

Supplementary Data

Rapid quantification of murine bile acids using liquid chromatography-tandem mass spectrometry

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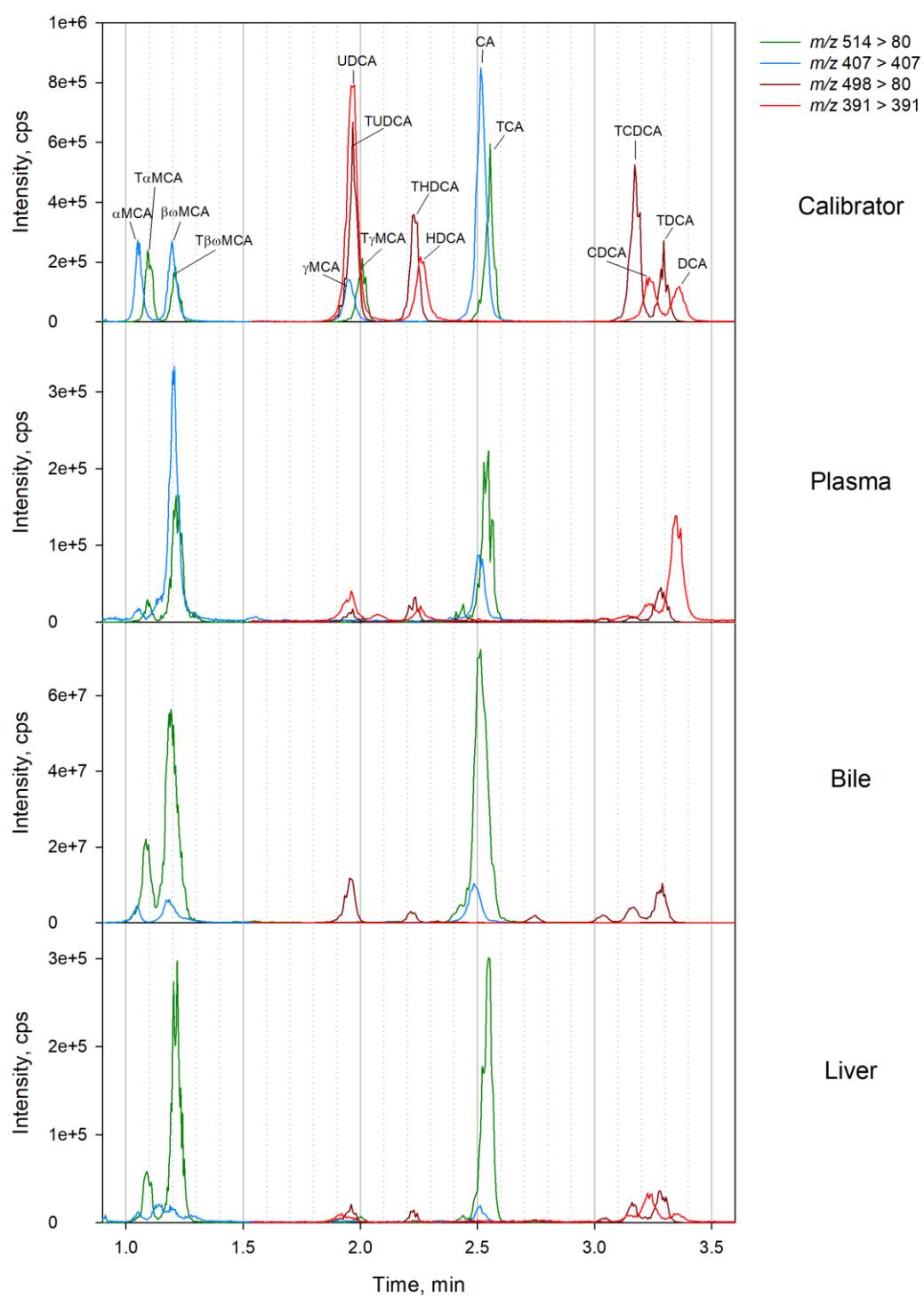


Figure S1: Chromatogram of calibrator, murine plasma, bile and liver. Displayed are SRM traces for calibrator level 3, plasma (sample volume 50 μ l), bile and liver samples.

Analyte	RT [min]	Mass transition [m/z]	DP [V]	CE [V]	IS
GαMCA	1.06	464.3 → 74	-110	-94	D5-αMCA
αMCA	1.07	407.3 → 407.3	-125	-30	D5-αMCA
TαMCA	1.13	514.3 → 79.9	-240	-156	D4-TαMCA
GβωMCA	1.21	464.3 → 74	-110	-94	D5-βMCA
βωMCA	1.22	407.3 → 407.3	-125	-30	D5-βMCA
TβωMCA	1.25	514.3 → 79.9	-240	-156	D4-TβMCA
GUDCA	1.99	448.3 → 74	-85	-84	D4-GUDCA
γMCA	1.99	407.3 → 407.3	-125	-30	D5-γMCA
GγMCA	2.02	464.3 → 74	-110	-94	D5-γMCA
TγMCA	2.06	514.3 → 79.9	-240	-156	D4-TγMCA
UDCA	2.00	391.3 → 391.3	-155	-30	D4-UDCA
		391.3 → 373.35	-45	-45	
TUDCA	2.02	498.3 → 79.9	-175	-164	D5-TUDCA
GHDCa	2.26	448.3 → 74	-85	-84	D5-HDCa
THDCa	2.28	498.3 → 79.9	-175	-164	D5-HDCa
HDCA	2.29	391.3 → 391.3	-155	-30	D5-HDCa
CA	2.55	407.3 → 407.3	-125	-30	D4-CA
		407.3 → 343.2	-45	-45	
GCA	2.58	464.3 → 74	-110	-94	D4-GCA
TCA	2.60	514.3 → 79.9	-240	-156	D5-TCA
GCDCA	3.23	448.3 → 74	-85	-84	D4-GCDCA
TCDCa	3.23	498.3 → 79.9	-175	-164	D5-TCDCa
CDCA	3.28	391.3 → 391.3	-155	-30	D4-CDCA
TDCA	3.35	498.3 → 79.9	-175	-164	D5-TDCA
GDCA	3.36	448.3 → 74	-85	-84	D4-GDCA
DCA	3.40	391.3 → 391.3	-155	-30	D4-DCA
		391.3 → 345.2	-45	-45	
TLCA	4.07	482.3 → 79.9	-165	-120	D5-TLCA
GLCA	4.09	432.3 → 74	-105	-74	D4-GLCA
LCA	4.32	375.3 → 375.3	-155	-30	D4-LCA
D5-αMCA	1.06	412.3 → 412.3	-125	-30	-
D4-TαMCA	1.13	518.3 → 79.9	-240	-156	-
D5-βMCA	1.21	412.3 → 412.3	-125	-30	-
D4-TβMCA	1.25	518.3 → 79.9	-240	-156	-
D4-GUDCA	1.98	452.3 → 74	-85	-84	-
D5-γMCA	1.98	412.3 → 412.3	-125	-30	-
D4-UDCA	1.99	395.3 → 395.3	-155	-30	-
		395.3 → 377.3	-45	-45	
D5-TUDCA	2.01	395.3 → 377.4	-175	-164	-
D4-TγMCA	2.05	503.3 → 79.9	-240	-156	-
D5-HDCa	2.28	518.3 → 79.9	-155	-30	-
D4-CA	2.55	396.3 → 396.3	-30	-30	-
		396.3 → 347.2	-125	-45	
D4-GCA	2.57	411.3 → 347.2	-110	-94	-
D5-TCA	2.59	411.3 → 411.3	-240	-156	-
D4-GCDCA	3.22	468.3 → 74	-85	-84	-

D5-TCDCA	3.22	519.3 → 79.9	-175	-164	-
D4-CDCA	3.26	452.3 → 74	-155	-30	-
D4-GDCA	3.34	503.3 → 79.9	-85	-84	-
D5-TDCA	3.34	395.3 → 395.3	-175	-164	-
D4-DCA	3.39	395.3 → 395.3	-155	-30	-
		395.3 → 349.2		-45	
D5-TLCA	4.05	452.3 → 74	-165	-120	-
D4-GLCA	4.08	395.3 → 349.2	-105	-74	-
D4-LCA	4.30	395.3 → 395.3	-155	-30	-

Table S1: BA analytical details.

Shown are retention time, mass transition, declustering potential (DP), collision energy (CE), and internal standard (IS) used for quantification for the monitored bile acid species. For the unconjugated BA UDCA, CA and DCA, two mass transitions were monitored.