Supporting Information for

Rapid Determination and Conversion Study of 5-Hydroxymethylfurfural and Its Derivatives in Glucose Injection

Cheng Wang^a, Yajing Hou^a, Yuanyuan Lin^a, Yitong Xie^a, Di Wei^a, Nan Zhou^b, Huaizhen He^{a*}

^a School of Pharmacy, Xi'an Jiaotong University, Xi'an 710061, China.

^b Department of Pharmacy, Shaanxi Provincial People's Hospital, Xi'an, China

^{*}E-mail: hehuaizhen@mai.xjtu.edu.cn; Tel: +86-29-82657740, Fax: +86-29-82655451

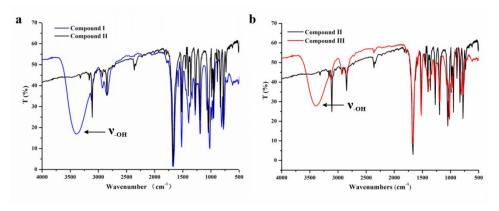


Figure S1. Comparison of typical IR spectra for Compounds I-III.

Chemical Formula: C₆H₆O₃

Exact Mass: 126.03 Molecular Weight: 126.11

m/z: 126.03 (100.0%), 127.04 (6.5%)

Elemental Analysis: C, 57.14; H, 4.80; O, 38.06

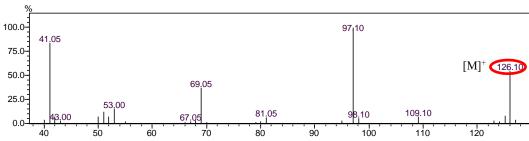
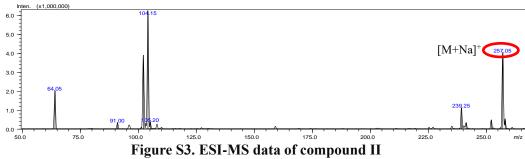


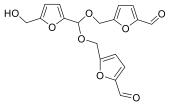
Figure S2. GC-MS data of compound I

Chemical Formula: C₁₂H₁₀O₅ Exact Mass: 234.05

Molecular Weight: 234.21

m/z: 234.05 (100.0%), 235.06 (13.0%), 236.06 (1.0%) Elemental Analysis: C, 61.54; H, 4.30; O, 34.16





Chemical Formula: C₁₈H₁₆O₈ Exact Mass: 360.08 Molecular Weight: 360.32

m/z: 360.08 (100.0%), 361.09 (19.5%), 362.09 (1.8%), 362.09 (1.6%) Elemental Analysis: C, 60.00; H, 4.48; O, 35.52

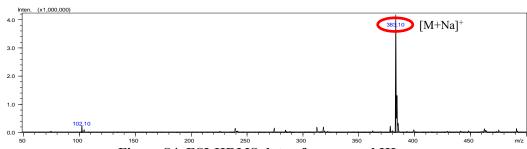


Figure S4. ESI-HRMS data of compound III

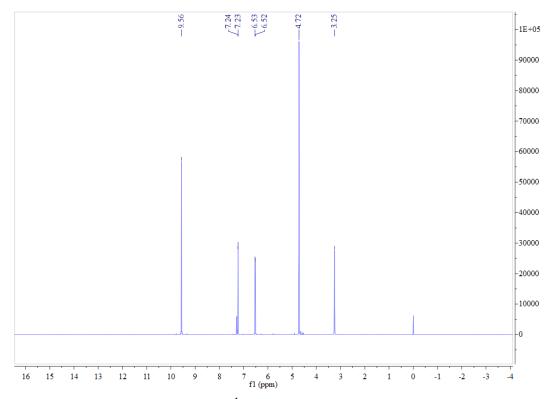


Figure S5. ¹H NMR of compound I

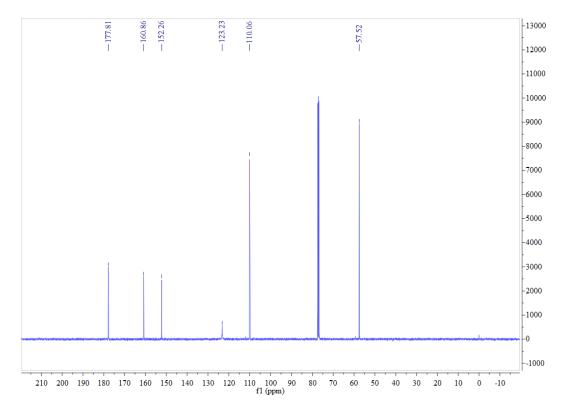


Figure S6. 13 C NMR of compound I

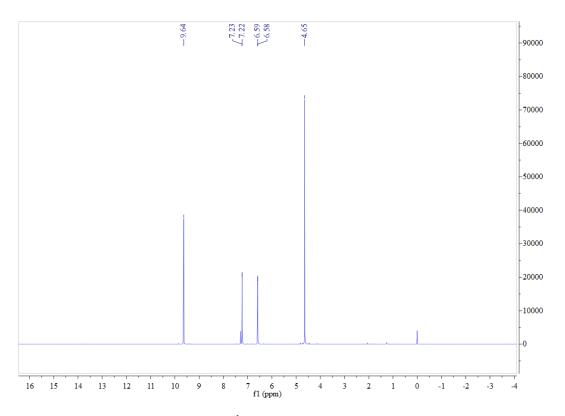


Figure S7. ¹H NMR of compound II

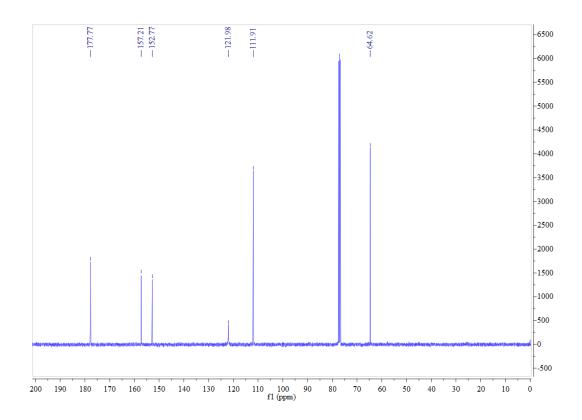


Figure S8. ¹³C NMR of compound II

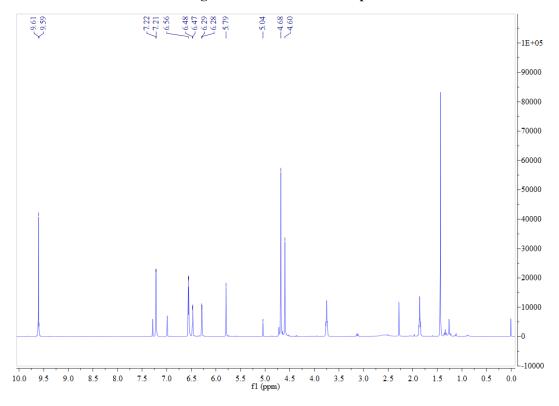


Figure S9. ¹H NMR of compound III

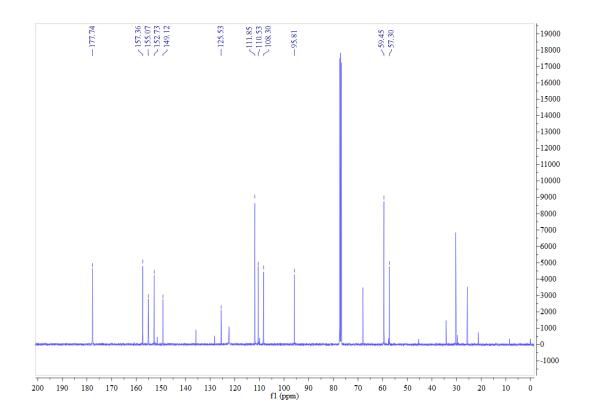


Figure S10. ¹³C NMR of compound III

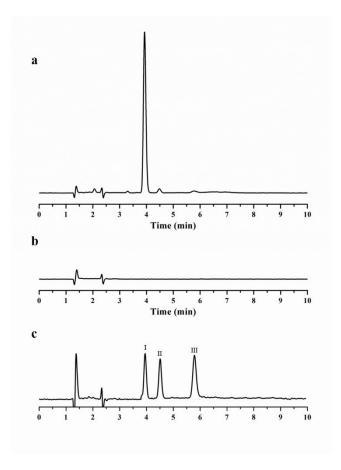


Figure S11. HPLC for sample, control and standard (a: HPLC for glucose injection; b: HPLC for control; c: HPLC for standard compounds.