Table 2: Extraction methods for GC-MS analysis breath collected in sampling bags.

| Extraction method | Adsorbent phase | Protocol | Desorption method | Sample storage conditions | Analysis method | GC-MS system | GC-column | Sensibility | Ref. |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| NTD | PDMS, Carbopack-X, Carboxen 1000 | air pump, 30mL/min | **Thermal Desorption** at 260°C (2min) | not specified | GC-MS | 6890 A gas chromatograph coupled with a 5975 Inert XL MSD (Agilent) | DB-624 (Agilent) 60m × 0.32mm × 1.8µm | **ppb** | [1] |
| NTD | 80 mg Carbotrap-B and 260 mg Carbopack-X | air pump, 30mL/min | **Thermal Desorption Unit TD-100** (Markes International). Desorption at 320 °C for 10 min using helium as an inert carrier gas with a flow rate of 50 mL/min. **Cryo-focusing** onto a cold trap kept at −20 °C filled with graphitized carbon blacks. The temperature of the cold trap is then rapidly raised to 340 °C hold for 2 min | samples are extracted immediately after sampling and analyzed on the same day (within a few hours) | GC-ToF-MS | 7890B Gas Chromatograph (Agilent) coupled with a Bench-TOFdx time-of-flight mass spectrometer (Five Technologies) | apolar column Restek-Q-Bond 30m x 0.25mm x 8μm | **ppb** | [2] |
| SPME | PDMS | 60min at 37°C | **Thermal desorption** at 250°C in a splitless mode (3min) | not specified | GC-MS | Gas Chromatograph Mass Spectrometer GCMS-QP2010/ PLUS (Shimadzu) | Rtx-1 (Restek) 30m × 0.25mm× 0.25µm | **not specified** | [3] |
| SPME | Carboxen, PDMS | 10min at 40°C | **Thermal desorption** at 290°C in a splitless mode (1 min) | not specified | GC-MS | 7890 Gas Chromatograph (Agilent) coupled with a mass selective detector MSD type 5975C (Agilent) | PoraBond Q column (Varian) 25m × 0.32mm x 5μm | **ppb** | [4] |
| SPME | DVB, Carboxen, PDMS | 60min at 22°C | **Thermal desorption** at 250°C in a splitless mode (2min) | storage at 22°C for no longer than 6 hours | GCxGC-ToF-MS | GC 7890A (Agilent) with a dual stage jet cryogenic modulator (licensed from Zoex) and a secondary oven coupled to a high-speed ToF mass spectrometer (LECO) | 1D column: HP-5 column (J&W Scientific Inc.) 30m × 0.32mm x 0.25µm 2D column: DB-FFAP (J&W Scientific Inc.) 0.79m × 0.25mm x 0.25µ | **ppq (pg/L)** | [5] |
| SPME | Carboxen, PDMS | 25min at room temperature | **Thermal desorption** at 270°C in a splitless mode (5min) | samples were analyzed within 6h | GC-MS | Finnigan Trace GC Ultra coupled to a Polaris Q Quadrupole Ion Trap GC-MS system | DB-624 (Agilent) 30m × 0.25mm × 1.4µm | **ppt** | [6] |
| TF-SPME | PDMS Thin-Film, 5% Carboxen | 3h at 25°C | **Thermal Desorption** at 270°C for 5 min in tapered glass TD tube (5 mm I.D) at 270°C with a helium flow rate of 60mL/min. **Cryo-focusing** at -120°C in a cooled injection system (CIS). The CIS is then heated to 270°C at 12°C/s | Samples are analyzed immediately after the 3h of extraction | GC-MS | GC-MS 6890/5973(Hewlett Packard) | SLBTM-5MB (Sigma-Aldrich) 30m × 0.25mm × 0.25μm | **ppb** | [7] |
| Trapping in TD tube | Carbotrap C, Carbopack C | air pump | **Thermal Desorption** at 250°C for 8min with helium flowing at 10mL/min. **Cryo-focusing** at -150°C. Injection at 250°C over 1.5min | not specified | GC-MS | HP 5890 Series II Plus GC coupled to 5972 MSD (Hewlett-Packard) | HP5MS 30m x 0.25mm x 0.25µm | **not specified** | [8] |
| Trapping in TD tube | Tenax | air pump, 250mL/min | **Thermal Desorption** at 300°C for 3 minutes. **Cryo-focusing** into a Tenax TA cold trap at −150°C, which was heated after 2 minutes to 280°C at 20°C/s | storage at 4°C for no longer than 2 weeks | GC-MS | 6890 N GC (Agilent) coupled to a quadrupole mass spectrometer 5975 MSD (Agilent) | VF1-MS 30m × 0.25mm x 1 µm | **ppb** | [9] |
| Trapping in TD tube | Tenax TA | air pump, 100mL/min | **Thermal Desorption** at 270°C for 5 min under 60mL/min flow. **Cryo-focusing** on a Tenax cold trap at 0°C; injection in splitless mode at constant 3mL/min total flow | stored at 4 °C until analysis | GC-MS and electronic nose | GCMS-QP2010 (Shimadzu) | SLB-5 MS (Sigma-Aldrich) 30m x 0.25mm x 0.5 | **ppb** | [10] |
| Trapping in TD tube | Tenax, Carbograph, Carboxen | air pump, 200mL/min | **Thermal Desorption** at 270°C for 10min. C**ryo-focusing** at 10°C. The cold trap is subsequently heated to 300°C | storage at 4°C for no longer than 2 weeks | GCxGC BenchTOF-MS | 7890B GC (Agilent) fitted with a flow modulator and a three-way splitter plate coupled to a flame ionization detector and a time-of-flight mass spectrometer with electron ionization (SepSolve). | 1D column: Stabilwax (Restek) 30m × 0.25mm × 0.25μm 2D column: Rtx-200 MS (Restek) 5m × 0.25mm × 0.1μm | **ppq (pg/L)** | [11] |
| Headspace | no adsorbent phase | Gas Syringe 50 mL/min and flow path temperature of 150 ℃ | **Thermal Desorption;** a multiple channel thermal desorption system (UNITYxrTM) with an auto-sampler CIA Advantage-xrTM (Markes) is used to sample 100 mL of exhaled breath from each of the Tedlar bags at a flow rate of 50 mL/min and flow path temperature of 150 ℃ | room temperature no longer than 24h | GC-MS | Trace GC-Ultra gas chromatograph attached to an ISQ Mass Spectrometer (GC-MS, Thermo Scientific) | Rtx-VMS (Restek) 30m × 0.25mm x 1.40μm | **ppm** | [12] |

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