

# Mass Spectrum SmartFormula Report

## Analysis Info

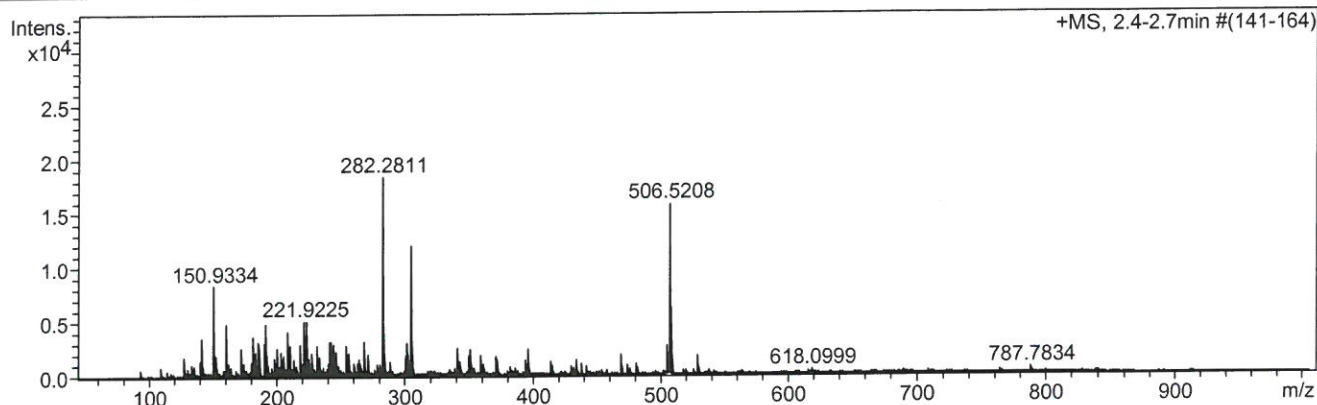
Analysis Name E:\Data2\Kilian\KC-3-Tolbusethyn000001.d  
 Method Tune\_low\_pos.m  
 Sample Name Tolbusethyn  
 Comment

Acquisition Date 2016-05-10 18:45:26

Operator Carin Larsson  
 Instrument / Ser# micrOTOF 125

## Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSig ma	rdb	e <sup>-</sup> Conf	N-Rul e
205.0346	1	C 11 H 16 Na S	0.00	203.0865	-1948.1	-9501.3	435.3	3.5	even	ok
	2	C 7 H 16 Na O 3 S	100.00	203.0712	-1963.4	-9575.7	523.3	-0.5	even	ok
	3	C 6 H 16 N 2 Na O 2 S	0.00	203.0825	-1952.1	-9521.0	525.4	-0.5	even	ok
	4	C 12 H 16 N S	0.00	206.0998	1065.2	5195.2	586.1	5.5	even	ok
	5	C 10 H 16 Na O S	0.00	207.0814	2046.8	9982.8	654.6	2.5	even	ok
	6	C 9 H 16 N 2 Na S	0.00	207.0926	2058.0	10037.6	655.8	2.5	even	ok
	7	C 7 H 16 N 3 O 2 S	0.00	206.0958	1061.2	5175.6	694.7	1.5	even	ok
	8	C 6 H 16 N 5 O S	0.00	206.1070	1072.4	5230.4	697.6	1.5	even	ok
227.0864	9	C 8 H 16 N O 3 S	0.00	206.0845	1049.9	5120.8	781.0	1.5	even	ok
	1	C 8 H 16 N 2 Na O 2 S	12.55	227.0825	-3.9	-17.1	57.0	1.5	even	ok
	2	C 9 H 16 Na O 3 S	0.00	227.0712	-15.1	-66.6	59.8	1.5	even	ok
	3	C 6 H 16 N 6 Na S	0.00	227.1049	18.6	81.8	61.3	1.5	even	ok
	4	C 7 H 16 N 4 Na O S	0.05	227.0937	7.4	32.4	63.0	1.5	even	ok
	5	C 13 H 16 Na S	100.00	227.0865	0.1	0.6	79.4	5.5	even	ok
	6	C 11 H 16 N O 2 S	0.00	226.0896	-996.7	-4389.2	663.1	4.5	even	ok
	7	C 10 H 16 N 3 O S	0.00	226.1009	-985.5	-4339.7	664.2	4.5	even	ok
	8	C 9 H 16 N 5 S	0.00	226.1121	-974.3	-4290.3	665.3	4.5	even	ok
	9	C 7 H 16 N O 5 S	0.00	226.0744	-1012.0	-4456.4	782.3	0.5	even	ok
	10	C 6 H 16 N 3 O 4 S	0.00	226.0856	-1000.7	-4406.9	783.6	0.5	even	ok

