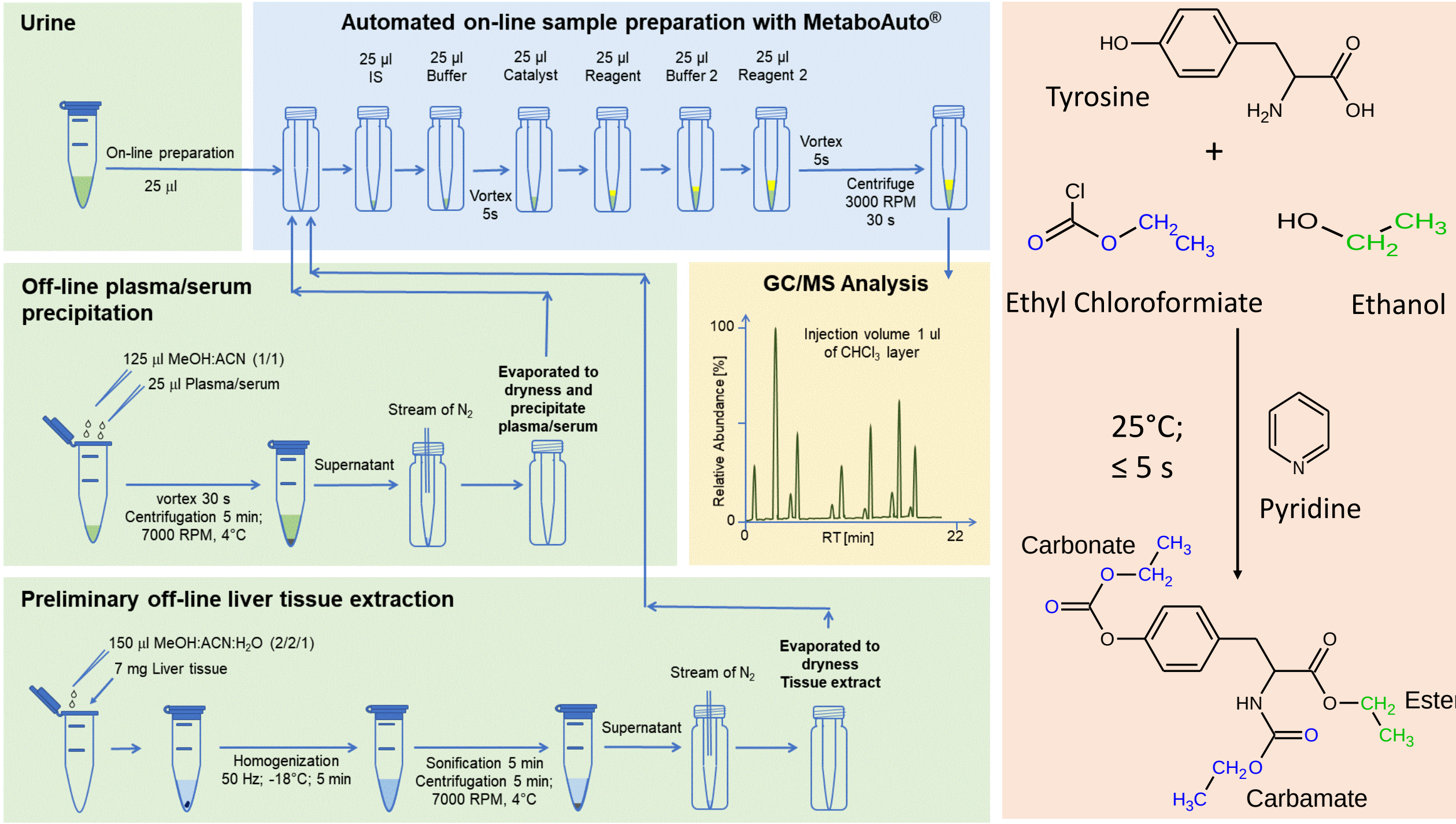
MetaboAuto® - Automated Sample Preparation Platform for on-line GC-MS Metabolomics

METABO AUTO®

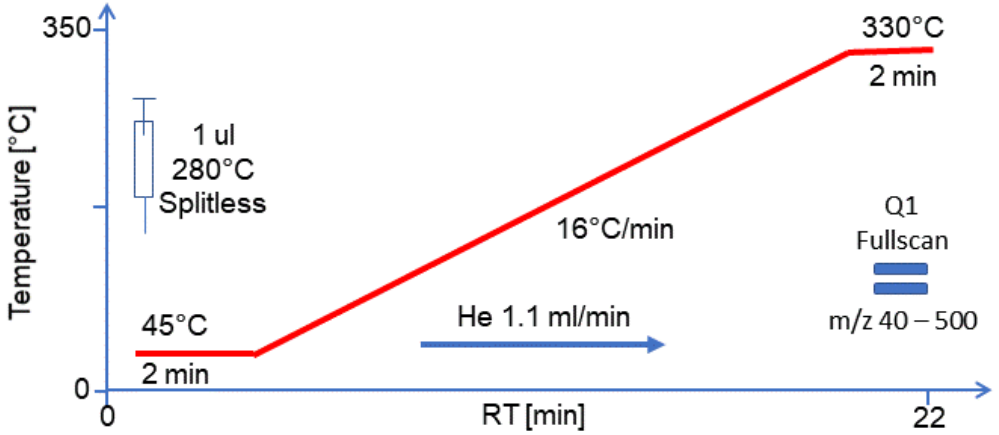
Automated Sample Preparation Platform for on-line GC/MS Metabolomics (MetaboAuto®)

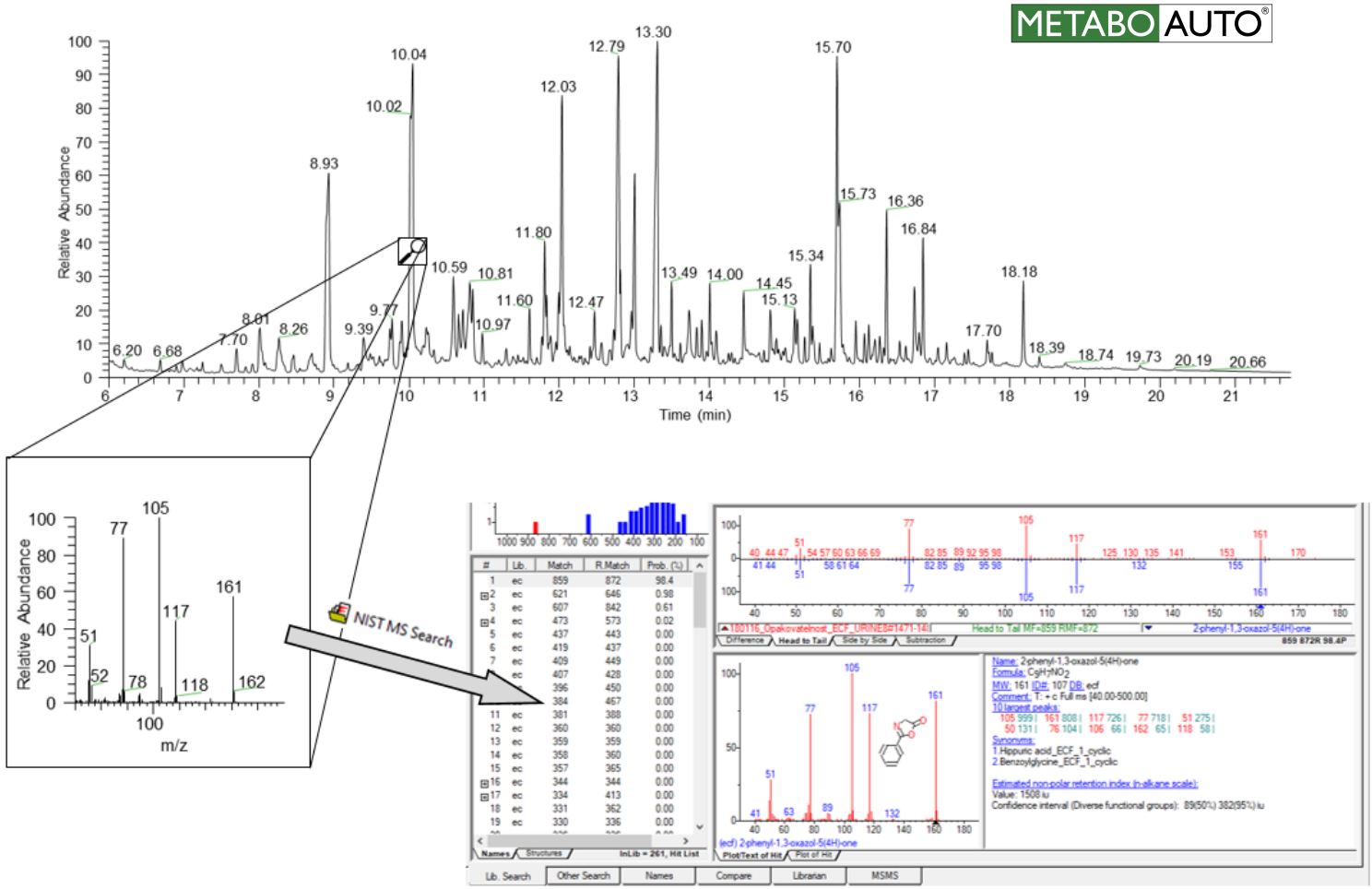
GC-MS Application Note

- Metabolite coverage: amino acids, organic acids, small peptides, biogenic amines
- The developed sample preparation workflow involves immediate, in-situ derivatization with ethyl chloroformate in an aqueous biological matrix.
- The derivatized metabolites concomitantly migrate into an immiscible organic phase (simultaneous derivatization + liquid liquid microextraction workflow).
- Automated Qual/Quan utility for the Thermo Scientific (Xcalibur, TraceFinder) data processing software
- Automated sample preparation in stand-alone or on-line regime integrated with the autosampler function.


Urine
On-line preparation
25 µl
Automated on-line sample preparation with MetaboAuto®
25 µl IS
25 µl Buffer
25 µl Catalyst
25 µl Reagent
25 µl Buffer 2
25 µl Reagent 2
Vortex 5s
Vortex 5s
Centrifuge 3000 RPM 30 s
Off-line plasma/serum precipitation
125 µl MeOH:ACN (1/1)
25 µl Plasma/serum
vortex 30 s
Centrifugation 5 min;
7000 RPM, 4°C
Supernatant
Stream of N2
Evaporated to dryness and precipitate plasma/serum
GC/MS Analysis
Injection volume 1 ul of CHCl3 layer
Relative Abundance [%]
100
0
0
RT [min]
22
Preliminary off-line liver tissue extraction
150 µl MeOH:ACN:H2O (2/2/1)
7 mg Liver tissue
Homogenization
50 Hz; -18°C; 5 min
Sonification 5 min
Centrifugation 5 min;
7000 RPM, 4°C
Supernatant
Stream of N2
Evaporated to dryness Tissue extract
Tyrosine
HO
O
H2N
OH
+
Cl
O
O
CH2
CH3
HO
CH2
CH3
Ethyl Chloroformiate
Ethanol
25°C;
≤ 5 s
N
Pyridine
Carbonate
CH3
O—CH2
O
O
HN
O
O—CH2
Ester
CH3
O
CH2O
H3C
Carbamate

MetaboAuto® EI spectral library

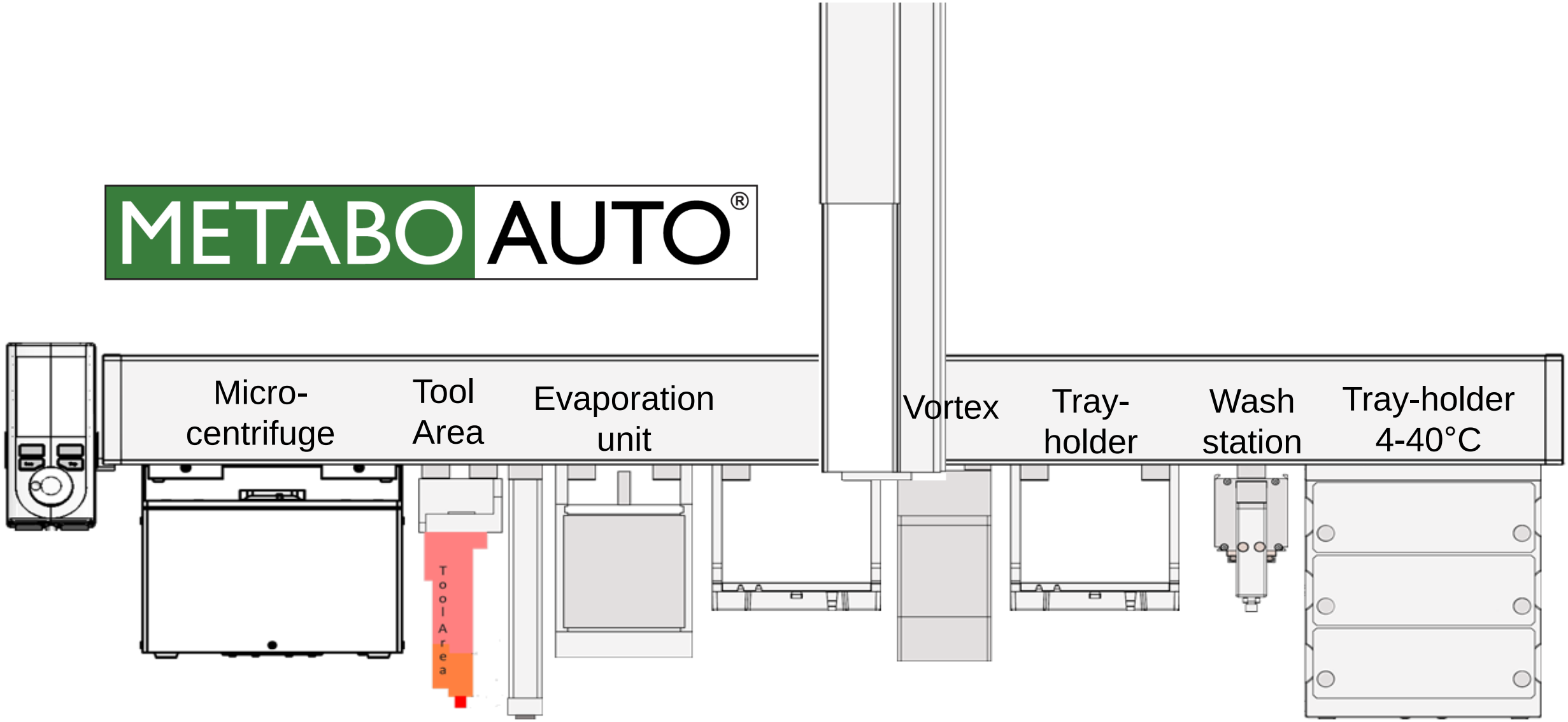




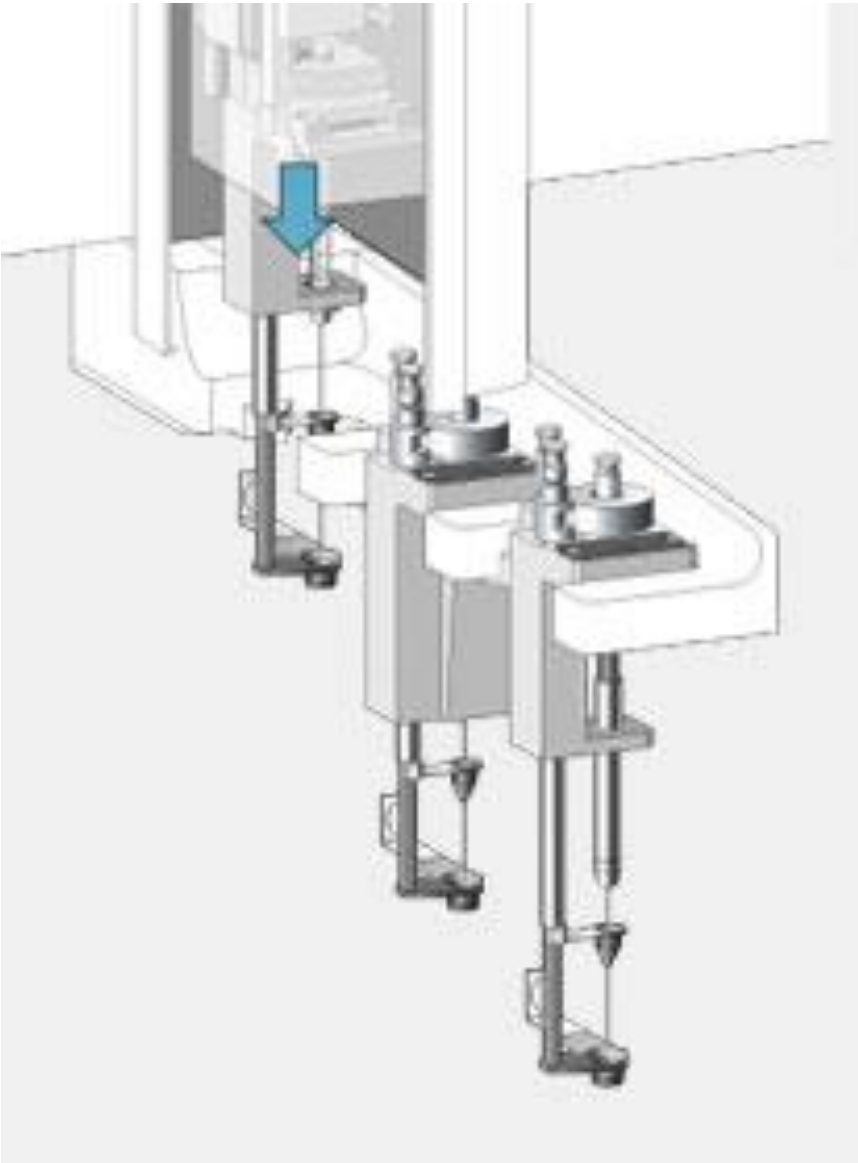
Metabolite library containing EI mass spectra of > 250 protic metabolite derivatives and their structures that can be uploaded into the NIST® mass spectral library.

RTC modular platform

METABO AUTO®



Robotic Tool Change



Liquid Syringe Tools
57mm or 85mm
1.2µL / 5µL / 10µL /100µL /
250µL / 500µL / 1 mL / 10 m

LC-MS Tool

Headspace Tools
Syringe temp. 40°C up
to 150°C in 1°C steps

Pipette Tool
200µL or 1000µL
tips

SPME Arrow Tool
SPME Fibers sorbents:
PDMS, DVB, PA, Carbon
WR, PDMS/Carbon WR,
PDMS/Carbon WR/DVB

ITEX Dynamic
Headspace Tool
Tenax TA trap
Temperature
range: 40 - 350°C

Centrifuge

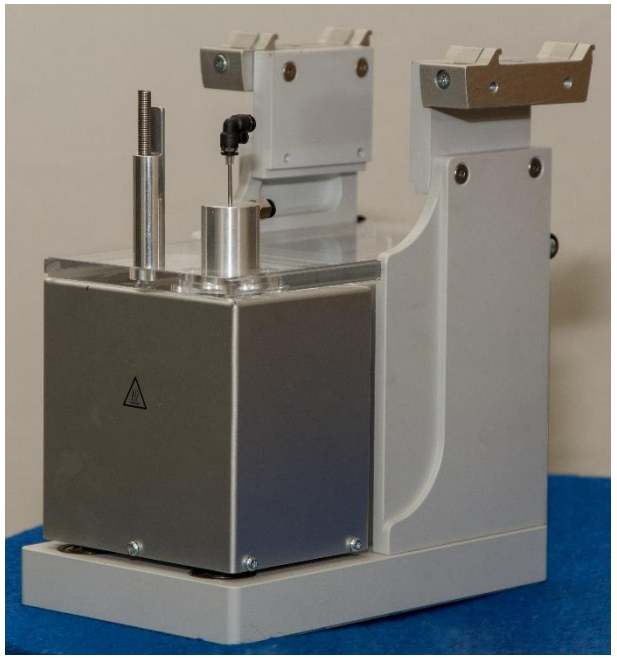
Protein precipitation
Phase separation

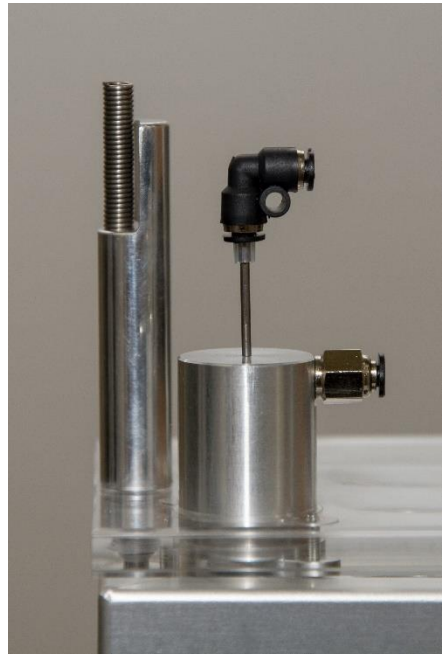
Relative centrifugal force

2000 x g with Centrifuge Combi
5000 x g with Centrifuge 2 mL

Centrifuge Combi: 2 mL (6x) + 10 mL / 20 mL (2x)
Centrifuge: 2 mL (8x)

Evaporation unit
N_2 Needel





N_2 or He, Ar, Air

2 mL; 10 mL / 20 mL

(30-80°C)

Sample Storage

Room Temperature Storage

Tray Holde

3x MTP (Multi Titer Plate)
3x DW (Deep Well Plate)
3x VT12 (12 x 40ml)
3x VT15 (15 x 10/20ml)
3x VT54 (54 x 2ml)
3x VT70 (70 x 1ml)
1x R60 (60 x 10/20ml)

Deep 96-Well Plate

Temperature Controlled Storage

Peltier Stack 4°C- 40°C

2x MTP (Multi Titer Plate)
2x DW (Deep Well Plate)
2x VT12 (12 x 40ml)
2x VT15 (15 x 10mL)
2x VT54 (54 x 2mL)
2x VT70 (70 x 1mL)

6x MTP (Multi Titer Plate)
6x DW (Deep Well Plate)
6x VT12 (12 x 40ml)
6x VT15 (15 x 10mL)
6x VT54 (54 x 2mL)
6x VT70 (70 x 1mL)

Mixing Modules

Vortex

Room Temperature

Agitation speed
0 - 2000rpm

Optional adapter for
2mL, 10mL or 20mL vials

Agitator

Temperature range
30° - 200°C

Agitation speed
250 - 750rpm

Optional adapter for
2mL or 10mL vials

Wash Modules

Fast Wash Module

Two different wash solvents (e.g. aqueous and organic)

Integrated pumps - active wash solvent delivery

Large Wash Module

2x Wash Vials
100ml
1x Waste Port

Standard Wash Module

4x Wash Vials 10mL
1x Waste Vial 10mL

Other modules available for the RTC platform

Barcode Reader Module

DeCapper Module

Opens/Closes 2, 10, 20 mL screw cap vials

Valve Drive Module

Sample injection, Column switiching online LC-LC-MS or SPE-LC-MS

SPME Arrow Conditioning Module

Conditioning of SPME Arrow and SPME fibers, max. 350°C

Heatex Stirrer Module

For powerful mixing and heating in sample prep. and SPME Arrow

Temperature 30° - 150°C
Stirring speed 1600 rpm
20mL vials

Dilutor

For efficient and accurate addition of larger amounts of liquids.