

Quadrupole Time-of-Flight Liquid Chromatograph Mass Spectrometer

# OAD-TOF system

**UFMS**  
ULTRA FAST MASS SPECTROMETRY



# **OAD-TOF system**

Quadrupole Time-of-Flight Liquid Chromatograph Mass Spectrometer

## **Radicalize Your Mass Spectrometer**

to Solve Unanswered Questions

### **Innovative fragmentation technology**

Introduction of neutral radicals in positive and negative modes

### **Surprisingly simple**

Effortless operation and reliable results

### **Creating endless possibilities**

Diverse analytical needs can be met

The OAD-TOF system is a QTOF LCMS that realizes OAD (Oxygen Attachment Dissociation), Shimadzu's proprietary fragmentation technology. It allows the analysis of the position of carbon-carbon double bonds in lipids and other organic compounds. Combined with the LCMS-9050, which boasts world-class high mass accuracy and fast polarity switching, it enables the creation of innovative applications.



# Innovative fragmentation technology

## Introduction of neutral radicals in positive and negative modes

The OAD-TOF system is equipped with an OAD RADICAL SOURCE I, which enables Oxygen Attachment Dissociation (OAD) analysis, an innovative fragmentation that utilizes Shimadzu's proprietary radical reaction. It can measure fragment ions that cannot be obtained by conventional collision-induced dissociation (CID), where ions are fragmented by collision with an inert gas such as argon or nitrogen. The irradiating oxygen radicals specifically oxidize/dissociate double bonds between carbons, which is useful for structure estimation of organic compounds such as lipids. The technique can be applied to monovalent ions and negative ions, which have been difficult to fragment using radical reactions by electrons and anions, and provides completely new structural information.

### Radical source

Neutral radicals such as O/OH/H radicals are generated by microwave discharge of raw material gases (water vapor and hydrogen gas) in a vacuum. The neutral radicals are introduced into the OAD cell through a quartz tube.

### OAD cell

Precursor ions are reacted with neutral radicals generated in a radical source and fragmented. A collision gas (argon) can be introduced, and conventional CID fragmentation is also possible by setting the collision energy (CE).

### UF-FlightTube™

Precise temperature control is achieved due to an optimized heater and heater sensor layout and a robust control system. This minimizes the effects of any room temperature variations to enable stable mass accuracy over long periods. It also reduces the time and trouble required for mass calibration.

### *iRef TOF*™

The unique electrode shape achieves an ideal electric potential distribution that increases energy-focusing, while also inhibiting trajectory divergence and flight time lengthening during ion reflection.



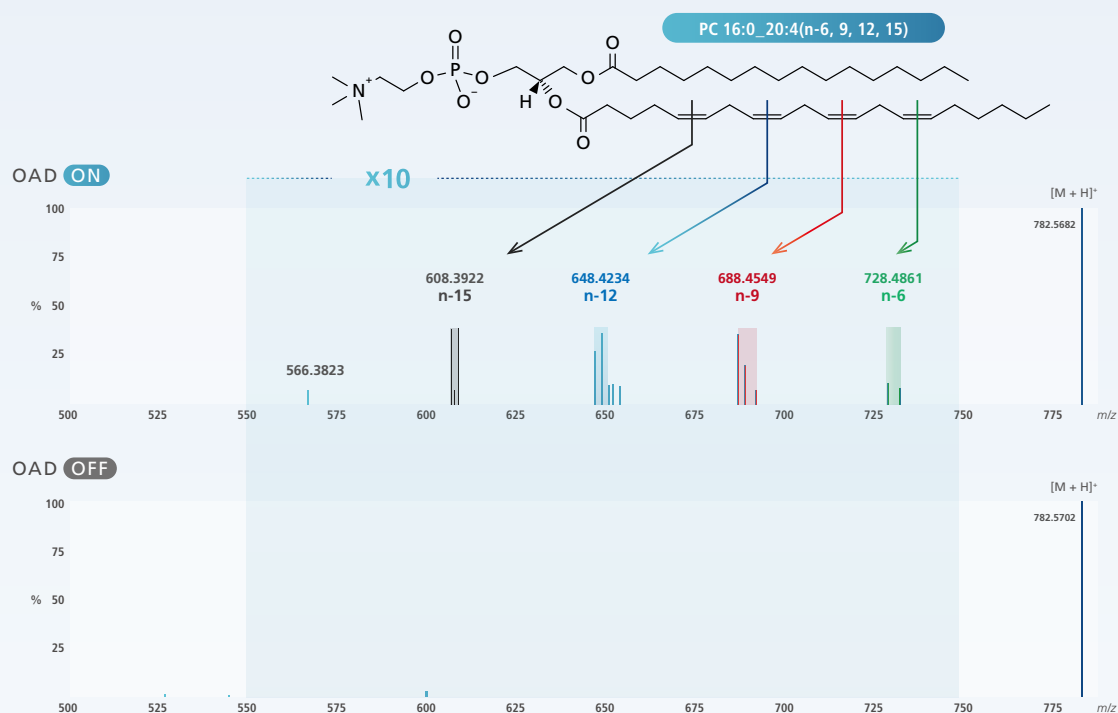
For LCMS-9050, click the button below.

Product



## What is OAD (oxygen attachment dissociation)?

CID preferentially dissociates weak chemical bonds. In the case of lipids, CID can determine the basic structure of lipids and polar groups, and the carbon composition of side chains (number of carbons and double bonds). With OAD, oxygen radicals react specifically with the double bonds between carbons, causing dissociation. By measuring fragment ions specific to the double bond, the position of the double bond can be determined.



## Positive/negative polarity switching opens possibilities for new applications

Shimadzu's breakthrough innovation challenges the common belief that TOF instruments cannot undergo efficient polarity switching. With the capability to achieve low-ppm mass measurement accuracies in short switching intervals, possibilities are now open to enhance the workflow with greater confidence and ease.

### Achieving both polarity switching and Mass accuracy

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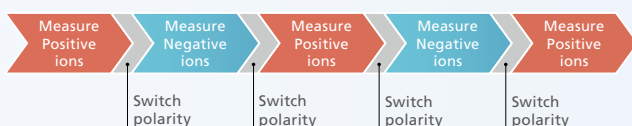
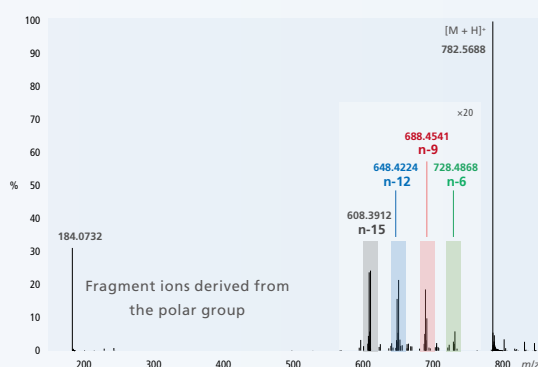


Illustration of Switching between Positive and Negative Ion Modes

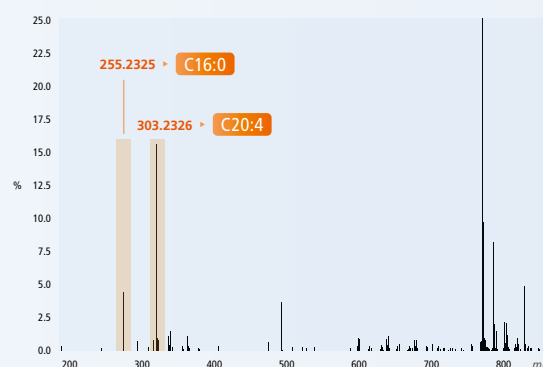
The LCMS-9050 features a proprietary high-precision electrical circuit and the UFstabilization™ algorithm (patent pending) that make polarity switching both fast and stable.

### Increasing workflow efficiency with polarity switching

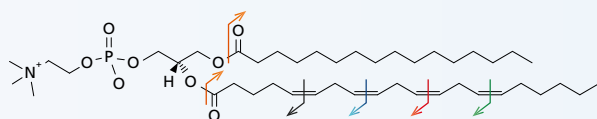
Analysis that was previously performed twice in positive ion mode and negative ion mode can now be performed in one analysis, improving the analysis throughput. In addition, positive and negative ions can be detected in the pretreated sample under the same conditions without any time lag, improving the reliability of the analytical data.



Positive Ion Mode Measurement (OAD)



Negative Ion Mode Measurement (CID)



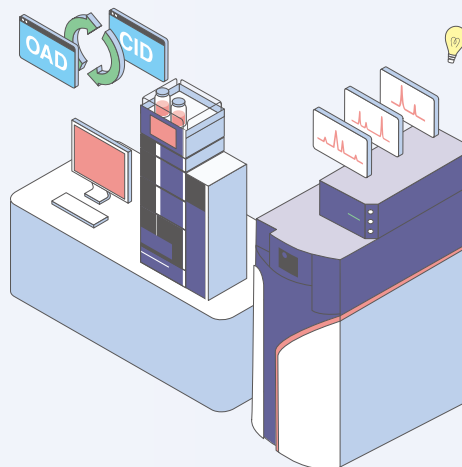
PC (36:4) and other lipids were detected in mouse liver samples in both positive ion and negative ion modes. Taking measurements in both positive ion and negative ion modes enables more accurate structural estimates of compounds.

# Surprisingly simple

Effortless operation and reliable results

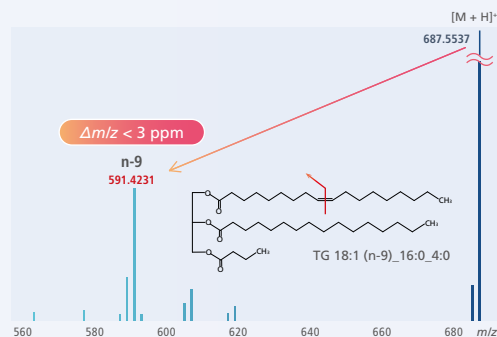
## Easy to switch between CID and OAD

CID is also possible with the OAD RADICAL SOURCE I installed. No special software is required, and LabSolutions™ LCMS control and analysis software for LCMS-9050 can easily switch between OAD and CID for analysis. Acquisition of a large amount of structural information by OAD and CID can lead to new discoveries in lipids and other organic compounds.



## Reliable structure estimation with high mass accuracy

The high mass accuracy achieved with the LCMS-9050 remains unchanged even with OAD. High-quality MS/MS data within  $\pm 3$  ppm enables reliable structure estimation of compounds, including determination of the position of carbon-carbon double bonds.





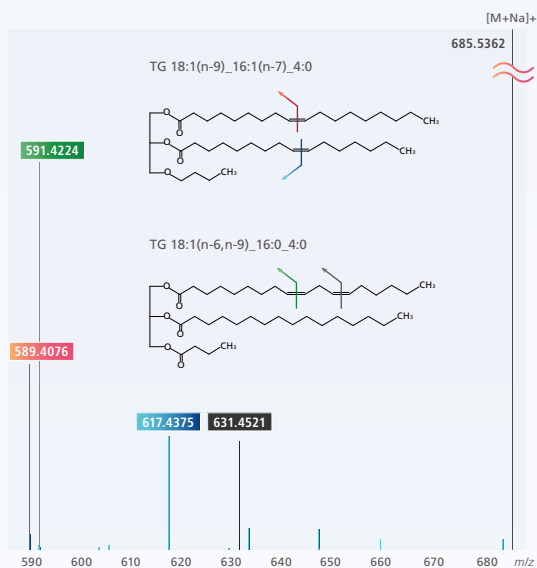
# Creating endless possibilities

Diverse analytical needs can be met

The OAD-TOF system can be used in combination with various options compatible with the LCMS-9050. The DPiMS™ QT, Kit for Direct Probe Ionization Mass Spectrometer, can be installed in place of the standard ESI unit for rapid analysis with simple pretreatment. It can also be connected to the Nexera™ UC supercritical fluid chromatography (SFC) system. This is especially useful for profiling lipids, where vast numbers of isomers exist.

## DPiMS

Kit for Direct Probe Ionization Mass Spectrometer



Lipids in butter were analyzed using DPiMS in combination with the OAD-TOF system. Specific fragment ions derived from OAD were observed with only a simple pretreatment, which is a feature of DPiMS, and the double bond position of triacylglycerol was quickly estimated.

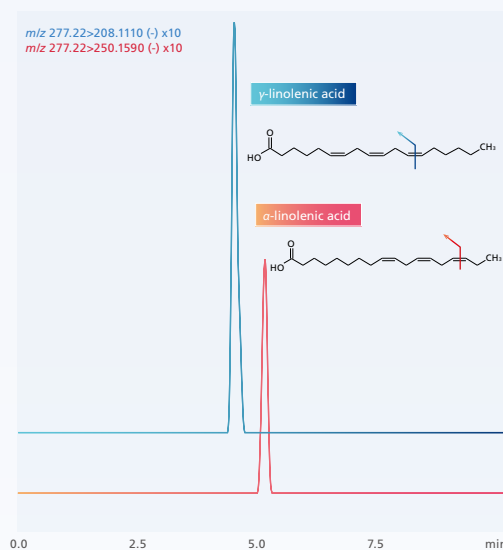
DPiMS QT, click the button below.

Product



## Nexera UC

Supercritical Fluid Extraction (SFE)-  
Supercritical Fluid Chromatography (SFC)



$\alpha$ -linolenic acid and  $\gamma$ -linolenic acid with different double bond positions were analyzed using Nexera UC and the OAD-TOF system. Isomers with similar structures were completely separated by SFC and detected with specific fragment ions derived from OAD, enabling highly accurate analysis. OAD can also be adapted to monovalent negative ions such as fatty acids.

Nexera UC, click the button below.

Product

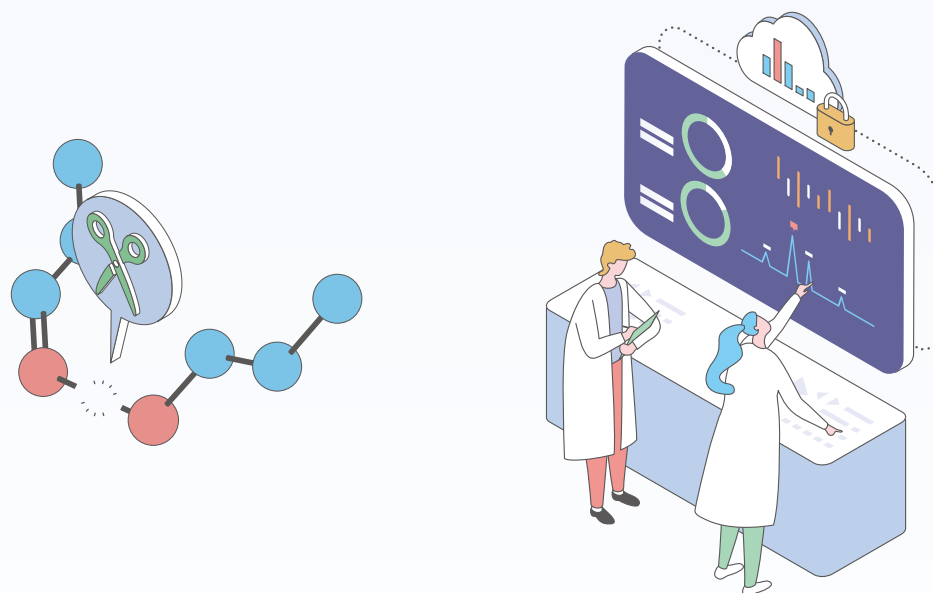
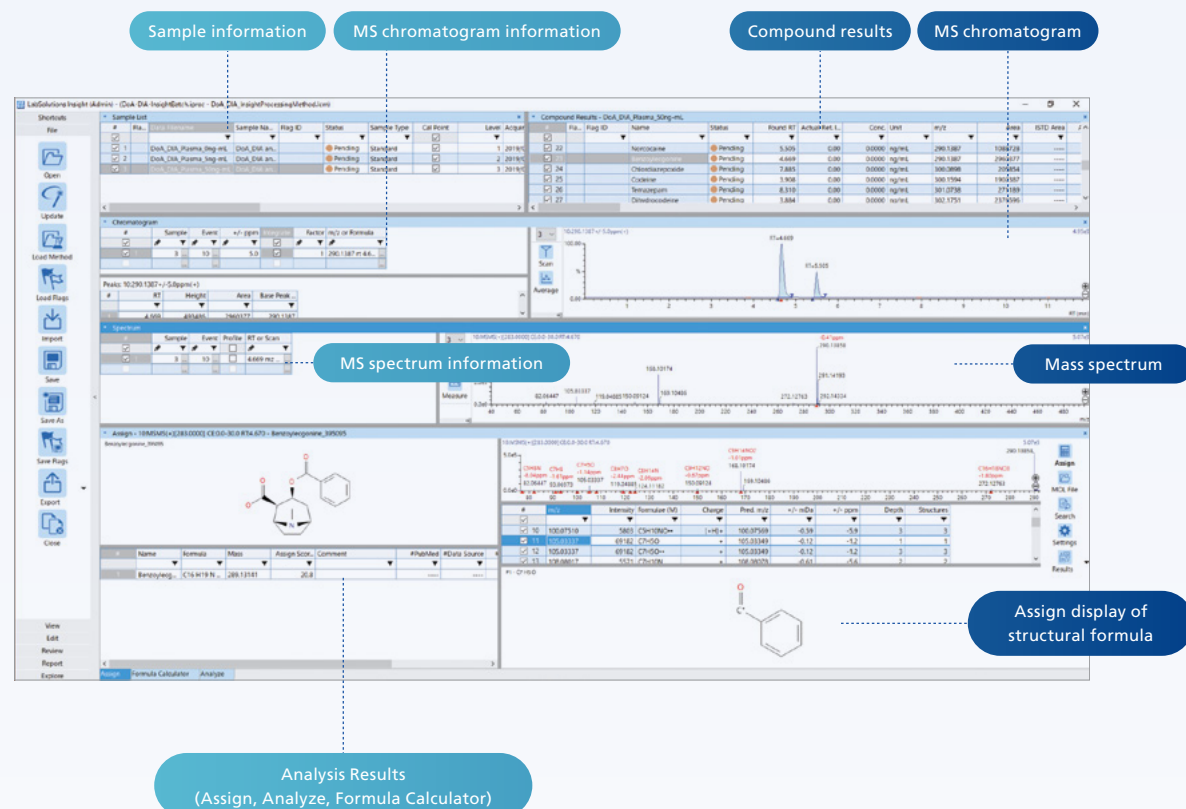




# LabSolutions Insight Explore™

Software supports everything from qualitative analysis to quantitative analysis

Explore software not only facilitates quantitative analysis of a large number of samples, but also comes with features for reliable library searching, elucidation of compound structure and sample composition, and multivalent ion analysis, making full use of MS data with high resolution and mass precision.



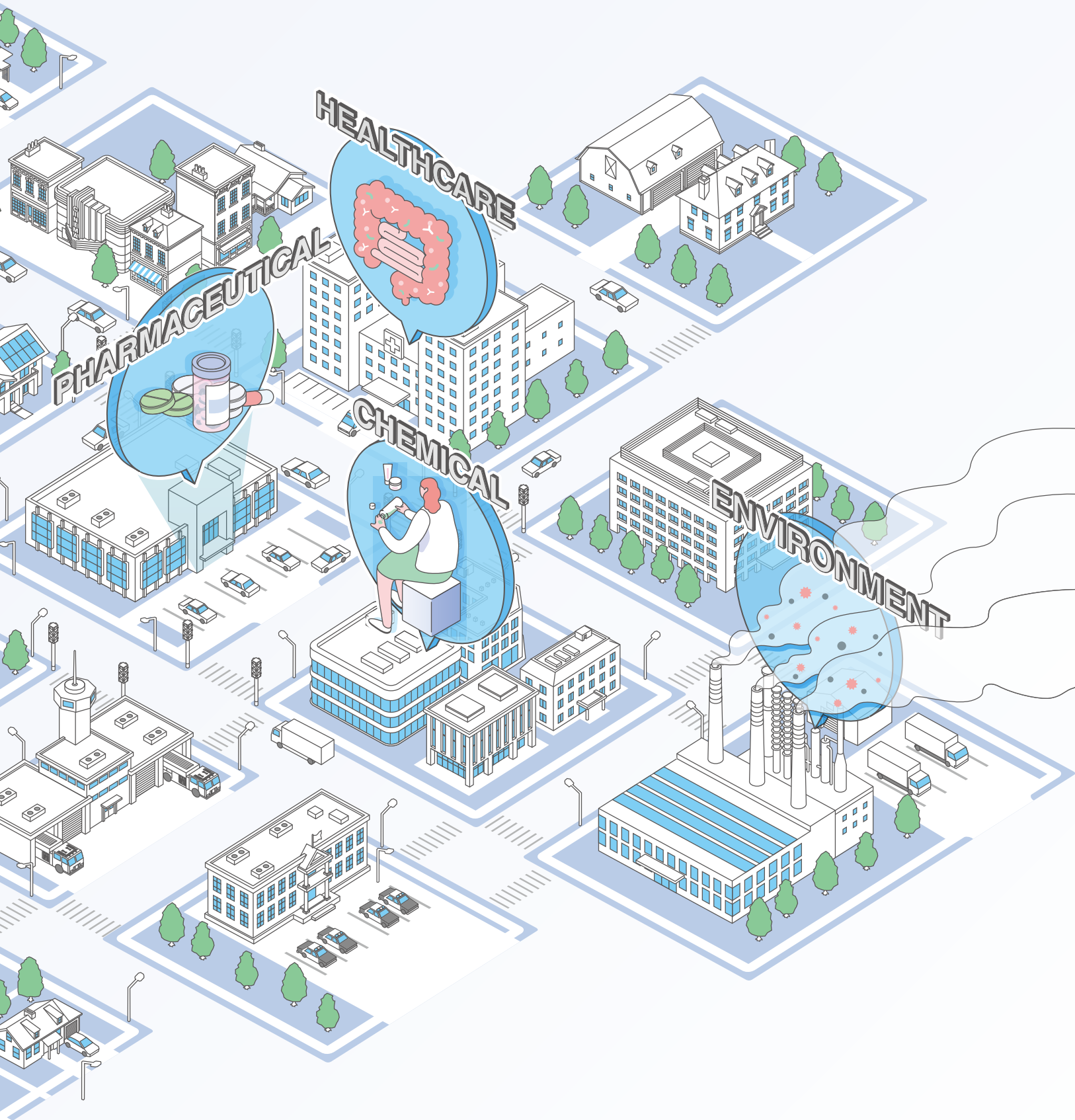
## Future possibilities envisioned by the OAD-TOF system

Our everyday environment is filled with organic compounds. Some organic compounds have double bonds between the carbons, and the number and position of these bonds greatly affect the properties of the compound.

The OAD-TOF system reveals the position of double bonds that cannot be determined by conventional CID. The use of this new technology may bring about the development of higher quality and more functional products, the further clarification of biological processes, and the realization of a healthier and longer-lived society.

The OAD-TOF system is an analytical solution that will revolutionize society in the near future.





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