Supplementary Information

Fast Screening of Solvents for Simultaneous Extraction of Furfural, 5-Hydroxymethylfurfural and Levulinic Acid from Aqueous Solution Using SMD Solvation Free Energies

Ellen V. Dalessandro and Josefredo R. Pliego Jr.*

Departamento de Ciências Naturais, Universidade Federal de São João del-Rei, 36301-160 São João del-Rei-MG, Brazil

*e-mail: pliego@ufsj.edu.br

Table S1. Solvation free energies of furfural in 179 solvents calculated by the SMD model and the X3LYP/6-31(+)G(d) electronic density

Solvent	ΔG_{solv} / (kcal mol^{-1})	$\Delta\Delta G_{solv}$ (w $\rightarrow$ org) / (kcal mol^{-1})
Propanal	–6.39	–3.57
Bromoethane	–6.33	–3.51
2-Bromopropane	–6.33	–3.51
2-Pentanone	–6.33	–3.51
1,1,1-Trichloroethane	–6.33	–3.51
Butanone	–6.31	–3.49
1-Chloropropane	–6.31	–3.49
sec-Butyl chloride	–6.29	–3.47
Tributyl phosphate	–6.29	–3.47
4-Methyl-2-pentanone	–6.27	–3.45
3-Pentanone	–6.26	–3.44
Butanonitrile	–6.21	–3.39
Butanal	–6.20	–3.38
Fluorobenzene	–6.19	–3.37
Benzaldehyde	–6.18	–3.36
2-Hexanone	–6.17	–3.35
4-Heptanone	–6.16	–3.34
1-Bromo-2-methylpropane	–6.15	–3.33
1-Bromopropane	–6.11	–3.29
2-Nitropropane	–6.07	–3.25
Benzonitrile	–6.06	–3.24
2-Heptanone	–6.06	–3.24
o-Dichlorobenzene	–6.06	–3.24
Diphenyl ether	–6.06	–3.24
Propanonitrile	–6.06	–3.24
Acetone	–6.04	–3.22
Nitrobenzene	–6.04	–3.22
Ethanethiol	–6.04	–3.22
5-Nonanone	–6.03	–3.21
1-Nitropropane	–6.02	–3.2
Pyridine	–6.02	–3.2

Pentanal	–6.00	–3.18
Ethyl formate	–5.99	–3.17
2-Methylpyridine	–5.99	–3.17
3-Methylpyridine	–5.99	–3.17
4-Methylpyridine	–5.98	–3.16
2-Octanone	–5.98	–3.16
Iodoethane	–5.97	–3.15
1-Chloropentane	–5.93	–3.11
2,4-Dimethylpyridine	–5.93	–3.11
Chlorobenzene	–5.91	–3.09
N,*N*-Dimethylacetamide	–5.89	–3.07
Methyl formate	–5.89	–3.07
Acetophenone	–5.87	–3.05
1-Iodopropane	–5.86	–3.04
2,6-Dimethylpyridine	–5.85	–3.03
Diethyl ether	–5.83	–3.01
Iodomethane	–5.82	–3
o-Nitrotoluene	–5.82	–3
Diethyl sulfide	–5.81	–2.99
1-Bromopentane	–5.79	–2.97
1-Iodobutane	–5.79	–2.97
Bromobenzene	–5.78	–2.96
N,*N*-Dimethylformamide	–5.78	–2.96
Dimethyl disulfide	–5.77	–2.95
1-Chlorohexane	–5.76	–2.94
Ethyl acetate	–5.74	–2.92
Nitroethane	–5.73	–2.91
Methyl acetate	–5.72	–2.9
Cyclopentanone	–5.70	–2.88
Tetrahydrofuran	–5.69	–2.87
Methyl propanoate	–5.68	–2.86
1-Iodopentane	–5.66	–2.84
Propyl acetate	–5.66	–2.84
Benzyl chloride	–5.65	–2.83
Cyclohexanone	–5.65	–2.83

Dichloromethane	–5.64	–2.82
Methyl butanoate	–5.62	–2.8
o-Chlorotoluene	–5.60	–2.78
Acetonitrile	–5.55	–2.73
Diisopropyl ether	–5.51	–2.69
Butyl acetate	–5.50	–2.68
Iodobenzene	–5.47	–2.65
1-Bromooctane	–5.45	–2.63
Pentyl acetate	–5.44	–2.62
cis-Dichloroethylene	–5.42	–2.6
Methyl benzoate	–5.40	–2.58
1-Fluorooctane	–5.38	–2.56
Ethylphenyl ether	–5.33	–2.51
Anisole	–5.25	–2.43
1,2-Dichloroethane	–5.22	–2.4
Nitromethane	–5.14	–2.32
Dimethyl sulfoxide	–5.11	–2.29
Thiophene	–5.01	–2.19
Carbon tetrachloride	–5.00	–2.18
Benzene	–4.98	–2.16
Toluene	–4.92	–2.1
Dibromomethane	–4.89	–2.07
Dibutyl ether	–4.84	–2.02
o-Xylene	–4.84	–2.02
Ethylbenzene	–4.80	–1.98
1-Iodohexadecane	–4.79	–1.97
Xylene (mixture)	–4.77	–1.95
Carbon disulfide	–4.75	–1.93
m-Xylene	–4.75	–1.93
Isopropylbenzene	–4.74	–1.92
Diethylamine	–4.70	–1.88
E-2-Pentene	–4.70	–1.88
p-Xylene	–4.70	–1.88
Tetralin	–4.70	–1.88
Triethylamine	–4.68	–1.86

1-Pentene	–4.68	–1.86
Mesitylene	–4.67	–1.85
Perfluorobenzene	–4.67	–1.85
tert-Butylbenzene	–4.67	–1.85
Trichloroethene	–4.67	–1.85
1,2,4-Trimethylbenzene	–4.65	–1.83
1-Hexene	–4.63	–1.81
p-Isopropyltoluene	–4.63	–1.81
sec-Butylbenzene	–4.63	–1.81
Chloroform	–4.62	–1.8
n-Butylbenzene	–4.60	–1.78
Tetrachloroethene	–4.59	–1.77
Thiophenol	–4.57	–1.75
1,1,2-Trichloroethane	–4.57	–1.75
2-Propanol	–4.55	–1.73
2-Methyl-2-propanol	–4.49	–1.67
2,2,4-Trimethylpentane	–4.46	–1.64
2-Methylpentane	–4.46	–1.64
n-Pentane	–4.45	–1.63
2,4-Dimethylpentane	–4.43	–1.61
2-Butanol	–4.39	–1.57
n-Hexane	–4.38	–1.56
Ethanol	–4.36	–1.54
n-Heptane	–4.32	–1.5
Methylcyclohexane	–4.28	–1.46
Cyclopentane	–4.27	–1.45
n-Octane	–4.27	–1.45
1,2-Dibromoethane	–4.25	–1.43
1-Propanol	–4.24	–1.42
2-Methyl-1-propanol	–4.23	–1.41
n-Nonane	–4.23	–1.41
cis-1,2-Dimethylcyclohexane	–4.22	–1.4
n-Undecane	–4.22	–1.4
Dipropylamine	–4.21	–1.39
n-Decane	–4.20	–1.38

Propylamine	–4.20	–1.38
Cyclohexane	–4.18	–1.36
n-Dodecane	–4.14	–1.32
trans-Decalin	–4.12	–1.3
1-Butanol	–4.08	–1.26
2-Propen-1-ol	–4.08	–1.26
Decalin (*cis*/*trans* mixture)	–4.07	–1.25
N-Methylaniline	–4.07	–1.25
n-Pentadecane	–4.07	–1.25
n-Hexadecane	–4.05	–1.23
Methanol	–4.04	–1.22
cis-Decalin	–4.02	–1.2
Butylamine	–4.01	–1.19
1-Pentanol	–4.00	–1.18
Tetrahydrothiophene-*S*,*S*-dioxide	–3.94	–1.12
Pentylamine	–3.91	–1.09
Phenylmethanol	–3.90	–1.08
2-Methoxyethanol	–3.90	–1.08
1-Hexyne	–3.89	–1.07
Cyclopentanol	–3.86	–1.04
1-Hexanol	–3.86	–1.04
1-Heptanol	–3.74	–0.92
1,4-Dioxane	–3.66	–0.84
trans-Dichloroethylene	–3.64	–0.82
1-Octanol	–3.61	–0.79
Aniline	–3.56	–0.74
Bromoform	–3.52	–0.7
N-Methylformamide (*E*/*Z* mixture)	–3.47	–0.65
1-Nonanol	–3.43	–0.61
1-Decanol	–3.25	–0.43
Diiodomethane	–3.01	–0.19
Water	–2.82	0
2,2,2-Trifluoroethanol	–1.88	0.94
m-Cresol	–1.72	1.1
o-Cresol	–1.60	1.22

1,2-Ethanediol	–0.50	2.32
Acetic acid	–0.30	2.52
Formamide	0.45	3.27
Propanoic acid	0.64	3.46
Formic acid	0.85	3.67
Butanoic acid	0.97	3.79
Pentanoic acid	1.30	4.12
Hexanoic acid	1.45	4.27

Table S2. Solvation free energies of 5-hydroxymethylfurfural in 179 solvents calculated by the SMD model and the X3LYP/6-31(+)G(d) electronic density

Solvent	ΔG_{solv} / (kcal mol^{-1})	$\Delta\Delta G_{solv}$ (w $\rightarrow$ org) / (kcal mol^{-1})
Tributyl phosphate	–9.51	–3.21
Propanal	–8.92	–2.62
2-Pentanone	–8.91	–2.61
Butanone	–8.88	–2.58
4-Methyl-2-pentanone	–8.83	–2.53
3-Pentanone	–8.82	–2.52
Acetone	–8.72	–2.42
2-Hexanone	–8.71	–2.41
4-Heptanone	–8.70	–2.40
Butanal	–8.69	–2.39
Benzaldehyde	–8.65	–2.35
Butanonitrile	–8.61	–2.31
N,*N*-Dimethylacetamide	–8.61	–2.31
2-Bromopropane	–8.59	–2.29
2-Methylpyridine	–8.59	–2.29
Bromoethane	–8.57	–2.27
2-Heptanone	–8.57	–2.27
Pyridine	–8.56	–2.26
1,1,1-Trichloroethane	–8.56	–2.26
2,4-Dimethylpyridine	–8.55	–2.25
3-Methylpyridine	–8.55	–2.25

5-Nonanone	–8.54	–2.24
4-Methylpyridine	–8.53	–2.23
1-Chloropropane	–8.52	–2.22
Propanonitrile	–8.52	–2.22
sec-Butyl chloride	–8.52	–2.22
2-Octanone	–8.48	–2.18
Benzonitrile	–8.45	–2.15
2,6-Dimethylpyridine	–8.45	–2.15
Pentanal	–8.45	–2.15
N,*N*-Dimethylformamide	–8.42	–2.12
2-Nitropropane	–8.42	–2.12
Fluorobenzene	–8.40	–2.10
Nitrobenzene	–8.38	–2.08
Diphenyl ether	–8.38	–2.08
1-Bromo-2-methylpropane	–8.36	–2.06
Ethyl formate	–8.36	–2.06
Acetophenone	–8.34	–2.04
Ethanethiol	–8.33	–2.03
1-Nitropropane	–8.33	–2.03
1-Bromopropane	–8.30	–2.00
Methyl formate	–8.23	–1.93
Diethyl ether	–8.20	–1.90
o-Dichlorobenzene	–8.20	–1.90
Iodoethane	–8.18	–1.88
Cyclopentanone	–8.13	–1.83
Diethyl sulfide	–8.12	–1.82
Cyclohexanone	–8.11	–1.81
Ethyl acetate	–8.11	–1.81
Methyl acetate	–8.09	–1.79
o-Nitrotoluene	–8.09	–1.79
Tetrahydrofuran	–8.09	–1.79
Nitroethane	–8.08	–1.78
1-Chloropentane	–8.05	–1.75
Methyl propanoate	–8.05	–1.75
Chlorobenzene	–8.04	–1.74

Dimethyl disulfide	–8.04	–1.74
1-Iodopropane	–8.04	–1.74
Propyl acetate	–8.03	–1.73
Iodomethane	–7.98	–1.68
Methyl butanoate	–7.97	–1.67
Benzyl chloride	–7.95	–1.65
1-Iodobutane	–7.95	–1.65
Bromobenzene	–7.91	–1.61
1-Bromopentane	–7.91	–1.61
Dichloromethane	–7.89	–1.59
1-Chlorohexane	–7.85	–1.55
Butyl acetate	–7.83	–1.53
Diisopropyl ether	–7.81	–1.51
Acetonitrile	–7.80	–1.50
1-Iodopentane	–7.78	–1.48
Pentyl acetate	–7.76	–1.46
Methyl benzoate	–7.75	–1.45
2-Propanol	–7.72	–1.42
Dimethyl sulfoxide	–7.71	–1.41
Ethanol	–7.66	–1.36
o-Chlorotoluene	–7.65	–1.35
cis-Dichloroethylene	–7.62	–1.32
Methanol	–7.59	–1.29
Iodobenzene	–7.57	–1.27
Nitromethane	–7.56	–1.26
2-Methyl-2-propanol	–7.56	–1.26
Ethylphenyl ether	–7.54	–1.24
2-Butanol	–7.52	–1.22
1-Propanol	–7.51	–1.21
1-Bromooctane	–7.49	–1.19
2-Methyl-1-propanol	–7.49	–1.19
1,2-Dichloroethane	–7.43	–1.13
Anisole	–7.41	–1.11
2-Propen-1-ol	–7.38	–1.08
1-Fluorooctane	–7.36	–1.06

1-Butanol	–7.30	–1.00
1-Pentanol	–7.20	–0.90
Diethylamine	–7.19	–0.89
Triethylamine	–7.12	–0.82
Dibromomethane	–7.03	–0.73
Dibutyl ether	–7.01	–0.71
1-Hexanol	–7.01	–0.71
2-Methoxyethanol	–6.99	–0.69
Thiophene	–6.99	–0.69
Benzene	–6.94	–0.64
Phenylmethanol	–6.93	–0.63
1,1,2-Trichloroethane	–6.89	–0.59
Chloroform	–6.86	–0.56
N-Methylformamide (*E*/*Z* mixture)	–6.86	–0.56
Toluene	–6.86	–0.56
1-Heptanol	–6.85	–0.55
Carbon tetrachloride	–6.83	–0.53
Cyclopentanol	–6.82	–0.52
o-Xylene	–6.78	–0.48
Propylamine	–6.78	–0.48
Ethylbenzene	–6.72	–0.42
1-Iodohexadecane	–6.70	–0.40
Xylene (mixture)	–6.69	–0.39
Thiophenol	–6.68	–0.38
1-Octanol	–6.67	–0.37
m-Xylene	–6.66	–0.36
Isopropylbenzene	–6.65	–0.35
Tetralin	–6.65	–0.35
Carbon disulfide	–6.62	–0.32
N-Methylaniline	–6.61	–0.31
p-Xylene	–6.61	–0.31
Mesitylene	–6.59	–0.29
Trichloroethene	–6.58	–0.28
1,2,4-Trimethylbenzene	–6.57	–0.27
Dipropylamine	–6.56	–0.26

tert-Butylbenzene	–6.56	–0.26
Butylamine	–6.55	–0.25
p-Isopropyltoluene	–6.53	–0.23
sec-Butylbenzene	–6.51	–0.21
E-2-Pentene	–6.49	–0.19
n-Butylbenzene	–6.46	–0.16
1-Pentene	–6.46	–0.16
1-Nonanol	–6.43	–0.13
Pentylamine	–6.42	–0.12
1-Hhexene	–6.39	–0.09
Perfluorobenzene	–6.38	–0.08
Tetrachloroethene	–6.33	–0.03
Water	–6.30	0.00
1,2-Dibromoethane	–6.27	0.03
Tetrahydrothiophene-*S*,*S*-dioxide	–6.25	0.05
1-Decanol	–6.18	0.12
2,2,4-Trimethylpentane	–6.12	0.18
2-Methylpentane	–6.11	0.19
n-Pentane	–6.10	0.20
2,4-Dimethylpentane	–6.08	0.22
Aniline	–6.07	0.23
n-Hexane	–6.01	0.29
n-Heptane	–5.95	0.35
Methylcyclohexane	–5.91	0.39
n-Octane	–5.89	0.41
Cyclopentane	–5.88	0.42
cis-1,2-Dimethylcyclohexane	–5.83	0.47
n-Nonane	–5.83	0.47
n-Undecane	–5.83	0.47
n-Decane	–5.79	0.51
Cyclohexane	–5.78	0.52
trans-Decalin	–5.73	0.57
n-Dodecane	–5.72	0.58
1,4-Dioxane	–5.71	0.59
Decalin (*cis*/*trans* mixture)	–5.66	0.64

1-Hexyne	–5.66	0.64
n-Pentadecane	–5.64	0.66
n-Hexadecane	–5.62	0.68
cis-Decalin	–5.60	0.70
Bromoform	–5.54	0.76
trans-Dichloroethylene	–5.30	1.00
Diiodomethane	–4.84	1.46
2,2,2-Trifluoroethanol	–4.68	1.62
m-Cresol	–4.58	1.72
o-Cresol	–4.29	2.01
1,2-Ethanediol	–3.47	2.83
Acetic acid	–2.72	3.58
Formamide	–2.15	4.15
Formic acid	–1.44	4.86
Propanoic acid	–1.35	4.95
Butanoic acid	–0.87	5.43
Pentanoic acid	–0.39	5.91
Hexanoic acid	–0.18	6.12

Table S3. Solvation free energies of levulinic acid in 179 solvents calculated by the SMD model and the X3LYP/6-31(+)G(d) electronic density

Solvent	ΔG_{solv} / (kcal mol^{-1})	$\Delta\Delta G_{solv}$ / (kcal mol^{-1})
Tributyl phosphate	–10.71	–4.29
2-Pentanone	–9.28	–2.86
N,*N*-Dimethylacetamide	–9.27	–2.85
Butanone	–9.25	–2.83
Propanal	–9.22	–2.80
4-Methyl-2-pentanone	–9.21	–2.79
3-Pentanone	–9.19	–2.77
2,4-Dimethylpyridine	–9.09	–2.67
2-Hexanone	–9.09	–2.67
4-Heptanone	–9.08	–2.66
Acetone	–9.06	–2.64

2-Methylpyridine	–9.06	–2.64
N,*N*-Dimethylformamide	–9.04	–2.62
2,6-Dimethylpyridine	–9.01	–2.59
Butanal	–9.00	–2.58
3-Methylpyridine	–8.98	–2.56
2-Heptanone	–8.96	–2.54
Pyridine	–8.96	–2.54
4-Methylpyridine	–8.95	–2.53
5-Nonanone	–8.93	–2.51
Benzaldehyde	–8.90	–2.48
2-Octanone	–8.88	–2.46
Butanonitrile	–8.80	–2.38
Pentanal	–8.77	–2.35
Propanonitrile	–8.70	–2.28
Acetophenone	–8.68	–2.26
Benzonitrile	–8.61	–2.19
Ethyl formate	–8.61	–2.19
2-Bromopropane	–8.57	–2.15
2-Nitropropane	–8.57	–2.15
2-Propanol	–8.57	–2.15
Cyclohexanone	–8.54	–2.12
Diethyl ether	–8.54	–2.12
Bromoethane	–8.52	–2.10
Cyclopentanone	–8.52	–2.10
Diphenyl ether	–8.51	–2.09
1,1,1-Trichloroethane	–8.50	–2.08
2-Methyl-2-propanol	–8.49	–2.07
Nitrobenzene	–8.48	–2.06
Dimethyl sulfoxide	–8.48	–2.06
Methyl formate	–8.48	–2.06
sec-Butyl chloride	–8.48	–2.06
Ethyl acetate	–8.47	–2.05
1-Nitropropane	–8.47	–2.05
Tetrahydrofuran	–8.47	–2.05
1-Chloropropane	–8.46	–2.04

Ethanethiol	–8.44	–2.02
Methyl acetate	–8.43	–2.01
Methyl propanoate	–8.40	–1.98
Propyl acetate	–8.39	–1.97
2-Butanol	–8.37	–1.95
Fluorobenzene	–8.37	–1.95
Acetonitrile	–8.34	–1.92
Diethyl sulfide	–8.34	–1.92
Methyl butanoate	–8.33	–1.91
1-Bromo-2-methylpropane	–8.32	–1.90
Ethanol	–8.31	–1.89
1-Bromopropane	–8.26	–1.84
Nitroethane	–8.23	–1.81
2-Methoxyethanol	–8.22	–1.80
Butyl acetate	–8.21	–1.79
Iodoethane	–8.19	–1.77
o-Nitrotoluene	–8.19	–1.77
Dimethyl disulfide	–8.18	–1.76
Benzyl chloride	–8.17	–1.75
Diisopropyl ether	–8.17	–1.75
1-Propanol	–8.16	–1.74
2-Methyl-1-propanol	–8.14	–1.72
Pentyl acetate	–8.14	–1.72
Diethylamine	–8.12	–1.70
Methyl benzoate	–8.11	–1.69
Methanol	–8.08	–1.66
o-Dichlorobenzene	–8.07	–1.65
1-Iodopropane	–8.05	–1.63
2-Propen-1-ol	–8.01	–1.59
1-Chloropentane	–8.00	–1.58
Chlorobenzene	–7.98	–1.56
Iodomethane	–7.97	–1.55
Triethylamine	–7.97	–1.55
1-Iodobutane	–7.97	–1.55
1-Butanol	–7.95	–1.53

1-Bromopentane	–7.89	–1.47
Bromobenzene	–7.88	–1.46
1-Pentanol	–7.84	–1.42
1-Chlorohexane	–7.81	–1.39
1-Iodopentane	–7.81	–1.39
Ethylphenyl ether	–7.79	–1.37
Phenylmethanol	–7.77	–1.35
Nitromethane	–7.71	–1.29
Dichloromethane	–7.71	–1.29
Cyclopentanol	–7.69	–1.27
1-Hexanol	–7.65	–1.23
Anisole	–7.62	–1.20
o-Chlorotoluene	–7.61	–1.19
Iodobenzene	–7.59	–1.17
N-Methylformamide (*E*/*Z* mixture)	–7.52	–1.10
Dipropylamine	–7.49	–1.07
1-Heptanol	–7.49	–1.07
1-Bromooctane	–7.48	–1.06
Dibutyl ether	–7.44	–1.02
Propylamine	–7.44	–1.02
cis-Dichloroethylene	–7.40	–0.98
1-Fluorooctane	–7.36	–0.94
1-Octanol	–7.31	–0.89
1,2-Dichloroethane	–7.30	–0.88
Butylamine	–7.21	–0.79
Thiophene	–7.10	–0.68
Pentylamine	–7.09	–0.67
N-Methylaniline	–7.07	–0.65
Benzene	–7.06	–0.64
1-Nonanol	–7.06	–0.64
Tetrahydrothiophene-*S*,*S*-dioxide	–7.02	–0.60
Toluene	–6.98	–0.56
Dibromomethane	–6.92	–0.50
o-Xylene	–6.91	–0.49
Ethylbenzene	–6.84	–0.42

Xylene (mixture)	–6.83	–0.41
1-Decanol	–6.81	–0.39
m-Xylene	–6.80	–0.38
Tetralin	–6.80	–0.38
Carbon tetrachloride	–6.79	–0.37
Isopropylbenzene	–6.79	–0.37
1-Iodohexadecane	–6.77	–0.35
Mesitylene	–6.77	–0.35
Trichloroethene	–6.77	–0.35
p-Xylene	–6.76	–0.34
Chloroform	–6.75	–0.33
Thiophenol	–6.74	–0.32
1,1,2-Trichloroethane	–6.74	–0.32
1,2,4-Trimethylbenzene	–6.74	–0.32
p-Isopropyltoluene	–6.72	–0.30
Aniline	–6.71	–0.29
tert-Butylbenzene	–6.70	–0.28
Carbon disulfide	–6.65	–0.23
sec-Butylbenzene	–6.65	–0.23
n-Butylbenzene	–6.59	–0.17
E-2-Pentene	–6.54	–0.12
1-Pentene	–6.52	–0.10
1-Hexene	–6.44	–0.02
Water	–6.42	0.00
1,4-Dioxane	–6.40	0.02
Perfluorobenzene	–6.35	0.07
Tetrachloroethene	–6.29	0.13
1,2-Dibromoethane	–6.27	0.15
2,2,4-Trimethylpentane	–6.11	0.31
2-Methylpentane	–6.10	0.32
n-Pentane	–6.09	0.33
2,4-Dimethylpentane	–6.07	0.35
n-Hexane	–6.00	0.42
n-Heptane	–5.93	0.49
Methylcyclohexane	–5.89	0.53

Cyclopentane	–5.87	0.55
n-Octane	–5.87	0.55
n-Nonane	–5.81	0.61
n-Undecane	–5.81	0.61
cis-1,2-Dimethylcyclohexane	–5.80	0.62
n-Secane	–5.77	0.65
Cyclohexane	–5.76	0.66
n-Dodecane	–5.70	0.72
trans-Decalin	–5.69	0.73
Decalin (*cis*/*trans* mixture)	–5.63	0.79
n-Pentadecane	–5.61	0.81
n-Hexadecane	–5.60	0.82
1-Hhexyne	–5.59	0.83
cis-Decalin	–5.56	0.86
Bromoform	–5.49	0.93
trans-Dichloroethylene	–5.29	1.13
Diiodomethane	–4.97	1.45
m-Cresol	–4.74	1.68
2,2,2-Trifluoroethanol	–4.72	1.70
o-Cresol	–4.46	1.96
1,2-Ethanediol	–4.12	2.30
Acetic acid	–2.92	3.50
Formamide	–2.54	3.88
Propanoic acid	–1.54	4.88
Formic acid	–1.40	5.02
Butanoic acid	–1.04	5.38
Pentanoic acid	–0.55	5.87
Hexanoic acid	–0.33	6.09

Table S4. Comparison between theoretical and experimental free energy of transfer from water to organic solvent

Solvent	K_c	Furfural	
		$\Delta\Delta G$ (w $\rightarrow$ org) / (kcal mol^{-1})	
	Experimental	Experimental	Theory
Toluene	5.3	–0.98	–2.10
Methyl benzoate	10.8	–1.41	–2.58
p-Xylene	2.9	–0.63	–1.88
1-Octanol	2.8	–0.61	–0.79
MIBK	9.5	–1.34	–3.45
Solvent	K_c	HMF	
		$\Delta\Delta G$ (w $\rightarrow$ org) / (kcal mol^{-1})	
	Experimental	Experimental	Theory
MIBK	1.04	–0.02	–2.53
1-Butanol	1.59	–0.27	–1.00
1-Pentanol	1.14	–0.08	–0.90
1-Hexanol	0.63	0.27	–0.71
1-Heptanol	0.33	0.66	–0.55

K_c is the partition coefficient.