Figure S-1: Acidic chemical oxidation yields of B, BH_2, BH_4, N, and NH_2, after 30 min of incubation according to ref. 29.

Table S-1. Analytical recovery and accuracy of the method, and within-run comparison between authentic and artificial cerebrospinal fluid (CSF) matrices.

Analytes	Added concentration (nmol/L)	Authentic CSF			Artificial CSF					p-value **
		Within-run (n = 6)			Within-run (n = 6)			Between-run (n = 10)		
		Measured concentration (nmol/L)	Analytical recovery (%)*	CV (%)	Measured concentration (nmol/L)	Analytical recovery (%)*	CV (%)	Measured concentration (nmol/L)	CV (%)	
N	0	2.5	-	7.3	-	-	-	-	-	-
	5	7.1	92.0	9.2	4.9	98.0	8.2	5.3	5.9	0.3605
	20	20.9	92.0	5.1	19.7	98.5	8.1	21.6	4.3	0.1280
	50	48.4	91.8	3.9	49.9	99.8	9.9	54.3	5.9	0.0936
	100	93.3	90.8	6.2	100.1	100.1	9.9	106.7	6.1	0.0752
NH2	0	7.5	-	8.9	-	-	-	-	-	-
	5	12.8	106.0	6.3	5.0	100.0	9.0	5.2	7.9	0.2190
	20	25.9	92.0	9.0	18.9	94.5	7.5	18.6	7.9	0.6631
	50	53.1	91.2	8.6	48.7	97.4	7.1	46.3	6.4	0.2144
	100	103.5	96.0	8.5	100.8	100.8	6.2	91.2	9.1	0.3015
BH4	0	n.d.	-	n.d.	-	-	-	-	-	-
	5	5.4	108.0	9.5	5.7	114.0	3.4	5.5	8.1	0.2099
	20	19.2	96.0	5.1	19.5	97.5	2.5	21.1	6.0	0.5169
	50	50.5	101.0	6.7	51.3	102.6	7.8	49.7	9.1	0.7162
	100	103.5	103.5	8.4	101.5	101.5	6.9	98.1	8.4	0.6701
B	0	25.2	-	4.6	-	-	-	-	-	-
	5	30.6	108.0	7.8	5.1	102.0	5.0	5.7	8.4	0.1664
	20	44.5	96.5	4.7	19.6	98.0	4.7	20.9	6.3	0.7544
	50	70.5	90.6	5.6	50.0	100.0	6.8	52.0	8.6	0.0516
	100	112.6	88.0	8.1	100.0	100.0	6.7	104.0	6.5	0.0506
BH2	0	28.7	-	1.9	-	-	-	-	-	-
	5	34.1	108.0	4.6	5.2	104.0	9.7	5.8	8.5	0.4040
	20	47.9	96.0	6.0	19.5	97.5	8.1	21.4	7.2	0.8275
	50	75.7	94.0	2.2	50.0	100.0	8.8	54.7	6.1	0.1497
	100	122.7	94.0	3.4	100.1	100.1	5.5	108.0	4.9	0.0558

* Analytical recovery was calculated according to the formulae: AR (%) = [(Final concentration − Initial concentration) / Added concentration] x 100
** p-value is obtained with a two-tailed Student's t-test for comparison of mean concentrations obtained between authenticCSF and artificial CSF after checking homogeneity of variances using Fisher's test.
(n.d. = not detected).

Table S-2. LOD, LOQ, and linearity data with spiked artificial CSF samples.

Analyte	LOD* nM	LOQ** nM	Slope	Intercept	R^2	Sy/x^a	Sa^b	Sb^c
B	1.2	3.6	0.1238	-0.016	0.990	0.48	0.0027	0.154
BH_2	1.8	5.0	0.0949	-0.023	0.990	0.30	0.0020	0.097
BH_4	1.7	5.0	0.0566	0.086	0.986	0.23	0.0014	0.074
N	0.9	2.7	0.1263	-0.027	0.981	0.67	0.0038	0.215
NH_2	1.5	4.5	0.1097	-0.093	0.991	0.38	0.0022	0.122

* Limit of detection for a signal to noise ratio of 3. ** Limit of quantitation. [a] Standard error of the estimate. [b] Standard error of the slope. [c] Standard error of the intercept.