Table S1. Optimized mass spectrometric parameters for MRM analyses

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Analyte 1** | **Precursor Ion (*m/z*)** | **Product Ion (*m/z*)** | **Q1 Pre-bias**  **(V)** | **CE**  **(V)** | **Q3 Pre-bias (V)** |
| ***N*-Lac-Gln** | **219.1** | **84.0** | **-18.0** | **-26.0** | **-17.0** |
| ***N*-Lac-Ile** | **204.1** | **158.1** | **-17.0** | **-11.0** | **-18.0** |
| ***N*-Lac-Leu** | **204.1** | **86.2** | **-17.0** | **-19.0** | **-17.0** |
| ***N*-Ac-Ser** | **148.2** | **60.1** | **-14.0** | **-18.0** | **-24.0** |
| ***N*-Ac-Glu** | **190.1** | **84.1** | **-16.0** | **-24.0** | **-18.0** |
| ***N*-Pyr-Leu** | **243.2** | **225.1** | **-12.0** | **-7.0** | **-17.0** |
| **Bz-Cadaverine** | **311.0** | **105.0** | **-13.0** | **-25.0** | **-20.0** |
| **Bz-Putrescine** | **297.0** | **105.0** | **-12.0** | **-26.0** | **-20.0** |
| **Bz-Spermidine** | **458.3** | **105.1** | **-12.0** | **-47.0** | **-21.0** |
| **Bz-Spermine** | **619.2** | **105.1** | **-26.0** | **-55.0** | **-12.0** |
| **Aqc-Ethanolamine** | **232.0** | **170.7** | **-18.0** | **-17.0** | **-19.0** |
| **Aqc-Methionine sulfoxide** | **336.0** | **170.9** | **-14.0** | **-25.0** | **-19.0** |
| **Aqc-GABA** | **274.0** | **171.0** | **-27.0** | **-20.0** | **-20.0** |
| **Aqc-Tyramine** | **308.2** | **171.0** | **-13.0** | **-23.0** | **-19.0** |
| **Aqc-Phenyethylamine** | **292.1** | **171.0** | **-24.0** | **-22.0** | **-19.0** |
| **Aqc-Tryptamine** | **331.1** | **171.0** | **-14.0** | **-30.0** | **-19.0** |
| **Aqc-Histamine** | **282.0** | **171.0** | **-24.0** | **-16.0** | **-19.0** |
| **Acetate-2NPH** | **193.9** | **122.1** | **19.0** | **14.0** | **21.0** |
| **Glycerate-2NPH** | **240.0** | **137.1** | **12.0** | **19.0** | **23.0** |
| **Lactate-2NPH** | **224.0** | **137.1** | **11.0** | **22.0** | **24.0** |
| **Malate-2NPH** | **403.0** | **208.2** | **11.0** | **19.0** | **20.0** |
| **Butyrate-2NPH** | **222.0** | **122.0** | **22.0** | **15.0** | **21.0** |
| **Caproate-****2NPH** | **250.0** | **220.2** | **12.0** | **12.0** | **21.0** |
| **Isocaproate-2NPH** | **250.0** | **122.2** | **12.0** | **16.0** | **21.0** |
| **Propionate-2NPH** | **208.0** | **122.0** | **10.0** | **14.0** | **19.0** |
| **Succinate-2NPH** | **386.9** | **234.2** | **14.0** | **16.0** | **14.0** |
| **Pyruvate-2NPH** | **356.9** | **137.0** | **18.0** | **23.0** | **24.0** |
| **Alpha-Ketobutyrate-2NPH** | **370.9** | **137.1** | **18.0** | **23.0** | **24.0** |
| **2-keto-3-methylbutyrate-2NPH** | **384.9** | **137.0** | **28.0** | **25.0** | **24.0** |
| **3-Methyl-2-oxovaleric acid-2NPH** | **399.0** | **137.0** | **30** | **25** | **24** |
| **4-Methyl-2-oxovaleric acid-2NPH** | **399.0** | **137.0** | **21** | **26** | **24** |
| **Heptanoate-2NPH** | **264.0** | **234.2** | **12.0** | **12.0** | **15.0** |

1Abbreviations are: Aqc, Bz-, Lac-, Pyr-, Ac-, 2NPH: 6-aminoquinolyl-*N*-hydroxysuccinimidyl carbamate, benzoyl-, lactoyl-, pyroglutamyl-, acetyl-, 2-nitrophenylhydrazine, respectively.