

Supporting Information

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

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Supporting Information Manuscript. This manuscript gives detailed results of experiments on substance P and on sesame oil.

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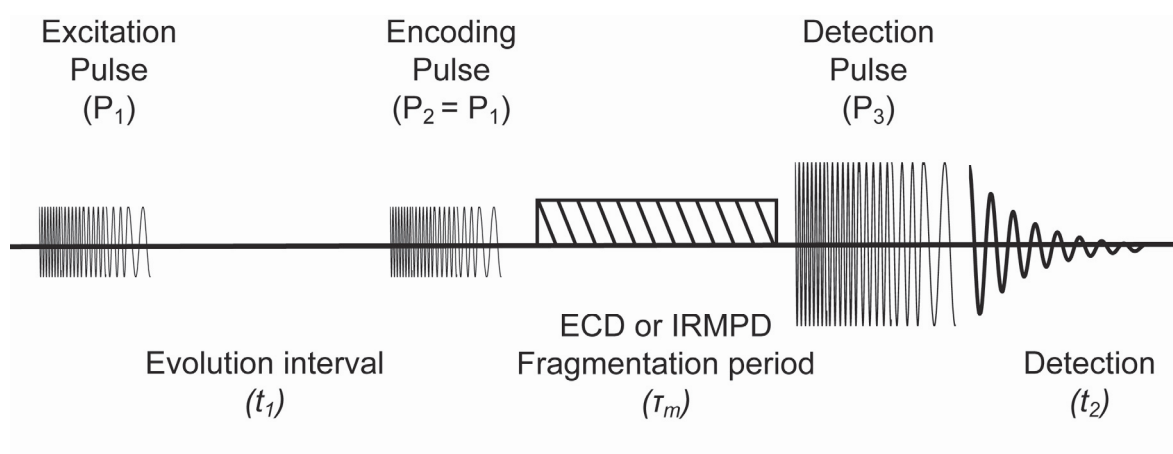
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Scheme S1. 2D FTICR MS pulse sequence.



The excitation and encoding pulses P_1 and P_2 are identical and have an overall duration of 723 μs each with 0.5 μs per frequency step. The P_1 pulse amplitude was tuned to decrease the fragment intensity to about half of the maximum. The detection pulse P_3 used the default settings for ion excitation in Apex/SolariX Control (100 V_{pp} amplitude and 20 μs per frequency step).

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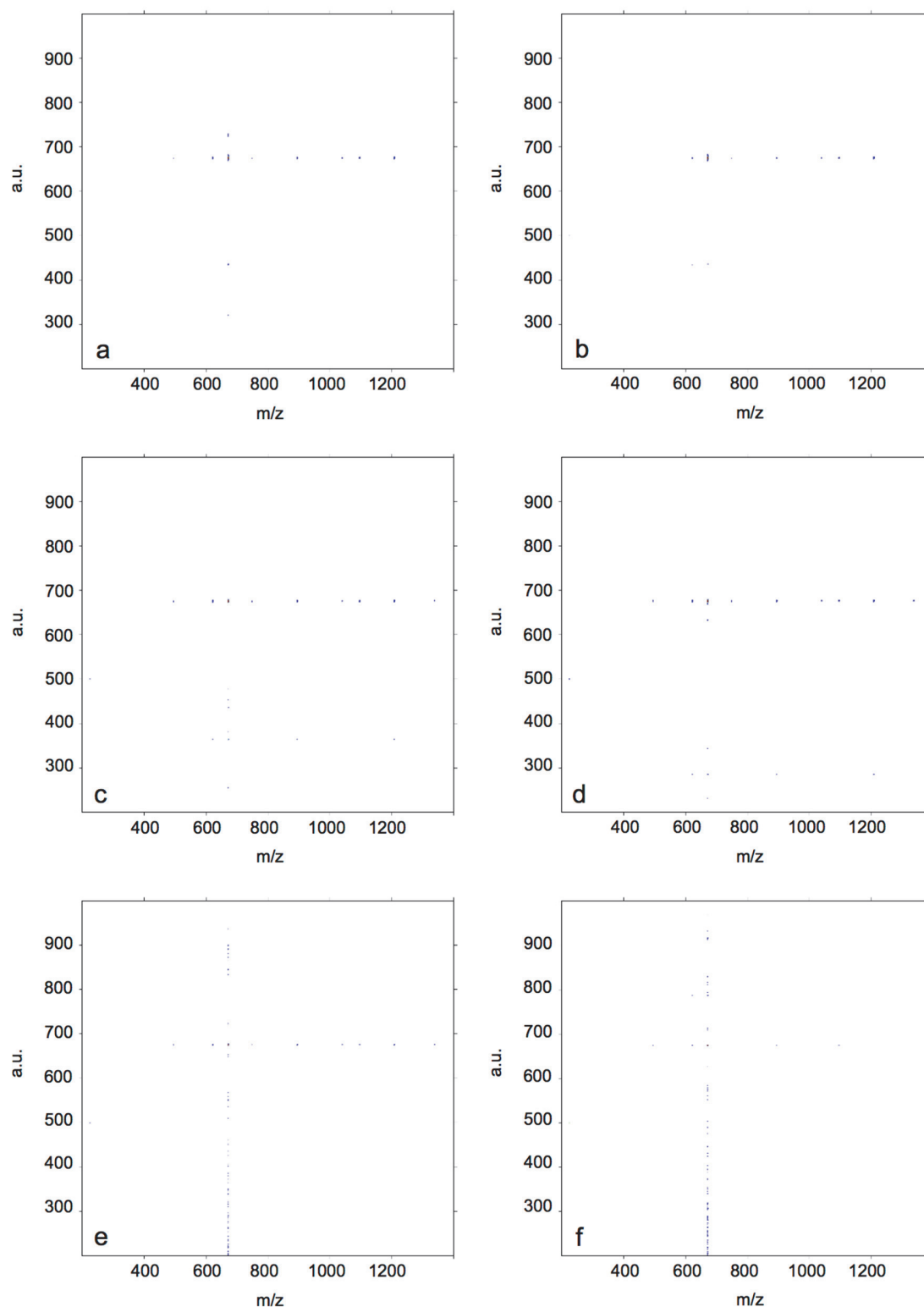


Figure S1. Full 2D spectrum at different NUS ratios. a) Classical acquisition (not-NUS, ie NUS 1), b) NUS 1/2, c) NUS 1/4, d) NUS 1/8, e) NUS 1/16, f) NUS 1/32.

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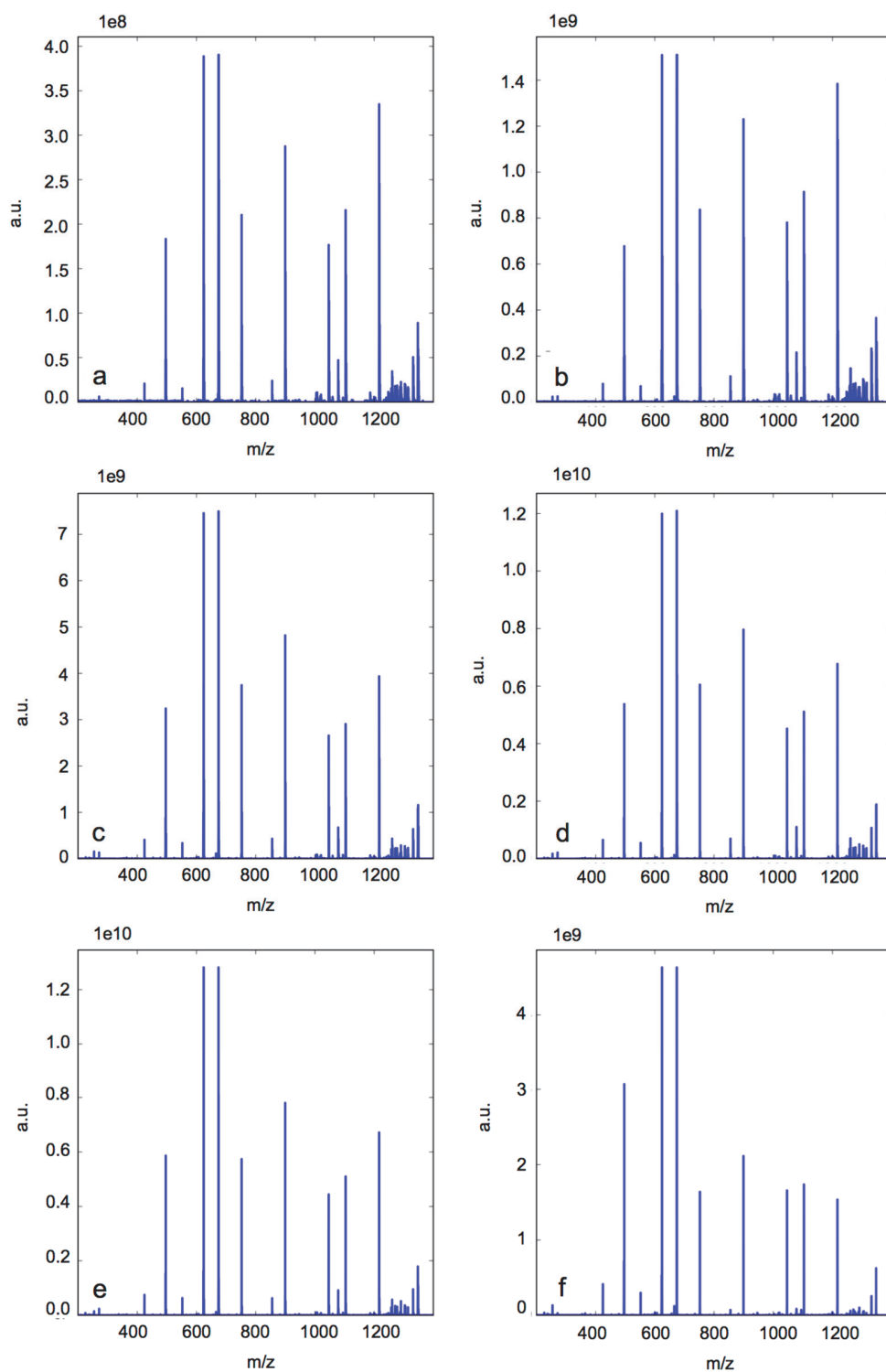


Figure S2. Fragment spectrum of the monoisotopic peak, normalized on the c_5 fragment, for different NUS ratios. a) Classical acquisition (not-NUS, ie NUS 1), b) NUS 1/2, c) NUS 1/4, d) NUS 1/8, e) NUS 1/16, f) NUS 1/32.

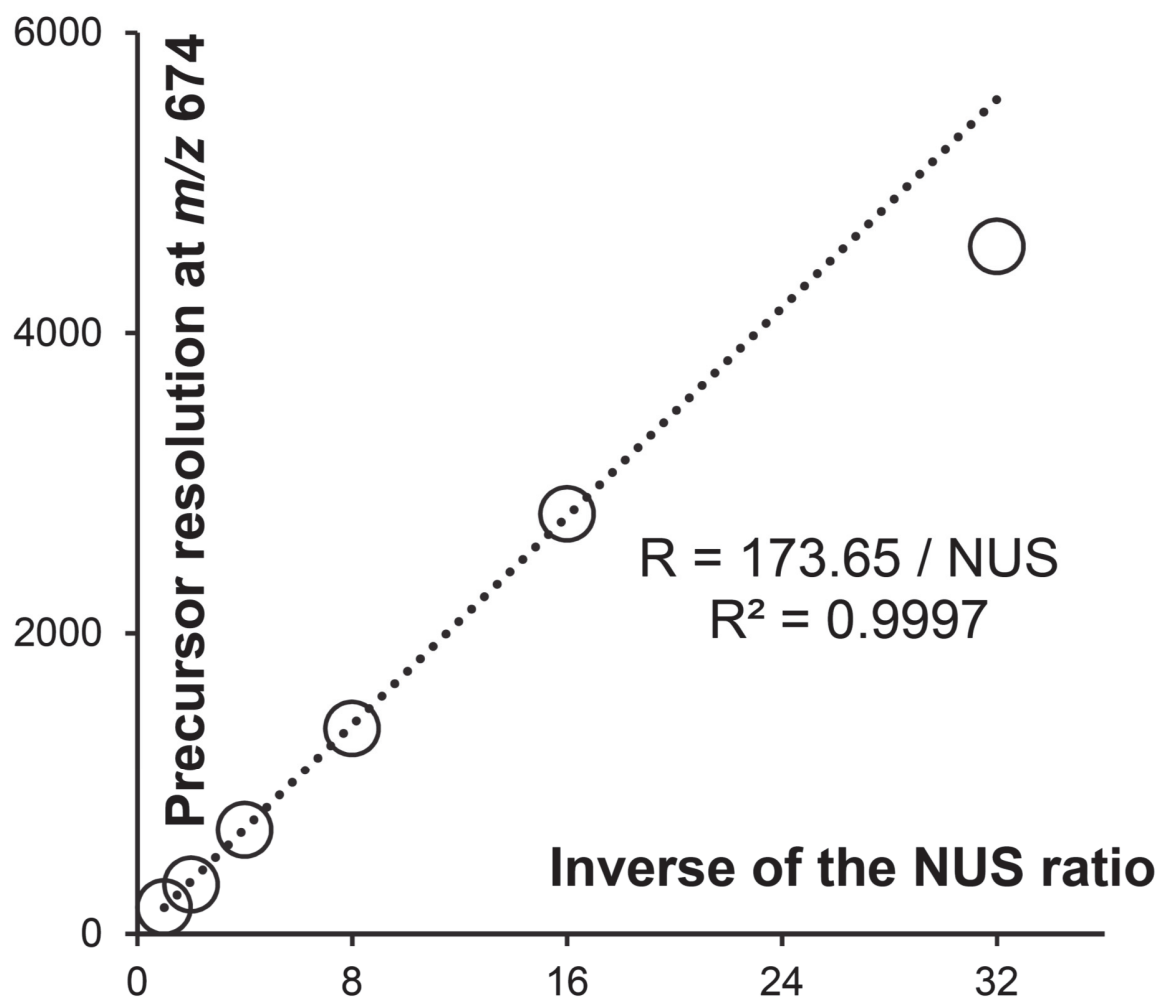


Figure S3. FWHM of the precursor peak as a function of the inverse of the NUS ratio.

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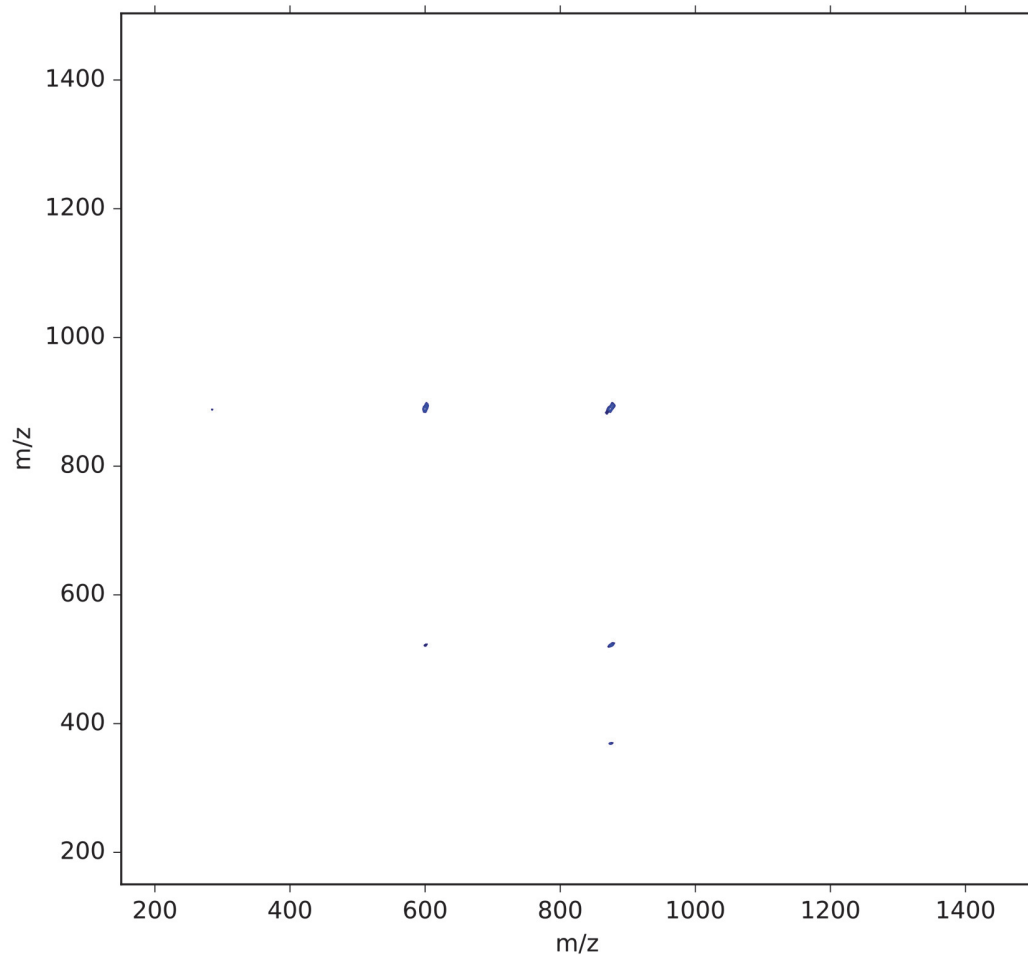


Figure S4. 2D FTICR spectra of sesame oil cationized by $^6\text{Li}^+$ and fragmented by IRMPD.

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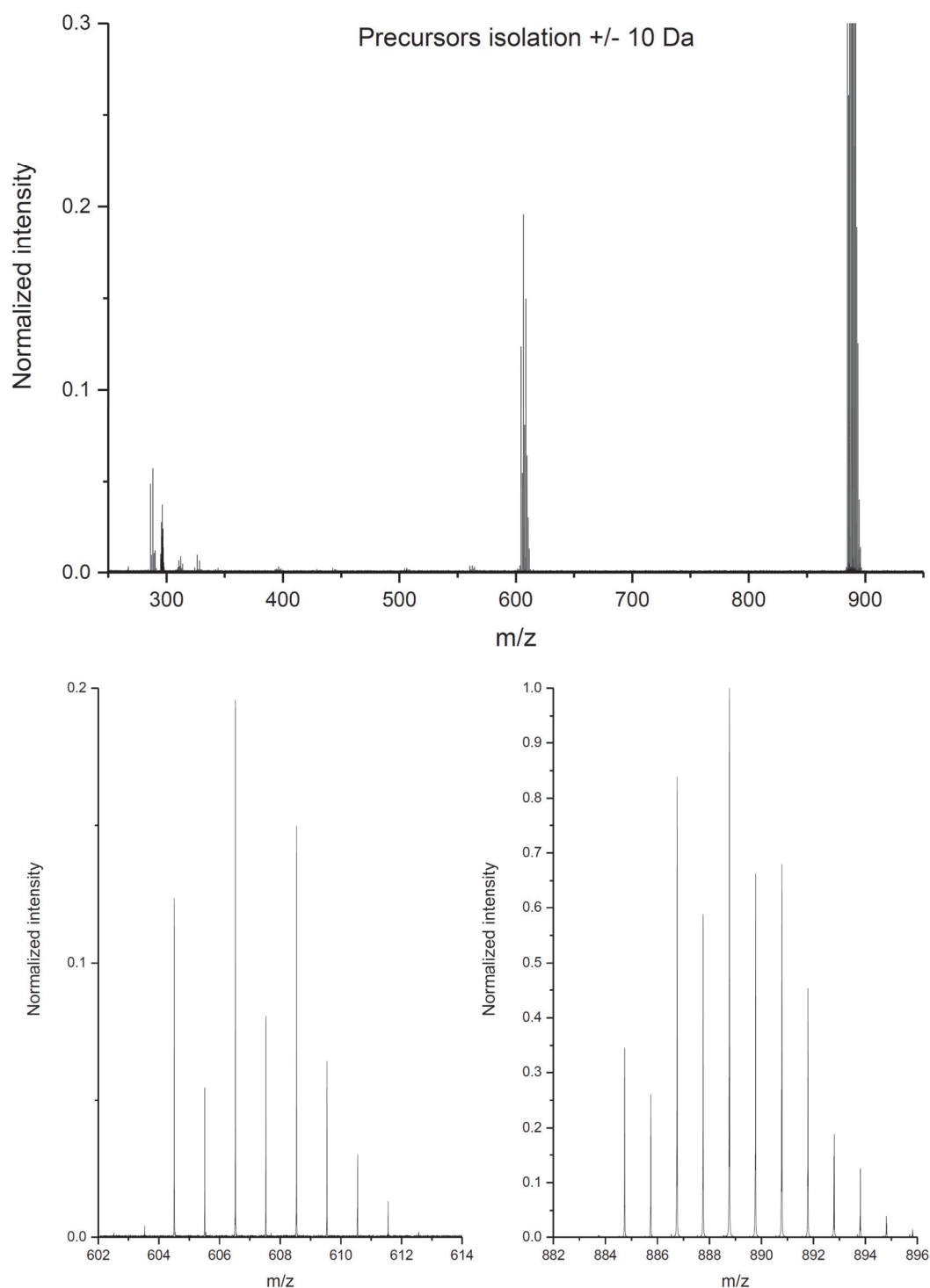


Figure S5a. Classical MS/MS FTICR spectra of sesame oil cationized by $^6\text{Li}^+$ and fragmented by IRMPD: upper panel full MS spectrum, right lower panel zoom on the precursor, left lower panel, zoom on fragments corresponding to the loss of a neutral fatty acid a) unselected precursors (quadrupole selection ± 10 m/z).

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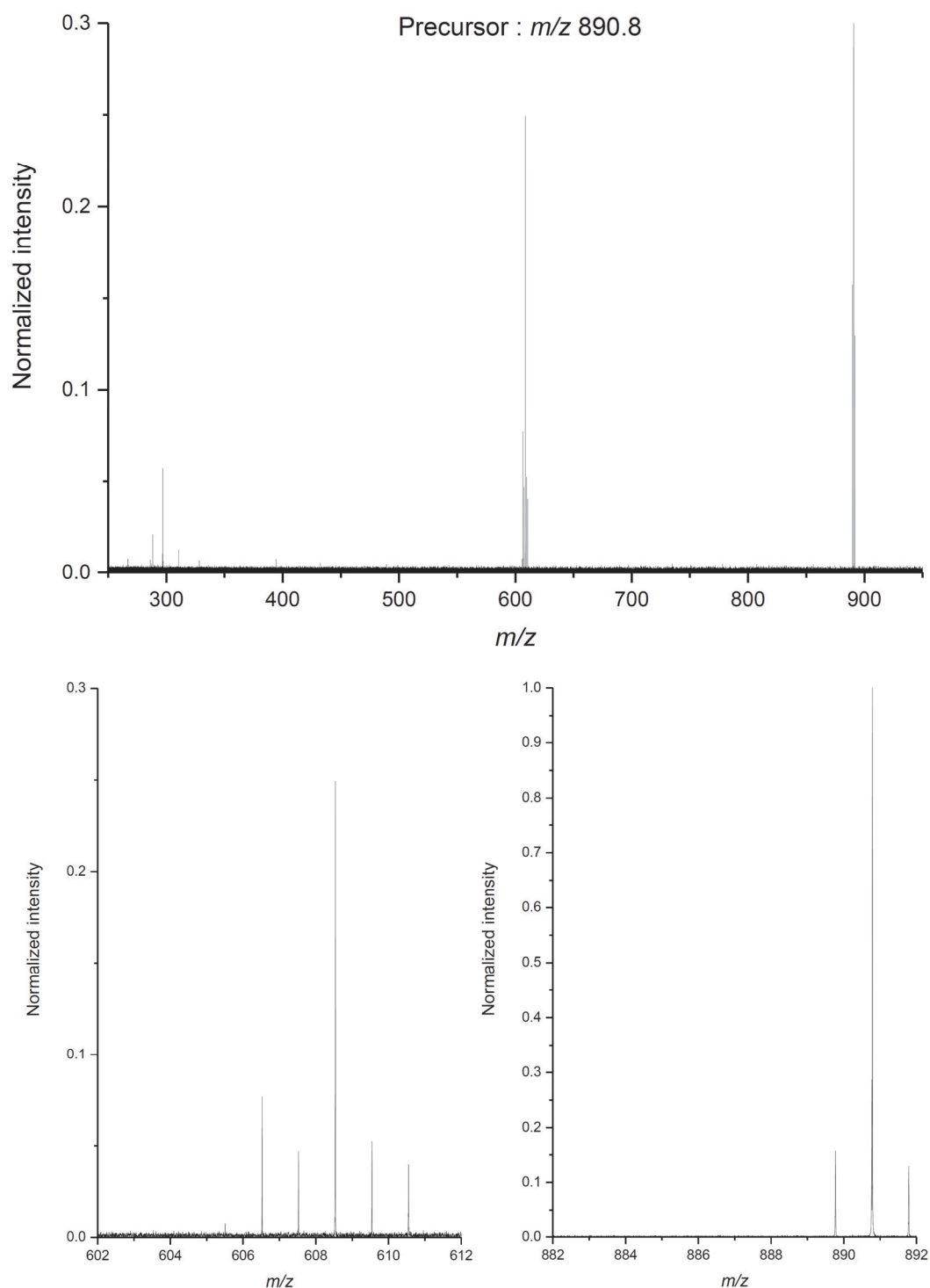


Figure S5b. Classical MS/MS FTICR spectra of sesame oil cationized by $^6\text{Li}^+$ and fragmented by IRMPD: upper panel full MS spectrum, right lower panel zoom on the precursor, left lower panel, zoom on fragments corresponding to the loss of a neutral fatty acid b) precursor m/z 890.8 (quadrupole selection ± 0.5 m/z).

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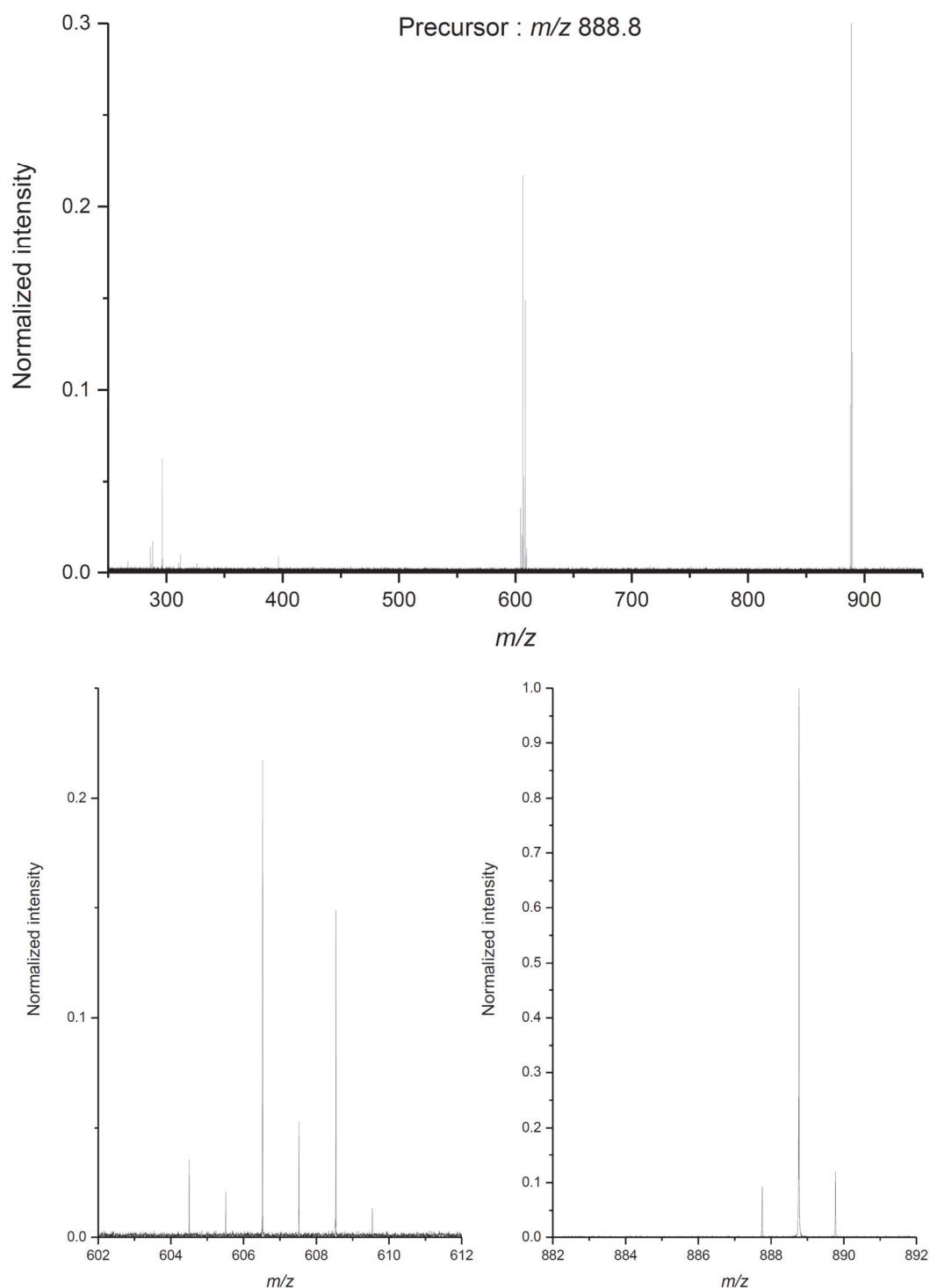


Figure S5c. Classical MS/MS FTICR spectra of sesame oil cationized by $^6\text{Li}^+$ and fragmented by IRMPD: upper panel full MS spectrum, right lower panel zoom on the precursor, left lower panel, zoom on fragments corresponding to the loss of a neutral fatty acid c) precursor m/z 888.8 (quadrupole selection ± 0.5 m/z).

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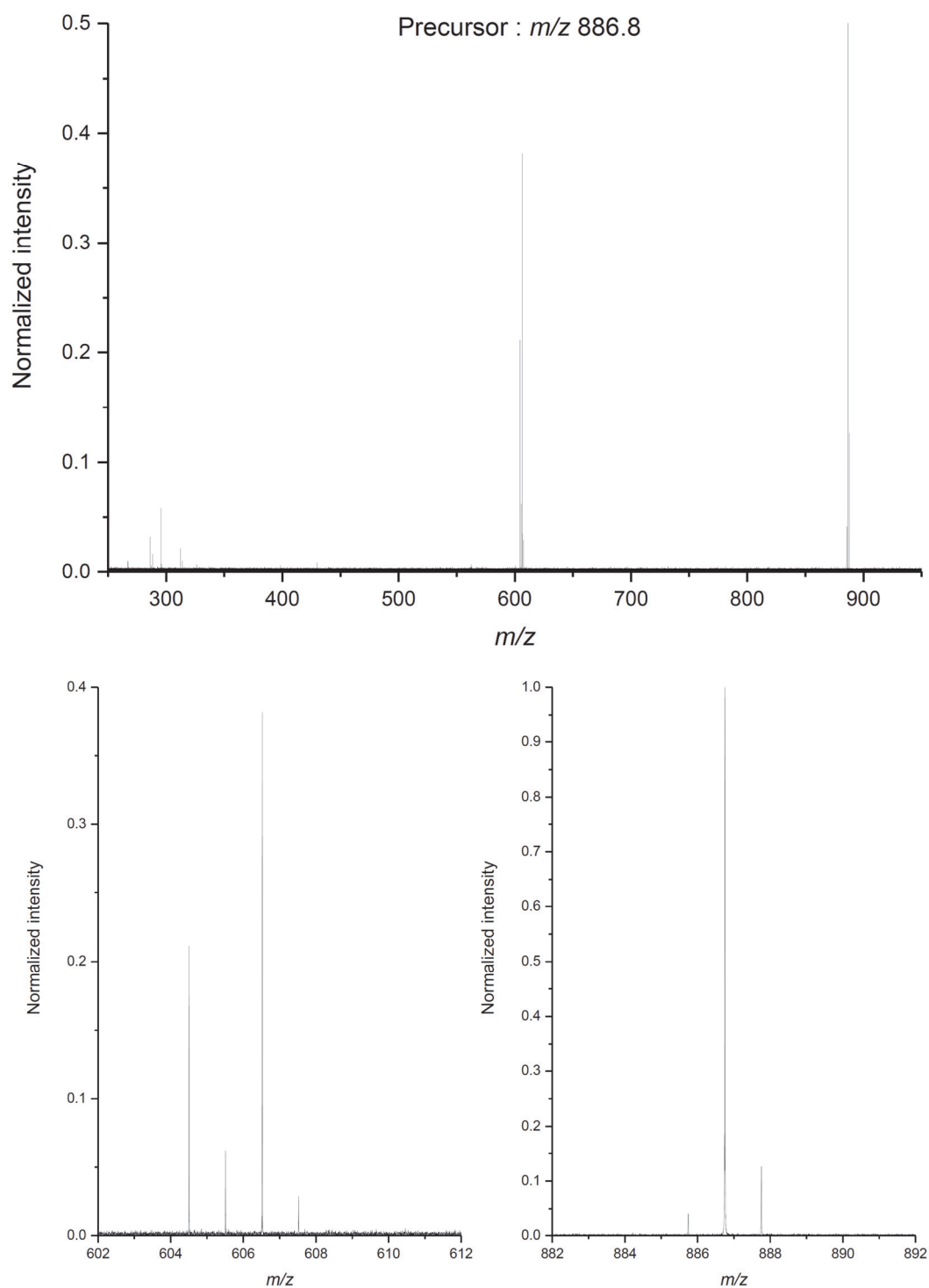


Figure S5d. Classical MS/MS FTICR spectra of sesame oil cationized by $^6\text{Li}^+$ and fragmented by IRMPD: upper panel full MS spectrum, right lower panel zoom on the precursor, left lower panel, zoom on fragments corresponding to the loss of a neutral fatty acid d) precursor m/z 886.8 (quadrupole selection ± 0.5 m/z).

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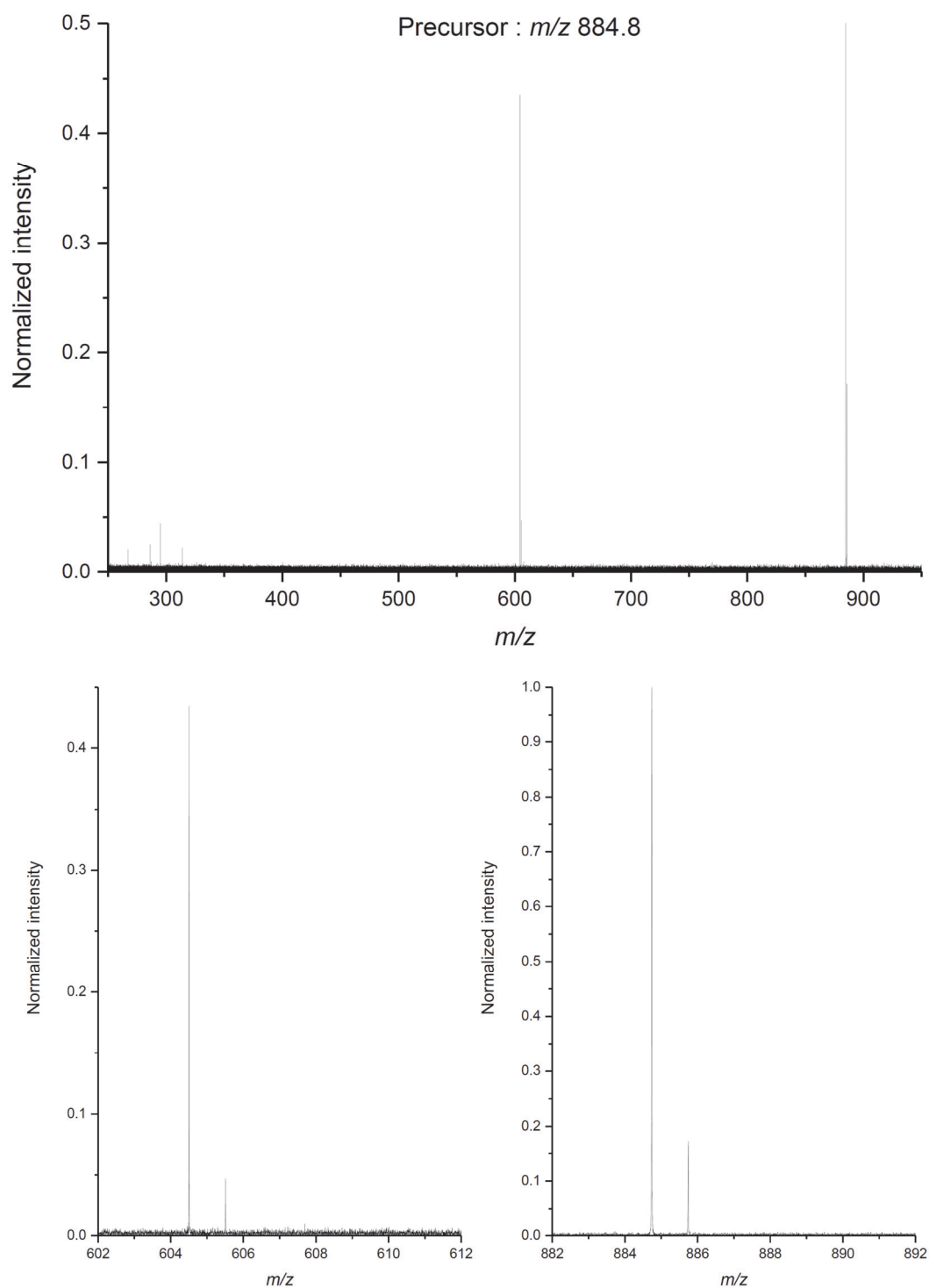


Figure S5e. Classical MS/MS FTICR spectra of sesame oil cationized by $^6\text{Li}^+$ and fragmented by IRMPD: upper panel full MS spectrum, right lower panel zoom on the precursor, left lower panel, zoom on fragments corresponding to the loss of a neutral fatty acid b) precursor m/z 884.7 (quadrupole selection ± 0.5 m/z).

Table S1. Interpretation of fragment spectrum of the monoisotopic peak for a classical acquisition (not-NUS, ie NUS 1).

		Classical acquisition (not NUS, ie NUS 1)						
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
1350.75922	MH ⁺ (+3)	1350.7557	-0.00352	-2.6	2.38E+07	6.08	26.67%	5624
1349.75128	MH ⁺ (+2)	1349.7562	0.00492	3.6	5.13E+07	13.11	57.50%	5581
1348.74334	MH ⁺ (+1)	1348.7466	0.00326	2.4	5.97E+07	15.27	66.98%	5548
1347.7354	MH ⁺	1347.7421	0.0067	5.0	8.91E+07	22.80	100.00%	5595
1333.73272	MH ⁺ -NH3 (+3)	1333.7286	-0.00412	-3.1	1.73E+07	4.43		5823
1332.72478	MH ⁺ -NH3 (+2)	1332.7249	0.00012	0.1	4.17E+07	10.66		5686
1331.71684	MH ⁺ -NH3 (+1)	1331.7236	0.00676	5.1	5.05E+07	12.93		5676
				1315.6942	1.50E+07	3.84		5805
				1314.6936	1.67E+07	4.27		6039
				1306.7248	1.43E+07	3.65		5914
				1305.7246	1.93E+07	4.94		6010
				1304.7313	1.66E+07	4.24		6118
1291.67294	m10 (+1)	1291.7237	0.05076	39.3	1.71E+07	4.37		6201
1290.665	m10	1290.7197	0.0547	42.4	2.29E+07	5.85		5931
				1289.6829	1.07E+07	2.75		5866
				1288.7291	1.33E+07	3.41		5689

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Classical acquisition (not NUS, ie NUS 1)							
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio
				1287.7329	1.74E+07	4.45	5920
				1278.704	1.38E+07	3.53	6228
				1277.7109	1.87E+07	4.79	5944
1275.6905	m5 / m6	1275.7063	0.0158	12.4	1.17E+07	2.98	5935
				1274.7214	1.72E+07	4.40	5905
				1273.689	1.39E+07	3.54	6479
				1271.7236	1.24E+07	3.17	6309
				1270.7166	1.81E+07	4.63	6166
				1262.6656	1.06E+07	2.72	5869
				1261.659	2.86E+07	7.31	5831
				1260.6585	3.46E+07	8.86	6094
				1258.7077	1.21E+07	3.09	6158
				1257.7092	1.54E+07	3.94	6151
				1247.662	1.16E+07	2.96	6183
1219.71872	c10 (+3)	1219.7077	-0.01102	-9.0	1.99E+07	5.10	5.94% 6355
1218.71078	c10 (+2)	1218.7051	-0.00568	-4.7	8.81E+07	22.52	26.27% 6101
1217.70284	c10 (+1)	1217.7021	-0.00074	-0.6	2.46E+08	62.84	73.28% 6172
1216.6949	c10	1216.6996	0.0047	3.9	3.35E+08	85.75	100.00% 6174

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Classical acquisition (not NUS, ie NUS 1)							
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio
				1186.6354	1.07E+07	2.74	6490
1105.62678	c9 (+2)	1105.6195	-0.00728	-6.6	4.40E+07	11.25	20.37% 6798
1104.61884	c9 (+1)	1104.6166	-0.00224	-2.0	1.43E+08	36.63	66.31% 6811
1103.6109	c9	1103.6143	0.0034	3.1	2.16E+08	55.24	100.00% 6819
1079.57074	z9 (+1)	1079.5652	-0.00554	-5.1	2.42E+07	6.19	50.94% 7021
1078.5628	z9	1078.5659	0.0031	2.9	4.75E+07	12.14	100.00% 7009
1048.60528	c8 (+2)	1048.5957	-0.00958	-9.1	3.42E+07	8.75	19.36% 7365
1047.59734	c8 (+1)	1047.594	-0.00334	-3.2	1.14E+08	29.09	64.34% 7209
1046.5894	c8	1046.5924	0.003	2.9	1.77E+08	45.22	100.00% 7226
				1007.5232	1.09E+07	2.78	8016
				1004.5563	1.05E+07	2.68	8002
901.53688	c7 (+2)	901.5272	-0.00968	-10.7	3.78E+07	9.67	13.15% 8438
900.52894	c7 (+1)	900.5251	-0.00384	-4.3	1.46E+08	37.43	50.88% 8378
899.521	c7	899.5219	0.0009	1.0	2.88E+08	73.57	100.00% 8372
				855.5069	2.41E+07	6.16	8901
754.46848	c6 (+2)	754.458	-0.01048	-13.9	1.74E+07	4.46	8.27% 10296
753.46054	c6 (+1)	753.454	-0.00654	-8.7	8.66E+07	22.14	41.09% 9994
752.4526	c6	752.4522	-0.0004	-0.5	2.11E+08	53.88	100.00% 10006

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Classical acquisition (not NUS, ie NUS 1)							
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio
676.38718	MH2+ (+4)	676.3739	-0.01328	-19.6	5.72E+07	14.63	10383
675.88321	MH2+ (+3)	675.8727	-0.01051	-15.6	2.53E+08	64.67	10840
				675.6692	1.39E+07	3.56	9786
675.37924	MH2+ (+2)	675.3719	-0.00734	-10.9	8.44E+08	215.77	10935
674.87527	MH2+ (+1)	674.8711	-0.00417	-6.2	2.00E+09	511.66	10998
674.3713	MH2+	674.3699	-0.0014	-2.1	3.09E+09	789.17	11120
				674.294	4.26E7	10.90	17233
				673.513	1.07E+07	2.75	15794
626.40988	c5 (+2)	626.3981	-0.01178	-18.8	2.28E+07	5.84	5.84% 12439
625.40194	c5 (+1)	625.3958	-0.00614	-9.8	1.33E+08	33.90	33.90% 12014
624.394	c5	624.3929	-0.0011	-1.8	3.91E+08	100.00	100.00% 11976
623.3862	c5 (-1)	623.3854	-0.0008	-1.3	4.94E+07	12.64	11915
552.3091	c9 ²⁺	552.3133	0.0042	7.6	1.55E+07	3.96	13142
497.34334	c4 (+1)	497.3372	-0.00614	-12.3	4.83E+07	12.36	26.35% 15032
496.3354	c4	496.3338	-0.0016	-3.2	1.83E+08	46.91	100.00% 15191
495.3276	c4 (-1)	495.3259	-0.0017	-3.4	4.75E+07	12.15	15255
				424.2523	2.08E+07	5.32	17995

Table S2. Interpretation of fragment spectrum of the monoisotopic peak for a NUS 1/2 acquisition.

		NUS 1/2							
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
1351.74322	MH ⁺ (+4)	1351.7581	0.01488	11.0		2.58E+07	1.70	7.03%	6279
1350.73528	MH ⁺ (+3)	1350.7575	0.02222	16.5		1.00E+08	6.60	27.30%	5648
1349.72734	MH ⁺ (+2)	1349.7545	0.02716	20.1		2.63E+08	17.32	71.64%	5592
1348.7194	MH ⁺ (+1)	1348.7626	0.0432	32.0		9.74E+07	6.42	26.55%	5418
1347.7116	MH ⁺	1347.7411	0.0295	21.9		3.67E+08	24.18	100.00%	5562
1334.71672	MH ⁺ -NH3 (+4)	1334.7255	0.00878	6.6		2.22E+07	1.46		9651
1333.70878	MH ⁺ -NH3 (+3)	1333.728	0.01922	14.4		7.92E+07	5.22		5997
1332.70084	MH ⁺ -NH3 (+2)	1332.7248	0.02396	18.0		2.18E+08	14.39		5657
1331.6929	MH ⁺ -NH3 (+1)	1331.7237	0.0308	23.1		2.33E+08	15.37		5700
					1316.7246	1.36E+07	0.89		10832
					1316.6158	1.46E+07	0.96		7740
					1315.7047	8.48E+07	5.59		7147
					1314.698	8.10E+07	5.34		5764
					1307.7076	1.35E+07	0.89		7779
					1306.7385	6.97E+07	4.60		8669
					1305.7215	9.31E+07	6.14		5746

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NUS 1/2									
m/z theoretical	Assignment (isotope)	m/z assigned	Mass shift	ppm	m/z unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
					1304.7709	9.14E+07	6.02		8382
					1303.7257	1.00E+08	6.61		5765
					1301.7556	1.46E+07	0.96		10765
1293.68882	m10 (+3)	1293.6811	-0.00772	-6.0		2.28E+07	1.50		10299
1292.68088	m10 (+2)	1292.6975	0.01662	12.9		4.17E+07	2.75		8513
1291.67294	m10 (+1)	1291.723	0.05006	38.8		6.60E+07	4.35		5918
1290.665	m10	1290.7237	0.0587	45.5		5.69E+07	3.75		5848
					1289.7971	2.83E+07	1.87		11205
					1289.7046	2.68E+07	1.76		5397
					1289.6371	3.11E+07	2.05		11241
					1288.7439	6.53E+07	4.30		10021
					1285.6974	1.20E+07	0.79		9354
1279.72226	m5 / m6 (+4)	1279.7019	-0.02036	-15.9		2.25E+07	1.48		9152
1278.71432	m5 / m6 (+3)	1278.7084	-0.00592	-4.6		5.77E+07	3.80		3537
1277.70638	m5 / m6 (+2)	1277.6931	-0.01328	-10.4		8.21E+07	5.41		5842
1276.69844	m5 / m6 (+1)	1276.7129	0.01446	11.3		2.24E+07	1.47		7522
1275.6905	m5 / m6	1275.726	0.0355	27.8		7.66E+07	5.05		5560
1274.72448	m11 (+2)	1274.7359	0.01142	9.0		6.00E+07	3.95		5812

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NUS 1/2									
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
1273.71654	m11 (+1)	1273.6908	-0.02574	-20.2		4.94E+07	3.26		4693
1272.7086	m11	1272.7151	0.0065	5.1		1.31E+07	0.87		8175
					1271.7174	6.14E+07	4.05		9343
					1270.7111	7.87E+07	5.19		6925
					1262.6357	5.22E+07	3.44		11306
					1261.6619	1.47E+08	9.70		5884
					1260.6585	1.47E+08	9.66		5995
					1258.69	7.33E+07	4.83		10007
					1257.7071	6.60E+07	4.35		6032
					1249.6948	4.17E+07	2.75		10055
					1248.6352	3.97E+07	2.61		10510
					1241.6911	1.76E+07	1.16		10841
					1240.638	1.58E+07	1.04		10431
					1233.678	1.20E+07	0.79		8864
1219.71872	c10 (+3)	1219.7057	-0.01302	-10.7		6.07E+07	4.00	4.38%	5852
1218.71078	c10 (+2)	1218.7069	-0.00388	-3.2		3.12E+08	20.55	22.51%	6064
					1217.9406	1.87E+07	1.23		10208
1217.70284	c10 (+1)	1217.7026	-0.00024	-0.2		1.14E+09	75.28	82.43%	6154

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		NUS 1/2							
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
1216.6949	c10	1216.6996	0.0047	3.9		1.39E+09	91.31	100.00%	6231
					1216.4428	1.27E+07	0.84		8905
					1204.6508	1.52E+07	1.00		9810
1200.67634	b10 (+1)	1200.6672	-0.00914	-7.6		1.38E+07	0.91	56.88%	10063
1199.6684	b10	1199.6905	0.0221	18.4		2.43E+07	1.60	100.00%	8019
1191.6343	y10	1191.6095	-0.0248	-20.8		1.04E+07	0.68		11666
					1187.6884	2.74E+07	1.81		9018
					1186.6212	3.37E+07	2.22		11162
1106.63472	c9 (+3)	1106.6109	-0.02382	-21.5		3.15E+07	2.08	3.45%	11935
1105.62678	c9 (+2)	1105.6203	-0.00648	-5.9		1.56E+08	10.26	17.01%	6678
					1104.8139	1.18E+07	0.78		12921
1104.61884	c9 (+1)	1104.6168	-0.00204	-1.8		6.44E+08	42.45	70.40%	6804
1103.6109	c9	1103.6149	0.004	3.6		9.15E+08	60.30	100.00%	6709
1094.5815	y9	1094.5753	-0.0062	-5.7		1.88E+07	1.24		9444
1080.55474	z9 (+1)	1080.5557	0.00096	0.9		1.23E+07	0.81	9.71%	6211
1079.5468	z9	1079.5658	0.019	17.6		1.27E+08	8.34	100.00%	6785
1078.539	y9 -NH3 (+1)	1078.5656	0.0266	24.7		2.17E+08	14.33		6932
					1060.5735	1.47E+07	0.97		12752

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance
Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

NUS 1/2									
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
1049.61322	c8 (+3)	1049.6193	0.00608	5.8	1059.5873	2.81E+07	1.85		13769
1048.60528	c8 (+2)	1048.596	-0.00928	-8.8		1.89E+07	1.25	2.42%	9455
1047.59734	c8 (+1)	1047.5941	-0.00324	-3.1		1.27E+08	8.35	16.22%	7281
1046.5894	c8	1046.5924	0.003	2.9		5.26E+08	34.67	67.33%	7242
						7.81E+08	51.48	100.00%	7079
					1021.53	1.64E+07	1.08		7155
					1020.5428	3.53E+07	2.32		14511
					1018.5504	1.07E+07	0.71		8611
					1008.5569	2.11E+07	1.39		11590
					1007.5164	2.50E+07	1.64		9734
					1007.4699	2.23E+07	1.47		11519
					1005.5475	2.37E+07	1.56		4584
					1004.5826	3.44E+07	2.27		10111
					1004.4933	2.61E+07	1.72		12541
					946.5182	1.07E+07	0.70		8889
902.54482	c7 (+3)	902.5243	-0.02052	-22.7		1.88E+07	1.24	1.53%	12735
901.53688	c7 (+2)	901.5294	-0.00748	-8.3		1.42E+08	9.36	11.54%	8479
900.52894	c7 (+1)	900.5242	-0.00474	-5.3		7.16E+08	47.21	58.21%	8320

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance
Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

NUS 1/2									
m/z theoretical	Assignment (isotope)	m/z assigned	Mass shift	ppm	m/z unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
899.521	c7	899.5219	0.0009	1.0		1.23E+09	81.11	100.00%	8413
					856.5093	4.87E+07	3.21		9408
754.46848	c6 (+2)	754.4585	-0.00998	-13.2	855.5079	1.13E+08	7.42		8574
753.46054	c6 (+1)	753.4545	-0.00604	-8.0		6.49E+07	4.27	7.75%	10067
752.4526	c6	752.4525	-1E-04	-0.1		4.02E+08	26.50	48.01%	9933
751.4448	c6 (-1)	751.4238	-0.021	-27.9		8.37E+08	55.19	100.00%	9976
676.38718	MH ²⁺ (+4)	676.3713	-0.01588	-23.5		2.45E+07	1.62		13194
675.88321	MH ²⁺ (+3)	675.8712	-0.01201	-17.8		7.03E+07	4.63		10838
						5.16E+08	34.02		11099
					675.6994	1.89E+07	1.24		16604
					675.6646	2.17E+07	1.43		12371
					675.636	1.48E+07	0.98		22276
					675.5551	1.35E+07	0.89		19818
675.37924	MH ²⁺ (+2)	675.3721	-0.00714	-10.6		2.59E+09	170.71		10892
					675.2299	3.08E+07	2.03		17706
					675.1908	2.22E+07	1.47		20636
					675.1592	2.08E+07	1.37		20501
					675.1224	2.29E+07	1.51		17941

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance
Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

NUS 1/2									
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
674.87527	MH ²⁺ (+1)	674.871	-0.00427	-6.3	675.0871	2.75E+07	1.81		19322
674.3713	MH ²⁺	674.3698	-0.0015	-2.2	675.0517	3.15E+07	2.08		20482
						8.32E+09	548.37		10999
						1.65E+10	1086.59		11186
					674.2937	2.30E+08	15.17		17226
					673.8217	2.07E+07	1.36		22124
					673.6689	1.16E+07	0.77		20532
					673.5557	2.42E+07	1.60		17517
					673.4858	1.58E+07	1.04		21134
					673.4136	1.43E+07	0.94		19065
					665.86	2.50E+07	1.65		14273
626.40988	c5 (+2)	626.3982	-0.01168	-18.6		7.90E+07	5.20	5.20%	12452
625.40194	c5 (+1)	625.3953	-0.00664	-10.6		6.38E+08	42.02	42.02%	11768
624.394	c5	624.3929	-0.0011	-1.8		1.52E+09	100.00	100.00%	11892
623.3862	c5 (-1)	623.3851	-0.0011	-1.8		2.28E+08	15.02		12083
607.3675	b5	607.3685	0.001	1.6		1.18E+07	0.78		16895
					606.3847	1.02E+07	0.67		13898
					553.3202	1.72E+07	1.13		9261

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance
Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

NUS 1/2							
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized Isotopic ratio
552.3091	c9 ²⁺	552.3124				6.91E+07	4.55
497.34334	c4 (+1)	497.3366				2.03E+08	13.39
496.3354	c4	496.3338				6.78E+08	29.97%
495.3276	c4 (-1)	495.3258				1.96E+08	44.69
						1.19E+07	100.00%
					425.2555	1.27E+07	12.90
					425.2504	0.79	0.84
					424.2523	27752	5.23
254.1612	b2	254.158				7.94E+07	1.56
						2.36E+07	43673

Table S3. Interpretation of fragment spectrum of the monoisotopic peak for a NUS 1/4 acquisition.

NUS 1/4									
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
1350.75922	MH ⁺ (+3)	1350.7823	0.02308	17.1		4.25E+07	0.57	3.67%	6602
1349.75128	MH ⁺ (+2)	1349.7531	0.00182	1.3		6.98E+08	9.29	60.21%	5216
1348.74334	MH ⁺ (+1)	1348.752	0.00866	6.4		1.16E+09	15.43	100.00%	5549
1347.7354	MH ⁺	1347.7399	0.0045	3.3		1.09E+09	14.52	94.07%	5642
1333.70878	MH ⁺ -NH3 (+2)	1333.7235	0.01472	11.0		2.71E+07	0.36		9496
1332.70084	MH ⁺ -NH3 (+1)	1332.7256	0.02476	18.6		4.04E+08	5.38		5880
1331.6929	MH ⁺ -NH3 +1)	1331.7234	0.0305	22.9		6.40E+08	8.52		5600
					1315.7342	8.74E+07	1.16		9077
					1314.6967	2.34E+08	3.11		6011
					1306.7347	4.48E+07	0.60		5641
					1305.7159	2.08E+08	2.77		5674
					1304.8106	7.42E+07	0.99		10477
					1304.7242	7.16E+07	0.95		3936
					1304.655	7.38E+07	0.98		8940
					1303.7287	2.71E+08	3.60		6193
					1302.7097	1.22E+07	0.16		5591

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance
Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

NUS 1/4									
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
					1301.76	2.65E+07	0.35		11136
					1293.6652	1.39E+07	0.18		5437
1291.67294	m10 (+1)	1291.719	0.04606	35.7		1.54E+08	2.06		5917
1290.665	m10	1290.7158	0.0508	39.4		2.90E+08	3.86		6075
					1288.7777	6.05E+07	0.81		9934
					1287.72	1.21E+08	1.61		7454
					1285.7249	1.79E+07	0.24		7575
					1284.785	1.90E+07	0.25		10800
					1284.7399	1.95E+07	0.26		9155
					1277.7069	2.25E+08	3.00		5172
					1275.7257	1.49E+08	1.99		5277
					1274.7228	2.31E+08	3.07		5061
					1273.7233	1.10E+08	1.47		10303
					1271.7506	5.98E+07	0.80		8867
					1270.7075	2.22E+08	2.96		8390
					1261.6633	2.84E+08	3.78		5897
					1260.6609	4.34E+08	5.78		5850
					1258.6982	8.76E+07	1.17		9052

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance
Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

NUS 1/4									
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
1257.6647	m7 / m8	1257.7056	0.0409	32.5		2.05E+08	2.73		6337
					1256.6642	3.06E+07	0.41		3754
					1253.6746	2.24E+07	0.30		8697
					1249.7288	4.60E+07	0.61		10544
					1249.6575	4.35E+07	0.58		6747
					1248.6563	4.56E+07	0.61		6277
					1247.7053	6.77E+07	0.90		8264
					1244.6608	1.05E+07	0.14		5974
					1243.6635	1.36E+07	0.18		8010
					1240.6756	4.08E+07	0.54		11159
					1232.6385	2.10E+07	0.28		8529
1219.71872	c10 (+3)	1219.7192	0.00048	0.4		2.67E+07	0.36	0.68%	8116
1218.71078	c10 (+2)	1218.7243	0.01352	11.1		6.05E+07	0.81	1.53%	6680
					1217.9511	4.52E+07	0.60		10681
1217.70284	c10 (+1)	1217.7036	0.00076	0.6		2.17E+09	28.83	54.93%	6263
1216.6949	c10	1216.7004	0.0055	4.5		3.94E+09	52.49	100.00%	6346
					1204.6614	1.58E+07	0.21		5045
					1203.6667	3.28E+07	0.44		9223

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance
Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

NUS 1/4									
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
1199.6684	b10	1199.6611	-0.0073	-6.1	1201.5976	2.12E+07	0.28		12527
						5.20E+07	0.69	100.00%	7388
1191.6343	y10	1191.6314	-0.0029	-2.4	1199.6062	5.14E+07	0.68		11753
1189.6187	Y10	1189.5942	-0.0245	-20.6		2.39E+07	0.32		11079
						2.02E+07	0.27		12043
					1187.6551	2.83E+07	0.38		7021
					1187.592	2.86E+07	0.38		6917
					1186.6438	7.15E+07	0.95		6128
1105.62678	c9 (+2)	1105.6286	0.00182	1.6		4.41E+07	0.59	1.52%	12330
1104.61884	c9 (+1)	1104.6182	-0.00064	-0.6		1.32E+09	17.60	45.42%	6848
1103.6109	c9	1103.6155	0.0046	4.2		2.91E+09	38.76	100.00%	6761
					1094.5723	8.48E+07	1.13		11108
1086.5843	b9	1086.6056	0.0213	19.6		1.21E+07	0.16		11373
1080.55474	z9 (+1)	1080.5792	0.02446	22.6		1.01E+08	1.34	23.94%	7990
1079.5468	z9	1079.5719	0.0251	23.2		4.22E+08	5.61	100.00%	7126
1078.539	y9 -NH3	1078.567	0.028	26.0		6.81E+08	9.07		7325
					1077.5488	2.81E+07	0.37		8645
					1060.5639	1.91E+07	0.25		10567

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance
Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

NUS 1/4								
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio
1048.60528	c8 (+2)	1048.6195	0.01422	13.6	1059.6058	6.34E+07	0.84	10408
1047.59734	c8 (+1)	1047.5961	-0.00124	-1.2		3.63E+07	0.48	13822
1046.5894	c8	1046.5928	0.0034	3.2		1.12E+09	14.90	6845
						2.66E+09	35.38	7082
					1045.5602	1.71E+07	0.23	13182
					1031.5934	1.08E+07	0.14	11273
					1031.5673	1.04E+07	0.14	8226
1029.5629	b8	1029.5628	-1E-04	-0.1		1.28E+07	0.17	9330
					1022.4944	2.09E+07	0.28	12924
					1021.558	2.36E+07	0.31	11830
					1021.5293	2.54E+07	0.34	14780
					1020.5387	7.89E+07	1.05	12957
					1018.5376	1.12E+07	0.15	14941
					1017.5768	4.90E+07	0.65	11215
					1008.5495	2.98E+07	0.40	12031
					1008.4955	4.00E+07	0.53	14737
					1007.4909	8.87E+07	1.18	13064
					1005.5373	3.26E+07	0.43	12994

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance
Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

NUS 1/4									
m/z theoretical	Assignment (isotope)	m/z assigned	Mass shift	ppm	m/z unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
					1004.5154	8.79E+07	1.17		12983
					1003.5646	2.33E+07	0.31		10688
					1002.5885	1.17E+07	0.16		9756
					986.5795	1.57E+07	0.21		15189
					946.5152	2.84E+07	0.38		9160
					933.5082	2.28E+07	0.30		12497
					933.4852	2.37E+07	0.32		14957
901.53688 c7 (+2)		901.5363	-0.00058	-0.6		5.69E+07	0.76	1.18%	10434
900.52894 c7 (+1)		900.5243	-0.00464	-5.2		1.65E+09	21.93	34.16%	8059
899.521 c7		899.5222	0.0012	1.3		4.82E+09	64.20	100.00%	8673
					898.5481	2.66E+07	0.35		16299
882.4944 b7		882.497	0.0026	2.9		1.98E+07	0.26		12773
					857.5131	2.02E+07	0.27		17775
					856.5111	1.88E+08	2.50		8789
					855.5066	4.33E+08	5.77		7993
					839.4859	1.15E+07	0.15		14241
754.46848 c6 (+2)		754.4635	-0.00498	-6.6		3.55E+07	0.47	0.95%	14141
753.46054 c6 (+1)		753.4547	-0.00584	-7.8		1.01E+09	13.43	26.90%	9388

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance
Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

NUS 1/4									
m/z theoretical	Assignment (isotope)	m/z assigned	Mass shift	ppm	m/z unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
752.4526	c6	752.4523	-0.0003	-0.4		3.75E+09	49.92	100.00%	10309
					751.4332	9.42E+07	1.25		18598
735.426	b6	735.4223	-0.0037	-5.0		1.60E+07	0.21		11465
					734.4389	1.12E+07	0.15		19195
					708.4366	1.53E+07	0.20		10885
					675.9396	1.77E+07	0.24		22212
675.88321	MH ²⁺ (+3)	675.883	-0.00021	-0.3		3.98E+08	5.29		12605
675.37924	MH ²⁺ (+2)	675.3747	-0.00454	-6.7		1.23E+09	16.39		12050
					675.2992	5.62E+07	0.75		14473
					675.2242	5.96E+07	0.79		22180
					675.0785	3.83E+07	0.51		19150
					675.0439	4.31E+07	0.57		22097
					675.0153	9.90E+07	1.32		17928
674.87527	MH ²⁺ (+1)	674.8711	-0.00417	-6.2		1.55E+10	206.69		10934
					674.7019	8.41E+07	1.12		18827
674.3713	MH ²⁺	674.3697	-0.0016	-2.4		5.48E+10	729.56		11305
					673.5938	2.64E+07	0.35		22483
					665.8588	1.16E+08	1.54		16486

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance
Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

NUS 1/4									
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
626.40988	c5 (+2)	626.3998	-0.01008	-16.1	656.852	1.89E+07	0.25		10169
625.40194	c5 (+1)	625.3952	-0.00674	-10.8		4.54E+07	0.60	0.60%	14813
624.394	c5	624.3925	-0.0015	-2.4		1.71E+09	22.74	22.74%	11525
623.3862	c5 (-1)	623.3841	-0.0021	-3.4		7.51E+09	100.00	100.00%	12048
607.3675	b5	607.3701	0.0026	4.3		1.02E+09	13.51		12400
						3.36E+07	0.45		12786
					606.3779	3.43E+07	0.46		12604
					600.337	3.26E+07	0.43		21645
					553.323	3.34E+07	0.44		19855
552.3091	c9 ²⁺	552.3125	0.0034	6.2		3.38E+08	4.50		12399
					524.3035	1.64E+07	0.22		18518
497.34334	c4 (+1)	497.3365	-0.00684	-13.8		5.42E+08	7.21	16.71%	14872
496.3354	c4	496.3334	-0.002	-4.0		3.24E+09	43.19	100.00%	15255
495.3276	c4 (-1)	495.3256	-0.002	-4.0		8.82E+08	11.74		15291
479.3089	b4	479.3065	-0.0024	-5.0		1.20E+07	0.16		20506
					478.3209	2.02E+07	0.27		20610
					453.3268	2.16E+07	0.29		30506
					425.2538	3.07E+07	0.41		28387

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Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

NUS 1/4									
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
382.2561 b3		382.2523	-0.0038	-9.9	424.2521	4.09E+08	5.45		17663
						1.17E+07	0.16		32853
					364.2445	2.20E+07	0.29		24399
					354.1759	1.01E+07	0.13		13291
					271.1864	1.35E+08	1.79		28639
					270.1801	1.57E+07	0.21		55436
					254.159	1.58E+08	2.10		46992
					243.1451	1.17E+07	0.16		56376
					243.1433	1.22E+07	0.16		53572
					237.1329	2.04E+07	0.27		28226
					226.153	1.28E+07	0.17		42999
					226.1177	3.02E+07	0.40		55868

Table S4. Interpretation of fragment spectrum of the monoisotopic peak for a NUS 1/8 acquisition.

		NUS 1/8							
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio	Resolutio n
1350.73528	MH ⁺ (+3)	1350.7586	0.02332	17.3		5.53E+07	0.46	2.93%	8950
1349.72734	MH ⁺ (+2)	1349.7526	0.02526	18.7		1.93E+08	1.60	10.23%	6044
1348.7194	MH ⁺ (+1)	1348.7468	0.0274	20.3		1.89E+09	15.63	100.00%	6405
1347.7116	MH ⁺	1347.7353	0.0237	17.6		1.88E+09	15.51	99.27%	5432
1332.70084	MH ⁺ -NH3 (+2)	1332.7177	0.01686	12.7		9.83E+07	0.81		5781
1331.6929	MH ⁺ -NH3 (+1)	1331.7191	0.0262	19.7		1.07E+09	8.88		5097
					1314.6827	3.71E+08	3.07		5290
					1305.7188	3.46E+08	2.86		3458
					1303.7219	4.55E+08	3.77		6133
					1301.7091	2.56E+07	0.21		7279
					1292.6791	4.01E+07	0.33		5703
					1292.6191	3.86E+07	0.32		8043
					1291.7399	4.65E+07	0.38		5893
1290.665	m10	1290.7155	0.0505	39.1		5.03E+08	4.16		5864
					1289.7092	7.47E+07	0.62		7230
					1287.7523	1.31E+08	1.08		7475

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NUS 1/8							
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio
				1284.7133	2.65E+07	0.22	9156
				1277.6968	3.95E+08	3.26	5570
				1275.8314	2.33E+07	0.19	10992
				1274.7155	3.76E+08	3.11	7731
				1273.6571	1.03E+08	0.85	6408
				1270.8003	1.43E+08	1.18	8836
				1261.6745	6.51E+07	0.54	6734
				1260.6532	7.12E+08	5.89	5624
1257.68854	m7 / m8 (+1)	1257.6984	0.00986	7.8	3.45E+08	2.86	6517
1256.6806	m7 / m8	1256.6752	-0.0054	-4.3	3.49E+07	0.29	5937
				1253.6683	3.59E+07	0.30	11462
				1249.6591	6.51E+07	0.54	7063
				1247.6373	9.27E+07	0.77	9836
				1245.6728	1.14E+07	0.09	8823
				1243.6301	2.11E+07	0.17	7504
				1240.6966	3.71E+07	0.31	7600
				1234.6647	1.03E+07	0.09	11611
				1232.6586	2.55E+07	0.21	9607

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance
Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

NUS 1/8							
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio Resolution
1219.71872 c10 (+3)		1219.7007	-0.01802 -14.8	1221.6584	1.12E+07	0.09	9984
1218.71078 c10 (+2)		1218.6971	-0.01368 -11.2		1.88E+07	0.16	5436
1217.70284 c10 (+1)		1217.7046	0.00176 1.4		1.03E+08	0.85	10800
1216.6949 c10		1216.6969	0.002 1.6		4.63E+08	3.83	7139
1215.6871 c10 (-1)		1215.7119	0.0248 20.4		6.77E+09	56.03	6005
					1.13E+07	0.09	7608
				1204.5967	1.76E+07	0.15	10107
				1203.6956	4.04E+07	0.33	11413
				1202.6042	1.30E+07	0.11	11495
				1201.6269	1.96E+07	0.16	9581
1199.6684 b10		1199.6606	-0.0078 -6.5		8.18E+07	0.68	6849
1191.6343 y10		1191.648	0.0137 11.5		2.30E+07	0.19	9841
				1189.5943	2.81E+07	0.23	11076
				1186.6805	7.20E+07	0.60	10487
				1130.5868	1.49E+07	0.12	8685
				1115.595	1.36E+07	0.11	9200
1105.62678 c9 (+2)		1105.6082	-0.01858 -16.8		6.01E+07	0.50	10851
1104.61884 c9 (+1)		1104.6186	-0.00024 -0.2		3.09E+08	2.56	7212

		NUS 1/8							
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio	Resolutio n
1103.6109	c9	1103.6116	0.0007	0.6		5.11E+09	42.28	100.00%	7059
1094.5815	y9	1094.5972	0.0157	14.3		9.62E+07	0.80		4389
1086.5843	b9	1086.5921	0.0078	7.2		1.99E+07	0.16		7163
1080.55474	z9 (+1)	1080.5743	0.01956	18.1		4.41E+07	0.37	12.54%	7246
1079.5468	z9	1079.5726	0.0258	23.9		3.52E+08	2.91	100.00%	8070
1078.539	y9 -NH3	1078.5639	0.0249	23.1		1.11E+09	9.17		6758
					1077.5503	4.54E+07	0.38		10778
			-		1059.6222	5.44E+07	0.45		9163
1048.60528	c8 (+2)	1048.6207	0.01542	14.7		3.65E+07	0.30	0.80%	7250
1047.59734	c8 (+1)	1047.5975	0.00016	0.2		2.72E+08	2.25	6.00%	7987
1046.5894	c8	1046.5891	-0.0003	-0.3		4.54E+09	37.52	100.00%	7230
					1045.5734	1.67E+07	0.14		8728
					1031.5601	1.23E+07	0.10		6914
1029.5629	b8	1029.5535	-0.0094	-9.1		1.77E+07	0.15		5447
					1022.5303	2.11E+07	0.17		10126
					1020.534	7.58E+07	0.63		7679
					1017.5276	6.29E+07	0.52		11825
					1007.523	1.02E+08	0.84		7343

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NUS 1/8							
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio
				1004.5405	1.05E+08	0.86	10189
				1003.591	3.05E+07	0.25	6904
				1002.5843	1.58E+07	0.13	9168
				1002.5623	1.62E+07	0.13	13765
				986.5592	1.91E+07	0.16	12036
				948.4899	1.03E+07	0.09	6812
				946.5148	4.74E+07	0.39	12802
				933.5014	3.14E+07	0.26	11781
901.53688 c7 (+2)		901.5465	0.00962	10.7	4.73E+07	0.39	0.59%
900.52894 c7 (+1)		900.5236	-0.00534	-5.9	4.21E+08	3.49	5.29%
899.521 c7		899.5189	-0.0021	-2.3	7.97E+09	65.91	100.00%
898.5132 c7 (-1)		898.5151	0.0019	2.1	3.53E+07	0.29	
882.4944 b7		882.4897	-0.0047	-5.3	2.60E+07	0.22	
		881.4993			1.21E+07	0.10	8408
		856.5139			1.58E+08	1.31	10173
		855.505			7.07E+08	5.85	9532
		839.4869			1.62E+07	0.13	12990
		756.423			1.74E+07	0.14	16047

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance
Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

		NUS 1/8							
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio	Resolutio n
753.46054	c6 (+1)	753.4533	-0.00724	-9.6		2.44E+08	2.02		10976
752.4526	c6	752.4491	-0.0035	-4.7	752.5488	4.73E+07	0.39		13158
751.4448	c6 (-1)	751.4458	0.001	1.3		6.10E+09	50.46		9503
735.426	b6	735.4233	-0.0027	-3.7		9.21E+07	0.76		12462
						2.59E+07	0.21		12265
					734.4453	1.49E+07	0.12		10881
					708.4362	1.45E+07	0.12		17089
					676.0145	4.22E+07	0.35		21322
675.88321	MH ²⁺ (+3)	675.8779	-0.00531	-7.9		4.30E+08	3.55		17571
675.37924	MH ²⁺ (+2)	675.3719	-0.00734	-10.9		1.95E+09	16.16		11135
					675.2866	3.26E+07	0.27		19683
674.87527	MH ²⁺ (+1)	674.8719	-0.00337	-5.0		6.48E+09	53.63		11097
674.3713	MH ²⁺	674.3685	-0.0028	-4.2		9.66E+10	799.28		11100
					665.8543	1.31E+08	1.09		10274
					656.8515	2.77E+07	0.23		11928
625.40194	c5 (+1)	625.3958	-0.00614	-9.8		3.78E+08	3.13	3.13%	12287
624.394	c5	624.3911	-0.0029	-4.6		1.21E+10	100.00	100.00%	11133
623.3862	c5 (-1)	623.3831	-0.0031	-5.0		1.60E+09	13.27		12028

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Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

NUS 1/8							
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio
607.3675 b5		607.3585	-0.009	-14.8	4.79E+07	0.40	18771
600.3378 b10 ²⁺				606.3813	4.76E+07	0.39	17155
		600.3361	-0.0017	-2.8	3.98E+07	0.33	12591
				591.3329	1.17E+07	0.10	17672
				581.388	1.25E+07	0.10	16613
				565.3529	1.46E+07	0.12	9542
552.3091 c9 ²⁺		552.3113	0.0022	4.0	5.49E+08	4.54	13308
497.34334 c4 (+1)		497.3368	-0.00654	-13.2	2.14E+07	0.18	25938
496.3354 c4		496.3327	-0.0027	-5.4	1.51E+08	1.25	2.79%
495.3276 c4 (-1)		495.3247	-0.0029	-5.9	5.40E+09	44.63	100.00%
479.3089 b4		479.3045	-0.0044	-9.2	1.43E+09	11.85	14865
					1.42E+07	0.12	16520
				478.3238	2.74E+07	0.23	23433
				453.3272	2.15E+07	0.18	24574
				424.2516	6.58E+08	5.44	17498
382.2561 b3		382.2544	-0.0017	-4.4	1.25E+07	0.10	14865
				364.2426	2.99E+07	0.25	21816
				356.2756	1.57E+07	0.13	29498

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Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

NUS 1/8							
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio
							Resolution
		354.1753		1.37E+07	0.11		27820
		254.1598		1.76E+08	1.45		38773
		243.1436		1.34E+07	0.11		34591
		237.1329		2.95E+07	0.24		36946
		226.1536		1.61E+07	0.13		26690
		226.1169		3.59E+07	0.30		22630

Table S5. Interpretation of fragment spectrum of the monoisotopic peak for a NUS 1/16 acquisition.

NUS 1/16									
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
1350.75922	MH ⁺ (+3)	1350.7732	0.01398	10.3		6.95E+07	0.53	3.88%	8726
1349.75128	MH ⁺ (+2)	1349.7442	-0.00708	-5.2		2.26E+08	1.74	12.64%	5959
1348.74334	MH ⁺ (+1)	1348.7251	-0.01824	-13.5		1.10E+09	8.44	61.27%	7561
1347.7354	MH ⁺	1347.7285	-0.0069	-5.1		1.79E+09	13.78	100.00%	5930
					1332.7259	1.06E+08	0.81		6567
					1331.6975	9.63E+08	7.40		8392
					1314.6991	2.92E+08	2.24		4059
					1305.6985	3.29E+08	2.53		9032
					1303.7216	3.66E+08	2.82		7426
					1301.7689	2.84E+07	0.22		6812
1292.68088	m10 (+2)	1292.7054	0.02452	19.0		5.63E+07	0.43		7582
1291.67294	m10 (+1)	1291.7178	0.04486	34.7		6.22E+07	0.48		7433
1290.665	m10	1290.7165	0.0515	39.9		5.22E+08	4.01		6673
					1289.6997	7.37E+07	0.57		8829
					1288.6217	2.46E+07	0.19		10769
					1287.7334	1.26E+08	0.97		5805

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NUS 1/16							
m/z theoretical	Assignment (isotope)	m/z assigned	Mass shift	ppm	m/z unassigned	Relative intensity	Normalized Isotopic ratio Resolution
					1284.7216	2.62E+07	0.20 7464
					1277.6856	3.19E+08	2.45 5414
					1273.6741	1.05E+08	0.81 7738
					1267.6417	1.01E+07	0.08 4692
					1261.6548	7.88E+07	0.61 7983
					1260.6905	5.33E+08	4.10 7126
					1260.6249	5.74E+08	4.42 7702
1256.6806	m7 / m8	1256.6645	-0.0161	-12.8		3.88E+07	0.30 10208
					1253.6656	3.13E+07	0.24 6038
					1249.6546	6.29E+07	0.48 4681
1247.648	m1	1247.6341	-0.0139	-11.1		7.99E+07	0.61 4000
					1245.6803	1.23E+07	0.09 3308
					1243.6456	2.36E+07	0.18 6069
1242.7106	da11	1242.6789	-0.0317	-25.5		1.13E+07	0.09 11495
					1240.6667	4.00E+07	0.31 7393
					1234.6392	1.49E+07	0.11 8307
					1233.6611	1.05E+07	0.08 11171
					1232.6602	2.53E+07	0.19 6864

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance
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NUS 1/16								
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio
					1221.6463	1.07E+07	0.08	6815
1218.71078	c10 (+2)	1218.7157	0.00492	4.0		1.46E+08	1.12	2.18%
					1218.6737	1.42E+08	1.09	8872
1217.70284	c10 (+1)	1217.7054	0.00256	2.1		6.19E+08	4.76	9.21%
1216.6949	c10	1216.6959	0.001	0.8		6.72E+09	51.63	100.00%
1215.6871	c10 (-1)	1215.7121	0.025	20.6		1.31E+07	0.10	9039
					1214.5869	1.18E+07	0.09	12089
					1204.6139	1.86E+07	0.14	5466
					1203.6833	3.59E+07	0.28	5962
					1202.6111	1.83E+07	0.14	7238
					1201.6415	2.00E+07	0.15	8033
1199.6684	b10	1199.6534	-0.015	-12.5		7.72E+07	0.59	100.00%
1191.6343	y10	1191.6341	-0.0002	-0.2		2.58E+07	0.20	8167
					1190.6127	1.12E+07	0.09	10371
1189.6187	Y10	1189.6169	-0.0018	-1.5		2.46E+07	0.19	7323
					1186.6432	7.28E+07	0.56	7359
1182.6418	b10 -NH3	1182.6463	0.0045	3.8		1.15E+07	0.09	8418
					1175.6546	1.05E+07	0.08	7483

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NUS 1/16							
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized Isotopic ratio Resolution
					1130.5706	1.21E+07	0.09 6584
					1115.5856	1.27E+07	0.10 6489
1105.62678 c9 (+2)		1105.6236	-0.00318	-2.9		8.01E+07	0.62 1.57% 9852
1104.61884 c9 (+1)		1104.6057	-0.01314	-11.9		4.37E+08	3.36 8.56% 8750
1103.6109 c9		1103.6189	0.008	7.2		5.11E+09	39.29 100.00% 4334
1094.5815 y9		1094.5842	0.0027	2.5		9.38E+07	0.72 8602
1086.5843 b9		1086.5743	-0.01	-9.2		2.04E+07	0.16 6743
1080.55474 z9 (+1)		1080.5669	0.01216	11.3		5.58E+07	0.43 22.71% 7209
1079.5468 z9		1079.5548	0.008	7.4		2.46E+08	1.89 100.00% 11808
1078.539 y9 -NH3		1078.5744	0.0354	32.8		9.19E+08	7.07 8813
					1078.541	9.10E+08	7.00 9628
					1077.5539	4.04E+07	0.31 7199
					1076.5687	1.05E+07	0.08 11154
					1059.6037	5.40E+07	0.41 8847
1048.60528 c8 (+2)		1048.5967	-0.00858	-8.2		6.57E+07	0.51 1.47% 6417
1047.59734 c8 (+1)		1047.5926	-0.00474	-4.5		3.64E+08	2.80 8.14% 6494
1046.5894 c8		1046.5847	-0.0047	-4.5		4.47E+09	34.38 100.00% 6060
1045.5816 c8 (-1)		1045.5655	-0.0161	-15.4		1.79E+07	0.14 9950

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance
Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

NUS 1/16							
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized Isotopic ratio Resolution
1029.5629 b8		1031.5697				1.38E+07	0.11 8239
		1029.5469	-0.016	-15.5		1.65E+07	0.13 5966
					1022.508	2.28E+07	0.18 9829
					1020.5408	7.93E+07	0.61 6350
					1018.5474	1.02E+07	0.08 6943
					1017.5569	4.98E+07	0.38 6906
					1008.5141	3.63E+07	0.28 13427
					1007.5142	1.02E+08	0.78 8556
					1004.5365	1.02E+08	0.78 8814
					1003.5787	3.02E+07	0.23 8145
					1002.5745	1.46E+07	0.11 12134
					986.5629	1.67E+07	0.13 4578
					948.4683	1.30E+07	0.10 9513
					946.5087	4.24E+07	0.33 6732
					933.5037	2.86E+07	0.22 8970
901.53688 c7 (+2)		901.5276	-0.00928	-10.3		7.17E+07	0.55 0.91% 7079
900.52894 c7 (+1)		900.5219	-0.00704	-7.8		5.27E+08	4.05 6.72% 6798
899.521 c7		899.514	-0.007	-7.8		7.85E+09	60.35 100.00% 7901

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance
Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

NUS 1/16									
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
898.5132	c7 (-1)	898.5212	0.008	8.9		2.98E+07	0.23		7965
882.4944	b7	882.4995	0.0051	5.8		2.52E+07	0.19		8027
					881.5042	1.40E+07	0.11		8401
					856.5054	1.29E+08	0.99		11618
					855.508	6.28E+08	4.83		7647
					839.4769	1.77E+07	0.14		11158
					756.4249	1.55E+07	0.12		12427
754.46848	c6 (+2)	754.4619	-0.00658	-8.7		3.23E+07	0.25	0.56%	14269
753.46054	c6 (+1)	753.4509	-0.00964	-12.8		3.30E+08	2.54	5.74%	11078
					752.5445	2.25E+07	0.17		18925
752.4526	c6	752.4512	-0.0014	-1.9		5.75E+09	44.19	100.00%	7787
751.4448	c6 (-1)	751.4433	-0.0015	-2.0		8.68E+07	0.67		13408
735.426	b6	735.423	-0.003	-4.1		2.70E+07	0.21		13692
					734.4391	1.53E+07	0.12		6477
					708.4339	1.65E+07	0.13		9577
676.38718	MH ²⁺ (+4)	676.3765	-0.01068	-15.8		5.69E+07	0.44		13396
675.88321	MH ²⁺ (+3)	675.883	-0.00021	-0.3		2.37E+08	1.82		18422
675.37924	MH ²⁺ (+2)	675.3728	-0.00644	-9.5		1.37E+09	10.54		14366

NUS 1/16

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Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

NUS 1/16									
m/z theoretical	Assignment (isotope)	m/z assigned	Mass shift	ppm	m/z unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
496.3354 c4	c4 (-1)	496.3323	-0.0031	-6.2		5.89E+09	45.30	100.00%	13462
495.3276 c4 (-1)		495.3243	-0.0033	-6.7		1.55E+09	11.88		14581
479.3089 b4		479.3064	-0.0025	-5.2		1.57E+07	0.12		20530
					478.3212	2.43E+07	0.19		15080
	b3				453.3274	1.99E+07	0.15		24174
					424.2513	7.54E+08	5.80		17256
382.2561 b3		382.2543	-0.0018	-4.7		1.24E+07	0.10		27383
					364.2428	2.74E+07	0.21		19818
	b2				356.2749	1.17E+07	0.09		29183
					354.1741	1.43E+07	0.11		24575
254.1612 b2		254.1592	-0.002	-7.9		1.45E+08	1.12		31040
					243.1436	1.43E+07	0.11		29220
	b2 -NH3					2.73E+07	0.21		37061
237.1346 b2 -NH3		237.1326	-0.002	-8.4		1.53E+07	0.12		36350
					226.1528	3.40E+07	0.26		34814
					224.7898	8.19E+07	0.63		31193

Table S6. Interpretation of fragment spectrum of the monoisotopic peak for a NUS 1/32 acquisition.

NUS 1/32									
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
					1314.6906	3.08E+07	0.7		9444
					1303.689	4.19E+07	0.9		9128
					1301.7581	1.45E+07	0.3		6521
					1287.7194	4.70E+07	1.0		6914
					1273.6736	4.62E+07	1.0		7159
					1260.7161	5.33E+07	1.2		10760
					1260.6594	5.97E+07	1.3		9347
					1256.6544	1.63E+07	0.4		6237
					1253.6858	1.14E+07	0.2		2774
					1203.6823	1.57E+07	0.3		7045
1199.6684	b10	1199.6668	-0.0016	-1.3		4.01E+07	0.9	100.00%	6561
					1191.6266	1.22E+07	0.3		7703
					1189.6136	1.02E+07	0.2		8583
		1103.6289	0.018	16.3		1.75E+09	37.8	100.00%	10093
		1094.5715	-0.01	-9.1		7.20E+07	1.6		8447
1086.5843	b9	1086.5778	-0.0065	-6.0		1.16E+07	0.3		7073

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Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

NUS 1/32									
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio	Resolution
1077.539	y9 -NH3	1077.5548	0.0158	14.7		3.46E+07	0.7		6490
1046.5894	c8	1046.6326	0.0432	41.3		1.27E+09	27.5	100.00%	12186
1029.5629	b8	1029.5549	-0.008	-7.8	1274.7263	1.28E+07	0.3		7373
					1020.5309	3.54E+07	0.8		9253
					1017.5446	2.79E+07	0.6		9293
					1003.5788	1.63E+07	0.4		9726
					986.5473	1.05E+07	0.2		11345
					946.5158	3.14E+07	0.7		9048
					933.5107	1.38E+07	0.3		9647
899.521	c7	899.5228	0.0018	2.0		1.74E+09	37.5	100.00%	8171
882.4944	b7	882.4895	-0.0049	-5.6		1.88E+07	0.4		9051
					855.5016	7.09E+07	1.5		11205
752.4526	c6	752.4437	-0.0089	-11.8		1.64E+09	35.4	100.00%	6466
735.426	b6	735.4215	-0.0045	-6.1		1.73E+07	0.4		10080
674.3713	MH ²⁺	674.3678	-0.0035	-5.2		7.41E+10	1600.1		10170
					665.8546	1.21E+08	2.6		12197
					656.8511	2.23E+07	0.5		8415
624.394	c5	624.4026	0.0086	13.8		4.63E+09	100.0	100.00%	20318

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NUS 1/32								
<i>m/z</i> theoretical	Assignment (isotope)	<i>m/z</i> assigned	Mass shift	ppm	<i>m/z</i> unassigned	Relative intensity	Normalized	Isotopic ratio
623.3862	c5 (-1)	623.3809	-0.0053	-8.5		5.29E+08	11.4	21488
607.3675	b5	607.3631	-0.0044	-7.2		3.07E+07	0.7	13984
600.3378	b10 ²⁺	600.3353	-0.0025	-4.2	606.3798	2.65E+07	0.6	13143
					552.3167	2.99E+08	6.5	14710
496.3354	c4	496.3304	-0.005	-10.1		3.09E+09	66.7	19802
495.3276	c4 (-1)	495.3246	-0.003	-6.1		7.27E+08	15.7	100.00%
					478.3232	1.60E+07	0.3	21188
					424.2501	4.16E+08	9.0	20347
					364.2433	2.44E+07	0.5	18950
					354.1745	1.46E+07	0.3	23187
254.1612	b2	254.1592	-0.002	-7.9		1.33E+08	2.9	26919
					243.1432	1.02E+07	0.2	19945
237.1346	b2 -NH3	237.1328	-0.0018	-7.6		2.02E+07	0.4	30816
					226.1528	1.34E+07	0.3	30073
					226.1169	3.35E+07	0.7	30311
								41377
								29131

Table S7. Observed isotopic distribution of 10 major fragments from the monoisotopic peak compared to the theoretical distribution calculated with the IsoPatrn software (the closest are in green, incorrect patterns in red).

Parent	frag isotope	NUS 1		NUS 2		NUS 4		NUS 8		NUS 16		NUS 32		Theoretical isotopic ratio %
		Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	
MH ⁺	Mono	8.91E+07	100.00%	3.67E+08	100.00%	1.09E+09	93.97%	1.88E+09	99.47%	1.79E+09	100.00%	0	0.00%	100
	1 st	5.97E+07	67.00%	9.74E+07	26.54%	1.16E+09	100.00%	1.89E+09	100.00%	1.10E+09	61.39%	0	0.00%	0
	2 nd	5.13E+07	57.58%	2.63E+08	71.66%	6.98E+08	60.17%	1.93E+08	10.21%	2.26E+08	12.61%	0	0.00%	0
	3 rd	2.38E+07	26.71%	1.00E+08	27.25%	4.25E+07	3.66%	5.53E+07	2.93%	6.95E+07	3.88%	0	0.00%	0
c10	Mono	3.35E+08	100.00%	1.39E+09	100.00%	3.94E+09	100.00%	6.77E+09	100.00%	6.72E+09	100.00%	0	0.00%	100
	1 st	2.46E+08	73.43%	1.14E+09	82.01%	2.17E+09	55.08%	4.63E+08	6.84%	6.19E+08	9.21%	0	0.00%	0
	2 nd	8.81E+07	26.30%	3.12E+08	22.45%	6.05E+07	1.54%	1.03E+08	1.52%	1.46E+08	2.17%	0	0.00%	0
	3 rd	1.99E+07	5.94%	6.07E+07	4.37%	2.67E+07	0.68%	1.88E+07	0.28%	0.00E+00	0.00%	0	0.00%	0
b10	Mono	0.00E+00	0.00%	2.43E+07	100.00%	5.20E+07	100.00%	8.18E+07	100.00%	7.72E+07	100.00%	4.01E+07	100.00%	100
	1 st	0.00E+00	0.00%	1.38E+07	56.79%	2.12E+07	0.00%	2.03E+07	24.82%	0.00E+00	0.00%	0	0.00%	0
	2 nd	0.00E+00	0.00%	0.00E+00	0.00%	2.12E+07	0.00%	1.95E+07	23.84%	0.00E+00	0.00%	0	0.00%	0

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Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

Parent MONO	frag isotope	NUS 1		NUS 2		NUS 4		NUS 8		NUS 16		NUS 32		Theoretical isotopic ratio %
		Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	
	3 rd	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	1.30E+07	15.89%	0.00E+00	0.00%	0	0.00%	0
c9	Mono	2.16E+08	100.00%	9.15E+08	100.00%	2.91E+09	100.00%	5.11E+09	100.00%	5.11E+09	100.00%	1.75E+09	100.00%	100
	1 st	1.43E+08	66.20%	6.44E+08	70.38%	1.32E+09	45.36%	3.09E+08	6.05%	4.37E+08	8.55%	0	0.00%	0
	2 nd	4.40E+07	20.37%	1.56E+08	17.05%	4.41E+07	1.52%	6.01E+07	1.18%	8.01E+07	1.57%	0	0.00%	0
	3 rd	0.00E+00	0.00%	3.15E+07	3.44%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0	0.00%	0
z9	Mono	4.75E+07	100.00%	1.27E+08	100.00%	4.22E+08	100.00%	3.52E+08	100.00%	2.46E+08	100.00%	0	0.00%	100
	1 st	2.42E+07	50.95%	1.23E+08	96.85%	1.01E+08	23.93%	4.41E+07	12.53%	5.58E+07	22.68%	0	0.00%	0
	2 nd	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0	0.00%	0
	3 rd	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0	0.00%	0
c8	Mono	1.77E+08	100.00%	7.81E+08	100.00%	2.66E+09	100.00%	4.54E+09	100.00%	4.47E+09	100.00%	1.27E+09	100.00%	100
	1 st	1.14E+08	64.41%	5.26E+08	67.35%	1.12E+09	42.11%	2.72E+08	5.99%	3.64E+08	8.14%	0	0.00%	0
	2 nd	3.42E+07	19.32%	1.27E+08	16.26%	3.63E+07	1.36%	3.65E+07	0.80%	6.57E+07	1.47%	0	0.00%	0
	3 rd	0.00E+00	0.00%	1.89E+07	2.42%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0	0.00%	0
C7	Mono	2.88E+08	100.00%	1.23E+09	100.00%	4.82E+09	100.00%	7.97E+09	100.00%	7.85E+09	100.00%	1.74E+09	100.00%	100
	1 st	1.46E+08	50.69%	7.16E+08	58.21%	1.65E+09	34.23%	4.21E+08	5.28%	5.27E+08	6.71%	0	0.00%	0
	2 nd	3.78E+07	13.13%	1.42E+08	11.54%	5.69E+07	1.18%	4.73E+07	0.59%	7.17E+07	0.91%	0	0.00%	0

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Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

Parent MONO	frag isotope	NUS 1		NUS 2		NUS 4		NUS 8		NUS 16		NUS 32		Theoretical isotopic ratio %
		Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	
	3 rd	0.00E+00	0.00%	1.88E+07	1.53%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0	0.00%	0
c6	Mono	2.11E+08	100.00%	8.37E+08	100.00%	3.75E+09	100.00%	6.10E+09	100.00%	5.75E+09	100.00%	1.64E+09	100.00%	100
	1 st	8.66E+07	41.04%	4.02E+08	48.03%	1.01E+09	26.93%	2.43E+08	3.98%	3.30E+08	5.74%	0	0.00%	0
	2 nd	1.74E+07	8.25%	6.49E+07	7.75%	3.55E+07	0.95%	0.00E+00	0.00%	3.23E+07	0.56%	0	0.00%	0
	3 rd	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0	0.00%	0
c5	Mono	3.91E+08	100.00%	1.52E+09	100.00%	7.51E+09	100.00%	1.21E+10	100.00%	1.30E+10	100.00%	4.63E+09	100.00%	100
	1 st	1.33E+08	34.02%	6.38E+08	41.97%	1.71E+09	22.77%	3.78E+08	3.12%	5.85E+08	4.50%	0	0.00%	0
	2 nd	2.28E+07	5.83%	7.90E+07	5.20%	4.54E+07	0.60%	0.00E+00	0.00%	4.12E+07	0.32%	0	0.00%	0
	3 rd	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0	0.00%	0
c4	Mono	1.83E+08	100.00%	6.78E+08	100.00%	3.24E+09	100.00%	5.40E+09	100.00%	5.89E+09	100.00%	3.09E+09	100.00%	100
	1 st	4.83E+07	26.39%	2.03E+08	29.94%	5.42E+08	16.73%	1.51E+08	2.80%	2.17E+08	3.68%	0	0.00%	0
	2 nd	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0	0.00%	0
	3 rd	0.00E+00	0.00%	0.00E+00	0.00%	0	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0	0.00%	0

Table S8. Observed isotopic distribution of 10 major fragments from the 1st isotopic peak compared to the theoretical distribution calculated with the IsoPatrn software (the closest are in green, incorrect patterns in red).

Parent	frag isotope	NUS 1		NUS 2		NUS 4		NUS 8		NUS 16		NUS 32		Theoretical isotopic ratio %
		Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	
MH ⁺	Mono	8.31E+07	100.00%	2.79E+08	100.00%	5.16E+08	43.00%	3.79E+08	16.92%	1.69E+08	6.60%	0	0.00%	0.015
	1 st	5.67E+07	68.23%	5.96E+07	21.36%	1.04E+09	86.67%	2.06E+09	91.96%	1.92E+09	75.00%	1.31E+08	100.00%	100
	2 nd	5.05E+07	60.77%	2.34E+08	83.87%	1.20E+09	100.00%	2.24E+09	100.00%	2.56E+09	100.00%	0	0.00%	0
	3 rd	2.58E+07	31.05%	1.28E+08	45.88%	2.60E+08	21.67%	2.21E+08	9.87%	3.85E+08	15.04%	0	0.00%	0
c10	Mono	3.10E+08	32.33%	1.06E+09	89.83%	1.76E+09	48.22%	1.83E+09	27.94%	9.42E+08	12.96%	0	0.00%	9.535
	1 st	2.47E+08	25.76%	1.18E+09	100.00%	3.65E+09	100.00%	6.55E+09	100.00%	7.27E+09	100.00%	8.60E+08	100.00%	100
	2 nd	9.59E+08	100.00%	4.27E+08	36.19%	6.46E+08	17.70%	3.68E+08	5.62%	7.61E+08	10.47%	0	0.00%	0
	3 rd	2.39E+07	2.49%	1.09E+08	9.24%	2.14E+07	0.59%	1.02E+08	1.56%	0.00E+00	0.00%	0	0.00%	0
b10	Mono	0.00E+00	0.00%	1.96E+07	100.00%	2.53E+07	87.85%	1.32E+07	36.26%	1.84E+07	48.81%	0	0.00%	10.16
	1 st	0.00E+00	0.00%	1.42E+07	72.45%	2.88E+07	100.00%	3.64E+07	100.00%	3.77E+07	100.00%	1.22E+07	100.00%	100
	2 nd	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	1.47E+07	38.99%	0	0.00%	0
	3 rd	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	2.40E+07	63.66%	0	0.00%	0
c9	Mono	1.99E+08	100.00%	6.85E+08	100.00%	1.33E+09	60.18%	1.69E+09	42.46%	8.50E+08	18.93%	0	0.00%	21.659
	1 st	1.42E+08	71.36%	6.58E+08	96.06%	2.21E+09	100.00%	3.98E+09	100.00%	4.49E+09	100.00%	3.27E+08	100.00%	100
	2 nd	4.79E+07	24.07%	2.14E+08	31.24%	3.35E+08	15.16%	1.63E+08	4.10%	3.99E+08	8.89%	0	0.00%	0

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance
Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

Parent FIRST	frag isotope	NUS 1		NUS 2		NUS 4		NUS 8		NUS 16		NUS 32		Theoretical isotopic ratio %
		Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	
	3 ^d	1.00E+07	5.03%	5.33E+07	7.78%	0.00E+00	0.00%	0.00E+00	0.00%	3.23E+07	0.72%	0	0.00%	0
z9	Mono	4.36E+07	100.00%	1.58E+08	100.00%	3.48E+08	52.65%	4.70E+08	37.30%	1.70E+08	12.59%	0	0.00%	22.984
	1 st	2.47E+07	56.65%	1.40E+08	88.61%	6.61E+08	100.00%	1.26E+09	100.00%	1.35E+09	100.00%	0	0.00%	100
	2 nd	0.00E+00	0.00%	2.87E+07	18.16%	2.09E+08	31.62%	3.23E+08	25.63%	4.44E+08	32.89%	0	0.00%	0
	3 ^d	0.00E+00	0.00%	1.09E+07	6.90%	0.00E+00	0.00%	0.00E+00	0.00%	2.93E+07	2.17%	0	0.00%	0
c8	Mono	1.62E+08	100.00%	5.82E+08	100.00%	1.21E+09	65.05%	1.64E+09	48.24%	7.67E+08	20.18%	0	0.00%	26.863
	1 st	1.13E+08	69.75%	5.33E+08	91.58%	1.86E+09	100.00%	3.40E+09	100.00%	3.80E+09	100.00%	2.67E+08	100.00%	100
	2 nd	3.73E+07	23.02%	1.72E+08	29.55%	2.71E+08	14.57%	1.25E+08	3.68%	3.19E+08	8.39%	0	0.00%	0
	3 ^d	0.00E+00	0.00%	3.15E+07	5.41%	0.00E+00	0.00%	0.00E+00	0.00%	2.34E+07	0.62%	0	0.00%	0
C7	Mono	2.64E+08	100.00%	8.76E+08	100.00%	2.40E+09	87.27%	3.77E+09	76.01%	2.01E+09	36.09%	0	0.00%	52.553
	1 st	1.44E+08	54.55%	7.09E+08	80.94%	2.75E+09	100.00%	4.96E+09	100.00%	5.57E+09	100.00%	3.05E+08	100.00%	100
	2 nd	4.12E+07	15.61%	1.89E+08	21.58%	3.26E+08	11.85%	1.29E+08	2.60%	3.82E+08	6.86%	0	0.00%	0
	3 ^d	0.00E+00	0.00%	3.61E+07	4.12%	0.00E+00	0.00%	0.00E+00	0.00%	3.16E+07	0.57%	0	0.00%	0
c6	Mono	1.91E+08	100.00%	5.65E+08	100.00%	2.07E+09	100.00%	3.52E+09	100.00%	2.39E+09	70.09%	0	0.00%	91.29
	1 st	8.51E+07	44.55%	3.89E+08	68.85%	1.67E+09	80.68%	3.03E+09	86.08%	3.41E+09	100.00%	1.63E+08	100.00%	100
	2 nd	1.91E+07	10.00%	8.34E+07	14.76%	1.51E+08	7.29%	6.72E+07	1.91%	1.79E+08	5.25%	0	0.00%	0

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance
Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

Parent	frag isotope	NUS 1		NUS 2		NUS 4		NUS 8		NUS 16		NUS 32		Theoretical isotopic ratio %
		Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	
		0.00E+00	0.00%	1.16E+07	2.05%	0.00E+00	0.00%	0.00E+00	0.00%	1.27E+07	0.37%	0	0.00%	0
	3 rd													
c5	Mono	3.53E+08	100.00%	9.94E+08	100.00%	4.62E+09	100.00%	8.42E+09	100.00%	7.44E+09	100.00%	0	0.00%	100
	1 st	1.29E+08	36.54%	6.03E+08	60.66%	2.87E+09	62.12%	5.07E+09	60.21%	5.72E+09	76.88%	4.57E+08	100.00%	78.898
	2 nd	2.42E+07	6.86%	1.03E+08	10.36%	2.09E+08	4.52%	1.02E+08	1.21%	2.39E+08	3.21%	0	0.00%	0
	3 rd	0.00E+00	0.00%	1.12E+07	1.13%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0	0.00%	0
c4	Mono	1.65E+08	100.00%	4.39E+08	100.00%	2.12E+09	100.00%	3.87E+09	100.00%	3.90E+09	100.00%	0	0.00%	100
	1 st	4.68E+07	28.36%	1.87E+08	42.60%	9.25E+08	43.63%	1.60E+09	41.34%	1.76E+09	45.13%	5.08E+08	100.00%	56.073
	2 nd	0.00E+00	0.00%	0.00E+00	0.00%	3.43E+07	1.62%	0.00E+00	0.00%	2.11E+07	0.54%	0	0.00%	0
	3 rd	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0	0.00%	0

Table S9. Observed isotopic distribution of 10 major fragments from the 2nd isotopic peak compared to the theoretical distribution calculated with the IsoPatrn software (the closest are in green, incorrect patterns in red).

Parent	frag isotope	NUS 1		NUS 2		NUS 4		NUS 8		NUS 16		NUS 32		Theoretical isotopic ratio %
		Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	
SECOND	MH ⁺	7.71E+07	100.00%	2.13E+08	100.00%	3.44E+07	5.21%	1.57E+08	31.78%	1.63E+08	18.38%	0	0.00%	0
		5.35E+07	69.39%	7.11E+07	33.38%	3.58E+08	54.24%	3.36E+08	68.02%	4.57E+08	51.52%	0	0.00%	0.024
		4.86E+07	63.04%	1.89E+08	88.73%	6.60E+08	100.00%	2.48E+08	50.20%	8.87E+08	100.00%	0	0.00%	100
		2.59E+07	33.59%	1.26E+08	59.15%	5.19E+08	78.64%	4.94E+08	100.00%	8.22E+08	92.67%	0	0.00%	0
c10	Mono	2.87E+08	100.00%	8.09E+08	76.32%	9.83E+08	65.97%	4.97E+08	39.76%	7.87E+08	39.75%	0	0.00%	18.099
	1 st	2.38E+08	82.93%	1.06E+09	100.00%	1.49E+09	100.00%	5.04E+08	40.32%	1.24E+09	62.63%	0	0.00%	17.571
	2 nd	9.63E+07	33.55%	4.41E+08	41.60%	1.22E+09	81.88%	1.25E+09	100.00%	1.98E+09	100.00%	0	0.00%	100
	3 rd	2.51E+07	8.75%	1.28E+08	12.08%	2.27E+08	15.23%	9.59E+07	7.67%	9.38E+07	4.74%	0	0.00%	0
b10	Mono	0.00E+00	0.00%	1.55E+07	100.00%	0.00E+00	0.00%	0.00E+00	0.00%	1.43E+07	76.88%	0	0.00%	18.39
	1 st	0.00E+00	0.00%	1.28E+07	82.58%	0.00E+00	0.00%	0.00E+00	0.00%	1.63E+07	87.63%	0	0.00%	18.707
	2 nd	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	1.86E+07	100.00%	0	0.00%	100
	3 rd	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0	0.00%	0
c9	Mono	1.84E+08	100.00%	5.19E+08	88.87%	1.07E+08	11.92%	3.61E+08	55.45%	5.61E+08	50.54%	0	0.00%	26.118
	1 st	1.37E+08	74.46%	5.84E+08	100.00%	8.98E+08	100.00%	3.42E+08	52.53%	9.33E+08	84.05%	0	0.00%	39.497
	2 nd	4.82E+07	26.20%	2.19E+08	37.50%	6.28E+08	69.93%	6.51E+08	100.00%	1.11E+09	100.00%	0	0.00%	100

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance
Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

Parent	frag isotope	NUS 1		NUS 2		NUS 4		NUS 8		NUS 16		NUS 32		Theoretical isotopic ratio %
		Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	
z9	3 rd	1.07E+07	5.82%	6.07E+07	10.39%	7.12E+07	7.93%	0.00E+00	0.00%	3.18E+07	2.86%	0	0.00%	0
	Mono	4.00E+07	100.00%	1.19E+08	92.97%	4.63E+07	16.59%	1.18E+08	56.73%	1.28E+04	0.00%	0	0.00%	5.296
	1 st	2.42E+07	60.50%	1.28E+08	100.00%	2.79E+08	100.00%	1.21E+08	58.17%	3.02E+08	71.90%	0	0.00%	34.661
	2 nd	0.00E+00	0.00%	3.43E+07	26.80%	2.49E+08	89.25%	2.08E+08	100.00%	4.20E+08	100.00%	0	0.00%	100
c8	3 rd	0.00E+00	0.00%	1.40E+07	10.94%	4.88E+07	17.49%	0.00E+00	0.00%	4.97E+07	11.83%	0	0.00%	0
	Mono	1.50E+08	100.00%	4.43E+08	94.06%	1.23E+08	16.44%	3.13E+08	59.73%	5.07E+08	53.76%	0	0.00%	31.337
	1 st	1.09E+08	72.67%	4.71E+08	100.00%	7.48E+08	100.00%	3.03E+08	57.82%	8.51E+08	90.24%	0	0.00%	49.075
	2 nd	3.75E+07	25.00%	1.76E+08	37.37%	5.11E+08	68.32%	5.24E+08	100.00%	9.43E+08	100.00%	0	0.00%	100
C7	3 rd	0.00E+00	0.00%	4.10E+07	8.70%	3.76E+07	5.03%	0.00E+00	0.00%	2.85E+07	3.02%	0	0.00%	0
	Mono	2.42E+08	100.00%	6.44E+08	100.00%	4.18E+08	36.03%	5.64E+08	100.00%	1.03E+09	70.07%	0	0.00%	60.421
	1 st	1.38E+08	57.02%	6.16E+08	95.65%	1.16E+09	100.00%	5.12E+08	90.78%	1.47E+09	100.00%	0	0.00%	93.416
	2 nd	4.13E+07	17.07%	1.91E+08	29.66%	6.16E+08	53.10%	5.54E+08	98.23%	1.19E+09	80.95%	0	0.00%	100
c6	3 rd	0.00E+00	0.00%	4.21E+07	6.54%	6.50E+07	5.60%	0.00E+00	0.00%	2.85E+07	1.94%	0	0.00%	0
	Mono	1.74E+08	100.00%	4.00E+08	100.00%	5.15E+08	71.63%	2.69E+08	97.46%	9.24E+08	98.30%	0	0.00%	81.43
	1 st	8.15E+07	46.84%	3.34E+08	83.50%	7.19E+08	100.00%	1.76E+08	63.77%	9.40E+08	100.00%	0	0.00%	100
	2 nd	1.95E+07	11.21%	8.20E+07	20.50%	2.93E+08	40.75%	2.76E+08	100.00%	5.61E+08	59.68%	0	0.00%	64.522

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Parent	frag isotope	NUS 1		NUS 2		NUS 4		NUS 8		NUS 16		NUS 32		Theoretical isotopic ratio %
		Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	
	3 rd	2.00E+07	11.49%	1.38E+07	3.45%	4.09E+08	56.88%	0.00E+00	0.00%	1.64E+07	1.74%	0	0.00%	0
c5	Mono	3.22E+08	100.00%	6.89E+08	100.00%	1.50E+09	100.00%	4.08E+08	100.00%	2.70E+09	100.00%	0	0.00%	100
	1 st	1.24E+08	38.51%	5.11E+08	74.17%	1.32E+09	88.00%	0.00E+00	0.00%	1.95E+09	72.22%	0	0.00%	97.866
	2 nd	2.40E+07	7.45%	1.03E+08	14.95%	3.97E+08	26.47%	0.00E+00	0.00%	7.72E+08	28.59%	0	0.00%	45.728
	3 rd	0.00E+00	0.00%	1.19E+07	1.73%	2.30E+07	1.53%	0.00E+00	0.00%	1.63E+07	0.60%	0	0.00%	0
c4	Mono	1.50E+08	100.00%	3.01E+08	100.00%	8.08E+08	100.00%	6.32E+08	100.00%	1.41E+09	100.00%	0	0.00%	100
	1 st	4.45E+07	29.67%	1.56E+08	51.83%	4.60E+08	56.93%	3.67E+08	58.07%	6.38E+08	45.25%	0	0.00%	74.904
	2 nd	0.00E+00	0.00%	0.00E+00	0.00%	6.10E+07	7.55%	3.89E+07	6.16%	5.48E+07	3.89%	0	0.00%	24.758
	3 rd	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0	0.00%	0

Table S10. Observed isotopic distribution of 10 major fragments produced from the 3rd isotopic peak compared to the theoretical distribution calculated with the IsoPatm software (the closest are in green, incorrect patterns in red).

Parent	frag isotope	NUS 1		NUS 2		NUS 4		NUS 8		NUS 16		NUS 32		Theoretical Isotopic ratio %
		Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	
MH ⁺	Mono	6.10E+07	100.00%	1.20E+08	100.00%	2.45E+07	7.78%	9.50E+07	20.56%	9.49E+07	40.04%	0	0.00%	0
	1 st	4.48E+07	73.44%	7.13E+07	59.42%	5.86E+07	18.60%	3.08E+08	66.67%	1.79E+08	75.53%	0	0.00%	0
	2 nd	4.21E+07	69.02%	1.08E+08	90.00%	2.13E+08	67.62%	3.15E+08	68.18%	2.37E+08	100.00%	0	0.00%	0.033
	3 rd	2.40E+07	39.34%	1.02E+08	85.00%	3.15E+08	100.00%	4.62E+08	100.00%	1.35E+08	56.96%	0	0.00%	100
c10	Mono	2.25E+08	100.00%	4.63E+08	61.00%	6.32E+07	10.97%	5.09E+08	60.17%	3.90E+08	96.53%	0	0.00%	3.854
	1 st	2.08E+08	92.44%	7.59E+08	100.00%	2.60E+08	45.14%	8.46E+08	100.00%	4.04E+08	100.00%	0	0.00%	46.912
	2 nd	9.02E+07	40.09%	3.96E+08	52.17%	5.76E+08	100.00%	6.28E+08	74.23%	2.71E+08	67.08%	0	0.00%	24.715
	3 rd	2.57E+07	11.42%	1.39E+08	18.31%	3.92E+08	68.06%	5.95E+08	70.33%	2.84E+08	70.30%	0	0.00%	100
b10	Mono	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0	0.00%	4.182
	1 st	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0	0.00%	47.598
	2 nd	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0	0.00%	26.297
	3 rd	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0	0.00%	100
c9	Mono	1.43E+08	100.00%	2.92E+08	70.87%	8.39E+07	28.63%	3.65E+08	69.92%	2.66E+08	65.84%	0	0.00%	12.209
	1 st	1.18E+08	82.52%	4.12E+08	100.00%	1.95E+08	66.55%	5.22E+08	100.00%	2.91E+08	72.03%	0	0.00%	66.585
	2 nd	4.50E+07	31.47%	1.94E+08	47.09%	2.93E+08	100.00%	3.85E+08	73.75%	1.47E+08	36.39%	0	0.00%	55.219

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Parent THIRD	frag isotope	NUS 1		NUS 2		NUS 4		NUS 8		NUS 16		NUS 32		Theoretical Isotopic ratio %
		Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	
	3 ^d	1.10E+07	7.69%	6.32E+07	15.34%	1.10E+08	37.54%	9.64E+07	18.47%	4.04E+08	100.00%	0	0.00%	100
z9	Mono	3.07E+07	100.00%	6.65E+07	72.92%	2.13E+07	17.90%	1.06E+08	62.72%	7.72E+07	88.33%	0	0.00%	1.229
	1 st	2.16E+07	70.36%	9.12E+07	100.00%	3.86E+07	32.44%	1.69E+08	100.00%	8.74E+07	100.00%	0	0.00%	10.694
	2 nd	0.00E+00	0.00%	3.67E+07	40.24%	1.19E+08	100.00%	1.49E+08	88.17%	7.57E+07	86.61%	0	0.00%	46.41
	3 ^d	0.00E+00	0.00%	1.66E+07	18.20%	5.84E+07	49.08%	6.59E+07	38.99%	2.41E+07	27.57%	0	0.00%	100
c8	Mono	1.16E+08	100.00%	2.54E+08	77.20%	7.60E+07	31.28%	3.59E+08	84.27%	2.60E+08	100.00%	0	0.00%	17.777
	1 st	9.48E+07	81.72%	3.29E+08	100.00%	1.86E+08	76.54%	4.26E+08	100.00%	2.44E+08	93.85%	0	0.00%	80.115
	2 nd	3.52E+07	30.34%	1.55E+08	47.11%	2.43E+08	100.00%	3.22E+08	75.59%	1.30E+08	50.00%	0	0.00%	68.676
	3 ^d	0.00E+00	0.00%	4.38E+07	13.31%	6.40E+07	26.34%	9.09E+07	21.34%	4.17E+07	16.04%	0	0.00%	100
C7	Mono	1.87E+08	100.00%	3.46E+08	83.37%	1.95E+08	58.38%	8.14E+08	100.00%	5.05E+08	100.00%	0	0.00%	37.531
	1 st	1.19E+08	63.64%	4.15E+08	100.00%	3.34E+08	100.00%	7.48E+08	91.89%	3.83E+08	75.84%	0	0.00%	100
	2 nd	3.84E+07	20.53%	1.65E+08	39.76%	3.05E+08	91.32%	4.66E+08	57.25%	1.90E+08	37.62%	0	0.00%	86.978
	3 ^d	0.00E+00	0.00%	4.42E+07	10.65%	9.54E+07	28.56%	8.24E+07	10.12%	4.67E+07	9.25%	0	0.00%	67.464
c6	Mono	1.32E+08	100.00%	1.98E+08	90.00%	2.10E+08	78.07%	6.85E+08	100.00%	3.86E+08	100.00%	0	0.00%	56.47
	1 st	6.96E+07	52.73%	2.20E+08	100.00%	2.69E+08	100.00%	5.07E+08	74.01%	2.48E+08	64.25%	0	0.00%	100
	2 nd	1.77E+07	13.41%	6.85E+07	31.14%	1.59E+08	59.11%	2.92E+08	42.63%	9.71E+07	25.16%	0	0.00%	72.335

Nonuniform Sampling Acquisition of Two-Dimensional Fourier Transform Ion Cyclotron Resonance
Mass Spectrometry for Increased Mass Resolution of Tandem Mass Spectrometry Precursor Ions

Parent THIRD	frag isotope	NUS 1		NUS 2		NUS 4		NUS 8		NUS 16		NUS 32		Theoretical Isotopic ratio %
		Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	Intensity	Isotopic ratio %	
	3 rd	0.00E+00	0.00%	1.49E+08	67.73%	0.00E+00	0.00%	3.80E+07	5.55%	2.12E+07	5.49%	0	0.00%	34.411
c5	Mono	2.43E+08	100.00%	3.28E+08	100.00%	5.02E+08	94.72%	1.56E+09	100.00%	7.95E+08	100.00%	0	0.00%	73.667
	1 st	1.05E+08	43.21%	3.28E+08	100.00%	5.30E+08	100.00%	9.95E+08	63.78%	4.58E+08	57.61%	0	0.00%	100
	2 nd	2.19E+07	9.01%	8.68E+07	26.46%	2.30E+08	43.40%	4.53E+08	29.04%	1.54E+08	19.37%	0	0.00%	57.959
	3 rd	0.00E+00	0.00%	1.09E+07	3.32%	3.86E+07	7.28%	4.33E+07	2.78%	2.45E+07	3.08%	0	0.00%	20.003
c4	Mono	1.14E+08	100.00%	1.38E+08	100.00%	2.66E+08	100.00%	6.84E+08	100.00%	3.09E+08	100.00%	0	0.00%	98.253
	1 st	3.74E+07	32.81%	9.67E+07	70.07%	1.99E+08	74.81%	4.07E+08	59.50%	1.13E+08	36.57%	0	0.00%	100
	2 nd	0.00E+00	0.00%	0.00E+00	0.00%	3.54E+07	13.31%	4.33E+07	6.33%	2.22E+07	7.18%	0	0.00%	44.152
	3 rd	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0.00E+00	0.00%	0	0.00%	10.77

Table S11. Theoretical fragmentation of the sesame oil major triglycerides cationized by $^6\text{Li}^+$ and fragmented by IRMPD.

Common name	Abbreviated formula	Molecular formula	m/z cationized by $^6\text{Li}^+$	Loss of oleic acid acid (-O) ^a		Loss of linolenic acid acid (-L) ^b	
				Molecular formula	m/z cationized by $^6\text{Li}^+$	Molecular formula	m/z cationized by $^6\text{Li}^+$
Triolein	OOO	$\text{C}_{57}\text{H}_{104}\text{O}_6$	890.798	$\text{C}_{39}\text{H}_{70}\text{O}_4$	608.542	-	-
	OOL or OLO	$\text{C}_{57}\text{H}_{102}\text{O}_6$	888.782	$\text{C}_{39}\text{H}_{68}\text{O}_4$	606.526	$\text{C}_{39}\text{H}_{70}\text{O}_4$	608.542
	OLL or LOL	$\text{C}_{57}\text{H}_{100}\text{O}_6$	886.767	$\text{C}_{39}\text{H}_{66}\text{O}_4$	604.511	$\text{C}_{39}\text{H}_{68}\text{O}_4$	606.526
Trilinolein	LLL	$\text{C}_{57}\text{H}_{98}\text{O}_6$	884.751	-	-	$\text{C}_{39}\text{H}_{66}\text{O}_4$	604.511

^aO: oleic acid ($\text{C}_{18}\text{H}_{34}\text{O}_2$)

^bL: Linolenic acid ($\text{C}_{18}\text{H}_{32}\text{O}_2$)