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Supplementary material

Table S1 Summary of within- and between-run accuracy data for IQ-1 in rat biosamples.

Matrix	Level	Concentration (ng/mL or ng/g)	Accuracy %	
			Within-run %	Between-run %
Brain	LLOQ	1.5	105 ± 8	99 ± 5
	LQC	4.5	102 ± 7	104 ± 6
	MQC	600	97 ± 5	98 ± 8
	HQC	1800	99 ± 7	96 ± 5
Heart	LLOQ	1.5	100 ± 10	99 ± 9
	LQC	4.5	102 ± 8	103 ± 11
	MQC	600	98 ± 8	96 ± 4
	HQC	1800	92 ± 5	94 ± 6
Liver	LLOQ	1.5	99 ± 8	97 ± 5
	LQC	4.5	97 ± 5	99 ± 7
	MQC	2400	90 ± 4	91 ± 5
	HQC	7200	88 ± 4	90 ± 4
Kidney	LLOQ	1.5	92 ± 8	93 ± 8
	LQC	4.5	95 ± 10	97 ± 9
	MQC	780	100 ± 12	98 ± 10
	HQC	2400	98 ± 7	96 ± 8
Lung	LLOQ	1.5	91 ± 8	94 ± 9
	LQC	4.5	95 ± 9	97 ± 8
	MQC	780	100 ± 10	98 ± 7
	HQC	2400	99 ± 9	99 ± 8
Spleen	LLOQ	1.5	101 ± 12	100 ± 13
	LQC	4.5	105 ± 13	99 ±10
	MQC	400	96 ± 6	98 ± 9
	HQC	1200	97 ± 7	94 ± 6
Muscle	LLOQ	1.5	103 ± 10	102 ± 9
	LQC	4.5	100 ± 8	99 ± 8
	MQC	780	96 ± 7	95 ± 7
	HQC	2400	97 ± 8	97 ± 9
Fat	LLOQ	1.5	105 ± 10	107 ± 12
	LQC	4.5	103 ± 9	108 ± 11
	MQC	400	100 ± 8	100 ±10
	HQC	1200	98 ± 8	97 ± 9
Duodenum	LLOQ	1.5	106 ± 12	108 ± 10
	LQC	4.5	102 ± 13	105 ± 12
	MQC	1600	101 ± 10	99 ± 9
	HQC	4800	98 ± 9	98 ± 9
Lymph*	LLOQ	1.0	106 ± 9	104 ± 8
	LQC	3.0	108 ± 10	107 ± 9

	MQC	1050	100 ± 8	102 ± 10
	HQC	3200	98 ± 7	99 ± 8
Matrix	**Level**	**Concentration (ng/mL or ng/g)**	**Accuracy %**	
			Within-run %	**Between-run%**
Bile*	LLOQ	1.0	104 ± 6	103 ± 6
	LQC	3.0	103 ± 7	104 ± 8
	MQC	1050	100 ± 8	99 ± 9
	HQC	3200	97 ± 6	98 ± 8

Values are presented as Mean ± SD;

LLOQ - lower limit of quantitation; LQC - low-quantitation level; MQC - medium quantitation level; HQC - high-quantitation level;

Summary of within- and between-run accuracy data for IQ-1 in rat plasma is provided in our previous publication.[16]

Table S2 Summary of within- and between-run accuracy data for IQ-18 in rat biosamples.

Matrix	Level	Concentration (ng/mL or ng/g)	Accuracy %	
			Within-run %	Between-run %
Brain	LLOQ	1.5	105 ± 8	102 ± 7
	LQC	4.5	105 ± 7	100 ± 6
	MQC	1600	98 ± 6	97 ± 7
	HQC	4800	96 ± 5	95 ± 5
Heart	LLOQ	1.5	110 ± 10	102 ± 10
	LQC	4.5	106 ± 9	104 ± 7
	MQC	600	100 ± 8	98 ± 7
	HQC	1800	97 ± 6	94 ± 5
Liver	LLOQ	1.5	100 ± 9	102 ± 8
	LQC	4.5	92 ± 7	94 ± 7
	MQC	2400	90 ± 6	91 ± 5
	HQC	7200	92 ± 6	93 ± 7
Kidney	LLOQ	1.5	103 ± 10	101 ± 8
	LQC	4.5	102 ± 9	100 ± 7
	MQC	800	98 ± 7	96 ± 6
	HQC	2400	95 ± 4	97 ± 8
Lung	LLOQ	1.5	105 ± 9	108 ± 7
	LQC	4.5	100 ± 8	99 ± 7
	MQC	800	91 ± 7	96 ± 5
	HQC	2400	94 ± 8	95 ± 5
Spleen	LLOQ	1.5	104 ± 8	102 ± 7
	LQC	4.5	100 ± 7	98 ± 8
	MQC	400	98 ± 6	97 ± 7
	HQC	1200	95 ± 4	96 ± 5
Muscle	LLOQ	1.5	108 ± 10	105 ± 8
	LQC	4.5	105 ± 8	107 ± 9
	MQC	600	100 ± 7	99 ± 7
	HQC	1800	98 ± 6	96 ± 5
Fat	LLOQ	1.5	100 ± 7	102 ± 9
	LQC	4.5	103 ± 10	105 ± 9
	MQC	800	92 ± 6	94 ± 7
	HQC	2400	94 ± 5	97 ± 8
Duodenum	LLOQ	1.5	105 ± 9	106 ± 11
	LQC	4.5	107 ± 10	108 ± 12
	MQC	1600	100 ± 8	100 ± 9
	HQC	4800	98 ± 7	96 ± 5
Lymph*	LLOQ	1.0	104 ± 10	102 ± 9
	LQC	3.0	102 ± 7	103 ± 8
	MQC	1050	100 ± 6	101 ± 7
	HQC	3200	98 ± 5	97 ± 4

Matrix	Level	Concentration (ng/mL or ng/g)	Accuracy %	
			Within-run %	Between-run%
Bile*	LLOQ	1.0	100 ± 10	98 ± 9
	LQC	3.0	101 ± 11	100 ± 10
	MQC	5350	99 ± 8	97 ± 7
	HQC	16000	96 ± 6	94 ± 5

1 Values are presented as Mean ± SD;
2 LLOQ - lower limit of quantitation; LQC - low-quantitation level; MQC - medium quantitation level; HQC - high-
3 quantitation level;
4 Summary of within- and between-run accuracy data for IQ-18 in rat plasma is provided in our previous publication.[16]

Table S3 Recovery, matrix effect, and stability of IQ-1 in rat biosamples.

Matrix	Level	Concentration (ng/mL or ng/g)	Recovery (%)	IS-normalized matrix factor	Stability			
					Freeze-thaw[1]	Autosampler[2]	RT[3]	−80°C[4]
Brain	LQC	4.5	91 ± 6	0.92 ± 0.09	104 ± 10	90 ± 5	97 ± 7	89 ± 5
	HQC	1800	88 ± 4	1.01 ± 0.05	99 ± 8	94 ± 6	102 ± 11	92 ± 7
Heart	LQC	4.5	89 ± 5	0.93 ± 0.08	103 ± 9	98 ± 7	110 ±12	93 ± 9
	HQC	1800	88 ± 4	1.01 ± 0.09	110 ± 7	99 ± 8	105 ± 10	95 ± 11
Liver	LQC	4.5	93 ± 7	0.89 ± 0.06	106 ± 10	100 ± 9	94 ± 5	94 ± 9
	HQC	7200	91 ± 5	0.90 ± 0.05	110 ± 8	98 ± 7	91 ± 6	102 ± 13
Kidney	LQC	4.5	91 ± 2	0.93 ± 0.09	104 ± 7	99 ± 7	109 ± 13	88 ± 6
	HQC	2400	88 ± 3	1.00 ± 0.08	108 ± 8	102 ± 9	103 ± 11	90 ± 7
Lung	LQC	4.5	90 ± 4	0.93 ± 0.09	99 ± 7	105 ± 10	99 ± 8	104 ± 10
	HQC	2400	89 ± 4	0.95 ± 0.08	102 ± 10	103 ± 9	94 ± 6	108 ± 9
Spleen	LQC	4.5	88 ± 3	0.94 ± 0.06	100 ± 5	105 ± 9	88 ± 5	110 ± 12
	HQC	1200	91 ± 4	0.97 ± 0.07	104 ± 6	107 ± 10	92 ± 6	108 ± 10
Muscle	LQC	4.5	89 ± 5	0.99 ± 0.05	101 ± 5	92 ± 5	93 ± 7	105 ± 9
	HQC	2400	88 ± 3	0.98 ± 0.07	99 ± 6	97 ± 7	97 ± 7	102 ± 9
Fat	LQC	4.5	90 ± 6	1.09 ± 0.12	100 ± 8	95 ± 5	101± 10	100 ± 8
	HQC	1200	88 ± 4	1.12 ± 0.07	99 ± 7	97 ± 6	106 ± 9	92 ± 7
Duodenum	LQC	4.5	89 ± 5	0.96 ± 0.08	88 ± 6	89 ± 8	101 ± 9	100 ± 10
	HQC	4800	92 ± 8	0.98 ± 0.09	91 ± 7	93 ± 7	95 ± 6	89 ± 6
Lymph*	LQC	3.0	90 ± 6	0.86 ± 0.05	95 ± 5	101 ± 8	103 ± 11	98 ± 8
	HQC	3200	93 ± 4	0.90± 0.06	97 ± 6	100 ± 9	108 ± 10	104 ± 12
Bile*	LQC	3.0	89 ± 5	0.90 ± 0.08	98 ± 5	103 ± 10	100 ± 12	89 ± 5
	HQC	3200	94 ± 3	0.91 ± 0.07	102 ± 7	102 ± 11	104 ± 9	94 ± 8

Values are presented as Mean ± SD;
LQC - low-quantitation level; HQC - high-quantitation level; RT- room temperature;
For the marked matrices (*) concentration values are expressed in ng/mL;
Every level of QC had replicate samples in recovery, stability test (n=6) and matrix effect assessment (n=4);
[1] Samples subjected to 3 freeze/thaw cycles (−80°C/RT); [2] Samples stored at autosampler at 15°C for 24 h; [3]Samples stored at RT for 6h; [4]Samples stored at −80°C for 30 days;
Recovery, matrix effect, and stability of IQ-1 in rat plasma is presented in our previous publication.[16]

Table S4 Recovery, matrix effect, and stability of metabolite IQ-18 in rat biosamples.

Matrix	Level	Concentration (ng/mL or ng/g)	Recovery (%)	IS-normalized matrix factor	Stability			
					Freeze-thaw[1]	Autosampler[2]	RT[3]	−80°C[4]
Brain	LQC	4.5	90 ± 5	0.94 ± 0.09	96 ± 6	110 ± 9	97 ± 8	100 ± 8
	HQC	4800	89 ± 4	1.00 ± 0.07	98 ± 7	105 ± 10	102 ±10	108 ± 10
Heart	LQC	4.5	88 ± 4	0.90 ± 0.06	94 ± 5	91 ± 7	97 ± 9	103 ± 7
	HQC	1800	88 ± 4	0.92 ± 0.07	111 ± 9	94 ± 6	87 ± 7	101 ± 9
Liver	LQC	4.5	91 ± 6	0.87 ± 0.05	99 ± 7	104 ± 8	88 ± 8	108 ± 12
	HQC	7200	90 ± 5	0.90 ± 0.06	96 ± 5	112 ± 9	89 ± 9	106 ± 11
Kidney	LQC	4.5	92 ± 4	0.91 ± 0.08	91 ± 4	97 ± 7	87 ± 6	97 ± 9
	HQC	2400	88 ± 3	1.00 ± 0.07	105 ± 11	89 ± 5	106 ± 5	92 ± 8
Lung	LQC	4.5	91 ± 6	0.91 ± 0.08	95 ± 9	109 ± 7	104 ± 10	88 ± 6
	HQC	2400	89 ± 5	0.93± 0.09	92 ± 7	103 ± 8	90 ± 9	108 ± 12
Spleen	LQC	4.5	88 ± 4	0.94 ± 0.07	103 ± 13	90 ± 6	96 ± 7	109 ± 11
	HQC	1200	90 ± 5	0.96 ± 0.06	112 ± 11	100 ± 11	94 ± 5	98 ± 9
Muscle	LQC	4.5	89 ± 4	0.94 ± 0.06	94 ± 10	87 ± 7	98 ± 8	91 ± 8
	HQC	1800	88 ± 5	0.97 ± 0.08	90 ± 8	95 ± 9	88 ± 4	102 ± 10
Fat	LQC	4.5	89 ± 6	1.00 ± 0.10	102 ± 9	91 ± 10	89 ± 6	104 ± 12
	HQC	2400	88 ± 4	1.11 ± 0.09	96 ± 10	109 ± 12	101 ± 10	105 ± 11
Duodenum	LQC	4.5	90 ± 6	0.89 ± 0.06	89 ± 7	100 ± 9	93 ± 7	98 ± 8
	HQC	4800	92 ± 7	0.93 ± 0.05	91 ± 6	95 ± 8	96 ± 7	94 ± 7
Lymph*	LQC	3.0	91 ± 5	0.88 ± 0.08	97 ± 8	96 ± 10	106 ± 9	99 ± 9
	HQC	3200	92 ± 6	0.89± 0.07	99 ± 9	94 ± 8	102 ± 12	108 ± 7
Bile*	LQC	3.0	90 ± 5	0.91 ± 0.09	100 ± 12	100 ± 11	104 ± 10	103 ±10
	HQC	16000	92 ± 6	0.93 ± 0.10	108 ± 14	105 ± 13	103 ± 9	99 ± 8

Values are presented as Mean ± SD;
LQC - low-quantitation level; HQC - high-quantitation level; RT- room temperature;
For the marked matrices (*) concentration values are expressed in ng/mL;
Every level of QC had replicate samples in recovery, stability test (n=6) and matrix effect assessment (n=4);
[1] Samples subjected to 3 freeze/thaw cycles (−80°C/RT); [2] Samples stored at autosampler at 15°C for 24 h; [3]Samples stored at RT for 6h; [4]Samples stored at −80°C for 30 days;
Recovery, matrix effect, and stability of IQ-1 in rat plasma is presented in our previous publication.[16]