Ion-pairing chromatography and amine derivatization provide complementary approaches for the targeted LC-MS analysis of the polar metabolome

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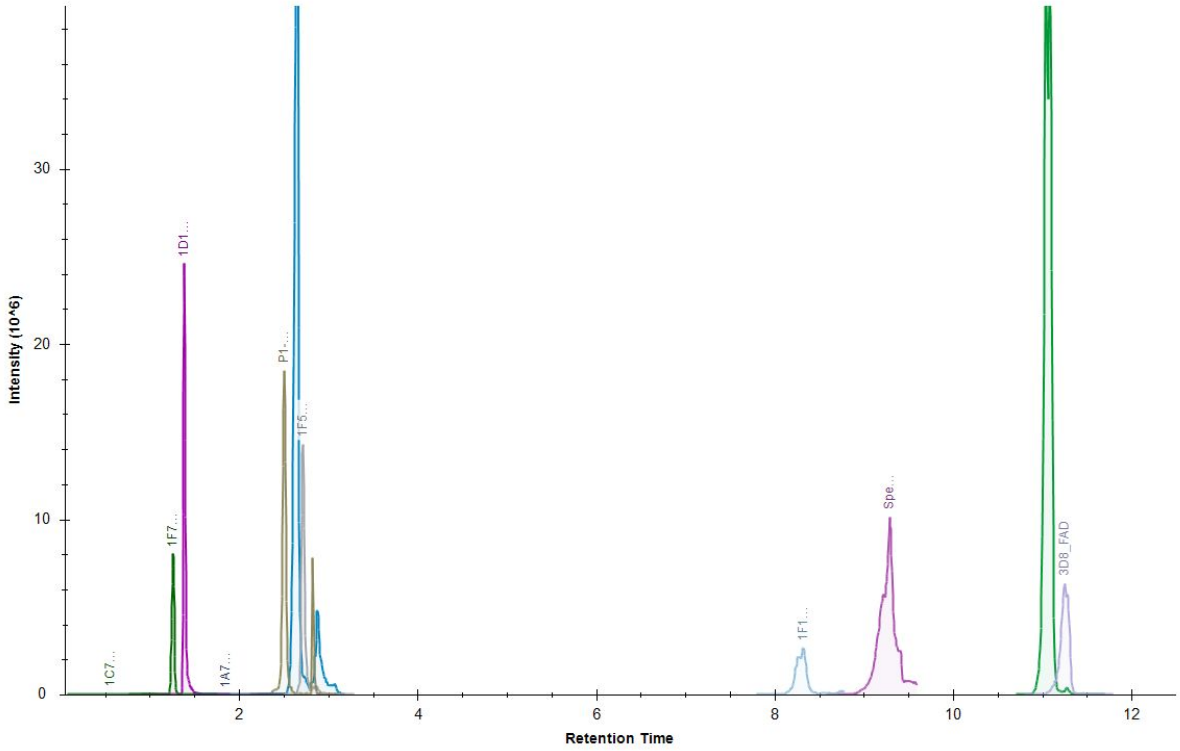
Figure S5. Correlations between NMR, AccQ-Tag, and ion-pairing data (for three different transitions) for 2-aminoadipate.

Table S1. Settings used for liquid chromatography-mass spectrometry experiments.

	AccQ-Tag RPLC	RPLC POS	IPC	RPLC NEG
LC unit	ACQUITY Binary Solvent Manager (Waters Corporation) + CTC Pal autosampler	UFLX XR (Shimadzu)	ACQUITY Binary Solvent Manager (Waters Corporation) + CTC Pal autosampler	ACQUITY Binary Solvent Manager (Waters Corporation) + CTC Pal autosampler
Mobile phase A	0.1 % Formic acid water	0.1 % Formic acid water	10mM of tributylamine + 15mM of acetic acid + acetylacetone (0.02% v/v) in water	0.1 % Formic acid water
Mobile phase B	0.1 % Formic acid Acetonitrile	0.1 % Formic acid Acetonitrile	80% methanol and 20% isopropanol	0.1 % Formic acid Acetonitrile
Flow rate	0.6 ml/min	0.4 ml/min	0.4 ml/min	0.4 ml/min
Column temperature	50 ℃	45 ℃	45 ℃	45 ℃
Column	Waters HSS T3 (1.8 µm, 2.1 x 150 mm)	Waters HSS T3 (1.8 µm, 2.1 x 100 mm)	Waters HSS T3 (1.8 µm, 2.1 x 100 mm)	Waters HSS T3 (1.8 µm, 2.1 x 100 mm)
Injection volume	5 µl	5 µl	5 µl	5 µl
Gradient	0.1 to 12 min from 1% solvent B to 28% solvent B; at a flow rate of 0.6 mL/min. Post-acquisition wash and recovery steps took 2.65 min in total and went up to 100% B, and 1 min at initial conditions for equilibration.	0min 1%; 0.5 min, 1% B; 10 min, 55% B; 11 min, 100% B; 12 min, 100% B; 12.5 min, 1% B; 14.5 min, 1% B.	0-0.5 min: 0% B; 0.5-6 min: 0% B-5%B; 4-6min: 5%B; 6-6.5 min: 5-20% B; 6.5-8.5 min: 20% B; 8.5-14min: 20-55%B; 14-15 min: 55-100% B; 15-17min: 100%B; 17-18min 100-0% B. 3 min at initial conditions before next injection cycle starts.	0min: 99% A; 0.5min: 99%A; 10 min: 45%A; 11min: 0%A; 12 min: 0%A; 12.5min: 99%A; 14.5 min: 99%A. Linear gradient between all times
MS type	Waters XEVO TQ-S (Waters Corporation)	QTRAP 5500 MS/MS system [Applied Biosystem (CA, USA)]	Waters XEVO TQ-S (Waters Corporation)	Waters XEVO TQ-S (Waters Corporation)
Ion mode	POS	POS	NEG	NEG
Source parameters	capillary voltage, 1.5 kV; source temperature, 150°C; cone voltage: 40 V;	De-clustering, entrance and collision cell exit potentials were set to 30 V, 10 V and 10 V, respectively.	capillary voltage, 1.5 kV; source temperature, 150°C; cone voltage: 40 V;	capillary voltage, 2 kV; source temperature, 150°C; cone voltage: 40 V;
AdditIonal source settings:	desolvation temperature 600°C; desolvation gas flow, 1000 L/h; cone gas flow, 150 L/h; nebuliser gas 7.0 bar; collision gas, 0.15 mL/min.	Curtain gas, 40 psi; collision gas, medium; ionspray voltage, 5500 V; temperature, 550°C; ion source gas 1 and 2, 40 and 60 psi, respectively.	desolvation temperature 600°C; desolvation gas flow, 1000 L/h; cone gas flow, 150 L/h; nebuliser gas 7.0 bar; collision gas, 0.15 mL/min.	desolvation temperature 300°C; desolvation gas flow, 1000 L/h; cone gas flow, 150 L/h; nebuliser gas 7.0 bar; collision gas, 0.15 mL/min.

Figure S1.



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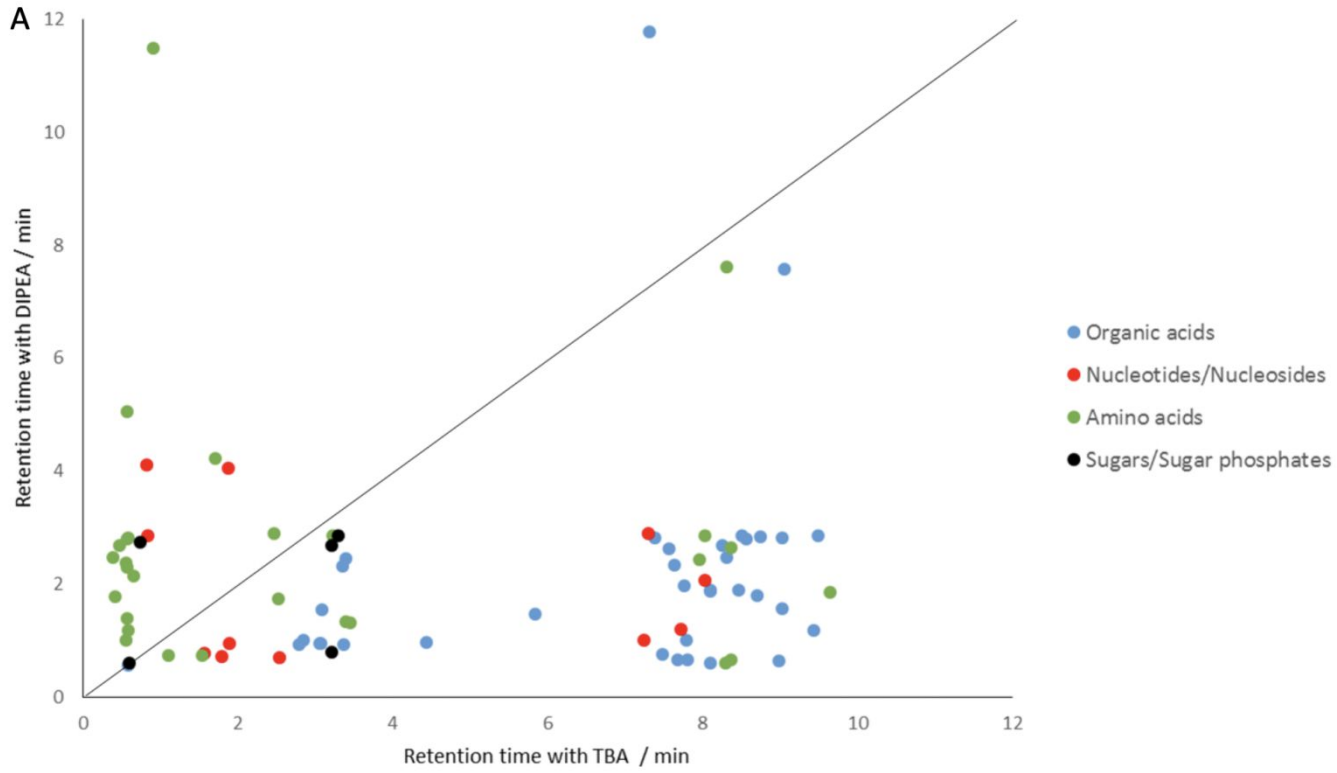

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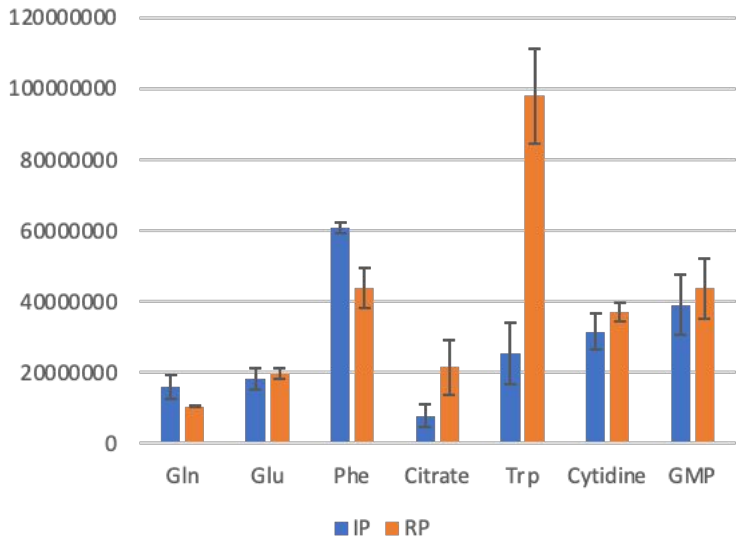

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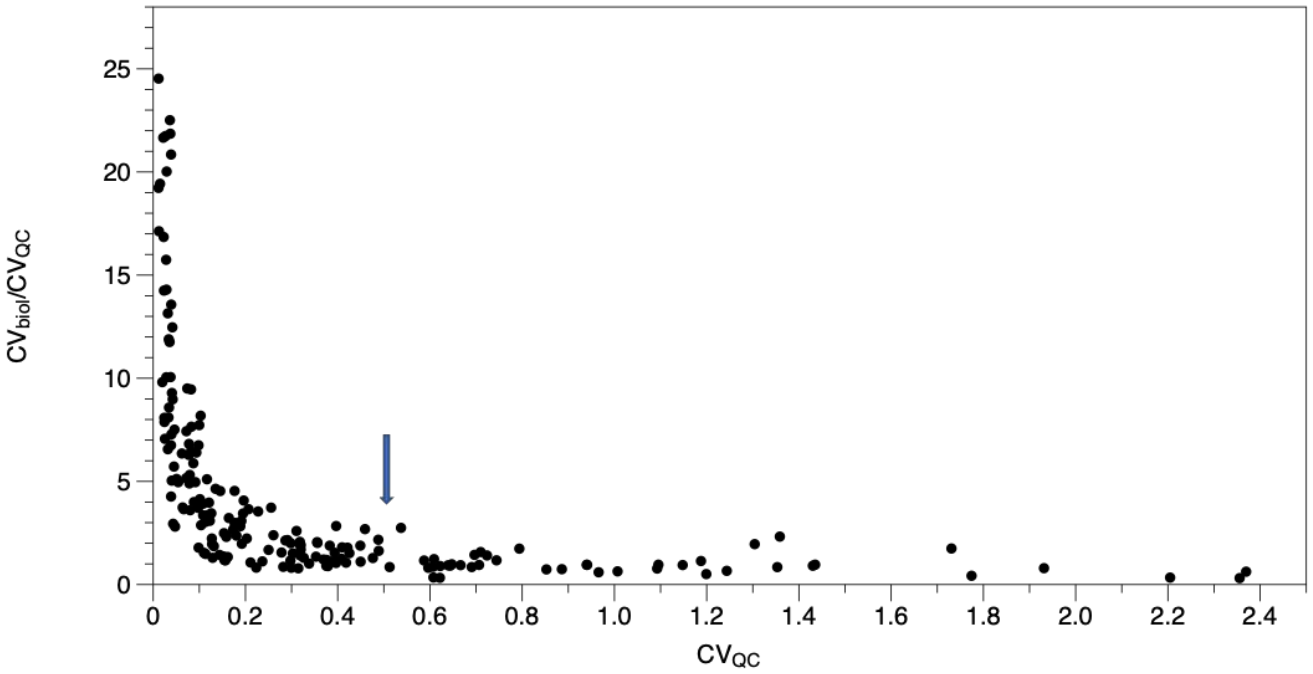

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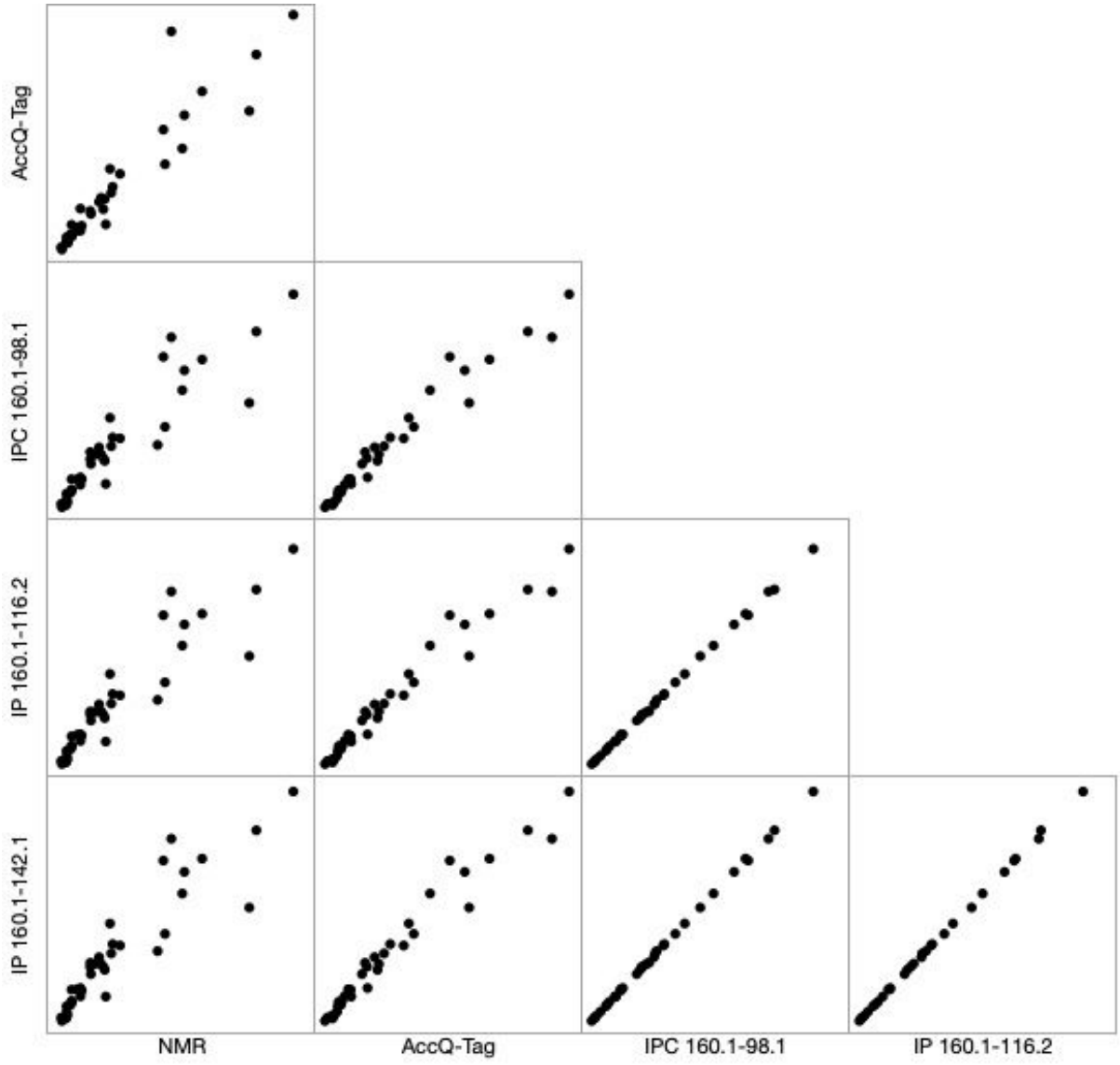
Figure S5



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