

Supplementary Information

deMix: Decoding Deuterated Distributions from Heterogeneous Protein States via HDX-MS

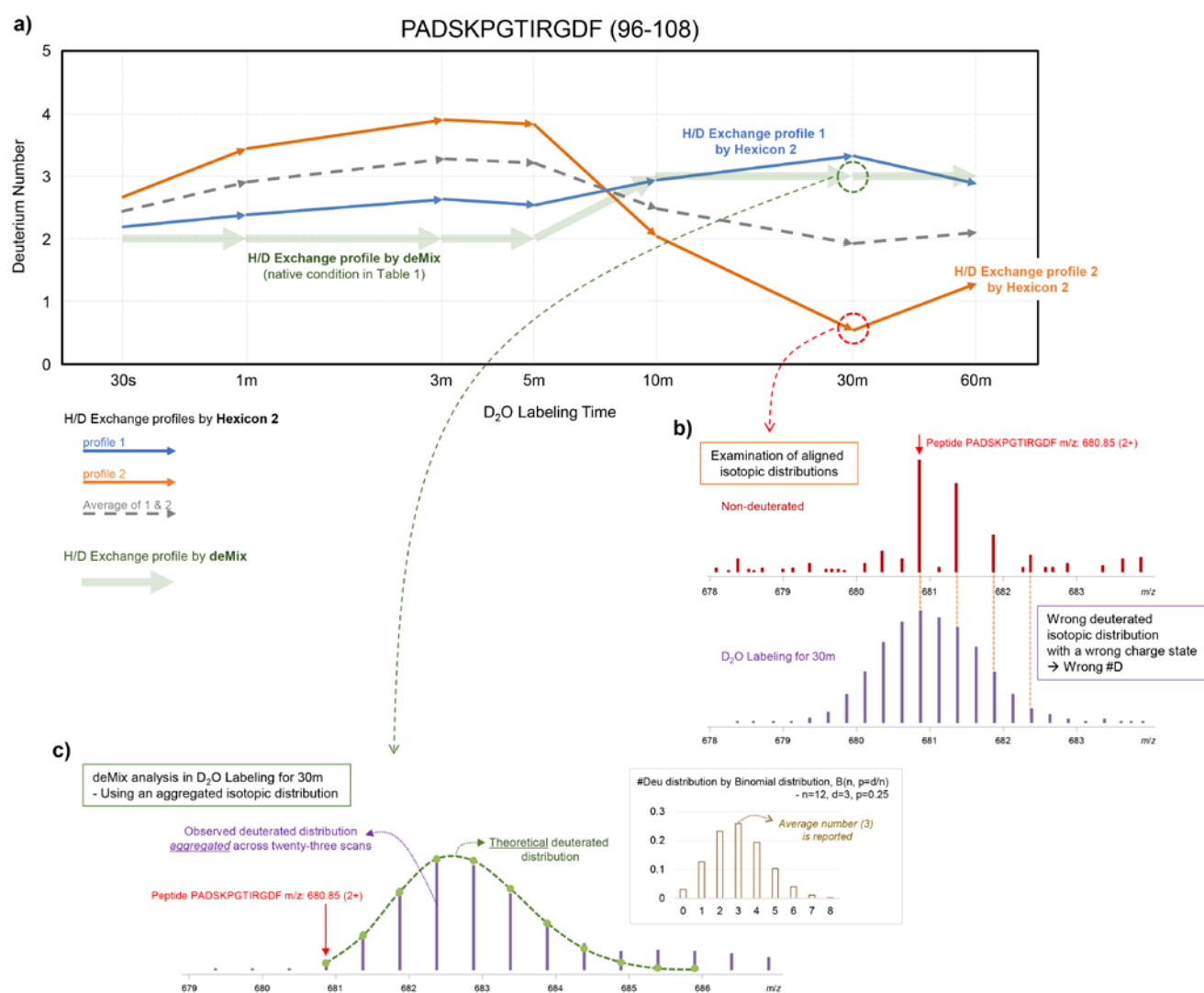
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Supplementary Figure S1.



Supplementary Figure S1. a) Hexicon 2 showed incompatible H/D exchange results (blue and orange lines) for a peptide ‘PADSKPGTIRGDF’. b) The exchange profile 2 (orange line) turned out to be wrong. The charge state of non-deuterated distribution (red peaks) was 2+, while 4+ (by peak spacing) for the aligned deuterated distribution (violet peaks). Different isotopic distributions of 2+ and 4+ charge states overlap in their isotopic peaks as shown in the figure if m/z values of any peaks are matched. c) deMix uses an aggregated isotopic distribution over elution time and in the figure violet peaks were aggregated from twenty-three scans. The aggregation prevents misleading analysis due to intervention of overlapped or noisy isotopic peaks. deMix interprets deuteration level as binomial distribution (inset) and reports the average number as the final deuterium number (3 in the figure).