SUPPLEMENTARY INFORMATION

Solvatochromic sensor array for the identification of common organic solvents

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Experimental procedure:

Eighteen spots were printed on polypropylene membrane (0.2 μm pore size, Sterlitech Corporation). Seven solvatochromic dyes, including 4 positive solvatochromic dyes (Nile Red, Disperse Orange 25, Disperse Orange 3, and Phenol Blue) and 3 negative solvatochromic dyes (Merocyanine 540, Reichardt's Dye and 1-Ethyl-4-(2-hydroxystyryl)pyridinium iodide), were used. All dyes and solvents were reagent grade, obtained from Sigma-Aldrich, and used without further purification.

For colorimetric sensor array printing, the formulations were loaded into an 18–hole Teflon ink well (40 μL). Sensor arrays were printed using an array of 18 floating slotted pins arranged linearly; pins were dipped into the ink well and brought into contact with the polypropylene membrane, transferring to membrane ~400 μm diameter spots of each formulation. The printing protocol for spots used in the collection of diffuse reflectance spectra is the same as above except larger diameter floating slotted pins were used to print ~1 mm diameter spots (equivalent to the approximate read diameter of the reflectance probe). Once printed, all arrays were stored in a glove bag under nitrogen for more than 3 days to ensure evaporation of solvent vapors.

Three mass flow controllers were used to control the total flow rate passing over the colorimetric sensor array. The total flow rate was 500 sccm and the analyte concentration was 10% (v/v) its saturated vapor pressure. The analyte concentration was obtained by flowing nitrogen at 50 sccm through a bubbler with 40 ml of pure solvent. This saturated stream was diluted with dry nitrogen for a total flow of 500 sccm using another mass flow controller. Typically, a dry nitrogen control stream (500 sccm) was passed over the array for two minutes, followed by five minutes of analyte flow. Images of the array were collected using a flatbed scanner after 2 min of dry nitrogen and after 5 min of analyte exposure. The RGB values for the pixels corresponding to the center two-thirds of each spot were averaged to avoid spot edge artifacts using a customized software package, SpotFinder (iSense). All experiments were run in quintuplicate.

For each trial, a color change profile was obtained by subtracting the RGB values of the "before" image (2 min dry nitrogen) from the "after" image (5 min analyte). This yields a 54-dimensional vector (i.e., 18 changes in red, green, and blue values) that quantitatively describes the color change of the array upon exposure to an analyte; this vector, or color pattern, is unique for each analyte. The color change profiles were compiled into a library database; standard chemometric analyses including principal component analysis (PCA) and hierarchical cluster analysis (HCA) were performed on the database using a multi-variance statistical package (MVSP, Kovach Computing Services). For all HCA, minimum variance (i.e., Ward's method) was used for classification.

Diffuse reflectance spectra were obtained using a B&W tek Prime-X spectrometer with 2.5 nm resolution, a reflectance accessory from StellarNet, Inc. with seven 400 μm illuminating fibers and a 600 μm read fiber in a 7 around 1 configuration and a deuterium/tungsten light source (190-1100 nm). Each spectrum was processed by first removing 4 points (from 485.35-487.76 nm) and 8 points (from 654.08-659.42 nm) due to the presence of hydrogen emission lines (characteristic of the deuterium light source), which would distort the signal in those regions. Next, each spectrum was put through a 20-point Savitzky-Golay smoothing filter. Figure 4a was also normalized from 0-1 to more clearly illustrate the observed wavelength shift.

Table S1. A summary of solvatochromic dyes and their categories.

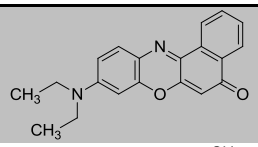
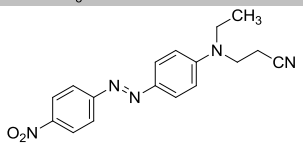
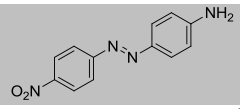
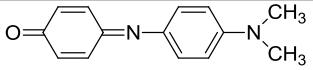
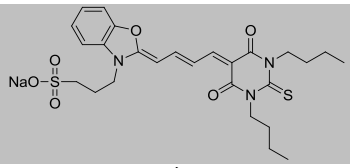
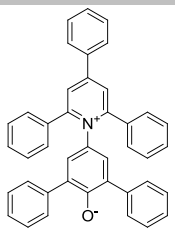
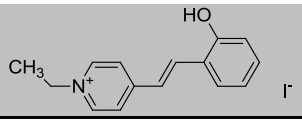
Number	Solvatochromic Category	Dye name (abbreviation)	Molecular Structure
1	positive	Nile Red (NR)	
2	positive	Disperse Orange #25 (DO25)	
3	positive	Disperse Orange #3 (DO3)	
4	positive	N,N-Dimethylindoaniline (Phenol Blue, PB)	
5	negative	Merocyanine 540 (M540)	
6	negative	Reichardt's Dye (R)	
7	negative	1-Ethyl-4-(2-hydroxystyryl)pyridinium Iodide (EHPI)	

Table S2. A summary of matrices and their concentrations for printing.

Name	Class	Composition	Concentration (v/v% in ME[a])
A	polar hydrogen bonding	Glycerol	10
B	polar hydrophobic (ionic liquid)	1-Butyl-3-methylimidazolium Hexafluorophosphate	10
C	relative nonpolar hydrophobic	Benzyl Butyl Phthalate	30
D	non-polar hydrophobic	Dow Diffusion Oil	10

[a]ME =2-methoxyethanol

Table S3. A complete list of solvatochromic dye-matrix combination.

Spot #	Dye	Amount (mg)	Matrix
1	NR	1	A
2	NR	1	B
3	NR	1	C
4	DO25	5	A
5	DO25	5	B
6	DO25	5	C
7	DO3	10	A
8	DO3	10	B
9	DO3	8	C
10	PB	3	A
11	PB	5	B
12	PB	3	C
13	M540	1.5	C
14	M540	1.5	D
15	R	15	C
16	R	15	D
17	EHPI	2	C
18	EHPI	4	D

Table S4. Summary of chosen analytes and their empirical $E_T(30)$ values.

	Analyte Name	$E_T(30)$ (kcal·mol^{-1})
1	Benzene	34.3
2	1,4-Dioxane	36.0
3	1,1,1-Trichloroethane	36.2
4	Tetrahydrofuran	37.4
5	1,2-Dibromoethane	38.3
6	Acetone	42.2
7	Dimethyl Formamide	43.2
8	Dimethyl Sulfoxide	45.1
9	1-Hexanol	48.8
10	Ethanol	51.9
11	Water	63.1

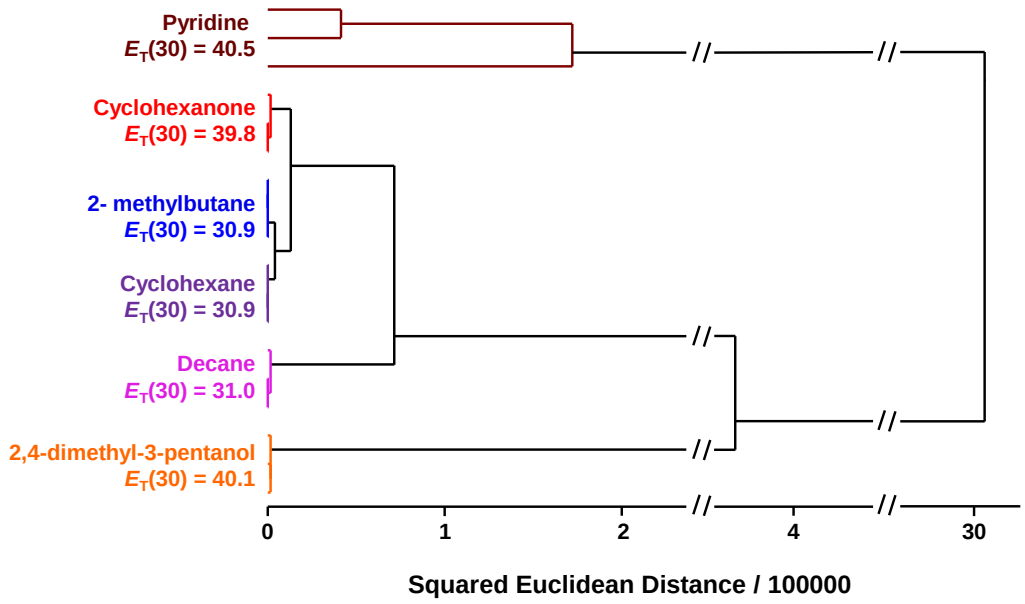


Figure S1. Hierarchical cluster analysis of the colorimetric array response to two groups of three common organic solvents with similar $E_T(30)$ values (given in kcal·mol^{-1}) at 10% of their saturation vapor pressure after 5 min of exposure. Each analyte was run in triplicate. The HCA used minimum variance (i.e., Ward's method) for clustering. Clustering appears independent of $E_T(30)$ and even analytes with the same $E_T(30)$ value are clearly separable, further demonstrating the colorimetric array probes more than just solvent polarity.

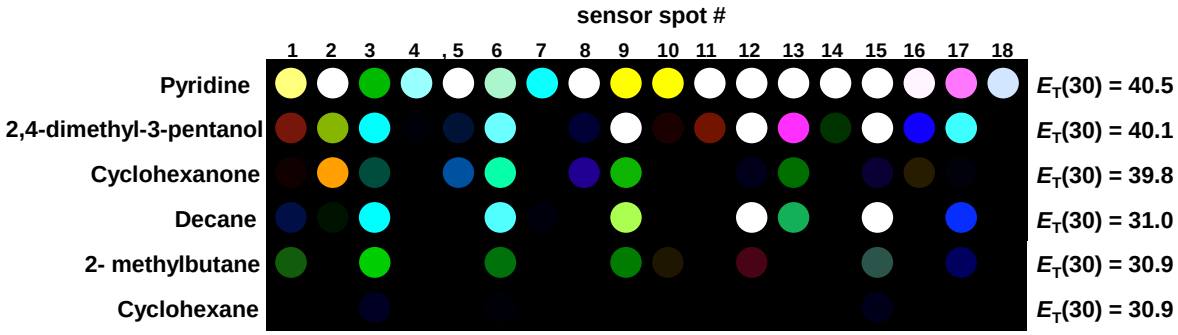


Figure S2. Difference maps showing the colorimetric sensor array response to two groups of three common organic solvents with similar $E_T(30)$ values (given in kcal·mol^{-1}) at 10% of their saturation vapor pressure after 5 min of exposure (averages of three trials each are shown). A color range of 1.5 - 8.5 was expanded to 8-bit color range (i.e., 0-255) for visualization. Response patterns show no obvious correlation to the analytes' $E_T(30)$ value.

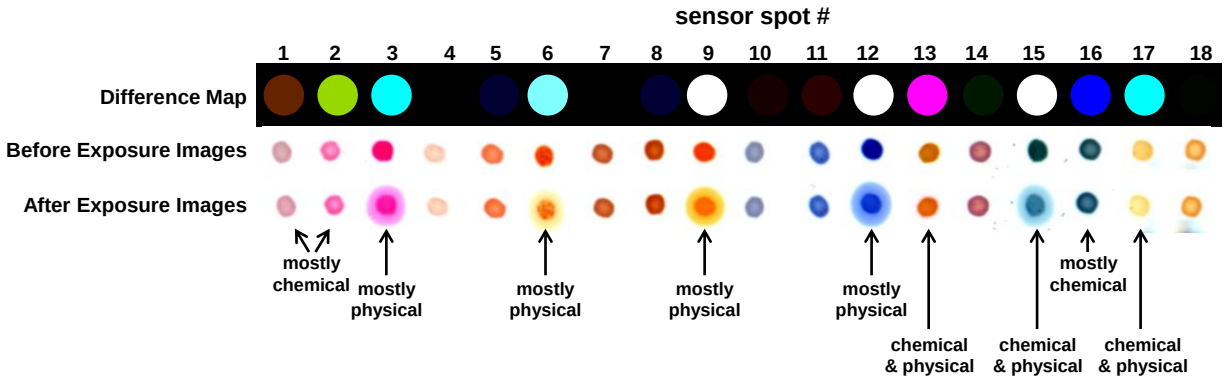


Figure S3. A typical array response for the solvatochromic sensor array. This particular experiment shows the response to 2,4-dimethyl-3-pentanol at 10% of its saturation vapor pressure. Top: difference map of 5 minute exposure time with color range of 1.5 - 8.5 expanded to 8-bit color range (i.e., 0-255) for visualization. Middle: raw images before exposure. Bottom: raw images after 5 minutes of exposure. Given below the images is the assignment of the primary reason for changes in RGB values: color changes are attributable to both chemical (i.e., analyte-dye interactions) and physical (i.e., spot blooming and refractive index alteration) changes.

Table S5. Color Difference Database (11 analytes plus a control).

	1	2	3	4	5	6	7	8	9	10	11	12	13	14
0% humidity control_1	-1.18	-3.44	-0.85	-13.19	8.38	5.50	0.00	0.36	6.56	6.65	2.17	1.89	2.19	7.63
0% humidity control_2	8.40	-4.01	3.00	3.57	2.01	2.43	0.00	-9.61	-7.93	17.02	-2.08	0.84	8.74	-3.87
0% humidity control_3	-1.20	6.15	5.85	-0.03	22.51	11.61	0.00	1.02	-0.36	-3.02	8.47	10.38	-2.20	18.81
0% humidity control_4	-1.30	0.28	-5.83	-5.00	6.42	5.05	0.00	-6.04	-21.26	-2.55	1.30	6.04	-3.84	9.54
0% humidity control_5	-5.50	4.62	10.97	-7.97	18.71	10.60	0.00	4.84	5.31	-4.77	4.79	0.71	-0.54	11.33
0% humidity control_6	-2.43	1.54	4.13	-11.78	12.57	-3.63	0.00	-24.33	-26.34	-0.17	0.57	4.70	6.14	3.40
0% humidity control_7	1.81	-5.87	-0.16	-5.69	2.57	-4.29	0.00	-8.21	-10.43	-1.80	3.35	-3.43	-1.60	2.27
1,4-dioxane_1	6.87	10.79	17.28	106.69	-74.13	4.51	0.00	45.78	-0.10	1.98	5.12	10.58	7.34	8.66
1,4-dioxane_2	-8.64	1.08	2.12	84.18	-78.38	-8.17	0.00	30.35	-13.19	2.59	7.98	5.67	-8.21	-12.86
1,4-dioxane_3	6.68	6.09	6.24	76.72	-57.89	0.59	0.00	38.23	-2.12	3.61	9.49	4.06	8.03	-11.21
1,4-dioxane_4	1.51	8.92	9.64	90.15	-62.79	3.57	0.00	42.16	0.84	3.16	6.33	1.89	2.89	-3.80
1,4-dioxane_5	1.13	17.73	12.94	93.00	-40.75	17.34	0.00	54.26	18.79	4.48	2.74	-12.77	4.39	0.21
1,1,1-trichloroethane_1	-1.79	1.03	-17.13	-20.97	30.65	-11.24	0.00	-120.54	-88.49	-3.67	-0.54	-8.49	-5.02	9.67
1,1,1-trichloroethane_2	-10.64	2.00	-5.84	-24.43	14.81	-14.17	0.00	-115.24	-87.67	-9.73	11.83	-4.06	-12.11	-9.84
1,1,1-trichloroethane_3	0.75	-4.06	-5.67	-5.46	20.17	-6.27	0.00	-69.13	-41.90	-2.76	2.38	2.76	-10.27	-1.73
1,1,1-trichloroethane_4	-7.19	0.11	-10.00	-14.54	-0.86	-16.17	0.00	-67.13	-36.11	-11.89	-4.33	-4.81	2.33	-14.87
1,1,1-trichloroethane_5	-1.40	5.73	-9.03	-12.60	10.86	-15.78	0.00	-70.43	-48.81	-9.14	5.19	-2.91	2.97	0.22
acetone_1	4.04	-6.94	9.23	154.91	-149.02	-17.35	0.00	-60.18	-45.05	-2.38	-1.41	1.35	-0.40	1.35
acetone_2	7.08	12.91	16.43	154.65	-124.65	-12.15	0.00	5.90	28.30	7.67	11.89	14.52	9.94	-7.08
acetone_3	9.11	1.49	2.85	116.50	-74.66	-15.81	0.00	-7.01	9.87	10.36	18.72	12.16	2.10	-3.18
acetone_4	23.17	25.87	28.49	147.66	-60.16	16.57	0.00	15.18	38.23	15.11	34.62	25.42	27.02	27.14
acetone_5	28.20	17.86	16.52	171.75	-125.45	-0.87	0.00	4.81	24.26	21.59	19.85	14.49	25.10	11.68
1,2-dibromoethane_1	13.99	45.12	56.78	52.27	3.40	50.10	0.00	-33.96	-44.20	3.40	28.79	34.13	1.63	3.17
1,2-dibromoethane_2	6.47	5.22	6.75	26.55	-42.43	0.52	0.00	30.18	25.79	2.74	7.53	-5.21	-10.40	-6.23
1,2-dibromoethane_3	-1.70	9.32	14.70	22.02	-28.69	11.24	0.00	46.19	55.69	6.73	7.93	8.61	1.02	3.14
1,2-dibromoethane_4	19.97	23.25	28.13	39.69	4.30	35.96	0.00	57.18	65.70	22.61	22.01	22.56	19.83	5.24
1,2-dibromoethane_5	0.83	12.30	12.18	27.75	-7.51	22.11	0.00	65.44	69.90	-0.99	14.14	1.65	2.50	-0.47
DMF_1	21.99	13.05	-1.32	370.45	-319.03	-58.12	0.00	-41.09	16.40	11.02	5.78	5.31	9.06	-28.35
DMF_2	17.32	4.34	7.90	343.41	-294.73	-53.66	0.00	-36.70	29.19	7.60	-4.86	-4.86	-0.99	-26.34
DMF_3	14.46	6.00	1.31	335.81	-285.83	-53.36	0.00	-37.47	28.74	1.27	-0.11	-1.61	-3.71	-21.08
DMF_4	8.81	4.77	-3.50	374.84	-336.42	-64.78	0.00	-29.19	40.30	-8.62	-1.56	-9.99	-9.58	-13.90
DMF_5	9.72	1.84	2.17	254.54	-193.13	-36.86	0.00	-42.90	29.08	-4.93	0.21	3.11	-13.34	-15.74
DMSO_1	19.21	7.93	-0.80	187.40	-76.16	-10.39	0.00	-31.67	23.39	1.72	9.28	1.91	-4.18	-24.76
DMSO_2	21.83	23.34	28.01	192.62	-73.35	24.21	0.00	-4.08	55.72	7.60	8.02	-5.76	-5.53	-29.66
DMSO_3	16.90	24.62	22.60	167.55	-62.40	10.66	0.00	-35.35	22.70	6.47	16.94	12.11	-3.96	1.27
DMSO_4	19.31	18.63	16.60	182.52	-70.64	8.16	0.00	-23.70	33.94	5.26	11.41	2.75	-4.56	-17.72
DMSO_5	20.52	15.64	13.61	190.01	-74.75	6.91	0.00	-17.88	39.55	4.66	8.65	-1.92	-4.86	-27.21
ethanol_1	20.03	19.35	11.85	9.30	4.94	19.07	0.00	-37.95	47.49	17.70	36.65	19.65	17.40	9.55
ethanol_2	16.99	17.63	14.91	-0.73	3.94	21.59	0.00	-41.20	42.62	10.97	20.93	16.73	14.33	2.81
ethanol_3	19.70	16.85	20.41	24.00	-1.80	21.38	0.00	-50.40	33.67	22.18	19.51	18.83	21.12	12.42
ethanol_4	21.26	29.52	26.03	13.95	20.25	33.39	0.00	-38.32	47.15	12.03	25.29	14.54	11.33	18.10
ethanol_5	21.84	11.90	18.60	22.43	8.38	6.97	0.00	-39.40	-35.19	14.43	4.65	13.30	26.43	5.73
THF_1	-10.00	-7.24	-3.03	-66.27	52.65	-0.65	0.00	-70.21	-35.46	-0.16	-1.35	-5.30	-5.78	8.33
THF_2	-18.54	-9.84	-6.43	-83.83	56.65	8.43	0.00	-91.84	-72.32	-11.51	-5.89	4.16	-10.05	14.60
THF_3	-9.51	1.30	-9.40	-58.38	39.95	-2.43	0.00	-72.54	-57.03	7.19	2.00	1.41	4.54	-25.29
THF_4	-7.08	-0.75	10.70	-66.22	35.73	-4.16	0.00	-80.54	-58.05	2.98	6.43	6.76	-5.51	-17.73
THF_5	-9.46	-5.89	0.65	-66.59	43.78	-2.38	0.00	-28.43	-1.30	-6.38	0.76	11.02	2.92	7.14
1-hexanol_1	-6.54	-23.14	-8.27	-4.43	-6.81	-9.63	0.00	25.95	-32.27	-12.16	-15.19	-10.16	-3.30	-2.92
1-hexanol_2	2.86	-6.22	-13.19	14.81	-24.00	-5.51	0.00	37.78	-28.59	9.79	-10.38	-2.86	-4.81	6.43
1-hexanol_3	-9.68	1.62	-1.03	20.70	-22.81	-13.51	0.00	26.71	-44.22	-3.02	-0.60	-1.51	4.54	-15.14
1-hexanol_4	-10.59	-1.51	-7.62	-1.51	0.00	-10.11	0.00	38.81	-29.62	1.02	5.45	-2.43	-0.16	4.54
1-hexanol_5	-3.78	-8.49	-1.68	1.35	-8.86	-13.29	0.00	33.30	-27.13	-0.27	5.79	-2.92	-0.91	3.30
benzene_1	-1.32	14.70	31.91	29.07	13.73	59.45	0.00	89.60	91.97	15.76	22.04	23.22	15.90	18.88
benzene_2	1.18	7.45	6.92	60.58	-52.82	6.89	0.00	58.90	40.55	9.25	8.68	12.28	14.59	13.29
benzene_3	15.38	25.58	46.09	53.85	15.79	57.01	0.00	74.10	56.68	15.05	6.23	19.73	11.91	4.72
benzene_4	5.05	19.76	30.40	52.61	-31.18	20.91	0.00	54.92	52.72	10.53	4.77	8.62	7.88	9.75
benzene_5	5.07	16.87	28.83	49.03	-13.62	36.06	0.00	69.38	60.48	12.65	10.43	15.96	12.57	11.66
water_1	2.17	0.03	-6.28	10.98	-17.84	-1.81	0.00	-7.76	-0.68	2.69	-3.12	-7.06	5.12	1.93
water_2	-1.89	-0.45	1.32	-3.30	-8.74	-5.83	0.00	-0.12	6.78	4.98	4.17	-1.85	-1.20	3.63
water_3	-5.05	3.21	6.47	-7.65	3.37	8.99	0.00	7.32	14.56	2.57	5.73	-1.25	-3.98	4.95
water_4	-0.94	3.26	-2.17	-5.36	-2.21	1.48	0.00	3.19	8.78	1.91	-2.81	0.52	-5.97	1.68
water_5	-3.33	-9.68	-3.80	-10.69	-4.84	-5.15	0.00	-12.11	-5.05	-1.51	-8.59	-5.43	-3.44	-14.18

	15	16	17	18	19	20	21	22	23	24	25	26	27	28
0% humidity control_1	9.72	3.02	6.06	5.94	-3.16	2.38	-0.40	3.19	0.19	3.28	-1.86	-2.62	2.03	-4.41
0% humidity control_2	-2.08	2.22	-7.67	7.77	10.12	-7.15	5.45	7.67	-3.70	2.10	2.86	-8.94	4.62	-2.80
0% humidity control_3	24.37	-13.21	-7.41	-1.91	1.14	-2.88	-4.65	3.89	20.98	8.10	-3.35	1.06	-0.09	2.06
0% humidity control_4	7.06	-3.30	-3.38	-2.67	-3.87	-2.78	1.06	-4.16	2.10	1.94	-11.82	-14.23	2.76	1.39
0% humidity control_5	10.86	-1.81	2.19	2.55	-3.85	-0.66	0.69	6.61	14.77	11.33	-8.23	-13.12	-3.52	1.91
0% humidity control_6	10.88	-7.20	-12.28	-10.88	3.40	0.35	0.85	0.44	9.74	6.70	-9.23	-12.80	-2.83	-4.60
0% humidity control_7	-4.10	-4.56	-5.62	-5.28	-0.17	-2.50	-4.55	3.09	8.07	6.04	-5.12	-7.05	0.34	-5.90
1,4-dioxane_1	17.18	5.43	66.69	39.60	9.96	5.92	2.74	1.37	-21.59	-34.19	35.94	54.21	-13.22	8.40
1,4-dioxane_2	-8.33	-14.13	34.95	5.52	1.23	5.43	-0.54	-6.72	-37.59	-34.47	-20.34	-36.46	-8.43	9.89
1,4-dioxane_3	-1.68	0.90	41.30	22.80	0.78	-1.03	7.70	0.95	-37.87	-28.60	20.88	23.46	-4.82	15.37
1,4-dioxane_4	1.16	-0.58	50.69	26.69	7.08	3.87	3.28	1.76	-27.47	-30.78	13.11	13.55	-8.20	11.47
1,4-dioxane_5	-2.55	5.50	59.82	38.84	16.35	5.17	3.24	11.44	-12.81	-25.84	15.98	13.00	-6.33	12.20
1,1,1-trichloroethane_1	7.14	-21.67	-178.60	-127.51	-0.76	8.70	-5.41	4.48	1.30	-3.84	-38.97	-97.02	-13.68	1.25
1,1,1-trichloroethane_2	-14.00	-33.41	-135.46	-85.52	-5.41	5.78	-4.54	-13.13	-14.59	-5.40	-36.11	-80.75	-10.97	-5.40
1,1,1-trichloroethane_3	-12.97	-6.32	-108.76	-70.22	-1.62	-0.32	-12.44	-8.65	-18.49	-8.81	-34.49	-59.89	-2.00	-4.27
1,1,1-trichloroethane_4	-10.11	-17.78	-128.44	-88.00	-3.83	1.30	-9.56	-16.59	-22.11	-9.51	-10.70	-63.36	-11.46	-6.92
1,1,1-trichloroethane_5	1.78	-13.40	-97.13	-56.38	-3.13	3.78	0.21	-2.06	-6.00	-1.72	-20.21	-49.41	-6.00	-10.76
acetone_1	-16.73	-28.13	2.93	29.42	-5.67	-6.68	-1.91	-5.02	-82.24	-87.32	-8.23	-34.36	-4.91	-30.40
acetone_2	-17.86	-8.52	38.42	61.66	7.67	2.92	5.71	1.77	-58.24	-68.49	5.05	-13.10	-10.92	-19.49
acetone_3	-9.11	-12.75	14.32	38.78	-2.22	-8.68	-3.89	-5.75	-60.65	-60.65	7.32	-6.63	-7.29	-14.98
acetone_4	11.51	-1.03	11.82	31.32	23.86	19.32	16.57	10.85	-42.54	-41.91	15.01	-29.88	-6.82	13.98
acetone_5	-2.53	3.47	20.63	27.16	16.40	5.52	6.16	7.32	-53.14	-63.15	22.38	-7.59	-2.88	21.69
1,2-dibromoethane_1	8.05	26.07	-30.98	-129.14	43.31	73.75	52.49	7.19	9.75	-4.75	18.38	41.13	-5.67	32.74
1,2-dibromoethane_2	-7.39	6.02	28.09	10.81	2.50	-0.09	0.23	2.12	-7.91	-8.33	2.50	2.91	-2.50	9.94
1,2-dibromoethane_3	9.37	10.46	45.20	30.51	6.56	0.90	7.50	-2.20	-7.37	-10.60	28.13	34.13	0.00	13.29
1,2-dibromoethane_4	16.80	28.49	44.74	33.06	21.62	5.83	11.54	23.69	6.09	4.96	30.59	35.06	5.12	18.59
1,2-dibromoethane_5	7.20	4.51	60.30	42.86	-0.14	4.34	2.45	-2.43	-1.01	-1.96	29.97	51.30	0.92	11.14
DMF_1	-6.40	-4.72	-64.64	5.09	-17.96	-41.32	-11.40	-15.86	-300.32	-148.89	-110.98	-175.82	18.65	21.90
DMF_2	-4.06	-8.40	-75.83	-2.43	-17.87	-36.98	-5.50	-27.16	-318.23	-156.56	-124.03	-192.64	20.03	10.15
DMF_3	2.20	-14.44	-66.48	2.82	-19.94	-40.56	-12.07	-21.80	-343.17	-169.65	-117.37	-180.09	17.78	30.20
DMF_4	13.31	-22.82	-62.92	0.88	-30.92	-51.83	-21.35	-16.00	-458.06	-220.44	-117.95	-180.10	16.31	30.06
DMF_5	5.97	-21.83	-62.54	7.74	-13.00	-32.12	-10.03	-28.18	-296.05	-152.69	-116.51	-171.80	16.12	58.69
DMSO_1	27.71	-16.87	-55.84	12.32	-15.32	-29.31	-7.79	-66.84	-370.62	-106.29	-144.35	-202.50	23.81	63.12
DMSO_2	28.43	-9.82	-48.31	14.37	-3.70	-17.61	5.15	-58.43	-400.73	-155.14	-131.92	-187.35	19.59	135.46
DMSO_3	52.27	-13.85	-56.24	2.95	-8.85	-22.33	-3.77	-70.16	-382.98	-140.29	-145.91	-200.07	19.94	117.24
DMSO_4	36.14	-13.51	-53.46	9.88	-9.29	-23.08	-2.14	-65.14	-384.78	-133.91	-140.73	-196.64	21.11	105.27
DMSO_5	28.07	-13.35	-52.07	13.35	-9.51	-23.46	-1.32	-62.64	-385.68	-130.72	-138.14	-194.93	21.70	99.29
ethanol_1	3.77	11.52	24.85	31.12	17.51	7.41	11.07	19.35	-0.02	-2.55	17.75	-2.53	-1.70	29.19
ethanol_2	2.05	14.65	0.92	-1.68	5.17	4.23	6.40	7.84	0.82	-2.83	11.44	4.35	0.47	23.95
ethanol_3	15.05	17.60	12.53	25.87	9.23	0.45	5.69	13.83	18.29	12.55	14.98	-5.78	-11.04	24.38
ethanol_4	15.20	1.41	5.19	4.65	7.41	13.81	6.91	13.71	10.50	8.36	14.33	5.36	-0.28	27.75
ethanol_5	-1.46	24.87	10.06	6.54	19.62	3.24	-9.02	13.84	-9.52	-4.54	9.25	22.27	4.54	-2.05
THF_1	3.08	-28.65	-127.73	-108.81	-3.19	8.86	0.05	-2.05	22.43	14.54	-29.51	-46.06	-1.19	-13.24
THF_2	13.46	-25.68	-108.33	-62.11	-0.27	18.11	2.81	-8.33	23.03	19.79	-44.00	-64.49	-3.62	-6.65
THF_3	-27.89	-7.08	-102.05	-71.19	12.54	9.41	-12.59	-7.35	8.65	5.08	-13.57	-28.92	-0.54	-24.38
THF_4	-23.46	-14.32	-105.35	-68.65	2.00	8.70	-2.22	-8.48	13.08	13.19	-33.63	-50.22	0.27	-8.76
THF_5	9.94	-15.36	-109.14	-56.21	10.81	14.75	6.05	-4.11	15.40	16.76	-22.22	-41.52	-2.48	-9.95
1-hexanol_1	-9.08	-11.19	-8.70	-9.08	3.46	13.41	2.65	-1.46	-6.06	-7.73	-3.30	6.71	-3.46	-2.59
1-hexanol_2	-7.68	-14.17	-13.41	-14.54	0.60	7.51	-2.43	-0.70	0.00	-5.08	12.21	6.81	-2.76	-13.30
1-hexanol_3	-18.87	8.76	-6.32	-18.87	-0.75	6.49	-4.60	8.60	-11.68	-8.38	-2.87	-0.27	0.22	-0.16
1-hexanol_4	-3.95	-6.27	-6.60	-8.11	-0.27	14.97	2.00	2.59	-2.43	-1.35	-7.94	-0.92	4.97	-4.27
1-hexanol_5	-7.08	4.00	-8.33	-19.46	0.71	15.30	-2.11	-8.06	10.49	-5.35	4.76	12.22	-3.94	0.92
benzene_1	29.99	5.27	76.50	46.45	8.08	1.89	6.28	17.62	7.88	7.34	34.81	48.54	0.14	28.51
benzene_2	17.51	23.39	96.07	61.86	7.22	17.37	11.64	-2.43	-3.32	-7.92	34.15	49.59	-9.37	10.74
benzene_3	16.31	6.89	53.95	29.27	20.77	27.89	21.24	8.48	-2.67	3.52	31.84	22.09	-8.71	27.40
benzene_4	25.72	18.22	71.95	46.85	-0.40	-0.09	5.45	0.45	-14.66	-7.03	25.23	57.48	12.58	12.58
benzene_5	22.38	13.44	74.62	46.11	8.92	11.76	11.15	6.03	-3.19	-1.02	31.51	44.43	-1.34	19.81
water_1	0.21	5.12	-4.06	-3.61	3.35	-1.82	0.64	6.68	-6.40	-3.06	5.05	-3.09	-2.62	5.38
water_2	-5.41	-0.02	13.12	14.80	-3.49	3.85	-3.77	-1.44	-2.38	-4.34	-2.38	-2.43	1.68	-0.02
water_3	4.96	-5.45	9.25	10.91	-8.40	-2.90	-0.97	-7.27	0.35	-0.76	1.01	3.89	0.52	-2.24
water_4	5.26	-1.06	11.02	2.72	-1.39	1.61	1.89	-7.39	-2.86	-5.73	-2.83	1.21	0.28	-3.12
water_5	-6.04	-2.05	-7.13	5.62	-1.49	-7.29	4.02	2.88	-5.03	2.22	2.43	5.00	-0.33	9.34

	29	30	31	32	33	34	35	36	37	38	39	40	41	42
0% humidity control_1	0.99	3.63	5.17	6.35	4.27	-2.08	-6.45	-11.05	-3.51	-2.15	-16.47	6.35	6.51	-19.00
0% humidity control_2	-4.25	-1.96	6.70	5.08	7.39	-0.40	-3.95	-3.87	10.12	4.89	-10.07	4.43	4.88	-10.10
0% humidity control_3	0.77	0.97	9.84	14.26	2.51	-0.85	-0.49	-4.16	3.33	10.64	-8.00	4.32	1.06	-6.18
0% humidity control_4	-1.86	-0.94	8.43	13.47	8.42	-1.32	-5.05	-14.54	-1.89	-1.89	-14.89	11.85	12.94	-10.59
0% humidity control_5	-2.74	-1.61	6.02	7.01	-0.73	-8.33	-9.61	-18.85	3.90	-1.96	-14.13	7.62	14.18	-18.06
0% humidity control_6	1.70	1.47	9.69	16.12	5.57	-8.69	-10.46	-17.66	10.40	3.64	-11.35	2.64	8.88	-18.29
0% humidity control_7	-8.56	-0.56	6.42	5.33	11.19	-3.68	-5.20	-2.78	0.63	7.12	-9.25	6.85	2.98	-2.69
1,4-dioxane_1	12.96	3.87	-51.30	-37.57	-20.25	11.99	0.94	3.19	8.07	-17.44	4.86	-1.09	-14.42	26.22
1,4-dioxane_2	6.26	2.17	-39.10	-31.05	-8.87	13.24	5.24	20.91	8.45	0.87	9.32	-13.72	-11.04	24.64
1,4-dioxane_3	6.23	6.40	-40.76	-35.30	-25.91	6.75	-4.72	4.27	-0.52	-13.93	1.88	-4.32	-18.92	28.51
1,4-dioxane_4	9.83	5.34	-42.39	-31.83	-15.35	15.67	9.76	11.27	5.35	-9.97	4.67	-2.18	-11.80	31.17
1,4-dioxane_5	13.85	8.90	-38.40	-23.41	-6.38	30.70	37.57	16.71	5.38	-9.37	2.60	10.40	-2.83	45.31
1,1,1-trichloroethane_1	-3.14	-5.73	14.37	-0.70	-3.13	-64.21	-72.65	-116.22	-14.33	-50.32	-75.79	-1.46	-0.59	-25.46
1,1,1-trichloroethane_2	-7.14	-3.08	-7.02	-8.81	-1.83	-62.65	-61.89	-105.57	-34.05	-52.37	-71.73	-4.75	4.22	-12.11
1,1,1-trichloroethane_3	-3.19	-6.54	4.97	-7.73	-2.98	-43.68	-43.30	-77.41	-5.46	-16.71	-47.24	-2.81	7.78	-3.67
1,1,1-trichloroethane_4	-10.32	-4.16	-18.00	-14.11	-1.30	-27.40	-27.79	-55.79	10.16	2.97	-35.62	-5.89	14.33	-9.19
1,1,1-trichloroethane_5	-8.21	-9.51	16.27	-2.17	5.46	-36.75	-34.21	-65.08	0.92	-11.08	-42.81	7.30	3.41	-8.97
acetone_1	14.73	4.11	-198.30	-184.90	-46.11	4.28	0.87	13.90	-10.64	-25.20	-13.00	-9.61	-25.70	37.73
acetone_2	11.80	6.68	-153.36	-137.60	-33.63	9.65	13.08	27.92	23.86	0.10	8.48	11.59	1.41	28.15
acetone_3	3.05	-4.91	-87.20	-77.81	-22.02	2.81	2.39	0.62	13.78	-5.10	-7.06	5.40	-13.21	31.90
acetone_4	18.76	6.56	-95.32	-92.09	-27.21	-2.43	-2.55	-3.87	-4.08	-40.47	-28.96	11.75	-14.99	35.82
acetone_5	23.23	8.70	-90.74	-86.60	-11.23	-14.96	-18.97	-20.37	29.33	0.99	4.53	14.04	-2.19	48.28
1,2-dibromoethane_1	39.60	35.25	-30.54	-7.79	23.13	27.75	52.37	101.76	14.94	43.42	12.91	0.93	-3.73	28.57
1,2-dibromoethane_2	6.23	3.44	-24.40	-7.20	5.17	15.50	20.65	33.06	5.66	25.14	-1.30	7.81	1.42	22.14
1,2-dibromoethane_3	8.75	6.35	-33.20	-18.91	-14.51	15.19	23.34	42.45	12.55	24.75	10.34	5.15	-1.86	25.25
1,2-dibromoethane_4	20.70	24.78	-3.87	9.72	15.36	14.06	20.58	49.13	12.11	27.36	8.97	20.55	16.30	52.69
1,2-dibromoethane_5	22.54	10.26	-29.48	-16.02	-13.90	-3.61	-4.08	23.76	-39.15	-21.85	-26.78	-39.81	-41.91	5.41
DMF_1	8.09	3.11	-142.18	-129.22	-52.34	-15.72	-13.57	-25.49	-34.00	-312.31	213.21	8.29	-23.36	72.52
DMF_2	-1.68	3.31	-146.91	-146.83	-59.82	-8.97	-3.40	4.18	-3.56	-330.50	205.76	2.52	-40.73	75.96
DMF_3	8.39	1.05	-157.82	-151.22	-65.42	-10.40	-4.53	-4.34	-38.80	-323.59	309.98	-2.17	-37.92	74.95
DMF_4	10.95	-4.93	-241.56	-235.75	-107.99	-10.17	-3.07	1.46	-109.41	-352.47	623.36	-13.24	-55.95	82.81
DMF_5	16.21	2.70	-100.62	-93.08	-41.53	-6.73	1.93	2.47	-8.21	-299.06	197.59	-6.27	-31.65	68.51
DMSO_1	20.67	-1.96	-37.71	-7.97	-17.82	-5.71	-2.52	-0.62	17.25	-353.02	397.01	-2.74	-36.79	79.15
DMSO_2	58.60	21.50	-30.52	2.27	13.71	-3.02	9.62	35.68	26.76	-359.43	438.53	11.23	-26.50	99.84
DMSO_3	42.55	3.18	-62.96	-25.25	-11.92	-11.84	0.57	4.72	4.86	-369.16	414.49	-6.53	-40.66	101.08
DMSO_4	40.61	7.57	-43.73	-10.32	-5.34	-6.86	2.56	13.26	16.29	-360.54	416.68	0.65	-34.65	93.36
DMSO_5	39.63	9.77	-34.12	-2.85	-2.06	-4.37	3.55	17.53	22.01	-356.23	417.77	4.25	-31.65	89.50
ethanol_1	21.50	16.33	-4.43	3.63	5.61	-0.35	16.90	33.48	33.04	-18.88	18.39	10.95	1.32	41.95
ethanol_2	22.45	16.35	4.18	24.78	26.99	-8.23	8.45	16.47	40.30	-7.20	33.41	19.92	6.39	46.94
ethanol_3	26.60	12.35	-26.03	-13.17	-14.65	-11.52	-2.06	14.77	37.00	-19.84	21.80	28.98	23.43	60.89
ethanol_4	34.24	18.08	1.55	15.36	17.84	-4.51	13.57	29.66	36.65	-8.12	28.30	26.26	27.68	57.00
ethanol_5	4.59	7.95	-7.84	-21.68	-6.22	9.95	-1.25	1.78	39.40	-13.50	27.60	6.20	3.28	44.91
THF_1	-6.43	4.76	31.03	13.84	-1.79	-17.19	-10.27	-22.00	29.24	64.37	-48.00	1.83	20.71	-21.25
THF_2	-17.14	-4.49	55.41	33.30	26.33	-15.13	-8.75	-64.27	28.00	58.05	-68.97	-5.40	13.84	-27.78
THF_3	-23.46	-24.27	13.46	9.30	-14.86	-23.62	-29.84	-72.59	25.51	45.25	-65.29	-5.40	23.51	-34.48
THF_4	-13.41	-3.03	5.13	-11.08	-13.14	-14.21	-12.92	-37.30	26.59	63.95	-67.08	-0.59	17.90	-27.25
THF_5	-12.22	-4.22	19.19	18.05	3.13	-31.51	-28.86	-61.46	14.06	45.52	-83.36	3.03	6.60	-21.79
1-hexanol_1	-14.32	-12.64	6.43	3.19	-5.35	2.38	-10.81	-22.11	-6.38	117.30	-75.84	-15.84	10.60	-12.54
1-hexanol_2	1.40	-13.19	8.48	-6.38	-11.30	-2.11	-14.11	-52.43	-0.43	81.46	-41.89	-14.43	3.84	-3.57
1-hexanol_3	-12.21	-5.51	-6.54	-20.33	-14.27	5.14	-9.46	-17.19	-8.76	74.06	-54.98	-7.62	1.51	-8.16
1-hexanol_4	-0.22	-0.38	4.76	0.48	6.05	3.35	-5.46	-5.40	-45.62	29.30	-19.19	-19.03	8.27	-3.46
1-hexanol_5	1.94	-4.64	15.08	3.29	-5.62	8.06	-9.79	-19.19	-18.76	53.19	-49.90	-0.59	2.54	-4.59
benzene_1	25.84	26.64	15.86	31.57	39.34	20.29	17.70	52.43	0.87	12.84	-4.46	31.88	45.29	50.12
benzene_2	16.21	15.51	-41.60	-18.72	2.55	26.45	40.78	87.22	21.68	25.61	16.31	1.88	-5.64	24.19
benzene_3	24.92	23.46	4.20	14.44	-0.07	15.45	16.80	39.95	19.14	27.61	18.01	8.26	-4.79	11.40
benzene_4	18.39	16.95	-37.21	-20.06	3.97	27.63	30.18	49.81	17.58	30.33	22.40	0.85	-6.49	35.92
benzene_5	21.34	20.64	-14.69	1.81	11.45	22.46	26.37	57.35	14.82	24.10	13.07	10.72	7.09	30.41
water_1	-1.20	2.69	11.73	8.12	4.49	0.00	1.11	7.74	13.35	7.20	-4.11	7.64	-2.43	-6.25
water_2	7.38	0.24	10.62	18.17	2.29	2.31	7.01	11.94	2.51	-5.66	-14.75	-1.18	-2.67	-5.61
water_3	16.19	6.13	7.08	15.06	3.96	2.13	3.10	13.92	11.06	22.90	1.04	4.91	11.26	12.51
water_4	3.73	1.04	3.52	8.02	-5.31	0.26	4.29	3.06	8.54	3.31	-0.62	5.92	8.35	2.72
water_5	2.39	3.59	11.49	7.36	-4.25	-0.47	1.04	5.78	15.19	8.29	-5.76	7.39	-5.74	-4.88

	43	44	45	46	47	48	49	50	51	52	53	54
0% humidity control_1	-2.71	-13.71	3.14	2.43	1.21	1.54	-12.82	-18.08	-6.96	-4.65	8.75	-4.62
0% humidity control_2	2.08	-11.33	8.04	4.17	0.04	-3.02	-4.48	-9.06	-17.65	6.44	3.42	-4.88
0% humidity control_3	-5.50	-9.01	2.15	13.12	7.38	7.93	-3.40	-11.54	-11.77	3.82	9.37	5.12
0% humidity control_4	10.27	-0.10	12.94	1.96	1.46	2.36	-0.47	-17.89	-17.87	2.50	-1.56	-6.89
0% humidity control_5	4.69	-2.95	11.04	-5.40	-1.01	2.57	-7.98	-16.83	-15.91	4.20	2.22	-2.78
0% humidity control_6	-10.47	-22.54	-7.27	-0.78	-3.00	0.16	-15.48	-18.92	-24.55	-0.52	-0.38	-4.98
0% humidity control_7	2.24	-6.98	7.04	4.75	-0.69	-2.12	-8.36	-9.68	-21.26	3.87	-1.16	-5.01
1,4-dioxane_1	-8.78	27.61	-14.61	-6.70	1.61	-10.06	-10.40	-4.60	-7.48	7.77	17.20	23.60
1,4-dioxane_2	0.26	30.73	-3.23	-11.87	-6.38	-9.96	-7.69	10.62	11.80	4.56	10.12	0.12
1,4-dioxane_3	6.84	31.18	3.71	-6.66	-8.12	-5.57	-1.54	6.98	5.02	-0.52	-2.74	4.25
1,4-dioxane_4	1.75	31.43	-1.31	-9.62	-5.18	-8.00	-2.56	7.07	6.85	6.80	11.36	12.77
1,4-dioxane_5	8.66	36.18	8.90	-13.26	-7.81	-6.39	9.37	15.27	18.05	15.39	20.87	23.10
1,1,1-trichloroethane_1	-51.95	-59.62	-63.08	15.35	19.51	-4.71	-1.35	11.35	29.19	-8.16	-3.35	2.87
1,1,1-trichloroethane_2	-83.84	-93.62	-97.95	-13.84	-3.57	-23.94	-14.71	-19.19	-76.97	-20.54	-4.60	-14.16
1,1,1-trichloroethane_3	-49.95	-52.60	-58.65	-4.75	5.08	-4.00	-0.22	-11.03	-32.64	-3.08	4.59	-2.70
1,1,1-trichloroethane_4	-60.16	-65.51	-74.22	-3.57	6.27	-6.70	-5.14	-0.97	-35.40	-11.46	-8.54	-4.71
1,1,1-trichloroethane_5	-64.43	-69.41	-76.17	-2.17	1.83	0.32	-11.19	-20.87	-44.33	2.38	-11.14	-6.64
acetone_1	-24.95	-18.33	-31.04	-32.76	-26.00	-12.41	-55.22	-27.89	-9.25	-6.04	8.43	15.12
acetone_2	5.19	19.28	7.22	-15.03	-15.60	4.70	8.24	25.37	12.34	14.09	28.43	33.06
acetone_3	0.82	12.51	3.82	-21.97	-23.46	-5.22	-1.32	-3.14	-16.33	8.31	12.67	18.55
acetone_4	-8.97	-6.21	-19.63	-21.43	-26.99	-6.09	23.18	27.26	22.87	27.04	22.82	13.90
acetone_5	-24.24	-13.78	-30.45	-22.84	-14.26	6.40	18.46	28.91	28.72	20.70	34.90	27.66
1,2-dibromoethane_1	155.77	130.14	214.60	4.09	0.57	20.01	14.16	52.58	56.45	12.81	10.26	-5.88
1,2-dibromoethane_2	225.44	188.11	280.87	22.25	16.24	29.09	11.87	21.97	28.20	4.36	14.16	15.00
1,2-dibromoethane_3	208.07	191.98	286.46	12.56	6.79	12.69	13.73	19.54	66.15	14.44	21.67	10.22
1,2-dibromoethane_4	223.15	202.60	290.41	22.89	22.25	36.43	23.15	24.52	44.86	23.13	22.65	23.27
1,2-dibromoethane_5	193.69	186.13	261.08	9.04	5.55	14.33	13.62	36.60	42.53	3.87	19.78	17.67
DMF_1	-8.05	22.09	-31.13	-40.94	-28.50	-7.01	2.01	75.38	43.61	9.49	0.59	20.91
DMF_2	-17.04	18.81	-46.63	-32.38	-27.05	-15.65	-0.38	81.56	7.79	13.41	13.90	21.47
DMF_3	-14.01	20.47	-36.25	-36.91	-32.02	-14.71	-7.90	109.14	47.53	2.47	13.55	22.91
DMF_4	-16.14	17.84	-35.99	-48.83	-51.51	-23.98	-17.61	194.86	86.01	-16.31	33.02	36.72
DMF_5	-14.82	23.13	-31.24	-25.48	-21.00	-12.20	-15.63	84.76	52.72	3.31	6.71	12.55
DMSO_1	-12.67	21.41	-21.03	-16.97	-3.00	-1.18	-4.03	60.27	-1.27	-0.99	6.78	11.42
DMSO_2	-7.81	21.88	-16.97	3.45	6.28	11.99	0.00	106.69	59.82	6.61	24.69	45.82
DMSO_3	-4.89	30.68	-10.17	-25.18	-19.47	-14.07	-1.98	74.86	-12.56	-3.31	15.17	10.03
DMSO_4	-8.46	24.66	-16.06	-12.90	-5.40	-1.09	-2.00	80.61	15.33	0.77	15.55	22.42
DMSO_5	-10.24	21.65	-19.00	-6.76	1.64	5.40	-2.02	83.48	29.28	2.81	15.74	28.62
ethanol_1	-30.87	-62.91	191.55	-22.99	-18.15	54.11	7.20	30.06	13.97	11.00	17.65	17.11
ethanol_2	-31.41	-73.46	187.50	1.65	-4.06	75.03	22.02	53.45	34.53	21.90	38.63	48.15
ethanol_3	-16.07	-44.79	210.12	6.85	-0.87	77.95	36.03	61.76	46.96	23.12	53.78	74.59
ethanol_4	-32.50	-72.38	196.84	15.97	12.77	85.90	34.12	75.79	45.45	26.67	68.74	79.74
ethanol_5	64.33	73.18	346.76	-11.09	-34.48	100.34	38.65	73.78	36.97	24.55	50.30	80.20
THF_1	-25.13	-62.92	-12.64	23.73	22.10	2.11	-2.00	-16.10	-60.48	-4.71	-13.89	-2.16
THF_2	-64.38	-102.21	-54.82	24.27	20.37	8.60	-4.22	-32.38	-82.44	-11.13	-6.38	-4.87
THF_3	-16.81	-56.27	-11.30	27.08	21.94	2.87	8.06	12.27	-44.59	4.33	-4.97	-12.97
THF_4	-23.46	-58.38	-10.81	27.46	11.13	8.60	4.27	-4.97	-70.17	-6.33	-6.59	-0.75
THF_5	-46.06	-103.84	-48.38	23.52	17.35	7.84	1.03	-17.68	-68.27	-8.16	-1.35	2.33
1-hexanol_1	73.46	102.05	-161.84	14.64	28.05	-46.27	-3.78	-22.22	-40.38	-10.22	-13.78	-8.59
1-hexanol_2	60.81	86.33	-135.95	22.16	42.38	-40.75	0.38	4.70	-15.79	-8.76	-8.81	-5.19
1-hexanol_3	55.89	76.81	-131.52	18.81	38.00	-39.41	-9.13	-27.51	-40.97	-6.81	-6.43	-10.54
1-hexanol_4	44.05	79.35	-139.73	9.35	27.89	-38.54	-8.65	10.81	-10.64	-21.67	-10.49	-9.52
1-hexanol_5	66.65	70.27	-126.00	21.73	27.03	-38.86	-9.79	1.24	-17.79	-2.92	-10.06	-6.82
benzene_1	4.15	19.02	15.38	13.22	6.40	45.59	5.66	36.30	40.85	22.96	54.52	66.88
benzene_2	22.80	61.55	45.76	-16.68	-20.46	-4.98	22.85	37.47	38.66	16.54	23.03	15.32
benzene_3	22.31	58.71	37.88	-23.34	-27.09	-13.02	9.01	27.54	33.98	11.47	27.21	12.60
benzene_4	27.98	60.82	45.05	0.54	5.74	11.31	10.05	14.18	38.40	5.03	5.52	14.49
benzene_5	19.31	50.03	36.02	-6.57	-8.85	9.73	11.89	28.87	37.97	14.00	27.57	27.32
water_1	1.39	3.54	10.60	4.70	-9.82	24.66	15.58	3.44	22.80	13.38	6.49	24.78
water_2	-3.21	5.22	7.86	1.53	-5.21	30.16	10.08	7.55	9.47	6.58	14.85	21.73
water_3	-9.67	9.08	12.51	-5.62	-6.39	28.75	-2.43	18.50	34.27	-4.77	2.33	23.72
water_4	-8.90	2.78	2.92	21.60	12.79	47.91	7.01	13.62	35.32	10.10	-0.07	8.52
water_5	-0.78	4.06	7.03	3.92	-14.86	22.91	9.04	-0.75	25.46	10.50	3.02	25.96