

New Precursors to 3-Sulfanylhexasan-1-ol? Investigating the Keto-Enol Tautomerism of 3-S-Glutathionylhexanal

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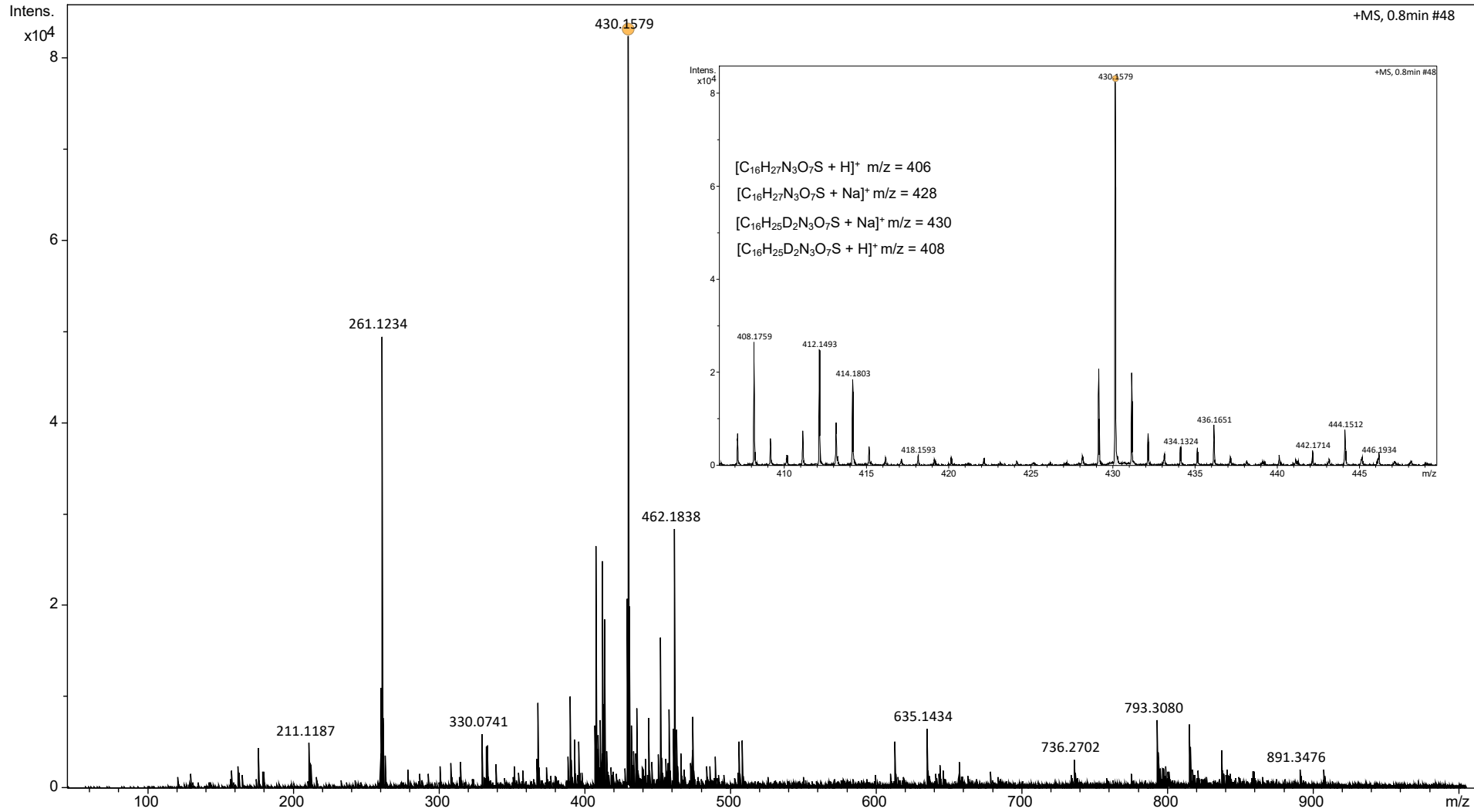
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Supporting Information

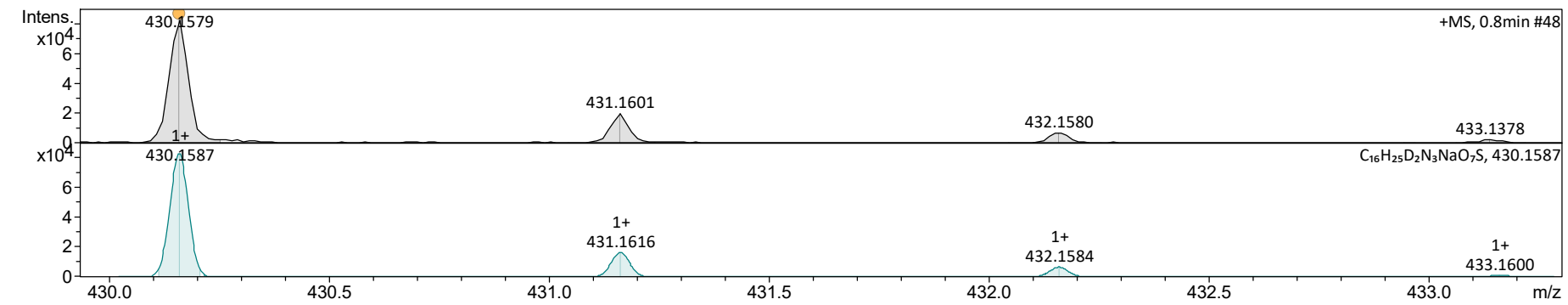
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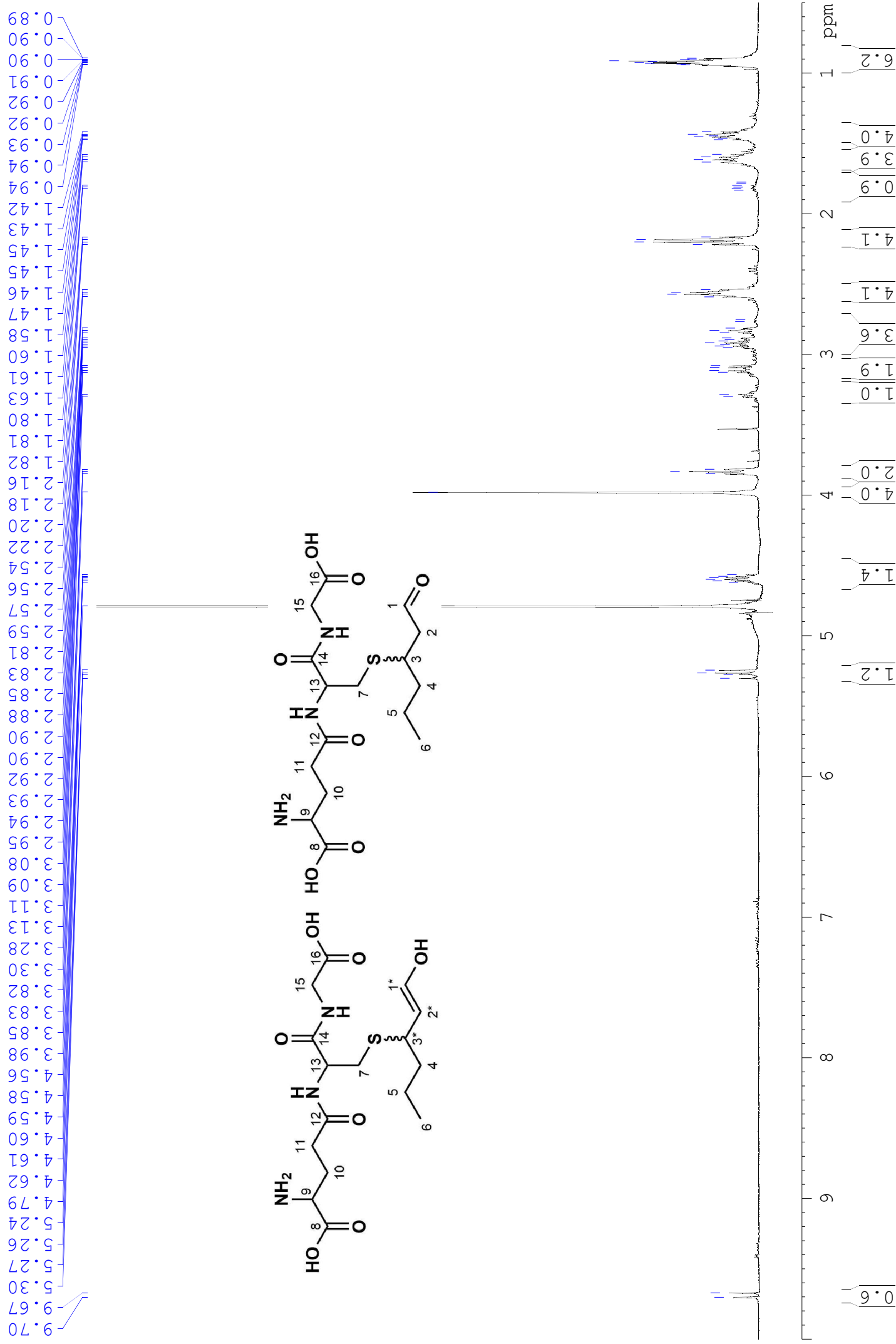
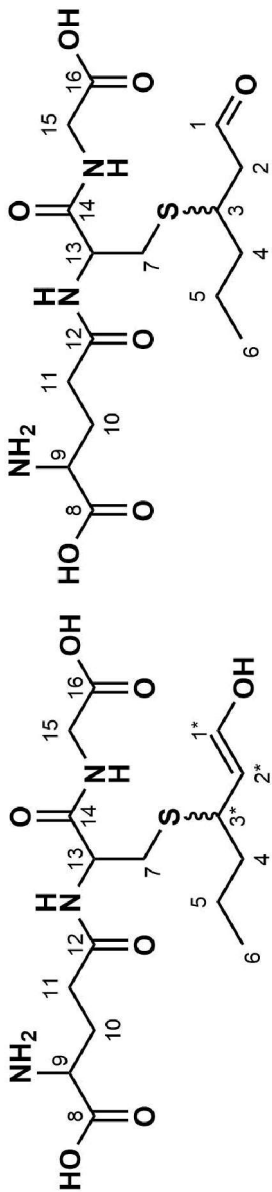
1. HRMS Spectra of Glut-3SH-al-*d*₂
2. ¹H NMR of Glut-3SH-al
3. ¹³C NMR of Glut-3SH-al



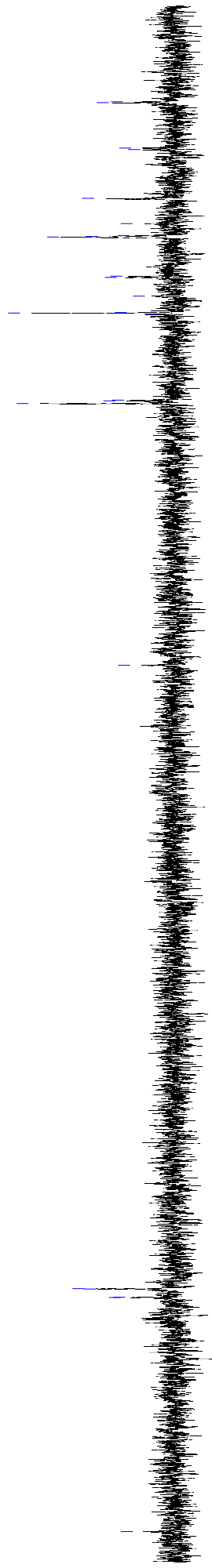
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar	Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C	430.1579	1	C ₁₆ H ₂₅ D ₂ N ₃ NaO ₇ S	430.1587	-2.1	23.7	1	100.00	4.5	even	ok
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min											
Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste											





200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



206.4
174.8
174.7
173.6
173.6
89.2
41.8
41.5
41.5
39.3
36.7
36.6
31.3
31.2
31.1
29.4
26.0
19.4
19.2
13.1
13.0