

Table S1. Cal14.1a's structures conformations after molecular dynamics.

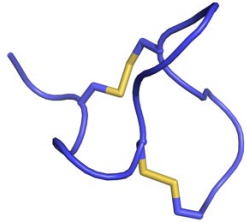
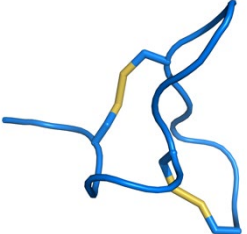
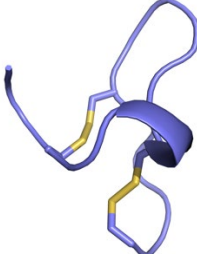
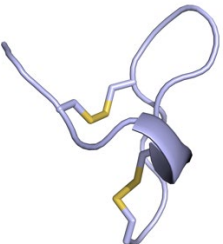
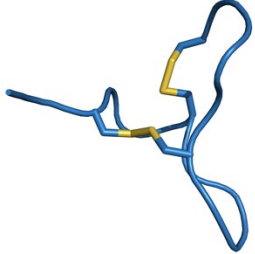
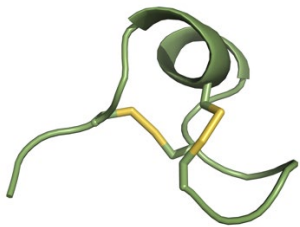
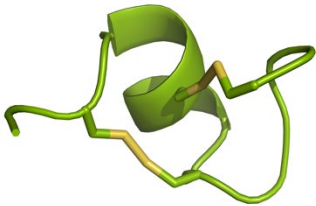


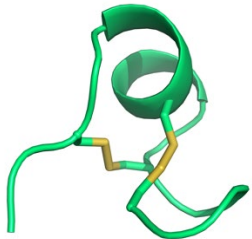
Conformation	Number of structures	Existence time (ns)
1		315 3.15
2		667 6.67
3		870 8.70
4		538 5.38
5		110 1.10

Table S2. Cal14.1b's structures conformations after molecular dynamics.

Conformation	Number of structures	Existence time (ns)
1		204 2.04
2		564 5.64
3		795 7.95
4		738 7.38
5		199 1.99