

Mass Spectrum SmartFormula Report

Analysis Info

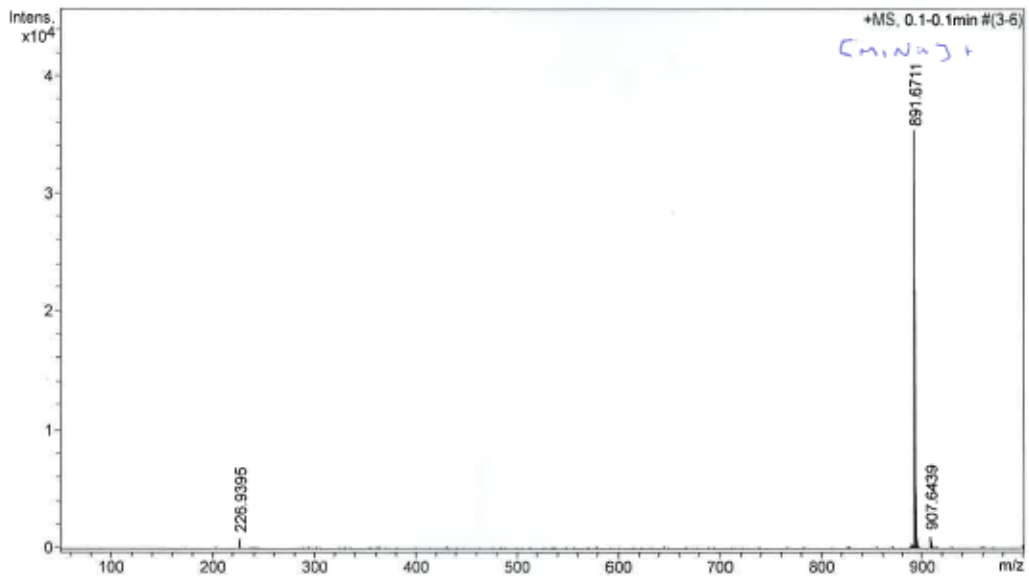
Analysis Name D:\Data\Mass Spectrometry Service\70127-000001.d
Method LM MS 50 to 1100.m
Sample Name Caldwell-SC-5-2
Comment

Acquisition Date 8/23/2018 9:53:42 AM

Operator user
Instrument / Ser# micrOTOF-Q 74

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive
Scan Begin	50 m/z		
Scan End	1100 m/z		



Formula	z	m/z	Meas. m/z	err [ppm]	err [mDa]
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Mass Spectrum SmartFormula Report

Analysis Info

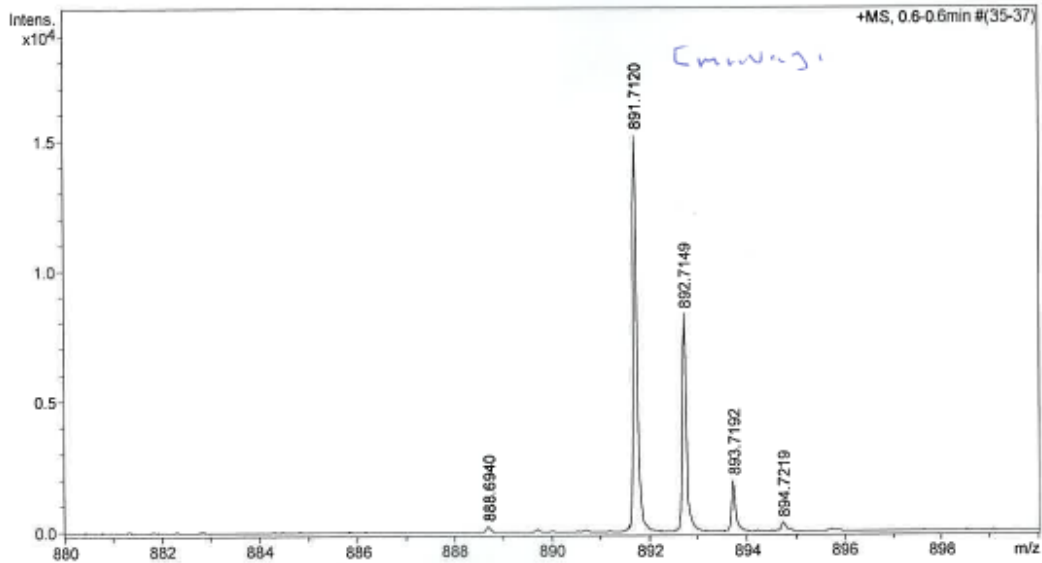
Analysis Name D:\Data\Mass Spectrometry Service\70127-000002.d
Method LM MS 50 to 1100.m
Sample Name Caldwell-SC-5-2
Comment

Acquisition Date 8/23/2018 9:53:49 AM

Operator user
Instrument / Ser# micrOTOF-Q 74

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive
Scan Begin	50 m/z		
Scan End	1100 m/z		



Formula	z	m/z	Meas. m/z	err [ppm]	err [mDa]
C ₅₉ H ₈₄ D ₆ NaO ₄	1+	891.7108	891.7120	-1.3	-1.2