

Supporting Information

For

Redox-neutral tri-/difluoromethylation of *para*-quinone methides with sodium sulfinates

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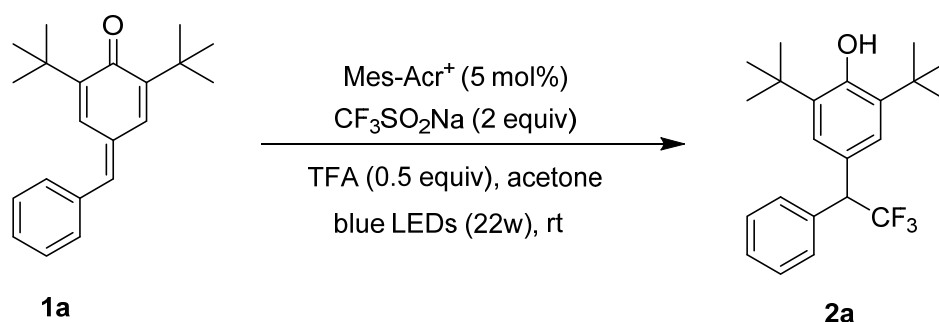
1. General remarks

^1H NMR spectra were recorded on 400 or 600 MHz (100 or 150 MHz for ^{13}C NMR, 376 or 564 MHz for ^{19}F NMR) agilent NMR spectrometer with CDCl_3 as the solvent and tetramethylsilane (TMS) as the internal standard. Chemical shifts were reported in parts per million (ppm, δ scale) downfield from TMS at 0.00 ppm and referenced to the CDCl_3 at 7.26 ppm (for ^1H NMR) or 77.16 ppm (for ^{13}C NMR). HRMS was recorded on a GCT PremierTM(CI) Mass Spectrometer. Infrared (FT-IR) spectra were recorded on a Varian 1000FT-IR, ν_{max} in cm^{-1} . Melting points were measured using SGW, X-4B and values are uncorrected. All commercially available reagents and solvents were used as received unless otherwise specified. The substrates we are readily prepared according to known methods (*Org. Lett.* **2015**, 17, 3390–3393; *Macromolecules* **2013**, 46, 5924–5928).

2. General procedure for synthesis of *p*-quinone methides

In a Dean-Stark apparatus, a mixture of aldehyde (1 equiv.) and 2,6-di-*tert*-butylphenol (1 equiv.) in toluene (0.25 M) was placed and refluxed. Piperidine (2 equiv.) was added to this reaction mixture in a drop-wise manner within an hour and the resultant mixture was stirred at reflux temperature for 12 h. The reaction mixture was cooled to 100 °C and acetic anhydride (2 equiv.) was added and the resulting solution was stirred for 30 more minutes at the same temperature. The reaction mixture was then cooled to room temperature and poured in to ice cold water (50 mL) and extracted with dichloromethane (50 mL $\times$ 2). The combined organic layer was dried over anhydrous sodium sulphate, filtered and concentrated under reduced pressure. The residue was purified by silica gel column chromatography to obtain a pure *p*-quinone methide.

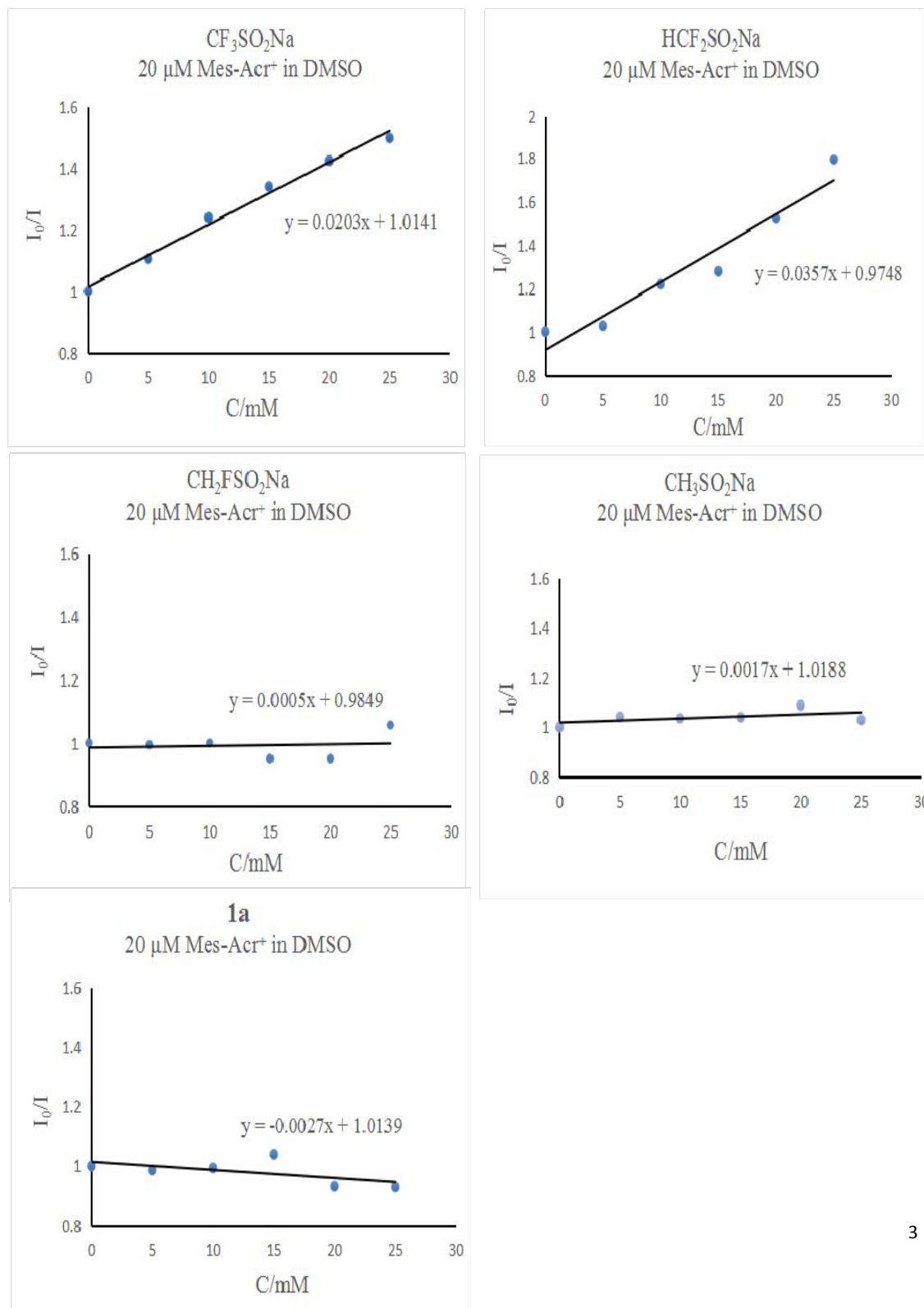
3. Typical experimental procedure



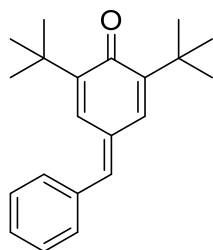
To a suspension of **1a** (58.8 mg, 0.2 mmol), CF₃SO₂Na (62.4 mg, 0.4 mmol) and *N*-methyl-9-mesityl acridinium perchlorate (4.1 mg, 0.01 mmol) in acetone (2 mL) was added TFA (7.7 μL , 0.1 mmol) at rt. The resulting mixture was stirred upon 22W blue LEDs irradiation under argon balloon. After the reaction was finished, the solvent was removed under reduced pressure and the residue was purified by flash column chromatography on silica gel to give **2a** as colorless oil (71.0 mg, 98% yield).

4. Fluorescence quenching experiments

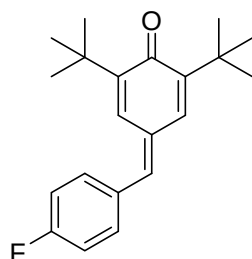
Emission intensities were recorded using LS55 Luminescence Spectrometer for all experiments. All Mes-Acr⁺ solutions were excited at 450 nm and the emission intensity was collected at 490-570 nm. In a typical experiment, the DMSO solution of Mes-Acr⁺ (0.02 mM) was added the appropriate amount of quencher in a screw-top 1.0 cm quartz cuvette. After degassing with nitrogen for 10 min, the emission spectra of the samples were collected. The results showed that CF₃SO₂Na and HCF₂SO₂Na quenched the photoexcited Mes-Acr⁺ effectively.



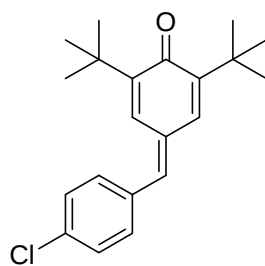
4. Characterization of the substrates and products



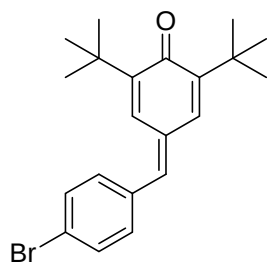
4-Benzylidene-2,6-di-tert-butylcyclohexa-2,5-dien-1-one (1a): ^1H NMR (600 MHz, CDCl_3) δ 7.54 (d, $J = 2.2$ Hz, 1H), 7.48 – 7.43 (m, 4H), 7.41 – 7.37 (m, 1H), 7.19 (s, 1H), 7.03 (d, $J = 2.3$ Hz, 1H), 1.35 (s, 9H), 1.32 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3) δ 186.6, 149.5, 147.9, 142.6, 136.0, 135.2, 132.1, 130.4, 129.2, 128.9, 127.9, 35.6, 35.1, 29.67, 29.65.



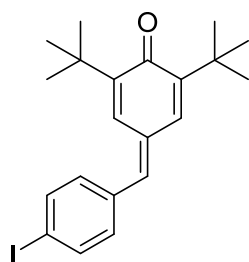
2,6-Di-tert-butyl-4-(4-fluorobenzylidene)cyclohexa-2,5-dien-1-one (1b): ^1H NMR (400 MHz, CDCl_3) δ 7.49 – 7.40 (m, 3H), 7.19 – 7.10 (m, 3H), 7.00 (s, 1H), 1.33 (s, 9H), 1.30 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3) δ 186.7, 163.17 (d, $J_{\text{C-F}} = 251.3$ Hz), 149.7, 148.0, 141.1, 135.1, 132.3 (d, $J_{\text{C-F}} = 8.2$ Hz), 132.22 (d, $J_{\text{C-F}} = 3.4$ Hz), 132.0, 127.5, 116.1 (d, $J_{\text{C-F}} = 21.8$ Hz), 35.6, 35.2, 29.7, 29.6.



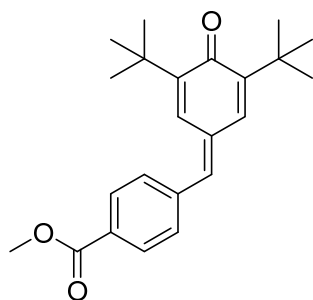
2,6-Di-tert-butyl-4-(4-chlorobenzylidene)cyclohexa-2,5-dien-1-one (1c): ^1H NMR (400 MHz, CDCl_3) δ 7.46 – 7.40 (m, 3H), 7.38 (d, $J = 8.3$ Hz, 2H), 7.11 (s, 1H), 6.99 (s, 1H), 1.33 (s, 9H), 1.30 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3) δ 186.7, 149.9, 148.2, 140.8, 135.3, 135.0, 134.5, 132.5, 131.6, 129.2, 127.4, 35.6, 35.2, 29.68, 29.65.



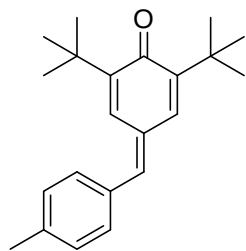
4-(4-Bromobenzylidene)-2,6-di-tert-butylcyclohexa-2,5-dien-1-one (1d): ^1H NMR (400 MHz, CDCl_3) δ 7.56 (d, $J = 8.0$ Hz, 2H), 7.43 (s, 1H), 7.30 (d, $J = 8.0$ Hz, 2H), 7.07 (s, 1H), 6.98 (s, 1H), 1.32 (s, 9H), 1.29 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3) δ 186.6, 149.8, 148.2, 140.7, 134.9, 134.9, 132.5, 132.1, 131.8, 127.3, 123.6, 35.6, 35.1, 29.7, 29.6.



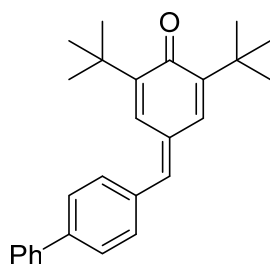
2,6-Di-tert-butyl-4-(4-iodobenzylidene)cyclohexa-2,5-dien-1-one (1e): ^1H NMR (400 MHz, CDCl_3) δ 7.78 (d, $J = 7.5$ Hz, 2H), 7.43 (s, 1H), 7.17 (d, $J = 7.5$ Hz, 2H), 7.06 (s, 1H), 6.98 (s, 1H), 1.32 (s, 9H), 1.29 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3) δ 186.6, 149.9, 148.2, 140.9, 138.1, 135.4, 135.0, 132.6, 131.9, 127.3, 95.5, 35.6, 35.2, 29.7, 29.6.



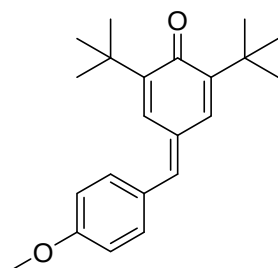
Methyl 4-((3,5-di-tert-butyl-4-oxocyclohexa-2,5-dien-1-ylidene)methyl)benzoate (1f): ^1H NMR (400 MHz, CDCl_3) δ 8.11 (d, $J = 7.6$ Hz, 2H), 7.51 (d, $J = 7.6$ Hz, 2H), 7.45 (s, 1H), 7.17 (s, 1H), 7.01 (s, 1H), 3.95 (s, 3H), 1.33 (s, 9H), 1.29 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3 , overlapping peaks) δ 186.7, 166.7, 150.1, 148.6, 140.6, 140.5, 134.9, 133.5, 130.3, 130.0, 127.5, 52.5, 35.7, 35.2, 29.67, 29.65.



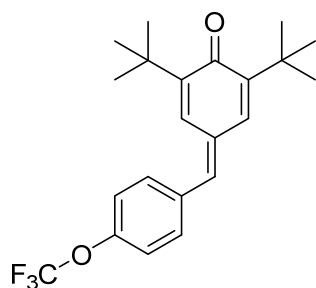
2,6-Di-tert-butyl-4-(4-methylbenzylidene)cyclohexa-2,5-dien-1-one (1g): ^1H NMR (400 MHz, CDCl_3) δ 7.56 (s, 1H), 7.37 (d, $J = 7.7$ Hz, 2H), 7.25 (d, $J = 7.6$ Hz, 2H), 7.16 (s, 1H), 7.01 (s, 1H), 2.40 (s, 3H), 1.34 (s, 9H), 1.31 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3) δ 186.6, 149.2, 147.6, 143.0, 139.7, 135.4, 133.3, 131.5, 130.5, 129.7, 128.0, 35.6, 35.1, 29.69, 29.65, 21.6.



4-([1,1'-Biphenyl]-4-ylmethylene)-2,6-di-tert-butylcyclohexa-2,5-dien-1-one (1h): ^1H NMR (400 MHz, CDCl_3) δ 7.71 (d, $J = 8.0$ Hz, 2H), 7.67 (d, $J = 7.5$ Hz, 2H), 7.62 (s, 1H), 7.57 (d, $J = 8.0$ Hz, 2H), 7.49 (t, $J = 7.4$ Hz, 2H), 7.40 (t, $J = 7.2$ Hz, 1H), 7.22 (s, 1H), 7.06 (s, 1H), 1.37 (s, 9H), 1.35 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3) δ 186.7, 149.5, 147.9, 142.2, 142.0, 140.1, 135.3, 135.1, 132.1, 131.1, 129.1, 128.0, 127.9, 127.5, 127.2, 35.6, 35.2, 29.73, 29.68.

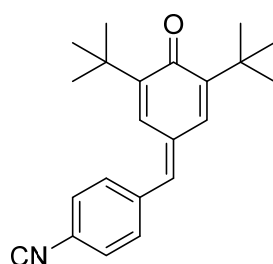


2,6-Di-tert-butyl-4-(4-methoxybenzylidene)cyclohexa-2,5-dien-1-one (1i): ^1H NMR (400 MHz, CDCl_3) δ 7.56 (s, 1H), 7.44 (d, $J = 8.4$ Hz, 2H), 7.13 (s, 1H), 7.02 – 6.96 (m, 3H), 3.87 (s, 3H), 1.33 (s, 9H), 1.32 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3) δ 186.6, 160.7, 149.1, 147.3, 142.8, 135.5, 132.3, 130.6, 128.8, 127.9, 114.6, 55.5, 35.6, 35.1, 29.72, 29.66.



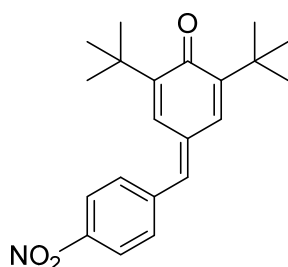
2,6-Di-tert-butyl-4-(4-(trifluoromethoxy)benzylidene)cyclohexa-2,5-dien-1-one

(1j): ^1H NMR (400 MHz, CDCl_3) δ 7.48 (d, $J = 8.4$ Hz, 2H), 7.43 (s, 1H), 7.30 (d, $J = 8.2$ Hz, 2H), 7.13 (s, 1H), 7.00 (s, 1H), 1.33 (s, 9H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 186.7, 150.0, 149.6, 148.3, 140.3, 135.0, 134.6, 132.7, 131.8, 127.3, 121.2, 120.55 (d, $J_{\text{C-F}} = 258.0$ Hz), 35.6, 35.2, 29.7, 29.6.



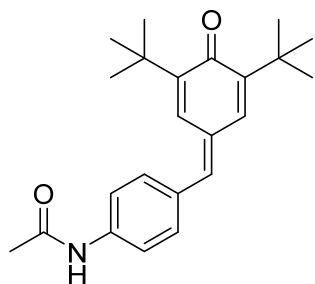
4-((3,5-Di-tert-butyl-4-oxocyclohexa-2,5-dien-1-ylidene)methyl)benzonitrile (1k):

^1H NMR (400 MHz, CDCl_3) δ 7.73 (d, $J = 8.0$ Hz, 2H), 7.53 (d, $J = 8.0$ Hz, 2H), 7.35 (s, 1H), 7.11 (s, 1H), 7.00 (s, 1H), 1.32 (s, 9H), 1.28 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 186.5, 150.6, 149.0, 140.5, 139.0, 134.6, 134.1, 132.5, 130.7, 126.8, 118.6, 112.2, 35.7, 35.3, 29.62, 29.59.

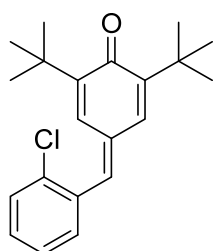


2,6-Di-tert-butyl-4-(4-nitrobenzylidene)cyclohexa-2,5-dien-1-one (1l):

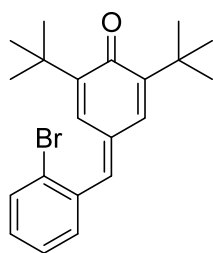
^1H NMR (400 MHz, CDCl_3) δ 8.31 (d, $J = 8.3$ Hz, 2H), 7.59 (d, $J = 8.3$ Hz, 2H), 7.37 (s, 1H), 7.15 (s, 1H), 7.01 (s, 1H), 1.33 (s, 9H), 1.29 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3) δ 186.6, 150.9, 149.3, 147.6, 142.5, 138.4, 134.6, 134.5, 130.9, 126.8, 124.1, 35.8, 35.3, 29.7, 29.6.



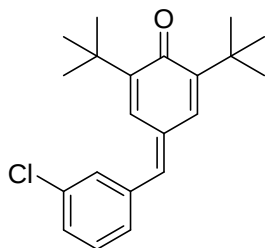
(4-((3,5-Di-tert-butyl-4-oxocyclohexa-2,5-dien-1-ylidene)methyl)phenyl)acetamide (1m): ^1H NMR (400 MHz, CDCl_3) δ 7.69 (s, 1H), 7.64 (d, $J = 7.8$ Hz, 2H), 7.52 (s, 1H), 7.43 (d, $J = 8.0$ Hz, 2H), 7.12 (s, 1H), 7.00 (s, 1H), 2.22 (s, 3H), 1.32 (s, 9H), 1.30 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3) δ 186.7, 168.7, 149.4, 147.7, 142.2, 139.0, 135.4, 131.9, 131.5, 131.5, 127.9, 119.8, 35.6, 35.1, 29.70, 29.65, 24.9.



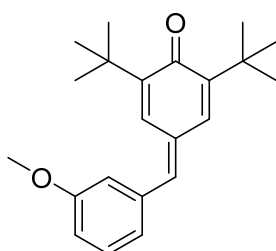
2,6-Di-tert-butyl-4-(2-chlorobenzylidene)cyclohexa-2,5-dien-1-one (1n): ^1H NMR (400 MHz, CDCl_3) δ 7.51 – 7.45 (m, 1H), 7.44 – 7.38 (m, 1H), 7.38 – 7.32 (m, 2H), 7.32 – 7.28 (m, 2H), 7.07 (s, 1H), 1.34 (s, 9H), 1.27 (s, 9H); ^{13}C NMR (151 MHz, CDCl_3 , Overlapping peaks) δ 186.7, 149.8, 148.4, 138.7, 135.0, 134.8, 134.2, 133.0, 132.3, 130.3, 130.1, 127.8, 126.8, 35.6, 35.2, 29.6.



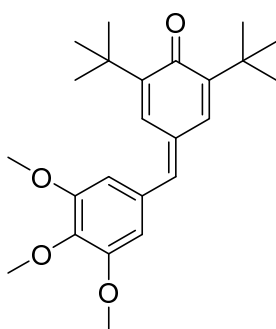
4-(2-Bromobenzylidene)-2,6-di-tert-butylcyclohexa-2,5-dien-1-one (1o): ^1H NMR (400 MHz, CDCl_3) δ 7.69 (d, $J = 7.9$ Hz, 1H), δ 7.44 – 7.36 (m, 2H), 7.31 – 7.21 (m, 3H), 7.08 (s, 1H), 1.35 (s, 9H), 1.27 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3) δ 186.7, 149.8, 148.4, 140.9, 136.0, 134.7, 133.4, 132.7, 132.4, 130.4, 127.8, 127.4, 125.2, 35.6, 35.3, 29.6.



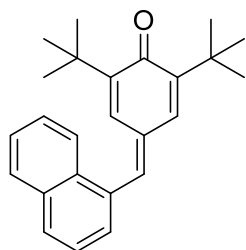
2,6-Di-tert-butyl-4-(3-chlorobenzylidene)cyclohexa-2,5-dien-1-one (1p): ^1H NMR (400 MHz, CDCl_3) δ 7.43 (d, $J = 3.4$ Hz, 2H), 7.39 – 7.28 (m, 3H), 7.08 (s, 1H), 6.99 (s, 1H), 1.33 (s, 9H), 1.30 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3) δ 186.6, 150.0, 148.4, 140.2, 137.7, 134.9, 134.8, 133.0, 130.2, 130.1, 129.0, 128.4, 127.4, 35.6, 35.2, 29.64, 29.63.



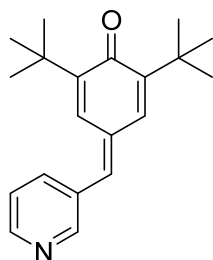
2,6-Di-tert-butyl-4-(3-methoxybenzylidene)cyclohexa-2,5-dien-1-one (1q): ^1H NMR (400 MHz, CDCl_3) δ 7.56 (s, 1H), 7.36 (t, $J = 7.8$ Hz, 1H), 7.16 (s, 1H), 7.05 (d, $J = 7.5$ Hz, 1H), 7.01 (s, 1H), 6.99 (s, 1H), 6.95 (d, $J = 8.2$ Hz, 1H), 3.85 (s, 3H), 1.34 (s, 9H), 1.31 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3) δ 186.7, 159.9, 149.5, 148.0, 142.5, 137.3, 135.2, 132.2, 129.9, 128.0, 123.1, 115.4, 115.3, 55.4, 35.6, 35.1, 29.71, 29.65.



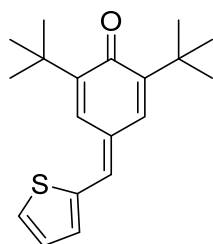
2,6-Di-tert-butyl-4-(3,4,5-trimethoxybenzylidene)cyclohexa-2,5-dien-1-one (1r): ^1H NMR (400 MHz, CDCl_3) δ 7.56 (s, 1H), 7.07 (s, 1H), 6.94 (s, 1H), 6.66 (s, 2H), 3.86 (s, 3H), 3.83 (s, 6H), 1.27 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 186.3, 153.3, 149.1, 147.5, 142.6, 139.2, 135.1, 131.4, 131.3, 127.7, 107.7, 60.9, 56.1, 35.4, 34.9, 29.6, 29.5.



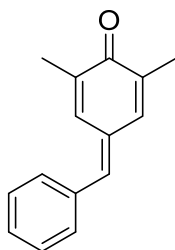
2,6-Di-tert-butyl-4-(naphthalen-1-ylmethylene)cyclohexa-2,5-dien-1-one (1s): ^1H NMR (400 MHz, CDCl_3) δ 8.08 – 8.00 (m, 1H), 7.92 (d, $J = 6.9$ Hz, 2H), 7.78 (s, 1H), 7.61 – 7.52 (m, 3H), 7.49 (d, $J = 6.9$ Hz, 1H), 7.39 (s, 1H), 7.20 (s, 1H), 1.39 (s, 9H), 1.25 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3) δ 186.9, 149.4, 148.1, 140.6, 134.8, 133.8, 133.4, 132.9, 132.1, 129.9, 129.5, 128.9, 128.7, 126.9, 126.6, 125.4, 124.8, 35.5, 35.2, 29.7, 29.6.



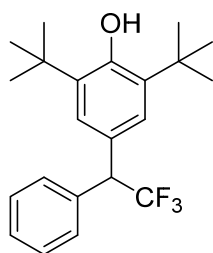
2,6-Di-tert-butyl-4-(pyridin-3-ylmethylene)cyclohexa-2,5-dien-1-one (1t): ^1H NMR (400 MHz, CDCl_3) δ 8.67 (s, 1H), 8.56 (d, $J = 4.3$ Hz, 1H), 7.73 (d, $J = 7.8$ Hz, 1H), 7.42 – 7.31 (m, 2H), 7.08 (s, 1H), 6.99 (s, 1H), 1.29 (s, 9H), 1.25 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3) δ 186.5, 150.9, 150.2, 149.5, 148.5, 137.7, 137.0, 134.6, 133.6, 131.9, 126.9, 123.6, 35.6, 35.1, 29.6, 29.5.



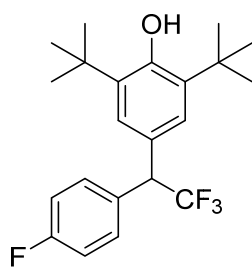
2,6-Di-tert-butyl-4-(thiophen-2-ylmethylene)cyclohexa-2,5-dien-1-one (1u): ^1H NMR (400 MHz, CDCl_3) δ 7.86 (s, 1H), 7.55 (d, $J = 4.9$ Hz, 1H), 7.32 (d, $J = 3.0$ Hz, 1H), 7.18 (s, 1H), 7.14 – 7.07 (m, 1H), 6.95 (s, 1H), 1.37 (s, 9H), 1.32 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 186.3, 149.4, 147.5, 139.4, 135.3, 134.2, 134.1, 131.3, 129.1, 128.0, 127.1, 35.8, 35.1, 29.72, 29.66.



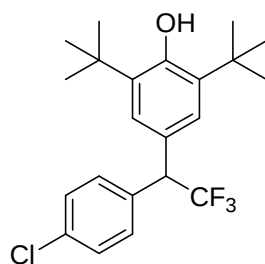
4-Benzylidene-2,6-dimethylcyclohexa-2,5-dien-1-one (1v): ^1H NMR (600 MHz, CDCl_3) δ 7.48 (s, 1H), 7.42 – 7.39 (m, 4H), 7.38 – 7.34 (m, 1H), 7.09 (s, 1H), 6.98 (s, 1H), 2.03 (s, 6H); ^{13}C NMR (150 MHz, CDCl_3 , overlapping peaks) δ 186.9, 142.6, 138.7, 137.2, 135.3, 131.4, 131.1, 130.2, 129.1, 128.5, 16.7, 16.0.



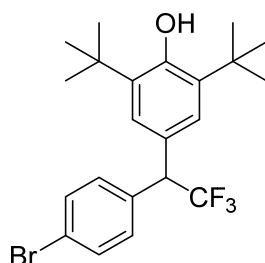
2,6-Di-tert-butyl-4-(2,2,2-trifluoro-1-phenylethyl)phenol (2a): Colorless oil; 98% yield (71 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.43 (d, $J = 7.3$ Hz, 2H), 7.38 (t, $J = 7.3$ Hz, 2H), 7.35 – 7.29 (m, 1H), 7.19 (s, 2H), 5.23 (s, 1H), 4.60 (q, $J = 10.1$ Hz, 1H), 1.44 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 153.6, 136.2, 136.0, 129.2, 128.7, 127.8, 126.6 (q, $J_{\text{C-F}} = 280.6$ Hz), 126.1, 125.9, 55.7 (q, $J_{\text{C-F}} = 27.2$ Hz), 34.5, 30.4; ^{19}F NMR (564 MHz, CDCl_3) δ -65.96 (d, $J = 10.1$ Hz, 3F); FT-IR (thin film, KBr): ν (cm^{-1}) 3638, 2958, 1149, 1104, 714; HRMS (CI) calcd $\text{C}_{22}\text{H}_{27}\text{F}_3\text{O}$ $[\text{M}]^+$: 364.2014, found: 364.2016.



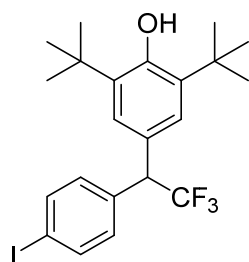
2,6-Di-tert-butyl-4-(2,2,2-trifluoro-1-(4-fluorophenyl)ethyl)phenol (2b): White solid; m.p. 84-86 $^{\circ}\text{C}$; 71% yield (54 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.41 – 7.33 (m, 2H), 7.14 (s, 2H), 7.06 (t, $J = 8.5$ Hz, 2H), 5.24 (s, 1H), 4.58 (q, $J = 10.0$ Hz, 1H), 1.43 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 162.4 (d, $J_{\text{C-F}} = 246.7$ Hz), 153.6, 136.2, 132.0, 130.9 (d, $J_{\text{C-F}} = 8.0$ Hz), 126.5 (q, $J_{\text{C-F}} = 280.5$ Hz), 125.9, 125.8, 115.7 (d, $J_{\text{C-F}} = 21.5$ Hz), 54.9 (q, $J_{\text{C-F}} = 27.4$ Hz), 34.5, 30.4; ^{19}F NMR (564 MHz, CDCl_3) δ -66.25 (d, $J = 10.1$ Hz, 3F), -114.70 – -114.78 (m, 1F); FT-IR (thin film, KBr): ν (cm^{-1}) 3633, 2961, 1190, 1097, 802; HRMS (CI) calcd $\text{C}_{22}\text{H}_{26}\text{F}_4\text{O}$ $[\text{M}]^+$: 382.1920, found: 382.1927.



2,6-Di-tert-butyl-4-(1-(4-chlorophenyl)-2,2,2-trifluoroethyl)phenol (2c): White solid; m.p. 83-87 °C; 83% yield (66 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.37 – 7.29 (m, 4H), 7.12 (s, 2H), 5.24 (s, 1H), 4.56 (q, $J = 10.0$ Hz, 1H), 1.42 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 153.7, 136.2, 134.7, 133.8, 130.5, 128.9, 126.4 (q, $J_{\text{C-F}} = 280.5$ Hz), 125.8, 125.6, 55.0 (q, $J_{\text{C-F}} = 27.4$ Hz), 34.5, 30.4; ^{19}F NMR (564 MHz, CDCl_3) δ -66.15 (d, $J = 10.0$ Hz, 3F); FT-IR (thin film, KBr): ν (cm^{-1}) 3621, 2923, 1184, 1095, 806; HRMS (CI) calcd $\text{C}_{22}\text{H}_{26}^{35}\text{ClF}_3\text{O}$ $[\text{M}]^+$: 398.1624, found: 398.1617.

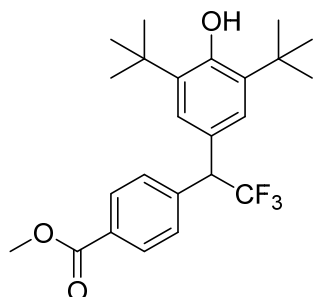


(1-(4-Bromophenyl)-2,2,2-trifluoroethyl)-2,6-di-tert-butylphenol (2d): White solid; m.p. 104-107 °C; 79% yield (70 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.47 (d, $J = 7.8$ Hz, 2H), 7.25 (d, $J = 7.9$ Hz, 2H), 7.10 (s, 2H), 5.22 (s, 1H), 4.53 (q, $J = 9.6$ Hz, 1H), 1.41 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 153.7, 136.2, 135.2, 131.9, 130.9, 126.3 (q, $J_{\text{C-F}} = 280.5$ Hz), 125.8, 125.5, 122.0, 55.1 (q, $J_{\text{C-F}} = 27.5$ Hz), 34.5, 30.4; ^{19}F NMR (564 MHz, CDCl_3) δ -66.12 (d, $J = 10.0$ Hz, 3F); FT-IR (thin film, KBr): ν (cm^{-1}) 3626, 2966, 1182, 1105, 722; HRMS (CI) calcd $\text{C}_{22}\text{H}_{26}^{79}\text{BrF}_3\text{O}$ $[\text{M}]^+$: 442.1119, found: 442.1121.

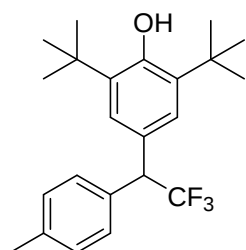


2,6-Di-tert-butyl-4-(2,2,2-trifluoro-1-(4-iodophenyl)ethyl)phenol (2e): White solid; m.p. 102-105 °C; 90% yield (88 mg); ^1H NMR (600 MHz, CDCl_3) δ 7.70 (d, $J = 8.4$ Hz, 2H), 7.15 (d, $J = 8.2$ Hz, 2H), 7.13 (s, 2H), 5.24 (s, 1H), 4.53 (q, $J = 10.0$ Hz, 1H), 1.43 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 153.7, 137.9, 136.2, 135.9, 131.1, 126.3 (q, $J_{\text{C-F}} = 280.6$ Hz), 125.8, 125.5, 93.6, 55.2 (q, $J_{\text{C-F}} = 27.5$ Hz), 34.5, 30.4; ^{19}F NMR (564 MHz, CDCl_3) δ -66.05 (d, $J = 10.0$ Hz, 3F); FT-IR (thin film, KBr): ν (cm^{-1})

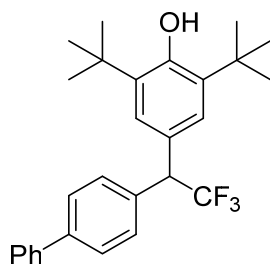
3617, 2957, 1184, 1108, 770; HRMS (CI) calcd C₂₂H₂₆F₃IO [M]⁺: 490.0981, found: 490.0968.



Methyl 4-(1-(3,5-di-tert-butyl-4-hydroxyphenyl)-2,2,2-trifluoroethyl)benzoate (2f): White solid; m.p. 46-48 °C; 83% yield (70 mg); ¹H NMR (400 MHz, CDCl₃) δ 8.04 (d, *J* = 7.8 Hz, 2H), 7.49 (d, *J* = 7.8 Hz, 2H), 7.13 (s, 2H), 5.26 (s, 1H), 4.65 (q, *J* = 9.8 Hz, 1H), 3.92 (s, 3H), 1.41 (s, 18H); ¹³C NMR (150 MHz, CDCl₃) δ 166.8, 153.8, 141.2, 136.2, 130.0, 129.6, 129.2, 126.3 (q, *J*_{C-F} = 280.6 Hz), 125.9, 125.3, 55.5 (q, *J*_{C-F} = 27.5 Hz), 52.3, 34.5, 30.3; ¹⁹F NMR (564 MHz, CDCl₃) δ -65.86 (d, *J* = 9.9 Hz, 3F); FT-IR (thin film, KBr): ν (cm⁻¹) 3937, 2956, 1721, 1435, 1152; HRMS (CI) calcd C₂₄H₂₉F₃O₃ [M + H]⁺: 423.2147, found: 423.2152.

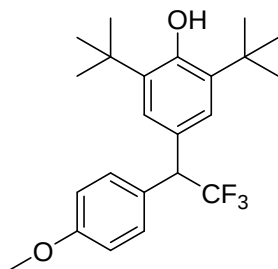


2,6-Di-tert-butyl-4-(2,2,2-trifluoro-1-(*p*-tolyl)ethyl)phenol (2g): White solid; m.p. 90-93 °C; 80% yield (61 mg); ¹H NMR (400 MHz, CDCl₃) δ 7.31 (d, *J* = 7.7 Hz, 2H), 7.21 – 7.15 (m, 4H), 5.21 (s, 1H), 4.56 (q, *J* = 10.2 Hz, 1H), 2.36 (s, 3H), 1.44 (s, 18H); ¹³C NMR (150 MHz, CDCl₃) δ 153.5, 137.5, 136.0, 133.2, 129.4, 129.0, 126.7 (d, *J*_{C-F} = 280.5 Hz), 126.3, 125.9, 55.4 (q, *J*_{C-F} = 27.2 Hz), 34.5, 30.4, 21.2; ¹⁹F NMR (564 MHz, CDCl₃) δ -66.10 (d, *J* = 10.2 Hz, 3F); FT-IR (thin film, KBr): ν (cm⁻¹) 3613, 2921, 1151, 1102, 639; HRMS (CI) calcd C₂₃H₂₉F₃O [M]⁺: 378.2171, found: 378.2163.

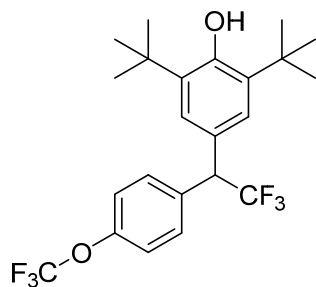


4-(1-([1,1'-Biphenyl]-4-yl)-2,2,2-trifluoroethyl)-2,6-di-tert-butylphenol (2h):

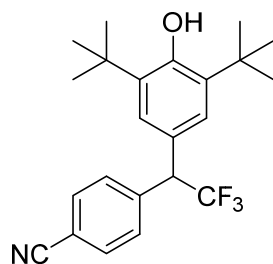
White solid; m.p. 148-150 °C; 77% yield (68 mg); ¹H NMR (400 MHz, CDCl₃) δ 7.65 – 7.57 (m, 4H), 7.54 – 7.42 (m, 4H), 7.37 (t, *J* = 7.0 Hz, 1H), 7.23 (s, 2H), 5.25 (s, 1H), 4.64 (q, *J* = 10.0 Hz, 1H), 1.45 (s, 18H); ¹³C NMR (150 MHz, CDCl₃) δ 153.6, 140.7, 140.6, 136.1, 135.2, 129.6, 128.9, 127.6, 127.5, 127.5 (q, *J*_{C-F} = 280.6 Hz), 127.2, 126.0, 125.9, 55.4 (q, *J*_{C-F} = 27.3 Hz), 34.5, 30.4; ¹⁹F NMR (564 MHz, CDCl₃) δ -65.94 (d, *J* = 10.1 Hz, 3F); FT-IR (thin film, KBr): ν (cm⁻¹) 3619, 2963, 1145, 1103, 698; HRMS (CI) calcd C₂₈H₃₁F₃O [M]⁺: 440.2327, found: 440.2321.



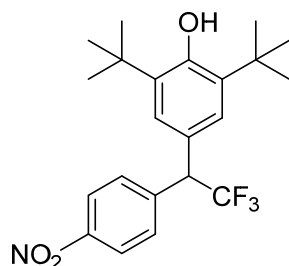
2,6-Di-tert-butyl-4-(2,2,2-trifluoro-1-(4-methoxyphenyl)ethyl)phenol (2i): White solid; m.p. 95-98 °C; 83% yield (65 mg); ¹H NMR (400 MHz, CDCl₃) δ 7.32 (d, *J* = 8.4 Hz, 2H), 7.16 (s, 2H), 6.90 (d, *J* = 8.5 Hz, 2H), 5.21 (s, 1H), 4.54 (q, *J* = 10.2 Hz, 1H), 3.81 (s, 3H), 1.43 (s, 18H); ¹³C NMR (150 MHz, CDCl₃) δ 159.1, 153.5, 136.0, 130.3, 128.3, 126.4, 126.9 (q, *J*_{C-F} = 280.5 Hz), 125.8, 114.1, 55.4, 54.8 (q, *J*_{C-F} = 27.2 Hz), 34.5, 30.4; ¹⁹F NMR (564 MHz, CDCl₃) δ -66.30 (d, *J* = 10.2 Hz, 3F); FT-IR (thin film, KBr): ν (cm⁻¹) 3598, 2961, 1146, 1030, 802; HRMS (CI) calcd C₂₃H₃₀F₃O₂ [M + H]⁺: 395.2198, found: 395.2188.



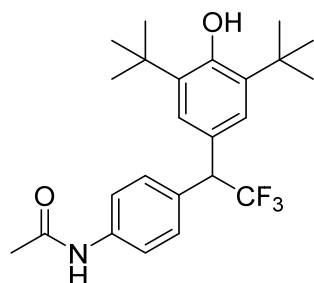
2,6-Di-tert-butyl-4-(2,2,2-trifluoro-1-(4-(trifluoromethoxy)phenyl)ethyl)phenol (2j): White solid; m.p. 46-49 °C; 79% yield (71 mg); ¹H NMR (400 MHz, CDCl₃) δ 7.43 (d, *J* = 8.3 Hz, 2H), 7.22 (d, *J* = 8.2 Hz, 2H), 7.14 (s, 2H), 5.25 (s, 1H), 4.60 (q, *J* = 9.9 Hz, 1H), 1.43 (s, 18H); ¹³C NMR (100 MHz, CDCl₃) δ 153.8, 148.9, 136.3, 134.9, 130.6, 126.4 (q, *J*_{C-F} = 280.5 Hz), 125.8, 125.5, 121.1, 120.6 (q, *J*_{C-F} = 257.2 Hz), 55.0 (q, *J*_{C-F} = 27.5 Hz), 34.5, 30.3; ¹⁹F NMR (376 MHz, CDCl₃) δ -57.85 (s, 3F), -66.13 (d, *J* = 10.0 Hz, 3F); FT-IR (thin film, KBr): ν (cm⁻¹) 3640, 2960, 1255, 1105, 808; HRMS (CI) calcd C₂₃H₂₇F₆O₂ [M + H]⁺: 449.1915, found: 449.1910.



2,6-Di-tert-butyl-4-(2,2,2-trifluoro-1-(4-isocyanophenyl)ethyl)phenol (2k): White solid; m.p. 99-101 °C; 69% yield (53 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.66 (d, J = 7.8 Hz, 2H), 7.51 (d, J = 7.8 Hz, 2H), 7.09 (s, 2H), 5.28 (s, 1H), 4.64 (q, J = 9.6 Hz, 1H), 1.41 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 153.9, 141.4, 136.5, 132.5, 129.9, 126.0 (q, $J_{\text{C-F}}$ = 280.6 Hz), 125.8, 124.7, 118.6, 111.9, 55.5 (q, $J_{\text{C-F}}$ = 27.7 Hz), 34.5, 30.3; ^{19}F NMR (564 MHz, CDCl_3) δ -65.83 (d, J = 9.8 Hz, 3F); FT-IR (thin film, KBr): ν (cm^{-1}) 3631, 2959, 2231, 1437, 1154; HRMS (CI) calcd $\text{C}_{23}\text{H}_{27}\text{F}_3\text{NO}$ $[\text{M} + \text{H}]^+$: 390.2045, found: 390.2054.

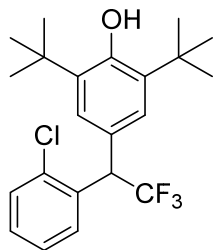


2,6-Di-tert-butyl-4-(2,2,2-trifluoro-1-(4-nitrophenyl)ethyl)phenol (2l): White solid; m.p. 120-122 °C; 68% yield (56 mg); ^1H NMR (400 MHz, CDCl_3) δ 8.22 (d, J = 8.5 Hz, 2H), 7.57 (d, J = 8.4 Hz, 2H), 7.10 (s, 2H), 5.29 (s, 1H), 4.70 (q, J = 9.7 Hz, 1H), 1.41 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 154.0, 147.5, 143.4, 136.5, 130.1, 126.0 (q, $J_{\text{C-F}}$ = 280.7 Hz), 125.8, 124.6, 124.0, 55.4 (q, $J_{\text{C-F}}$ = 27.8 Hz), 34.5, 30.3; ^{19}F NMR (564 MHz, CDCl_3) δ -65.86 (d, J = 9.7 Hz, 3F); FT-IR (thin film, KBr): ν (cm^{-1}) 3605, 2920, 1523, 1119, 850; HRMS (CI) calcd $\text{C}_{22}\text{H}_{27}\text{F}_3\text{NO}_3$ $[\text{M} + \text{H}]^+$: 410.1943, found: 410.1930.

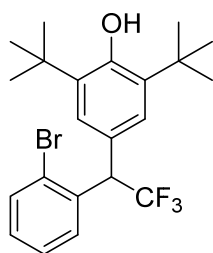


N-(4-(1-(3,5-di-tert-butyl-4-hydroxyphenyl)-2,2,2-trifluoroethyl)phenyl)acetamide (2m): White solid; m.p. 208-214 °C; 67% yield (57 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.49 (d, J = 8.2 Hz, 2H), 7.41 (s, 1H), 7.33 (d, J = 8.1 Hz, 2H), 7.13 (s, 2H), 5.21 (s, 1H), 4.53 (q, J = 10.0 Hz, 1H), 2.16 (s, 3H), 1.41 (s, 18H); ^{13}C NMR (100 MHz, CDCl_3) δ 168.6, 153.5, 137.5, 136.1, 132.0, 129.8, 126.5 (d, $J_{\text{C-F}}$ = 280.5 Hz),

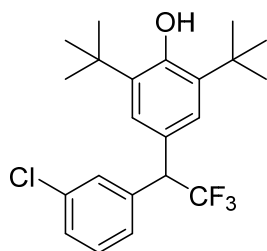
126.0, 125.8, 120.0, 55.1 (q, J_{C-F} = 54.7, 27.3 Hz), 34.5, 30.4, 24.7; ^{19}F NMR (564 MHz, CDCl_3) δ -66.16 (d, J = 9.7 Hz, 3F); FT-IR (thin film, KBr): ν (cm^{-1}) 3620, 3910, 2959, 1148, 1103; HRMS (CI) calcd $\text{C}_{24}\text{H}_{31}\text{F}_3\text{NO}_2$ $[\text{M} + \text{H}]^+$: 422.2307, found: 422.2317.



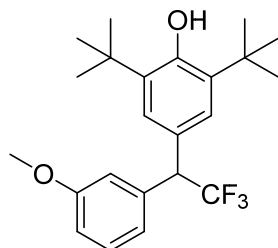
2,6-Di-tert-butyl-4-(1-(2-chlorophenyl)-2,2,2-trifluoroethyl)phenol (2n): White solid; m.p. 100-103 °C; 90% yield (72 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.68 (d, J = 7.7 Hz, 1H), 7.41 (d, J = 7.8 Hz, 1H), 7.32 (t, J = 7.4 Hz, 1H), 7.28 – 7.21 (m, 1H), 7.18 (s, 2H), 5.34 – 5.17 (m, 2H), 1.42 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 153.7, 136.0, 134.7, 134.2, 130.2, 129.2, 129.0, 127.2, 126.5 (d, J_{C-F} = 280.5 Hz), 126.2, 124.9, 51.0 (q, J_{C-F} = 27.9 Hz), 34.5, 30.4; ^{19}F NMR (564 MHz, CDCl_3) δ -65.48 (d, J = 10.1 Hz, 3F); FT-IR (thin film, KBr): ν (cm^{-1}) 3629, 2960, 1123, 1102, 755; HRMS (CI) calcd $\text{C}_{22}\text{H}_{26}^{35}\text{ClF}_3\text{O}$ $[\text{M}]^+$: 398.1624, found: 398.1629.



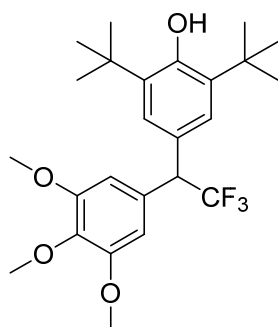
4-(1-(2-Bromophenyl)-2,2,2-trifluoroethyl)-2,6-di-tert-butylphenol (2o): White solid; m.p. 103-107 °C; 80% yield (71 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.69 (d, J = 7.7 Hz, 1H), 7.61 (d, J = 8.0 Hz, 1H), 7.36 (t, J = 7.6 Hz, 1H), 7.20 (s, 2H), 7.19 – 7.13 (m, 1H), 5.34 – 5.16 (m, 2H), 1.43 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 153.7, 136.0, 135.9, 133.6, 129.3, 129.3, 127.8, 126.5 (q, J_{C-F} = 280.7 Hz), 126.2, 125.7, 124.9, 53.7 (q, J_{C-F} = 27.8 Hz), 34.5, 30.4; ^{19}F NMR (564 MHz, CDCl_3) δ -65.36 (d, J = 10.1 Hz, 3F); FT-IR (thin film, KBr): ν (cm^{-1}) 3630, 2957, 1122, 1101, 754; HRMS (CI) calcd $\text{C}_{22}\text{H}_{26}^{79}\text{BrF}_3\text{O}$ $[\text{M}]^+$: 442.1119, found: 442.1108.



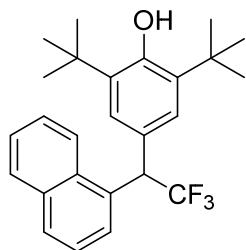
2,6-Di-tert-butyl-4-(1-(3-chlorophenyl)-2,2,2-trifluoroethyl)phenol (2p): White solid; m.p. 99-102 °C; 82% yield (65 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.40 (s, 1H), 7.33 – 7.29 (m, 3H), 7.15 (s, 2H), 5.26 (s, 1H), 4.56 (q, $J = 9.9$ Hz, 1H), 1.44 (s, 18H); ^{13}C NMR (100 MHz, CDCl_3) δ 153.8, 138.1, 136.2, 134.6, 130.0, 129.5, 128.1, 127.2, 126.3 (q, $J_{\text{C-F}} = 280.5$ Hz), 125.9, 125.3, 55.3 (q, $J_{\text{C-F}} = 27.6$ Hz), 34.5, 30.3; ^{19}F NMR (564 MHz, CDCl_3) δ -65.98 (d, $J = 10.0$ Hz, 3F); FT-IR (thin film, KBr): ν (cm^{-1}) 3636, 2956, 1143, 1108, 693; HRMS (CI) calcd $\text{C}_{22}\text{H}_{27}^{35}\text{ClF}_3\text{O}$ $[\text{M} + \text{H}]^+$: 399.1703, found: 399.1691.



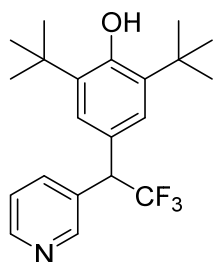
2,6-Di-tert-butyl-4-(2,2,2-trifluoro-1-(3-methoxyphenyl)ethyl)phenol (2q): White solid; m.p. 74-77 °C; 83% yield (65 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.31 – 7.22 (m, 1H), 7.16 (s, 2H), 7.00 (d, $J = 7.6$ Hz, 1H), 6.94 (s, 1H), 6.84 (d, $J = 7.8$ Hz, 1H), 5.20 (s, 1H), 4.53 (q, $J = 10.1$ Hz, 1H), 3.79 (s, 3H), 1.41 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 159.8, 153.6, 137.6, 136.0, 129.7, 126.6 (q, $J_{\text{C-F}} = 280.5$ Hz), 125.93, 125.88, 121.5, 115.3, 113.0, 55.6 (q, $J_{\text{C-F}} = 54.7, 27.4$ Hz), 55.3, 34.5, 30.4; ^{19}F NMR (564 MHz, CDCl_3) δ -65.96 (d, $J = 10.1$ Hz, 3F); FT-IR (thin film, KBr): ν (cm^{-1}) 3614, 2962, 1264, 1144, 698; HRMS (CI) calcd $\text{C}_{23}\text{H}_{30}\text{F}_3\text{O}_2$ $[\text{M} + \text{H}]^+$: 395.2198, found: 395.2186.



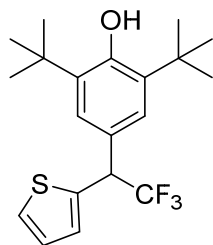
2,6-Di-tert-butyl-4-(2,2,2-trifluoro-1-(3,4,5-trimethoxyphenyl)ethyl)phenol (2r): Colorless oil; 73% yield (66 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.20 (s, 2H), 6.63 (s, 2H), 5.22 (s, 1H), 4.48 (q, $J = 10.0$ Hz, 1H), 3.87 – 3.82 (m, 9H), 1.43 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 153.7, 153.3, 137.7, 136.1, 131.4, 126.5 (q, $J_{\text{C-F}} = 280.9$ Hz), 125.8, 125.7, 106.5, 61.0, 56.2, 55.7 (q, $J_{\text{C-F}} = 27.3$ Hz), 34.5, 30.4; ^{19}F NMR (564 MHz, CDCl_3) δ -66.15 (d, $J = 10.1$ Hz, 3F); FT-IR (thin film, KBr): ν (cm^{-1}) 3636, 2956, 1237, 1007, 700; HRMS (CI) calcd $\text{C}_{25}\text{H}_{34}\text{F}_3\text{O}_4$ $[\text{M} + \text{H}]^+$: 455.2409, found: 455.2408.



2,6-Di-tert-butyl-4-(2,2,2-trifluoro-1-(naphthalen-1-yl)ethyl)phenol (2s): White solid; m.p. 153-158 °C; 70% yield (58 mg); ^1H NMR (400 MHz, CDCl_3) δ 8.04 (d, J = 8.2 Hz, 1H), 7.92 – 7.75 (m, 3H), 7.59 – 7.43 (m, 3H), 7.22 (s, 2H), 5.45 (q, J = 9.8 Hz, 1H), 5.18 (s, 1H), 1.39 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 153.6, 135.9, 134.2, 131.9, 131.8, 129.2, 128.6, 127.0 (q, $J_{\text{C-F}}$ = 280.7 Hz), 126.7, 126.2, 125.9, 125.8, 125.7, 125.4, 123.2, 50.4 (q, $J_{\text{C-F}}$ = 27.2 Hz), 34.5, 30.4; ^{19}F NMR (376 MHz, CDCl_3) δ -64.82 (d, J = 10.8 Hz); ^{19}F NMR (564 MHz, CDCl_3) δ -64.82 (d, J = 10.8 Hz, 3F); FT-IR (thin film, KBr): ν (cm^{-1}) 3616, 2920, 1182, 1103, 772; HRMS (CI) calcd $\text{C}_{26}\text{H}_{29}\text{F}_3\text{O}$ $[\text{M}]^+$: 414.2171, found: 414.2156.

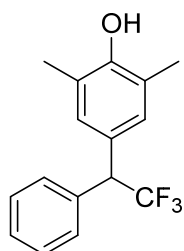


2,6-Di-tert-butyl-4-(2,2,2-trifluoro-1-(pyridin-3-yl)ethyl)phenol (2t): Colorless liquid; 43% yield (31 mg); ^1H NMR (400 MHz, CDCl_3) 8.65 – 8.52 (m, 2H), 7.76 (d, J = 7.3 Hz, 1H), 7.34 – 7.28 (m, 1H), 7.12 (s, 2H), 5.29 (s, 1H), 4.60 (q, J = 9.7 Hz, 1H), 1.41 (s, 18H); ^{13}C NMR (100 MHz, CDCl_3) δ 153.9, 150.4, 149.0, 136.44, 136.40, 132.2, 126.2 (q, $J_{\text{C-F}}$ = 280.7 Hz), 125.8, 124.8, 123.7, 53.4 (q, $J_{\text{C-F}}$ = 28.0 Hz), 34.5, 30.3; ^{19}F NMR (564 MHz, CDCl_3) δ -66.11 (d, J = 10.3 Hz, 3F); FT-IR (thin film, KBr): ν (cm^{-1}) 3638, 2957, 1578, 1155, 865; HRMS (CI) calcd $\text{C}_{21}\text{H}_{27}\text{F}_3\text{NO}$ $[\text{M} + \text{H}]^+$: 366.2045, found: 366.2040.

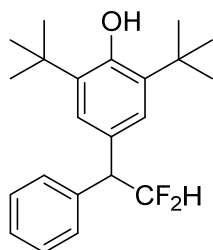


2,6-Di-tert-butyl-4-(2,2,2-trifluoro-1-(thiophen-2-yl)ethyl)phenol (2u): Yellowish oil; 20% yield (15 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.25 (s, 1H), 7.21 (s, 2H), 7.09 – 7.06 (m, 1H), 7.01 – 6.95 (m, 1H), 5.24 (s, 1H), 4.79 (q, J = 9.5 Hz, 1H), 1.42 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 154.0, 138.1, 136.1, 127.5, 126.9, 125.9, 125.8 (q, $J_{\text{C-F}}$ = 280.6 Hz), 125.7, 125.5, 51.3 (q, $J_{\text{C-F}}$ = 28.8 Hz), 34.5, 30.4; ^{19}F NMR (564

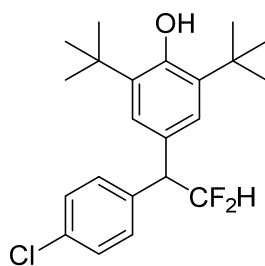
MHz, CDCl₃) δ -68.01 (d, J = 9.9 Hz, 3F); FT-IR (thin film, KBr): ν (cm⁻¹) 3637, 2957, 1435, 1251, 701; HRMS (CI) calcd C₂₀H₂₆F₃OS [M + H]⁺: 371.1656, found: 371.1660.



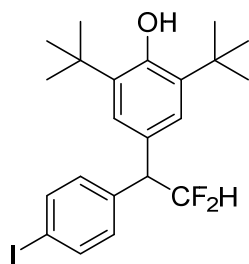
2,6-Dimethyl-4-(2,2,2-trifluoro-1-phenylethyl)phenol (2v): Yellowish oil; 34% yield (19 mg); ¹H NMR (600 MHz, CDCl₃) δ 7.37 (d, J = 7.5 Hz, 2H), 7.34 (t, J = 7.5 Hz, 2H), 7.30 (t, J = 7.0 Hz, 1H), 6.97 (s, 2H), 4.65 (s, 1H), 4.54 (q, J = 10.1 Hz, 1H), 2.22 (s, 6H); ¹³C NMR (150 MHz, CDCl₃) δ 152.1, 136.1, 129.4, 129.1, 128.8, 127.8, 127.1, 126.5 (q, J_{C-F} = 280.4 Hz), 123.4, 55.0 (q, J_{C-F} = 27.4 Hz), 16.1; ¹⁹F NMR (564 MHz, CDCl₃) δ -66.06 (d, J = 10.1 Hz, 3F); FT-IR (thin film, KBr): ν (cm⁻¹) 3447, 2925, 1259, 1105, 699; HRMS (CI) calcd C₁₆H₁₆F₃O [M + H]⁺: 281.1153, found: 281.1146.



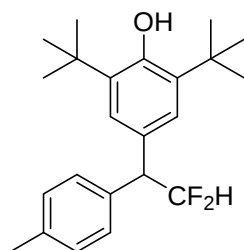
2,6-Di-tert-butyl-4-(2,2-difluoro-1-phenylethyl)phenol (3a): Yellowish oil; 81% yield (56 mg); ¹H NMR (400 MHz, CDCl₃) δ 7.38 – 7.32 (m, 4H), 7.31 – 7.27 (m, 1H), 7.10 (s, 2H), 6.26 (td, J = 56.1, 4.3 Hz, 1H), 5.18 (s, 1H), 4.31 (td, J = 16.3, 4.2 Hz, 1H), 1.42 (s, 18H); ¹³C NMR (150 MHz, CDCl₃) δ 153.2, 137.8, 136.1, 129.2, 128.7, 127.8, 127.4, 125.8, 117.4 (t, J_{C-F} = 244.5 Hz), 55.2 (t, J_{C-F} = 20.4 Hz), 34.5, 30.4; ¹⁹F NMR (564 MHz, CDCl₃) δ -117.26 (ddd, J = 276.9, 56.1, 15.5 Hz, 1F), -118.26 (ddd, J = 276.9, 56.2, 16.9 Hz, 1F); FT-IR (thin film, KBr): ν (cm⁻¹) 3636, 2958, 1436, 1055, 699; HRMS (CI) calcd C₂₂H₂₉F₂O [M + H]⁺: 347.2186, found: 347.2181.



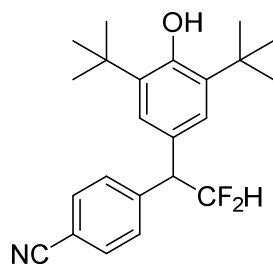
2,6-Di-tert-butyl-4-(1-(4-chlorophenyl)-2,2-difluoroethyl)phenol (3b): Yellowish oil; 63% yield (48 mg); ^1H NMR (600 MHz, CDCl_3) δ 7.31 (d, $J = 8.1$ Hz, 2H), 7.25 (d, $J = 7.7$ Hz, 2H), 7.05 (s, 2H), 6.21 (td, $J = 56.0, 3.9$ Hz, 1H), 5.19 (s, 1H), 4.35 – 4.21 (m, 1H), 1.41 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 153.4, 136.3, 136.2, 133.3, 130.6, 128.8, 127.3, 125.6, 117.1 (t, $J_{\text{C-F}} = 244.8$ Hz), 54.5 (t, $J_{\text{C-F}} = 20.5$ Hz), 34.5, 30.4; ^{19}F NMR (564 MHz, CDCl_3) δ -116.82 (ddd, $J = 278.0, 55.9, 14.5$ Hz, 1F), -119.10 (ddd, $J = 278.0, 56.1, 18.2$ Hz, 1F); FT-IR (thin film, KBr): ν (cm^{-1}) 3635, 2958, 1436, 1053, 810; HRMS (CI) calcd $\text{C}_{22}\text{H}_{28}^{35}\text{ClF}_2\text{O}$ $[\text{M} + \text{H}]^+$: 381.1797, found: 381.1788.



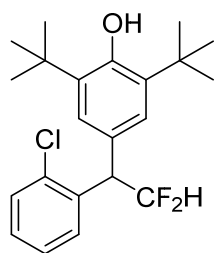
2,6-Di-tert-butyl-4-(2,2-difluoro-1-(4-iodophenyl)ethyl)phenol (3c): White solid; m.p. 115-117 °C; 70% yield (66 mg); ^1H NMR (600 MHz, CDCl_3) δ 7.67 (d, $J = 8.2$ Hz, 2H), 7.08 (d, $J = 8.1$ Hz, 2H), 7.06 (s, 2H), 6.22 (td, $J = 56.0, 3.9$ Hz, 1H), 5.20 (s, 1H), 4.29 – 4.21 (m, 1H), 1.42 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 153.4, 137.7, 137.4, 136.3, 131.3, 127.2, 125.6, 117.0 (t, $J_{\text{C-F}} = 244.8$ Hz), 93.1, 54.7 (t, $J_{\text{C-F}} = 20.5$ Hz), 34.5, 30.4; ^{19}F NMR (564 MHz, CDCl_3) δ -116.73 (ddd, $J = 278.1, 55.8, 14.4$ Hz, 1F), -119.06 (ddd, $J = 278.1, 56.1, 18.2$ Hz, 1F); FT-IR (thin film, KBr): ν (cm^{-1}) 3616, 2957, 1434, 1208, 799; HRMS (CI) calcd $\text{C}_{22}\text{H}_{27}\text{F}_2\text{IO}$ $[\text{M}]^+$: 472.1075, found: 472.1089.



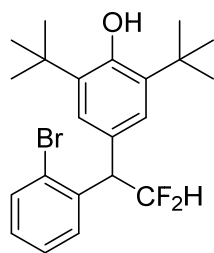
2,6-Di-tert-butyl-4-(2,2-difluoro-1-(p-tolyl)ethyl)phenol (3d): White solid; m.p. 83-86 °C; 58% yield (42 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.23 (d, $J = 7.7$ Hz, 2H), 7.16 (d, $J = 7.7$ Hz, 2H), 7.11 (s, 2H), 6.24 (td, $J = 56.2, 4.1$ Hz, 1H), 5.17 (s, 1H), 4.27 (td, $J = 16.5, 3.8$ Hz, 1H), 2.34 (s, 3H), 1.42 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 153.2, 137.0, 136.0, 134.7, 129.4, 129.0, 128.0, 125.7, 117.5 (t, $J_{\text{C-F}} = 244.4$ Hz), 54.9 (t, $J_{\text{C-F}} = 20.4$ Hz), 34.5, 30.4, 21.2; ^{19}F NMR (564 MHz, CDCl_3) δ -117.18 (ddd, $J = 276.4, 56.1, 15.5$ Hz, 1F), -118.32 (ddd, $J = 276.4, 56.3, 17.0$ Hz, 1F); FT-IR (thin film, KBr): ν (cm^{-1}) 3611, 2959, 1436, 1109, 799; HRMS (CI) calcd $\text{C}_{23}\text{H}_{31}\text{F}_2\text{O}$ $[\text{M} + \text{H}]^+$: 361.2343, found: 361.2335.



2,6-Di-tert-butyl-4-(2,2-difluoro-1-(4-isocyanophenyl)ethyl)phenol (3e): White solid; m.p. 40-44 °C; 42% yield (31 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.63 (d, J = 8.0 Hz, 1H), 7.44 (d, J = 8.0 Hz, 1H), 7.04 (s, 1H), 6.25 (td, J = 55.7, 3.5 Hz, 1H), 5.24 (s, 1H), 4.45 – 4.30 (m, 1H), 1.41 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3) δ 153.5, 142.8, 136.4, 132.2, 130.0, 126.3, 125.5, 118.7, 116.6 (t, $J_{\text{C-F}}$ = 245.3 Hz), 111.2, 54.9 (t, $J_{\text{C-F}}$ = 20.5 Hz), 34.4, 30.2; ^{19}F NMR (564 MHz, CDCl_3) δ -116.18 (ddd, J = 279.8, 55.5, 13.5 Hz, 1F), -119.59 (ddd, J = 279.8, 55.9, 19.2 Hz, 1F); FT-IR (thin film, KBr): ν (cm^{-1}) 3632, 2959, 2229, 1436, 810; HRMS (CI) calcd $\text{C}_{23}\text{H}_{28}\text{F}_2\text{NO}$ $[\text{M} + \text{H}]^+$: 372.2139, found: 372.2143.

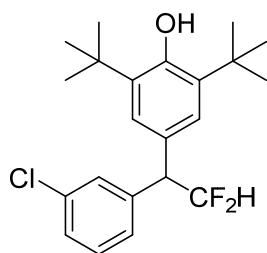


2,6-Di-tert-butyl-4-(1-(2-chlorophenyl)-2,2-difluoroethyl)phenol (3f): White solid; m.p. 59-64 °C; 66% yield (50 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.50 (d, J = 7.6 Hz, 1H), 7.41 (d, J = 7.7 Hz, 1H), 7.29 (t, J = 7.4 Hz, 1H), 7.22 (t, J = 7.2 Hz, 1H), 7.13 (s, 2H), 6.31 (td, J = 55.9, 4.3 Hz, 1H), 5.18 (s, 1H), 4.92 (td, J = 16.3, 4.2 Hz, 1H), 1.42 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 153.3, 136.0, 135.9, 134.8, 130.2, 129.7, 128.6, 127.1, 126.4, 126.0, 117.1 (t, $J_{\text{C-F}}$ = 244.8 Hz), 50.9 (t, $J_{\text{C-F}}$ = 21.2 Hz), 34.5, 30.4; ^{19}F NMR (564 MHz, CDCl_3) δ -117.39 (ddd, J = 277.8, 56.0, 15.5 Hz, 1F), -118.89 (ddd, J = 277.8, 55.8, 16.8 Hz, 1F); FT-IR (thin film, KBr): ν (cm^{-1}) 3630, 2958, 1434, 1060, 751; HRMS (CI) calcd $\text{C}_{22}\text{H}_{27}^{35}\text{ClF}_2\text{O}$ $[\text{M}]^+$: 380.1718, found: 380.1721.

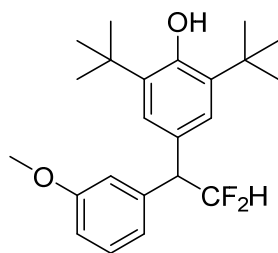


4-(1-(2-Bromophenyl)-2,2-difluoroethyl)-2,6-di-tert-butylphenol (3g): White solid; m.p. 81-84 °C; 62% yield (53 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.60 (d, J = 7.9 Hz,

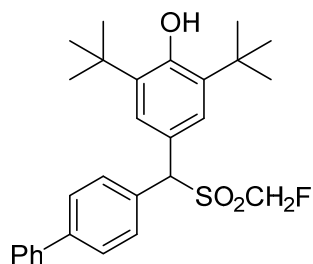
1H), 7.50 (d, $J = 7.7$ Hz, 1H), 7.33 (t, $J = 7.5$ Hz, 1H), 7.16 – 7.11 (m, 3H), 6.30 (td, $J = 55.9, 3.7$ Hz, 1H), 5.18 (s, 1H), 4.93 (td, $J = 16.3, 3.6$ Hz, 1H), 1.42 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 153.3, 137.5, 136.0, 133.5, 129.7, 128.8, 127.7, 126.5, 126.0, 125.7, 117.2 (t, $J_{\text{C-F}} = 244.9$ Hz), 53.4 (t, $J_{\text{C-F}} = 21.2$ Hz), 34.5, 30.4; ^{19}F NMR (564 MHz, CDCl_3) δ -117.39 (ddd, $J = 277.8, 56.0, 15.6$ Hz, 1F), -119.02 (ddd, $J = 277.7, 55.8, 16.8$ Hz, 1F); FT-IR (thin film, KBr): ν (cm^{-1}) 3631, 2958, 1435, 1022, 749; HRMS (CI) calcd $\text{C}_{22}\text{H}_{27}^{79}\text{BrF}_2\text{O}$ $[\text{M}]^+$: 424.1213, found: 424.1223.



2,6-Di-tert-butyl-4-(2,2-difluoro-1-(3-methoxyphenyl)ethyl)phenol (3h): White solid; m.p. 68-70 °C; 52% yield (42 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.50 (d, $J = 7.6$ Hz, 1H), 7.40 (d, $J = 7.8$ Hz, 1H), 7.29 (t, $J = 7.5$ Hz, 1H), 7.22 (t, $J = 7.3$ Hz, 1H), 7.13 (s, 2H), 6.31 (td, $J = 55.9, 4.3$ Hz, 1H), 5.18 (s, 1H), 4.92 (td, $J = 16.3, 4.1$ Hz, 1H), 1.41 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 153.3, 136.0, 135.9, 134.7, 130.2, 129.7, 128.6, 127.0, 126.4, 126.0, 117.1 (t, $J_{\text{C-F}} = 244.8$ Hz), 50.9 (t, $J_{\text{C-F}} = 21.2$ Hz), 34.5, 30.4; ^{19}F NMR (564 MHz, CDCl_3) δ -117.39 (ddd, $J = 277.8, 56.0, 15.5$ Hz, 1F), -118.89 (ddd, $J = 277.7, 55.8, 16.8$ Hz, 1F); FT-IR (thin film, KBr): ν (cm^{-1}) 3630, 2959, 1434, 1060, 751; HRMS (CI) calcd $\text{C}_{22}\text{H}_{28}^{35}\text{ClF}_2\text{O}$ $[\text{M} + \text{H}]^+$: 381.1797, found: 381.1796.

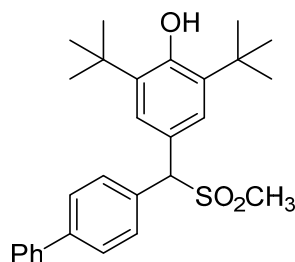


2,6-Di-tert-butyl-4-(2,2-difluoro-1-(3-methoxyphenyl)ethyl)phenol (3i): Colorless oil; 59% yield (45 mg); ^1H NMR (600 MHz, CDCl_3) δ 7.28 – 7.23 (m, 1H), 7.10 (s, 2H), 6.92 (d, $J = 7.6$ Hz, 1H), 6.87 (s, 1H), 6.81 (d, $J = 8.2$ Hz, 1H), 6.23 (td, $J = 56.1, 4.3$ Hz, 1H), 5.16 (s, 1H), 4.26 (td, $J = 16.1, 4.2$ Hz, 1H), 3.79 (s, 3H), 1.41 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 159.8, 153.3, 139.3, 136.1, 129.6, 127.6, 125.7, 121.5, 117.4 (t, $J_{\text{C-F}} = 244.6$ Hz), 115.3, 112.5, 55.3, 55.3 (t, $J_{\text{C-F}} = 20.5$ Hz), 34.5, 30.4; ^{19}F NMR (564 MHz, CDCl_3) δ -117.24 (ddd, $J = 276.8, 56.1, 15.5$ Hz, 1F), -118.14 (ddd, $J = 276.9, 56.2, 16.6$ Hz, 1F); FT-IR (thin film, KBr): ν (cm^{-1}) 3634, 2957, 1434, 1053, 771; HRMS (CI) calcd $\text{C}_{23}\text{H}_{31}\text{F}_2\text{O}_2$ $[\text{M} + \text{H}]^+$: 377.2292, found: 377.2297.



4-([1,1'-Biphenyl]-4-yl((fluoromethyl)sulfonyl)methyl)-2,6-di-tert-butylphenol

(4a): White solid; m.p. 51-55 °C; 59% yield (55 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.74 (d, J = 8.2 Hz, 2H), 7.65 (d, J = 8.2 Hz, 2H), 7.59 (d, J = 7.5 Hz, 2H), 7.49 – 7.42 (m, 4H), 7.37 (t, J = 7.2 Hz, 1H), 5.54 (s, 1H), 5.36 (s, 1H), 4.92 (d, J = 46.9 Hz, 2H), 1.45 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3) δ 154.9, 142.2, 140.3, 136.8, 130.9, 130.4, 129.0, 127.94, 127.87, 127.3, 126.9, 121.7, 88.3 (d, $J_{\text{C-F}}$ = 219.2 Hz), 70.8, 34.6, 30.4; ^{19}F NMR (564 MHz, CDCl_3) δ -211.91 (td, J = 46.9, 1.9 Hz, 1F); FT-IR (thin film, KBr): ν (cm^{-1}) 3629, 2957, 1434, 1140, 740; HRMS (CI) calcd $\text{C}_{28}\text{H}_{34}\text{FO}_3\text{S}$ $[\text{M} + \text{H}]^+$: 469.2213, found: 469.2223.

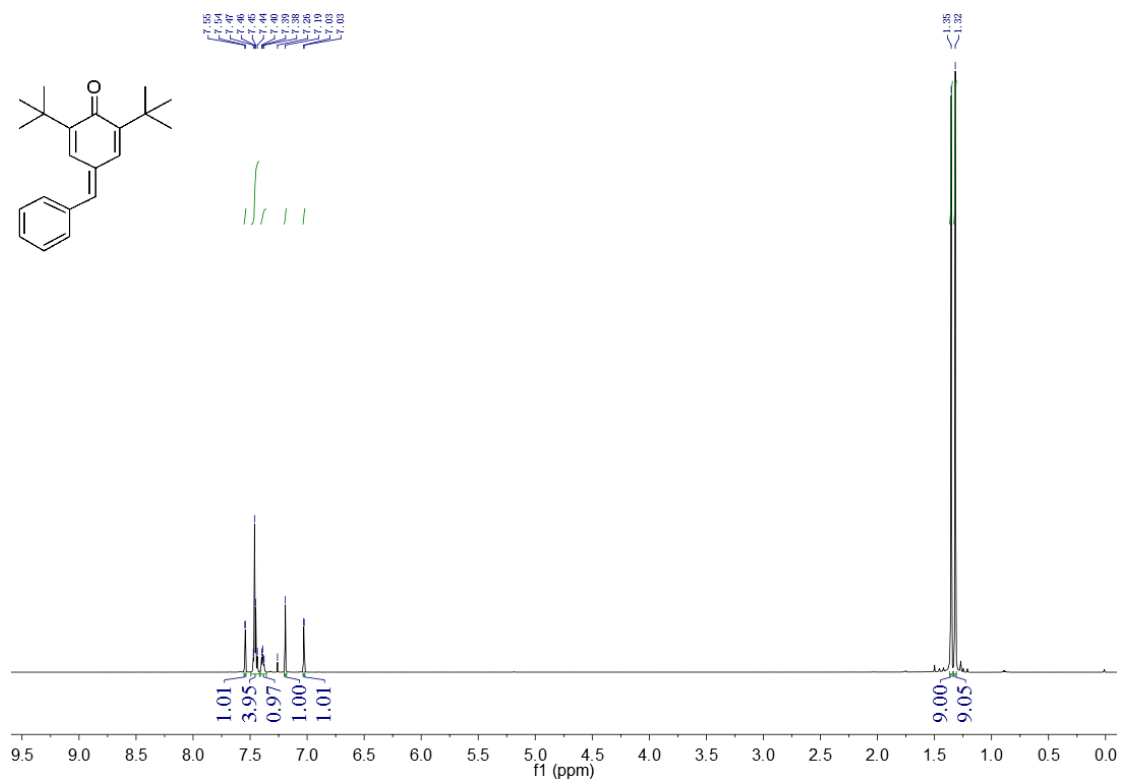


4-([1,1'-Biphenyl]-4-yl(methylsulfonyl)methyl)-2,6-di-tert-butylphenol (4b):

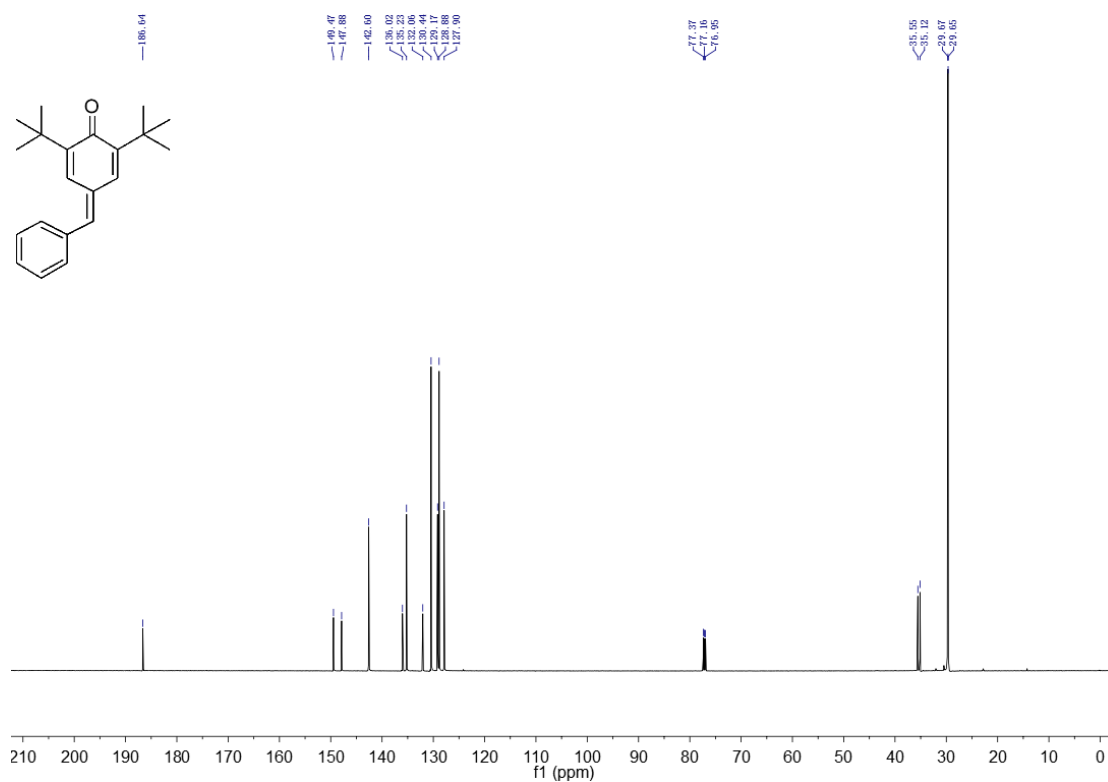
White solid; m.p. 75-80 °C; 58% yield (52 mg); ^1H NMR (400 MHz, CDCl_3) δ 7.73 (d, J = 8.2 Hz, 2H), 7.64 (d, J = 8.2 Hz, 2H), 7.58 (d, J = 7.4 Hz, 2H), 7.49 – 7.41 (m, 4H), 7.36 (t, J = 7.2 Hz, 1H), 5.33 (s, 1H), 5.29 (s, 1H), 2.78 (s, 3H), 1.45 (s, 18H); ^{13}C NMR (150 MHz, CDCl_3 , overlapping peaks) δ 154.6, 141.7, 140.4, 136.5, 132.3, 130.2, 128.9, 127.7, 127.2, 126.6, 123.2, 74.8, 40.0, 34.6, 30.4; FT-IR (thin film, KBr): ν (cm^{-1}) 3629, 2956, 1435, 1133, 730; HRMS (CI) calcd $\text{C}_{28}\text{H}_{35}\text{O}_3\text{S}$ $[\text{M} + \text{H}]^+$: 451.2307, found: 451.2304.

5. NMR Spectra for the substrates and products

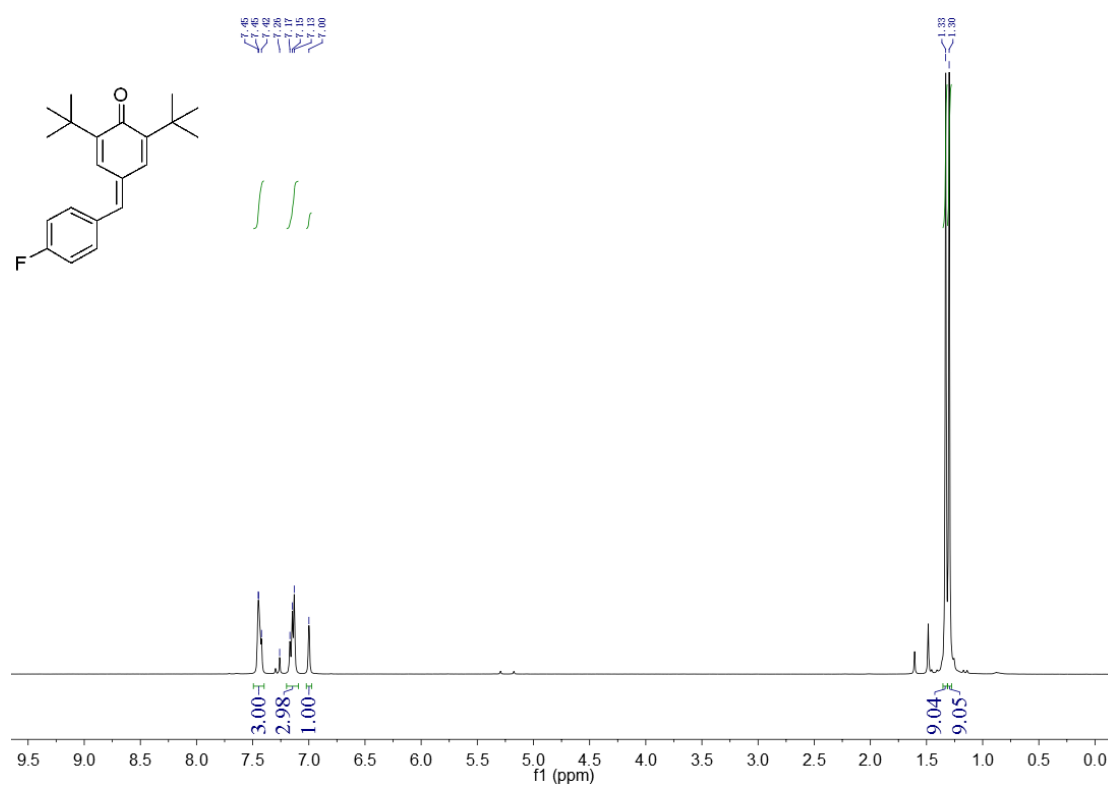
¹H NMR of **1a**



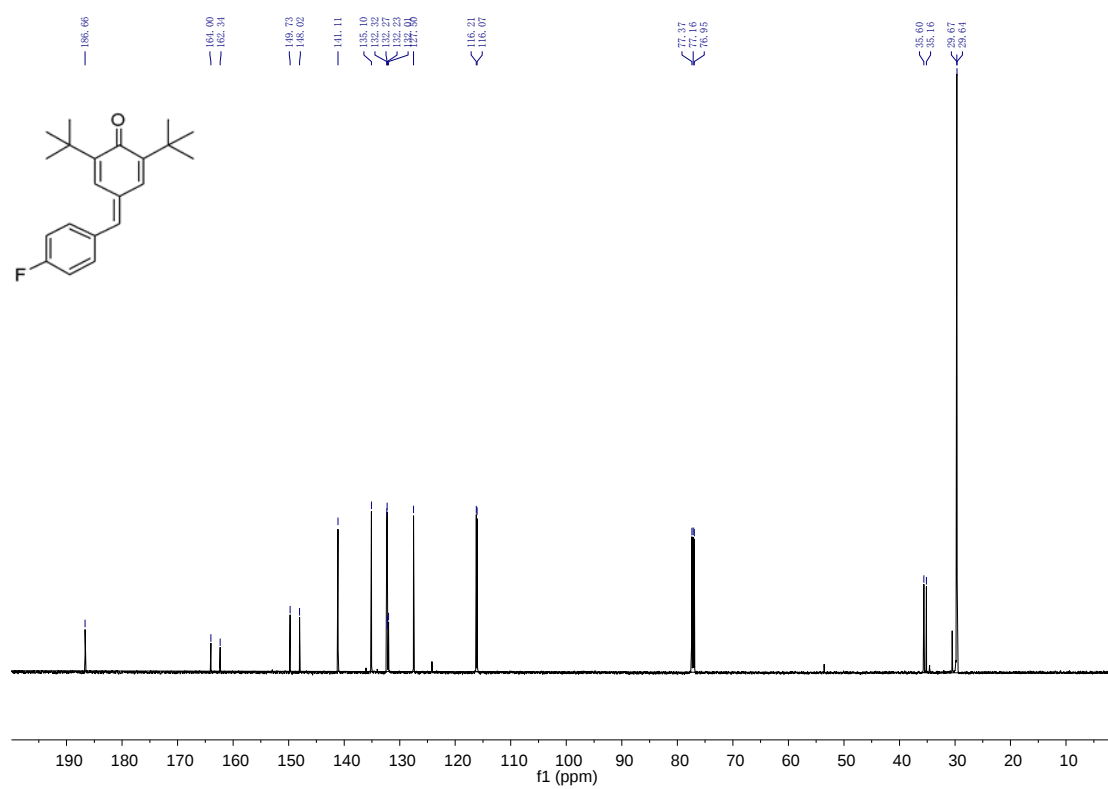
¹³C NMR of **1a**



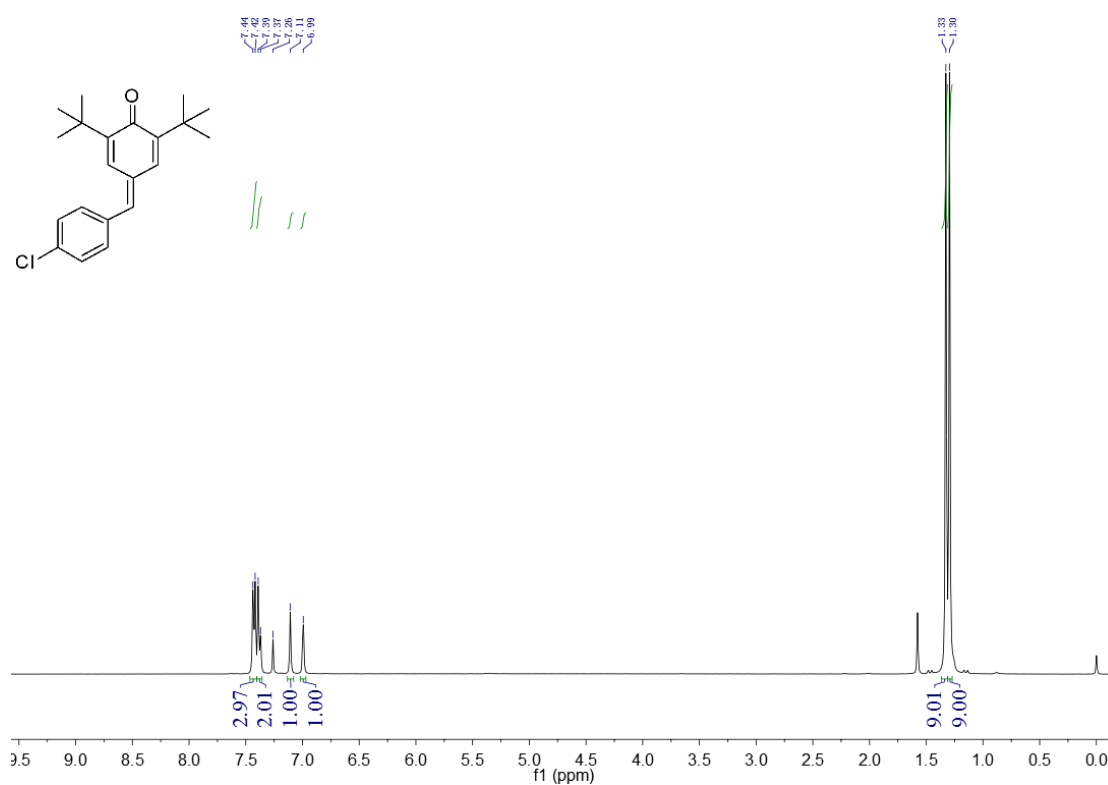
¹H NMR of **1b**



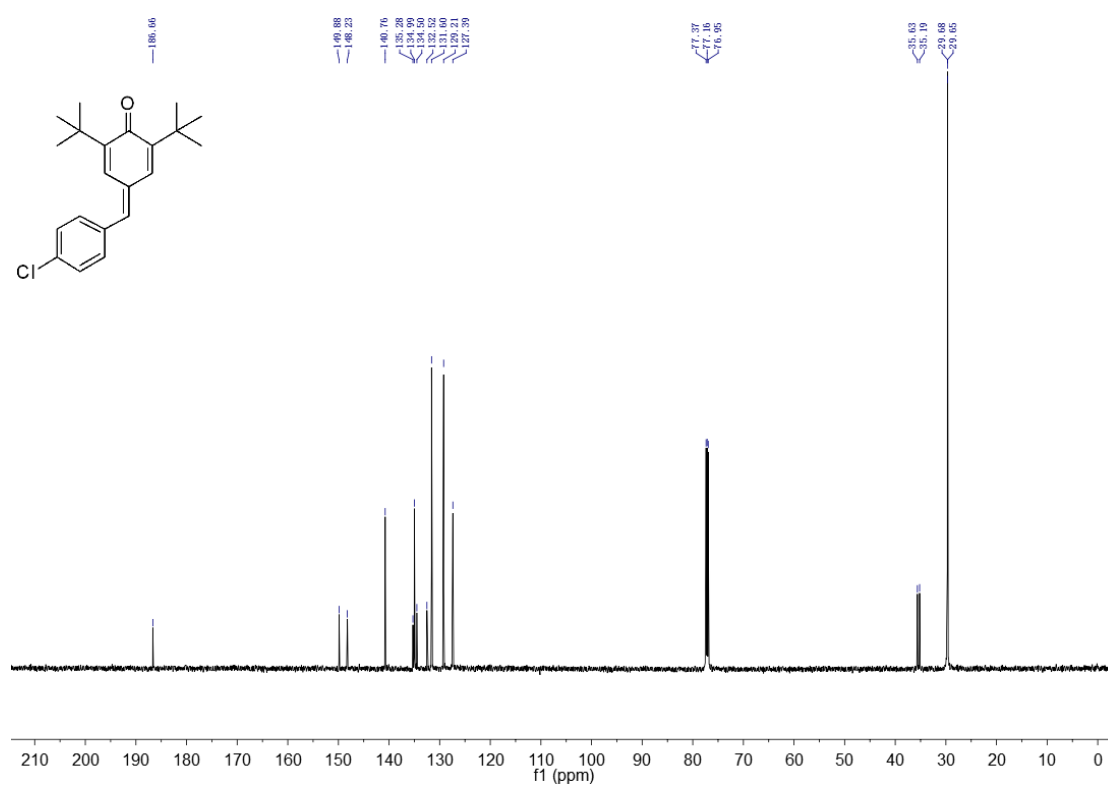
¹³C NMR of **1b**



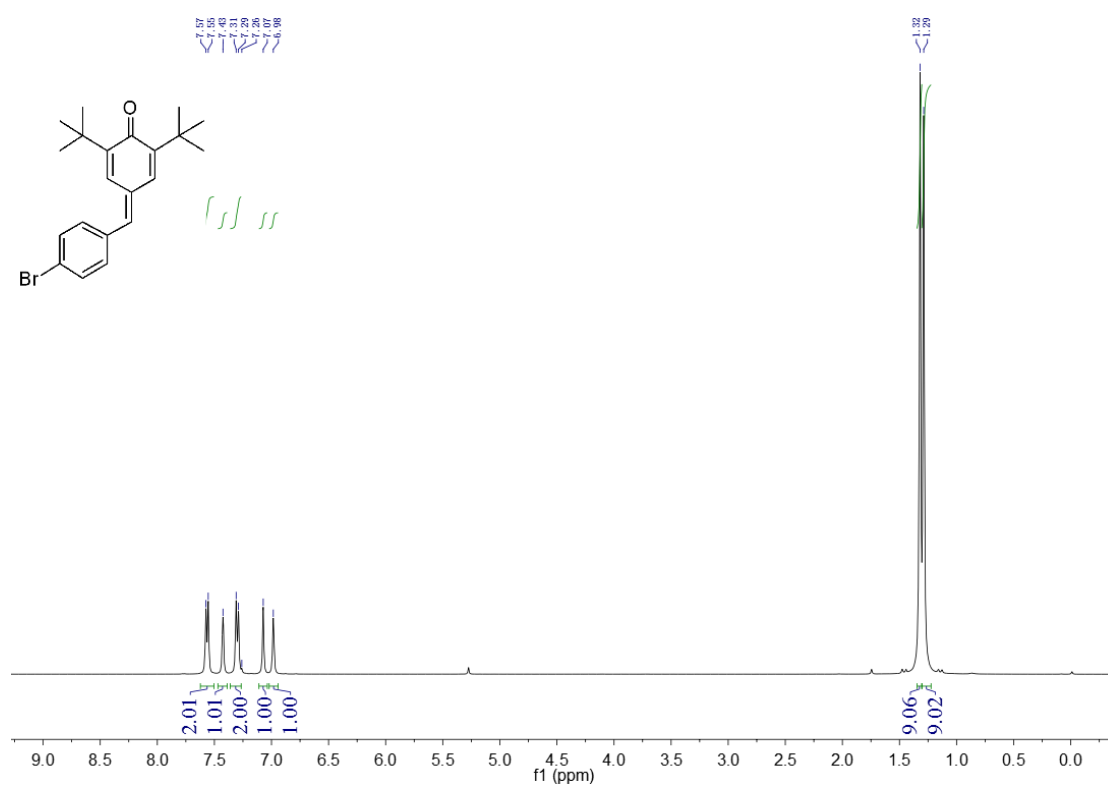
¹H NMR of **1c**



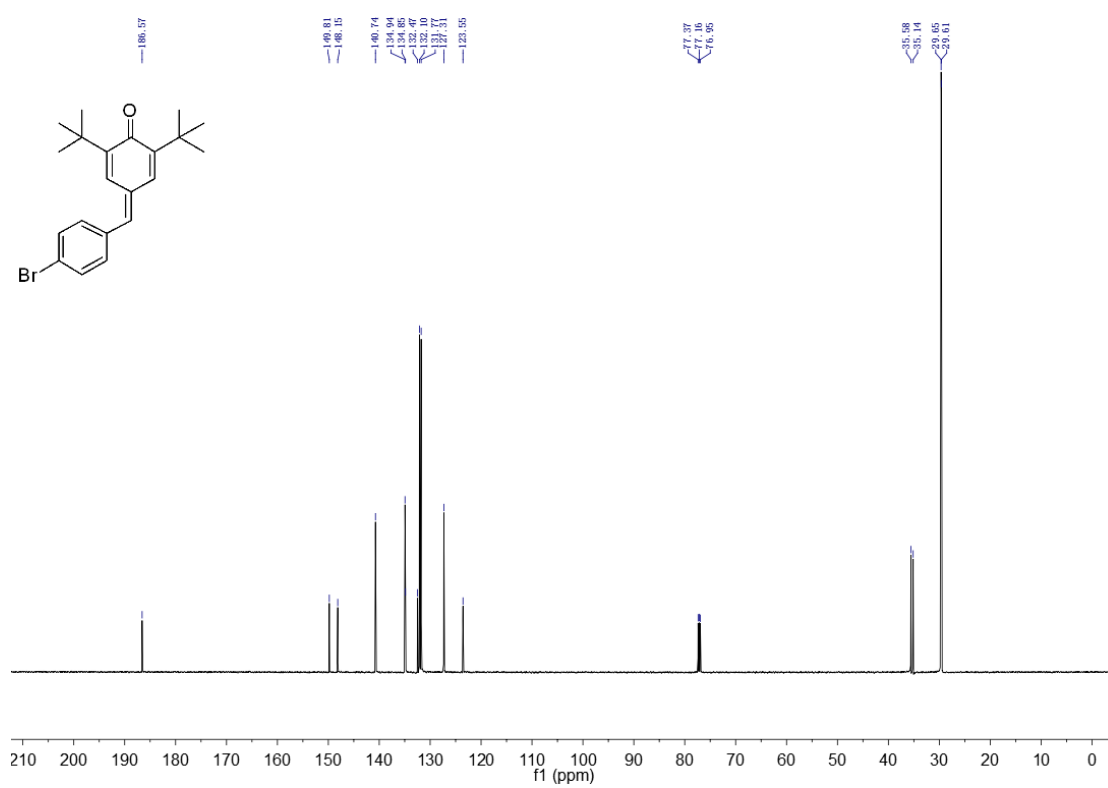
¹³C NMR of **1c**



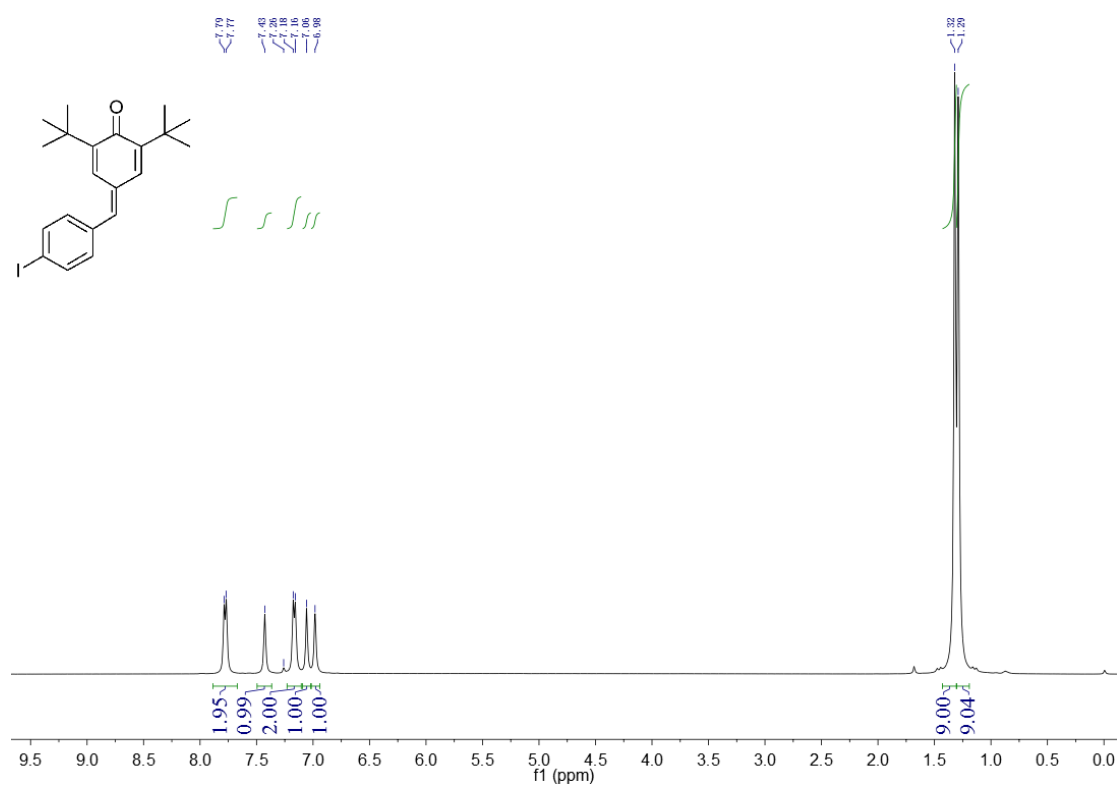
¹H NMR of **1d**



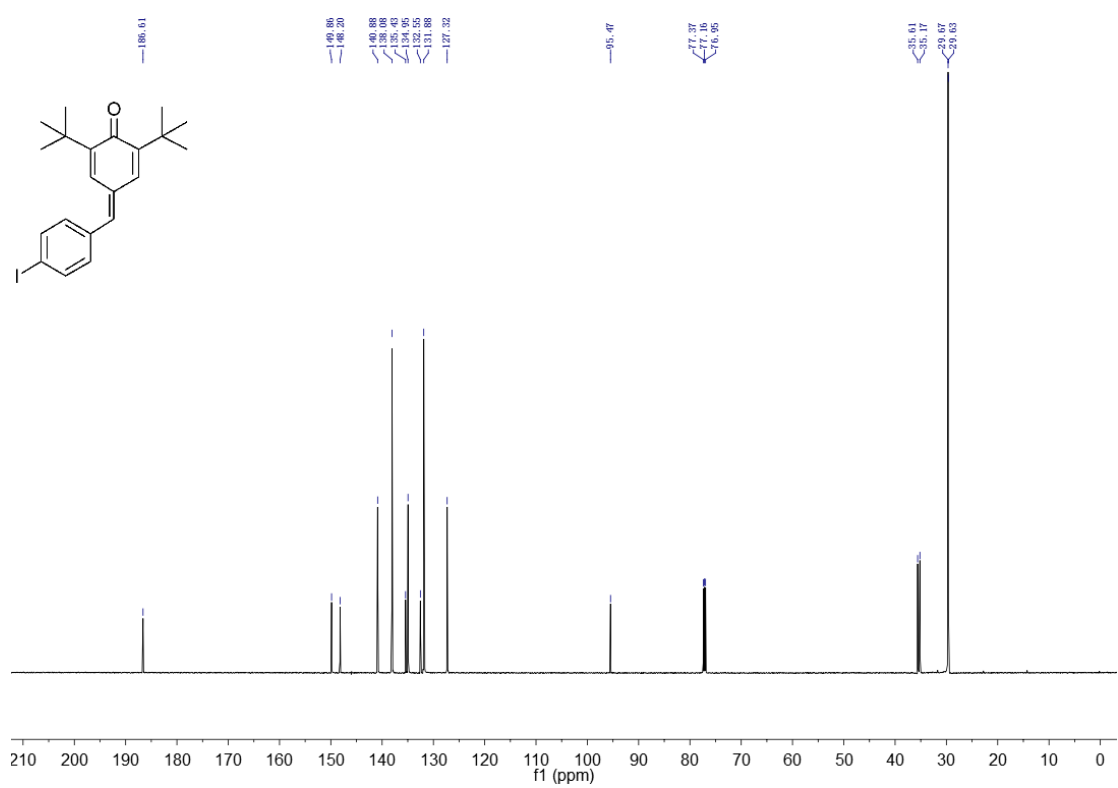
¹³C NMR of **1d**



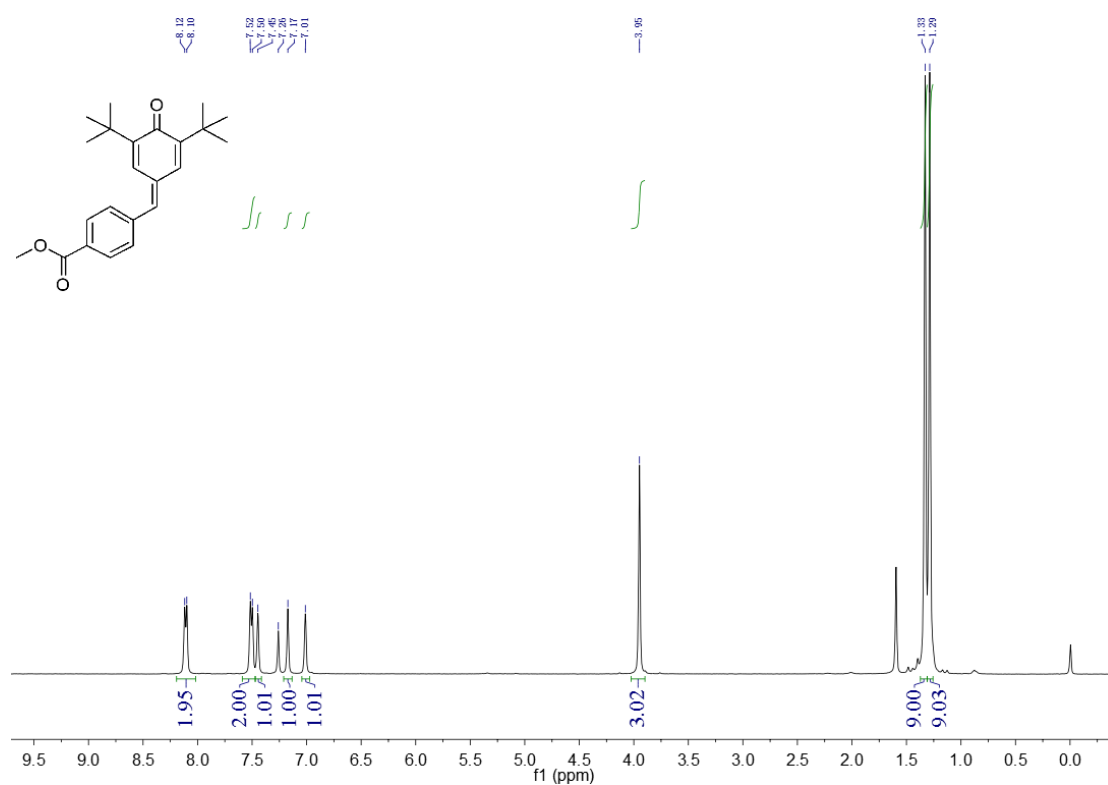
¹H NMR of **1e**



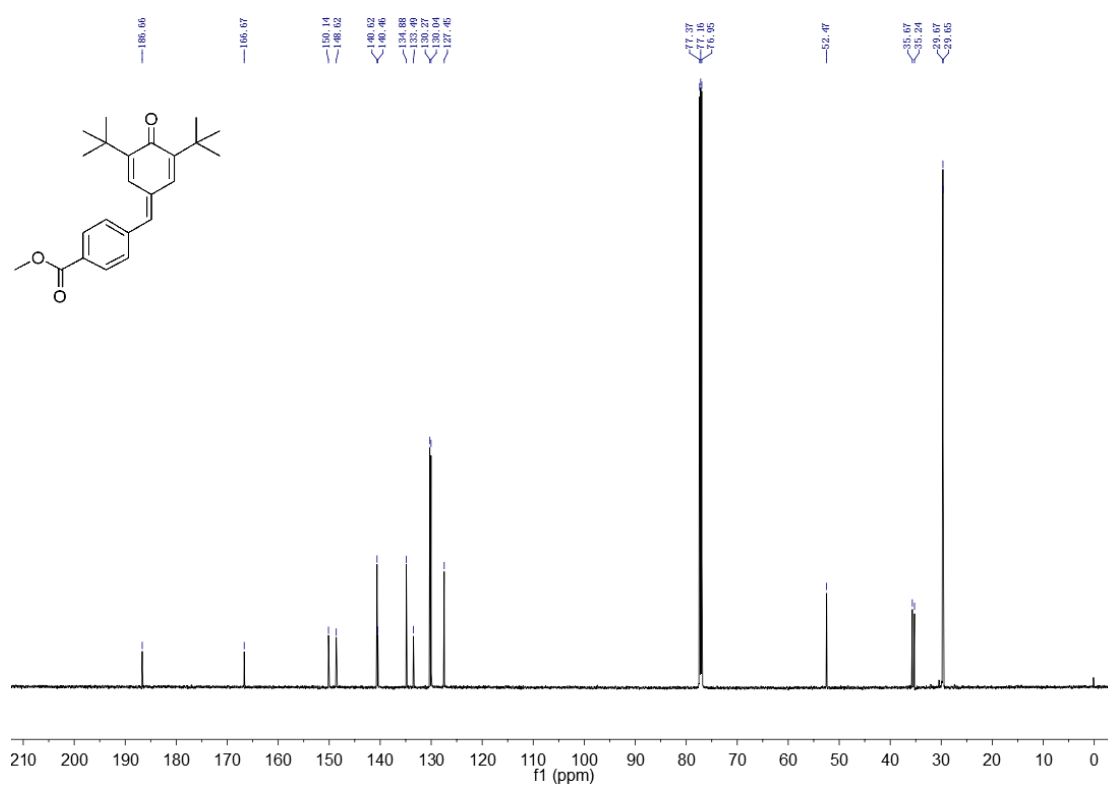
¹³C NMR of **1e**



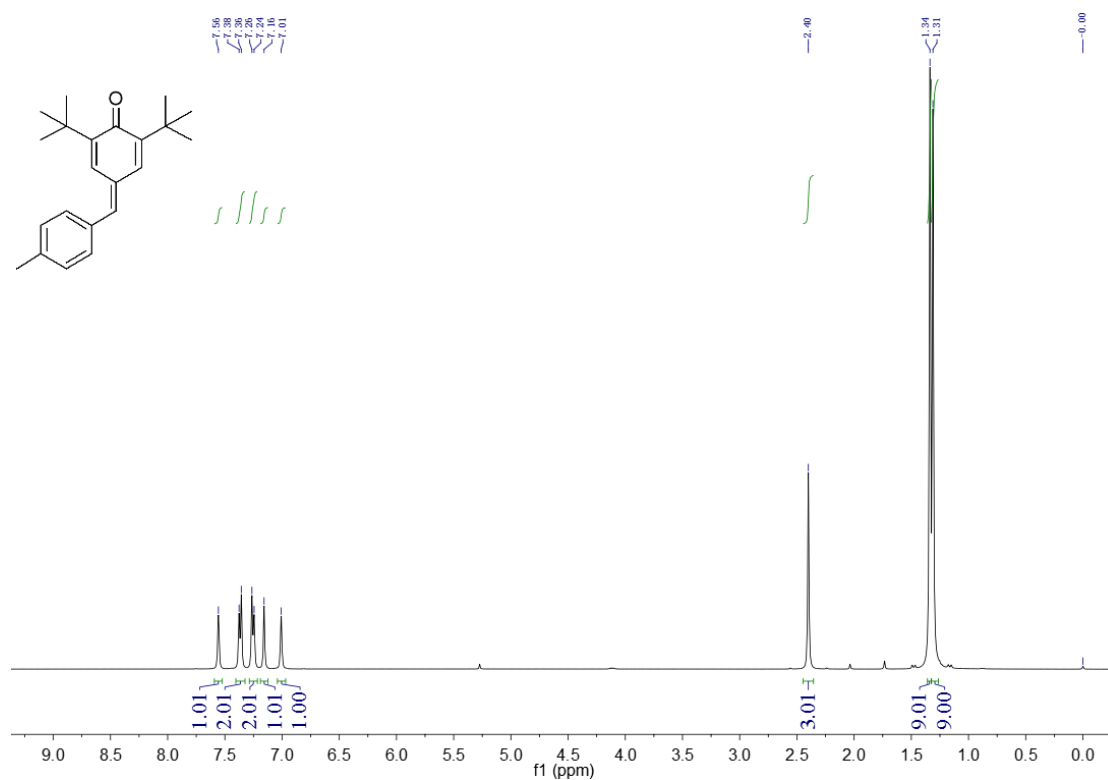
¹H NMR of **1f**



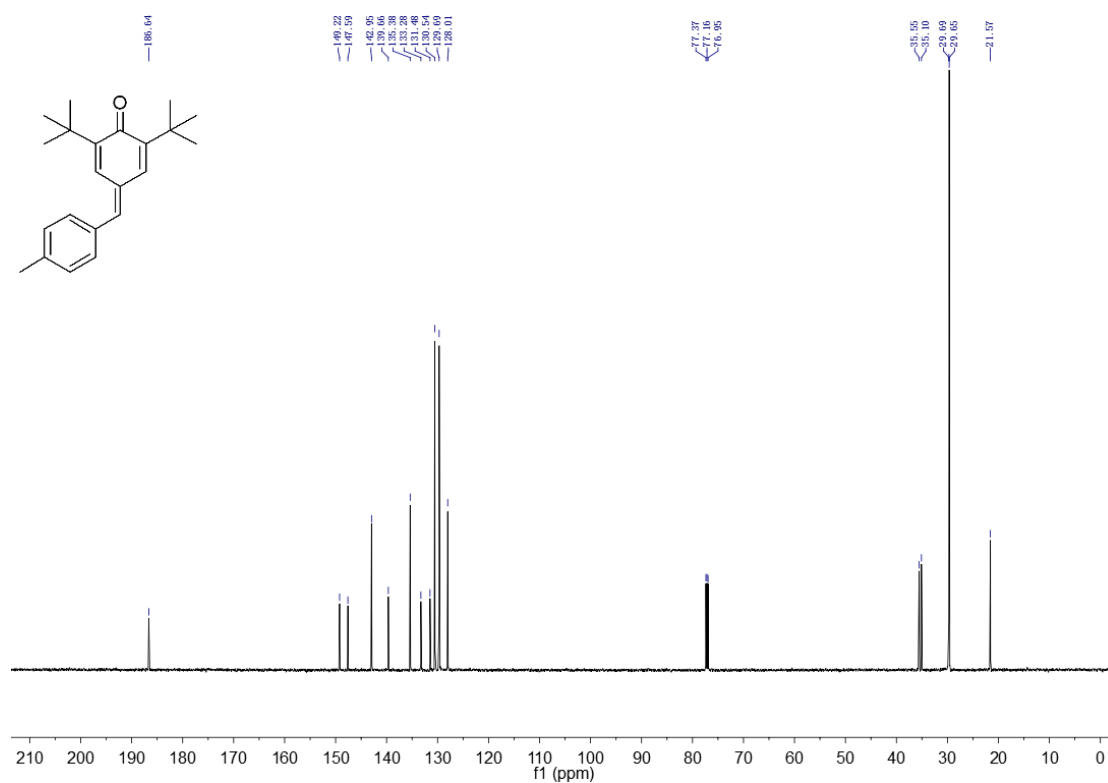
¹³C NMR of **1f**



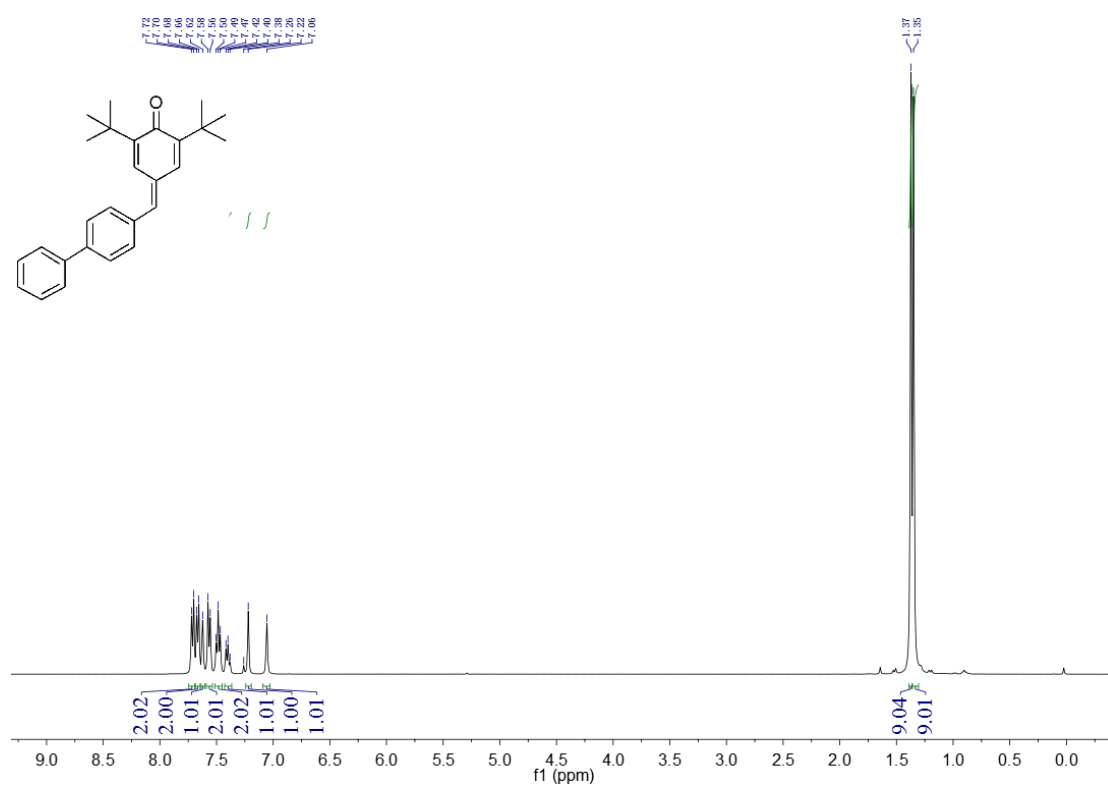
¹H NMR of **1g**



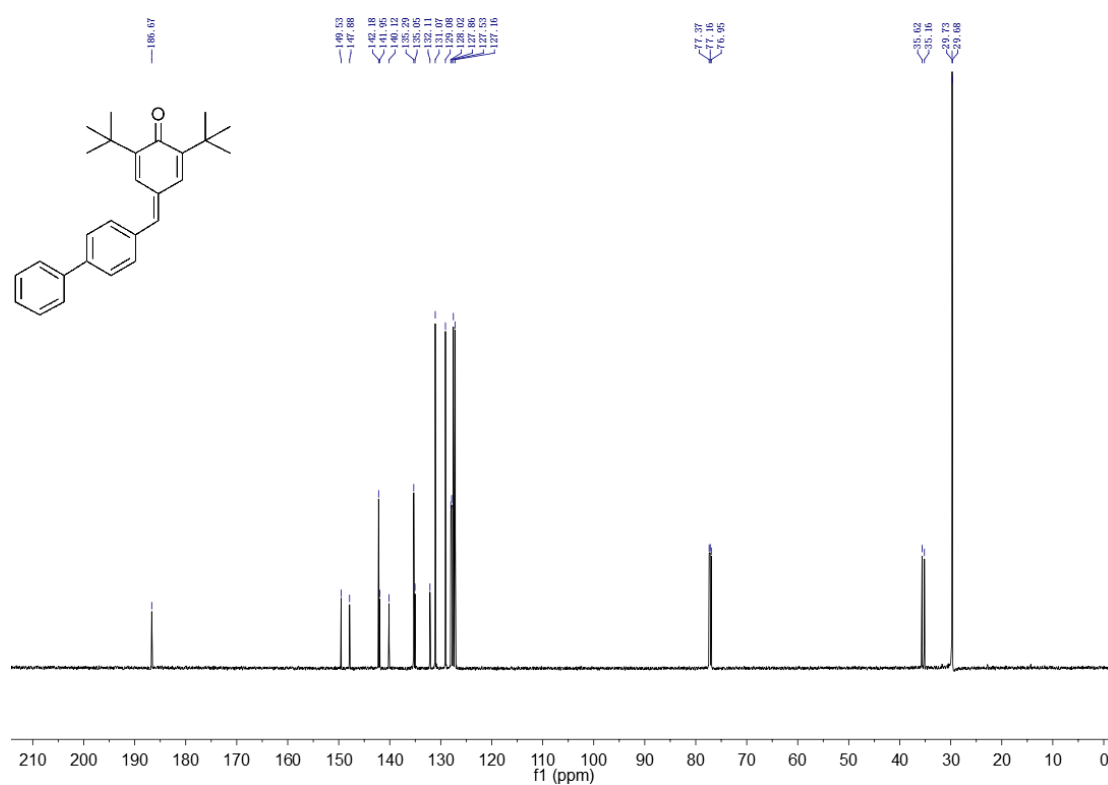
¹³C NMR of **1g**



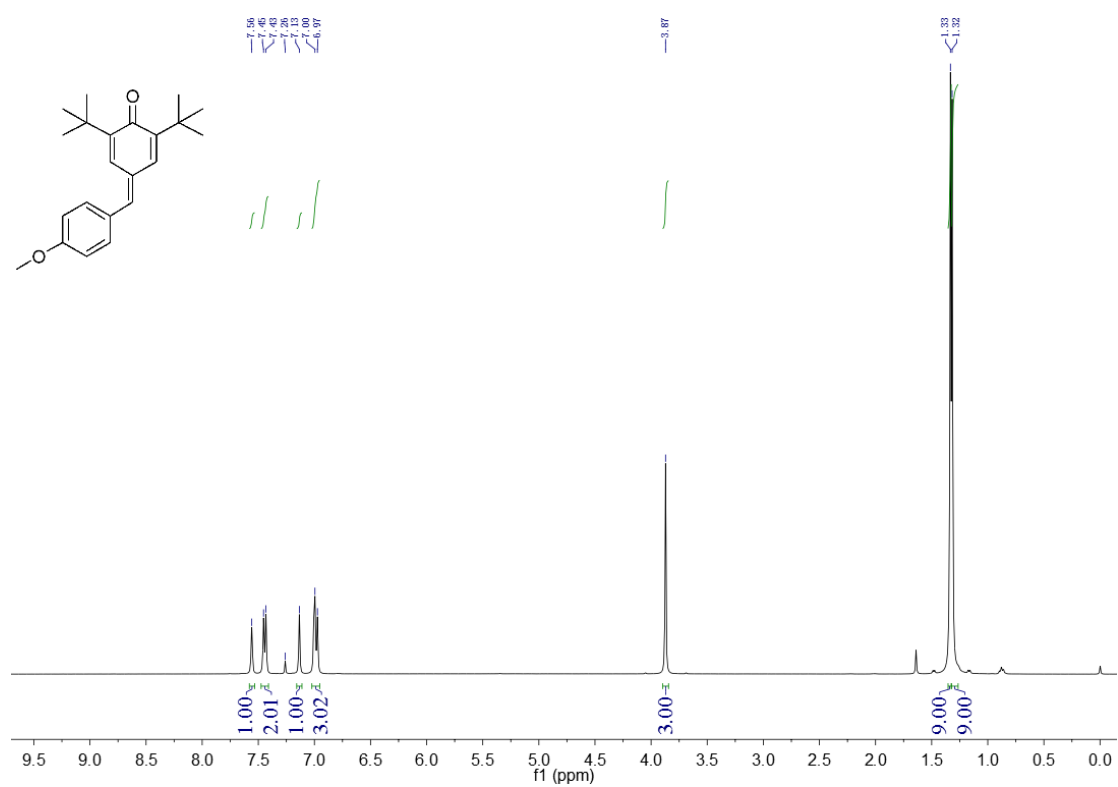
¹H NMR of **1h**



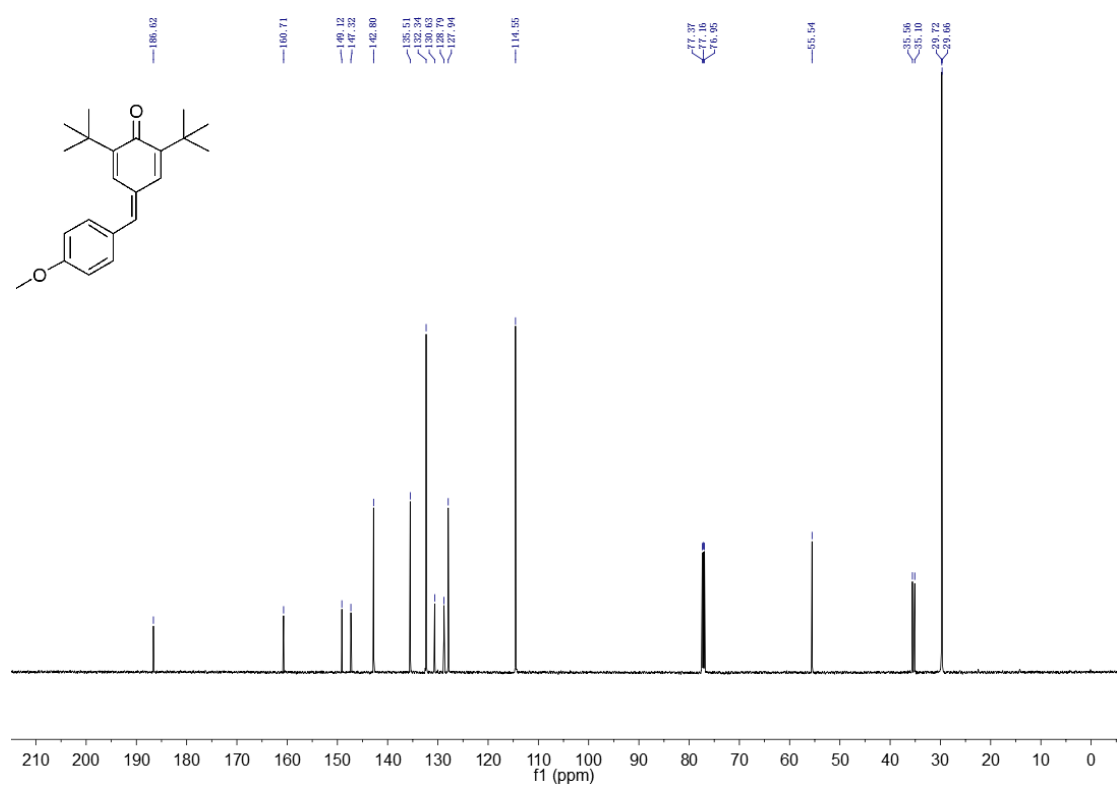
¹³C NMR of **1h**



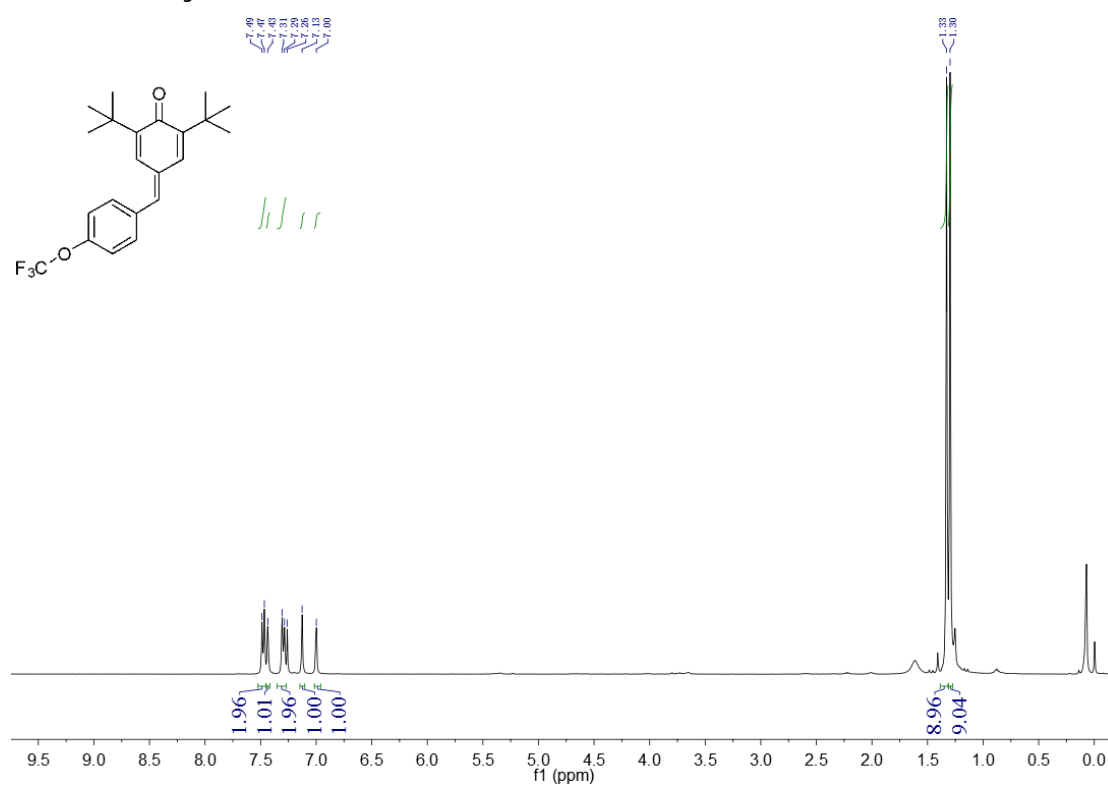
¹H NMR of **1i**



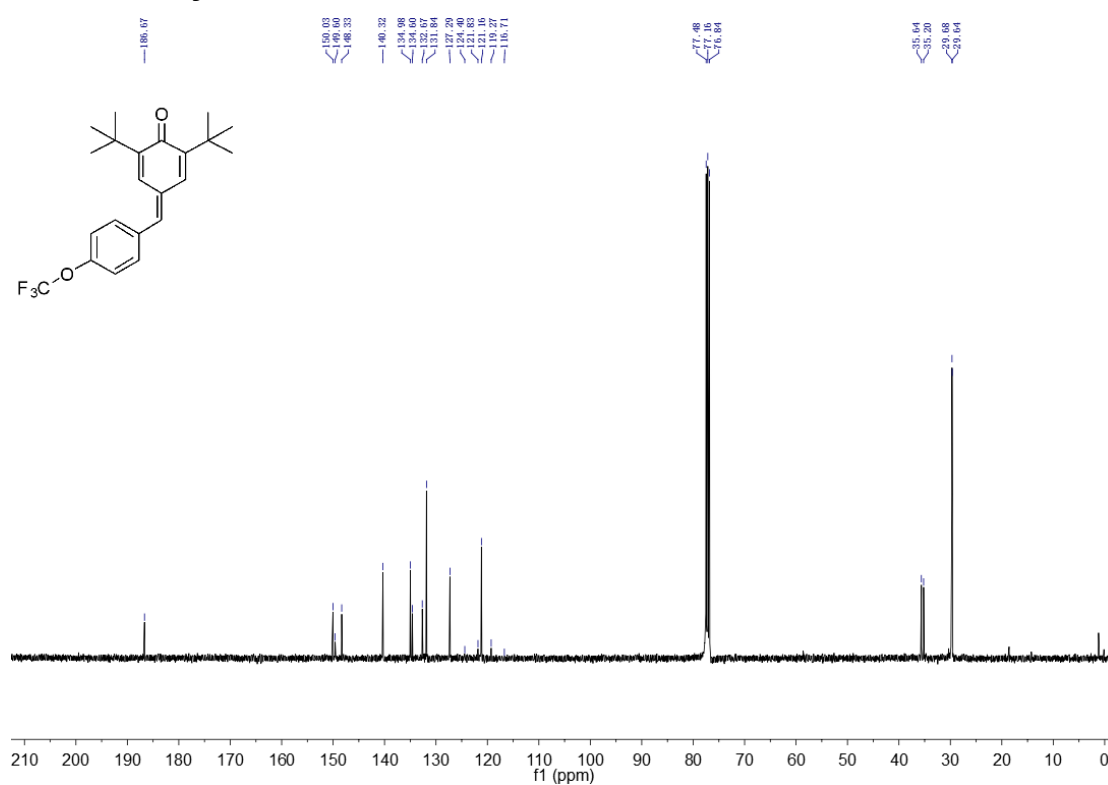
¹³C NMR of **1i**



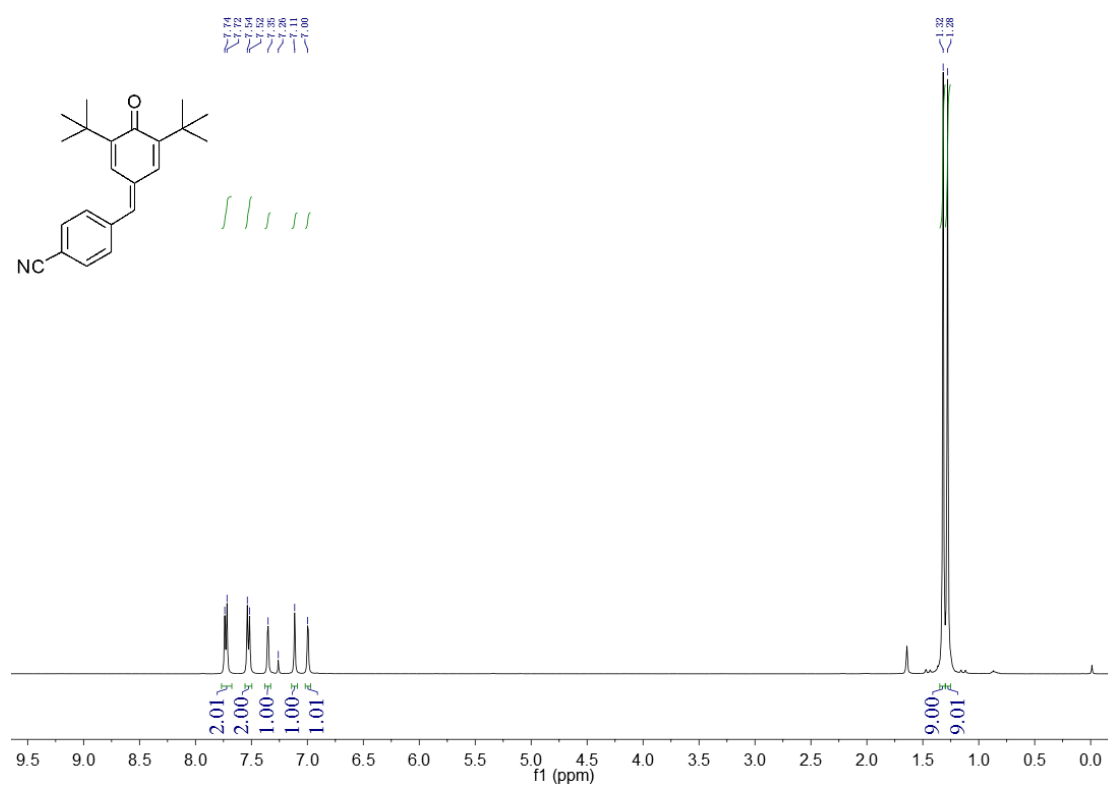
¹H NMR of **1j**



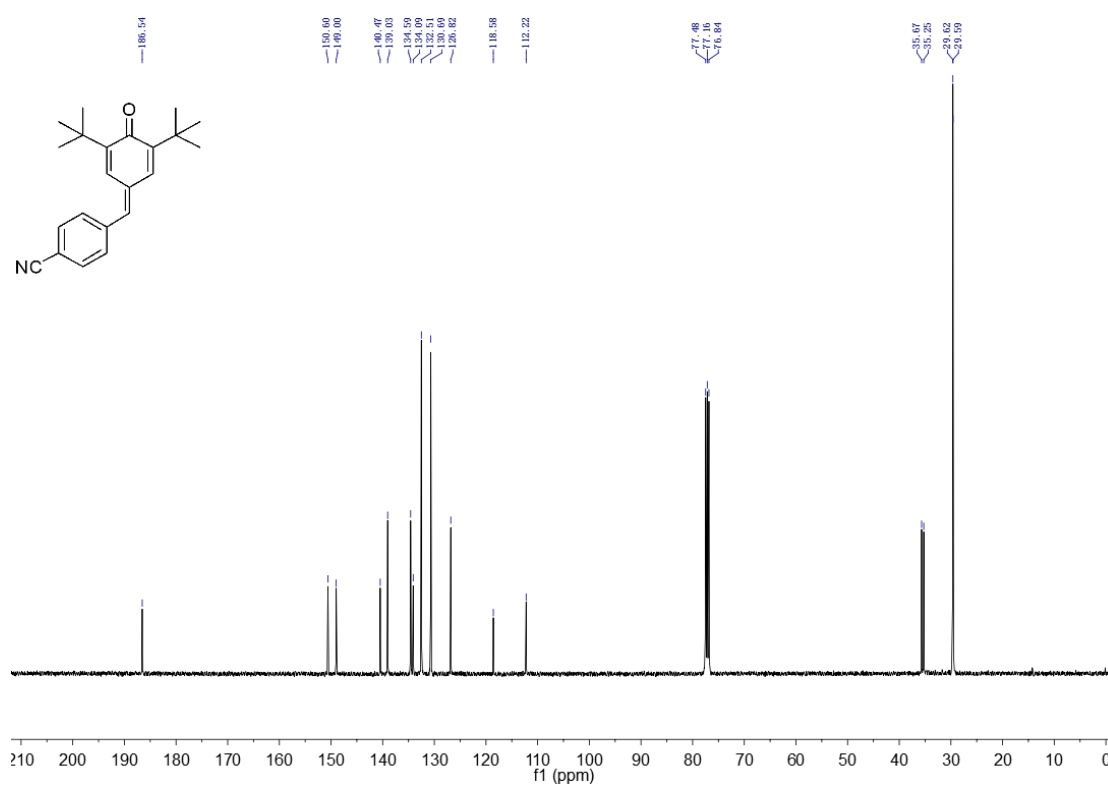
¹³C NMR of **1j**



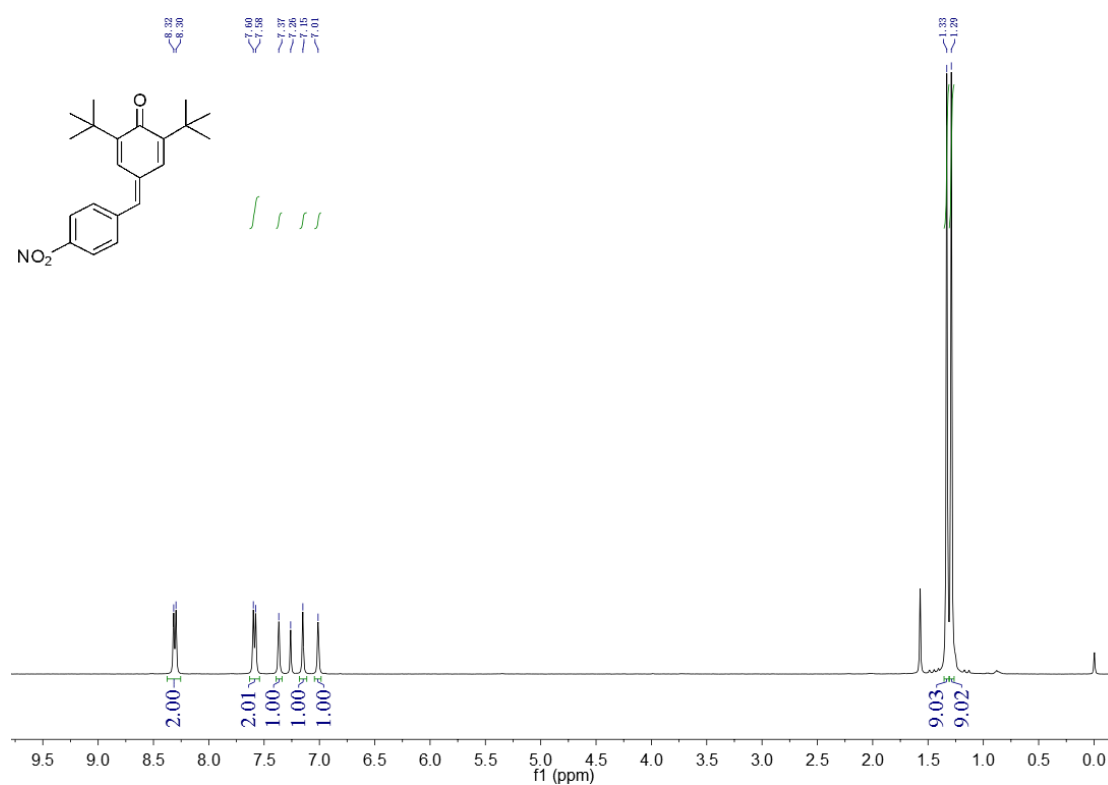
¹H NMR of **1k**



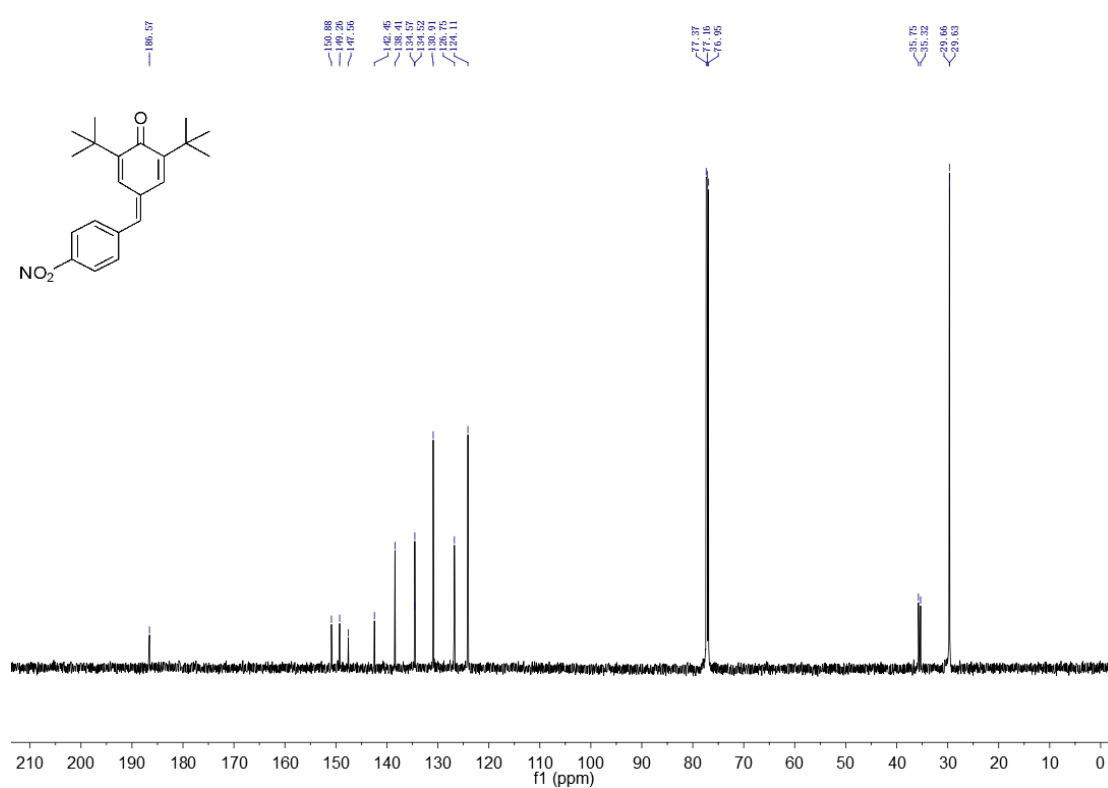
¹³C NMR of **1k**



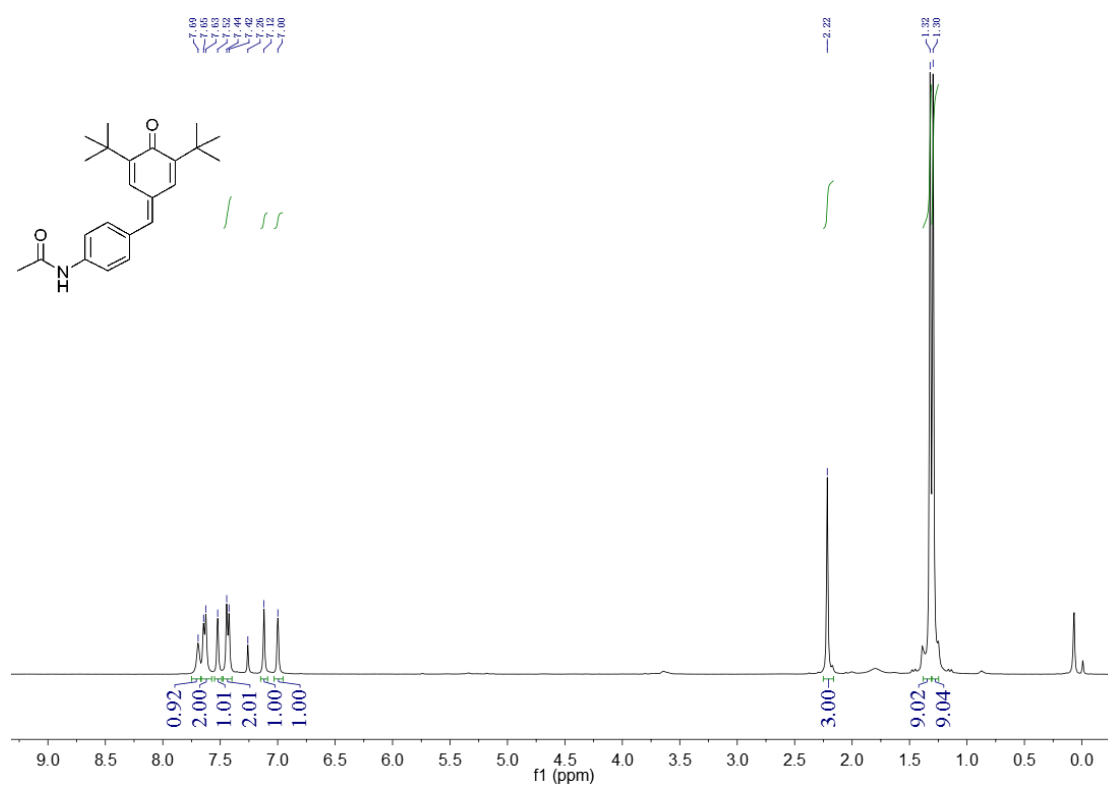
¹H NMR of **11**



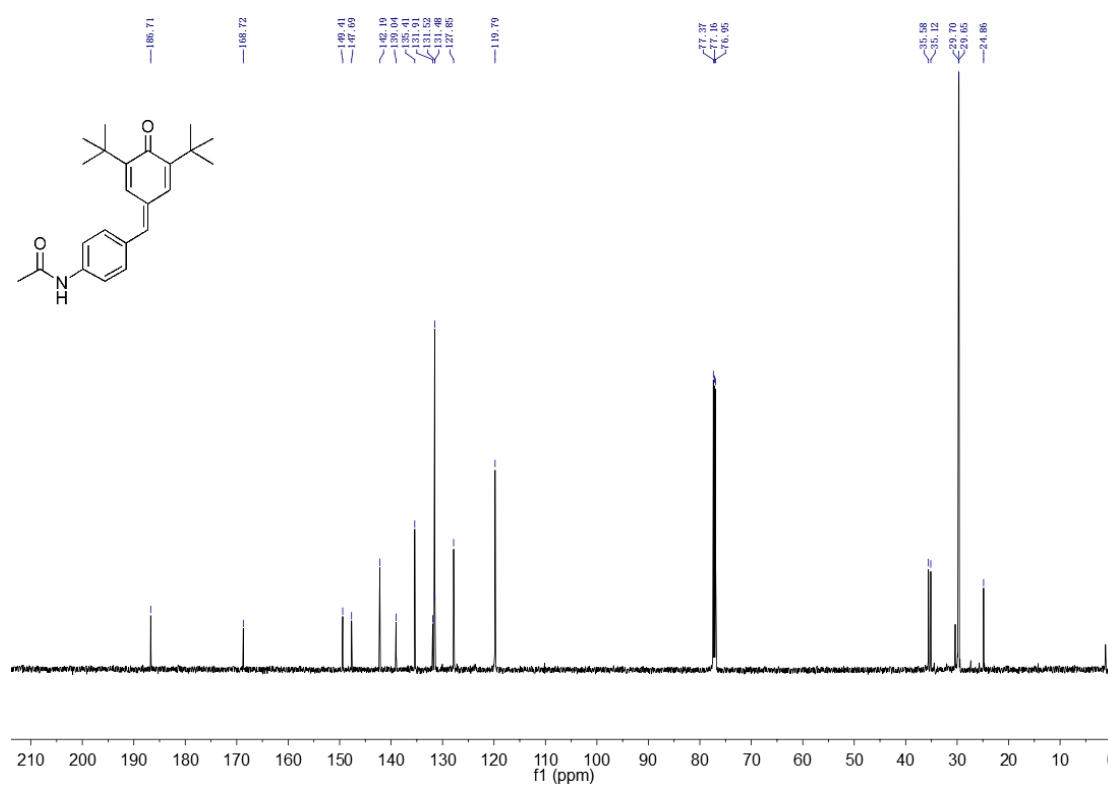
¹³C NMR of **11**



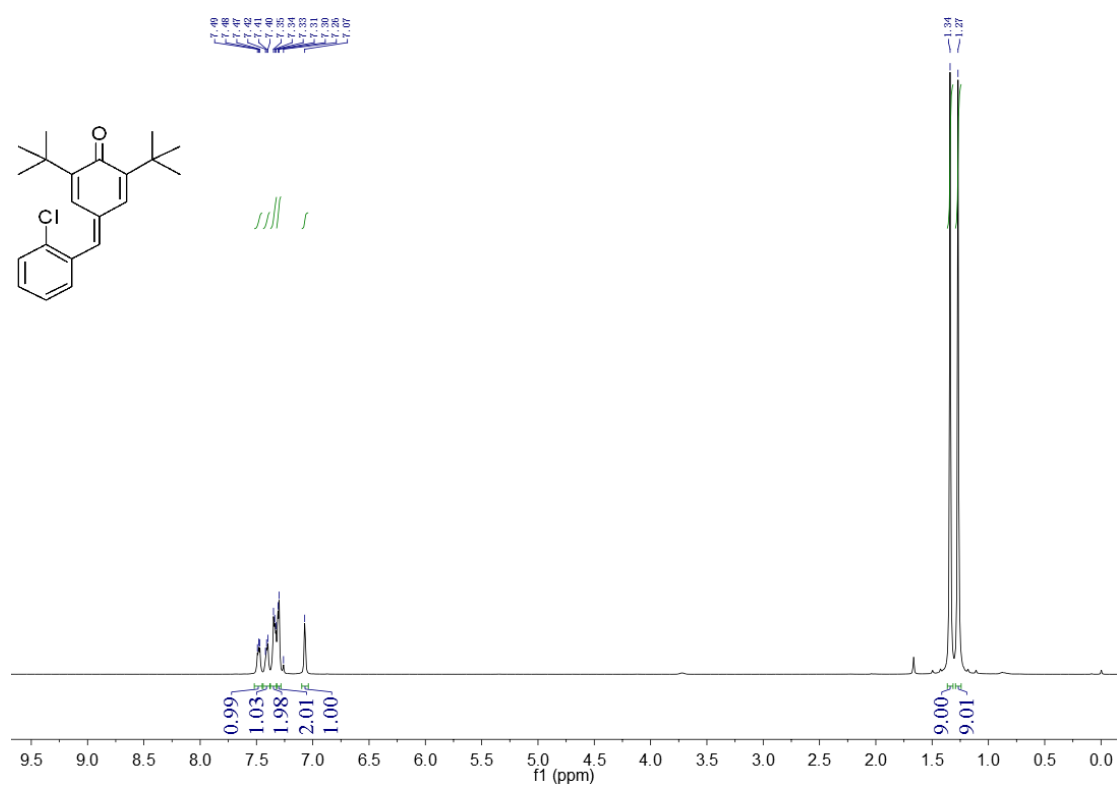
¹H NMR of **1m**



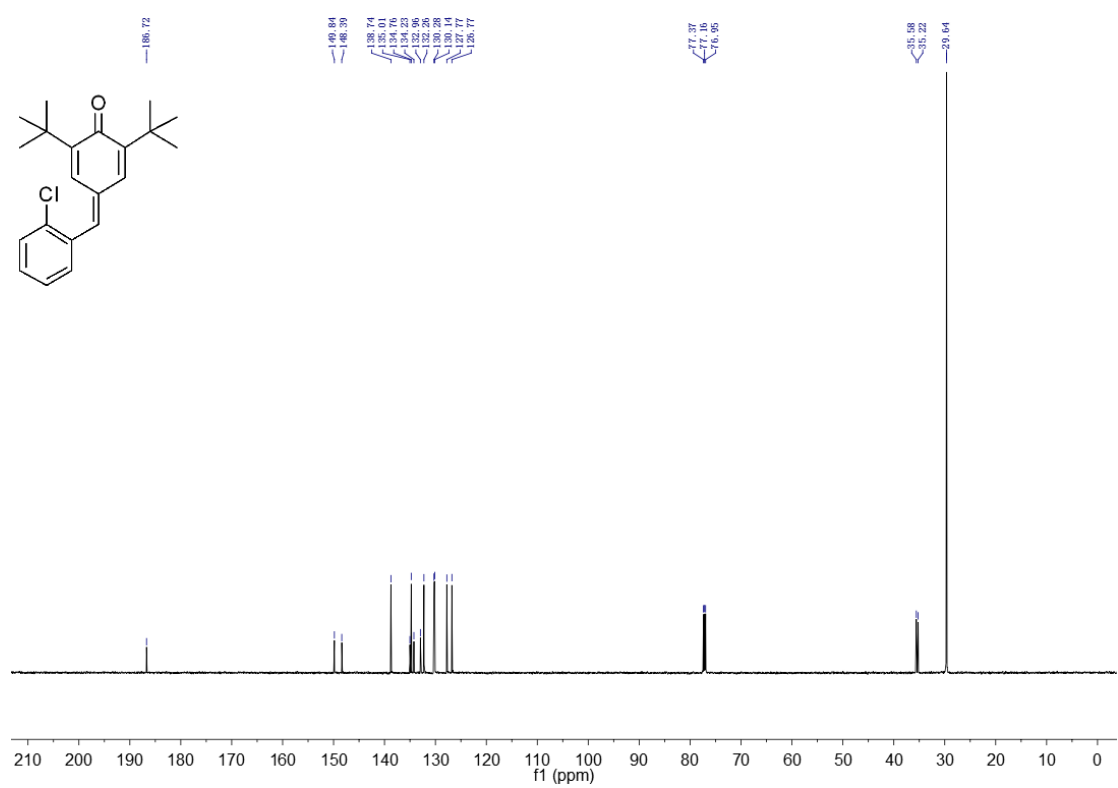
¹³C NMR of **1m**



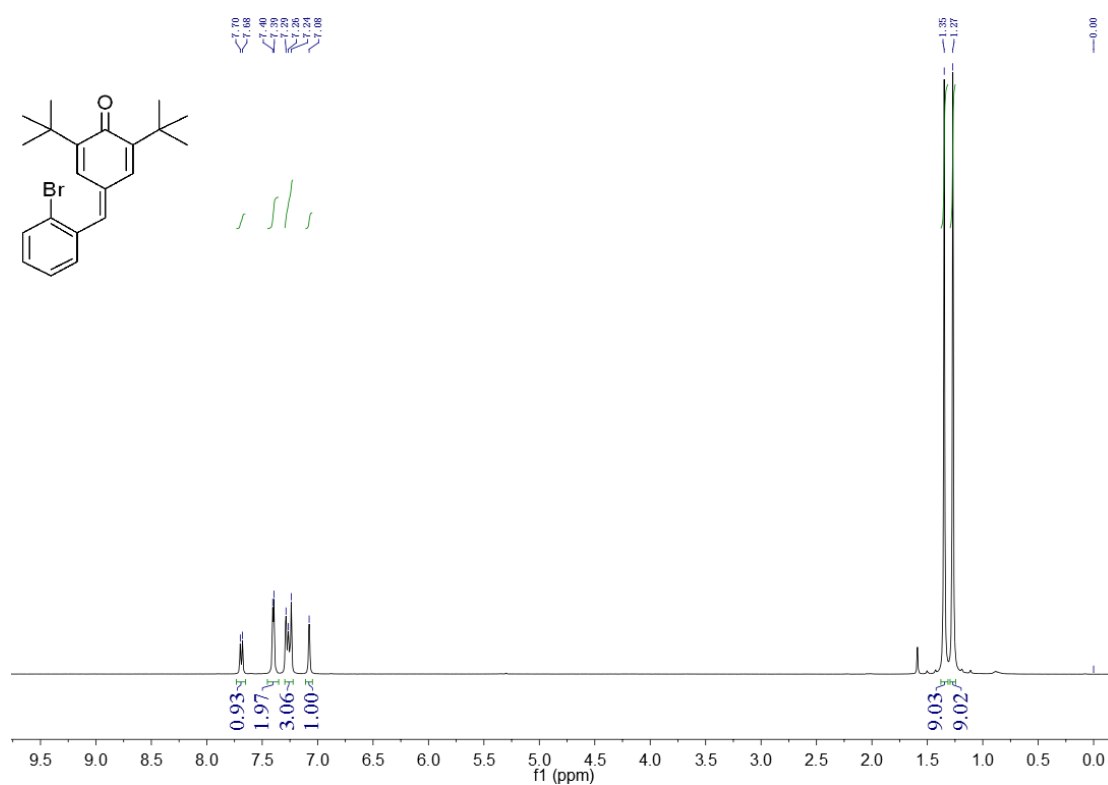
¹H NMR of **1n**



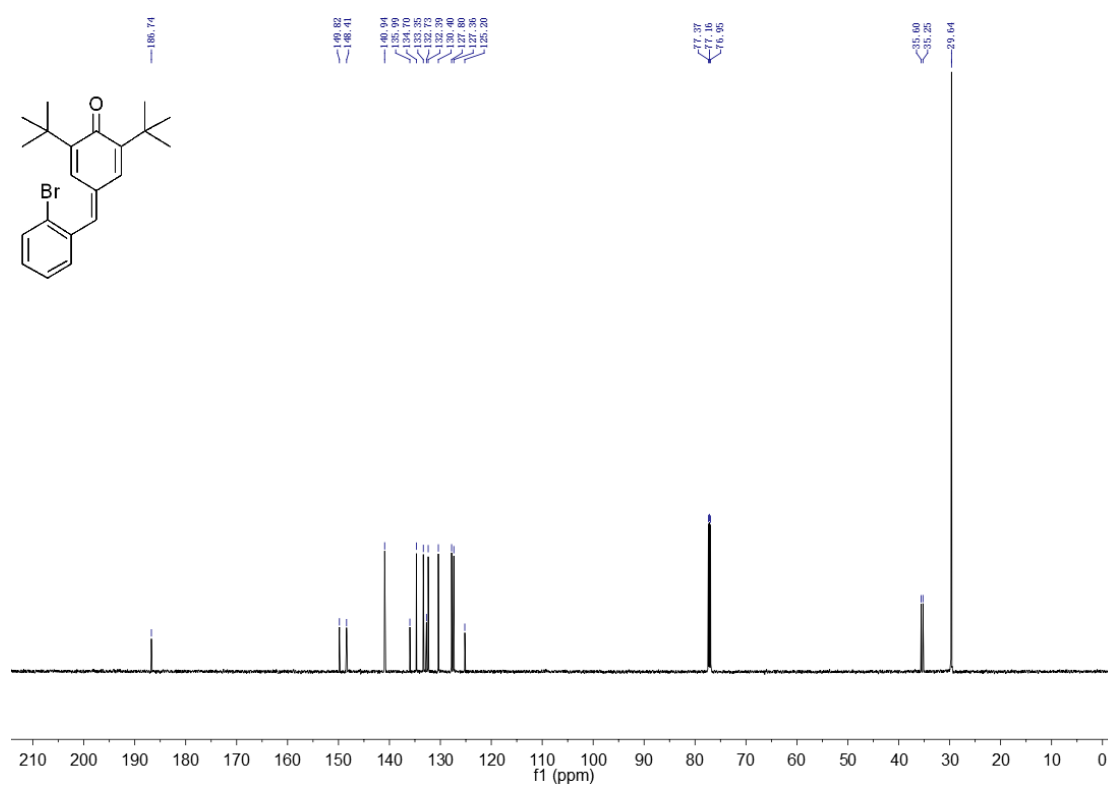
¹³C NMR of **1n**



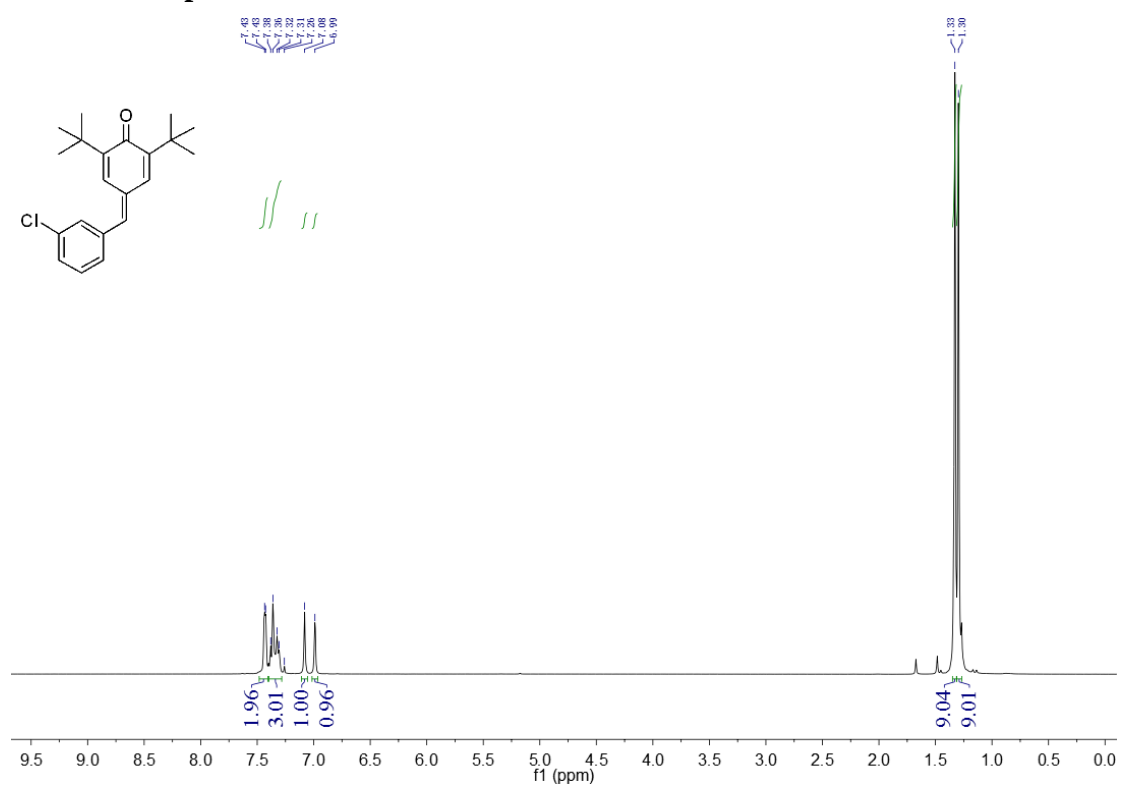
¹H NMR of **1o**



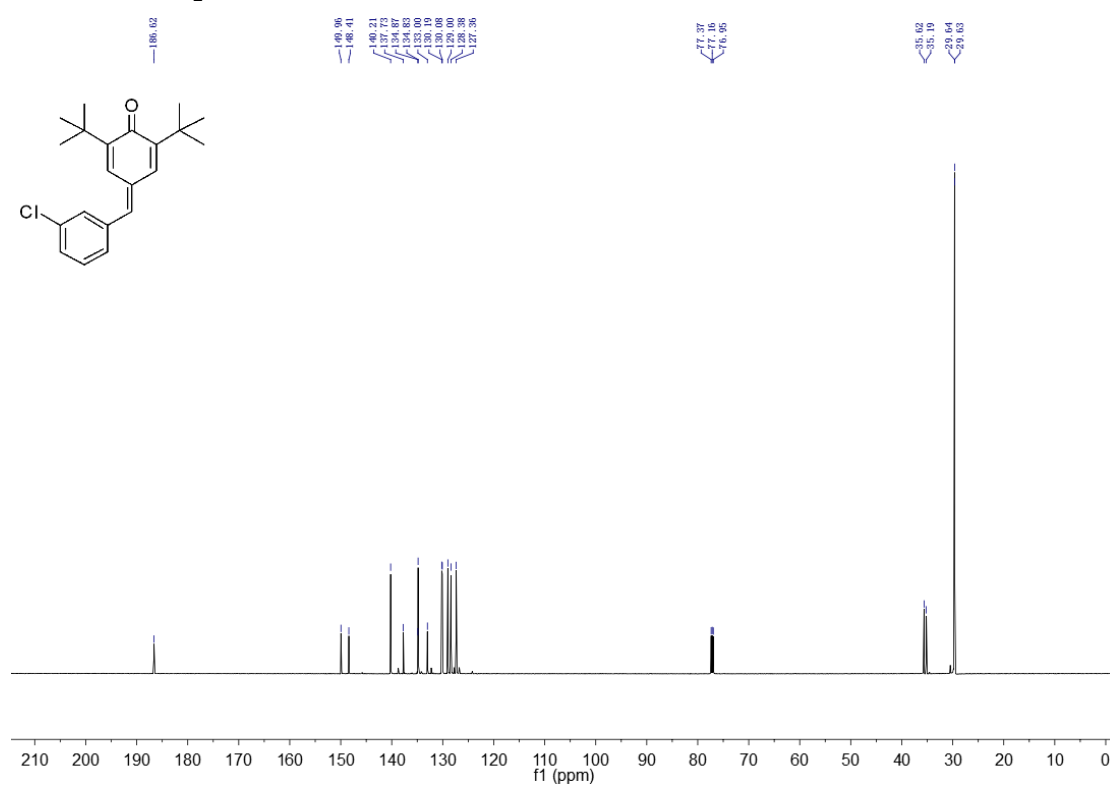
¹³C NMR of **1o**



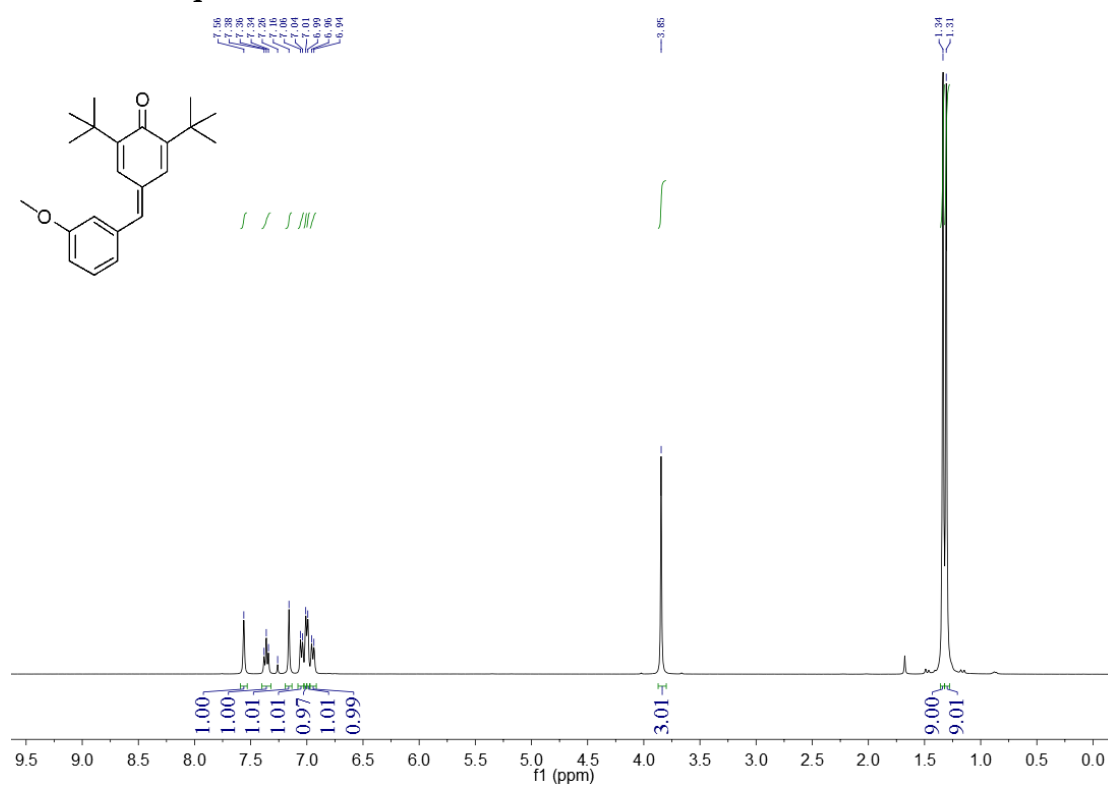
¹H NMR of **1p**



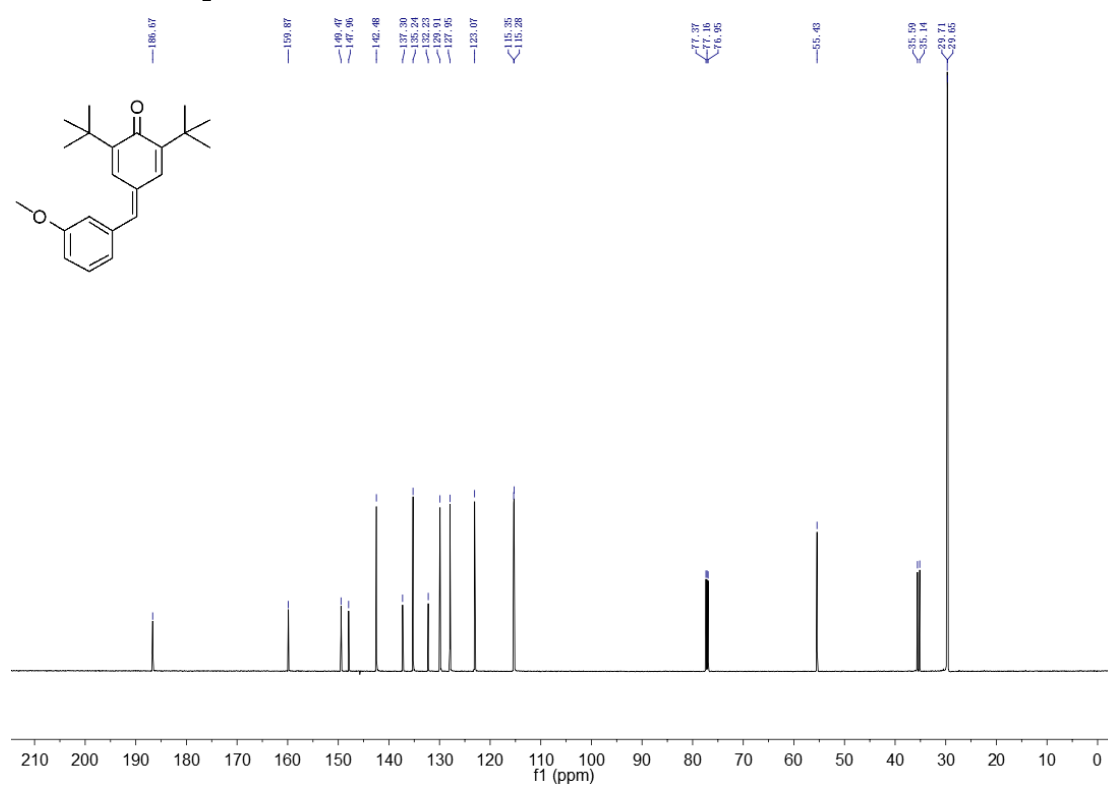
¹³C NMR of **1p**



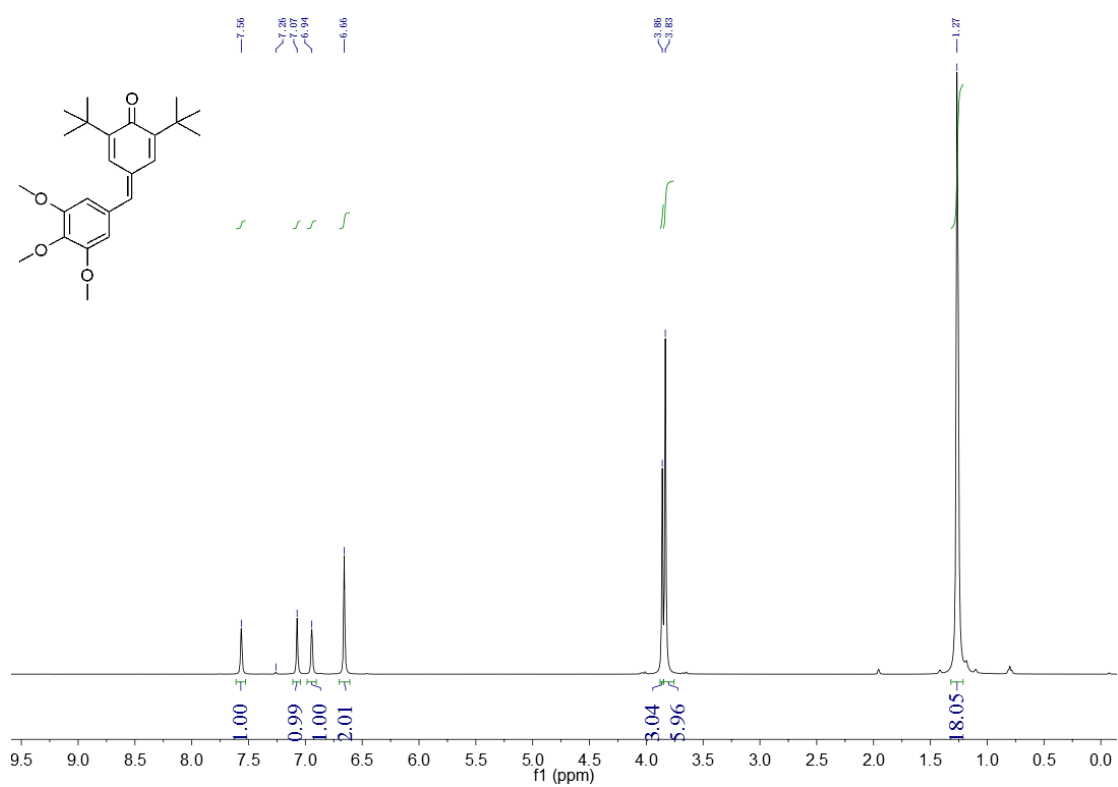
¹H NMR of **1q**



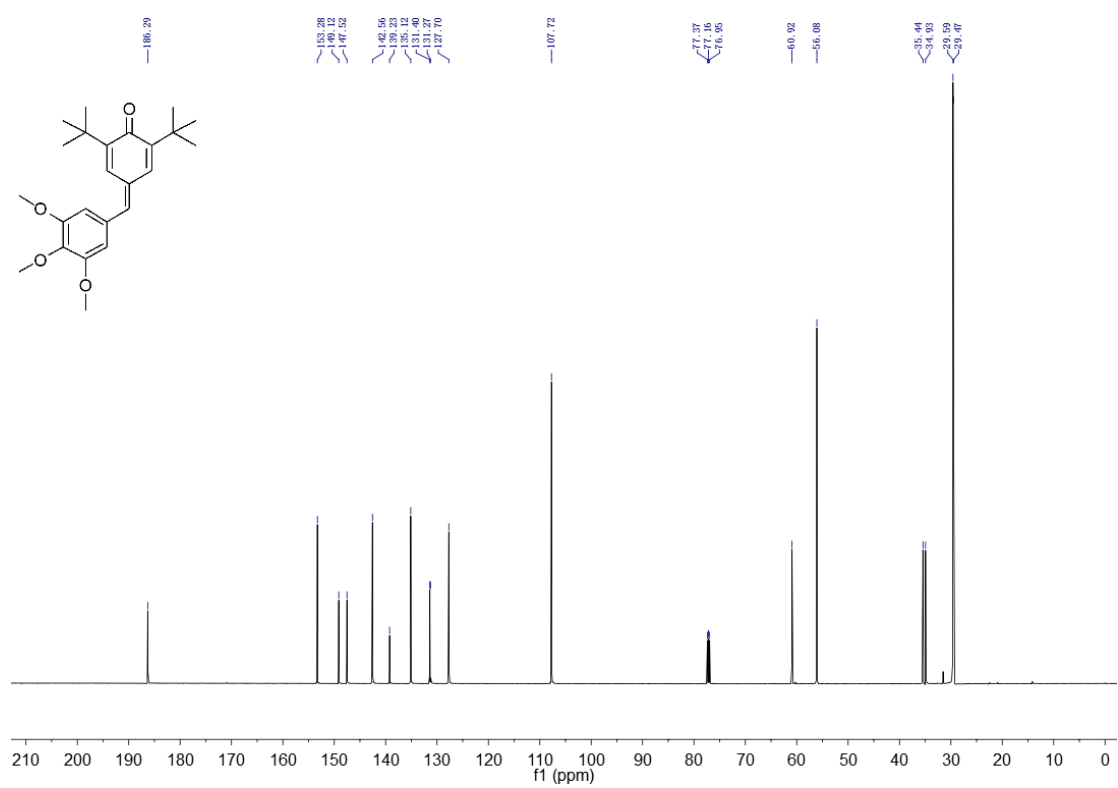
¹³C NMR of **1q**



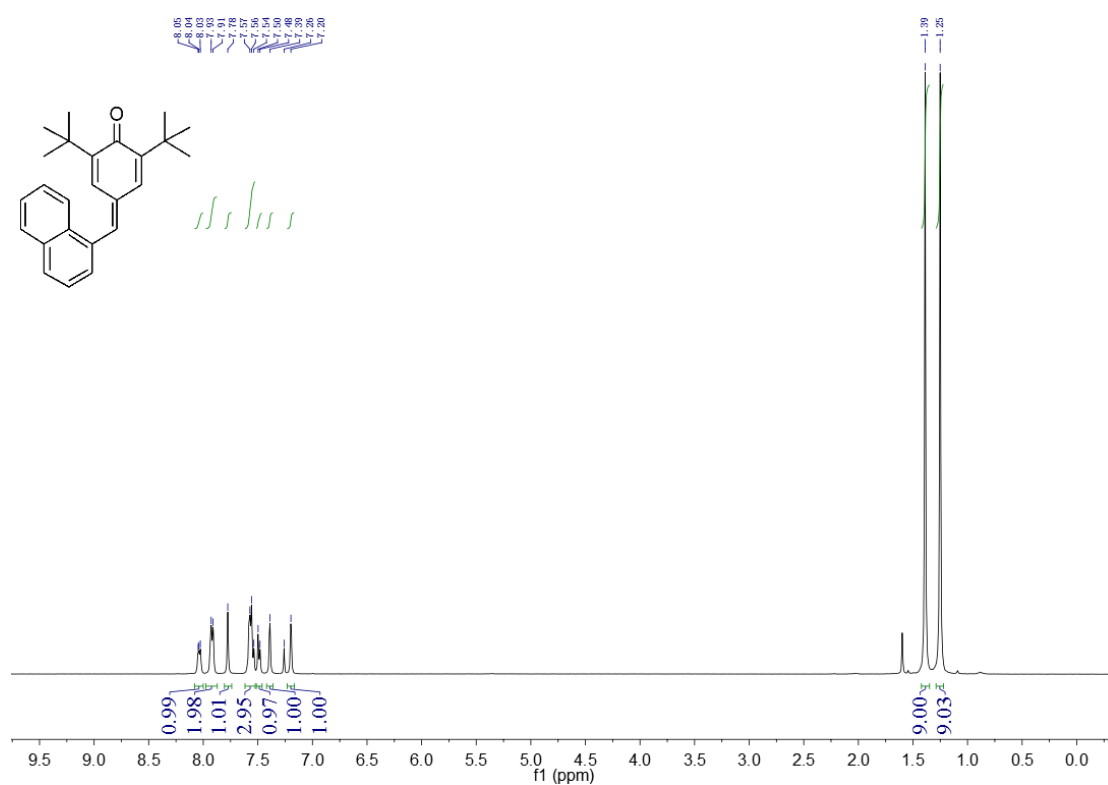
¹H NMR of **1r**



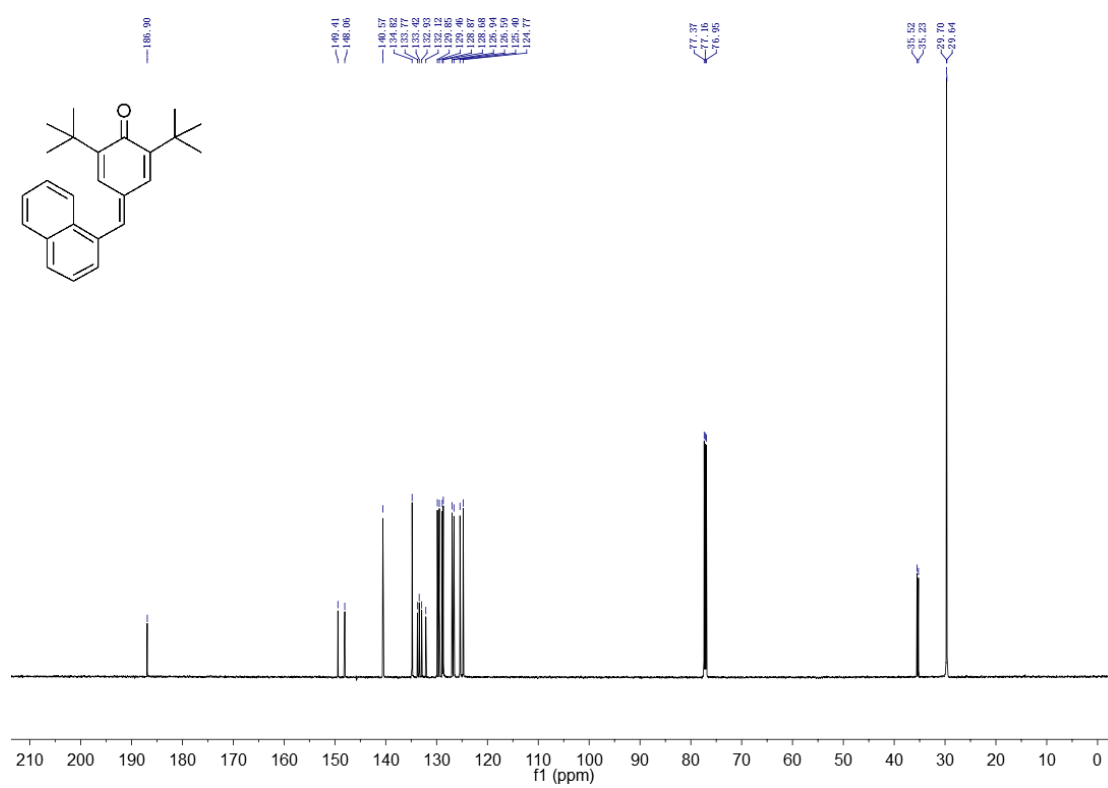
¹³C NMR of **1r**



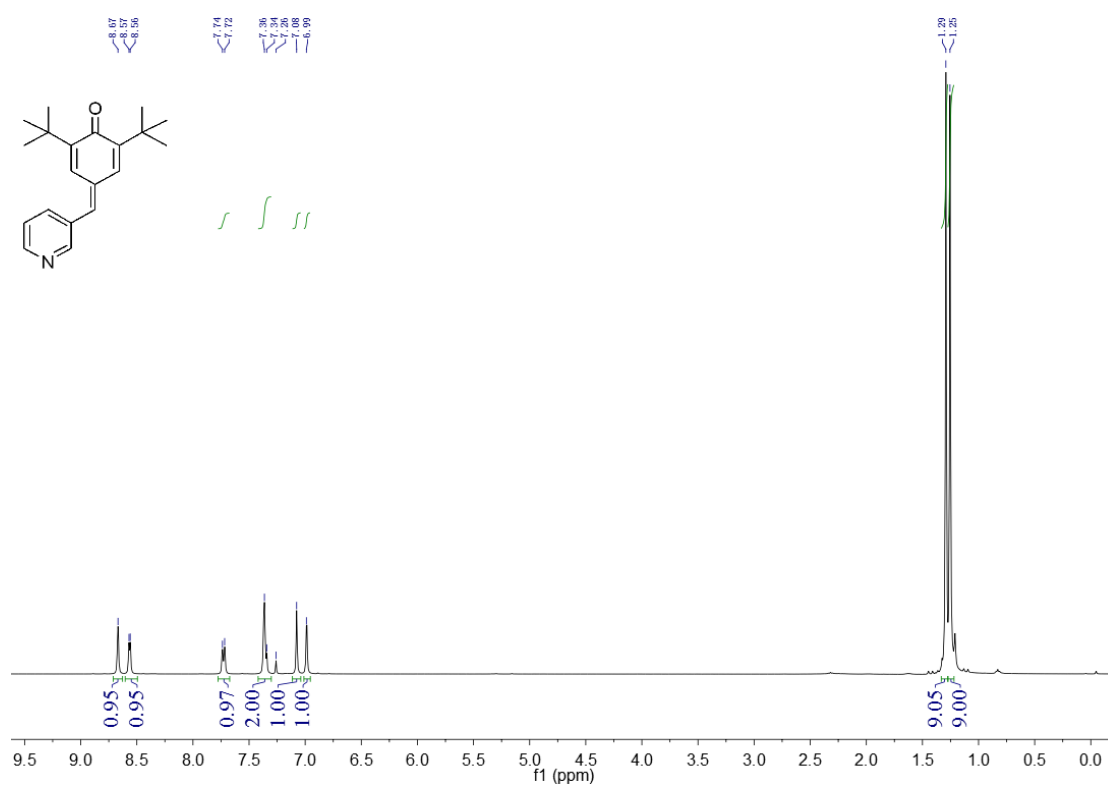
¹H NMR of **1s**



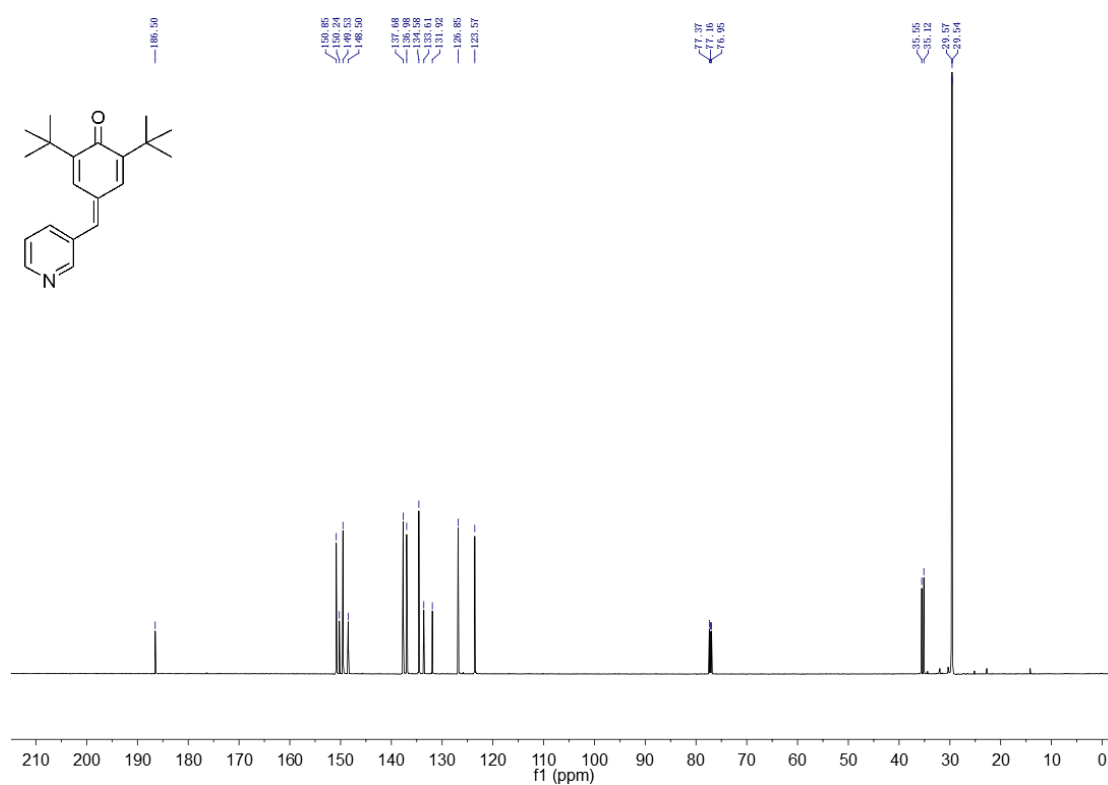
¹³C NMR of **1s**



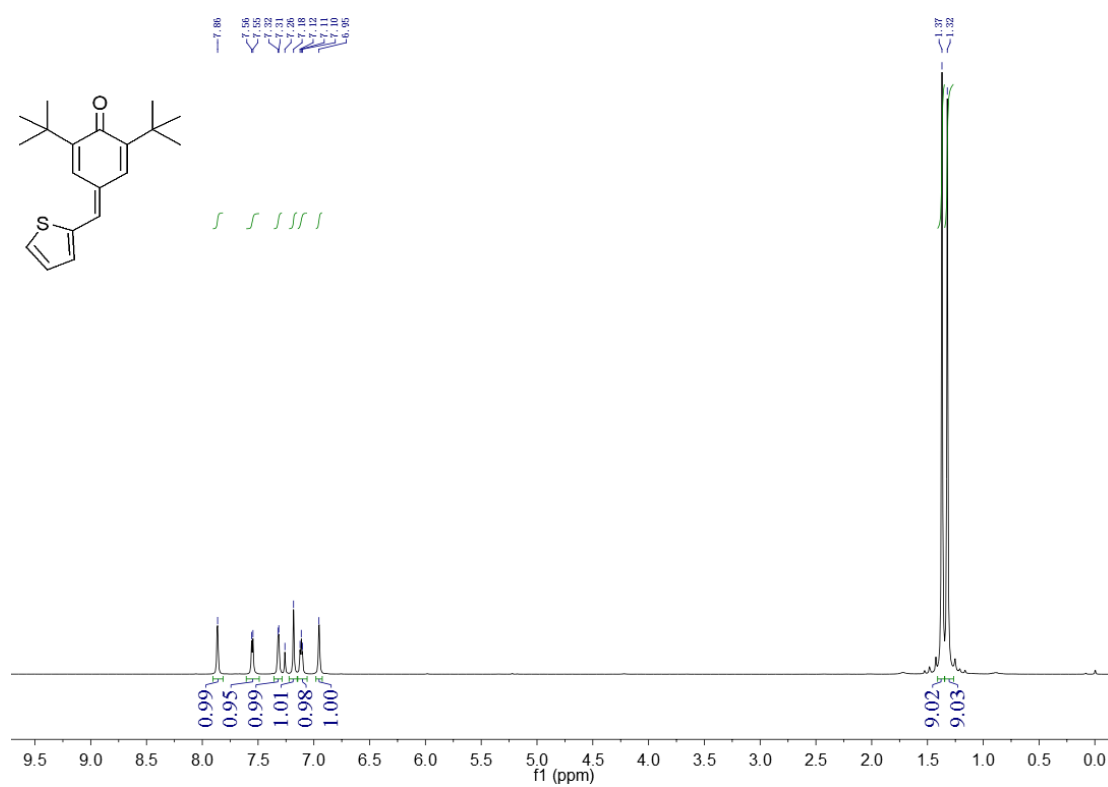
¹H NMR of **1t**



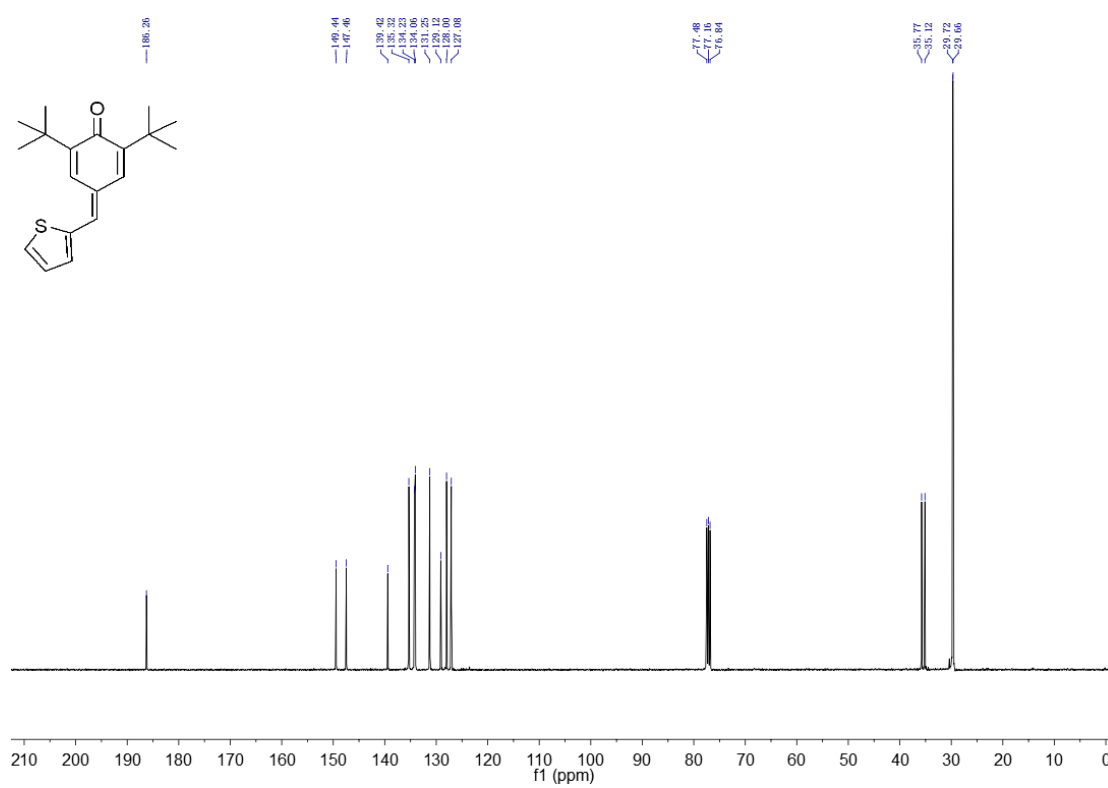
¹³C NMR of **1t**



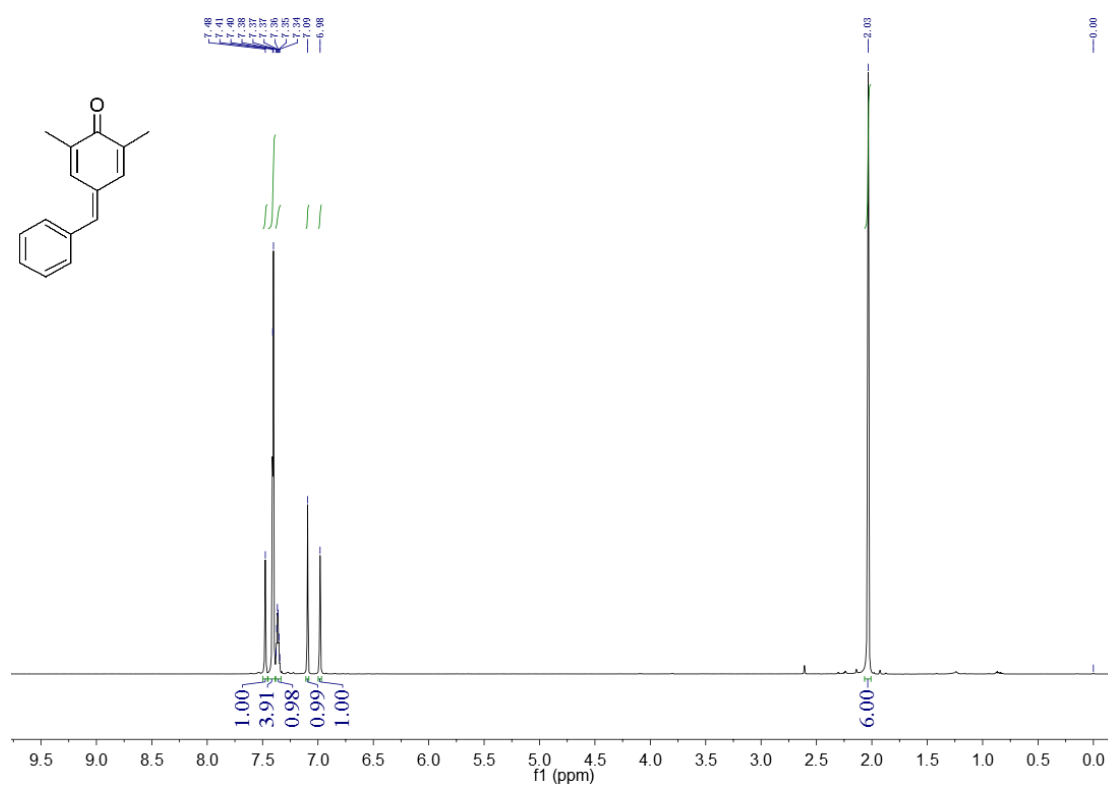
¹H NMR of **1u**



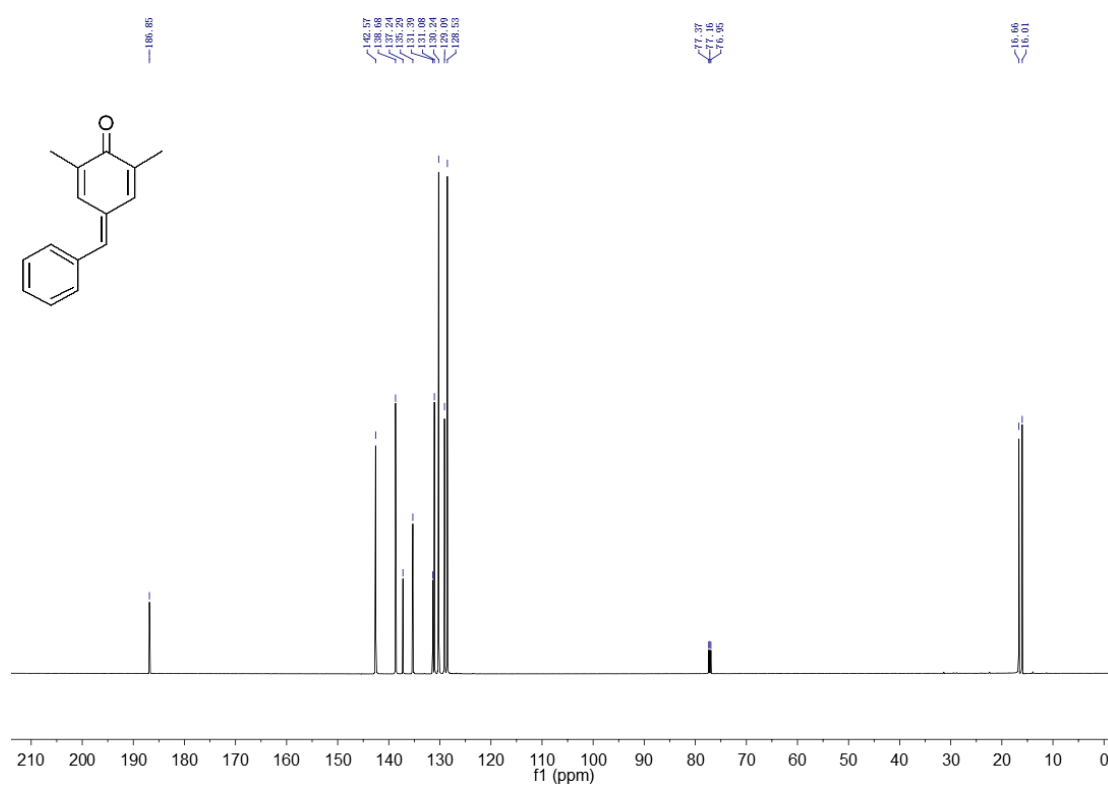
¹³C NMR of **1u**



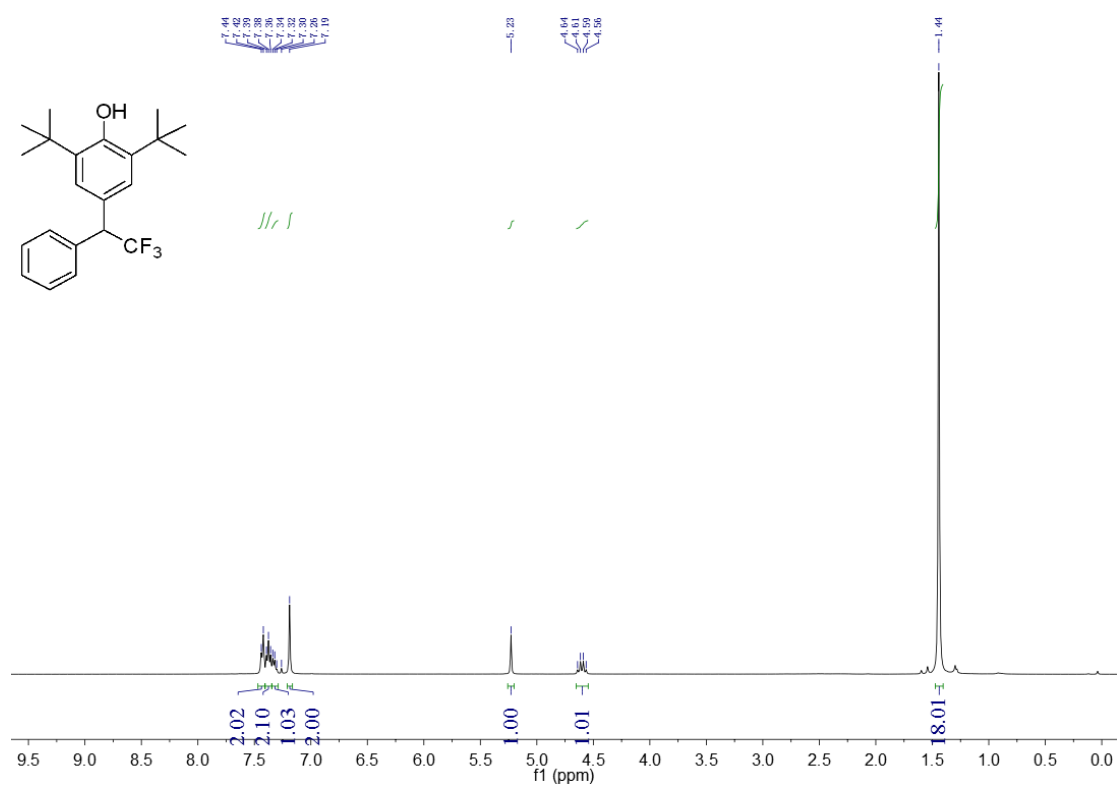
¹H NMR of **1v**



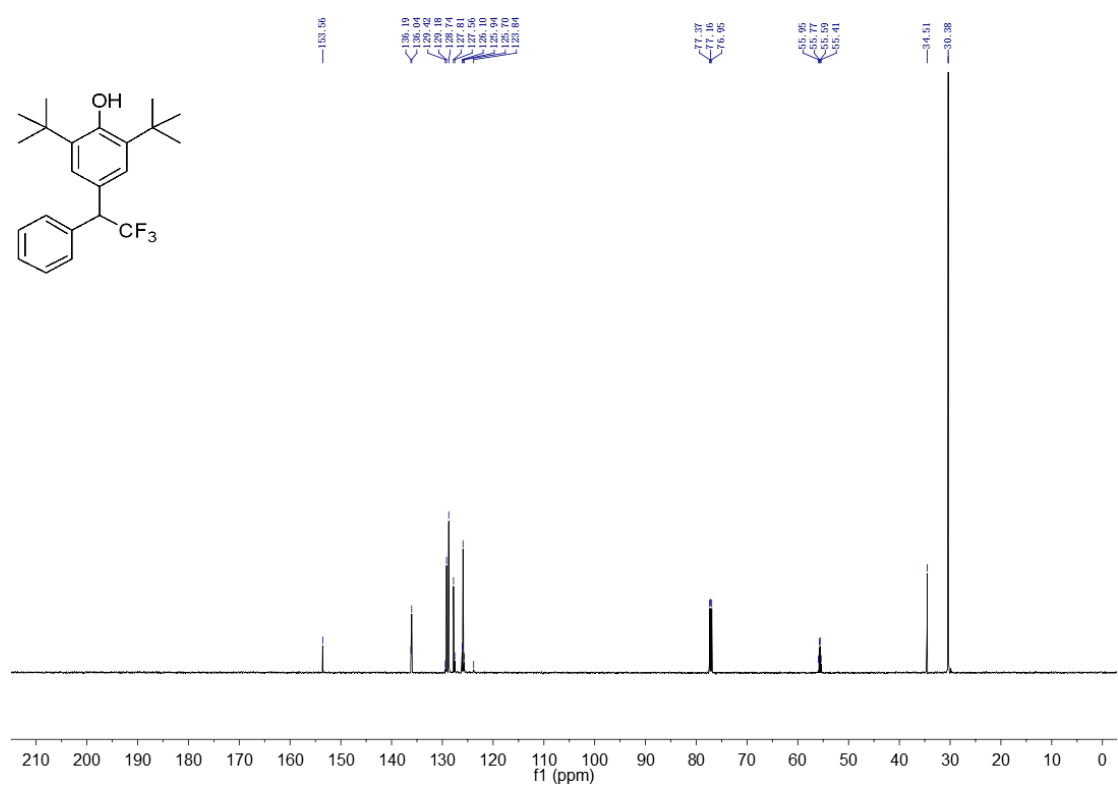
¹³C NMR of **1v**



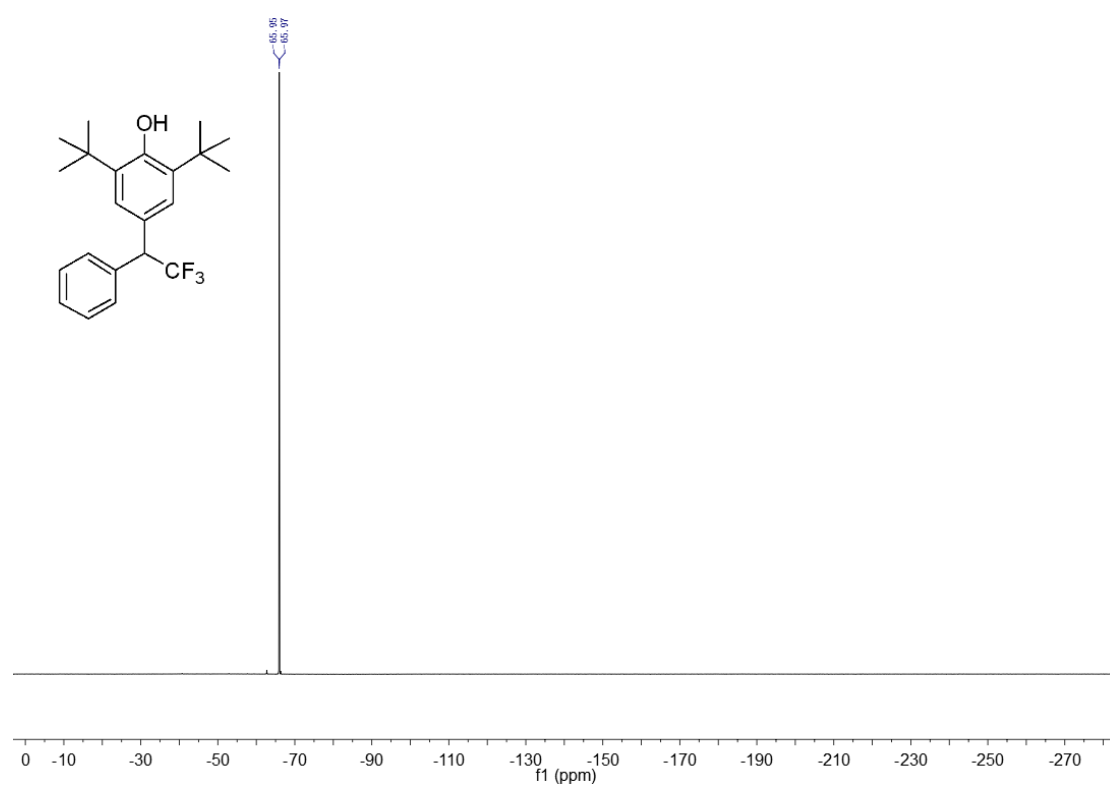
¹H NMR of **2a**



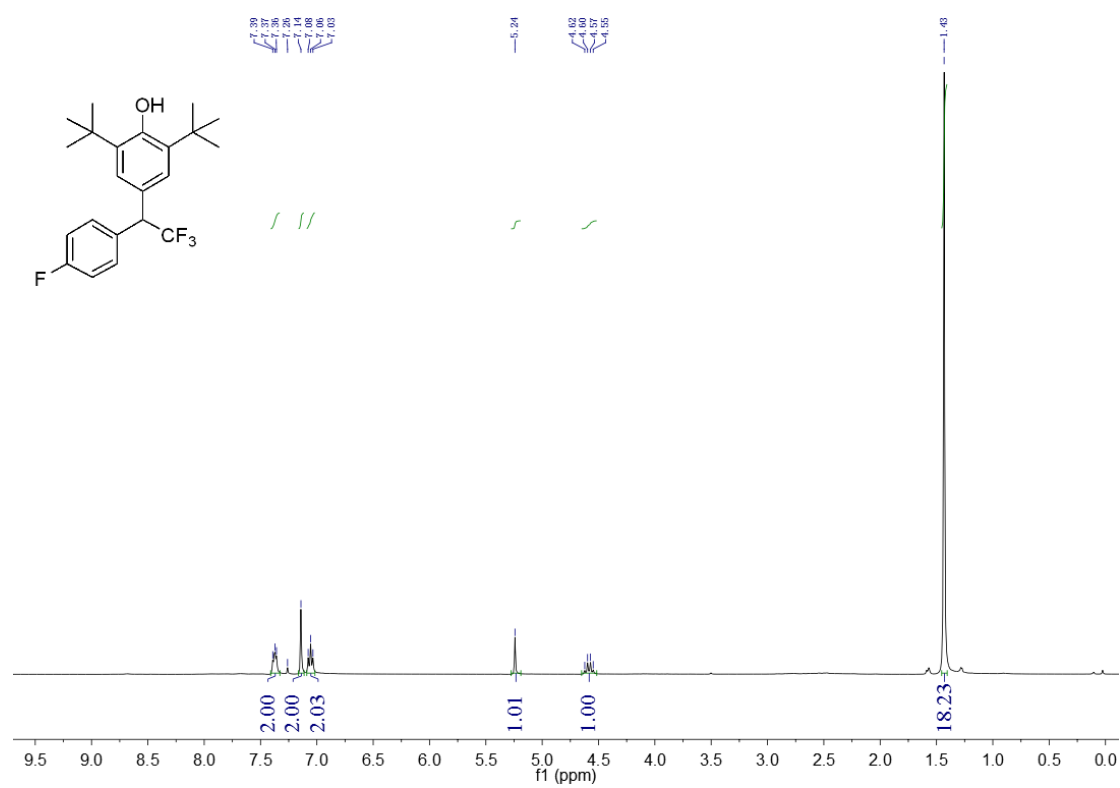
¹³C NMR of **2a**



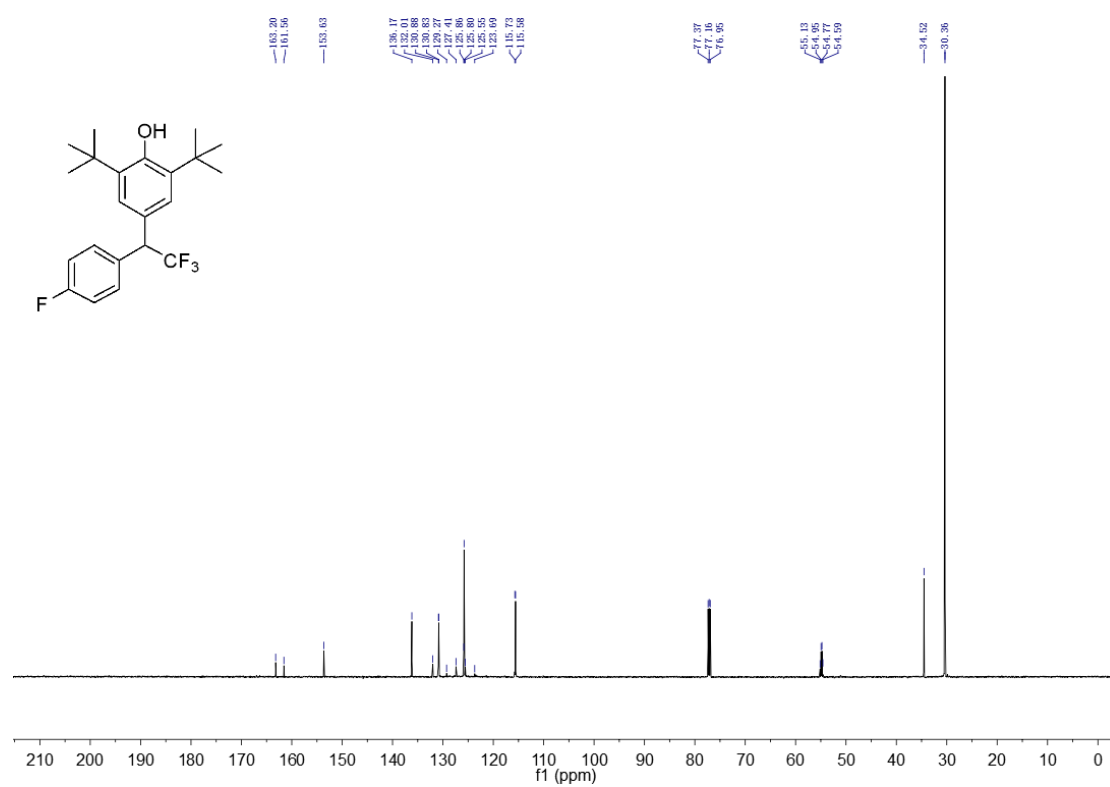
¹⁹F NMR of **2a**



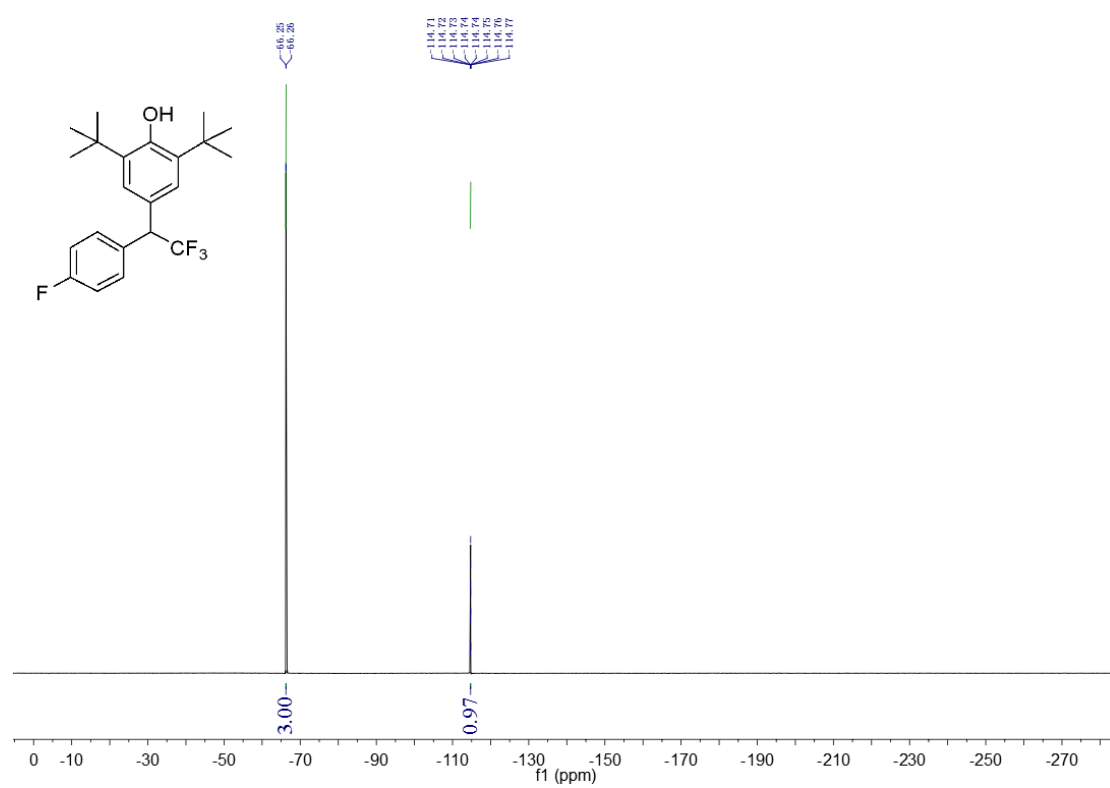
¹H NMR of **2b**



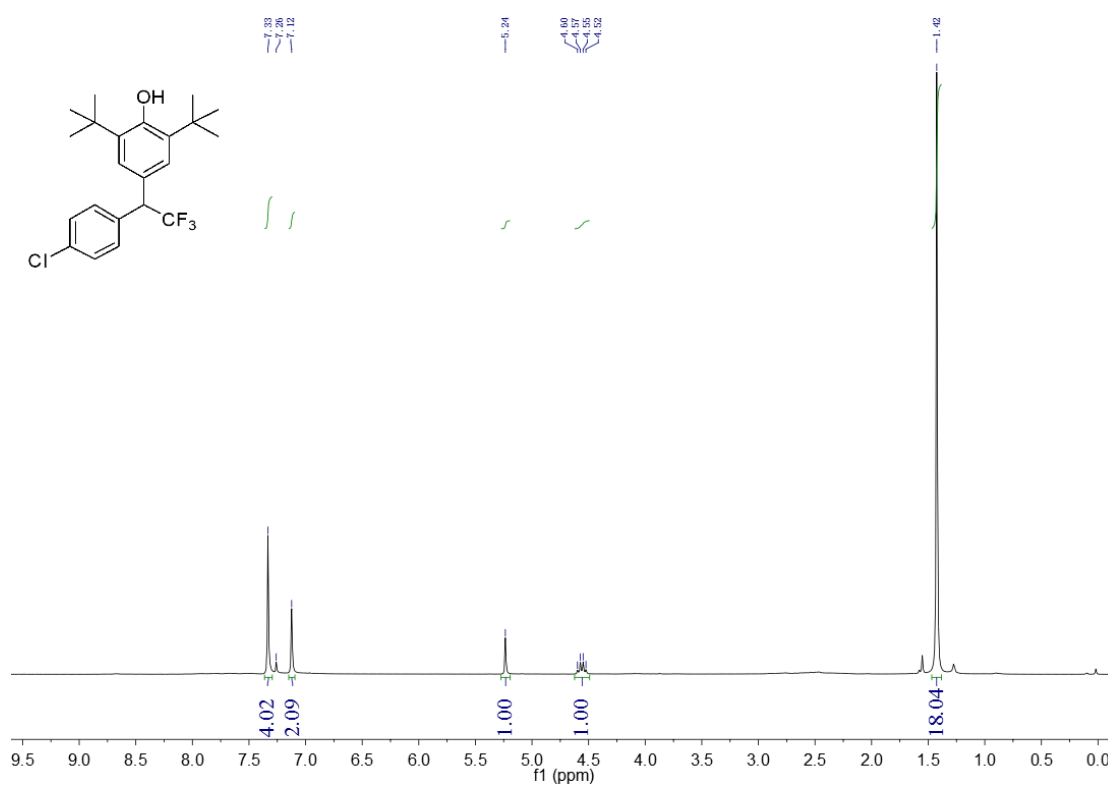
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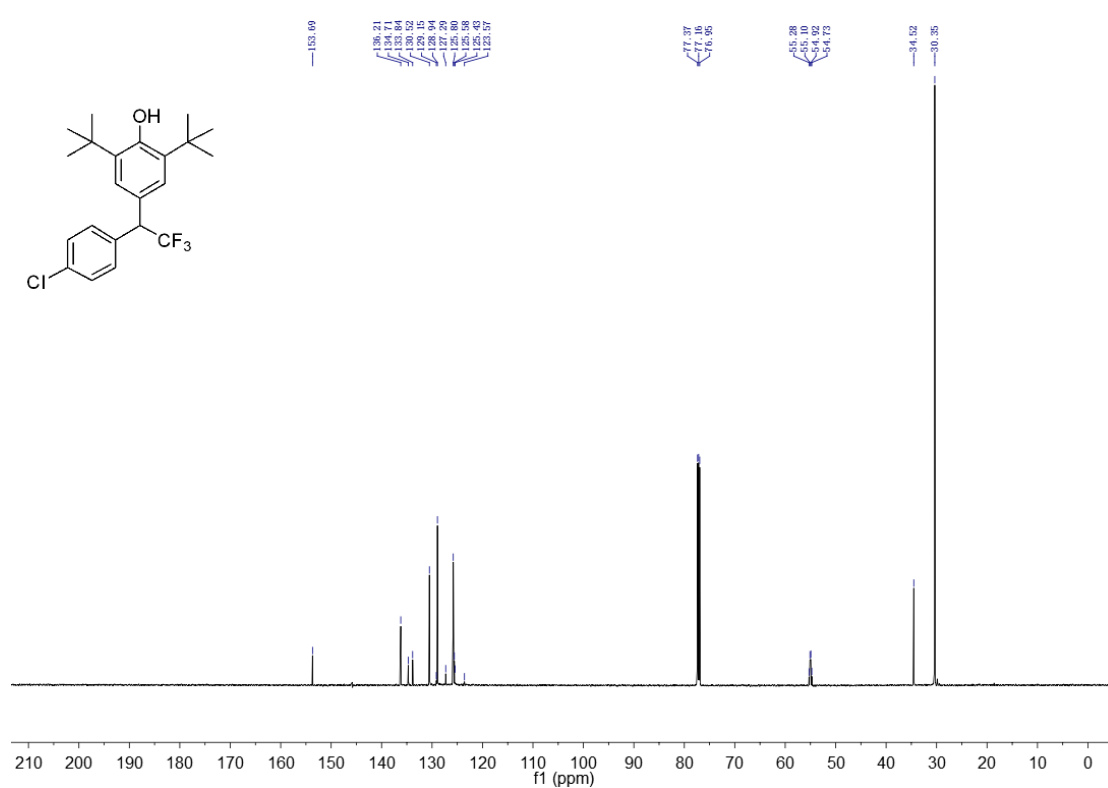
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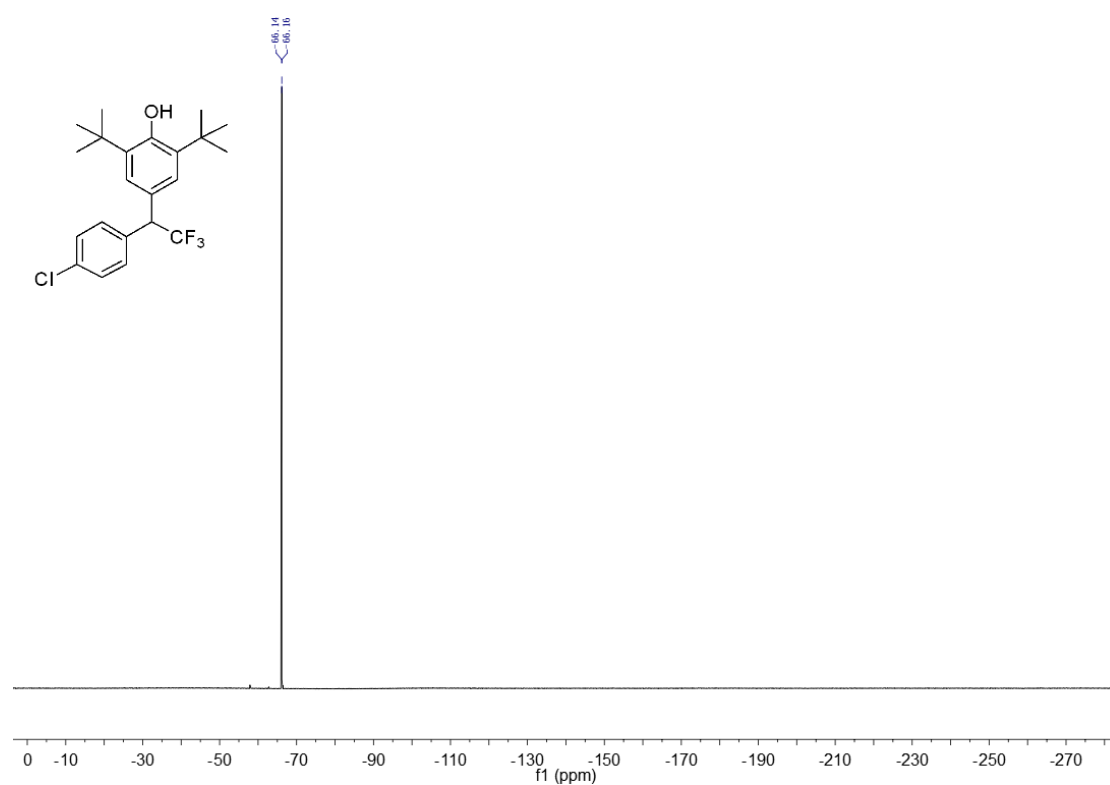
¹H NMR of 2c



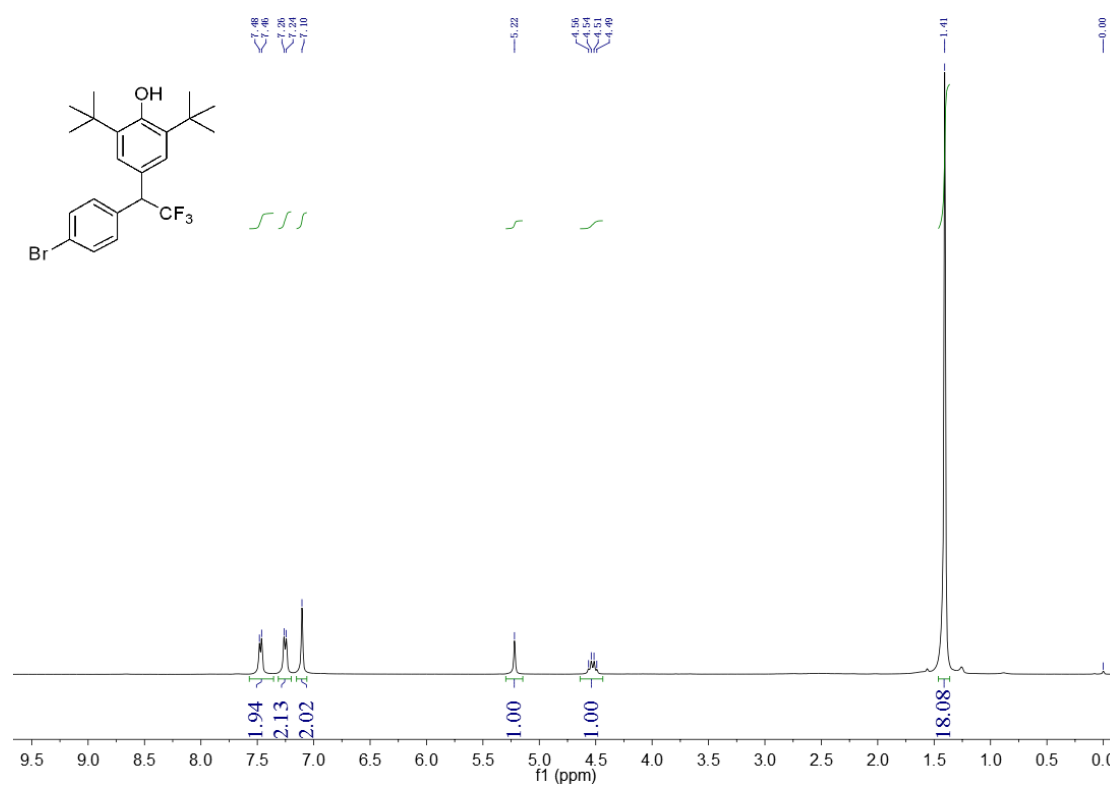
¹³C NMR of 2c



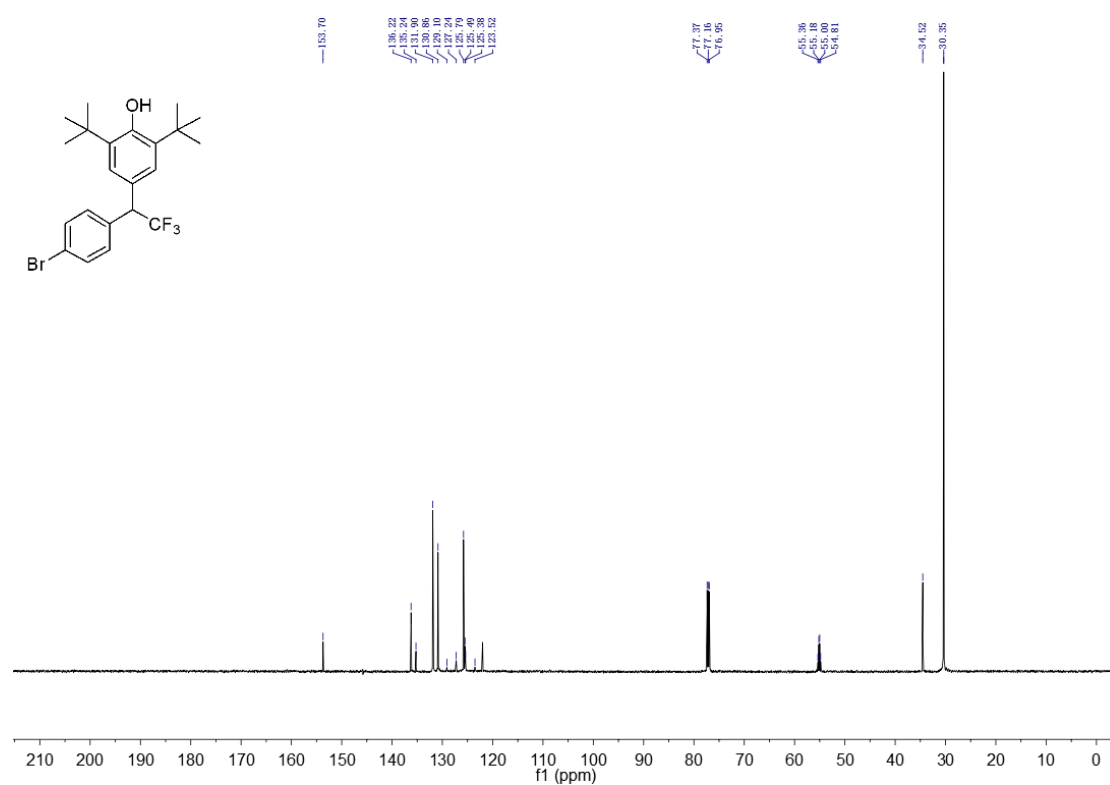
¹⁹F NMR of **2c**



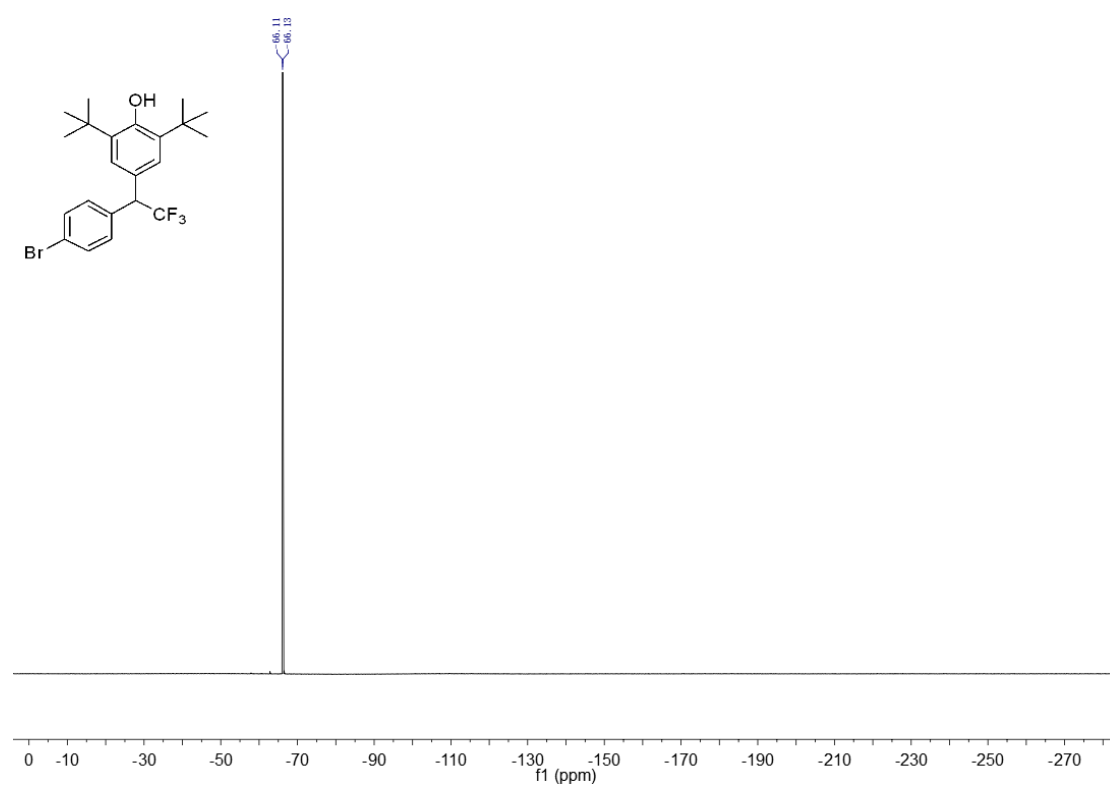
¹H NMR of **2d**



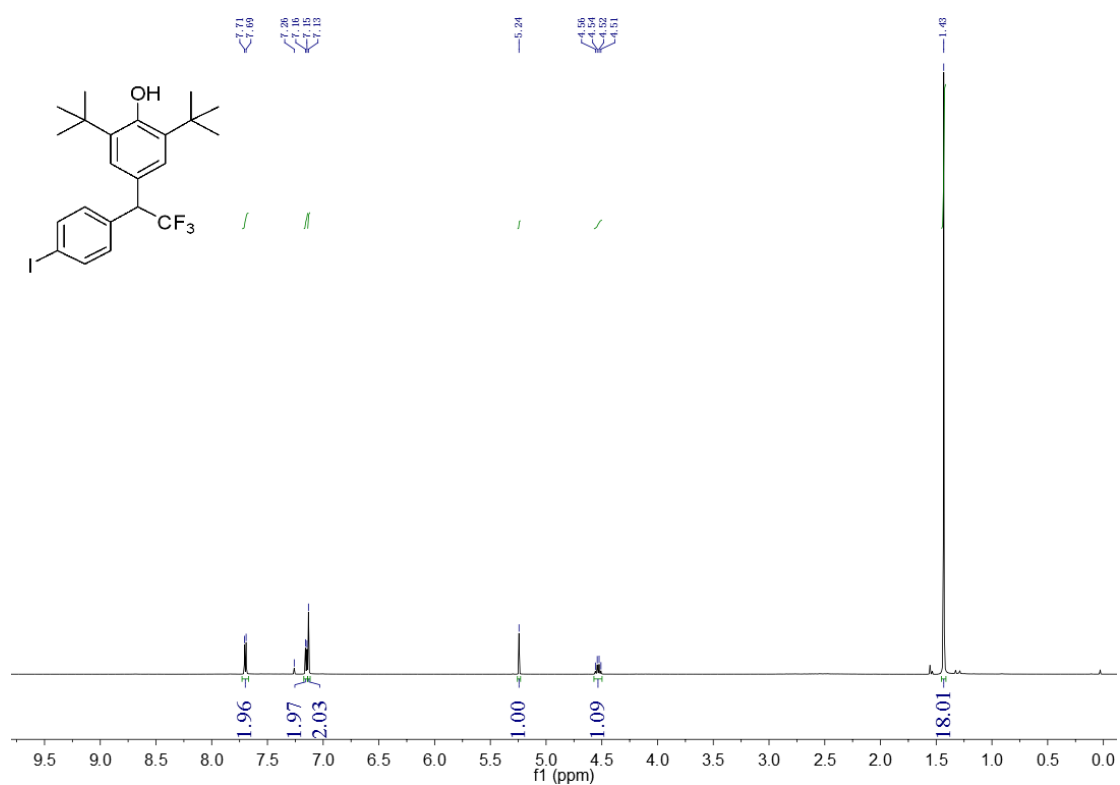
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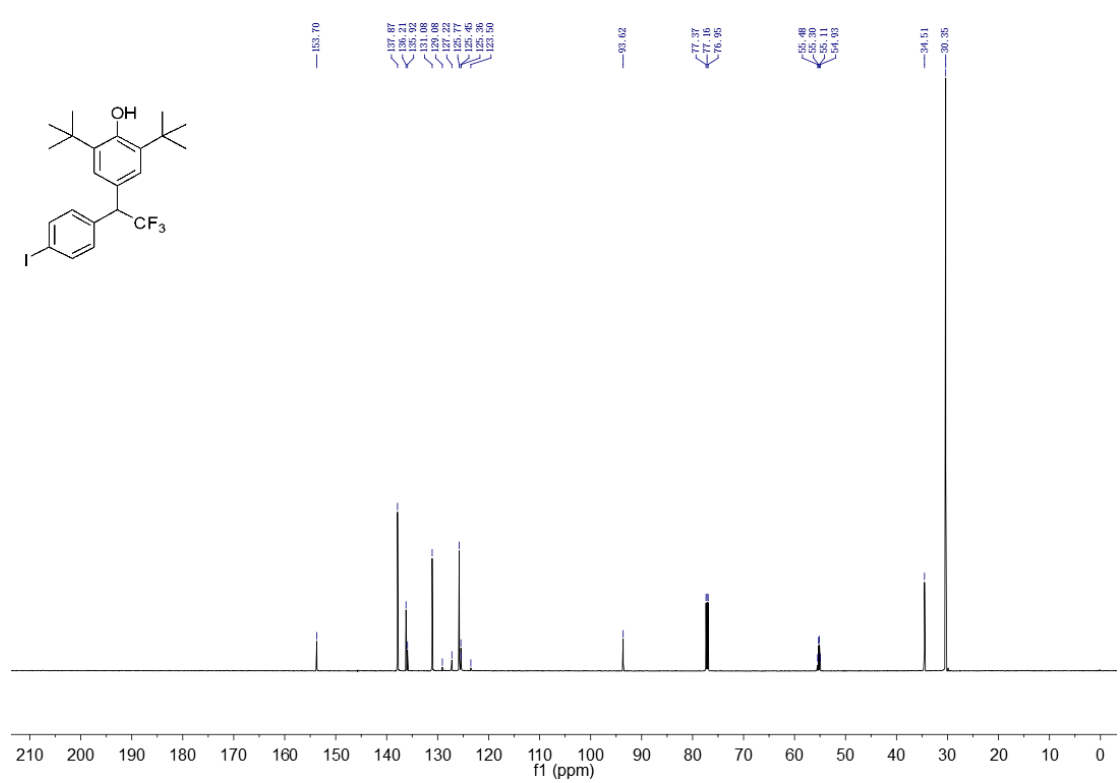
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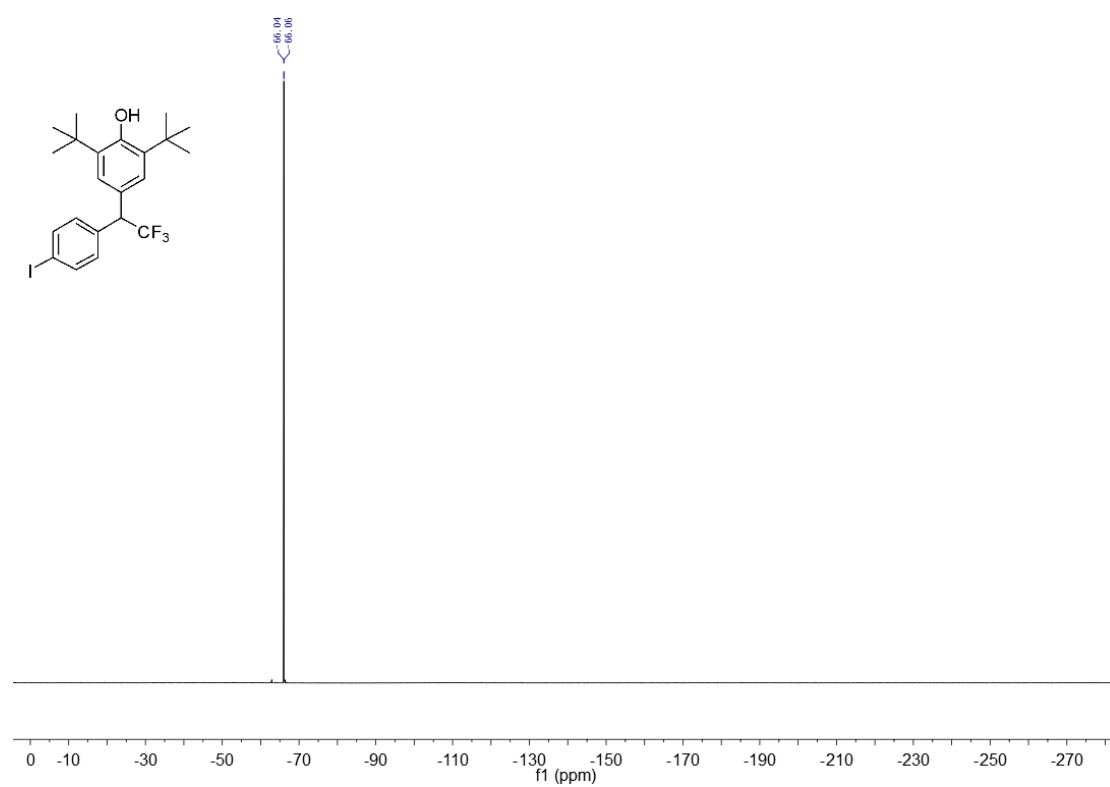
¹H NMR of 2e



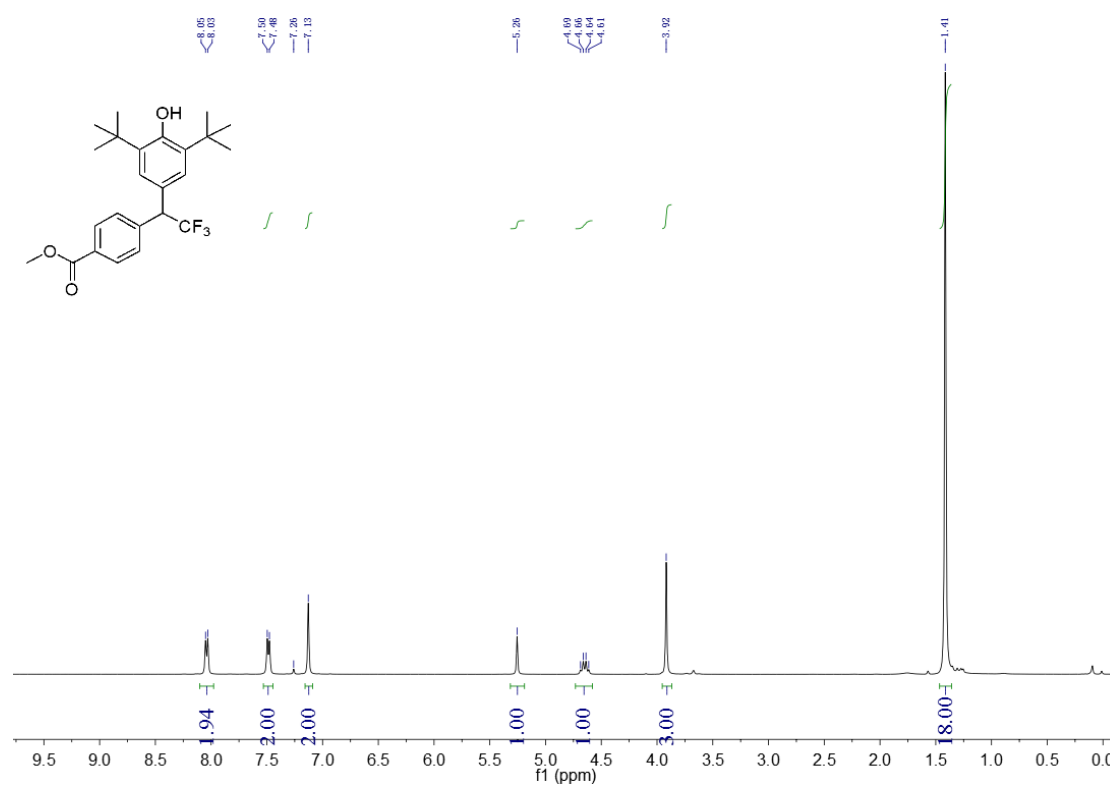
¹³C NMR of 2e



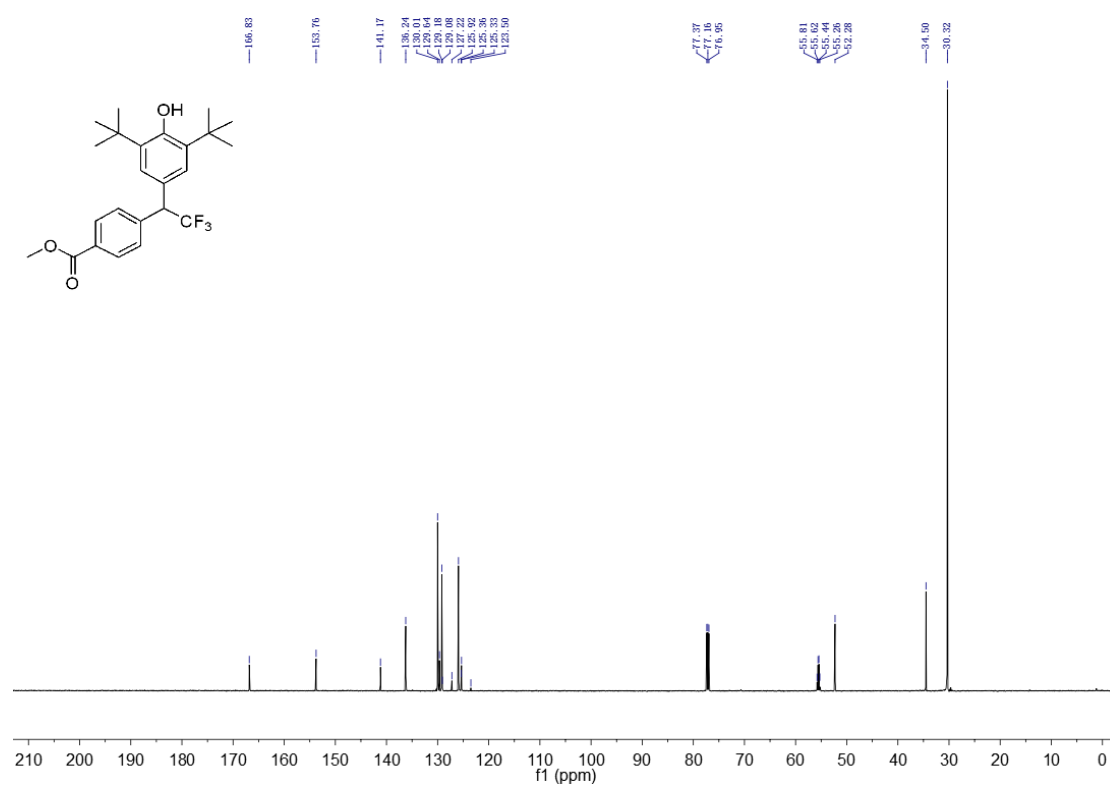
¹⁹F NMR of **2e**



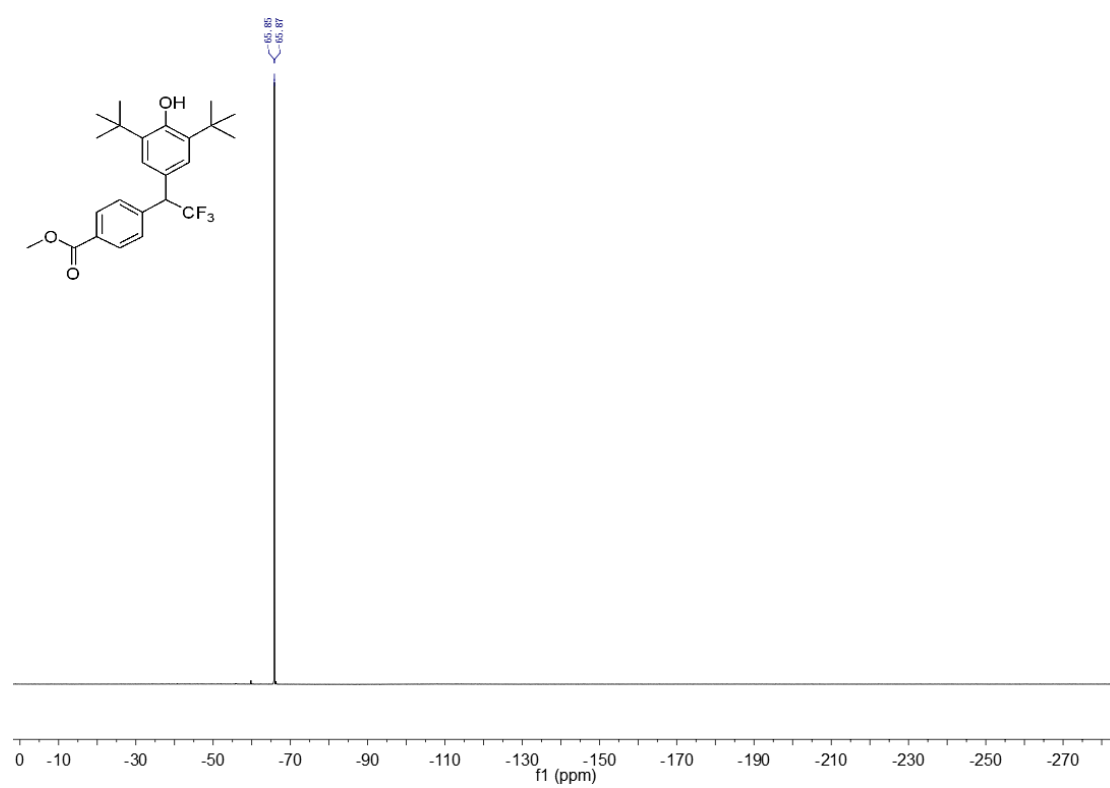
¹H NMR of **2f**



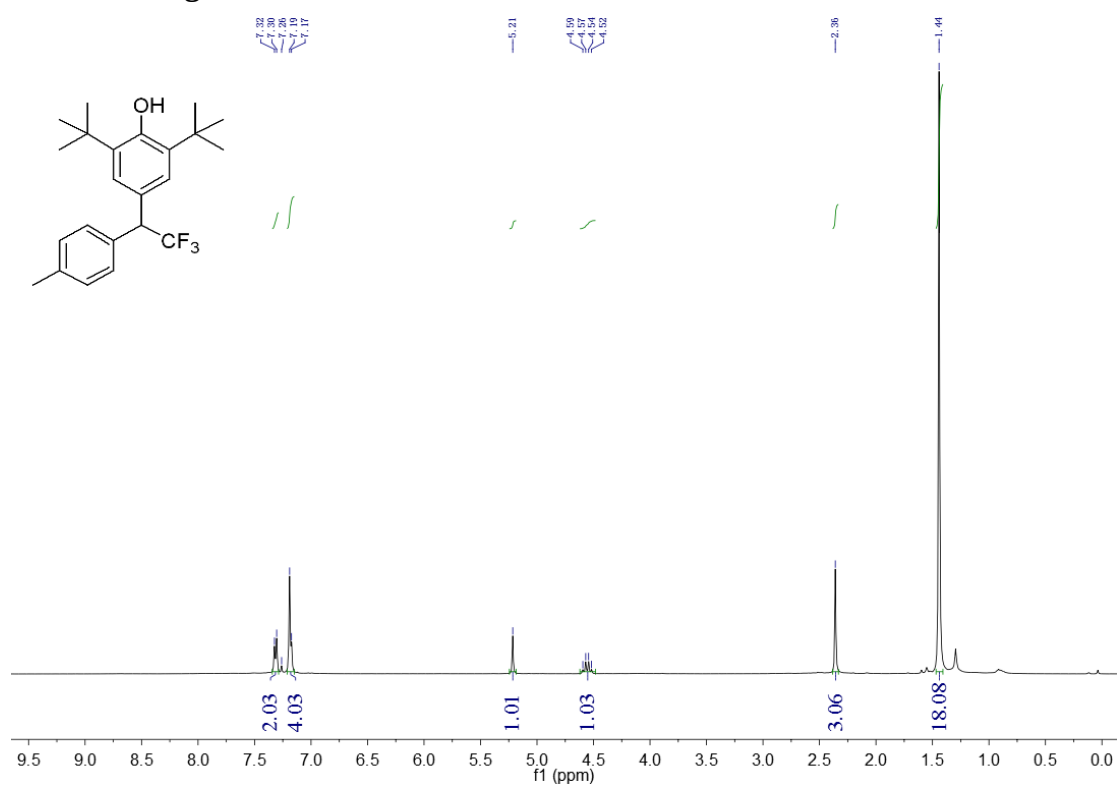
¹³C NMR of **2f**



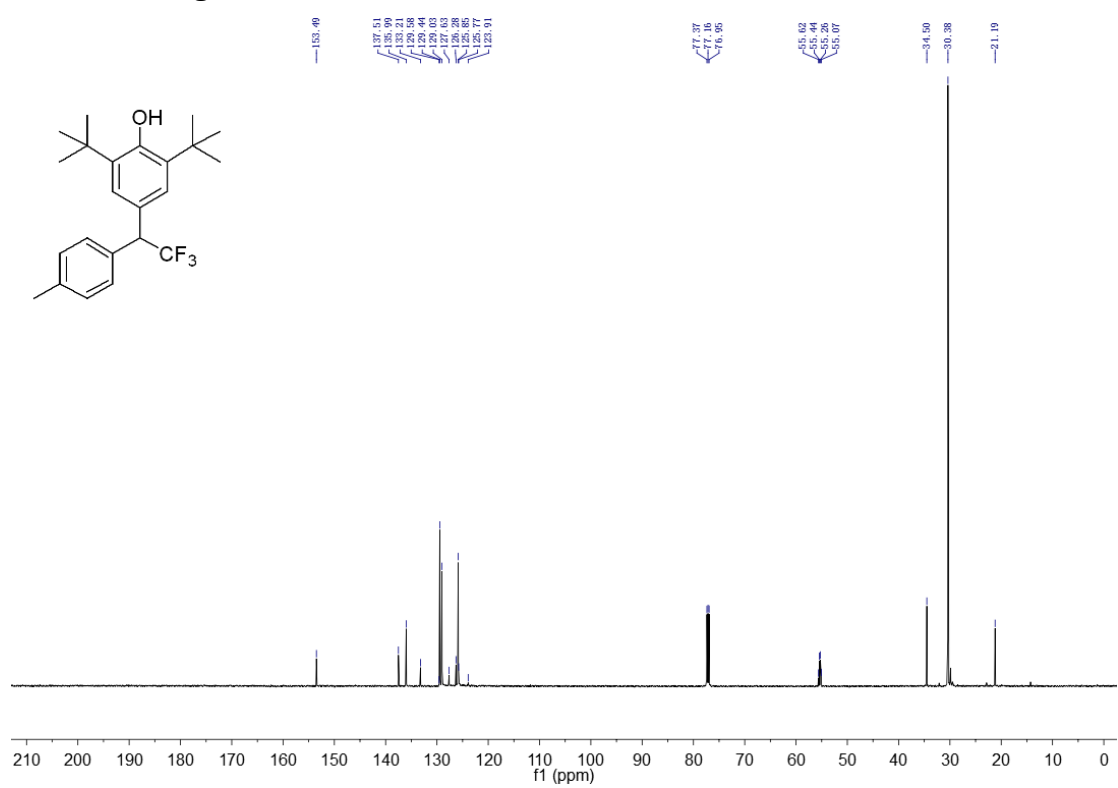
¹⁹F NMR of **2f**



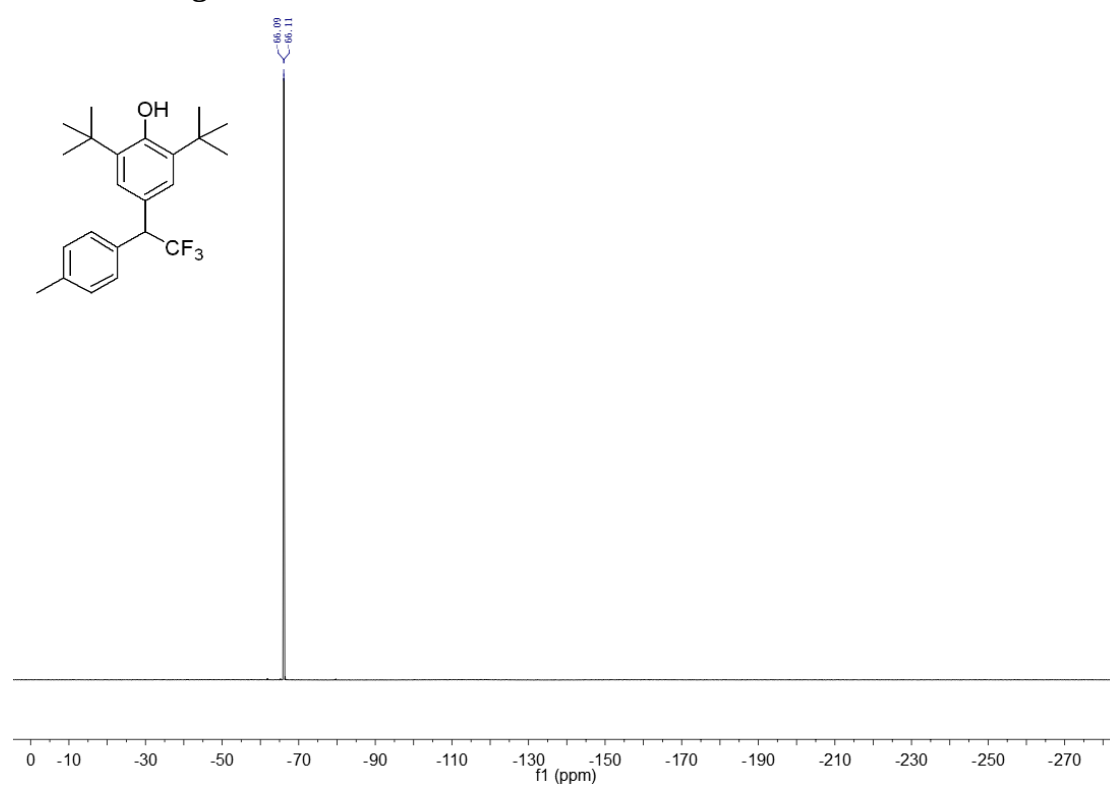
¹H NMR of **2g**



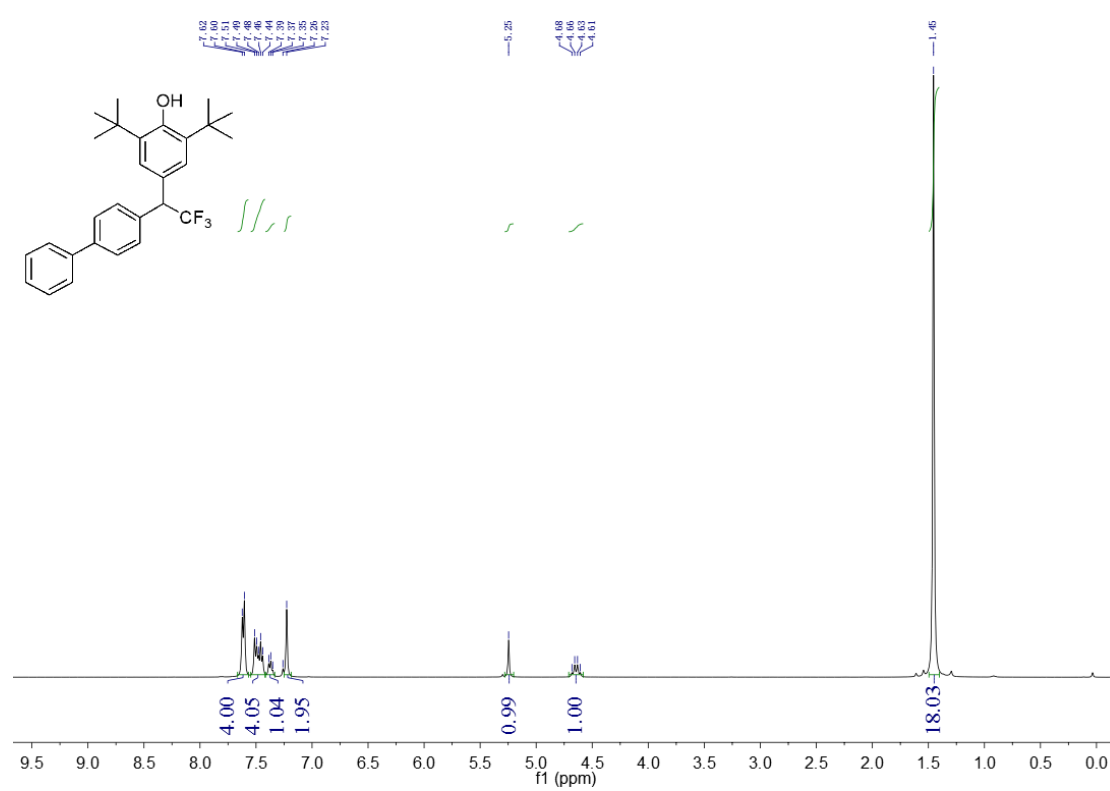
¹³C NMR of **2g**



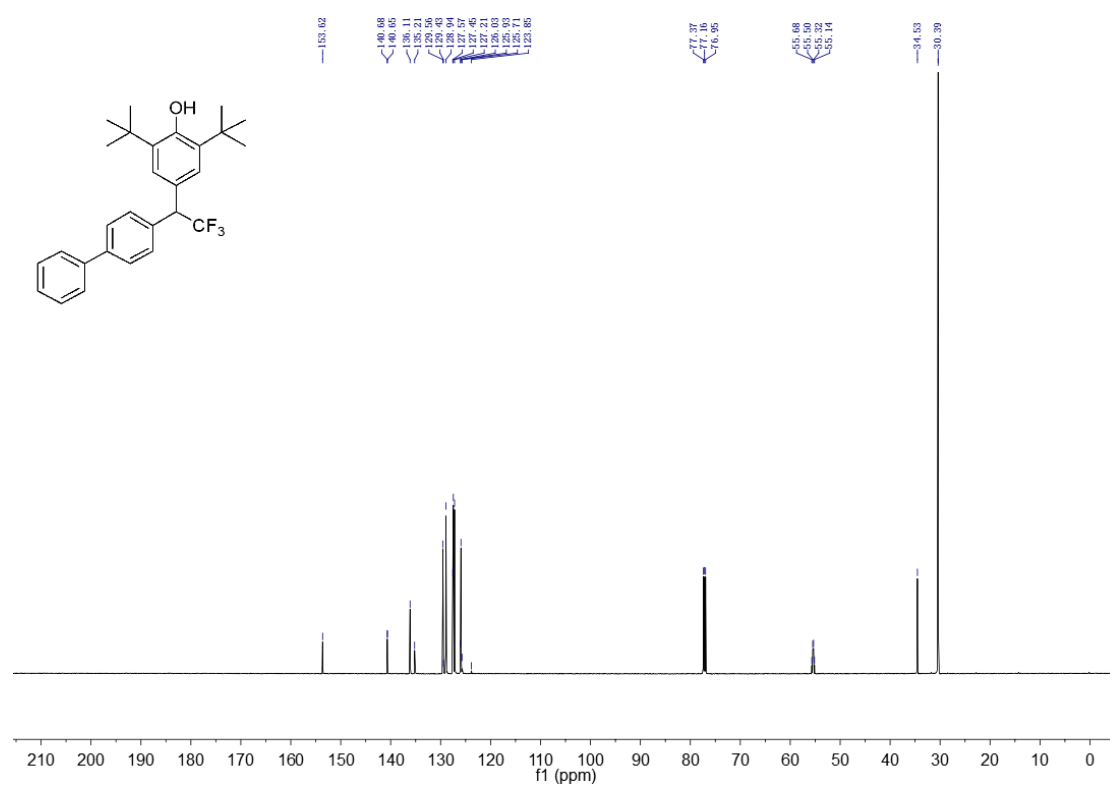
¹⁹F NMR of **2g**



¹H NMR of **2h**



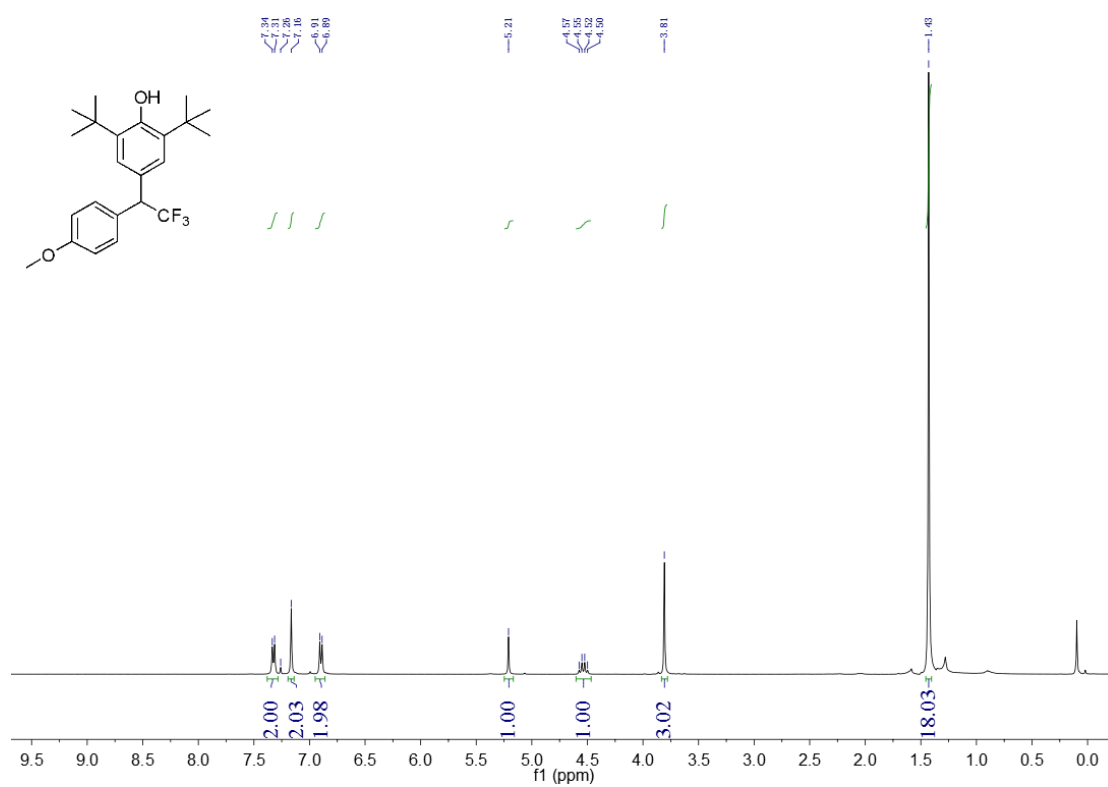
¹³C NMR of **2h**



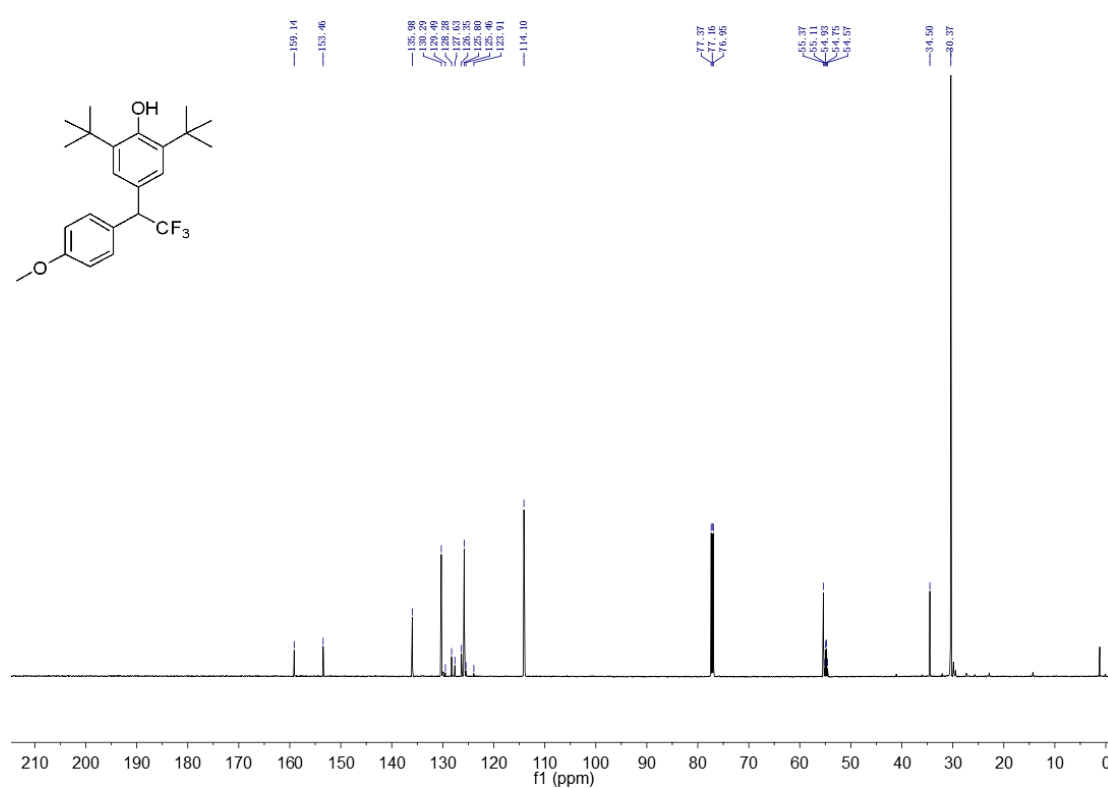
¹⁹F NMR of **2h**



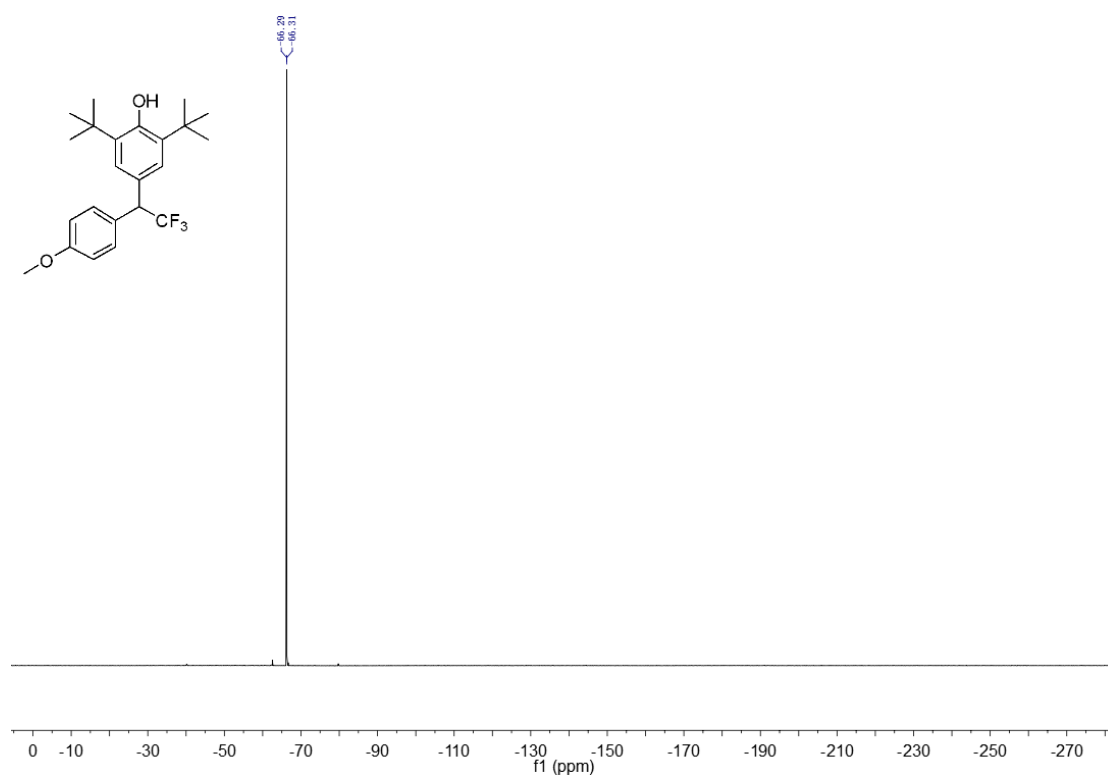
¹H NMR of **2i**



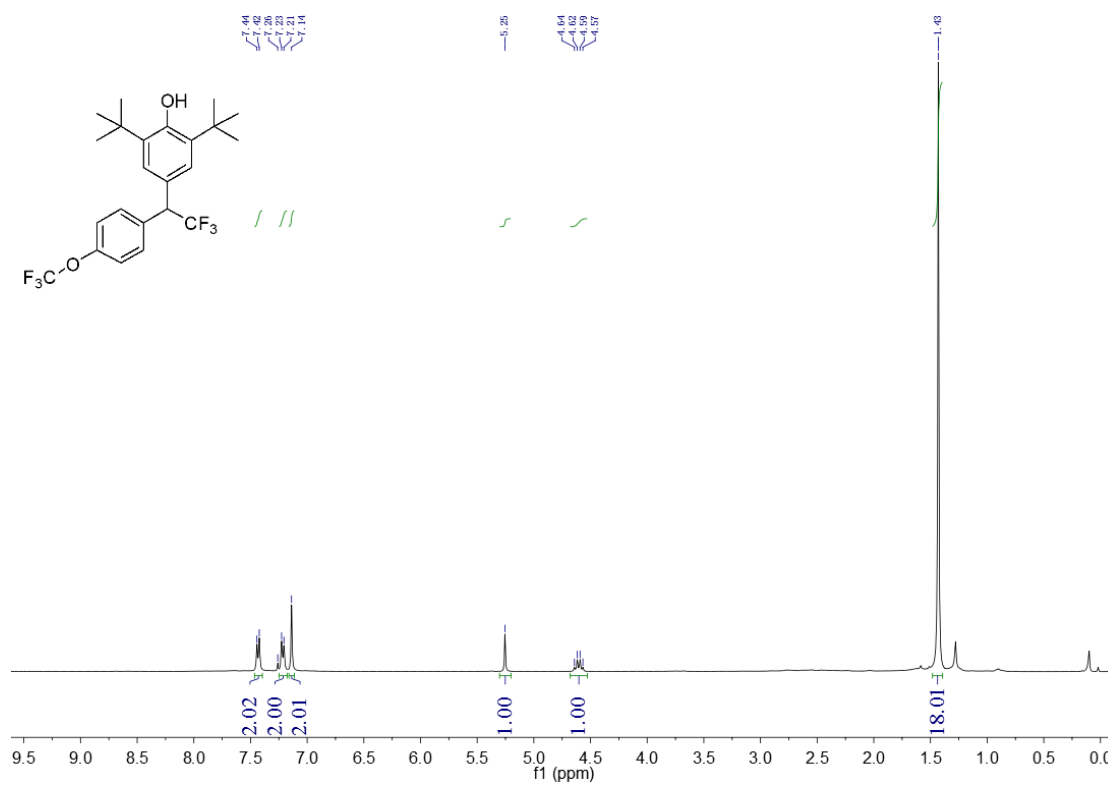
¹³C NMR of **2i**



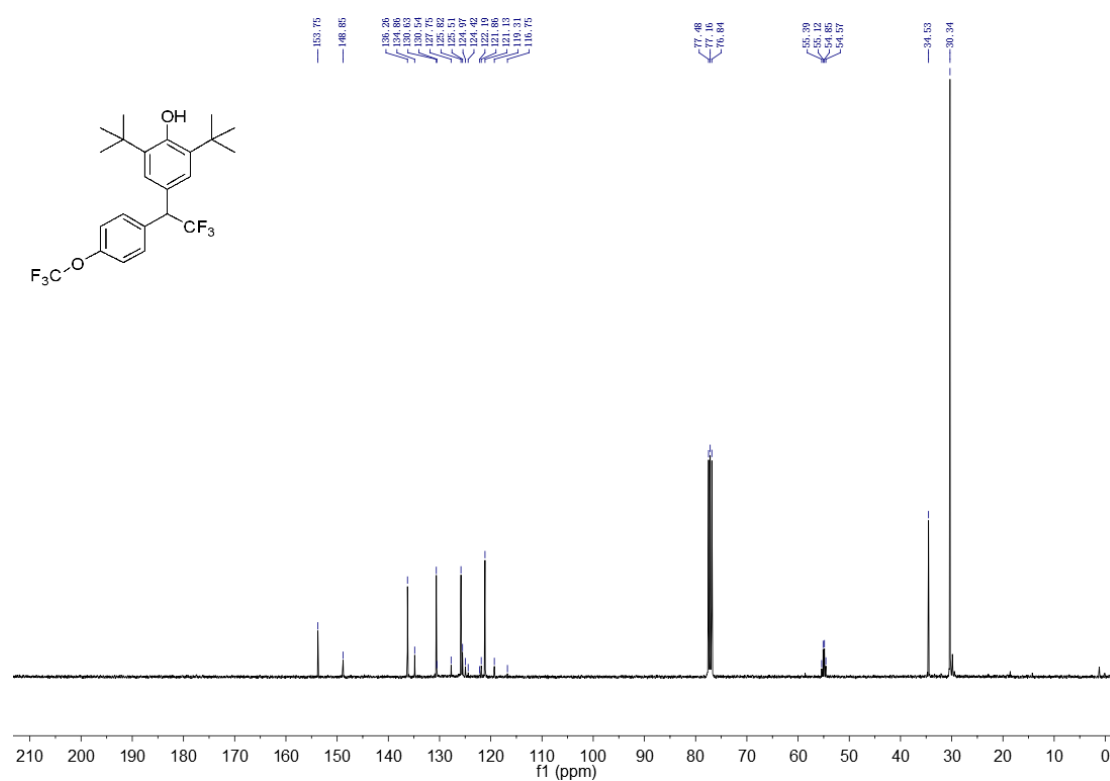
¹⁹F NMR of **2i**



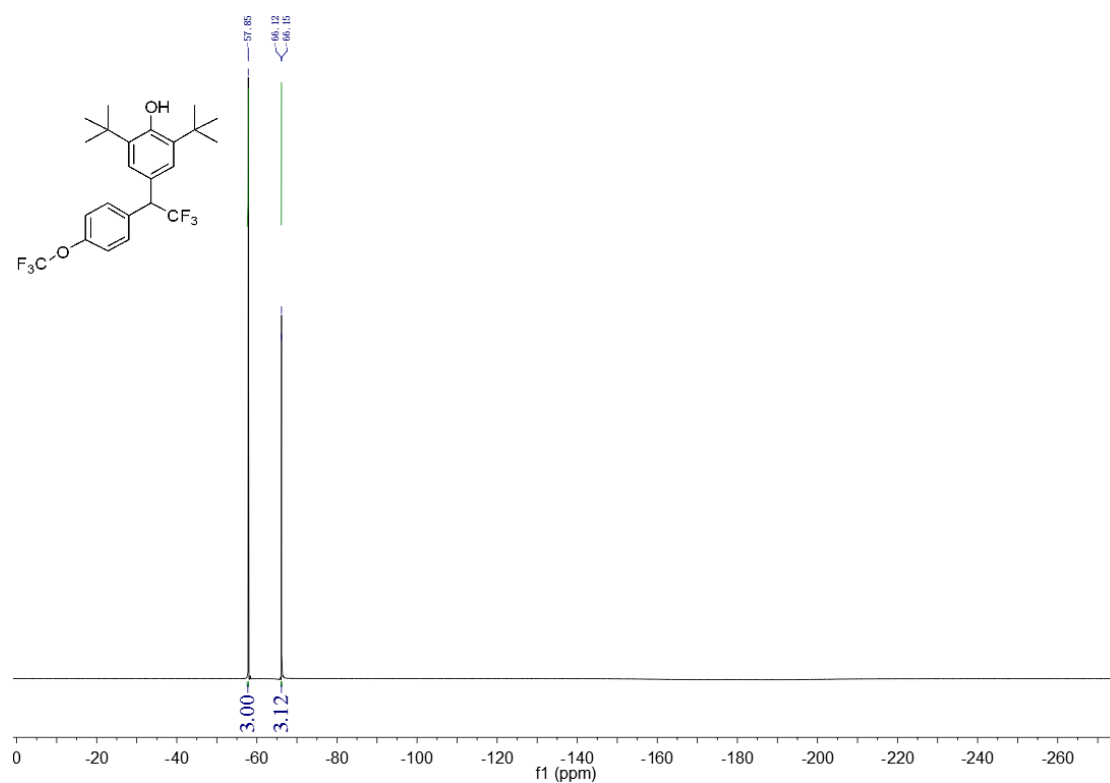
¹H NMR of **2j**



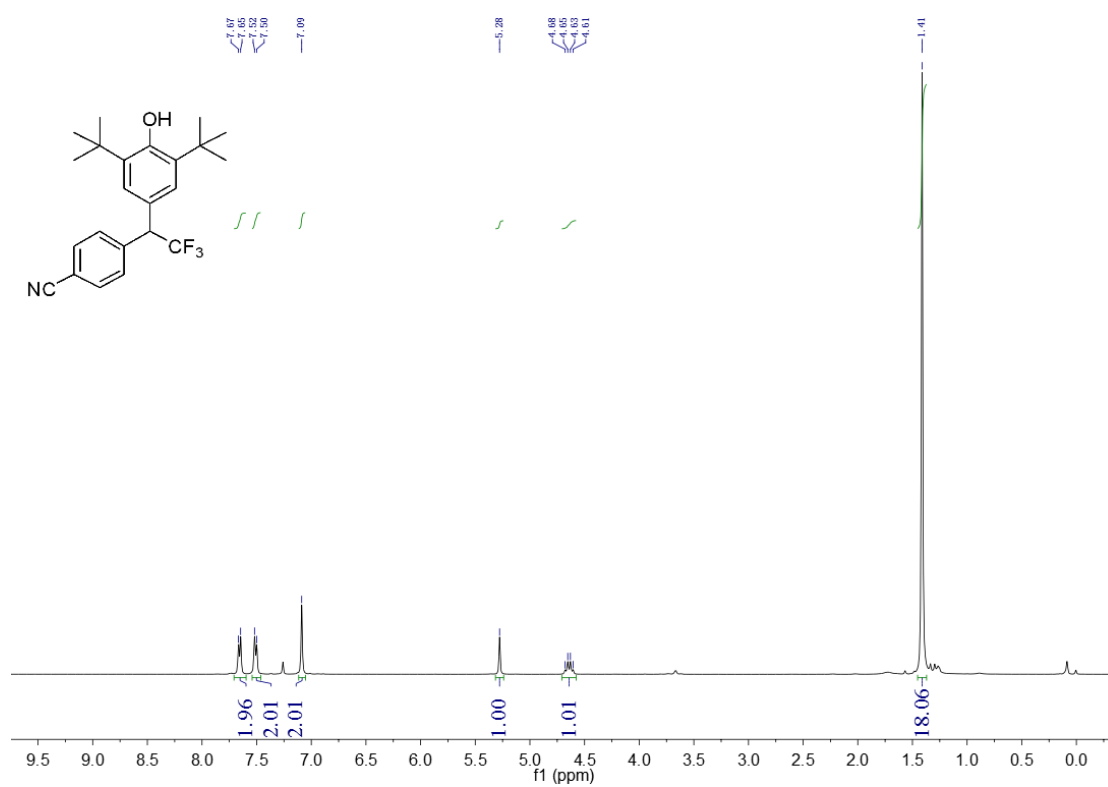
¹³C NMR of **2j**



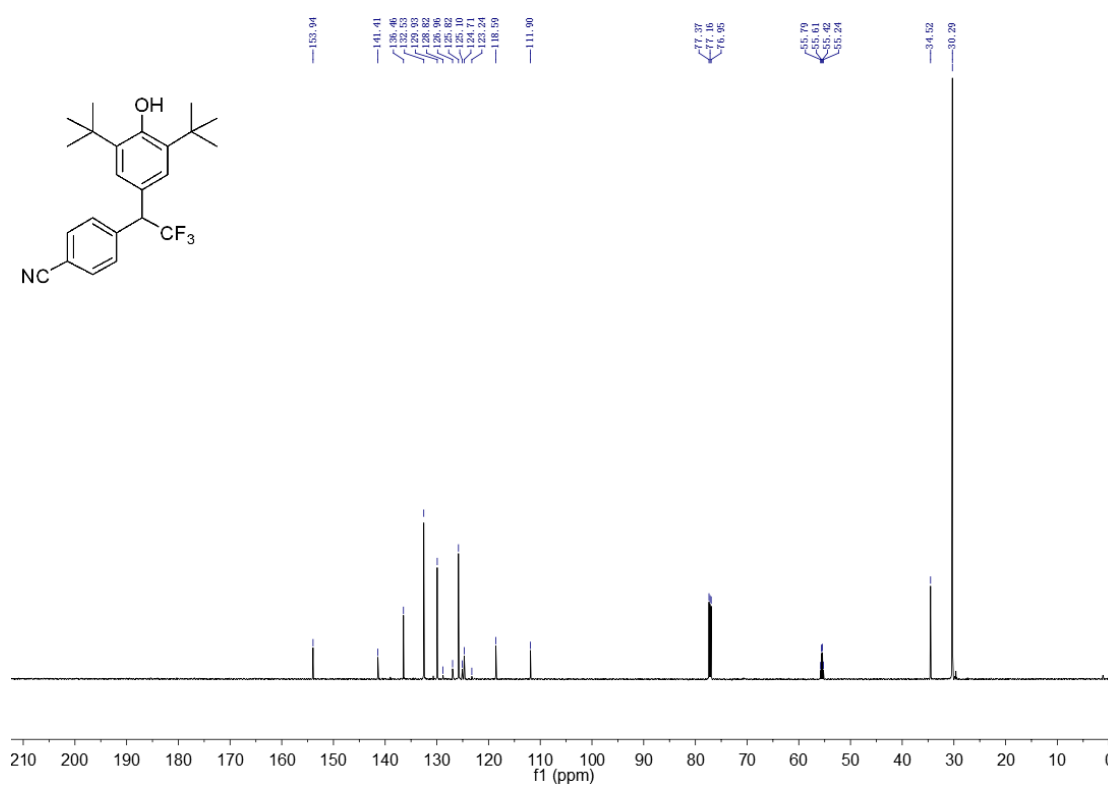
¹⁹F NMR of **2j**



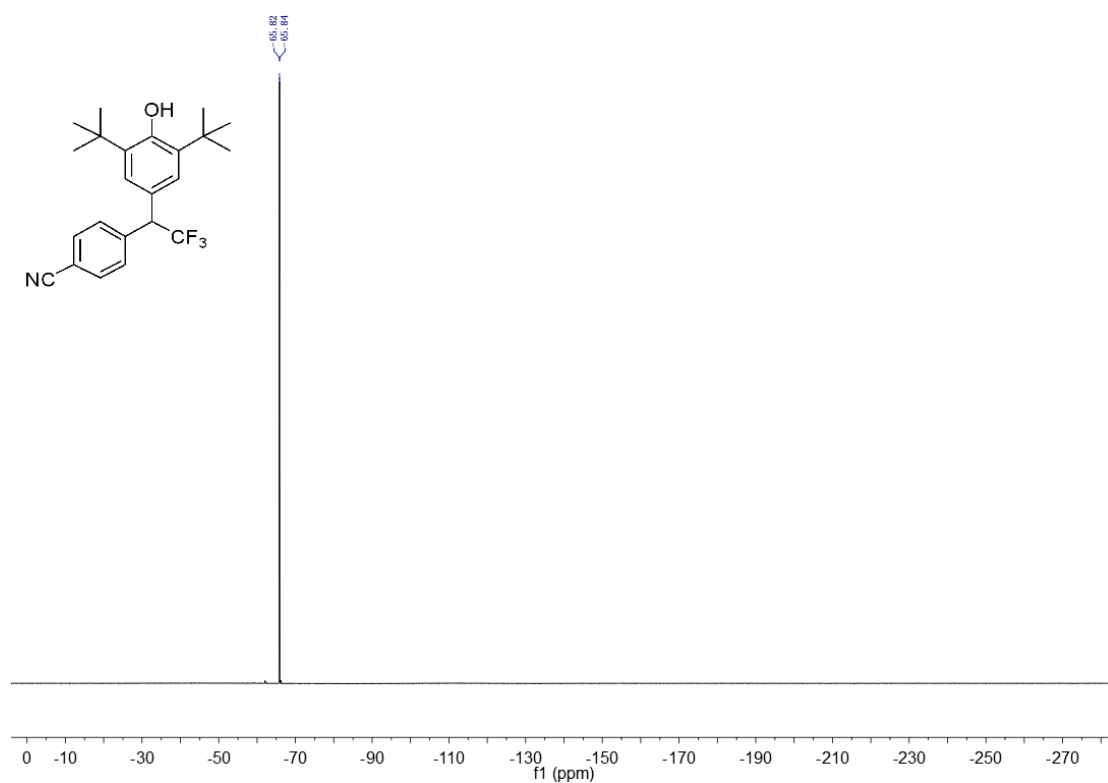
¹H NMR of **2k**



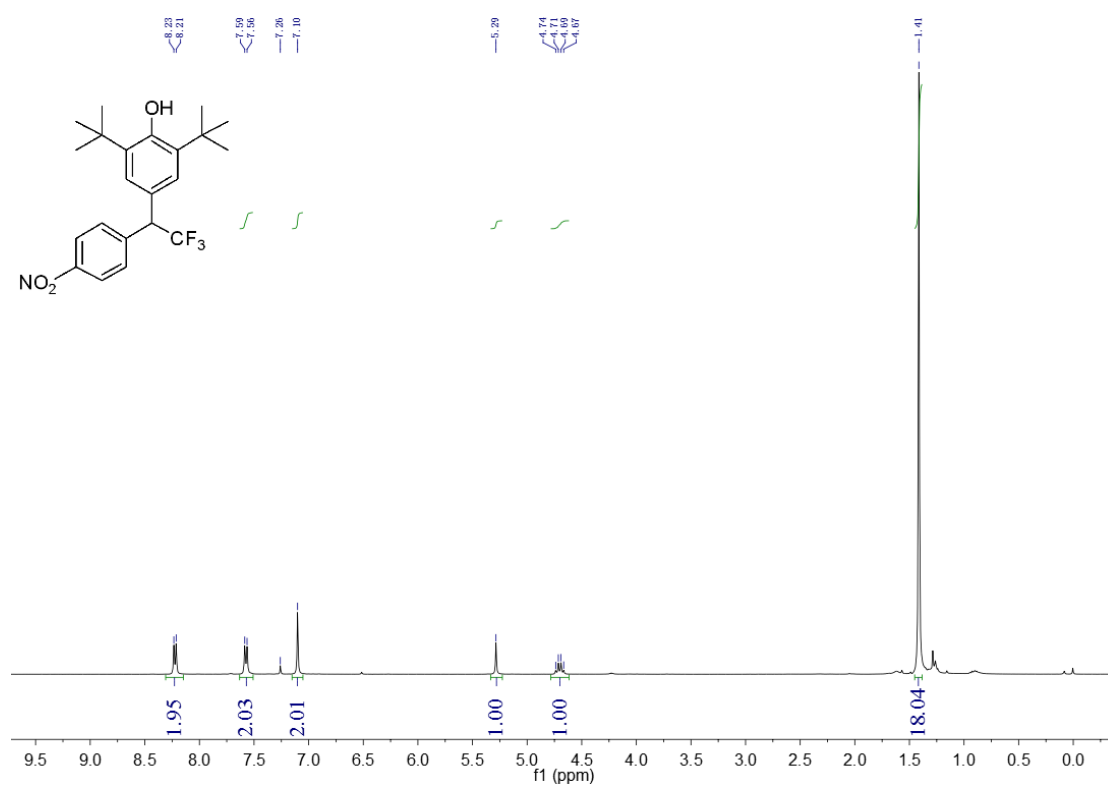
¹³C NMR of **2k**



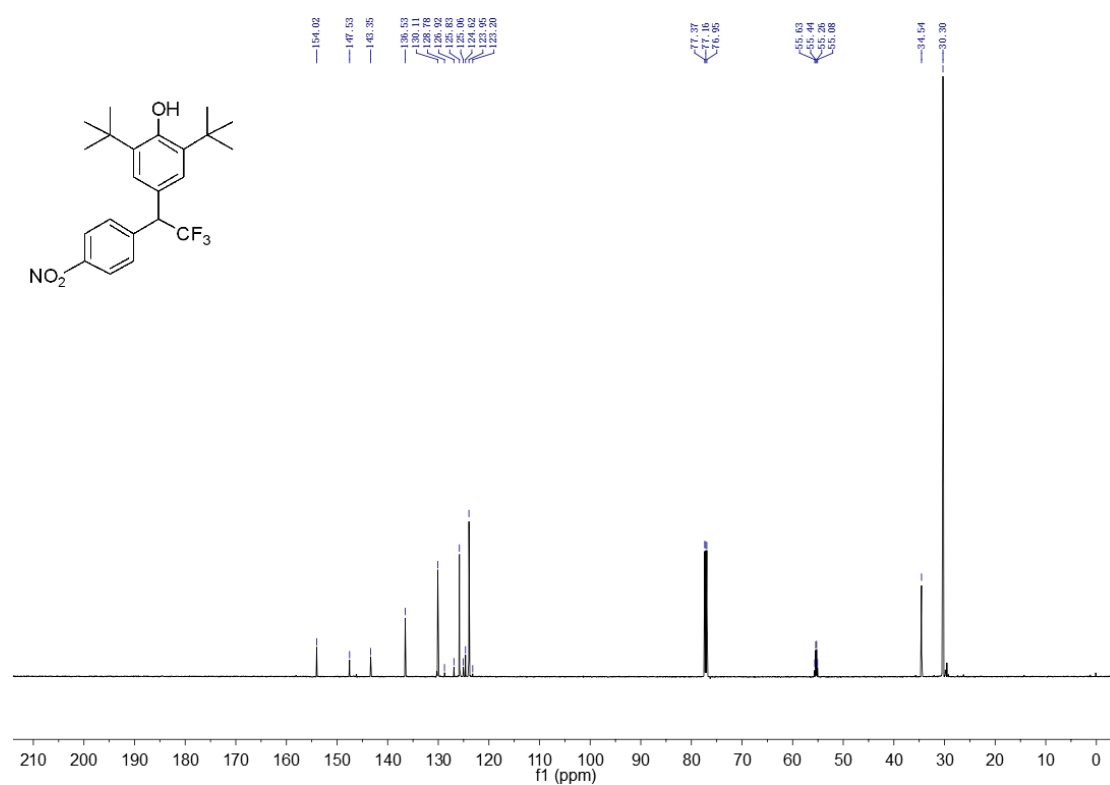
¹⁹F NMR of **2k**



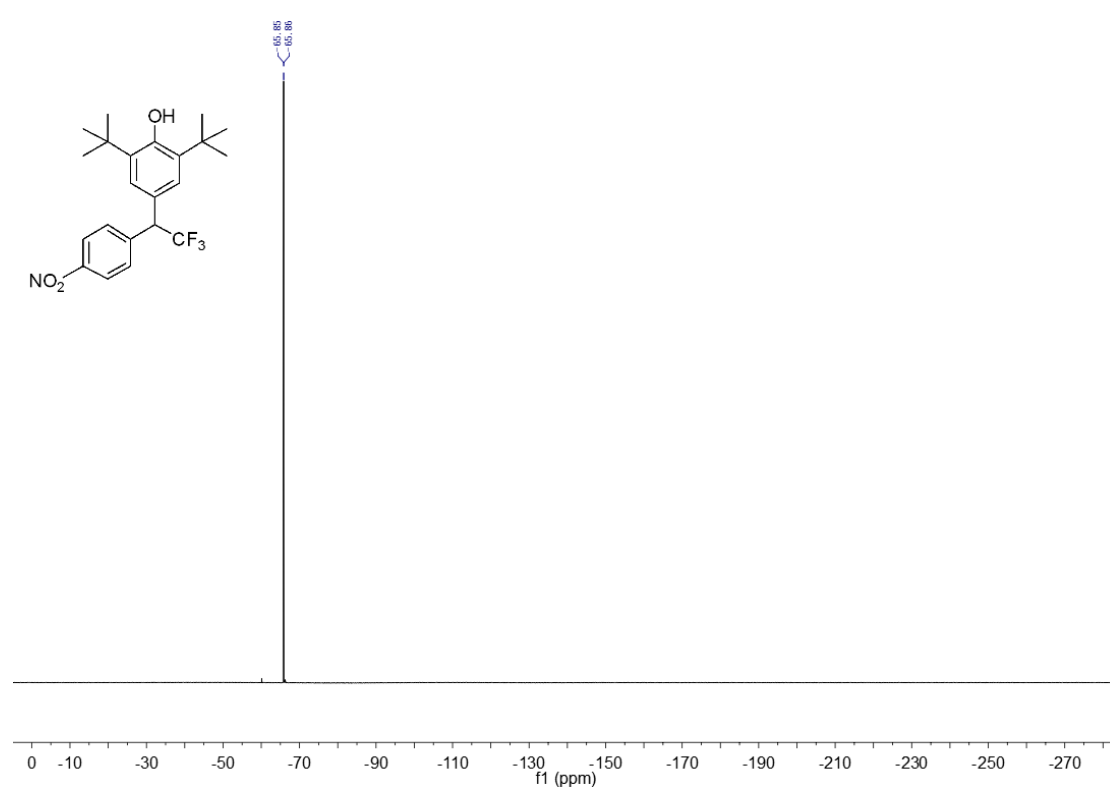
¹H NMR of **2l**



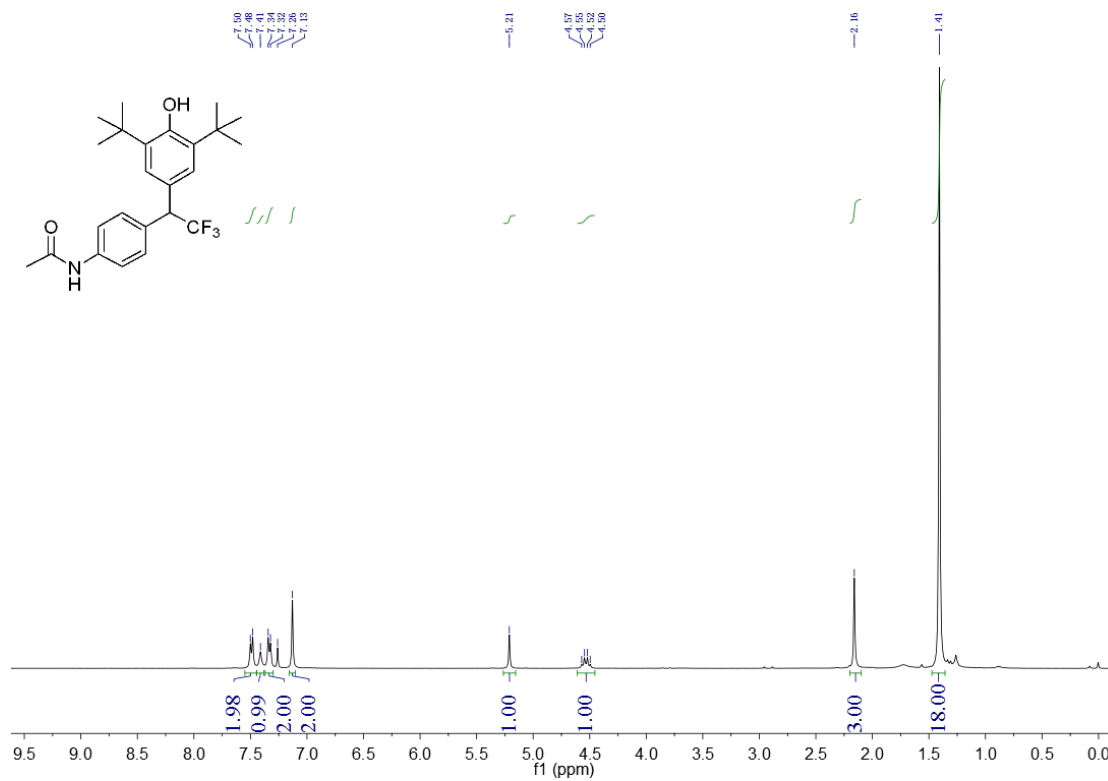
¹³C NMR of **2l**



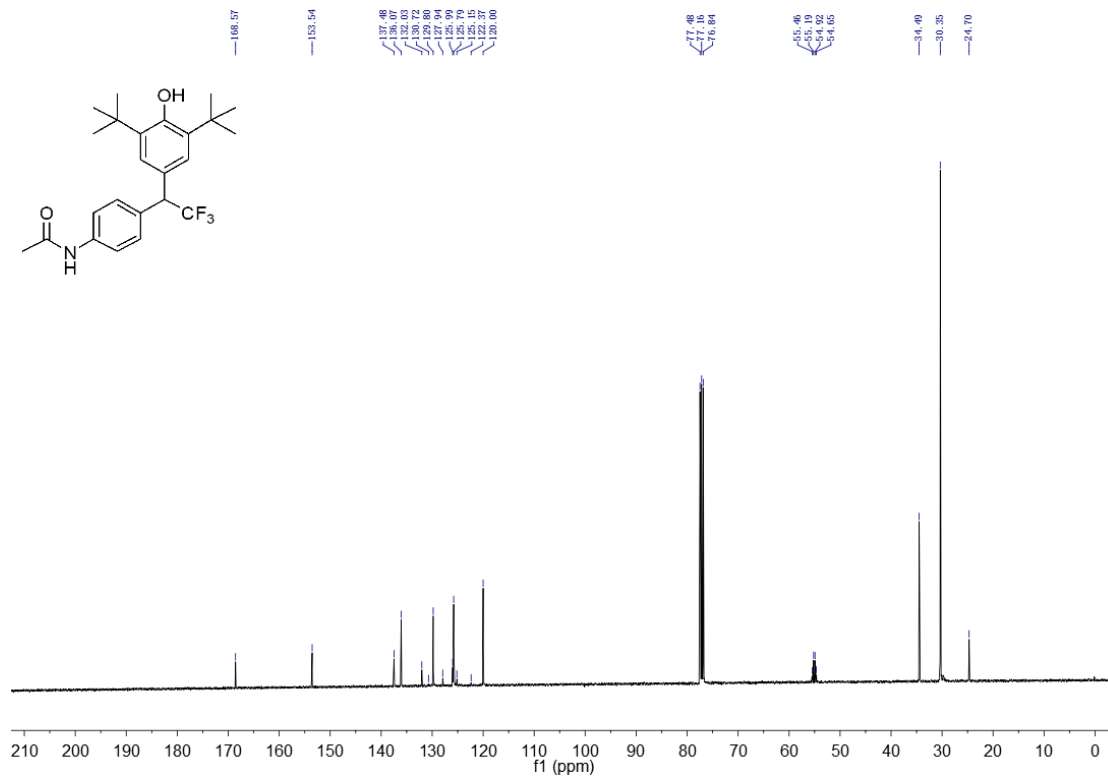
¹⁹F NMR of **2l**



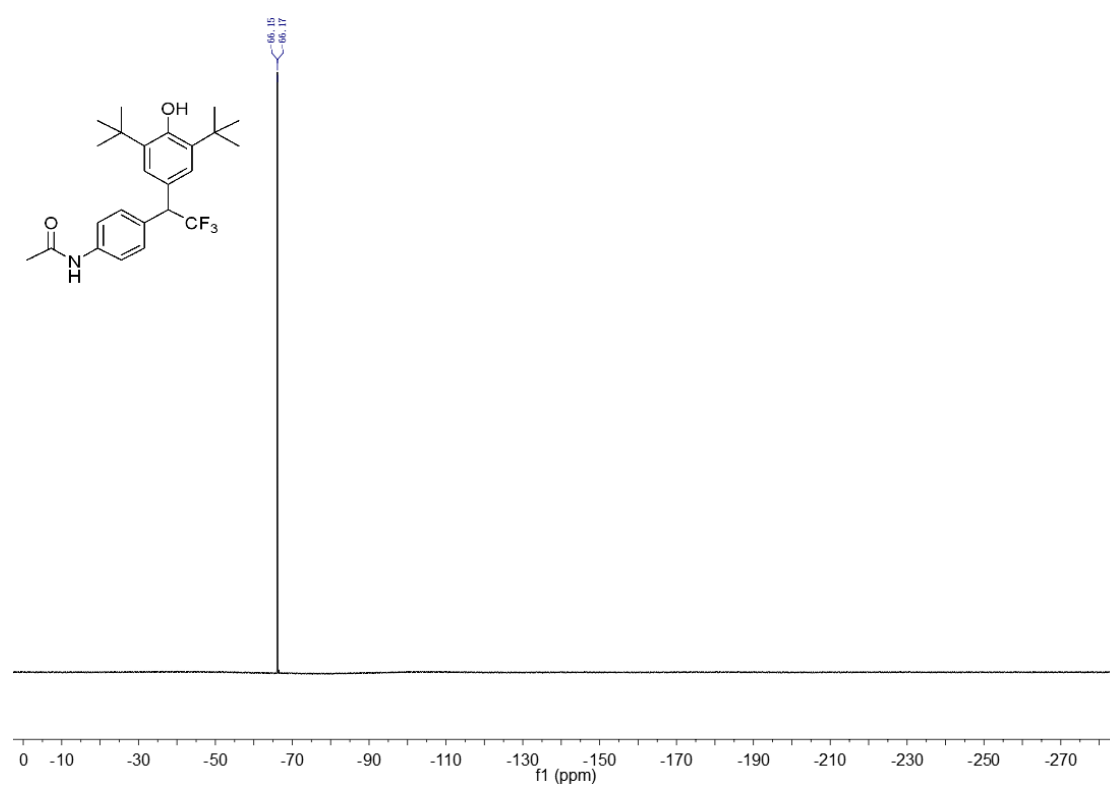
¹H NMR of **2m**



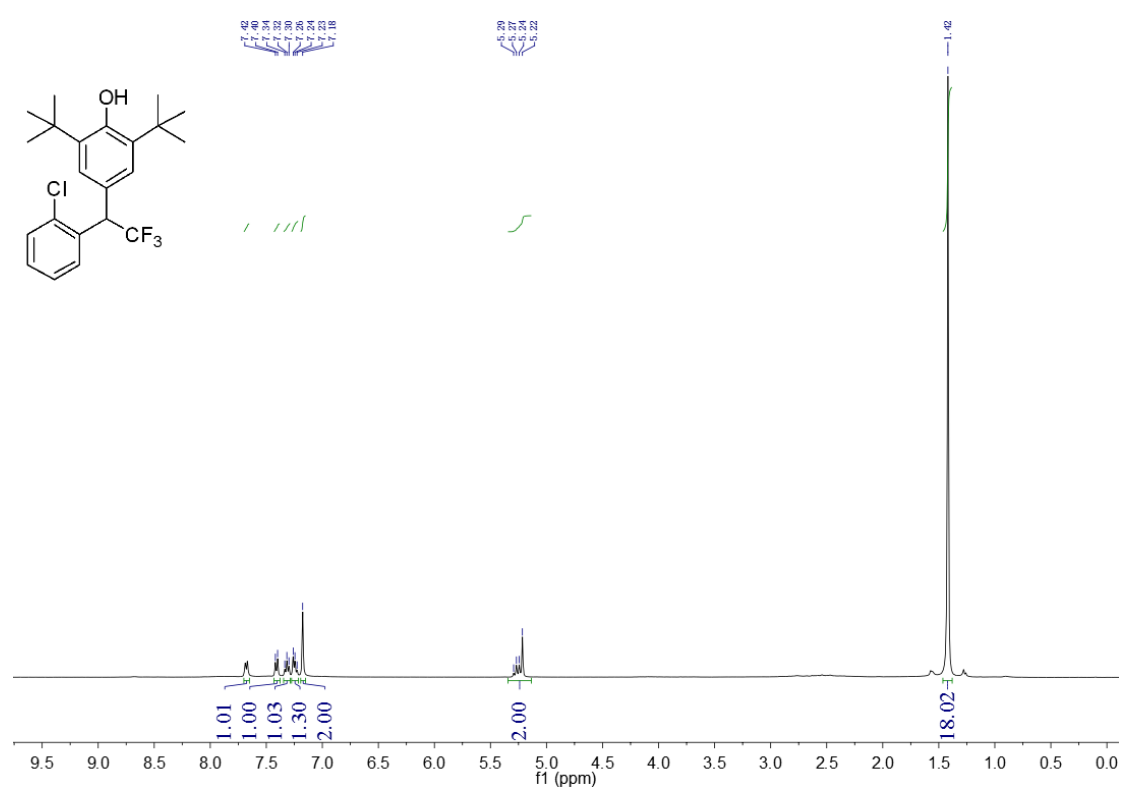
¹³C NMR of **2m**



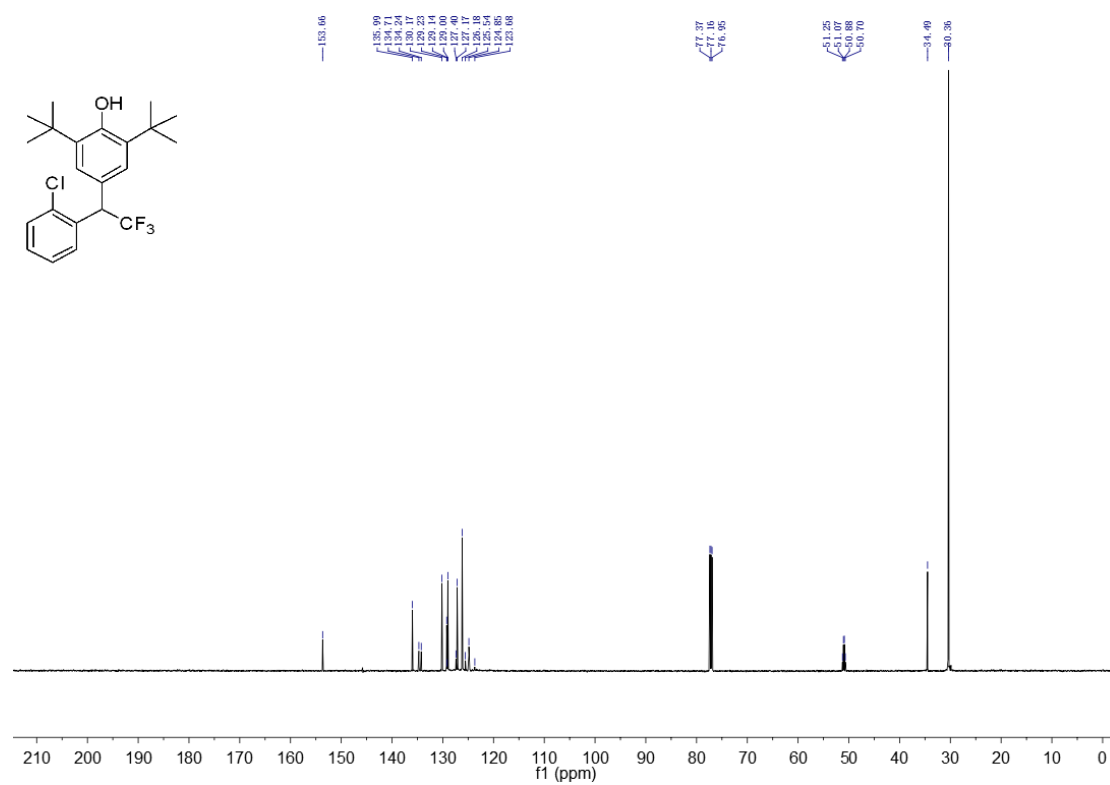
¹⁹F NMR of **2m**



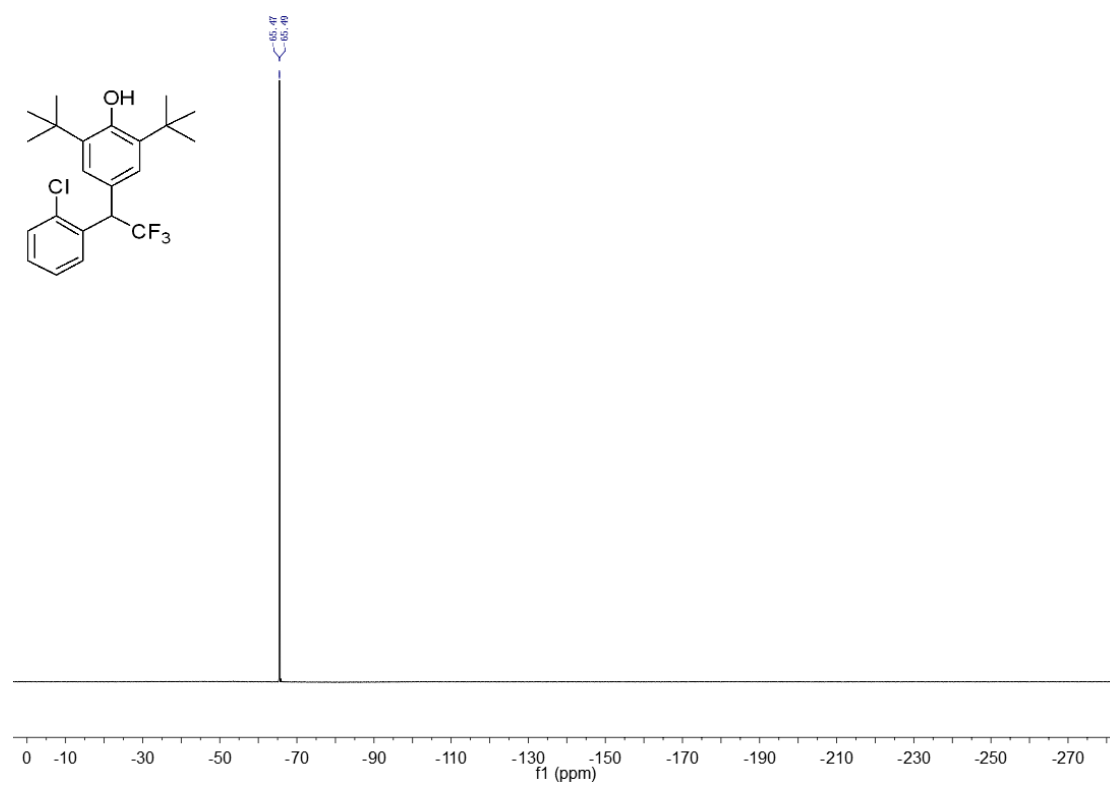
¹H NMR of **2n**



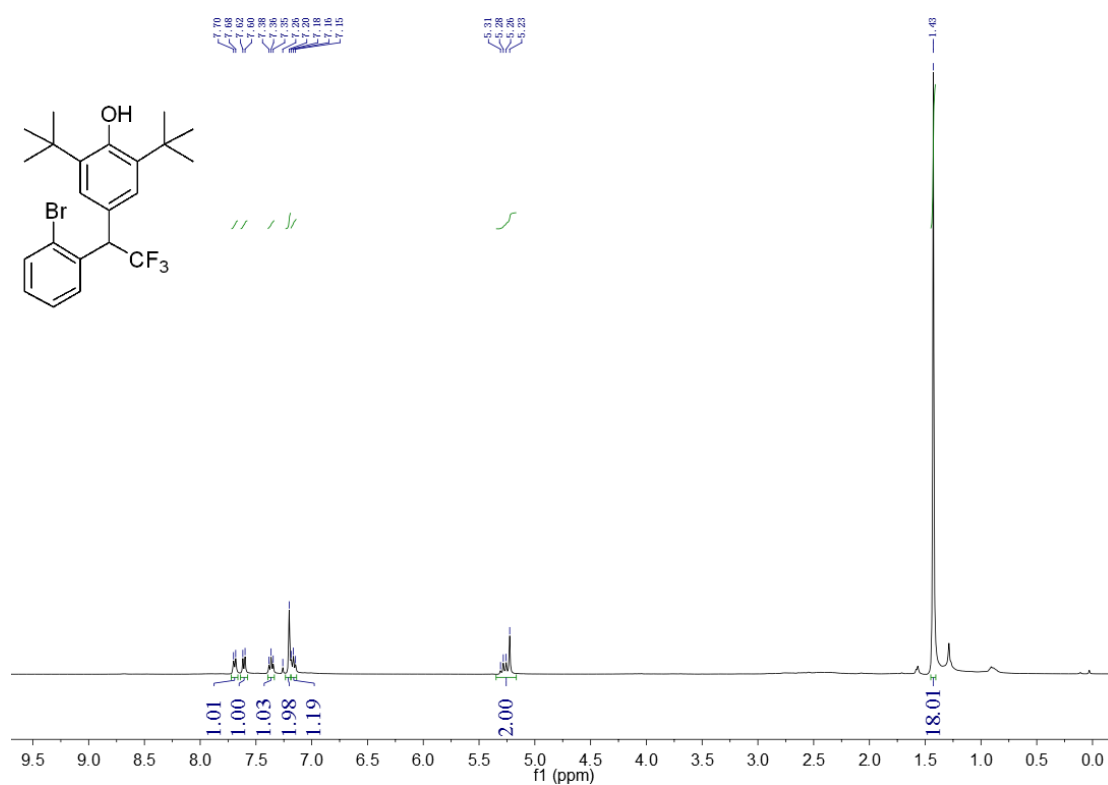
¹³C NMR of **2n**



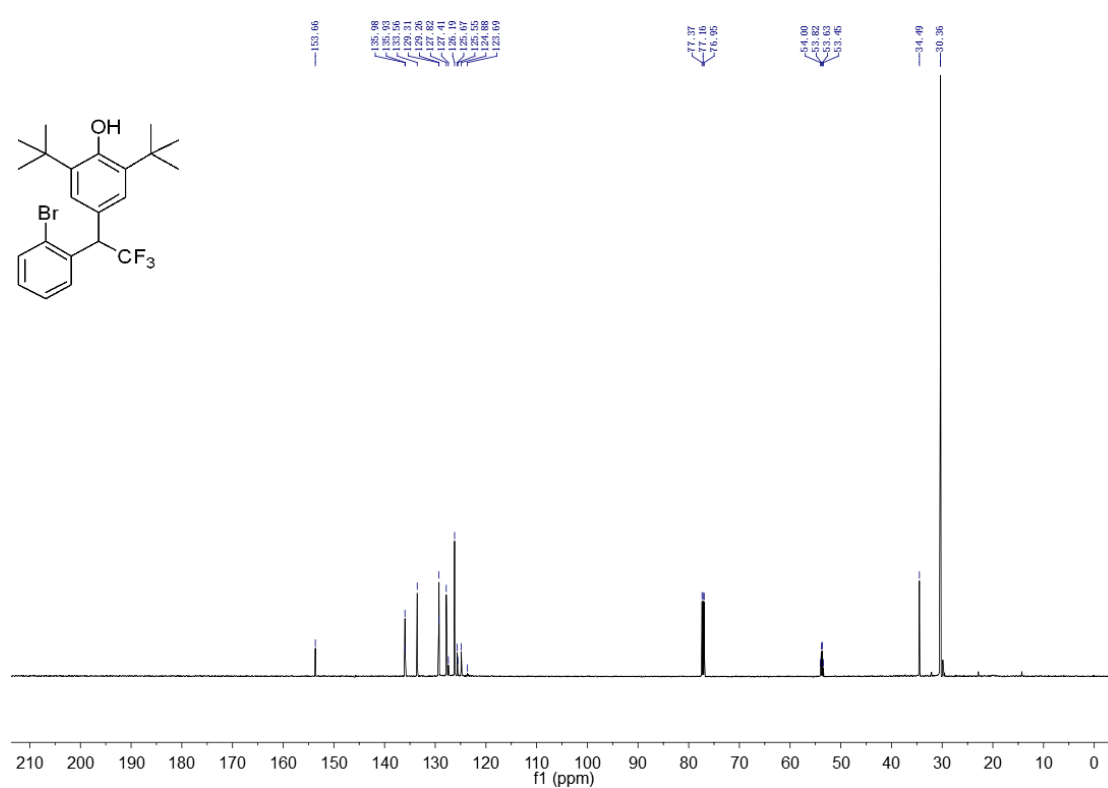
¹⁹F NMR of **2n**



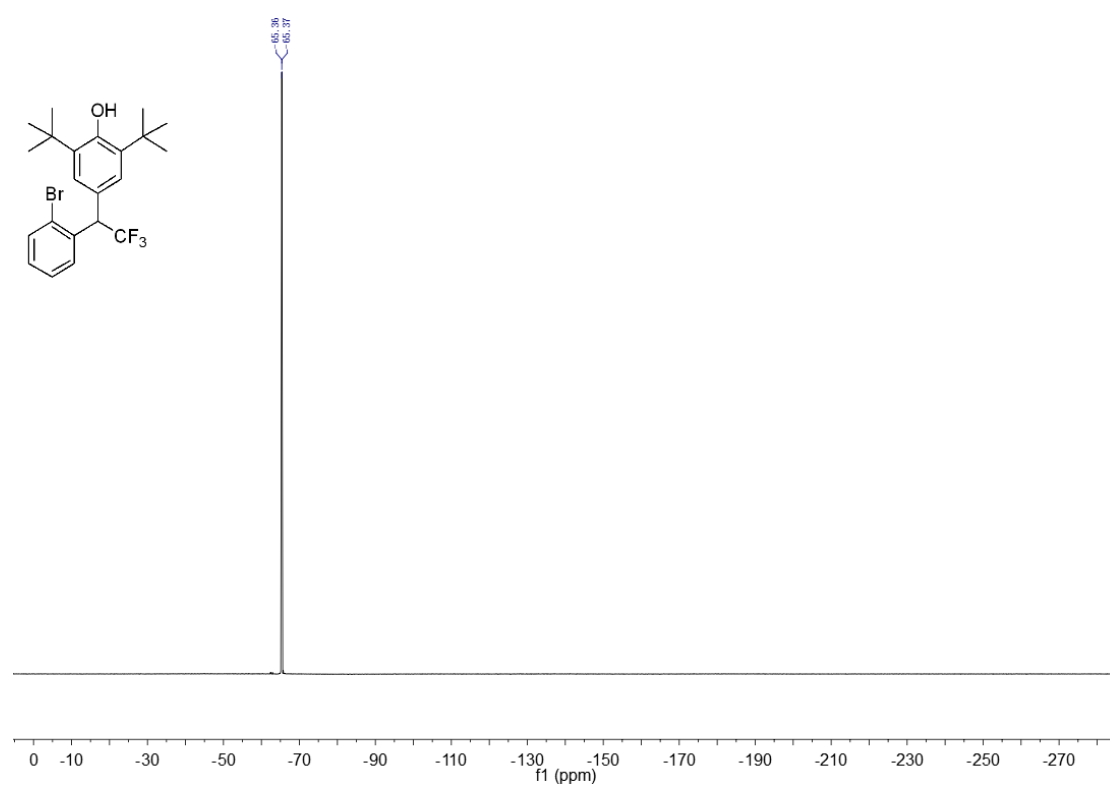
¹H NMR of **2o**



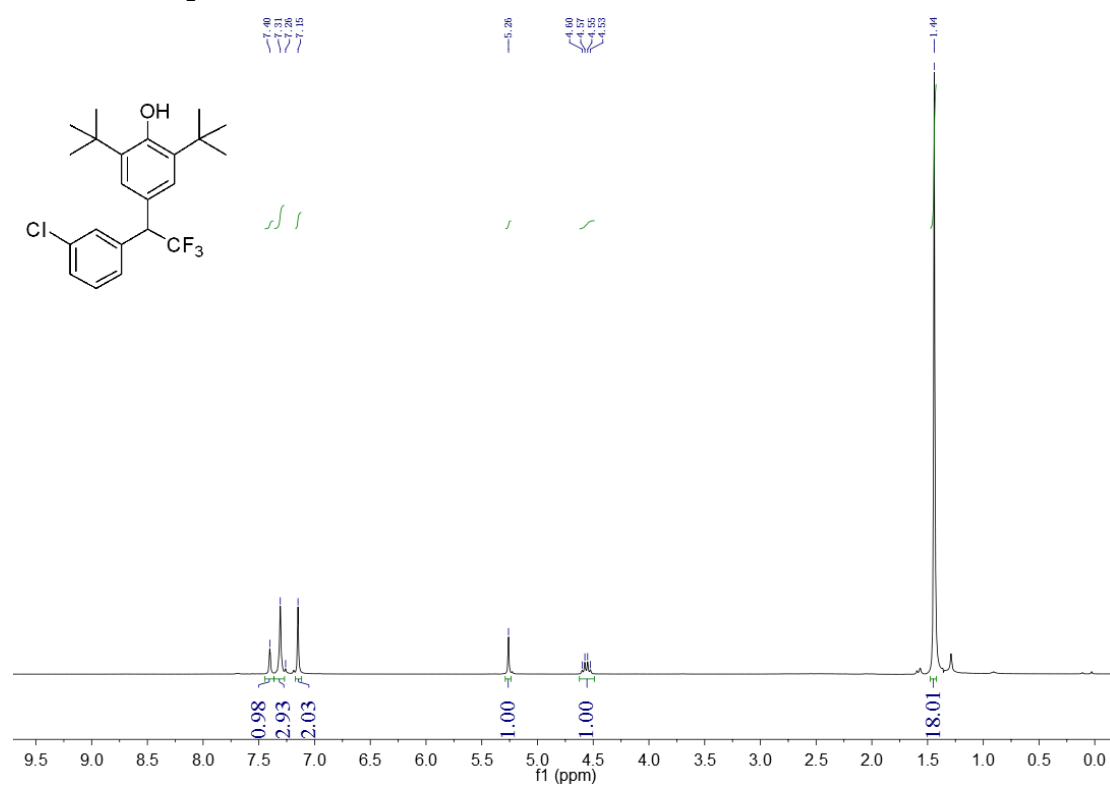
¹³C NMR of **2o**



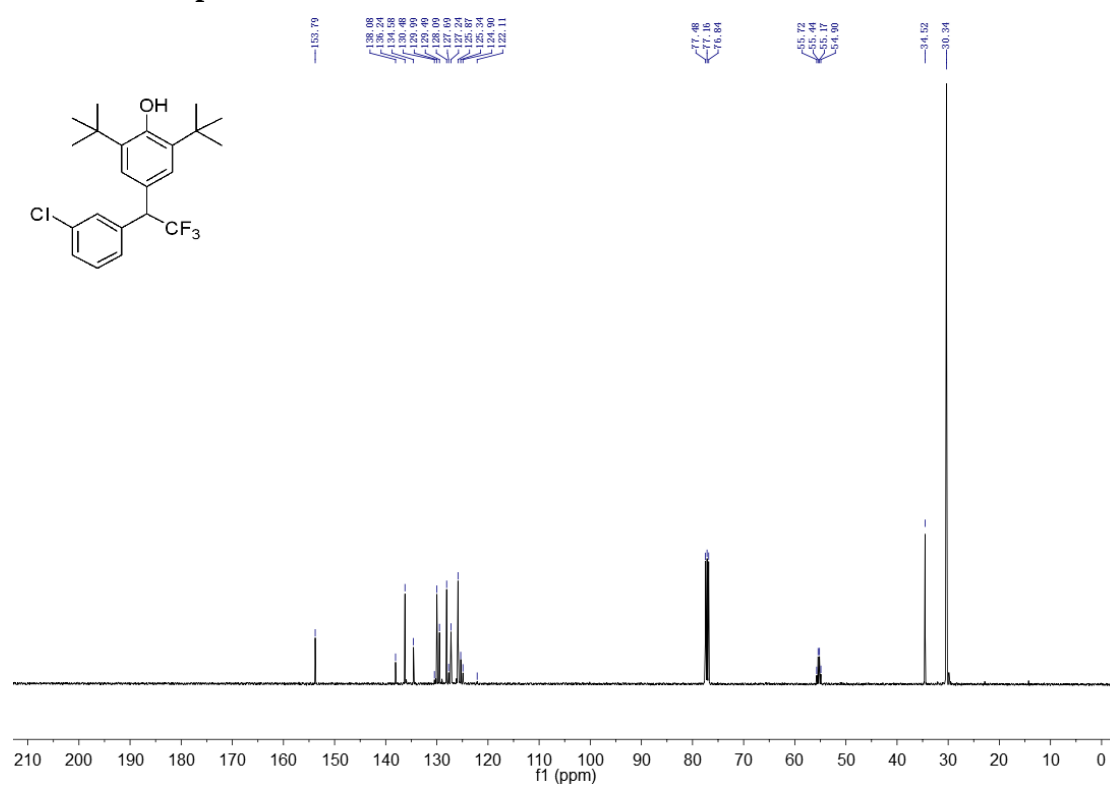
¹⁹F NMR of **2o**



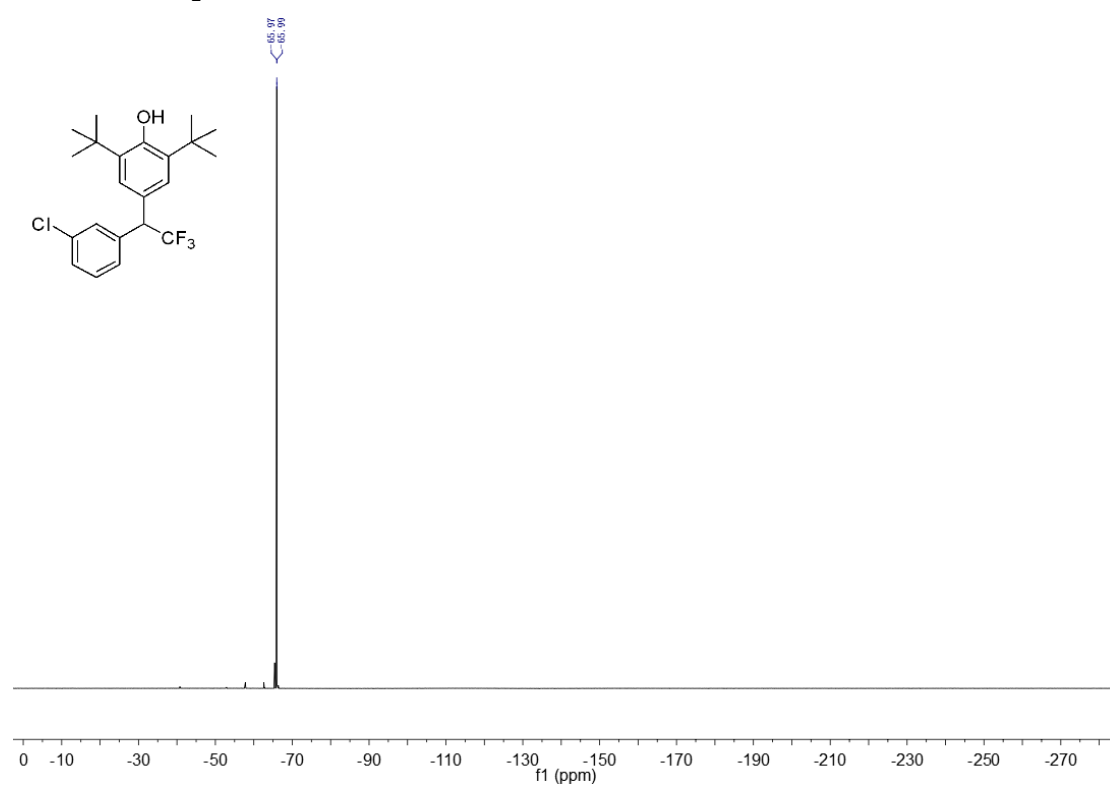
¹H NMR of **2p**



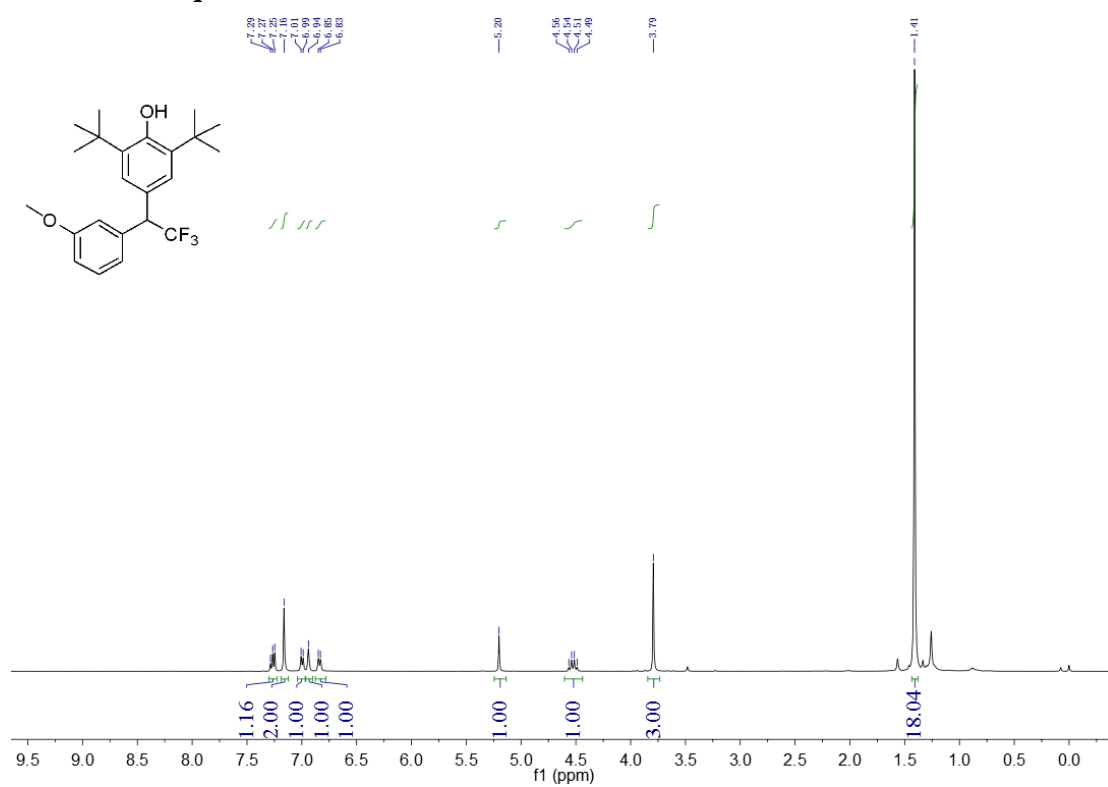
¹³C NMR of **2p**



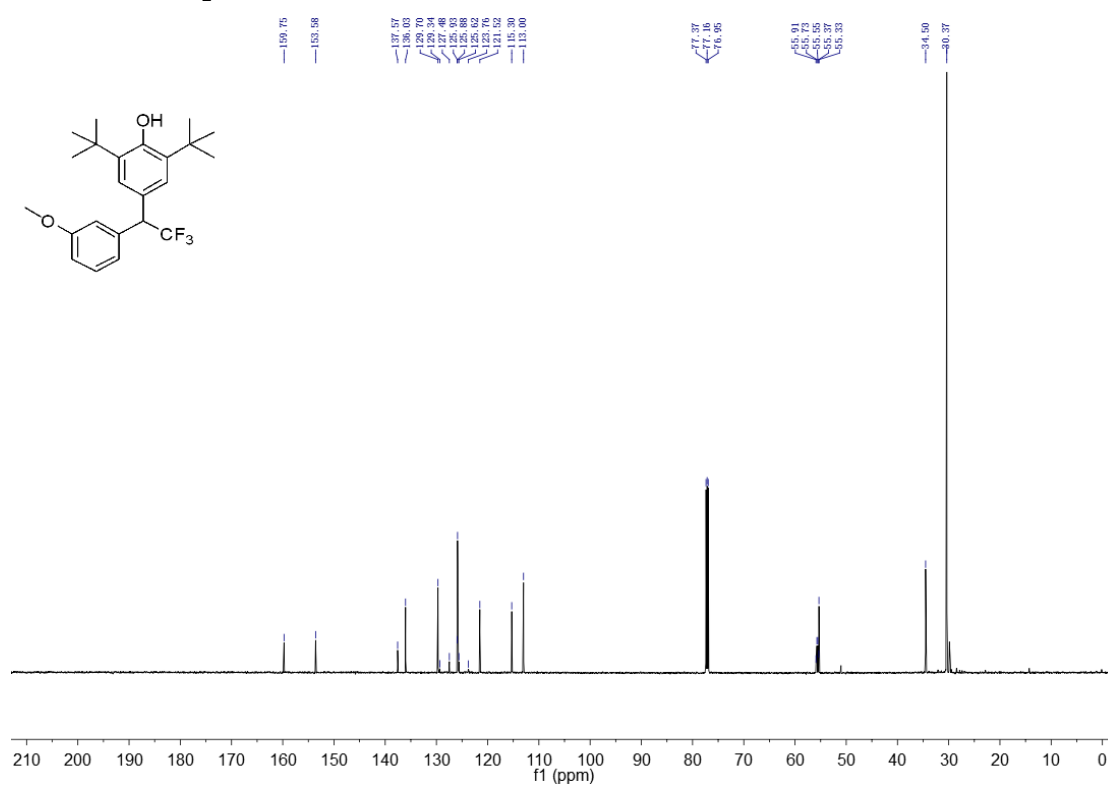
¹⁹F NMR of **2p**



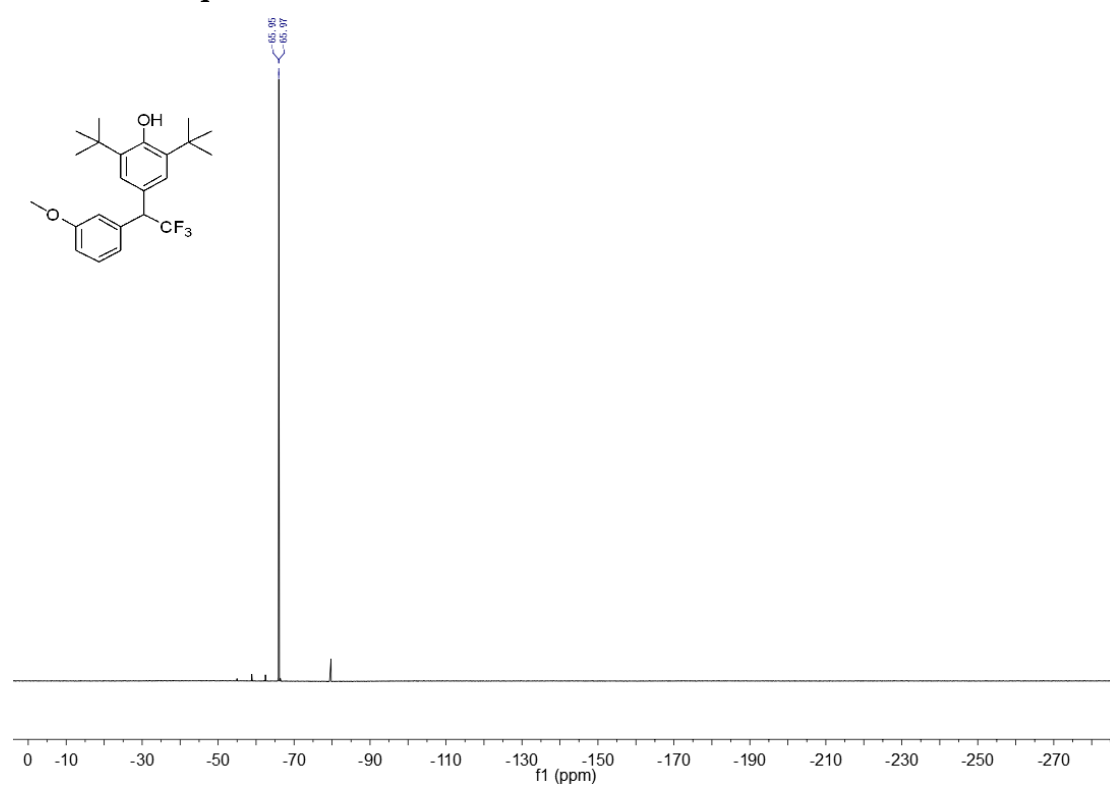
¹H NMR of **2q**



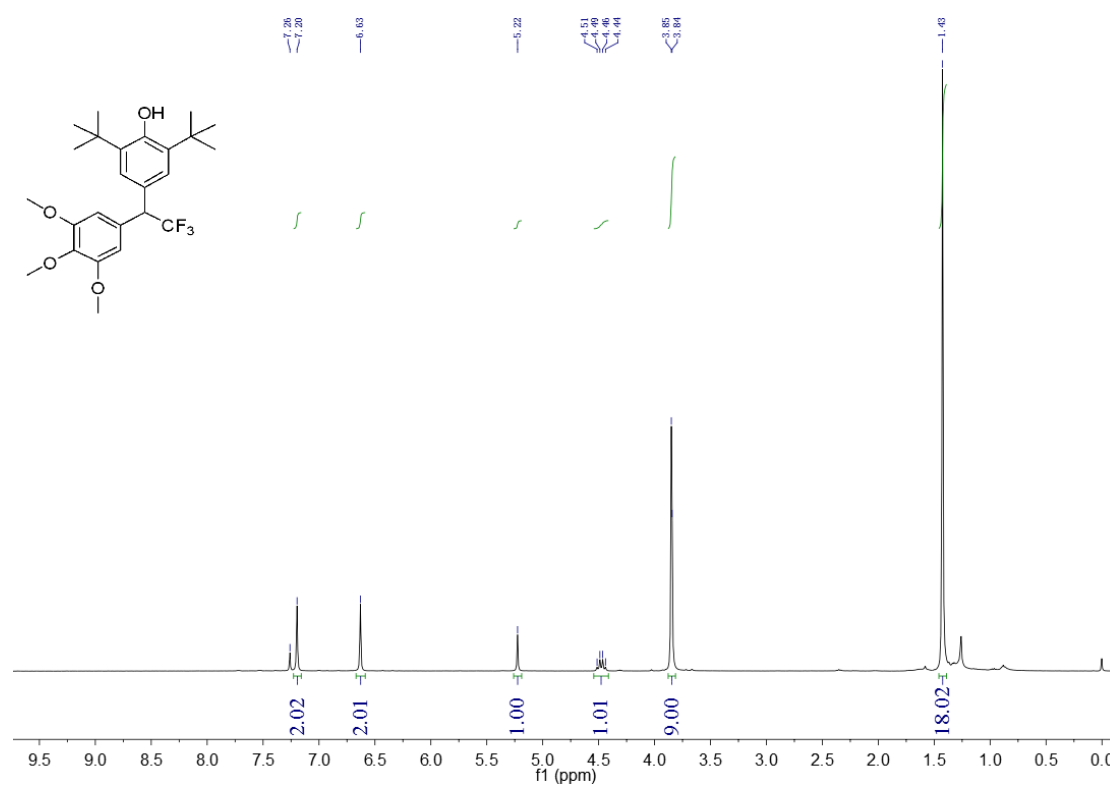
¹³C NMR of **2q**



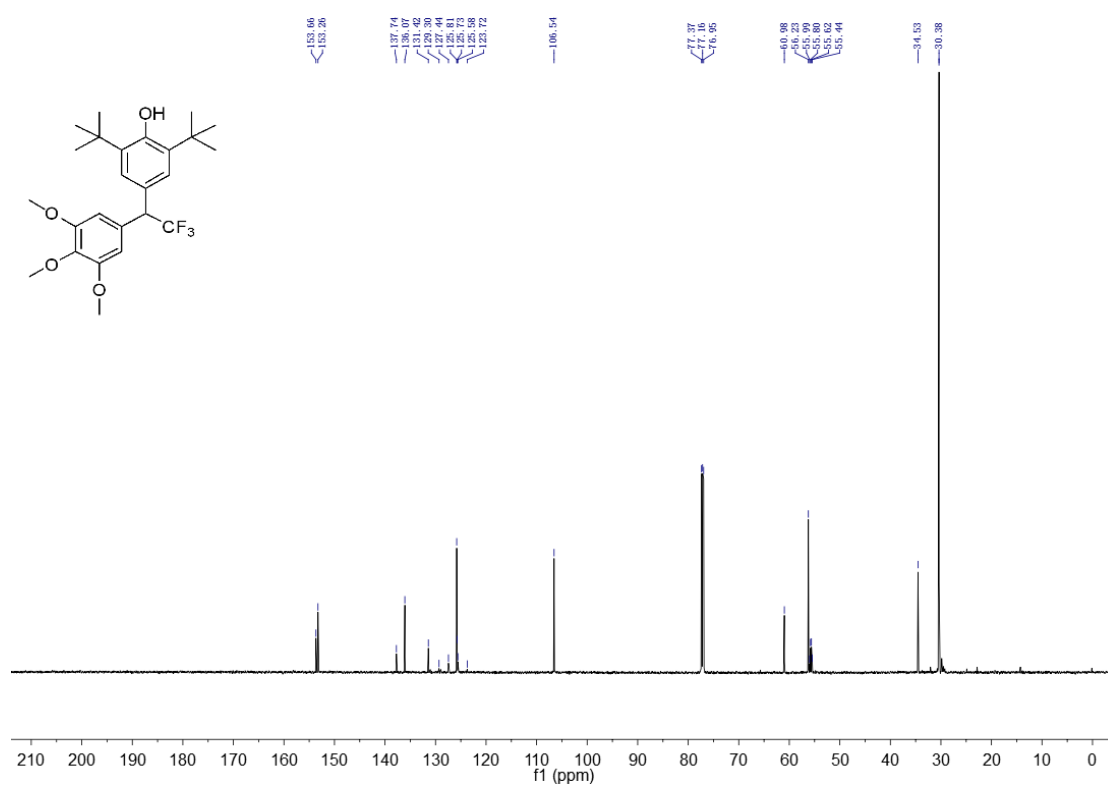
¹⁹F NMR of **2q**



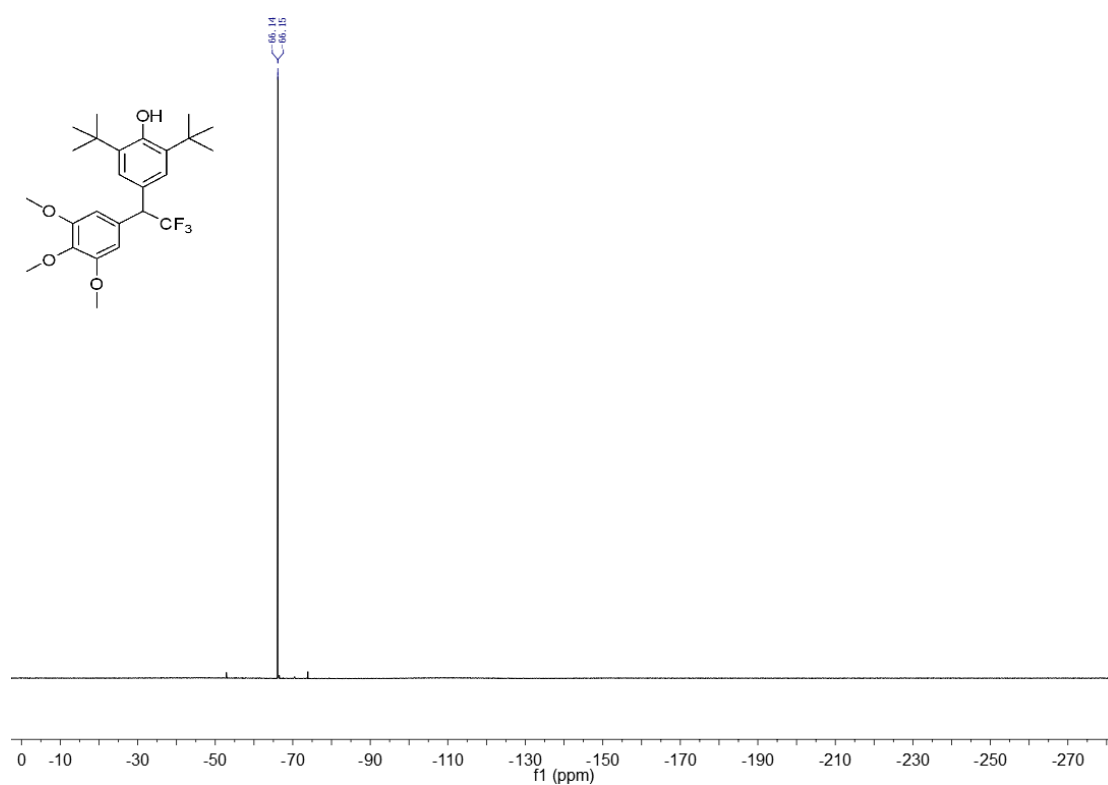
¹H NMR of **2r**



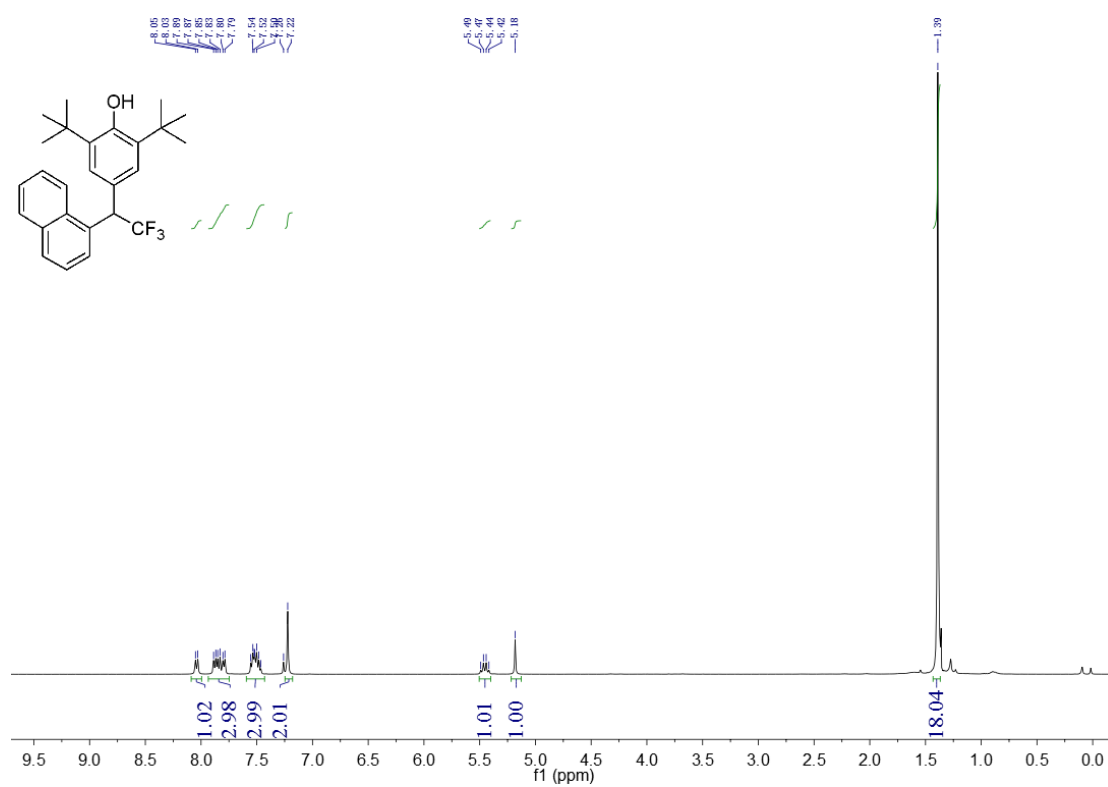
¹³C NMR of **2r**



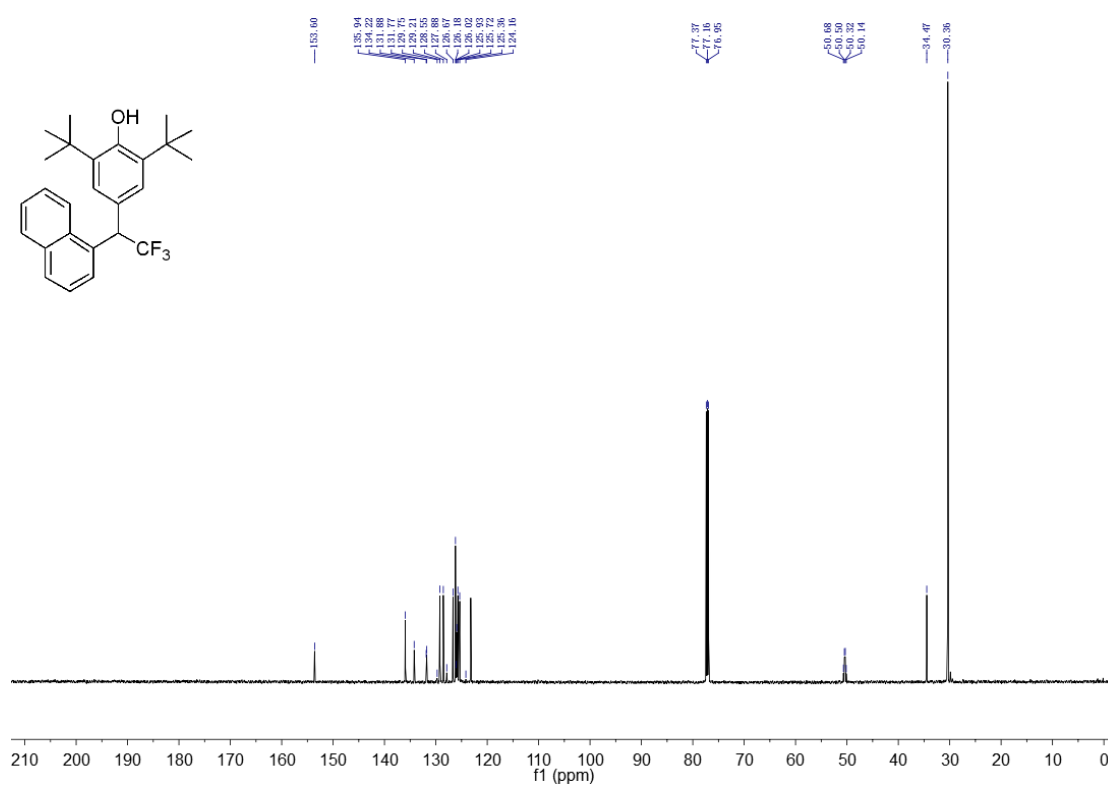
¹⁹F NMR of **2r**



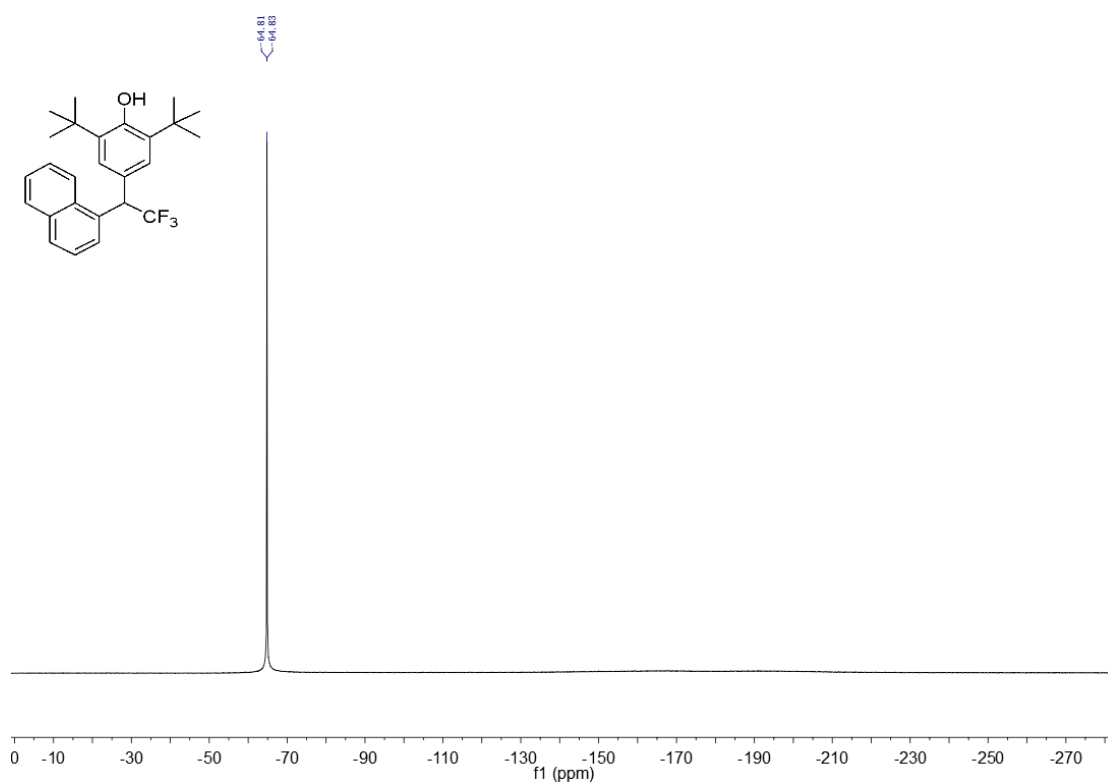
¹H NMR of 2s



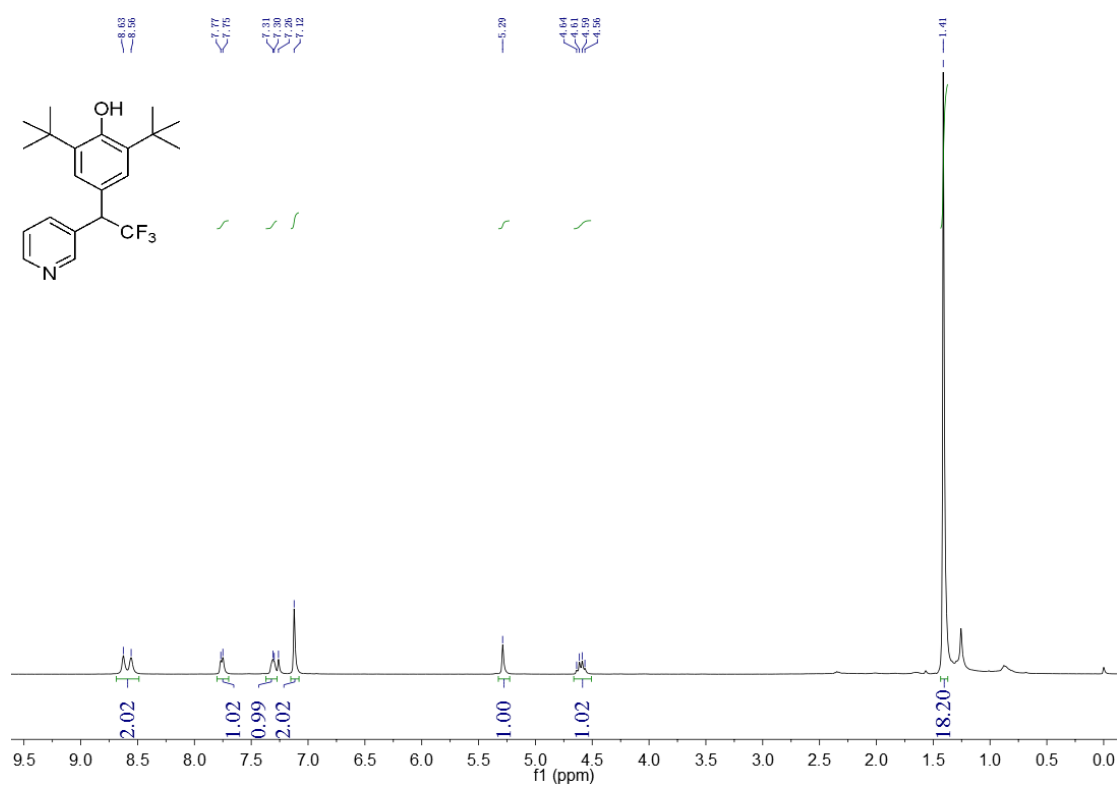
¹³C NMR of 2s



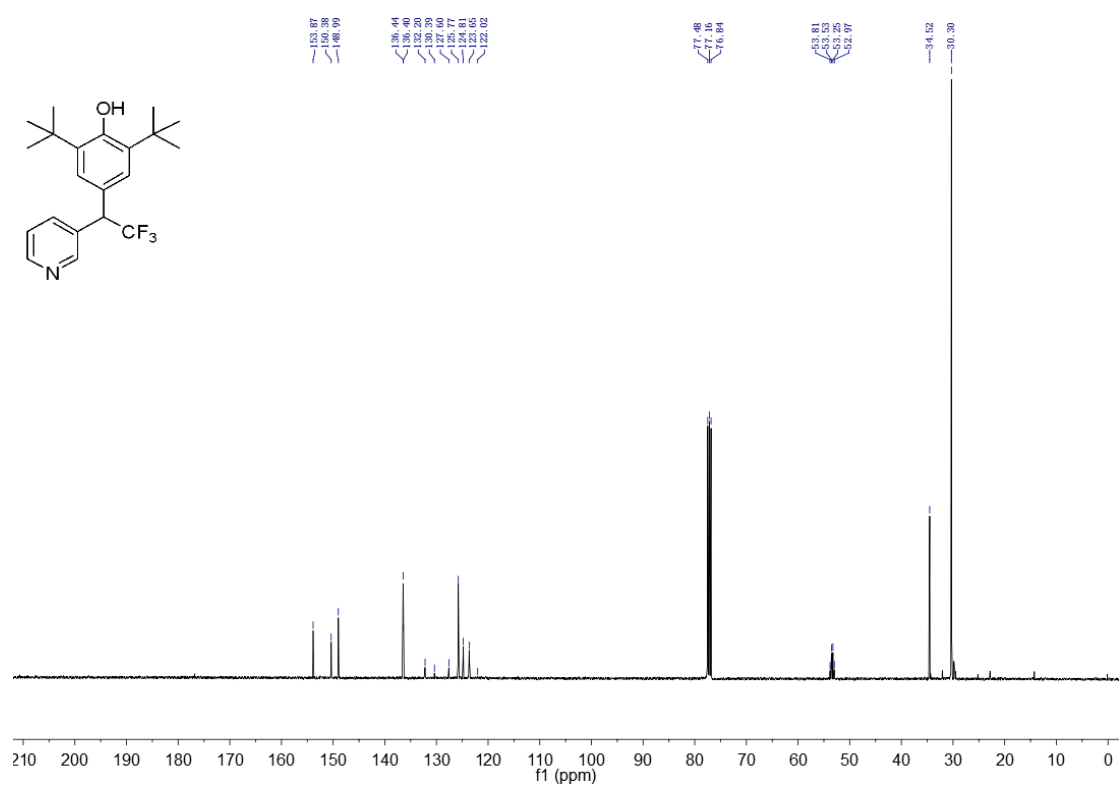
¹⁹F NMR of **2s**



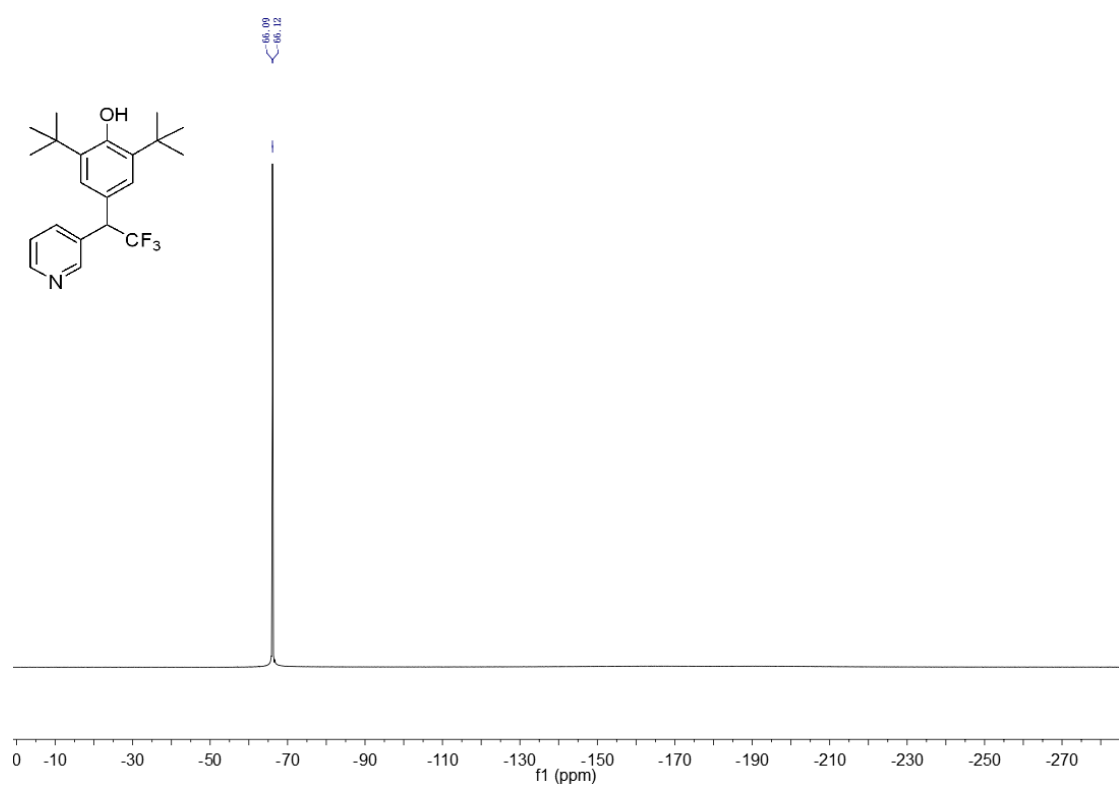
¹H NMR of **2t**



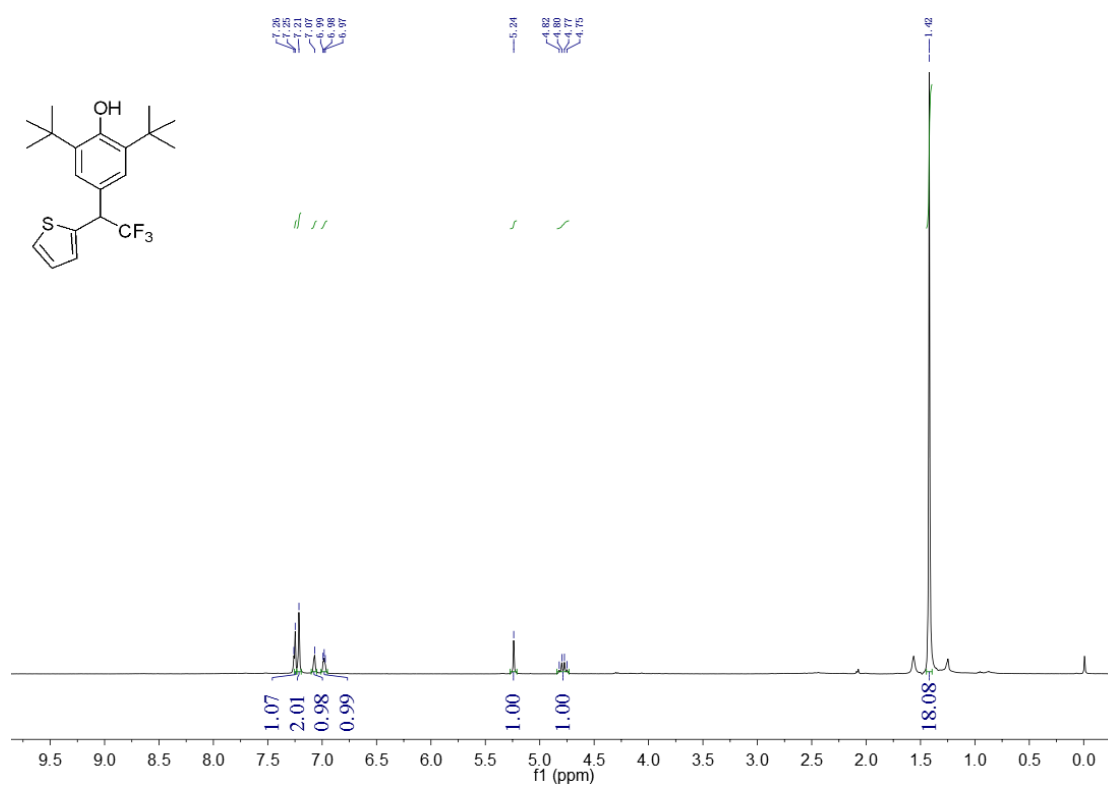
¹³C NMR of **2t**



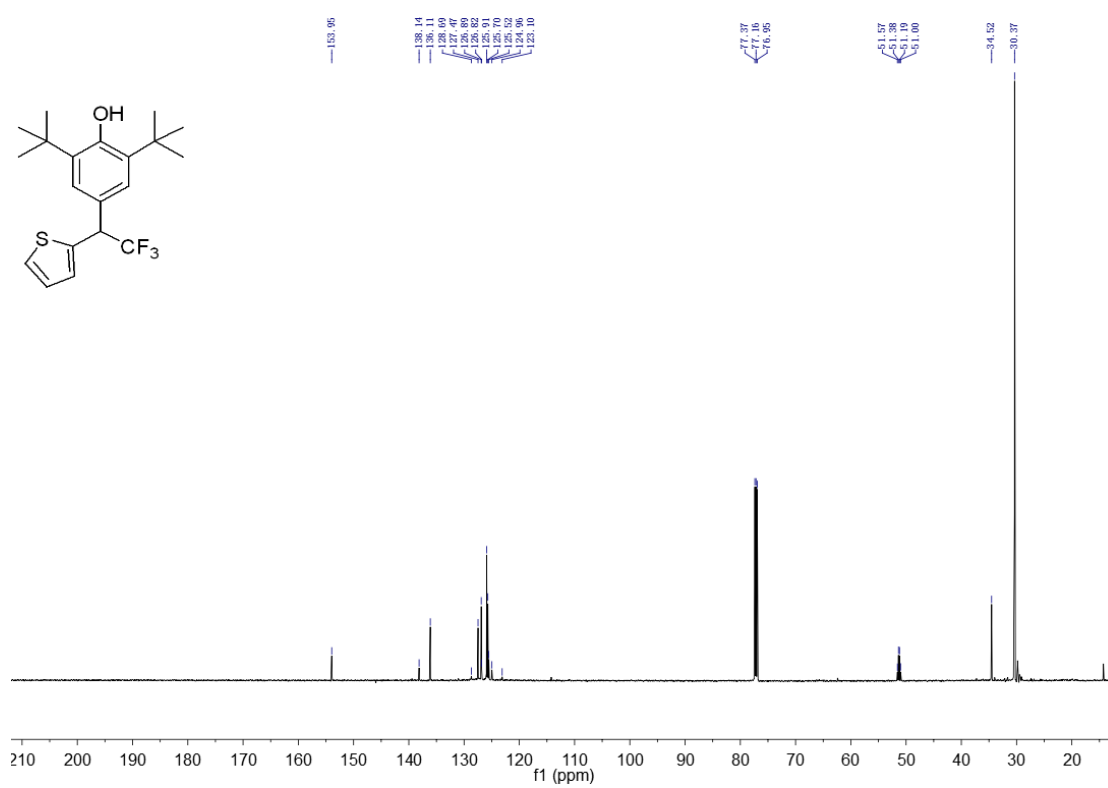
¹⁹F NMR of **2t**



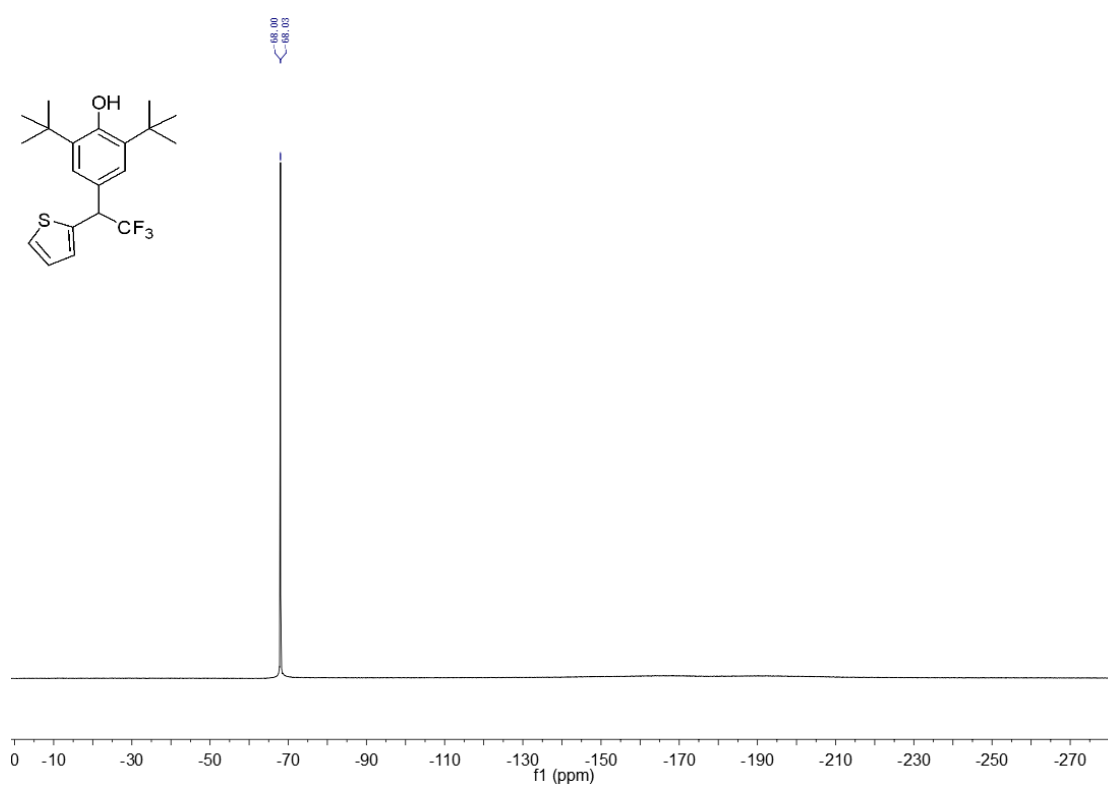
¹H NMR of **2u**



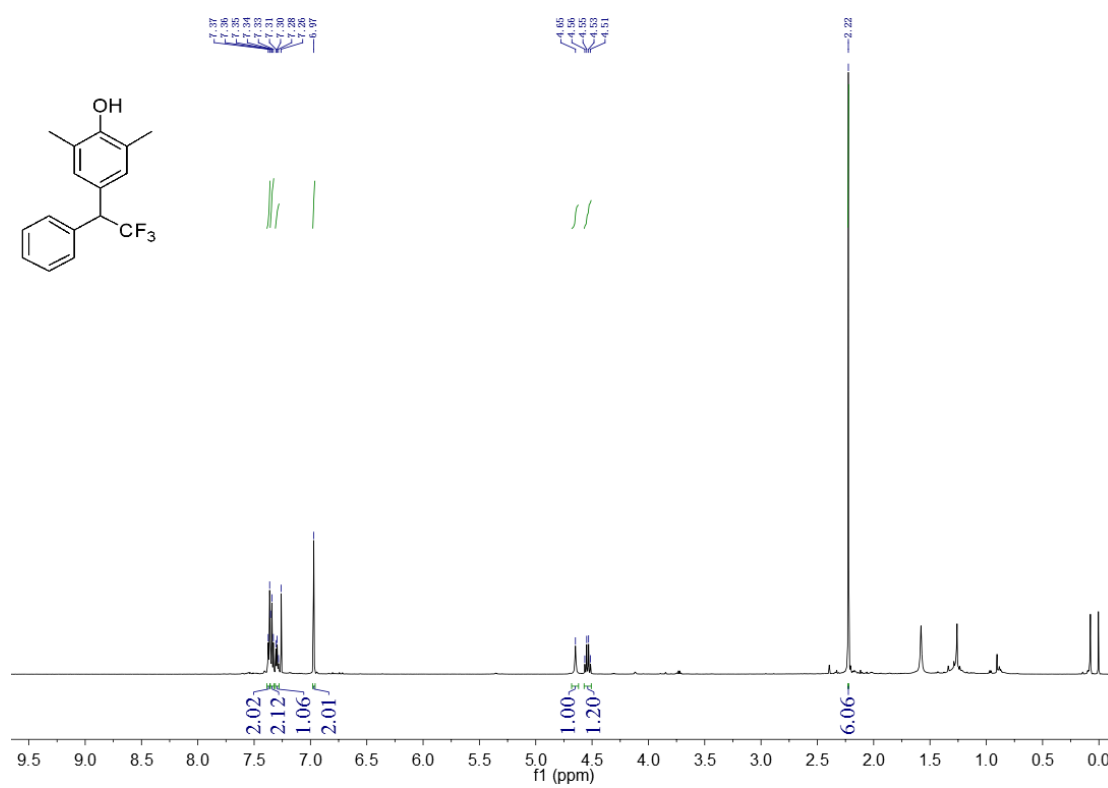
¹³C NMR of **2u**



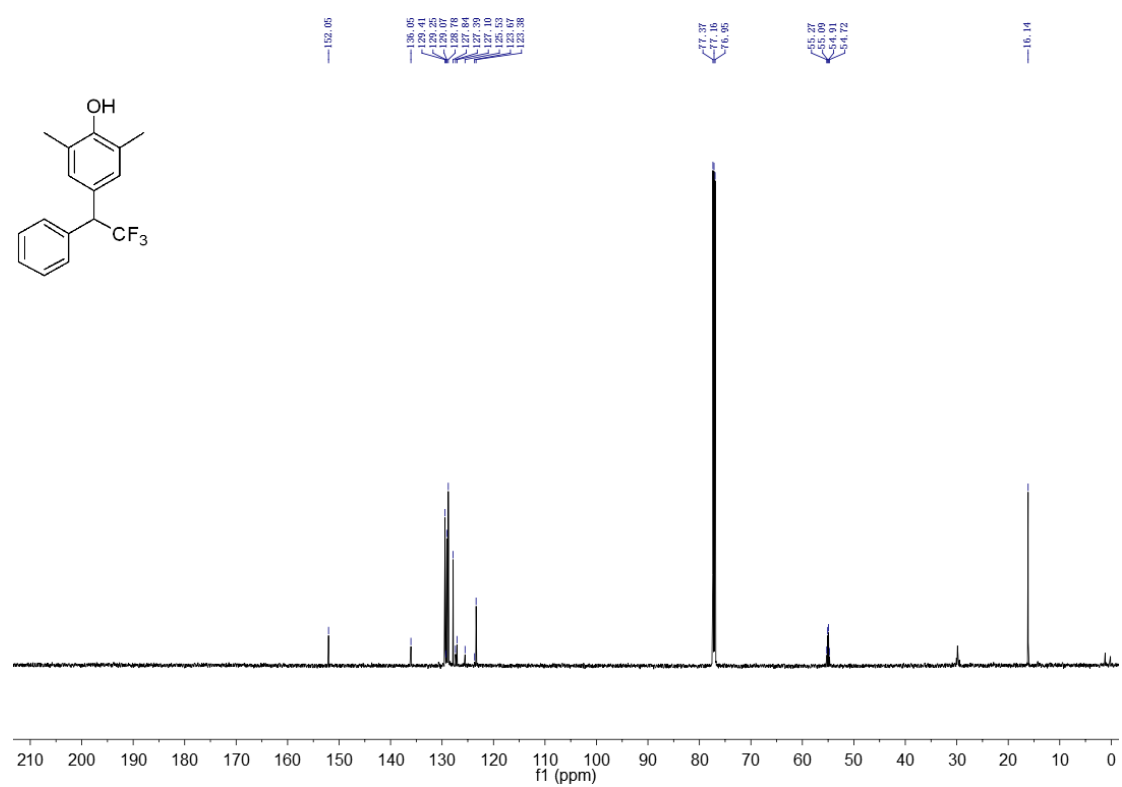
¹⁹F NMR of **2u**



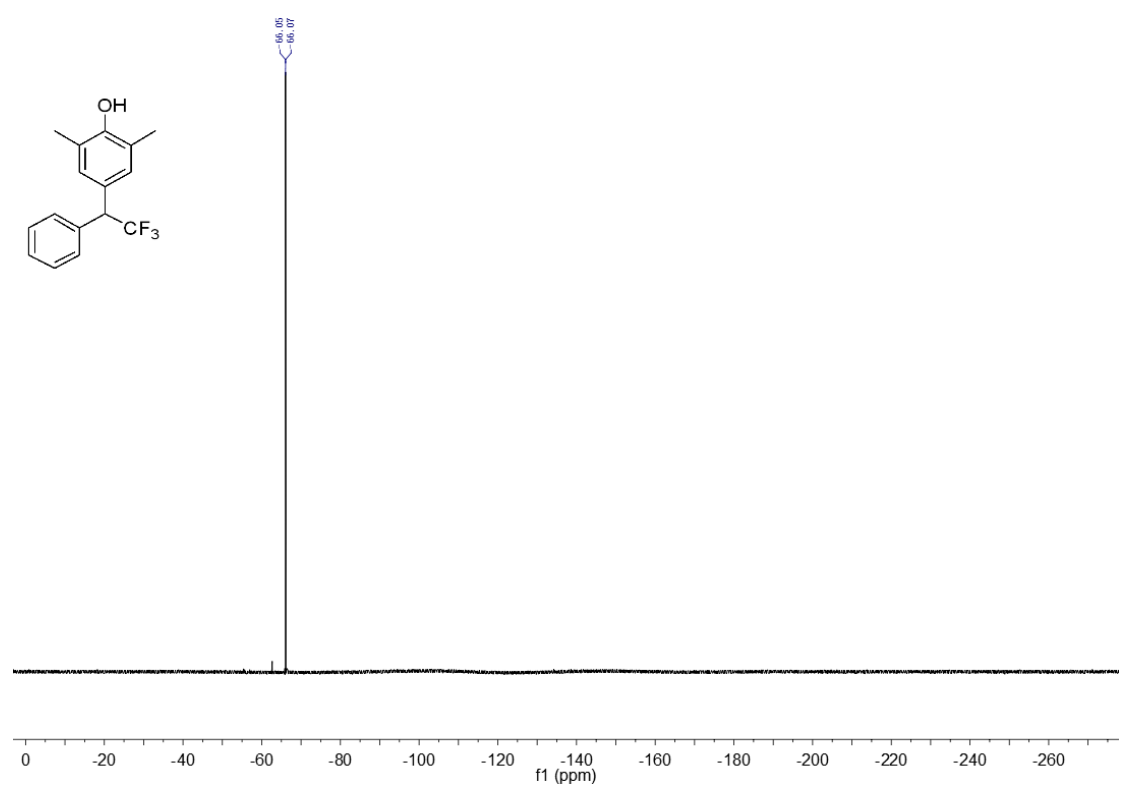
¹H NMR of **2v**



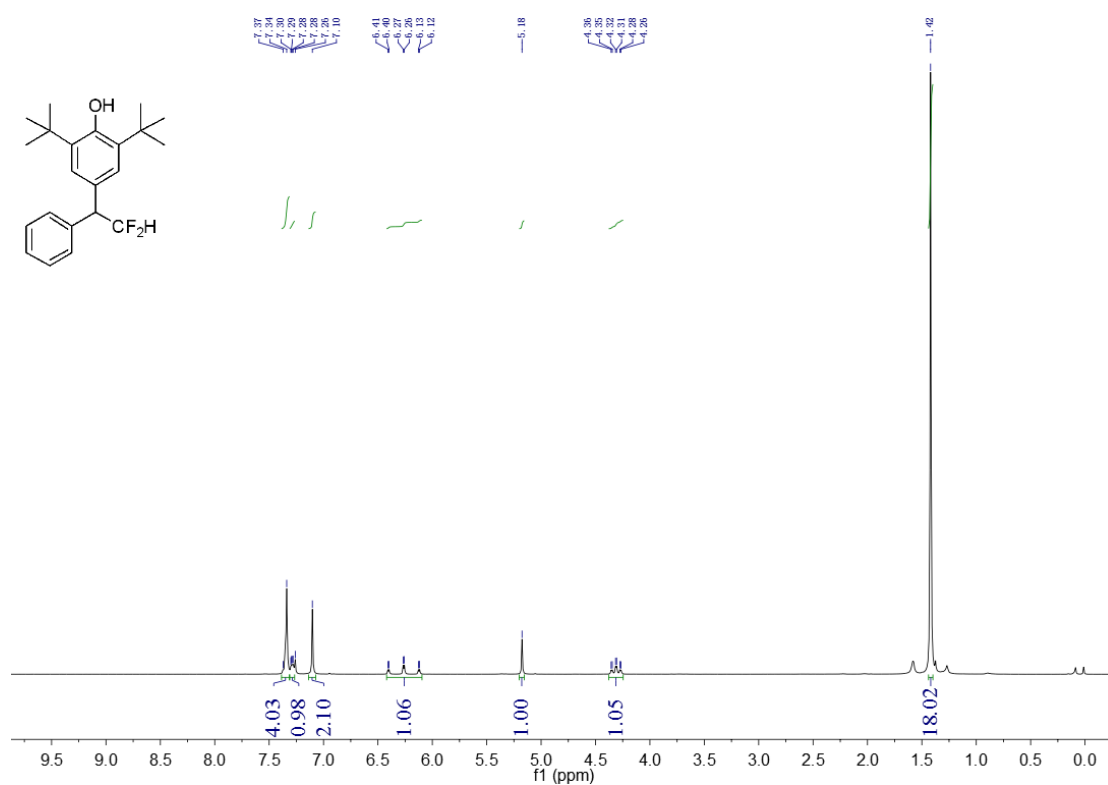
¹³C NMR of **2v**



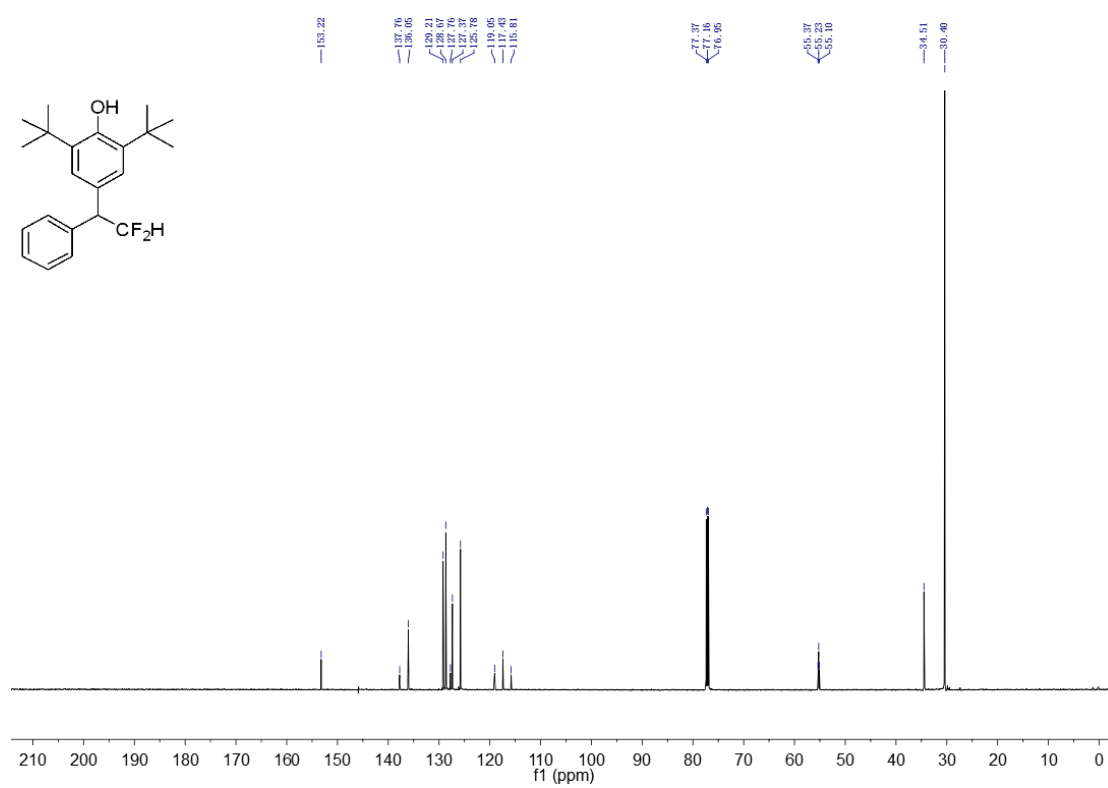
¹⁹F NMR of **2v**



¹H NMR of **3a**



¹³C NMR of **3a**



Chemical structure: CC(C)(C)c1cc(C(C)(C)C)c(C(F)(F)O)c1C(F)(F)Oc2ccccc2

¹³C NMR spectrum (ppm):

- 116.95, 116.98, 117.05, 117.12, 117.44, 117.47, 117.54, 117.57, 117.95, 117.98, 118.08, 118.44, 118.44, 118.54, 118.57

Integration values: 0.99, 1.00

Chemical structure: CC(C)(C)c1cc(O)c(C(C)(C)C)cc1C(CF)C2=CC=C(Cl)C=C2

¹H NMR spectrum (CDCl₃) showing peaks at 7.1-7.3 ppm (aromatic, 5H), 6.2 ppm (aromatic, 1H), 5.1 ppm (CH-OH, 1H), 4.3 ppm (CH₂, 2H), and 1.4 ppm (tert-butyl, 18H). Integration values are shown below the peaks.

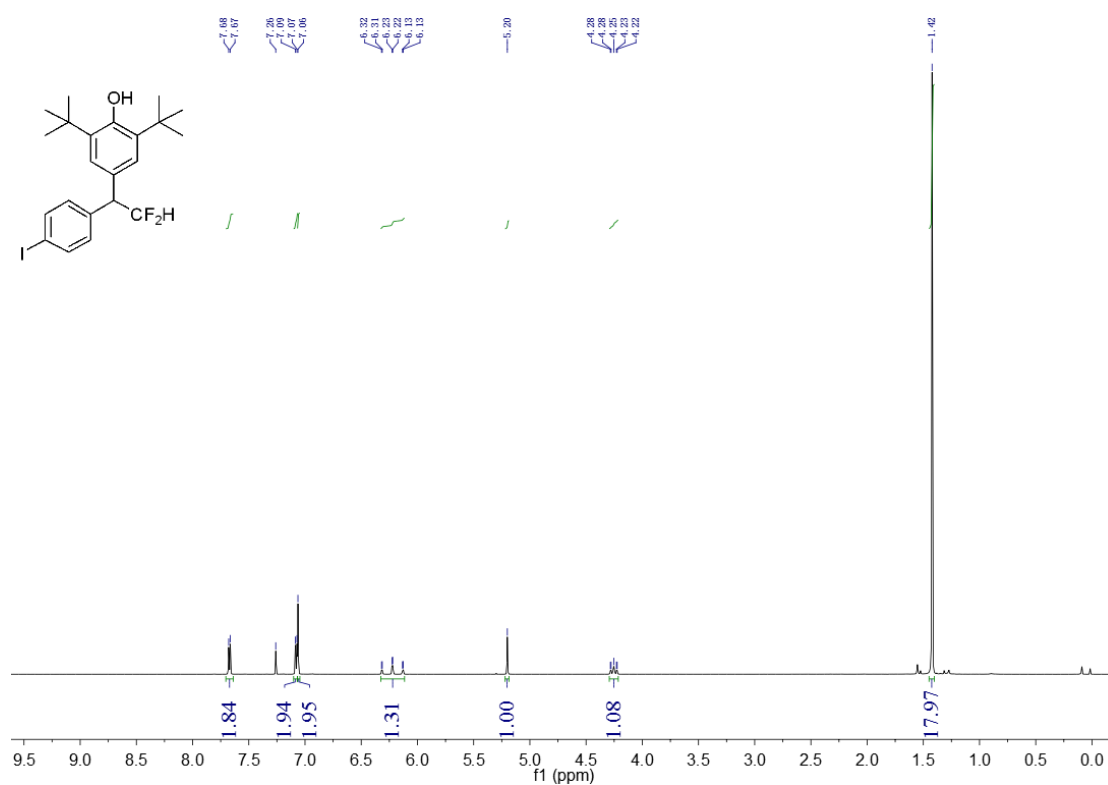
Chemical structure of 2-(4-chlorophenyl)-2-(4-tert-butyl-2-hydroxyphenyl)ethanol (1) is shown. The ¹³C NMR spectrum (CDCl₃) displays peaks at the following chemical shifts (ppm): 153.36, 136.25, 136.16, 133.34, 130.44, 128.81, 127.29, 125.64, 118.73, 117.10, 115.48, 77.37, 77.16, 76.95, 54.66, 54.53, 54.39, 34.53, and 30.38.

Chemical structure: CC(C)(C)c1cc(O)cc(C(F)(F)c2ccc(Cl)cc2)c1

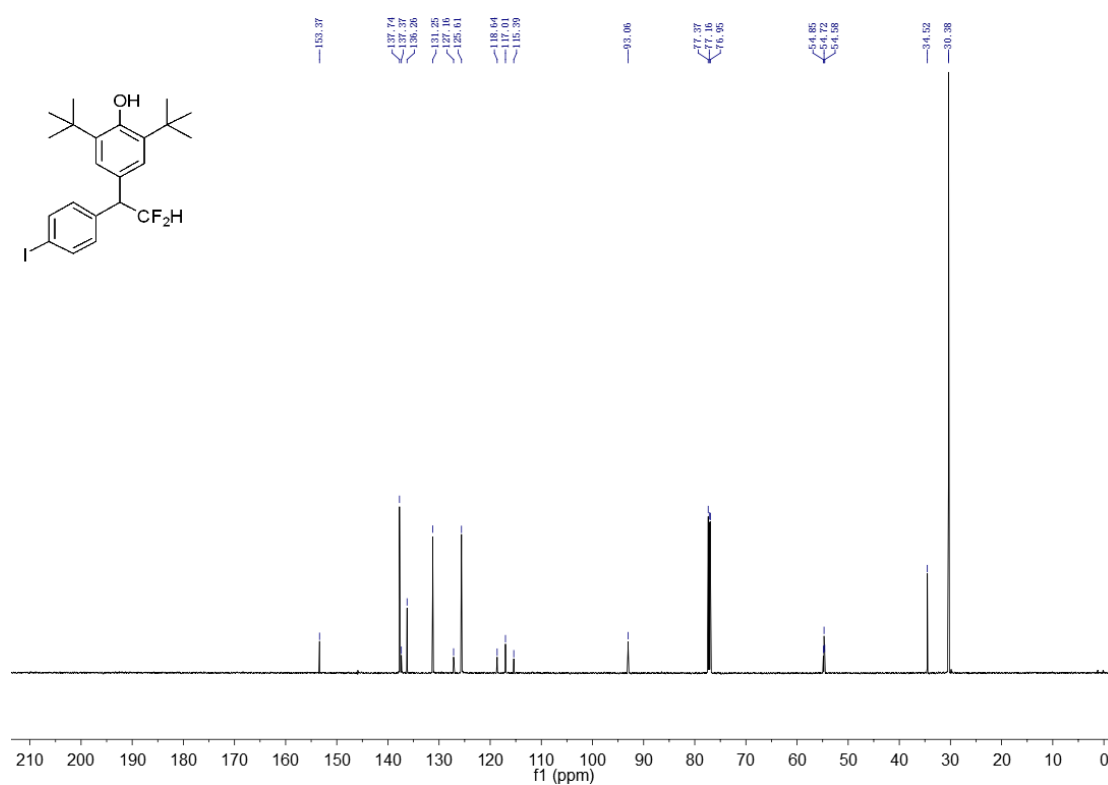
¹³C NMR spectrum (ppm):

- 116.51, 116.54, 116.61, 116.64, 117.01, 117.03, 117.05, 117.13, 117.15, 117.17, 117.19, 117.21, 117.23, 117.25, 117.27, 117.29, 117.31, 117.33, 117.35, 117.37, 117.39, 117.41, 117.43, 117.45, 117.47, 117.49, 117.51, 117.53, 117.55, 117.57, 117.59, 117.61, 117.63, 117.65, 117.67, 117.69, 117.71, 117.73, 117.75, 117.77, 117.79, 117.81, 117.83, 117.85, 117.87, 117.89, 117.91, 117.93, 117.95, 117.97, 117.99, 118.01, 118.03, 118.05, 118.07, 118.09, 118.11, 118.13, 118.15, 118.17, 118.19, 118.21, 118.23, 118.25, 118.27, 118.29, 118.31, 118.33, 118.35, 118.37, 118.39, 118.41, 118.43, 118.45, 118.47, 118.49, 118.51, 118.53, 118.55, 118.57, 118.59, 118.61, 118.63, 118.65, 118.67, 118.69, 118.71, 118.73, 118.75, 118.77, 118.79, 118.81, 118.83, 118.85, 118.87, 118.89, 118.91, 118.93, 118.95, 118.97, 118.99, 119.01, 119.03, 119.05, 119.07, 119.09, 119.11, 119.13, 119.15, 119.17, 119.19, 119.21, 119.23, 119.25, 119.27, 119.29, 119.31, 119.33, 119.35, 119.37, 119.39, 119.41, 119.43, 119.45, 119.47, 119.49, 119.51, 119.53, 119.55, 119.57, 119.59, 119.61, 119.63, 119.65, 119.67, 119.69, 119.71, 119.73, 119.75, 119.77, 119.79, 119.81, 119.83, 119.85, 119.87, 119.89, 119.91, 119.93, 119.95, 119.97, 119.99, 120.01, 120.03, 120.05, 120.07, 120.09, 120.11, 120.13, 120.15, 120.17, 120.19, 120.21, 120.23, 120.25, 120.27, 120.29, 120.31, 120.33, 120.35, 120.37, 120.39, 120.41, 120.43, 120.45, 120.47, 120.49, 120.51, 120.53, 120.55, 120.57, 120.59, 120.61, 120.63, 120.65, 120.67, 120.69, 120.71, 120.73, 120.75, 120.77, 120.79, 120.81, 120.83, 120.85, 120.87, 120.89, 120.91, 120.93, 120.95, 120.97, 120.99, 121.01, 121.03, 121.05, 121.07, 121.09, 121.11, 121.13, 121.15, 121.17, 121.19, 121.21, 121.23, 121.25, 121.27, 121.29, 121.31, 121.33, 121.35, 121.37, 121.39, 121.41, 121.43, 121.45, 121.47, 121.49, 121.51, 121.53, 121.55, 121.57, 121.59, 121.61, 121.63, 121.65, 121.67, 121.69, 121.71, 121.73, 121.75, 121.77, 121.79, 121.81, 121.83, 121.85, 121.87, 121.89, 121.91, 121.93, 121.95, 121.97, 121.99, 122.01, 122.03, 122.05, 122.07, 122.09, 122.11, 122.13, 122.15, 122.17, 122.19, 122.21, 122.23, 122.25, 122.27, 122.29, 122.31, 122.33, 122.35, 122.37, 122.39, 122.41, 122.43, 122.45, 122.47, 122.49, 122.51, 122.53, 122.55, 122.57, 122.59, 122.61, 122.63, 122.65, 122.67, 122.69, 122.71, 122.73, 122.75, 122.77, 122.79, 122.81, 122.83, 122.85, 122.87, 122.89, 122.91, 122.93, 122.95, 122.97, 122.99, 123.01, 123.03, 123.05, 123.07, 123.09, 123.11, 123.13, 123.15, 123.17, 123.19, 123.21, 123.23, 123.25, 123.27, 123.29, 123.31, 123.33, 123.35, 123.37, 123.39, 123.41, 123.43, 123.45, 123.47, 123.49, 123.51, 123.53, 123.55, 123.57, 123.59, 123.61, 123.63, 123.65, 123.67, 123.69, 123.71, 123.73, 123.75, 123.77, 123.79, 123.81, 123.83, 123.85, 123.87, 123.89, 123.91, 123.93, 123.95, 123.97, 123.99, 124.01, 124.03, 124.05, 124.07, 124.09, 124.11, 124.13, 124.15, 124.17, 124.19, 124.21, 124.23, 124.25, 124.27, 124.29, 124.31, 124.33, 124.35, 124.37, 124.39, 124.41, 124.43, 124.45, 124.47, 124.49, 124.51, 124.53, 124.55, 124.57, 124.59, 124.61, 124.63, 124.65, 124.67, 124.69, 124.71, 124.73, 124.75, 124.77, 124.79, 124.81, 124.83, 124.85, 124.87, 124.89, 124.91, 124.93, 124.95, 124.97, 124.99, 125.01, 125.03, 125.05, 125.07, 125.09, 125.11, 125.13, 125.15, 125.17, 125.19, 125.21, 125.23, 125.25, 125.27, 125.29, 125.31, 125.33, 125.35, 125.37, 125.39, 125.41, 125.43, 125.45, 125.47, 125.49, 125.51, 125.53, 125.55, 125.57, 125.59, 125.61, 125.63, 125.65, 125.67, 125.69, 125.71, 125.73, 125.75, 125.77, 125.79, 125.81, 125.83, 125.85, 125.87, 125.89, 125.91, 125.93, 125.95, 125.97, 125.99, 126.01, 126.03, 126.05, 126.07, 126.09, 126.11, 126.13, 126.15, 126.17, 126.19, 126.21, 126.23, 126.25, 126.27, 126.29, 126.31, 126.33, 126.35, 126.37, 126.39, 126.41, 126.43, 126.45, 126.47, 126.49, 126.51, 126.53, 126.55, 126.57, 126.59, 126.61, 126.63, 126.65, 126.67, 126.69, 126.71, 126.73, 126.75, 126.77, 126.79, 126.81, 126.83, 126.85,

¹H NMR of 3c



¹³C NMR of 3c



[illegible]

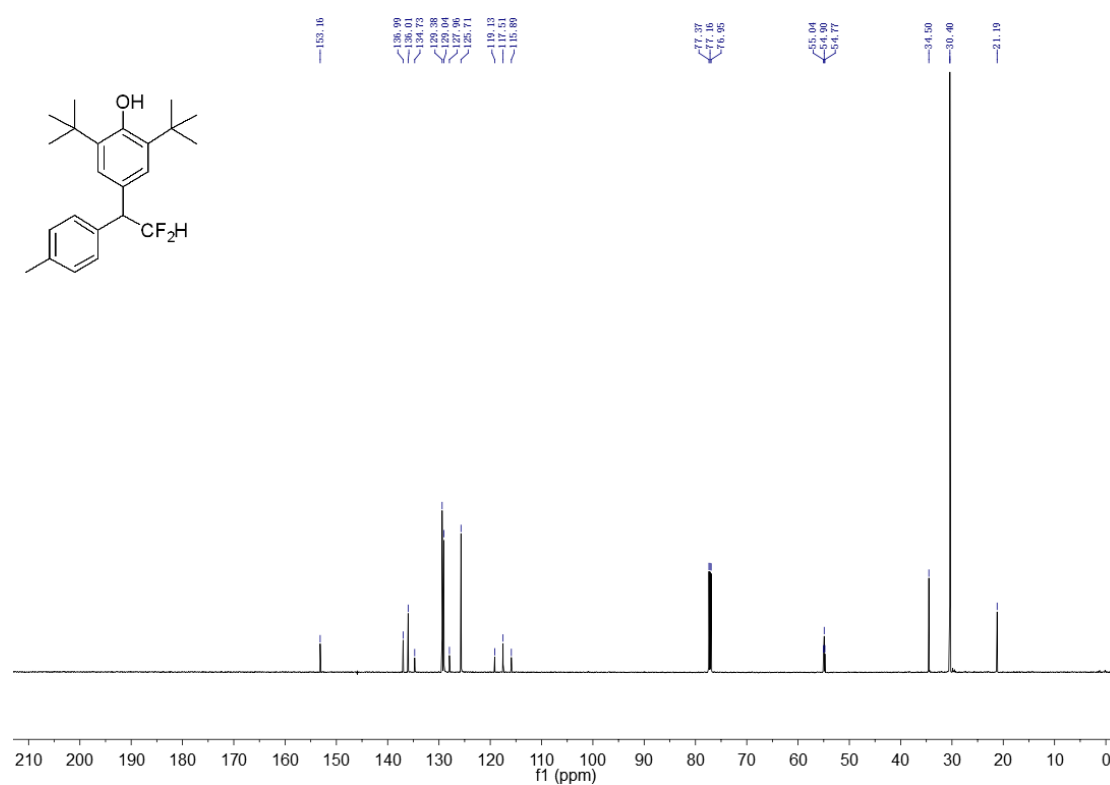
¹H NMR Spectrum (400 MHz, CDCl₃)

Chemical Structure: 1-(4-(tert-butyl)-2-hydroxyphenyl)-4-(pentafluorophenyl)ethan-1-ol

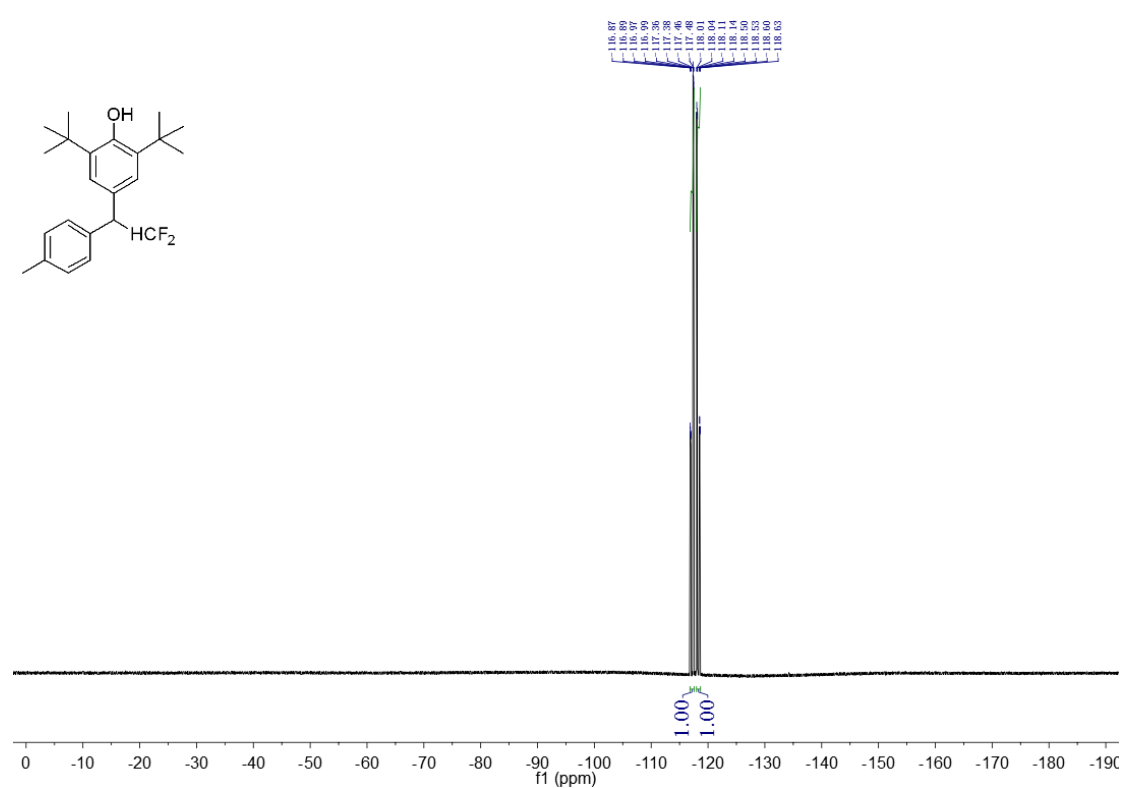
Chemical Shifts (ppm): 7.26, 7.24, 7.22, 7.17, 7.15, 7.13, 7.11, 6.39, 6.38, 6.35, 6.24, 6.11, 6.10, 5.17, 4.32, 4.31, 4.29, 4.27, 4.25, 2.34, 1.42.

Integration Values: 1.97, 1.99, 2.00, 1.01, 1.00, 1.01, 3.00, 18.00.

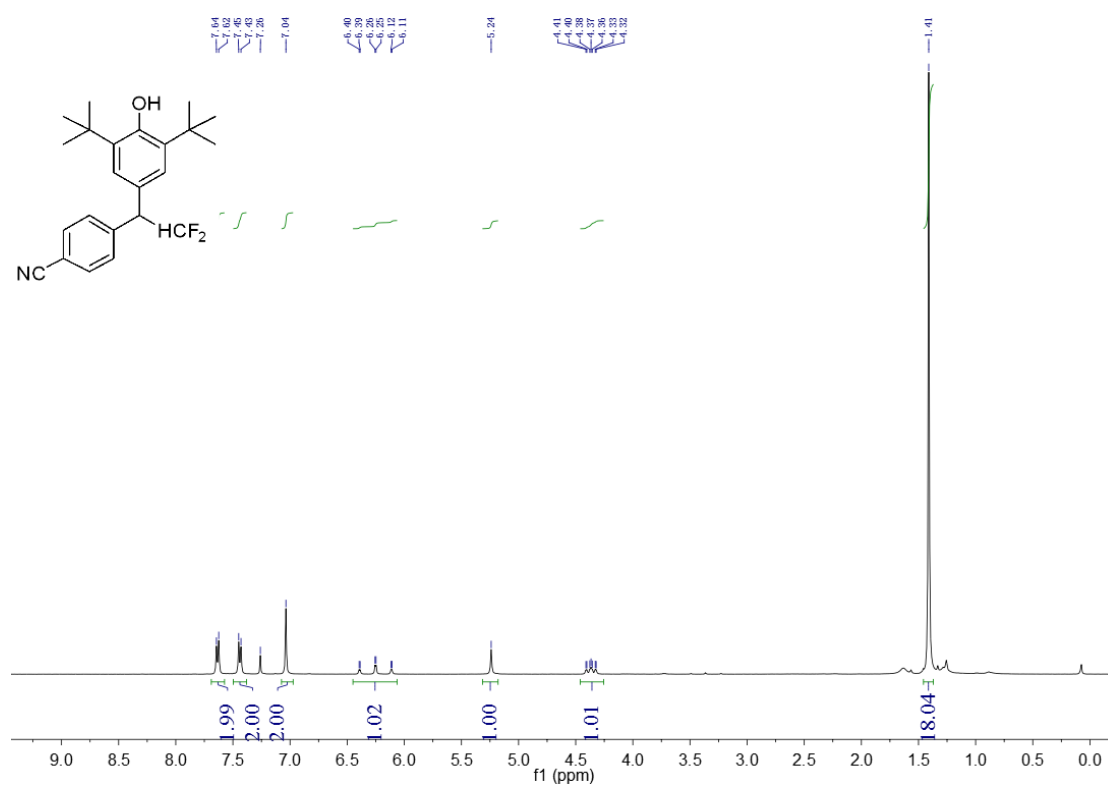
¹³C NMR of **3d**



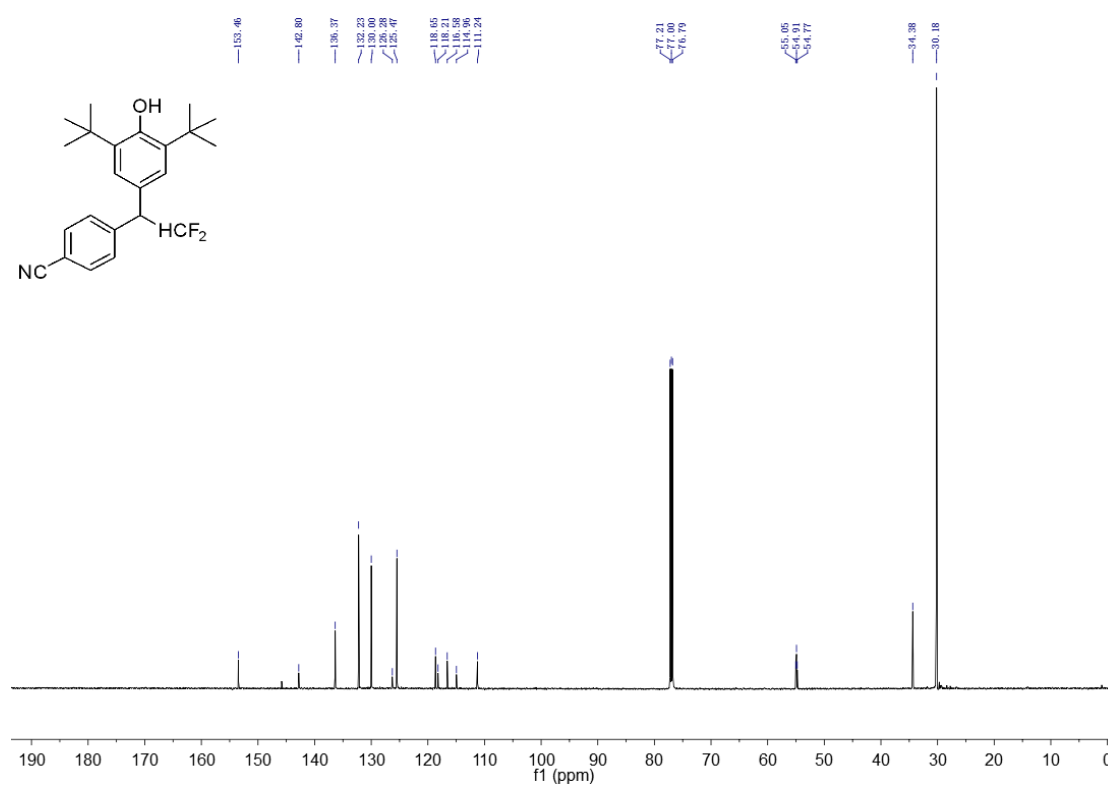
¹⁹F NMR of **3d**



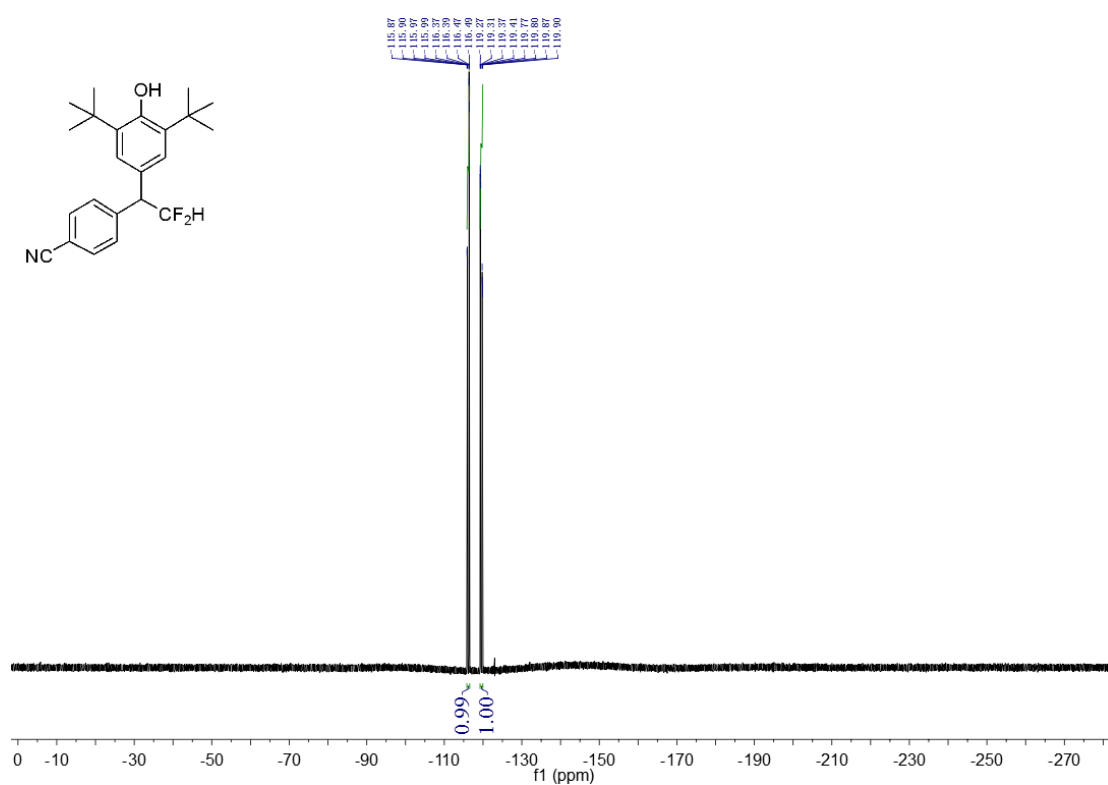
¹H NMR of 3e



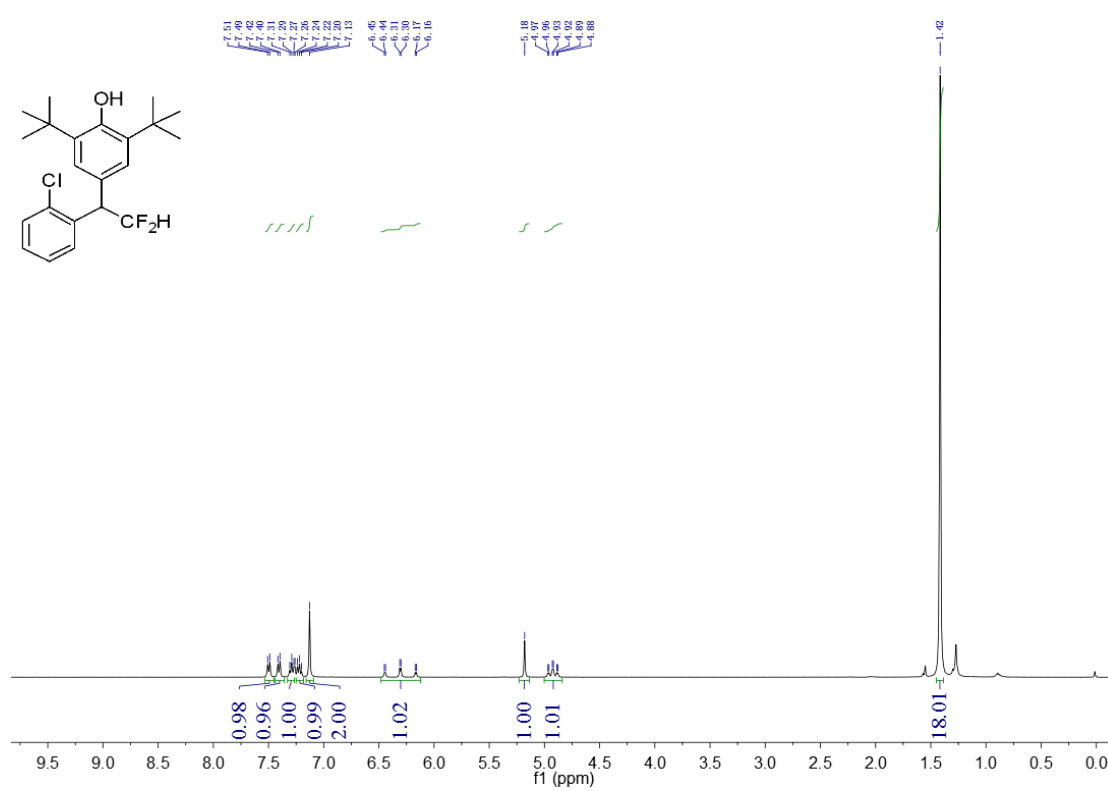
¹³C NMR of 3e



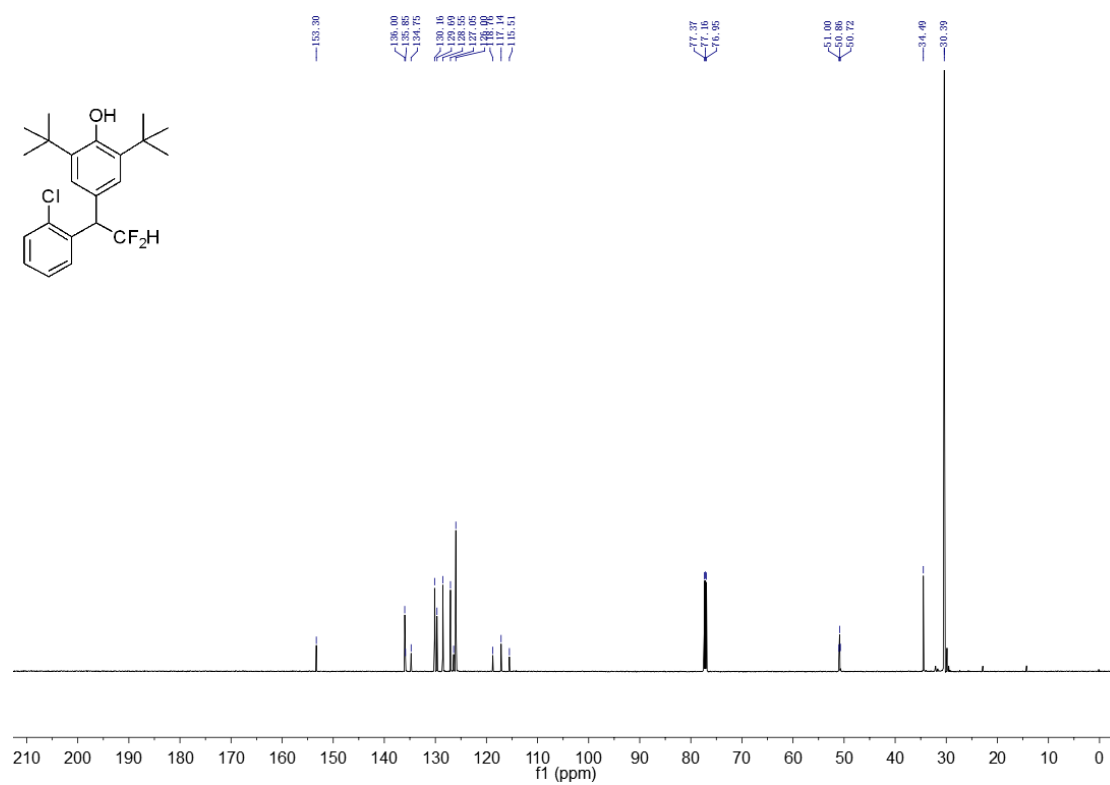
¹⁹F NMR of **3e**



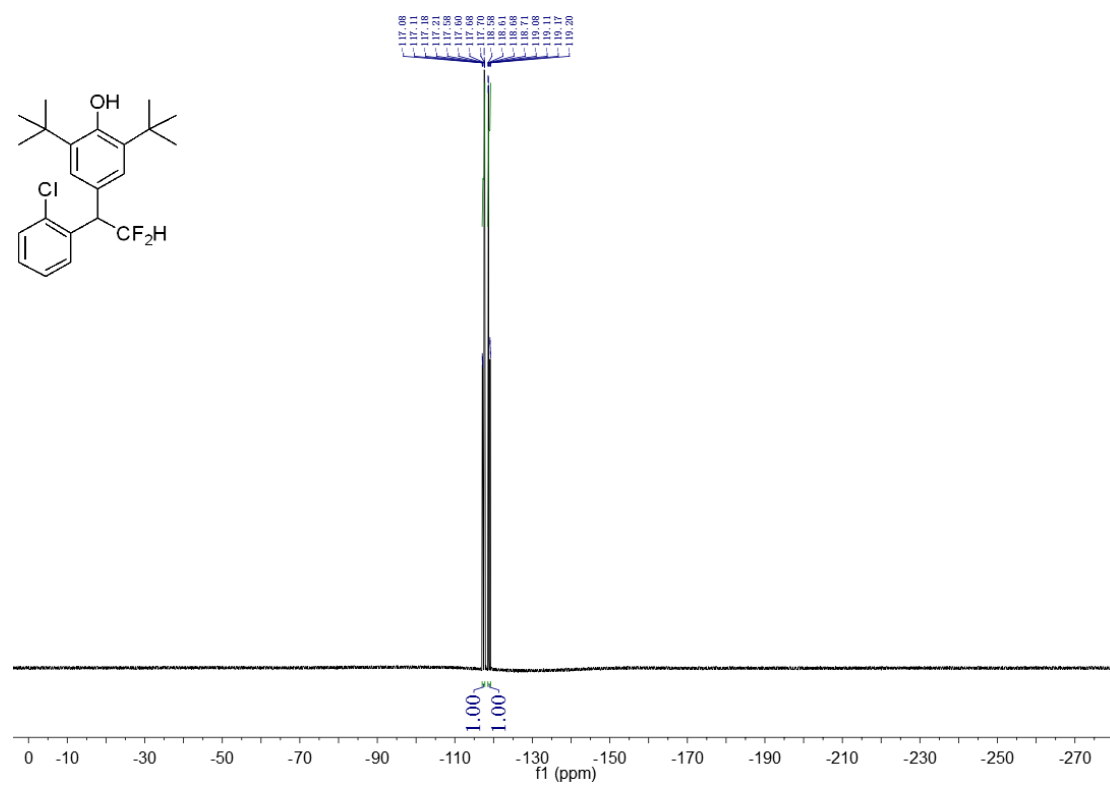
¹H NMR of **3f**



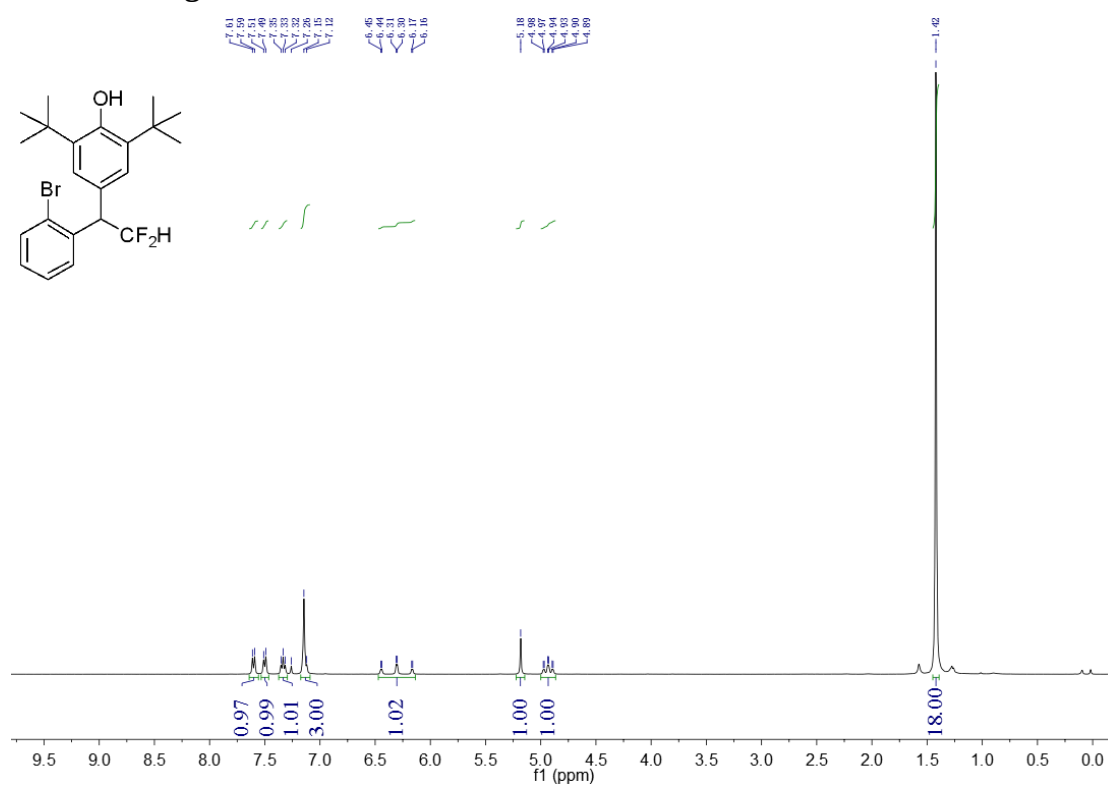
¹³C NMR of **3f**



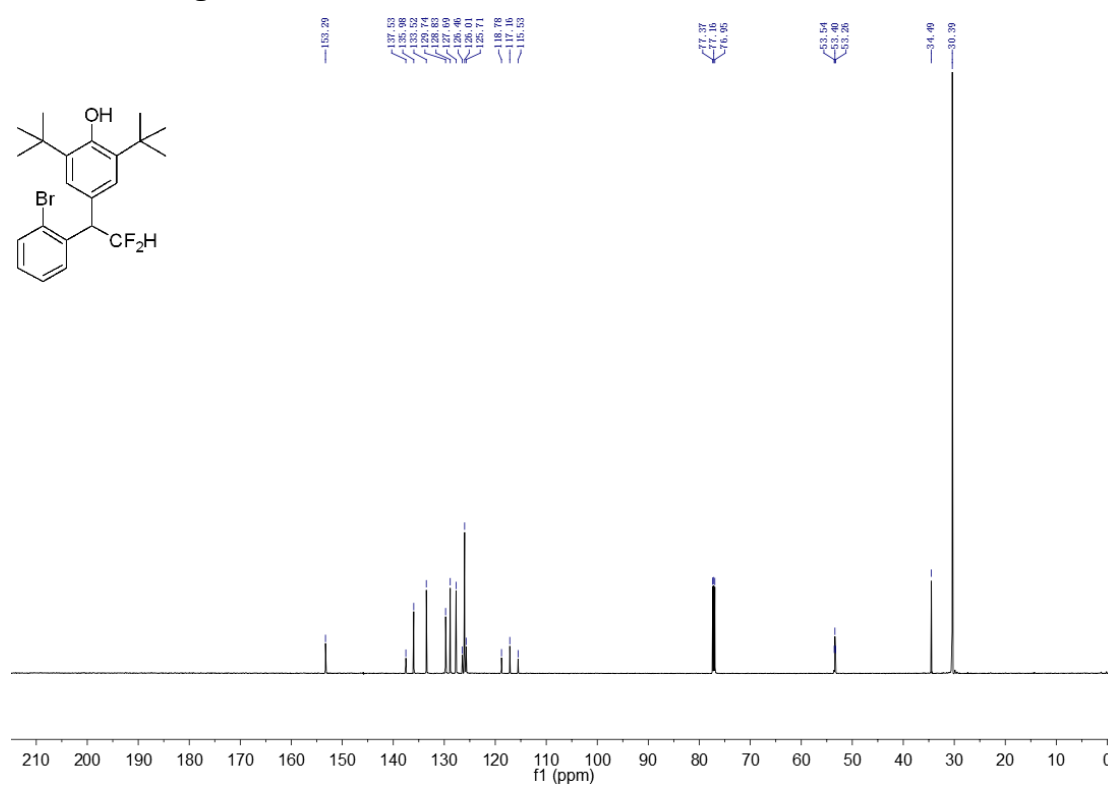
¹⁹F NMR of **3f**



¹H NMR of **3g**



¹³C NMR of **3g**



Chemical structure: CC(C)(C)c1cc(C(C)(C)C)c(C(O)C(Cc2ccccc2Br)C(F)(F)F)c1

¹H NMR spectrum (ppm):

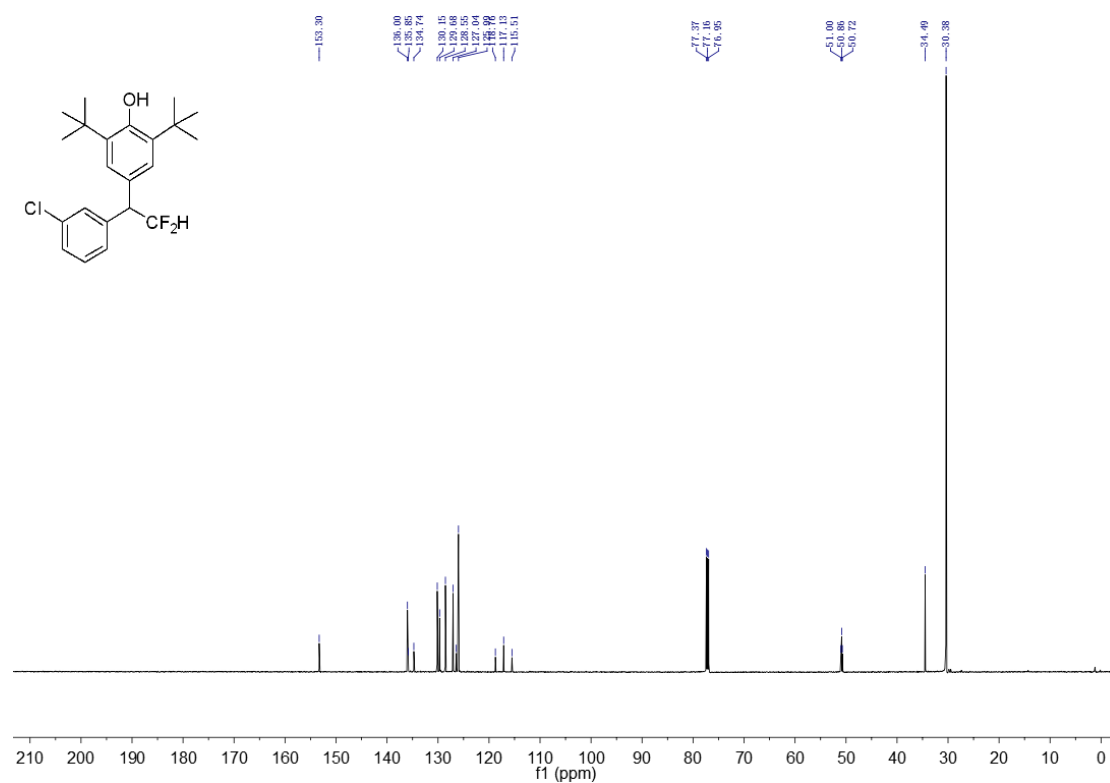
- 117.08 (broad peak, integration 0.99)
- 117.10, 117.18, 117.29, 117.57, 117.60, 117.66, 117.70, 117.71 (multiplet, integration 1.00)
- 118.65, 118.68, 118.71 (multiplet)
- 119.30, 119.32, 119.33 (multiplet)

Chemical structure: Cc1cc(Cc2ccc(Cl)cc2)c(O)c(C)c1

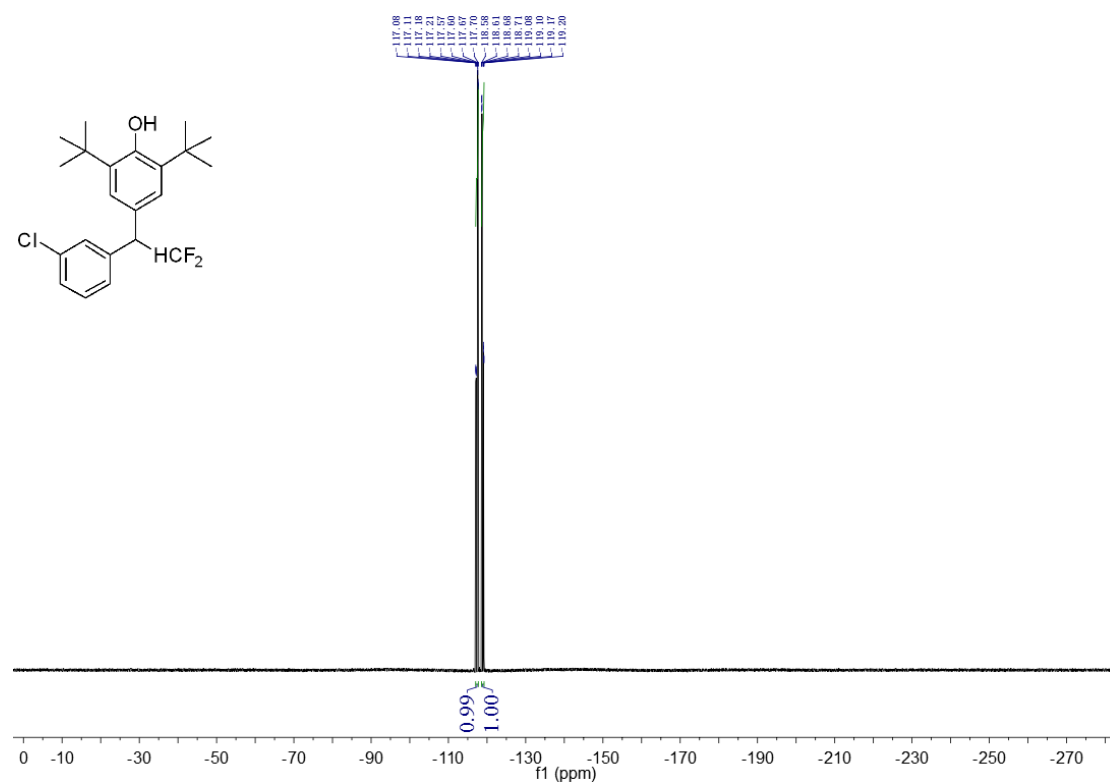
¹H NMR spectrum (ppm):

- 7.51, 7.49, 7.41, 7.39, 7.37, 7.35, 7.22, 7.20, 7.13 (multiplet, 4.00H)
- 6.46, 6.44, 6.43, 6.30, 6.17, 6.16 (doublet, 1.01H)
- 4.89, 4.88, 4.87, 4.86, 4.85, 4.84, 4.83, 4.82, 4.81, 4.80, 4.79, 4.78, 4.77, 4.76, 4.75, 4.74, 4.73, 4.72, 4.71, 4.70, 4.69, 4.68, 4.67, 4.66, 4.65, 4.64, 4.63, 4.62, 4.61, 4.60, 4.59, 4.58, 4.57, 4.56, 4.55, 4.54, 4.53, 4.52, 4.51, 4.50, 4.49, 4.48, 4.47, 4.46, 4.45, 4.44, 4.43, 4.42, 4.41, 4.40, 4.39, 4.38, 4.37, 4.36, 4.35, 4.34, 4.33, 4.32, 4.31, 4.30, 4.29, 4.28, 4.27, 4.26, 4.25, 4.24, 4.23, 4.22, 4.21, 4.20, 4.19, 4.18, 4.17, 4.16, 4.15, 4.14, 4.13, 4.12, 4.11, 4.10, 4.09, 4.08, 4.07, 4.06, 4.05, 4.04, 4.03, 4.02, 4.01, 4.00, 3.99, 3.98, 3.97, 3.96, 3.95, 3.94, 3.93, 3.92, 3.91, 3.90, 3.89, 3.88, 3.87, 3.86, 3.85, 3.84, 3.83, 3.82, 3.81, 3.80, 3.79, 3.78, 3.77, 3.76, 3.75, 3.74, 3.73, 3.72, 3.71, 3.70, 3.69, 3.68, 3.67, 3.66, 3.65, 3.64, 3.63, 3.62, 3.61, 3.60, 3.59, 3.58, 3.57, 3.56, 3.55, 3.54, 3.53, 3.52, 3.51, 3.50, 3.49, 3.48, 3.47, 3.46, 3.45, 3.44, 3.43, 3.42, 3.41, 3.40, 3.39, 3.38, 3.37, 3.36, 3.35, 3.34, 3.33, 3.32, 3.31, 3.30, 3.29, 3.28, 3.27, 3.26, 3.25, 3.24, 3.23, 3.22, 3.21, 3.20, 3.19, 3.18, 3.17, 3.16, 3.15, 3.14, 3.13, 3.12, 3.11, 3.10, 3.09, 3.08, 3.07, 3.06, 3.05, 3.04, 3.03, 3.02, 3.01, 3.00, 2.99, 2.98, 2.97, 2.96, 2.95, 2.94, 2.93, 2.92, 2.91, 2.90, 2.89, 2.88, 2.87, 2.86, 2.85, 2.84, 2.83, 2.82, 2.81, 2.80, 2.79, 2.78, 2.77, 2.76, 2.75, 2.74, 2.73, 2.72, 2.71, 2.70, 2.69, 2.68, 2.67, 2.66, 2.65, 2.64, 2.63, 2.62, 2.61, 2.60, 2.59, 2.58, 2.57, 2.56, 2.55, 2.54, 2.53, 2.52, 2.51, 2.50, 2.49, 2.48, 2.47, 2.46, 2.45, 2.44, 2.43, 2.42, 2.41, 2.40, 2.39, 2.38, 2.37, 2.36, 2.35, 2.34, 2.33, 2.32, 2.31, 2.30, 2.29, 2.28, 2.27, 2.26, 2.25, 2.24, 2.23, 2.22, 2.21, 2.20, 2.19, 2.18, 2.17, 2.16, 2.15, 2.14, 2.13, 2.12, 2.11, 2.10, 2.09, 2.08, 2.07, 2.06, 2.05, 2.04, 2.03, 2.02, 2.01, 2.00, 1.99, 1.98, 1.97, 1.96, 1.95, 1.94, 1.93, 1.92, 1.91, 1.90, 1.89, 1.88, 1.87, 1.86, 1.85, 1.84, 1.83, 1.82, 1.81, 1.80, 1.79, 1.78, 1.77, 1.76, 1.75, 1.74, 1.73, 1.72, 1.71, 1.70, 1.69, 1.68, 1.67, 1.66, 1.65, 1.64, 1.63, 1.62, 1.61, 1.60, 1.59, 1.58, 1.57, 1.56, 1.55, 1.54, 1.53, 1.52, 1.51, 1.50, 1.49, 1.48, 1.47, 1.46, 1.45, 1.44, 1.43, 1.42, 1.41, 1.40, 1.39, 1.38, 1.37, 1.36, 1.35, 1.34, 1.33, 1.32, 1.31, 1.30, 1.29, 1.28, 1.27, 1.26, 1.25, 1.24, 1.23, 1.22, 1.21, 1.20, 1.19, 1.18, 1.17, 1.16, 1.15, 1.14, 1.13, 1.12, 1.11, 1.10, 1.09, 1.08, 1.07, 1.06, 1.05, 1.04, 1.03, 1.02, 1.01, 1.00, 0.99, 0.98, 0.97, 0.96, 0.95, 0.94, 0.93, 0.92, 0.91, 0.90, 0.89, 0.88, 0.87, 0.86, 0.85, 0.84, 0.83, 0.82, 0.81, 0.80, 0.79, 0.78, 0.77, 0.76, 0.75, 0.74, 0.73, 0.72, 0.71, 0.70, 0.69, 0.68, 0.67, 0.66, 0.65, 0.64, 0.63, 0.62, 0.61, 0.60, 0.59, 0.58, 0.57, 0.56, 0.55, 0.54, 0.53, 0.52, 0.51, 0.50, 0.49, 0.48, 0.47, 0.46, 0.45, 0.44, 0.43, 0.42, 0.41, 0.40, 0.39, 0.38, 0.37, 0.36, 0.35, 0.34, 0.33, 0.32, 0.31, 0.30, 0.29, 0.28, 0.27, 0.26, 0.25, 0.24, 0.23, 0.22, 0.21, 0.20, 0.19, 0.18, 0.17, 0.16, 0.15, 0.14, 0.13, 0.12, 0.11, 0.10, 0.09, 0.08, 0.07, 0.06, 0.05, 0.04, 0.03, 0.02, 0.01, 0.00
- 1.41 (singlet, 18.00H)

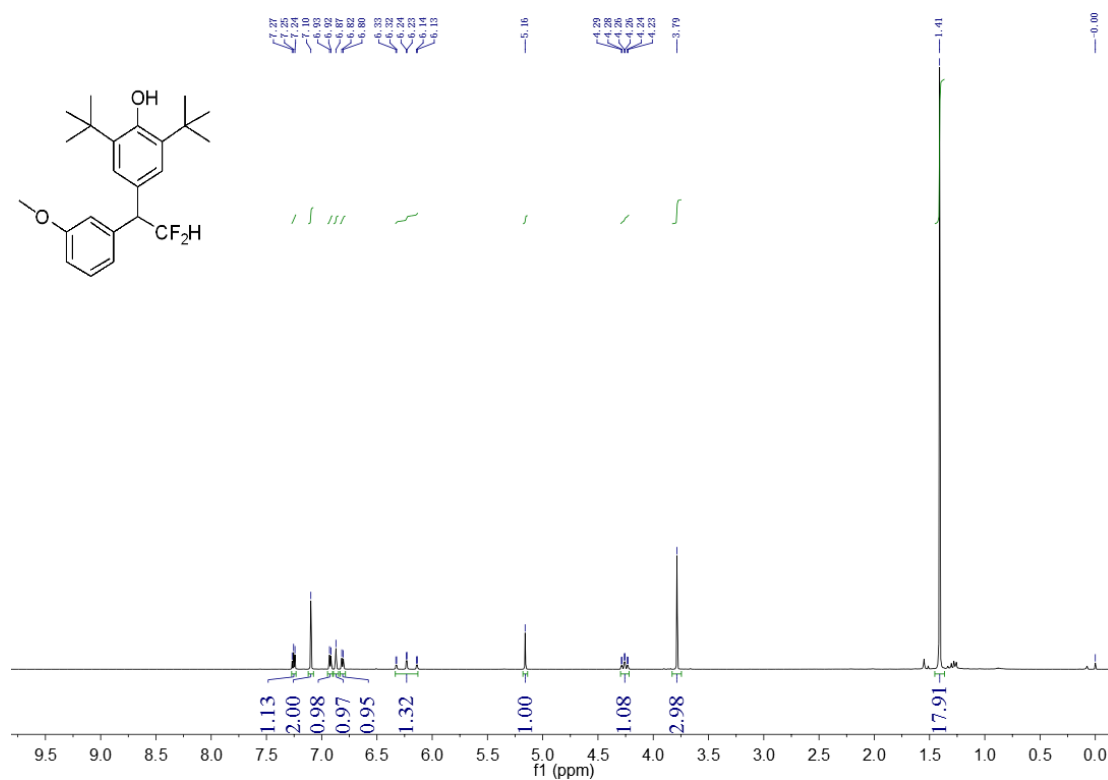
¹³C NMR of **3h**



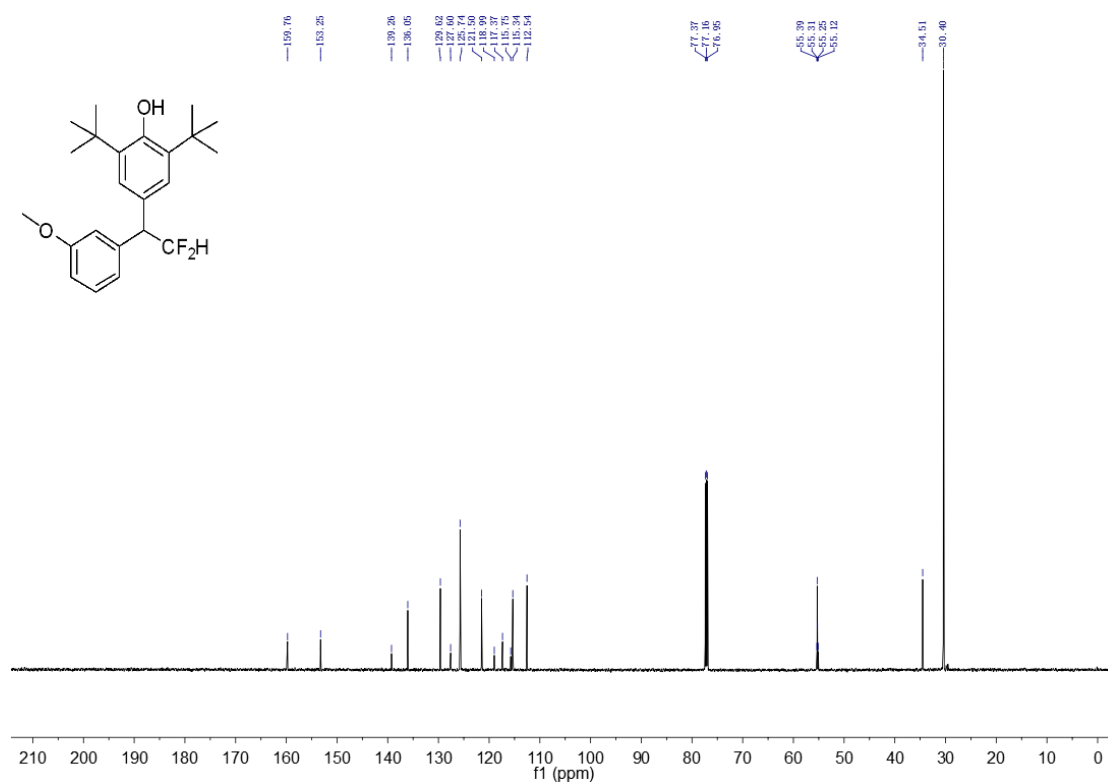
¹⁹F NMR of **3h**



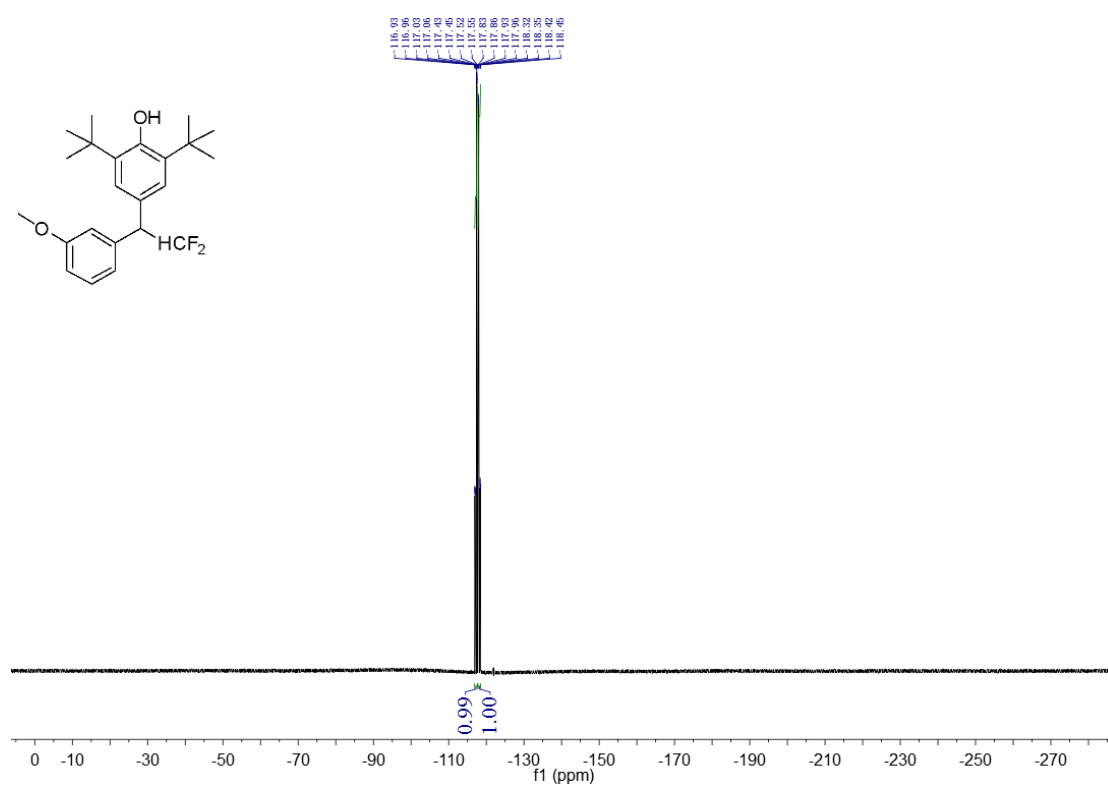
¹H NMR of **3i**



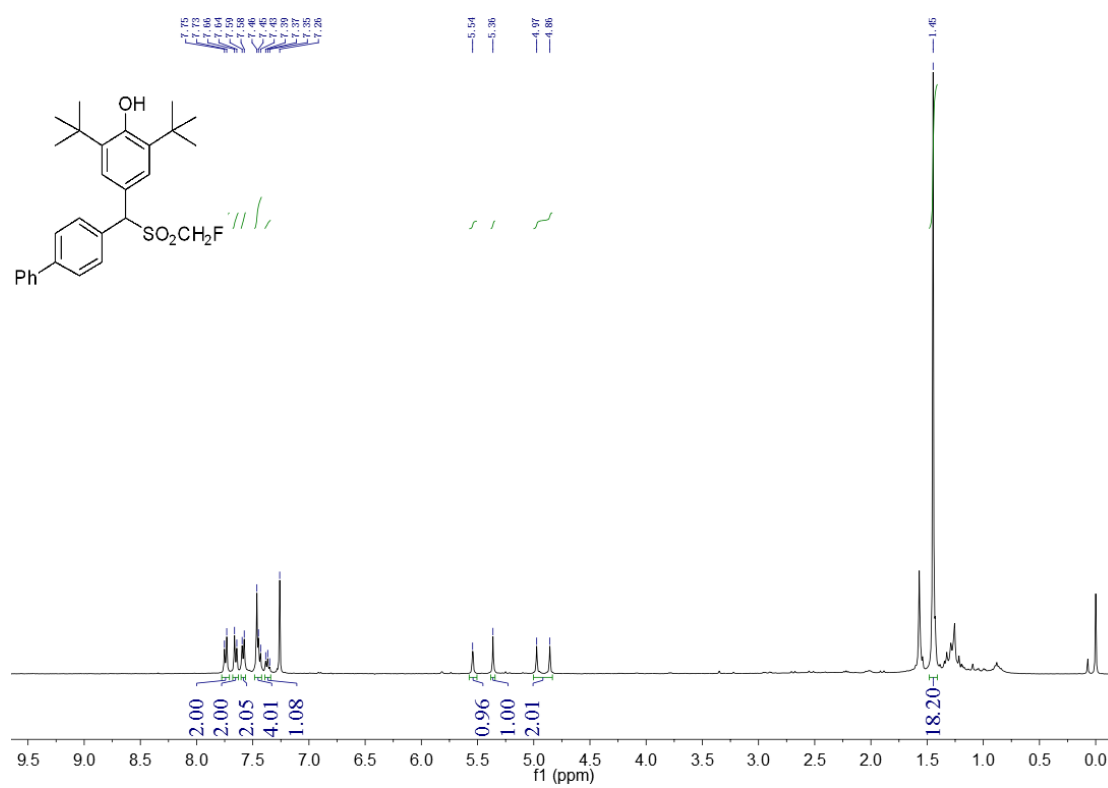
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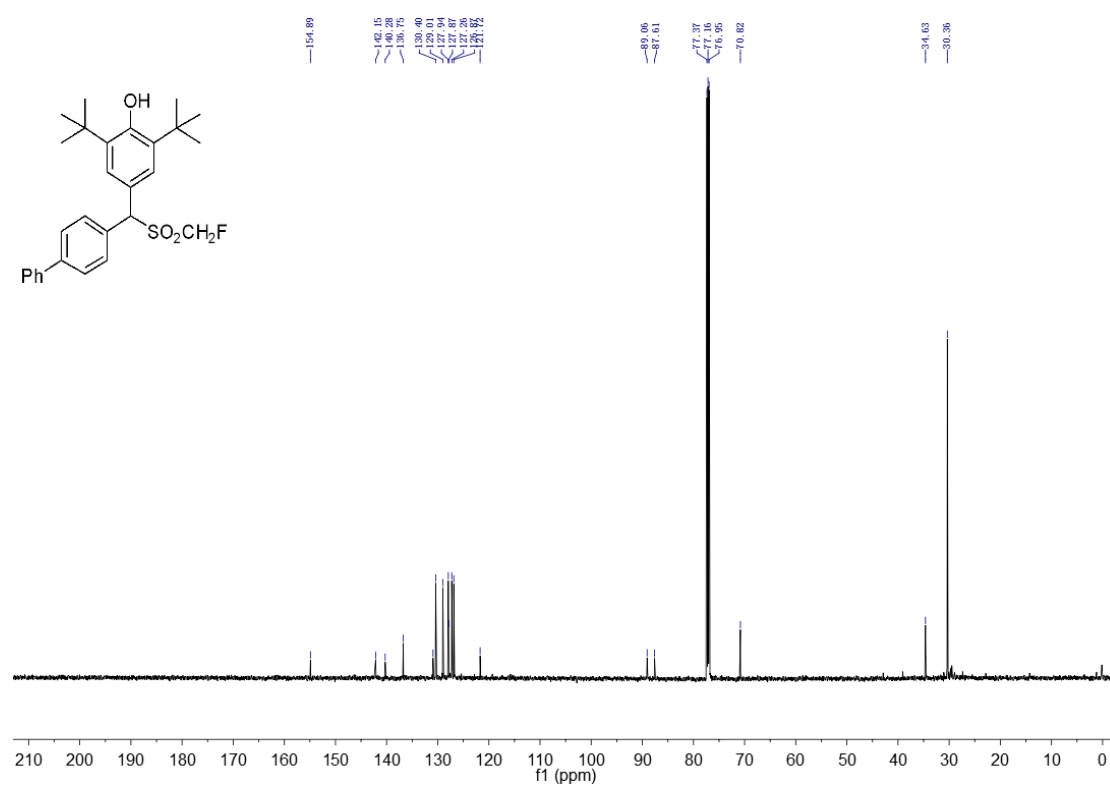
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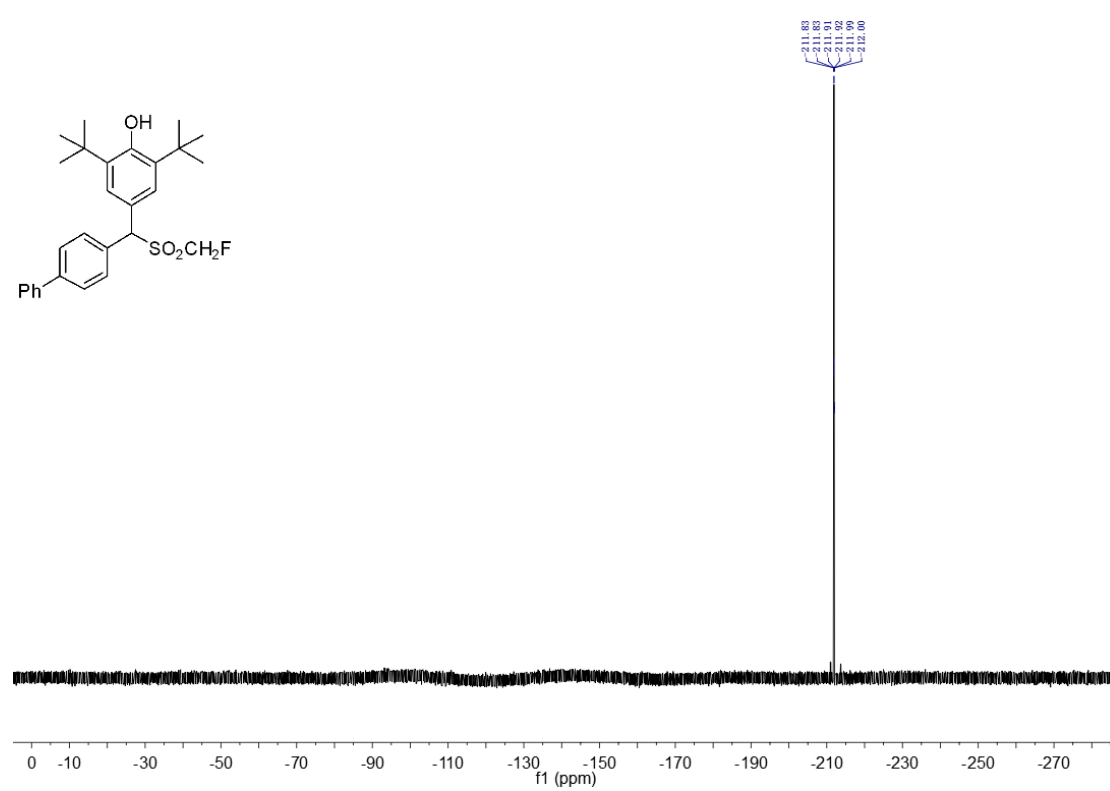
¹H NMR of **4a**



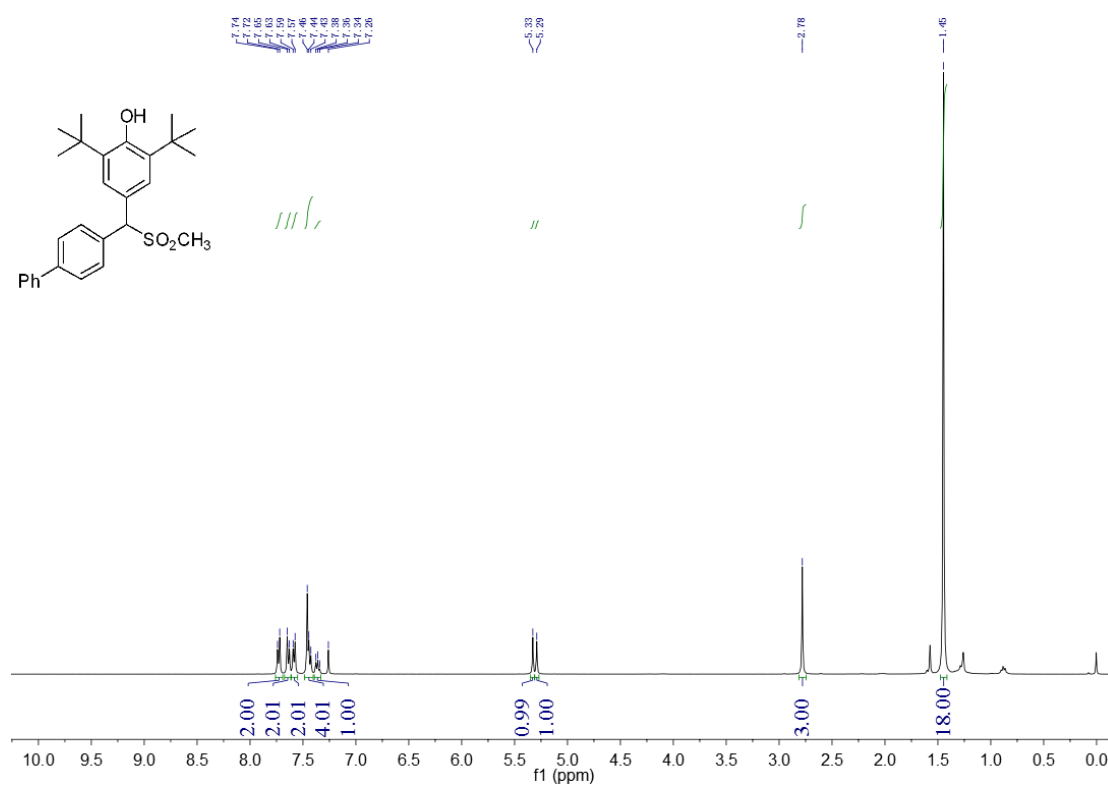
¹³C NMR of **4a**



¹⁹F NMR of **4a**



¹H NMR of **4b**



¹³C NMR of **4b**

