Supporting Information

Localization of Post-Translational Modifications in Peptide Mixtures via High-Resolution Differential Ion Mobility Separations Followed by Electron Transfer Dissociation

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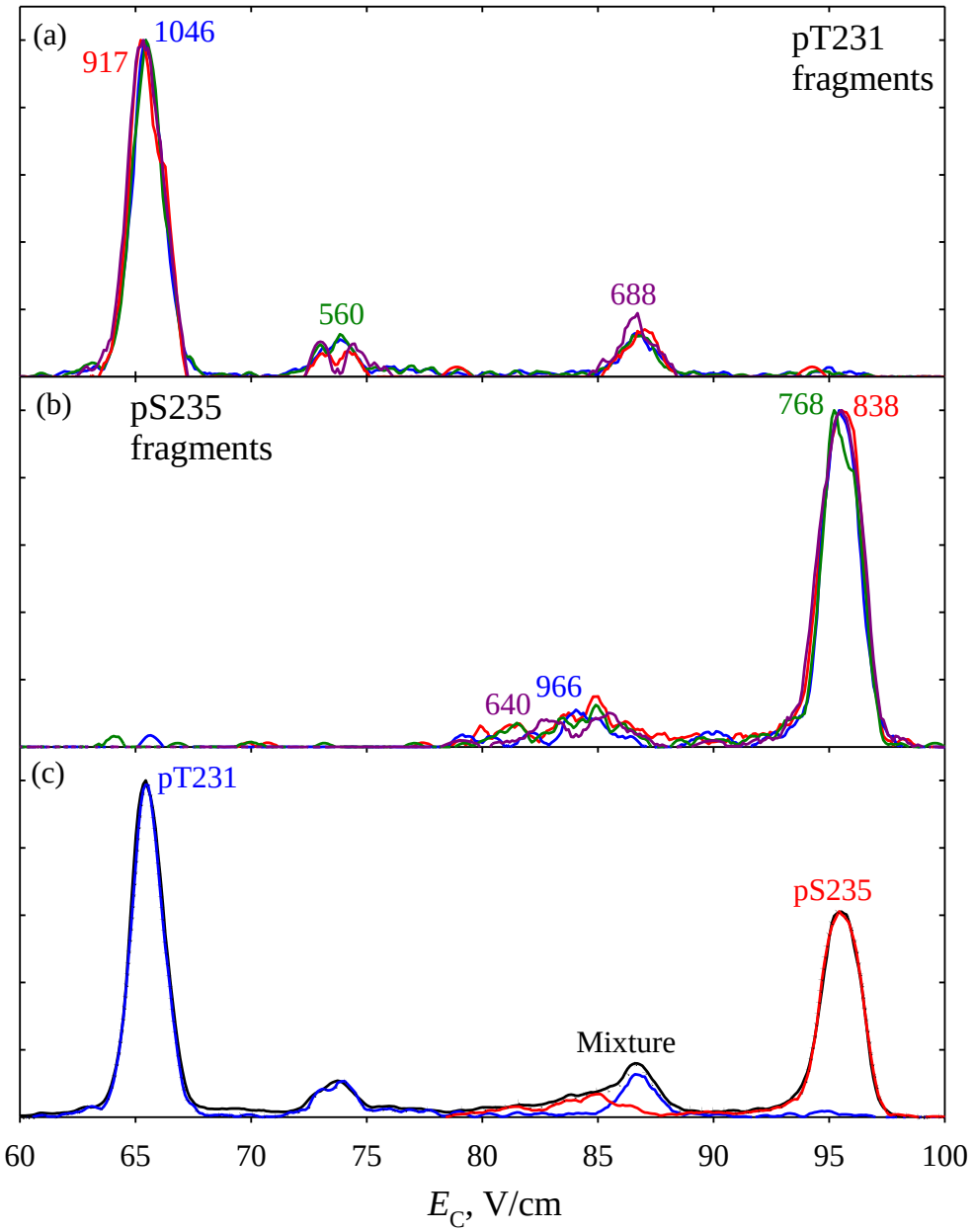
Figures S1 - S4

Figures show the detailed results of FAIMS/ETD scans at 30% and 40% He and the analysis of fragments for spectral reconstruction.

Procedures for spectral processing

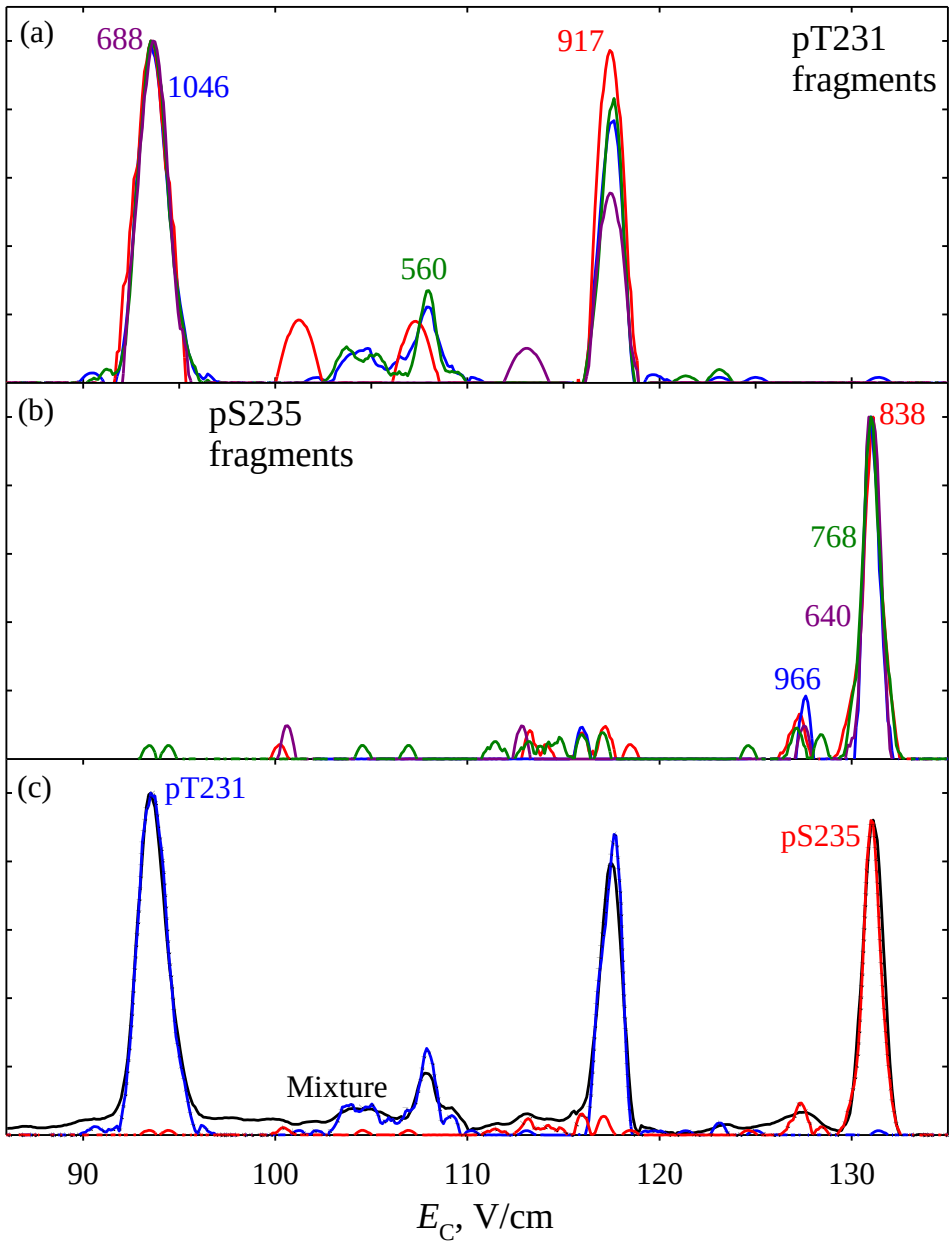
Raw E_C traces for fragment m/z (including the isotopic distribution) were extracted using the operating software of Thermo instrument (Excalibur), downloaded as unformatted text files into Sigma Plot 11.0, and converted to the V/cm scale by custom transforms. They were smoothed in the negative exponential mode with the polynomial degree of 2 and the sampling proportion and number of intervals varied depending on the ion signal and s/n ratio to eliminate most noise but retain the real features. However, we forced identical parameters on the spectra for different fragments from same acquisition to permit accurate point-by-point scaling and addition or subtraction.

Fig. S1



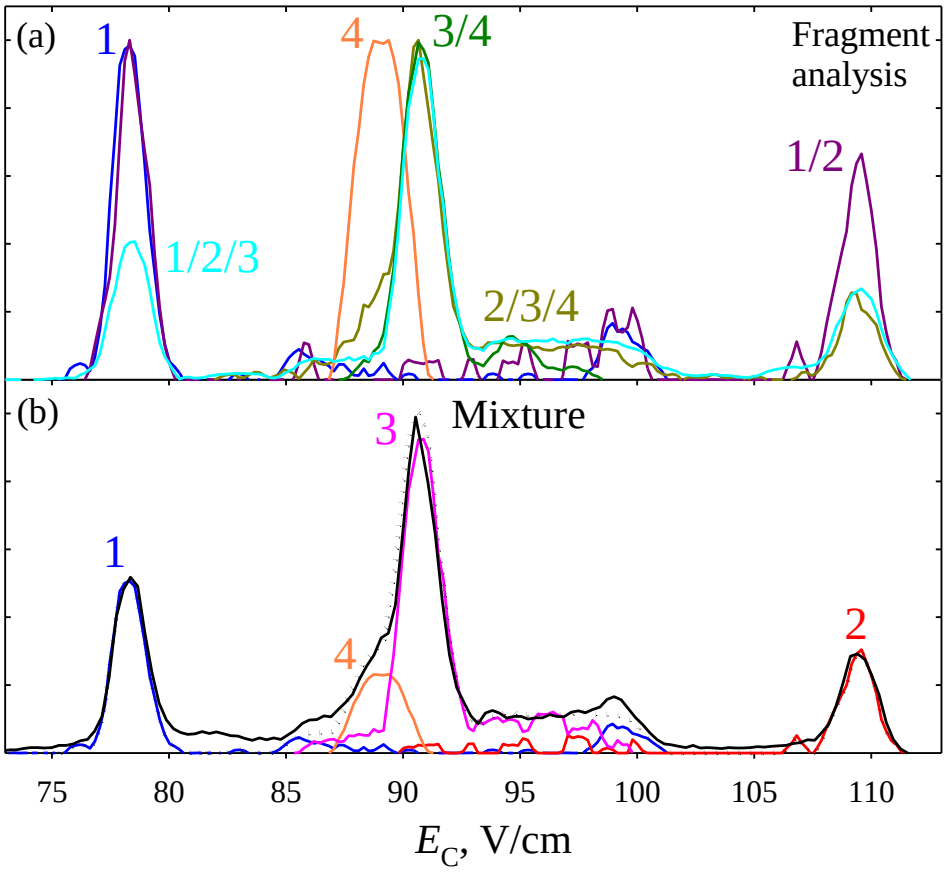
FAIMS spectra for the pT^{231} and pS^{235} variants at 30% He obtained from the ETD fragments of precursor mixture: (a, b) normalized spectra for the fragments of pT^{231} and pS^{235} with the *m*/*z* values as labeled, (c) measured trace (line) with the scaled spectra for both species produced by summing the spectra for all unique fragments of each above, and the mixture spectrum reconstructed by adding the two (dotted line).

Fig. S2



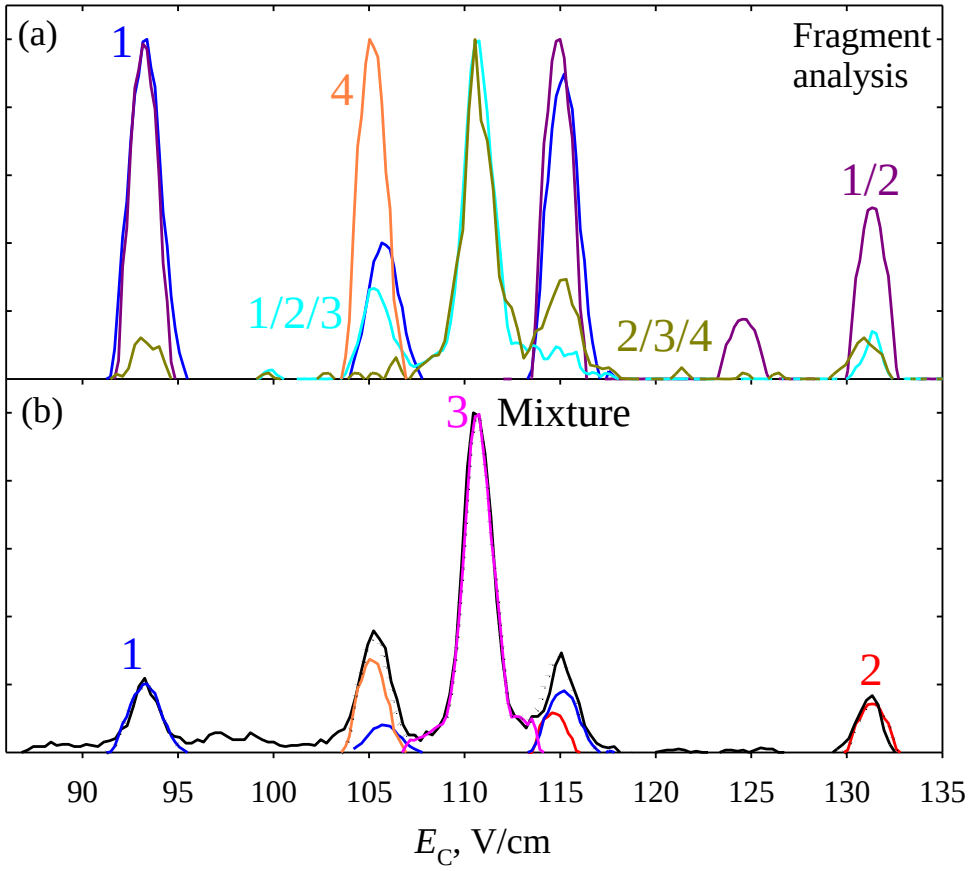
Same as Fig. S1 at 40% He.

Fig. S3



Reconstruction of FAIMS spectra for the four variants at 30% He from the ETD fragments of equimolar precursor mixture: (a) normalized spectra for the precursors or their groups derived by summing the spectra for all distinguishing fragments, (b) measured trace (line) with the scaled spectra for individual species derived from above data, and the mixture spectrum obtained by adding the two (dotted line).

Fig. S4



Same as Fig. S3 at 40% He.