ACQUITY QDa Detector – Starting Point Settings and Optimization Guidelines

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This quick reference card is intended to provide recommendations for successful use of the ACQUITY QDa Detector. Conditions are described that are reasonable starting points for most methods. Additional tips are included to assist in optimizing a method further. Please also consult Waters literature "Mass Data Terminology, Considerations, and Interpretation" (Document number 715004945).

SOLVENTS AND BUFFERS

- Refer to the newest version of the *ACQUITY QDa Detector Overview and Maintenance Guide* on the Waters website (Document number 715003956) for a list of tested solvents.
- Non-volatile buffers such as phosphate are not recommended for use with the QDa, even at levels lower than 1 mM. These components lead to reduced sensitivity and can foul the source.
- High purity solvents are recommended for best performance.

FLOW RATE

- The optimum performance plateau for flow rate into the QDa is between 0.3 and 0.8 mL/min.
- The upper flow rate limit is 2 mL/min.
- Flow rates less than 0.3 mL/min, require evaluation (see Capillary Voltage and Probe Temperature sections).
- Less than 0.2 mL/min is not recommended.

CONE VOLTAGE

- Do not assume that the cone voltage value from another instrument will be appropriate for QDa.
- Start at 15 V in positive mode and 30 V in negative mode.
- When optimizing for increased sensitivity, test higher and lower cone voltages:
  - Increase in 3 V steps. Note that the signal might be reduced because of in-source fragmentation.
  - Decrease in 2 V steps. Note that the signal might be reduced because of reduced ion transfer.
- In some experiments, a higher cone voltage is deliberately used to create fragment ions characteristic of the analyte. Use twice the optimum cone voltage for your analyte of interest as a starting point.

CAPILLARY VOLTAGE

- For positive ionization, use 0.8 kV for most flow rates.
  - For flow rates near 0.3 mL/min or isocratic mobile phases above 80% organic, increase to 1.5 kV.
- For negative ionization use 0.8 kV at all flow rates.

PROBE TEMPERATURE

- Set the probe temperature to 600°C for flow rates greater than 0.3 mL/min.
- Set the probe temperature to 300°C when the flow rate is less than 0.3 mL/min.

PURIFICATION SYSTEMS

- For the make-up flow composition of LC prep systems (typically 0.5 mL/min into the QDa):

Compound types	Mobile phase composition	Capillary voltage	Probe temperature
Most compounds	50% water : 50% acetonitrile + 0.01% formic acid	0.8 kV	500°C
Early eluting polar compounds	90% water : 10% acetonitrile + 0.01% formic acid	0.8 kV	600°C

- For the make-up flow composition for SFC prep systems (typically 0.4 to 0.7 mL/min into the QDa), use 85% methanol : 15% water + 0.1% formic acid. Set the capillary voltage to 1.5 kV, and probe temperature to 600°C.

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ISOCRATIC SOLVENT MANAGER / SPLIT AND DILUTE SYSTEM

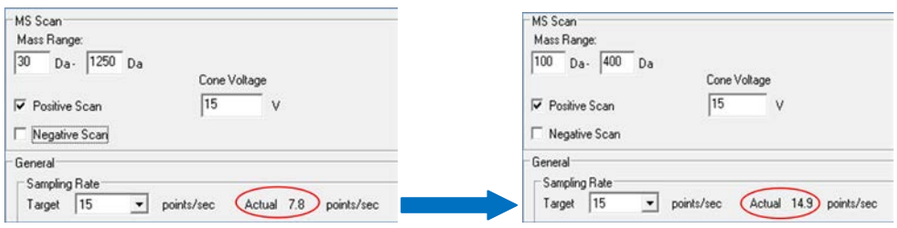
- A typical composition of make-up solvent is 90% water : 10% acetonitrile + 0.01% formic acid.
  - Other make-up solvents and additives can provide improved signal-to-noise ratio for particular analytes.
  - The split ratio will change if alternative make-up solvents with differing viscosities are used. Consult the *Isocratic Solvent Manager Overview and Maintenance Guide* (Document number 715004208).
- Start with the restrictor module number 5 or 10 and select a larger restrictor number to align the detector range, if necessary. Higher number restrictors reduce signal intensity but also increase peak broadening and retention time offset.
- Flow rate considerations:
  - Increasing make-up flow with respect to LC eluent flow reduces the proportion of sample transferred, which results in reduced QDa signal.
  - Decreasing make-up flow with respect to LC eluent flow increases the proportion of sample transferred, which results in increased QDa signal.

SAMPLING RATE

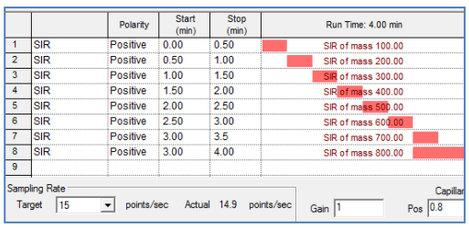
- For quantitative analysis, set sampling rate to achieve 12-15 points per peak (for example, 5 points/sec for a 3 second peak).
- For qualitative analysis, set the sampling rate to achieve 8-10 points per peak.
- The software automatically calculates the maximum possible sampling rate of an experiment based upon the number and type of functions, as well as the mass range for any MS scan. If the desired sampling rate for that type of experiment cannot be reached, an Actual sampling rate lower than the Target sampling rate appears.

To increase the achievable Actual sampling rate for an experiment:

- Set a reduced mass range specific to the analytes of interest:



- Reduce the number of overlapping functions by setting windows based upon known retention times:



Single ION Recording (SIR) recommendations

Select the minimum sampling rate to fully characterize a peak. This results in optimal signal to noise and reproducibility. Selecting a higher than needed sampling rate can lower the signal-to-noise ratio and impact data quality.

MS scan recommendations

In MS Scan mode, the slower a scan (lower sampling rate), the better the quality of spectral data in terms of sensitivity and dynamic range. Select the smallest mass range that covers the analytes of interest to lower the scan speed.

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