Electronic Supplementary Information

SOLUTE-INDUCED PERTURBATION OF METHANOL-WATER ASSOCIATION

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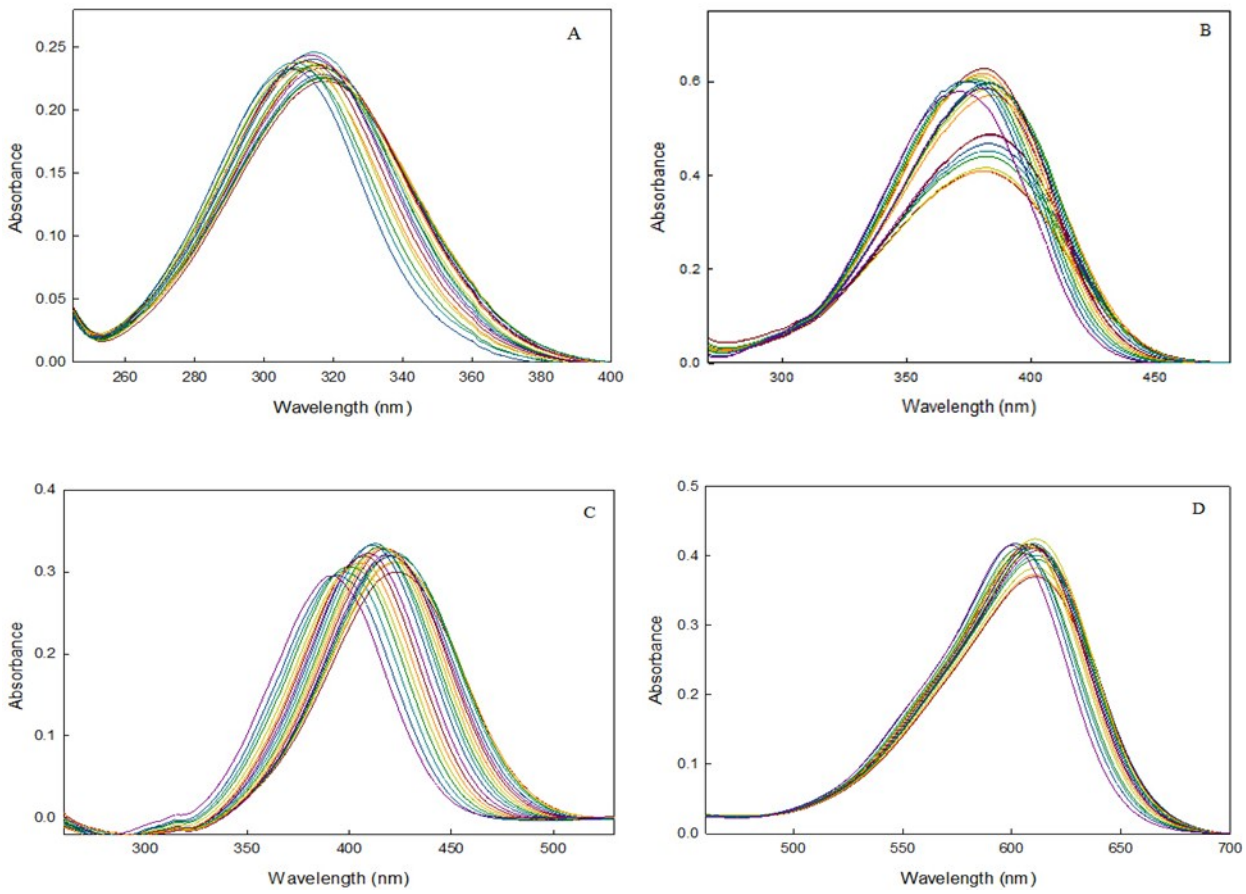

Fig. S1 Changes in absorption spectra of equal concentration of four dyes in 0-1 mole fraction of methanol water. Dyes molecules are 4-nitroanisol (A),4-nitroaniline (B), N, N dimethyl- 4-nitroaniline (C) and indigo carmine (D).

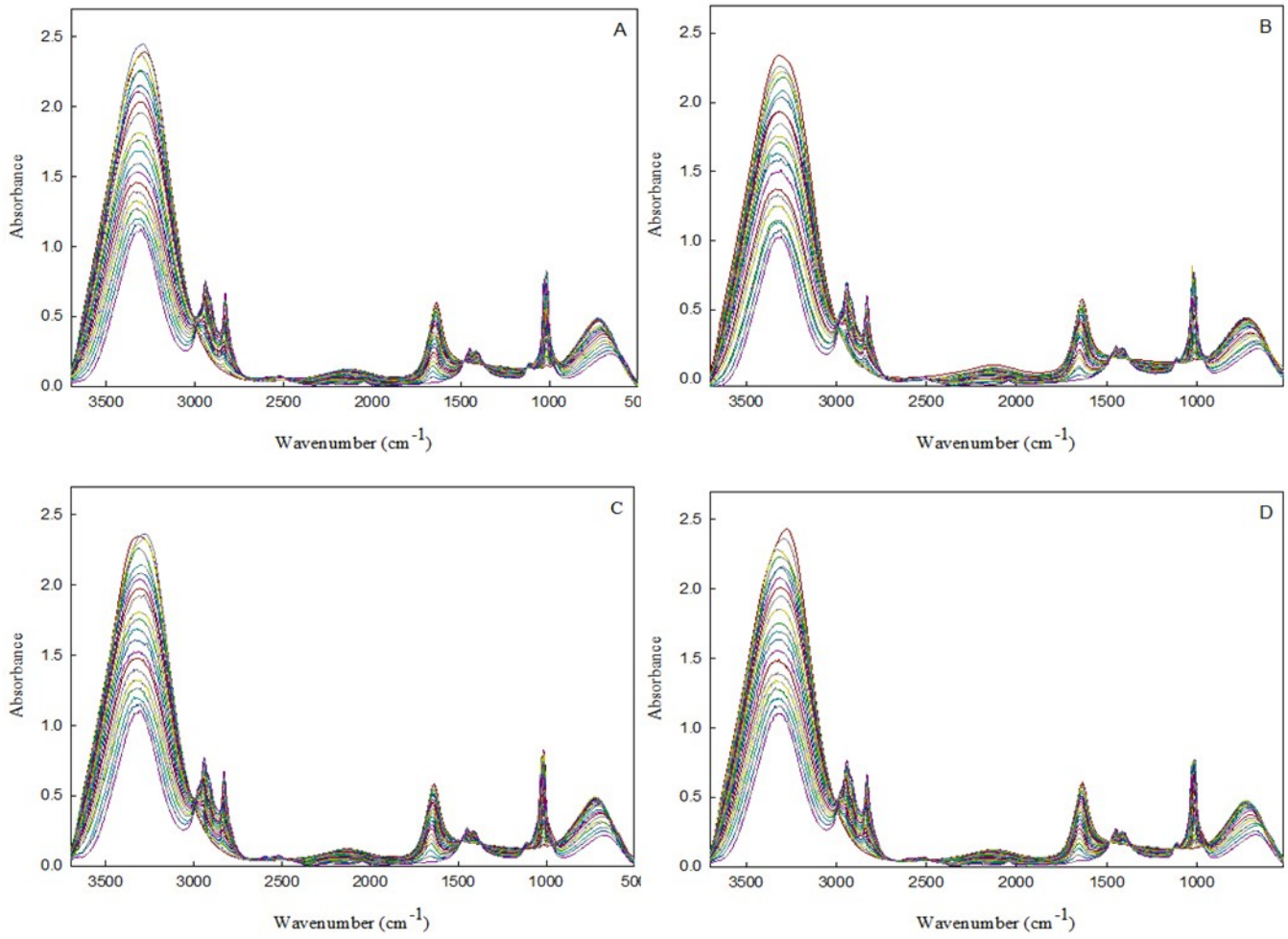

Fig. S2 Changes in infrared spectra of equal concentration of four dyesas solvatochromic probe in methanol-water mixtures.Methanol mole fractions varying from 0 to 1.00. Dyes molecules as probes are4-nitroanisol (A), 4-nitroaniline (B), N, N dimethyl- 4- nitroaniline (C) and indigo carmine (D).

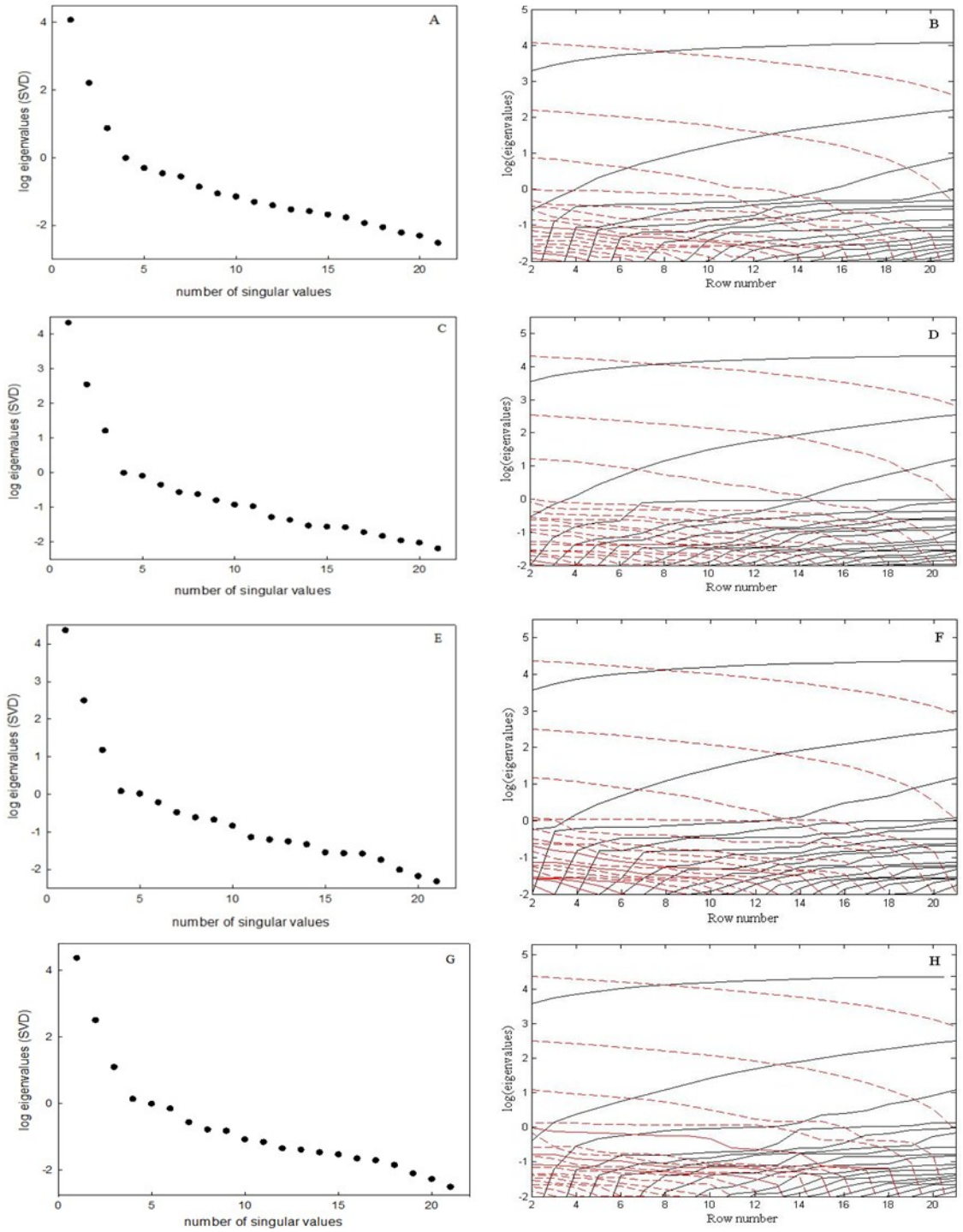

Fig. S3 Plot of log(EV) vs. number of principle components obtained from SVD (A, C, E, G and I) and logarithm of eigenvalues as obtained byevolving factor analysis (B, D, F, H, J) for data matrix of five Probes for IR and UV augmented matric. Probes are 4-nitroanisol (A and B), N, N dimethyl- 4- Nitroaniline (C and D), 4-nitroaniline (E and F) and indigo carmine (G and H).

Table S1 SVD analysis results for augmented spectra of UV–Vis and IR of different dyes.

Dye solvated solvent	Factor no	Log (EV)	Log (REV)	RSD	RMS
4-nitroanisol	**1**	4.07	-0.54	0.64	0.064
	2	2.20	-2.39	0.15	0.015
	3	0.87	-3.69	0.078	0.0080
	4	-0.012	-4.56	0.062	0.0063
	5	-0.31	-4.83	0.052	0.0052
	6	-0.47	-4.96	0.043	0.0044
4-nitroaniline	**1**	4.33	-0.51	0.97	0.075
	2	2.58	-2.25	0.22	0.016
	3	1.21	-3.60	0.092	0.0071
	4	0.058	-4.73	0.075	0.0058
	5	-0.091	-4.85	0.062	0.0048
	6	-0.36	-5.09	0.053	0.0041
N,N dimethyl4-nitroaniline	**1**	4.36	-0.53	0.89	0.065
	2	2.49	-2.38	0.21	0.016
	3	1.17	-3.66	0.099	0.0073
	4	0.080	-4.74	0.083	0.0061
	5	0.013	-4.78	0.067	0.0049
	6	-0.22	-4.98	0.055	0.0041
Indigo carmine	**1**	4.37	-0.49	0.89	0.068
	2	2.50	-2.33	0.20	0.015
	3	1.09	-3.72	0.098	0.0075
	4	0.14	-4.65	0.079	0.0061
	5	-0.0094	-4.77	0.063	0.0048
	6	-0.15	-4.89	0.048	0.0037
Augmented Data	**1**	4.90	-0.51	1.72	0.069
	2	3.06	-2.33	0.41	0.016
	3	1.71	-3.67	0.22	0.0087
	4	0.65	-4.69	0.19	0.0077
	5	0.55	-4.77	0.16	0.0067
	6	0.45	-4.85	0.14	0.0059