

Additional file 4. Mass spectrometer parameters for the detection of methylmalonic acid, homocysteine, and methylcitric acid.

Analyte	Cone voltage (V)	Collision energy (eV)	MRM transition	Retention time (min)
MMA	15	10	117>73	0.89
MMA-d ₃	15	10	120>76	0.89
Hcys	60	15	136>90	0.57
Hcys-d ₈	60	15	140>94	0.57
MCA	30	13	205>125	0.95
MCA-d ₃	30	13	208>128	0.95

Hcys: homocysteine; Hcys-d₈: homocysteine (3,3,3',3',4,4,4',4'-d₈); MCA: methylcitric acid; MCA-d₃: MCA-d₃: 2-methyl-d₃-citric acid; MMA: methylmalonic acid; MMA-d₃: isotopically labeled methylmalonic acid; MRM: multiple reaction monitoring.