Supporting information:

Table A. Proline residue isomerization state, relative stability and protonation site of the candidate structures proposed in Figures 2 and 3.

	$Prol^3$	$Prol^7$	Potential Energy kJ/mol	Protonation Site
A	Trans	Trans	-1103	N term, Arg4
B	Cis	Cis	-1656	N term, Lys1
C	Trans	Trans	-1264	N term, Arg4
D	Cis	Trans	-1624	N term, Lys1
E	Trans	Trans	-1184	N term, Arg4
F	Cis	Cis	-1017	N term, Arg4, Arg6
G	Cis	Trans	-1288	N term, Lys1,Arg6
H	Trans	Cis	-1187	N term, Arg4, Arg6
I	Trans	Cis	-1310	N term, Lys1,Arg6
J	trans	Cis	-1085	N term, Lys1,Arg6

Footnote: Energy comparison should be made between the same protonation sites.

PDB files of candidate structures proposed. (separate file)