Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information: Crystallization behavior of polyvinylidene fluoride (PVDF) in NMP/DMF solvents : a molecular dynamics study

Anseong Park,[a] Je-Yeon Jung,[a] Seungtae Kim,[a] WooJin Kim,[b] Min Young Seo,[b] Sangdeok Kim,[a] YongJoo Kim,*[b] Won Bo Lee,*[a]

[a]School of Chemical and Biological Engineering and Institute of Chemical Processes, Seoul National University, Seoul 08826, Republic of Korea. Tel: +82 (0)2 880 1529; E-mail: wblee@snu.ac.kr

[b]School of Advanced Materials Engineering, KookMin University, Seoul 02707, Republic of Korea. Tel: +82 (0)2 910 4685; E-mail: cjyjee@kookmin.ac.kr

Table S1 Number of molecules in each simulated system.

NMP	PVDF	wt %	DMF	PVDF	wt %
1030	216	67.06	1395	216	67.09
1030	162	60.42	1395	162	60.46
1030	108	50.44	1395	108	50.48
1030	90	45.90	1395	90	45.93
1030	72	40.43	1395	72	40.46
1030	54	33.73	1395	54	33.76
1030	40	27.38	1395	40	27.41
1030	25	19.07	1395	25	19.09
1030	11	9.40	1395	11	9.40

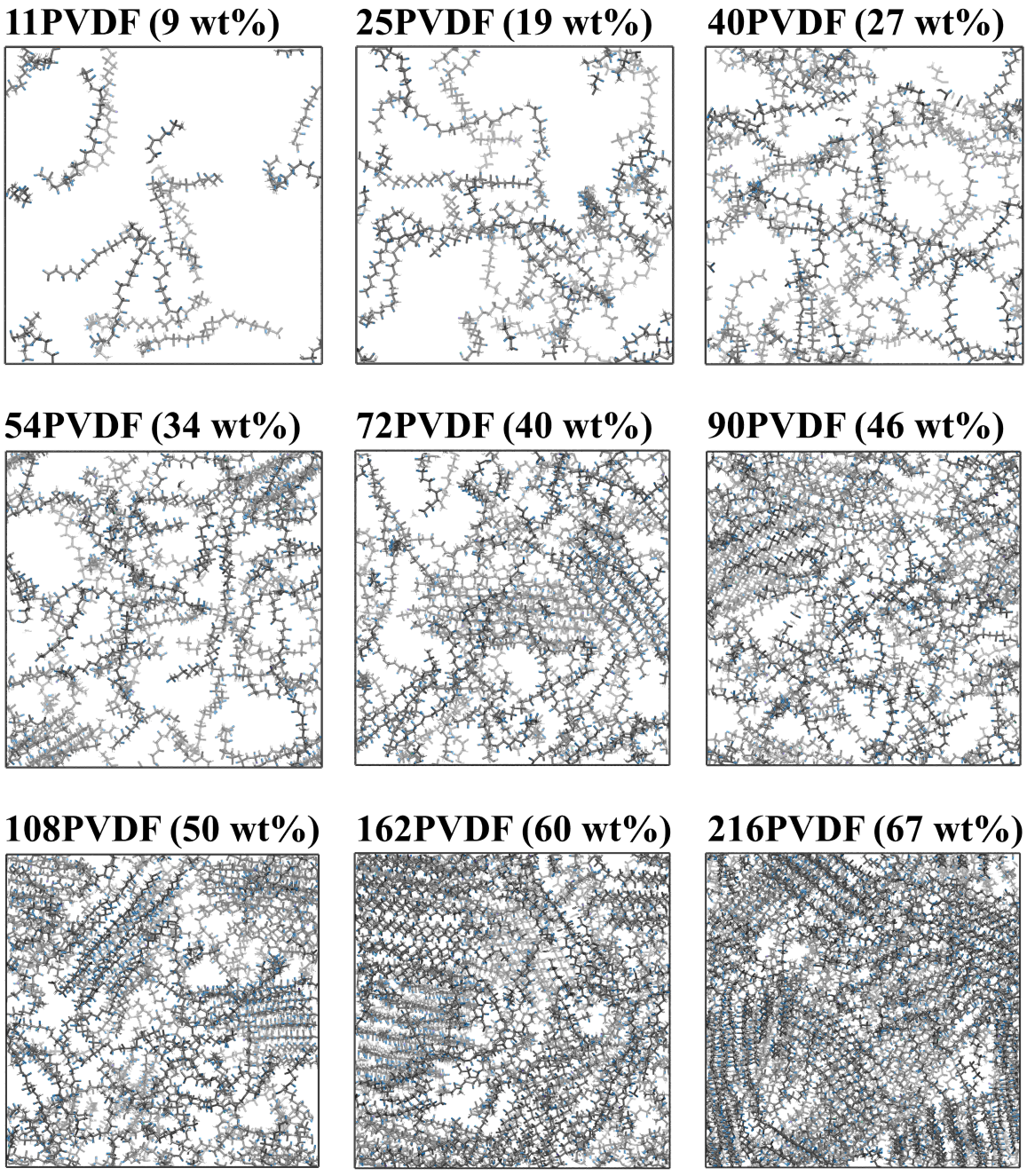

Figure S1 Simulation snapshots of varying PVDF wt% in NMP solvent.

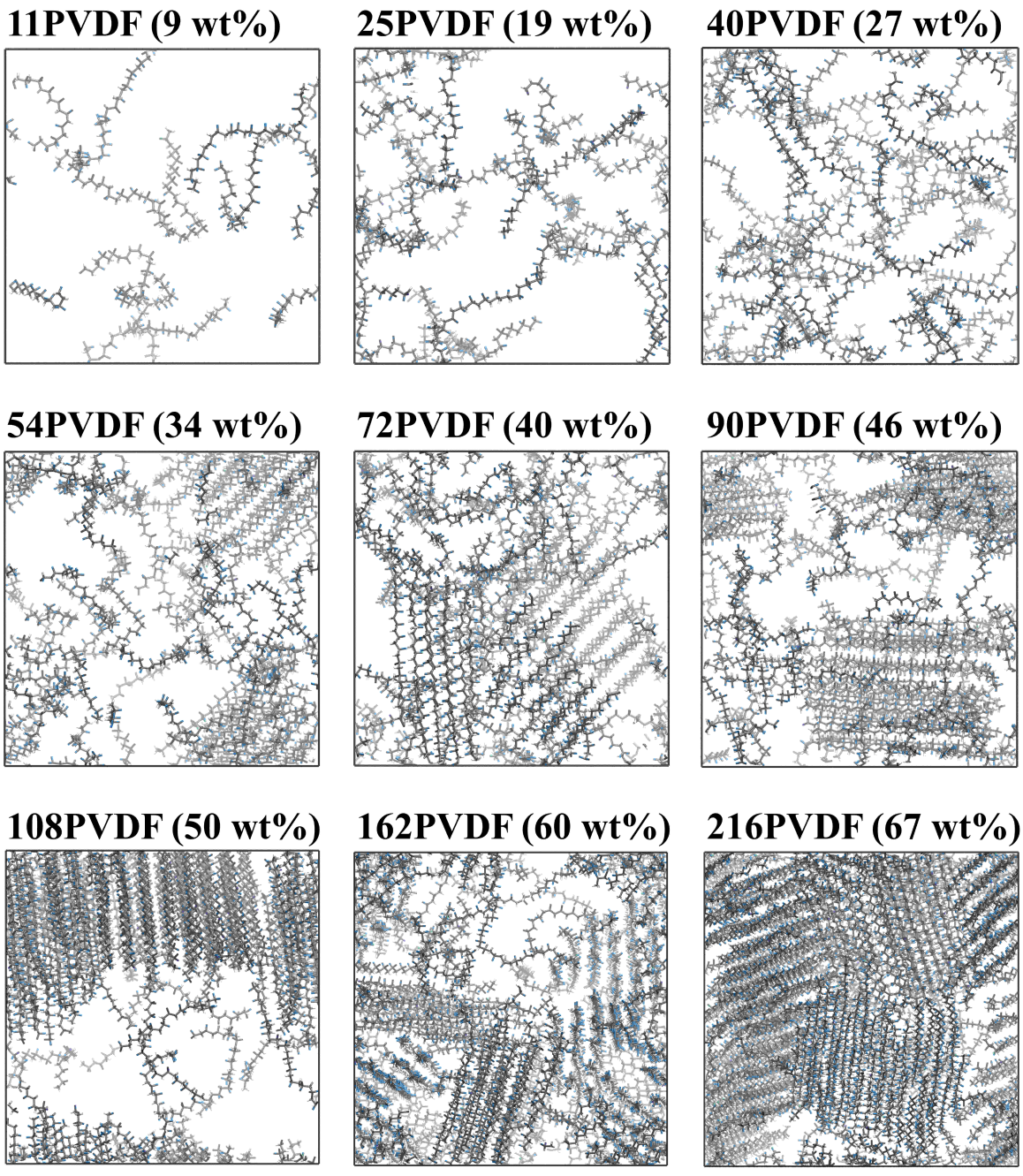

Figure S2 Simulation snapshots of varying PVDF wt% in DMF solvent.

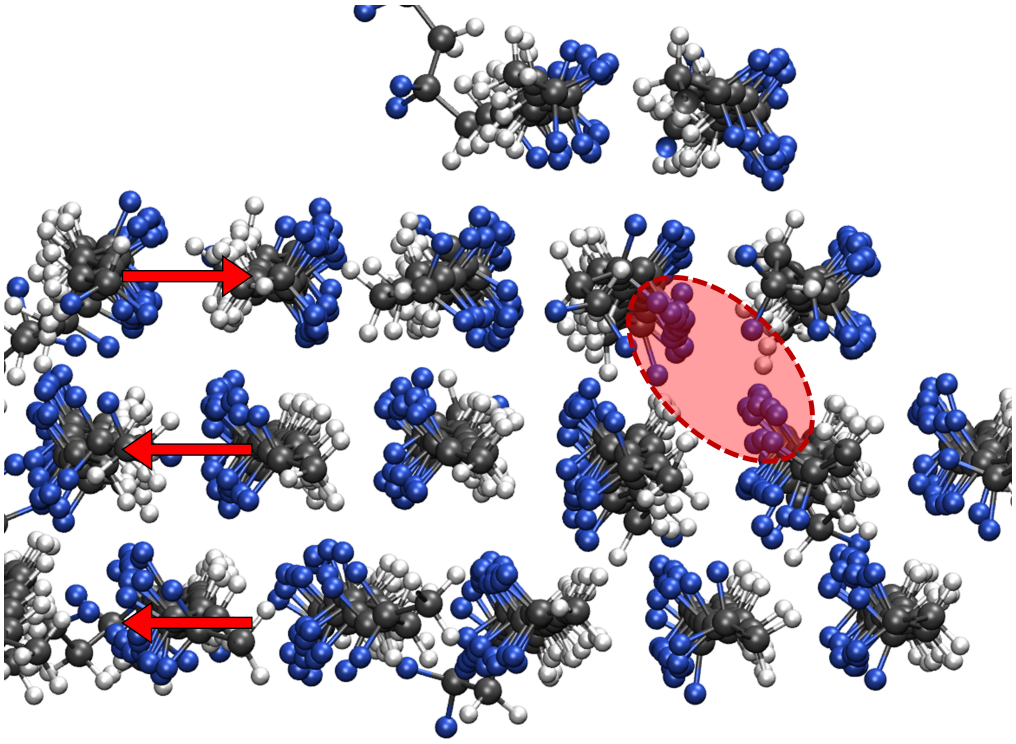

Figure S3 Simulation snapshot of aligned β phase PVDF chains at 34 wt% of PVDF in DMF.

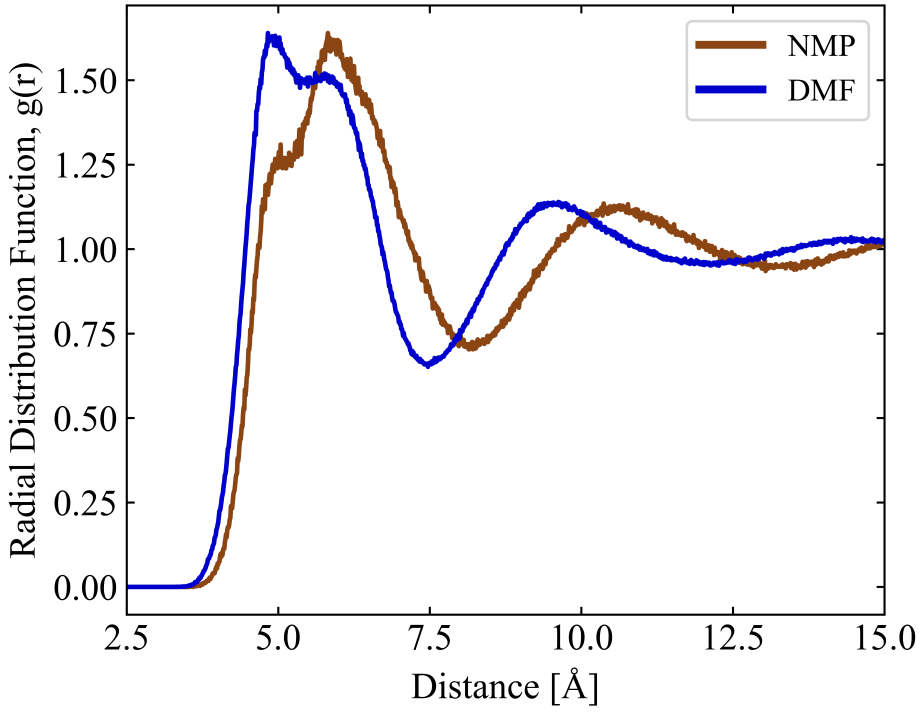

Figure S4 Radial distribution functions of NMP-NMP and DMF-DMF.

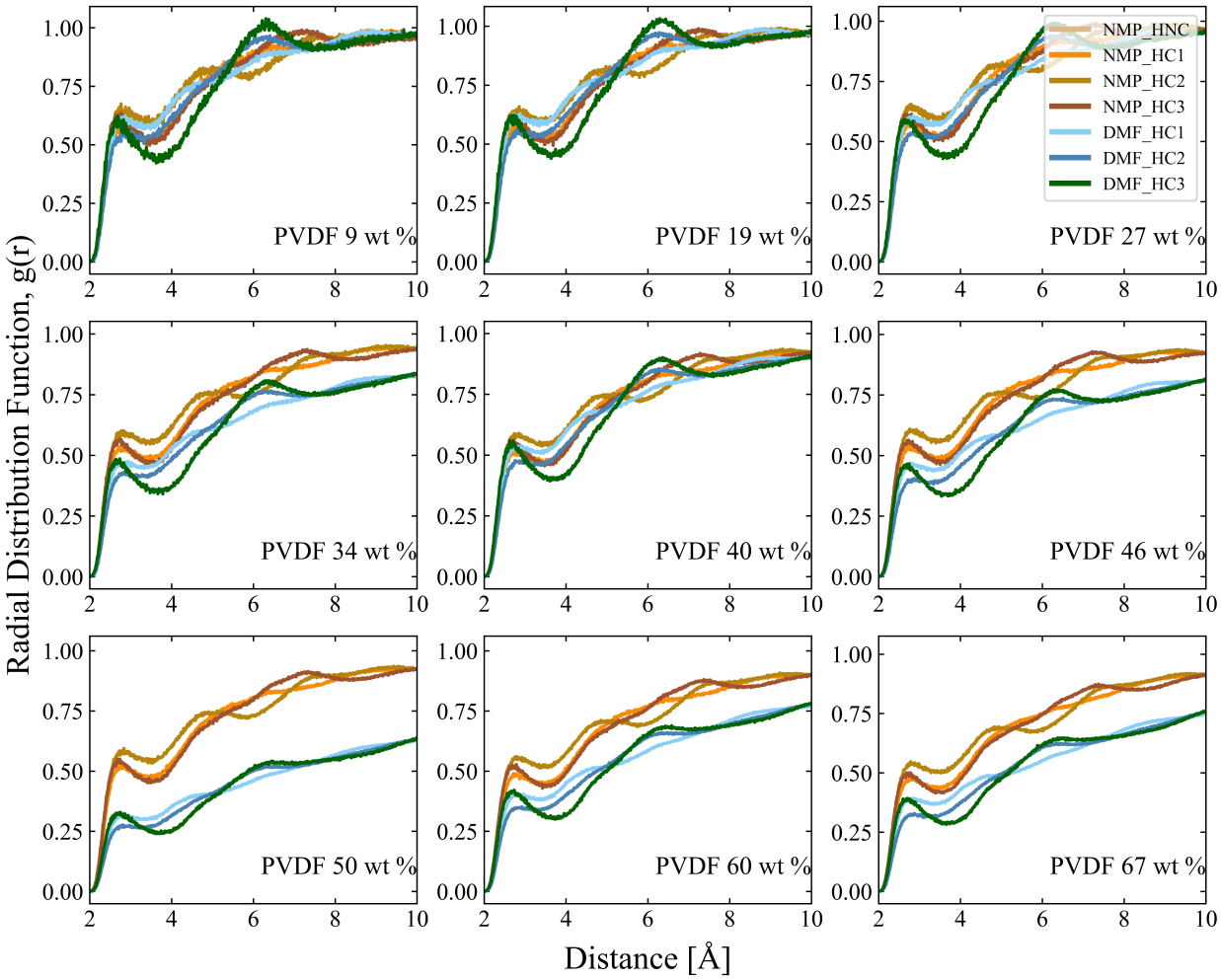

Figure S5 Radial distribution function of PVDF fluorine and solvent hydrogen atom groups. Plots are shown in order of increasing PVDF wt%.

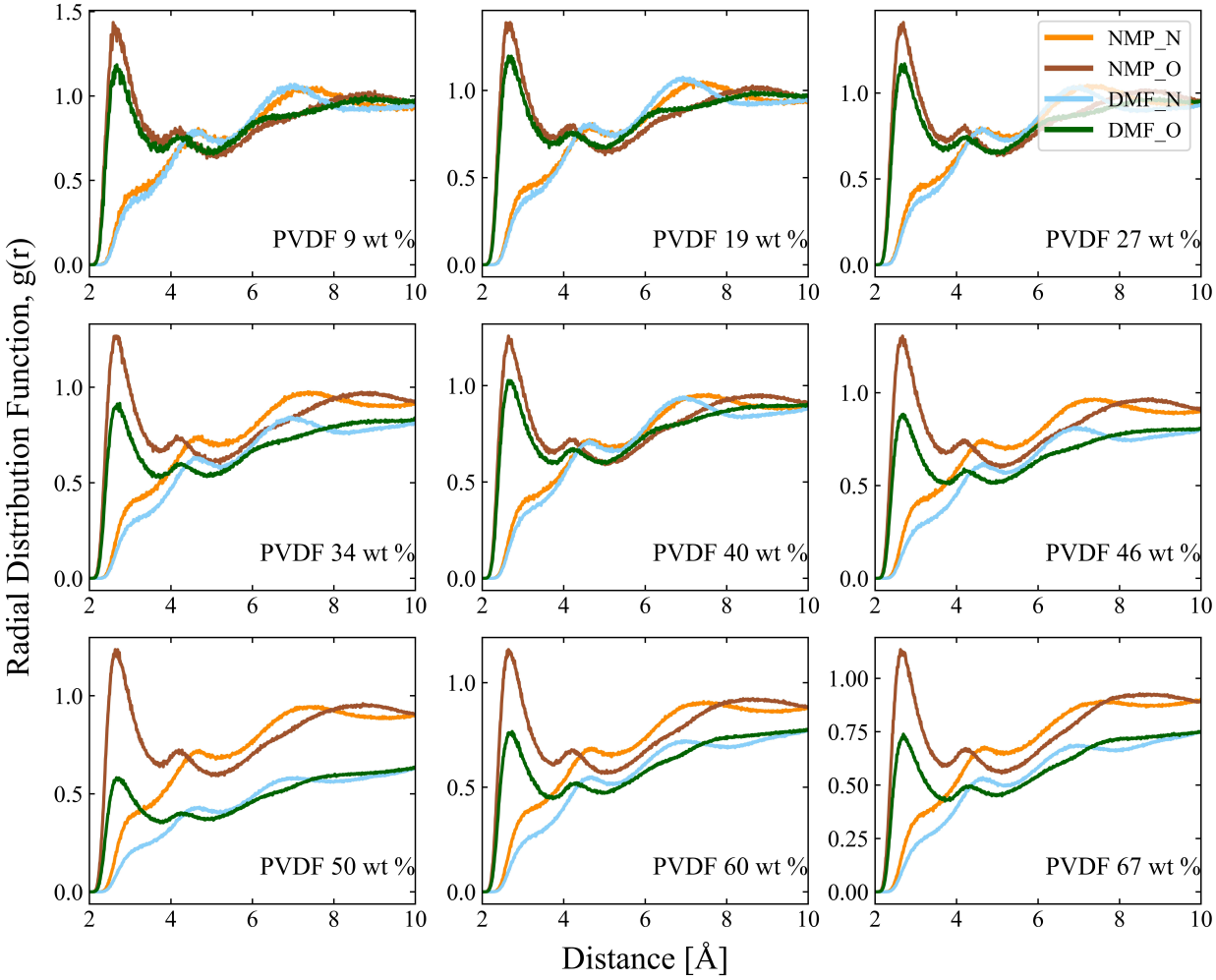

Figure S6 Radial distribution function of PVDF hydrogen groups and solvent N/O atoms. Plots are shown in order of increasing PVDF wt%.

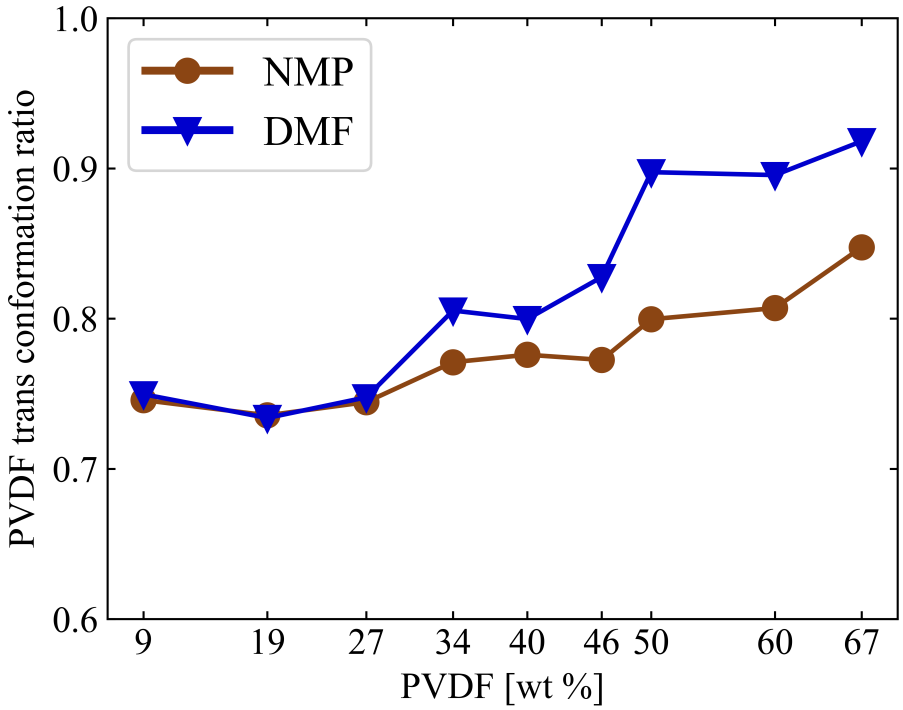

Figure S7 Ratio of *trans* structure PVDF within 3.8 Å from NMP and DMF, respectively.