

# Package ‘qqqMS’

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**Type** Package

**Title** Peak Detection for MRM-MS data

**Version** 0.0.99

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**Description** Simple wrappers for using post-acquisition processing of Multiple Reaction Monitoring (MRM) Mass Spectrometry (MS) data using xcms.

**License** GPL (>= 3)

**Depends** xcms, methods

**Imports** MSnbase

**Suggests** testthat, covr

**Encoding** UTF-8

**LazyData** true

**RoxygenNote** 6.0.1

**NeedsCompilation** no

## R topics documented:

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extract_targets	<i>Extract Targets</i>
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## Description

Extract Targets

**Usage**

```
extract_targets(features, targets)
```

**Arguments**

- |          |  |
|----------|--|
| features | a list which has been produced using the <a href="#">integrate_peaks</a> function  |
| targets  | a <code>data.frame</code> of MRM-MS targets to extract the the <code>xcms</code> processed object. targets must contain the following columns; <ul style="list-style-type: none"> <li>• <b>name</b> the generic name of the target</li> <li>• <b>mz</b> the m/z value of the target (as it appears in the raw file)</li> <li>• <b>rt</b> the approximate retention time of the target</li> </ul> |

**Value**

a `data.frame` of feature values for only those which corresponds to an identified target

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integrate_peaks	<i>Detect and integrate MRM-MS features</i>
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**Description**

Detect and integrate MRM-MS features

**Usage**

```
integrate_peaks(files, phenoData)
```

**Arguments**

- |           |   |
|-----------|---|
| files     | a character vector of <code>.mzML</code> files which have been converted from MRM-MS <code>.mzML</code> to LC-MS style <code>.mzML</code> files using <code>MRMConverter</code>   |
| phenoData | a <code>data.frame</code> . <code>phenoData</code> must contain the following columns; <ul style="list-style-type: none"> <li>• <b>fileName</b> file name</li> <li>• <b>name</b> sample name</li> </ul> Providing these two columns are present; <code>phenoData</code> can contain as many other columns as the user wishes. |

**Value**

a list of two elements

- values values for the integrated peak areas of all features detected
- definitions a `data.frame` of feature definitions. See [XCMSnExp-class](#) for more details

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