C146-E273

SHIMADZU
Excellence in Science

5 Dimensional Comprehensive Chromatography System

5D Ultra-e

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LC-GC×GC-MS/MS System

Online HPLC
Comprehensive Two Dimensional Gas Chromatograph
Triple Quadrupole Mass Spectrometer

Five Dimensions for Analysis with Greater Separation and Selectivity

The 5D Ultra-e is a unique system that combines a comprehensive two-dimensional gas chromatograph and triple quadrupole mass spectrometer with an HPLC system connected online. This system is the only one of its kind in the world.
The online HPLC system enhances the power of comprehensive 2D GC analysis and simultaneously improves productivity by increasing automation. Furthermore, the GC×GC system combined with an ultra fast triple quadrupole mass spectrometer allows both untargeted analysis as well as targeted analysis of components in complex samples.
Consequently, the five dimensions provided by the LC-GC×GC-MS/MS system opens the road to analysis with even higher separation and higher selectivity.

This LC-GC×GC-MS/MS system was developed by the group led by Prof. Dr. Luigi Mondello at the University of Messina and Chromaleont S. r. l. in Italy and developed into a product by Shimadzu Corporation.

Components

The system includes HPLC (Prominence) units, LC-GC transfer unit (AOC-5000 Plus and OPTIC-4PTV), GC×GC unit (GC-2010 Plus and ZX-2), and a MS/MS (GCMS-TQ8040). After the sample is injected into the Prominence HPLC, it is separated by normal-phase chromatography. Then the AOC-5000 Plus injects only the target fraction into the OPTIC-4PTV GC inlet. After separating the fraction in the GC×GC with a double-oven and ZX-2 thermal modulator, the analytes are detected by the GCMS-TQ8040. This entire series of analytical steps can be executed entirely from the 5D Solution integrated software, which means that the resulting data can be analyzed using ChromSquare 2D chromatography data analysis software.

Step 1: HPLC Separation

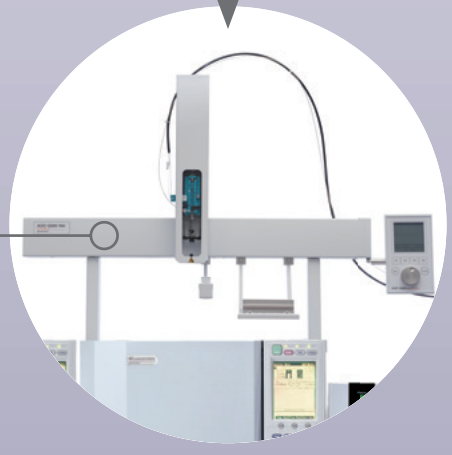
Prominence

- Separate samples with complex matrices.
- Units can be customized based on analytical targets.

Step 2: Online Injection

AOC-5000 Plus

- Inject only the LC fraction with the required components into the GC unit.
- Allows different injection volumes since no loops or valves are used.



Step 3: Concentration and Injection to GC

OPTIC-4PTV*1

- Collect eluted components in the insert.
- The temperature program efficiently eliminates solvent components.

Step 4: 2D-GC Separation

GC-2010 Plus × 2 with ZX-2*2

- Powerfully separates components that cannot be separated with one-dimensional chromatography.
- Independent temperature control of first and second GC dimensions by double ovens provides analytical flexibility.
- The ZX-2 modulator requires no liquid nitrogen.

Step 5: MS/MS Analysis

GCMS-TQ8040

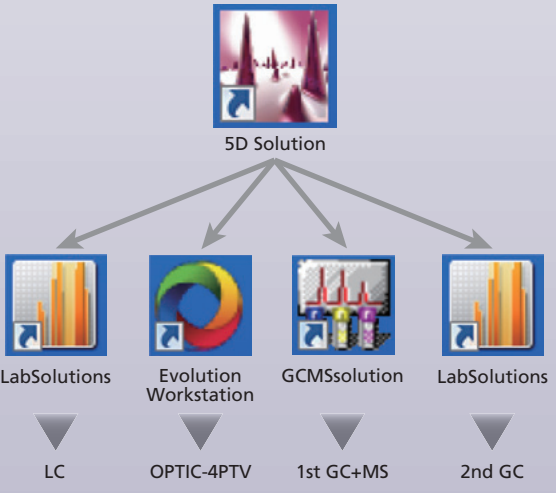
- The ultra fast MS/MS accurately analyzes separated components.
- Scan/MRM can be used for simultaneous targeted and untargeted analysis.

*1: The OPTIC-4PTV is a product of GL Sciences Inc. in Japan.
*2: The ZX-2 is a product of Zoex Corporation in the United States.

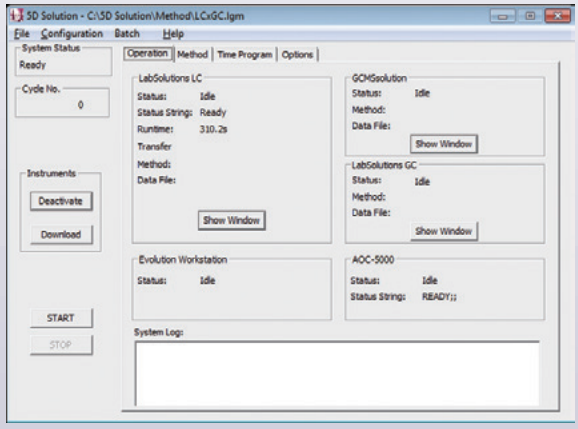
Software

5D Solution Integrated Software

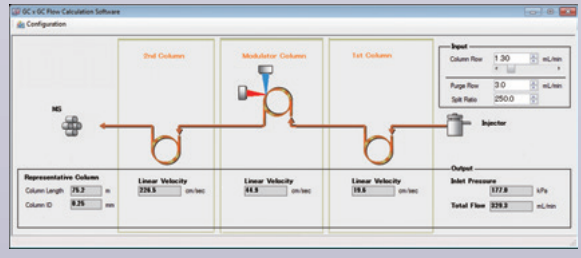
Dedicated software is used to control each unit of the LC-GC×GC-MS/MS system. However, 5D Solution collectively manages all of these control software programs, so that analysis can be started with a single click. Furthermore, continuous analysis of multiple samples can be performed.
The included linear velocity calculation software allows the user to view the calculated linear velocity values of the first and second columns while the optimal column inlet pressures are being specified, which provides powerful assistance for determining analytical conditions for comprehensive 2D-GC analysis.



5D Solution

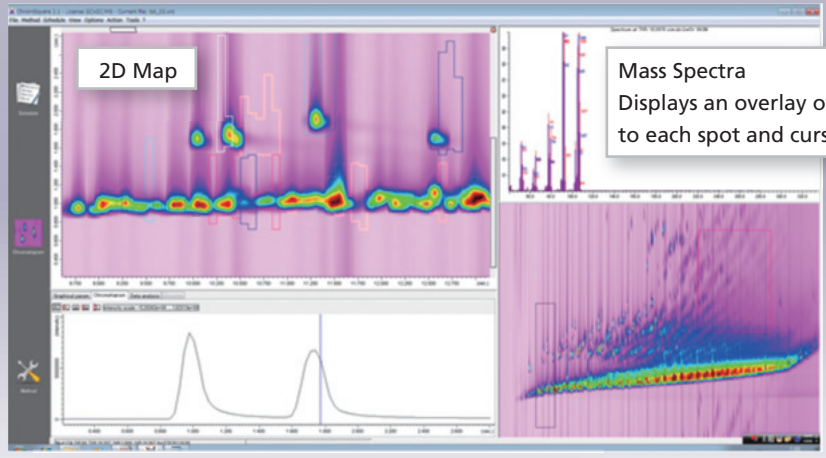


Linear Velocity Calculation Software



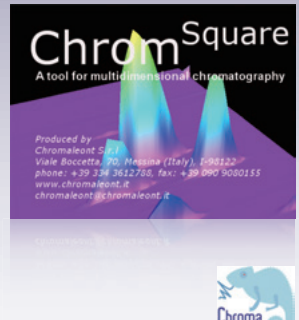
ChromSquare 2D-GC Data Analysis Software

ChromSquare 2D-GC data analysis software converts data obtained from the LC-GCxGC-MS/MS system to contour data (2D map). Chromatogram peaks appear as spots on the contour lines. These spots are used for qualitative and quantitative analysis. ChromSquare is able to display a summary of the corresponding second-dimensional chromatogram, mass spectrum, and analytical data together with 2D maps, which makes it easy to perform data analysis.



Mass Spectra
Displays an overlay of mass spectra corresponding to each spot and cursor position.

Displays the second-dimensional chromatogram corresponding to the cursor position.



ChromSquare is a product of Chromaleont S.r.l. in Italy.

Application

Comprehensive Analysis of Coal Tar and Analysis of Sulfur Compounds

GC×GC is often used for comprehensive sample measurements because of its superior separation capabilities. Nevertheless, GC×GC can be inadequate for extremely complex samples. For example, attempting to measure coal tar diluted with dichloromethane directly by GC×GC-MS/MS (Q3 Scan) results in an extremely complicated 2D map (see Fig. 1).
In contrast, Figs. 2 to 4 show the results from analyzing the same sample using LC-GC×GC-MS/MS. Three fractions separated by type using LC were then consecutively measured by GC×GC-MS/MS. The simplified 2D map obtained by HPLC separation allows even more detailed comprehensive analysis.

Analysis by GC×GC-MS/MS

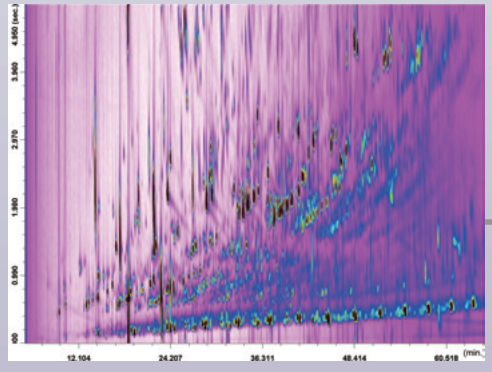


Fig. 1 2D Map (Q3 Scan) Obtained by Direct Injection into a GC×GC-MS/MS System

A wide variety of sulfur compounds is present in fossil fuels in low concentrations, which make analysis vulnerable to matrix effects. Therefore, the LC-GC×GC-MS/MS system is especially useful in such cases, due to its high selectivity and high detection sensitivity.
Fig. 5 shows the MRM measurement results of the sulfur compounds (dibenzothiophene) contained in the second fraction. This shows that MS/MS was able to selectively detect each isomer of dibenzothiophene.

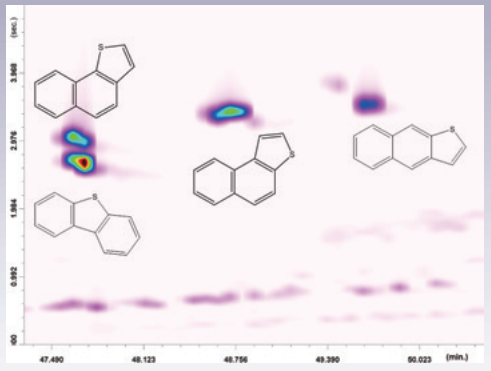


Fig. 5 2D Map (MRM) of Dibenzothiophene in the Second Fraction

Online Separation by LC

Analysis by LC-GC×GC-MS/MS

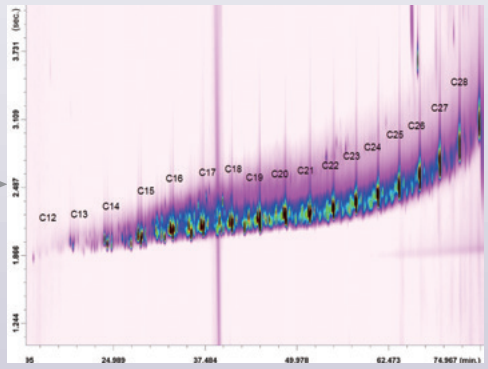


Fig. 2 2D Map of First Fraction (Q3 Scan) (Non-Aromatic Hydrocarbons)

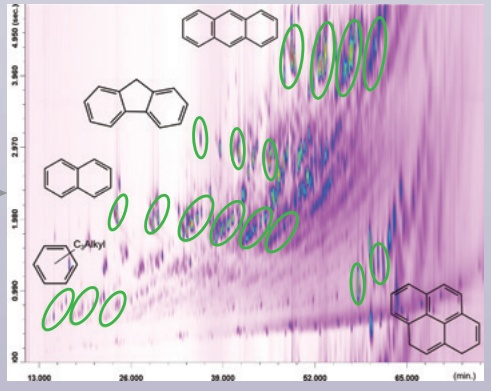


Fig. 3 2D Map of Second Fraction (Q3 Scan) (Aromatic Compounds)

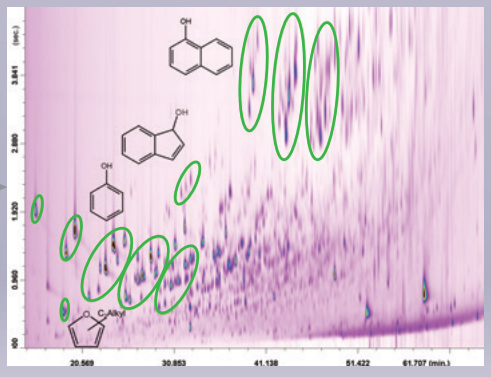


Fig. 4 2D Map of Third Fraction (Q3 Scan) (Oxygenated Compounds)

Data was provided by Prof. Dr. Luigi Mondello at the University of Messina and Chromaleont S. r. l. in Italy.
Optimizing conditions for customer application requirements is necessary. Please contact us for more details.

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Printed in Japan 3655-10421-20AIT