Information Sheet

Semi Polar Metabolites QC Mix

Catalog Number SBR00052

Product Description

Metabolomics is the profiling study of small molecules (metabolites) from biochemical processes and pathways,[1,2] which are mostly characterized from samples of stool,[3] serum/plasma,[4] urine,[5] cerebrospinal fluid,[6] and saliva.[7] Metabolomics deals with diverse areas like microbiome,[8] nutrition[9], diseases[10] and agriculture[11], where metabolites are analyzed by two main approaches: targeted and untargeted metabolomics. Targeted metabolomics[12,13] is the analysis of known specific chemical group such as: short chain fatty acids,[16] bile acids, lipids,[17] and amino acids.[18] Untargeted metabolomics[14,15] is the analysis of all unknown chemical compounds in a single sample.

Liquid chromatography-mass spectrometry (LC-MS) is the main method for metabolite profiling in metabolomics analysis.[19,20]

In order to assess any variations in the LC-MS-based metabolomics analysis data, it is recommended to add an additional known QC (quality control) sample at the beginning of every analytical experiment batch with additional QC sample injections after every 4-10 unknown samples injections into the workflow steps.[19,21,22] The known QC sample evaluates any drifting phenomenon like intensity values, ion suppression or other changes in the retention time of the materials peaks in the LC-MS data.

The Semi Polar Metabolites QC Mix is a ready-to-use solution for mass spectroscopy workflows. By utilizing the QC mix, the user will be able to assess drifting and ion suppression phenomena. The Semi Polar Metabolites QC Mix is comprised of 9 components (see Table 1), containing bile acids, aromatic carboxylic acids, and nucleosides.

Components

Table 1.
Components in the Semi Polar Metabolites QC Mix

No.	Metabolite name	Empirical Formula	Exact mass	Concentration (µg/mL)	Concentration (µM)
1	Uridine	$C_9H_{12}N_2O_6$	244.0695	10	40.95
2	Adenosine	$C_{10}H_{13}N_5O_4$	267.0967	5	18.71
3	Guanosine	$C_{10}H_{13}N_5O_5$	283.0916	5	17.65
4	4-Hydroxybenzoic acid	$C_7H_6O_3$	138.0316	10	72.40
5	Vanillic acid	$C_8H_8O_4$	168.0422	20	118.94
6	Melatonin	$C_{13}H_{16}N_2O_2$	232.1211	2.5	10.76
7	Taurocholic acid	$C_{26}H_{45}NO_7S$	515.2916	2	3.72
8	Cholic acid	$C_{24}H_{40}O_5$	408.2875	2.5	5.81
9	Hyodeoxycholic acid	$C_{24}H_{40}O_4$	392.2926	2.5	6.37

Equipment Required but Not Provided

- ACQUITY UPLC HSS T3 1.8 µm, 100Å 2.1 × 150 mm, Waters Catalog Number 186003540

Precautions and Disclaimer

For R&D use only. Not for drug, household, or other uses. Please consult the Safety Data Sheet for information regarding hazards and safe handling practices.

Storage/Stability

The product is shipped at ambient temperature. Store at +2 °C to +8 °C upon receipt.

Preparation Instructions

The Semi Polar Metabolites QC Mix is a ready-to-use solution supplied in a crimp top (Silicone/PTFE liner) amber vial.

Procedure

Experimental procedures provided here are an example of how to use the products. The results may vary under different experimental parameters.

Mass Spectrometry Conditions:

Instrument: Bruker™ Q-Tof Impact II
Source Type: ESI

Method A:

Ion Polarity: Negative
Capillary: 5500 V
Nebulizer: 2.2 Bar
Dry gas temperature: 200 ºC
Dry gas: 8L/min

Method B:

Ion Polarity: Positive
Capillary: 4500 V
Nebulizer: 2.2 Bar
Dry gas temperature: 200 ºC
Dry gas: 8L/min

LC conditions:

Column: ACQUITY UPLC HSS T3 1.8 µm 2.1 × 150 mm
Column oven temperature: 35 ºC
Flow rate: 0.4 ml/min
Injection volume: 1 µL
Gradient: See Table 2

Table 2.

Time (min)	Acetonitrile [%]	Water + 0.1% Formic acid [%]
0	2	98
2	2	98
17	70	30
19	2	98
26	2	98

Figure 1.
Method A: BPC chromatogram of MS ESI$^-$ of Semi Polar Metabolites QC Mix and table of peak assignments (Table 3). Note: Adenosine is not detected under negative ion polarity.

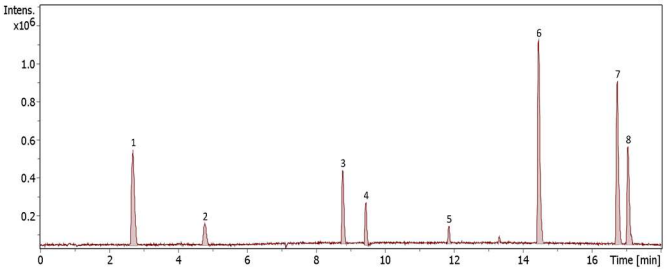

Table 3.

Peak no.	Metabolite name	Rt (min)
1	Uridine	2.7
2	Guanosine	4.7
3	4-Hydroxybenzoic acid	8.8
4	Vanillic acid	9.5
5	Melatonin	11.9
6	Taurocholic acid	14.5
7	Cholic acid	16.8
8	Hyodeoxycholic acid	17.1

Figure 2.
Method B: BPC chromatogram of MS ESI$^+$ of Semi Polar Metabolites QC Mix and table of peak assignments (Table 4).

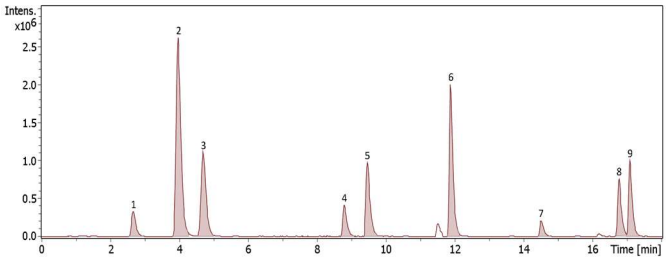

Table 4.

Peak no.	Metabolite name	Rt (min)
1	Uridine	2.7
2	Adenosine	4.0
3	Guanosine	4.7
4	4-Hydroxybenzoic acid	8.8
5	Vanillic acid	9.5
6	Melatonin	11.9
7	Taurocholic acid	14.5
8	Cholic acid	16.8
9	Hyodeoxycholic acid	17.1

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