

Supporting Information

Fluorination-Triggered Tandem Cyclization of Styrene-type Carboxylic Acid to Access 3-Aryl Isocoumarin Derivatives under Microwave Irradiation

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1. Screening the reaction condition

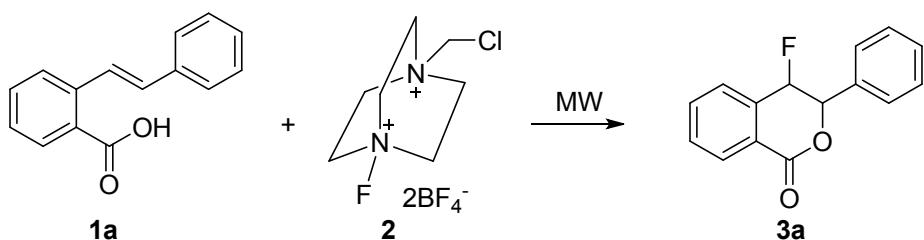


Table S1 Screening the molar ratio of reaction substrates^a

Entry	The molar ratio of 1a and 2	Yields (%) ^b
1	2:1	50
2	1:1	58
3	1:1.2	63
4	1:1.5	70
5	1:2.0	61

^a Reaction conditions: (E)-2-styrylbenzoic acid **1a** (0.2 mmol, 44.8 mg), Selectflour reagent **2**, in 3.0 mL CH₃CN solvent, 100 °C for 0.5 h.

^b Isolated yield.

2. Copies of spectra of products

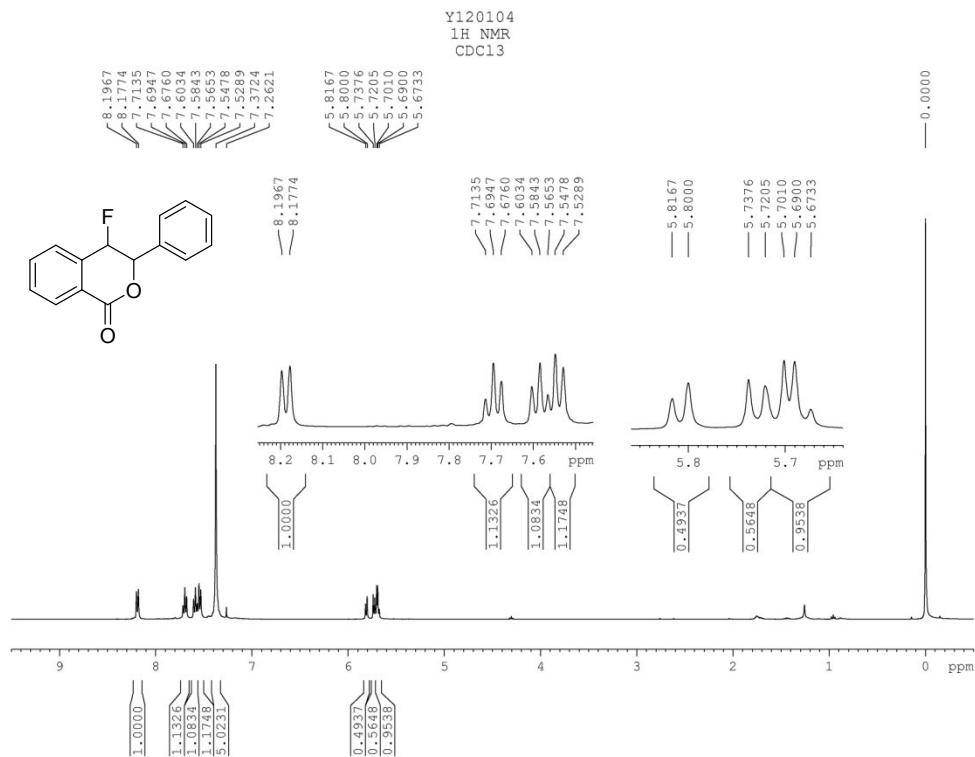


Fig. 1 ^1H NMR spectrum of compound **3a**

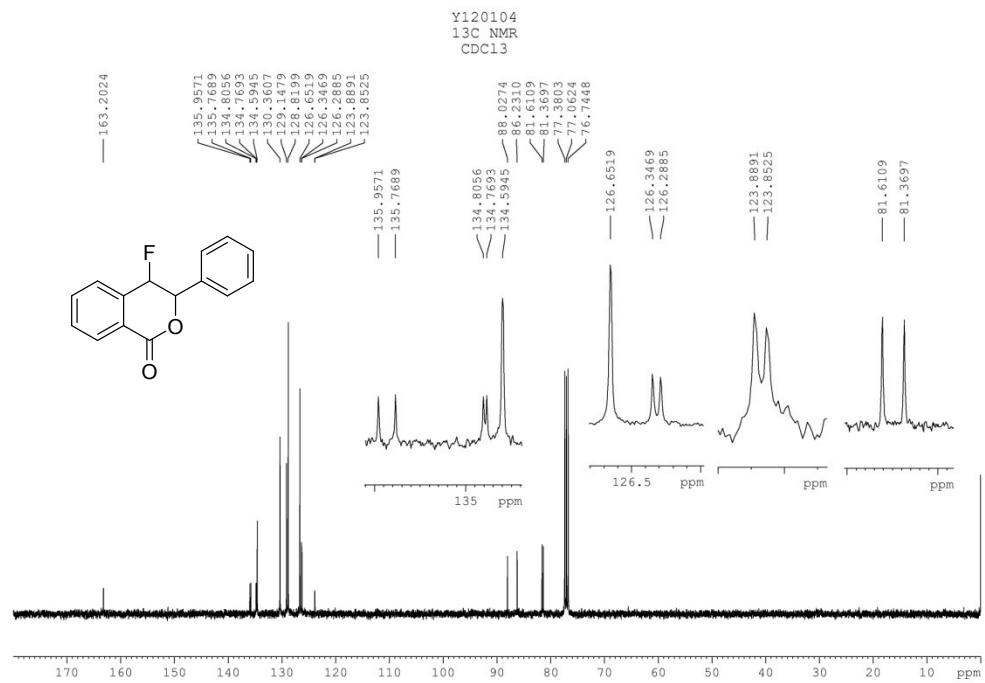


Fig. 2 ^{13}C NMR spectrum of compound **3a**

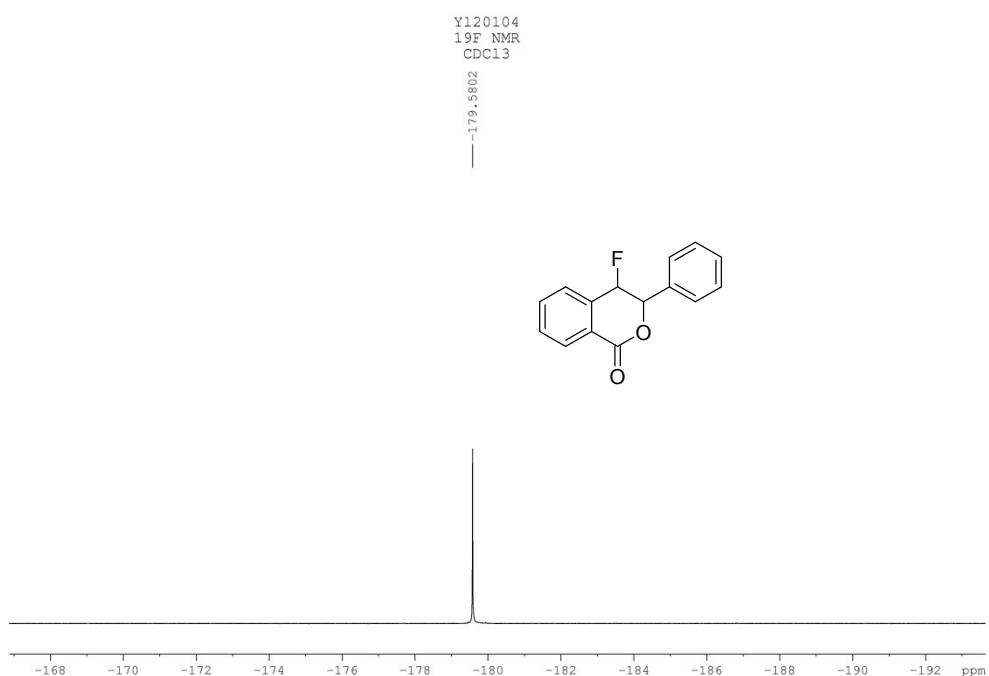


Fig. 3 ^{19}F NMR spectrum of compound **3a**

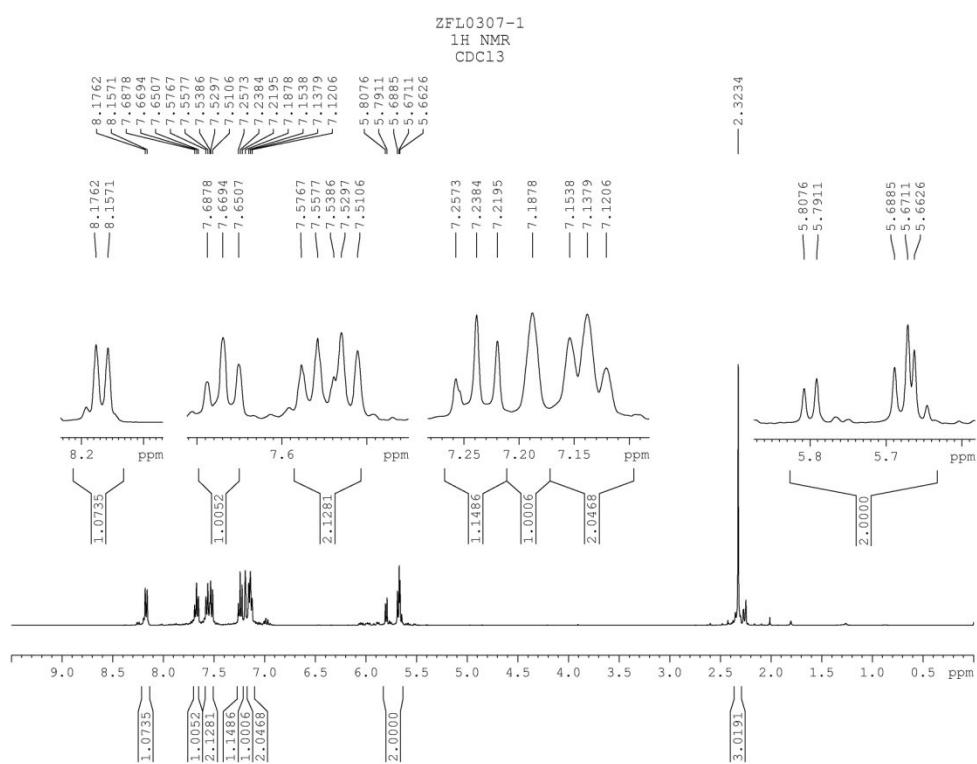


Fig. 4 ^1H NMR spectrum of compound **3b**

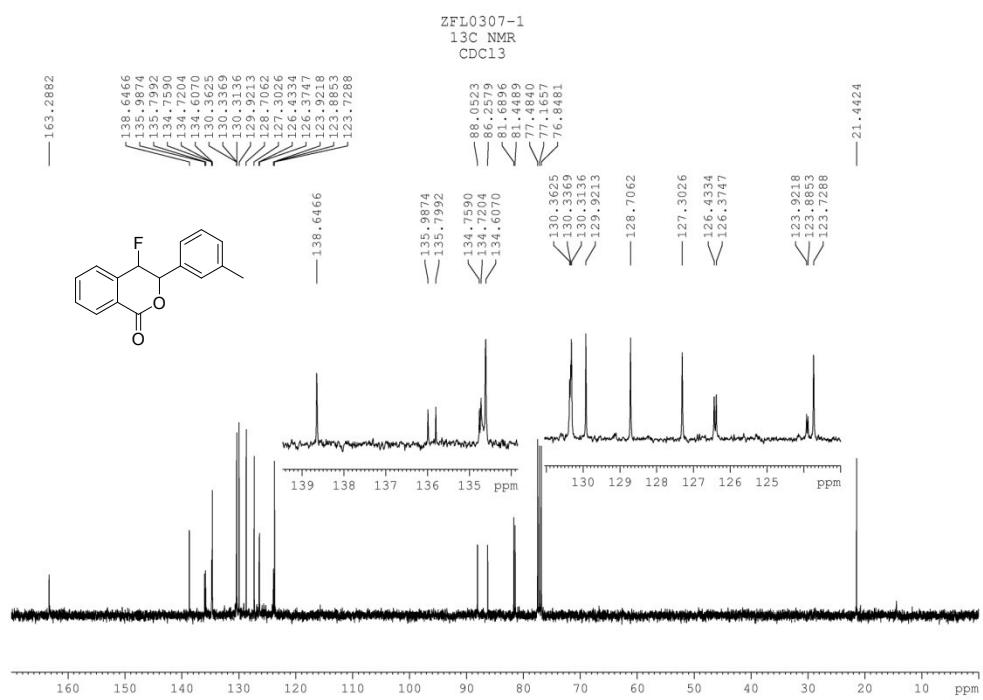


Fig. 5 ^{13}C NMR spectrum of compound 3b

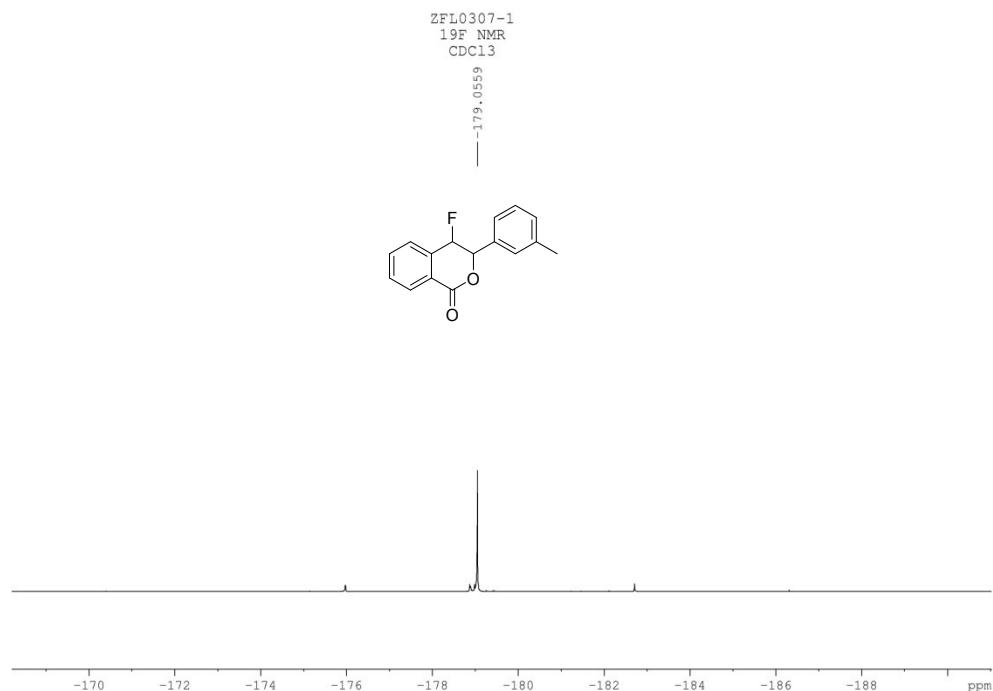


Fig. 6 ^{19}F NMR spectrum of compound 3b

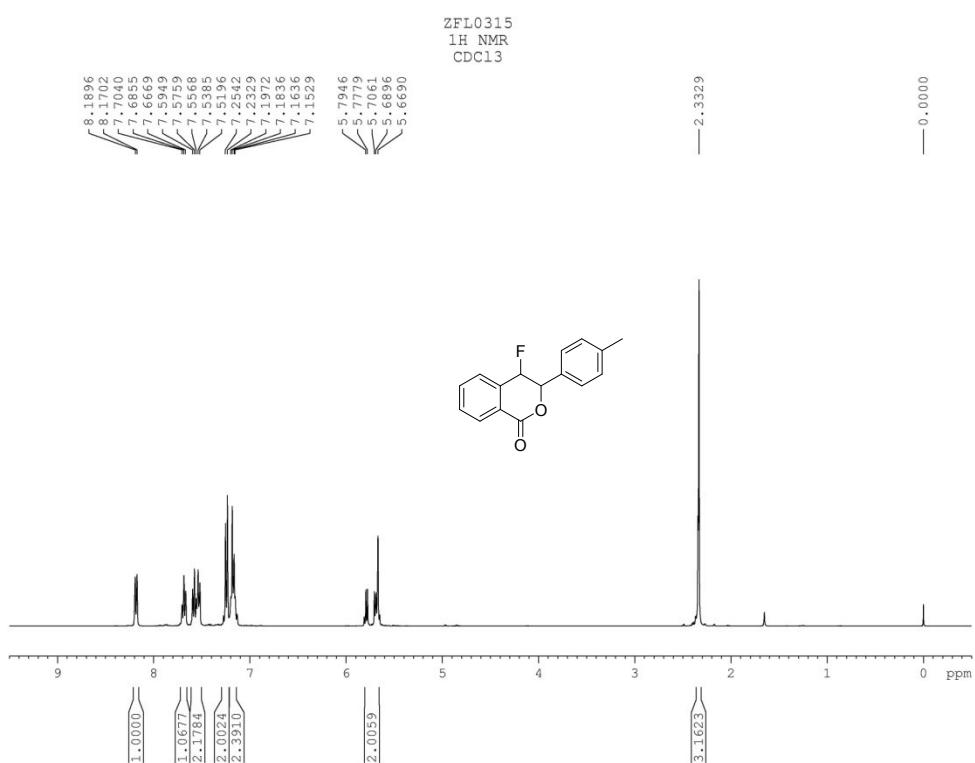


Fig. 7 ¹H NMR spectrum of compound 3c

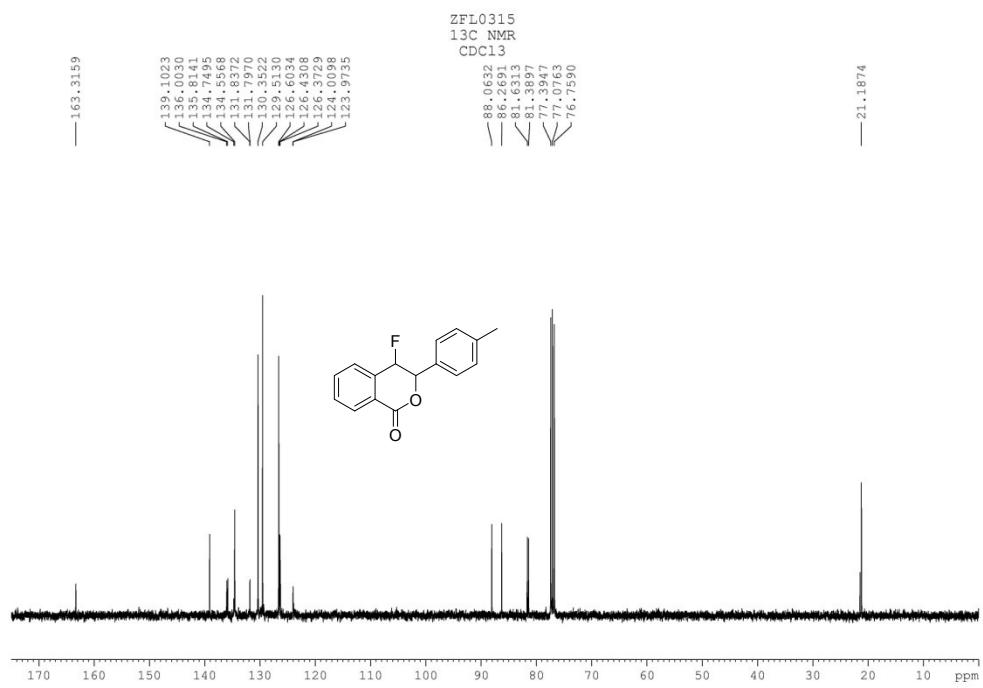


Fig. 8 ¹³C NMR spectrum of compound 3c

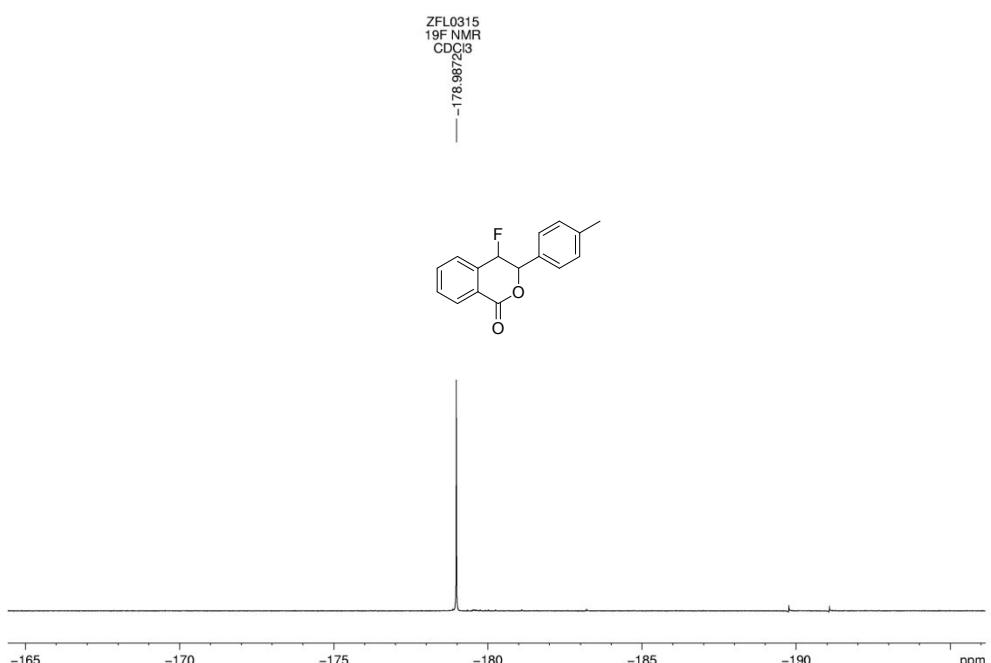


Fig. 9 ^{19}F NMR spectrum of compound **3c**

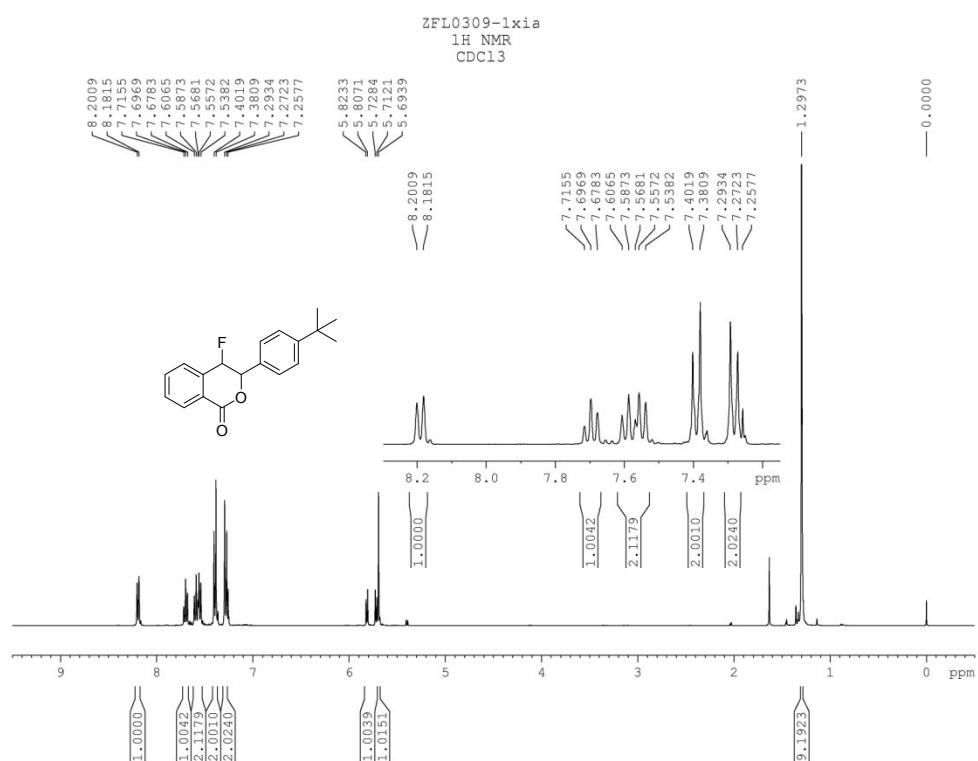


Fig. 10 ^1H NMR spectrum of compound **3d**

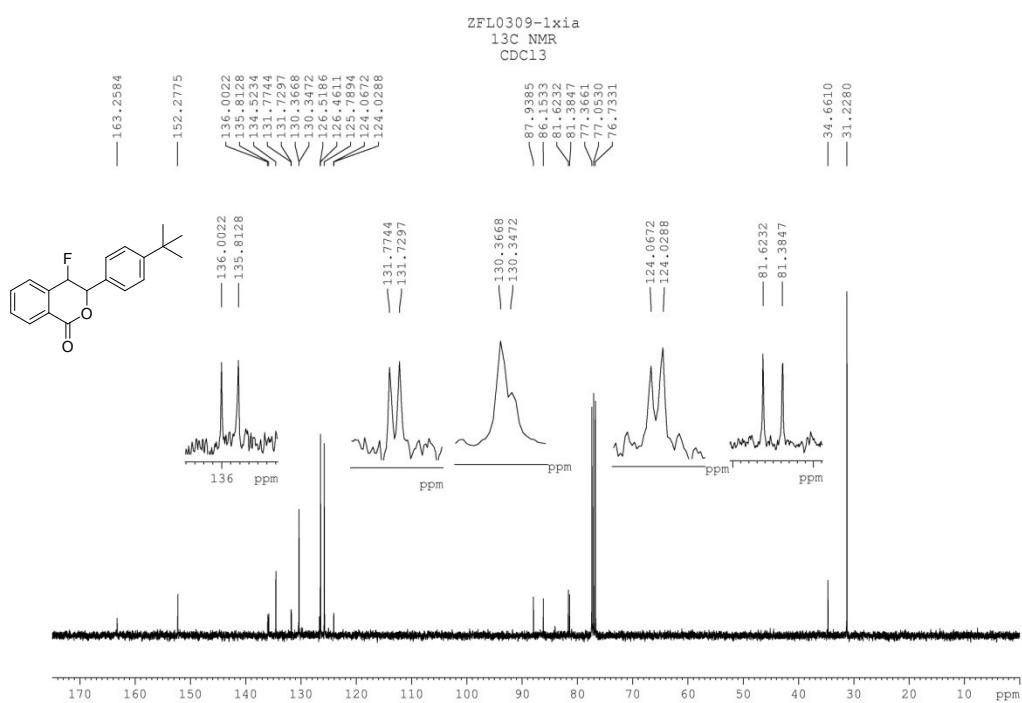


Fig. 11 ^{13}C NMR spectrum of compound **3d**

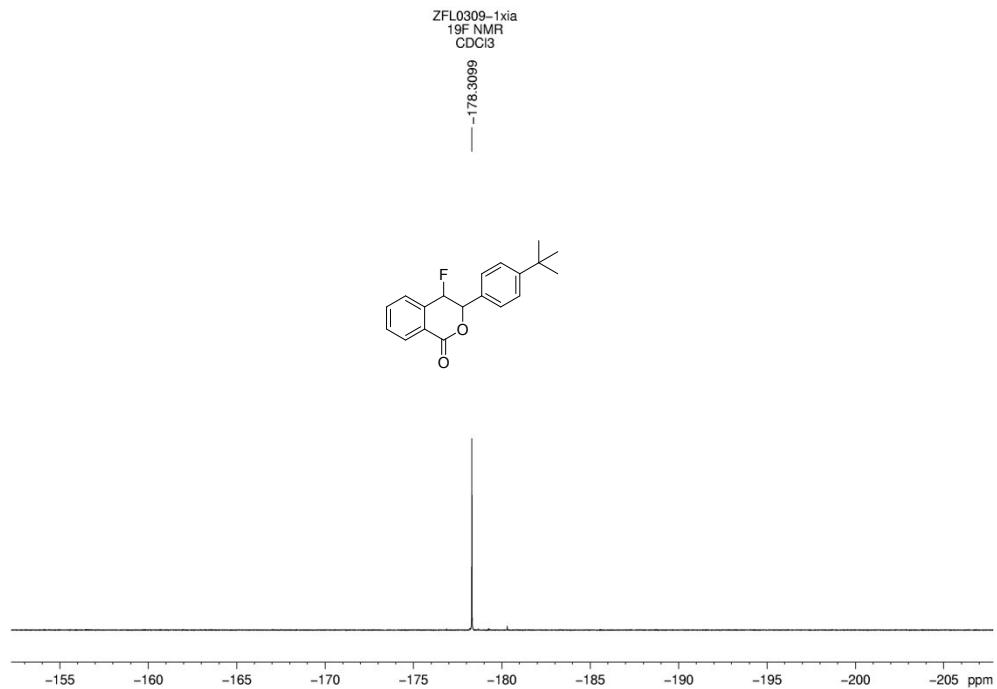


Fig. 12 ^{19}F NMR spectrum of compound **3d**

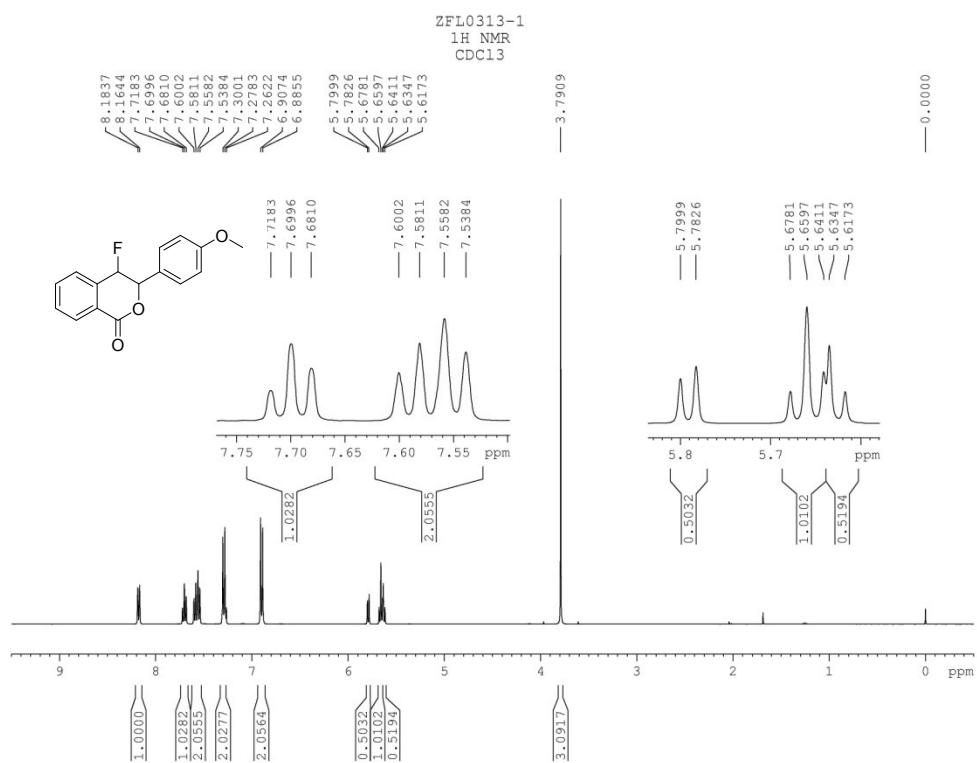


Fig. 13 ¹H NMR spectrum of compound 3e

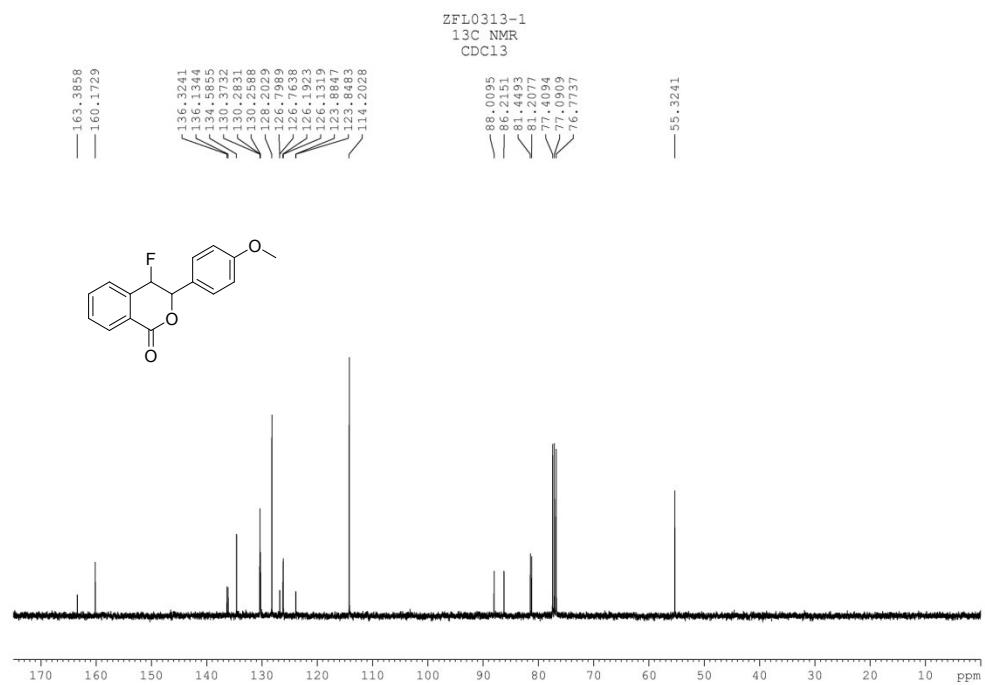


Fig. 14 ¹³C NMR spectrum of compound 3e

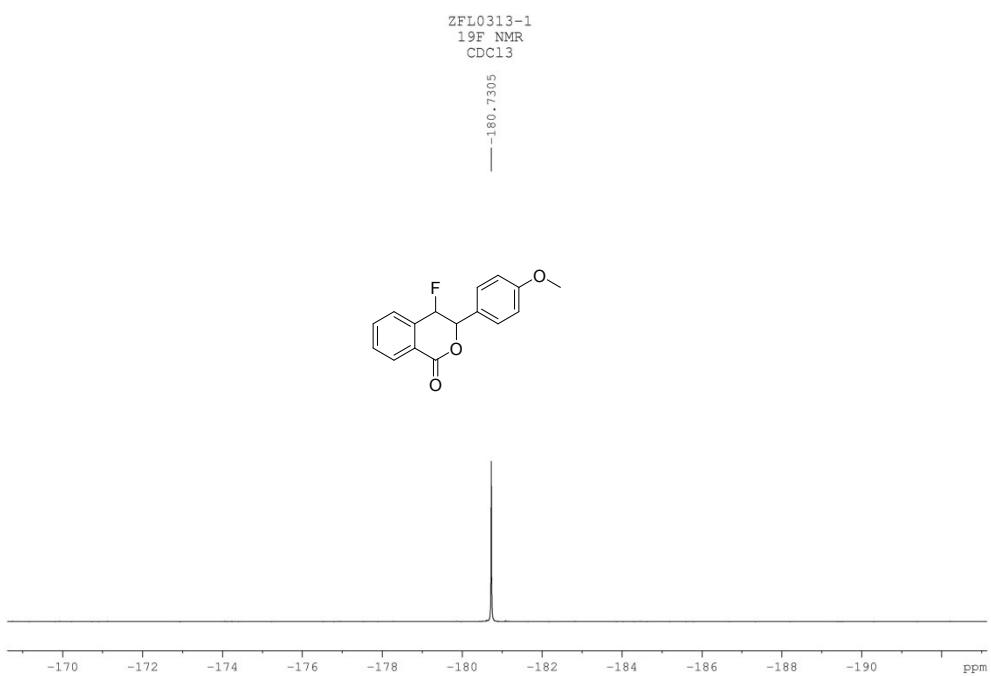


Fig. 15 ¹⁹F NMR spectrum of compound **3e**

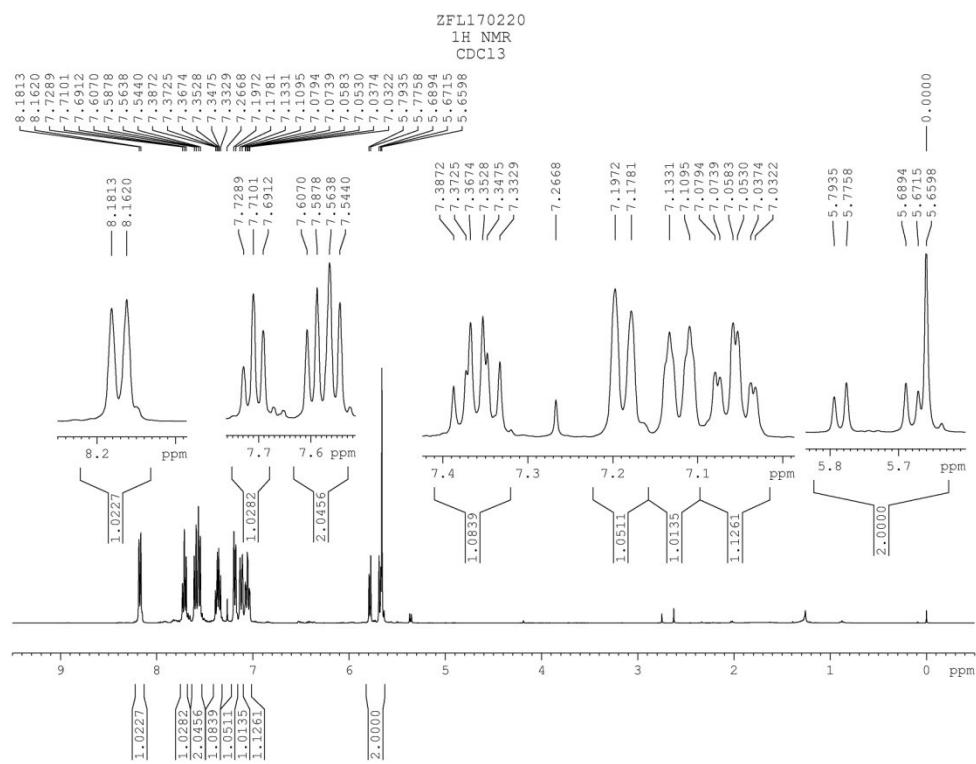


Fig. 16 ¹H NMR spectrum of compound **3f**

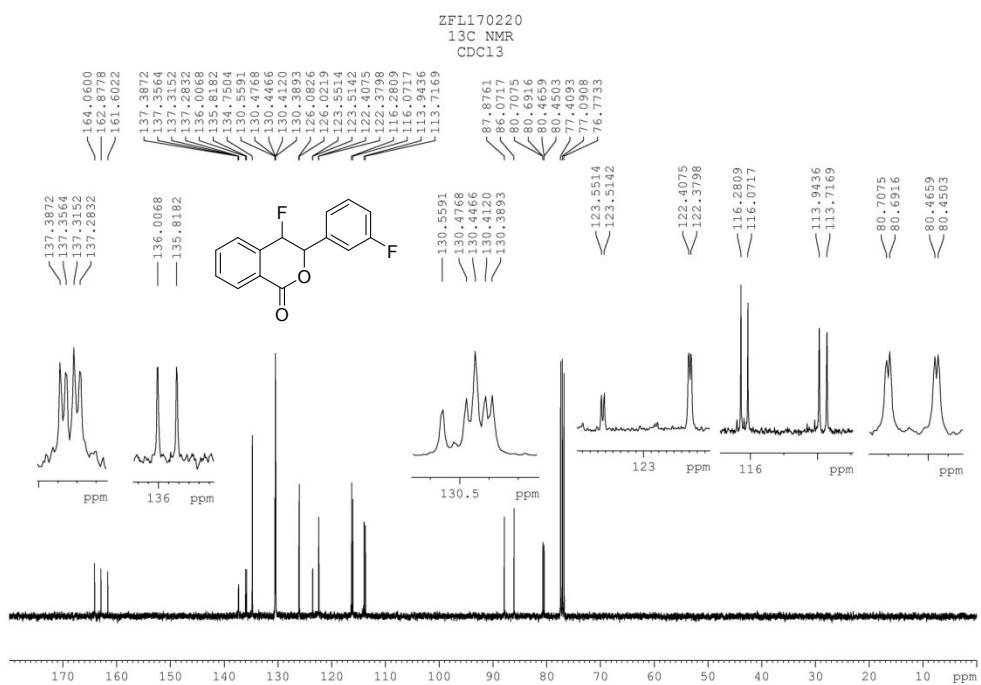


Fig. 17 ^{13}C NMR spectrum of compound **3f**

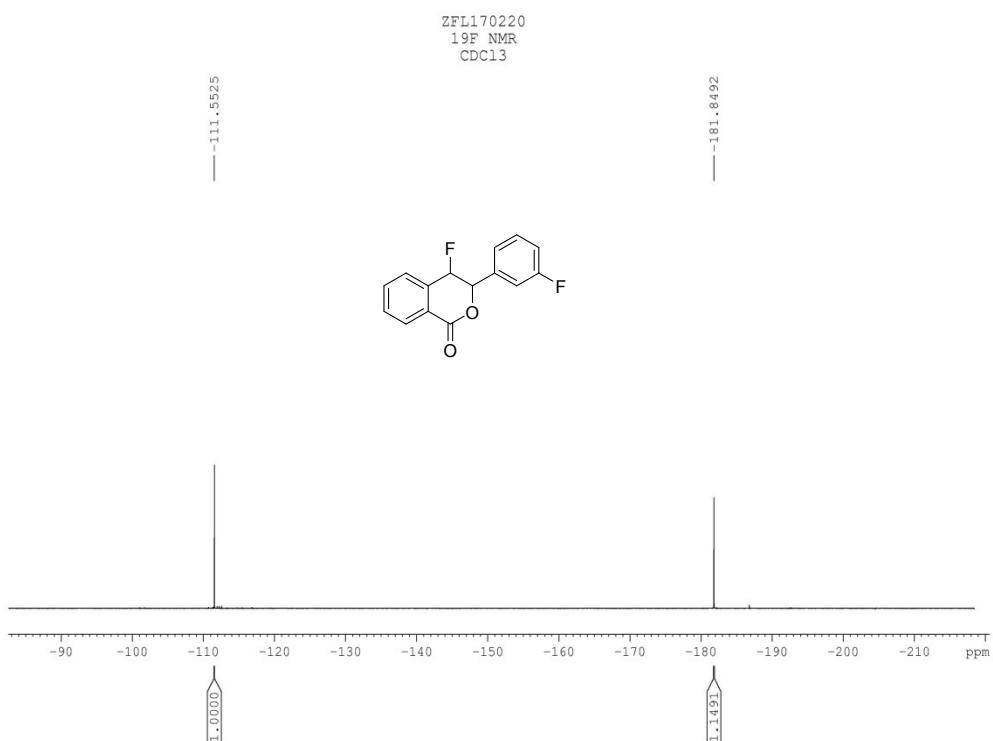


Fig. 18 ^{19}F NMR spectrum of compound **3f**

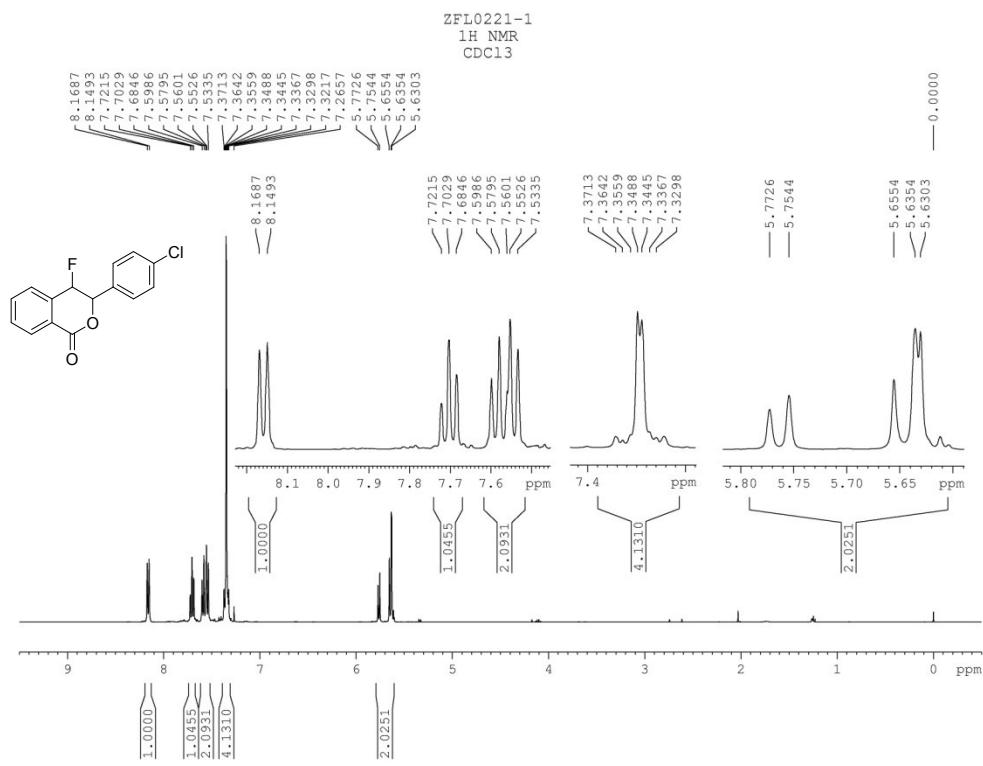


Fig. 19 ^1H NMR spectrum of compound **3g**

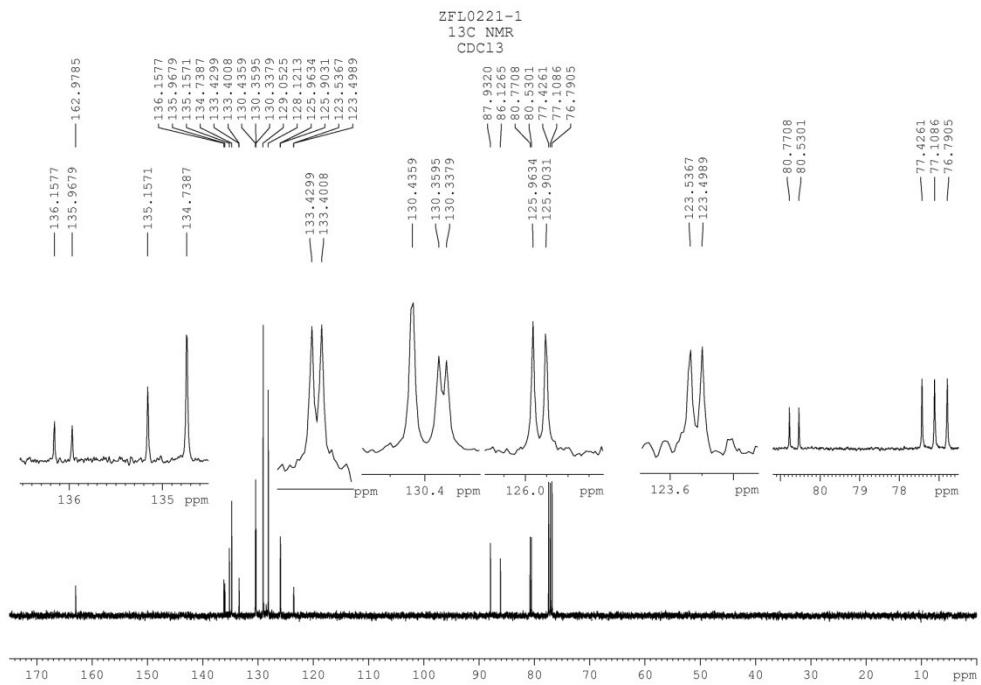


Fig. 20 ^{13}C NMR spectrum of compound **3g**

ZFL0221-1
¹⁹F NMR
CDCl₃

— -182.7481

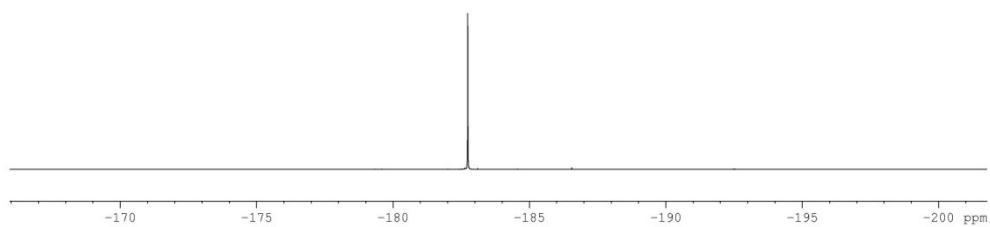
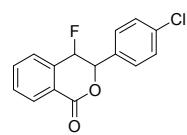


Fig. 21 ¹⁹F NMR spectrum of compound 3g

ZFL0314-1-3
¹H NMR
CDCl₃

— 0.0000

</

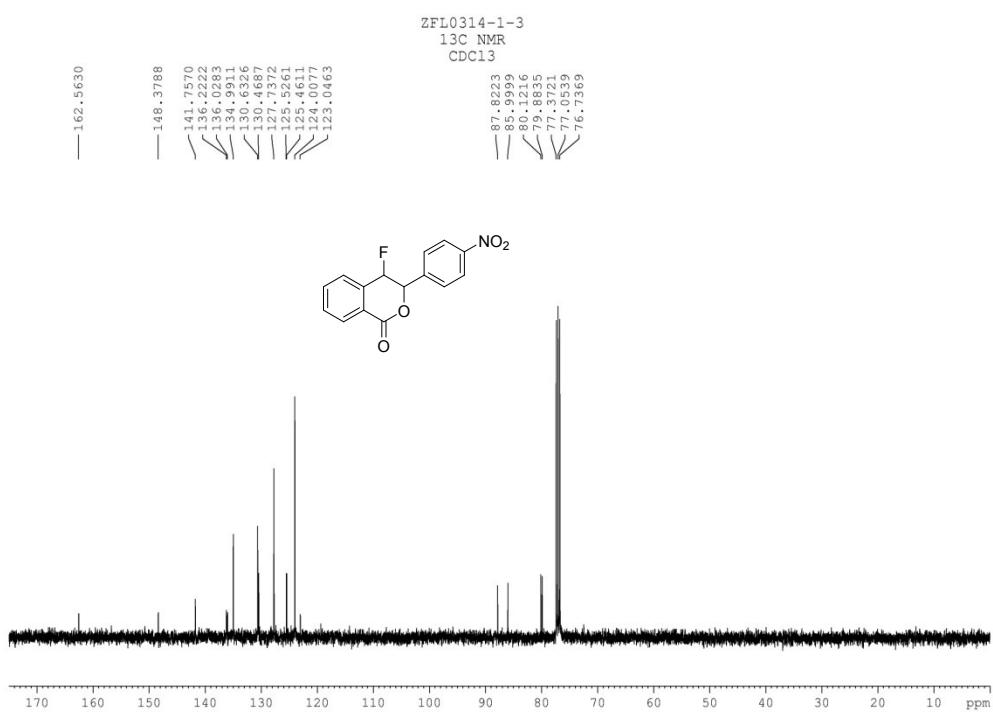


Fig. 23 ¹³C NMR spectrum of compound **3h**

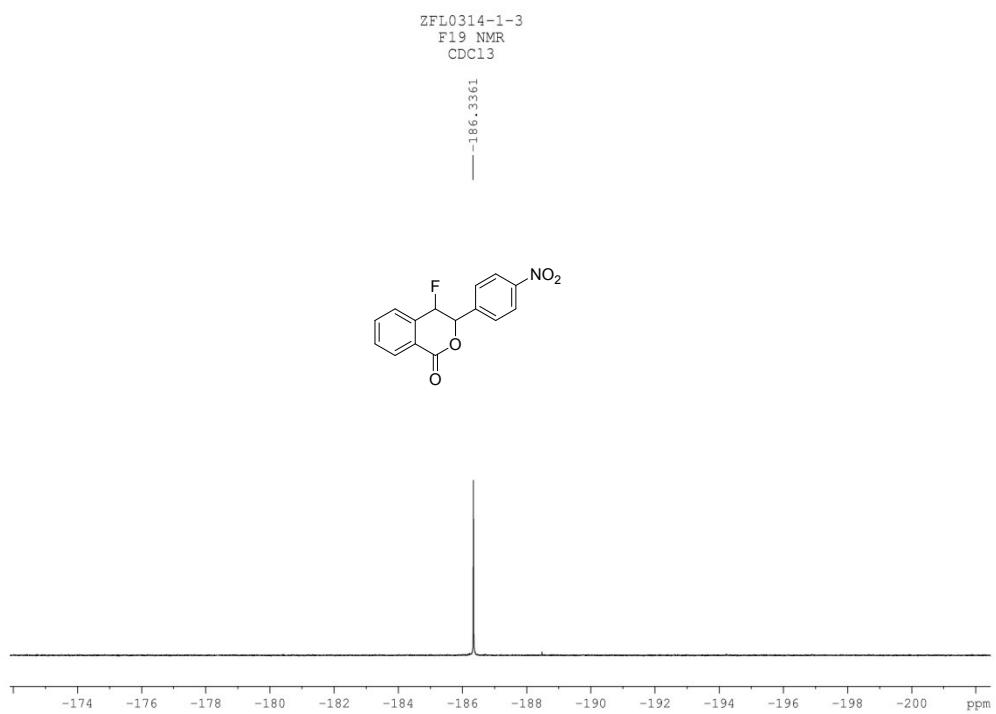


Fig. 24 ¹⁹F NMR spectrum of compound **3h**

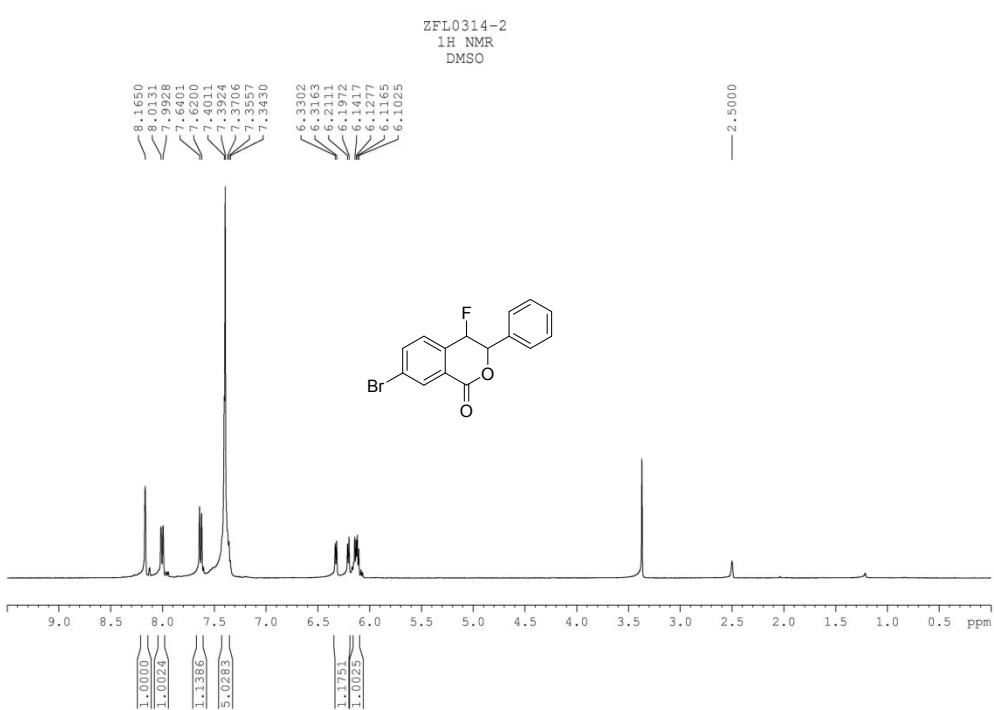


Fig. 25 ^1H NMR spectrum of compound **3i**

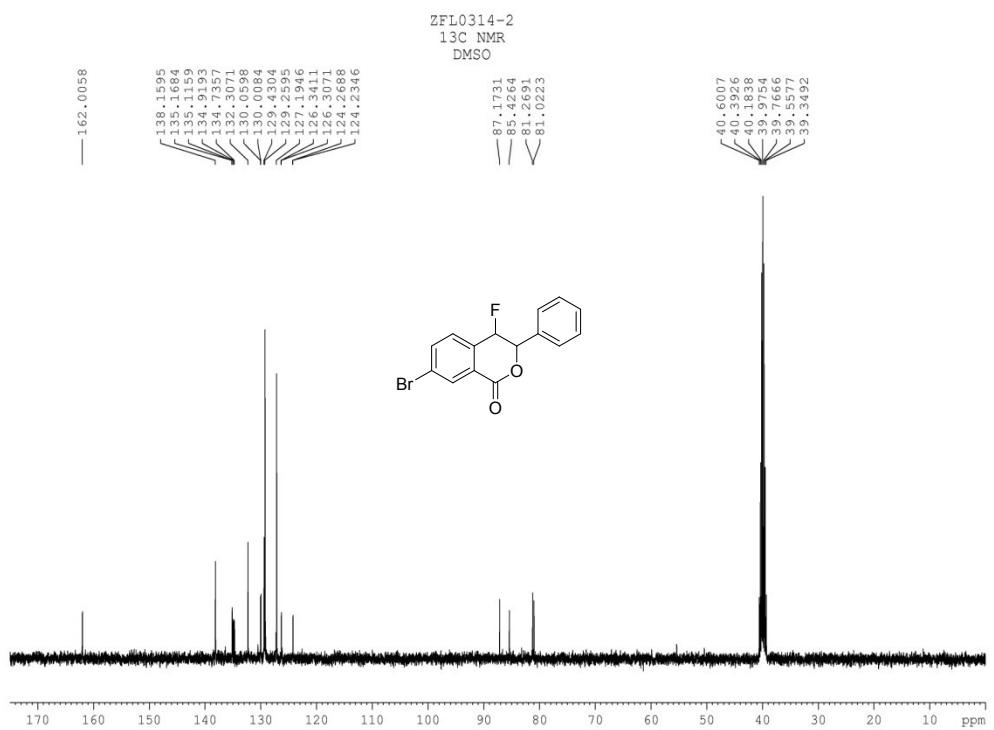


Fig. 26 ^{13}C NMR spectrum of compound **3i**

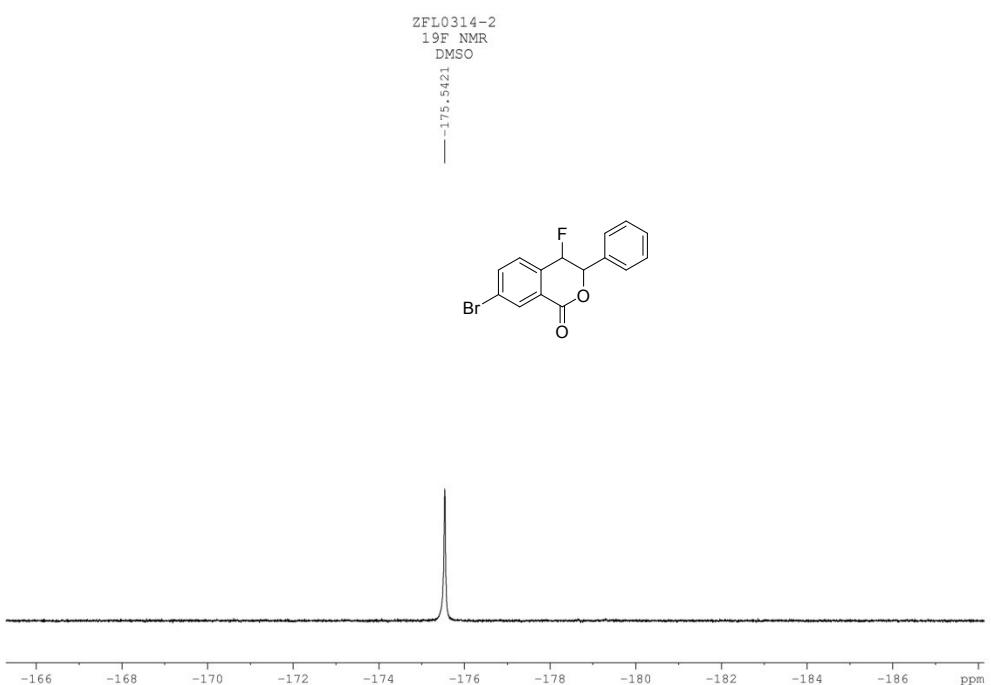


Fig. 27 ^{19}F NMR spectrum of compound **3i**

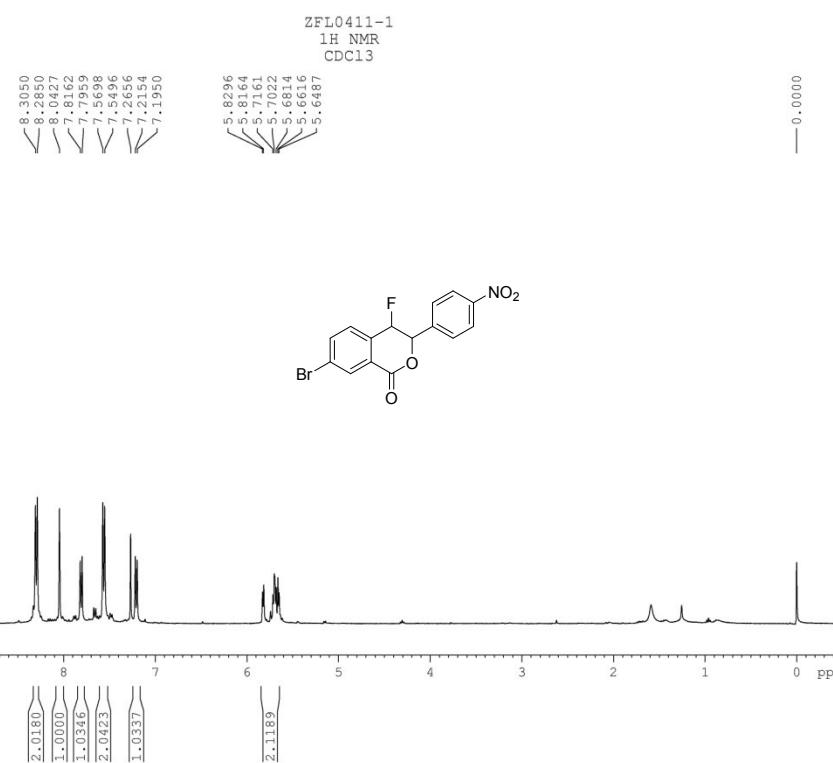


Fig. 28 ^1H NMR spectrum of compound **3j**

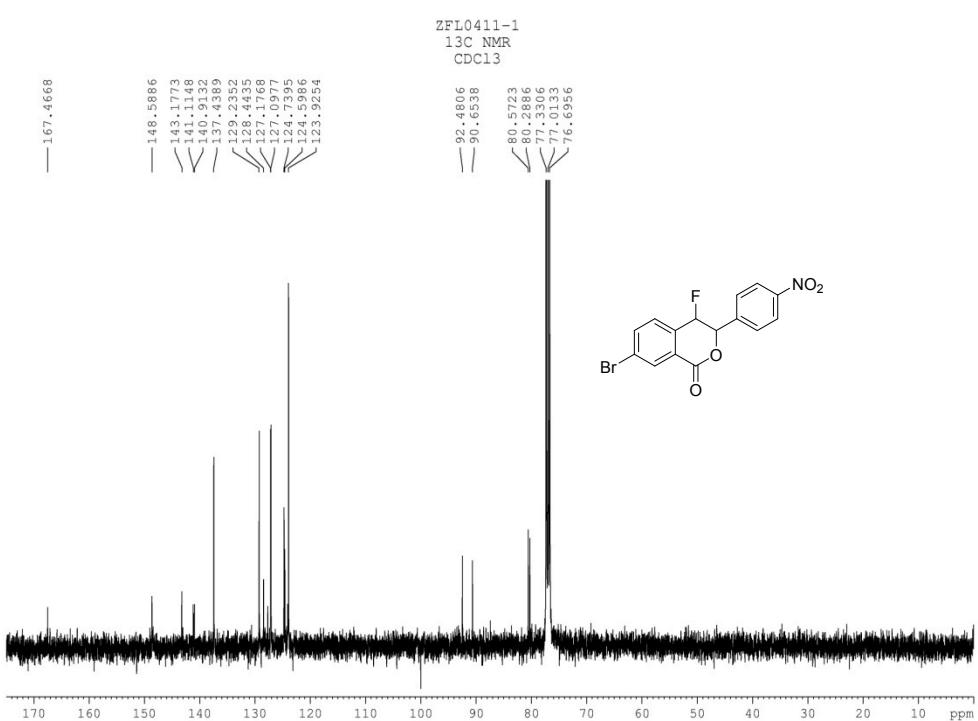


Fig. 29 ¹³C NMR spectrum of compound 3j

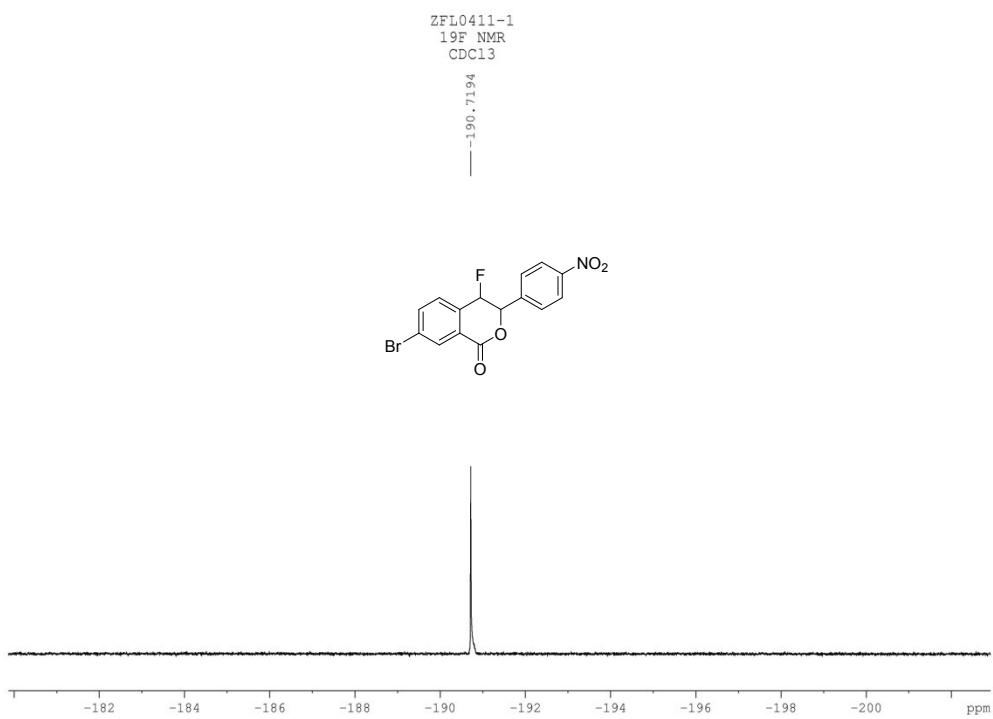


Fig. 30 ¹⁹F NMR spectrum of compound 3j

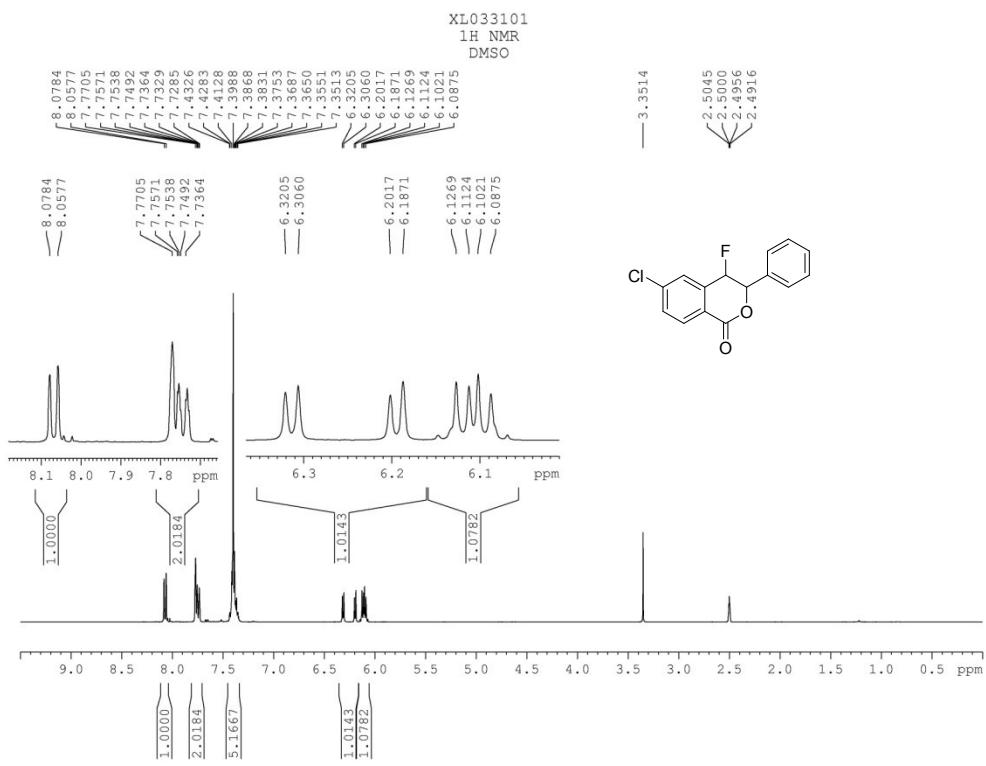


Fig. 31 ^1H NMR spectrum of compound **3k**

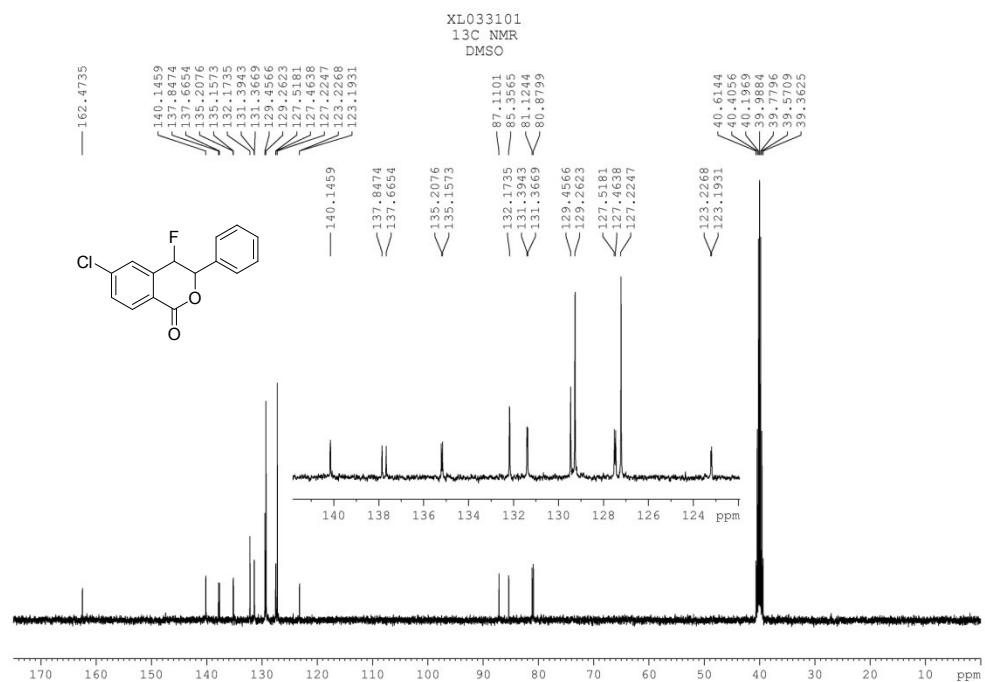


Fig. 32 ^{13}C NMR spectrum of compound **3k**

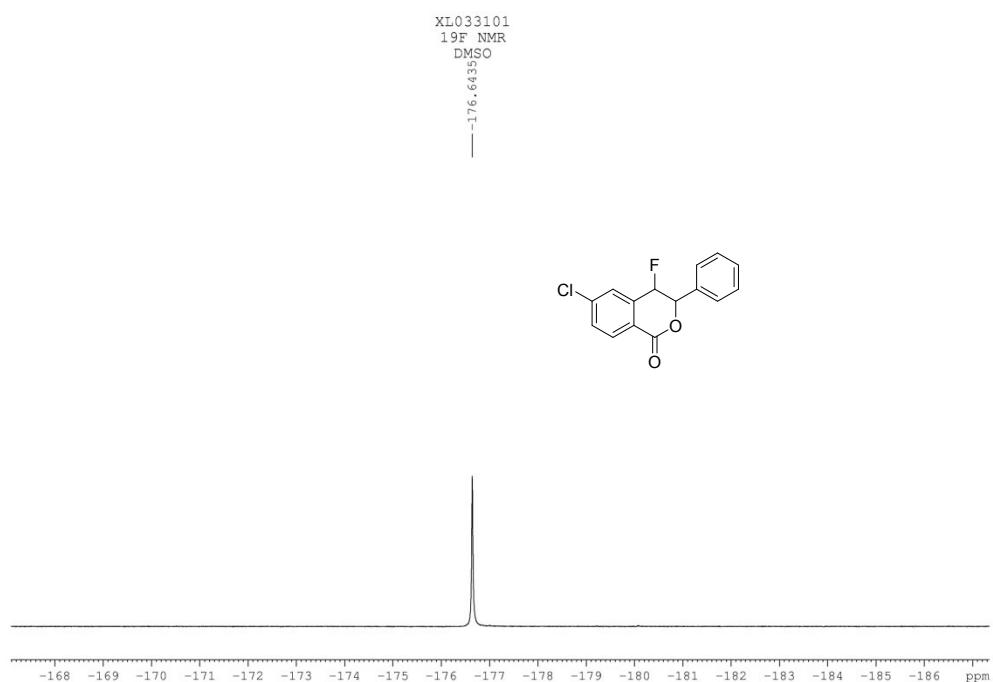


Fig. 33 ^{19}F NMR spectrum of compound **3k**

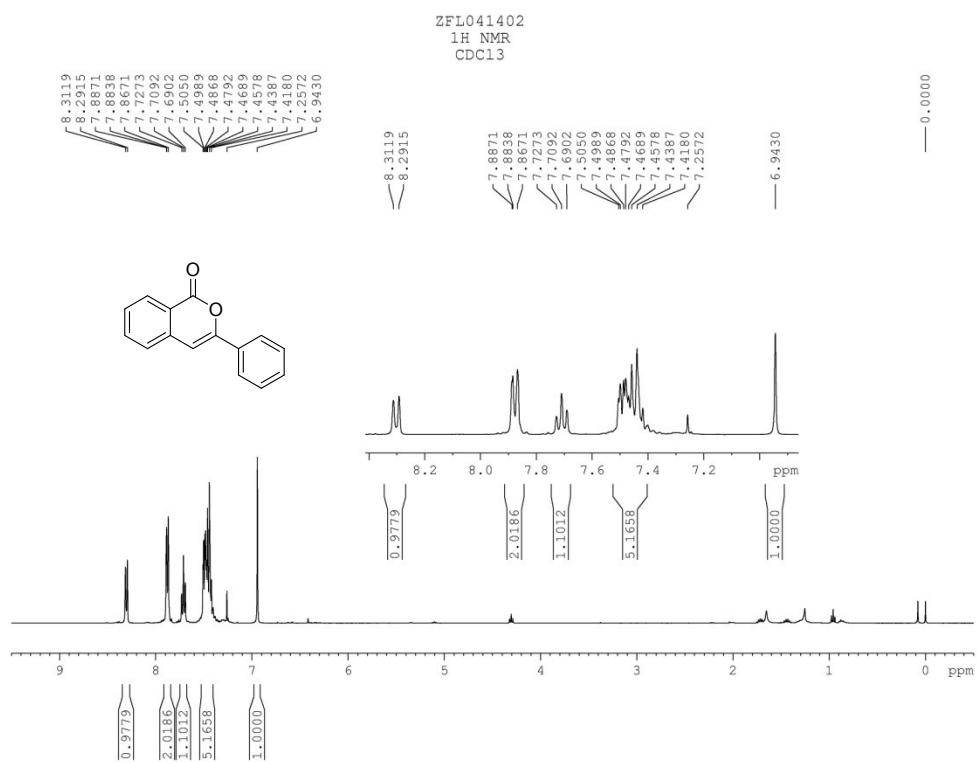


Fig. 34 ^1H NMR spectrum of compound **4a**

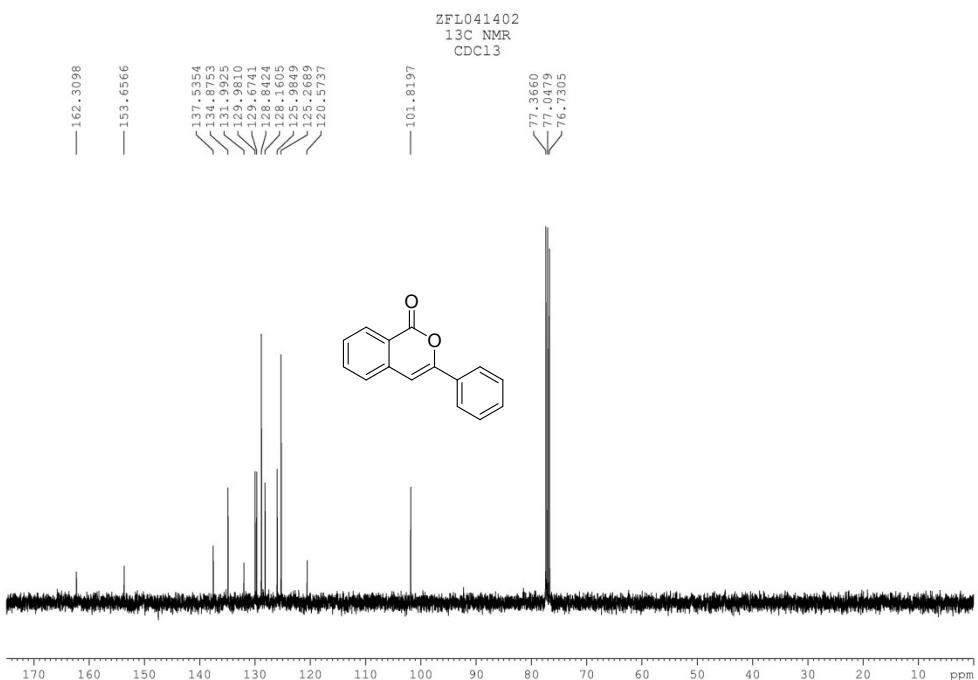


Fig. 35 ^{13}C NMR spectrum of compound **4a**

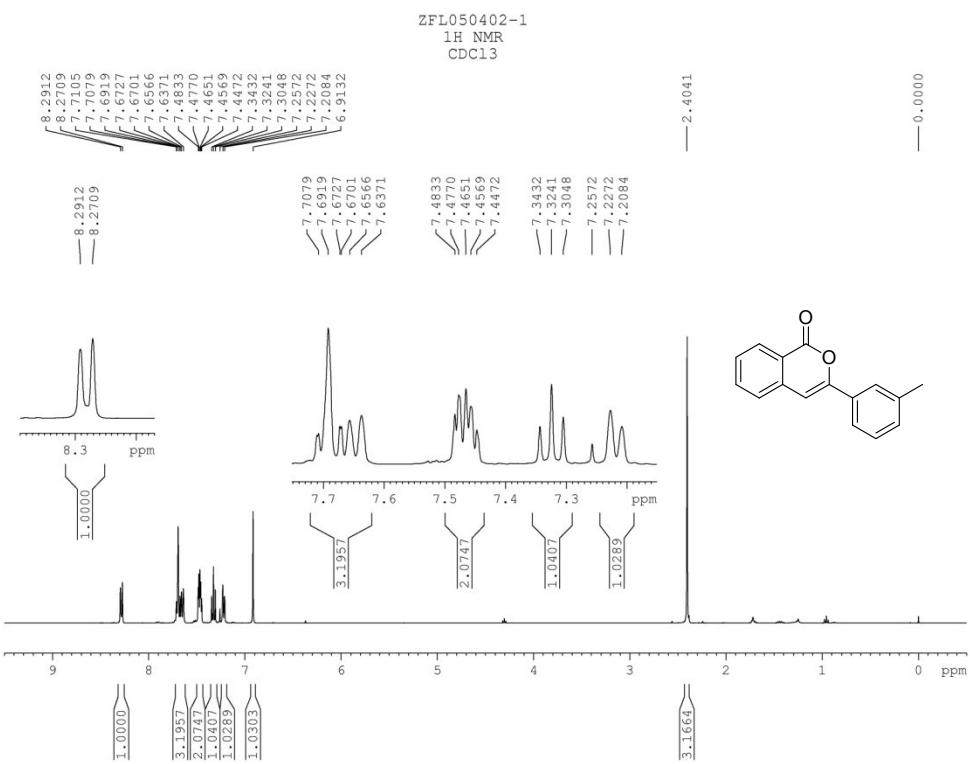


Fig. 36 ^1H NMR spectrum of compound **4b**

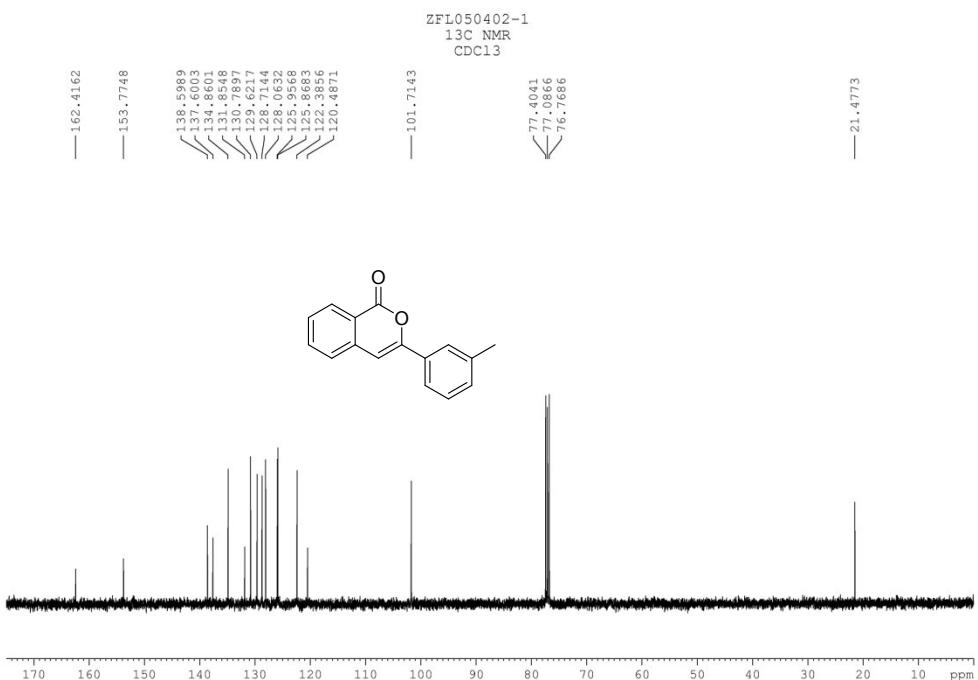


Fig. 37 ¹³C NMR spectrum of compound **4b**

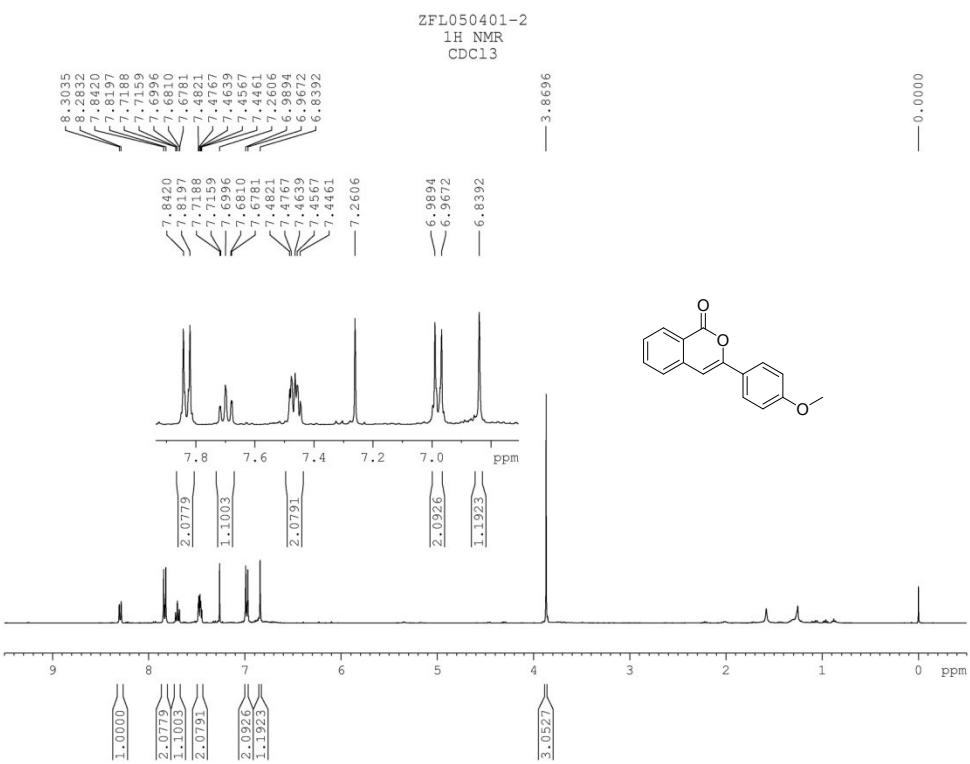


Fig. 38 ¹H NMR spectrum of compound **4c**

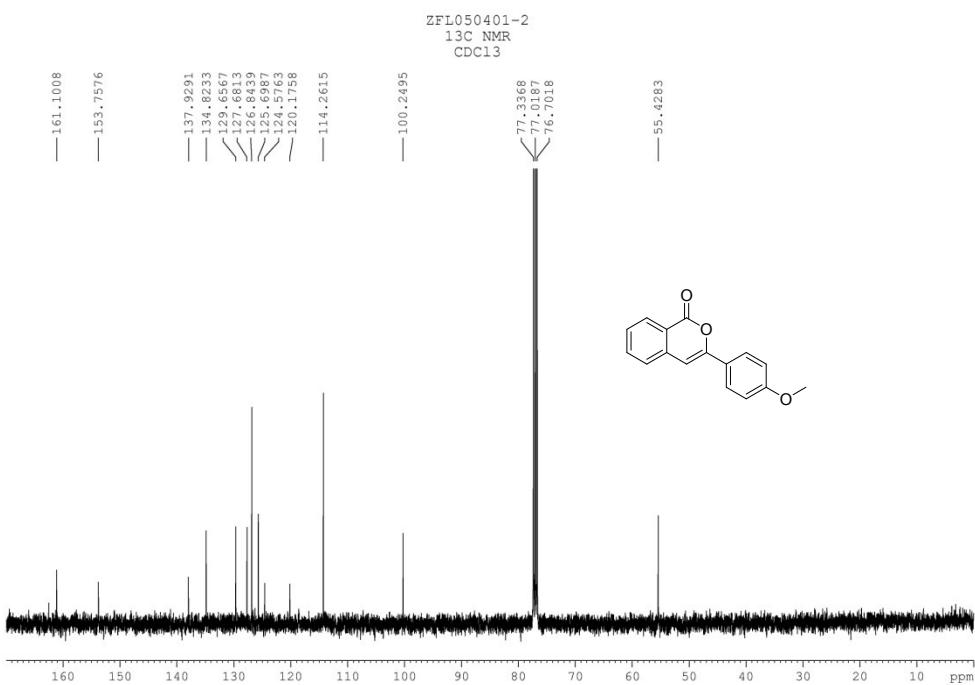


Fig. 39 ^{13}C NMR spectrum of compound **4c**

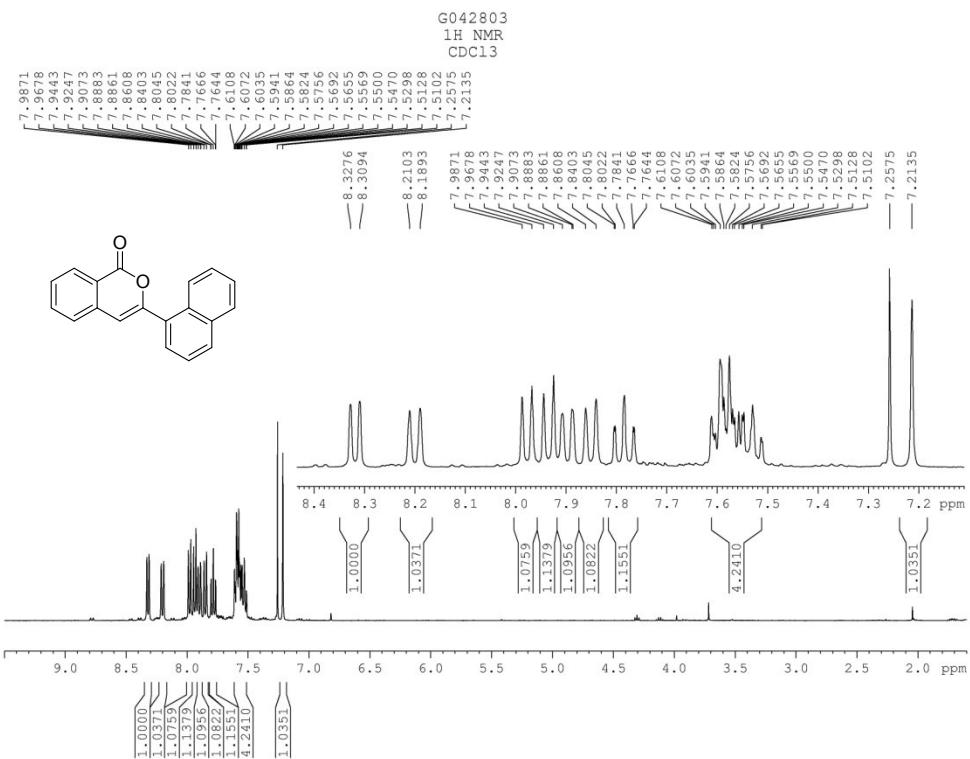


Fig. 40 ^1H NMR spectrum of compound **4d**

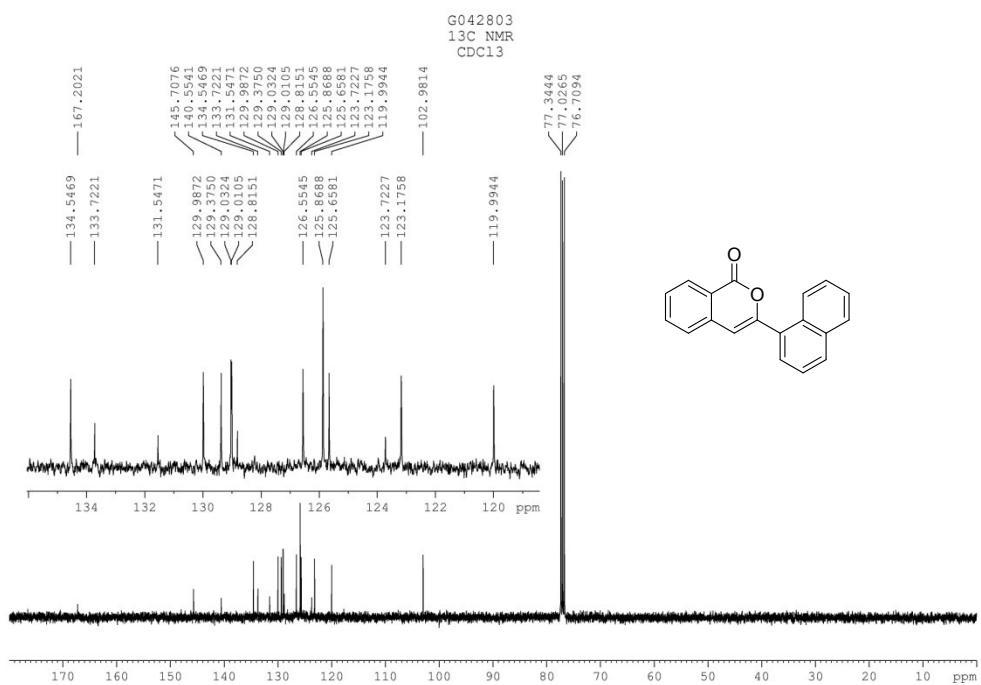


Fig. 41 ^{13}C NMR spectrum of compound **4d**

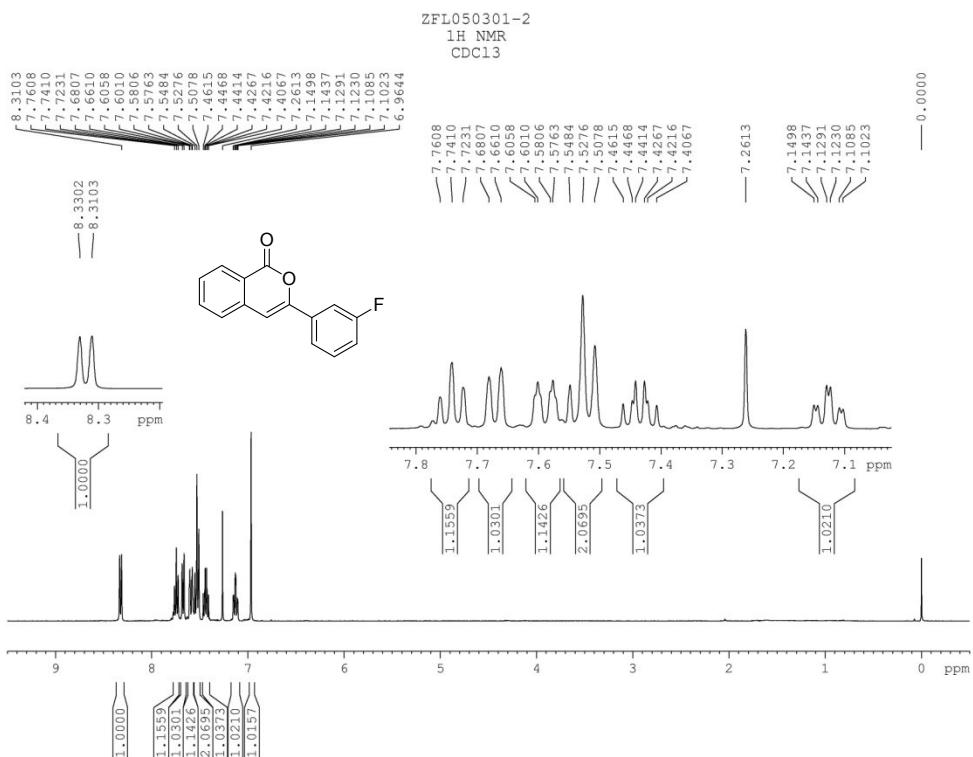


Fig. 42 ^1H NMR spectrum of compound **4e**

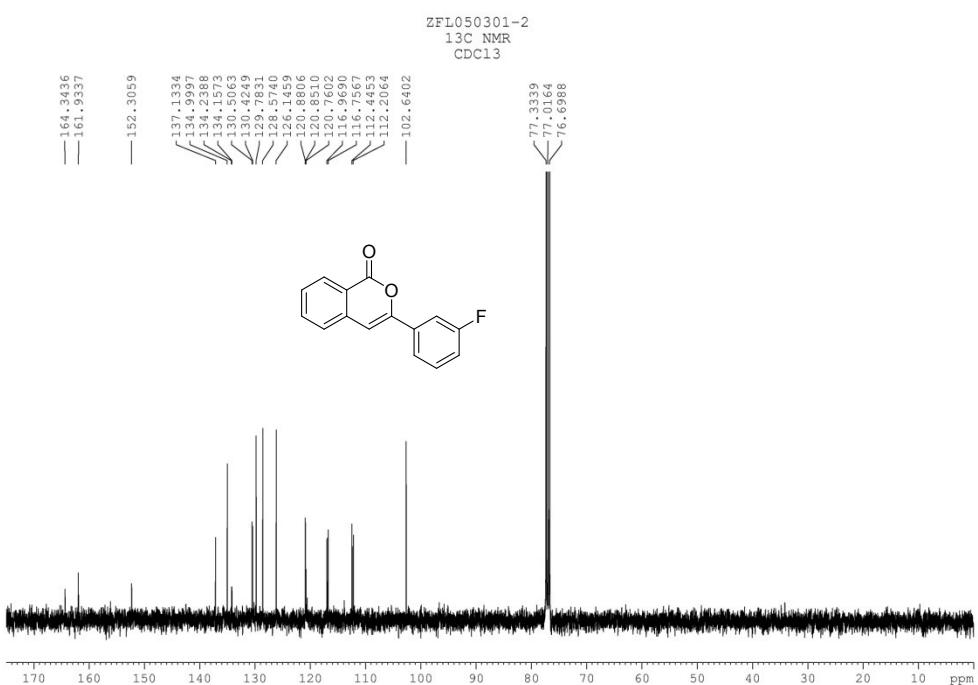


Fig. 43 ¹³C NMR spectrum of compound 4e

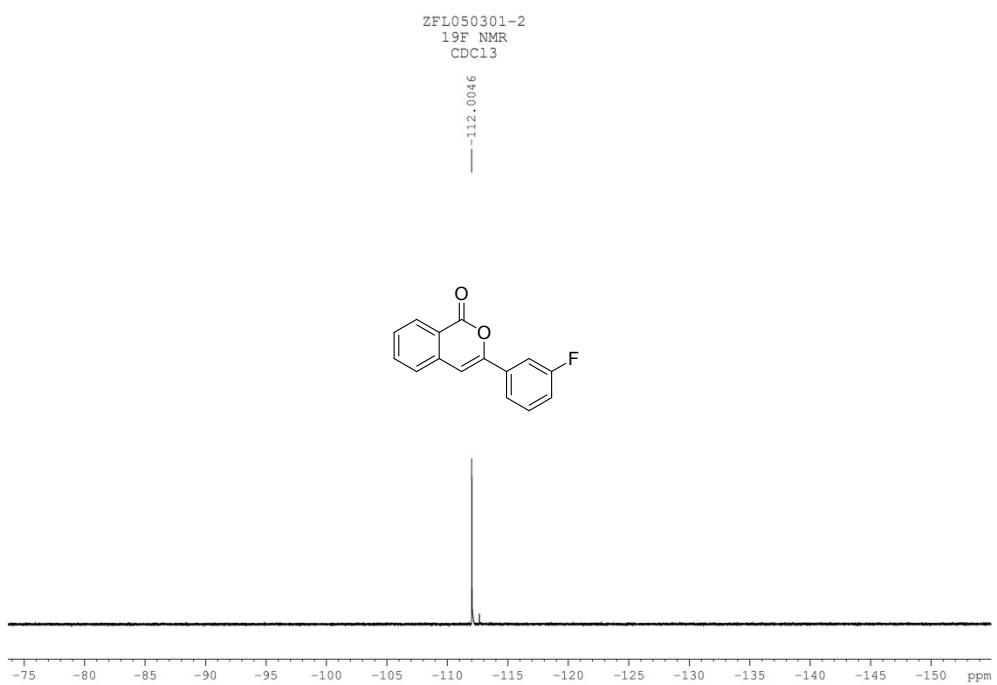


Fig. 44 ¹⁹F NMR spectrum of compound 4e

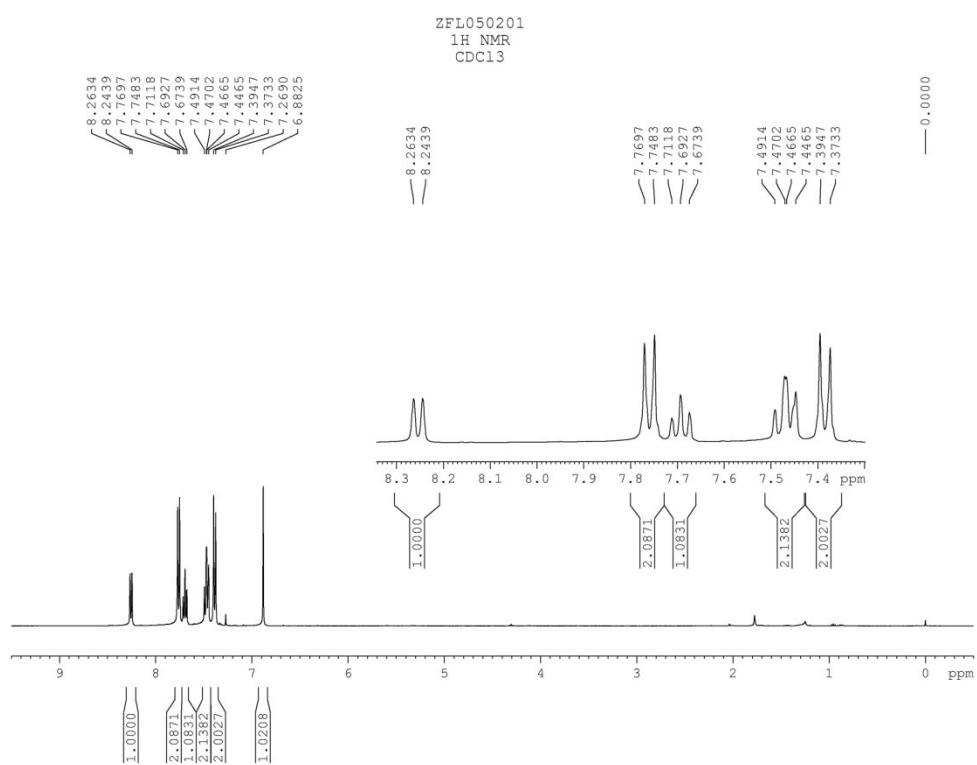


Fig. 45 ¹H NMR spectrum of compound 4f

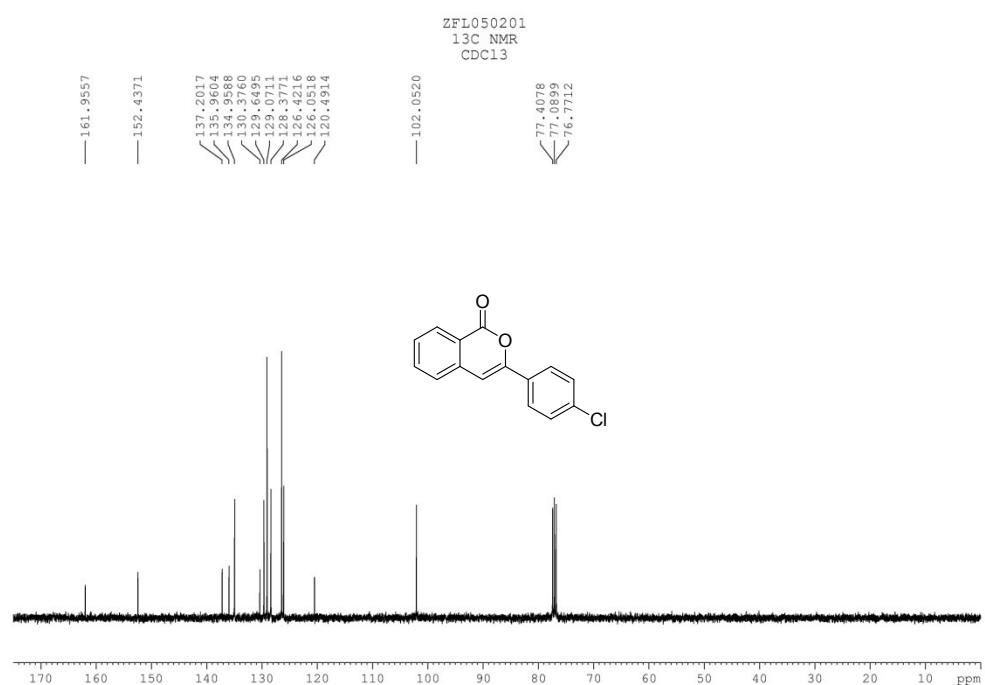


Fig. 46 ¹³C NMR spectrum of compound 4f

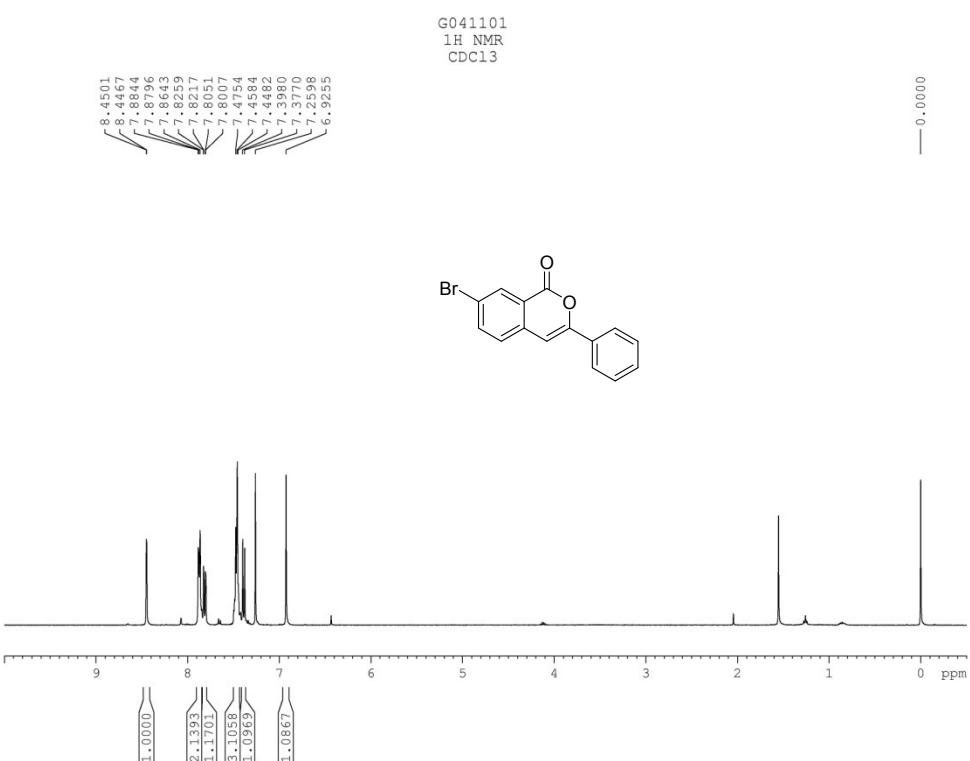


Fig. 47 ¹H NMR spectrum of compound **4g**

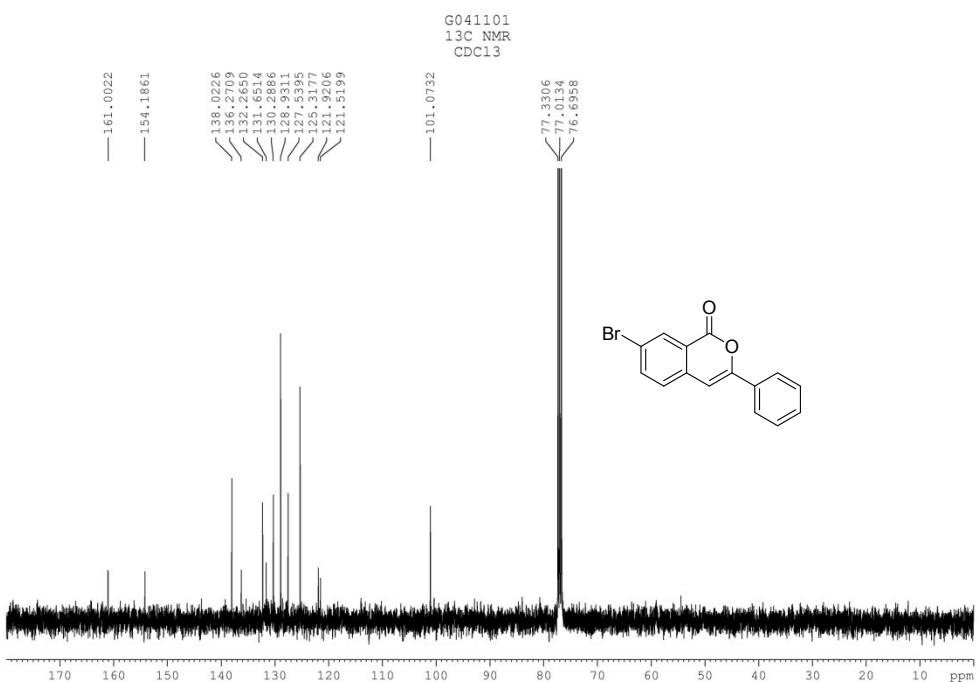


Fig. 48 ¹³C NMR spectrum of compound **4g**