



Simplified Operation of Thin Surface-induced Dissociation Devices

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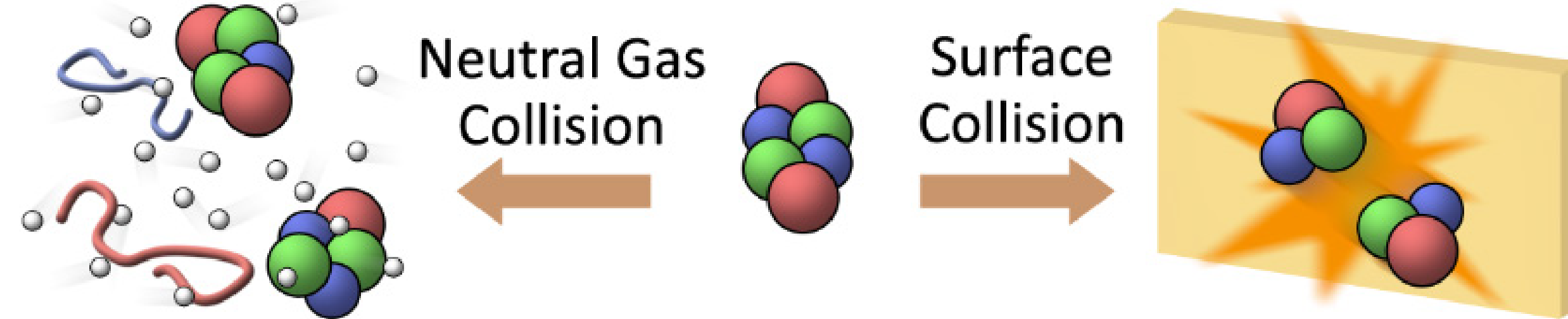
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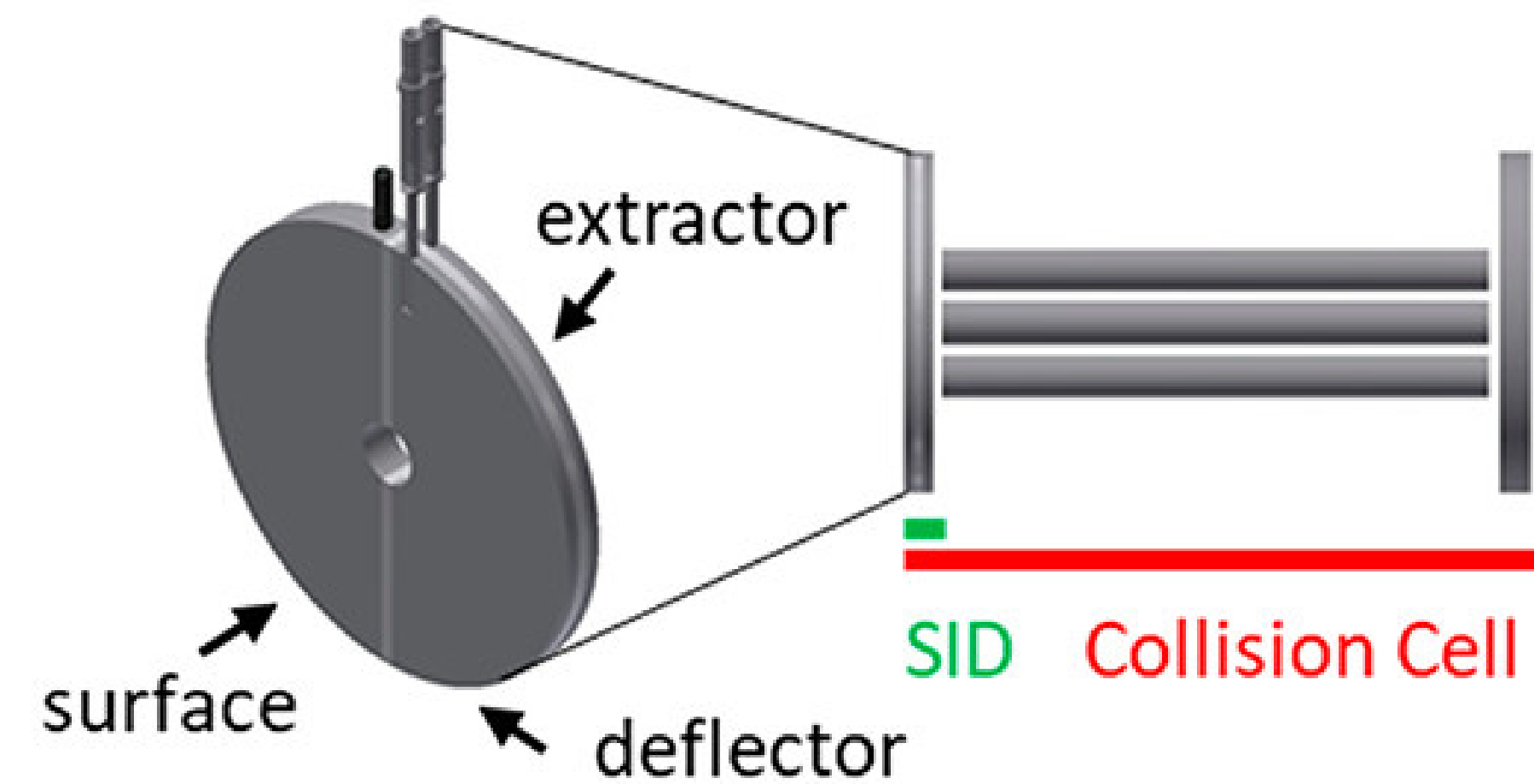
Introduction and Background

• Surface-induced dissociation (SID) involves ion – surface collisions instead of ion – neutral collisions.¹



• SID causes native-like protein complexes to dissociate at the weakest subunit interfaces, revealing information about subunit connectivity and topology.²

• Thin SID devices feature electrodes occupying ~3 mm along the ion beam instead of 1.5 – 3 cm.³



• Thin SID devices have 3 independent electrodes which simplifies tuning requirements (previous devices had up to 10 electrodes).

• Waters Corp. operates a commercialized thin SID device in the SELECT SERIES Cyclic IMS with the surface and extractor at the same voltage, which possibly influences ion transmission efficiency.⁴

• Thus, we are investigating the effect of tuning the extractor relative to the surface voltage to determine the effect on ion transmission and observed SID product ions.

Instrumentation and Methods

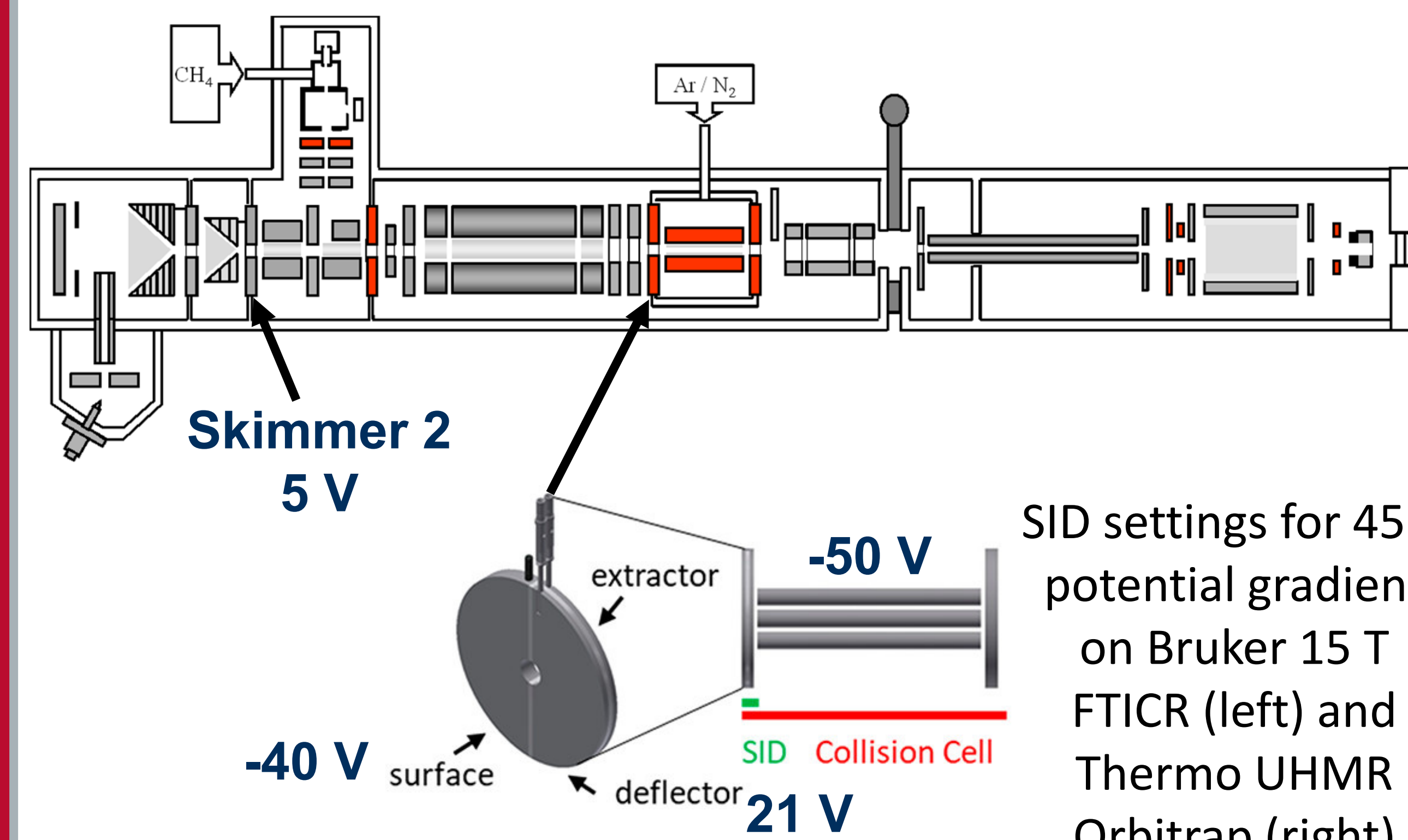
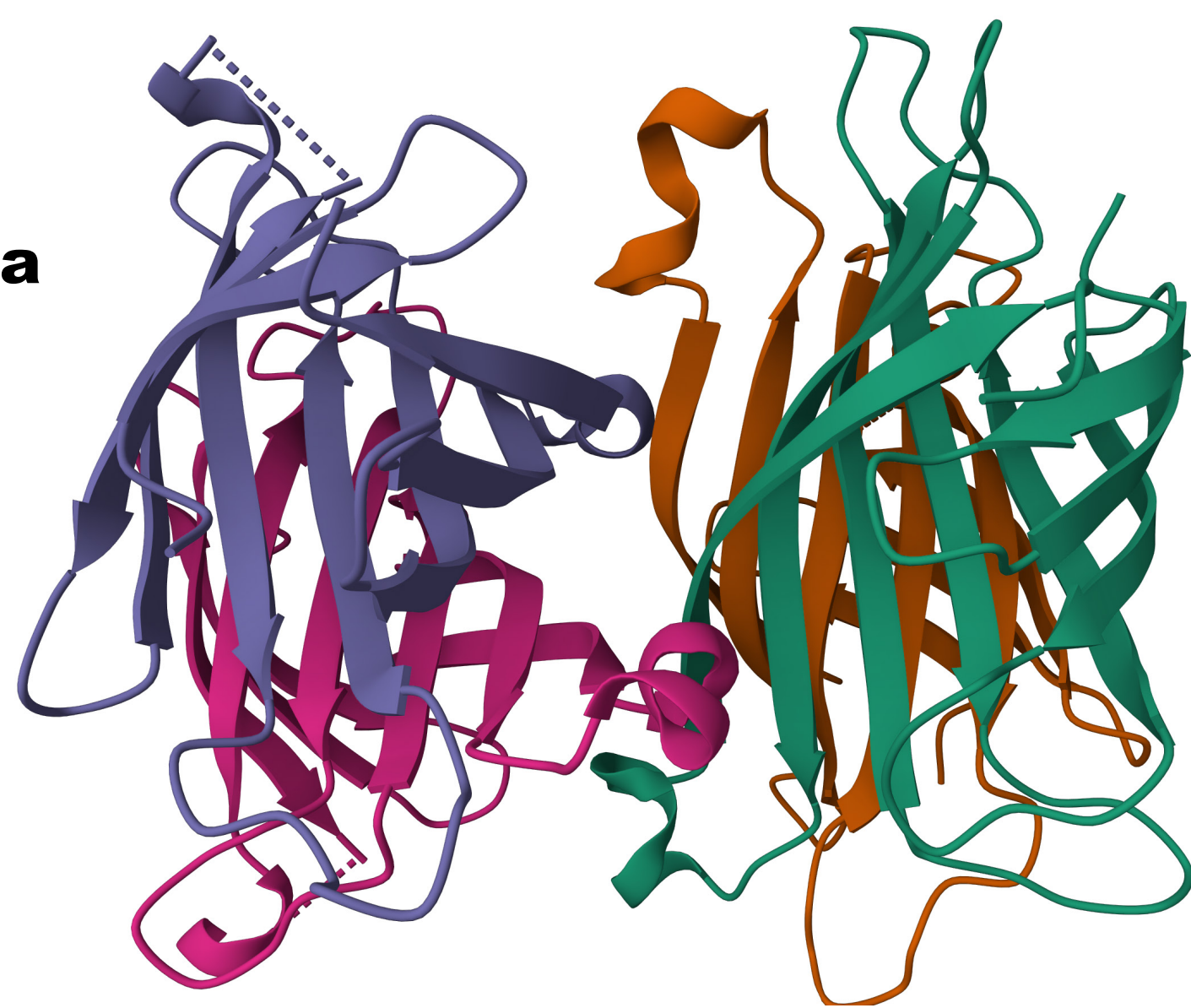
• Bruker solarix XR 15 T FTICR with 3 mm long SID device, replacing the RF collision cell's entrance lens.

• Thermo Scientific Q Exactive Ultra-High Mass Range (UHMR) Orbitrap mass spectrometer with 3 mm long SID device, which replaces the end cap electrode of an e-MSion ExD device, allowing post-ECD and post-ECnOD SID.

Apo-Streptavidin 53 kDa

(PDB: 1SWB)

Tetramer via dimer of dimers topology



SID settings for 45 V potential gradient on Bruker 15 T FTICR (left) and Thermo UHMR Orbitrap (right)

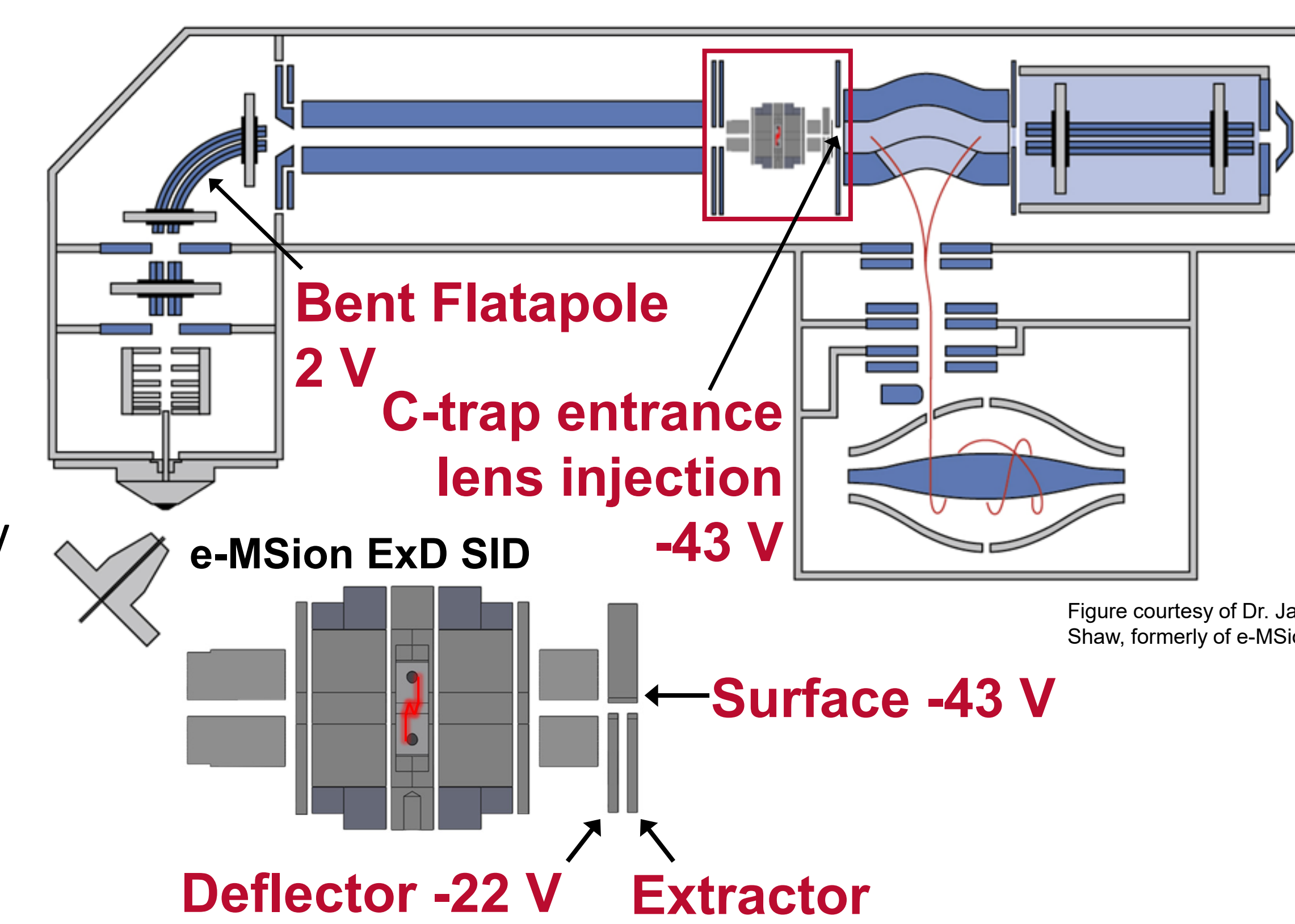
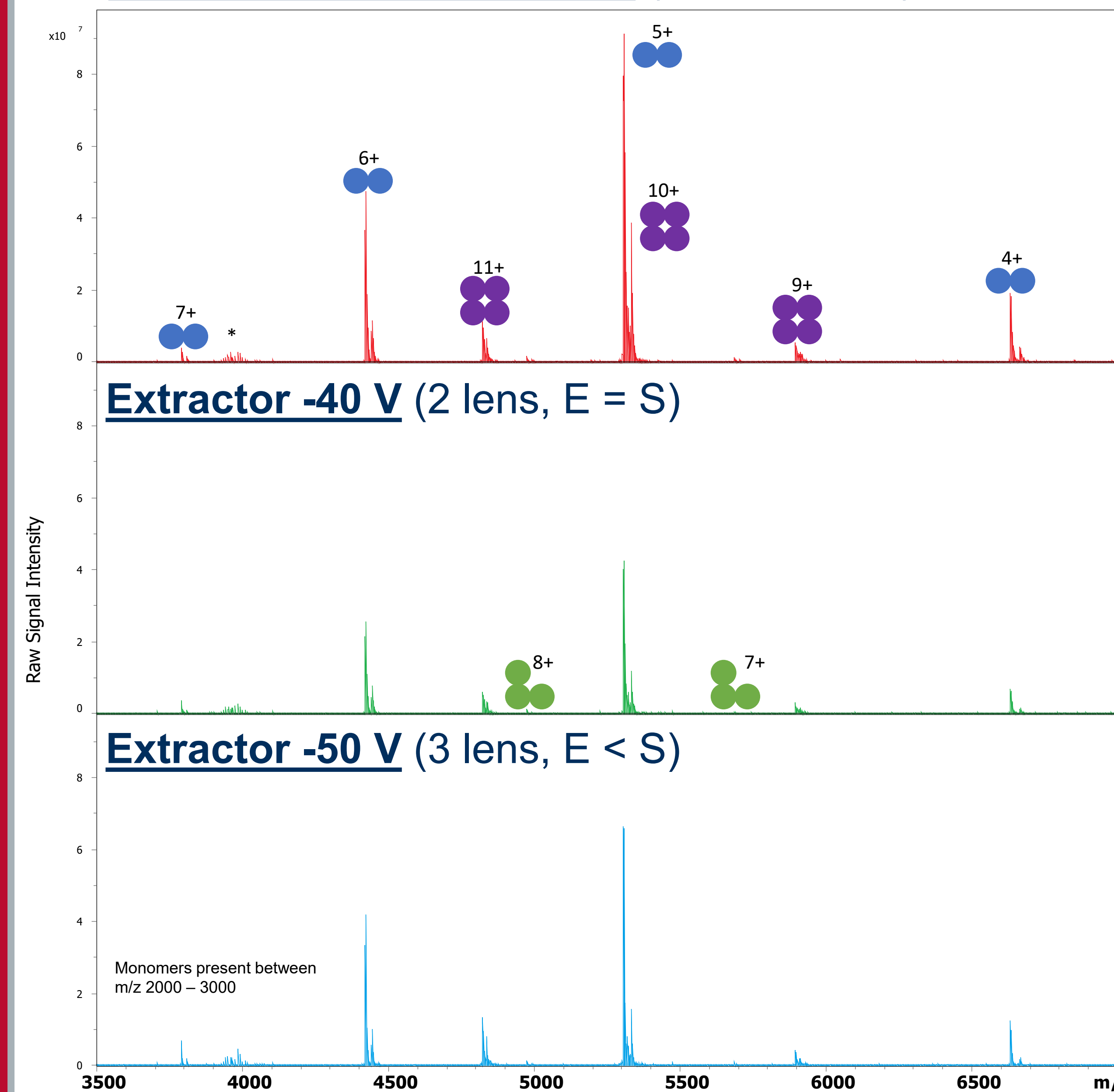
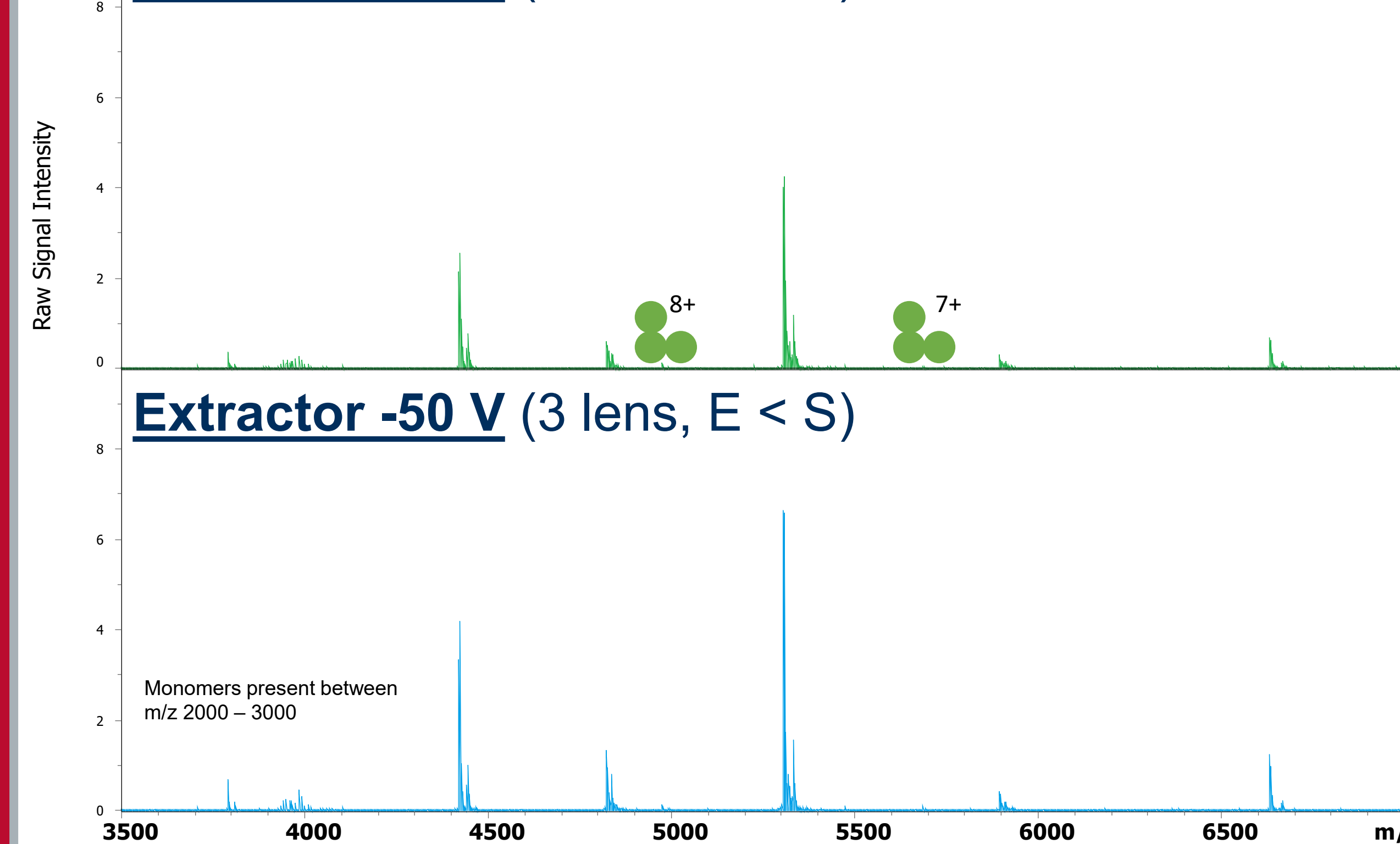


Figure courtesy of Dr. Jared Shaw, formerly of e-MSion.

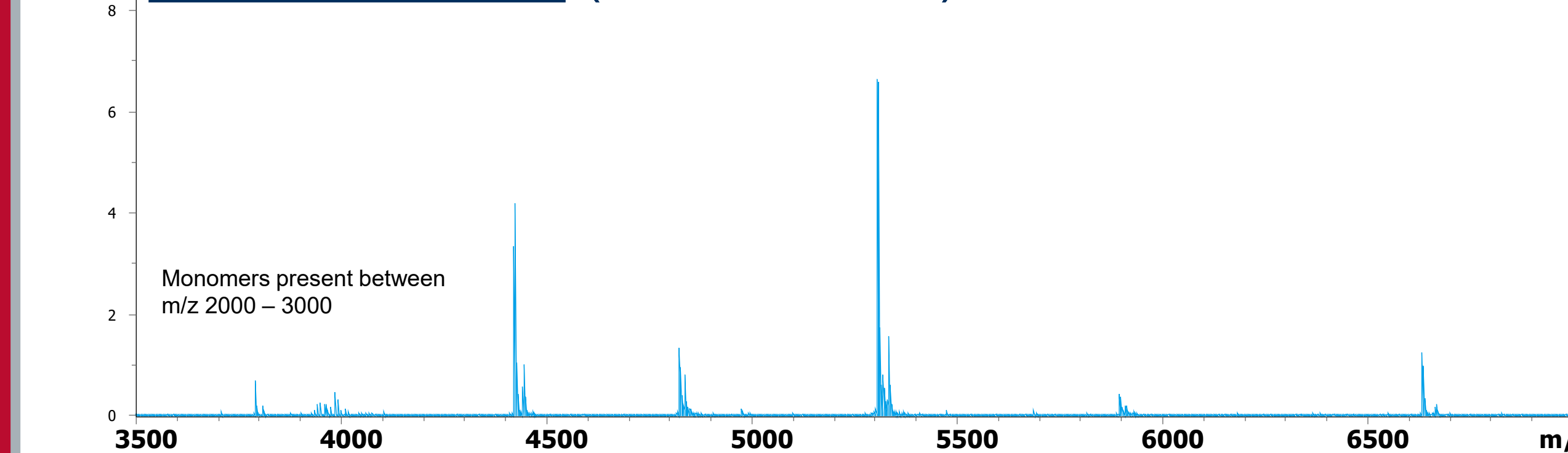
FTICR with Extractor -32 V (3 lens, E > S)



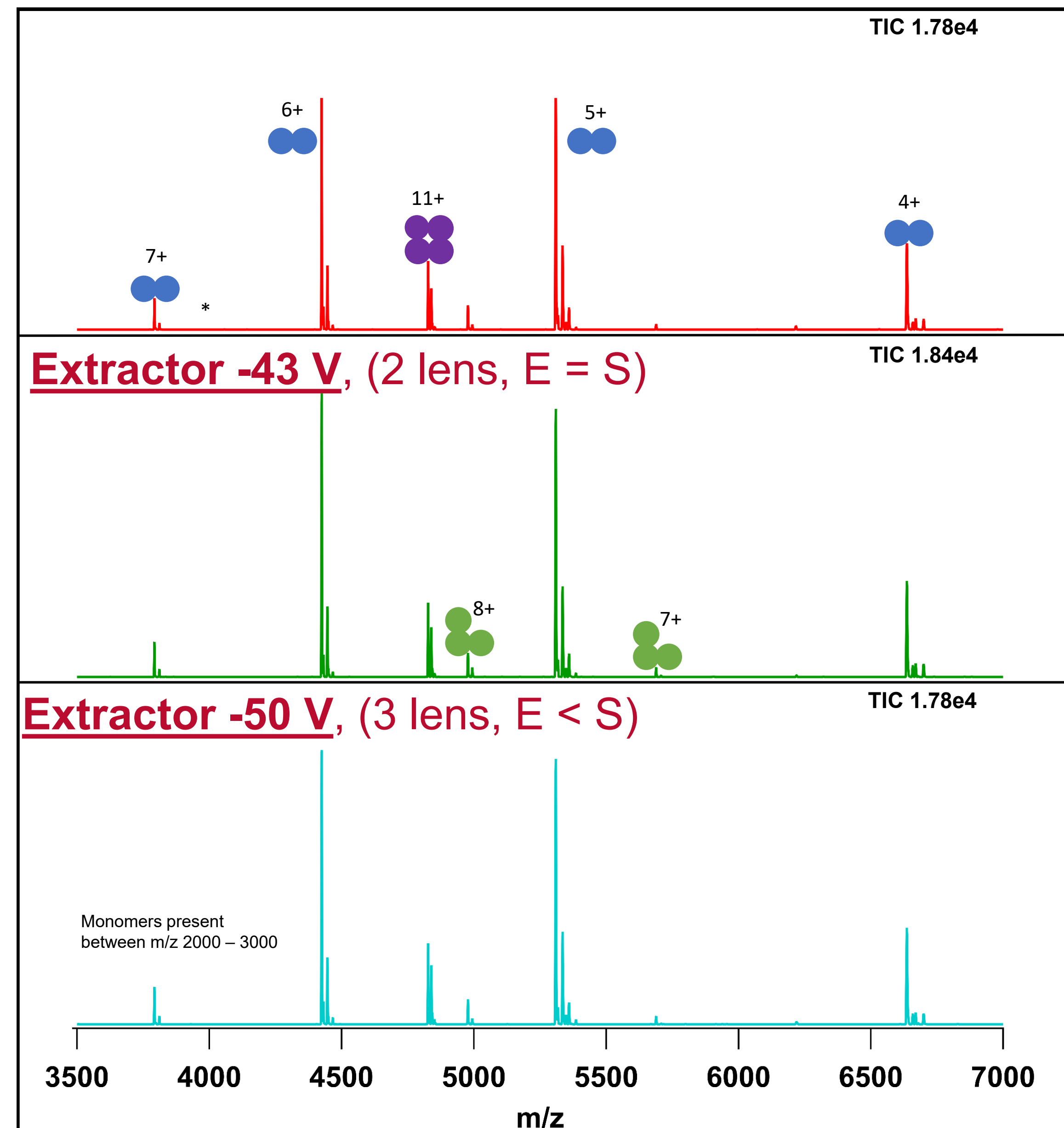
Extractor -40 V (2 lens, E = S)



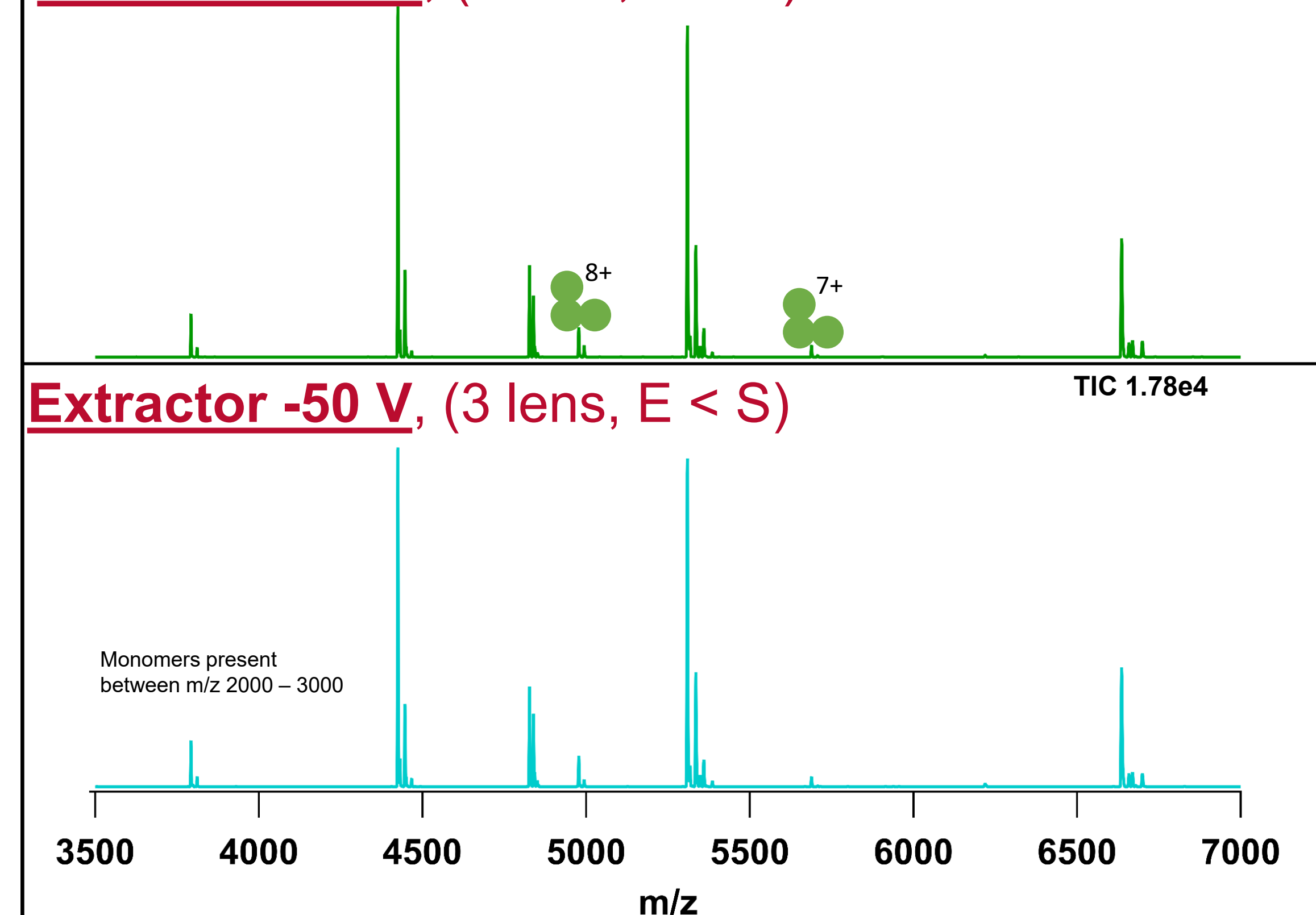
Extractor -50 V (3 lens, E < S)



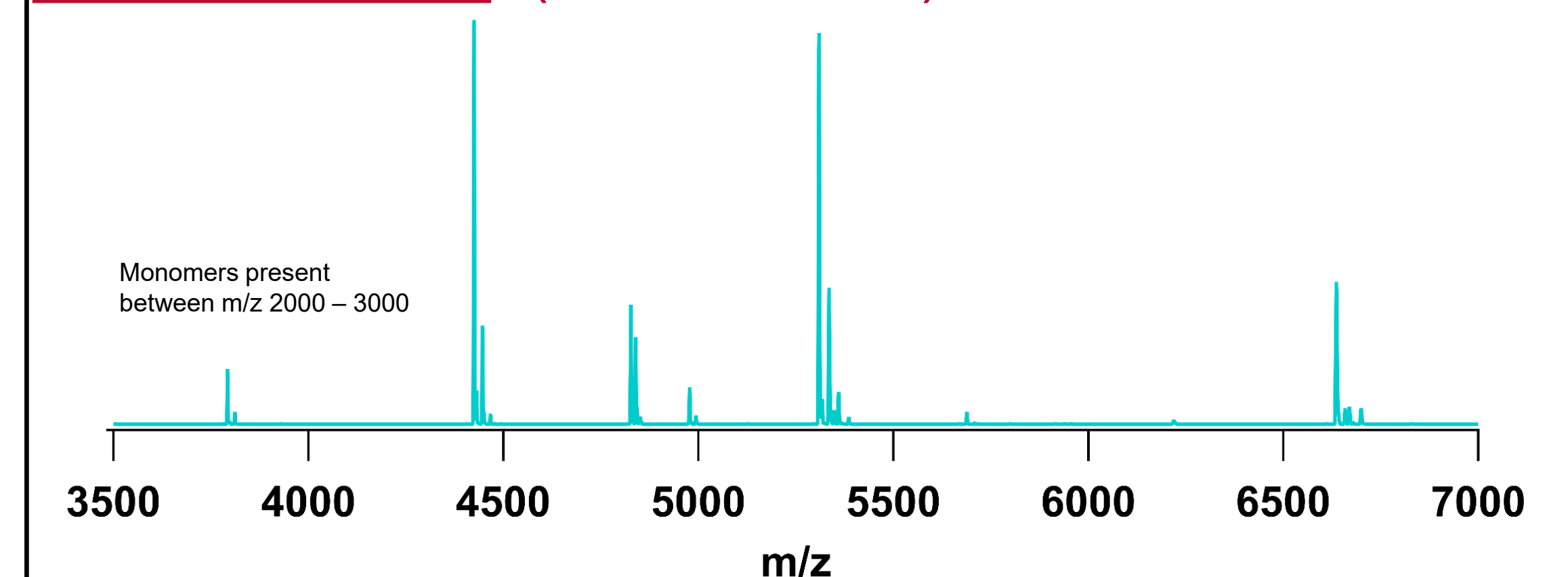
UHMR with Extractor -40 V, (3 lens, E > S)



Extractor -43 V, (2 lens, E = S)

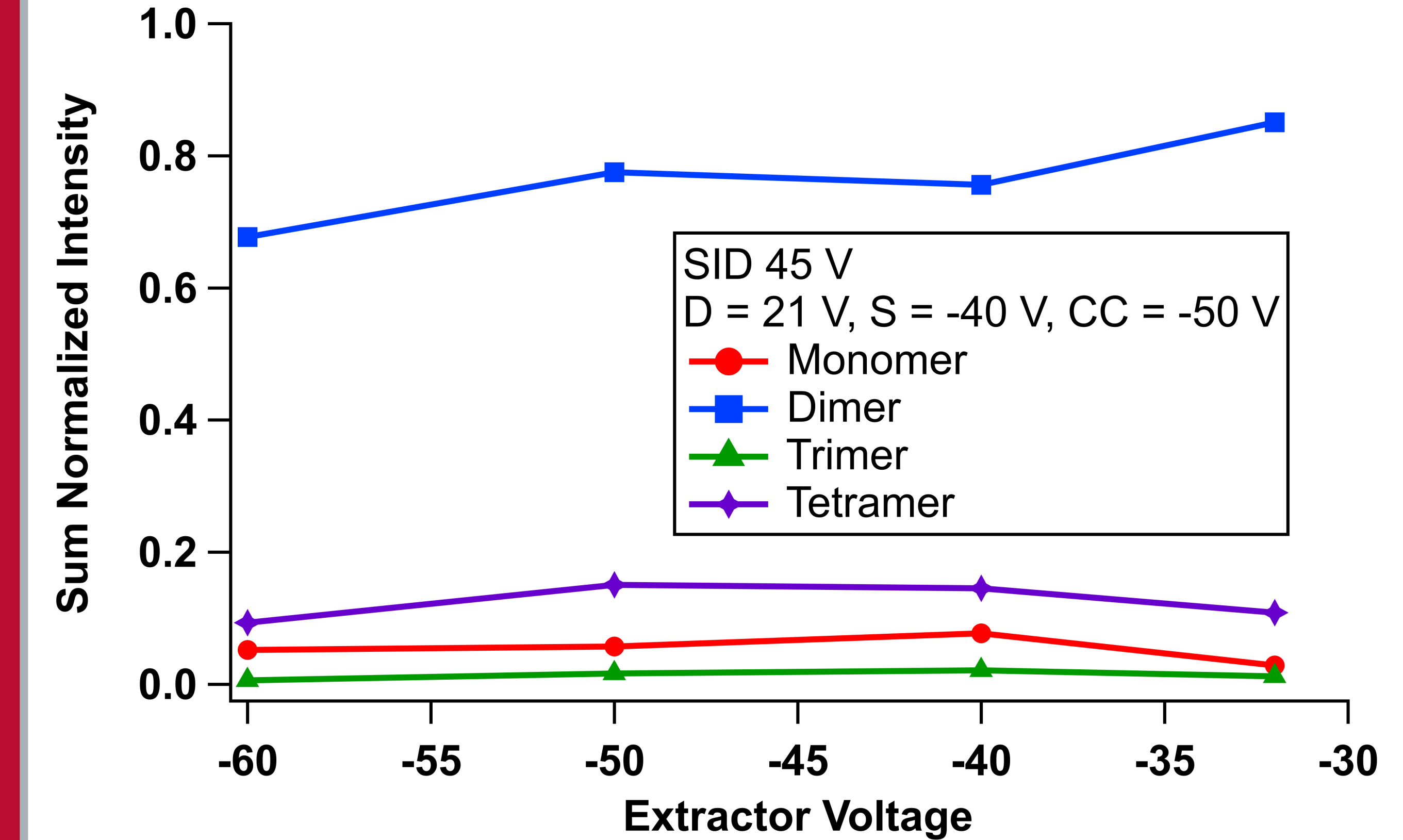


Extractor -50 V, (3 lens, E < S)

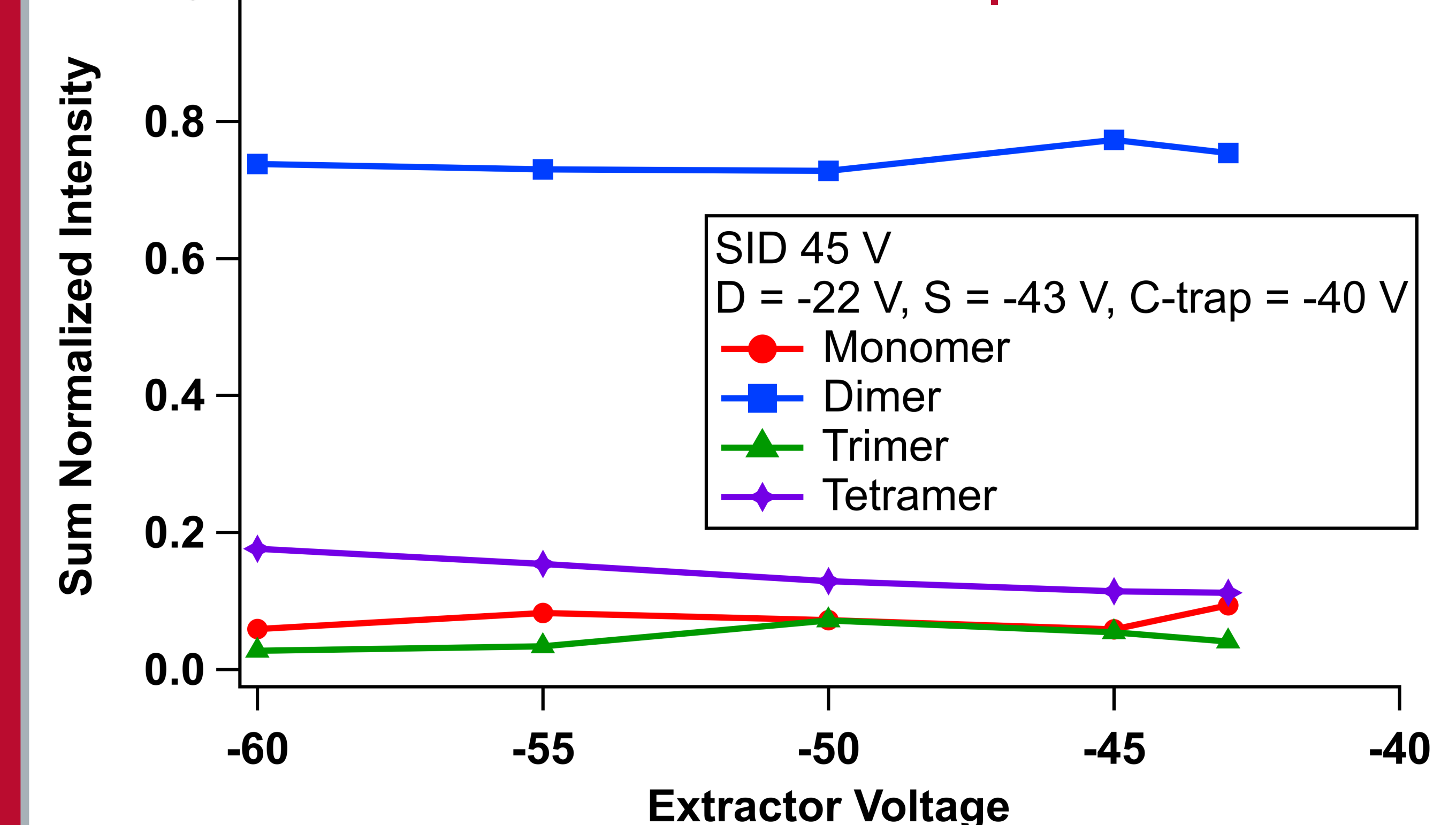


Tuning the extractor higher than, equal to, and lower than the surface voltage had minimal effect on observed spectra and signal intensity.

SA on FTICR



SA on UHMR Orbitrap



References

- (1) Snyder, D. T.; Harvey, S. R.; Wysocki, V. H., Surface-induced Dissociation Mass Spectrometry as a Structural Biology Tool. *Chem. Rev.* **2022**, *122* (8), 7442-7487.
- (2) Harvey, S. R.; Seffernick, J. T.; Quintyn, R. S.; Song, Y.; Ju, Y.; Yan, J.; Sahasrabudhe, A. N.; Norris, A.; Zhou, M.; Behrman, E. J.; Lindert, S.; Wysocki, V. H., Relative interfacial cleavage energetics of protein complexes revealed by surface collisions. *Proc. Natl. Acad. Sci. U.S.A.* **2019**, *116* (17), 8143-8148.
- (3) Snyder, D. T.; Panczyk, E. M.; Somogyi, A.; Kaplan, D. A.; Wysocki, V., Simple and Minimally Invasive SID Devices for Native Mass Spectrometry. *Anal. Chem.* **2020**, *92* (16), 11195-11203.
- (4) Snyder, D. T.; Jones, B. J.; Lin, Y.-F.; Cooper-Shepherd, D. A.; Hewitt, D.; Wildgoose, J.; Brown, J. M.; Langridge, J. I.; Wysocki, V. H., Surface-induced dissociation of protein complexes on a cyclic ion mobility spectrometer. *Analyst* **2021**, *146* (22), 6861-6873.

Acknowledgments

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