# Benzothiazole and Derivatives by LC-MS/MS

ACE® Ultra-inert UHPLC & HPLC Columns

**Application #AN4840**

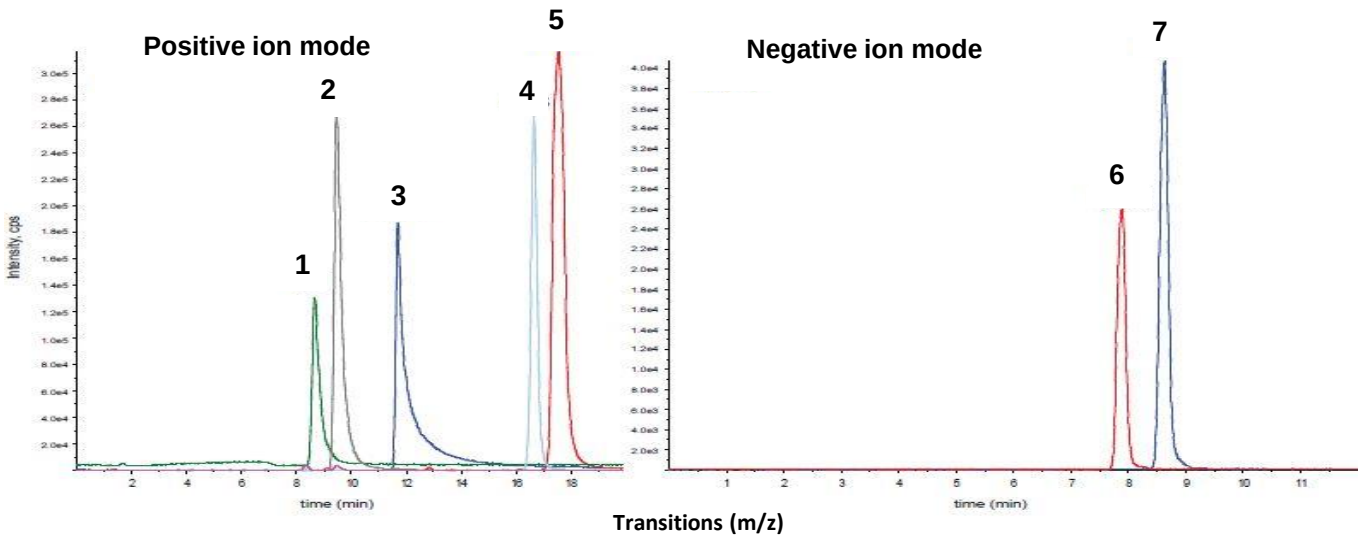
**Conditions**

| | |
|---|---|
| Column: | ACE 3 C8 |
| Dimensions: | 50 x 2.1 mm |
| Part Number: | ACE-112-0502 |
| Mobile Phase: | A: 0.1% formic acid in $H_2O$<br>B: 0.1% formic acid in MeCN |

| Positive mode | | Negative mode | |
|---|---|---|---|
| Time (mins) | %B | Time (mins) | %B |
| 0 | 5 | 0 | 5 |
| 5 | 50 | 2 | 5 |
| 10 | 95 | 5 | 50 |
| 23 | 95 | 9 | 50 |
| 23.1 | 5 | 9.1 | 5 |
| 28.1 | 5 | 12.1 | 5 |

| | |
|---|---|
| Flow Rate: | 0.12 mL/min |
| Injection: | 5 µL |
| Detection: | Sciex API 2000 LC-MS/MS, TurboIonSpray in positive and negative MRM modes, Ion spray voltage: ± 4200V, Ion source temperature: 120°C |
| Sample: | Benzothiazoles in street run-off wastewater due to tyre tread wear. |

Benzothiazoles are commonly used as vulcanisation accelerators in rubber production, but also as biocides and corrosion inhibitors in antifreeze and are widespread environmental pollutants in wastewater.




**Transitions (m/z)**

| Analyte | Quantifier | Confirmatory |
|---|---|---|
| 1. Benzothiazole | 136 > 109 | 136 > 65 |
| 2. 2-Methylbenzothiazole | 150 > 109 | 150 > 65 |
| 3. 2-Methylthiobenzothiazole | 182 > 167 | 182 > 109 |
| 4. *N*-Cyclohexyl-2-benzothiazole sulphenamide | 265 > 166 | 265 > 183 |
| 5. 2,2'-Dithiobisbenzothiazole | 333 > 167 | 333 > 109 |
| 6. 2-Mercaptobenzoxazole | 150 > 58 | 150 > 118 |
| 7. 2-Mercaptobenzothiazole | 166 > 134 | 166 > 58 |

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