

Fundamental of GC-MS/MS



GCMS-TQseries

- **GCMS-TQseries is Shimadzu gas chromatograph-Tandem mass spectrometer (GC-MS/MS).**
- **GC-MS is a combination of two different analytical techniques, Gas Chromatography and Mass Spectrometry.**

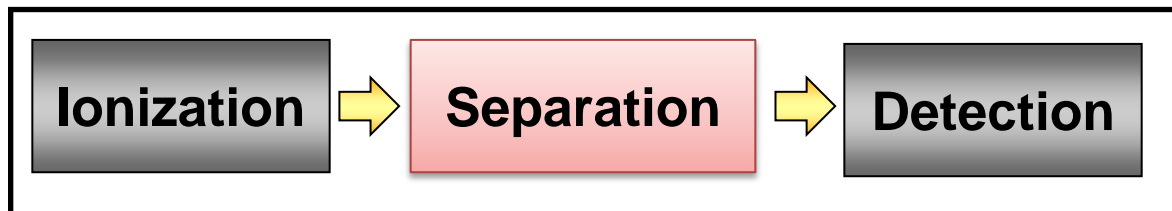


Triple Quadrupole GCMS

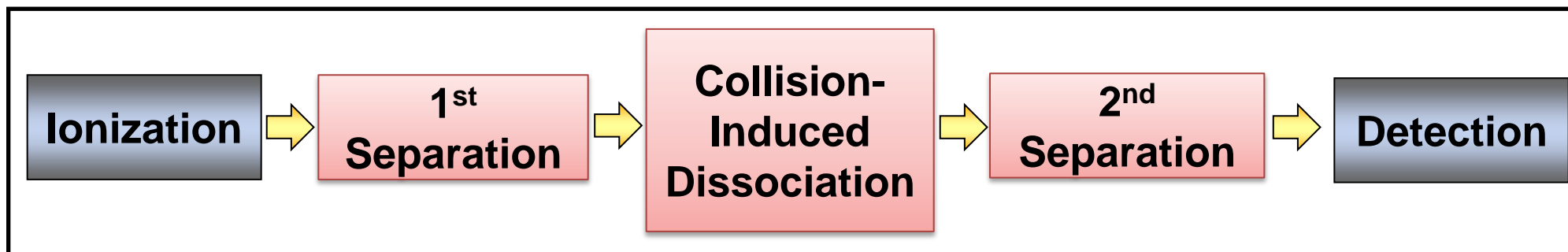


Tandem Mass Spectrometry

Mass Spectrometry (MS)



Tandem Mass Spectrometry (MS/MS)

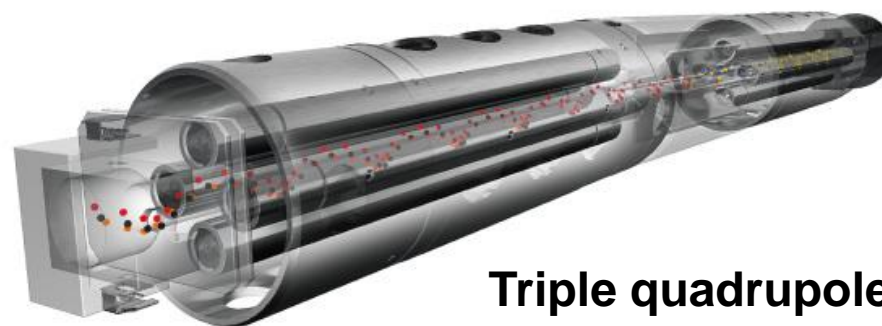


- **Tandem MS** refers to MS/MS system that use the same mass analyzers (e.g. Triple Quadrupole).
- **Hybrid MS** refers to MS/MS system with different MS system (e.g. Quadrupole-TOF)

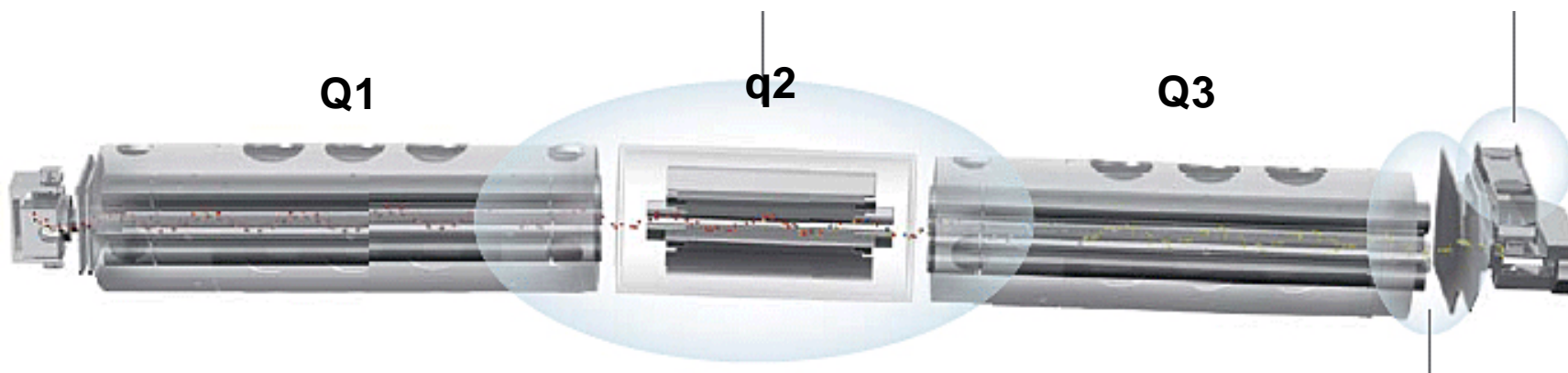
Single quadrupole vs Triple quadrupole



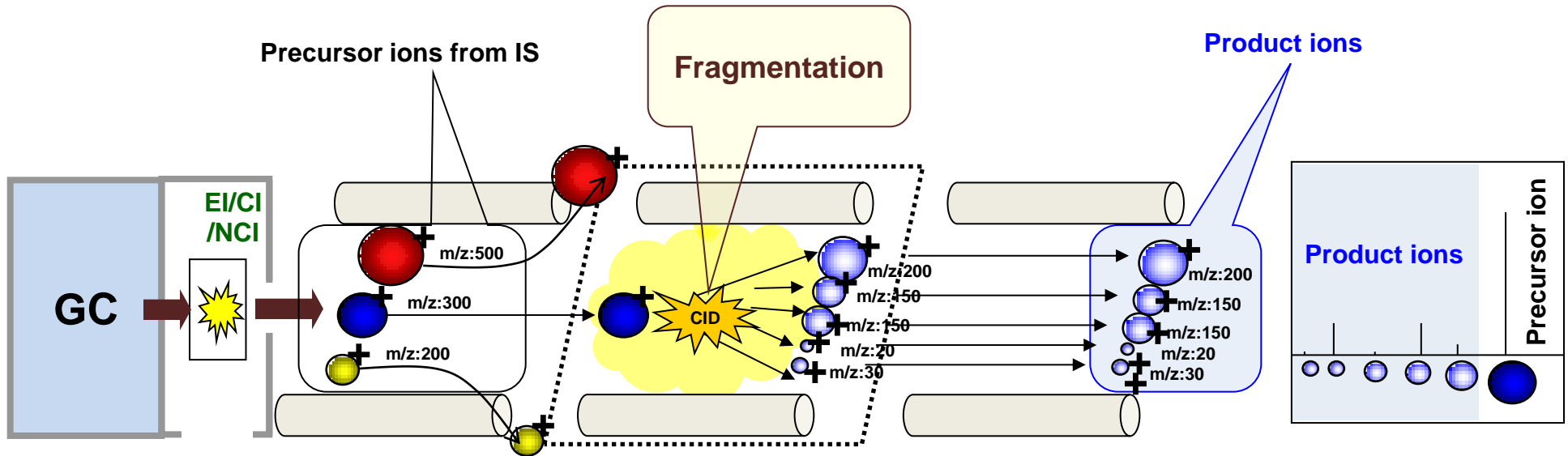
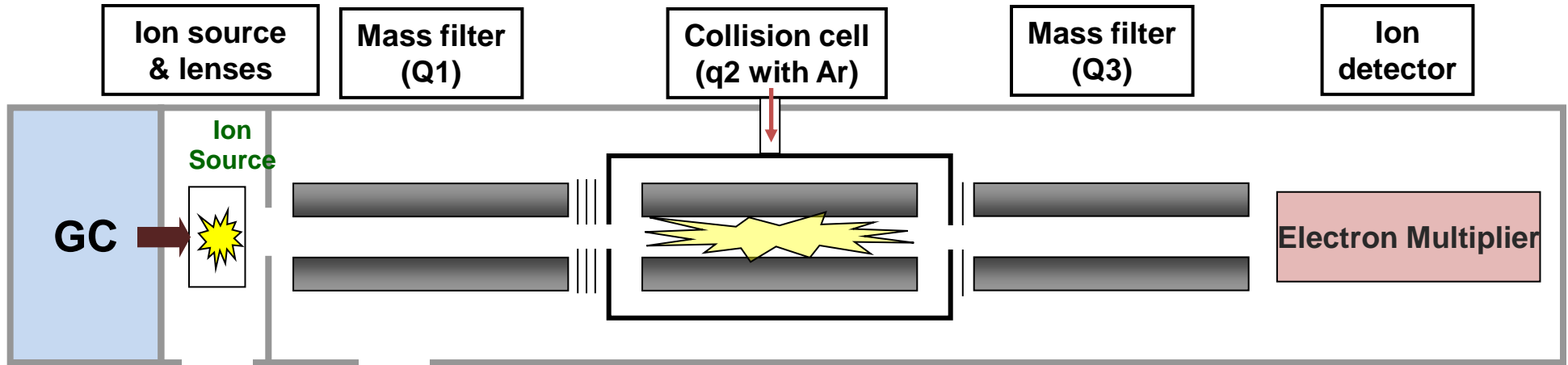
Single quadrupole



Triple quadrupole

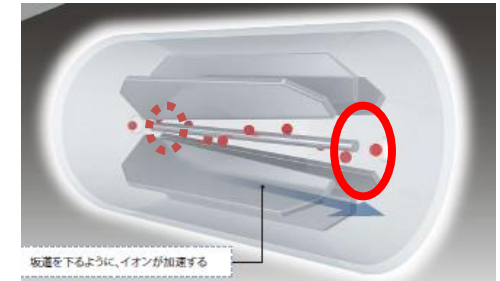


Terminology in GC-MS/MS

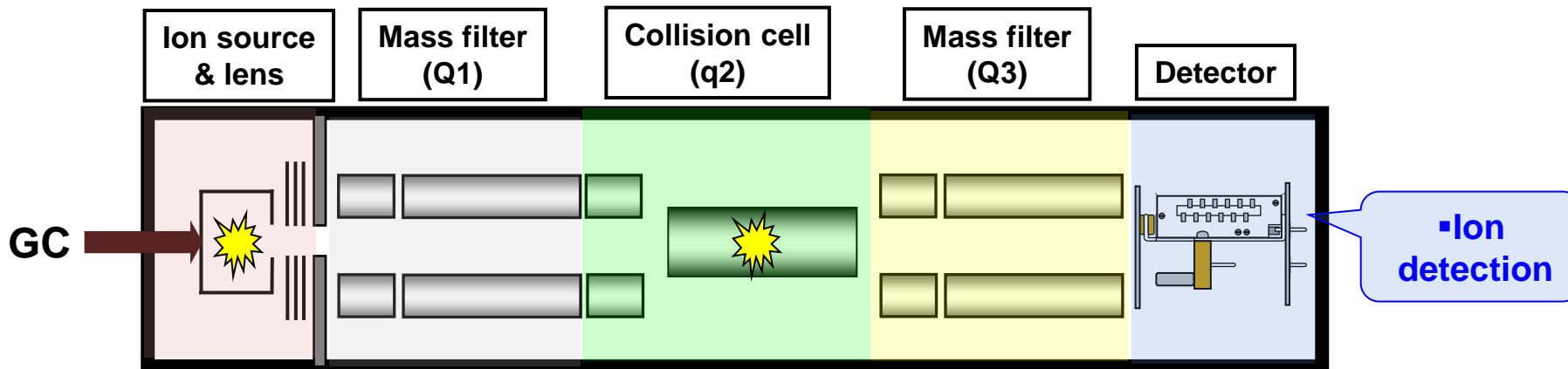


Collision Cell (q2)

- Located between Q1 and Q3
 - Collision-induced dissociation (CID) of ions take place in CC
 - Ions are accelerated with sufficient kinetic energy in CC and collide with the inert gas molecules (i.e. Ar atoms)
 - Collision-induced dissociation
 - Kinetic energy supplied = Collision Energy (CE)
- Functions of CC
 - Accelerate ions to lead CID
 - Ensure that fragment ions produced are not lost
 - Sweep remaining ions out
- Optimum CE is specific to each precursor ion
 - To obtain good intensity of highly selective product ion fragments for sensitive quantification in MRM mode.



Analysis Modes of GC-MS/MS

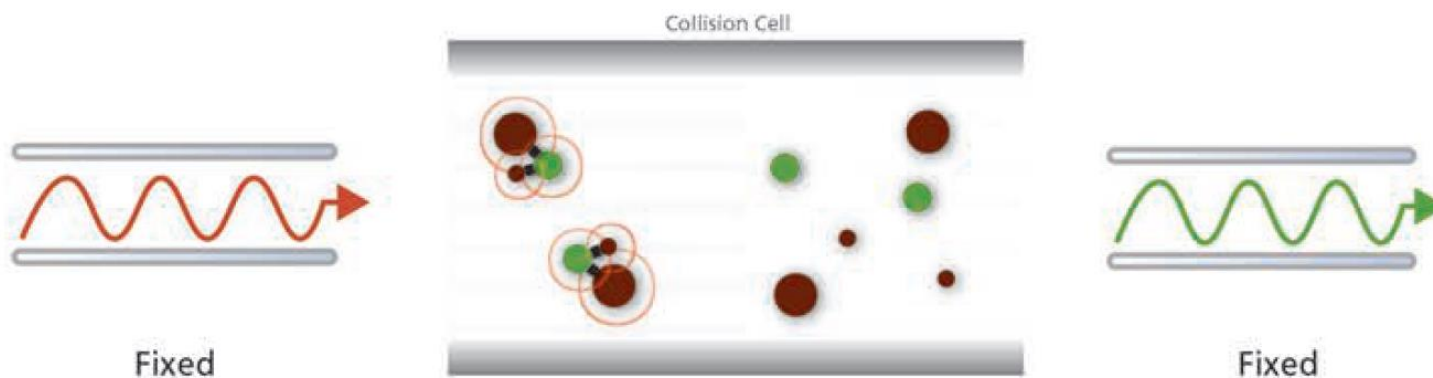
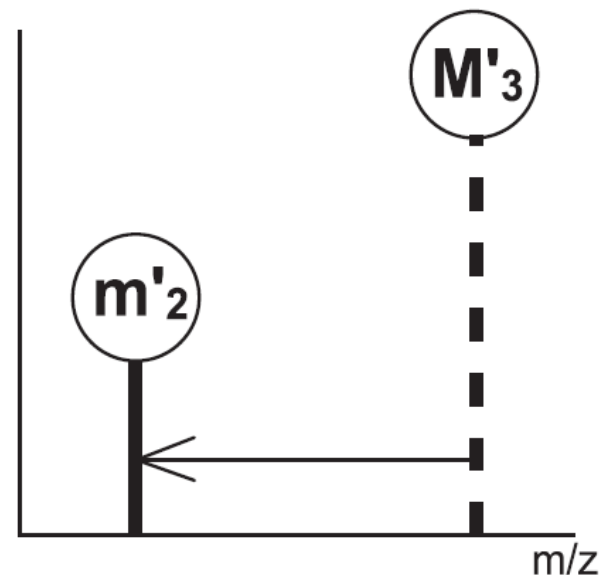


Acquisition mode	Q1	q2 (CC)	Q3	Analysis
Q1 Scan	Scan	Through	Through	Qualitative
Q3 Scan	Through	Through	Scan	Qualitative
Q1 SIM	SIM	Through	Through	Quantitative
Q3 SIM	Through	Through	SIM	Quantitative
Product Ion Scan	SIM	Selected ions fragmented	Scan	Qualitative
Precursor Ion Scan	Scan	All ions fragmented	SIM	Qualitative
MRM	SIM	Selected ions fragmented	SIM	Quantitative
Neutral Loss Scan	Scan	All ion fragmented	Scan	Qualitative
FASST	Through	Through	Scan	Qualitative
(Simultaneous Acquisition of Scan/MRM)	SIM	Selected ions are fragmented	SIM	Quantitative

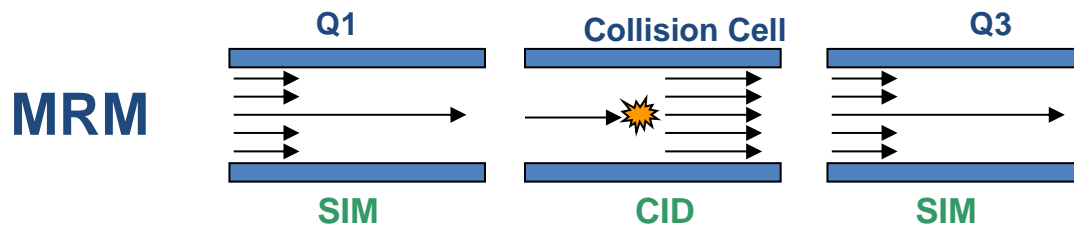
- CID gas **ON** → for all acquisition modes
- CID gas **OFF** → only Q3 Scan, Q3 SIM and FASST (Q3 Scan/Q3 SIM) are available

MRM; Multiple Reaction Monitoring

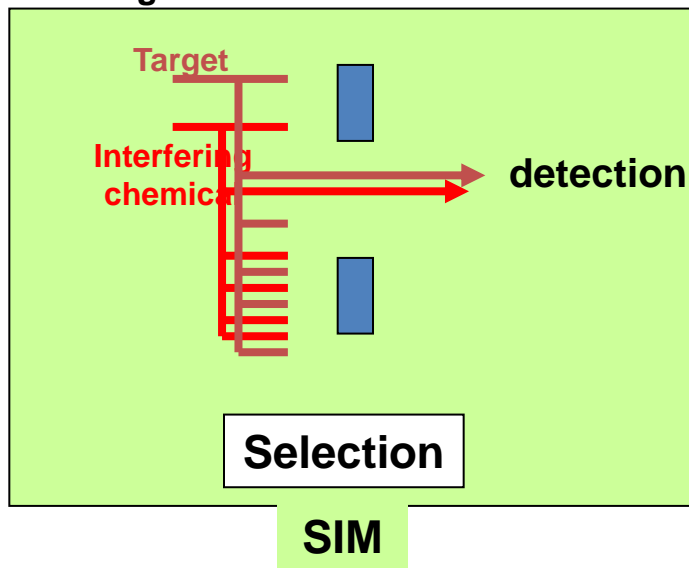
- The analysis method in this mode involves fixing both Q1 and Q3 to a specific m/z and selectively analyzing ions.
- Product ions, which are generated in CID (Collision-induced dissociation) and subsequently selected in Q3, contain structural information of precursor ions.



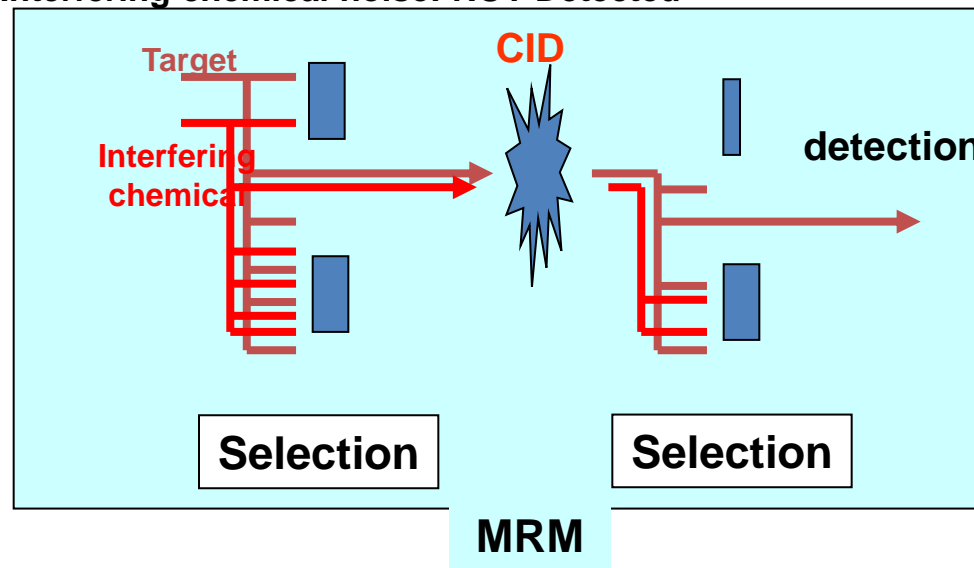
MRM Mode



Interfering chemical noise: Detected

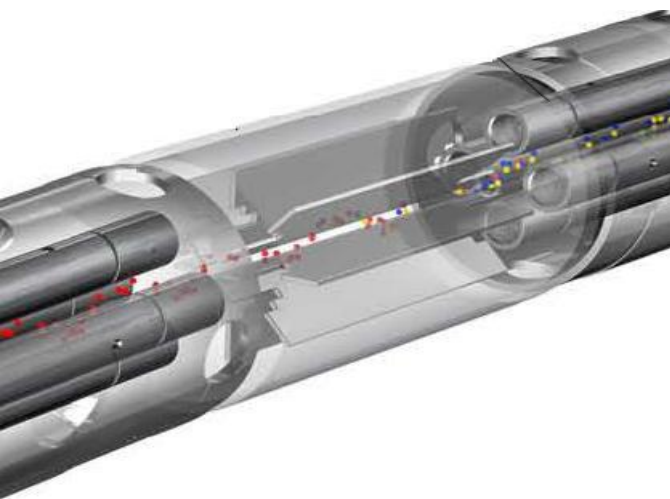


Interfering chemical noise: NOT Detected

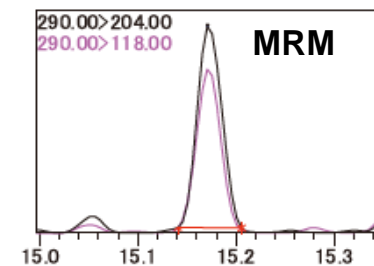
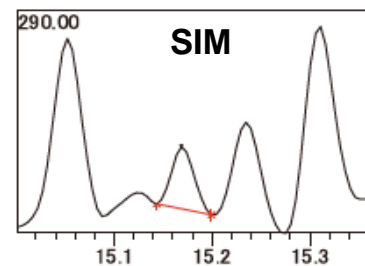


MRM Mode (VS SIM Mode)

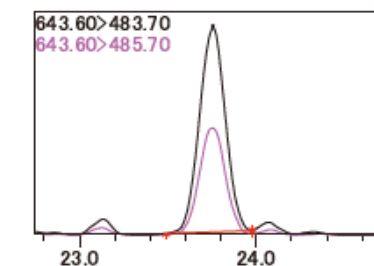
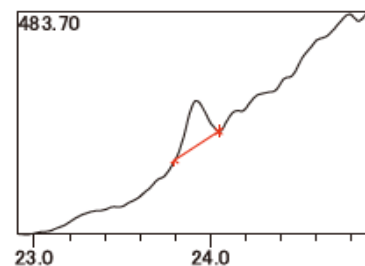
MRM mode provides Enhanced selectivity



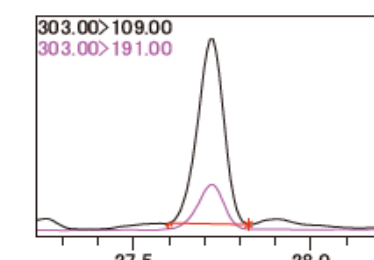
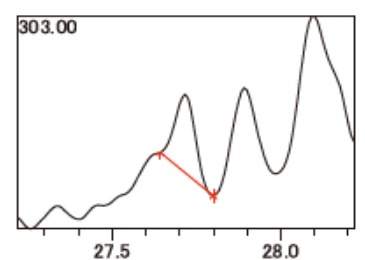
Detection of trace components in high matrix samples



Foods: Analysis of residual pesticides (1 ppb isoprothiolane) in ginger



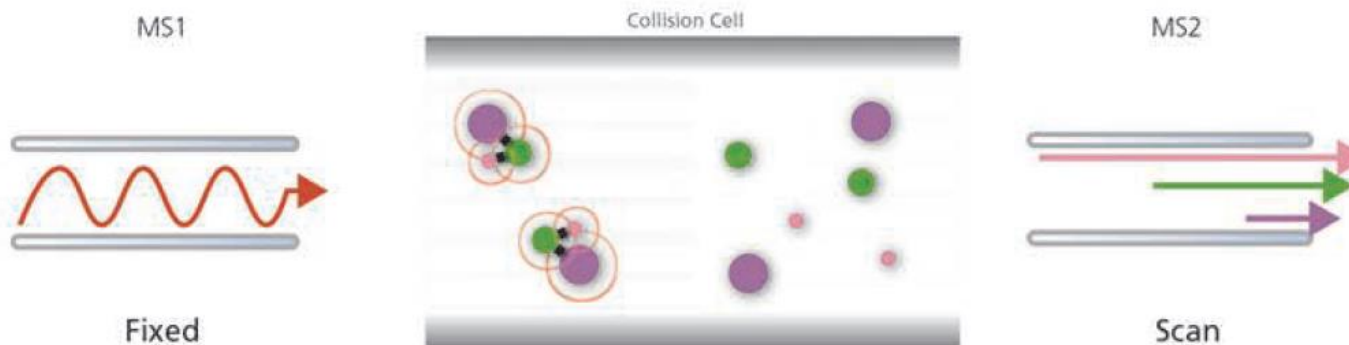
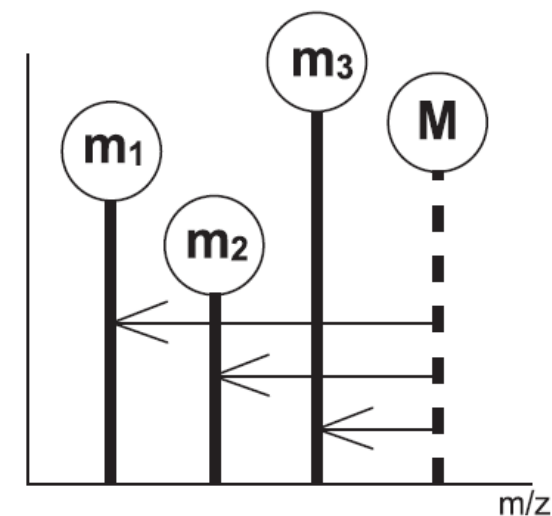
Environment: Analysis of PBDEs (hexa-BDE/BDE-153) in sediment



Life Sciences: Analysis of metabolites (suberic acid) in rat urine

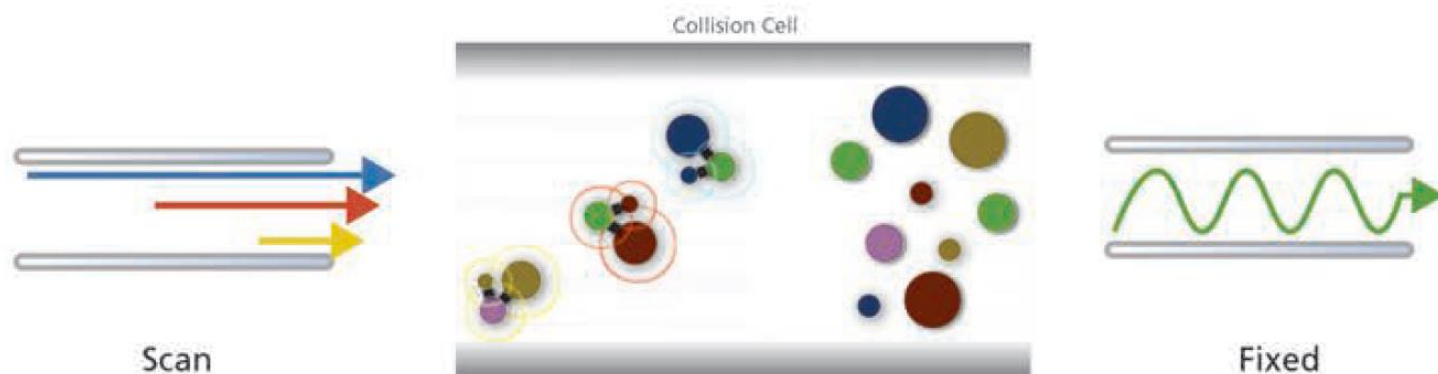
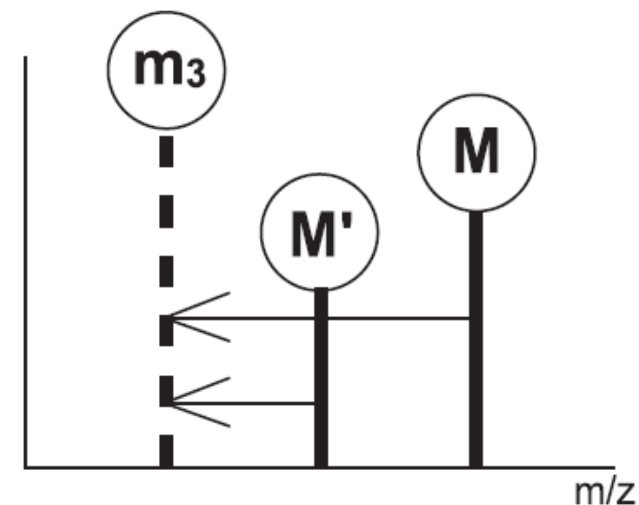
Product Ion Scan

- **Precursor ions are selected** in Q1 and sent to the collision cell.
- These ions collided with argon or other inert gas molecules in the collision cell to cause fragmentation by CID
- Generated product ions are scanned in Q3 to detect and record the signal.
- With a controlled analytical condition, product ion mass spectrum could serve as the finger print data for qualitative study of the substructures.



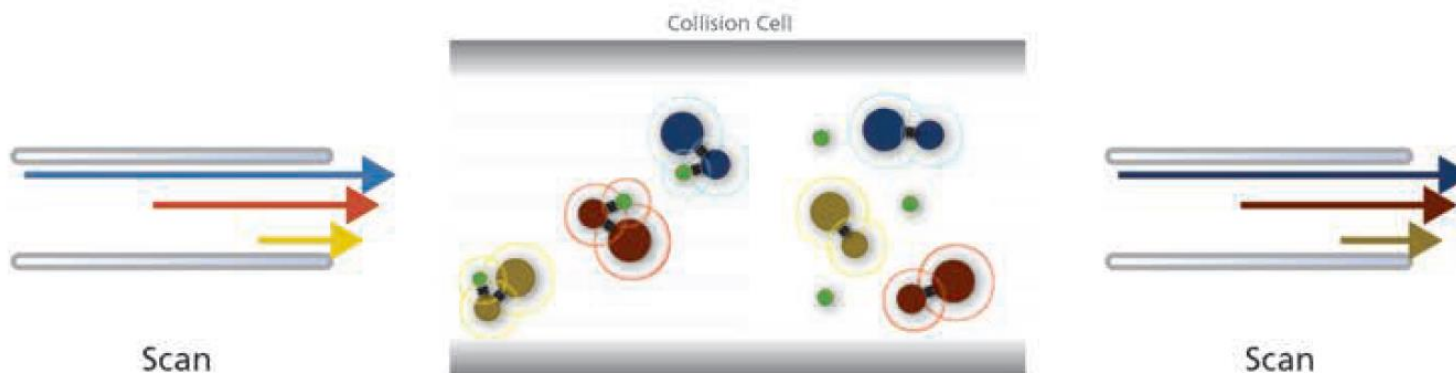
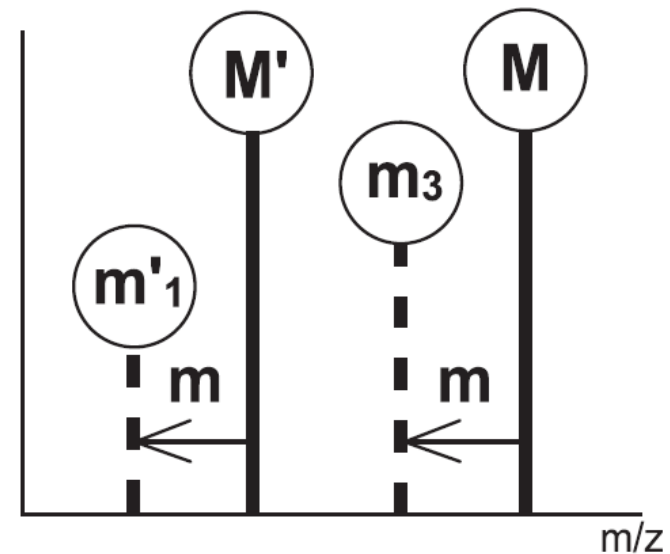
Precursor Ion Scan

- This acquisition mode involves performing scanning in Q1, fixing Q3 to a specific m/z , and selectively detects the **selected product ions with Q3 SIM**. Subsequently, track and record the precursor ions in Q1 Scan.
- This allows the examination of precursor ions with common product ions .
- For screening molecules with common substructures.

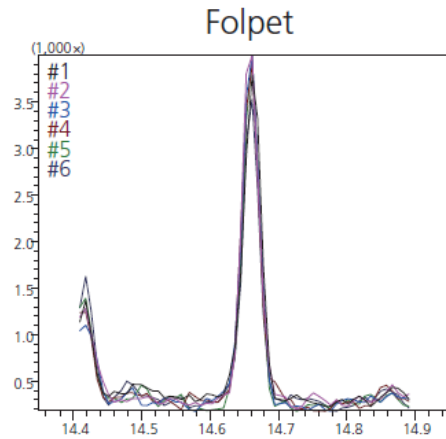


Neutral Loss Scan

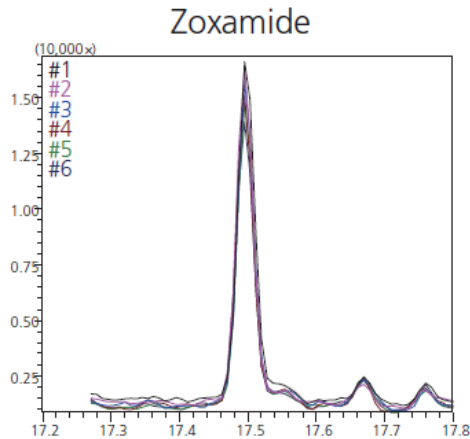
- Performing **simultaneously Q1 scan and Q3 scan** by tracking the m/z difference constant between the two mass filters. Record the precursors with specific NL in Q1 Scan.
- The constant difference of m/z between precursor and production pair is the lost of neutral fragment from the precursor ion.
- This allows the screening of precursor ions with common neutral fragments detached by CID.
- Suitable for screening molecules with common substructures.



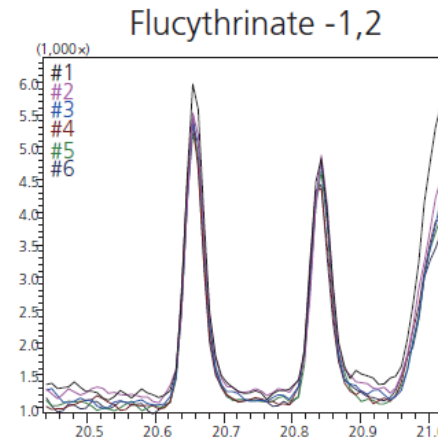
Smart MRM



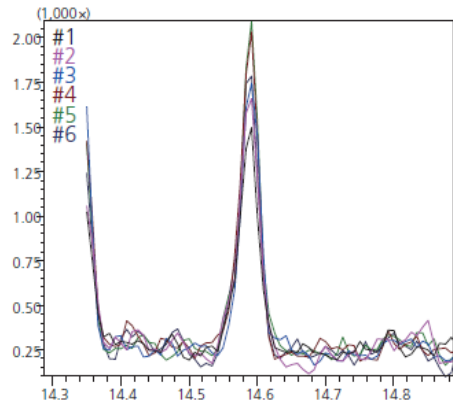
%RSD = 8.3%
S/N = 35.6



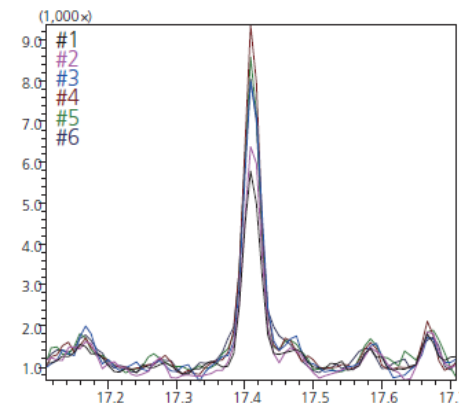
%RSD = 5.9%
S/N = 66.2



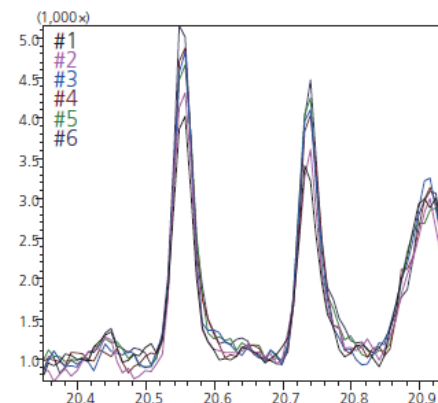
%RSD = 6.0, 4.8%
S/N = 34.2, 25.8



%RSD = 15.2%
S/N = 16.0



%RSD = 24.0%
S/N = 21.0



%RSD = 9.1, 11.3%
S/N = 16.1, 11.3

- #1 Chlorpyrifos
- #2 Ethionazin
- #3 Dichlorfenant metololite
- #4 Fipronil
- #5 Flusulfon metololite
- #6 Dorsotophos
- #7 Triketazin
- #8 2,6-Dichlorbenzamid
- #9 Benflacarb
- #10 Dorsobenzofos
- #11 Benfluralin
- #12 Monocrotophos
- #13 Sulfotep
- #14 Carbofent
- #15 Dialeto-1
- #16 Phorate
- #17 alpha-HCH
- #18 Dialeto-2
- #19 Desmediphan deg
- #20 Thiometon
- #21 Hexachlorbenzene
- #22 Dieldrin
- #23 Dieldrin
- #24 Simazine

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- #3 Dichlorfenant metololite
- #4 Fipronil
- #5 Flusulfon metololite
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THANKS YOU

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