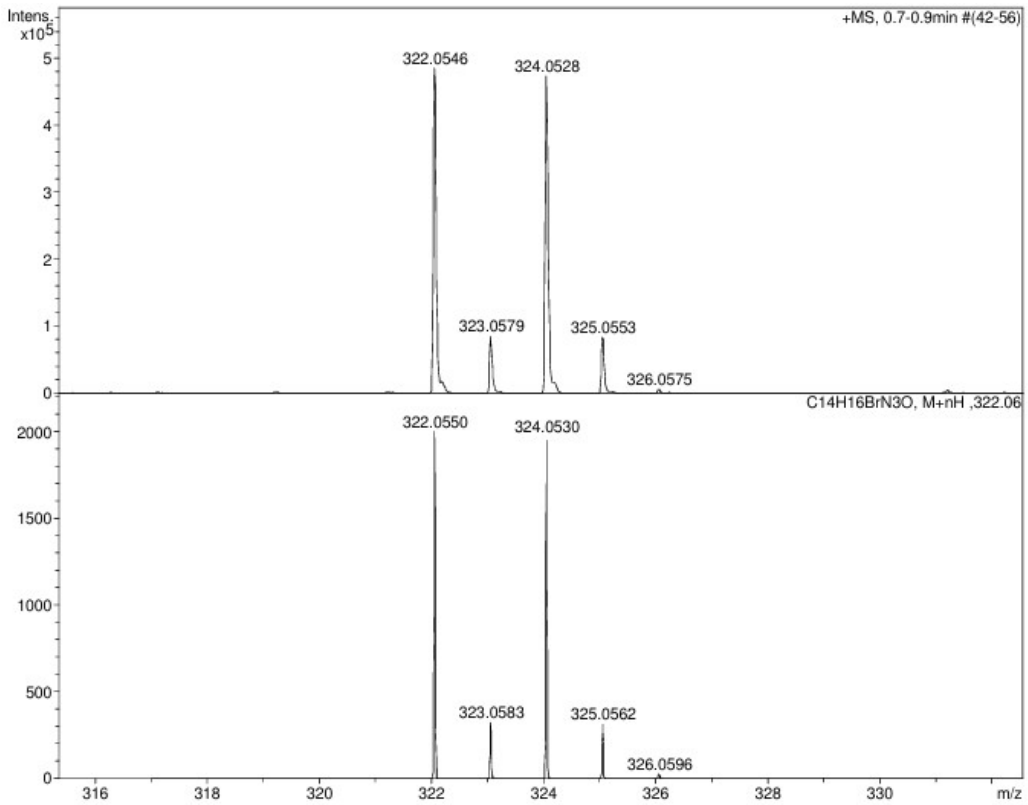
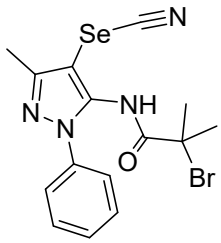


Figure-124: HRMS spectrum of compound **9**



NMR and HRMS spectra of compound 10



2-Bromo-2-methyl-N-(3-methyl-1-phenyl-4-selenocyanato-1H-pyrazol-5-yl)propanamide, ***10***

Grey powder, m.p. 122-124°C, yield 76% (0.97 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.45 (s, 1H), 7.55 – 7.46 (m, 4H), 7.44 – 7.37 (m, 1H), 2.36 (s, 3H), 1.91 (s, 6H). ^{77}Se NMR (57 MHz, DMSO) δ 157.12. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 170.78, 150.84, 138.58, 138.08, 129.19, 128.00, 123.19, 102.99, 95.08, 58.68, 30.64, 13.12. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{15}H_{16}BrN_4OSe$]$^{+}$: 426.9664; found: 426.9669.

Figure-125: ^{1}H NMR spectrum (300 MHz) of **10** in DMSO-d_6

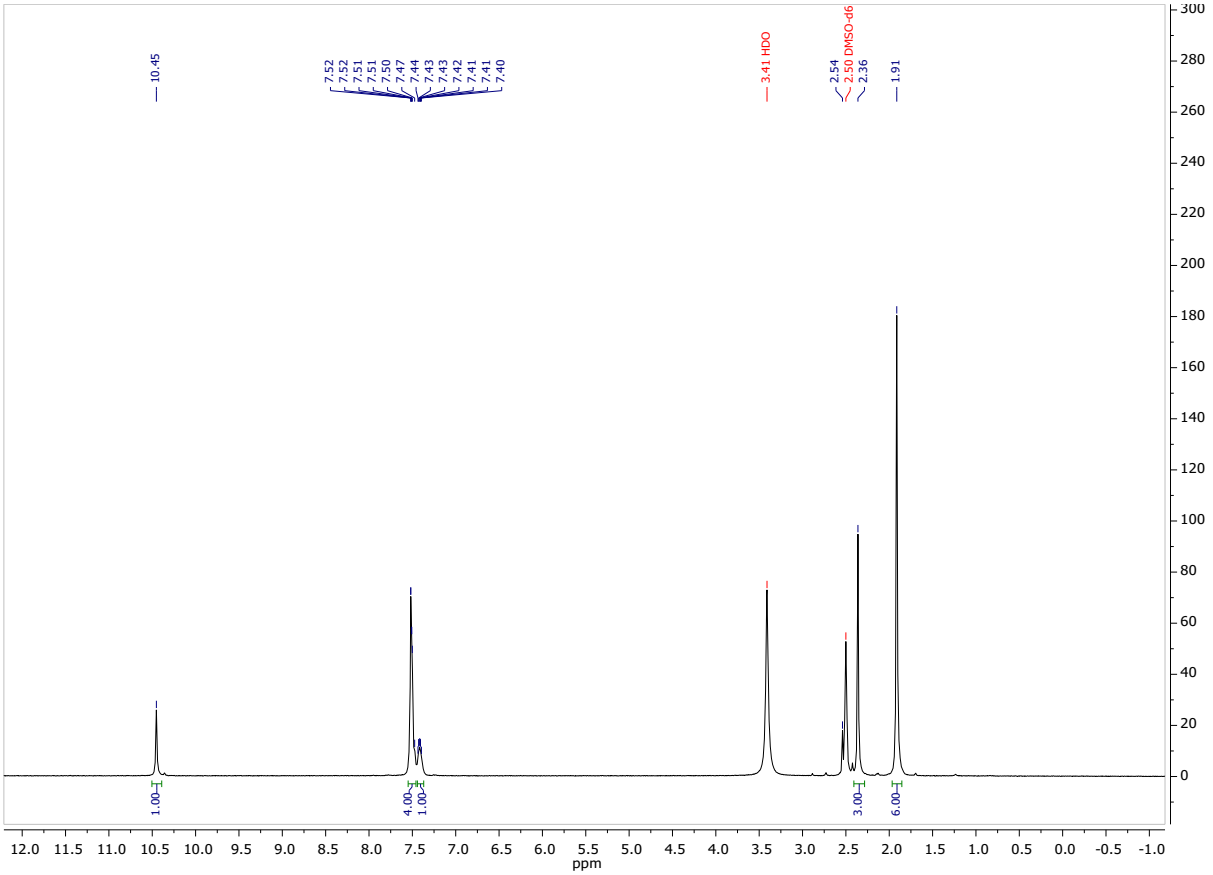


Figure-126: ^{77}Se NMR spectrum (57 MHz) of **10** in DMSO-d_6

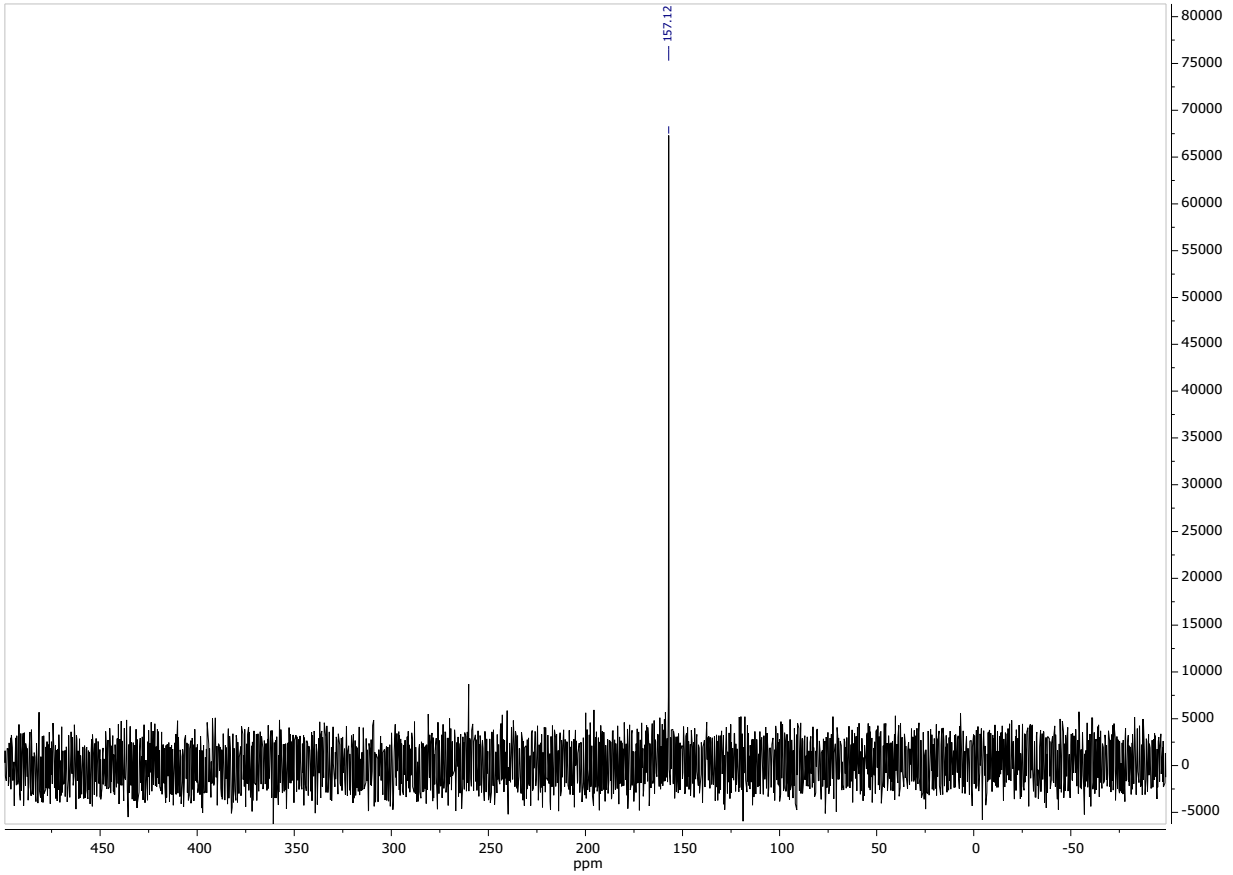


Figure-127: ^{13}C NMR spectrum (76 MHz) of **10** in DMSO-d_6

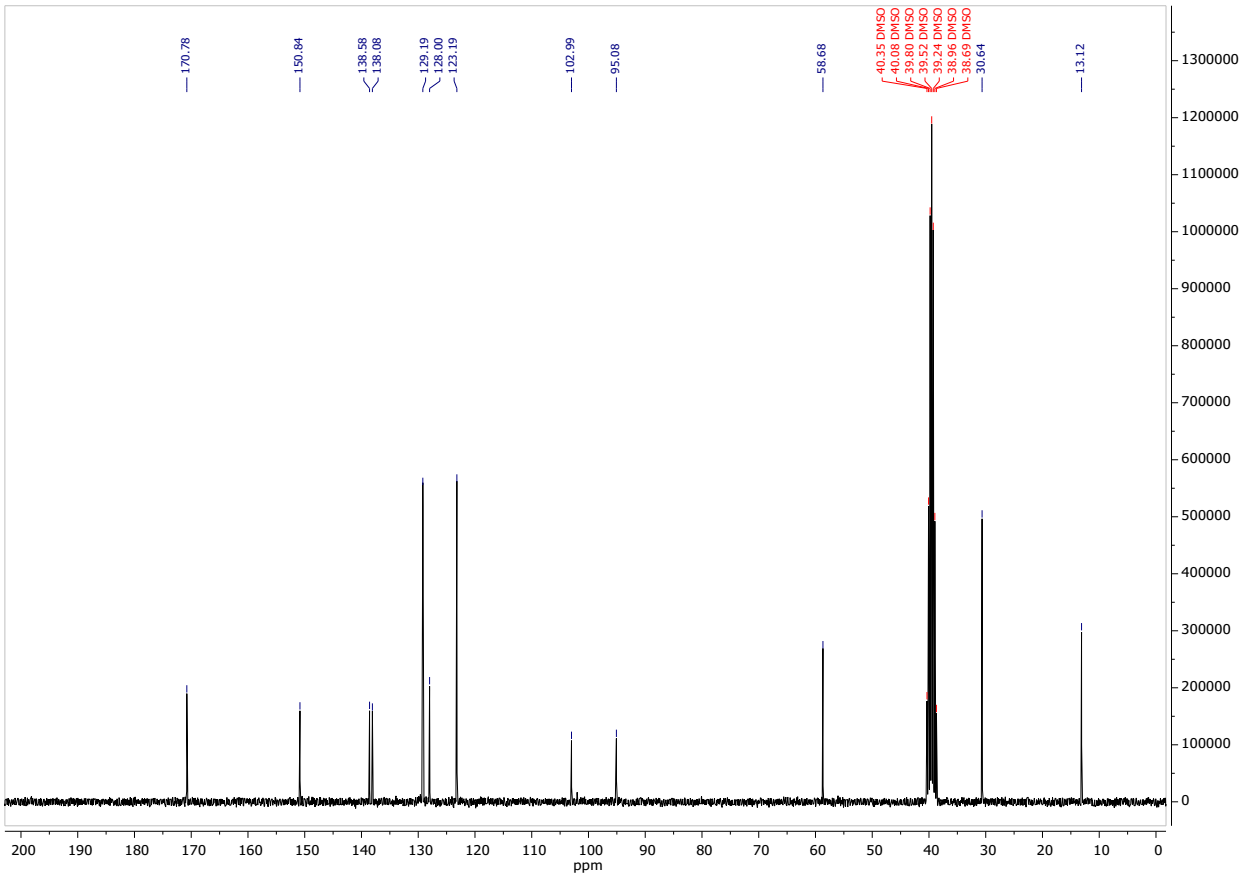
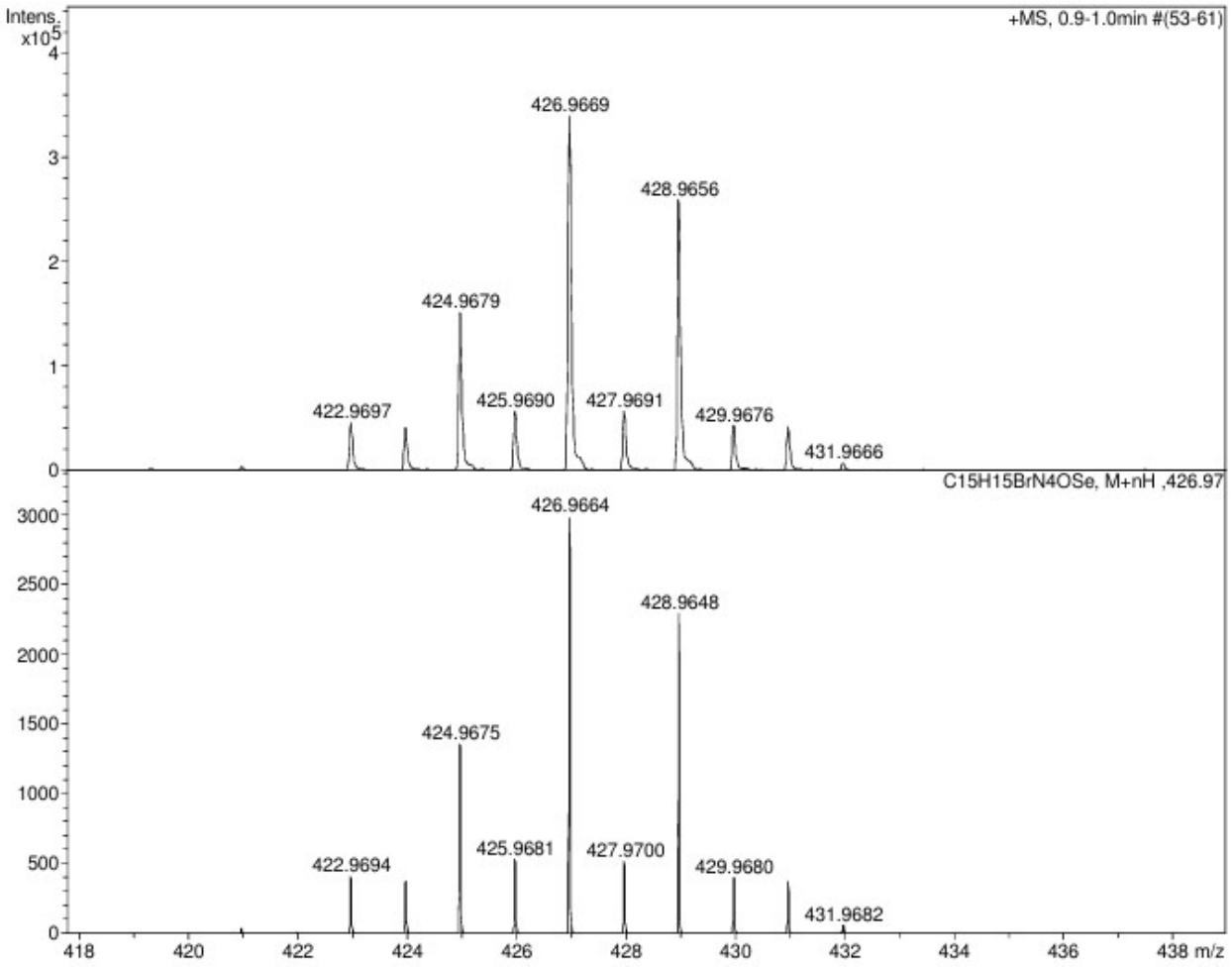
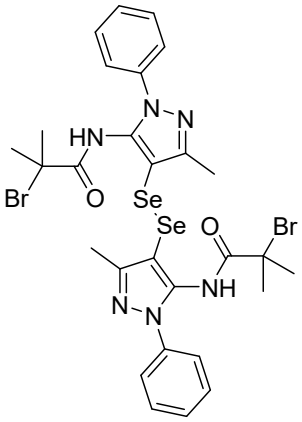


Figure-128: HRMS spectrum of compound **10**



NMR and HRMS spectra of compound 11



N,N'-(diselanediylbis(3-methyl-1-phenyl-1H-pyrazole-4,5-diyl))bis(2-bromo-2-methylpropanamide), ***11***

Yellow powder, m.p. 151-153°C, yield 59% (0.19 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 9.70 (s, 2H), 7.52 – 7.45 (m, 8H), 7.40 – 7.34 (m, 2H), 2.26 (s, 6H), 1.73 (s, 12H). ^{77}Se NMR (57 MHz, DMSO) δ 326.99. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 171.10, 152.21, 138.35, 138.13, 129.18, 127.65, 122.68, 103.43, 58.59, 30.60, 13.15. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{28}H_{31}Br_2N_6O_2Se_2$]$^{+}$: 800.9206; found: 800.9138.

Figure-129: ^{1}H NMR spectrum (300 MHz) of **11** in DMSO-d_6

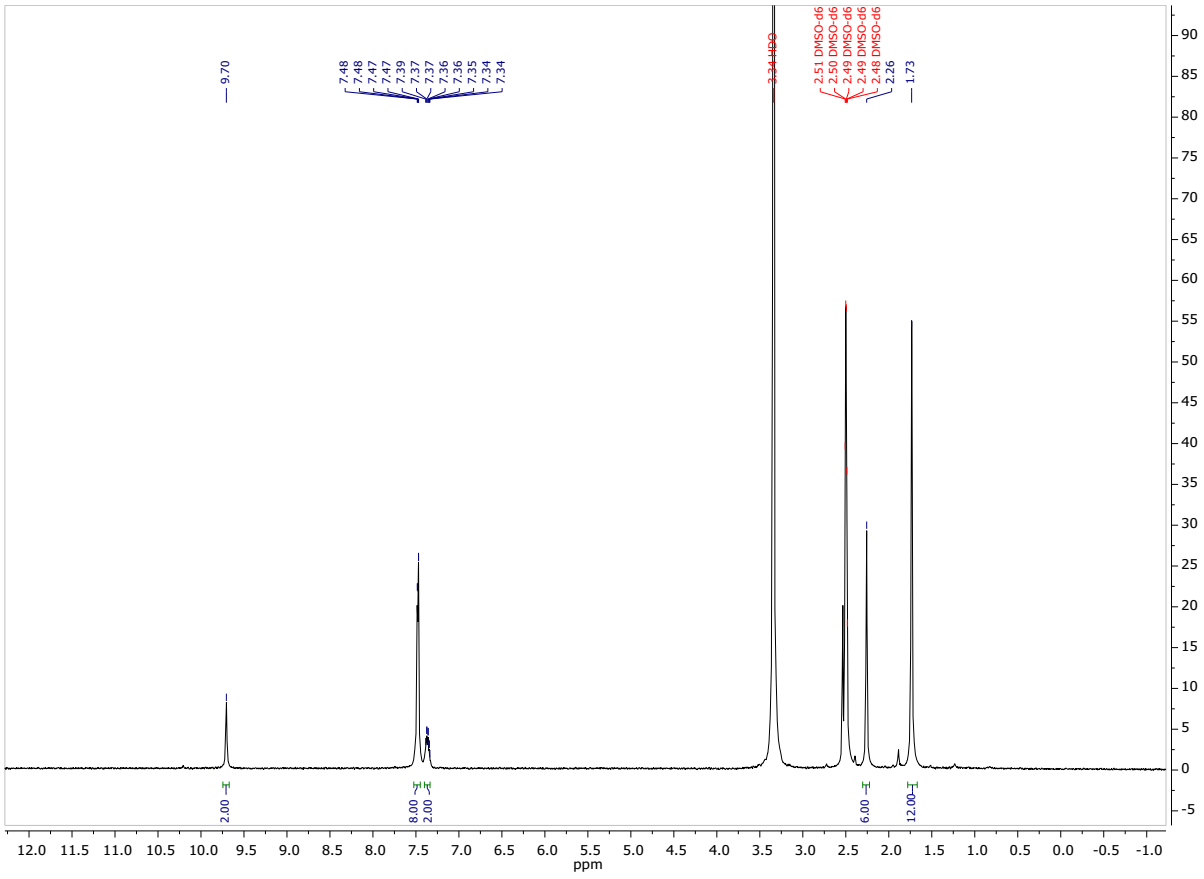


Figure-130: ^{77}Se NMR spectrum (57 MHz) of **11** in DMSO-d_6

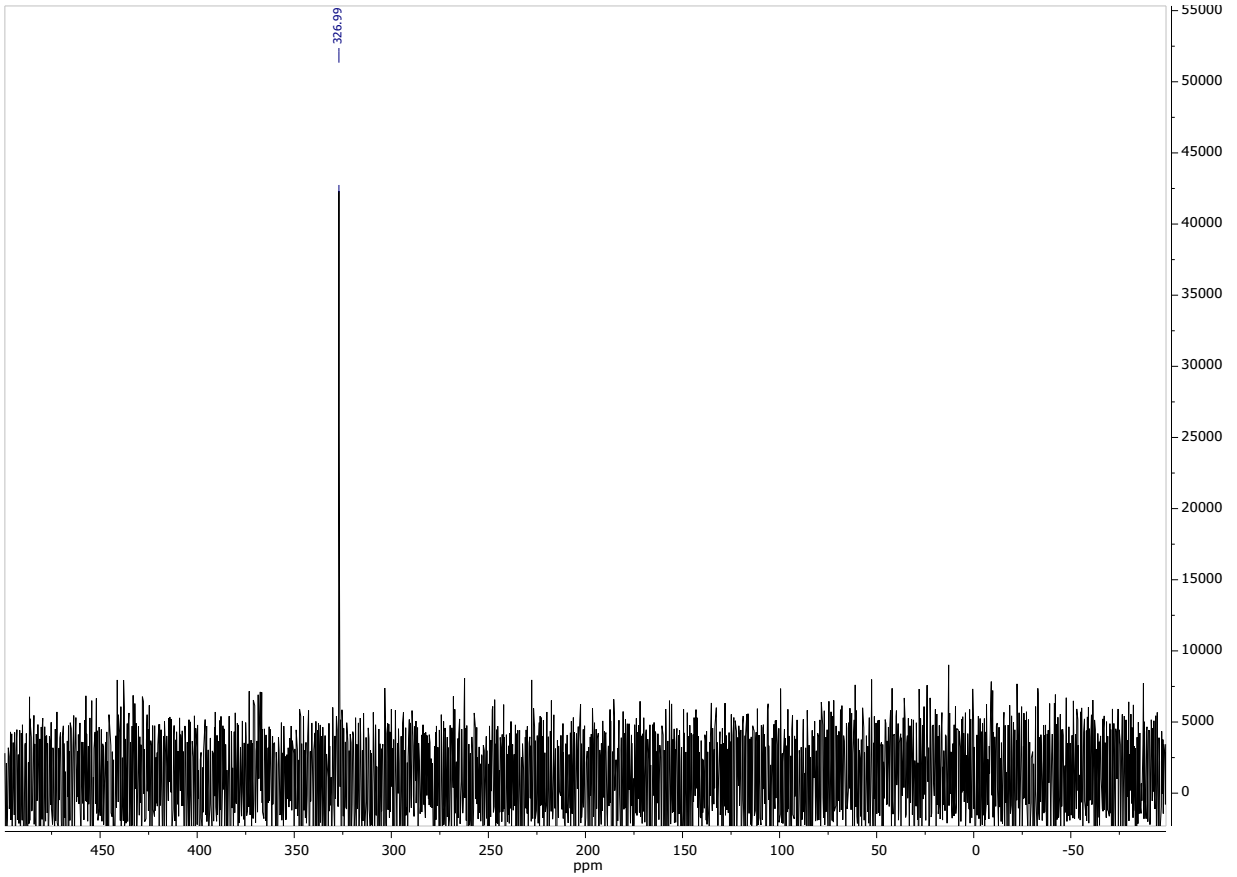


Figure-131: ^{13}C NMR spectrum (76 MHz) of **11** in DMSO-d_6

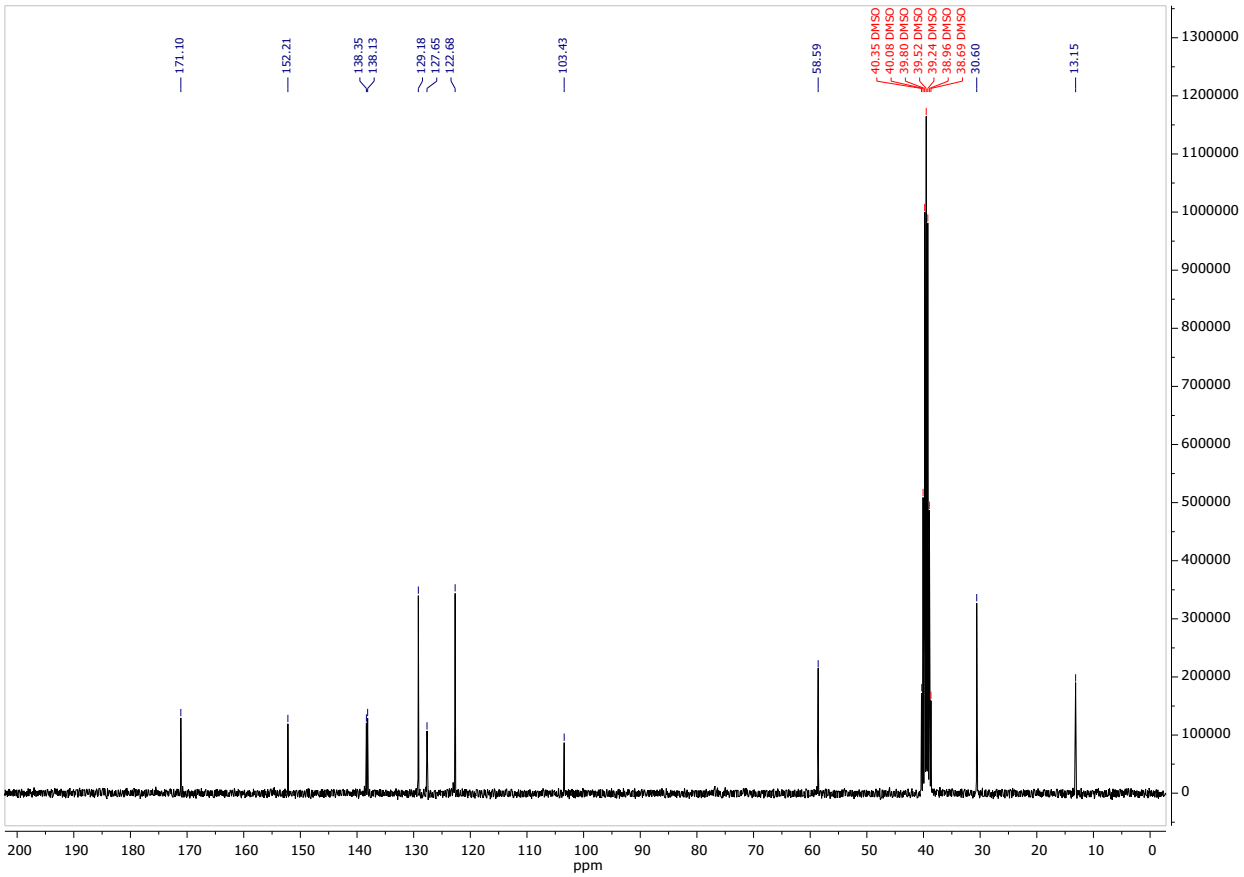
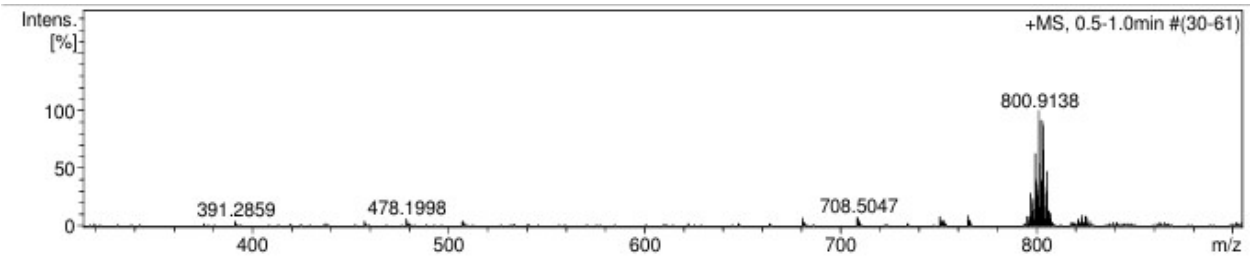
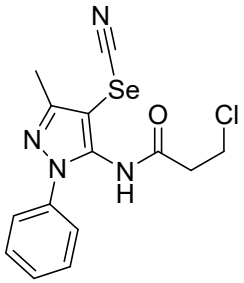


Figure-132: HRMS spectrum of compound **11**



NMR and HRMS spectra of compound 14



3-Chloro-N-(3-methyl-1-phenyl-4-selenocyanato-1H-pyrazol-5-yl)propanamide, ***14***

Grey powder, m.p. 124-126°C, yield 64% (0.71 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.56 (s, 1H), 7.54 – 7.48 (m, 4H), 7.46 – 7.39 (m, 1H), 3.82 (t, J = 6.1 Hz, 2H), 2.85 (t, J = 6.1 Hz, 2H), 2.35 (s, 3H). ^{77}Se NMR (57 MHz, DMSO) δ 160.97. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 169.76, 150.57, 138.24, 137.99, 129.31, 128.04, 123.49, 103.34, 94.31, 40.30, 38.13, 13.11. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{14}H_{14}ClN_4OSe$]$^{+}$: 369.0014; found: 369.0022.

Figure-133: ^{1}H NMR spectrum (300 MHz) of **14** in DMSO-d_6

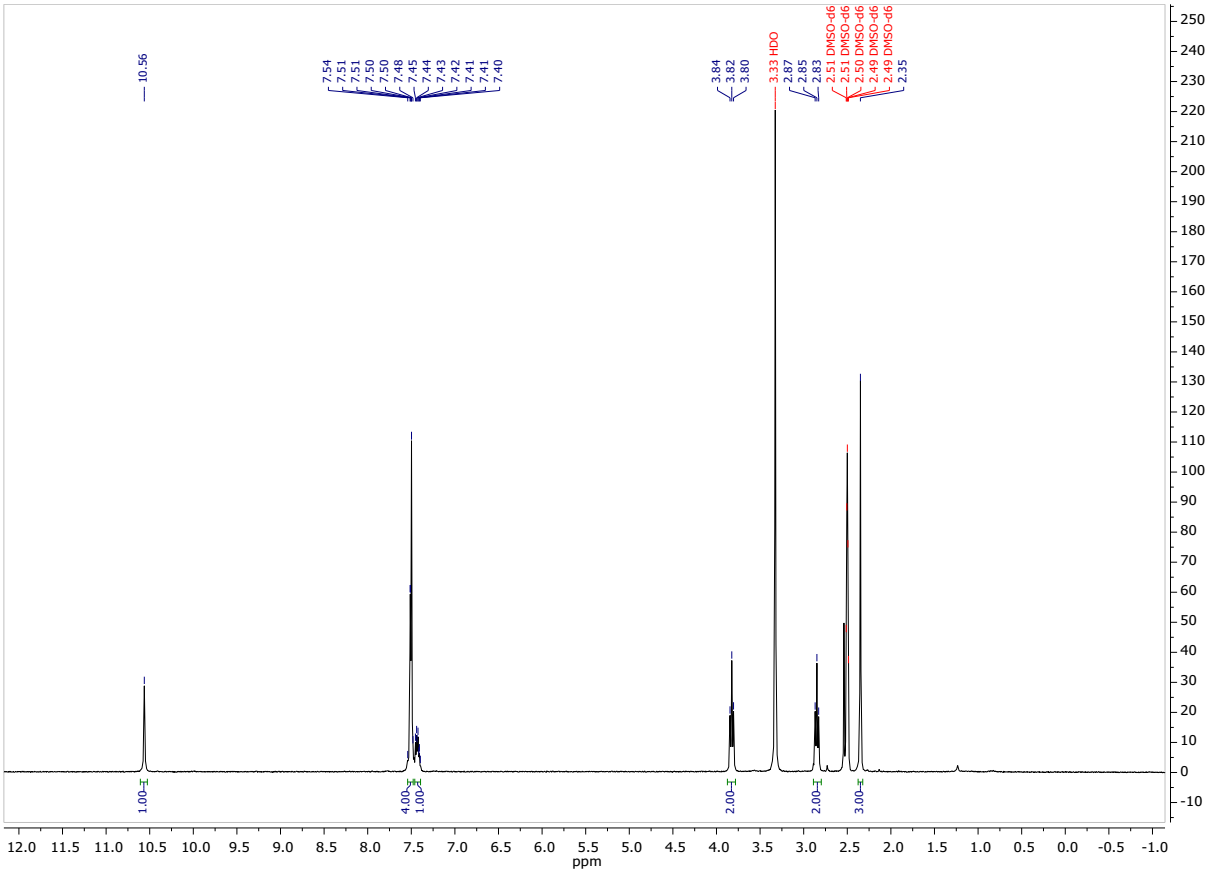


Figure-134: ^{77}Se NMR spectrum (57 MHz) of **14** in DMSO-d_6

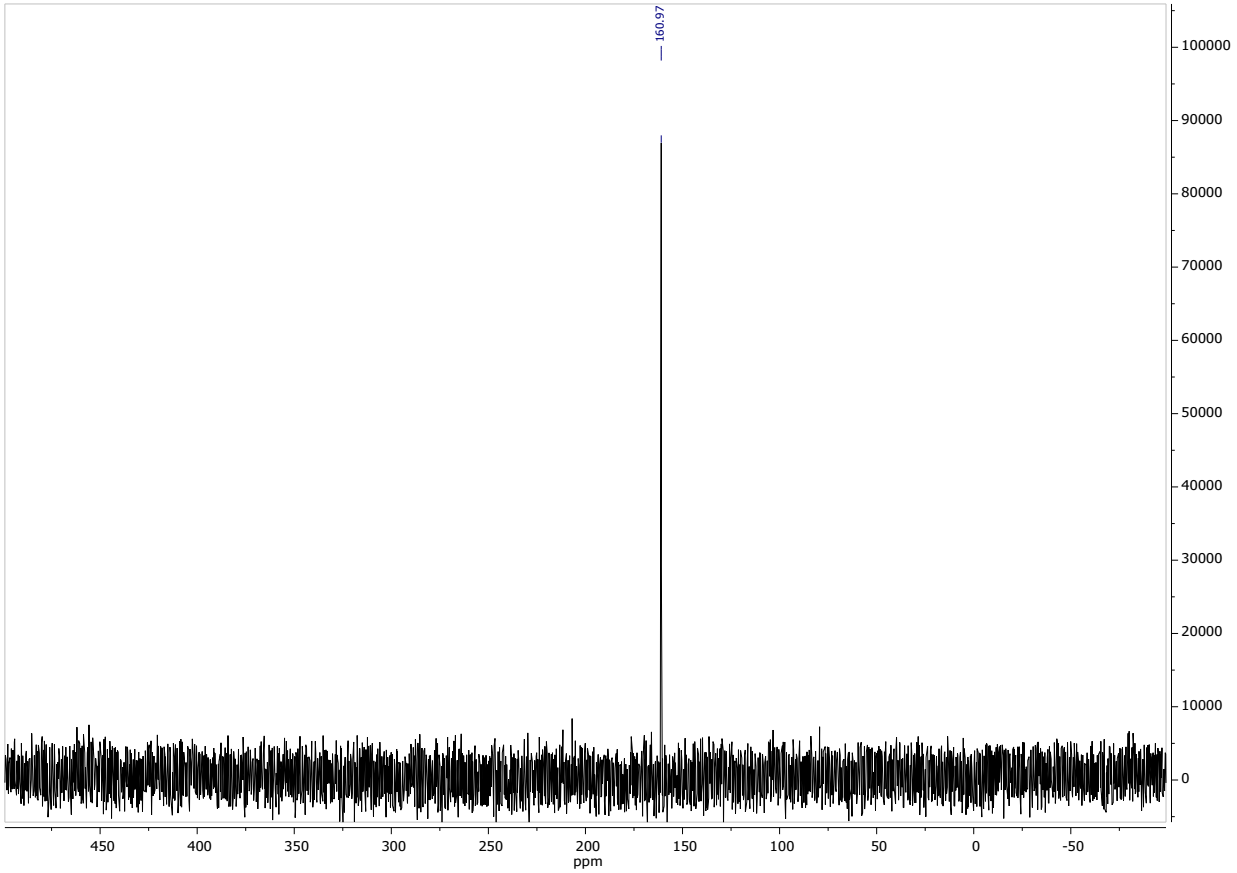


Figure-135: ^{13}C NMR spectrum (76 MHz) of **14** in DMSO-d_6

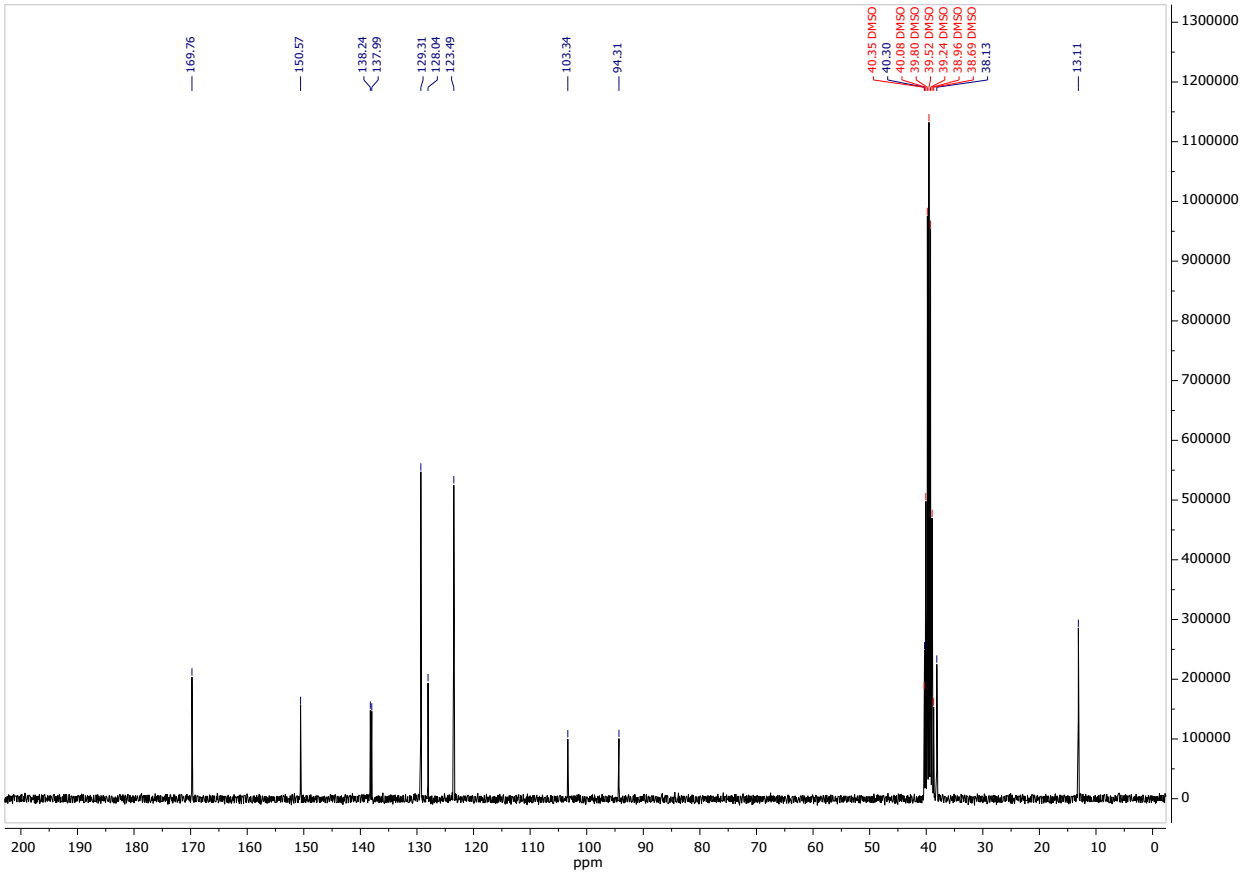
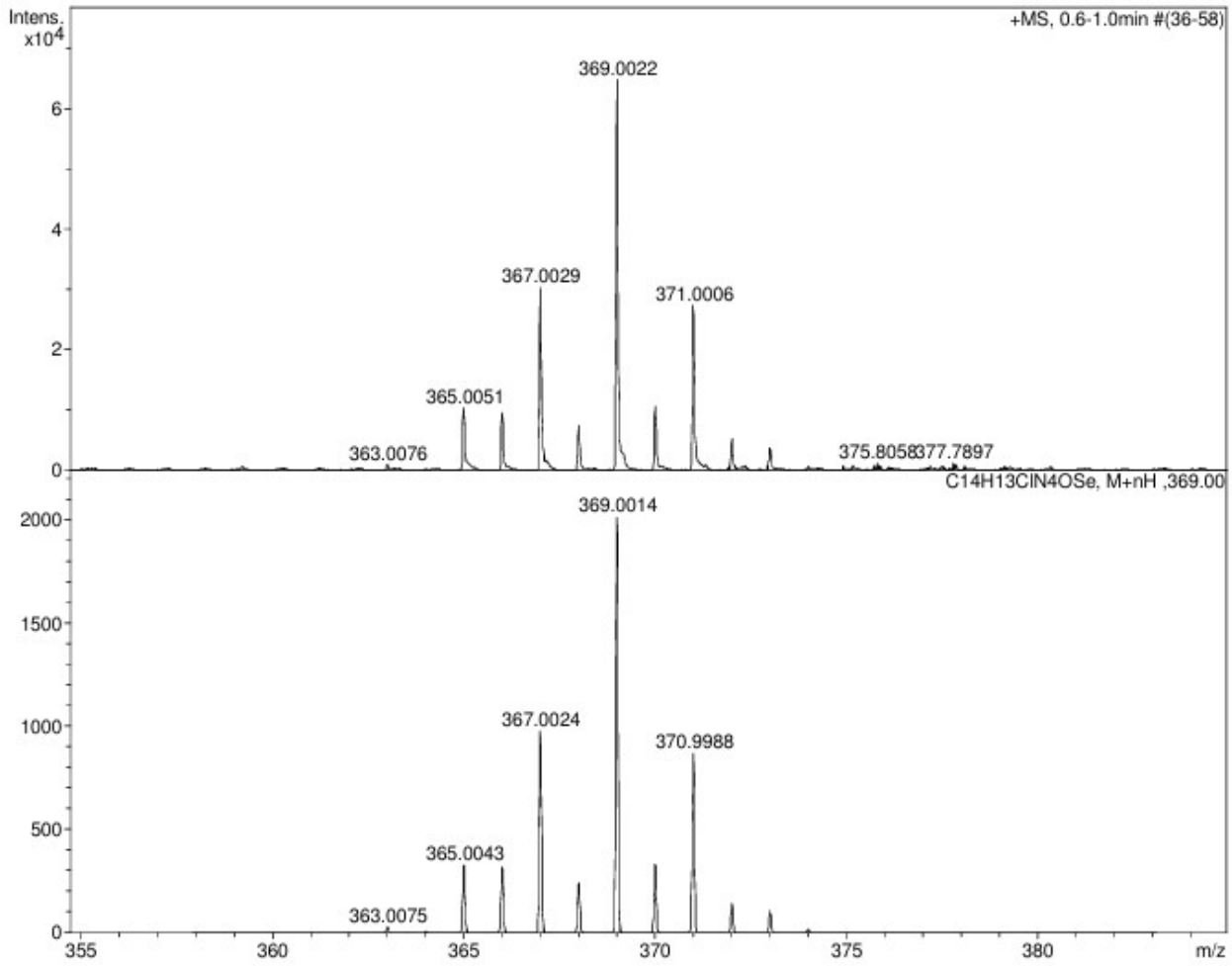
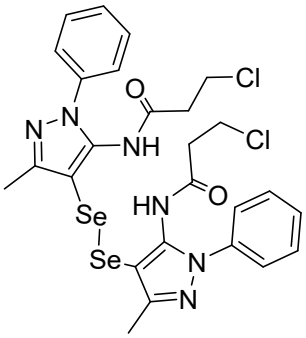


Figure-136: HRMS spectrum of compound **14**



NMR and HRMS spectra of compound 15



N,N'-(diselanediylbis(3-methyl-1-phenyl-1H-pyrazole-4,5-diyl))bis(3-chloropropanamide), ***15***

Orange powder, m.p. 150-152°C, yield 85% (0.23 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.13 (s, 2H), 7.52 – 7.44 (m, 8H), 7.41 – 7.35 (m, 2H), 3.74 (t, J = 6.1 Hz, 4H), 2.73 (t, J = 6.1 Hz, 4H), 2.13 (s, 6H). ^{77}Se NMR (57 MHz, DMSO) δ 328.69. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 169.64, 151.89, 138.65, 138.36, 129.16, 127.60, 123.06, 102.32, 40.23, 38.12, 13.01. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{26}H_{27}Cl_2N_6O_2Se_2$]$^{+}$: 684.9894; found: 684.9887.

Figure-137: ^{1}H NMR spectrum (300 MHz) of **15** in DMSO-d_6

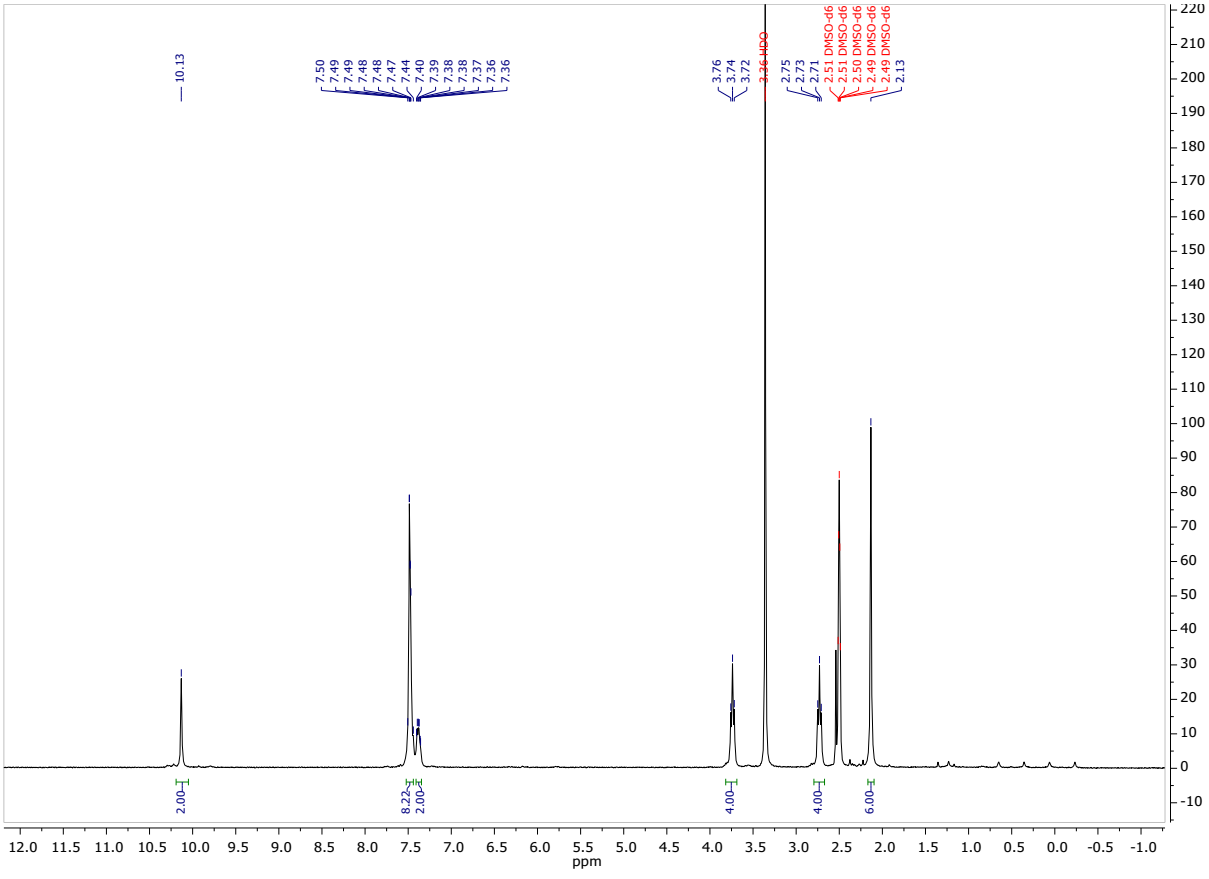


Figure-138: ^{77}Se NMR spectrum (57 MHz) of **15** in DMSO-d_6

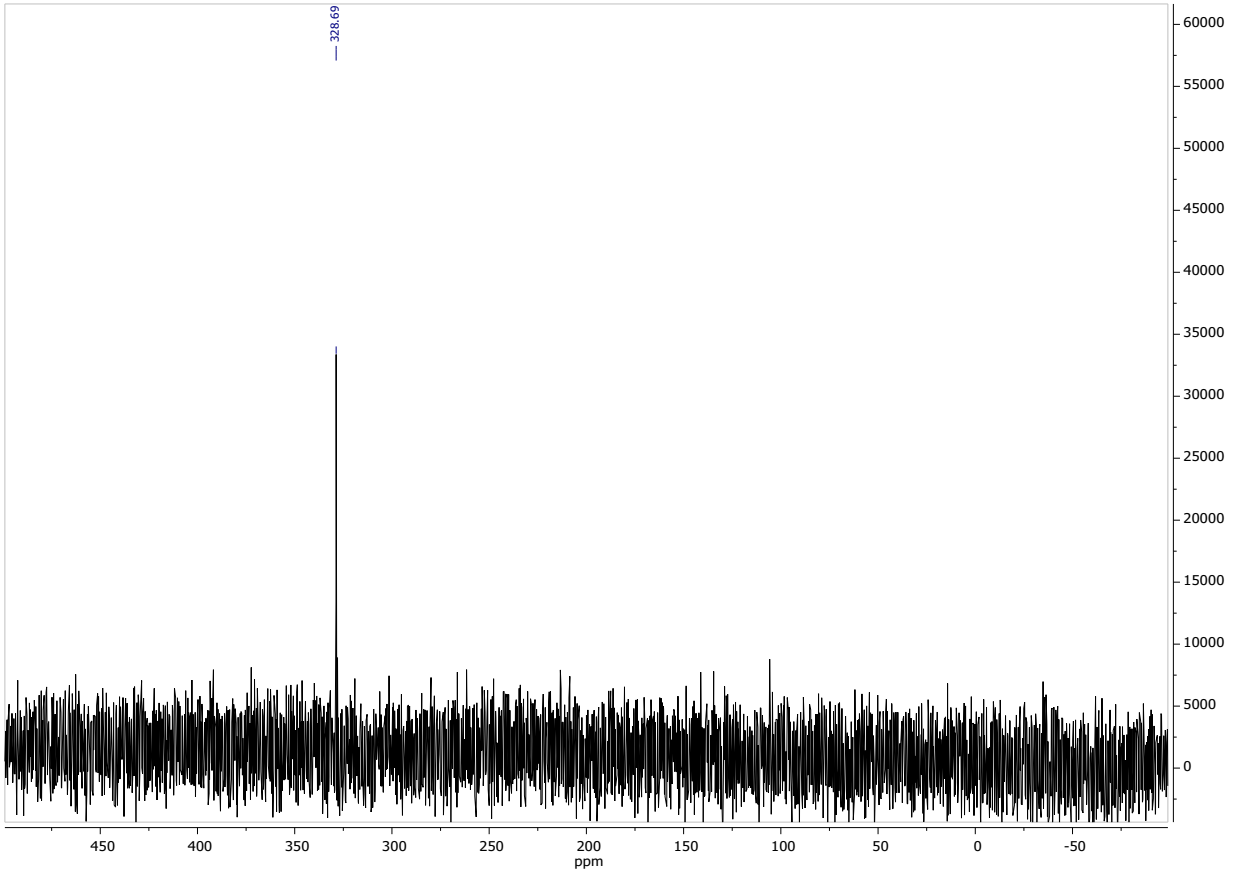


Figure-139: ^{13}C NMR spectrum (76 MHz) of **15** in DMSO-d_6

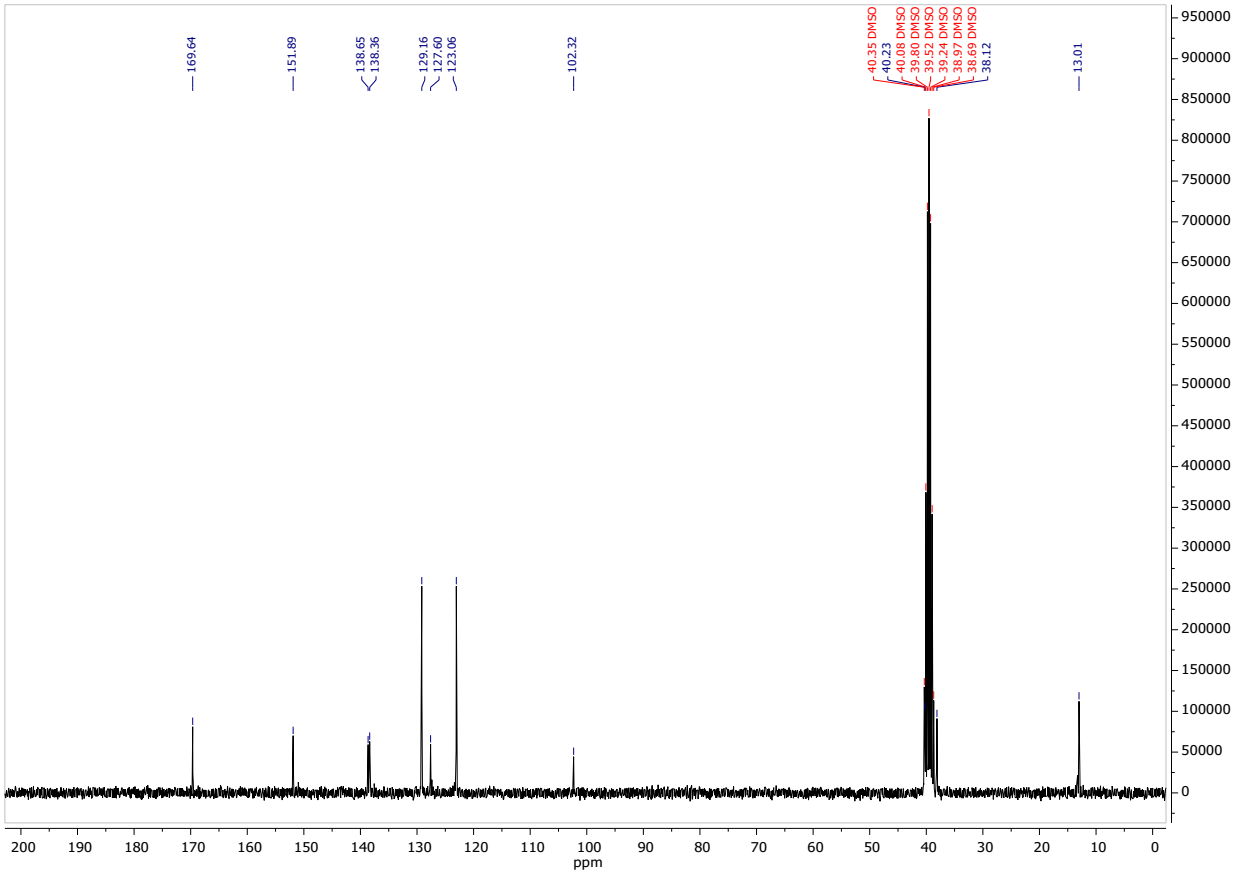
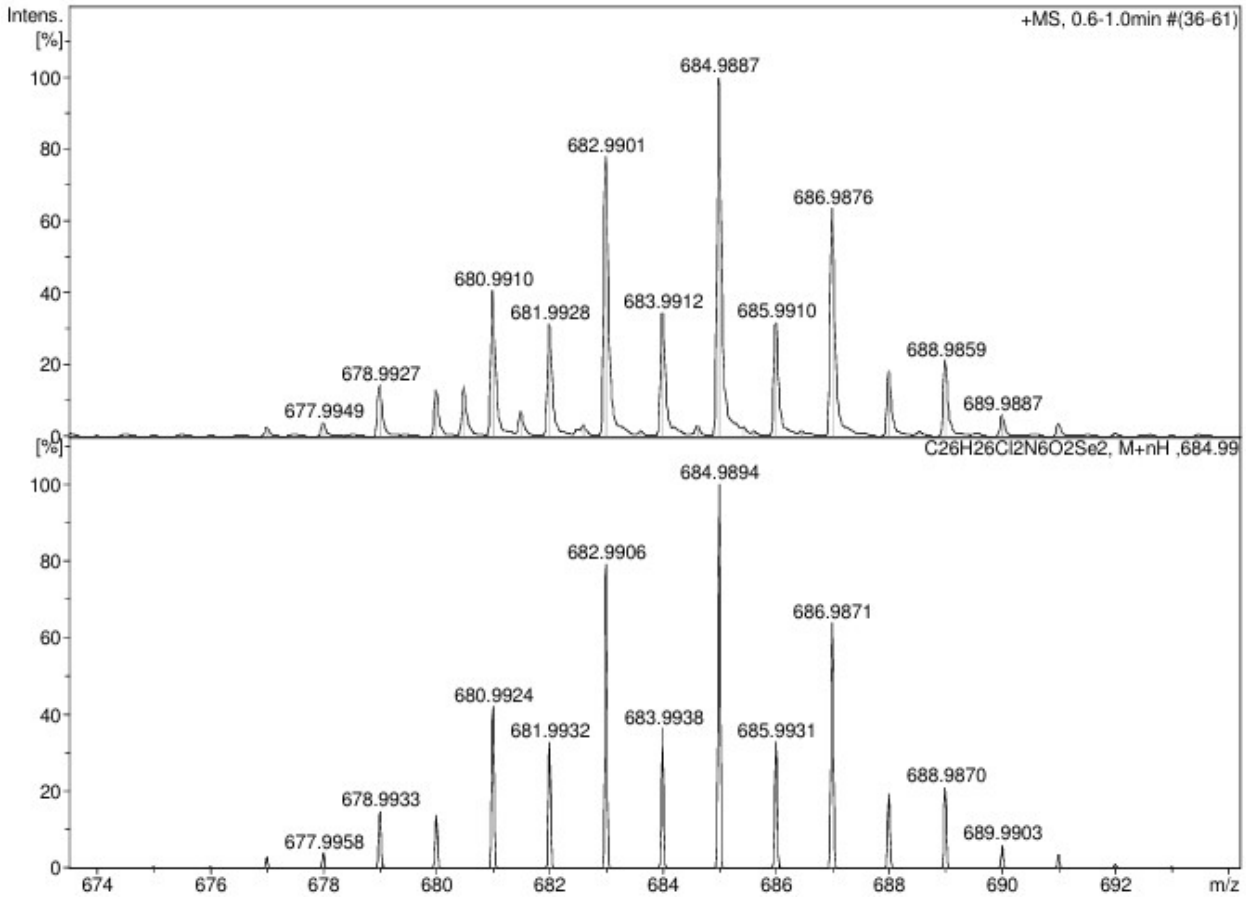
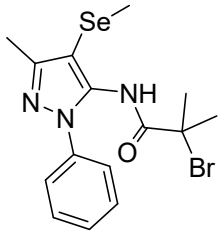


Figure-140: HRMS spectrum of compound **15**



NMR and HRMS spectra of compound 17



2-Bromo-2-methyl-N-(3-methyl-4-(methylselanyl)-1-phenyl-1H-pyrazol-5-yl)propanamide, ***17a***

White powder, m.p. 151-153^{o}C, yield 62% (0.10 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.05 (s, 1H), 7.50 – 7.43 (m, 4H), 7.38 – 7.32 (m, 1H), 2.30 (s, 3H), 2.05 (s, 3H), 1.88 (s, 6H).^{77}Se NMR (57 MHz, DMSO) δ 0.28. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 171.36, 151.55, 138.54, 138.43, 129.15, 127.57, 123.11, 102.71, 59.02, 31.00, 13.38, 8.35. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{15}H_{19}BrN_3OSe$]$^{+}$: 415.9868; found: 415.9860.

Figure-141: ^{1}H NMR spectrum (300 MHz) of **17a** in DMSO-d_6

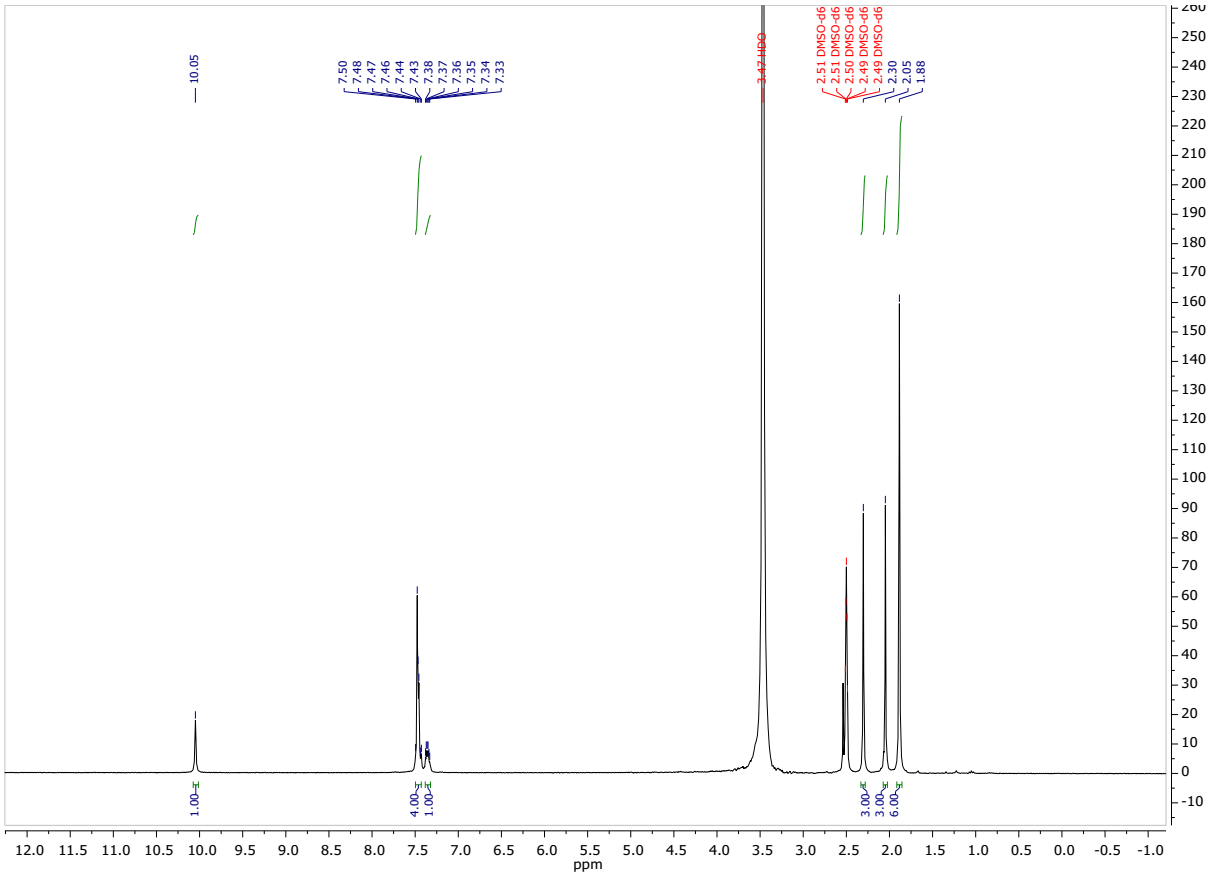


Figure-142: ^{77}Se NMR spectrum (57 MHz) of **17a** in DMSO-d_6

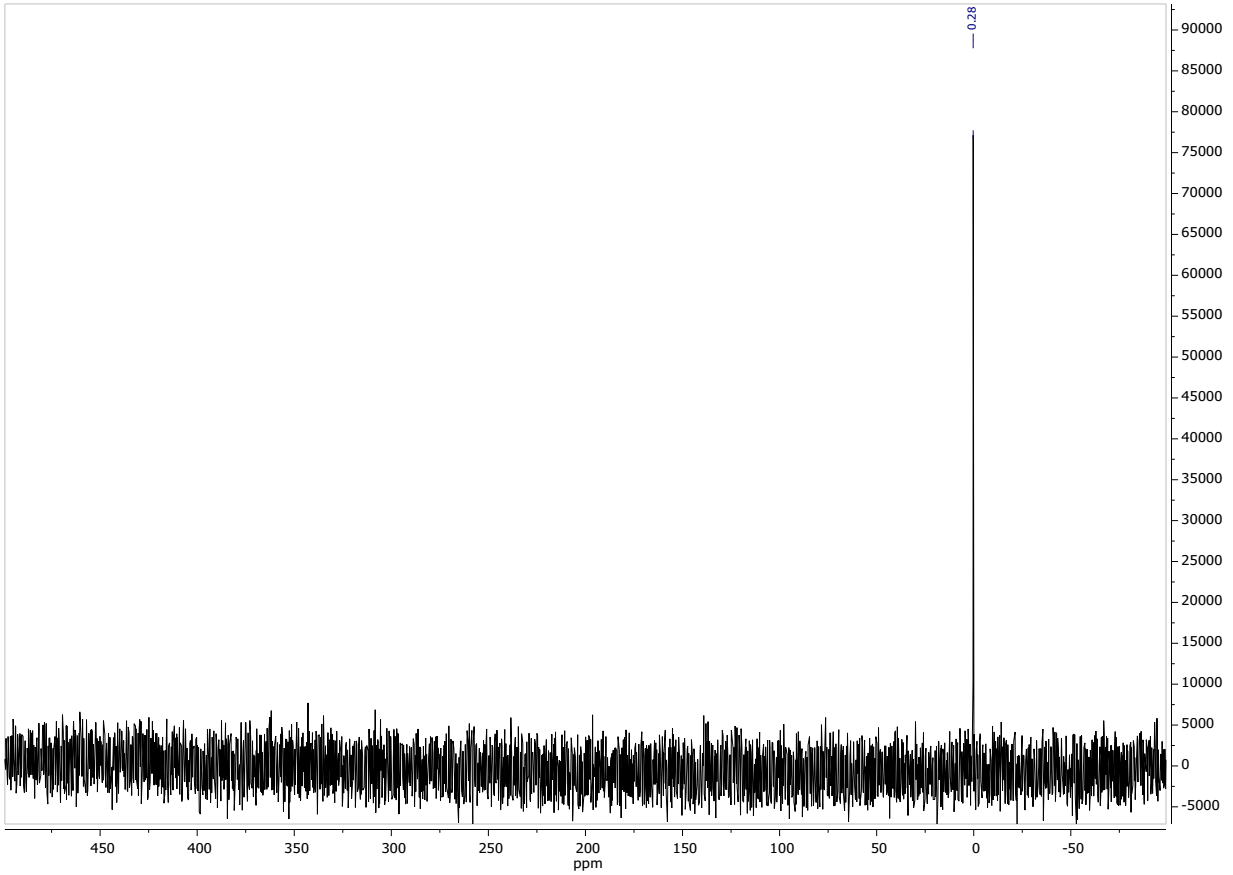


Figure-143: ^{13}C NMR spectrum (76 MHz) of **17a** in DMSO-d_6

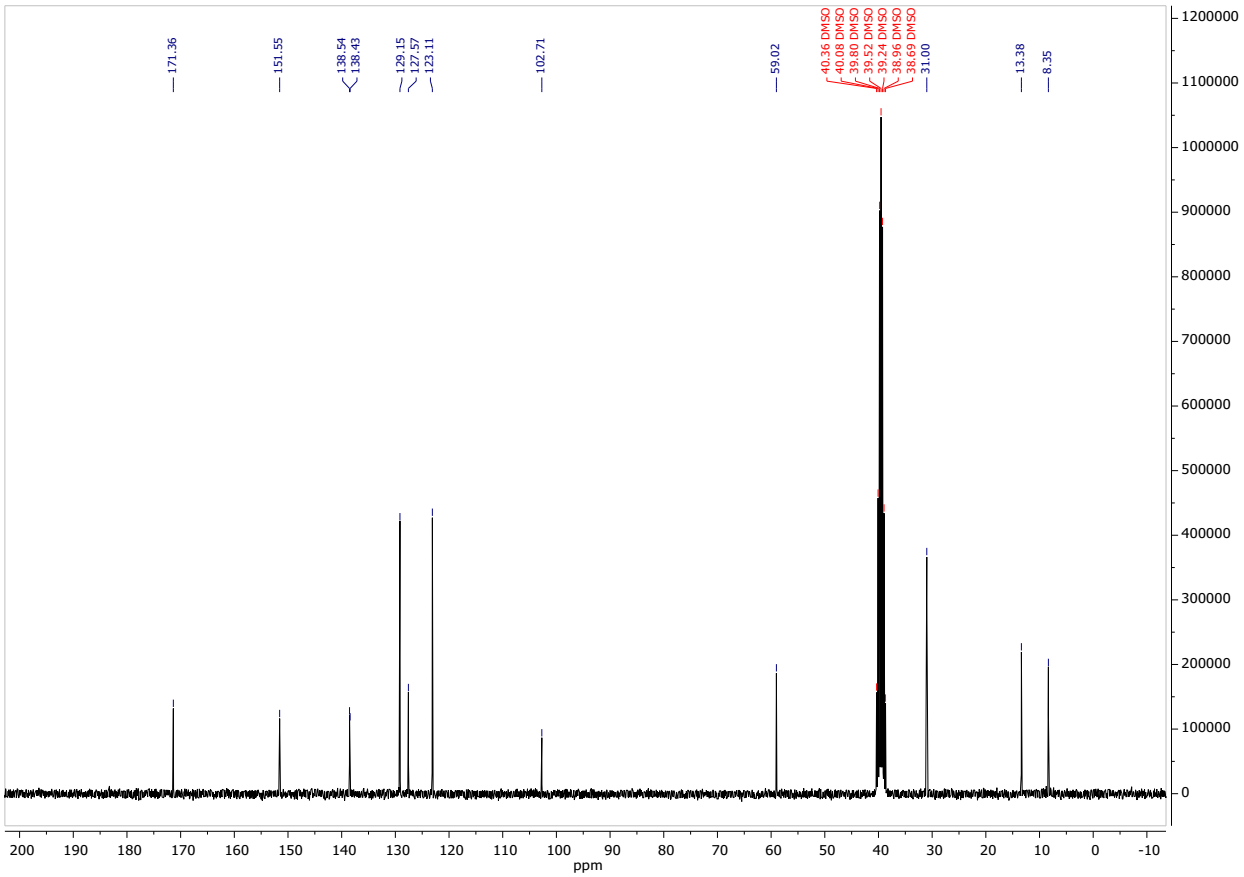
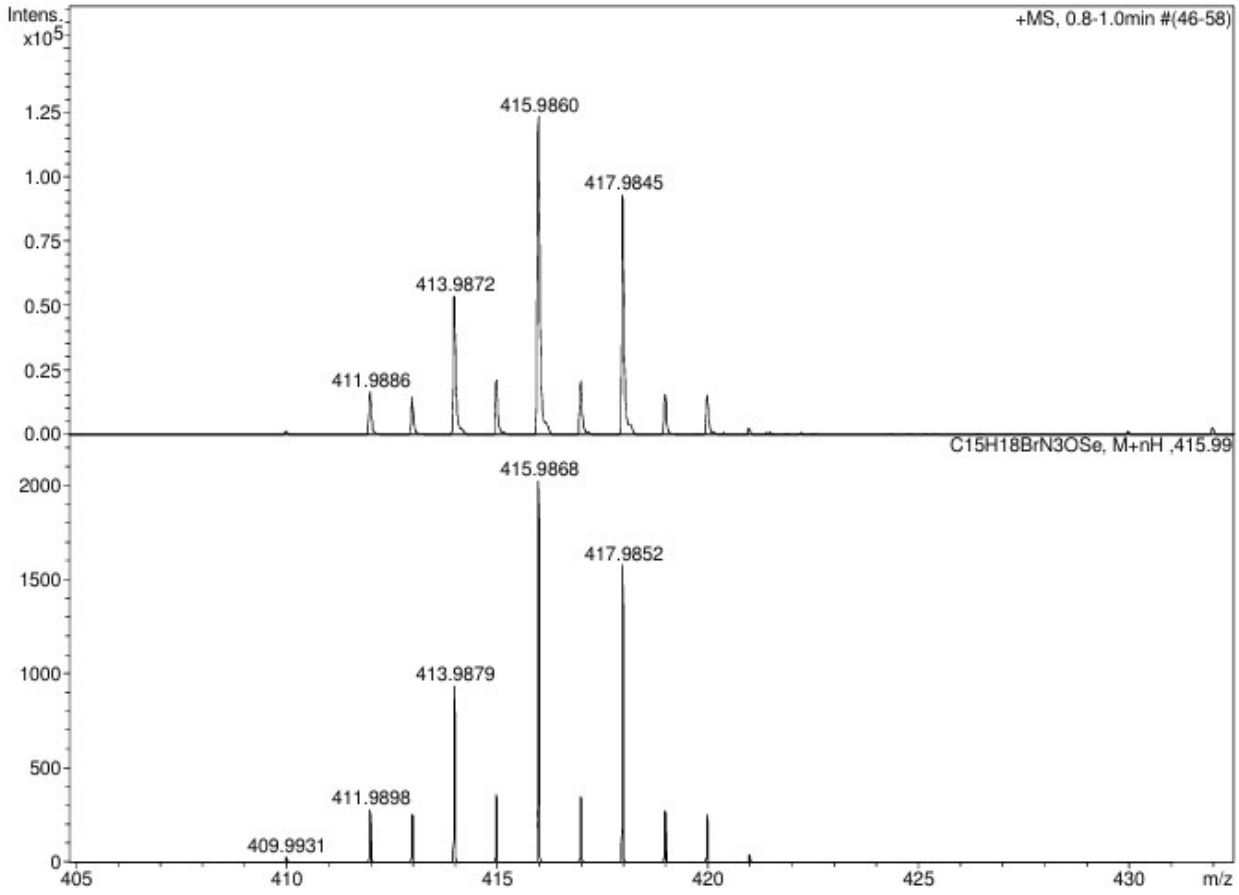
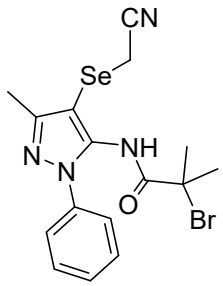


Figure-144: HRMS spectrum of compound **17a**





2-Bromo-N-(4-((cyanomethyl)selanyl)-3-methyl-1-phenyl-1H-pyrazol-5-yl)-2-methylpropanamide, ***17b***

Grey powder, m.p. 130-132°C, yield 65% (0.11 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.19 (s, 1H), 7.57 – 7.46 (m, 4H), 7.44 – 7.37 (m, 1H), 3.54 (s, 2H), 2.40 (s, 3H), 1.91 (s, 6H). ^{77}Se NMR (57 MHz, DMSO) δ 158.81. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 171.40, 152.61, 139.75, 138.13, 129.11, 127.75, 123.01, 119.07, 100.22, 58.81, 30.75, 13.21, 7.60. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for [$C_{16}H_{18}BrN_4OSe$]$^{+}$: 440.9821; found: 440.9814.

Figure-145: ^{1}H NMR spectrum (300 MHz) of **17b** in DMSO-d_6

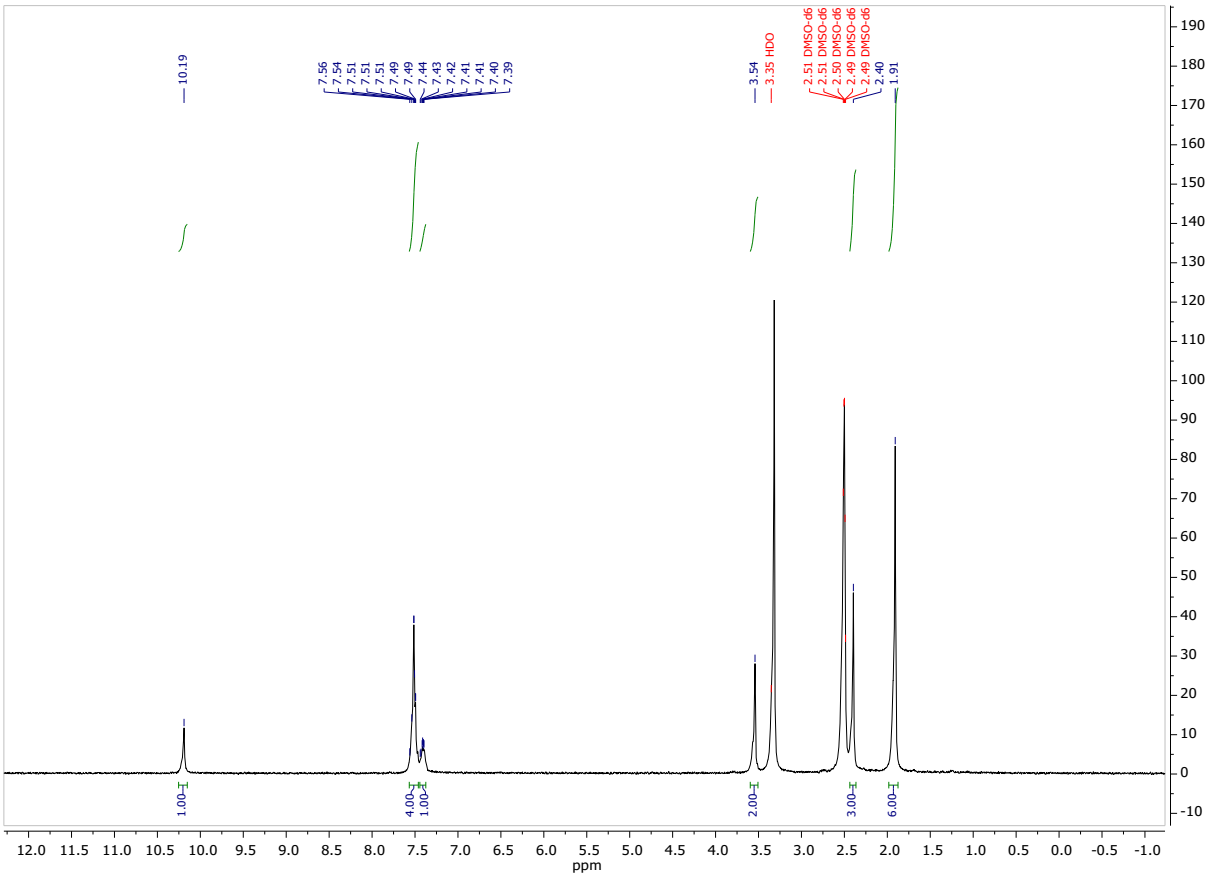


Figure-146: ^{77}Se NMR spectrum (57 MHz) of **17b** in DMSO-d_6

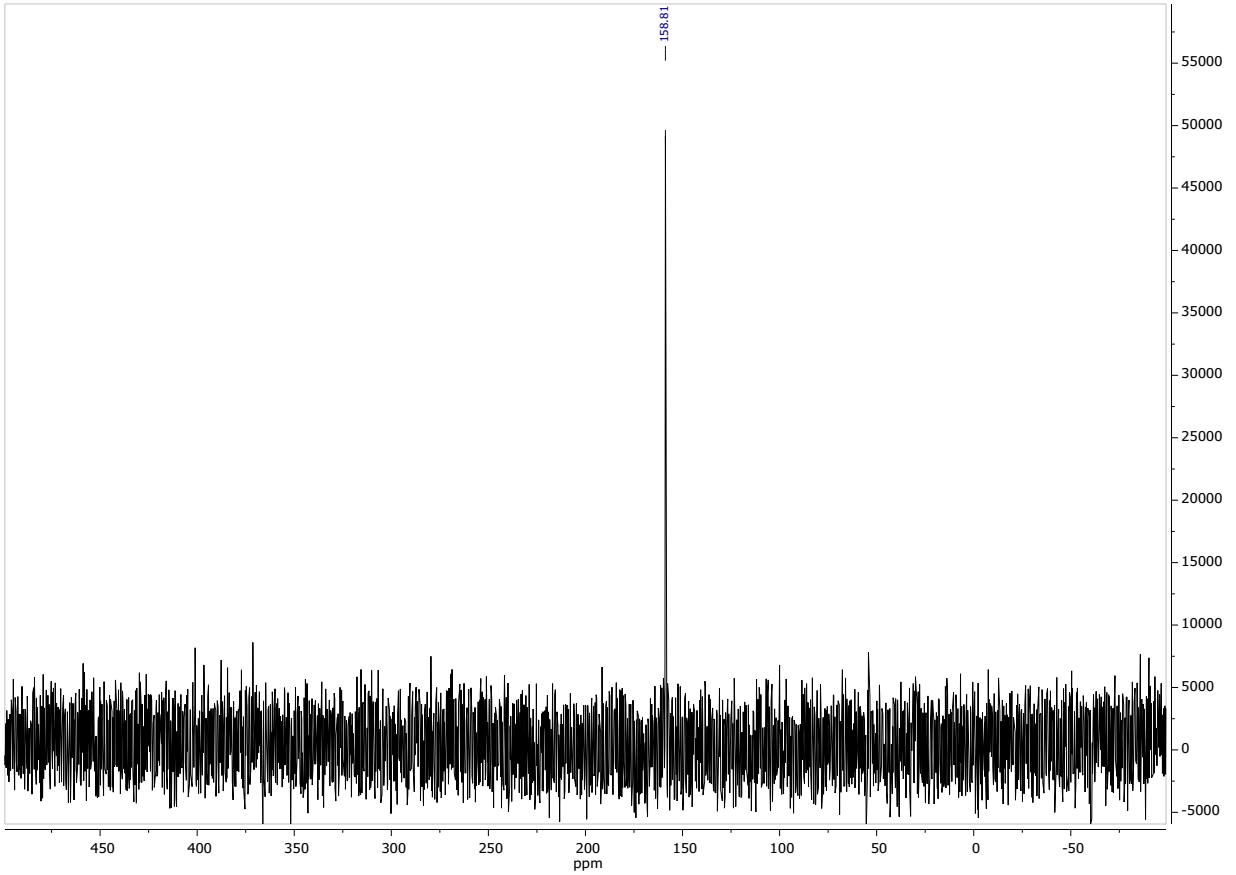


Figure-147: ^{13}C NMR spectrum (76 MHz) of **17b** in DMSO-d_6

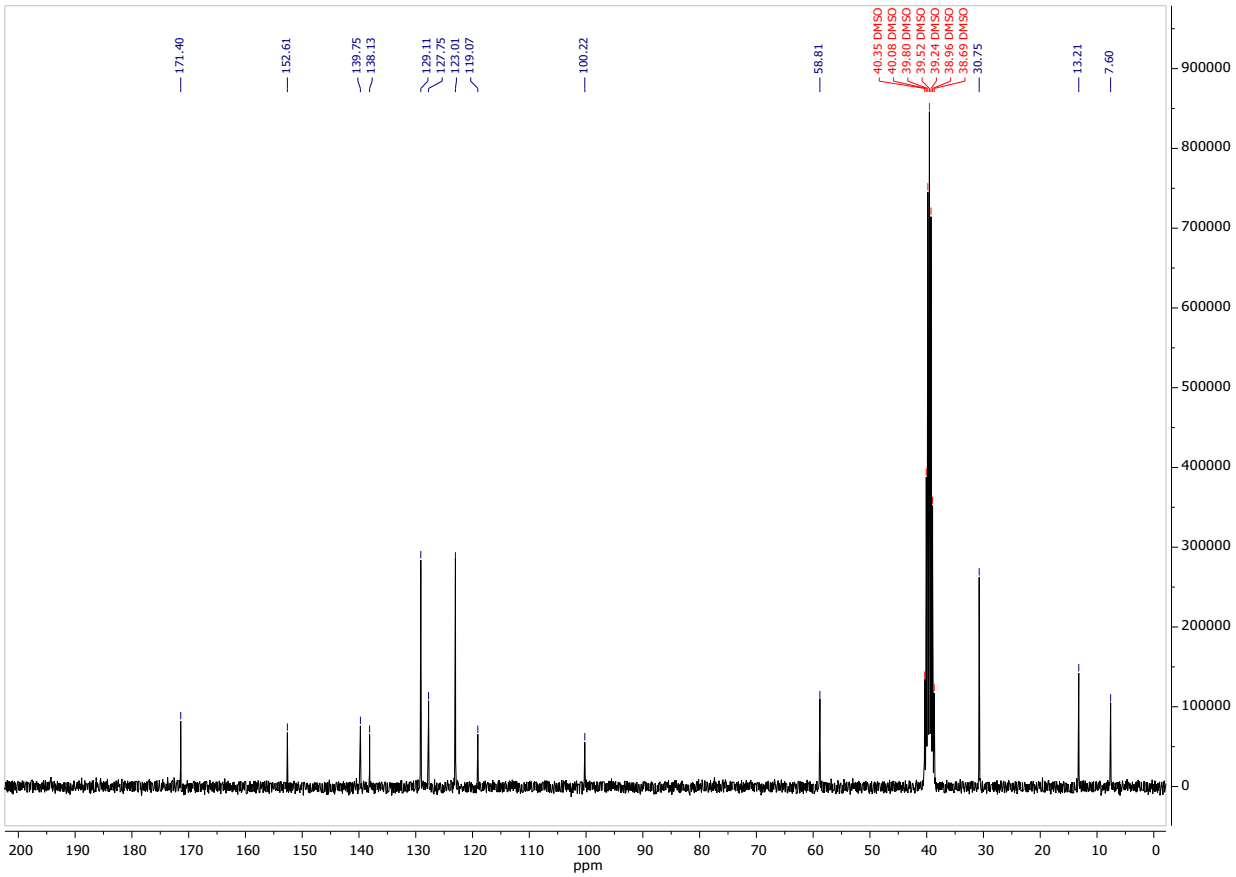
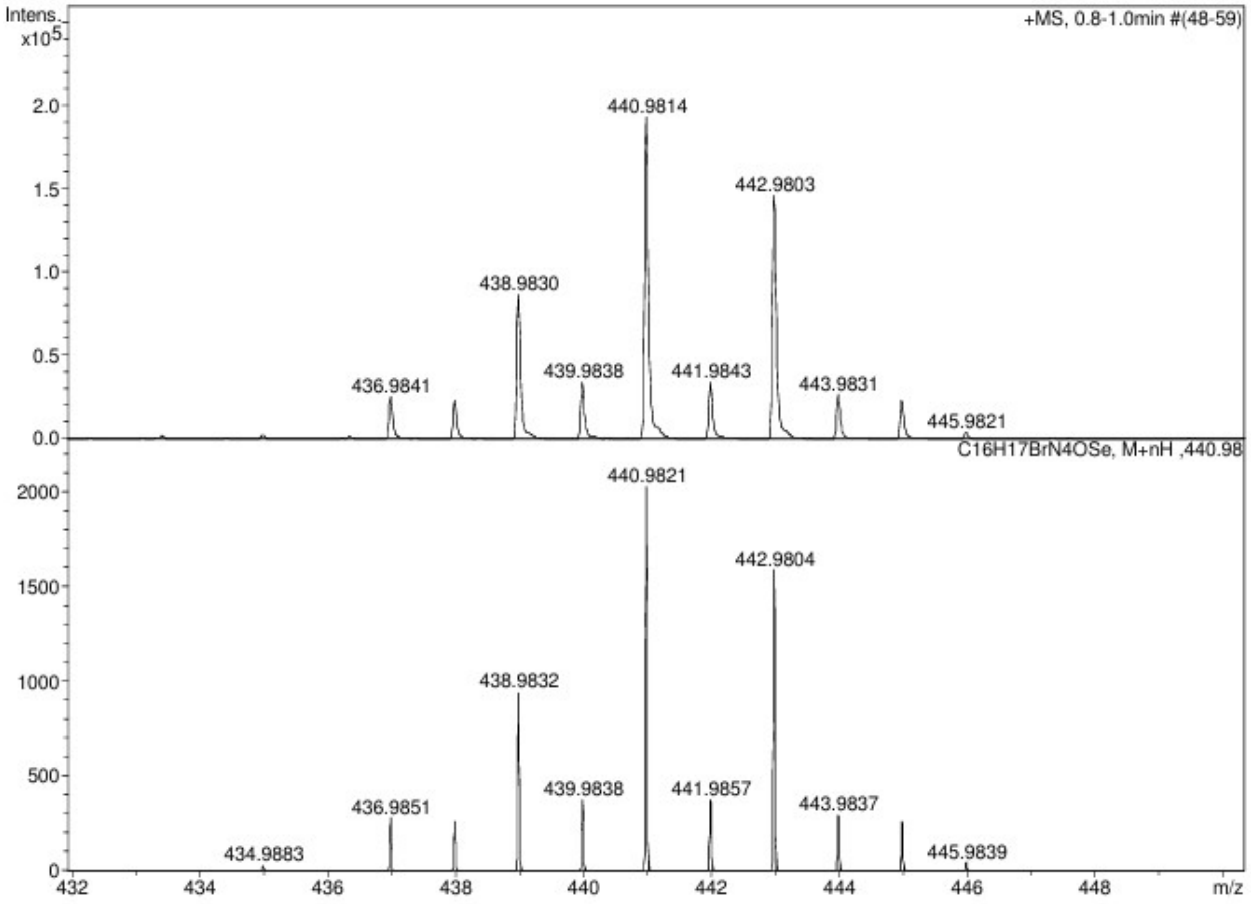
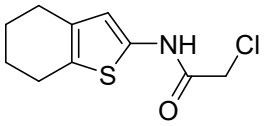


Figure-148: HRMS spectrum of compound **17b**



NMR and HRMS spectra of compound 19



2-Chloro-N-(4,5,6,7-tetrahydrobenzo[b]thiophen-2-yl)acetamide, ***19***

Grey powder, m.p. 185-187°C, yield 87% (0.80 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 11.24 (s, 1H), 6.40 (s, 1H), 4.22 (s, 2H), 2.61 – 2.55 (m, 2H), 2.48 – 2.40 (m, 2H), 1.78 – 1.64 (m, 4H). ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 162.70, 135.60, 131.57, 126.49, 112.49, 42.61, 24.91, 23.76, 23.24, 22.59. HRMS (ESI-TOF): m/z [M+H]$^{+}$: calcd for $[C_{10}H_{13}ClN_4OS]^{+}$: 230.0401; found: 230.0404.

Figure-149: ^{1}H NMR spectrum (300 MHz) of **19** in DMSO-d_6

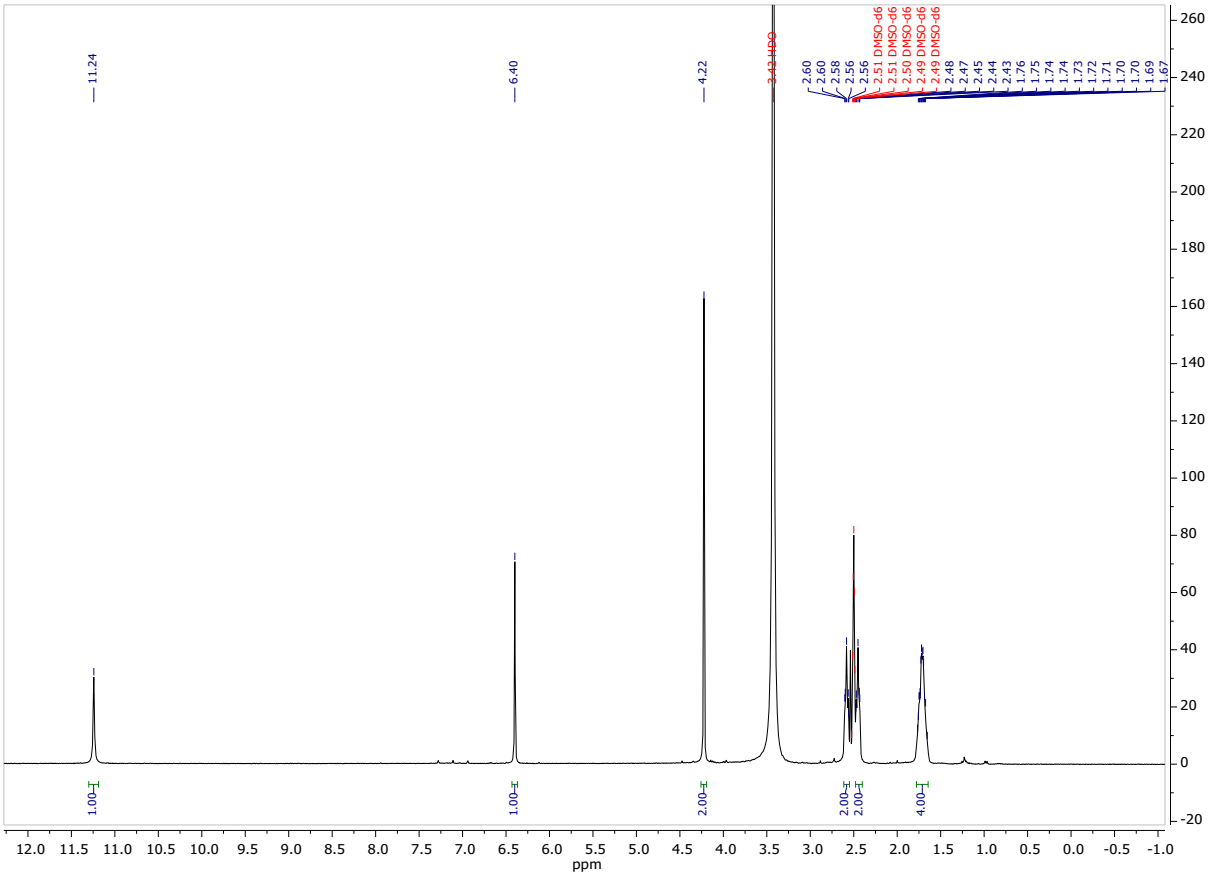


Figure-150: ^{13}C NMR spectrum (76 MHz) of **19** in DMSO-d_6

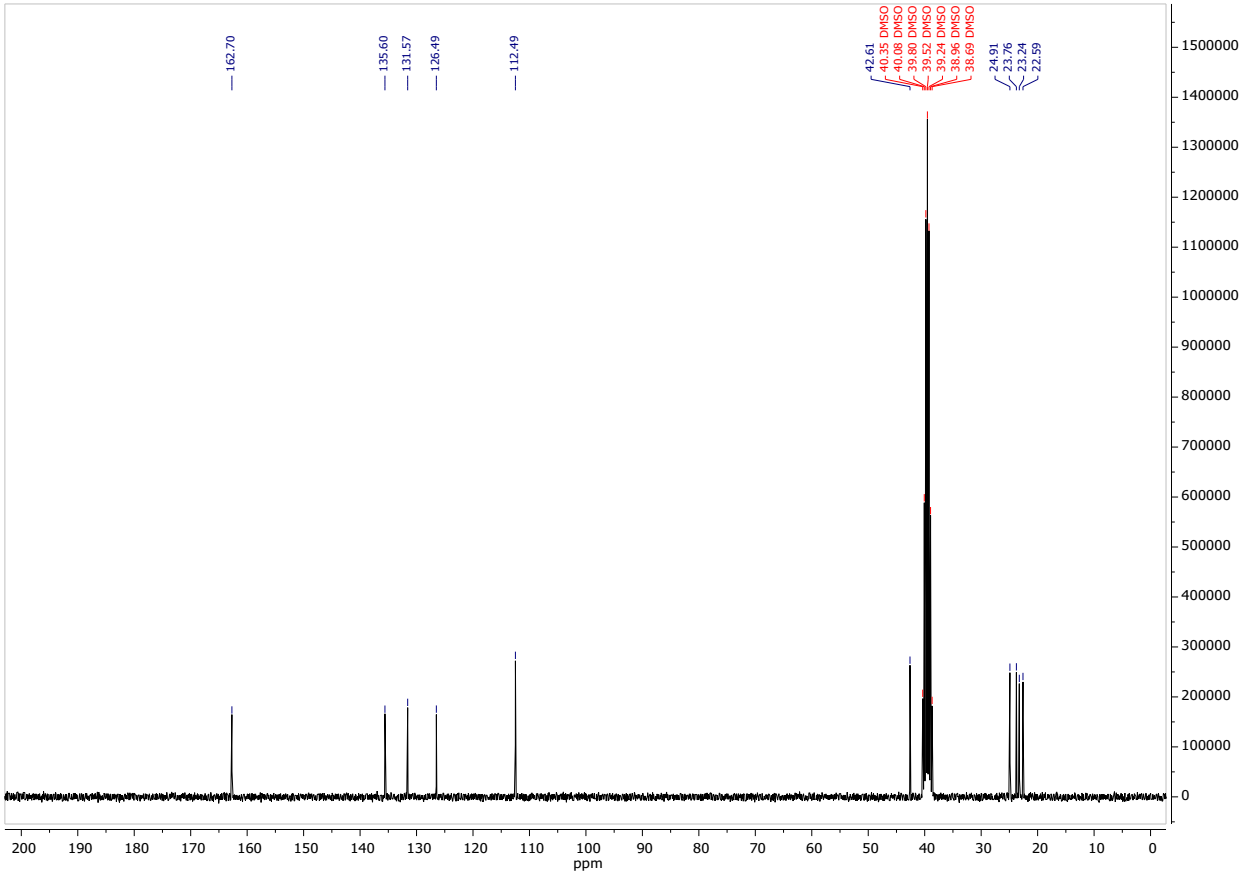
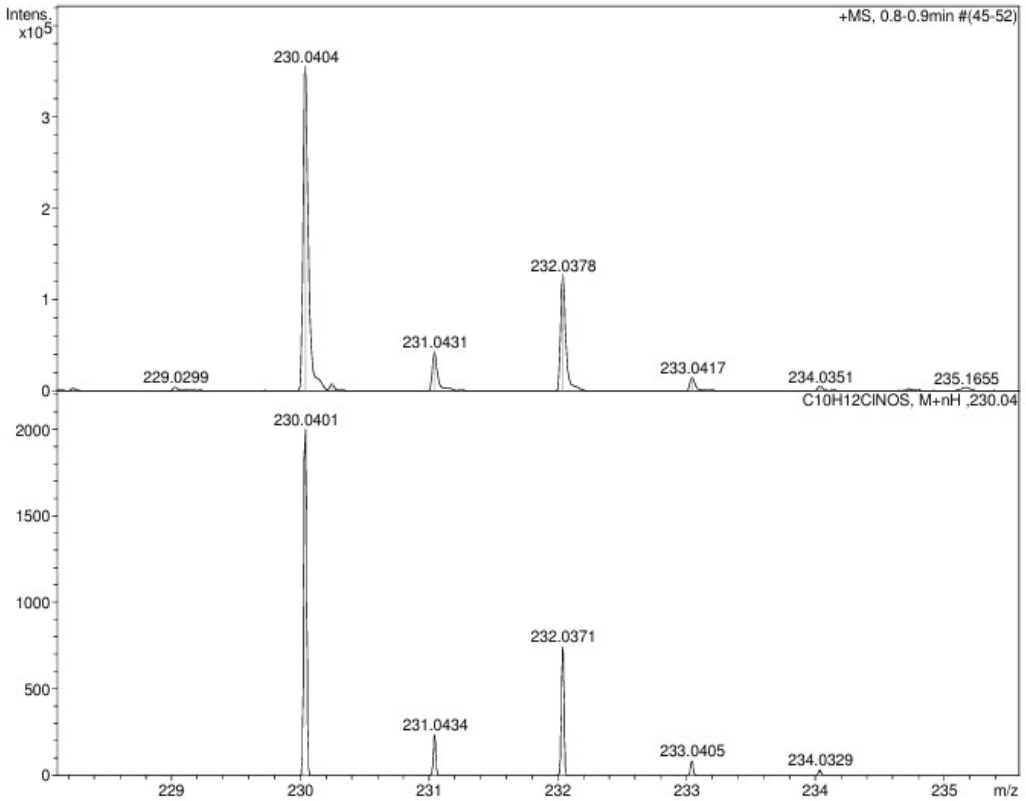
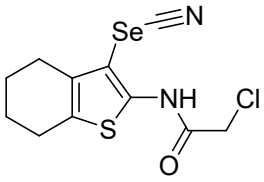


Figure-151: HRMS spectrum of compound **19**



NMR and HRMS spectra of compound 20



2-Chloro-N-(3-selenocyanato-4,5,6,7-tetrahydrobenzo[b]thiophen-2-yl)acetamide, ***20***

Grey powder, m.p. 119-121°C, yield 79% (0.53 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.82 (s, 1H), 4.48 (s, 2H), 2.69 – 2.62 (m, 2H), 2.60 – 2.54 (m, 2H), 1.82 – 1.74 (m, 4H). ^{77}Se NMR (57 MHz, DMSO) δ 172.39. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 164.61, 139.15, 133.34, 128.97, 104.31, 102.25, 42.35, 25.19, 23.93, 22.89, 22.23. HRMS (ESI-TOF): m/z $[M+H]^+$: calcd for $[C_{11}H_{12}ClN_2OSSe]^+$: 334.9515; found: 334.9504.

Figure-152: ^{1}H NMR spectrum (300 MHz) of **20** in DMSO-d_6

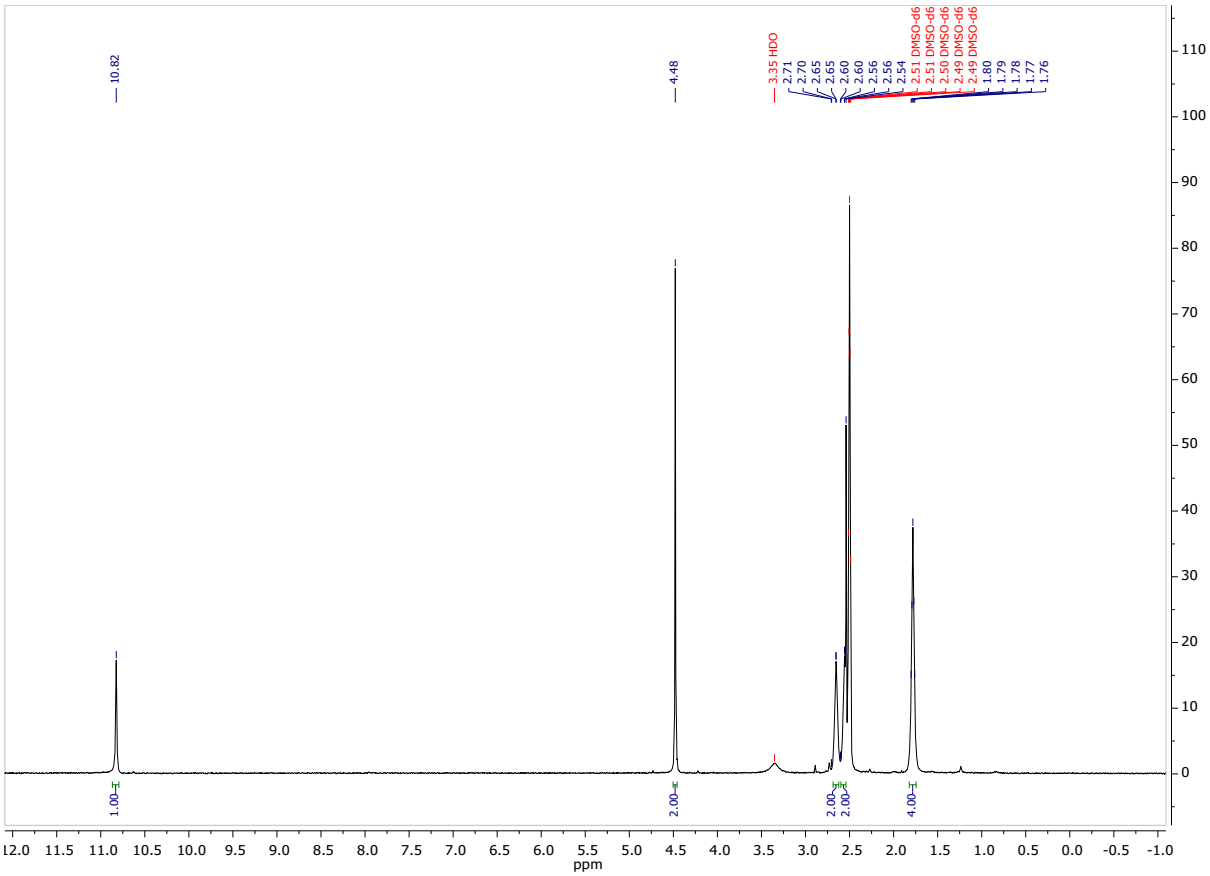


Figure-153: ^{77}Se NMR spectrum (57 MHz) of **20** in DMSO-d_6

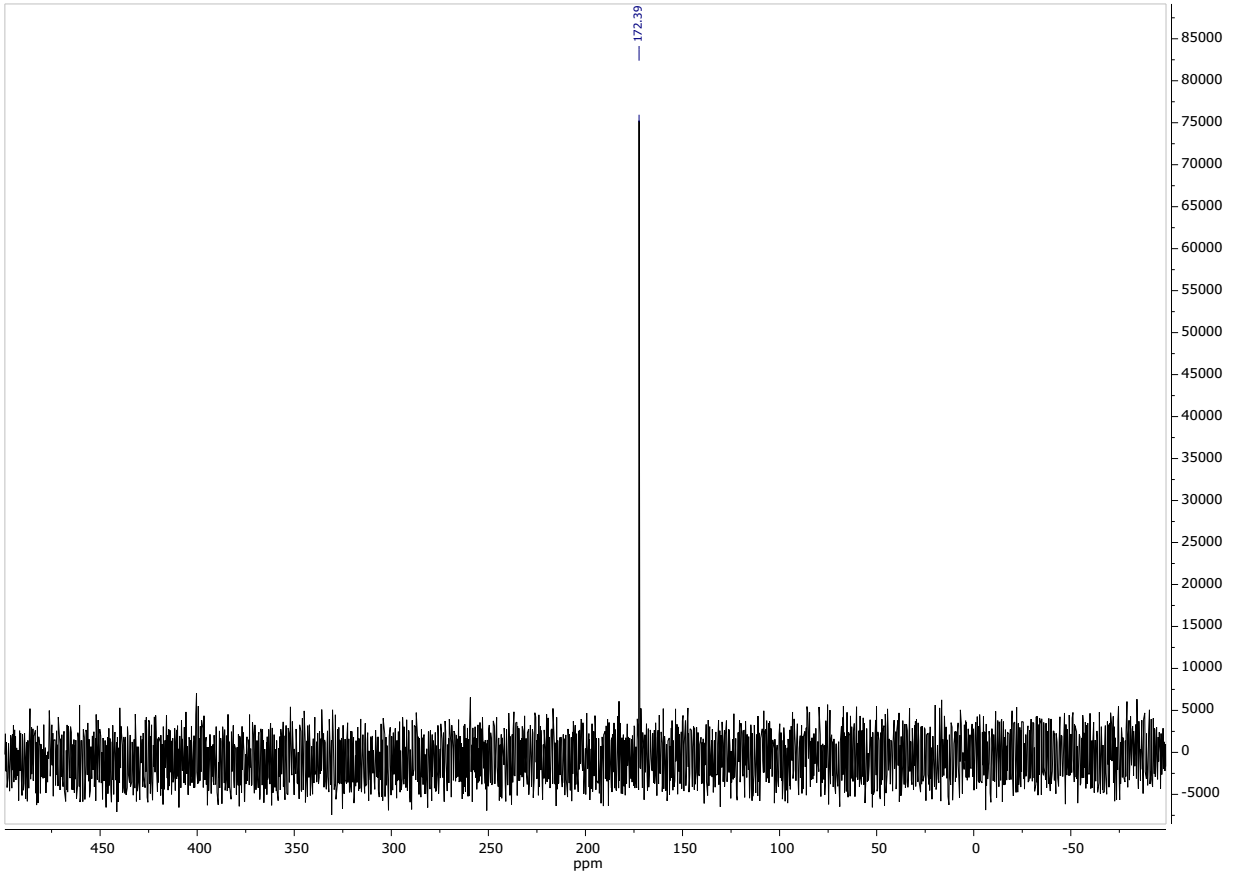


Figure-154: ^{13}C NMR spectrum (76 MHz) of **20** in DMSO-d_6

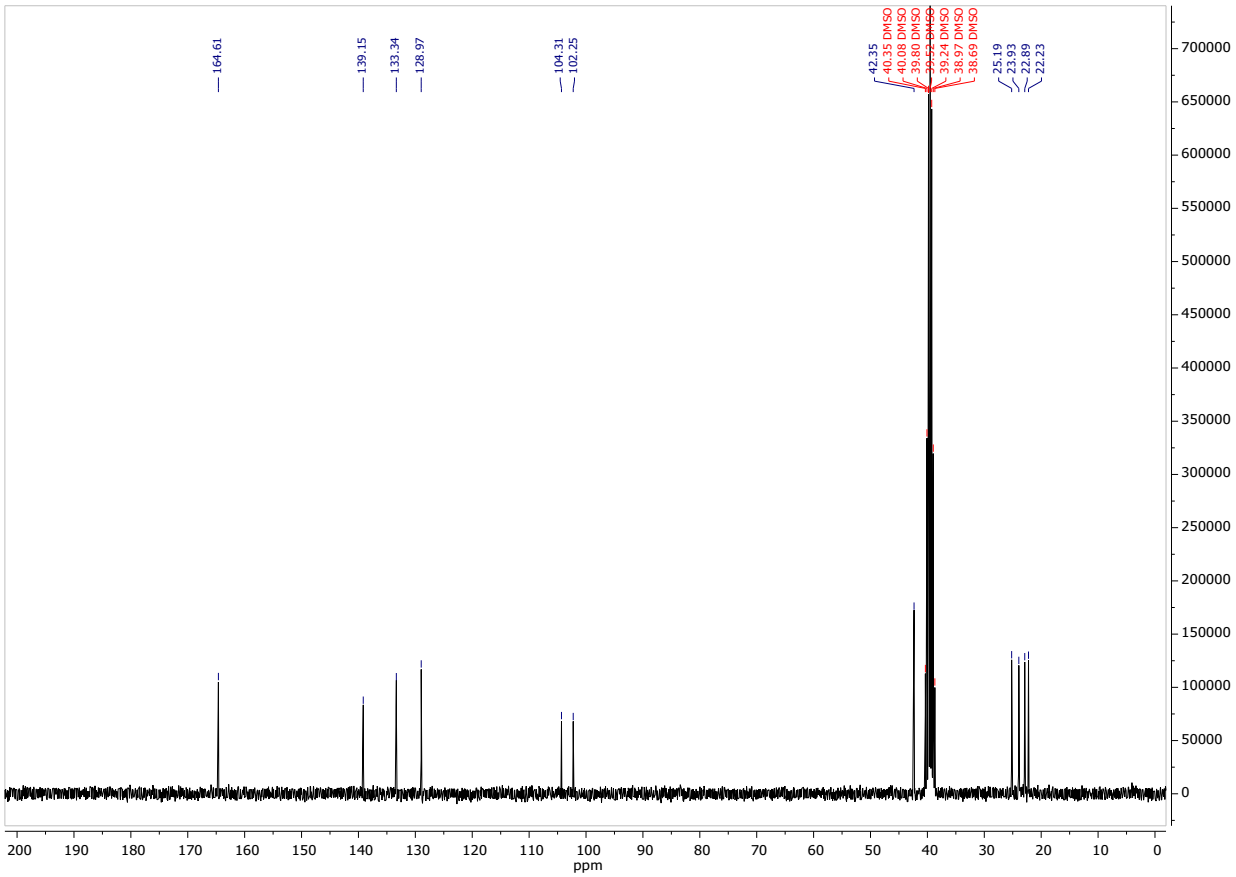
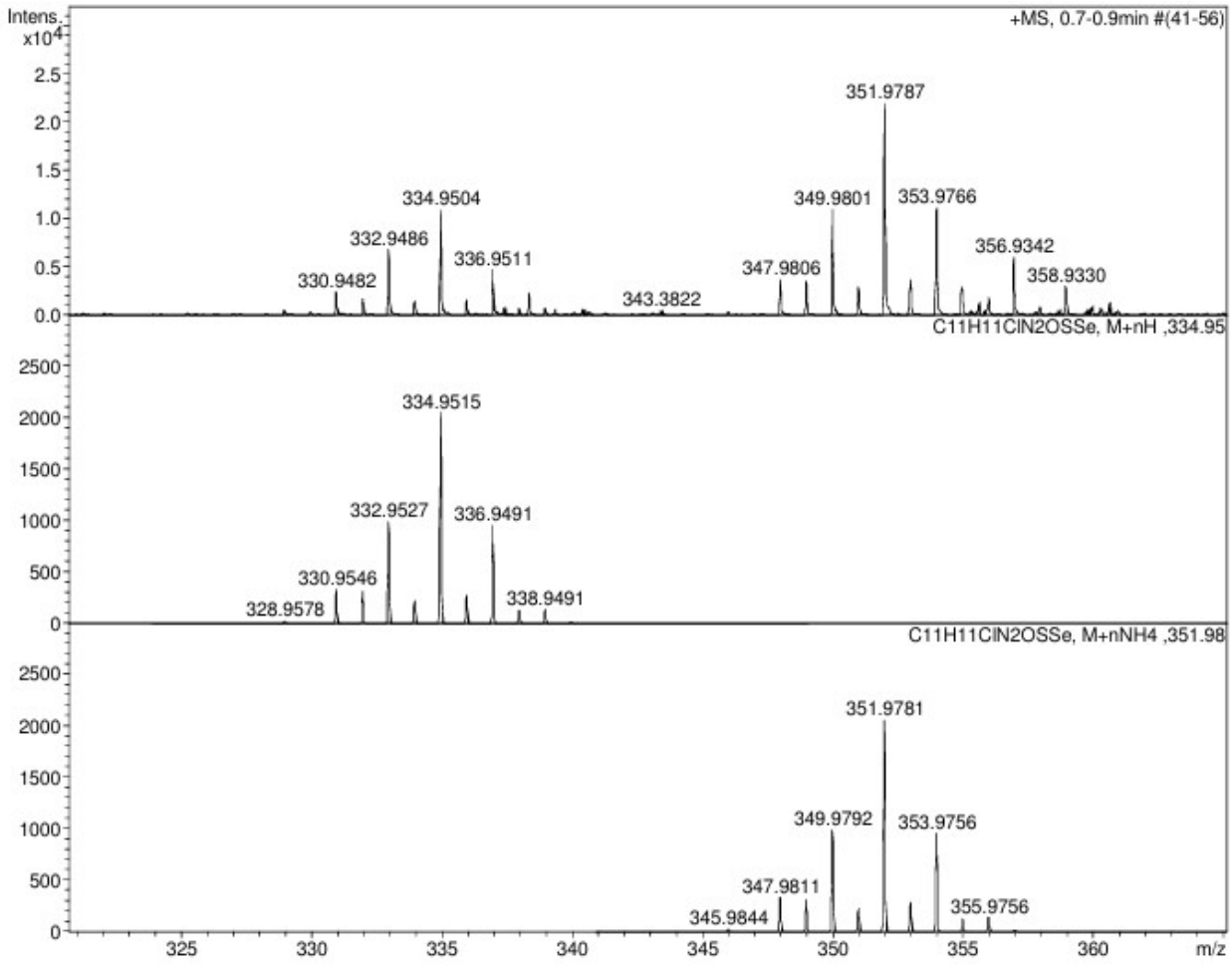
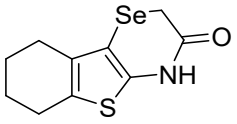


Figure-155: HRMS spectrum of compound **20**



NMR and HRMS spectra of compound 21



6,7,8,9-Tetrahydro-2H-benzo[4,5]thieno[3,2-b][1,4]selenazin-3(4H)-one, ***21***

Yellow powder, m.p. 223-225°C, yield 65% (0.07 g)

^{1}H NMR (300 MHz, DMSO-d_6) δ 10.54 (s, 1H), 3.33 (s, 2H), 2.62 – 2.57 (m, 2H), 2.35 – 2.28 (m, 2H), 1.77 – 1.69 (m, 4H). ^{77}Se NMR (57 MHz, DMSO) δ 131.51. ^{13}C{^{1}H} NMR (76 MHz, DMSO) δ 164.67, 132.47, 131.98, 125.66, 103.83, 24.70, 23.98, 22.99, 22.09, 20.66. HRMS (ESI-TOF): m/z [M-H]$^{+}$: calcd for [$C_{10}H_{10}NOSSe$]$^{+}$: 271.9642; found: 271.9642.

Figure-156: ^{1}H NMR spectrum (300 MHz) of **21** in DMSO-d_6

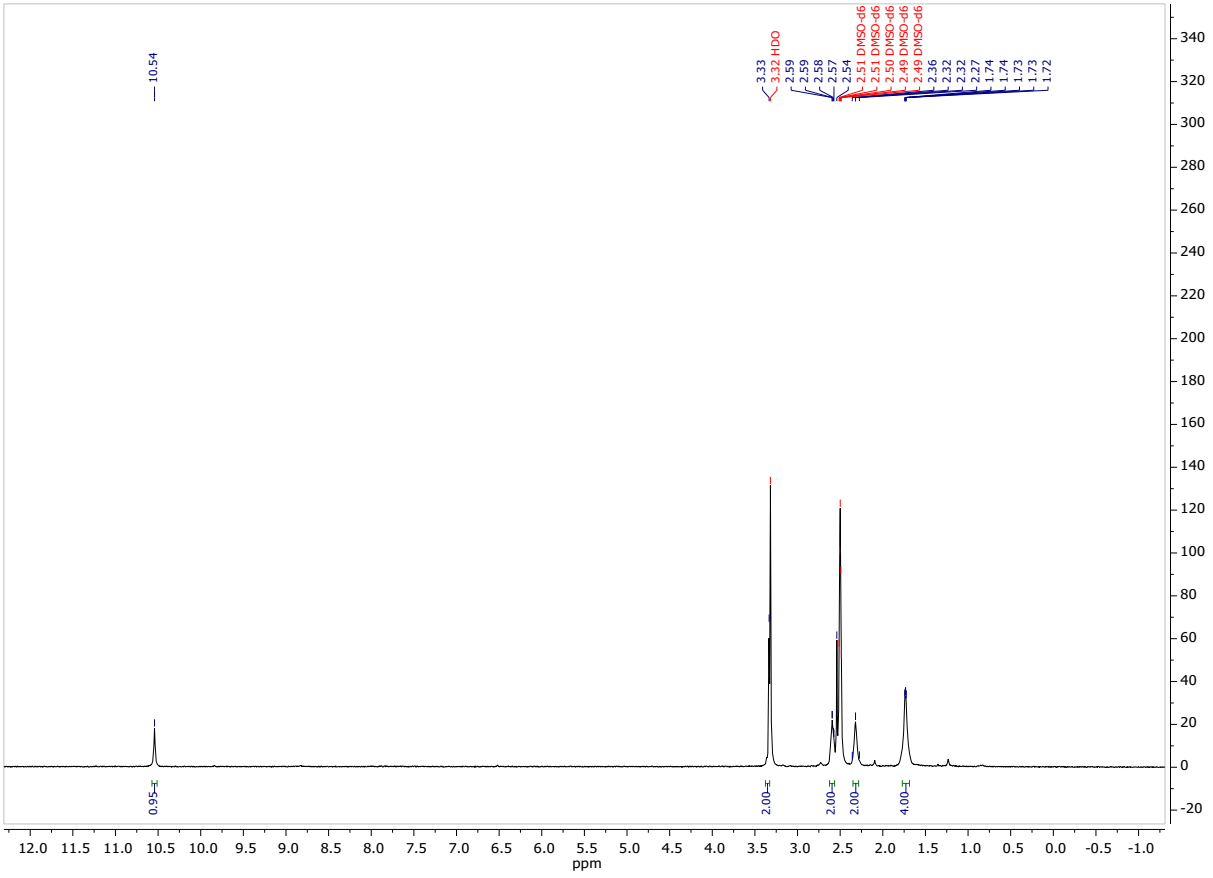


Figure-157: ^{77}Se NMR spectrum (57 MHz) of **21** in DMSO-d_6

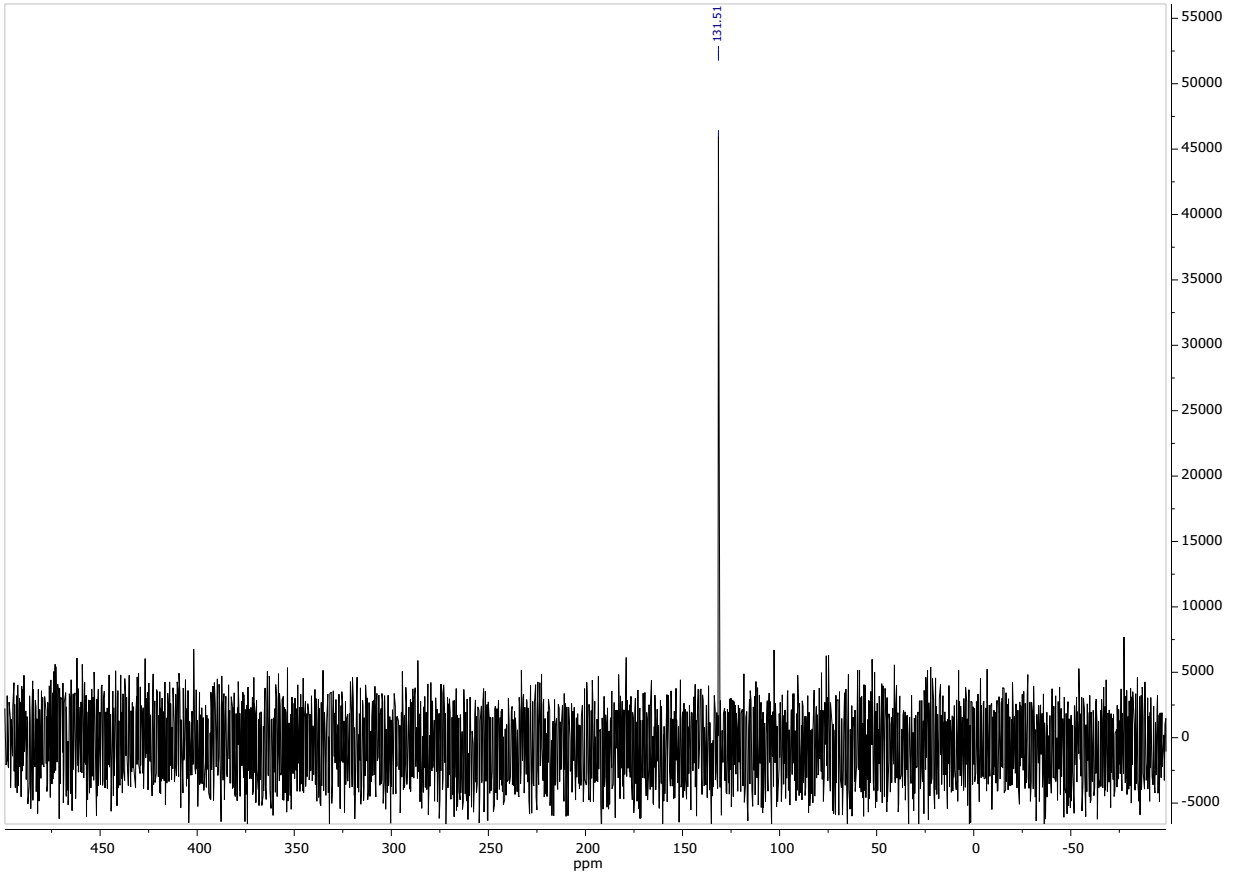


Figure-158: ^{13}C NMR spectrum (76 MHz) of **21** in DMSO-d_6

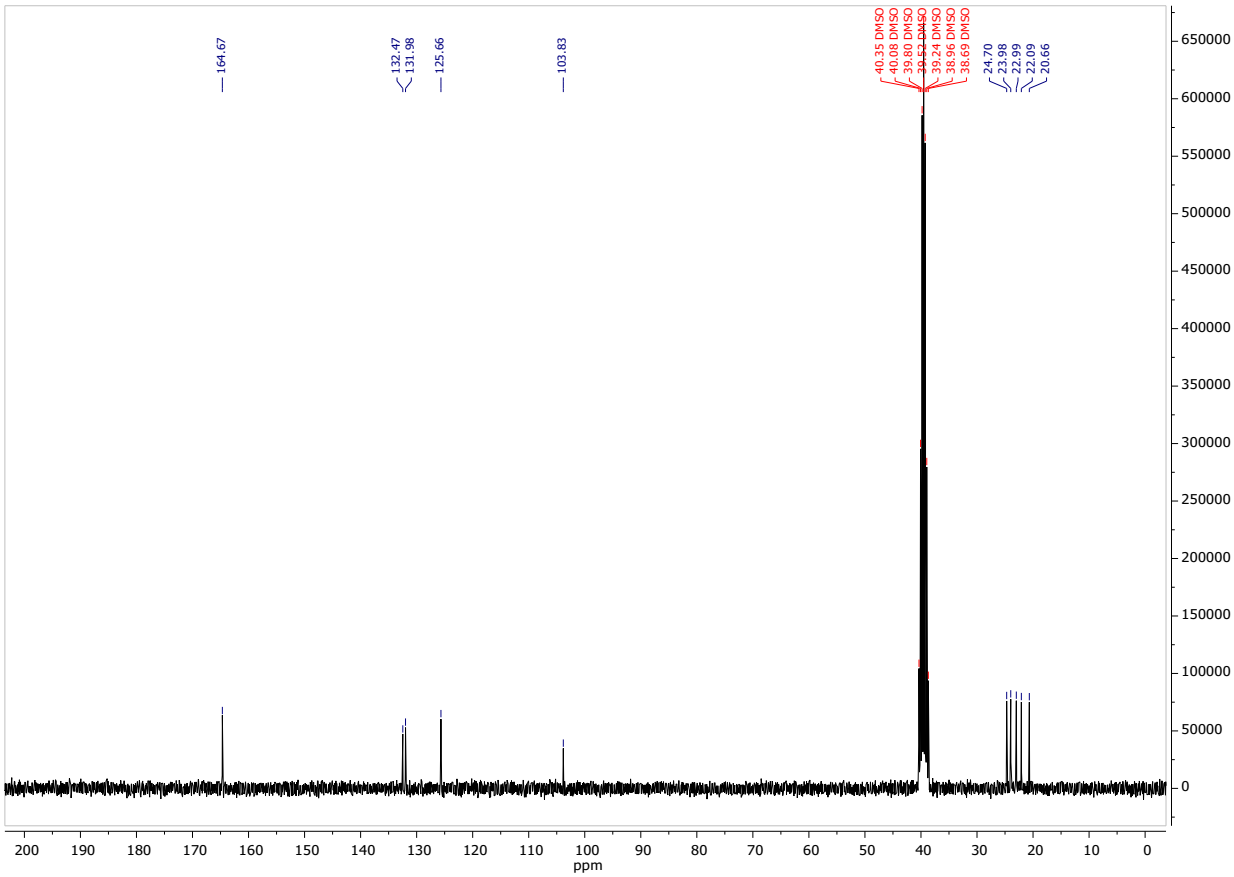
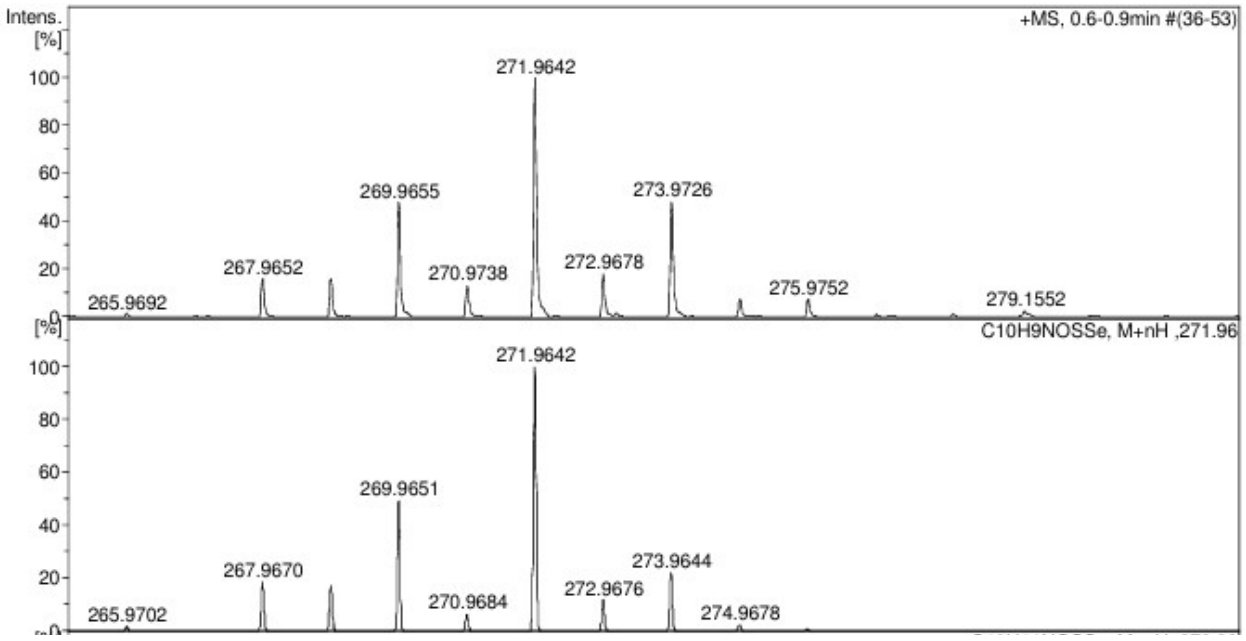


Figure-159: HRMS spectrum of compound **21**



Crystallographic data for compound 6i

Table 1. Crystal data and structure refinement for **6i**.

Identification code	2506169	
Empirical formula	C14 H15 N3 O Se	
Formula weight	320.25	
Temperature	291.0 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2_1/n	
Unit cell dimensions	a = 7.8853(3) Å	a= 90°.
	b = 7.8504(3) Å	b= 93.193(2)°.
	c = 21.1466(9) Å	g = 90°.
Volume	1307.00(9) $Å^3$	
Z	4	
Density (calcd)	1.628 g/cm^3	
Absorption coefficient	2.868 mm^{-1}	
F(000)	648	
Crystal size	0.319 x 0.154 x 0.036 mm^3	
Theta range for data collection	2.768 to 31.547°.	
Index ranges	-11<=h<=11, -11<=k<=11, -31<=l<=31	
Reflections collected	50591	
Independent reflections	4373 [R(int) = 0.0404]	
Observed reflections	3854	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7462 and 0.5646	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4373 / 0 / 179	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0225, wR2 = 0.0528	
R indices (all data)	R1 = 0.0284, wR2 = 0.0556	
Largest diff. peak and hole	0.477 and -0.594 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6i**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Se(7)	5961(1)	4835(1)	9177(1)	15(1)
O(5)	7852(1)	6991(1)	7740(1)	19(1)
N(1)	1607(1)	3433(1)	8133(1)	15(1)
N(4)	5282(1)	5706(1)	7685(1)	13(1)
C(8)	4058(2)	4347(2)	8624(1)	13(1)
C(9)	2490(2)	3525(2)	8689(1)	14(1)
C(18)	1771(2)	2845(2)	9277(1)	18(1)
N(2)	2613(1)	4191(1)	7703(1)	13(1)
C(10)	2117(2)	4154(2)	7046(1)	13(1)
C(11)	3251(2)	3540(2)	6620(1)	14(1)
C(12)	2723(2)	3420(2)	5980(1)	14(1)
C(16)	3918(2)	2779(2)	5502(1)	19(1)
C(13)	1058(2)	3879(2)	5791(1)	15(1)
C(14)	-76(2)	4486(2)	6221(1)	15(1)
C(17)	-1882(2)	4920(2)	6011(1)	19(1)
C(15)	476(2)	4648(2)	6856(1)	14(1)
C(3)	4077(2)	4770(2)	7992(1)	12(1)
C(5)	6901(2)	5910(2)	7942(1)	15(1)
C(6)	7458(2)	4684(2)	8465(1)	16(1)

Table 3. Bond lengths [Å] and angles [°] for **6i**.

Se(7)-C(8) 1.8894(12)	C(9)-C(8)-Se(7) 134.76(9)
Se(7)-C(6) 1.9674(13)	C(3)-C(8)-Se(7) 119.99(9)
O(5)-C(5) 1.2251(16)	C(3)-C(8)-C(9) 105.19(10)
N(1)-C(9) 1.3359(16)	N(1)-C(9)-C(8) 110.85(11)
N(1)-N(2) 1.3743(14)	N(1)-C(9)-C(18) 120.74(11)
N(4)-C(3) 1.3893(16)	C(8)-C(9)-C(18) 128.39(11)
N(4)-C(5) 1.3688(15)	C(9)-C(18)-H(18A) 109.5
N(4)-H(4) 0.845(19)	C(9)-C(18)-H(18B) 109.5
C(8)-C(9) 1.4083(17)	C(9)-C(18)-H(18C) 109.5
C(8)-C(3) 1.3797(16)	H(18A)-C(18)-H(18B) 109.5
C(9)-C(18) 1.4929(18)	H(18A)-C(18)-H(18C) 109.5
C(18)-H(18A) 0.9600	H(18B)-C(18)-H(18C) 109.5
C(18)-H(18B) 0.9600	N(1)-N(2)-C(10) 119.96(10)
C(18)-H(18C) 0.9600	C(3)-N(2)-N(1) 110.89(10)
N(2)-C(10) 1.4228(15)	C(3)-N(2)-C(10) 128.91(10)
N(2)-C(3) 1.3541(15)	C(11)-C(10)-N(2) 119.25(11)
C(10)-C(11) 1.3904(17)	C(15)-C(10)-N(2) 118.53(11)
C(10)-C(15) 1.3891(16)	C(15)-C(10)-C(11) 122.12(11)
C(11)-H(11) 0.9300	C(10)-C(11)-H(11) 120.5
C(11)-C(12) 1.3956(17)	C(10)-C(11)-C(12) 118.91(11)
C(12)-C(16) 1.5069(18)	C(12)-C(11)-H(11) 120.5
C(12)-C(13) 1.3982(17)	C(11)-C(12)-C(16) 120.58(11)
C(16)-H(16A) 0.9600	C(11)-C(12)-C(13) 119.01(11)
C(16)-H(16B) 0.9600	C(13)-C(12)-C(16) 120.40(11)
C(16)-H(16C) 0.9600	C(12)-C(16)-H(16A) 109.5
C(13)-H(13) 0.9300	C(12)-C(16)-H(16B) 109.5
C(13)-C(14) 1.3945(18)	C(12)-C(16)-H(16C) 109.5
C(14)-C(17) 1.5074(17)	H(16A)-C(16)-H(16B) 109.5
C(14)-C(15) 1.3935(17)	H(16A)-C(16)-H(16C) 109.5
C(17)-H(17A) 0.9600	H(16B)-C(16)-H(16C) 109.5
C(17)-H(17B) 0.9600	C(12)-C(13)-H(13) 119.1
C(17)-H(17C) 0.9600	C(14)-C(13)-C(12) 121.79(11)
C(15)-H(15) 0.9300	C(14)-C(13)-H(13) 119.1
C(5)-C(6) 1.5137(18)	C(13)-C(14)-C(17) 120.94(11)
C(6)-H(6A) 0.9700	C(15)-C(14)-C(13) 118.86(11)
C(6)-H(6B) 0.9700	C(15)-C(14)-C(17) 120.18(12)
	C(14)-C(17)-H(17A) 109.5
C(8)-Se(7)-C(6) 90.23(5)	C(14)-C(17)-H(17B) 109.5
C(9)-N(1)-N(2) 105.52(10)	C(14)-C(17)-H(17C) 109.5
C(3)-N(4)-H(4) 119.0(13)	H(17A)-C(17)-H(17B) 109.5
C(5)-N(4)-C(3) 121.58(11)	H(17A)-C(17)-H(17C) 109.5
C(5)-N(4)-H(4) 116.4(13)	H(17B)-C(17)-H(17C) 109.5

C(10)-C(15)-C(14)	119.27(11)	N(4)-C(5)-C(6)	116.21(11)
C(10)-C(15)-H(15)	120.4	Se(7)-C(6)-H(6A)	109.4
C(14)-C(15)-H(15)	120.4	Se(7)-C(6)-H(6B)	109.4
C(8)-C(3)-N(4)	128.66(11)	C(5)-C(6)-Se(7)	111.06(8)
N(2)-C(3)-N(4)	123.71(11)	C(5)-C(6)-H(6A)	109.4
N(2)-C(3)-C(8)	107.52(11)	C(5)-C(6)-H(6B)	109.4
O(5)-C(5)-N(4)	121.27(12)	H(6A)-C(6)-H(6B)	108.0
O(5)-C(5)-C(6)	122.47(11)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **6i**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Se(7)	15(1)	18(1)	12(1)	-2(1)	-3(1)	2(1)
O(5)	13(1)	22(1)	22(1)	0(1)	1(1)	-4(1)
N(1)	13(1)	17(1)	14(1)	0(1)	2(1)	-1(1)
N(4)	11(1)	16(1)	13(1)	1(1)	-1(1)	0(1)
C(8)	14(1)	16(1)	11(1)	-1(1)	-1(1)	1(1)
C(9)	14(1)	14(1)	13(1)	0(1)	2(1)	2(1)
C(18)	21(1)	20(1)	14(1)	2(1)	4(1)	0(1)
N(2)	10(1)	19(1)	11(1)	0(1)	0(1)	-2(1)
C(10)	12(1)	15(1)	11(1)	0(1)	-1(1)	-2(1)
C(11)	11(1)	16(1)	14(1)	1(1)	-1(1)	-1(1)
C(12)	13(1)	15(1)	14(1)	0(1)	1(1)	-2(1)
C(16)	17(1)	24(1)	15(1)	-3(1)	1(1)	1(1)
C(13)	16(1)	16(1)	13(1)	1(1)	-2(1)	-2(1)
C(14)	11(1)	15(1)	17(1)	2(1)	-2(1)	-2(1)
C(17)	14(1)	23(1)	20(1)	2(1)	-3(1)	0(1)
C(15)	11(1)	16(1)	15(1)	1(1)	0(1)	-1(1)
C(3)	11(1)	14(1)	11(1)	-2(1)	-1(1)	1(1)
C(5)	11(1)	17(1)	16(1)	-3(1)	0(1)	1(1)
C(6)	12(1)	20(1)	18(1)	0(1)	-1(1)	3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **6i**.

	x	y	z	U(eq)
H(18A)	1380	3773	9526	28
H(18B)	2634	2225	9518	28
H(18C)	838	2099	9165	28
H(11)	4344	3216	6758	17
H(16A)	3307	2065	5199	28
H(16B)	4814	2134	5714	28
H(16C)	4394	3729	5288	28
H(13)	697	3778	5366	18
H(17A)	-2596	4792	6361	29
H(17B)	-2265	4170	5674	29
H(17C)	-1935	6077	5863	29
H(15)	-247	5083	7149	17
H(6A)	8615	4944	8614	20
H(6B)	7437	3530	8301	20
H(4)	4950(20)	6420(30)	7405(9)	24(5)

Table 6. Torsion angles [°] for **6i**.

Se(7)-C(8)-C(9)-N(1)-176.62(10)	C(10)-C(11)-C(12)-C(16) 179.38(12)
Se(7)-C(8)-C(9)-C(18)4.9(2)	C(10)-C(11)-C(12)-C(13) -1.59(18)
Se(7)-C(8)-C(3)-N(4)-7.33(18)	C(11)-C(10)-C(15)-C(14) 1.74(19)
Se(7)-C(8)-C(3)-N(2)176.44(8)	C(11)-C(12)-C(13)-C(14) 1.32(19)
O(5)-C(5)-C(6)-Se(7)123.68(12)	C(12)-C(13)-C(14)-C(17) -178.02(12)
N(1)-N(2)-C(10)-C(11)-126.57(12)	C(12)-C(13)-C(14)-C(15) 0.50(19)
N(1)-N(2)-C(10)-C(15)49.99(16)	C(16)-C(12)-C(13)-C(14) -179.66(12)
N(1)-N(2)-C(3)-N(4)-174.93(11)	C(13)-C(14)-C(15)-C(10) -2.00(18)
N(1)-N(2)-C(3)-C(8) 1.53(14)	C(17)-C(14)-C(15)-C(10) 176.54(11)
N(4)-C(5)-C(6)-Se(7)-58.74(13)	C(15)-C(10)-C(11)-C(12) 0.09(19)
C(9)-N(1)-N(2)-C(10)173.62(11)	C(3)-N(4)-C(5)-O(5)-165.42(12)
C(9)-N(1)-N(2)-C(3)-1.19(14)	C(3)-N(4)-C(5)-C(6)16.98(17)
C(9)-C(8)-C(3)-N(4)175.01(12)	C(3)-C(8)-C(9)-N(1) 0.52(14)
C(9)-C(8)-C(3)-N(2)-1.22(14)	C(3)-C(8)-C(9)-C(18)-177.92(12)
N(2)-N(1)-C(9)-C(8) 0.38(14)	C(3)-N(2)-C(10)-C(11)47.19(19)
N(2)-N(1)-C(9)-C(18)178.96(11)	C(3)-N(2)-C(10)-C(15)-136.25(13)
N(2)-C(10)-C(11)-C(12)176.52(11)	C(5)-N(4)-C(3)-C(8)20.53(19)
N(2)-C(10)-C(15)-C(14)-174.72(11)	C(5)-N(4)-C(3)-N(2)-163.79(12)
C(10)-N(2)-C(3)-N(4)10.9(2)	C(6)-Se(7)-C(8)-C(9)149.44(13)
C(10)-N(2)-C(3)-C(8)-172.68(12)	C(6)-Se(7)-C(8)-C(3)-27.38(11)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **6i** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(4)-H(4)...N(1)#1	0.845(19)	2.27(2)	3.0829(15)	161.7(17)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,y+1/2,-z+3/2