

## **An Efficient Selectfluor-Mediated Oxidative Thio- and Seleno-Cyanation of Diversely Substituted Indoles and Carbazoles**

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\*Kenneth.Laali@unf.edu

Fig S1. <sup>1</sup>H and <sup>13</sup>C NMR spectra of the compound 2

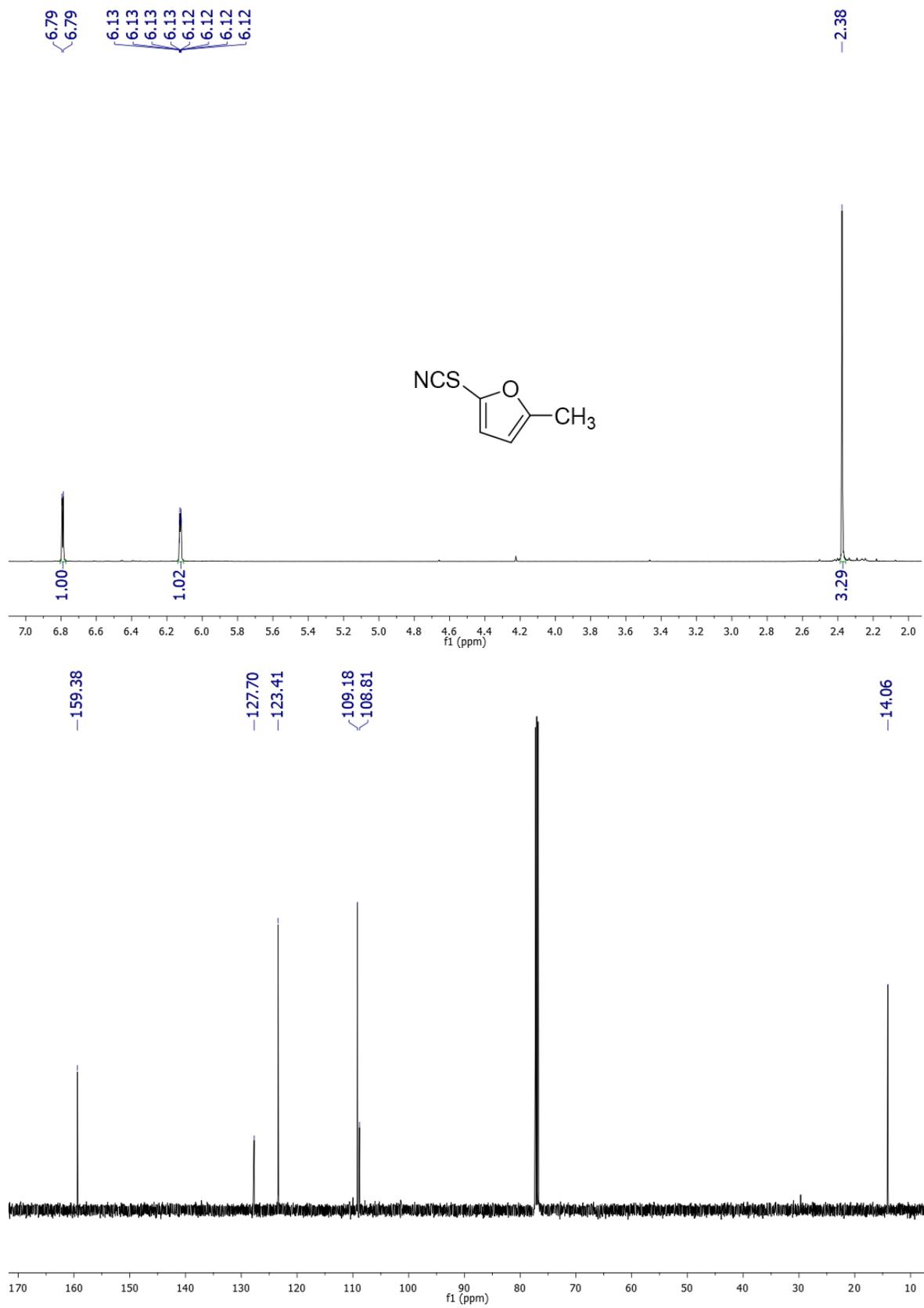


Fig S2. <sup>1</sup>H and <sup>13</sup>C NMR spectra of the compound 4a

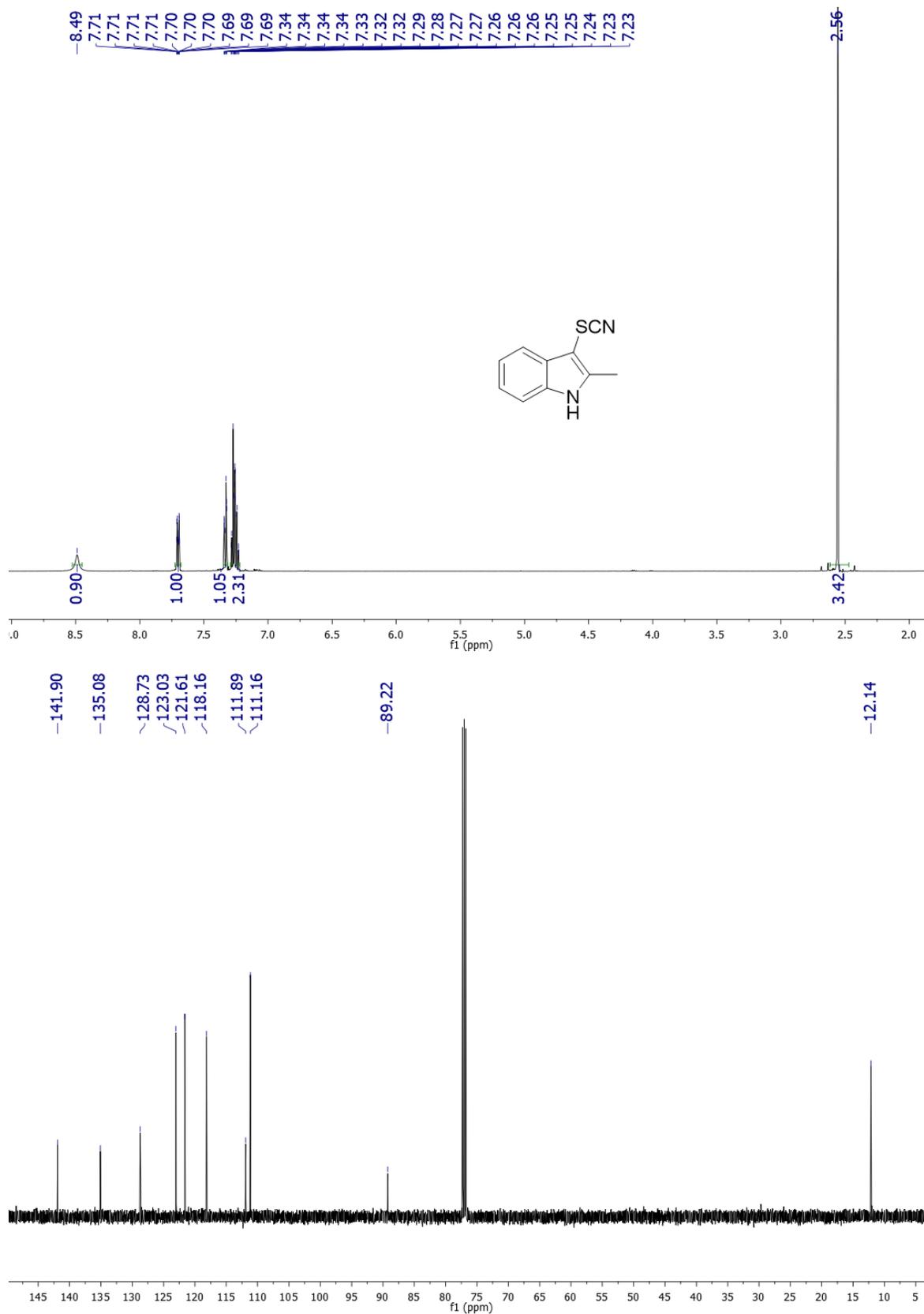
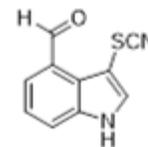
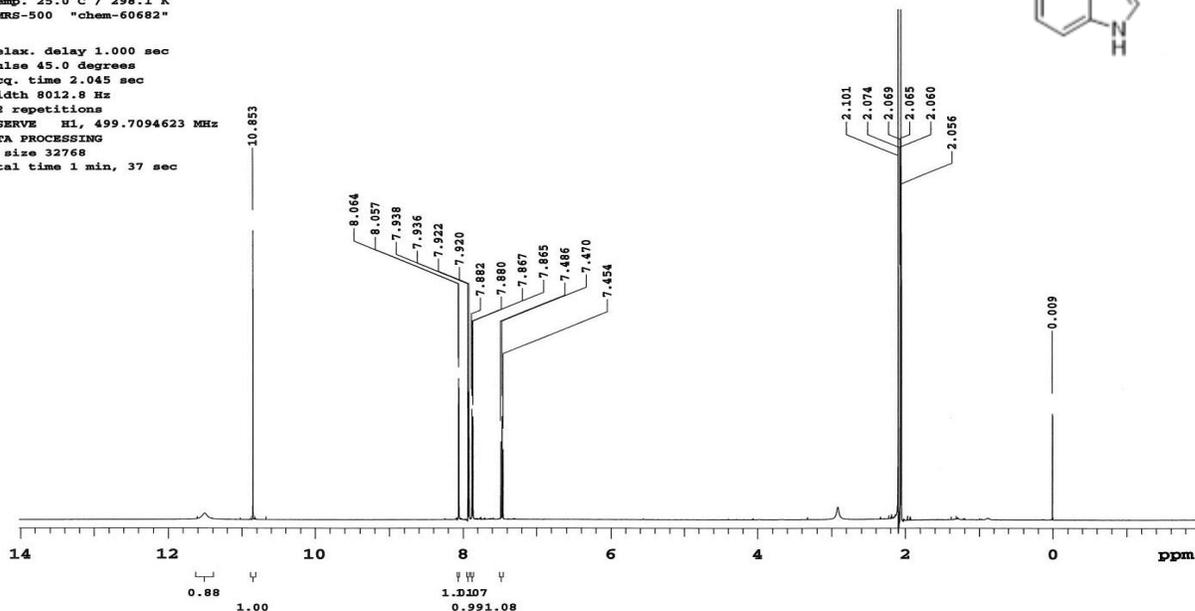


Fig S3. <sup>1</sup>H and <sup>13</sup>C NMR spectra of the compound 4b



indole-4-cho-3-scN  
Pulse Sequence: s2pul  
Solvent: acetone  
Temp. 25.0 C / 298.1 K  
VNMRS-500 "chem-60682"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.045 sec  
Width 8012.8 Hz  
32 repetitions  
OBSERVE H1, 499.7094623 MHz  
DATA PROCESSING  
FT size 32768  
Total time 1 min, 37 sec



indole-4-cho-3-scN  
Pulse Sequence: s2pul  
Solvent: acetone  
Temp. 25.0 C / 298.1 K  
User: 1-14-87  
VNMRS-500 "chem-60682"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.049 sec  
Width 31250.0 Hz  
1920 repetitions  
OBSERVE C13, 125.6520442 MHz  
DECOUPLE H1, 499.7119609 MHz  
Power 44 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65336  
Total time 1 hr, 5 min, 33 sec

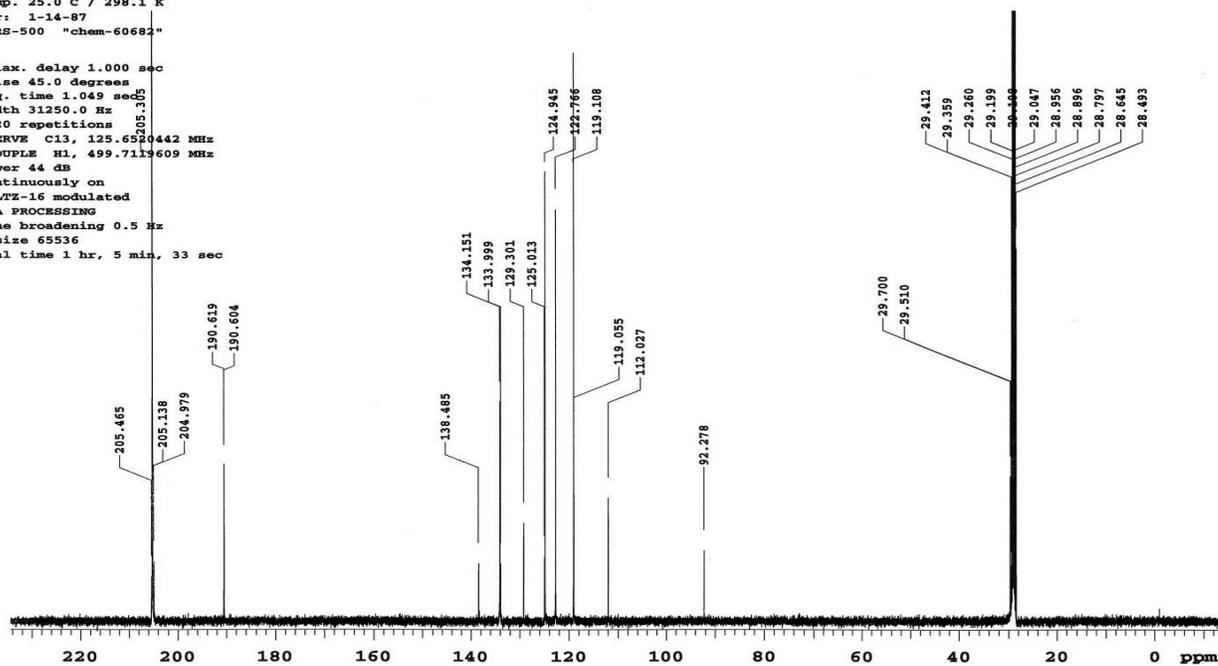


Fig S4.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of the compound 4c

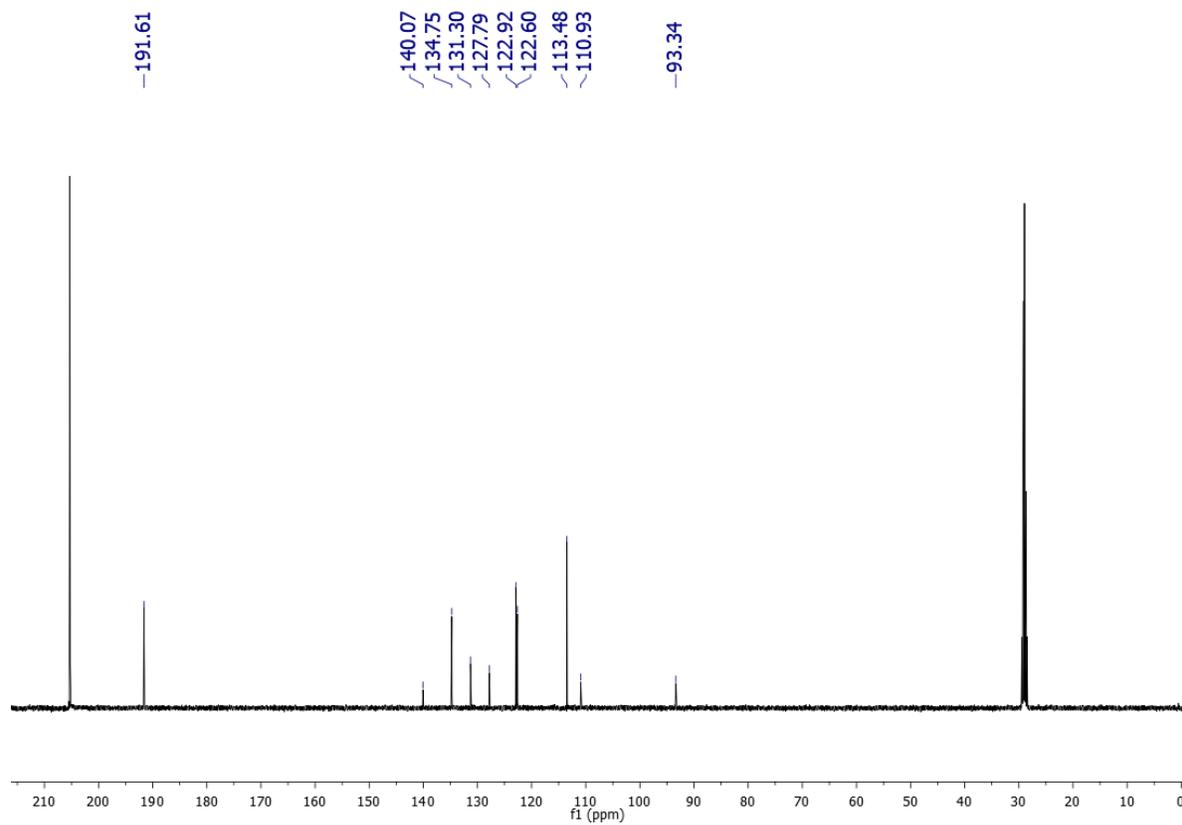
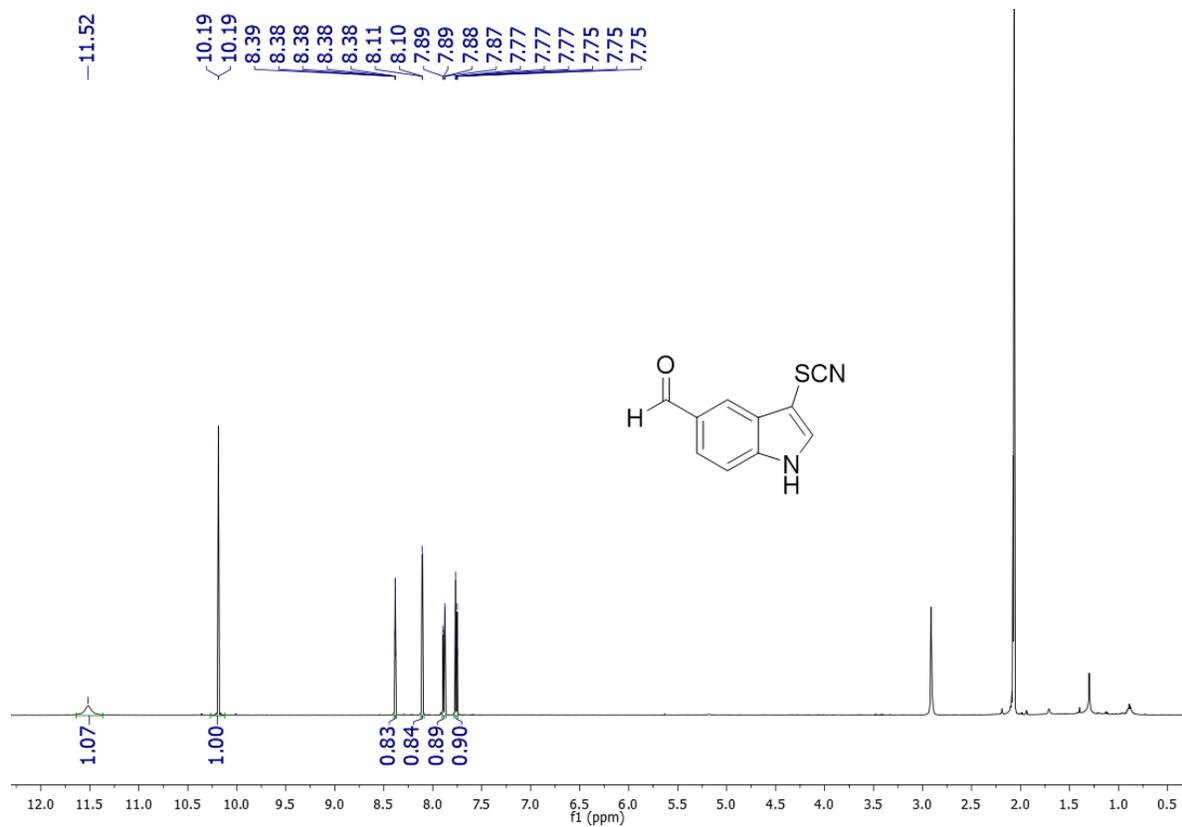
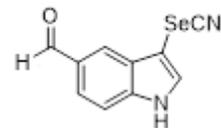
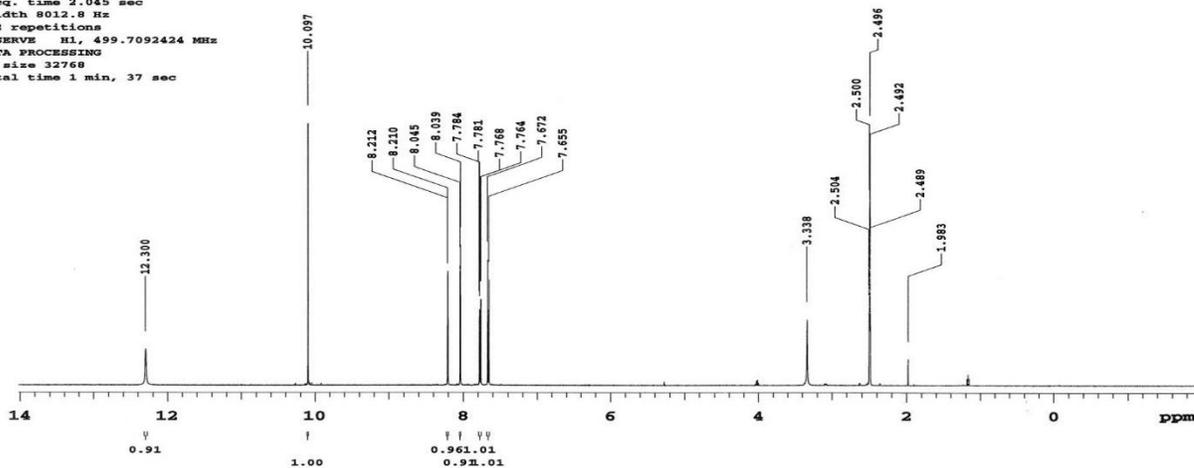


Fig S5. <sup>1</sup>H, <sup>13</sup>C and <sup>77</sup>Se NMR spectra of the compound 5c



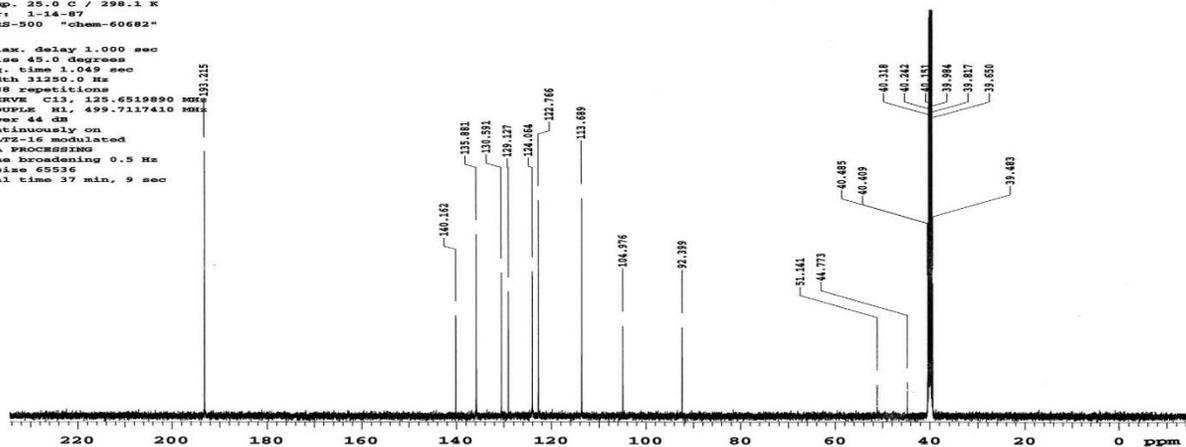
Indole\_5\_SeCN\_Reaction\_2

Pulse Sequence: s2pul  
 Solvent: dmsc  
 Temp. 25.0 C / 298.1 K  
 VNMRS-500 "chem-60682"  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 2.045 sec  
 Width 8012.8 Hz  
 32 repetitions  
 OBSERVE H1, 499.7092424 MHz  
 DATA PROCESSING  
 FT size 32768  
 Total time 1 min, 37 sec



Indole\_5\_SeCN\_C13

Pulse Sequence: s2pul  
 Solvent: dmsc  
 Temp. 25.0 C / 298.1 K  
 User: 1-14-87  
 VNMRS-500 "chem-60682"  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.049 sec  
 Width 31290.0 Hz  
 1089 repetitions  
 OBSERVE C13, 125.6519890 MHz  
 DECOUPLE H1, 499.7117410 MHz  
 Power 44 dB  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 0.5 Hz  
 FT size 65536  
 Total time 37 min, 9 sec



SeCN\_15\_aid

Pulse Sequence: s2pul  
 Solvent: cdcl3  
 Temp. 25.0 C / 298.1 K  
 User: 1-14-87  
 VNMRS-500 "chem-60682"  
 Relax. delay 25.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.311 sec  
 Width 50000.0 Hz  
 32 repetitions  
 OBSERVE Se77, 95.3016605 MHz  
 DECOUPLE H1, 499.7093674 MHz  
 Power 44 dB  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 0.5 Hz  
 FT size 131072  
 Total time 14 min, 2 sec



Fig S6. <sup>1</sup>H and <sup>13</sup>C NMR spectra of the compound 4d

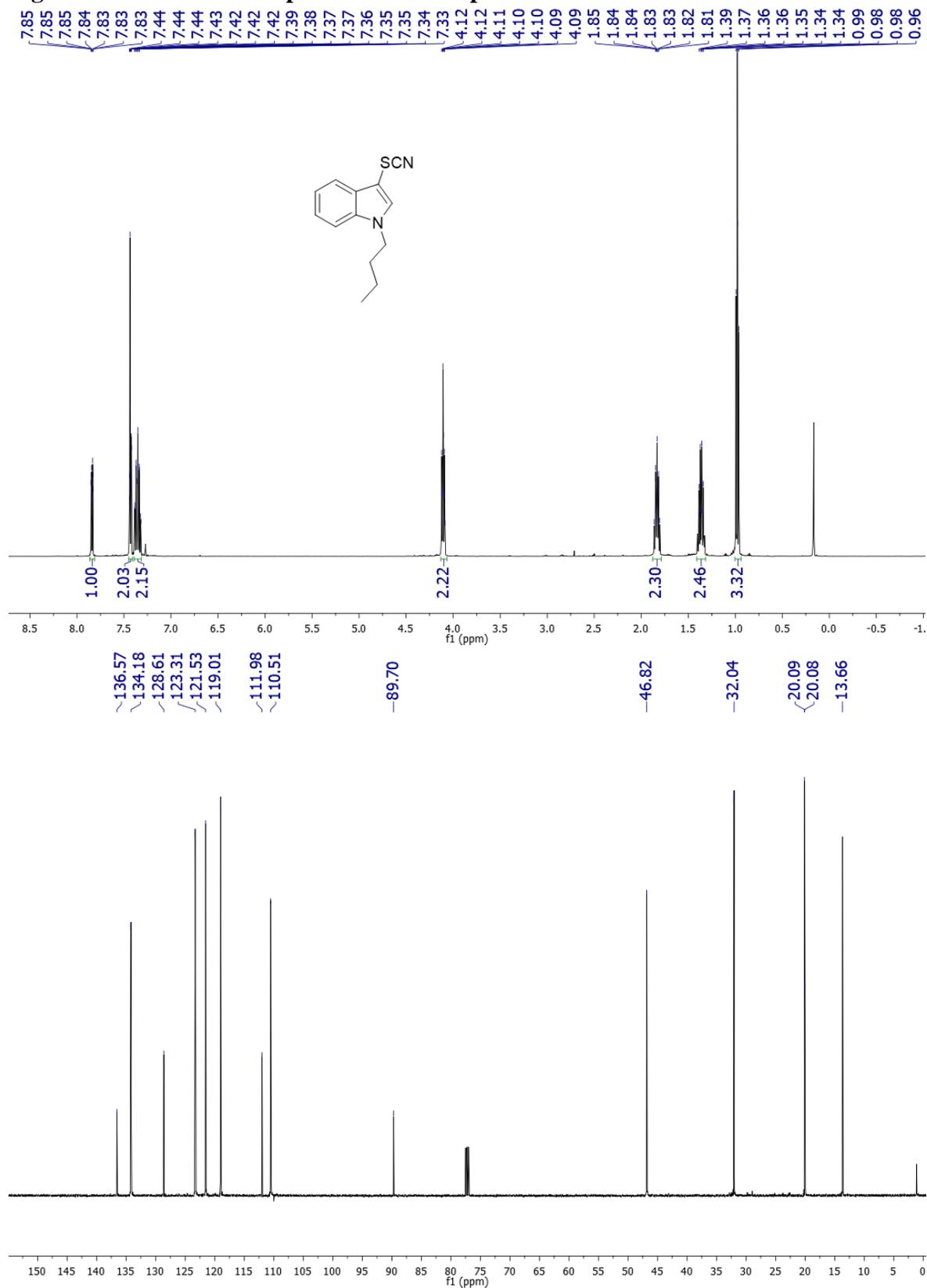


Fig S7.  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{77}\text{Se}$  NMR spectra of the compound 5d

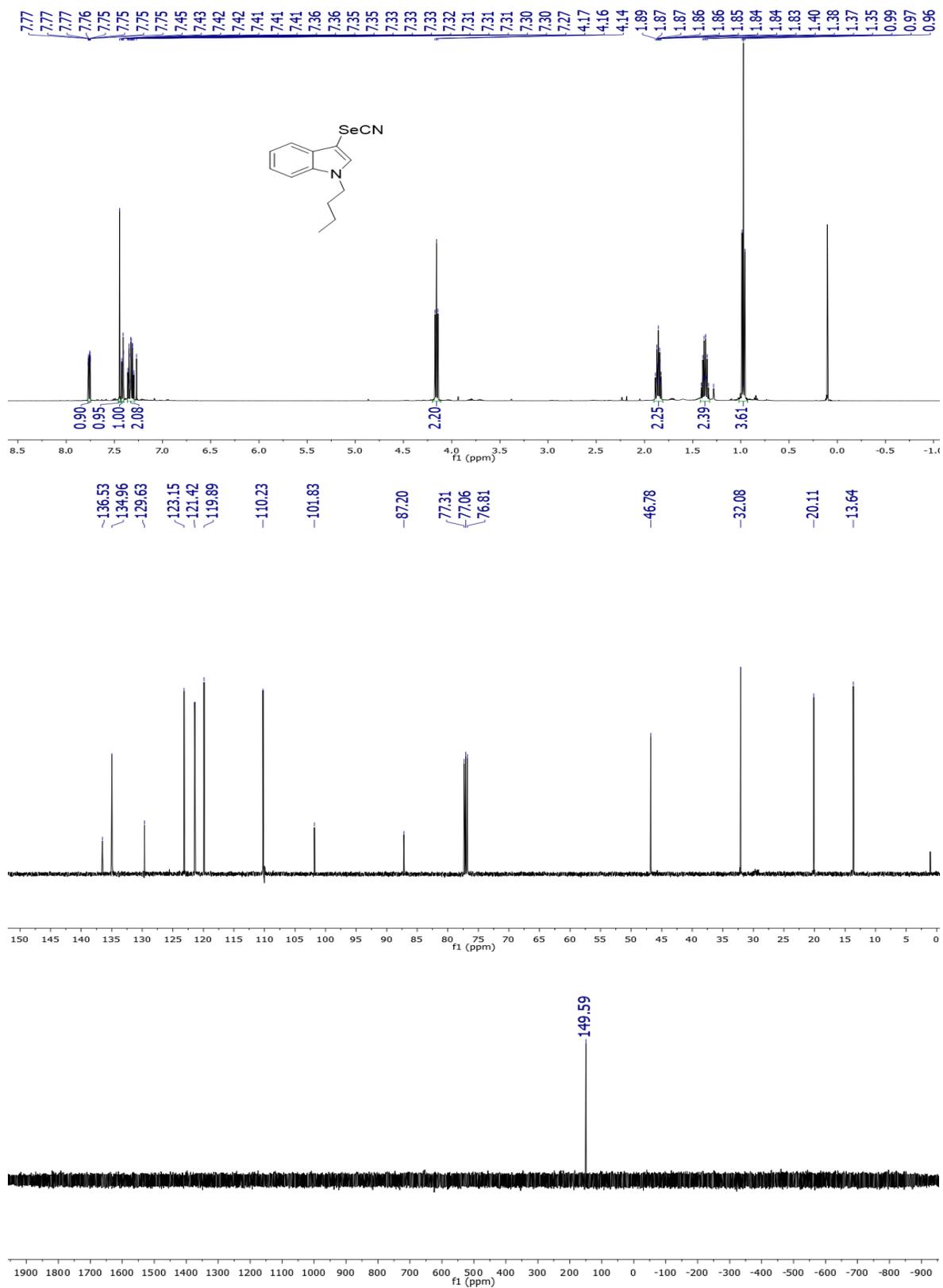


Fig S8. <sup>1</sup>H and <sup>13</sup>C NMR spectra of the compound 4e

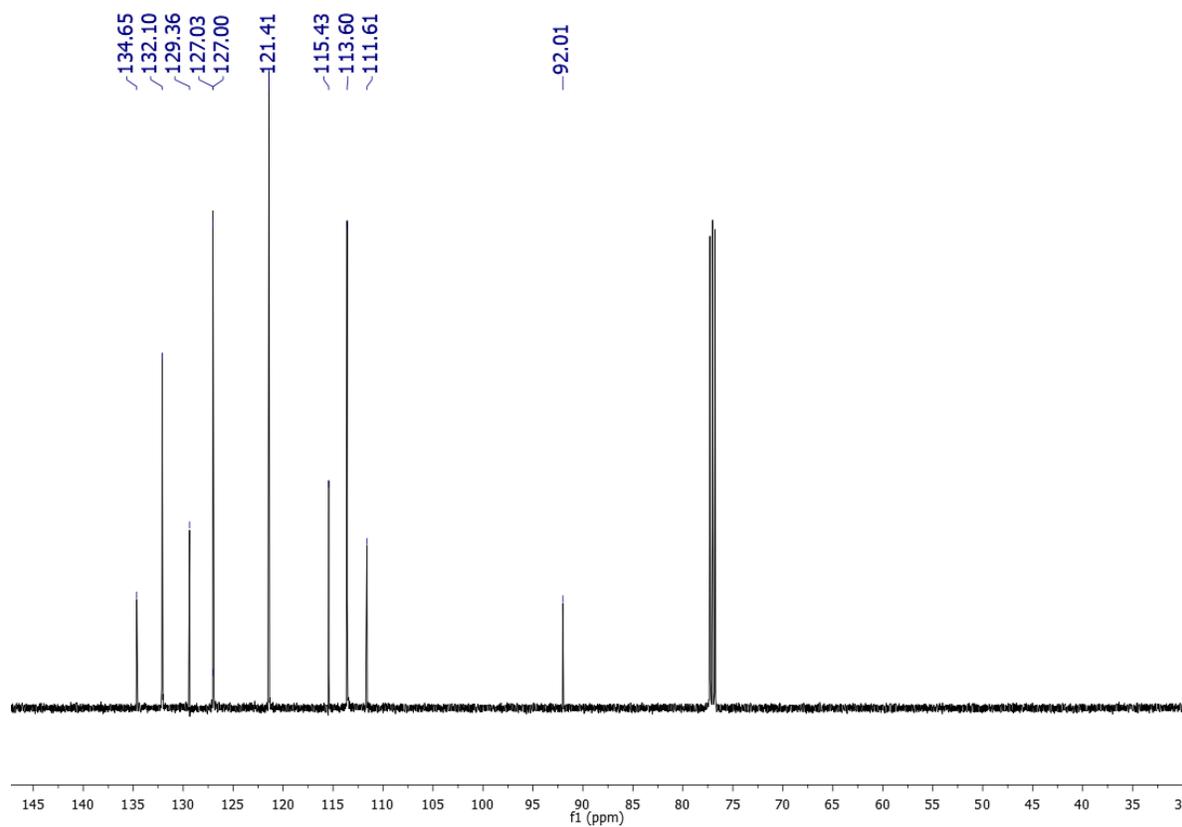
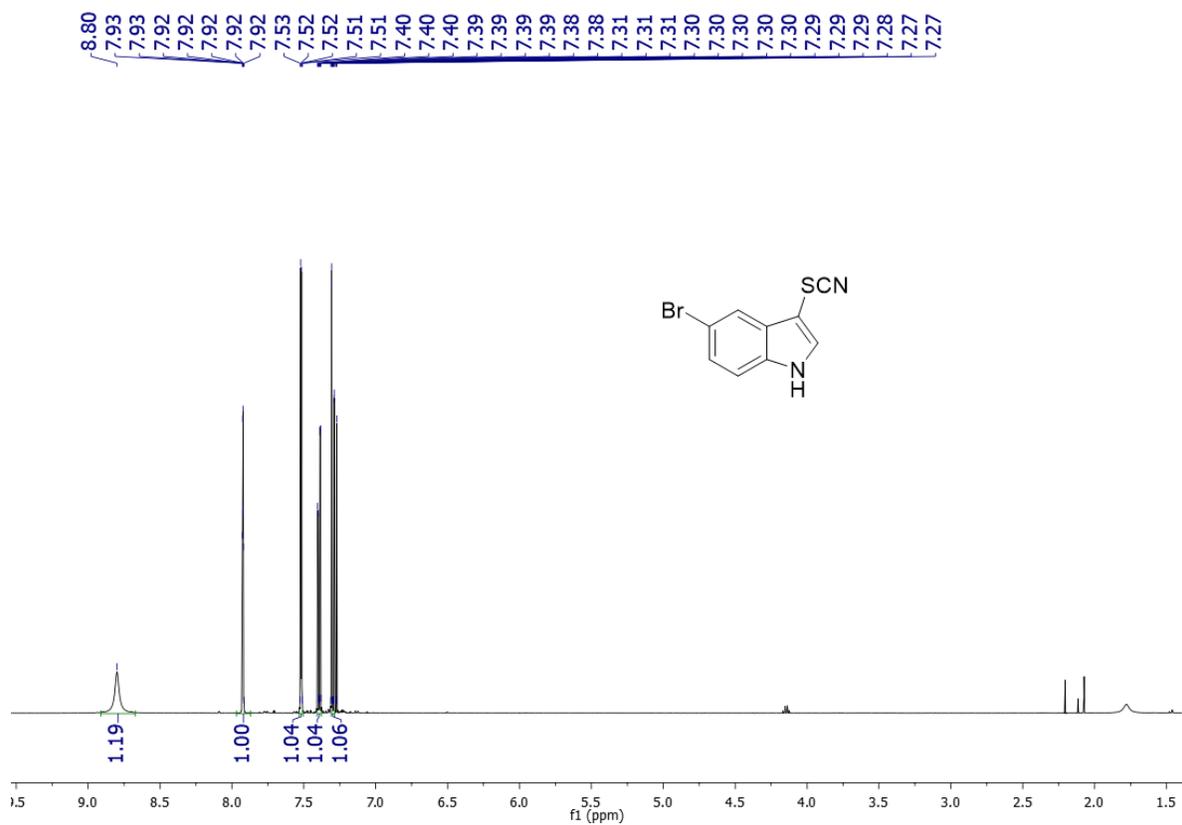
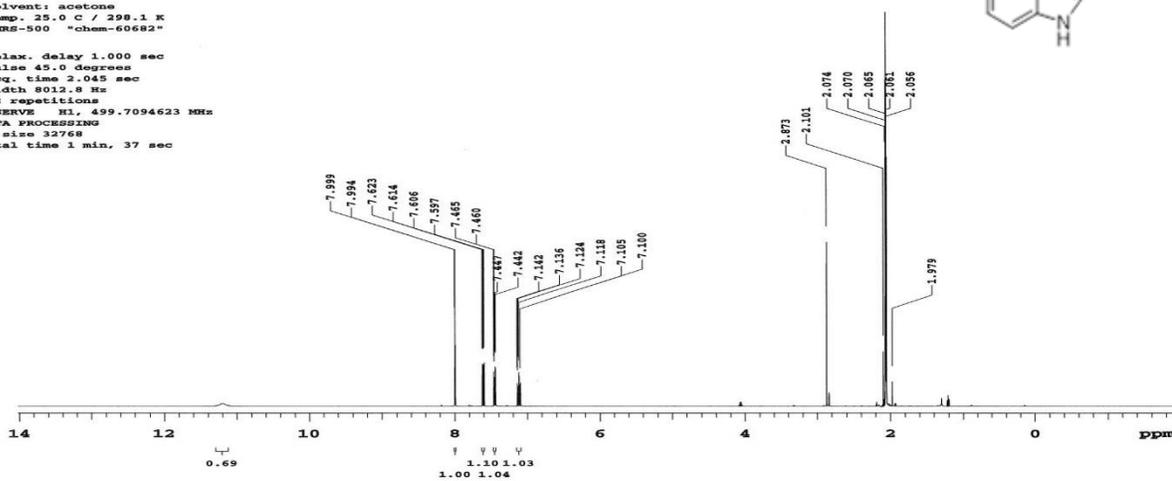
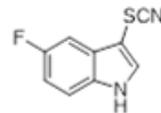




Fig S10. <sup>1</sup>H, <sup>19</sup>F and <sup>13</sup>C NMR spectra of the compound 4f

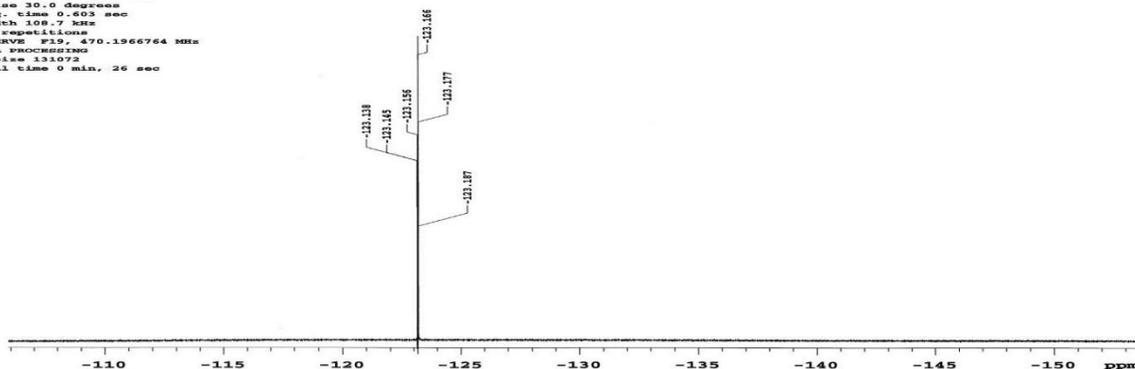
5-F-Indole-3-SCN\_Column\_Purified

Pulse Sequence: s2pul  
 Solvent: acetone  
 Temp. 25.0 C / 298.1 K  
 VNMRS-500 "chem-60682"  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 2.045 sec  
 Width 8012.8 Hz  
 32 repetitions  
 OBSERVE H1, 499.7094623 MHz  
 DATA PROCESSING  
 FT size 32768  
 Total time 1 min, 37 sec



5-F-Indole-3-SCN\_Column\_Purified

Pulse Sequence: s2pul  
 Solvent: acetone  
 Temp. 25.0 C / 298.1 K  
 VNMRS-500 "chem-60682"  
 Relax. delay 1.000 sec  
 Pulse 30.0 degrees  
 Acq. time 0.603 sec  
 Width 106.7 kHz  
 16 repetitions  
 OBSERVE F19, 470.1966764 MHz  
 DATA PROCESSING  
 FT size 131072  
 Total time 0 min, 26 sec



5-F-Indole-3SCN\_C13

Pulse Sequence: s2pul  
 Solvent: acetone  
 Temp. 25.0 C / 298.1 K  
 UBOX: 1-14-87  
 VNMRS-500 "chem-60682"  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.049 sec  
 Width 32220.0 Hz  
 3220 repetitions  
 OBSERVE C13, 125.629442 MHz  
 DECOUPLE H1, 499.711609 MHz  
 Power: 4 dB  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 0.5 Hz  
 FT size 65536  
 Total time 2 hr, 11 sec

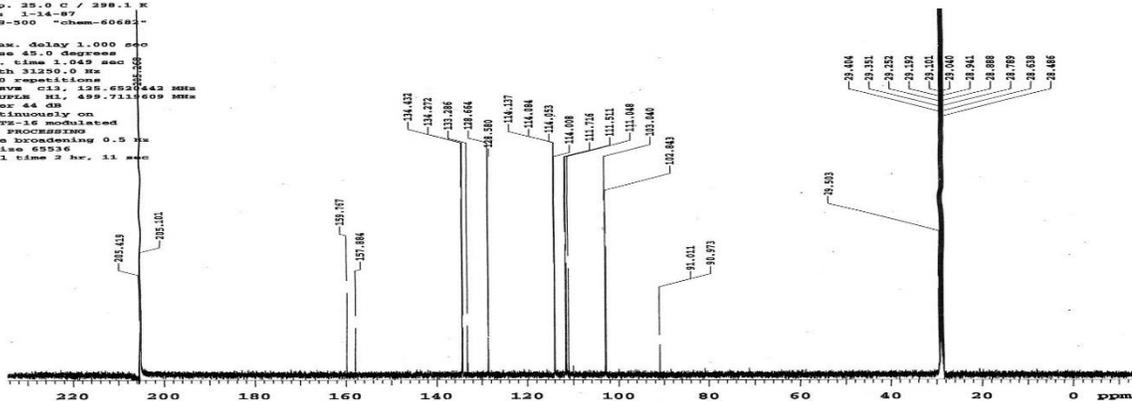
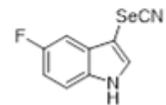


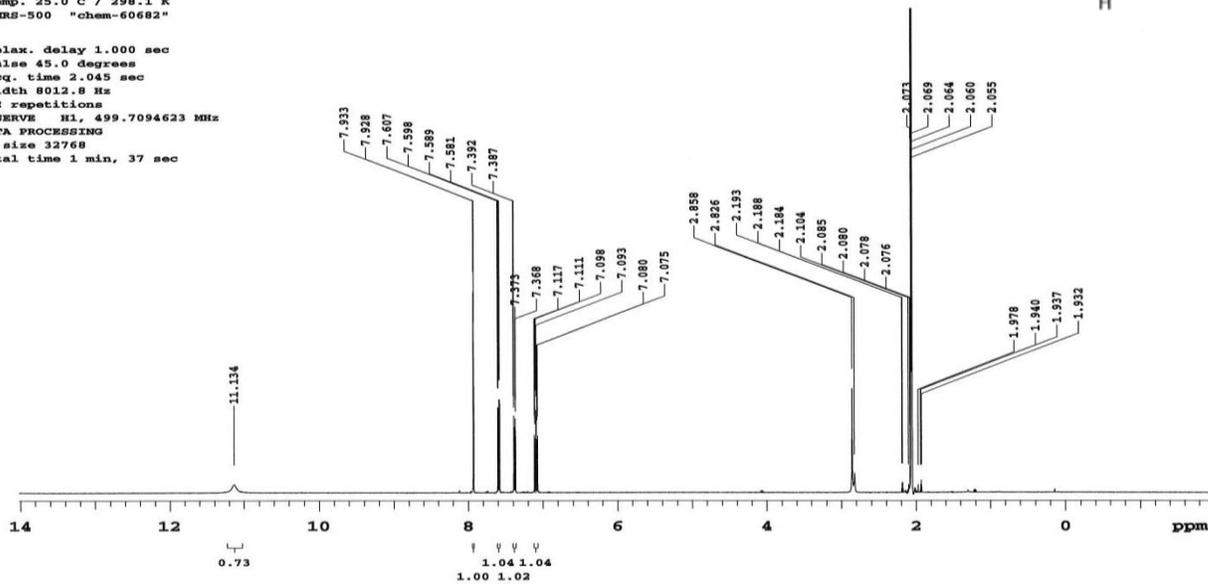
Fig S11.  $^1\text{H}$ ,  $^{19}\text{F}$ ,  $^{13}\text{C}$  and  $^{77}\text{Se}$  NMR spectra of the compound 5f



5-F-3-SeCN\_Indole

Pulse Sequence: s2pul  
Solvent: acetone  
Temp. 25.0 C / 298.1 K  
VMRS-500 "chem-60682"

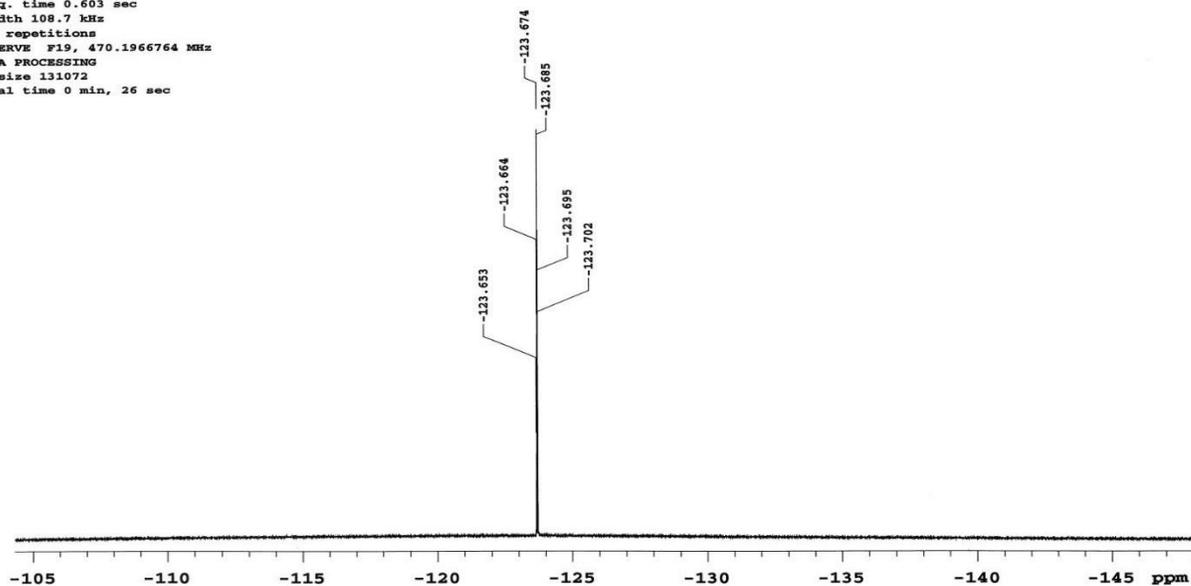
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.045 sec  
Width 8012.8 Hz  
32 repetitions  
OBSERVE H1, 499.7094623 MHz  
DATA PROCESSING  
FT size 32768  
Total time 1 min, 37 sec



5-F-3-SeCN\_Indole

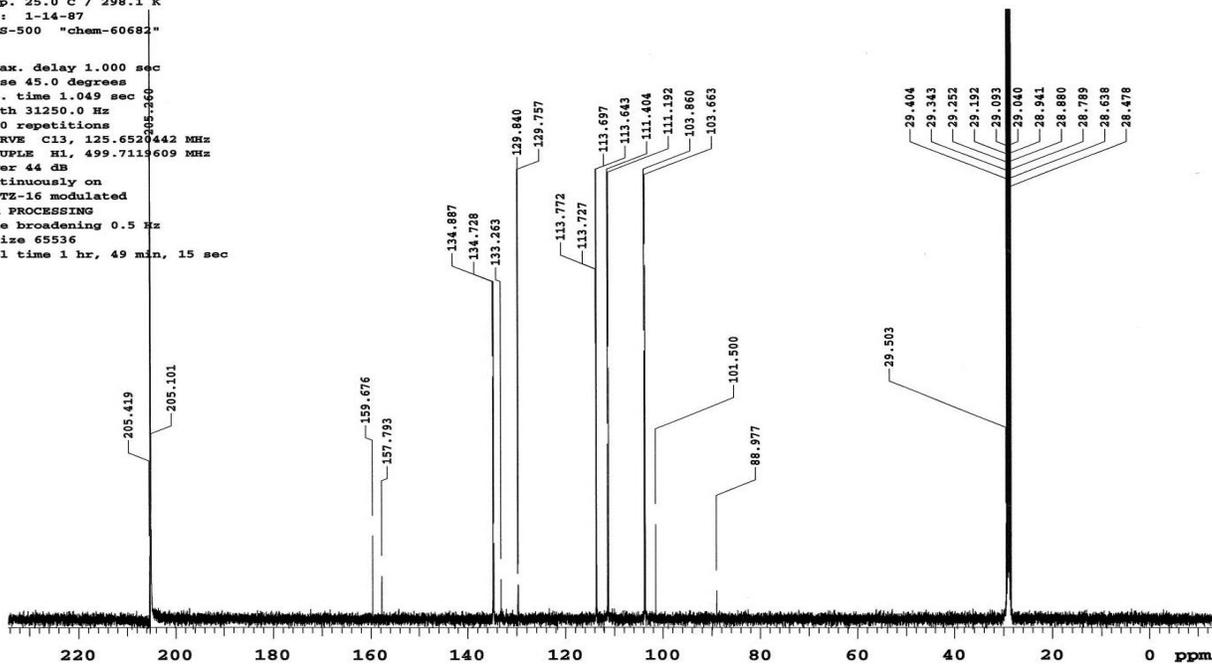
Pulse Sequence: s2pul  
Solvent: acetone  
Temp. 25.0 C / 298.1 K  
VMRS-500 "chem-60682"

Relax. delay 1.000 sec  
Pulse 30.0 degrees  
Acq. time 0.603 sec  
Width 108.7 kHz  
16 repetitions  
OBSERVE F19, 470.1966764 MHz  
DATA PROCESSING  
FT size 131072  
Total time 0 min, 26 sec



-F-3-SeCN\_Indole

Pulse Sequence: s2pul  
Solvent: acetone  
Temp. 25.0 C / 298.1 K  
User: 1-14-87  
VNMRS-500 "chem-60682"  
  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.049 sec  
Width 31250.0 Hz  
3200 repetitions  
OBSERVE C13, 125.6520442 MHz  
DECOUPLE H1, 499.7119609 MHz  
Power 44 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 hr, 49 min, 15 sec



5-F-3-SeCN\_Indole

Pulse Sequence: s2pul  
Solvent: acetone  
Temp. 25.0 C / 298.1 K  
User: 1-14-87  
VNMRS-500 "chem-60682"  
  
Relax. delay 5.000 sec  
Pulse 45.0 degrees  
Acq. time 0.944 sec  
Width 277.8 kHz  
32 repetitions  
OBSERVE Se77, 95.3021551 MHz  
DECOUPLE H1, 499.7119609 MHz  
Power 44 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 524288  
Total time 3 min, 10 sec

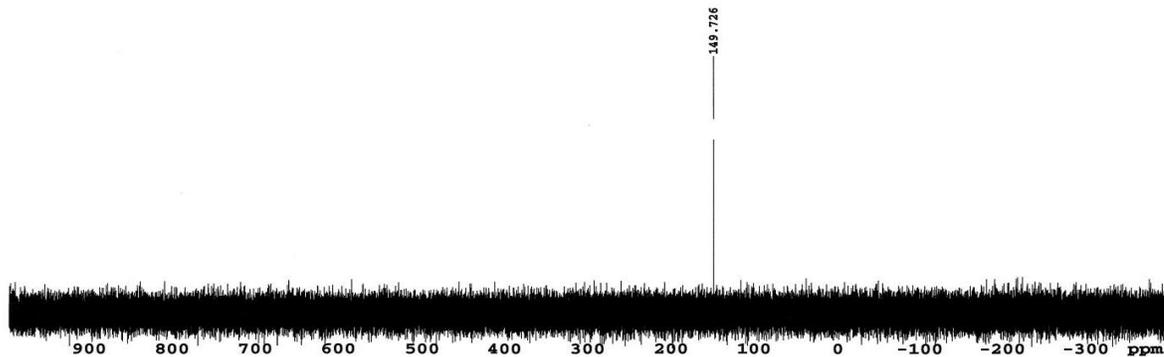


Fig S12. <sup>1</sup>H, <sup>19</sup>F and <sup>13</sup>C NMR spectra of the compound 4g

N-Bu-Indole\_5-F\_3-SCN

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

VNMR-500 "chem-60682"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.048 sec

Width 8012.8 Hz

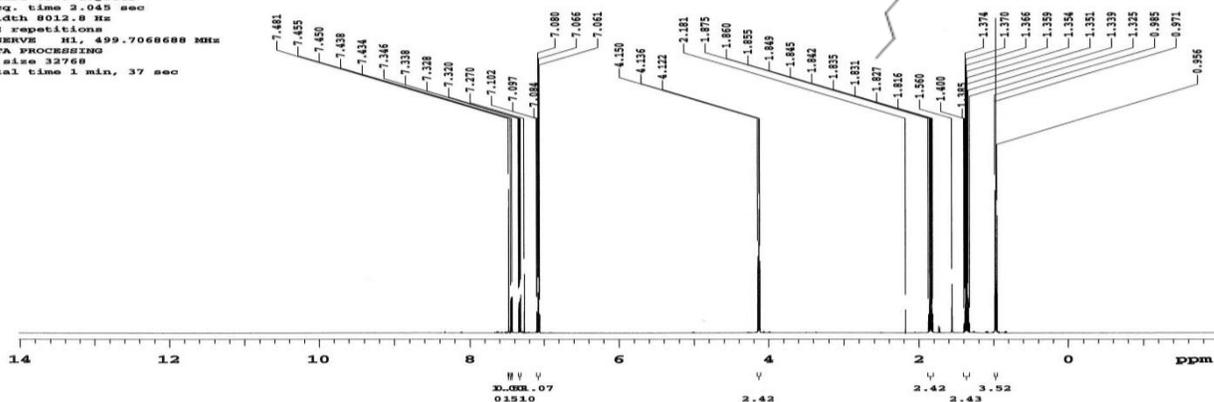
32 repetitions

OBSERVE H1, 499.7068688 MHz

DATA PROCESSING

FT size 32768

Total time 1 min, 37 sec



N-Bu-Indole\_5-F\_3-SCN

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

VNMR-500 "chem-60682"

Relax. delay 1.000 sec

Pulse 30.0 degrees

Acq. time 0.603 sec

Width 109.7 kHz

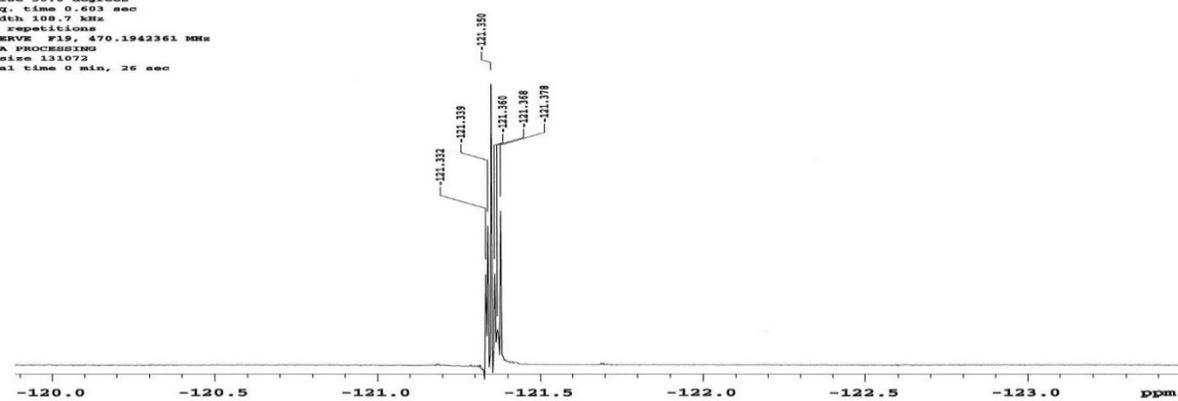
16 repetitions

OBSERVE F19, 470.1942361 MHz

DATA PROCESSING

FT size 131072

Total time 0 min, 26 sec



N-Bu-Indole-5-F-3-SCN

Pulse Sequence: s2pul

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Year: 1-14-87

VNMR-500 "chem-60682"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.049 sec

Width 31250.0 Hz

2944 repetitions

OBSERVE C13, 125.6513921 MHz

DECOUPLE H1, 499.7093674 MHz

Power 44 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 1 hr, 40 min, 31 sec

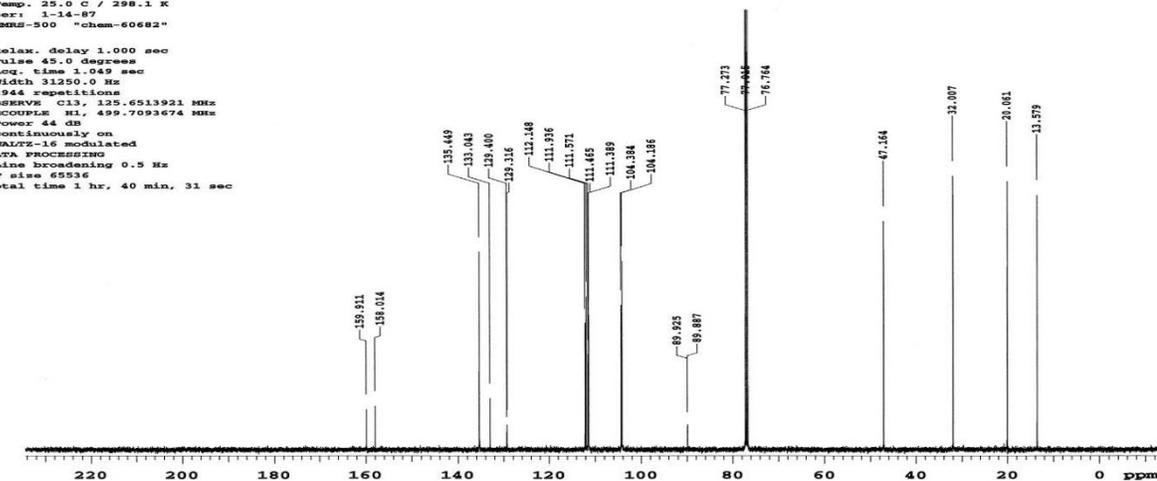
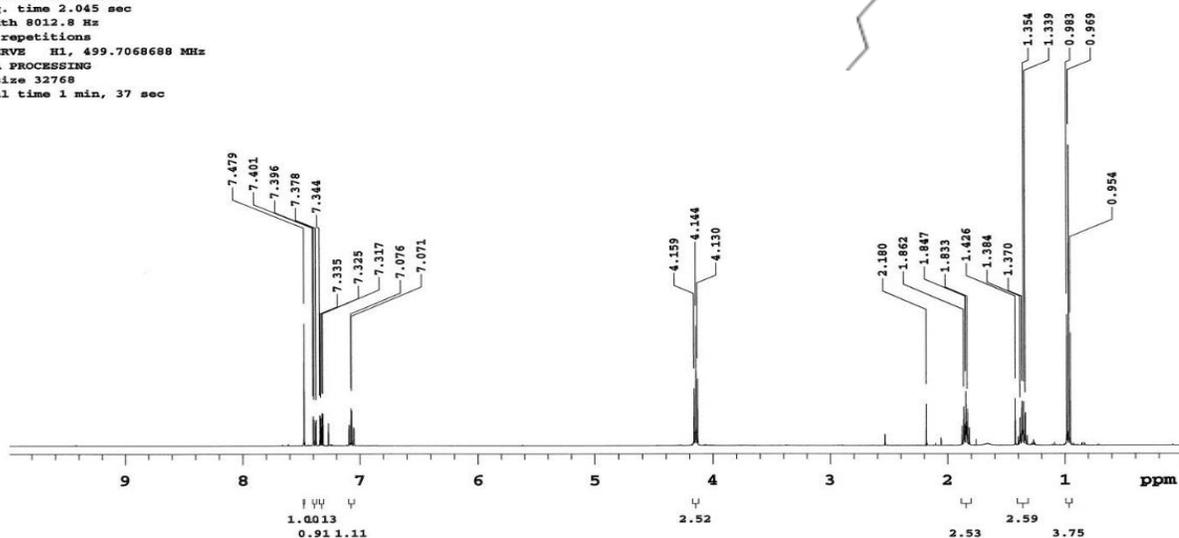
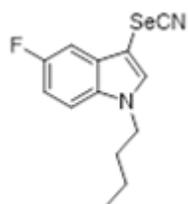


Fig S13.  $^1\text{H}$ ,  $^{19}\text{F}$  and  $^{13}\text{C}$  and  $^{77}\text{Se}$  NMR spectra of the compound 5g

N-Bu\_Indole\_5-F\_3-SeCN

Pulse Sequence: s2pul  
Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
VNMR5-500 "chem-60682"

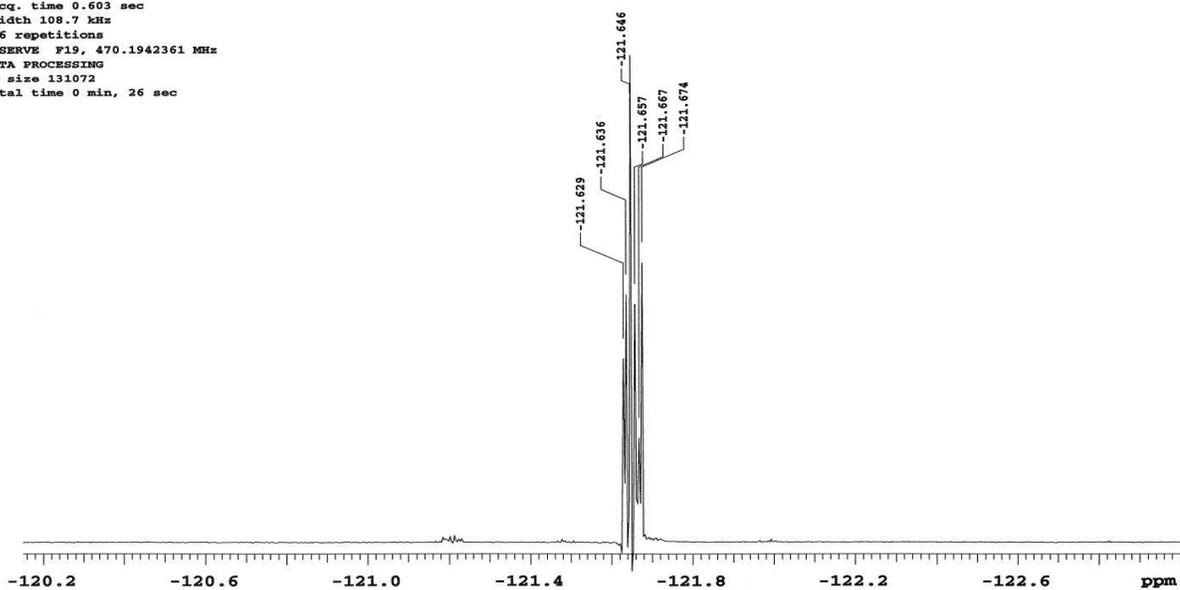
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.045 sec  
Width 8012.8 Hz  
32 repetitions  
OBSERVE H1, 499.7068688 MHz  
DATA PROCESSING  
FT size 32768  
Total time 1 min, 37 sec



N-Bu\_Indole\_5-F\_3-SeCN

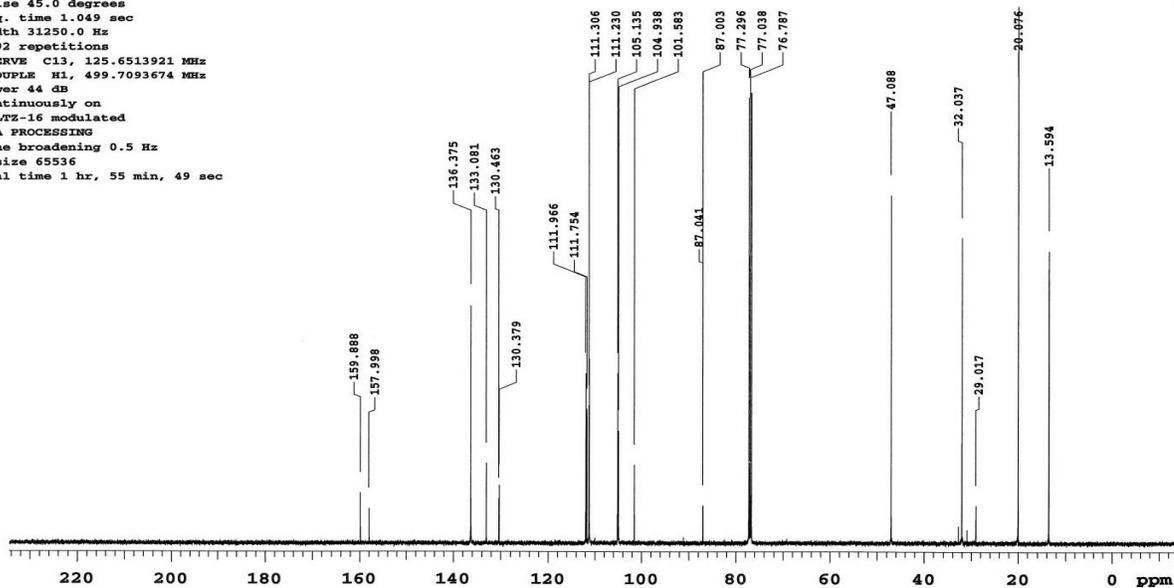
Pulse Sequence: s2pul  
Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
VNMR5-500 "chem-60682"

Relax. delay 1.000 sec  
Pulse 30.0 degrees  
Acq. time 0.603 sec  
Width 108.7 MHz  
16 repetitions  
OBSERVE F19, 470.1942361 MHz  
DATA PROCESSING  
FT size 131072  
Total time 0 min, 26 sec



n-Bu-Indole-5F-3SeCN  
Pulse Sequence: s2pul  
Solvent: cdcl3  
Temp: 25.0 C / 298.1 K  
User: 1-14-87  
VMRS-500 "chem-60682"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.049 sec  
Width 31250.0 Hz  
3392 repetitions  
OBSERVE C13, 125.6513921 MHz  
DECOUPLE H1, 499.7093674 MHz  
Power 44 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1 hr, 55 min, 49 sec



N-Bu\_Indole\_5-F\_3-SeCN  
Pulse Sequence: s2pul  
Solvent: cdcl3  
Temp: 25.0 C / 298.1 K  
User: 1-14-87  
VMRS-500 "chem-60682"

Relax. delay 5.000 sec  
Pulse 45.0 degrees  
Acq. time 0.944 sec  
Width 277.8 kHz  
32 repetitions  
OBSERVE Se77, 95.3016605 MHz  
DECOUPLE H1, 499.7093674 MHz  
Power 44 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 524288  
Total time 3 min, 10 sec

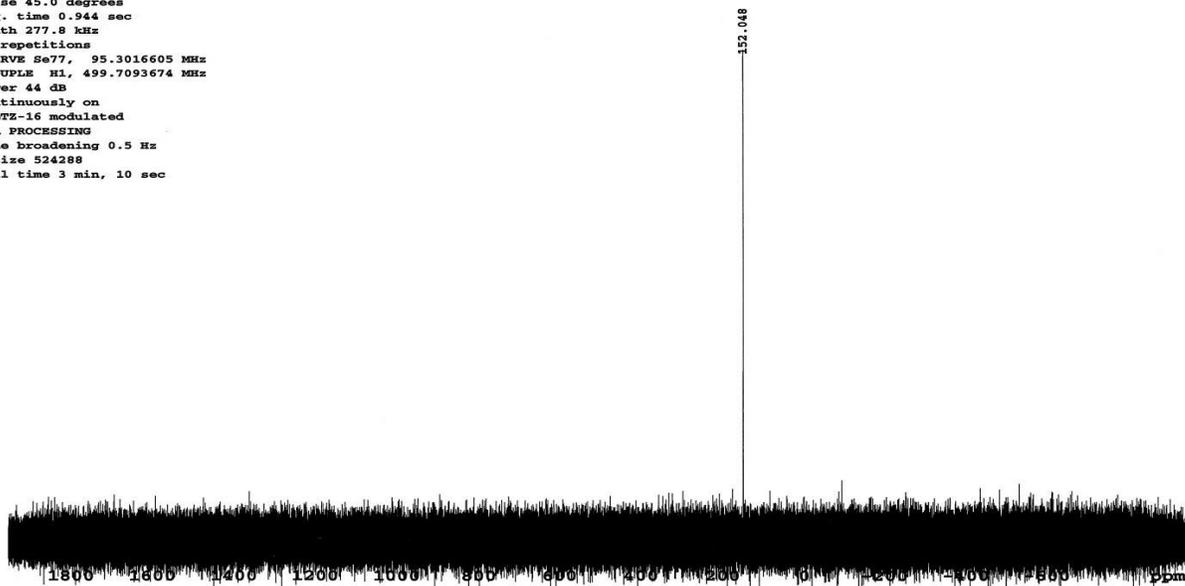


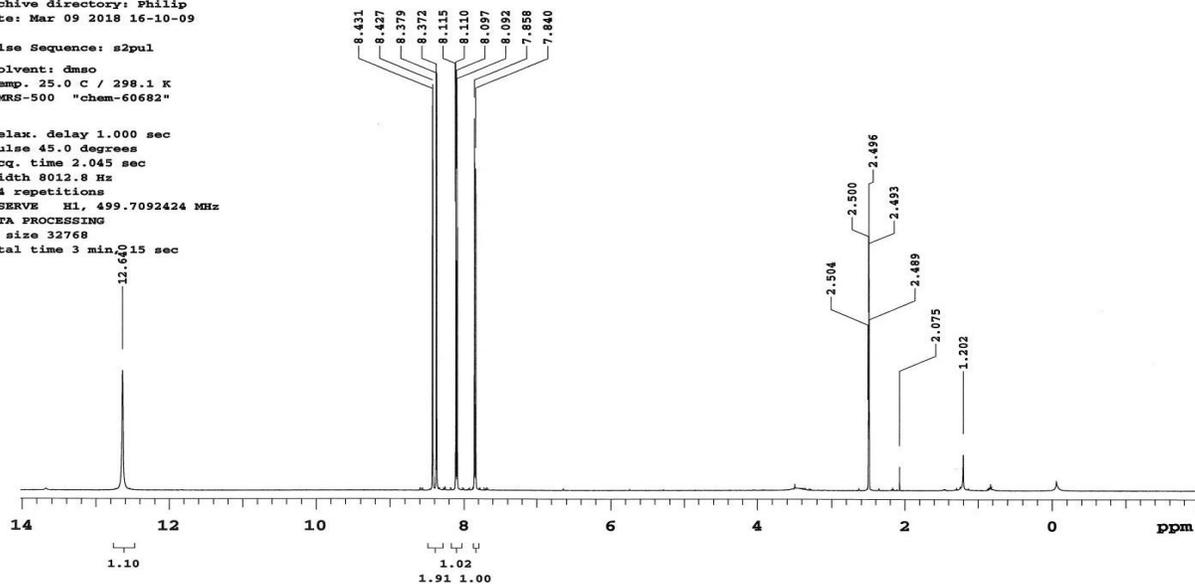
Fig S14. <sup>1</sup>H and <sup>13</sup>C NMR spectra of the compound 4h

Varian VNMR5 500 NMR  
Spectrometer  
SN#P008521

Sample ID number: 6nitroindole  
Project Number:  
Chemist:  
Sample concentration: n/a  
mg/Operator:  
Philip  
Archive directory: Philip  
Date: Mar 09 2018 16-10-09

Pulse Sequence: s2pul  
Solvent: dmsc  
Temp. 25.0 C / 298.1 K  
VNMR5-500 "chem-60682"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.045 sec  
Width 8012.8 Hz  
64 repetitions  
OBSERVE H1, 499.7092424 MHz  
DATA PROCESSING  
FT size 32768  
Total time 3 min, 15 sec



Varian VNMR5 500 NMR  
Spectrometer  
SN#P008521

Sample ID number:  
6nitroindolescn  
Project Number:  
Chemist:  
Sample concentration: n/a  
mg/Operator:  
Philip  
Archive directory: Philip  
Date: Mar 09 2018 16-13-41

Pulse Sequence: s2pul  
Solvent: dmsc  
Temp. 25.0 C / 298.1 K  
User: 1-14-87  
VNMR5-500 "chem-60682"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.049 sec  
Width 31250.0 Hz  
512 repetitions  
OBSERVE C13, 125.6519890 MHz  
DECOUPLE H1, 499.7117410 MHz  
Power 44 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 17 min, 29 sec

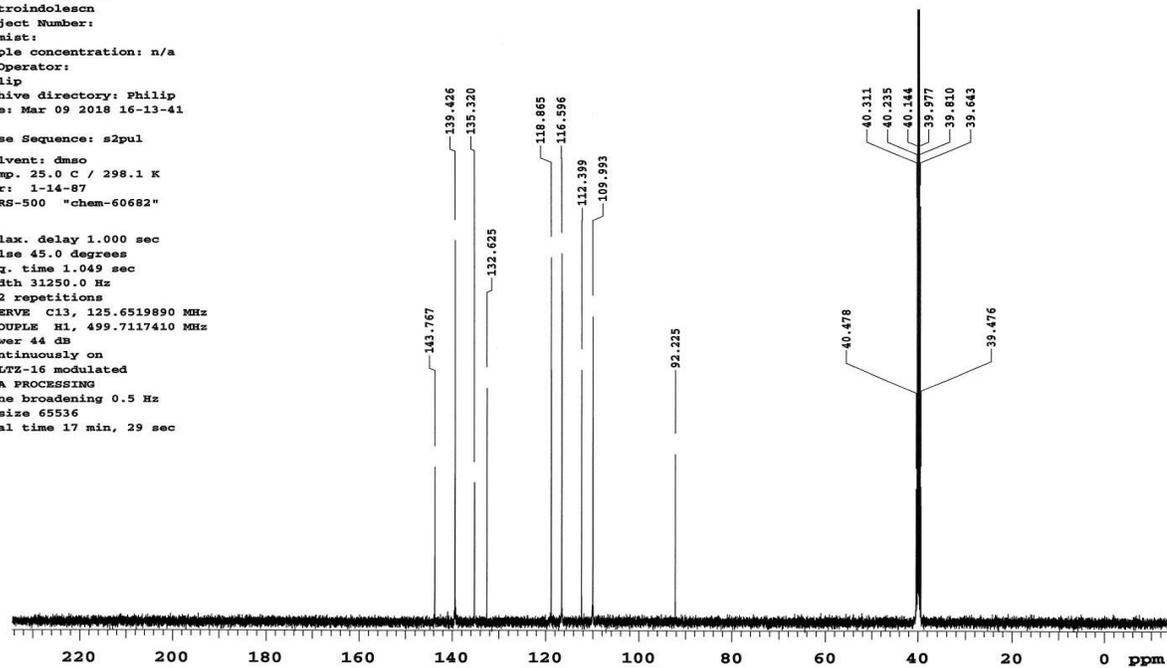


Fig S15.  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{77}\text{Se}$  NMR spectra of the compound 5h

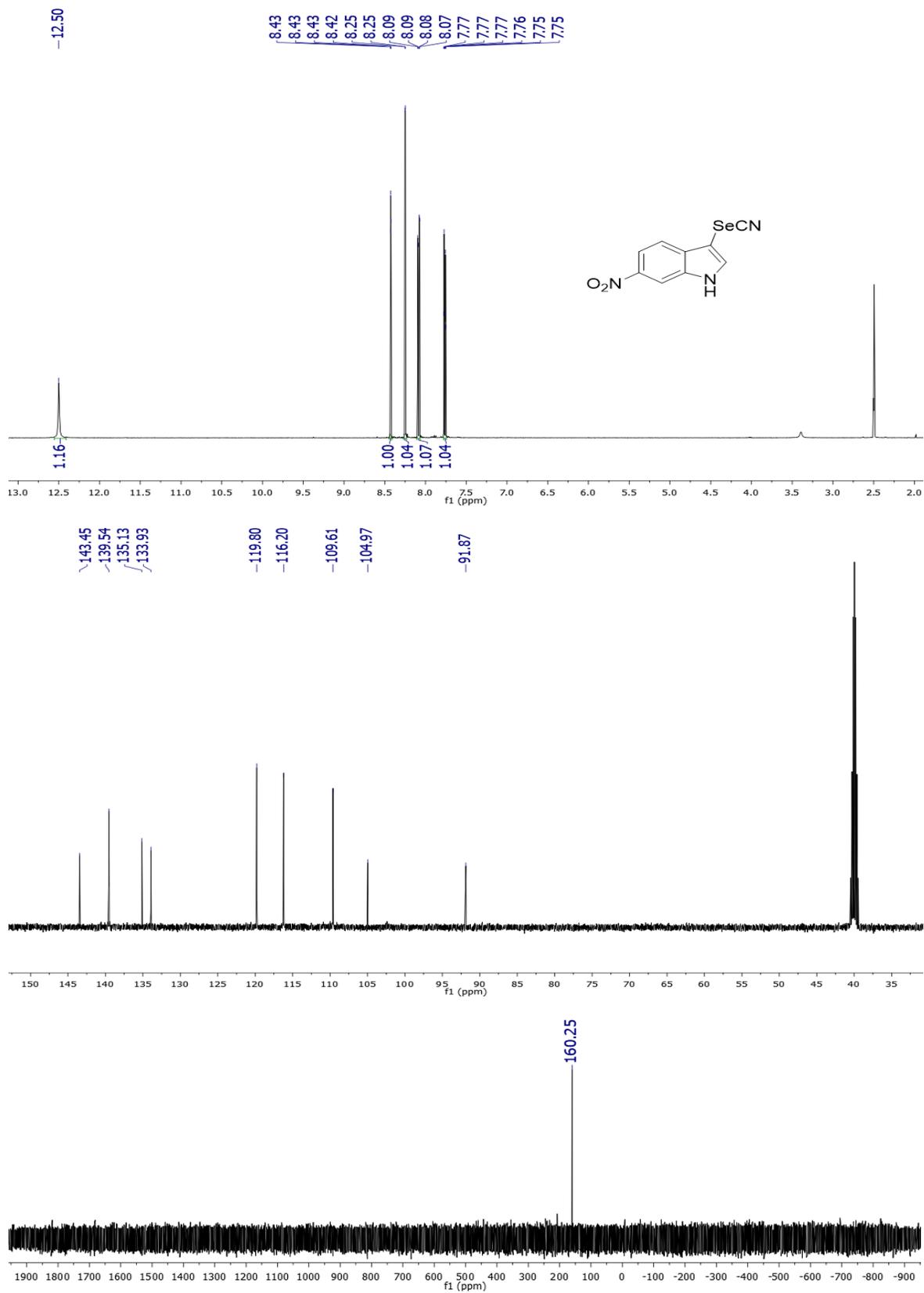
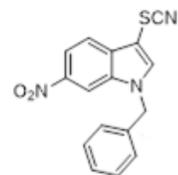


Fig S16. <sup>1</sup>H and <sup>13</sup>C NMR spectra of the compound 4i



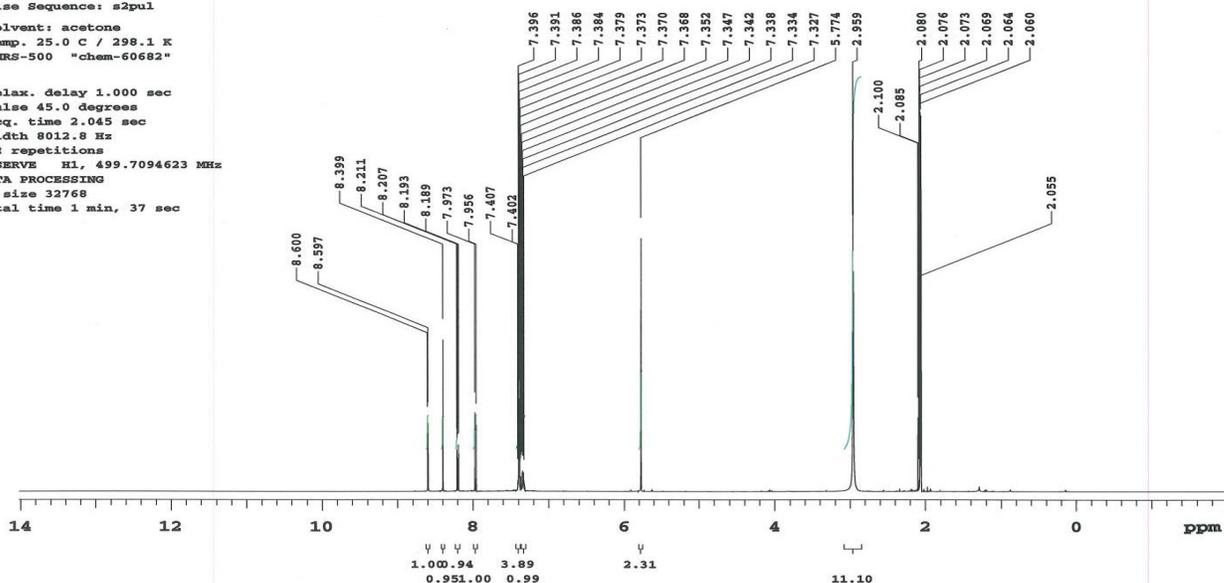
Varian VMRS 500 NMR  
Spectrometer  
SN#P008521

Sample ID number: 6nitroindole  
Sample concentration: n/a mg  
Operator: Philip  
Archive directory: Philip  
Date: Mar 29 2018 12-36-31

Pulse Sequence: s2pul

Solvent: acetone  
Temp. 25.0 C / 298.1 K  
VMRS-500 "chem-60682"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.045 sec  
Width 8012.8 Hz  
32 repetitions  
OBSERVE H1, 499.7094623 MHz  
DATA PROCESSING  
FT size 32768  
Total time 1 min, 37 sec



nitro\_indole\_benzyl\_scn

Pulse Sequence: s2pul

Solvent: acetone  
Temp. 25.0 C / 298.1 K  
User: 1-14-87  
VMRS-500 "chem-60682"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.049 sec  
Width 31250.0 Hz  
1000 repetitions  
OBSERVE C13, 125.6520442 MHz  
DECOUPLE H1, 499.7119609 MHz  
Power 44 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 34 min, 9 sec

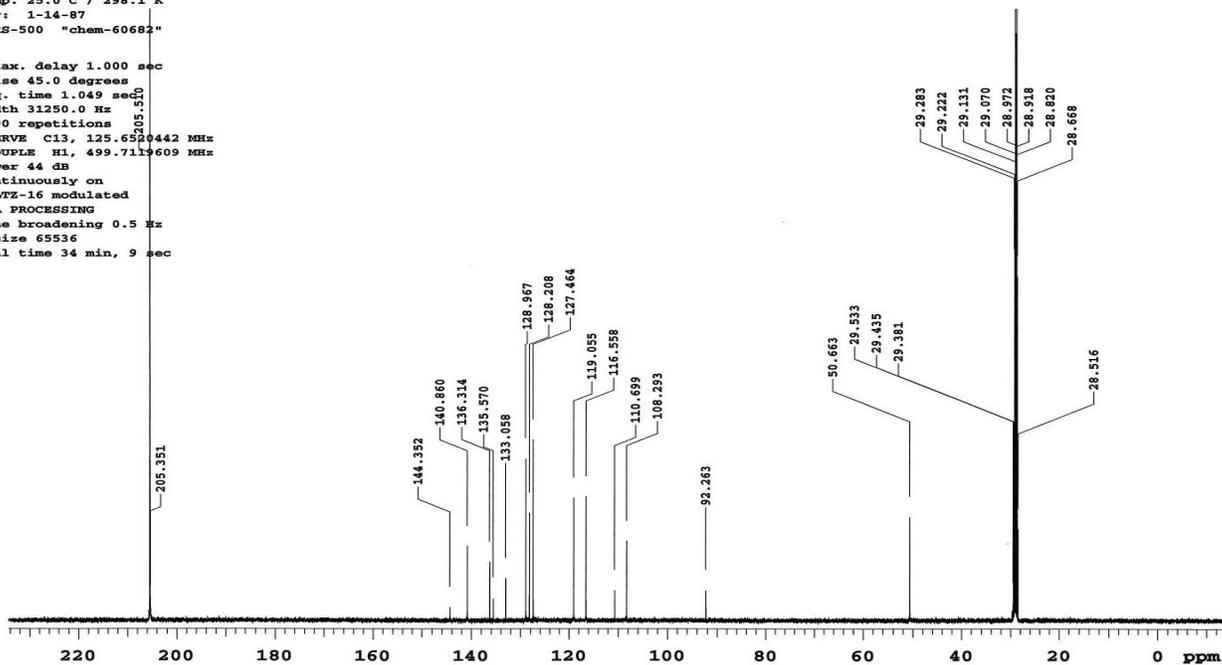


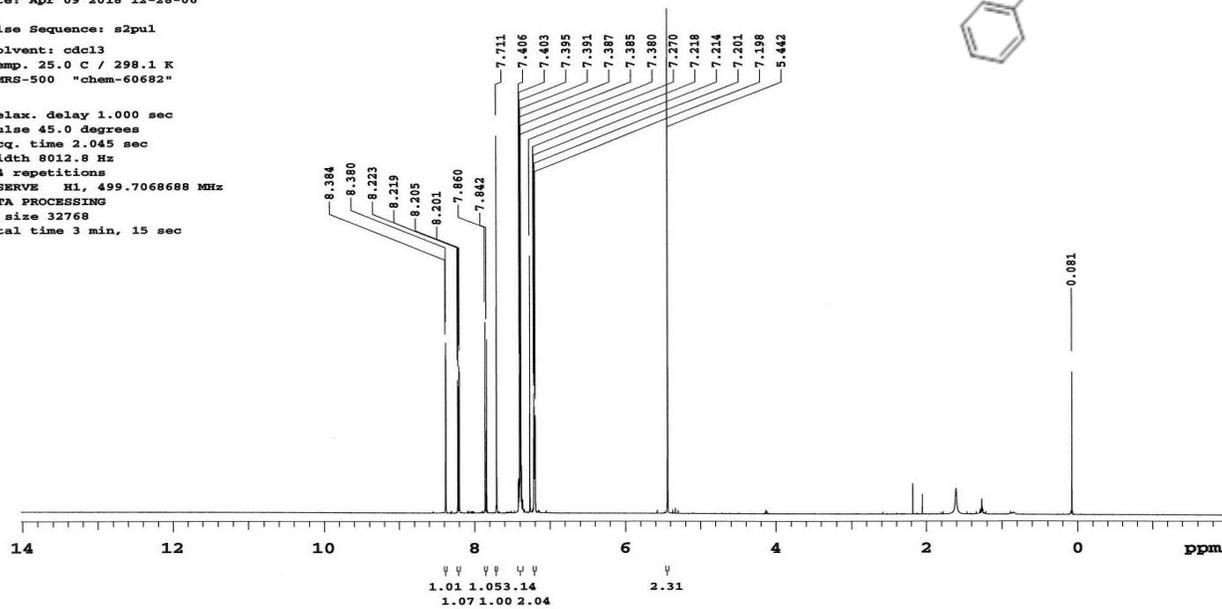
Fig S17. <sup>1</sup>H and <sup>13</sup>C NMR spectra of the compound 5i

Varian VNMR5 500 NMR  
Spectrometer  
SN#P008521

Sample ID number: n  
Sample concentration: n/a mg  
Operator: Philip  
Archive directory: Philip  
Date: Apr 09 2018 12-28-06

Pulse Sequence: s2pul  
Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
VNMR5-500 "chem-60682"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.045 sec  
Width 8012.8 Hz  
64 repetitions  
OBSERVE H1, 499.7068688 MHz  
DATA PROCESSING  
FT size 32768  
Total time 3 min, 15 sec



6-nitro\_n\_bz\_secn\_indole

Pulse Sequence: s2pul  
Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
User: 1-14-87  
VNMR5-500 "chem-60682"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.049 sec  
Width 31250.0 Hz  
256 repetitions  
OBSERVE C13, 125.6513921 MHz  
DECOUPLE H1, 499.7093674 MHz  
Power 44 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 8 min, 44 sec

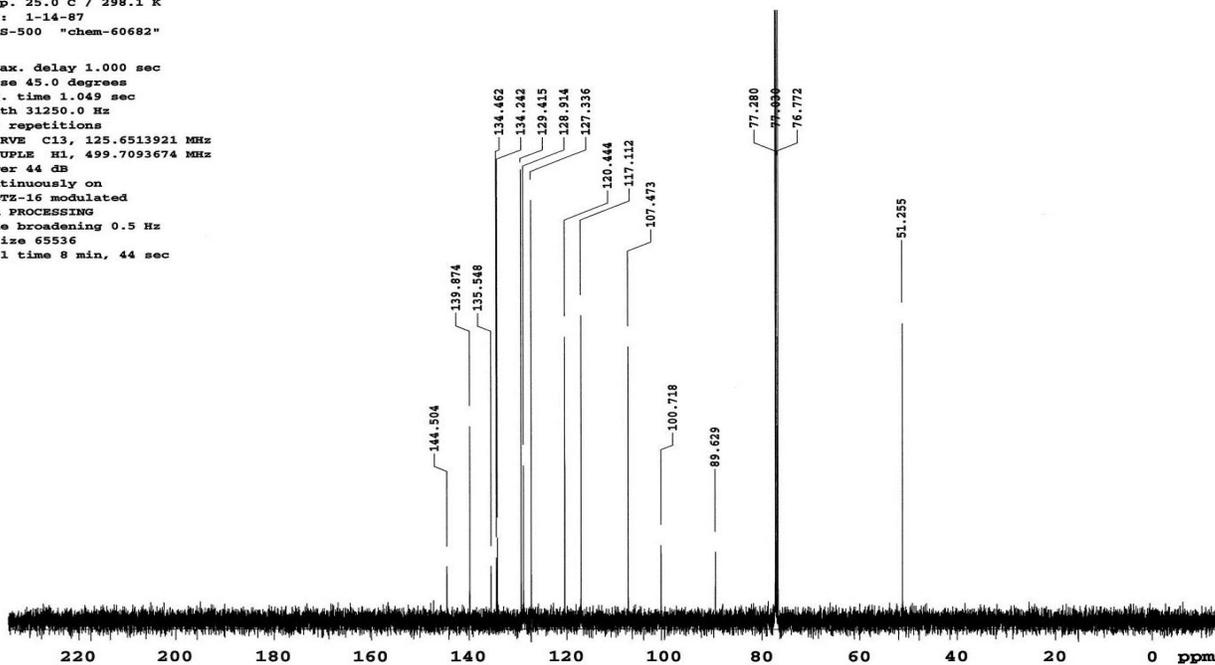


Fig S18.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of the compound 4j

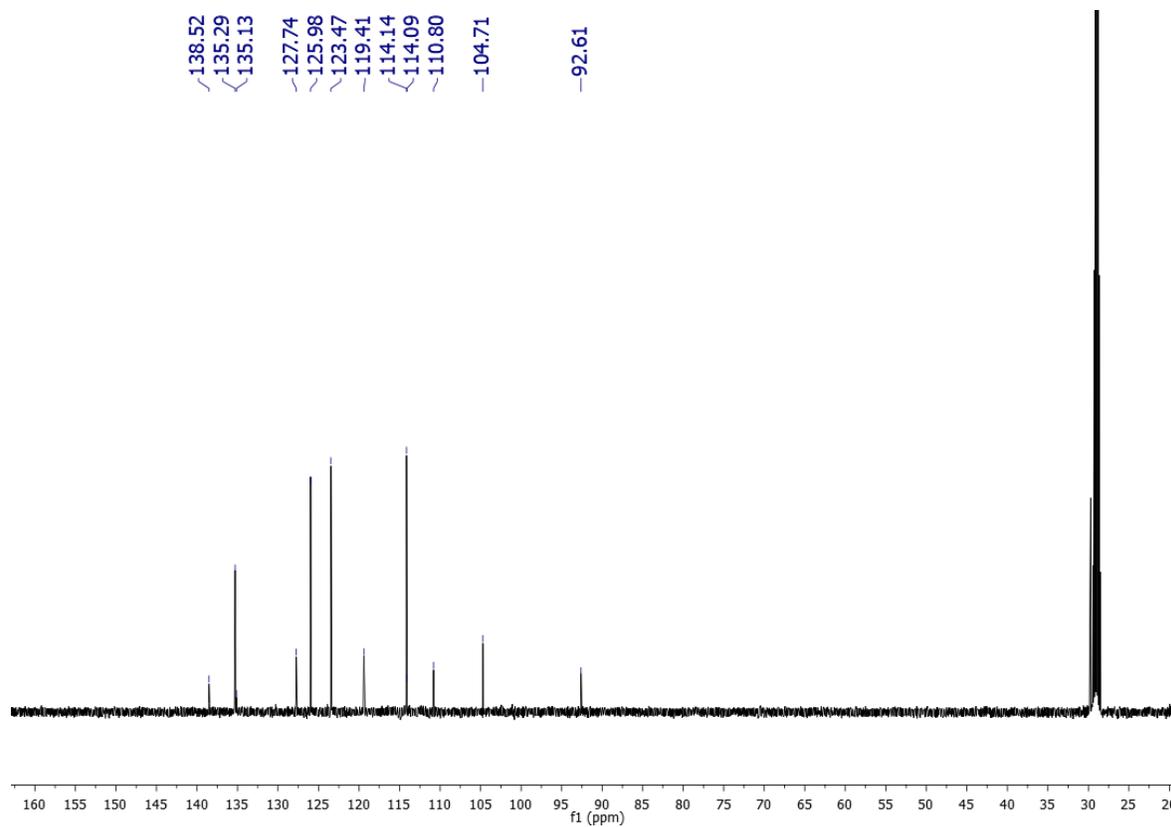
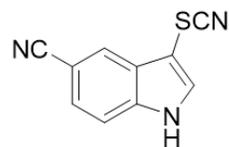
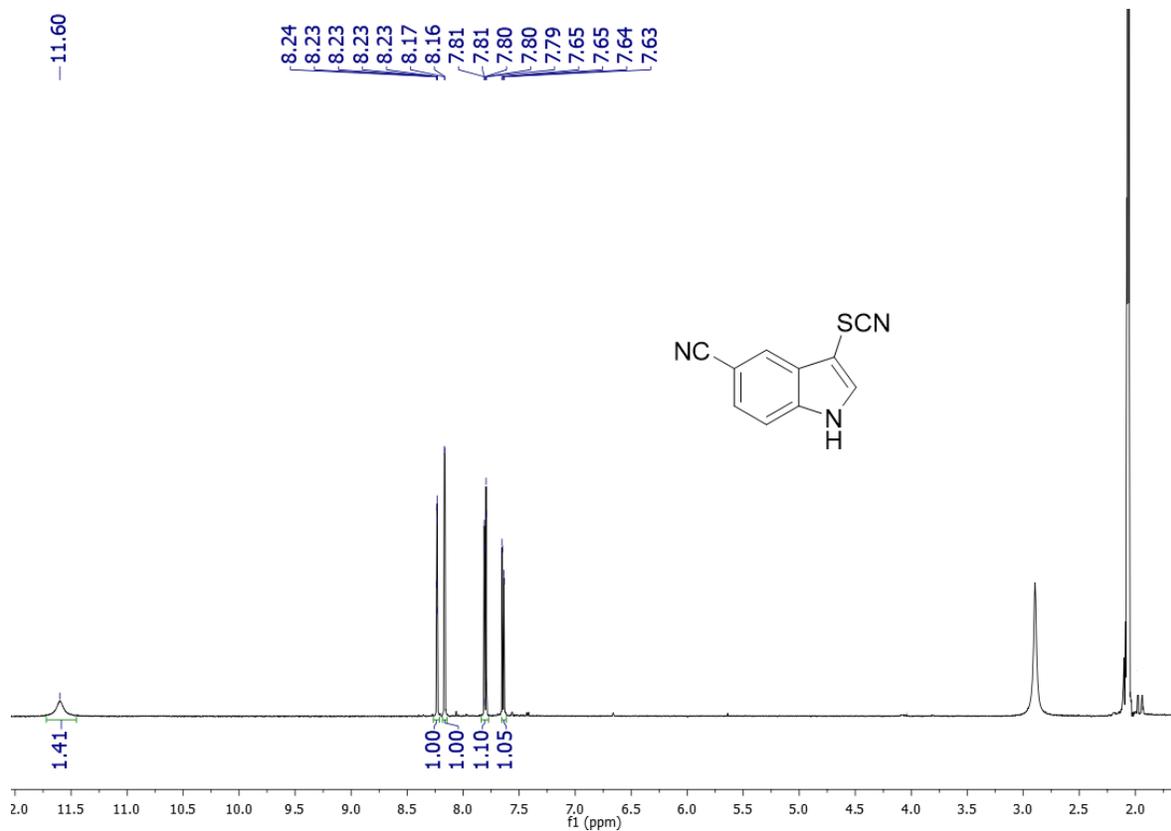




Fig S20.  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{77}\text{Se}$  NMR spectra of the compound 8a

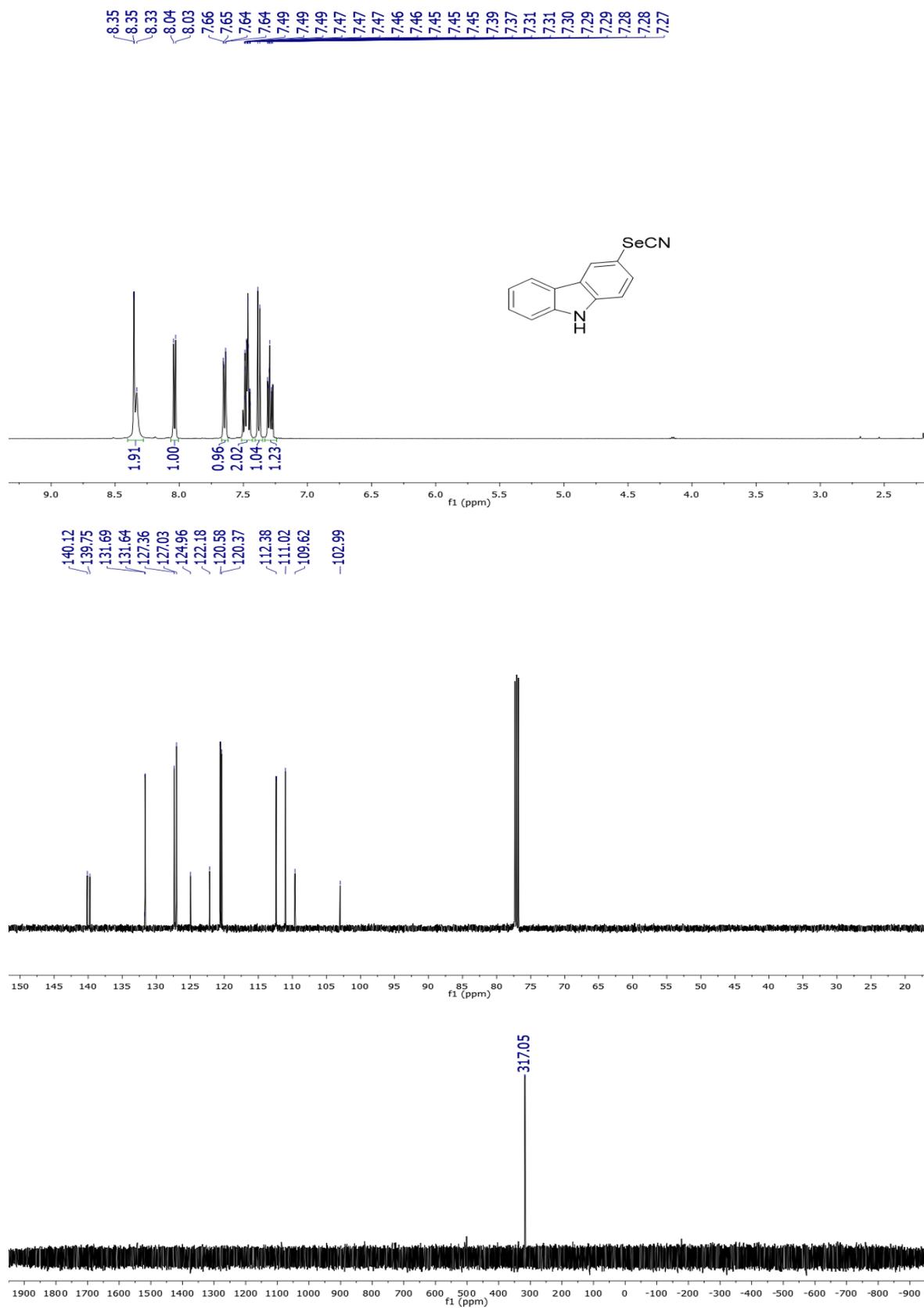


Fig S21. <sup>1</sup>H and <sup>13</sup>C NMR spectra of the compound 7b

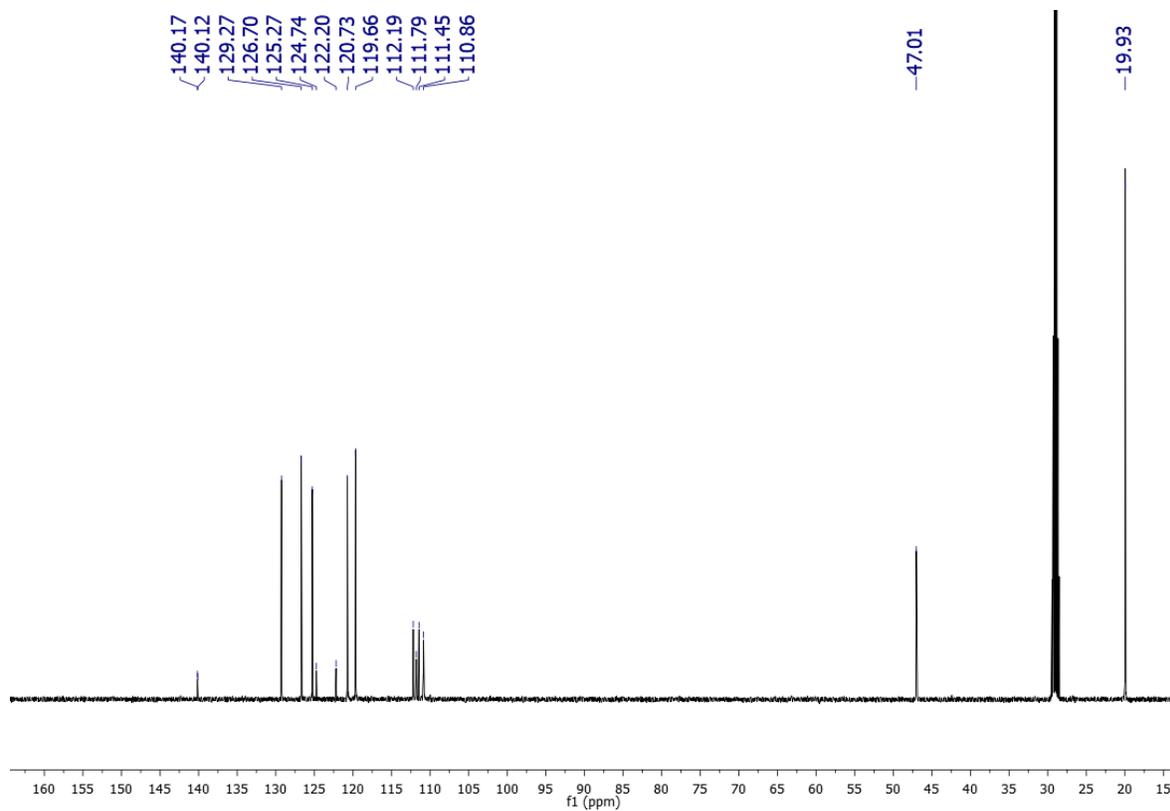
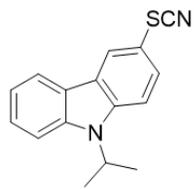
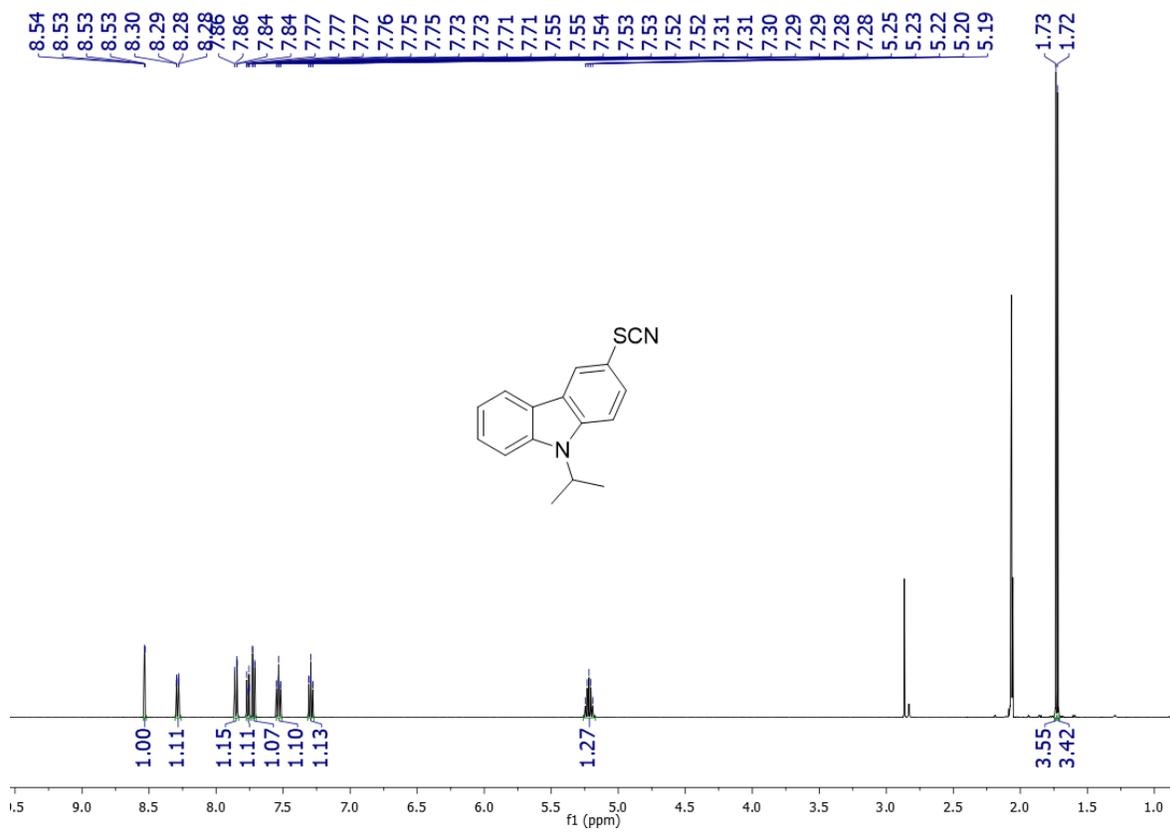


Fig S22.  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{77}\text{Se}$  NMR spectra of the compound 8b

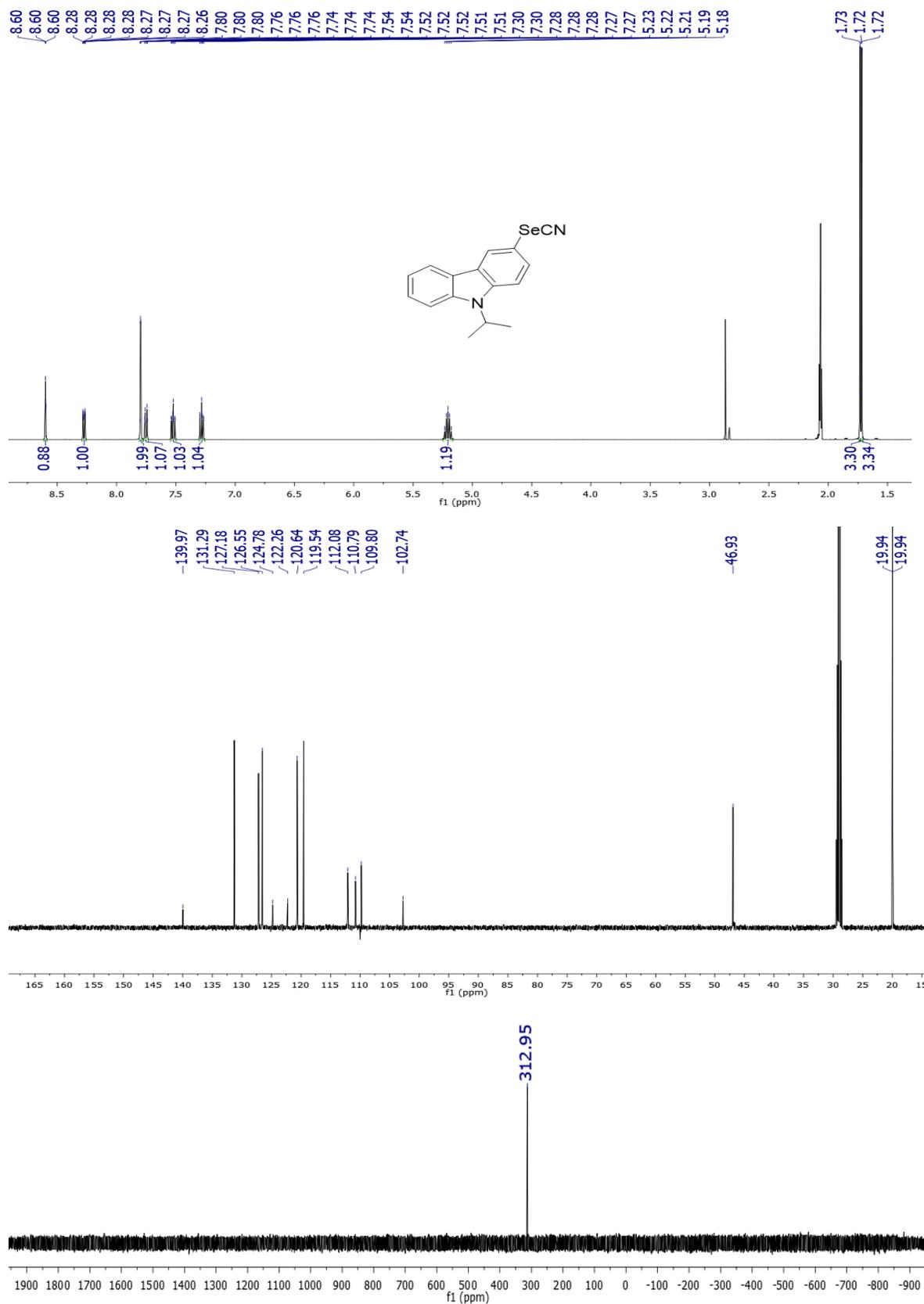


Fig S23.  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{77}\text{Se}$  NMR spectra of the compound 9

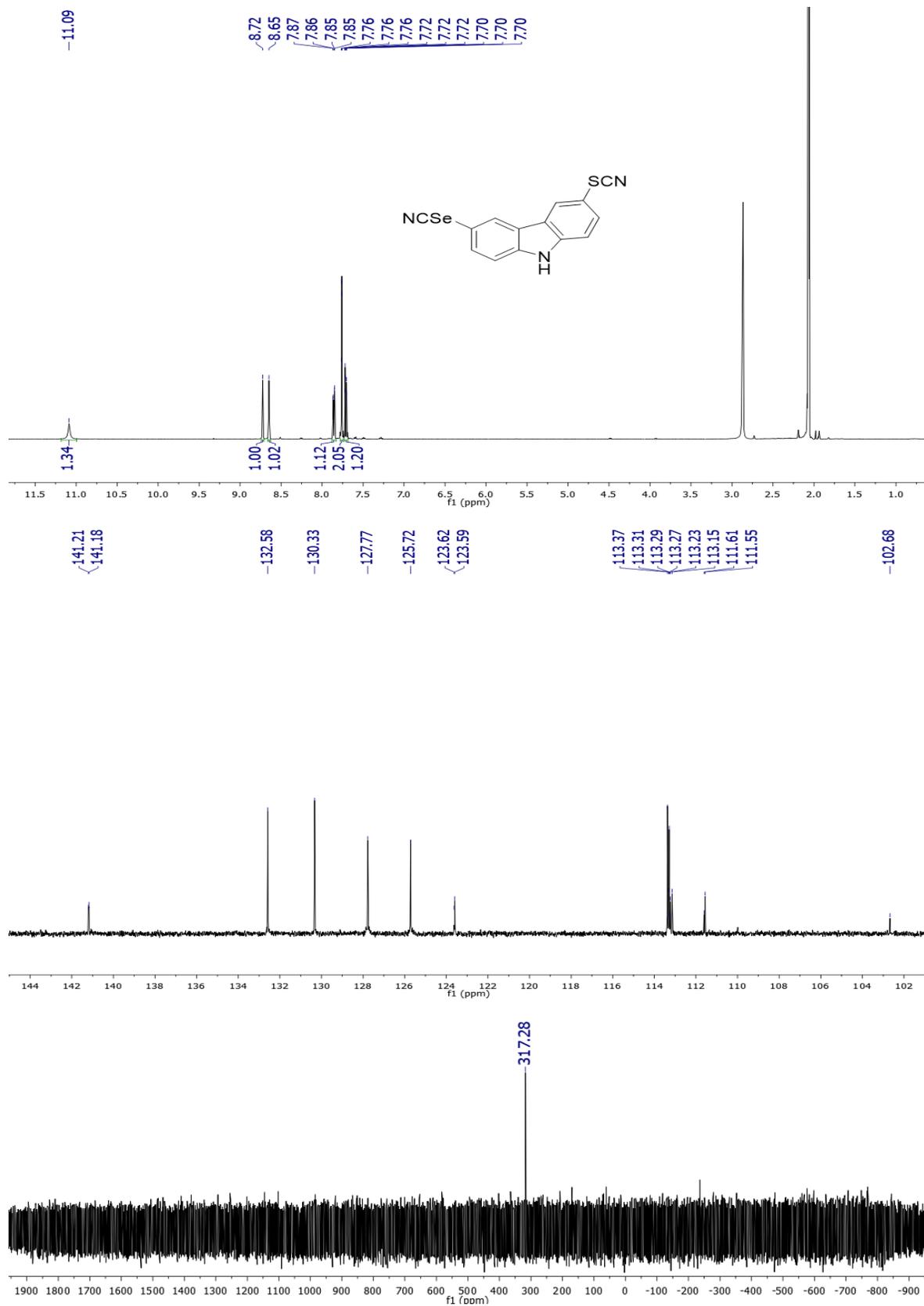


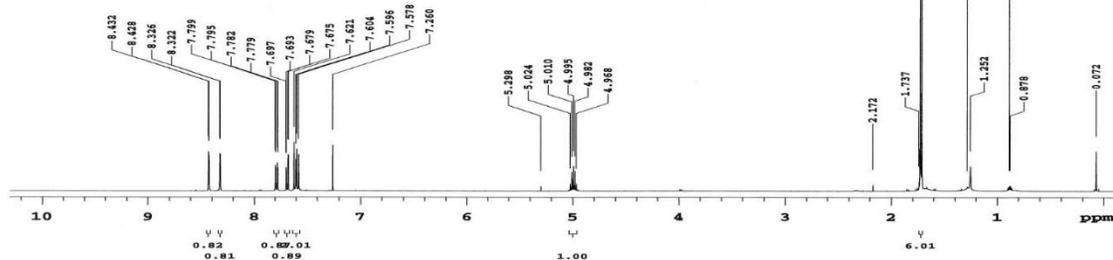
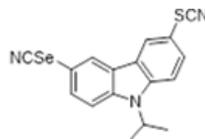
Fig S24.  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{77}\text{Se}$  NMR spectra of the compound 10

Varian VNMRS 500 NMR  
Spectrometer  
SN#P008521

Sample ID number: carbasole  
Sample concentration: n/a mg  
Operator: Philip  
Archive directory: Philip  
Date: May 07 2018 11-40-00

Pulse Sequence: s2pul  
Solvent: cdcl3  
Temp: 25.0 C / 298.1 K  
VNMRS-500 "chem-60682"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.045 sec  
Width 8012.8 Hz  
32 repetitions  
OBSERVE H1, 499.7068735 MHz  
DATA PROCESSING  
FT size 32768  
Total time 1 min, 37 sec

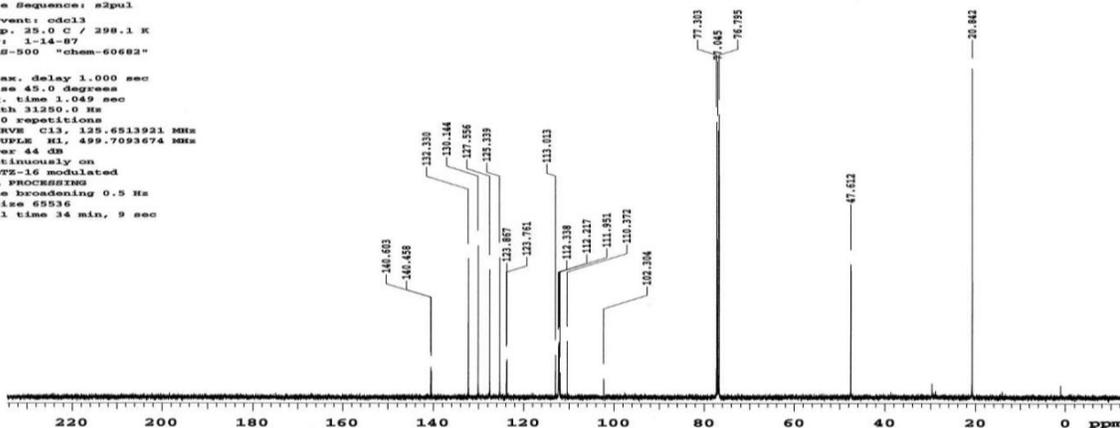


Varian VNMRS 500 NMR  
Spectrometer  
SN#P008521

Sample ID number: carbasole  
Sample concentration: n/a mg  
Operator: Philip  
Archive directory: Philip  
Date: May 07 2018 12-26-57

Pulse Sequence: s2pul  
Solvent: cdcl3  
Temp: 25.0 C / 298.1 K  
User: 1-14-87  
VNMRS-500 "chem-60682"

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 3.049 sec  
Width 31250.0 Hz  
1000 repetitions  
OBSERVE C13, 125.6513951 MHz  
DECOUPLE H1, 499.7093674 MHz  
Power 44 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 14 min, 9 sec



di\_iso

Pulse Sequence: s2pul  
Solvent: cdcl3  
Temp: 25.0 C / 298.1 K  
User: 1-14-87  
VNMRS-500 "chem-60682"

Relax. delay 5.000 sec  
Pulse 45.0 degrees  
Acq. time 0.944 sec  
Width 277.8 MHz  
32 repetitions  
OBSERVE Se77, 95.3016605 MHz  
DECOUPLE H1, 499.7093674 MHz  
Power 44 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 254288  
Total time 3 min, 10 sec

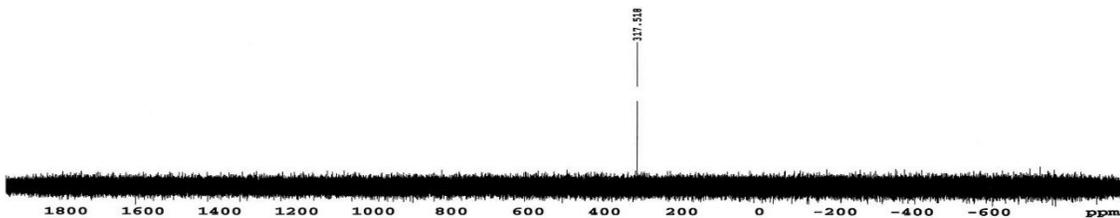


Fig S25. <sup>1</sup>H and <sup>13</sup>C NMR spectra of the compound 11b

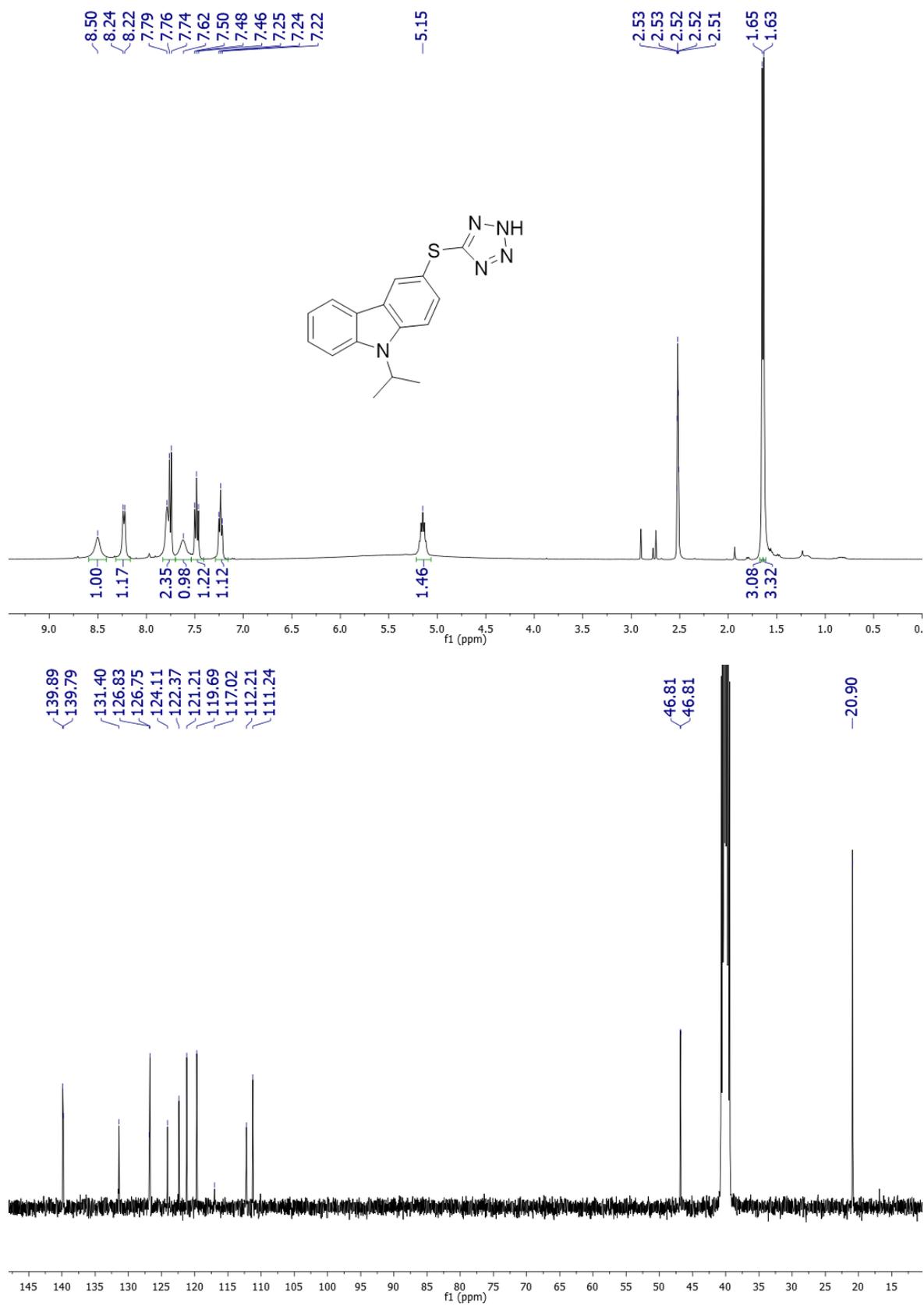


Fig S26. <sup>1</sup>H and <sup>13</sup>C NMR spectra of the compound 12b

