Conformational Study of N-terminal Prion Peptides by Molecular Dynamics Simulations

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Table 1. Proportions of secondary structures in PrP from MD simulations

	β-Sheet	Coil	β-Bridge	Bend	Turn	Helix	3-Helix	π -Helix
PrP _H without lons	3.08	52.46	4.42	37.12	2.77	0.15	0.00	0.00
PrP _N without lons	0.23	47.54	4.38	34.46	9.08	0.62	0.00	3.69
PrP _H with lons	0.00	45.96	6.35	42.62	4.88	0.00	0.19	0.00
PrP _N with lons	0.00	59.12	1.08	38.00	1.65	0.15	0.00	0.00