Supporting Information

Homotropic Cooperativity of Human Liver Microsomal Cytochrome P450 3A Enzymes in Thalidomide 5-Hydroxylation and Formation of a Glutathione Conjugate

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Contents

Figure S1. ESI-LC-MS/MS chromatogram and mass spectrum of 5-hydroxythalidomide. A) ESI-LC-MS/MS chromatogram of 5-hydroxythalidomide (*m/z* 273). B) CID spectrum of the t_R 4.31 min peak in part A.

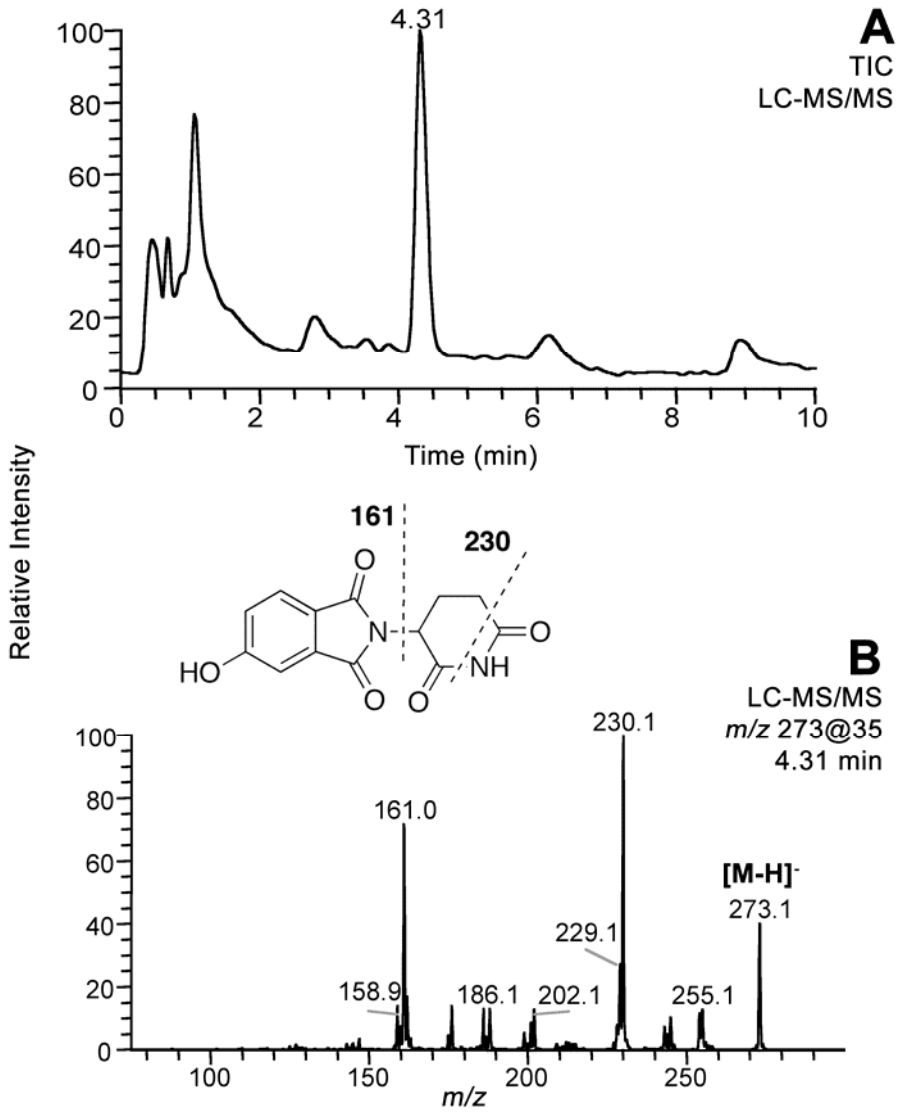


Figure S2. ESI-LC-HRMS chromatogram and mass spectrum of the 5-hydroxythalidomide-GSH conjugate. A) Extracted ion chromatogram of the 5-hydroxythalidomide-GSH conjugate, *m/z* 580. B) HR-MS spectrum of the t_R 3.42 min peak in part A.

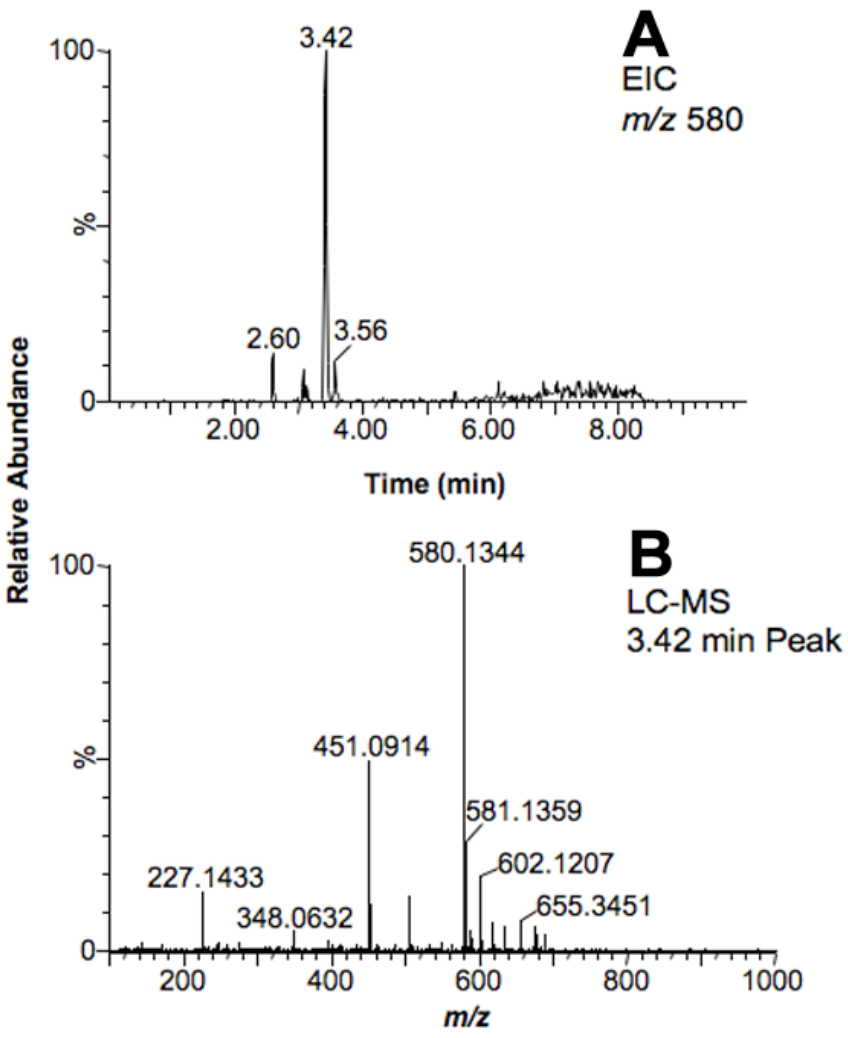
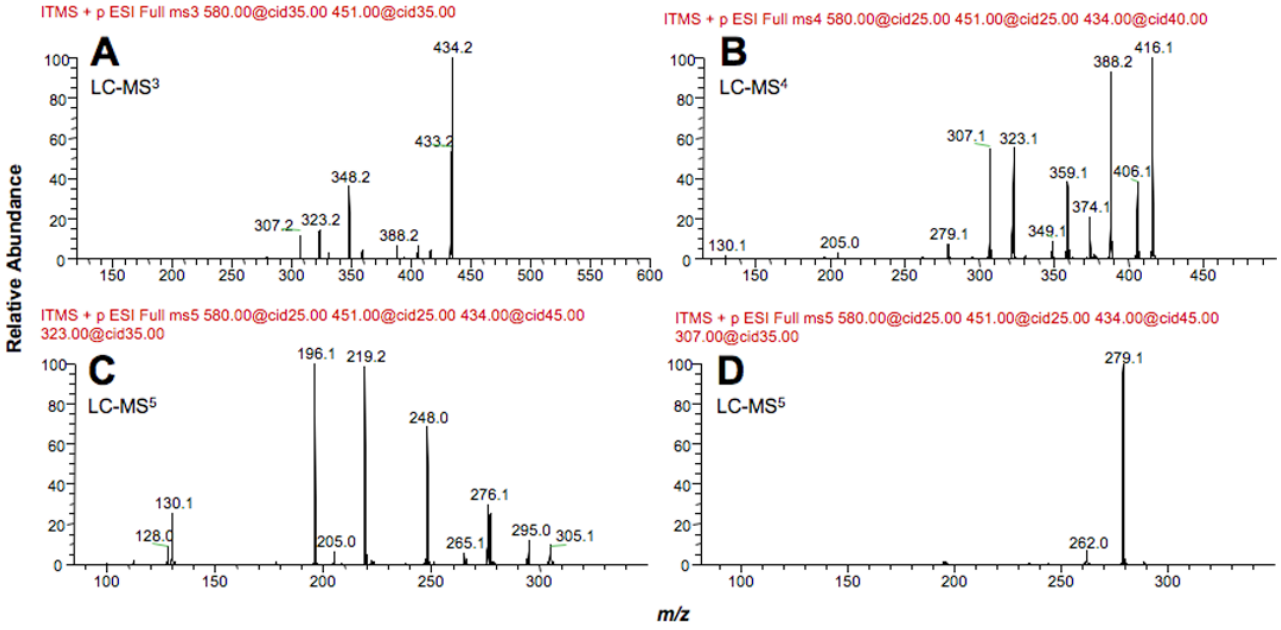


Figure S3. ESI-LC-MS^n spectrum of the 5-hydroxythalidomide-GSH conjugate. A) MS^3 spectra of ions *m/z* 580@35, 451@35 B) MS^4 spectra of ions *m/z* 580@35, 451@25, 434@40 C) MS^5 spectra of ions *m/z* 580@35, 451@25, 434@45, 323@35 D) MS^5 spectra of ions *m/z* 580@35, 451@25, 434@45, 307@35



Scheme S1. Proposed mechanism for formation of a GSH conjugate of 5-hydroxythalidomide