

SUPPLEMENTAL MATERIAL

Supplemental Figure 1. EDD spectrum of T1 [M-5H+1Na]⁴⁻.

Supplemental Figure 2. IRMPD spectrum of T1 [M-5H+1Na]⁴⁻.

Supplemental Figure 3. EDD spectrum of T2 [M-5H+2Na]³⁻.

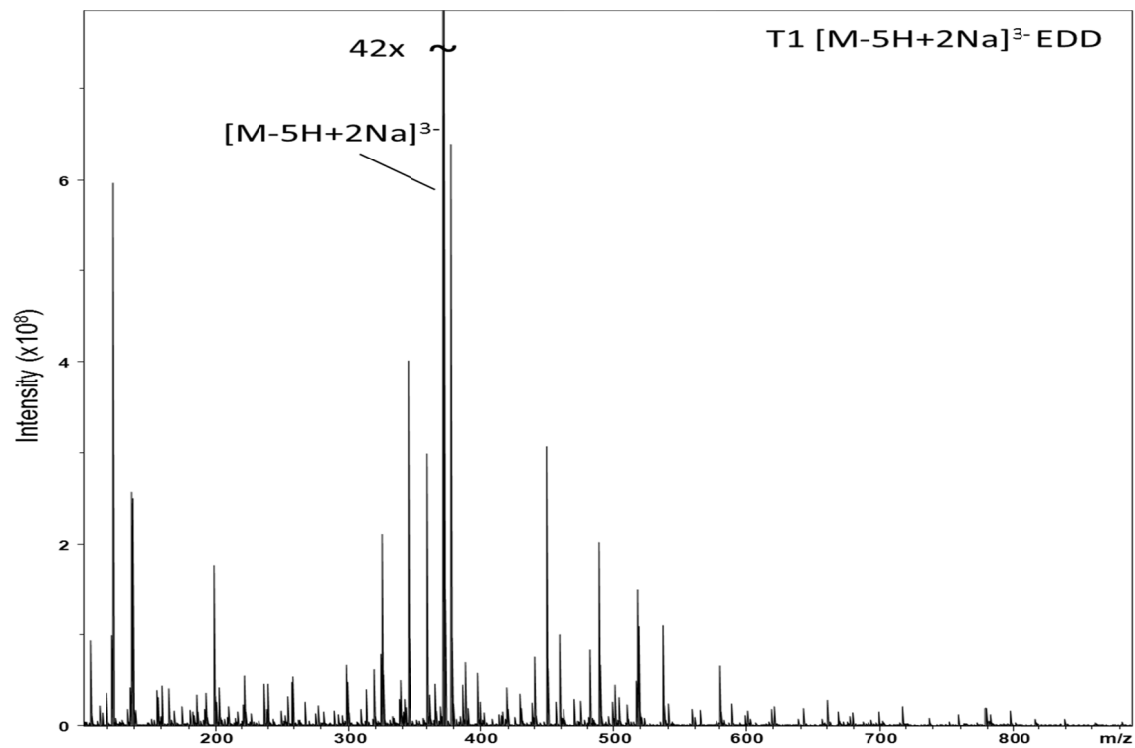
Supplemental Figure 4. IRMPD spectrum of T2 [M-5H+2Na]³⁻.

Supplemental Figure 5. EDD spectrum of T2 [M-5H+3Na]²⁻.

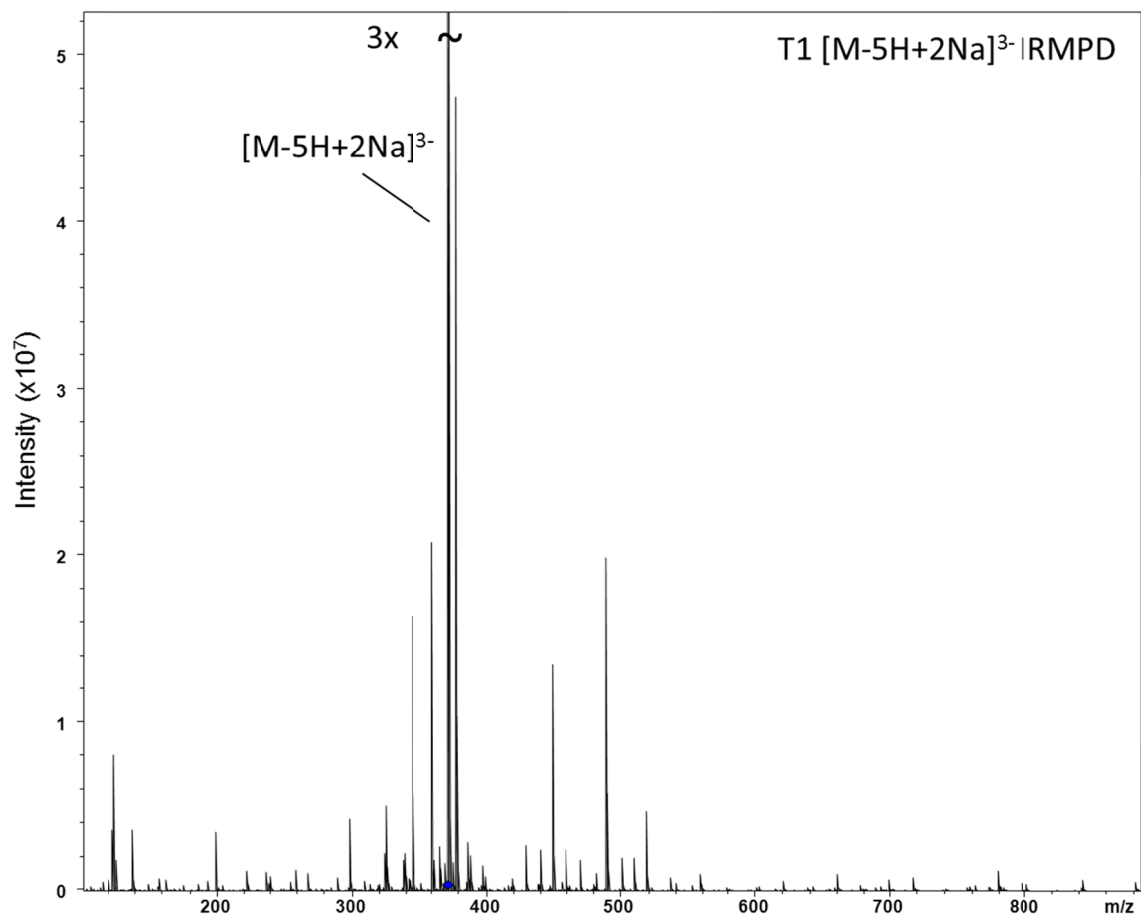
Supplemental Figure 6. IRMPD spectrum of T2 [M-5H+3Na]²⁻.

Supplemental Tables 1-6. Mass-to-charge, intensity, and assignment lists for the six supplemental figures.

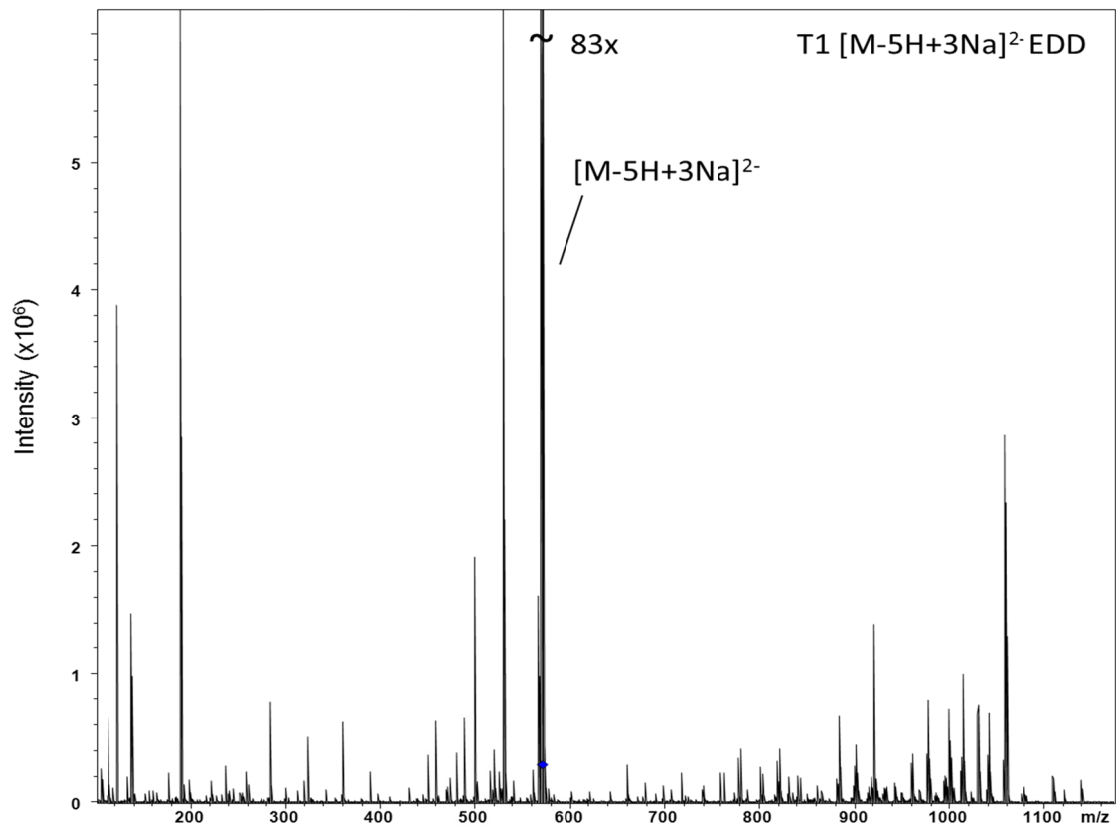
Supplemental Figure 1. EDD spectrum of T1 $[M-5H+1Na]^4$.



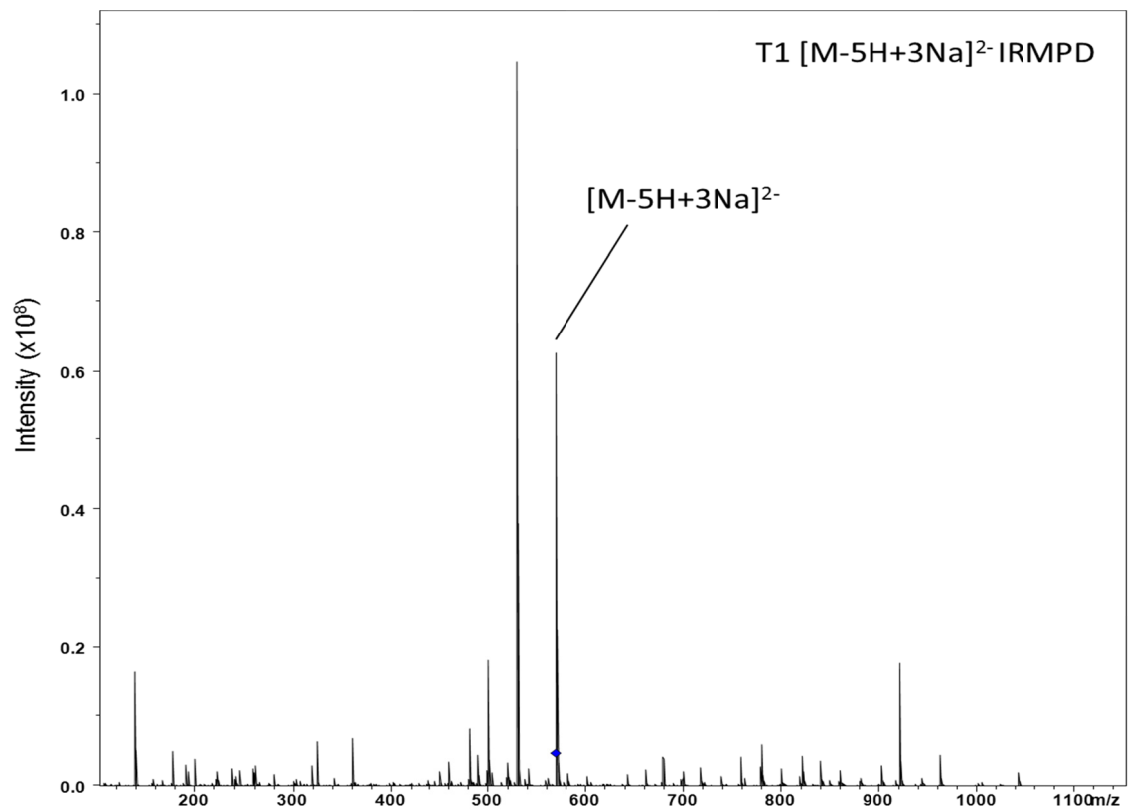
Supplemental Figure 2. IRMPD spectrum of T1 $[M-5H+1Na]^{4-}$.



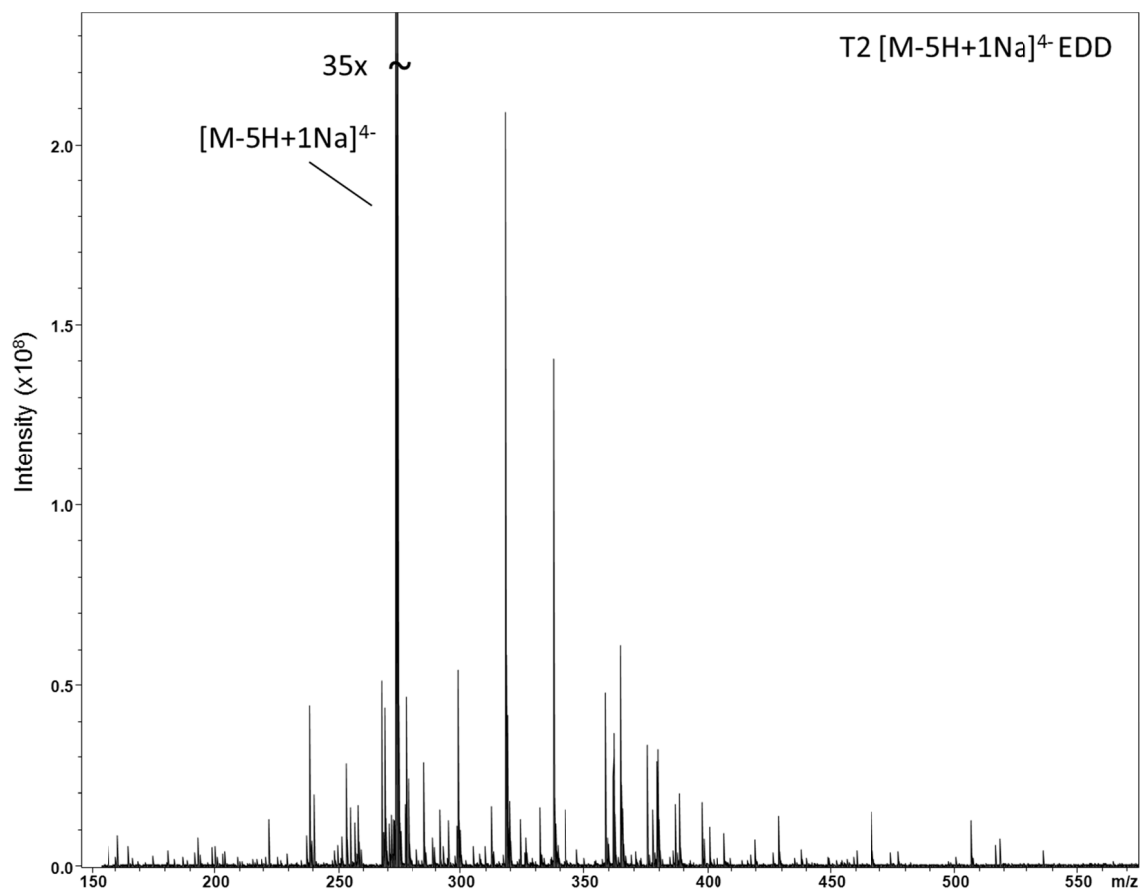
Supplemental Figure 3. EDD spectrum of T2 $[M-5H+2Na]^{3-}$.



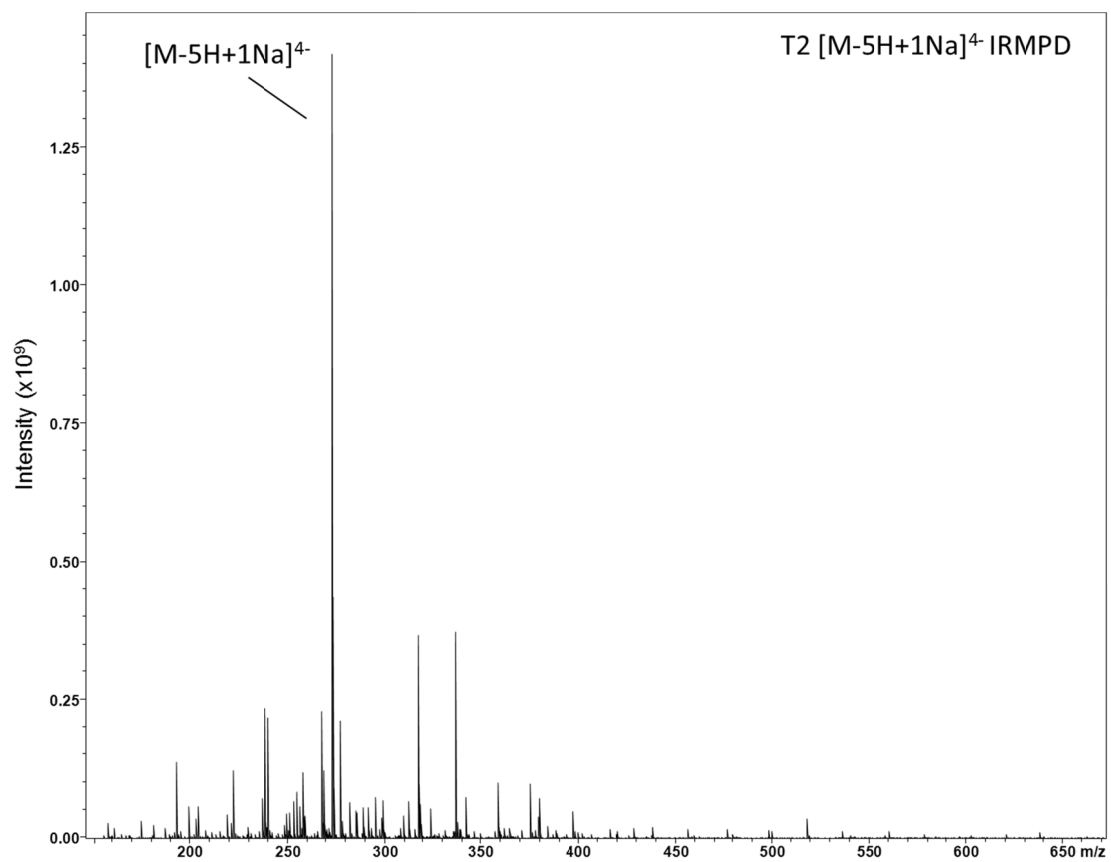
Supplemental Figure 4. IRMPD spectrum of T2 $[M-5H+2Na]^{3-}$.



Supplemental Figure 5. EDD spectrum of T2 $[M-5H+3Na]^{2-}$.



Supplemental Figure 6. IRMPD spectrum of T2 $[M-5H+3Na]^{2-}$.



Supplemental Table 1. Assignment list for T1 EDD [M-5H+2Na]³⁻.

Mass to charge	Assignment	Intensity
157.0145	B1-SO3	396835
159.9688	0,2X1+Na	104742
168.9815	1,4X0	165041
175.025	C1-SO3	214800
190.9635	1,4X0+Na	72573
208.9763	1,5A1	101303
228.9724	0,2A2+Na	46777
230.9581	1,5A1+Na	39992
236.9711	B1	461972
238.4948	B2-SO3	188129
240.0184	Z1-SO3	463682
243.9898	B3	76422
249.4857	B2-SO3+Na	171559
254.9816	C1	321708
258.029	Y1-SO3	481996
258.491	C2-SO3+Na	118248
258.491	Z2+Na	118248
258.953	B1+Na	536894
262.0004	Z1-SO3+Na	65777
267.4964	Y2+Na	265095
276.9636	C1+Na	221575
279.496	2,4A3-SO3+Na	41636
289.4642	B2+Na	164165
296.9919	2,4A2	45501
298.4693	C2+Na	668513
298.6589	0,2A3+2Na	483850
299.9464	2,4X0+Na	50868
300.4549	B2+2Na	143226
306.3202	0,2X3-SO3+2Na	51149
309.4601	C2+2Na	190656
318.3378	[M-5H+2Na]-2SO3	82040
318.9741	2,4A2+Na	623495
319.4746	2,4A3+Na	111848
321.9284	2,4X1+2Na	63868
325.3112	0,2A4+2Na	2121157
326.5113	B3-SO3	65597
330.4653	2,4A3+2Na	67501
332.972	0,2X3+2Na	106712
333.472	3,5A3+Na	89223
337.5016	B3-SO3+Na	293729
340.956	2,4A2+2Na	153622

341.957	Z1+Na	289630
344.9902	[M-5H+2Na]-SO3	4031306
346.5071	C3-SO3+Na	95534
348.4924	B3-SO3+2Na	55059
357.013	0,2A2-SO3	88667
357.4972	C3-SO3+2Na	70974
359.9676	Y1+Na	3008673
371.642	[M-5H+2Na]	2.54E+08
377.48	B3+Na	6400287
378.5026	2,4A4-SO3+Na	291591
378.9952	0,2A2-SO3+Na	250576
386.4853	C3+Na	455087
387.9625	1,5X1+Na	698516
388.0089	Y3-SO3+Na	127082
388.4709	B3+2Na	430552
389.9945	Z3-SO3+2Na	83345
397.4762	C3+2Na	456490
398.9999	Y3-SO3+2Na	267307
401.9783	0,2X1+Na	146455
408.5135	0,2A4-2SO3+2Na	79750
412.9463	3,5A2+Na	132147
416.0502	C2-2SO3	157832
416.0502	Z2-SO3	157832
418.4813	2,4A4+2Na	420654
420.0215	B2-2SO3+Na	185291
429.9728	Z3+2Na	201159
438.032	C2-2SO3+Na	252650
438.032	Z2-SO3+Na	252650
438.9782	Y3+2Na	101597
448.4919	0,2A4-SO3+2Na	3085258
456.0427	Y2-SO3+Na	269774
458.9519	0,2A2+Na	999111
459.9833	0,2X3-SO3+2Na	83613
471.9839	1,5A2-SO3+Na	55612
480.9339	2,4A3-2SO3+Na	835446
480.9339	0,2A2+2Na	835446
484.0375	1,5X2-SO3+Na	66197
488.4704	0,2A4+2Na	2042376
494.9858	1,5A4-SO3+Na	106425
499.9786	B2-SO3+Na	449297
514.0183	Y2	53169
517.9899	C2-SO3+Na	1088170
517.9899	Z2+Na	1088170
521.9607	B2-SO3+Na	90334
535.9997	Y2+Na	1095966

539.9712	C2-SO3+2Na	252326
539.9712	Z2+2Na	252326
557.9822	Y2+2Na	186986
560.0008	2,4A3-SO3+Na	96254
563.9948	1,5X2+Na	181140
581.981	2,4A3-SO3+2Na	68918
585.9769	1,5X2+2Na	41169
587.9944	3,5A3-SO3+Na	241132
597.9449	C2+Na	115866
601.9167	B2+2Na	73886
619.9288	C2+2Na	216384
667.9516	3,5A3+Na	159748
676.0122	B3-SO3+Na	105858
678.0563	2,4A4-2SO3+2Na	144005
697.9923	B3-SO3+2Na	158961
701.0414	Z3-2SO3+2Na	61099
716.0038	C3-SO3+2Na	219992
736.0315	2,4A4-SO3+Na	89983
758.0133	2,4A4-SO3+2Na	131751
777.9498	B3+2Na	202292
780.996	Z3-SO3+2Na	129160
795.9598	C3+2Na	167666
815.9876	2,4A4+Na	75532
837.9715	2,4A4+2Na	82497
860.9527	Z3+2Na	38664
897.9915	0,2A4-SO3+2Na	623776
911.0231	1,5A4-SO3+2Na	46424
977.9492	0,2A4+2Na	222468

Supplemental Table 2. Assignment list for T1 IRMPD $[M-5H+2Na]^{3-}$.

Mass to charge	Assignment	Intensity
157.0141	B1-SO3	282331
168.4891	1,4X0	151345
175.0247	C1-SO3	324090
208.9761	1,5A1	86311
230.9579	1,5A1+Na	37156
236.971	B1	1112796
240.0183	Z1-SO3	824600
254.9816	C1	518297
258.0289	Y1-SO3	1237239
258.953	B1+Na	687126
276.9633	C1+Na	160779

296.9924	2,4A2	61685
299.947	2,4X0+Na	48240
318.338	2,4A2+Na	100593
341.9571	Z1+Na	738805
359.9677	Y1+Na	2.09E+07
401.9785	0,2X1+Na	85594
	0,2A4-	
408.5137	2SO3+2Na	116834
416.0505	3,5A2+Na	327721
416.0505	C2-2SO3	327721
416.0505	Z2-SO3	327721
420.022	B2-2SO3+Na	301326
438.0324	C2-2SO3+Na	404226
438.0324	Z2-SO3+Na	404226
448.4922	0,2A4-SO3+2Na	1.35E+07
456.0431	Y2-SO3+Na	510704
458.9523	0,2A2+Na	2427837
459.9839	0,2A2+2Na	282862
459.9839	2,4A3-2SO3+Na	282862
517.9895	C2-SO3+Na	4743104
517.9895	Z2+Na	4743104
521.9611	B2-SO3+Na	211992
539.9712	C2-SO3+2Na	484964
539.9712	Z2+2Na	484964
581.9825	2,4A3-SO3+2Na	69780
601.9179	B2+2Na	256814
619.9286	C2+2Na	620254
676.012	B3-SO3+Na	306051
697.9935	B3-SO3+2Na	658144
701.0399	Z3-2SO3+2Na	129597
716.0046	C3-SO3+2Na	825034
777.9502	B3+2Na	1181595
795.9614	C3+2Na	459297

Supplemental Table 3. Assignment list for T1 EDD [M-5H+3Na]²⁻.

Mass to charge	Assignment	Intensity
157.0144	B1-SO3	102844
236.9711	B1	297045
240.0185	Z1-SO3	101585
254.9816	C1	52708
258.0289	Y1-SO3	244188
258.9531	B1+Na	186366
299.9465	2,4X0+Na	123418

318.9742	2,4A2+Na	182899
341.957	Z1+Na	107125
359.9677	Y1+Na	633143
387.9627	1,5X1+Na	249732
408.4671	C3+3Na	56253
429.4728	2,4A4+3Na	121963
458.9523	0,2A2+Na	65351
459.4829	0,2A4-SO3+3Na	644672
470.9741	0,2X3-SO3+3Na	130126
480.9341	0,2A2+2Na	398615
489.0015	[M-5H+3Na]- 2SO3	663773
499.4612	0,2A4+3Na	1929554
517.9898	C2-2SO3+Na	107698
517.9898	Z2+Na	107698
521.9595	B2-SO3+Na	125404
528.9798	[M-5H+3Na]- SO3	1.85E+07
539.9711	C2-SO3+2Na	178297
539.9711	Z2+2Na	178297
568.9572	[M-5H+3Na]	4.66E+08
574.0727	B3-2SO3	69637
581.982	2,4A3-SO3+2Na	68381
601.9165	B2+2Na	95144
619.9273	C2+2Na	94622
641.9114	C2+3Na	88755
678.0572	2,4A4- 2SO3+2Na	159513
689.9324	3,5A3+2Na	75908
697.9929	B3-SO3+2Na	137132
716.0039	C3-SO3+2Na	238591
719.975	B3-SO3+3Na	62327
737.9863	C3-SO3+3Na	110489
758.0135	2,4A4-SO3+2Na	239352
777.9503	B3+2Na	358800
779.9959	2,4A4-SO3+3Na	421830
799.9317	B3+3Na	287863
802.9803	Z3-SO3+3Na	234074
817.9411	C3+3Na	330363
820.9902	Y3-SO3+3Na	424621
848.9847	1,5X3-SO3+3Na	78975
859.9527	2,4A4+3Na	142647
882.9364	Z3+3Na	678431
900.9459	Y3+3Na	452782
919.9737	0,2A4-SO3+3Na	1399915
933.0044	1,5A4-	129271

	2SO3+3Na	
998.9475	1,3X3+3Na	734558
1012.9618	1,5A4-SO3+3Na	1004778

Supplemental Table 4. Assignment list for T1 IRMPD $[M-5H+3Na]^{2-}$.

Mass to charge	Assignment	Intensity
157.0141	B1-SO3	1034068
236.971	B1	2536377
240.0182	Z1-SO3	1456490
254.9816	C1	152103
258.0289	Y1-SO3	2525270
258.9529	B1+Na	1923001
318.974	2,4A2+Na	2949576
341.9571	Z1+Na	1080697
359.9678	Y1+Na	6893068
408.467	C3+3Na	292040
429.4725	2,4A4+3Na	436660
458.9523	0,2A2+Na	170506
459.4828	0,2A4-SO3+3Na	3510766
470.9741	0,2X3-SO3+3Na	500842
480.9342	0,2A2+2Na	8303582
489.002	[M-5H+3Na]- 2SO3	4528610
499.4617	0,2A4+3Na	1.82E+07
510.9535	0,2X3+3Na	6.27E+04
517.9891	C2-2SO3+Na	1219788
517.9891	Z2+Na	1219788
521.9604	B2-SO3+Na	772256
528.9797	[M-5H+3Na]-SO3	1.05E+08
539.9706	C2-SO3+2Na	2473787
539.9706	Z2+2Na	2473787
568.9591	[M-5H+3Na]	6.27E+07
581.9818	2,4A3-SO3+2Na	766054
601.9177	B2+2Na	211454
619.9285	C2+2Na	68789
641.9102	C2+3Na	342435
678.0568	2,4A4-2SO3+2Na	4262703
697.9927	B3-SO3+2Na	2092767
716.0045	C3-SO3+2Na	2670661
719.975	B3-SO3+3Na	612496
737.9863	C3-SO3+3Na	1371535
758.0149	2,4A4-SO3+2Na	4243902
777.9504	B3+2Na	2751249

779.9967	2,4A4-SO3+3Na	6080427
799.9316	B3+3Na	2493273
802.9799	Z3-SO3+3Na	344374
820.989	Y3-SO3+3Na	4390506
848.9854	1,5X3-SO3+3Na	809915
859.9521	2,4A4+3Na	2236197
900.9475	Y3+3Na	184437
919.9755	0,2A4-SO3+3Na	1.77E+07

Supplemental Table 5. Assignment list for T2 EDD [M-5H+1Na]⁴⁺.

Mass to charge	Assignment	Intensity
157.0142	B1-SO3	5875684
159.9685	0,2X0	2829679
175.0248	C1-SO3	3179816
208.976	1,5A2	2803316
236.971	B1	8931601
238.4945	B2-SO3	4.49E+07
240.0181	Z1	2.01E+07
247.4994	Z2	2005447
249.4854	B2-SO3+Na	6366833
251.0094	Y3-SO3	2586241
251.3171	B3-SO3+Na	8599503
252.9952	[M-5H+1Na]-SO3	2.87E+07
254.9814	C1	1.65E+07
256.5053	Y2	1.24E+07
258.0287	Y1	1.72E+07
258.4908	C2-SO3+Na	7055631
258.4908	Z2+Na	7055631
258.9526	B1+Na	5103257
267.4964	Y2+Na	5.15E+07
270.5024	1,5X2	9006814
271.3244	2,4A4-SO3+Na	1.20E+07
272.9842	[M-5H+1Na]	7.61E+09
276.6461	C3	1810990
276.9633	C1+Na	1.60E+07
277.056	0,2A2-SO3	1832615
277.9697	B3+Na	2.46E+07
278.4727	B2	6418101
278.9855	Z3+Na	2623243
282.0284	B2+0,2X3-2SO3	4.97E+06
283.9733	C3+Na	2148350
284.989	Y3+Na	2.88E+07

286.0236	1,5X1	4243123
288.5014	0,2X3+C3-2SO3	8.31E+06
289.4637	B2+Na	5729569
291.3312	0,2A4+Na-SO3	1.60E+07
294.3212	1,5X3+Na	2741881
294.974	Y2+C3+Na	1.32E+07
295.067	0,2A4+Y2-SO3	1.69E+07
298.4696	C2+Na	1.15E+07
298.9927	0,2X3+Na-SO3	5.47E+07
301.9645	B2+Z3	2.05E+06
307.4743	C3+Y3+Na	3.32E+07
307.5206	0,2A3+Y3-SO3	3.93E+06
309.5062	0,2A4+Z3+Na-SO3	5.87E+06
317.9838	0,2A4+Na	2.10E+08
318.9739	2,4A2	1.09E+07
319.4741	2,4A3+Na	6162577
323.9464	B2+Z3+Na	1.32E+07
328.0338	Z3-2SO3	1.55E+06
328.48	2,4A4+Y3+Na	2.37E+06
333.4716	3,5A3	2807337
336.9847	2,4A4+Y2+Na	1.41E+08
337.5012	B3-2SO3+Na	5603611
341.9573	C2+Z3+Na	1.59E+07
341.9573	B2+Y3+Na	1.59E+07
346.5071	C3-2SO3+Na	5162066
349.4853	0,2A4+Z3+Na	2.67E+06
357.0141	0,2A2-SO3	2302914
358.4902	0,2A4+Y3+Na	4.87E+07
363.4829	1,5A3-SO3+Na	2819717
364.3156	[M-5H+1Na]	6.19E+07
374.0241	0,2A4+Y2	3.40E+07
377.4802	B3-SO3+Na	1.60E+07
378.9954	0,2A4+Z2+Na	2.92E+07
383.9681	2,4A4+Z2+Na	3.11E+06
385.4777	C3"-SO3+Na	4.84E+06
386.4852	C3-SO3+Na	1.74E+07
388.0095	Y3-SO3+Na	2.03E+07
397.0061	0,2A4+Y2+Na	1.79E+07
398.0394	B2-2SO3	7902932
401.9801	0,2X1+Na	1.44E+02
420.0224	B2-SO3+Na	1.79E+06
437.5005	0,2A4+SO3+Na	5009506
438.033	Z2-SO3+Na	2304060
438.033	C2-2SO3+Na	2304060
458.9528	0,2A2+Na	2819384

466.0104	[M-5H+1Na]-2SO3	1.54E+07
499.9778	B2-SO3+Na	3079758
517.9891	Z2+Na	8164487
517.9891	C2-SO3+Na	8164487
535.9996	Y2+Na	4851433

Supplemental Table 6. Assignment list for T2 IRMPD [M-5H+1Na]⁴⁺.

Mass to charge	Assignment	Intensity
157.0142	B1-SO3	2.76E+07
159.9686	0,2X0	5453812
175.0248	C1-SO3	5945994
208.9762	1,5A2	5887199
217.0352	2,4A2-SO3	3732966
230.958	1,5A2+Na	9379930
236.971	B1	7.27E+07
238.4945	B2-SO3	2.35E+08
240.0183	Z1	2.18E+08
247.4998	Z2	6567858
247.4998	B2-SO3+Na	6567858
251.0094	Y3-SO3	9655881
251.3174	B3-SO3+Na	4.67E+07
252.9951	[M-5H+1Na]-SO3	6.70E+07
254.9815	C1	8.35E+07
256.5052	Y2	5.75E+07
257.3211	C3-SO3+Na	3122238
258.0289	Y1	1.19E+08
258.4909	C2-SO3+Na	3.91E+07
258.4909	Z2+Na	3.91E+07
258.9529	B1+Na	4.15E+07
262.0003	Z1+Na	5071776
267.4961	Y2+Na	2.32E+08
270.5026	1,5X2	6101854
271.3244	2,4A4-SO3+Na	1.86E+07
272.9841	[M-5H+1Na]	1.43E+09
276.6457	C3	1997545
276.9635	C1+Na	1.14E+08
277.0564	0,2A2-SO3	1.46E+07
277.9697	B3+Na	3.26E+07
278.4728	B2	1.01E+07
280.0109	Y1+Na	1962248
283.9732	C3+Na	2359447
284.9888	Y3+Na	5.07E+07

289.4638	B2+Na	2.10E+07
291.3314	0,2A4+Na-SO3	5.52E+07
294.3206	1,5X3+Na	1915628
296.9923	2,4A2	4661362
298.4693	C2+Na	3.69E+07
298.9922	0,2X3+Na-SO3	6.80E+07
312.5131	1,5A2-SO3	3539757
317.9835	0,2A4+Na	3.70E+08
318.9742	2,4A2	2.76E+07
319.4746	2,4A3+Na	2.62E+07
323.5042	1,5A3-2SO3+Na	3908828
328.0346	Z3-2SO3	3064199
333.4719	3,5A3	2973538
337.5014	B3-2SO3+Na	1.20E+07
346.5069	C3-2SO3+Na	6101481
357.0136	0,2A2-SO3	1.22E+07
363.4821	1,5A3-SO3+Na	4743244
377.4797	B3-SO3+Na	1.58E+07
378.9953	0,2A4+Z2+Na	3.95E+07
386.4848	C3-SO3+Na	7514338
388.0084	Y3-SO3+Na	1.58E+07
398.0401	B2-2SO3	1.31E+07
401.9784	0,2X1+Na	9317717
416.0507	Z2-SO3	1.76E+07
416.0507	C2-2SO3	1.76E+07
420.0217	B2-SO3+Na	1.36E+07
437.5011	0,2A4+SO3+Na	6398904
438.0324	Z2-SO3+Na	2.02E+07
438.0324	C2-2SO3+Na	2.02E+07
458.061	2,4A3-2SO3	3828315
458.9521	0,2A2+Na	6446910
499.979	B2-SO3+Na	1.23E+07
517.9894	Z2+Na	3.63E+07
517.9894	C2-SO3+Na	3.63E+07
535.9999	Y2+Na	1.34E+07
560.0002	2,4A3+Na-SO3	1.37E+07