

**Table S2: Monitored transitions in LC-MS/MS negative mode of DMH and the IS.**

Compounds	Molecular ion [M-2H] <sup>2-</sup> /2 (m/z)	Fragment (m/z)	DP (volts)	CE (volts)	CXP (volts)
Dimethylheptanoyl-CoA	452.6	408 (quantifier)	-120	-30	-15
	452.6	134 (qualifier)	-120	-34	-3
21:0 Coenzyme A	538.8	408 (quantifier)	-105	-34	-19
	538.8	134 (qualifier)	-105	-36	-7