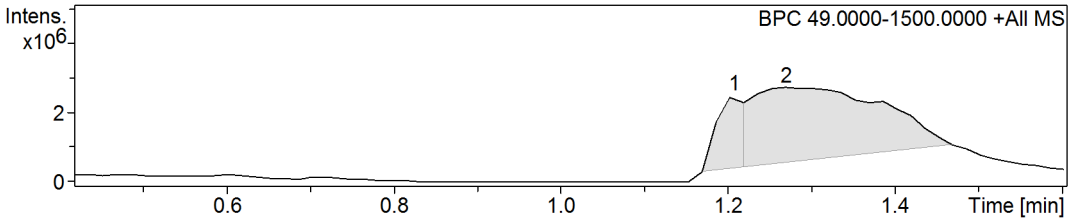
School of Chemistry Mass Spectrometry Service

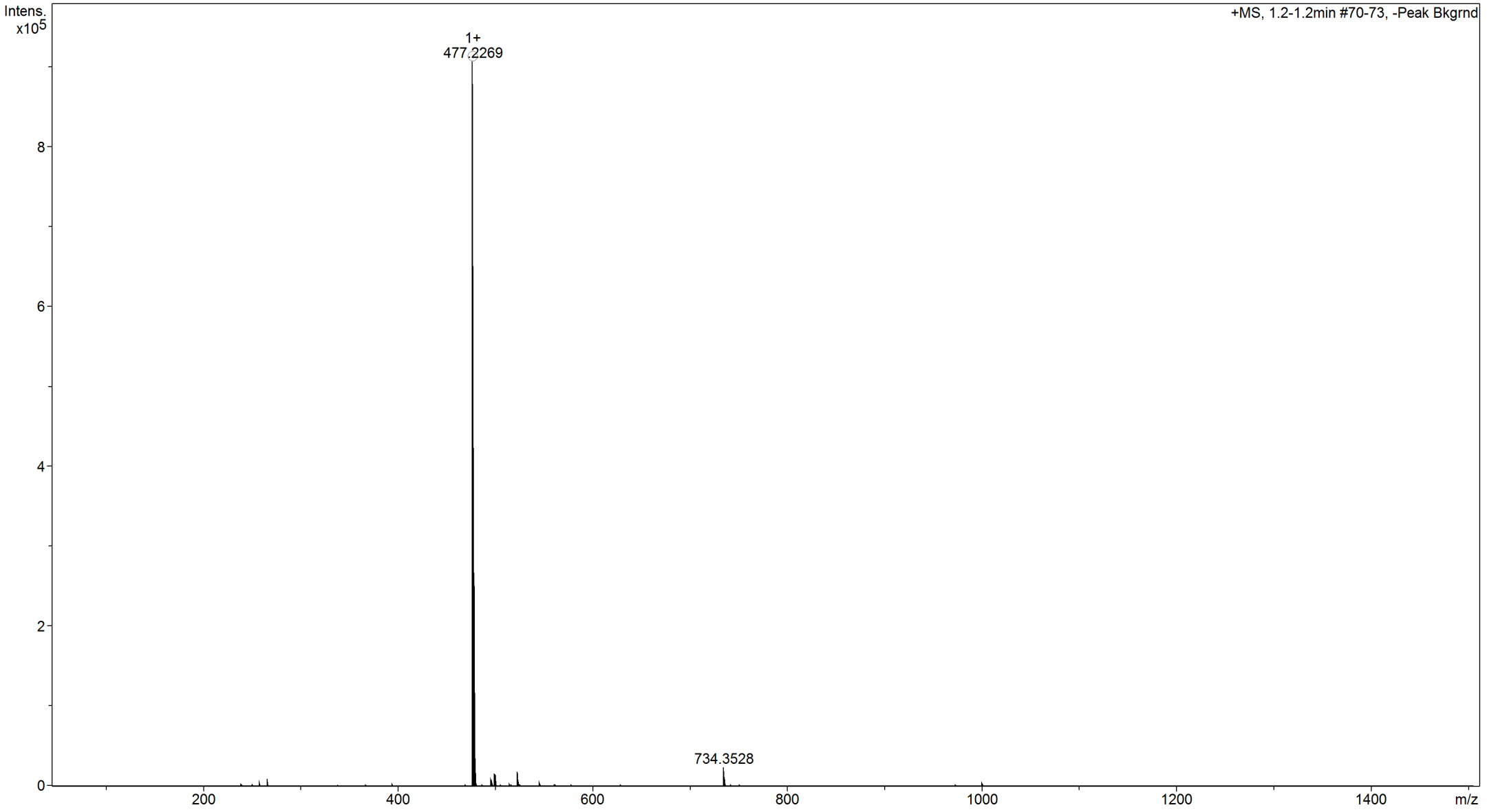
SampleID	ER ligand 1				**Submitter**	Emily Ratcliffe	
Sample Description							
Analysis Name	D:\Data\malcolmhalcrow\cm15esjr\ER ligand 1_259914_RA3_01_53587.d				**Supervisor**	Malcolm Halcrow	
Method	3a_AccMass_Loop_Positive.m				**Acquisition Date**	05/02/2019 11:05:33	
Instrument	maXis impact	**Source Type**	ESI	**Ion Polarity**	Positive	**Scan Begin**	50 m/z	**Scan End**	1500 m/z

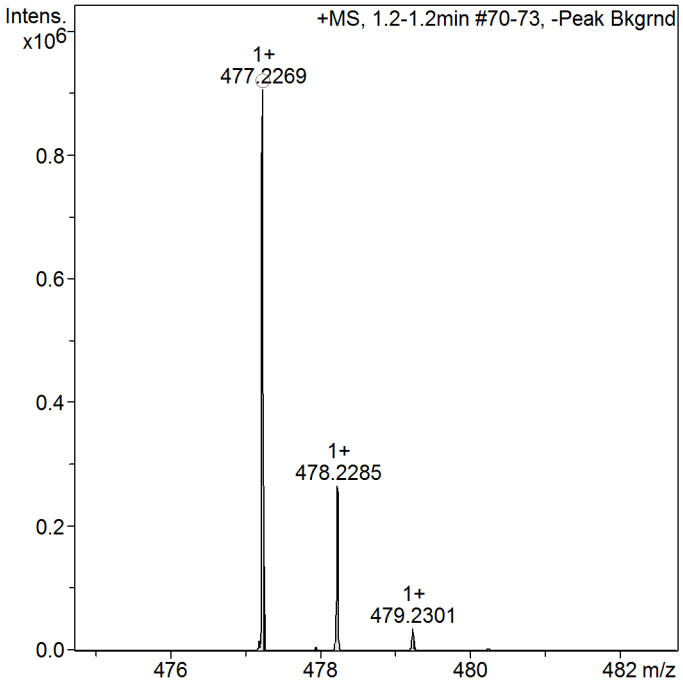


Summary of Results

Name	RT	BPC Area(%)	UV Area(%)	Confirm Formula Results
Cmpd 1, 1.2 min	1.21	16.1	no uv	
Cmpd 2, 1.3 min	1.27	83.9	no uv	

Cmpd 1, 1.2 min


Intens.
x10^5
+MS, 1.2-1.2min #70-73, -Peak Bkgrnd
1+
477.2269
734.3528
8
6
4
2
0
200
400
600
800
1000
1200
1400
m/z



Smart Formula Parameter	Value
Expected Formula	
Adducts Considered	
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

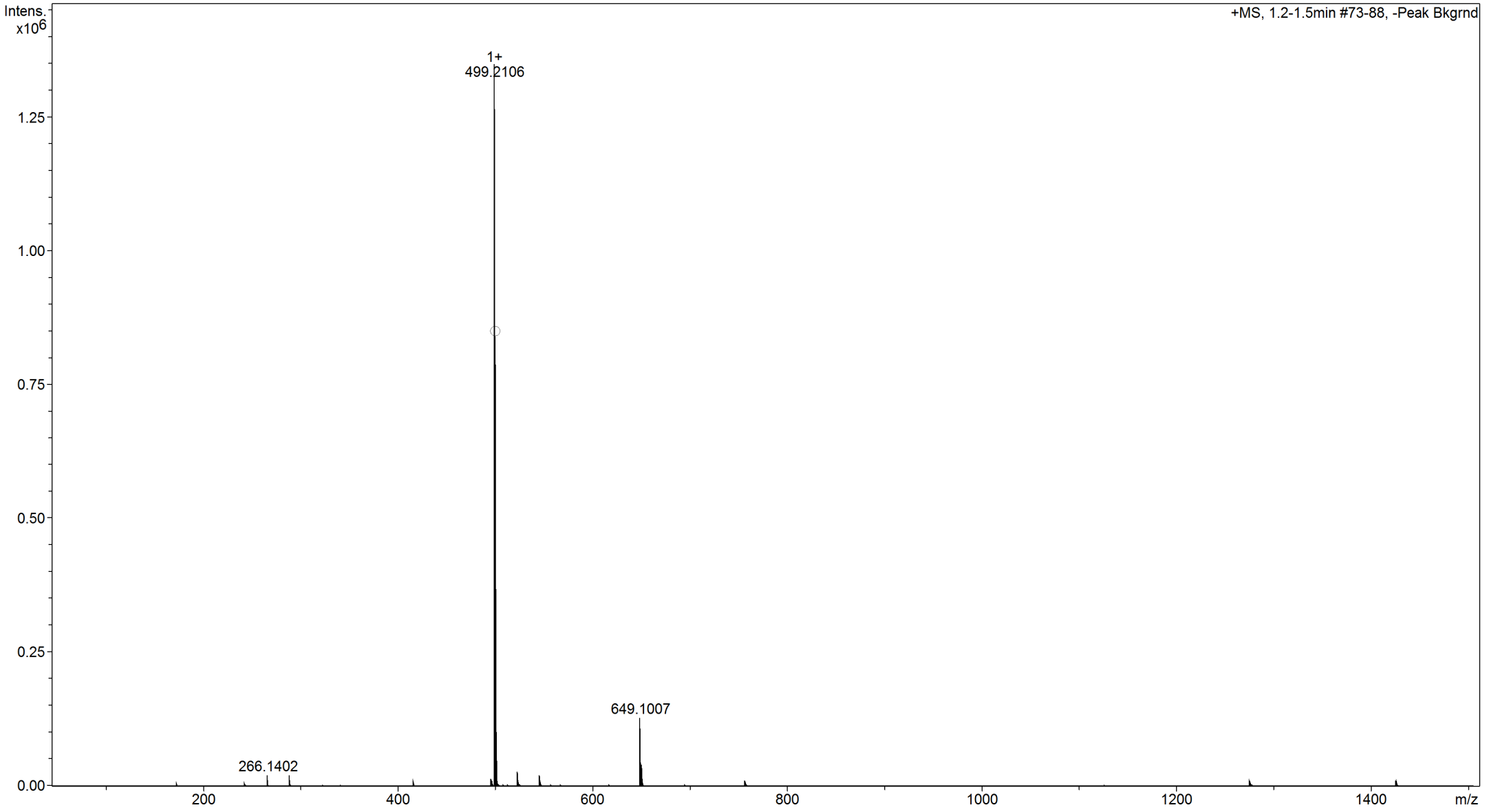
Confirm/Find Formula Results

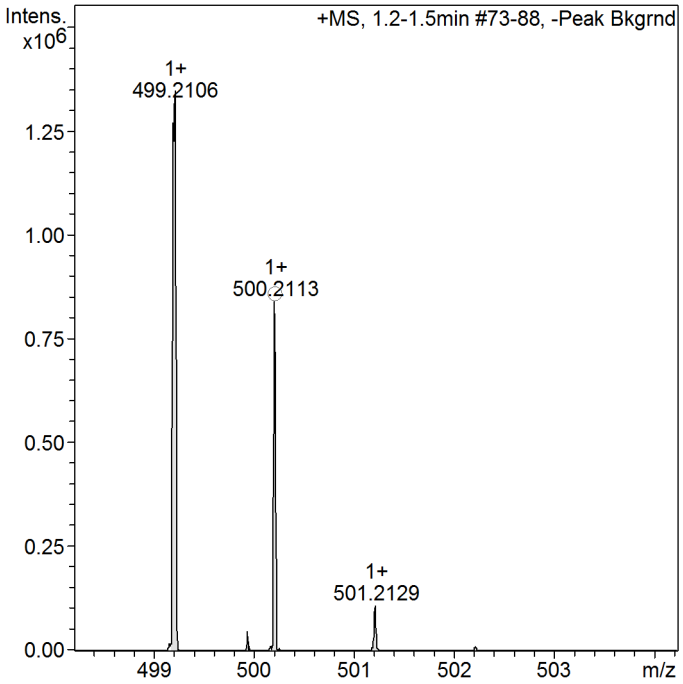
The section below shows the results of formula calculation. If an expected formula was provided and found these are the results that are listed. If no formula was provided or no matches were found the system has attempted to determine the formula constrained by the parameters listed to the left

Cmpd 1, 1.2 min

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
477.226926	C26H25N10	1+	477.225817	-1.1	-2.3	15.7	48.85	C26H24N10	M+H
	C29H33O6	1+	477.227165	0.2	0.5	16.6	100.00	C29H32O6	M+H
	C30H29N4O2	1+	477.228503	1.6	3.3	26.3	38.49	C30H28N4O2	M+H
	C26H25N10	1+	477.225817	-1.1	-2.3	15.7	48.85	C26H21N9	M+NH4
	C30H29N4O2	1+	477.228503	1.6	3.3	26.3	38.49	C30H25N3O2	M+NH4
	C28H30N4NaO2	1+	477.226097	-0.8	-1.7	17.3	100.00	C28H30N4O2	M+Na
	C31H31N2Na2	1+	477.227714	0.8	1.7	31.2	100.00	C31H32N2	M+Na2-H
	C16H27N14Na2O	1+	477.228217	1.3	2.7	39.7	60.07	C16H28N14O	M+Na2-H
	C26H25N10	1+	477.225817	-1.1	-2.3	15.7	48.85	C13H12N5	2M+H
	C30H29N4O2	1+	477.228503	1.6	3.3	26.3	38.49	C15H14N2O	2M+H
	C28H30N4NaO2	1+	477.226097	-0.8	-1.7	17.3	100.00	C14H15N2O	2M+Na

Cmpd 2, 1.3 min


Intens.
x10^6
+MS, 1.2-1.5min #73-88, -Peak Bkgrnd
1+
499.2106
649.1007
266.1402
1.25
1.00
0.75
0.50
0.25
0.00
200
400
600
800
1000
1200
1400
m/z



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Expected Formula	
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Formula Search Maximum	
Algorithm Parameters	
Tolerance	4 ppm
Match to Isotope Pattern(mSigma)	40
Electron Configuration	even
Estimate No of Carbons	yes
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Cmpd 2, 1.3 min

Meas. m/z	Ion Formula	z	m/z	err [mDa]	err [ppm]	mSigma	Score	Sum Formula	Adduct
500.211330	C6H18N27O2	1+	500.213129	1.8	3.6	21.9	100.00	C6H17N27O2	M+H
	C6H18N27O2	1+	500.213129	1.8	3.6	21.9	100.00	C6H14N26O2	M+NH4
	C7H20N25Na2	1+	500.212341	1.0	2.0	23.4	100.00	C7H21N25	M+Na2-H