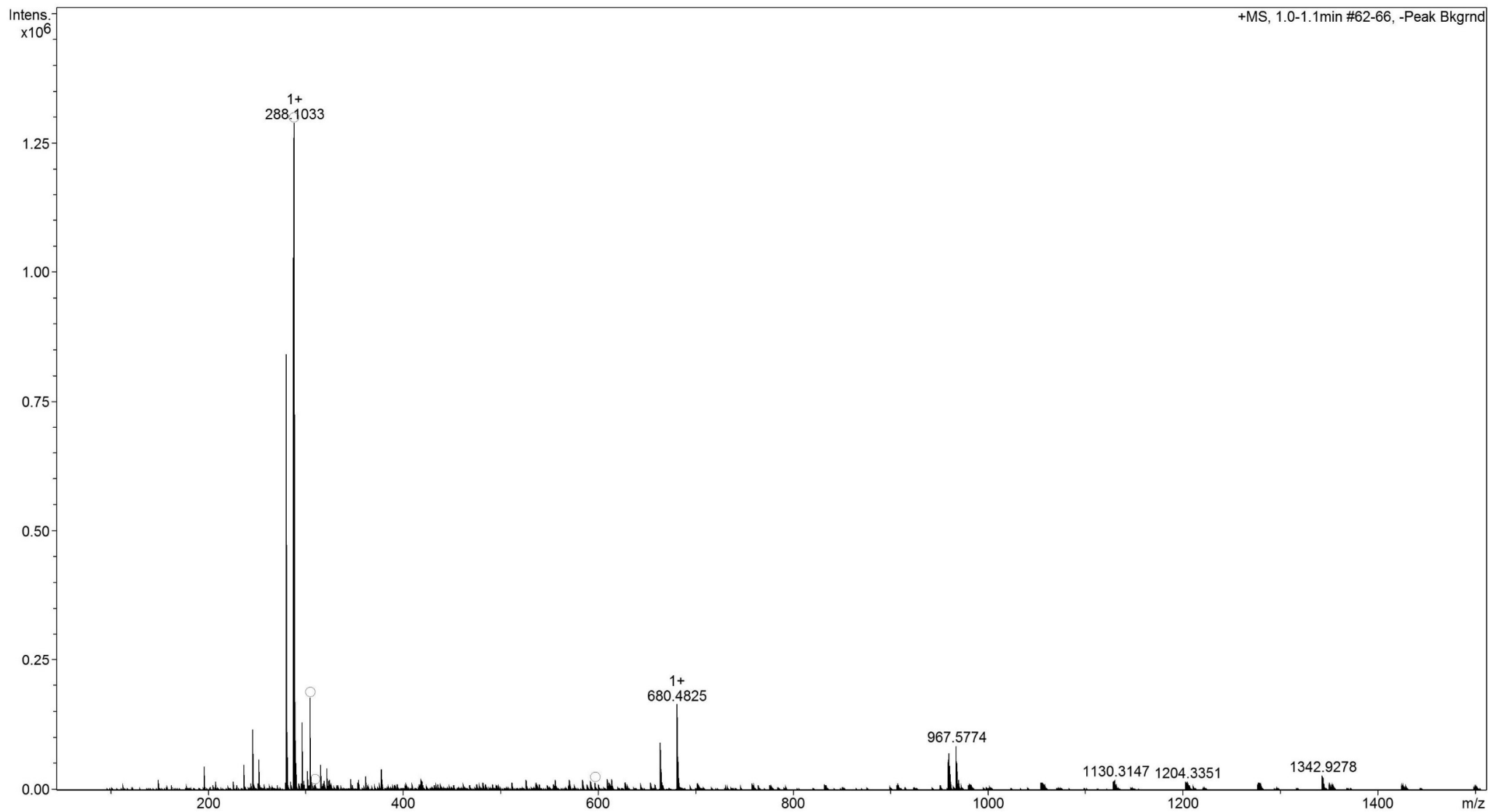
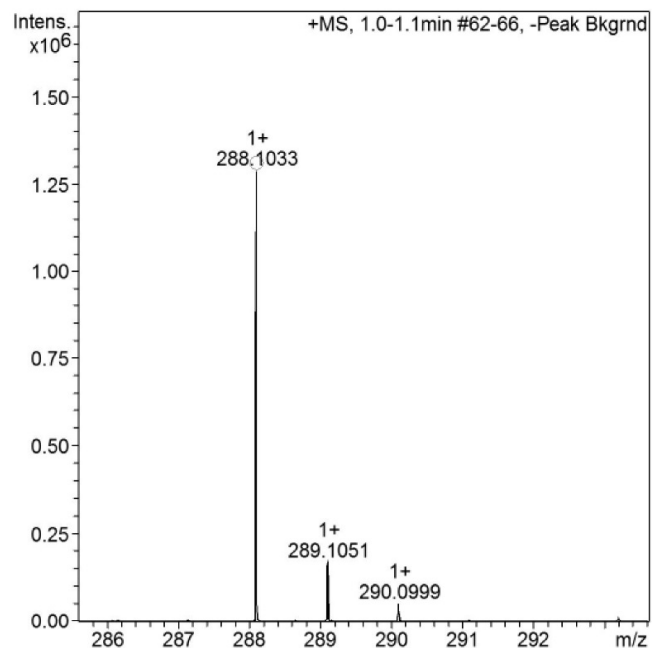


Cmpd 3, 1.1 min





## Confirm/Find Formula Results

The section below shows the results of formula calculation. If an expected formula was provided and found these are the results that are listed. If no formula was provided or no matches were found the system has attempted to determine the formula constrained by the parameters listed to the left

### Cmpd 3, 1.1 min

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
288.103285	C12H14N7S	1+	288.102591	0.7	2.4	19.3	100.00	C12 H13 N7 S	M+H
305.129304	C12H17N8S	1+	305.129140	-0.2	-0.5	13.7	100.00		M+NH4
310.084363	C12H13N7NaS	1+	310.084535	-0.2	-0.6	29.8	100.00		M+Na
597.180480	C24H26N14NaS2	1+	597.179850	-0.6	-1.1	27.3	100.00		2M+Na

Smart Formula Parameter	Value
Expected Formula	C12H13N7S
Adducts Considered	;M+H;;M+NH4;;M+Na;;M+K;;M+Na 2-H;;2M+H;;2M+Na;

Smart Formula Search Parameters  
CHNO and adducts considered  
implicitly

Formula Search Minimum	
Formula Search Maximum	S 2

Algorithm Parameters	
Tolerance	4 ppm
Match to Isotope Pattern(mSigma)	40
Electron Configuration	even
Estimate No of Carbons	yes
Filter by H/C Ratio	0 < H/C < 3
Number of Double Bonds & Rings	0 < rings&DB < 80