Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for the Manuscript "Responses of polar organic compounds to different ionic environment in aqueous media are interrelated"

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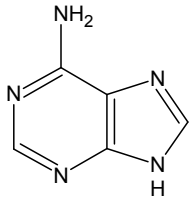
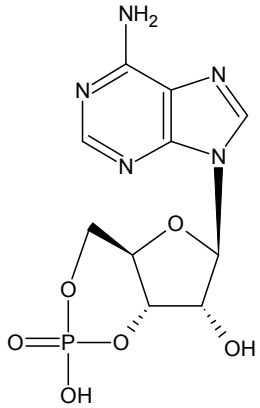
Figure S1. Structures of compounds examined:

Adenine



Adenosine



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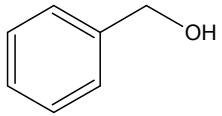

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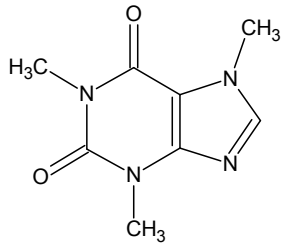

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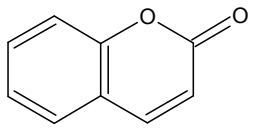
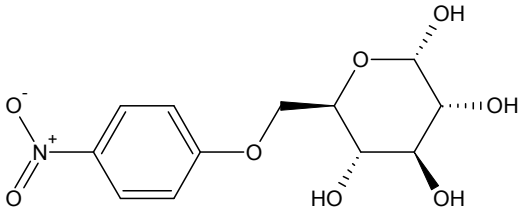


p-Nitrophenyl-α-D-glucopyranoside



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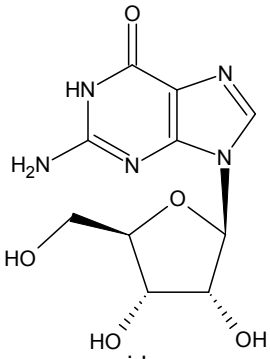

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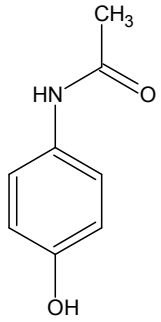

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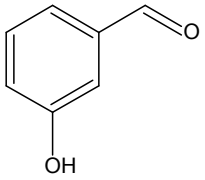

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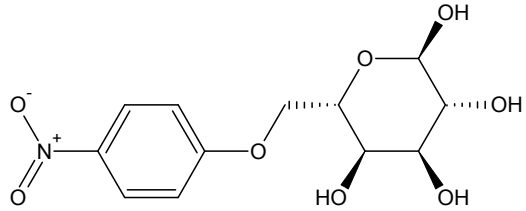

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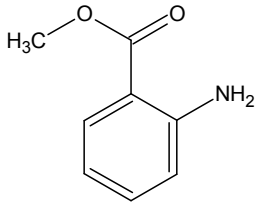

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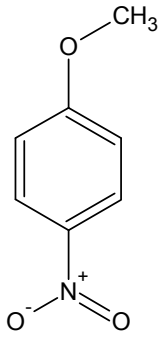

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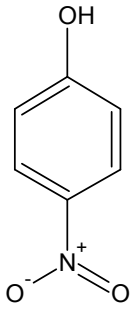

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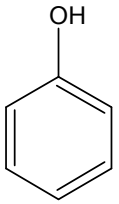

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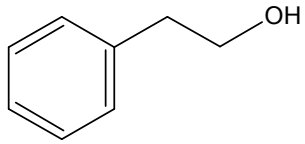
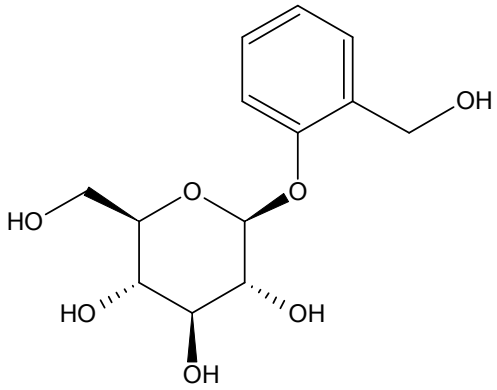


D-(-)-Salicin



Vanillin

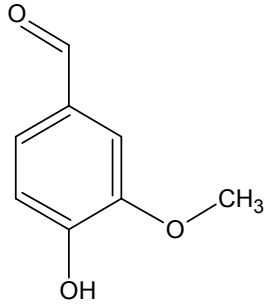


Table S1. Solubility (logS) of compounds in aqueous Na_2SO_4 solutions

Compounds	$[Na_2SO_4]$, M				
	0	0.25	0.5	0.75	1.0
Adenine	2.097	-2.224	-2.284	(-2.326)[c]	(-2.397)[c]
Adenosine	-1.710	-2.772	-2.757	-2.752	-2.752
Benzyl alcohol	-0.401	-0.538	-0.642	-0.788	-0.910
Caffeine	-0.845	-1.066	-1.240	-1.415	-1.658
Coumarin	-1.934	-2.035	-2.163	-2.292	-2.444
Glucoside[a]	-1.519	-1.638	-1.721	-1.836	-1.961
Guanosine	(-2.775)[c]	(-2.690)[c]	-2.666	-2.670	-2.687
4-Hydroxyacetanilide	-1.033	-1.169	-1.283	-1.407	-1.556
3-Hydroxybenzaldehyde	-1.141	-1.222	-1.312	-1.409	-1.490
Mannoside[b]	-1.788	-1.917	-2.000	-2.114	-2.260
Methyl Anthranilate	(-1.914)[c]	-1.963	-2.143	-2.347	-2.553
4-Nitroanisole	(-2.409)[c]	-3.102	-3.340	-3.640	-3.955
4-Nitrophenol	-0.939	-1.084	-1.166	-1.264	-1.399
Phenol	-0.029	-0.176	-0.302	-0.431	-0.556
2-Phenylethanol	-0.740	-0.888	-0.989	-0.978	-1.278
D-(-)-Salicin	-0.823	-0.951	-1.064	-1.172	-1.278
Vanillin	-1.155	-1.319	-1.413	-1.558	-1.719

[a] *p*-Nitrophenyl-α-D-glucopyranoside

[b] *p*-Nitrophenyl-α-D-mannopyranoside

[c] Solubility values in paranthesis were not included in calculations of salting-out constants

Table S2. Solubility (logS) of compounds in aqueous NaCl solutions

Compounds	[NaCl], M				
	0	0.5	1.0	1.5	2.0
Adenine	(-2.097)[c]	0.005728	-2.242	-2.281	-2.369
Adenosine	-1.710	0.018964	-1.722	-1.806	-1.889
Benzyl alcohol	(-0.401)[c]	0.358	-0.446	-0.525	-0.718
Caffeine	-0.845	0.1032	-0.986	-1.017	-1.186
Coumarin	-1.934	0.01029	-1.988	-2.035	-2.211
Glucoside[a]	-1.519	0.0250	-1.602	-1.650	-1.772
Guanosine	(-2.775)[c]	0.001631	-2.788	-2.752	-2.635
4-Hydroxyacetanilide	-1.033	0.0708	-1.150	-1.211	-1.400
3-Hydroxybenzaldehyde	-1.141	0.062707	-1.203	-1.274	-1.398
Mannoside[b]	-1.788	0.0134	-1.873	-1.936	-2.022
Methyl Anthranilate	(-1.914)[c]	0.0126	-1.900	-2.102	-2.222
4-Nitroanisole	-2.409	0.000797	-3.099	-3.272	-3.437
4-Nitrophenol	-0.939	0.08212	-1.086	-1.166	-1.297
Phenol	-0.029	0.697247	-0.157	-0.262	-0.448
2-Phenylethanol	-0.740	0.1512	-0.820	-0.910	(-1.017)[c]
D-(-)-Salicin	-0.823	0.12	-0.921	-1.011	-1.167
Vanillin	-1.155	0.05107	-1.292	-1.380	-1.538

[a] *p*-Nitrophenyl-α-D-glucopyranoside

[b] *p*-Nitrophenyl-α-D-mannopyranoside

[c] Solubility values in paranthesis were not included in calculations of salting-out constants

Table S3. Solubility (logS) of compounds in aqueous $NaClO_4$ solutions

Compounds	[$NaClO_4$], M				
	0	0.5	1.0	1.5	2.0
Adenine	(-2.097)[c]	-2.144	-2.082	-2.039	-2.004
Adenosine	(-1.710)[c]	-1.558	-1.503	-1.434	-1.375
Benzyl alcohol	-0.401	-0.426	-0.465	-0.510	-0.536
Coumarin	-1.934	-1.862	-1.742	-1.752	-1.685
Glucoside[a]	(-1.519)[c]	-1.497	(-2.472)[c]	-1.474	-1.461
Guanosine	(-2.775)[c]	-2.653	-2.524	-2.390	-2.305
4-Hydroxyacetanilide	-1.033	-1.073	-1.102	(-1.130)[c]	(-1.158)[c]
3-Hydroxybenzaldehyde	-1.141	-1.122	-1.109	-1.114	-1.098
Mannoside[b]	-1.788	-1.744	-1.692	-1.664	(-1.664)
Methyl Anthranilate	(-1.914)[c]	-1.849	-1.861	-1.724	-1.736
4-Nitroanisole	(-2.409)[c]	-2.851	-2.812	-2.695	-2.671
4-Nitrophenol	-0.939	(-0.970)[c]	-0.962	-0.970	-0.985
Phenol	-0.029	-0.099	-0.161	-0.249	-0.284
2-Phenylethanol	-0.740	-0.773	-0.812	-0.854	-0.892
D-(-)-Salicin	-0.823	(-0.883)[c]	-0.918	-0.962	-1.000
Vanillin	-1.155	-1.148	-1.121	-1.112	-1.082

[a] *p*-Nitrophenyl-α-D-glucopyranoside

[b] *p*-Nitrophenyl-α-D-mannopyranoside

[c] Solubility values in paranthesis were not included in calculations of salting-out constants

Table S4. Solubility (logS) of compounds in aqueous NaSCN solutions

Compounds	[NaSCN], M				
	0	0.5	1.0	1.5	2.0
Adenine	(-2.097)[c]	-2.123	-2.072	-2.033	-1.992
Adenosine	(-1.710)[c]	-1.567	-1.485	-1.382	-1.303
Benzyl alcohol	-0.401	-0.401	-0.346	-0.362	-0.360
Coumarin	-1.934	-1.817	-1.740	(-1.671)[c]	(-1.637)[c]
Glucoside[a]	(-1.519)[c]	-1.511	-1.454	-1.390	-1.338
Guanosine	(-2.775)[c]	-2.64	-2.477	-2.344	-2.228
4-Hydroxyacetanilide	-1.033	-1.031	-1.029	(-1.037)[c]	(-1.053)[c]
3-Hydroxybenzaldehyde	-1.141	-1.126	-1.109	-1.099	-1.075
Mannoside[b]	-1.788	-1.692	-1.601	-1.510	-1.440
Methyl Anthranilate	-1.914	-1.821	-1.787	-1.769	(-1.790)[c]
4-Nitroanisole	(-2.409)[c]	-2.841	-2.751	-2.706	-2.626
4-Nitrophenol	-0.939	-0.939	-0.898	-0.863	-0.856
Phenol	-0.029	-0.044	-0.067	-0.078	-0.106
2-Phenylethanol	-0.740	-0.695	-0.660	-0.620	-0.580
D-(-)-Salicin	(-0.823)[c]	-0.829	(-0.842)[c]	-0.827	-0.826
Vanillin	-1.155	-1.115	-1.055	-0.991	-0.955

[a] *p*-Nitrophenyl-α-D-glucopyranoside

[b] *p*-Nitrophenyl-α-D-mannopyranoside

[c] Solubility values in paranthesis were not included in calculations of salting-out constants

Table S5. Setschenow constants k_{salt} reported in the literature

Compound	k_{Na2SO4}	k_{NaCl}	k_{NaClO4}	Data from
Adenine	0.24	0.06	-0.12	[S1]
Benzene	0.548	0.195	-0.106	[S4]
Caffeine	0.76 ± 0.01	0.17 ± 0.007	-0.55 ± 0.03	[S2]
Cytosine	0.00	-0.06	-0.13	[S1]
Deoxyadenosine	0.45	0.11	-0.26	[S1]
Naphthalene	0.668	0.222	0.113	[S3]
Pyrene	0.732	0.208	0.105	[S3]
Perylene	0.609	0.259	0.166	[S3]
Theobromine	0.42 ± 0.003	0.056 ± 0.05	-0.37 ± 0.02	[S2]
Theophylline	0.47 ± 0.02	0.11 ± 0.01	-0.38 ± 0.01	[S2]
Thymine	0.16	0.02	-0.20	[S1]
Toluene	0.67 ± 0.024	0.22 ± 0.029	-0.139	[S5]

S1. Robinson D.R., Grant M.E. The effects of aqueous salt solutions on the activity coefficients of purine and pyrimidine bases and their relation to the denaturation of deoxyribonucleic acid by salts. J. Biol. Chem., 1966, 241, 4030-4042.

S2. Al-Maaieh, A., Flanagan, D.R. Salt effects on caffeine solubility, distribution, and self-association. J. Pharm. Sci., 2002, 91, 1000-1008.

S3. Schlautman, M.A., Yun, S., Carraway, E.R., Lee, J.H., Herbert, B.E. Testing a surface tension-based model to predict the salting out of polycyclic aromatic hydrocarbons in model environmental solutions. Water Res., 2004, 38, 3331-3339.

S4. McDevit W., Long F.A. The activity coefficients of benzene in aqueous salt solutions. J. Am. Chem. Soc., 1952, 74, 1773-1777.

S5. Poulson S.R., Harrington R.R., Drever J.I. The solubility of toluene in aqueous salt solutions. Talanta, 1999, 48, 633-641.

Table S6. Setschenow constants k_{salt} values reported in the literature for compounds indicated*

#	Compound	k_{salt} Na_2SO_4	k_{salt} NaCl	k_{salt} NaClO4	k_{salt} NaSCN
1	AG1E	-0.02	-0.04	-0.08	-0.03
2	AG2E	0.2	0.05	0	-0.1
3	AG3E	0.36	0.11	0.03	-0.21
4	AG4E	0.52	0.05	-0.32	-0.26
5	Formamide	0.55	0.09	-0.21	-0.09
6	Acetamide	0.56	0.16	-0.03	0
7	N-Methylacetamide	0.58	0.13	-0.13	0.01

* AG1E – acetylglycine ethyl ester; AG2E – acetyldiglycine ethyl ester; AG3E – acetyltriglycine ethyl ester; AG4E – acetyltetraglycine ethyl ester; data taken from P. K. Nandi, D. R. Robinson, J. Am. Chem. Soc., 1972, 94, 1299

Table S7. Partition coefficients of polar organic compounds in aqueous PEG-8000-sodium sulfate two-phase systems with different salt additives at the concentrations indicated

	NaCl	$NaClO_4$	NaSCN	NaH_2PO_4	NaCl	$NaClO_4$	NaSCN	NaH_2PO_4	Data from
Compounds	~0.10 M				~1.10 M				
Adenine	2.8	3.78	3.7	2.61					[S6]
Adenosine	2.897	3.113	3.074	2.631	4.208	2.662	2.63	2.182	[S7]
AMP	0.88	0.65	0.678	1.41					[S6]
ADP	0.6	0.4	0.431	0.86					[S6]
ATP	0.46	0.26	0.29	0.57					[S6]
4-Aminophenol	3.49	4.14	3.983	-	5.246	5.759	4.83	-	[S7]
Caffeine	1.969	2.38	2.265	2.125	2.376	2.04	1.863	5.2	[S7]
Glucoside[a]	2.348	2.69	2.589	2.542	3.355	3.423	2.869	8.8	[S7]
Guanosine	1.718	1.75	1.739	1.804	2.335	1.391	1.529	2.877	[S7]
4-Hydroxyacetanilide	6.657	8.969	8.5	7.36	14.31	15.649	9.9	42	[S7]
3-Hydroxybenzaldehyde	5.63	7.9	7.4	6.347	10.859	15.9	9.3	33.6	[S7]
Mannoside[b]	2.309	2.706	2.649	2.553	3.432	3.883	3.139	9.32	[S7]
4-Nitroanisole	5.838	8.591	7.7	6.7	11.551	20.908	10.4	69	[S7]
Phenol	5.701	7.7	7.4	6.2	12	17	10.1	37	[S7]
D-(-)-Salicin	2.054	2.178	2.175	2.256	2.944	2.661	2.606	6.2	[S7]
1,3,5-Trihydroxybenzene	12.5	16.2	15.54	-	31.7	20.8	14.64	-	[S7]

[a] *p*-Nitrophenyl-α-D-glucopyranoside; [b] *p*-Nitrophenyl-α-D-mannopyranoside

S6. da Silva, N., Ferreira, L.A., Mikheeva, L.M., Teixeira, J., Zaslavsky, B.Y. Origin of salt additive effect on solute partitioning in aqueous PEG- sodium sulfate two-phase system. J. Chromatogr. A, 2014, 1337, 3-8.

S7. Ferreira, L. A., Teixeira, J. A., Mikheeva, L. M., Chait, A., Zaslavsky, B.Y. Effect of salt additives on partition of nonionic solutes in aqueous PEG–sodium sulfate two-phase system J. Chromatogr. A, 2011, 1218, 5031-5039.