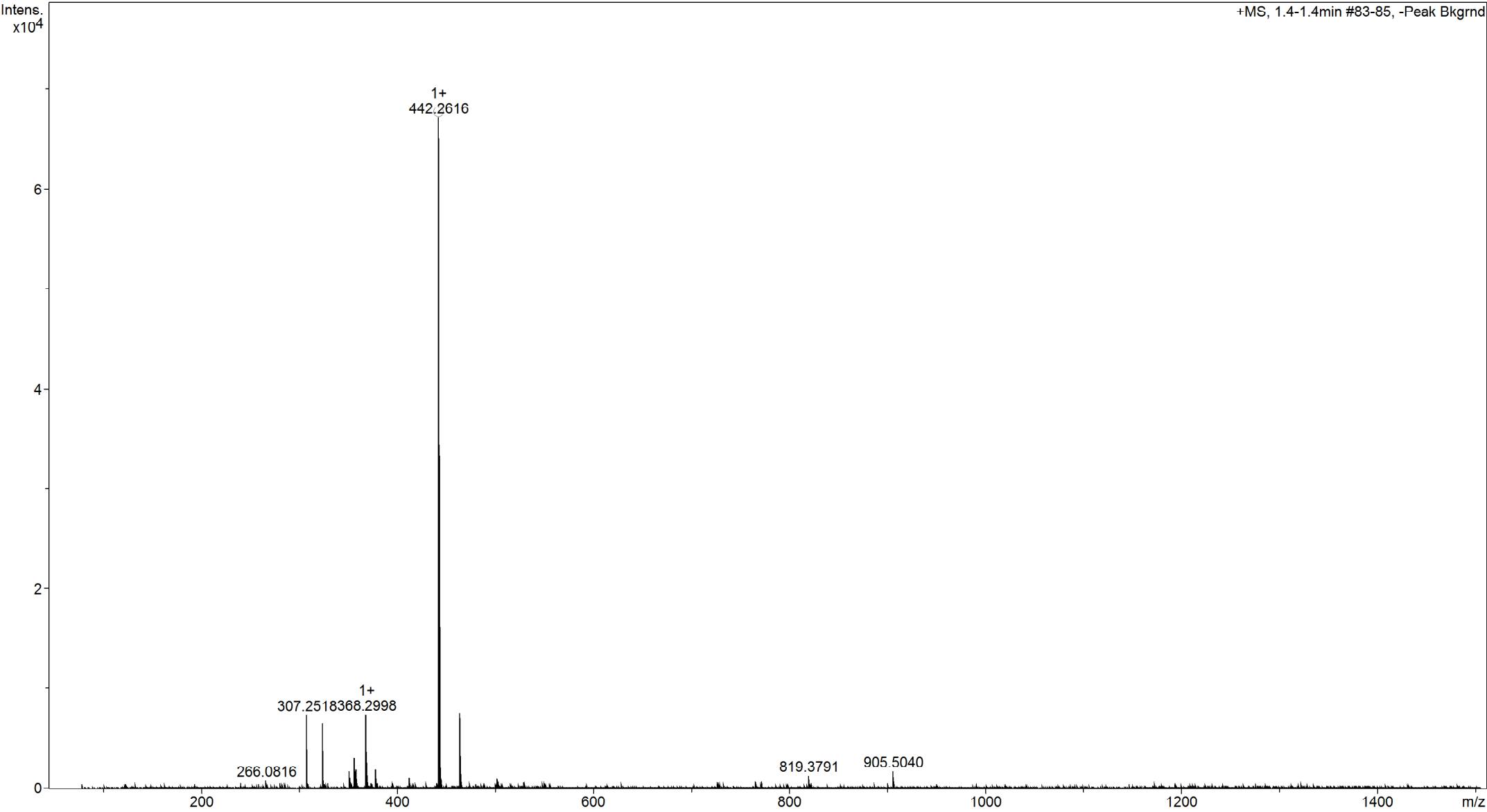
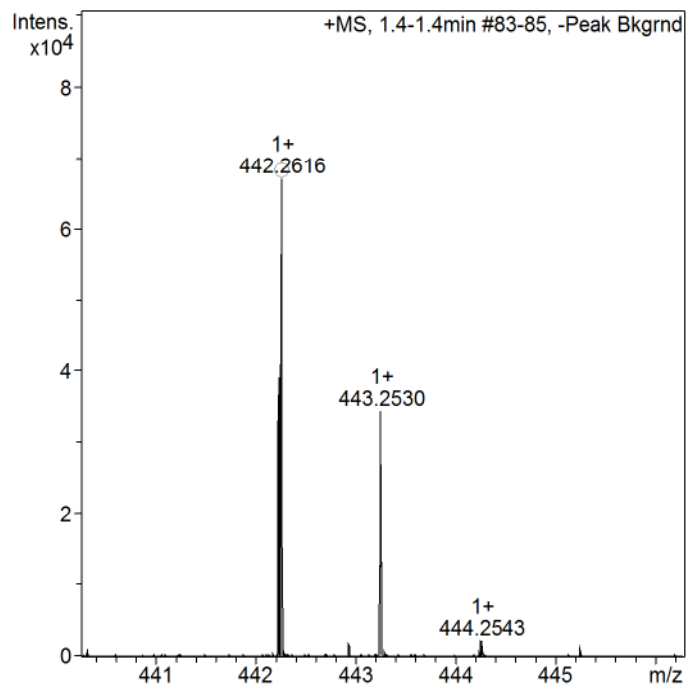


Cmpd 4, 1.4 min





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 4, 1.4 min

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
442.261608	C15H36N7O8	1+	442.261988	0.4	0.9	n.a.	-1.#J	C15 H35 N7 O8	M+H
	C12H28N17O2	1+	442.260640	-1.0	-2.2	n.a.	-1.#J	C12 H27 N17 O2	M+H
	C27H32N5O	1+	442.260137	-1.5	-3.3	n.a.	-1.#J	C27 H31 N5 O	M+H
	C16H32N11O4	1+	442.263325	-1.7	-3.9	n.a.	-1.#J	C16 H31 N11 O4	M+H
	C15H36N7O8	1+	442.261988	0.4	0.9	n.a.	-1.#J	C15 H32 N6 O8	M+NH4
	C12H28N17O2	1+	442.260640	-1.0	-2.2	n.a.	-1.#J	C12 H24 N16 O2	M+NH4
	C27H32N5O	1+	442.260137	-1.5	-3.3	n.a.	-1.#J	C27 H28 N4 O	M+NH4
	C16H32N11O4	1+	442.263325	-1.7	-3.9	n.a.	-1.#J	C16 H28 N10 O4	M+NH4
	C15H29N15Na	1+	442.262257	0.6	1.5	n.a.	-1.#J	C15 H29 N15	M+Na
	C14H33N11NaO4	1+	442.260919	0.7	1.6	n.a.	-1.#J	C14 H33 N11 O4	M+Na
	C27H37KN3	1+	442.261906	-0.3	-0.7	n.a.	-1.#J	C27 H37 N3	M+K
	C12H33KN15O	1+	442.262409	-0.8	-1.8	n.a.	-1.#J	C12 H33 N15 O	M+K
	C17H34N9Na2O2	1+	442.262536	-0.9	-2.1	n.a.	-1.#J	C17 H35 N9 O2	M+Na2-H
	C13H30N15Na2	1+	442.259851	-1.8	-4.0	n.a.	-1.#J	C13 H31 N15	M+Na2-H

Smart Formula Parameter	Value
Expected Formula	C24H27N9
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

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