

S1 Table. Analysis of selected reaction monitoring (SRM) parameters and internal standards for bile acids.

Analytes	SRM transition	Fragmentor	Collision	Internal standard
		voltage (V)	Energy (eV)	
CA	m/z 407 \rightarrow 407	230	0	3, 7, 12- ^{18}O]CA
GCA	m/z 464 \rightarrow 74	210	45	3, 7- ^{18}O]GCA
TCA	m/z 514 \rightarrow 80	300	95	3, 7- ^{18}O]GCA
CDCA	m/z 391 \rightarrow 391	210	0	3, 7- ^{18}O , $^2\text{H}_2$]GCDCA
GCDCA	m/z 448 \rightarrow 74	200	40	3, 7- ^{18}O , $^2\text{H}_2$]GCDCA
TDCA	m/z 498 \rightarrow 80	290	90	3, 12- ^{18}O , $^2\text{H}_2$]TDCA
DCA	m/z 391 \rightarrow 391	200	0	3- ^{18}O , $^2\text{H}_2$]GLCA
GDCA	m/z 448 \rightarrow 74	200	40	3, 7- ^{18}O , $^2\text{H}_2$]GCDCA
TDCA	m/z 498 \rightarrow 80	290	75	3, 12- ^{18}O , $^2\text{H}_2$]TDCA
UDCA	m/z 391 \rightarrow 391	230	0	3, 7, 12- ^{18}O]CA
GUDCA	m/z 448 \rightarrow 74	200	40	3, 7- ^{18}O]GCA
TUDCA	m/z 498 \rightarrow 80	290	75	3, 7- ^{18}O]GCA
LCA	m/z 375 \rightarrow 375	190	0	3- ^{18}O , $^2\text{H}_2$]GLCA
GLCA	m/z 432 \rightarrow 74	190	40	3- ^{18}O , $^2\text{H}_2$]GLCA
TLCA	m/z 482 \rightarrow 80	280	75	3- ^{18}O , $^2\text{H}_2$]TLCA
3, 7, 12- ^{18}O]CA	m/z 413 \rightarrow 413	230	0	
3, 7- ^{18}O]GCA	m/z 470 \rightarrow 74	210	45	
3, 7- ^{18}O , $^2\text{H}_2$]GCDCA	m/z 454 \rightarrow 74	200	40	
3, 12- ^{18}O , $^2\text{H}_2$]TDCA	m/z 504 \rightarrow 80	290	75	
3- ^{18}O , $^2\text{H}_2$]GLCA	m/z 435 \rightarrow 74	190	40	
3- ^{18}O , $^2\text{H}_2$]TLCA	m/z 485 \rightarrow 80	280	75	