NIS Promoted Carbochalcogenation of Styrenes: Regioselective C-3 Alkylation of Pyrazolo[1,5-*a*]pyrimidines

Abhinay S. Chillal, [†a] Varsha Kumari, [†a] and Umesh A. Kshirsagar*[a]

[a]Department of Chemistry, Indian Institute of Technology Indore, Khandwa Road, Indore 453552, INDIA.

Corresponding author e-mail: uakshirsagar@iiti.ac.in

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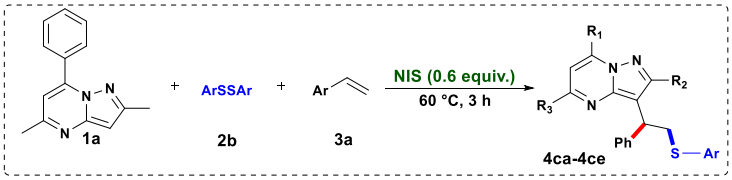
General Information

All chemicals and reagents that were procured from commercial suppliers (TCI, Spectrochem, BLD pharma) are used without further purification. All reactions were conducted in pre-dried screw cap test tubes made of borosilicate glass. Thin layer chromatography was carried out on aluminium sheets pre-coated with Merck silica gel $60F_{254}$ and visualised under UV light (254 nm). The organic solutions were concentrated using the Heidolph rotary evaporator under reduced pressure. Product isolation was accomplished through column chromatography on silica gel with a mesh size of 100-200 using hexanes and ethyl acetate as eluent. Nuclear magnetic resonance spectra (^{1}H, ^{13}C, ^{19}F) were obtained using a Fourier transform nuclear magnetic resonance spectrometer, including the Bruker Avance 500MHz model. $CDCl_3$ served as the solvent for spectroscopic acquisition, with chemical shifts indicated in δ values (parts per million) relative to tetramethylsilane. High-resolution mass spectrometric analyses (HRMS) were performed using an electrospray ionization time-of-flight mass spectrometer (ESI-TOF-MS), comprising Dionex Ultimate 3000 and YL9100 components. Melting points were measured with an electrothermal apparatus. All the starting materials and substrates were synthesized according to literature reports.[1,3]

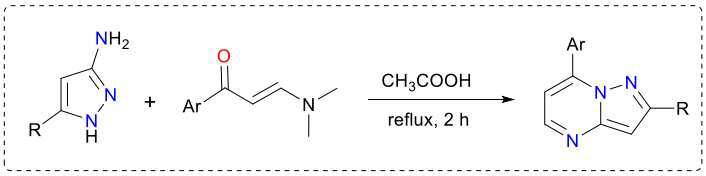
Table S1. Optimization of the Reaction Conditions for carbosulfenylation reaction[a]



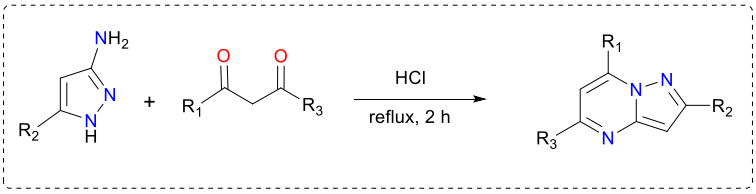
Sr No.	Oxidant (equiv.)	Solvent	Yield[b] (%)
1	NIS (1.0)	ACN	43
2	NIS (1.0)	DMSO	15
3	NIS (1.0)	H_2O	ND
4	NIS (1.0)	PEG-400	Trace
5	NIS (1.0)	-	64
6	**NIS (0.6)**	**-**	**62**
7	NIS (0.5)	-	48
8[c]	NIS (0.6)	-	32
9[d]	NIS (0.6)	-	21
10[e]	NIS (0.6)	-	22
11[f]	NIS (0.6)	-	33
12[g]	NIS (0.6)	-	61
13	-	-	NR

[a]Reaction condition: **1a** (0.2 mmol), **2ba** (0.1 mmol), **3aa** (0.60 mmol), 60 ºC, 3 h; [b]Isolated yield; [c]2.5 equiv. of styrene was used, [d]2.0 equiv. of styrene was used, [e]Reaction at rt, [f]Reaction at 40 ºC, [g]Reaction at 80 ºC.

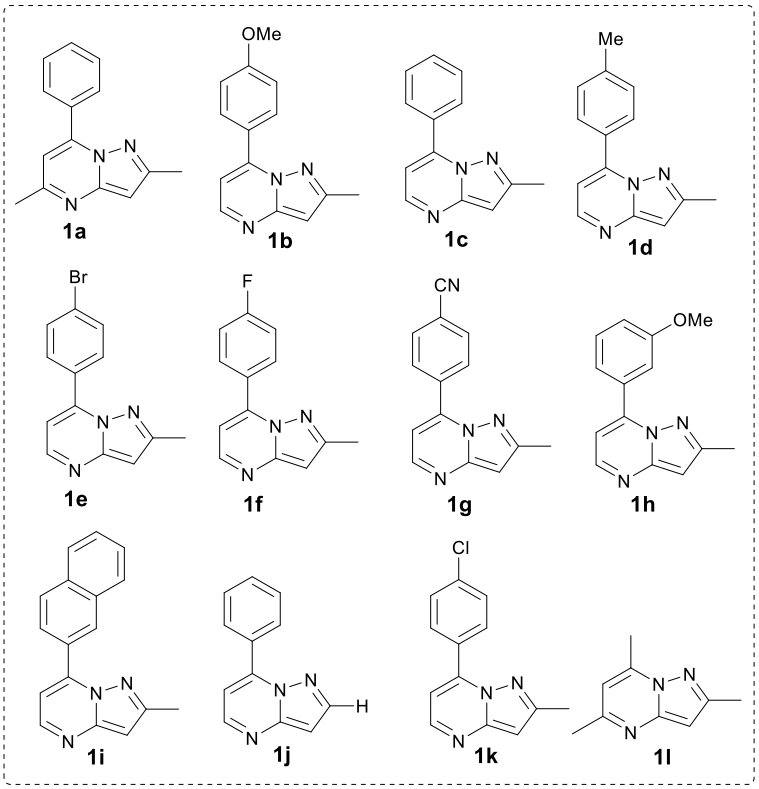
Preparation of starting materials



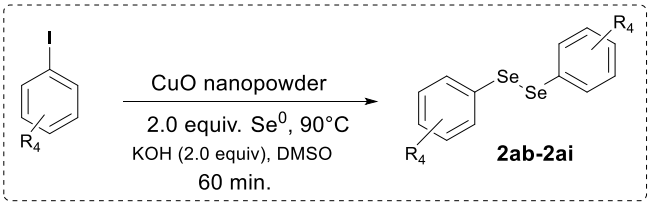
General procedure for the synthesis of substituted pyrazolo[1,5-*a*]pyrimidines:[1a] In an oven-dried round bottom flask (RB), a mixture of substituted amino pyrazoles (1.0 mmol, 1.0 equiv.) and enones (1.0 mmol, 1.0 equiv.) in acetic acid (AcOH) (1.0 mL) was refluxed in an oil bath in stirring condition. The reaction was monitored by TLC analysis. After completing the reaction, the mixture was subjected to extraction using DCM and water. The organic layer was evaporated to obtain the crude pyrazolo[1,5-*a*]pyrimidine derivatives which were purified by column chromatography using 100-200 mesh silica gel and a gradient elution of ethyl acetate-hexane (1:9 to 1:4). Product conformation was done through ^{1}H and ^{13}C NMR spectroscopic analysis.



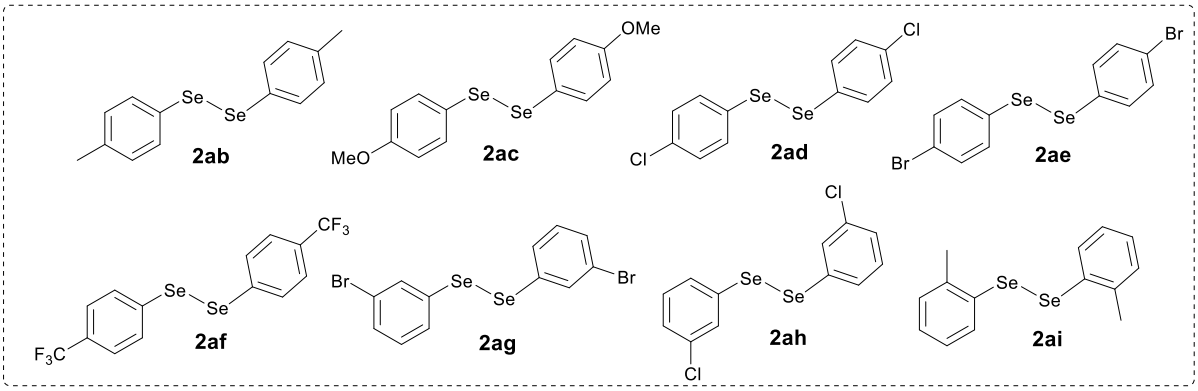
General procedure for the synthesis of substituted pyrazolo[1,5-*a*]pyrimidines:[1b] In an oven-dried round bottom flask(RB), substituted amino pyrazoles (1.0 mmol, 1.0 equiv.) and diketones (1.0 mmol, 1.0 equiv.) were taken. The reaction mixture was refluxed with vigorous stirring in an oil bath after adding 1.0 mL of HCl. The reaction progress was effectively monitored through TLC analysis. Upon completion of the reaction, the mixture was extracted with DCM and water. The organic layer was evaporated to obtain the crude pyrazolo[1,5-*a*]pyrimidine derivatives. Product conformation was done through ^{1}H and ^{13}C NMR spectroscopic analysis.



Products **1a-1l** were already synthesized by us in our previous work and the same products were used as it is for this work.[2]

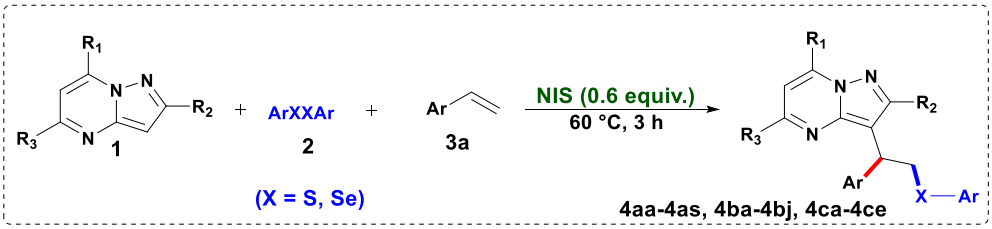


General procedure for synthesis of substituted diselenides:[3] Under nitrogen atmosphere a solution containing selenium metal (Se^0) (2.0 mmol), copper oxide (CuO) nanoparticles (10.0 mol%) and halides (1.0 mmol) in dry DMSO (2.0 mL) was stirred. Potassium hydroxide (KOH) (2 equivalents) were added. The reaction mixture was heated in an oil bath, and the progress was monitored using TLC. After the reaction was completed, the mixture was cooled and then purified by column chromatography to isolate the desired diselenides. The identity of the products was confirmed through ^1H and ^{13}C NMR spectroscopic analysis.



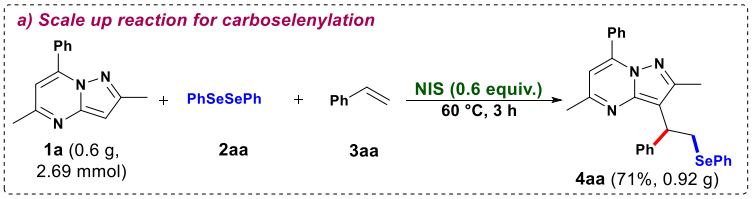
We already synthesized products **2ab**-**2ai** in our previous work[2] and the same products were used as it is for this work.

General experimental procedure for the preparation of C3 alkylated pyrazolo[1,5-*a*]pyrimidine derivatives:



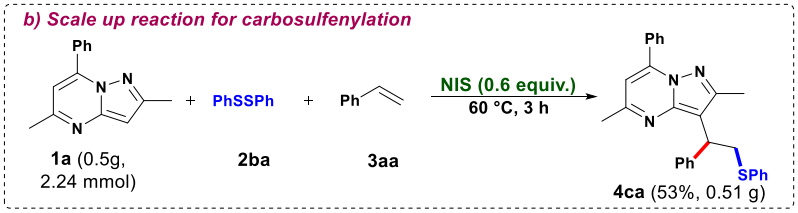
In an oven-dried reaction vessel, substituted pyrazolo[1,5-*a*]pyrimidines **1** (0.2 mmol, 1 equiv.), diorganyl dichalcogenides **2** (0.1mmol, 0.5 equiv.), substituted styrene **3a** (2.5-3.0 equiv.) and NIS (0.6 equiv.) were taken and stirred in an oil bath at 60 °C for 3 hours. Reaction progress was monitored via TLC analysis. After completion, the crude product was purified by silica gel column chromatography (100-200 mesh) to give the desired product. Product confirmation was done using ^{1}H and ^{13}C NMR and HRMS analysis.

Experimental procedure for the scale-up synthesis of 2,5-dimethyl-7-phenyl-3-(1-phenyl-2-(phenylselanyl)ethyl)pyrazolo[1,5-*a*]pyrimidine (4aa):



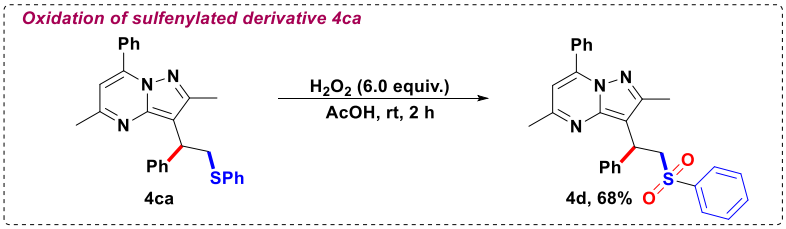
2,5-Dimethyl-7-phenylpyrazolo[1,5-*a*]pyrimidine **1a** (0.6 g, 2.69 mmol), diphenyl diselenide **2aa** (1.34 mmol, 0.5 equiv.), styrene **3aa** (6.72 mmol, 2.5 equiv.) and NIS (0.6 equiv.) were taken and stirred in an oil bath at 60 °C for 3 hours. Reaction progress was monitored via TLC analysis. After completion, the crude product was purified by silica gel column chromatography (100-200 mesh) to give the desired product **4aa** in 71% yield. Product confirmation was done using ^{1}H and ^{13}C NMR and HRMS analysis.

Experimental procedure for the scale-up synthesis of 2,5-Dimethyl-7-phenyl-3-(1-phenyl-2-(phenylthio)ethyl)pyrazolo[1,5-*a*]pyrimidine (4ca):



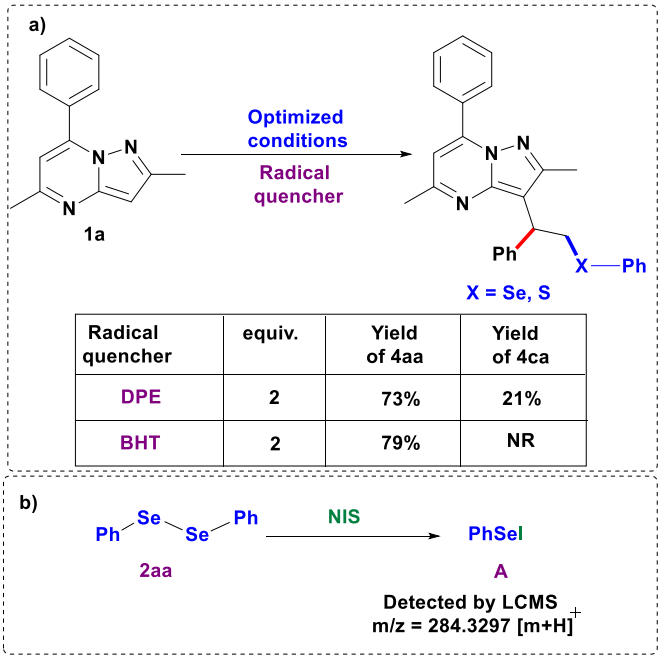
2,5-Dimethyl-7-phenylpyrazolo[1,5-*a*]pyrimidine **1a** (0.5 g, 2.24 mmol), diphenyl disulfide **2ba** (1.12 mmol, 0.5 equiv.), styrene **3aa** (6.72 mmol, 3.0 equiv.) and NIS (0.6 equiv.) were taken in a round bottom flask and stirred in an oil bath at 60 °C for 3 hours. Reaction progress was monitored via TLC analysis. After completion, the crude product was purified by silica gel column chromatography (100-200 mesh) to give the desired product **4ca** in 53% yield. Product confirmation was done using ^{1}H and ^{13}C NMR and HRMS analysis.

Experimental procedure for the oxidation of sulfenylated derivative 4ca:



2,5-dimethyl-7-phenyl-3-(1-phenyl-2-(phenylthio)ethyl)pyrazolo[1,5-*a*]pyrimidine **4ca** (40.0 mg, 1.0 equiv.), 30% H_2O_2 (6.0 equiv.), glacial acetic acid (100 µL) were taken in a 10mL round bottom flask equipped with a magnetic stir bar. The reaction was stirred at room temperature for the duration of 2 hours and the reaction progress was checked using TLC. After completion, reaction mixture was neutralised using $NaHCO_3$ solution and extracted with ethyl acetate (3 X 5mL). Combined organic layers were dried using Na_2SO_4, and concentrated under vacuum. Crude product was purified by silica gel column chromatography (100-200 mesh) to give desired product **4d** in 68% yield.

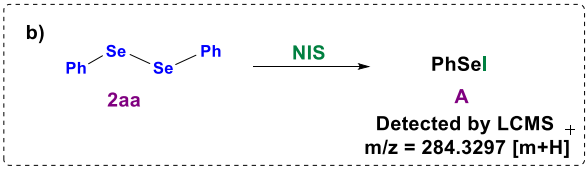
Procedure for control Experiments:



Radical quencher	equiv.	Yield of 4aa	Yield of 4ca
DPE	2	73%	21%
BHT	2	79%	NR

Scheme S5. Control experiments and detection of intermediates

Control experiments for C3 alkylation of pyrazolo[1,5-a]pyrimidines: In an oven-dried reaction vessel, substituted pyrazolo[1,5-*a*]pyrimidines **1aa** (0.2mmol, 1.0 equiv.), diphenyl dichacogenides **2** (0.1mmol, 0.5 equiv.), styrene **3aa** (0.22 mmol, 2.5-3 equiv.), NIS (0.6 equiv.) and radical scavengers (DPE/ BHT, 2.0 equiv.) were taken and stirred in an oil bath at 60 °C for 3 hours. Reaction progress was monitored via TLC analysis. After completion, the crude product was purified by silica gel column chromatography to give the desired product. ^{1}H and ^{13}C NMR did product confirmation.



Control experiment for the detection of intermediates involved in selenylation reaction: An oven-dried screw-capped test tube was taken with a magnetic stir bar. Diphenyl diselenide (**2aa**) (0.5 equiv., 0.1 mmol), NIS (0.6 equiv.) and ACN (1.5 mL) were added to the test tube. The reaction mixture was stirred at 60 °C for 3 hours. After completion of the reaction, 100µL aliquote of the reaction mixture was taken and diluted with 1.5 mL of MeOH and immediately analyzed using LCMS analysis.

Electron Paramagnetic Resonance Spectroscopy (EPR) Study:

To check whether the reaction proceeds via a radical pathway or not , Electron paramagnetic resonance (EPR) spectra were recorded on a Bruker Biospin GmbH spectrometer at 120K temperature, and the spectra were measured at a Microwave frequency of 9.4 GHz at the X-band. The sample required for EPR analysis was prepared in MeCN solvent.

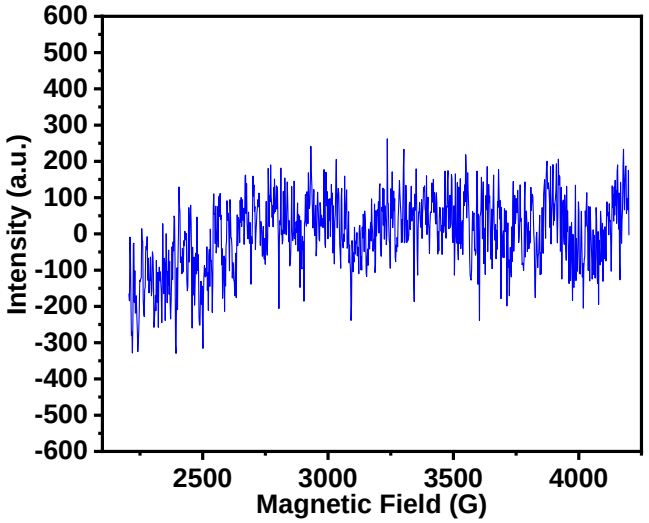


Figure S1. EPR spectrum for carboselenylation reaction mixture

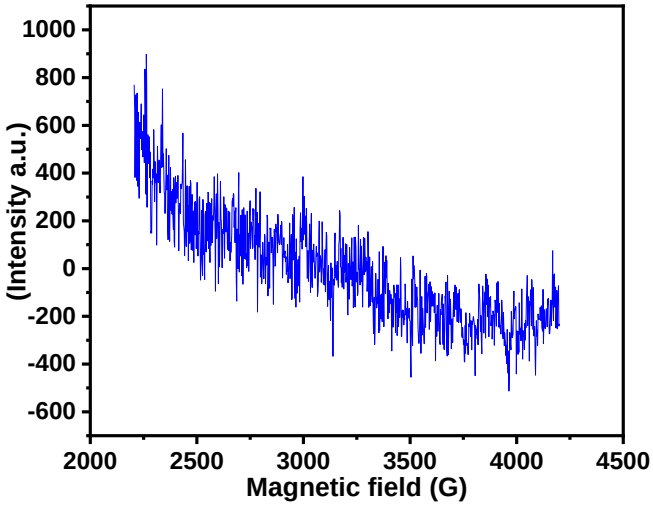
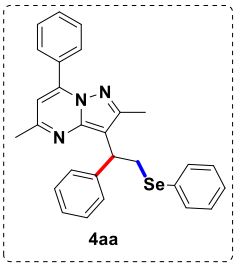


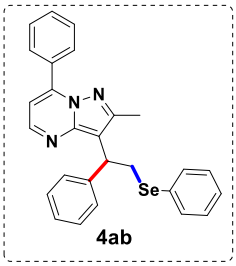
Figure S2. EPR spectrum for carbosulfenylation reaction mixture

Characterization data of compounds (4aa-4as, 4ba-4bj, 4ca-4ce, 4d):



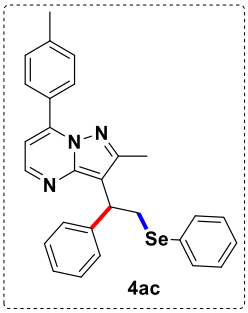
4aa

2,5-Dimethyl-7-phenyl-3-(1-phenyl-2-(phenylselanyl)ethyl)pyrazolo[1,5-*a*]pyrimidine(4aa): Yellow oil; 88% (85 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.91 (q, *J* = 3.7 Hz, 2H), 7.45 (s, 5H), 7.41 – 7.36 (m, 2H), 7.22 (d, *J* = 7.9 Hz, 2H), 7.11 (s, 4H), 6.52 (d, *J* = 3.8 Hz, 1H), 4.37 (d, *J* = 4.3 Hz, 1H), 4.36 – 4.29 (m, 1H), 3.68 (dd, *J* = 11.1, 4.7 Hz, 1H), 2.53 (s, 3H), 2.27 (s, 3H); **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 157.2, 153.1, 147.5, 145.1, 144.8, 133.1, 131.6, 130.7, 130.6, 129.2, 128.7, 128.6, 128.5, 127.8, 126.7, 126.5, 107.9, 107.5, 43.5, 33.1, 25.0, 13.4; **HRMS** (ESI, *m/z*): Calculated for $C_{28}H_{26}N_3Se$ $[M+H]^+$: 484.1288, found 484.1283.



4ab

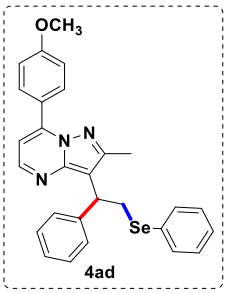
2-Methyl-7-phenyl-3-(1-phenyl-2-(phenylselanyl)ethyl)pyrazolo[1,5-*a*]pyrimidine (4ab): Yellow oil; 87% (81.7 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.32 (d, *J* = 4.4 Hz, 1H), 7.94 (td, *J* = 4.6, 4.1, 2.2 Hz, 2H), 7.47 – 7.41 (m, 5H), 7.40 – 7.34 (m, 2H), 7.23 – 7.19 (m, 2H), 7.14 – 7.07 (m, 4H), 6.67 – 6.61 (m, 1H), 4.41 (dd, *J* = 10.4, 5.6 Hz, 1H), 4.33 – 4.27 (m, 1H), 3.69 (dd, *J* = 11.8, 5.6 Hz, 1H), 2.31 (s, 3H); **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 153.4, 147.7, 145.8, 144.5, 133.0, 131.4, 130.9, 130.4, 129.3, 128.8, 128.7, 128.6, 127.7, 126.7, 126.6, 109.1, 106.5, 43.4, 33.1, 13.4; **HRMS** (ESI, *m/z*): Calculated for $C_{27}H_{24}N_3Se$ $[M+H]^+$: 470.1132, found 470.1132.



4ac

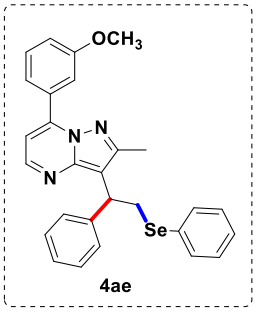
2-Methyl-3-(1-phenyl-2-(phenylselanyl)ethyl)-7-(p-tolyl)pyrazolo[1,5-*a*]pyrimidine (4ac): Orange oil; 73% (72 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.41 (d, *J* = 4.3 Hz, 1H), 7.95 (d, *J* = 8.2 Hz, 2H), 7.51 (d, *J* = 7.2 Hz, 2H), 7.47 – 7.43 (m, 2H), 7.37 (d, *J* = 8.2 Hz, 2H), 7.30 (t, *J* = 7.6 Hz, 2H), 7.23 – 7.16 (m, 4H), 6.74 (d, *J* = 4.3 Hz, 1H), 4.49 (dd, *J* = 10.4, 5.6 Hz, 1H), 4.40 – 4.34 (m, 1H), 3.77 (dd, *J* = 11.9, 5.6 Hz, 1H), 2.46 (s, 3H), 2.40 (s, 3H). **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 153.3, 147.8, 147.7, 146.0, 144.6, 141.3, 133.1,

130.5, 129.4, 129.2, 128.8, 128.6, 128.5, 127.8, 126.7, 126.6, 109.0, 106.2, 43.5, 33.1, 21.6, 13.4; **HRMS** (ESI, *m/z*): Calculated for $C_{28}H_{26}N_3Se$ $[M+H]^+$: 484.1288, found 484.1290.



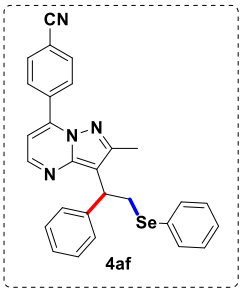
4ad

7-(4-Methoxyphenyl)-2-methyl-3-(1-phenyl-2-(phenylselanyl)ethyl)pyrazolo[1,5-*a*]pyrimidine(4ad): Brown oil; 82% (82 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.39 (d, *J* = 4.3 Hz, 1H), 8.06 (d, *J* = 8.9 Hz, 2H), 7.50 (d, *J* = 9.2 Hz, 2H), 7.44 (dd, *J* = 6.6, 3.1 Hz, 2H), 7.29 (t, *J* = 7.6 Hz, 2H), 7.23 – 7.14 (m, 4H), 7.06 (d, *J* = 9.0 Hz, 2H), 6.72 (d, *J* = 4.3 Hz, 1H), 4.48 (dd, *J* = 10.5, 5.6 Hz, 1H), 4.41 – 4.30 (m, 1H), 3.89 (s, 3H), 3.76 (dd, *J* = 11.9, 5.6 Hz, 1H), 2.39 (s, 3H). **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 161.7, 153.22, 147.8, 147.7, 145.6, 144.6, 133.1, 131.0, 130.5, 128.8, 128.6, 127.8, 126.7, 126.6, 123.6, 114.1, 108.9, 105.8, 55.5, 43.4, 33.1, 13.4; **HRMS** (ESI, *m/z*): Calculated for $C_{28}H_{26}N_3OSe$ $[M+H]^+$: 500.1237, found 500.1240.



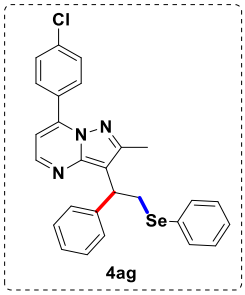
4ae

7-(3-Methoxyphenyl)-2-methyl-3-(1-phenyl-2-(phenylselanyl)ethyl)pyrazolo[1,5-*a*]pyrimidine(4ae): Yellow oil; 87% (86.8 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.38 (d, *J* = 4.3 Hz, 1H), 7.63 – 7.60 (m, 1H), 7.55 – 7.47 (m, 3H), 7.45 – 7.40 (m, 3H), 7.28 (d, *J* = 7.5 Hz, 2H), 7.20 – 7.14 (m, 4H), 7.06 (dd, *J* = 8.2, 3.0 Hz, 1H), 6.71 (d, *J* = 4.3 Hz, 1H), 4.48 (dd, *J* = 10.5, 5.6 Hz, 1H), 4.40 – 4.32 (m, 1H), 3.84 (s, 3H), 3.75 (dd, *J* = 11.9, 5.6 Hz, 1H), 2.38 (s, 3H); **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 159.5, 153.3, 147.7, 147.6, 145.6, 144.5, 133.0, 132.5, 130.3, 129.7, 128.7, 128.5, 127.7, 126.7, 126.6, 121.7, 116.6, 114.8, 109.1, 106.5, 55.4, 43.4, 33.0, 13.4; **HRMS** (ESI, *m/z*): Calculated for $C_{28}H_{26}N_3OSe$ $[M+H]^+$: 500.1237, found 500.1238.



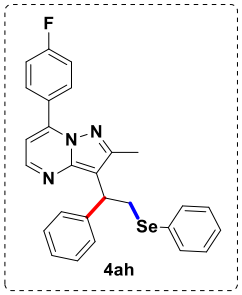
4af

4-(2-Methyl-3-(1-phenyl-2-(phenylselanyl)ethyl)pyrazolo[1,5-*a*]pyrimidin-7-yl)benzonitrile(4af): Orange oil; 78% (77.1 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.42 (d, *J* = 4.3 Hz, 1H), 8.11 (d, *J* = 8.5 Hz, 2H), 7.80 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 7.9 Hz, 2H), 7.38 (dd, *J* = 6.5, 3.1 Hz, 2H), 7.26 – 7.21 (m, 2H), 7.20 – 7.08 (m, 4H), 6.72 (d, *J* = 4.3 Hz, 1H), 4.42 (dd, *J* = 10.6, 5.4 Hz, 1H), 4.36 – 4.25 (m, 1H), 3.69 (dd, *J* = 11.8, 5.4 Hz, 1H), 2.33 (s, 3H); **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 153.9, 147.6, 144.3, 143.6, 135.7, 133.1, 132.5, 130.2, 130.0, 128.9, 128.7, 127.7, 126.9, 126.8, 118.3, 114.4, 109.8, 106.9, 43.4, 33.1, 13.3; **HRMS** (ESI, *m/z*): Calculated for $C_{28}H_{23}N_4Se$ $[M+H]^+$: 495.1084, found 495.1083.



4ag

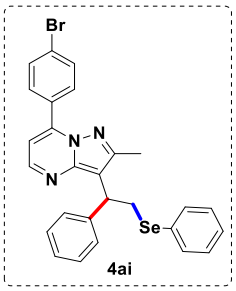
7-(4-Chlorophenyl)-2-methyl-3-(1-phenyl-2-(phenylselanyl)ethyl)pyrazolo[1,5-*a*]pyrimidine(4ag): Yellow jelly; 91% (91.5 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.33 (d, *J* = 4.4 Hz, 1H), 7.90 (d, *J* = 8.5 Hz, 2H), 7.43 (t, *J* = 7.6 Hz, 4H), 7.39 – 7.31 (m, 2H), 7.24 – 7.18 (m, 2H), 7.17 – 7.02 (m, 4H), 6.62 (d, *J* = 4.6 Hz, 1H), 4.45 – 4.36 (m, 1H), 4.34 – 4.23 (m, 1H), 3.74 – 3.58 (m, 1H), 2.31 (d, *J* = 2.6 Hz, 3H). **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 153.5, 147.7, 147.6, 144.6, 144.5, 137.0, 133.0, 130.6, 130.4, 129.7, 129.0, 128.8, 128.6, 127.7, 126.7, 126.6, 109.3, 106.3, 43.4, 33.0, 13.3; **HRMS** (ESI, *m/z*): Calculated for $C_{27}H_{23}ClN_3Se$ $[M+H]^+$: 504.0739, found 504.0739.



4ah

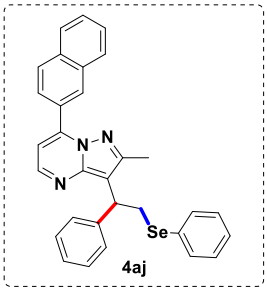
7-(4-Fluorophenyl)-2-methyl-3-(1-phenyl-2-(phenylselanyl)ethyl)pyrazolo[1,5-*a*]pyrimidine(4ah): Yellow gummy mass; 91% (88.6 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.33 (d, *J* = 4.3 Hz, 1H), 7.97 (dd, *J* = 8.7, 5.5 Hz, 2H), 7.42 (d, *J* = 7.8 Hz, 2H), 7.36 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.21 (t, *J* = 7.6 Hz, 2H), 7.18 – 7.08 (m, 6H), 6.62 (d, *J* = 4.4 Hz, 1H), 4.41

(dd, *J* = 10.5, 5.5 Hz, 1H), 4.29 (t, *J* = 11.1 Hz, 1H), 3.68 (dd, *J* = 11.8, 5.6 Hz, 1H), 2.31 (s, 3H). **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 165.1, 163.1, 153.5, 147.7, 147.6, 144.7, 144.5, 133.0, 131.5, 131.4, 130.4, 128.8, 128.6, 127.7, 127.4, 127.3 126.7, 126.6, 115.9, 115.8, 109.2, 106.3, 43.4, 33.0, 13.3; **HRMS** (ESI, *m/z*): Calculated for $C_{27}H_{23}FN_3Se$ $[M+H]^+$: 488.1037, found 488.1037.



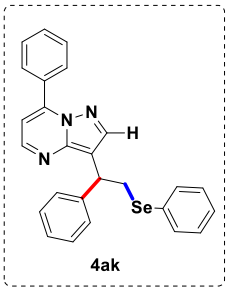
4ai

7-(4-Bromophenyl)-2-methyl-3-(1-phenyl-2-(phenylselanyl)ethyl)pyrazolo[1,5-*a*]pyrimidine(4ai):Yellow oil; 87% (95.2 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.38 (d, *J* = 4.4 Hz, 1H), 7.91 – 7.84 (m, 2H), 7.68 – 7.61 (m, 2H), 7.46 – 7.41 (m, 2H), 7.41 – 7.36 (m, 2H), 7.25 (s, 1H), 7.24 – 7.21 (m, 1H), 7.18 – 7.10 (m, 4H), 6.69 (d, *J* = 4.3 Hz, 1H), 4.43 (dd, *J* = 10.5, 5.6 Hz, 1H), 4.36 – 4.26 (m, 1H), 3.70 (dd, *J* = 11.9, 5.5 Hz, 1H), 2.33 (s, 3H); **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 153.6, 147.7, 147.6, 144.8, 144.5, 133.1, 132.0, 130.9, 130.4, 130.2, 128.8, 128.6, 127.8, 126.8, 126.7, 125.5, 109.4, 106.3, 43.5, 33.0, 13.4; **HRMS** (ESI, *m/z*): Calculated for $C_{27}H_{23}BrN_3Se$ $[M+H]^+$: 548.0234, found 548.0231.



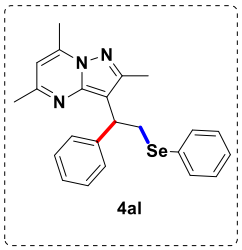
4aj

2-Methyl-7-(naphthalen-2-yl)-3-(1-phenyl-2-(phenylselanyl)ethyl)pyrazolo[1,5-*a*]pyrimidine(4aj): Orange oil; 71% (73.7 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.49 (s, 1H), 8.37 (d, *J* = 4.1 Hz, 1H), 7.98 (d, *J* = 8.5 Hz, 1H), 7.89 (t, *J* = 9.5 Hz, 2H), 7.83 (d, *J* = 9.2 Hz, 1H), 7.48 (dd, *J* = 15.2, 7.7 Hz, 4H), 7.43 – 7.37 (m, 2H), 7.24 (d, *J* = 7.8 Hz, 2H), 7.18 – 7.09 (m, 4H), 6.75 (d, *J* = 4.3 Hz, 1H), 4.46 (dd, *J* = 10.5, 5.6 Hz, 1H), 4.34 (t, *J* = 11.1 Hz, 1H), 3.73 (dd, *J* = 11.9, 5.6 Hz, 1H), 2.35 (s, 3H); **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 153.4, 147.7, 145.9, 144.5, 134.4, 133.0, 132.9, 130.4, 129.8, 129.0, 128.8, 128.7, 128.6, 128.2, 127.8, 127.7, 127.6, 126.7, 126.6, 126.5, 125.7, 109.2, 106.8, 43.4, 33.0, 13.4; **HRMS** (ESI, *m/z*): Calculated for $C_{31}H_{26}N_3Se$ $[M+H]^+$: 520.1289, found 520.1288.



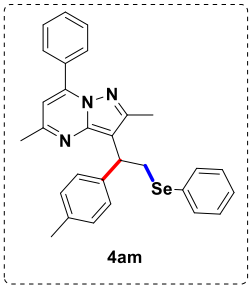
4ak

7-phenyl-3-(1-phenyl-2-(phenylselanyl)ethyl)pyrazolo[1,5-*a*]pyrimidine(4ak): Yellow oil; 83% (75.5 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.38 (d, *J* = 4.3 Hz, 1H), 8.02 (s, 1H), 7.92 (dd, *J* = 6.7, 3.1 Hz, 2H), 7.50 – 7.45 (m, 3H), 7.40 (dd, *J* = 7.2, 2.4 Hz, 4H), 7.24 (d, *J* = 7.9 Hz, 2H), 7.14 (ddd, *J* = 16.2, 5.9, 1.9 Hz, 4H), 6.73 (d, *J* = 4.3 Hz, 1H), 4.73 – 4.62 (m, 1H), 3.97 (dd, *J* = 12.0, 9.1 Hz, 1H), 3.61 (dd, *J* = 12.1, 6.9 Hz, 1H); **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 148.1, 146.8, 146.5, 144.0, 143.5, 132.8, 131.0, 130.9, 130.6, 129.2, 128.9, 128.7, 128.6, 127.7, 126.7, 112.5, 107.3, 42.6, 34.0; **HRMS** (ESI, *m/z*): Calculated for $C_{26}H_{22}N_3Se$ $[M+H]^+$: 456.0975, found 456.0989.



4al

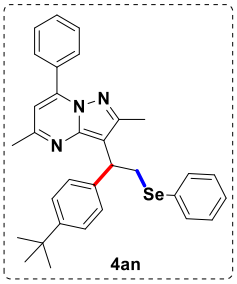
2,5,7-trimethyl-3-(1-phenyl-2-(phenylselanyl)ethyl)pyrazolo[1,5-*a*]pyrimidine(4al):Brown oil; 79% (66.5 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.45 – 7.39 (m, 4H), 7.26 – 7.22 (m, 2H), 7.17 (q, *J* = 3.6 Hz, 4H), 6.42 (s, 1H), 4.42 – 4.31 (m, 2H), 3.70 (dd, *J* = 11.3, 5.2 Hz, 1H), 2.64 (s, 3H), 2.54 (s, 3H), 2.33 (s, 3H); **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 157.3, 152.8, 146.5, 144.7, 144.4, 133.0, 130.6, 128.8, 128.6, 127.8, 126.8, 126.6, 108.0, 107.7, 43.2, 33.4, 24.9, 17.2, 13.2; **HRMS** (ESI, *m/z*): Calculated for $C_{23}H_{24}N_3Se$ $[M+H]^+$: 422.1131, found 422.1135.



4am

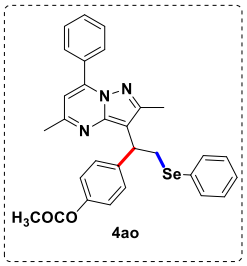
2,5-Dimethyl-7-phenyl-3-(2-(phenylselanyl)-1-(p-tolyl)ethyl)pyrazolo[1,5-*a*]pyrimidine(4am): Yellow jelly; 85% (84.5 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.95 – 7.89 (m, 2H), 7.48 – 7.44 (m, 3H), 7.41 – 7.36 (m, 2H), 7.34 (d, *J* = 8.1 Hz, 2H), 7.14 – 7.08 (m, 3H), 7.04 (d, *J* = 8.1 Hz, 2H), 6.52 (s, 1H), 4.37 (dd, *J* = 10.2, 5.3 Hz, 1H), 4.34 – 4.27 (m, 1H), 3.69 (dd, *J* = 11.4, 5.5 Hz, 1H), 2.54 (s, 3H), 2.28 (s, 3H), 2.24 (s, 3H); **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 157.2, 153.1, 147.4, 145.1, 141.9, 136.0, 133.0, 131.6, 130.7,

129.3, 129.2, 129.1, 128.7, 128.6, 127.7, 126.6, 108.1, 107.4, 43.0, 33.2, 25.0, 21.1, 13.4; **HRMS** (ESI, *m/z*): Calculated for $C_{29}H_{28}N_3Se$ $[M+H]^+$: 498.1445, found 498.1452.



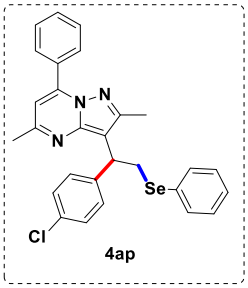
4an

3-(1-(4-(tert-butyl)phenyl)-2-(phenylselanyl)ethyl)-2,5-dimethyl-7-phenylpyrazolo[1,5-*a*]pyrimidine(4an): Orange oil; 82% (88.4 mg)**;** ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 8.00 (dd, *J* = 6.6, 3.1 Hz, 2H), 7.57 – 7.52 (m, 3H), 7.49 – 7.42 (m, 4H), 7.33 (d, *J* = 8.4 Hz, 2H), 7.22 – 7.15 (m, 3H), 6.61 (s, 1H), 4.44 (d, *J* = 7.9 Hz, 2H), 3.77 – 3.67 (m, 1H), 2.63 (s, 3H), 2.38 (s, 3H), 1.32 (s, 9H); ^{13}**C {**^{1}**H} NMR** (126 MHz, $CDCl_3$) δ 157.1, 153.2, 149.2, 147.4, 145.1, 141.9, 133.1, 131.6, 130.7, 130.6, 129.3, 128.7, 128.6, 127.5, 126.6, 125.4, 108.1, 107.4, 43.1, 34.5, 33.3, 31.5, 25.0, 13.6; **HRMS** (ESI, *m/z*): Calculated for $C_{32}H_{34}N_3Se$ $[M+H]^+$: 540.1915, found 540.1915.



4ao

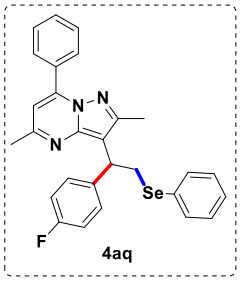
4-(1-(2,5-Dimethyl-7-phenylpyrazolo[1,5-*a*]pyrimidin-3-yl)-2-(phenylselanyl)ethyl)phenyl acetate(4ao): Yellow jelly; 78% (84.4 mg); ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 7.89 – 7.83 (m, 2H), 7.42 – 7.37 (m, 5H), 7.31 (dd, *J* = 6.6, 3.1 Hz, 2H), 7.07 – 7.02 (m, 3H), 6.88 (d, *J* = 8.7 Hz, 2H), 6.48 (s, 1H), 4.33 – 4.23 (m, 2H), 3.59 (dd, *J* = 10.9, 4.5 Hz, 1H), 2.47 (s, 3H), 2.22 (s, 3H), 2.14 (s, 3H); ^{13}**C {**^{1}**H} NMR** (126 MHz, $CDCl_3$) δ 168.5, 156.2, 152.0, 148.1, 146.3, 144.1, 141.3, 132.0, 130.4, 129.6, 129.3, 128.1, 127.7, 127.6, 127.5, 125.6, 120.3, 106.5, 106.4, 41.8, 32.1, 23.9, 20.1, 12.2; **HRMS** (ESI, *m/z*): Calculated for $C_{30}H_{27}N_3O_2SeNa$ $[M+Na]^+$: 564.1163, found 564.1162.



4ap

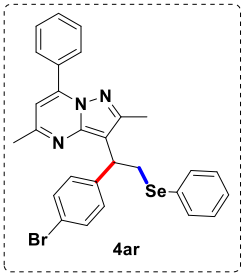
3-(1-(4-Chlorophenyl)-2-(phenylselanyl)ethyl)-2,5-dimethyl-7-phenylpyrazolo[1,5-*a*]pyrimidine(4ap):Yellow oil; 71% (73.4 mg); ^{1}**H NMR** (500 MHz, $CDCl_3$) δ 7.97 (dd, *J* =

6.7, 3.1 Hz, 2H), 7.54 – 7.51 (m, 3H), 7.43 – 7.39 (m, 4H), 7.23 (d, *J* = 8.5 Hz, 2H), 7.19 – 7.15 (m, 3H), 6.61 (s, 1H), 4.42 – 4.36 (m, 1H), 4.31 – 4.25 (m, 1H), 3.71 (dd, *J* = 11.9, 6.0 Hz, 1H), 2.61 (s, 3H), 2.31 (s, 3H); **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 157.5, 153.1, 147.2, 145.5, 143.2, 133.2, 132.3, 131.5, 130.9, 130.4, 129.3, 129.2, 128.8, 128.7, 128.6, 126.9, 107.6, 107.5, 42.9, 33.0, 25.0, 13.4; **HRMS** (ESI, *m/z*): Calculated for $C_{28}H_{25}ClN_3Se$ $[M+H]^+$: 518.0896, found 518.0904.



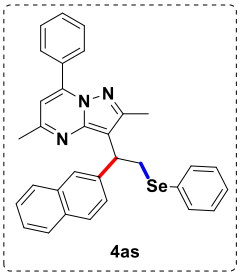
4aq

3-(1-(4-Fluorophenyl)-2-(phenylselanyl)ethyl)-2,5-dimethyl-7-phenylpyrazolo[1,5-*a*]pyrimidine(4aq):Yellow oil; 89% (89.2 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.03 – 7.95 (m, 2H), 7.57 – 7.51 (m, 3H), 7.50 – 7.41 (m, 4H), 7.23 – 7.14 (m, 3H), 7.02 – 6.93 (m, 2H), 6.62 (s, 1H), 4.43 (dd, *J* = 9.9, 6.0 Hz, 1H), 4.31 (dd, *J* = 12.0, 10.0 Hz, 1H), 3.73 (dd, *J* = 11.9, 6.0 Hz, 1H), 2.62 (s, 3H), 2.34 (s, 3H); **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 162.3, 160.4, 157.2, 152.8, 147.1, 145.1, 140.3, 140.3, 132.9, 131.3, 130.5, 130.2, 129.1, 129.0, 128.9, 128.5, 128.4, 126.5, 115.1, 114.9, 107.6, 107.3, 42.5, 33.0, 24.7, 13.1; **HRMS** (ESI, *m/z*): Calculated for $C_{28}H_{25}FN_3Se$ $[M+H]^+$: 502.1194, found 502.1193.



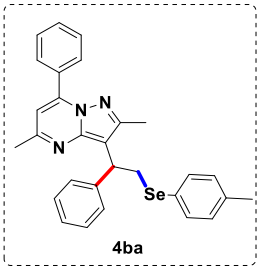
4ar

3-(1-(4-Bromophenyl)-2-(phenylselanyl)ethyl)-2,5-dimethyl-7-phenylpyrazolo[1,5-*a*]pyrimidine(4ar): Brown oil; 68% (76.3 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.98 (dd, *J* = 6.6, 3.1 Hz, 2H), 7.66 – 7.46 (m, 4H), 7.42 (dd, *J* = 6.6, 3.1 Hz, 2H), 7.38 (d, *J* = 1.7 Hz, 3H), 7.20 – 7.15 (m, 3H), 6.62 (s, 1H), 4.39 (dd, *J* = 9.9, 6.0 Hz, 1H), 4.31 – 4.23 (m, 1H), 3.72 (dd, *J* = 12.0, 6.0 Hz, 1H), 2.61 (s, 3H), 2.32 (s, 3H); **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 157.5, 153.1, 147.3, 145.4, 143.7, 133.2, 131.6, 131.5, 130.8, 130.3, 129.7, 129.3, 128.8, 128.7, 126.8, 120.4, 107.6, 107.5, 42.9, 32.9, 25.0, 13.4; **HRMS** (ESI, *m/z*): Calculated for $C_{28}H_{25}BrN_3Se$ $[M+H]^+$: 562.0391, found 562.0380.



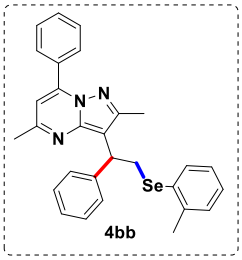
4as

2,5-Dimethyl-3-(1-(naphthalen-2-yl)-2-(phenylselanyl)ethyl)-7-phenylpyrazolo[1,5-*a*]pyrimidine(4as):Brown jelly; 81% (86.4 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.00 (dd, *J* = 6.8, 3.0 Hz, 2H), 7.86 (s, 1H), 7.82 – 7.74 (m, 3H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.57 – 7.50 (m, 3H), 7.50 – 7.39 (m, 4H), 7.23 – 7.14 (m, 3H), 6.63 (s, 1H), 4.70 – 4.55 (m, 1H), 4.44 (t, *J* = 11.1 Hz, 1H), 3.86 (dd, *J* = 12.0, 5.9 Hz, 1H), 2.65 (s, 3H), 2.36 (s, 3H); **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 157.4, 153.4, 147.4, 145.4, 142.1, 133.6, 133.1, 132.4, 131.6, 130.8, 130.7, 129.3, 128.8, 128.7, 128.3, 127.9, 127.7, 126.8, 126.7, 126.0, 125.9, 125.5, 107.9, 107.6, 43.5, 33.0, 25.0, 13.5; **HRMS** (ESI, *m/z*): Calculated for $C_{32}H_{28}N_3Se$ $[M+H]^+$: 534.1445, found 534.1445.



4ba

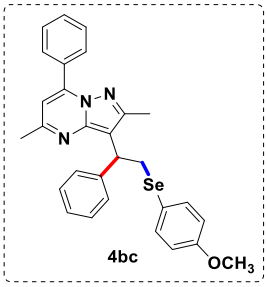
2,5-Dimethyl-7-phenyl-3-(1-phenyl-2-(p-tolylselanyl)ethyl)pyrazolo[1,5-a]pyrimidine(4ba): Yellow jelly; 80% (79.5 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.92 (dd, *J* = 6.8, 3.0 Hz, 2H), 7.50 – 7.39 (m, 5H), 7.28 (s, 2H), 7.21 (t, *J* = 7.6 Hz, 2H), 7.12 (t, *J* = 7.3 Hz, 1H), 6.92 (d, *J* = 8.1 Hz, 2H), 6.53 (s, 1H), 4.38 (dd, *J* = 10.5, 5.4 Hz, 1H), 4.29 (t, *J* = 11.1 Hz, 1H), 3.62 (dd, *J* = 11.7, 5.5 Hz, 1H), 2.54 (s, 3H), 2.28 (s, 3H), 2.22 (s, 3H); **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 157.2, 153.2, 147.4, 145.2, 144.9, 136.6, 133.6, 131.6, 130.7, 129.5, 129.3, 128.6, 128.5, 127.8, 126.7, 126.5, 108.0, 107.4, 43.5, 33.4, 25.0, 21.2, 13.4; **HRMS** (ESI, *m/z*): Calculated for $C_{29}H_{28}N_3Se$ $[M+H]^+$: 498.1445, found 498.1444.



4bb

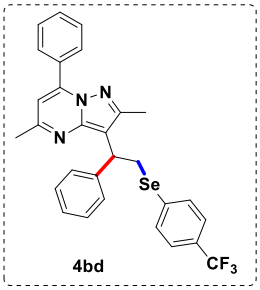
2,5-Dimethyl-7-phenyl-3-(1-phenyl-2-(o-tolylselanyl)ethyl)pyrazolo[1,5-a]pyrimidine(4bb): Yellow jelly; 86% (85.5 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.95 (dd, *J* = 6.8, 2.8 Hz, 2H), 7.54 – 7.45 (m, 5H), 7.40 (d, *J* = 7.8 Hz, 1H), 7.28 – 7.23 (m, 2H), 7.17 (t, *J* = 7.4 Hz, 1H), 7.06 (dd, *J* = 13.4, 7.5 Hz, 2H), 7.03 – 6.96 (m, 1H), 6.58 (s, 1H), 4.43 (dd, *J* = 10.4, 5.5 Hz, 1H), 4.35 (t, *J* = 10.9 Hz, 1H), 3.71 – 3.60 (m, 1H), 2.58 (s, 3H), 2.31 (d, *J* =

2.0 Hz, 6H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 157.3, 153.2, 147.4, 145.2, 144.9, 139.9, 132.6, 131.6, 131.6, 130.8, 129.7, 129.3, 128.7, 128.6, 127.9, 126.7, 126.6, 126.2, 108.1, 107.5, 43.3, 32.0, 24.99, 22.58, 13.44; **HRMS** (ESI, *m/z*): Calculated for $C_{29}H_{28}N_3Se$ $[M+H]^+$: 498.1445, found 498.1441.



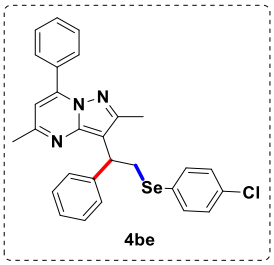
4bc

3-(2-((4-Methoxyphenyl)selanyl)-1-phenylethyl)-2,5-dimethyl-7-phenylpyrazolo[1,5-*a*]pyrimidine(4bc): Yellow oil; 87% (89.3 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.99 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.58 – 7.51 (m, 3H), 7.48 (d, *J* = 7.5 Hz, 2H), 7.35 (d, *J* = 8.7 Hz, 2H), 7.30 – 7.25 (m, 2H), 7.18 (t, *J* = 7.4 Hz, 1H), 6.70 (d, *J* = 8.7 Hz, 2H), 6.59 (s, 1H), 4.42 (dd, *J* = 10.7, 5.0 Hz, 1H), 4.34 (t, *J* = 11.1 Hz, 1H), 3.75 (s, 3H), 3.61 (dd, *J* = 11.7, 5.1 Hz, 1H), 2.60 (s, 3H), 2.37 (s, 3H); **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 159.1, 157.2, 153.2, 147.9, 145.1, 145.0, 135.8, 131.6, 130.7, 129.3, 128.6, 128.5, 127.8, 126.5, 120.3, 114.3, 107.9, 107.4, 55.3, 43.7, 33.9, 25.0, 13.5; **HRMS** (ESI, *m/z*): Calculated for $C_{29}H_{28}N_3OSe$ $[M+H]^+$: 514.1394, found 514.1395.



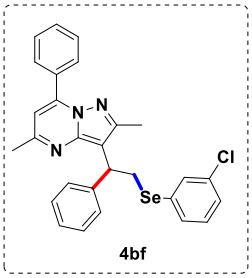
4bd

2,5-Dimethyl-7-phenyl-3-(1-phenyl-2-((4-(trifluoromethyl)phenyl)selanyl)ethyl)pyrazolo[1,5-*a*]pyrimidine(4bd): Yellow gummy mass; 88% (97.0 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.98 (dt, *J* = 5.2, 3.0 Hz, 2H), 7.56 – 7.50 (m, 5H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.38 (d, *J* = 8.4 Hz, 2H), 7.30 (t, *J* = 7.6 Hz, 2H), 7.22 (d, *J* = 7.3 Hz, 1H), 6.60 (s, 1H), 4.58 – 4.35 (m, 2H), 3.80 (dd, *J* = 11.3, 5.0 Hz, 1H), 2.59 (s, 3H), 2.36 (s, 3H); **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 157.4, 153.2, 147.4, 145.3, 144.5, 136.4, 132.4, 131.4, 130.9, 129.3, 128.7, 128.6, 128.4, 127.9, 126.8, 125.3 (q, *J* = 3.9 Hz), 107.7, 107.5, 43.8, 33.1, 25.0, 13.5; **HRMS** (ESI, *m/z*): Calculated for $C_{29}H_{25}F_3N_3Se$ $[M+H]^+$: 552.1162, found 552.1165.



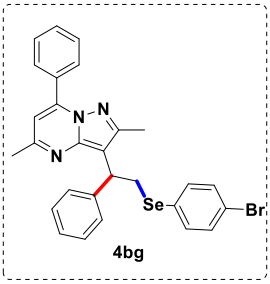
4be

3-(2-((4-Chlorophenyl)selanyl)-1-phenylethyl)-2,5-dimethyl-7-phenylpyrazolo[1,5-a]pyrimidine(4be): Brown oil; 84% (86.9 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.02 (dd, *J* = 6.5, 3.3 Hz, 2H), 7.61 – 7.47 (m, 5H), 7.36 – 7.27 (m, 4H), 7.25 – 7.18 (m, 1H), 7.10 (dd, *J* = 8.5, 2.1 Hz, 2H), 6.61 (s, 1H), 4.44 (m, 2H), 3.70 (m, 1H), 2.60 (s, 3H), 2.39 (s, 3H); **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 157.3, 153.1, 147.4, 145.1, 144.7, 134.8, 132.9, 131.5, 130.8, 129.3, 128.6, 128.5, 127.8, 126.6, 107.6, 107.4, 44.0, 33.9, 24.9, 13.4; **HRMS** (ESI, *m/z*): Calculated for $C_{28}H_{25}ClN_3Se$ $[M+H]^+$: 518.0896, found 518.0897.



4bf

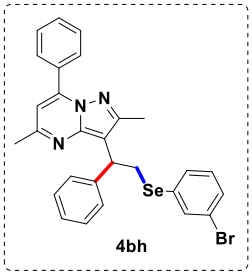
3-(2-((3-Chlorophenyl)selanyl)-1-phenylethyl)-2,5-dimethyl-7-phenylpyrazolo[1,5-*a*]pyrimidine(4bf): Yellow oil; 84% (86.9 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.97 (dd, *J* = 6.7, 3.1 Hz, 2H), 7.56 – 7.46 (m, 5H), 7.40 (s, 1H), 7.30 – 7.22 (m, 3H), 7.19 (t, *J* = 7.9 Hz, 1H), 7.09 (d, *J* = 8.1 Hz, 1H), 7.03 (t, *J* = 7.9 Hz, 1H), 6.60 (s, 1H), 4.56 – 4.29 (m, 2H), 3.72 (dd, *J* = 11.1, 4.7 Hz, 1H), 2.61 (s, 3H), 2.35 (s, 3H); **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 157.4, 153.1, 147.4, 145.2, 144.6, 134.2, 132.5, 132.3, 131.5, 130.9, 130.7, 129.6, 129.3, 128.6, 128.5, 127.8, 126.7, 126.7, 107.6, 107.5, 43.8, 33.3, 25.0, 13.4; **HRMS** (ESI, *m/z*): Calculated for $C_{28}H_{25}ClN_3Se$ $[M+H]^+$: 518.0896, found 518.0901.



4bg

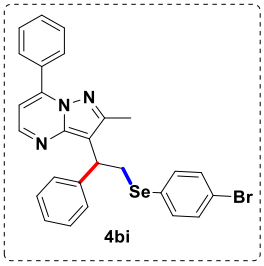
3-(2-((4-bromophenyl)selanyl)-1-phenylethyl)-2,5-dimethyl-7-phenylpyrazolo[1,5-*a*]pyrimidine(4bg): Yellow oil; 82% (92.0 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.04 – 7.97 (m, 2H), 7.57 – 7.48 (m, 5H), 7.29 (t, *J* = 7.6 Hz, 2H), 7.22 (s, 5H), 6.61 (s, 1H), 4.45 (dd, *J* = 10.7, 4.9 Hz, 1H), 4.38 (t, *J* = 11.2 Hz, 1H), 3.67 (dd, *J* = 11.6, 4.9 Hz, 1H), 2.59 (s, 3H), 2.38 (s, 3H); **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 157.3, 153.2, 147.3, 145.2, 144.7, 135.1, 131.6,

131.5, 130.8, 129.5, 129.3, 128.7, 128.6, 127.8, 126.7, 121.0, 107.7, 107.4, 44.1, 33.6, 25.0, 13.5; **HRMS** (ESI, *m/z*): Calculated for $C_{28}H_{25}BrN_3Se$ $[M+H]^+$: 562.0391, found 562.0397.



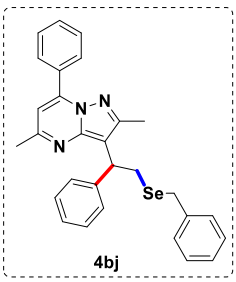
4bh

3-(2-((3-Bromophenyl)selanyl)-1-phenylethyl)-2,5-dimethyl-7-phenylpyrazolo[1,5-a]pyrimidine(4bh): Yellow oil; 82% (92.0 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.97 (dd, *J* = 6.8, 3.0 Hz, 2H), 7.64 – 7.42 (m, 6H), 7.30 – 7.25 (m, 4H), 7.19 (t, *J* = 7.3 Hz, 1H), 6.98 (t, *J* = 7.9 Hz, 1H), 6.61 (s, 1H), 4.56 – 4.25 (m, 2H), 3.71 (dd, *J* = 11.4, 5.0 Hz, 1H), 2.63 (s, 3H), 2.34 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 157.5, 153.2, 147.4, 145.3, 144.6, 135.4, 132.7, 131.6, 131.5, 130.8, 130.0, 129.7, 129.4, 128.7, 128.6, 127.9, 126.7, 122.5, 107.7, 107.6, 43.8, 33.4, 25.1, 13.5; **HRMS** (ESI, *m/z*): Calculated for $C_{28}H_{25}BrN_3Se$ $[M+H]^+$: 562.0391, found 562.0389.



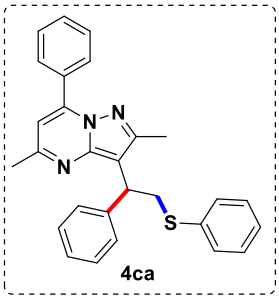
4bi

3-(2-((4-Bromophenyl)selanyl)-1-phenylethyl)-2-methyl-7-phenylpyrazolo[1,5-a]pyrimidine(4bi): Yellow oil; 78% (85.3 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.37 (d, *J* = 4.3 Hz, 1H), 8.07 – 8.01 (m, 2H), 7.57 – 7.52 (m, 3H), 7.48 (d, *J* = 9.9 Hz, 2H), 7.32 – 7.26 (m, 2H), 7.21 (d, *J* = 2.7 Hz, 5H), 6.75 (d, *J* = 4.3 Hz, 1H), 4.46 (q, *J* = 6.5, 5.3 Hz, 1H), 4.41 – 4.28 (m, 1H), 3.68 (ddd, *J* = 14.6, 5.2, 2.5 Hz, 1H), 2.40 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 153.5, 147.8, 146.0, 144.4, 134.9, 131.7, 131.3, 131.1, 129.4, 129.3, 128.8, 128.7, 127.8, 126.8, 121.1, 108.9, 106.5, 44.0, 33.5, 13.5; **HRMS** (ESI, *m/z*): Calculated for $C_{27}H_{23}BrN_3Se$ $[M+H]^+$: 5548.0234, found 548.0232.



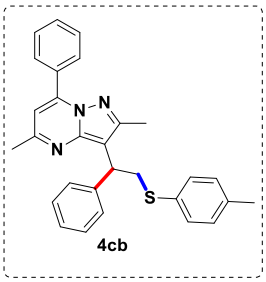
4bj

3-(2-(benzylselanyl)-1-phenylethyl)-2,5-dimethyl-7-phenylpyrazolo[1,5-*a*]pyrimidine(4bj): Yellow oil; 67% (66.6 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.96 (dd, *J* = 6.6, 3.1 Hz, 2H), 7.53 – 7.47 (m, 3H), 7.39 (d, *J* = 8.5 Hz, 2H), 7.29 – 7.25 (m, 4H), 7.25 – 7.22 (m, 2H), 7.21 – 7.12 (m, 2H), 6.61 (s, 1H), 4.26 (dd, *J* = 9.7, 6.6 Hz, 1H), 3.86 (dd, *J* = 12.1, 9.6 Hz, 1H), 3.71 (s, 2H), 3.42 (dd, *J* = 12.1, 6.7 Hz, 1H), 2.60 (s, 3H), 2.27 (s, 3H); **^{13}C {^{1}H} NMR** (126 MHz, $CDCl_3$) δ 157.4, 153.2, 147.5, 145.4, 144.9, 140.1, 131.6, 130.8, 129.3, 129.0, 128.7, 128.6, 128.5, 127.9, 126.7, 126.5, 108.5, 107.5, 43.3, 29.5, 27.8, 25.0, 13.6; **HRMS** (ESI, *m/z*): Calculated for $C_{29}H_{28}N_3Se$ $[M+H]^+$: 498.1445, found 498.1448.



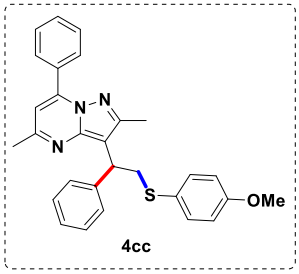
4ca

2,5-Dimethyl-7-phenyl-3-(1-phenyl-2-(phenylthio)ethyl)pyrazolo[1,5-*a*]pyrimidine(4ca): Brown oil; 62% (54.0 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.98 – 7.93 (m, 2H), 7.54 – 7.49 (m, 3H), 7.47 (d, *J* = 7.2 Hz, 2H), 7.29 (t, *J* = 7.2 Hz, 3H), 7.24 (d, *J* = 4.6 Hz, 1H), 7.22 – 7.15 (m, 3H), 7.12 (t, *J* = 7.3 Hz, 1H), 6.60 (s, 1H), 4.34 (d, *J* = 9.3 Hz, 2H), 3.81 – 3.72 (m, 1H), 2.59 (s, 3H), 2.28 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 157.4, 153.3, 147.6, 145.3, 144.2, 136.5, 131.7, 130.7, 130.1, 129.3, 128.8, 128.7, 128.6, 128.0, 126.7, 126.1, 107.6, 107.5, 42.4, 39.0, 25.1, 13.4; **HRMS** (ESI, *m/z*): Calculated for $C_{28}H_{26}N_3S$ $[M+H]^+$: 436.1842, found 436.1841.

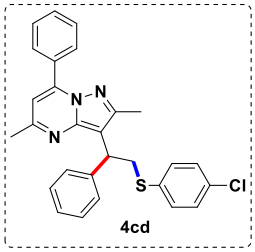


4cb

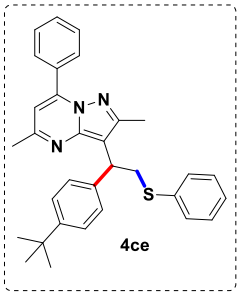
2,5-Dimethyl-7-phenyl-3-(1-phenyl-2-(p-tolylthio)ethyl)pyrazolo[1,5-*a*]pyrimidine(4cb): Yellow jelly; 56% (50.2 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.97 (dd, *J* = 6.0, 3.9 Hz, 2H), 7.57 – 7.41 (m, 5H), 7.26 (d, *J* = 15.1 Hz, 2H), 7.22 – 7.13 (m, 3H), 7.01 (d, *J* = 7.9 Hz, 2H), 6.60 (s, 1H), 4.32 (d, *J* = 12.7 Hz, 2H), 3.70 (dd, *J* = 11.2, 4.2 Hz, 1H), 2.60 (s, 3H), 2.29 (d, *J* = 10.8 Hz, 6H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 157.3, 153.4, 147.4, 145.3, 144.3, 136.2, 132.7, 131.6, 130.9, 130.8, 129.5, 129.3, 128.7, 128.6, 128.0, 126.6, 107.6, 107.5, 42.5, 39.4, 25.0, 21.2, 13.5; **HRMS** (ESI, *m/z*): Calculated for $C_{29}H_{28}N_3S$ $[M+H]^+$: 450.1998, found 450.1993.



3-(2-((4-Methoxyphenyl)thio)-1-phenylethyl)-2,5-dimethyl-7-phenylpyrazolo[1,5-*a*]pyrimidine(4cc): Yellow oil; 61% (57.3 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.99 (dd, *J* = 6.4, 2.9 Hz, 2H), 7.54 (d, *J* = 4.7 Hz, 3H), 7.46 (d, *J* = 7.3 Hz, 2H), 7.29 – 7.24 (m, 4H), 7.18 (t, *J* = 7.3 Hz, 1H), 6.73 (d, *J* = 8.7 Hz, 2H), 6.64 (s, 1H), 4.52 (d, *J* = 11.1 Hz, 1H), 4.25 (t, *J* = 11.7 Hz, 1H), 3.75 (s, 3H), 3.65 (d, *J* = 18.5 Hz, 1H), 2.69 (s, 3H), 2.33 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 158.9, 157.6, 154.0, 146.3, 144.0, 133.7, 131.2, 129.5, 128.8, 128.6, 128.0, 126.6, 114.3, 107.7, 107.5, 55.4, 42.4, 40.4, 24.6, 13.7; **HRMS** (ESI, *m/z*): Calculated for $C_{29}H_{28}N_3OS$ $[M+H]^+$: 466.1948, found 466.1946.

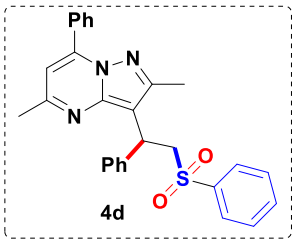


3-(2-((4-Chlorophenyl)thio)-1-phenylethyl)-2,5-dimethyl-7-phenylpyrazolo[1,5-*a*]pyrimidine(4cd): Yellow oil; 60% (55.8 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.98 (dd, *J* = 6.6, 2.6 Hz, 2H), 7.56 – 7.47 (m, 5H), 7.28 (t, *J* = 7.4 Hz, 2H), 7.22 – 7.17 (m, 3H), 7.13 (d, *J* = 8.4 Hz, 2H), 6.62 (s, 1H), 4.43 – 4.27 (m, 2H), 3.72 (dd, *J* = 12.5, 5.2 Hz, 1H), 2.62 (s, 3H), 2.33 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 157.5, 153.5, 147.1, 145.6, 143.9, 135.1, 132.1, 131.7, 131.4, 131.0, 129.4, 128.8, 128.7, 128.6, 128.0, 126.8, 107.6, 107.3, 42.8, 39.3, 25.0, 13.5; **HRMS** (ESI, *m/z*): Calculated for $C_{28}H_{25}ClN_3S$ $[M+H]^+$: 470.1452, found 470.1452.



3-(1-(4-(tert-butyl)phenyl)-2-(phenylthio)ethyl)-2,5-dimethyl-7-phenylpyrazolo[1,5-*a*]pyrimidine(4ce): Brown oil; 57% (53.1 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.98 (dd, *J* = 6.8, 3.0 Hz, 2H), 7.55 – 7.50 (m, 3H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 8.2 Hz, 4H), 7.23 – 7.19 (m, 2H), 7.15 – 7.10 (m, 1H), 6.62 (s, 1H), 4.47 – 4.28 (m, 2H), 3.75 (dd, *J* = 12.4, 5.2

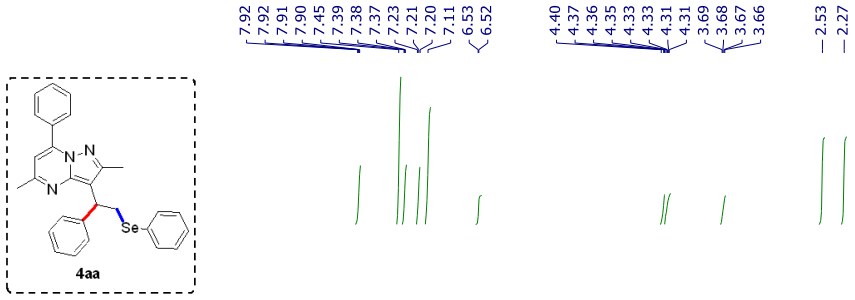
Hz, 1H), 2.64 (s, 3H), 2.33 (s, 3H), 1.29 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.4, 153.6, 149.3, 147.0, 145.6, 141.1, 136.7, 131.5, 130.9, 130.0, 129.4, 128.7, 128.6, 127.6, 125.9, 125.5, 107.7, 107.5, 41.9, 38.9, 34.5, 31.5, 24.8, 13.5; **HRMS** (ESI, *m/z*): Calculated for $C_{32}H_{34}N_3S$ $[M+H]^+$: 492.2468, found 492.2464.

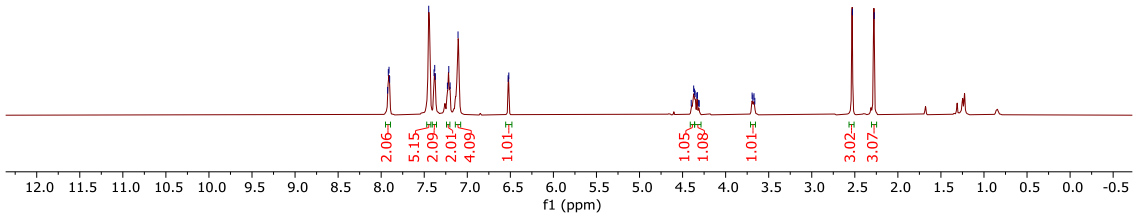


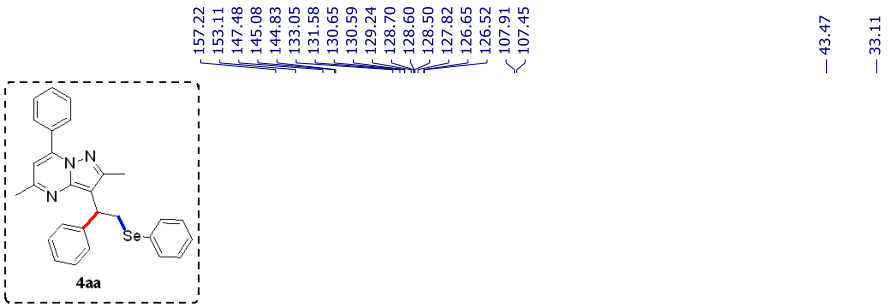
2,5-Dimethyl-7-phenyl-3-(1-phenyl-2-(phenylsulfonyl)ethyl)pyrazolo[1,5-*a*]pyrimidine(4d): Off white solid; m.p. 184-186 °C; 68% (29.2 mg); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.91 – 7.81 (m, 2H), 7.56 – 7.49 (m, 3H), 7.49 – 7.44 (m, 2H), 7.43 – 7.36 (m, 2H), 7.26 (d, *J* = 7.3 Hz, 2H), 7.17 (dd, *J* = 19.0, 7.4 Hz, 2H), 7.06 (t, *J* = 7.8 Hz, 2H), 6.45 (s, 1H), 5.31 (dd, *J* = 14.6, 11.4 Hz, 1H), 4.73 (dd, *J* = 11.5, 3.3 Hz, 1H), 3.68 (dd, *J* = 14.6, 3.2 Hz, 1H), 2.51 (s, 3H), 2.47 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 157.3, 152.9, 146.9, 145.0, 142.8, 139.5, 132.1, 131.2, 131.0, 129.1, 128.9, 128.8, 127.7, 127.5, 127.3, 127.1, 107.3, 105.3, 59.2, 38.0, 24.9, 13.1; **HRMS** (ESI, *m/z*): Calculated for $C_{28}H_{25}N_3O_2SNa$ $[M+Na]^+$: 490.1565, found 490.1564.

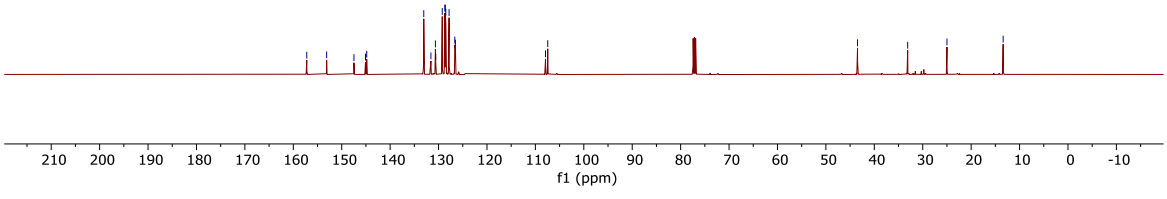
NMR spectra of compounds

4aa (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)

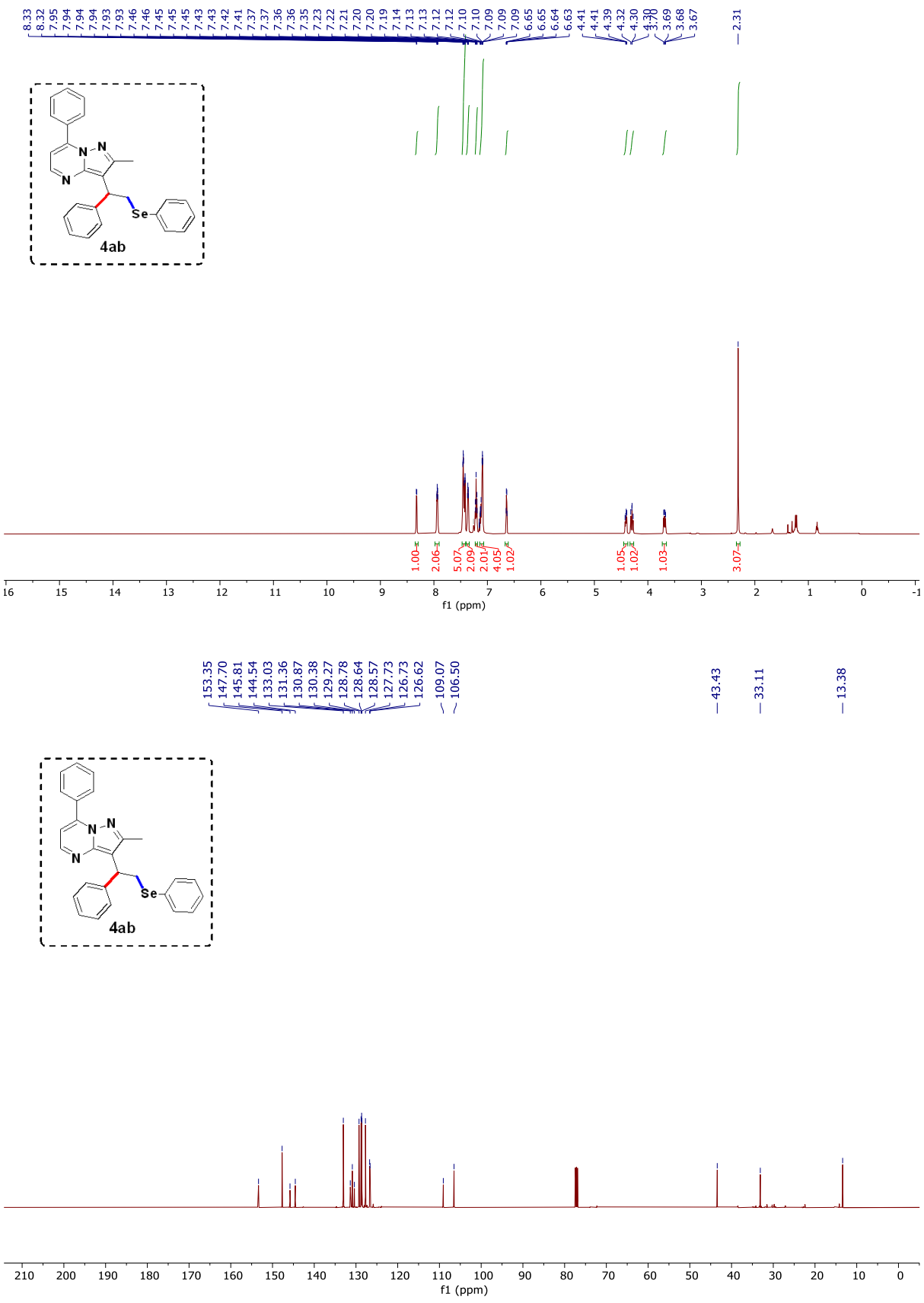




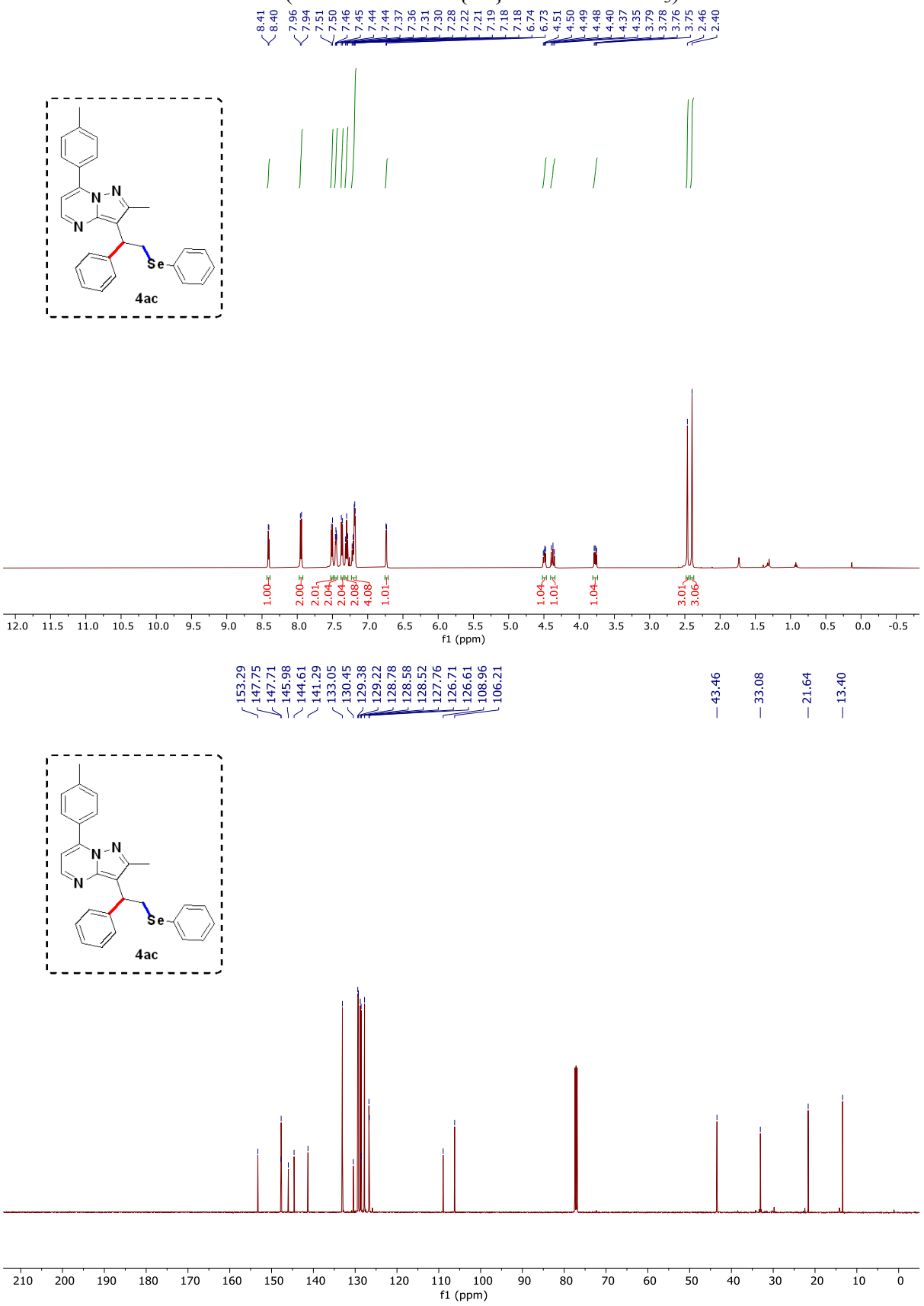




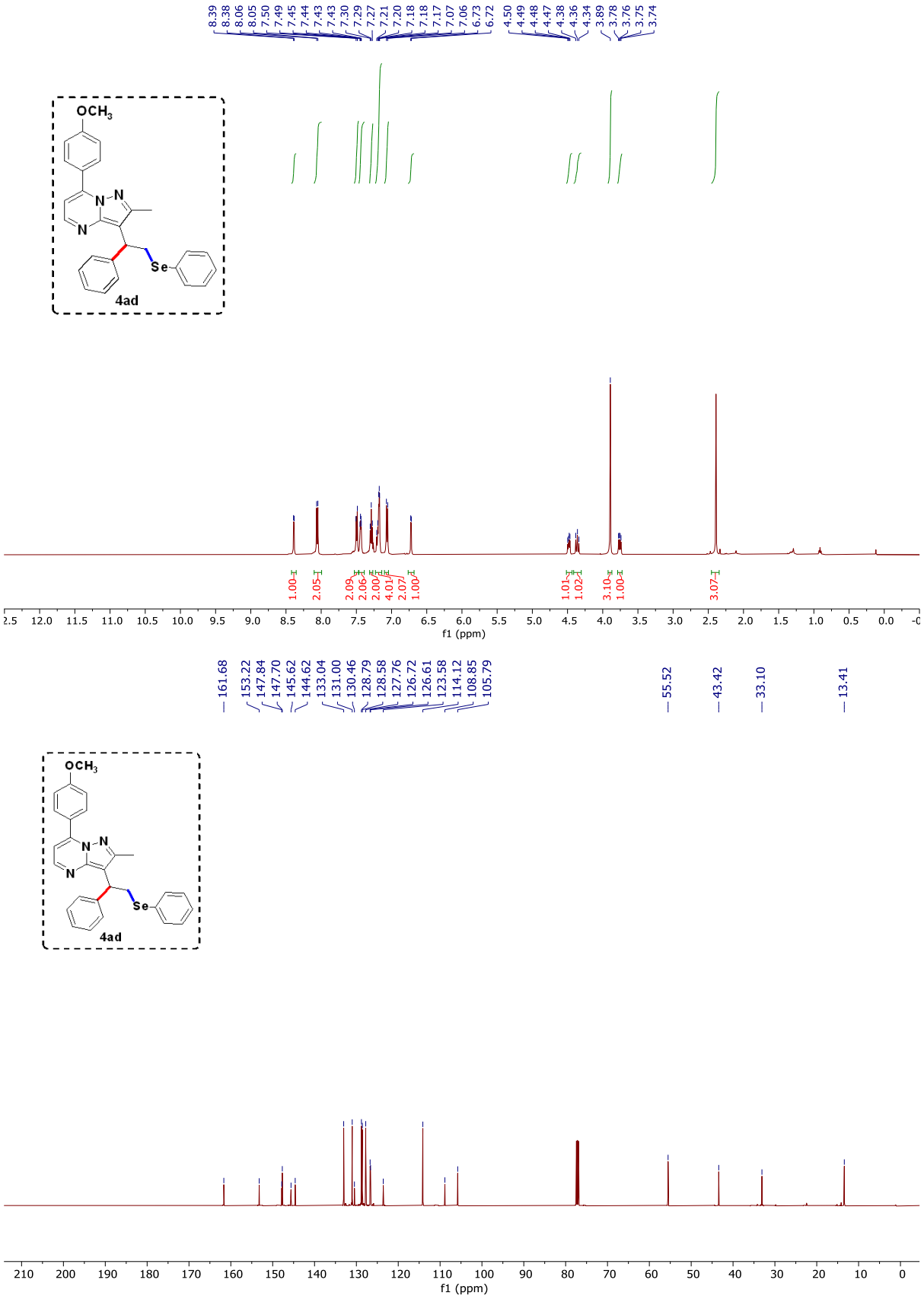
4ab (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-CDCl$_3$)



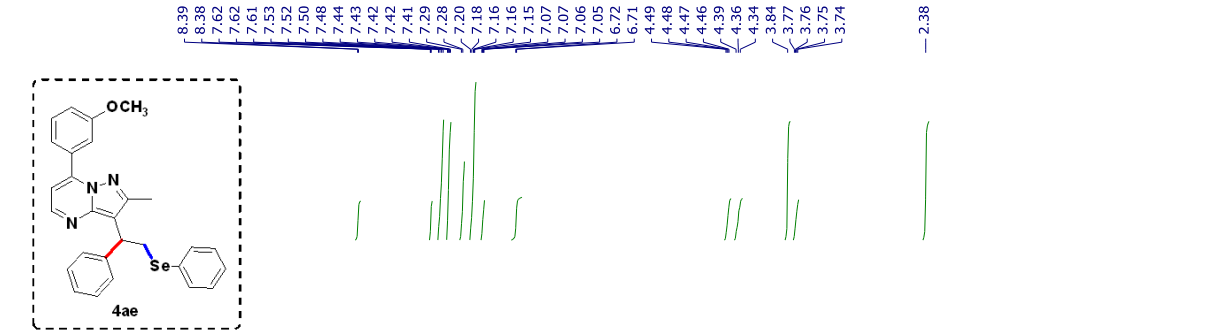
4ac (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)

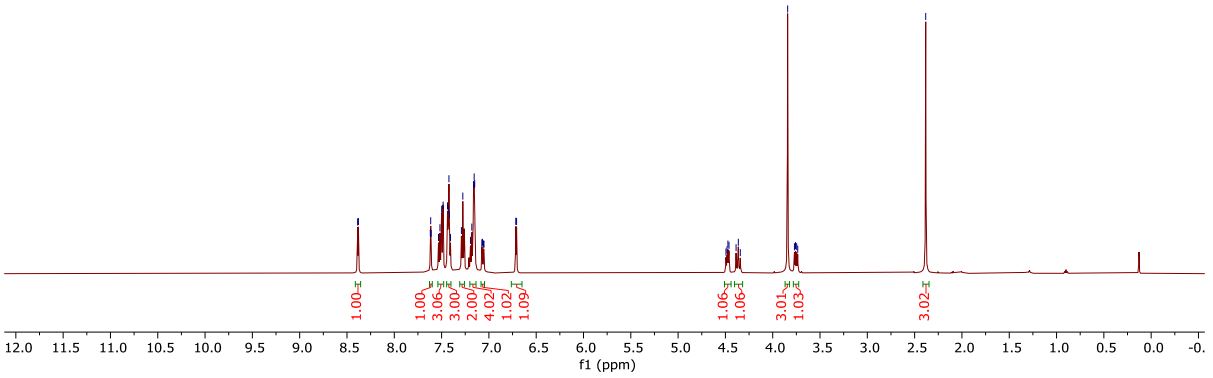


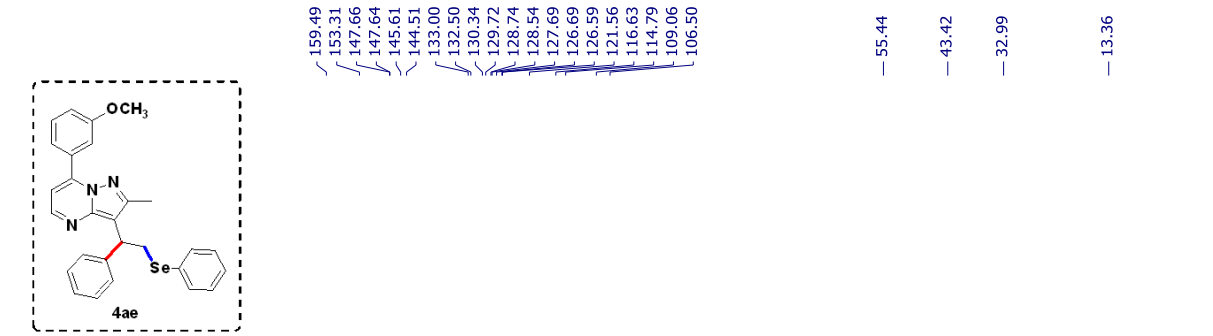
4ad (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)

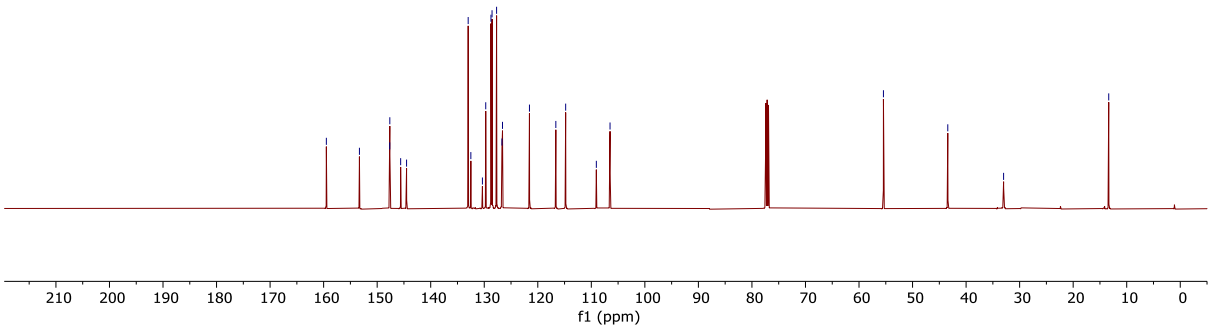


4ae (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)

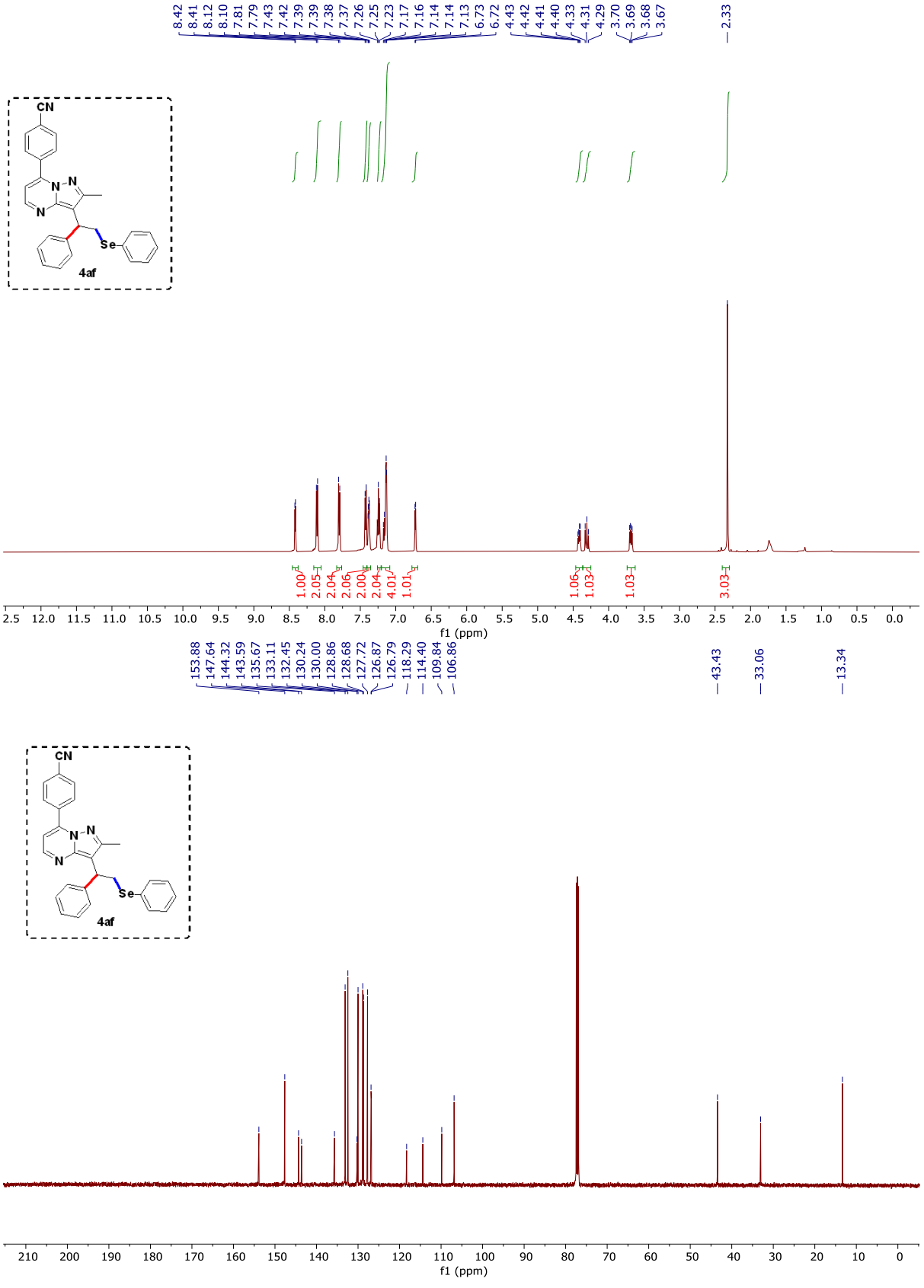




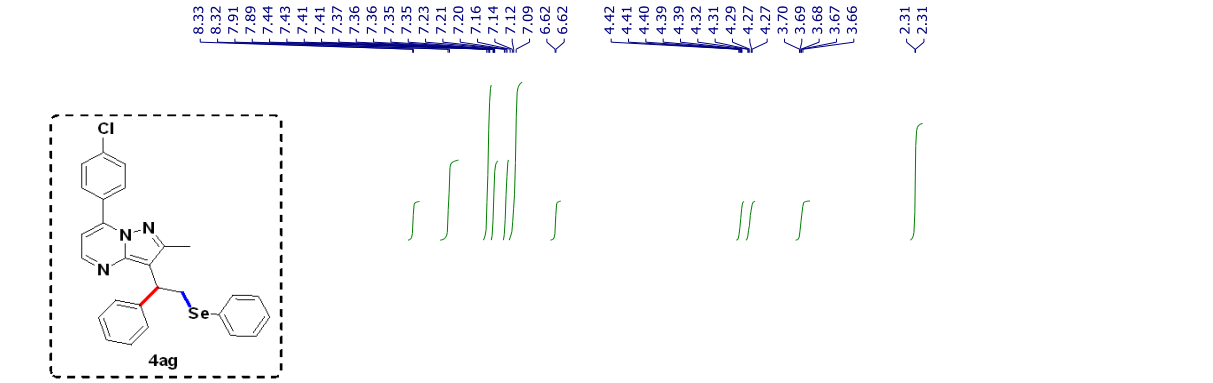


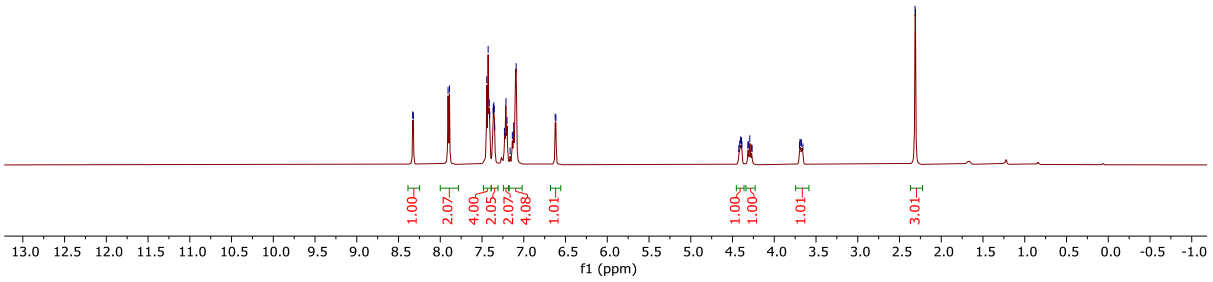


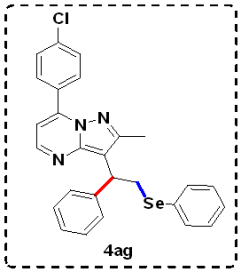
4af (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)

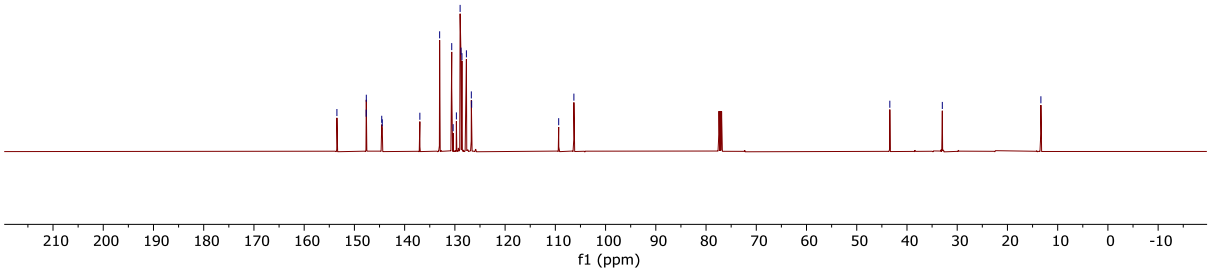


4ag (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)

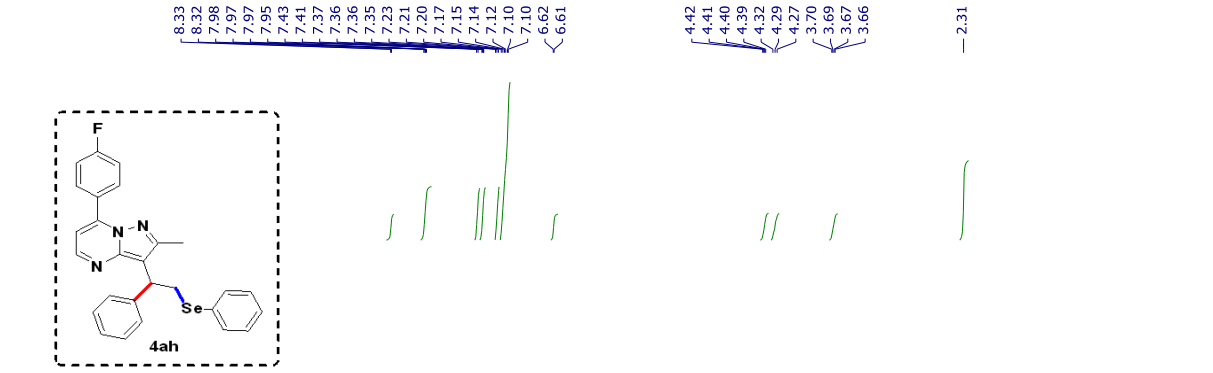


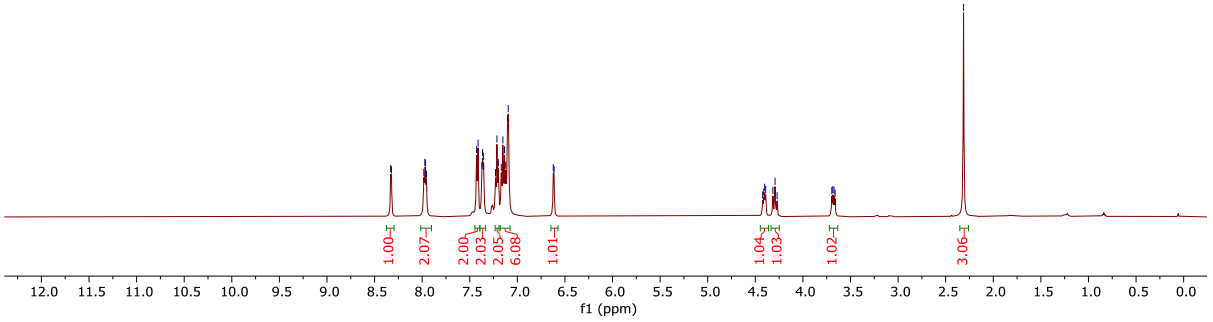


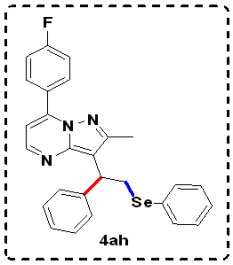


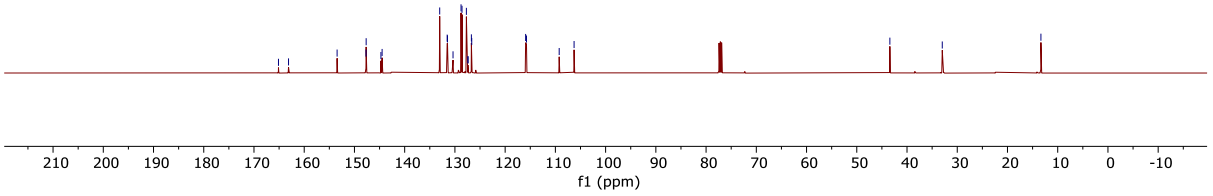


4ah (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-CDCl$_3$)

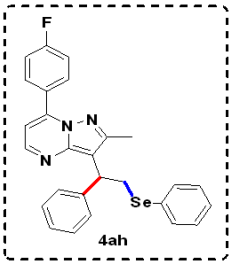




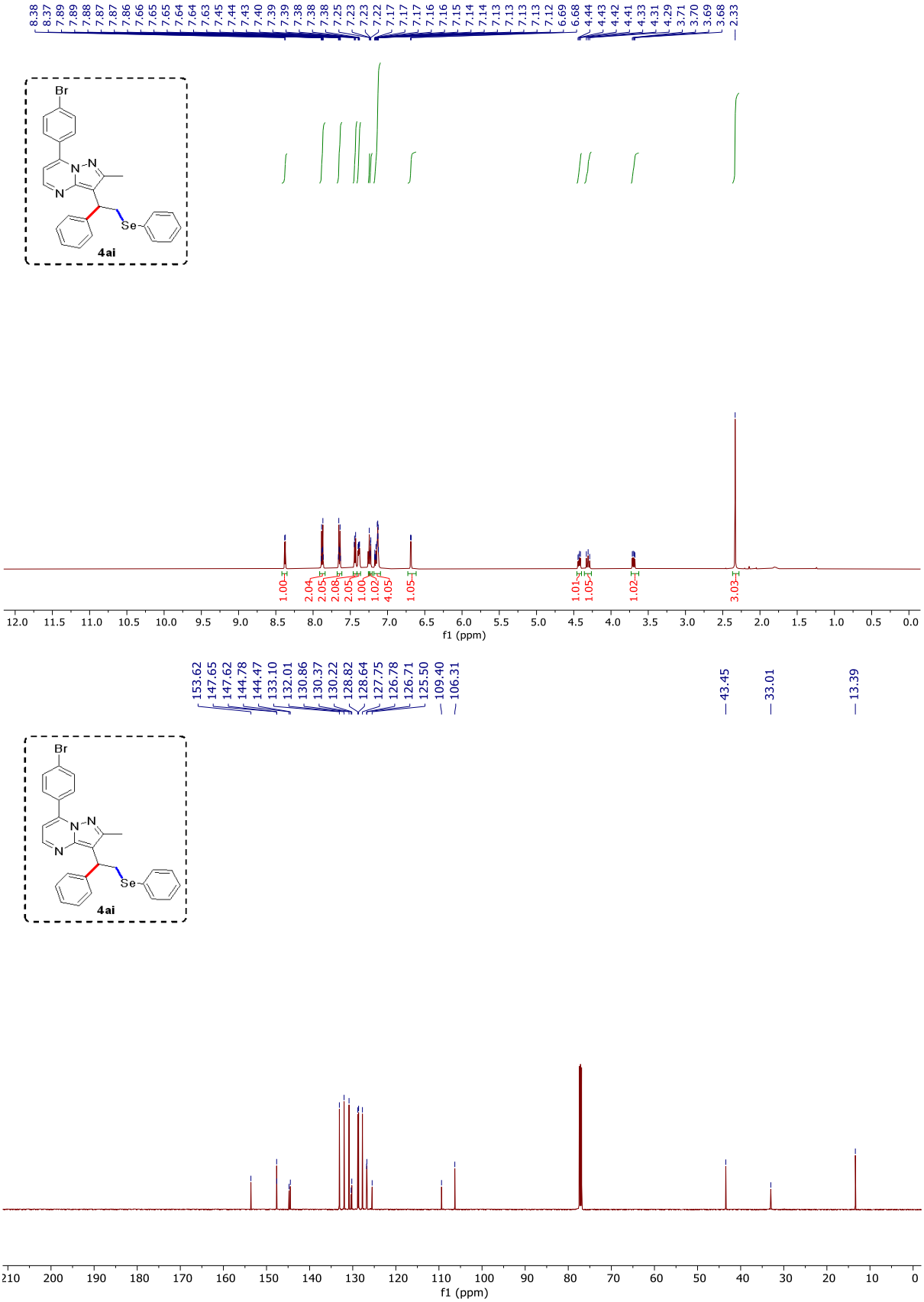




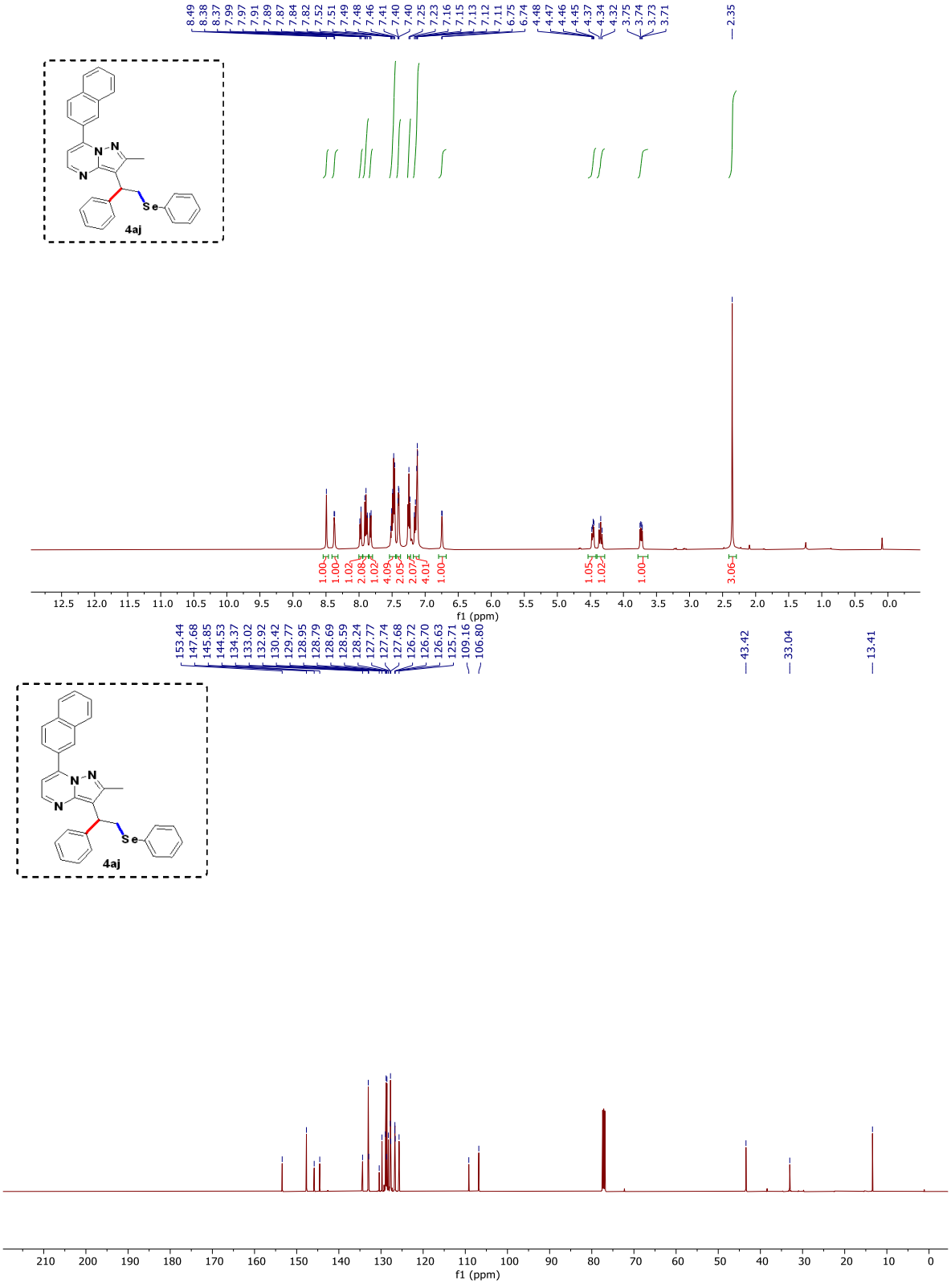
4ah (^{19}F NMR 471 MHz, $CDCl_3$)



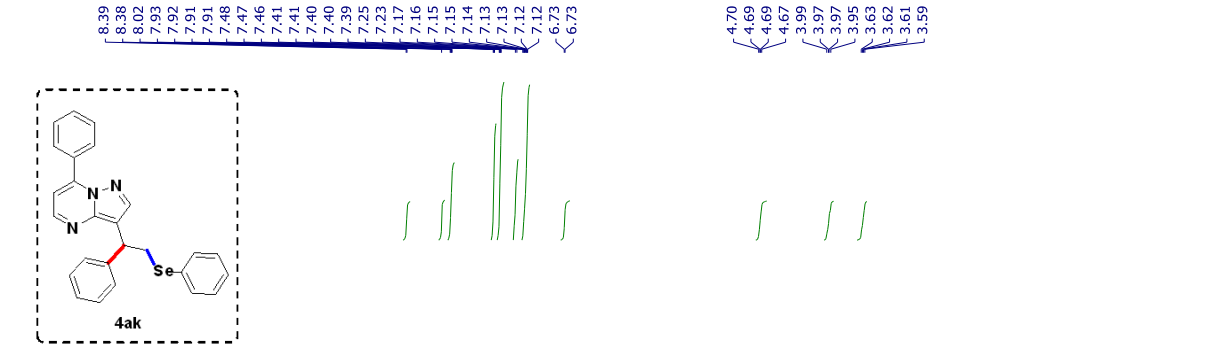
4ai (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-CDCl$_3$)

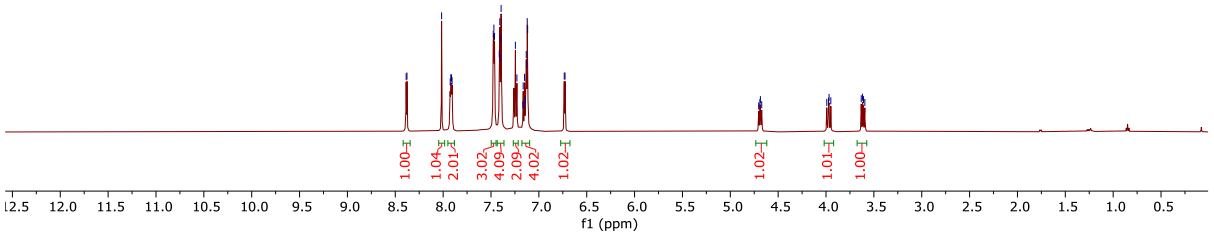


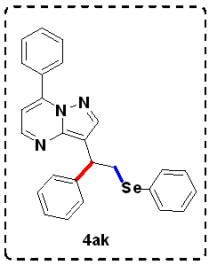
4aj (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)

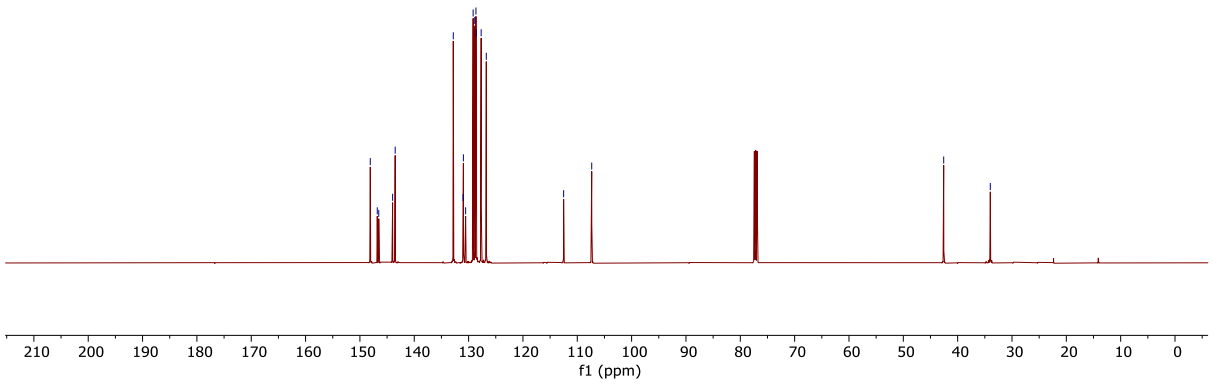


4ak (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)

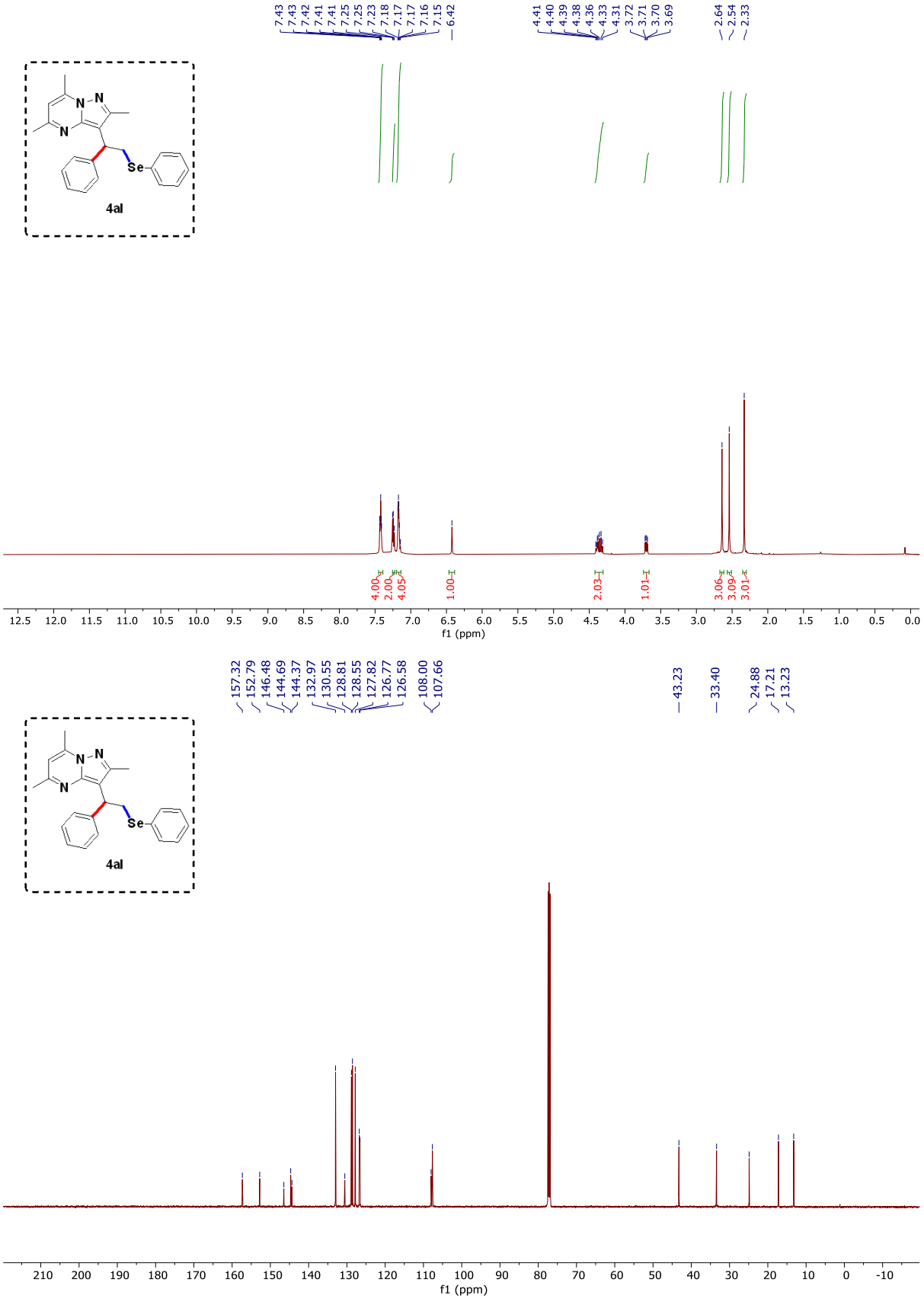




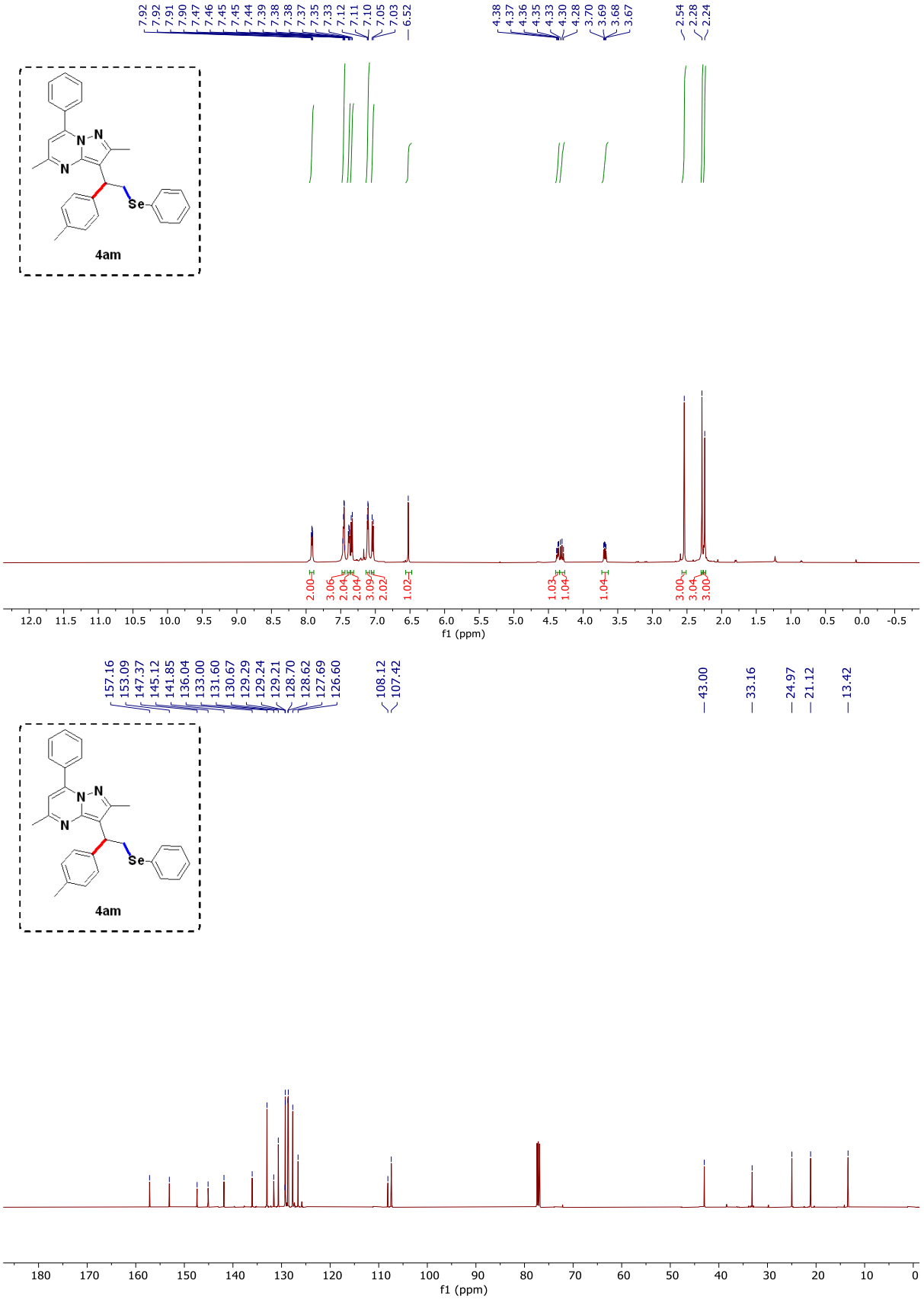




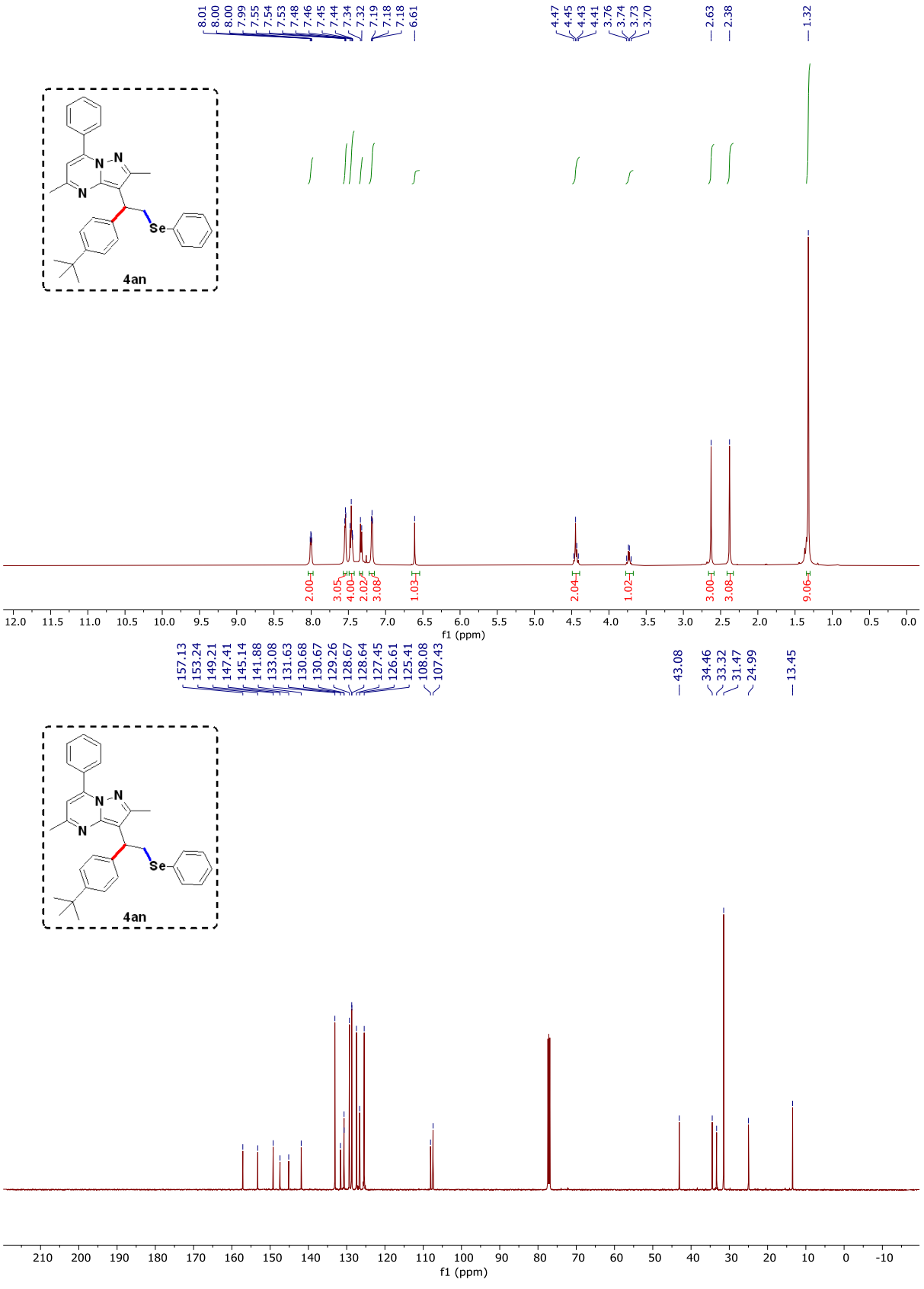
4al (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)



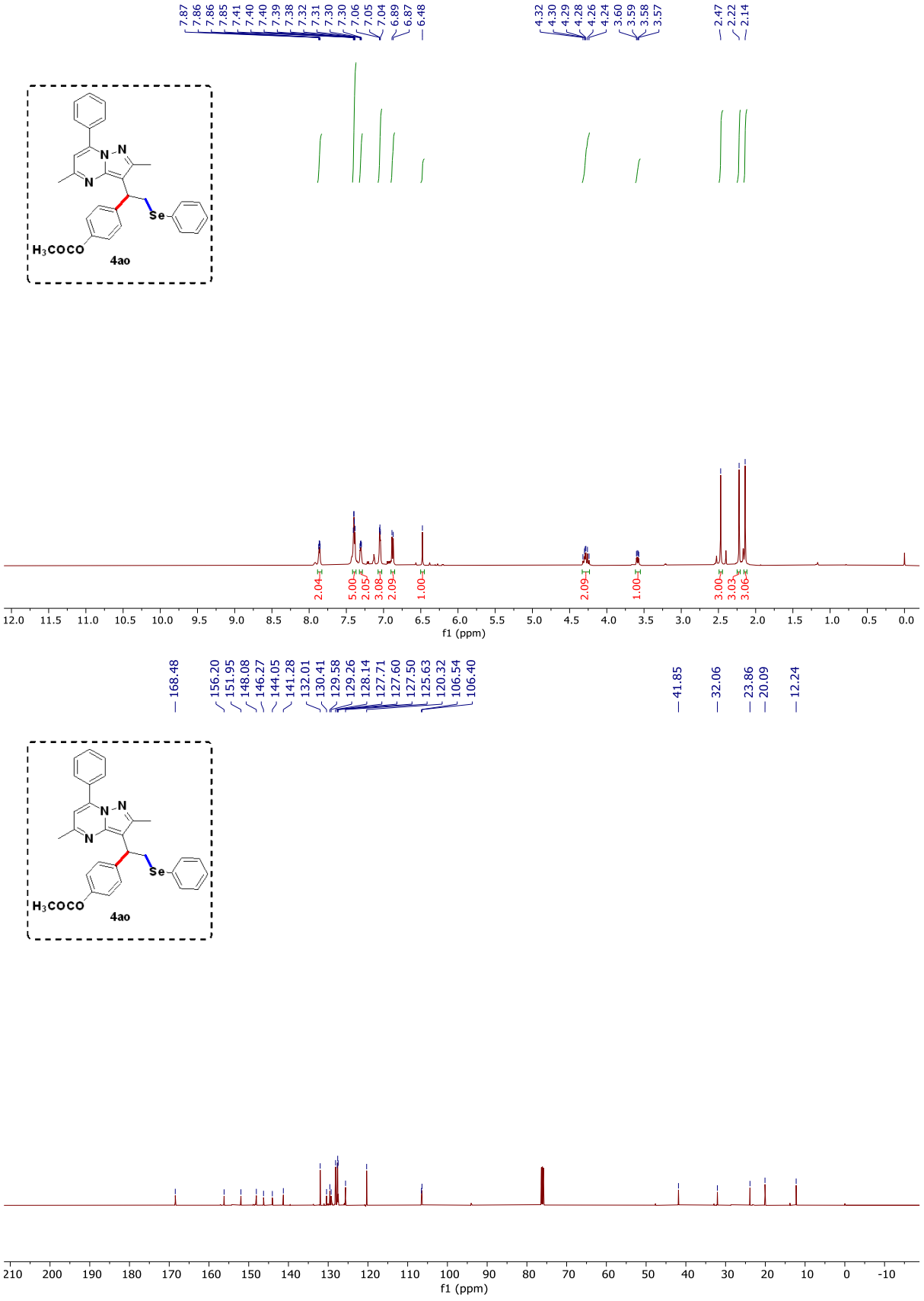
4am (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)



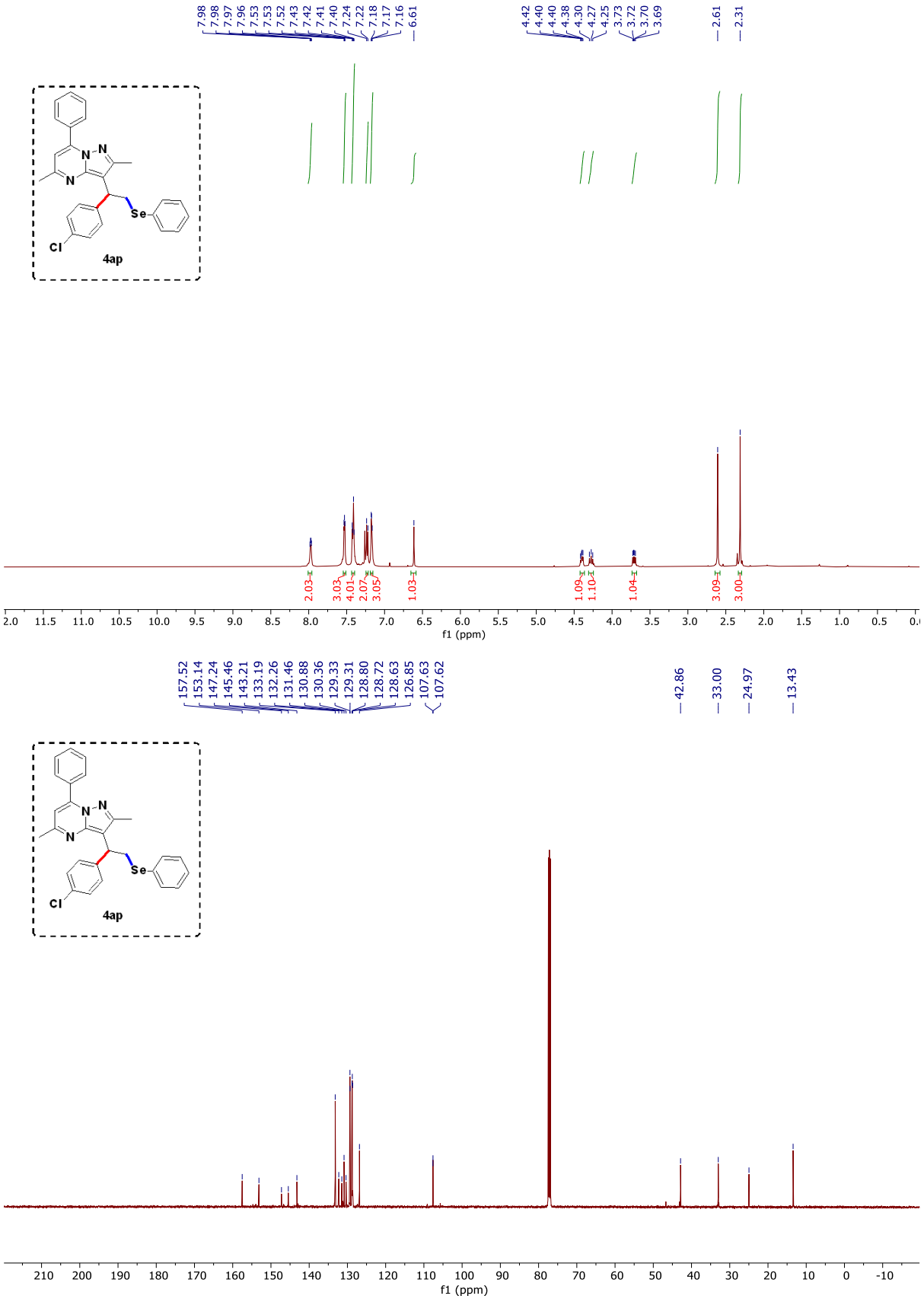
4an (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)



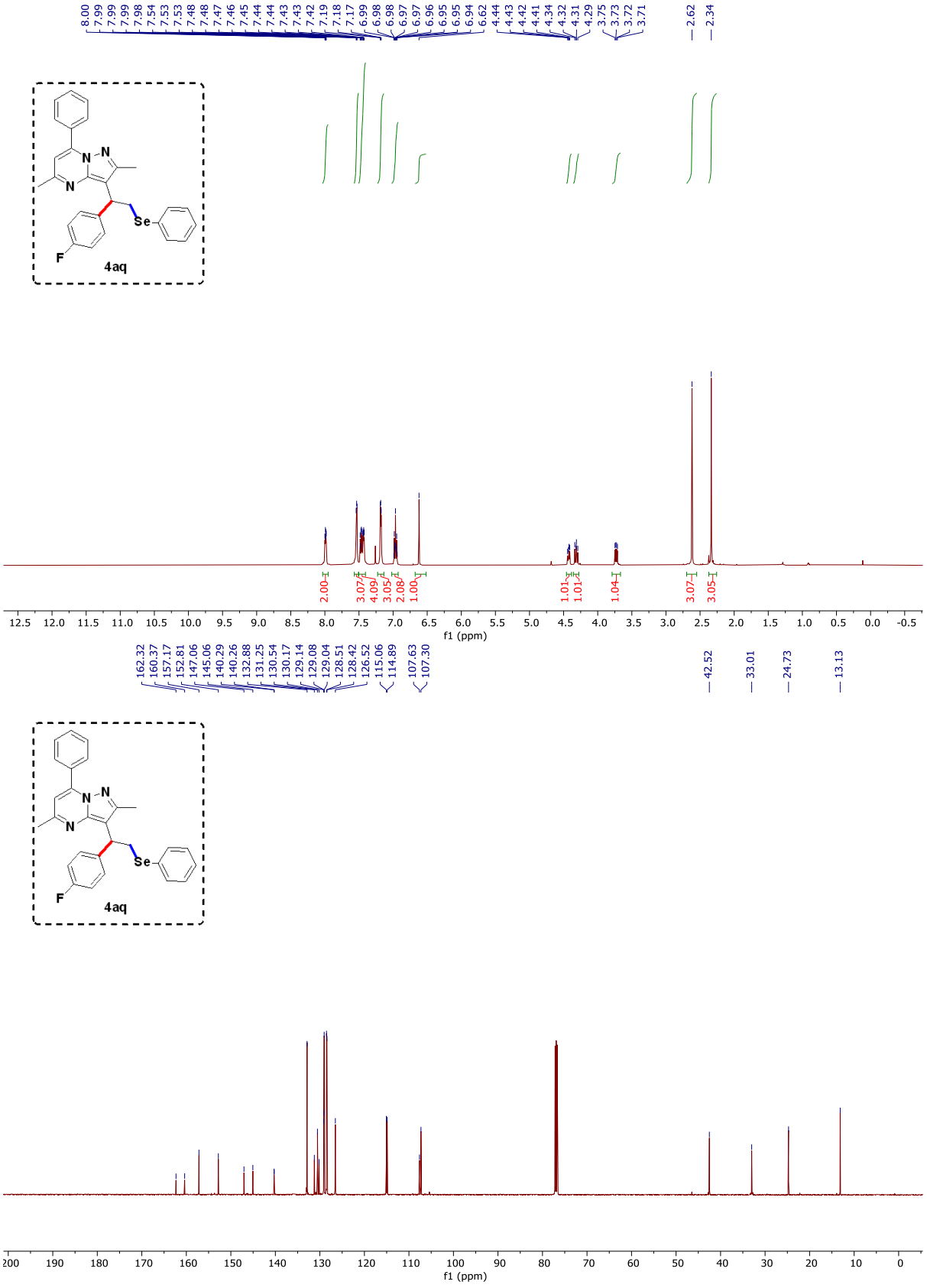
4ao (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-CDCl$_3$)



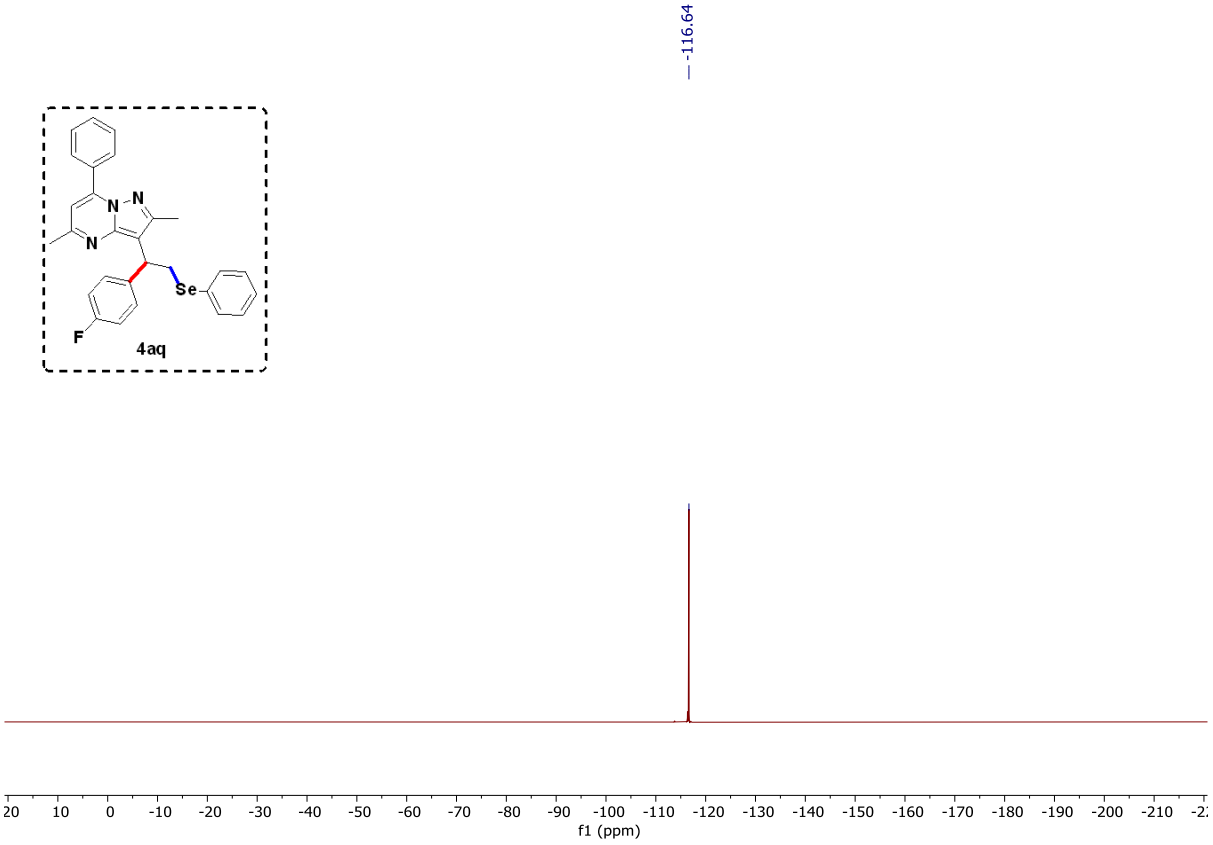
4ap (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-CDCl$_3$)



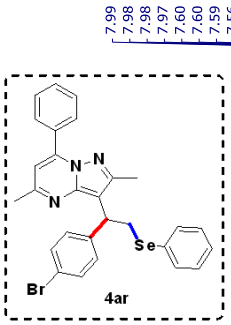
4aq (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)

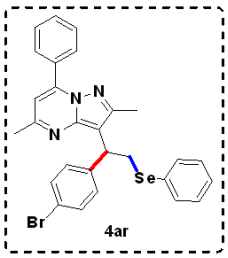


4ah (^{19}F NMR 471 MHz, $CDCl_3$)

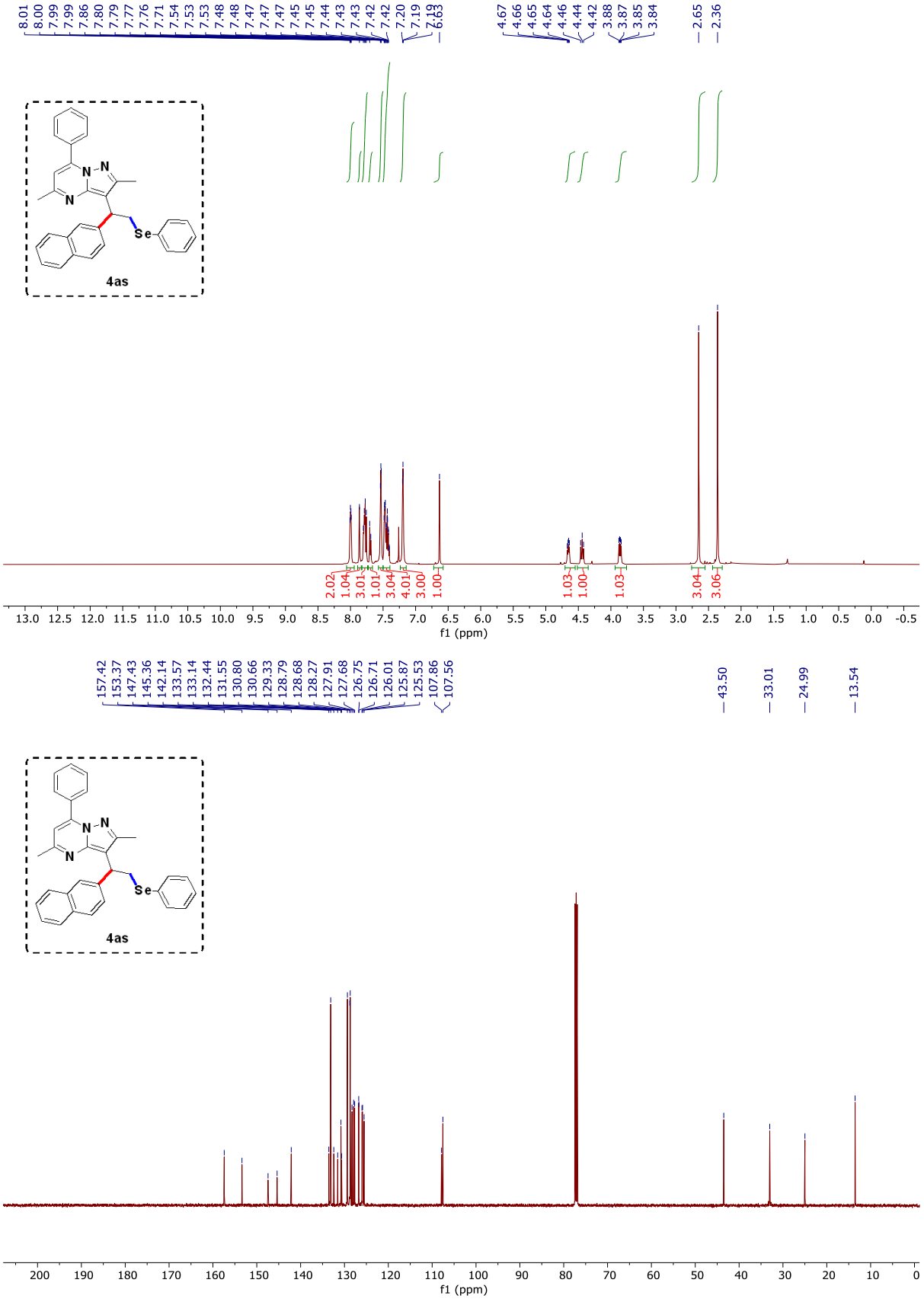


4ar (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)

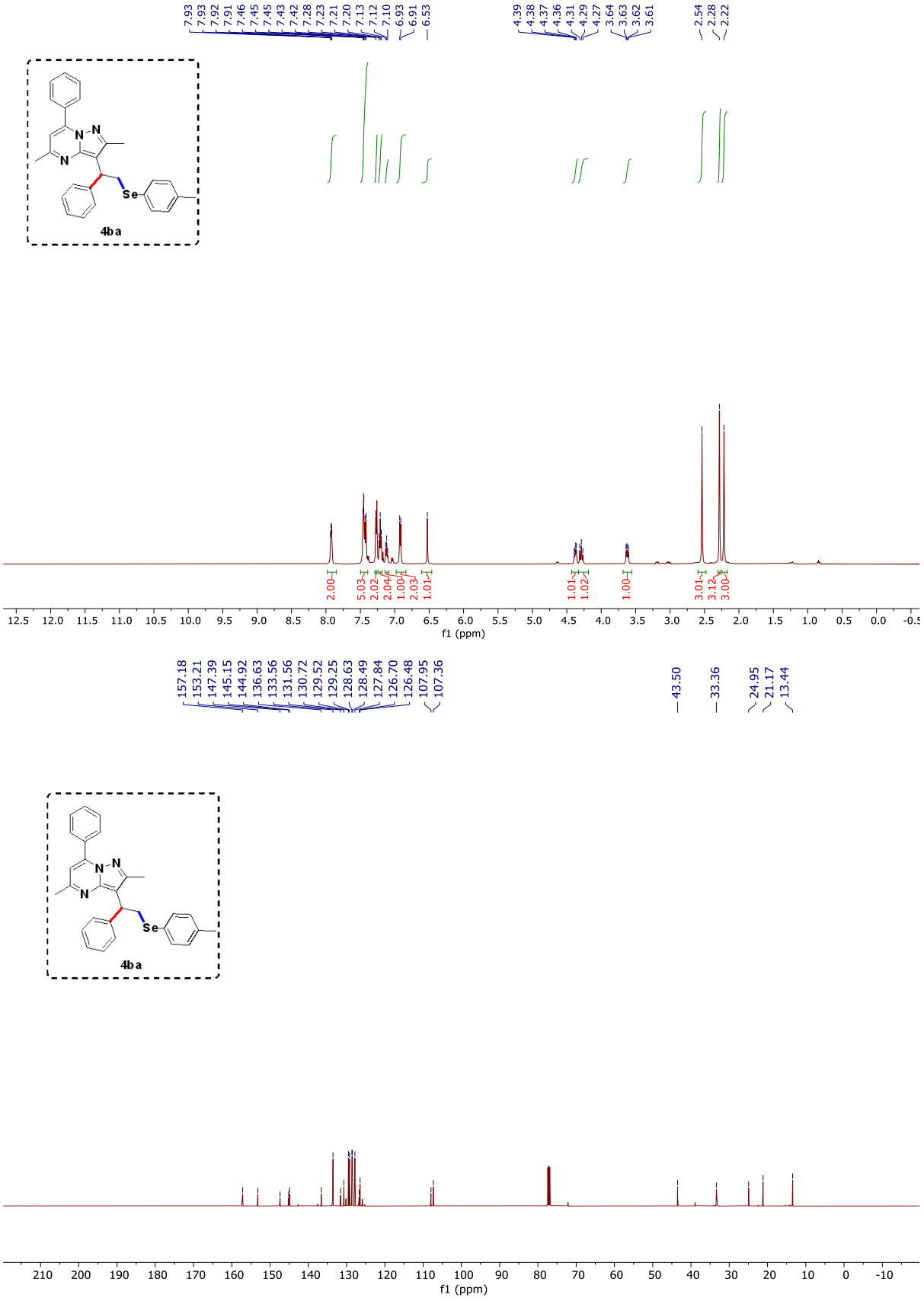




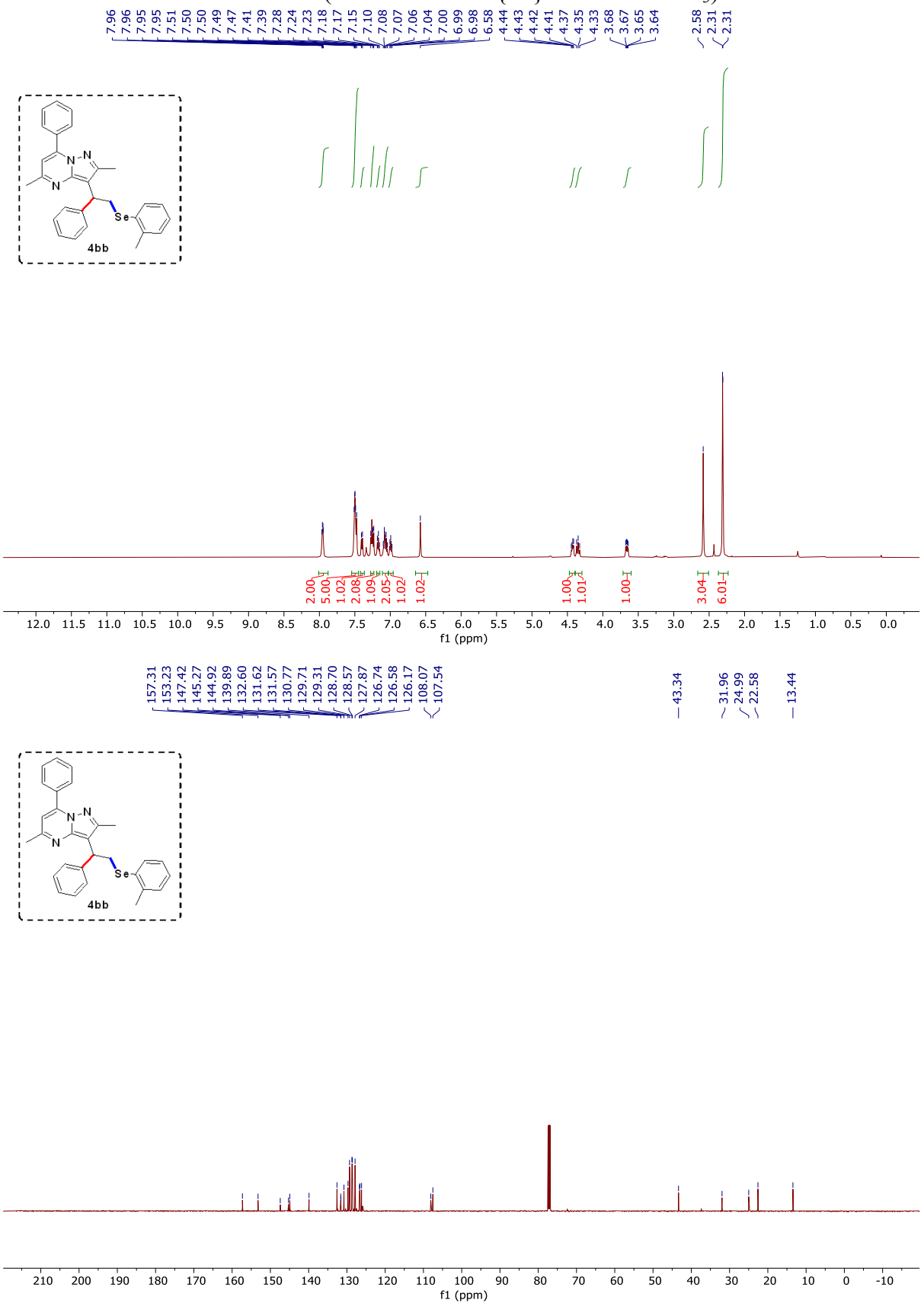
4as (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-CDCl$_3$)



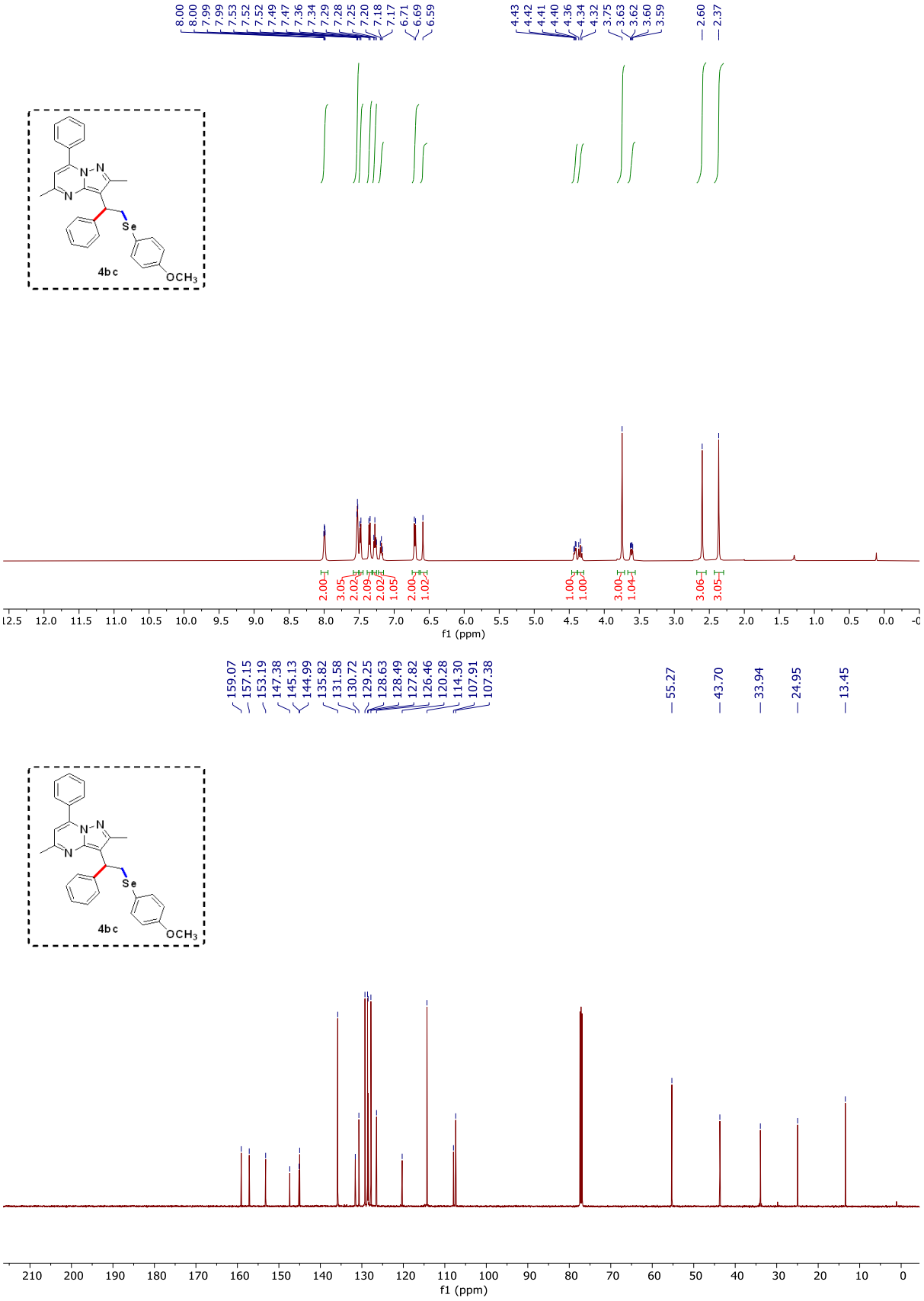
4ba (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)



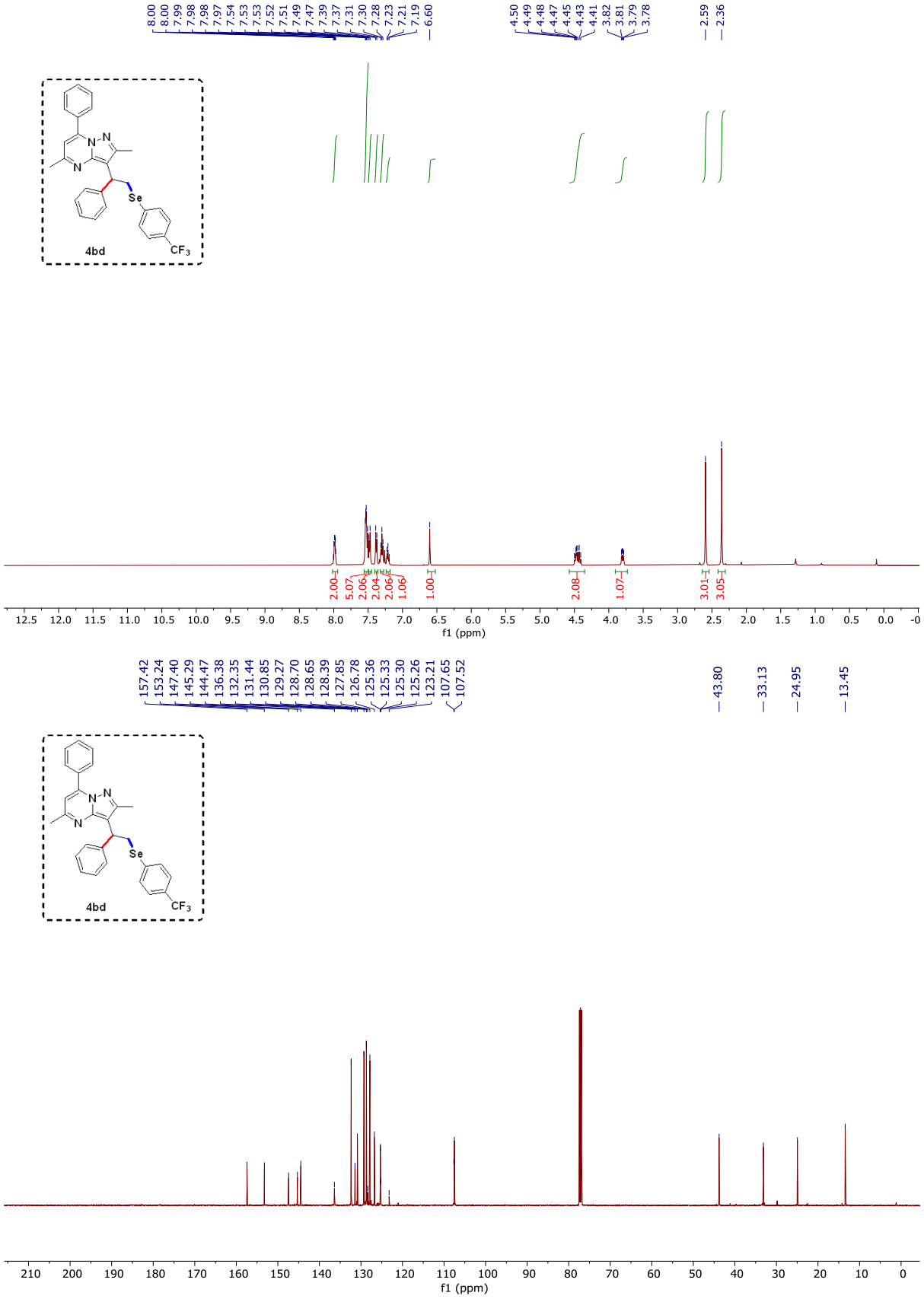
4bb (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)



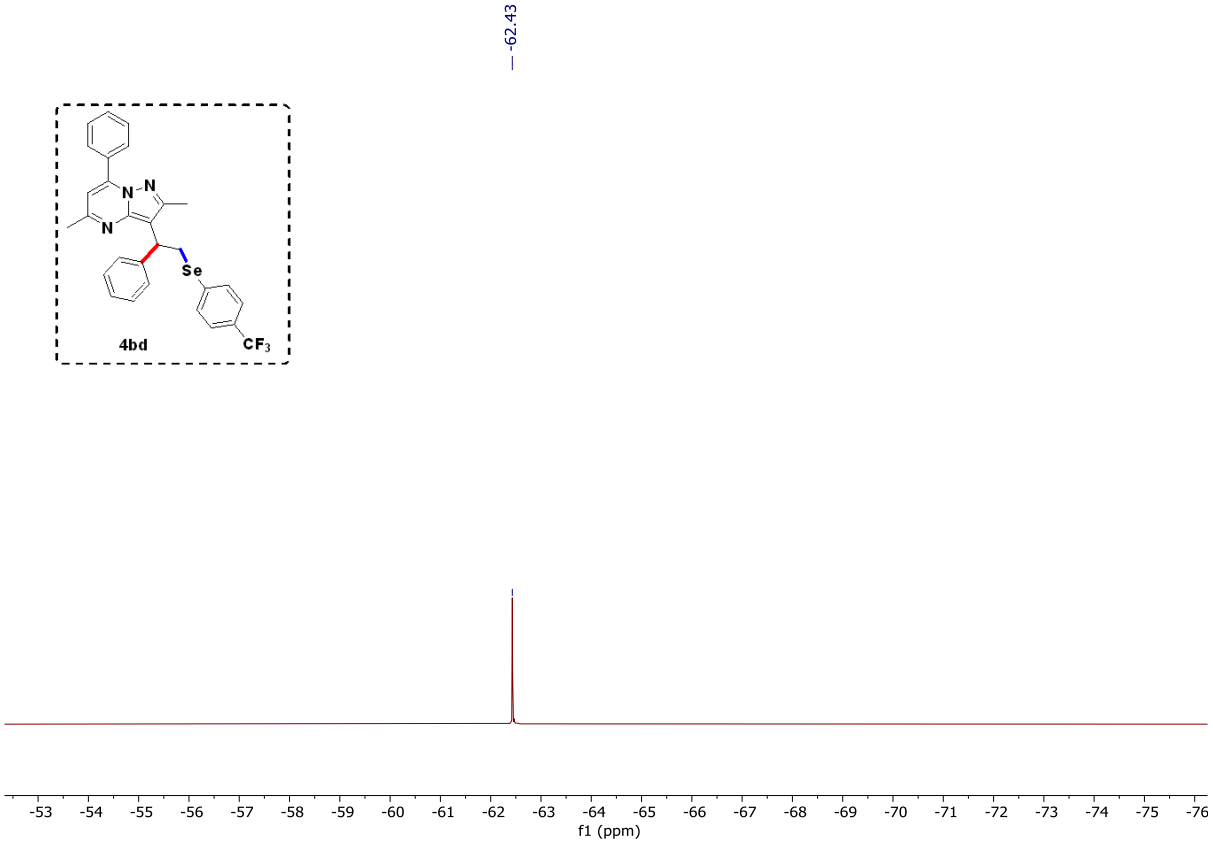
4bc (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-CDCl$_3$)



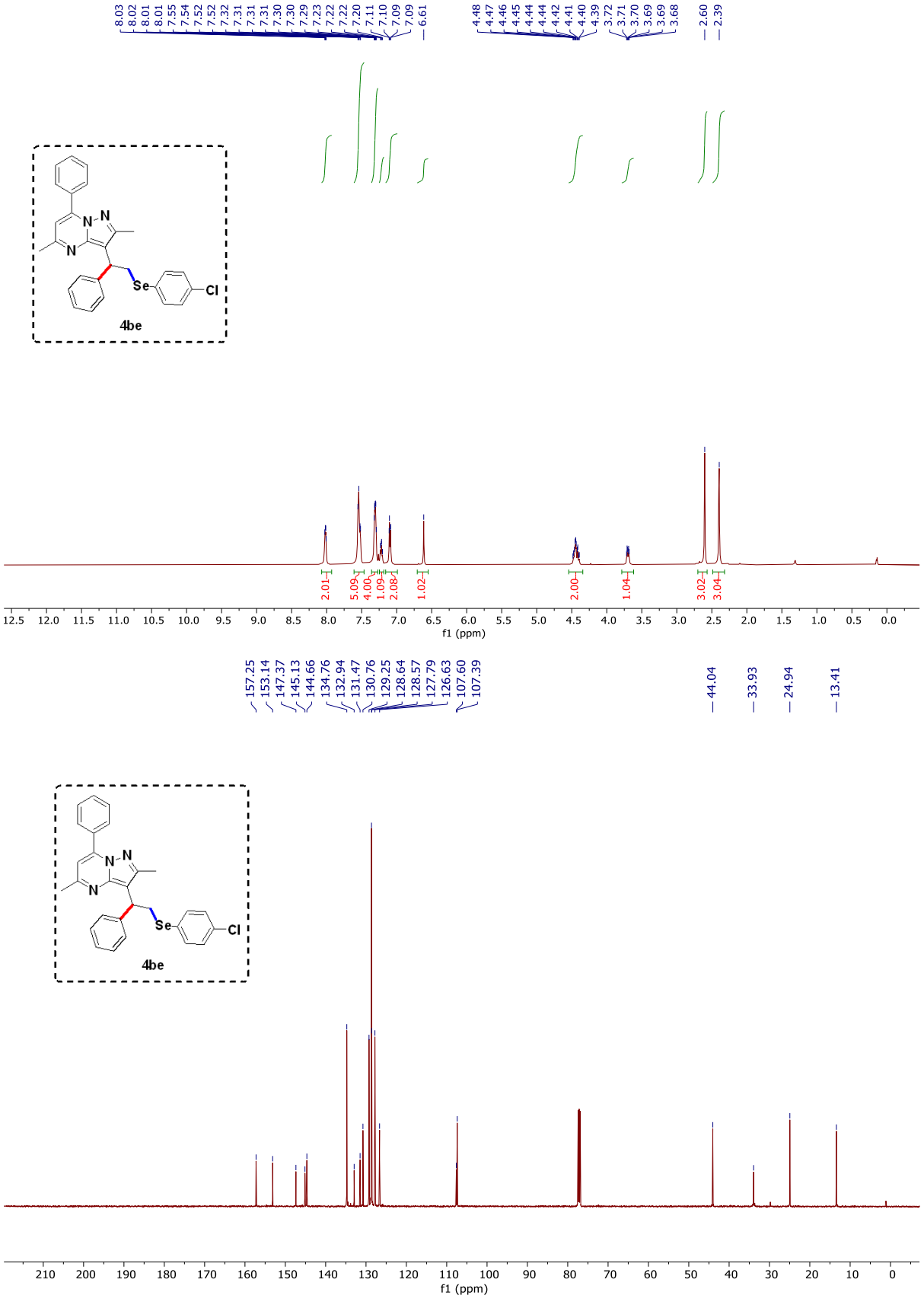
4bd (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-CDCl$_3$)



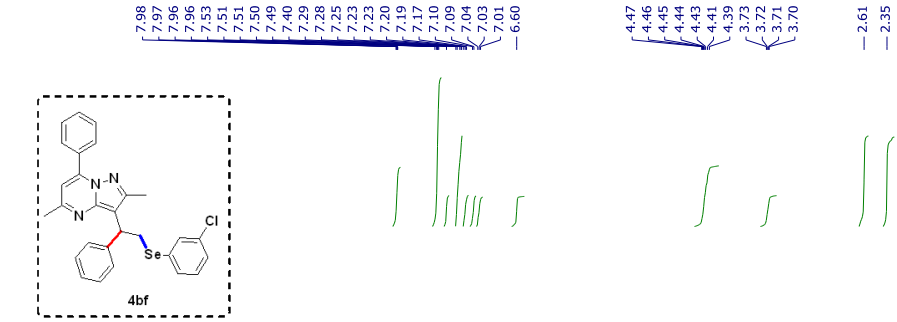
4bd (^{19}F NMR 471 MHz, $CDCl_3$)

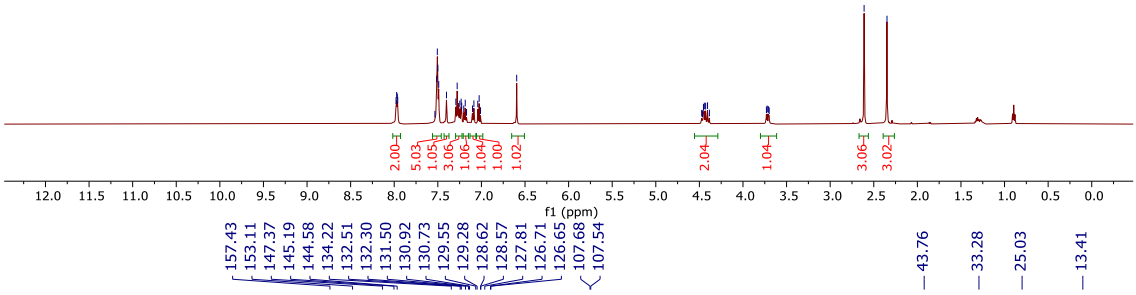


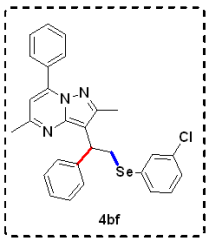
4be (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)

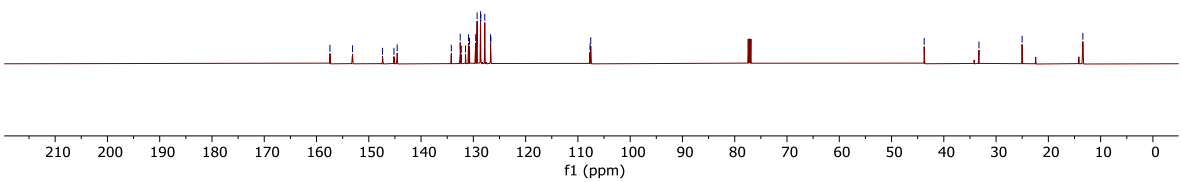


4bf (^{1}H 500MHz/ ^{13}C{^{1}H}126MHz-CDCl$_3$)

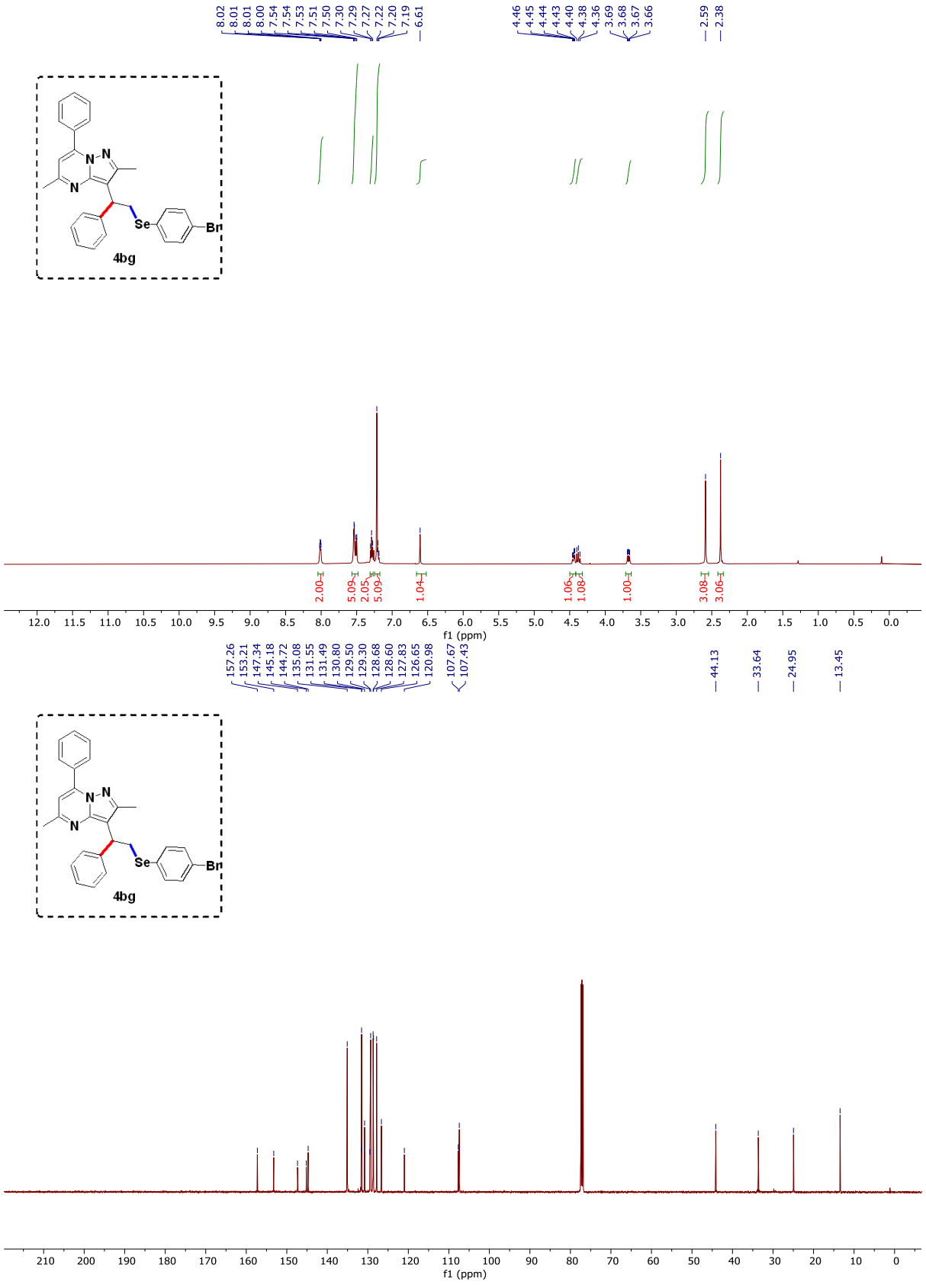




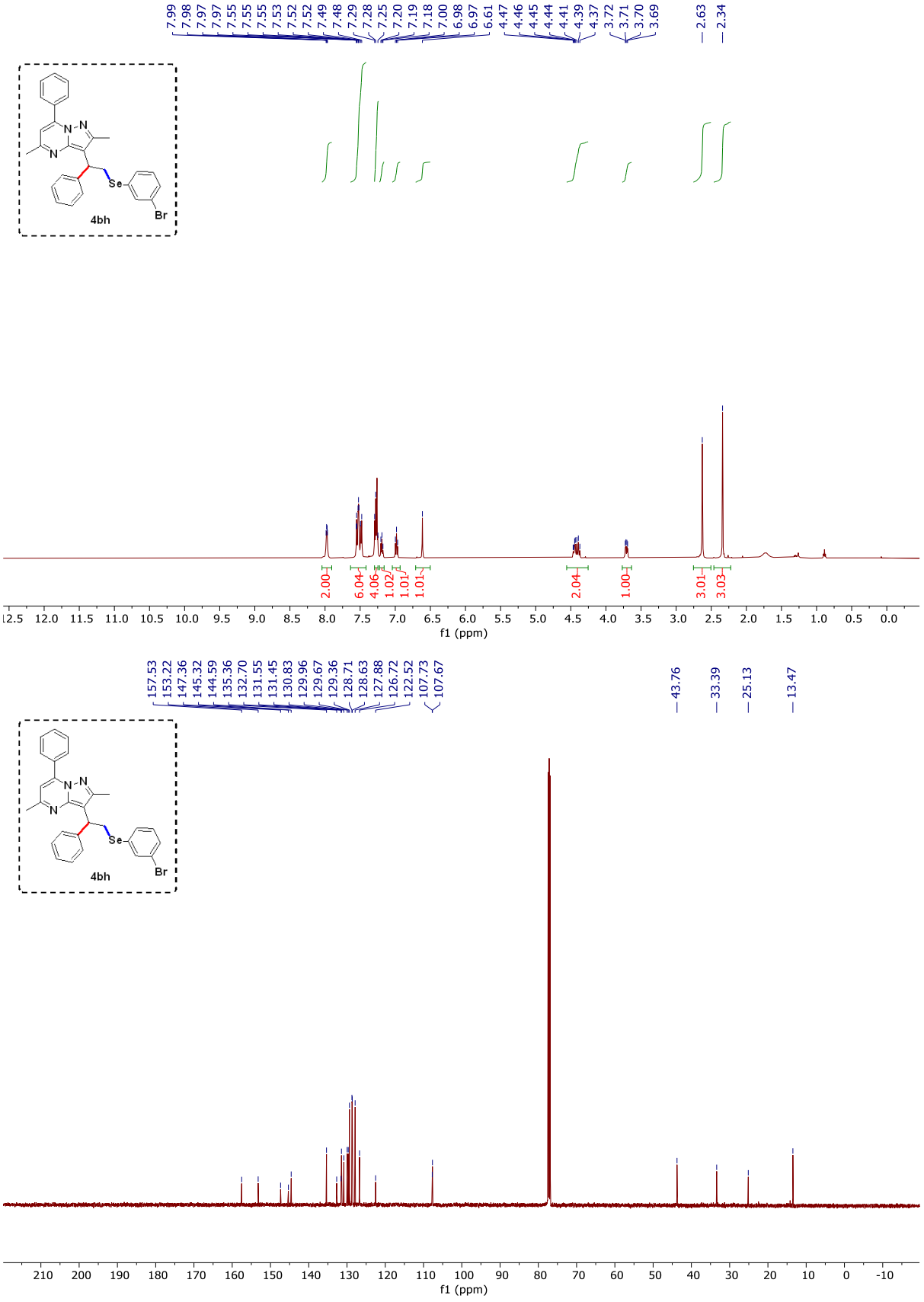




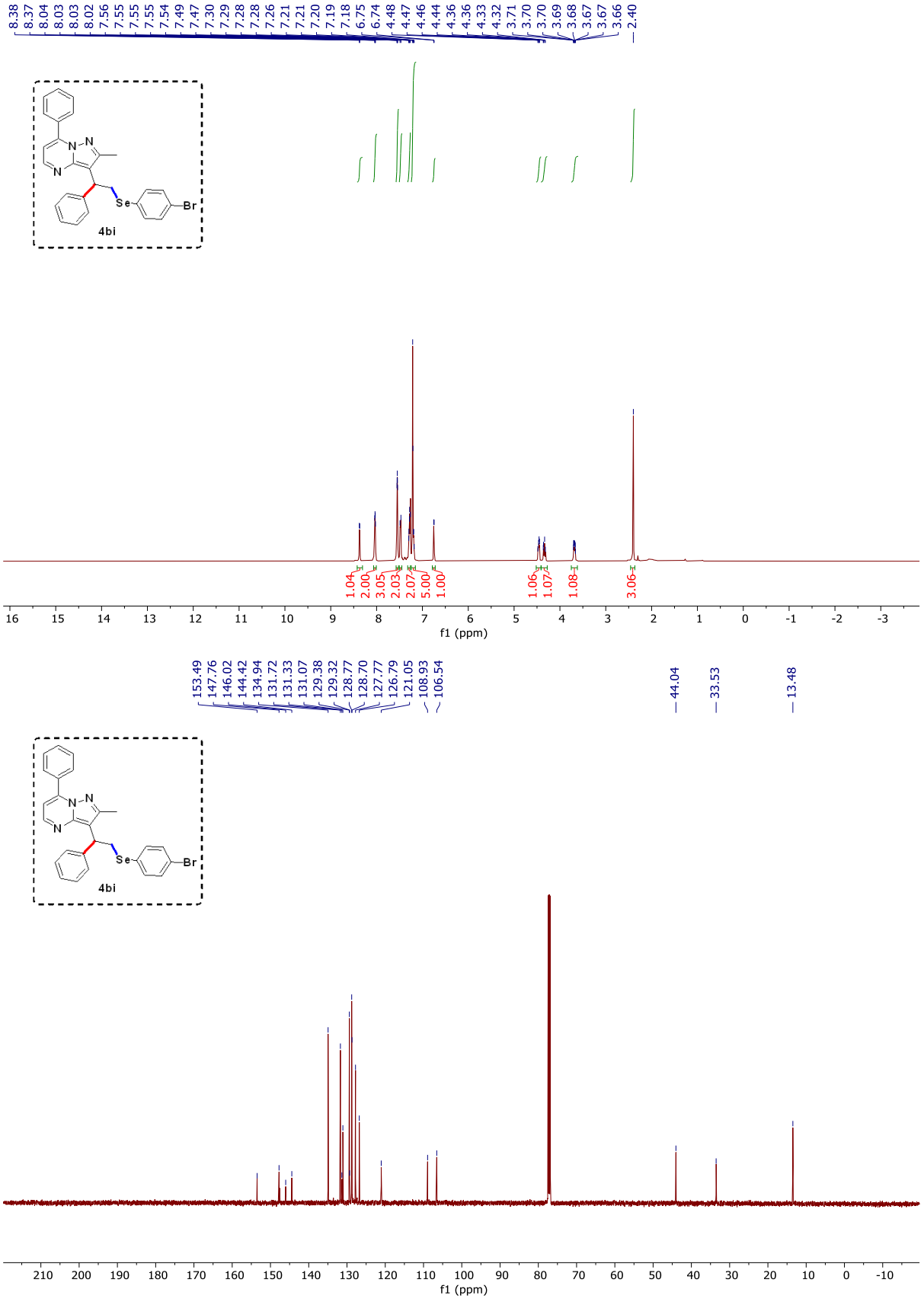
4bg (^{1}H 500MHz/ ^{13}C{^{1}H}126MHz-CDCl$_3$)



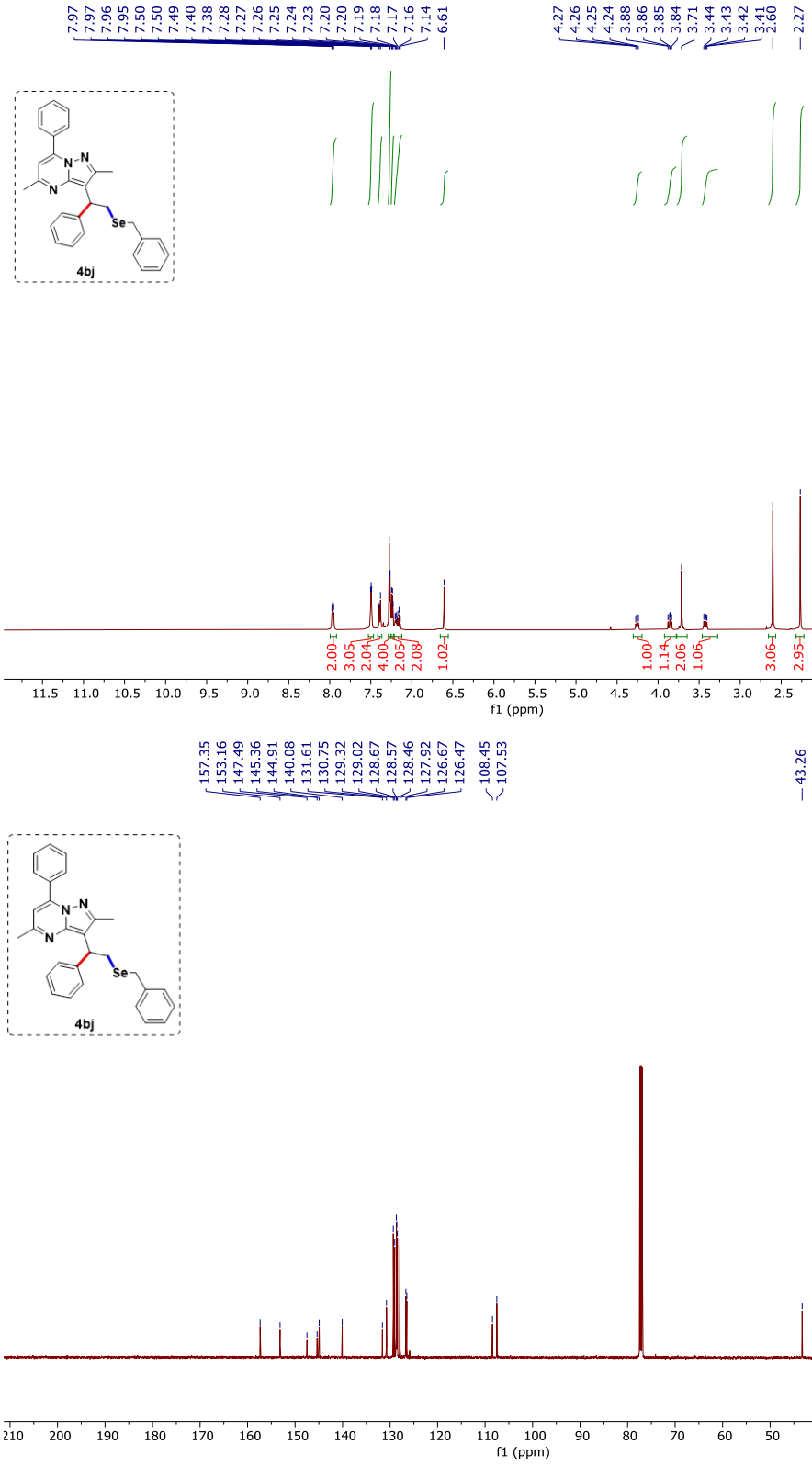
4bh (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-CDCl$_3$)



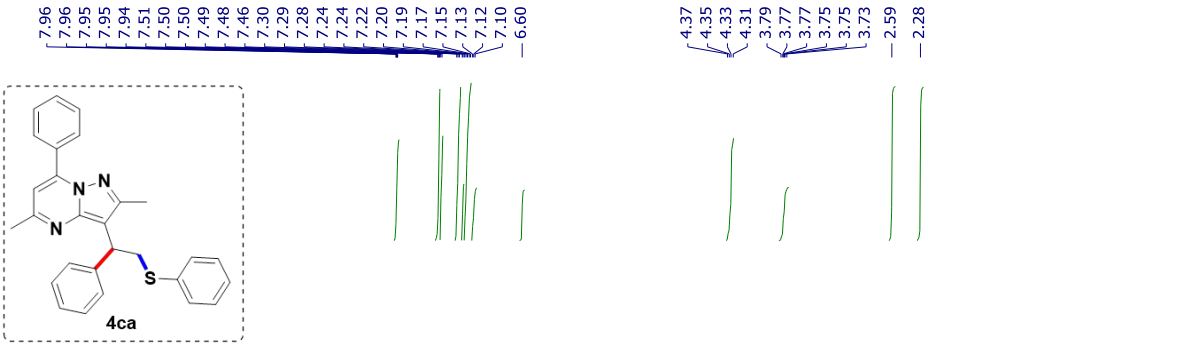
4bi (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)

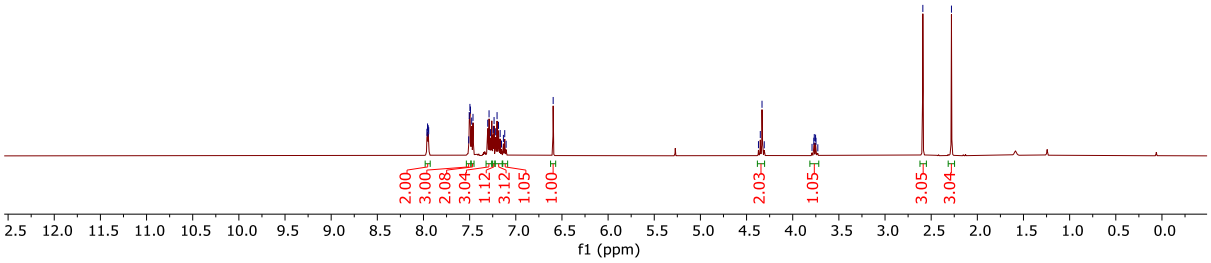


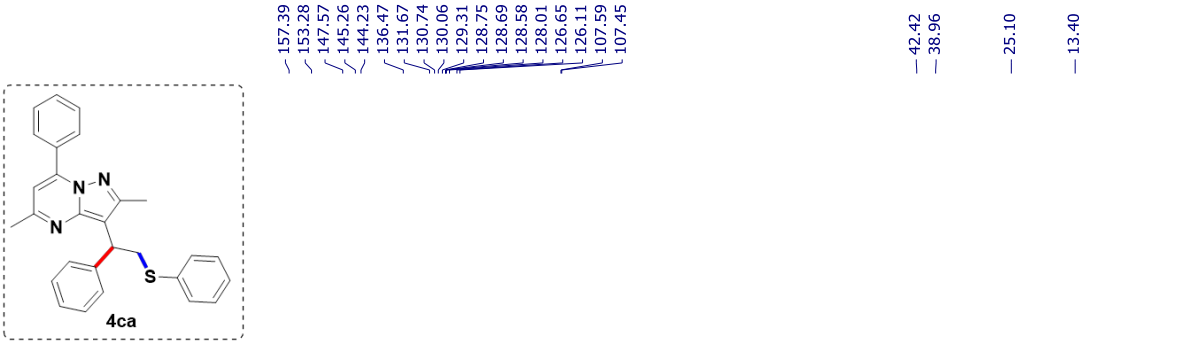
4bj (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)

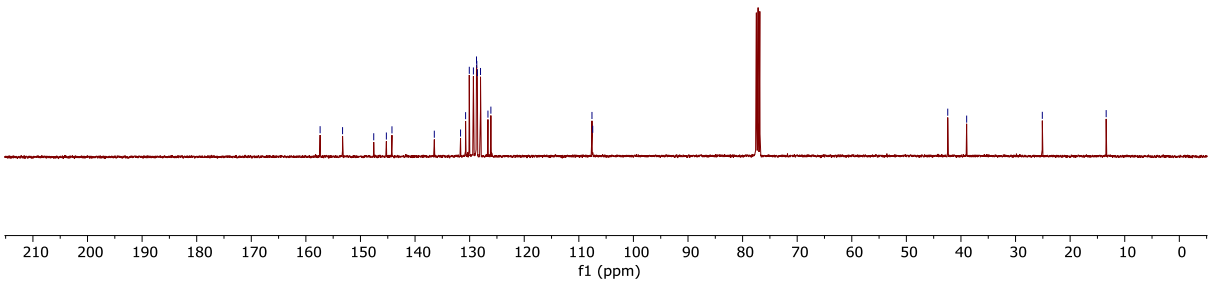


4ca (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)

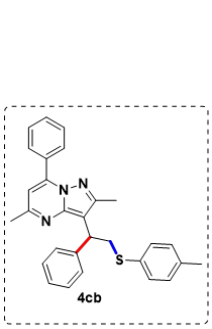


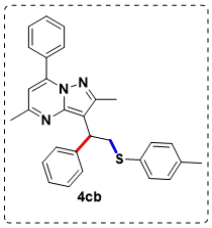




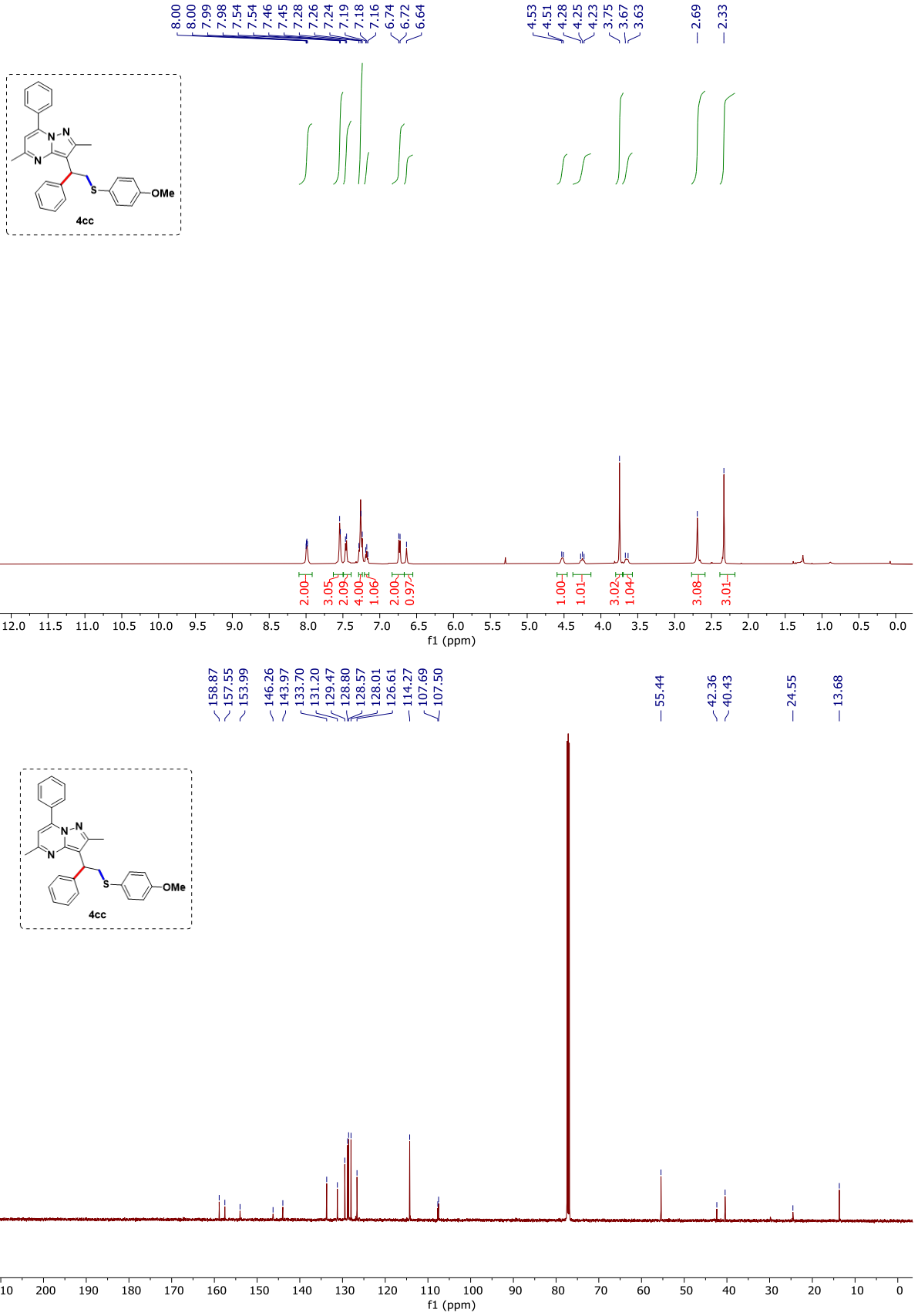


4cb (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-CDCl$_3$)

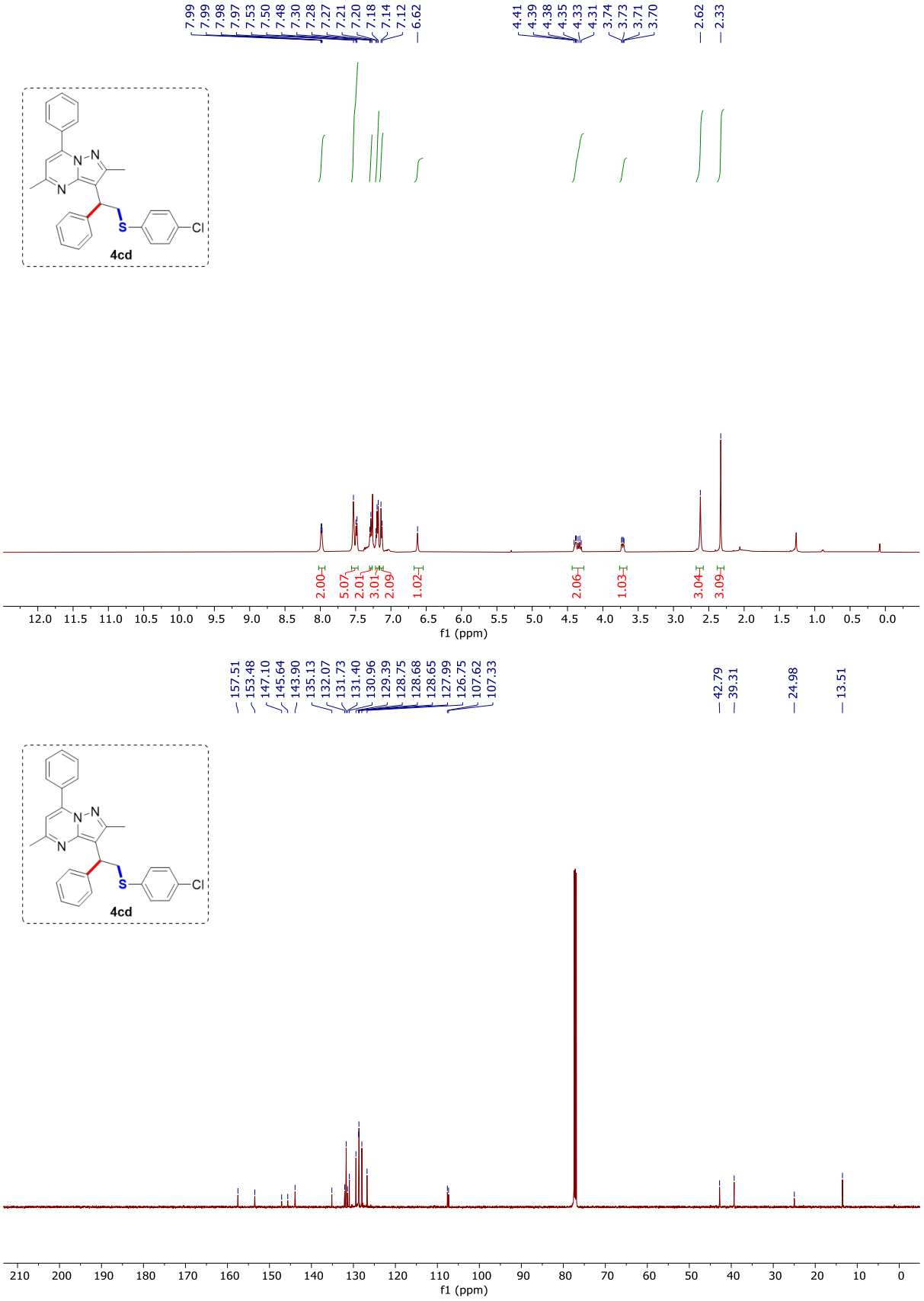




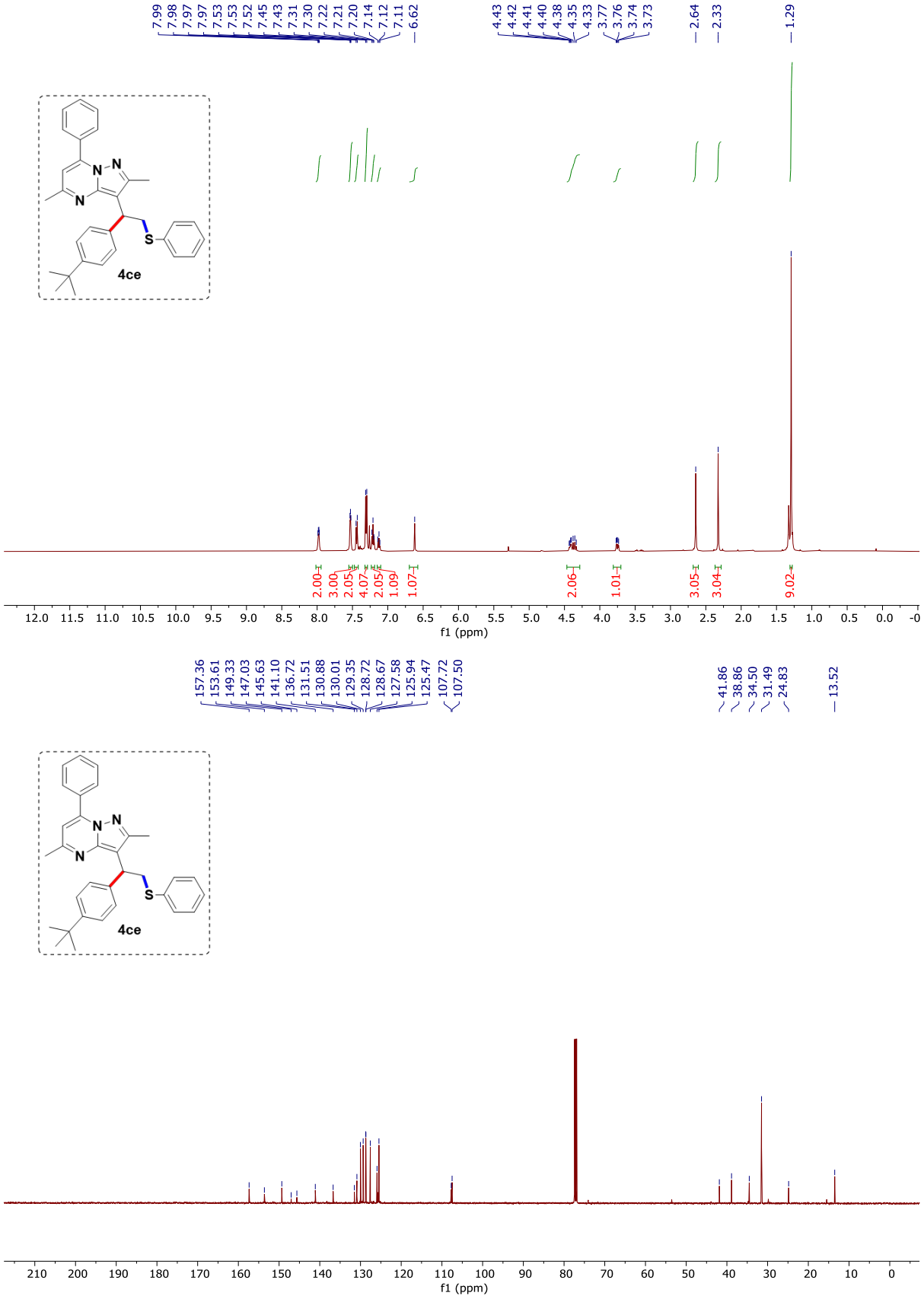
4cc (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)



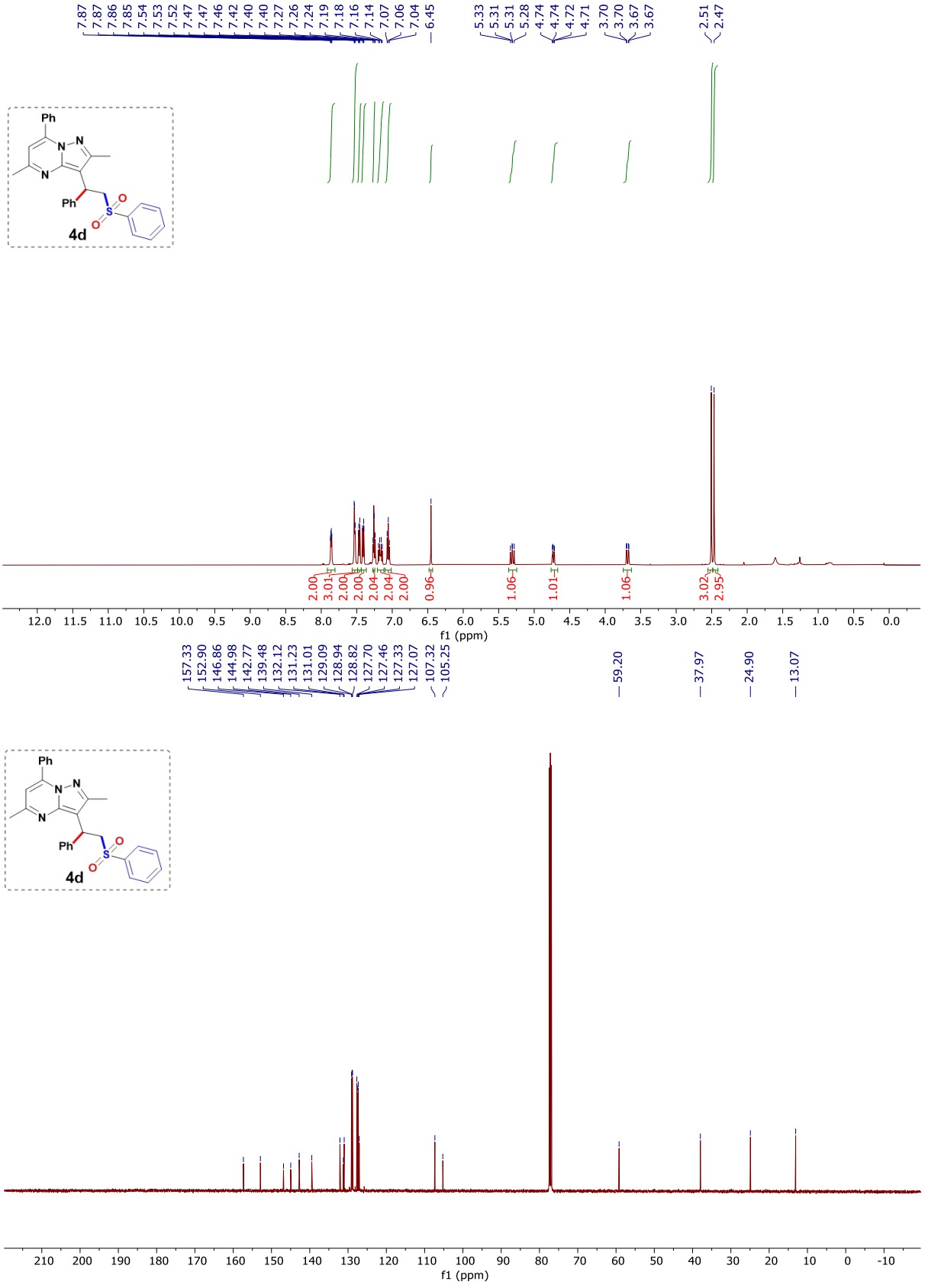
4cd (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)



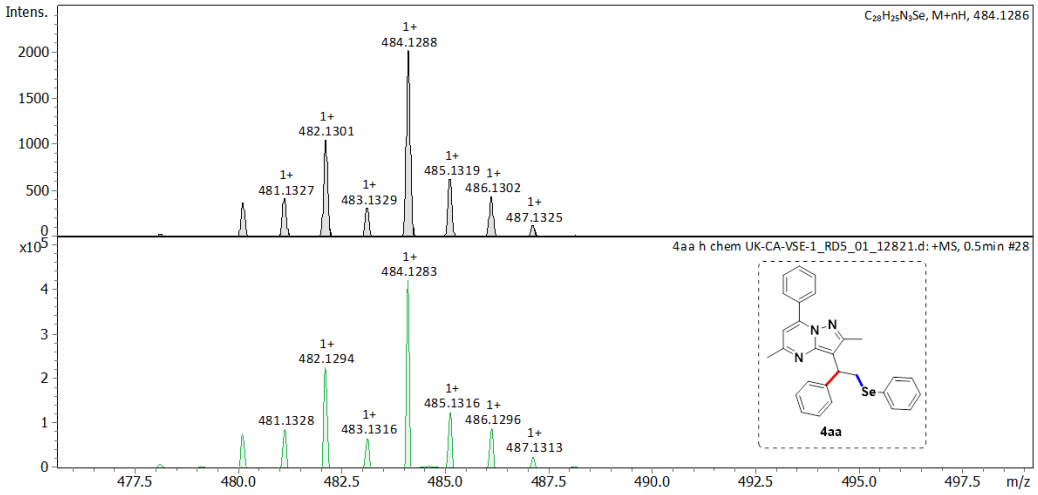
4ce (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)

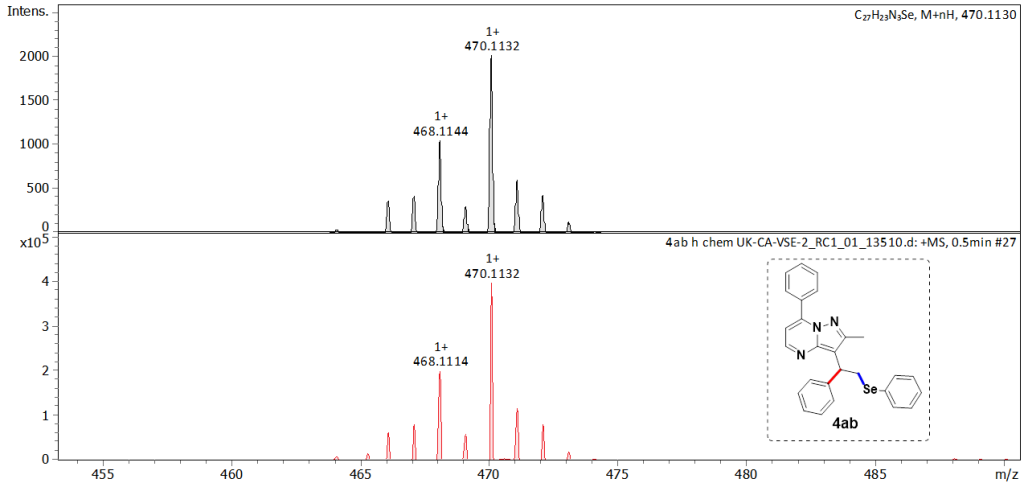


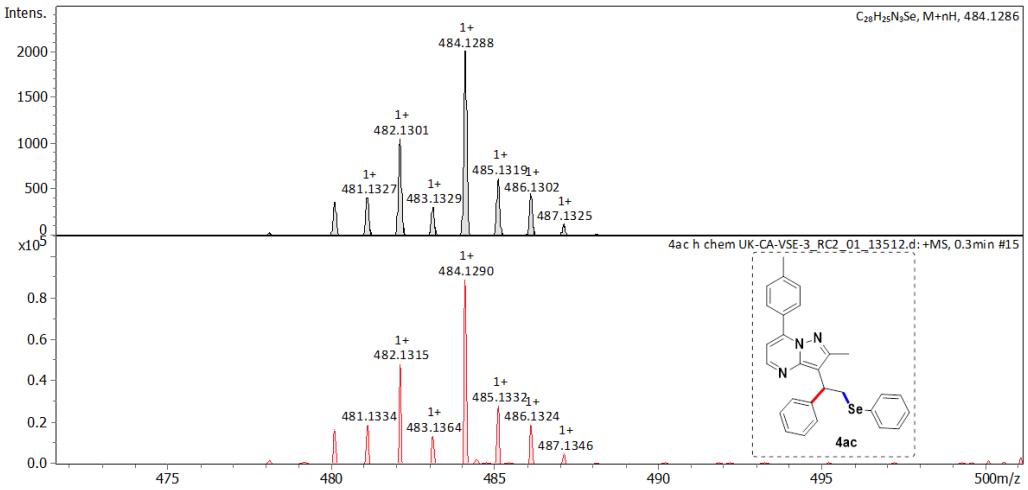
4d (^{1}H 500MHz/ ^{13}C{^{1}H} 126MHz-$CDCl_3$)

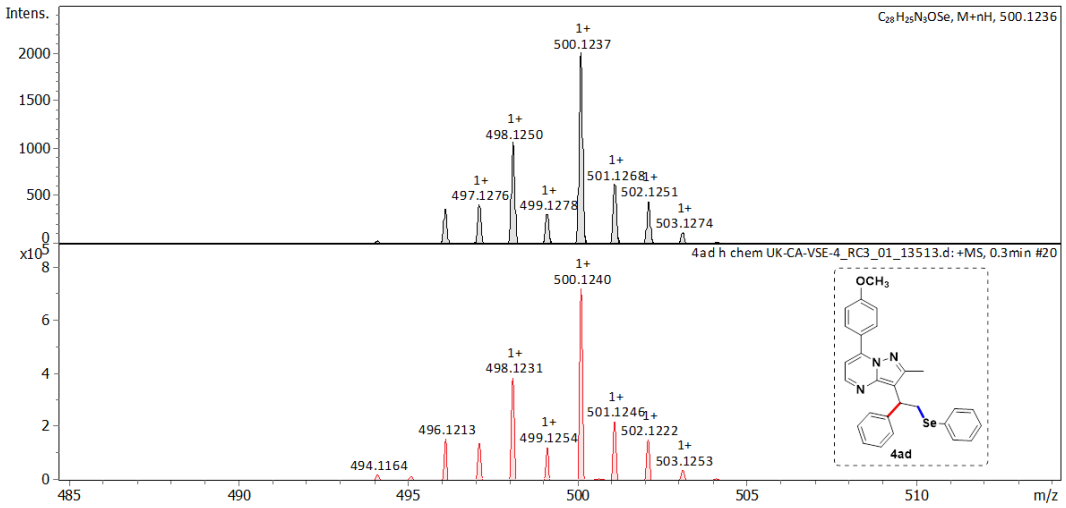


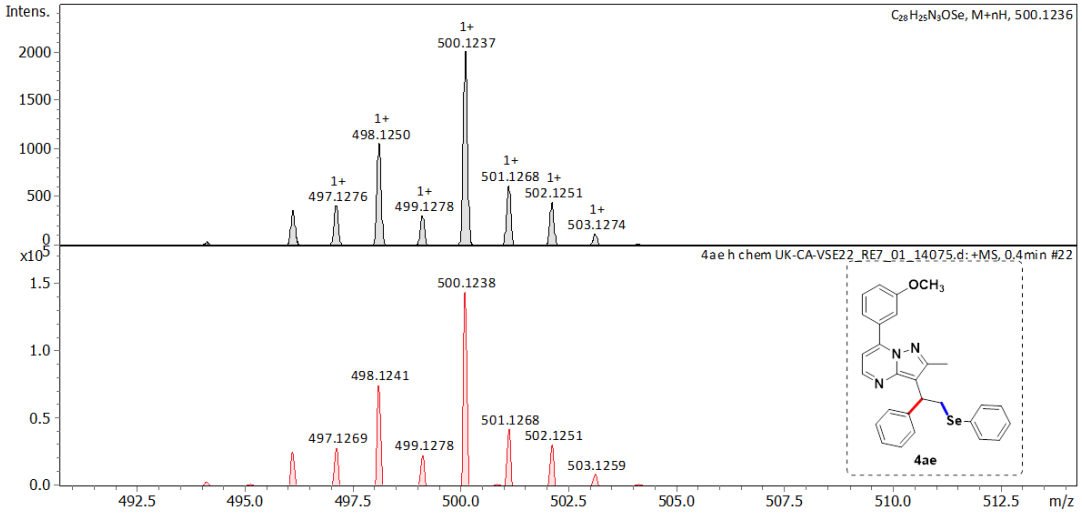
HRMS spectra of the compounds (**4aa-4at**, **4ba-4bj**, **4ca-4ce, 4d**)

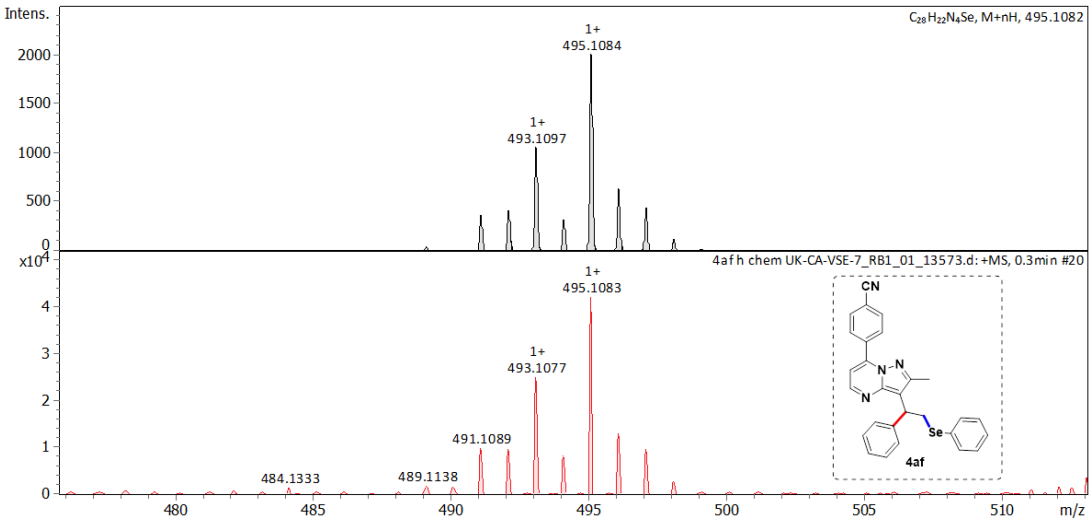


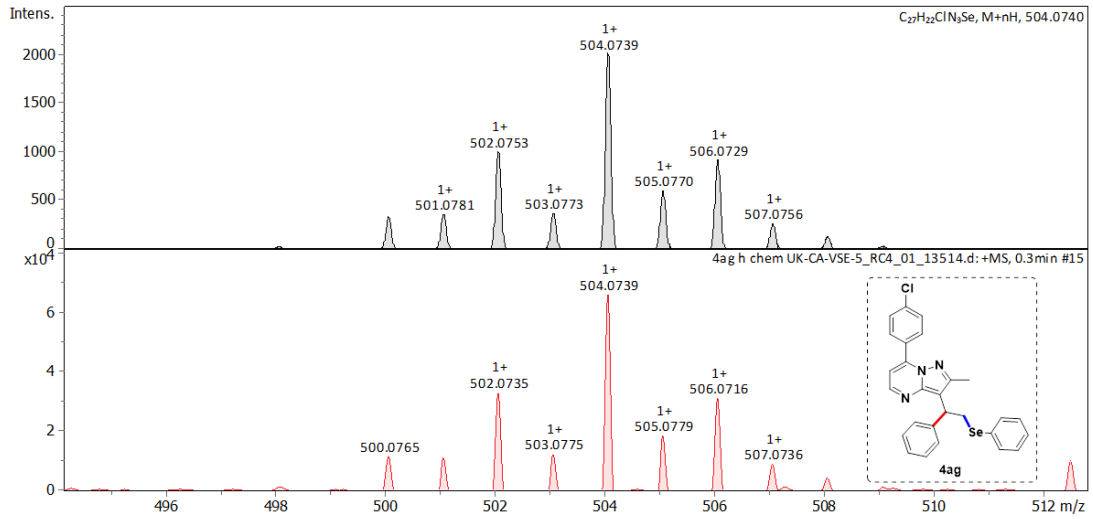


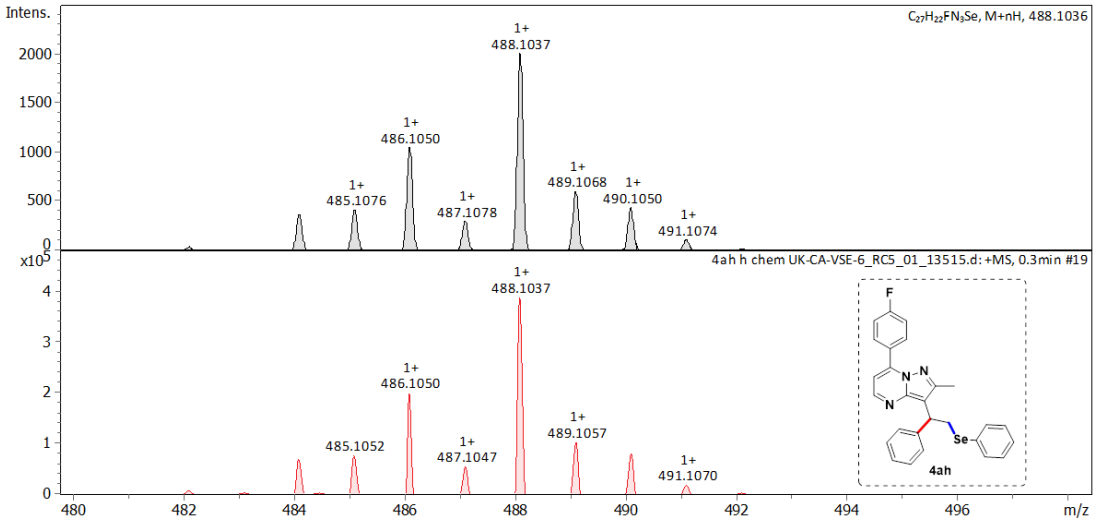


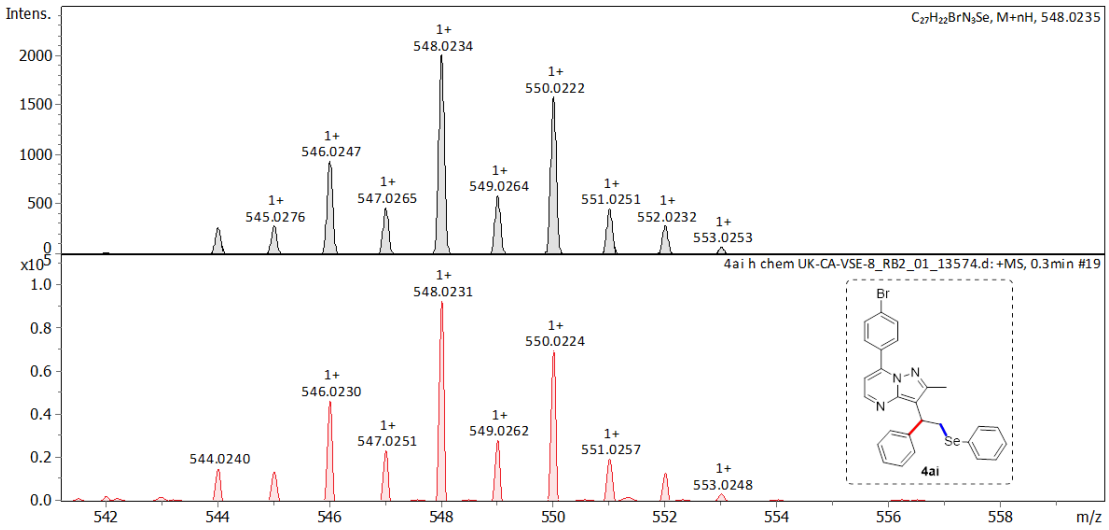

Intens.
C28H25N3OSe, M+nH, 500.1236
1+ 500.1237
1+ 498.1250
1+ 497.1276
1+ 499.1278
1+ 501.1268
1+ 502.1251
1+ 503.1274
4ad h chem UK-CA-VSE-4_RC3_01_13513.d: +MS, 0.3min #20
1+ 500.1240
1+ 498.1231
1+ 501.1246
1+ 502.1222
1+ 499.1254
1+ 503.1253
496.1213
494.1164
OCH3
Se
4ad
m/z

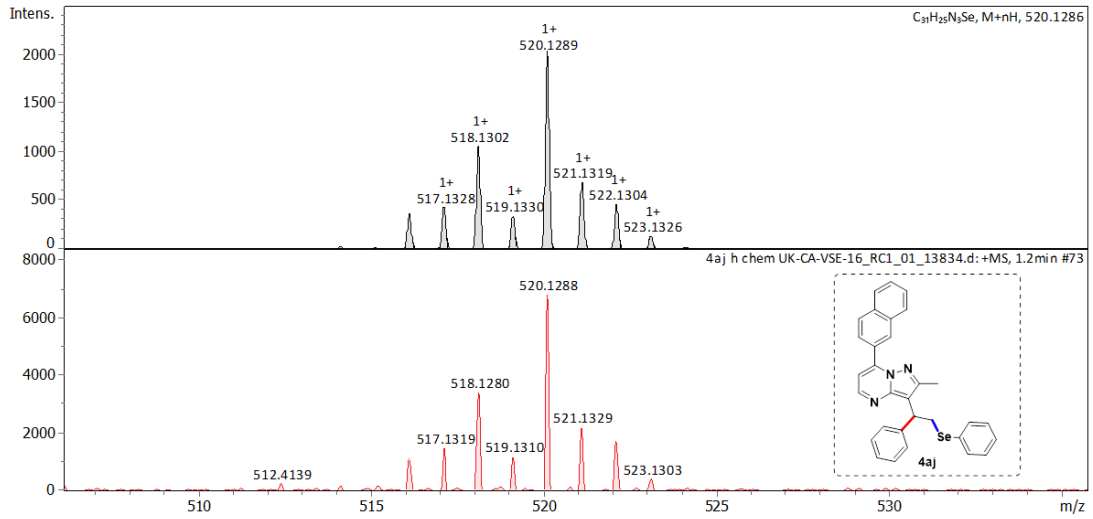

Intens.
C28H25N3OSe, M+nH, 500.1236
1+ 500.1237
1+ 498.1250
1+ 497.1276
1+ 499.1278
1+ 501.1268
1+ 502.1251
1+ 503.1274
4ae h chem UK-CA-VSE22_RE7_01_14075.d: +MS, 0.4min #22
500.1238
498.1241
497.1269
499.1278
501.1268
502.1251
503.1259
OCH3
Se
4ae
m/z

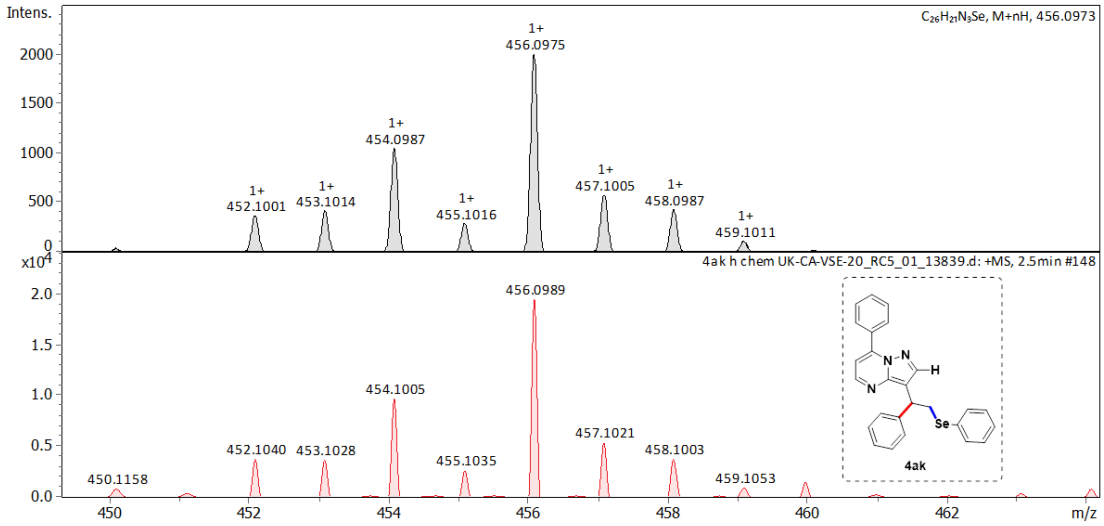

Intens.
C28H22N4Se, M+nH, 495.1082
1+ 495.1084
1+ 493.1097
4af h chem UK-CA-VSE-7_RB1_01_13573.d: +MS, 0.3min #20
1+ 495.1083
1+ 493.1077
491.1089
484.1333
489.1138
CN
Se
4af
m/z

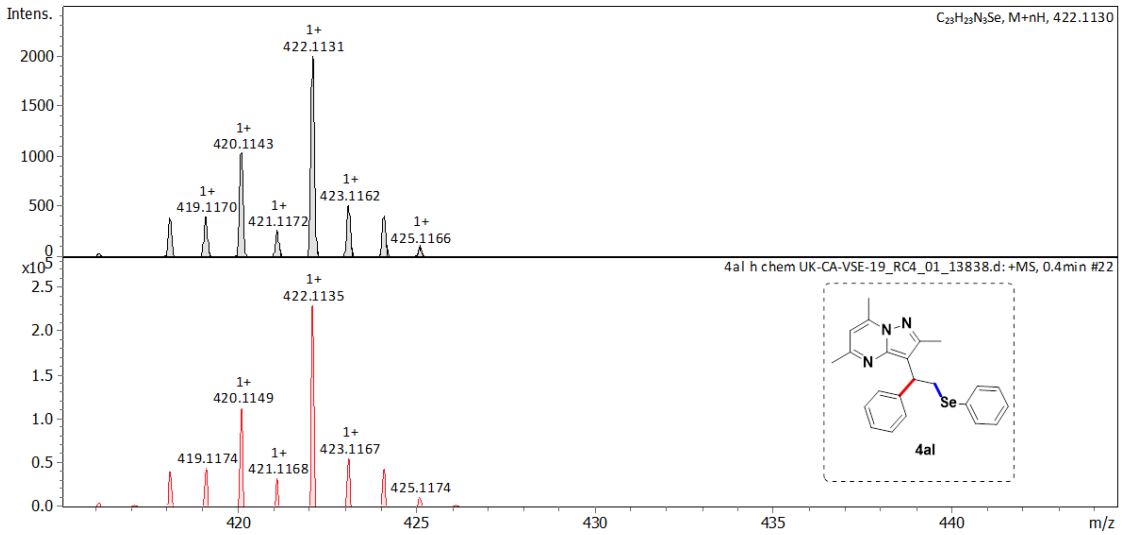

Intens.
C27H22ClN3Se, M+nH, 504.0740
1+ 504.0739
1+ 502.0753
1+ 501.0781
1+ 503.0773
1+ 506.0729
1+ 505.0770
1+ 507.0756
x10^4
4ag h chem UK-CA-VSE-5_RC4_01_13514.d: +MS, 0.3min #15
1+ 504.0739
1+ 502.0735
1+ 506.0716
1+ 505.0779
1+ 503.0775
500.0765
1+ 507.0736
Cl
N
N
Se
4ag
m/z

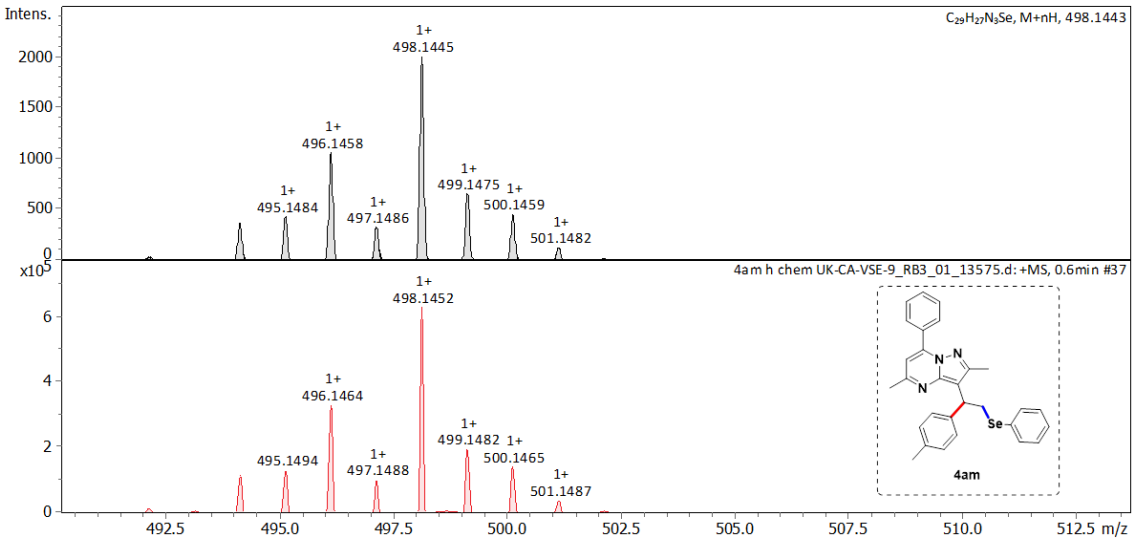

Intens.
C27H22FN3Se, M+nH, 488.1036
1+ 488.1037
1+ 486.1050
1+ 485.1076
1+ 489.1068
1+ 490.1050
1+ 487.1078
1+ 491.1074
x10^5
4ah h chem UK-CA-VSE-6_RC5_01_13515.d: +MS, 0.3min #19
1+ 488.1037
1+ 486.1050
485.1052
1+ 489.1057
1+ 487.1047
1+ 491.1070
F
N
N
Se
4ah
m/z

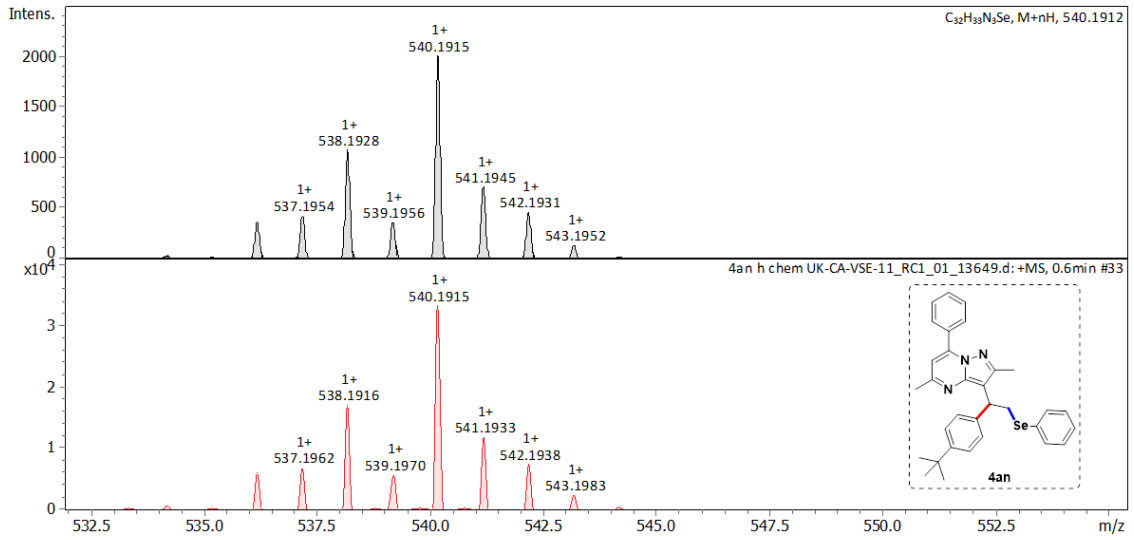

Intens.
C27H22BrN3Se, M+nH, 548.0235
1+ 548.0234
1+ 550.0222
1+ 546.0247
1+ 547.0265
1+ 549.0264
1+ 545.0276
1+ 551.0251
1+ 552.0232
1+ 553.0253
x10^5
4ai h chem UK-CA-VSE-8_RB2_01_13574.d: +MS, 0.3min #19
1+ 548.0231
1+ 550.0224
1+ 546.0230
1+ 547.0251
1+ 549.0262
1+ 551.0257
544.0240
1+ 553.0248
Br
N
N
Se
4ai
m/z


Intens.
C31H25N3Se, M+nH, 520.1286
1+ 520.1289
1+ 518.1302
1+ 521.1319
1+ 517.1328
1+ 519.1330
1+ 522.1304
1+ 523.1326
4aj h chem UK-CA-VSE-16_RC1_01_13834.d: +MS, 1.2min #73
520.1288
518.1280
521.1329
517.1319
519.1310
512.4139
523.1303
4aj
m/z


Intens.
C26H21N3Se, M+nH, 456.0973
1+ 456.0975
1+ 454.0987
1+ 452.1001
1+ 453.1014
1+ 455.1016
1+ 457.1005
1+ 458.0987
1+ 459.1011
x10^4
4ak h chem UK-CA-VSE-20_RC5_01_13839.d: +MS, 2.5min #148
456.0989
454.1005
457.1021
452.1040
453.1028
458.1003
455.1035
450.1158
459.1053
4ak
m/z


Intens.
C23H23N3Se, M+nH, 422.1130
1+ 422.1131
1+ 420.1143
1+ 419.1170
1+ 423.1162
1+ 421.1172
1+ 425.1166
x10^5
4al h chem UK-CA-VSE-19_RC4_01_13838.d: +MS, 0.4min #22
1+ 422.1135
1+ 420.1149
1+ 423.1167
419.1174
1+ 421.1168
425.1174
4al
m/z


Intens.
C29H27N3Se, M+nH, 498.1443
1+ 498.1445
1+ 496.1458
1+ 495.1484
1+ 497.1486
1+ 499.1475
1+ 500.1459
1+ 501.1482
x10^5
4am h chem UK-CA-VSE-9_RB3_01_13575.d: +MS, 0.6min #37
1+ 498.1452
1+ 496.1464
495.1494
1+ 497.1488
1+ 499.1482
1+ 500.1465
1+ 501.1487
Se
4am
492.5
495.0
497.5
500.0
502.5
505.0
507.5
510.0
512.5 m/z


Intens.
C32H33N3Se, M+nH, 540.1912
1+ 540.1915
1+ 538.1928
1+ 537.1954
1+ 539.1956
1+ 541.1945
1+ 542.1931
1+ 543.1952
x10^4
4an h chem UK-CA-VSE-11_RC1_01_13649.d: +MS, 0.6min #33
1+ 540.1915
1+ 538.1916
1+ 537.1962
1+ 539.1970
1+ 541.1933
1+ 542.1938
1+ 543.1983
Se
4an
532.5
535.0
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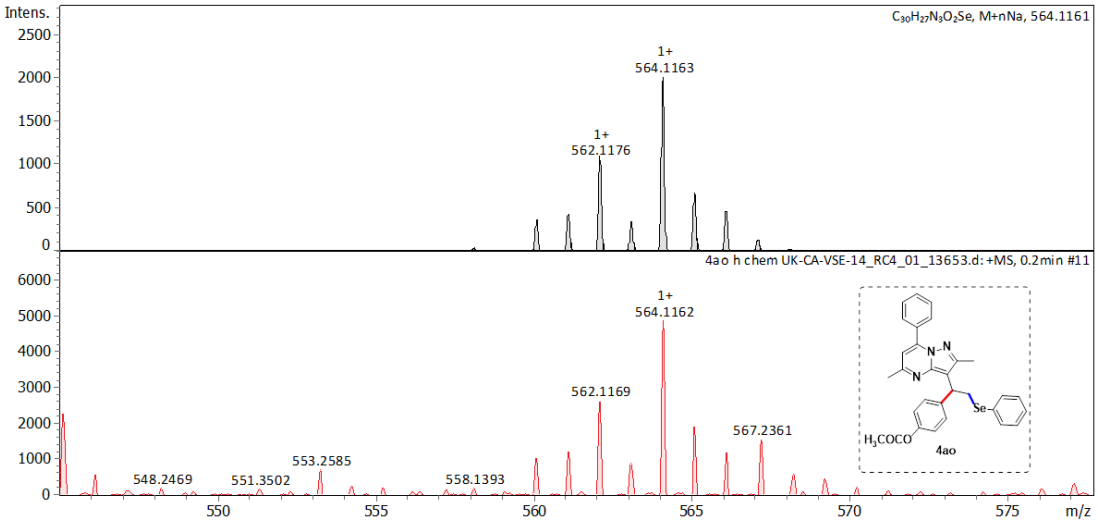
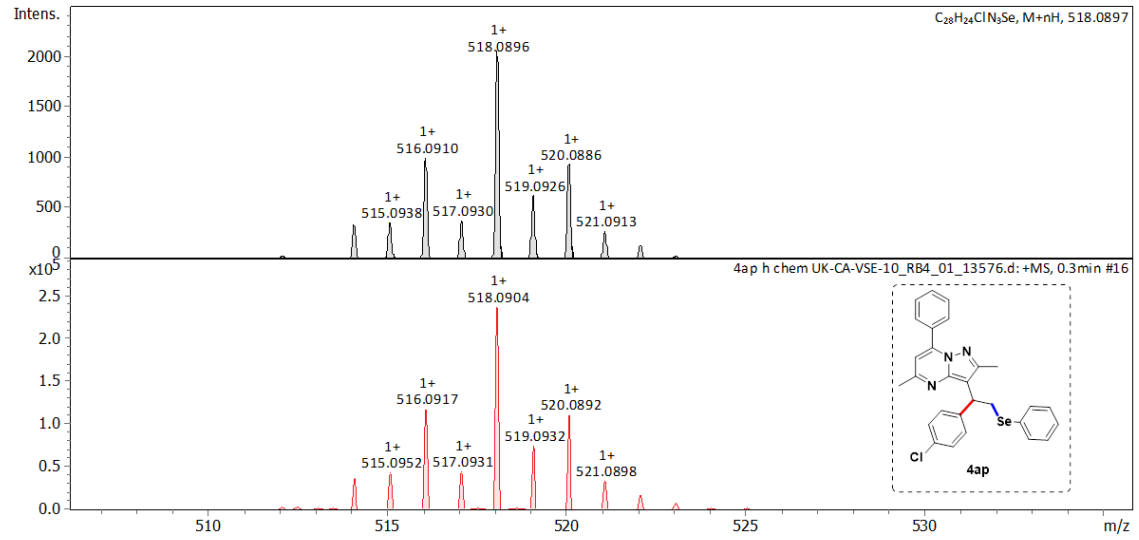
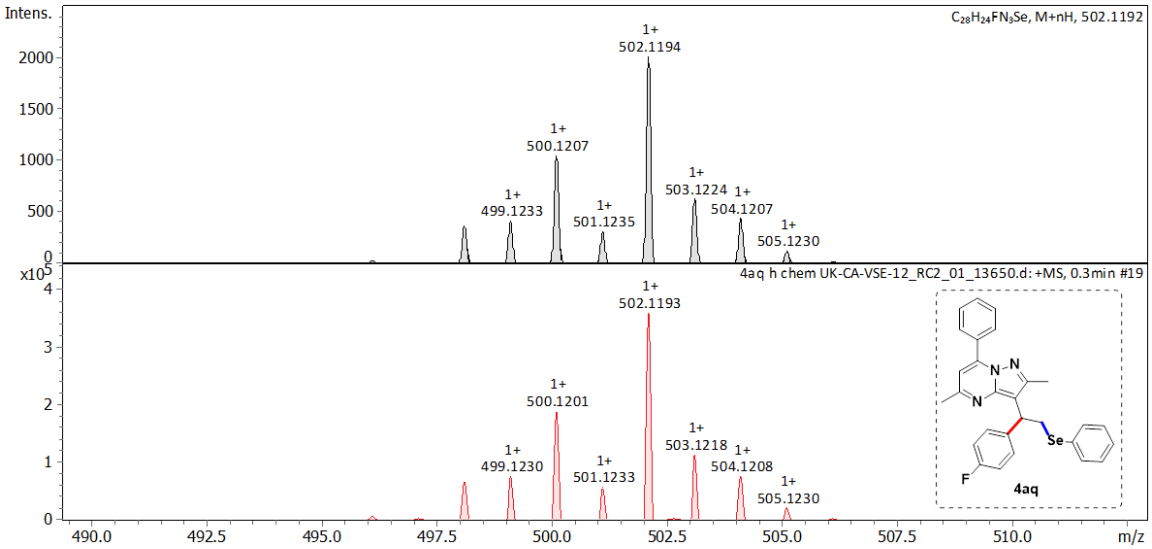
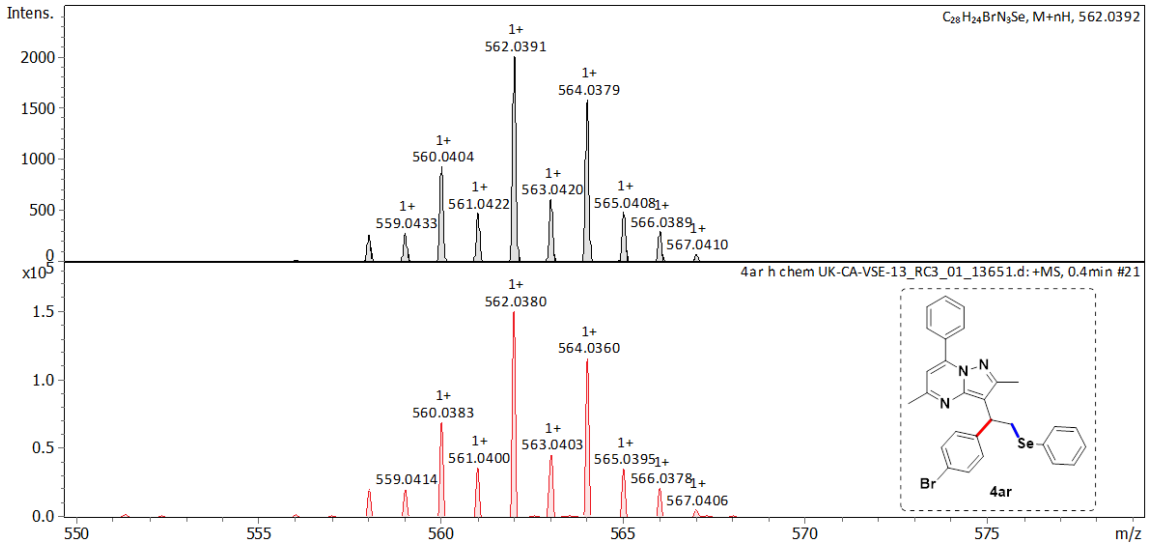
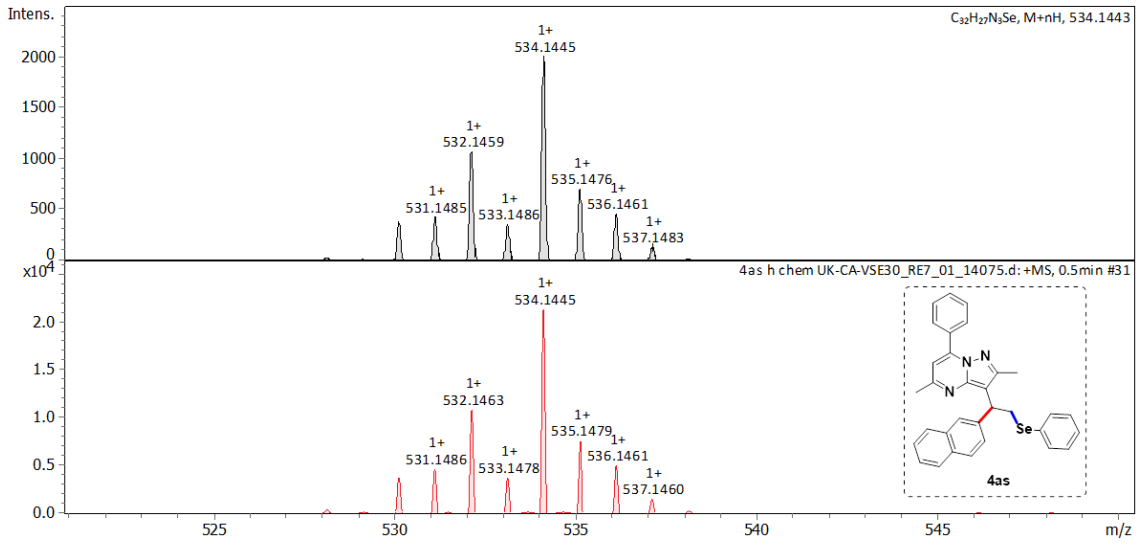
542.5
545.0
547.5
550.0
552.5
m/z

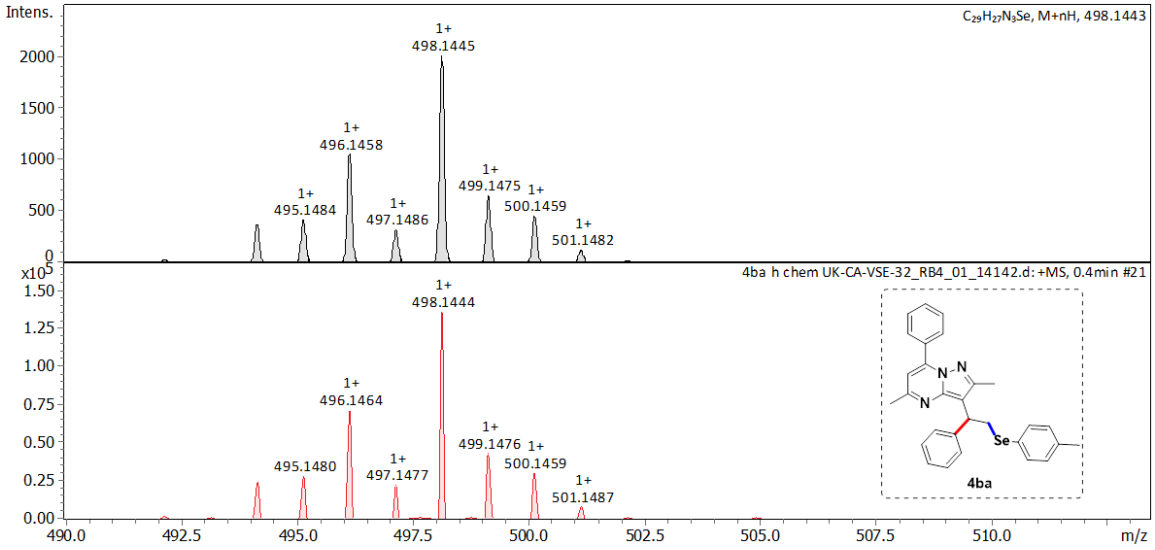

Intens.
C30H27N3O2Se, M+nNa, 564.1161
1+ 564.1163
1+ 562.1176
4ao h chem UK-CA-VSE-14_RC4_01_13653.d: +MS, 0.2min #11
1+ 564.1162
562.1169
567.2361
553.2585
548.2469
551.3502
558.1393
H3COCO
Se
4ao
550
555
560
565
570
575
m/z

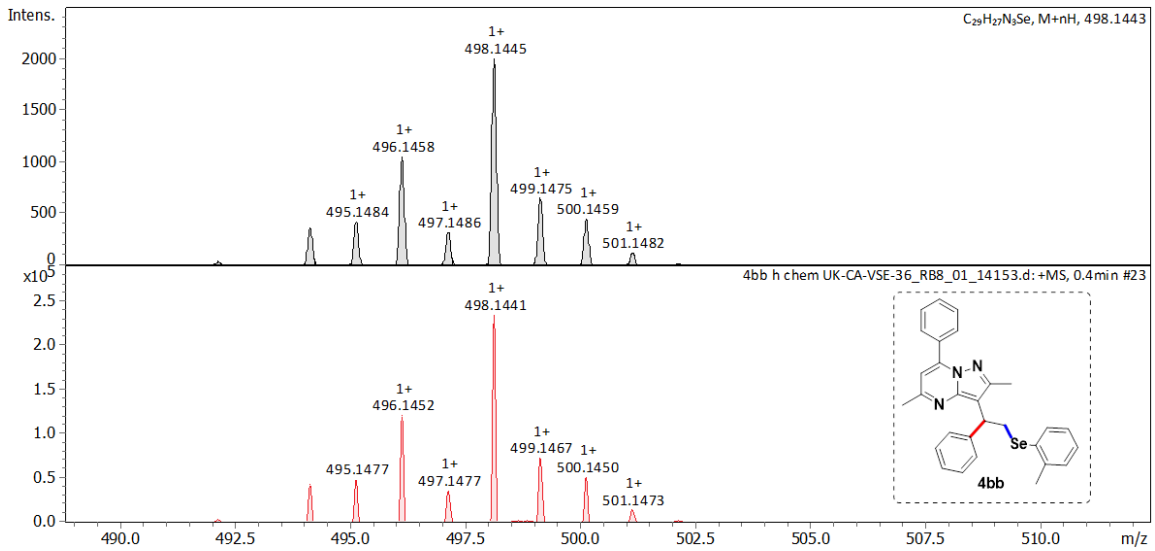

Intens.
$C_{28}H_{24}ClN_3Se$, M+nH, 518.0897
1+ 518.0896
1+ 516.0910
1+ 520.0886
1+ 519.0926
1+ 515.0938
1+ 517.0930
1+ 521.0913
4ap h chem UK-CA-VSE-10_RB4_01_13576.d: +MS, 0.3min #16
1+ 518.0904
1+ 516.0917
1+ 520.0892
1+ 519.0932
1+ 515.0952
1+ 517.0931
1+ 521.0898
Cl
Se
4ap
m/z

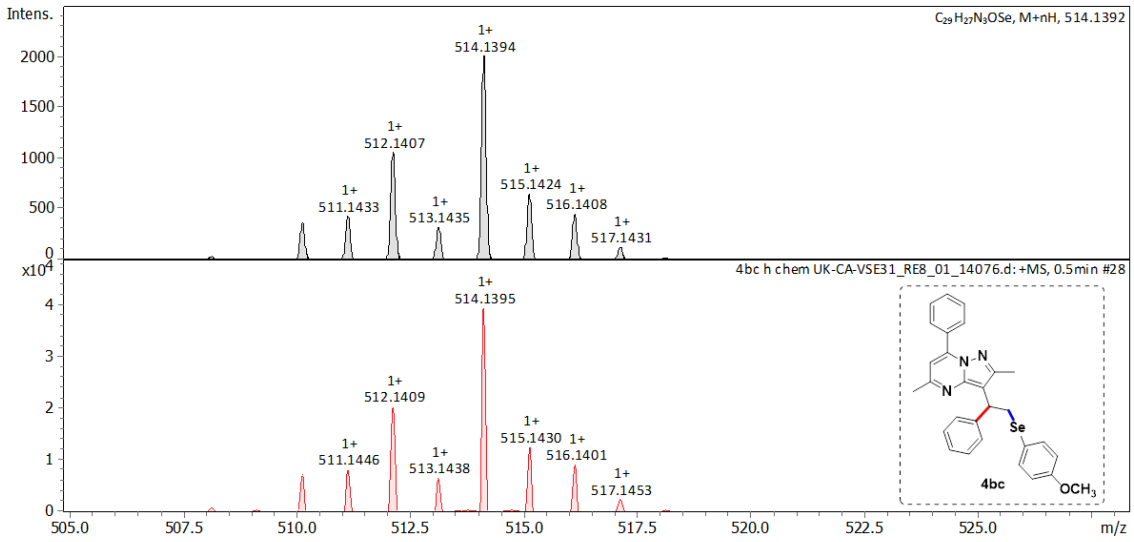

Intens.
$C_{28}H_{24}FN_3Se$, M+nH, 502.1192
1+ 502.1194
1+ 500.1207
1+ 503.1224
1+ 499.1233
1+ 501.1235
1+ 504.1207
1+ 505.1230
4aq h chem UK-CA-VSE-12_RC2_01_13650.d: +MS, 0.3min #19
1+ 502.1193
1+ 500.1201
1+ 503.1218
1+ 499.1230
1+ 501.1233
1+ 504.1208
1+ 505.1230
F
Se
4aq
m/z

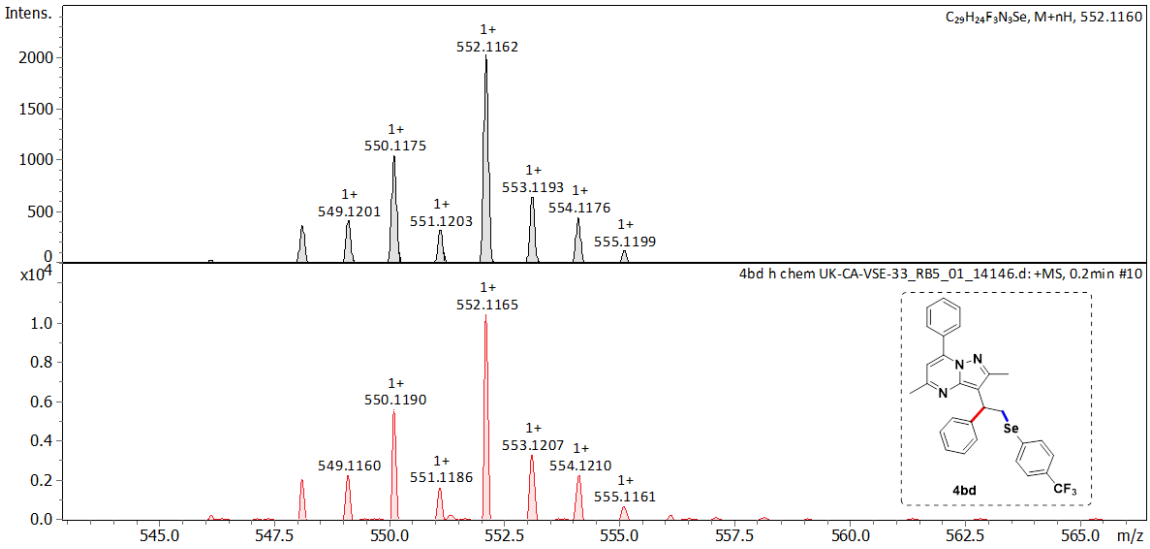

Intens.
$C_{28}H_{24}BrN_3Se$, M+nH, 562.0392
1+ 562.0391
1+ 564.0379
1+ 560.0404
1+ 563.0420
1+ 561.0422
1+ 565.0408
1+ 559.0433
1+ 566.0389
1+ 567.0410
4ar h chem UK-CA-VSE-13_RC3_01_13651.d: +MS, 0.4min #21
1+ 562.0380
1+ 564.0360
1+ 560.0383
1+ 563.0403
1+ 561.0400
1+ 565.0395
559.0414
1+ 566.0378
1+ 567.0406
Br
Se
4ar
m/z

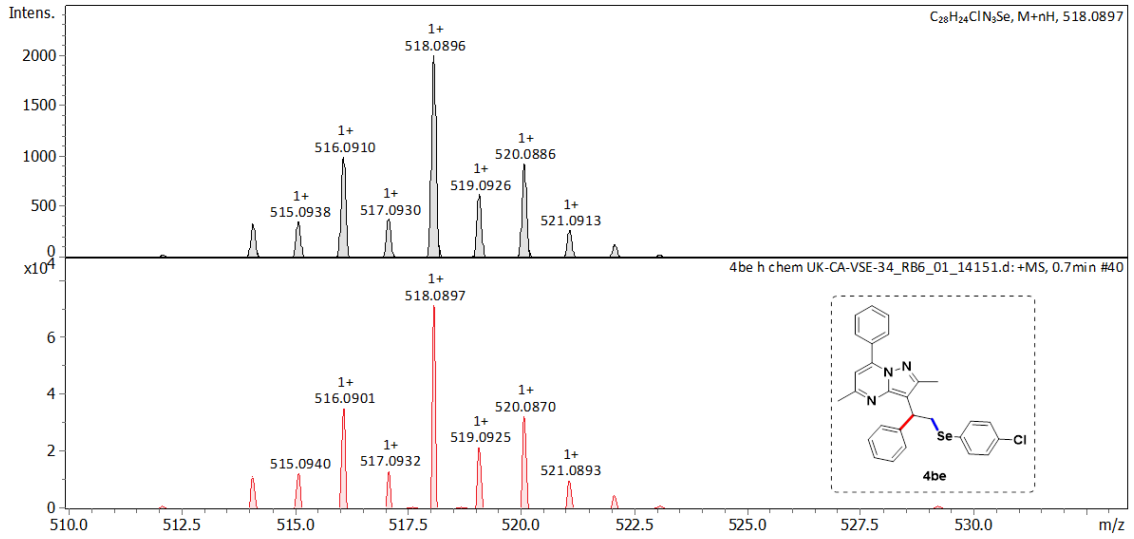

Intens.
$C_{32}H_{27}N_3Se$, M+nH, 534.1443
1+ 534.1445
1+ 532.1459
1+ 531.1485
1+ 533.1486
1+ 535.1476
1+ 536.1461
1+ 537.1483
4as h chem UK-CA-VSE30_RE7_01_14075.d: +MS, 0.5min #31
1+ 534.1445
1+ 532.1463
1+ 531.1486
1+ 533.1478
1+ 535.1479
1+ 536.1461
1+ 537.1460
4as
m/z

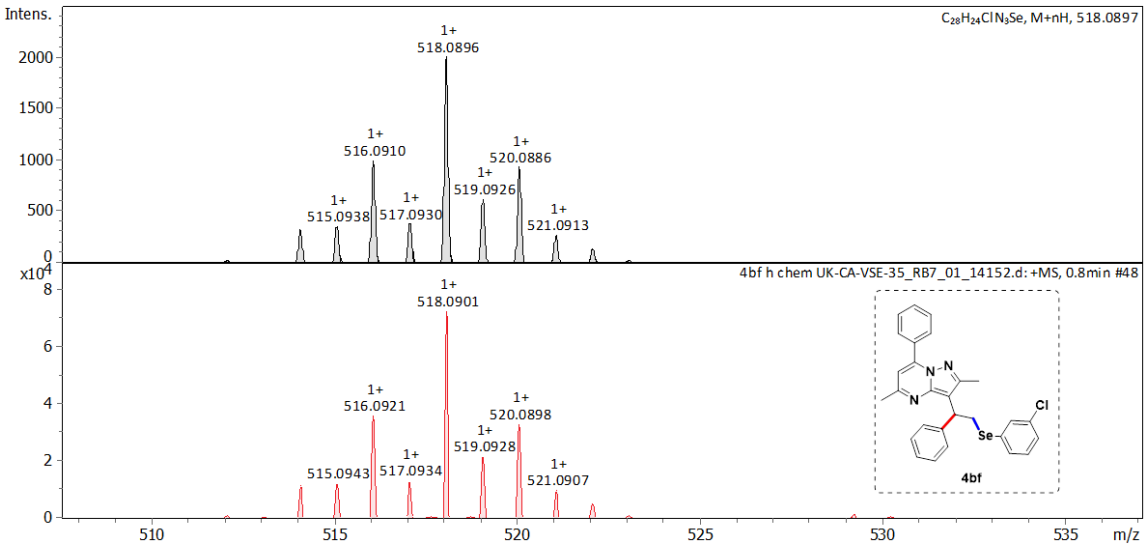

Intens.
$C_{29}H_{27}N_3Se$, M+nH, 498.1443
1+ 498.1445
1+ 496.1458
1+ 495.1484
1+ 497.1486
1+ 499.1475
1+ 500.1459
1+ 501.1482
4ba h chem UK-CA-VSE-32_RB4_01_14142.d: +MS, 0.4min #21
1+ 498.1444
1+ 496.1464
1+ 495.1480
1+ 497.1477
1+ 499.1476
1+ 500.1459
1+ 501.1487
4ba
m/z

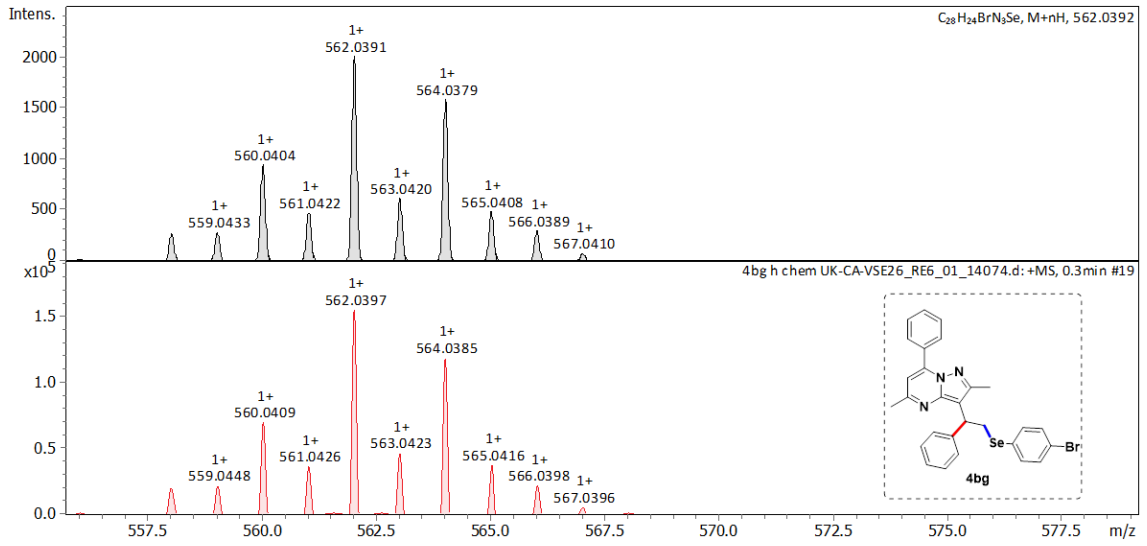

Intens.
$C_{29}H_{27}N_3Se$, M+nH, 498.1443
1+ 498.1445
1+ 496.1458
1+ 495.1484
1+ 497.1486
1+ 499.1475
1+ 500.1459
1+ 501.1482
4bb h chem UK-CA-VSE-36_RB8_01_14153.d: +MS, 0.4min #23
1+ 498.1441
1+ 496.1452
1+ 495.1477
1+ 497.1477
1+ 499.1467
1+ 500.1450
1+ 501.1473
4bb
m/z

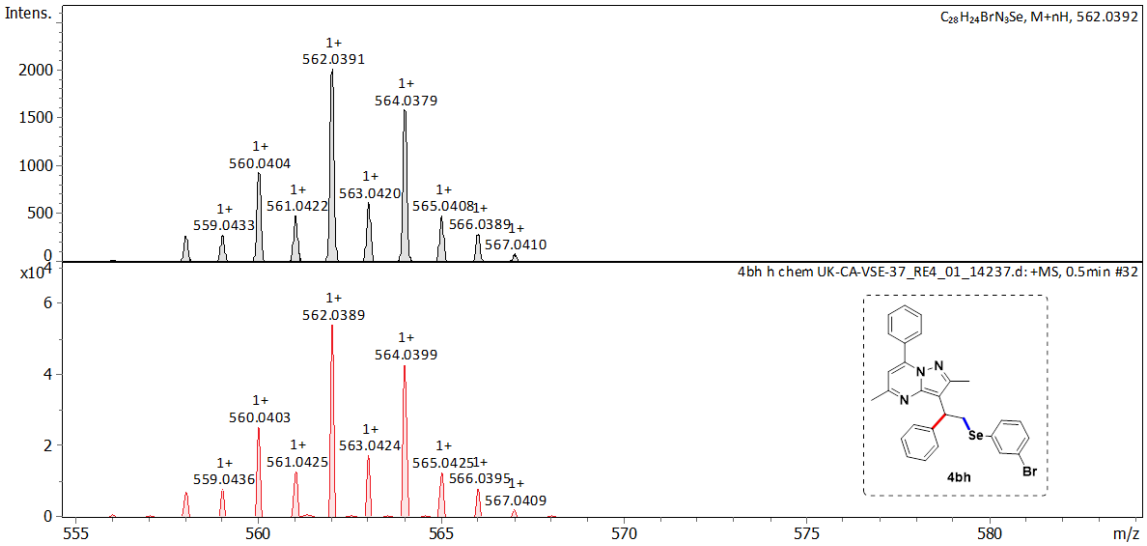

Intens.
$C_{29}H_{27}N_3OSe$, M+nH, 514.1392
1+ 514.1394
1+ 512.1407
1+ 511.1433
1+ 513.1435
1+ 515.1424
1+ 516.1408
1+ 517.1431
4bc h chem UK-CA-VSE31_RE8_01_14076.d: +MS, 0.5min #28
1+ 514.1395
1+ 512.1409
1+ 511.1446
1+ 513.1438
1+ 515.1430
1+ 516.1401
1+ 517.1453
4bc
m/z

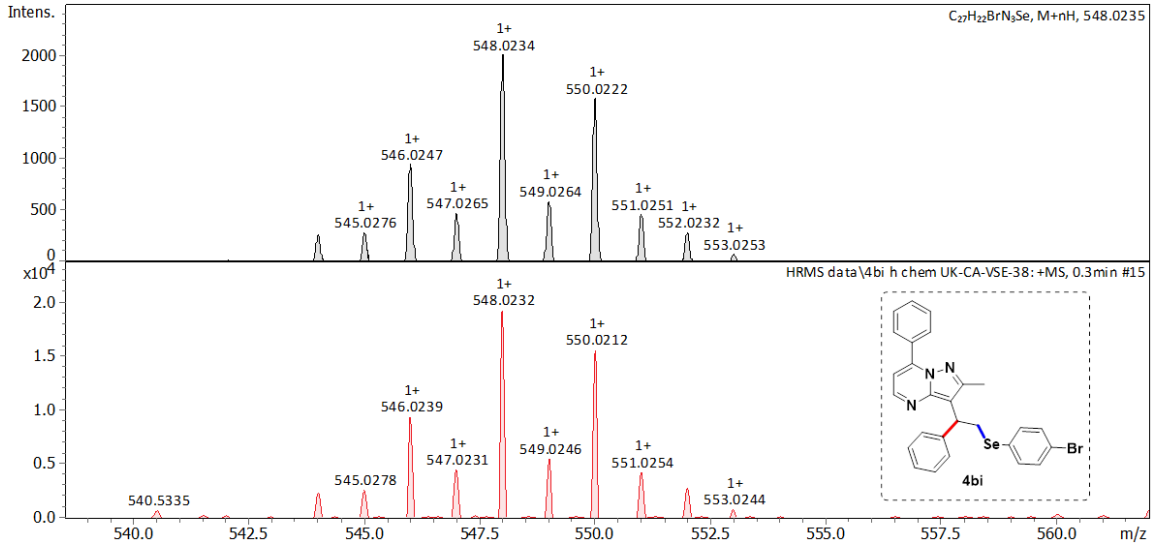

Intens.
$C_{29}H_{24}F_3N_3Se$, M+nH, 552.1160
1+ 552.1162
1+ 550.1175
1+ 549.1201
1+ 551.1203
1+ 553.1193
1+ 554.1176
1+ 555.1199
4bd h chem UK-CA-VSE-33_RB5_01_14146.d: +MS, 0.2min #10
1+ 552.1165
1+ 550.1190
1+ 549.1160
1+ 551.1186
1+ 553.1207
1+ 554.1210
1+ 555.1161
4bd
m/z

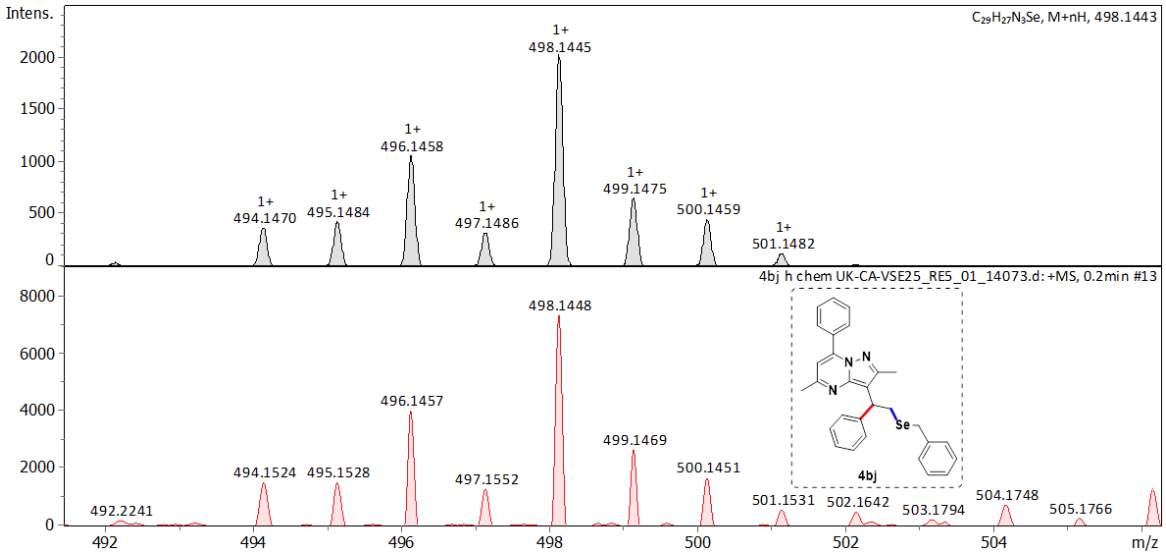

Intens.
$C_{28}H_{24}ClN_3Se$, M+nH, 518.0897
1+ 518.0896
1+ 516.0910
1+ 515.0938
1+ 517.0930
1+ 519.0926
1+ 520.0886
1+ 521.0913
4be h chem UK-CA-VSE-34_RB6_01_14151.d: +MS, 0.7min #40
1+ 518.0897
1+ 516.0901
1+ 515.0940
1+ 517.0932
1+ 519.0925
1+ 520.0870
1+ 521.0893
4be
m/z

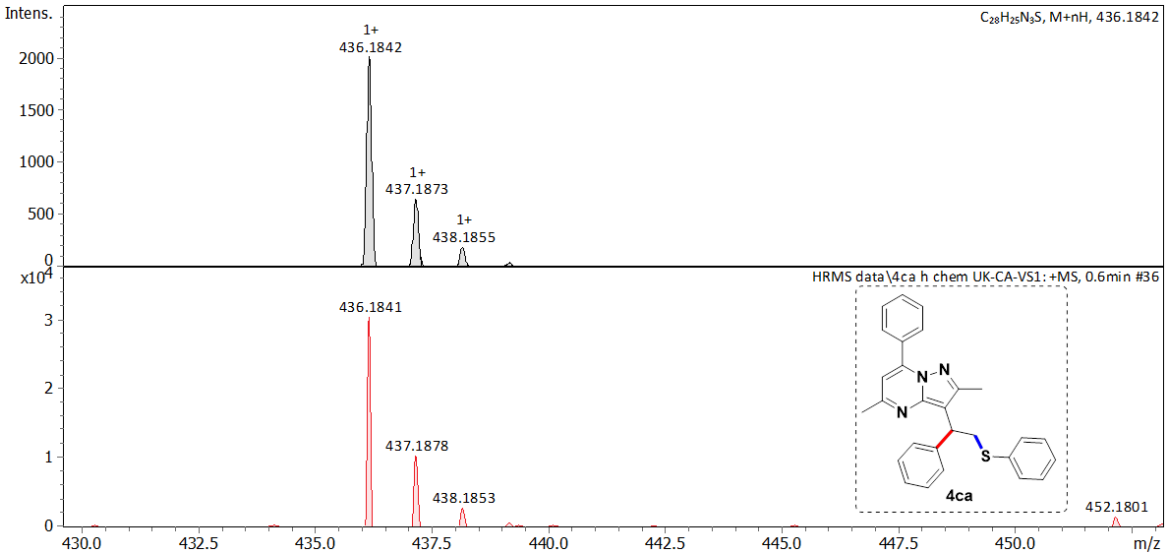

Intens.
C28H24ClN3Se, M+nH, 518.0897
1+ 518.0896
1+ 516.0910
1+ 520.0886
1+ 519.0926
1+ 515.0938
1+ 517.0930
1+ 521.0913
x10^4
4bf h chem UK-CA-VSE-35_RB7_01_14152.d: +MS, 0.8min #48
1+ 518.0901
1+ 516.0921
1+ 520.0898
1+ 519.0928
1+ 515.0943
1+ 517.0934
1+ 521.0907
Cl
Se
4bf
m/z

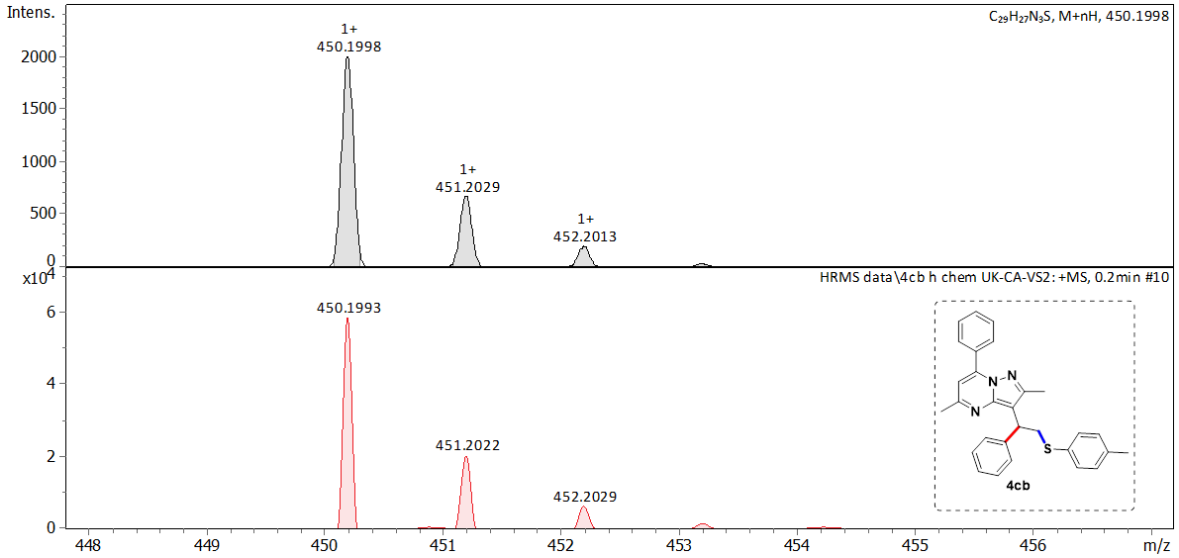

Intens.
C28H24BrN3Se, M+nH, 562.0392
1+ 562.0391
1+ 564.0379
1+ 560.0404
1+ 563.0420
1+ 561.0422
1+ 565.0408
1+ 559.0433
1+ 566.0389
1+ 567.0410
x10^5
4bg h chem UK-CA-VSE26_RE6_01_14074.d: +MS, 0.3min #19
1+ 562.0397
1+ 564.0385
1+ 560.0409
1+ 563.0423
1+ 561.0426
1+ 565.0416
1+ 559.0448
1+ 566.0398
1+ 567.0396
Se
Br
4bg
m/z

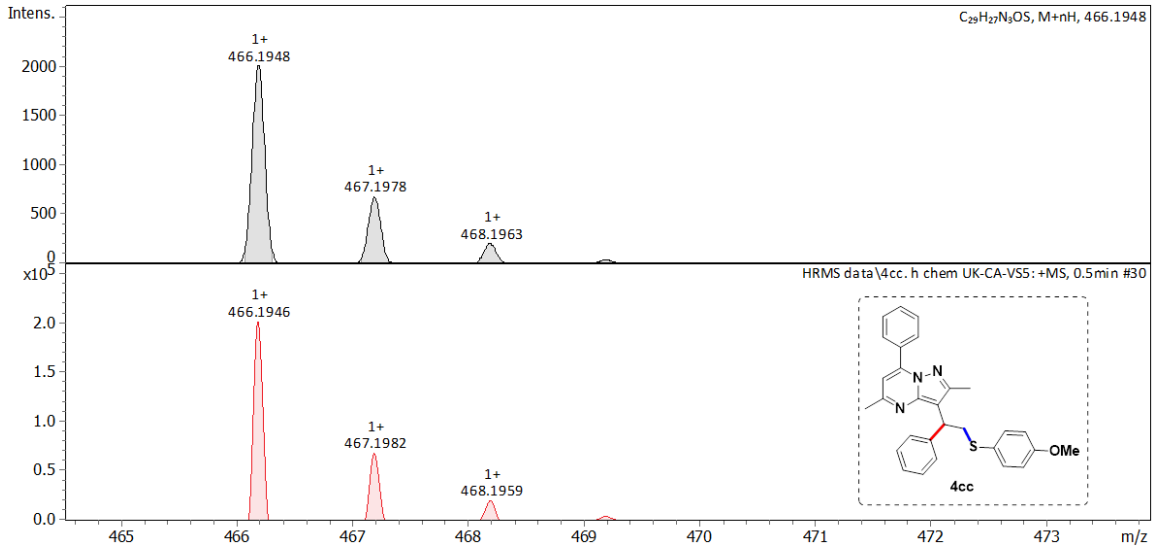

Intens.
C28H24BrN3Se, M+nH, 562.0392
1+ 562.0391
1+ 564.0379
1+ 560.0404
1+ 563.0420
1+ 561.0422
1+ 565.0408
1+ 559.0433
1+ 566.0389
1+ 567.0410
x10^4
4bh h chem UK-CA-VSE-37_RE4_01_14237.d: +MS, 0.5min #32
1+ 562.0389
1+ 564.0399
1+ 560.0403
1+ 563.0424
1+ 561.0425
1+ 565.0425
1+ 559.0436
1+ 566.0395
1+ 567.0409
Se
Br
4bh
m/z

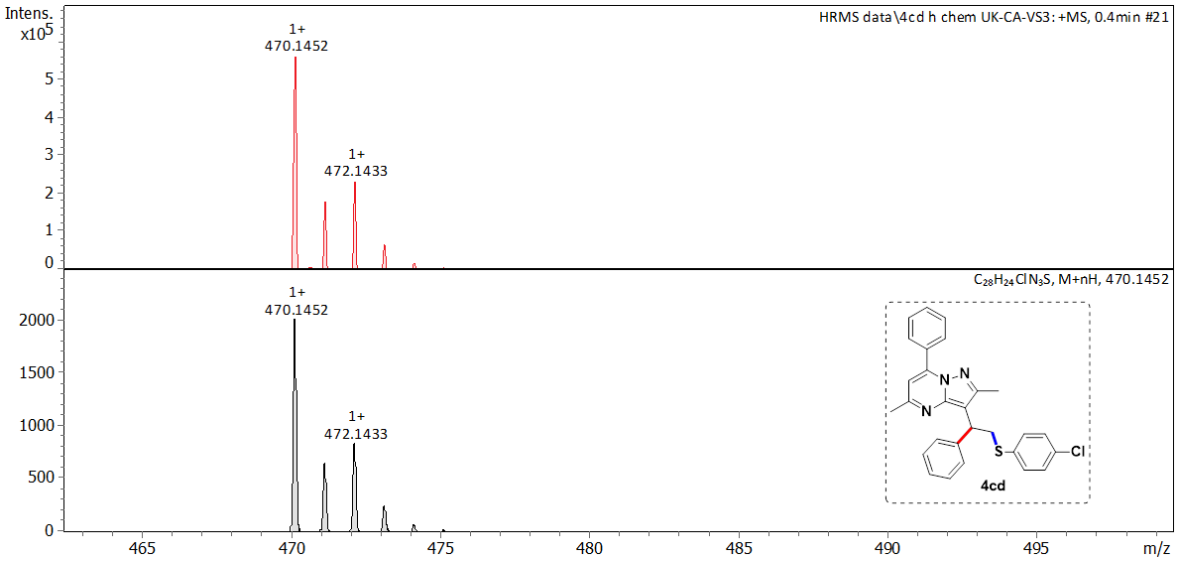

Intens.
C27H22BrN3Se, M+nH, 548.0235
1+ 548.0234
1+ 550.0222
1+ 546.0247
1+ 547.0265
1+ 549.0264
1+ 545.0276
1+ 551.0251
1+ 552.0232
1+ 553.0253
x10^4
HRMS data\4bi h chem UK-CA-VSE-38: +MS, 0.3min #15
1+ 548.0232
1+ 550.0212
1+ 546.0239
1+ 547.0231
1+ 549.0246
1+ 551.0254
1+ 545.0278
1+ 553.0244
540.5335
4bi
m/z

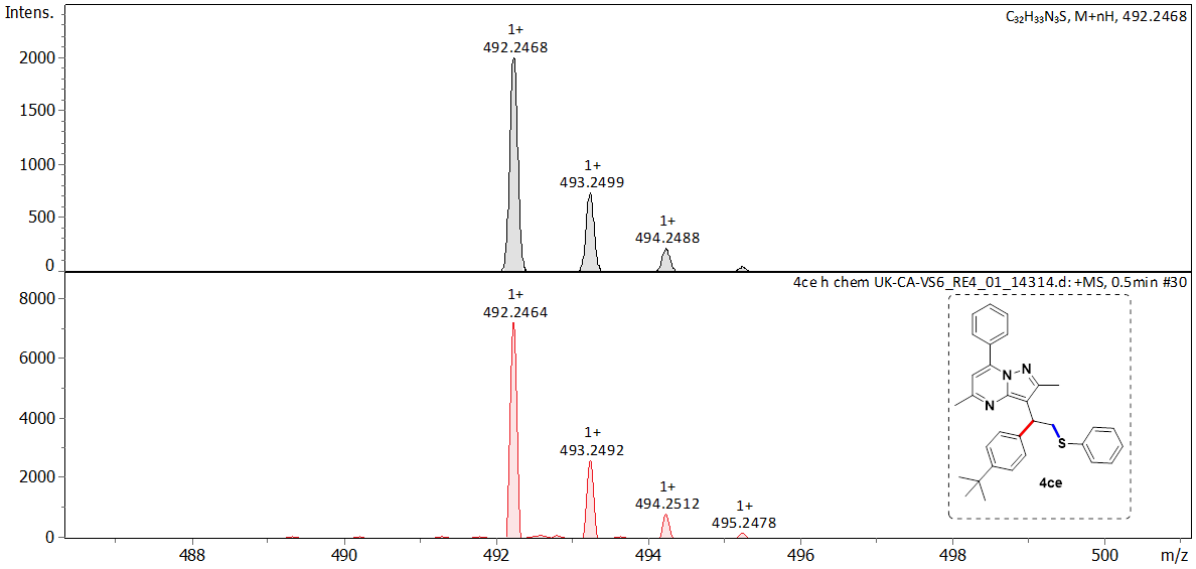

Intens.
C29H27N3Se, M+nH, 498.1443
1+ 498.1445
1+ 496.1458
1+ 494.1470
1+ 495.1484
1+ 497.1486
1+ 499.1475
1+ 500.1459
1+ 501.1482
4bj h chem UK-CA-VSE25_RE5_01_14073.d: +MS, 0.2min #13
498.1448
496.1457
499.1469
494.1524
495.1528
497.1552
500.1451
492.2241
501.1531
502.1642
503.1794
504.1748
505.1766
4bj
m/z

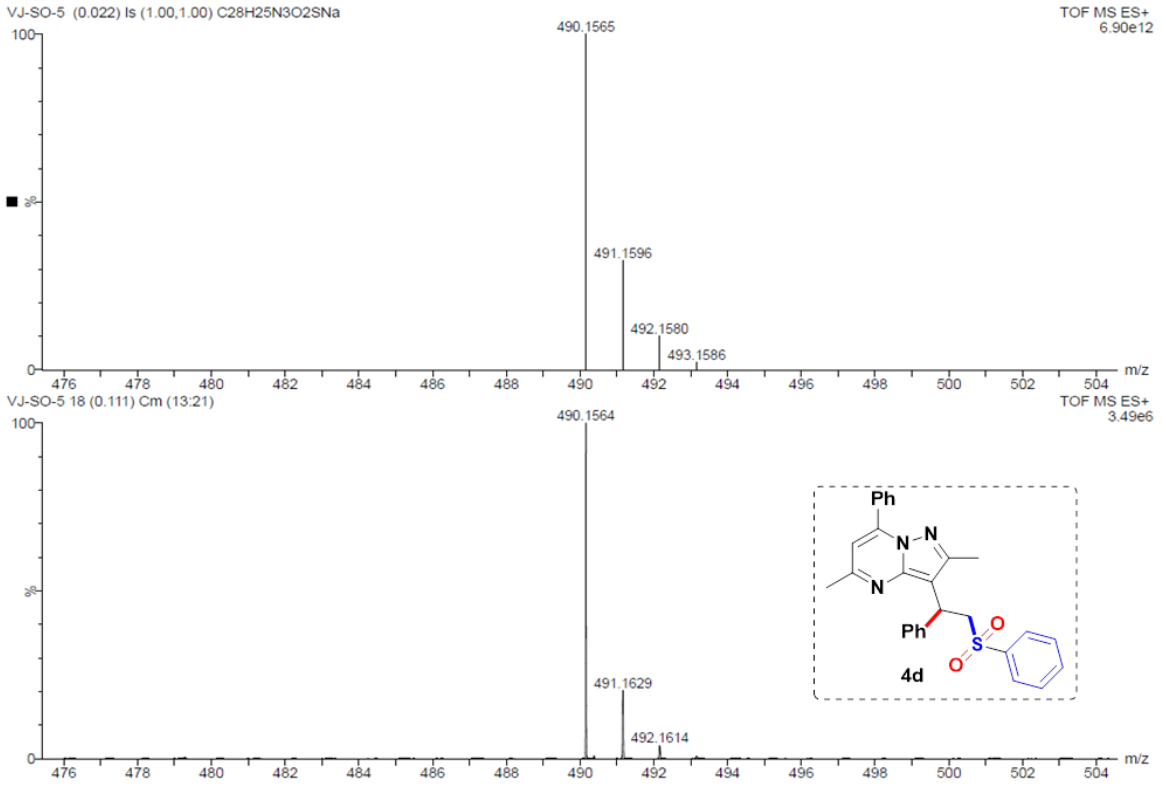

Intens.
C28H25N3S, M+nH, 436.1842
1+ 436.1842
1+ 437.1873
1+ 438.1855
x10^4
HRMS data\4ca h chem UK-CA-VS1: +MS, 0.6min #36
436.1841
437.1878
438.1853
452.1801
4ca
m/z


Intens.
C29H27N3S, M+nH, 450.1998
1+
450.1998
1+
451.2029
1+
452.2013
HRMS data\4cb h chem UK-CA-VS2: +MS, 0.2min #10
450.1993
451.2022
452.2029
4cb
m/z


Intens.
C29H27N3OS, M+nH, 466.1948
1+
466.1948
1+
467.1978
1+
468.1963
HRMS data\4cc. h chem UK-CA-VS5: +MS, 0.5min #30
1+
466.1946
1+
467.1982
1+
468.1959
OMe
4cc
m/z


Intens.
HRMS data\4cd h chem UK-CA-VS3: +MS, 0.4min #21
1+
470.1452
1+
472.1433
C28H24ClN3S, M+nH, 470.1452
1+
470.1452
1+
472.1433
Cl
4cd
m/z


Intens.
C32H33N3S, M+nH, 492.2468
1+
492.2468
1+
493.2499
1+
494.2488
4ce h chem UK-CA-VS6_RE4_01_14314.d: +MS, 0.5min #30
1+
492.2464
1+
493.2492
1+
494.2512
1+
495.2478
4ce
m/z


VJ-SO-5 (0.022) Is (1.00,1.00) C28H25N3O2SNa
TOF MS ES+
6.90e12
490.1565
491.1596
492.1580
493.1586
m/z
VJ-SO-5 18 (0.111) Cm (13:21)
TOF MS ES+
3.49e6
490.1564
491.1629
492.1614
Ph
Ph
4d
m/z

References

1) a) M. A. P. Martins, E. Scapin, C. P. Frizzo, F. A. Rosa, H. G. Bonacorso, N. Zanatta, *J Braz Chem Soc*, **2009**, *20*, 205-213; b) L. Yin and J. Liebscher, *Synthesis*, **2004**, *2004*, 2329-2334.
2) Chillal, A. S.; Bhawale, R. T.; Kshirsagar, U. A., *ChemistrySelect* **2024**, *9*, e202304815.
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