

Caption for supplementary figures

Figure S1. Typical full scan mass spectra of GHB-EDC_A / GHB-EDC_B (**a**) and D₆-GHB-EDC_A / D₆-GHB-EDC_B (**b**) derivatives, and accurate mass measurements data of the four MH⁺ ions.

Figure S2. Derivatization yields of the GHB-EDC derivatives at different temperature and time reaction conditions.

Figure S3. Stability of GHB-EDC derivatives kept at different temperatures and times before instrumental injection.

Figure S4. MH⁺ collision-induced product ion spectra (merging of collision energies at 10, 25, 50 eV) of GHB-EDC, BHB-EDC, and BHisoB-EDC for both type A and type B derivatives.