

Gas Chromatograph Mass Spectrometer

GCMS-TQ8040

UFMS
ULTRA FAST MASS SPECTROMETRY





GCMS-TQ8040 *with* Smart Technologies

Smart Productivity, Smart Operation, Smart Performance

Finally, a triple quadrupole GCMS **Smart** enough for everyday use in your laboratory.



The Shimadzu GCMS-TQ8040 is the first triple quadrupole with **Smart Productivity** for high efficiency sample throughput, **Smart Operation** for quick and easy method development, and **Smart Performance** for low detection limits and Scan/MRM. These three smart technologies contribute to **Smart MRM**, and provide the most accurate, cost-effective, and easy-to-use triple quadrupole GCMS you have ever imagined.

Smart Productivity

Simultaneous multi-component analysis is now possible for hundreds of target compounds, dramatically improving productivity. Smart MRM produces GC-MS/MS methods with up to 32,768 transitions in a single run.

> | P. 6 to **Smart Productivity**



Smart Operation

GC-MS/MS analysis requires multiple settings that can be confusing to the average operator. With **Smart MRM**, the GCMS-TQ8040 software sets the analytical conditions automatically, making method development painless, fast, and easy.

> | P. 8 to **Smart Operation**

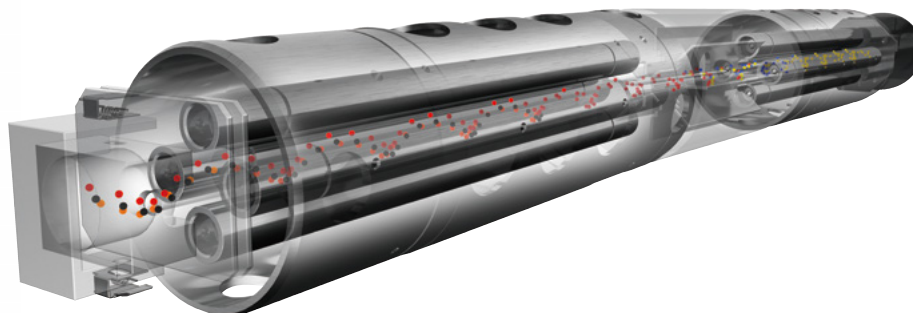


Smart Productivity Operation Performance

Smart Performance

The exceptionally efficient ion source and collision cell provide low detection limits. High-speed scanning control (Advanced Scanning Speed Protocol, or ASSP) and simultaneous Scan/MRM analysis mode provide high-quality library searchable fragmentation spectra, and accurate low-level quantitative data in a single analysis.

> | P. 12 to **Smart Performance**



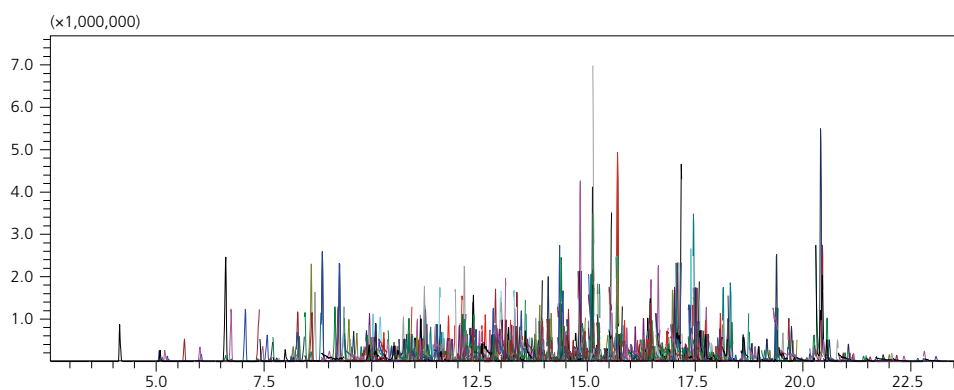
Smart Productivity

▮ Innovative Technologies that Improve Accuracy and Throughput

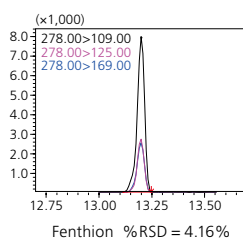
UFMS in the Multiple Reaction Mode can acquire over 800 transitions per second and over 32,000 transitions in a single analysis. The **Smart MRM** technology automatically adjusts the analytical dwell time for each transition, only acquiring data during peak elution, to fully optimize sensitivity. For example, analysis of more than 400 pesticides that used to require two or three methods can now be accomplished in a single acquisition method created by **Smart MRM**, significantly increasing laboratory throughput.

The UFMS technology guarantees a minimum of ten data points across each peak for optimum sensitivity and repeatability. Highly accurate, low-level detection of multiple components in complex matrices is finally possible by UFMS and **Smart MRM**.

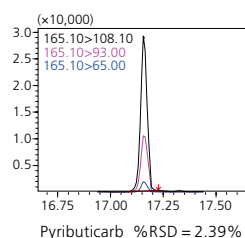
> | P. 9 to **Smart MRM**



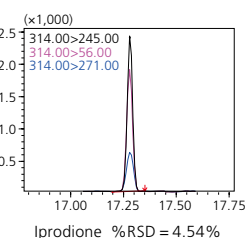
Simultaneous Analysis of 439 Pesticides Using UFMS and **Smart MRM**



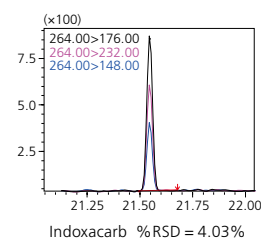
Fenthion %RSD = 4.16%



Pyributicarb %RSD = 2.39%

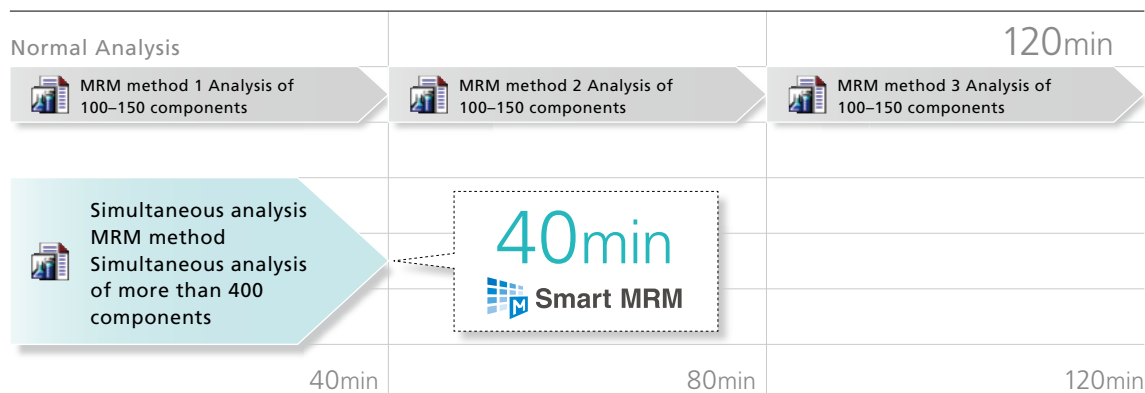


Iprodione %RSD = 4.54%



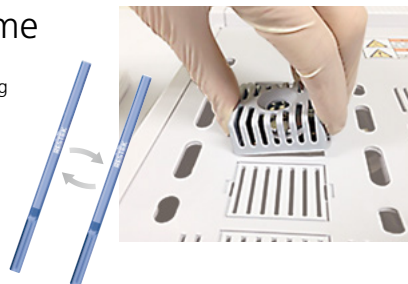
Indoxacarb %RSD = 4.03%

Mass chromatogram and %RSD (5 ppb)



Reduce Analysis Costs and Minimize Downtime

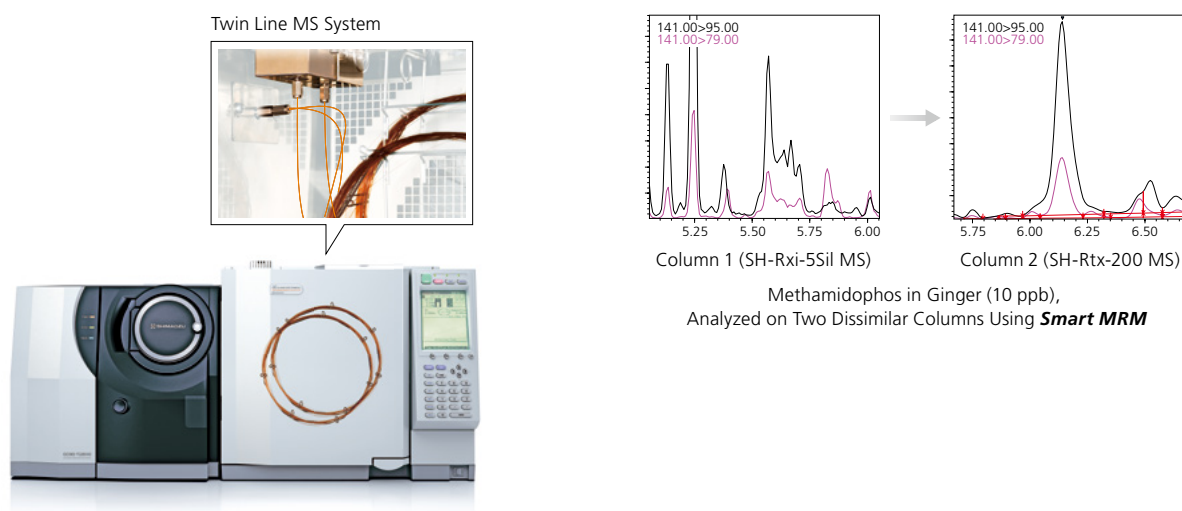
If simultaneous, multi-component analysis can be performed in 1/2 to 1/3 the time of existing systems, then two to three times the number of samples can be analyzed in the same period of time, and return on investment is improved. In addition, the frequency of maintenance, such as replacing glass liners and columns, is reduced, thereby minimizing downtime.



Twin Line MS System Eliminates the Need to Vent the MS

The GCMS-TQ8040 is capable of accepting installation of two narrow-bore capillary columns into the MS simultaneously. This allows you to switch applications without venting the MS.

Simply decide which column is best for your analysis and choose the associated injection port.



CID gas control is a method parameter, allowing acquisition of GC-MS and GC-MS/MS data in the same batch. By coupling this with the Twin Line MS System, analysis of phenols by SIM and analysis of pesticides by MRM are possible in a single batch without venting the MS.

	Method File	Data File	
1	Phenols_SIM.qgm	DATA_01.qgd	SIM GC-MS (CID gas-Off)
2	Phenols_SIM.qgm	DATA_02.qgd	
3	Phenols_SIM.qgm	DATA_03.qgd	
4	Pesticide_MRM.qgm	DATA_04.qgd	MRM GC-MS/MS (CID gas-On)
5	Pesticide_MRM.qgm	DATA_05.qgd	

Run SQ and TQ Methods in a Single Sequence

*) The Twin Line MS System requires an optional installation kit and is limited to certain column dimensions.

Smart Operation

Smart MRM

Smart MRM makes method development quick and easy.

Whether starting from scratch to optimize transitions and collision energies for new compounds, or starting from an MRM database of known target analytes to build a custom MRM method,

Smart MRM takes the stress and difficulty out of method development.

Pesticide Residue Analysis



Metabolic Component Analysis



Environmental Pollutant Analysis



Forensic Toxicological Analysis



Serial	Type	Acq. Mode	Method No.	Compound Name (S)	Ref. Index	Case	Type	m/z	CE	Ratio	Type	m/z	CE	Ratio
1	Target	MRM	1	Aldicarb deg.	887	0 - 00 - 0	T	118.1x102.1	8	100.00	Ref 1	118.1x102.1	8	100.00
2	Target	MRM	1	DDP	1057	108 - 00 - 1	T	121.1x45.0	4	100.00	Ref 1	121.1x77.0	8	48.00
3	Target	MRM	1	Aldicarb deg.	1134	0 - 00 - 0	T	80.0x66.0	6	100.00	Ref 1	80.0x66.0	4	3.94
4	Target	MRM	1	Chlorfentazine deg.	1194	0 - 00 - 0	T	137.0x102.0	14	100.00	Ref 1	137.0x75.0	26	37.61
5	Target	MRM	1	Pyrimethanil	1201	1000 - 00 - 1	T	99.0x71.0	8	100.00	Ref 1	99.0x54.0	26	6.13
6	Target	MRM	1	Methamidophos	1240	1008 - 00 - 8	T	141.0x96.0	8	100.00	Ref 1	141.0x126.0	4	18.74
7	Target	MRM	1	Dichlorvos	1248	62 - 73 - 7	T	185.0x93.0	14	100.00	Ref 1	185.0x109.0	14	28.66
8	Target	MRM	1	Permethrin	1265	0 - 00 - 0	T	149.1x71.1	8	100.00	Ref 1	149.1x102.1	6	67.94
9	Target	MRM	1	Azinphos	1290	00 - 71 - 0	T	138.1x66.0	6	100.00	Ref 1	138.1x110.1	6	53.98
10	Target	MRM	1	Dichlorodant	1348	1104 - 60 - 6	T	170.9x100.0	24	100.00	Ref 1	170.9x130.0	14	101.88
11	Target	MRM	1	EPFC	1359	789 - 84 - 4	T	189.1x128.1	4	100.00	Ref 1	189.1x68.0	12	22.86
12	Target	MRM	1	Biphenyl	1393	92 - 62 - 4	T	154.1x126.1	22	100.00	Ref 1	154.1x115.1	24	74.03

MRM Optimization Tool



Smart Database

Smart MRM



Smart Database

■ Compounds and Optimized Transitions

The Shimadzu “Smart Database” is a database of related compounds (e.g. pesticides, drugs, metabolites, etc.) with optimized transitions and collision energies, CAS registry numbers, and Retention Indices (RI). The user can select from hundreds of pre-registered compounds

in one of the “Smart Database” files, or add their own optimized transitions. The user selects the compounds to be analyzed, and **Smart MRM** builds the MRM or Scan/MRM acquisition method from the “Smart Database” with the push of a button.

Smart MRM

■ Automatic Method Creation

For multi-component analyses, with hundreds of compounds and up to 32,768 transitions, adjusting the loop and dwell times for optimum sensitivity can be complex and difficult. Shimadzu's **Smart MRM**

technology creates MRM and Scan/MRM methods by automatically adjusting the analytical dwell times for each transition in a method.

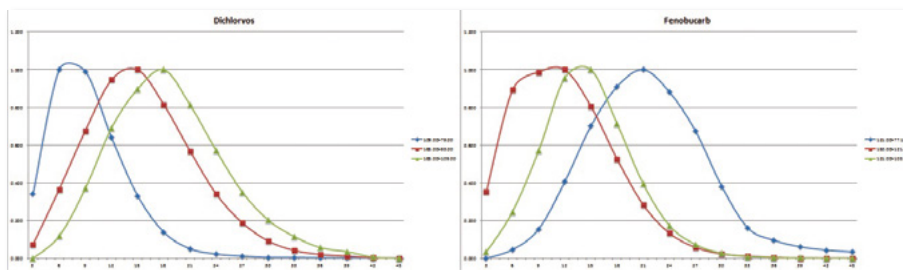
The screenshot displays the Smart MRM software interface. On the left, a table lists compounds with columns for Serial, Target, Acq. Mode, Method No., Compound Name, and Type. In the center, the 'MRM,SRM Parameter' dialog box is open, showing 'Loop Time (MRM, SRM)' set to 6.3 sec and 'Required Processing Time: R.T.s' set to 6.3 min. Below this, the 'Scan Parameter' dialog box is visible, showing 'Scan Range: Start m/z - End m/z' set to 2 - 1000 and 'Acquisition Time: Start R.T. - End R.T.' set to 1 - 30 min. On the right, a list of compounds is shown, including 200, 201, 202, 203, 204, 205, 206, 207, 208, 209, 210, 211, 212, 213, 214, 215, 216, 217, 218, 219, 220, 221, 222, 223, 224, 225, 226, 227, 228, 229, 230, 231, 232, 233, 234, 235, 236, 237, 238, 239, 240, 241, 242, 243, 244, 245, 246, 247, 248, 249, 250, 251, 252, 253, 254, 255, 256, 257, 258, 259, 260, 261, 262, 263, 264, 265, 266, 267, 268, 269, 270, 271, 272, 273, 274, 275, 276, 277, 278, 279, 280, 281, 282, 283, 284, 285, 286, 287, 288, 289, 290, 291, 292, 293, 294, 295, 296, 297, 298, 299, 300, 301, 302, 303, 304, 305, 306, 307, 308, 309, 310, 311, 312, 313, 314, 315, 316, 317, 318, 319, 320, 321, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 336, 337, 338, 339, 340, 341, 342, 343, 344, 345, 346, 347, 348, 349, 350, 351, 352, 353, 354, 355, 356, 357, 358, 359, 360, 361, 362, 363, 364, 365, 366, 367, 368, 369, 370, 371, 372, 373, 374, 375, 376, 377, 378, 379, 380, 381, 382, 383, 384, 385, 386, 387, 388, 389, 390, 391, 392, 393, 394, 395, 396, 397, 398, 399, 400, 401, 402, 403, 404, 405, 406, 407, 408, 409, 410, 411, 412, 413, 414, 415, 416, 417, 418, 419, 420, 421, 422, 423, 424, 425, 426, 427, 428, 429, 430, 431, 432, 433, 434, 435, 436, 437, 438, 439, 440, 441, 442, 443, 444, 445, 446, 447, 448, 449, 450, 451, 452, 453, 454, 455, 456, 457, 458, 459, 460, 461, 462, 463, 464, 465, 466, 467, 468, 469, 470, 471, 472, 473, 474, 475, 476, 477, 478, 479, 480, 481, 482, 483, 484, 485, 486, 487, 488, 489, 490, 491, 492, 493, 494, 495, 496, 497, 498, 499, 500, 501, 502, 503, 504, 505, 506, 507, 508, 509, 510, 511, 512, 513, 514, 515, 516, 517, 518, 519, 520, 521, 522, 523, 524, 525, 526, 527, 528, 529, 530, 531, 532, 533, 534, 535, 536, 537, 538, 539, 540, 541, 542, 543, 544, 545, 546, 547, 548, 549, 550, 551, 552, 553, 554, 555, 556, 557, 558, 559, 560, 561, 562, 563, 564, 565, 566, 567, 568, 569, 570, 571, 572, 573, 574, 575, 576, 577, 578, 579, 580, 581, 582, 583, 584, 585, 586, 587, 588, 589, 590, 591, 592, 593, 594, 595, 596, 597, 598, 599, 600, 601, 602, 603, 604, 605, 606, 607, 608, 609, 610, 611, 612, 613, 614, 615, 616, 617, 618, 619, 620, 621, 622, 623, 624, 625, 626, 627, 628, 629, 630, 631, 632, 633, 634, 635, 636, 637, 638, 639, 640, 641, 642, 643, 644, 645, 646, 647, 648, 649, 650, 651, 652, 653, 654, 655, 656, 657, 658, 659, 660, 661, 662, 663, 664, 665, 666, 667, 668, 669, 670, 671, 672, 673, 674, 675, 676, 677, 678, 679, 680, 681, 682, 683, 684, 685, 686, 687, 688, 689, 690, 691, 692, 693, 694, 695, 696, 697, 698, 699, 700, 701, 702, 703, 704, 705, 706, 707, 708, 709, 710, 711, 712, 713, 714, 715, 716, 717, 718, 719, 720, 721, 722, 723, 724, 725, 726, 727, 728, 729, 730, 731, 732, 733, 734, 735, 736, 737, 738, 739, 740, 741, 742, 743, 744, 745, 746, 747, 748, 749, 750, 751, 752, 753, 754, 755, 756, 757, 758, 759, 760, 761, 762, 763, 764, 765, 766, 767, 768, 769, 770, 771, 772, 773, 774, 775, 776, 777, 778, 779, 780, 781, 782, 783, 784, 785, 786, 787, 788, 789, 790, 791, 792, 793, 794, 795, 796, 797, 798, 799, 800, 801, 802, 803, 804, 805, 806, 807, 808, 809, 810, 811, 812, 813, 814, 815, 816, 817, 818, 819, 820, 821, 822, 823, 824, 825, 826, 827, 828, 829, 830, 831, 832, 833, 834, 835, 836, 837, 838, 839, 840, 841, 842, 843, 844, 845, 846, 847, 848, 849, 850, 851, 852, 853, 854, 855, 856, 857, 858, 859, 860, 861, 862, 863, 864, 865, 866, 867, 868, 869, 870, 871, 872, 873, 874, 875, 876, 877, 878, 879, 880, 881, 882, 883, 884, 885, 886, 887, 888, 889, 890, 891, 892, 893, 894, 895, 896, 897, 898, 899, 900, 901, 902, 903, 904, 905, 906, 907, 908, 909, 910, 911, 912, 913, 914, 915, 916, 917, 918, 919, 920, 921, 922, 923, 924, 925, 926, 927, 928, 929, 930, 931, 932, 933, 934, 935, 936, 937, 938, 939, 940, 941, 942, 943, 944, 945, 946, 947, 948, 949, 950, 951, 952, 953, 954, 955, 956, 957, 958, 959, 960, 961, 962, 963, 964, 965, 966, 967, 968, 969, 970, 971, 972, 973, 974, 975, 976, 977, 978, 979, 980, 981, 982, 983, 984, 985, 986, 987, 988, 989, 990, 991, 992, 993, 994, 995, 996, 997, 998, 999, 1000. A small icon of a document with a checkmark is shown to the right of the list.

MRM Optimization Tool

■ Optimize MRM Transitions Automatically

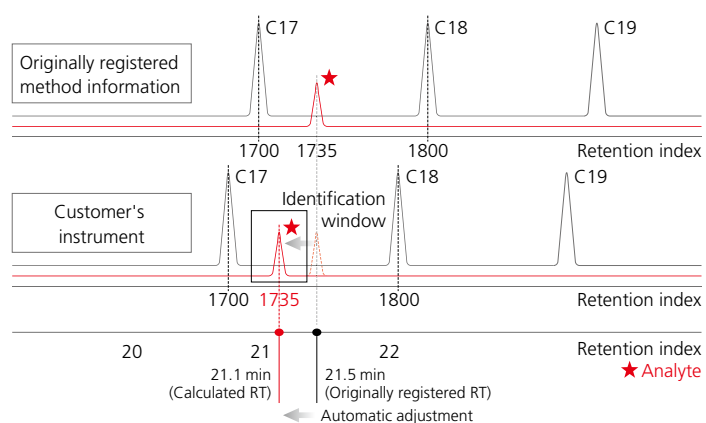
Determining and optimizing MRM transitions for new compounds can require significant development time. The “MRM Optimization Tool” automates the process by collecting product ion scan data and finding the optimum collision energy for each transition.

Once established, the transitions are registered to one of the Shimadzu “Smart Database” files, and the MRM or Scan/MRM methods are created using **Smart MRM**.



GC/MSsolution for Quick, Error-Free Operation

Automatic Adjustment of Compound Retention Time (AART) (Automatic Adjustment of Retention Time)



The AART function adjusts the retention times of target components based on linear retention indices (LRI) and the retention times of n-alkanes. The AART function easily adjusts acquisition and processing method parameters simultaneously.

1 n-alkane analysis

2 AART execution

3 Adjustment of retention times

Automatic Adjustment of Retention Time (AART) (File) (Edit) (View) (Tools) (Help)

The retention time is the compound name of the compound. It is modified for the following table. In addition, it can be used to modify the retention time of the compound parameters for some of the compounds.

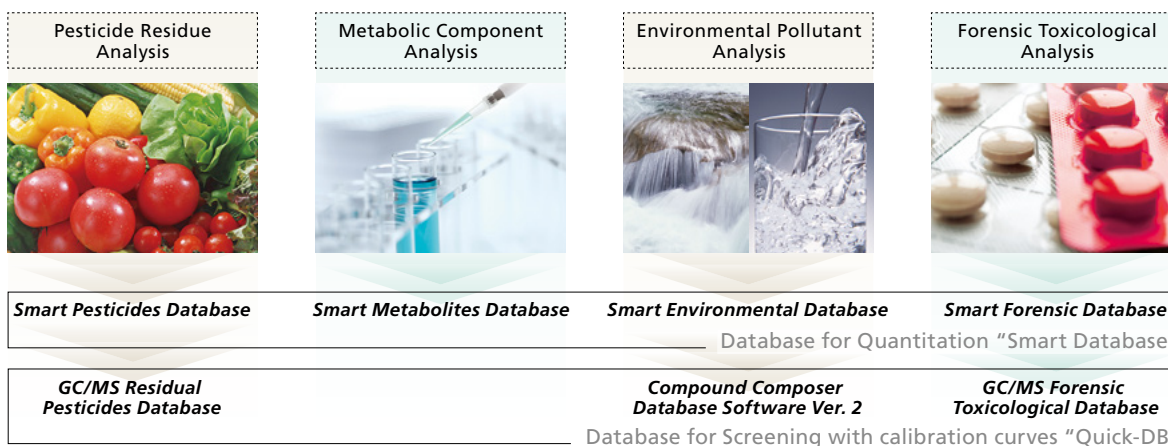
Compound Name	Retention Time (min)	Retention Time (min)	Retention Time (min)
1,2-Dichloroethane	1.561	1.564	-0.003
1,2-Dichlorobenzene	1.745	1.746	-0.001
1,2-Dichloroethane	1.968	1.960	0.008
1,2-Dichloroethane	5.192	5.174	0.018
1,2-Dichloroethane	6.292	6.267	0.025
1,2-Dichloroethane	6.782	6.761	0.021
1,2-Dichloroethane	7.098	7.075	0.023
1,2-Dichloroethane	7.157	7.132	0.025
1,2-Dichloroethane	7.542	7.517	0.025
1,2-Dichloroethane	9.588	9.554	0.034
1,2-Dichloroethane	10.857	10.822	0.035
1,2-Dichloroethane	11.299	11.263	0.036
1,2-Dichloroethane	11.579	11.544	0.035

Compound Name	Predicted RT	Measured RT	RT Error
Mono-BDE (BDE-001)	1.561	1.564	-0.003
Mono-BDE (BDE-002)	1.745	1.746	-0.001
Mono-BDE (BDE-003)	1.968	1.960	0.008
Di-BDE (BDE-010)	5.192	5.174	0.018
Di-BDE (BDE-007)	6.292	6.267	0.025
Di-BDE (BDE-008&BDE011)	6.782	6.761	0.021
Di-BDE (BDE-012)	7.098	7.075	0.023
Di-BDE (BDE-013)	7.157	7.132	0.025
Di-BDE (BDE-015)	7.542	7.517	0.025
Tri-BDE (BDE-030)	9.588	9.554	0.034
Tri-BDE (BDE-032)	10.857	10.822	0.035
Tri-BDE (BDE-017)	11.299	11.263	0.036
Tri-BDE (BDE-025)	11.579	11.544	0.035

Updating compound retention times for low- to high-boiling compounds is simple and accurate.

GC/MS Database

To begin a GC-MS/MS analysis, the analytical conditions and information about the compound to be analyzed must be set and these tasks require a lot of effort. To facilitate the start of GC-MS/MS analyses, Shimadzu has preset the required information in databases.



LabSolutions Insight

Multi-analyte Data Review

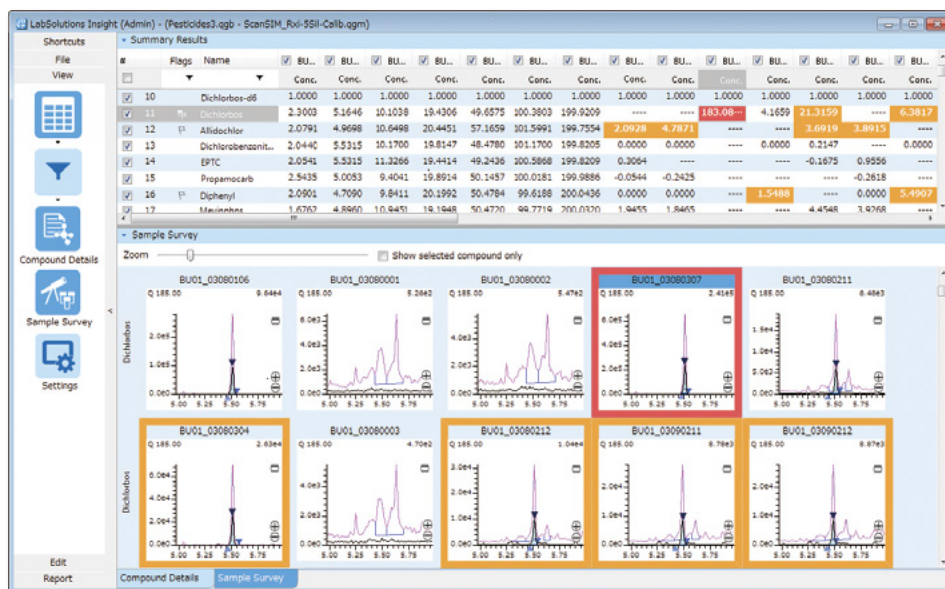
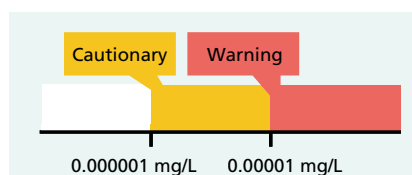
With LabSolutions Insight software, quantitative results for a complete series of data files can be displayed side-by-side for comparison and QC review. All of the chromatograms for a selected target compound can be displayed simultaneously, making it easy to review the detected peaks and confirm the quantitative results. Color-coded QA/QC flags quickly identify any outliers that require further examination.

Color-coded QA/QC Flags

In LabSolutions Insight, quantitative results can be compared to established criteria, and any outliers are color-coded for easy identification and further review. Five color-coded criteria levels can be defined, making it easy to determine which data points are outliers, and which specific QC criteria were not met. Any changes made to calibration curves or manual peak integration are immediately reflected in the color-coded flags.

Example of Using Flags for Quantitative Review

The example below illustrates how an orange flag was set to identify moldy odor compound concentrations that exceeded a defined cautionary limit of 1.0 ppt (part-per-trillion), and a red flag was used as a warning to identify those which had exceeded 10 ppt. In the figure below, quantitative results are tabulated at the top of the screen, while the bottom of the screen simultaneously displays peak identification and integration. Both views include the color-coded flags.



System Configurations Using Multiple Client Computers

Data acquired from multiple analytes can be reviewed or confirmed using client computers connected via a LAN or other network. If multiple systems are used, data obtained from each system can be reviewed from any client computer. Even in the case of multiple analysts using the same system, the ability to separate analytical work from measurement work improves work efficiency.

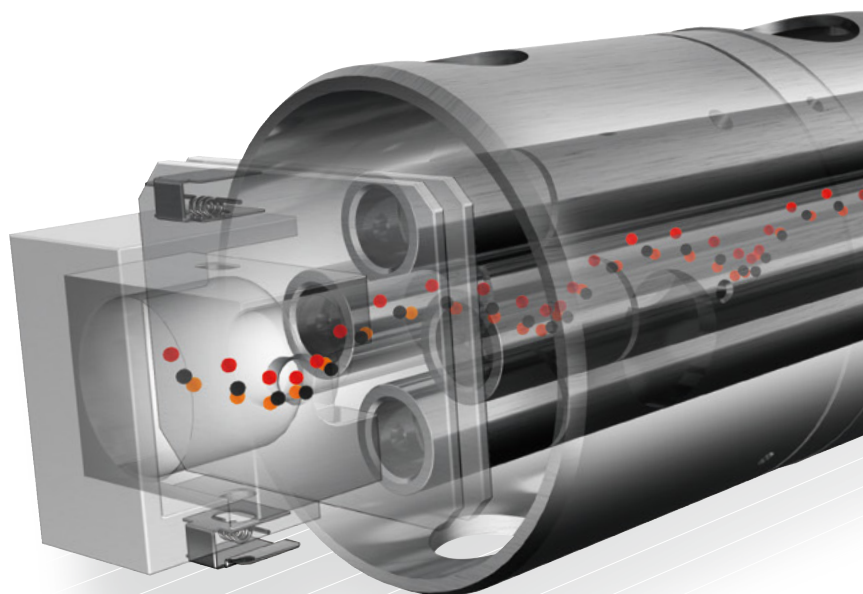
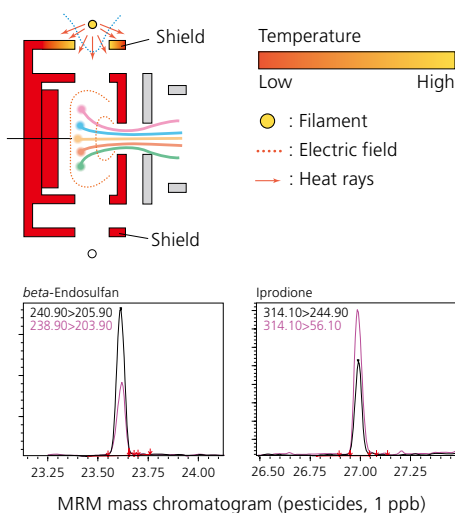
* LabSolutions Insight is the optional software.

Smart Performance

■ High-Sensitivity Ion Source

The effect of the filament's electric potential on the ion source is reduced by placing more distance between the filament and ion source box. In addition, a shield blocks out radiant heat generated

from the filament to ensure the ion source box temperature remains uniform. Since this prevents any active spots within the ion source, it provides higher sensitivity for analysis. (Patent: US7939810)

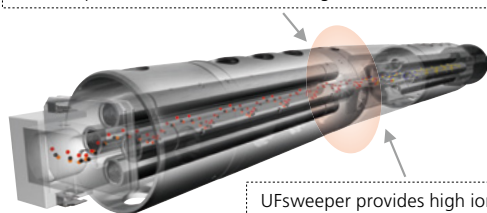


■ Sensitivity and Repeatability in Single GC/MS Mode

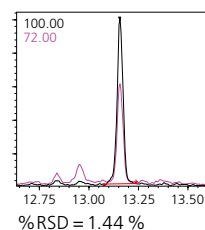
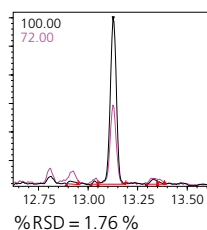
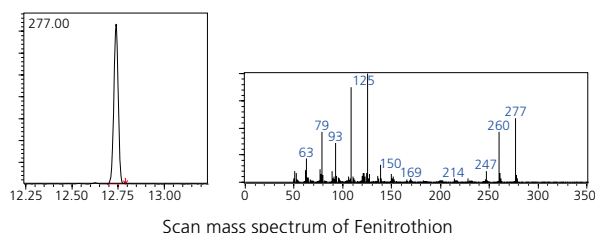
The high-efficiency ion source provides the foundation of an ion generation and transmission system, which creates and then delivers ions to the detector, resulting in a GC/MS with the maximum possible sensitivity and repeatability. These features

are not realized just for MRM measurements by GC-MS/MS, but also for scan and SIM measurements in single quadrupole modes, even with the most reactive compounds.

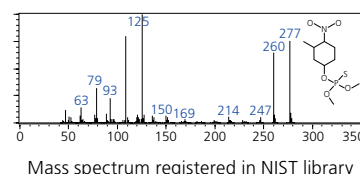
Q1 with post-rod achieves outstanding ion transfer efficiency



Ufsweeper provides high ion transfer efficiency

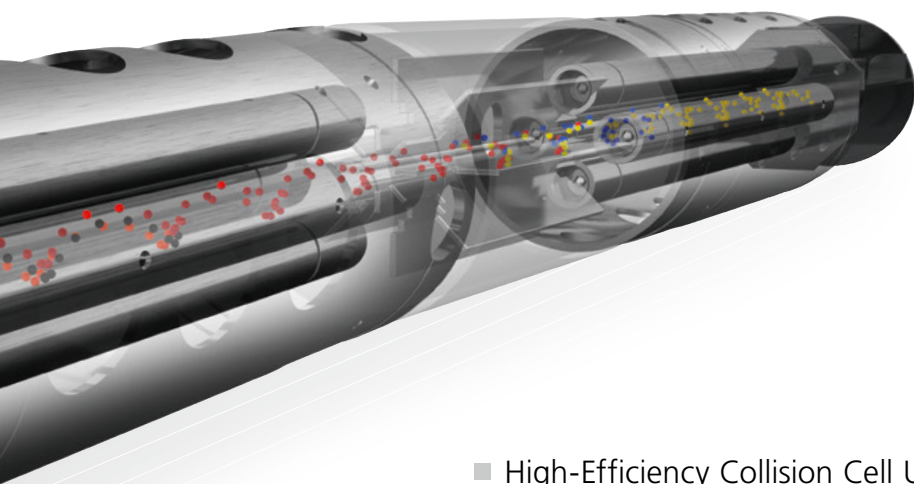


Thiobencarb 5 ppb
Left: GCMS-QP2010 Ultra, Right: GCMS-TQ8040
(for RSD determination, n = 5)



■ OFF-AXIS Ion Optics

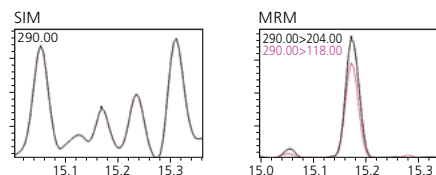
Lower detection limits are achieved by OFF-AXIS Ion Optics (Patent Pending). Meta-stable and neutral ions are removed without sacrificing sensitivity. Helium buffer gas is not required in the CID cell.



■ High-Efficiency Collision Cell UFsweeper™

UFGS
ULTRA FAST MASS SPECTROMETRY

Shimadzu's proprietary UFsweeper technology achieves high-speed MRM analysis at speeds up to 800 transitions per second. It sweeps residual ions from the collision cell to provide high-efficiency CID and fast ion transport. Rapid ion removal minimizes cross-talk and enables trace analysis (patent pending).



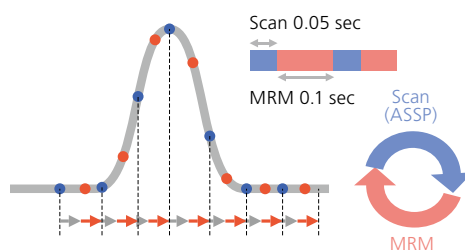
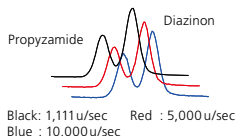
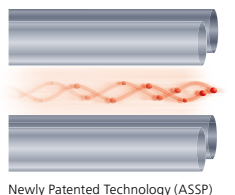
Analysis of residual pesticides (Isoprothiolane 1 ppb)

■ High-Speed Scanning Control (Advanced Scanning Speed Protocol, ASSP™)

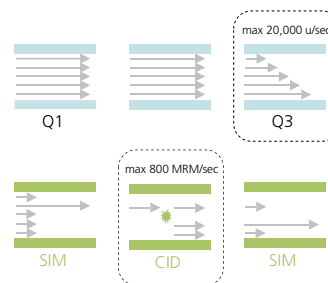
UFGS
ULTRA FAST MASS SPECTROMETRY

ASSP achieves scan speeds of 20,000 u/second. The rod bias voltage is dynamically optimized during ultrahigh-speed data acquisition, thereby minimizing the drop in sensitivity that would otherwise occur above 10,000 u/second. This is necessary for maintaining sensitivity at high scan speeds and acquiring superior mass spectra when

performing product ion scans or simultaneous scan and MRM measurement in the Scan/MRM mode. (Patent: US6610979). Scan/MRM simultaneous analysis is possible by coupling high-speed scanning with high-speed MRM.



By switching rapidly between scan and MRM modes, data can be acquired using both modes in the same analysis.



Smart Options

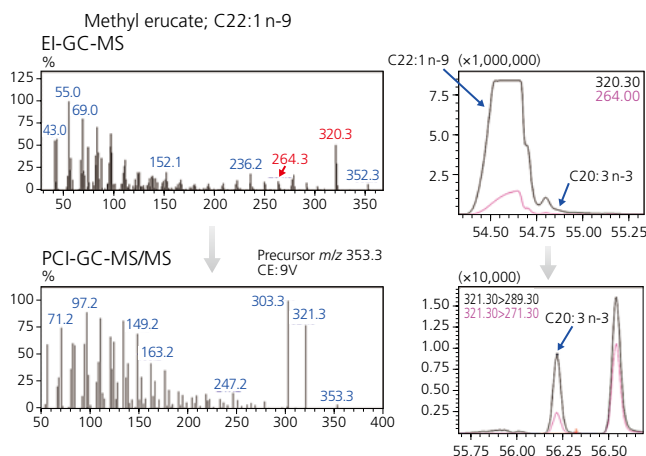
▧ Various System Configurations

For GC-MS/MS analysis, different system configurations may be required depending on the application and sample-introduction needs. The GCMS-TQ8040 offers a wide variety of system configurations and sample-introduction devices to enable an expanded range of applications.



▧ Chemical Ionization and Negative Chemical Ionization

In addition to commonly-used electron ionization (EI), both chemical ionization (CI) and negative chemical ionization (NCI) are available for the GCMS-TQ8040. The CI mode is a “soft ionization” technique, used to detect many compounds not possible by EI, and is suited for confirmation of molecular weight. The NCI mode can be used to detect functional groups having a high electron affinity such as halogens. Any of three types of reagent gases (methane, isobutane, or ammonia) can be used.

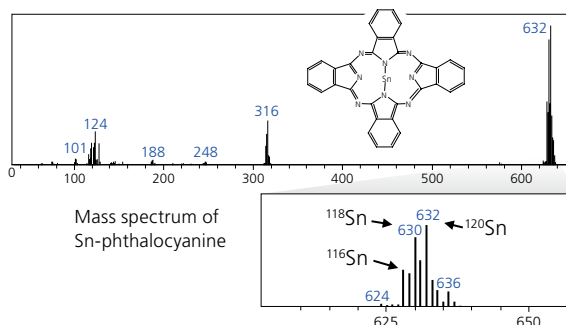


▧ DI-2010 Direct Sample Inlet Device



The DI probe allows a sample to be introduced directly into the ion source without passing through a GC column. It is an effective technique for obtaining mass spectra of synthetic compounds that do not chromatograph well. A DI system can be

incorporated into a standard GC-MS configuration without making any changes to the GC. It is then possible to switch between conventional GC column chromatography and DI analysis without making any hardware changes.



Components that are thermally degradable or difficult to vaporize are not suited to GC analysis. Their mass spectra can be obtained easily using the DI probe. Above is an example of Sn-phthalocyanine spectra obtained using the DI probe.

HS-20 Headspace Sampler

The GCMS-TQ8040 can also be used as a single quadrupole GC-MS. In combination with the HS-20 headspace sampler, it can analyze residual solvents in pharmaceuticals. If highly toxic impurities are discovered, even trace quantities can be quantified using MRM analysis.

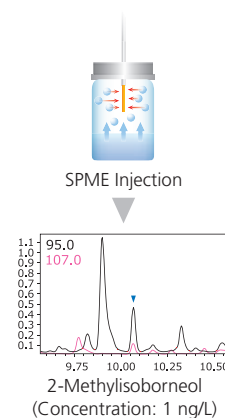
The HS-20 transfer line is built into the GC, so combination with a liquid sample injector using the AOC-20 as well as switchover operations are easy.



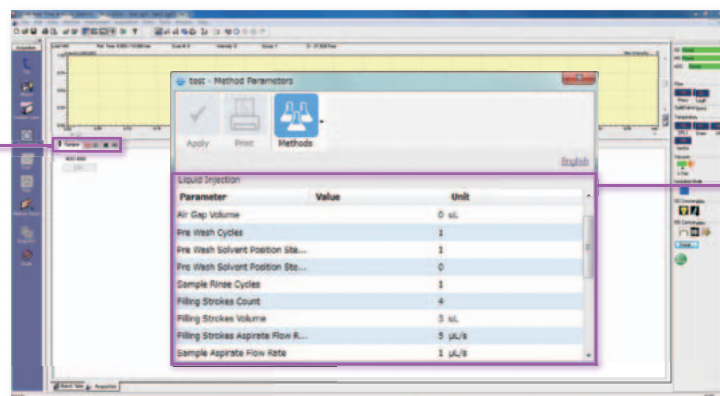
AOC-6000 Multifunctional Autosampler

The AOC-6000 is compatible with three sample injection methods: liquid sample injection, headspace injection, and solid phase micro extraction (SPME) injection. The sample injection method can be selected to suit the form of the sample and the components subject to analysis.

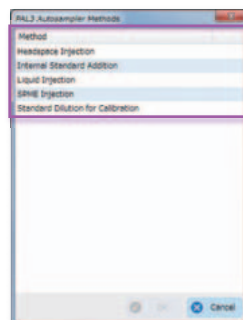
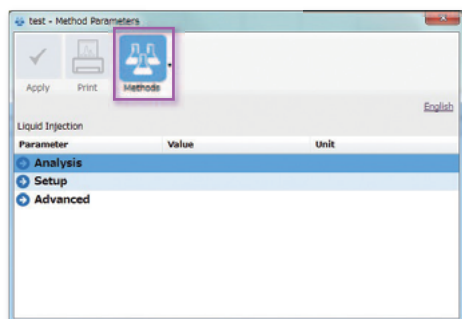
Condition setting and control can be performed from the GCMSolution software for GC/MS. The AOC-6000 and GC/MS analysis conditions are recorded in the data measured, so management of analysis accuracy is easily performed. General analysis conditions are preconfigured, so you can start your analysis quickly.



GC/MS and the AOC-6000 are controlled from the same software, simplifying method selection and analysis conditions settings.



AOC-6000 analysis conditions are stored in the measurement data file.



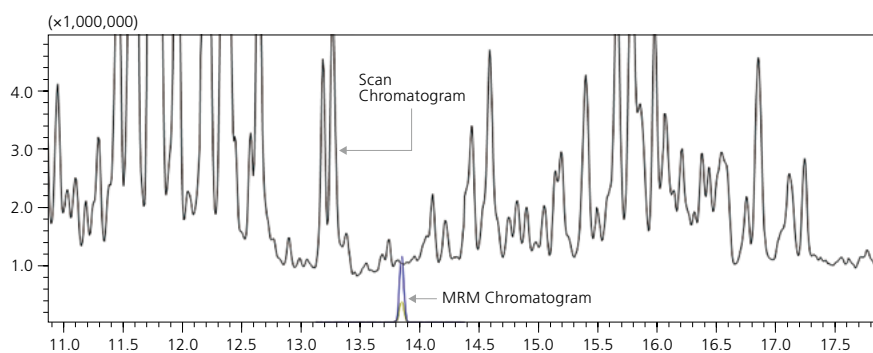
Typical analysis conditions are preconfigured, so analysis can start immediately just by changing some parameters, or using the preconfigured conditions as they are.

Smart Solutions using GCMS-TQ8040

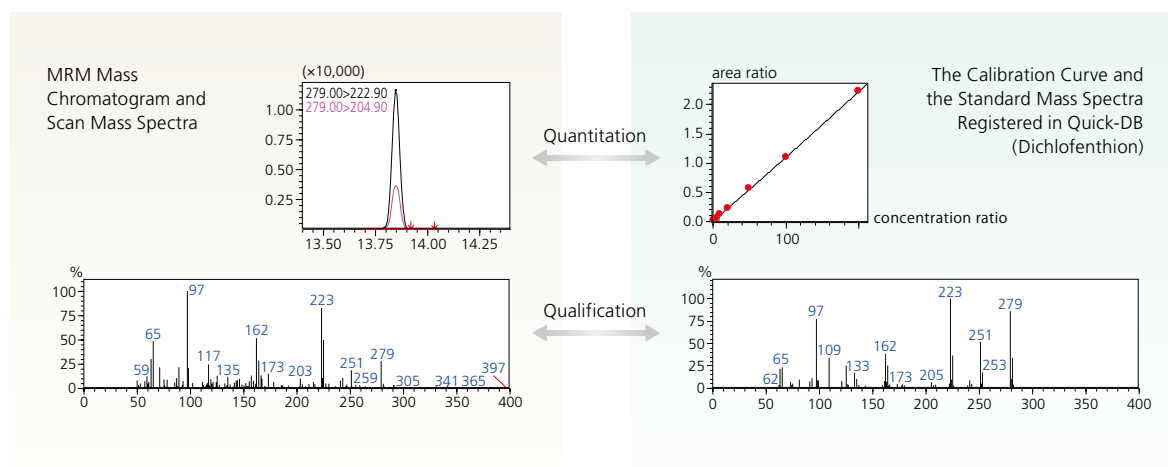
▨ Pesticide Quick-DB

Pesticide Quick-DB is a software package that contains Scan/MRM and Scan/SIM acquisition methods and pre-stored calibration curves for more than 450 pesticides. The **Pesticide Quick-DB** uses isotopically labeled pesticide surrogates as internal standards for each compound class to enable rapid, semi-quantitative results. In addition, Scan/MRM simultaneously acquires qualitative mass spectra for confirmation. When used with the Twin Line MS System, detected compounds can also be confirmed on a second, dissimilar column without venting the MS.

Pesticide Residue Analysis



Analysis of Pesticides in a Cabbage Extract Using Scan/MRM



Quantitative Results Using a Database (10 ng/mL pesticide added)

Compound Name	Conc. (ng/mL)	Compound Name	Conc. (ng/mL)
Dichlorvos	11.60	Fenitrothion	8.28
Acephate	9.53	Linuron	9.02
<i>gamma</i> -BHC	10.20	Isoxathion	9.99
Diazinon	10.29	<i>beta</i> -Endosulfan	8.53
Iprobenfos	10.74	<i>o,p'</i> -DDT	9.77
Dichlofenthion	8.21	EPN	11.16
Carbaryl	10.28	Etofenprox	10.18
Metalaxyl	9.57	Azoxystrobin	10.20

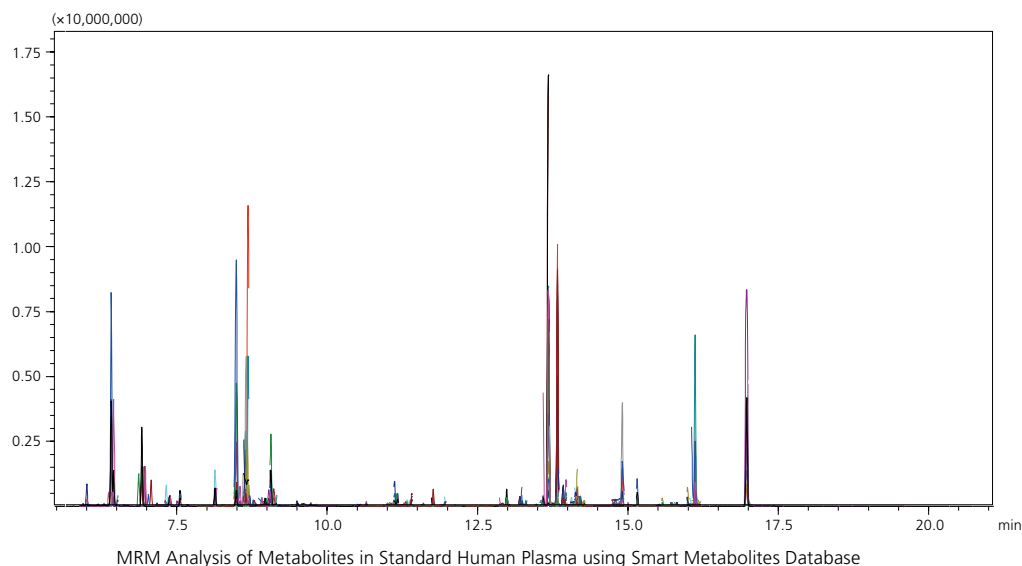
Metabolite Database

Biological samples such as blood serum contain large amounts of interfering co-extractants. Due to co-elution of components, some compounds cannot be reliably analyzed using single quadrupole GC-MS. MRM measurements eliminate the effect of interfering background matrices, and enable the targeted compounds to be accurately and reliably identified.

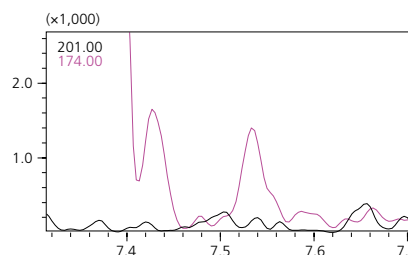
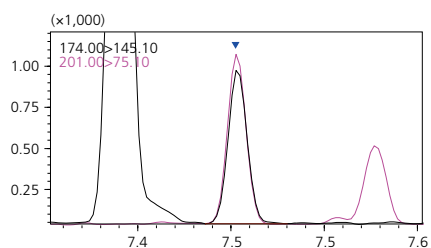
Smart Metabolites Database registers MRM information of 475 metabolites mainly contained in biological samples such as blood, urine and cells.

The database used in conjunction with the Shimadzu GCMS-TQ8040, which supports high speed MRM analysis, allows the acquisition of simultaneous measurement of 475 metabolites.

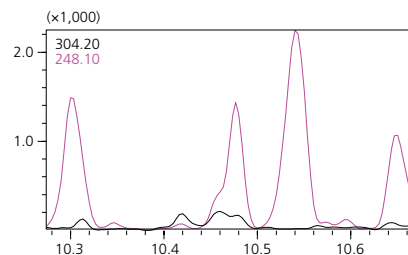
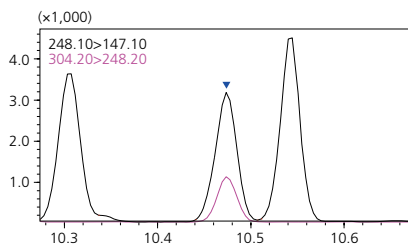
Metabolic Component Analysis



Valproic acid-TMS



3-Aminoisobutyric acid-3TMS

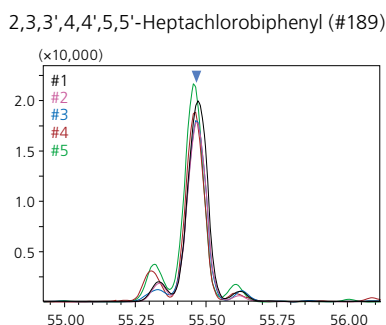
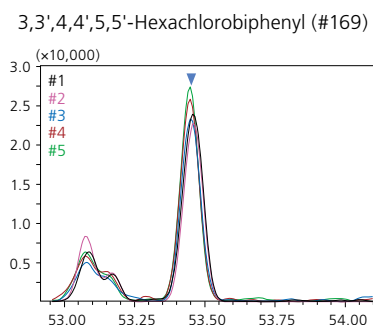
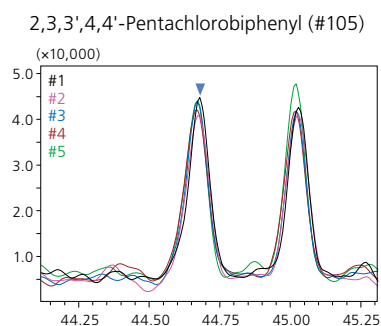
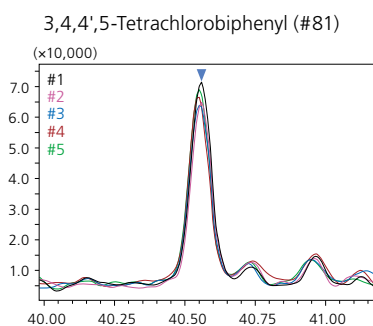


Comparison of MRM (Left) and Scan (Right) Mass Chromatograms for Metabolites in Standard Human Plasma

Smart Environmental Database

Persistent organic pollutants (POPs) are known to have an adverse impact on plants and animals. They are subject to analysis in a variety of samples. MRM measurements can be started quickly using **Smart Environmental Database**, which is registered with more than 500 POP compounds including polychlorinated biphenyls. Thanks to the high selectivity of MRM, even trace quantities of compounds can be detected with high sensitivity.

Environmental Pollutant Analysis



MRM Mass Chromatogram (100 fg/μL) of Polychlorinated Biphenyls Added to Transformer Oil (Diluted 1/1000), and Repeated Analysis Accuracy

Compound Name	%RSD (n=5)
3,4,4',5-Tetrachlorobiphenyl (#81)	3.70
3,3',4,4'-Tetrachlorobiphenyl (#77)	6.19
2',3,4,4',5-Pentachlorobiphenyl (#123)	3.50
2,3',4,4',5-Pentachlorobiphenyl (#118)	8.30
2,3,4,4',5-Pentachlorobiphenyl (#114)	6.30
2,3,3',4,4'-Pentachlorobiphenyl (#105)	2.81
3,3',4,4',5-Pentachlorobiphenyl (#126)	8.28
2,3',4,4',5,5'-Hexachlorobiphenyl (#167)	2.95
2,3,3',4,4',5-Hexachlorobiphenyl (#156)	8.05
2,3,3',4,4',5'-Hexachlorobiphenyl (#157)	8.04
3,3',4,4',5,5'-Hexachlorobiphenyl (#169)	5.53
2,3,3',4,4',5,5'-Heptachlorobiphenyl (#189)	8.24

Note: Figures in brackets to the right of compound names are the IUPAC numbers for each polychlorinated biphenyl.

Forensic Database

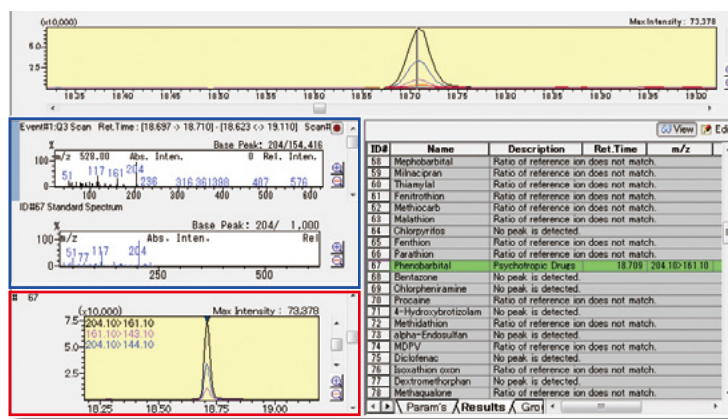
With GC-MS/MS MRM mode, interferences in biological sample and forensic toxicological substances can be separated out, enabling high sensitivity detection. The **Smart Forensic Database** for MRM is registered with a total of 201 forensic toxicological substances often involved in poisonings, such as drugs of abuse, psychotropic drugs, pharmaceuticals and pesticides, it is easy to create the Scan/MRM method. Scan data obtained with simultaneous Scan/MRM measurements can be analyzed using the **Forensic Quick-DB** for scan, which is used to screen for forensic toxicological substances. MRM data can be used for trace quantity analyses of toxicological substances often involved in poisonings, which are registered in the **Smart Forensic Database**, while the scan data can be used to screen for drugs of abuse using the **Forensic Quick-DB**, which is replete with designer drugs.

Forensic Toxicological Analysis

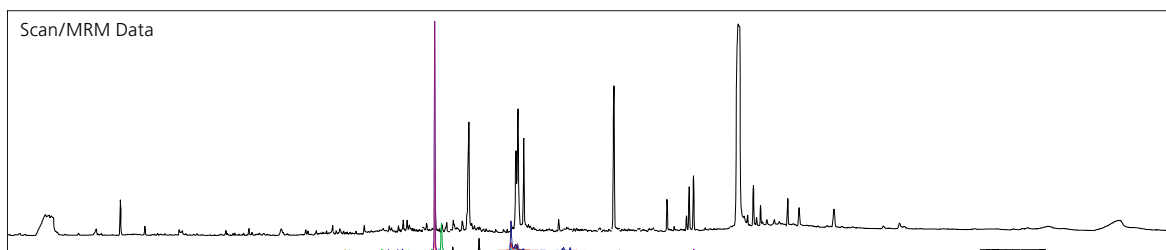


Improved Identification Reliability via Confirmation Using Scan Mass Spectrum

High Sensitivity, High Separation Detection via MRM Mass Chromatograms

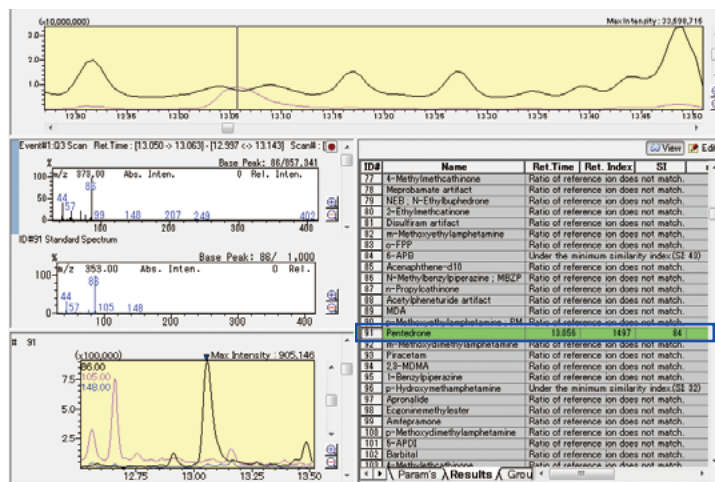
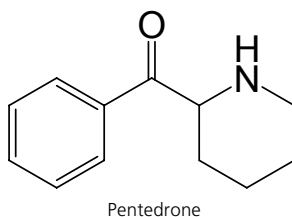


MRM Data + Smart Forensic Database



Scan Data + Forensic Quick-DB

Detection of Pentedrone, a Type of Cathinones





Shimadzu Corporation

www.shimadzu.com/an/

For Research Use Only. Not for use in diagnostic procedure.

This publication may contain references to products that are not available in your country. Please contact us to check the availability of these products in your country.

Company names, product/service names and logos used in this publication are trademarks and trade names of Shimadzu Corporation or its affiliates, whether or not they are used with trademark symbol "TM" or "®". Third-party trademarks and trade names may be used in this publication to refer to either the entities or their products/services. Shimadzu disclaims any proprietary interest in trademarks and trade names other than its own.

The contents of this publication are provided to you "as is" without warranty of any kind, and are subject to change without notice. Shimadzu does not assume any responsibility or liability for any damage, whether direct or indirect, relating to the use of this publication.