Elemental Composition Determination of Unknown Organometallic Compounds with Mass Spectral Accuracy

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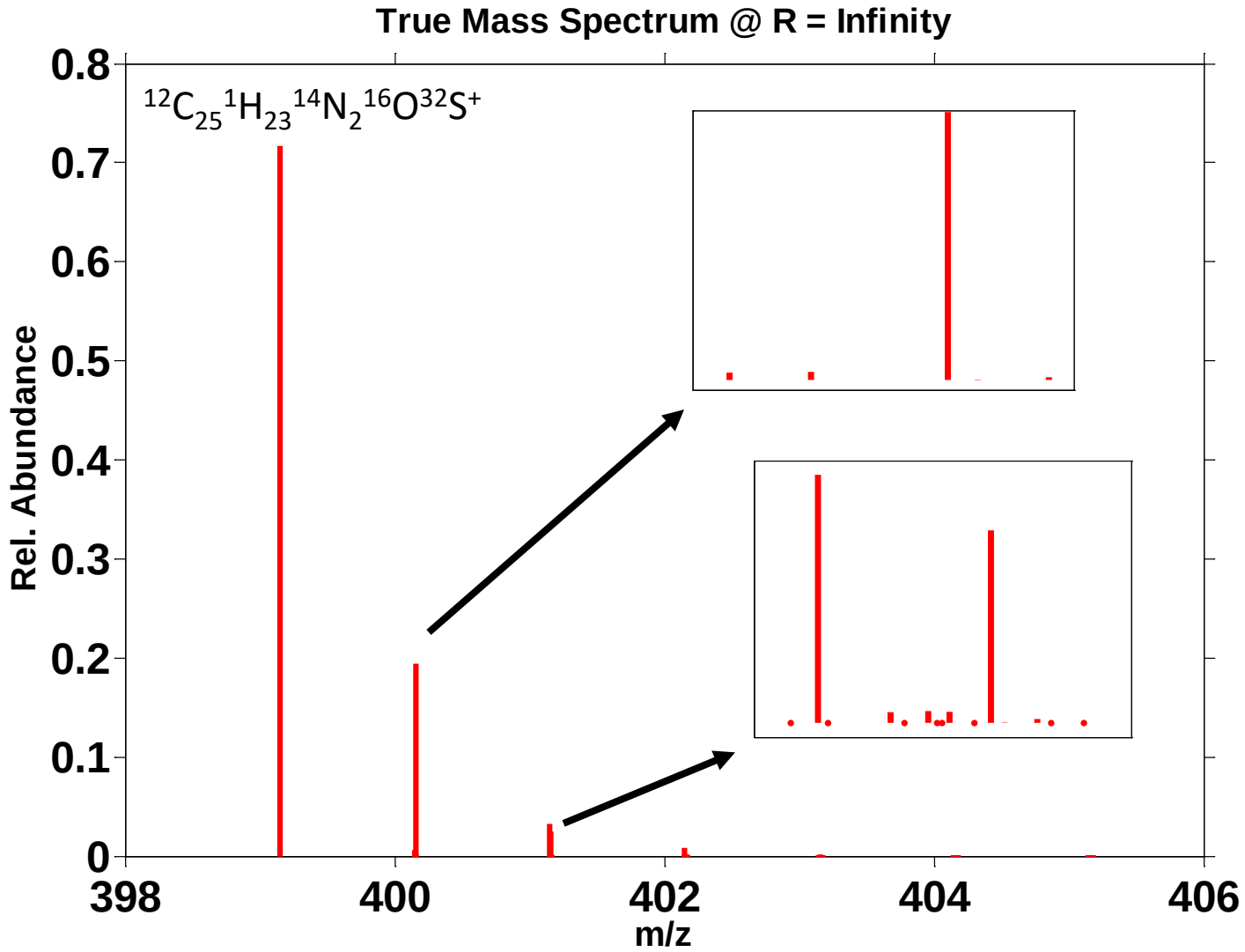
Elemental Composition and Mass Spec Measurement (e.g., $C_{25}H_{23}N_2OS^+$)



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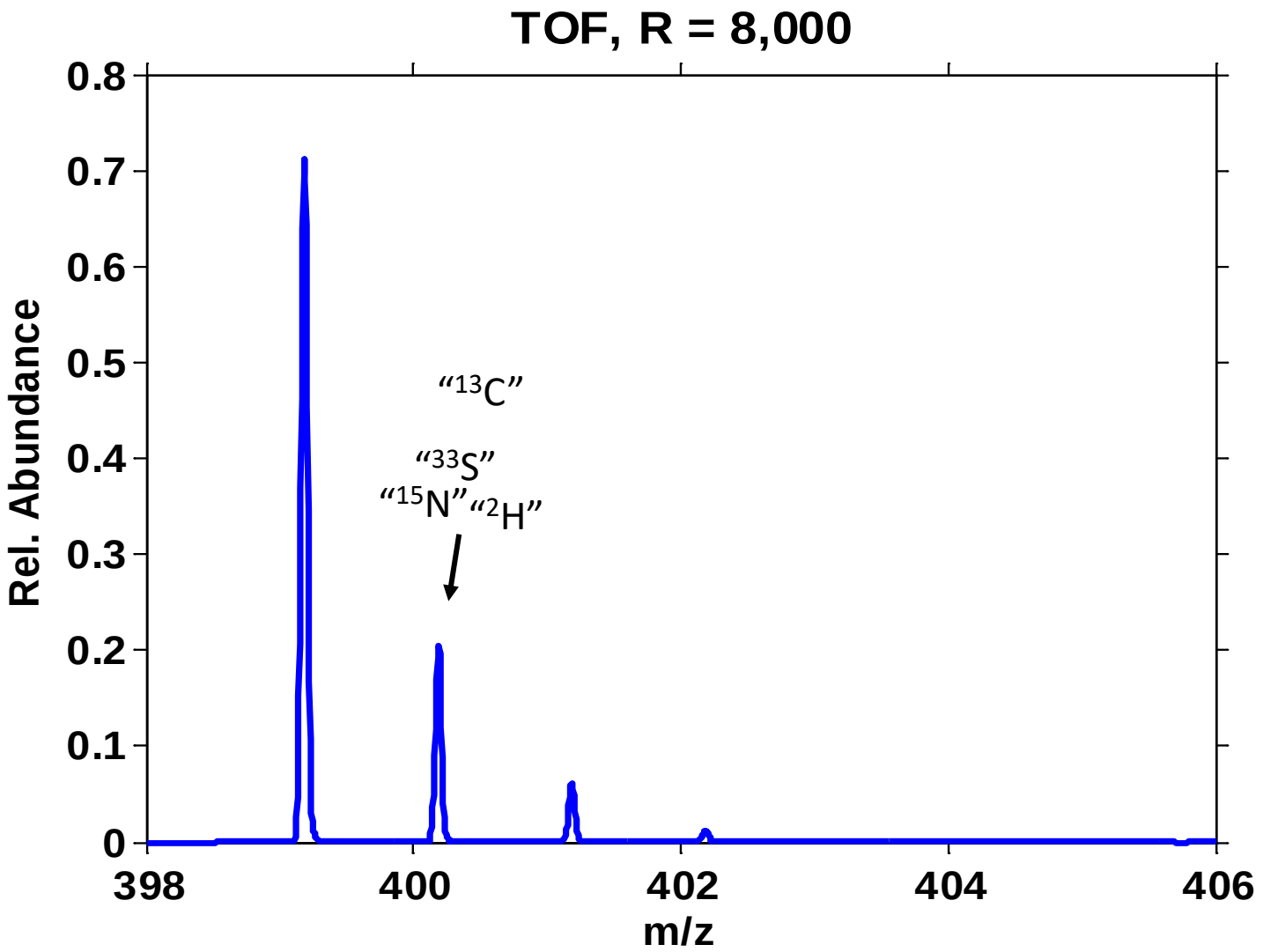
Elemental Composition and Mass Spec Measurement (e.g., $C_{25}H_{23}N_2OS^+$): Baseline Resolved w/HiRes



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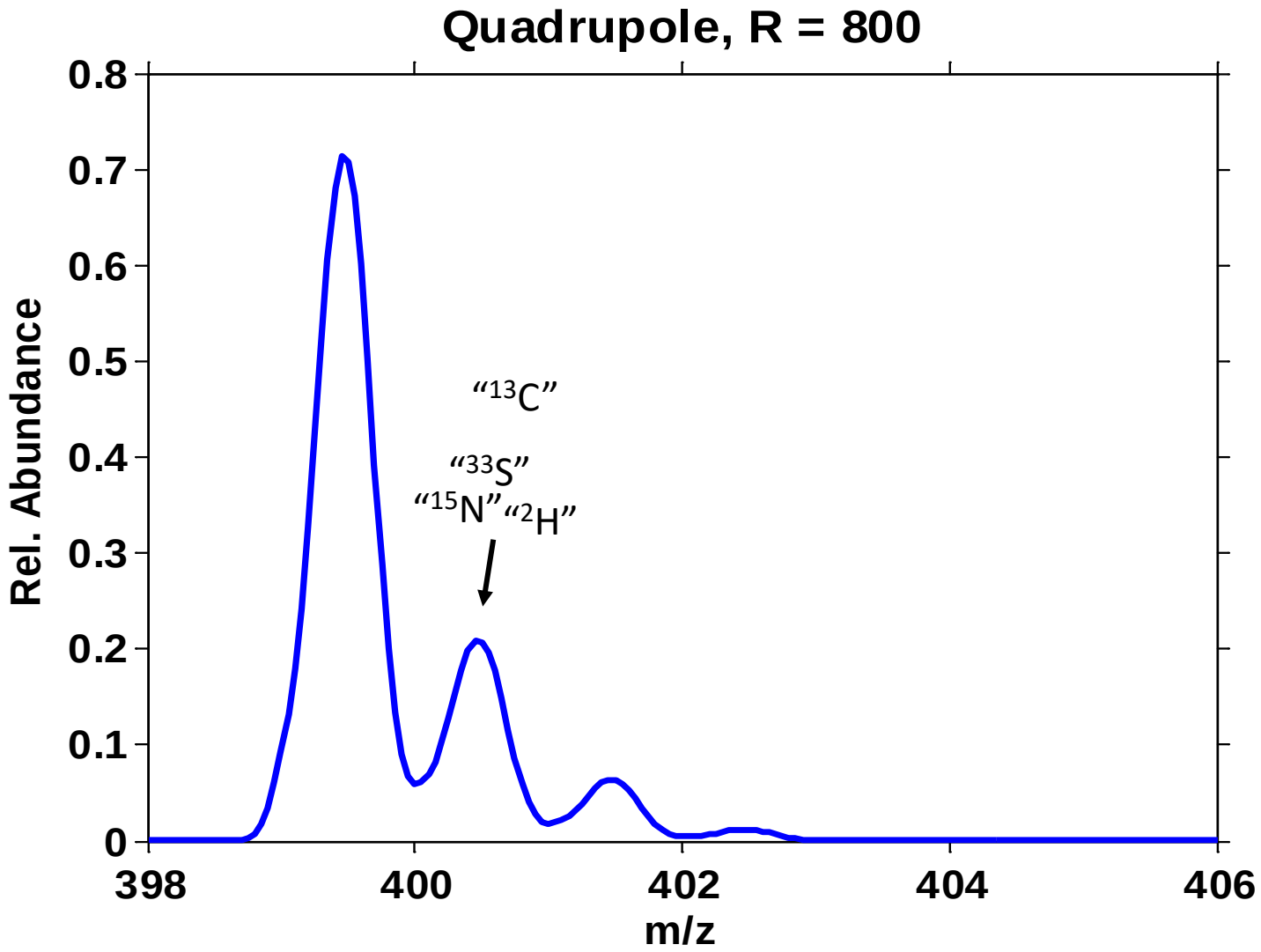
Elemental Composition and Mass Spec Measurement (e.g., $C_{25}H_{23}N_2OS^+$): Baseline Unresolved @ Unit Mass



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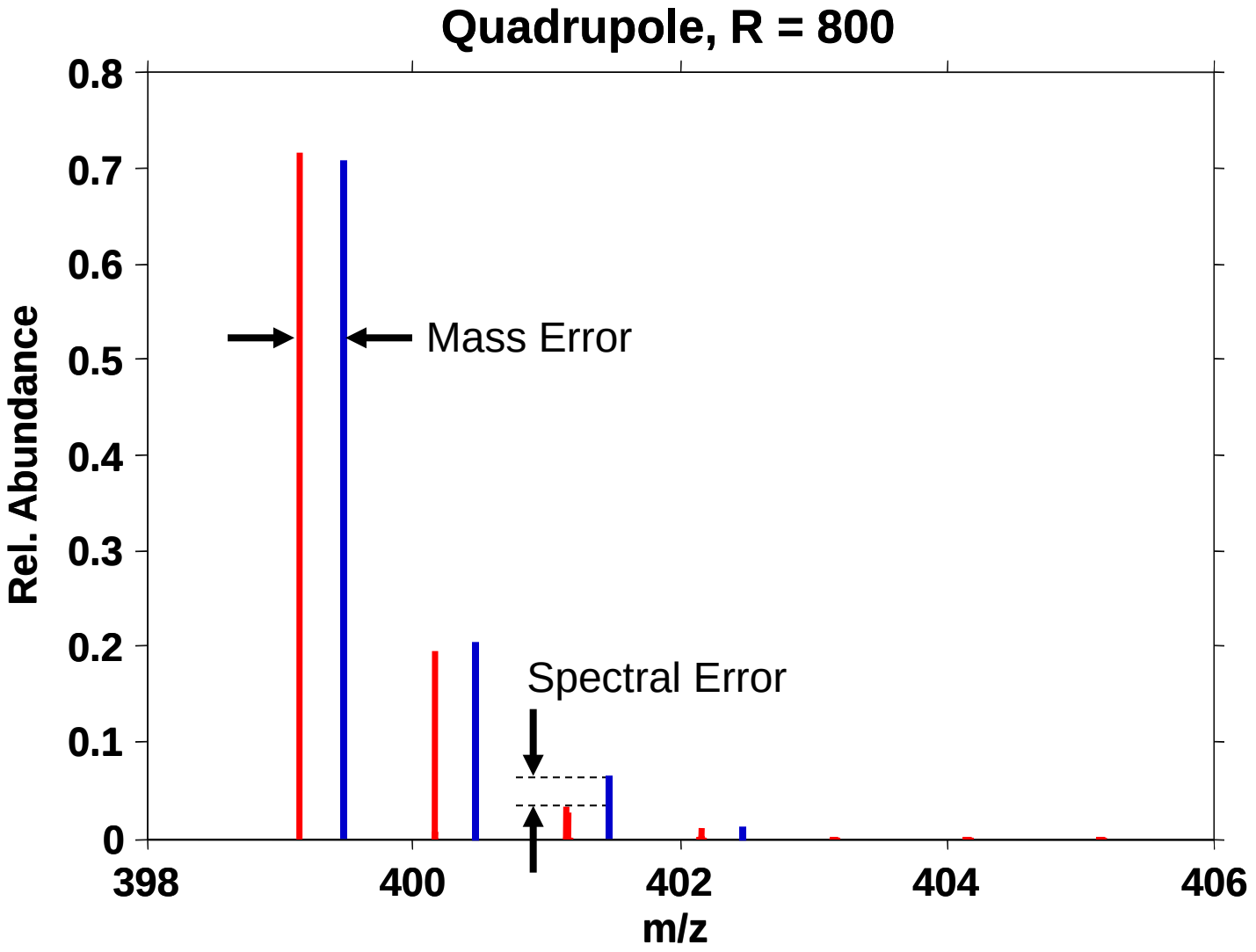
Elemental Composition and Mass Spec Measurement (e.g., $C_{25}H_{23}N_2OS^+$)



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Entirely Different MS Calibration

TrueCal: True & Fully Calibrated MS (Cerno only)

Raw Profile MS and True MS

m/z-Only Calibration (conventional calibration)

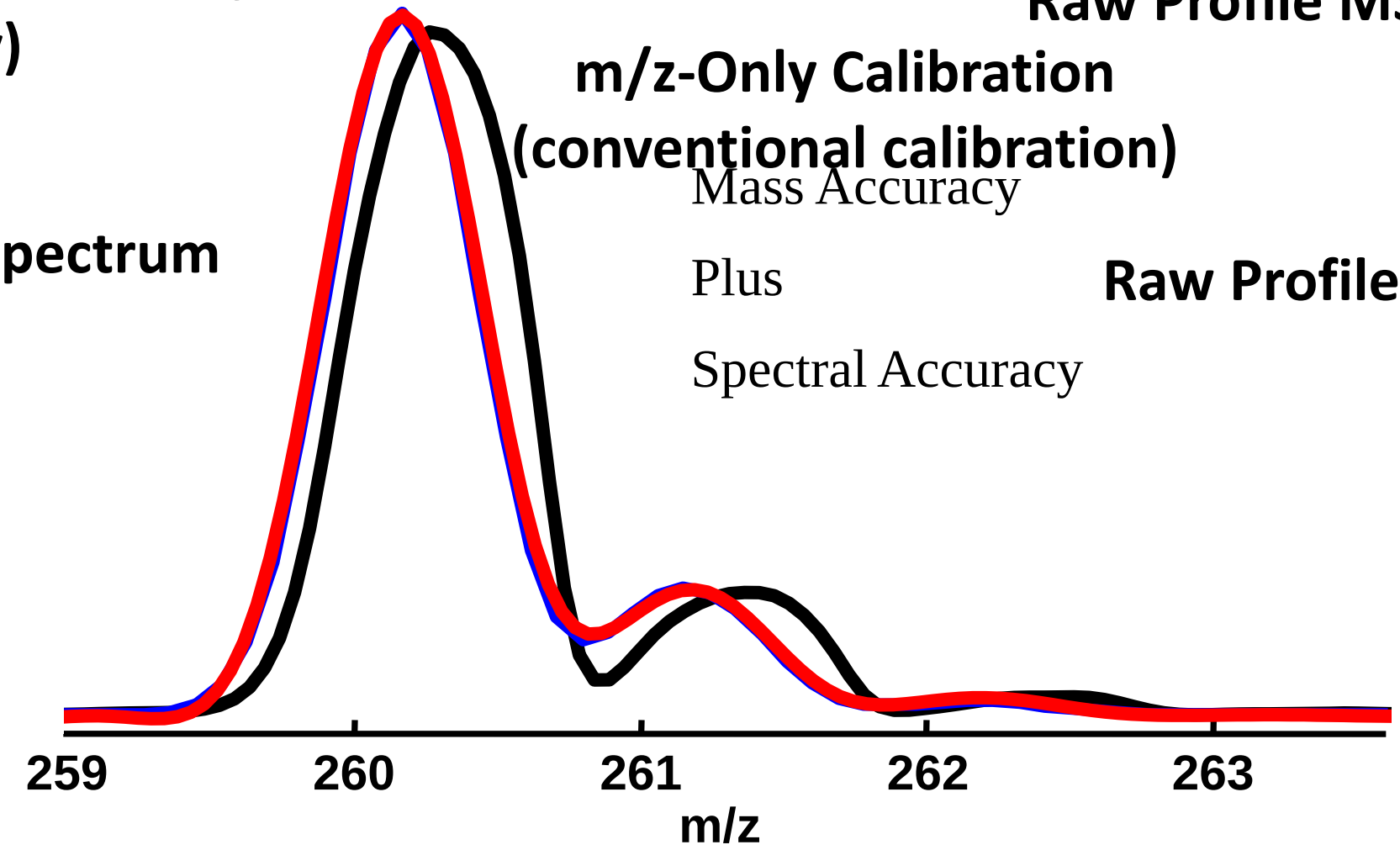
Mass Accuracy

Plus

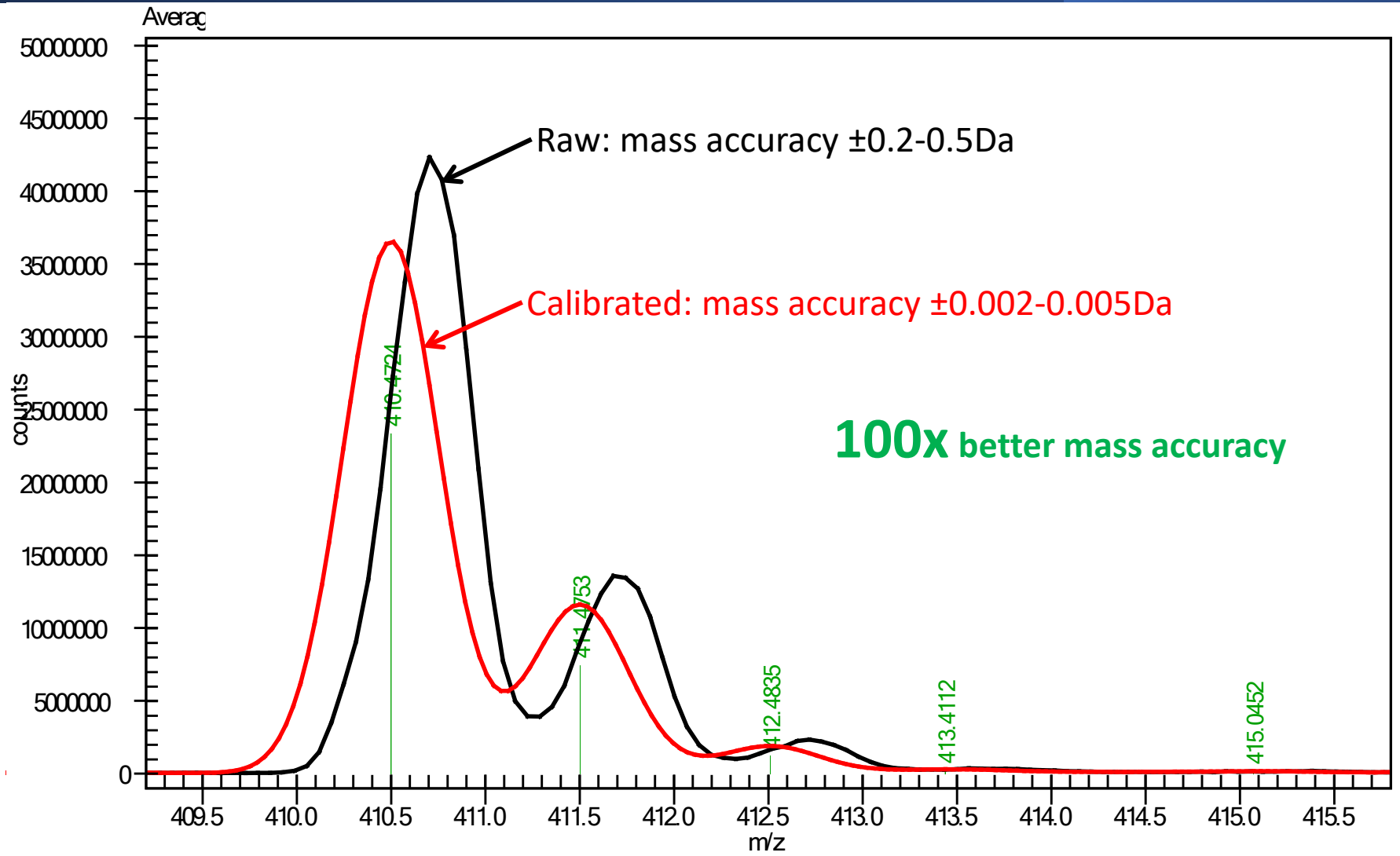
Spectral Accuracy

True Mass Spectrum

Raw Profile Mass Spectrum



The Unparalleled Gain in Performance



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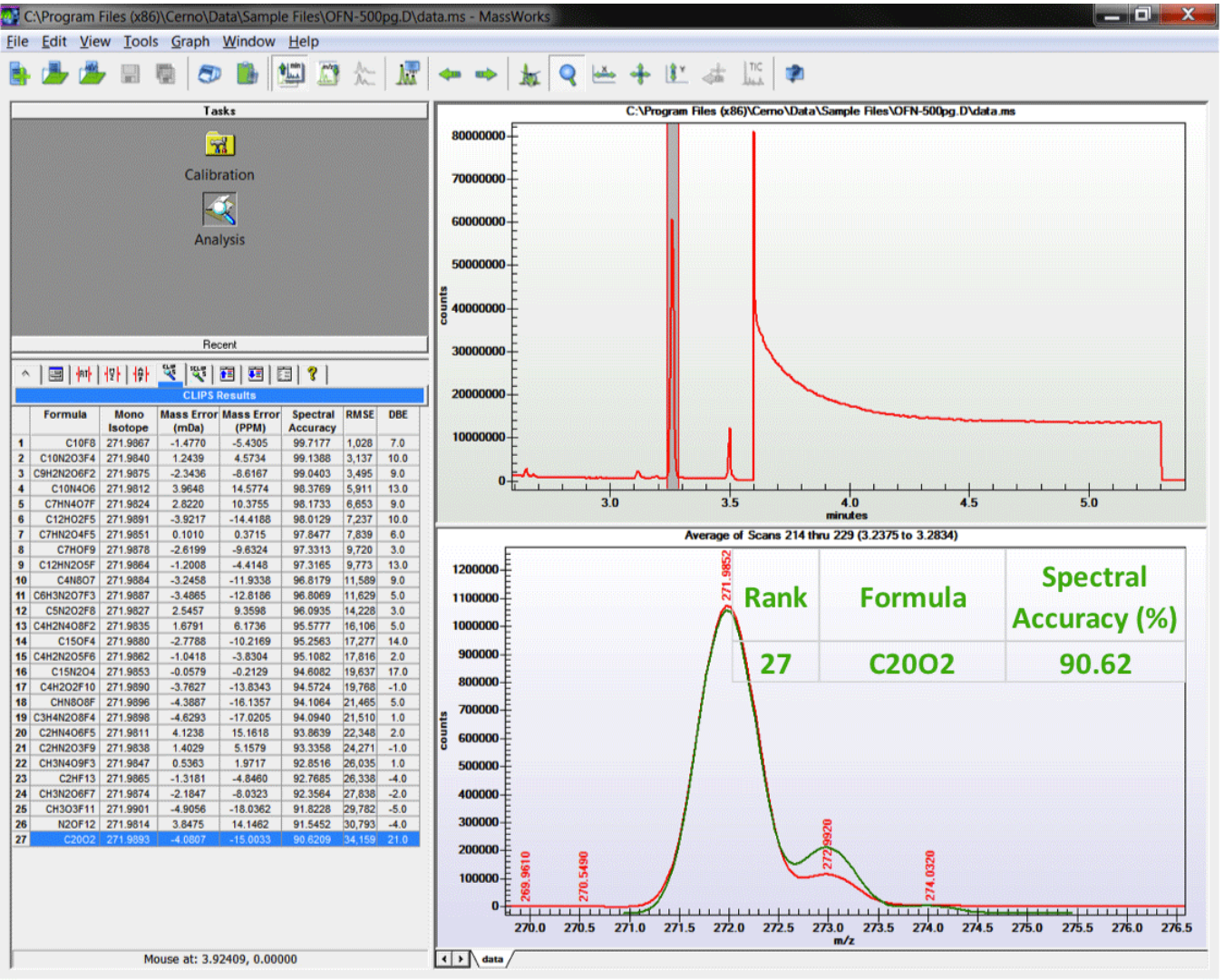
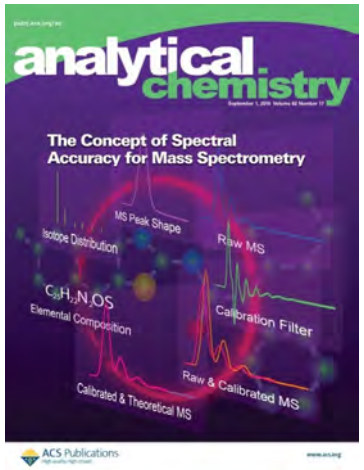
The Unparalleled Gain in Performance



	Formula	Mono Isotope	Mass Error (mDa)	Mass Error (PPM)	Spectral Accuracy	RMSE	DBE
1	C10F8	271.9867	-1.4770	-5.4305	99.7177	1,028	7.0
2	C10N2O3F4	271.9840	1.2439	4.5734	99.1388	3,137	10.0
3	C9H2N2O6F2	271.9875	-2.3436	-8.6167	99.0403	3,495	9.0
4	C10N4O6	271.9812	3.9648	14.5774	98.3769	5,911	13.0
5	C7HN4O7F	271.9824	2.8220	10.3755	98.1733	6,653	9.0
6	C12HO2F5	271.9891	-3.9217	-14.4188	98.0129	7,237	10.0
7	C7HN2O4F5	271.9851	0.1010	0.3715	97.8477	7,839	6.0
8	C7HOF9	271.9878	-2.6199	-9.6324	97.3313	9,720	3.0
9	C12HN2O5F	271.9864	-1.2008	-4.4148	97.3165	9,773	13.0
10	C4N8O7	271.9884	-3.2458	-11.9338	96.8179	11,589	9.0
11	C6H3N2O7F3	271.9887	-3.4865	-12.8186	96.8069	11,629	5.0
12	C5N2O2F8	271.9827	2.5457	9.3598	96.0935	14,228	3.0
13	C4H2N4O8F2	271.9835	1.6791	6.1736	95.5777	16,106	5.0
14	C15OF4	271.9880	-2.7788	-10.2169	95.2563	17,277	14.0
15	C4H2N2O5F6	271.9862	-1.0418	-3.8304	95.1082	17,816	2.0
16	C15N2O4	271.9853	-0.0579	-0.2129	94.6082	19,637	17.0
17	C4H2O2F10	271.9890	-3.7627	-13.8343	94.5724	19,768	-1.0
18	CHN8O8F	271.9896	-4.3887	-16.1357	94.1064	21,465	5.0
19	C3H4N2O8F4	271.9898	-4.6293	-17.0205	94.0940	21,510	1.0
20	C2HN4O6F5	271.9811	4.1238	15.1618	93.8639	22,348	2.0
21	C2HN2O3F9	271.9838	1.4029	5.1579	93.3358	24,271	-1.0
22	CH3N4O9F3	271.9847	0.5363	1.9717	92.8516	26,035	1.0
23	C2HF13	271.9865	-1.3181	-4.8460	92.7685	26,338	-4.0
24	CH3N2O6F7	271.9874	-2.1847	-8.0323	92.3564	27,838	-2.0
25	CH3O3F11	271.9901	-4.9056	-18.0362	91.8228	29,782	-5.0
26	N2OF12	271.9814	3.8475	14.1462	91.5452	30,793	-4.0
27	C20O2	271.9893	-4.0807	-15.0033	90.6209	34,159	21.0

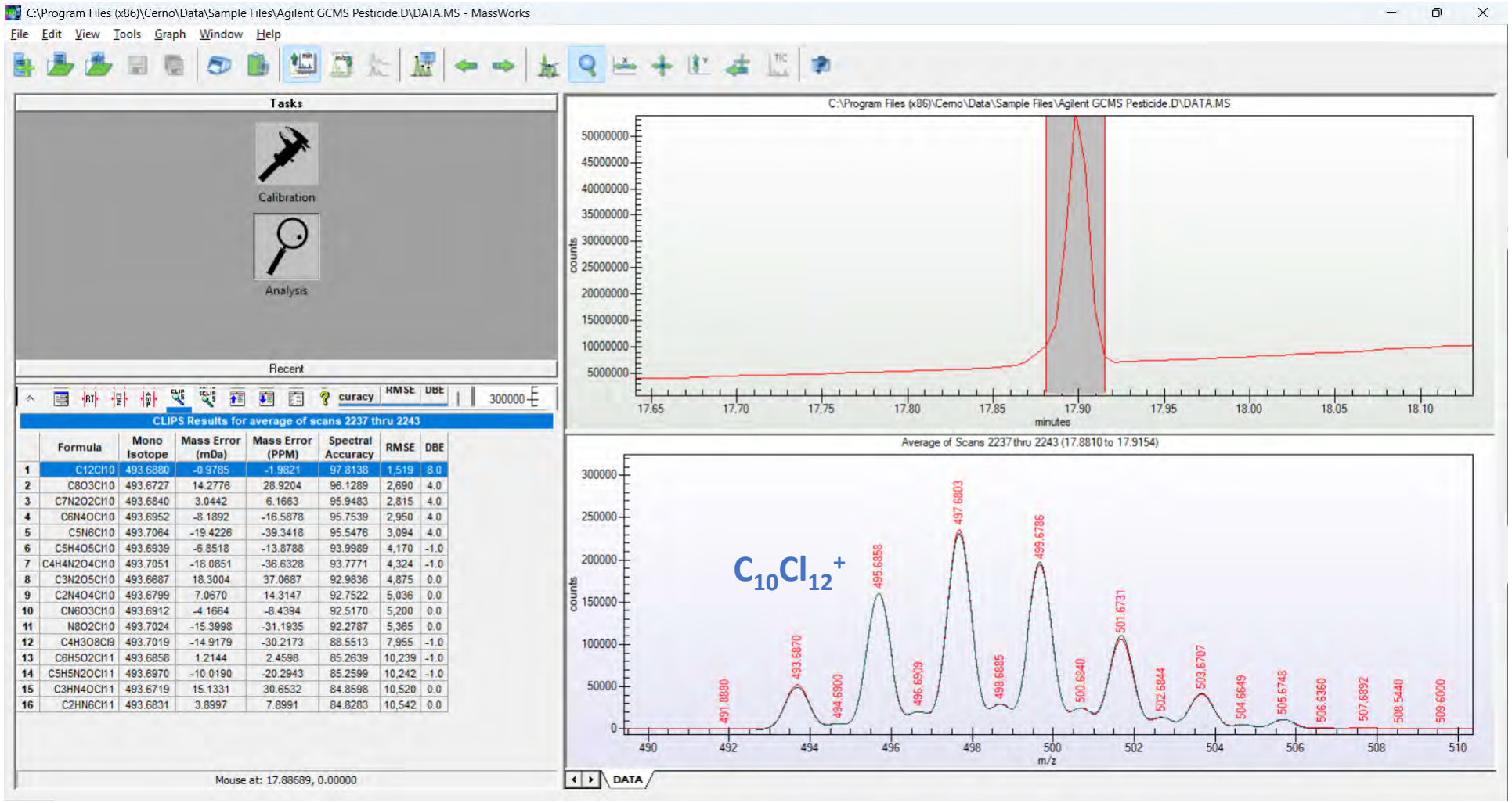
- Measured MS accurately compared to theoretical MS
- The concept of Spectral Accuracy
- Elemental composition determination with even single quad
- Further enhance HiRes MS (TOF/Orbitrap)
- Education/Teaching tools

Selected Publications



Wang, Y. et al *Anal. Chem.* **2010**, *82*, 7055-7062 (17)

Weak Monoisotopic Peak: Cl/Br-Containing (z=1, Unit Mass Resolution)



	Formula	Mono Isotope	Mass Error (mDa)	Mass Error (PPM)	Spectral Accuracy	RMSE	DBE
1	C12Cl10	493.6880	-0.9785	-1.9821	97.8138	1,519	8.0
2	C8O3Cl10	493.6727	14.2776	28.9204	96.1289	2,690	4.0
3	C7N2O2Cl10	493.6840	3.0442	6.1663	95.9483	2,815	4.0
4	C6N4OCl10	493.6952	-8.1892	-16.5878	95.7539	2,950	4.0
5	C5N6Cl10	493.7064	-19.4226	-39.3418	95.5476	3,094	4.0
6	C5H4O5Cl10	493.6939	-6.8518	-13.8788	93.9989	4,170	-1.0
7	C4H4N2O4Cl10	493.7051	-18.0851	-36.6328	93.7771	4,324	-1.0
8	C3N2O5Cl10	493.6687	18.3004	37.0687	92.9836	4,875	0.0
9	C2N4O4Cl10	493.6799	7.0670	14.3147	92.7522	5,036	0.0
10	CN6O3Cl10	493.6912	-4.1664	-8.4394	92.5170	5,200	0.0
11	N8O2Cl10	493.7024	-15.3998	-31.1935	92.2787	5,365	0.0
12	C4H3O8Cl9	493.7019	-14.9179	-30.2173	88.5513	7,955	-1.0
13	C6H5O2Cl11	493.6858	1.2144	2.4598	85.2639	10,239	-1.0
14	C5H5N2OCl11	493.6970	-10.0190	-20.2943	85.2599	10,242	-1.0
15	C3HN4OCl11	493.6719	15.1331	30.6532	84.8598	10,520	0.0
16	C2HN6Cl11	493.6831	3.8997	7.8991	84.8283	10,542	0.0

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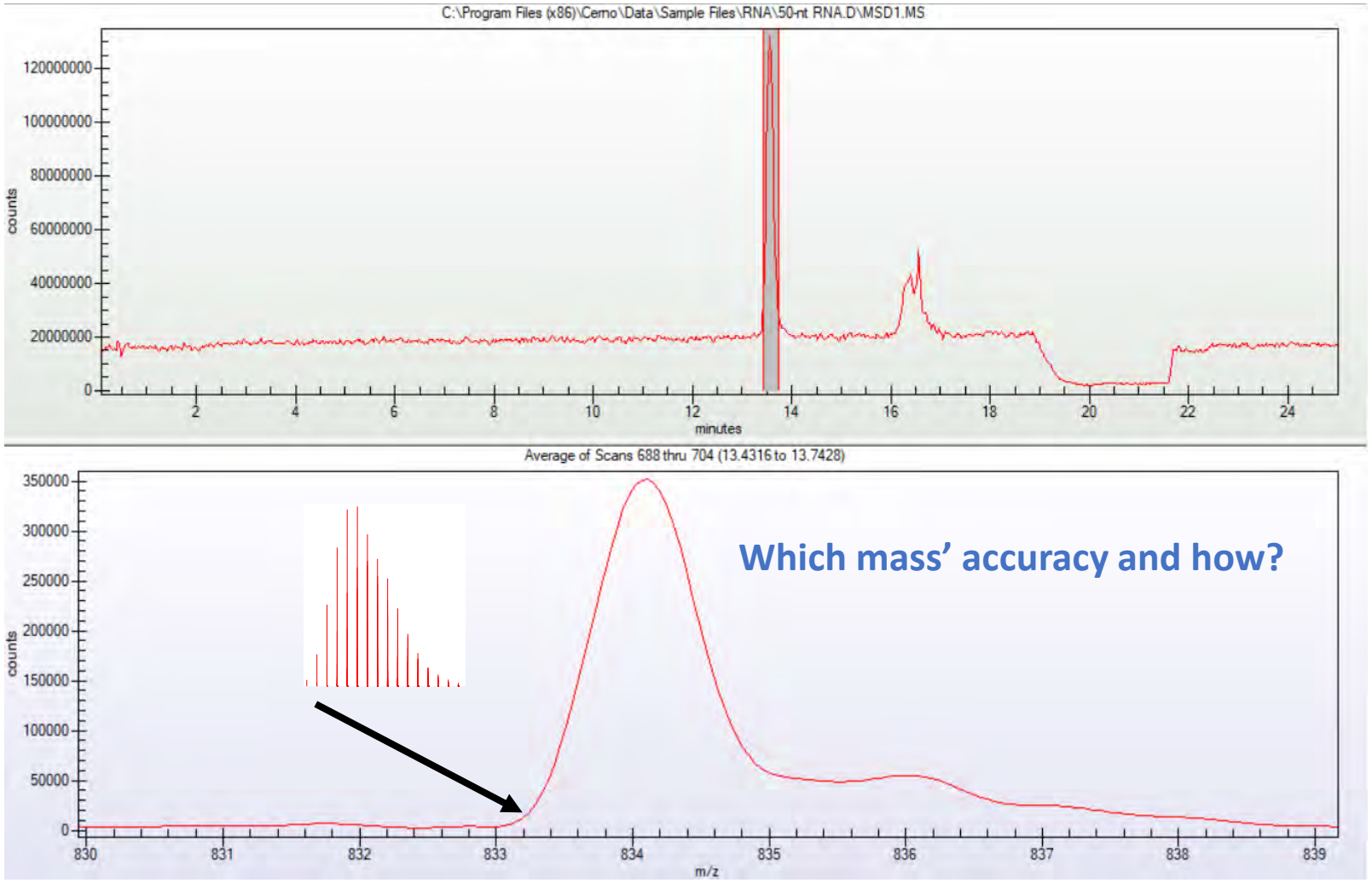
Monoisotopic Peak Goes Missing: 50-nt RNA, z=-19, Unit Mass Resolution

Seq: 5′-HO-UAUUCAAGUUACACUCAAGAAGGAAUAAUUUCUAAACCGUUACCAUUACU-OH-3′



Neutral formula:
$C_{474}H_{585}N_{182}O_{345}P_{49}$
Exact Monoisotopic Mass:
15,862.0969

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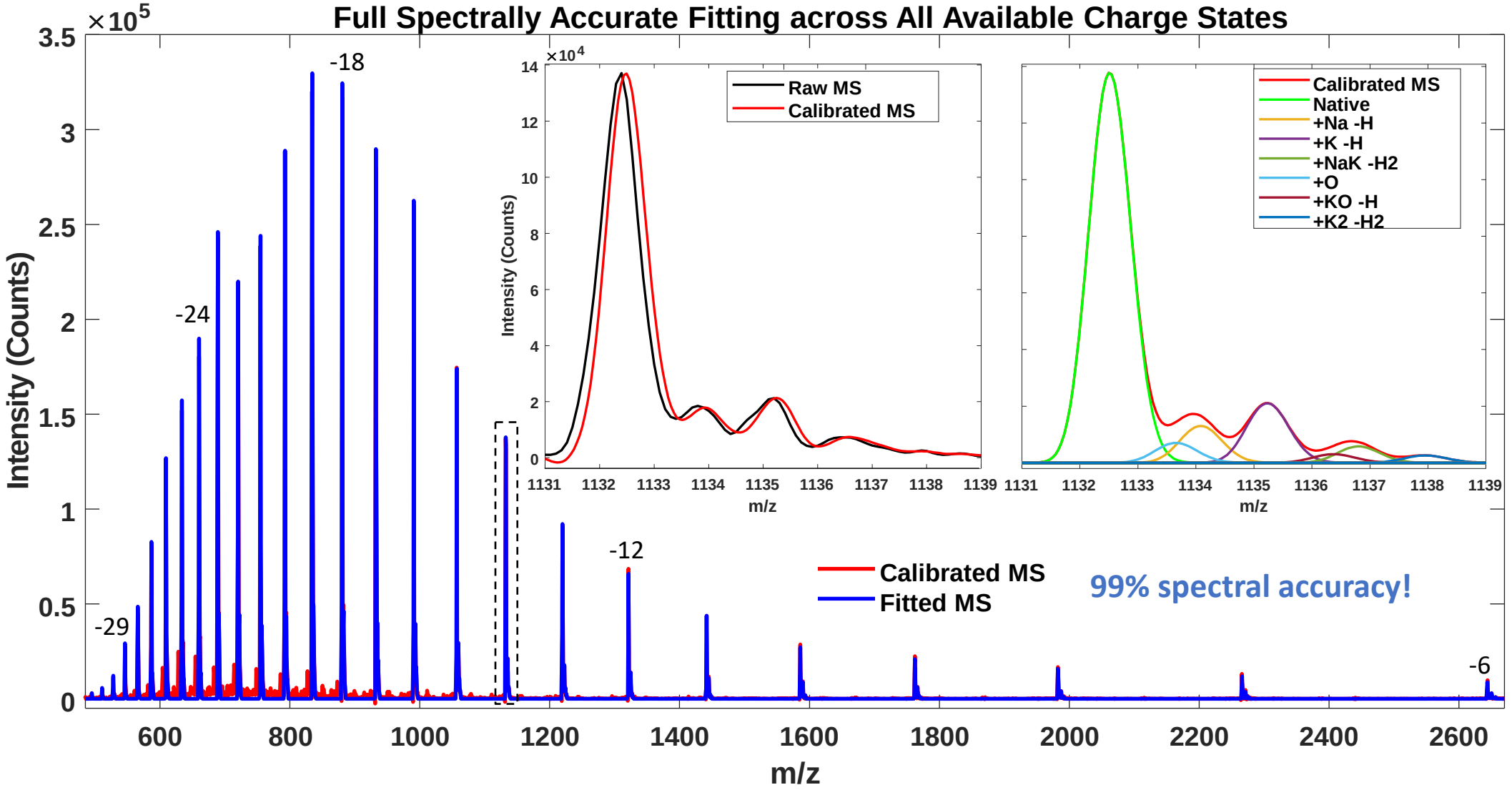
Monoisotopic Peak Goes Missing: 50-nt RNA, z=-14, Unit Mass Resolution



Wang, Y. et al
ASMS Poster 2021

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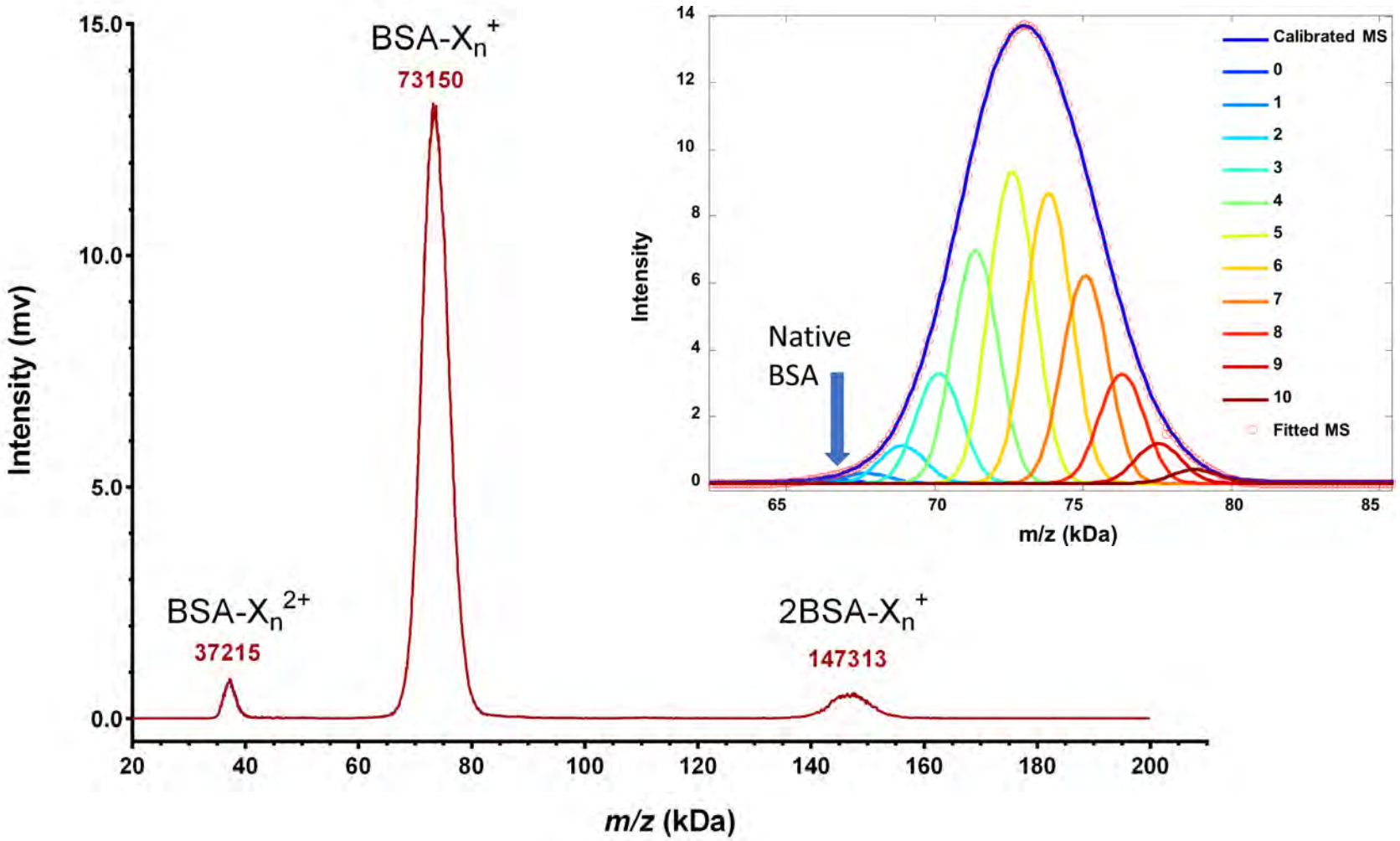
Monoisotopic Peak Goes Missing: BSA, z=1-2, MALDI TOF MS



Lai, C. et al
ASMS Poster 2017

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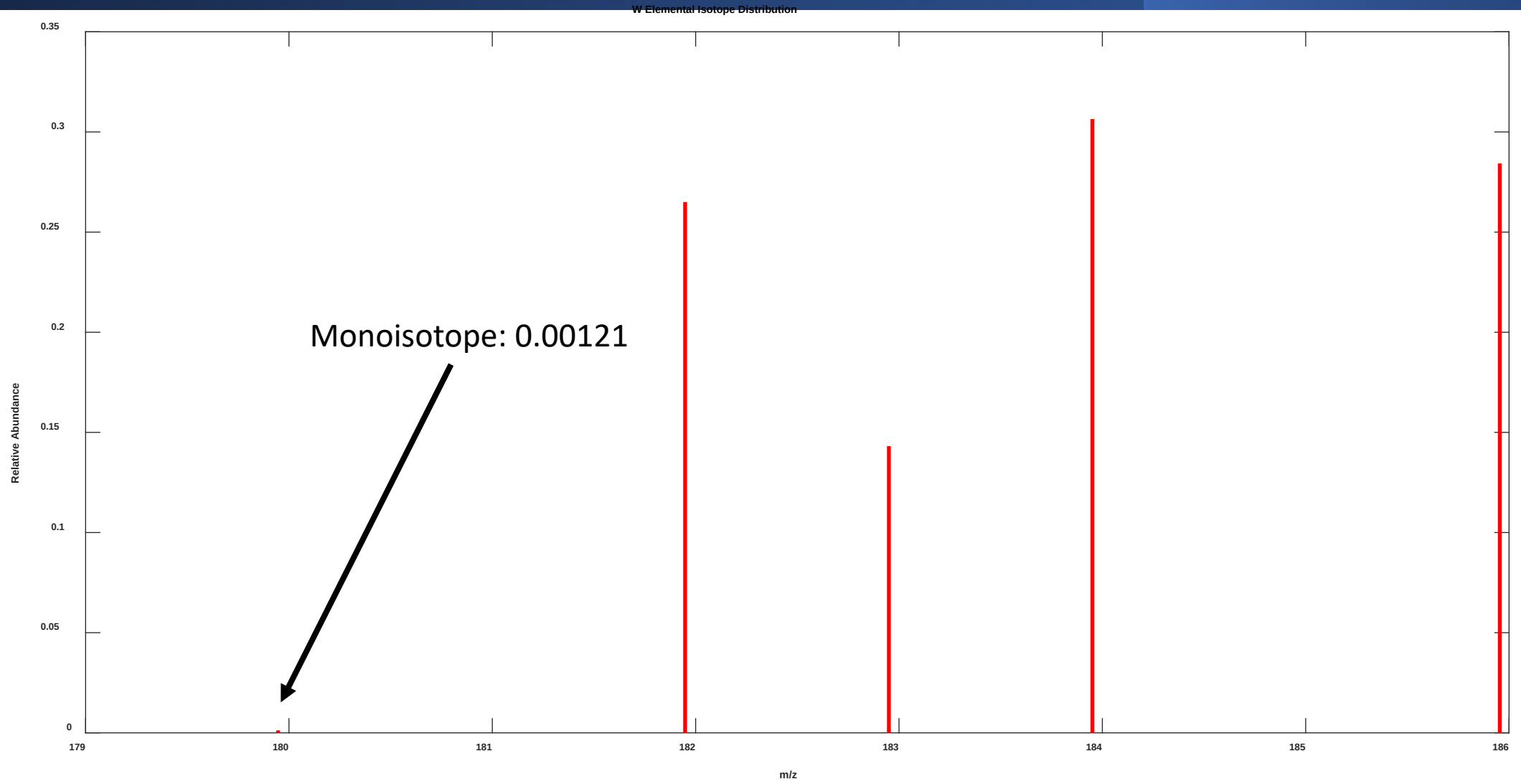
Monoisotopic Peak Goes Missing: W-containing, Any Resolution



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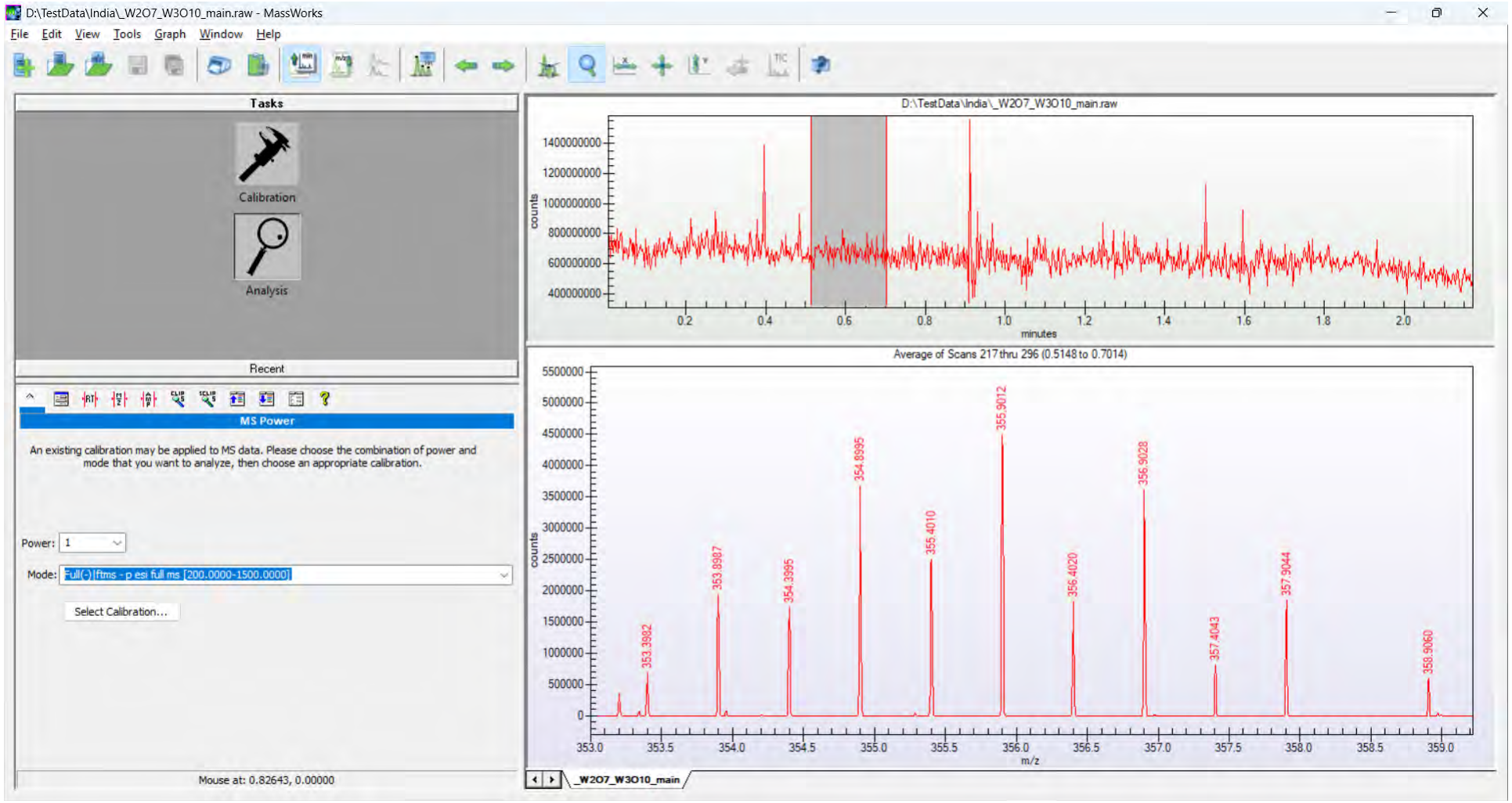
Monoisotopic Peak Goes Missing: W-containing, z=-2, Orbitrap LC/MS, ESI-



Data courtesy of Mr. Abhijit Nandy & Prof. Shibdas Banerjee, Department of Chemistry, Indian Institute of Science Education and Research Tirupati

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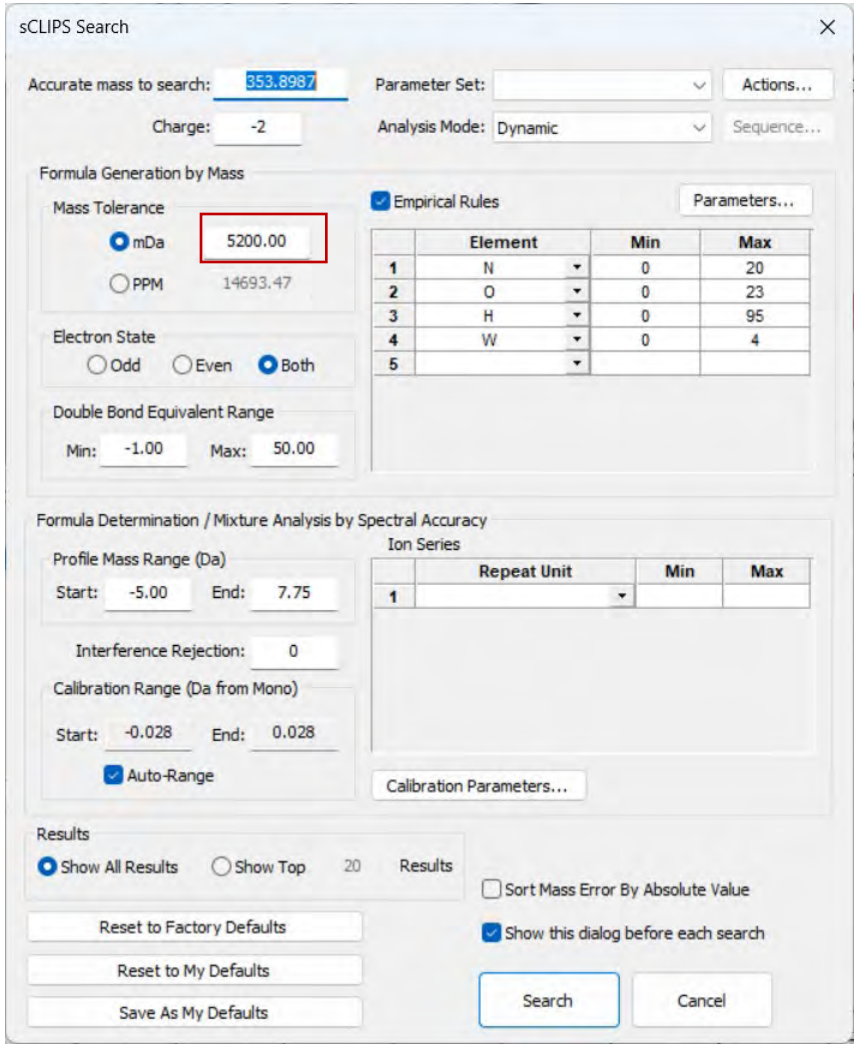
Monoisotopic Peak Goes Missing: W-containing, z=-2, Orbitrap LC/MS, ESI-



Wide open mass tolerance ±5.2Da

Spectral Accuracy search only

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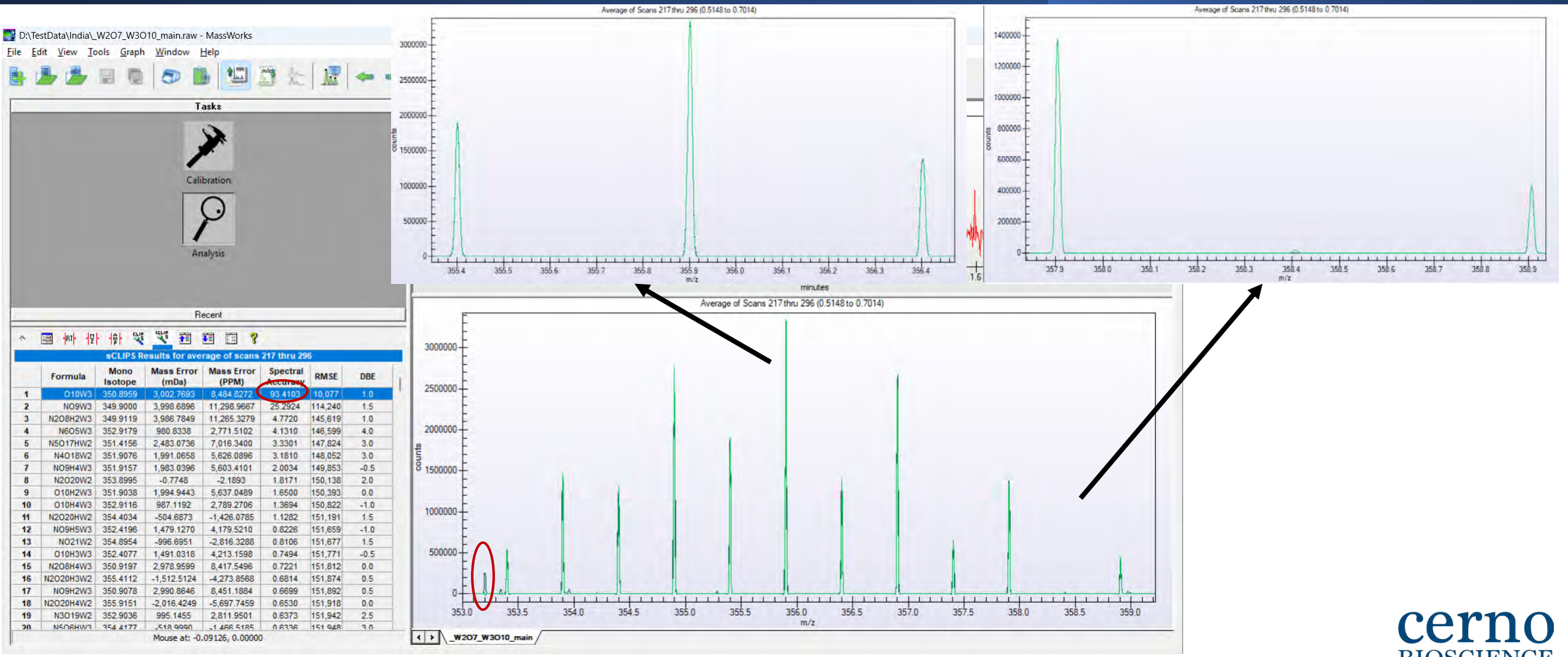
Monoisotopic Peak Goes Missing: W-containing, z=-2, Orbitrap LC/MS, ESI-



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Summary

- Mass accuracy is important and clearly defined when there is observable monoisotope
- Spectral Accuracy is always well defined regardless
- Peak shape calibration is key to achieve high Spectral Accuracy at any resolution
- Spectral Accuracy enables accurate mixture analysis
- It is possible to search for unknown elemental composition based on Spectral Accuracy alone (computational efficiency)
- Compounds with metal ions are amenable to Spectral Accuracy analysis
- Next step: organometallic compounds with Hg, Cr, Sn etc.

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Further Info & Acknowledgement

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Acknowledgement

- Many early adopters
- Many “out-of-box” scientists/researchers

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