Supporting Information

Ensuring Fact-Based Metabolite Identification in LC-MS-Based Metabolomics

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Table S1: Examples[#] of identifications showing unrealistic elution orders in RPLC-MS systems*

	RT(min)	Metabolites Names and characteristic LogKow values
Example 1	2.99	*LysoPC(15:0)*
	3.41	Phenylalanine
	3.62	Glucose
	4.27	Citric acid
	9.14	Lactic acid
	8.11	Aspartic acid -4.32
	8.29	*LysoPC(15:0)*
	9.53	Lactic acid -0.65
Example 2	4.27	*Palmitic acid* 6.96
	4.50	1-Methylhistamine
	4.60	5-Hydroxy-L-tryptophan
	4.86	L-Lysine -2.99
	5.08	*2-Hydroxydecanedioic acid*
	5.09	Asymmetric dimethylarginine
	5.09	4-Hydroxynonenal
	5.09	L-alpha-Aminobutyric acid
Example 3	2.09	Isocitric acid -2.01
	2.21	*Arachidonic acid 8.07*
	2.49	*18-Hydroxycorticosterone*
	3.55	Glucose -2.89
	3.67	*11-Dehydrocorticosterone 1.77*
	4.45	L-Leucine
	5.09	D-Ornithine
	5.24	Mevalonic acid-5P
	5.31	Glycine -3.41
	6.91	*Eicosadienoic acid 8.50*
	7.56	Deoxyuridine -1.19
Example 4	3.37	*PC(18:1(9Z)/0:0)*
	3.76	*Arachidonic acid 8.07*
	5.21	*Lysopc(16:1(9Z)/0:0)*
	11.79	*Lysopc(18:1(11Z))*
	13.18	L-Asparagine -4.99
	13.22	*PC(18:2(9Z,12Z)/18:1(11Z))*
	17.95	Glutathione
	21.13	Guanosine diphosphate -5.55

*Apolar analytes = italics, more polar analytes = normal font

LogKow were obtained from Chemspider. RPLC theory dictates that increase in analyte log Kow results to increase in t_R. Here this relationship is not observed and values are clearly in disarray.

The numbers are reproduced as found in their sources but in some cases t_R values have been reduced to 2 digits.

[#]Studies are anonymised.