A Novel Model System for Investigating Molecular Dynamics: Selenosteroids

Izabella Jastrzebska[1]*, Marta Malinowska[1], Tomasz Pawlak[2], Anna Kamińska[3], Marcin Górecki[3], Rafał Dolot[2], Piotr Paluch[2]

[1] Faculty of Chemistry, University of Białystok, Ciołkowskiego 1K, 15-254 Białystok, Poland

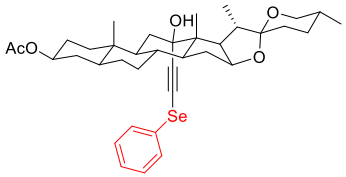
[2] Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, 90-363 Łódź, Sienkiewicza 112, Poland

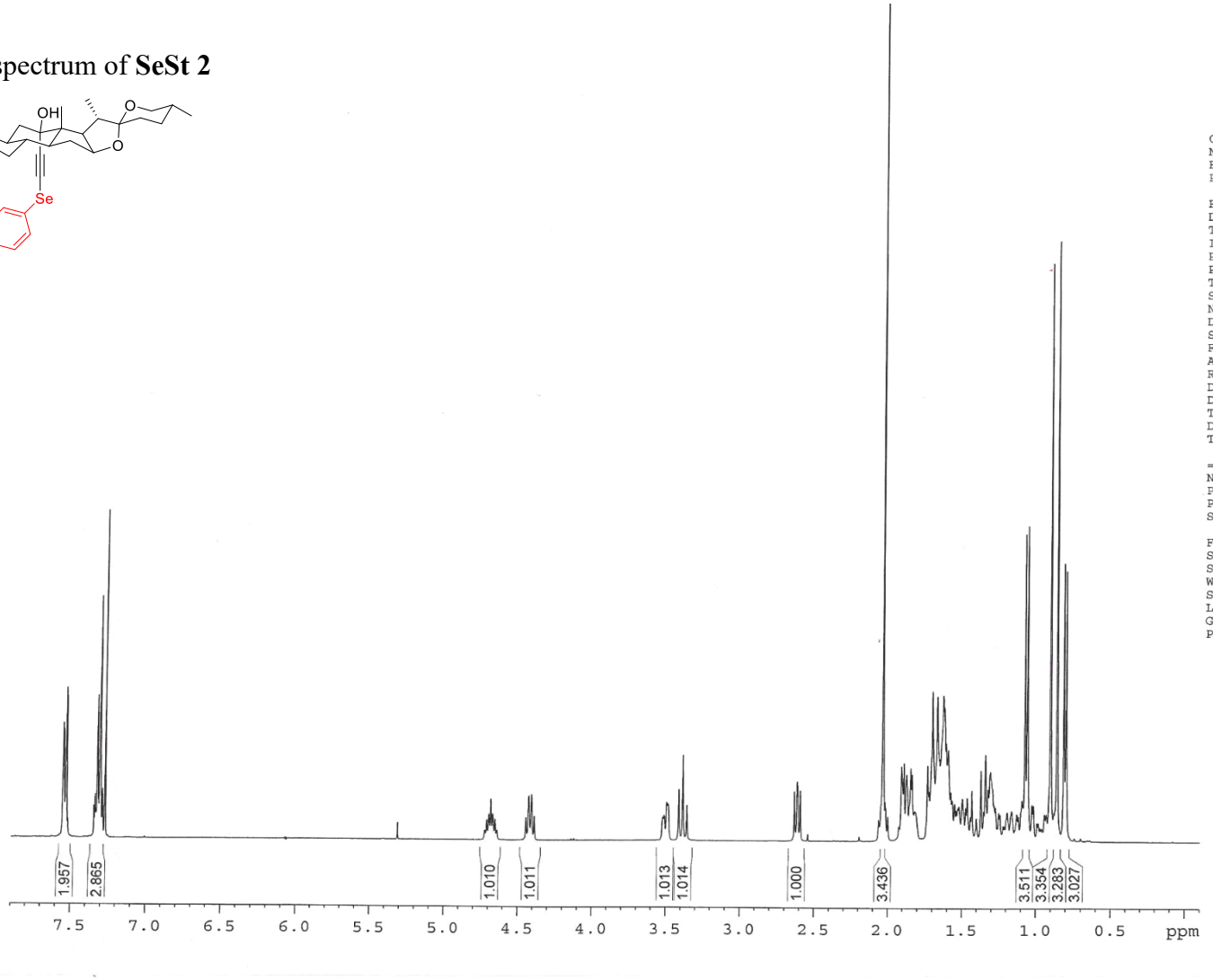
[3] Institute of Organic Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland

E-mail: i.jastrzebska@uwb.edu.pl

Supporting information

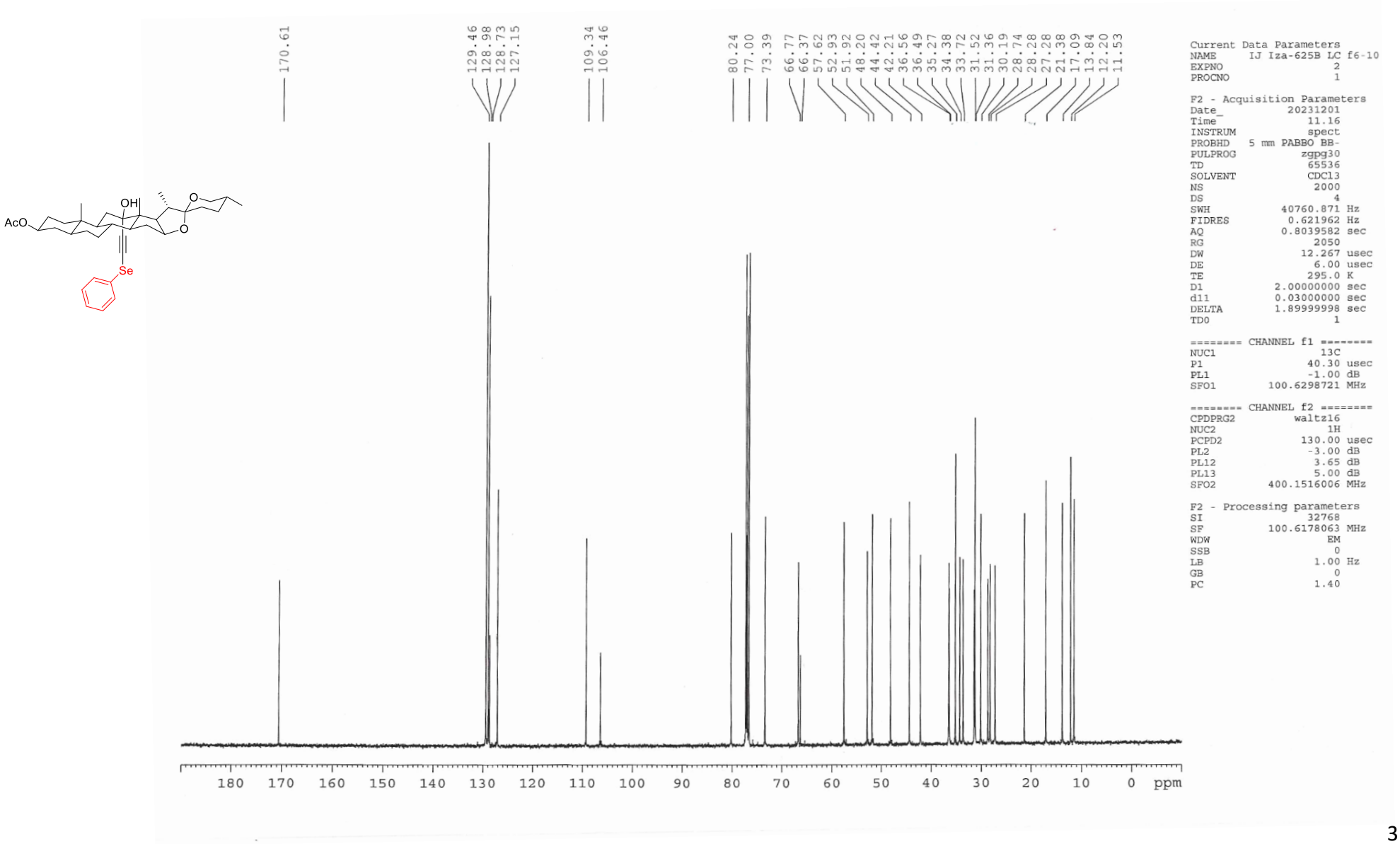
^{1}H NMR spectrum of **SeSt 2**



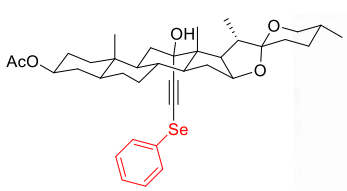


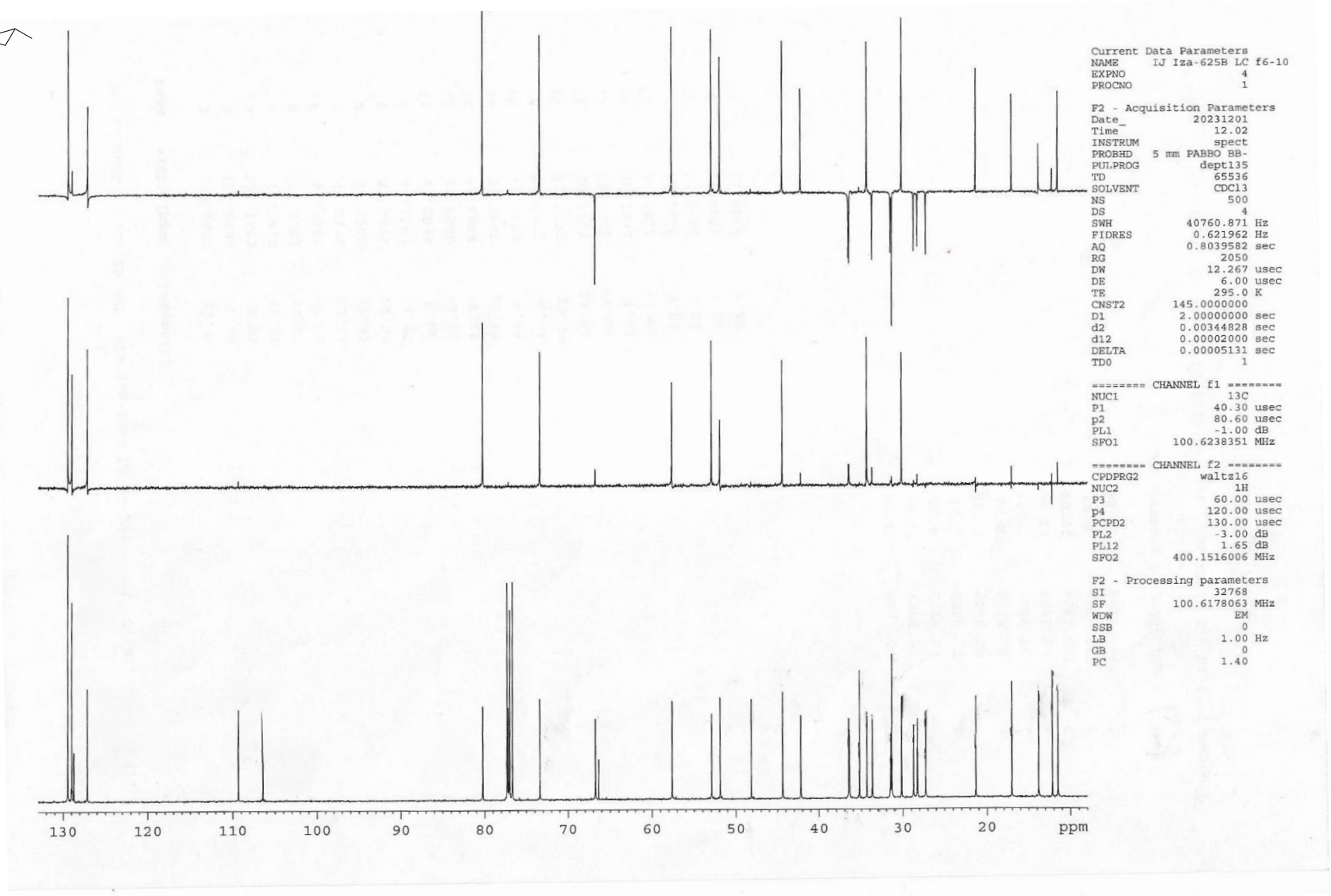

```
Current Data Parameters
NAME      IJ Iza-625B LC f6-10
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20231129
Time                 12.21
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                    400
DS                      0
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                    406
DW                 60.800 usec
DE                  8.00 usec
TE                 294.0 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 35.00 usec
PL1                -3.00 dB
SFO1         400.1524711 MHz

F2 - Processing parameters
SI                  32768
SF           400.1500000 MHz
WDW                    GM
SSB                     0
LB                 -0.20 Hz
GB                    0.2
PC                   1.00
```

^{13}C NMR spectrum of **SeSt 2**

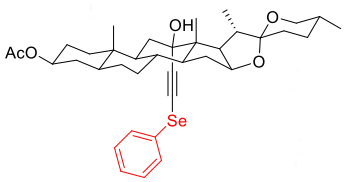


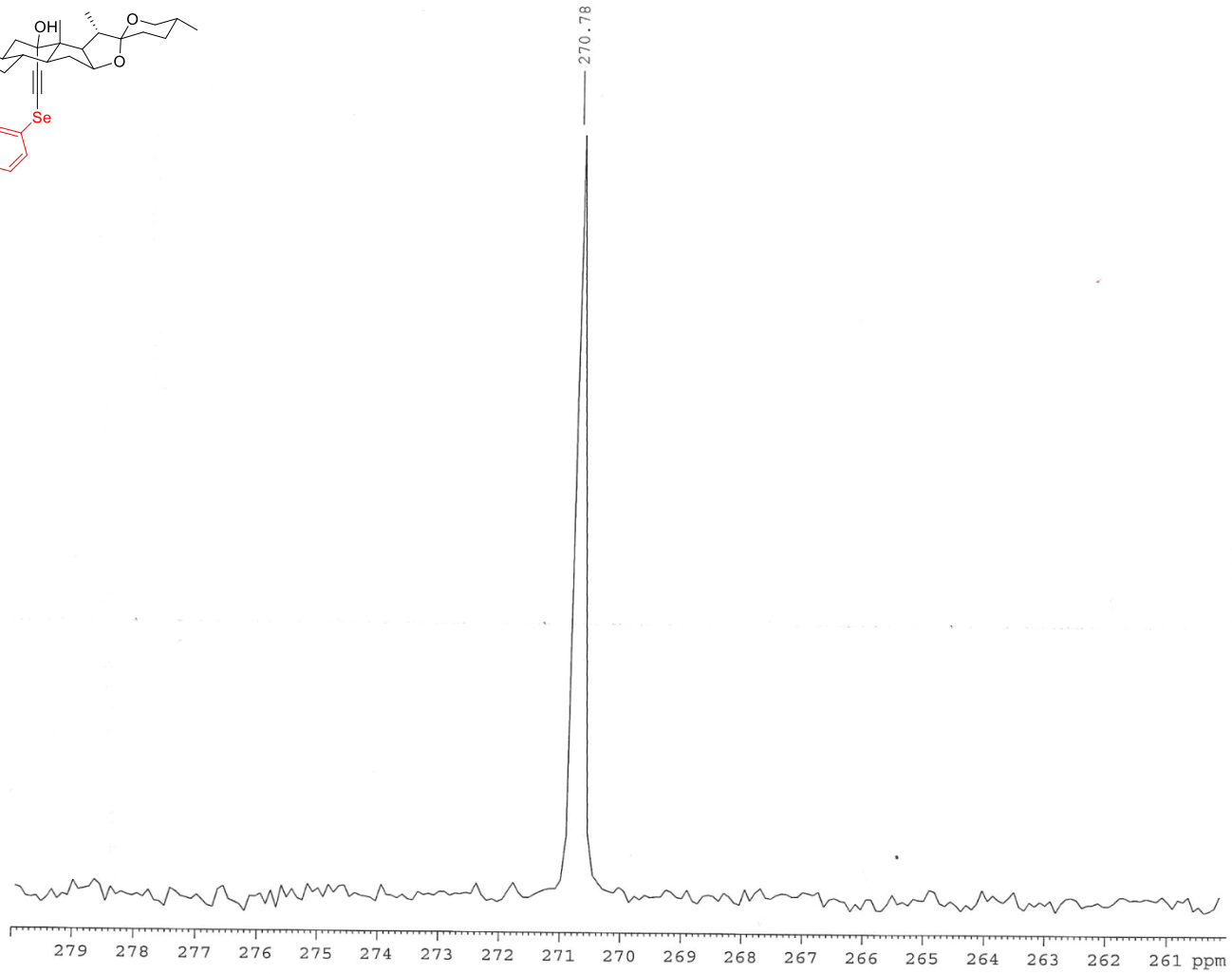
^{13}C NMR spectrum of **SeSt 2**





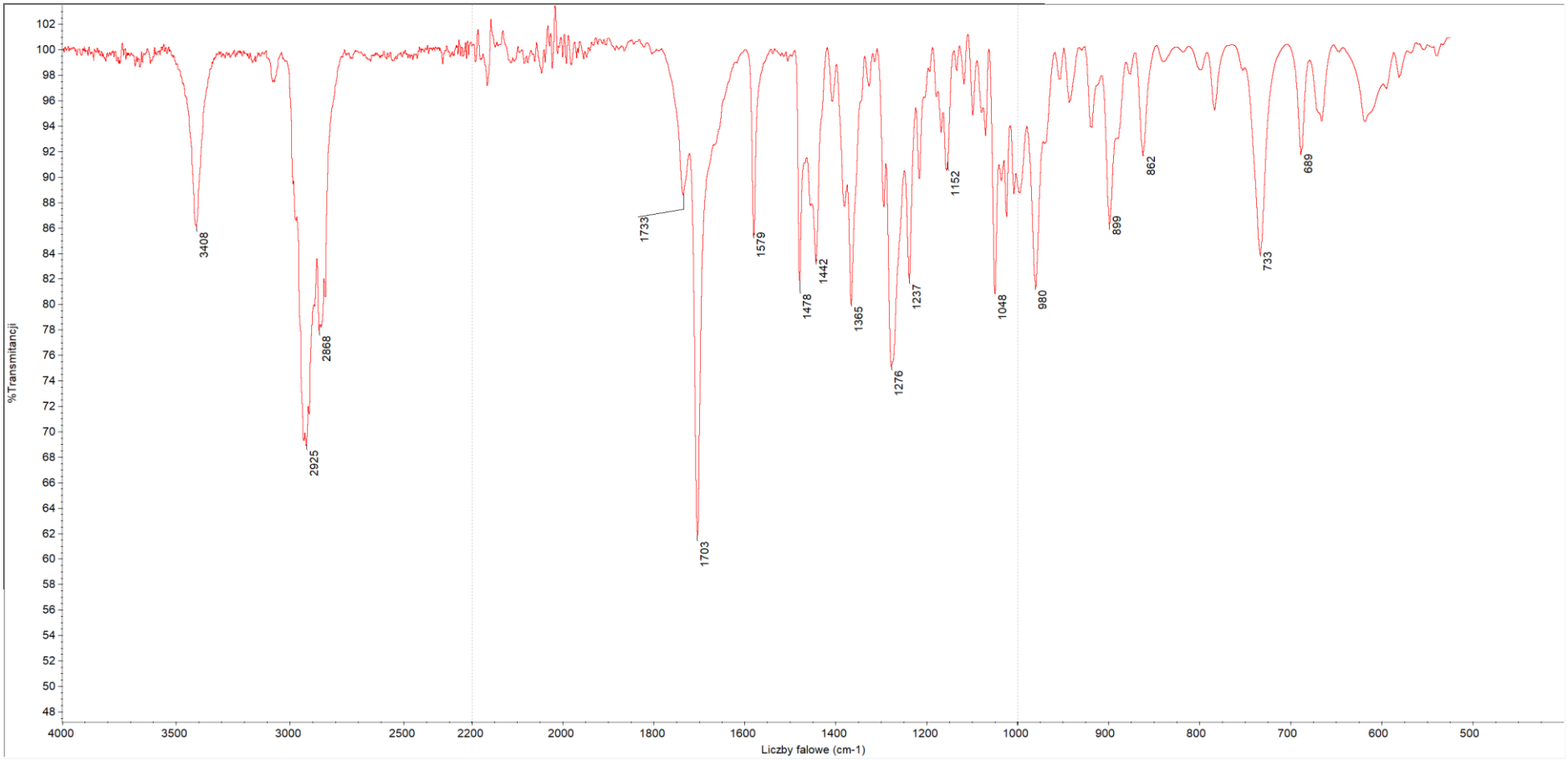
^{77}Se NMR spectrum of **SeSt 2**



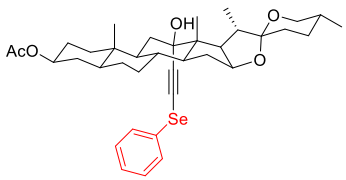



```
Current Data Parameters
NAME          IJ Iza-625B
EXPNO                   8
PROCNO                  1

F2 - Acquisition Parameters
Date_            20240724
Time               18.32
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG               zg
TD                 65536
SOLVENT            CDCl3
NS                 29180
DS                     4
SWH          217391.297 Hz
FIDRES         3.317128 Hz
AQ             0.1507828 sec
RG                  2050
DW                2.300 usec
DE                6.00 usec
TE                 0.0 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                77Se
P1                35.00 usec
PL1                1.00 dB
SFO1         76.3146590 MHz

F2 - Processing parameters
SI                 32768
SF           76.3146808 MHz
WDW                   EM
SSB                    0
LB                 3.00 Hz
GB                     0
PC                  1.40
```

IR spectrum of **SeSt 2**



SI - MS spectrum of **SeSt 2**



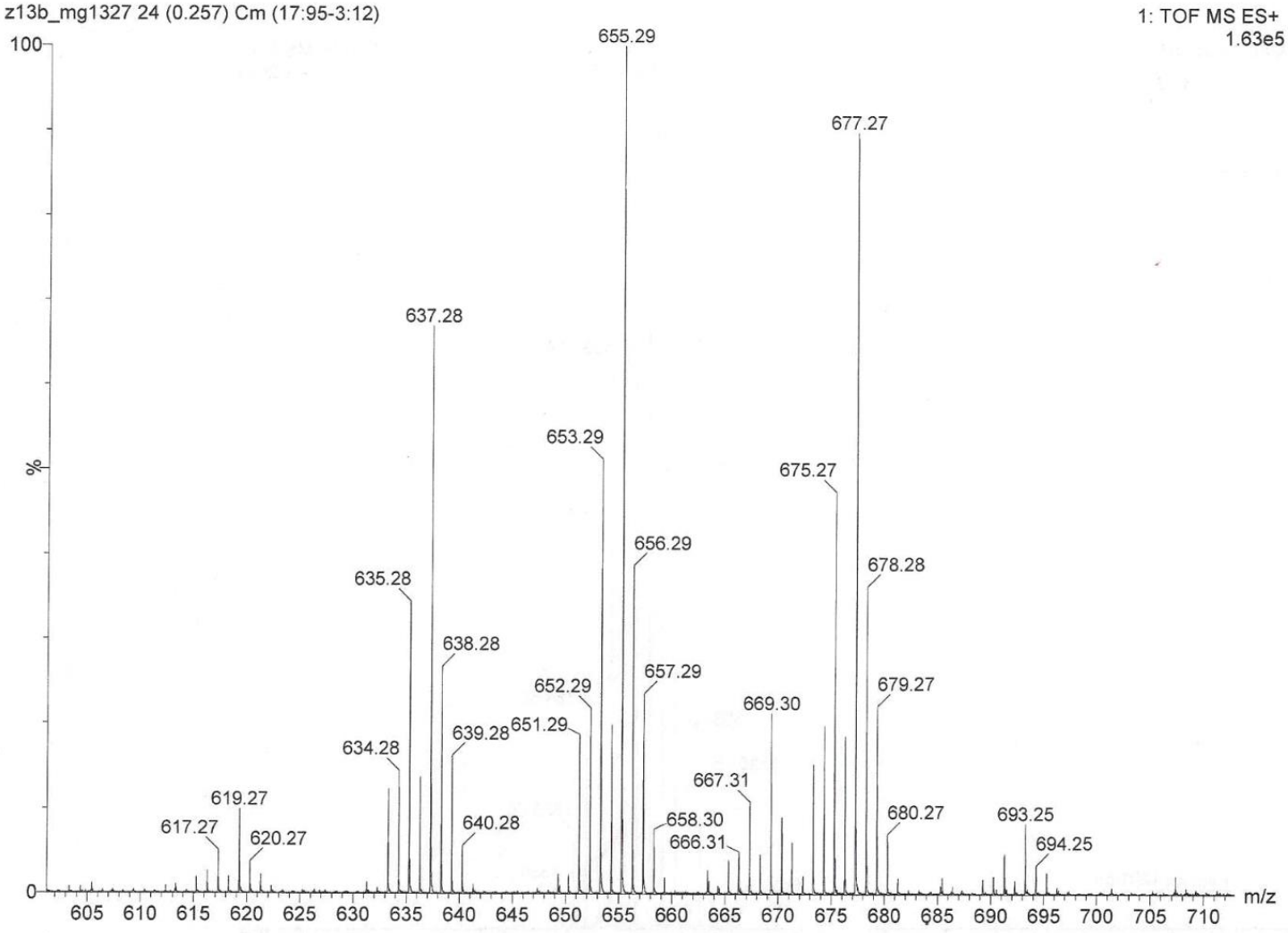


Table S1. Crystal structure, data collection and refinement parameters of the **SeSt 1** and **SeSt 2** studied in this research.

Compound	**SeSt 1**	**SeSt 2**
Crystal data		
CCDC	2453626	2453627
Chemical formula	$C_{37}H_{50}O_5Se$	$C_{37}H_{50}O_5Se$
Formula weight	653.73	653.73
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1$	$P2_1$
Temperature (K)	99.99(10)	100.00(10)
a [Å]	15.9668(1)	13.4375(3)
b [Å]	14.1741(1)	7.2022(2)
c [Å]	29.7960(2)	18.0356(5)
α [°]	90	90
β [°]	93.898(1)	105.267(2)
γ [°]	90	90
V [Å^3]	6727.68(8)	1683.88(8)
Z	8	2
Z'	4	1
d_{calc} [g/cm^3]	1.291	1.289
Crystal dimensions [mm]	0.60 × 0.10 × 0.05	0.95 × 0.10 × 0.03
Radiation type	CuKα	CuKα
μ [mm^{-1}]	1.829	1.827
Data collection		
Reflections measured	103082	25149
Range/indices (h, k, l)	-20, 20 -17, 16 -36, 37	-16, 16 -8, 9 -22, 19
θ (max, min) [°]	77.047, 2.774	77.224, 2.539
Total no. of unique data	25936	6387
No. of observed data, I > 2σ(I)	24722	5814
R_{int}	0.059	0.090
Refinement		
R [$F^2 > 2\sigma$ (F^2)]	0.079	0.094
$wR(F^2)$	0.211	0.218
S	1.092	1.170
No. of reflections	25936	6387
No. of parameters	1569	389
No. of restraints	1	1
H-atom treatment	H atoms treated by constrained refinement	H atoms treated by constrained refinement
Δρ (min, max), e/Å^3	-1.01/1.55	-0.91/2.26

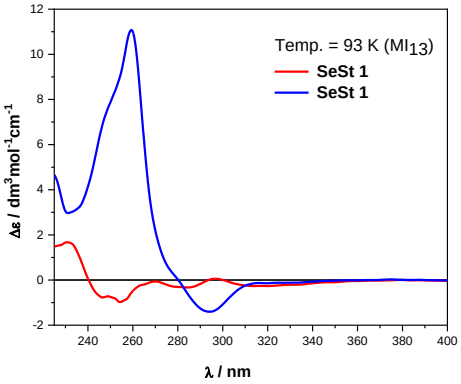
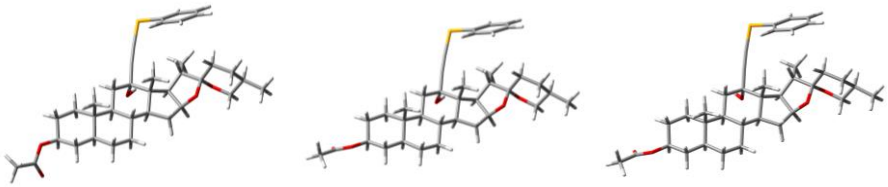


Figure S1. ECD spectra of **SeSt 1** and **SeSt 2** recorded at 93 K in MI_{13}.

Table S2. Relative energies and populations at 298 K based on DFT-optimized conformers of **SeSt 1** and **SeSt 2** within 1 kcal mol^{-1} calculated at the ωB97X-D/6-311+G(d,p) level with the three representative torsion angles.

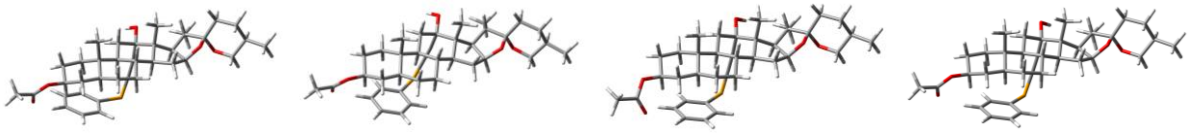
Conf.	ΔE / kcal mol^{-1}	Pop. /%	α / deg	β / deg	C36–O4–C3–C2 / deg
Rotor SeSt 1					
SeSt 1a	0.00	45.10	–5.8	+122.1	+155.2
SeSt 1b	0.10	38.18	–5.0	+122.1	+83.2
SeSt 1c	0.59	16.71	–6.1	+120.1	+83.0
Rotor SeSt 2					
SeSt 2a	0.00	43.45	+13.8	+89.8	+85.7
SeSt 2b	0.37	23.08	+8.3	+100.2	+90.6
SeSt 2c	0.40	21.94	+10.0	+97.7	+150.3
SeSt 2d	0.78	11.54	+3.8	+97.6	+91.1

Rotor SeSt 1



SeSt 1a **SeSt 1b** **SeSt 1c**

Rotor SeSt 2



SeSt 2a **SeSt 2b** **SeSt 2c** **SeSt 2d**

Figure S2. The stable conformers of rotors **SeSt 1** and **SeSt** within 1 kcal/mol calculated at the ωB97X-D/6-311+G(d,p) level of theory.