

A Novel Model System for Investigating Molecular Dynamics: Selenosteroids

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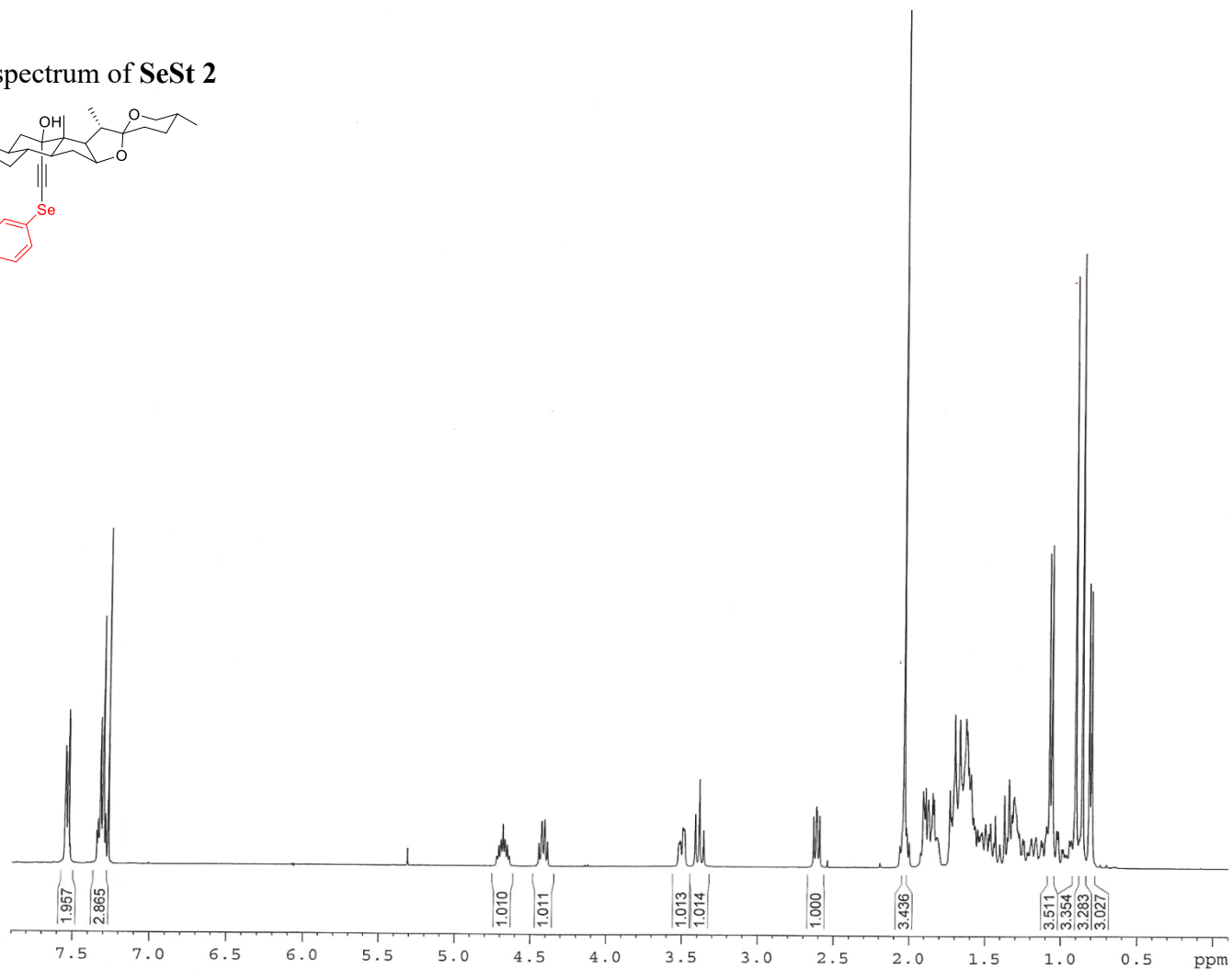
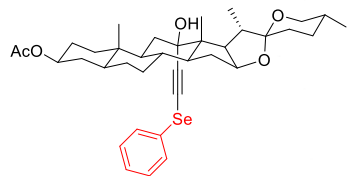
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¹H NMR spectrum of SeSt 2



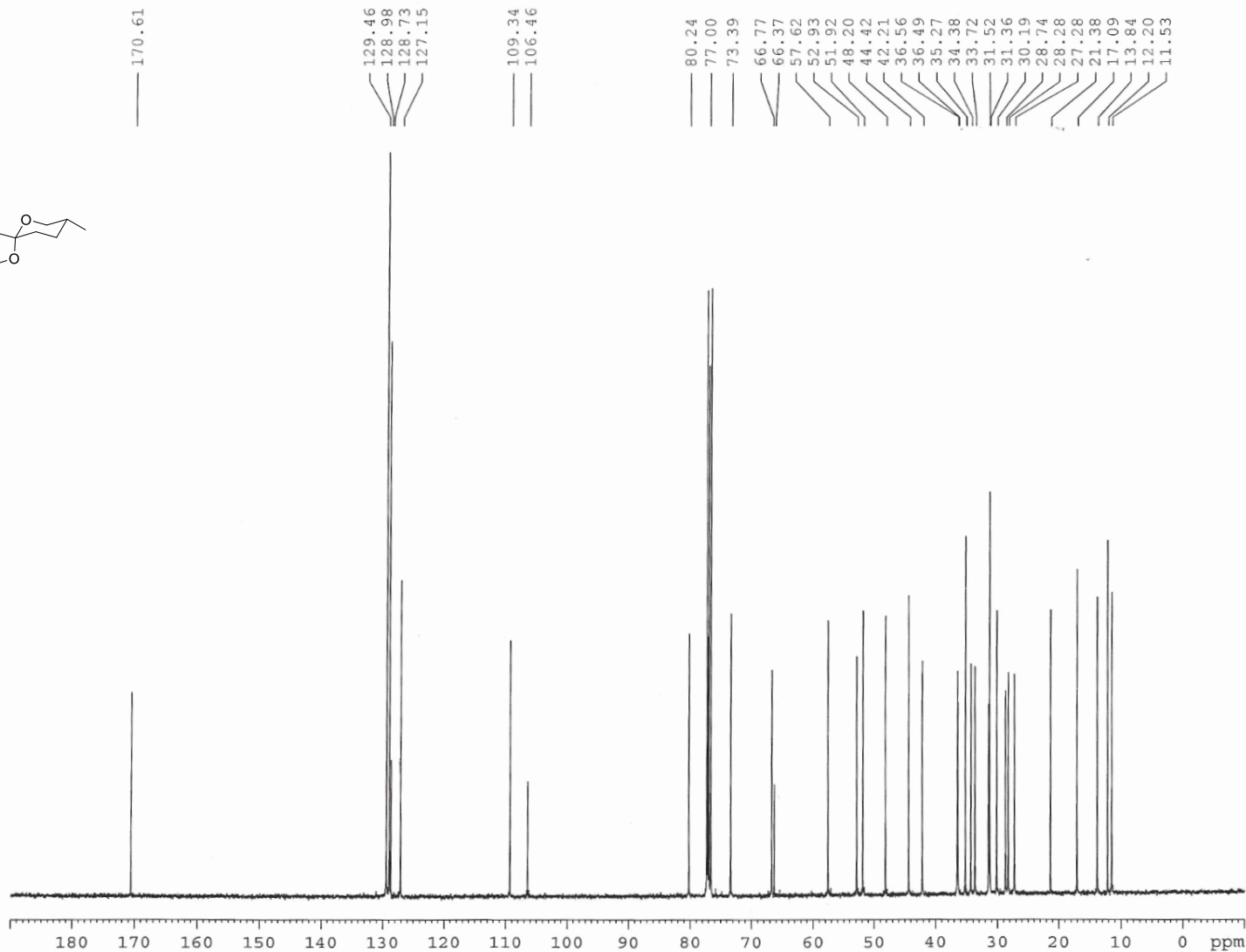
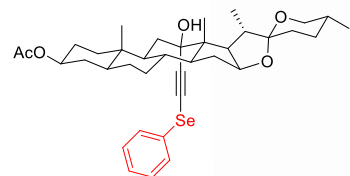
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TDO 1

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¹³C NMR spectrum of SeSt 2



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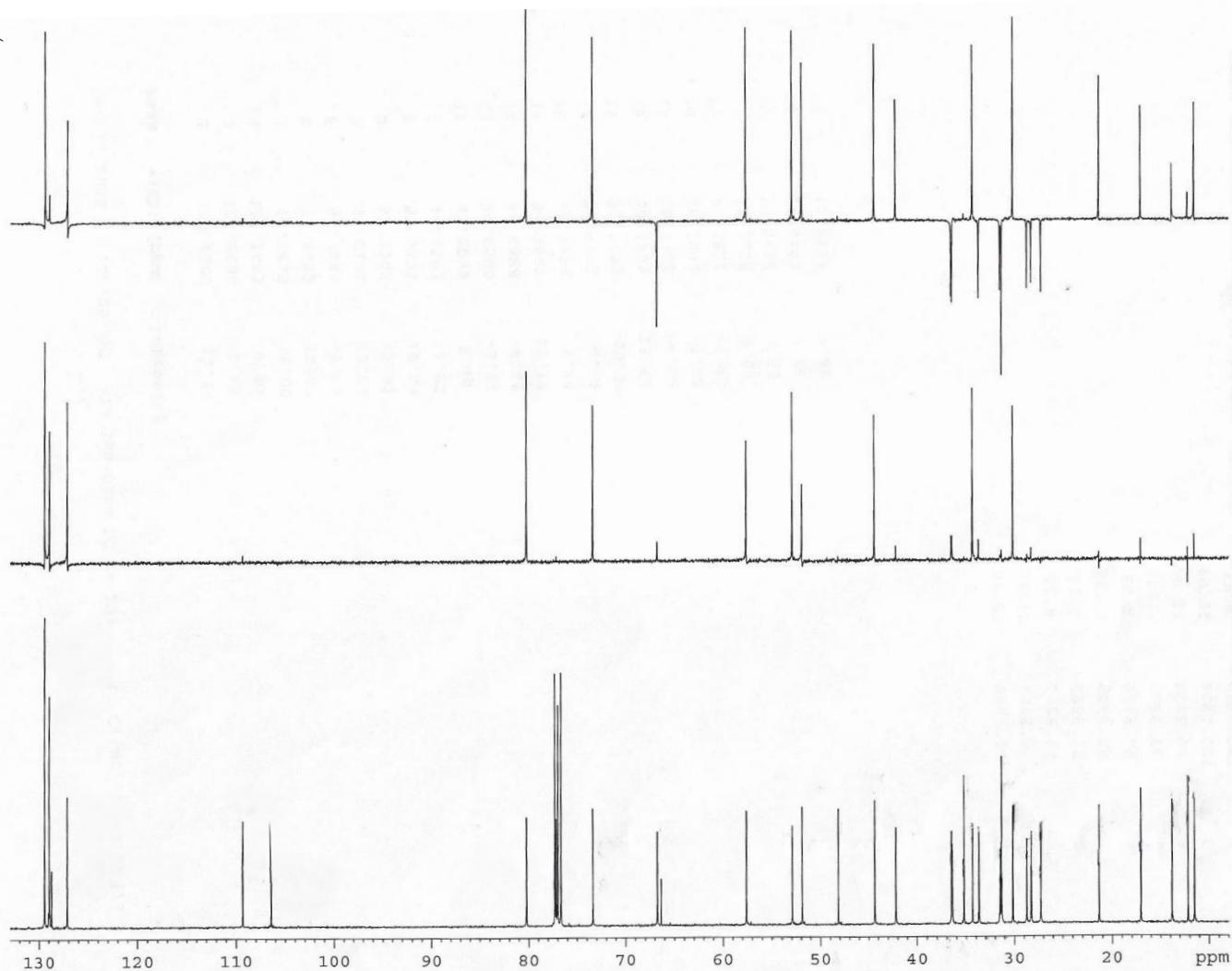
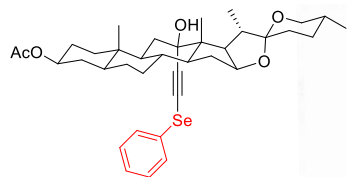
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 DS 4
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F2 - Processing parameters
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¹³C NMR spectrum of SeSt 2



Current Data Parameters
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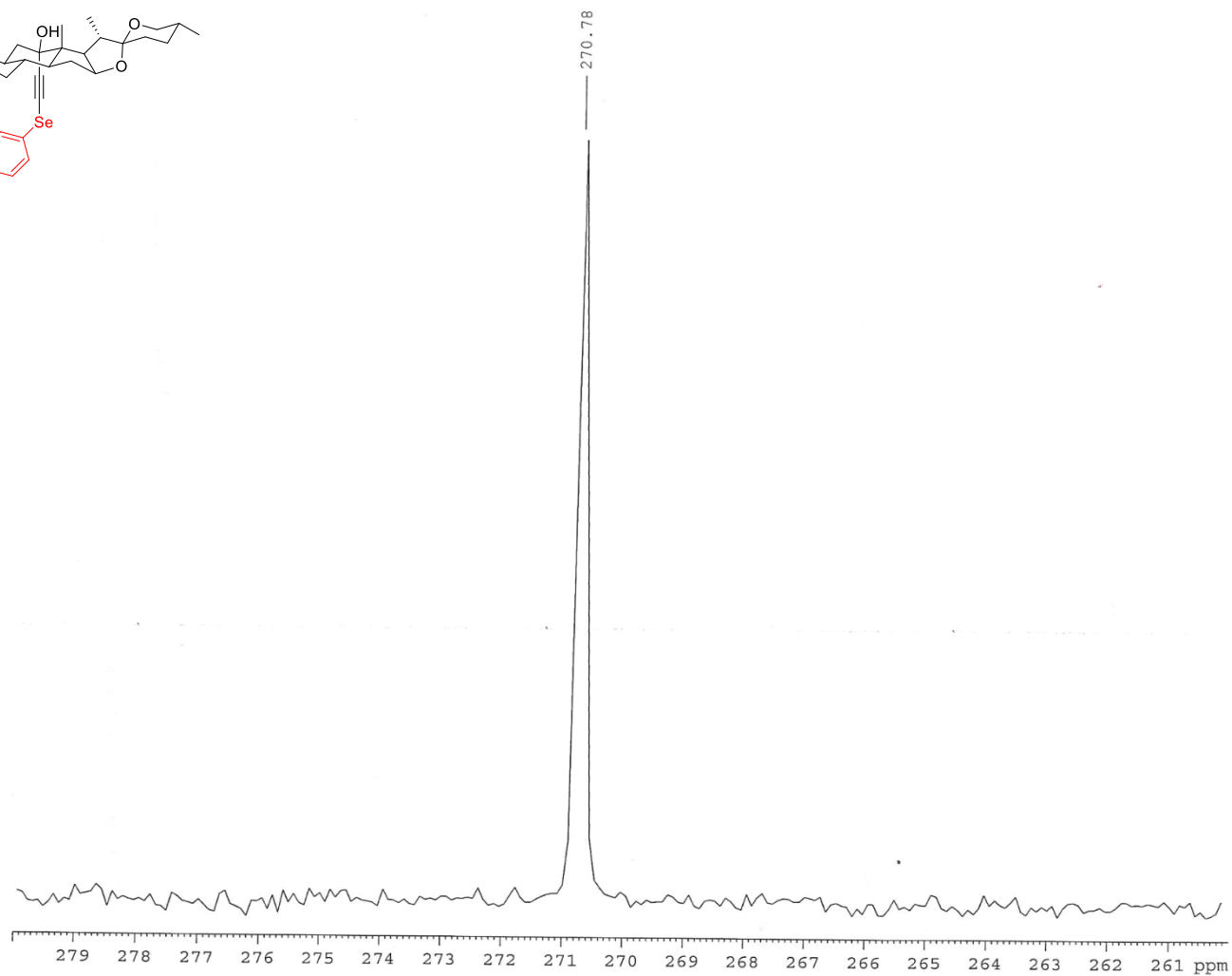
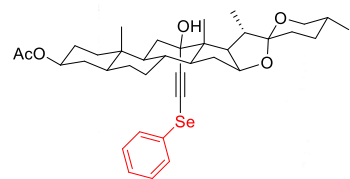
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RG 2050
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DE 6.00 usec
TE 295.0 K
CNST2 145.0000000
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d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00005131 sec
TD0 1

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p2 80.60 usec
PL1 -1.00 dB
SFO1 100.6238351 MHz

----- CHANNEL f2 -----
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P3 60.00 usec
p4 120.00 usec
PCPD2 130.00 usec
PL2 -3.00 dB
PL12 1.65 dB
SFO2 400.1516006 MHz

F2 - Processing parameters
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⁷⁷Se NMR spectrum of SeSt 2



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D1         2.00000000 sec
TDO        1

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PL1        1.00 dB
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IR spectrum of SeSt 2

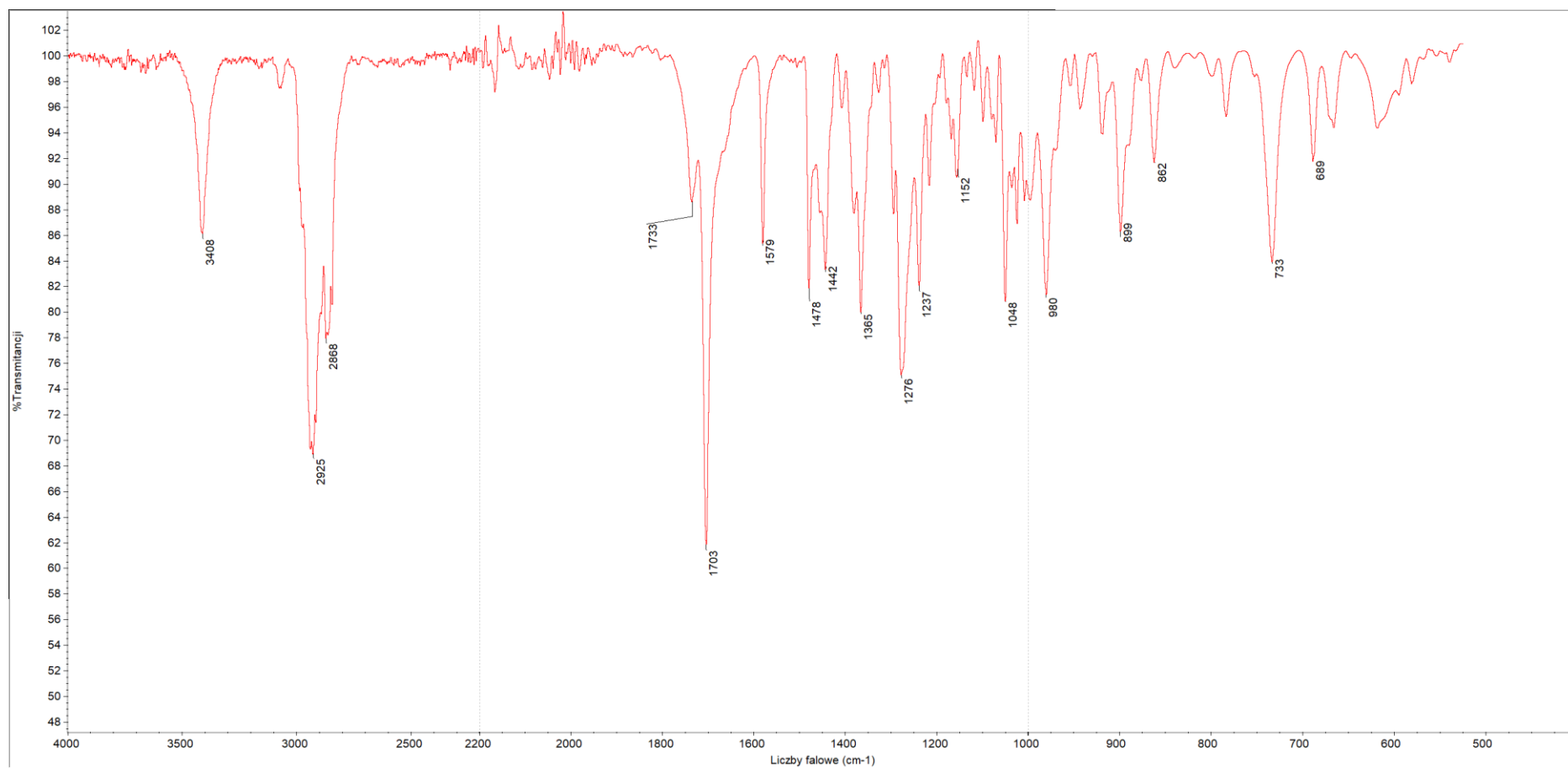


Table S1. Crystal structure, data collection and refinement parameters of the **SeSt 1** and **SeSt 2** studied in this research.

Compound	SeSt 1	SeSt 2
Crystal data		
CCDC	2453626	2453627
Chemical formula	C ₃₇ H ₅₀ O ₅ Se	C ₃₇ H ₅₀ O ₅ Se
Formula weight	653.73	653.73
Crystal system	Monoclinic	Monoclinic
Space group	<i>P</i> 2 ₁	<i>P</i> 2 ₁
Temperature (K)	99.99(10)	100.00(10)
<i>a</i> [Å]	15.9668(1)	13.4375(3)
<i>b</i> [Å]	14.1741(1)	7.2022(2)
<i>c</i> [Å]	29.7960(2)	18.0356(5)
α [°]	90	90
β [°]	93.898(1)	105.267(2)
γ [°]	90	90
<i>V</i> [Å ³]	6727.68(8)	1683.88(8)
<i>Z</i>	8	2
<i>Z'</i>	4	1
<i>d</i> _{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	CuK α	CuK α
μ [mm ⁻¹]	1.829	1.827
Data collection		
Reflections measured	103082	25149
Range/indices (<i>h</i> , <i>k</i> , <i>l</i>)	-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>I</i> > 2 σ (<i>I</i>)	24722	5814
<i>R</i> _{int}	0.059	0.090
Refinement		
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)]	0.079	0.094
<i>wR</i> (<i>F</i> ²)	0.211	0.218
<i>S</i>	1.092	1.170
No. of reflections	25936	6387
No. of parameters	1569	389
No. of restraints	1	1
H-atom treatment	<u>H atoms treated by constrained refinement</u>	<u>H atoms treated by constrained refinement</u>
$\Delta\rho$ (min, max), e/Å ³	-1.01/1.55	-0.91/2.26

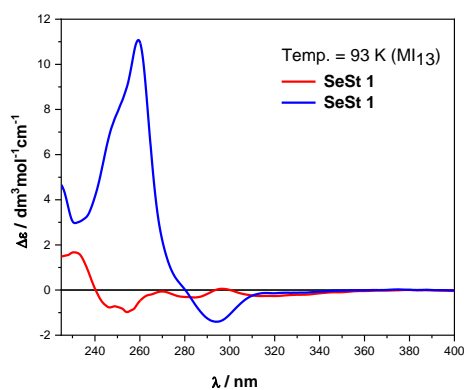
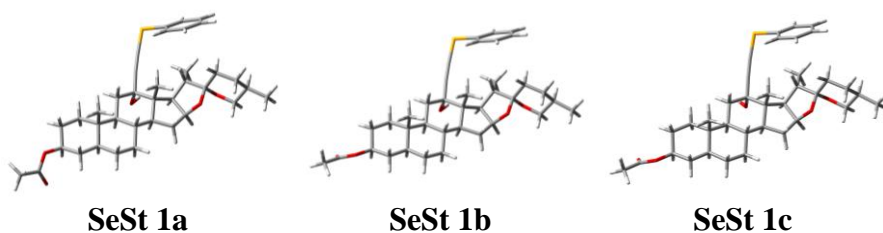


Figure S1. ECD spectra of **SeSt 1** and **SeSt 2** recorded at 93 K in MI_{13} .

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 $\omega B97X-D/6-311+G(d,p)$ 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



Rotor SeSt 2

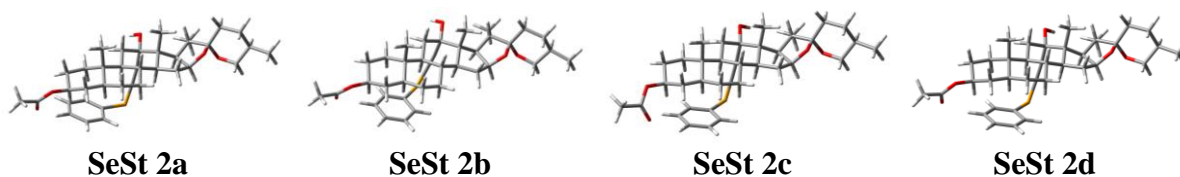


Figure S2. The stable conformers of rotors **SeSt 1** and **SeSt 2** within 1 kcal/mol calculated at the $\omega B97X-D/6-311+G(d,p)$ level of theory.