

SUPPORTING INFORMATION

Bioactivation of Fluorinated 2-Aryl-benzothiazole Anti-tumor Molecules by Human Cytochrome P450s 1A1 and 2W1 and Deactivation by Cytochrome P450 2S1

Wang, K., and Guengerich, F. P. (2012) *Chem. Res. Toxicol.* 25, 000-000

Figure S1. Selective NOE NMR spectra of GW 610

Figure S2. ¹H NMR spectrum of **4c'**

Figure S3. ¹H NMR and HH COSY spectra of **8a**

Figure S4. ¹H NMR spectrum of **8b**

Figure S5. UV spectra of GW610, **4b**, **4c**, and **4c'**

Figure S6. HPLC chromatograms of incubations of GW 610 with P450 2W1 using **4b** as internal standard

Figure S7. HPLC chromatograms of incubations of 5F 203 with P450s 2W1 and 1A1

Figure S8. HPLC chromatograms and UV spectra of synthetic **10**, **11**, and **9**

Figure S9. LC-MS chromatograms and spectra of **4c** and **4c'**

Figure S10. LC-MS chromatograms of 5F 203 oxidation products formed by P450s 2W1 and 1A1

Figure S11. LC-MS/MS and LC-MS³ chromatograms and CID spectra showing the presence of a dGuo adduct derived from synthetic **10**.

Figure S1. Selective NOE NMR spectra of GW 610

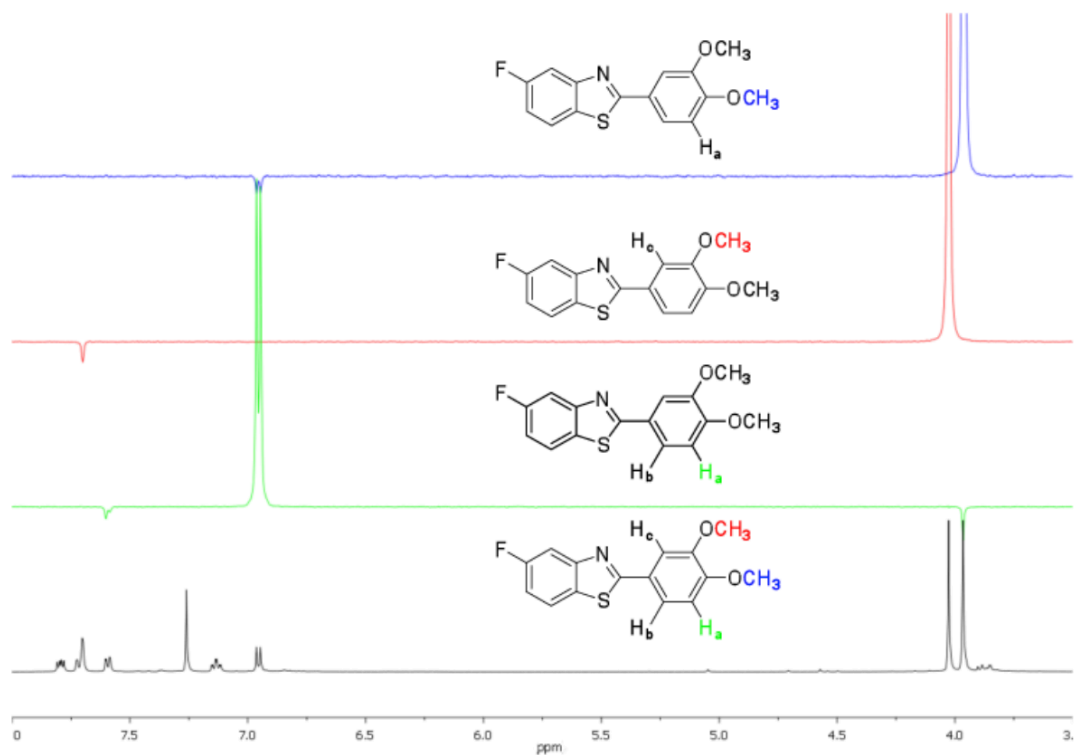


Figure S2. ^1H NMR spectrum of **4c'**

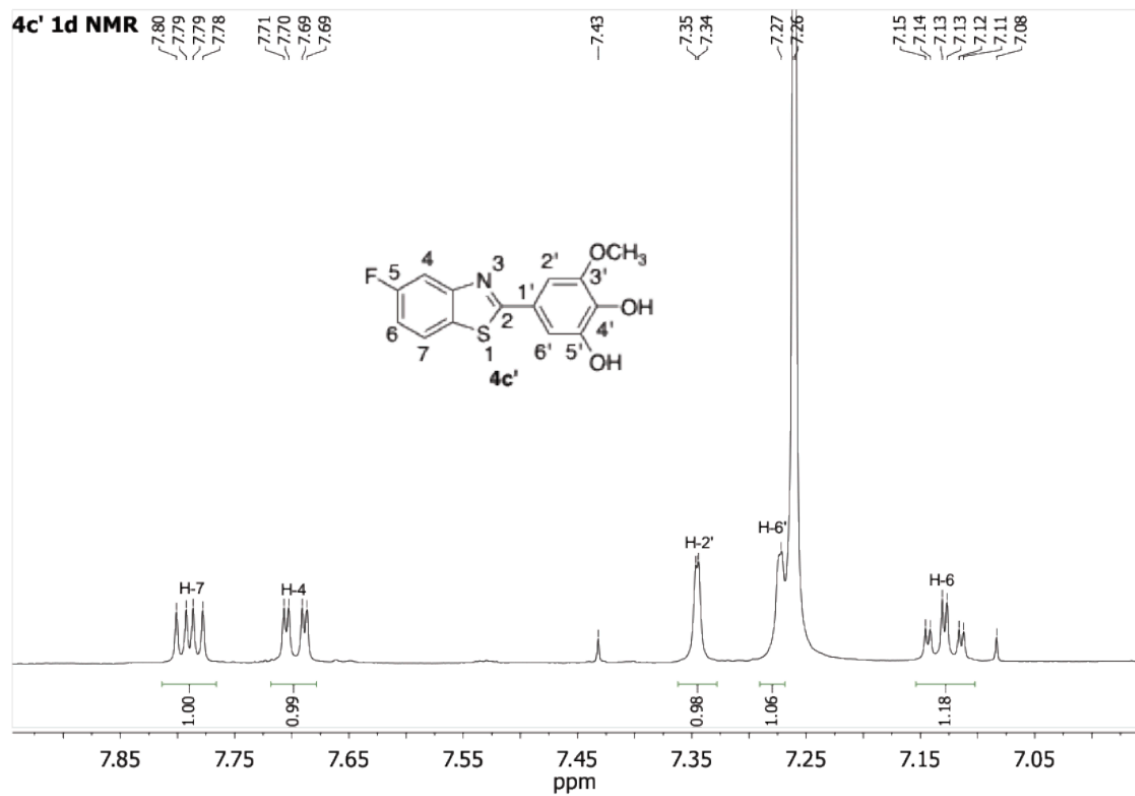


Figure S3. ^1H NMR and HH COSY spectra of **8a**

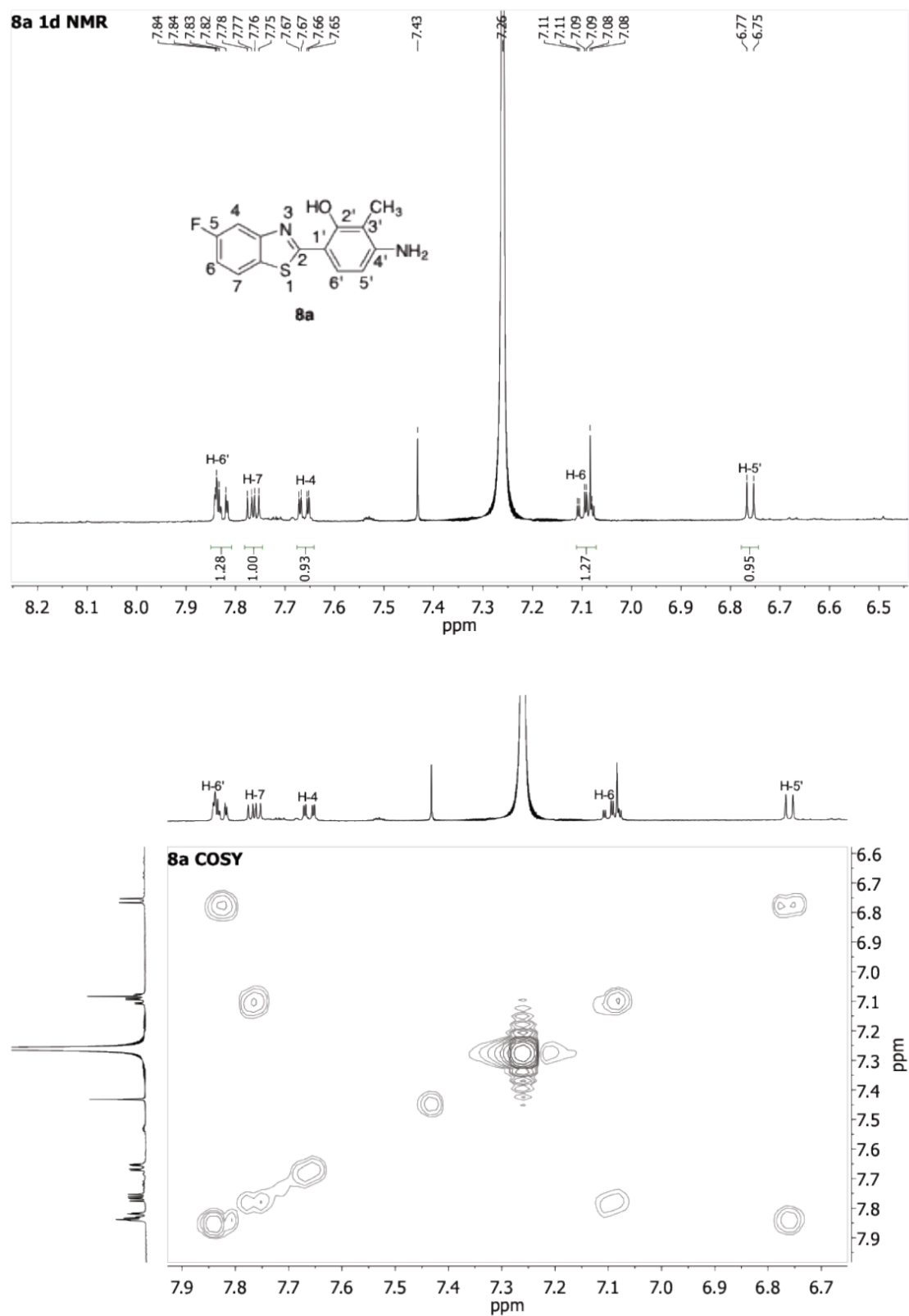


Figure S4. ^1H NMR spectrum of **8b**

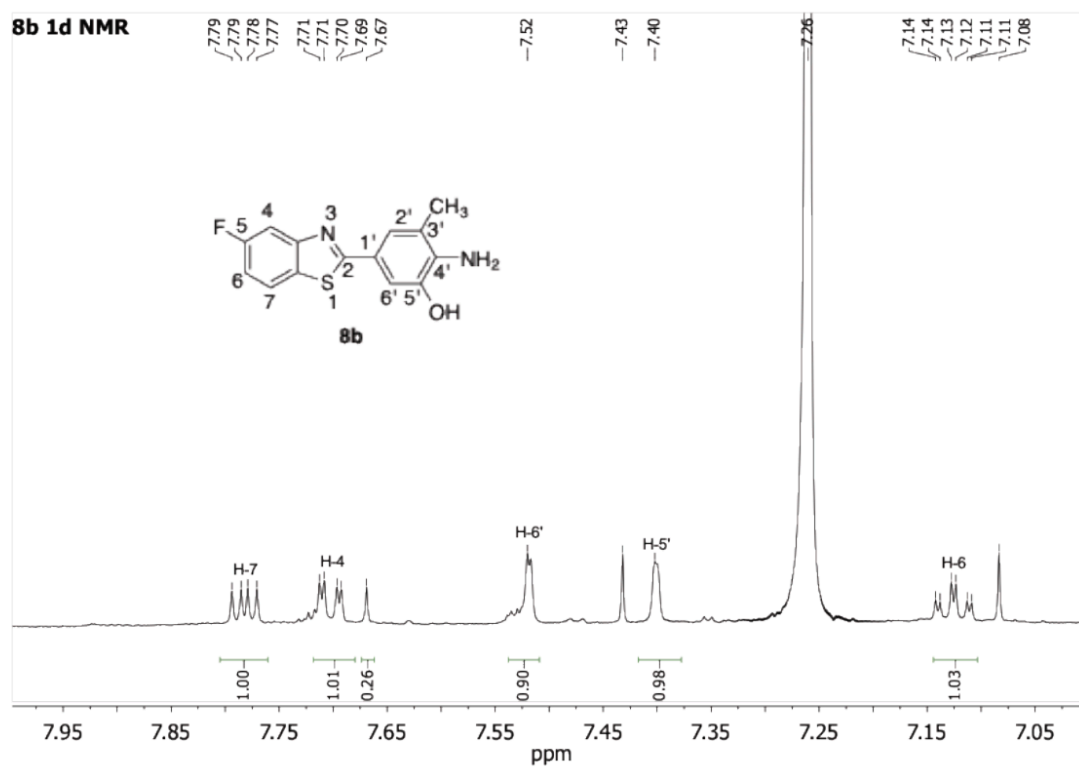


Figure S5. UV spectra of GW610, **4b**, **4c**, and **4c'**

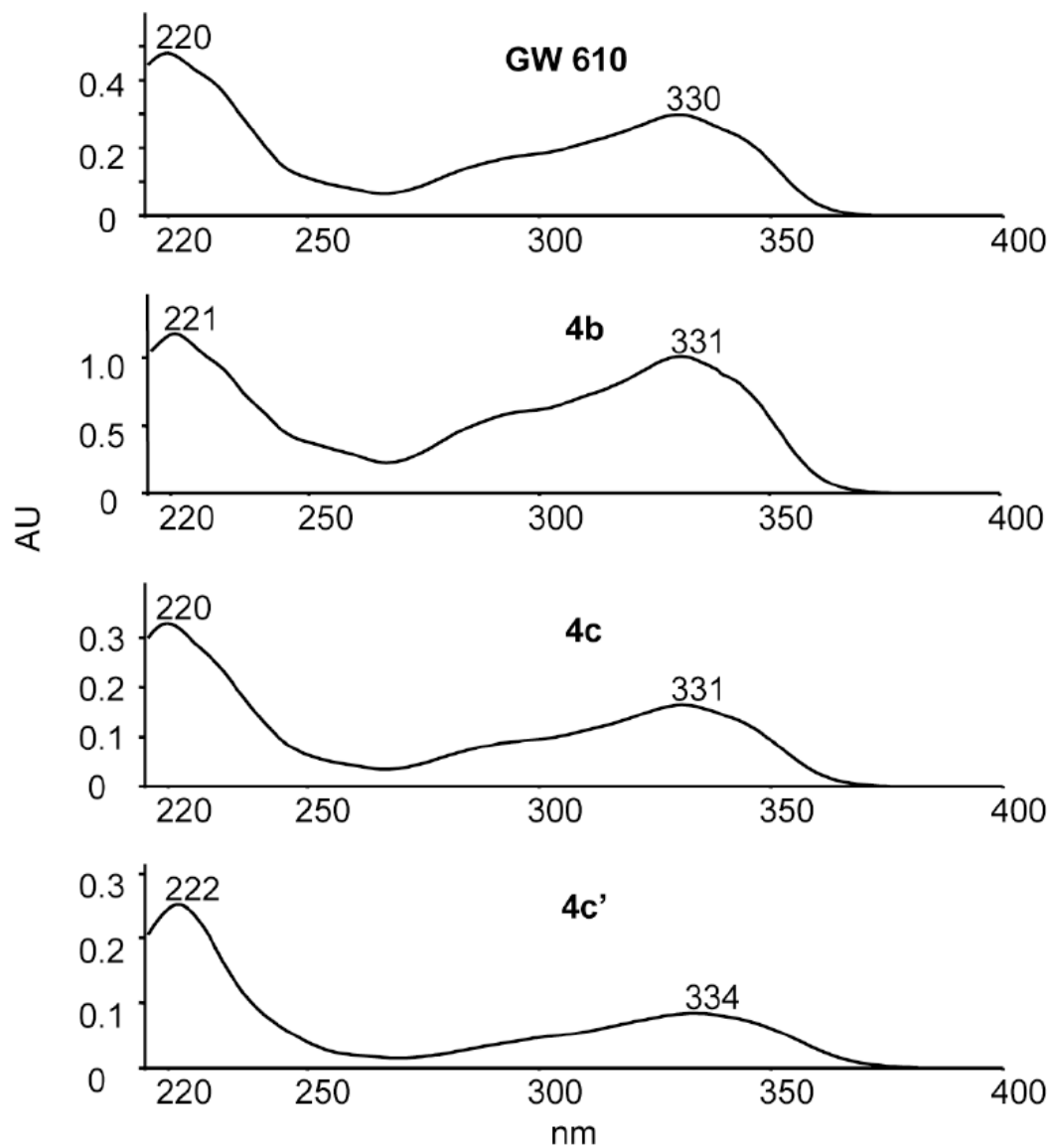
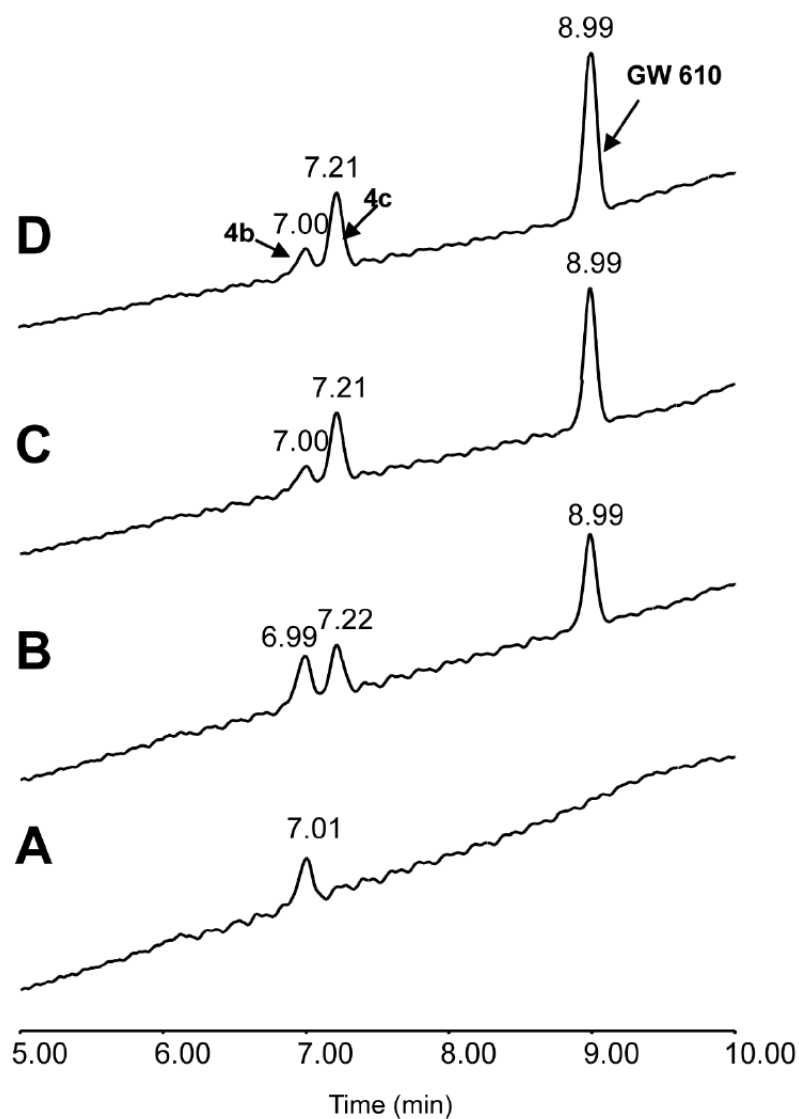


Figure S6. HPLC chromatograms* of incubations of GW 610 with P450 2W1 using **4b** as internal standard



(A) **4b** (1 μ M).

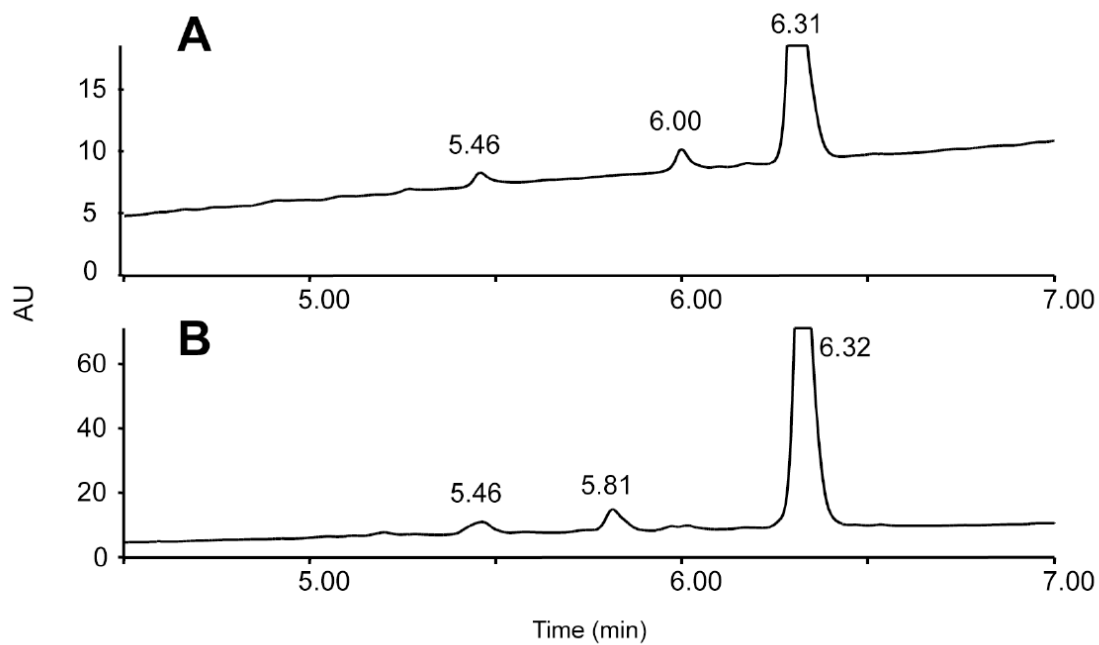
(B) GW 610 (4 μ M) incubated with P450 2W1 for 10 min, then **4b** (1 μ M) was added.

(C) GW 610 (8 μ M) incubated with P450 2W1 for 10 min, then **4b** (1 μ M) was added.

(D) GW 610 (12 μ M) incubated with P450 2W1 for 10 min, then **4b** (1 μ M) was added.

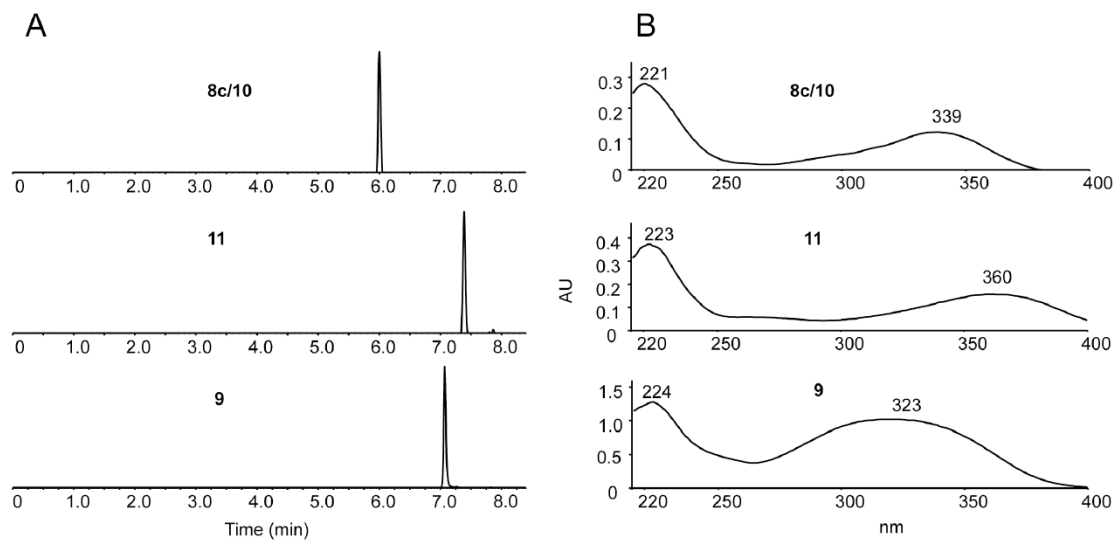
***4b** (t_R 7.01 min), **4c** (t_R 7.22 min), GW 610 (t_R 8.99 min)

Figure S7. HPLC chromatograms of incubations of 5F 203 with P450s 2W1 and 1A1



(A) Incubation of 5F 203 with P450 2W1, **8a** (t_R 5.46 min), **10** (t_R 6.00 min), 5F 203 (t_R 6.31 min). (B) Incubation of 5F 203 with P450 1A1, **8a** (t_R 5.46 min), **8b** (t_R 5.81 min), 5F 203 (t_R 6.32 min).

Figure S8. HPLC chromatograms and UV spectra of synthetic **10**, **11**, and **9**



(A) HPLC chromatograms of synthetic **10**, **11**, and **9**

(B) UV spectra of synthetic **10**, **11**, and **9**

Figure S9. LC-MS chromatograms and spectra of **4c** and **4c'**

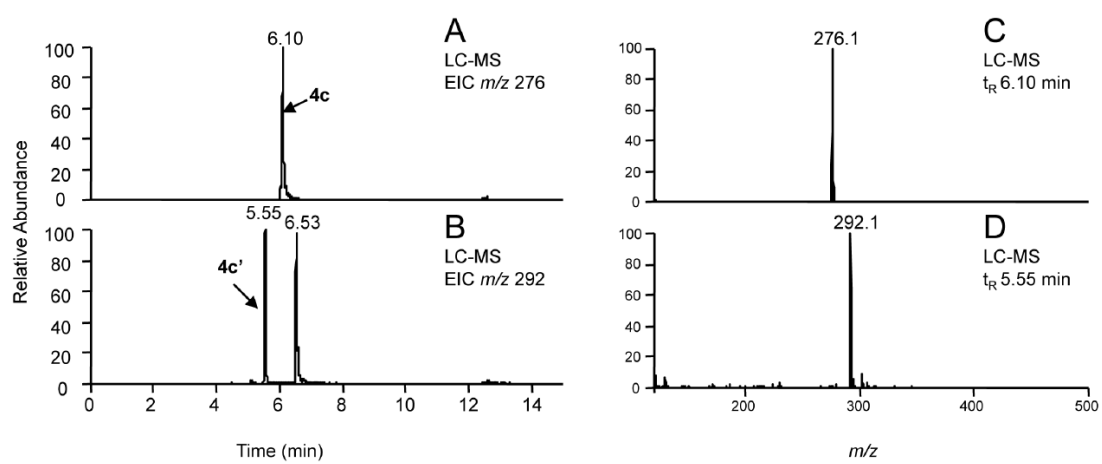
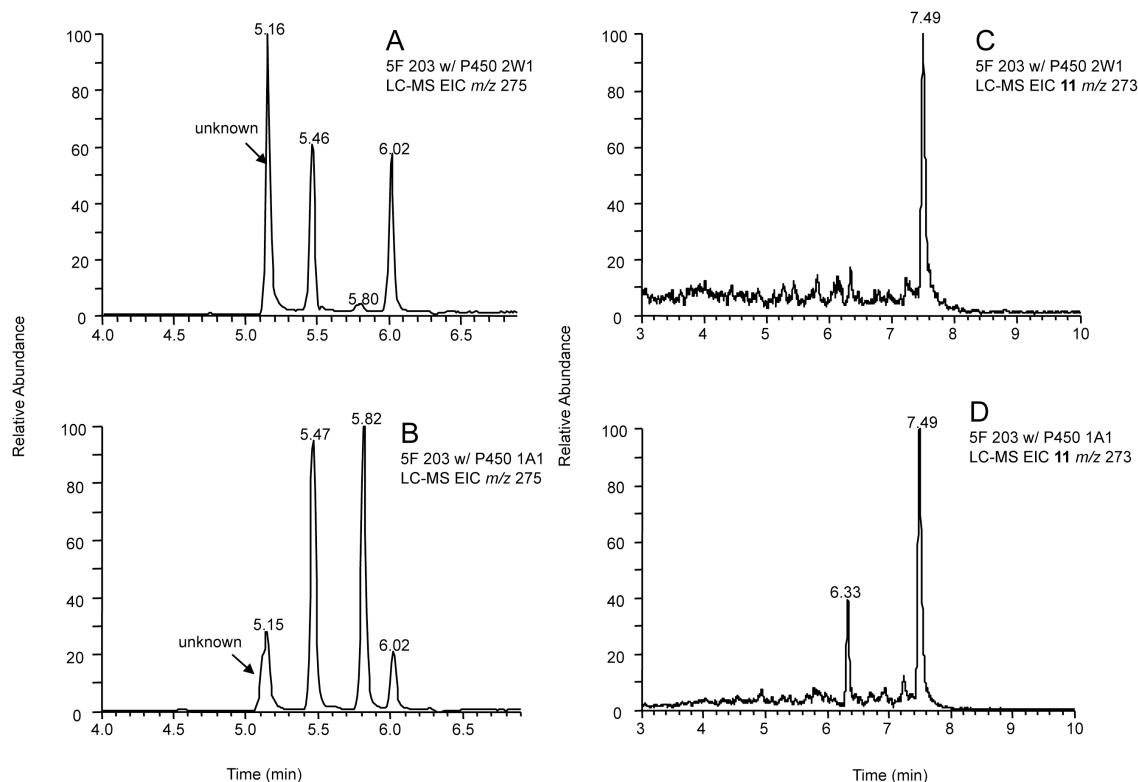
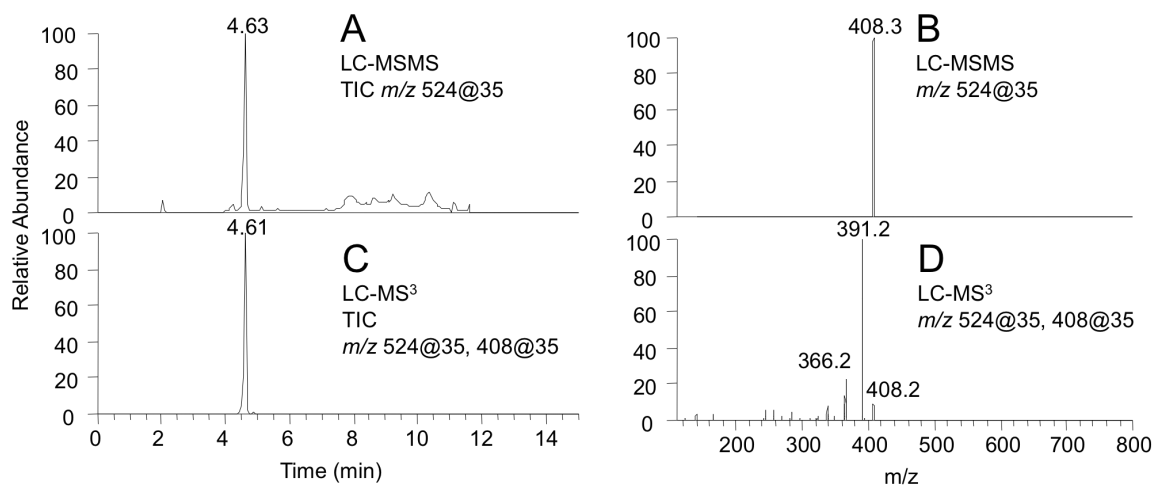


Figure S10. LC-MS chromatograms of 5F 203 oxidation products formed by P450s 2W1 and 1A1



(A) Extracted ion chromatogram of m/z 275 (from incubation of 5F 230 with P450 2W1, **8a**, t_R 5.46 min, **8b**, t_R 5.80 min, **10**, t_R 6.02 min). (B) Extracted ion chromatogram of m/z 275, (from incubation of 5F 230 with P450 1A1, **8a**, t_R 5.47 min, **8b**, t_R 5.82 min, **10**, t_R 6.02 min). (C) Extracted ion chromatogram of m/z 273 (from incubation of 5F 230 with P450 2W1, **11**, t_R 7.49 min). (D) Extracted ion chromatogram of m/z 273 (from incubation of 5F 230 with P450 1A1, **11**, t_R 7.49 min).

Figure S11. LC-MS/MS and LC-MS³ chromatograms and CID spectra showing the presence of a dGuo adduct with derived from synthetic **10**.



(A) Total ion chromatogram of m/z 524 product ion. (B) LC-MS/MS spectrum of the peak at t_R 4.63 min. (C) Total ion chromatogram of CID of the m/z 408 product ion. (D) LC-MS³ spectrum of the peak at t_R 4.61 min.