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S U P P L E M E N T A R Y M A T E R I A L

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An Ebselen-like Catalyst with Enhanced GPx Activity via a Selenol Intermediate

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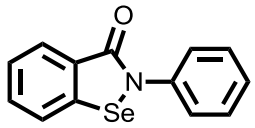
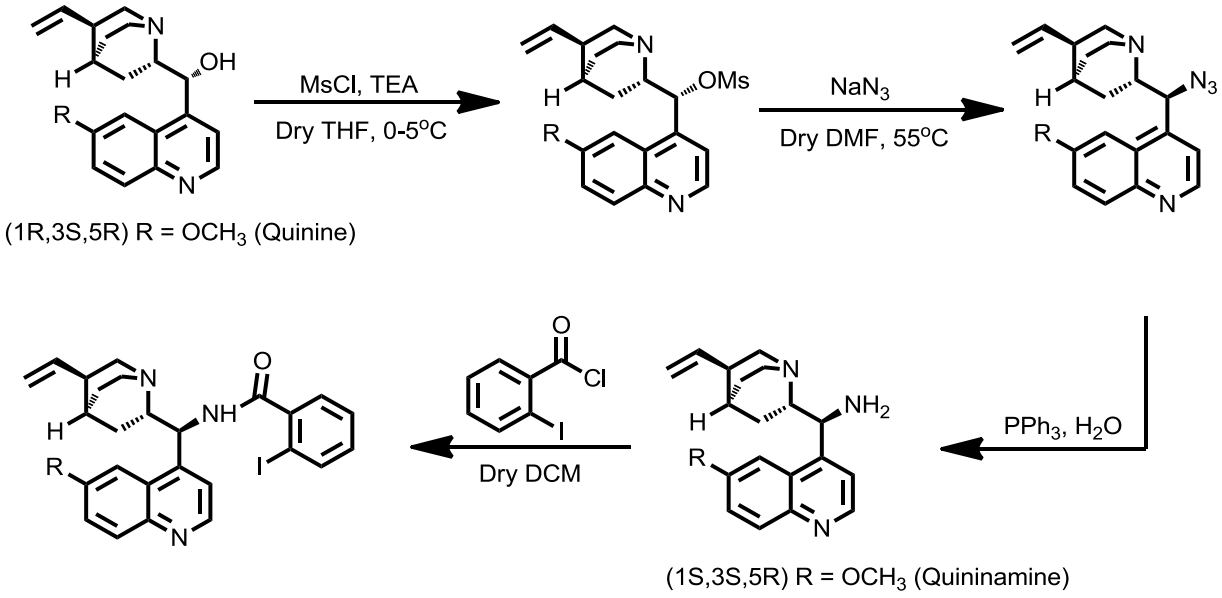
General experimental details

All NMR experiments were carried out on 400 or 500 MHz spectrometers in DMSO-d_6 or $CDCl_3$ and NMR chemical shifts are reported in ppm referenced to the solvent peaks of $CDCl_3$ (7.26 ppm for ^{1}H and 77.0 (± 0.1) ppm for ^{13}C, respectively) or DMSO-d_6 (2.50 ppm for ^{1}H and 39.50 ppm for ^{13}C, respectively). Some of ^{77}Se NMR spectra were recorded in CD_3OD solvent. High resolution mass spectra (HRMS) are reported for ions of ^{80}Se. Mass analysis is performed on quadruple-time of flight (Q-TOF) mass spectrometer equipped with an ESI source (+ve). Melting points are uncorrected. DMF with sure seal septa, selenium powder (60 mesh size), copper iodide, and 1, 10-phenanthroline were used as received from Aldrich. Grinded anhydrous K_2CO_3 powder was used which was grinded using mortar, dried in oven at 160 ^{o}C for 6 h and stored in a desiccator. Selenium- nitrogen coupling reactions were carried out under nitrogen atmosphere. Substituted benzoyl chlorides were prepared from respective benzoic acids by refluxing with excess of thionyl chloride otherwise prepared according to reported procedure. Excess of thionyl chloride was removed under vacuo and resulted residue was used for amide preparation without further purification. Silica gel (60-120 mesh size) was used for column chromatography. TLC analysis of reaction mixtures was performed using silica gel plates. Se-N heterocycles **1a**, **1e**, **1g**-**1i**, **1n**, **1p**-**1r** were prepared according to our previously reported method.[1, 2]



2-phenylbenzo[d][1,2]selenazol-3(2H)-one (1a):[1] Yield 82%, mp 180-182 °C (180-181 °C).[1]Please see figures S1-S4 for characterization data.



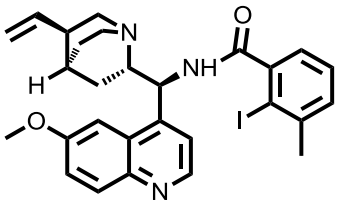
Scheme 1. Synthesis of Quininamine, and Corresponding 2-Iodo-benzamides

(1S)-(6-Methoxyquinolin-4-yl)((2S,4S,5R)-5-vinylquinuclidin-2-yl)methanamine (Quininamine), A Typical Procedure:[3]In a 100 mL capacity round bottom flask, quinine (3.0 g, 9.2 mmol) was dissolved in 60 mL of dry THF. Reaction mixture was cooled to 0 ^{o}C in an ice-bath. Then, triethylamine (2.3 g, 23.1 mmol) was added to the reaction mixture and stirred for 15 minutes. Then, mesyl chloride (1.6 g, 13.8 mmol) diluted with 15 mL of dry THF was added drop wise through dropping funnel to the reaction mixture. Reaction mixture was maintained at 0-5 ^{o}C for 4h. After this, reaction mixture was added to 60 mL of distilled water and was extracted with ethyl acetate (50 mL x 3). Ethyl acetate layer was dried over Na_2SO_4 and evaporated under reduced pressure to obtain crude product which was purified by column chromatography over silica gel (mobile phase: ethyl acetate). Yield 3.35 g (90%).

Prepared mesylate compound (1.5 g, 3.7 mmol) was dissolved in 15 mL of anhydrous DMF followed by addition of sodium azide (0.3 g, 4.5 mmol). Reaction mixture was

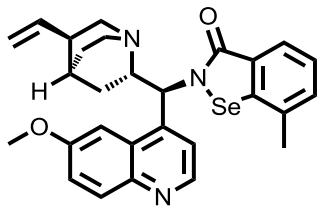
maintained at 60 ^{o}C for 20h. Then, reaction mixture was added into 80 mL of saturated aqueous sodium bicarbonate solution and stirred for 6h. Reaction mixture was extracted with ethyl acetate (40 mL x 3). Ethyl acetate layer was dried over Na_2SO_4 and evaporated under reduced pressure to give corresponding azide. Yield 1.10 g (85%).

Formed azide derivative (1.0 g, 2.86 mmol) was exposed to Staudinger reduction by treating with triphenyl phosphine (0.9 g, 3.4 mmol) in THF (25 mL). Reaction mixture was maintained at 60 ^{o}C for 4h followed by addition of water (7 mL). Then it was stirred for 10h at room temperature. Completion of reaction was monitored by TLC (mobile phase: ethyl acetate). The reaction mixture was concentrated *in vacuo* and the residue was partitioned between CH_2Cl_2 and 2N HCl (1:1, 80 mL). The mixture was vigorously shaken and the aqueous phase was separated and washed with CH_2Cl_2 (40 x 2 mL). The aqueous layer was basified with conc. NaOH solution and extracted with ethyl acetate (50 mL x 3). Ethyl acetate layer was dried over Na_2SO_4 and evaporated under reduced pressure to give corresponding amine. Yield 0.74 g (80%). ^{1}H NMR (400 MHz, $CDCl_3$) δ8.64 (d, *J* = 4.5 Hz, 1H), 7.94 (d, *J* = 9.2 Hz, 1H), 7.56 (s, 1H), 7.36 (s, 1H), 7.28 (dd, *J* = 9.2, 2.5 Hz, 1H), 5.70 (quintet, *J* = 8.8 Hz, 1H), 4.90 (m, 2H), 4.50 (s, 1H) 3.86 (s, 3H), 3.09 (m, 3H), 2.70 (m, 2H), 2.24 (m, 4H), 1.48 (m, 3H), 1.33 (t, *J* = 11.8 Hz, 1H) ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.6, 147.9, 147.1, 144.0, 141.7, 131.7, 128.8, 121.2, 119.9, 114.3, 101.9, 62.3, 56.3, 55.5, 40.9, 39.8, 29.6, 28.1, 27.5, 26.0. HRMS-ES^{+}*m/z*: 324.2078 (Calculated for $C_{20}H_{25}N_3O$ + H^{+}: 324.2070).



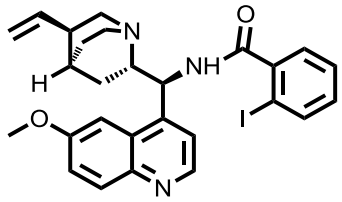
2-Iodo-N-((1S)-(6-methoxyquinolin-4-yl)((2S,4S,5R)-5-vinylquinuclidin-2-yl)methyl)-3-methylbenzamide (Substrate for 1b): In a 100 mL capacity round bottom flask, 2-iodo-3-

methylbenzoyl chloride (0.3 g, 1.0 mmol) was dissolved in 40 mL of dry dichloromethane. Reaction mixture was cooled to 0-5 ^{o}C. To this, quininamine (0.38 g, 1.1 mmol) and triethylamine (0.32 g, 3.2 mmol) in 40 mL of dry dichloromethane was added drop wise. Reaction mixture was maintained at room temperature for 3h and then poured in 50 mL of distilled water. After vigorous shaking, dichloromethane layer was separated, dried over Na_2SO_4 and then solvent was evaporated under reduced pressure at 40 ^{o}C to obtain light yellow solid. Yield 0.55 g (91%), mp above 225 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ8.72 (s, 1H), 8.02 (d, *J* = 9.2 Hz, 1H), 7.74 (bs, 1H), 7.45 (d, *J* = 4.1 Hz, 1H), 7.37 (dd, *J* = 9.2, 2.5 Hz, 1H), 7.25-7.15 (m, 3H), 7.01 (bs, 1H), 5.75-5.63 (m, 1H), 5.06-4.76 (m, 3H), 4.03- 3.89 (m, 3H), 3.28-3.17 (m, 2H), 2.83-2.58 (m, 4H), 2.42 (s, 3H), 2.32-2.25 (m, 1H), 1.72-1.54 (m, 4H) ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.1, 157.9, 147.8, 147.5, 144.8, 143.7, 142.7, 141.5, 141.2, 131.8, 130.3, 128.0, 125.2, 121.7, 118.9, 114.7, 102.3, 99.0, 56.0, 55.8, 53.4, 46.1, 41.3, 39.5, 29.1, 27.9, 27.4, 10.5. HRMS-ES^{+}*m/z*: 568.1468 (Calculated for $C_{28}H_{30}IN_3O_2 + H^{+}$: 568.1455).



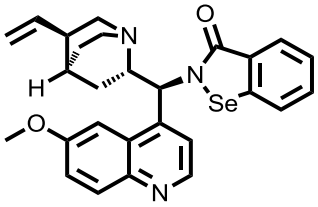
2-((1S)-(6-Methoxyquinolin-4-yl)((2S,4S,5R)-5-vinylquinuclidin-2-yl)methyl)-7-methylbenzo[d][1,2]selenazol-3(2H)-one (1b): Isoselenazolone **1b** was synthesized from 2-iodo-N-((1S)-(6-methoxyquinolin-4-yl)((2S,4S,5R)-5-vinylquinuclidin-2-yl)methyl)-3-methylbenzamide (0.4 g, 0.7 mmol), KO^{t}Bu (0.12 g, 1.05 mmol), selenium powder (67 mg, 0.8 mmol) in DMF (7 mL) and refluxed for 10h at 110 ^{o}C under nitrogen atmosphere. Progress of reaction was monitored by TLC. Standard workup gave dark brown colored oil, which was purified by column chromatography by using ethyl acetate over silica gel gave

brown solid. Yield 0.26 g (71%), mp decomposed after 155 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ8.78 (d, *J* = 4.4 Hz, 1H), 7.97 (d, *J* = 9.2 Hz, 2H), 7.81 (s, 1H), 7.38-7.23 (m, 4H), 6.38 (s, 1H), 5.94 (q, *J* = 8.4 Hz, 1H), 5.14-5.03 (m, 2H), 3.98 (s, 3H), 3.67-3.44 (m, 2H), 3.27 (t, *J* = 12.0 Hz, 1H), 2.84-2.67 (m, 2H), 2.38-2.28 (m, 1H), 2.2 (s, 3H), 2.03-1.79 (m, 3H), 1.68-1.49 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.6, 162.5, 158.5, 147.1, 144.9, 142.7, 141.6, 132.7, 131.9, 131.6, 127.3, 126.7, 126.1, 122.7, 118.5, 114.6, 101.8, 58.5, 56.0, 53.7, 41.6, 39.5, 36.4, 31.4, 29.7, 28.2, 27.6, 20.2. ^{77}Se NMR δ 835.1 ppm. HRMS-ES^{+}*m/z*: 520.1484 (Calculated for $C_{28}H_{29}N_3O_2Se + H^{+}$: 520.1499).



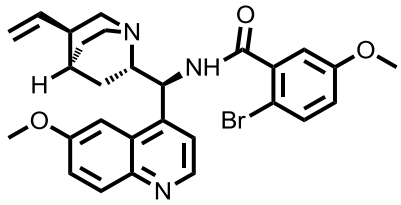
2-Iodo-N-((1S)-(6-methoxyquinolin-4-yl)((2S,4S,5R)-5-vinylquinuclidin-2-yl)methyl)benzamide (Substrate for 1c): In a 100 mL capacity round bottom flask, 2-iodobenzoyl chloride (0.34 g, 1.3 mmol) was dissolved in a 20 mL of dry dichloromethane. Reaction mixture was cooled to 0 ^{o}C. To this, quininamine (0.5 g, 1.5 mmol) and triethyl amine (0.4 g, 3.8 mmol) in 20 mL of dry dichloromethane was added drop wise. Reaction mixture was maintained at room temperature for 3h and then poured in 40 mL of distilled water. After vigorous shaking, dichloromethane layer was separated, dried over Na_2SO_4 and solvent was evaporated under reduced pressure at 40 ^{o}C to obtain light brown solid. Yield 0.65 g (92 %), mp 94-96 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ8.77 (s, 1H), 8.06 (d, *J* = 9.2 Hz, 1H), 7.80 (d, *J* = 7.5 Hz, 1H), 7.76 (s, 1H), 7.50 (s, 1H), 7.42 (d, *J* = 9.3 Hz, 1H), 7.33 (s, 2H), 7.20 (s, 1H) 7.09 (t, *J* = 6.1 Hz, 1H), 5.75 (quintet, *J* = 8.5 Hz, 1H), 5.0 (m, 2H), 4.01 (s, 3H), 3.25 (m, 3H), 2.74 (m, 3H), 2.74 (m, 3H), 2.32 (s, 2H), 1.70 (m, 3H), 1.52 (t, *J* = 11.0 Hz, 1H) ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.0, 157.8, 147.5, 144.9, 141.9, 141.2, 139.9,

135.3, 131.9, 131.04, 128.9, 128.4, 128.0, 121.6,115.0, 114.7, 102.2, 92.3, 56.0, 55.8, 45.97, 41.3, 39.3, 29.7, 27.9, 27.4, 26.3. HRMS-ES$^+$ *m/z*: 554.1300 (Calculated for $C_{27}H_{28}IN_3O_2$ + H^+: 554.1299).

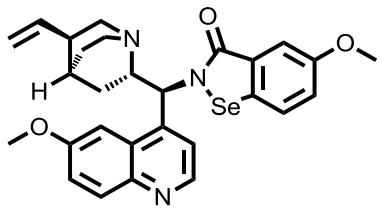


2-((1S)-(6-Methoxyquinolin-4-yl)((2S,4S,5R)-5-vinylquinuclidin-2-yl)methyl)benzo[d][1,2]selenazol-3(2H)-one (1c): In a 25 mL capacity round bottom flask DMF (7 mL) was taken followed by sequential addition of KO^{t}Bu (0.12 g, 1.1 mmol) and selenium powder (0.068 g, 0.9 mmol) at 0-5 ^{o}C. Then, reaction mixture was brought to room temperature and stirred for 15 minutes which resulted in a brownish-green colored solution of potassium *tert*-butoxyselenolate (KSeO^{t}Bu). After that, 2-iodo-N-((1S)-(6-methoxyquinolin-4-yl)((2S,4S,5R)-5-vinylquinuclidin-2-yl)methyl)benzamide (0.4 g, 0.7 mmol) was added in a lot and reaction mixture was refluxed at 110 ^{o}C for 20h. Progress of reaction was monitored by TLC. Reaction mixture was poured into saturated aqueous sodium bicarbonate solution (70 mL) and stirred for 3h. Product was extracted by ethyl acetate (30.0 mL x 3). Combined ethyl acetate layer was washed with distilled water (50 mL), dried over sodium sulphate and ethyl acetate was distilled under reduced pressure at 40 ^{o}C. Resulted dark brown colored oil was purified by column chromatography using ethyl acetate over silica gel. Yield 0.3 g (84%) mp 214-216 ^{o}C.^{1}H NMR (400 MHz, $CDCl_3$) δ8.77 (d, *J* = 4.5 Hz, 1H), 8.06-7.84 (m, 3H), 7.64-7.54 (m, 1H), 7.46 (t, *J* = 7.5 Hz, 1H), 7.39-7.27 (m, 3H), 6.49-6.25 (m, 1H), 6.04-5.79 (m, 1H), 5.20-5.01 (m, 2H), 3.97 (s, 3H), 3.79-3.55 (m, 2H), 3.28 (t, *J* = 12 Hz, 1H), 2.83-2.74 (m, 2H), 2.42-2.30 (m, 1H), 2.07-1.88 (m, 2H), 1.81-1.73 (m, 1H), 1.71-1.56 (m, 2H) ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.1, 166.9, 158.5, 147.1, 144.9, 142.9, 141.7, 139.1, 131.8,

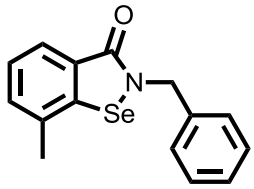
131.6, 128.8, 127.6, 126.0, 124.0, 122.8, 118.5, 114.6., 101.8, 58.6, 56.2, 56.0, 53.8, 41.5, 39.5, 29.7, 27.7, 27.6. ^{77}Se NMR δ 858.1 ppm. HRMS-ES^{+}*m*/*z*: 506.1352 (Calculated for $C_{27}H_{27}N_3O_2{}^{80}Se + H^+$: 506.1343).



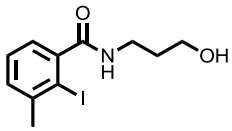
2-Bromo-5-methoxy-N-((1S)-(6-methoxyquinolin-4-yl)((2S,4S,5R)-5-vinylquinuclidin-2-yl)methyl)benzamide (Substrate for 1d): In a 100 mL capacity round bottom flask, 2-bromo-5-methoxybenzoyl chloride (0.4 g, 1.6 mmol) was dissolved in 30 mL of dry dichloromethane. Reaction mixture was cooled to 0-5 ^{o}C. To this, mixture of quininamine (0.6 g, 1.9 mmol) and triethyl amine (0.48 g, 4.8 mmol) diluted with 30 mL of dry dichloromethane was added drop wise. Then, Reaction mixture was maintained at room temperature for 3 hours and then poured in 50 mL of distilled water. After vigorous shaking, dichloromethane layer was separated, dried over Na_2SO_4 and then solvent was evaporated under reduced pressure at 40 ^{o}C to obtain light brown viscous oil. Yield 0.77 g (90%), ^{1}H NMR (400 MHz, $CDCl_3$) δ8.69 (d, *J* = 4.5 Hz, 1H), 7.98 (d, *J* = 9.2 Hz, 1H), 7.66 (s, 1H), 7.42 (d, *J* = 4.5 Hz, 1H), 7.38-7.30 (m, 2H),6.97 (s, 1H), 6.72 (dd, *J* = 8.8, 3.1 Hz, 1H), 5.65 (quintet, *J* = 8.6 Hz, 1H), 5.12-4.77 (m, 3H), 3.93 (s, 3H), 3.67 (s, 3H), 3.37-3.16 (m, 3H), 2.80-2.66 (m, 2H), 2.33-2.25 (m, 1H), 1.71-1.58 (m, 3H), 1.52-1.40 (m, 1H), 1.05 (s, 1H) ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 158.8, 157.8, 147.8, 147.6, 144.8, 141.5, 141.2, 138.1, 134.1, 131.7, 121.6, 117.7, 115.0, 114.7, 114.5, 109.5, 102.1, 56.0, 55.7, 55.6, 46.0, 41.1, 39.7, 39.5, 27.9, 27.5, 27.4. HRMS-ES^{+}*m*/*z*: 536.1538 (Calculated for $C_{28}H_{30}BrN_3O_3 + H^+$: 536.1543).



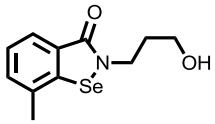
5-Methoxy-2-((1S)-(6-methoxyquinolin-4-yl)((2S,4S,5R)-5-vinylquinuclidin-2-yl)methyl)benzo[d][1,2]selenazol-3(2H)-one (1d): Isoselenazolone **1d** was synthesized from 2-bromo-5-methoxy-N-((1S)-(6-methoxyquinolin-4-yl)((2S,4S,5R)-5-vinylquinuclidin-2-yl)methyl)benzamide (0.5 g, 0.9 mmol), KO^{t}Bu (0.15 g, 1.35 mmol), selenium powder (85 mg, 1.08 mmol) in DMF (8 mL) and refluxed for 12h at 110 ^{o}C under nitrogen atmosphere. Progress of reaction was monitored by TLC. Standard workup gave dark brown colored oil, which was purified by column chromatography using ethyl acetate: hexane (9:1) over silica gel gave off white solid. Yield 0.35 g (70%), mp 190-192 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ8.77 (s, 1H), 8.05-7.85 (m, 2H), 7.45-7.30 (m, 4H), 7.15-7.02 (s, 1H), 6.50-6.20 (m, 1H), 6.05-5.80 (m, 1H), 5.20-5.0 (m, 2H), 4.0 (s, 3H), 3.80 (s, 3H), 3.60 (s, 2H), 3.27 (t, *J* = 12.0 Hz, 1H), 2.85-2.70 (m, 2H), 2.35 (s, 1H), 1.90 (s, 1H), 1.80-1.50 (m, 4H) ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.9, 158.8, 147.2, 144.9, 142.7, 141.4, 132.2, 132.1, 131.6, 128.6, 128.4, 124.9, 122.7, 121.7, 118.4, 114.8, 110.7, 101.8, 60.4, 58.8, 56.0, 55.6, 53.9, 41.6, 39.4, 31.9, 29.7, 27.6. ^{77}Se NMR δ 867.6 ppm. HRMS-ES$^+$ *m/z*: 536.1451



2-benzyl-7-methylbenzo[d][1,2]selenazol-3(2H)-one (1e):[1] Yield (85%), mp 74-76 °C.(74-76 °C).[1] Please see figures S29-S32 for characterization data.

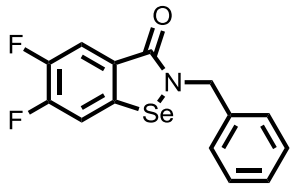


N-(3-hydroxypropyl)-2-iodo-3-methylbenzamide (Substrate for 1f): 2-Iodo-3-methylbenzoyl chloride (0.4 g, 1.4 mmol) was dissolved in dry CH_2Cl_2 (30 mL) in a single neck flask and cooled to 0 ^oC. 3-amino-1-propanol (0.13 g, 1.7 mmol) and triethylamine (0.42 g, 4.2 mmol) in 30 mL CH_2Cl_2 were slowly added to 2-iodo-3-methylbenzoyl chloride solution by dropping funnel. Resulted reaction mixture stirred for 1 h at 0 ^oC and 3 h at room temperature. After this water (50 mL) was added to reaction flask and stirred for 30 min. CH_2Cl_2 (50 mL) was added to reaction mixture and water layer separated by separating funnel. CH_2Cl_2 layer was washed with 10% HCl (25 mL), and then with water (25 mL). Dichloromethane layer dried over Na_2SO_4, evaporated on rotary evaporator under *vacuo*. Resulted solid was passed through silica gel using CH_2Cl_2 to obtain pure amide. Yield 0.42 g (92%). mp 88-90 °C.^{1}H NMR (400 MHz, $CDCl_3$) δ7.24-7.11 (m, 2H), 7.09-6.97 (m, 1H), 6.62-6.12 (m, 1H), 3.79-3.66 (m, 2H), 3.59-3.46 (m, 2H), 3.08 (bs, 1H), 2.43 (s, 3H), 1.80-1.70 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.5, 143.6, 143.0, 130.5, 128.1, 125.1, 99.3, 59.7, 36.9, 31.9, 29.2. HRMS-ES$^+$*m/z*: 320.0163 (Calculated for $C_{11}H_{14}INO_2$ + H^+: 320.0142).

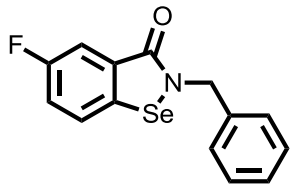


2-(3-hydroxypropyl)-7-methylbenzo[d][1,2]selenazol-3(2H)-one (1f): Isoselenazolone **1f** was synthesized from corresponding N-(3-hydroxypropyl)-2-iodo-3-methylbenzamide (0.4 g, 1.25 mmol), CuI (60 mg, 0.3 mmol), 1,10-phenanthroline (56 mg, 0.3 mmol), selenium powder (0.12 g, 1.5 mmol), and K_2CO_3 (0.52 g, 3.75 mmol) in DMF (7 mL) and refluxing for 24 h at 110^{o}C under nitrogen atmosphere. Progress of reaction was monitored by TLC. After

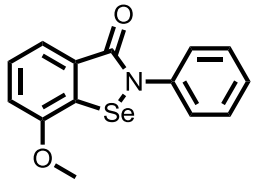
this, reaction mixture was poured over dilute HCl (40 mL) and stirred for 5 h. Product was extracted by using ethyl acetate (40.0 mL x 3). Combined ethyl acetate layer was washed with distilled water (40 mL x 2), dried over sodium sulphate and ethyl acetate was distilled under reduced pressure at 40^{o} C. resulted crude product was purified by column chromatography using [dichloromethane : methanol (95:5)] over silica gel to get colourless viscous oil. Yield 0.30 g (88%). ^{1}H NMR (400 MHz, $CDCl_3$) δ7.84-7.79 (m, 1H), 7.36-7.31 (m, 2H), 3.97 (t, *J* = 6.2 Hz, 2H) 2H), 3.88 (bs, 1H), 3.54 (t, *J* = 5.6 Hz, 2H), 2.30 (s, 3H), 1.84 (quartet, *J* = 6.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.8, 139.2, 132.9, 132.2, 127.1, 126.6, 126.2, 57.9, 41.3, 32.7, 20.4. ^{77}Se NMR δ 878.7 ppm. HRMS-ES^{+}*m/z*: 272.0207 (Calculated for $C_{11}H_{13}NO_2Se + H^{+}$: 272.0185).



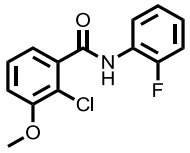
2-benzyl-5, 6-difluorobenzo[d][1,2]selenazol-3(2H)-one (1g):[1] Yield (85%), mp 187-188 °C(187-188 °C).[1]Please see figures S40-S43 for characterization data.



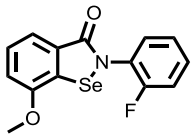
2-benzyl-5-fluorobenzo[d][1,2]selenazol-3(2H)-one (1h):[1]Yield (87%), mp 177-179°C.(177-179 °C).[1]Please see figures S44-S47 for characterization data.



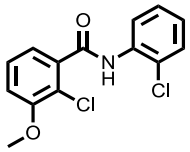
7-methoxy-2-phenylbenzo[d][1,2]selenazol-3(2H)-one (1i):[2] Yield (55%), mp 137-139°C.(138-141 °C).[2] Please see figures S48-S51 for characterization data.



2-Chloro-N-(2-fluorophenyl)-3-methoxybenzamide (Substrate for 1j): 2-Chloro-3-methoxybenzoyl chloride (0.5 g, 2.4 mmol) was dissolved in dry CH_2Cl_2 (25 mL) in a single neck flask and cooled to 0 ^oC. 2-Fluoro aniline (0.32 g, 2.9 mmol) and triethylamine (0.73 g, 7.2 mmol) in 40 mL CH_2Cl_2 were slowly added to 2-Chloro-3-methoxybenzoyl chloride solution by dropping funnel. Resulted reaction mixture stirred for 1 h at 0 ^oC and 3 h at room temperature. After this water (50 mL) was added to reaction flask and stirred for 30 min. CH_2Cl_2 (50 mL) was added to reaction mixture and water layer separated by separating funnel. CH_2Cl_2 layer was washed with 10% HCl (25 mL), and then with water (25 mL). Dichloromethane layer dried over Na_2SO_4, evaporated on rotary evaporator under *vacuo*. Resulted solid was passed through silica gel using CH_2Cl_2 to obtain pure amide. Yield 0.63 g (92%). mp 112-114 °C. ^1H NMR (400 MHz, $CDCl_3$) δ8.47 (t, J = 7.9 Hz, 1H), 8.05 (s, 1H), 7.35-7.27 (m, 2H), 7.21-7.15 (m, 1H), 7.12-7.07 (m, 2H), 7.06-7.01 (m, 1H), 3.93 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 155.5, 153.8, 151.4, 136.6, 128.0, 126.2, 126.1, 124.85, 124.77, 124.71, 124.68, 121.9, 121.4, 119.5, 115.0, 114.8, 113.9, 56.4. HRMS-ES$^+$ m/z: 280.0554 (Calculated for $C_{14}H_{11}ClFNO_2 + H^+$: 280.0535)

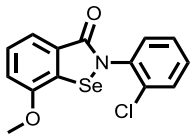


2-(2-Fluorophenyl)-7-methoxybenzo[d][1,2]selenazol-3(2H)-one (**1j**): Se-N heterocycle **1j** was synthesized from corresponding 2-chloro-N-(2-fluorophenyl)-3-methoxybenzamide (0.3 g, 1.0 mmol), CuI (100 mg, 0.5 mmol), 1,10-phenanthroline (95 mg, 0.5 mmol), selenium powder (0.1 g, 1.3 mmol), and K_2CO_3 (0.36 g, 2.6 mmol) in DMF (5 mL) and refluxing for 16 h at 110^{o}C under nitrogen atmosphere. Progress of reaction was monitored by TLC. After this, reaction mixture poured over brine solution (60 mL) and stirred for 3 h. Product was extracted by using ethyl acetate (40.0 mL x 3). Combined ethyl acetate layer was washed with distilled water (40 mL x 2), dried over sodium sulphate and ethyl acetate was distilled under reduced pressure at 40^{o} C. resulted light brown colored oil, which was purified by column chromatography using hexane : ethyl acetate (8:2) over silica gel gave white colored crystalline compound. Yield 0.24 g (71%). mp 140-142 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ7.7 (d, *J* = 7.7 Hz, 1H), 7.3-7.5 (m, 3H), 7.2 (m, 2H), 7.06 (d, *J* = 7.9 Hz, 1H), 3.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 130.0, 129.84, 129.76, 128.3, 128.2, 127.2, 126.2, 126.1, 124.63, 124.59, 121.3, 116.96, 116.77, 112.4, 56.2. ^{77}Se NMR δ 976.2 ppm. HRMS-ES^{+}*m/z*: 323.9947 (Calculated for $C_{14}H_{10}FNO_2{}^{80}Se + H^{+}$: 323.9934).



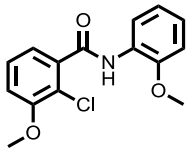
2-Chloro-N-(2-chlorophenyl)-3-methoxybenzamide (Substrate for 1k): 2-Chloro-3-methoxybenzoyl chloride (0.5 g, 2.4 mmol) was dissolved in dry CH_2Cl_2 (25 mL) in a single neck flask and cooled to 0 ^{o}C. 2-Chloro aniline (0.37 g, 2.9 mmol) and triethylamine (0.73 g, 7.2 mmol) in 40 mL CH_2Cl_2 were slowly added to 2-Chloro-3-methoxybenzoyl

chloridesolution by dropping funnel. Resulted reaction mixture stirred for 1 h at 0 ^{o}C and 3 h at room temperature. After this water (50 mL) was added to reaction flask and stirred for 30 min. CH_2Cl_2 (50 mL) was added to reaction mixture and water layer separated by separating funnel. CH_2Cl_2 layer was washed with 10% HCl (25 mL), and then with water (25 mL). Dichloromethane layer dried over Na_2SO_4, evaporated on rotary evaporator under *vacuo*. Resulted solid was passed through silica gel using CH_2Cl_2 to obtain pure amide. Yield 0.68 g (95%). mp 126-128 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ8.55 (t, *J* = 8.2 Hz, 1H), 8.32 (s, 1H), 7.41-7.36 (m, 1H), 7.35-7.27 (m, 3H), 7.11-7.02 (m, 2H), 3.93 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 155.5, 136.7, 134.5, 129.1, 128.0, 127.8, 125.1, 123.1, 121.8, 121.4, 119.6, 113.9, 56.4. HRMS-ES^{+}*m/z*: 296.0252 (Calculated for $C_{14}H_{11}Cl_2NO_2$ + H^{+}: 296.0240)

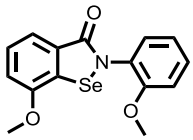


2-(2-Chlorophenyl)-7-methoxybenzo[d][1,2]selenazol-3(2H)-one (**1k**): Se-N heterocycle **1k** was synthesized from corresponding 2-chloro-N-(2-chlorophenyl)-3-methoxybenzamide(0.4 g, 1.3 mmol), CuI (130 mg, 0.7 mmol), 1,10-phenanthroline (120 mg, 0.7 mmol), selenium powder (0.13 g, 1.6 mmol), and K_2CO_3 (0.47 g, 3.4 mmol) in DMF (7 mL) and refluxing for 16 h at 110^{o}C under nitrogen atmosphere. Progress of reaction was monitored by TLC. After this, reaction mixture poured over brine solution (80 mL) and stirred for 3 h. Product was extracted by using ethyl acetate (50.0 mL x 3). Combined ethyl acetate layer was washed with distilled water (50 mL x 2), dried over sodium sulphate and ethyl acetate was distilled under reduced pressure at 40^{o} C. resulted light brown colored oil, which was purified by column chromatography using hexane : ethyl acetate (8:2) over silica gel gave white colored crystalline compound. Yield 0.35 g (76%). mp 176-178 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ7.7 (d, *J* = 7.8 Hz, 1H), 7.4-7.52 (m, 2H), 7.34 (m, 2H), 7.07 (d, *J* = 7.95

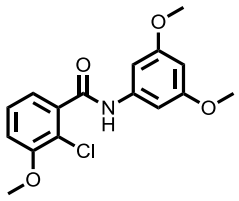
Hz, 2H), 3.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 153.8, 135.9, 133.9, 131.0, 130.7, 130.0, 128.3, 127.7, 127.2, 121.3, 112.4, 56.2. ^{77}Se NMR δ 966.7 ppm. HRMS-ES$^+$*m/z*: 339.9651 (Calculated for $C_{14}H_{10}ClNO_2{}^{80}Se + H^+$: 339.9636).



2-Chloro-3-methoxy-N-(2-methoxyphenyl) benzamide (Substrate for 1l): 2-Chloro-3-methoxybenzoyl chloride (0.5 g, 2.4 mmol) was dissolved in dry CH_2Cl_2 (25 mL) in a single neck flask and cooled to 0 ^{o}C. 2-Methoxy aniline (0.35 g, 2.9 mmol) and triethylamine (0.73 g, 7.2 mmol) in 40 mL CH_2Cl_2 were slowly added to 2-Chloro-3-methoxybenzoyl chloride solution by dropping funnel. Resulted reaction mixture stirred for 1 h at 0 ^{o}C and 3 h at room temperature. After this water (50 mL) was added to reaction flask and stirred for 30 min. CH_2Cl_2 (50 mL) was added to reaction mixture and water layer separated by separating funnel. CH_2Cl_2 layer was washed with 10% HCl (25 mL), and then with water (25 mL). Dichloromethane layer dried over Na_2SO_4, evaporated on rotary evaporator under *vacuo*. Resulted solid was passed through silica gel using CH_2Cl_2 to obtain pure amide. Yield 0.65 g (92%). mp 108-110 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ8.53 (d, *J* = 8.0 Hz, 1H), 8.41 (s, 1H), 7.35-7.25 (m, 2H), 7.11-6.97 (m, 3H), 6.89 (d, *J* = 8.1 Hz, 1H), 3.93 (s, 3H), 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 155.4, 148.2, 137.5, 127.8, 127.6, 124.2, 121.4, 121.2, 120.0, 119.6, 113.5, 110.1, 56.5, 55.8. HRMS-ES$^+$*m/z*: 292.0745 (Calculated for $C_{15}H_{14}ClNO_3 + H^+$: 292.0735)

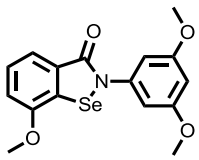


7-Methoxy-2-(2-methoxyphenyl)benzo[d][1,2]selenazol-3(2H)-one (**1l**): Se-N heterocycle **1l** was synthesized from corresponding 2-chloro-3-methoxy-N-(2-methoxyphenyl)benzamide (0.3 g, 1.0 mmol), CuI (98 mg, 0.5 mmol), 1,10-phenanthroline (93 mg, 0.5 mmol), selenium powder (0.097 g, 1.2 mmol), and K_2CO_3 (0.36 g, 2.6 mmol) in DMF (5 mL) and refluxing for 12 h at 110^{o}C under nitrogen atmosphere. Progress of reaction was monitored by TLC. After this, reaction mixture poured over brine solution (60 mL) and stirred for 3 h. Product was extracted by using ethyl acetate (40.0 mL x 3). Combined ethyl acetate layer was washed with distilled water (40 mL x 2), dried over sodium sulphate and ethyl acetate was distilled under reduced pressure at 40^{o} C. resulted light brown colored oil, which was purified by column chromatography using hexane : ethyl acetate (8:2) over silica gel gave white colored crystalline compound. Yield 0.21 g (61%). mp 151-153 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ7.75 (d, *J* = 7.7 Hz, 1H), 7.5 (m, 3H), 7.05 (m, 3H), 4.0 (s, 3H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 155.4, 154.2, 129.9, 129.6, 128.5, 127.93, 127.87, 127.13, 121.2, 120.8, 112.3, 112.0, 56.2, 30.1. ^{77}Se NMR δ 958.7 ppm. HRMS-ES^{+}*m/z*: 336.0147 (Calculated for $C_{15}H_{13}NO_3{}^{80}Se + H^{+}$: 336.0134).



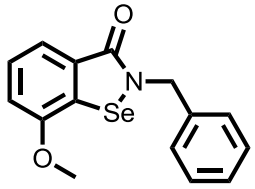
2-Chloro-N-(3, 5-dimethoxyphenyl)-3-methoxybenzamide (Substrate for 1m): 2-Chloro-3-methoxybenzoyl chloride (0.5 g, 2.4 mmol)was dissolved in dry CH_2Cl_2 (25 mL) in a single neck flask and cooled to 0 ^{o}C. 3, 5-Dimethoxy aniline (0.44 g, 2.9 mmol) and

triethylamine (0.73 g, 7.2 mmol) in 40 mL CH_2Cl_2 were slowly added to 2-Chloro-3-methoxybenzoyl chloride solution by dropping funnel. Resulted reaction mixture stirred for 1 h at 0 ^oC and 3 h at room temperature. After this water (50 mL) was added to reaction flask and stirred for 30 min. CH_2Cl_2 (50 mL) was added to reaction mixture and water layer separated by separating funnel. CH_2Cl_2 layer was washed with 10% HCl (25 mL), and then with water (25 mL). Dichloromethane layer dried over Na_2SO_4, evaporated on rotary evaporator under *vacuo*. Resulted solid was passed through silica gel using CH_2Cl_2 to obtain pure amide. Yield 0.75 g (96%). mp 52-54 °C. ^1H NMR (400 MHz, $CDCl_3$) δ7.81 (s, 1H), 7.30-7.15 (m, 2H), 6.98 (d, *J* = 8.0 Hz, 1H), 6.86 (d, *J* = 2.0 Hz, 2H), 6.26 (t, *J* = 2.1 Hz, 1H), 3.90 (s, 3H), 3.77 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.7, 161.1, 155.4, 139.4, 137.1, 127.9, 121.1, 119.3, 113.6, 98.2, 97.2, 56.5, 55.4. HRMS-ES$^+$ *m/z*: 322.0854 (Calculated for $C_{16}H_{16}ClNO_4 + H^+$: 322.0841).

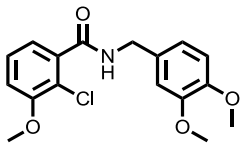


2-(3,5-Dimethoxyphenyl)-7-methoxybenzo[d][1,2]selenazol-3(2H)-one (**1m**): Se-N heterocycle **1m** was synthesized from corresponding 2-chloro-N-(3,5-dimethoxyphenyl)-3-methoxybenzamide (0.35 g, 1.1 mmol), CuI (104 mg, 0.55 mmol), 1,10-phenanthroline (98 mg, 0.55 mmol), selenium powder (0.103 g, 1.3 mmol), and K_2CO_3 (0.38 g, 2.7 mmol) in DMF (6 mL) and refluxing for 16 h at 110^oC under nitrogen atmosphere. Progress of reaction was monitored by TLC. After this, reaction mixture poured over brine solution (80 mL) and stirred for 3 h. Product was extracted by using ethyl acetate (40.0 mL x 3). Combined ethyl acetate layer was washed with distilled water (40 mL x 2), dried over sodium sulphate and ethyl acetate was distilled under reduced pressure at 40^o C. resulted light brown colored oil, which was purified by column chromatography using hexane : ethyl acetate (8:2) over silica

gel gave white colored crystalline compound. Yield 0.26 g (65%). mp 88-90 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ7.72 (d, *J* = 7.8 Hz, 1H), 7.46 (t, *J* = 7.9 Hz, 2H), 7.09 (m, 1H), 6.9 (d, *J* = 2.2 Hz, 2H), 6.4 (t, *J* = 2.2 Hz, 1H), 4.0 (s, 3H), 3.84 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.0, 161.1, 154.1, 141.0, 129.1, 128.3, 127.0, 121.1, 112.3, 103.5, 99.2, 56.0, 55.5. ^{77}Se NMR δ 947.6 ppm. HRMS-ES^{+}*m/z*: 366.0237 (Calculated for $C_{16}H_{15}NO_4{}^{80}Se$ + H^{+}: 366.0240).



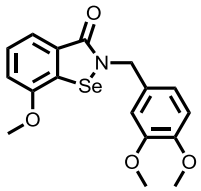
2-benzyl-7-methoxybenzo[d][1,2]selenazol-3(2H)-one (1n):[2] Yield 67%, mp 66-68 °C (66-68 °C).[2] Please see figures S80-S83 for characterization data.



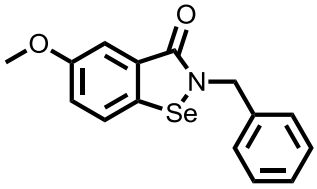
2-Chloro-N-(3,4-dimethoxybenzyl)-3-methoxybenzamide (Substrate for 1o):

2-Chloro-3-methoxybenzoyl chloride (0.3 g, 1.5 mmol) was dissolved in dry CH_2Cl_2 (20 mL) in a single neck flask and cooled to 0 ^{o}C. (3,4-dimethoxyphenyl)methanamine (0.29 g, 1.7 mmol) and triethylamine (0.45 g, 4.5 mmol) in 30 mL CH_2Cl_2 were slowly added to 2-Chloro-3-methoxybenzoyl chloride solution by dropping funnel. Resulted reaction mixture stirred for 1 h at 0 ^{o}C and 3 h at room temperature. After this water (50 mL) was added to reaction flask and stirred for 30 min. CH_2Cl_2 (50 mL) was added to reaction mixture and water layer separated by separating funnel. CH_2Cl_2 layer was washed with 10% HCl (25 mL), and then with water (25 mL). Dichloromethane layer dried over Na_2SO_4, evaporated on rotary evaporator under *vacuo*. Resulted solid was passed through silica gel using CH_2Cl_2 to

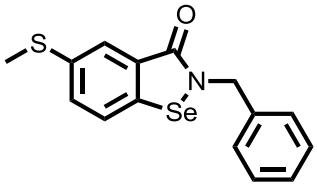
obtain pure amide. Yield 0.46 g (94%). mp 126-128 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ7.23 (t, *J* = 8.0 Hz, 1H), 7.17-7.09 (m, 1H), 6.94 (d, *J* = 8.1 Hz, 1H), 6.90 (s, 1H), 6.88-6.83 (m, 1H), 6.81-6.77 (m, 1H), 6.36 (s, 1H), 4.55 (d, *J* = 5.7 Hz, 2H), 3.87 (s, 3H), 3.84 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 155.3, 149.2, 148.5, 137.0, 130.3, 127.8, 121.1, 120.1, 119.3, 113.3, 111.2, 111.1, 56.4, 55.94, 55.89, 43.5. HRMS-ES^{+}*m/z*: 336.1009 (Calculated for $C_{17}H_{18}ClNO_4 + H^{+}$: 336.0997).



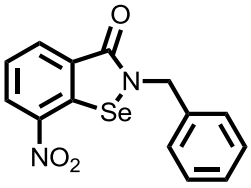
2-(3,4-Dimethoxybenzyl)-7-methoxybenzo[d][1,2]selenazol-3(2H)-one (**1o**): Se-N heterocycle **1o** was synthesized from corresponding 2-chloro-N-(3,4-dimethoxybenzyl)-3-methoxybenzamide (0.4 g, 1.2 mmol), CuI (113 mg, 0.6 mmol), 1,10-phenanthroline (107 mg, 0.6 mmol), selenium powder (0.113 g, 1.4 mmol), and K_2CO_3 (0.41 g, 3.0 mmol) in DMF (8 mL) and refluxing for 24 h at 110^{o}C under nitrogen atmosphere. Progress of reaction was monitored by TLC. After this, reaction mixture was poured over brine solution (80 mL) and stirred for 3 h. Product was extracted by using ethyl acetate (40.0 mL x 3). Combined ethyl acetate layer was washed with distilled water (40 mL x 2), dried over sodium sulphate and ethyl acetate was distilled under reduced pressure at 40^{o} C. resulted light brown colored oil, which was purified by column chromatography using hexane : ethyl acetate (6:4) over silica gel gave light brown heavy oil. Yield 0.39 g (86%).^{1}H NMR (400 MHz, $CDCl_3$) δ7.63 (d, *J* = 7.8 Hz, 1H), 7.36 (t, *J* = 7.8 Hz, 1H), 6.9 (m, 4H), 4.9 (s, 2H), 3.85 (d, *J* = 4.8 Hz, 6H), 3.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.3, 154.3, 149.3, 149.2, 129.8, 129.0, 127.9, 127.5, 121.2, 120.5, 111.8, 111.6, 111.0, 55.93, 55.88, 55.86, 43.8. ^{77}Se NMR δ 862.4 ppm. HRMS-ES^{+}*m/z*: 380.0396 (Calculated for $C_{17}H_{17}NO_4{}^{80}Se + H^{+}$: 380.0396).



2-benzyl-5-methoxybenzo[d][1,2]selenazol-3(2H)-one (1p):[2] Yield 76%, mp 124-126 °C (124-126 °C).[2] Please see figures S91-S94 for characterization data.



2-benzyl-5-(methylthio) benzo[d][1,2]selenazol-3(2H)-one (1q):[2] Yield 35%, mp 138-140 °C (139-141 °C).[2] Please see figures S95-S98 for characterization data.



2-benzyl-7-nitrobenzo[d][1,2]selenazol-3(2H)-one (1r):[1] Yield 87%, mp 110-112 °C (110-111 °C).[1] Please see figures S99-S102 for characterization data.

^{77}Se NMR study of isoselenazolone 1b and intermediates 2b, 3b and 5b

^{77}Se is a very sensitive NMR active nucleus and it is easily influenced by the chemical environment. Moreover, isoselenazolones and all other intermediates, i.e. RSeSPh, RSeH, RSeOH are expected to show large differences in their chemical shift values. Therefore, ^{77}Se NMR technique was used for mechanistic investigation. Stock solution for PhSH was made by dissolving 200 mg of PhSH in 10 mL of CD_3OD.

Isoselenazolone 1b: In a clean and dry NMR tube isoselenazolone **1b** was dissolved in 0.6 mL of deuterated methanol and resulting solution was monitored for 15 hours by ^{77}Se NMR spectroscopy. A peak was observed at 851 ppm (See Figure S106)

Reaction of isoselenazolone 1b with one equivalent of PhSH: In a clean and dry NMR tube **1b** (30 mg, 0.06 mmol) was dissolved in 0.3 mL CD_3OD. To that PhSH (0.3 mL in CD_3OD, 0.06 mmol) was added in a lot. NMR tube was shaken well and resulting solution was monitored for 10 hours by ^{77}Se NMR spectroscopy. A peak was observed at -0.3 ppm (See Figure S107).

Reaction of isoselenazolone 1b with two equivalent of PhSH: In a NMR tube containing **1b** (30 mg, 0.06 mmol), solution of PhSH (0.6 mL, 0.12 mmol) in deuterated methanol was added and ^{77}Se NMR was recorded with 10000 scans. A peak was observed at 4.8 ppm (See Figure S109)

Detection of selenenic acid intermediate 5b: Isoselenazolone **1b**, PhSH and H_2O_2 were mixed in a (1:2:1) stoichiometry in CD_3OD and NMR spectrum was recorded for 10 hours. Peaks observed at 1093 ppm and 851 ppm (See Figures S115-S116)

Mass spectrometry study of isoselenazolone 1b and intermediates 2b, 3b and 5b

Isoselenazolone **1b** and intermediates **2b**, **3b** and **5b** were analysed by mass (LCMS) spectrometry. HPLC grade methanol was used as solvent medium for experiments. All the experiments were performed by direct injection method in ESI mode.

Isoselenazolone 1b: Freshly prepared solution of **1b** in methanol was analysed by mass spectrometry and peak observed at *m*/*z*: 520.1484(Calculated for $C_{28}H_{29}N_3O_2Se + H^+$) (See Figure S14)

Reaction of isoselenazolone 1b with one equivalent of PhSH: A freshly prepared (1:1) mixture of **1b** and PhSH in methanol was analysed mass spectrometrically and peaks were observed at *m*/*z*: 630.1726 (Calculated for $C_{34}H_{35}N_3O_2SSe + H^+$) and *m*/*z*: 520.1540 (Calculated for $C_{28}H_{31}N_3O_2Se - H^+$) attributed to selenenylsulfide **2b** and selenol **3b** respectively. (See Figure S108)

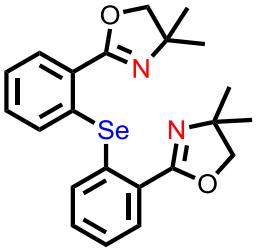
Reaction of isoselenazolone 1b with two equivalent of PhSH: A freshly prepared (1:2) mixture of **1b** and PhSH in methanol was analysed mass spectrometrically and peaks were observed at *m*/*z*: 520.1546 (Calculated for $C_{28}H_{31}N_3O_2Se - H^+$) attributed to selenol **3b**. (See Figure S110)

Reaction of isoselenazolone 1b with two equivalent of PhSH and one equivalent of hydrogen peroxide: A freshly prepared (1:2:1) mixture of **1b**, PhSH and H_2O_2 in methanol was analysed mass spectrometrically and peaks were observed at *m*/*z*: 536.1489 (Calculated for $C_{28}H_{31}N_3O_2Se- H^+$) attributed to selenenic acid **5b**. (See Figure S117)

^{77}Se NMR and mass spectrometric study of methyl selenide obtained by reaction of 1b, two equivalent of PhSH and excess of methyl iodide:

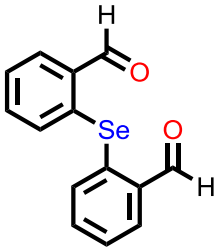
Isoselenazolone **1b** (30 mg, 0.06 mmol) and solution of PhSH (0.6 mL, 0.12 mmol) in deuterated methanol was mixed thoroughly. To this freshly prepared solution, excess of methyl iodide (24 mg, 0.17 mmol) was added in a lot. Resulted reaction mixture was shaken well and monitored by ^{77}Se NMR spectroscopy for 10 hours. A peak was observed at 124.8 ppm (See Figure S113). Similarly, mass spectrometric analysis in methanol gave peak at *m*/*z*: 536.1930 (Calculated for $C_{29}H_{33}N_3O_2Se + H^+$) attributed to methyl selenide. (See Figure S114).

^{77}Se NMR chemical shift comparison for organoselenium analogues having Se…X (X= N or O) interaction either via conjugation or non-conjugation with each other[4]



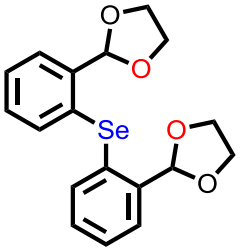
1.1

420 ppm



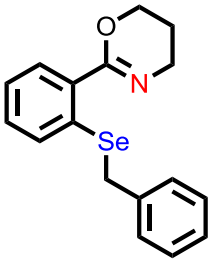
1.2

393 ppm



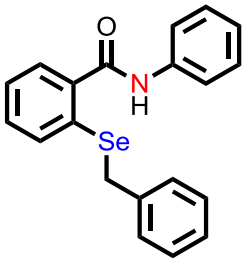
1.3

321 ppm



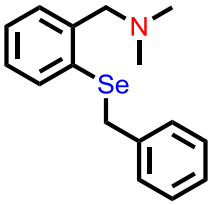
2.1

362 ppm



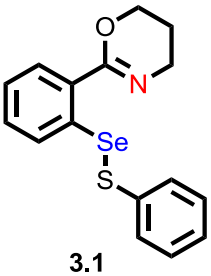
2.2

377 ppm



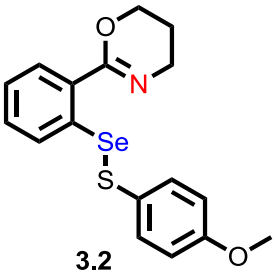
2.3

321 ppm



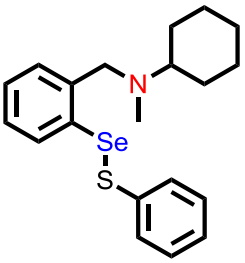
3.1

625 ppm



3.2

660 ppm



3.3

571.5 ppm

Figure S1 ^{1}H NMR of **1a**

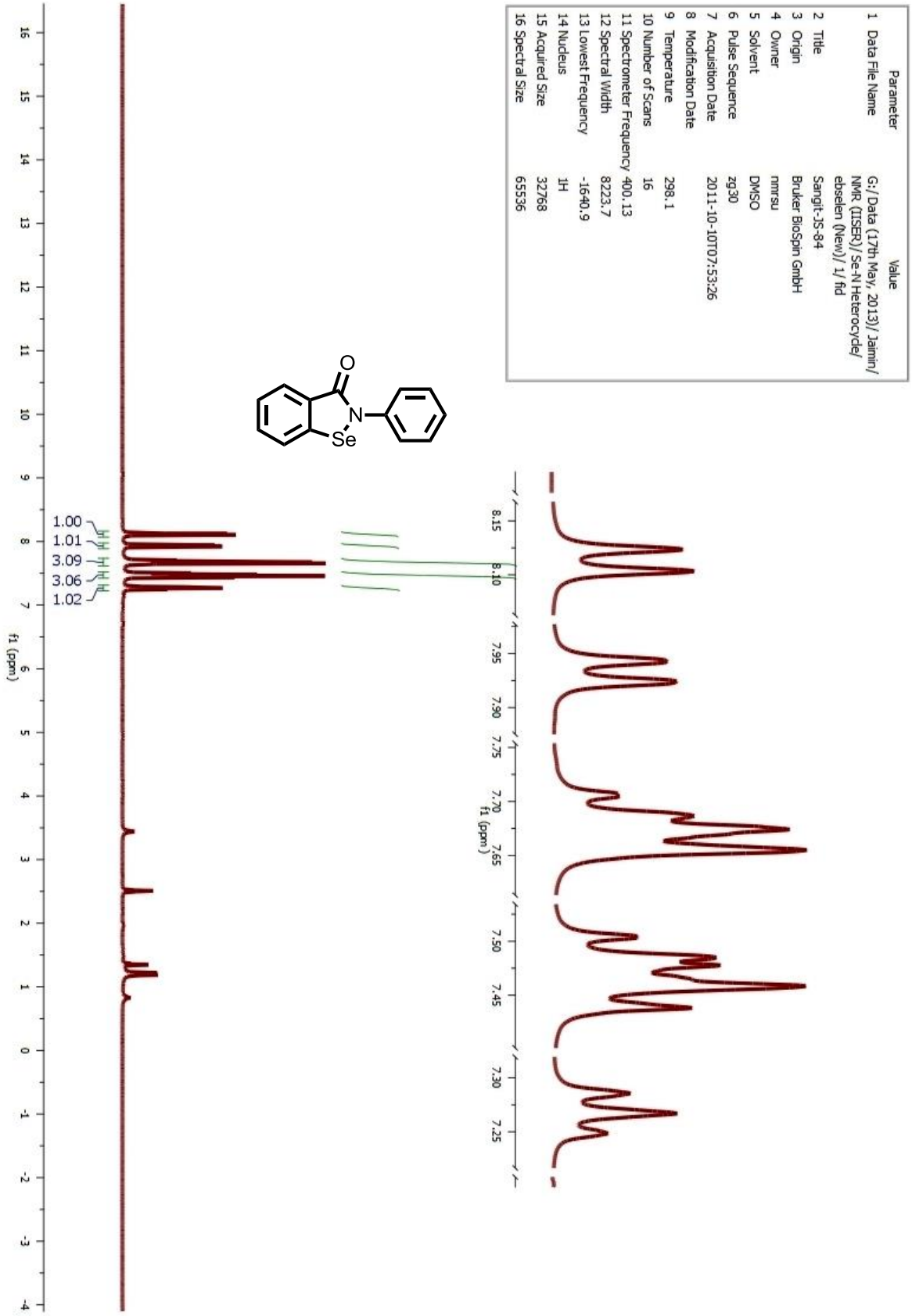


Figure S2 ^{13}C NMR for **1a**

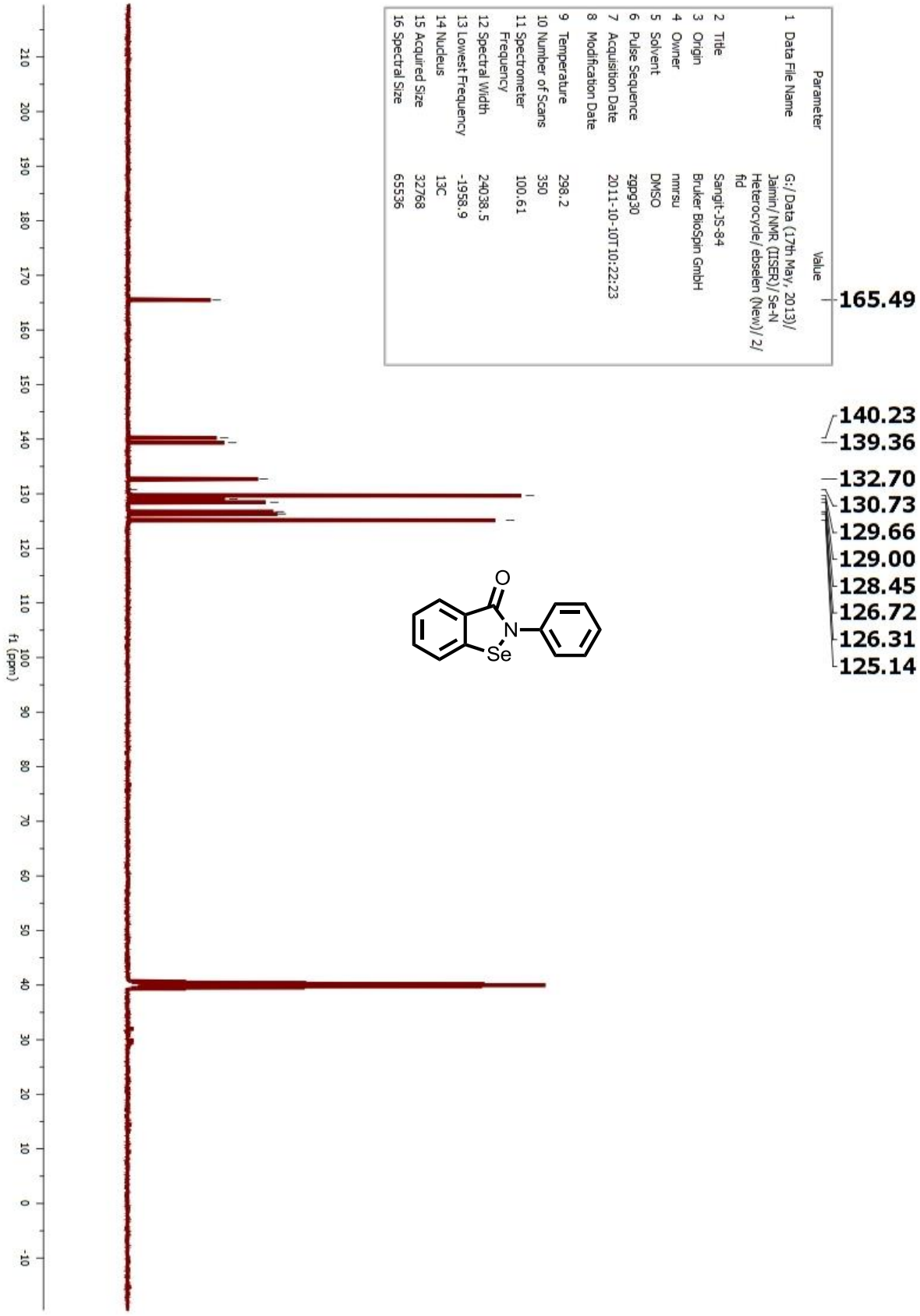


Figure S3 ^{77}Se NMR for **1a**

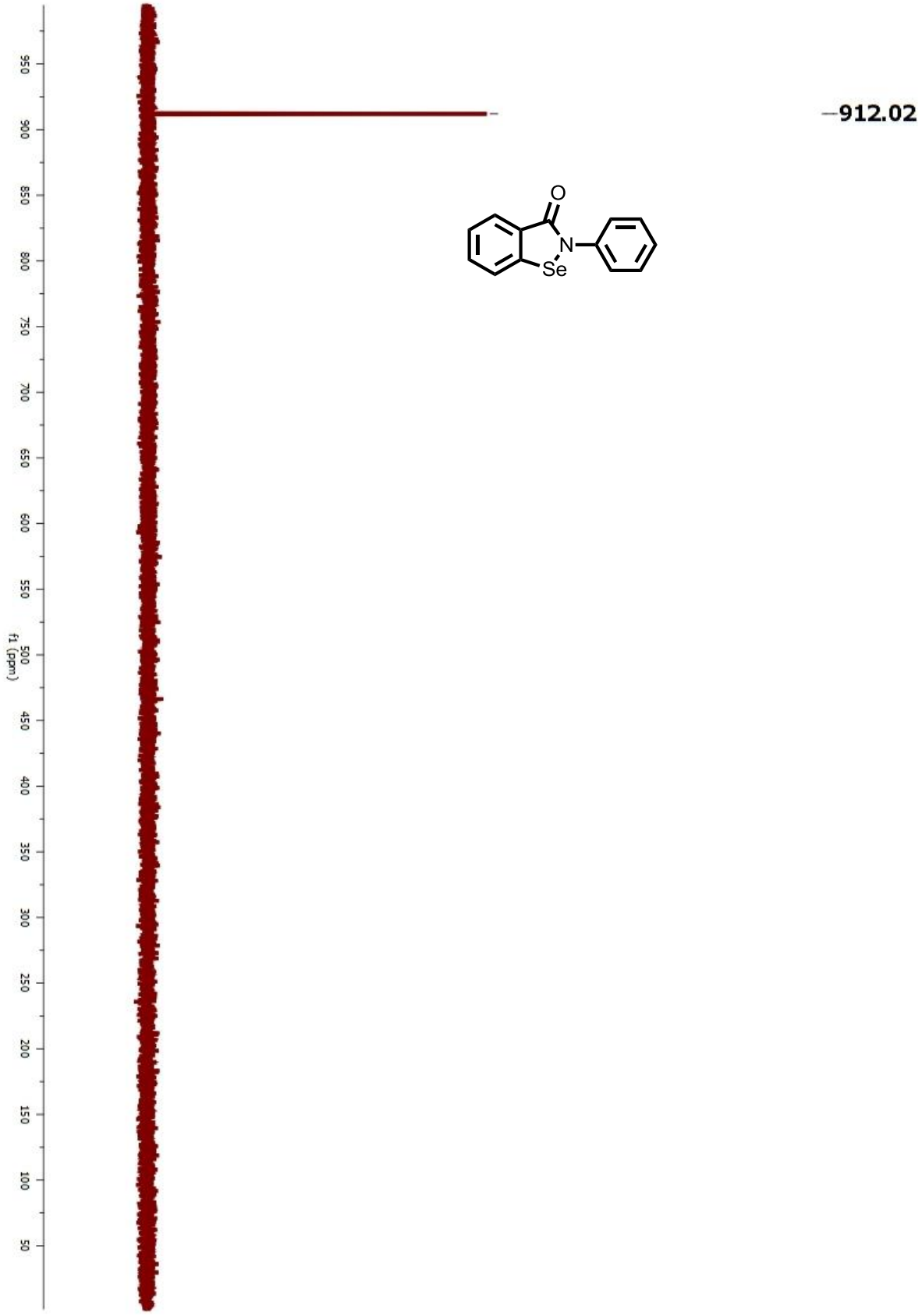


Figure S4 HRMS (ESI) spectrum of **1a**

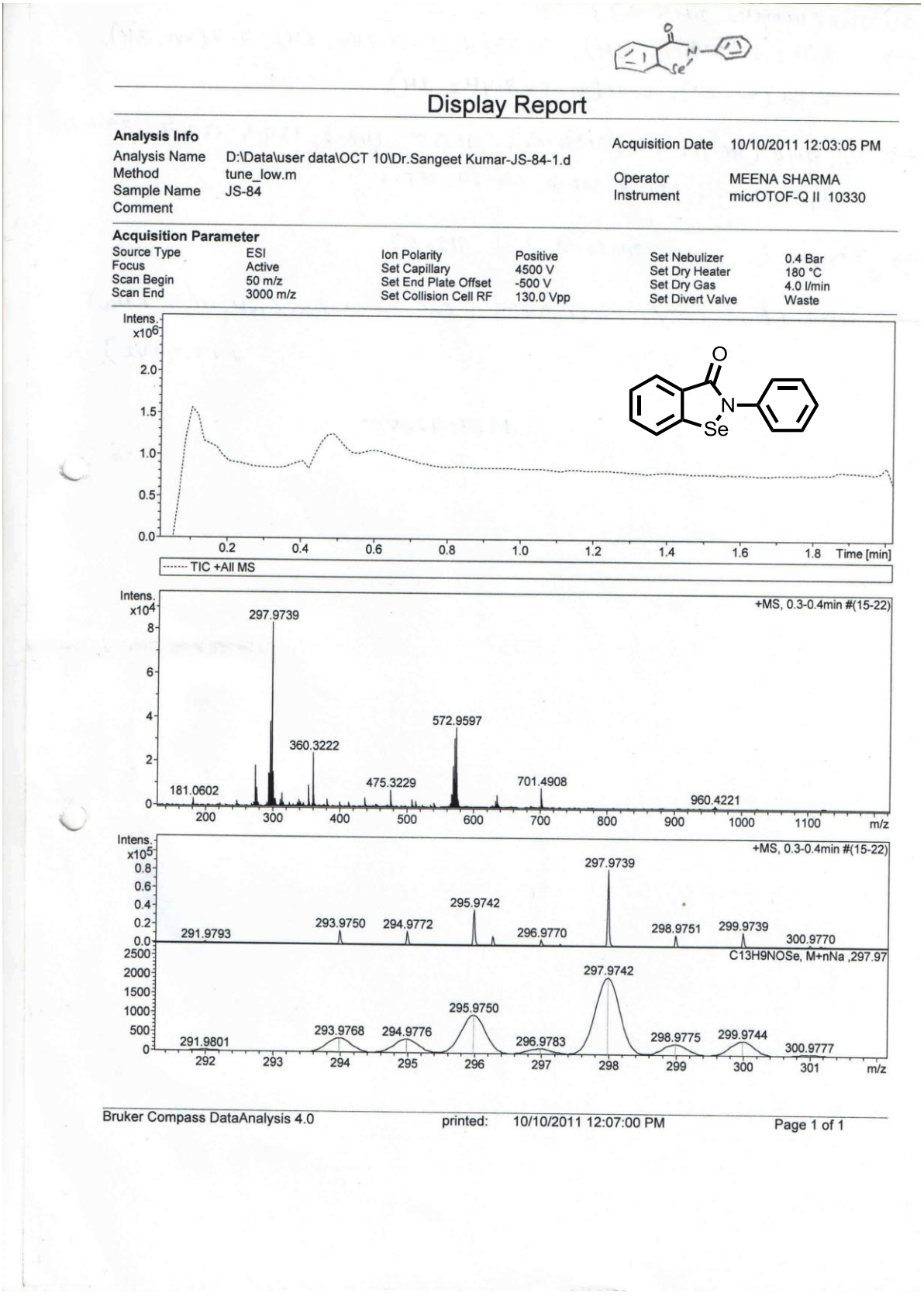


Figure S5 ^{1}H NMR of (1S)-(6-methoxyquinolin-4-yl)((2S,4S,5R)-5-vinylquinuclidin-2-yl)methanamine

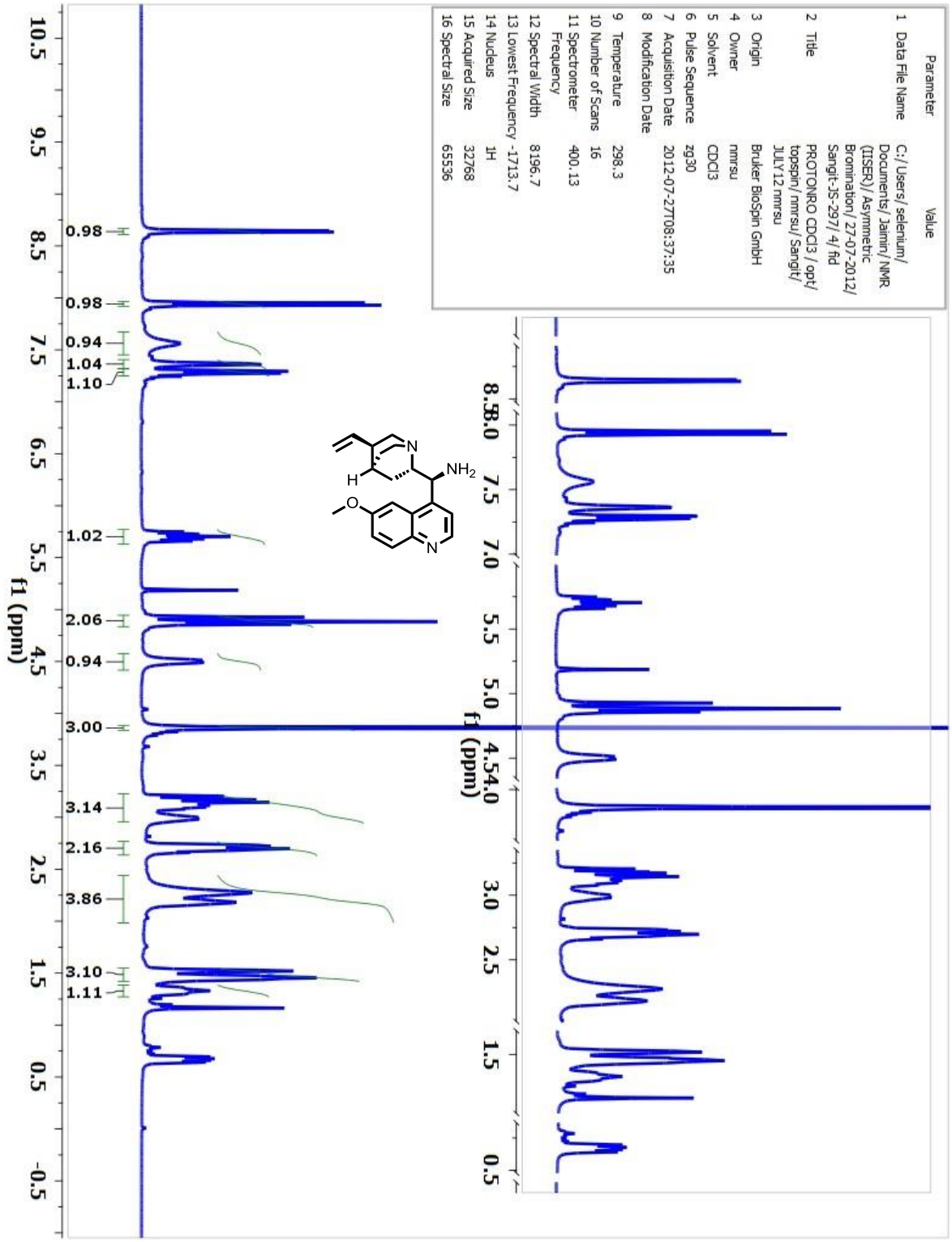


Figure S6 ^{13}C NMR of (1S)-(6-methoxyquinolin-4-yl)((2S,4S,5R)-5-vinylquinuclidin-2-yl)methanamine

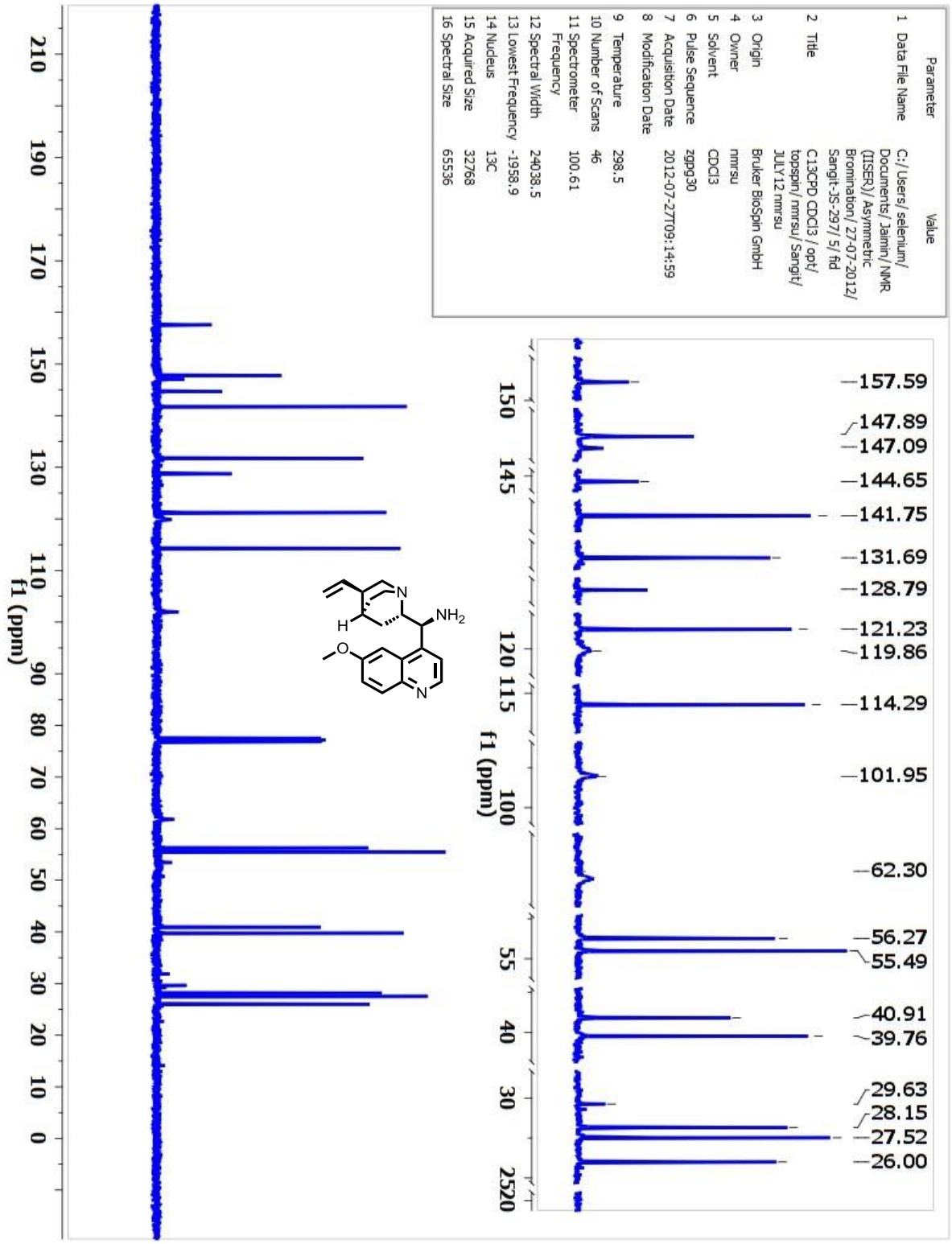


Figure S7 HRMS (ESI) of (1S)-(6-methoxyquinolin-4-yl)((2S,4S,5R)-5-vinylquinuclidin-2-yl)methanamine

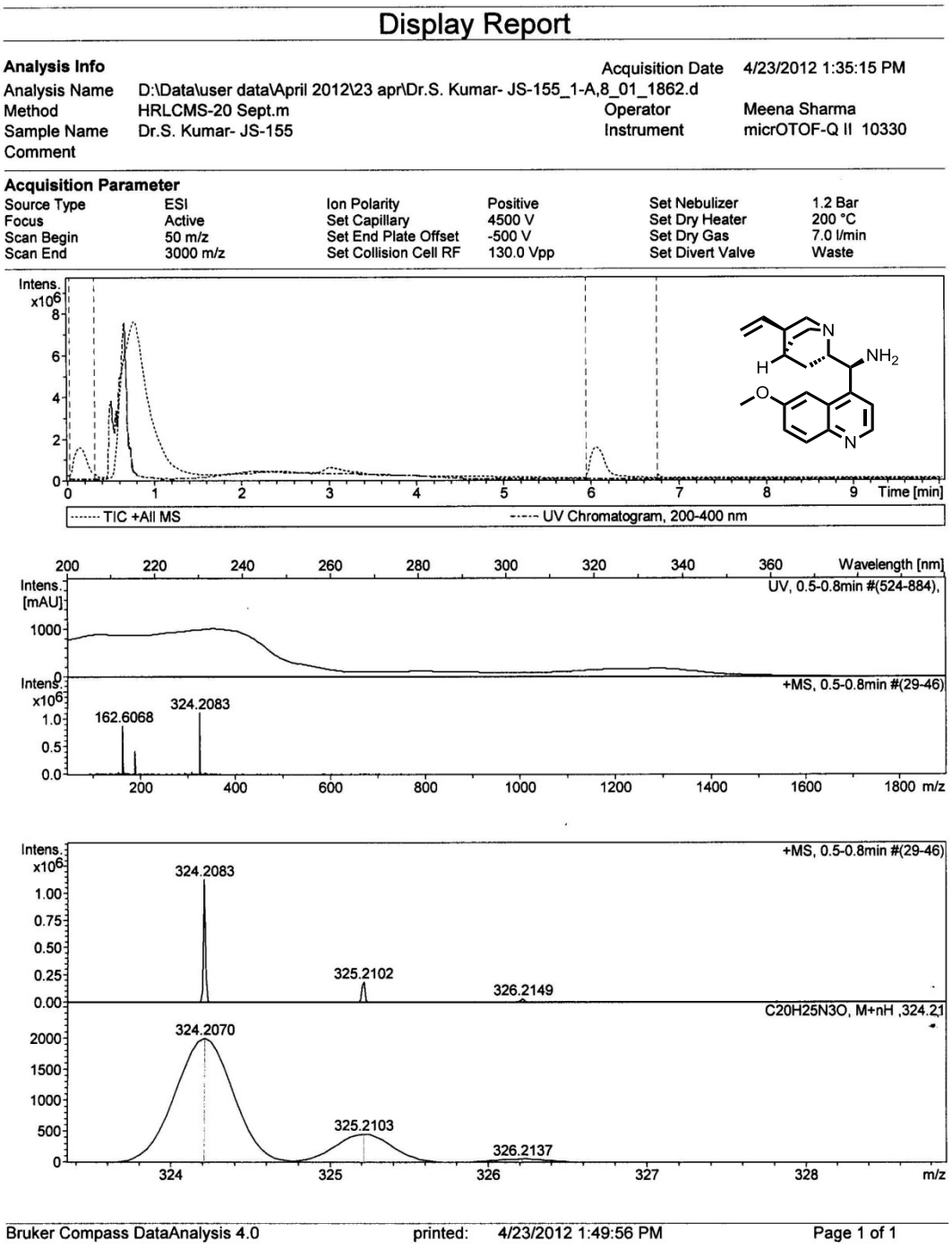


Figure S8 ^{1}H NMR of precursor of **1b**

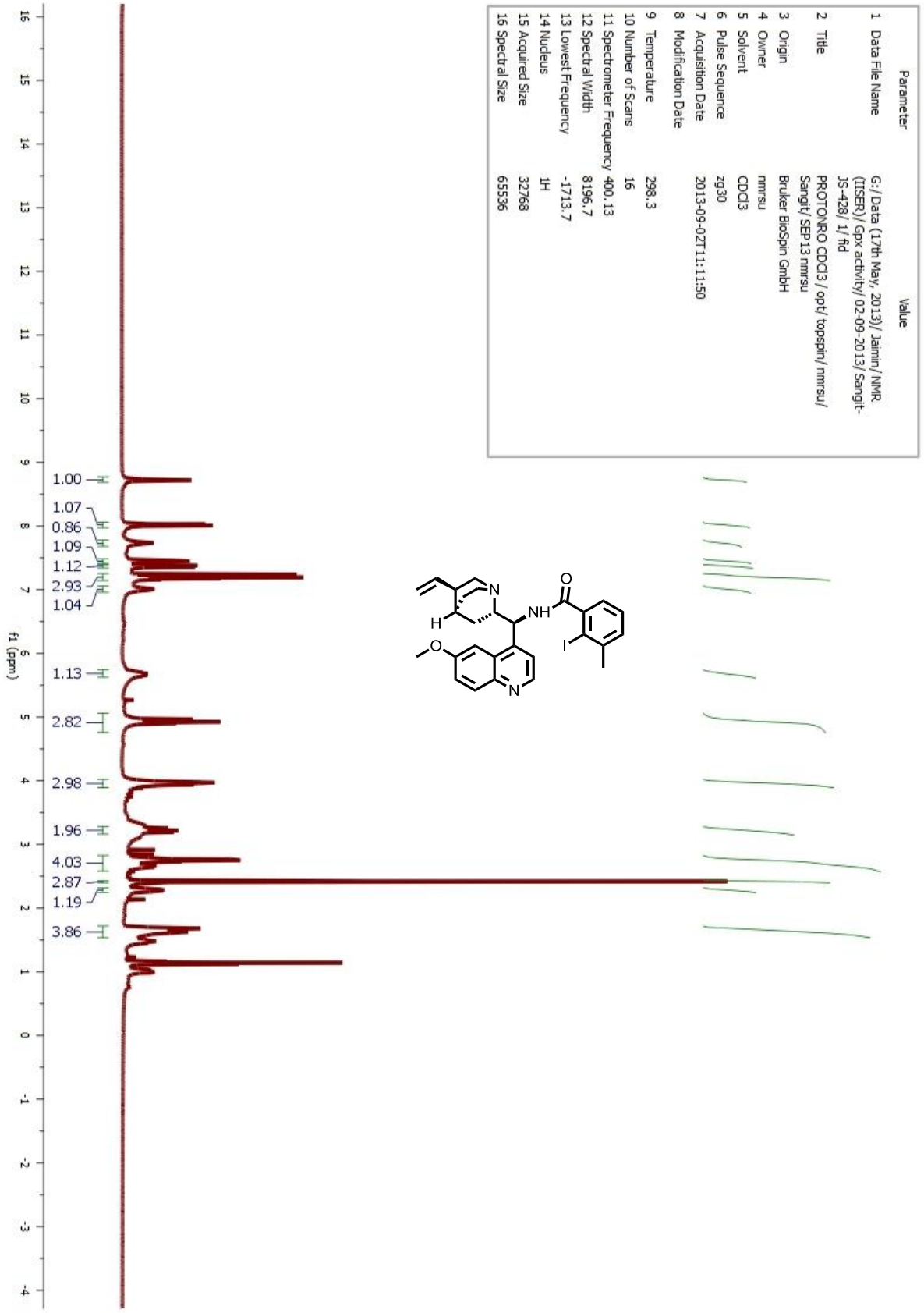


Figure S9 ^{13}C NMR of precursor of **1b**

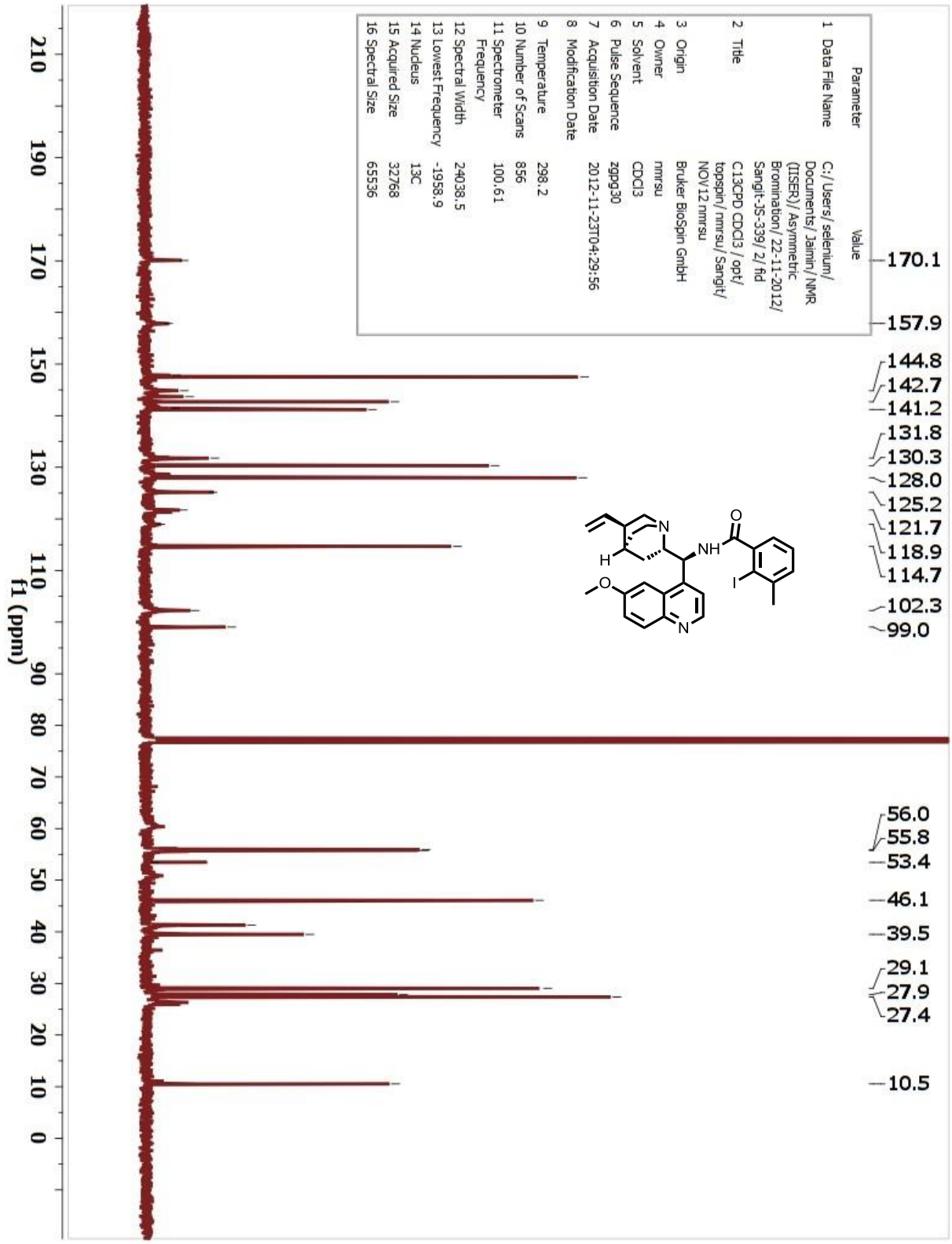


Figure S10HRMS (ESI) of precursor of **1b**

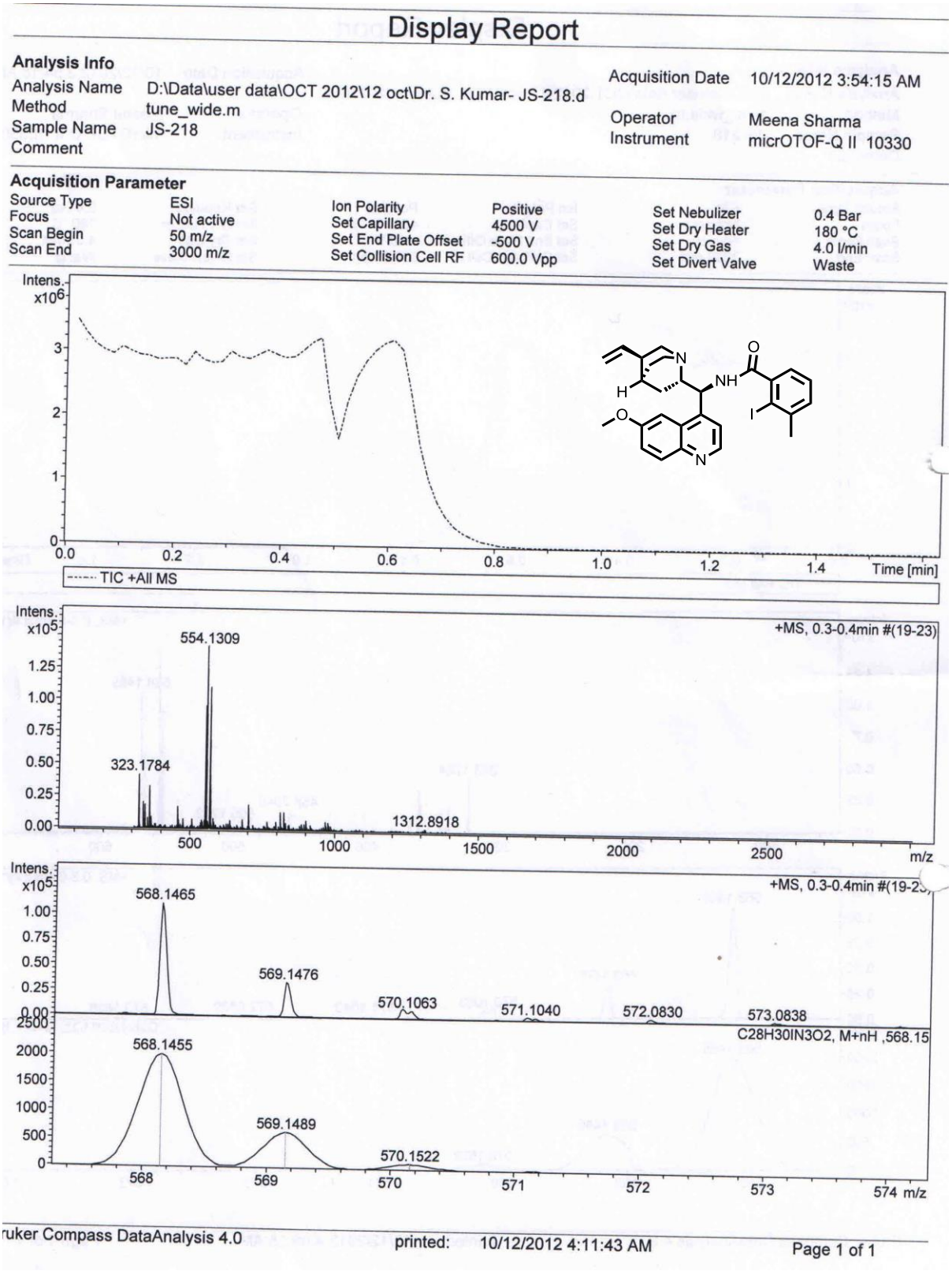


Figure S11 ^{1}H NMR of **1b**

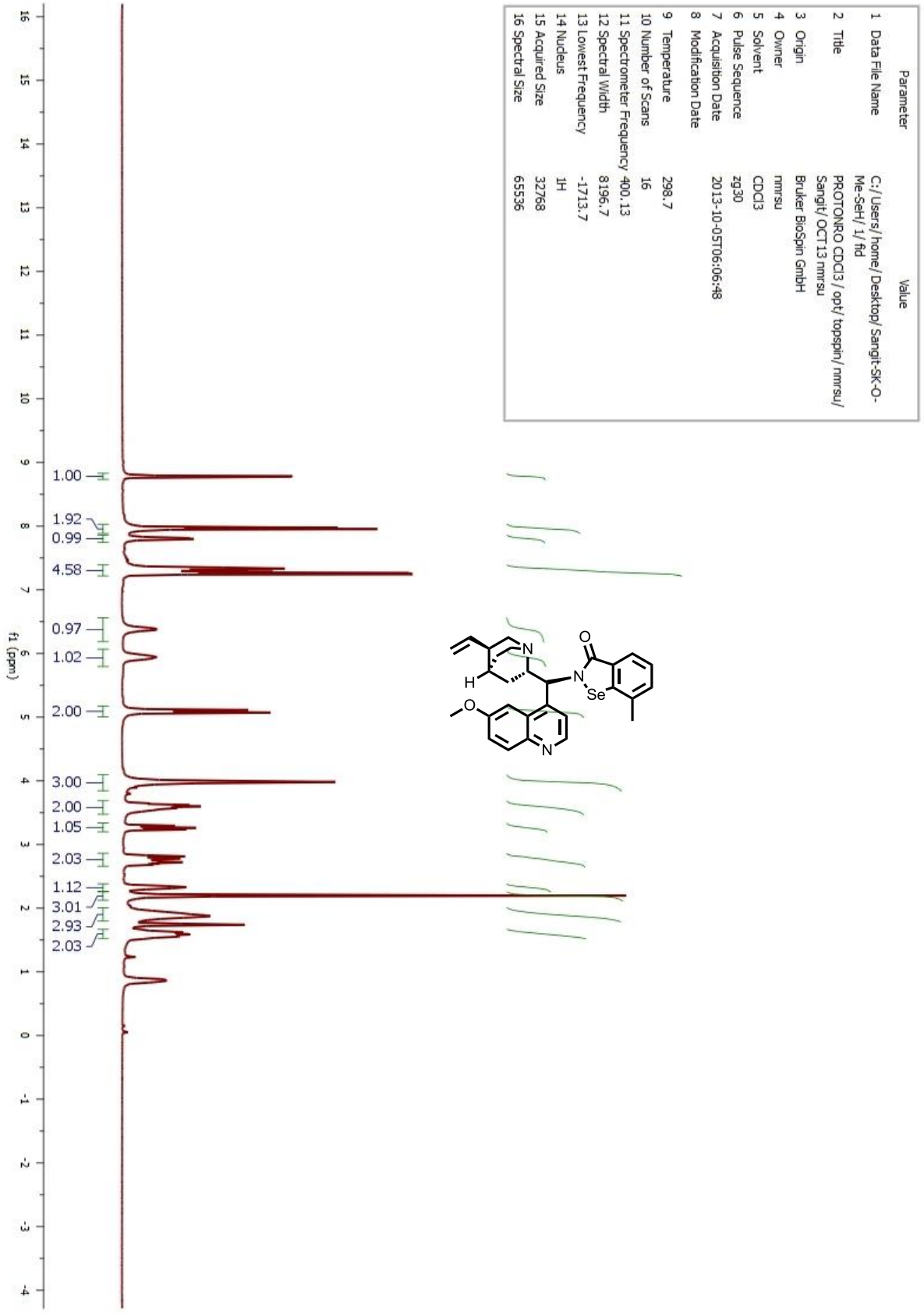


Figure S12 ^{13}C NMR of **1b**

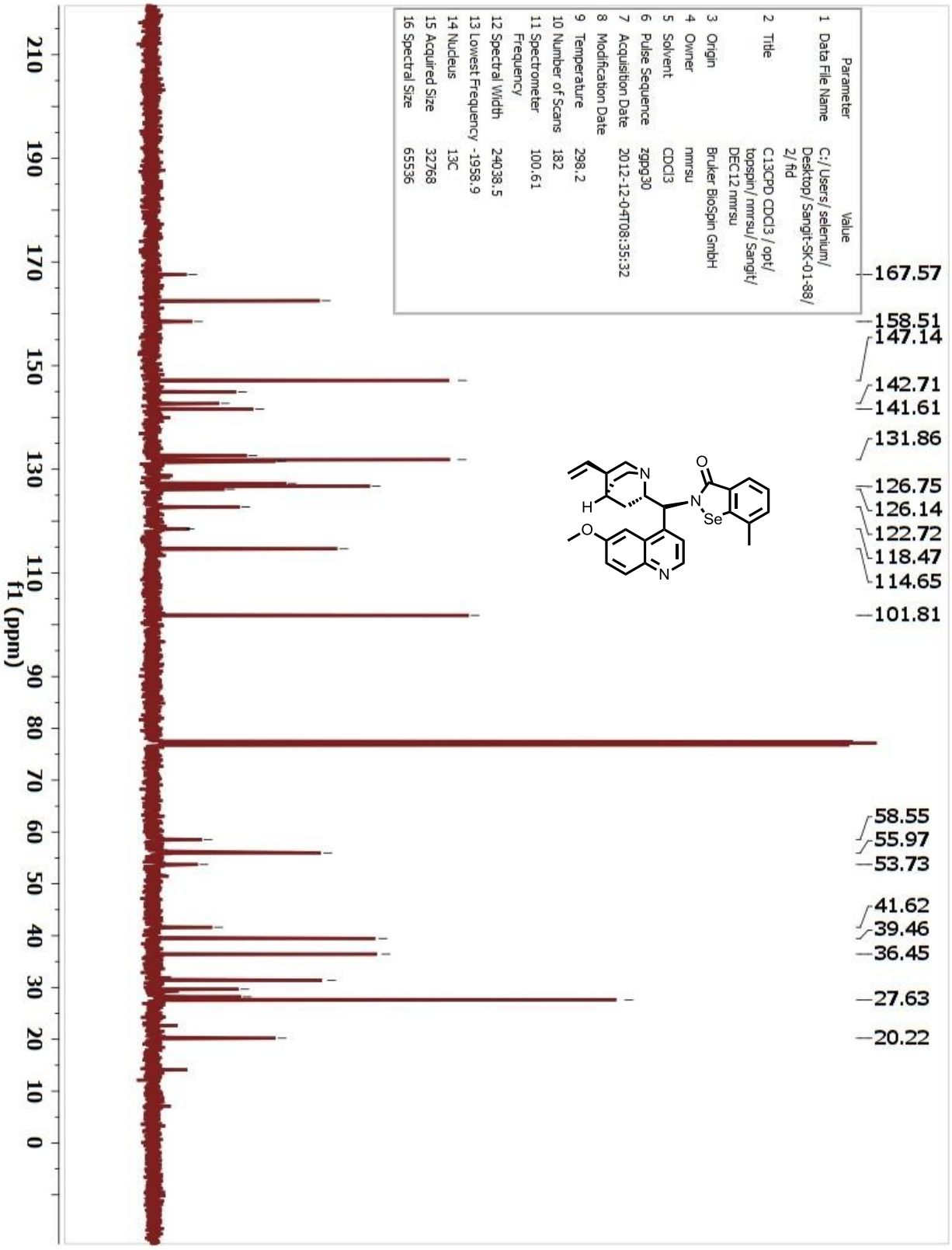


Figure S13 ^{77}Se NMR **1b**

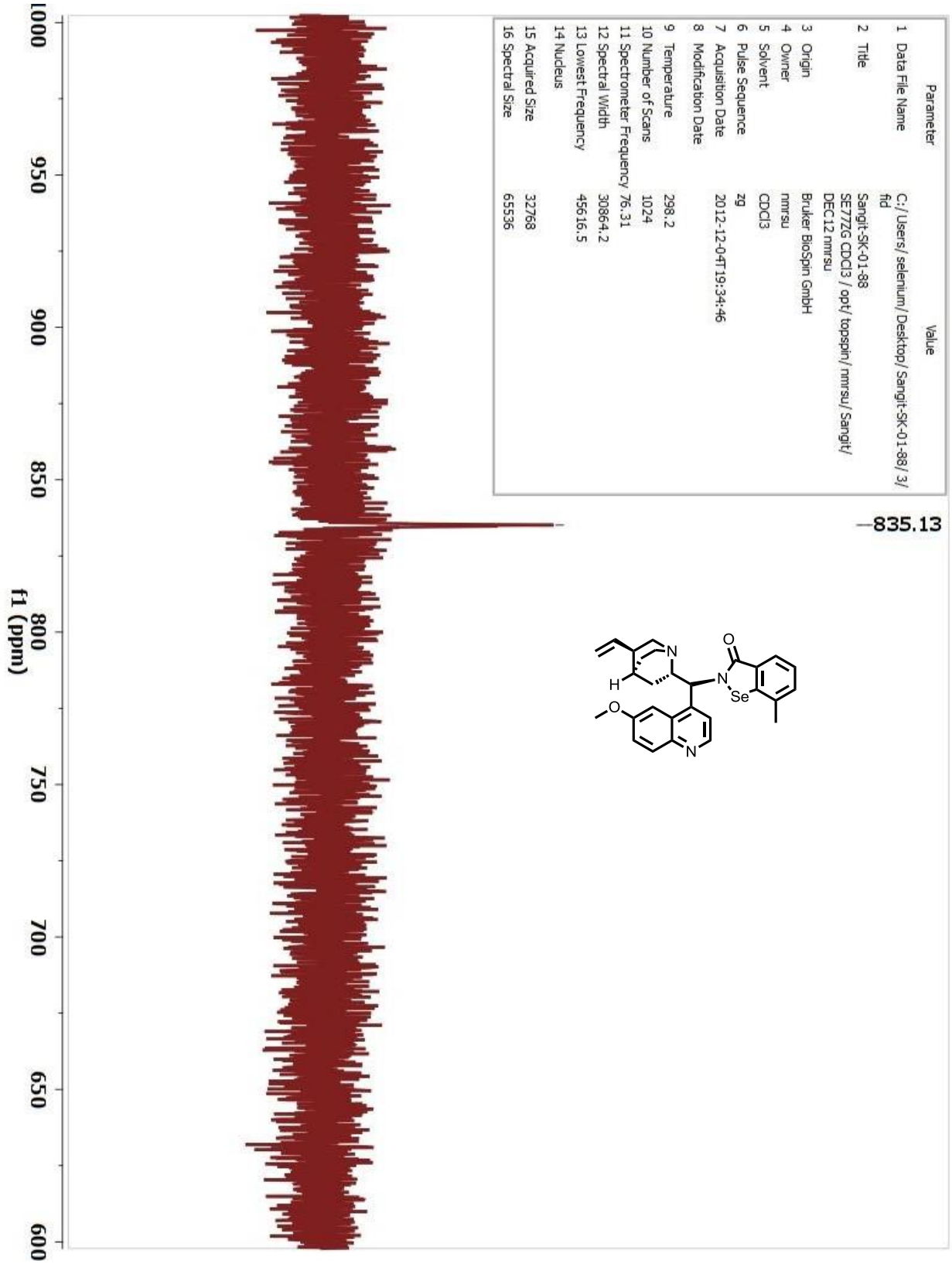


Figure S14 HRMS (ESI) of **1b**

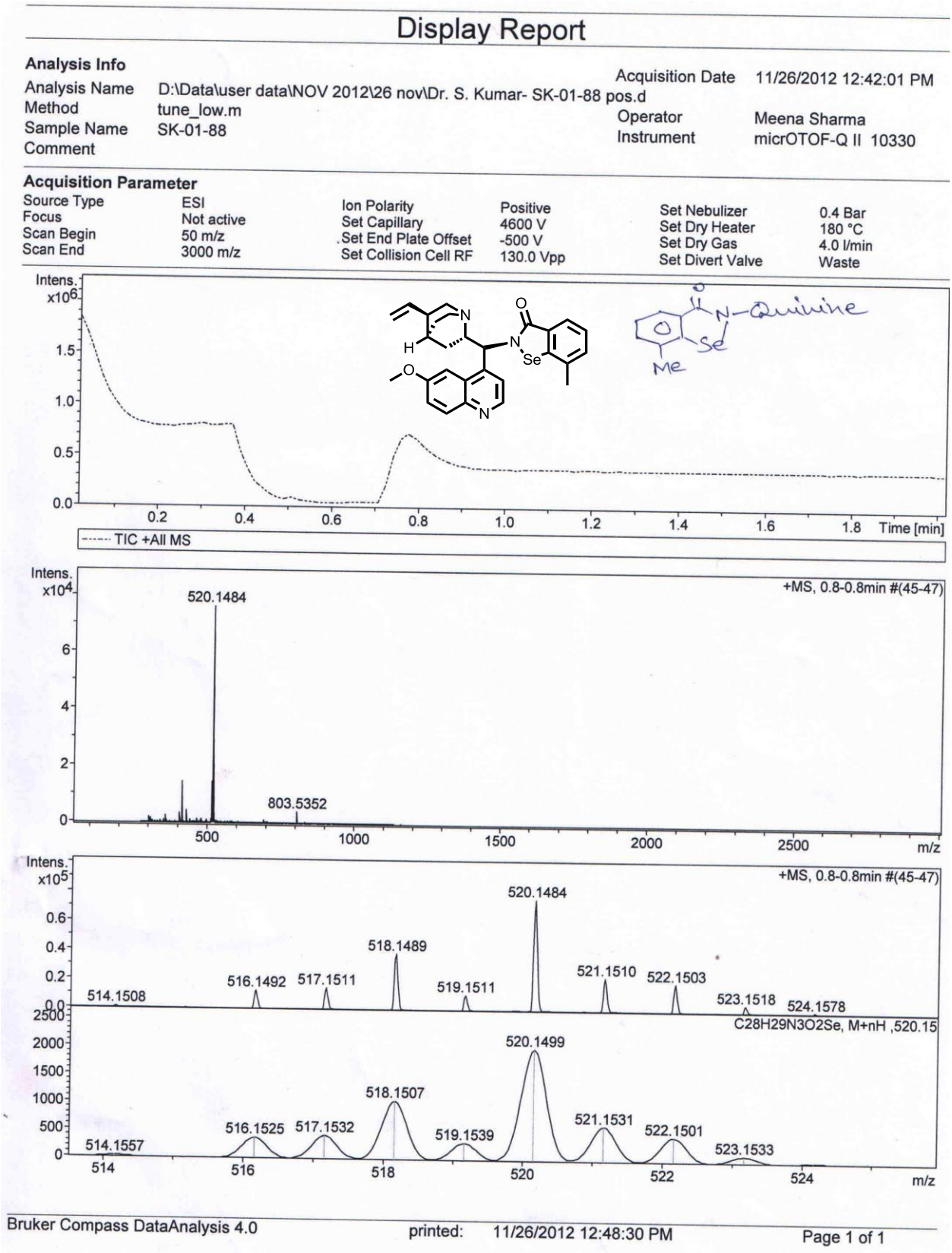


Figure S15 ^{1}H NMR of precursor of **1c**

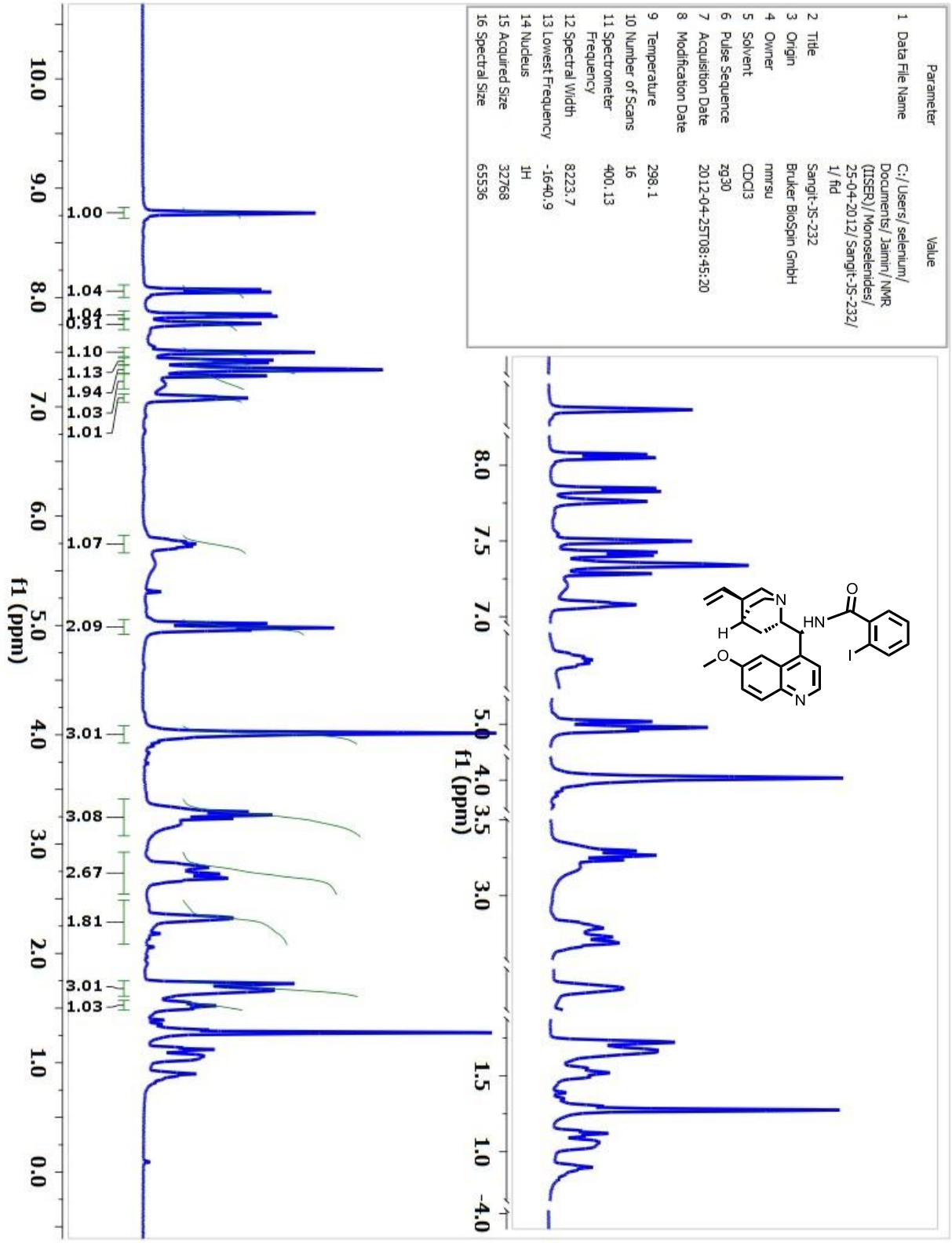


Figure S16 ^{13}C NMR of precursor of **1c**

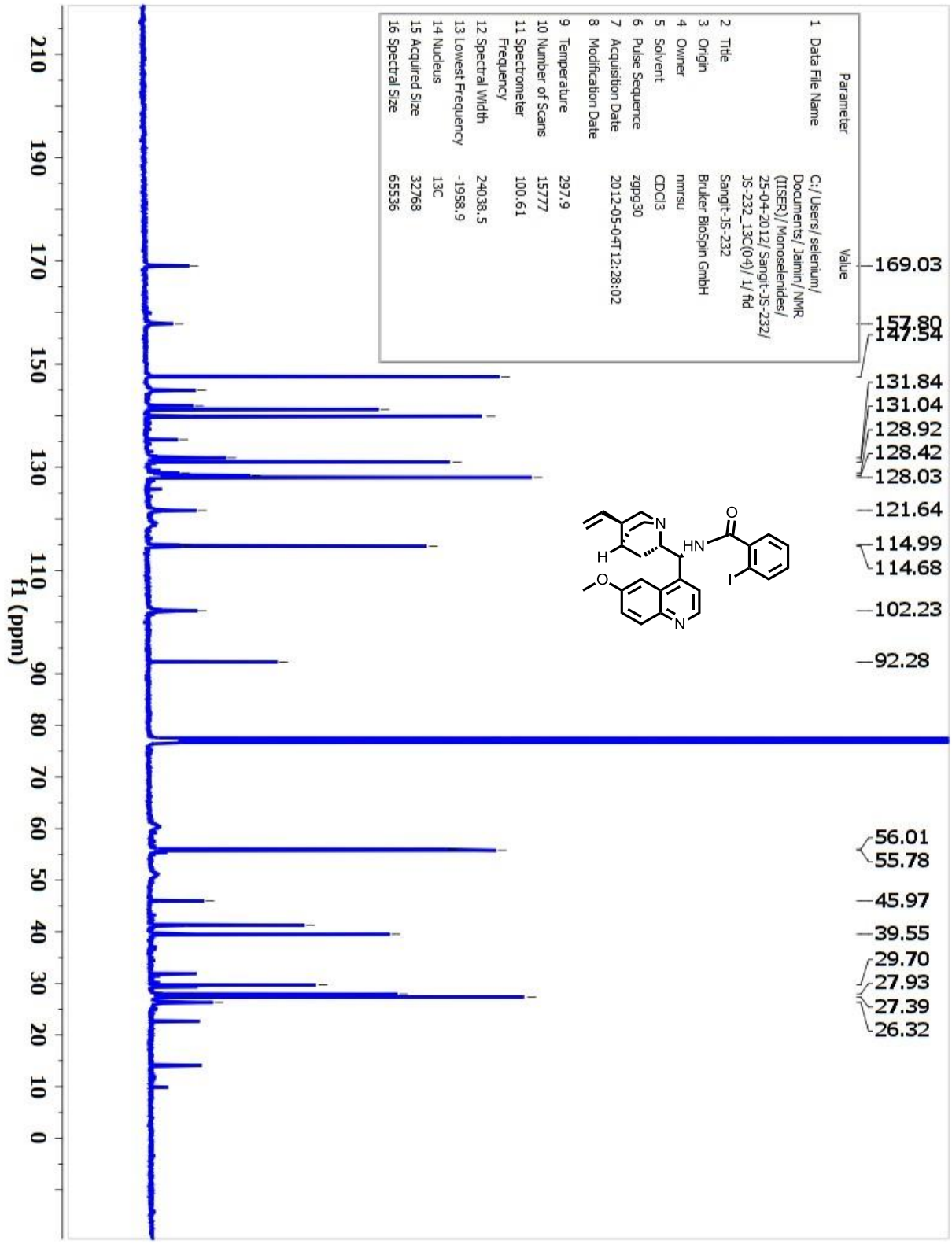


Figure S17 HRMS (ESI) of precursor of **1c**

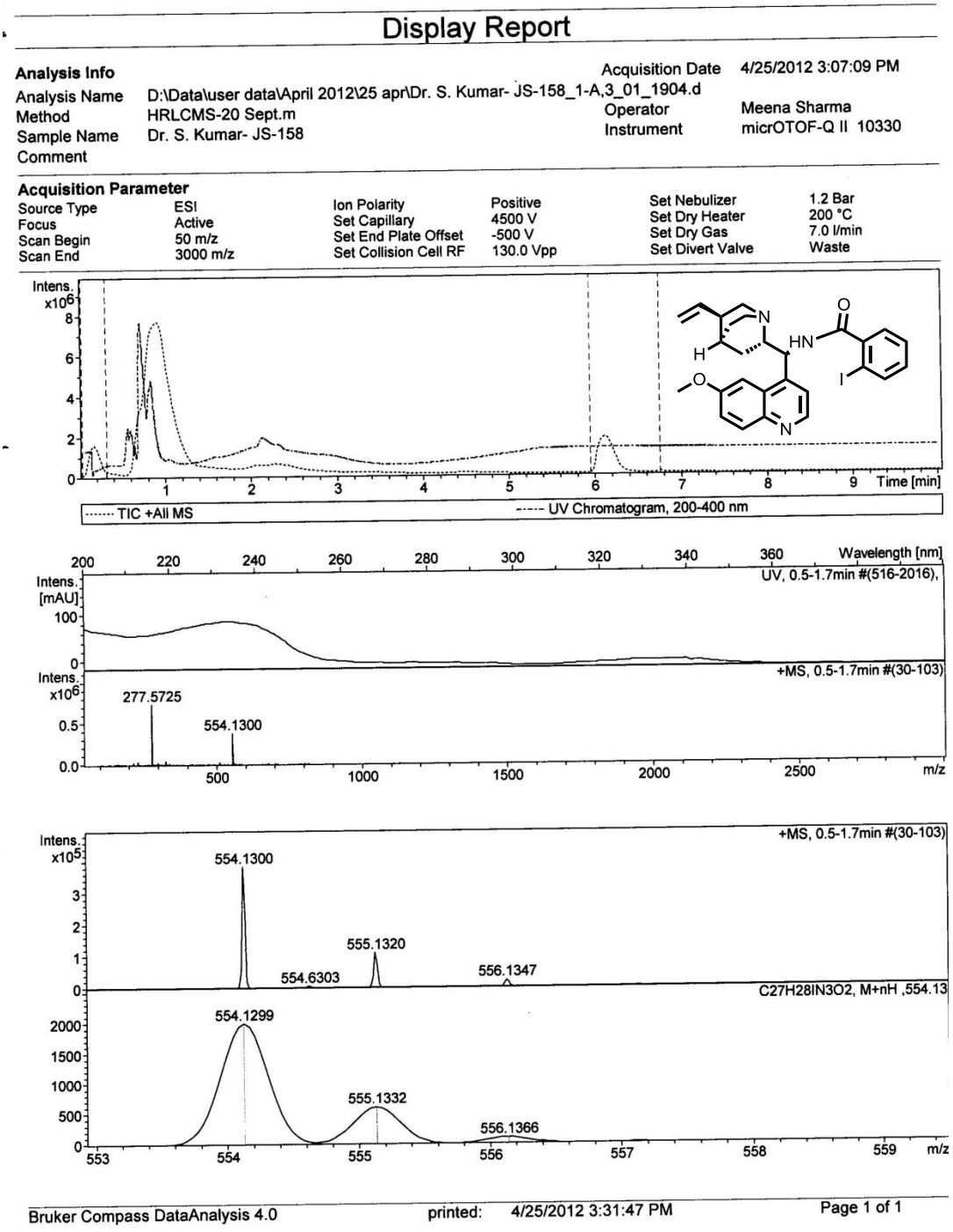


Figure S18 ^{1}H NMR of **1c**

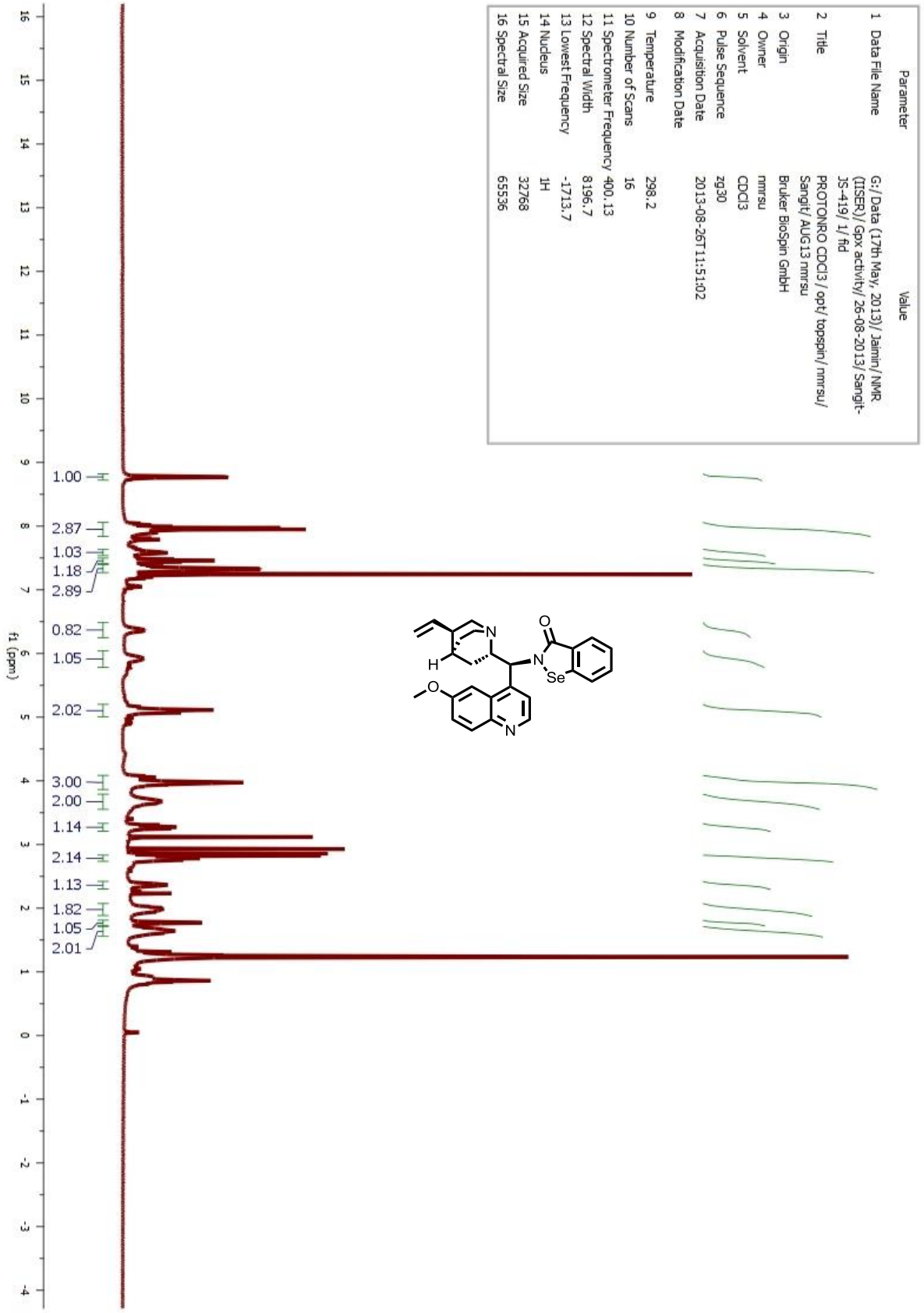


Figure S19 ^{13}C NMR of **1c**

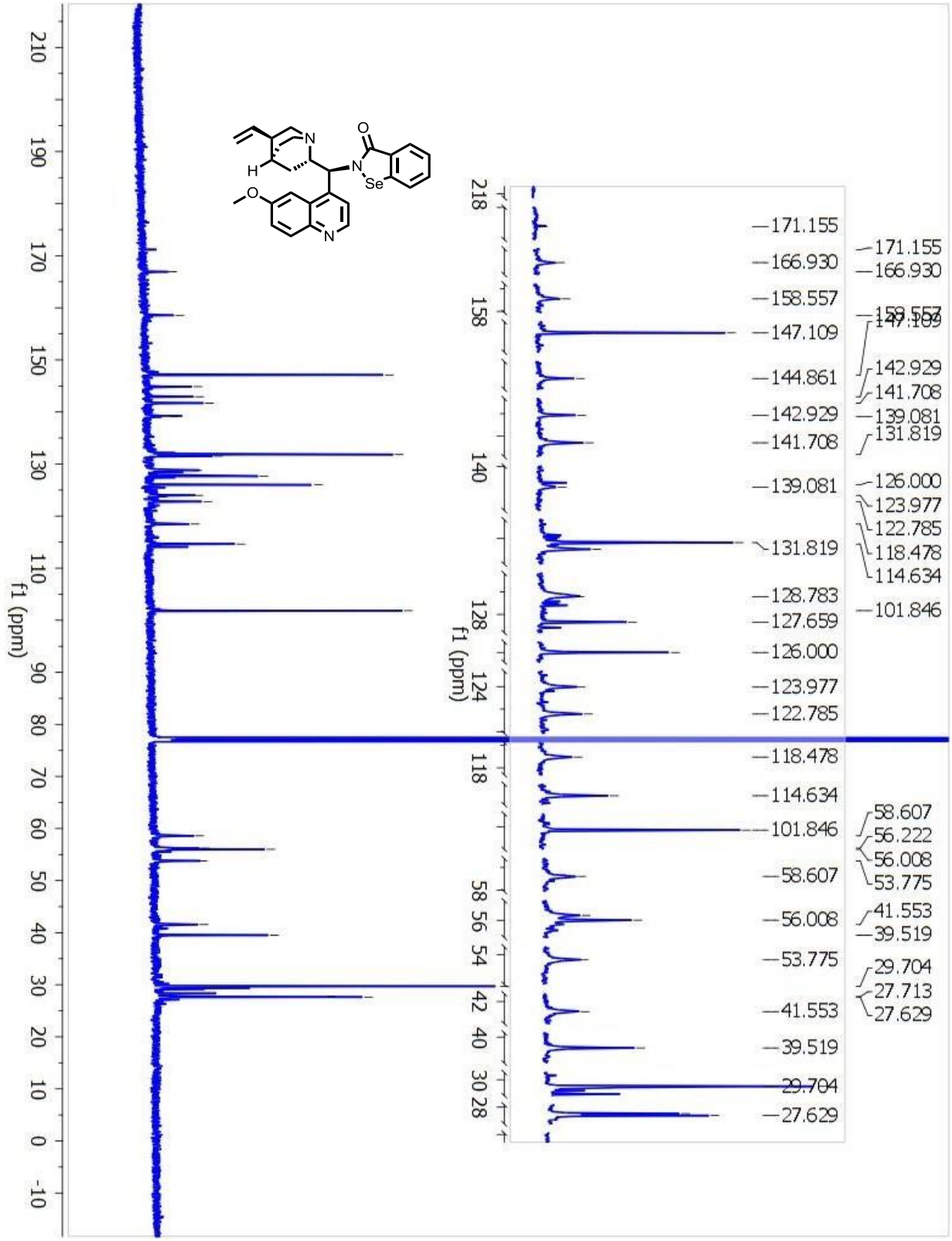


Figure S20 ^{77}Se NMR of **1c**

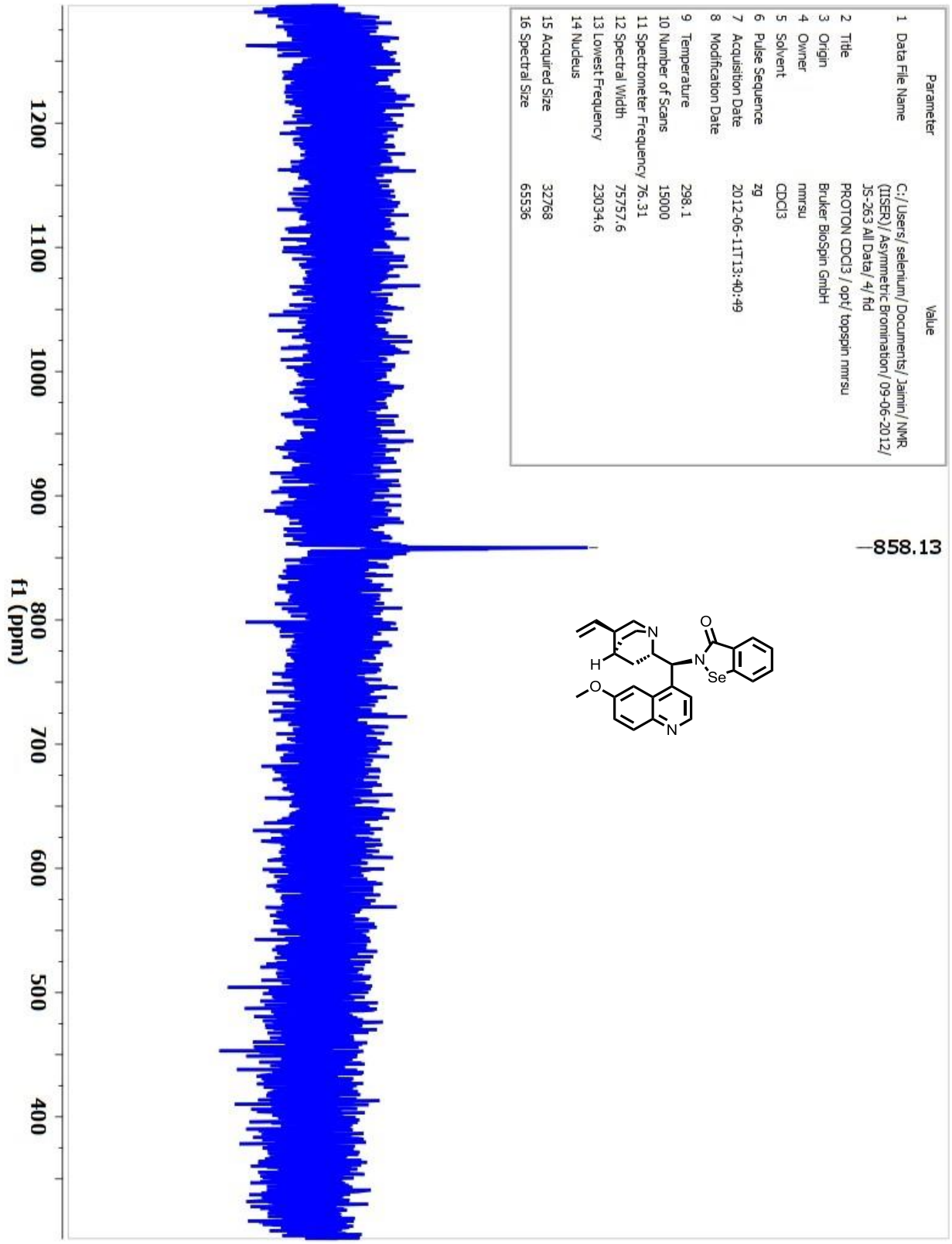


Figure S21 HRMS (ESI) of **1c**

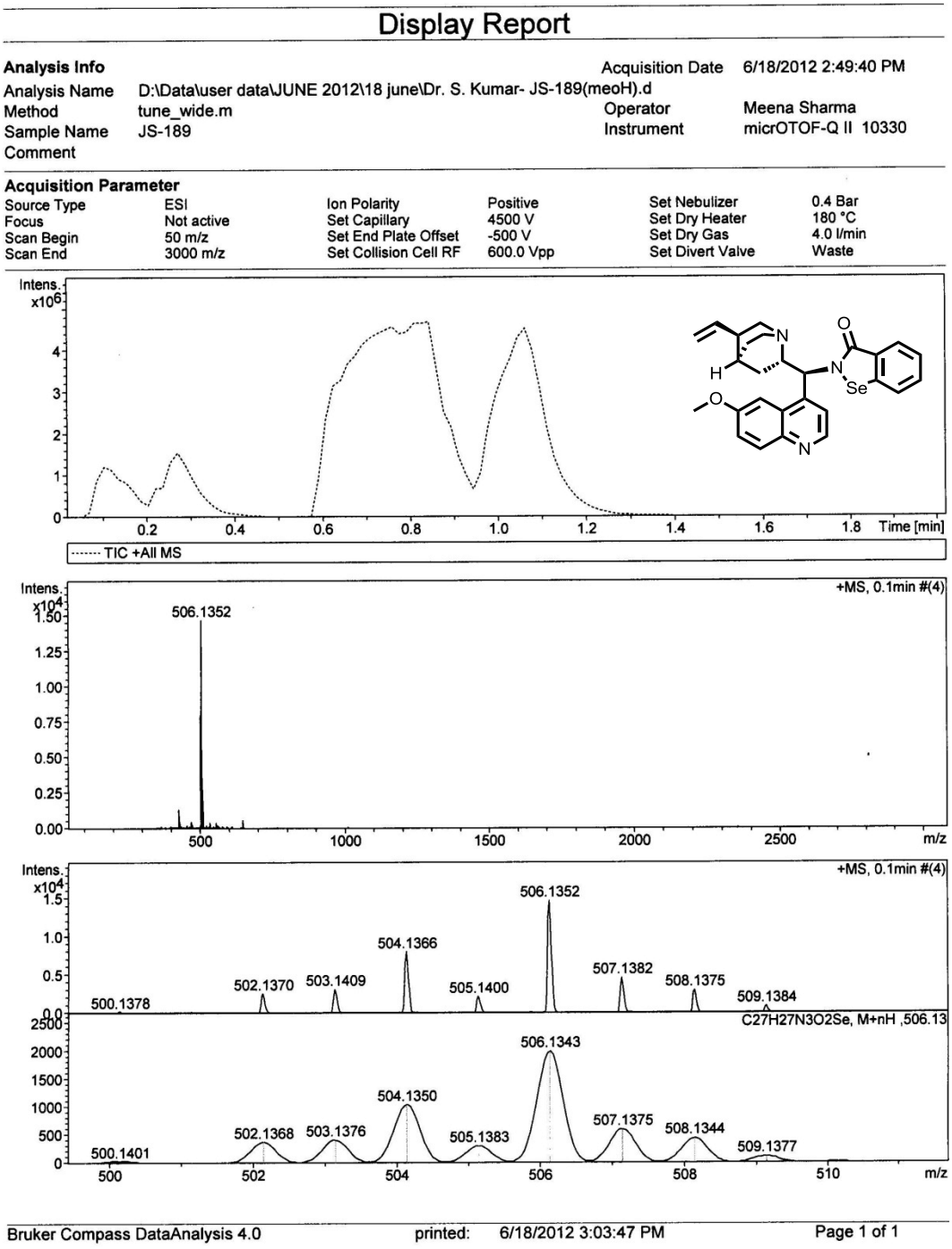


Figure S22 ^{1}H NMR of precursor of **1d**

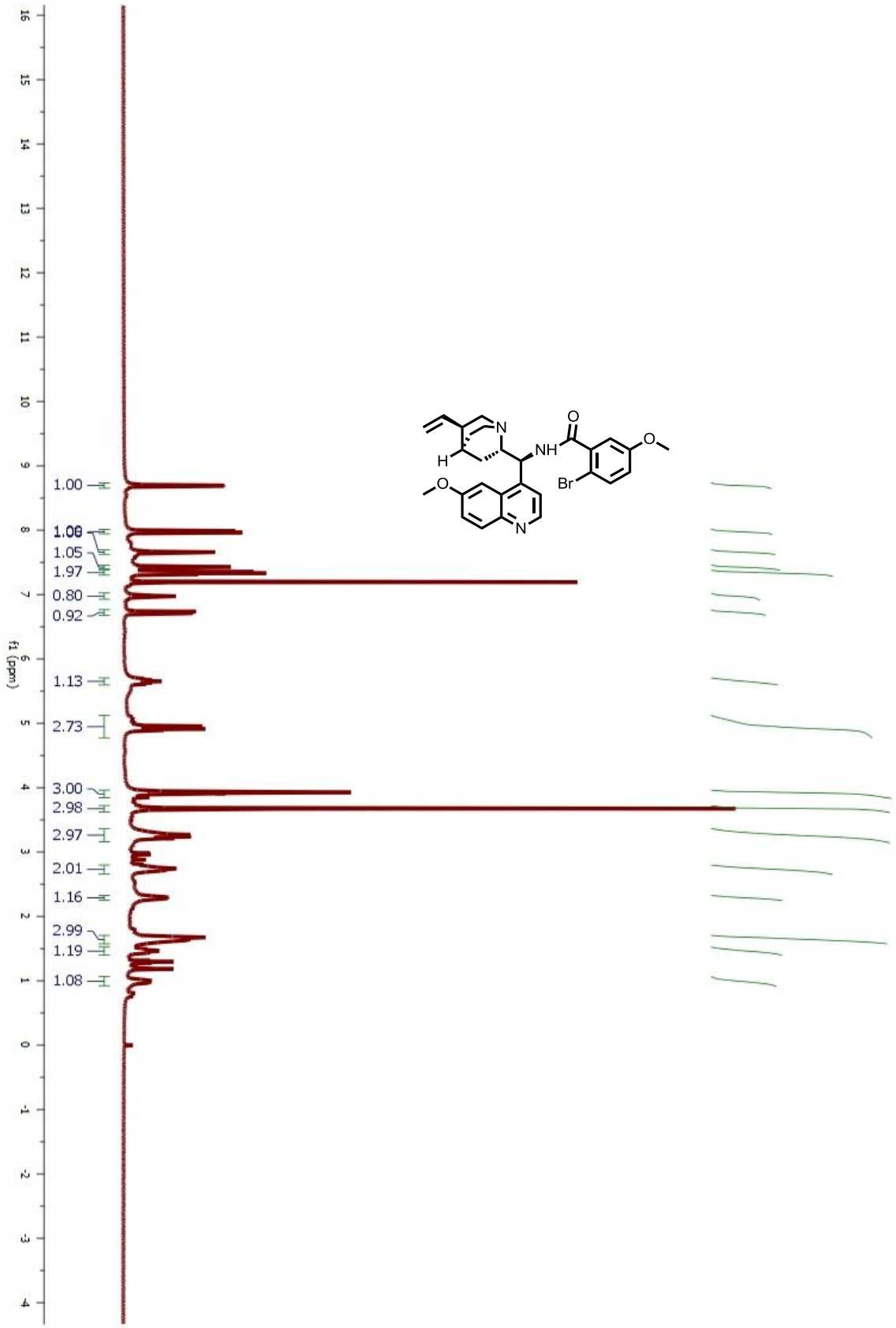


Figure S23 ^{13}C NMR of precursor of **1d**

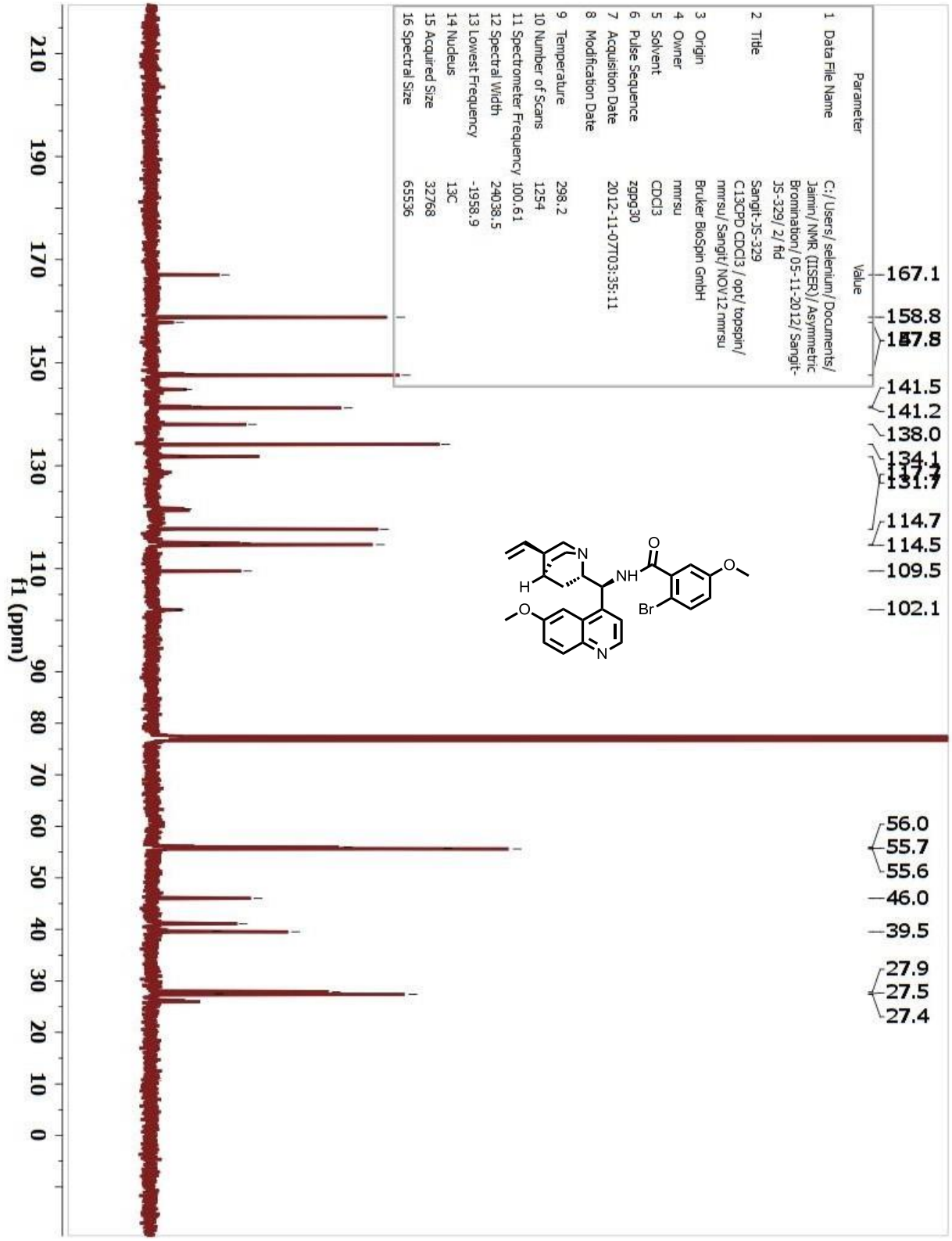


Figure S24 HRMS (ESI) of precursor of **1d**

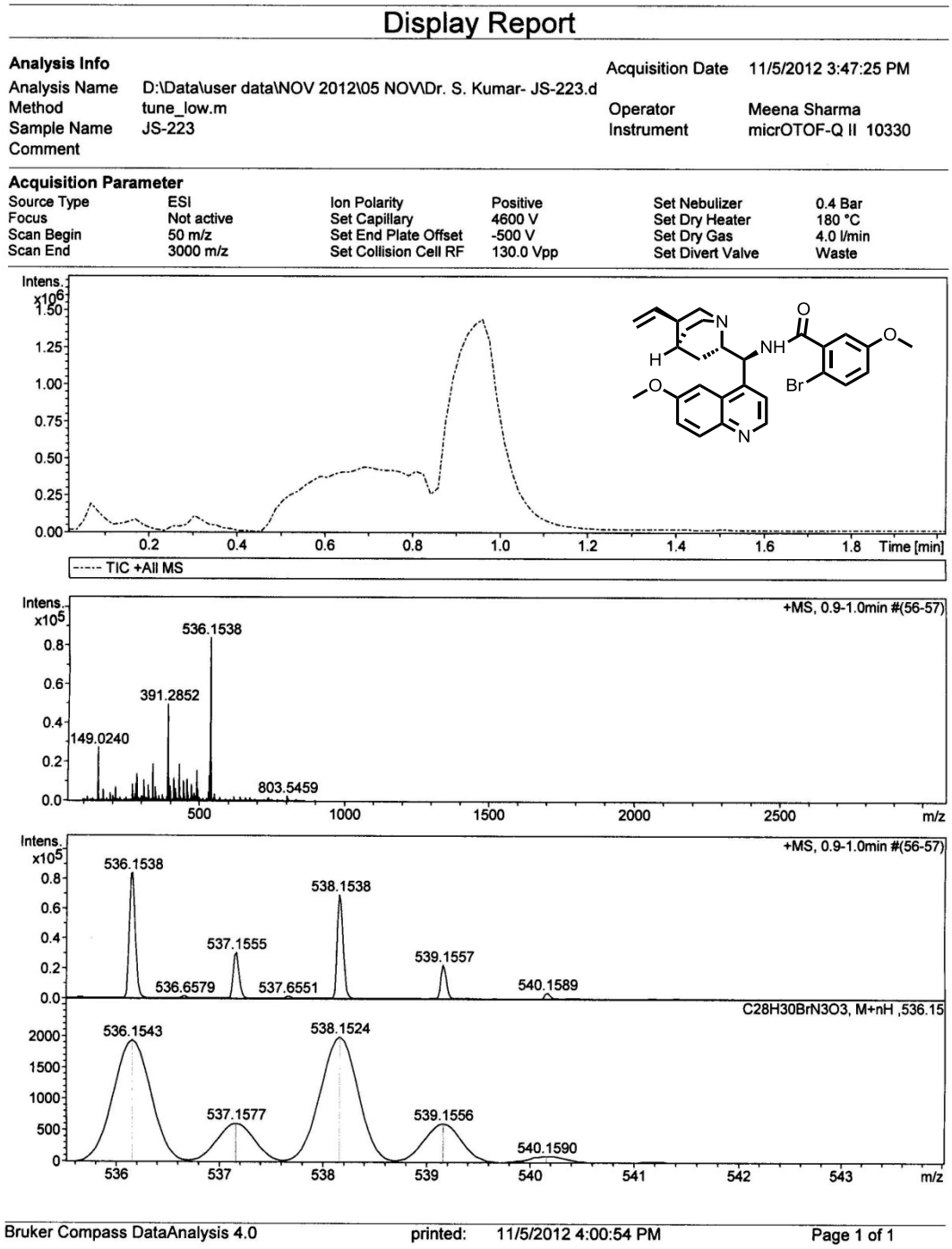


Figure S25 ^{1}H NMR of **1d**

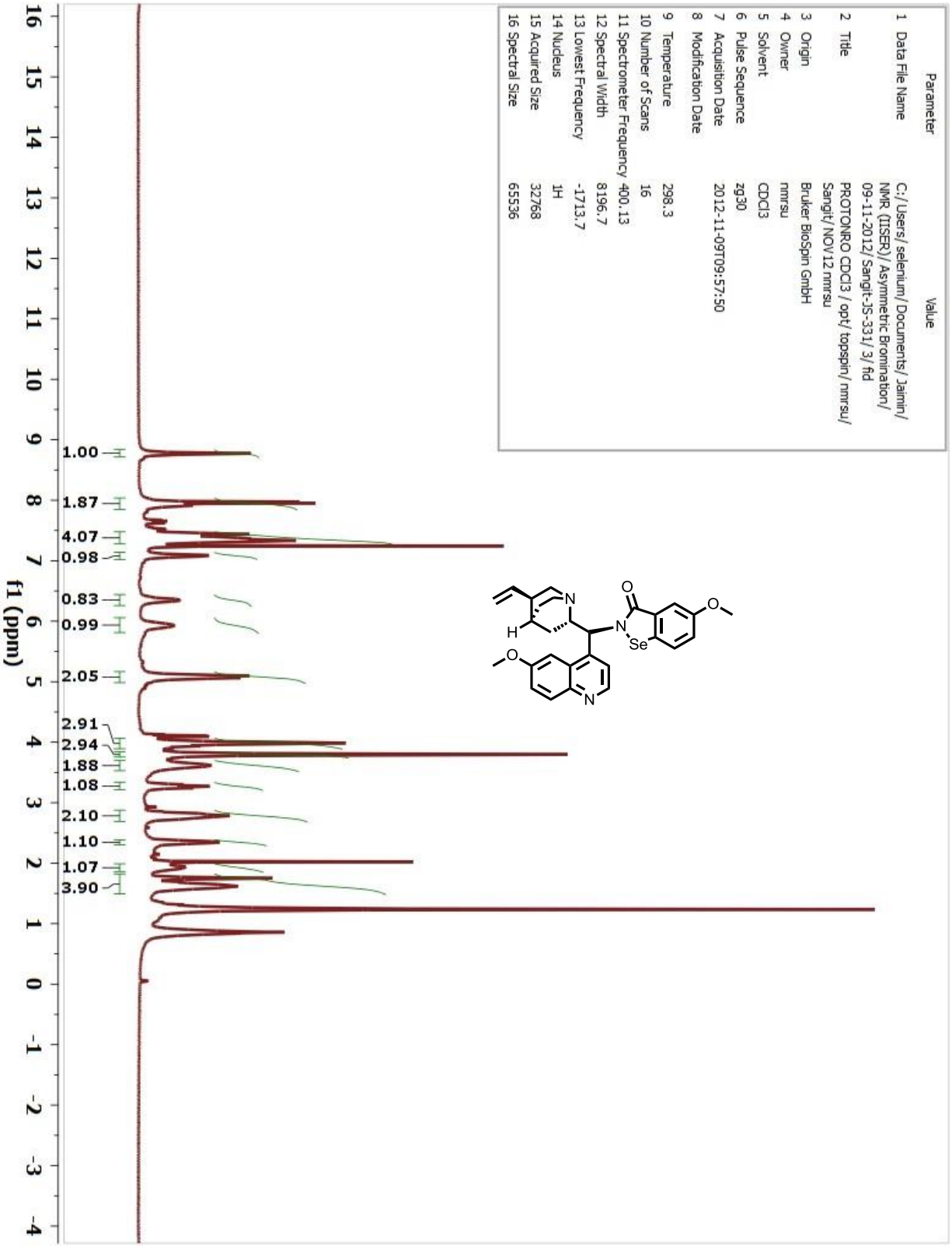


Figure S26 ^{13}C NMR of **1d**

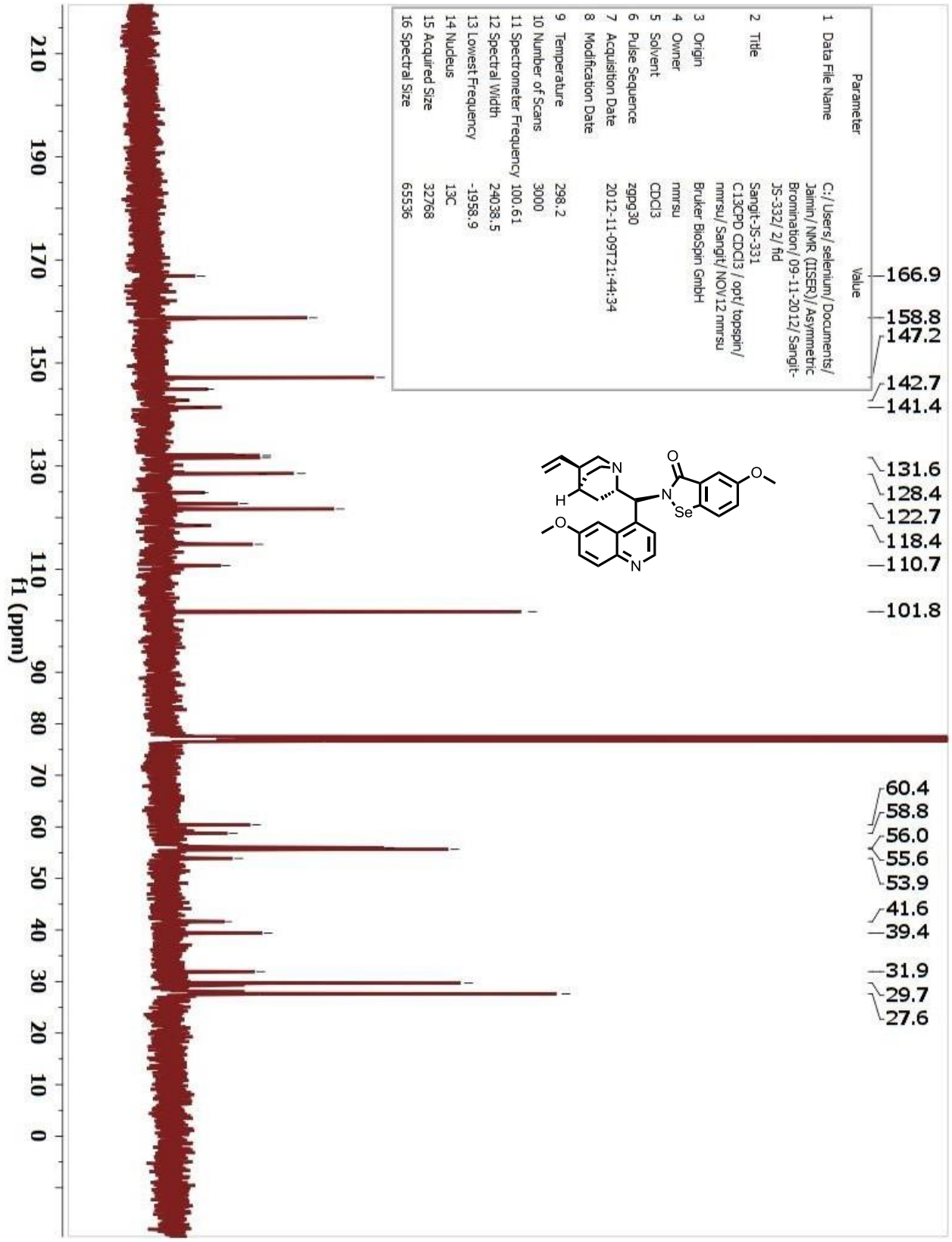


Figure S27 HRMS (ESI) of **1d**

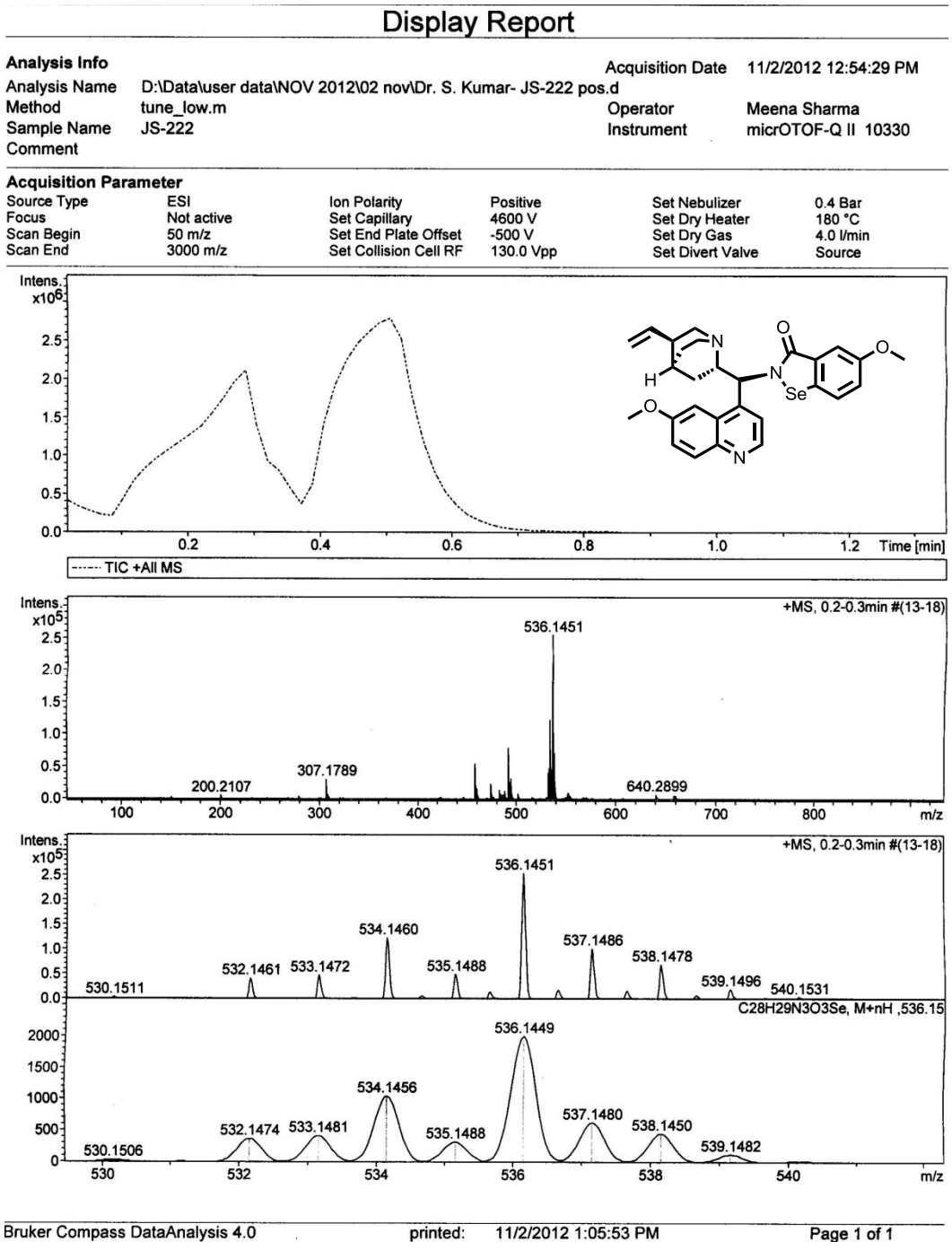


Figure S28 ^{77}Se NMR of **1d**

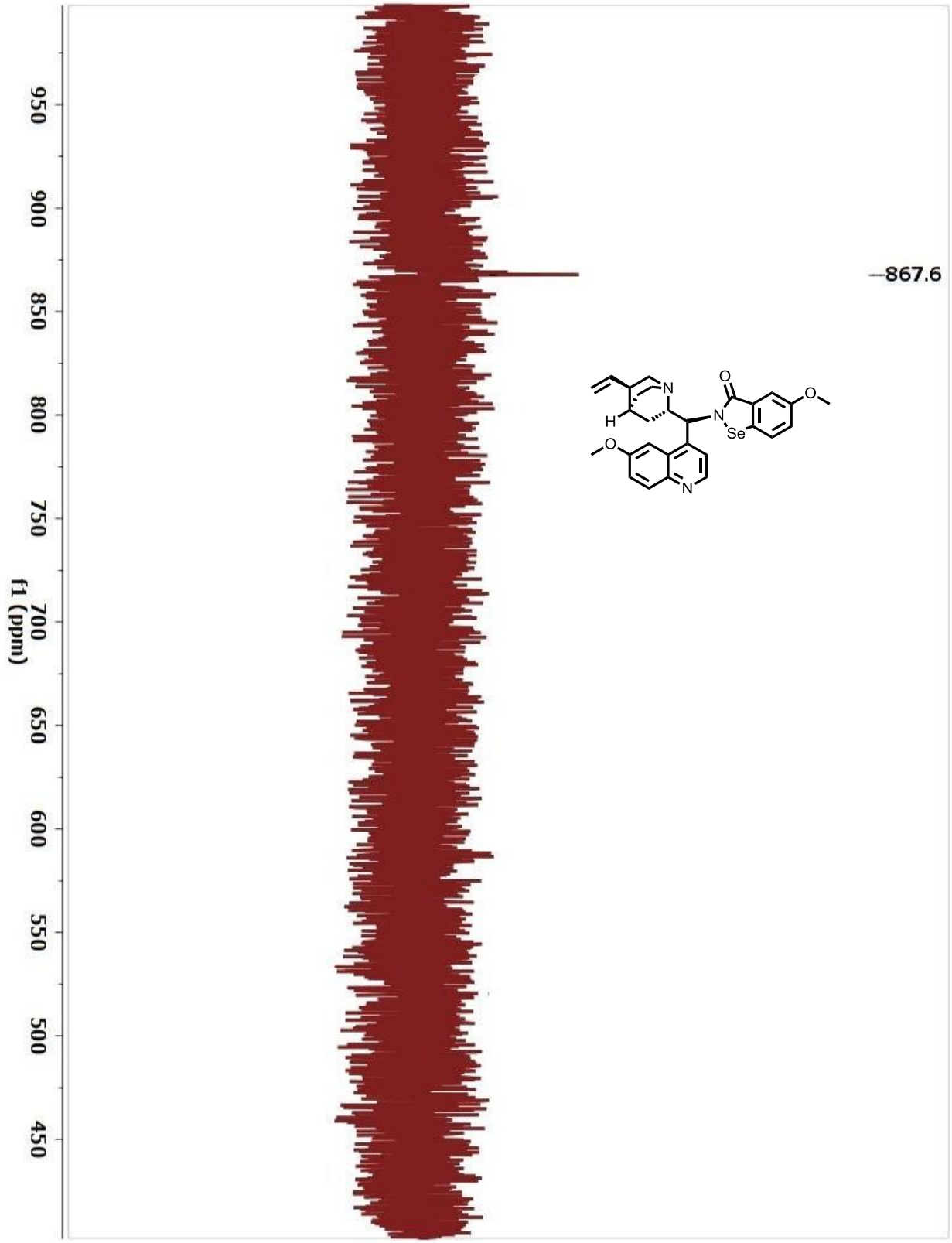


Figure S29 ^{1}H NMR of **1e**

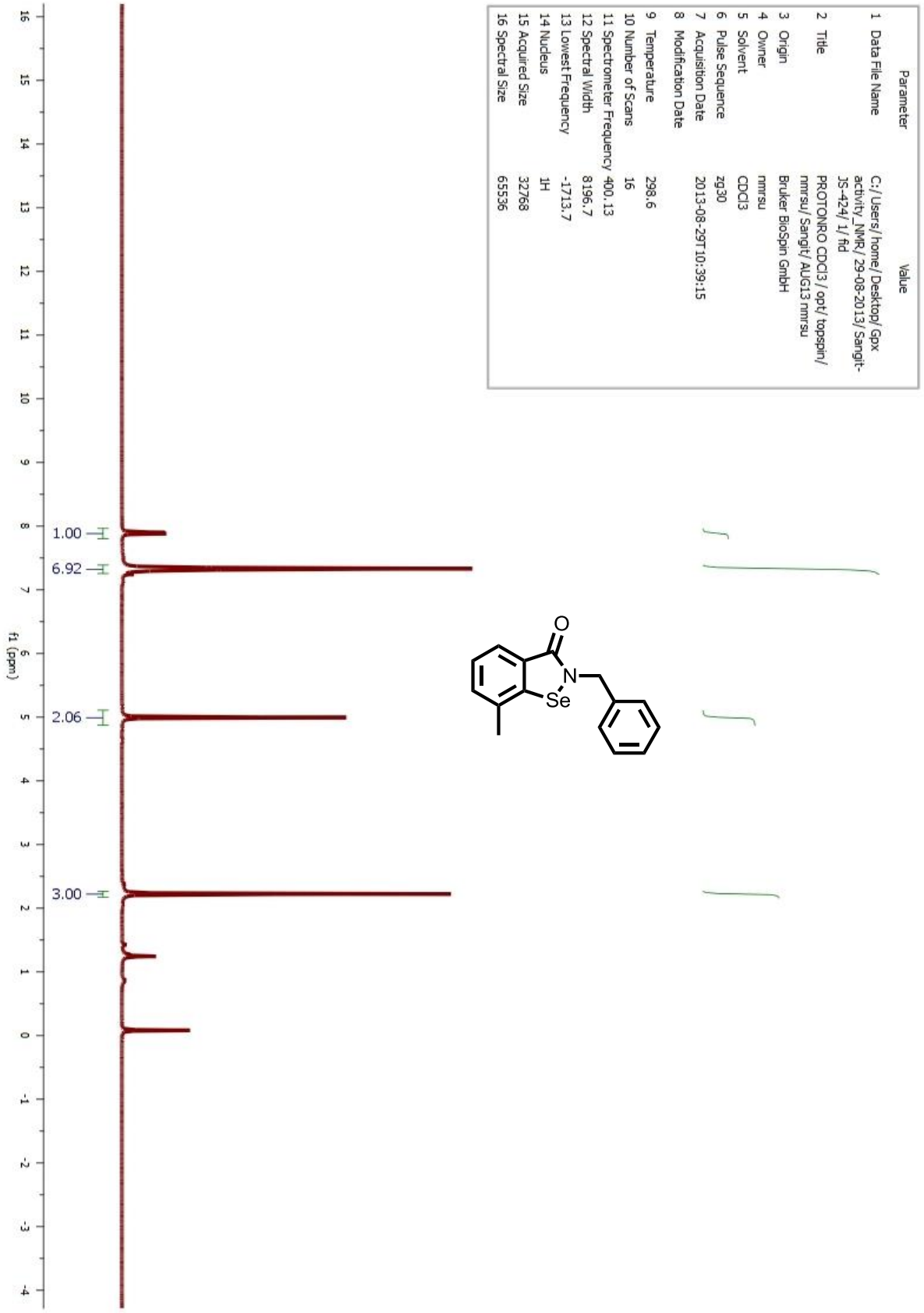


Figure S30 ^{13}C NMR of **1e**

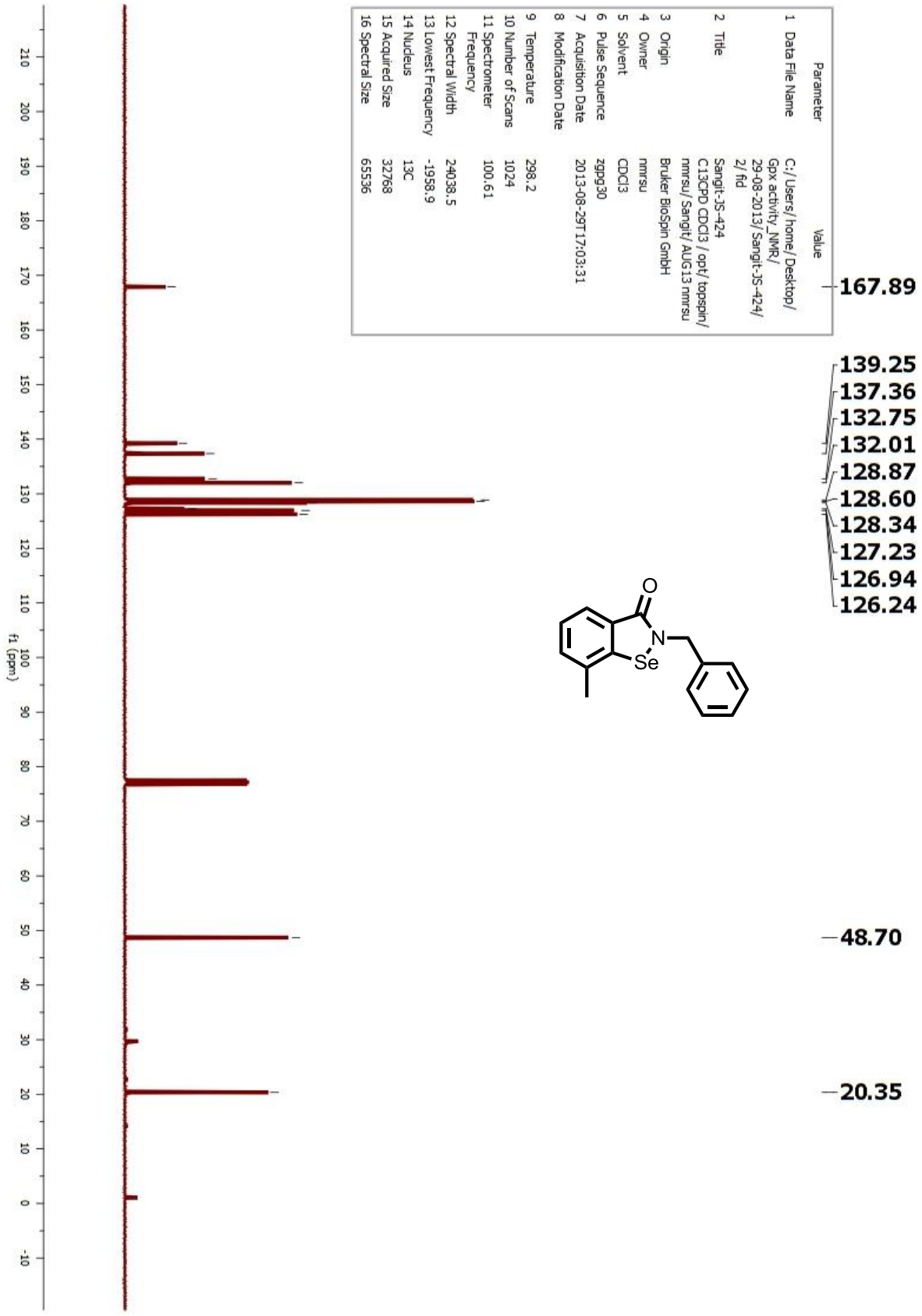
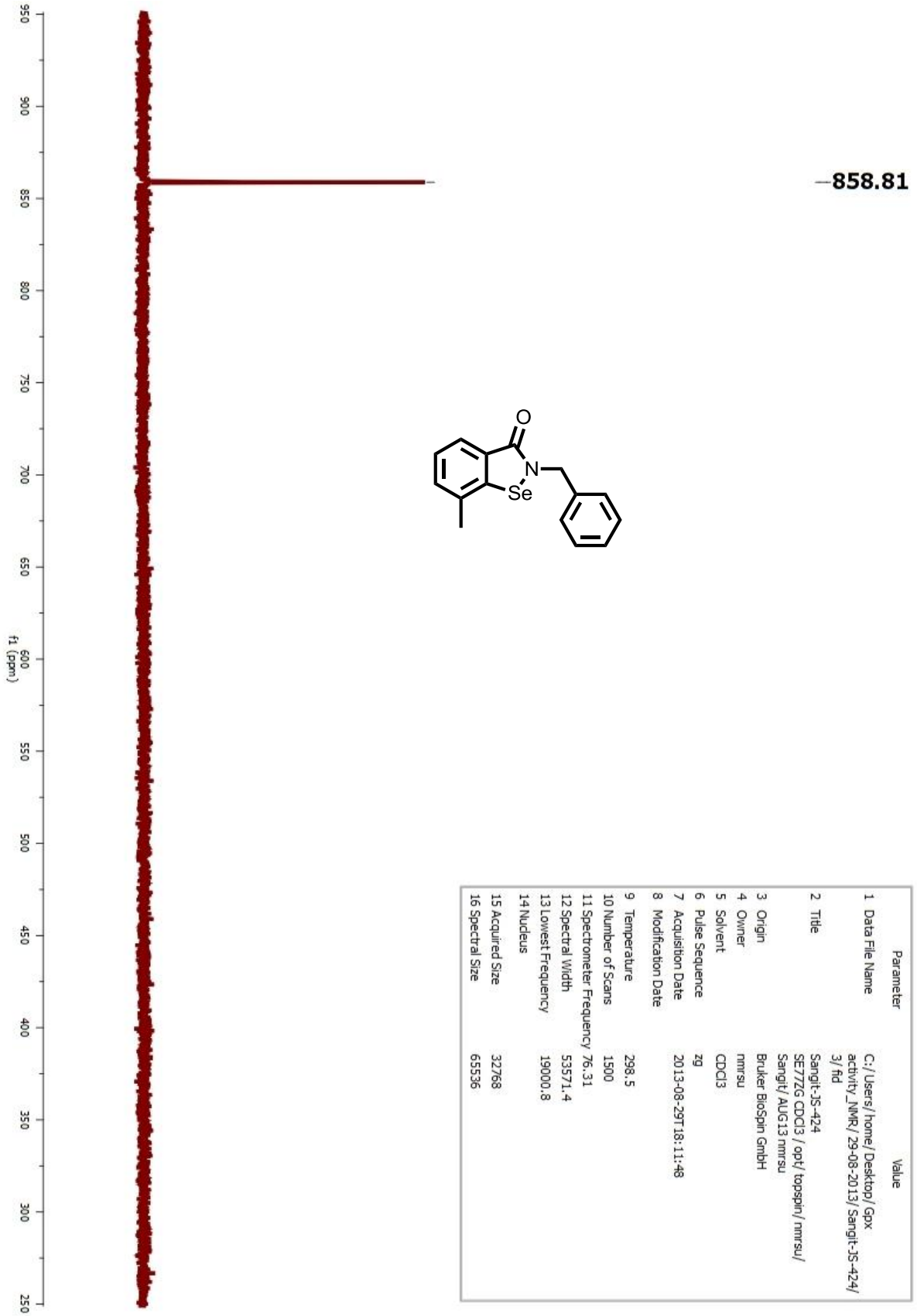


Figure S31 ^{77}Se NMR of **1e**



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7	Acquisition Date	2013-08-29T18:11:48
8	Modification Date	
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Figure S32 HRMS of **1e**

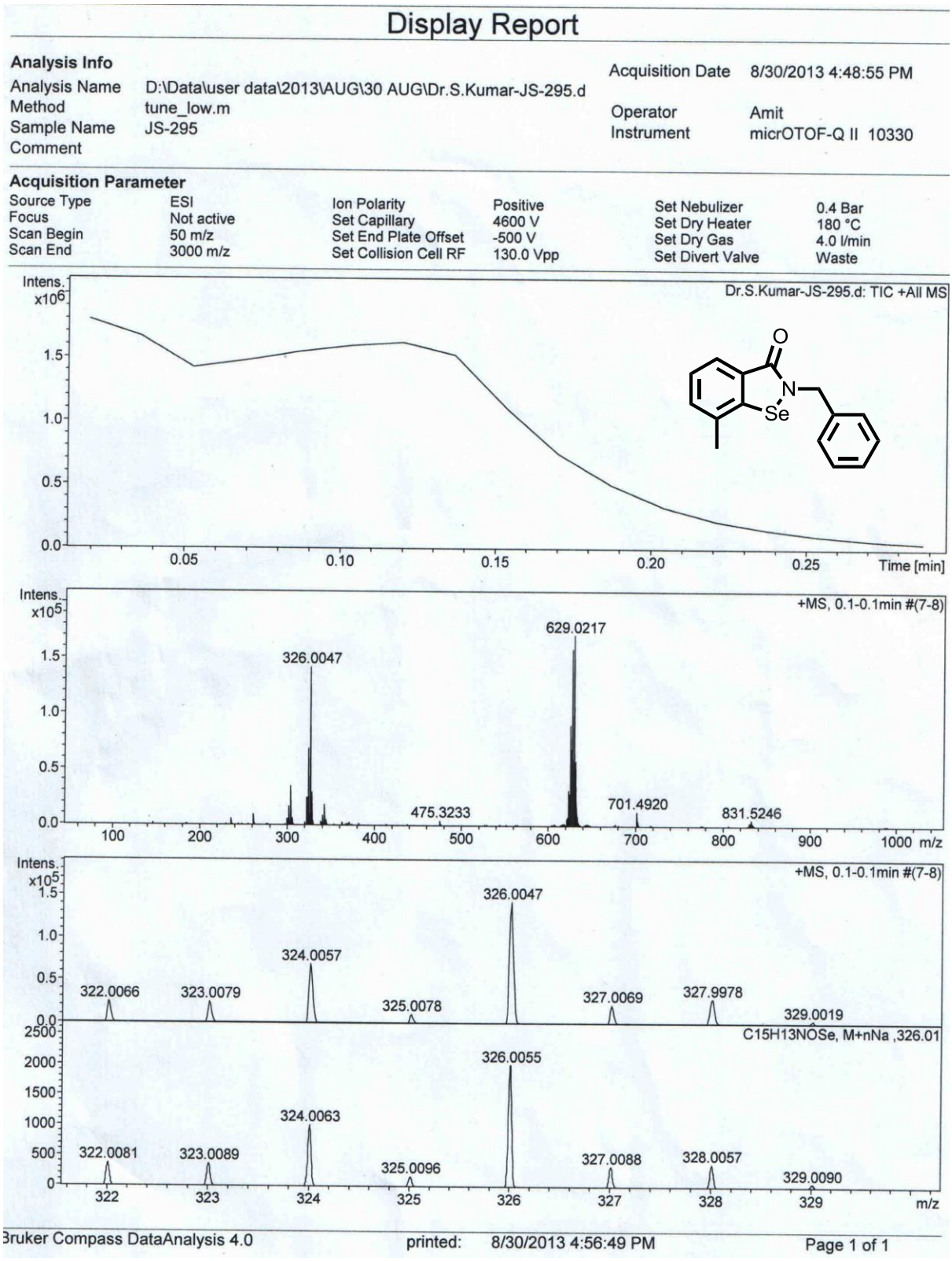


Figure S33 ^{1}H NMR of precursor of **1f**

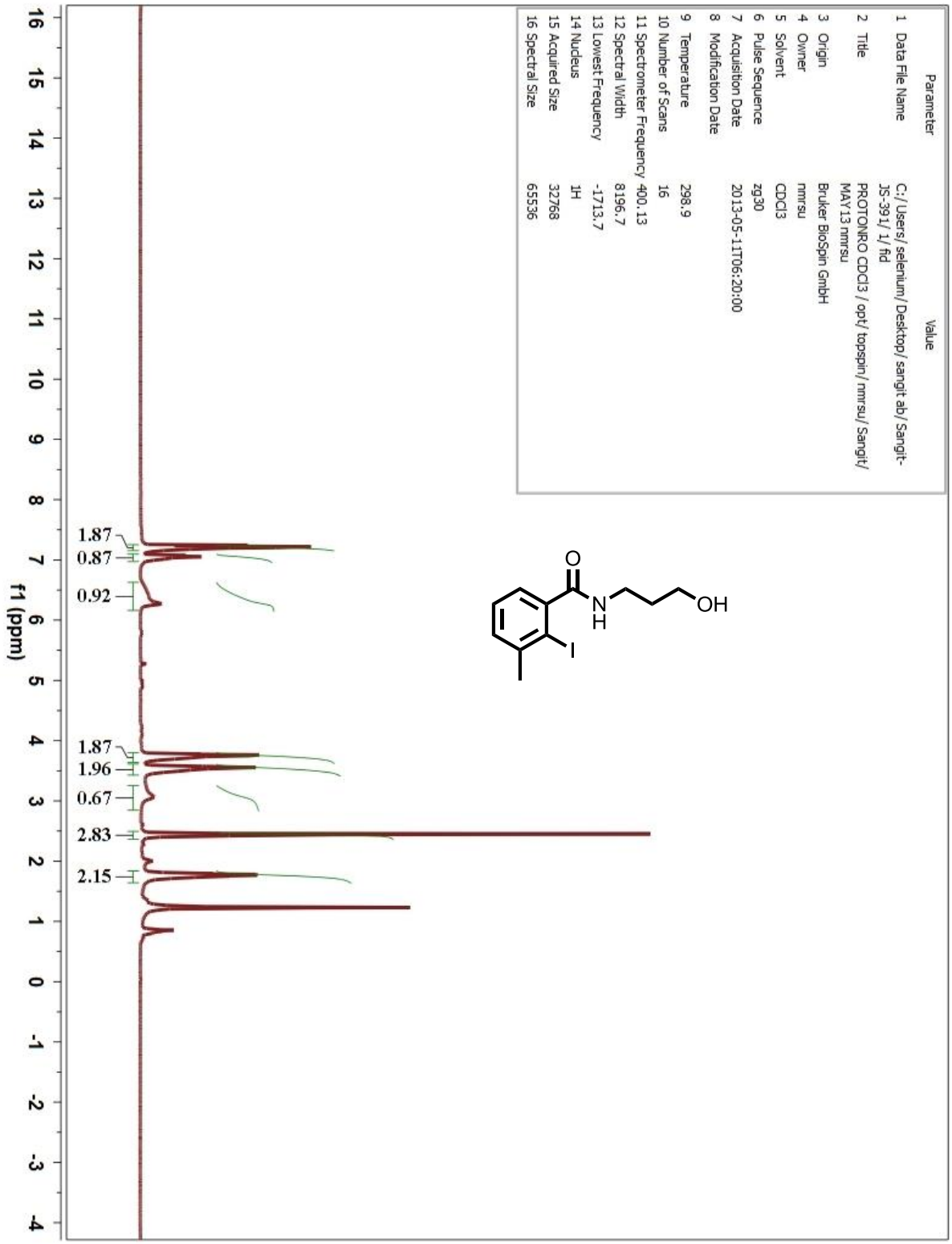


Figure S34 ^{13}C NMR of precursor of **1f**

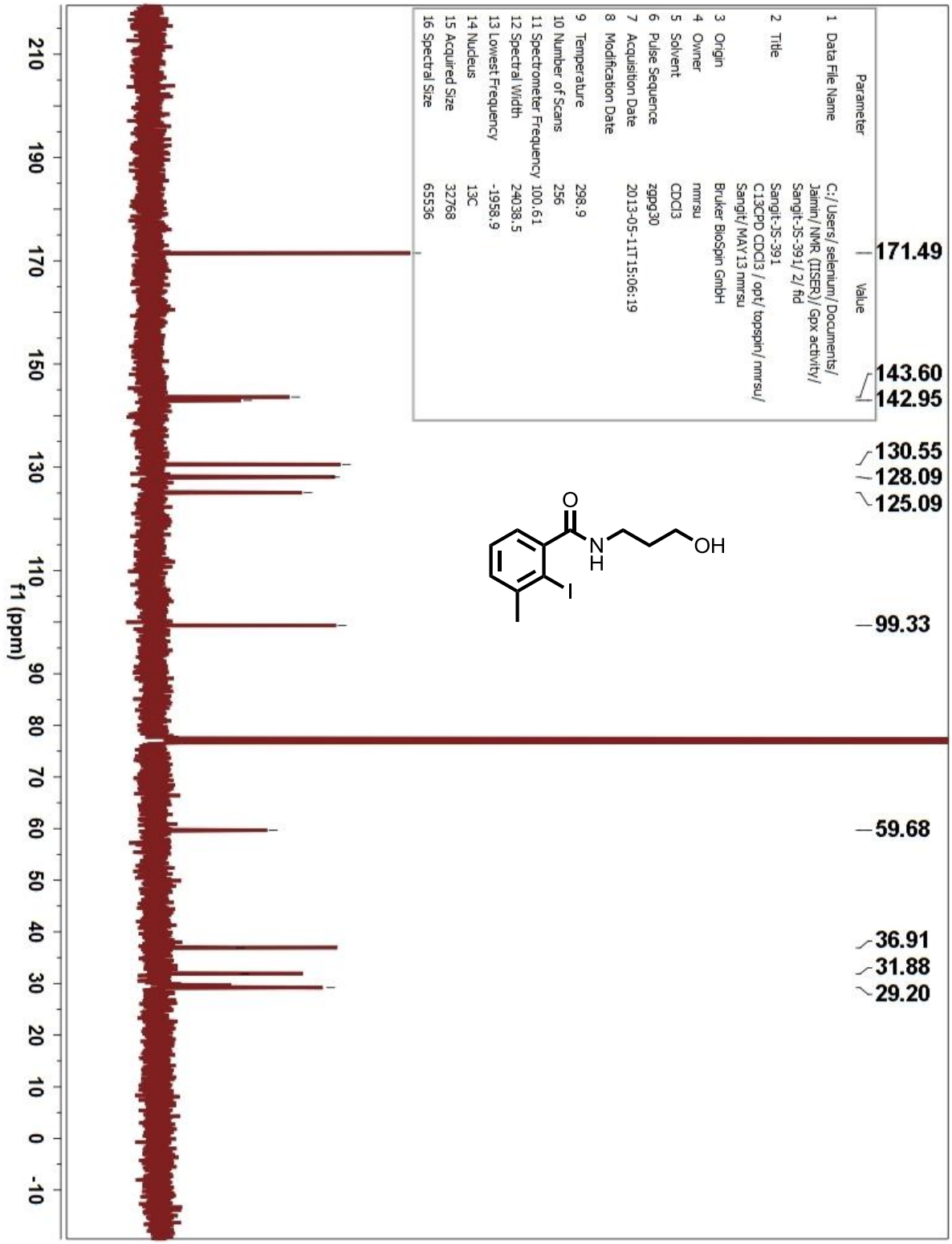


Figure S35 HRMS of precursor of **1f**

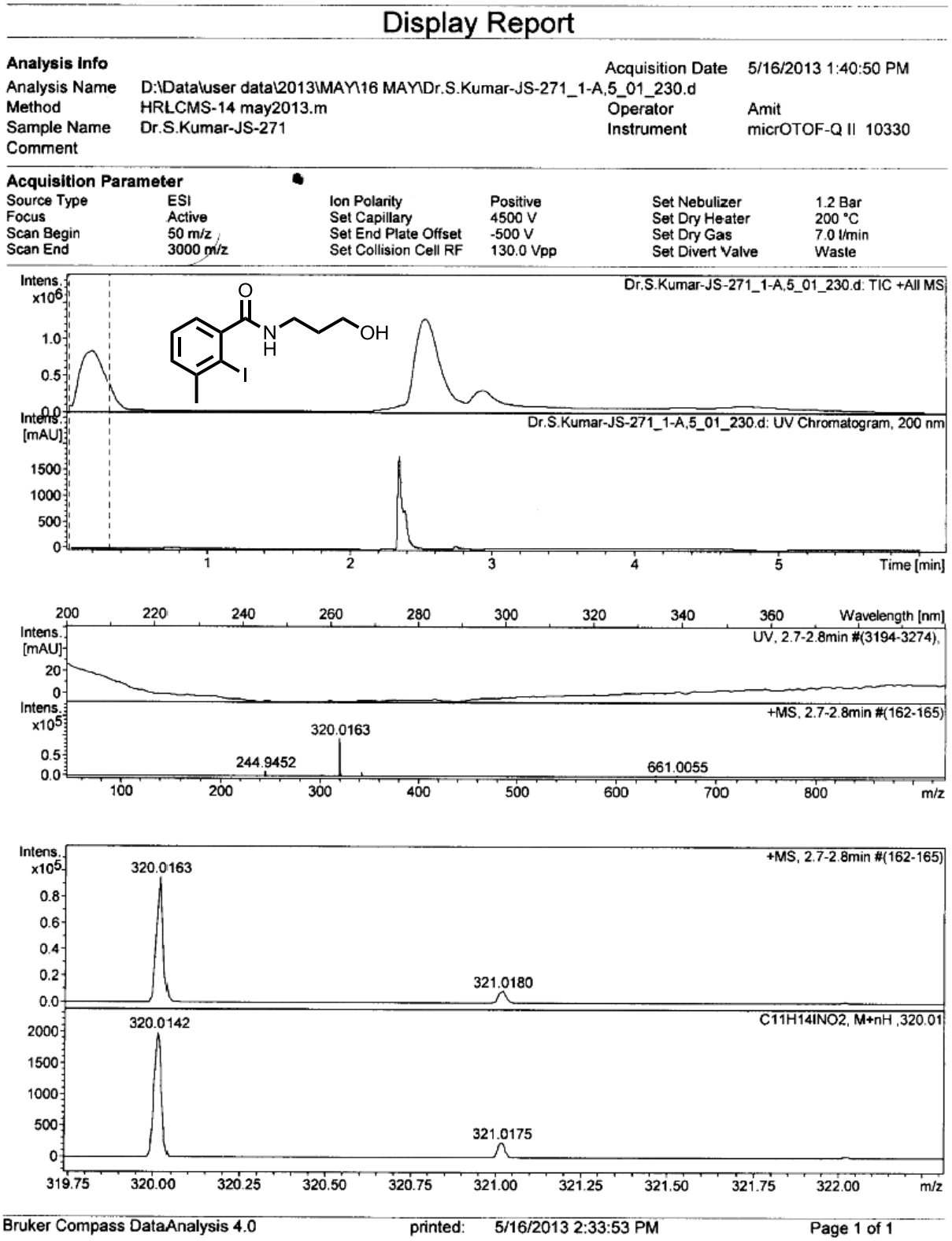


Figure S36 ^{1}H NMR of **1f**

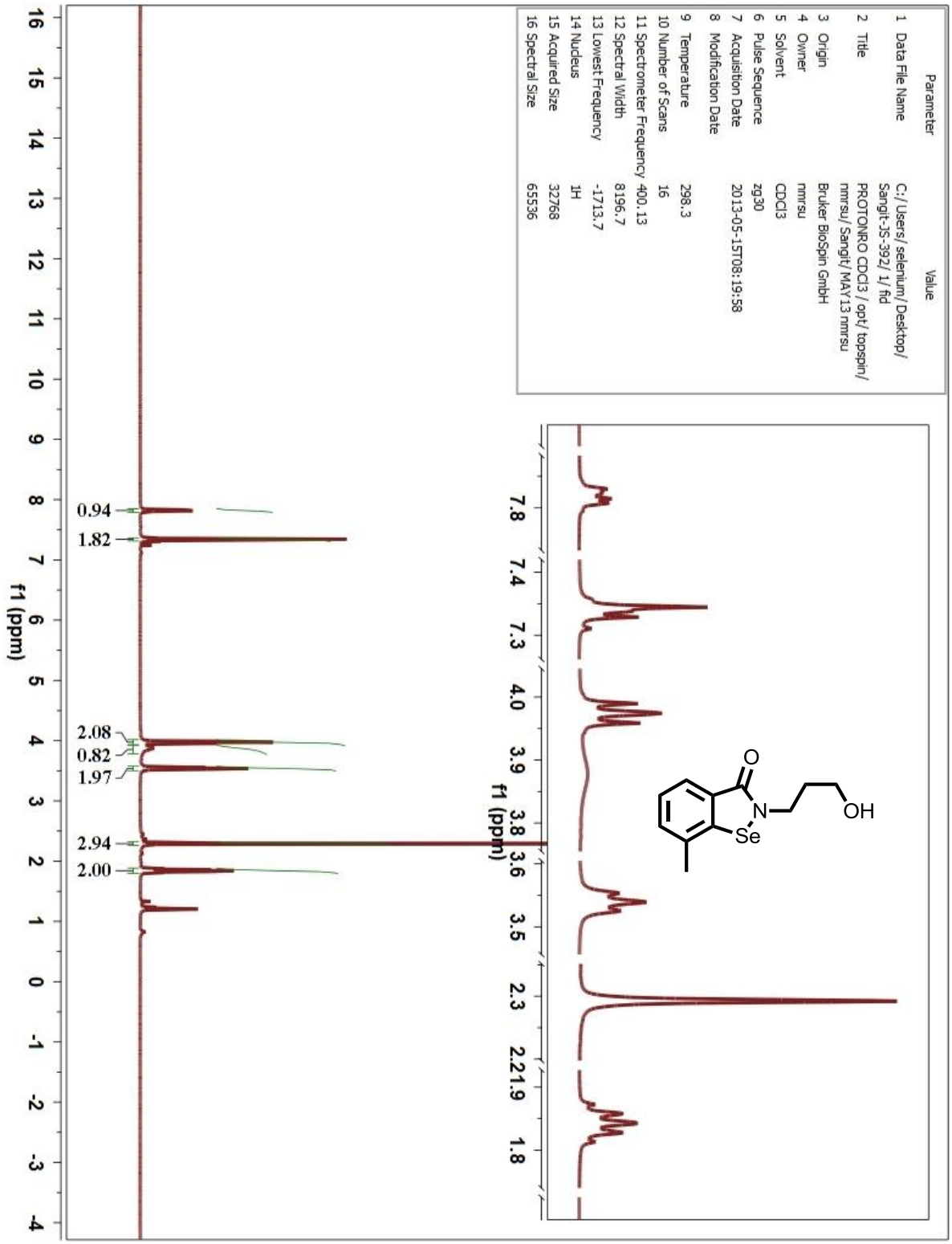


Figure S37 ^{13}C NMR of **1f**

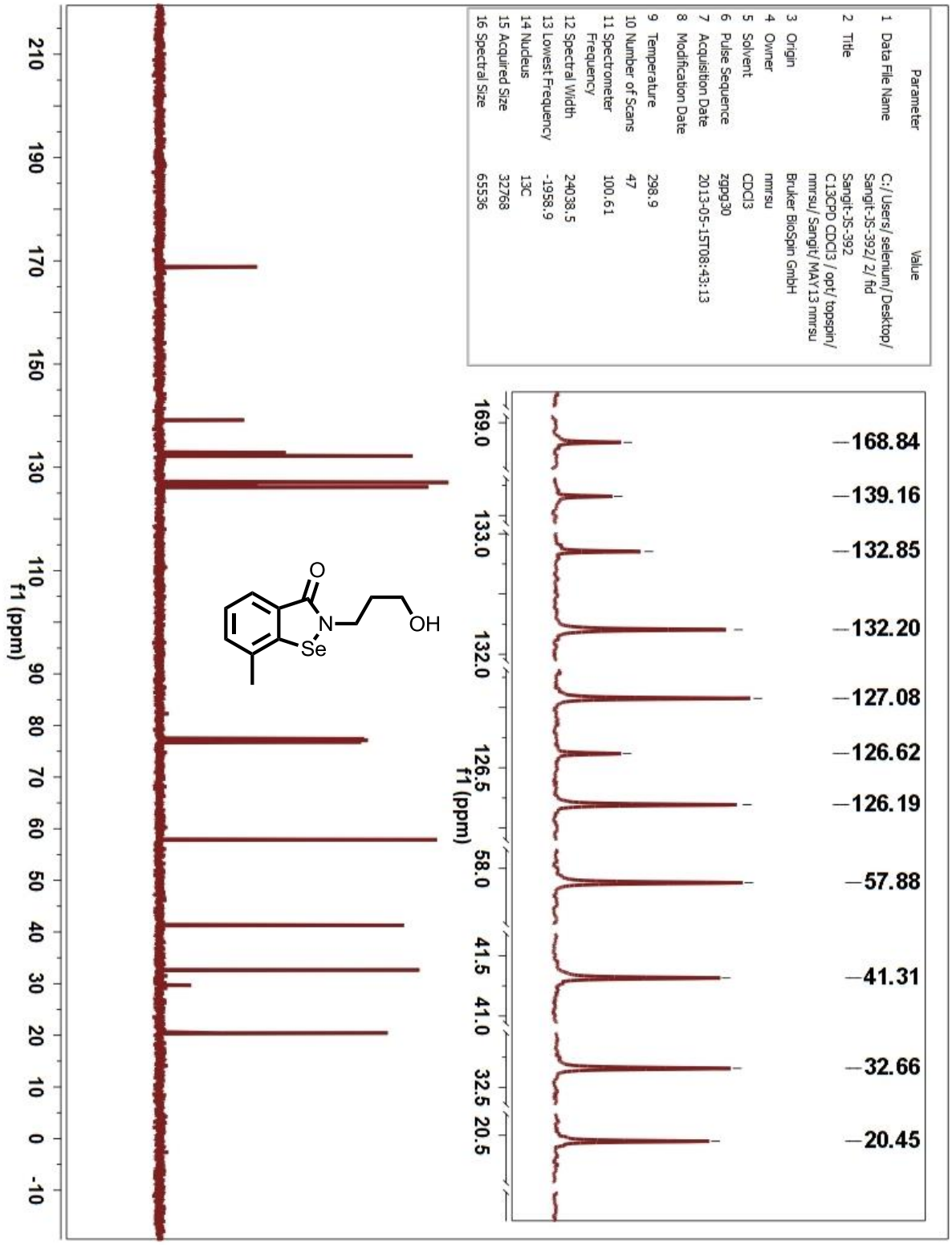
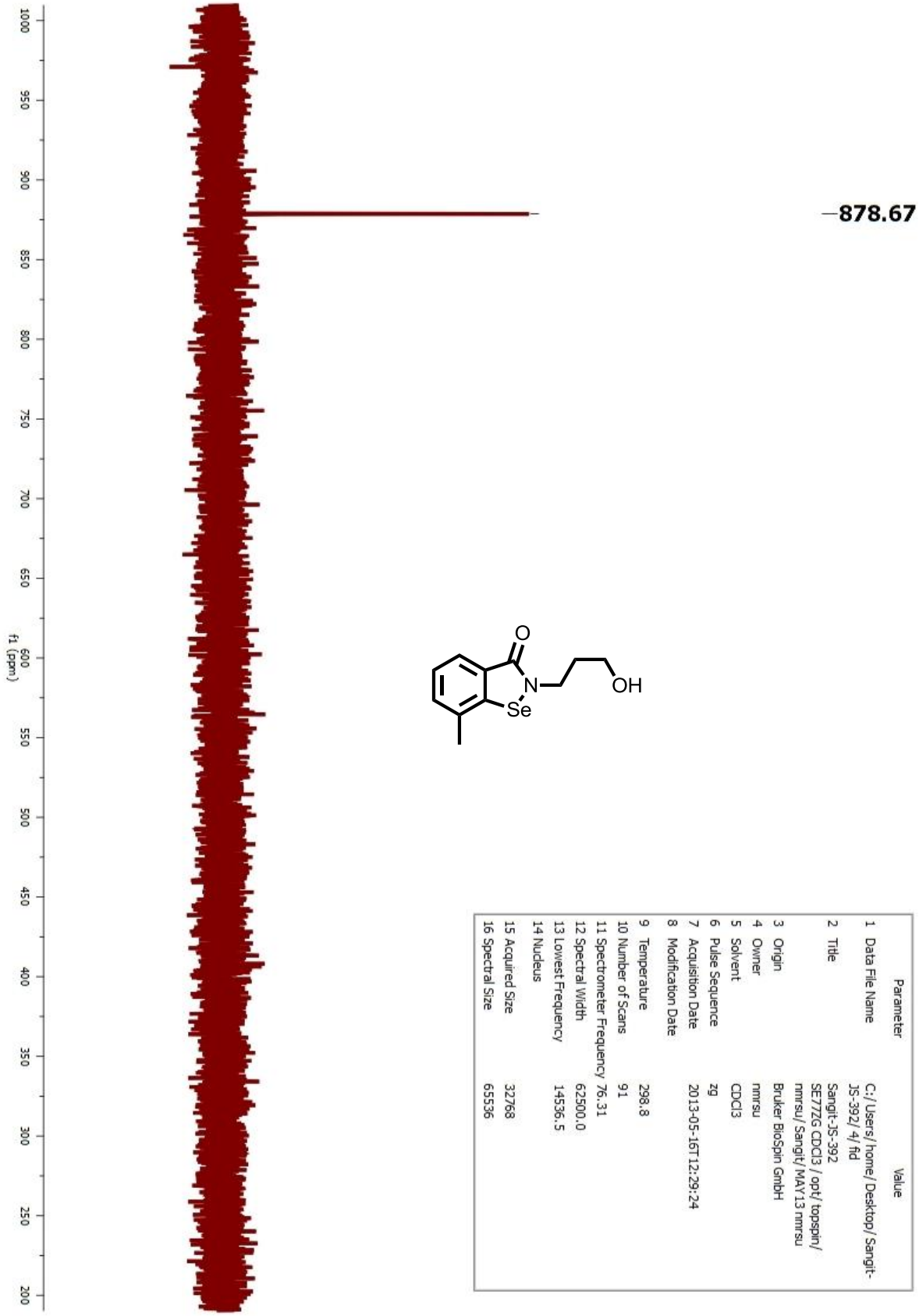


Figure S38 ^{77}Se NMR of **1f**



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3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	CDCl3
6	Pulse Sequence	zg
7	Acquisition Date	2013-05-16T12:29:24
8	Modification Date	
9	Temperature	298.8
10	Number of Scans	91
11	Spectrometer Frequency	76.31
12	Spectral Width	62500.0
13	Lowest Frequency	14536.5
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

Figure S39 HRMS of **1f**

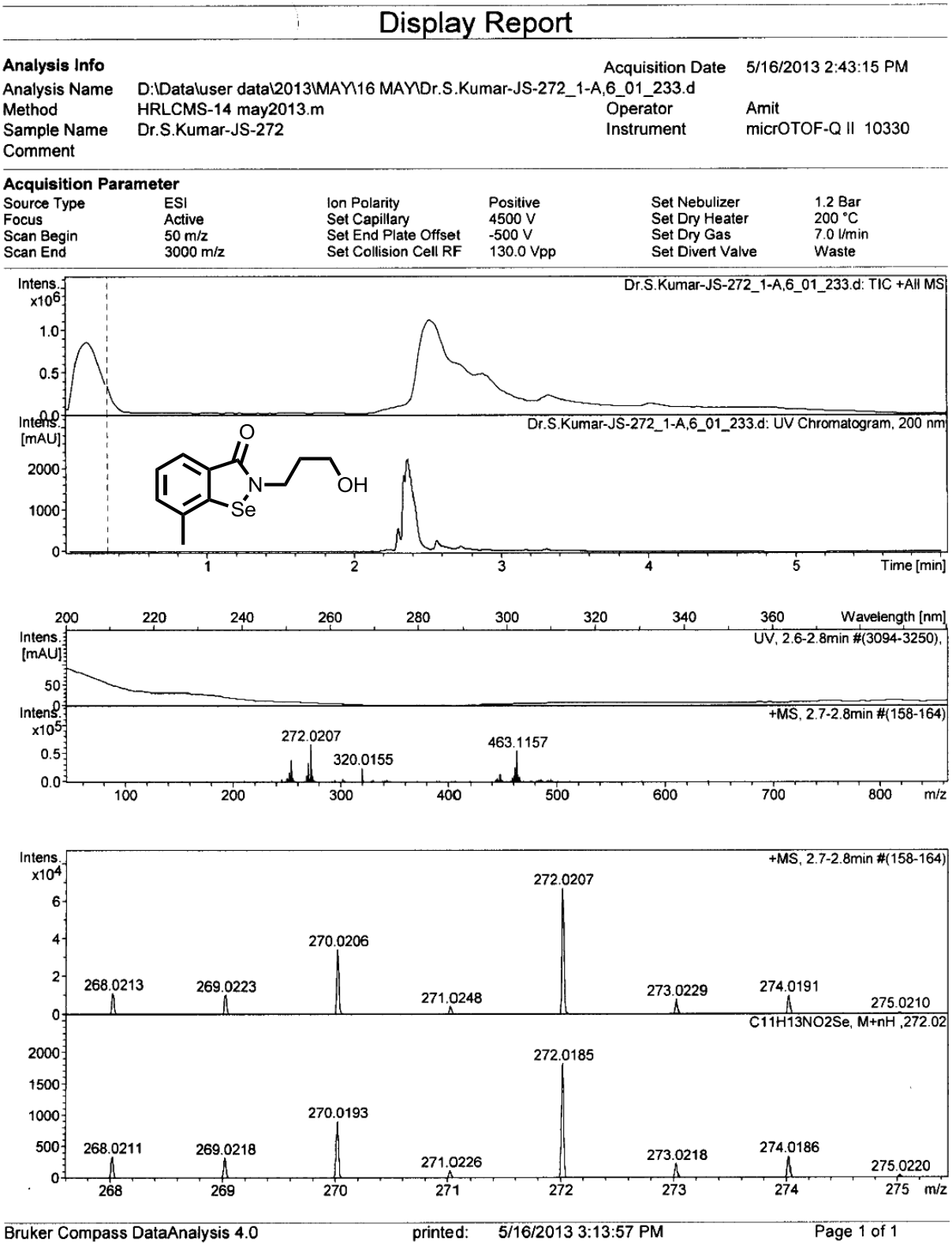


Figure S40 ^{1}H NMR of **1g**

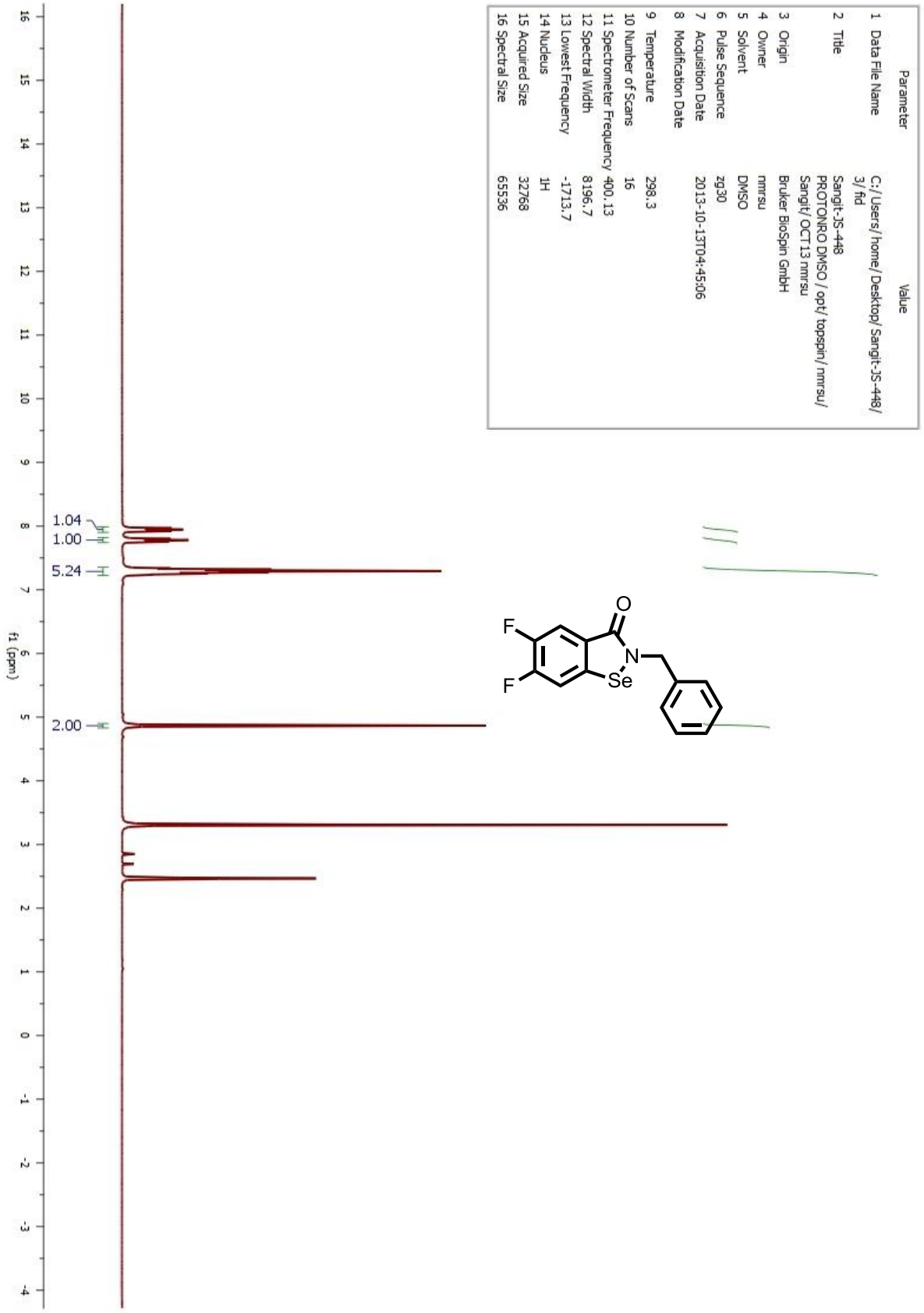


Figure S41 ^{13}C NMR of **1g**

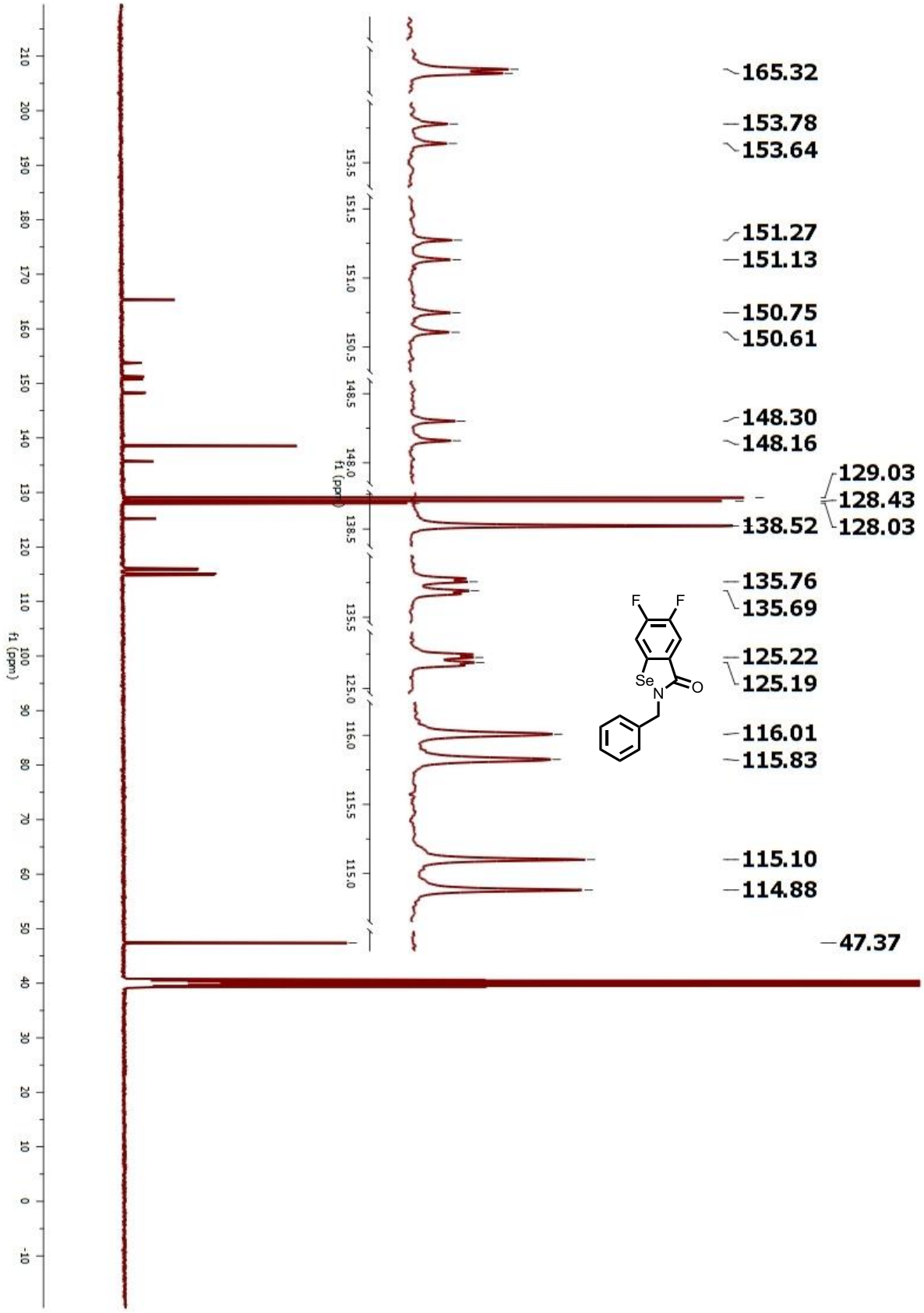
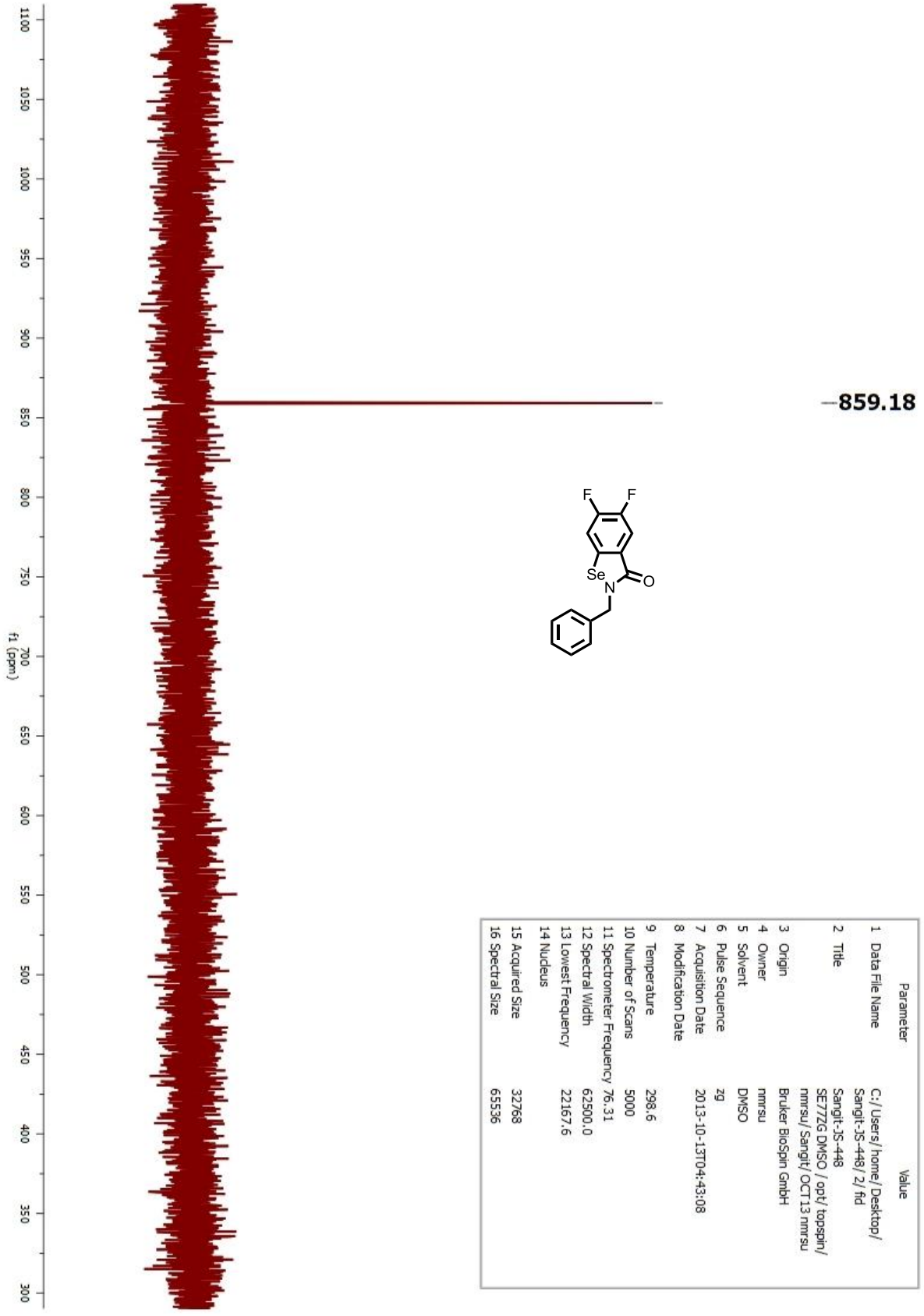


Figure S42 ^{77}Se NMR of **1g**



Parameter	Value
1 Data File Name	C:/Users/home/Desktop/Sangit-3S-448/2/fid
2 Title	Sangit-3S-448 SE77ZG DMSO /opt/topspin/nmrsu/Sangit/OCT13 nmrsu
3 Origin	Bruker BioSpin GmbH
4 Owner	nmrsu
5 Solvent	DMSO
6 Pulse Sequence	zg
7 Acquisition Date	2013-10-13T04:43:08
8 Modification Date	
9 Temperature	298.6
10 Number of Scans	5000
11 Spectrometer Frequency	76.31
12 Spectral Width	62500.0
13 Lowest Frequency	22167.6
14 Nucleus	
15 Acquired Size	32768
16 Spectral Size	65536

Figure S43 LRMS (ESI) spectrum of **1g** (*m/z* 326, calcd for $C_{14}H_9F_2ON^{80}Se + H^+$: 326).

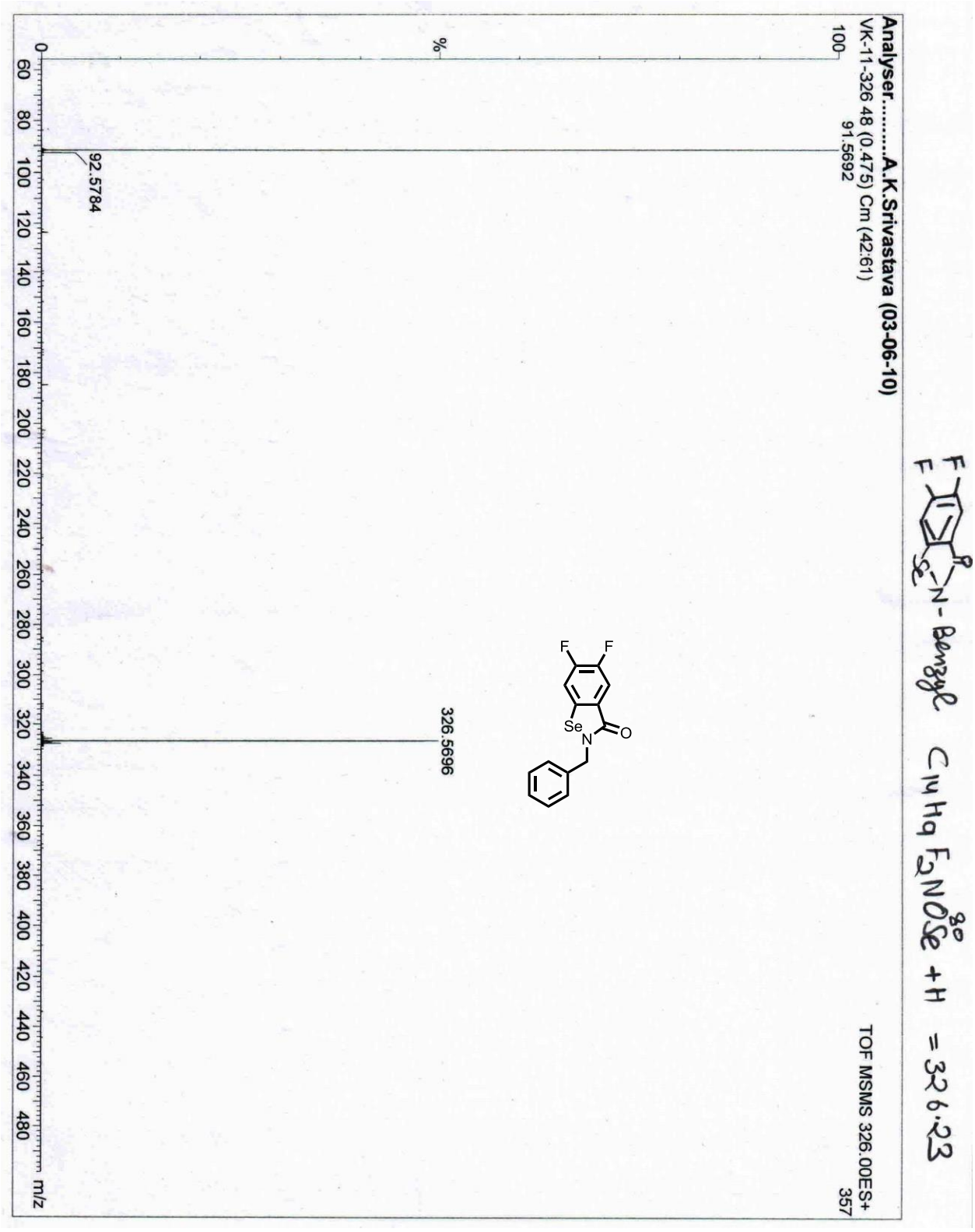


Figure S44 ^{1}H NMR of **1h**

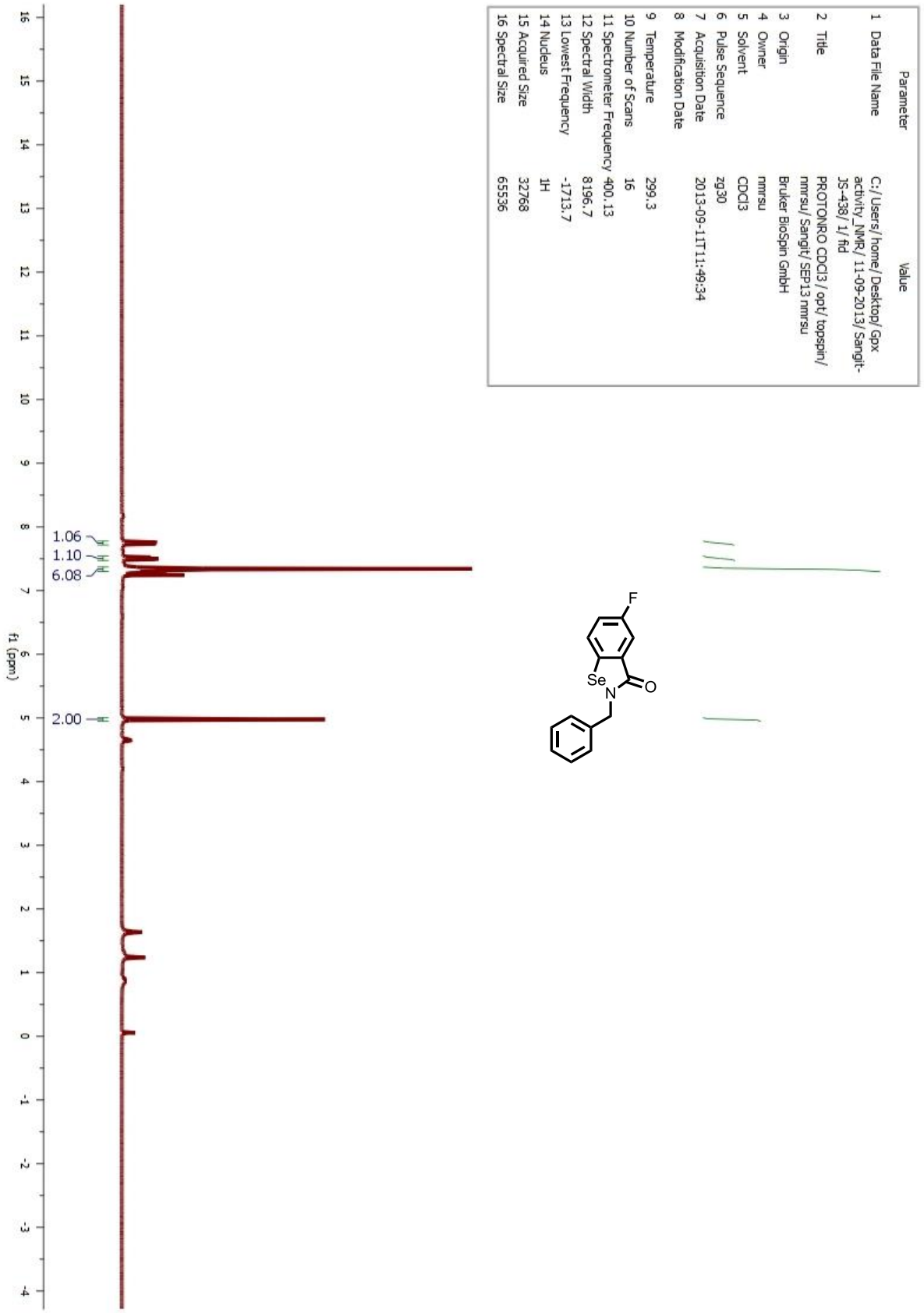


Figure S45 ^{13}C NMR of **1h**

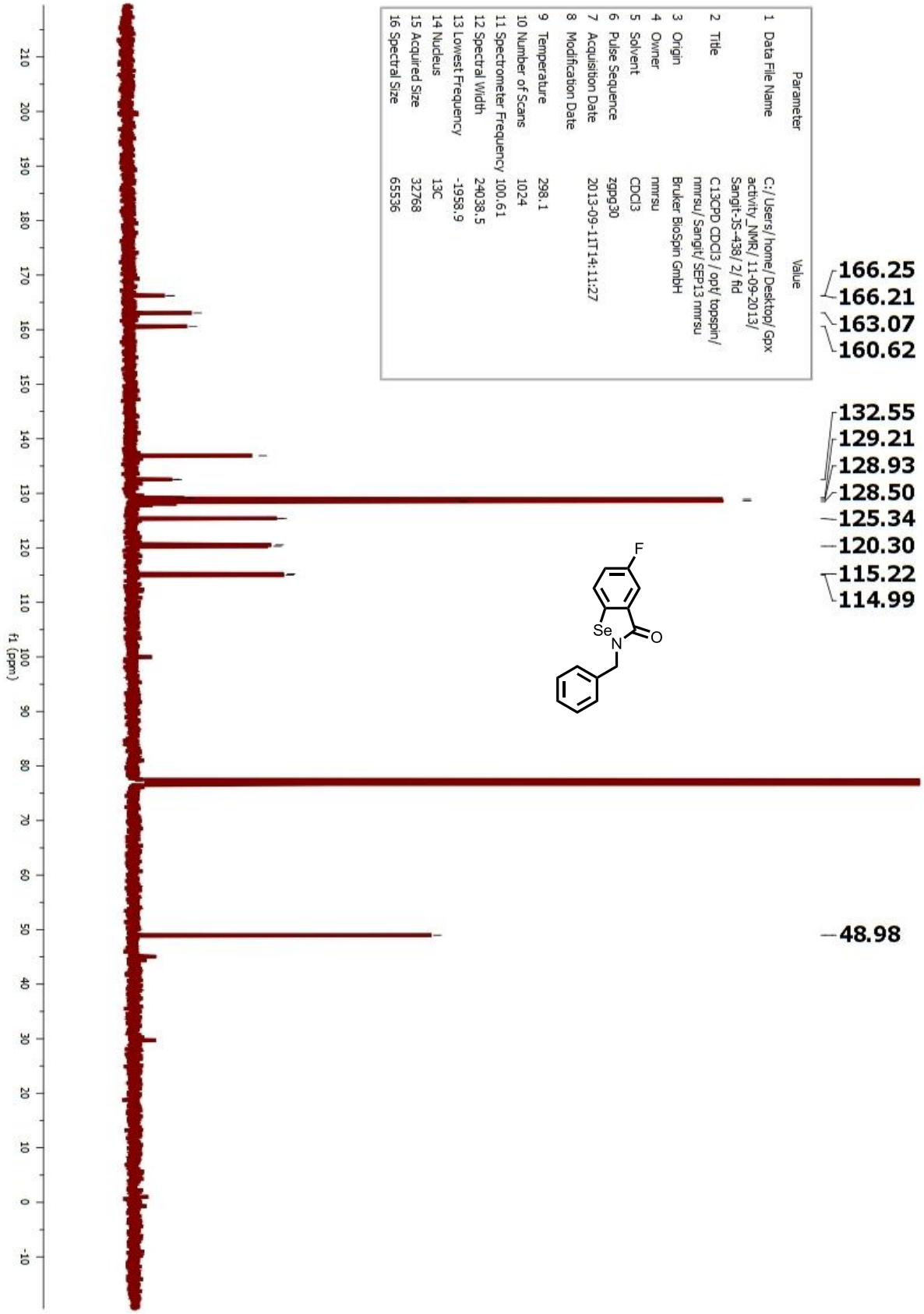
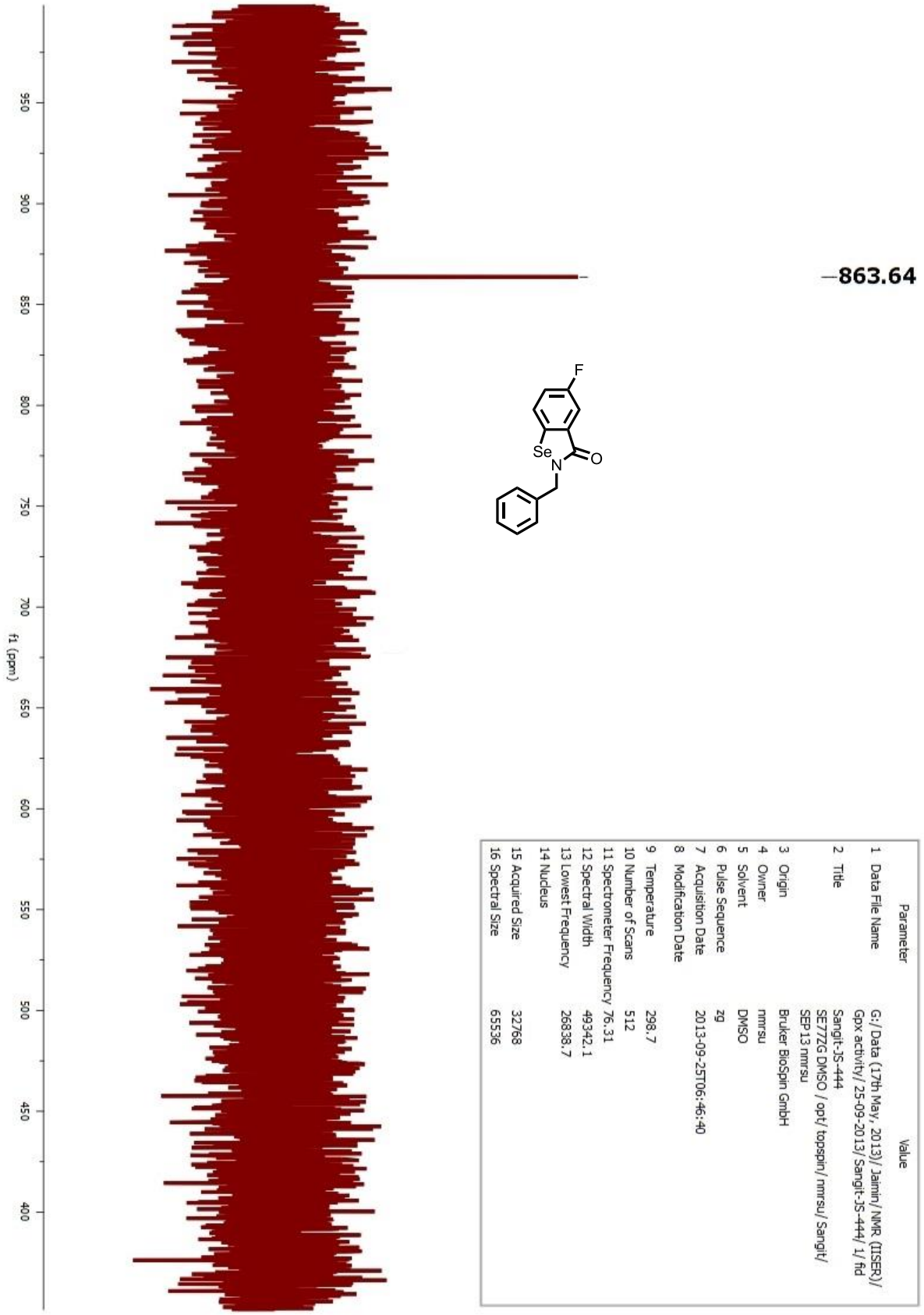


Figure S46 ^{77}Se of **1h**



	Parameter	Value
1	Data File Name	G:/Data (17th May, 2013)/Jaimin/NMR (IISER)/Gpx activity/25-09-2013/Sangit-JS-444/1/fid
2	Title	Sangit-JS-444 SE77ZG DMSO / opt/ topspin/ nmrsu/ Sangit/ SEP13 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	DMSO
6	Pulse Sequence	zg
7	Acquisition Date	2013-09-25T06:46:40
8	Modification Date	
9	Temperature	298.7
10	Number of Scans	512
11	Spectrometer Frequency	76.31
12	Spectral Width	49342.1
13	Lowest Frequency	26838.7
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

Figure S47 LRMS of **1h**

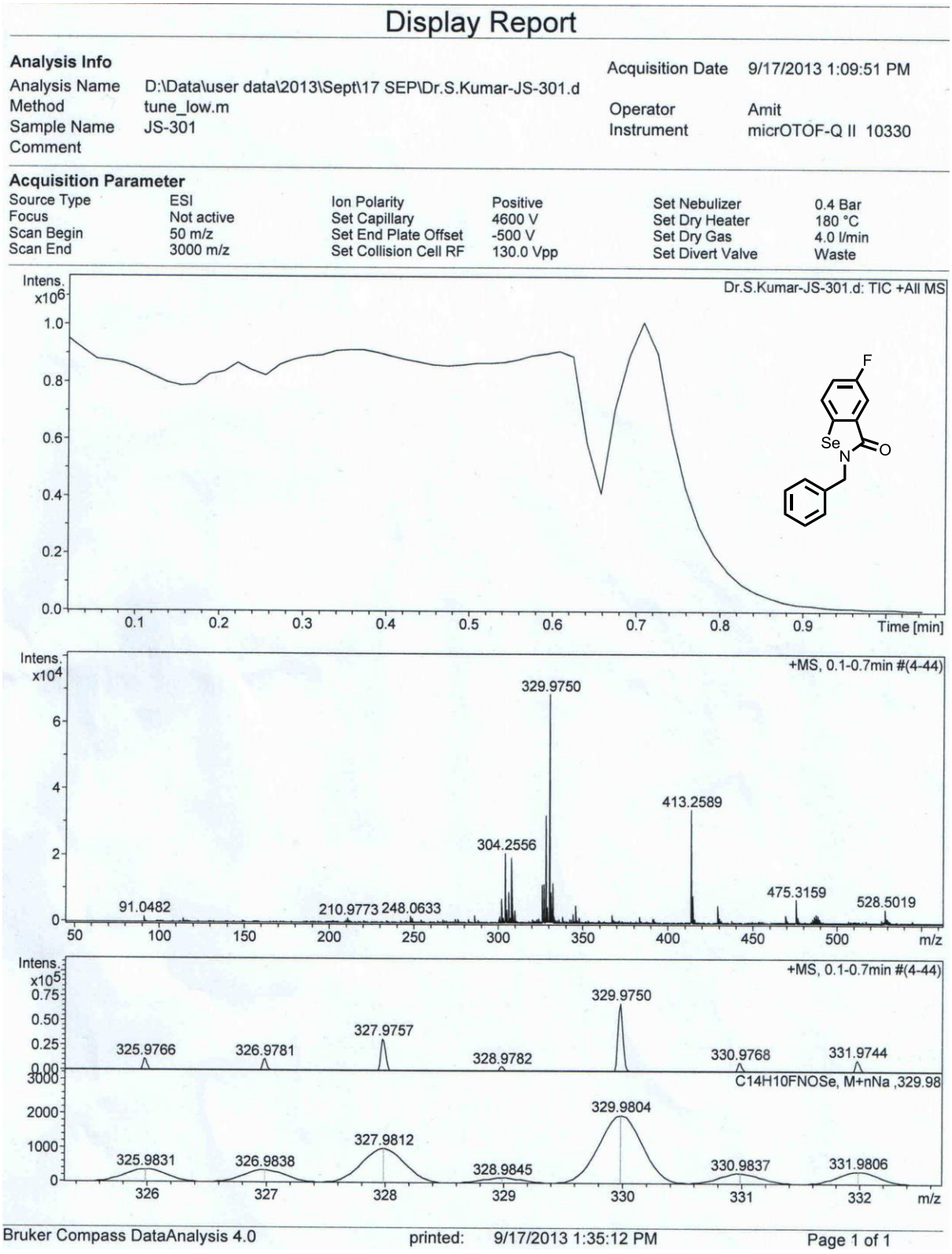


Figure S48 ^{1}H NMR of **1i**

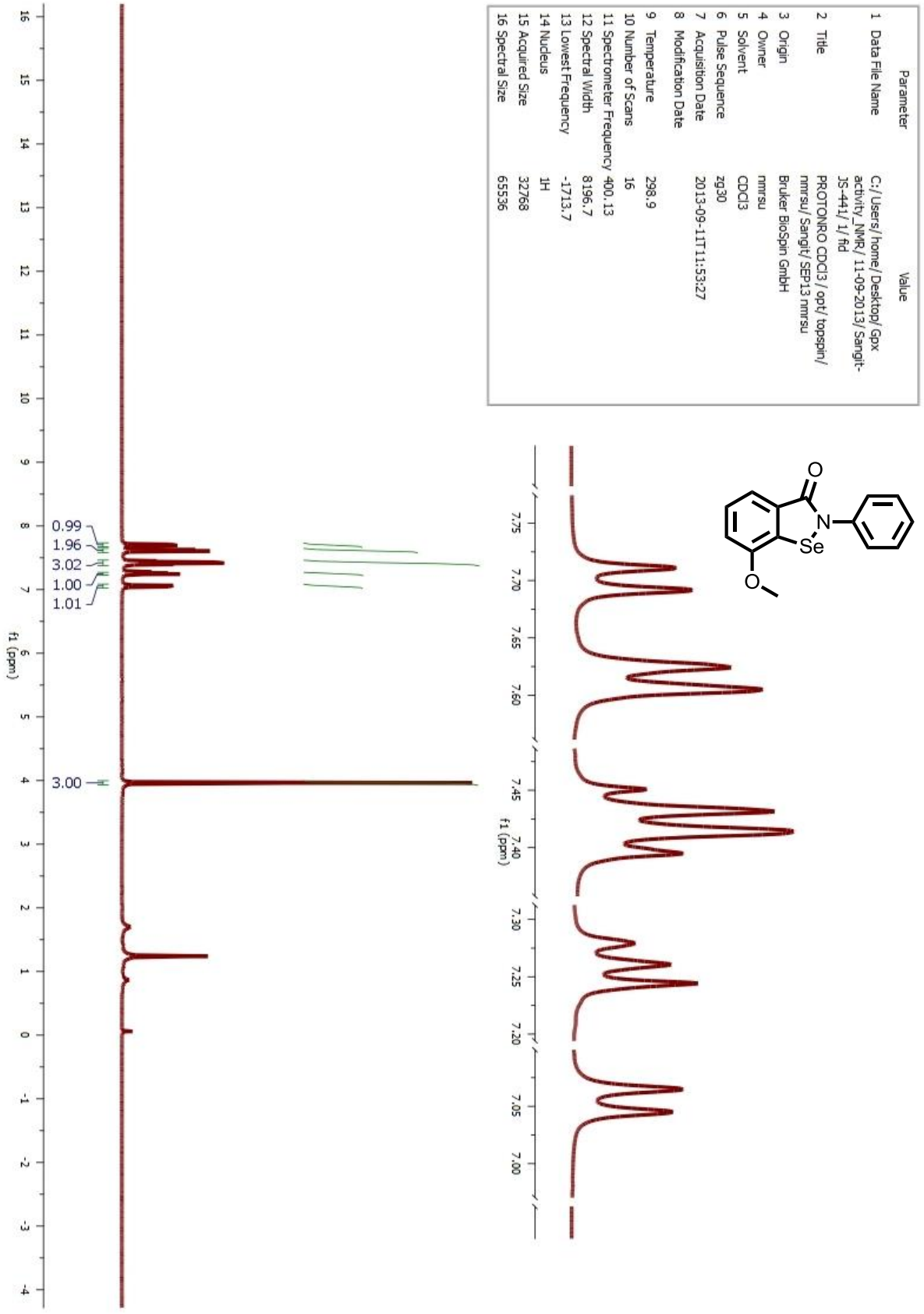


Figure S49 ^{13}C NMR of **1i**

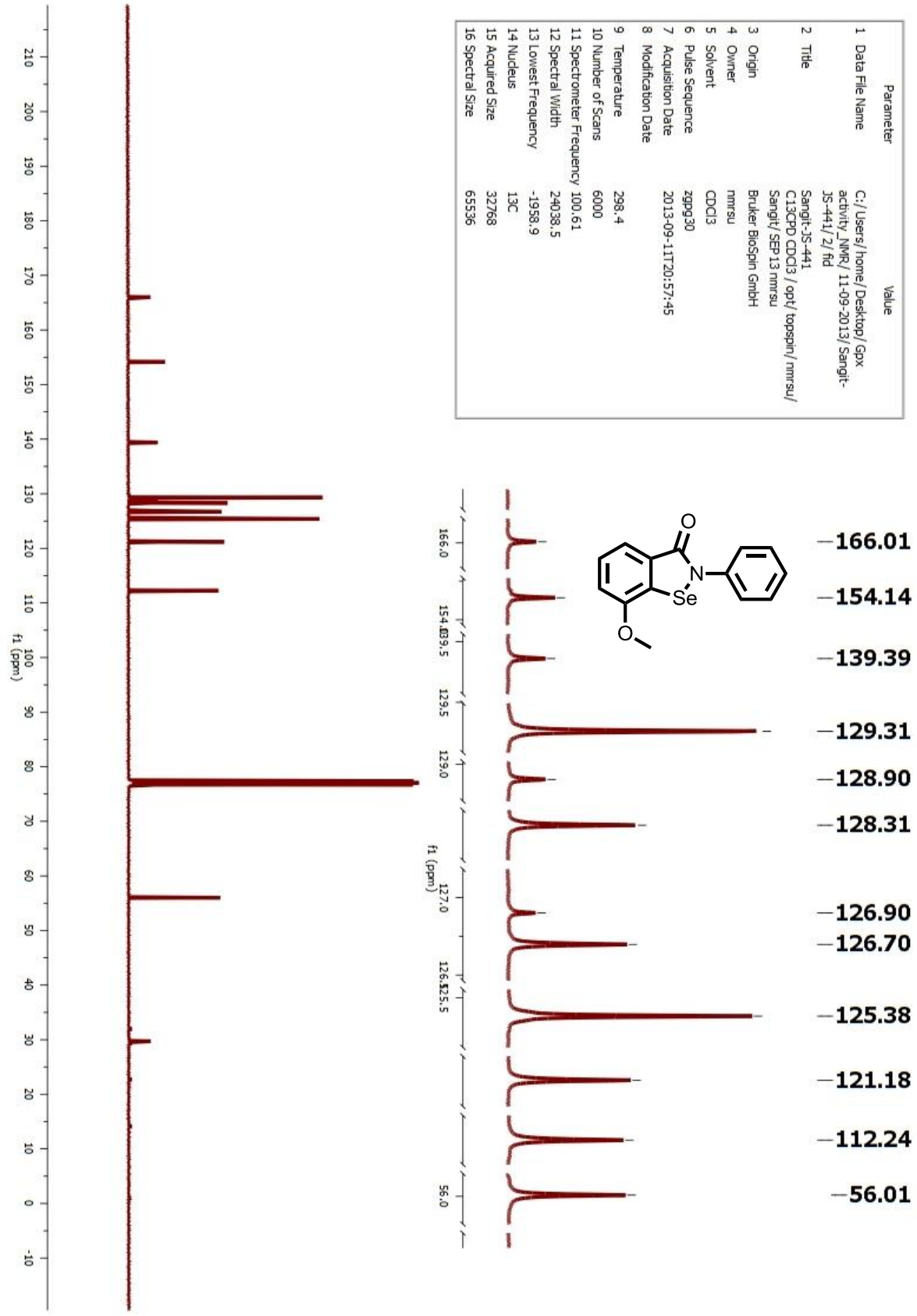
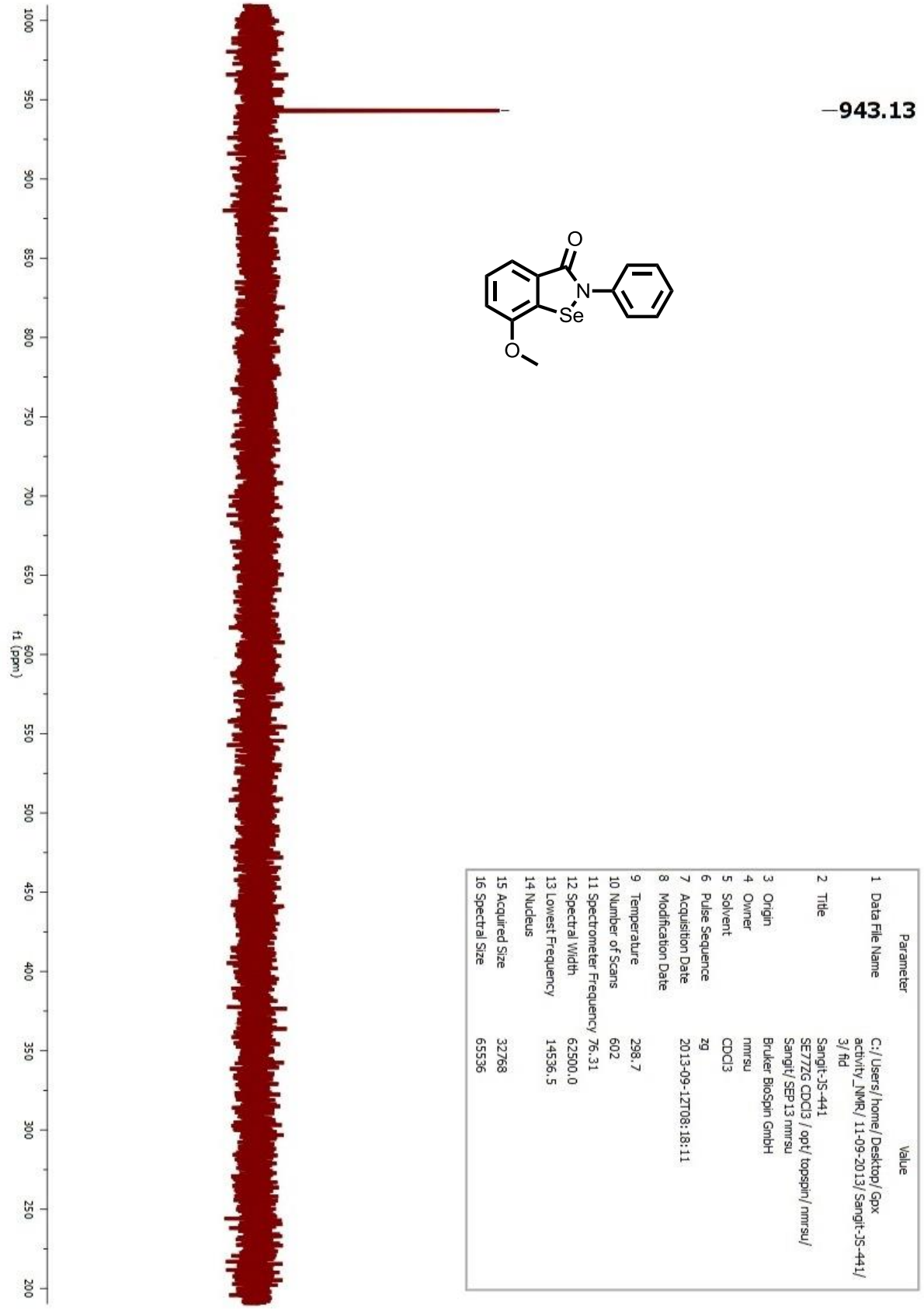


Figure S50 ^{77}Se NMR of **1i**



Parameter	Value
1 Data File Name	C:/ Users/ home/ Desktop/ Gpx activity_NMR/ 11-09-2013/ Sangit-JS-441/ 3/ fid
2 Title	Sangit-JS-441 SE77ZG CDCl3 / opt/ topspin/ nmrsu/ Sangit/ SEP 13 nmrsu
3 Origin	Bruker BioSpin GmbH
4 Owner	nmrsu
5 Solvent	CDCl3
6 Pulse Sequence	zg
7 Acquisition Date	2013-09-12T08:18:11
8 Modification Date	
9 Temperature	298.7
10 Number of Scans	602
11 Spectrometer Frequency	76.31
12 Spectral Width	62500.0
13 Lowest Frequency	14536.5
14 Nucleus	
15 Acquired Size	32768
16 Spectral Size	65536

Figure S51 HRMS of **1i**

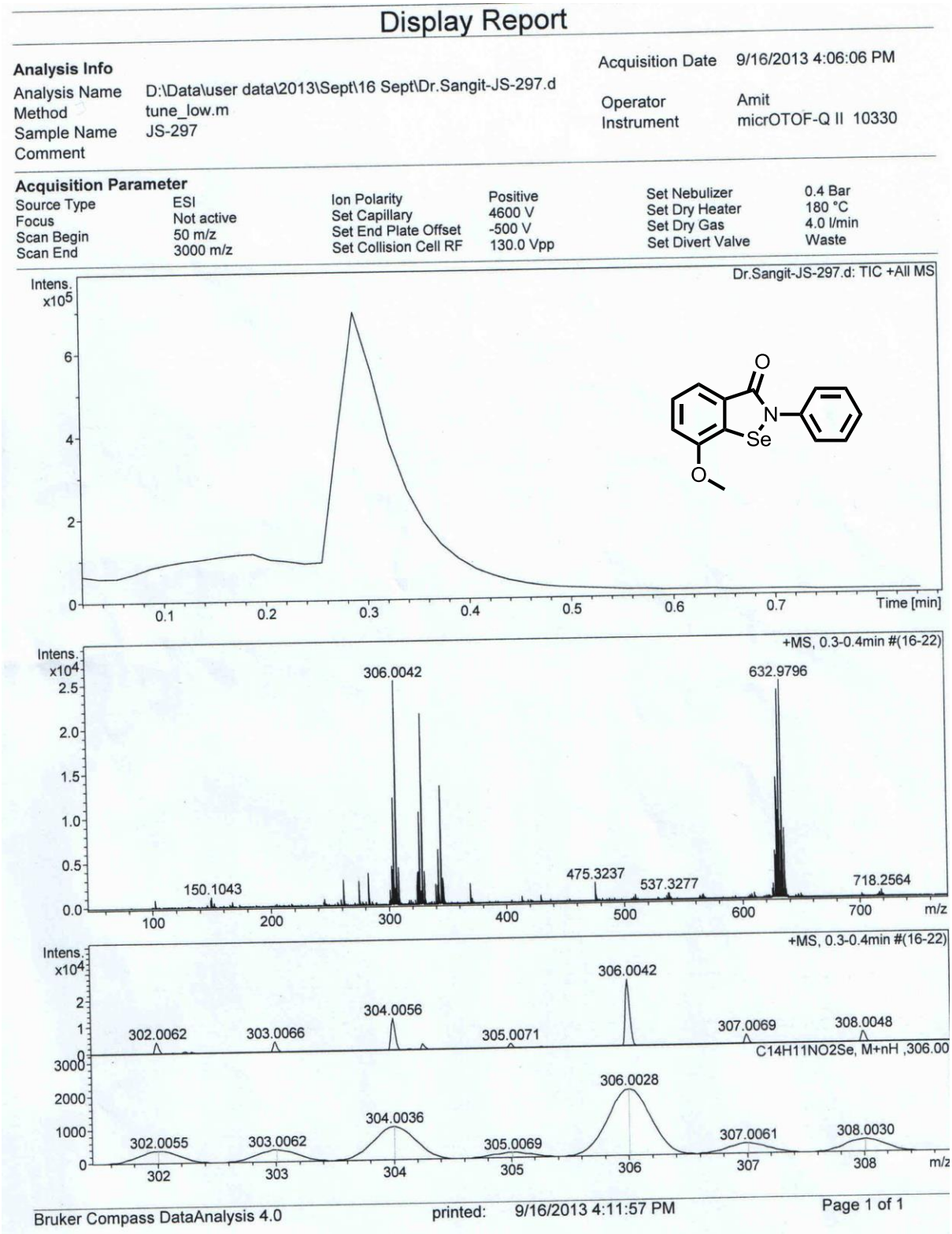


Figure S52 ^{1}H NMR of precursor of **1j**

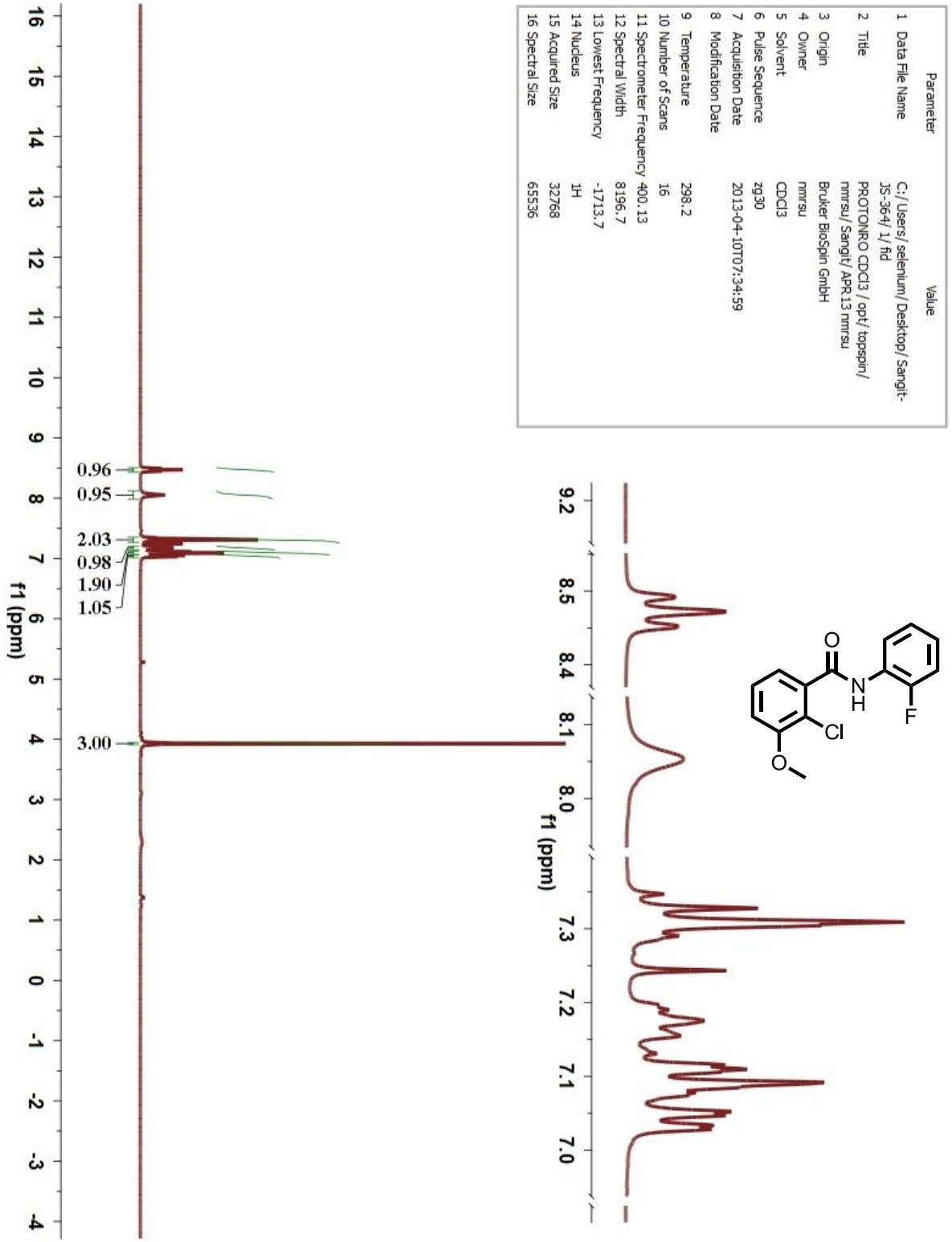


Figure S53 ^{13}C NMR of precursor of **1j**

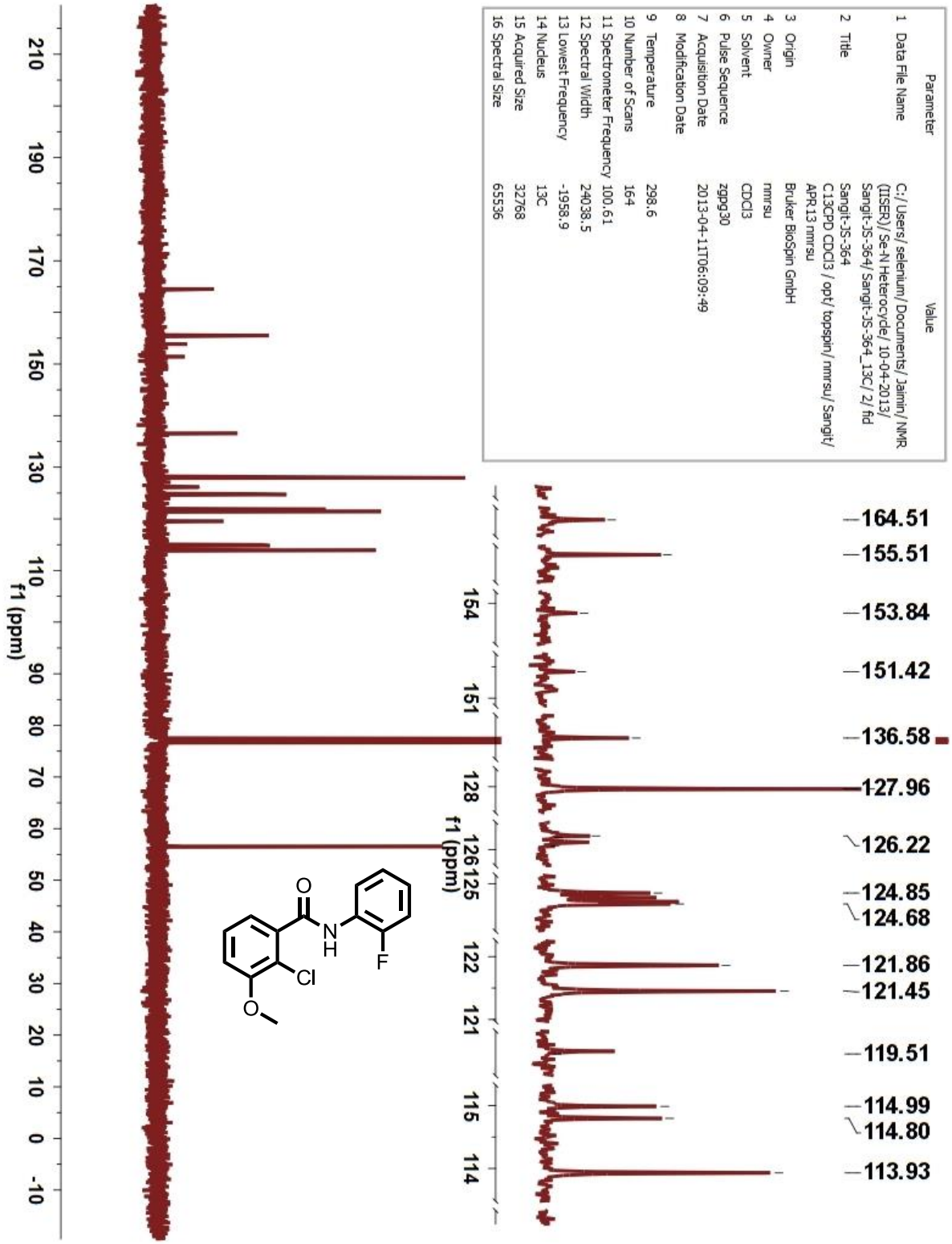


Figure S54 HRMS of precursor for **1j**

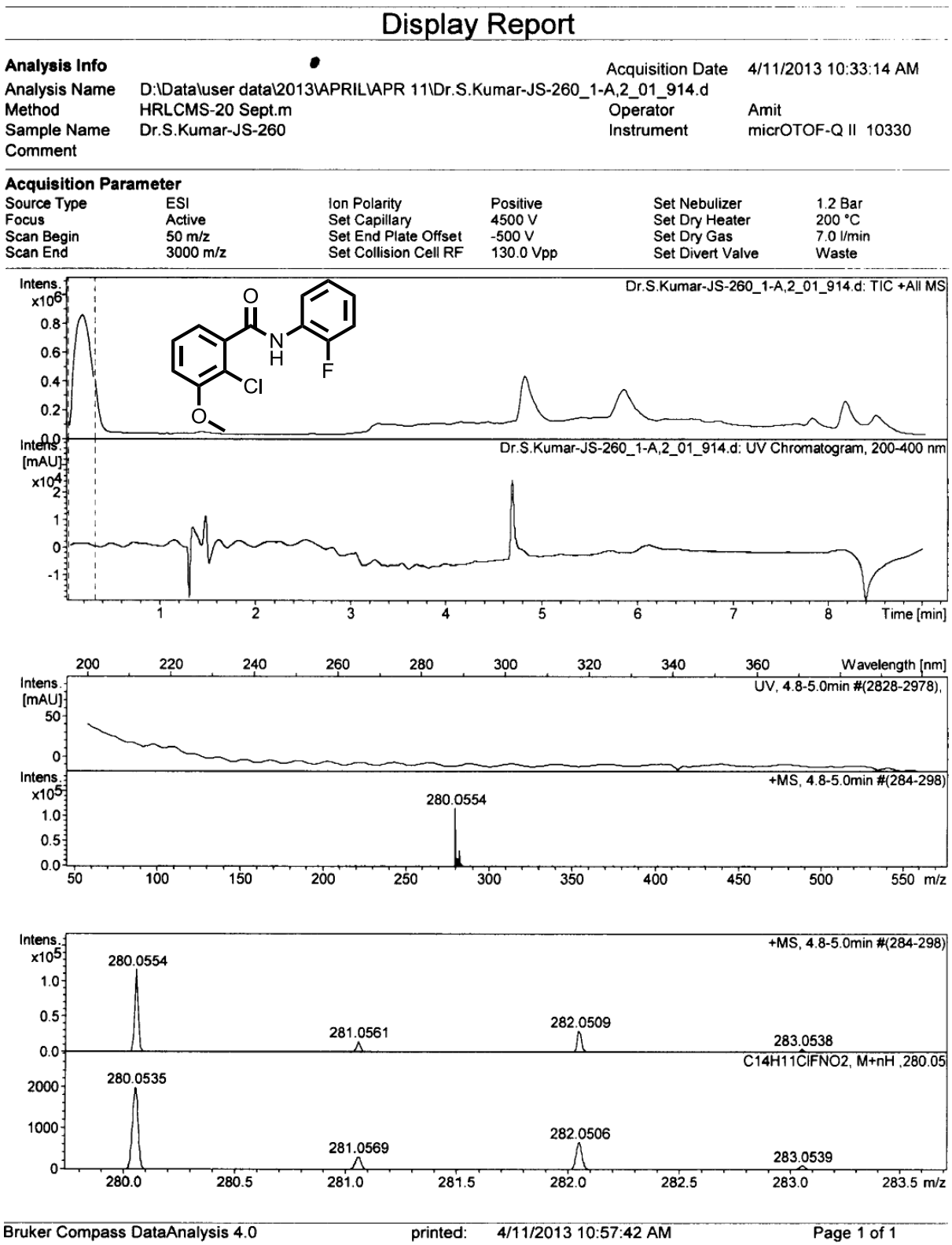


Figure S55 ^{1}H NMR of **1j**

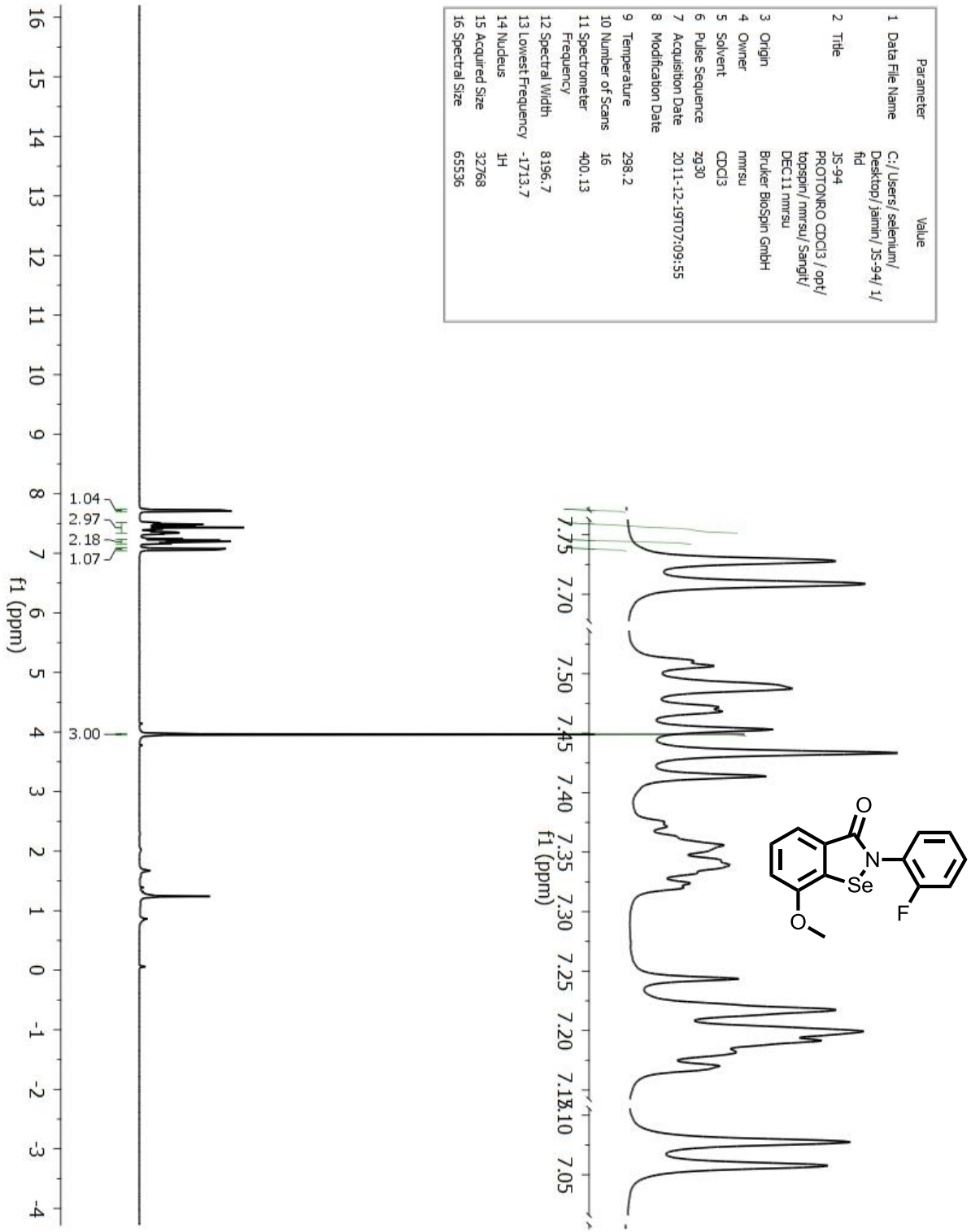


Figure S56 ^{13}C NMR of **1j**

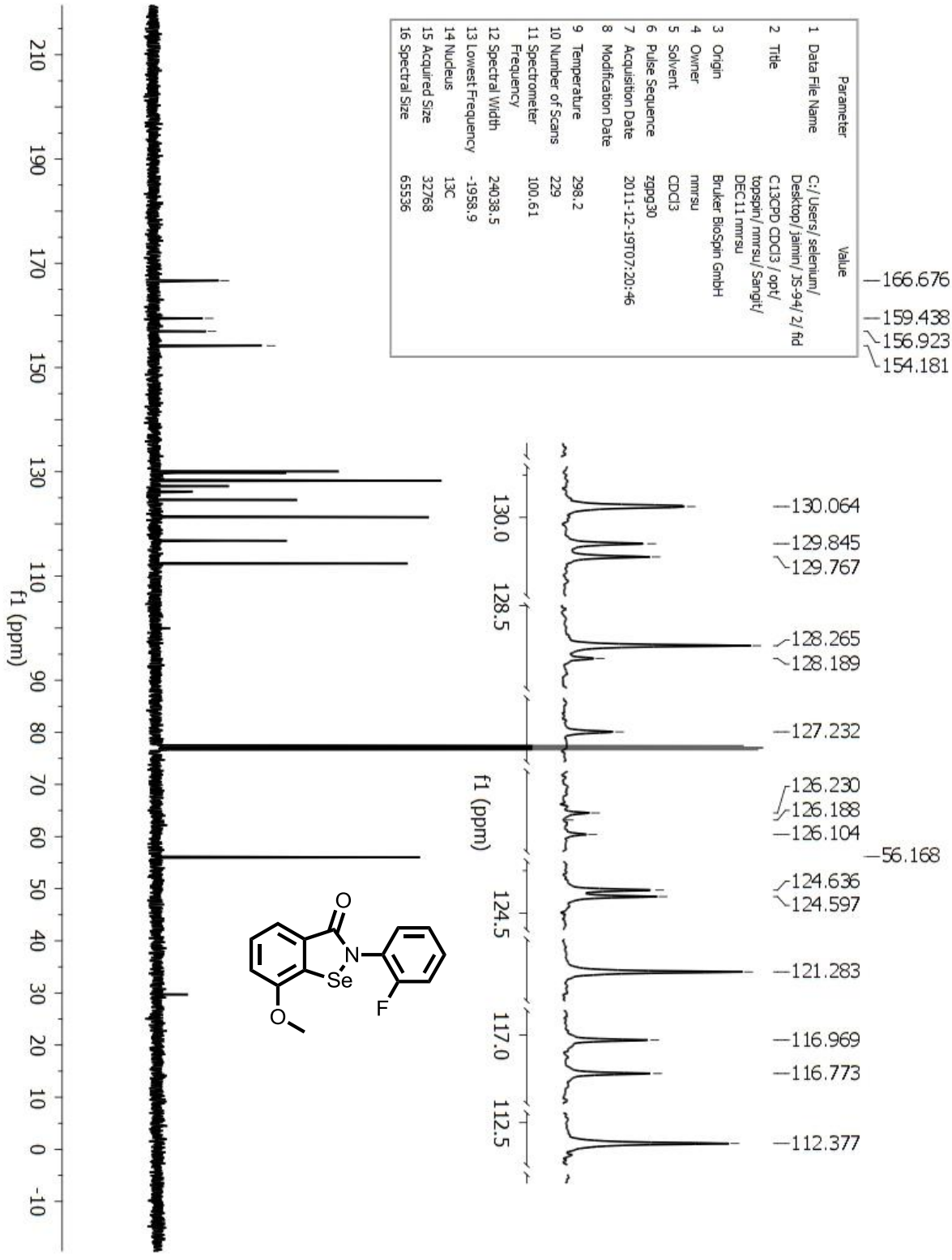


Figure S57 ^{77}Se NMR of **1j**

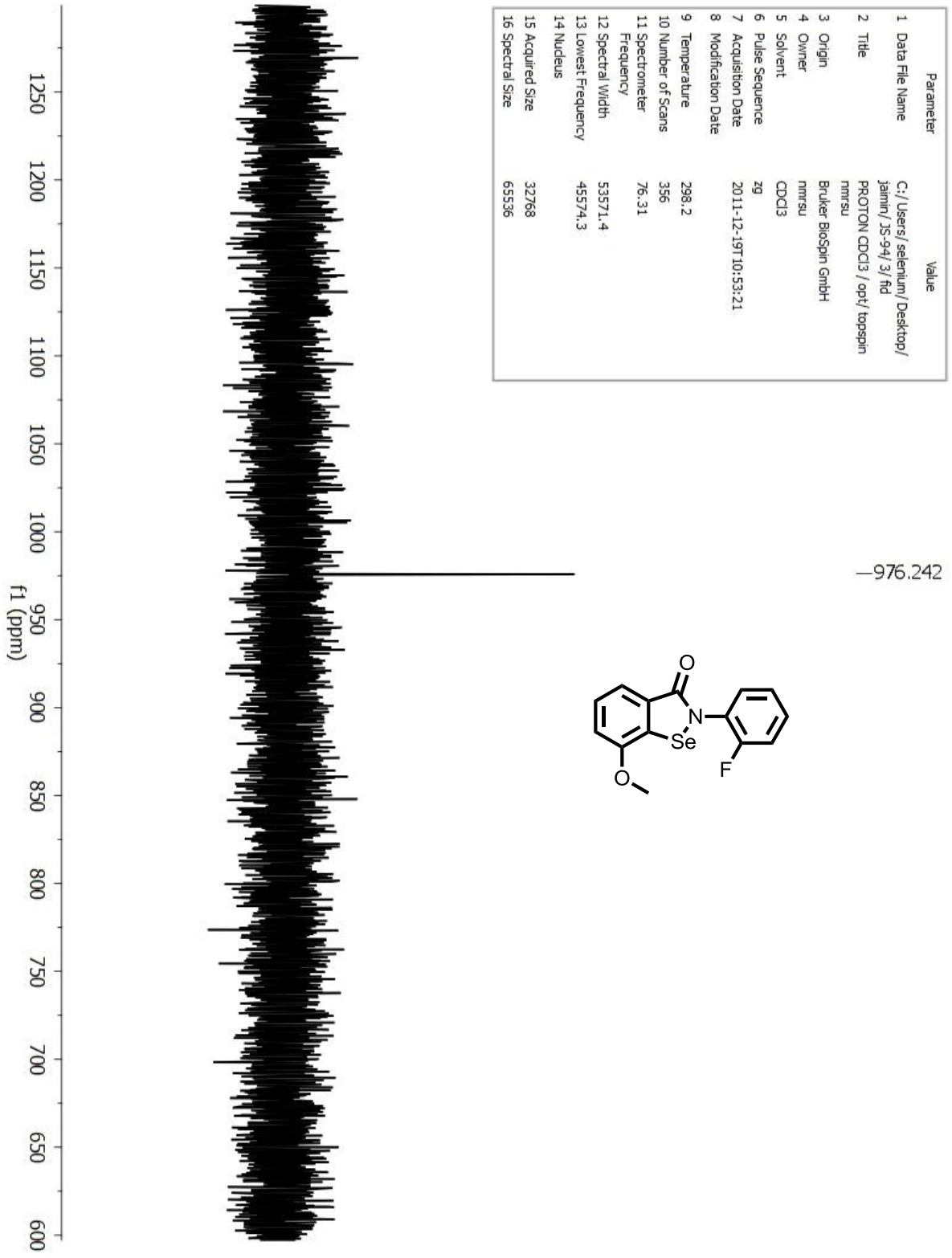


Figure S58 HRMSof**1j**

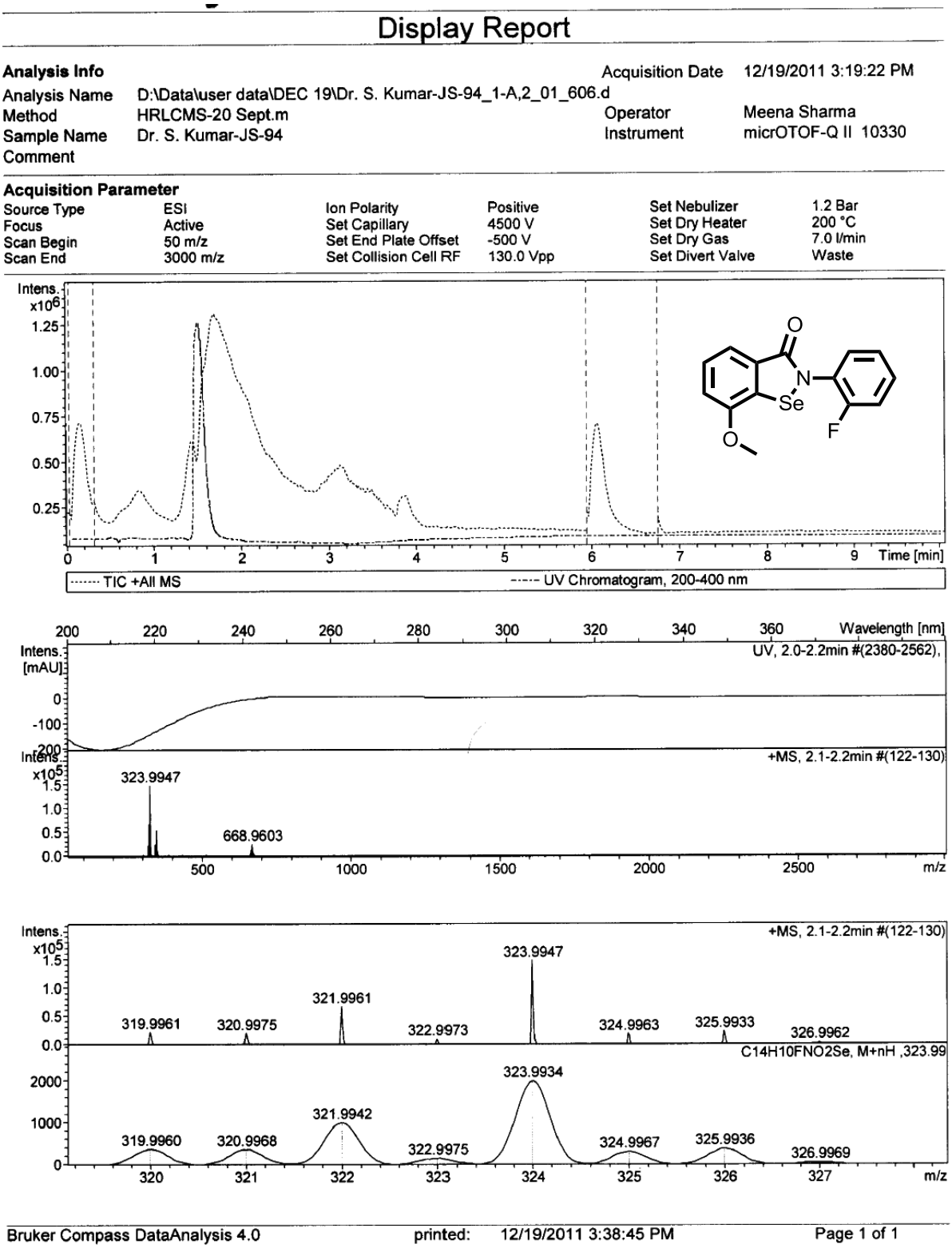


Figure S59 ^{1}H NMR of precursor of **1k**

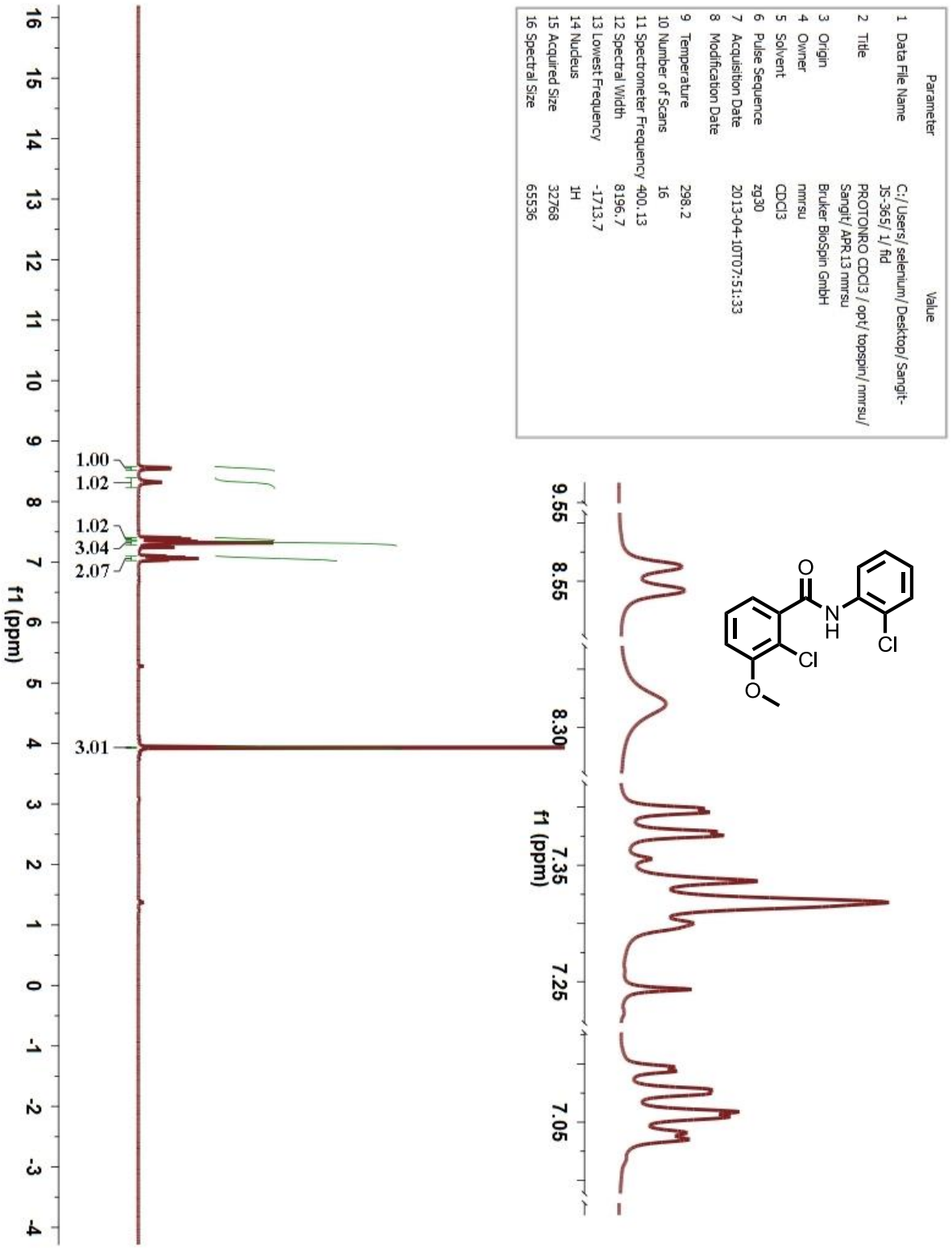


Figure S60 ^{13}C NMR of precursor of **1k**

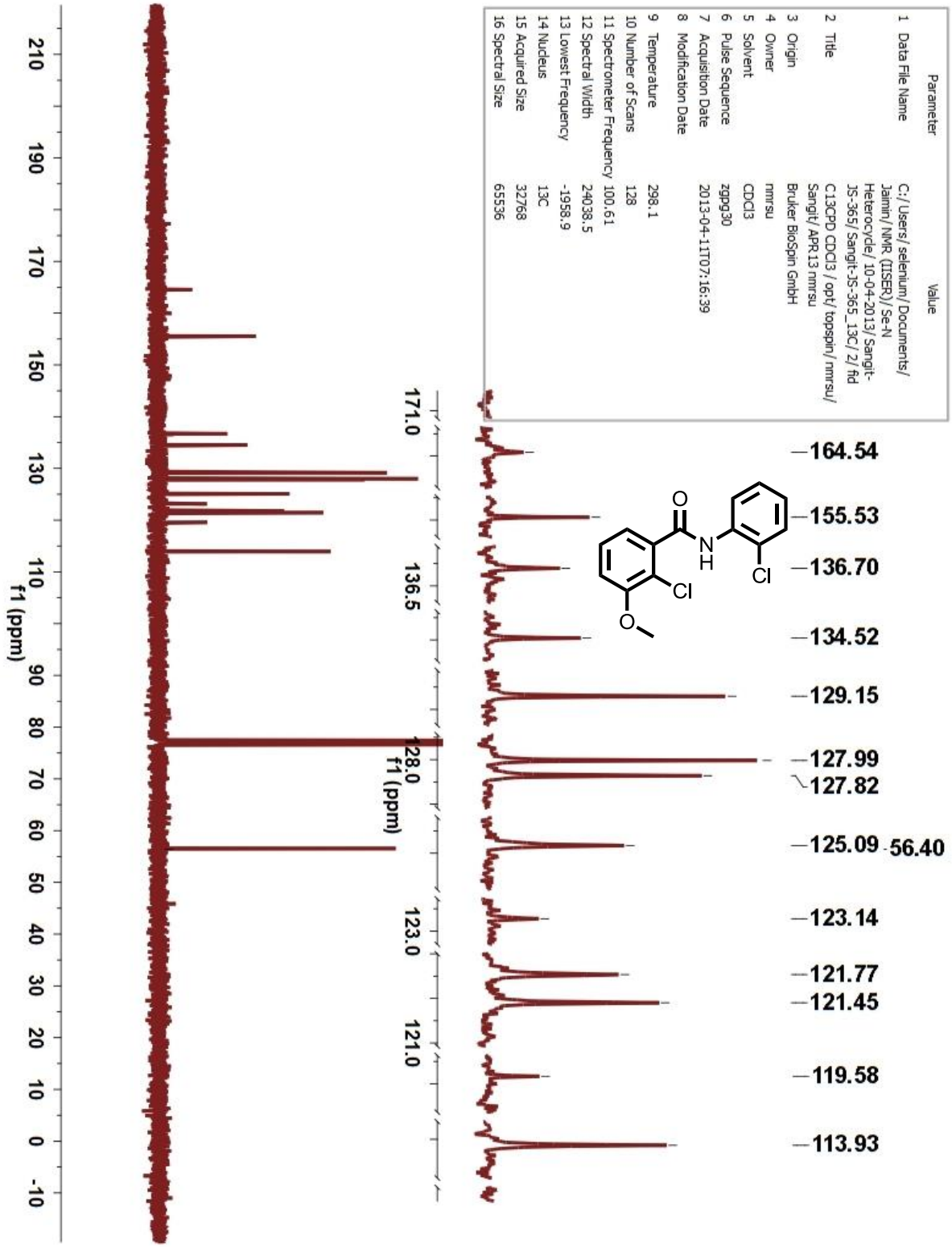


Figure S61 HRMS of precursor of **1k**

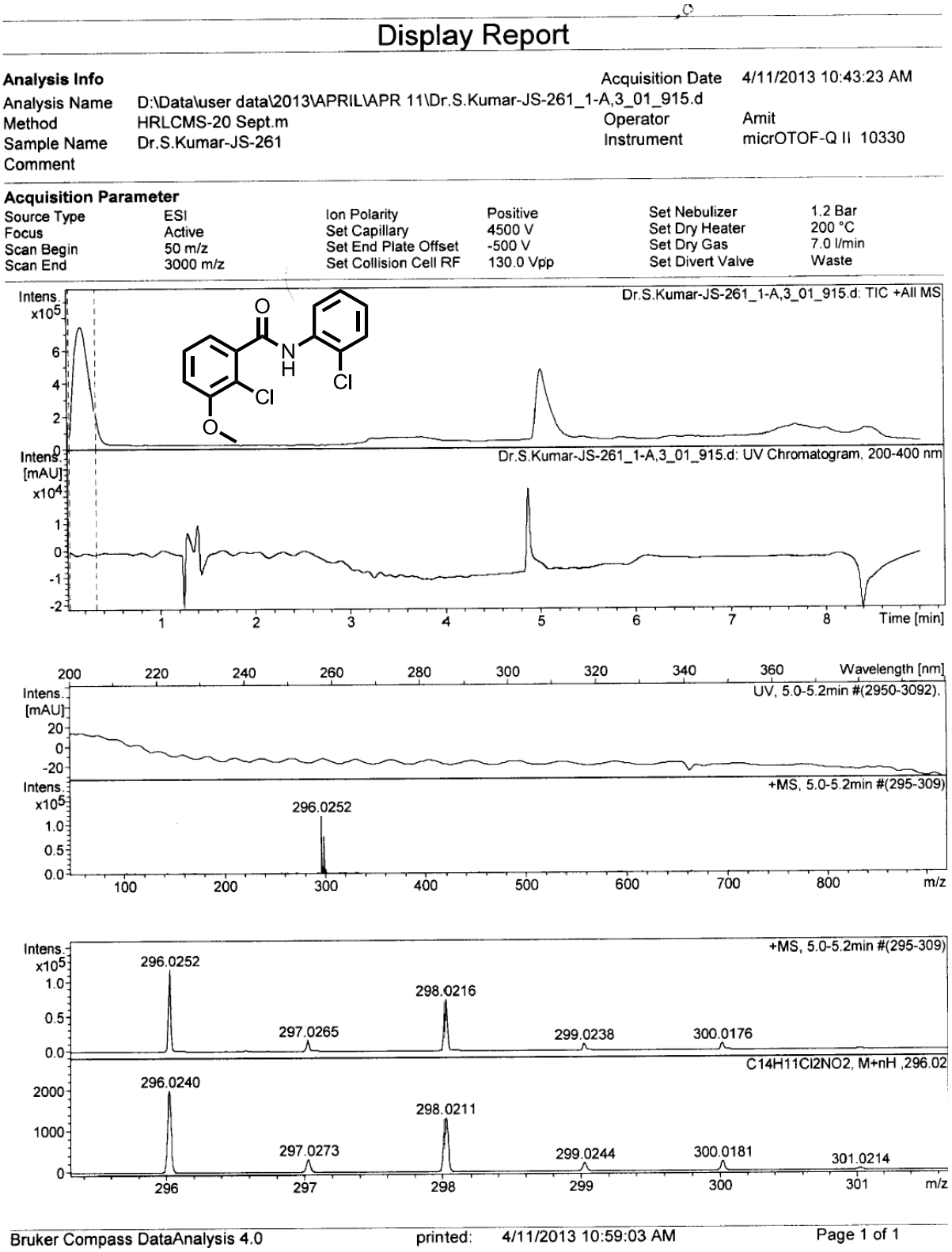


Figure S62 ^{1}H NMR of **1k**

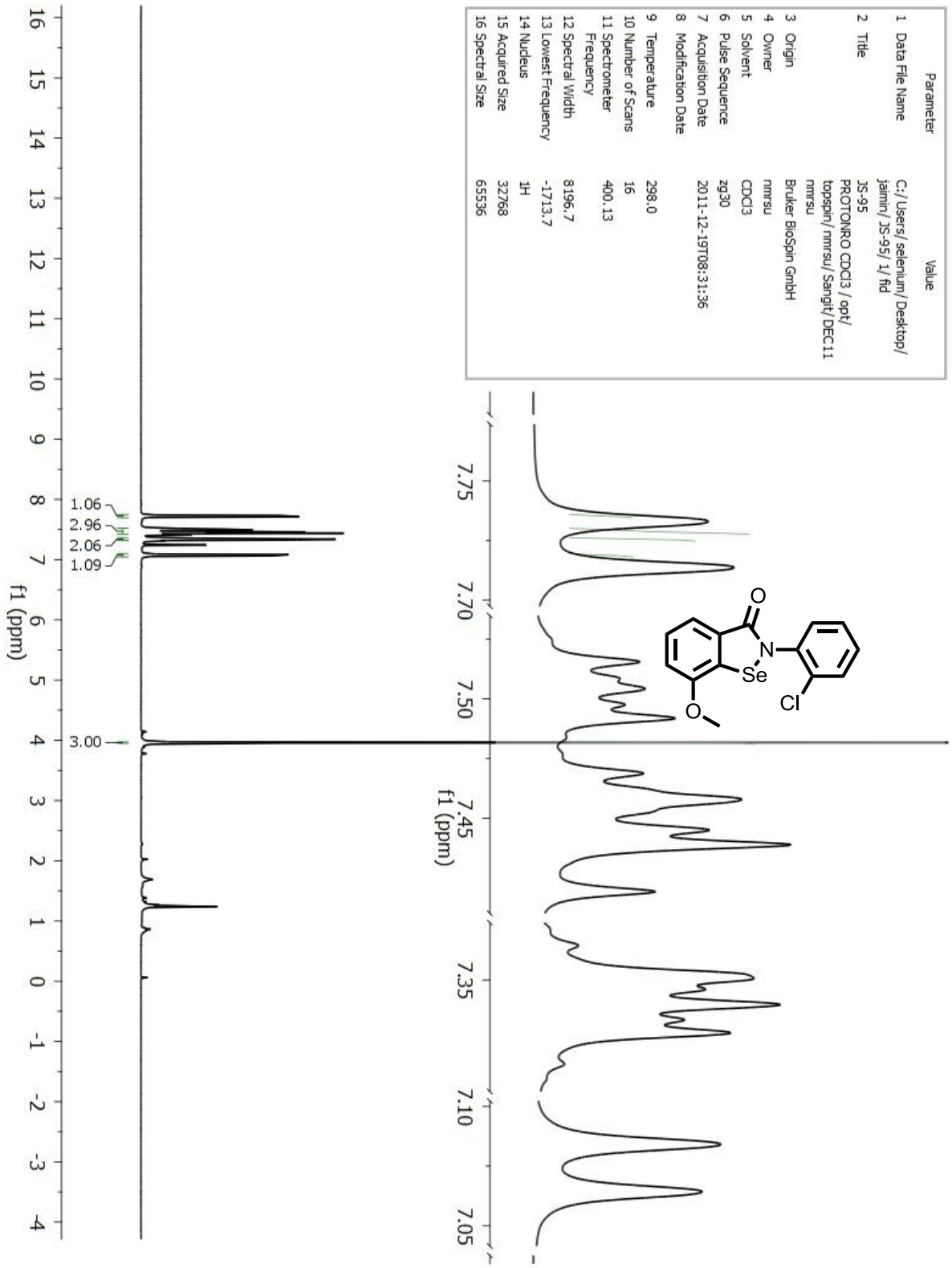


Figure S63 ^{13}C NMR of **1k**

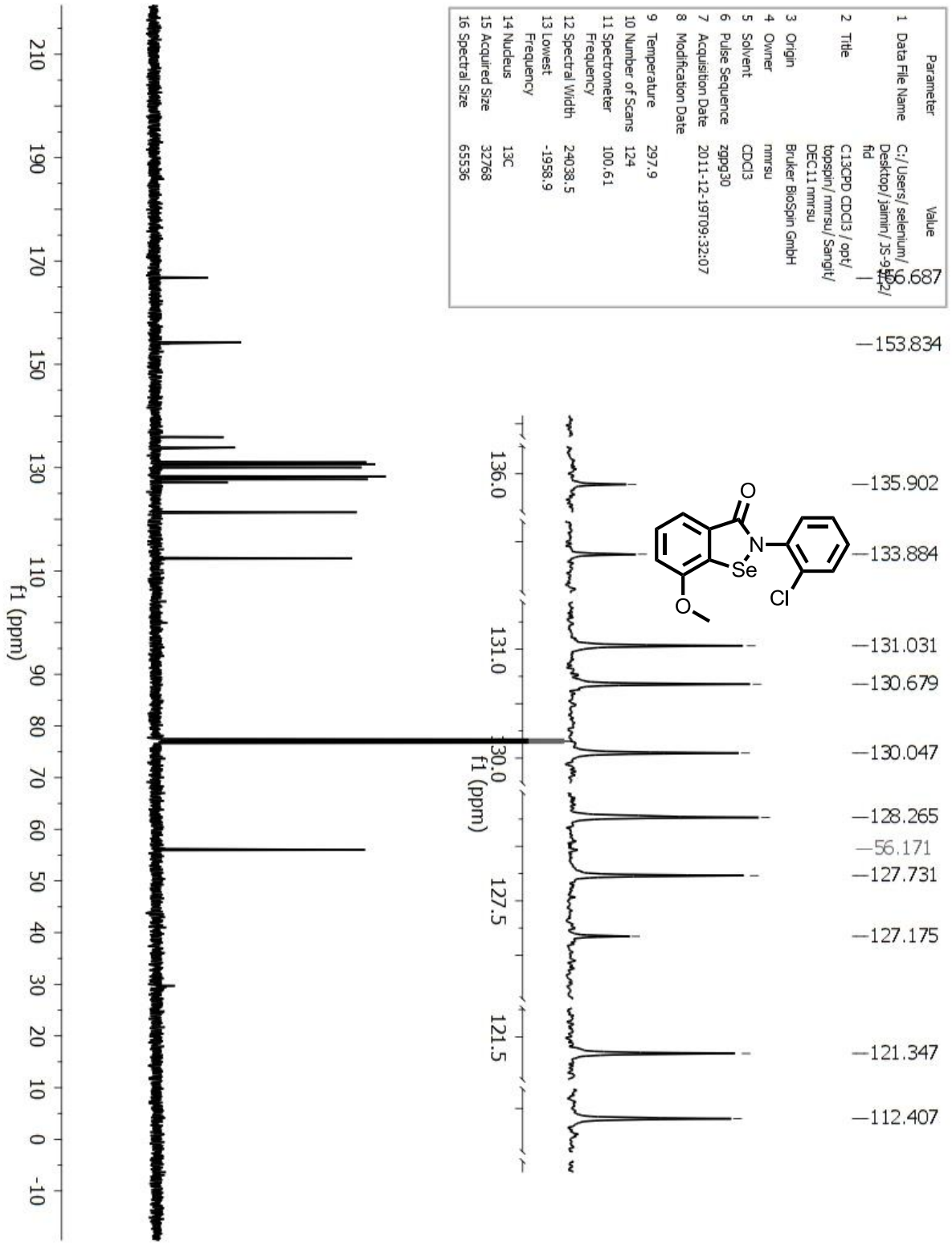


Figure S64 ^{77}Se NMR of **1k**

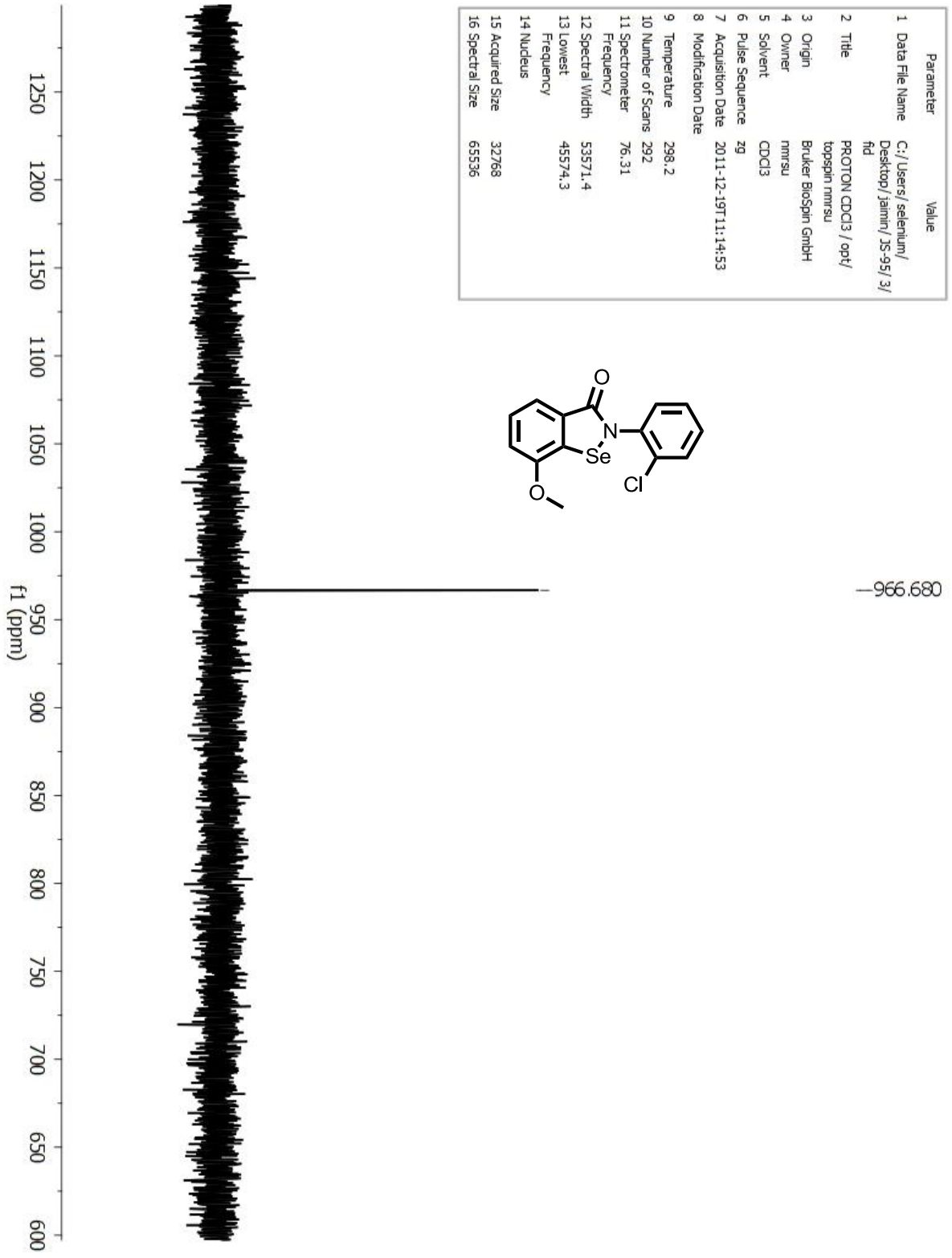


Figure S65 HRMS of **1k**

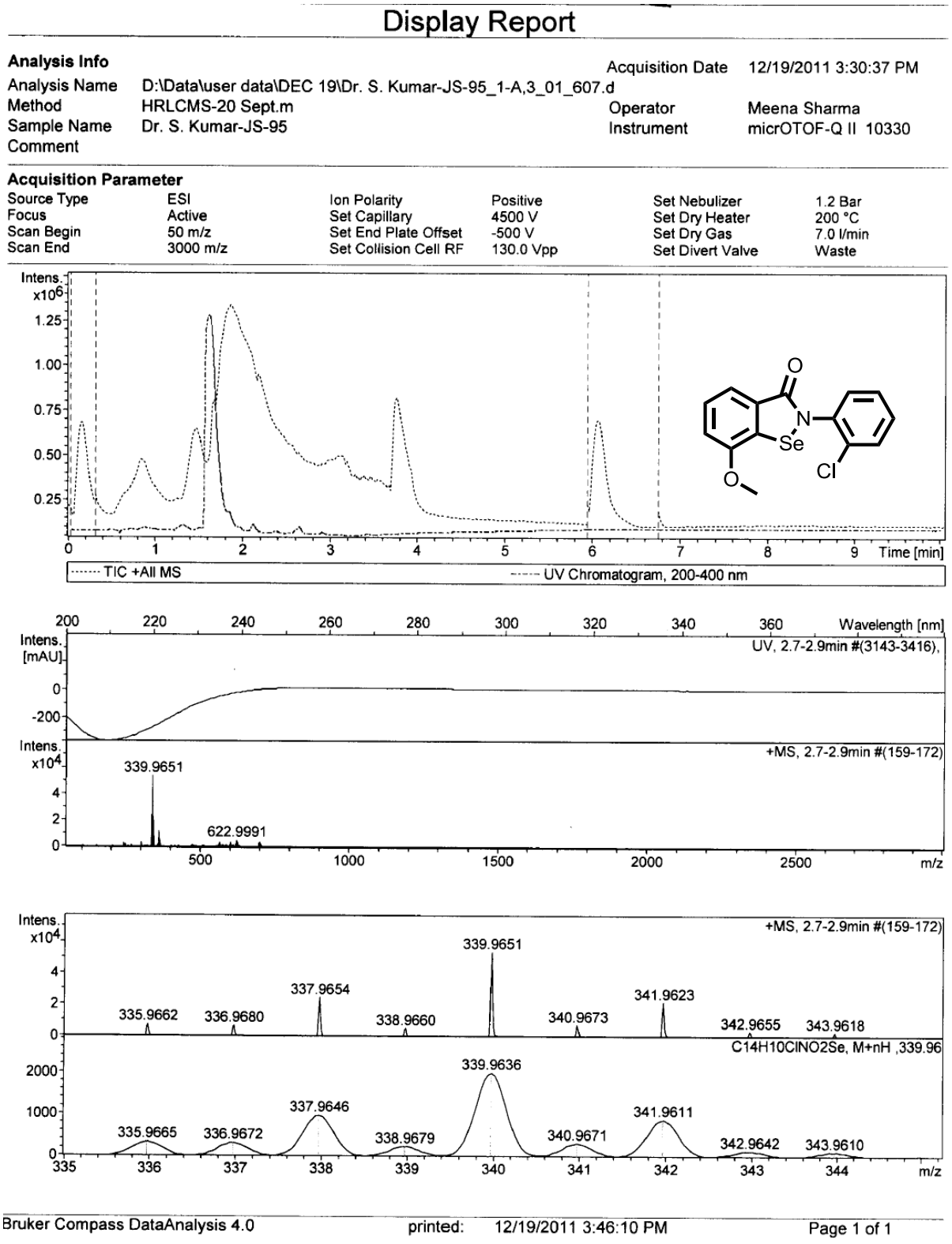


Figure S66 ^{1}H NMR of precursor of **1l**

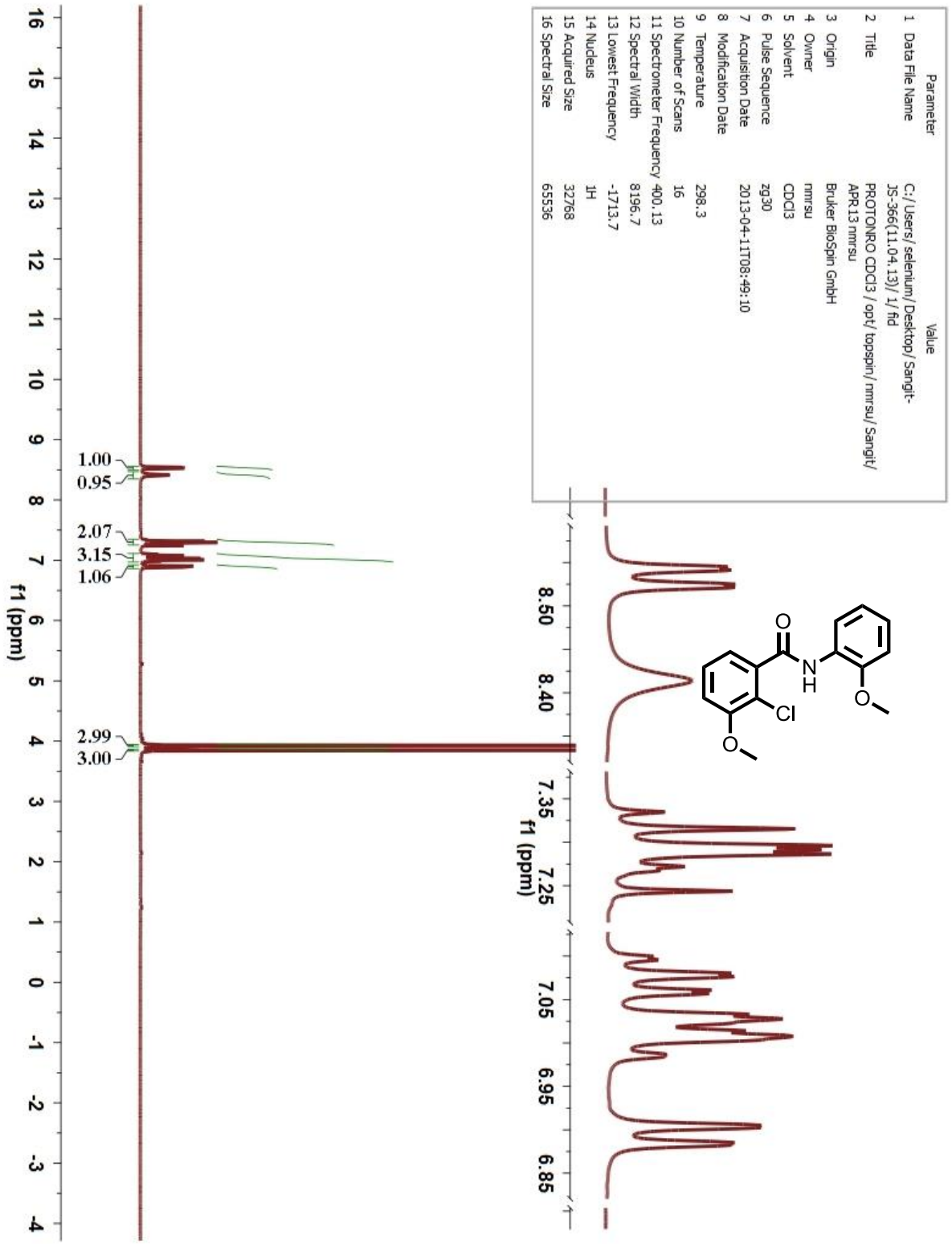


Figure S67 ^{13}C NMR of precursor of **1l**

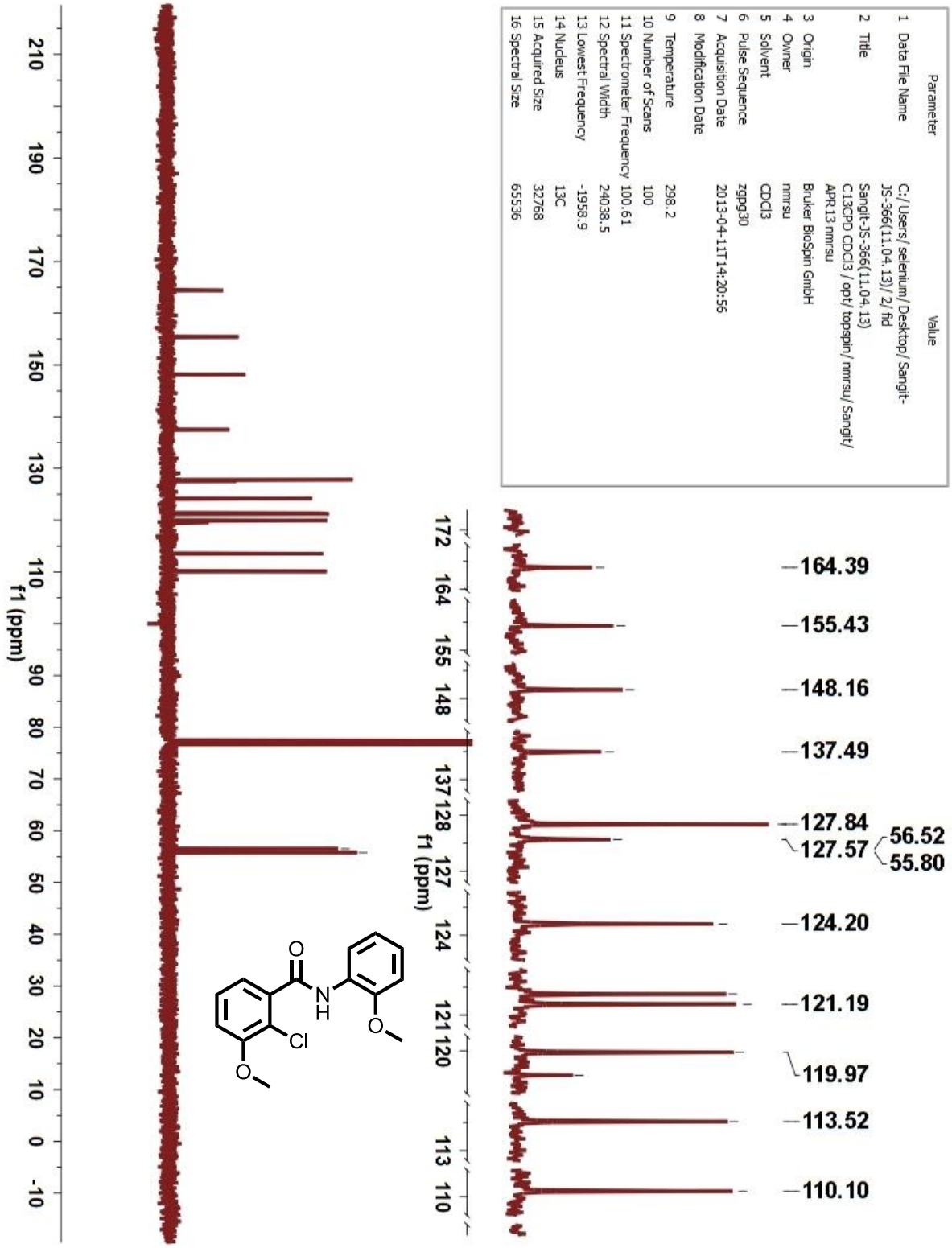


Figure S68 HRMS of precursor of **1l**

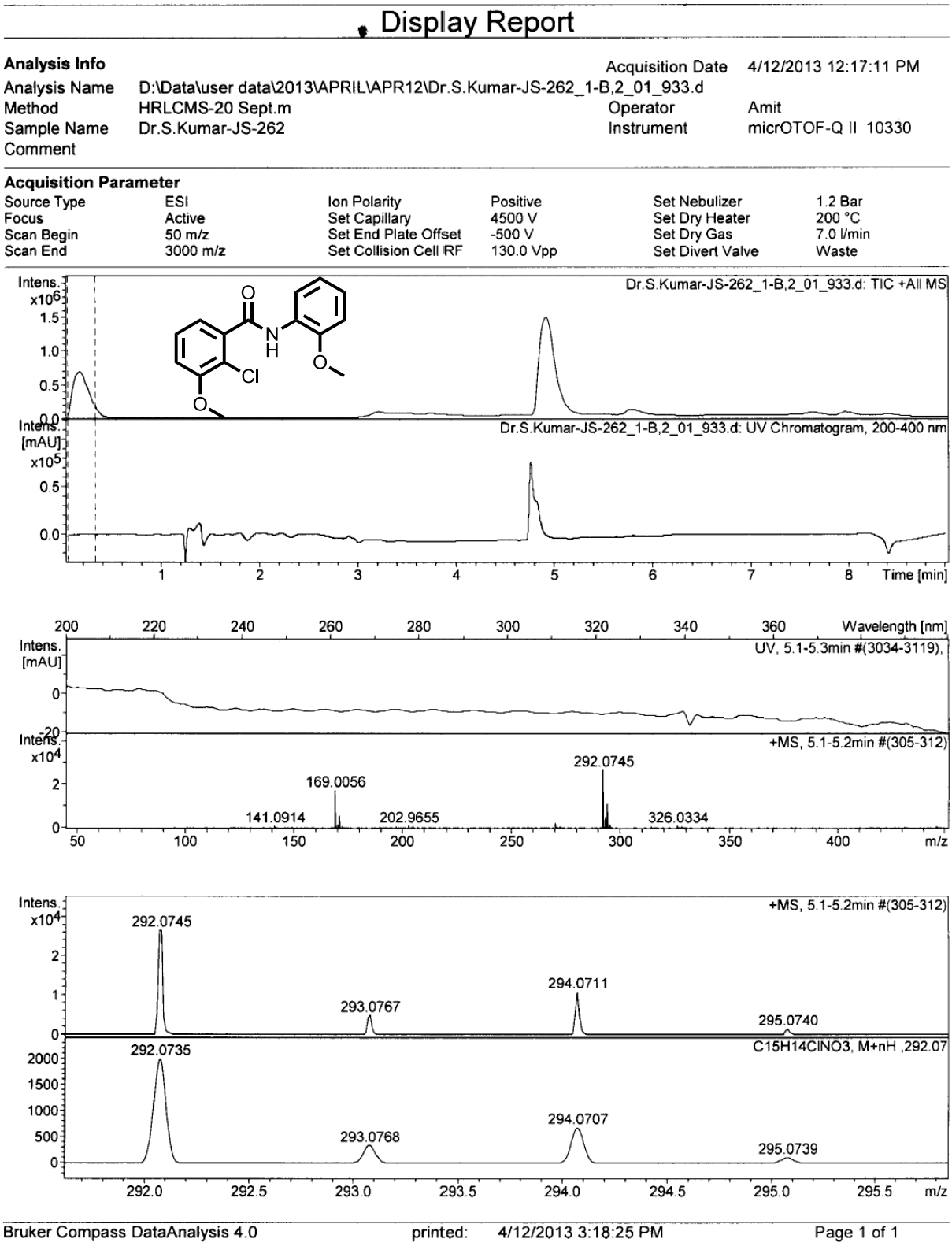


Figure S69 ^{1}H NMR of **1l**

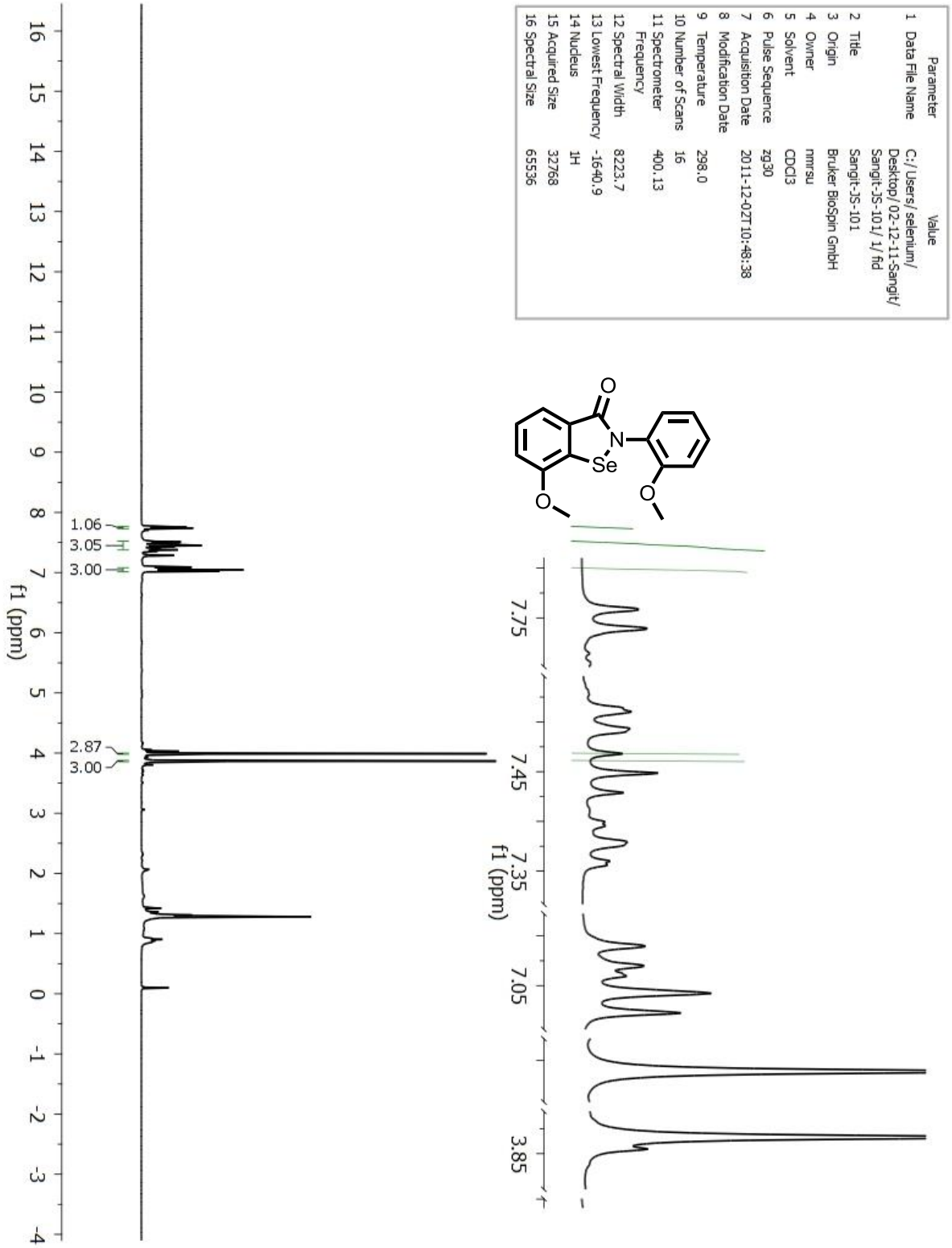


Figure S70 ^{13}C NMR of **1l**

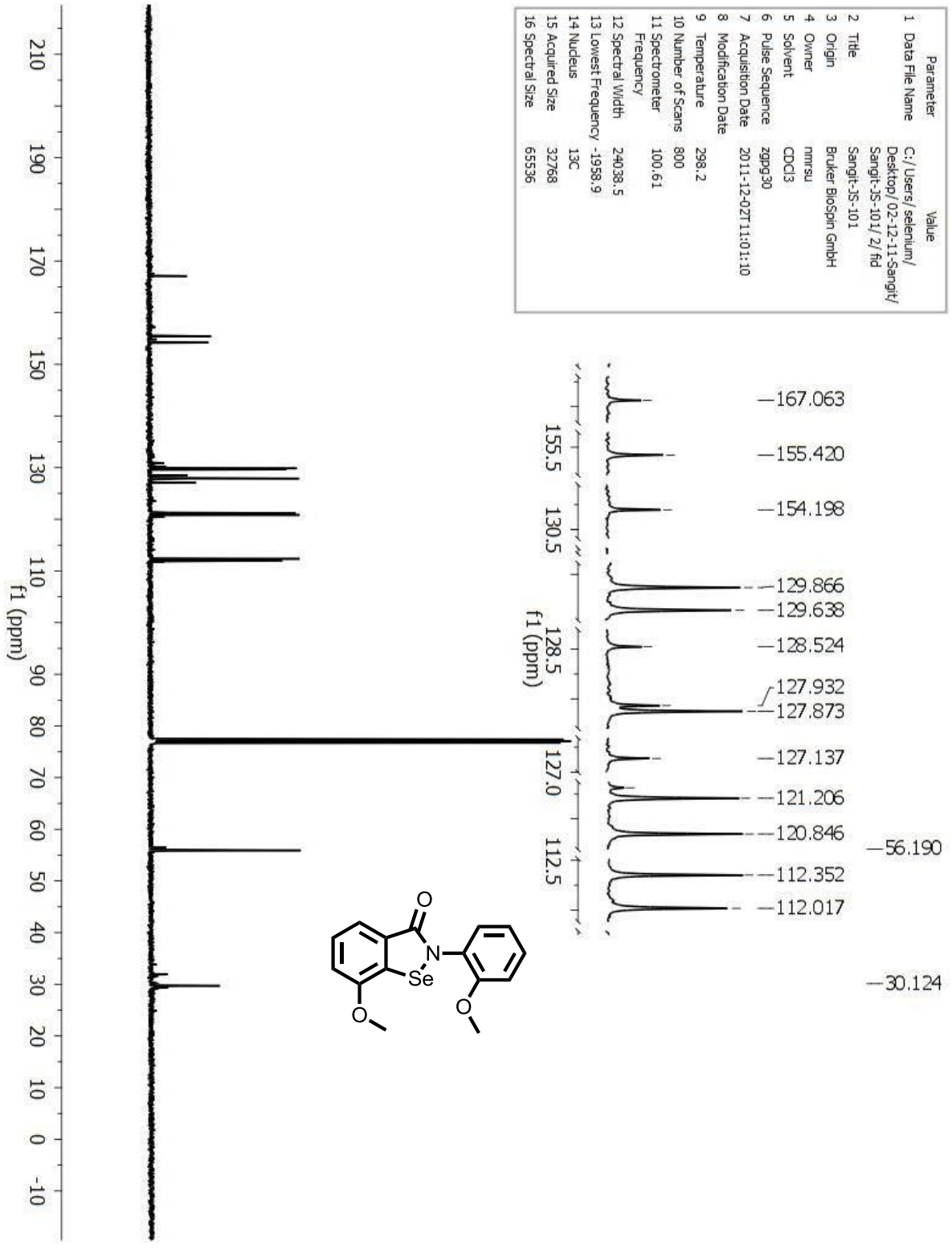


Figure S71 ^{77}Se NMR of **1l**

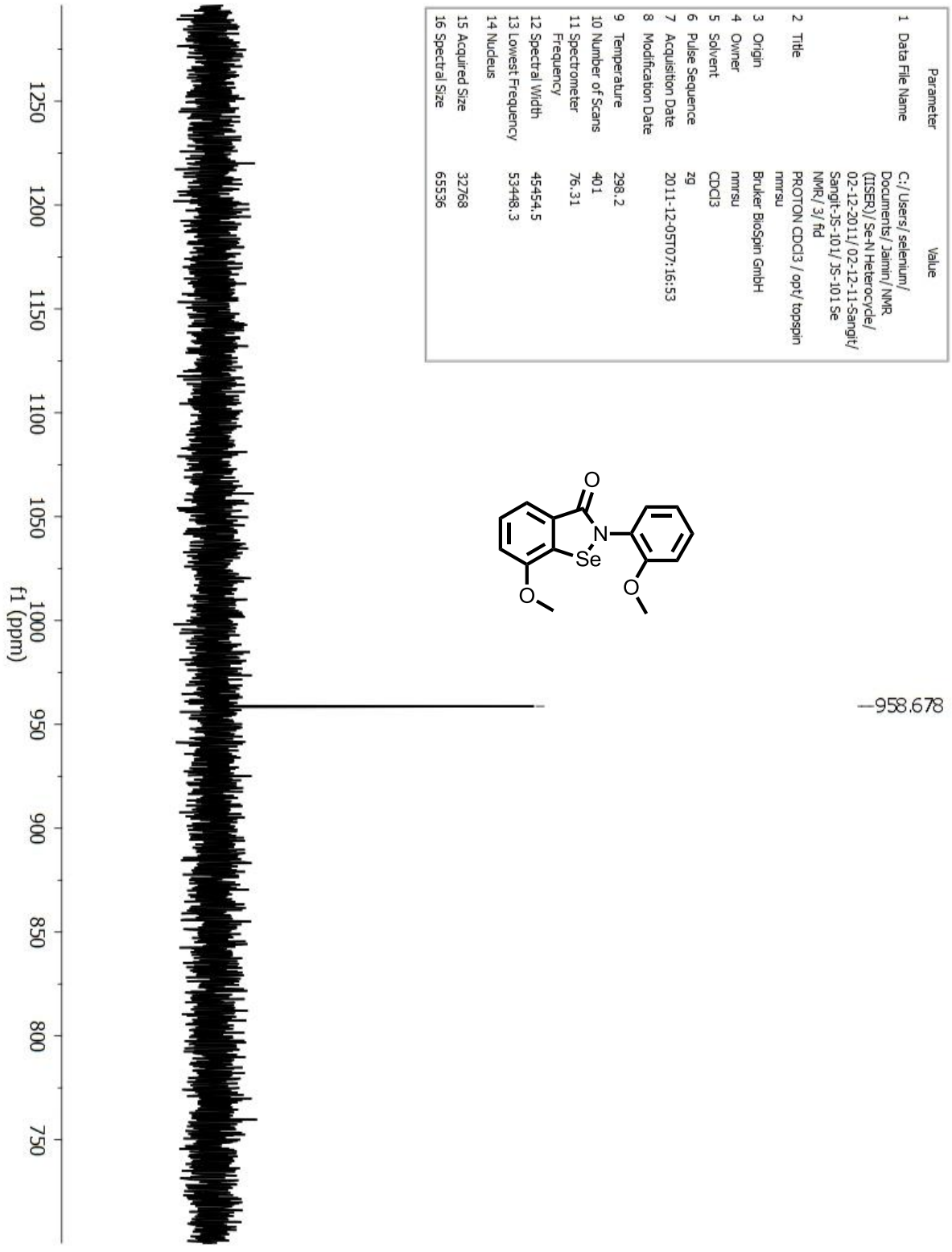


Figure S72 HRMS of **1l**

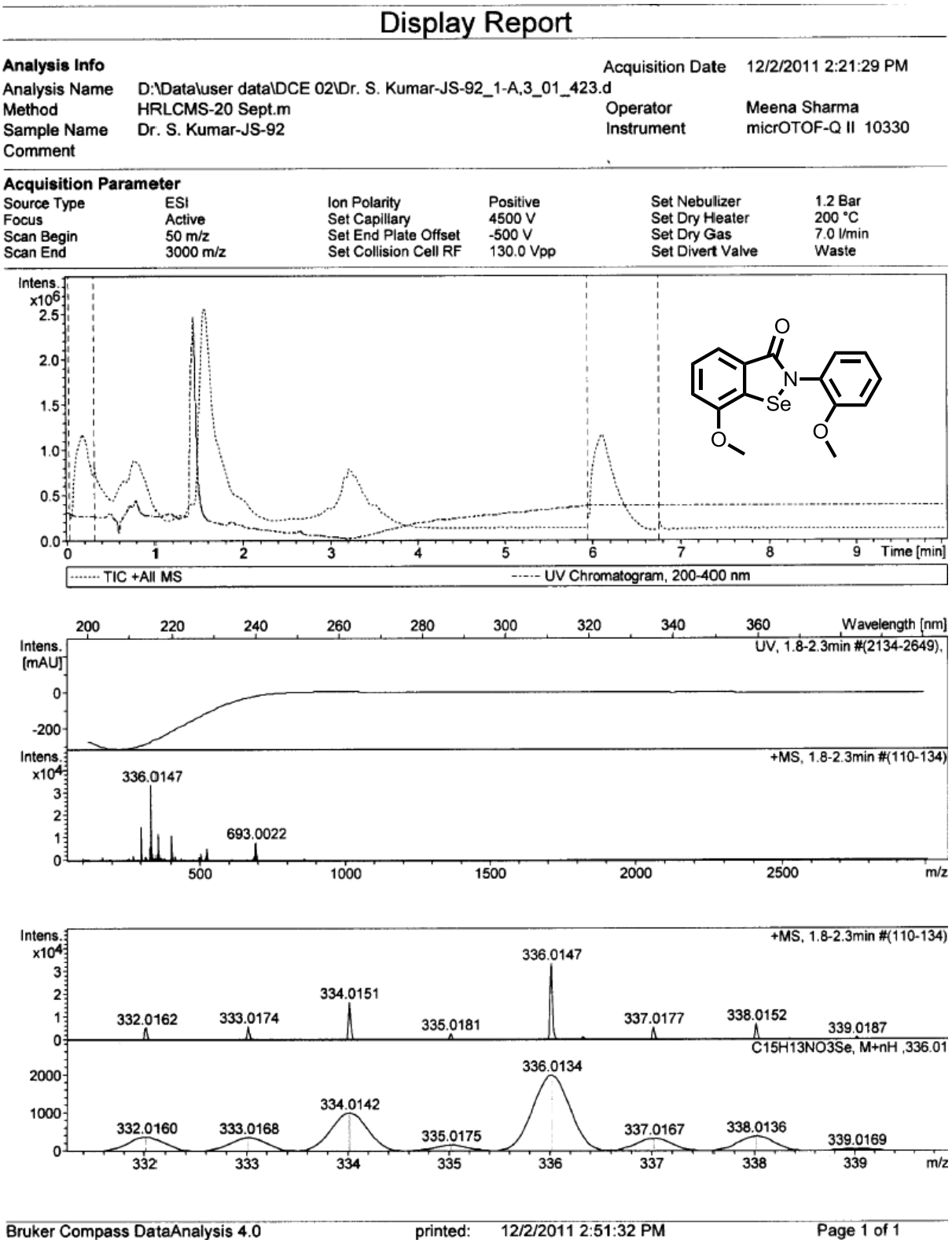


Figure S73 ^{1}H NMR of precursor of **1m**

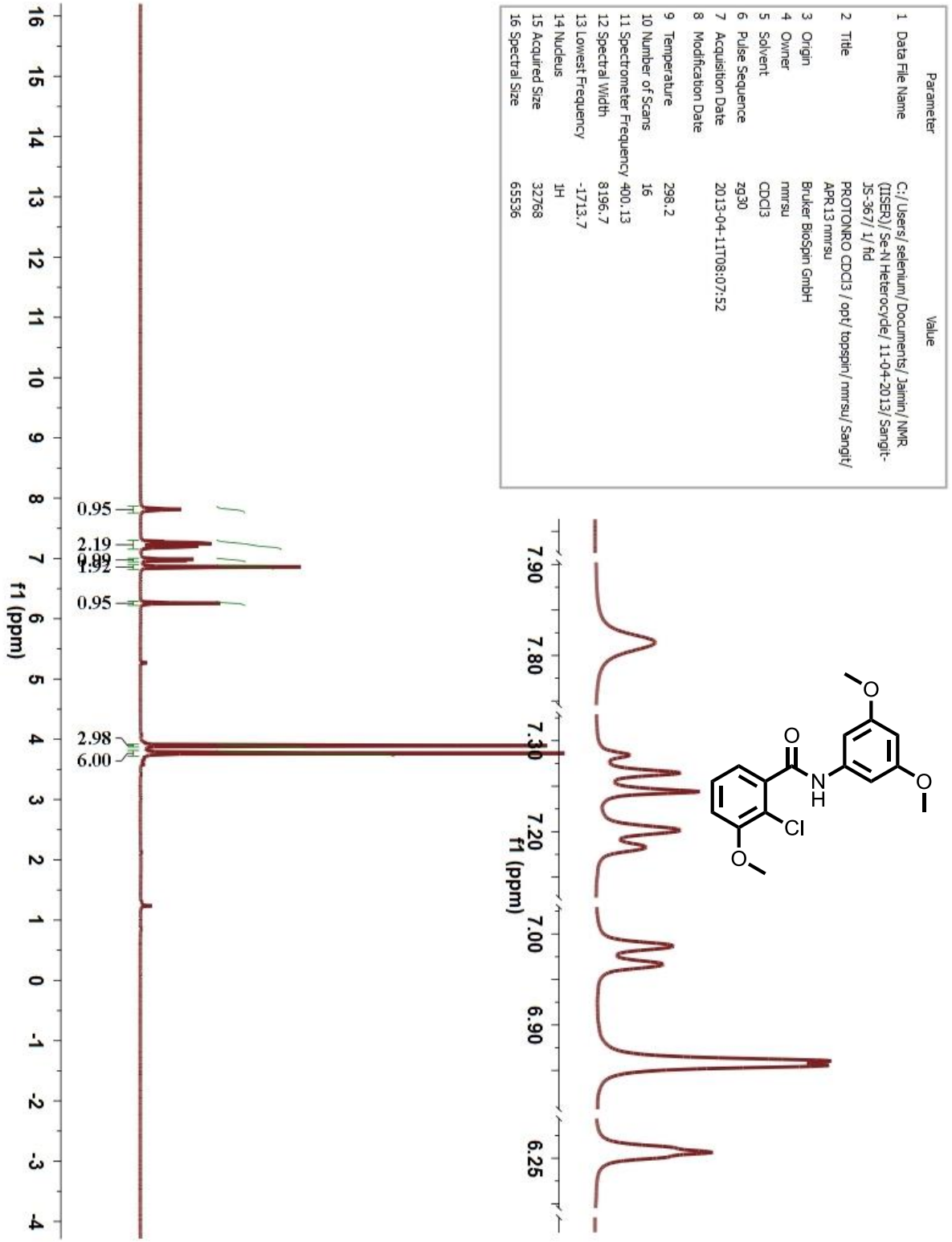


Figure S74 ^{1}H NMR of precursor of **1m**

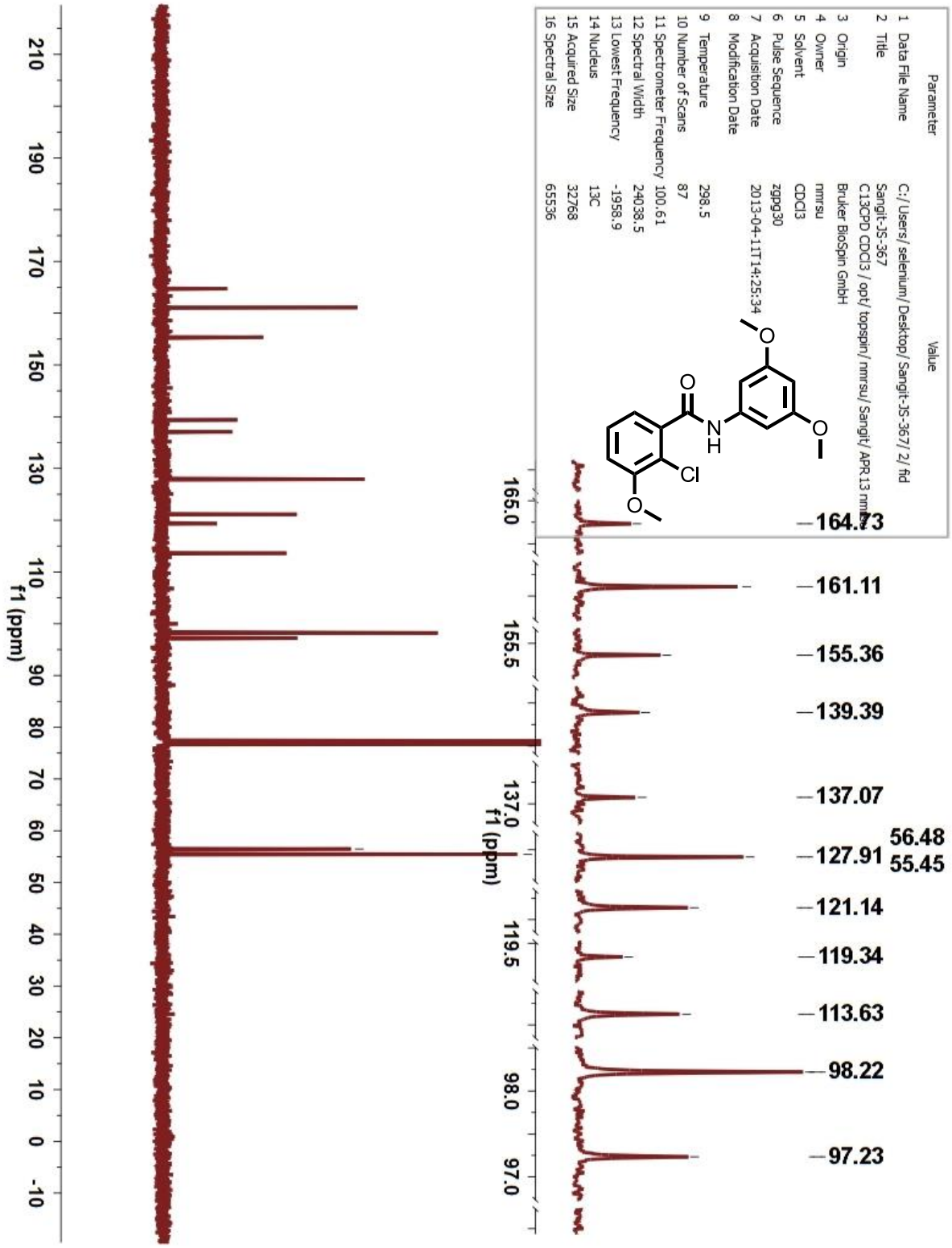


Figure S75 HRMS of precursor of **1m**

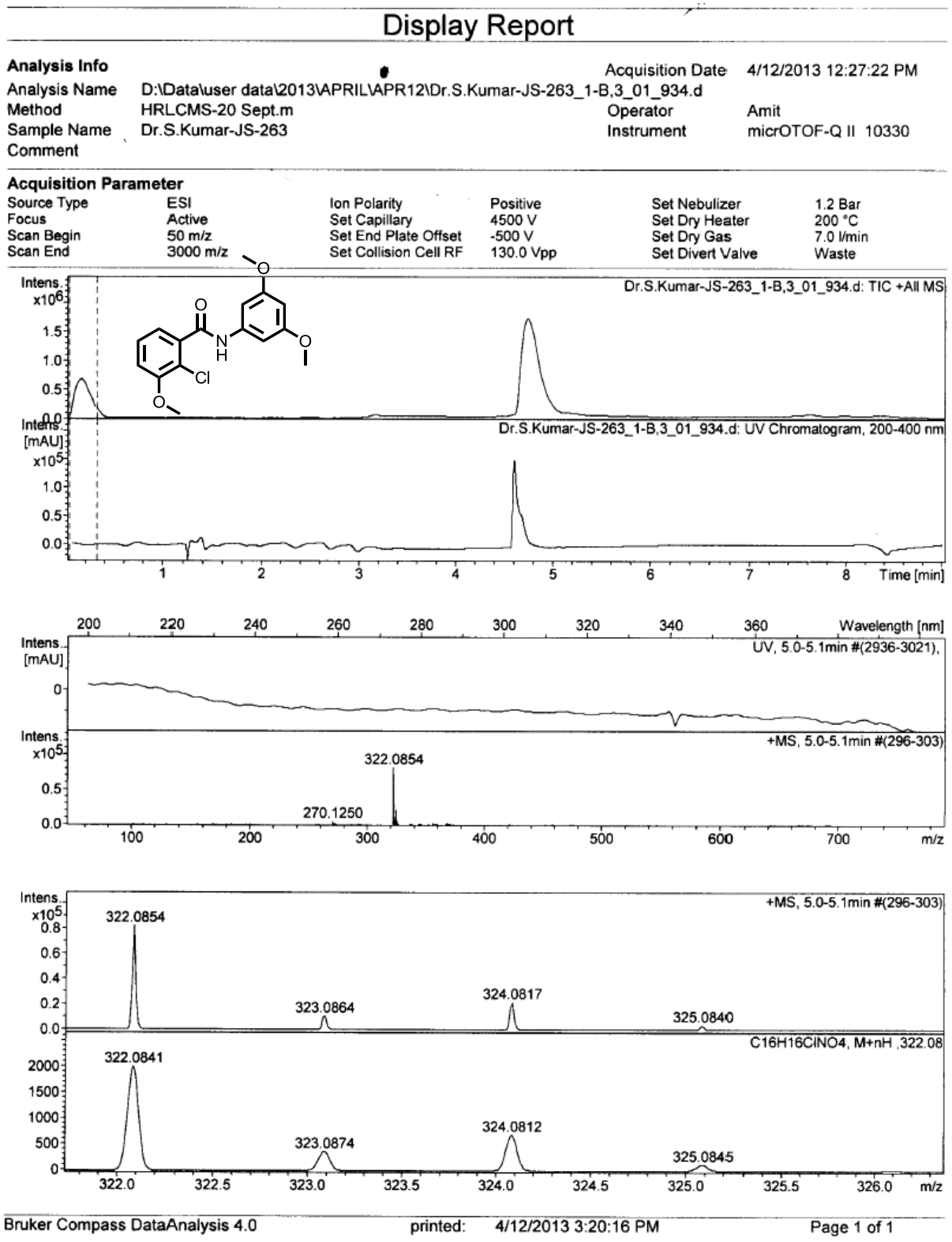


Figure S76 ^{1}H NMR of **1m**

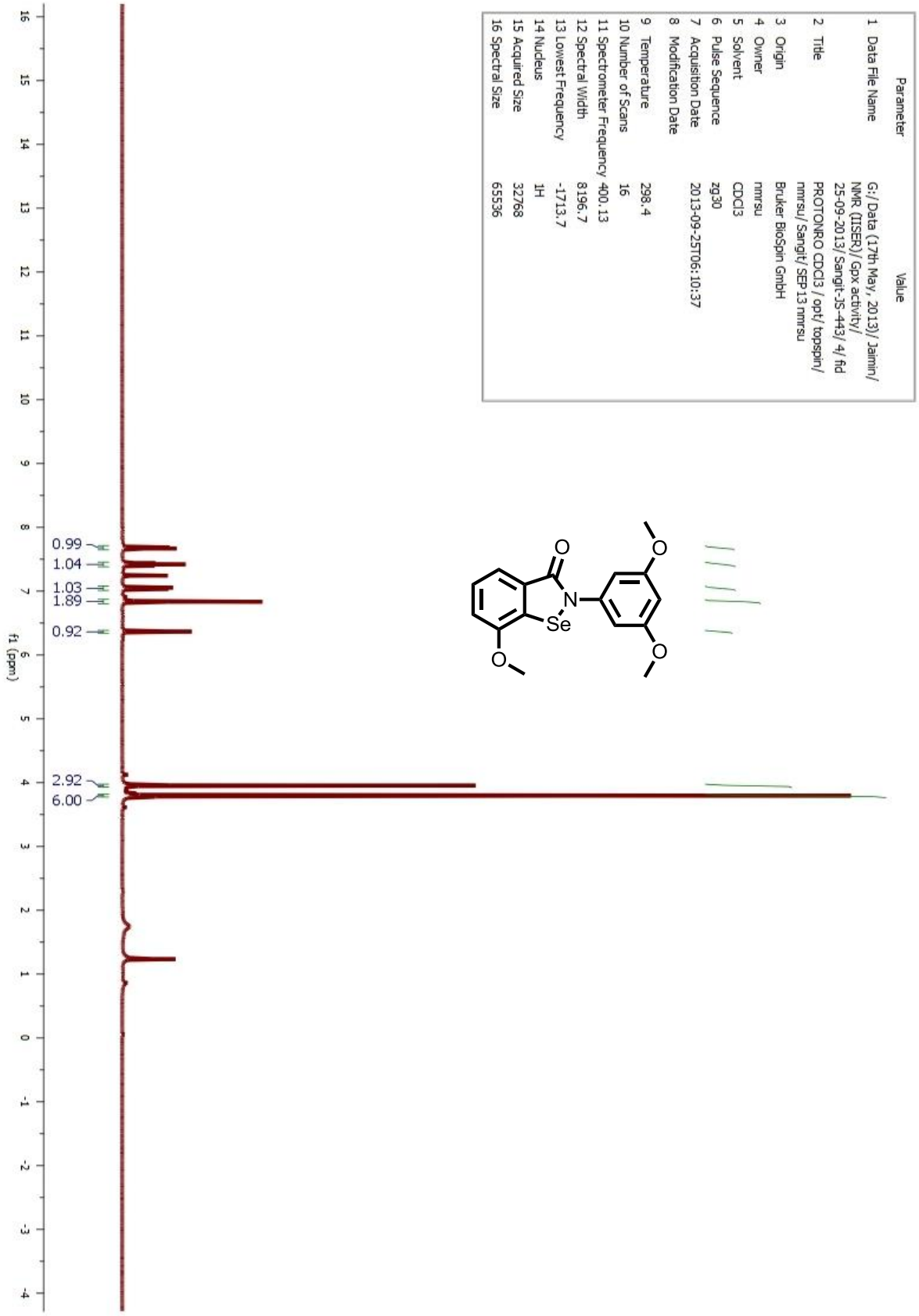


Figure S77 ^{13}C NMR of **1m**

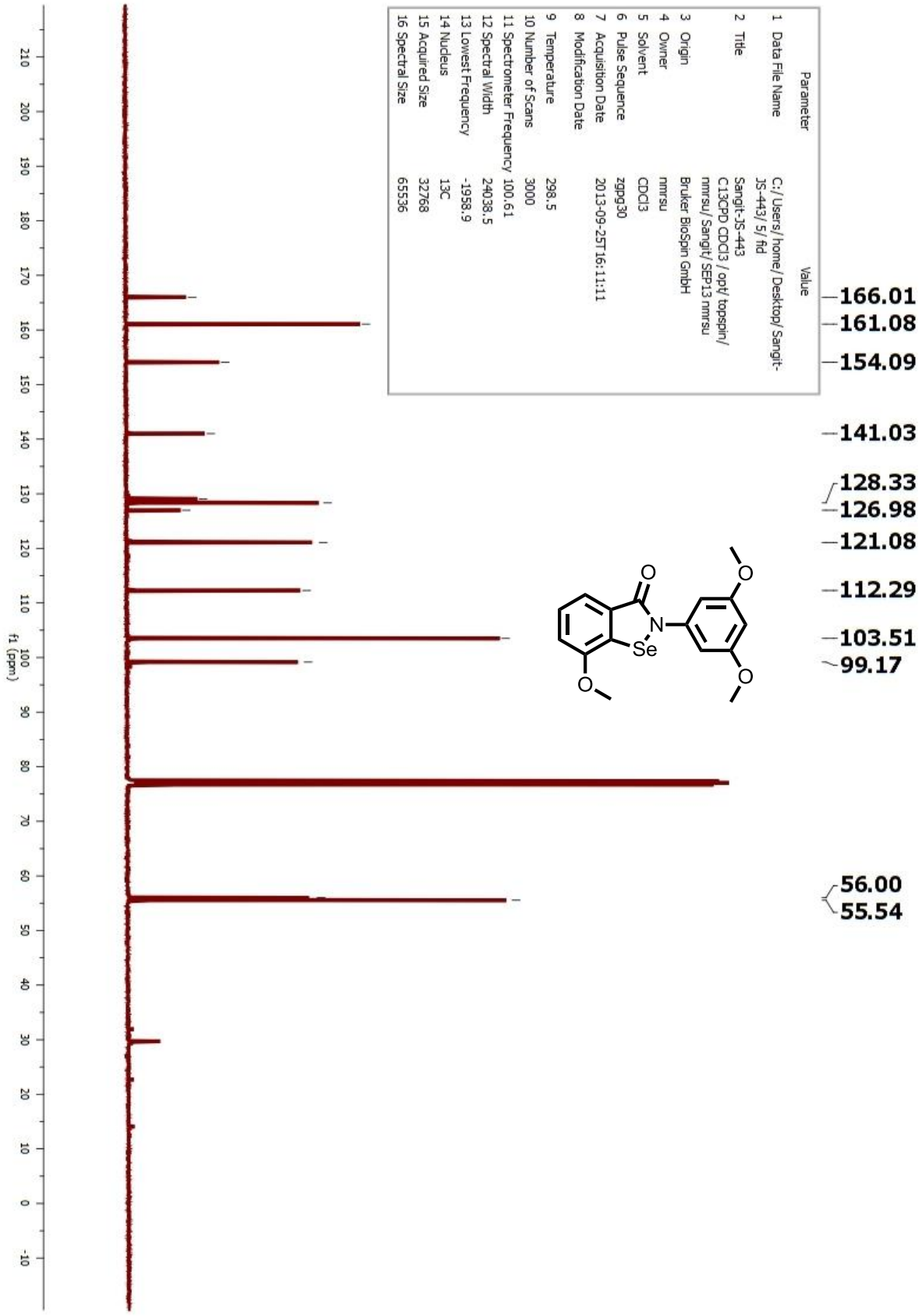


Figure S78 ^{77}Se NMR of **1m**

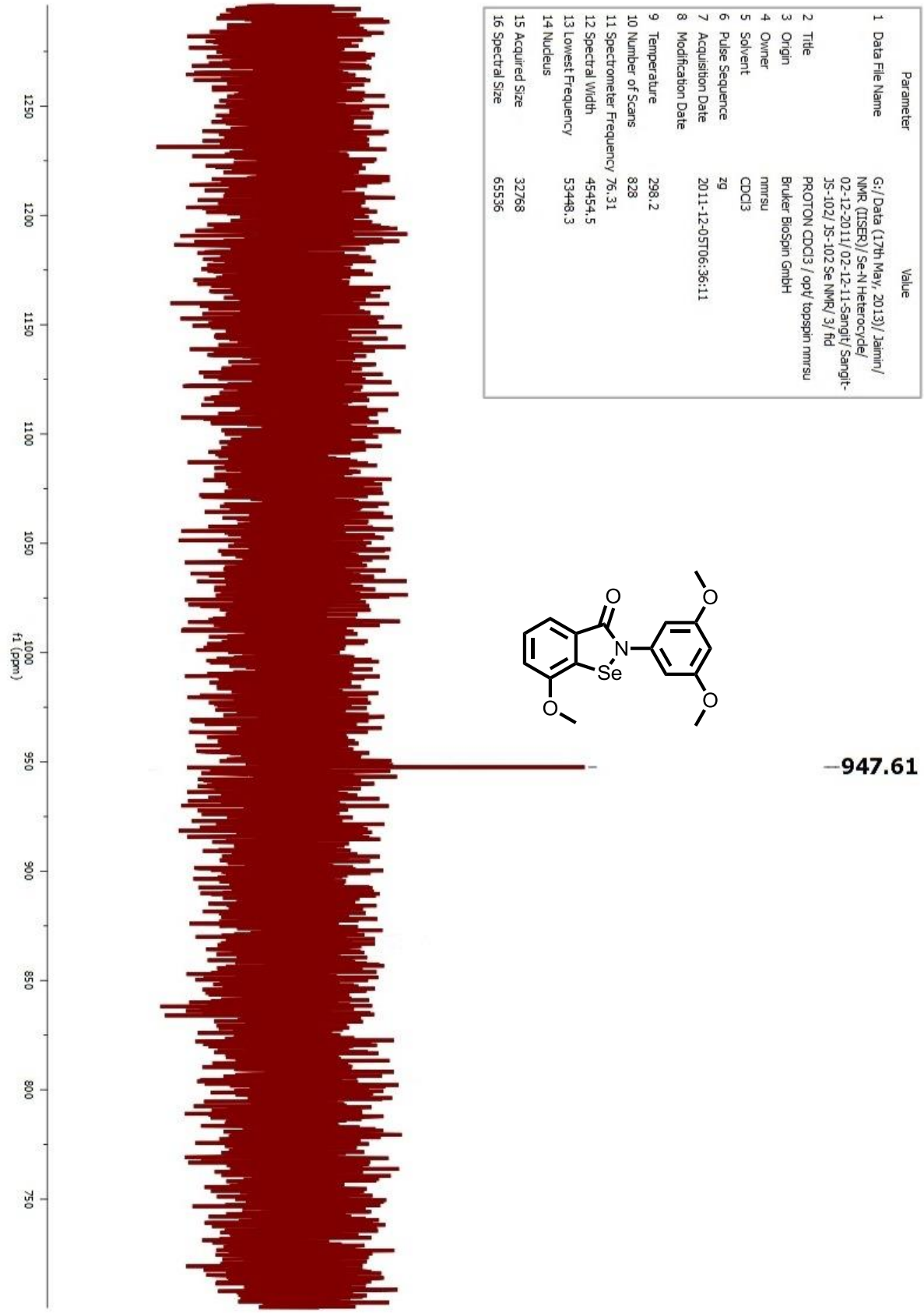


Figure S79 HRMS of **1m**

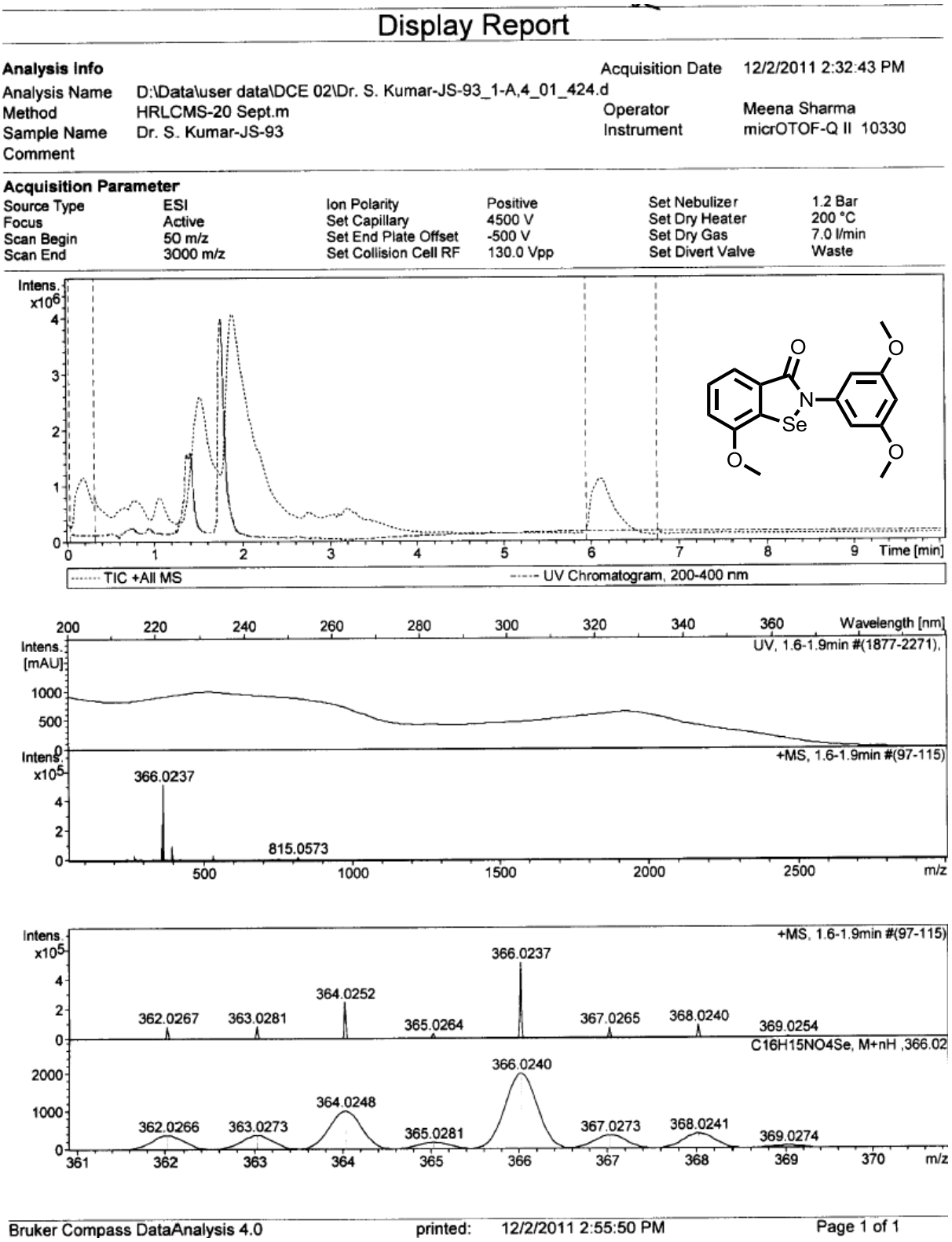


Figure S80 ^{1}H NMR of **1n**

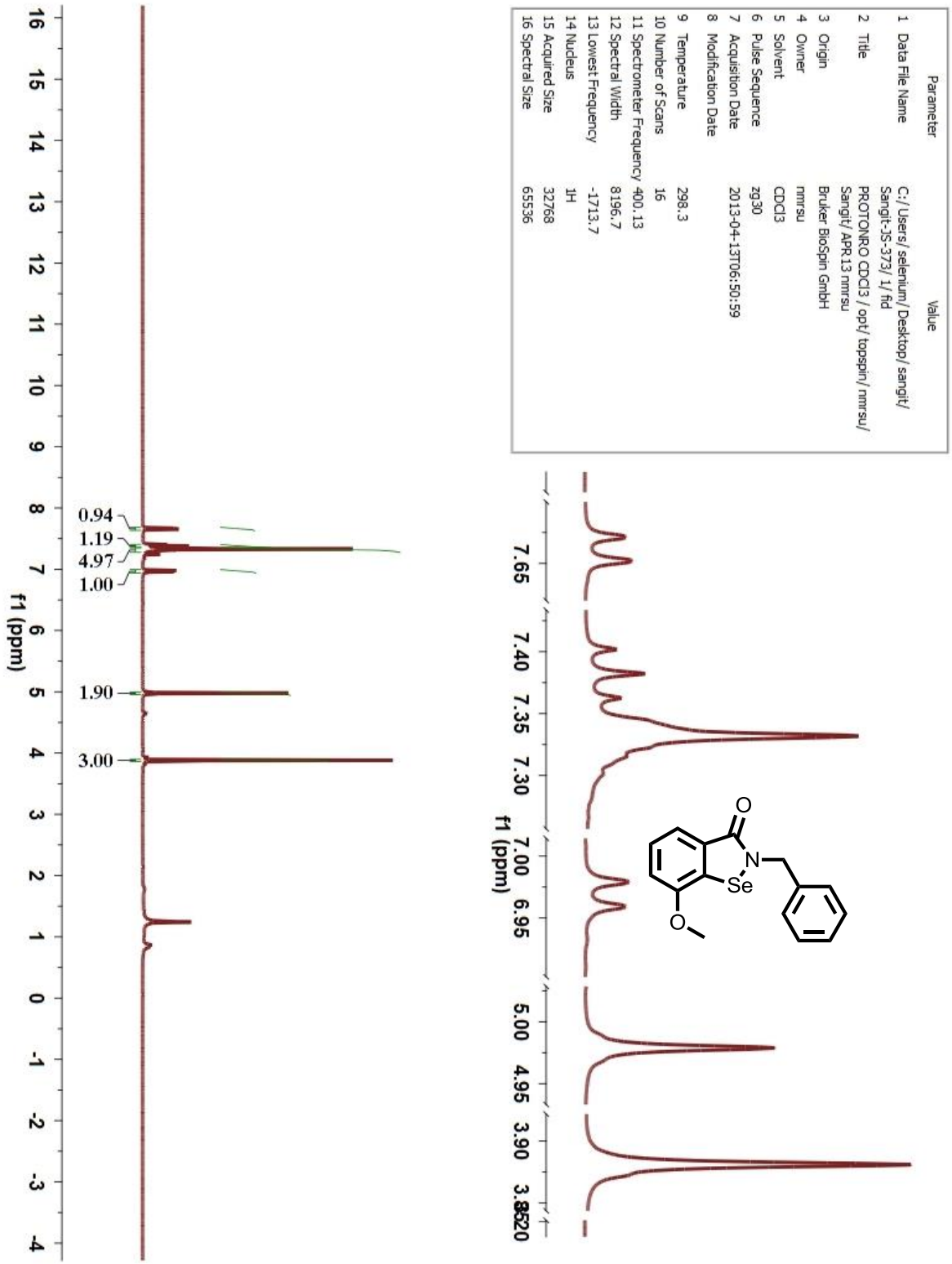


Figure S81 ^{13}C NMR of **1n**

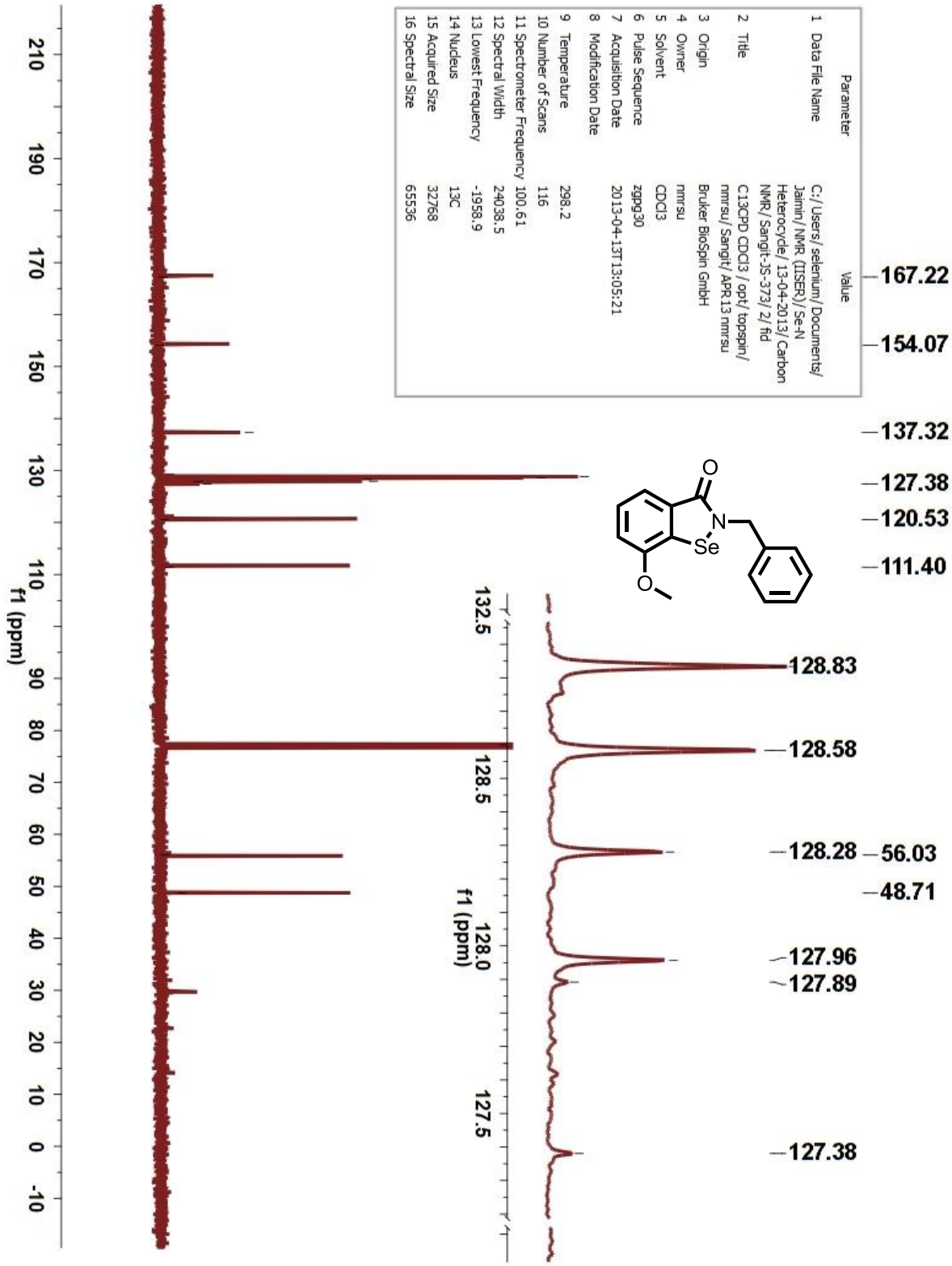


Figure S82 ^{77}Se NMR of **1n**

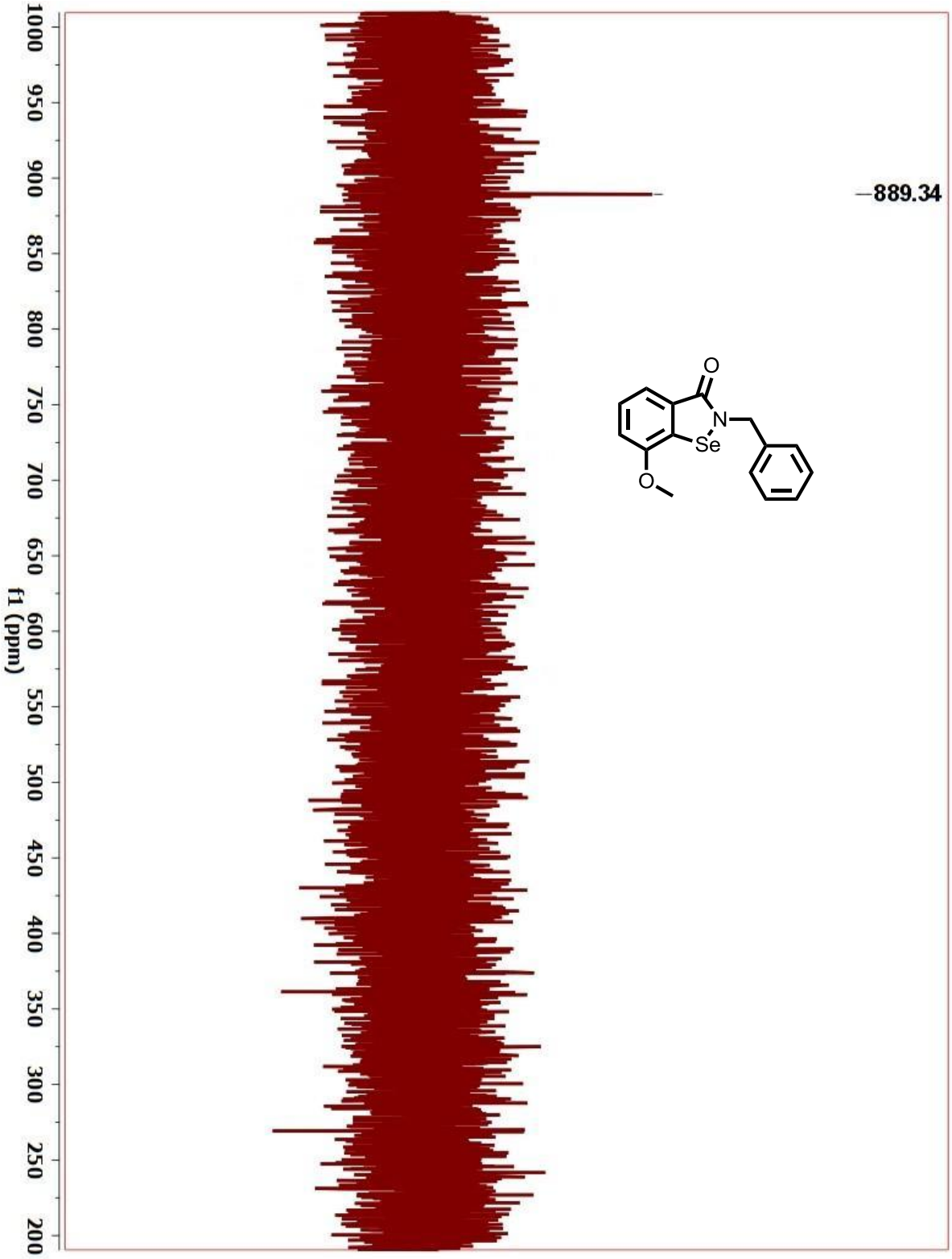


Figure S83 HRMS of **1n**

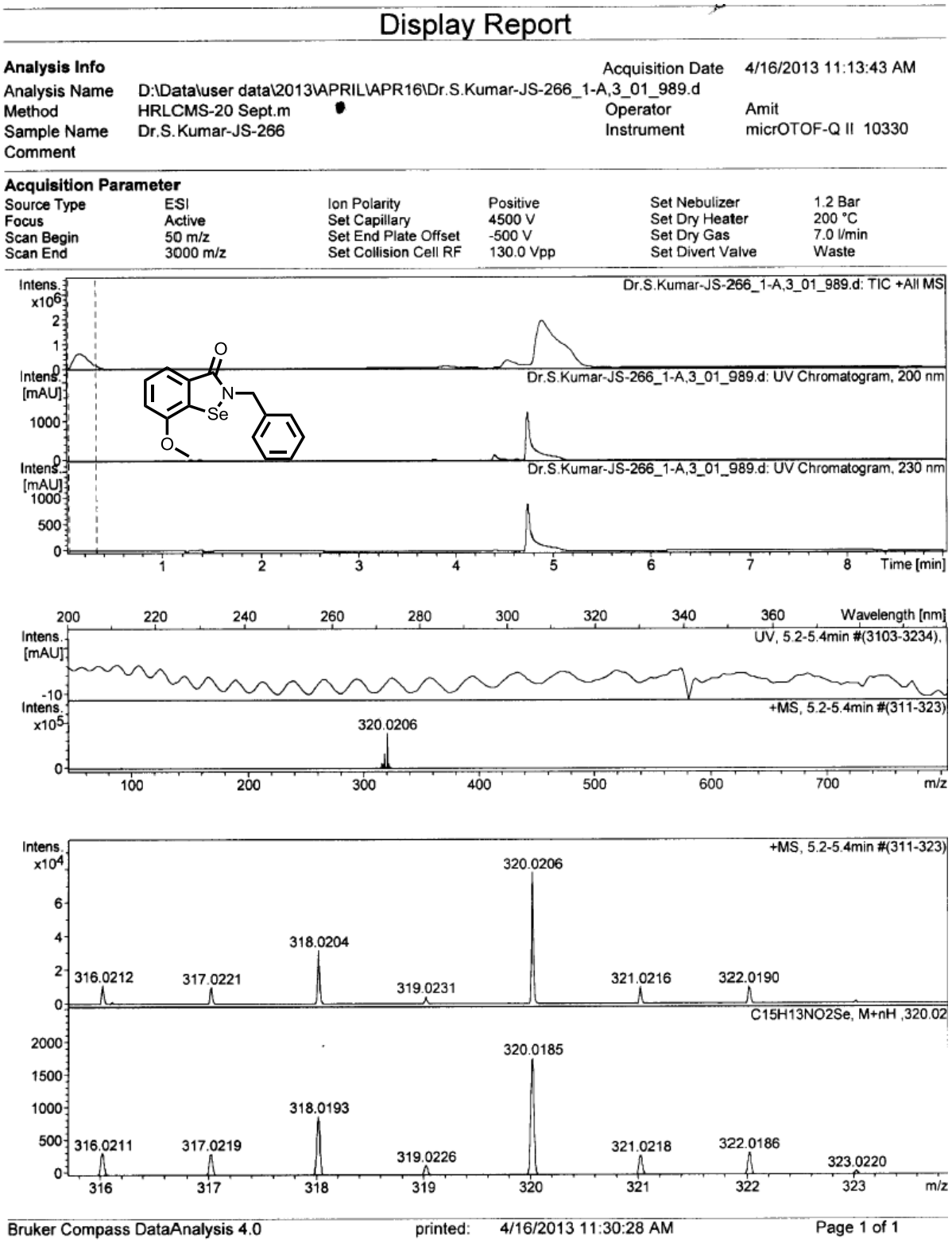


Figure S84 ^{1}H NMR of precursor of **1o**

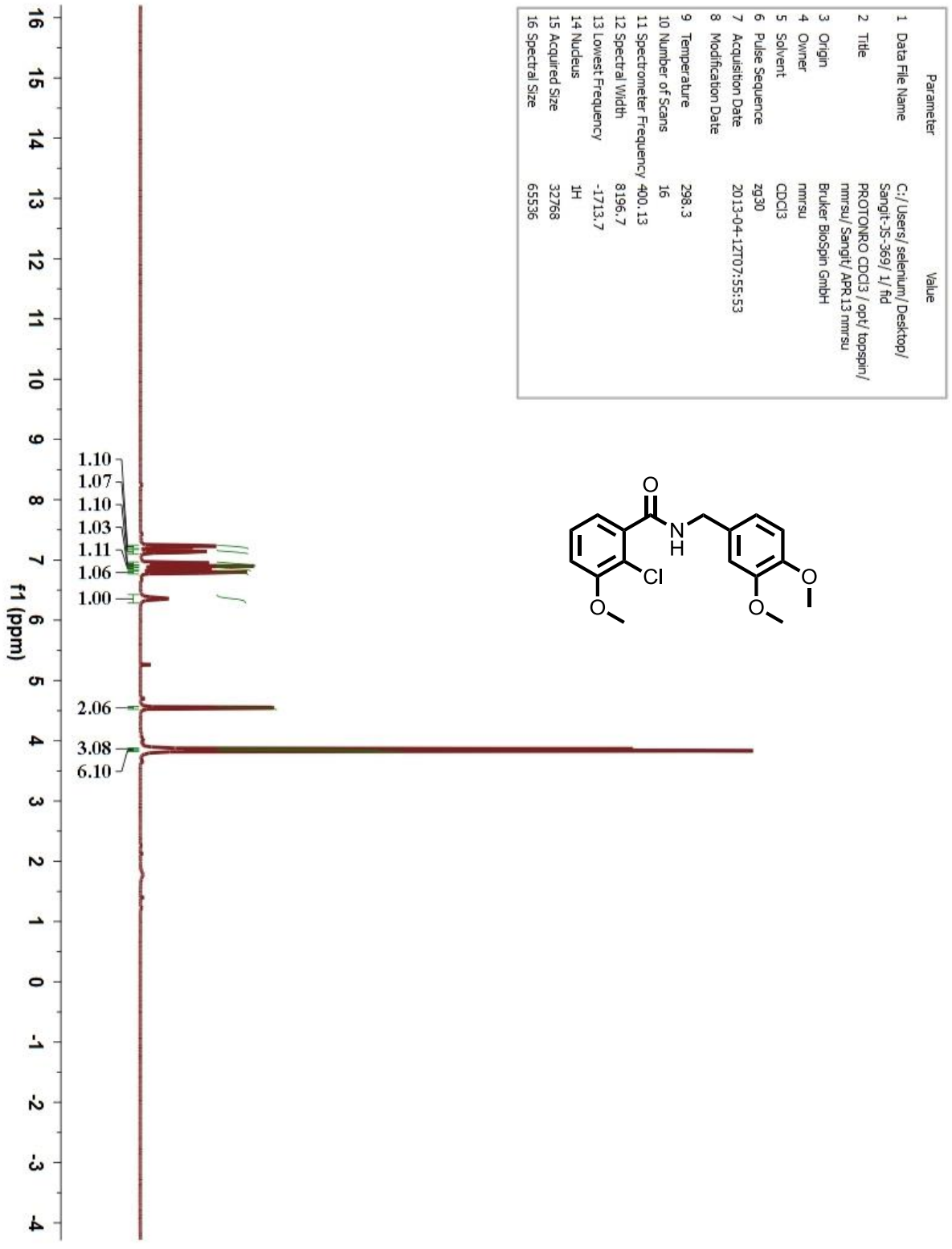


Figure S85 ^{13}C NMR of precursor of **1o**

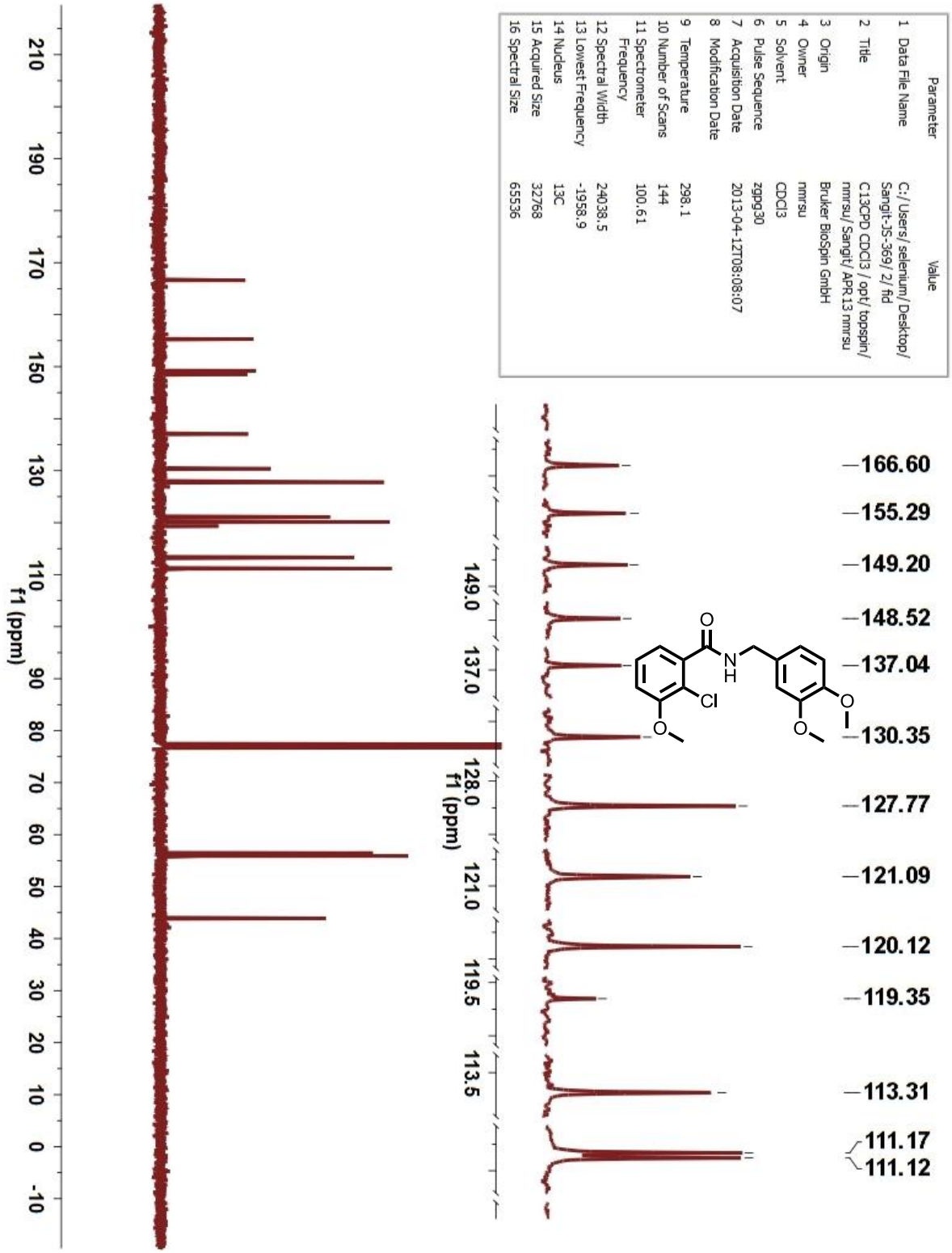


Figure S86 LRMS of precursor of **1o**

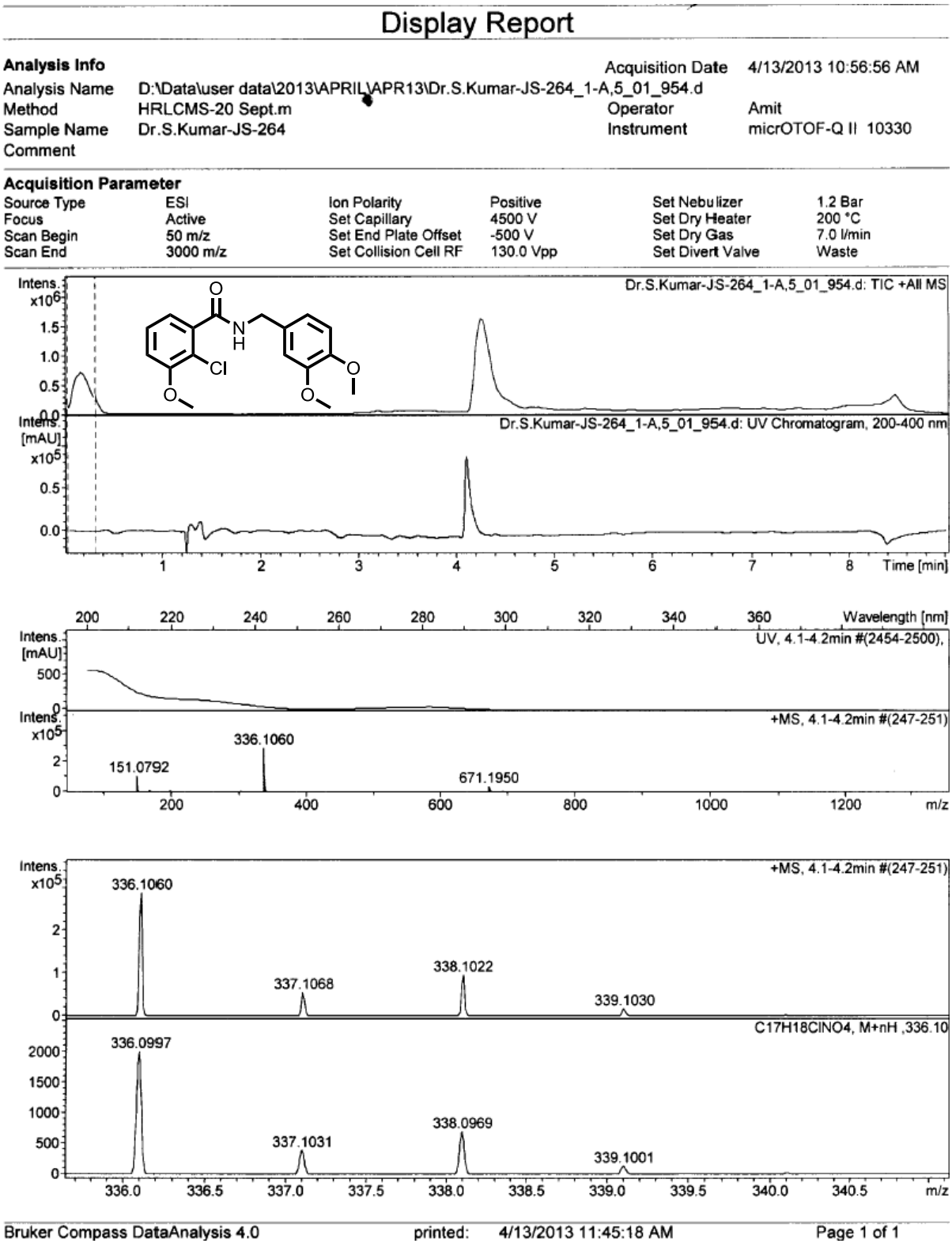


Figure S87 ^{1}H NMR of **1o**

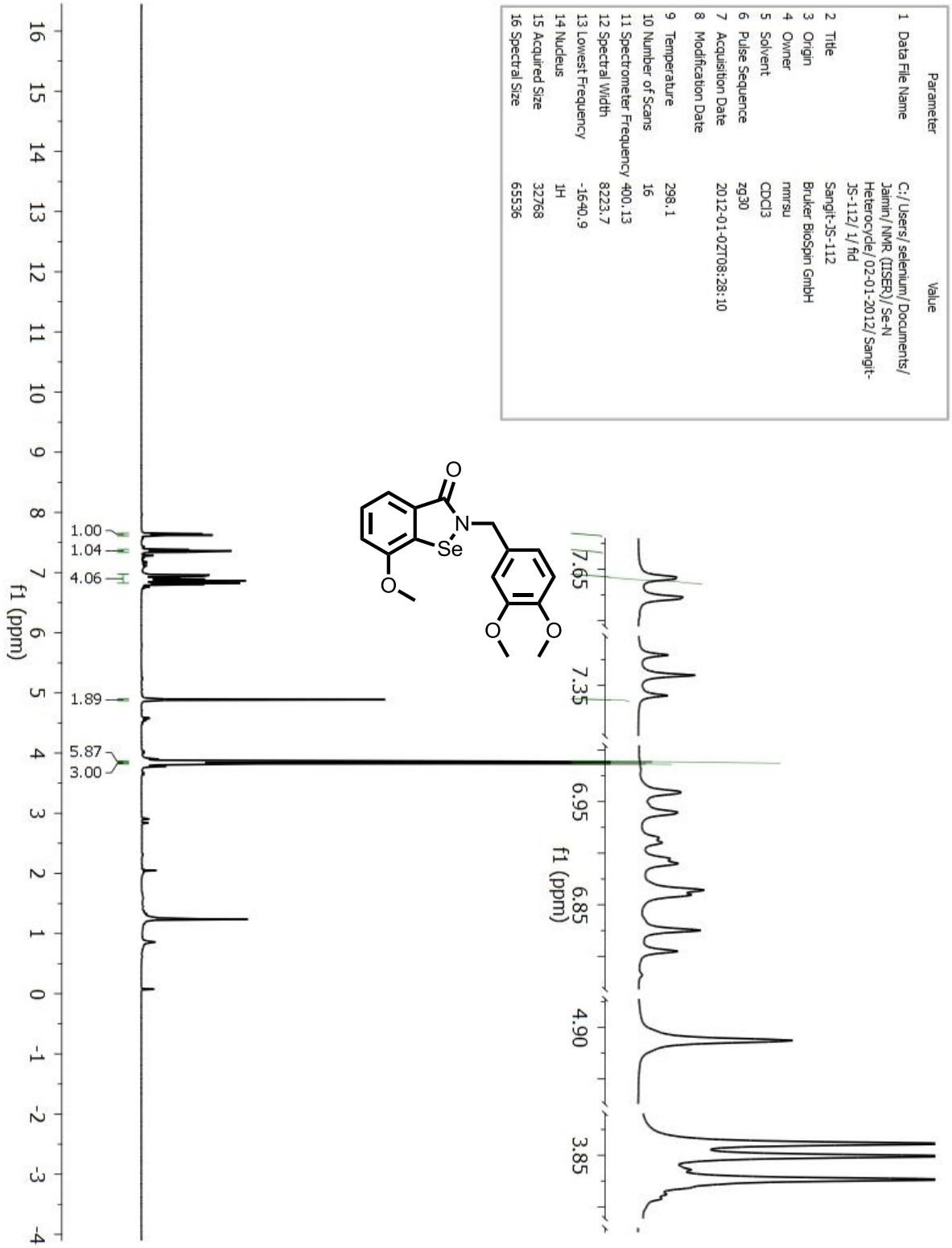


Figure S88 ^{13}C NMR of **1o**

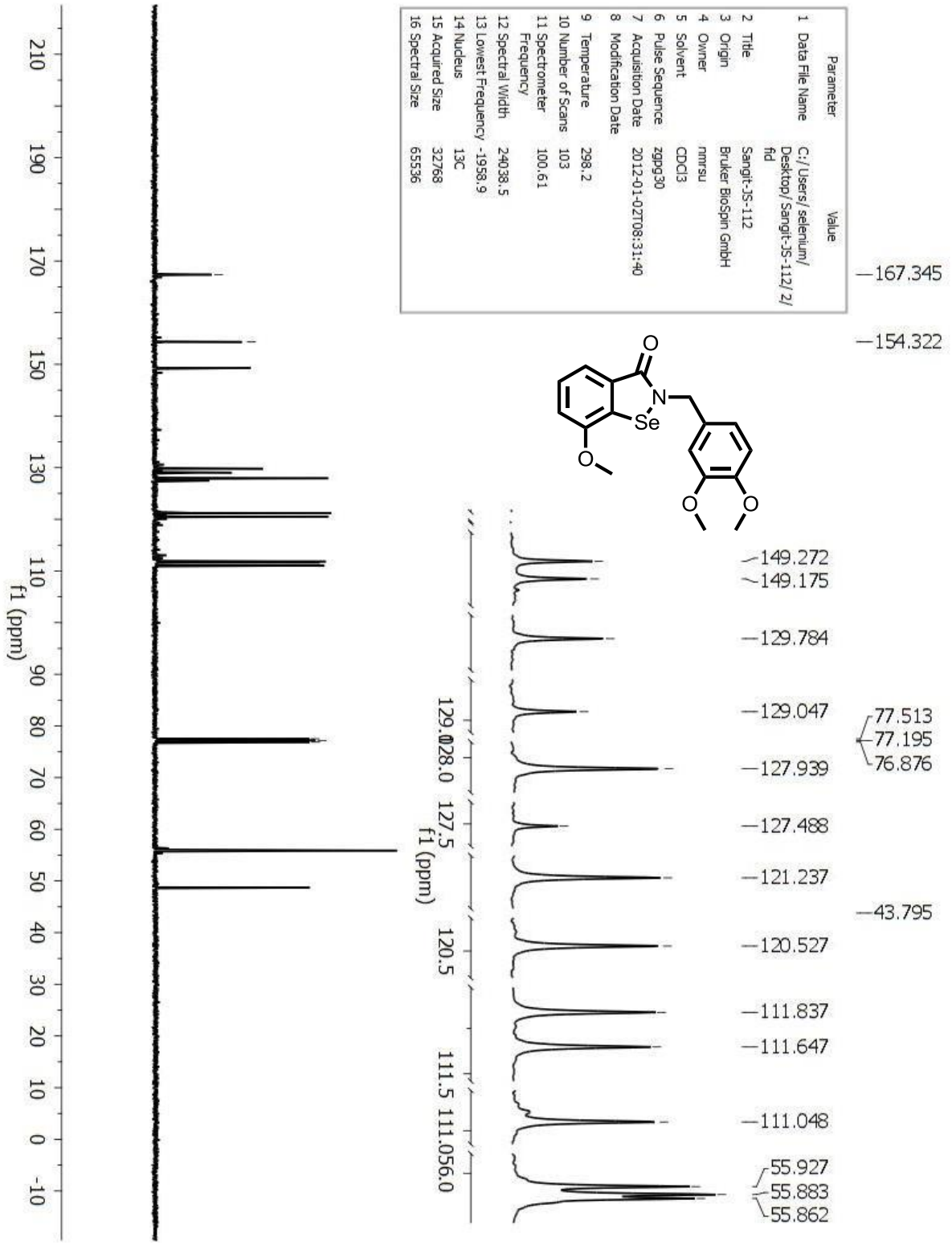
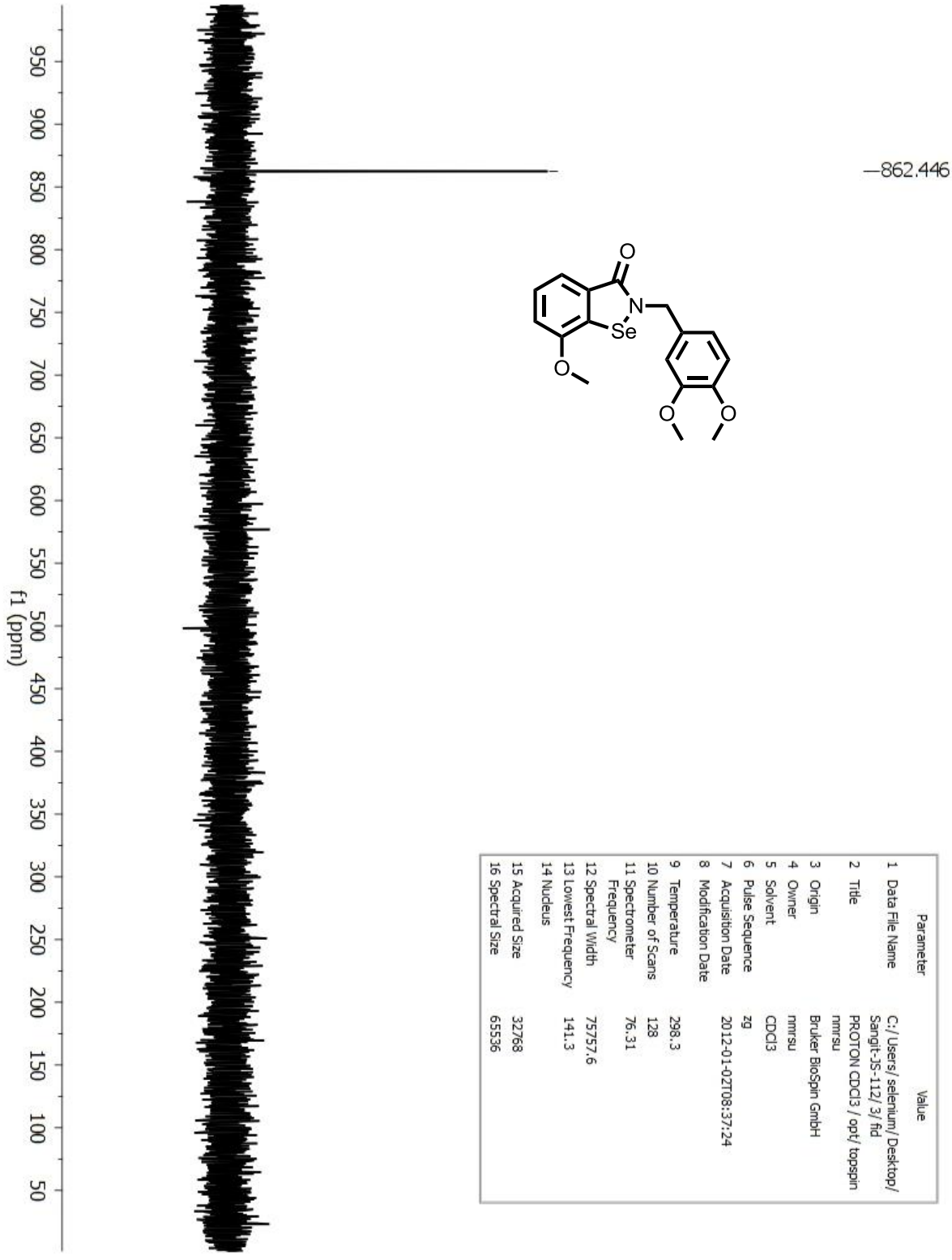


Figure S89 ^{77}Se NMR of **1o**



	Parameter	Value
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2	Title	PROTON CDCl3 / opt/ topspin nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	CDCl3
6	Pulse Sequence	zg
7	Acquisition Date	2012-01-02T08:37:24
8	Modification Date	
9	Temperature	298.3
10	Number of Scans	128
11	Spectrometer Frequency	76.31
12	Spectral Width	75757.6
13	Lowest Frequency	141.3
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

Figure S90 HRMS of **1o**

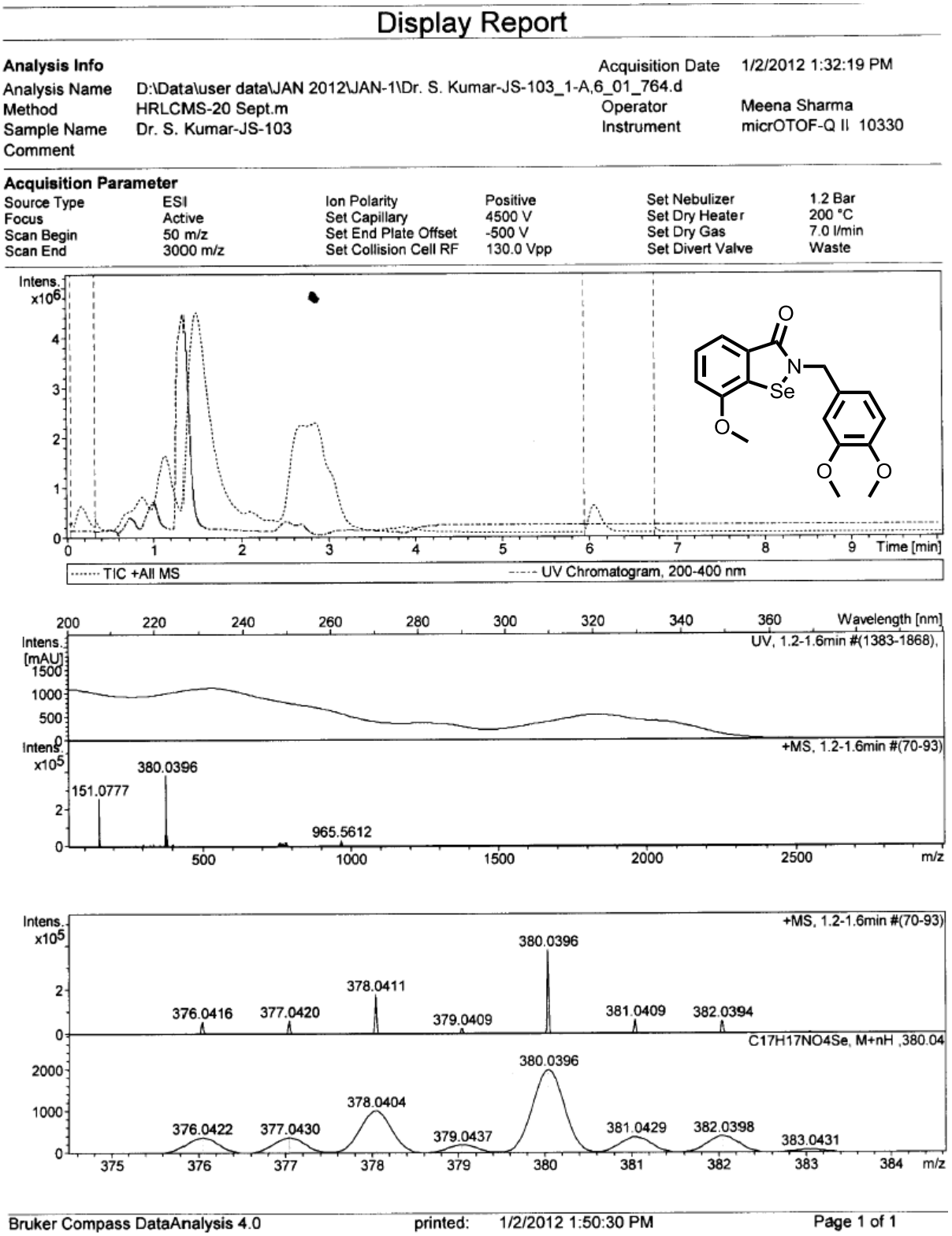


Figure S91 ^{1}H NMR of **1p**

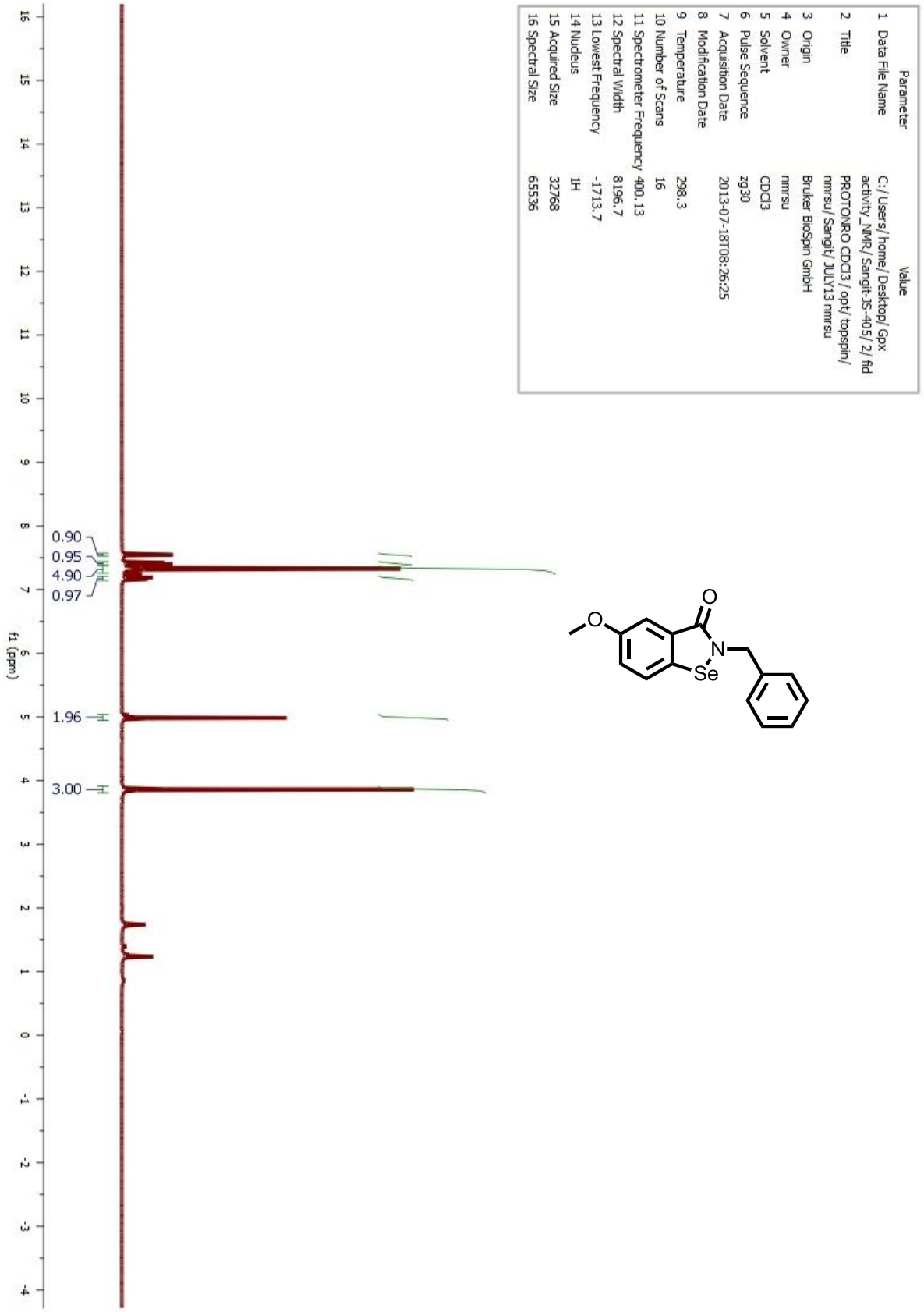


Figure S92 ^{13}C NMR of **1p**

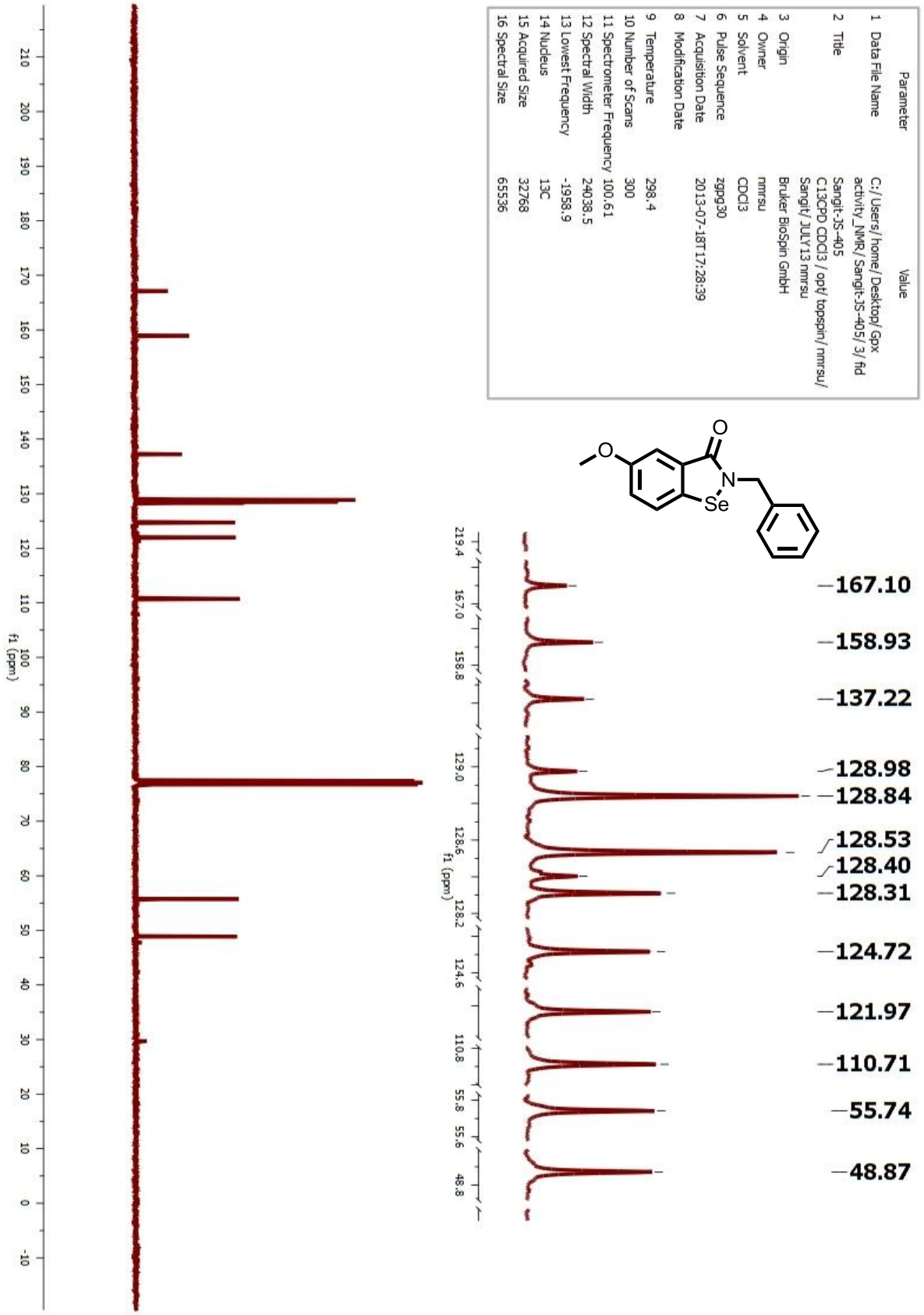
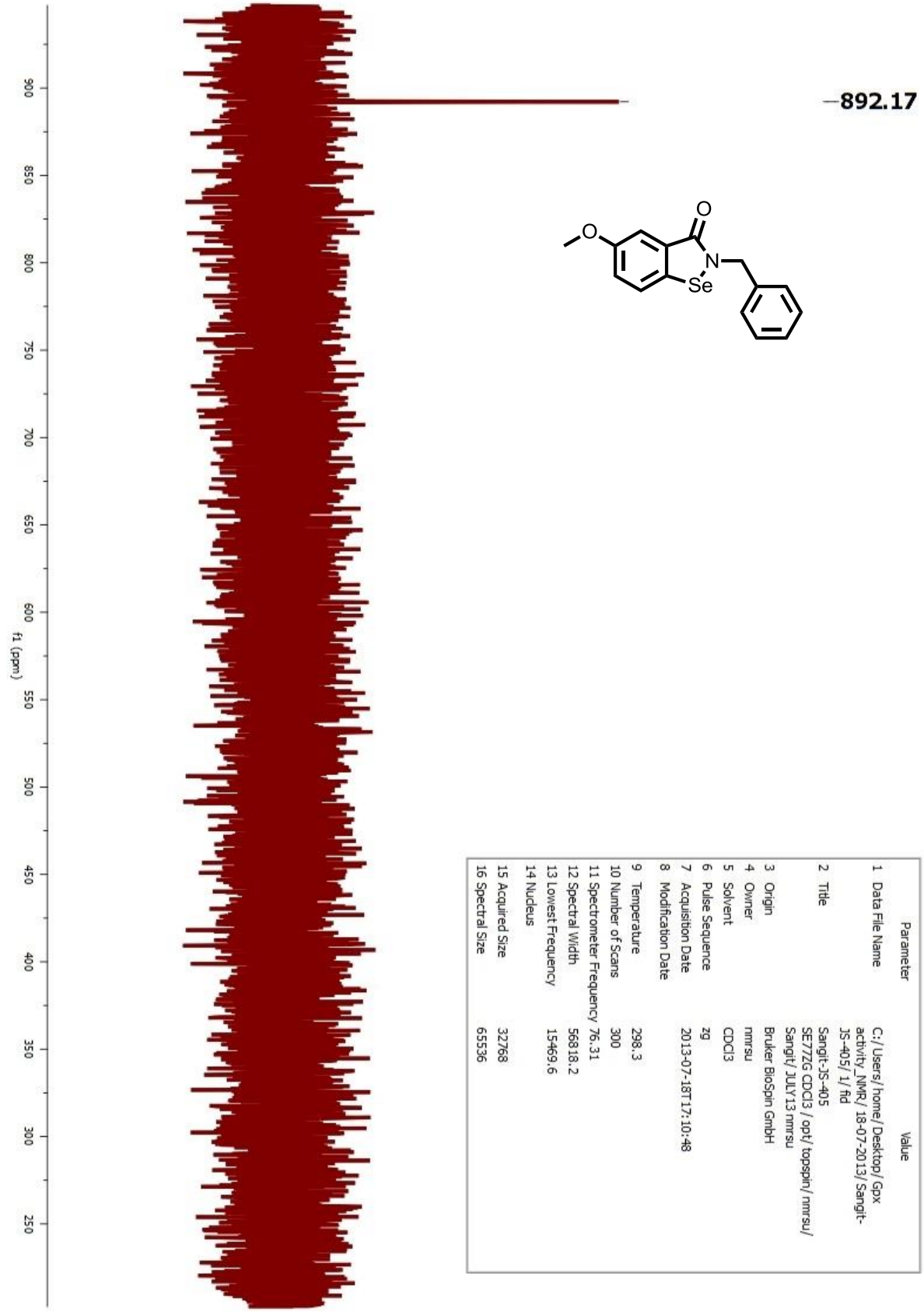


Figure S93 ^{77}Se NMR of **1p**



	Parameter	Value
1	Data File Name	C:/Users/home/Desktop/Gpx activity_NMR/ 18-07-2013/Sangit-JS-405/ 1/ fid
2	Title	Sangit-JS-405 SE77ZG CDCl3 / opt/ topspin/ nmrsu/ Sangit/ JULY13 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	CDCl3
6	Pulse Sequence	zg
7	Acquisition Date	2013-07-18T17:10:48
8	Modification Date	
9	Temperature	298.3
10	Number of Scans	300
11	Spectrometer Frequency	76.31
12	Spectral Width	56818.2
13	Lowest Frequency	15469.6
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

Figure S94 HRMS of **1p**

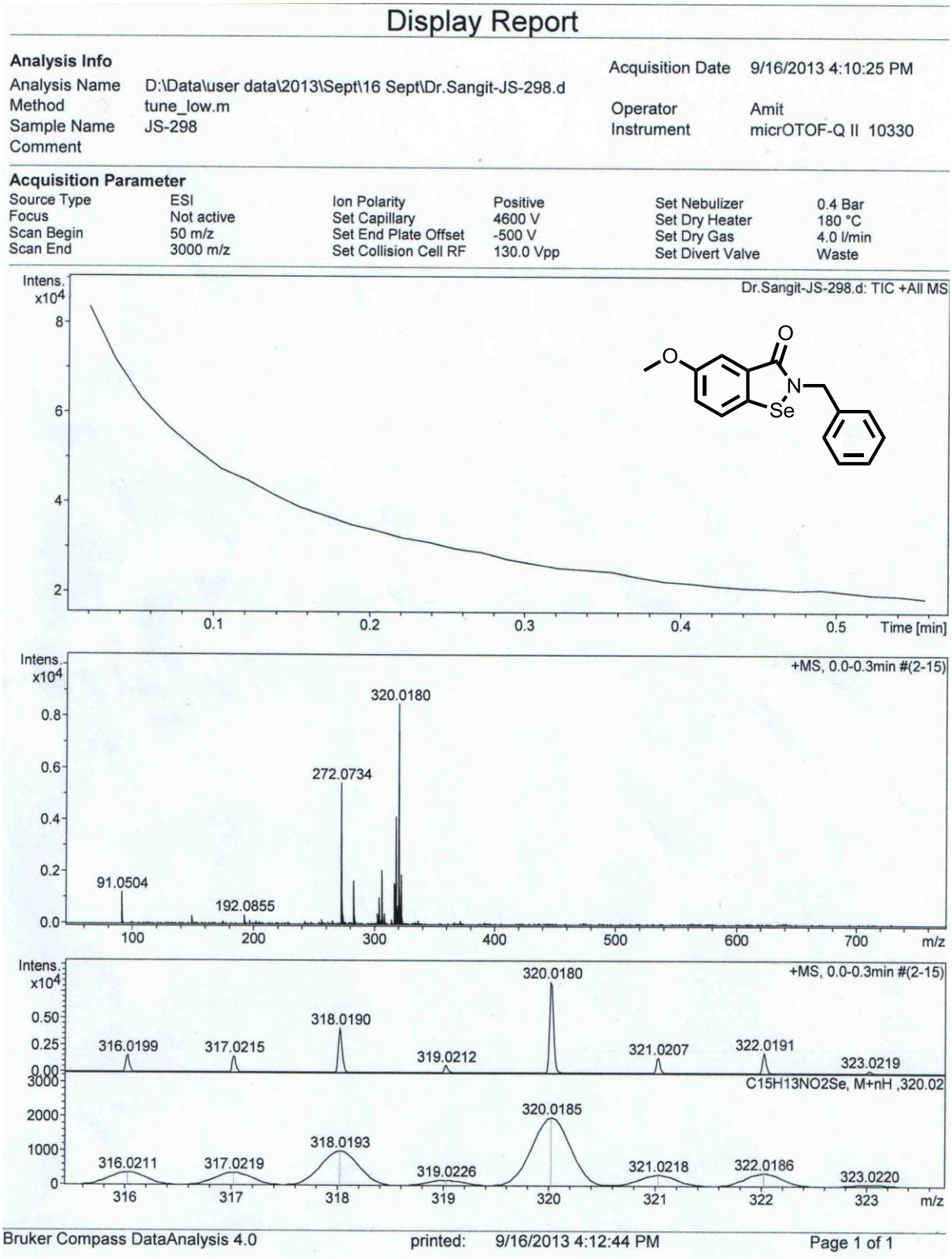


Figure S95 ^{1}H NMR of**1q**

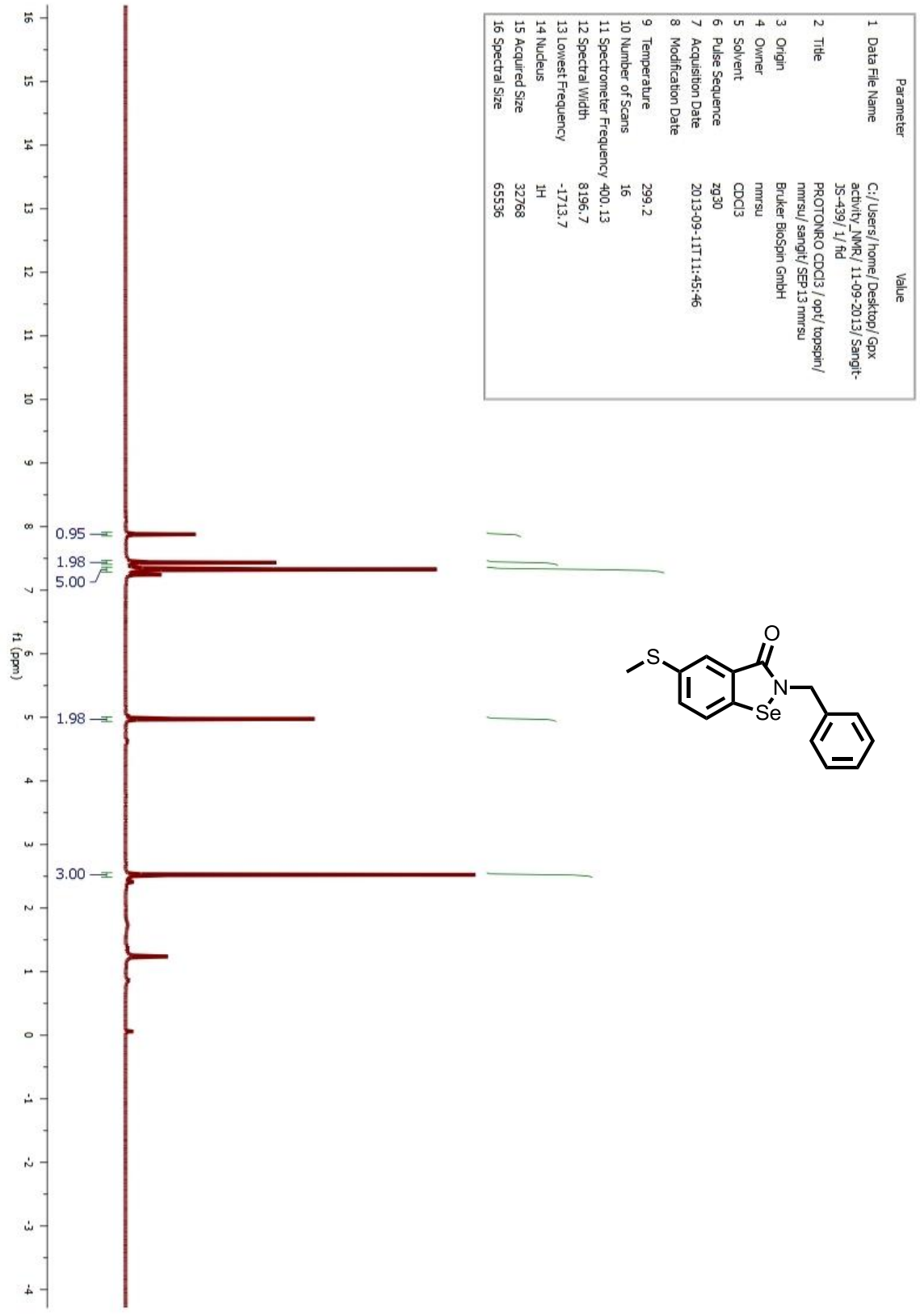


Figure S96 ^{13}C NMR of **1q**

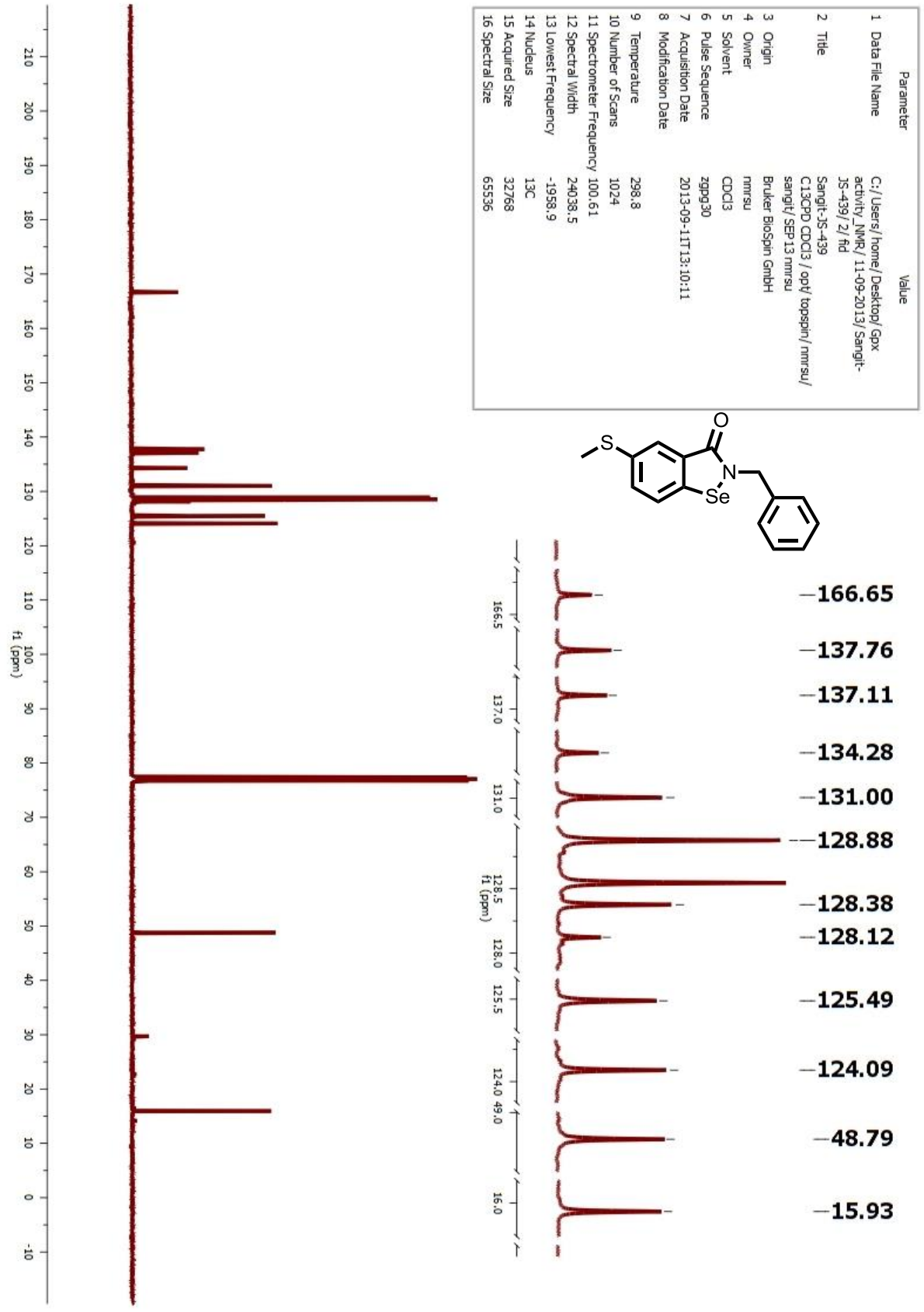
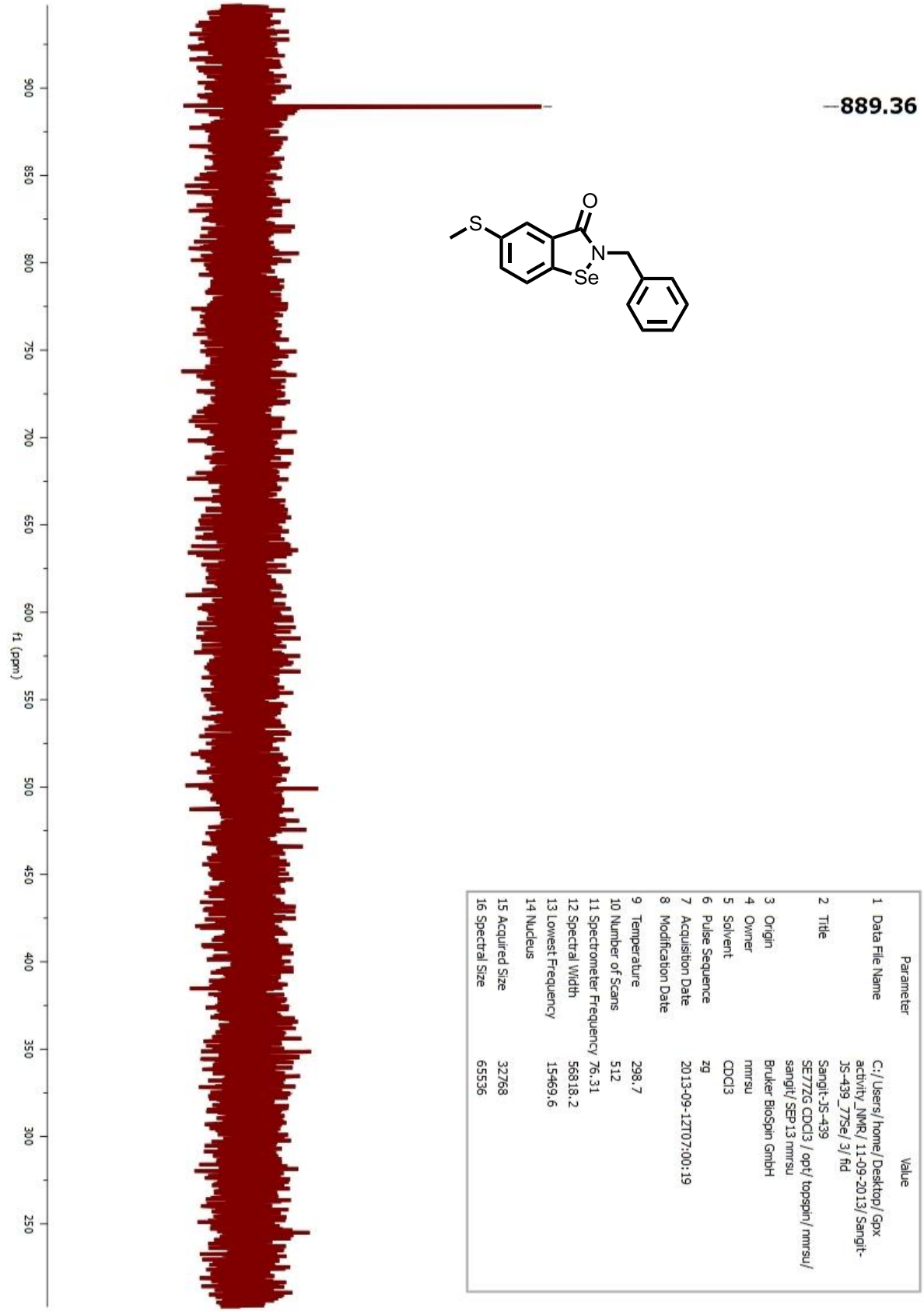


Figure S97 ^{77}Se NMR of **1q**



	Parameter	Value
1	Data File Name	C:/Users/home/Desktop/Gpx activity_NMR/11-09-2013/Sangit-JS-439_77Se/3/fid
2	Title	Sangit-JS-439 SE77ZG CDCl3 / opt/topspin/nmrsu/ sangit/SEP13 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	CDCl3
6	Pulse Sequence	zg
7	Acquisition Date	2013-09-12T07:00:19
8	Modification Date	
9	Temperature	298.7
10	Number of Scans	512
11	Spectrometer Frequency	76.31
12	Spectral Width	56818.2
13	Lowest Frequency	15469.6
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

Figure S98 LRMS of **1q**

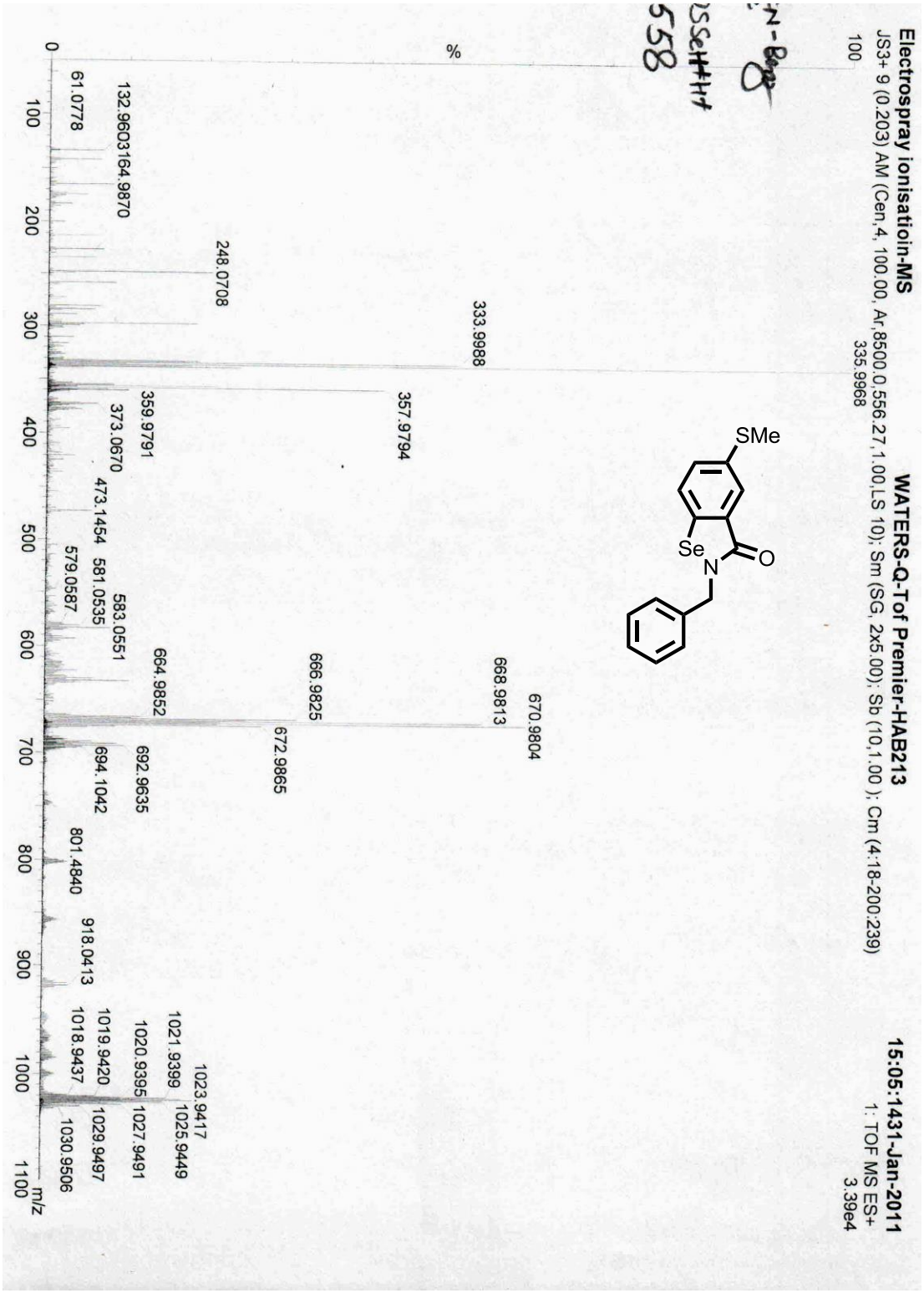


Figure S99 ^{1}H NMR of **1r**

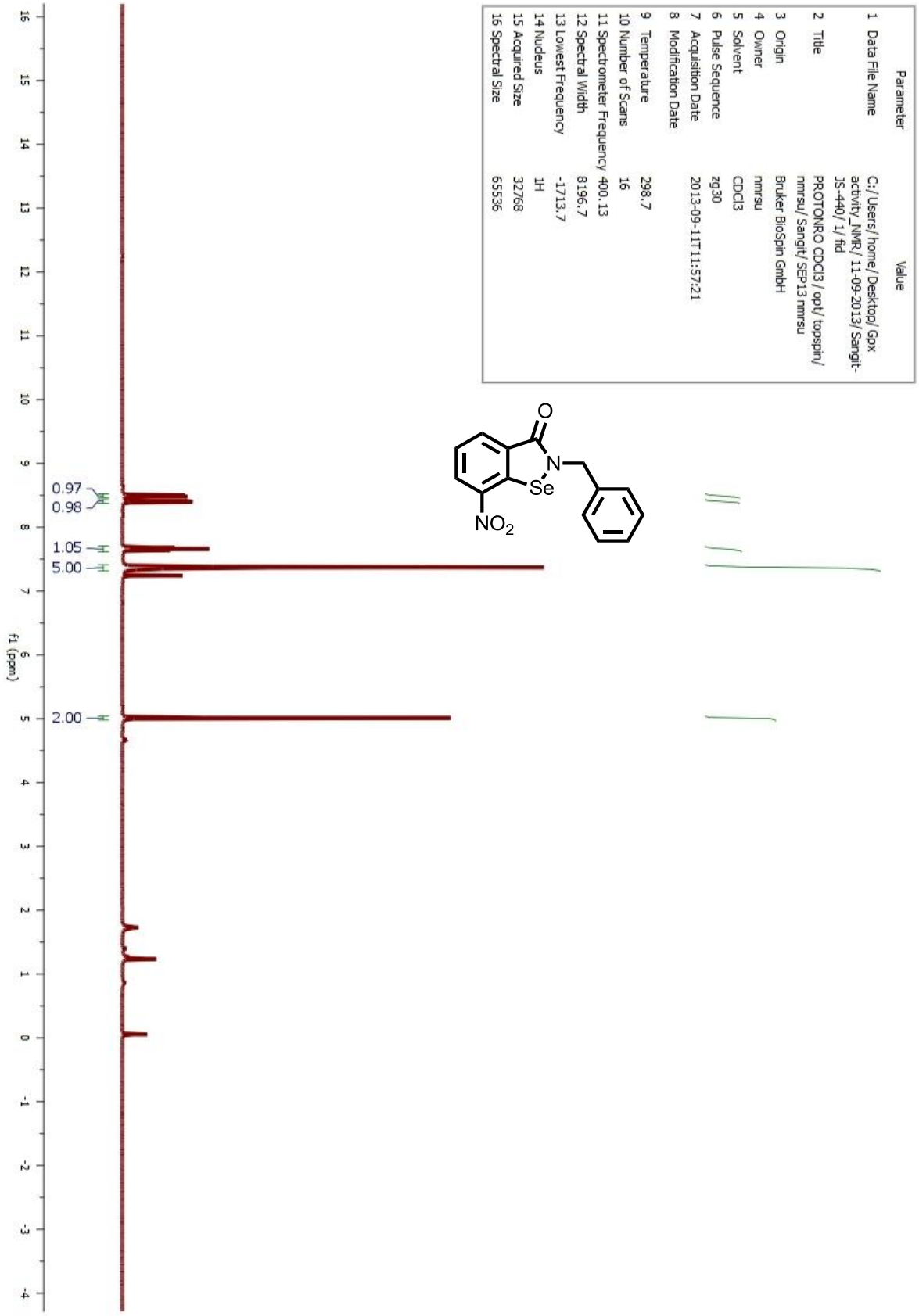


Figure S100 ^{13}C NMR of **1r**

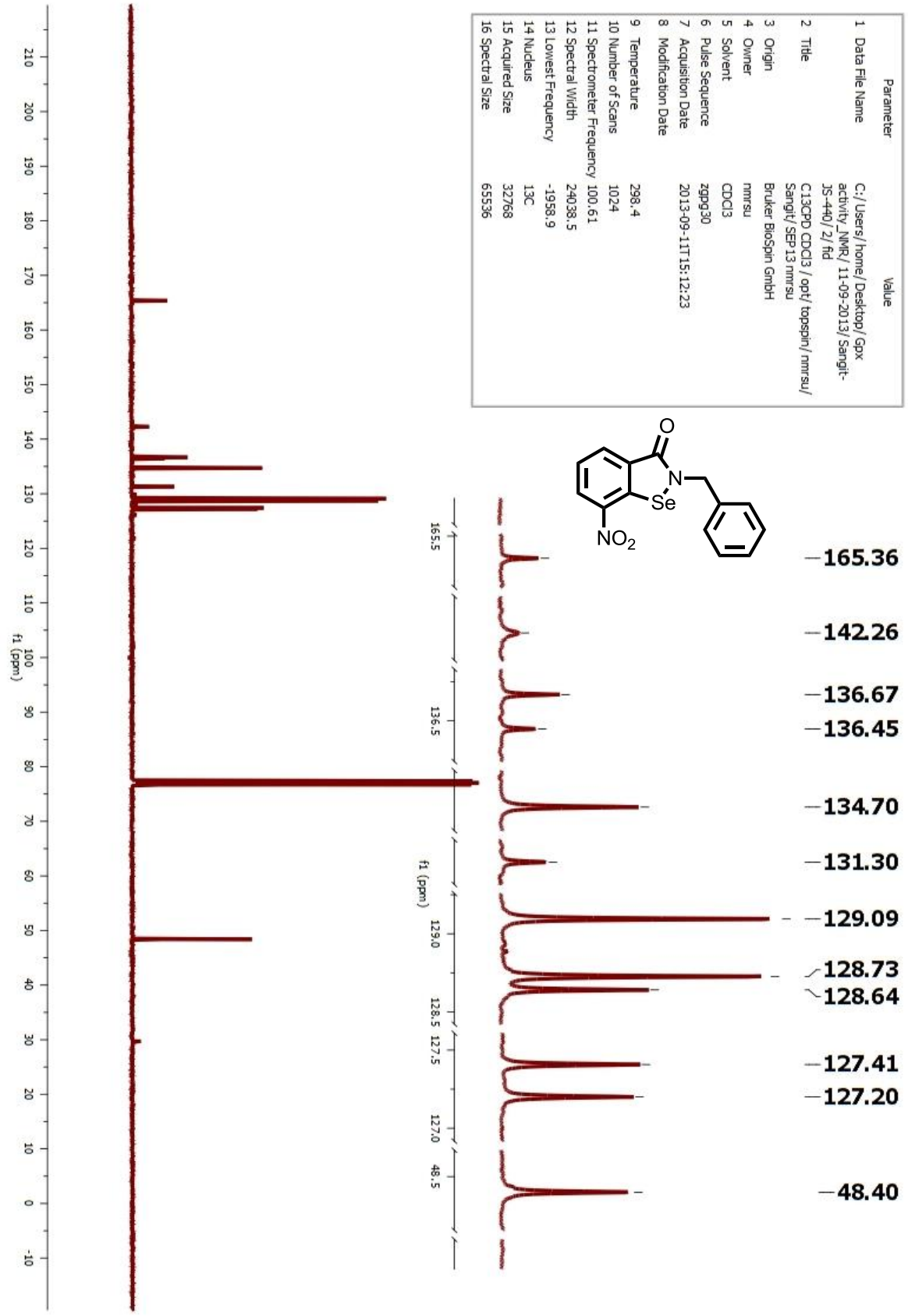
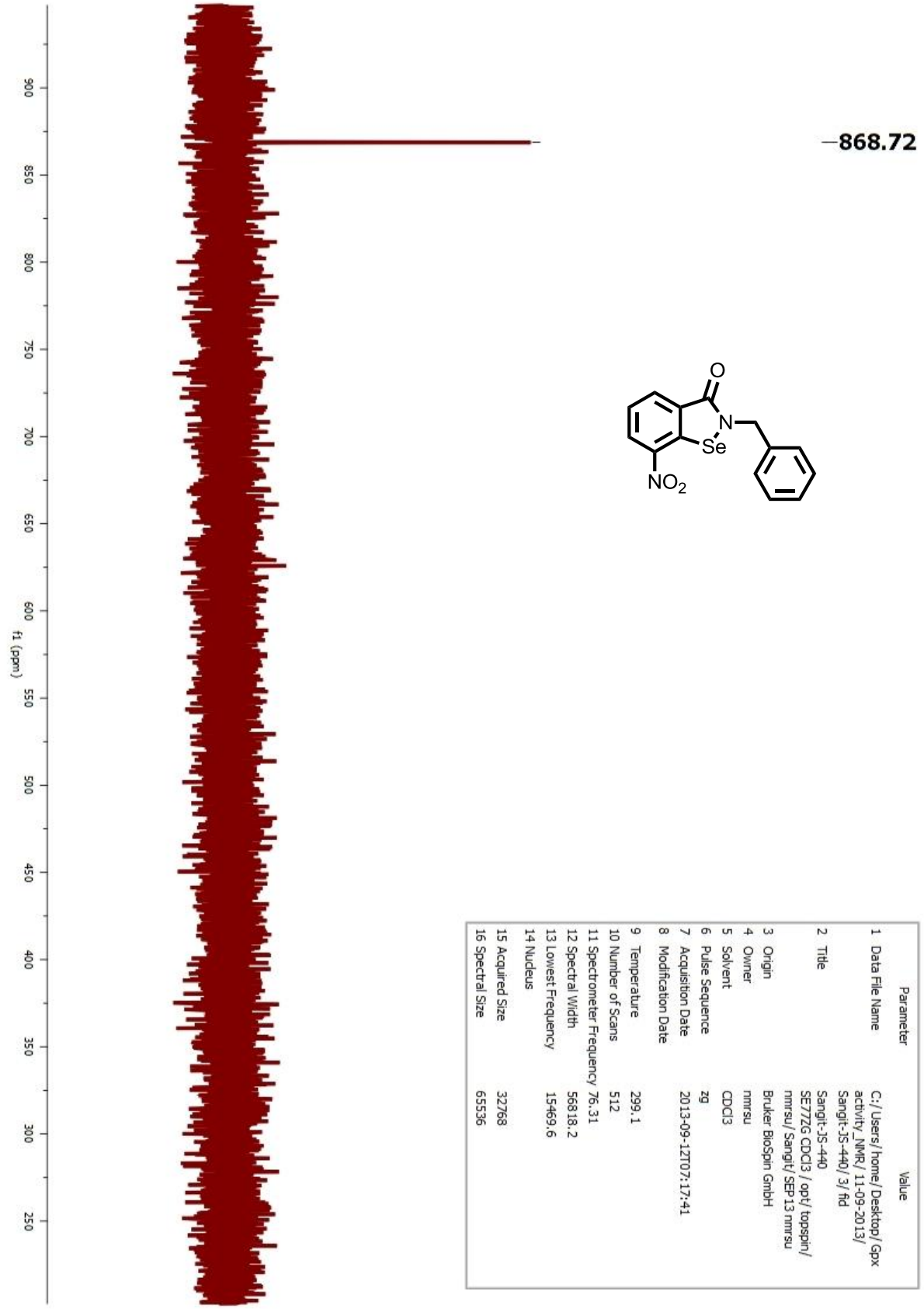
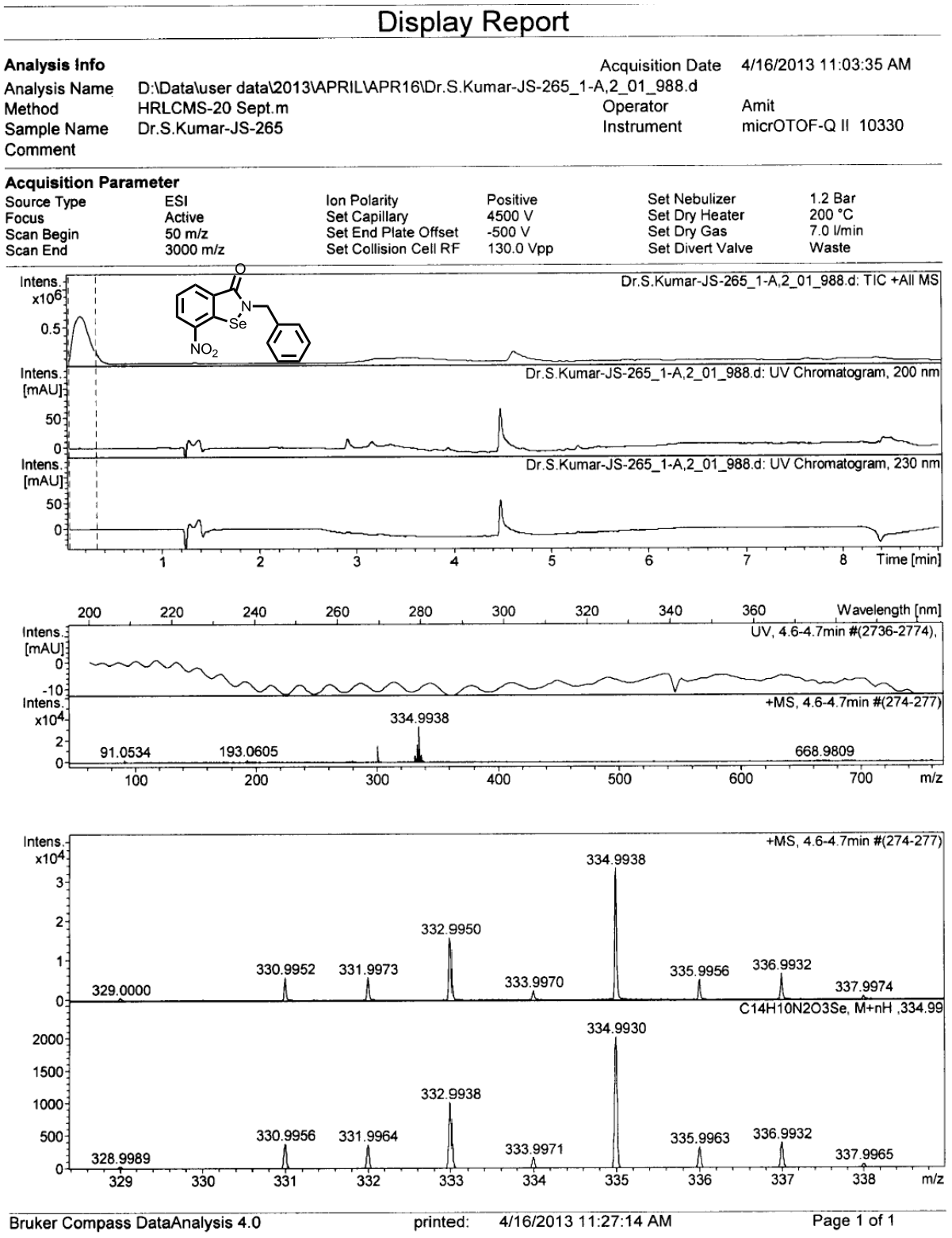


Figure S101 ^{77}Se NMR of **1r**



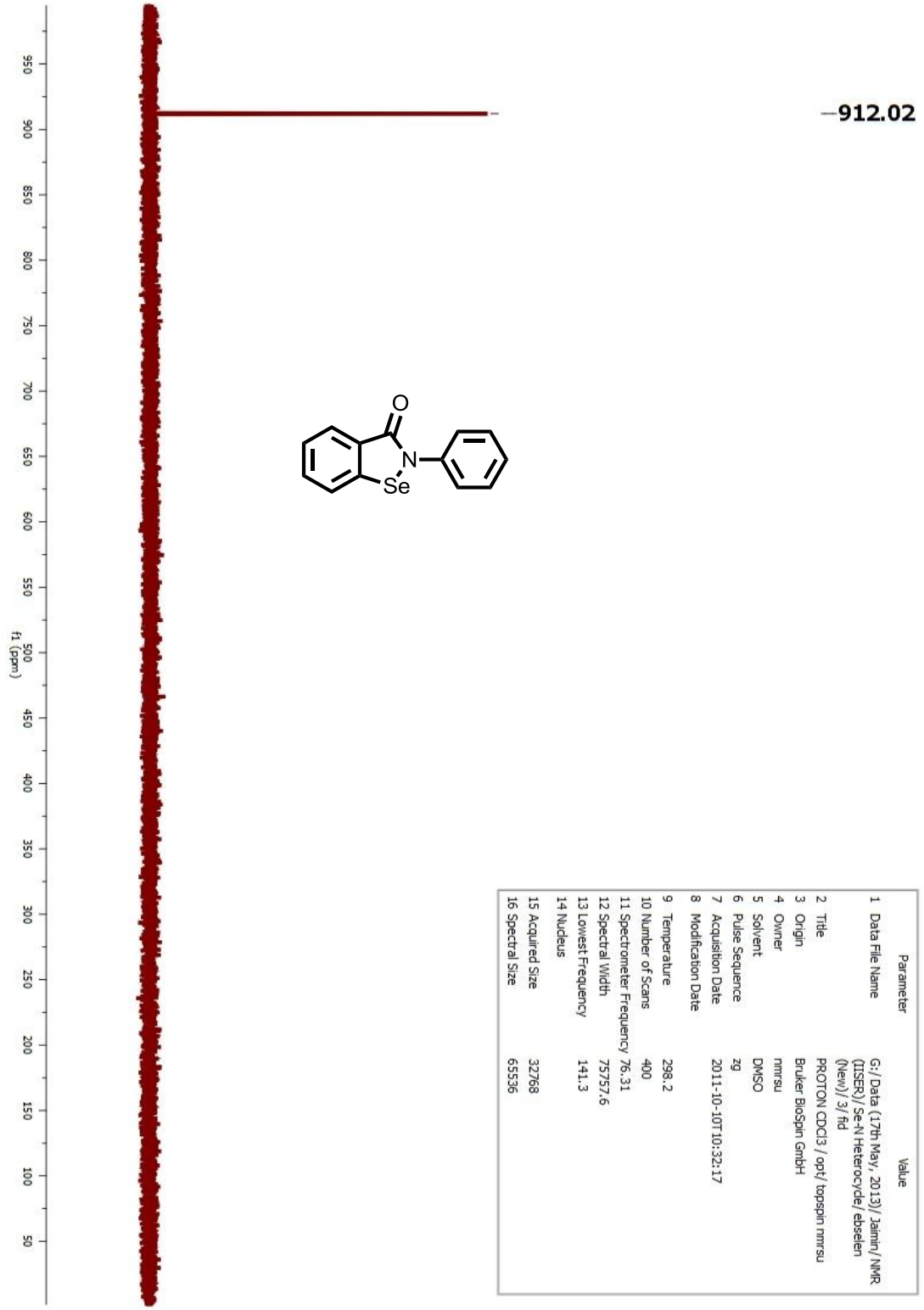
	Parameter	Value
1	Data File Name	C:/Users/home/Desktop/Gpx activity_NMR/11-09-2013/ Sangit-JS-440/3/fid
2	Title	Sangit-JS-440 SE77ZG CDCl3 / opt/topspin/ nmrsu/Sangit/SEP13 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	CDCl3
6	Pulse Sequence	zg
7	Acquisition Date	2013-09-12T07:17:41
8	Modification Date	
9	Temperature	299.1
10	Number of Scans	512
11	Spectrometer Frequency	76.31
12	Spectral Width	56818.2
13	Lowest Frequency	15469.6
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

Figure S102 HRMS of **1r**



Reaction of Isoselenazolones with PhSH Investigated by ^{77}Se NMR and Mass Spectrometry

Figure S103 ^{77}Se NMR of **1a**



	Parameter	Value
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2	Title	PROTON CDCl3 / opt/ topspin nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	DMSO
6	Pulse Sequence	zg
7	Acquisition Date	2011-10-10T10:32:17
8	Modification Date	
9	Temperature	298.2
10	Number of Scans	400
11	Spectrometer Frequency	76.31
12	Spectral Width	75757.6
13	Lowest Frequency	141.3
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

Figure S104 ^{77}Se NMR of **2a** obtained by the reaction of **1a + one equiv of PhSH**

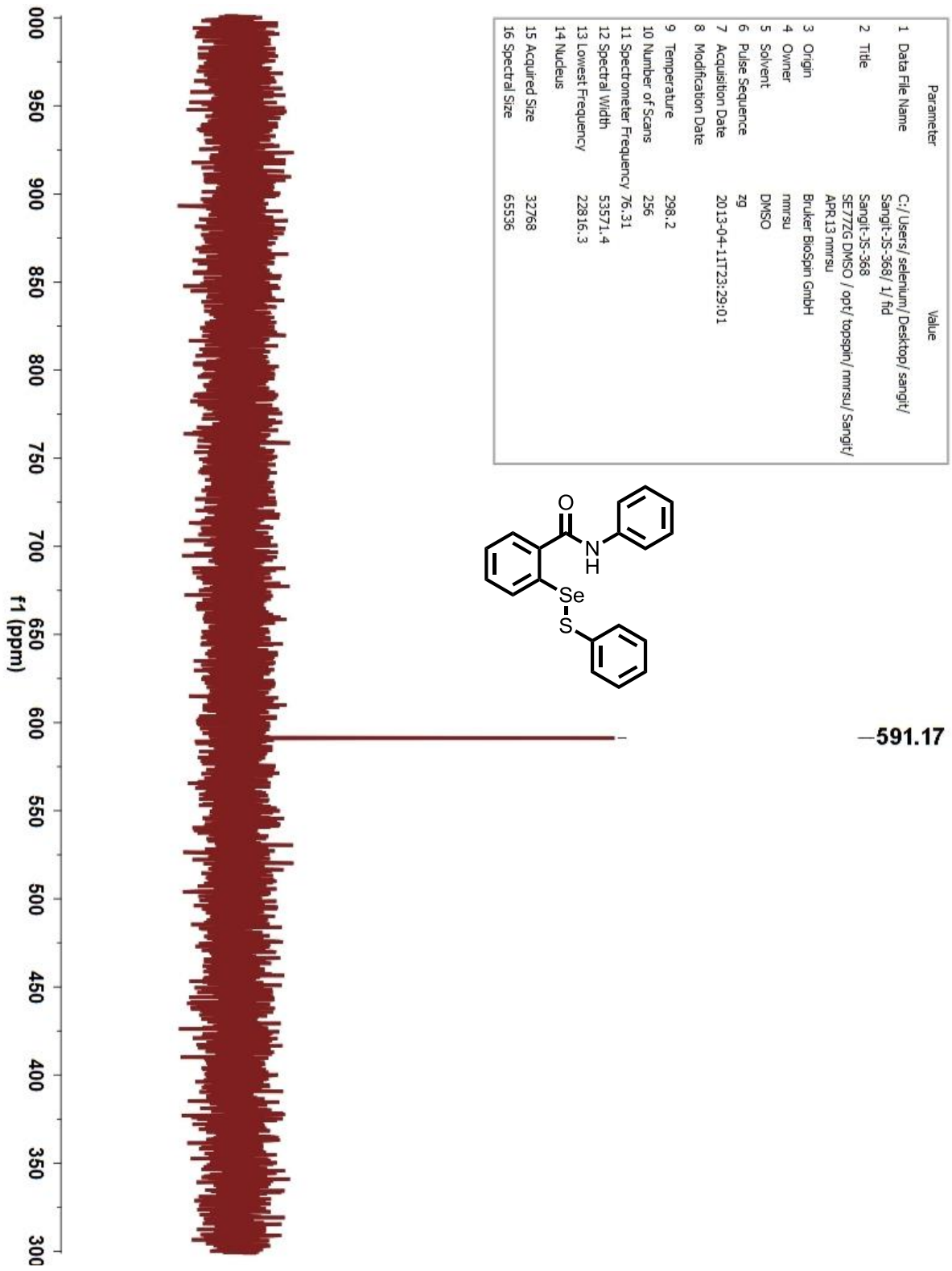
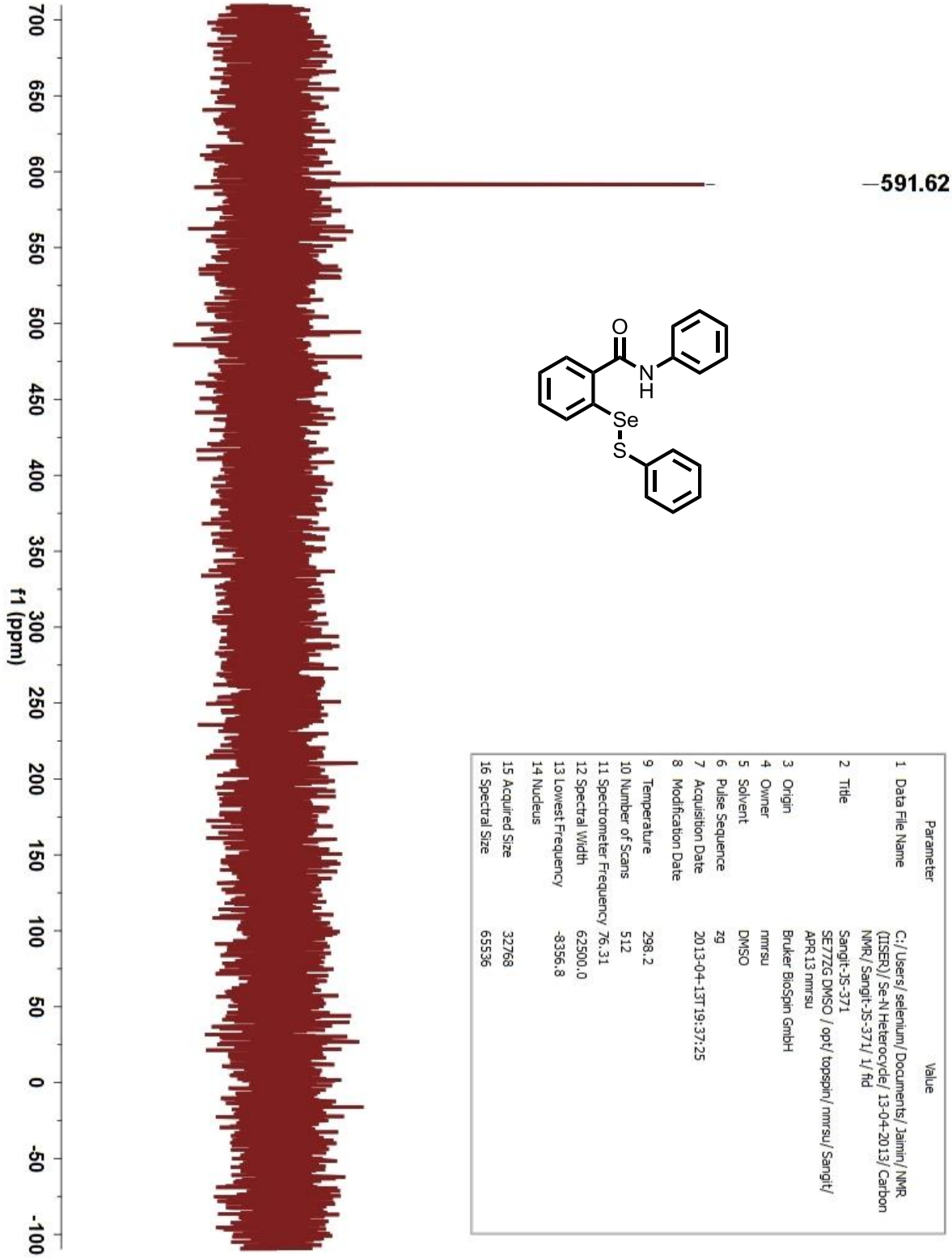
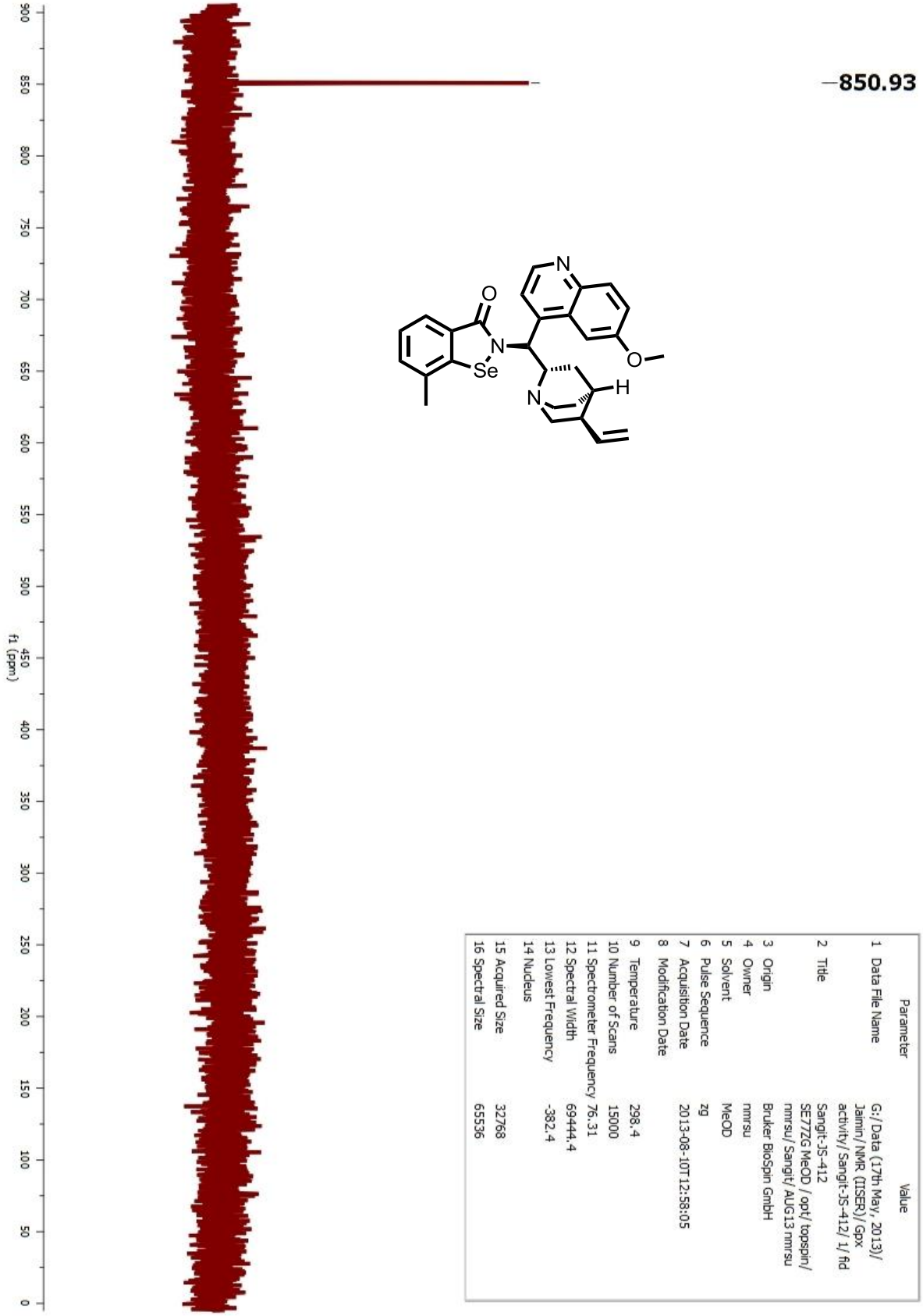


Figure S105 ^{77}Se NMR of **2a** obtained by the reaction of **1a + two equiv of PhSH**



	Parameter	Value
1	Data File Name	C:/Users/selenium/Documents/Jaimin/NMR (IISER)/Se-N Heterocycle/13-04-2013/Carbon NMR/Sangit-JS-371/1/fid
2	Title	Sangit-JS-371 SE77ZG DMSO / opt/ topspin/ nmrsu/ Sangit/ APR13 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	DMSO
6	Pulse Sequence	zg
7	Acquisition Date	2013-04-13T19:37:25
8	Modification Date	
9	Temperature	298.2
10	Number of Scans	512
11	Spectrometer Frequency	76.31
12	Spectral Width	62500.0
13	Lowest Frequency	-8356.8
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

Figure S106 ^{77}Se NMR of **1b**



	Parameter	Value
1	Data File Name	G:/Data (17th May, 2013)/ Jaimin/NMR (IISER)/Gpx activity/Sangit-JS-412/ 1/ fid
2	Title	Sangit-JS-412 SE77ZG MeOD / opt/ topspin/ nmrsu/ Sangit/ AUG13 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	MeOD
6	Pulse Sequence	zg
7	Acquisition Date	2013-08-10T12:58:05
8	Modification Date	
9	Temperature	298.4
10	Number of Scans	15000
11	Spectrometer Frequency	76.31
12	Spectral Width	69444.4
13	Lowest Frequency	-382.4
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

Figure S107 ^{77}Se NMR of selenol **3b** obtained by the reaction of **1b** + one quiv of **PhSH**

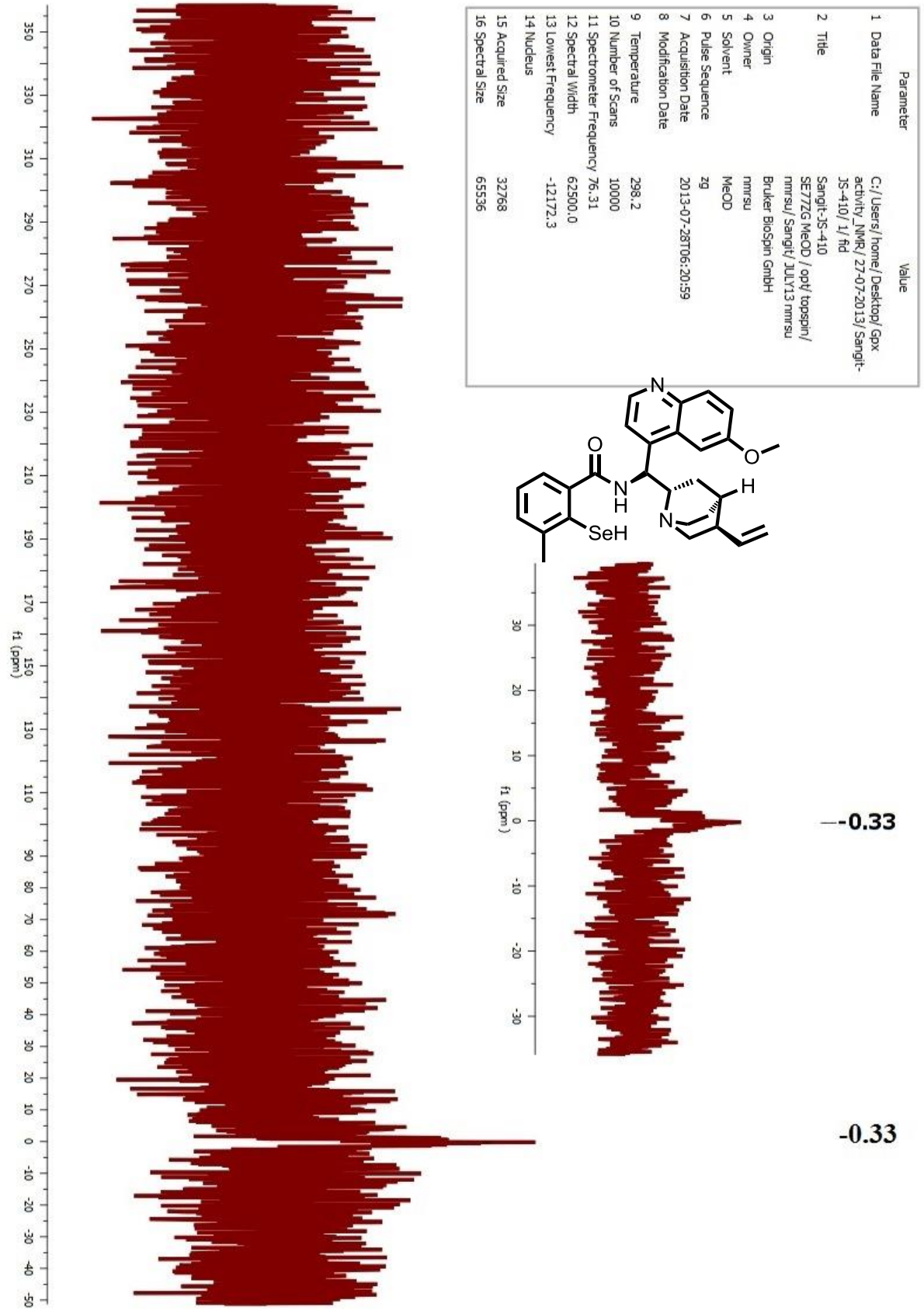


Figure S108 Mass spectra of **2b** obtained by the reaction of **1b** + **one equiv of PhSH**

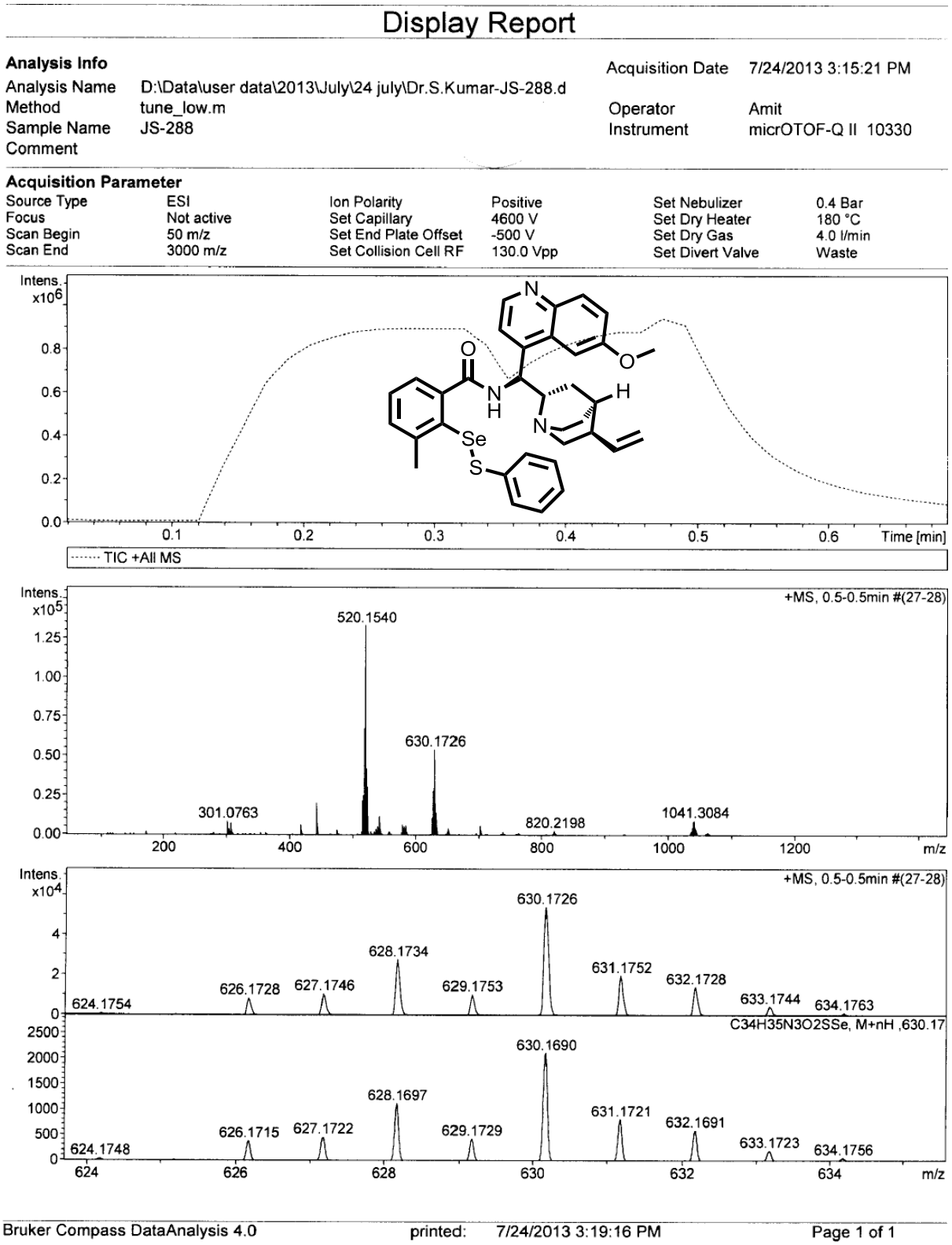


Figure S109 ^{77}Se NMR of selenol**3b** obtained by the reaction of **1b** + **two equiv of PhSH**

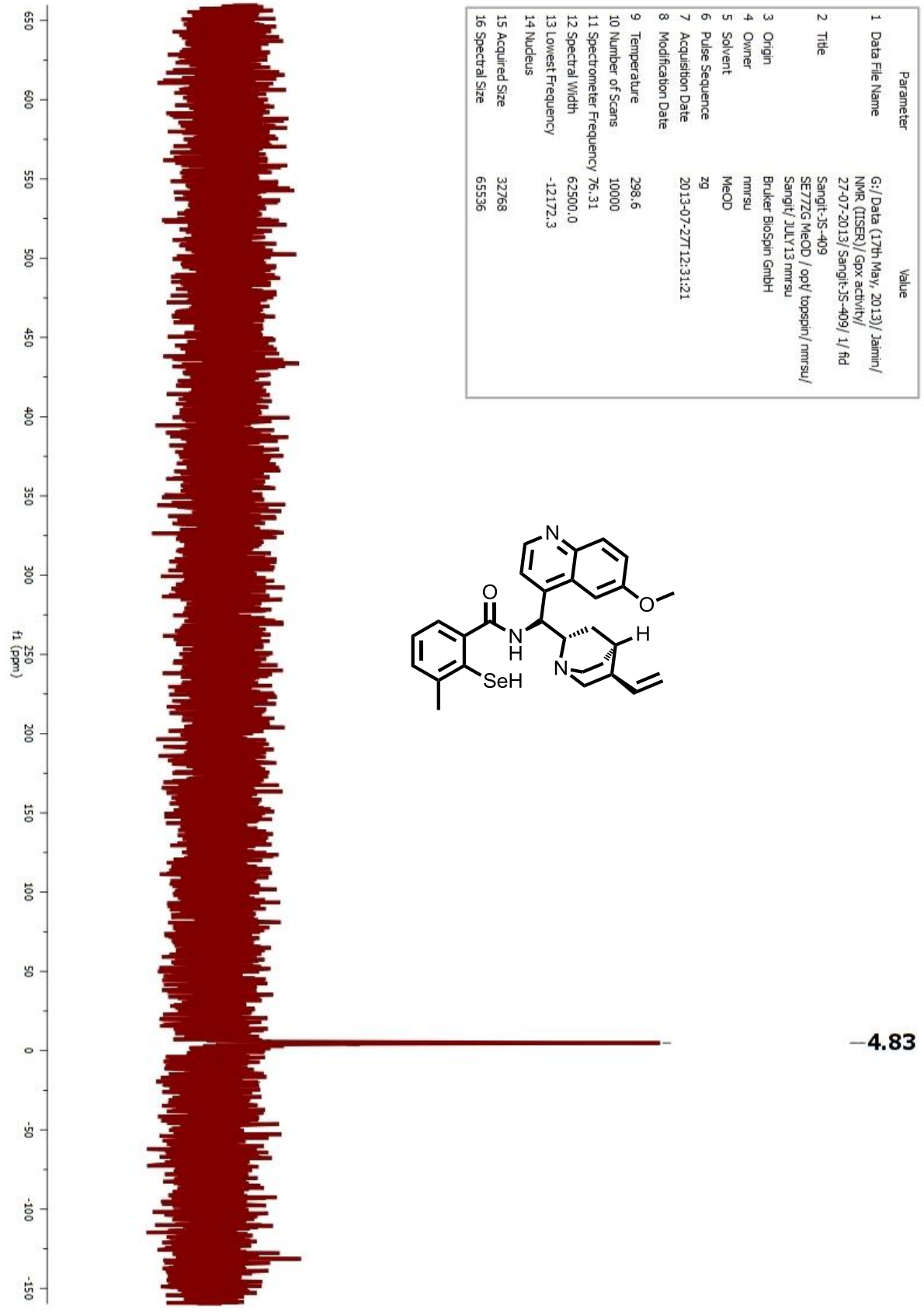


Figure S110 Mass spectra of selenol **3b** obtained by the reaction of **1b + two equiv of PhSH**

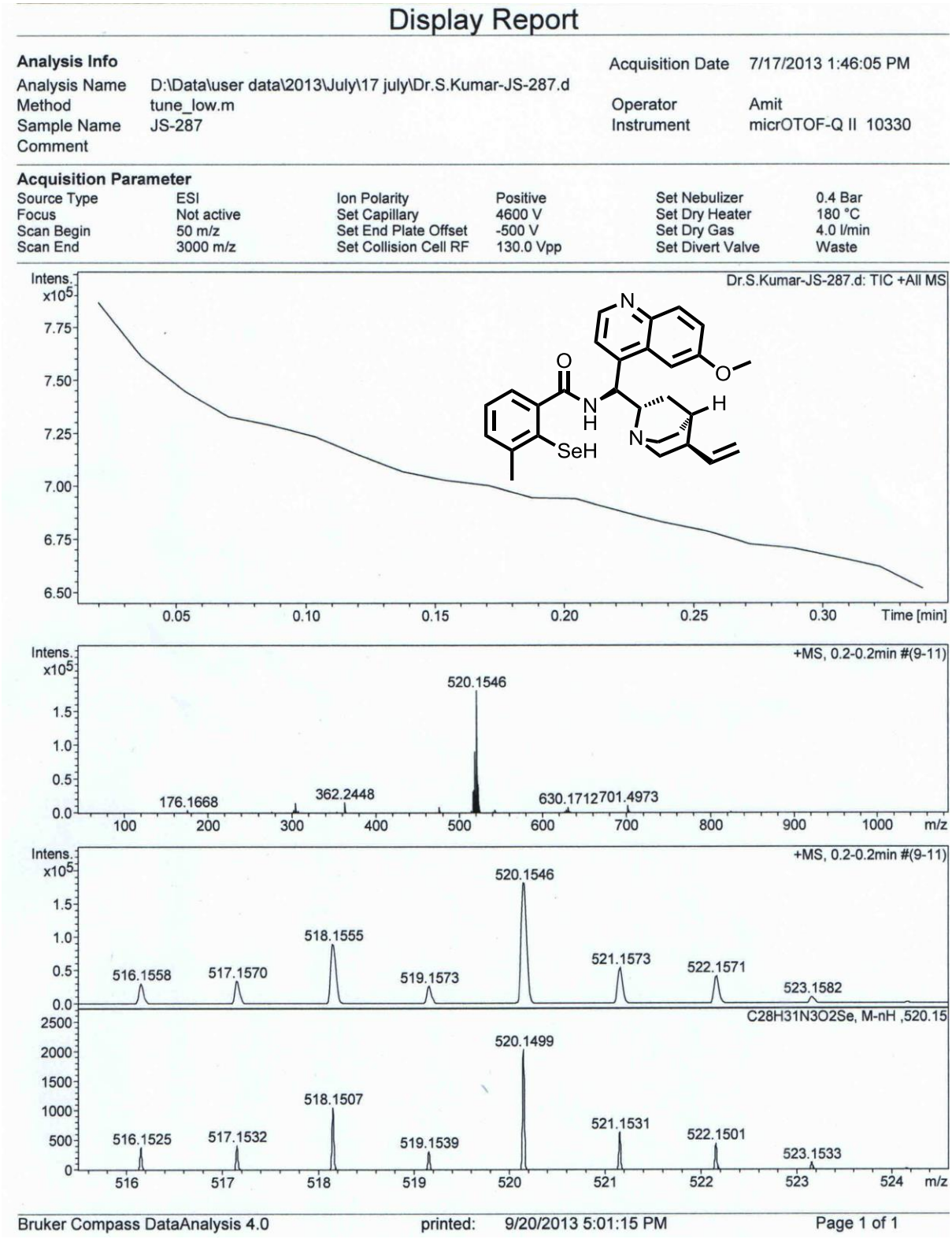


Figure S111 Mass spectra of selenol **3b** + **Na**

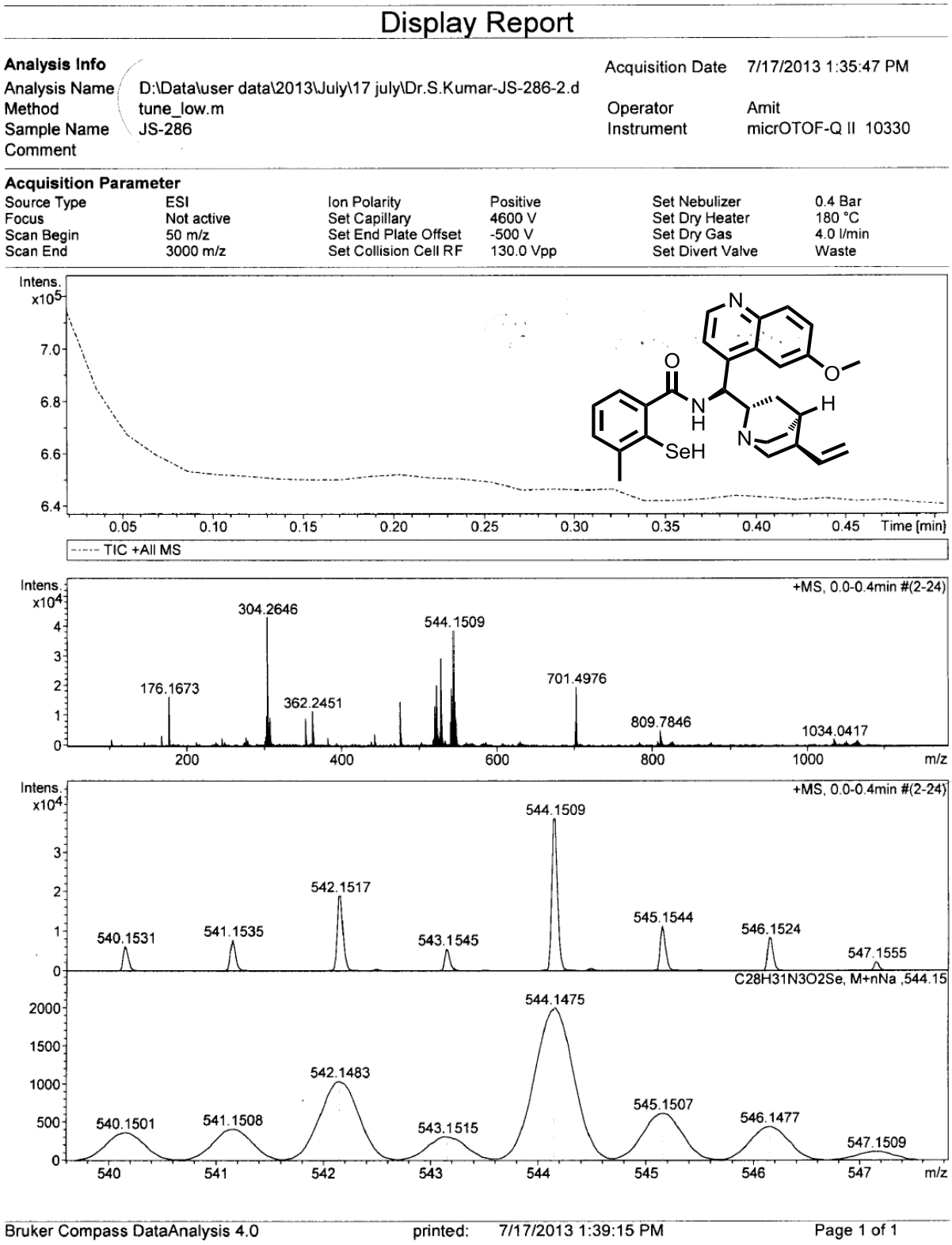


Figure S112 ^{77}Se NMR of **3b** after 2 weeks (spectra was obtained after 10,000 scans)

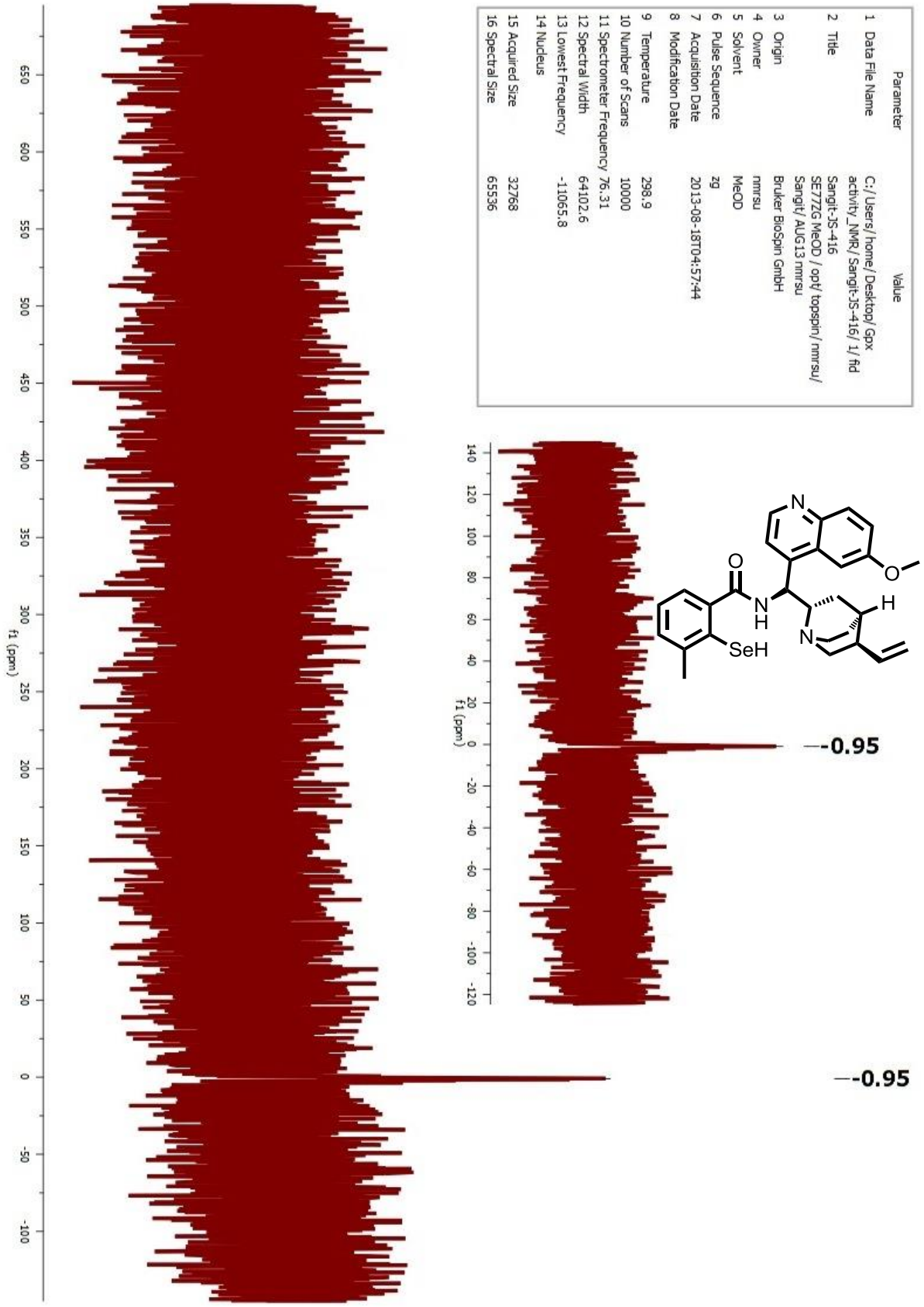


Figure S113 ^{77}Se NMR on the reaction of selenol **3b** with CH_3I (**1b + 2PhSH + CH_3I)**

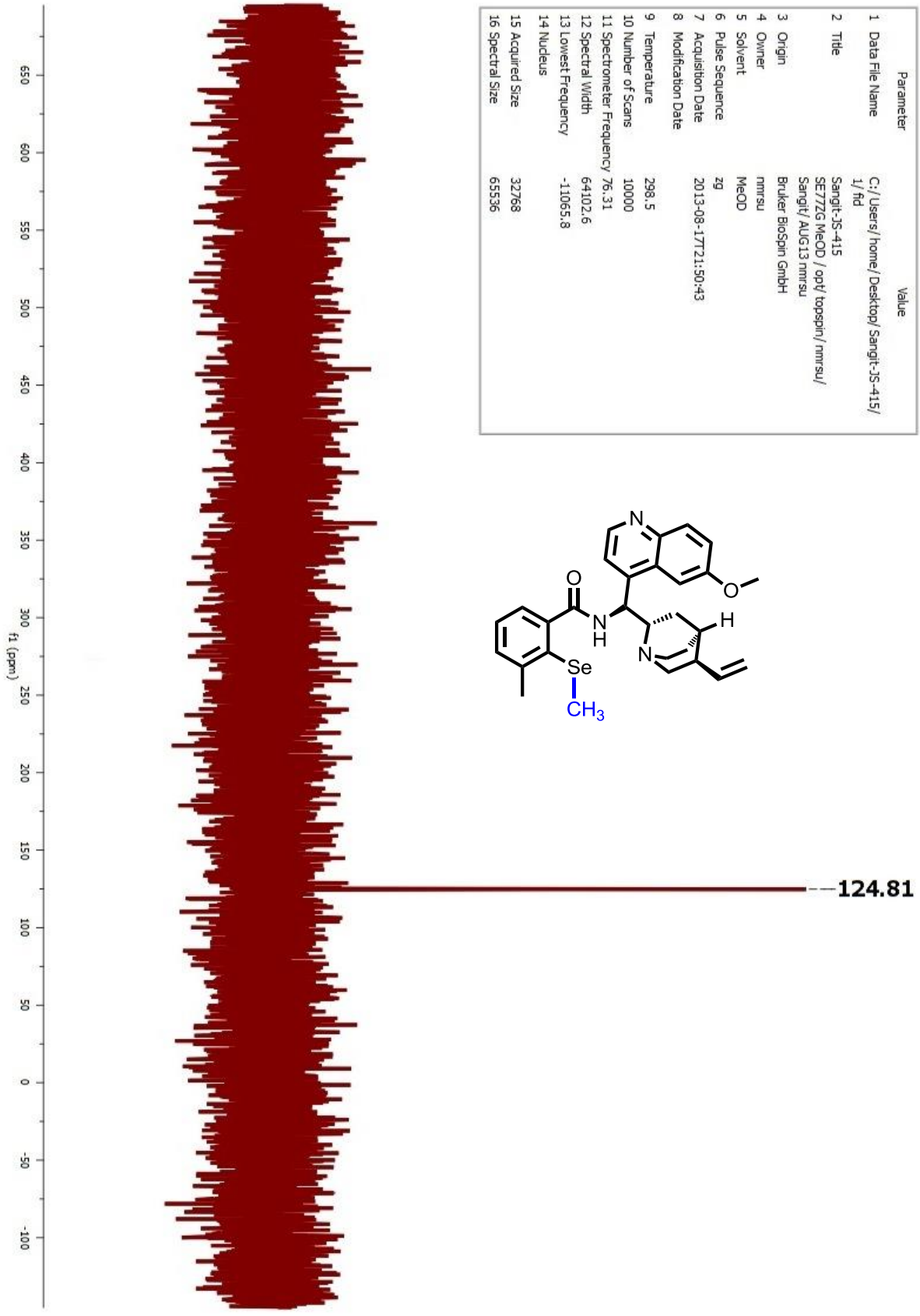


Figure S114 Mass spectra of on the reaction of selenol **3b** with CH_3I (**1b + 2PhSH + CH_3I)**

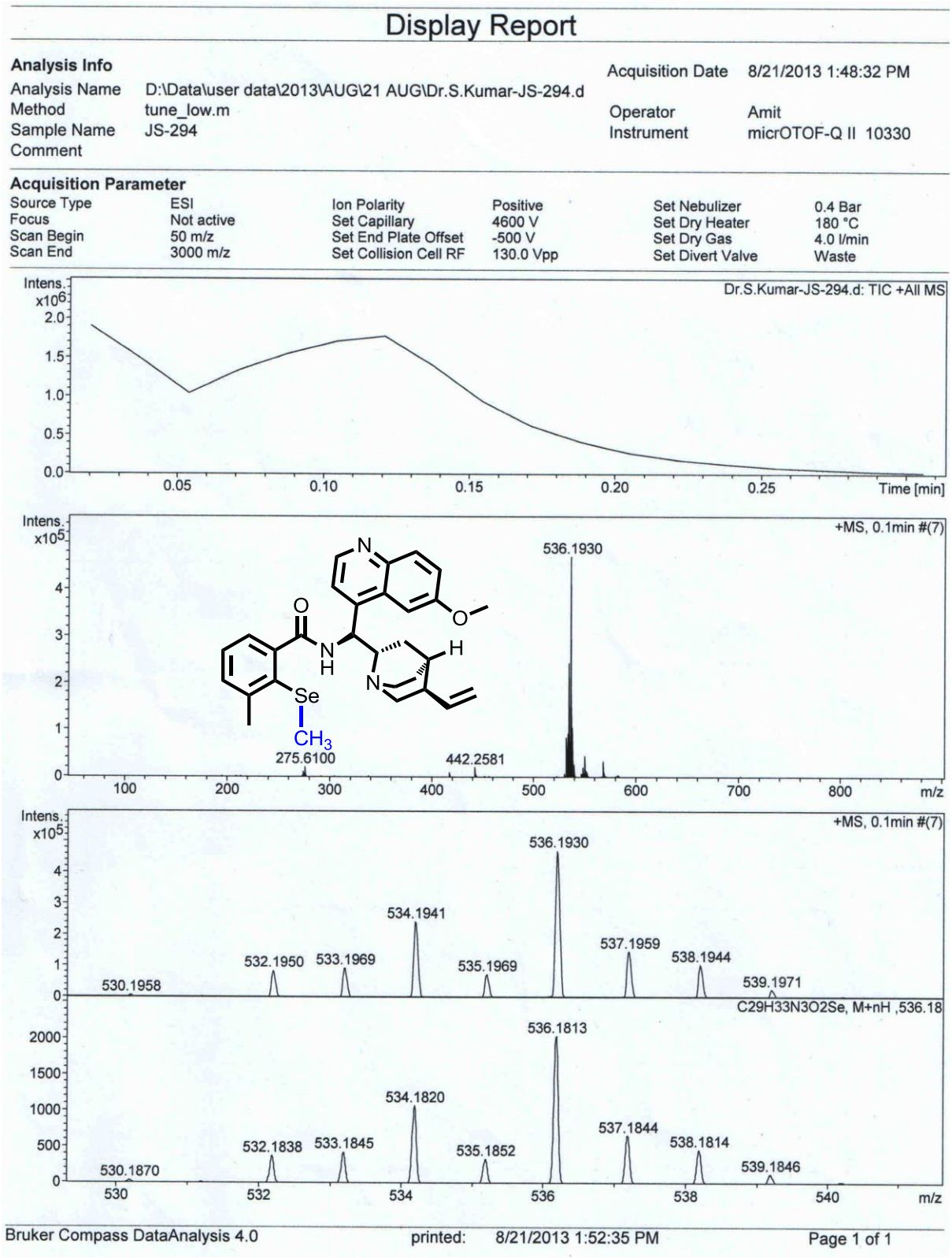


Figure S115 ^{77}Se NMR of **5b(1b + 2PhSH + H_2O_2)**(700-1300 ppm range)

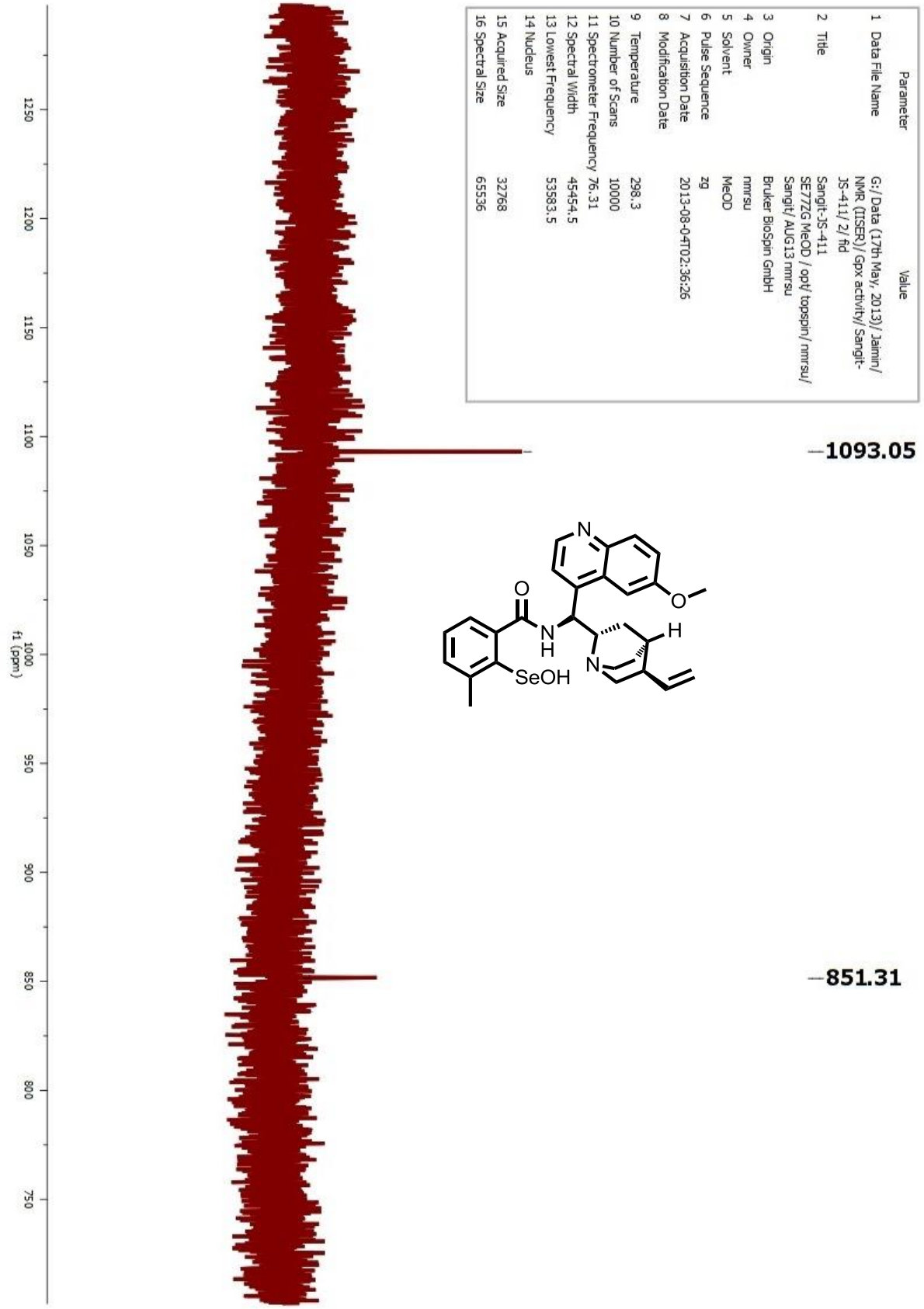
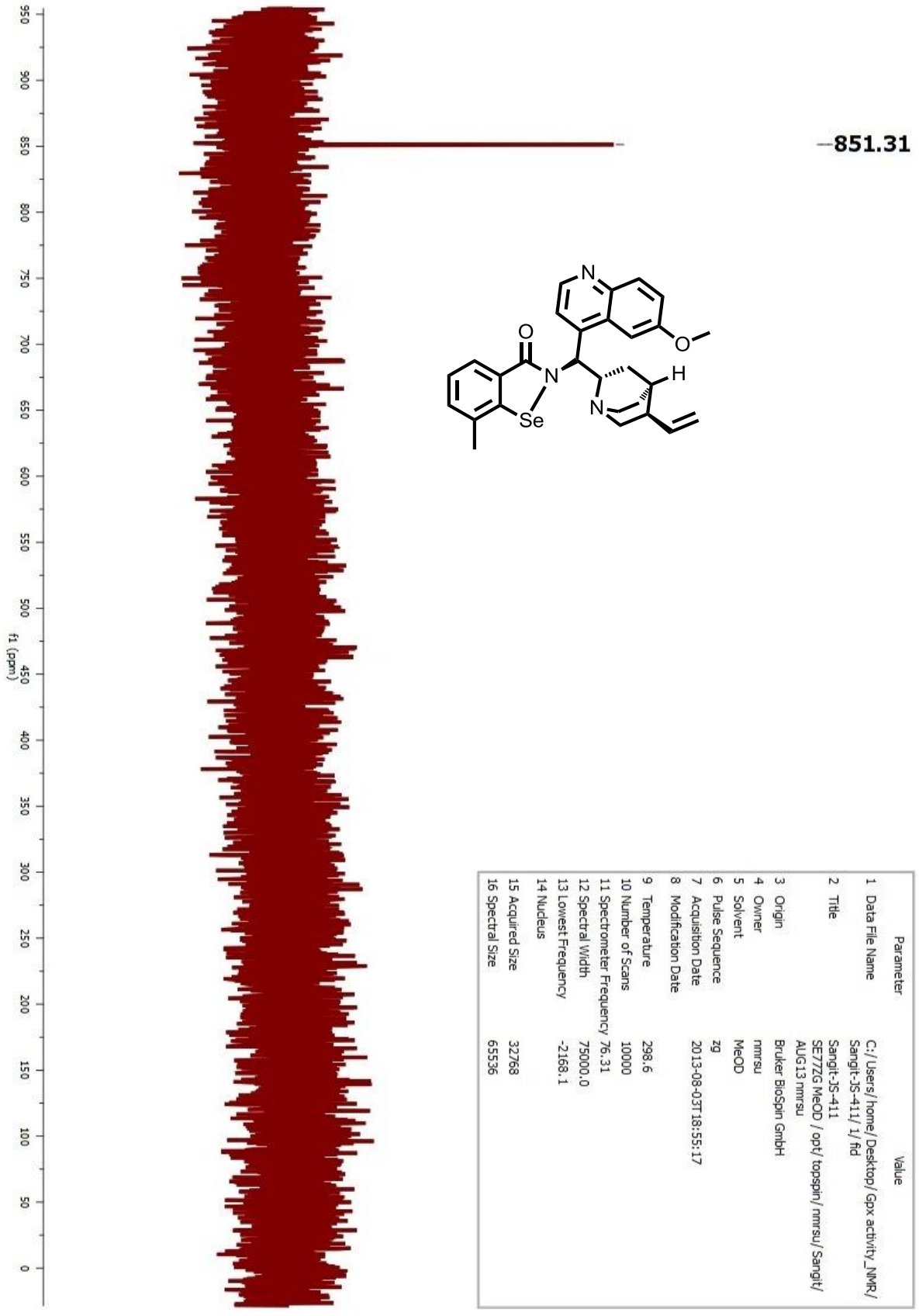


Figure S116 ^{77}Se NMR of (**1b + 2PhSH + H_2O_2**) (0-950 ppm range)



	Parameter	Value
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2	Title	Sangit-JS-411 SE77ZG MeOD / opt/ topspin/ nmrsu/ Sangit/ AUG13 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	MeOD
6	Pulse Sequence	zg
7	Acquisition Date	2013-08-03T18:55:17
8	Modification Date	
9	Temperature	298.6
10	Number of Scans	10000
11	Spectrometer Frequency	76.31
12	Spectral Width	75000.0
13	Lowest Frequency	-2168.1
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

Figure S117 LRMS for **5b**

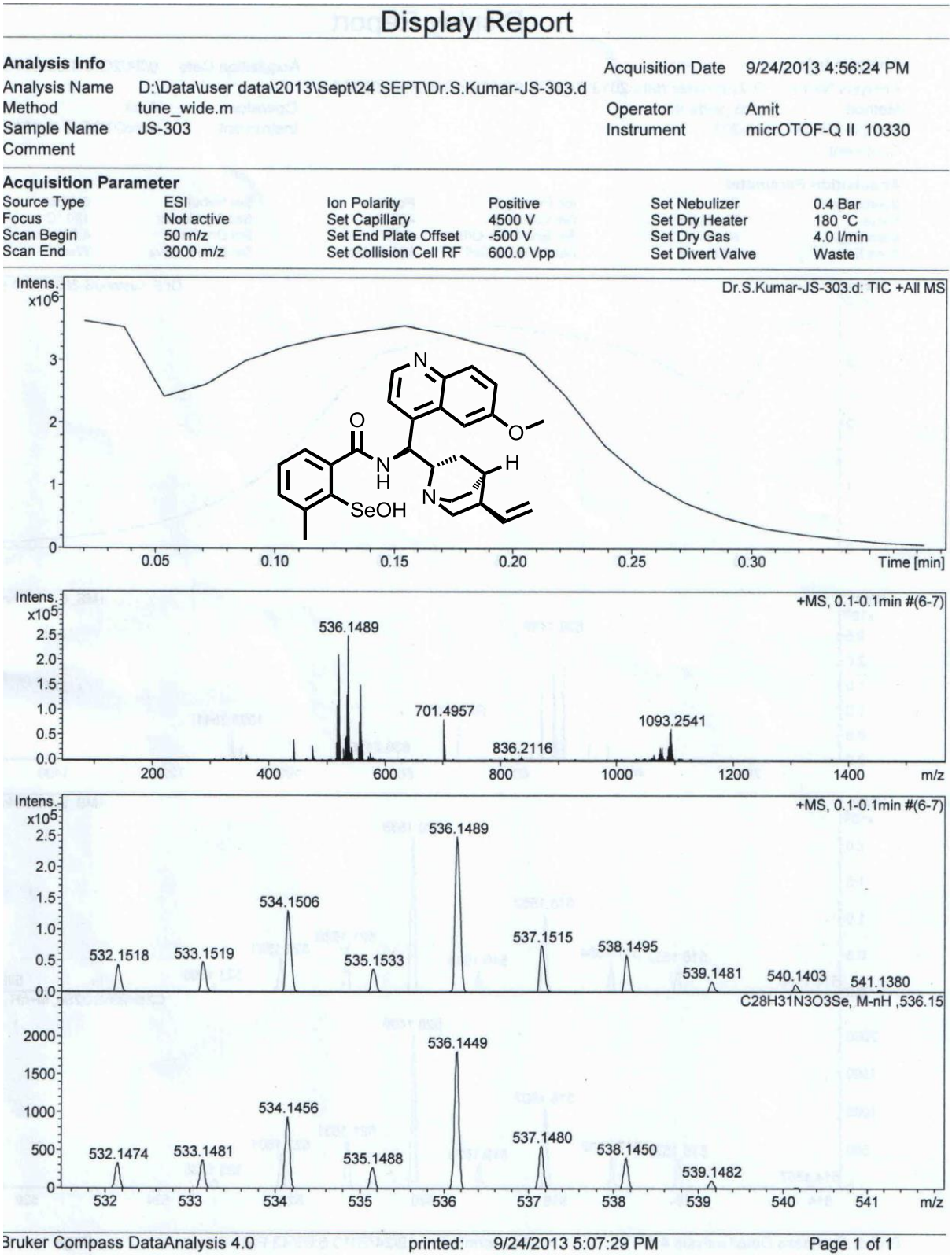
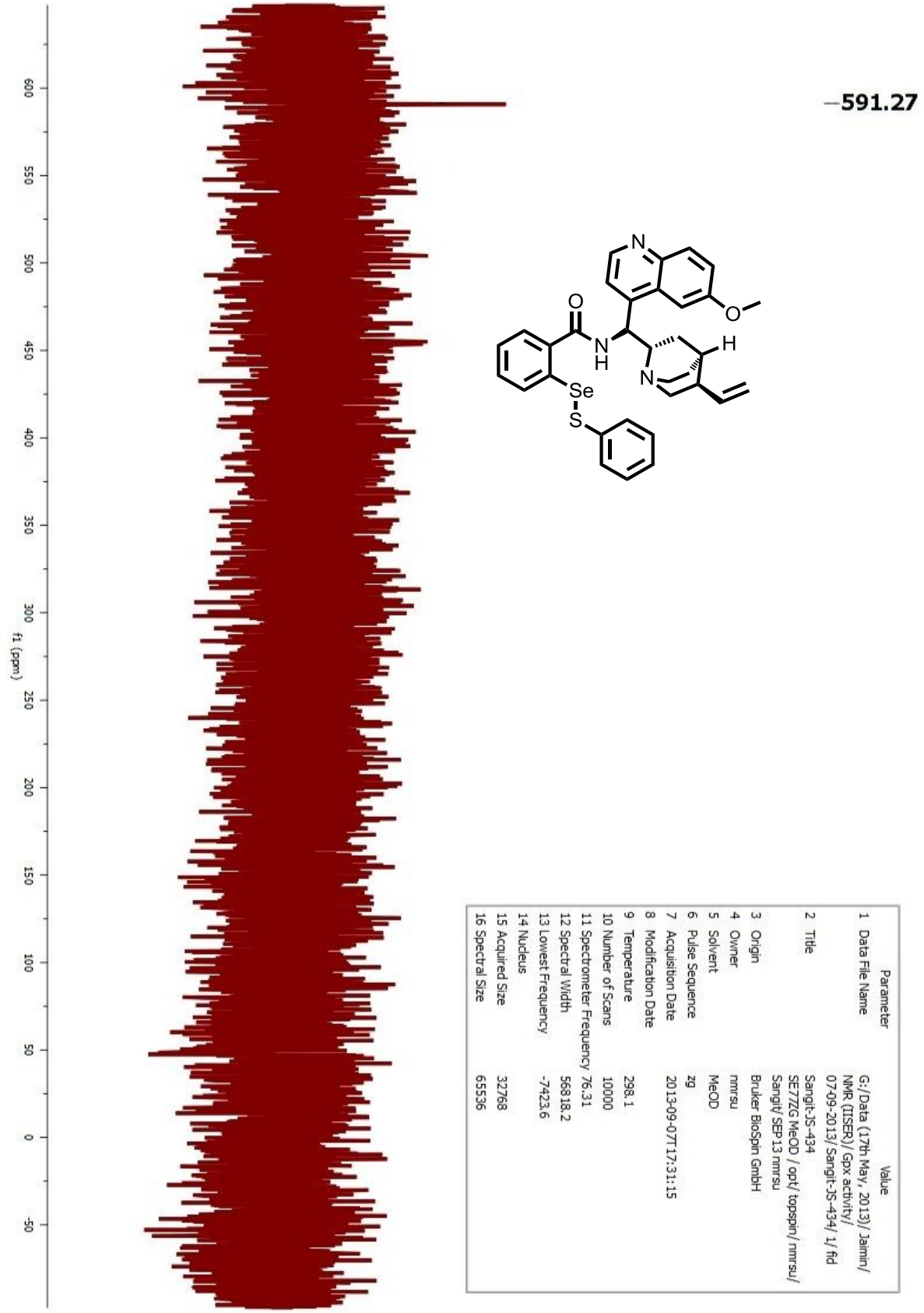
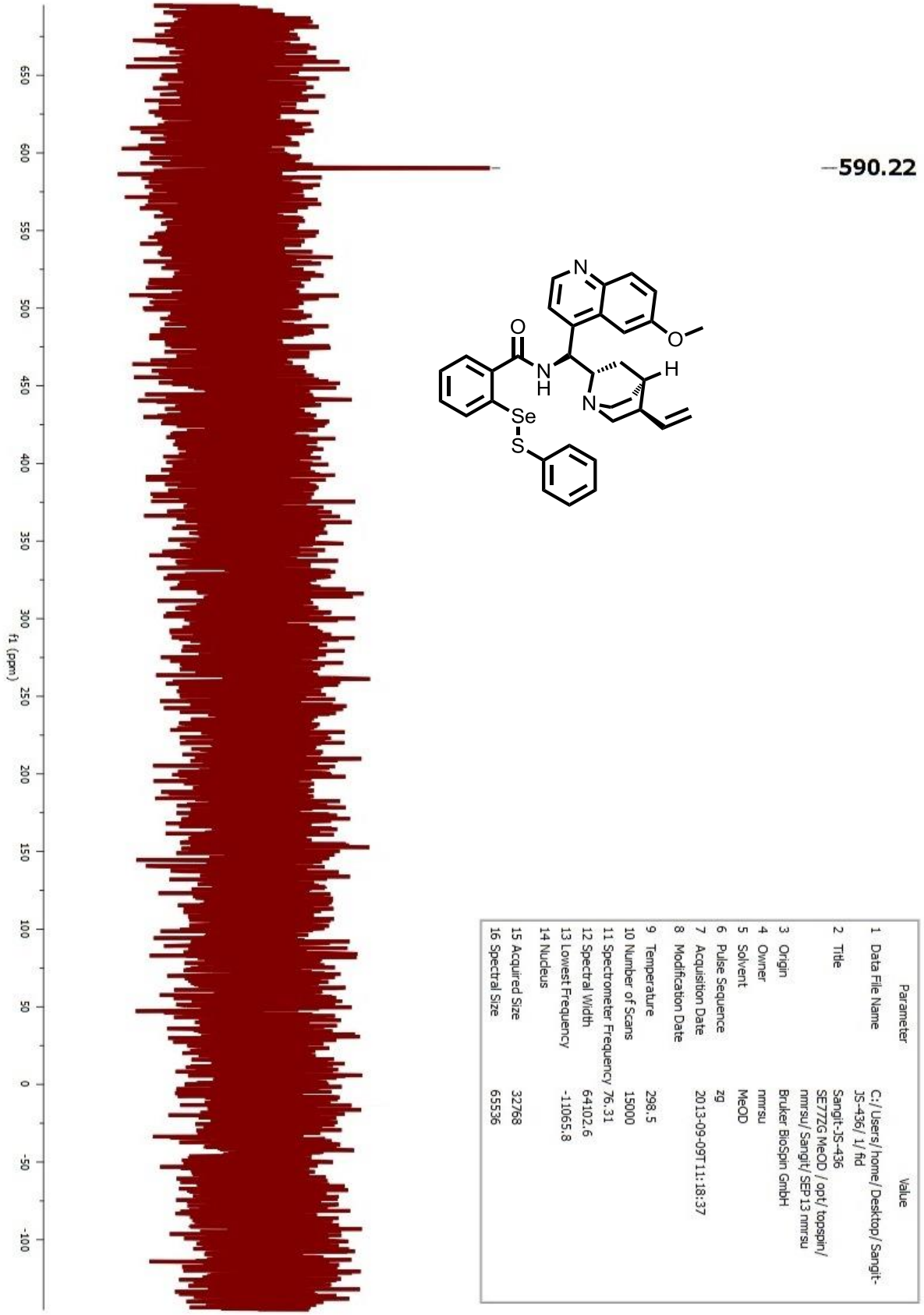


Figure S118 ^{77}Se NMR of (**1c** + **PhSH)**



	Parameter	Value
1	Data File Name	G:/Data (17th May, 2013)/ Jaimin/ NMR (IISER)/ Gpx activity/ 07-09-2013/ Sangit-JS-434/ 1/ fid
2	Title	Sangit-JS-434 SE77ZG MeOD / opt/ topspin/ nmrsu/ Sangit/ SEP 13 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	MeOD
6	Pulse Sequence	zg
7	Acquisition Date	2013-09-07T17:31:15
8	Modification Date	
9	Temperature	298.1
10	Number of Scans	10000
11	Spectrometer Frequency	76.31
12	Spectral Width	56818.2
13	Lowest Frequency	-7423.6
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

Figure S119 ^{77}Se NMR of (**1c + 2PhSH)**



	Parameter	Value
1	Data File Name	C:/ Users/ home/ Desktop/ Sangit-JS-436/ 1/ fid
2	Title	Sangit-JS-436 SE77ZG MeOD / opt/ topspin/ nmrsu/ Sangit/ SEP 13 nmrsu
3	Origin	Bruker BioSpin GmbH
4	Owner	nmrsu
5	Solvent	MeOD
6	Pulse Sequence	zg
7	Acquisition Date	2013-09-09T11:18:37
8	Modification Date	
9	Temperature	298.5
10	Number of Scans	15000
11	Spectrometer Frequency	76.31
12	Spectral Width	64102.6
13	Lowest Frequency	-11065.8
14	Nucleus	
15	Acquired Size	32768
16	Spectral Size	65536

Figure S120 ^{77}Se NMR of **2e** and **4e** obtained by the reaction of **1e** + one equiv of PhSH

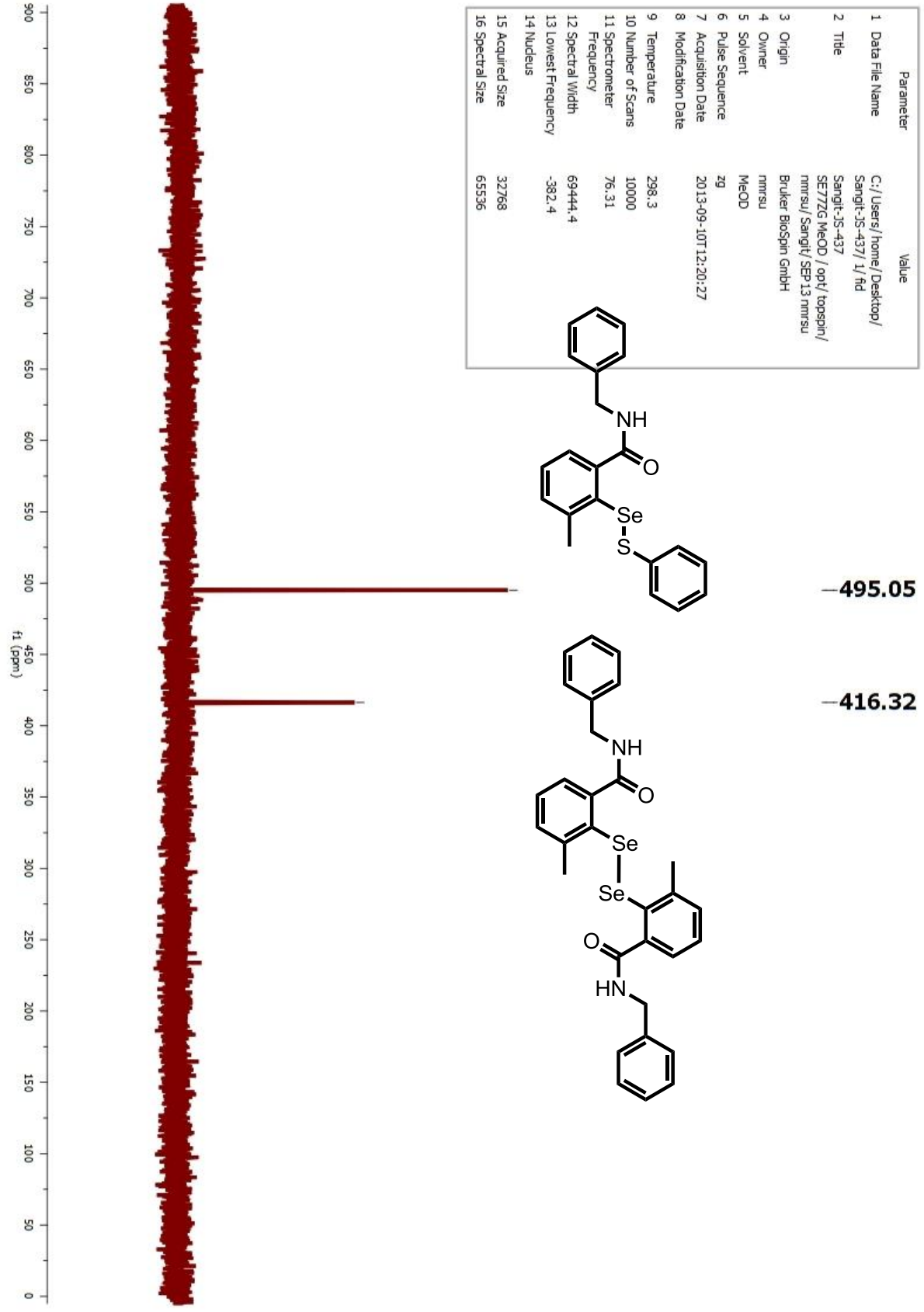


Figure S121 ^{77}Se NMR of **2e** and **4e** obtained by the reaction of **1e** + one equiv of PhSH

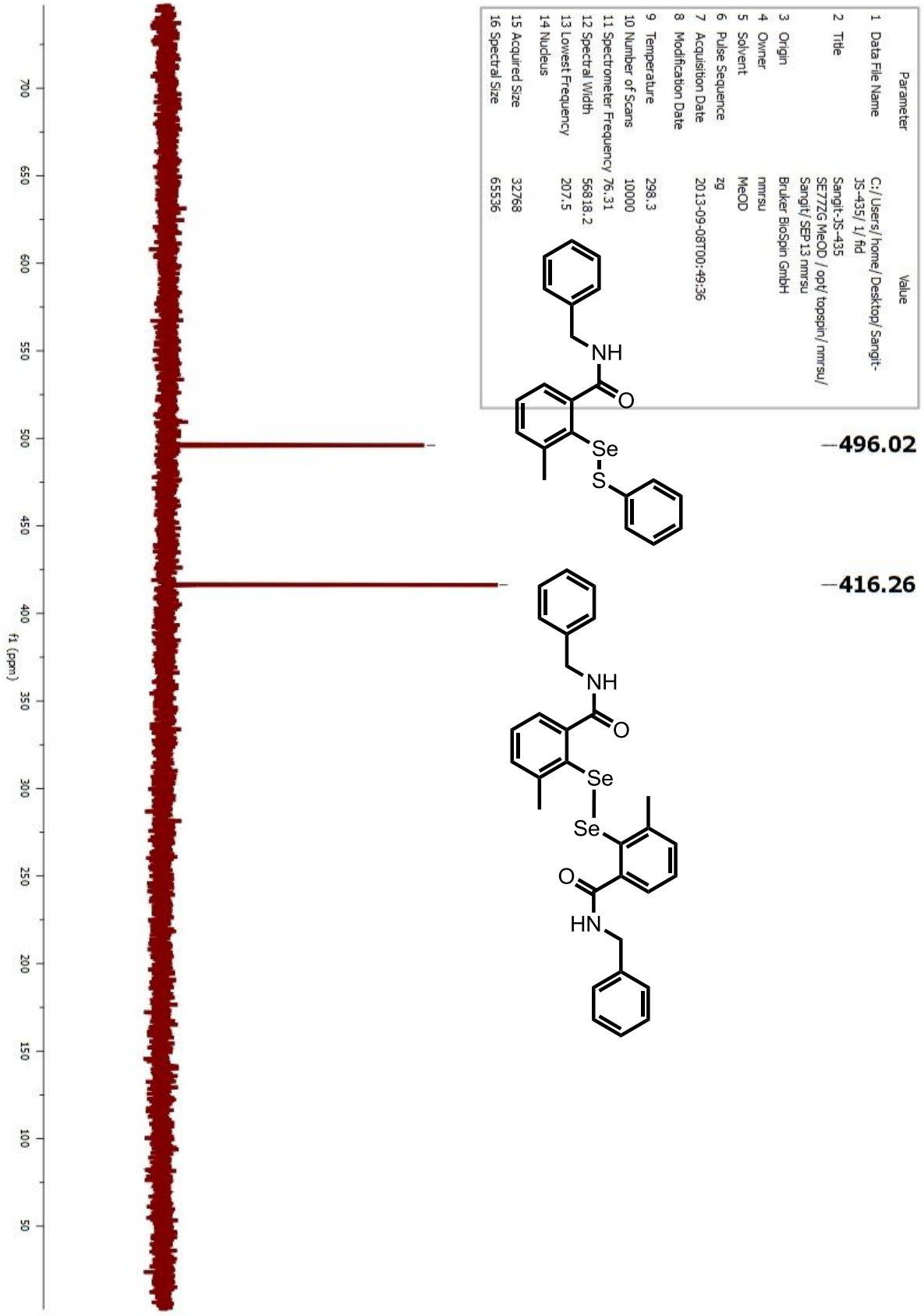


Figure S122 ^{77}Se NMR of **2n** and **4n** obtained by the reaction of **1n** + one equiv of **PhSH**

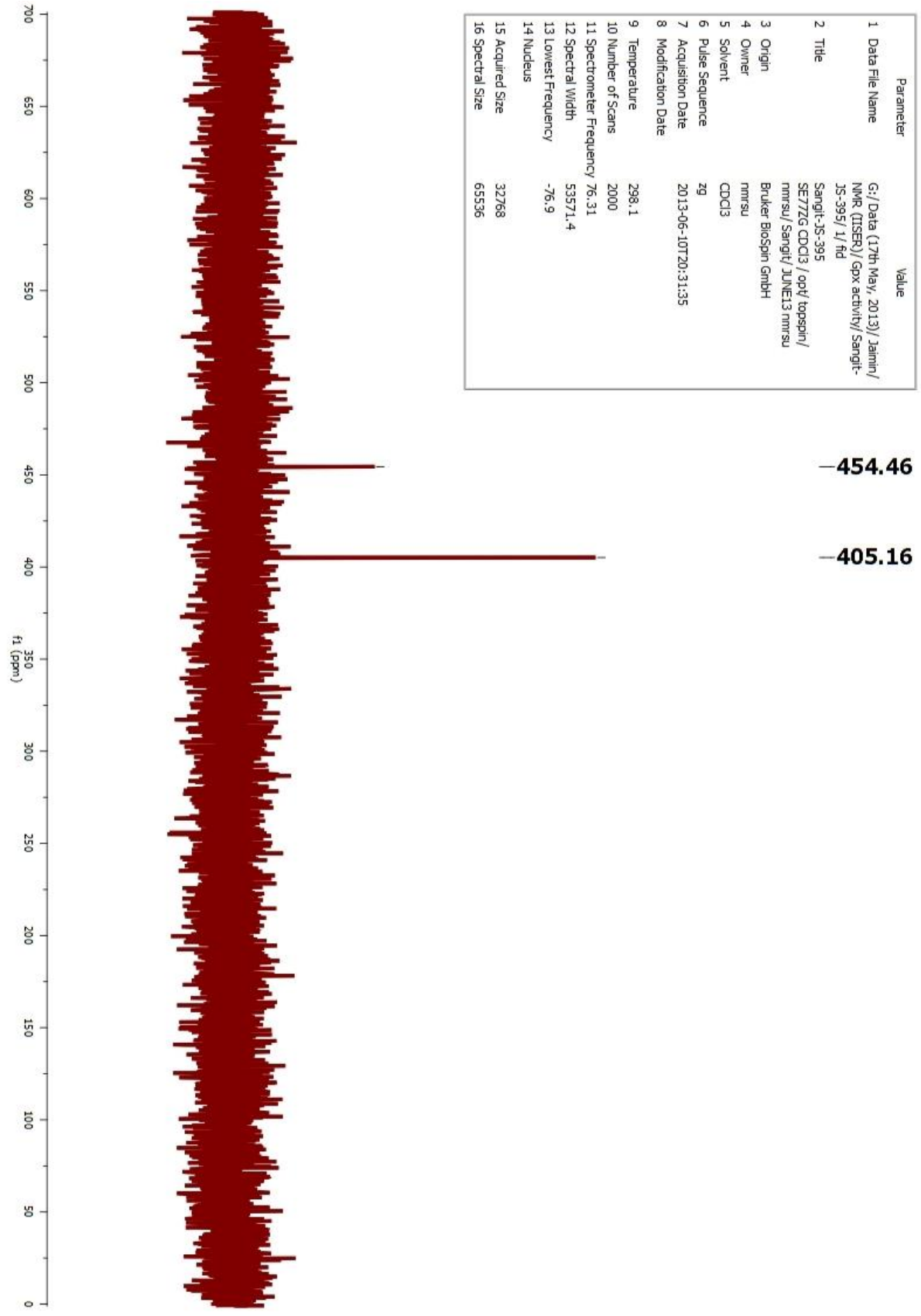


Figure S123 ^{77}Se NMR of (**1n + 2PhSH)**

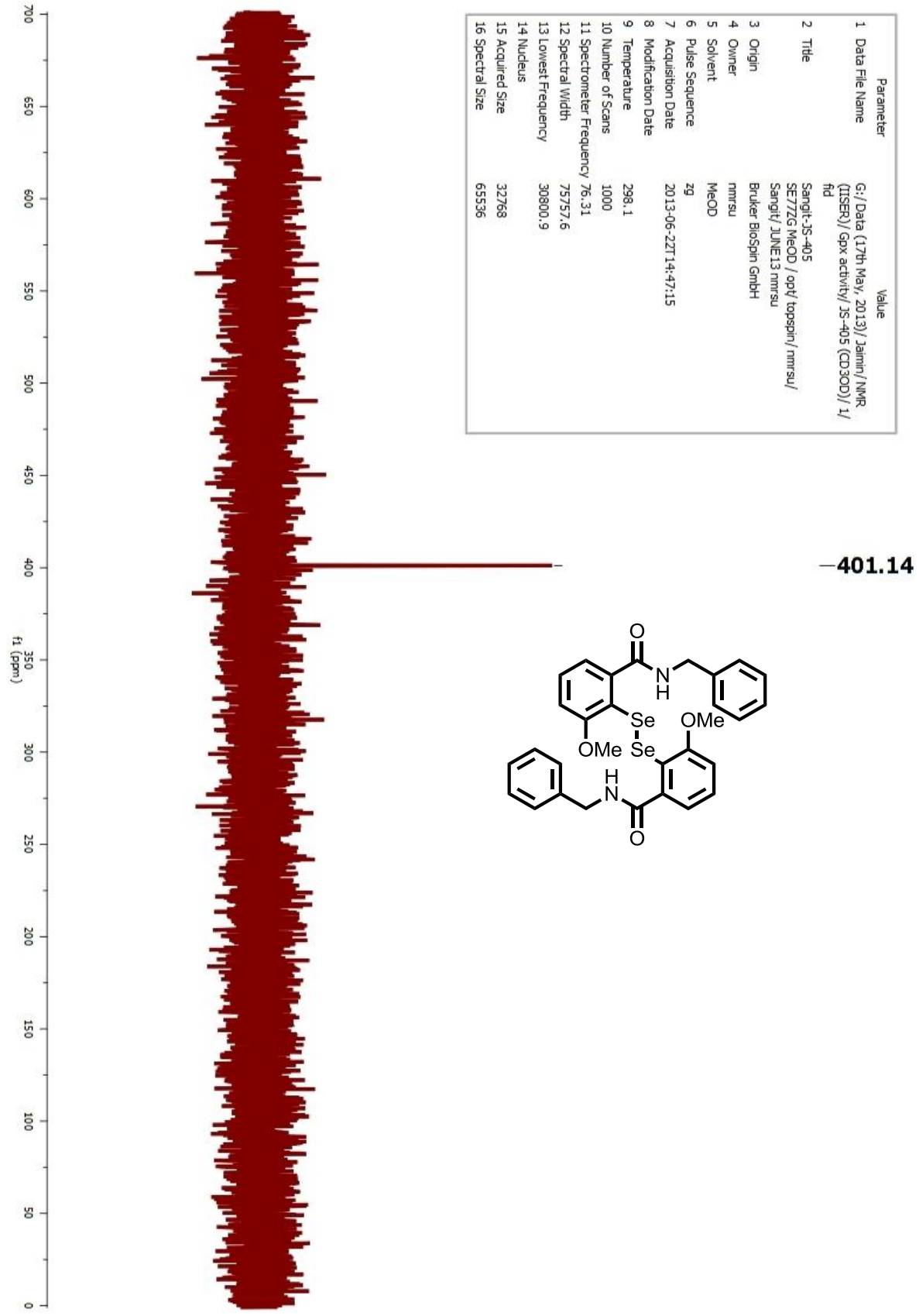
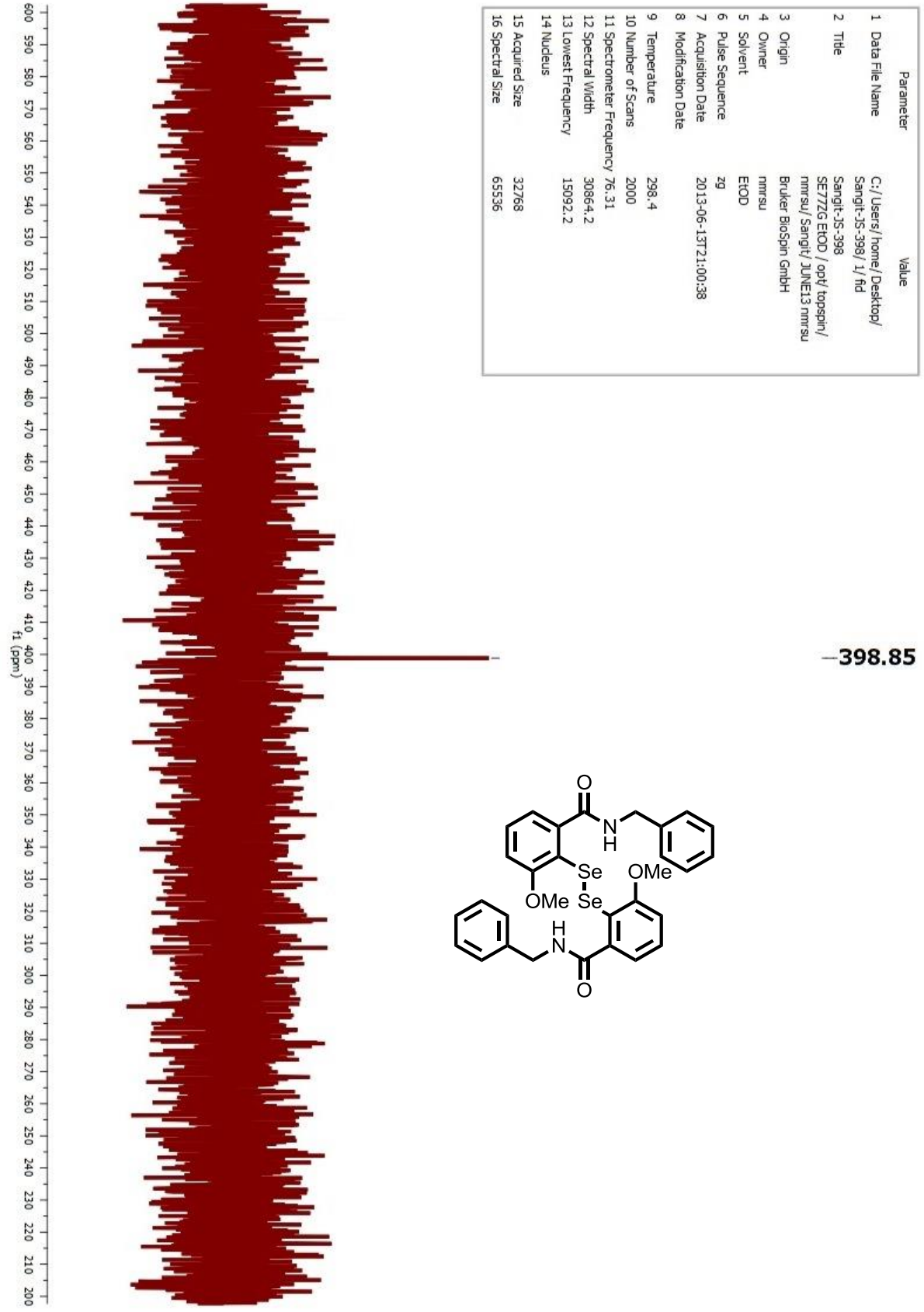
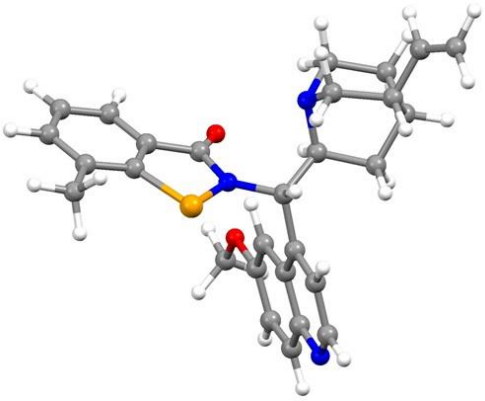


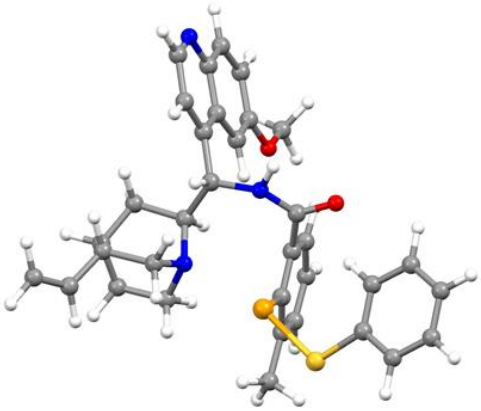
Figure S124 ^{77}Se NMR of authentic sample for diselenide of **1n**



Optimized geometry and co-ordinates for **1b** and **2b**



Compound 1b



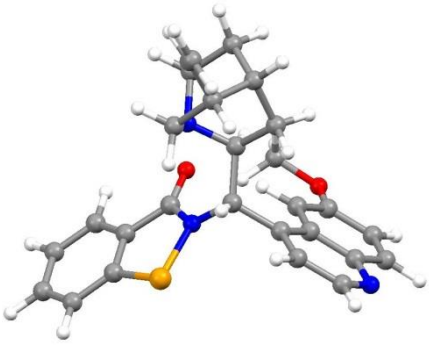
Compound 2b

C	-0.6659	-0.02306	0.62636	C	0.22704	-2.10346	3.09684
C	-1.74775	0.0191	-0.48274	C	1.16013	-1.19547	3.59079
N	-1.98475	-1.33422	-1.03075	C	1.84187	-0.31366	2.74155
C	-2.71221	-1.17132	-2.30196	C	1.55693	-0.36368	1.36138
C	-4.03246	-0.36486	-2.08873	C	0.58377	-1.24741	0.86148
C	-2.7921	-2.17126	-0.13167	C	-0.05645	-2.13645	1.73393
C	-4.2182	-1.5682	0.14877	Se	2.41263	0.85011	0.12366
C	-5.32806	-2.49578	-0.26199	N	-0.40845	-0.58415	-1.38706
C	-6.3019	-2.92901	0.541	C	0.35095	-1.43394	-0.6204
C	-4.24683	-0.18895	-0.56964	O	0.88822	-2.39311	-1.17272
H	-5.20416	0.30612	-0.37283	S	4.58871	0.33785	0.37201
C	-3.08675	0.64891	0.01068	C	5.01133	-0.92661	-0.83659
C	-0.43226	1.29698	1.36353	C	4.07277	-1.73499	-1.47907
C	0.09397	2.49377	0.76663	C	4.50468	-2.72375	-2.36394
C	0.50305	2.60461	-0.58265	C	5.86454	-2.91224	-2.61467
C	0.9922	3.80327	-1.07958	C	6.79972	-2.09809	-1.97159
O	1.35592	3.79934	-2.39457	C	6.37962	-1.10467	-1.08751
C	1.88997	4.98443	-2.96134	C	-1.42444	0.47545	-1.2266
C	1.09649	4.94306	-0.24291	C	-1.42632	1.25059	0.11052
C	0.71378	4.85388	1.07601	N	-0.16137	2.00114	0.29695
C	0.21097	3.64746	1.61995	C	-0.12142	2.51127	1.6849
N	-0.13496	3.65579	2.94142	C	-1.3377	3.43473	1.98594
C	-0.59753	2.53638	3.45007	C	-0.03973	3.15505	-0.61479
C	-0.76116	1.34504	2.70283	C	-1.22053	4.17544	-0.44542
C	4.12499	-2.86319	-2.07797	C	-0.7316	5.57535	-0.19111

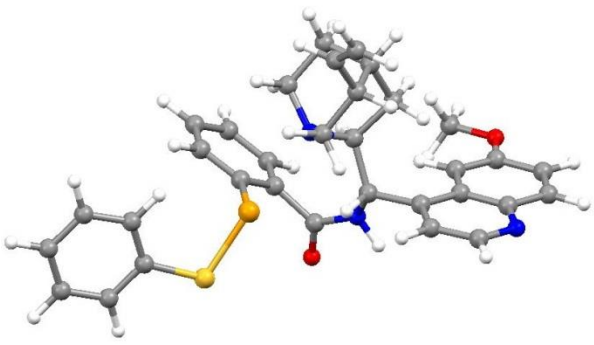
C	4.49321	-3.3589	-0.8179	C	-1.05042	6.64189	-0.92631
C	3.7847	-3.03094	0.34095	C	-2.13372	3.61048	0.67946
C	2.68158	-2.18493	0.17892	H	-2.98111	4.28717	0.8336
C	2.30001	-1.67971	-1.06424	C	-2.64254	2.2313	0.21688
C	3.02824	-2.01862	-2.20736	C	-2.79265	-0.04847	-1.69166
Se	1.54041	-1.55533	1.54675	C	-3.59676	-1.00982	-0.991
N	0.59738	-0.64862	0.19194	C	-3.25166	-1.5828	0.25247
C	1.11562	-0.78915	-1.08274	C	-4.07106	-2.51502	0.86809
O	0.67623	-0.23473	-2.08959	O	-3.62331	-3.00801	2.0598
C	4.16411	-3.54878	1.70378	C	-4.41472	-3.9699	2.74349
H	-1.0596	-0.70389	1.39081	C	-5.28992	-2.90795	0.2604
H	-1.36406	0.60544	-1.31445	C	-5.6516	-2.35916	-0.94911
H	-2.91976	-2.17334	-2.69541	C	-4.83223	-1.41009	-1.60838
H	-2.04191	-0.67641	-3.01112	N	-5.27184	-0.92785	-2.80769
H	-3.96827	0.6233	-2.56137	C	-4.50615	-0.05366	-3.42072
H	-4.88905	-0.87318	-2.54568	C	-3.26975	0.40598	-2.90447
H	-2.24699	-2.32723	0.80539	H	-0.27997	-2.78763	3.77132
H	-2.87837	-3.1585	-0.59993	H	1.37227	-1.16537	4.65694
H	-4.32632	-1.37757	1.22521	H	-0.76365	-2.86075	1.3437
H	-5.31071	-2.84274	-1.29676	H	-0.3849	-0.93168	-2.34154
H	-7.07604	-3.60662	0.19052	H	3.01484	-1.60621	-1.29111
H	-6.36219	-2.62189	1.58365	H	3.76231	-3.3512	-2.85016
H	-3.15483	0.65621	1.10642	H	6.1943	-3.68526	-3.30364
H	-3.15645	1.69359	-0.31387	H	7.86221	-2.22997	-2.16086
H	0.47038	1.75752	-1.25929	H	7.11105	-0.4685	-0.59536
H	2.11632	4.73957	-4.00069	H	-1.15738	1.21986	-1.98548
H	1.16702	5.81084	-2.93584	H	-1.46342	0.54297	0.94132
H	2.81317	5.2974	-2.45563	H	-0.09372	1.65147	2.3595
H	1.47835	5.88133	-0.62877	H	0.82747	3.04377	1.80281
H	0.78805	5.70741	1.74235	H	-1.01096	4.40411	2.37803
H	-0.86571	2.55065	4.50626	H	-1.98642	2.991	2.75099
H	-1.15507	0.4626	3.20179	H	0.92294	3.62753	-0.39221
H	4.7048	-3.14208	-2.95305	H	0.03177	2.80195	-1.64724
H	5.35418	-4.01811	-0.73415	H	-1.81626	4.19428	-1.368
H	2.7175	-1.61292	-3.16522	H	-0.05482	5.70463	0.65535

H	3.34543	-4.13234	2.14709	H	-0.66253	7.63124	-0.6993
H	4.38236	-2.72181	2.39362	H	-1.71225	6.56621	-1.78716
H	5.04827	-4.19095	1.65992	H	-3.1507	2.33852	-0.74804
				H	-3.3854	1.83543	0.91865
				H	-2.33179	-1.31836	0.75325
				H	-3.86511	-4.21181	3.65474
				H	-5.39907	-3.56579	3.0127
				H	-4.5468	-4.88287	2.14882
				H	-5.93677	-3.63613	0.73582
				H	-6.57801	-2.64146	-1.43887
				H	-4.86229	0.32399	-4.37867
				H	-2.69737	1.12798	-3.48233
				C	2.8437	0.65421	3.32091
				H	3.86189	0.25506	3.2477
				H	2.8376	1.59645	2.76538
				H	2.63137	0.8521	4.37643

Optimized geometry and co-ordinates for **1c** and **2c**



Compound 1c



Compound 2c

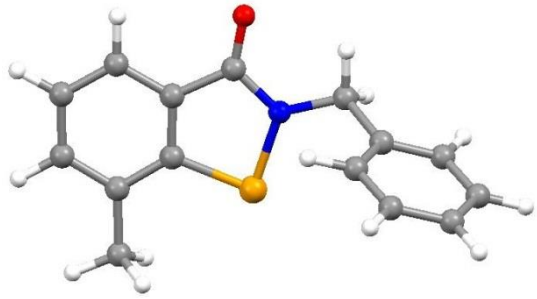
C	3.02348	4.43865	1.37123	C	1.54499	-2.48336	3.26467
C	3.06842	4.92423	0.05537	C	2.57696	-1.54568	3.18232
C	2.44639	4.23803	-0.98632	C	2.73789	-0.79509	2.0192
C	1.77016	3.05562	-0.6864	C	1.87008	-0.97508	0.93632
C	1.71989	2.56033	0.61989	C	0.83712	-1.91802	1.00694
C	2.35113	3.25458	1.65525	C	0.69403	-2.67713	2.17918
Se	0.84902	1.91087	-1.8734	Se	2.08341	0.11445	-0.636
N	0.45786	0.84358	-0.37436	N	-1.09773	-1.57125	-0.60862
C	0.97815	1.29436	0.82098	C	-0.03281	-2.3327	-0.16086

O	0.86694	0.71609	1.90453	O	0.11622	-3.46349	-0.60999
C	-0.50482	-0.2476	-0.62617	C	-1.32773	-0.1116	-0.70917
C	-1.45545	-0.51684	0.56709	C	-1.23437	0.63261	0.67425
N	-2.09661	0.73807	1.01622	N	0.03044	1.41923	0.73125
C	-2.72701	0.47386	2.32107	C	0.3272	1.74594	2.14114
C	-3.76643	-0.68697	2.21863	C	-0.85934	2.50558	2.80201
C	-3.13031	1.20841	0.08287	C	-0.07336	2.67964	-0.03146
C	-4.2793	0.15565	-0.13297	C	-1.16746	3.64287	0.55015
C	-5.63948	0.72023	0.17023	C	-0.59981	4.97052	0.97458
C	-6.66538	0.74913	-0.68258	C	-1.03432	6.1572	0.54709
C	-3.89945	-1.0805	0.73173	C	-1.8691	2.85873	1.6938
H	-4.66101	-1.85852	0.60954	H	-2.68935	3.46085	2.09913
C	-2.53511	-1.59218	0.22334	C	-2.42698	1.55623	1.08304
C	0.15759	-1.48107	-1.24572	C	-2.62239	0.09416	-1.48916
C	1.07622	-2.35433	-0.57627	C	-3.88694	-0.46538	-1.11096
C	1.53352	-2.16508	0.75724	C	-4.08209	-1.28498	0.03664
C	2.41999	-3.0632	1.32456	C	-5.33867	-1.77501	0.33933
O	2.92162	-2.96789	2.58488	O	-5.62888	-2.57272	1.40325
C	2.48629	-1.88492	3.40103	C	-4.56611	-2.96441	2.25979
C	2.88489	-4.18792	0.58984	C	-6.45511	-1.46278	-0.48442
C	2.46513	-4.3854	-0.69804	C	-6.29082	-0.67885	-1.59448
C	1.55982	-3.48304	-1.32279	C	-5.01286	-0.15956	-1.94559
N	1.20649	-3.75007	-2.61149	N	-4.93488	0.60939	-3.06753
C	0.3757	-2.91398	-3.19727	C	-3.7522	1.08814	-3.39356
C	-0.16783	-1.77903	-2.55644	C	-2.57851	0.85518	-2.64154
H	3.51681	4.98929	2.16669	S	3.58306	-1.13847	-1.74133
H	3.59555	5.84978	-0.15968	C	5.20362	-0.55354	-1.21393
H	2.48963	4.62191	-2.00137	C	5.41618	0.58594	-0.43124
H	2.29822	2.84874	2.66105	C	6.71588	0.97025	-0.09772
H	-1.14998	0.14287	-1.42144	C	7.8127	0.22953	-0.54
H	-0.86487	-0.85909	1.41416	C	7.59878	-0.90655	-1.32351
H	-1.93163	0.2459	3.03782	C	6.30405	-1.30052	-1.65888
H	-3.20336	1.40376	2.65253	H	1.41517	-3.07689	4.16541
H	-4.73776	-0.39013	2.63041	H	3.257	-1.40291	4.0177
H	-3.43773	-1.56063	2.79523	H	3.54366	-0.07298	1.9414

H	-3.53678	2.13815	0.49745
H	-2.66299	1.48356	-0.86879
H	-4.28151	-0.16937	-1.18231
H	-5.77367	1.1478	1.1656
H	-7.6263	1.17765	-0.41024
H	-6.58305	0.34394	-1.68957
H	-2.59442	-1.77775	-0.85679
H	-2.27887	-2.55017	0.69025
H	1.21186	-1.29482	1.31421
H	3.01994	-1.99554	4.34674
H	2.72034	-0.9155	2.94873
H	1.40485	-1.93281	3.57961
H	3.57736	-4.86761	1.07672
H	2.80967	-5.23047	-1.28542
H	0.10567	-3.13309	-4.22993
H	-0.85263	-1.14027	-3.10966

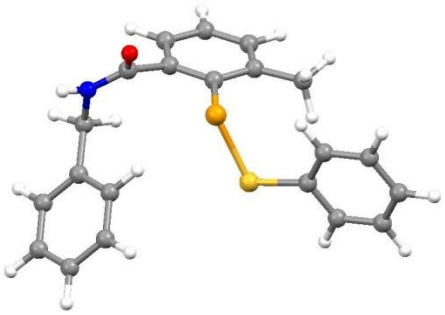
H	-0.0782	-3.43966	2.22087
H	-1.53471	-2.07991	-1.37235
H	-0.52769	0.30113	-1.33191
H	-1.12218	-0.14399	1.43587
H	0.55384	0.81605	2.66901
H	1.24222	2.34853	2.14599
H	-0.51245	3.40648	3.31955
H	-1.35075	1.87973	3.55718
H	0.91704	3.1474	-0.01669
H	-0.28866	2.44143	-1.07731
H	-1.9213	3.83597	-0.22404
H	0.23701	4.94048	1.67482
H	-0.58467	7.08749	0.88364
H	-1.85831	6.24412	-0.15873
H	-3.05519	1.8078	0.22347
H	-3.07354	1.0405	1.80166
H	-3.22636	-1.54225	0.64537
H	-5.01558	-3.60583	3.01963
H	-4.10179	-2.09547	2.74473
H	-3.79795	-3.52639	1.71336
H	-7.42341	-1.86838	-0.20857
H	-7.12486	-0.42998	-2.24264
H	-3.70161	1.69287	-4.29825
H	-1.63826	1.28029	-2.98313
H	4.56321	1.16601	-0.09201
H	6.86779	1.85913	0.5099
H	8.82233	0.53263	-0.27714
H	8.44281	-1.49534	-1.67365
H	6.14522	-2.19015	-2.26289

Optimized geometry and co-ordinates for **1e** and **2e**



Compound 1e

C	-4.29262	0.94333	0.76664
C	-4.2691	-0.44854	0.58928
C	-3.11657	-1.12217	0.17632
C	-1.98128	-0.33573	-0.05369
C	-1.98423	1.04965	0.12006
C	-3.14981	1.69989	0.53316
Se	-0.28382	-0.97071	-0.60475
N	0.26544	0.82308	-0.52193
C	-3.07024	-2.61508	-0.02031
C	-0.70754	1.74374	-0.16121
O	-0.50454	2.95209	-0.093
C	1.59762	1.21283	-0.95322
C	2.71651	0.49169	-0.22453
C	3.89899	0.17784	-0.90424
C	4.9611	-0.43662	-0.23951
C	4.84774	-0.75374	1.11491
C	3.66744	-0.45278	1.79807
C	2.60871	0.16601	1.13373
H	-5.21056	1.42644	1.08849
H	-5.17167	-1.02562	0.77692
H	-3.13226	2.77805	0.66055
H	-2.82686	-2.86971	-1.06103
H	-4.02686	-3.08485	0.22496
H	-2.29751	-3.07215	0.61329
H	1.64073	2.29266	-0.76773
H	1.701	1.06056	-2.03621
H	3.98941	0.41785	-1.96167

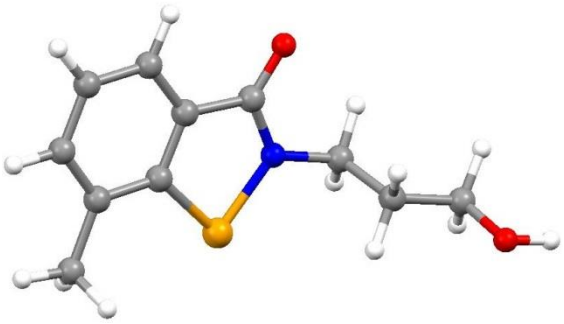


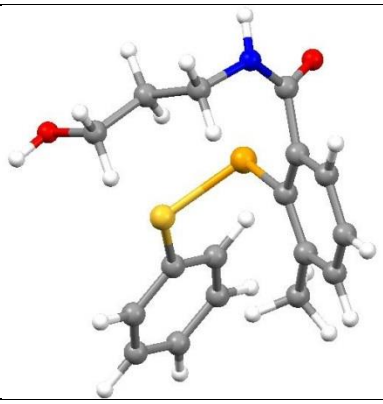
Compound 2e

C	-0.94244	3.79874	-1.63632
C	0.40197	3.44249	-1.68847
C	0.93008	2.42861	-0.87502
C	0.05197	1.7508	-0.01095
C	-1.29971	2.13606	0.08135
C	-1.79272	3.15461	-0.73975
Se	0.62842	0.30814	1.15546
N	-3.38322	1.06844	0.87799
C	2.40337	2.12446	-0.92975
C	-2.158	1.59085	1.19385
O	-1.77831	1.68633	2.35911
C	-3.78909	0.46775	-0.39329
C	-3.75372	-1.05177	-0.37601
C	-4.85524	-1.79091	-0.81838
C	-4.81599	-3.18705	-0.83103
C	-3.67241	-3.85597	-0.3946
C	-2.56994	-3.12319	0.05358
C	-2.60892	-1.7299	0.06406
S	1.38808	-1.18332	-0.31611
C	3.18479	-1.20979	-0.17767
C	3.86188	-1.90407	-1.19043
C	5.24925	-2.03543	-1.13706
C	5.97226	-1.47179	-0.0839
C	5.29432	-0.77828	0.91961
C	3.90505	-0.64903	0.88118
H	-1.32088	4.59468	-2.27156
H	1.07241	3.97085	-2.36183

H	5.87287	-0.67345	-0.78153	H	-2.83258	3.45622	-0.65139
H	5.67148	-1.23652	1.63383	H	-3.86603	0.72522	1.70284
H	3.57011	-0.70041	2.85185	H	2.95548	2.95997	-1.37061
H	1.6881	0.3912	1.66443	H	2.79499	1.93378	0.07393
				H	2.61286	1.23018	-1.52643
				H	-4.79936	0.81231	-0.64562
				H	-3.11965	0.85674	-1.1655
				H	-5.75055	-1.27215	-1.15543
				H	-5.68018	-3.74899	-1.17558
				H	-3.63991	-4.94223	-0.39977
				H	-1.67454	-3.63578	0.39433
				H	-1.75112	-1.16458	0.41957
				H	3.30566	-2.33798	-2.01752
				H	5.76494	-2.57462	-1.92742
				H	7.05328	-1.5721	-0.04632
				H	5.84587	-0.33664	1.74557
				H	3.38206	-0.11128	1.66611

Optimized geometry and co-ordinates for **1f** and **2f**





C	-3.60847	1.62012	0.55746	C	-2.32357	-2.86739	1.86062
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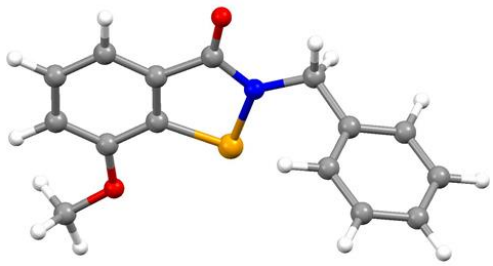
C	-2.89653	-0.71097	0.31996	C	-0.14759	-2.14259	1.02308
C	-1.62172	-0.22261	0.01052	C	-0.80783	-1.33417	0.08055
C	-1.33155	1.14223	-0.03078	C	-2.21233	-1.34082	-0.00865
C	-2.33236	2.07646	0.24718	C	-2.96615	-2.1006	0.89058
Se	-0.09798	-1.27079	-0.39982	Se	0.13022	-0.21203	-1.19944

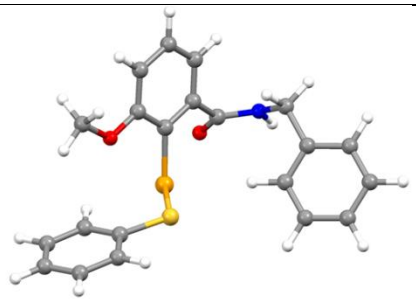
N	0.80366	0.36001	-0.62831
C	-3.16627	-2.19275	0.35287
C	0.06625	1.50188	-0.36051
O	0.53557	2.6353	-0.40786
C	2.2417	0.39198	-0.85452
C	3.05341	0.02147	0.3932
C	4.5551	0.06277	0.13933
O	5.20568	-0.33475	1.34053
H	-4.40283	2.32783	0.77601
H	-4.88334	-0.09617	0.83778
H	-2.08621	3.13351	0.21494
H	-2.52316	-2.6949	1.0888
H	-2.96128	-2.65335	-0.62343
H	-4.20614	-2.40825	0.61389
H	2.48097	-0.27846	-1.69015
H	2.46233	1.41675	-1.16859
H	2.80682	0.71625	1.20378
H	2.78073	-0.98429	0.73716
H	4.81389	-0.61217	-0.69488
H	4.85467	1.08081	-0.15991
H	6.1619	-0.27113	1.19696

N	-3.85563	0.26841	-0.90594
C	1.35292	-2.24444	1.08554
C	-2.90457	-0.68286	-1.17853
O	-2.66885	-1.06395	-2.32078
C	-3.78975	1.18497	0.23542
C	-2.74495	2.29112	0.03112
C	-2.52844	3.14563	1.27258
O	-1.58911	4.15883	0.93611
S	1.30083	1.16365	0.10423
C	3.02153	0.63282	0.01926
C	3.87664	1.18112	0.98573
C	5.24025	0.88927	0.95652
C	5.7608	0.04411	-0.02521
C	4.90506	-0.50411	-0.98186
C	3.54082	-0.21021	-0.96802
H	-2.9051	-3.46363	2.55834
H	-0.43261	-3.52045	2.645
H	-4.04948	-2.10368	0.8095
H	-4.23099	0.66274	-1.76381
H	1.65865	-3.15176	1.61532
H	1.77987	-2.26389	0.07832
H	1.79913	-1.38745	1.60158
H	-4.79094	1.60443	0.38824
H	-3.55194	0.59611	1.12589
H	-1.8019	1.81821	-0.26379
H	-3.04416	2.94428	-0.79891
H	-3.48653	3.58459	1.60209
H	-2.15784	2.51441	2.09725
H	-1.38742	4.65992	1.74056
H	3.47663	1.83283	1.75841
H	5.89426	1.31942	1.71059
H	6.82245	-0.18531	-0.04376
H	5.29834	-1.16254	-1.75213
H	2.87955	-0.63848	-1.71508

Optimized geometry and co-ordinates for **1n** and **2n**



C	-3.97377	1.46676	0.73903
C	-4.08564	0.07969	0.53107
C	-2.97631	-0.66043	0.12075
C	-1.7656	0.0128	-0.07603
C	-1.65614	1.3842	0.13233
C	-2.76852	2.12784	0.54349
Se	-0.14336	-0.78409	-0.61114
N	0.57073	0.95131	-0.48306
C	-0.31271	1.95638	-0.11841
O	0.00304	3.13876	-0.02497
C	1.93558	1.22246	-0.90317
C	2.97543	0.36472	-0.20605
C	2.83401	-0.00229	1.13859
C	3.82395	-0.75146	1.77422
C	4.96819	-1.14316	1.07591
C	5.11451	-0.7851	-0.26507
C	4.12075	-0.04	-0.90127
O	-2.94393	-2.0034	-0.11688
C	-4.14135	-2.74683	0.06443
H	-4.85239	2.01998	1.05794
H	-5.04139	-0.40672	0.69189
H	-2.66149	3.19665	0.69759
H	2.08794	2.28485	-0.67865
H	2.02455	1.10044	-1.99141
H	1.94019	0.29318	1.68036
H	3.70089	-1.03029	2.81746
H	5.738	-1.72777	1.57248



C	-0.64171	3.73176	-1.43221
C	3.72242	-2.36243	-0.88169
H	3.22919	0.08522	1.43002
H	5.70344	-0.06981	1.53149
H	6.92044	-1.68457	0.07767
H	5.63175	-3.15298	-1.46878
H	3.16559	-3.00895	-1.55569
H	2.95953	1.99179	-2.61166
H	3.4521	3.14249	-1.32947
H	4.13709	1.49083	-1.36393
H	-2.01746	-1.12428	0.31218
H	-2.19362	-3.57946	0.11477
H	-4.281	-4.62381	-0.74936
H	-6.19332	-3.18104	-1.42191
H	-6.01332	-0.71732	-1.23063
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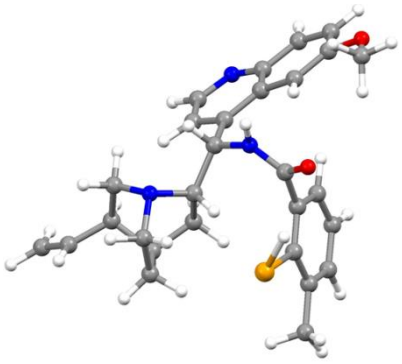
H	-3.17519	1.13286	-1.11204
H	-3.97869	0.90444	1.73558
H	-2.56826	3.62435	-0.46712
H	1.36785	3.64691	-2.18334
H	-0.90331	4.58802	-2.04754
C	3.76064	-0.62467	0.80525
C	5.15305	-0.71383	0.84998
C	5.83679	-1.6189	0.03581
C	5.11385	-2.44235	-0.82976
C	3.042	-1.45031	-0.06325
S	1.24639	-1.46619	-0.20687

H	5.99787	-1.09152	-0.81916	C	3.24599	2.08876	-1.55703
H	4.23563	0.23129	-1.94873	O	2.24467	1.56024	-0.698
H	-3.89015	-3.78128	-0.17473	C	-2.93014	-1.57043	-0.07581
H	-4.49465	-2.68737	1.10176	C	-3.03289	-2.95652	-0.18236
H	-4.93316	-2.39797	-0.61064	C	-4.20439	-3.54268	-0.66942
				C	-5.27599	-2.73406	-1.04767
				C	-5.17398	-1.34533	-0.93832
				C	-4.00274	-0.75209	-0.45662
				C	-3.88822	0.76125	-0.37127
				O	-1.81038	1.58423	2.47776
				C	-2.17342	1.59661	1.30359
				N	-3.44257	1.23606	0.93944
				Se	0.46042	-0.00066	1.26275
				C	-1.57835	3.18802	-0.55856
				C	-1.2317	2.08475	0.23219
				C	0.05075	1.52271	0.14661
				C	1.00371	2.10534	-0.71303
				C	0.64449	3.19923	-1.51192

Optimized geometry and co-ordinates for **3b**



Compound 3b

C	-0.89083	-1.78421	2.74265
C	0.28839	-2.46507	3.02904
C	1.15801	-2.87731	2.01046
C	0.81239	-2.58424	0.67845
C	-0.36957	-1.87932	0.3793
C	-1.22128	-1.49491	1.41988

Se	2.06757	-3.06997	-0.70213
N	-0.82764	-0.41869	-1.59844
C	-0.81338	-1.67192	-1.05154
O	-1.19985	-2.63263	-1.7207
C	-0.32692	0.88509	-1.12499
C	1.18788	0.6976	-0.67406
N	2.10466	1.31051	-1.67749
C	3.36378	0.536	-1.6424
C	3.92961	0.46435	-0.19234
C	2.42788	2.7116	-1.3699
C	3.13776	2.87704	0.02506
C	4.50335	3.49667	-0.09345
C	4.90072	4.6016	0.54031
C	3.1403	1.465	0.68008
H	3.57834	1.5298	1.68212
C	1.67095	0.99635	0.77458
C	-1.31044	1.70798	-0.2583
C	-2.71836	1.45248	-0.05879
C	-3.47039	0.38074	-0.63269
C	-4.81343	0.20815	-0.3551
O	-5.5837	-0.79238	-0.86181
C	-4.98583	-1.72776	-1.75242
C	-5.49772	1.1032	0.50891
C	-4.81985	2.16044	1.04846
C	-3.43893	2.38203	0.77638
N	-2.89615	3.50073	1.32809
C	-1.63478	3.74648	1.04899
C	-0.82717	2.89327	0.27242
H	-1.55526	-1.47904	3.54585
H	0.54393	-2.69415	4.06062
H	-2.14579	-0.97571	1.19226
H	1.01878	-3.46771	-1.67429
H	-1.12878	-0.45504	-2.56583
H	-0.22944	1.45779	-2.05369
H	1.35323	-0.36655	-0.82063

H	3.16285	-0.47046	-2.02361
H	4.06862	1.01888	-2.32887
H	5.00401	0.67785	-0.16653
H	3.79501	-0.55037	0.2047
H	3.07226	3.0842	-2.17433
H	1.5104	3.30757	-1.41695
H	2.5331	3.53319	0.66628
H	5.20514	2.99682	-0.76359
H	5.90023	5.00857	0.41204
H	4.23927	5.14375	1.21376
H	1.07473	1.75025	1.2934
H	1.59838	0.08286	1.37403
H	-2.98706	-0.30663	-1.30238
H	-5.77151	-2.44305	-2.00087
H	-4.63842	-1.23595	-2.67038
H	-4.14278	-2.25365	-1.28859
H	-6.55085	0.93072	0.70713
H	-5.31072	2.88072	1.69487
H	-1.20801	4.65962	1.46299
H	0.19686	3.1947	0.10052
C	2.42469	-3.62521	2.35308
H	2.48623	-4.56523	1.79279
H	3.32336	-3.04816	2.09967
H	2.46769	-3.8509	3.42258

Table 1.Summary of DFT calculations on **1b**, **1c**, **1e** at the B3LYP/6-31G(d) level and ^{77}Se NMR chemical shift calculated at the GIAO-B3LYP/6-311+G(d,p)//B3LYP/6-311+G(d,p) level along with experimental ^{77}Se NMR chemical shifts.

Isoselenazolone	$\mathbf{r_{Se\text{-}N\ [Å]}}$	**^{77}Se δ[ppm][a]**	**^{77}Se δ[ppm][b]**
1b	1.883 (1.855)	908.3	851.0
1c	1.881 (1.863)	972.7	858.1
1e	1.878 (1.859)	847.1	858.8

[a] Theoretical ^{77}Se NMR value referenced to the peak for Me_2Se. [b] Experimental ^{77}Se NMR value. The experimental values for Se-N bond length are given in parentheses.

Table 2.^{77}Se NMR chemical shift calculated at the GIAO-B3LYP/6-311+G(d,p)//B3LYP/6-311+G(d,p) level along with experimental ^{77}Se NMR chemical shifts for selenenyl sulphides **2b**, **2c** and **2e**.

Selenenylsulfide	**^{77}Se δ[ppm][a]**	**^{77}Se δ[ppm][b]**
2b	686.4	-
2c	761.5	591.3
2e	648.7	495.0

[a] Theoretical ^{77}Se NMR value referenced to the peak for Me_2Se. [b] Experimental ^{77}Se NMR value.

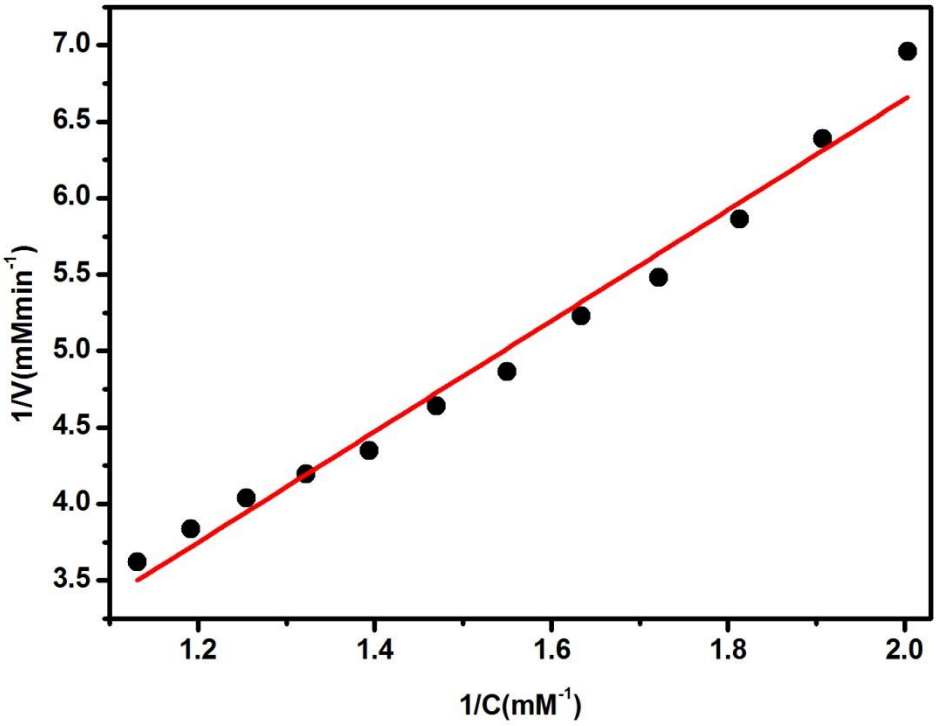
Procedure for thiol-peroxidase like activity

The thiol-peroxidase like activity was followed spectrophotometrically. The test mixture contained benzenethiol (1mM), organoselenium catalyst (0.01mM) and hydrogen peroxide (3.75mM). Reaction of model compound with PhSH and H_2O_2 were studied in methanol by following the appearance of diphenyl disulfide absorption at 305nm at 25 ^{o}C. Each initial reduction rate was measured at least three times by using 1.24$mM^{-1}cm^{-1}$ as the molar extinction coefficient for PhSSPh. Initial reduction rate for most active compounds **1b** was measured fifteen times.

Table 3.Reduction rates (v_o) obtained at the concentrations of catalyst **1b,** PhSH and H_2O_2werefixed to 0.01 mM, 1.0 mM and 3.75 mM respectively.

Time (Sec)	Absorbance	C_t (mM)	C (mM)	1/C (mM^{-1})	V ($mM.min^{-1}$)	1/V ($mM^{-1}.min$)
0	0.05766	0.907		-	-	-
5	0.0862	0.860967742	0.883983871	1.13124236	0.276193548	3.620649381
10	0.11315	0.8175	0.839233871	1.191562965	0.260806452	3.834260977
15	0.13875	0.776209677	0.796854839	1.254933711	0.247741935	4.036458333
20	0.16337	0.7365	0.756354839	1.322130763	0.238258065	4.197129705
25	0.18714	0.69816129	0.717330645	1.394057269	0.230032258	4.347216379
30	0.20942	0.662225806	0.680193548	1.470169781	0.215612903	4.637941352
35	0.23067	0.627951613	0.64508871	1.550174395	0.205645161	4.862745098
40	0.25043	0.596080645	0.612016129	1.633943866	0.191225806	5.229419703
45	0.26929	0.56566129	0.580870968	1.721552729	0.182516129	5.478967833
50	0.28692	0.537225806	0.551443548	1.81342225	0.170612903	5.861221403
55	0.3031	0.511129032	0.524177419	1.907751008	0.156580645	6.386485373
60	0.31795	0.487177419	0.499153226	2.003392843	0.143709677	6.958473625

Figure S125**.** Lineweaver-Burk plots obtained for **1b**.The initial concentration of H_2O_2 was fixed to3.75 mM. The initial PhSH concentration was 1 mM. (See Table 3)



Best Fit: 3.62461x + (-0.60177)

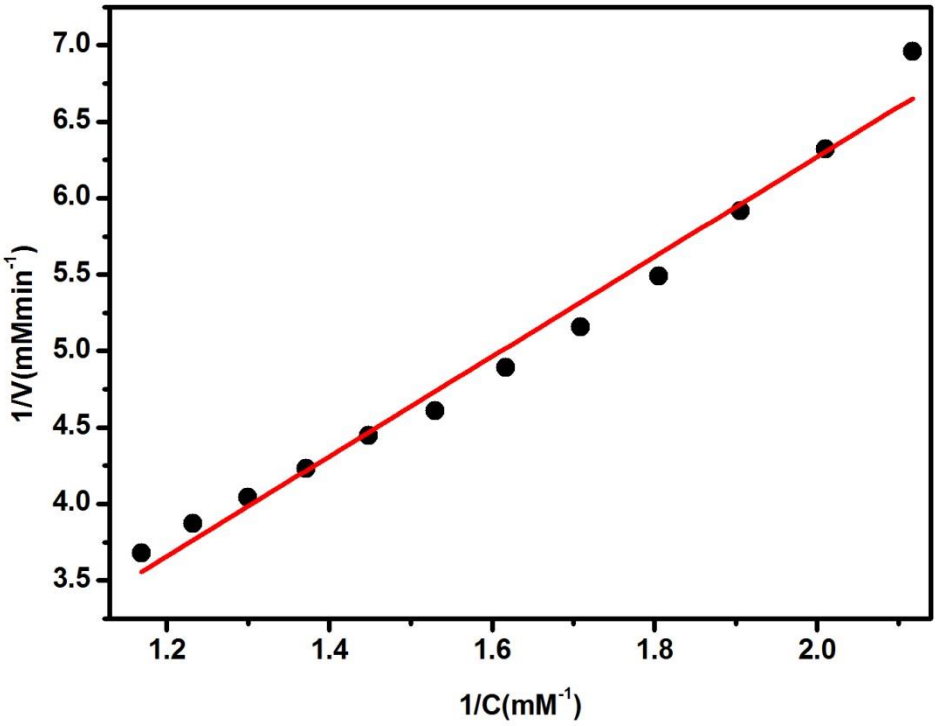
Adj-R-Square = 0.98015

ν_o = 330.8147 μMmin^{-1}

Table 4.Reduction rates (v_o) obtained at the concentrations of catalyst **1b,** PhSH and H_2O_2werefixed to 0.01 mM, 1.0 mM and 3.75 mM respectively.

Time (Sec)	Absorbance	C_t (mM)	C (mM)	1/C (mM^{-1})	V ($mM.min^{-1}$)	1/V ($mM^{-1}.min$)
0	0.07556	0.878129032		-	-	-
5	0.10364	0.83283871	0.855483871	1.16892911	0.271741935	3.679962013
10	0.13033	0.789790323	0.811314516	1.232567617	0.258290323	3.871612339
15	0.1559	0.748548387	0.769169355	1.300103799	0.247451613	4.041194108
20	0.18032	0.70916129	0.728854839	1.372015313	0.236322581	4.231504232
25	0.20355	0.671693548	0.690427419	1.448378167	0.224806452	4.448270914
30	0.22597	0.635532258	0.653612903	1.529957556	0.216967742	4.608980077
35	0.24709	0.601467742	0.6185	1.616814875	0.204387097	4.892676768
40	0.26712	0.56916129	0.585314516	1.70848317	0.19383871	5.158928274
45	0.28595	0.538790323	0.553975806	1.805132983	0.182225806	5.487696938
50	0.30342	0.510612903	0.524701613	1.905845104	0.169064516	5.914901736
55	0.31977	0.484241935	0.497427419	2.010343542	0.158225806	6.320081549
60	0.33462	0.460290323	0.472266129	2.11745018	0.143709677	6.958473625

Figure S126**.** Lineweaver-Burk plots obtained for **1b**.The initial concentration of H_2O_2 was fixed to3.75 mM. The initial PhSH concentration was 1 mM. (See Table 4)



Best Fit: 3.26531x + (-0.26101)

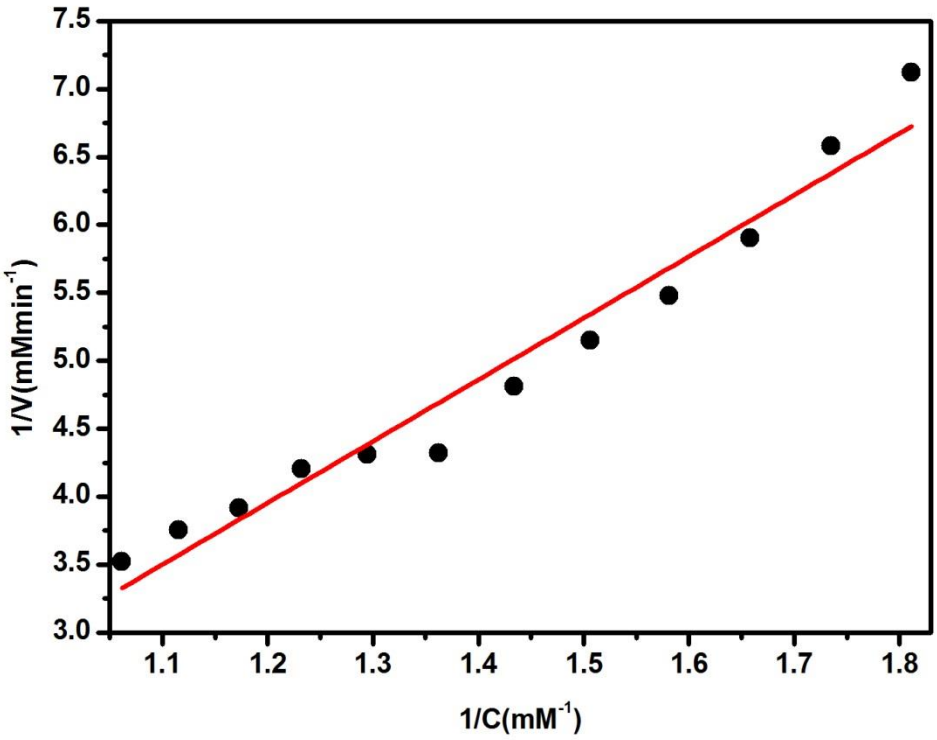
Adj-R-Square = 0.9807

ν_o = 332.8562µMmin^{-1}

Table 5.Reduction rates (v_o) obtained at the concentrations of catalyst **1b,** PhSH and H_2O_2werefixed to 0.01 mM, 1.0 mM and 3.75 mM respectively.

Time (Sec)	Absorbance	C_t (mM)	C (mM)	1/C (mM^{-1})	V ($mM.min^{-1}$)	1/V ($mM^{-1}.min$)
0	0.02114	0.965903226		-	-	-
5	0.05047	0.918596774	0.94225	1.061289467	0.28383871	3.523127628
10	0.07801	0.874177419	0.896387097	1.115589463	0.266516129	3.752118131
15	0.10441	0.831596774	0.852887097	1.172488133	0.255483871	3.914141414
20	0.129	0.791935484	0.811766129	1.231881898	0.237967742	4.202250237
25	0.15296	0.753290323	0.772612903	1.294309215	0.231870968	4.312743461
30	0.17687	0.714725806	0.734008065	1.362382852	0.231387097	4.321762164
35	0.19834	0.680096774	0.69741129	1.43387412	0.207774194	4.812917249
40	0.21841	0.647725806	0.66391129	1.506225326	0.194225806	5.148646404
45	0.23727	0.617306452	0.632516129	1.580987352	0.182516129	5.478967833
50	0.25478	0.589064516	0.603185484	1.657864831	0.169451613	5.901389682
55	0.27048	0.563741935	0.576403226	1.734896606	0.151935484	6.581740977
60	0.28499	0.54033871	0.552040323	1.811461879	0.140419355	7.121525385

Figure S127.Lineweaver-Burk plots obtained for **1b**.The initial concentration of H_2O_2 was fixed to3.75 mM. The initial PhSH concentration was 1 mM. (See Table 5)



Best Fit: 4.53264x + (-1.48475)

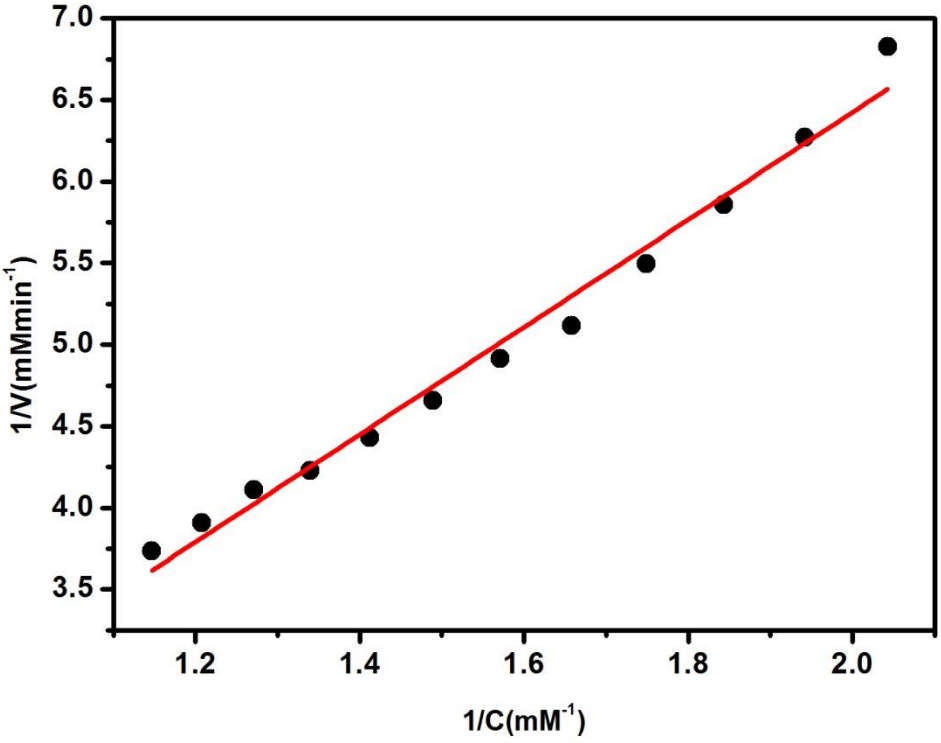
Adj-R-Square = 0.95732

ν_o = 328.0960µMmin^{-1}

Table 6.Reduction rates (v_o) obtained at the concentrations of catalyst **1b,** PhSH and H_2O_2werefixed to 0.01 mM, 1.0 mM and 3.75 mM respectively.

Time (Sec)	Absorbance	C_t (mM)	C (mM)	1/C (mM^{-1})	V ($mM.min^{-1}$)	1/V ($mM^{-1}.min$)
0	0.06562	0.89416129		-	-	-
5	0.093299	0.849517742	0.871839516	1.147000086	0.26786129	3.733275528
10	0.11973	0.806887097	0.828202419	1.20743429	0.255783871	3.909550654
15	0.14486	0.766354839	0.786620968	1.271260291	0.243193548	4.111951187
20	0.16929	0.726951613	0.746653226	1.339309823	0.236419355	4.229772138
25	0.19262	0.689322581	0.708137097	1.412155929	0.225774194	4.429204172
30	0.2148	0.653548387	0.671435484	1.489346369	0.214645161	4.658851818
35	0.23582	0.619645161	0.636596774	1.570853075	0.203419355	4.915953061
40	0.25601	0.587080645	0.603362903	1.657377334	0.195387097	5.118045237
45	0.27481	0.556758065	0.571919355	1.748498266	0.181935484	5.496453901
50	0.29245	0.528306452	0.542532258	1.843208372	0.170709677	5.857898715
55	0.30893	0.501725806	0.515016129	1.941686762	0.159483871	6.270226537
60	0.32407	0.477306452	0.489516129	2.042833608	0.146516129	6.825187142

Figure S128.Lineweaver-Burk plots obtained for **1b**.The initial concentration of H_2O_2 was fixed to3.75 mM. The initial PhSH concentration was 1 mM. (See Table 6)



Best Fit: 3.29305x + (-0.16066)

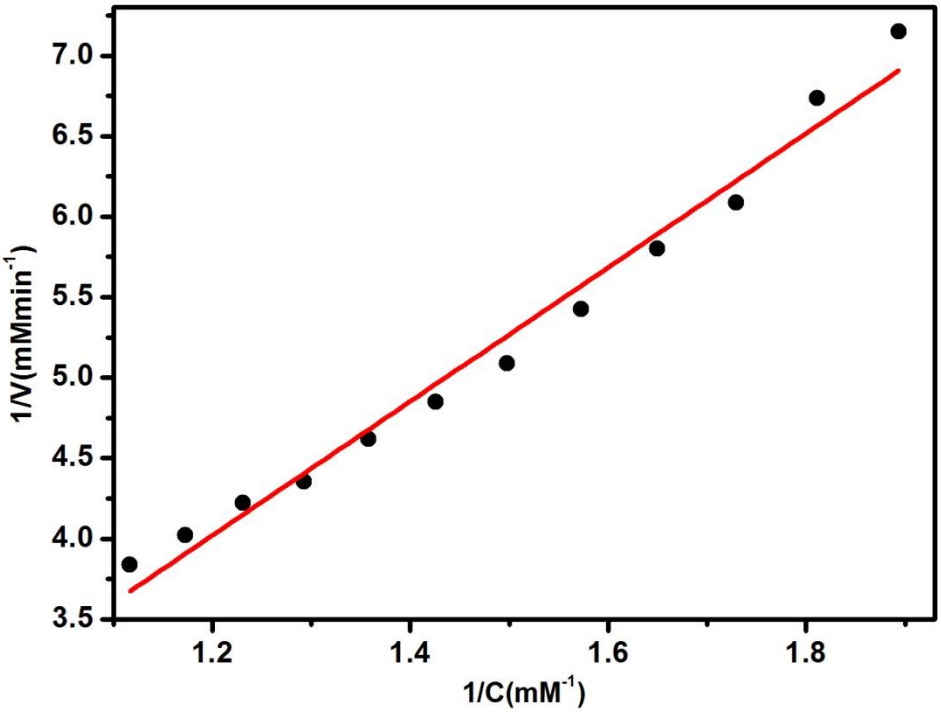
Adj-R-Square = 0.98294

ν_o = 319.245μMmin^{-1}

Table 7.Reduction rates (v_o) obtained at the concentrations of catalyst **1b,** PhSH and H_2O_2werefixed to 0.01 mM, 1.0 mM and 3.75 mM respectively.

Time (Sec)	Absorbance	C_t (mM)	C (mM)	1/C (mM^{-1})	V ($mM.min^{-1}$)	1/V ($mM^{-1}.min$)
0	0.05139	0.917112903		-	-	-
5	0.078299	0.87371129	0.895412097	1.116804211	0.260409677	3.840103063
10	0.10399	0.832274194	0.852992742	1.172342918	0.248622581	4.022160809
15	0.12847	0.792790323	0.812532258	1.230720368	0.236903226	4.221132898
20	0.15221	0.7545	0.773645161	1.292582246	0.229741935	4.352709913
25	0.17459	0.718403226	0.736451613	1.357862462	0.216580645	4.617217754
30	0.19589	0.684048387	0.701225806	1.426074156	0.206129032	4.851330203
35	0.2162	0.651290323	0.667669355	1.49774734	0.196548387	5.087805679
40	0.23525	0.620564516	0.635927419	1.572506499	0.184354839	5.42432196
45	0.25306	0.59183871	0.606201613	1.649616198	0.172354839	5.801983904
50	0.27004	0.564451613	0.578145161	1.72966941	0.164322581	6.085590891
55	0.28538	0.539709677	0.552080645	1.811329574	0.148451613	6.736201651
60	0.29983	0.516403226	0.528056452	1.893736923	0.13983871	7.151095732

Figure S129.Lineweaver-Burk plots obtained for **1b**.The initial concentration of H_2O_2 was fixed to3.75 mM. The initial PhSH concentration was 1 mM. (See Table 7)



Best Fit: 4.16162x + (-0.97343)

Adj-R-Square = 0.97997

ν_o = 313.666μMmin^{-1}

Figure S130.Graph representing linear dependency between initial reduction rates (v_0) and concentration of catalyst **1b**. Concentration of catalyst varied from 0.001mM to 0.009mM

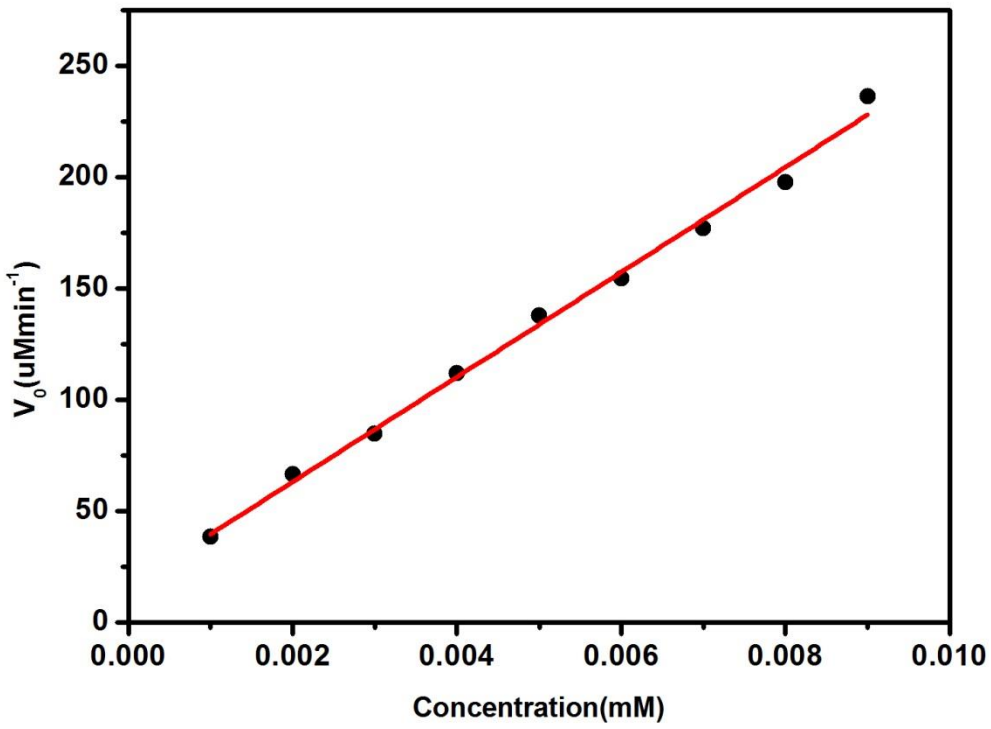
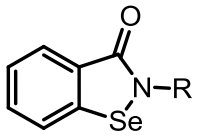
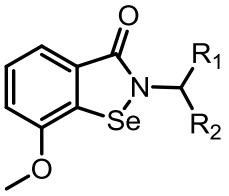


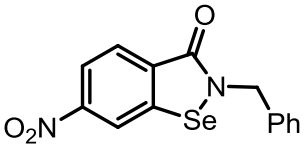
Chart1. Reduction rates (v_o) obtained for various isoselenazolone catalysts (0.01mM), PhSH (1.0 mM) and H_2O_2(3.7mM) respectively.



R, Benz 0.4(0.03)

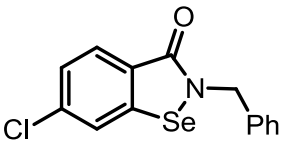


R_1, CH_3, R_2, 1-Naphth 4.3(0.02)

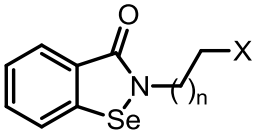


3.0 (0.1)

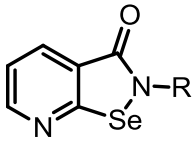
R, H 10.8(1.1)
R, CH_3 9.9(1.5)



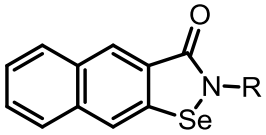
1.3(0.2)



X, OH, n, 2, 28.1(2.0)
X = NMe_2, n, 1, 0.2(0.03)



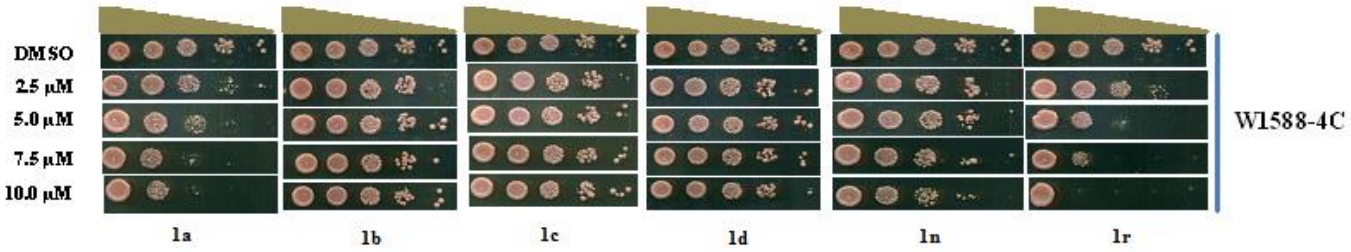
R nBu 2.9(0.1)
R Benz 5.7(0.4)
R Cyc-hex 4.5(0.2)



R Ph 21.7(2.8)
R Benz 0.5(0.05)

Procedure for growth sensitivity and growth curve assay

Figure S131 Growth sensitivity assay



To investigate the biological effect of ebselen and compounds **1b-1d**, **1n** and **1r** on the growth of yeast cells, growth assay was carried out by spot tests and growth curve assays. For spot test, serial dilutions of mid-log phase cultures of wild-type yeast strain W1588-4C (MATa ade2-1 can1-100 his3-11, 15 leu2-3, 112 trp1-1, ura3-1, RAD5+)[5] was made in autoclaved distilled water. Three microliter of each undiluted and 10-fold serially diluted cultures were spotted onto solid SCA (Synthetic complete + 2% Agar) plates containing DMSO (control) or different concentrations of compounds (2.5, 5.0, 7.5, 10 µM). All plates were incubated at 30°C and growth of the yeast cells was recorded after 72 hours by scanning SCA (Synthetic complete + 2% Agar) plates using a HP scanner. Isoselenazolones bearing quinine moiety **1b-1d** showed better cell growth than ebselen **1a** while nitro-substituted isoselenazolone **1r** showed minimum cell growth. Results obtained from growth sensitivity assay were further validated with most active compound **1b** by growth curve analysis and results were compared with that of ebselen **1a**.

Growth curve analysis was performed for compounds **1a** and **1b**. Yeast cells were treated with increasing dose of compounds **1a** and **1b** (10, 20 and 30 µM) in liquid SC media. Growth was monitored at OD_{600nm} (1 OD_{600} unit represents 10^7 cells/mL) for 11 hours at regular interval of 1hour by automated micro- plate spectrophotometer (Eon Biotek). Results obtained from spectrophotometer were processed using Gen5 2.03lnk software and growth

curve was generated.[6] Growth curve analysis was performed separately in three independent biological repeats and each time experiment was conducted in triplicate to ensure the reproducibility of the results.

The doubling time of WT yeast cells in presence or absence of compound **1a** or **1b** (30 μM) were calculated using the formula: Doubling time = t/g [Where, t = the time cultured; g = [log10 (N_t/N_0)]/0.3; N_0 = Number of cells or OD_{600} at start, N_t =Number of cells or OD_{600} at the end].[7]

OD_{600} values taken at 600 nm

DMSO

Time (hr)	First Repeat			Second Repeat			Third Repeat			Average	Standard Deviation
0	0.028	0.026	0.024	0.025	0.029	0.022	0.023	0.023	0.026	0.025111	0.002369
1	0.031	0.028	0.028	0.026	0.031	0.024	0.025	0.024	0.028	0.027222	0.002682
2	0.037	0.032	0.033	0.03	0.034	0.028	0.028	0.029	0.033	0.031556	0.003046
3	0.051	0.044	0.044	0.042	0.048	0.038	0.039	0.039	0.046	0.043444	0.004419
4	0.08	0.067	0.067	0.064	0.071	0.057	0.06	0.06	0.07	0.066222	0.007032
5	0.127	0.107	0.105	0.101	0.114	0.091	0.096	0.094	0.113	0.105333	0.011435
6	0.208	0.176	0.17	0.166	0.188	0.15	0.16	0.155	0.189	0.173556	0.018682
7	0.33	0.285	0.276	0.267	0.3	0.244	0.261	0.251	0.314	0.280889	0.029062
8	0.495	0.437	0.423	0.413	0.454	0.38	0.404	0.391	0.502	0.433222	0.043266
9	0.675	0.613	0.597	0.583	0.631	0.546	0.573	0.56	0.715	0.610333	0.05541
10	0.833	0.776	0.76	0.745	0.791	0.708	0.736	0.723	0.875	0.771889	0.054052
11	0.977	0.921	0.907	0.892	0.937	0.854	0.882	0.869	1.006	0.916111	0.050191

10 μM dose of 1a

Time (hr)	First Repeat			Second Repeat			Third Repeat			Average	Standard Deviation
0	0.033	0.032	0.031	0.032	0.032	0.029	0.029	0.028	0.026	0.030222	0.002333
1	0.035	0.032	0.032	0.032	0.032	0.03	0.029	0.028	0.027	0.030778	0.002489
2	0.037	0.034	0.033	0.034	0.034	0.032	0.03	0.03	0.028	0.032444	0.002744
3	0.044	0.041	0.04	0.041	0.04	0.038	0.037	0.036	0.034	0.039	0.003041
4	0.059	0.056	0.054	0.055	0.052	0.051	0.048	0.048	0.045	0.052	0.004472
5	0.085	0.08	0.078	0.079	0.072	0.072	0.069	0.069	0.065	0.074333	0.006481
6	0.13	0.124	0.121	0.12	0.109	0.111	0.106	0.105	0.101	0.114111	0.00993
7	0.206	0.196	0.191	0.191	0.171	0.176	0.168	0.166	0.159	0.180444	0.016009
8	0.323	0.31	0.301	0.301	0.269	0.279	0.272	0.262	0.252	0.285444	0.02413
9	0.478	0.463	0.449	0.447	0.407	0.419	0.409	0.395	0.384	0.427889	0.032471
10	0.648	0.63	0.61	0.612	0.564	0.58	0.57	0.55	0.536	0.588889	0.037962

11	0.806	0.8	0.767	0.768	0.714	0.735	0.726	0.7	0.684	0.744444	0.043192

20 µM dose of 1a

Time (hr)	First Repeat			Second Repeat			Third Repeat			Average	Standard Deviation
0	0.039	0.043	0.044	0.044	0.045	0.042	0.047	0.039	0.037	0.042222	0.00327
1	0.04	0.042	0.045	0.044	0.044	0.042	0.047	0.039	0.037	0.042222	0.003153
2	0.04	0.042	0.045	0.044	0.045	0.042	0.048	0.038	0.037	0.042333	0.003571
3	0.046	0.046	0.049	0.048	0.048	0.045	0.051	0.041	0.04	0.046	0.003606
4	0.055	0.053	0.056	0.056	0.056	0.052	0.058	0.048	0.047	0.053444	0.003812
5	0.066	0.067	0.07	0.069	0.07	0.065	0.072	0.06	0.059	0.066444	0.004503
6	0.09	0.091	0.095	0.092	0.095	0.087	0.095	0.081	0.081	0.089667	0.00559
7	0.133	0.133	0.14	0.133	0.14	0.128	0.137	0.118	0.117	0.131	0.008544
8	0.205	0.207	0.216	0.201	0.212	0.197	0.209	0.181	0.179	0.200778	0.013046
9	0.317	0.319	0.331	0.307	0.33	0.305	0.321	0.282	0.281	0.310333	0.01854
10	0.466	0.472	0.488	0.452	0.484	0.454	0.472	0.422	0.42	0.458889	0.024538
11	0.625	0.642	0.657	0.614	0.653	0.62	0.638	0.584	0.578	0.623444	0.028018

30 µM dose of 1a

Time (hr)	First Repeat			Second Repeat			Third Repeat			Average	Standard Deviation
0	0.047	0.052	0.046	0.048	0.057	0.063	0.051	0.052	0.047	0.051444	0.005548
1	0.049	0.056	0.047	0.048	0.054	0.061	0.052	0.051	0.048	0.051778	0.004577
2	0.049	0.056	0.049	0.048	0.057	0.06	0.053	0.051	0.048	0.052333	0.004416
3	0.05	0.057	0.048	0.049	0.055	0.062	0.054	0.051	0.049	0.052778	0.004631
4	0.052	0.059	0.051	0.051	0.057	0.064	0.056	0.054	0.051	0.055	0.004472
5	0.056	0.063	0.053	0.055	0.061	0.067	0.06	0.057	0.054	0.058444	0.00464
6	0.063	0.069	0.059	0.061	0.068	0.075	0.067	0.064	0.061	0.065222	0.005019
7	0.074	0.082	0.07	0.072	0.08	0.088	0.078	0.074	0.071	0.076556	0.00594
8	0.093	0.101	0.088	0.093	0.101	0.11	0.097	0.093	0.089	0.096111	0.006954
9	0.126	0.135	0.12	0.122	0.134	0.139	0.131	0.125	0.12	0.128	0.007
10	0.181	0.193	0.168	0.174	0.191	0.197	0.185	0.177	0.171	0.181889	0.010265
11	0.267	0.281	0.242	0.256	0.279	0.286	0.271	0.259	0.252	0.265889	0.014752

10 µM dose of 1b

Time (hr)	First Repeat			Second Repeat			Third Repeat			Average	Standard Deviation
0	0.027	0.027	0.025	0.028	0.024	0.025	0.025	0.025	0.024	0.025556	0.001424
1	0.029	0.029	0.027	0.03	0.026	0.027	0.028	0.027	0.025	0.027556	0.00159
2	0.033	0.033	0.031	0.033	0.03	0.03	0.032	0.03	0.028	0.031111	0.001764
3	0.045	0.045	0.043	0.045	0.041	0.042	0.045	0.041	0.039	0.042889	0.002261
4	0.068	0.067	0.065	0.068	0.062	0.063	0.068	0.063	0.06	0.064889	0.003018
5	0.109	0.108	0.105	0.108	0.101	0.102	0.108	0.1	0.096	0.104111	0.004567
6	0.181	0.177	0.174	0.179	0.165	0.171	0.179	0.165	0.158	0.172111	0.007928
7	0.29	0.288	0.284	0.288	0.27	0.277	0.289	0.268	0.258	0.279111	0.011483

8	0.442	0.442	0.437	0.439	0.415	0.428	0.438	0.413	0.402	0.428444	0.014842
9	0.615	0.617	0.611	0.613	0.589	0.6	0.61	0.585	0.573	0.601444	0.015653
10	0.774	0.78	0.774	0.772	0.751	0.763	0.769	0.747	0.734	0.762667	0.015362
11	0.918	0.928	0.92	0.918	0.897	0.91	0.915	0.892	0.878	0.908444	0.016094

20 µM dose of 1b

Time (hr)	First Repeat			Second Repeat			Third Repeat			Average	Standard Deviation
0	0.034	0.024	0.028	0.03	0.027	0.026	0.028	0.024	0.022	0.027	0.003606
1	0.036	0.026	0.029	0.031	0.028	0.028	0.029	0.025	0.024	0.028444	0.003575
2	0.042	0.03	0.034	0.035	0.032	0.031	0.032	0.028	0.028	0.032444	0.004304
3	0.053	0.041	0.045	0.048	0.044	0.042	0.042	0.038	0.039	0.043556	0.004667
4	0.075	0.064	0.068	0.071	0.067	0.063	0.061	0.058	0.06	0.065222	0.005518
5	0.113	0.1	0.109	0.112	0.106	0.1	0.096	0.091	0.094	0.102333	0.008016
6	0.18	0.166	0.179	0.184	0.174	0.165	0.156	0.151	0.156	0.167889	0.011973
7	0.285	0.268	0.289	0.295	0.281	0.266	0.254	0.246	0.255	0.271	0.017321
8	0.435	0.417	0.442	0.448	0.43	0.41	0.394	0.384	0.393	0.417	0.023243
9	0.608	0.59	0.619	0.623	0.604	0.58	0.56	0.551	0.563	0.588667	0.026655
10	0.771	0.752	0.779	0.788	0.765	0.744	0.722	0.713	0.722	0.750667	0.027212

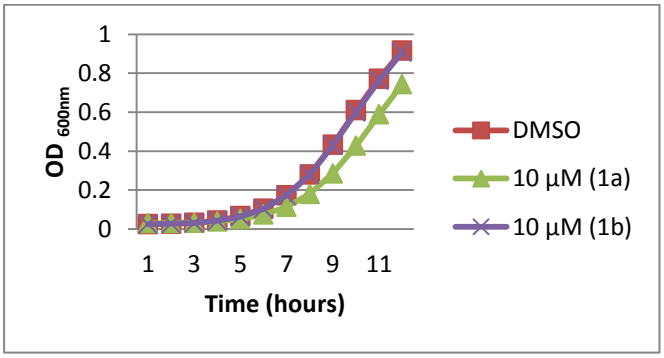
30 µM dose of 1b

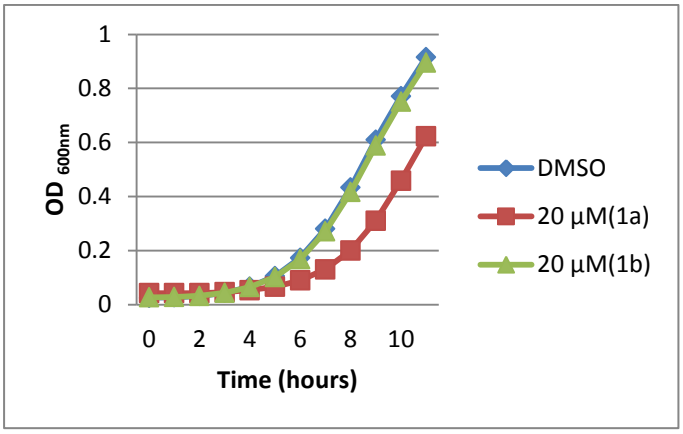
Time (hr)	First Repeat			Second Repeat			Third Repeat			Average	Standard Deviation
0	0.022	0.018	0.021	0.021	0.024	0.025	0.02	0.022	0.021	0.021556	0.002068
1	0.024	0.02	0.023	0.024	0.025	0.027	0.023	0.025	0.023	0.023778	0.001922
2	0.03	0.024	0.027	0.028	0.029	0.032	0.026	0.029	0.026	0.027889	0.002421
3	0.04	0.035	0.038	0.038	0.04	0.041	0.037	0.039	0.036	0.038222	0.001986
4	0.059	0.052	0.057	0.059	0.06	0.061	0.056	0.058	0.055	0.057444	0.002789
5	0.094	0.081	0.089	0.093	0.094	0.096	0.088	0.091	0.088	0.090444	0.004558
6	0.157	0.136	0.147	0.153	0.154	0.155	0.146	0.15	0.145	0.149222	0.006515
7	0.256	0.225	0.24	0.249	0.249	0.254	0.24	0.245	0.238	0.244	0.009513
8	0.396	0.356	0.376	0.388	0.386	0.394	0.376	0.381	0.374	0.380778	0.012204
9	0.564	0.52	0.54	0.557	0.554	0.562	0.543	0.55	0.542	0.548	0.013611
10	0.725	0.677	0.7	0.716	0.715	0.722	0.708	0.713	0.702	0.708667	0.014491

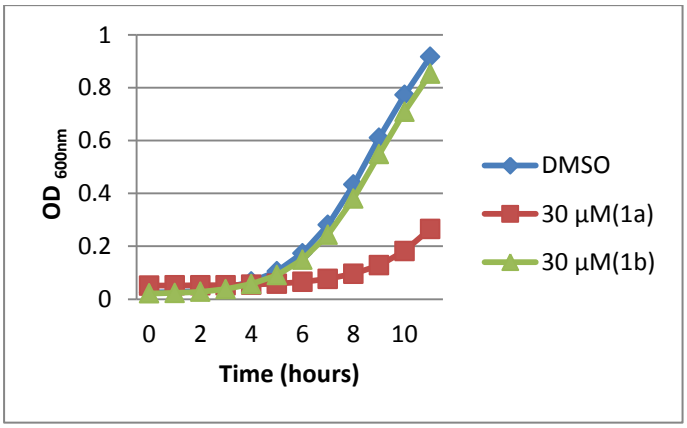
Average values calculated from nine independent samples

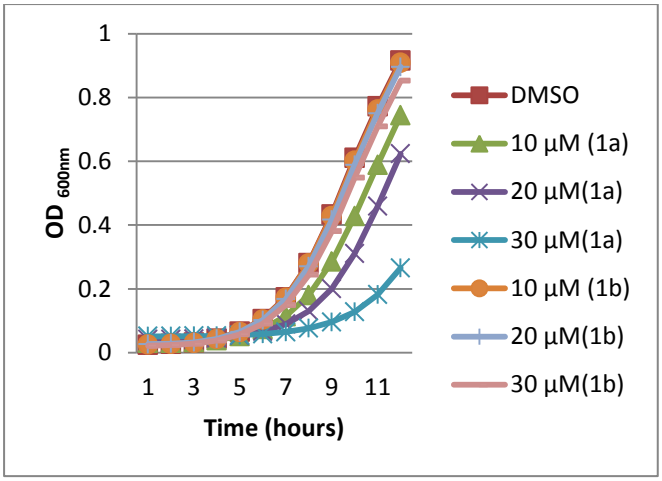
Time	DMSO	10 µM (1a)	20 µM(1a)	30 µM(1a)	10 µM (1b)	20 µM(1b)	30 µM(1b)
0	0.025111	0.030222	0.042222	0.051444	0.025556	0.027	0.021556
1	0.027222	0.030778	0.042222	0.051778	0.027556	0.028444	0.023778
2	0.031556	0.032444	0.042333	0.052333	0.031111	0.032444	0.027889
3	0.043444	0.039	0.046	0.052778	0.042889	0.043556	0.038222
4	0.066222	0.052	0.053444	0.055	0.064889	0.065222	0.057444
5	0.105333	0.074333	0.066444	0.058444	0.104111	0.102333	0.090444
6	0.173556	0.114111	0.089667	0.065222	0.172111	0.167889	0.149222
7	0.280889	0.180444	0.131	0.076556	0.279111	0.271	0.244

8	0.433222	0.285444	0.200778	0.096111	0.428444	0.417	0.380778
9	0.610333	0.427889	0.310333	0.128	0.601444	0.588667	0.548
10	0.771889	0.588889	0.458889	0.181889	0.762667	0.750667	0.708667





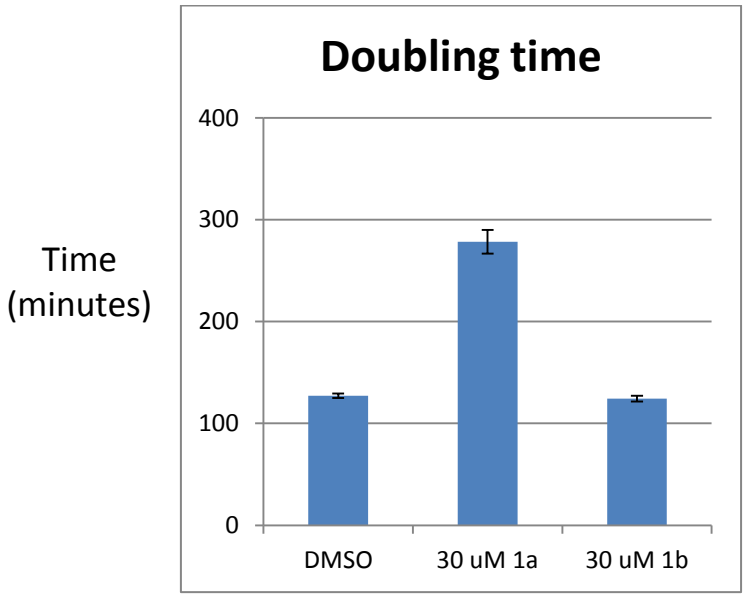




Calculation of doubling time of yeast cells grown at 30 µM concentration of ebselen (1a) and compound 1b

Samples	1	2	3	4	5	6	7	8	9	Average	Std. dev
DMSO	128.8	128.2	126	128	131.6	125	125.4	126	125.1	127.1222	2.204415
30 uM (1a)	263.4	271.2	275.5	273.3	288.1	302.4	273.9	284.9	272.4	278.3444	11.61799
30 uM (1b)	124.5	119.7	123.9	123.3	127.8	129.1	121.9	125	123.8	124.3333	2.831519

Samples	Average (min)	Standard Deviation
DMSO	127.1222	2.204415
30 uM 1a	278.3444	11.61799
30 uM 1b	124.3333	2.831519



Crystallographic details for compounds 1b, 1c and 1e

Data collection, structure solution and refinement:

Single crystal X-ray diffraction data of all the compounds were collected at 25 °C on a Bruker Apex II D8 Venture diffractometer equipped with CMOS detector. Data reduction and integration were performed by SAINT V7.685A12 and absorption corrections and scaling was done using SADABS. All the crystal structures were solved by direct methods using SIR 92 and refined by the full matrix least squares method using SHELXL97 present in the program suite WinGX. *ORTEP* of all the compounds were generated using ORTEP32 and molecular diagrams were generated using Mercury software. The non-hydrogen atoms were refined anisotropically and the hydrogen atoms bonded to C and N atoms were positioned geometrically and refined using a riding model. **Table 8-10** lists the crystallographic and refinement data of **1b**, **1c** and **1e** respectively.

Crystallographic modelling of disorder:

The ethenyl group at quinine moiety on compounds **1b** and **1c** displays disorder at two positions. The associated disorders were refined using PART command in SHELXL97 with occupancy ratio of 0.72(1): 0.28(1) and 0.87 (1): 0.13(1) for compounds **1b** and **1c** respectively. The thermal parameters of involved atoms were constrained to be equal by EADP command in SHELXL 97. The distance and angle restrain DFIX, DANG or SADI were applied in order to model the associated disorder in the ethenyl group. Crystallization of **1c** from ethanol at room temperature produces its solvates with one ethanol and one water molecules present in the asymmetric unit. The ethanol molecule found to disorder at two orientations with occupancy ratio 0.73(1): 0.27 (1) and was modelled with PART command in SHELXL97. The thermal parameters of involved atoms were constrained to be equal by

EADP command in SHELXL 97. The hydrogen atoms for water molecule and oxygen atom of ethanol molecule were located from the difference fourier.

Table 8: **Crystallographic and Refinement Data for 1b:**

DATA	(1b)
Molecular Formula	$C_{28}H_{29}N_3O_2Se$
Molecular weight	518.50
Wavelength	0.71073
CCDC No.	930741
Solvent system	Ethanol
Crystal System	Orthorhombic
Space Group	$P2_12_12_1$
a (Å)	9.2900(5)
b (Å)	16.2681(10)
c (Å)	16.8894(10)
α (^{0})	90
β (^{0})	90
γ (^{0})	90
Volume (Å^3)	2552.5(3)
Z	4
ρ (g/cm^3)	1.349
μ (mm^{-1})	1.500
F (000)	1072
$\theta_{min,\ max}$	2.41, 24.09
$h_{min,max}$;$k_{min,max}$; $l_{min,max}$	-10, 10; -17, 15; -19, 19
Treatment of hydrogen	Fixed
No. of reflections.	16444
No. unique/ observedreflections.	3449/3054
No. of parameters	316
R_all, R_obs	0.0361, 0.0275
wR_2_all, wR_2_obs	0.0616, 0.0590
$\Delta\rho_{min,max}$(eÅ^{-3})	-0.148, 0.240
GooF	1.052

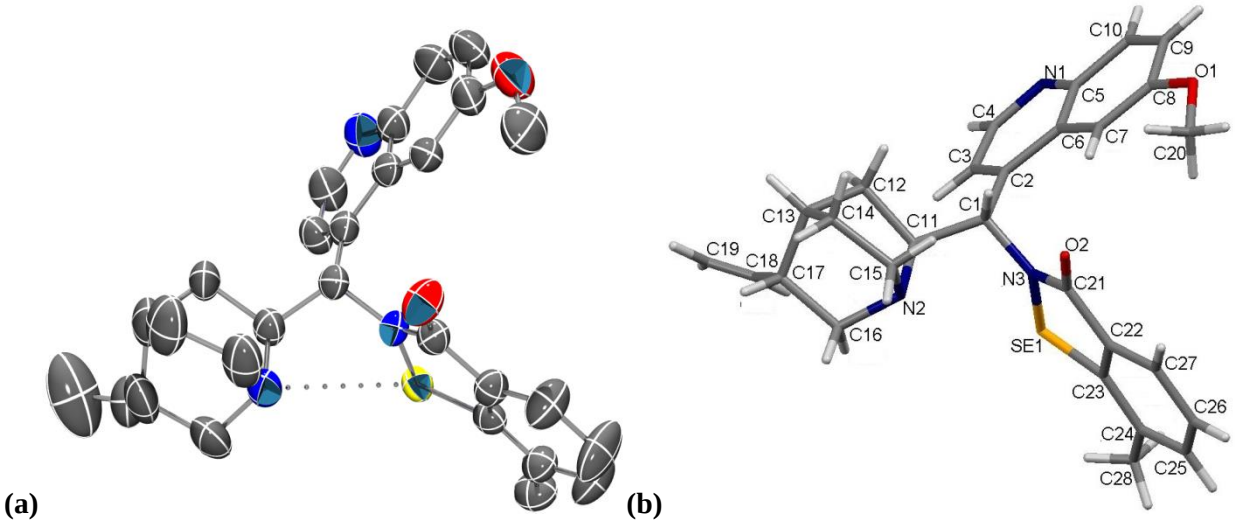
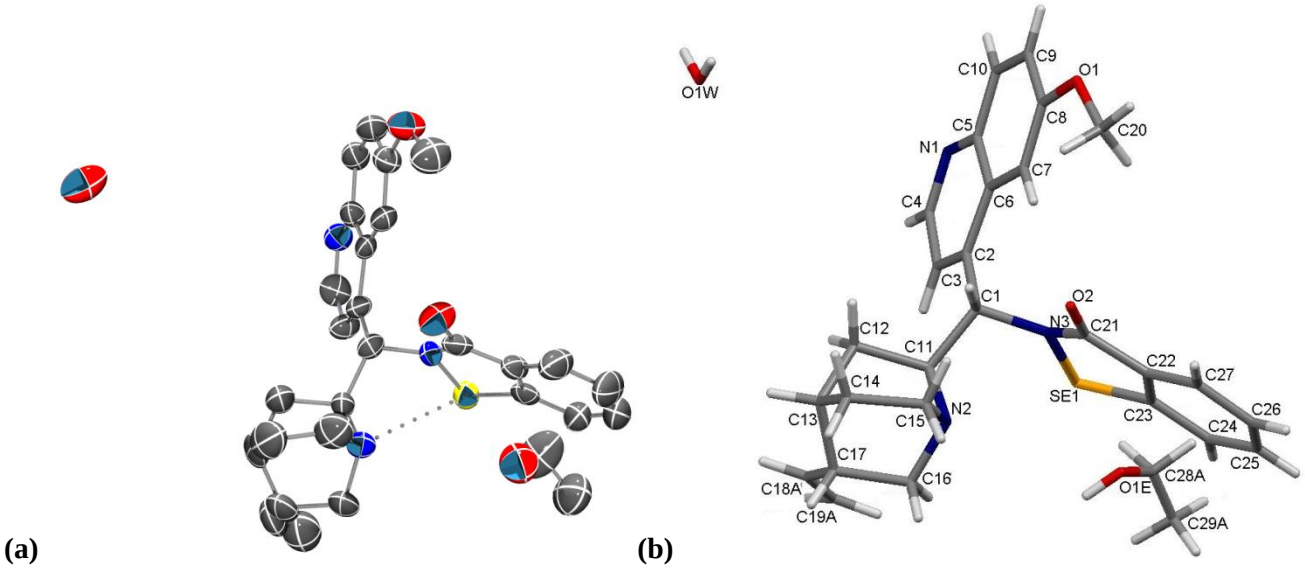


Figure 133 **(a)** *ORTEP* of **1b** drawn with 50% ellipsoidal properties. Hydrogen atoms were omitted for clarity. **(b)**Molecular diagram of **1b** displaying atom numbering scheme.

Table 9: **Crystallographic and Refinement Data for 1c:**

DATA	(1c)
Molecular Formula	$C_{27}H_{27}N_3O_2Se \cdot C_2H_6O \cdot H_2O$
Molecular weight	568.56
Wavelength	0.71073
CCDC No.	930742
Solvent system	Ethanol
Crystal System	Monoclinic
Space Group	$P2_1$
a (Å)	9.5877(15)
b (Å)	15.441(2)
c (Å)	10.1760(17)
α (^{0})	90
β (^{0})	112.072(9)
γ (^{0})	90
Volume (Å^3)	1396.1(4)
Z	2
ρ (g/cm^3)	1.352
μ (mm^{-1})	1.383
F (000)	592
$\theta_{min,\ max}$	2.29, 24.98
$h_{min,max}$;$k_{min,max}$; $l_{min,max}$	-8, 11; -18, 18; -12, 12
Treatment of hydrogen	Fixed
No. of reflections.	11855
No. unique/ observedreflections.	4768/ 3046
No. of parameters	363
R_all, R_obs	0.1002, 0.0441
wR_2_all, wR_2_obs	0.0801, 0.0716

$\Delta\rho_{min,max}$(eÅ^{-3})	-0.276, 0.576
GooF	0.921



(a) **(b)**

Figure 134. **(a)** O*RTEP* of **1c** drawn with 50% ellipsoidal properties. Hydrogen atoms were omitted for clarity. **(b)**Molecular diagram of **1c** displaying atom numbering scheme.

Table 10: **Crystallographic and Refinement Data for 1e:**

DATA	(1e)
Molecular Formula	$C_{15}H_{13}NOSe$
Molecular weight	302.22
Wavelength	0.71073
CCDC No.	953729
Solvent system	Dichloromethane
Morphology	Plate
Crystal System	Monoclinic
Space Group	$P2_1/c$
a (Å)	10.4368(2)
b (Å)	10.9926(2)
c (Å)	11.5312(2)
α (^{0})	90
β (^{0})	102.8070(10)
γ (^{0})	90
Volume (Å^3)	1290.03(4)
Z	4
ρ (g/cm^3)	1.556
μ (mm^{-1})	2.897
F (000)	608
$\theta_{min,\ max}$	2.00, 30.65
$h_{min,max}$;$k_{min,max}$; $l_{min,max}$	-14, 13; -15, 15; -16, 16
Treatment of hydrogen	Fixed
No. of reflections.	14580
No. unique/ observedreflections.	3981/3157

No. of parameters	164
R_all, R_obs	0.0395, 0.0271
wR_2_all, wR_2_obs	0.0749, 0.0693
$\Delta\rho_{min,max}$(eÅ^{-3})	-0.520, 0.280
GooF	1.021

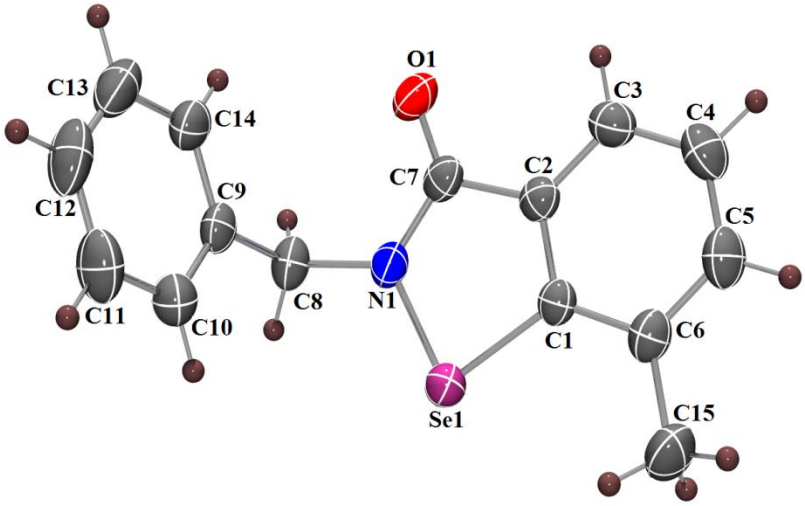


Figure 135.*ORTEP* of **1e**with 50% ellipsoidal properties. Hydrogen atoms were omitted for clarity.

Figure S136 ^{1}H NMR of potassium *tert*-butoxyselenolate

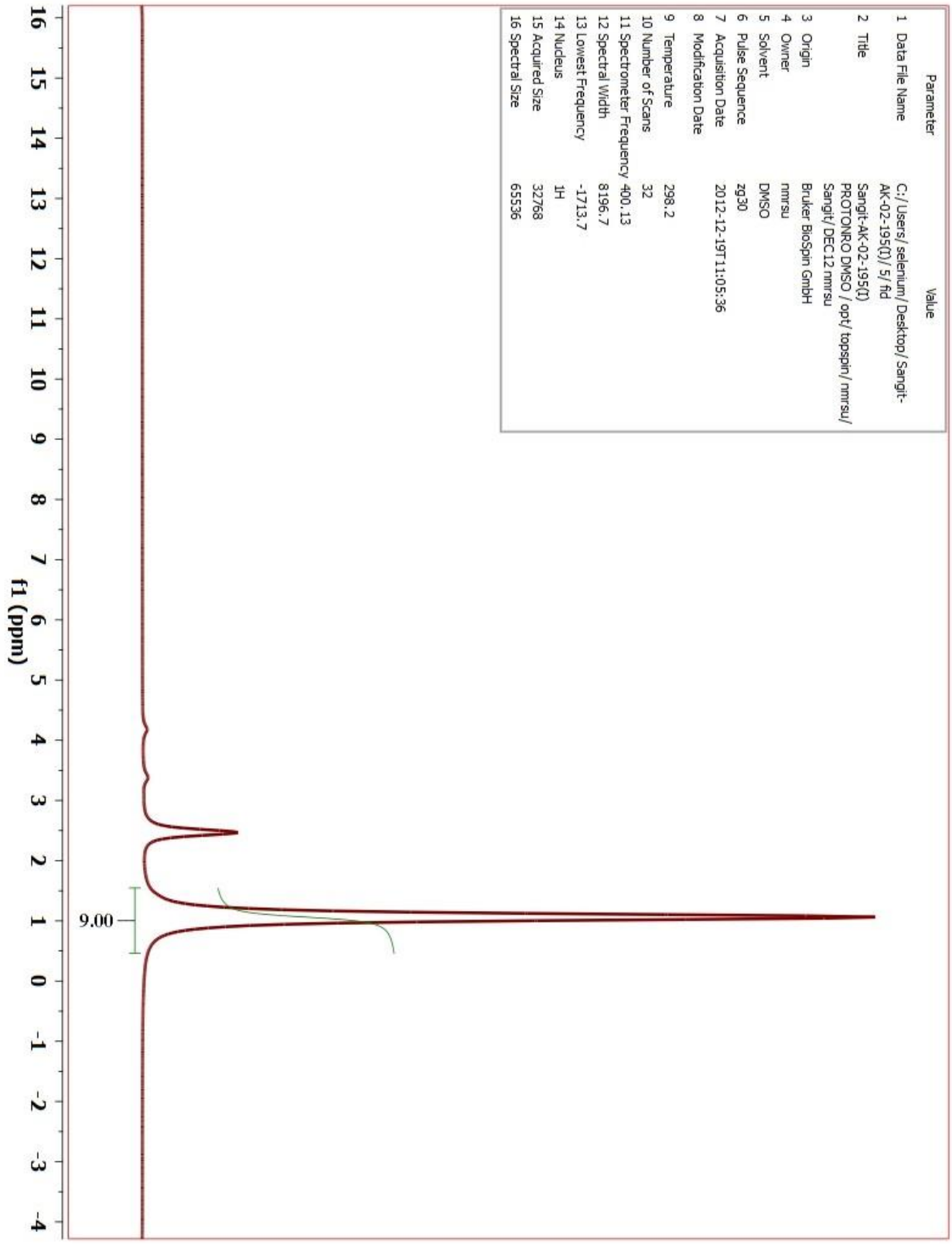


Figure S137 ^{13}C NMR of potassium *tert*-butoxyselenolate

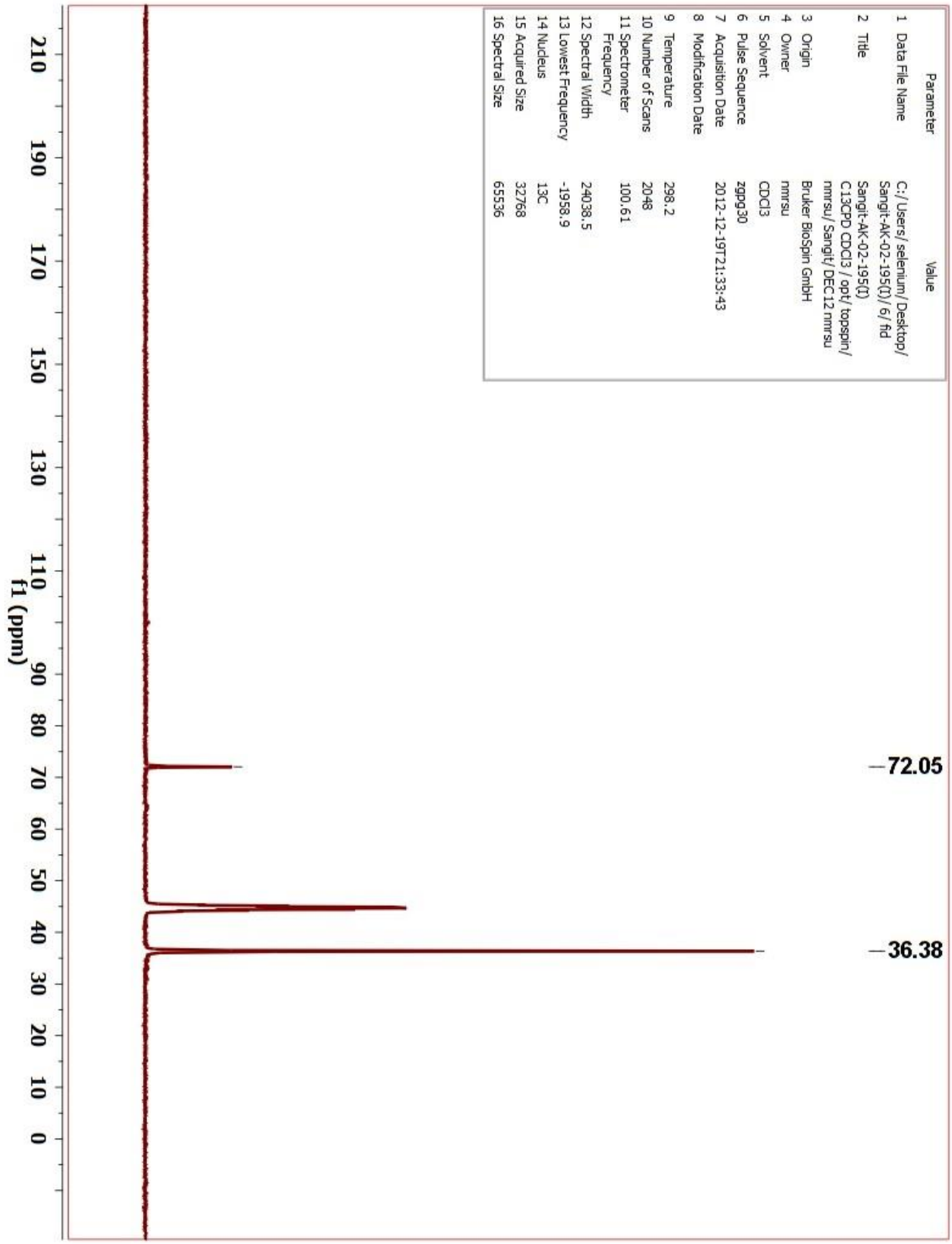


Figure S138 DEPT-135 NMR of potassium *tert*-butoxyselenolate

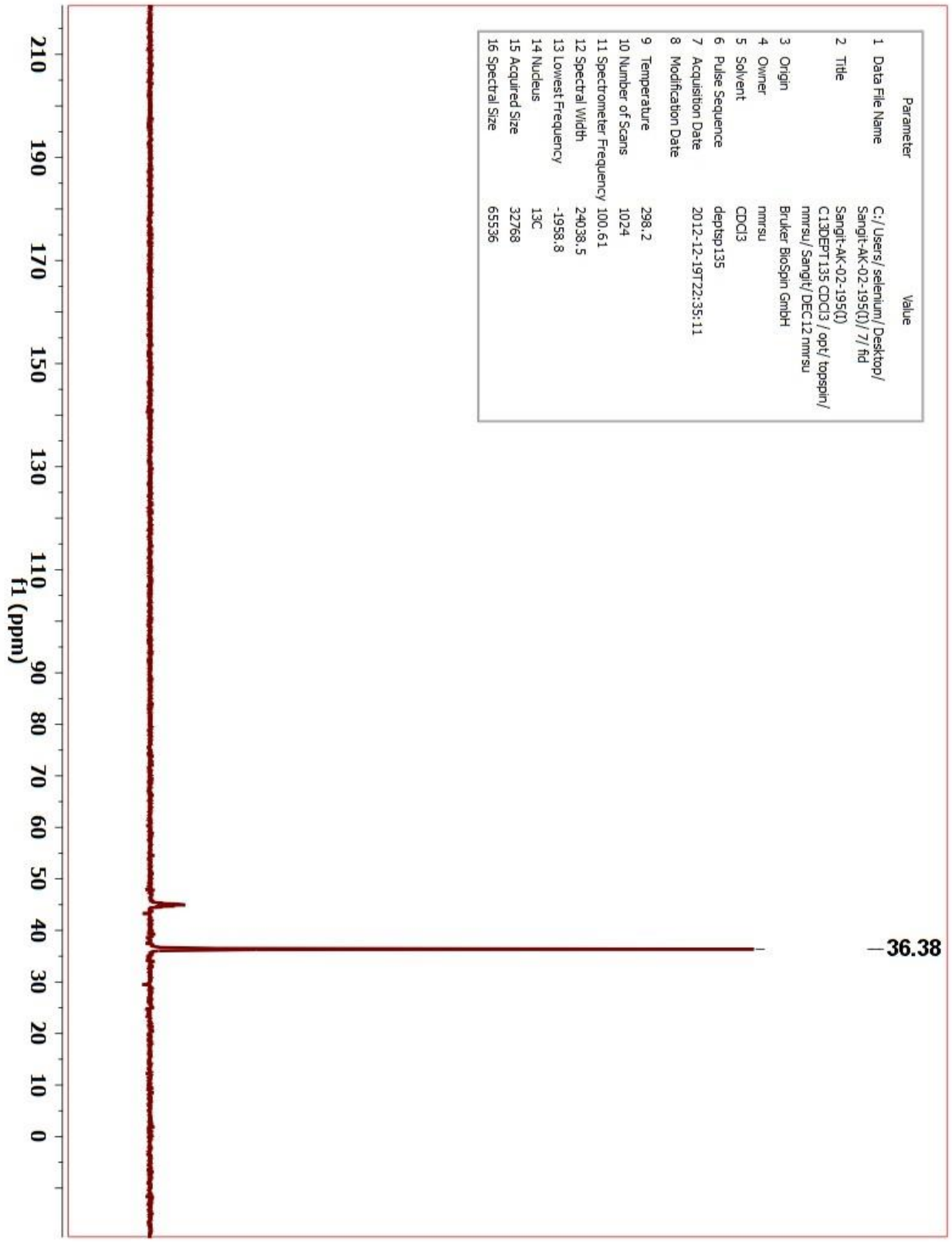
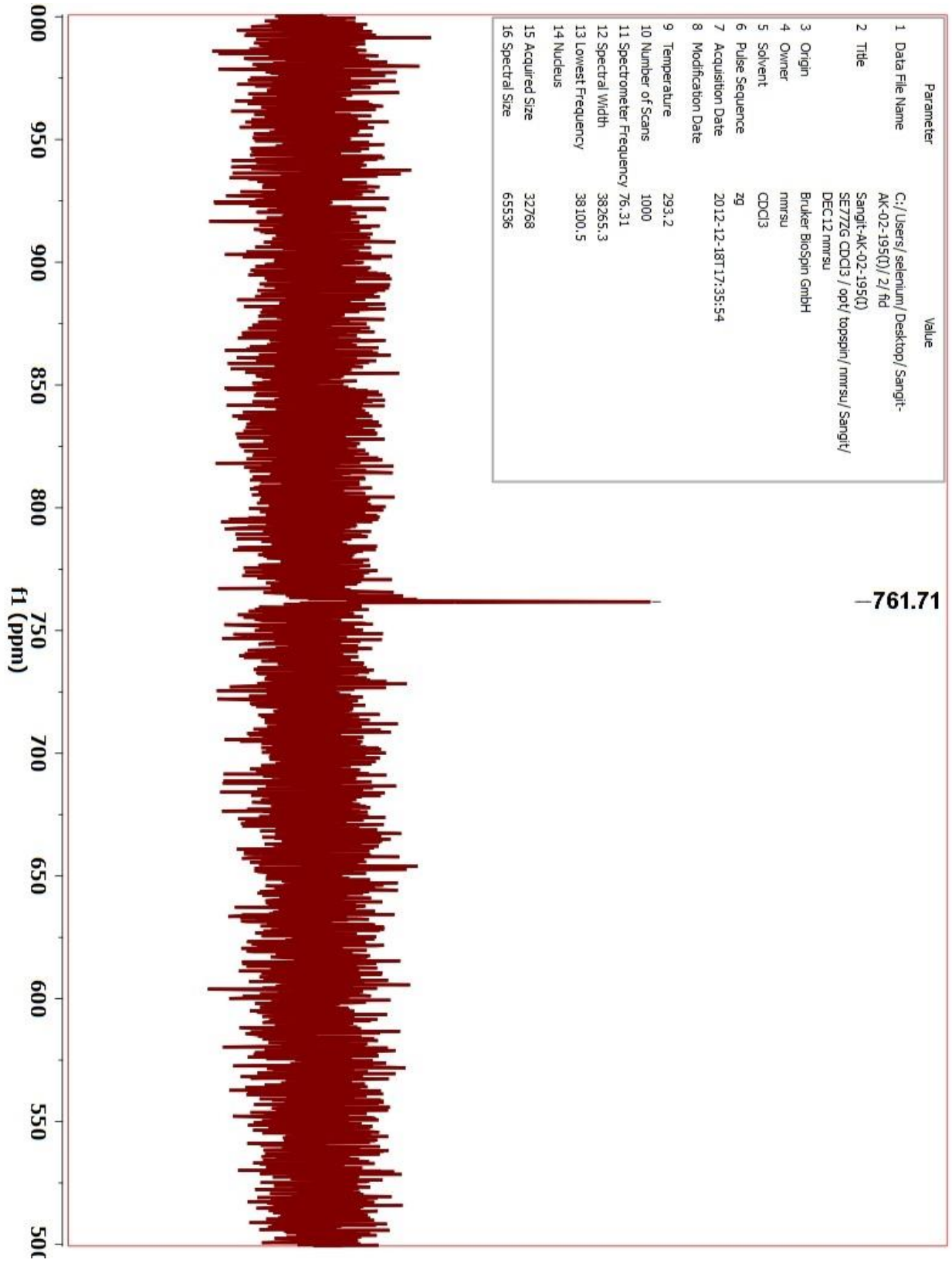


Figure S139 ^{77}Se NMR of potassium *tert*-butoxyselenolate



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