

Coated Blade Spray-Mass Spectrometry as a New Approach for the Rapid Characterization of Brain Tumors

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SUPPLEMENTARY MATERIALS

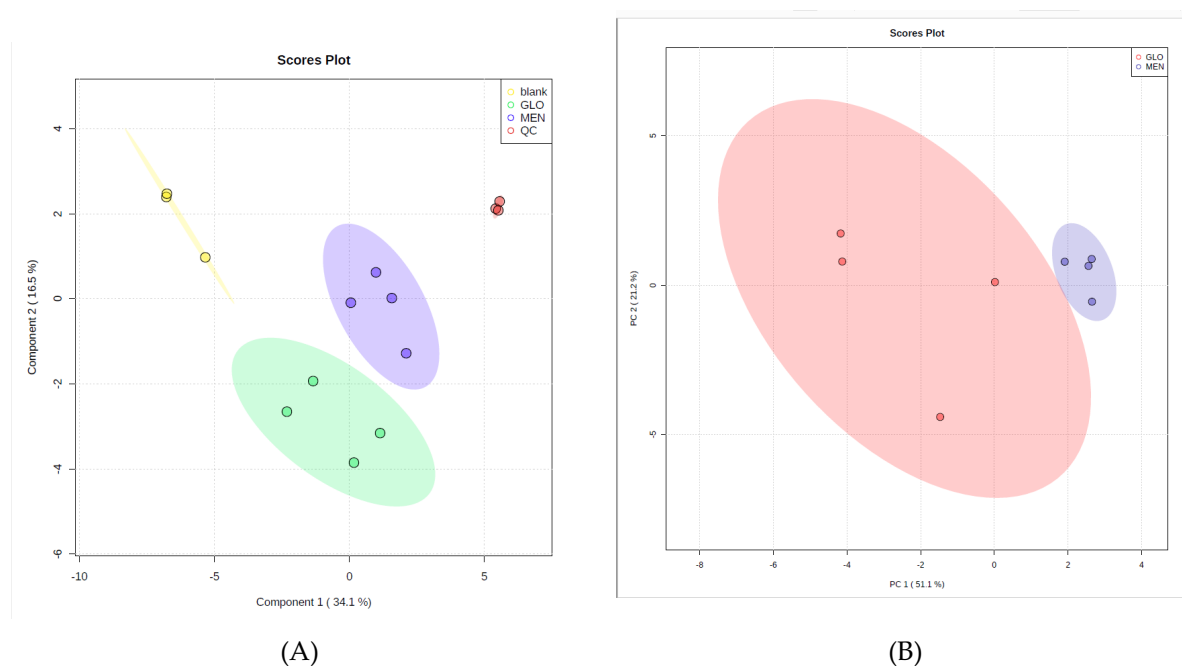


Figure S1. (A) Partial least squares data analysis (PLS-DA) of studied samples based on tentative lipids. Model passed permutation test with three components. R^2 were 0.98 and Q^2 at level 0.70; (B) Principal component analysis of meningiomas and gliomas based on tentative lipid with VIP-score above 1.0.

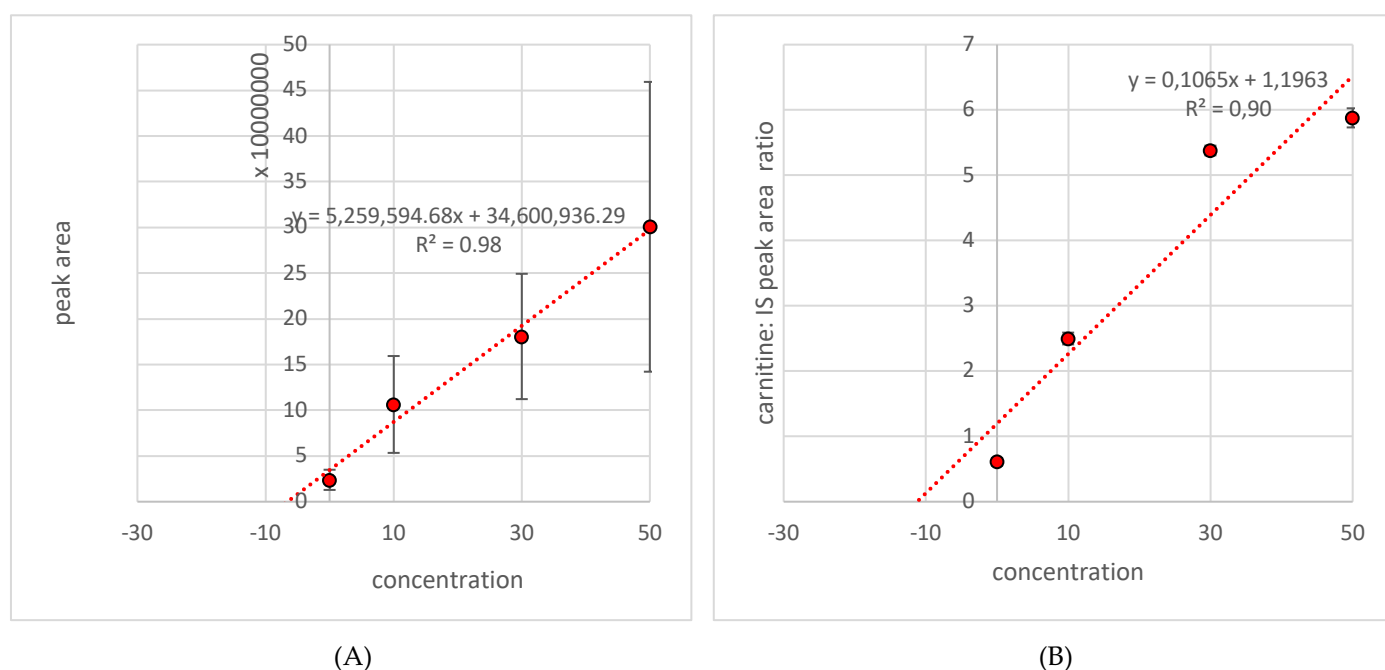


Figure S2. Standard addition curve of carnitine; (A) raw data; (B)- data normalized on internal standard (IS) area. Bars represent the standard deviation of peak areas and carnitine: IS peak area ratios.

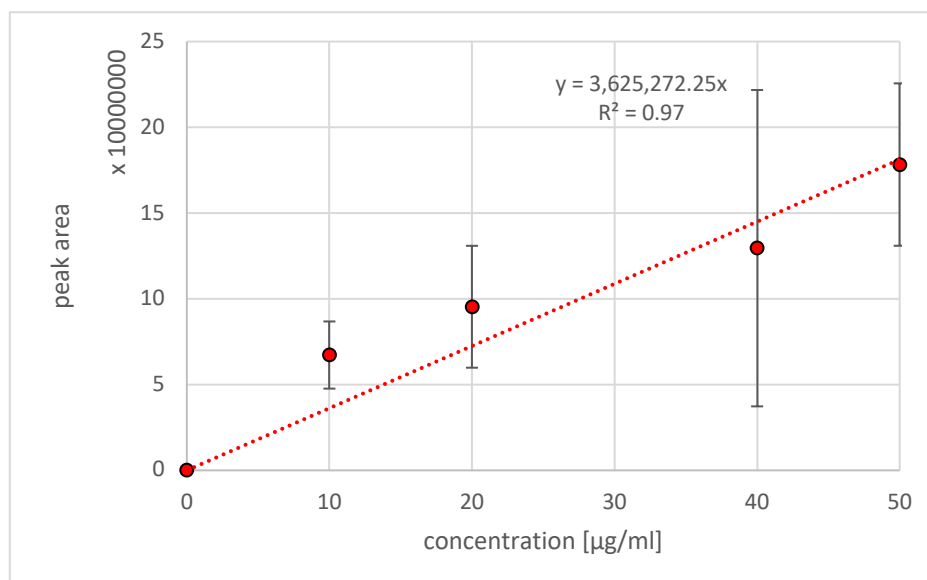
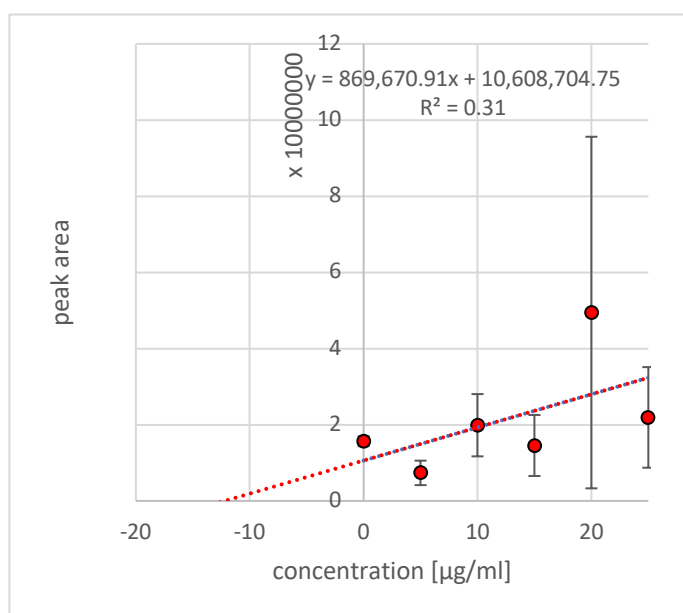
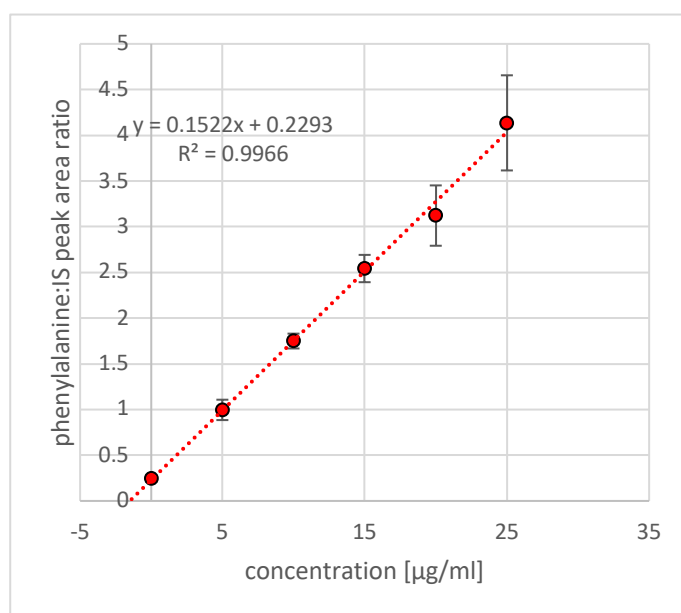


Figure S3. Calibration curve for carnitine(trimethyl-d9) in brain tumor homogenate. Bars represent the standard deviation of peak areas



(A)



(B)

Figure S4. Standard addition curve of phenylalanine; (A) raw data; (B)- data normalized on internal standard (IS) area. Bars represent the standard deviation of peak areas and phenylalanine: IS peak area ratios.

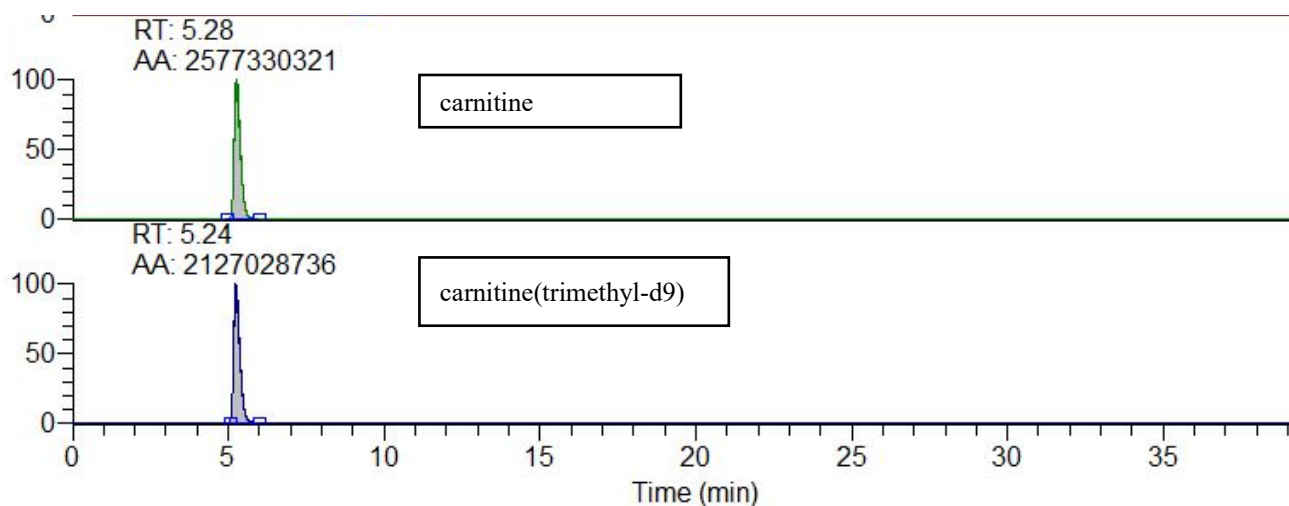


Figure S5. Comparison of the peak areas of the mixture of carnitine and its deuterated form in the concentration 10 ppm. The methodology of this analysis was presented in Bogusiewicz et al. (Bogusiewicz et al. 2020)* under metabolomics analysis on PFP column.

* Bogusiewicz, J.; Goryńska, P.Z.; Gaca, M.; Chmara, K.; Goryński, K.; Jaroch, K.; Paczkowski, D.; Furtak, J.; Harat, M.; Bojko, B. On-Site Sampling and Extraction of Brain Tumors for Metabolomics and Lipidomics Analysis. *J. Vis. Exp.* 2020, 2020, 159, doi:10.3791/61260.

Table S1. Peak areas and RSD for lipids used in the selection of desorption solvent for untargeted analysis.

sample [x] + phenylalanine	IPA:MeOH,1:3,v/v with 10 mM ammonium acetate and 1 mM acetic acid		IPA:MeOH,1:1,v/v with 10 mM ammonium acetate and 1 mM acetic acid	
	Average area	RSD	Average area	RSD ¹
PC C16-18:1	811259	23%	766728	51%
LPE 17:1	939323	9%	1000845	38%
PG 17:0-20:4	474606	28%	493471	53%
Sphingosine (d17:1)	2008763	23%	7106255	110%

¹relative standard deviation**Table S2.** Standard addition curve details for carnitine

Sample [x] + carnitine	Raw data		Normalized data	
	area	RSD	ratio	RSD ¹
x+50 ug/ml	300725268	62%	5.88	3%
x+30 ug/ml	428917804	46%	5.38	1%
x+10 ug/ml	106366685	59%	2.50	4%
X	23917467	39%	0.61	10%

¹relative standard deviation**Table S3.** Standard addition curve details for phenylalanine

sample [x] + phenylalanine	Raw data		Normalized data	
	area	RSD	ratio: standard/Deuter	RSD ¹
x+25 ug/ml	21928862	60%	4.14	13%
x+20 ug/ml	49460652	93%	3.12	11%
x+15 ug/ml	14558740	55%	2.54	6%
x+10 ug/ml	19881108	41%	1.75	5%
x+5 ug/ml	7364715	44%	1.00	11%
X	3023055	43%	0.24	13%

¹relative standard deviation