Supporting Information

Discovery of furanone-based radiopharmaceuticals for diagnostic targeting of COX-1 in ovarian cancer

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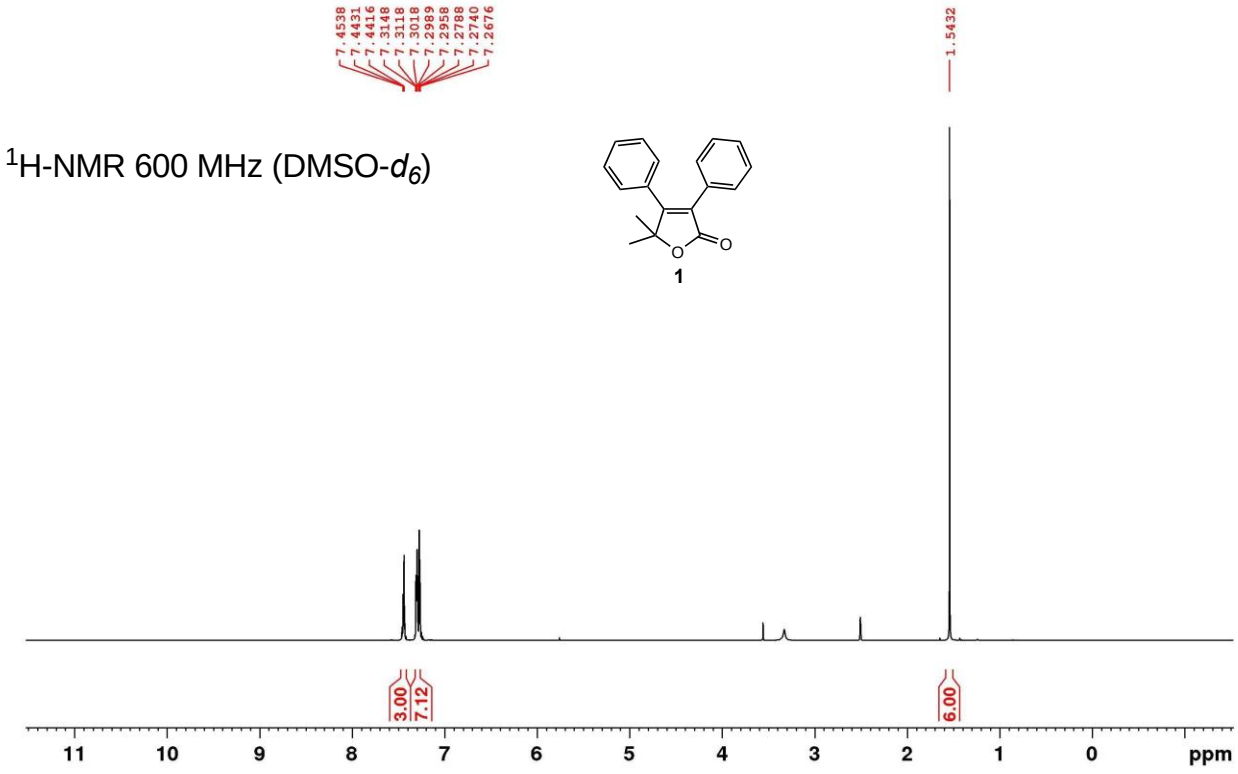

Figure S1. ^{1}H NMR spectrum of compound **1**.

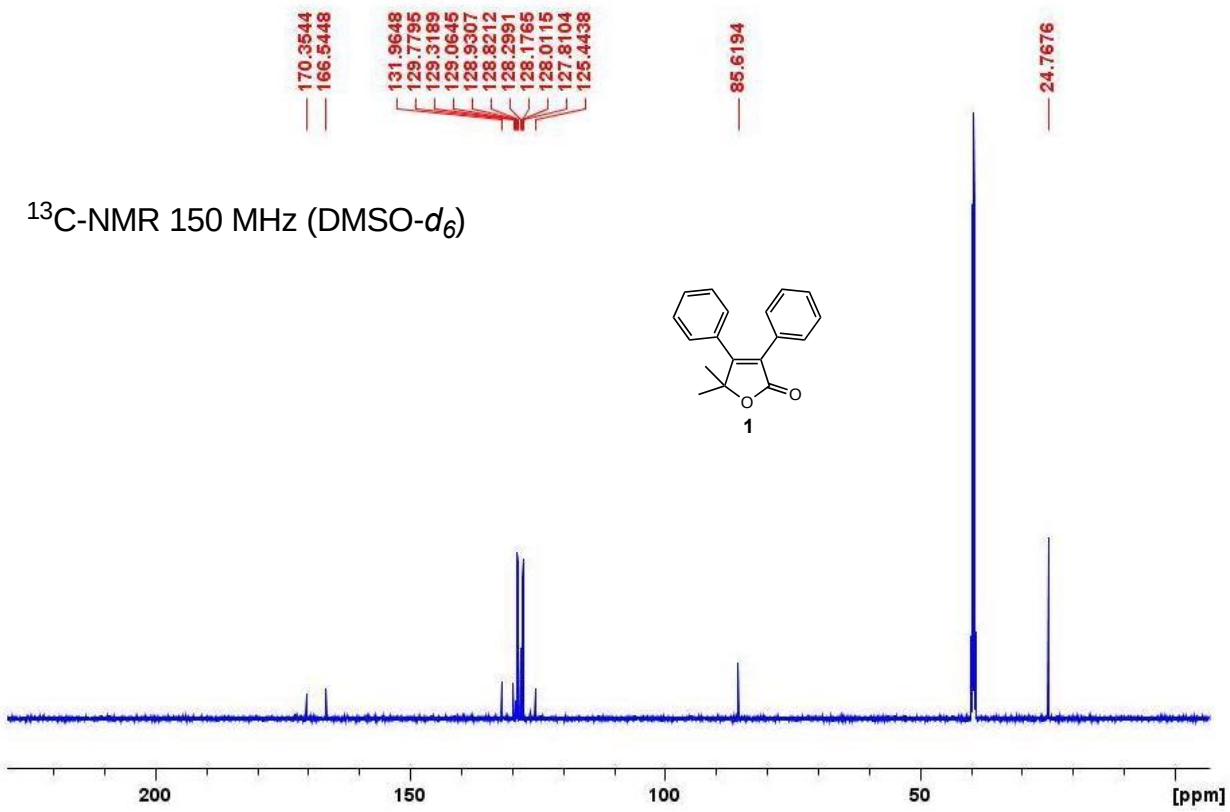

Figure S2. ^{13}C NMR spectrum of compound **1**.

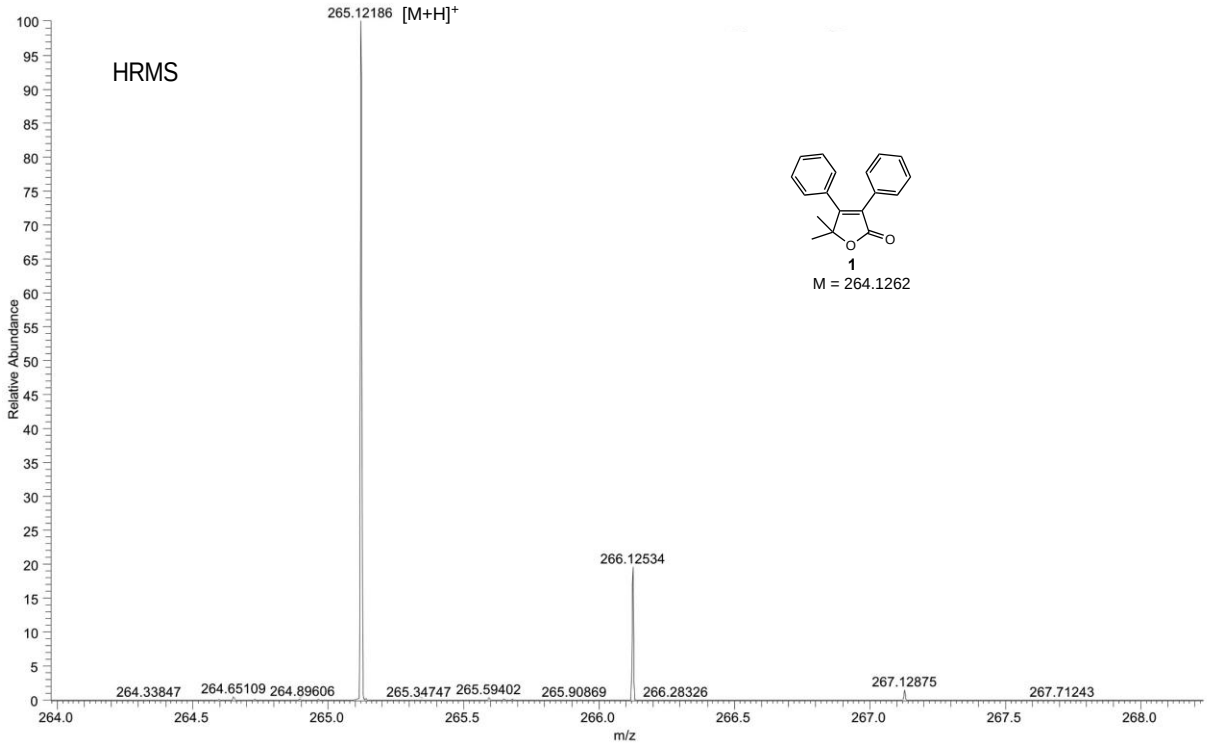

Figure S3 HRMS spectrum of compound **1,** *m/z* calculated for $[C_{18}H_{16}O_2 + H]^+$ 265.1262, found 265.1218.

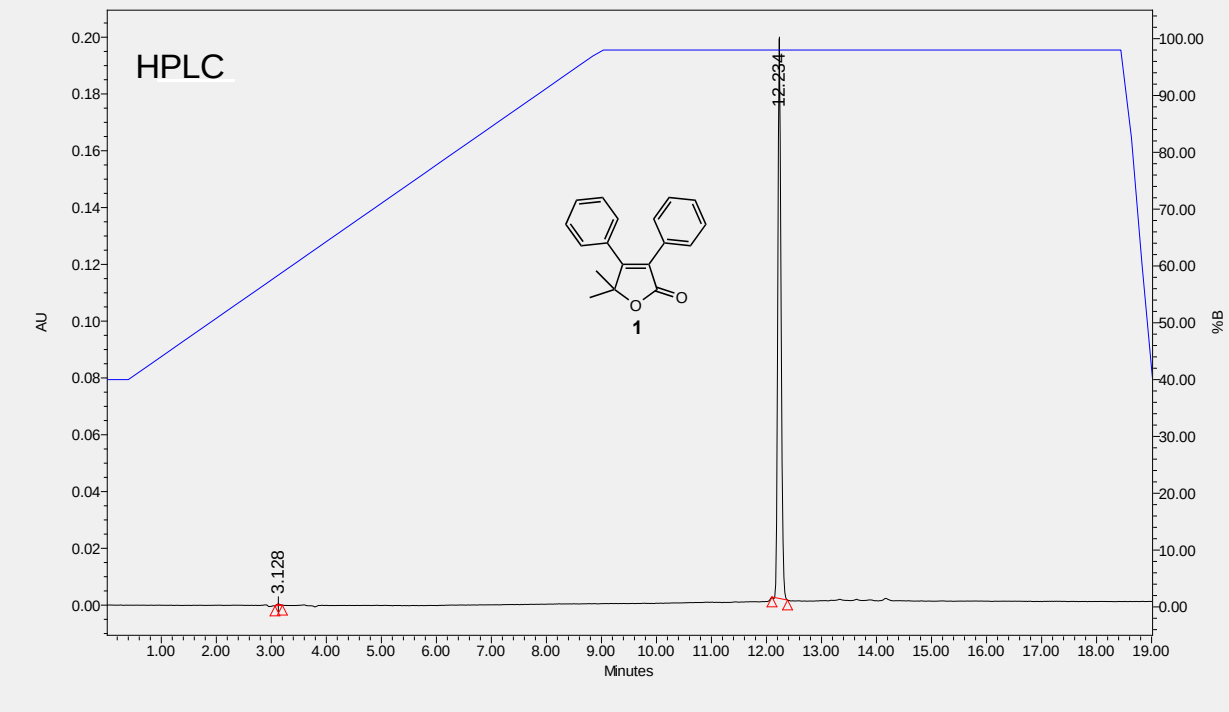

Figure S4. HPLC chromatogram of compound **1**.

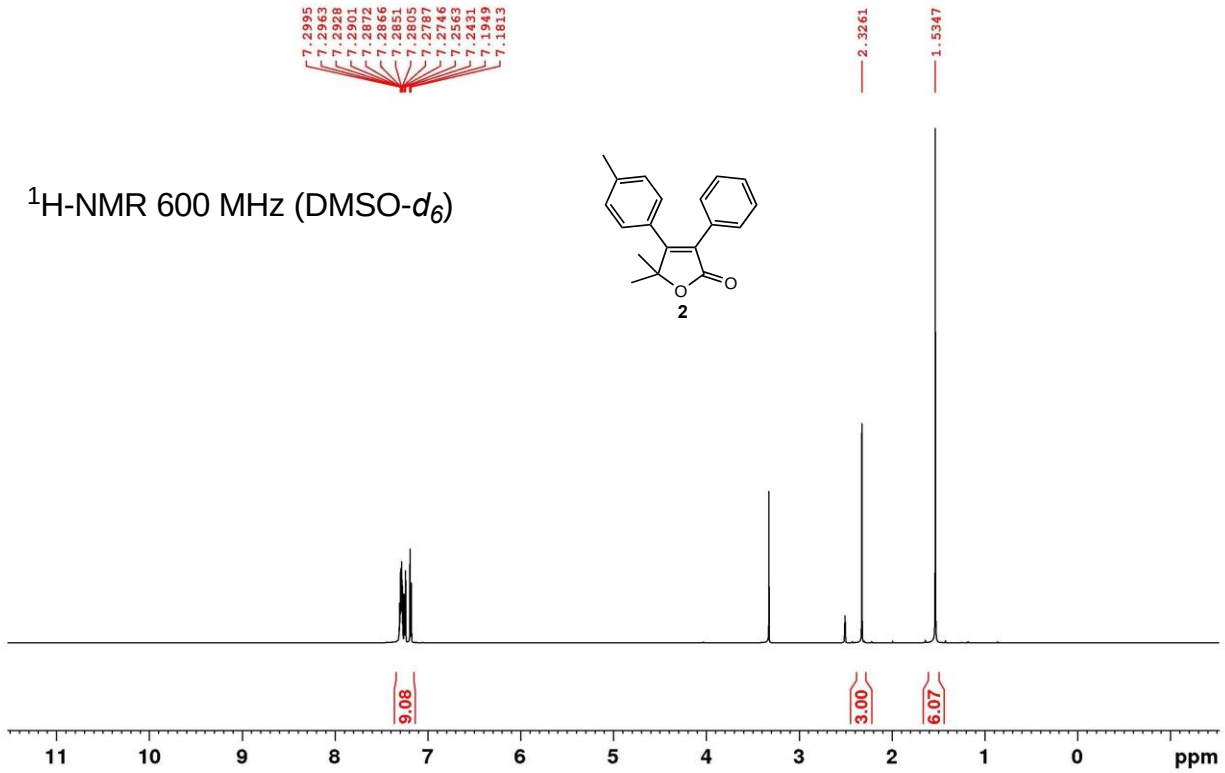

Figure S5. ^{1}H NMR spectrum of compound **2**.

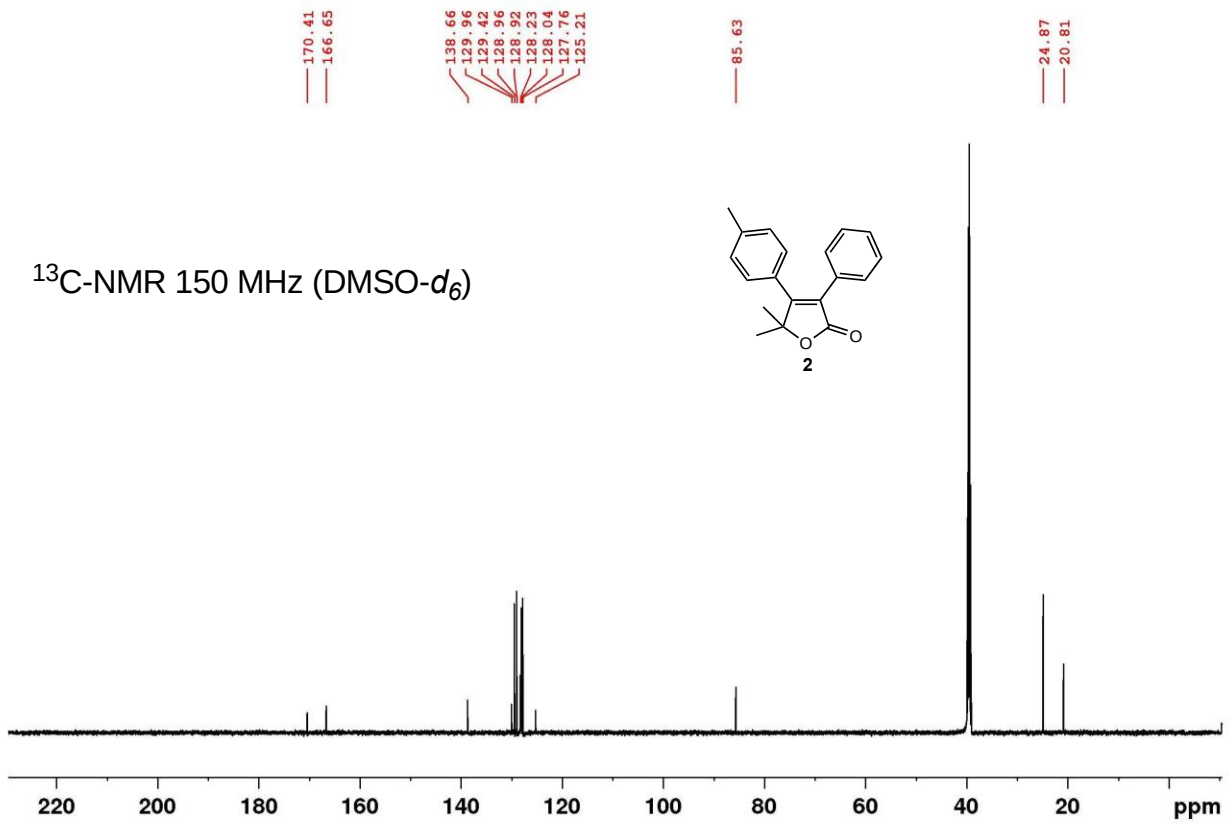

Figure S6. ^{13}C NMR spectrum of compound **2**.

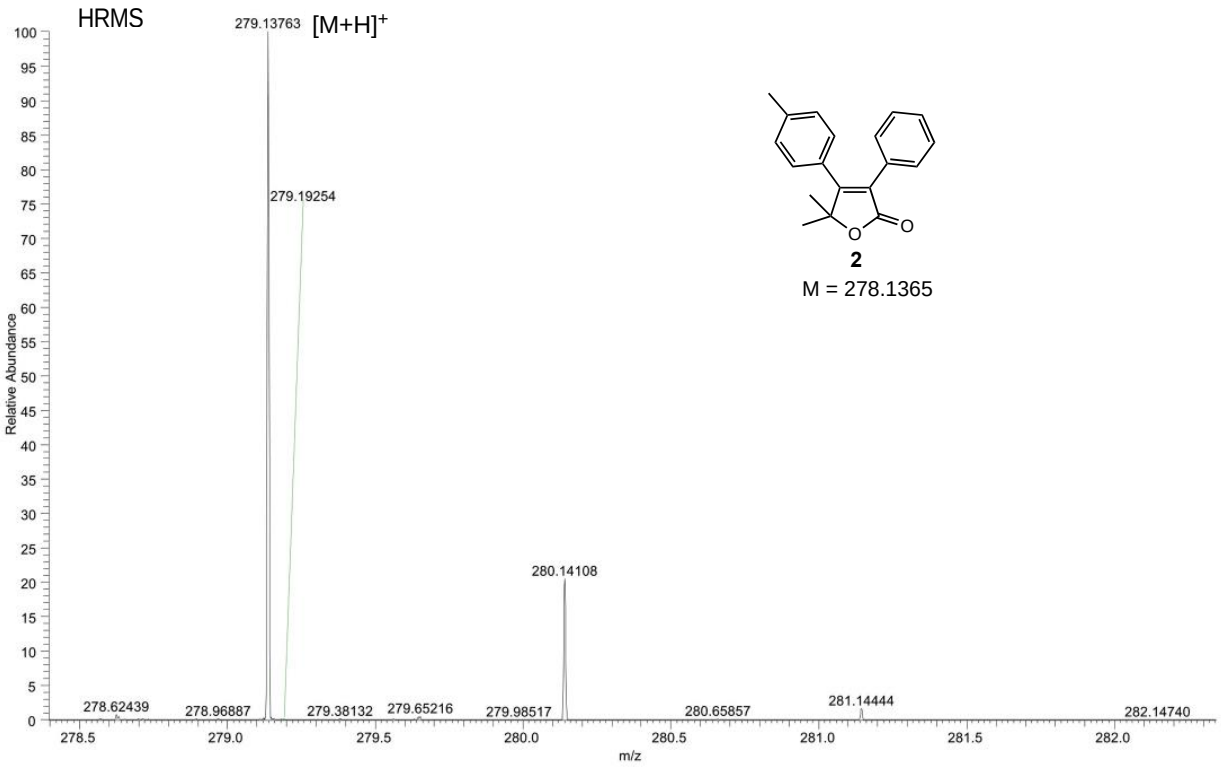

Figure S7. HRMS spectrum of compound **2,** *m/z* calculated for $[C_{19}H_{18}O_2 + H]^+$ 279.1365, found 279.1376.

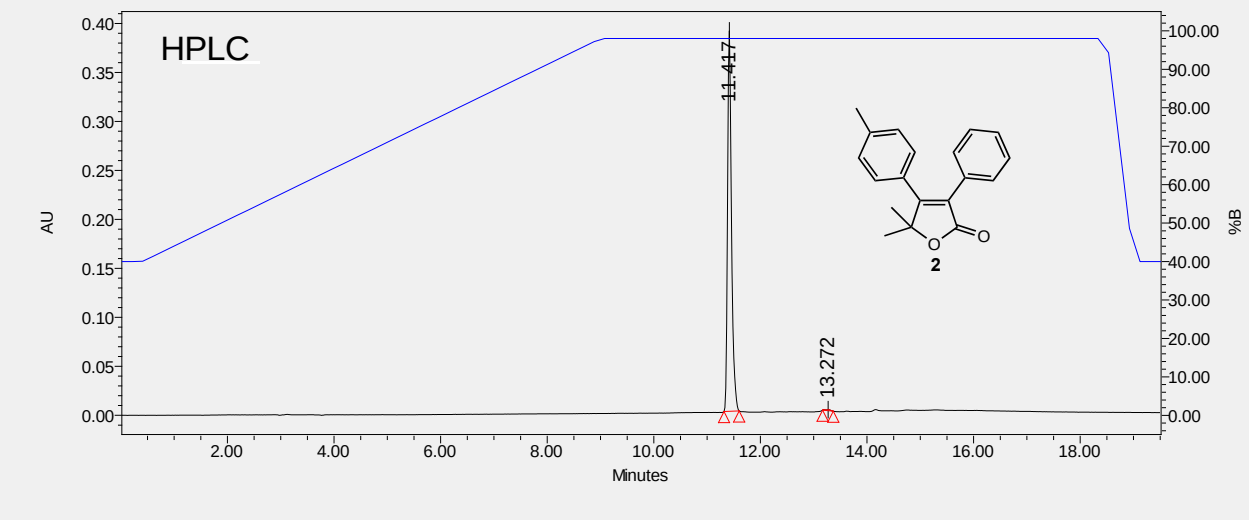

Figure S8. HPLC chromatogram of compound **2**.

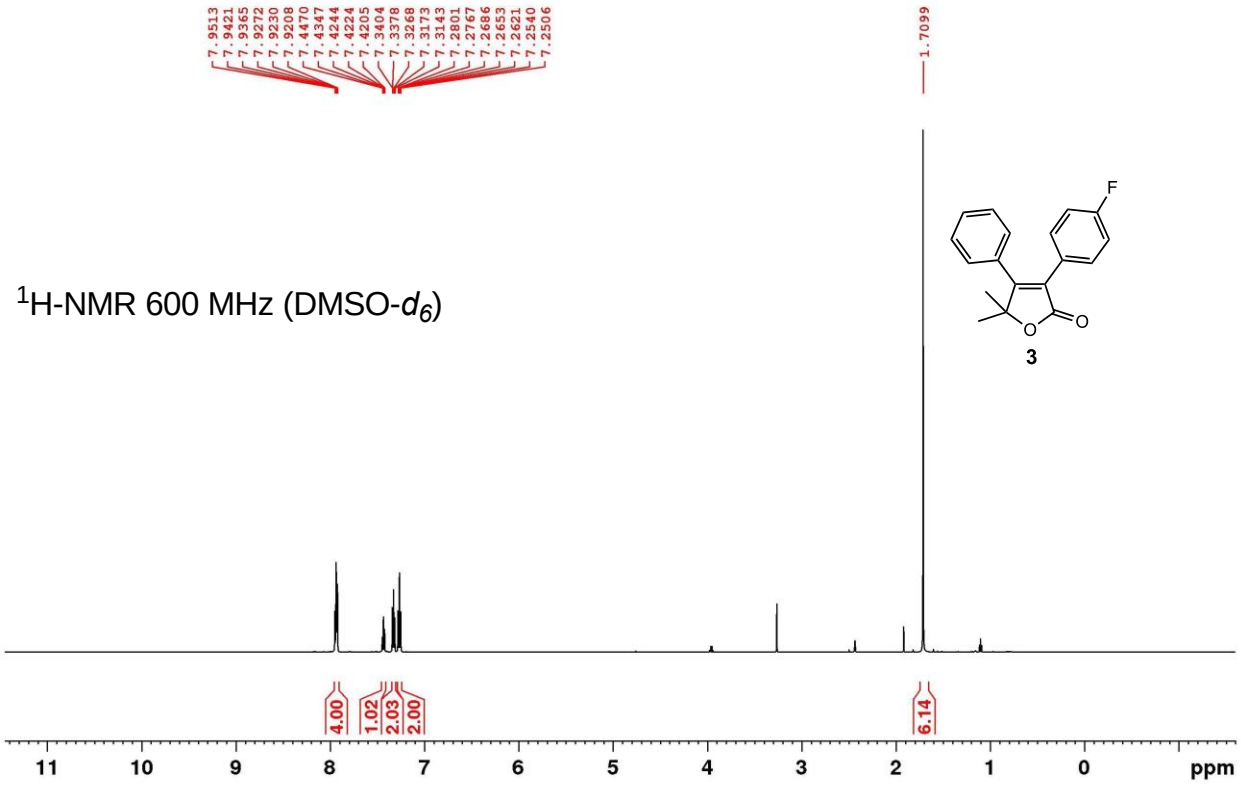

Figure S9. ^{1}H NMR spectrum of compound **3**.

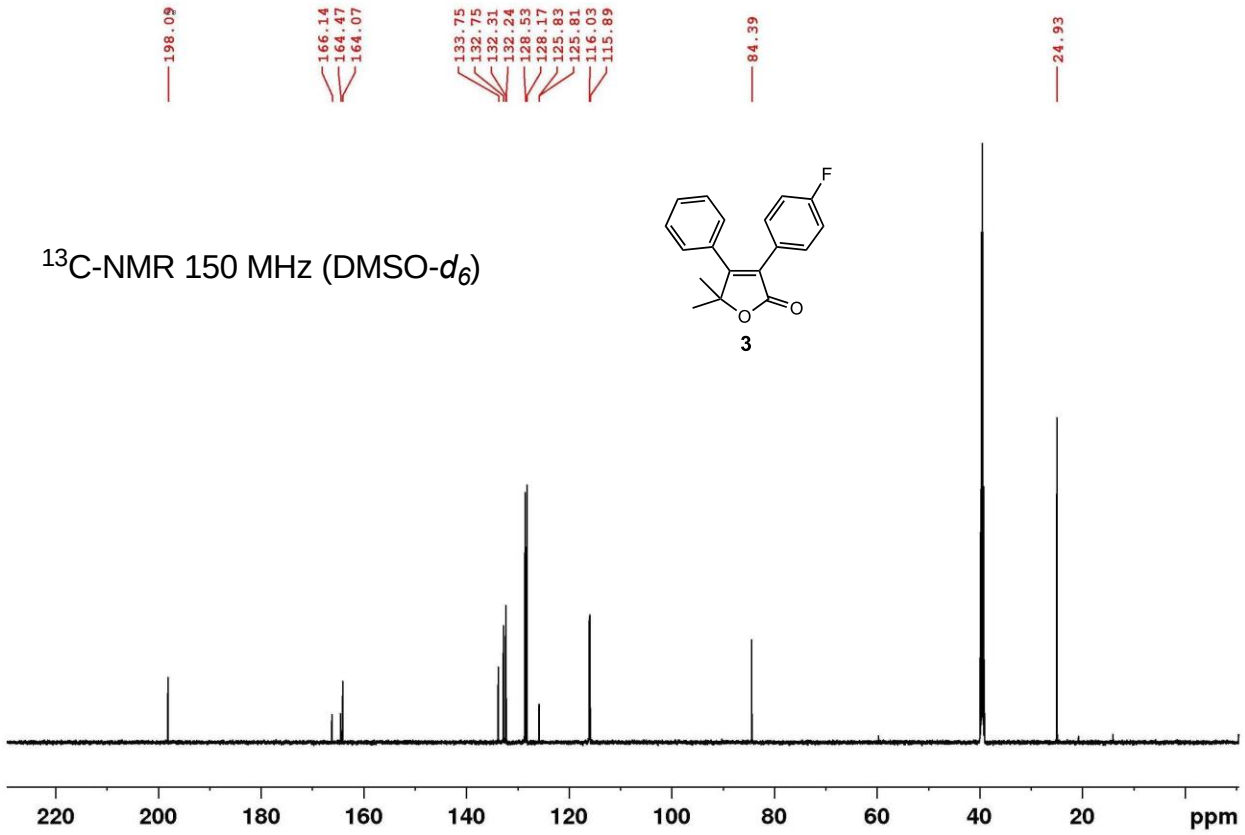

Figure S10. ^{13}C NMR spectrum of compound **3**.

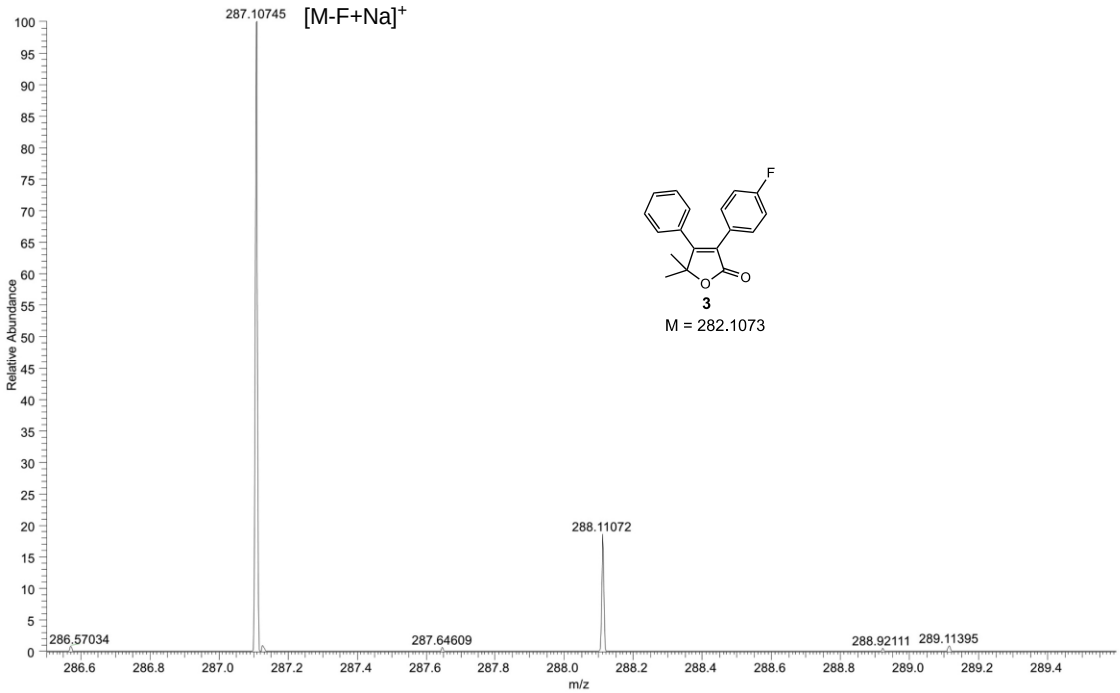

Figure S11. HRMS spectrum of compound **3,** *m/z* calculated for $[C_{18}H_{15}FO_2 - F + Na]^+$ 287.1073, found 287.1074.

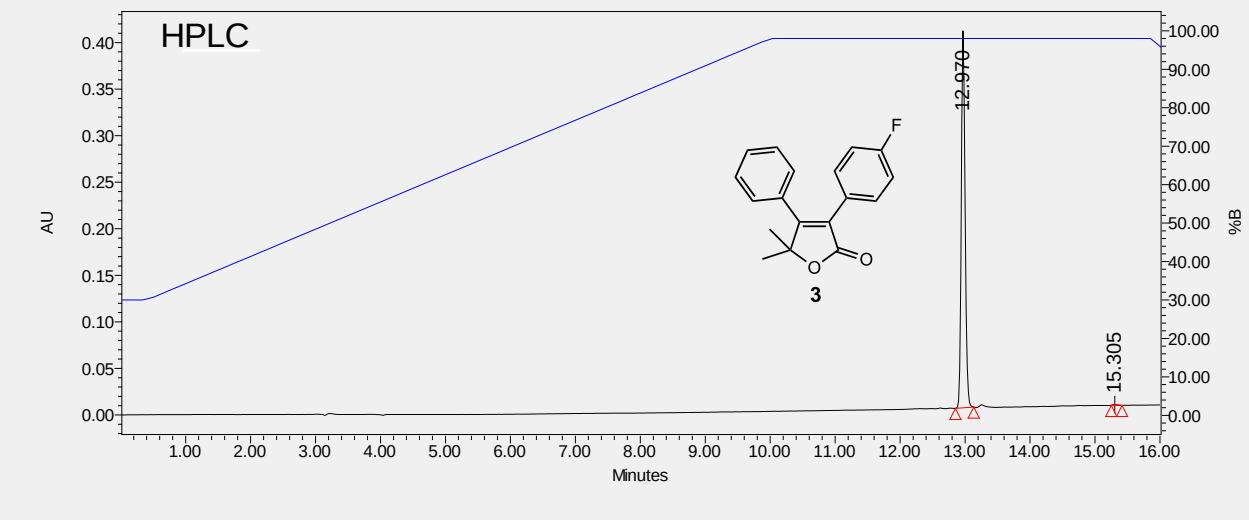

Figure S12. HPLC chromatogram of compound **3**.

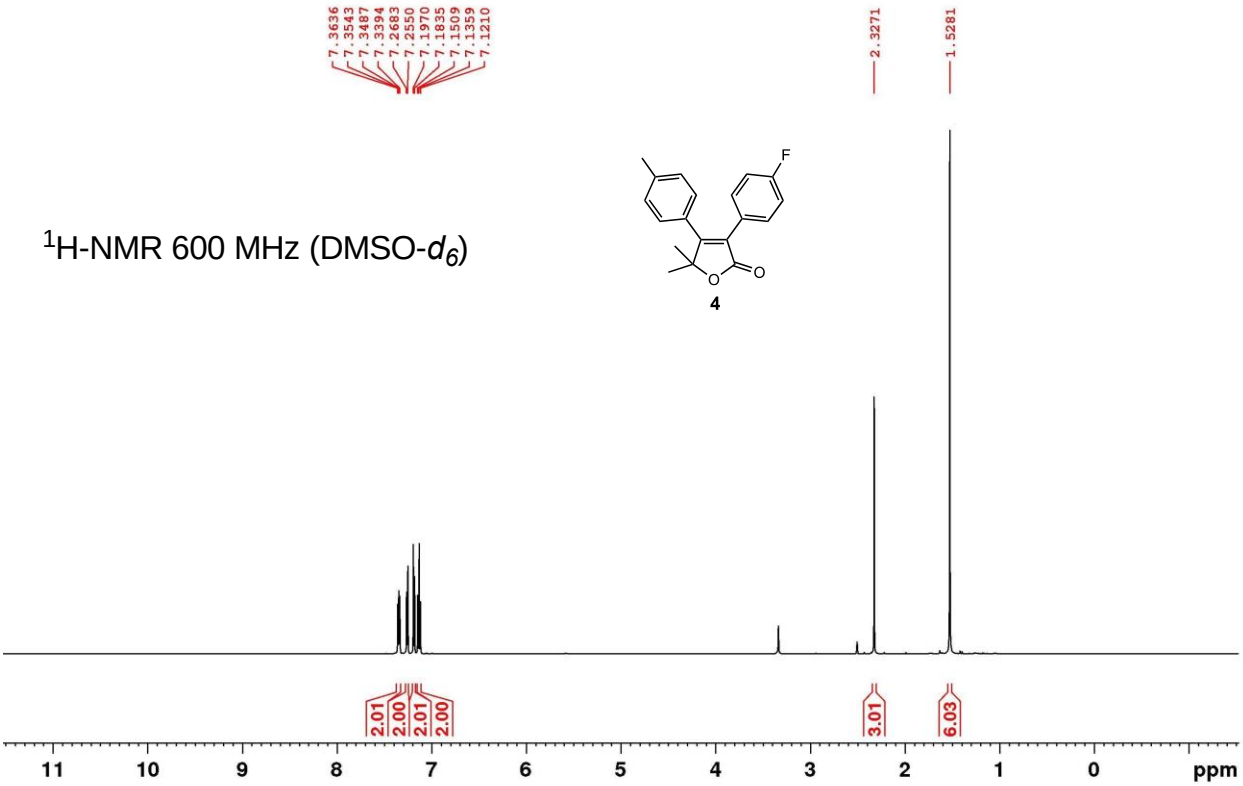

Figure S13. ^{1}H NMR spectrum of compound **4**.

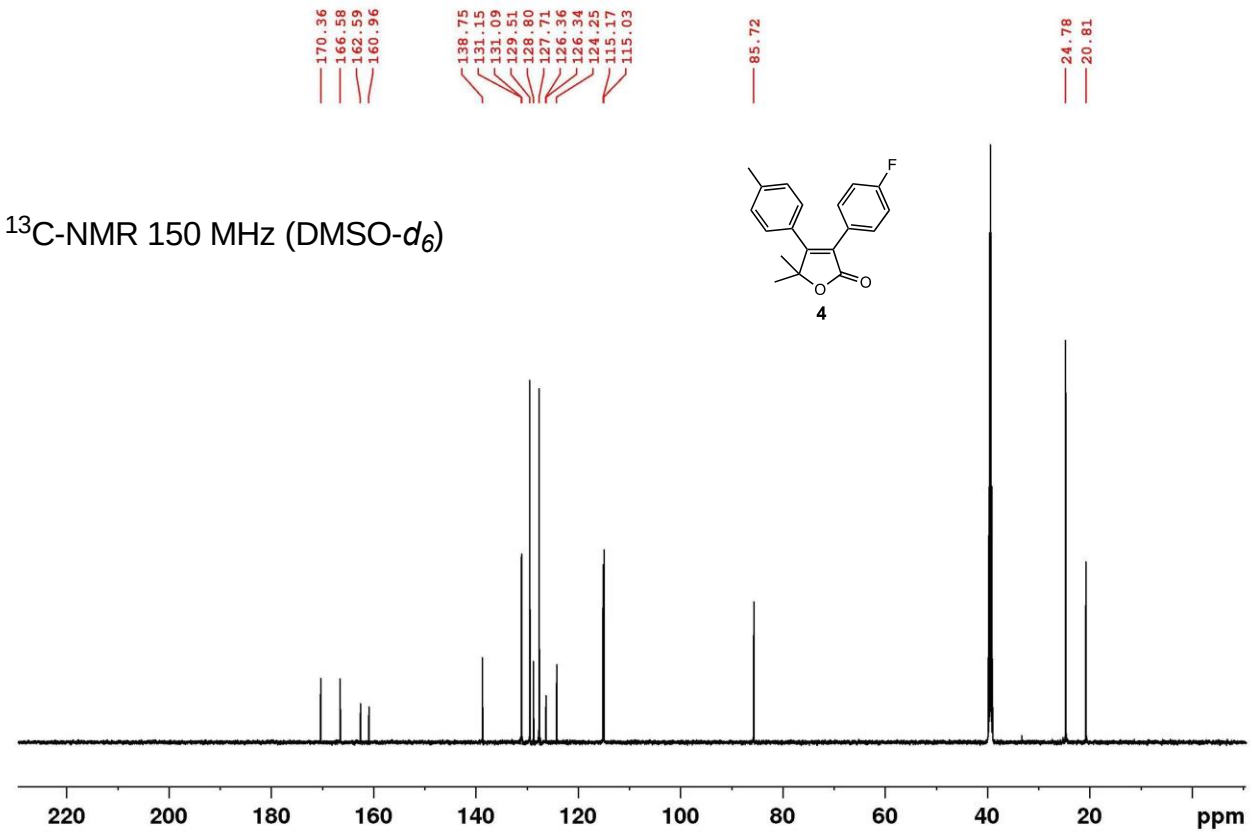

Figure S14. ^{13}C NMR spectrum of compound **4**.

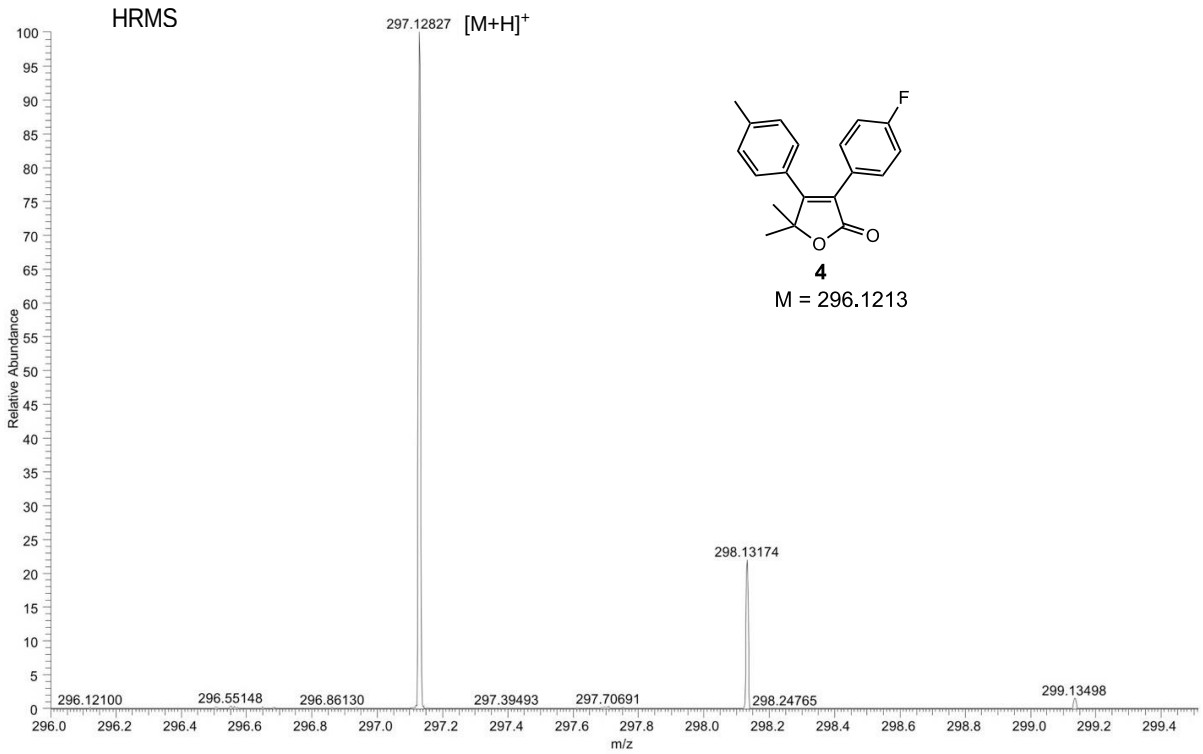

Figure S15. HRMS spectrum of compound **4,** *m/z* calculated for $[C_{19}H_{17}FO_2 + H]^+$ 297.1213, found 297.1282.

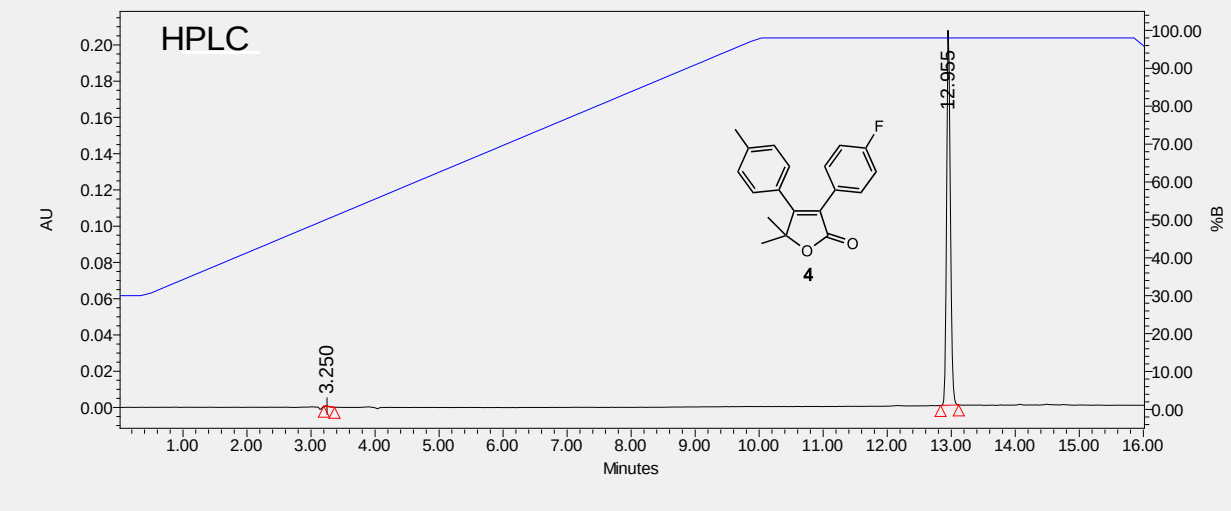

Figure S16. HPLC chromatogram of compound **4**.

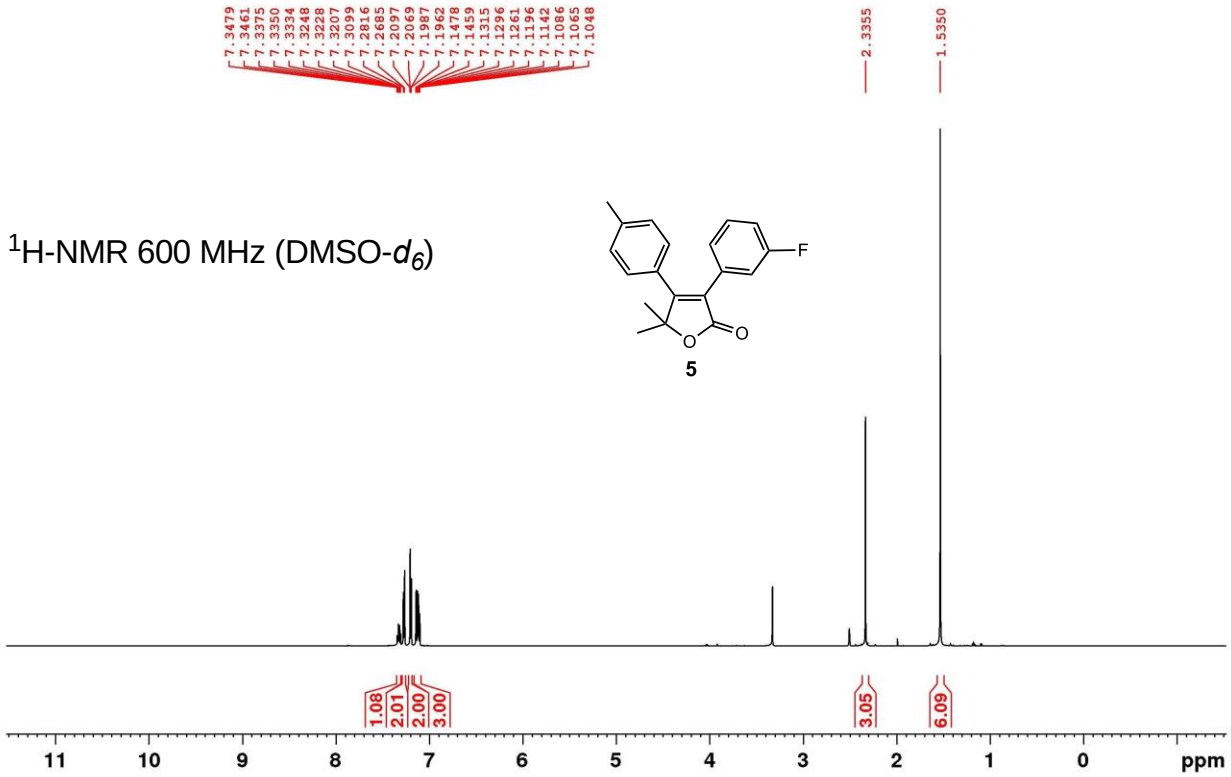

Figure S17. ^{1}H NMR spectrum of compound **5**.

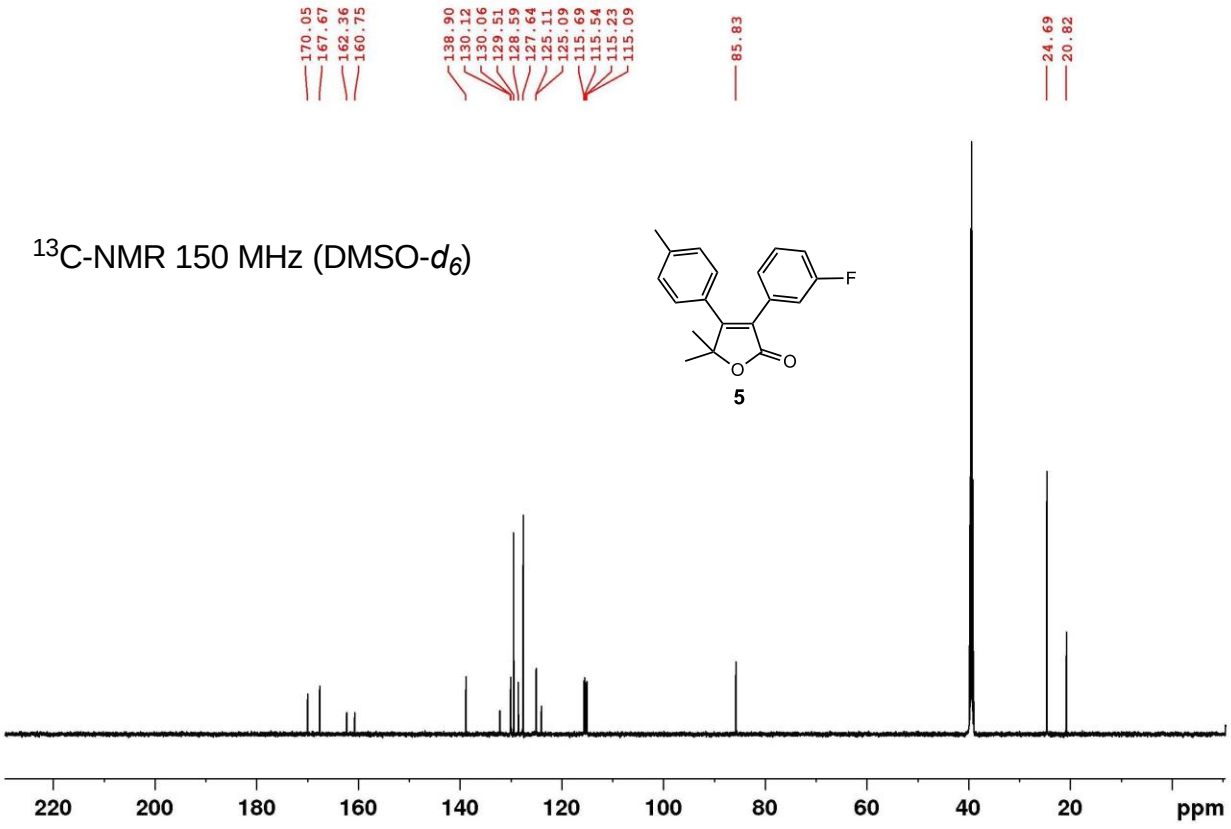

Figure S18. ^{13}C NMR spectrum of compound **5**.

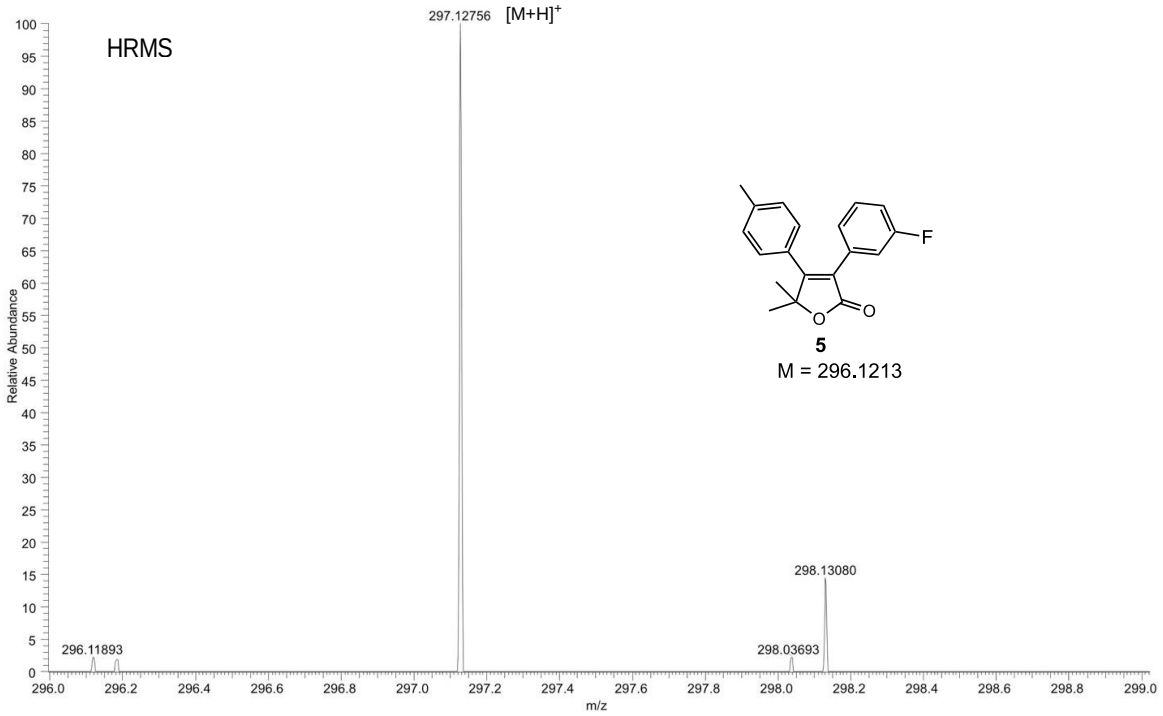

Figure S19. HRMS spectrum of compound **5,** *m/z* calculated for $[C_{19}H_{17}FO_2 + H]^+$ 297.1213, found 297.1275.

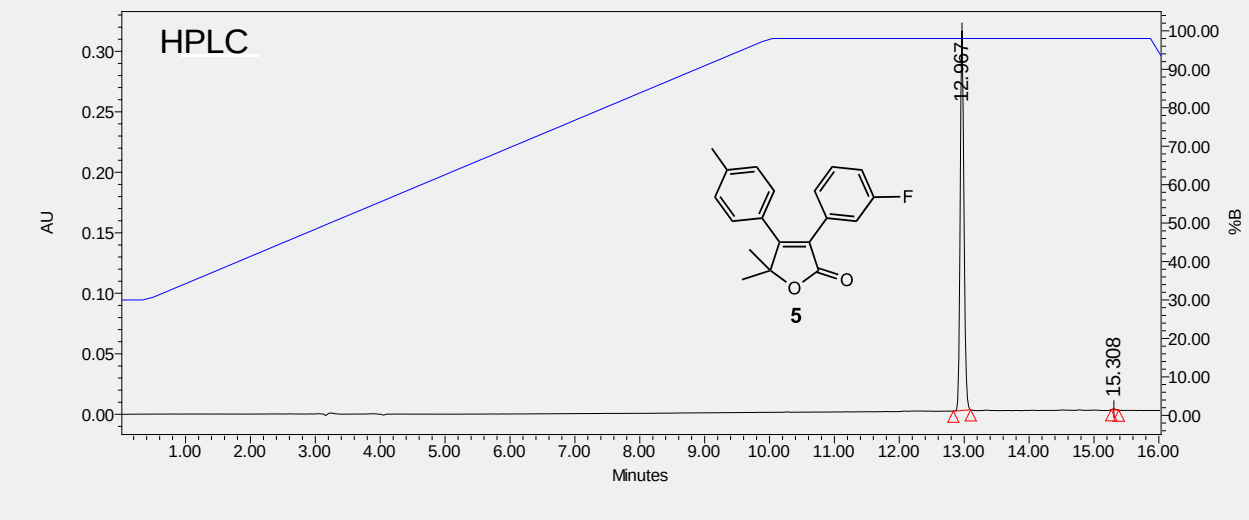

Figure S20. HPLC chromatogram of compound **5**.

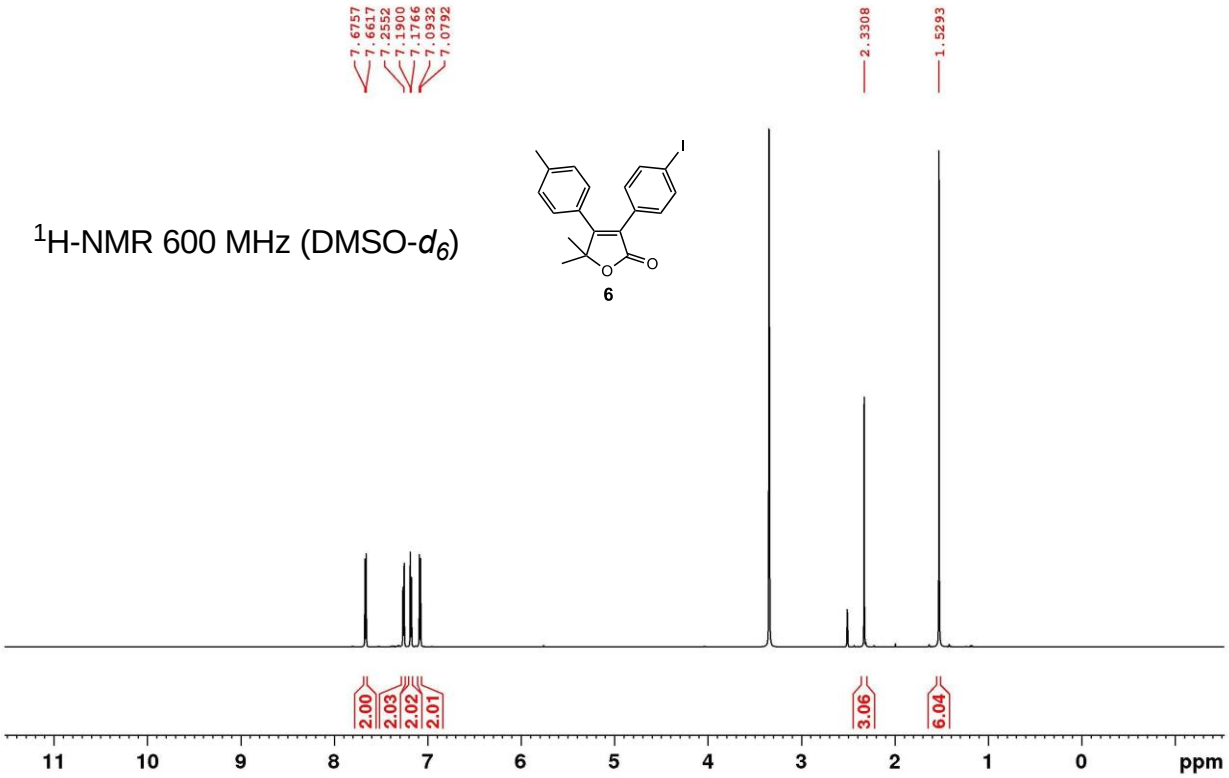

Figure S21. ^{1}H NMR spectrum of compound **6**.

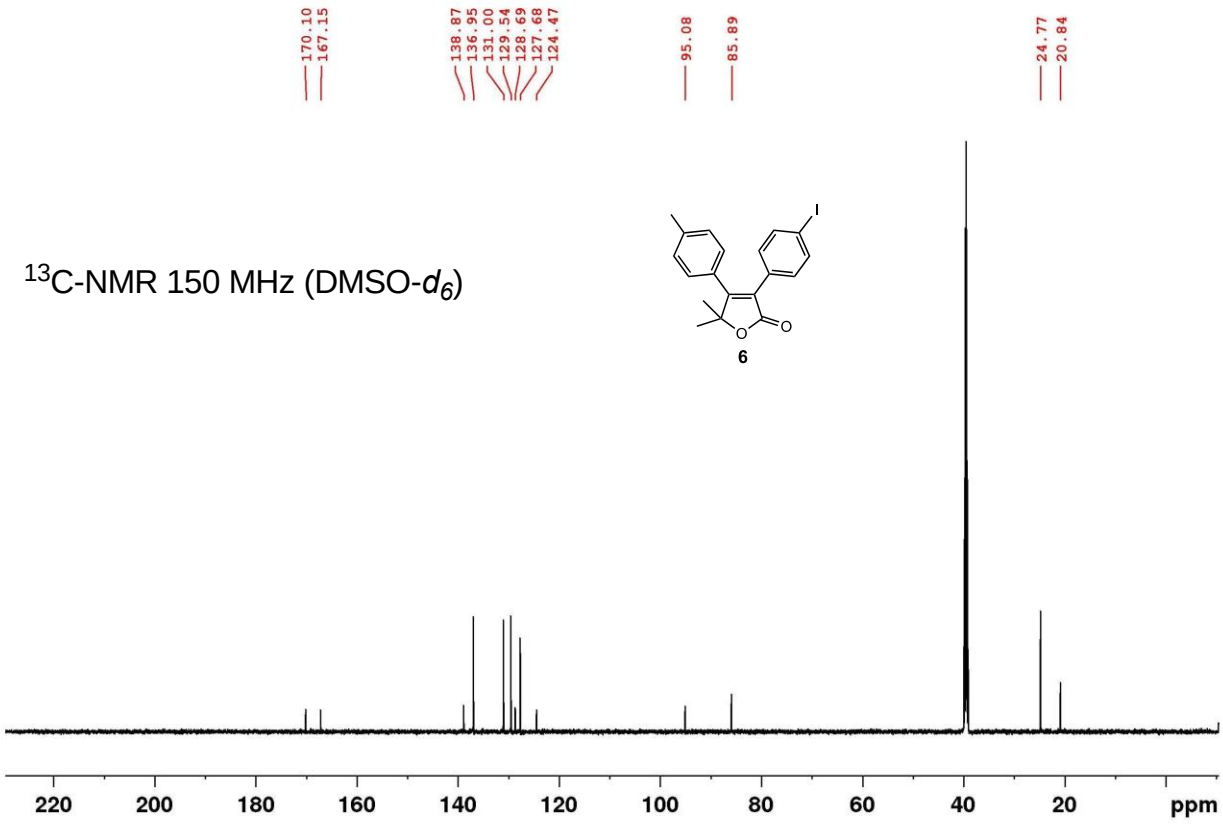

Figure S22. ^{13}C NMR spectrum of compound **6**.

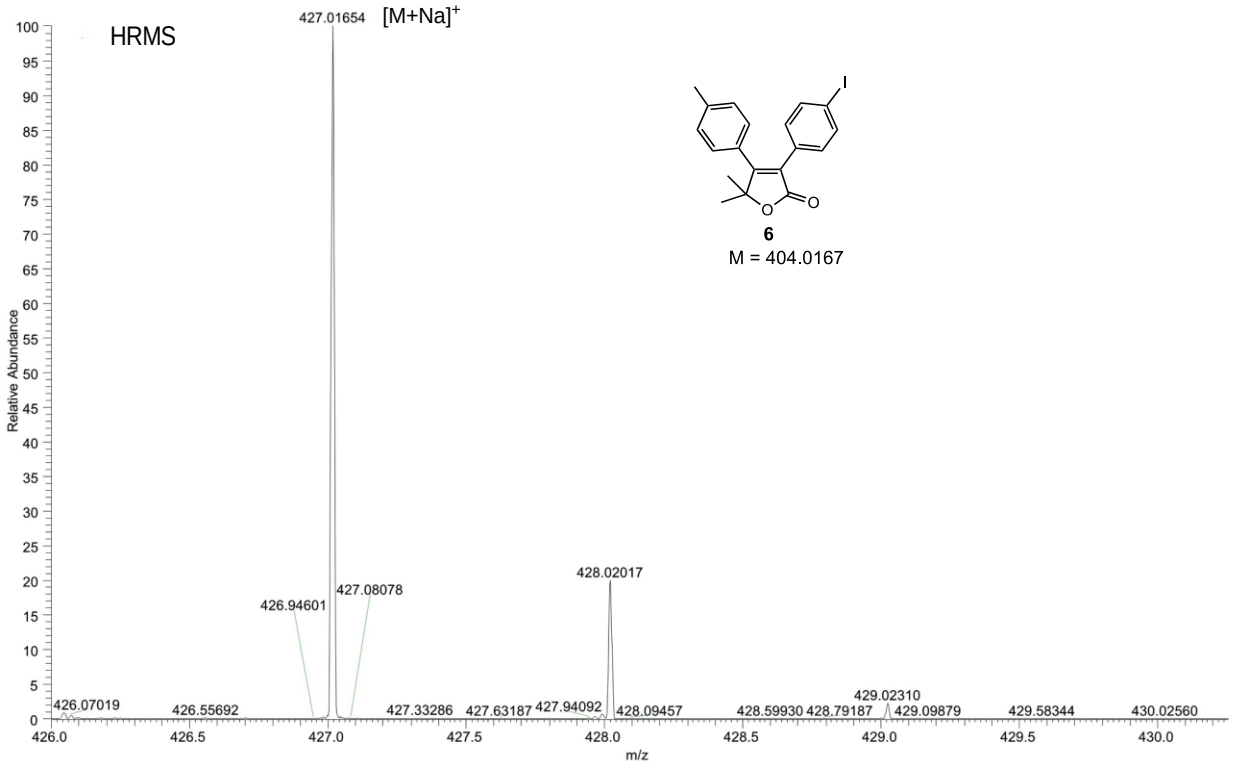

Figure S23. HRMS spectrum of compound **6,** *m/z* calculated for 427.0167 $[C_{19}H_{17}IO_2 + Na]^+$, found 427.0165.

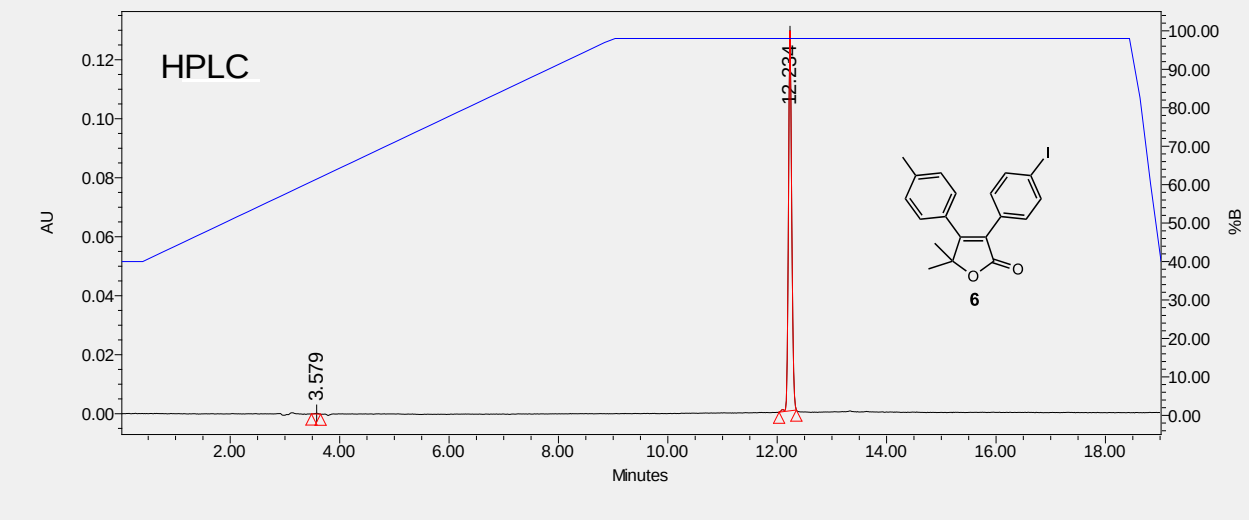

Figure S24. HPLC chromatogram of compound **6**.

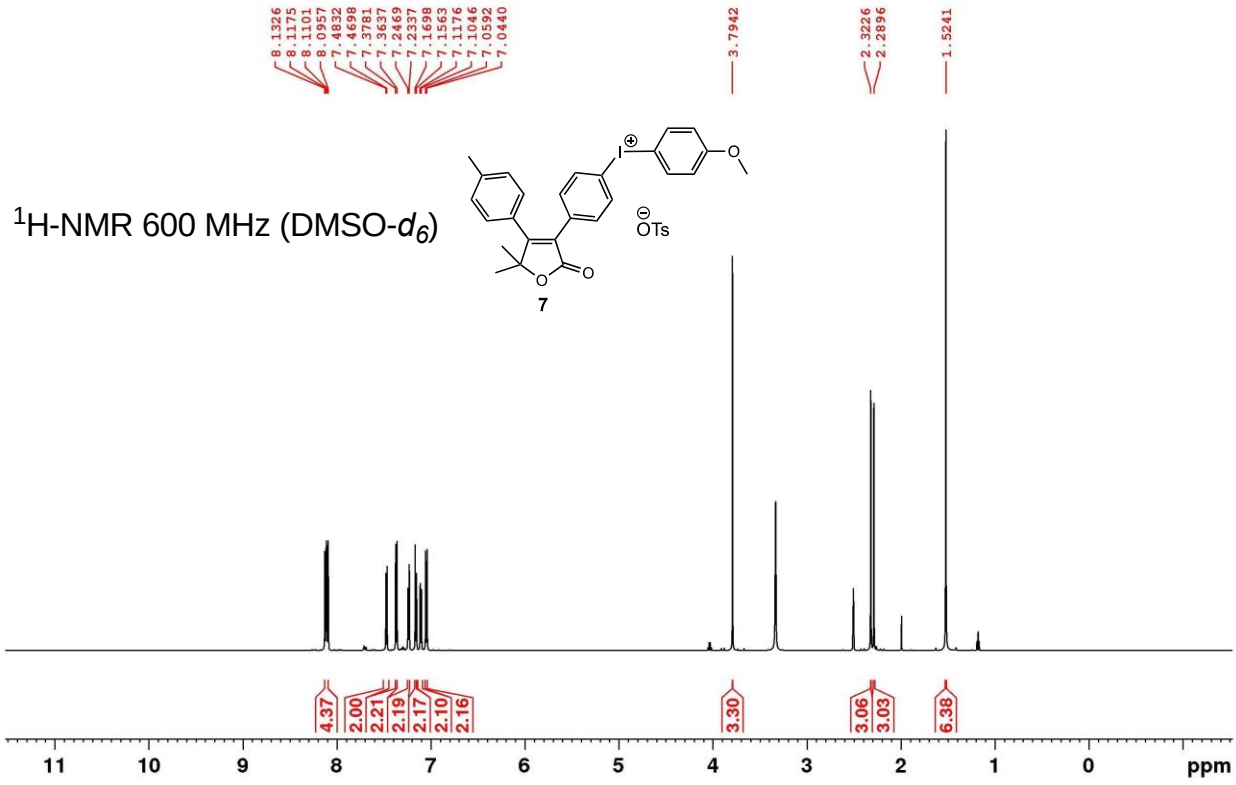

Figure S25. ^{1}H NMR spectrum of compound **7**.

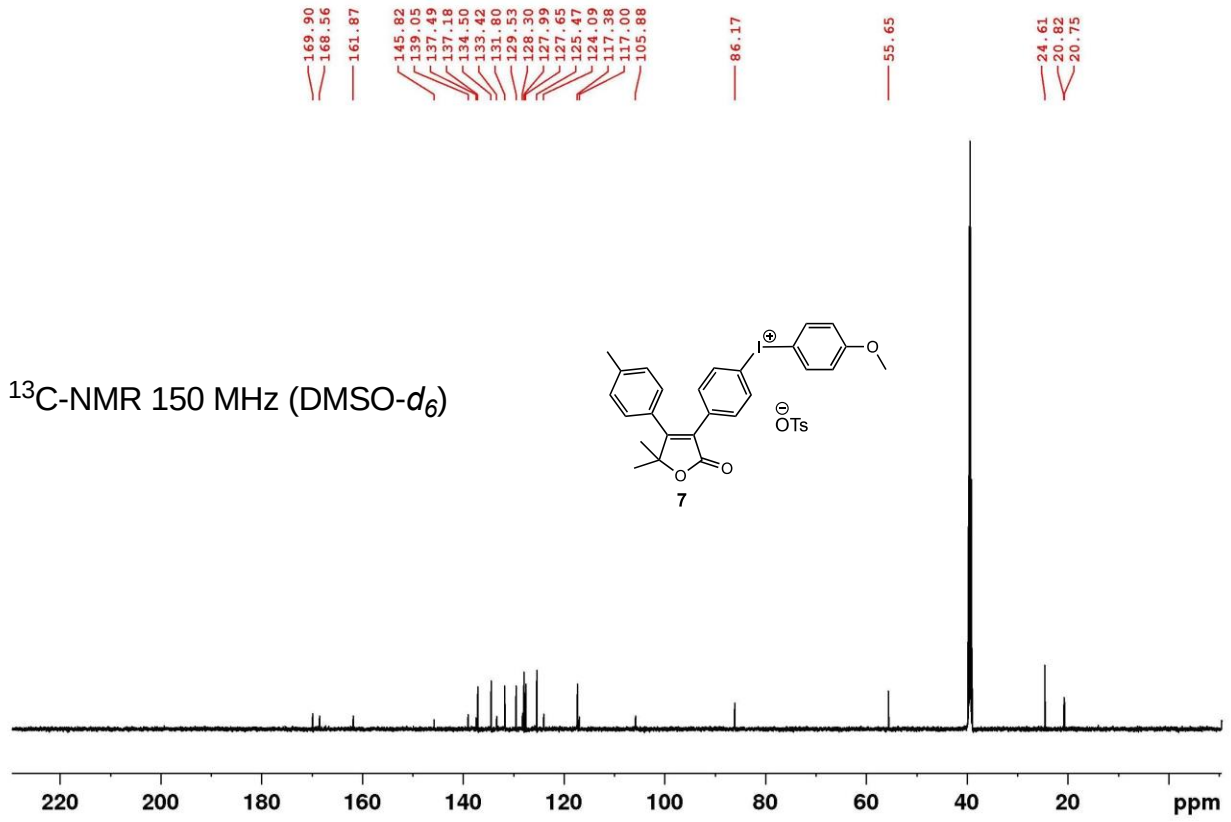

Figure S26. ^{13}C NMR spectrum of compound **7**.

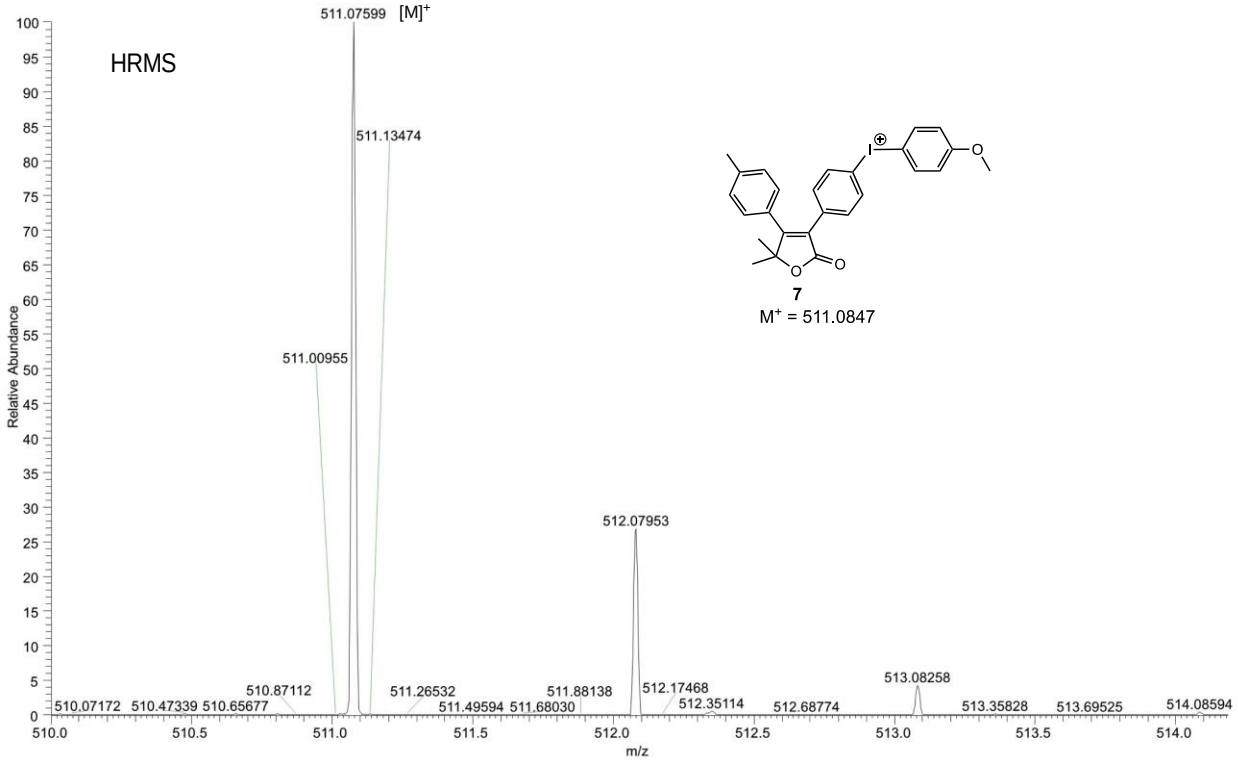

Figure S27. HRMS spectrum of compound **7,** *m/z* calculated for 511.0847 $[C_{26}H_{24}IO_3]^+$, found 511.0759.

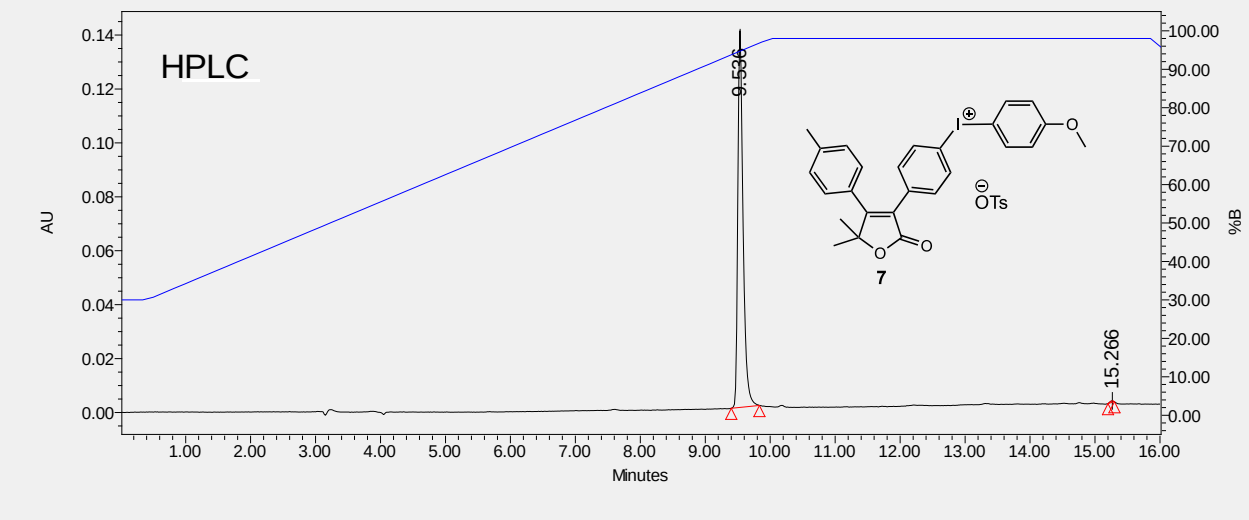

Figure S28. HPLC chromatogram of compound **7**.

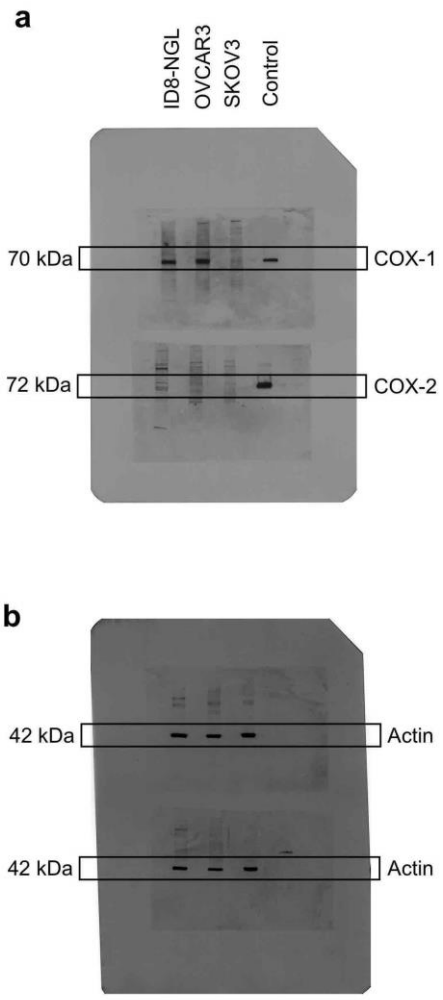

Figure S29: Full-length Western blots showing (a) COX-1 and COX-2 bands in ID8-NGL, OVCAR3 and SKOV3 cancer cells, and (b) actin bands as loading control.

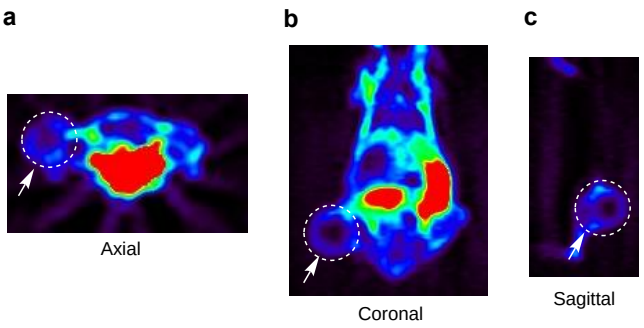

Figure S30: In vivo [^{18}F]FDF PET (650 μCi *(0.0241 GBq), intraperitoneal injection, t = 30 min*) images of a female nude mouse bearing a SKOV3/COX-1 subcutaneous xenograft tumor in (a) axial, (b) coronal, and (c) sagittal views.

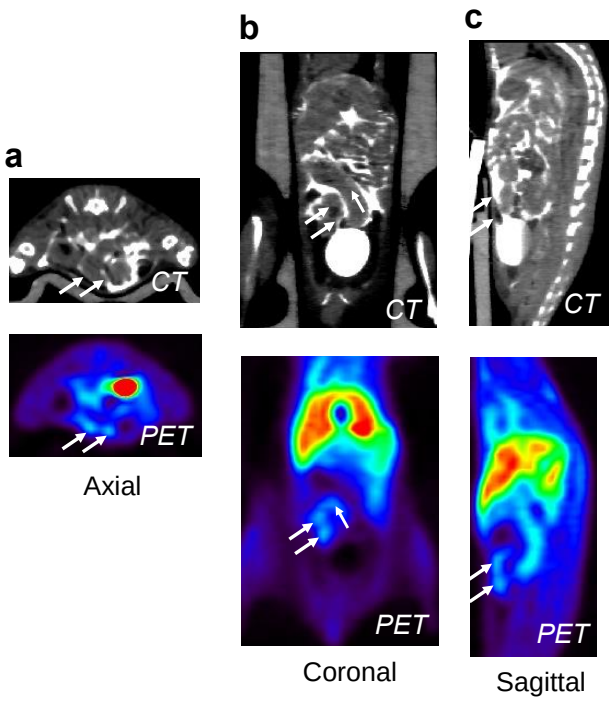

***Figure S31**: In vivo [^{18}F]FDF PET with (612 μCi (0.0226 GBq), retro-orbital injection, t = 5 min) images of a female nude mouse bearing a SKOV3/COX-1 intraperitoneal tumors in (a) axial, (b) coronal, and (c) sagittal views.*