

5-Selenization of Salicylic Acid Derivatives Yielded Isoform-specific 5-Lipoxygenase Inhibitors

(Supplementary Information)

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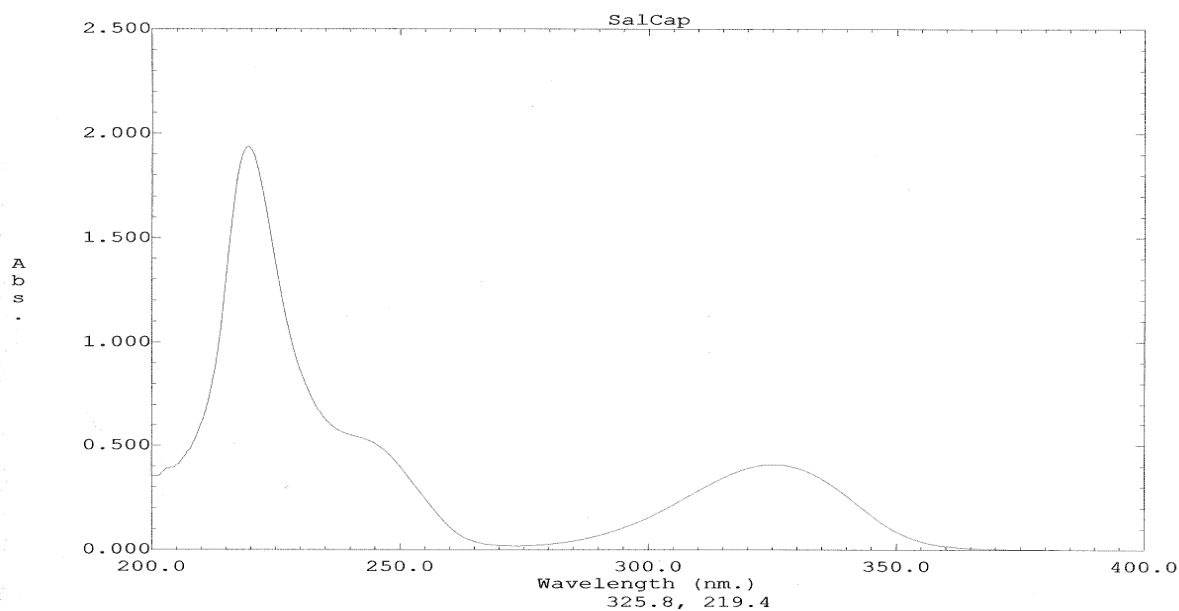
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Contents

1. Spectra of salicyloyl caproic acid.....	S2
2. Spectra of 2b	S4
3. Spectra of 3c	S8
4. Spectra of 3d	S11
5. Spectra of 3e	S15
6. Spectra of 4e	S19
7. Spectra of 5e	S23



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Figure SI-1. UV spectrum of salicyloyl caproic acid.

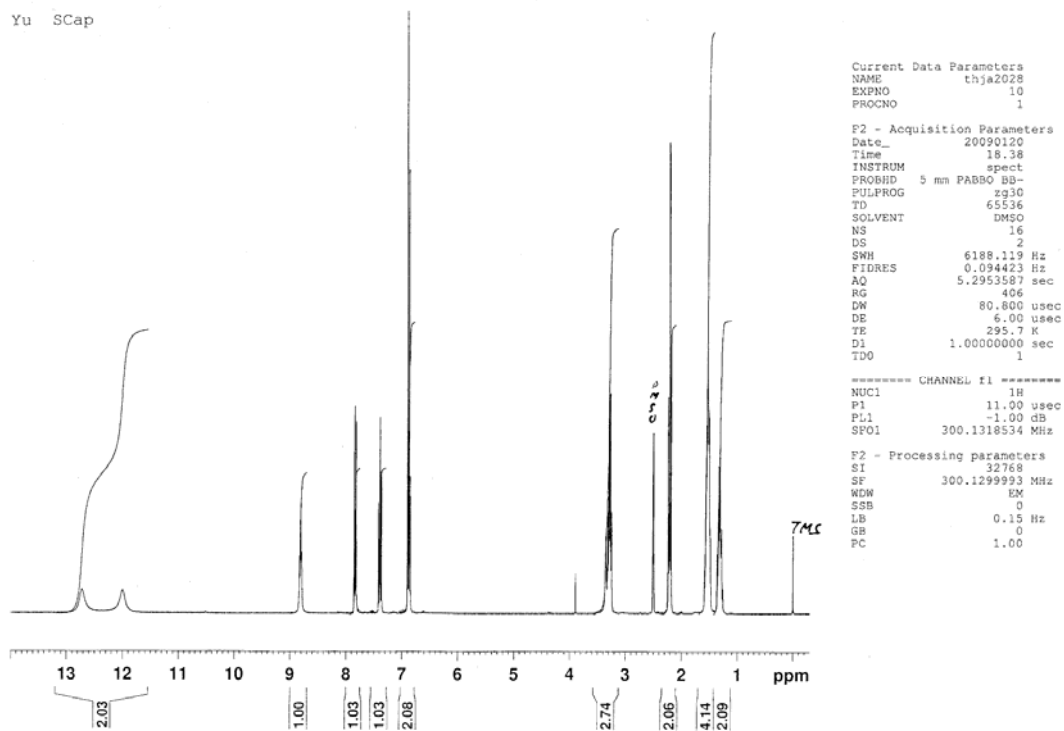


Figure SI-2. ¹H-NMR spectrum of salicyloyl caproic acid

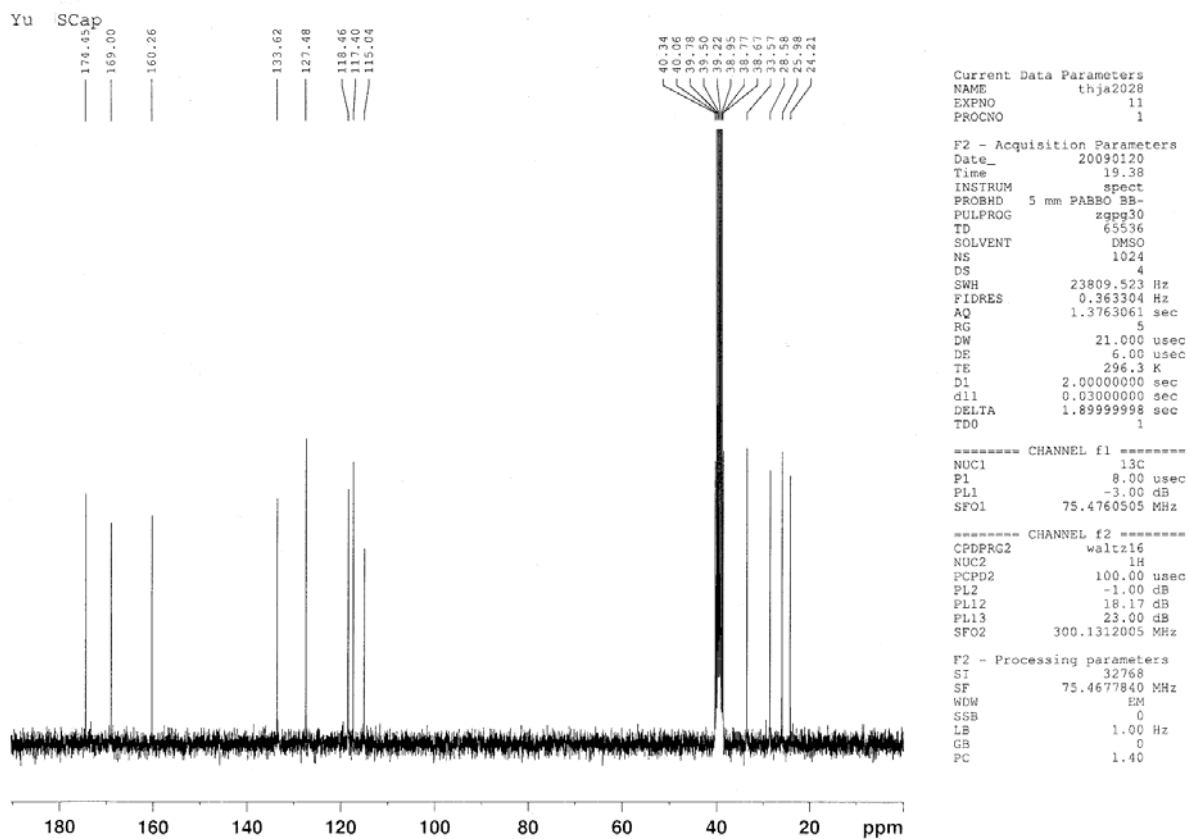


Figure SI-3. ^{13}C -NMR spectrum of salicyloyl caproic acid

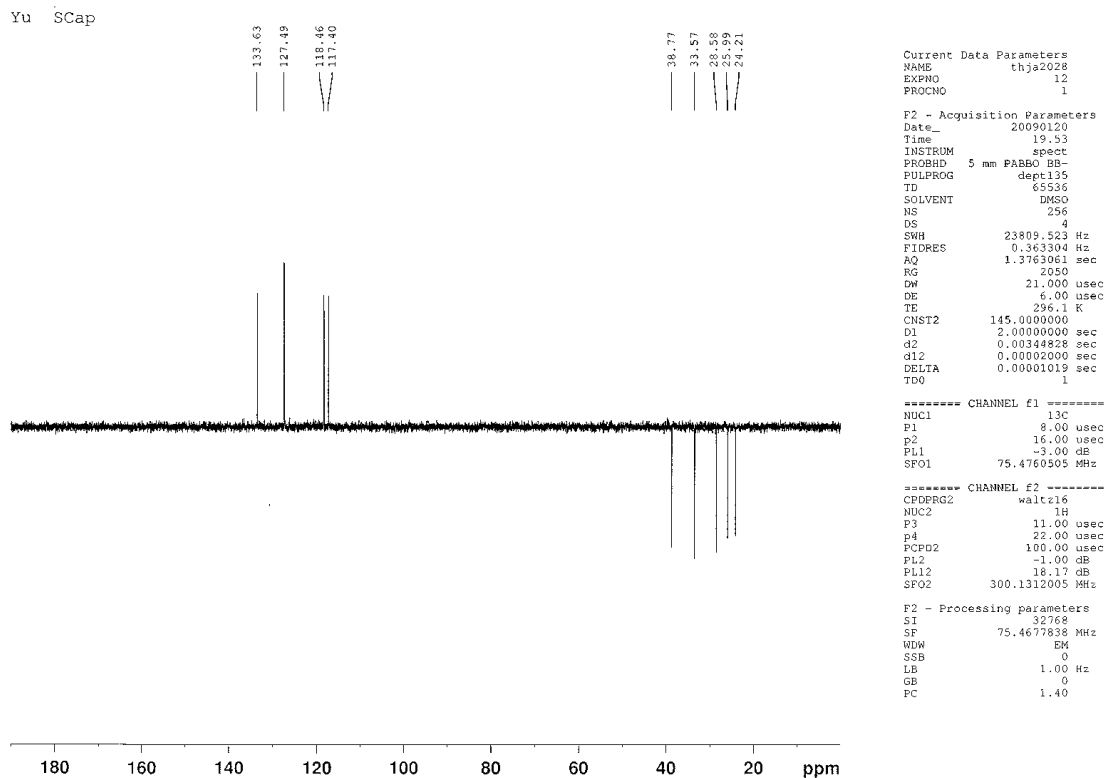


Figure SI-4. 2D-NMR spectrum (HMQC) of salicyloyl caproic acid

:\ms-daten-lin\...Yu_SCap_pos_07012009

07.01.2009 09:35:14

Yu SCap

u_SCap_pos_07012009#17-187 RT: 0.22-4.93 AV: 85 NL: 3.97E6
: FTMS + c NSI Full ms [100.00-600.00]

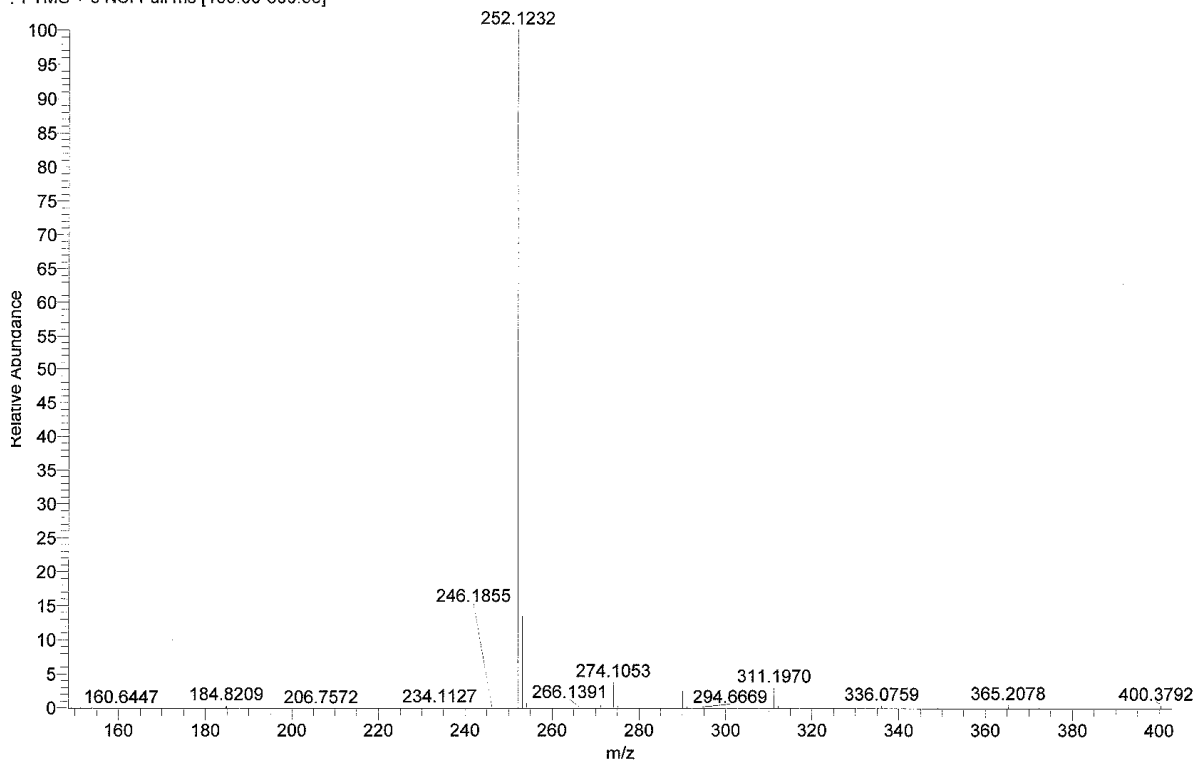


Figure SI-5. HR-MS spectrum of salicyloyl caproic acid

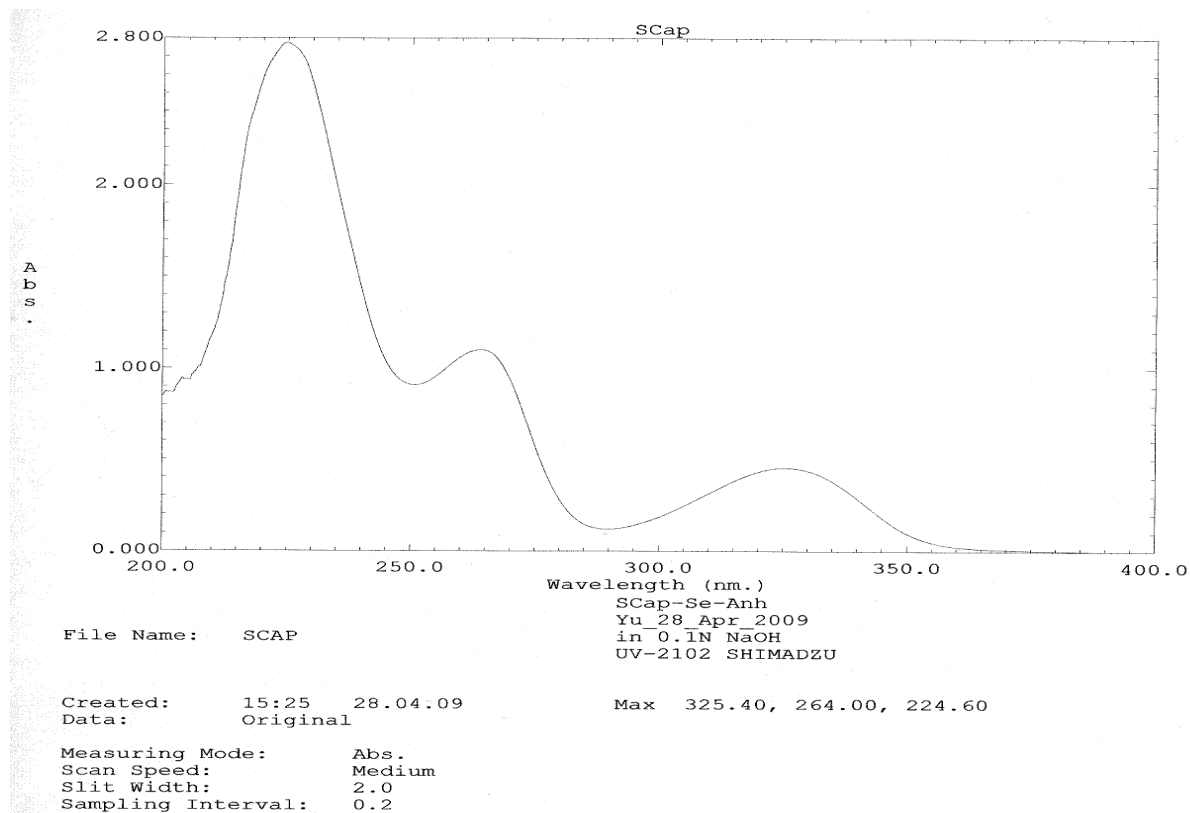


Figure SI-6. UV spectrum of **2b**

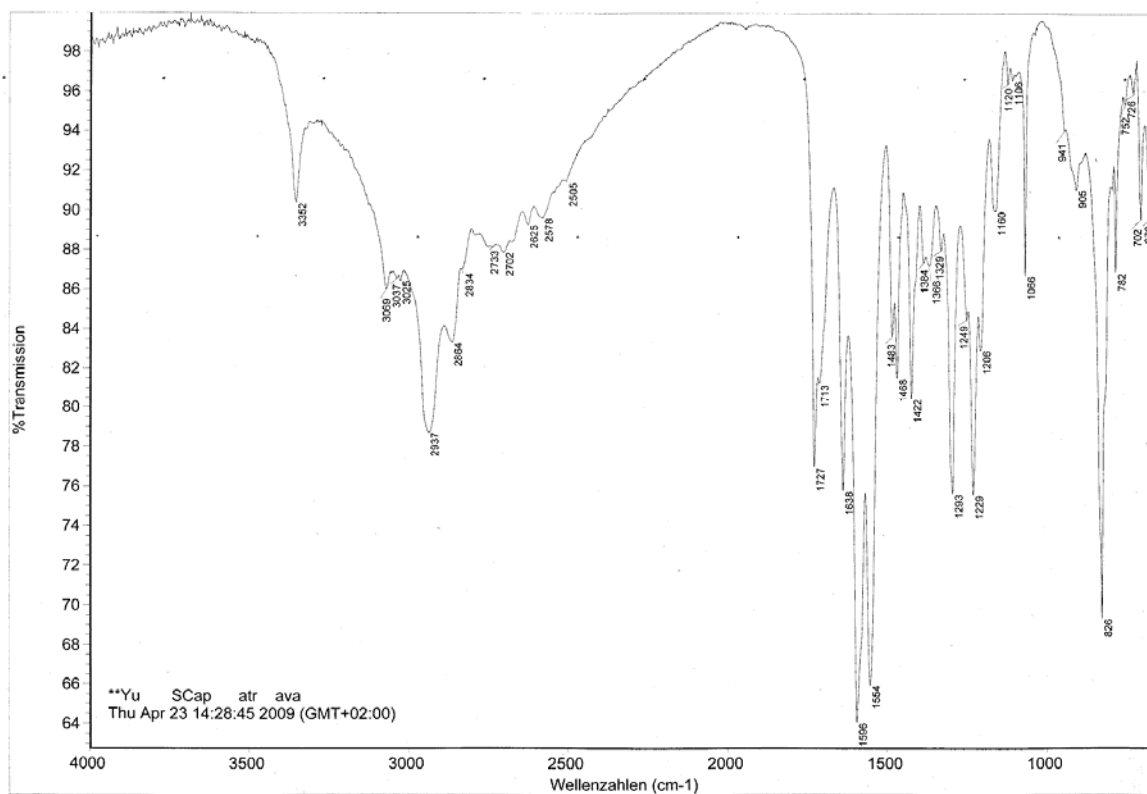


Figure SI-7. FT-IR spectrum of **2b**

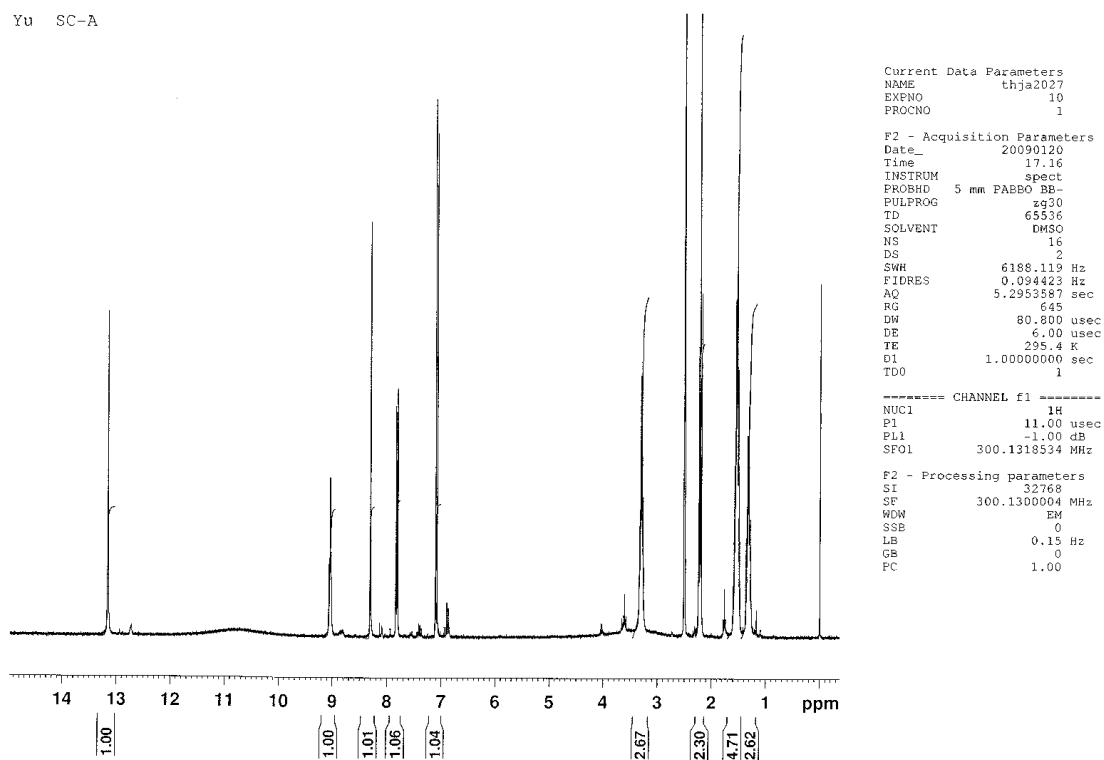


Figure SI-8. $^1\text{H-NMR}$ spectrum of **2b**

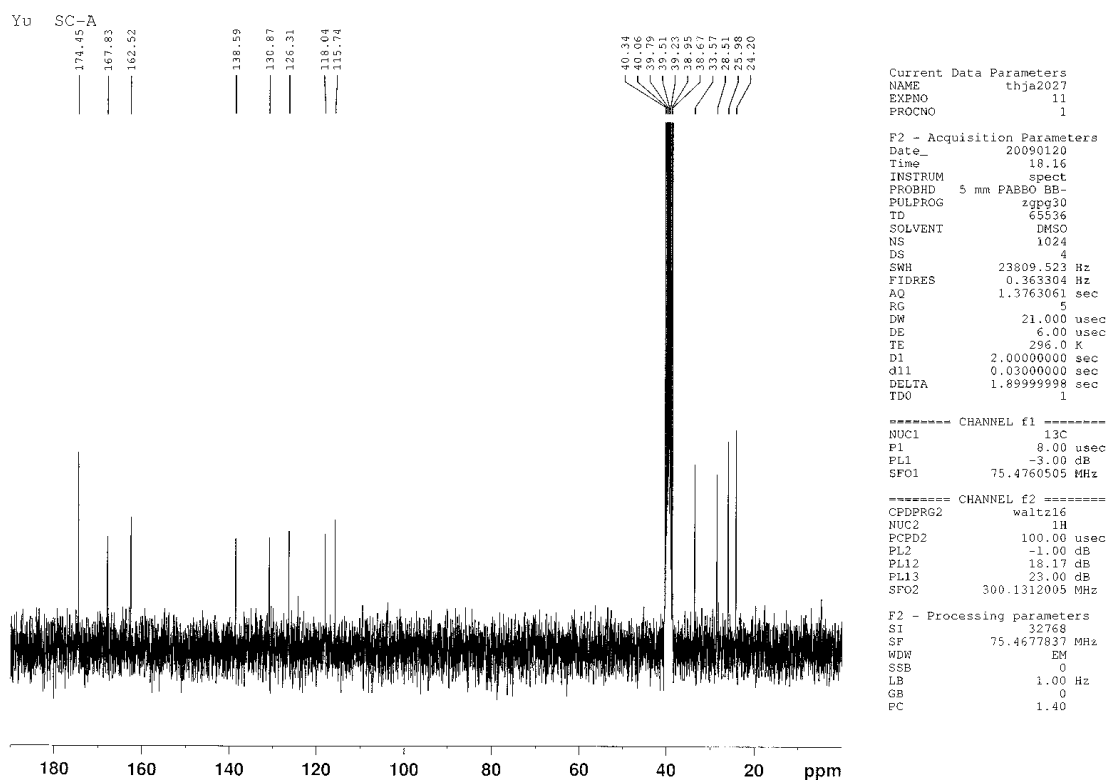


Figure SI-9. ^{13}C -NMR spectrum of **2b**

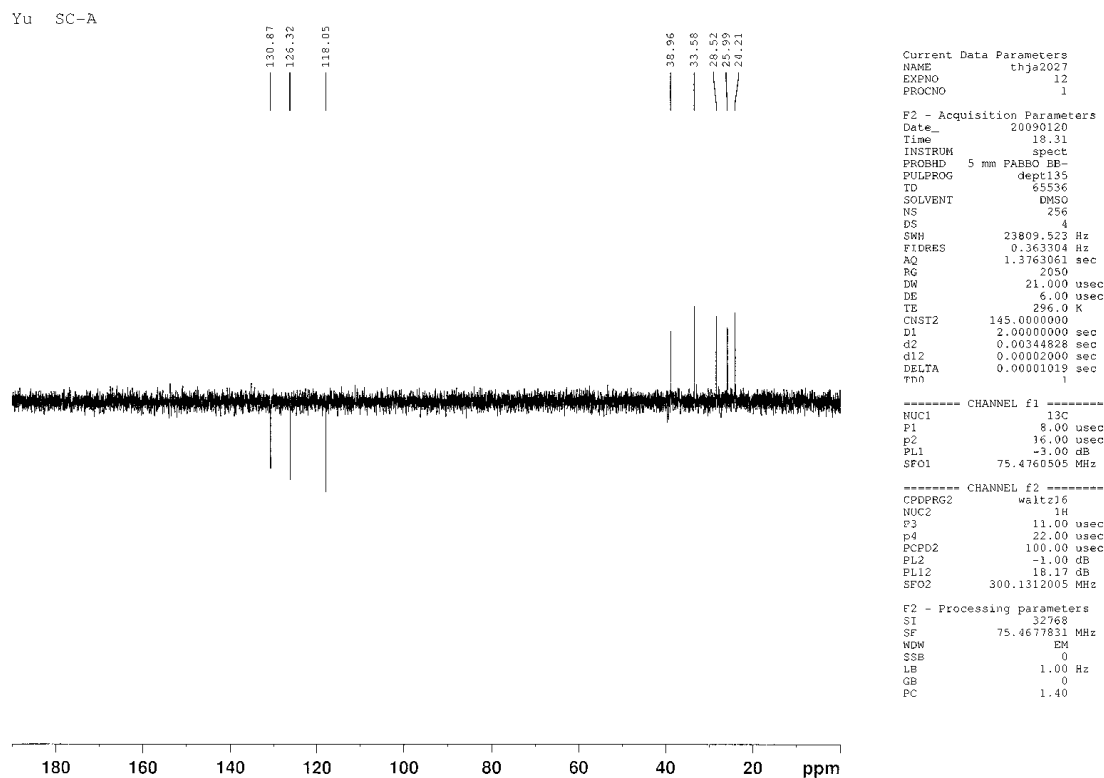


Figure SI-10. 2D-NMR spectrum (HMQC) of **2b**

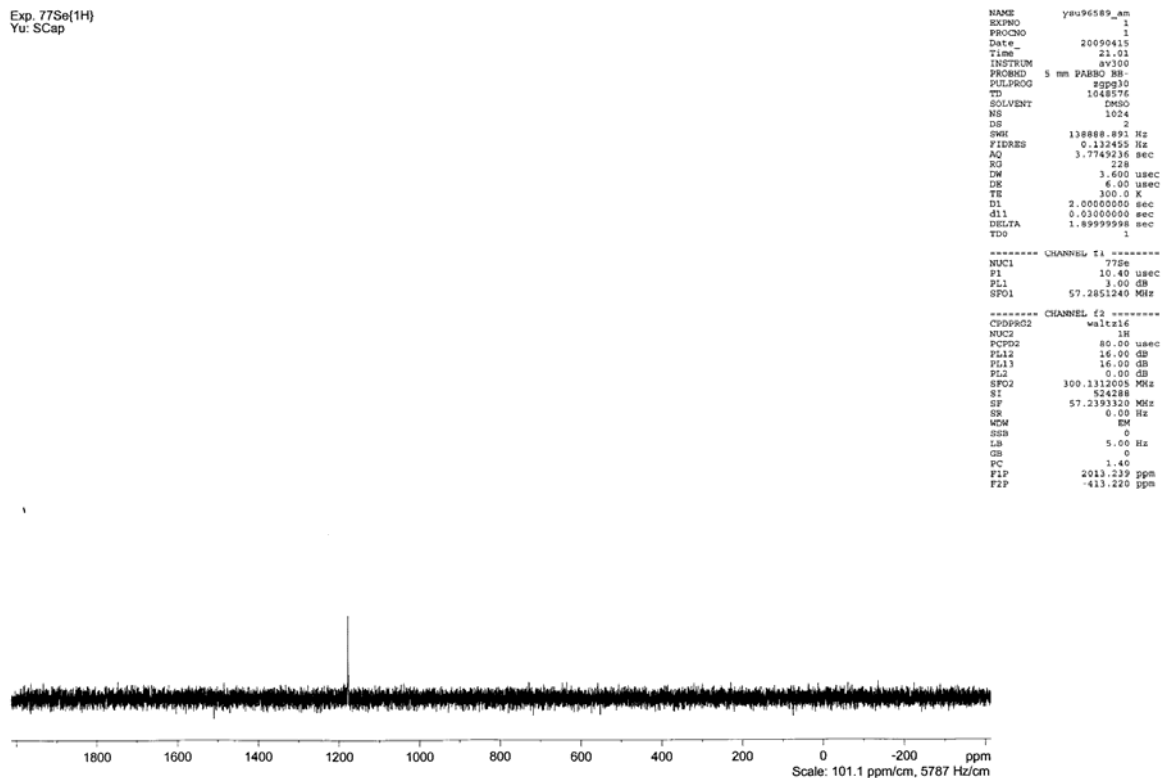


Figure SI-11. ^{77}Se -NMR spectrum of **2b**

:\ms-daten-lin\...\Yu_SC-A_pos_07012009

07.01.2009 09:41:13

Yu SC - A

u_SC-A_pos_07012009 #103-187 RT: 2.57-4.94 AV: 42 NL: 5.89E5
FTMS + c NSI Full ms [150.00-1300.00]

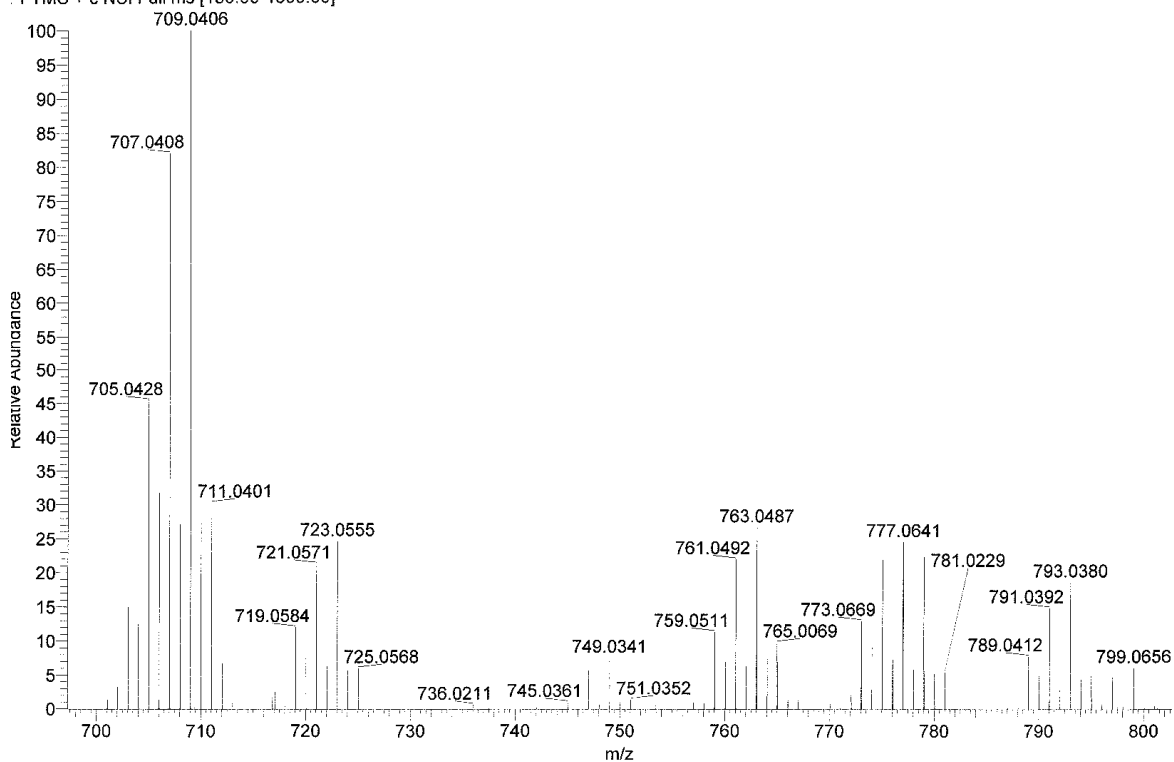


Figure SI-12. HR-MS spectrum of **2b**

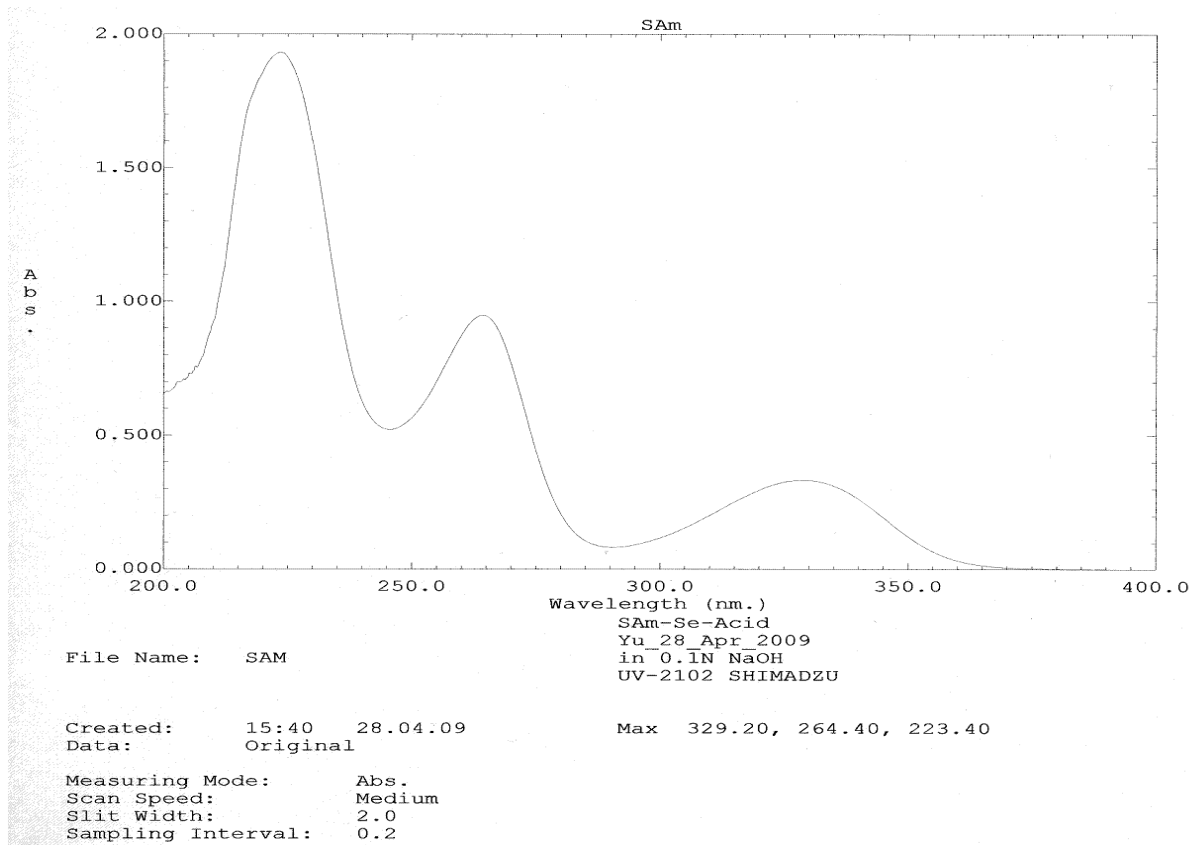


Figure SI-13. UV spectrum of **3c**

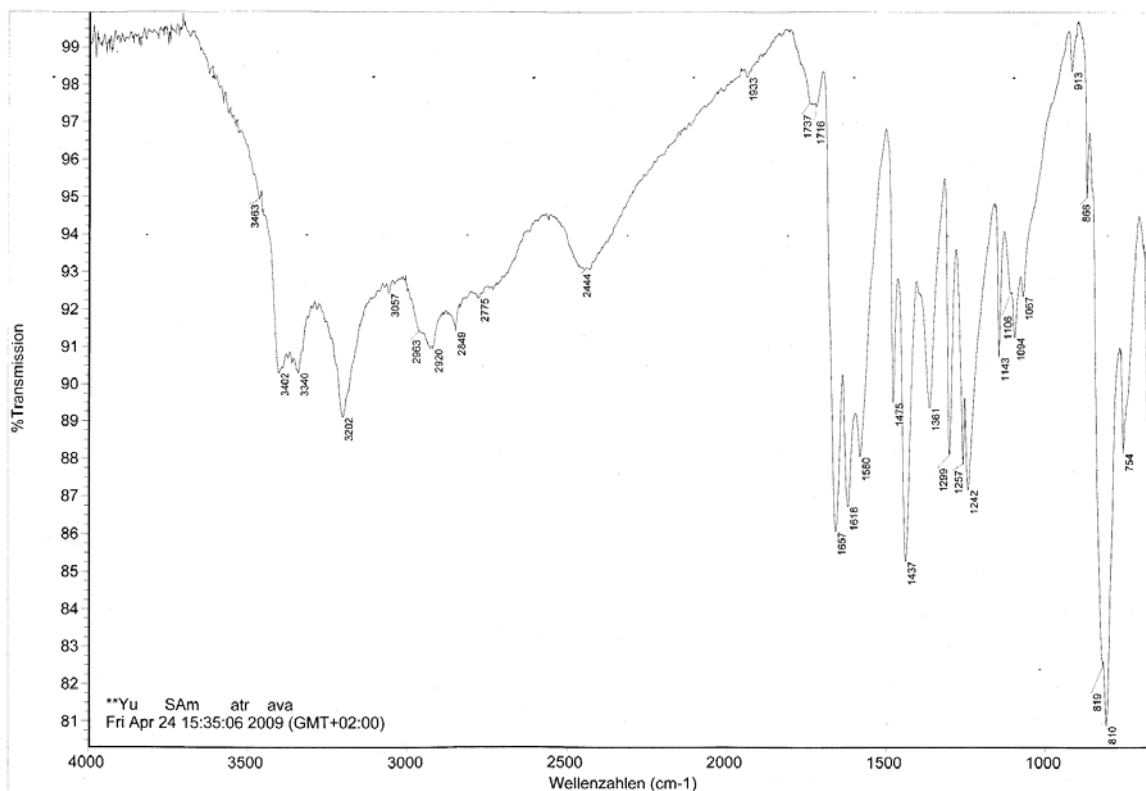
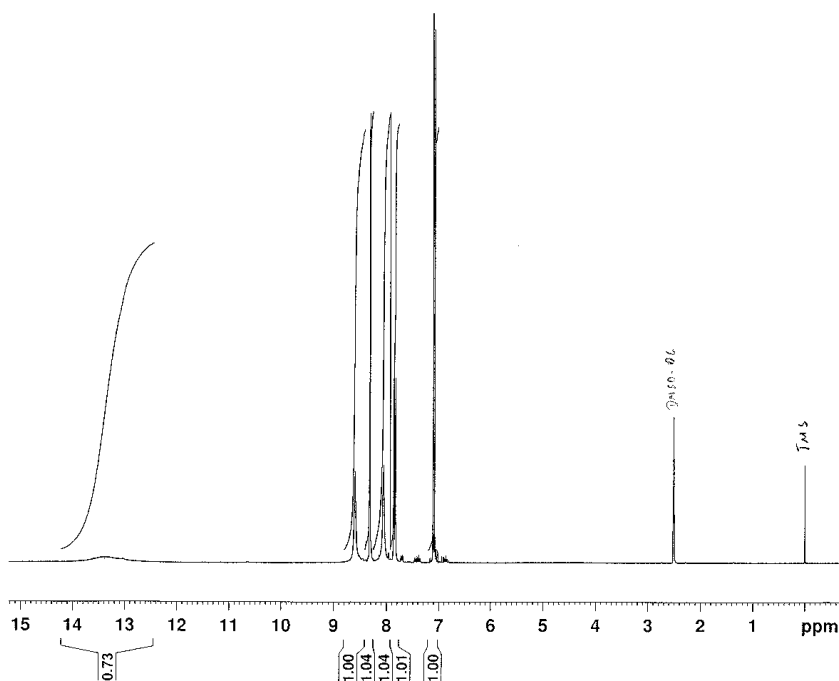


Figure SI-14. FT-IR spectrum of **3c**

Yu SAM-A



```
Current Data Parameters
NAME      thja2025
EXPNO    10
PROCNO   1

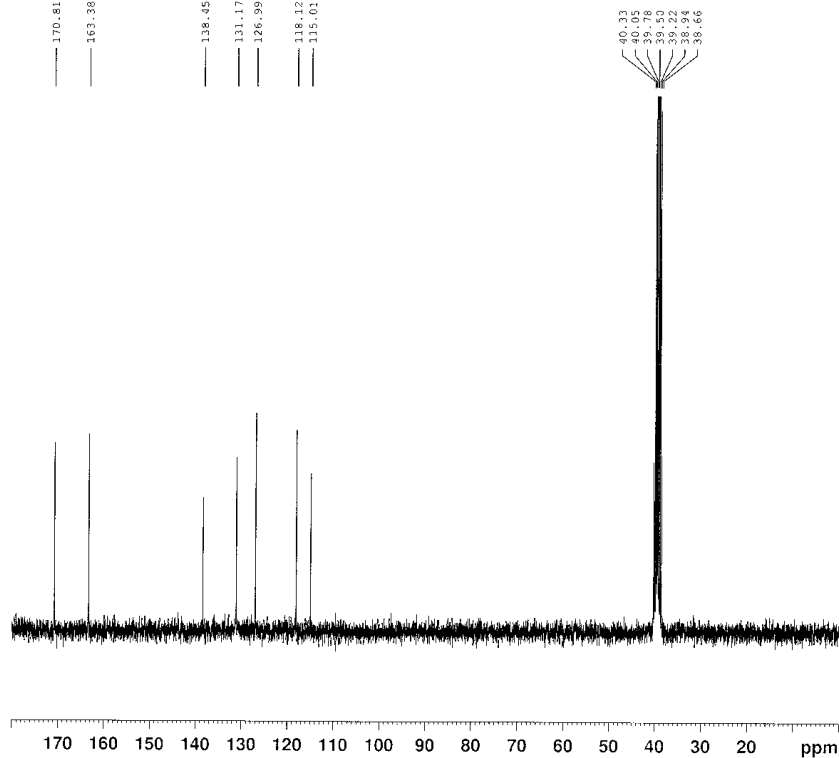
F2 - Acquisition Parameters
Date_    20090120
Time     15.00
INSTRUM spect
PROBHD   5 mm PABBO BB-
PULPROG zg30
TD       65536
SOLVENT  DMSO
NS       16
DS       2
SWH      6188.119 Hz
FIDRES   0.094423 Hz
AQ       5.2953587 sec
RG       512
DW       80.800 usec
DE       6.00 usec
TE       295.5 K
D1       1.0000000 sec
TD0      1

===== CHANNEL f1 =====
NUC1     1H
P1       11.00 usec
PL1     -1.00 dB
SFO1    300.1318534 MHz

F2 - Processing parameters
SI       32768
SF       300.1299990 MHz
WDW      EM
SSB      0
LB       0.15 Hz
GB       0
PC       1.00
```

Figure SI-15. ^1H -NMR spectrum of **3c**

Yu SAM-A



```
Current Data Parameters
NAME      thja2025
EXPNO    11
PROCNO   1

F2 - Acquisition Parameters
Date_    20090120
Time     15.05
INSTRUM spect
PROBHD   5 mm PABBO BB-
PULPROG zgpg30
TD       65536
SOLVENT  DMSO
NS       512
DS       4
SWH      23809.523 Hz
FIDRES   0.363304 Hz
AQ       1.3763061 sec
RG       5
DW       21.000 usec
DE       6.00 usec
TE       295.9 K
D1       2.0000000 sec
d11      0.0300000 sec
DELTA    1.89999998 sec
TD0      1

===== CHANNEL f1 =====
NUC1     13C
P1       8.00 usec
PL1     -3.00 dB
SFO1    75.4760505 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2     1H
PCPD2    100.00 usec
PL2     -1.00 dB
PL12    18.17 dB
PL13    23.00 dB
SFO2    300.1312005 MHz

F2 - Processing parameters
SI       32768
SF       75.4677821 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
```

Figure SI-16. ^{13}C -NMR spectrum of **3c**

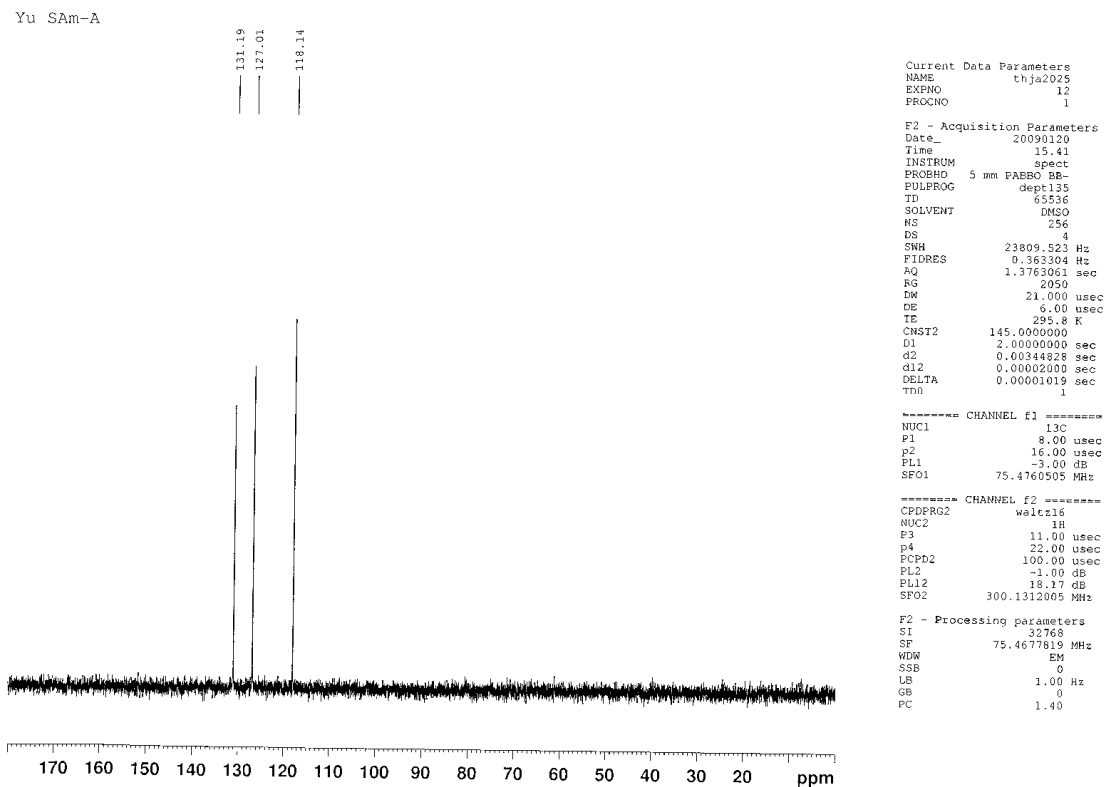


Figure SI-17. 2D-NMR spectrum (HMQC) of **3c**

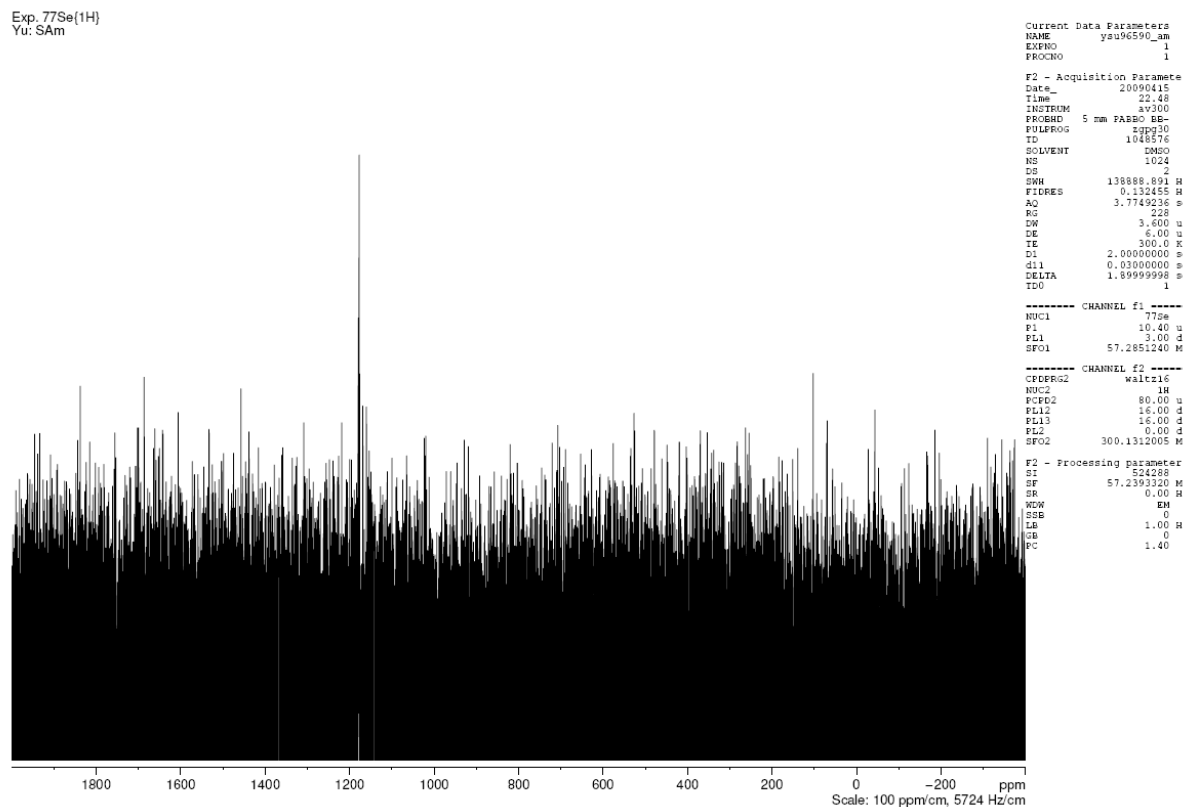


Figure SI-18. ^{77}Se -NMR spectrum of **3c**

Yu_FT_SAm-A_neg_21012009
in Methanol

21.01.2009 12:01:01

SAm - A

Yu_FT_SAm-A_neg_21012009 #8-88 RT: 0.38-4.54 AV: 81 NL: 1.76E4
T: FTMS - p ESI Full ms [195.00-900.00]

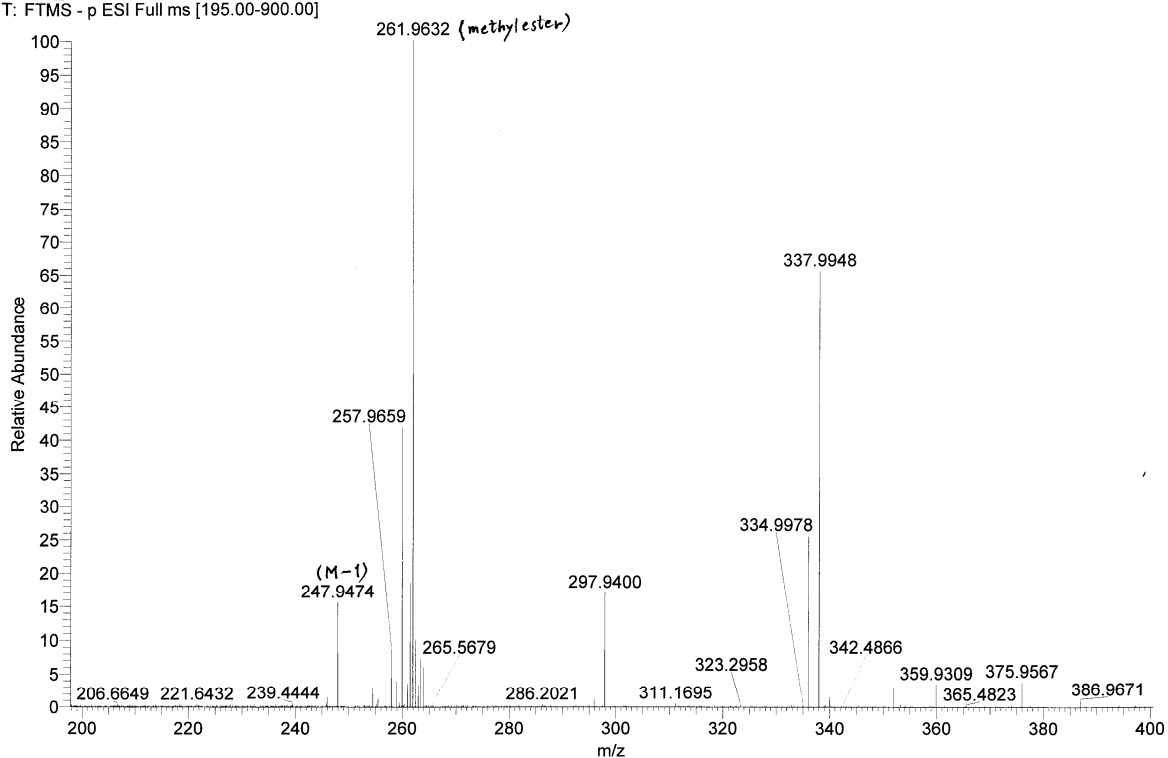


Figure SI-19. HR-MS spectrum of **3c**

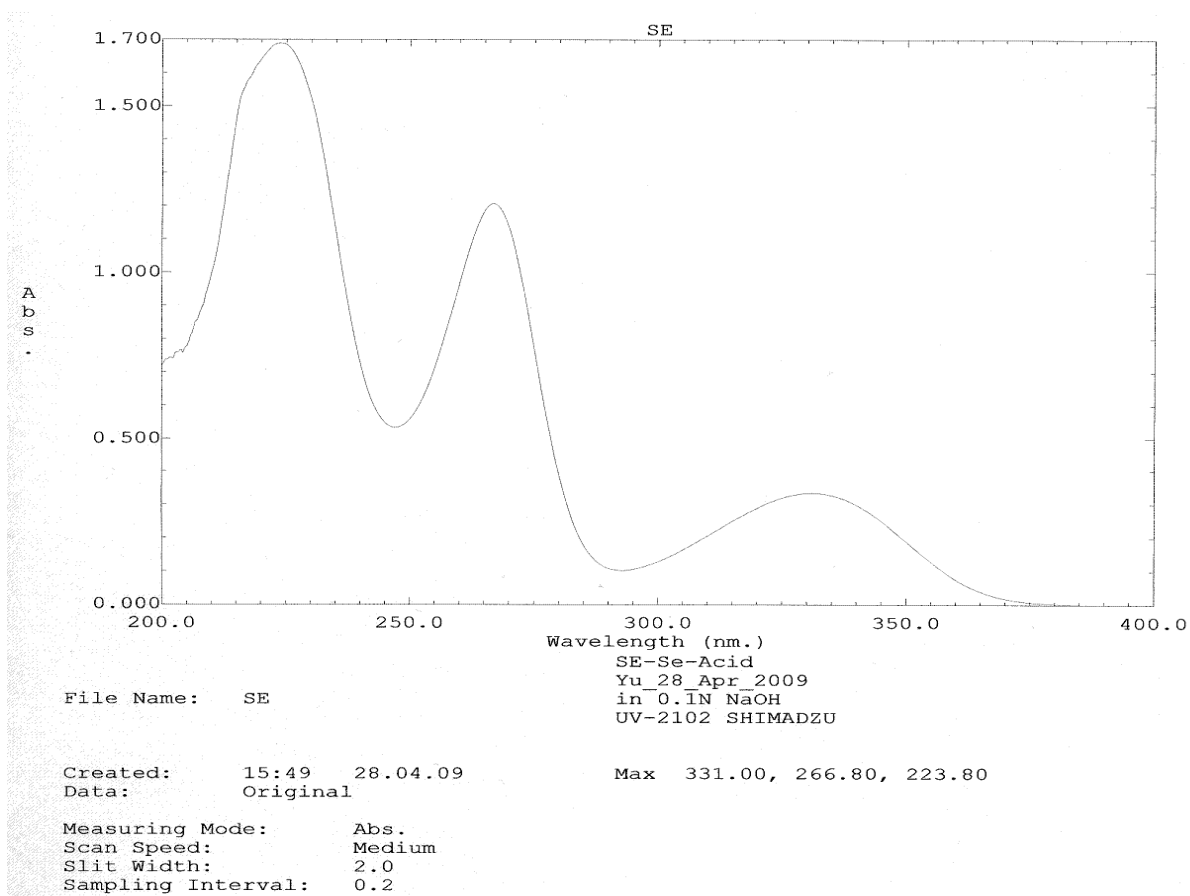


Figure SI-20. UV spectrum of **3d**

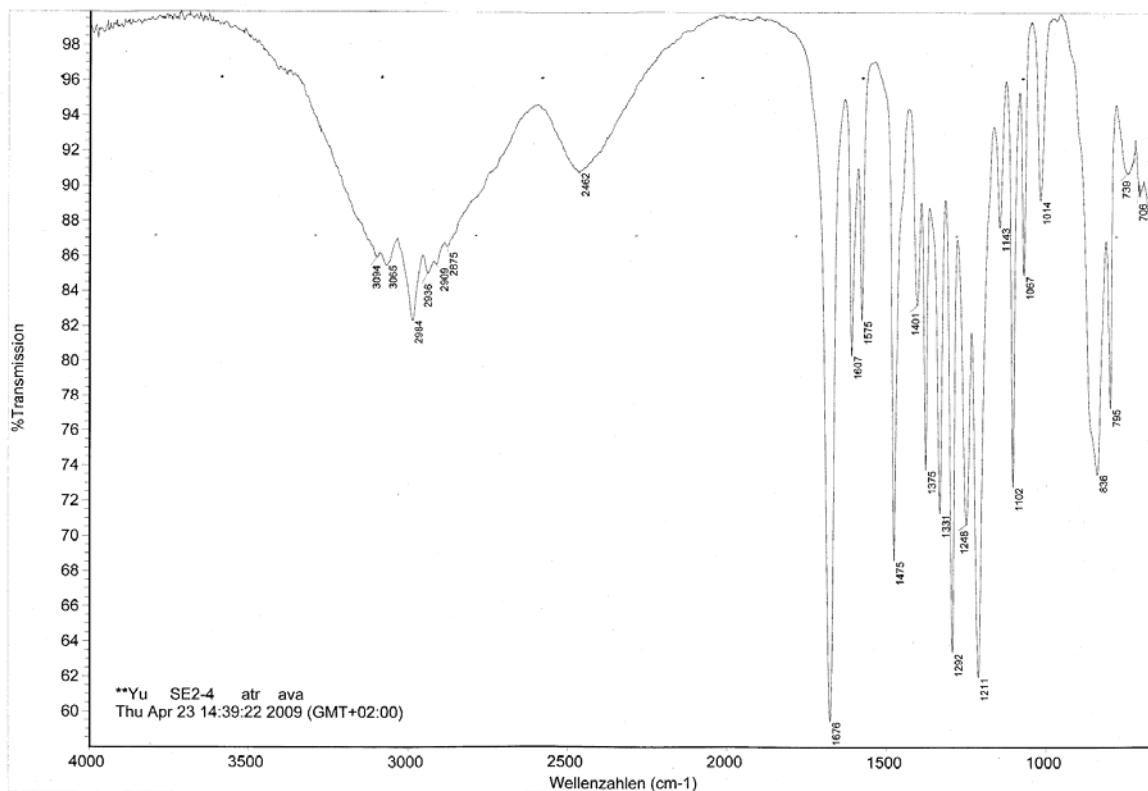


Figure SI-21. FT-IR spectrum of **3d**

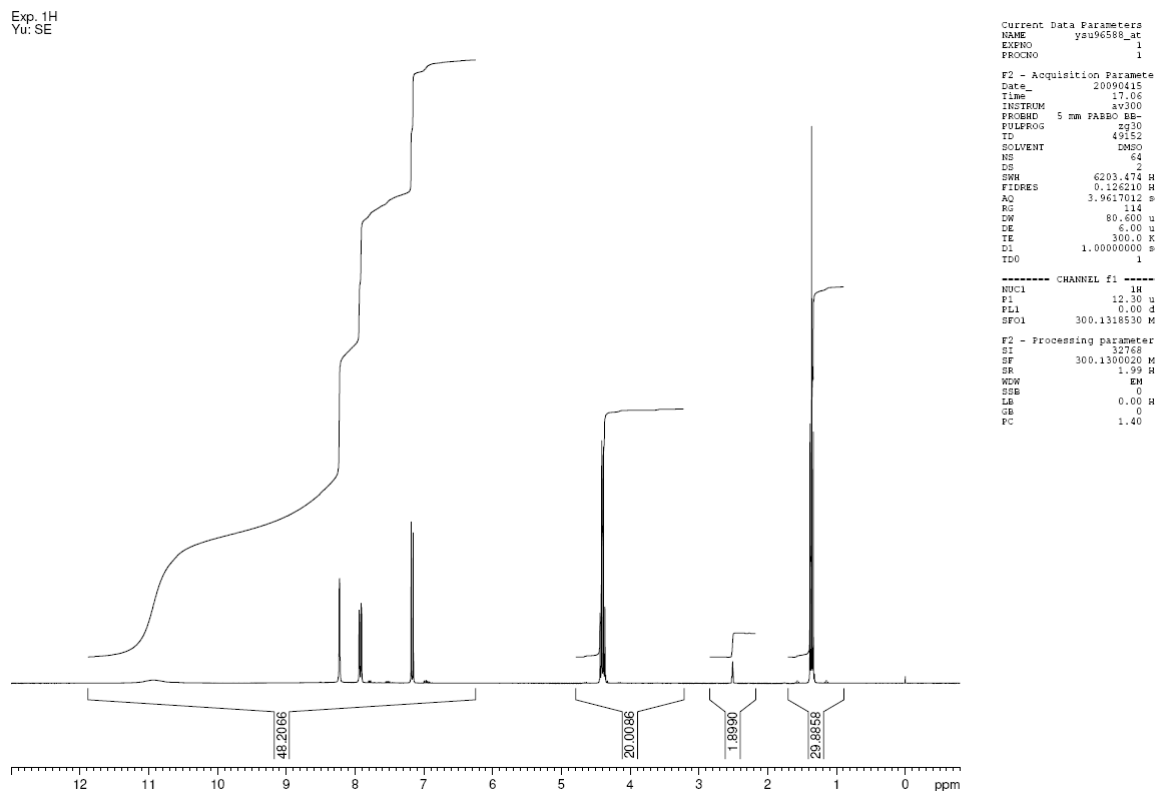


Figure SI-22. ^1H -NMR spectrum of **3d**

Exp. 13C-CPD
 Yu: SE

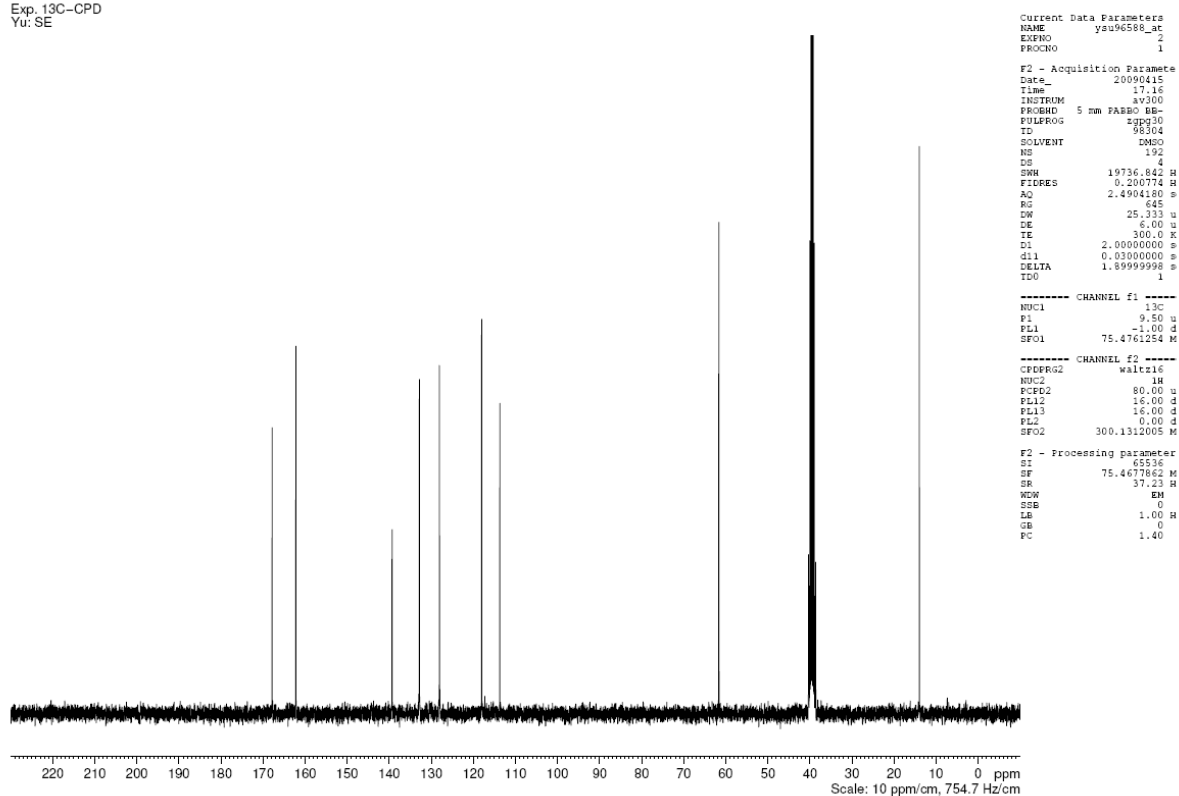


Figure SI-23. ¹³C-NMR spectrum of **3d**

Exp. 13C-Dept135
 Yu: SE

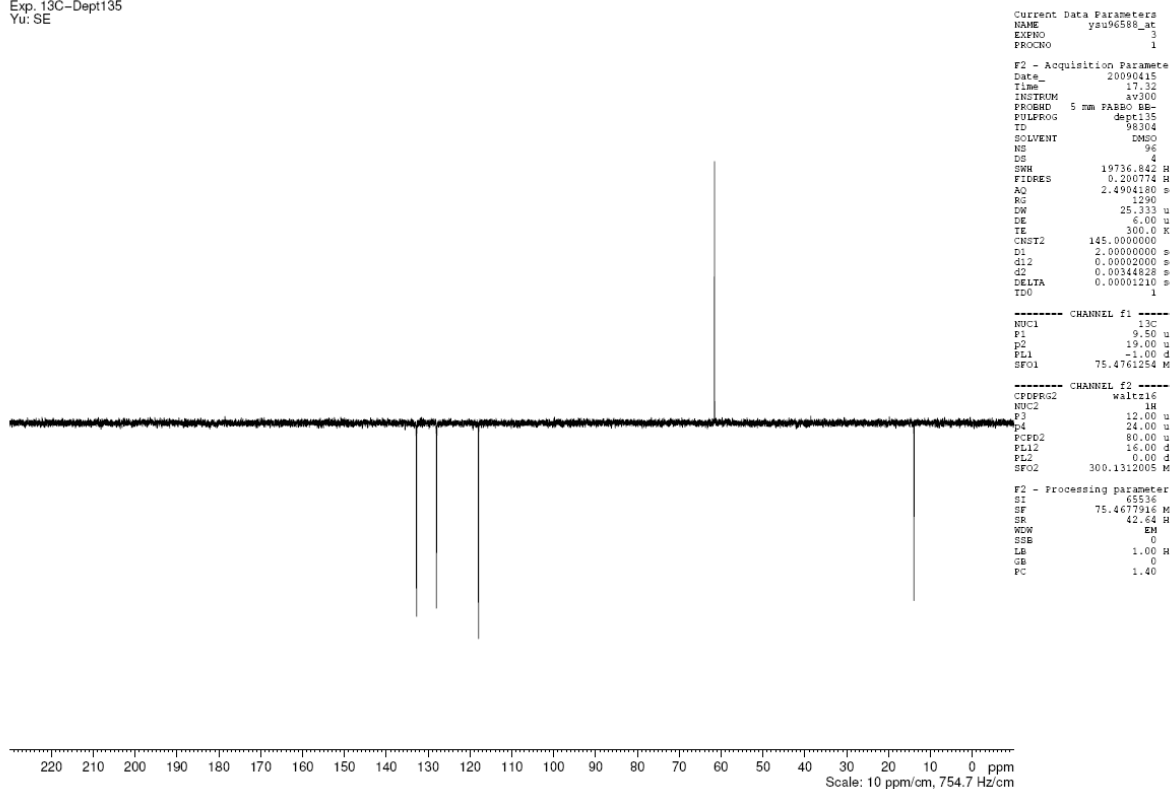


Figure SI-24. 2D-NMR spectrum (HMQC) of **3d**

Exp. ^{77}Se (1H)
Yu: SE

```
NAME ysu96588_a_k
EXPNO 4
PROCNO 1
Date_ 20090415
Time 19.15
INSTRUM ag300
PROBHD 5 mm PABBO B9-
PULPROG zgpg30
TD 1048576
SOLVENT DMSO
NS 1024
DS 2
SWH 139888.891 Hz
FIDRES 0.132455 Hz
AQ 3.7749216 sec
RG 128
DM 3.600 usec
DE 5.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.01000000 sec
DELTA 1.89999998 sec
ZD0 1

===== CHANNEL f1 =====
NUC1 77Se
P1 16.40 usec
PL1 3.00 dB
SFO1 57.2851240 MHz

===== CHANNEL f2 =====
CDEPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 15.00 dB
PL13 16.00 dB
PL2 0.00 dB
SFO2 300.1312005 MHz
SI 524288
SF 57.2393320 MHz
SR 0.00 Hz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40
F1P 2000.000 ppm
F2P -400.000 ppm
```

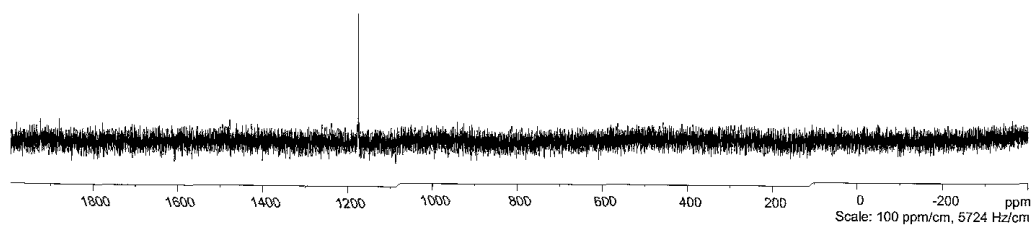


Figure SI-25. ^{77}Se -NMR spectrum of **3d**

SE1-6_Anionen_Spritze #1-23 RT: 0.02-0.64 AV: 23 NL: 1.72E7
T: FTMS - c ESI Full ms [150.00-2000.00]

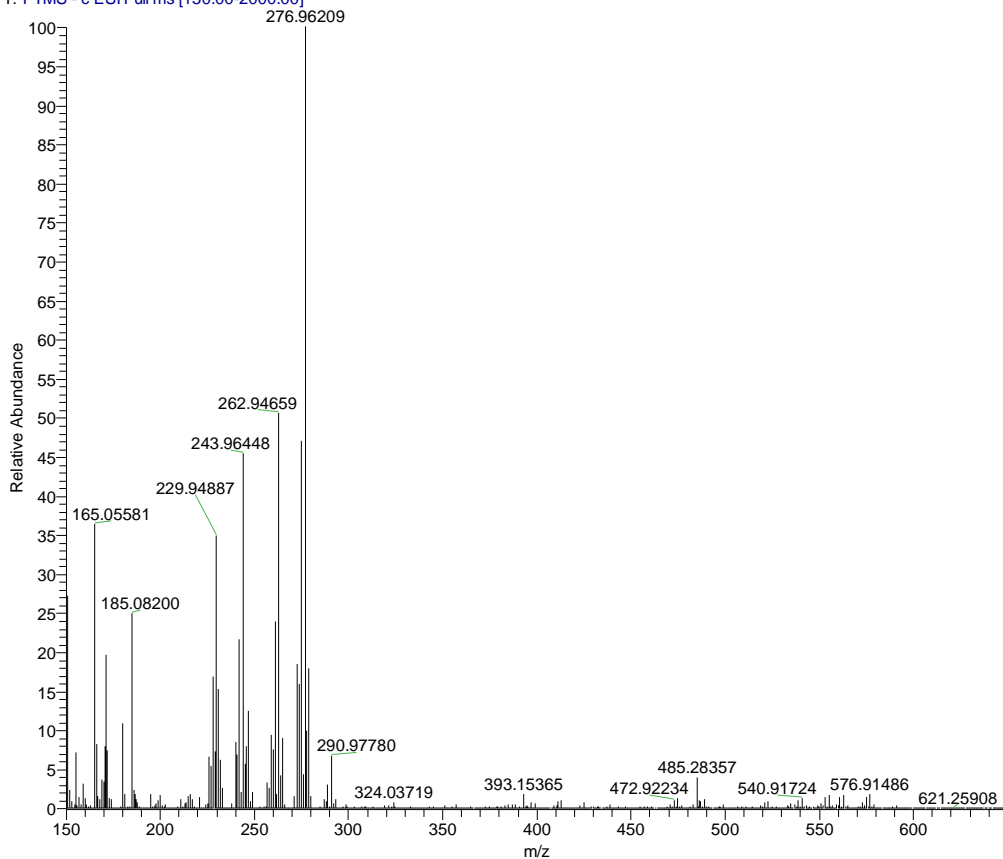
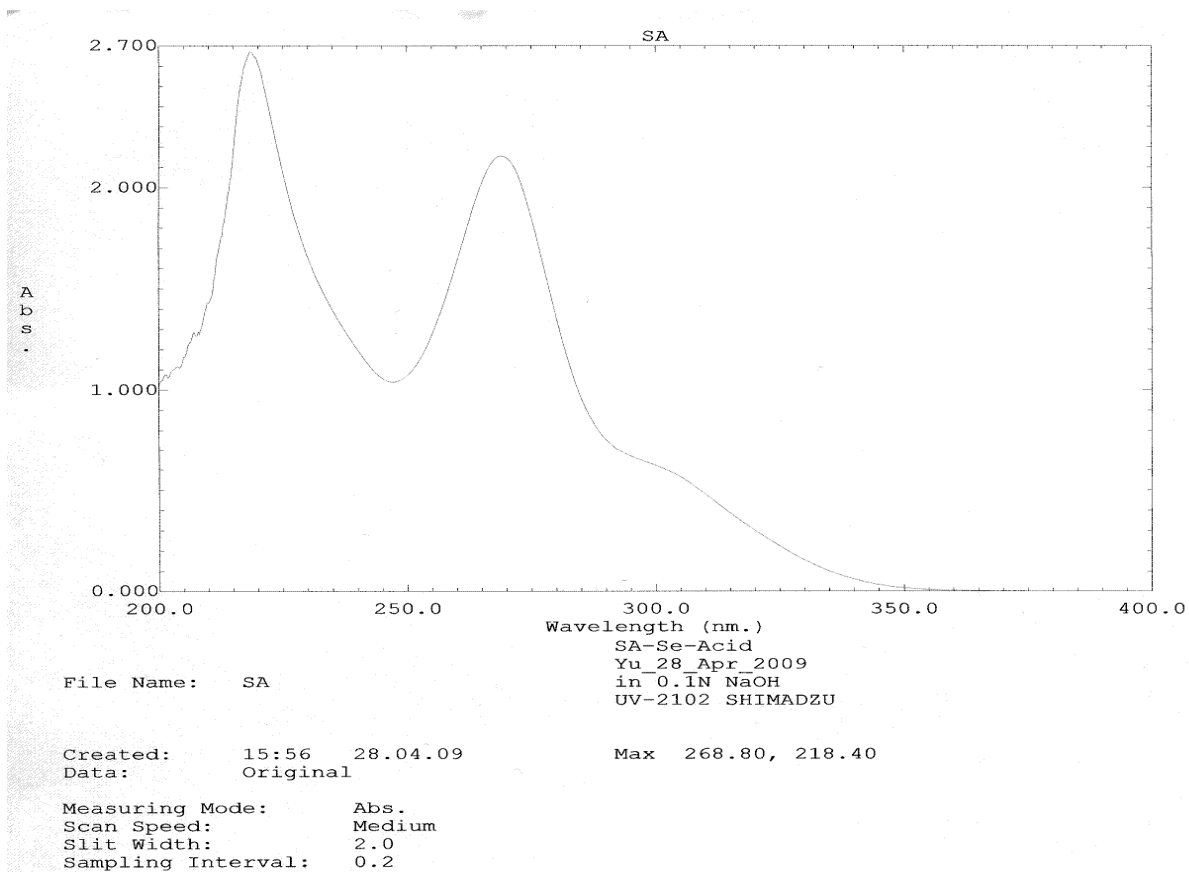
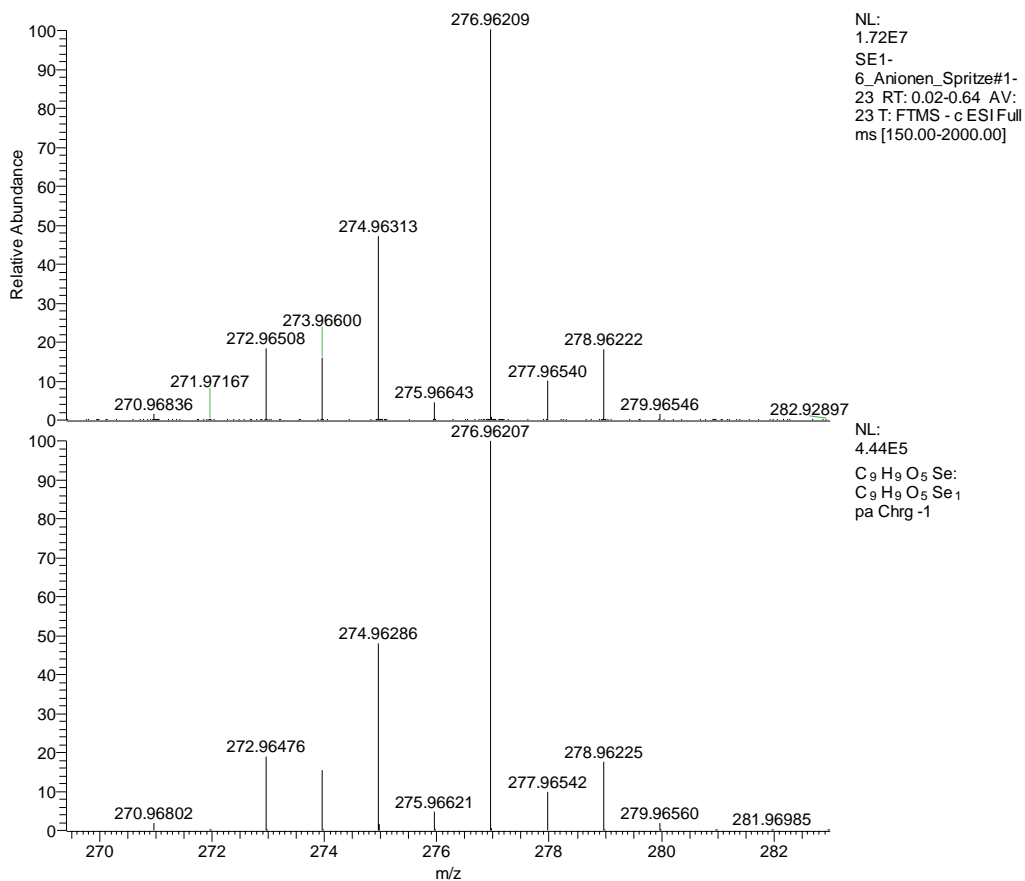


Figure SI-26. HR-MS spectrum (overview) of **3d**



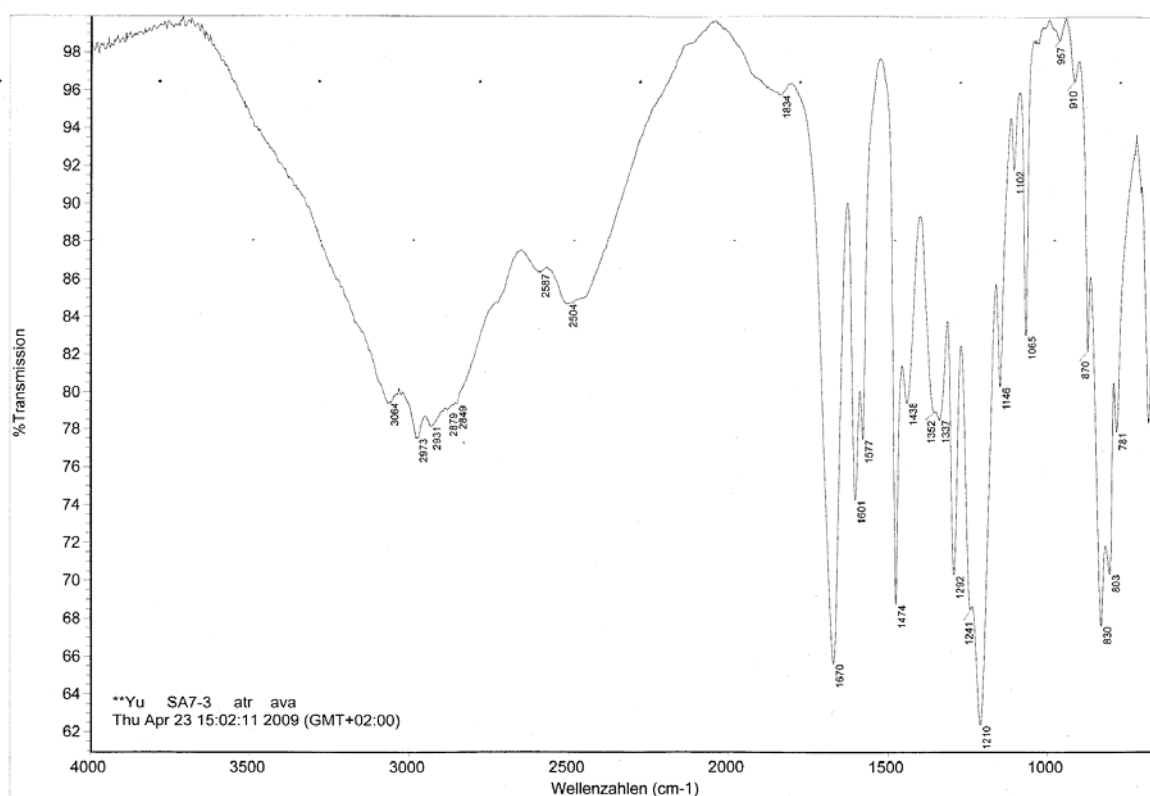


Figure SI-29. FT-IR spectrum of **3e**

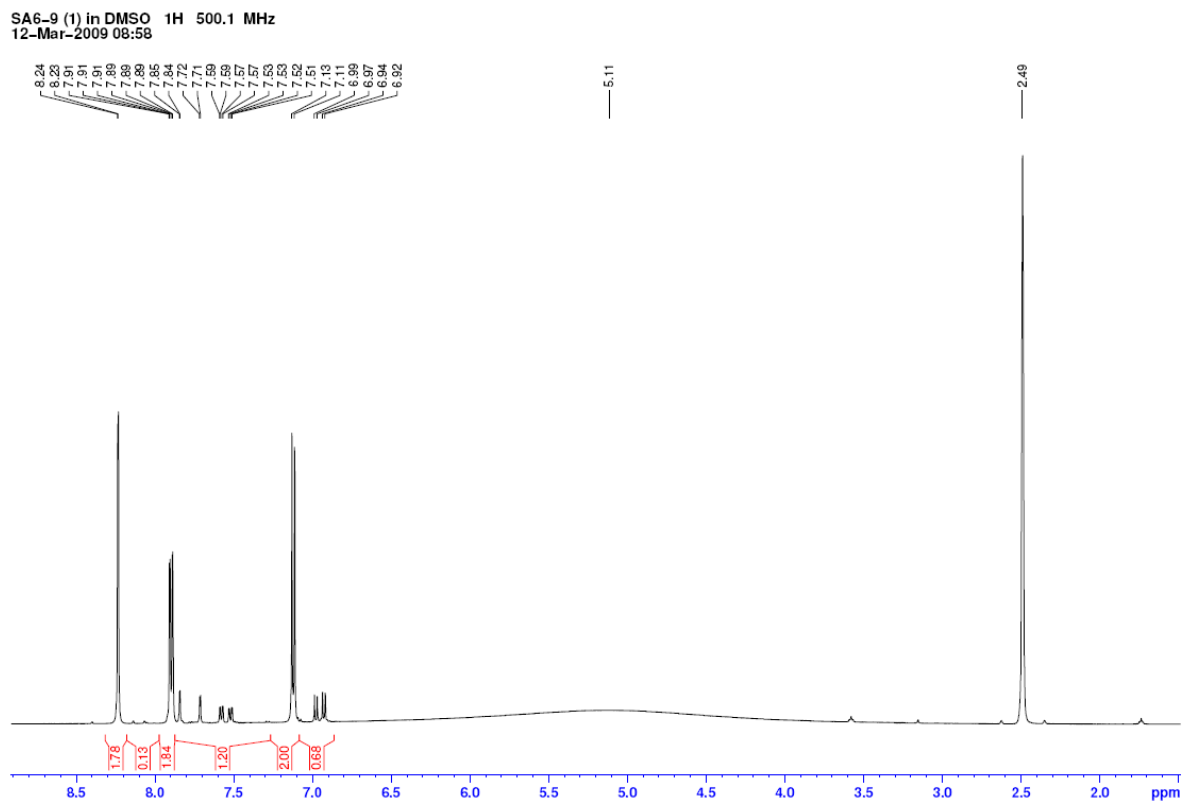


Figure SI-30. $^1\text{H-NMR}$ spectrum (overview) of **3e**

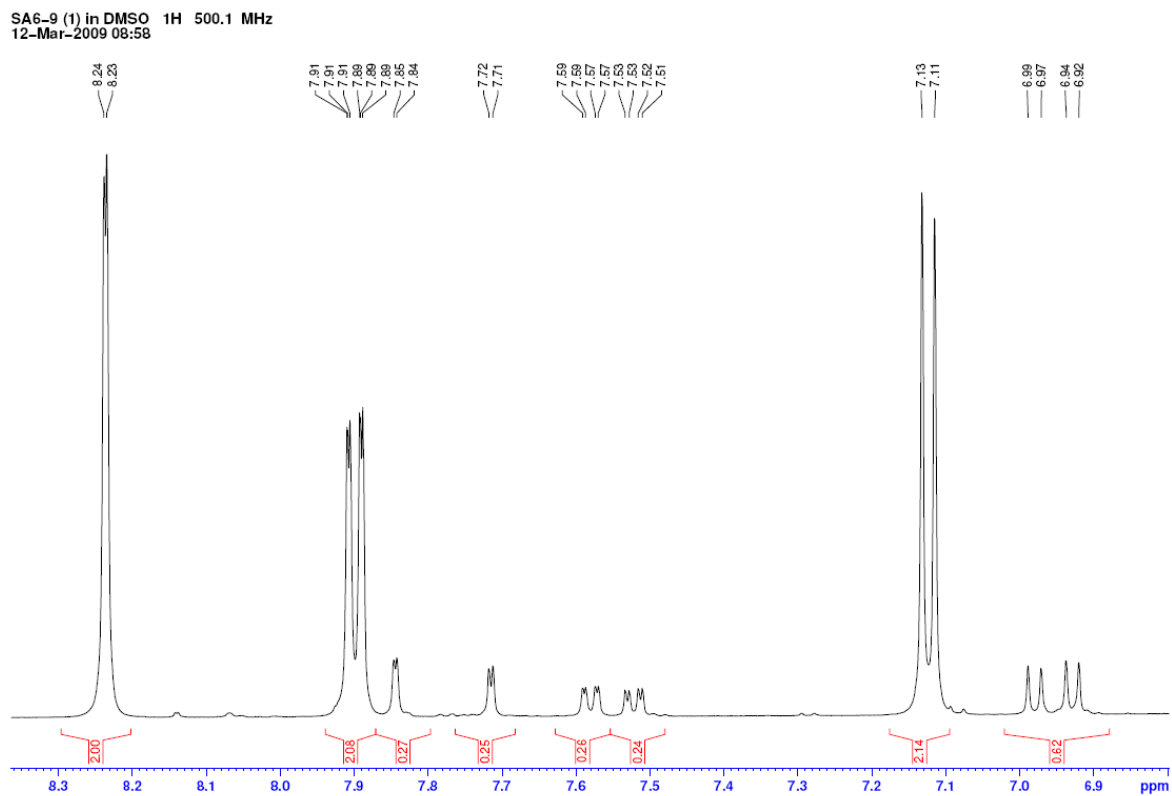


Figure SI-31. ^1H -NMR spectrum (expanded) of **3e**

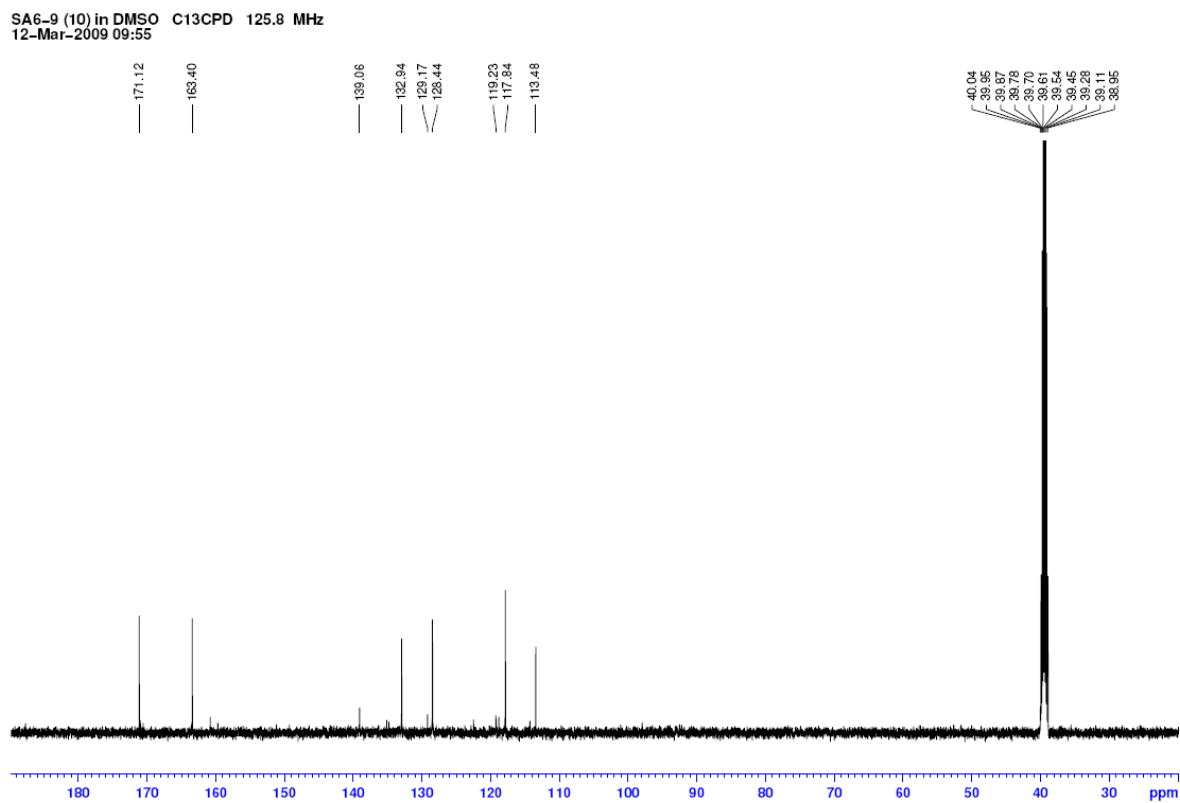


Figure SI-32. ^{13}C -NMR spectrum of **3e**

SA6-9 gs-HMQC Spektrum
 12-Mar-2009 09:29

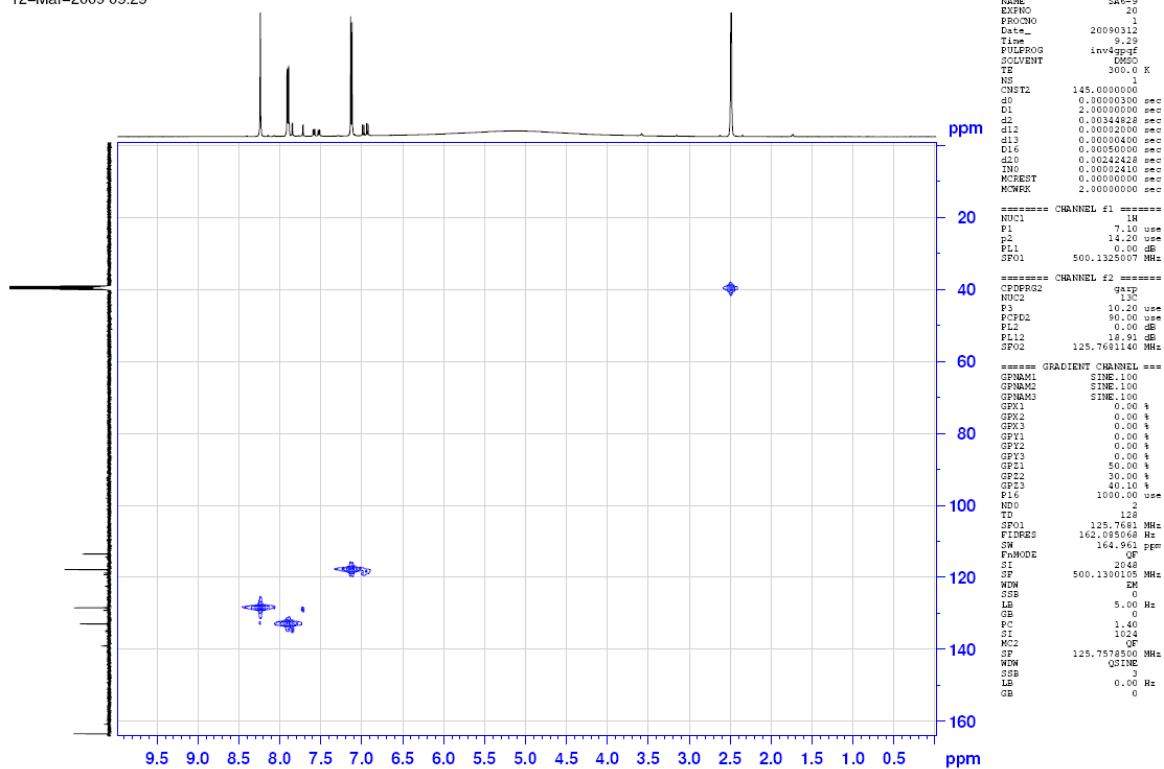


Figure SI-33. 2D-NMR spectrum (HMQC) of **3e**

Exp: 77Se(1H)
 Yu: SA

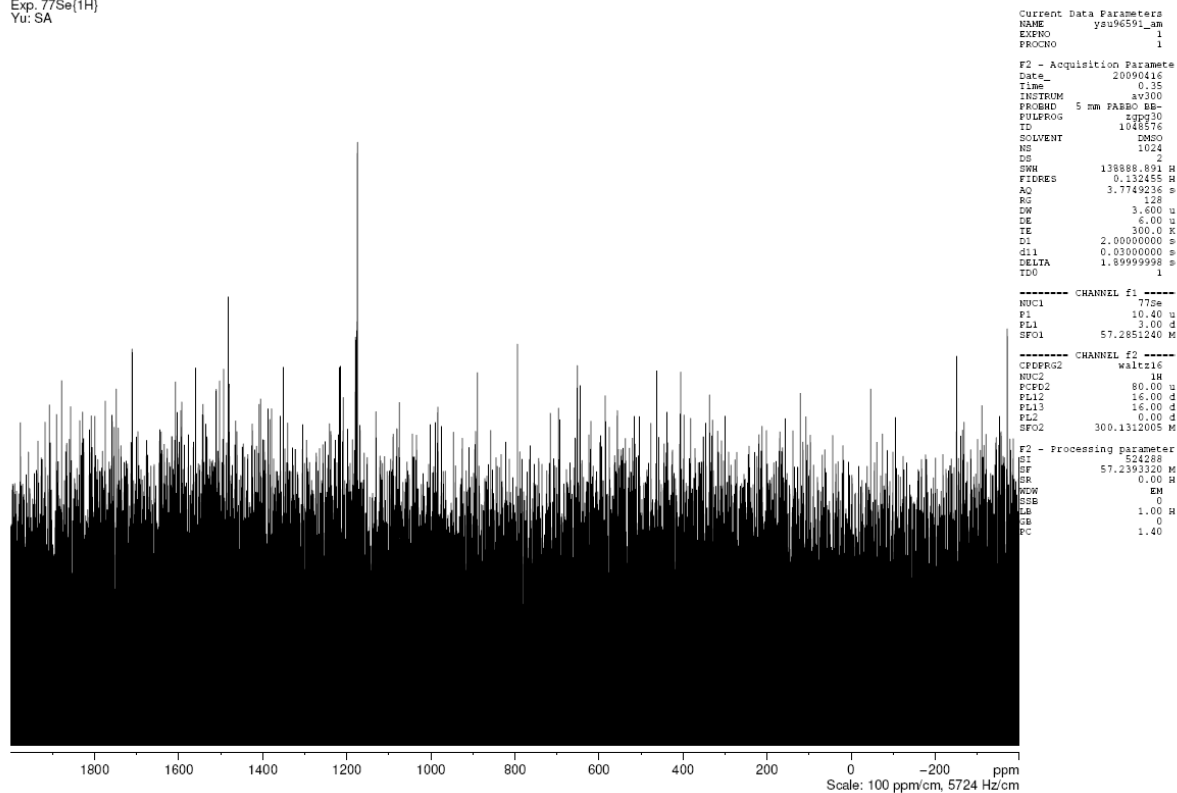


Figure SI-34. ^{77}Se -NMR spectrum of **3e**

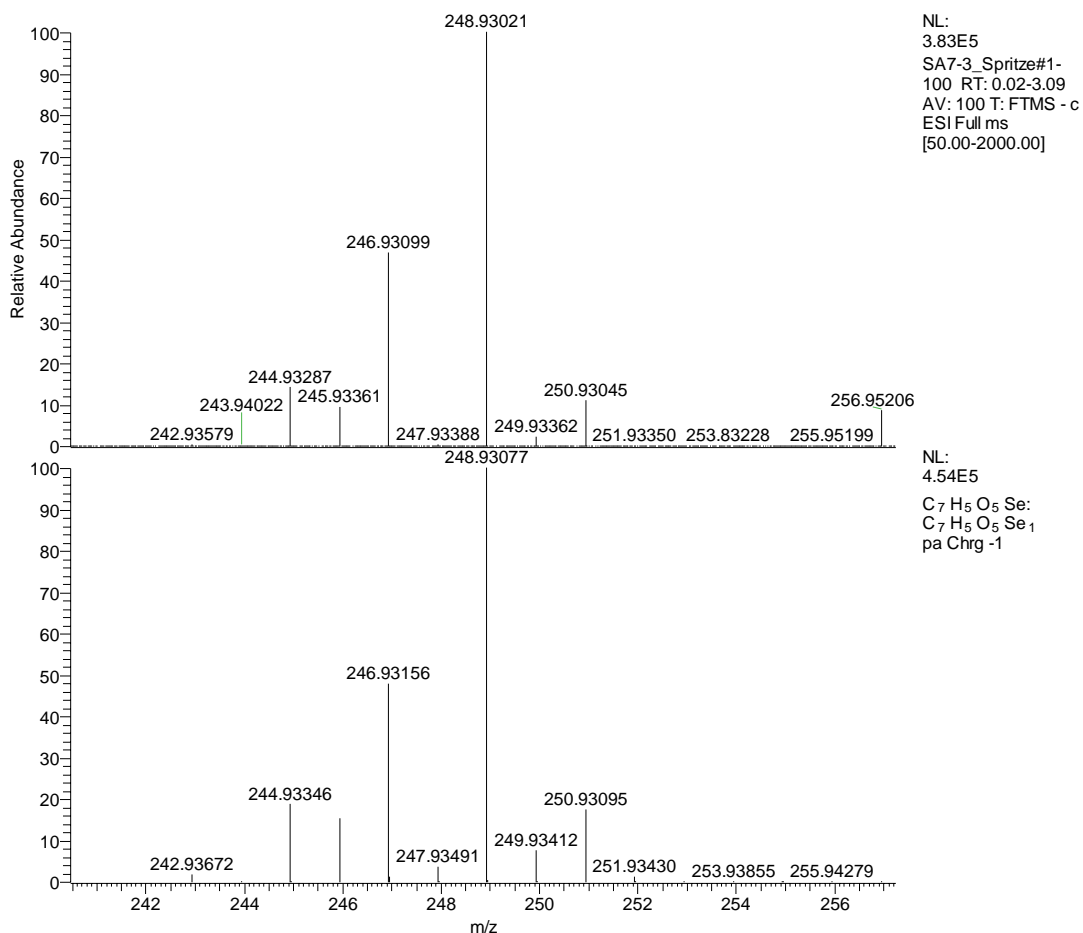


Figure SI-35. HR-MS spectrum (expanded) of **3e**

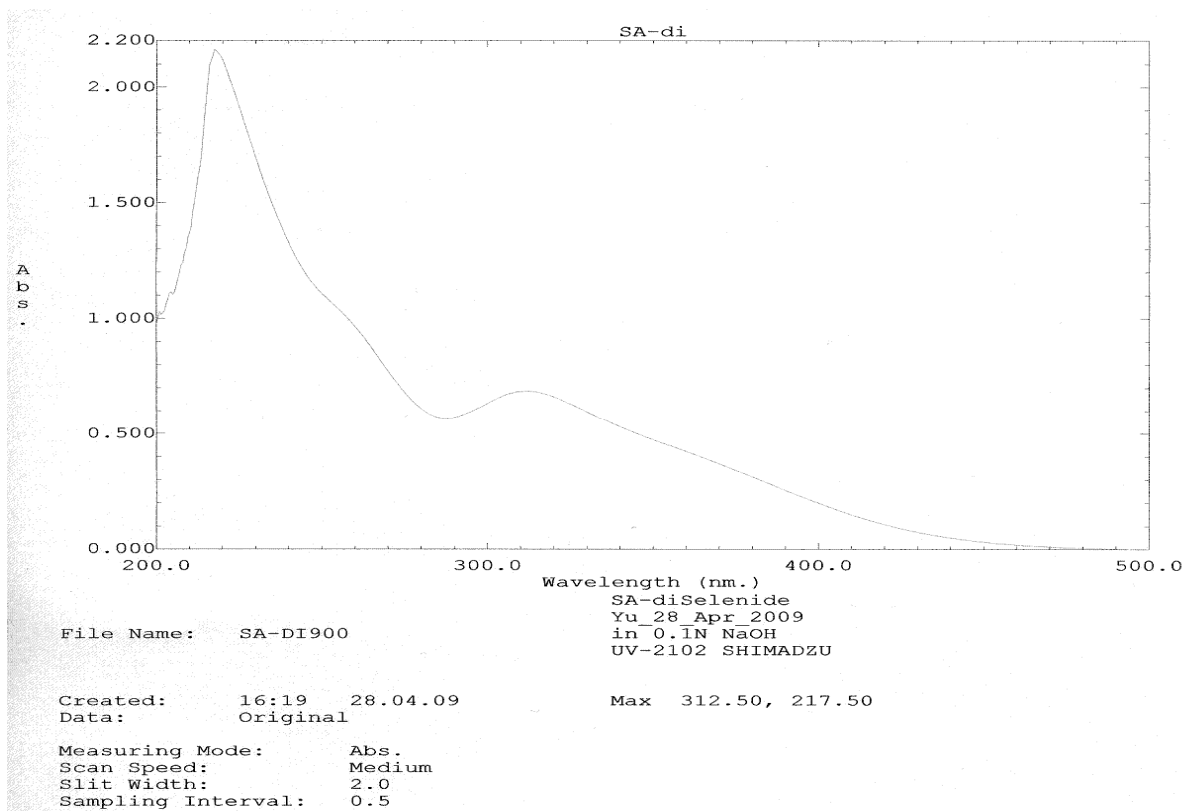


Figure SI-43. UV spectrum of **4e**

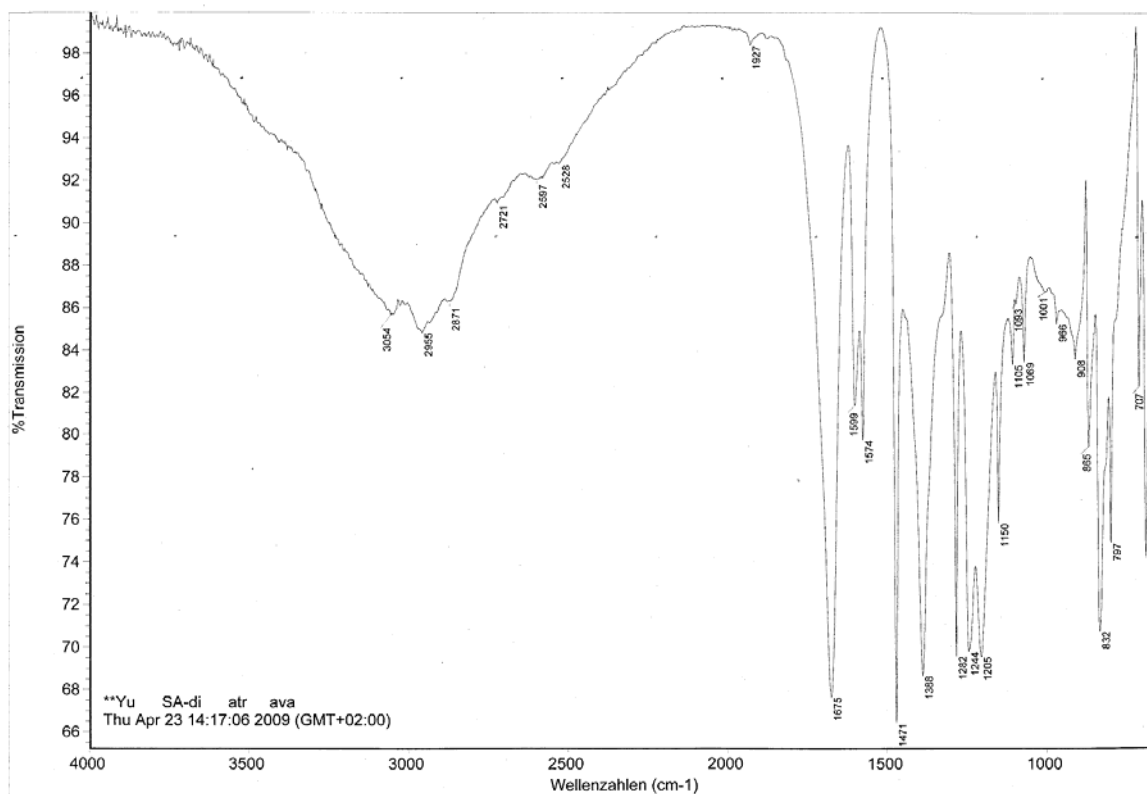


Figure SI-44. FT-IR spectrum of **4e**

SA7-6 (1) in DMSO
18-Mar-2009 08:50

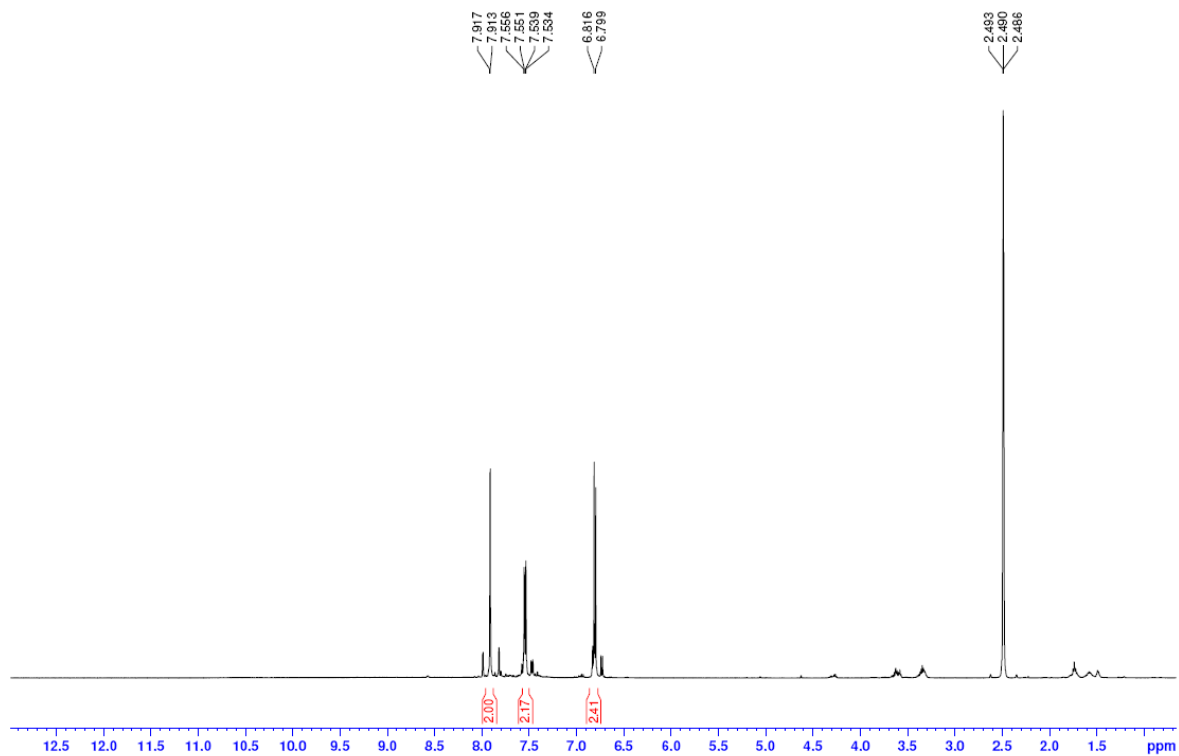


Figure SI-45. $^1\text{H-NMR}$ spectrum (overview) of **4e**

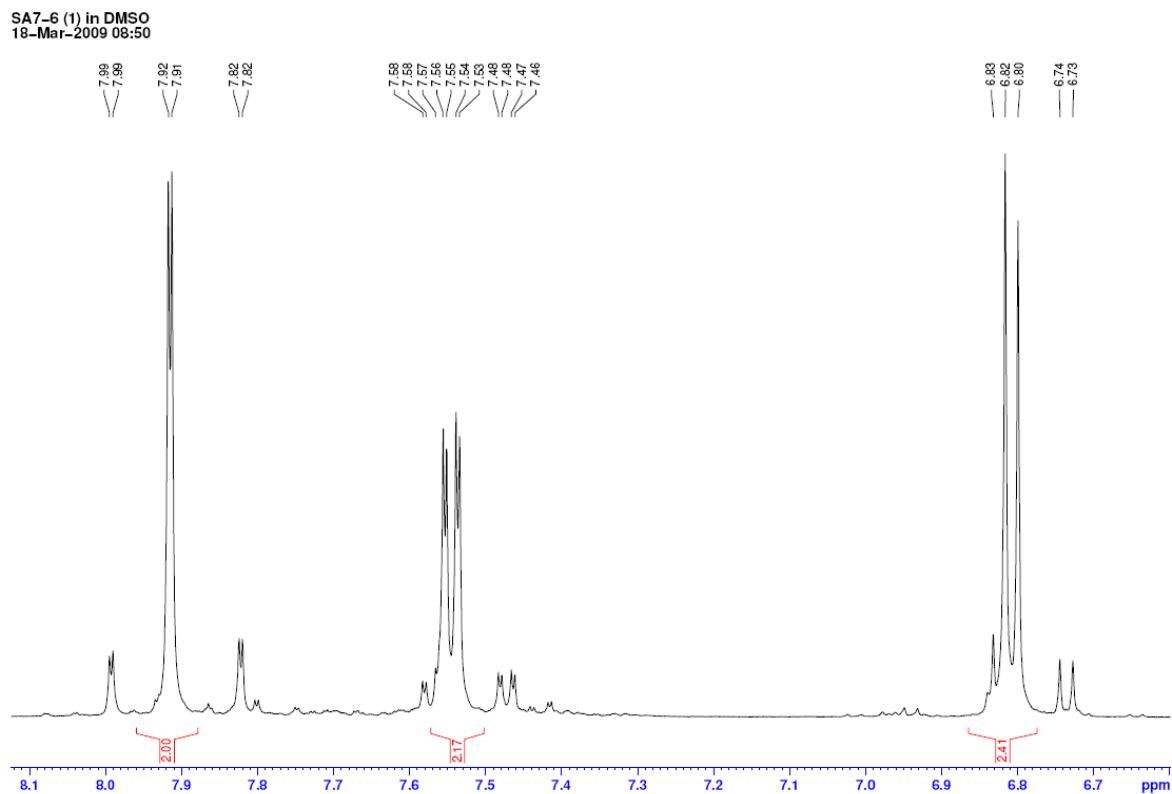


Figure SI-46. ^1H -NMR spectrum (expanded) of **4e**

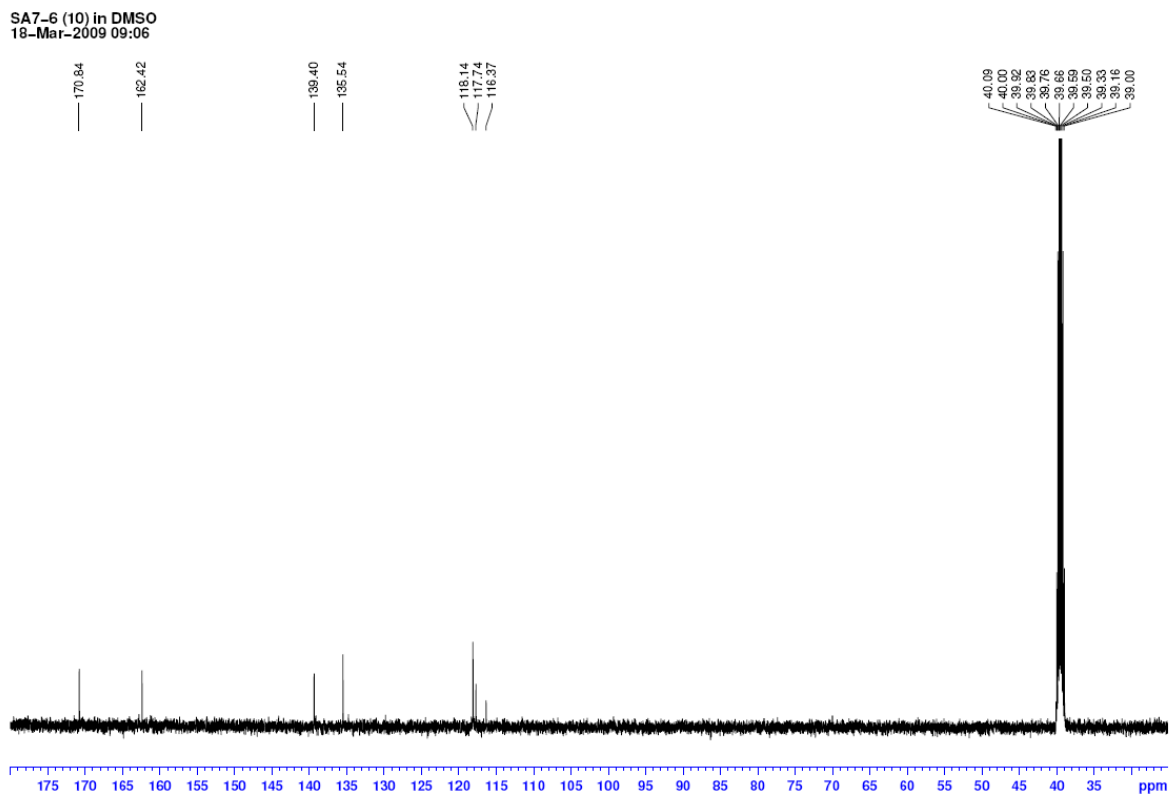


Figure SI-47. ^{13}C -NMR spectrum of **4e**

Exp. 77Se(1H)
Yu: SA-dj

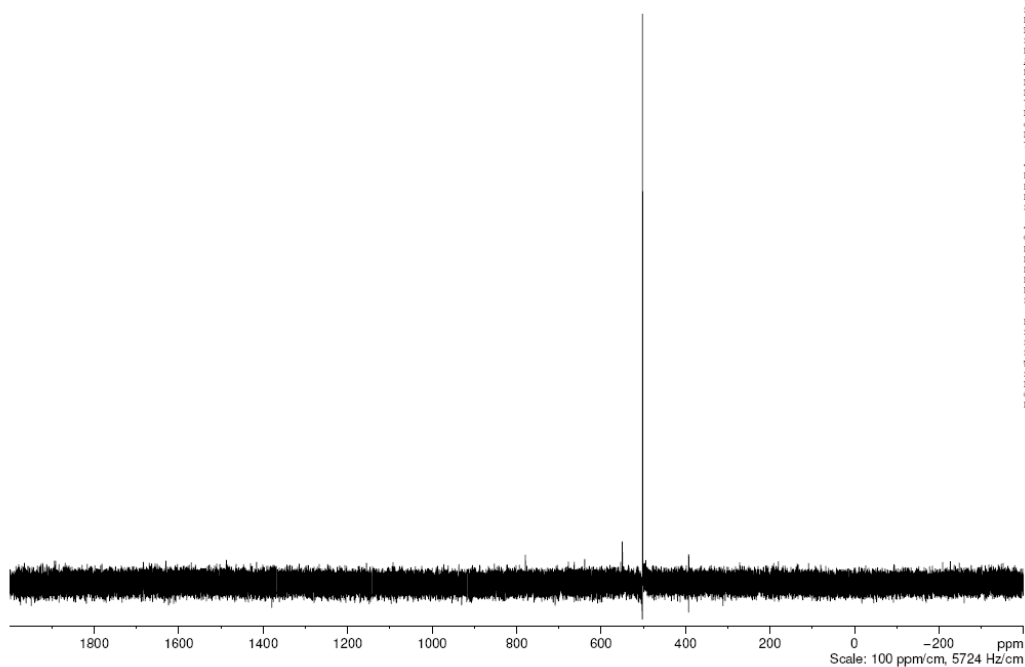


Figure SI-48. ^{77}Se -NMR spectrum of **4e**

SA7-6_Spritz #4-99 RT: 0.09-2.86 AV: 96 NL: 1.22E7
T: FTMS - c ESI Full ms [50.00-2000.00]

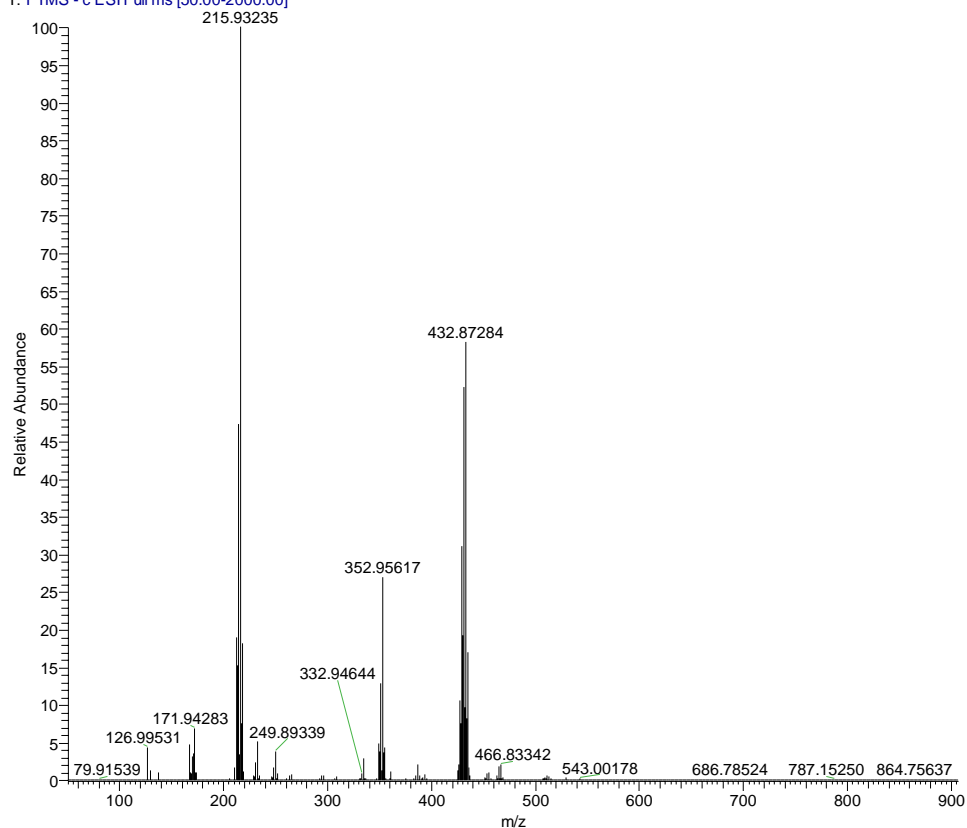


Figure SI-49. HR-MS spectrum (overview) of **4e**

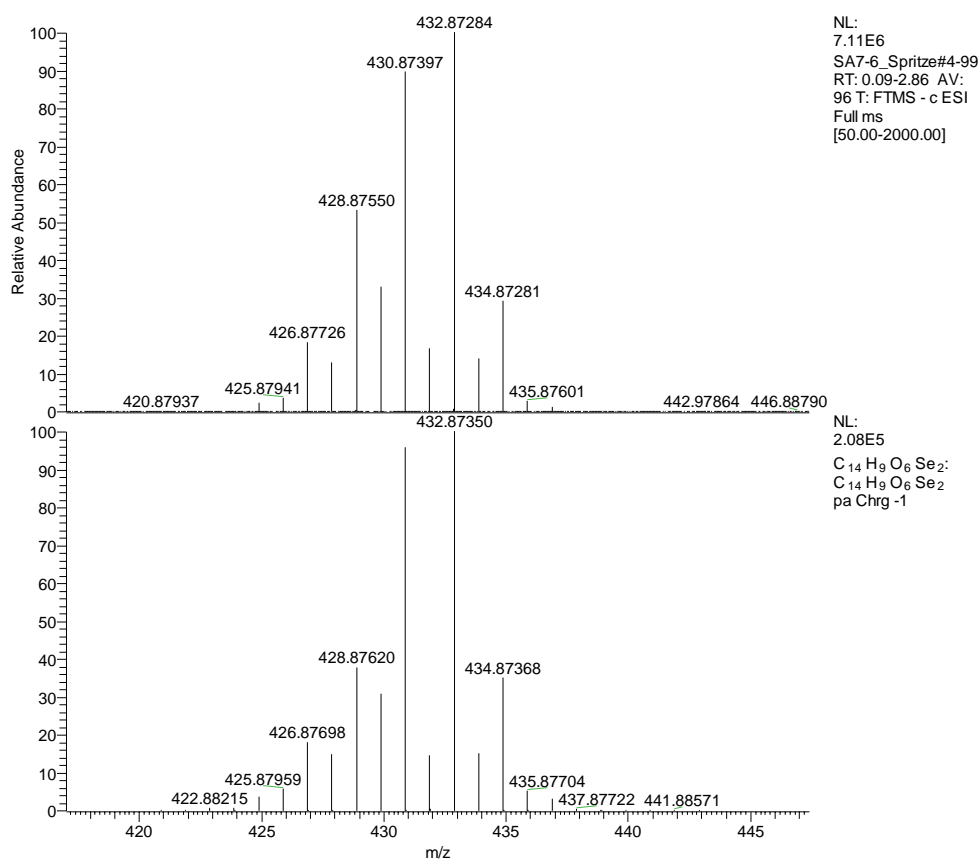


Figure SI-50. HR-MS spectrum (expanded) of **4e**

SA7-5 (1) in DMSO 1H 500.1 MHz
18-Mar-2009 08:17

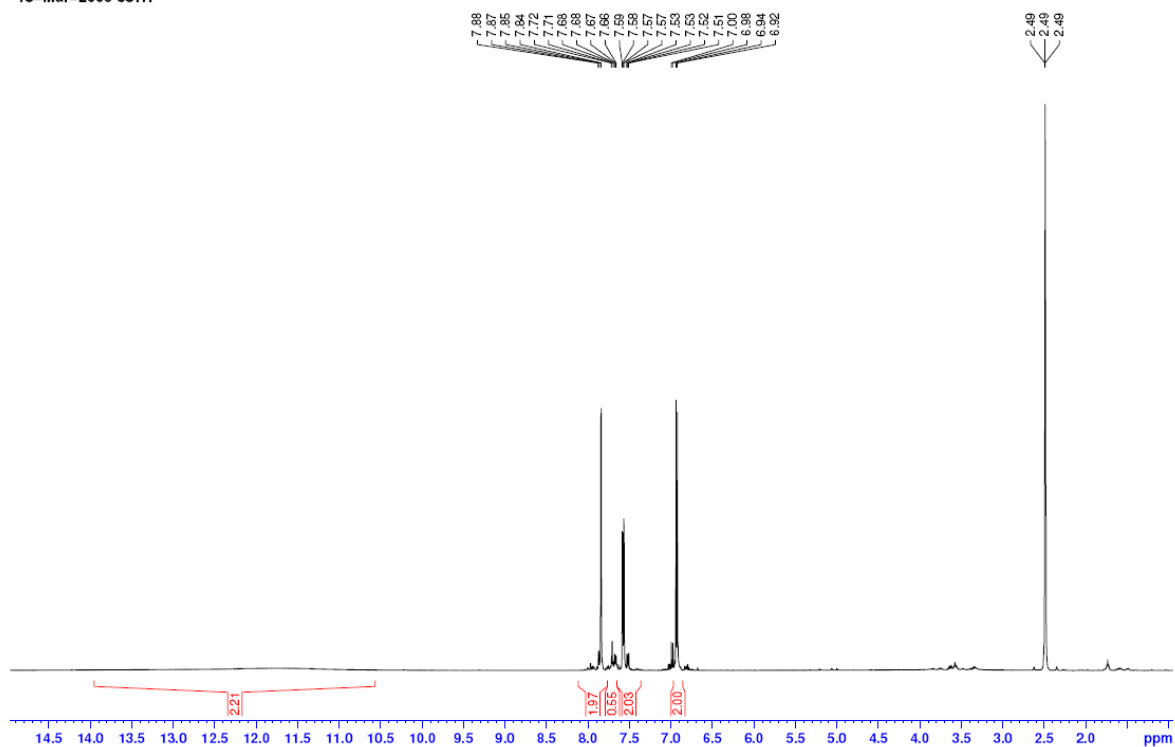


Figure SI-36. ¹H-NMR spectrum (overview) of **5e**

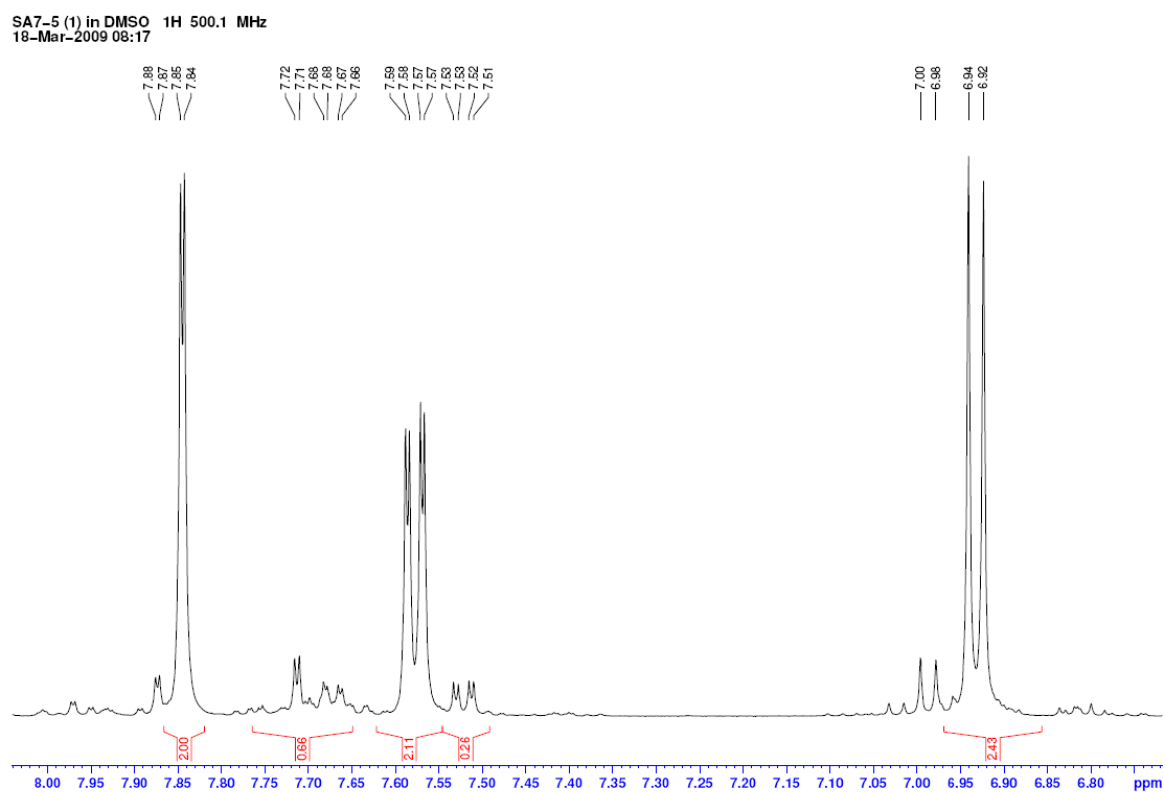


Figure SI-37. ^1H -NMR spectrum (expanded) of **5e**

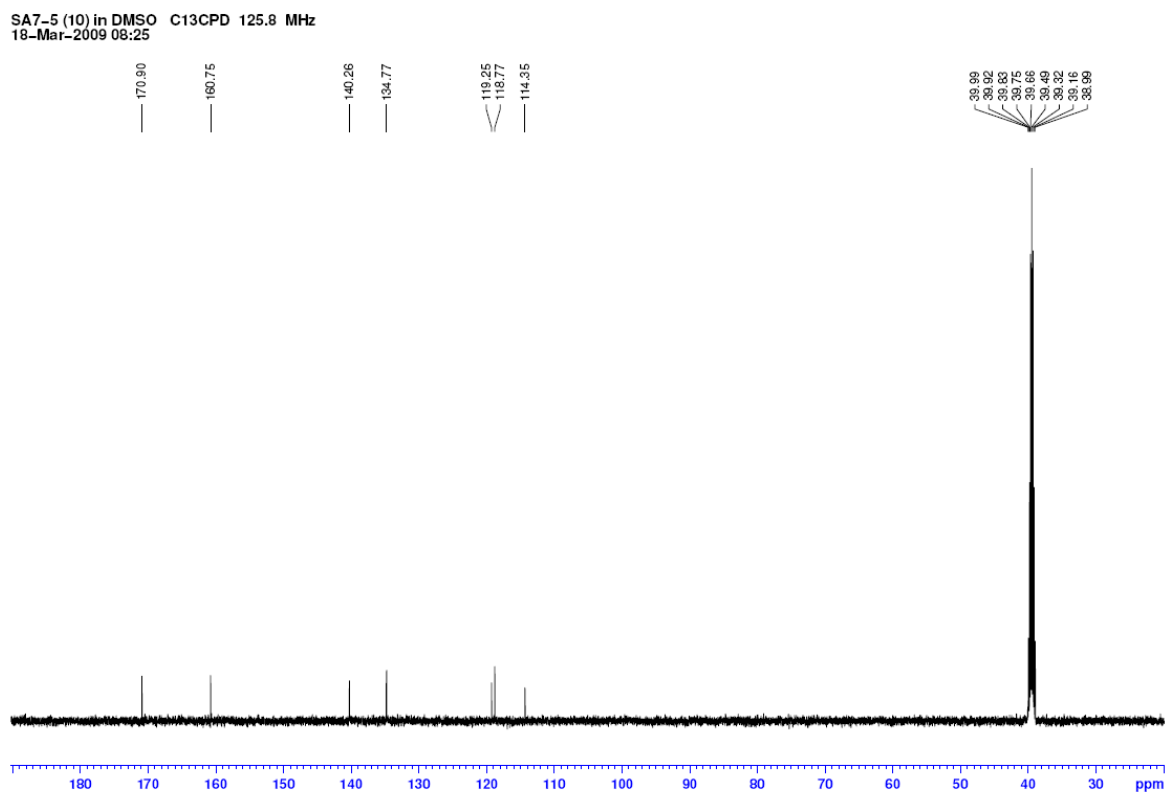


Figure SI-38. ^{13}C -NMR spectrum of **5e**

SA7-5 gs-HMOC Spektrum
 18-Mar-2009 08:27

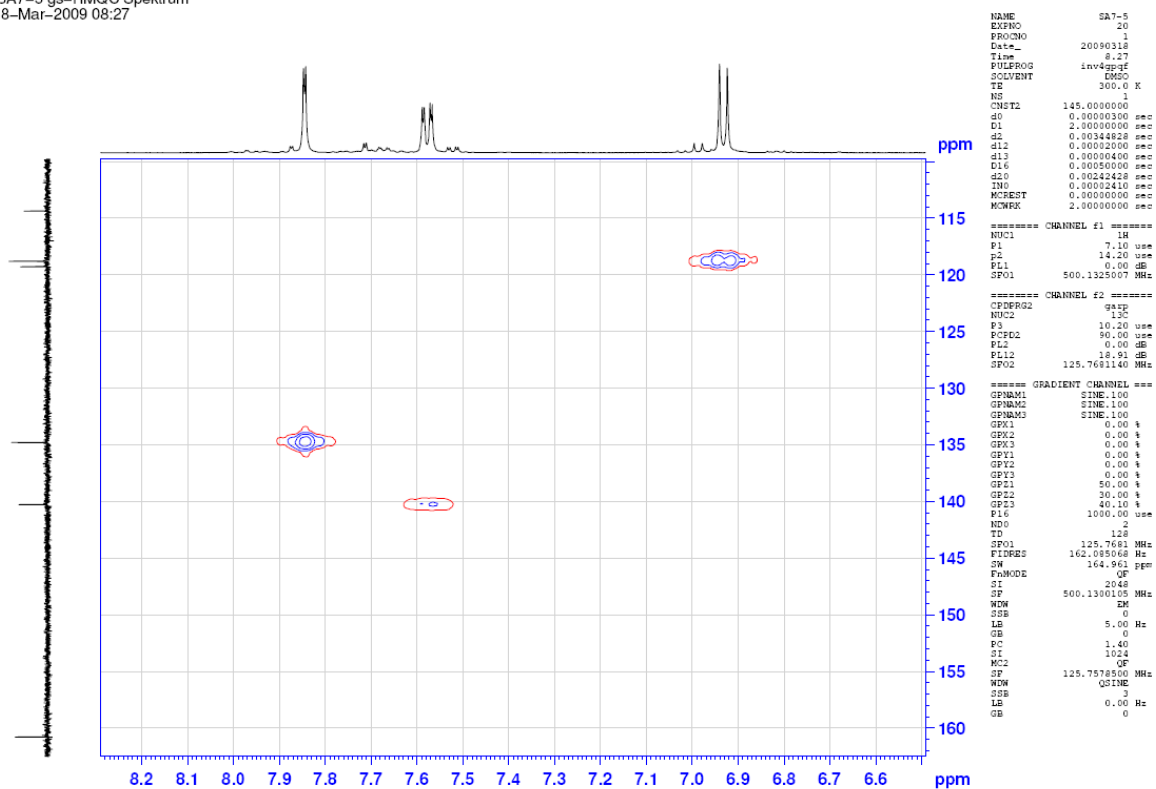


Figure SI-39. 2D-NMR spectrum (HMOC) of **5e**

Exp: 77Se(1H)
 Yu: SA-none

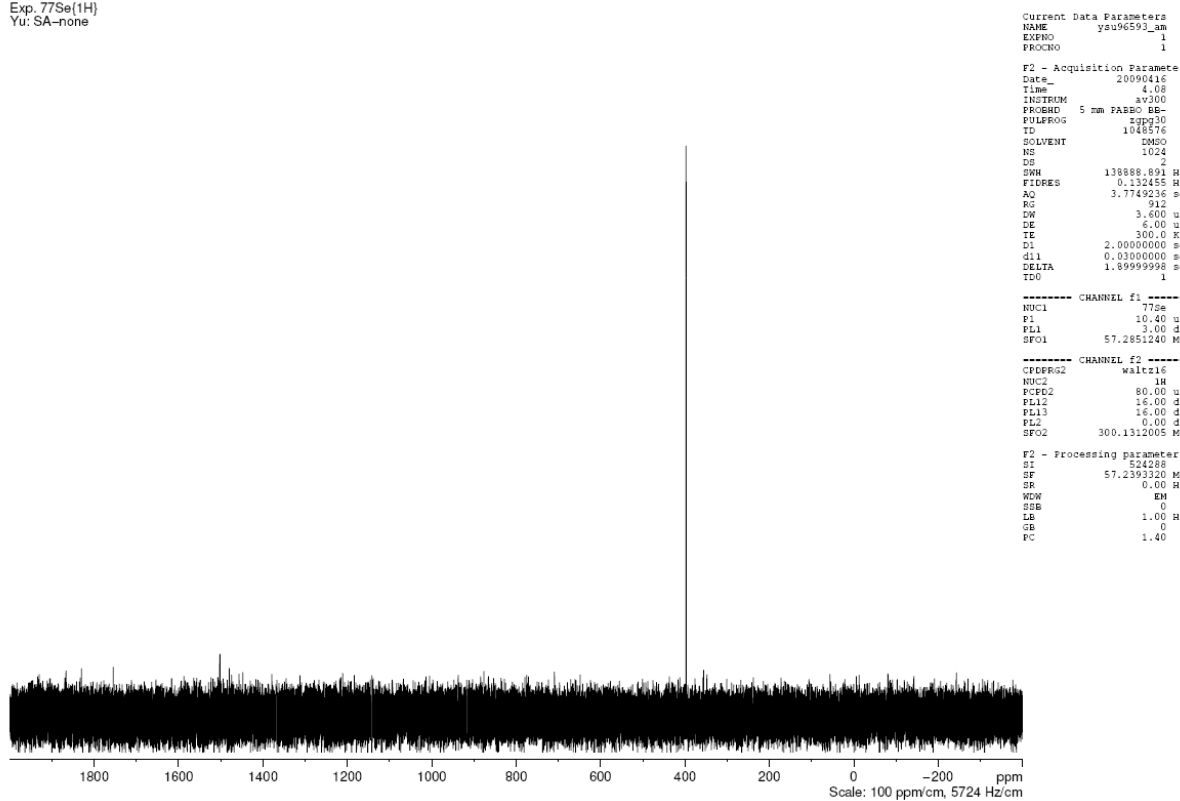


Figure SI-40. ⁷⁷Se-NMR spectrum of **5e**

SA7-5_Spritz#4-100 RT: 0.11-2.89 AV: 97 NL: 1.71E7
T: FTMS - c ESI Full ms [50.00-2000.00]

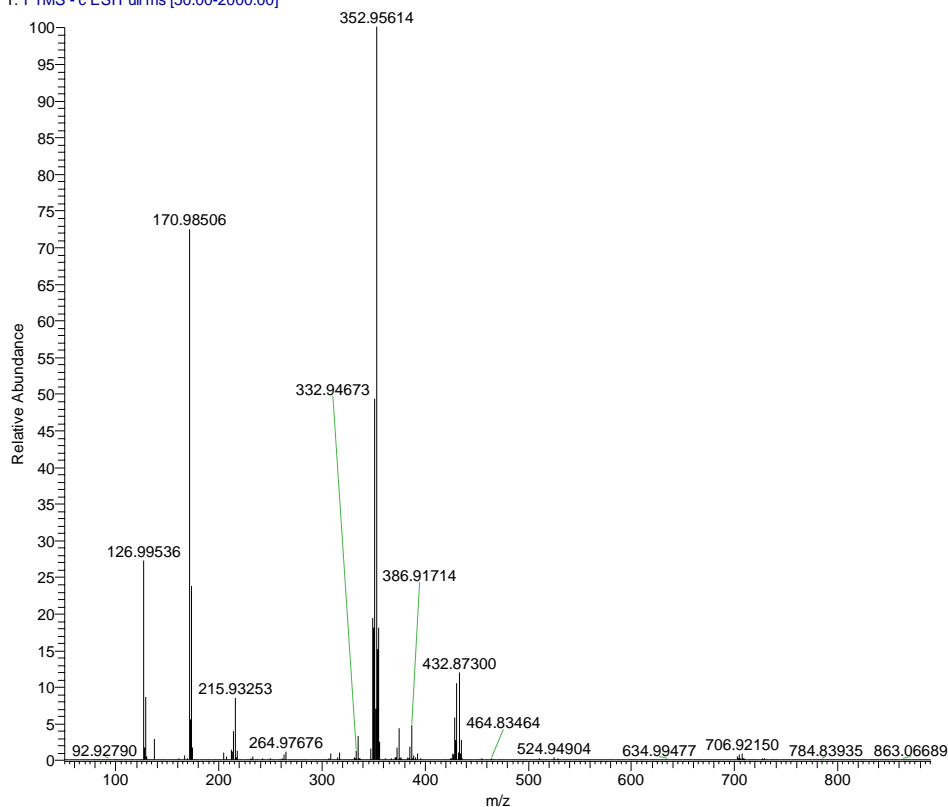


Figure SI-41. HR-MS spectrum (overview) of 5e

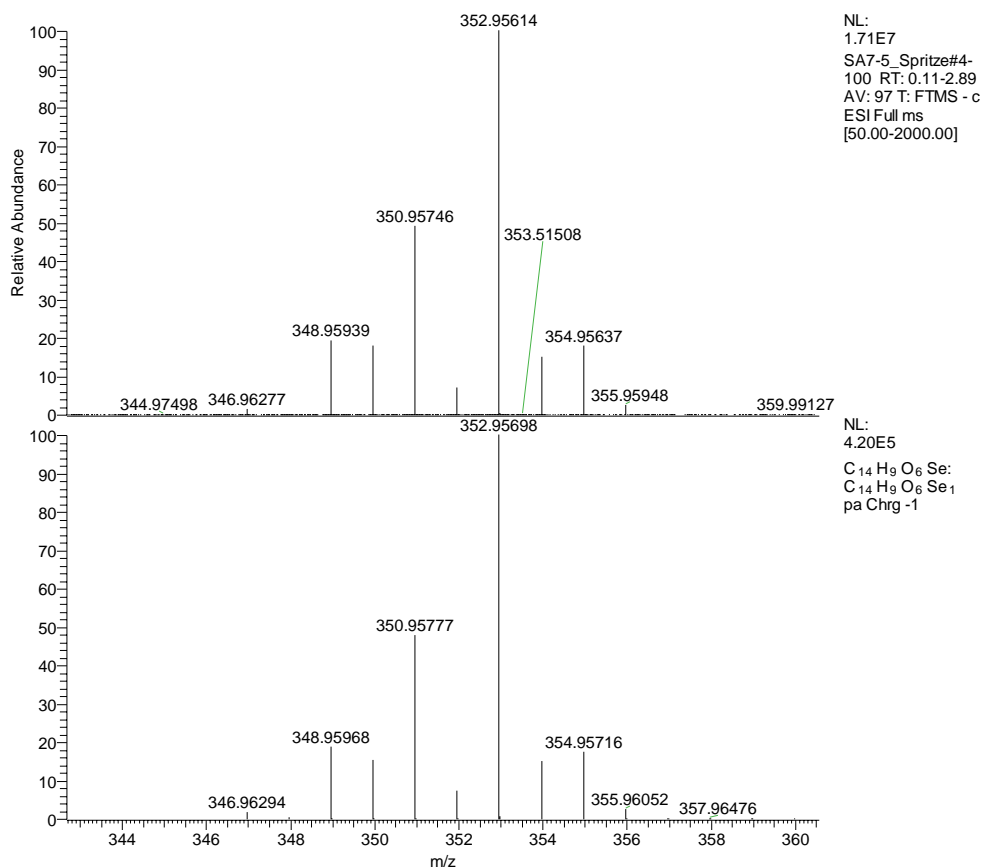


Figure SI-42. HR-MS spectrum (expanded) of 5e