

SUPPORTING INFORMATION FOR

Burial of the polymorphic residue 129 in amyloid fibrils of prion stop mutants

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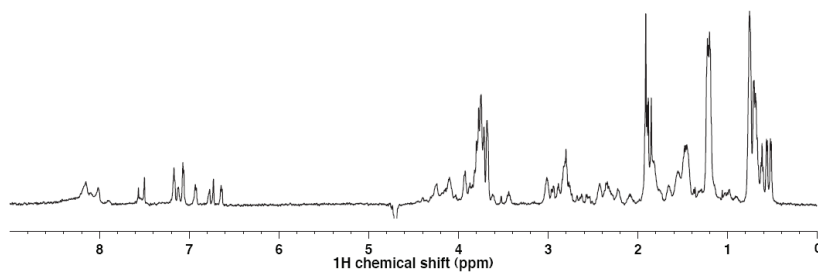


Figure S1. One-dimensional proton NMR spectrum of humPrP(108-143). The small dispersion in the amide proton (~8.2 ppm) and methyl region (0-1 ppm) demonstrates that monomeric humPrP(108-143) is disordered in solution.

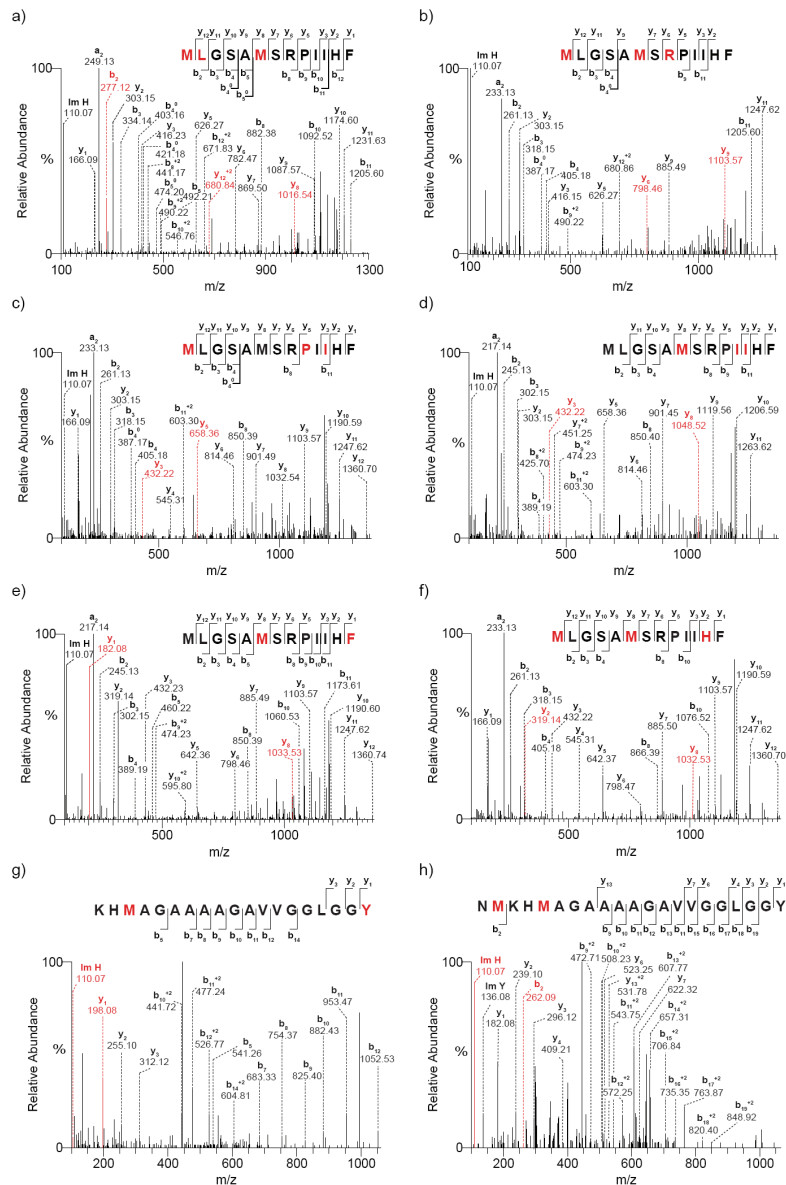


Figure S2. Tandem MS spectra of modified (oxidized) humPrP(108-143) peptides. The oxidized amino acid and its corresponding fragment ions containing the modification are depicted in red, b and y ions indicate fragmentation of the peptide bond conserving the charge to the N- or C- terminus, respectively; subindex 0 indicates loss of water. (i.e b-H₂O) a-f) Oxidized amino acids found in peptide ¹²⁹MLGSAMSRPIIHF¹⁴¹: a) M129, L130, M134 b) M129, M134 and R136; c) M129, P137 and I139; d) M134, I138, I139; e) M134 and F141 and f) M129, M134 and H140. g-h) Oxidized amino acids in the peptide 109-128: g) M112 and Y128 are oxidized, note the immonium ion of H (non modified); h) Modification in M109 and M112; of note immonium ions of H111 and Y128 are non-oxidized indicating that M112 is the actual oxidized residue. Spectra a-f) are from fibrillar samples, whereas spectra g-h) correspond to monomeric samples.