

HPST, s.r.o Písnická 372/20 142 00 Praha 4 Česká republika Tel.: +420 244 001 231 Fax: +420 244 011 235 E-mail: info@hpst.cz Web: www.hpst.cz IC: 25791079 DIČ: CZ25791079 Citibank a.s., Praha 6 č.ú.: 2504270118/2600

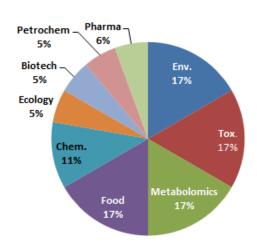


## Přehled aplikací GC-MS

Typ MS	Časové období	Celkem	Aplikace	Publikace	Ostatní
Celkem		671	118	513	40
QTOF	2011-2013	33	5	13	15
TQ	2008-2013	172	37	128	7
MSD	Aplikace: 2005-14 Publikace: 2013/14	466	76	372	18

<sup>\*</sup> Zdroj: Google Scholar, e-Library

### GC-QTOF 7200 Typy aplikací



# Aplikace GC-QTOF 7200 pro metabolomiku a expozomiku

The role of GC/Q-TOF in Exposomics

Authors: Anthony Macherone

Abstract: Kynurenine pathway of triphtophan metabolism, monitoring of some of the key

 Metabolic Profiling of Yeast Sterols Using the Agilent 7200 Series GC/Q-TOF System

Authors: Wu M., Onge R.S., Suresh S., Davis R. Peltz G.

HPST, s.r.o Písnická 372/20 142 00 Praha 4 Česká republika Tel.: +420 244 001 231 Fax: +420 244 011 235 E-mail: info@hpst.cz Web: www.hpst.cz IC: 25791079 DIČ: CZ25791079 Citibank a.s., Praha 6 č.ú.: 2504270118/2600

Abstract: Metabolic profiling of yeast sterols to precisely determine enzymatic targets for new potential antifungal drugs was performed using the Agilent 7200 series GC/Q-TOF System and Mass Profiler Professional (MPP) software. Targeted analysis of the relative levels of ergosterol biosynthesis pathway intermediates was combined with an untargeted approach, empowered by accurate mass high resolution GC/Q-TOF technology, to obtain the most comprehensive results. Full acquisition electron ionization (EI) spectral product ion spectral data to confirm the identity of the compounds accumulated ininformation was complemented with MS/MS accurate massyeast as a result of drug treatment.

#### Metabolomics of Opiate-Induced Changes in Murine Brain by GC/Q-TOF

Authors: Wu M., Zheng M., Clark D., Peltz G.

Abstract: A study was performed to elucidate opiate-induced metabolic changes in murine brain. The EI MS, EI MS/MS, and PCI capabilities of the Agilent 7200 Series GC/Q-TOF MS, in combination with Agilent MassHunter Software tools, enabled a very flexible and comprehensive workflow for identifying metabolomic differences.

#### • Analysis of Biomarkers in Crude Oil

Authors: David F.

Abstract: The analysis of biomarkers such as (alkyl-) dibenzothiophenes, hopanes, and steranes in crude oil is used in many petrochemical applications, including the characterization of oil sources and the identification of sources of oil spillage. The analysis is normally done by GC-MS after complex sample preparation and fractionation. Using a high resolution time-of-flight mass spectrometer, a diluted sample can be analysed without fractionation and the biomarkers of interest can be measured by exploiting the high selectivity of ion extraction at accurate mass.

#### Enhanced Metabolite Profi ling from Bark of Alangium Salviifolium Using LC/MS and GC/Q-TOF Techniques

Authors: Siddaiah C., Prakash H.S., Deepak S.A., Lateef S.S., Simha U.

Abstract: Traditional herbal remedies are used as alternative medicines for a number of diseases. Alangium salviifolium is one such plant, used as traditional medicinal plant. Several investigations have been performed using this plant extract to demonstrate its therapeutic value. However, very few attempts have been made to identify the extensive metabolite composition of this plant. In this Application Note, we performed metabolite profiling and identification from the bark of A. salviifolium by extracting the sample in organic and aqueous solvents. The organic and aqueous extracts were fraction collected using the Agilent 1260 Analytical Scale Fraction Collection System. Each of the fractions was analyzed by LC/MS and GC/Q-TOF techniques. The LC/MS/MS analyses were performed using HILIC chromatography, as well as three separate, orthogonal reverse phase columns. Data were collected using AJS source in both positive and negative ionization modes, followed by METLIN database or MS/MS library searches. Compounds from Alangium that could not be identified by database or library matching were subsequently searched against the ChemSpider (http://www.chemspider.com/) database of over 30 million structures using Agilent MSC software. To identify compounds generated by GC/Q-TOF, the data were searched against the Agilent-Fiehn GC/MS Metabolomics Library and Wiley/NIST libraries. The results of the combined GC libraries searches identified 62 compounds with a matching score > 70.

Using both techniques, a total of 1,016 compounds were detected, of which 511 were identified. A literature search revealed 81 out of 511 compounds had therapeutic properties against traditionally reported diseases such as cancer, microbial infections,

HPST, s.r.o Písnická 372/20 142 00 Praha 4 Česká republika Tel.: +420 244 001 231 Fax: +420 244 011 235 E-mail: info@hpst.cz Web: www.hpst.cz

IC: 25791079 DIČ: CZ25791079 Citibank a.s., Praha 6 č.ú.: 2504270118/2600

and so forth. Our study suggests that the use of fraction collection for metabolite enrichment, biphasic solvent extraction, and orthogonal column chemistries for metabolite separation, as well as complementary LC/MS and GC/MS detection, leads to greater metabolite detection coverage in medicinal plants.

#### **Targeted Exposomics: Profiling Urinary Organic Acids**

Authors: Macherone A., Hopkins J.

Abstract: Measuring the exposome or totality exposures over individuals' lifetime, offers new insight into exposure-response relationships (biological epidemiology) by determining and differentiating the causal pathways (exposure biology) and reactive pathways (systems biology) in chronic human disease. Through the application of discoverybased omics and targeted methodologies to measure the exposome, exposomics will identify new biomarkers of disease, guide methods to mitigate exposures, and ultimately lead to more personalized medical interventions. Volatile organic solvent exposure, such as benzene or toluene, is an example of an exposure biomarker (the causal disease pathway) that leads to primary and secondary disease traits as evidenced by perturbations in the urinary organic acid profile (the reactive disease pathway). This application note presents a top-down, targeted approach of measuring the urinary organic acid exposome using GC/MS and post-acquisition mass spectral deconvolution with targeting library searching