

Supplementary Information (Part 2) for:

Preparation and Certification of Natural and ⁸²Se-Labelled Selenomethionine Reference Materials

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Total Ion Chromatogram – SEES-1

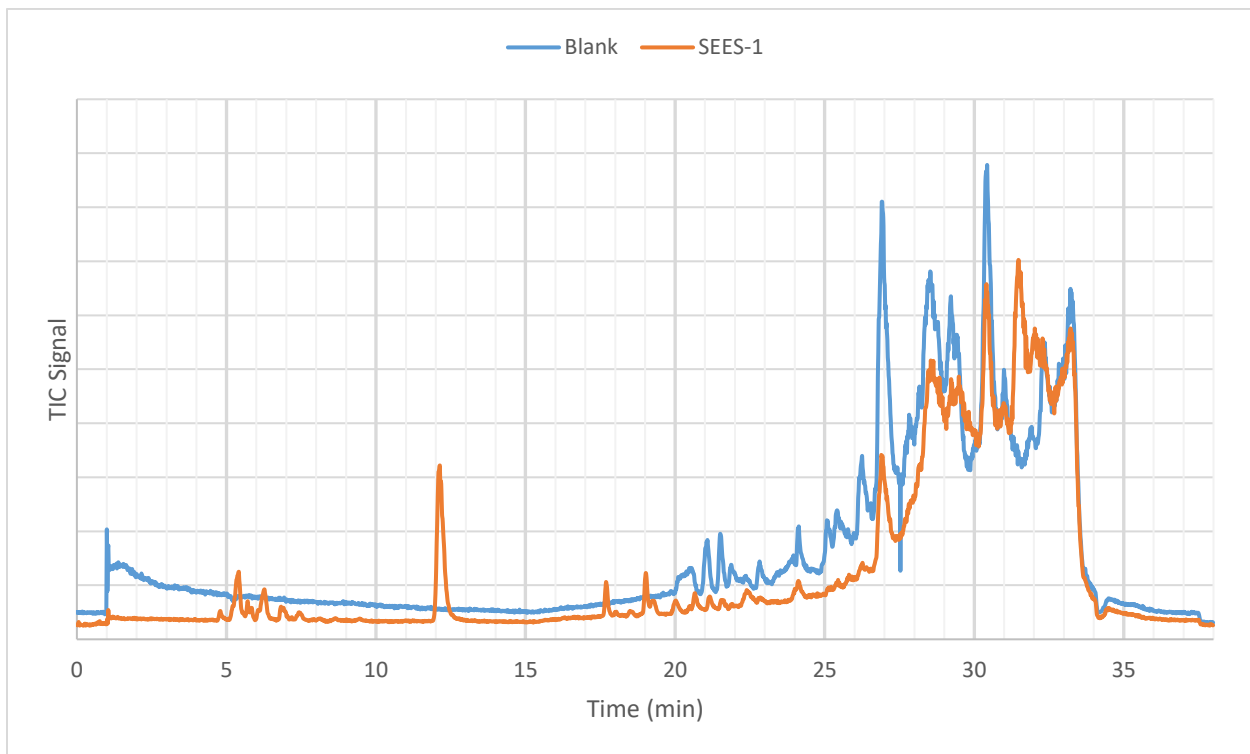


Figure S1: Total ion chromatogram (m/z 50 to 500) for a blank solution (deionized water) and for a SEES-1 standard solution of approximate concentration $25 \mu\text{g g}^{-1}$ ($\sim 10 \mu\text{g Se g}^{-1}$)

Selenomethionine

12.14 min (SeMet)

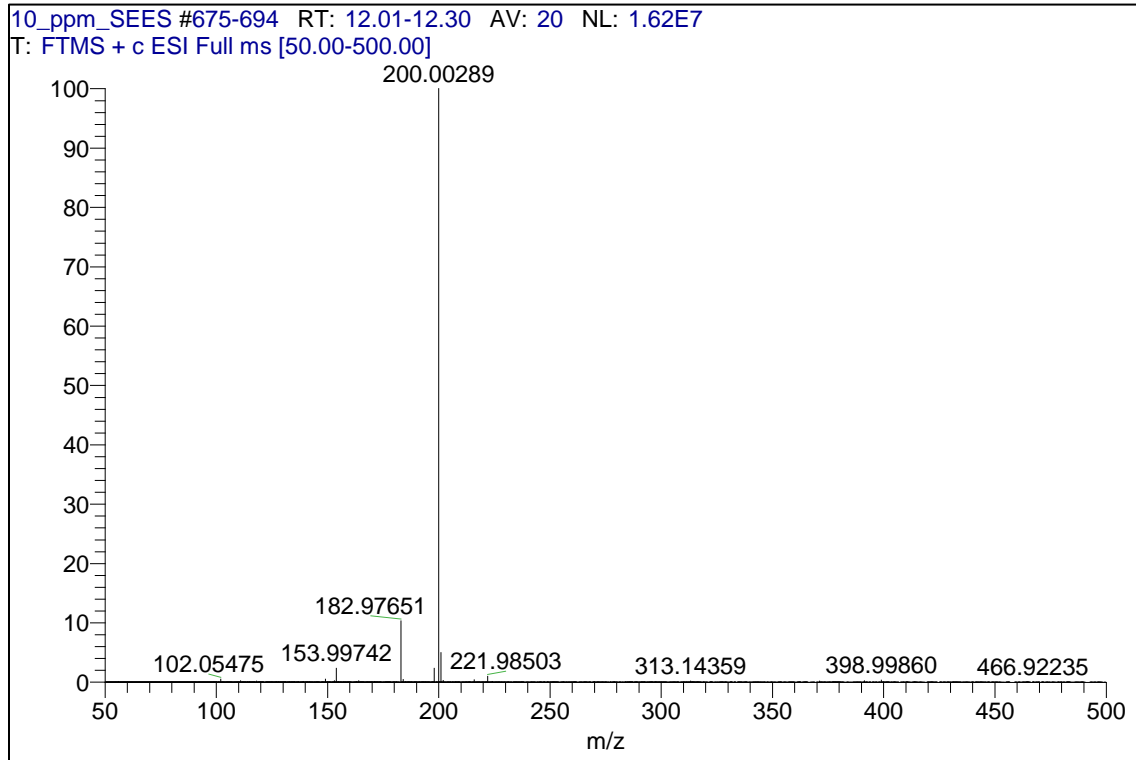


Figure S2: Mass spectrum, full scan from 12.01 min to 12.30 min

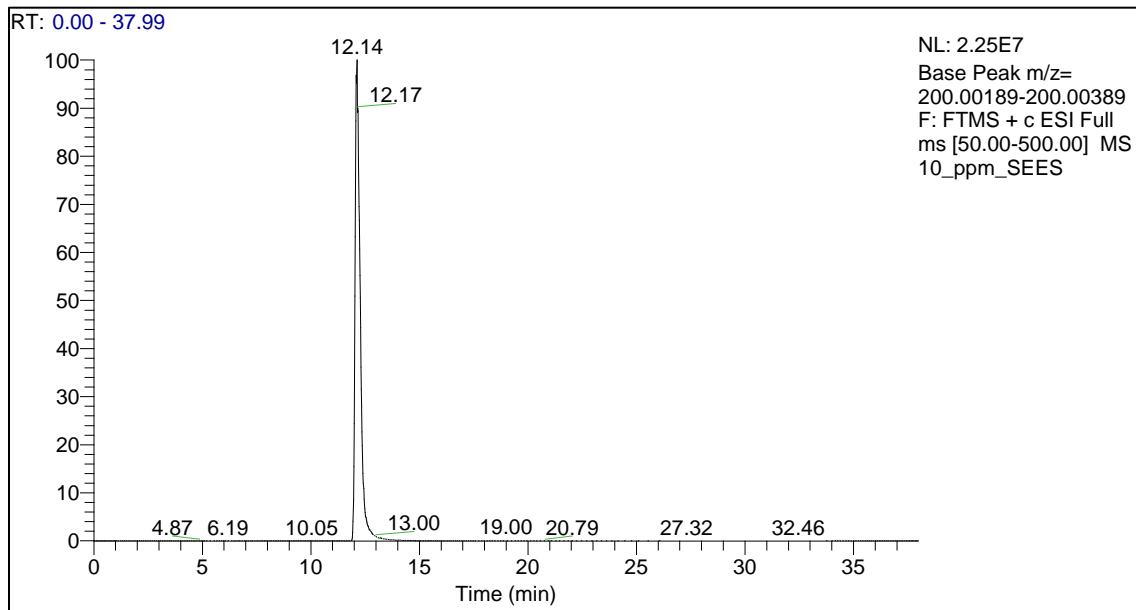


Figure S3: Extracted ion chromatogram for m/z 200

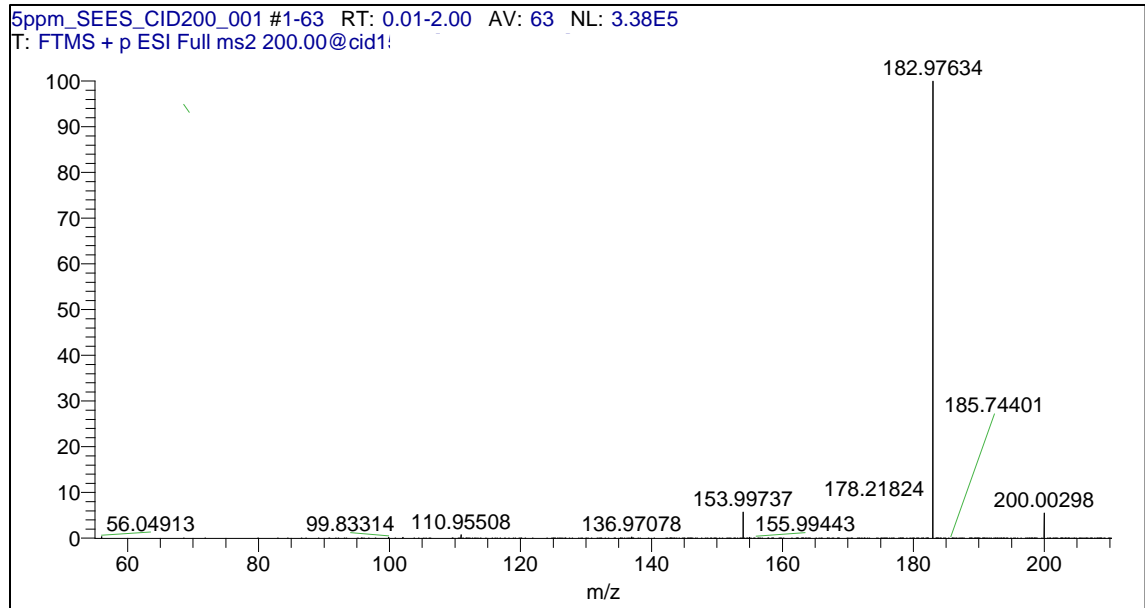


Figure S4: Collision induced dissociation of m/z 200, infusion of SEES-1 for (2 minute scan time)

Peak Identification:

Full Scan	200.00289	$C_5H_{12}NO_2^{82}Se^+$ (-0.326 ppm)
	182.97651	$C_5H_9O_2^{82}Se^+$ (0.568 ppm)
CID (200)	200.00298	$C_5H_{12}NO_2^{82}Se^+$ (0.124 ppm)
	182.97634	$C_5H_9O_2^{82}Se^+$ (-0.361 ppm) (-17 amu, -OH)

Impurity: 5.40 min Peak

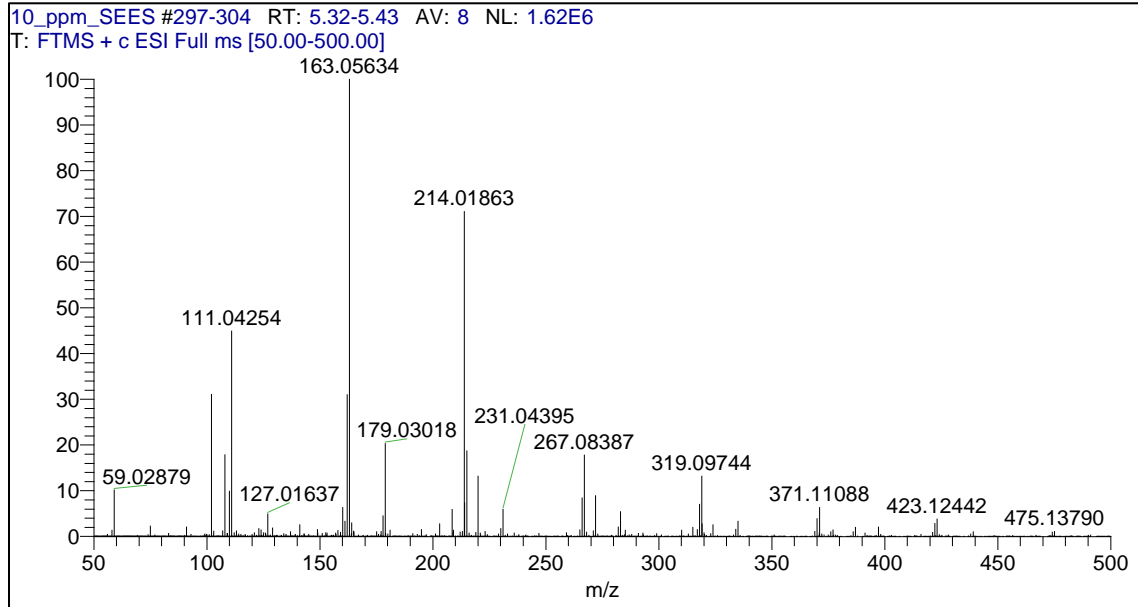


Figure S5: Mass spectrum, full scan from 5.32 min to 5.43 min

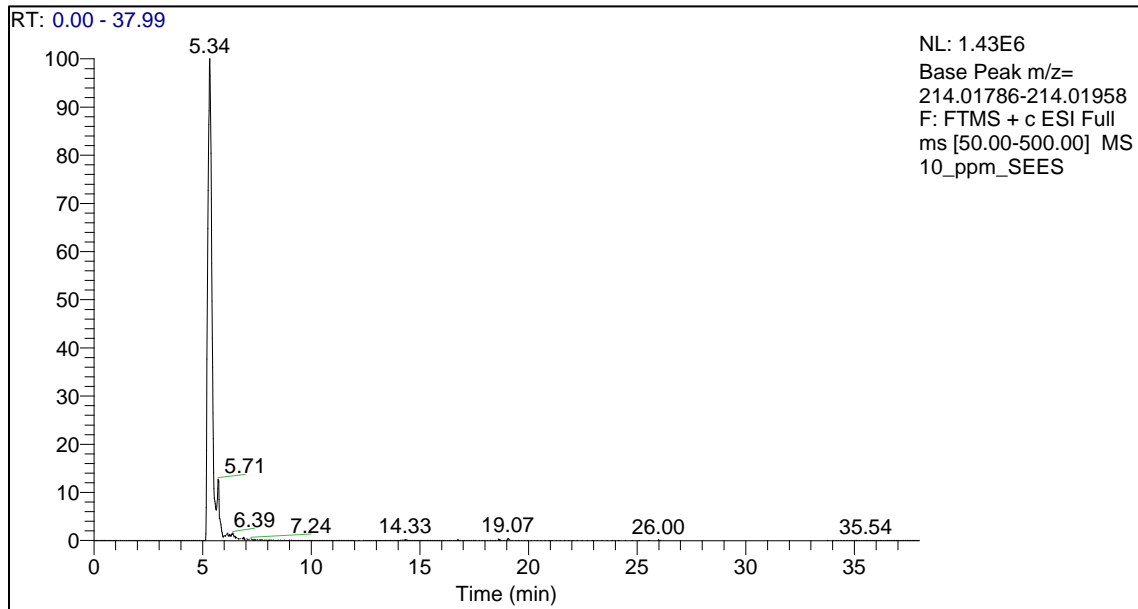


Figure S6: Extracted ion chromatogram for m/z 214

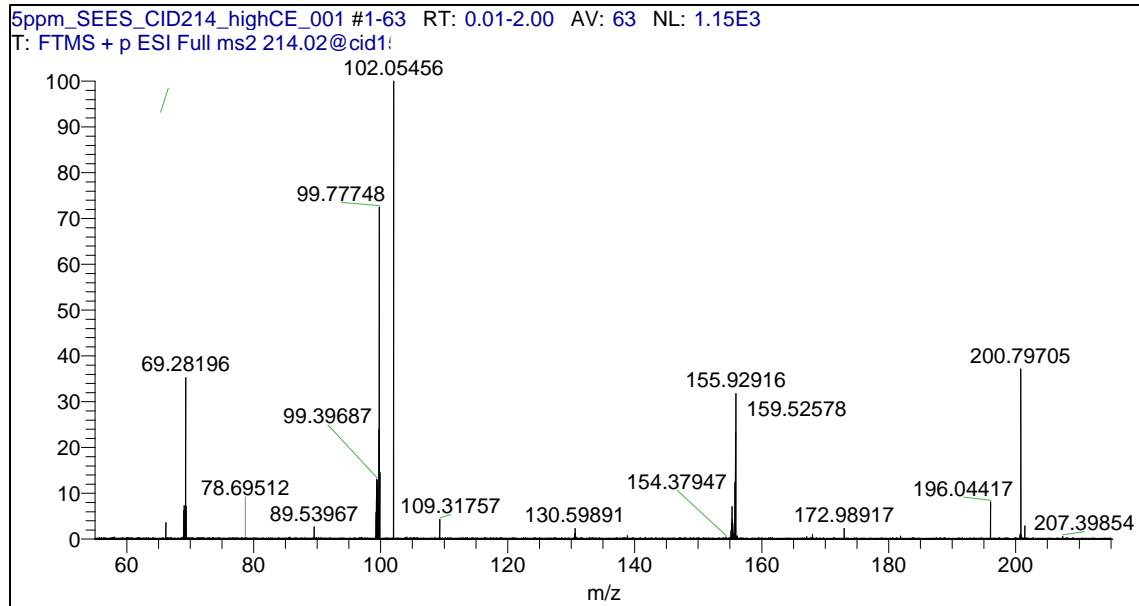


Figure S7: Collision induced dissociation of m/z 214, infusion of SEES-1 for (2 minute scan time)

Peak Identification

Full Scan 214.01863 $C_6H_{14}NO_2^{82}Se^+$ (0.116 ppm)

CID

Impurity: 5.83 min Peak

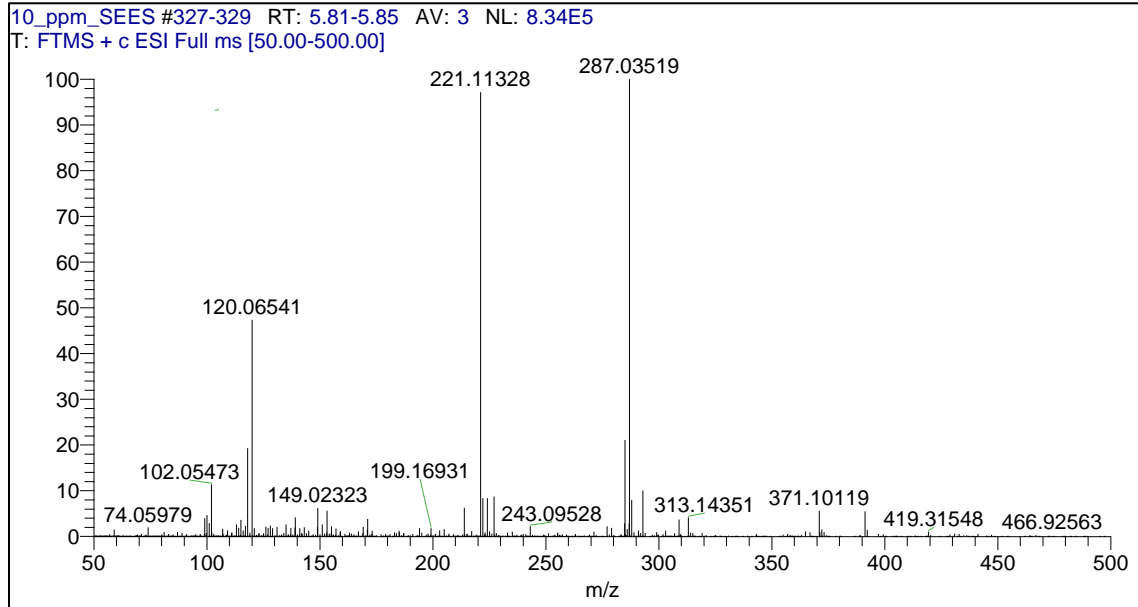


Figure S8: Mass spectrum, full scan from 5.81 min to 5.85 min

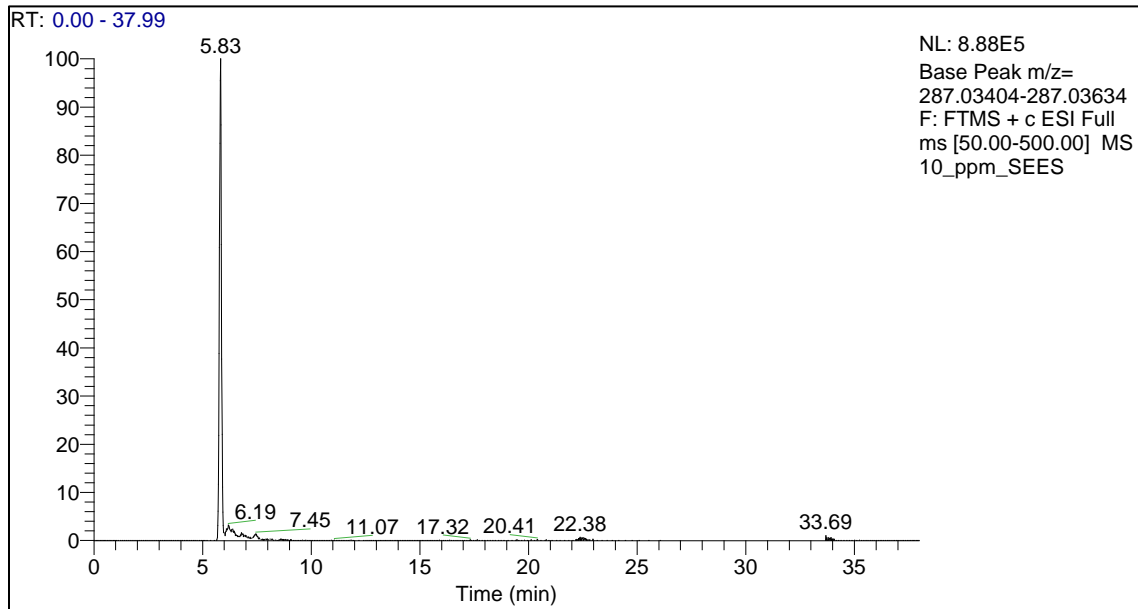


Figure S9: Extracted ion chromatogram for m/z 287

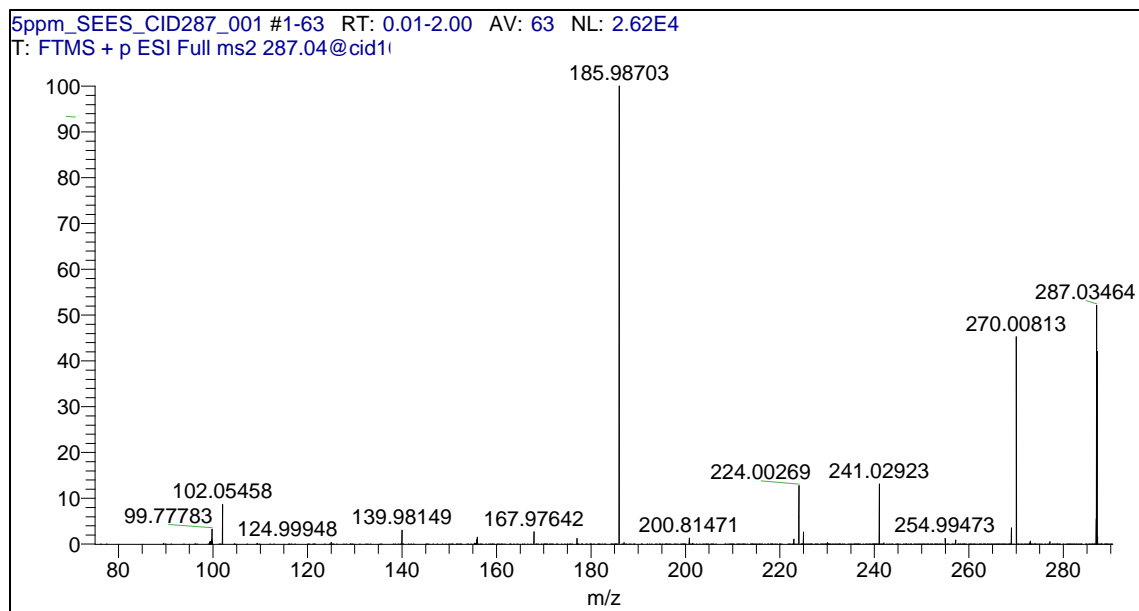


Figure S10: Collision induced dissociation of m/z 287, infusion of SEES-1 for (2 minute scan time)

Peak Identification

Full Scan	287.03519	$C_8H_{17}N_2O_4^{82}Se^+$ (0.719 ppm)
CID	287.03464	$C_8H_{17}N_2O_4^{82}Se^+$ (-1.197 ppm)
	185.98703	$C_4H_{10}NO_2^{82}Se^+$ (-1.479 ppm) (-101 amu, $-C_4H_7NO_2$)

Impurity: 6.89 min Peak

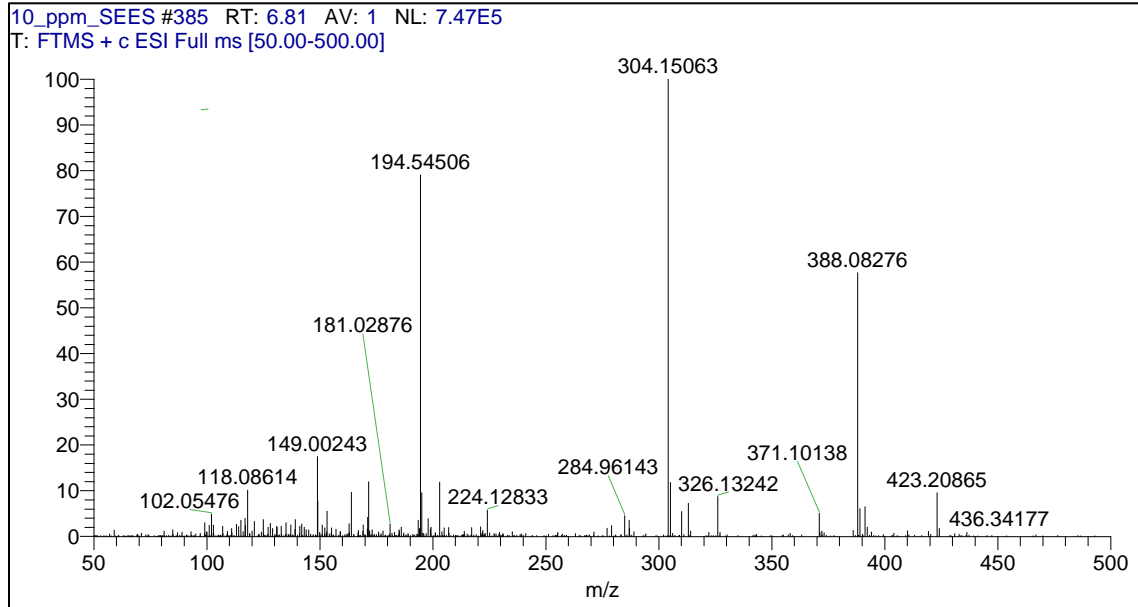


Figure S11: Mass spectrum, full scan at 6.81 min

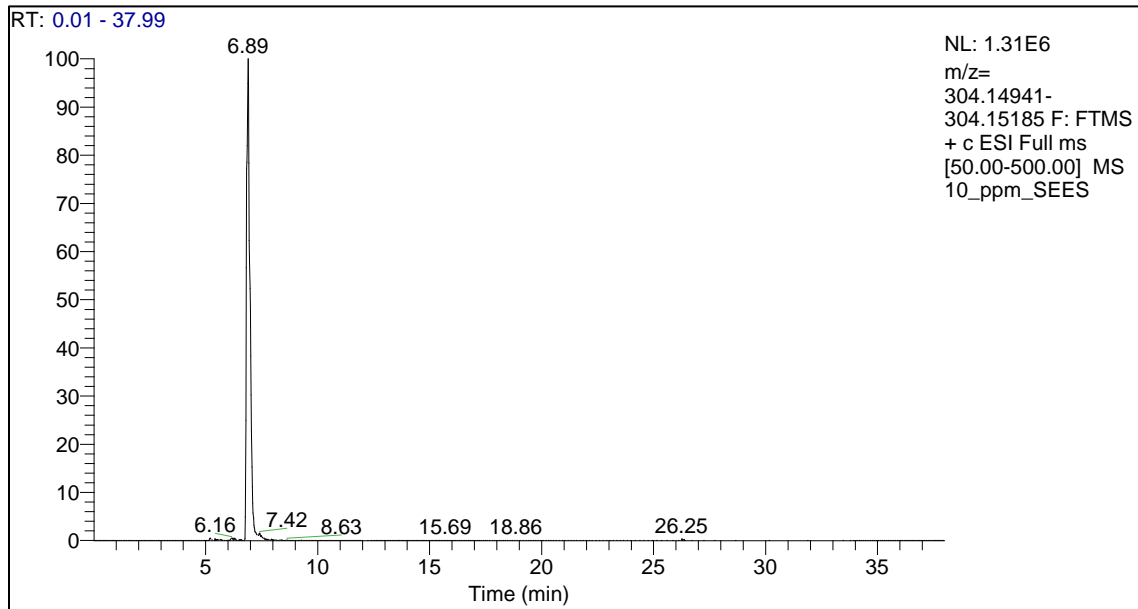


Figure S12: Extracted ion chromatogram for m/z 304

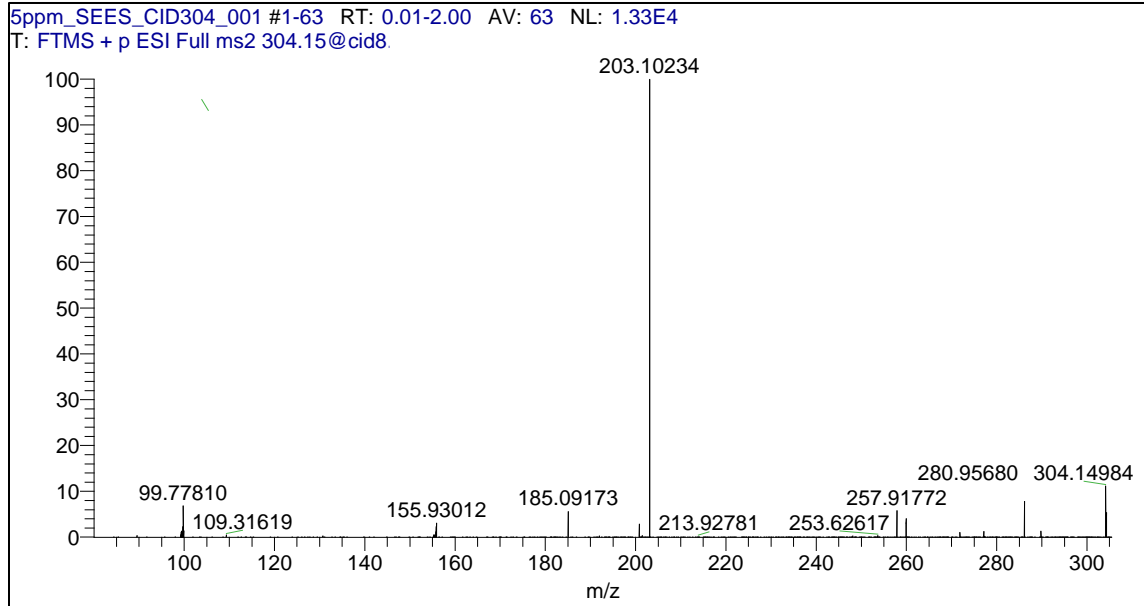


Figure S13: Collision induced dissociation of m/z 304, infusion of SEES-1 for (2 minute scan time)

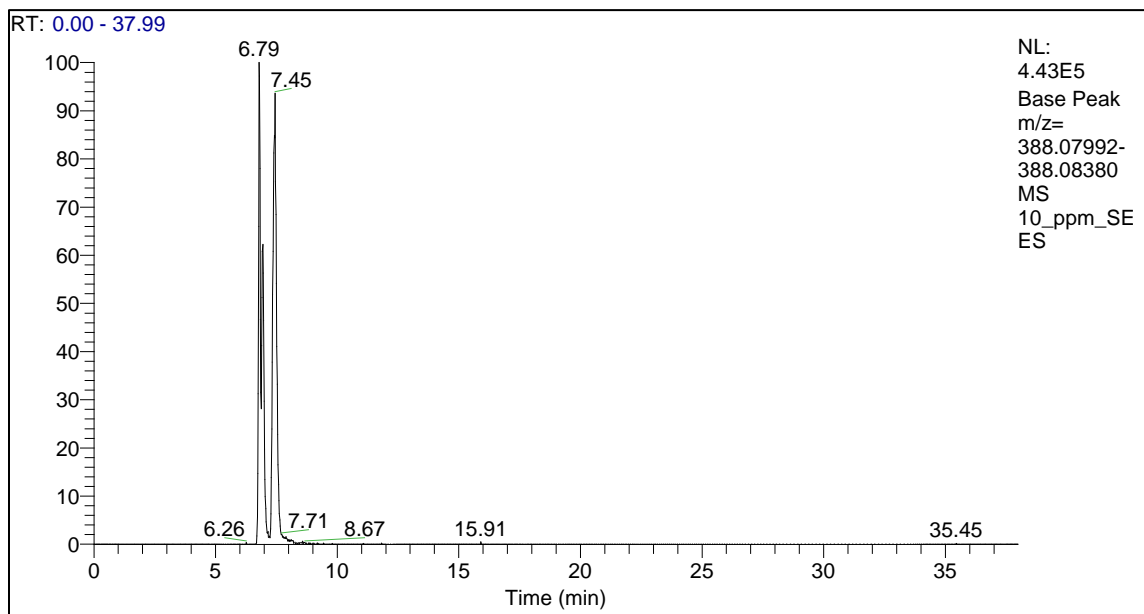


Figure S14: Extracted ion chromatogram for m/z 388

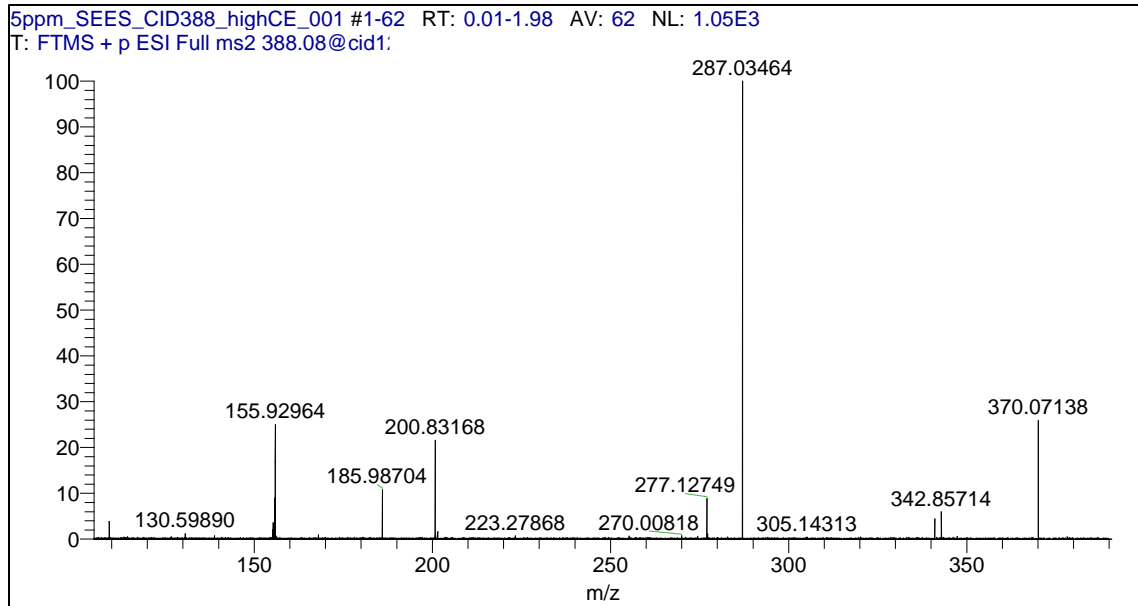


Figure S15: Collision induced dissociation of m/z 388, infusion of SEES-1 for (2 minute scan time)

Peak Identification

Full Scan	388.08276	$C_{12}H_{24}N_3O_6^{82}Se^+$ (0.256 ppm)
	304.15063	$C_{16}H_{30}^{82}Se^+$ (-0.896 ppm)
CID (304)	304.14984	$C_{16}H_{30}^{82}Se^+$ (-3.493 ppm)
	203.10234	$C_9H_{13}^{82}Se^+$ (413 ppm!!) (-101 amu, $-C_7H_{17}$)
CID (388)	388.08186	$C_{12}H_{24}N_3O_6^{82}Se^+$ (-2.066 ppm)
	370.07138	$C_{20}H_{22}N_3O_5^{82}Se^+$ (-1.992 ppm) (-18 amu, $-H_2O$)
	278.03464	$C_8H_{17}N_2O_4^{82}Se^+$ (-1.092 ppm) (-101 amu, $-C_4H_7NO_2$)
	185.98704	$C_4H_{10}NO_2^{82}Se^+$ (-1.425 ppm) (-202 amu, $-C_8H_{14}N_2O_4$)

Impurity: 7.45 min Peak

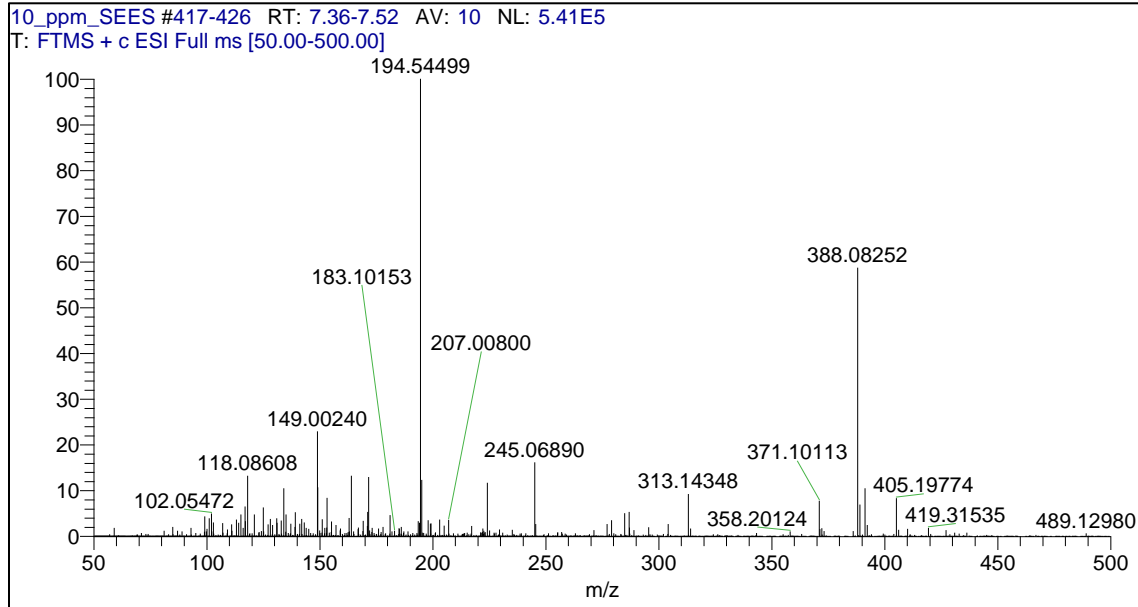


Figure S16: Mass spectrum, full scan from 7.36 min to 7.52 min

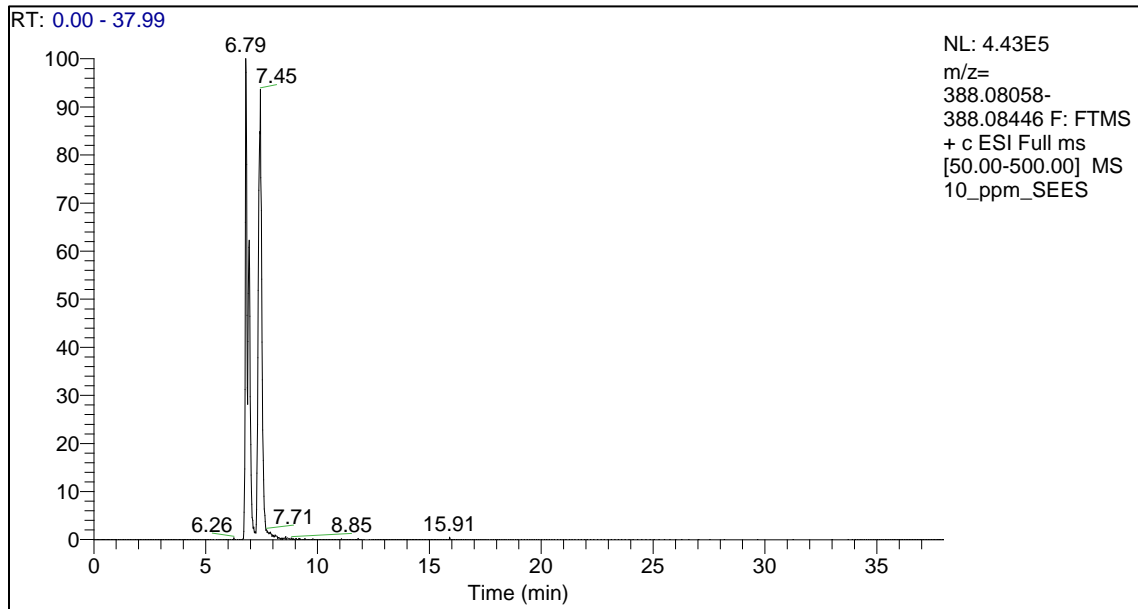


Figure S17: Extracted ion chromatogram for m/z 388

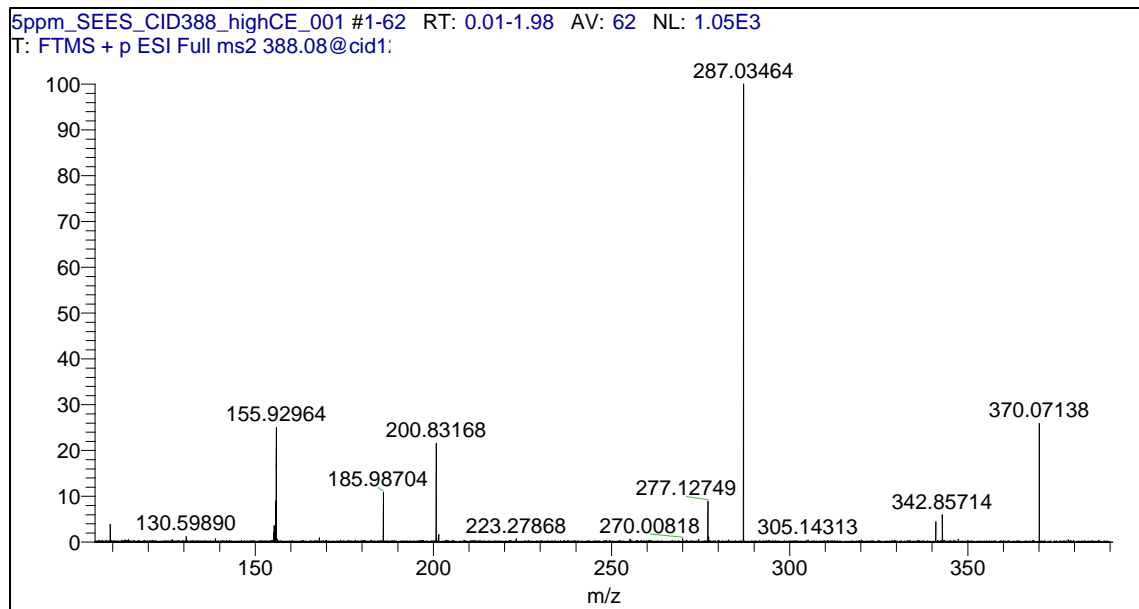


Figure S18: Collision induced dissociation of m/z 388, infusion of SEES-1 for (2 minute scan time)

Peak Identification

Full Scan	194.54500	$C_{12}H_{25}N_3O_6^{82}Se^{2+}$ (0.158 ppm)
	388.08252	$C_{12}H_{24}N_3O_6^{82}Se^+$ (0.256 ppm)
CID (388)	388.08186	$C_{12}H_{24}N_3O_6^{82}Se^+$ (-2.066 ppm)
	370.07138	$C_{20}H_{22}N_3O_5^{82}Se^+$ (-1.992 ppm) (-18 amu, $-H_2O$)
	278.03464	$C_8H_{17}N_2O_4^{82}Se^+$ (-1.092 ppm) (-101 amu, $-C_4H_7NO_2$)
	185.98704	$C_4H_{10}NO_2^{82}Se^+$ (-1.425 ppm) (-202 amu, $-C_8H_{14}N_2O_4$)

Impurities: 17.69 min & 19.02 Min Peaks

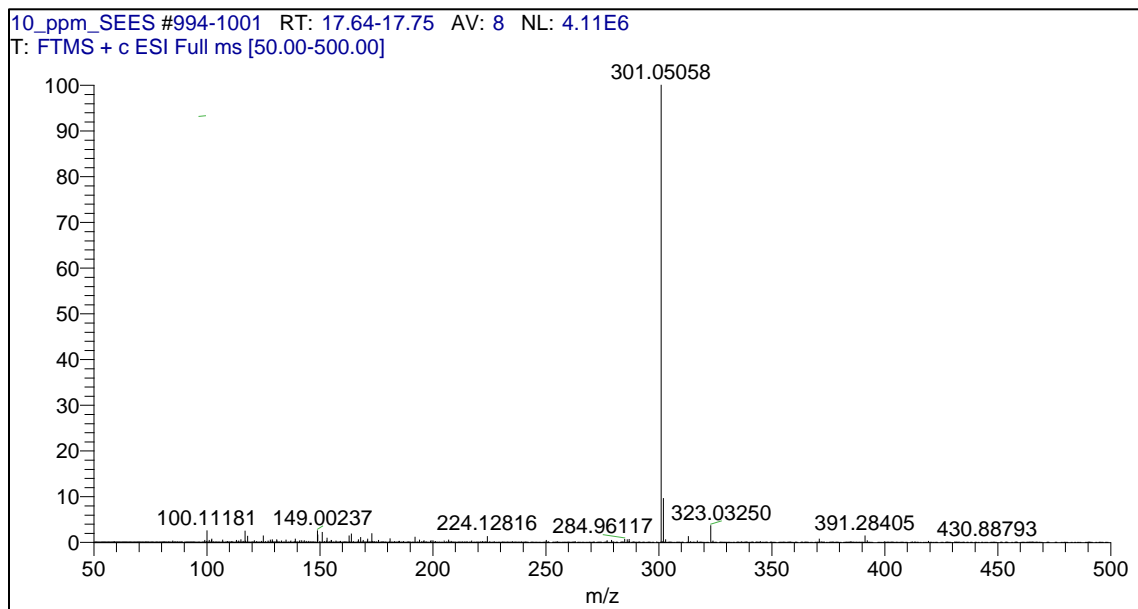


Figure S19: Mass spectrum, full scan from 17.69 min to 17.75 min

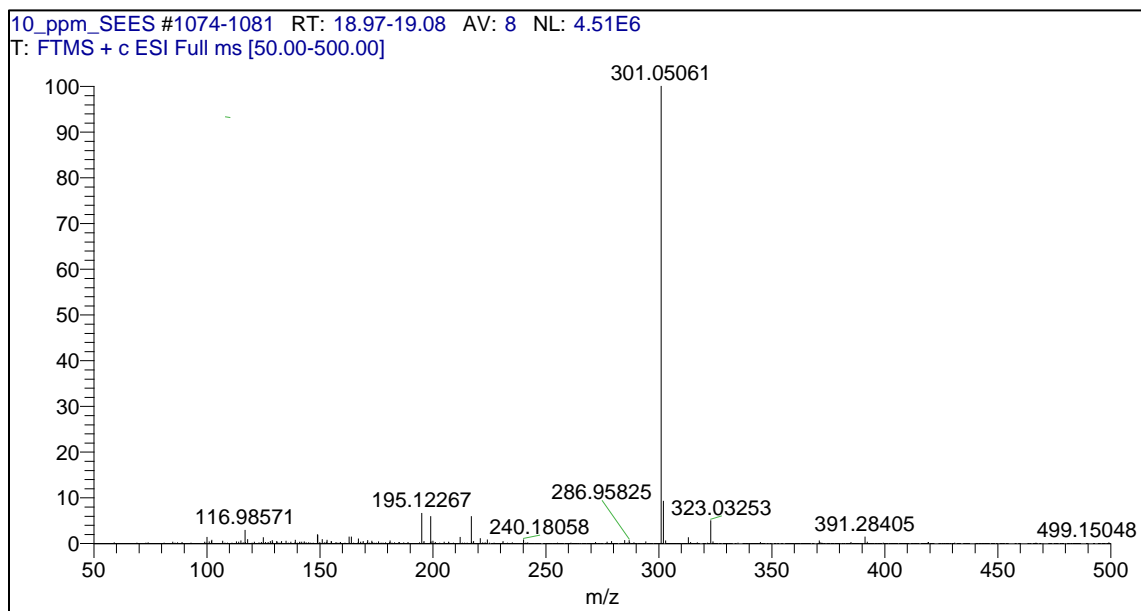


Figure S20: Mass spectrum, full scan from 18.97 min to 19.08 min

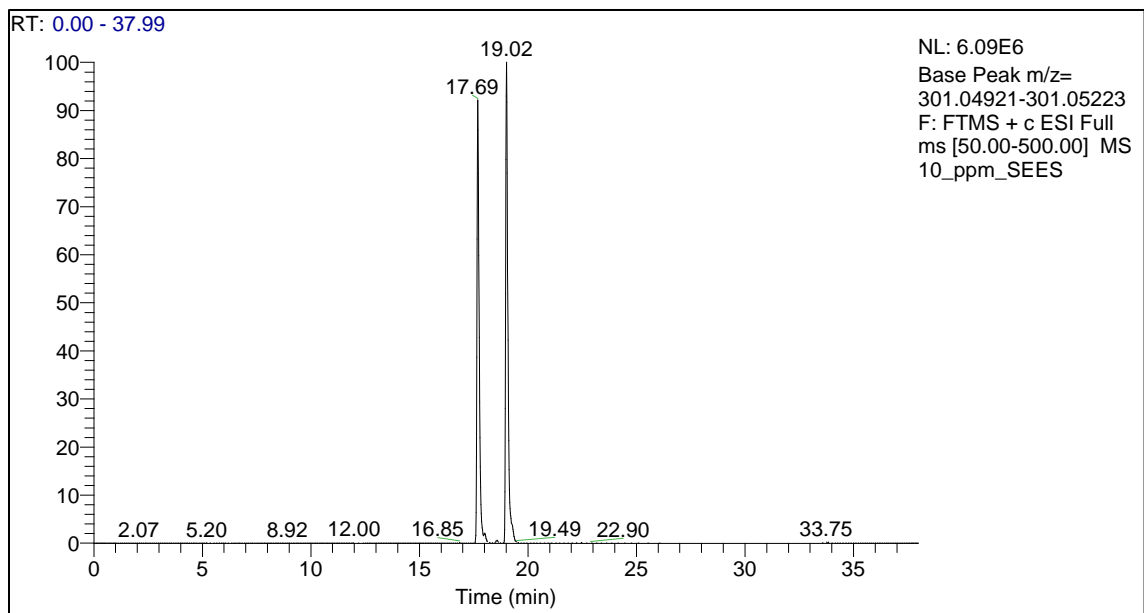


Figure S21: Extracted ion chromatogram for m/z 301

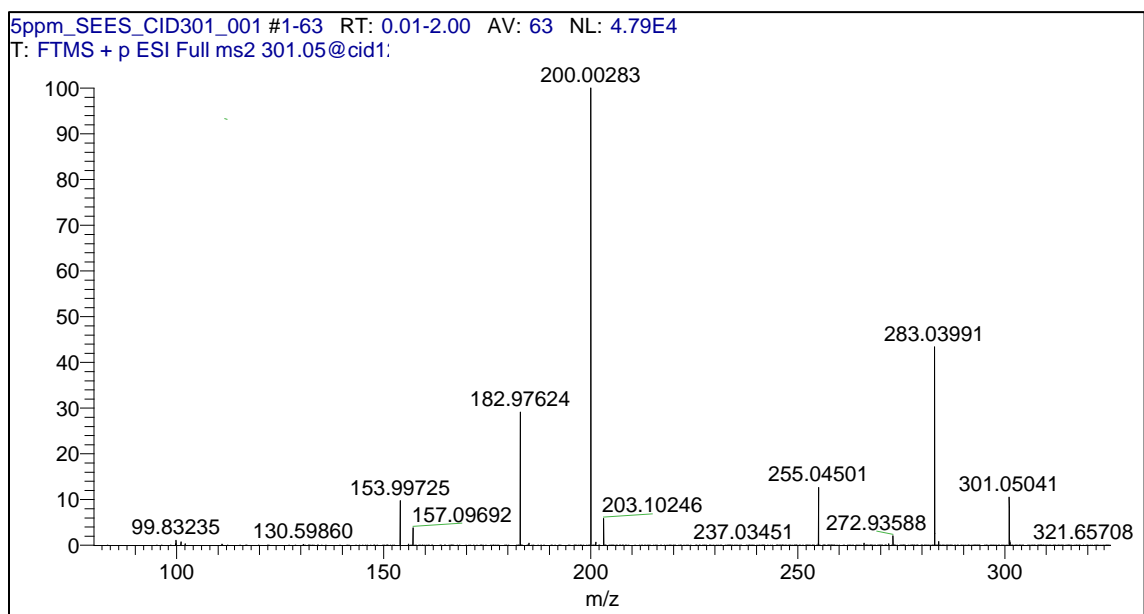


Figure S22: Collision induced dissociation of m/z 301, infusion of SEES-1 for (2 minute scan time)

Peak Identification

Full Scan	301.05058	$C_9H_{19}N_2O_4^{82}Se^+$ (-0.178 ppm, 17.7 min)
	301.05061	$C_9H_{19}N_2O_4^{82}Se^+$ (-0.078 ppm, 19.0 min)
CID	301.05041	$C_9H_{19}N_2O_4^{82}Se^+$ (-0.743 ppm)
	283.03991	$C_9H_{17}N_2O_3^{82}Se^+$ (-0.561 ppm) (-18 amu, $-H_2O$)
	255.04501	$C_8H_{17}O_2N_2^{82}Se^+$ (-0.566 ppm) (-46 amu, $-CH_2O_2$)
	200.00283	$C_5H_{12}NO_2^{82}Se^+$ (-0.626 ppm) (-101 amu, $-C_4H_7NO_2$)
	182.97624	$C_5H_9O_2^{82}Se^+$ (-0.908 ppm) (-118 amu, $-C_4H_{10}NO_2$)