

Supporting Information for An Improved Process for Industrial Production of Isosorbide-5-mononitrate: Recycling of Wastes

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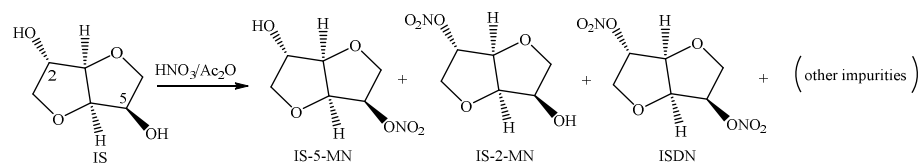
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1. Supplementary on the acetylated impurities in the direct nitration of IS.

During the process of direct nitration of IS (**Scheme S1**), series of acetylated side-products including isosorbide-2-acetate (IS-2-Ac), isosorbide-5-acetate (IS-5-Ac), isosorbide-2,5-diacetate (IS-2,5-DAc), isosorbide-2-acetate-5-nitrate (IS-2-Ac-5-MN), and isosorbide-5-acetate-2-nitrate (IS-5-Ac-2-MN) were detected by HPLC (**Figure S1**). However, the accumulation of acetylated side-products were much lower than nitration, where the total amount of acetylated side products was only 3% at the end of nitration reaction. And during the process of neutralization, IS-2-Ac, IS-5-Ac and IS-2,5-DAc were easily hydrolyzed by sodium hydroxide solution to form IS. IS-2-Ac-5-MN and IS-5-Ac-2-MN were hydrolyzed to give IS-5-MN and IS-2-MN respectively. Therefore, the main side-products in the direct nitration were IS-2-MN and ISDN.

Scheme S1. Direct nitration of IS.



other impurities including:

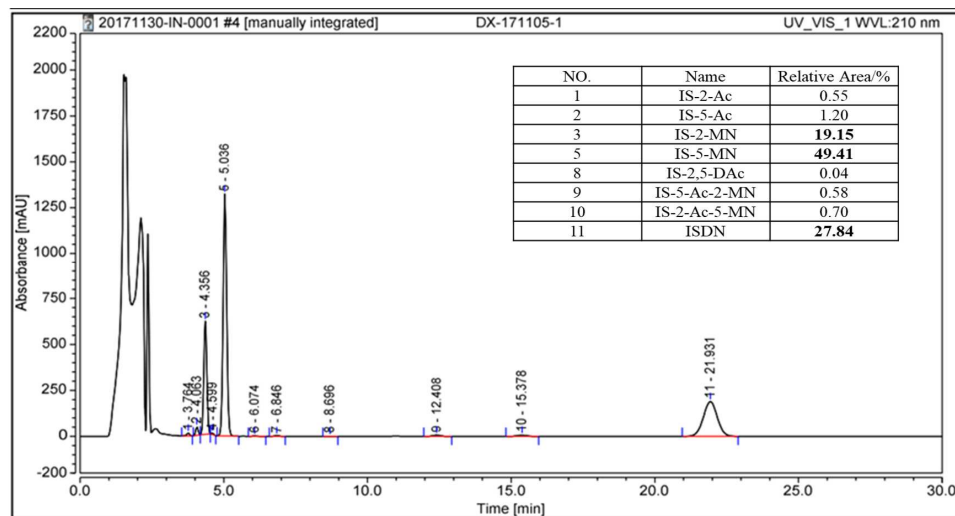
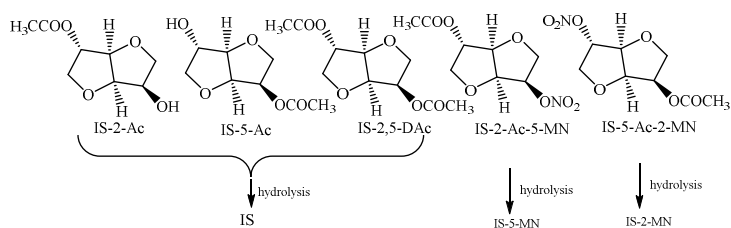
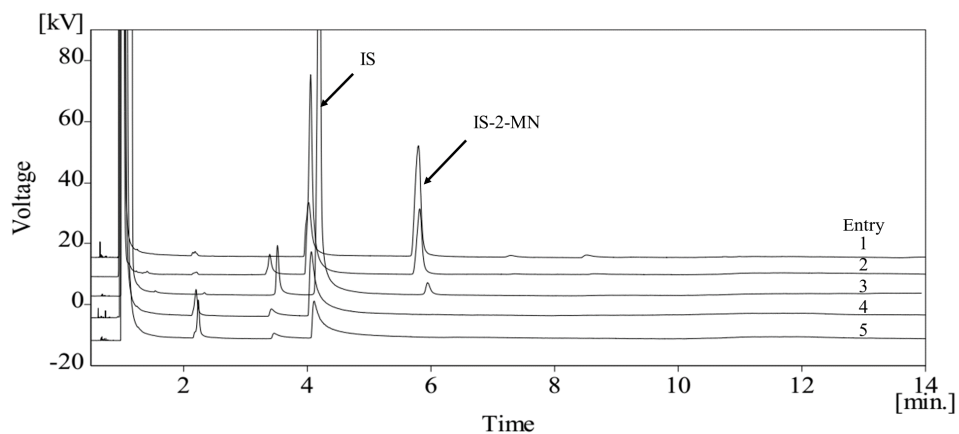
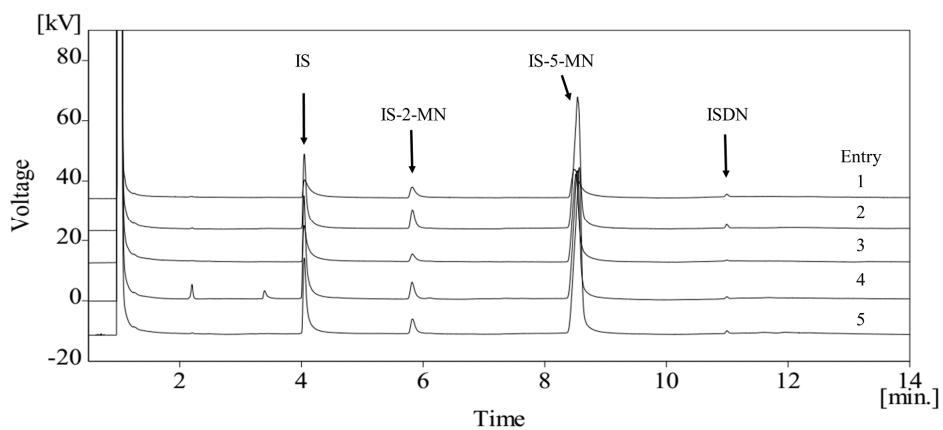


Figure S1. HPLC chromatogram of the direct nitration of IS.

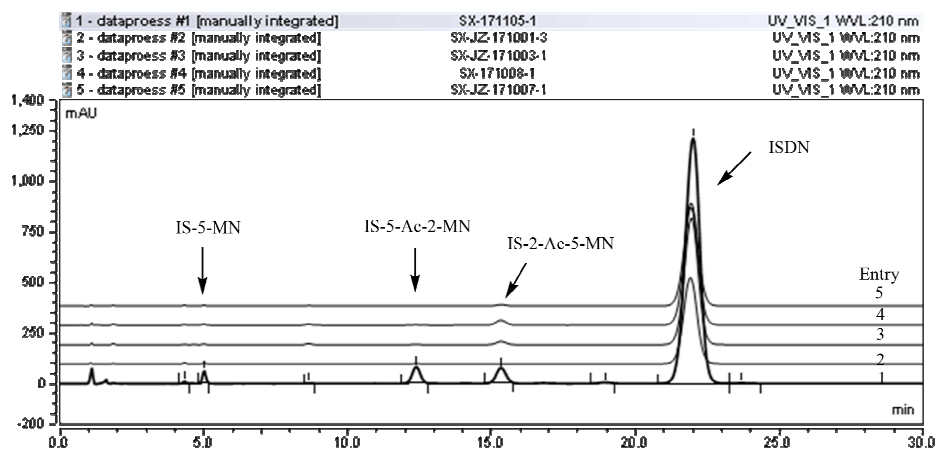
2. The relevant GC chromatograms in the **Table 2**.



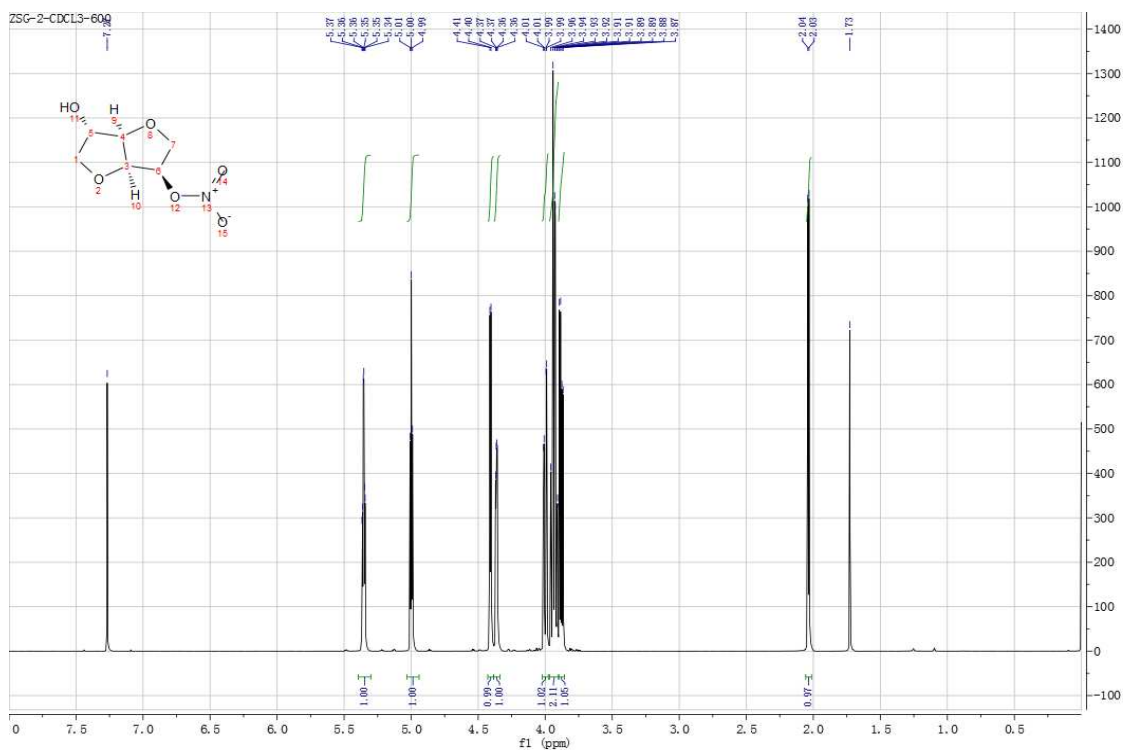
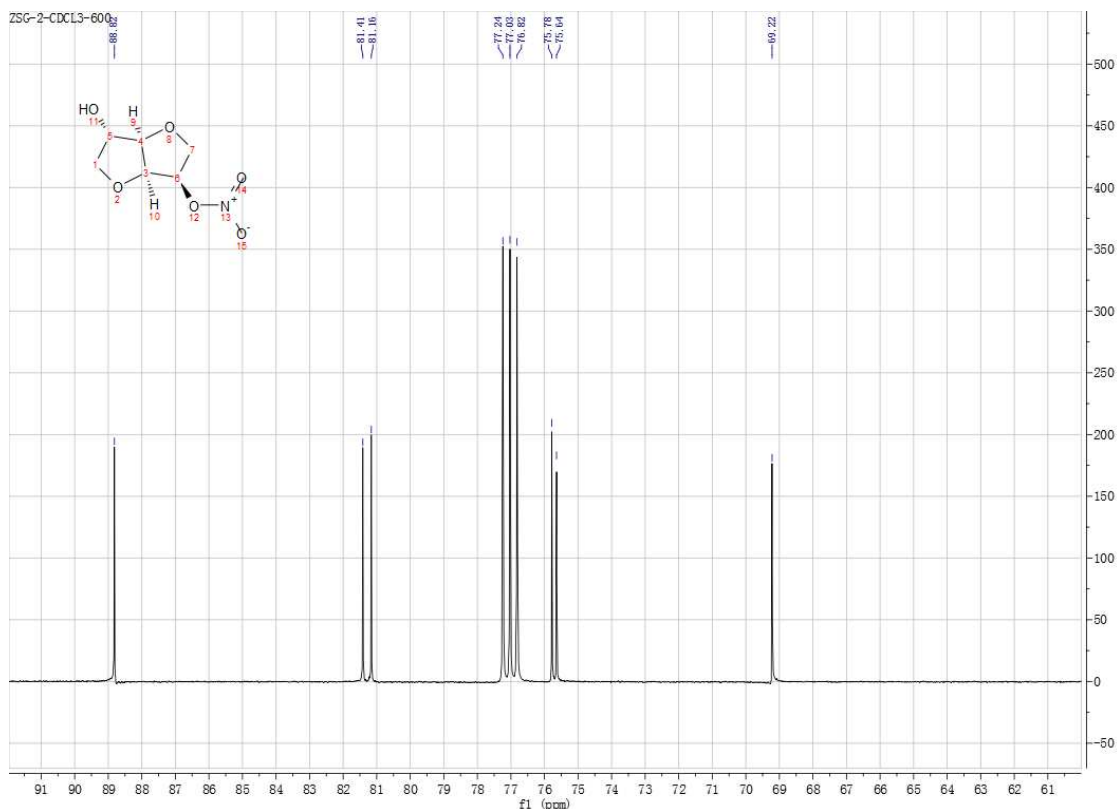
3. The relevant GC chromatograms in the **Table 5**.

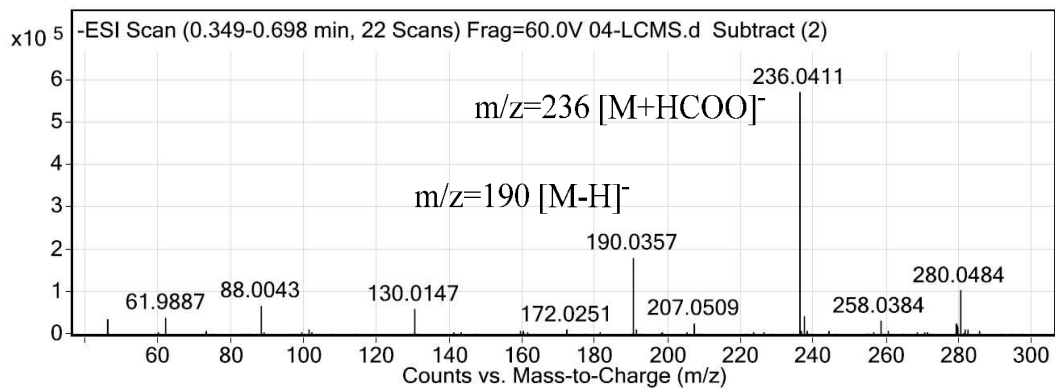


4. The relevant HPLC chromatograms in the **Table 4**.



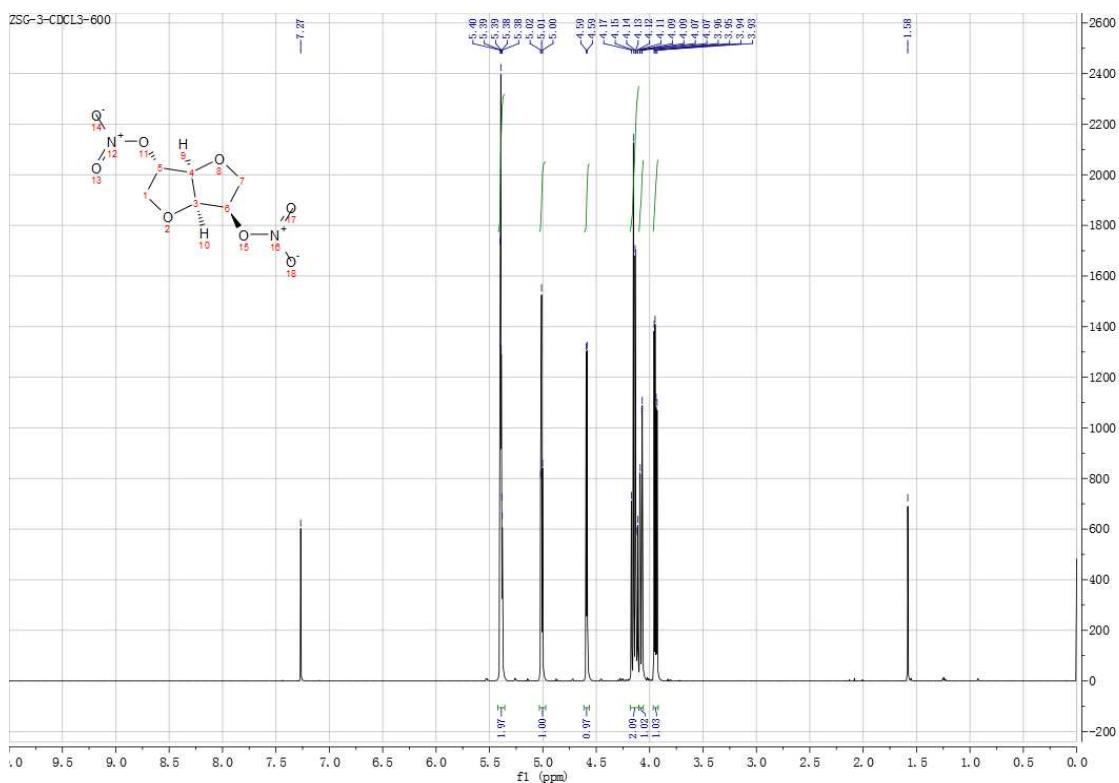
5. ^1H NMR, ^{13}C NMR, MS date of IS-5-MN

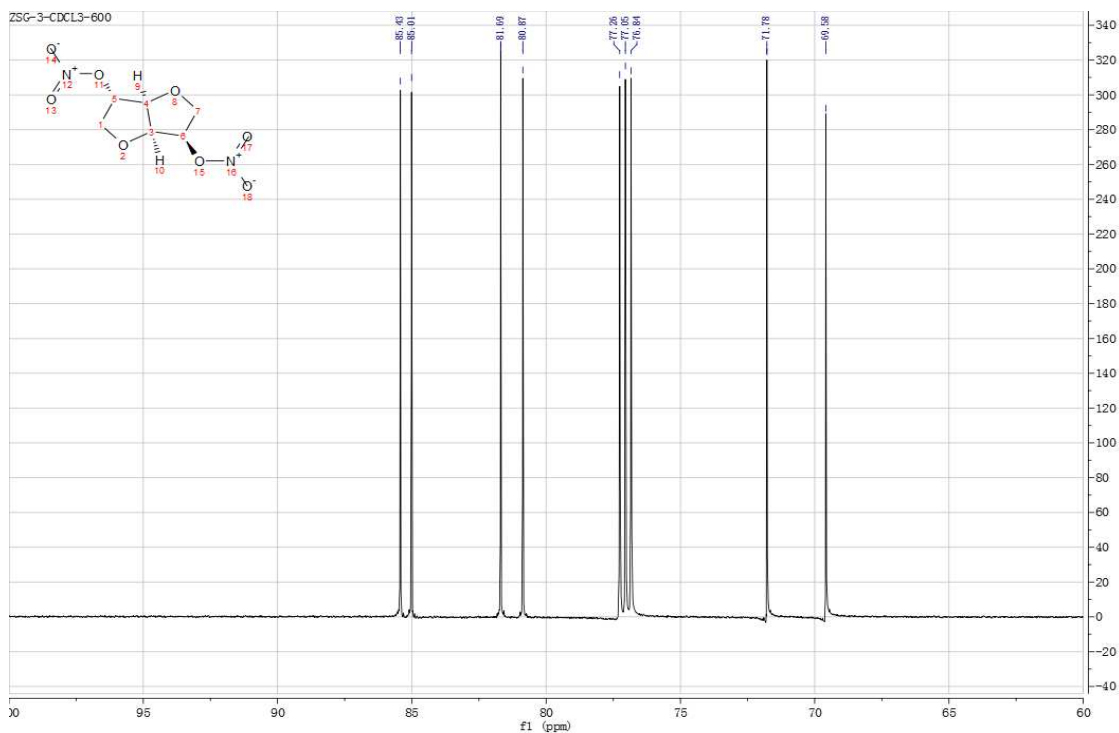
¹H NMR spectrum of IS-5-MN

^{13}C NMR spectrum of IS-5-MN

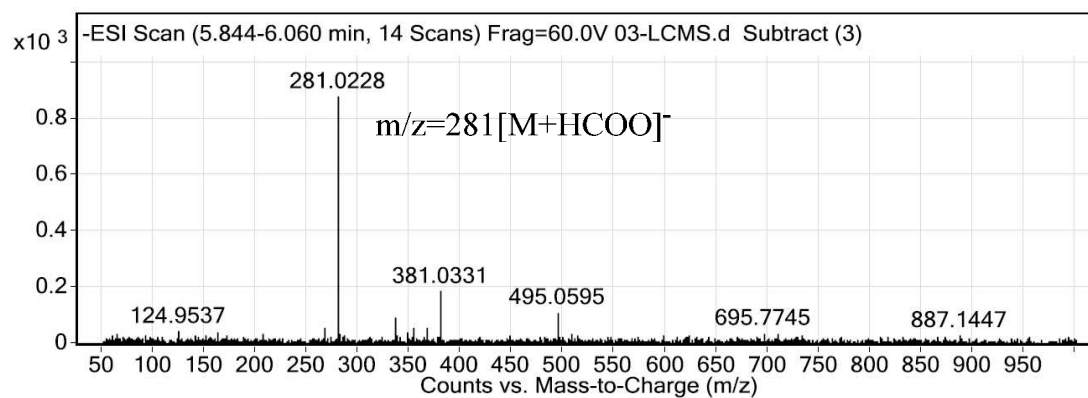
MS spectrum of IS-5-MN

6. ^1H NMR, ^{13}C NMR, MS date of ISDN

¹H NMR spectrum of ISDN

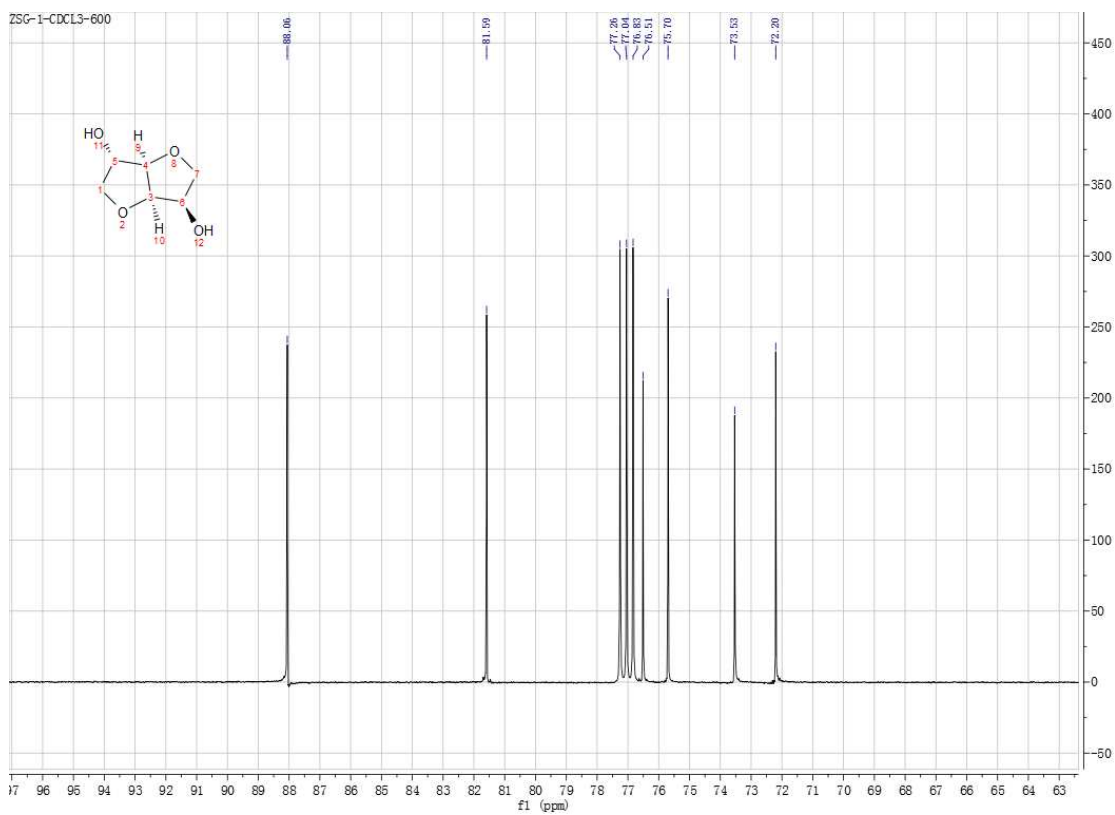
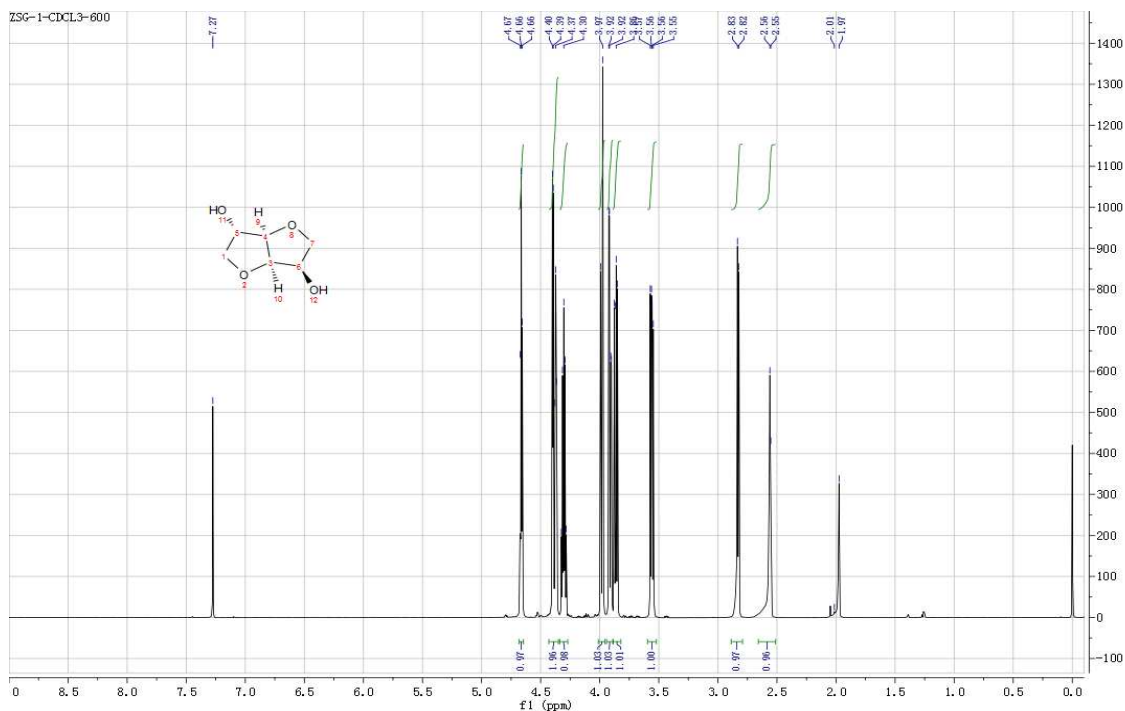


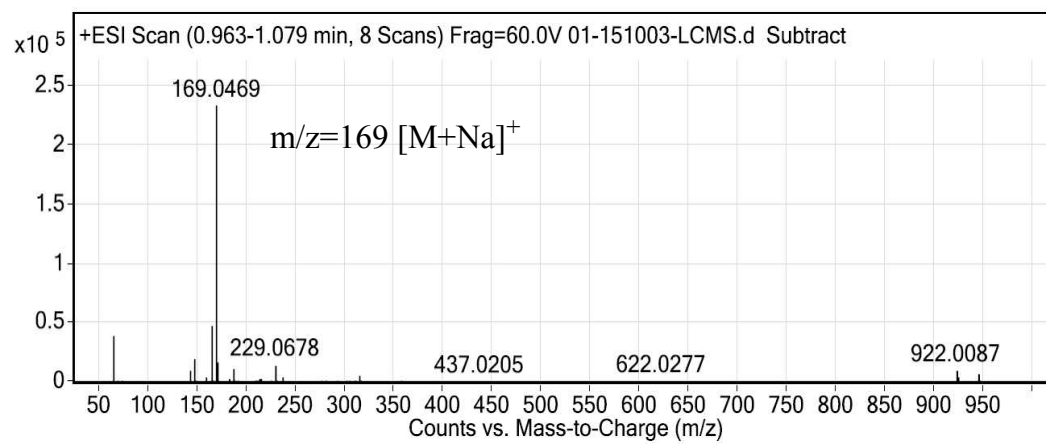
^{13}C NMR spectrum of ISDN



MS spectrum of ISDN

7. ^1H NMR, ^{13}C NMR, MS date of IS





MS spectrum of IS