

## Removal of 17 $\alpha$ -ethinylestradiol with Mn(III) and product identification

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With increasing concern about the contamination of aquatic environment by estrogenic pollutants, removal of synthetic estrogens has been widely studied. However, the degradation products have rarely identified. The purpose of this study is structurally to identify the oxidation products of 17 $\alpha$ -ethinylestradiol(EE2). Mn(III) was used as an oxidizing agent. To obtain the oxidation products, highly concentrated solution of EE2 (1 mM) was prepared in the mixture of water and a water-miscible organic solvent. From HPLC analysis of reaction products, single compound (I) was found to be predominant. From LC-MS, its molecular weight was found to be 294 and two hydrogens were believed to be removed from EE2 (M.W. 296) to form a C=C double bond. The structure of compound I was determined using <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, H-H COSY, HSQC, and HMBC. As minor products, isomeric dimers (M.W. 590) of EE2 as well as the products (M.W. 588) where EE2 was coupled to compound I were also formed during the Mn(III)-mediated oxidation of EE2. The work was financially supported by the ERC program of MOST/KOSEF (R11-2003-006-01001-1) through the Advanced Environmental Biotechnology Research Center at POSTECH.