Liquid chromatography?time-of-flight high-resolution mass spectrometry study and determination of the dansylated products of estrogens and their hydroxylated metabolites in water and wastewater

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 A method combining liquid chromatography with a dual-probe ultraspray electrospray ionization (ESI) source and time-of-flight high-resolution mass spectrometry (LC-ESI-TOF/MS) was developed for the simultaneous determination of four steroidal sex hormones, estrone (E1), 17?-estradiol (E2), 17?-ethinyl estradiol (EE2), and estriol (E3), as well as five of their hydroxylated metabolites, 2-hydroxyestrone (2-OHE1), 4-hydroxyestrone (4-OHE1), 16?-hydroxyestrone (16-OHE1), 2-hydroxyestradiol (2-OHE2), and 4-hydroxyestradiol (4-OHE2), in water samples in a short chromatographic run of 10 min. Derivatization of the analytes was optimized using dansyl chloride as the derivatizing agent. Under optimal positive ionization conditions, the following signals, which had not been previously reported, were observed (with theoretical values of m/z 377.1373 for 2- and 4-OHE1 and 378.1452 for 2- and 4-OHE2), corresponding to doubly derivatize