

Supplementary information

HPLC-EAT (Environmental Assessment Tool): A tool for profiling safety, health and environmental impacts of liquid chromatography methods

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Table 1 Safety, health and environmental factors for solvents commonly used in HPLC chromatography as determined by EHS method¹

	Safety				Health		Environment			S	H	E
Substance	Release potential	Fire/ Explos.	React./ Decom.	Acute toxicity	Irritation	Chronic toxicity	Persis- tency	Air Hazard	Water Hazard			
Acetone	0.698	1.000	0.000	0.297	0.625	0.184	0.126	0.184	0.000	1.995	0.809	0.310
Acetonitrile	0.615	1.000	0.600	0.510	0.625	0.431	0.341	0.431	0.000	2.724	1.056	0.772
Chloroform	0.684	0.000	0.000	0.394	0.625	0.800	0.457	0.800	0.178	1.077	1.425	1.435
Dichloromethane	0.753	1.000	0.600	0.265	0.349	0.289	0.023	0.289	0.031	2.618	0.638	0.343
Ethanol	0.580	1.000	0.000	0.292	0.000	0.204	0.282	0.204	0.000	1.872	0.204	0.485
Ethyl acetate	0.619	1.000	0.000	0.276	0.625	0.171	0.026	0.171	0.003	1.895	0.796	0.199
Heptane	0.557	1.000	0.000	0.368	0.625	0.159	0.430	0.159	0.500	1.925	0.784	1.089
Hexane (n)	0.661	1.000	0.000	0.343	0.625	0.349	0.426	0.349	0.325	2.004	0.974	1.100
Isooctane	0.630	1.000	0.000	0.000	0.330	0.000	0.680	0.000	0.875	1.630	0.330	1.555
Isopropanol	0.556	1.000	0.000	0.318	0.625	0.260	0.280	0.260	0.000	1.874	0.885	0.540
Methanol	0.646	1.000	0.000	0.267	0.113	0.317	0.000	0.317	0.000	1.912	0.430	0.317
Sulfuric acid 96%	0.000	0.000	0.800	0.956	1.000	1.000	0.485	1.000	0.500	1.756	2.000	1.985
<i>t</i> -butyl methyl ether	0.720	1.000	0.000	0.000	0.220	0.350	0.710	0.350	0.090	1.720	0.570	1.150
Tetrahydrofuran	0.667	1.000	0.000	0.298	0.625	0.365	0.535	0.365	0.000	1.965	0.990	0.900

Table 2 Six parameters of the GSK's solvent selection guide and their reciprocal values which have been used in our study to evaluate the greenness of the HPLC study cases

Solvent	Scores originally used in The GSK's solvent selection guide system ²						Reciprocal of the scores which are used in our study					
	Waste Recycling, incineration, VOC, and biotreatment	Environmental impact fate and effects on the environment	Health Acute and chronic effects on human health and exposure potential	Flammability & Explosion Storage and handling	Reactivity & Stability Factors affecting the stability of the solvent	Life cycle score	Waste	Environmental impact	Health	Flammability & Explosion	Reactivity & Stability	Life cycle score
Acetone	3	9	8	4	9	7	0.33	0.11	0.13	0.25	0.11	0.14
Acetonitrile	2	6	6	6	10	3	0.50	0.17	0.17	0.17	0.10	0.33
Chloroform	3	6	3	6	9	6	0.33	0.17	0.33	0.17	0.11	0.17
Dichloromethane	3	6	4	6	9	7	0.33	0.17	0.25	0.17	0.11	0.14
Ethanol	3	8	8	6	9	9	0.33	0.13	0.13	0.17	0.11	0.11
Ethyl acetate	4	8	8	4	8	6	0.25	0.13	0.13	0.25	0.13	0.17
Heptane	6	3	8	3	10	7	0.17	0.33	0.13	0.33	0.10	0.14
Hexane	5	3	4	2	10	7	0.20	0.33	0.25	0.50	0.10	0.14
Isooctane	6	4	8	3	10	7	0.17	0.25	0.13	0.33	0.10	0.14
Iso-propanol	3	9	8	6	8	4	0.33	0.11	0.13	0.17	0.13	0.25
Methanol	4	9	5	5	10	9	0.25	0.11	0.20	0.20	0.10	0.11
<i>t</i> -Butyl methyl ether	4	5	5	3	9	8	0.25	0.20	0.20	0.33	0.11	0.13
Tetrahydrofuran	3	5	6	3	4	4	0.33	0.20	0.17	0.33	0.25	0.25
Water	4	10	10	10	10	10	0.25	0.10	0.10	0.10	0.10	0.10

References

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2. R. K. Henderson, C. Jimenez-Gonzalez, D. J. C. Constable, S. R. Alston, G. G. A. Inglis, G. Fisher, J. Sherwood, S. P. Binks and A. D. Curzons, *Green Chem.*, 2011, <http://dx.doi.org/10.1039/C1030GC00918K>.