

Supporting information for

**Correlating solvation with conformational pathways of proteins
in alcohol-water mixtures: A THz spectroscopic insight**

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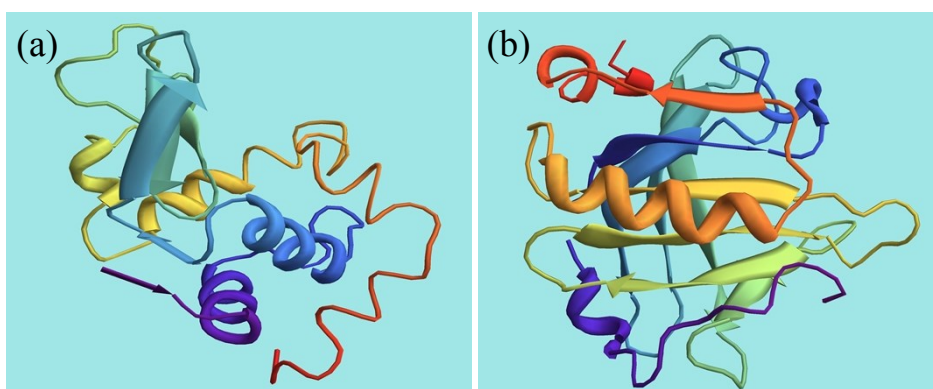
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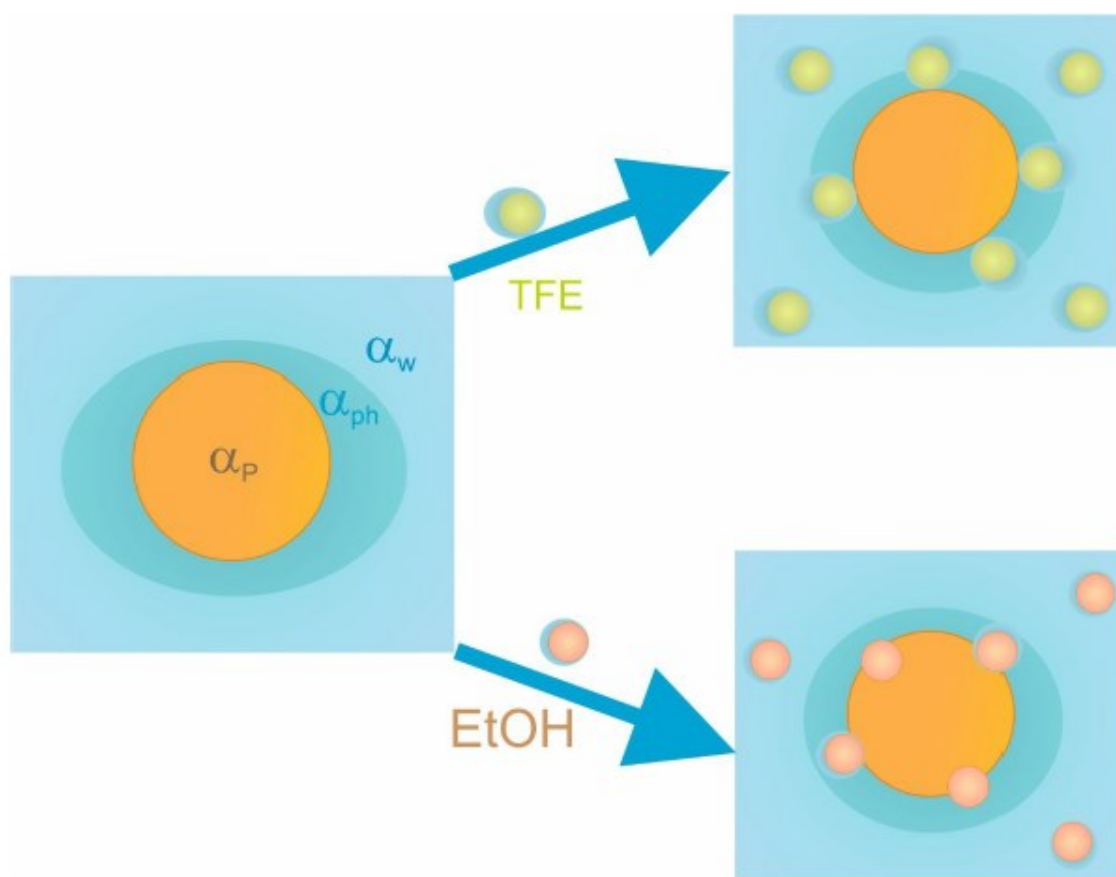
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Scheme S1. Crystalline structure of (a) lysozyme (1lyz)¹, (b) β -lg (3np0)² as obtained from protein data bank. [pdb files are viewed and modified in *Mathematica* 9]



Scheme S2. Schematic representation of the approached model for protein hydration in water and in presence of alcohols. The yellow sphere represents a protein which is assumed to be a void cavity in a dielectric. The dark shaded regions (α_{ph}) denote the protein hydration. This model is valid only for low concentration of alcohol.

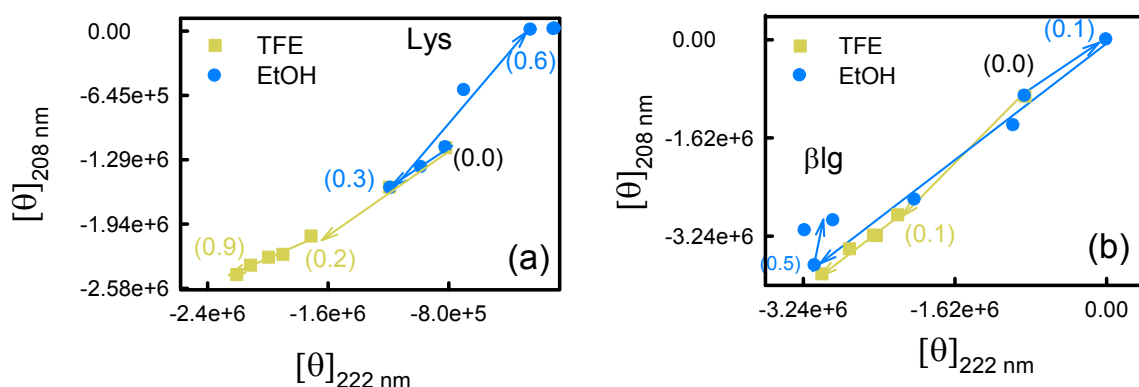


Figure S1. Phase diagram obtained from molar ellipticity ($[\theta]$) measured at 222 nm vs. 208 nm of (a) Lys and (b) β lg at different mole fractions of ethanol (blue symbols) and TFE (yellow symbols). Some representative mole fractions are shown within parenthesis. The arrows indicate increasing alcohol mole fraction. Molar ellipticity is expressed in $\text{deg cm}^2 \text{dmol}^{-1}$ unit.

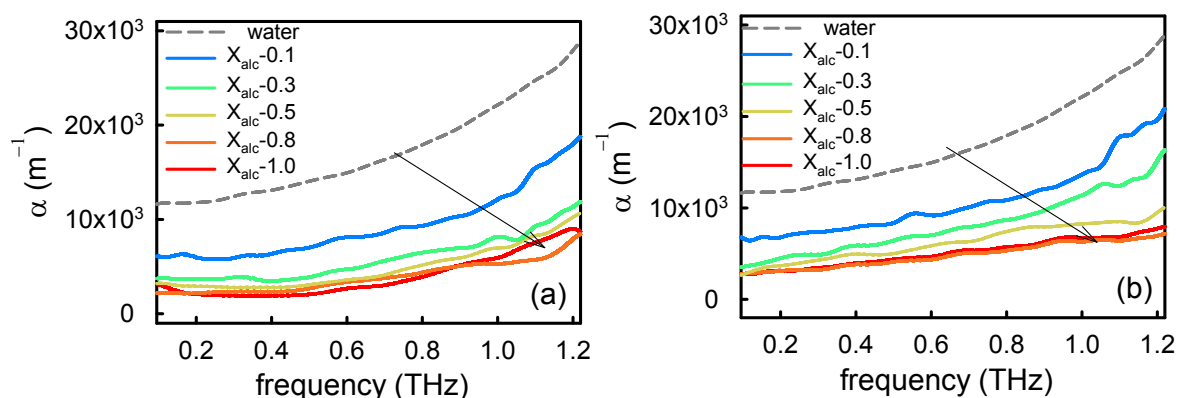


Figure S2. Absorption coefficient of water/alcohol binary mixture as a function of frequency for (a) ethanol (b) TFE.

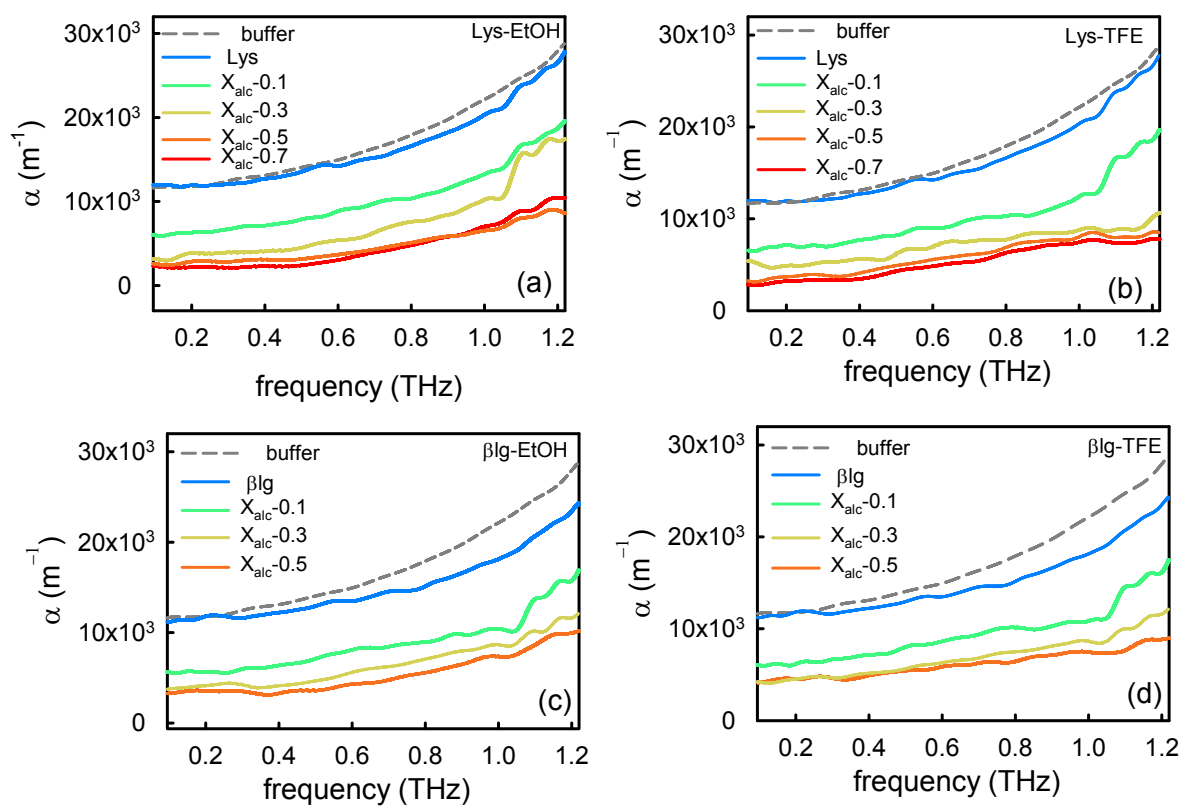


Figure S3. Some representative profile of the absorption coefficient as a function of frequency for Lysozyme in (a) ethanol/ water mixture, (b) TFE/ water mixture and β -lg in (c) ethanol/water mixture, (d) TFE/ water mixture.

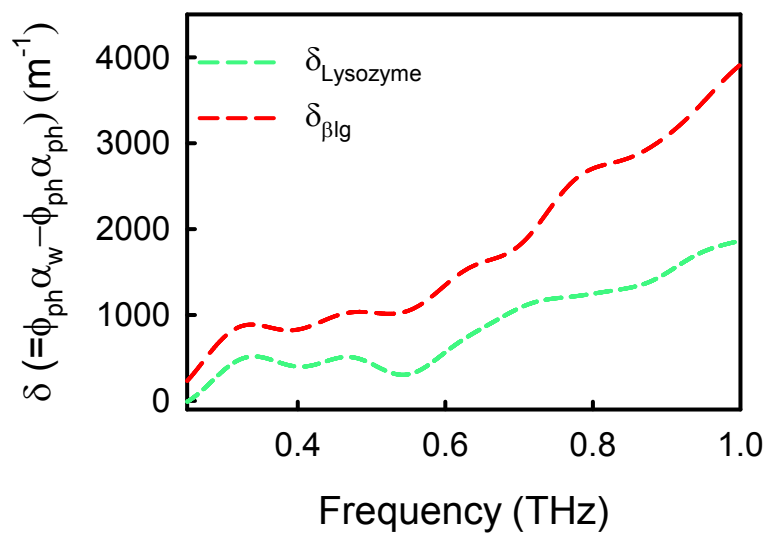


Figure S4. Change in the THz absorption, $\delta (= \phi_{ph}\alpha_w - \phi_{ph}\alpha_{ph})$ of two proteins due to the conversion of bulk water to protein hydration water.

Table S1. Secondary Structure of proteins in alcohols

X _{alcohol}	α -helix (%)	β -antiparallel (%)	β -parallel (%)	β -turn (%)	β -struct. (%)	Random Coil (%)
Lysozyme-ethanol						
0.0	27.19	15.82	8.68	17.74	42.24	30.57
0.1	29.48	14.63	8.41	18.00	41.04	29.48
0.3	32.89	12.77	8.07	18.18	39.02	28.09
0.4	20.23	19.02	9.67	16.56	45.25	34.52
0.45	14.20	25.46	10.11	15.35	50.92	34.88
0.6	12.99	28.98	9.78	15.31	54.07	32.94
0.8	12.23	30.78	9.75	15.14	55.67	32.10
Lysozyme-TFE						
0.1	33.68	12.46	7.93	18.23	38.62	27.70
0.3	48.68	5.41	6.29	17.44	29.14	22.18
0.4	53.76	3.88	5.65	16.74	26.27	19.97
0.6	55.86	3.09	5.41	16.22	24.72	19.42
0.7	59.58	2.19	5.04	15.44	22.67	17.75
β lg-ethanol						
0	20.58	19.96	9.41	16.80	46.17	33.25
0.1	21.26	23.75	8.63	17.44	49.82	28.92
0.15	30.53	15.86	8.03	18.37	42.26	27.21
0.2	45.31	7.26	6.60	18.04	31.90	22.79
0.3	60.29	2.78	4.78	16.13	23.69	16.02
0.4	66.74	1.53	3.93	14.50	19.96	13.30
0.5	70.57	0.97	3.44	13.53	17.94	11.49
0.6	69.26	0.96	3.63	13.45	18.04	12.70
0.9	67.85	0.51	3.97	11.90	16.38	15.77
β lg-TFE						
0.1	51.87	5.03	5.81	17.43	28.27	19.66
0.2	58.25	3.48	5.05	16.61	25.14	16.61
0.3	59.51	3.13	4.92	16.33	24.38	16.11
0.5	64.86	1.99	4.20	15.25	21.44	13.70
0.8	71.47	1.08	3.24	13.73	18.05	10.48

References:

1. R. Diamond, *J. Mol. Biol.*, 1974, **82**, 371-391
2. J. Locha, A. Politb, A. Gońreckib, P. Bonarekb, K. Kurpiewskaa, M. Dziedzicka-Wasylewskab and K. Lewin'skia, *J. Mol. Recognit.*, 2011, **24**, 341-349.