Title: Using UHPLC Q-Trap/MS as a Complementary Technique to In-depth Mine UPLC Q-TOF/MS Data for Identifying Modified Nucleosides in Urine

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Highlights

1. PBA extraction was more efficiently than the other solid phase extraction (HLB, MCX cartridges) and protein precipitation methods for extraction of cis-diol-containing biomolecules in this study.
2. It was a powerful method to comprehensively identify urinary nucleosides by combining UPLC Q-TOF/MS with UHPLC Q-Trap/MS.
3. Five urinary nucleosides were identified for the first time, including 4',5'-didehydro-5'-deoxyadenosine, 4',5'-didehydro-5'-deoxyinosine, isonicotinamide riboside, and 2 hypermodified nucleosides, peroxywybutosine and hydroxywybutosine. This was the first discovery of nucleoside peroxide from human urine.

Full Length Article

Using UHPLC Q-Trap/MS as a Complementary Technique to In-depth Mine UPLC Q-TOF/MS Data for Identifying Modified Nucleosides in Urine

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Abbreviations: UPLC Q-TOF/MS: ultraperformance liquid chromatography quadrupole time-of-flight mass spectrometry; UHPLC Q-Trap/MS: ultra-high performance liquid chromatography coupled with hybrid triple quadrupole linear ion trap mass spectrometer; SPE: solid phase extraction; MRM-EPI: multiple reaction monitoring trigger enhanced product ion scan; NL: neutral loss scan; PBA: phenylboronic acid; HMDB: Human Metabolome Database; LC/MS: liquid chromatography coupled with mass spectrometer; HDMS: high definition mass spectrometry; HLB: hydrophilic-lipophilic balance; MCX: mixed-mode cation exchange; IDA: information-dependent acquisition; EIC: extracted ion chromatogram.