Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supporting Information

The nucleation and growth of methane hydrates in the presence of phenylalanine and tryptophan: A comparative molecular dynamics simulations study

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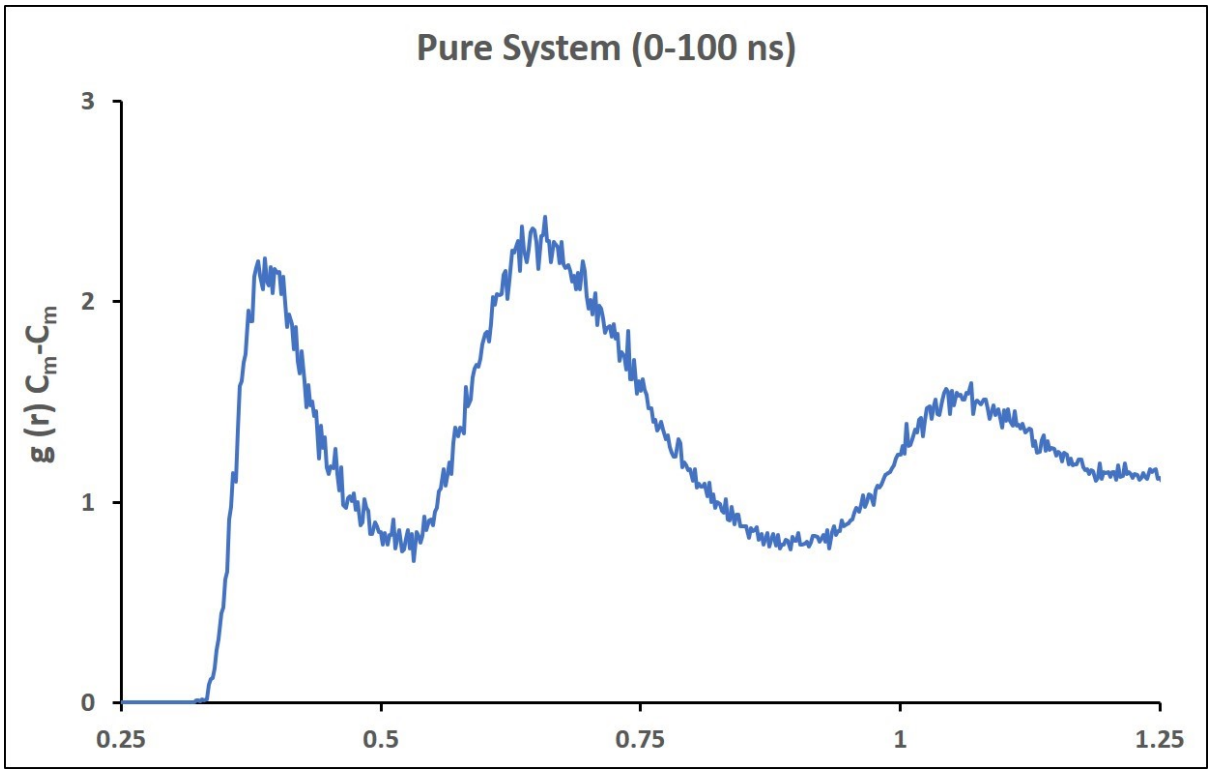

Figure S1: Radial distribution function for carbon atoms during the dispersion period (0-100 ns)

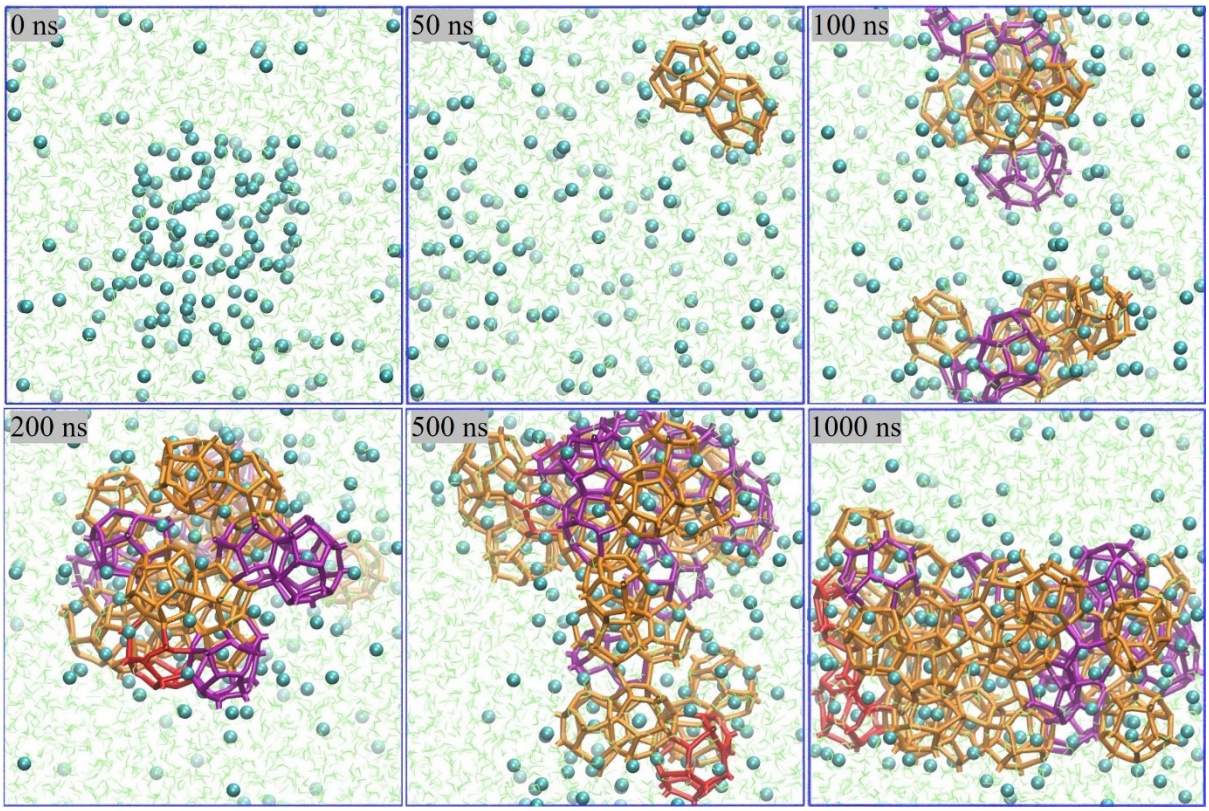

Figure S2: Snapshots of CH_4 hydrate growth in the Pure system at different time frames.

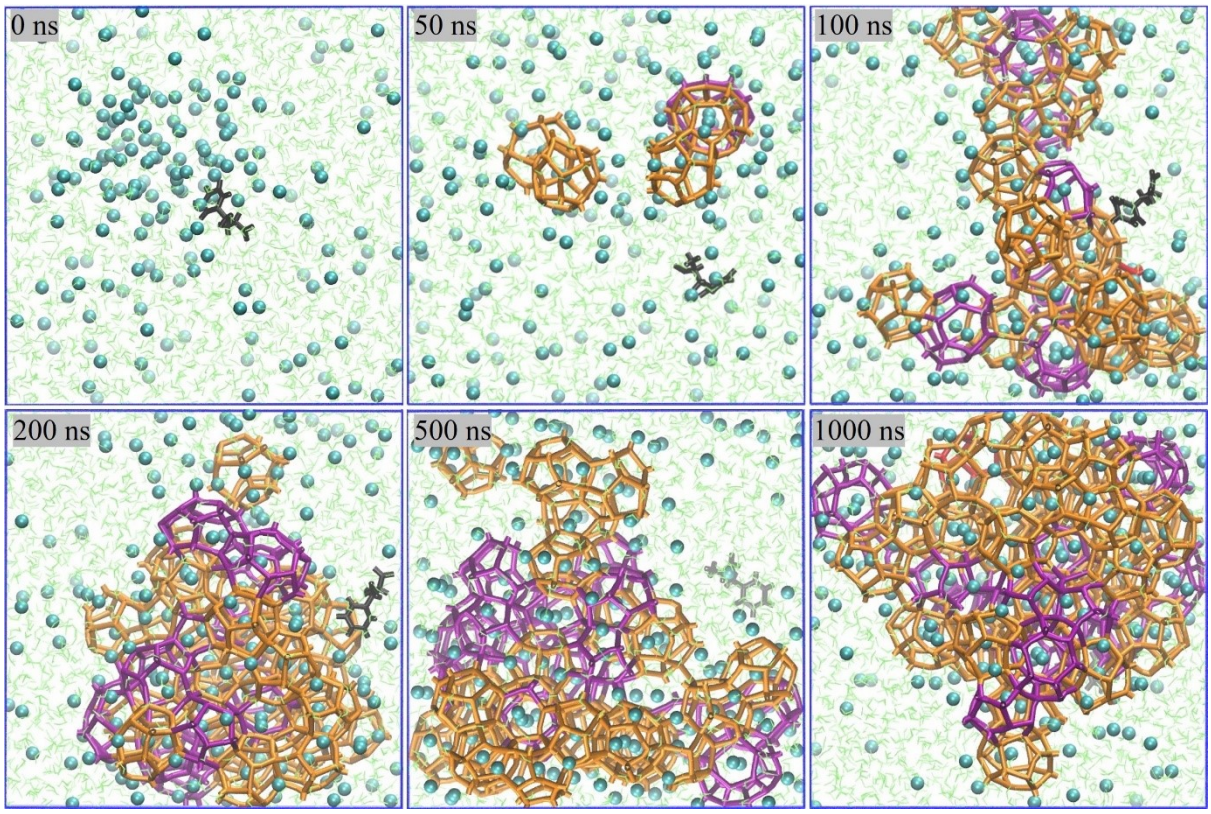

Figure S3: Snapshots of CH_4 hydrate growth in the 1-PHE system at different time frames.

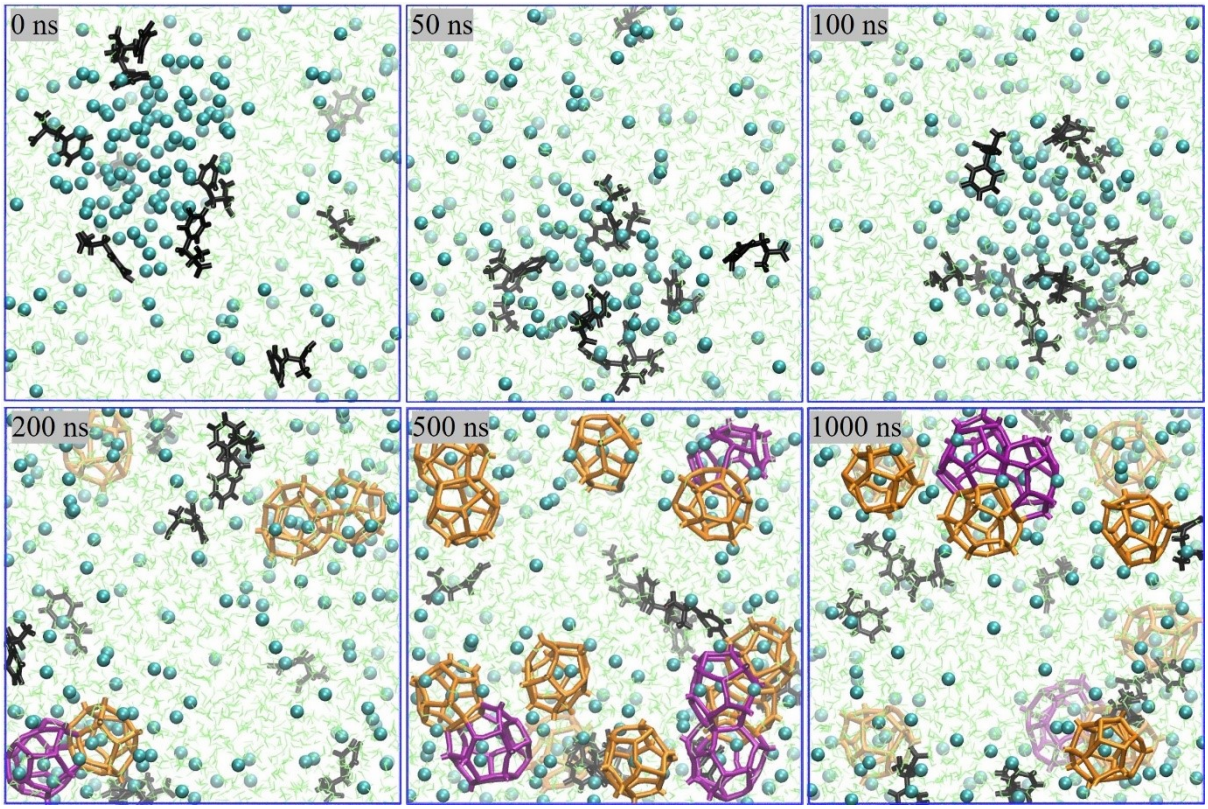

Figure S4: Snapshots of CH_4 hydrate growth in the 10-PHE system at different time frames.

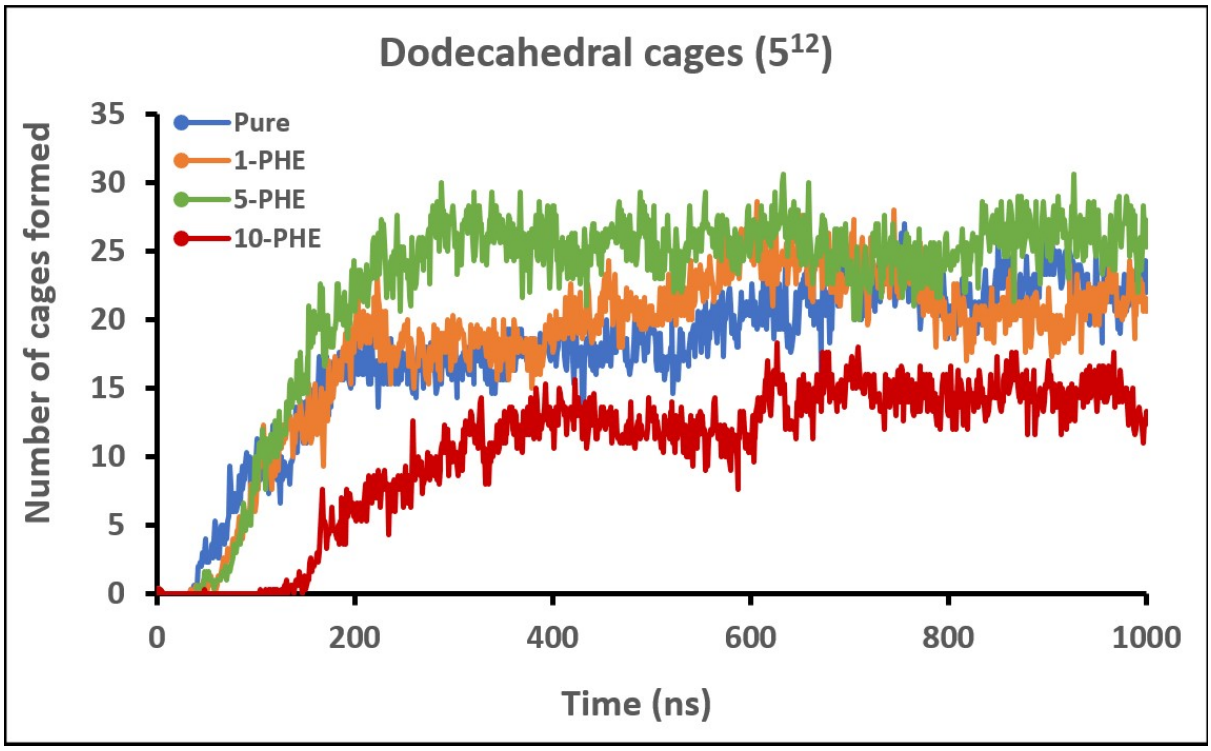

Figure S5: Number of dodecahedral cages formed during the simulations

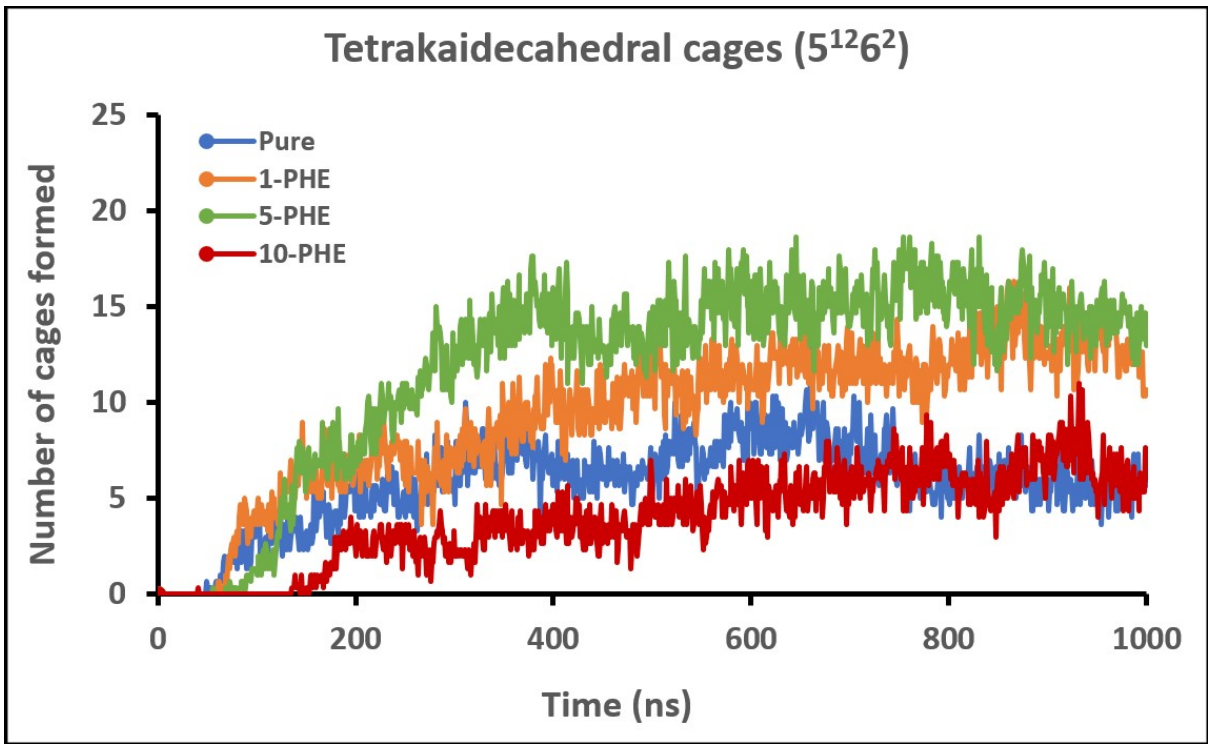

Figure S6: Number of tetrakaidecahedral cages formed during the simulations

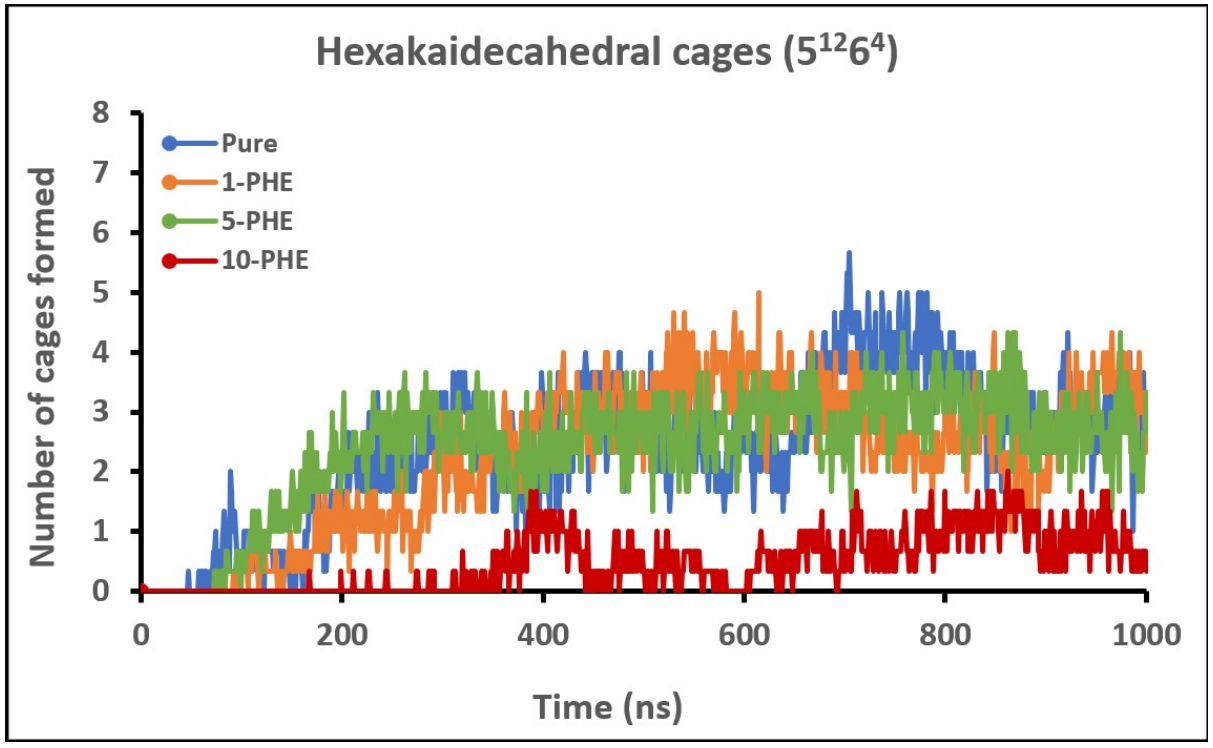

Figure S7: Number of hexakaidecahedral cages formed during the simulations

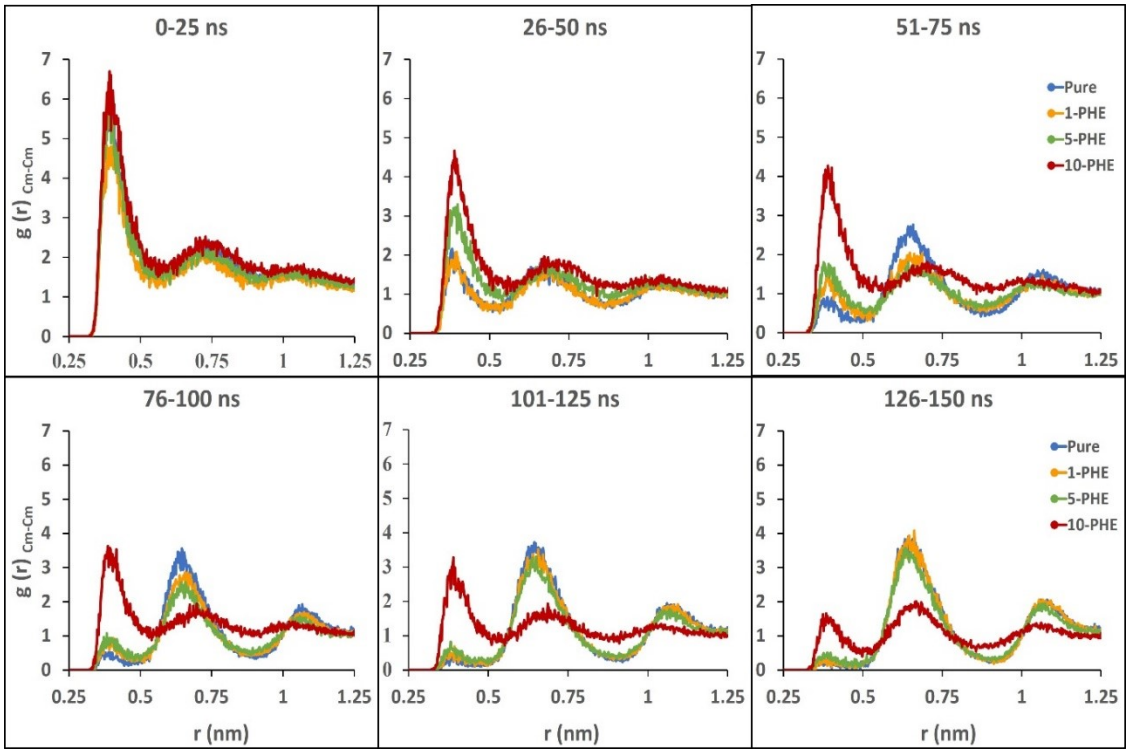

Figure S8: The radial distribution function for carbon atoms of methane molecules (C_m-C_m) for various phenylalanine systems at the time intervals of 25 ns.

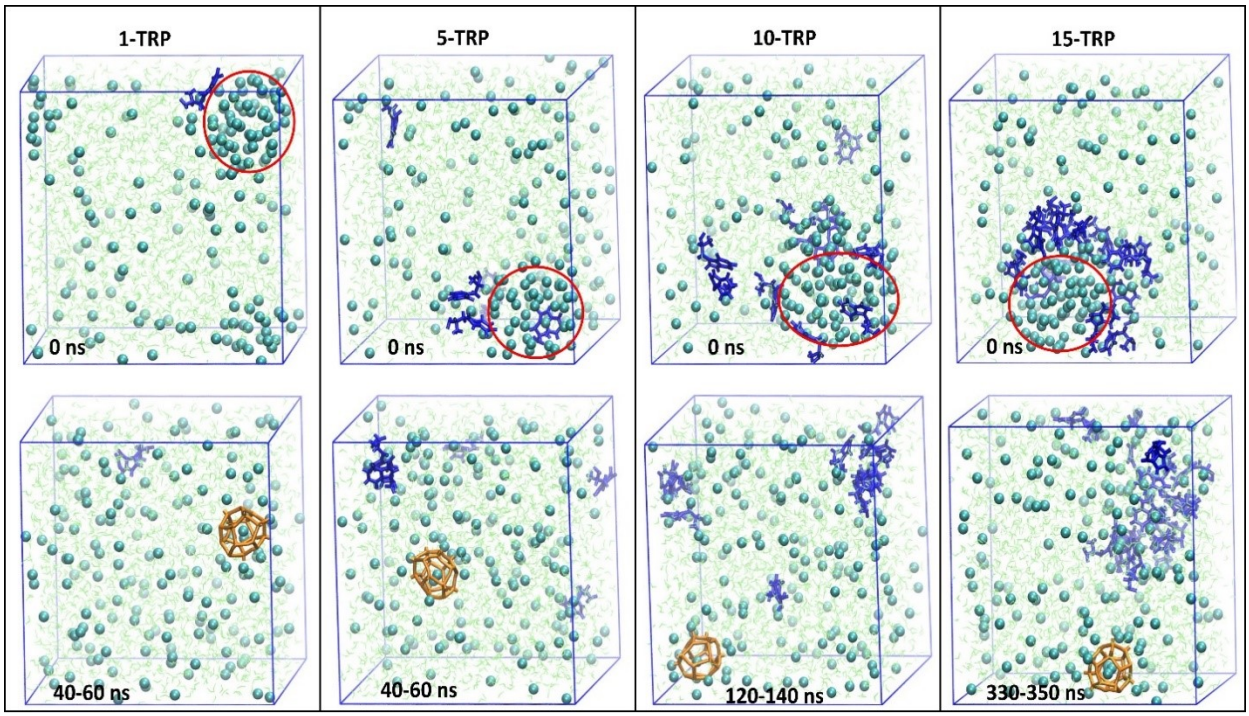

Figure S9. The initial stage of the nucleation of methane hydrate in the presence of tryptophan for its various concentrations. The top panel shows the configuration of the systems at the starting of the simulations and the bottom panel shows the configurations for the time period at which the first stable cage is formed. Methane molecules are shown as balls (cyan-colored), water molecules as lines (lime-colored), and tryptophan as bonds and stick (blue-colored). The methane molecules clustered in the initial configuration are encircled.

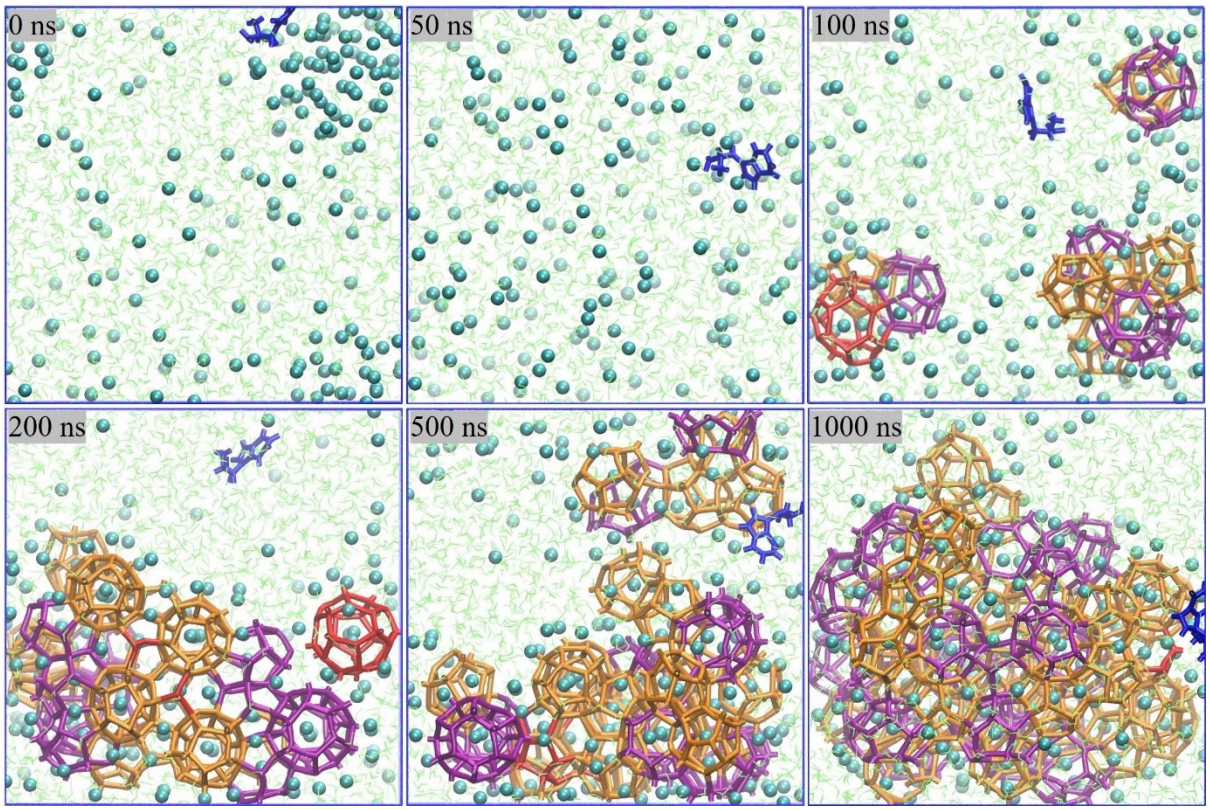

Figure S10: Snapshots of CH_4 hydrate growth in the 1-TRP system at different time frames.

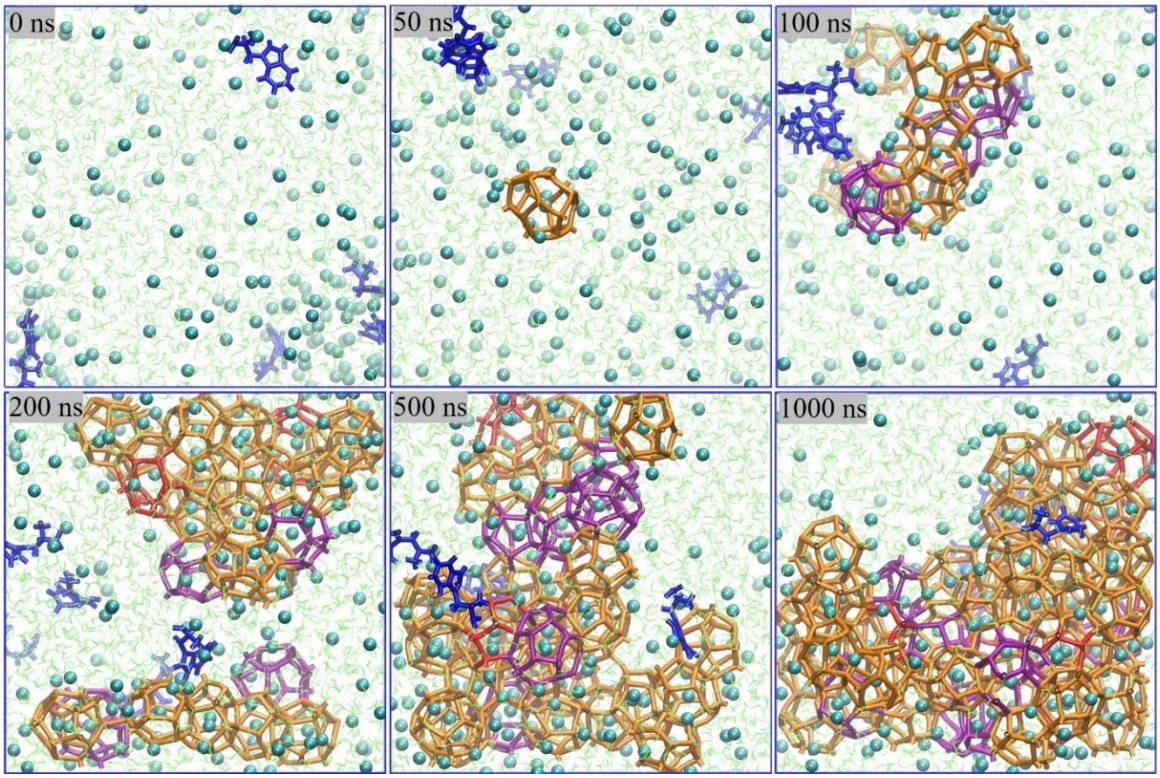

Figure S11: Snapshots of CH_4 hydrate growth in the 5-TRP system at different time frames.

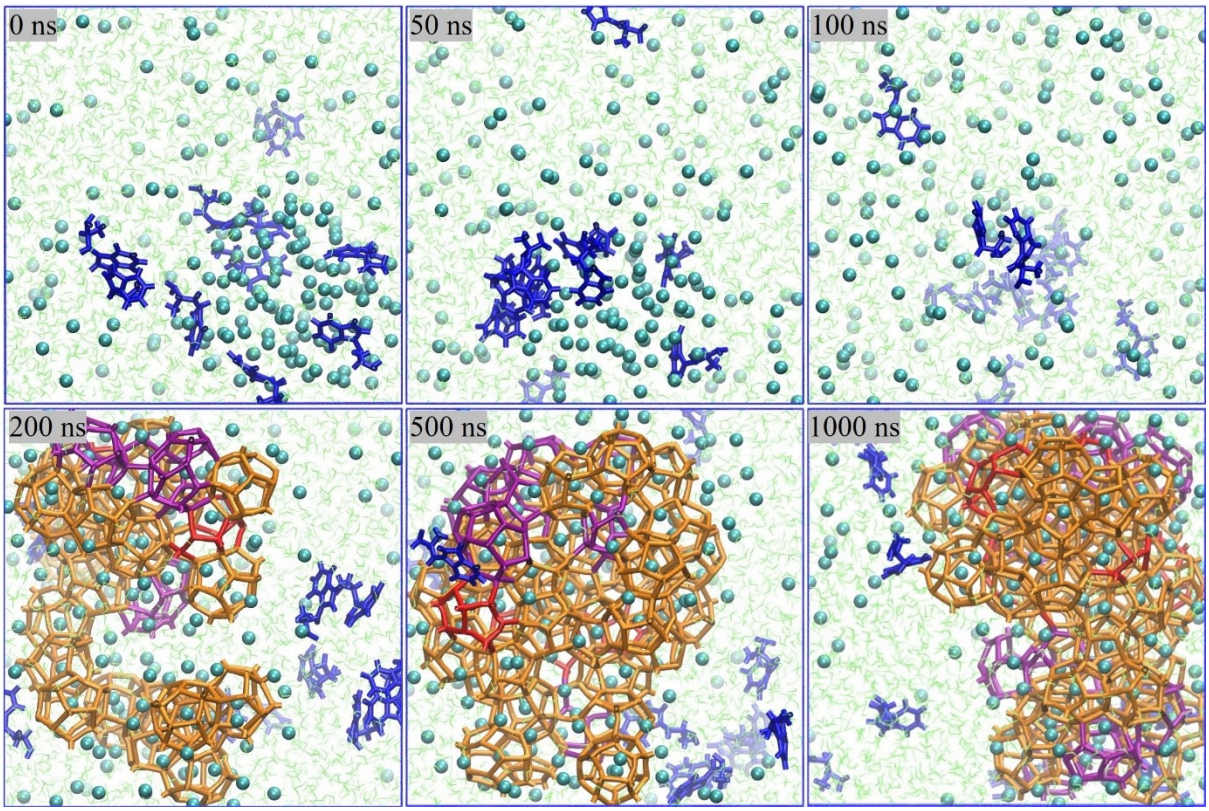

Figure S12: Snapshots of CH_4 hydrate growth in the 10-TRP system at different time frames.

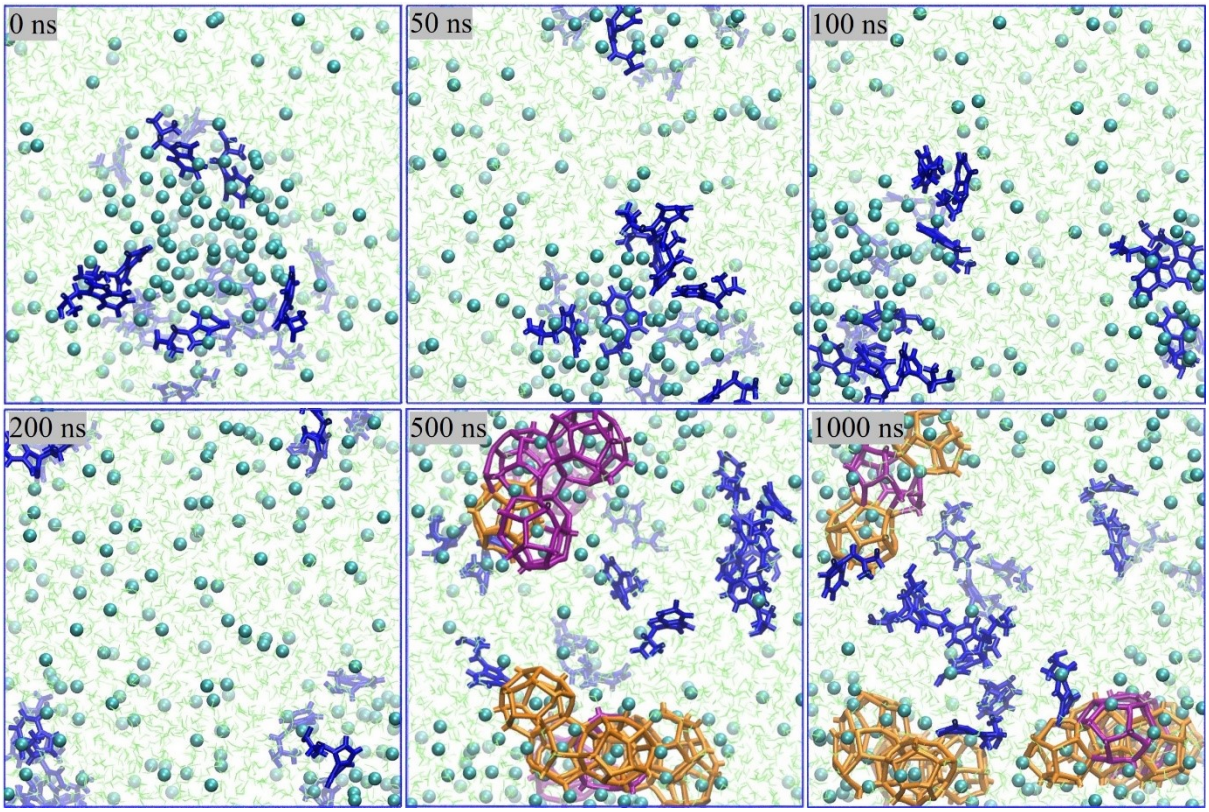

Figure S13: Snapshots of CH_4 hydrate growth in the 15-TRP system at different time frames.

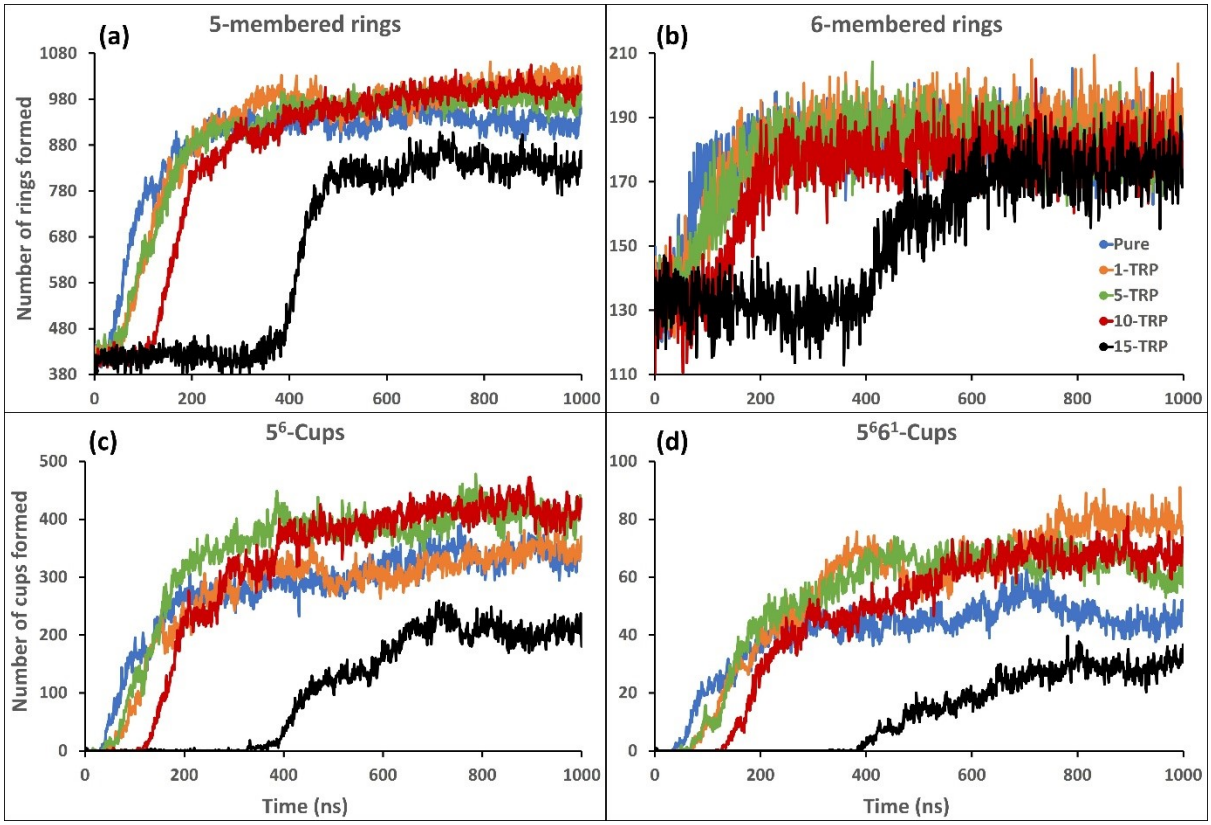

Figure 14. Number of **(a)** 5-membered rings, **(b)** 6-membered rings, **(c)** 5^6 cups, and **(d)** 5^66^1 cups formed during simulations in the presence of tryptophan.

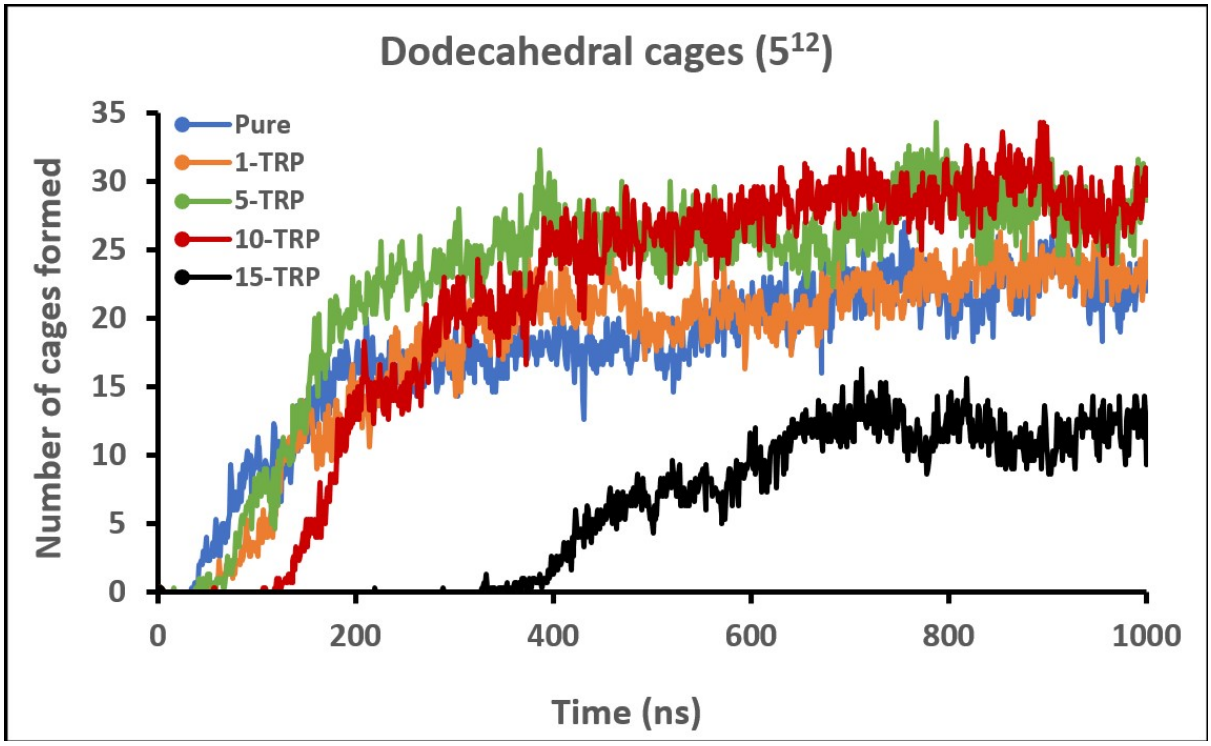

Figure S15: Number of dodecahedral cages formed during the simulations.

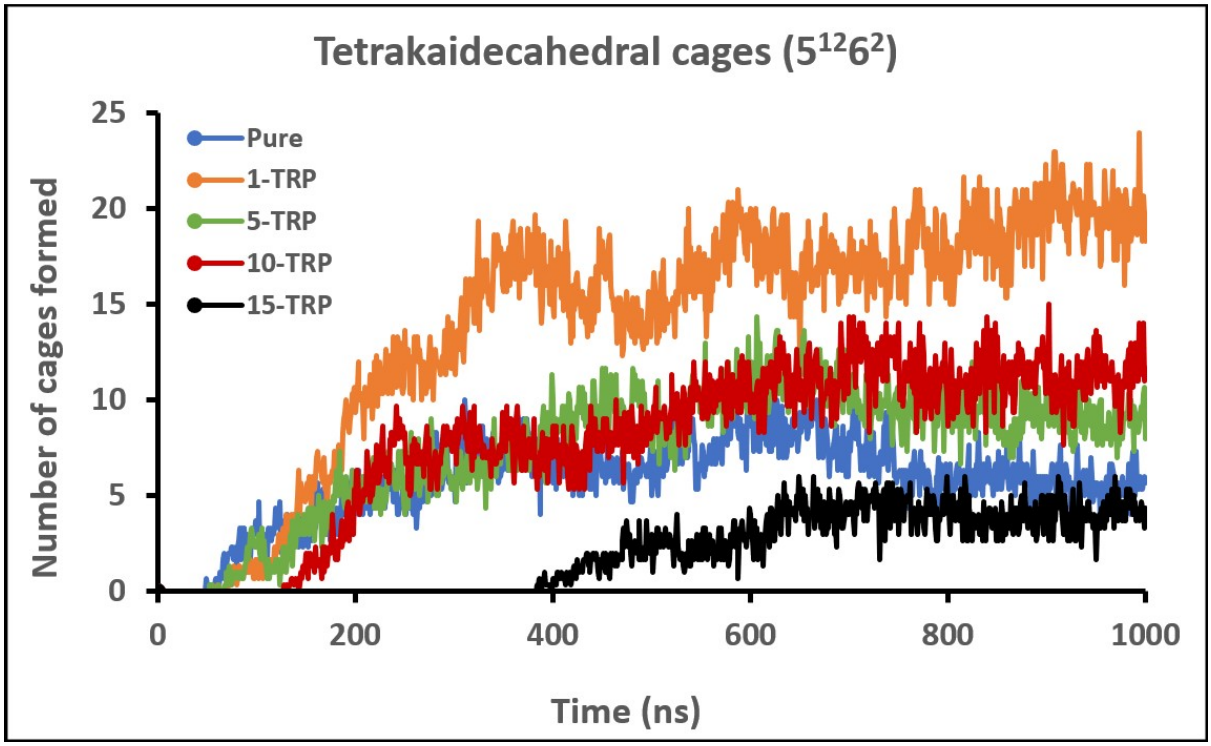

Figure S16: Number of tetrakaidecahedral cages formed during the simulations.

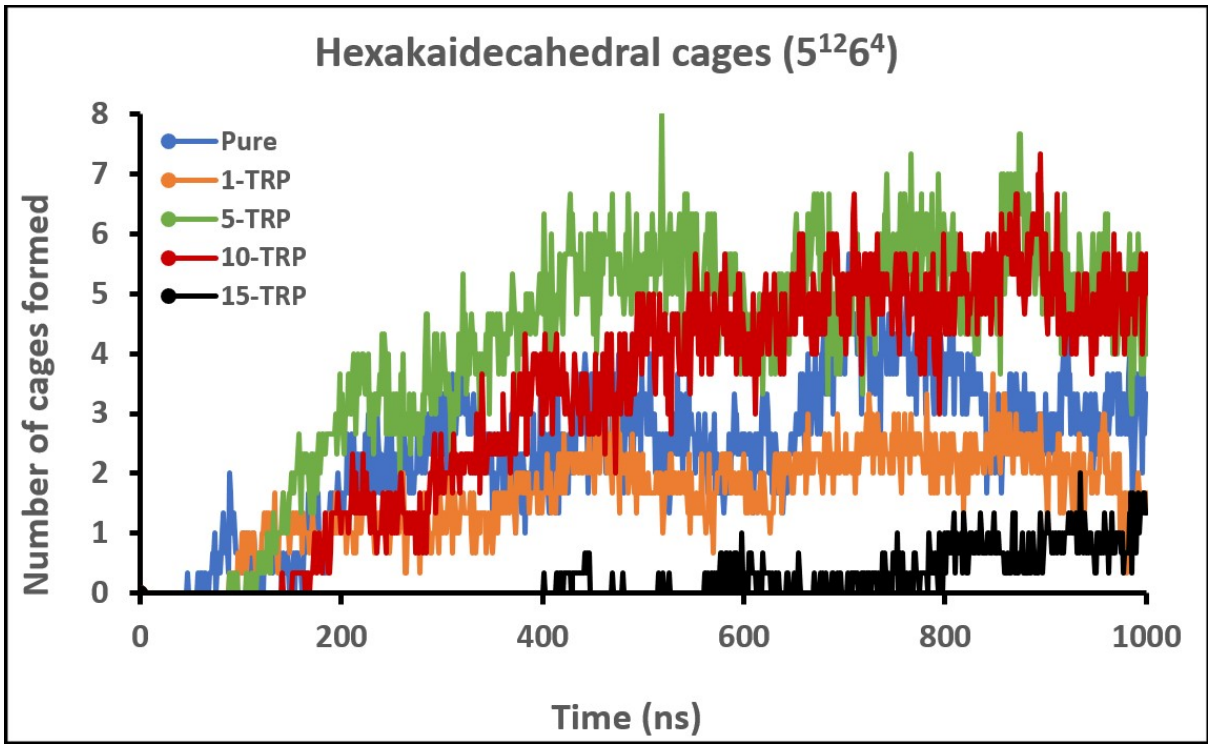

Figure S17: Number of hexakaidecahedral cages formed during the simulations.

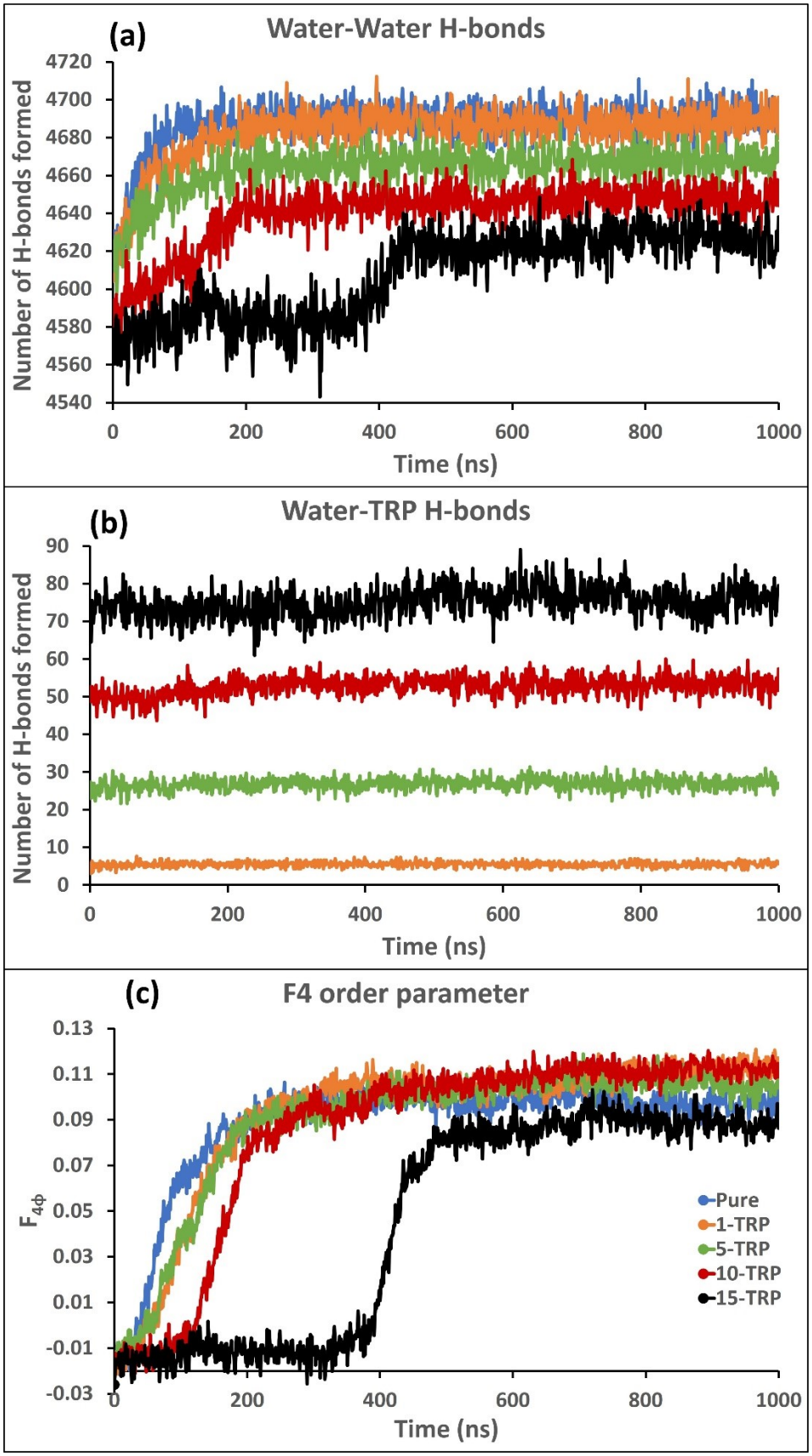

Figure S18. The number of hydrogen bonds formed between **(a)** water molecules, **(b)** water and phenylalanine molecules of all the systems during simulations. **(c)** F4 order parameter of water molecules during the simulations.

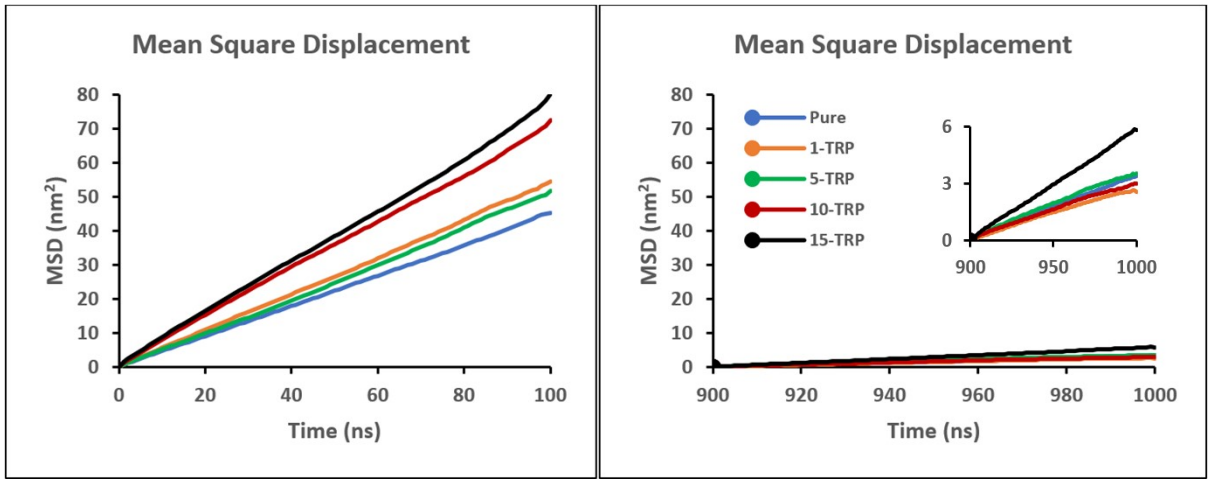

Figure S19. Mean square displacement of methane molecules during the simulations.

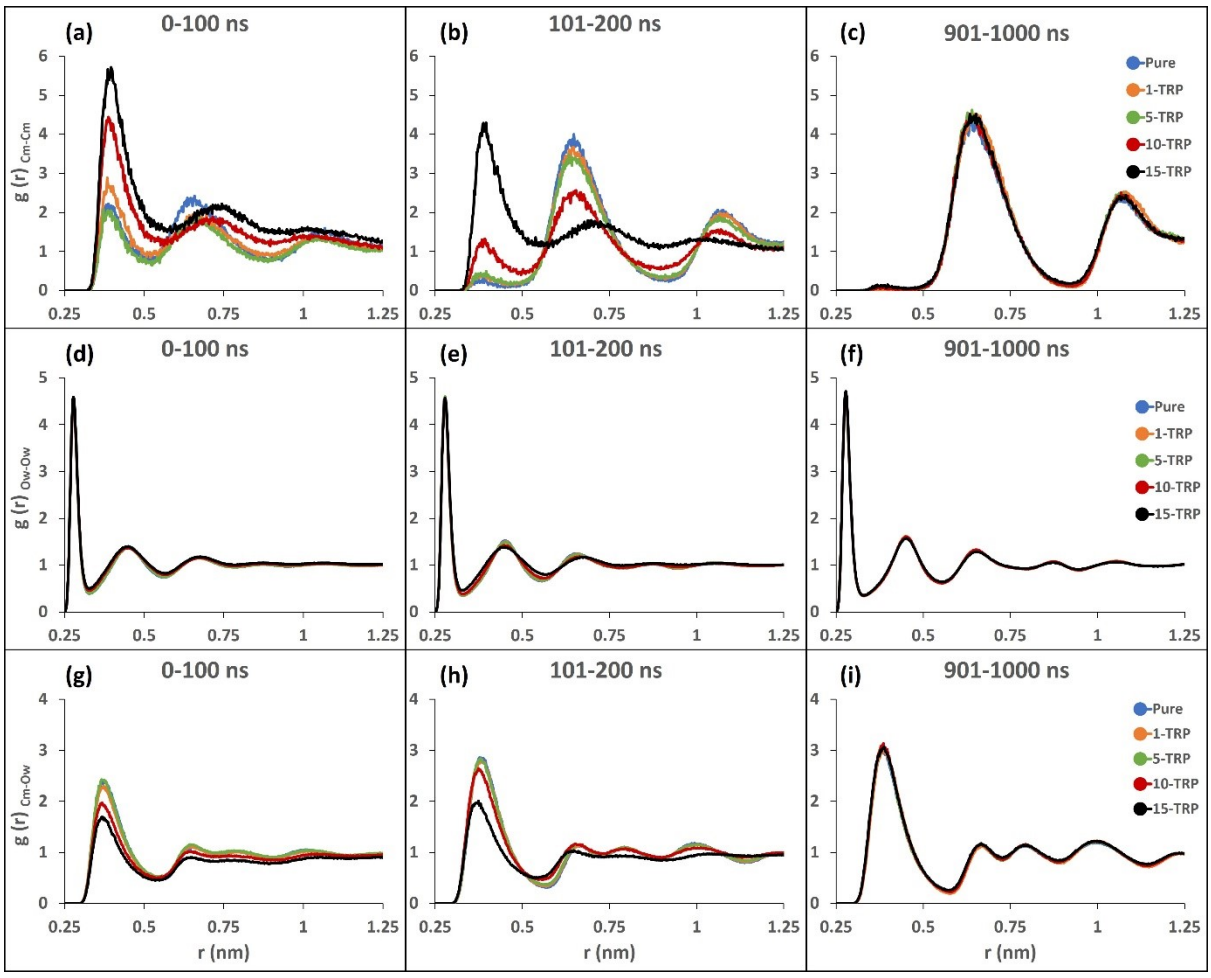

Figure S20. The radial distribution functions for different pairs of atoms in presence of varying concentrations of tryptophan.

The structural parameters of phenylalanine and tryptophan

Table S1: Lennard-jones parameters for phenylalanine

Atom	Sigma	Epsilon	Charges
N	3.25E-01	7.11E-01	-0.4688
H	1.07E-01	6.57E-02	0.3033
C	3.40E-01	4.58E-01	0.1925
H	1.96E-01	6.57E-02	0.0524
C	3.40E-01	4.58E-01	-0.0305
H	2.65E-01	6.57E-02	0.0377
C	3.40E-01	3.60E-01	-0.0426
C	3.40E-01	3.60E-01	-0.1317
H	2.60E-01	6.28E-02	0.1451
C	3.40E-01	3.60E-01	-0.1628
H	2.60E-01	6.28E-02	0.1386
C	3.40E-01	3.60E-01	-0.1115
H	2.60E-01	6.28E-02	0.1301
C	3.40E-01	3.60E-01	0.6553
O	2.96E-01	8.79E-01	-0.6703

Table S2: Lennard-jones parameters for tryptophan

Atom	Sigma	Epsilon	Charges
N	3.25E-01	7.11E-01	-0.2905
H	1.07E-01	6.57E-02	0.2659
C	3.40E-01	4.58E-01	0.0755
H	2.47E-01	6.57E-02	0.0663
C	3.40E-01	4.58E-01	-0.0421
H	2.65E-01	6.57E-02	0.0486
C	3.40E-01	3.60E-01	-0.1210
C	3.40E-01	3.60E-01	-0.1671
H	2.51E-01	6.28E-02	0.2326
N	3.25E-01	7.11E-01	-0.3382
H	1.07E-01	6.57E-02	0.3466
C	3.40E-01	3.60E-01	0.1184
C	3.40E-01	3.60E-01	0.0760
C	3.40E-01	3.60E-01	-0.2046
H	2.60E-01	6.28E-02	0.1422
C	3.40E-01	3.60E-01	-0.1970
H	2.60E-01	6.28E-02	0.1440
C	3.40E-01	3.60E-01	-0.1399
H	2.60E-01	6.28E-02	0.1395
C	3.40E-01	3.60E-01	-0.2136
H	2.60E-01	6.28E-02	0.1479
C	3.40E-01	3.60E-01	0.7246
O	2.96E-01	8.79E-01	-0.7197
O	2.96E-01	8.79E-01	-0.6748