Supporting Information

Analyzing the effects of protecting osmolytes on solute-water interactions by solvatochromic comparison method: I. Small organic compounds

Luisa A. Ferreira^a, Pedro Madeira,^b Vladimir N. Uversky,^{c,d,e}

and Boris Y. Zaslavsky^{a,*}

^aAnaliza, Inc., 3516 Superior Ave., Suite 4407B, Cleveland, OH, USA;

^bLaboratory of Separation and Reaction Engineering, Department of Chemical Engineering, Faculty of Engineering of the University of Porto, Rua Dr. Roberto Frias, 4200-465, Porto, Portugal;

^cDepartment of Molecular Medicine, Morsani College of Medicine, University of South Florida, Tampa, Florida 33612, USA;

^dDepartment of Biological Science, Faculty of Science, King Abdulaziz University, PO Box 80203, Jeddah 21589, Saudi Arabia;

^eLaboratory of Structural Dynamics, Stability and Folding of Proteins, Institute of Cytology, Russian Academy of Sciences, St. Petersburg, Russia



Figure S1: The solvatochromic absorption band of Reichardt's betaine dye for the coexisting phases in dextran-PEG-0.5 M sorbitol-0.01 M K/NaPB ATPS (K/NaPB – potassium/sodium phosphate buffer, pH 7.4).



Figure S2. An illustrative example of the output of the partition experiments. Concentration of a solute (phenol, 2-phenylethanol) in the top phase expressed as the UV absorbance at the maximum wavelength plotted against concentration of the same solute in the bottom phase. The slope of each curve represents the partition coefficient of a given solute under conditions indicated.

Table S1. Solvatochromic solvent parameters characterizing the dipolarity/polarizability π^* , the hydrogen bond donor acidity α , and hydrogen bond acceptor basicity β of the media in the coexisting phases of the aqueous two-phase systems: 12.0 wt% Dex-75 – 6.0 wt% PEG-8K - 0.01M K/NaPB, pH 7.4 and 12.0 wt% Dex-75 – 6.0 wt% PEG-8K - 0.5 M osmolyte - 0.01M K/NaPB, pH 7.4 (K/NaPB – sodium/potassium phosphate buffer).

_	Top Phase			Bottom Phase		
_	π*	α	β	π^*	α	β
0.01 M K/NaPB	1.101±0.002	1.039±0.003	0.618±0.001	1.143±0.001	1.090±0.001	0.612±0.003
0.5 M Sorbitol	1.122±0.001	1.013 ± 0.002	0.631±0.004	1.164±0.003	1.079±0.003	0.625±0.004
0.5 M Sucrose	1.132±0.002	$0.973 {\pm} 0.003$	0.634 ± 0.004	1.206±0.003	1.019 ± 0.004	0.611±0.004
0.5 M Trehalose	1.122±0.003	0.968 ± 0.002	0.640 ± 0.004	1.164±0.001	1.049 ± 0.002	0.634±0.003
0.5 M TMAO	1.101±0.001	$0.998 {\pm} 0.002$	0.643±0.001	1.132±0.002	1.072 ± 0.002	0.634 ± 0.008