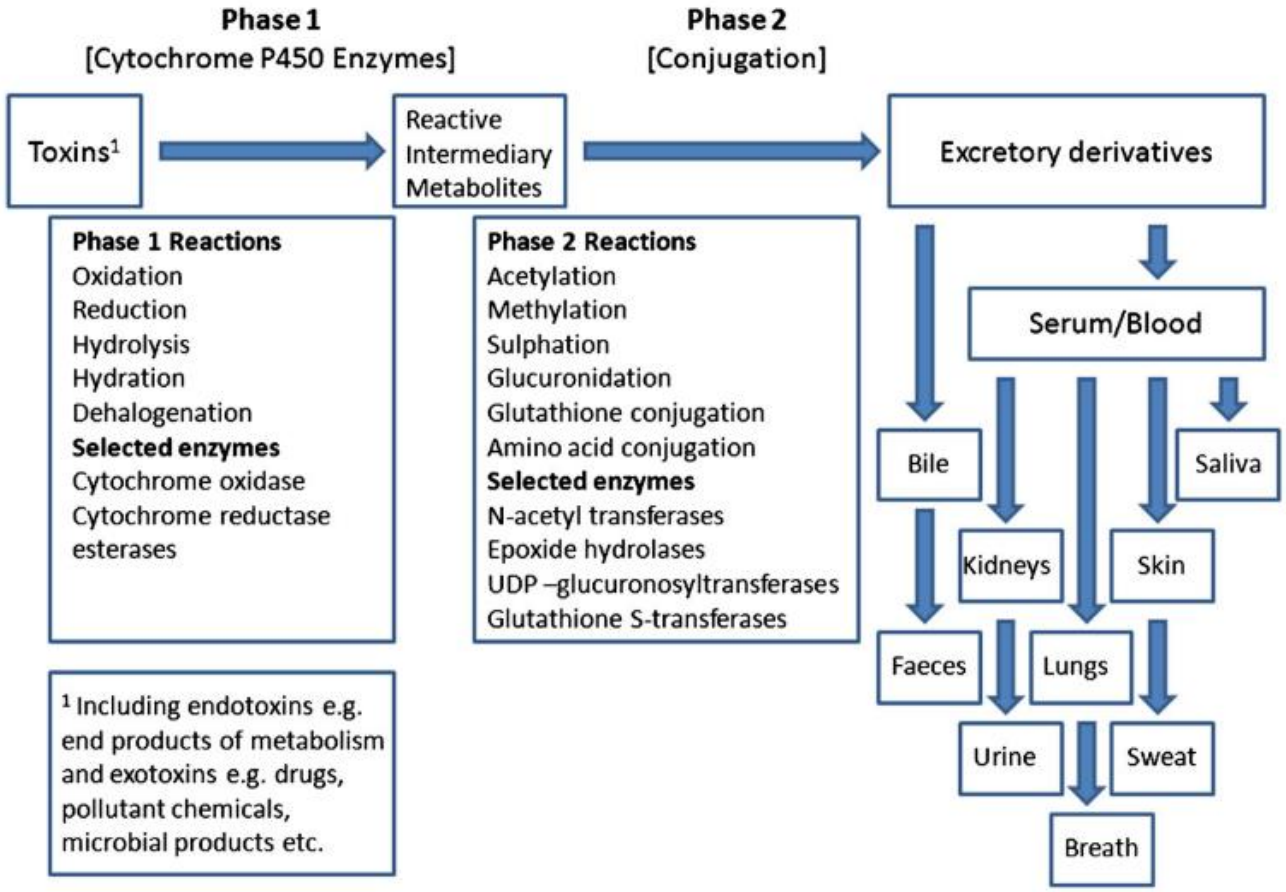
Université de Lille

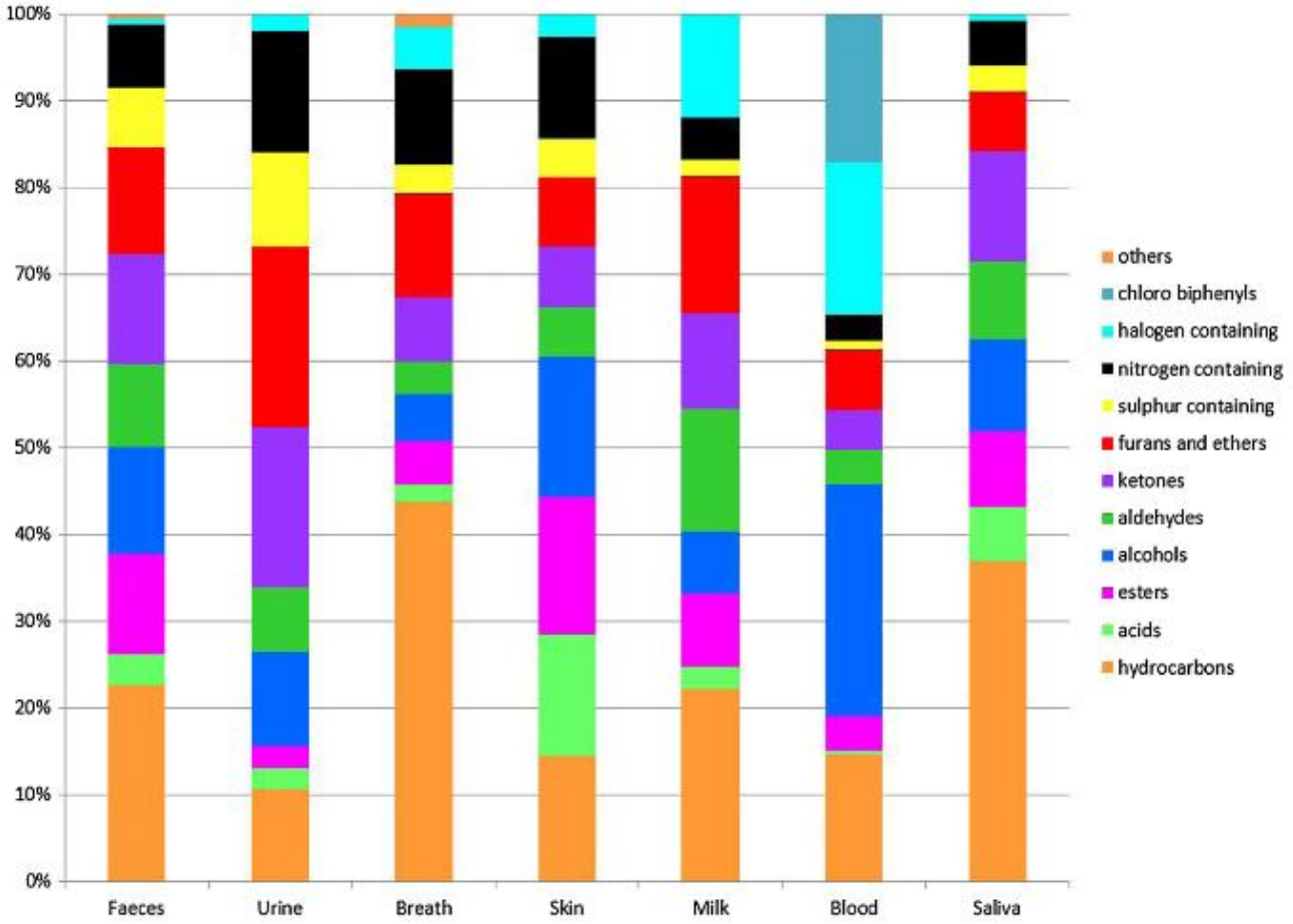
CM4
Volatile organic coumpounds

Chemical conversions undertaken by the liver



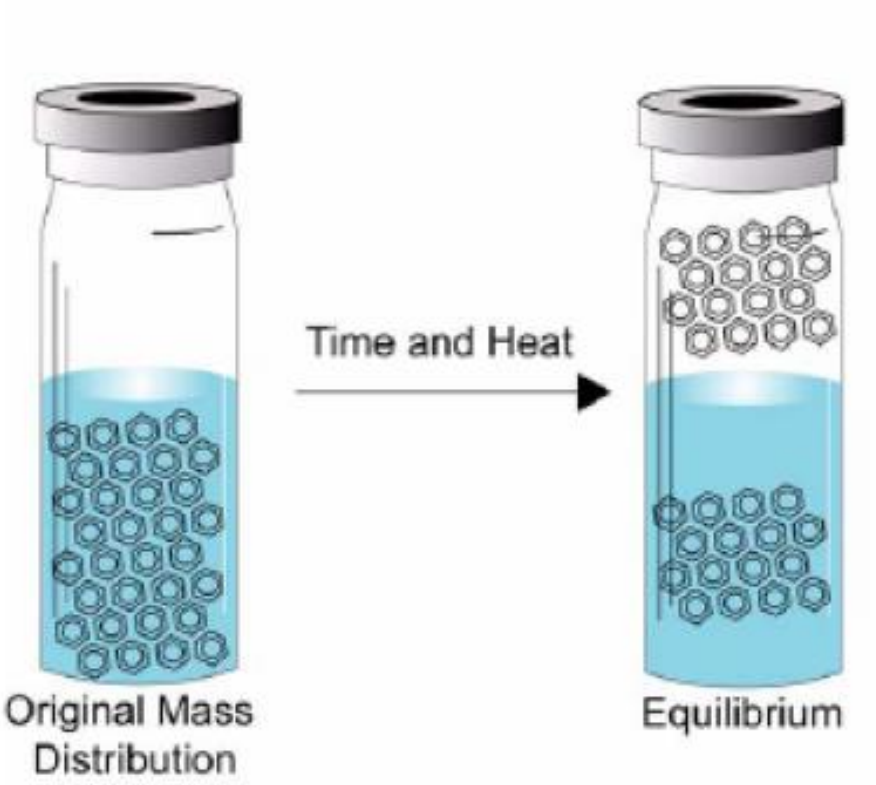
10.1088/1752-7155/8/1/014001

Relative numbers of detected compounds

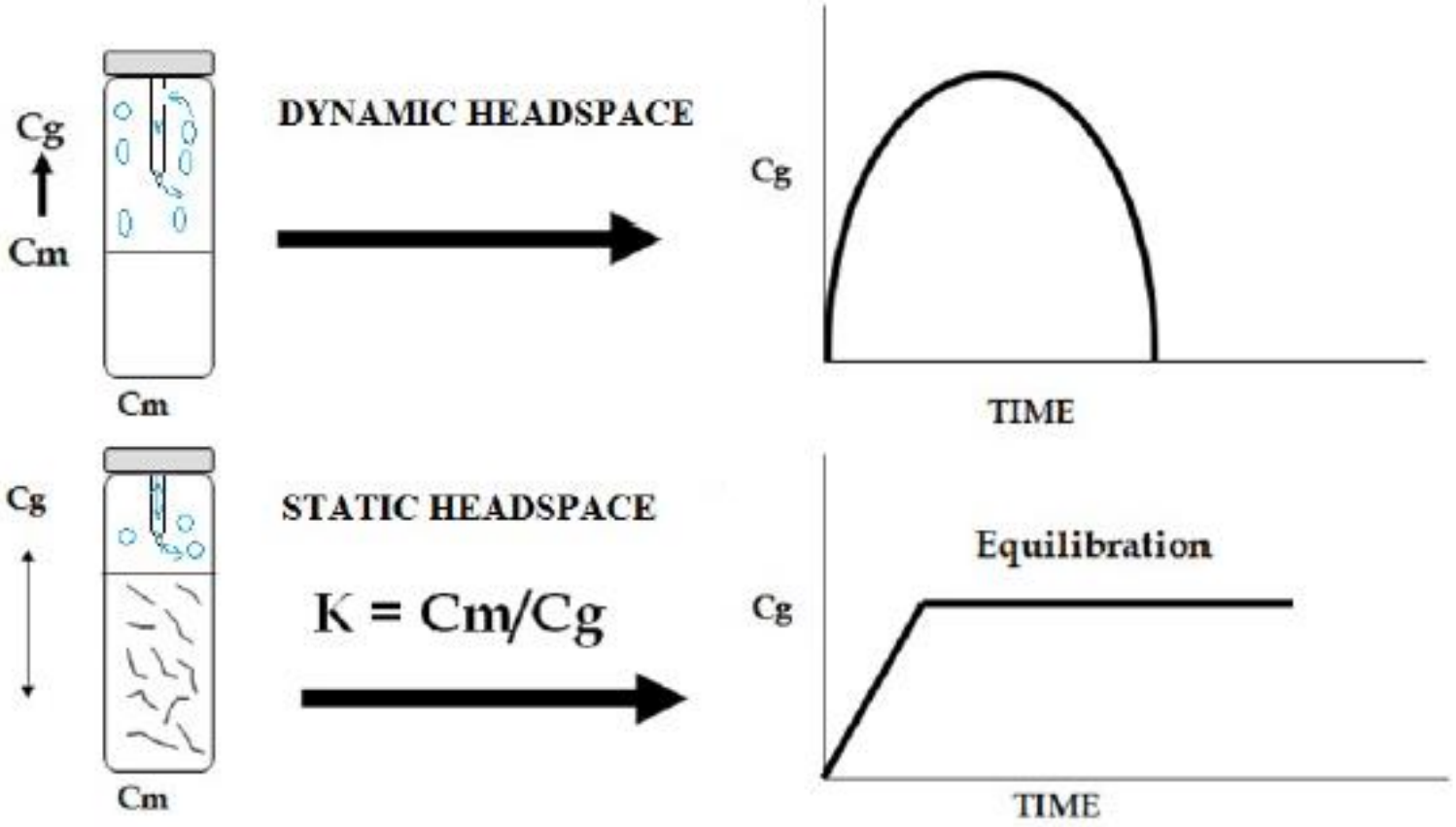


10.1088/1752-7155/8/1/014001

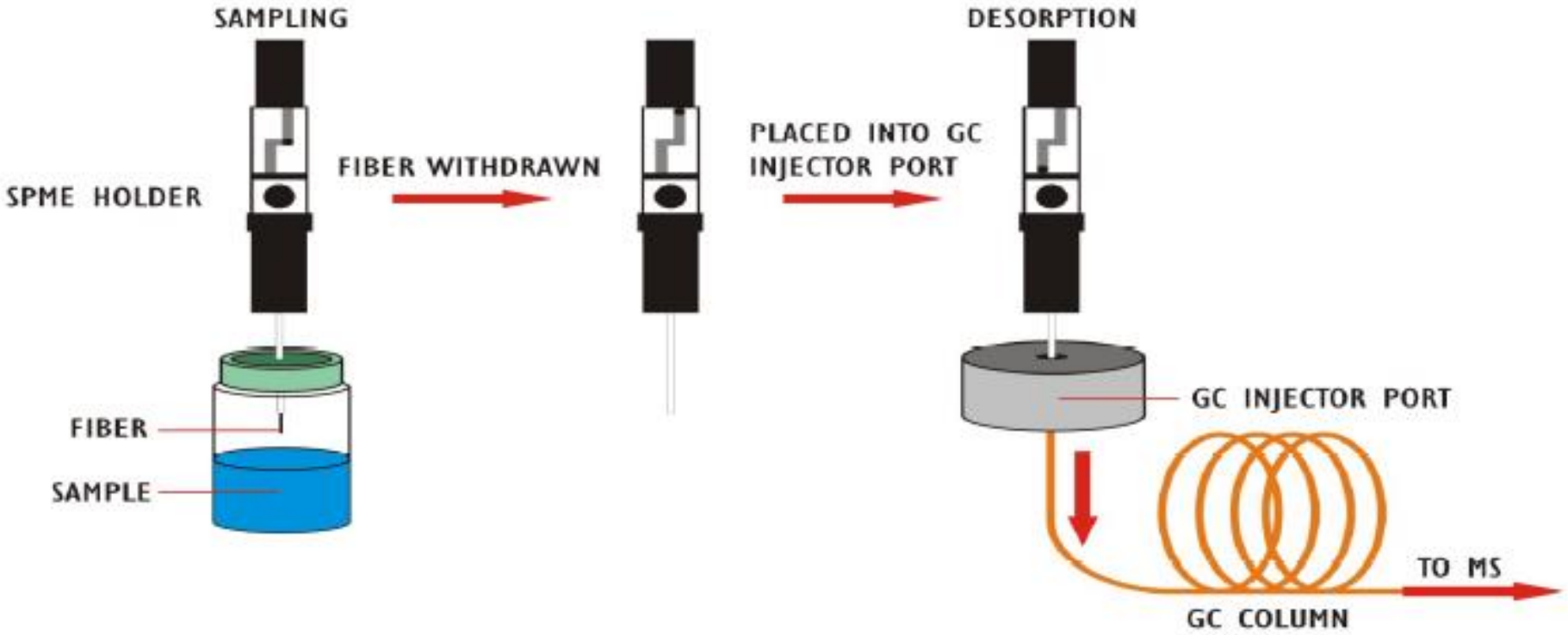
Headspace theory



Static vs dynamic headspace



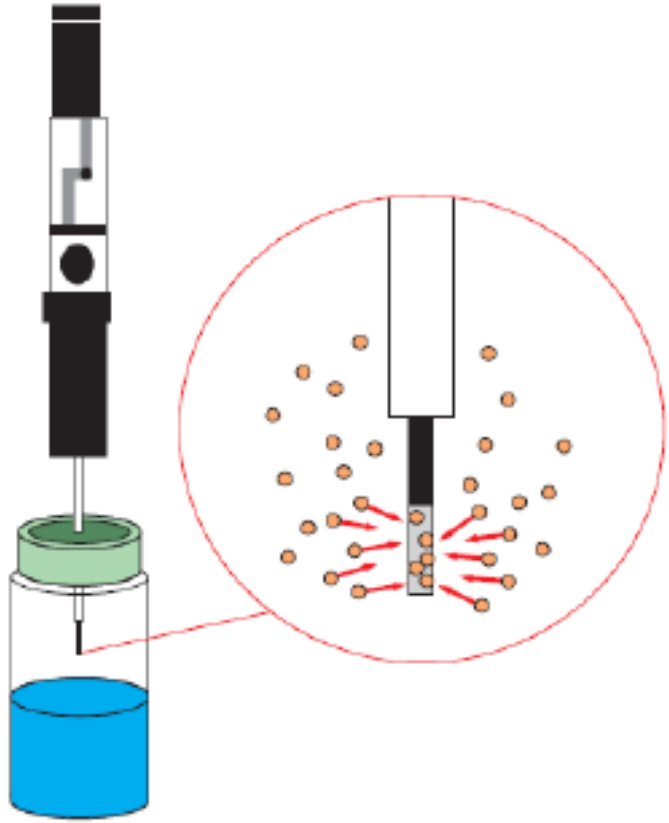
Solid phase microextraction (SPME)



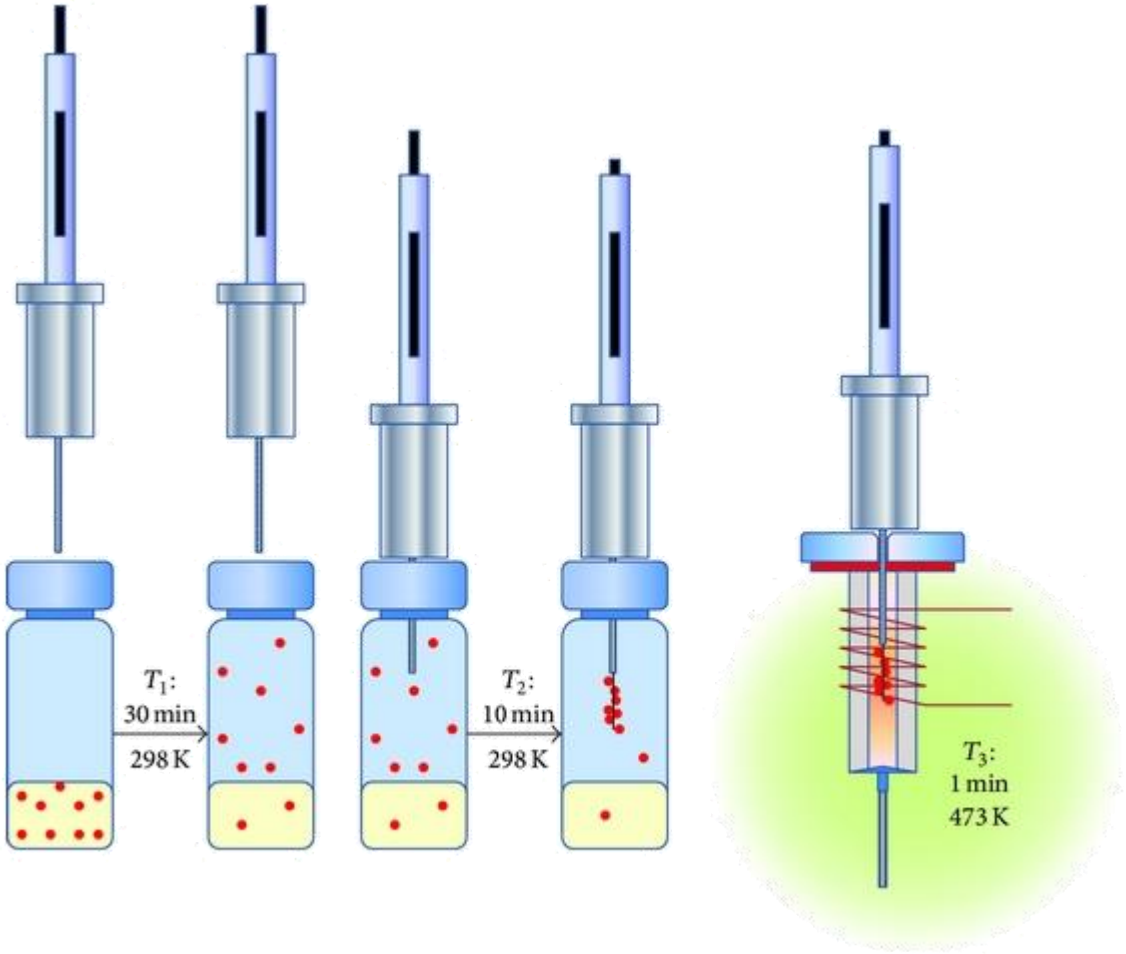
Solid phase microextraction (SPME)

Detection of VOCs

- Thin polymeric coating on a support where analytes are adsorbed onto according to their partition coefficient
- Extraction is maximum when the equilibrium is reached



Solid phase microextraction (SPME)



(SPME)
Detection of VOCs

Polymer coating and thickness	Recommended application	Mechanism	MW	Polarity
100 µm PDMS	Volatiles	Absorbent	60-275	Non-polar
30 µm PDMS	Non-polar semi-volatiles	Absorbent	80-500	Non-polar
7 µm PDMS	Non-polar high molecular weight compounds	Absorbent	125-600	Non-polar
60 µm PEG	Alcohols and polar compounds	Absorbent	40-275	Polar
85 µm PA	Polar semi-volatiles	Absorbent	80-300	Polar
75 µm/85 µm CAR/PDMS	Gases and low molecular weight compounds	Adsorbent	30-225	Bipolar
65 µm PDMS/DVB	Volatiles, amines and nitro-aromatic compounds	Adsorbent	50-300	Bipolar
60 µm PDMS/DVB	Amines, nitroaromatic and polar compounds (HPLC use only)	Adsorbent	50-300	Bipolar
50/30 µm DVB/CAR/PDMS on a StableFlex fiber	Flavour compounds: volatiles and semi-volatiles, C3-C20	Adsorbent	40-275	Bipolar
50/30 µm DVB/CAR/PDMS on a 2 cm StableFlex fiber	Trace compound analysis	Adsorbent	40-275	Bipolar

CAR: Carboxen; PDMS: Polydimethylsiloxane; DVB: Divinylbenzene; HPLC: High Performance Liquid Chromatography; PA: Polyacrylate; PEG: Carbowax-Polyethylene Glycol [19].

- Large variety of supports exist
  - ✓ *Fiber*
  - ✓ *Stir-bars*
  - ✓ *Needles*
  - ✓ *Syringes to small blades for the 96 well-plate*
- Excellent versatility of SPME in terms of sample volume

Analysis of volatile human urinary metabolome by solid-phase microextraction in combination with gas chromatography–mass spectrometry for biomarker discovery: Application in a pilot study to discriminate patients with renal cell carcinoma

Márcia Monteiro [a,*], Márcia Carvalho [a,b], Rui Henrique [c,d,e], Carmen Jerónimo [c,e], Nathalie Moreira [a,f], Maria de Lourdes Bastos [a], Paula Guedes de Pinho [a,*]

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[b] *CEBIMED, Faculdade de Ciências da Saúde, Universidade Fernando Pessoa, Porto, Portugal*
[c] *Cancer Biology & Epigenetics Group, Research Center of the Portuguese Oncology Institute – Porto, Rua Dr. António Bernardino de Almeida, Porto, Portugal*
[d] *Department of Pathology, Portuguese Oncology Institute – Porto, Rua Dr. António Bernardino de Almeida, Porto, Portugal*
[e] *Department of Pathology and Molecular Immunology, Institute of Biomedical Sciences Abel Salazar, University of Porto, Porto, Portugal*
[f] *CBQF – Center for Biotechnology and Fine Chemistry – Associated Laboratory, Faculty of Biotechnology, Catholic University of Portugal, Rua Dr. António Bernardino Almeida, 4200-072 Porto, Portugal*

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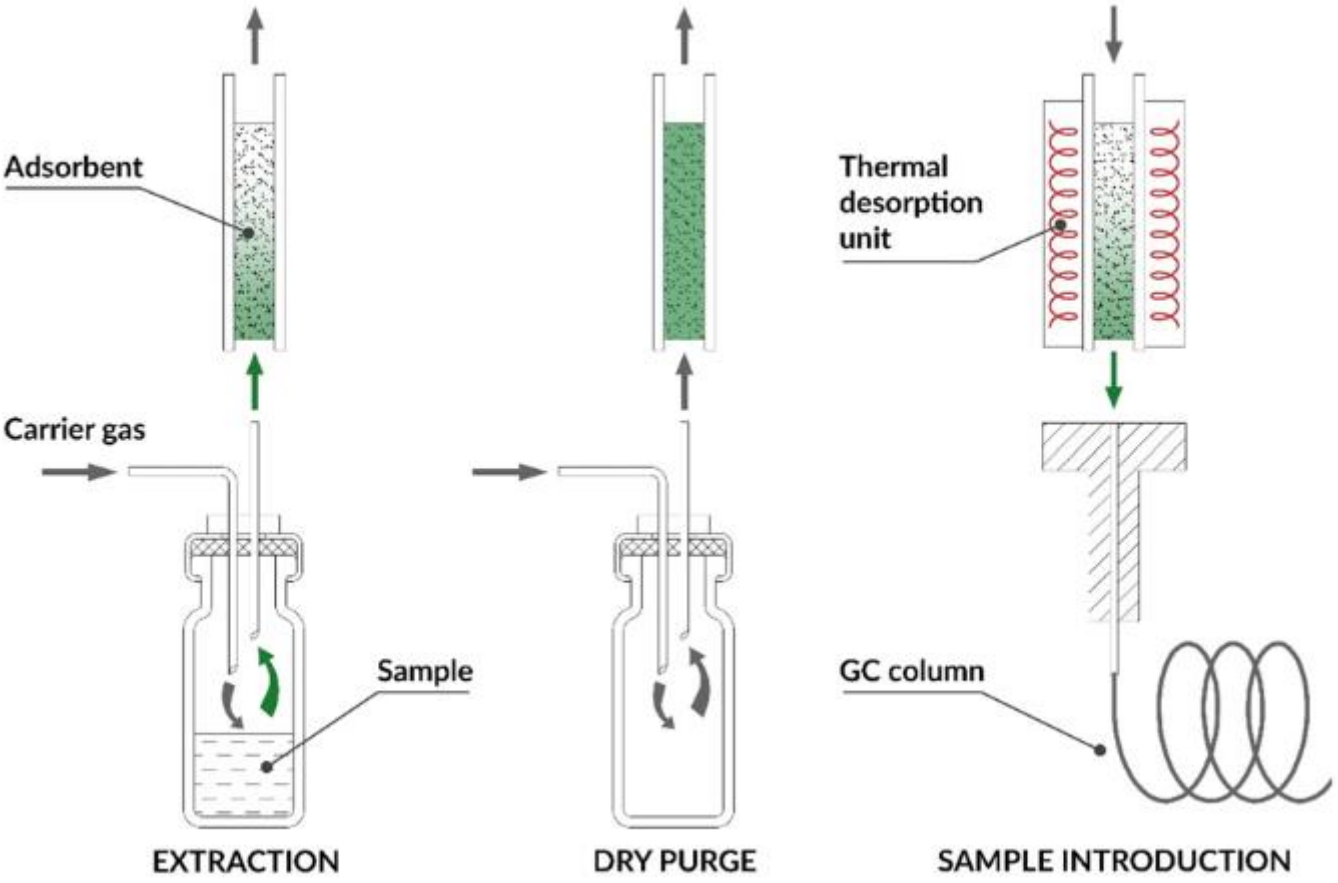
Anal Bioanal Chem (2014) 406:4649–4662
DOI 10.1007/s00216-014-7855-z

RESEARCH PAPER

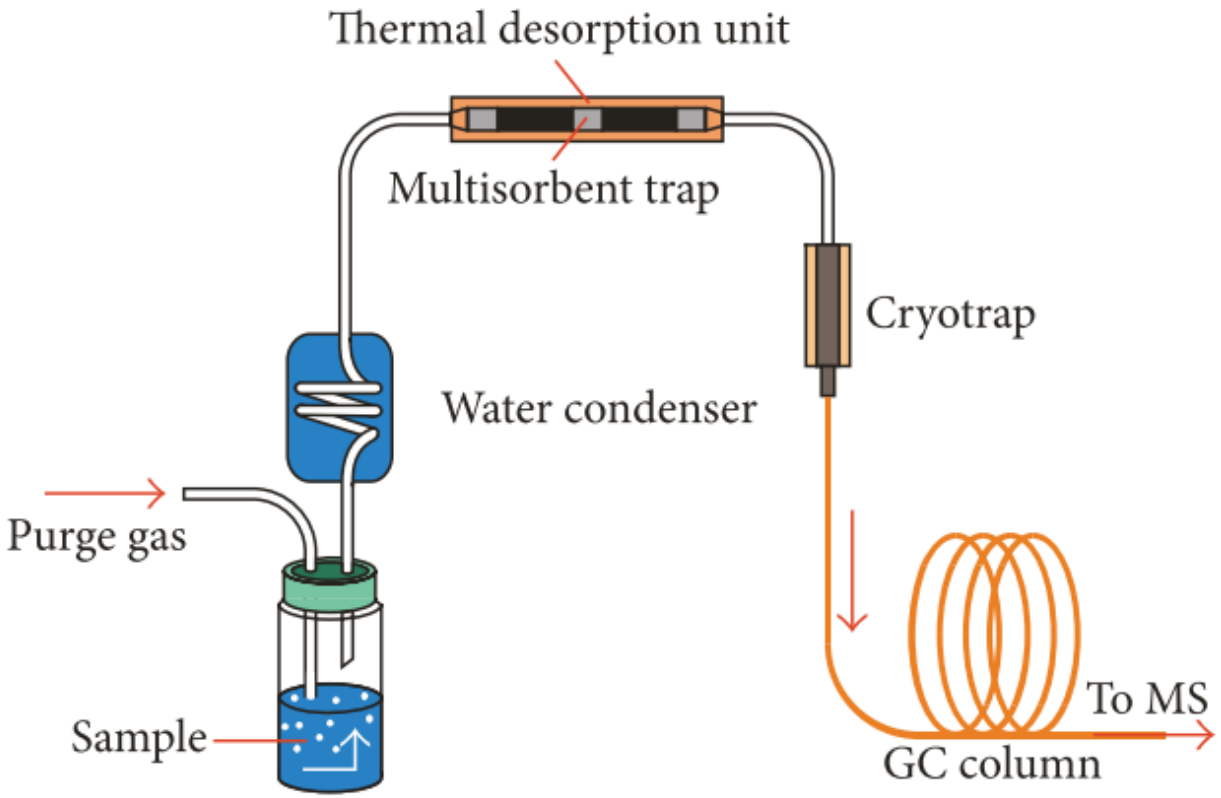
Use of solid-phase microextraction coupled to gas chromatography–mass spectrometry for determination of urinary volatile organic compounds in autistic children compared with healthy controls

Rosaria Cozzolino · Laura De Magistris · Paola Saggese · Matteo Stocchero · Antonella Martignetti · Michele Di Stasio · Antonio Malorni · Rosa Marotta · Floriana Boscaino · Livia Malorni

Thermal desorption tube



Thermal desorption unit



10.1155/2015/981458

British Journal of Cancer (2011) 105, 1894 – 1904

www.bjcancer.com

Investigation of urinary volatile organic metabolites as potential cancer biomarkers by solid-phase microextraction in combination with gas chromatography-mass spectrometry

CL Silva[1], M Passos[2] and JS Câmara[*,1]

[1]CQM/UMa – Centro de Química da Madeira, Centro de Ciências Exactas e da Engenharia, Universidade da Madeira, Campus Universitário da Penteada, Funchal 9000-390, Portugal; [2]Hospital Dr Nélio Mendonça, Avda. Luís de Camões, Funchal 9000, Portugal

DHS ou SHS???

Mochalski et al. Cancer Cell International 2013, 13:72
http://www.cancerci.com/content/13/1/72

CANCER CELL INTERNATIONAL

PRIMARY RESEARCH Open Access

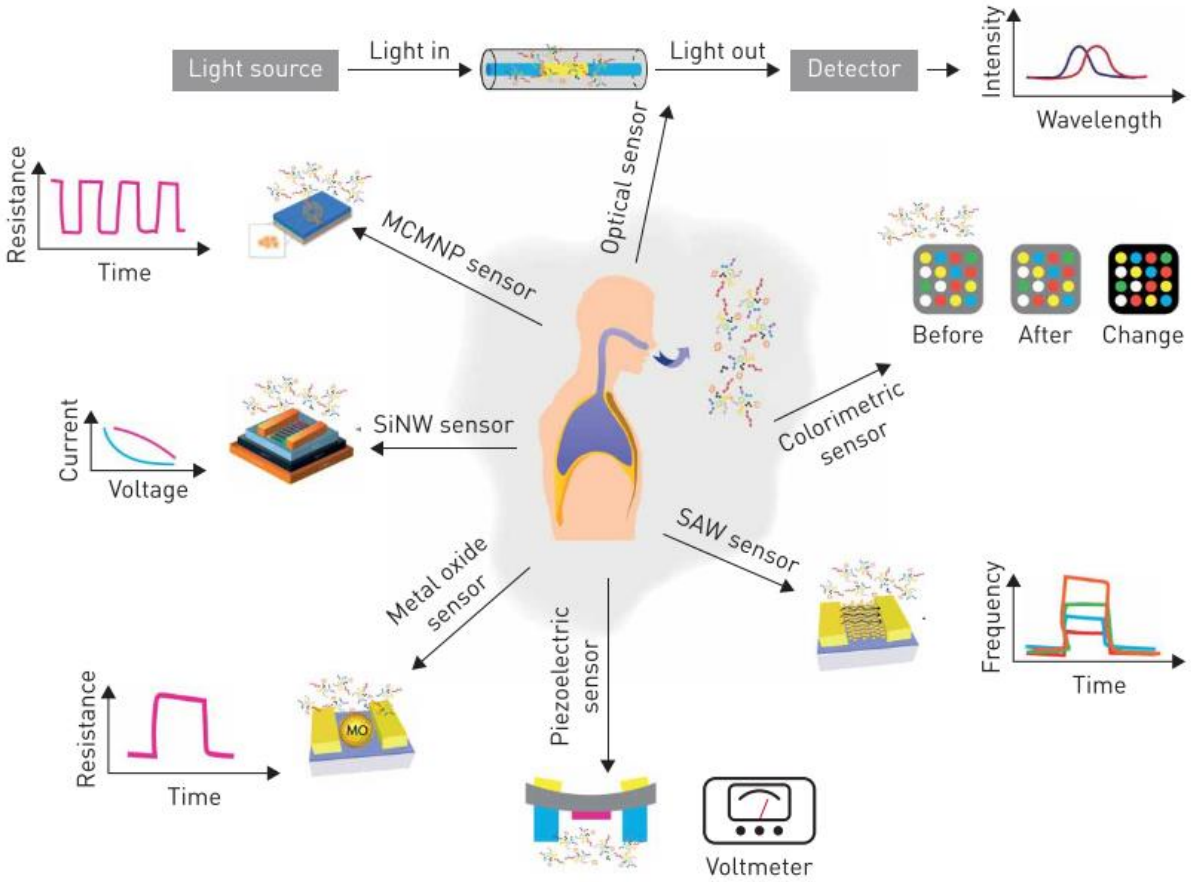
Release and uptake of volatile organic compounds by human hepatocellular carcinoma cells (HepG2) *in vitro*

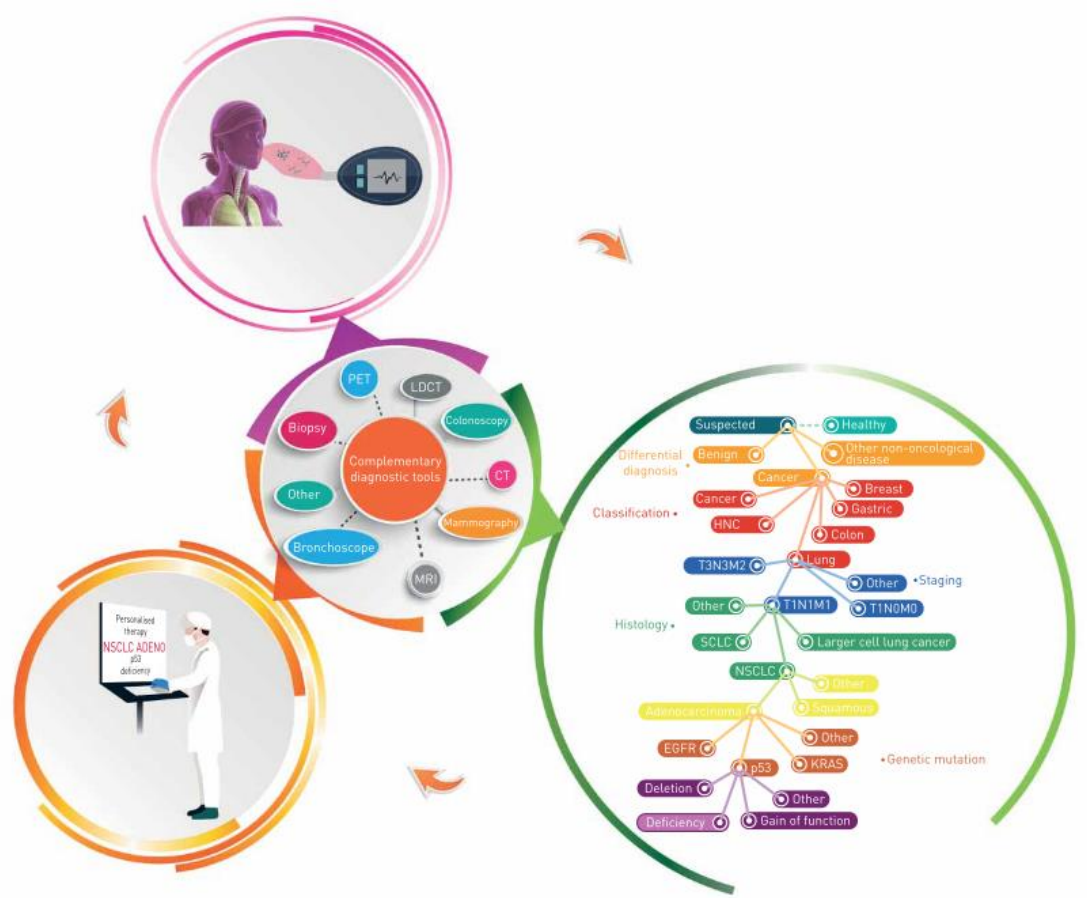
Paweł Mochalski[1*], Andreas Sponring[1,2], Julian King[1], Karl Unterkofler[1,3], Jakob Troppmair[4] and Anton Amann[1,2*]

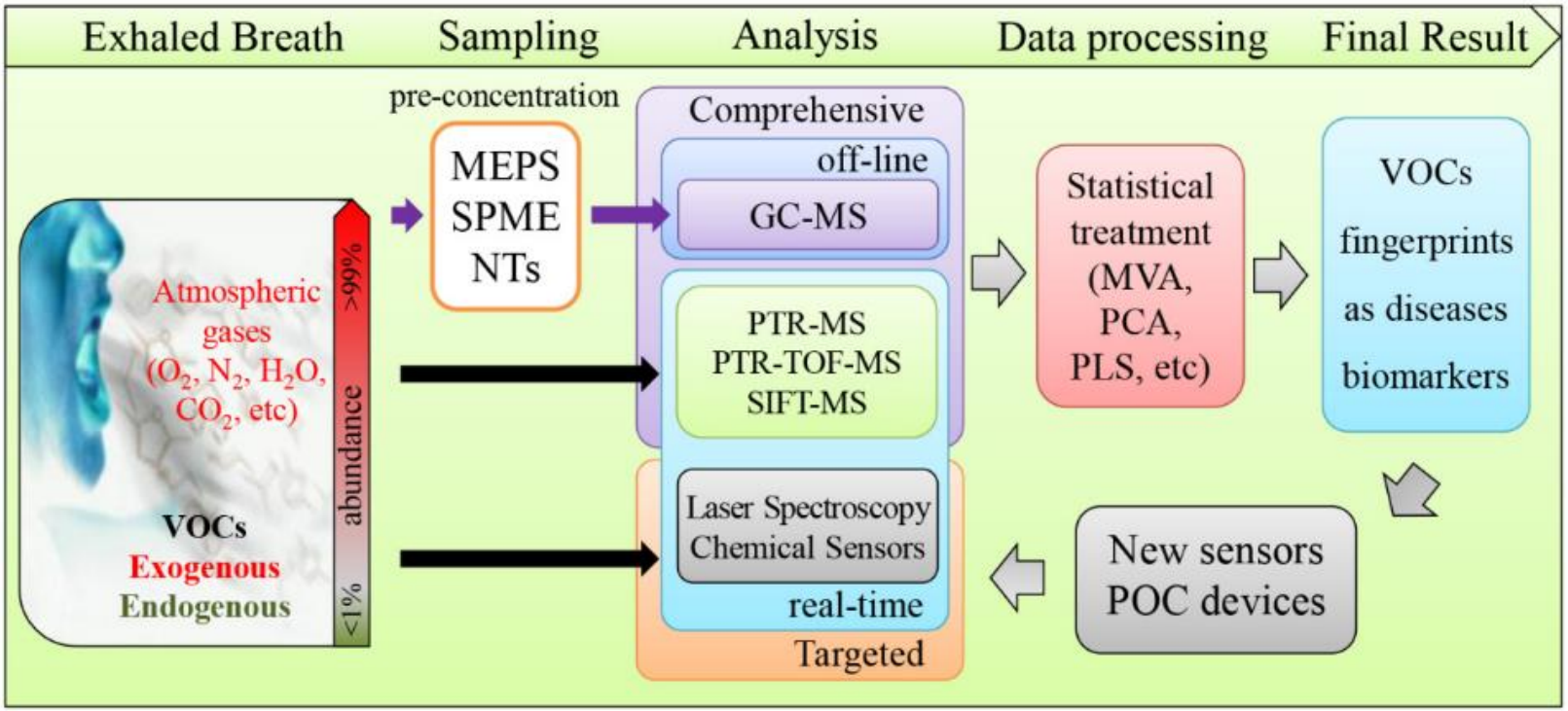
NTD

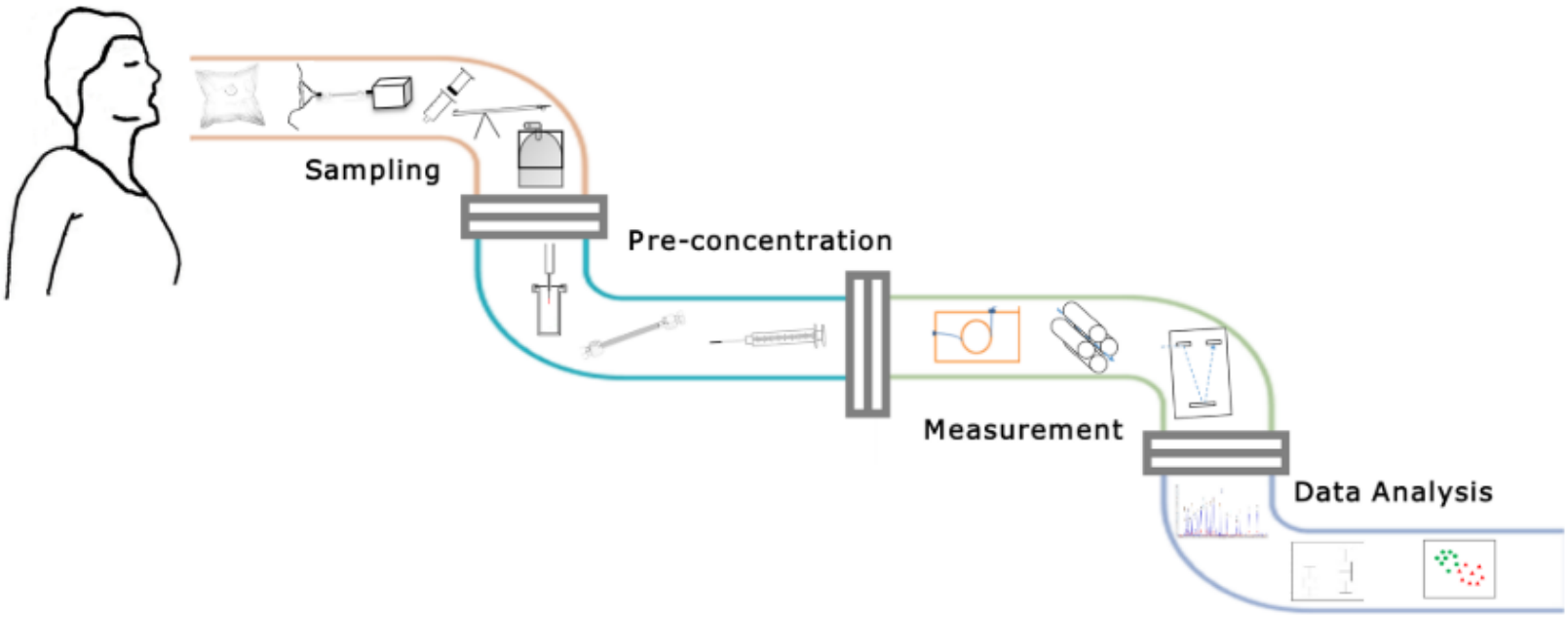
Breath analysis

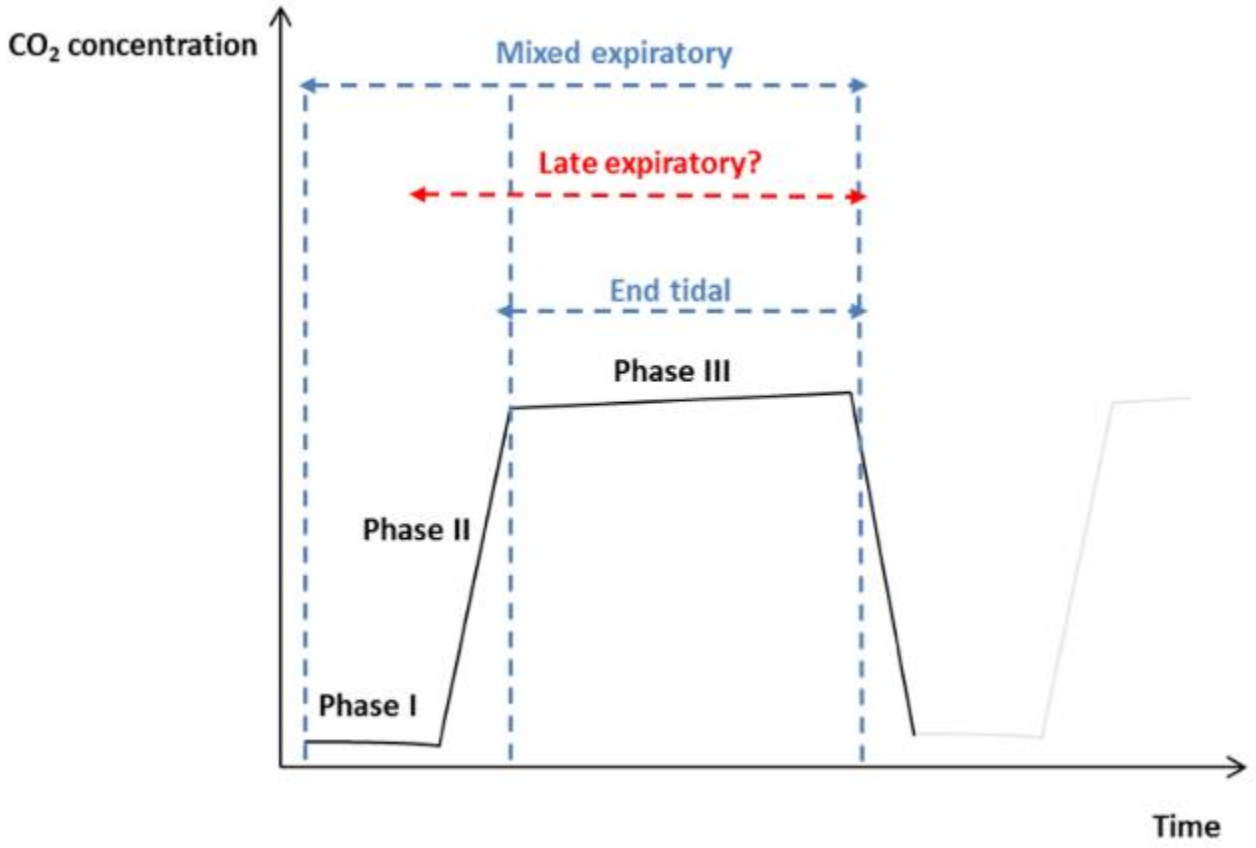
- http://dx.doi.org/10.1183/16000617.0002-2019
- 10.1007/s11306-017-1241-8
- 10.1109/mpuls.2020.2993684
- 10.3390/metabo5010003


Light source
Light in
Light out
Detector
Intensity
Wavelength
Optical sensor
Resistance
Time
MCMNP sensor
Before
After
Change
Current
Voltage
SiNW sensor
Colorimetric sensor
SAW sensor
Metal oxide sensor
Piezoelectric sensor
Frequency
Time
Resistance
Time
MO
Voltmeter


PET
LDCT
Biopsy
Colonoscopy
Complementary diagnostic tools
CT
Other
Mammography
Bronchoscope
MRI
Personalised therapy
NSCLC ADENO
p53 deficiency
Suspected
Healthy
Differential diagnosis
Benign
Other non-oncological disease
Cancer
Classification
Cancer
Breast
Gastric
HNC
Colon
T3N3M2
Lung
Other
•Staging
Other
T1N1M1
T1N0M0
Histology
SCLC
Larger cell lung cancer
NSCLC
Other
Adenocarcinoma
Squamous
Other
EGFR
p53
KRAS
•Genetic mutation
Deletion
Other
Deficiency
Gain of function


Exhaled Breath
Sampling
Analysis
Data processing
Final Result
pre-concentration
MEPS
SPME
NTs
Comprehensive
off-line
GC-MS
PTR-MS
PTR-TOF-MS
SIFT-MS
Laser Spectroscopy
Chemical Sensors
real-time
Targeted
Atmospheric gases (O_2, N_2, H_2O, CO_2, etc)
VOCs
Exogenous
Endogenous
>99%
abundance
<1%
Statistical treatment (MVA, PCA, PLS, etc)
VOCs fingerprints as diseases biomarkers
New sensors
POC devices


Sampling
Pre-concentration
Measurement
Data Analysis


CO_2 concentration
Mixed expiratory
Late expiratory?
End tidal
Phase III
Phase II
Phase I
Time