Supplemental Information: Application of UHPLC-ESI-MS/MS to Identify Free Radicals via Spin Trapping with BMPO

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Summary: 9 supporting figures

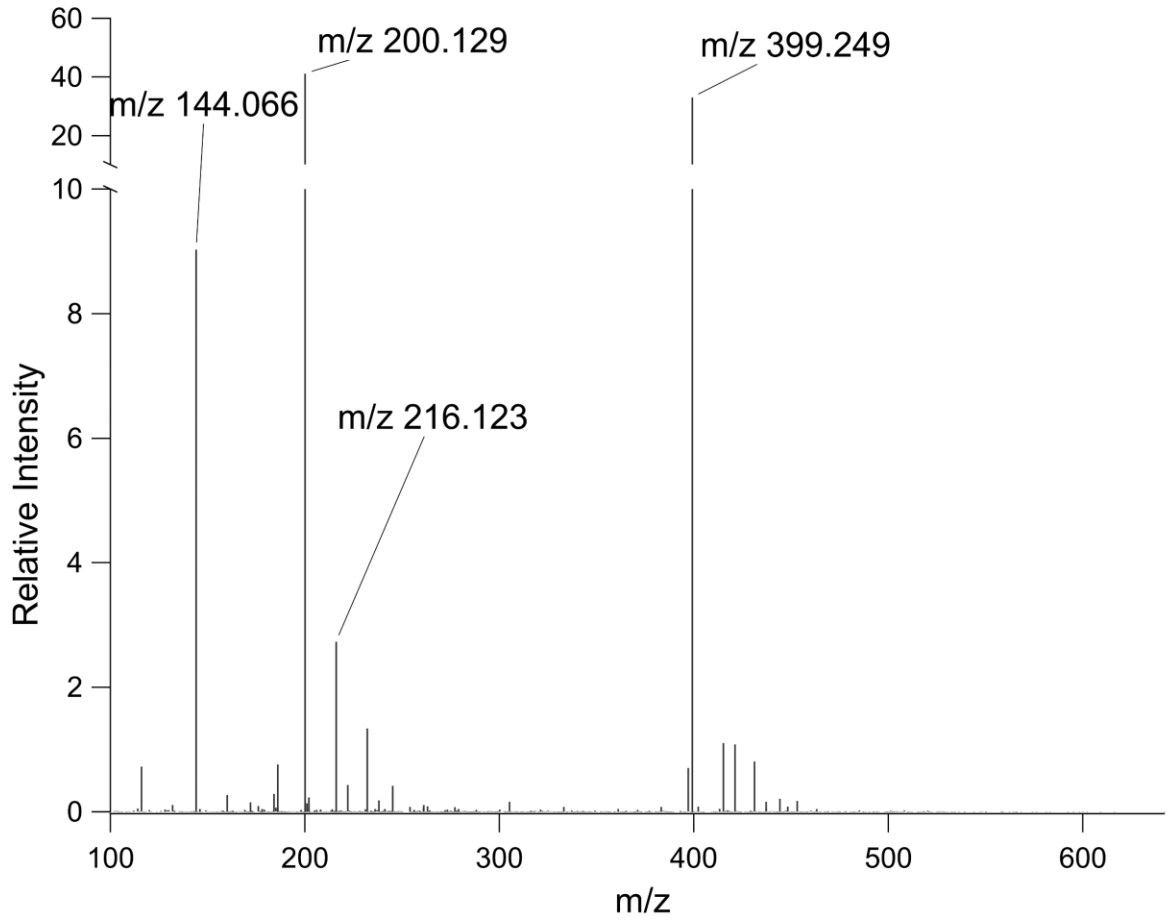

Figure S1: Positive ion mode mass spectrum of irradiated H_2O_2 and BMPO obtained by integration of the chromatogram over 1.6-16 min. A zoomed-in version of this mass spectrum is shown in Figure 4, along with assignments of the major peaks. Note that peaks corresponding to ^{13}C isomers were removed during processing.

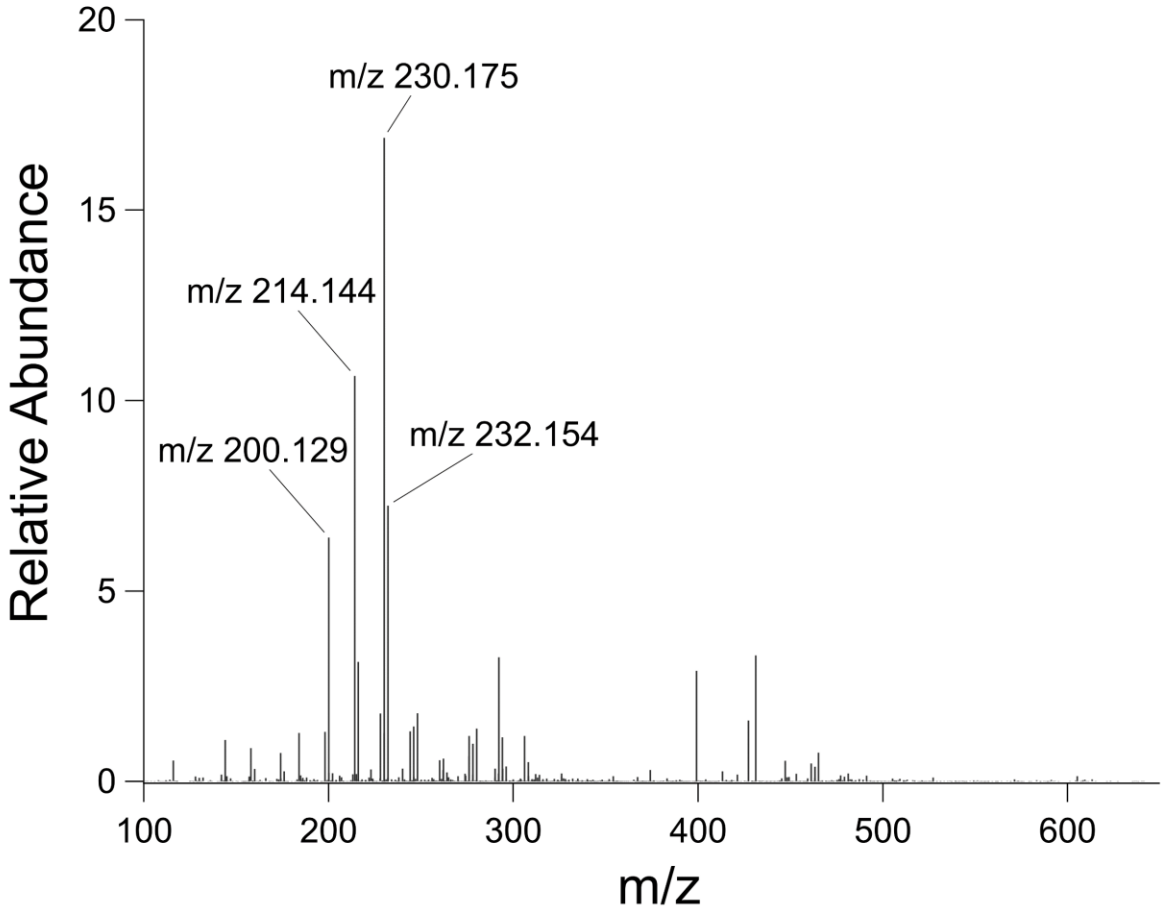

Figure S2: Positive ion mode mass spectrum of the products of OH oxidation of DMSO in the presence of 10 mM BMPO obtained by integration of the chromatogram over 1.6-16 min. A zoomed-in version of this mass spectrum is shown in Figure 6, along with assignments of the major peaks. Note that peaks corresponding to ^{13}C isomers were removed during processing.

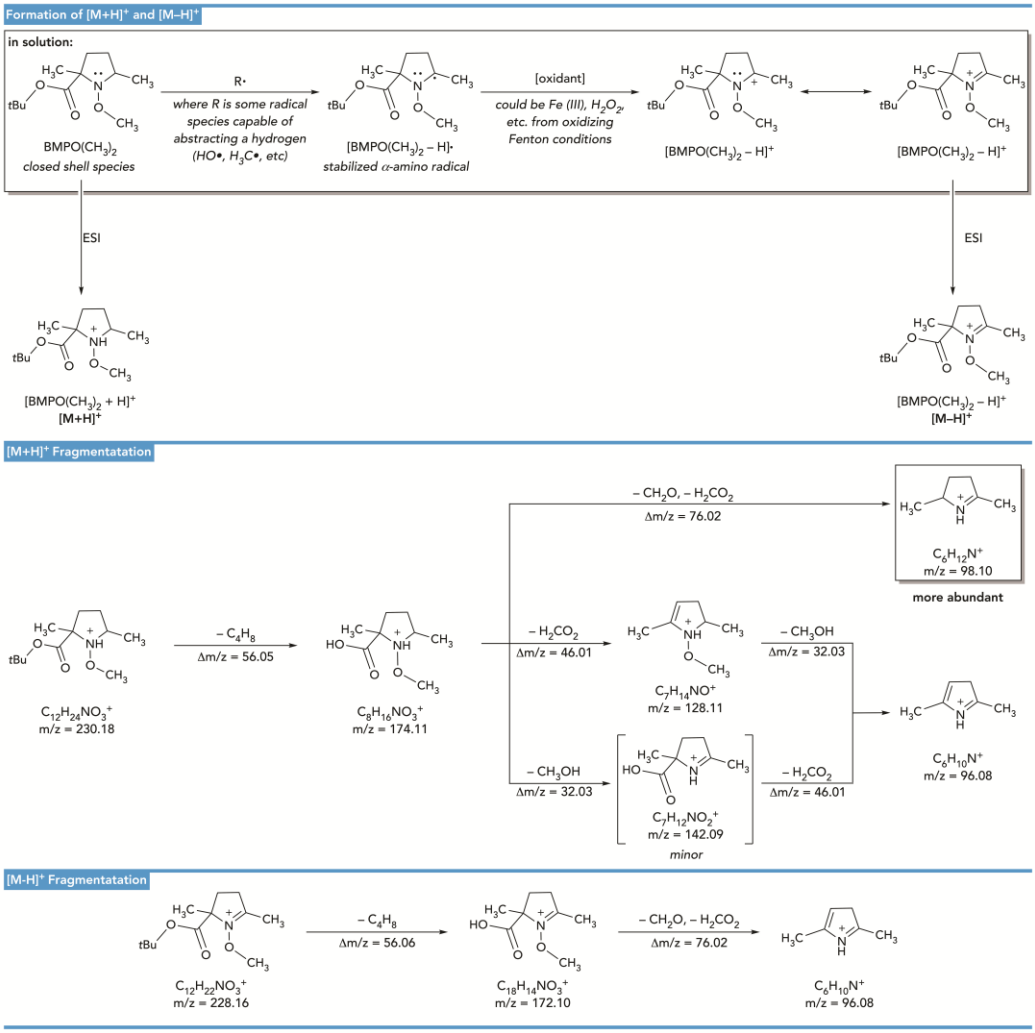

Figure S3: Fragmentation pathway for $BMPO(CH_3)_2$ di-adduct with proposed structures at each monoisotopic *m/z*.

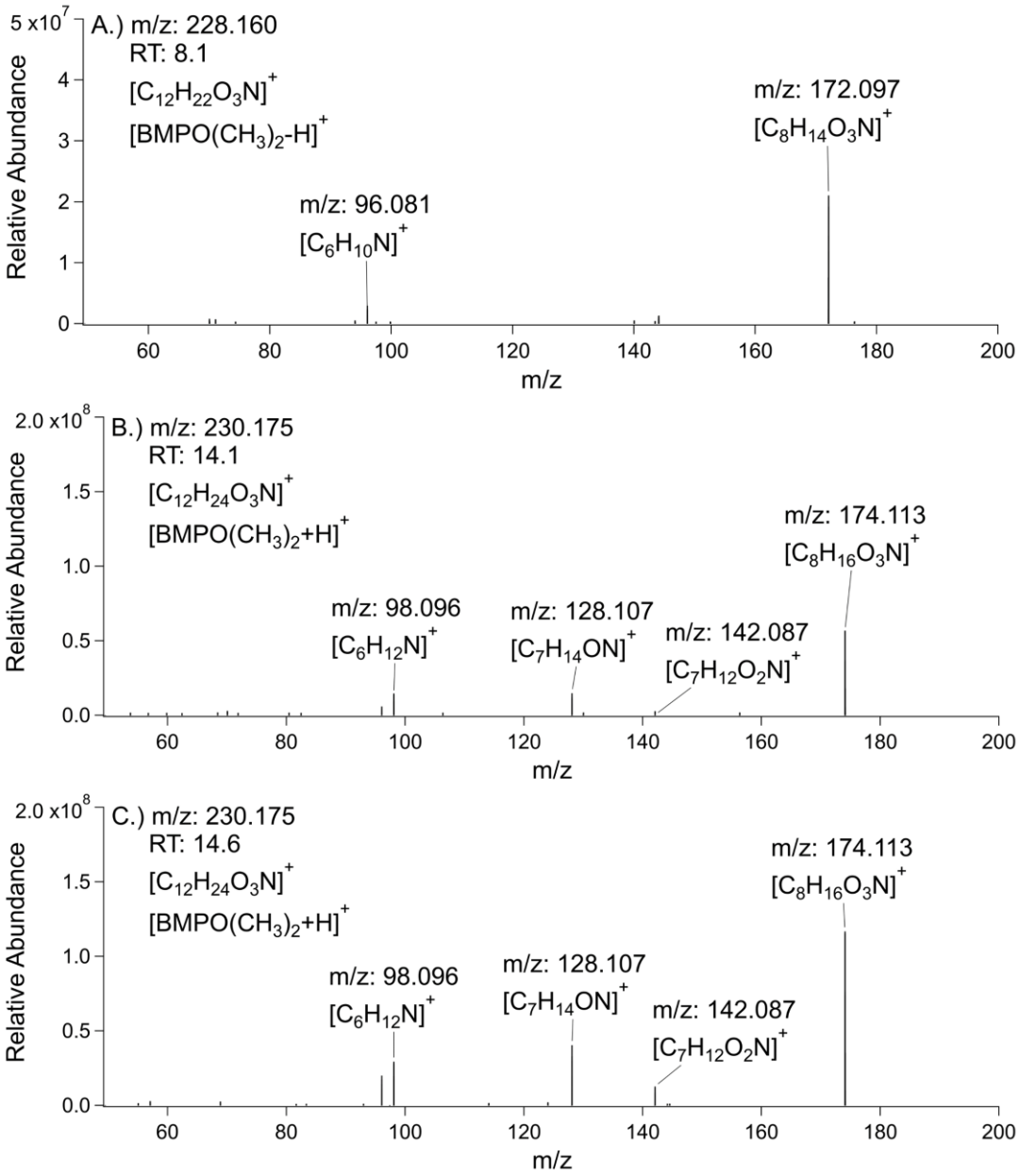

Figure S4: Sum of the fragmentation mass spectra recorded at collision energies 10, 30, and 50 for $BMPO(CH_3)_2$ di-adduct in the form $[M-H]^+$ at retention time 8.1 min (panel A) and $[M+H]^+$at retention times 14.1 min (panel B) and 14.6 min (panel C).

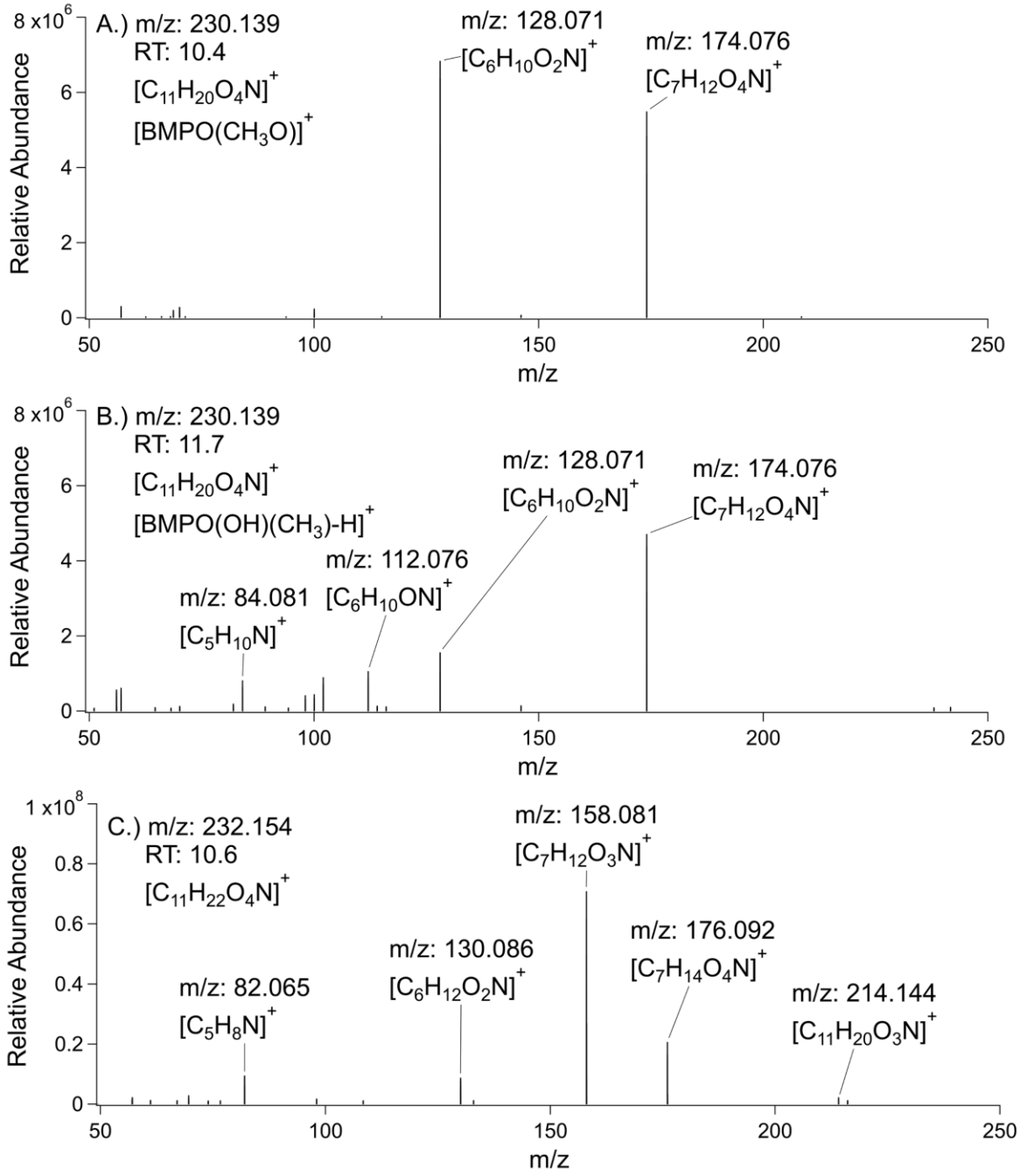

Figure S5: Sum of the fragmentation mass spectra recorded at collision energies 10, 30, and 50 for the oxidized $[M]^+$ BMPO(CH_3O) at retention time 10.4 min (panel A), $[M-H]^+$ ion of BMPO(OH)(CH_3) at 11.7 min (panel B), and either $[BMPO(CH_3O)+2H]^+$ or $[BMPO(OH)(CH_3)+H]^+$ at 10.6 min (panel C).

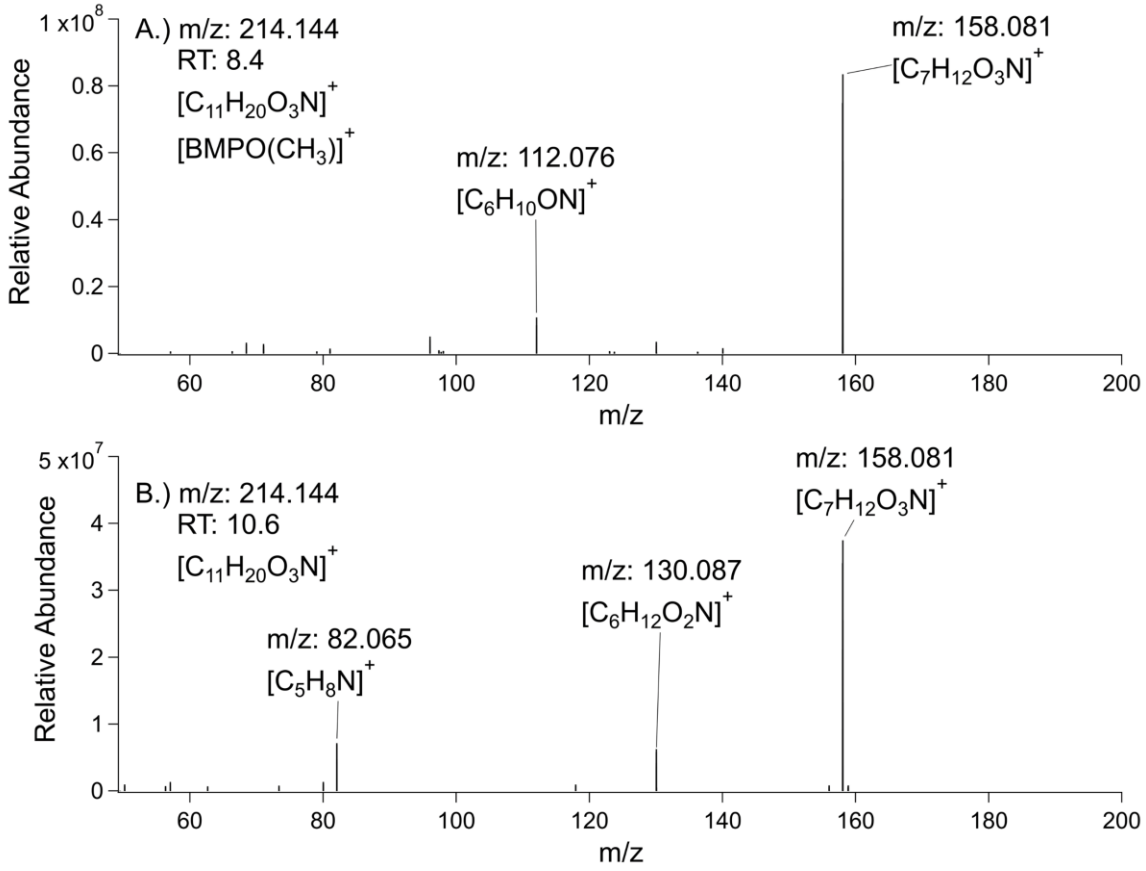

Figure S6: Sum of the fragmentation mass spectra recorded at collision energies 10, 30, and 50 for $[M]^+$ of $BMPO(CH_3)$ at retention time 8.3 min (panel A) and the dehydration fragment of *m/z* 232.154 ($[BMPO(CH_3O)+2H]^+$ or $[BMPO(OH)(CH_3)+H]^+$) at 10.6 min (panel B).

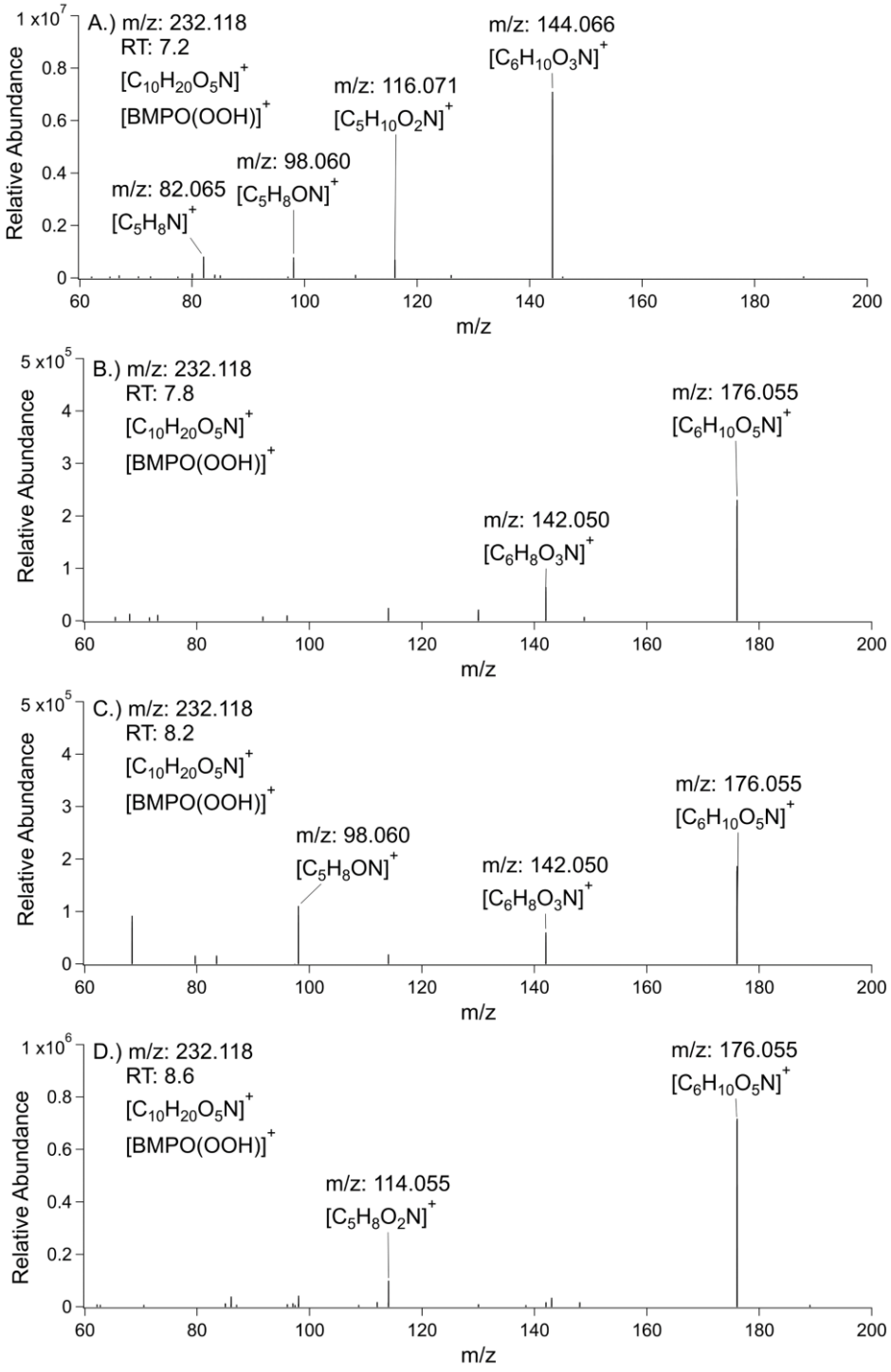

Figure S7: Sum of the fragmentation mass spectra recorded at collision energies 10, 30, and 50 for *m/z* 232.118 (BMPO(OOH) and BMPO(OH)$_2$) at retention times 7.2 min (panel A), 7.8 min (panel B), 8.2 min (panel C), and 8.6 min (panel D).

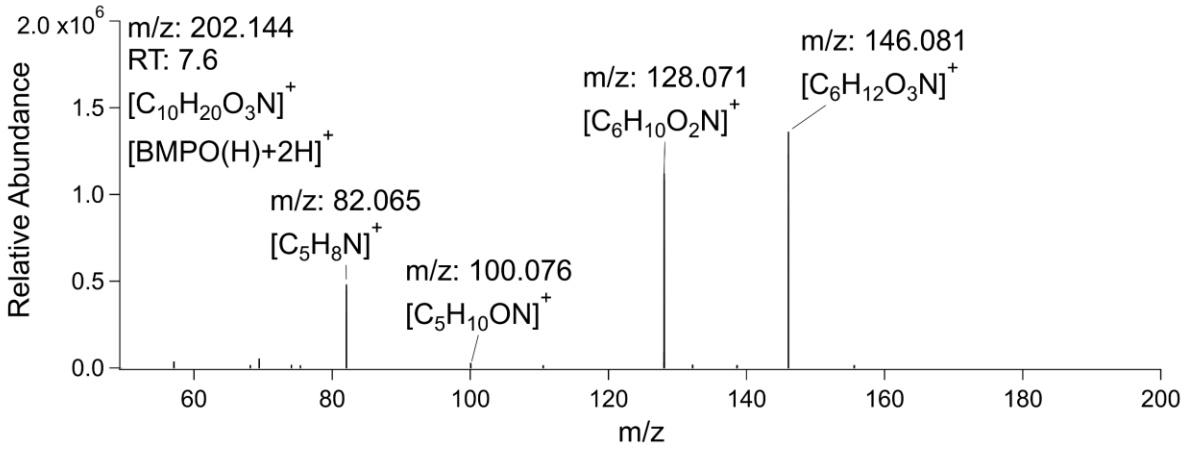

Figure S8: Sum of the fragmentation mass spectra recorded at collision energies 10, 30, and 50 for *m/z* 202.144 $[BMPO(H)+2H]^+$ at retention time 7.6 min.

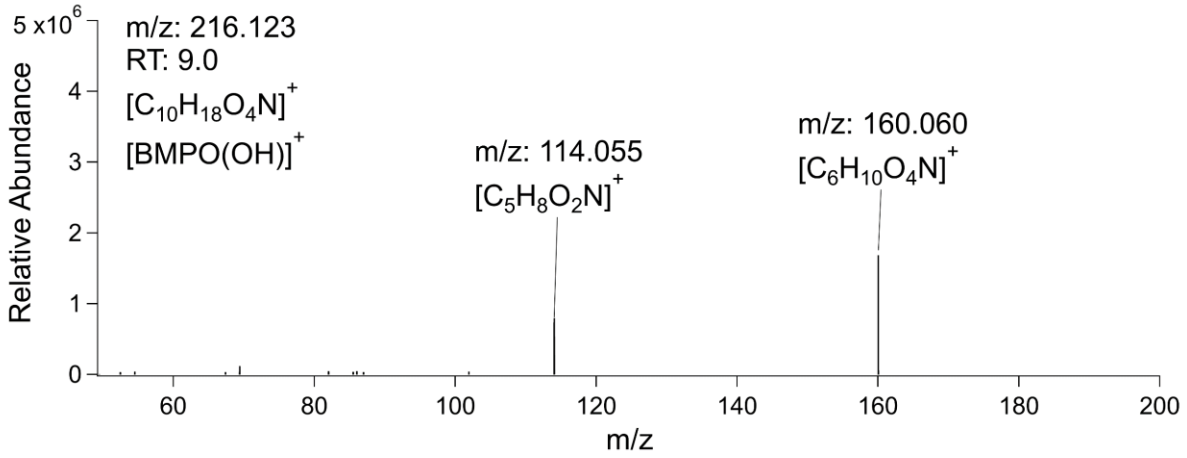

Figure S9: Sum of the fragmentation mass spectra recorded at collision energies 10, 30, and 50 for $[BMPO(OH)]^+$ *m/z* 216.123 at retention time 9.0 min.