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Helical Arylamide Foldamers: Structure Prediction by Molecular Dynamics Simulations

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Table S1. Percentage of helical (n > NUpT) or fully H-bonded conformations (n < NUpT, *italic numbers*)

	Tetramer			Octamer			Dodecamer		
	$CHCl_3$	MeOH	H_2O	$CHCl_3$	MeOH	H_2O	$CHCl_3$	MeOH	H_2O
I-OMe	*87.7*	*90.3*	*84.9*	*20.6*	*64.6*	*63.7*	0.5	99.8	99.6
I-F	*96.5*	*73.1*	*57.3*	*93.2*	*52.2*	*37.0*	90.8	46.4	87.7
I-Napy	*100*	*92.9*	*100*	*100*	*87.0*	*83.1*	100	100	100
II-OMe	*88.9*	*89.7*	*79.6*	*36.6*	*77.5*	*78.5*	10.2[a]	99.9	99.4
II-F	*96.7*	*71.4*	*52.6*	*86.6*	*32.0*	*35.8*	64.6[a]	31.7	86.3
II-Napy	*100*	*94.2*	*68.9*	*99.8*	*91.3*	*21.1*	98.7[a]	100	97.8
III-OMe	*95.8*	*92.2*	*88.6*	66.3[a]	99.5	100	86.6[a]	80.1[a]	95.1[a]
III-F	*97.3*	*59.0*	*43.0*	92.6	39.4	98.6	99.3	64.4	98.9
III-Py	*100*	*12.4*	*5.8*	100	100	100	100	100 (86.3)[b]	100 (6)[b]
III-Qn	100	100	100	100	100	100	100	100	100
III-Bf	90.5	55.8	91.9	100	97.3	100	90.6	99.6	100
IV-OMe	*93.9*	*91.2*	*93.2*	60.3[a]	66.6[a]	99.9	77.2[a]	74.4[a]	44.9[a]
IV-F	*96.0*	*66.2*	*40.8*	95.9	65.6	93.0	99.6	90.7	99.5
IV-Py	*100*	*23.5*	*9.4*	100	100 (93.0)[b]	100 (76.2)[b]	98.4	100 (76.1)[b]	100 (49.3)[b]
IV-Qn	100	100	99.8	100	100	100	100	100	100
IV-Bf	85.6	20.7	40.0	99.9	100 (77.7)[b]	100	99.9	100 (44.8)[b]	100 (94.5)[b]

[a] In these cases, no helical conformation was found (identified structures are elongated helices with no aromatic stacking, partially folded structures, etc.). The percentages shown are for fully H-bonded conformations, calculated as having all of the atomistic dihedral angles within the range that favours the intramolecular H-bonds.

[b] The 100% values are for helical conformation with or without one terminal group flipped 180º, and the percentage values in the parenthesis are for fully H-bonded conformations.

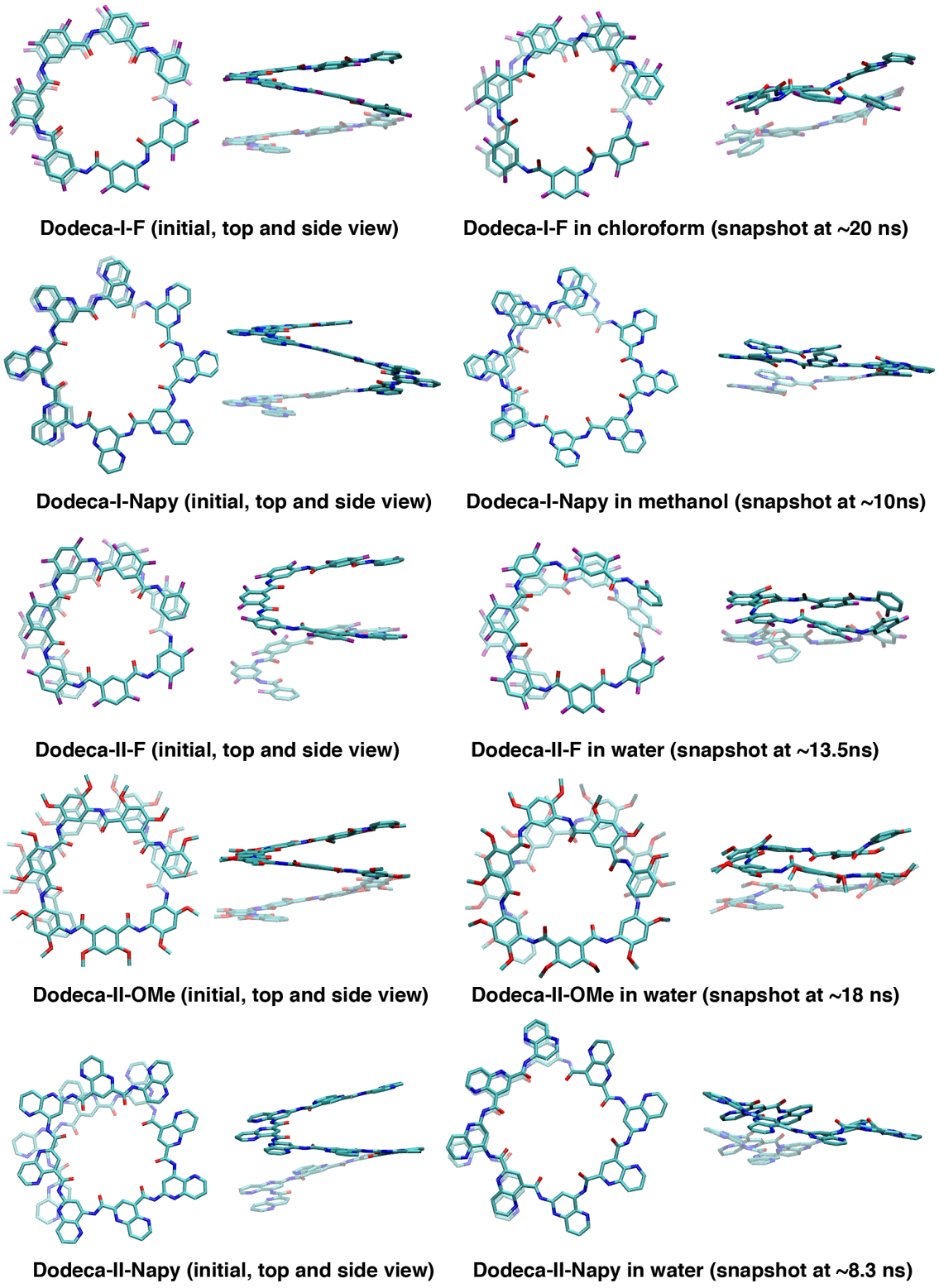

Figure S1. Examples of initial structures and snapshots from simulations of type **I** and **II** oligomers.

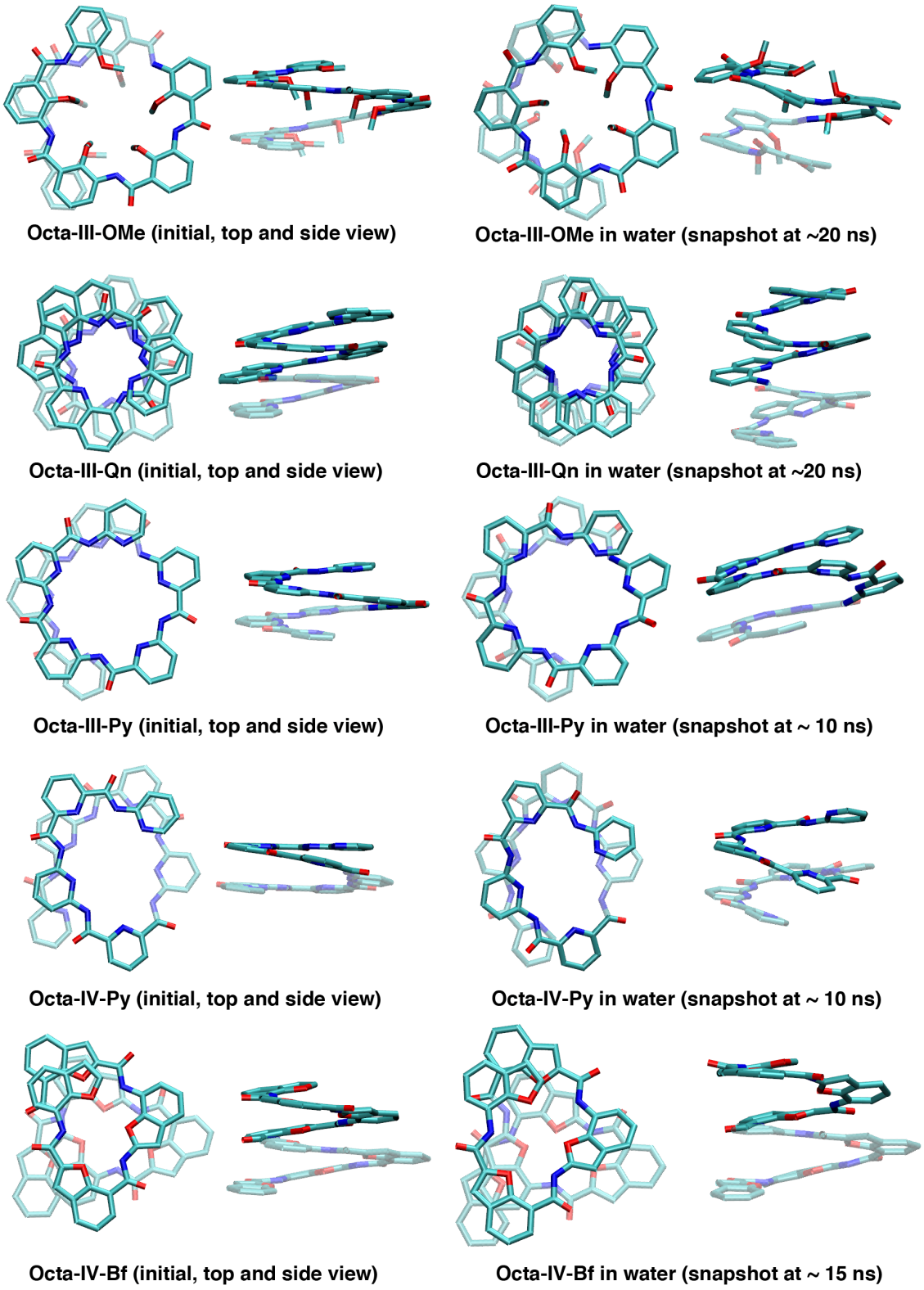

Figure S1-cont. Examples of initial structures and snapshots from simulations of type **III** and **IV** oligomers.

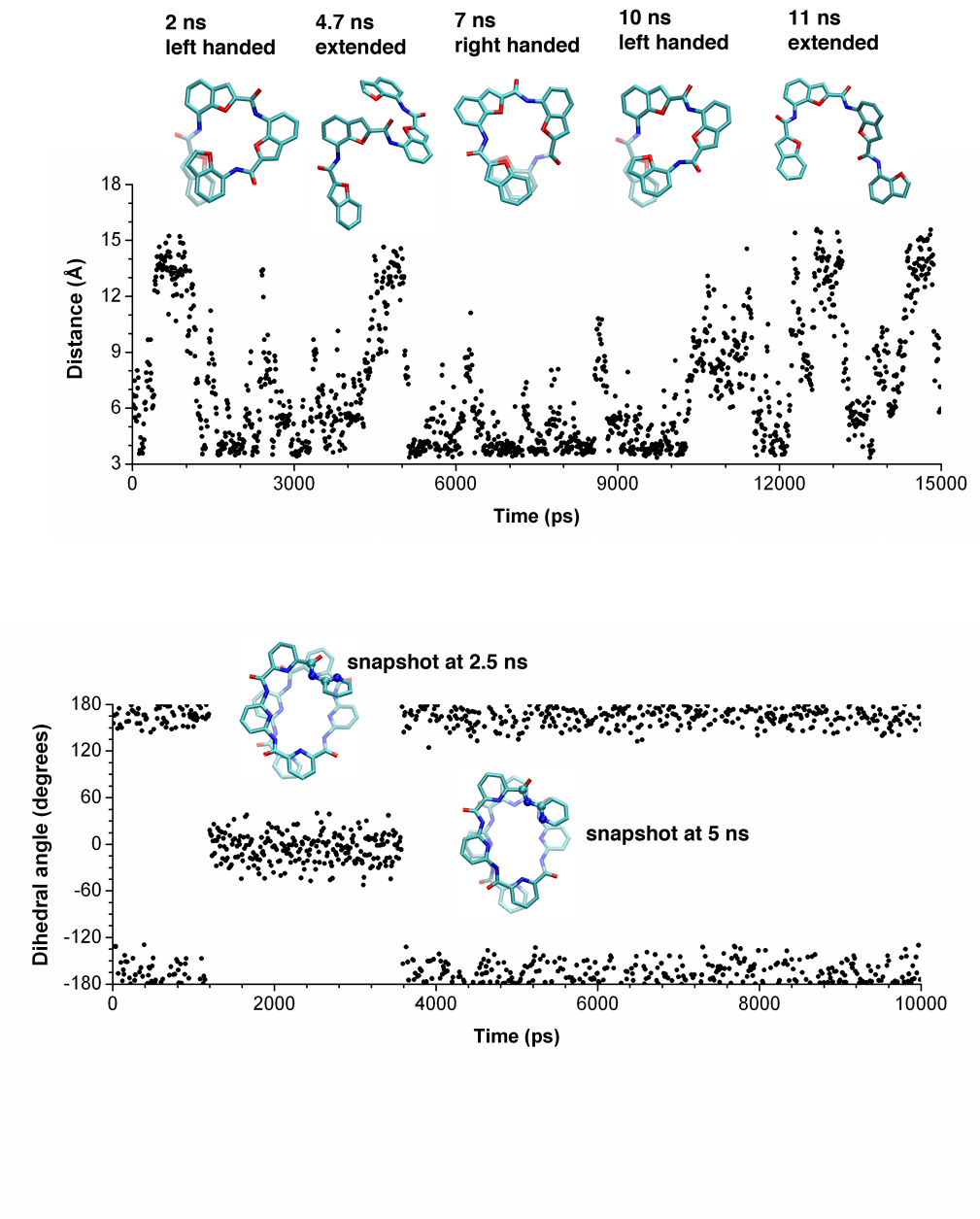

Figure S2. MD trajectory examples. Top: Distance between COMs of the *i*th and (*i*+NUpT)th aromatic ring is shown as a function of simulation time for **Tetra-III-Bf** in methanol. Snapshots of the tetramer at selected time intervals are shown to illustrate that folding/unfolding and helix handedness inversion have occurred. Bottom: The terminal N_a-C_a-N_p-C_p (depicted as ball and stick mode in the snapshots) dihedral angle is shown as a function of simulation time for **Octa-IV-Py** in water. Snapshots show helical conformation with and without the terminal group flipped 180°.