Mass Spectrometer Scan Types

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Types of Mass Spectrometer scans

Full Scan MS Q1 & Q3	Qualitative scan
Single ion Monitoring	Selective quantitative scan
Full Scan Product ion	Structural scan
Selected Reaction monitoring (SRM) and (MRM)	Quantitative target analyte scan
Precursor ion	Screening scan
Neutral loss	Screening scan
Data Dependent MS/MS scans from Full scan MS Neutral loss Precursor ion	Intelligent structural and screening scans

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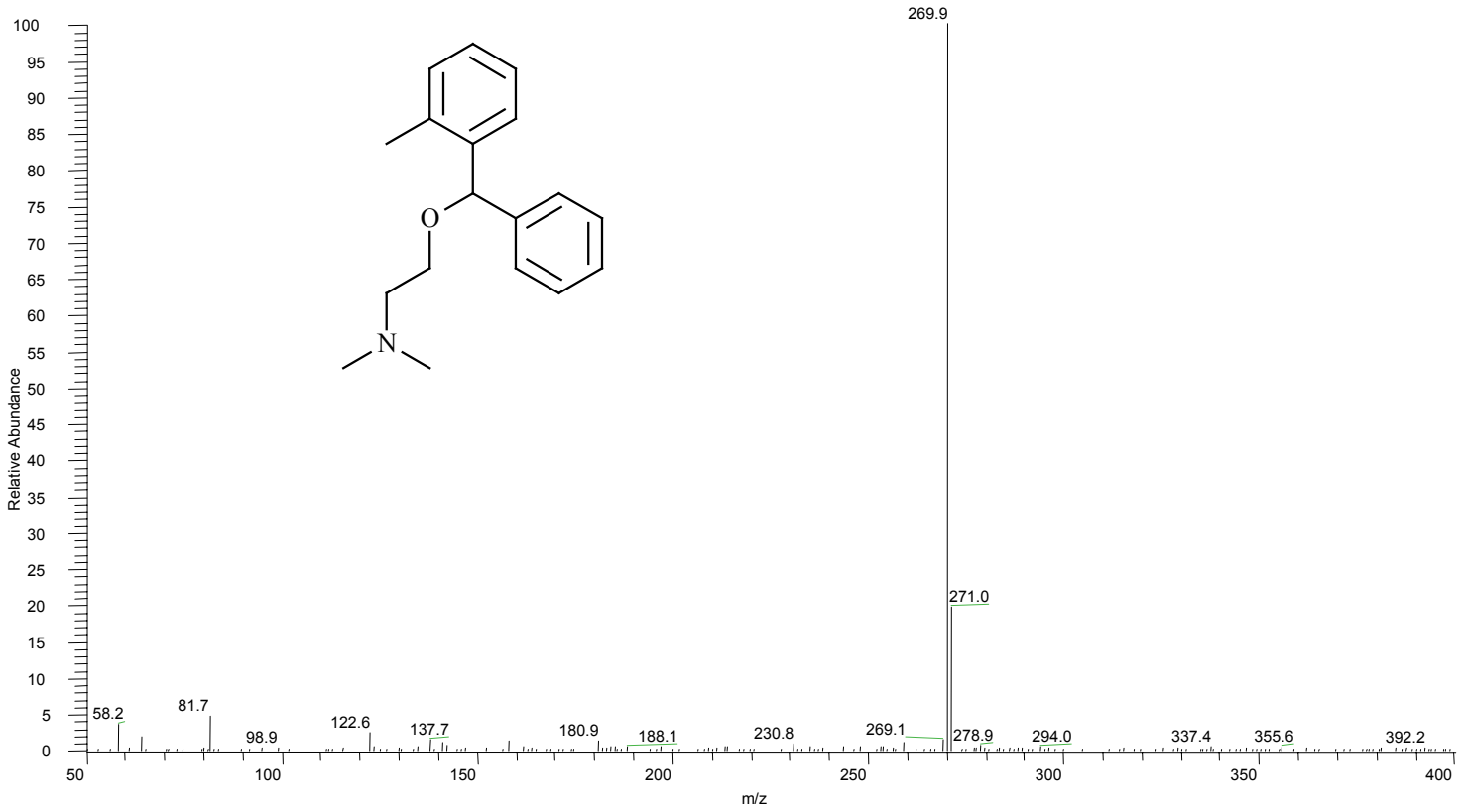
Full Scan MS of Orphenadrine

Scanning between 50 and 400 amu shows the molecular ion of Orphenadrine at m/z 269 – qualitative identification



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Single Ion Monitoring

Single (or Selected) Ion Monitoring (SIM) is used as a quantitative scan whereby the molecular ion of the analyte is monitored in a narrow amu window.

Eg Orphenadrine may be monitored at 269.9 +/- 0.3 amu (269.6 to 270.2)

Other analytes or an internal standard may be monitored in sequential scans.

SIM gives more sensitivity and better selectivity than monitoring Orphenadrine in full scan MS.

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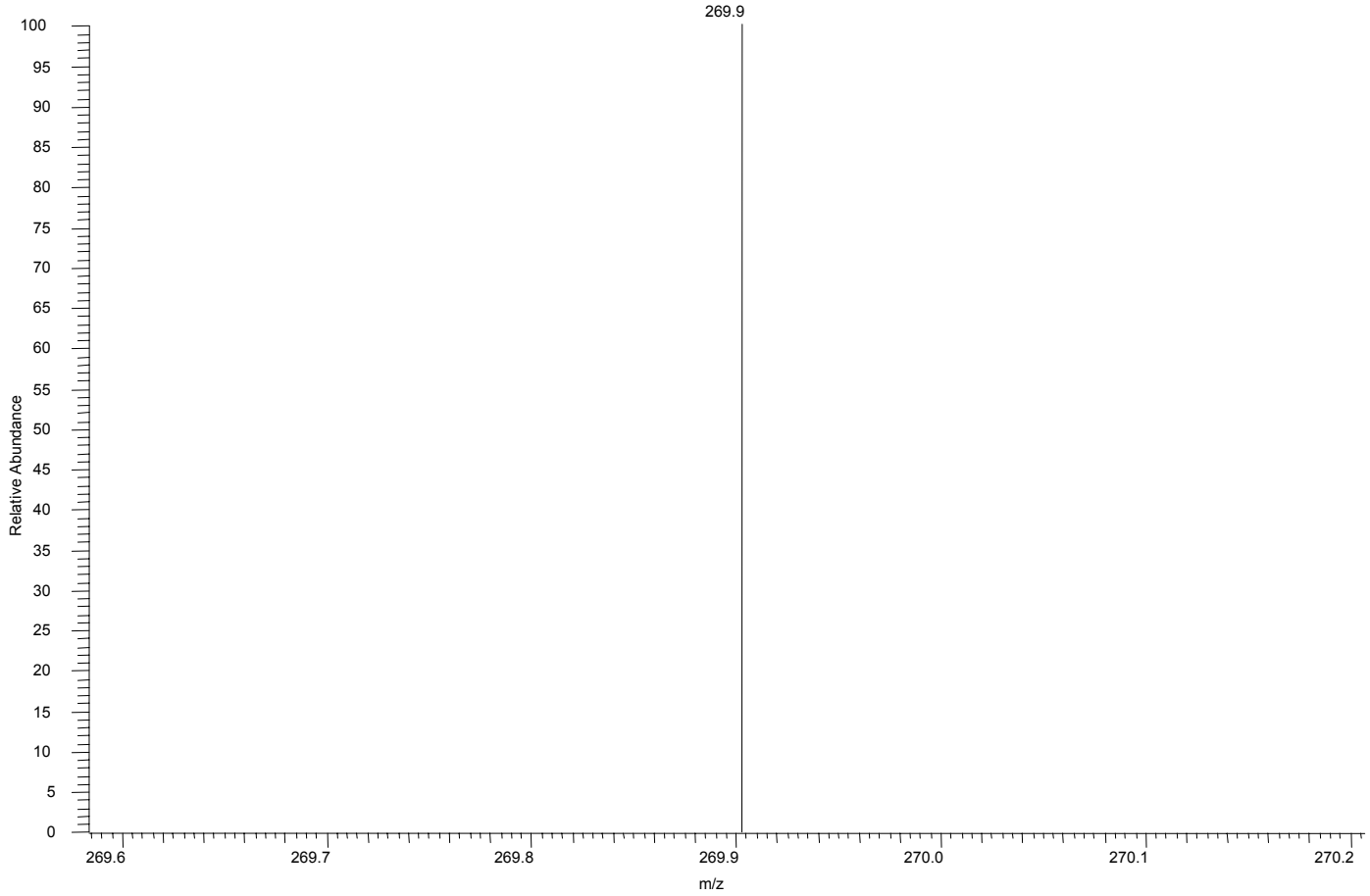
SIM of Orphenadrine

Orphenadrine monitored at 269.9 +/- 0.3 amu (269.6 to 270.2)



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Product ion scans

There are two types of product ion scans :

- Full Scan Product ion are used for qualitative applications to obtain structural information.
- Selected Reaction Monitoring Product ion scans are used for Quantitative target analysis

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What are product ion scans ?

- Product ion scans also know as daughter ion scans
- Q1 is set to allow only the transmission of one m/z
- The parent ion collides with Argon gas in Q2 to create fragment or product ions
- Product ions are scanned through Q3

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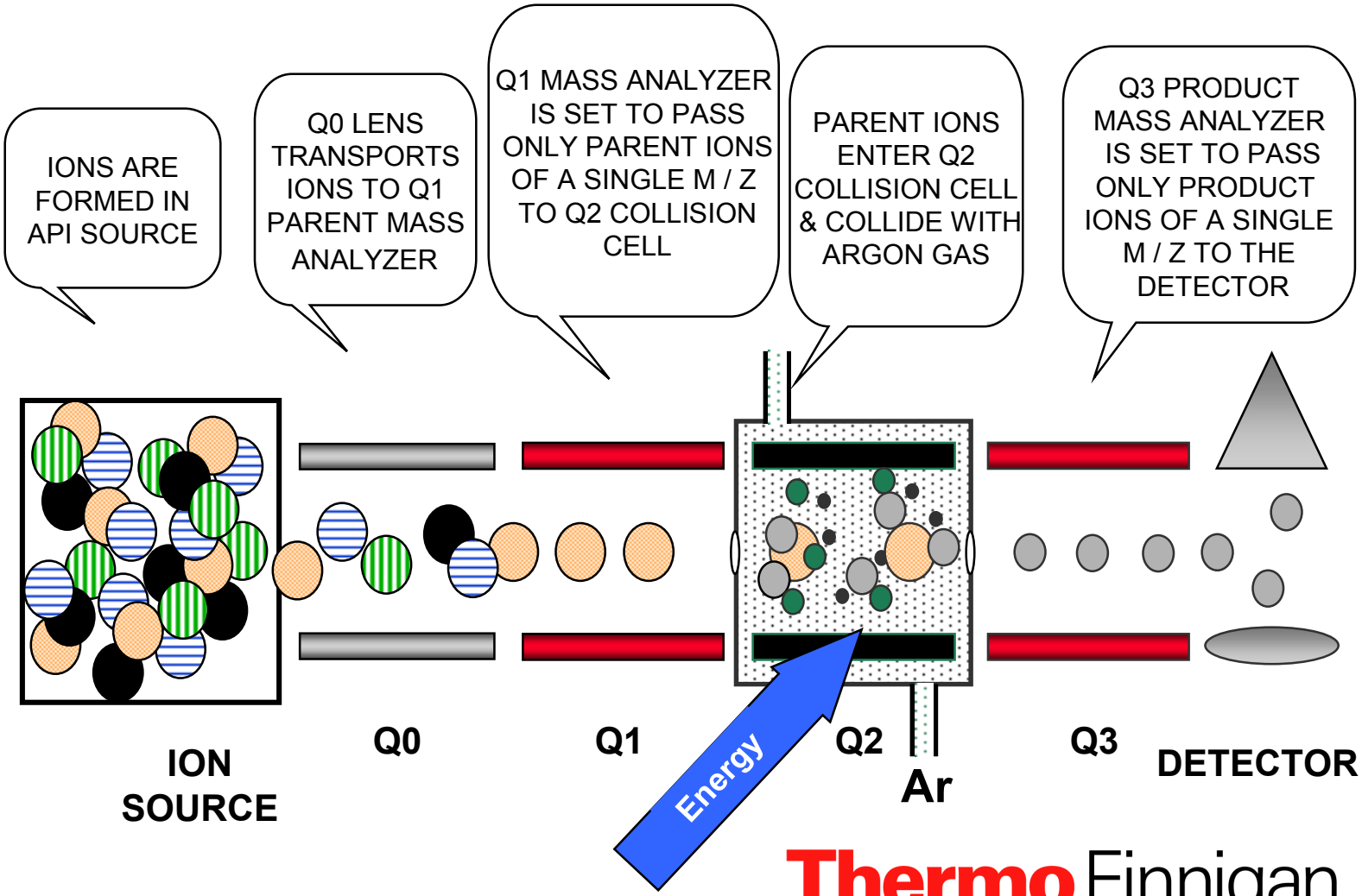
TSQ MS/MS SRM Product Ion Scan



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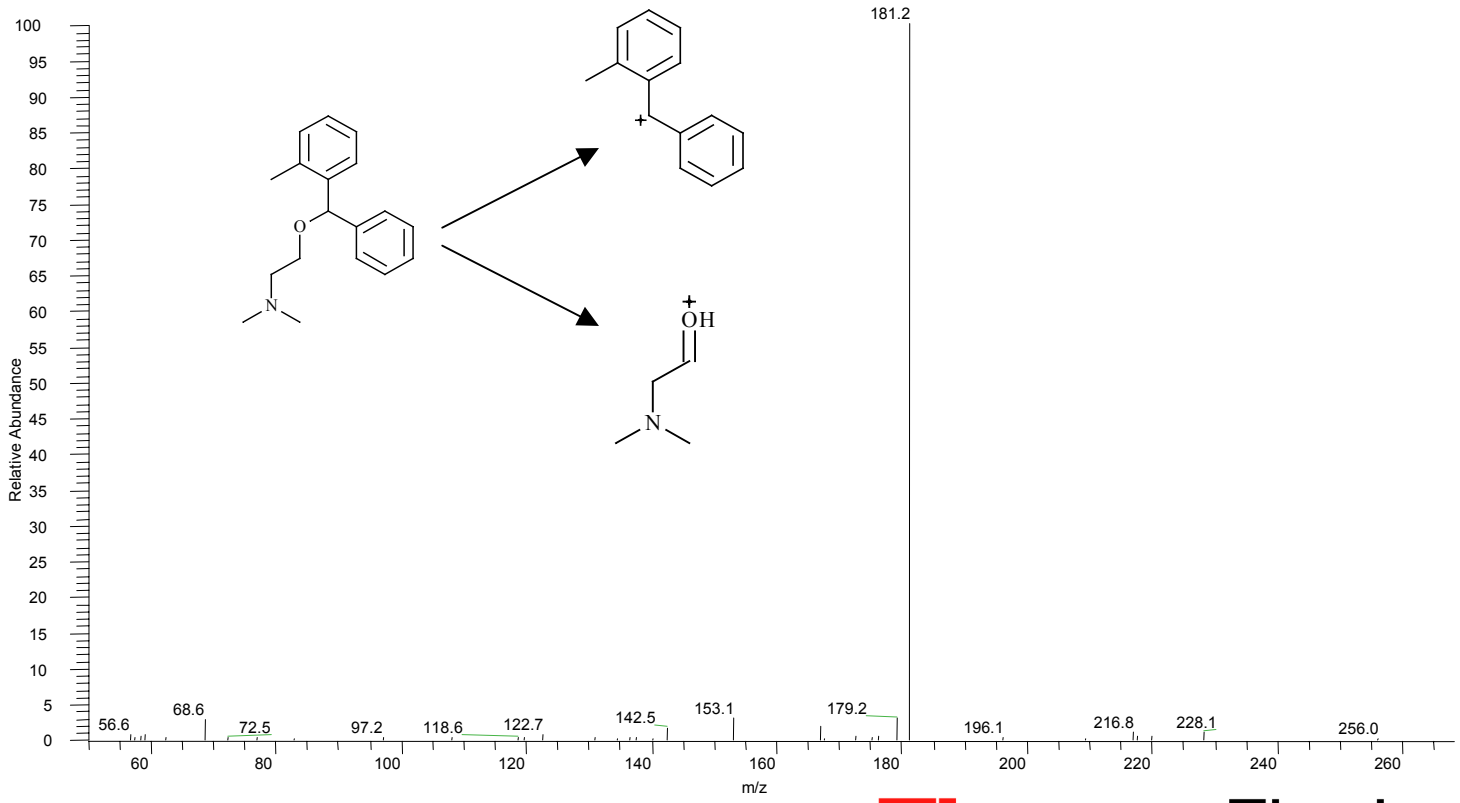
Full Scan Product Ion

Q1 is set to allow only the transmission of Orphenadrine m/z 269

Q3 is scanned between 50 to 268 amu - qualitative information



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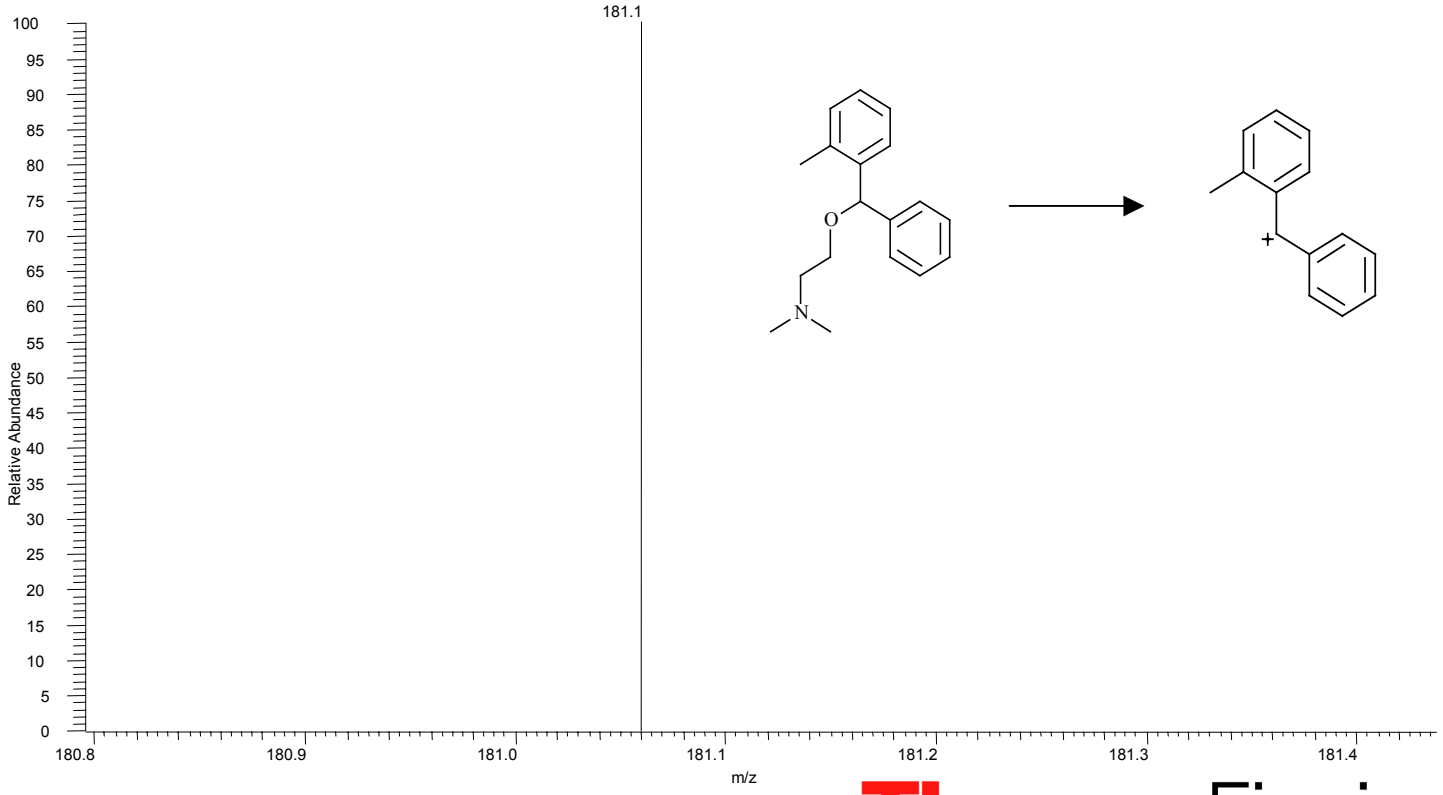
SRM Product Ion Scan

Q1 is set to allow only the transmission of Orphenadrine m/z 269.9

Q3 is scanned only to detect m/z 181.1 +/- 0.3

SRM provides best selectivity and signal to noise ratio for quantitation



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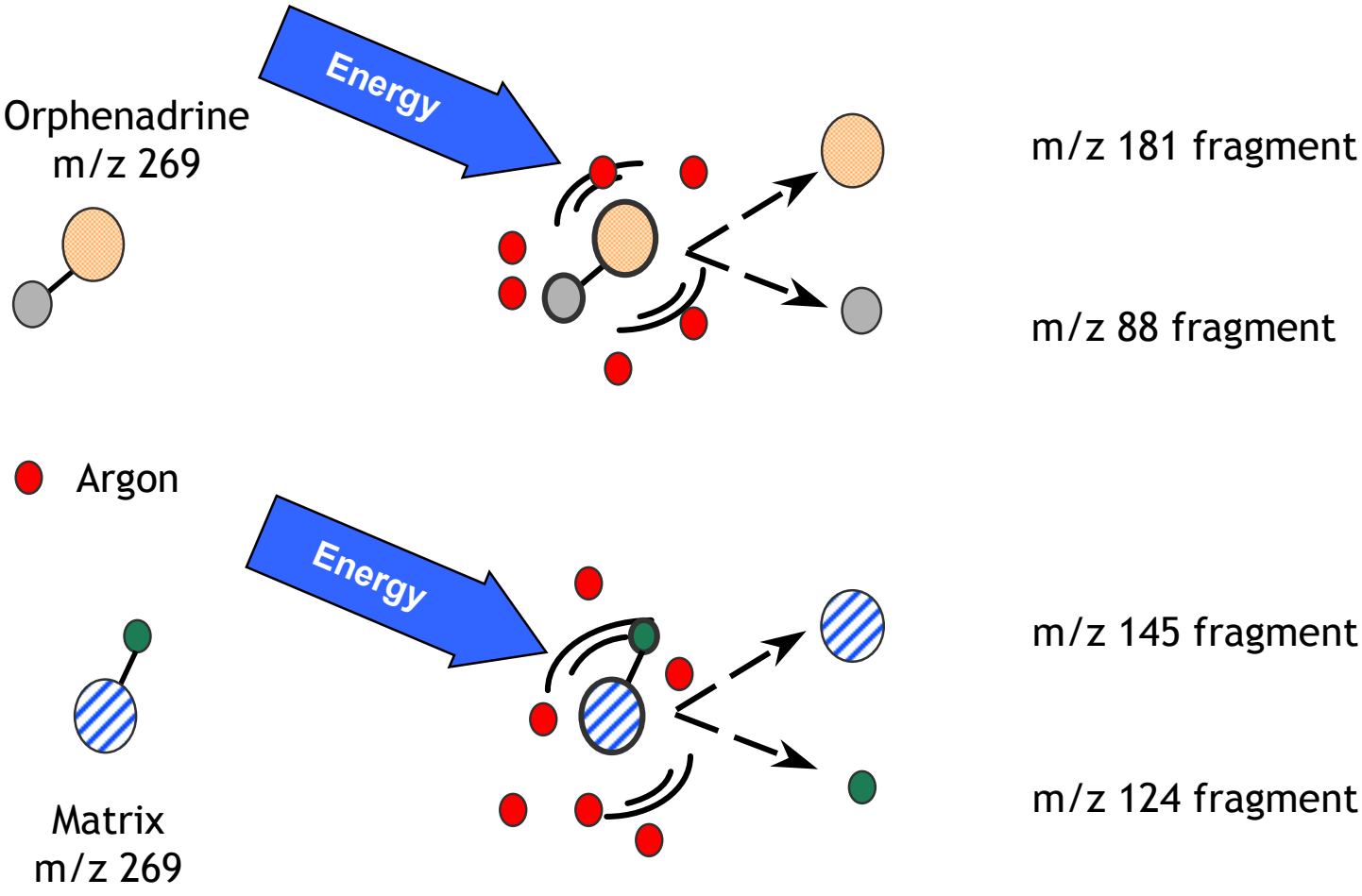
The Selectivity of SRM



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What are precursor ion scans ?

- Precursor ion scans also known as parent ion scans
- Q3 is set to allow only a fragment ion of one m/z to pass
- Q1 is scanned
- The precursor ions collide with Argon gas in Q2 to create fragment or product ions
- Only those compounds which give that specific fragment ion are detected

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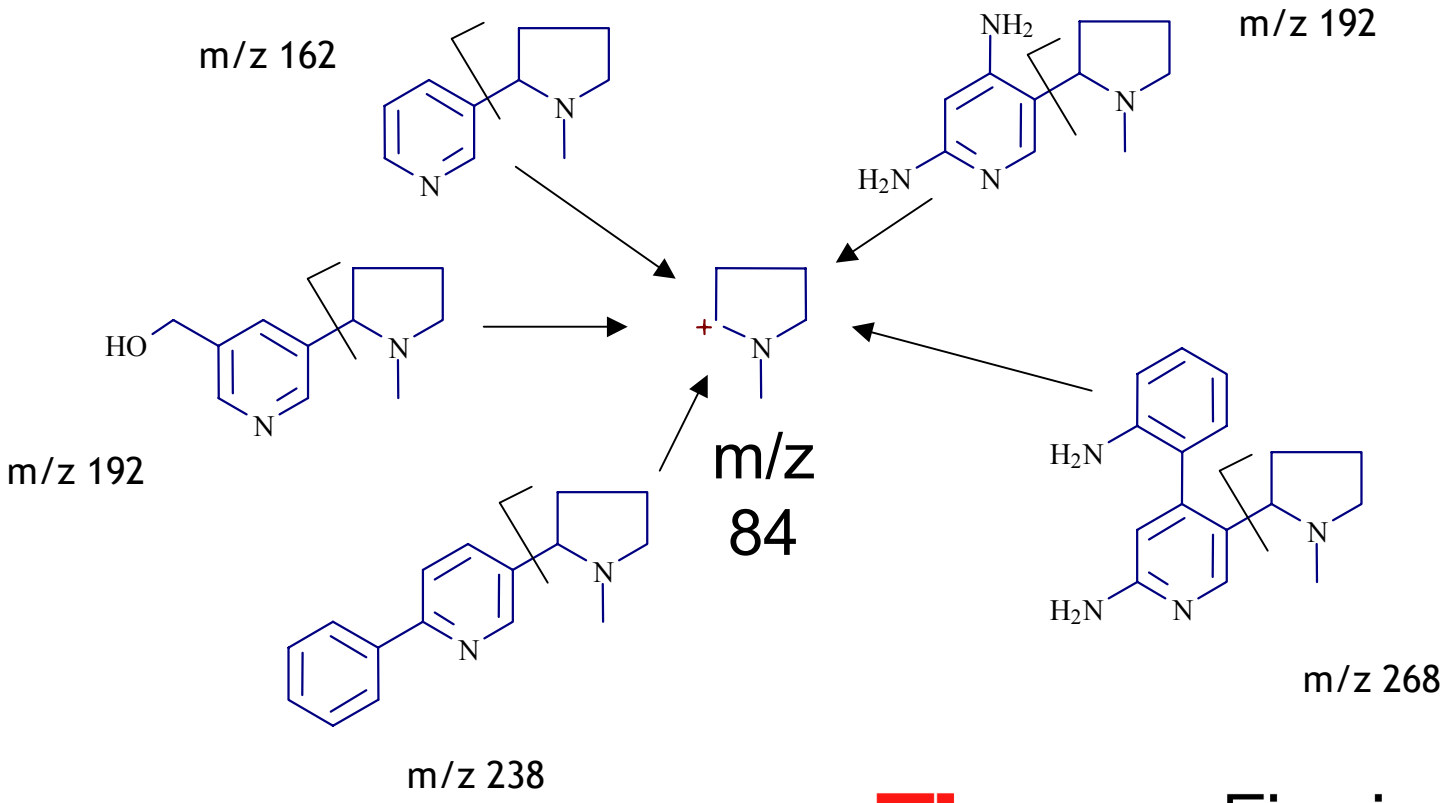
Precursor ion scans

Precursor ion scans are used for screening experiments where a group of compounds all give the same fragment ion



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What are neutral loss scans ?

- Both Q1 and Q3 are scanned together
- Q3 is offset by the neutral loss under investigation
- The precursor ions collide with Argon gas in Q2 to create fragment ions
- Only those compounds which give a fragment having that specific loss are detected

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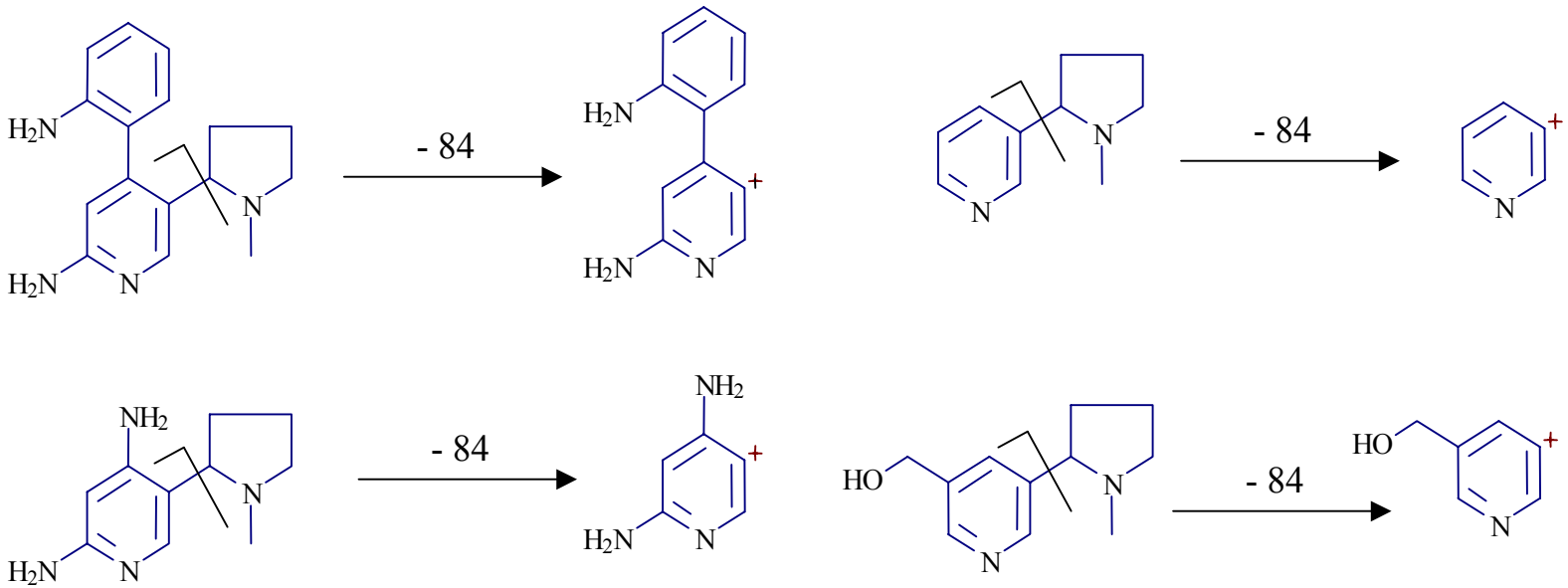
Neutral loss scans

Neutral loss scans are used for screening experiments where a group of compounds all give the same loss



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Data Dependent Experiments

- Ion Traps can run MS and data dependent product ion scans

- TSQ has three different data dependent modes
  - Full scan MS triggered
  - Neutral loss triggered
  - Precursor ion triggered

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TSQ Data Dependent Experiments

- In Full Scan MS data dependency the most intense ion above a preset signal threshold value eluting from the column is selected in Q1. This ion is fragmented in Q2 and scanned in Q3 in full scan MS/MS mode.

- In precursor ion data dependency a precursor ion is selected in Q3 and Q1 is scanned. When a fragmentation occurs which results in a precursor ion formation above a preset signal threshold then full scan MS/MS is performed on the parent.

- In Neutral loss data dependency Q1 and Q3 are set to detect the neutral loss of a specific mass. When a neutral loss occurs above a preset signal threshold then full scan MS/MS is performed on the parent ion.

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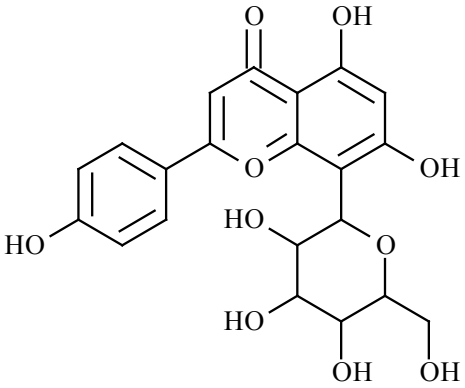
Flavonoid Data Dependent Examples

- Flavonoid aglycones can be identified by a m/z 153 product fragment ion

- Glycosylated flavonoids can be identified by a neutral loss of m/z 162
  - This equates to the loss of a hexose sugar unit



Apigenin glycoside

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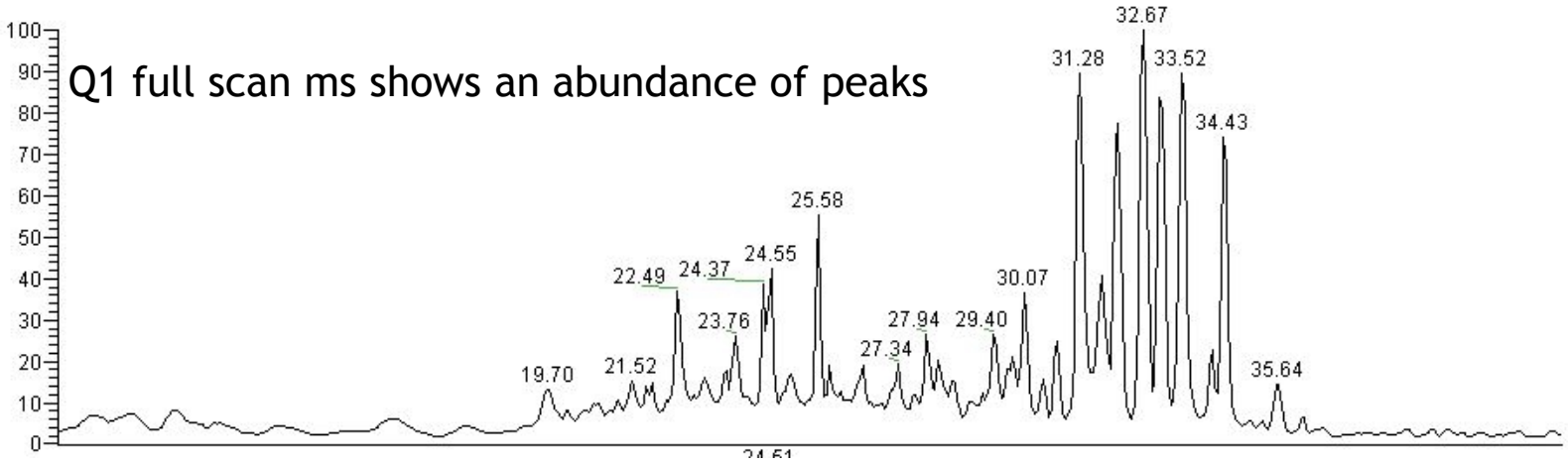
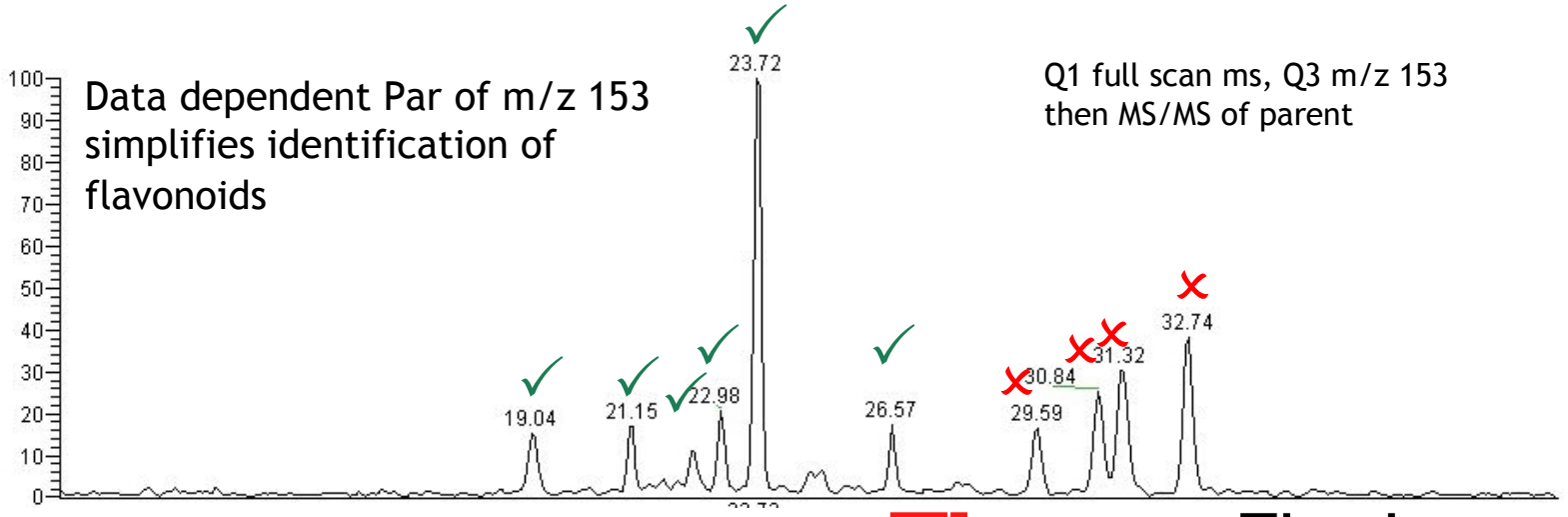
Flavonoids from Orange extracts





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Methods of MS/MS in TSQ

Q1	Collision Cell	Q3	Result
Fixed	Gas	Scanned	Product Ion
Scanned	Gas	Fixed	Parent Ion
Scanned	Gas	Scanned	Neutral Loss
Fixed m/z	Gas	Fixed m/z	SRM

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