

Prep-LC fraction	Prep-LC RRT	UHPLC RT (min)	UHPLC RRT	Metabolite
19	0.23	5.13	0.55	M21
		5.55	0.59	M19
20	0.24	5.13	0.55	M21
		5.55	0.59	M19
23	0.27	5.13	0.55	M21
		5.55	0.59	M19
50	0.60	3.32	0.35	M2
		4.20	0.45	M1
		5.13	0.55	M21
		5.55	0.59	M19
54	0.64	3.23	0.34	M2
		4.14	0.44	M1
		5.55	0.59	M19
59	0.70	4.14	0.44	M1
		6.03	0.64	M22
		6.54	0.70	M18
60	0.71	4.19	0.45	M1
		6.02	0.64	M22
		6.54	0.70	M18
65	0.77	4.17	0.44	M1
		7.48	0.79	M25
84	1.00	4.19	0.45	M1
		9.41	1.00	P

Footnote:

Prep-LC RRT calculated using (metabolite fraction number/parent fraction number)

UHPLC RRT calculated using (metabolite UHPLC RT (min)/parent UHPLC RT (min))

Bold highlighting signifies major component(s) by MS peak area counts (rank order only, not quantitative) and not possible where metabolites detected in same fraction but in opposing ionisation polarity (e.g. M21 and M19)

Table S1: Summary of UHPLC-MS/MS data for NMR fractions of single dose human urine (0-24 h pool) to confirm major components.