

Supplementary file for:

Bridging the polar and hydrophobic metabolome in single-run untargeted liquid chromatography-mass spectrometry dried blood spot metabolomics for clinical purposes

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Supplementary Table**Table S1.** Peak area (PA) and retention time (RT) relative standard deviation (RSD %) of selected compounds measured in a DBS injected three times each day during an analysis run of 11 days.

Compound	Average PA (a.u.) N=30	RSD % PA (a.u.) N=30	Average RT (min) N=30	RSD % RT (min) N=30
Ornithine	1.81E+07	4 %	1.62	0.3 %
Arginine	6.88E+06	3 %	1.75	0.4 %
Citrulline	1.75E+07	3 %	2.19	0.2 %
Valine	1.71E+08	9 %	2.50	0.1 %
Methionine	8.17E+06	7 %	3.05	0.2 %
Leucine	1.37E+08	6 %	3.33	0.3 %
Tyrosine	3.34E+07	5 %	4.10	0.3 %
Phenylalanine	6.73E+07	3 %	6.73	0.2 %
Acylcarnitine C0	5.16E+07	2 %	2.11	0.3 %
Acylcarnitine C2	3.10E+07	4 %	2.61	0.2 %
Acylcarnitine C3	1.02E+06	8 %	4.97	0.4 %
Acylcarnitine C8	2.09E+05	8 %	12.09	0.1 %
Acylcarnitine C14	3.35E+05	10 %	13.14	0.1 %
Acylcarnitine C16	2.90E+06	4 %	13.69	0.1 %
Acylcarnitine C18	1.14E+06	4 %	14.42	0.1 %

Supplementary Information

Number of detected features and annotated/identified metabolites

An example of the number of detected features and annotated/identified metabolites, using Compound Discoverer 2.1 (with standard settings and filters for a metabolomics workflow), in a dried blood spot positive ionization analysis: detected features: 11394. Annotated or identified metabolites: 1042.

Supplementary figures S1-S4 (chromatograms from other evaluated columns)

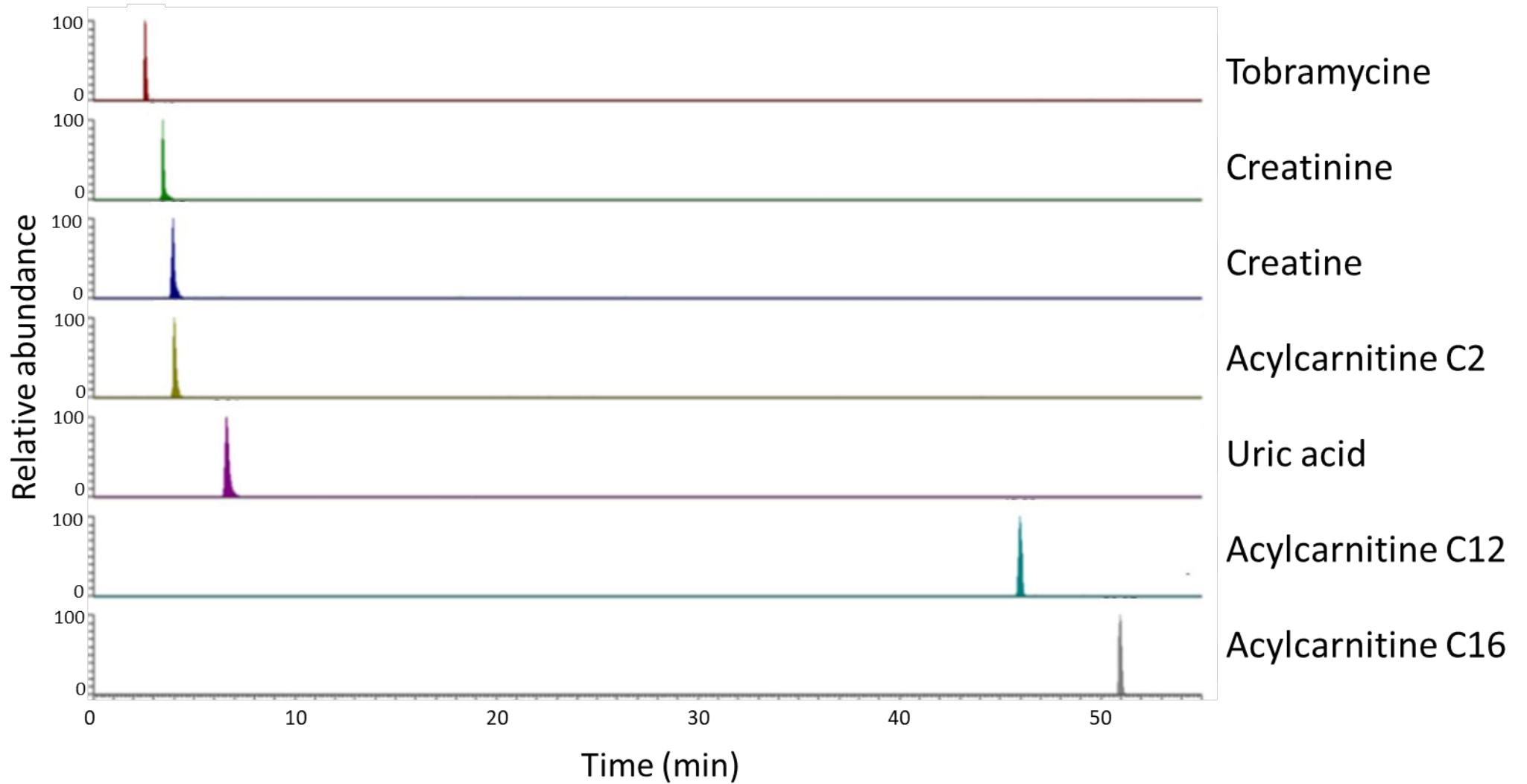


Figure S1. Extracted ion chromatograms of tobramycine, creatinine, creatine, acylcarnitine C2, uric acid, acylcarnitine C12 and acylcarnitine C16 using the Polaris C18-Ether column.

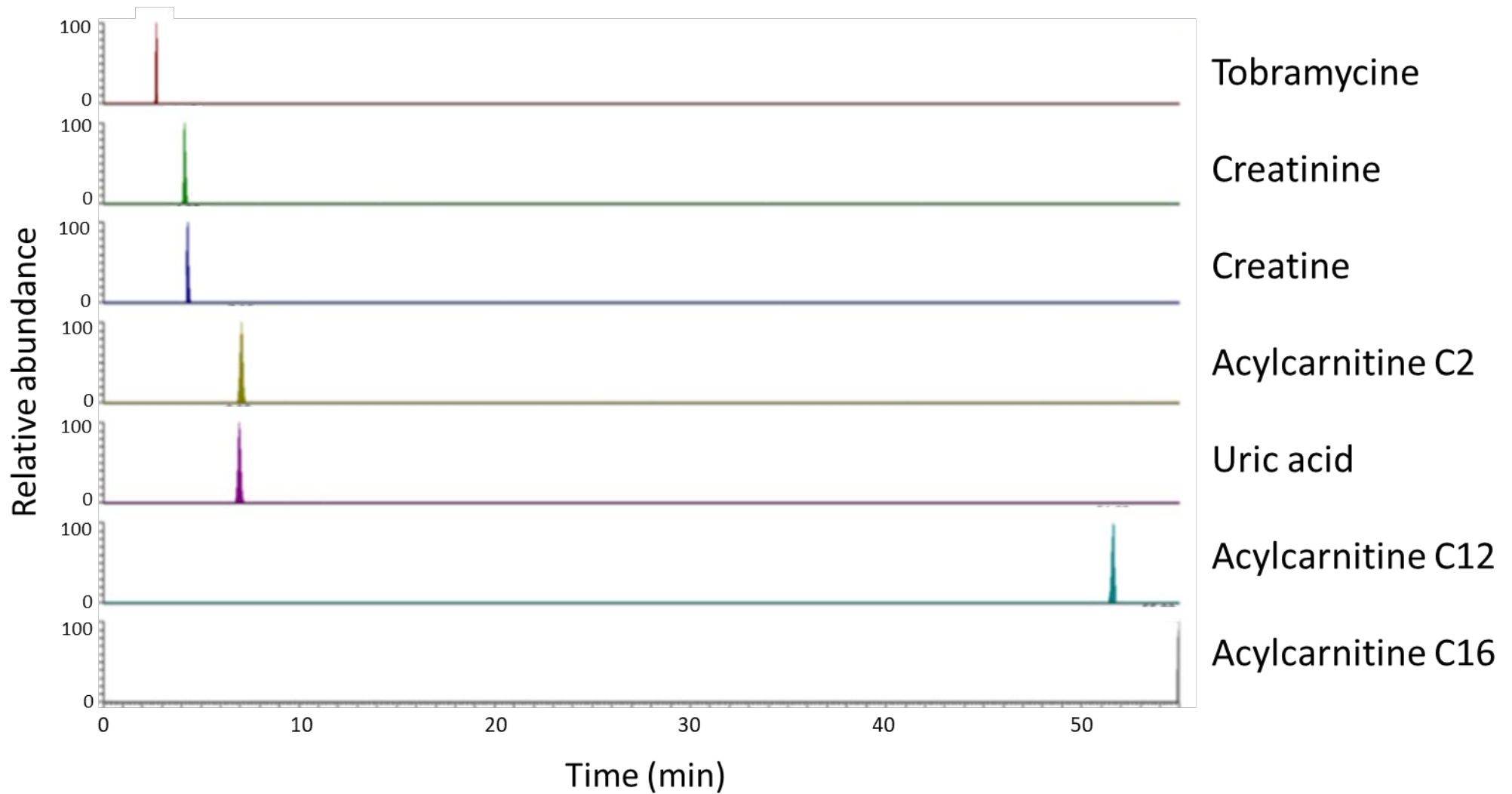


Figure S2. Extracted ion chromatograms of tobramycine, creatinine, creatine, acylcarnitine C2, uric acid, acylcarnitine C12 and acylcarnitine C16 using the ACE C18-PFP column.

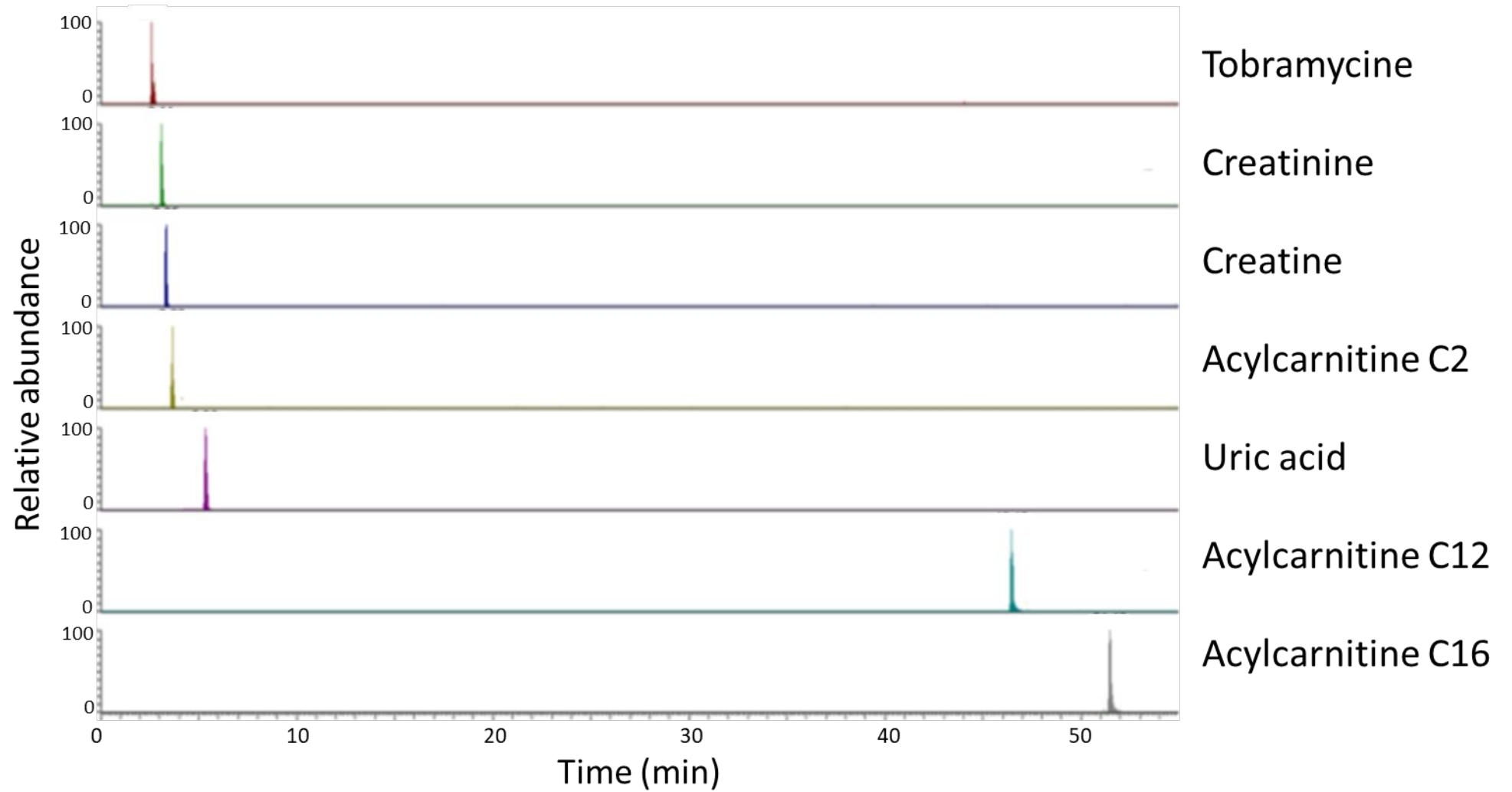


Figure S3. Extracted ion chromatograms of tobramycine, creatinine, creatine, acylcarnitine C2, uric acid, acylcarnitine C12 and acylcarnitine C16 using the Aeris Peptide XB-C18 column.

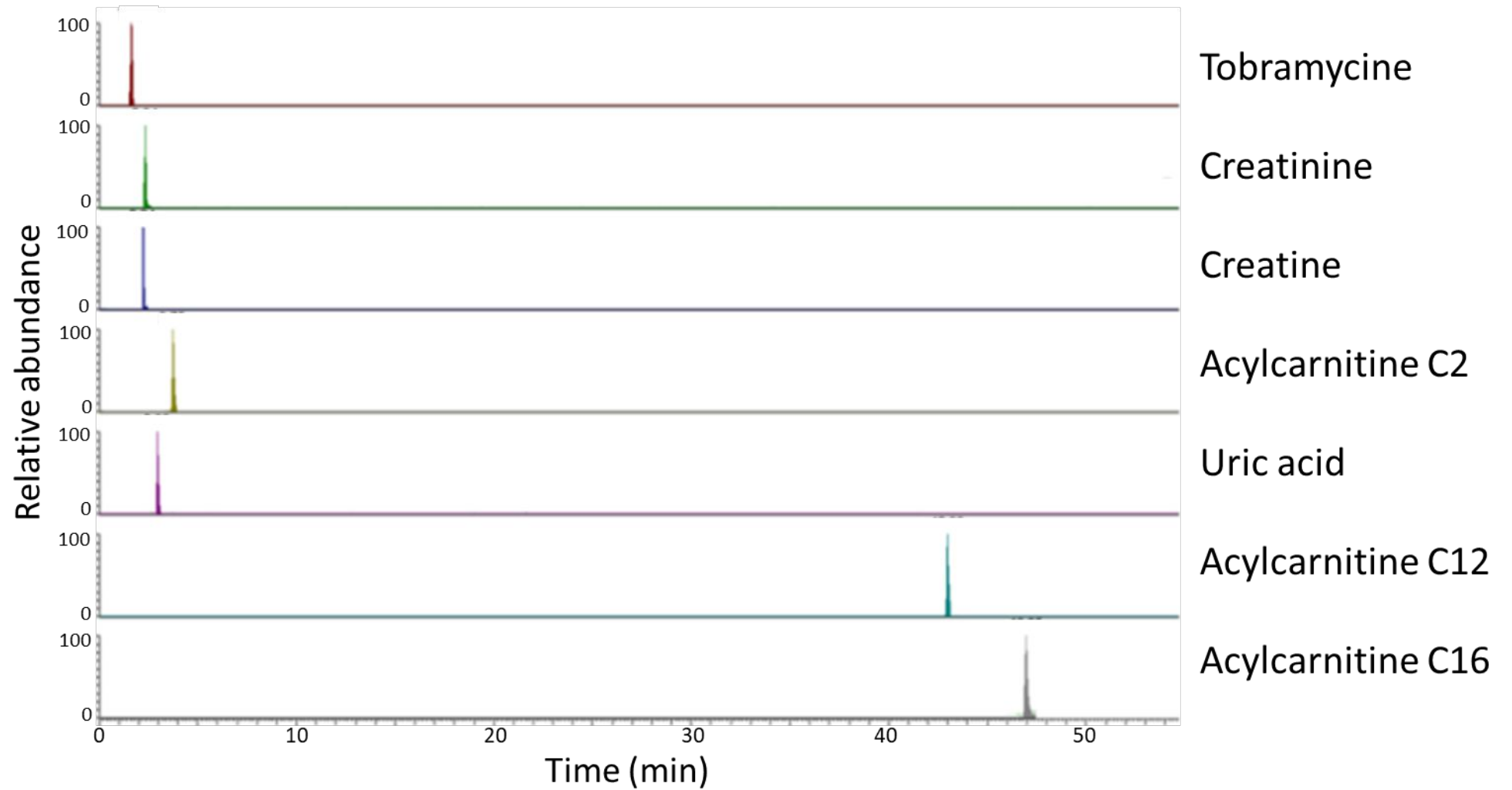


Figure S4. Extracted ion chromatograms of tobramycine, creatinine, creatine, acylcarnitine C2, uric acid, acylcarnitine C12 and acylcarnitine C16 using the Raptor Biphenyl column.