

SUPPLEMENTAL INFORMATION

Sensitive and selective quantification of free and total malondialdehyde in plasma using UHPLC-HRMS

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Running title: Quantification of free and total plasma MDA using UHPLC-HRMS

Supplemental Table S1 – Linearity assay using different concentrations of purified MDA-DNPH. Calibration equation was: $y=11.50x + 1.89$, weighing $1/x$, with $r^2=0.997$.

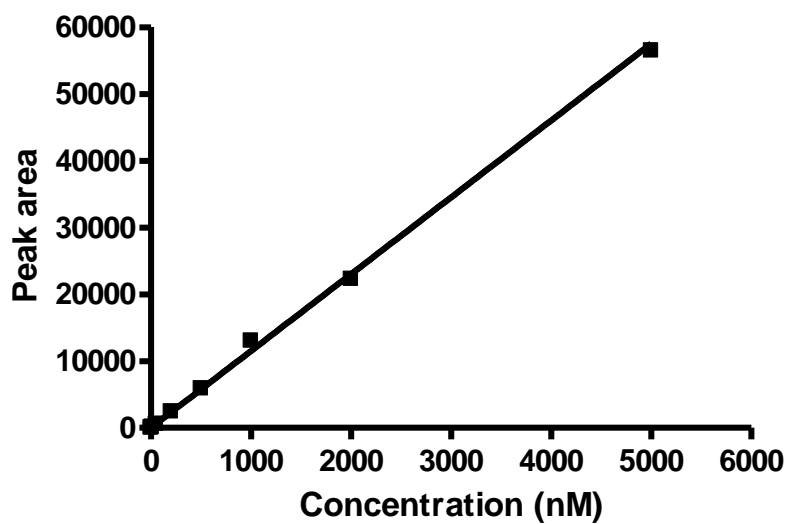
MDA-DNPH standards	Trace (m/z)	Predicted RT (min)	RT (min)	Back calculated concentration (ng mL ⁻¹)	Standard concentration (ng mL ⁻¹)	Accuracy (%)	Injection volume (μL)
Standard 1 ng mL ⁻¹	235.0462	2.87	2.88	1.07	1	106.8	2.5
Standard 2.5 ng mL ⁻¹	235.0462	2.87	2.88	2.55	2.5	102.1	2.5
Standard 5 ng mL ⁻¹	235.0462	2.87	2.87	4.66	5	93.3	2.5
Standard 10 ng mL ⁻¹	235.0462	2.87	2.87	10.23	10	102.3	2.5
Standard 50 ng mL ⁻¹	235.0462	2.87	2.88	47.91	50	95.8	2.5
Standard 200 ng mL ⁻¹	235.0462	2.87	2.87	211.86	200	105.9	2.5
Standard 500 ng mL ⁻¹	235.0462	2.87	2.87	508.71	500	101.7	2.5
Standard 1000 ng mL ⁻¹	235.0462	2.87	2.87	1134.25	1000	113.4	2.5
Standard 2000 ng mL ⁻¹	235.0462	2.87	2.88	1938.33	2000	96.9	2.5
Standard 5000 ng mL ⁻¹	235.0462	2.87	2.87	4908.94	5000	98.2	2.5

Supplemental Table S2 – Calibration assay using different concentrations of MDA salt with constant concentration (3000 nM) of D₂-MDA.

Calibration equation was: $y=0.0253x + 0.0085$, weighing: $1/x$, with $r^2=0.999$.

MDA standards	Trace (m/z)	Predicted RT (min)	RT (min)	Back calculated concentration (nM)	Accuracy (%)	Injection volume (μL)
Standard 32 nM	235.0462	2.87	2.86	30.8	96.3	2.5
Standard 80 nM	235.0462	2.87	2.86	82.4	103.0	2.5
Standard 321 nM	235.0462	2.87	2.86	334.9	104.3	2.5
Standard 803 nM	235.0462	2.87	2.86	757.2	94.3	2.5
Standard 1606 nM	235.0462	2.87	2.86	1641.0	102.2	2.5
Standard 6427 nM	235.0462	2.87	2.86	6422.7	99.9	2.5

Supplemental Figure S3 – Calibration curve obtained for the linearity assay using different concentrations of purified MDA-DNPH. Calibration equation was: $y=11.50x + 1.89$, weighing $1/x$, with $r^2=0.997$.



Supplemental Figure S4 – Calibration curve obtained using different concentrations of MDA

salt. Calibration equation was: $y=0.0253x + 0.0085$, weighing: $1/x$, with $r^2=0.999$.

