Capillary Electrophoresis Method for Analysis of Inorganic and Organic Anions Related to Habitability and the Search for Life

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Table of Contents

1. Metabolically relevant anions

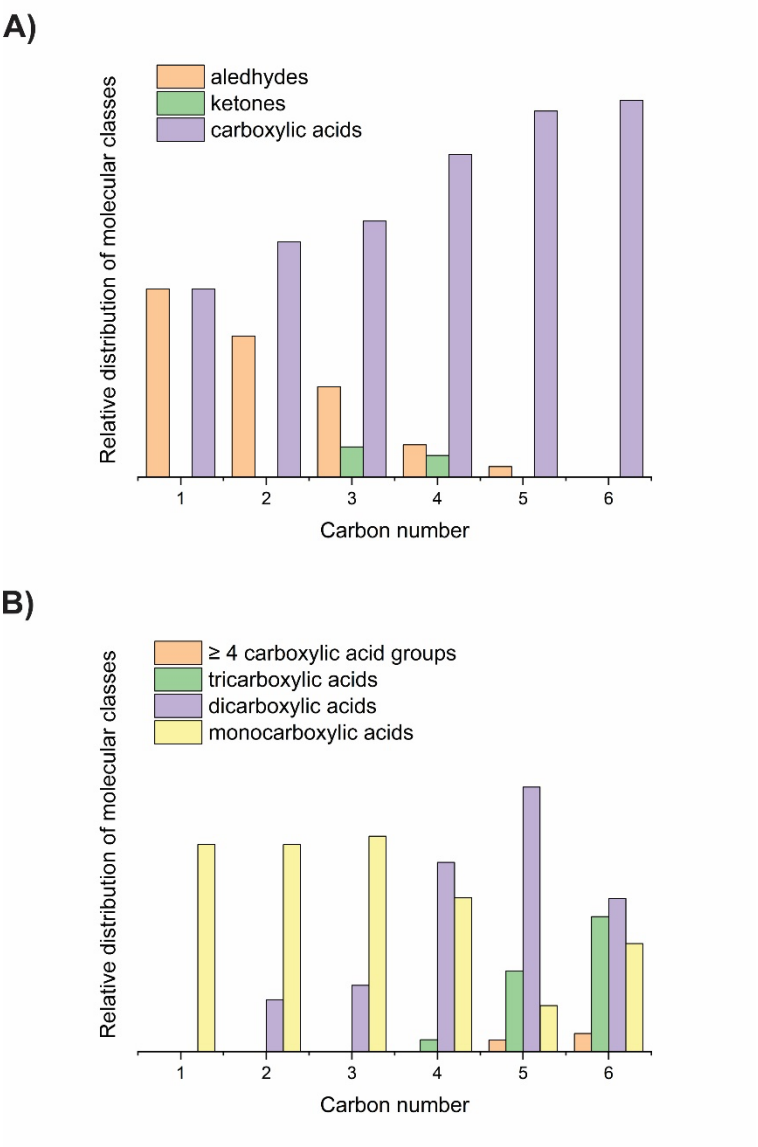

Figure S1: Distribution of the number of the relative number of (A) aldehydes, ketones, and carboxylic acid per carbon number and (B) carboxylic acids with one, two, three, or ≥ 4 carboxylic acid groups derived from the simulations conducted in Morowitz et al[1].

Table S1: Biologically relevant compounds with migration times tested during peak identification during analysis of *E. coli*.

Analyte	Migration Time (min)
oxaloacetic acid	5.9
α-ketoglutaric acid	6.8
α -hydroxyglutaric acid	7.5
glutaric acid	8.1
adenosine triphosphate	8.6
lactic acid	9.5
pyroglutamic acid	10.8
adenosine diphosphate	10.8

2. Sample matrix salinity interferences

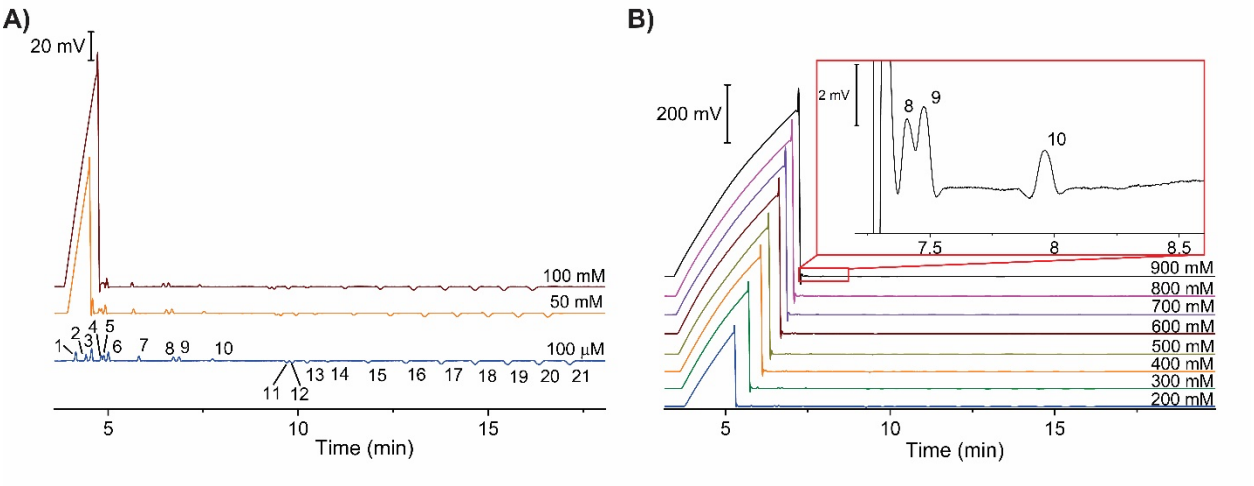

Figure S2: Electropherograms of a 100 µM standard mixture in a BGE composed of 50 mM triethylamine and 55 mM acetic acid, 5% glycerol (pH 5.5) with background concentrations of (A) 100 µM – 100 mM and (B) 200 mM – 900 mM of NaCl. Insert includes magnified peaks at the Cl^- peak front for a 900 mM background concentration. Injections were performed by applying 1 psi for 10 s and the separation voltage was -20 kV. Peaks are (1) chloride (2) nitrate (3) sulfate (4) perchlorate (5) chlorate (6) oxalic acid (7) formic acid (8) malic acid (9) citric acid (10) succinic acid (11) phosphate (12) suberic acid (13) α-hydroxyisobutyric acid (14) propionic acid (15) butanoic acid (16) pentanoic acid (17) hexanoic acid (18) heptanoic acid (19) octanoic acid (20) nonanoic acid (21) decanoic acid.

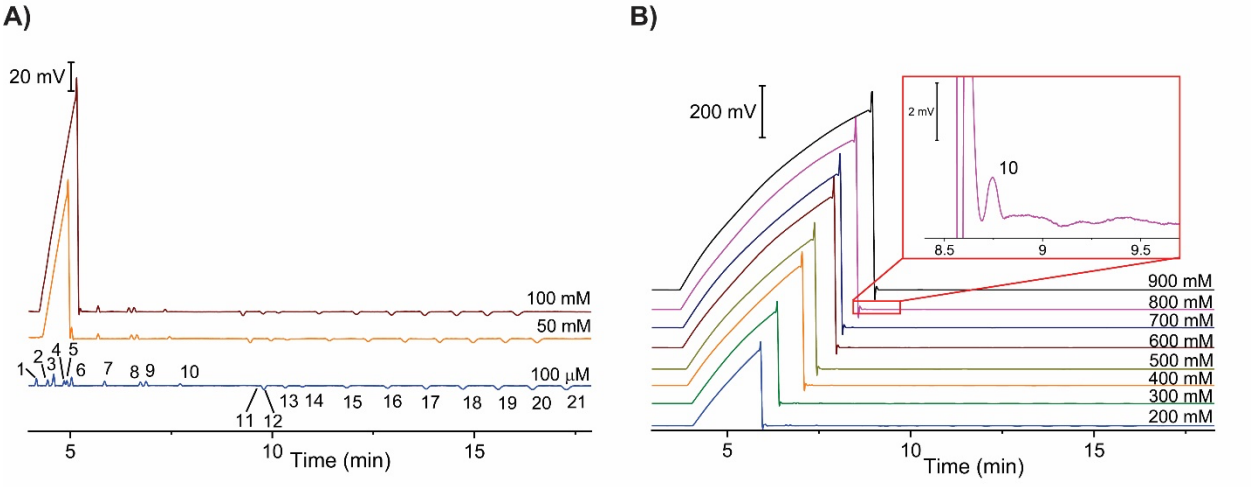

Figure S3: Electropherograms of a 100 µM standard mixture in a BGE composed of 50 mM triethylamine and 55 mM acetic acid, 5% glycerol (pH 5.5) with background concentrations of (A) 100 µM – 100 mM and (B) 200 mM – 900 mM of $MgSO_4$. Insert includes magnified peaks at the SO_4^{2-} peak front for an 800 mM background concentration. Injections were performed by applying 1 psi for 10 s and the separation voltage was -20 kV. Peaks are (1) chloride (2) nitrate (3) sulfate (4) perchlorate (5) chlorate (6) oxalic acid (7) formic acid (8) malic acid (9) citric acid (10) succinic acid (11) phosphate (12) suberic acid (13) α-hydroxyisobutyric acid (14) propionic acid (15) butanoic acid (16) pentanoic acid (17) hexanoic acid (18) heptanoic acid (19) octanoic acid (20) nonanoic acid (21) decanoic acid.

3. Analysis of *E coli* without subcritical water extraction

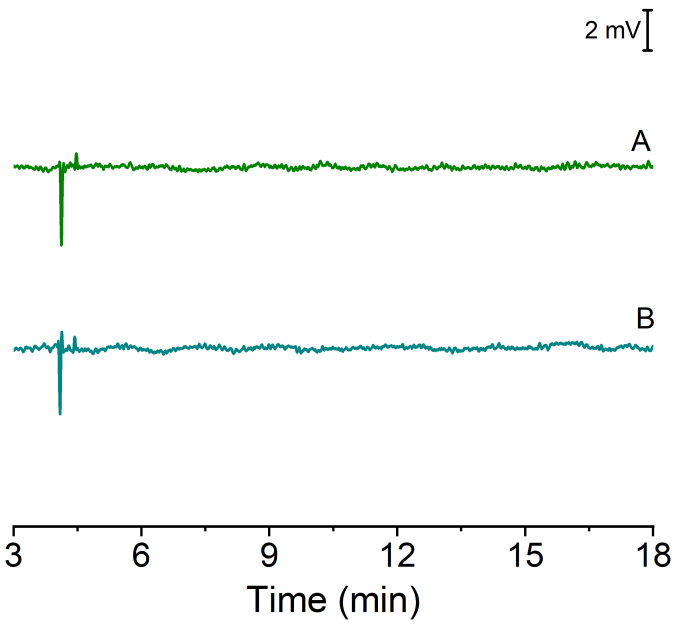

Figure S4: Electropherograms of (A) *E. coli* and (B) blank. The third rinse of *E coli* with 18 MΩ water was used as blank. Separation conditions: 50 mM TEA, 55 mM acetic acid, 5% glycerol at pH 5.5, injection for 1 sec at 10 psi, voltage -20 kV.

4. References

1. Morowitz, H. J.; Kostelnik, J. D.; Yang, J.; Cody, G. D., The origin of intermediary metabolism. *Proceedings of the National Academy of Sciences* **2000,** *97* (14), 7704-7708.