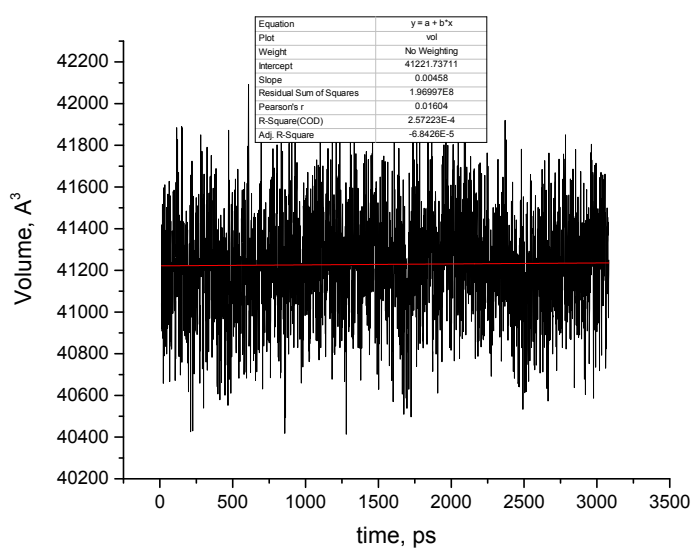
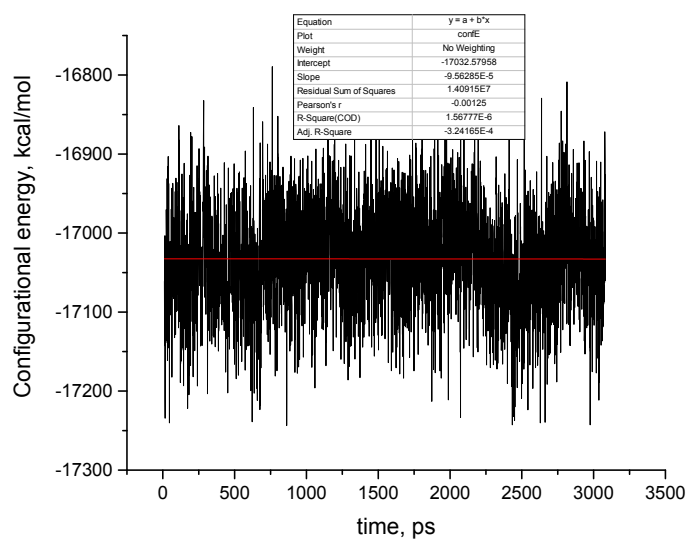


## Electronic Supplementary Information

### **Molecular dynamics simulations of aqueous glycine solutions**

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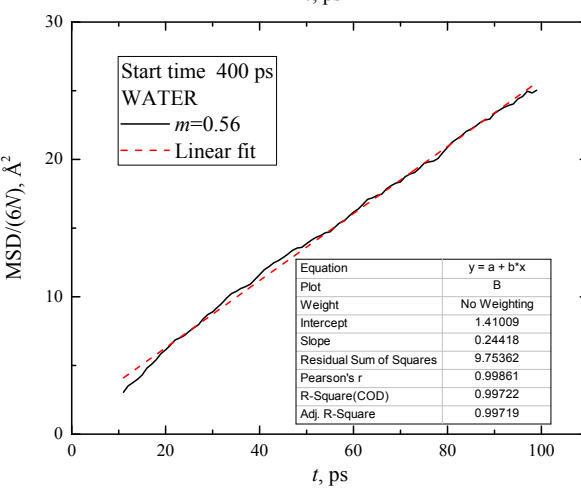
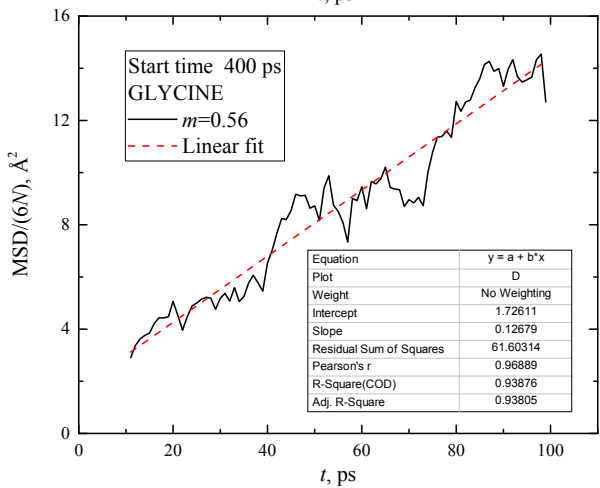
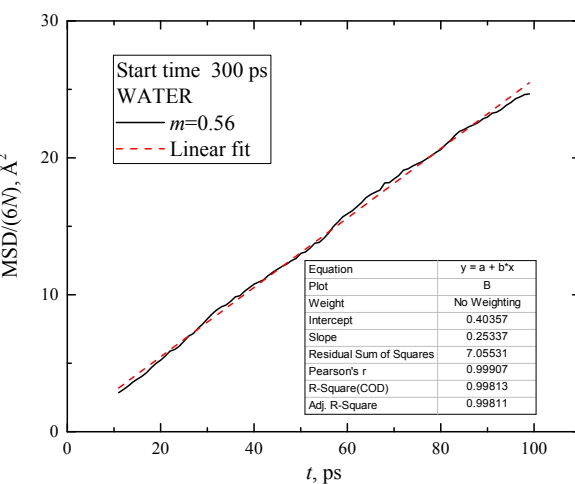
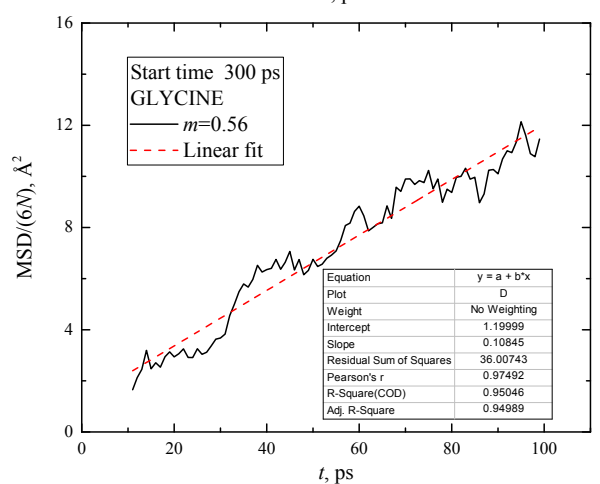
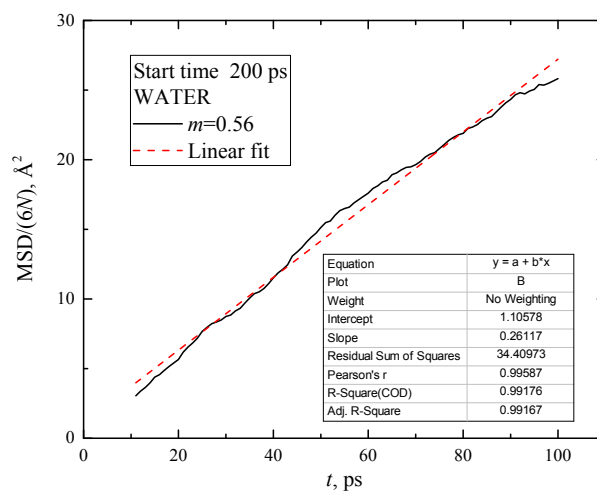
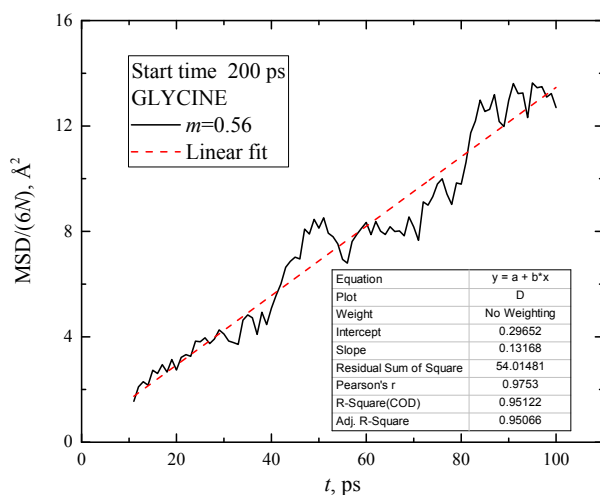
**Fig. S1.** Typical energy and volume fluctuations during the productive run.

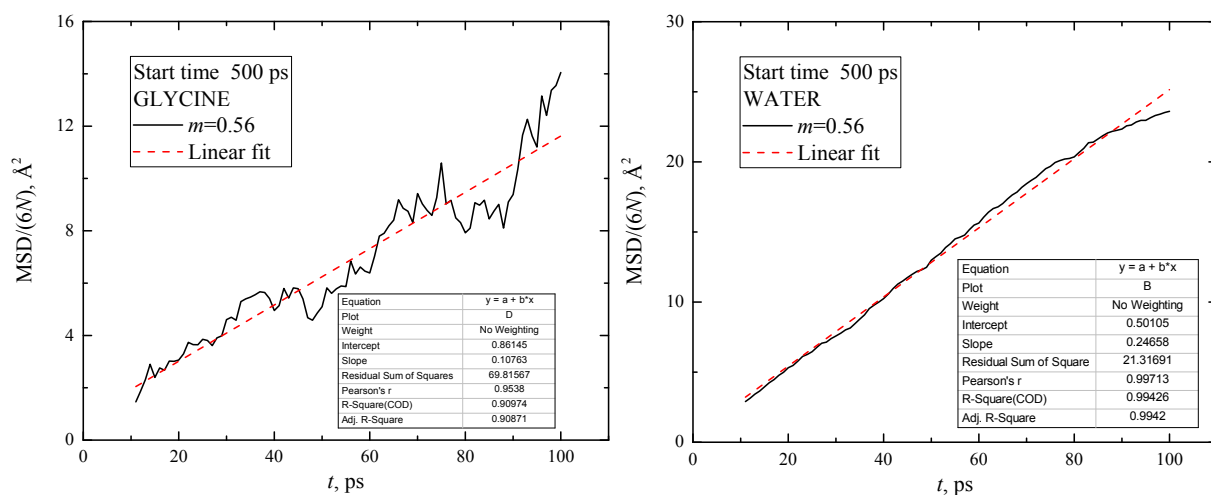
**Table S1. Duration of Simulations, ns**

T=300 K, Charge set	Number of glycine molecules in solution		
	N=12	N=36	N=72
CNDO	3.8	3.5	4.5
B3LYP	3.0	3.1	3.8
mB3LYP	3.4	3.0	3.4

Duration, ns (mB3LYP, N=72)		
Electric field	T=300 K	T=350 K
E=0 V/m	3.4	3.3
E=10 <sup>3</sup> V/m	4.0	3.3
E=10 <sup>4</sup> V/m	4.3	5.3

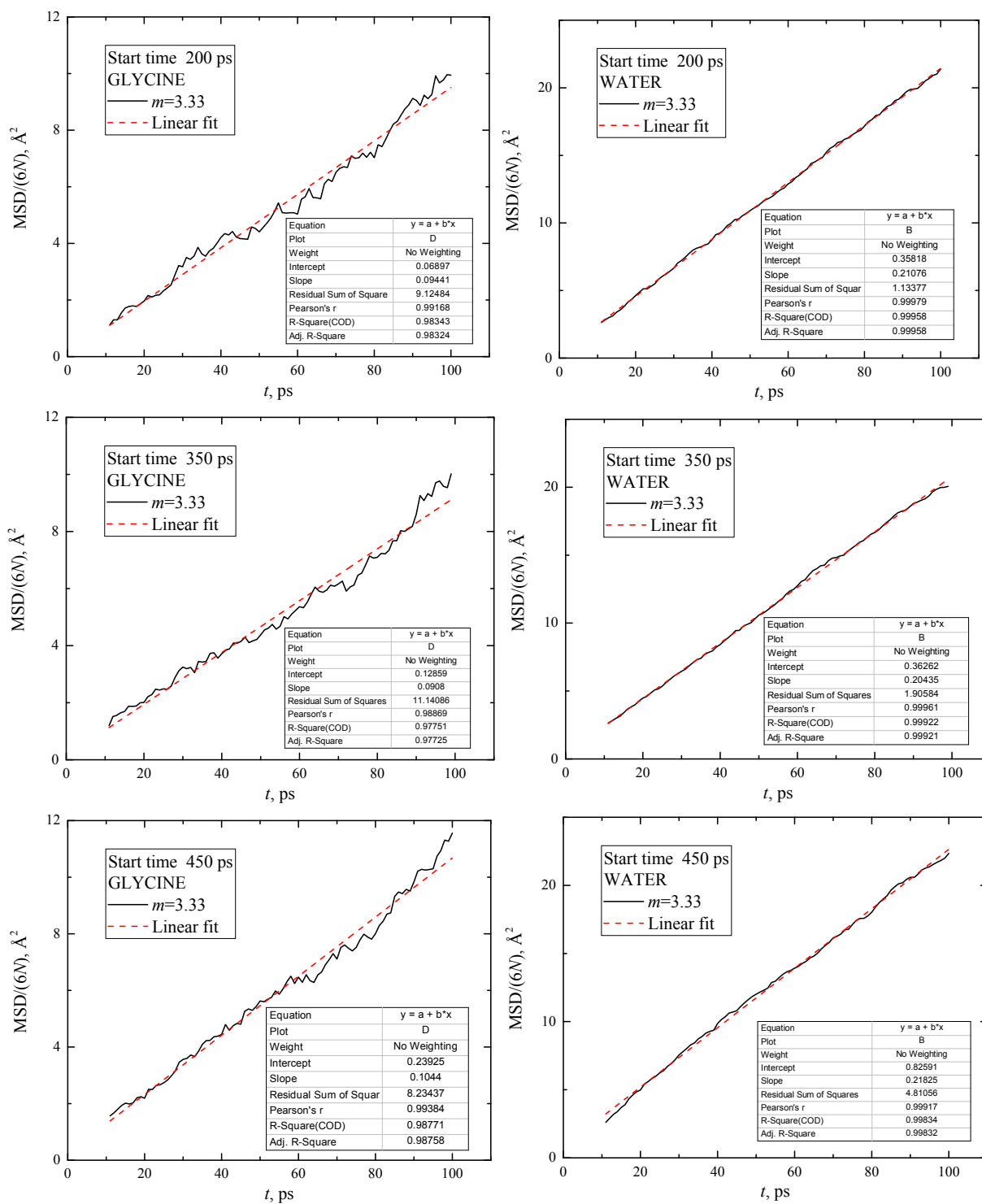
## Calculation of Diffusion Coefficients





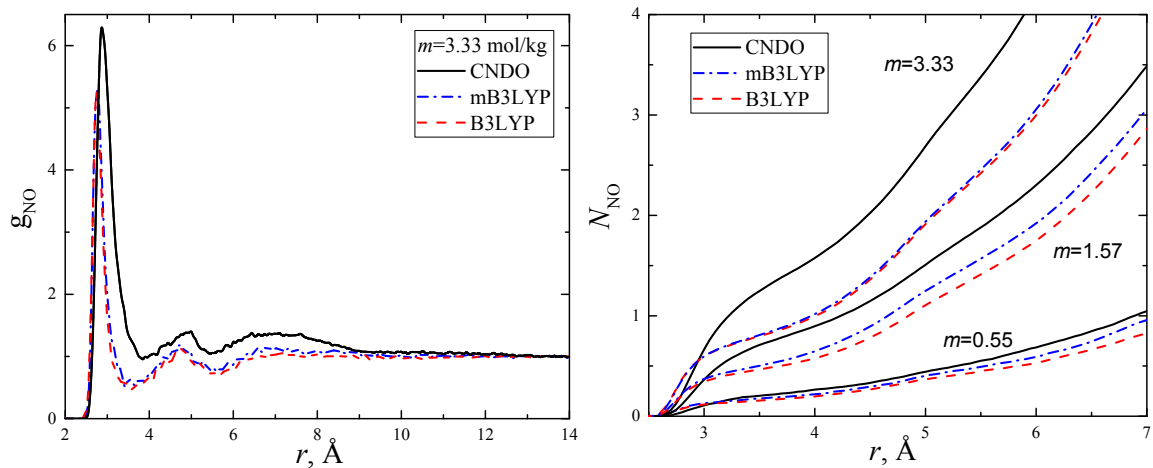
Mean	Standard Deviation	SE of mean	Lower 95% CI of Mean	Upper 95% CI of Mean
1.1865	0.12408	0.06204	0.98907	1.38393
2.5135	0.07636	0.03818	2.392	2.635

**Fig. S2.** Mean square displacement of glycine and water molecules during 100 ps time intervals on 0.5 ns trajectory due to diffusion at  $m=0.56$  mol/kg

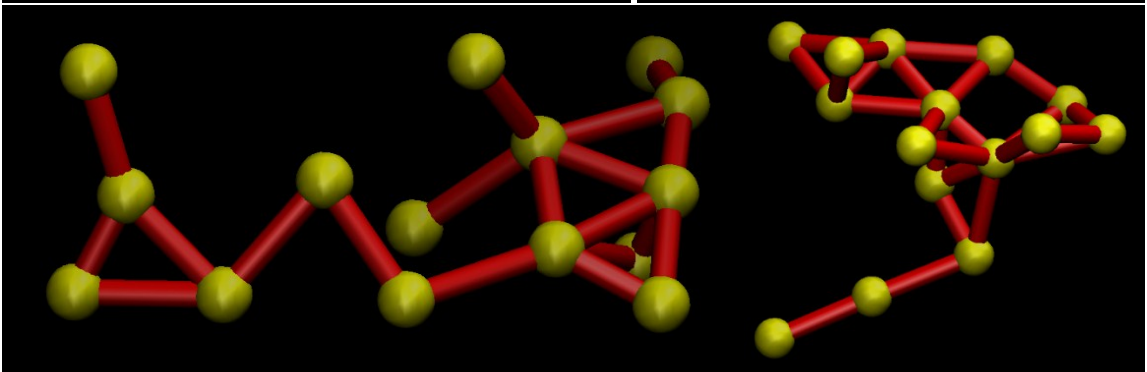
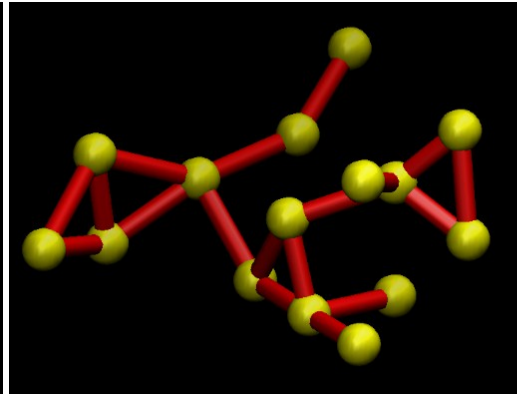
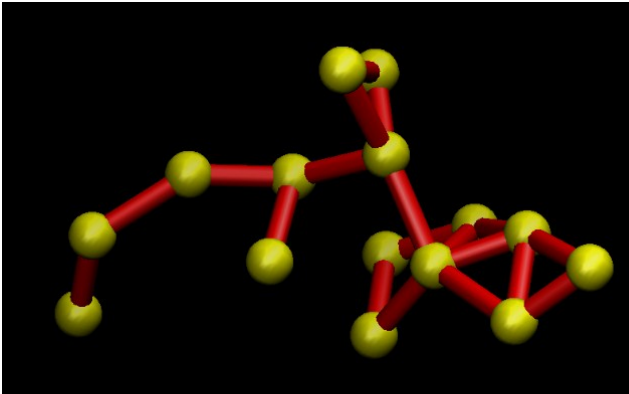
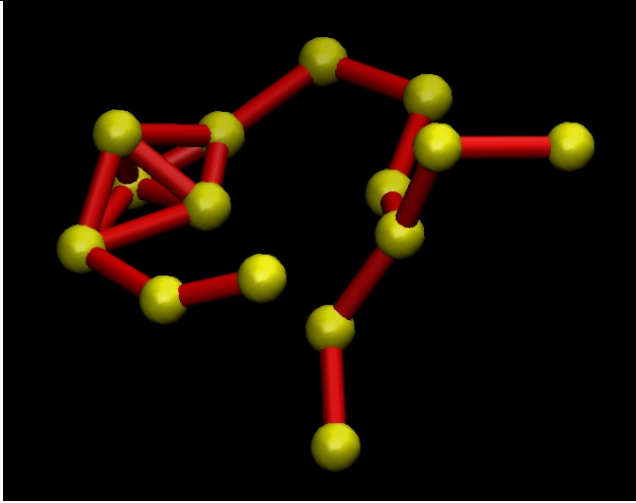
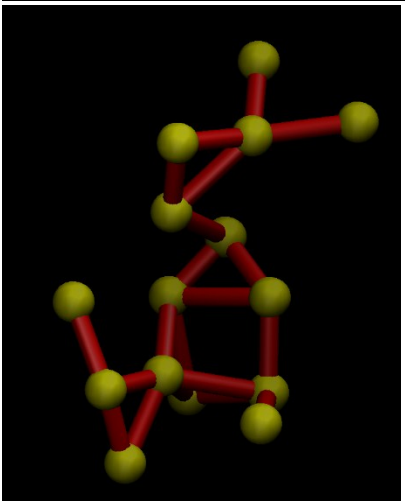
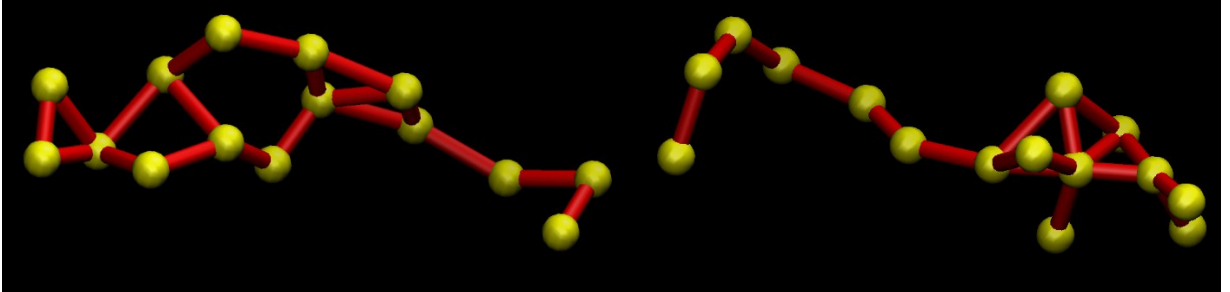
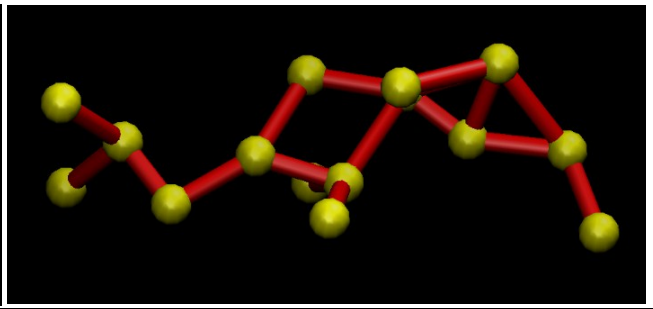
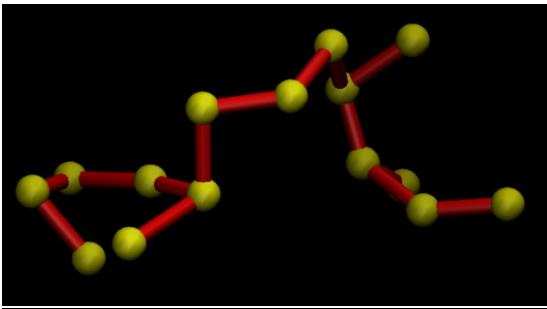


Mean	Standard Deviation	SE of mean	Lower 95% CI of Mean	Upper 95% CI of Mean
0.96533	0.07047	0.04068	0.79029	1.14038
2.11167	0.06957	0.04017	1.93884	2.28449

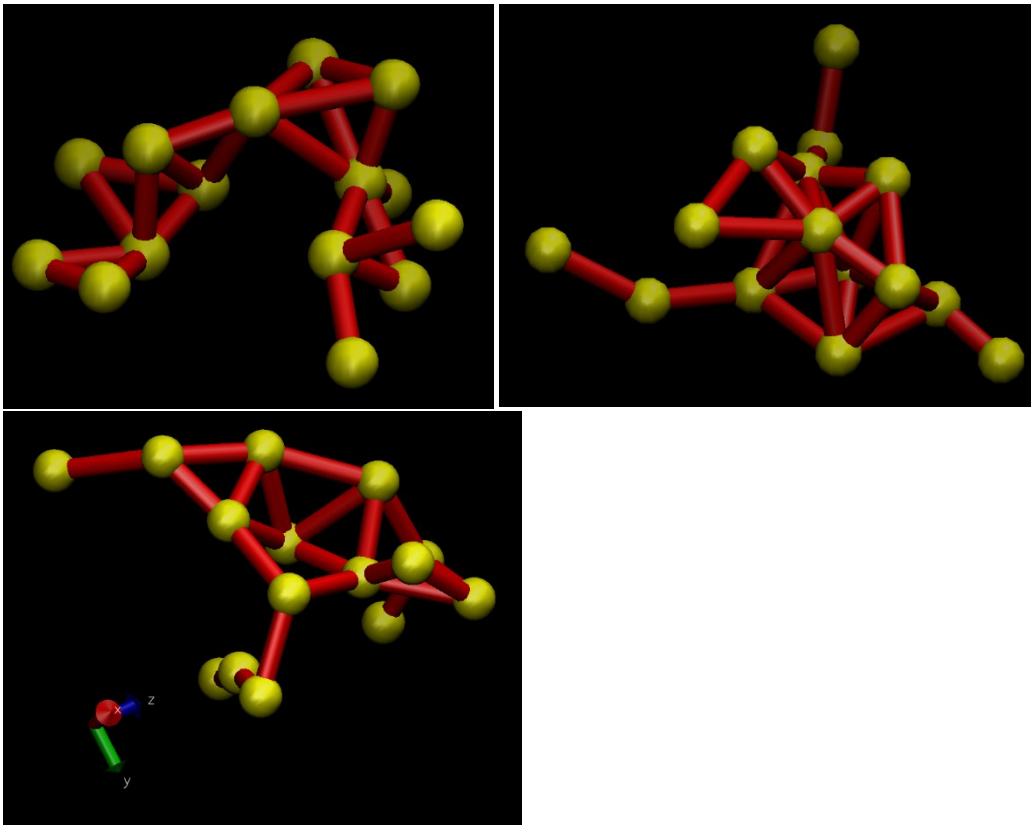
**Fig. S3.** Mean square displacement of glycine and water molecules during 100 ps time intervals due to diffusion at  $m=3.33$  mol/kg



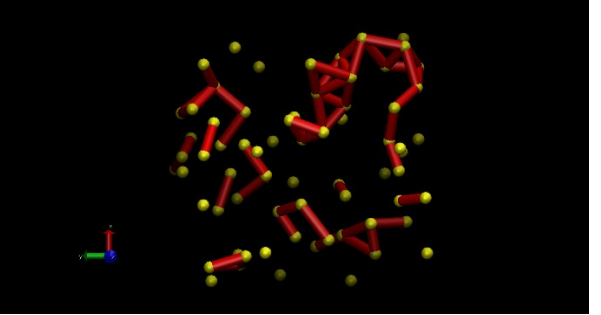
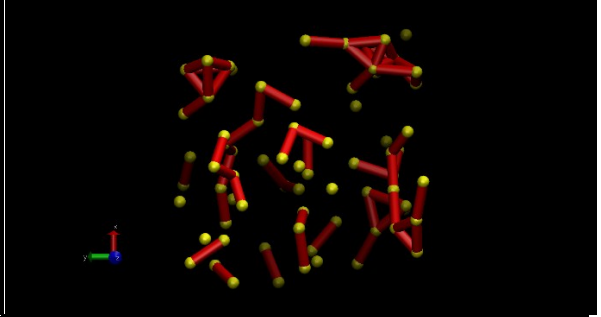
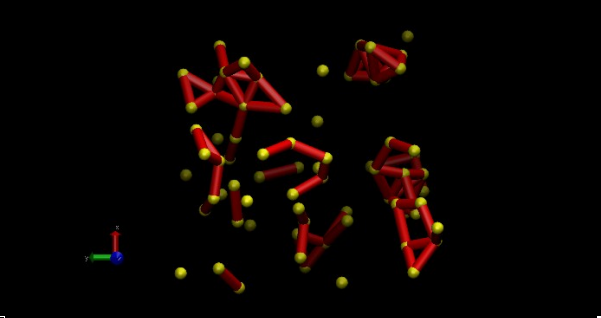
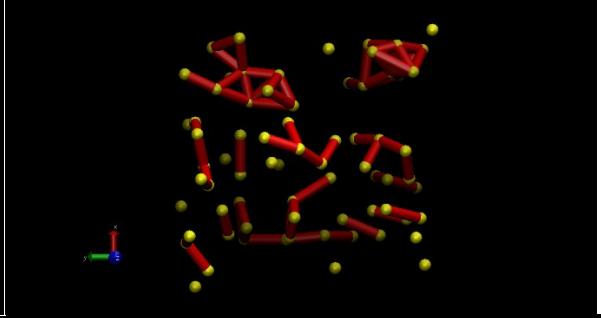
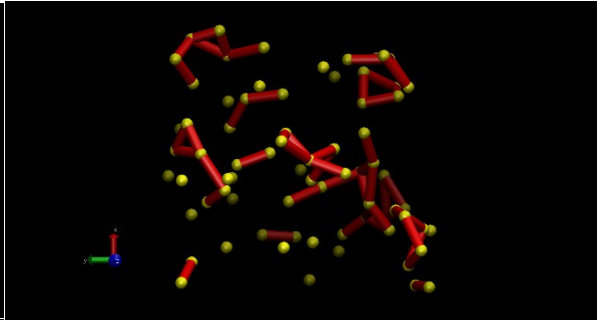
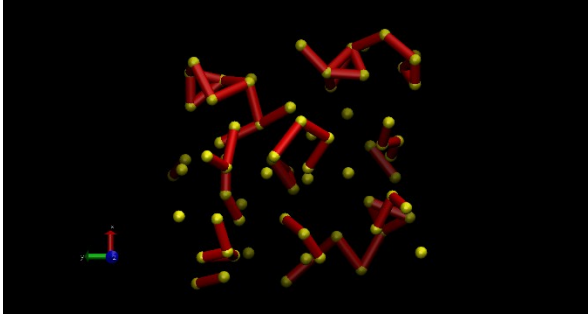
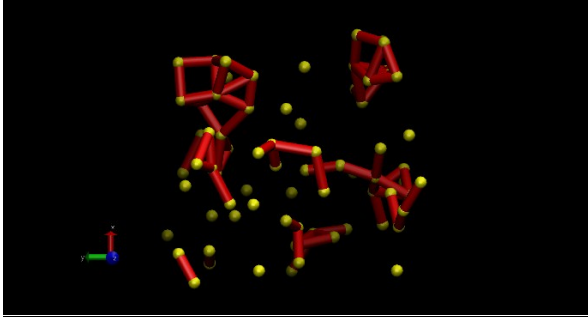
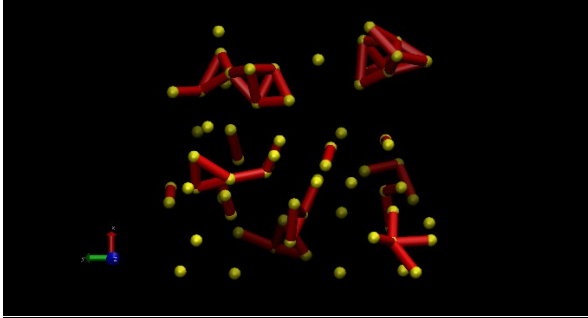
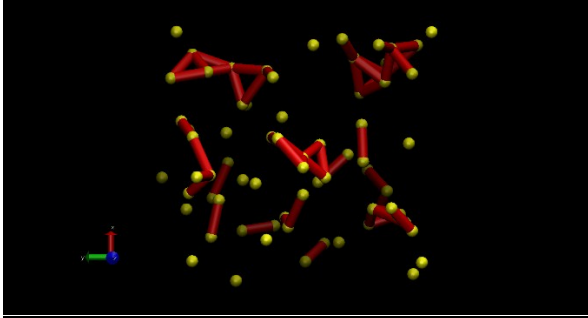
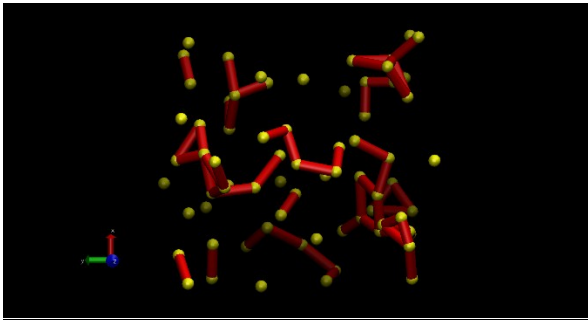
**Fig. S4** Radial distribution functions,  $g_{\text{NO}}(r)$ , and running coordination numbers,  $N_{\text{NO}}(r)$ , for nitrogens and oxygens of glycine in aqueous solutions with various solute concentrations,  $m$ .

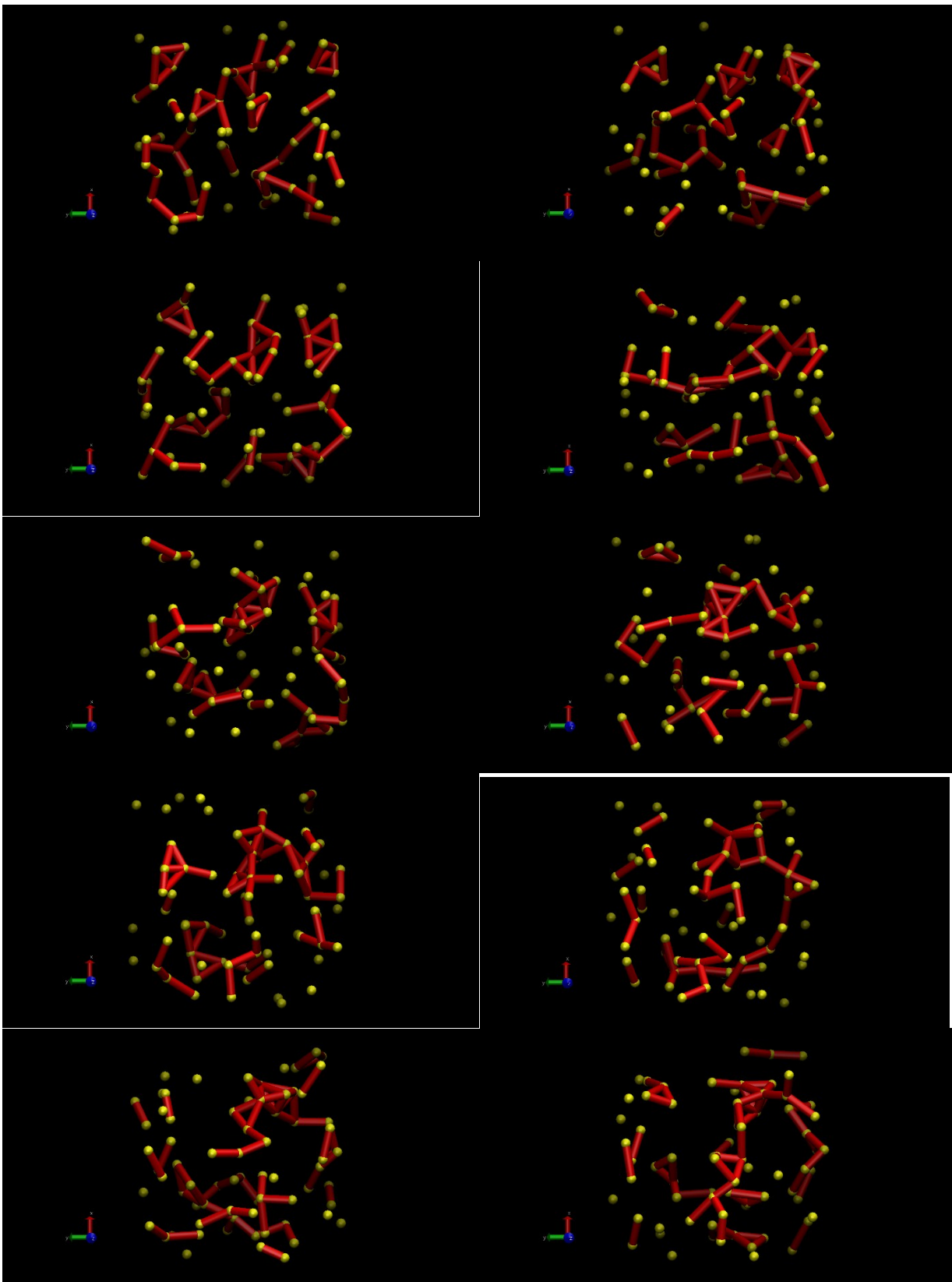




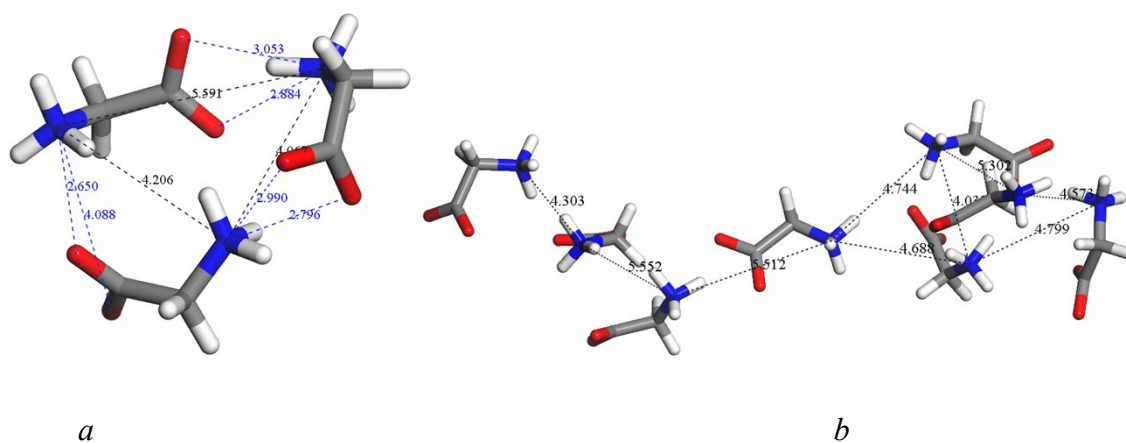


**Fig. S5.** Glycine clusters consisting from 15 glycine molecules, nitrogen atoms are presented by yellow balls. Sticks connect the nearest nitrogens.

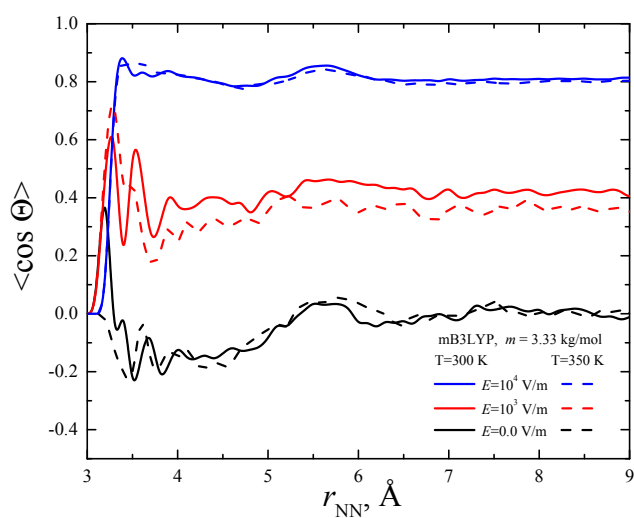




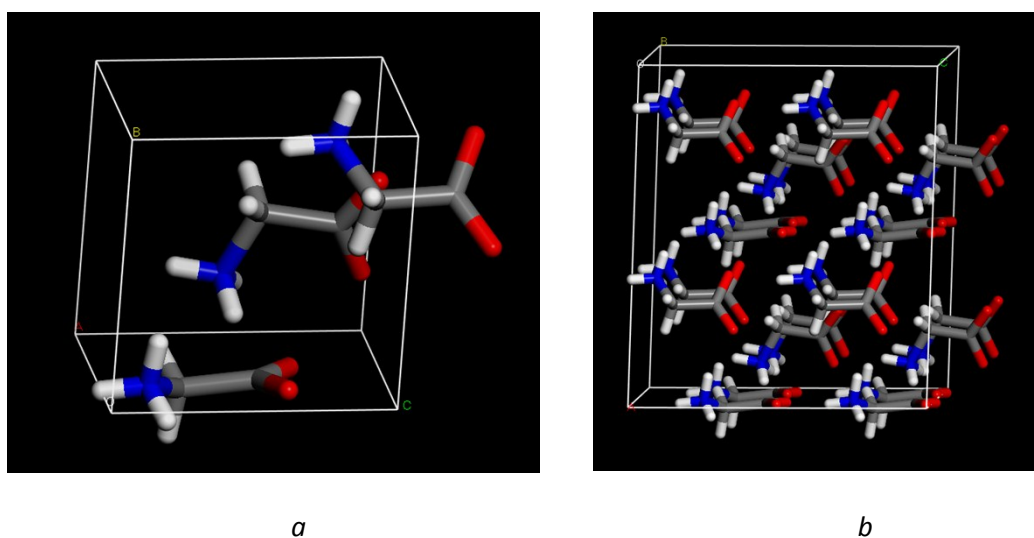
**Fig. S6.** Snapshots of the simulation box at  $m=3.33$  mol/kg. Nitrogen atoms are presented by yellow balls. Sticks connect the nearest nitrogens. Water molecules are not shown for clarity. Time interval between snapshots is equal to 10 ps.



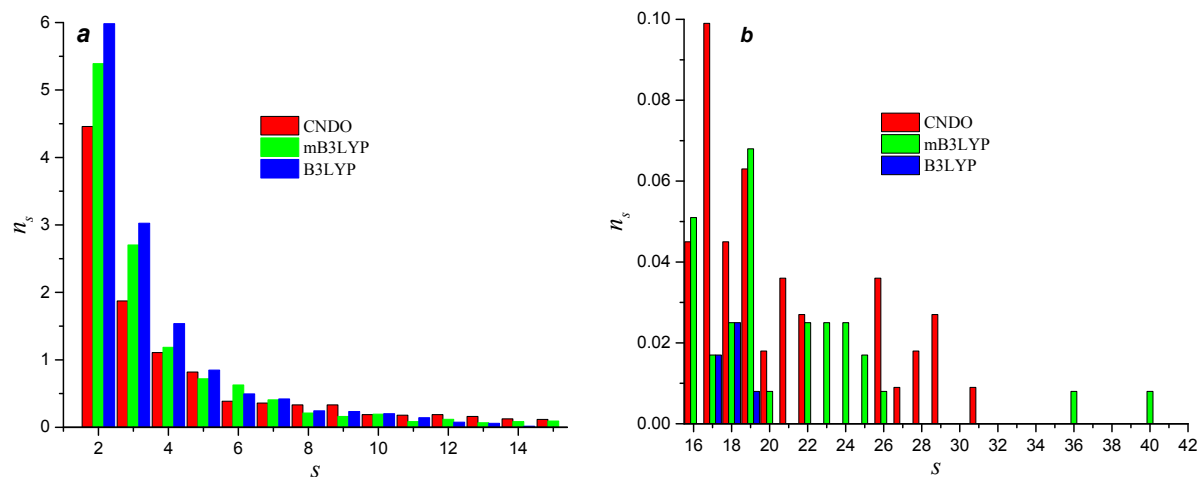
**Fig. S7.** Small glycine clusters in aqueous solution at  $m=3.33$  mol/kg



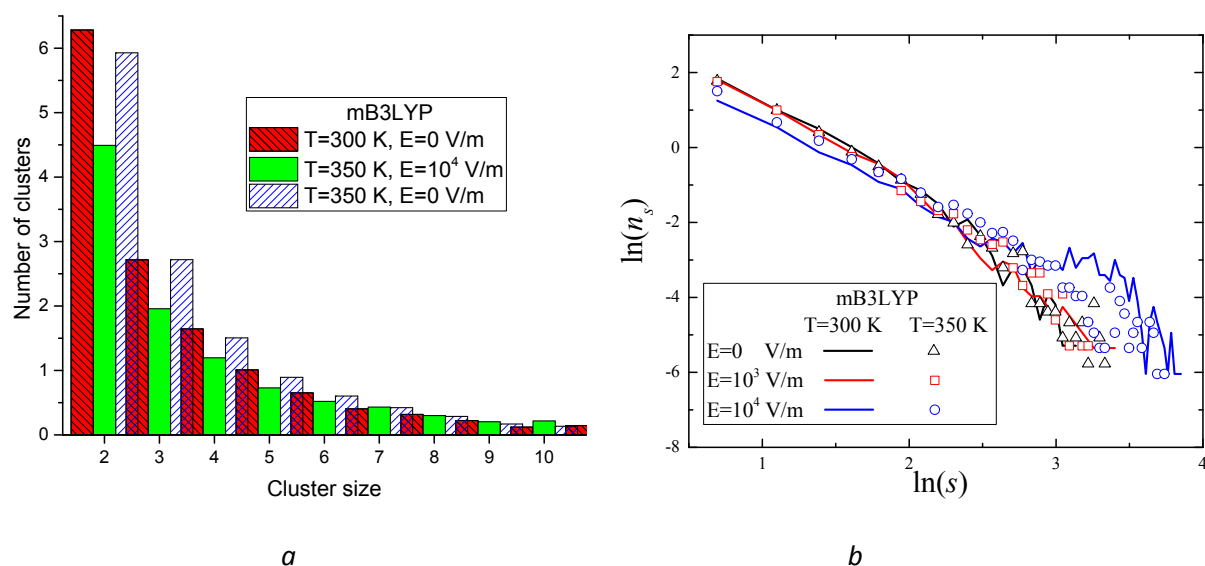
**Fig. S8.** Average cosine of the angle between vectors connecting carbon atoms ( $\text{H}_2\text{C} \rightarrow \text{CO}_2$ ) in two glycine molecules calculated without and with dc electric field ( $E=10^3$  and  $10^4$  V/m) applied to solution at  $m=3.33$  mol/kg ( $T=300$  K and  $350$  K)



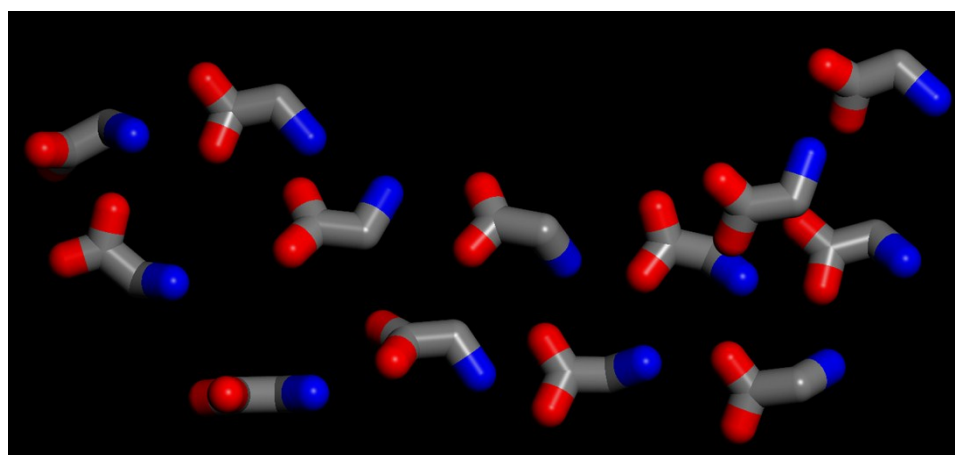
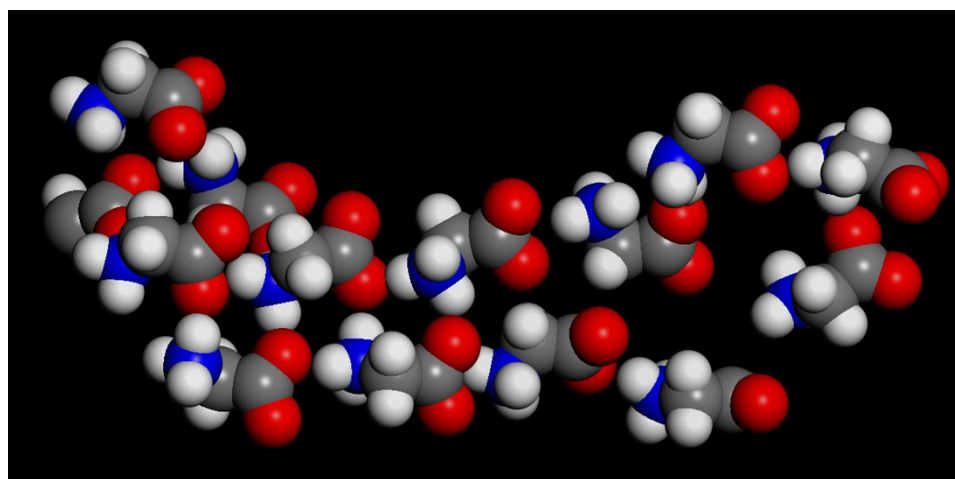
**Fig. S9.** (a) Crystallographic unit cell of  $\gamma$ -glycine, (b)  $2 \times 2 \times 2$  unit cells.



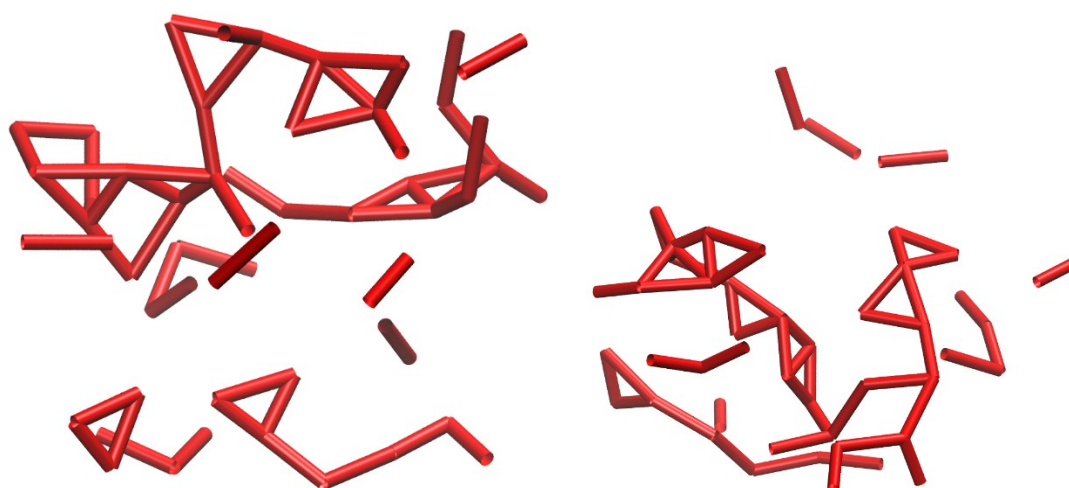
**Fig. S10.** Number of glycine clusters,  $n_s$ , in the saturated aqueous solution as a function of cluster size,  $s$ : (a) for small clusters, (b) for other clusters.



**Fig. S11.** Number of glycine clusters,  $n_s$ , in the saturated aqueous solution as a function of cluster size,  $s$ : (a) for small clusters, (b) for all clusters. The mB3LYP force field is used. Data calculated at 300 K and 350 K for solutions in the electric field and without the electric field are presented.

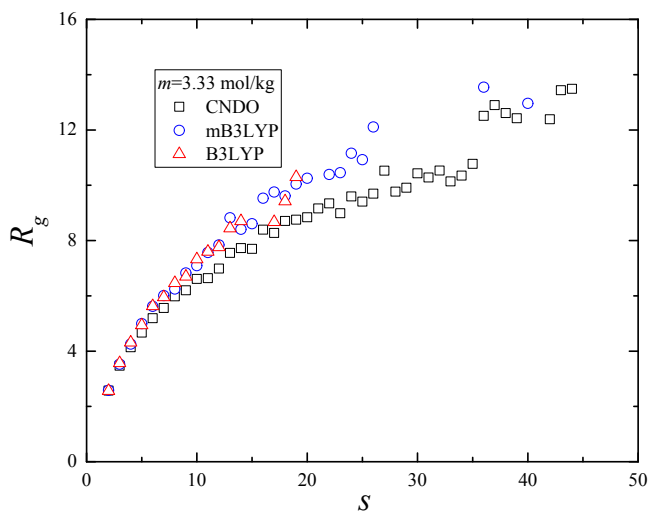


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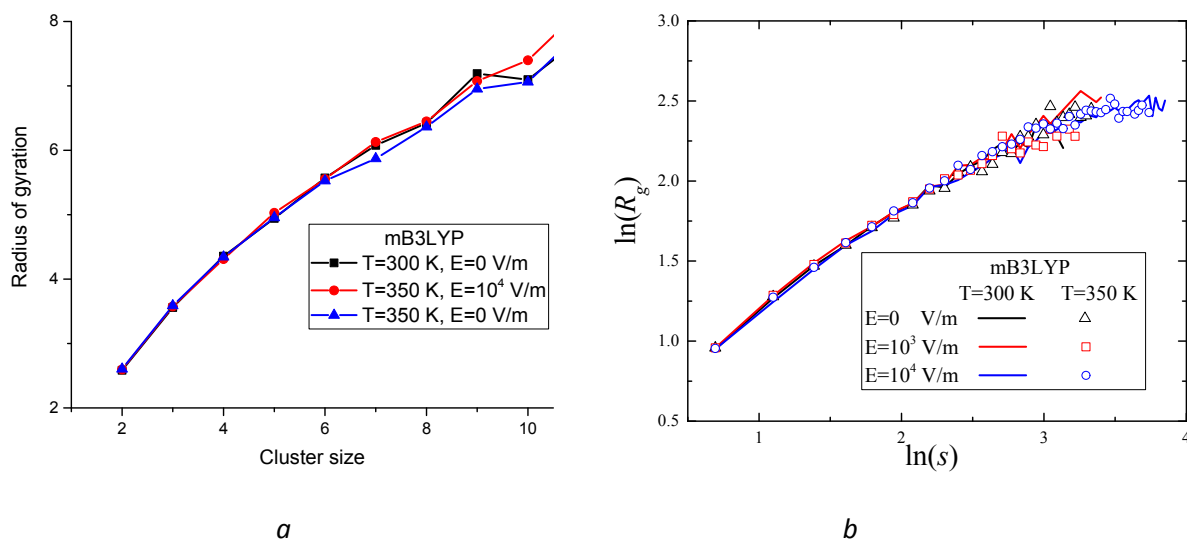


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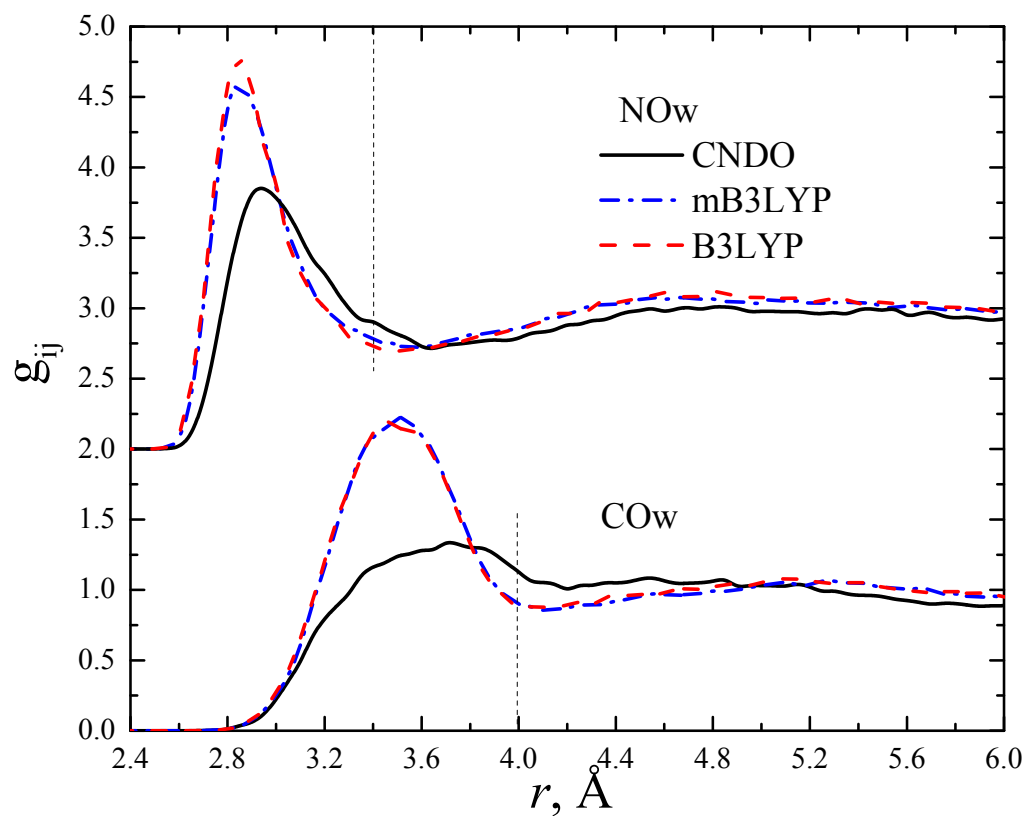
**Fig. S12.** Glycine clusters observed in aqueous solutions at  $m=3.33$  mol/kg and  $E=10^4$  V/m. (a) stripe-like clusters; (b) chain-like and stripe-like clusters, sticks connect the nearest nitrogens ( $r_{NN} < 6 \text{ \AA}$ ), water molecules and monomers are not shown for clarity.



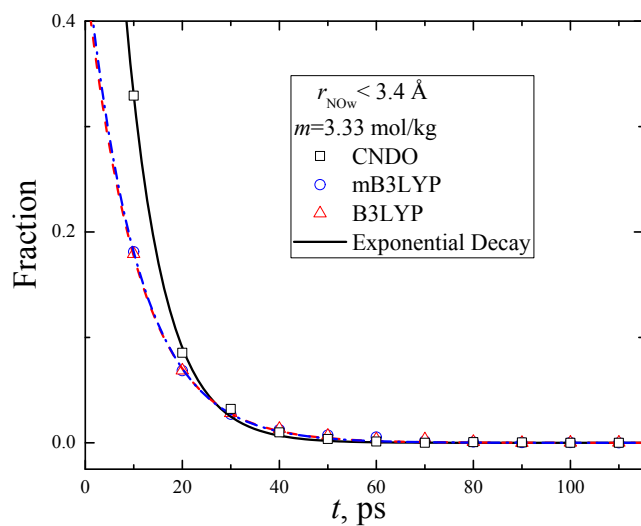
**Fig. S13.** Radius of gyration,  $R_g$ , of glycine clusters in the saturated aqueous solution as a function of cluster size,  $s$ .



**Fig. S14.** Radius of gyration,  $R_g$ , of glycine clusters in the saturated aqueous solution as a function of cluster size,  $s$ : (a) for small clusters, (b) for all clusters. The mB3LYP force field is used. Data calculated at 300 K and 350 K for solutions in the electric field and without the electric field are presented.

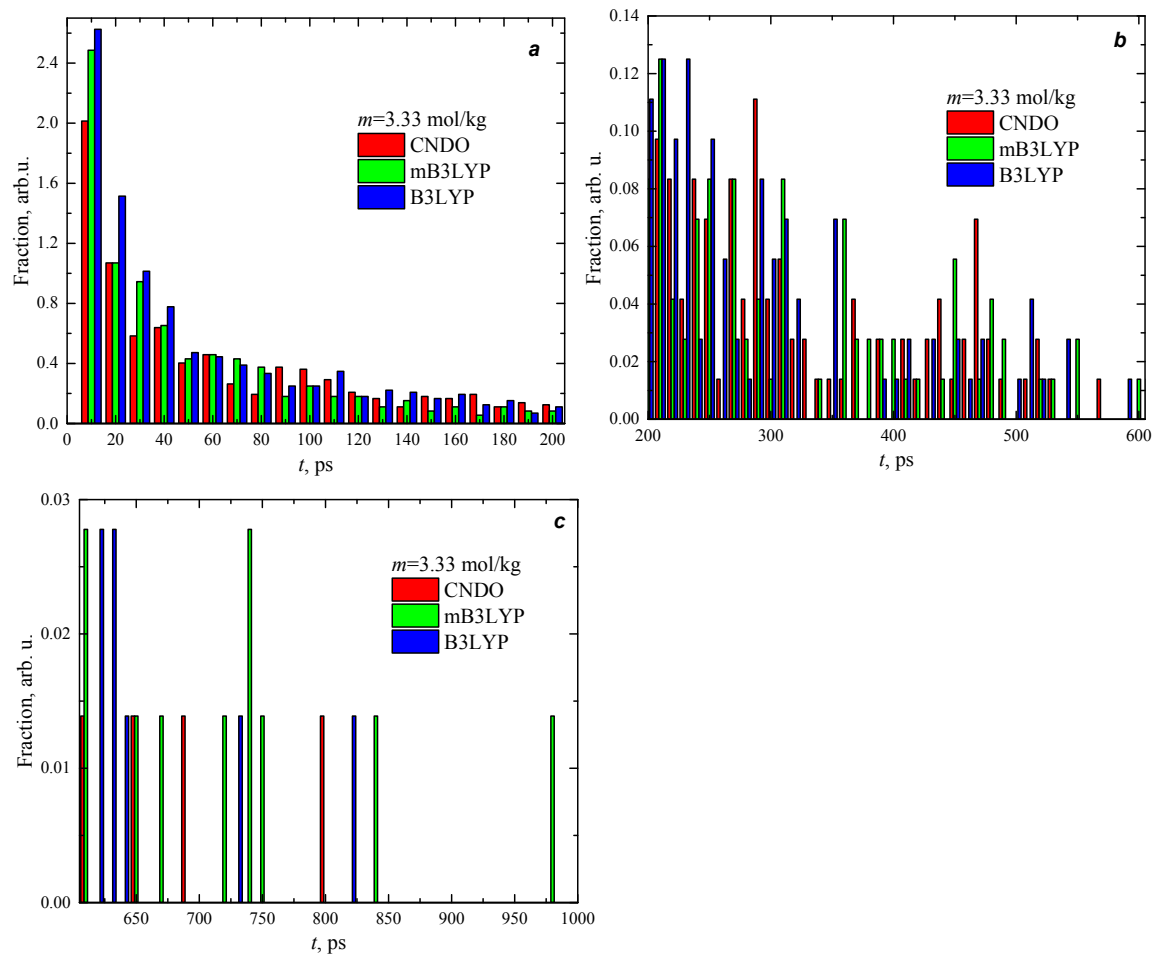


**Fig. S15.** Radial distribution functions,  $g(r)$ , of water oxygens with respect to nitrogens (NOW) and carbons of  $-\text{COO}$  groups (COW).



**Fig. S16.** Fractions of water molecules from the first hydration shells of  $-\text{NH}_3$  groups vs. lifetimes





**Fig. S17.** Fractions of glycine molecules vs. lifetimes.