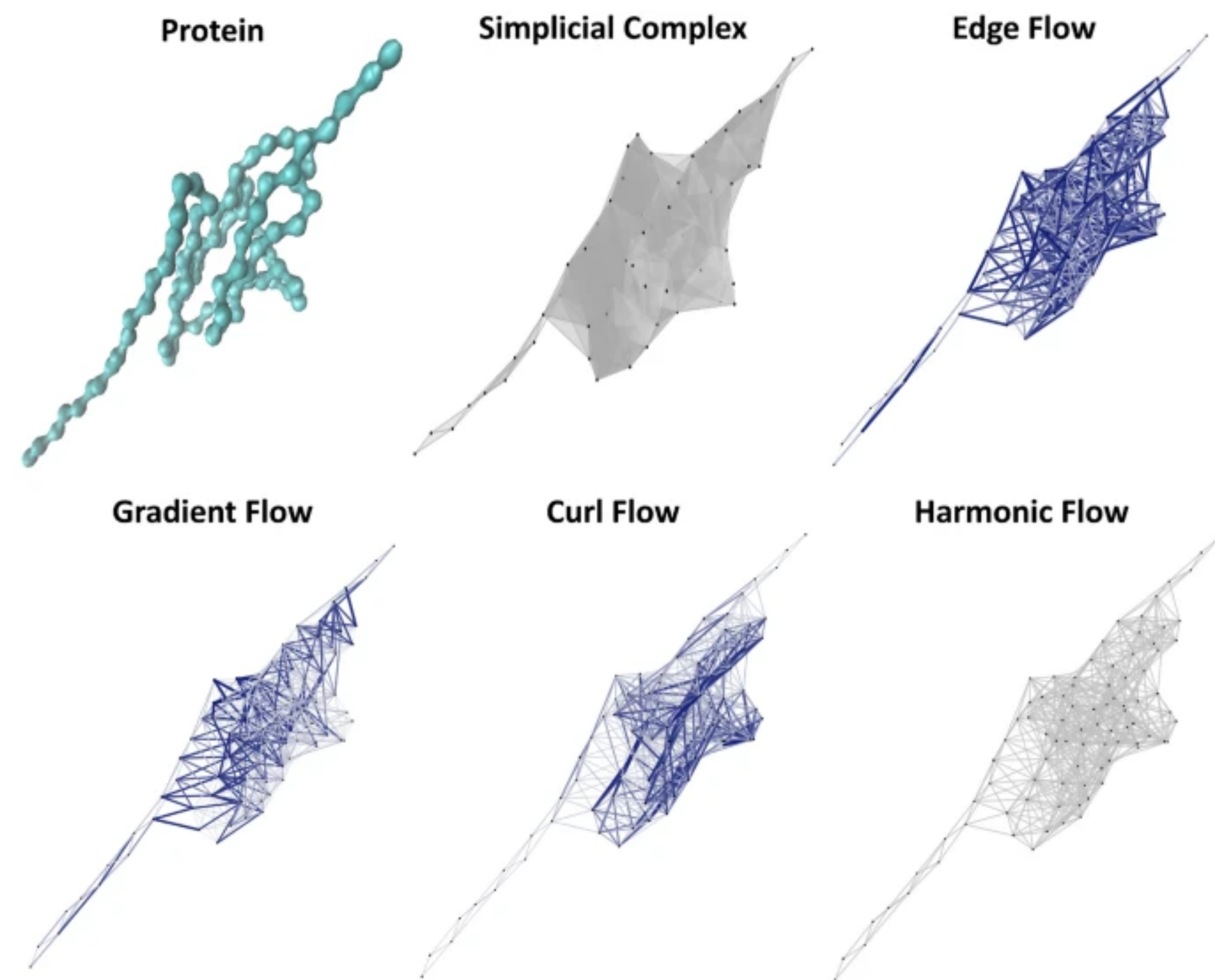
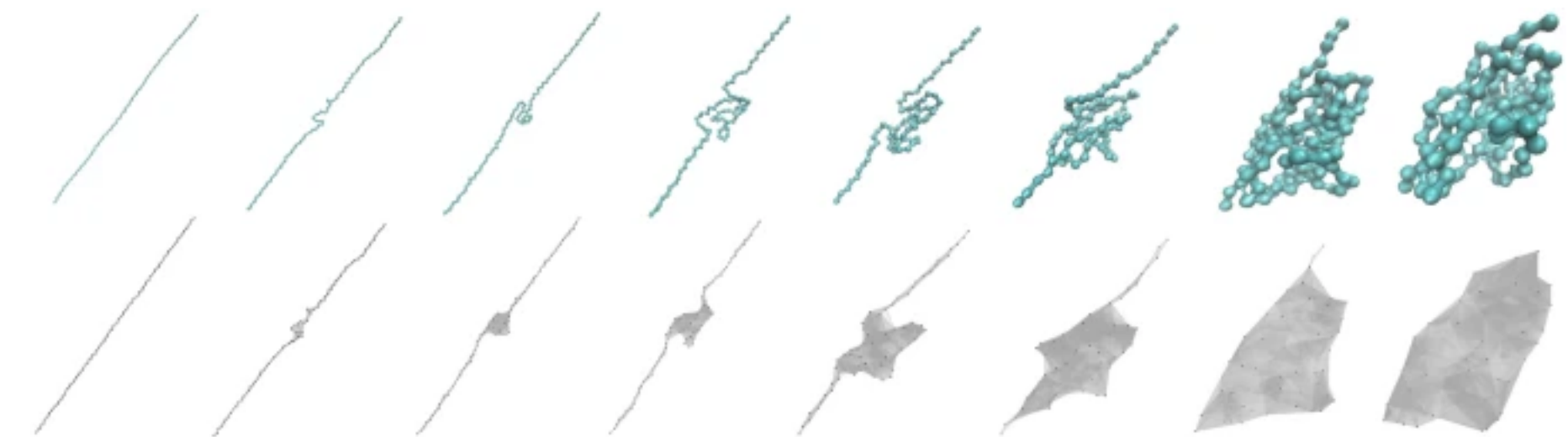


Ideas on molecular dynamics

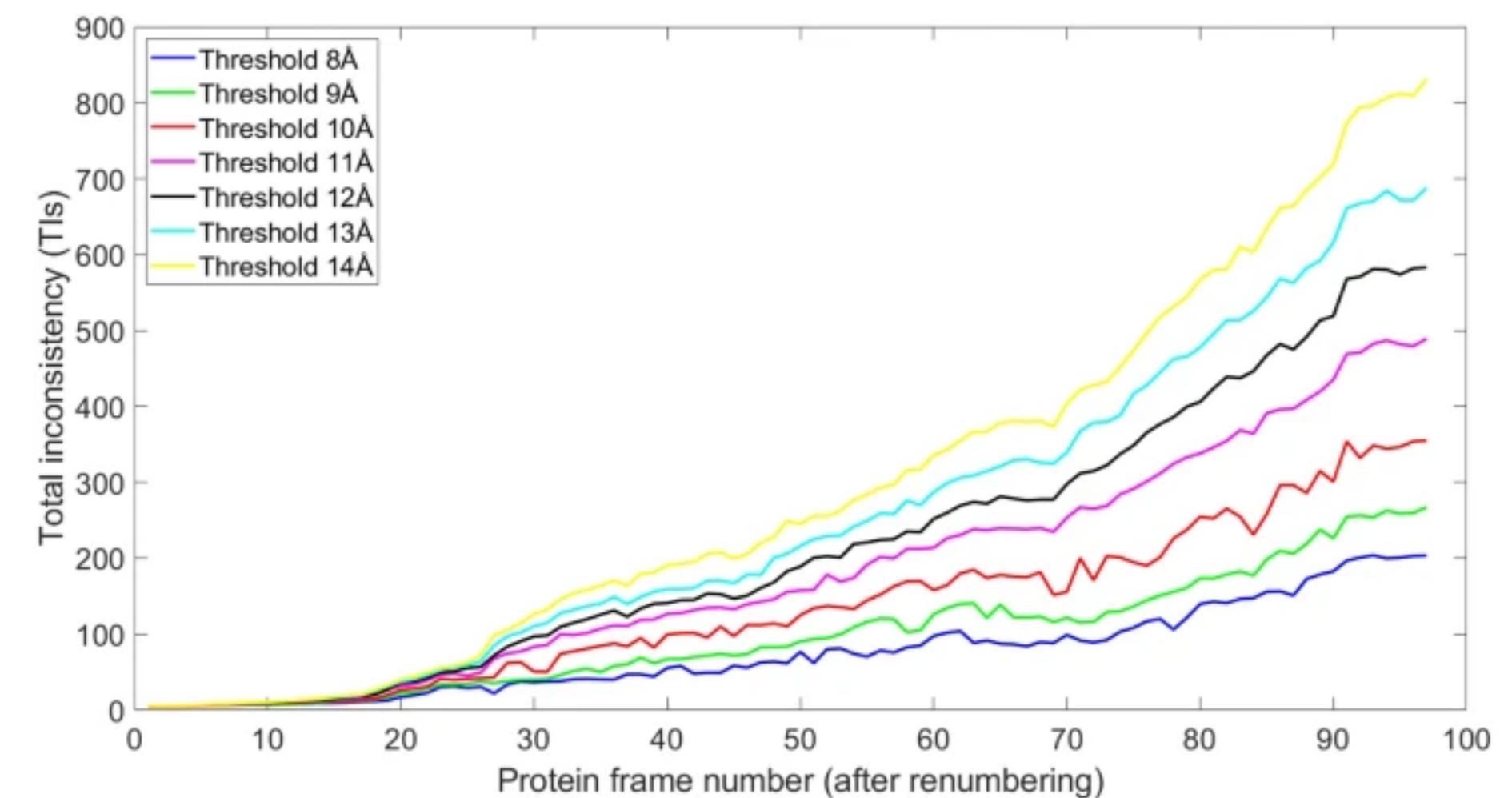
Wei, R.K.J., Wee, J., Laurent, V.E. *et al.* Hodge theory-based biomolecular data analysis. *Sci Rep* (2022)



gradient, curl, and harmonic, for a partially-folded protein



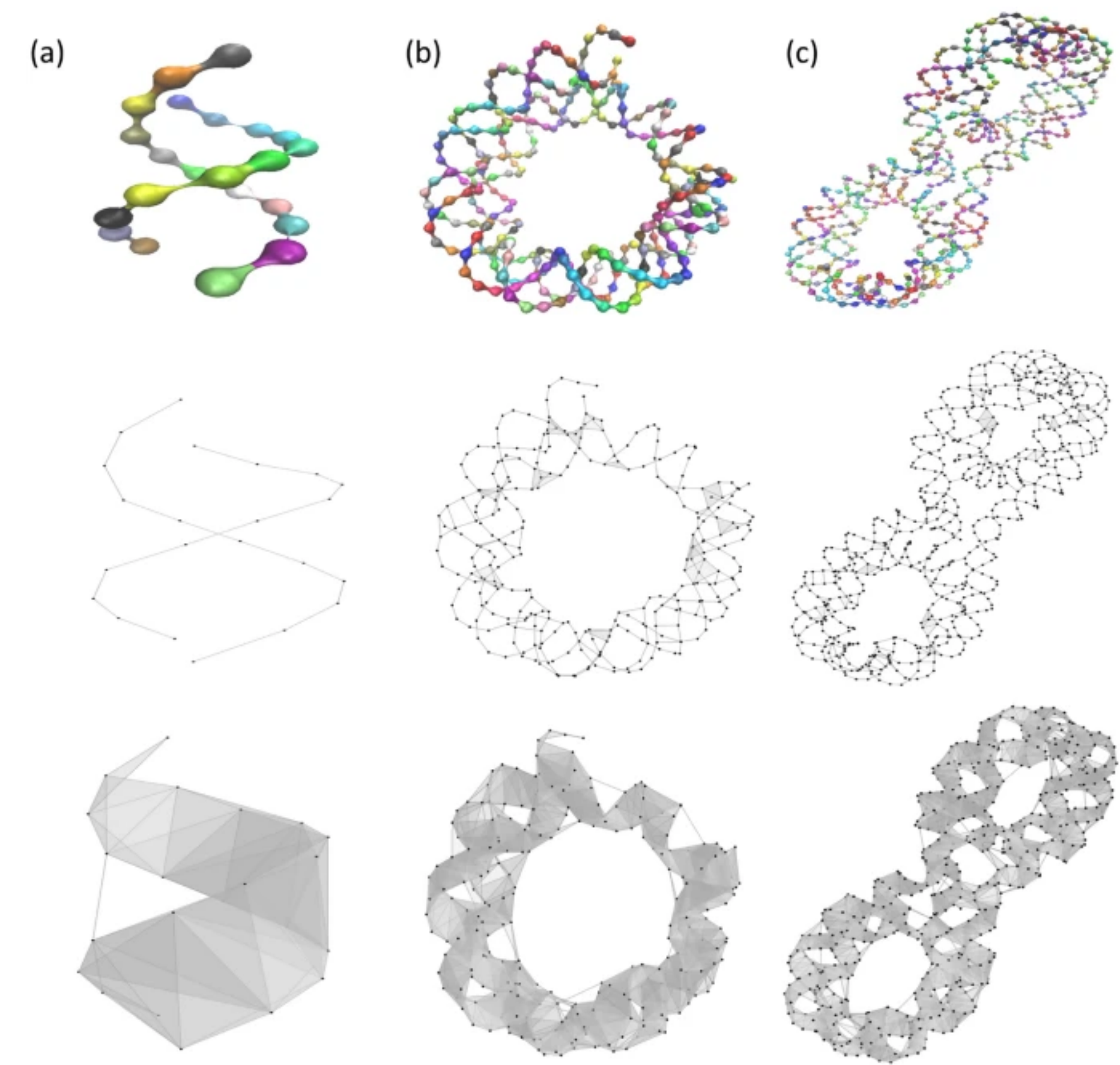
Eight configurations (after renumbering) extracted from the steered molecular dynamics simulation of Titin molecule, and their associated simplicial complexes.



(TI) for Titin configurations during the SMD simulations

Ideas on molecular dynamics

Wei, R.K.J., Wee, J., Laurent, V.E. *et al.* Hodge theory-based biomolecular data analysis. *Sci Rep* (2022)



	TIs			AIs		
Cutoff	DNA helix	Nucleosome	Tetranucleosome	DNA helix	Nucleosome	Tetranucleosome
10 Å	0.0	279.3223	631.4930	0.0	0.9599	0.9126
12 Å	0.0	302.6626	734.4815	0.0	1.0401	1.0614
14 Å	28.9381	653.4245	1590.3249	1.3154	2.2454	2.2982
16 Å	33.9428	739.7261	1774.1848	1.5429	2.5420	2.5639
18 Å	46.7132	987.8988	2530.9683	2.1233	3.3948	3.6575
20 Å	63.1120	1308.3067	3191.6790	2.8687	4.4959	4.6123

three DNA structures, including DNA helix (a), nucleosome (b), and tetranucleosome (c), and their corresponding simplicial complexes at two different cutoff distances