Supplementary Material (ESI) for Nanoscale

Supporting Information : Probing diameter-selective solubilisation of carbon nanotubes by reversible cyclic peptides using molecular dynamics simulations

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Contents

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Figure S6: Evidence of a stable helix configuration for the RC7/0.45 nm system starting from a helix geometry. **(a)** Sulfur-sulfur contacts as a function of time. **(b)** Percentage of radial coverage as a function of time.

Figure S7: Evidence of a two interpenetrating half-wrap geometries for the RC7/0.75 nm system starting from a two side-by-side cyclised-wrap configurations. **(a)** Snapshot of final conformation. **(b)** Sulfur-sulfur contacts as a function of time. **(c)** Percentage of radial coverage as a function of time.

Table S1. Carbon nanotube chiralities [(n,m) indices] used in this work.

D_a Label	(n,m)
0.45	(5,1)
0.55	(7,0)
0.65	(8,0)
0.75	(9,1)
0.85	(11,0)
0.95	(8,6)
1.05	(10,5)
1.15	(12,4)
1.25	(16,0)

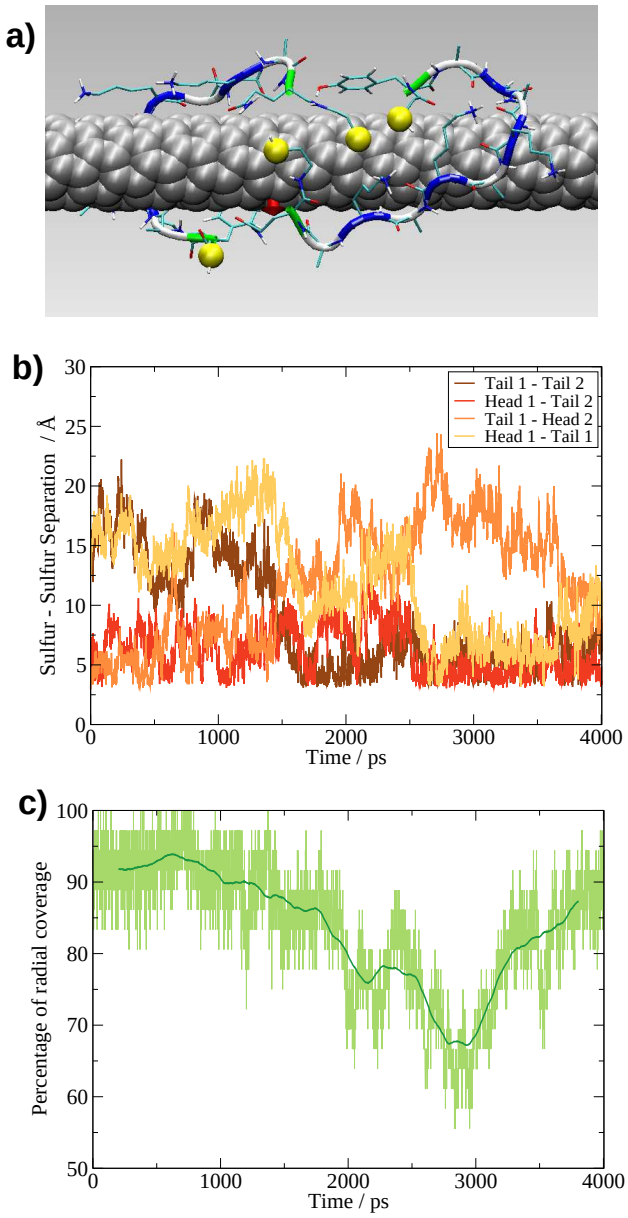

Figure S2: Evidence of formation of an interpenetrating half-wrap two-chain complex for the RC5/0.45 nm system. **(a)** Snapshot, with sulfur atoms indicated as yellow spheres. **(b)** Sulfur-sulfur non-bonded contacts as a function of time. **(c)** Percentage of radial coverage as a function of time. The dark line indicates the running average of this coverage.

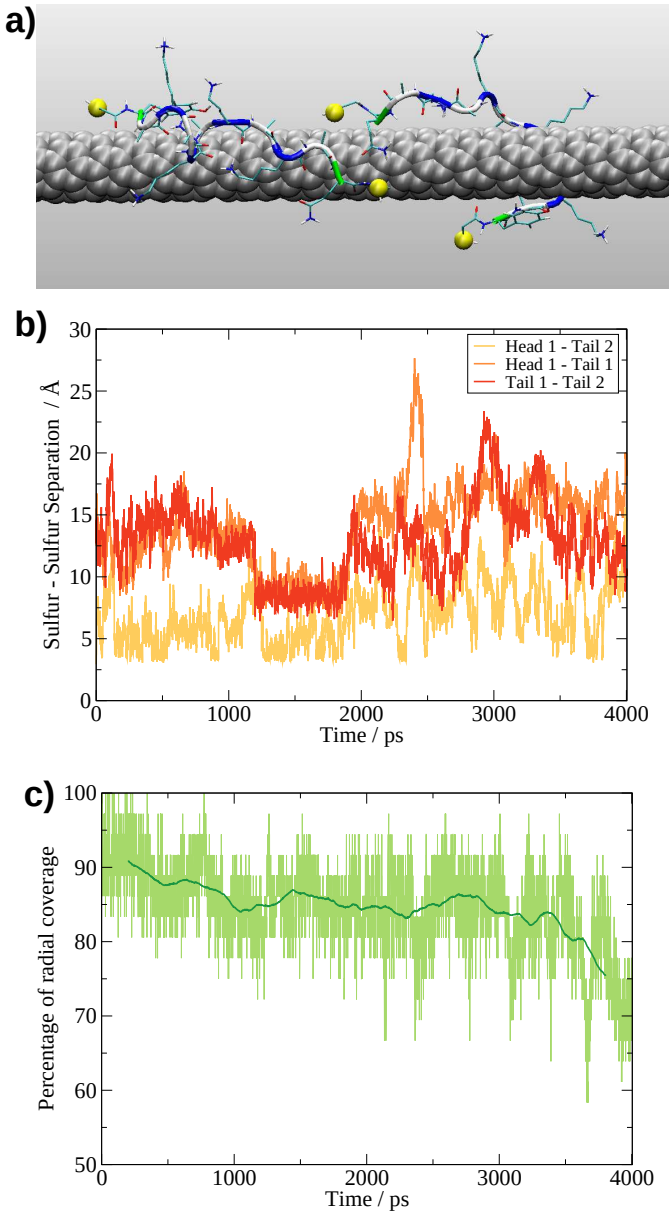

Figure S3: Evidence of formation of a 3-sulfur two-chain complex for the RC5/0.45 nm system. **(a)** Snapshot, with sulfur atoms indicated as yellow spheres. **(b)** Sulfur-sulfur contacts as a function of time. **(c)** Percentage of radial coverage as a function of time. The dark line indicates the running average of this coverage.

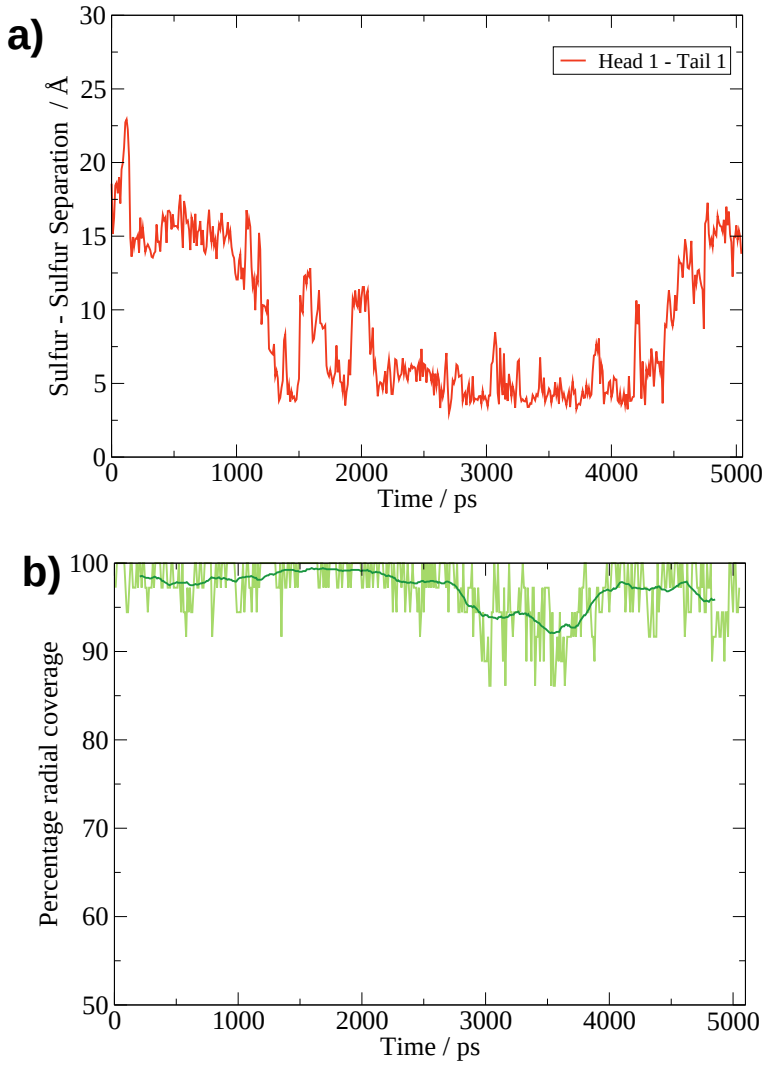

Figure S4: Evidence of two-chain complex for the RC7/0.75 nm system supporting a cyclised-wrap structure. **(a)** Sulfur-sulfur non-bonded contact as a function of time. **(b)** Percentage of radial coverage as a function of time. The dark line indicates the running average of this coverage.

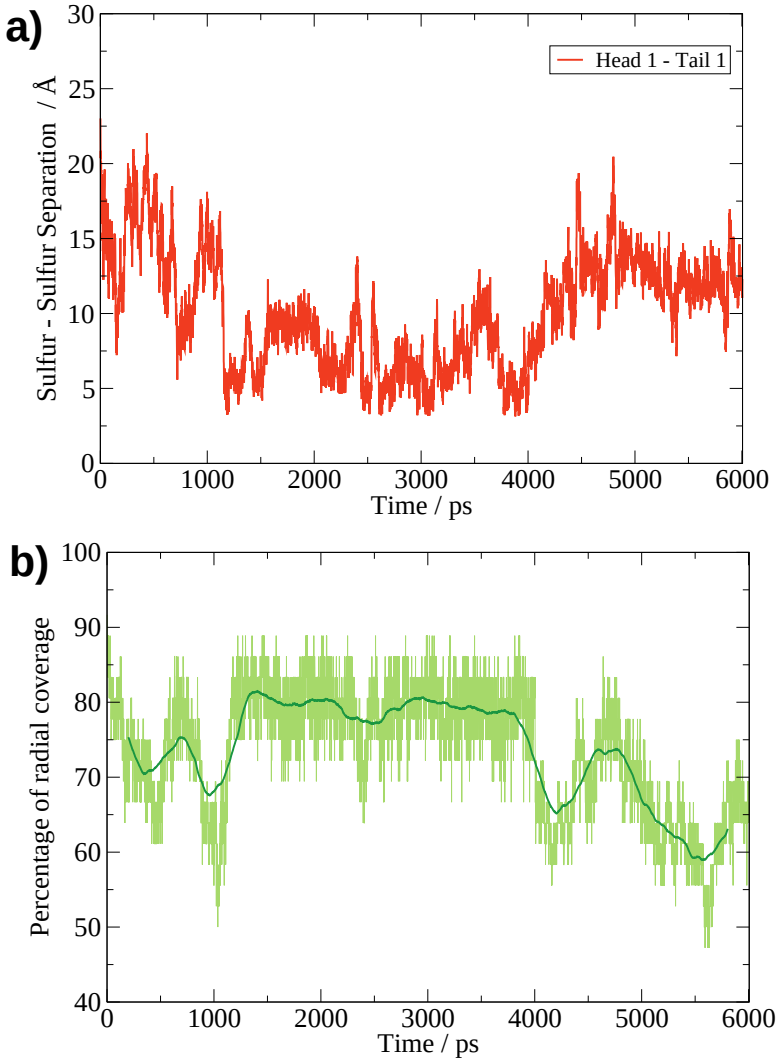

Figure S5: Evidence of cyclised wrap configuration for the RC5/0.45 nm system starting from a helix geometry. **(a)** Sulfur-sulfur contacts as a function of time. **(b)** Percentage of radial coverage as a function of time.

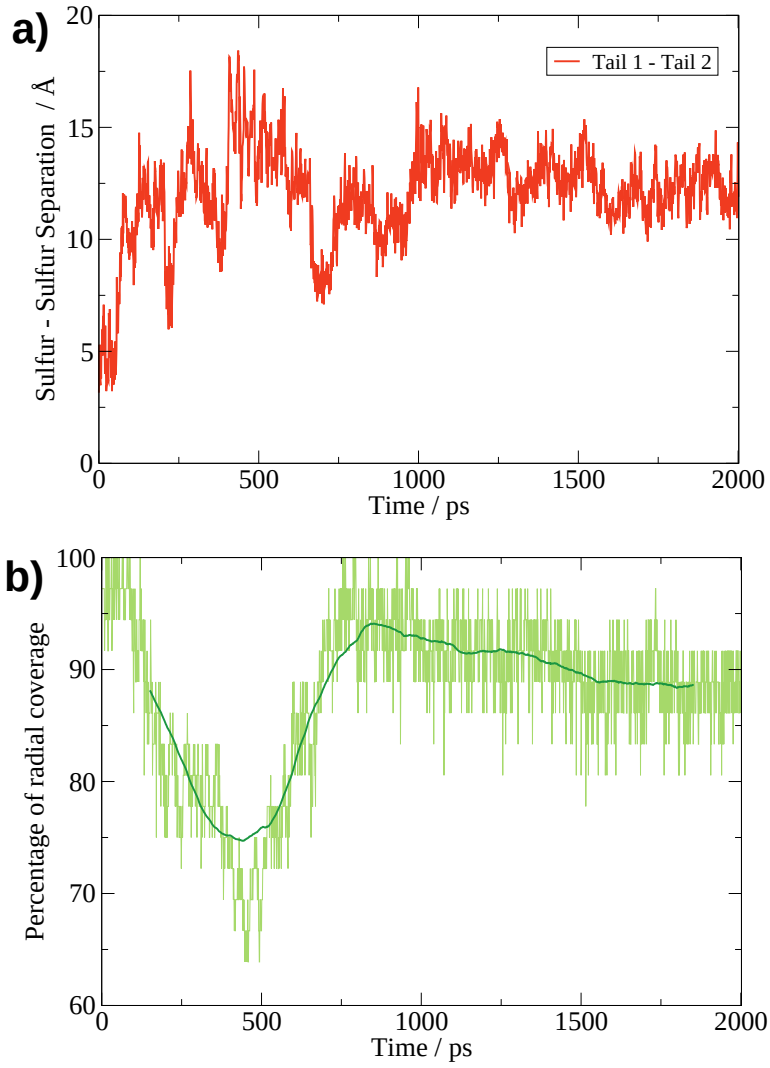

Figure S6: Evidence of a stable helix configuration for the RC7/0.45 nm system starting from a helix geometry. **(a)** Sulfur-sulfur contacts as a function of time. **(b)** Percentage of radial coverage as a function of time. The dark line indicates the running average of this coverage.

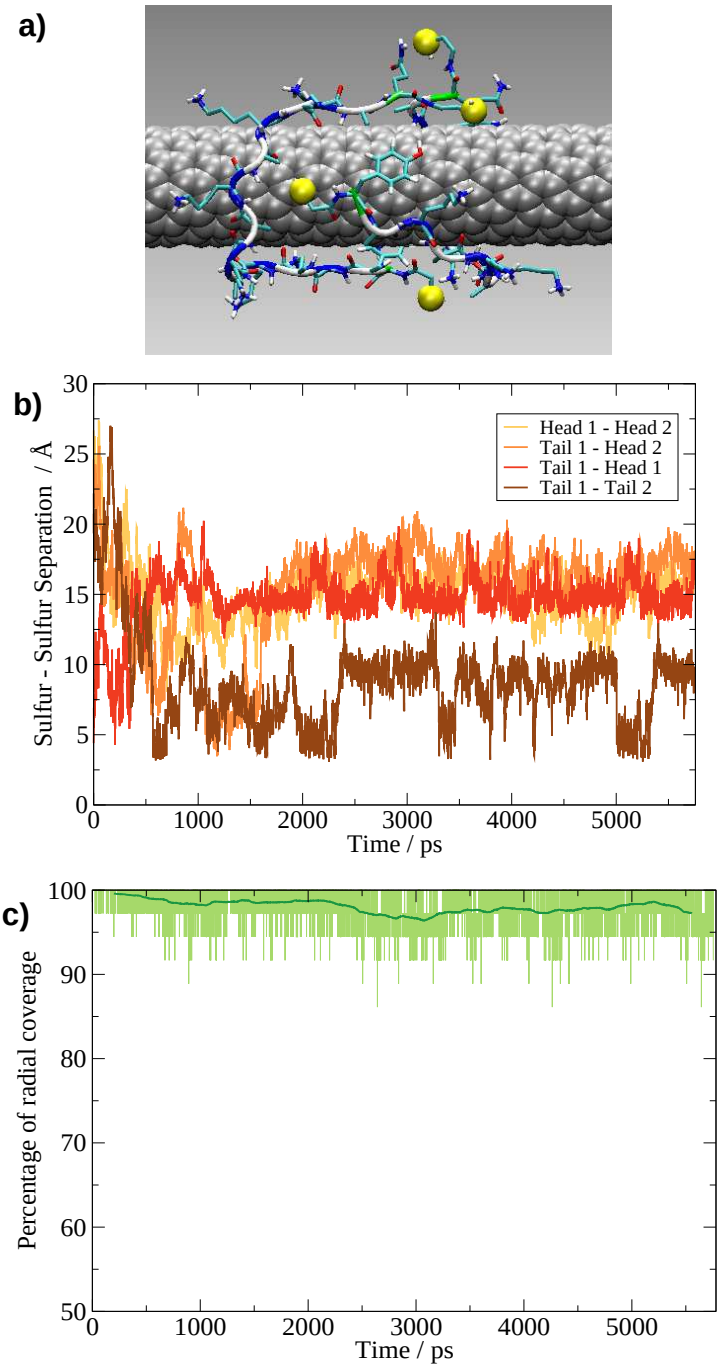

Figure S7: Evidence of a two interpenetrating half-wrap geometries for the RC7/0.75 nm system starting from a two side-by-side cyclised-wrap configurations. **(a)** Snapshot of final conformation, with sulfur atoms indicated as yellow spheres. **(b)** Sulfur-sulfur contacts as a function of time. **(c)** Percentage of radial coverage as a function of time. The dark line indicates the running average of this coverage.