

SUPPORTING INFORMATION

5,5'-Selenobis(1-benzyl-2-oxo-1,2-dihydropyridine-4-carbaldehyde)

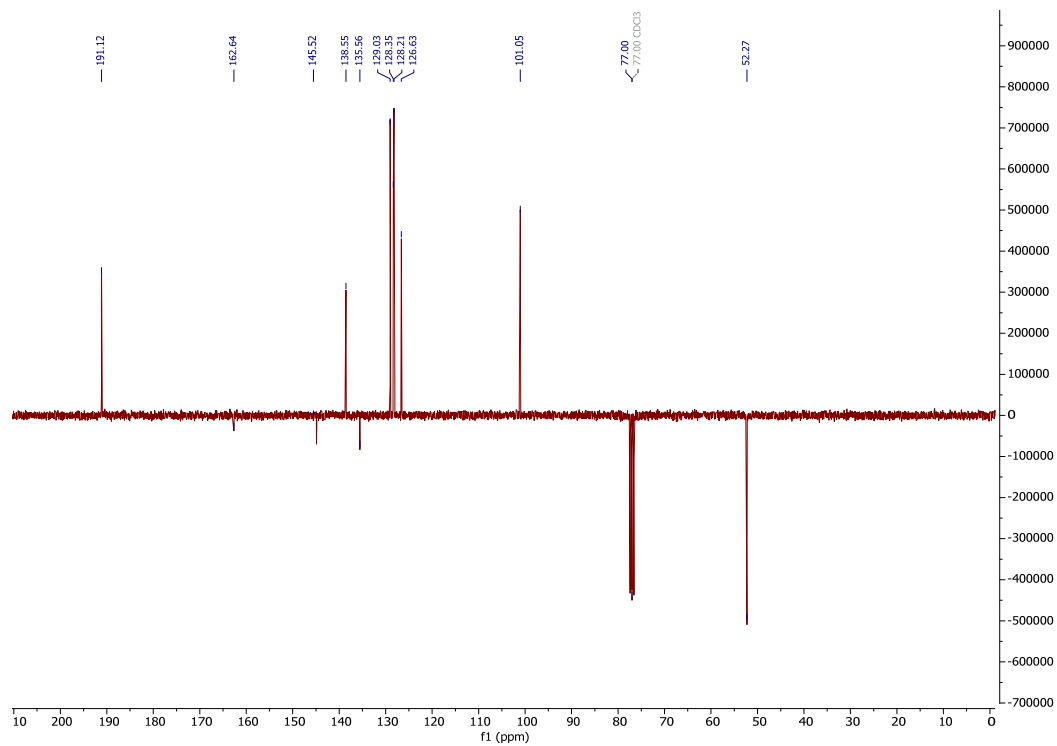
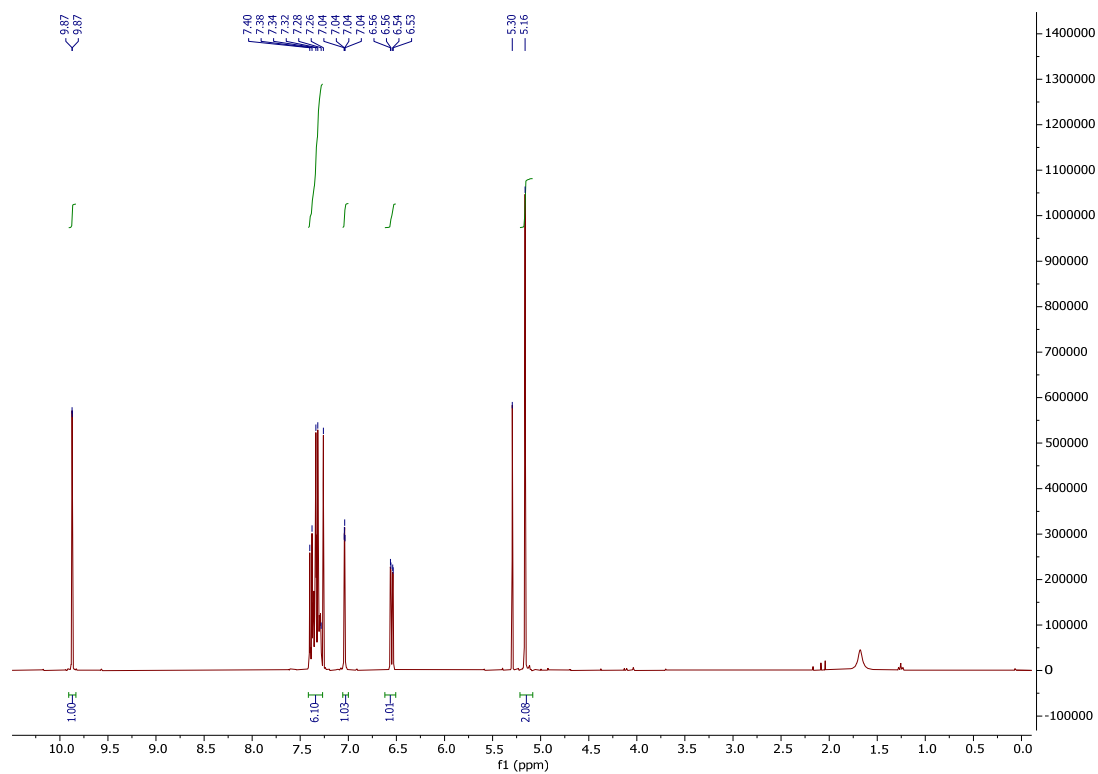
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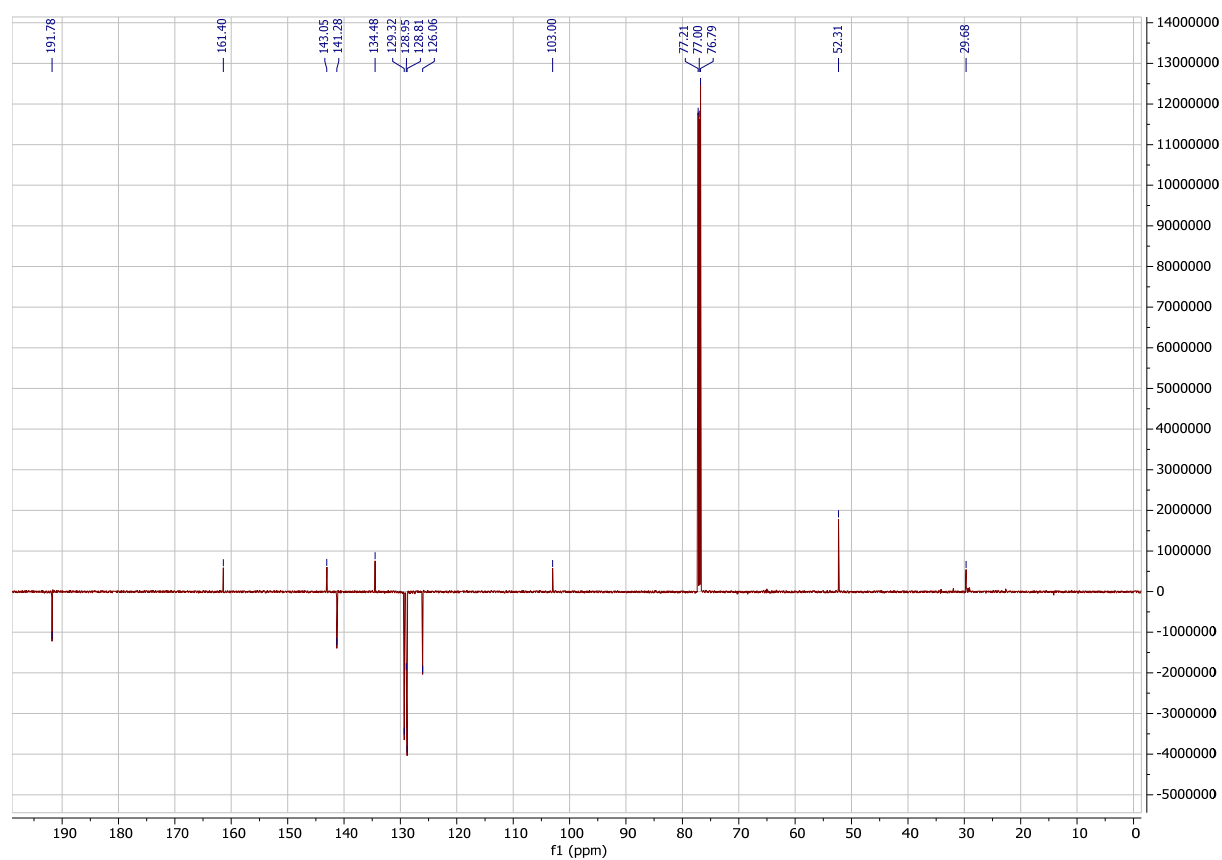
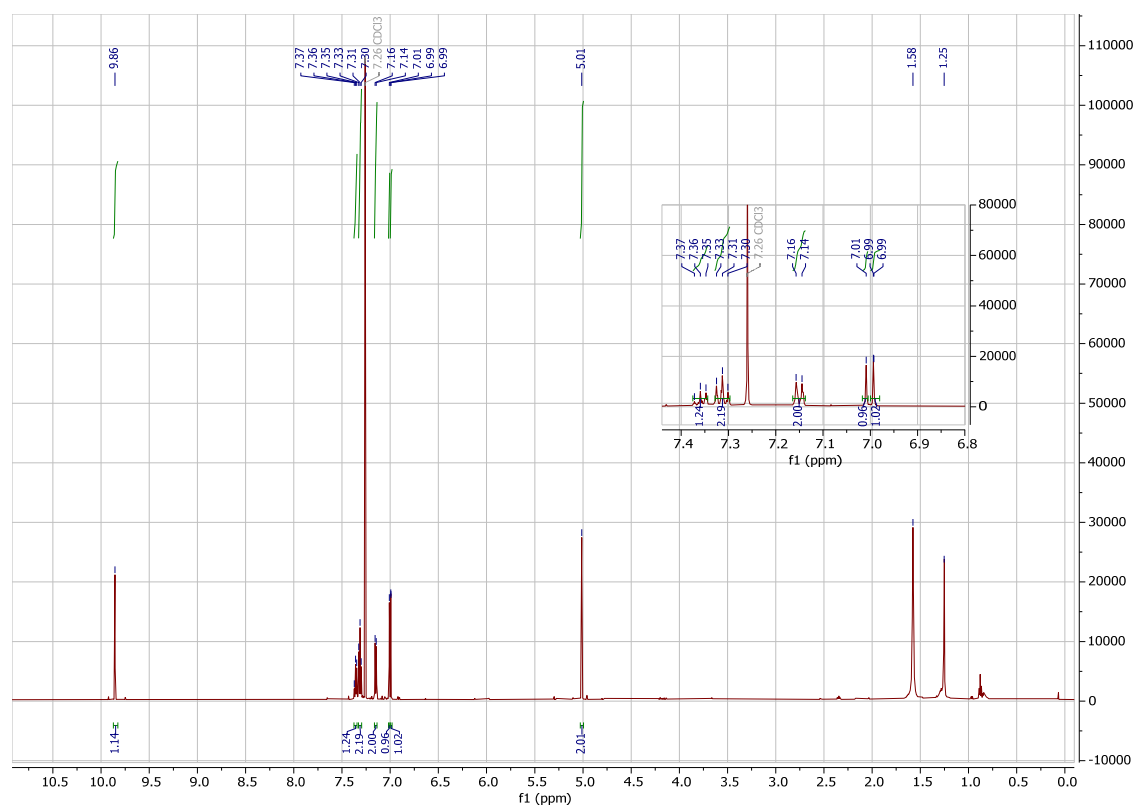
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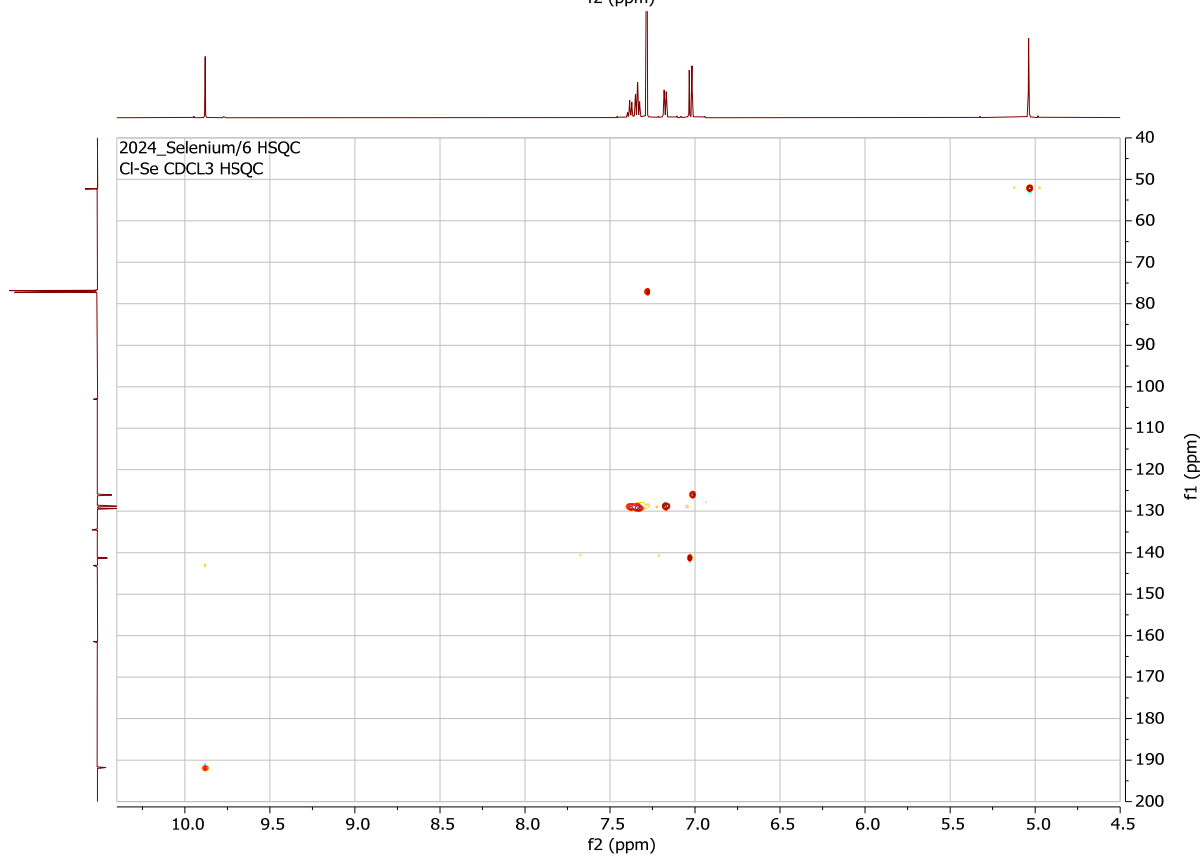
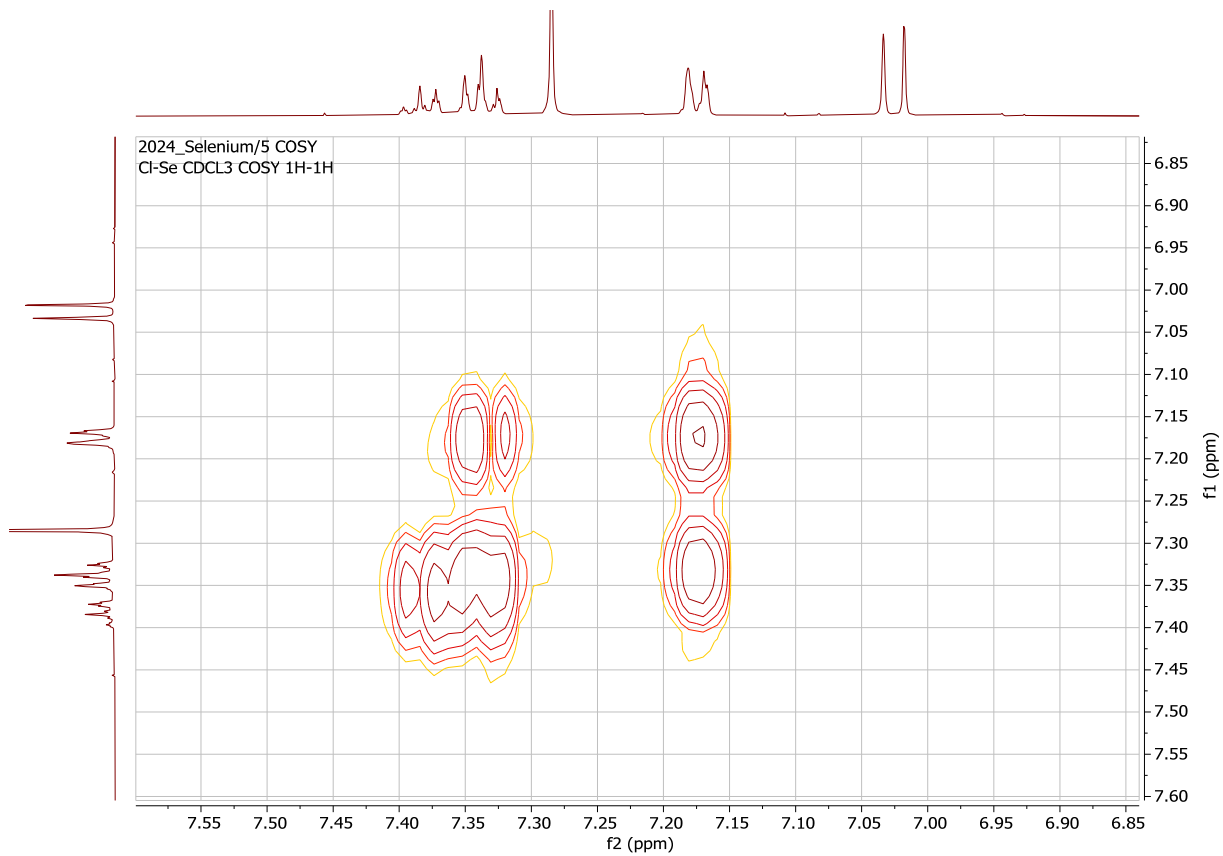
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Mass data for compound 3	6

Compound 2

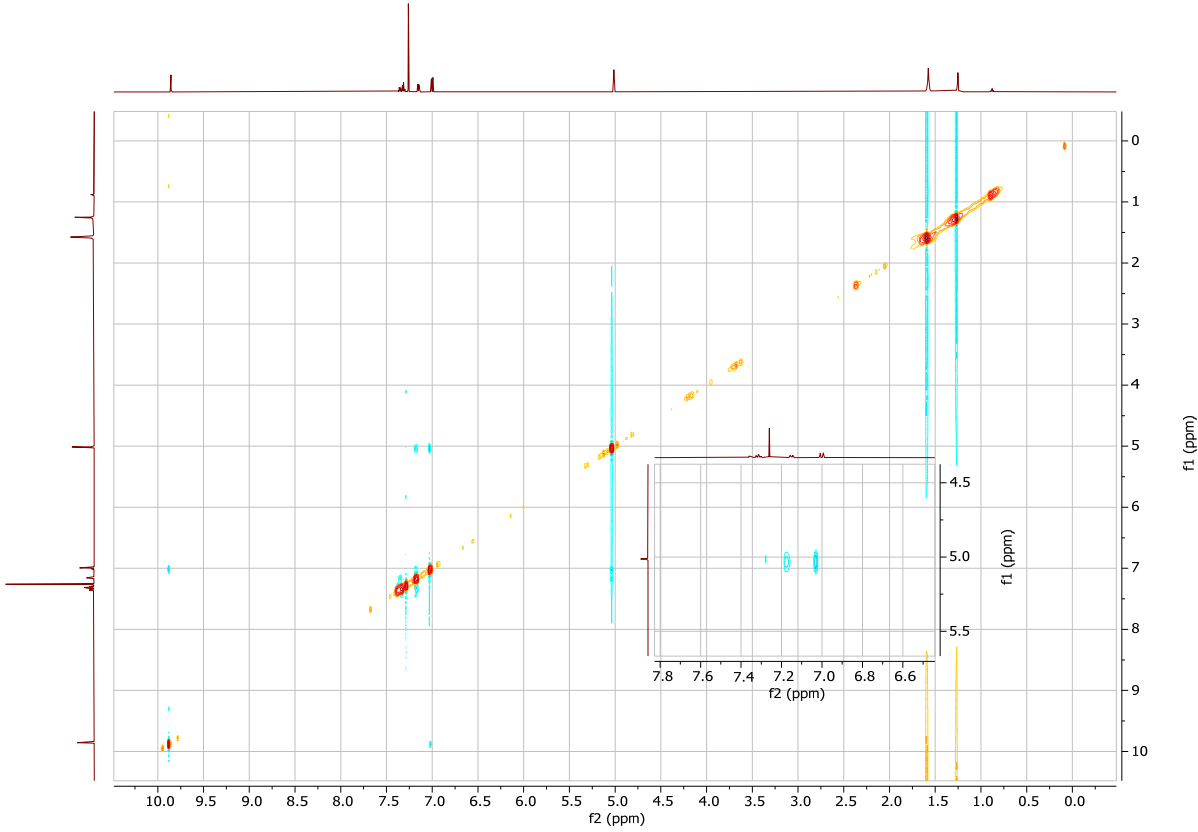


Compound 3 :





NOESY :



Multiple Mass Analysis: 2 mass(es) processed

Tolerance = 3.0 PPM / DBE: min = -5.0, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

932 formula(e) evaluated with 5 results within limits (up to 50 closest results for each mass)

Elements Used:

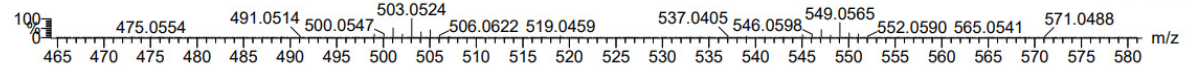
C: 0-100 H: 0-100 N: 0-4 O: 0-6 80Se: 0-1

Cone voltage =50V Xevo G2 QTOF #YCA210

22-Oct-2024 14:09:32

EG1-196Se-NEG-2 79 (0.515) AM2 (Ar,18000.0,0.00,0.00); Cm (72:87)

1: TOF MS ES-
3.20e+005



Minimum: 55.00
Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
503.0524	100.00	503.0537	-1.3	-2.6	24.0	360.8	0.398	67.17	C29 H17 N3 O 80Se
		503.0510	1.4	2.8	19.5	361.6	1.114	32.83	C26 H19 N2 O4 80Se
549.0565	78.70	549.0565	0.0	0.0	19.5	326.5	0.778	45.93	C27 H21 N2 O6 80Se
		549.0552	1.3	2.4	37.5	326.7	1.016	36.20	C41 H9 O3
		549.0578	-1.3	-2.4	42.0	327.4	1.722	17.87	C44 H7 N

Cone voltage =50V

Xevo G2 QTOF #YCA210

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EG1-196Se-NEG-2 79 (0.515) AM2 (Ar,18000.0,0.00,0.00); Cm (72:87)

1: TOF MS ES-
3.20e5

