

Supporting Information

Gertz et al. 1073/pnas.0800691105

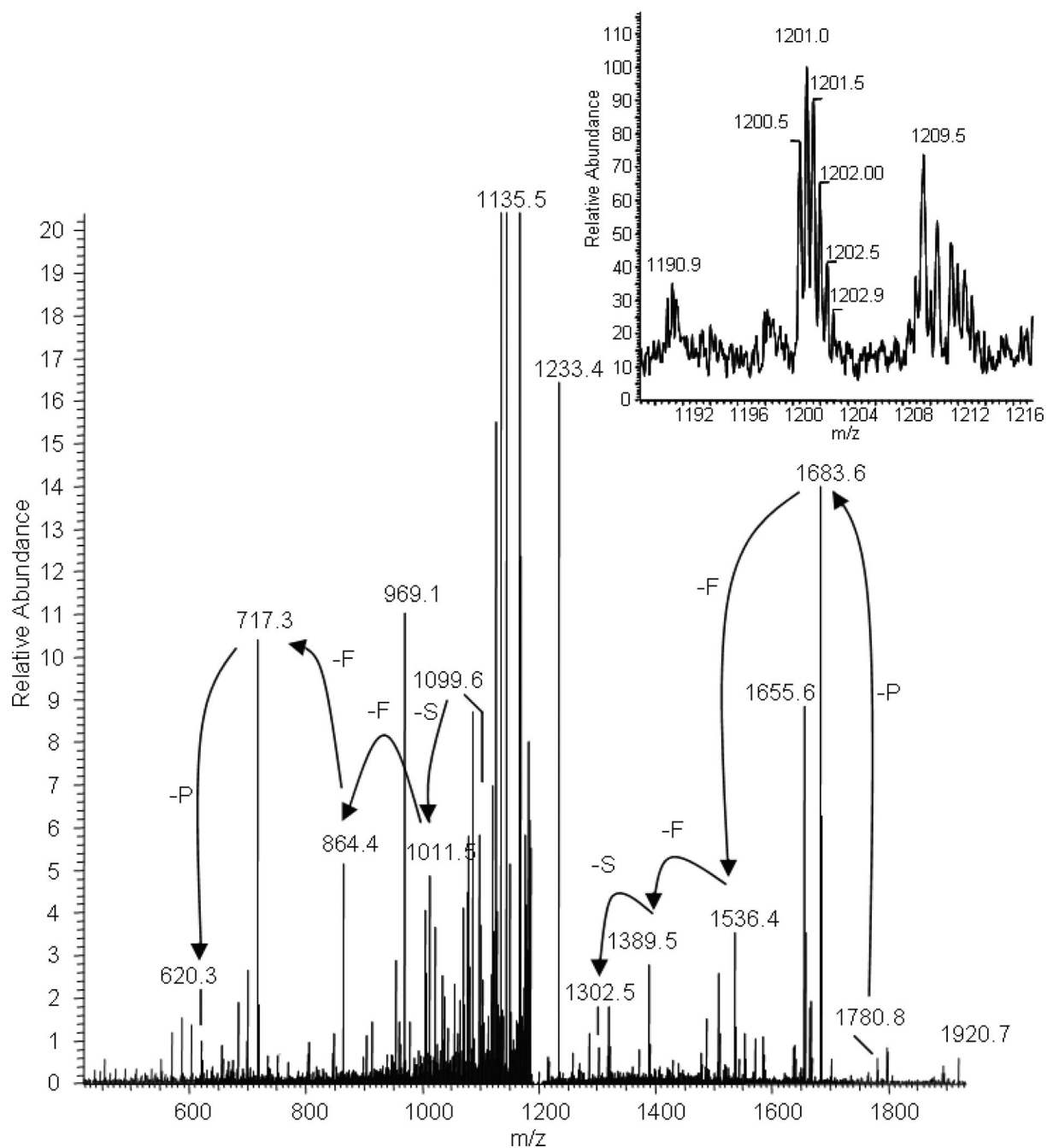


Fig. S1. MS/MS spectrum and MS spectrum (*Inset*) of the disulfide bridged peptide $L_{68}NSMRPFSC_{59}\text{-S-S-C}_{59}\text{SFFPRMSNL}_{68}$ with annotated y-ion series. Isotopic distribution of such peptide at $m/z = 1,200.5$ reveals doubly charged species.

a

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OrigSeq      : 1-----11-----21-----31-----41-----51-----61-----71-----81-----91-----101-----111-----121-----131-----141----- : OrigSeq
              : MDLLPKPKYNPLRNESSLSEEGASGTPPEELPSPSASSLGFILPPLPGDDSPPTLCSEFFPMSNLKLANFAGGRLGPKGEPKAAEDGEGSAGAALRDSGLLPLQDMNKLSGGGRRTRVEGGQLGGEWTRHGSEFVNKPTRGLWH
jalign       : -----EEEE-----H-HHHHHH-----HHHHHHHHHH-----HHH----- : jalign
jfreq        : -----EEEE-----EE-----HHHHH-----HHHHHH-----EEE-----EE-----E- : jfreq
jhmm         : -----EEE-E-----EEEE-----EE-----HHHHH-----HHHHHH-----EEE-----EE-----E- : jhmm
jnet         : -----EEEE-----EEE-----EE-----HHH--H-----EE--E-----E----- : jnet
jpsm         : -----EEEE-----EEE-----HHH--H-----EE--E-----E----- : jpsm

jpred        : -----EEEE-----EE-----HHH-----EEE-----EE----- : jpred

Lupas 14     : ----- : Lupas 14
Lupas 21     : ----- : Lupas 21
Lupas 28     : ----- : Lupas 28

Jnet_25      : B-BB--B--BB-BBBBBBBB--B-BBB-BBB--BB-B--BBBBBBBB-BB-B-BBBBBBB-BB--B--B--BBBBBBB-B--BB-BBB-BB-B--B--BBB--BBBB--BB--BBBBB-BB-BBBB : Jnet_25
Jnet_5       : -----B-----B-----B-B-B-----BBBB--B-B-B-----B-----B-----B-----B-----BB-----BB----- : Jnet_5
Jnet_0       : -----B-----B-----B-B-B-----BBBB--B-B-B-----B-----B-----B-----B-----BB-----BB----- : Jnet_0
Jnet Rel     : 3799899999998888765414589999999999986324789899999999983212422557534136888988888765323579877655577777886641222422447873047713241476335998655688765262 : Jnet Rel

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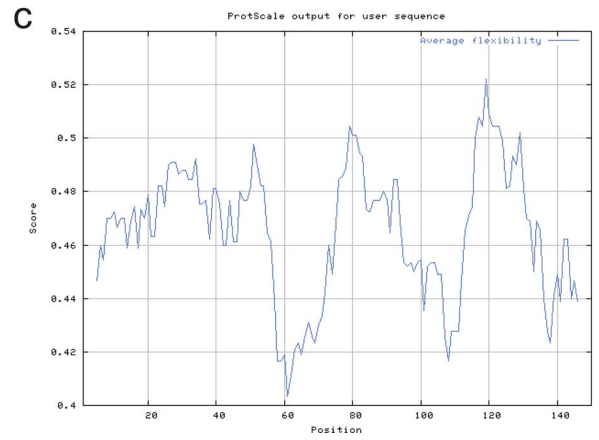
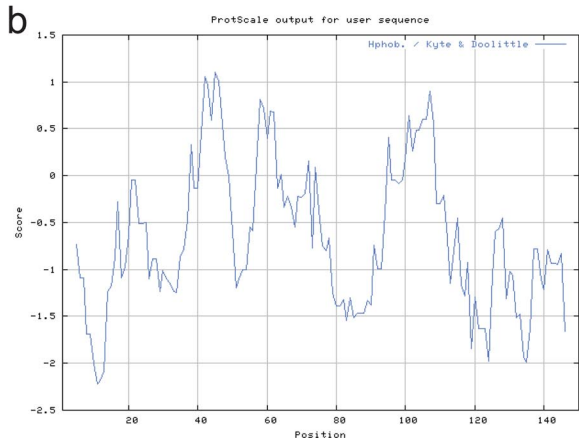


Fig. S2. Sequence analyses for p66CH2-CB using Jpred2 and Prot-Scale. (a) Secondary structure prediction for p66CH2-CB using the Jpred2 server (H: helix, E: extended). (b) Prediction of the hydrophobicity of p66CH2-CB using the scale of Kyte and Doolittle on the Prot-Scale server. (c) Prediction of the average flexibility of p66CH2-CB using the Prot-Scale server.