Data archive for:

Stabilization of non-native folds and programmable protein gelation in compositionally designed deep eutectic solvents

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Spectroscopic and scattering data from lysozyme (BSA) and bovine serum albumin (BSA) in the binary deep eutectic solvents 1:2 choline chloride:glycerol (1:2 ChCl:Glyc), 1:2 choline acetate:glycerol (1:2 ChAcO:Glyc), 1:2 choline chloride:acetic acid (1:2 ChCl:AcOH), and 1:2 choline chloride:urea (1:2 ChCl:Urea). Also, data for the characterization of the proteins in 10 mM, pH 7 phosphate buffer is included.

- UV-vis spectroscopy: The contribution from the solvent absorbance has been subtracted to each file.

Protein	Solvent	File
Lyz	1:2 ChCl:Glyc	UVv_Lyz_ChClG_sub.txt
Lyz	1:2 ChAcO:Glyc	UVv_Lyz_ChAcOG_sub.txt
Lyz	1:2 ChCl:AcOH	UVv_Lyz_ChClAcOH_sub.txt
Lyz	1:2 ChCl:Urea	UVv_Lyz_ChClU_sub.txt
Lyz	Phosphate buffer	UVv_Lyz_AqBuffer_sub.txt
BSA	1:2 ChCl:Glyc	UVv_BSA_ChClG_sub.txt
BSA	1:2 ChAcO:Glyc	UVv_BSA_ChAcOG_sub.txt
BSA	1:2 ChCl:AcOH	UVv_BSA_ChClAcOH_sub.txt
BSA	1:2 ChCl:Urea	UVv_BSA_ChClU_sub.txt
BSA	Phosphate buffer	UVv_BSA_AqBuffer_sub.txt

- Steady-state emission fluorescence: The signal from the solvent has been subtracted to each file. Proteins in 1:2 ChAcO:Glyc could not be characterized due to the strong absorbance of the solvent in the emission window of the protein.

Protein	Solvent	File
Lyz	1:2 ChCl:Glyc	Fluo295_Lyz_ChClG_sub.txt
Lyz	1:2 ChAcO:Glyc	Fluo295_Lyz_ChAcOG_sub.txt
Lyz	1:2 ChCl:Urea	Fluo295_Lyz_ChClU_sub.txt
Lyz	Phosphate buffer	Fluo295_Lyz_AqBuffer_sub.txt
BSA	1:2 ChCl:Glyc	Fluo295_BSA_ChClG_sub.txt
BSA	1:2 ChCl:AcOH	Fluo295_BSA_ChClAcOH_sub.txt
BSA	1:2 ChCl:Urea	Fluo295_BSA_ChClU_sub.txt
BSA	Phosphate buffer	Fluo295_BSA_AqBuffer_sub.txt

- Far-UV circular dichroism: The signal from the solvent has been subtracted to each file.

Protein	Solvent	File
Lyz	1:2 ChCl:Glyc	CD_Lyz_ChClG_sub.txt
Lyz	1:2 ChAcO:Glyc	CD_Lyz_ChAcOG_sub.txt
Lyz	1:2 ChCl:AcOH	CD_Lyz_ChClAcOH_sub.txt
Lyz	1:2 ChCl:Urea	CD_Lyz_ChClU_sub.txt
Lyz	Phosphate buffer	CD_Lyz_AqBuffer_sub.txt
BSA	1:2 ChCl:Glyc	CD_BSA_ChClG_sub.txt
BSA	1:2 ChAcO:Glyc	CD_BSA_ChAcOG_sub.txt
BSA	1:2 ChCl:AcOH	CD_BSA_ChClAcOH_sub.txt
BSA	1:2 ChCl:Urea	CD_BSA_ChClU_sub.txt
BSA	Phosphate buffer	CD_BSA_AqBuffer_sub.txt

- Small-angle neutron scattering: The contribution from the solvent scattering has been subtracted to each file. Please not that deuterated solvents were used in these experiments.

Protein	Solvent	File
Lyz	1:2 d_9-ChCl: d_8-Glyc	SANS_Lyz_ChClG_sub.dat
Lyz	1:2 d_{12}-ChAcO:d_8-Glyc	SANS_Lyz_ChAcOG_sub.dat
Lyz	1:2 d_9-ChCl:d_4-AcOH	SANS_Lyz_ChClAcOH_sub.dat
Lyz	1:2 d_9-ChCl:d_4-Urea	SANS_Lyz_ChClU_sub.dat
Lyz	Phosphate buffer	SANS_Lyz_AqBuffer_sub.dat
BSA	1:2 d_9-ChCl: d_8-Glyc	SANS_BSA_ChClG_sub.dat
BSA	1:2 d_{12}-ChAcO:d_8-Glyc	SANS_BSA_ChAcOG_sub.dat
BSA	1:2 d_9-ChCl:d_4-AcOH	SANS_BSA_ChClAcOH_sub.dat
BSA	1:2 d_9-ChCl:d_4-Urea	SANS_BSA_ChClU_sub.dat
BSA	Phosphate buffer	SANS_BSA_AqBuffer_sub.dat

- Excited-state emission fluorescence: The instrument response function (IRF) has been measured using a Ludox particle solution.

Protein	Solvent	File
Lyz	1:2 ChCl:Glyc	TCSPC_Lyz_ChClG.txt
Lyz	1:2 ChCl:AcOH	TCSPC_Lyz_ChClAcOH.txt
Lyz	Phosphate buffer	TCSPC_Lyz_AqBuffer.txt
IRF	Water	TCSPC_IRF.txt

Spectroscopic, scattering, and rheological data from lysozyme (BSA) in the ternary deep eutectic solvents 1:x:2-x choline chloride:glycerol (1:x:2-x ChCl:Glyc:AcOH), where x=1.9, 1.8, 1.75, 1.7, 1.65, 1.6, 1.5, 1.0, and 0.5.

- UV-vis spectroscopy: The contribution from the solvent absorbance has been subtracted to each file.

Protein	Solvent	File
Lyz	1:1.9:0.1 ChCl:Glyc:AcOH	UVv_Lyz_C1G19A01_sub.txt
Lyz	1:1.8:0.2 ChCl:Glyc:AcOH	UVv_Lyz_C1G18A02_sub.txt
Lyz	1:1.75:0.25 ChCl:Glyc:AcOH	UVv_Lyz_C1G175A025_sub.txt
Lyz	1:1.7:0.3 ChCl:Glyc:AcOH	UVv_Lyz_C1G17A03_sub.txt
Lyz	1:1.65:0.35 ChCl:Glyc:AcOH	UVv_Lyz_C1G165A035_sub.txt
Lyz	1:1.6:0.4 ChCl:Glyc:AcOH	UVv_Lyz_C1G16A04_sub.txt
Lyz	1:1.5:0.5 ChCl:Glyc:AcOH	UVv_Lyz_C1G15A05_sub.txt
Lyz	1:1:1 ChCl:Glyc:AcOH	UVv_Lyz_C1G1A1_sub.txt
Lyz	1:0.5:1.5 ChCl:Glyc:AcOH	UVv_Lyz_C1G05A15_sub.txt

- Far-UV circular dichroism: The contribution from the solvent absorbance has been subtracted to each file. The refolded sample by tuning the composition of the solvent from 1:1.5:0.5 ChCl:Glyc:AcOH to 1:1.8:0.2 ChCl:Glyc:AcOH has been labelled as CD_Lyz_CGAref_sub.txt and the inverse process as CD_Lyz_CGAunf_sub.txt.

Protein	Solvent	File
Lyz	1:1.9:0.1 ChCl:Glyc:AcOH	CD_Lyz_C1G19A01_sub.txt
Lyz	1:1.8:0.2 ChCl:Glyc:AcOH	CD_Lyz_C1G18A02_sub.txt
Lyz	1:1.75:0.25 ChCl:Glyc:AcOH	CD_Lyz_C1G175A025_sub.txt
Lyz	1:1.7:0.3 ChCl:Glyc:AcOH	CD_Lyz_C1G17A03_sub.txt
Lyz	1:1.65:0.35 ChCl:Glyc:AcOH	CD_Lyz_C1G165A035_sub.txt
Lyz	1:1.6:0.4 ChCl:Glyc:AcOH	CD_Lyz_C1G16A04_sub.txt
Lyz	1:1.5:0.5 ChCl:Glyc:AcOH	CD_Lyz_C1G15A05_sub.txt
Lyz	1:1:1 ChCl:Glyc:AcOH	CD_Lyz_C1G1A1_sub.txt
Lyz	1:0.5:1.5 ChCl:Glyc:AcOH	CD_Lyz_C1G05A15_sub.txt
Lyz	1:1.8:0.2 ChCl:Glyc:AcOH	CD_Lyz_CGAref_sub.txt
Lyz	1:0.5:1.5 ChCl:Glyc:AcOH	CD_Lyz_CGAunf_sub.txt

- Small-angle neutron scattering: The contribution from the solvent scattering has been subtracted to each file. Please not that deuterated solvents were used in these experiments. The refolded sample by tuning the composition of the solvent from 1:0.5:1.5 d_9-ChCl:d_8-Glyc:d_4-AcOH to 1:1.8:0.2 d_9-ChCl:d_8-Glyc:d_4-AcOH has been labelled as SANS_Lyz_CGGref_sub.txt and the inverse process as SANS_Lyz_CGGunf_sub.txt.

Protein	Solvent	File
Lyz	1:1.9:0.1 d_9-ChCl:d_8-Glyc:d_4-AcOH	SANS_Lyz_C1G19A01_sub.dat
Lyz	1:1.8:0.2 d_9-ChCl:d_8-Glyc:d_4-AcOH	SANS_Lyz_C1G18A02_sub.dat
Lyz	1:1.75:0.25 d_9-ChCl:d_8-Glyc:d_4-AcOH	SANS_Lyz_C1G175A025_sub.dat
Lyz	1:1.7:0.3 d_9-ChCl:d_8-Glyc:d_4-AcOH	SANS_Lyz_C1G17A03_sub.dat
Lyz	1:1.65:0.35 d_9-ChCl:d_8-Glyc:d_4-AcOH	SANS_Lyz_C1G165A035_sub.dat
Lyz	1:1.6:0.4 d_9-ChCl:d_8-Glyc:d_4-AcOH	SANS_Lyz_C1G16A04_sub.dat
Lyz	1:1.5:0.5 d_9-ChCl:d_8-Glyc:d_4-AcOH	SANS_Lyz_C1G15A05_sub.dat
Lyz	1:1:1 d_9-ChCl:d_8-Glyc:d_4-AcOH	SANS_Lyz_C1G1A1_sub.dat
Lyz	1:0.5:1.5 d_9-ChCl:d_8-Glyc:d_4-AcOH	SANS_Lyz_C1G05A15_sub.dat

- Excited-state emission fluorescence: The instrument response function has been measured using a Ludox particle solution.

Protein	Solvent	File
Lyz	1:1.9:0.1 ChCl:Glyc:AcOH	TCSPC_Lyz_C1G19A01_sub.txt
Lyz	1:1.8:0.2 ChCl:Glyc:AcOH	TCSPC_Lyz_C1G18A02_sub.txt
Lyz	1:1.7:0.3 ChCl:Glyc:AcOH	TCSPC_Lyz_C1G17A03_sub.txt
Lyz	1:1.5:0.5 ChCl:Glyc:AcOH	TCSPC_Lyz_C1G15A05_sub.txt
Lyz	1:1:1 ChCl:Glyc:AcOH	TCSPC_Lyz_C1G1A1_sub.txt
Lyz	1:0.5:1.5 ChCl:Glyc:AcOH	TCSPC_Lyz_C1G05A15_sub.txt

- Rheology:

The gelation of the system was checked for Lyz in 1:1:1 ChCl:Glyc:AcOH (labelled as “Gelation”) and the self-healing properties of the gel were characterized for Lyz in 1:0.5:1.5 ChCl:Glyc:AcOH (labelled as “Post1h”)

Protein	Solvent	File
Lyz	1:1:1 ChCl:Glyc:AcOH	Rheo_Lyz_C1G1G1_Gelation.txt
Lyz	1:1.8:0.2 ChCl:Glyc:AcOH	Rheo_Lyz_C1G18A02.txt
Lyz	1:1.7:0.3 ChCl:Glyc:AcOH	Rheo_Lyz_C1G17A03.txt
Lyz	1:1.5:0.5 ChCl:Glyc:AcOH	Rheo_Lyz_C1G15A05.txt
Lyz	1:1:1 ChCl:Glyc:AcOH	Rheo_Lyz_C1G1A1.txt
Lyz	1:0.5:1.5 ChCl:Glyc:AcOH	Rheo_Lyz_C1G05A15.txt
Lyz	1:0.5:1.5 ChCl:Glyc:AcOH	Rheo_Lyz_C1G05A15_Post1h.txt