Supplementary information

# Complete Capillary Electrophoresis Process on a Drone: Towards a Flying Micro-lab

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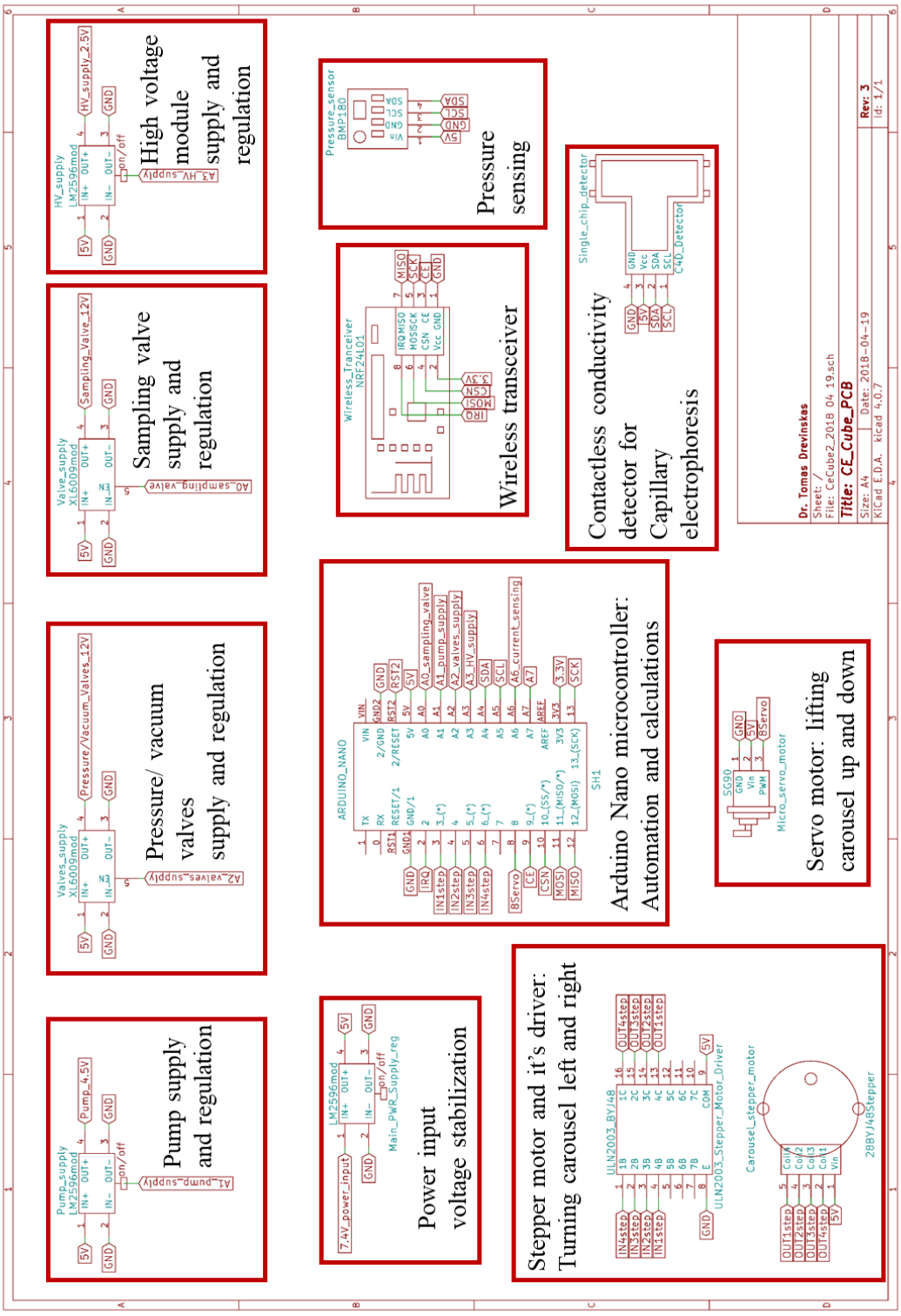
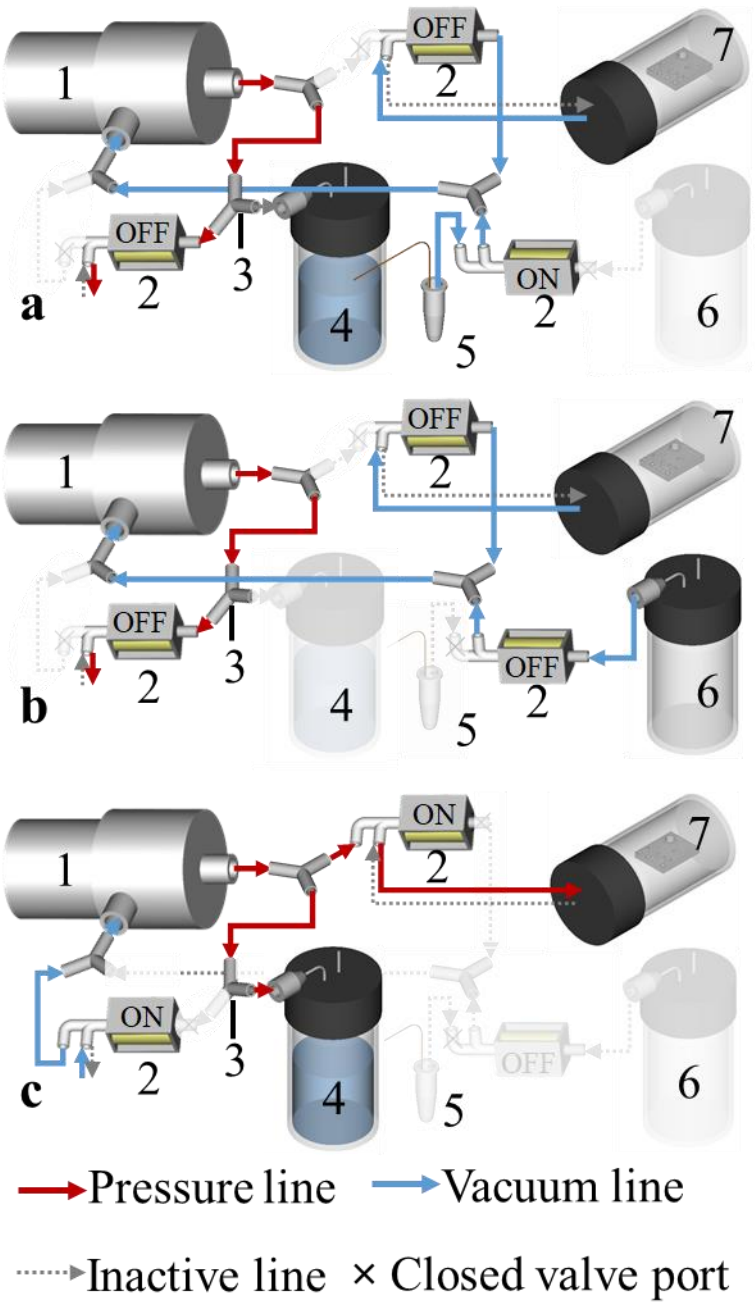
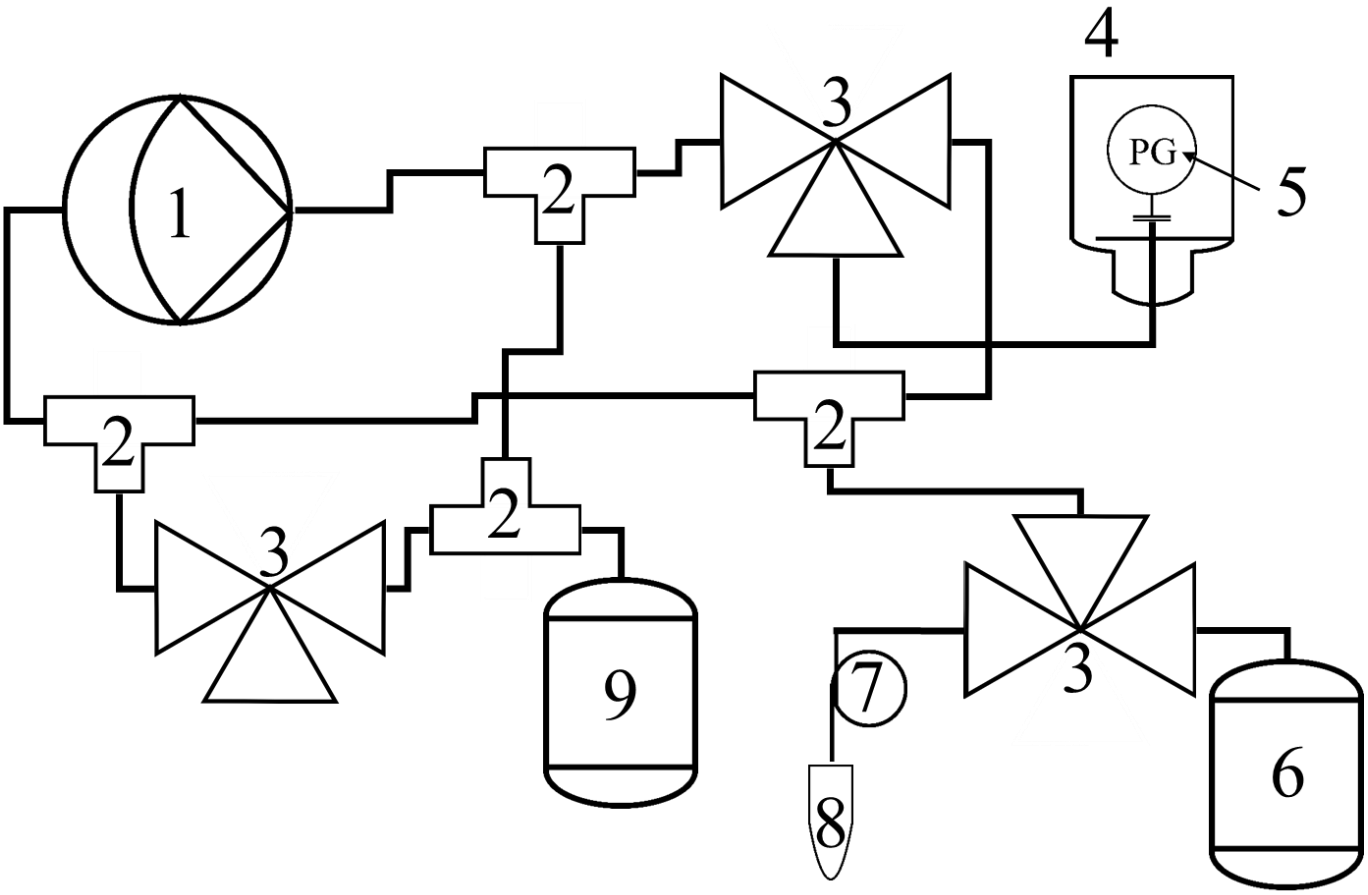


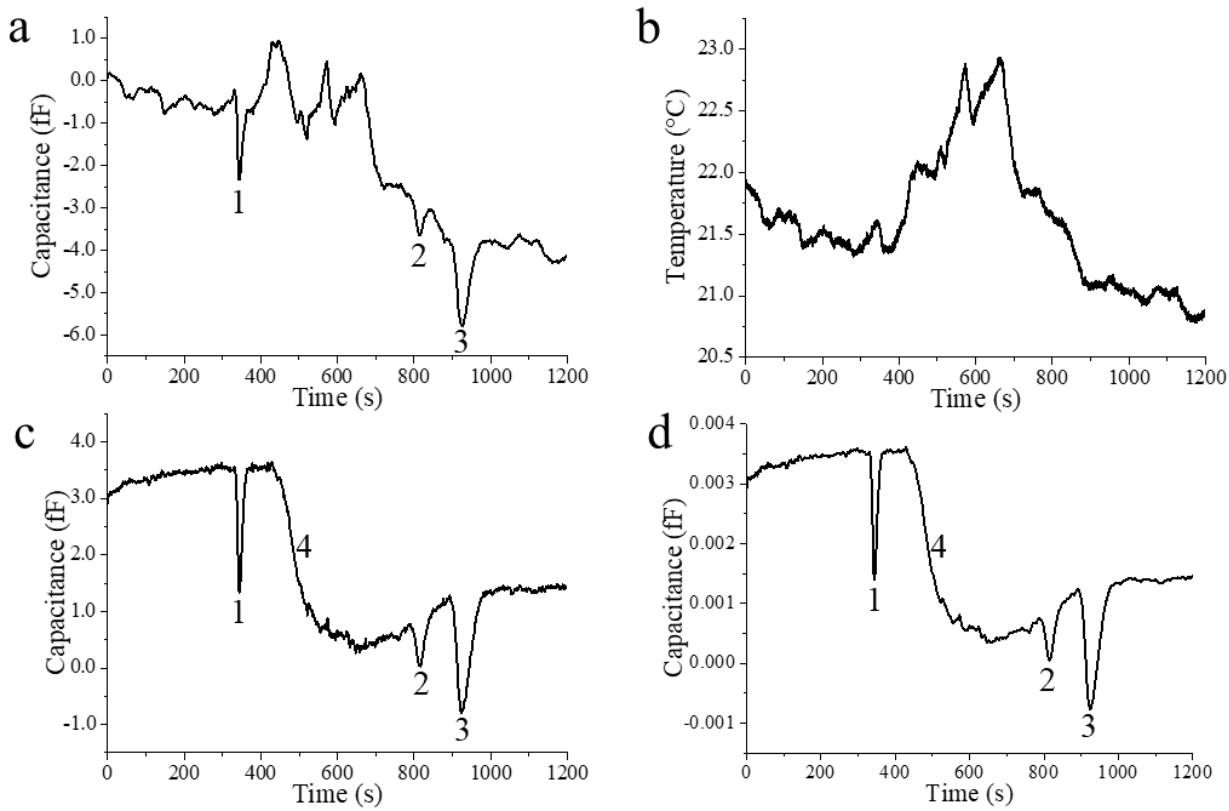

Supplementary Fig. S1. Schematic electrical wiring diagram. Designed using KiCAD.



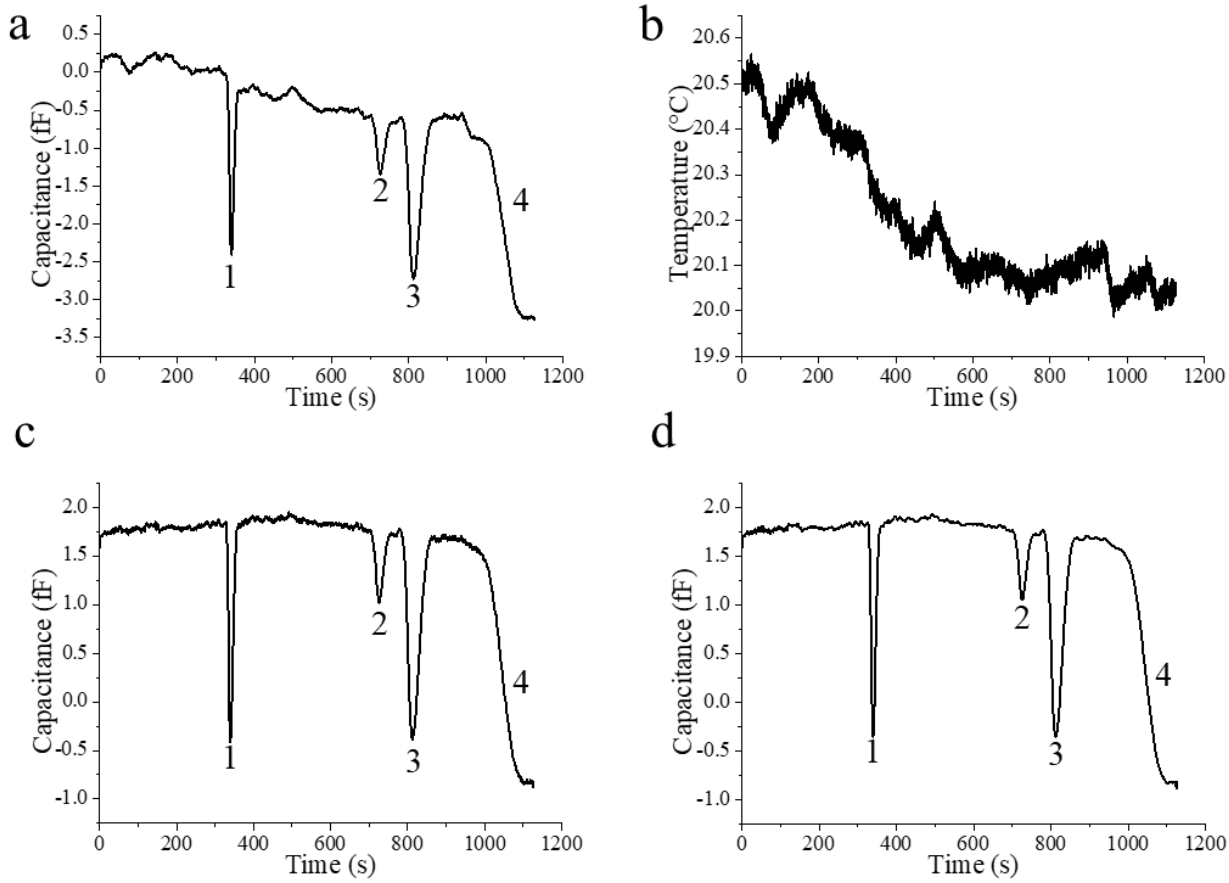

Supplementary Fig. S2. Schematic diagram of pressure, vacuum and liquid distribution system: (**a**) sampling mode, sample collection procedure from the air to the vial, (**b**) vacuum mode, capillary flushing procedure from the vial, (**c**) pressure mode, separation capillary flushing procedure from the BGE bottle. Numbers: 1 – pressure/ vacuum pump, 2 – 3-port, 2-way air valve, 3 – air split, 4 – BGE bottle, 5 – sample vial, 6 – waste bottle, 7 – bottle with pressure sensor



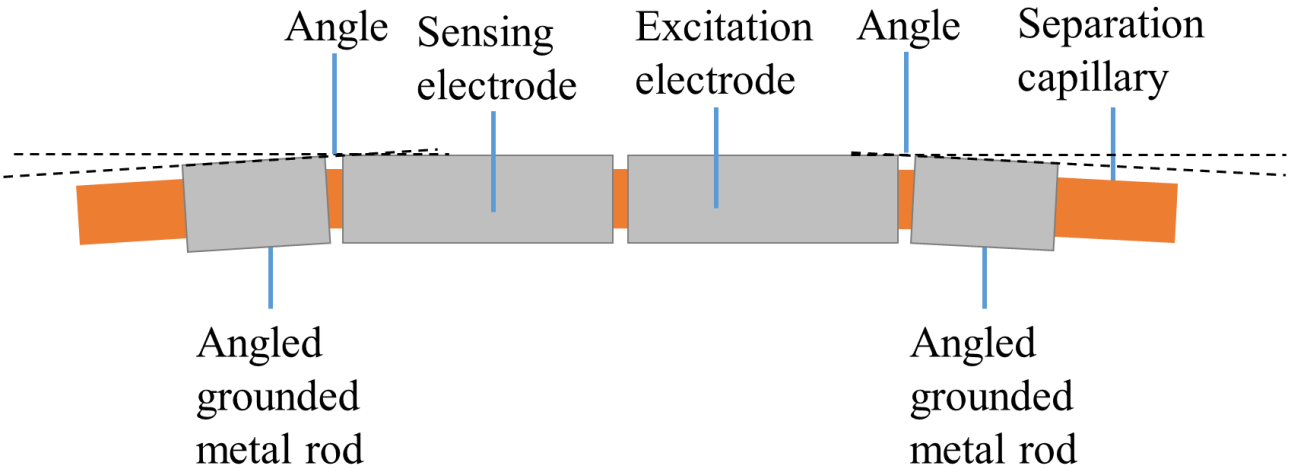

Supplementary Fig. S3 P&ID diagram of a pressure/ vacuum distribution system. Markings: (1) – mini diaphragm 6 V pressure/ vacuum pump, (2) 3-port air split, (3) 3-port 2-way solenoid valve, (4) Pressure/ vacuum gas bottle, (5) pressure sensor, (6) waste bottle, (7) fused silica capillary, (8) sample vial, (9) background electrolyte bottle.




Supplementary Fig. S4. Demonstration of signal compensation and conditioning, when analysis performed on a hovering drone. (a) Original electropherogram, (b) temperature change during analysis, (c) temperature-compensated electropherogram, (d) sensitivity-enhanced electropherogram. Peaks: 1 – $NH_4^+$, 2 – DEA, 3 – TEA, 4 – system valley. Average wind speed 7 m/ s, gusts up to 10 m/ s. Sampling – 32 min. Added volatile compounds: no more than 1.0 ppm $NH_3$, 1.3 ppm DEA, 1.0 ppm TEA. Separation conditions: BGE – 500 mM CH3COOH, injection at 10s×20 kPa, $L_{tot}$ 30 cm, $L_{eff}$ 23.5 cm, separation voltage potential + 4.0 kV, detection – C4D at 3.3 V 32 kHz square wave.




Supplementary Fig. S5. Demonstration of signal compensation and conditioning, when analysis performed on a landed drone. (a) Original electropherogram, (b) temperature change during analysis, (c) temperature-compensated electropherogram, (d) sensitivity-enhanced electropherogram. Peaks: 1 – $NH_4^+$, 2 – DEA, 3 – TEA, 4 – system valley. Average wind speed 7 m/ s, gusts up to 10 m/ s. Sampling – 32 min. Added volatile compounds: no more than 1.0 ppm $NH_3$, 1.3 ppm DEA, 1.0 ppm TEA. Separation conditions: BGE – 500 mM CH3COOH, injection at 10s×20 kPa, $L_{tot}$ 30 cm, $L_{eff}$ 23.5 cm, separation voltage potential + 4.0 kV, detection – C4D at 3.3 V 32 kHz square wave.




Supplementary Fig. S6. Schematic diagram representing how the capillary was fixed in order to prevent vibration caused effects on the detection

Supplementary Table S1. Calibration conditions and results

| No | Analyte | Calibration equation y= | $R^2$ | Average Precision (%) | Calibration Range (mM) | Background electrolyte | Injection | Ltot (cm)* | Leff (cm)* |
|---|---|---|---|---|---|---|---|---|---|
| 1 | $K^+$ | 0.3335x | 0.9964 | <10.3 | 0.0058-0.3700 | 500 mM $CH_3COOH$ | 10s×20kPa | 30 | 23.5 |
| 2 | $Ca^{2+}$ | 0.8642x | 0.9913 | <9.6 | 0.0059-0.3818 | | | | |
| 3 | $Na^+$ | 0.6226x | 0.9953 | <6.5 | 0.0039-0.2500 | | | | |
| 4 | $NH_4^+$ | 0.3363x | 0.9913 | <4.5 | 0.0133-0.3127 | | | | |
| 5 | Diethylamine | 0.7199x | 0.9984 | <2.2 | 0.0151-0.9680 | | | | |
| 6 | Triethylamine | 0.9175x | 0.9967 | <3.3 | 0.0112-0.7165 | | | | |
| 7 | BSA* | 18.202x | 0.9925 | <11.1 | 0.0005-0.0341 | | | | |
| 8 | Formic acid | 0.1212x + 0.0021 | 0.9922 | <11.6 | 0.0078-0.2500 | 150 mM AMP** | 10s×20kPa | 35 | 28.5 |
| 9 | Acetic acid | 0.2909x + 0.0023 | 0.9857 | <10.3 | 0.0078-0.2500 | | | | |
| 10 | Methylphosphonic acid | 0.2465x | 0.9935 | <3.8 | 0.0400-0.2000 | 10 mM MES***/L-His**** | 5s×20kPa | 35 | 28.5 |
| 11 | Ethylphosphonic acid | 0.0867x + 0.0022 | 0.9925 | <8.0 | 0.0400-0.1000 | | | | |
| 12 | Propylphosphonic acid | 0.0857x + 0.0028 | 0.9934 | <8.8 | 0.0400-0.1000 | | | | |
| 13 | Ethyl methylphosphonate | 0.0725x + 0.0011 | 0.9956 | <12.6 | 0.0400-0.1000 | | | | |
| 14 | Pinacoyl methylphosphonate | 0.0587x + 0.0007 | 0.9809 | <6.2 | 0.0400-0.1000 | | | | |

* BSA – Bovine serum albumin

** AMP - 2-Amino-2-methyl-1-propanol

*** MES - 2-(N-morpholino)ethanesulfonic acid

**** L-His - L-histidine

Supplementary Table S2. Sampling conditions

| No | Analyte | Reagent concentration | Method | Concentration in the air (ppm) | Added | Sampling Time (min) | Determined in collected sample (mM) |
|---|---|---|---|---|---|---|---|
| 1 | $CH_3COOH$ | 99.9 % | Evaporation | 79.3 | 10 µL | 16 | 0.0647 ± 0.0026 |
| 2 | $CH_3COOH$ | 99.9 % | Evaporation | 15.9 | 2 µL | 16 | 0.0229 ± 0.0013 |
| 3 | HCOOH | 99.9 % | Evaporation | 120.3 | 10 µL | 16 | 0.1074 ± 0.0114 |
| 4 | HCOOH | 99.9 % | Evaporation | 24.0 | 2 µL | 16 | 0.0490 ± 0.0036 |
| 5 | $NH_4^+$ | 25 % | Evaporation | 51.2 | 10 µL | 4 | 0.0381 ± 0.0108 |
| 6 | $NH_4^+$ | 25 % | Evaporation | 51.2 | 10 µL | 8 | 0.0985 ± 0.0070 |
| 7 | $NH_4^+$ | 25 % | Evaporation | 51.2 | 10 µL | 16 | 0.1297 ± 0.0072 |
| 8 | $NH_4^+$ | 0.5 % | Evaporation | 1.0 | 10 µL | 32 | 0.0184 ± 0.0009 |
| 9 | DEA* | 99.9 % | Evaporation | 43.9 | 10 µL | 4 | 0.0298 ± 0.0034 |
| 10 | DEA | 99.9 % | Evaporation | 43.9 | 10 µL | 8 | 0.0750 ± 0.0022 |
| 11 | DEA | 99.9 % | Evaporation | 43.9 | 10 µL | 16 | 0.0706 ± 0.0029 |
| 12 | DEA | 2.0 % | Evaporation | 1.3 | 15 µL | 32 | 0.0090 ± 0.0007 |
| 13 | TEA** | 99.9 % | Evaporation | 32.5 | 10 µL | 4 | 0.0209 ± 0.0035 |
| 14 | TEA | 99.9 % | Evaporation | 32.5 | 10 µL | 8 | 0.0577 ± 0.0037 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 15 | TEA | 99.9 % | Evaporation | 32.5 | 10 µL | 16 | 0.1102 ± 0.0038 |
| 16 | TEA | 2.0 % | Evaporation | 1.0 | 15 µL | 32 | 0.0384 ± 0.0042 |
| 17 | $K^+$ | 32 mg/ L | Ultrasonic atomization | N/A*** | N/A | 4 | 0.0303 ± 0.0020 |
| 18 | $K^+$ | 32 mg/ L | Ultrasonic atomization | N/A | N/A | 8 | 0.0305 ± 0.0023 |
| 19 | $K^+$ | 32 mg/ L | Ultrasonic atomization | N/A | N/A | 16 | 0.0391 ± 0.0044 |
| 20 | $Na^+$ | 1727 mg/ L | Ultrasonic atomization | N/A | N/A | 4 | 0.0750 ± 0.0080 |
| 21 | $Na^+$ | 1727 mg/ L | Ultrasonic atomization | N/A | N/A | 8 | 0.2006 ± 0.0104 |
| 22 | $Ca^{2+}$ | 552 mg/ L | Ultrasonic atomization | N/A | N/A | 4 | 0.0123 ± 0.0020 |
| 23 | $Ca^{2+}$ | 552 mg/ L | Ultrasonic atomization | N/A | N/A | 8 | 0.0331 ± 0.0024 |
| 24 | BSA**** | 1 mg/ mL | Ultrasonic atomization | N/A | N/A | 8 | 0.0034 ± 0.0006 |
| 25 | BSA | 1 mg/ mL | Ultrasonic atomization | N/A | N/A | 16 | 0.0076 ± 0.0003 |

DEA* - Diethylamine

TEA** - Triethylamine

N/A*** - Not applicable

BSA**** - Bovine serum albumin

$$LOQ = \frac{10\sigma}{S} (Supplementary\ equation\ S1)$$

[1]Where LOQ is the limit of quantification, S is the slope of calibration curve and σ is the standard deviation of the response.

$$C_{mg/L} = \frac{V_s \times C_{\%} \times \rho_s}{V_{box} \times 100\%} (Supplementary\ equation\ S2)$$

Where $C_{mg/L}$ – is the concentration of a substance in the air (mg/ L), $V_s$ – added solution (µL), $C_{\%}$ - percentage of substance solution (%), $\rho_s$ – solution density (mg/ µL), $V_{box}$ – volume of the box (L)

$$C_{ppm} = \frac{m \times 10^3}{V} \times \frac{24.46}{MW} \quad (Supplementary\ equation\ S3)$$

[2]Where $C_{ppm}$ - air concentration (ppm) by volume, at 25 °C and 760 mm Hg, m – actual mass of substance (mg), V – air volume (L), 24.46 – the volume (L) of 1 mole of gas (or evaporated substance) at 25 °C and pressure of 760 mm Hg, MW – molecular weight, grams/ mole.

References

(1) Ich. ICH Topic Q2 (R1) Validation of Analytical Procedures : Text and Methodology. *International Conference on Harmonization*. 2005, p 17.

(2) Air Concentration Calculations for Comparison to OSHA Standards. In *Niosh Manual of Analytical Methods (NMAM)*; Eller, P. M., Cassinelli, M. E., Eds.; U.S. Department of Health and Human Services: Cincinnati, Ohio, 1994; p A-2.