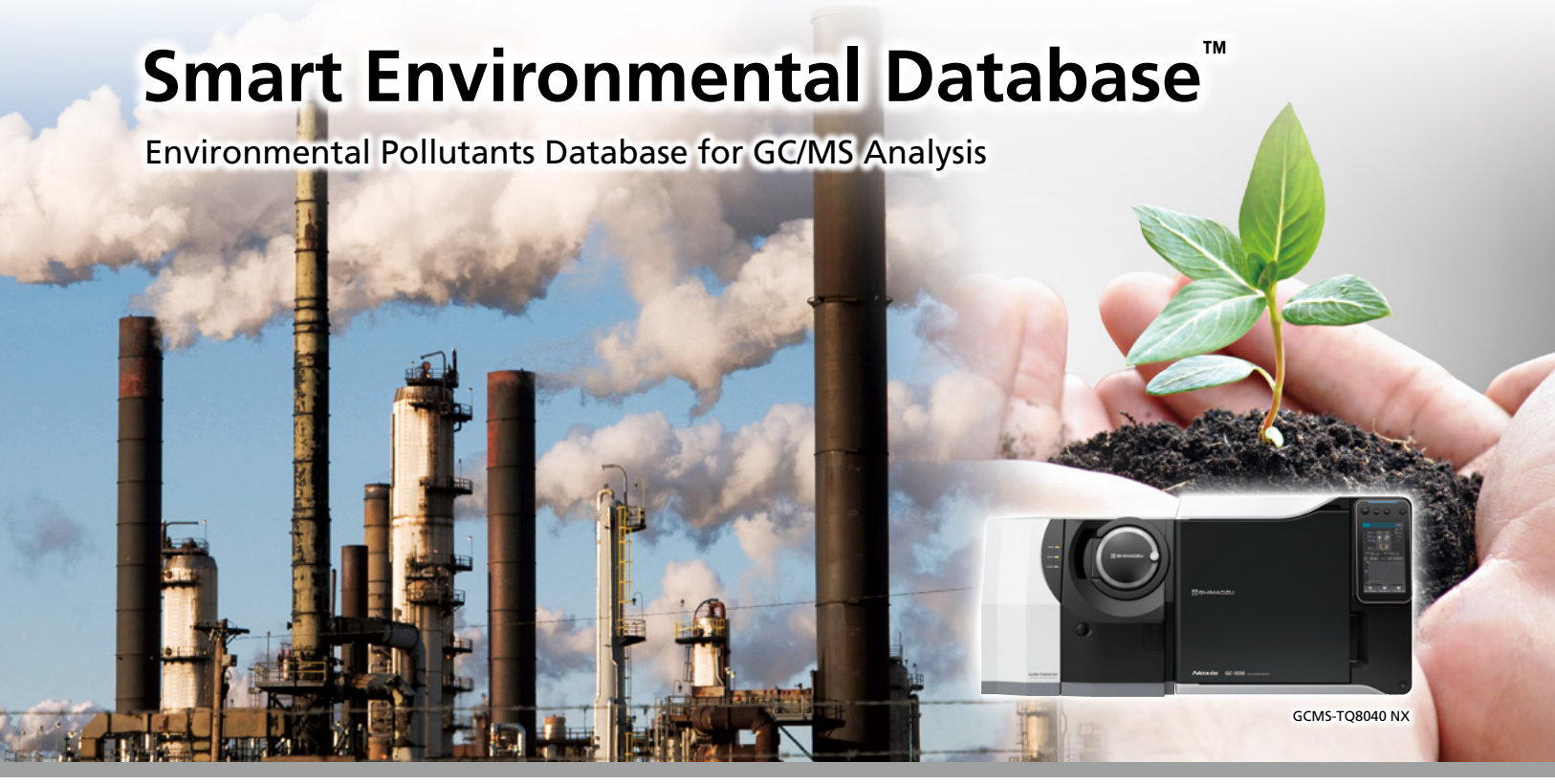
SHIMADZU
Excellence in Science

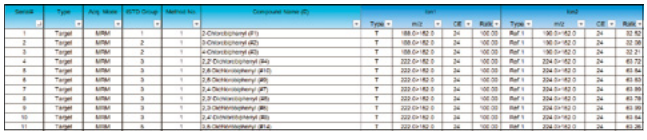
Smart Environmental Database™

Environmental Pollutants Database for GC/MS Analysis



Create MRM Methods for GC-MS/MS

The Shimadzu Smart Environmental Database contains all the information necessary to create MRM methods for over 500 environmental pollutants, including polychlorinated biphenyls (PCBs), brominated flame retardants (BFRs), dioxins, polycyclic aromatic hydrocarbons (PAHs), organochlorine pesticides (OCPs), and stable isotopically labeled compounds that are commonly used as Internal and Surrogate Standards. The database includes up to six fully optimized MRM transitions for all compounds, plus retention indices (RI) for setting correct retention times, CAS numbers, and other compound-specific information.
Optimized analytical methods for each compound class, including the recommended capillary column and GC oven program, are part of the database package to minimize start-up time.

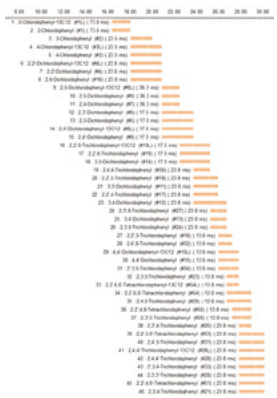


Accurate Retention Time Update via AART

The Automatic Adjustment of Retention Time (AART) function is a standard feature of all Shimadzu GCMS packages, and allows the user to quickly and easily perform multipoint retention time updates using the fundamental principle of Retention Indices. The Smart Database™ Series includes RIs for all registered compounds for easy implementation of the AART function.

Smart MRM Optimizes Methods Automatically

The Shimadzu Smart MRM™ feature allows the user to create fully optimized MRM and Scan/MRM methods automatically. GC-MS/MS Dwell, Event, and Loop times can be difficult to optimize when dozens, or even hundreds of compounds are to be analyzed simultaneously. The Smart MRM feature automatically determines the optimum Dwell, Event, and Loop settings using flexible MRM events, and creates MRM and Scan/MRM methods that provide the best sensitivity for all compounds in a single method.



Applicable Models: GCMS-TQ™ series

Operating Environment
OS: Microsoft® Windows® 7 Professional, Windows® 10 Professional
Excel: Microsoft® Excel® 2021, 2019 (32/64-bit version)
Microsoft® Excel® 2016 (32-bit version)
Workstation Software: GCMSsolution™, LabSolutions™ DB GCMS, LabSolutions CS

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Database Configuration

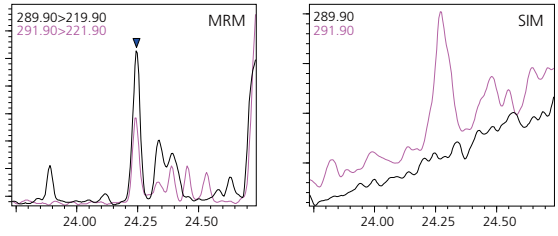
Registered Compounds	Number of Registered Compounds	Number of Registered Compounds Labeled with Stable Isotopes
Polychlorinated biphenyls	209	45
Brominated flame retardants	55	28
Dioxins	32	26
Polycyclic aromatic hydrocarbons	38	37
Organochlorine pesticides	32	25

The Smart Environmental Database consists of an Excel spreadsheet containing RIs, CAS numbers, and optimized MRM transitions for the compounds shown in the table above. It also includes method files for data acquisition and analysis, so analysis can begin with minimal start-up time.

Note: The retention indices registered in the database are calculated using the analysis conditions registered in the AART method file. If you are using the registered retention indices, use the identical conditions.

Sensitive Analysis via MRM

Analysis of PCB in River Water
(2,2',5,5'-Tetrachlorobiphenyl (#52) concentration in water of 0.080 ng/L)

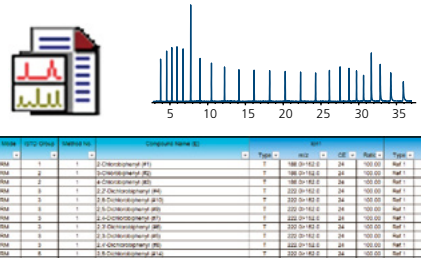


Analysis of environmental pollutants using the triple quadrupole MRM mode improves both sensitivity and selectivity, compared to the single quadrupole SIM mode, especially in cases where co-extracted contaminants might interfere with the analysis.

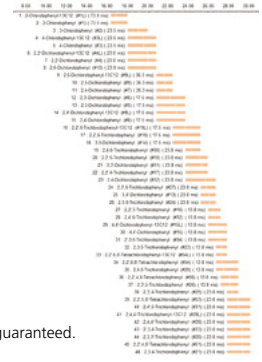
Procedure for Creating MRM Methods Using Smart Database

1. Analyze an aliquot of the *n*-alkane mixture.

2. Update retention times using the AART function.



3. Use Smart MRM to create the MRM or Scan/MRM method automatically from the Smart Environmental Database.



Remarks and Precautions

1. The accuracy of the information contained in the database and the usefulness of information obtained as a result of the use of this information is not guaranteed.
2. Be sure to test the qualitative and quantitative information obtained with this system using a standard sample for confirmation.
3. To reliably identify substances registered with this database, perform measurement using the system requirements of the method template file included with the product.

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