

S2 Tables. Validation Parameters

A: precision and accuracy for three different plasma concentrations (n=5)

	accuracy [%]			Coefficient of Variation [%]		
	25nM	100nM	1000nM	25nM	100nM	1000nM
CA Quanti	97.7	101.4	102.6	5.3	4.3	2.0
DCA Quanti	92.0	98.9	101.8	3.2	4.4	2.6
LCA Quanti	93.1	100.7	98.0	12.4	6.9	4.5
CDCA Quanti	106.3	107.0	99.5	2.3	3.0	5.7
TLCA Quanti	90.7	100.5	103.9	3.0	3.8	2.4
UDCA Quanti	95.5	101.2	102.3	6.3	2.8	2.6
TCDCA Quanti	97.8	103.4	98.8	4.1	3.6	3.0
GCA Quanti	107.8	101.2	97.6	4.0	2.5	2.7
GCDCA Quanti	107.3	102.0	100.1	9.4	3.0	6.1
TDCA Quanti	100.5	103.3	100.4	3.6	3.3	2.7
TCA Quanti	102.4	103.1	101.9	3.4	4.4	1.7
GUDCA Quanti	108.8	103.1	107.7	2.1	4.2	1.2
TUDCA Quanti	94.0	105.1	101.2	4.2	2.6	2.9
GDCA Quanti	114.6	106.5	101.2	5.1	4.5	3.6

B: Precision between batches (n=13) determined by pooled QC samples

	CA	DCA	LCA	CDCA	TLCA	UDCA	TCDC	GCA	GCDCA	TDCA	TCA	GUDCA	TUDCA	GDCA
CV (%)	4.6	6.7	10.8	6.6	n.a.	5.9	4.8	5.0	4.9	6.1	13.3	4.7	n.a.	5.2
Mean Concentration	331.2	425.2	19.9	439.4	n.a.	95.6	97.0	324.3	877.6	55.5	53.0	121.8	n.a.	301.6

C: Recovery and matrix effect (n=5) for spiked plasma samples c=250 nM

	CA	DCA	LCA	CDCA	TLCA	UDCA	TCDC	GCA	GCDCA	TDCA	TCA	GUDCA	TUDCA	GDCA
Recovery %	87.7	87.4	72.7	99.5	95.6	98.2	88.9	101.8	94.4	91.0	118.1	103.9	101.0	86.3
Matrix Effect %	65.4	99.9	88.2	102.6	100.9	83.6	123.0	124.9	79.4	75.0	92.5	73.9	96.9	110.8