**样品液质联用方法**

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| 项目 | 描述 | 制造商 |
| 液相系统 | Dionex Ultimate 3000 RSLC (HPG) | Thermo Fisher Scientific |
| 质谱系统 | Thermo Scientific Q Exactive Focus | Thermo Fisher Scientific |
| 离子源 | HESI-II | Thermo Fisher Scientific |

**色谱柱**

|  |  |  |
| --- | --- | --- |
| 类型 | 规格 | 制造商 |
| Waters Acquity uplc hss T3 1.8um | 100\*2.1 mm, | waters |

**离子源参数设置**

|  |  |
| --- | --- |
| 离子源参数 | 设定值 |
| Spray Voltage | 3.0 kV (+)/2.5 kV (-) |
| Capillary Temperature | 320°C |
| Sheath Gas | 35 arb |
| AUX Gas | 10 arb |
| Sweep Gas | 0 arb |
| Probe Heater Temperature | 350°C |
| S-Lens | 60 |

**梯度洗脱表**

|  |  |  |  |
| --- | --- | --- | --- |
| Time (min) | Flow (mL/min) | C（有机相）乙腈(0.1%甲酸) | B（水相）0.1%甲酸水 |
| 0 | 0.3 | 5 | 95 |
| 2 | 0.3 | 5 | 95 |
| 42 | 0.3 | 95 | 5 |
| 47 | 0.3 | 95 | 5 |
| 47.1 | 0.3 | 5 | 95 |
| 50 | 0.3 | 5 | 95 |
| 柱温：40°C | | | |

**质谱扫描参数设置**

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| --- | --- |
| 质谱扫描参数 | 设定值 |
| Scan mode | Full MS-ddms2 |
| Full MS scan range | 100 to 1500*m*/*z* |
| Spectrum data type | Profile |
| Resolution | Full MS: 70,000 |
| MS/MS: 17,500 |
| AGC target | Full MS:1e6 |
| MS/MS:2e5 |
| Maximum IT | Full MS: 100 ms |
| MS/MS: 50 ms |
| Loop count | 3 |
| MSX count | 1 |
| Isolation width | 1.5*m*/*z* |
| NCE (Stepped NCE) | 20, 40, 60 |
| Minimum AGC target | 8e3 |
| Intensity Threshold | 1.6e5 |
| Dynamic exclution | 5 s |