HILIC (1)
Instrument Name: Waters Xevo-TQ-S
Instrument Type: Triple quadrupole
MS Type: ESI
Ion Mode: Positive and Negative switching
MS acquisition Comments: The selected reaction monitoring (SRM) transitions were monitored
over a 5 to 10 minute window around the retention time. For most metabolites, two SRM
transitions were monitored, one for quantification and an additional for compound confirmation. Scheduling was set up to ensure at least 12 data points per peak were collected.
Data processing Comments: Data was processed as in Boysen and Heal et al. 2018. Analytical Chemistry.
Software/procedures used for feature assignments: Peaks were integrated using Skyline. Data was processed using quality control, and best-matched internal standard normalization.
MS parameters were as follows: capillary voltage of 0.5 kV, source temperature of 130 ∞C, cone gas flow at 150 L/h and desolvation gas flow at 1000 L/h, Desolvation temperature was 500 ∞C

HILIC (2)
Instrument Name: Thermo Q Exactive HF hybrid Orbitrap
Instrument Type: Orbitrap
MS Type: ESI
Ion Mode: Positive
MS acquisition Comments: Polarity switching was used with a scan range of 80 to 900 m/z and a resolution of 60,000.
A DDA method was used with a scan range of 90 to 900 m/z.
Data processing Comments: Data was processed as in Boysen and Heal et al. 2018. Analytical Chemistry.
Software/procedures used for feature assignments: Peaks were integrated using Skyline. Data was processed using quality control, and best-matched internal standard normalization.
MS parameters were as follows: capillary temperature was 320 ∞C, the H-ESI spray voltage was 3.3 kV, and the auxiliary gas heater temperature was 100 ∞C. The
S-lens RF level was 65. Sheath gas, auxiliary gas, and sweep gas flow rates were maintained
at 8, 3, and 0, respectively.

HILIC (3)
Instrument Name: Thermo Q Exactive HF hybrid Orbitrap
Instrument Type: Orbitrap
MS Type: ESI
Ion Mode: Negative
MS acquisition Comments: Polarity switching was used with a scan range of 80 to 900 m/z and a resolution of 60,000.
A DDA method was used with a scan range of 90 to 900 m/z.
Data processing Comments: Data was processed as in Boysen and Heal et

al. 2018. Analytical Chemistry.
Software/procedures used for feature assignments: Peaks were integrated using Skyline. Data was processed using quality control, and best-matched internal standard normalization.
MS parameters were as follows: capillary temperature was 320 ∞C, the H-ESI spray voltage was 3.3 kV, and the auxiliary gas heater temperature was 100 ∞C. The
S-lens RF level was 65. Sheath gas, auxiliary gas, and sweep gas flow rates were maintained
at 8, 3, and 0, respectively.

Reversed Phase (4)
Instrument Name: Thermo Q Exactive HF hybrid Orbitrap
Instrument Type: Orbitrap
MS Type: ESI
Ion Mode: Positive
MS acquisition Comments: A full scan method was used with a scan range of 90 to 900 m/z and a resolution of 120,000.
A DDA method was used with a scan range of 90 to 900 m/z.
Data processing Comments: Data was processed as in Boysen and Heal et al. 2018. Analytical Chemistry.
Software/procedures used for feature assignments: Peaks were integrated using Skyline. Data was processed using quality control, and best-matched internal standard normalization.
MS parameters were as follows: capillary temperature was 320 ∞C, the H-ESI spray voltage was 3.8 kV, and the auxiliary gas heater temperature was 100 ∞C. The
S-lens RF level was 65. Sheath gas, auxiliary gas, and sweep gas flow rates were maintained
at 40, 10, and 1, respectively.