Supporting Information

for

A Visible-Light-Induced Photocatalyst-Free Approach for C-3 Dicarbonyl Coumarins Production

Jinhu Xi, Xinjie Wu, Mengmeng Huang, Jung Keun Kim,* Jianye Zhang,
Yabo Li* and Yangjie Wu

College of Chemistry, Henan Key Laboratory of Chemical Biology and Organic Chemistry, Key Laboratory of Applied Chemistry of Henan Universities, Zhengzhou University, Zhengzhou 450052, P.R. China. E-mail: ybli@zzu.edu.cn, kim@zzu.edu.cn

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1. General information

All reactions were performed using quartz tube. Solvents were dried by standard methods before they were used. 3-Arylacetylene coumarins and 3-bromocoumarin were synthesized according to the literature.[1,2,3] Commercial grade reagents were used without further purification. $H_2{}^{18}O$ is purchased from Shanghai Yi Shi Chemical Co., purity 97%. Silica gel was purchased from Qing Dao Hai Yang Chemical Industry Co. All reactions were carried out with photoreactor (Serial No: PEA12) which was purchased from LUOYANG JINFENG ELECTROMECHANICAL EQUIPMENT CO., LTD. The LCD Digital Hotplate Magnetic Stirrer MS-H-Pro$^+$ and Digital Single Channel Adjustable Automatic Electronic Pipette Micropipette dPettee$^+$ were purchased from Dragon Laboratory Instruments Limited. ^{1}H NMR and ^{13}C NMR spectra were recorded on 400 and 100 MHz NMR instruments using $CDCl_3$ as the solvent and TMS as the internal standard. ^{19}F NMR spectra was recorded at 376.5 MHz on Bruker DPX-400, the chemical shifts δ are reported relative to $CFCl_3$ (δ = 0 ppm) as internal standard. The multiplicity of signals is designated by the following abbreviations: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd = doublet of doublet. High resolution mass spectra (HRMS) was obtained on an Agilent LC-MSD-Trap-XCT spectrometer with micromass MS software using electrospray ionisation (ESI). The UV/Vis absorption spectra was recorded on a Perkin Elmer Lambda 35 Spectrometer and the fluorescence emission spectra were recorded using a F-4500 FL spectrophotometer. The X-ray single crystal structure was determined by the Oxford Diffraction Xcalibur CCD single crystal diffractometer. The illuminance of LED light was tested by the ZDS-10 digital luxmeter from Suzhou Tianwei Instrument Co., Ltd.

2. Experimental procedures

2.1 General procedure for synthesis of 3-arylacetylene coumarins from alkyne esters[1]

To a reaction tube equipped with a magnetic stirring bar were added phenyl 3-phenylpropiolate (0.2 mmol), NIS (2 equiv.), MeCN (1.5 mL) stirred under 3 W blue LED (E = 5.00-5.15X10^4 lx, λ_{max} = 450-465 nm) under air atmosphere and at room temperature for 24 hours. Then $Pd(PPh_3)_2Cl_2$ (0.0144 g, 10 mol%), CuI (0.0039 g, 10 mol%), phenylacetylene (3 equiv.) and Et_3N (0.5 mL) were added. The obtained reaction mixture was heated at 60 ^{o}C for 12 hours under Ar atmosphere. The solvent

was removed under vacuum, and the residue was purified by flash chromatography on silica gel (eluent: petroleum ether/dichloromethane = 6:1/3:1, v/v) to give the desired compound **1**.

2.2 General procedure for the synthesis of 3-arylacetylene coumarins from 3-bromocoumarins[2,3]

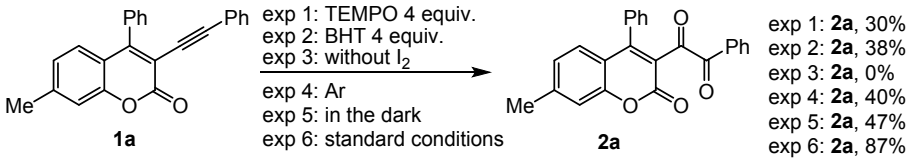
To a reaction tube equipped with a magnetic stirring bar were added 3-bromocoumarin (0.2 mmol), $Pd(PPh_3)_2Cl_2$ (0.0144 g, 10 mol%), CuI (0.0039 g, 10 mol%), phenylacetylene (3 equiv.) and Et_3N (0.5 mL) were added. The obtained reaction mixture was heated at 60 ^oC for 12 hours under Ar atmosphere. The solvent was removed under vacuum, and the residue was purified by flash chromatography on silica gel (eluent: petroleum ether/dichloromethane = 6:1/3:1, v/v) to give the desired compound **1**.

2.3 General procedure for the synthesis of C-3 dicarbonyl coumarins 2

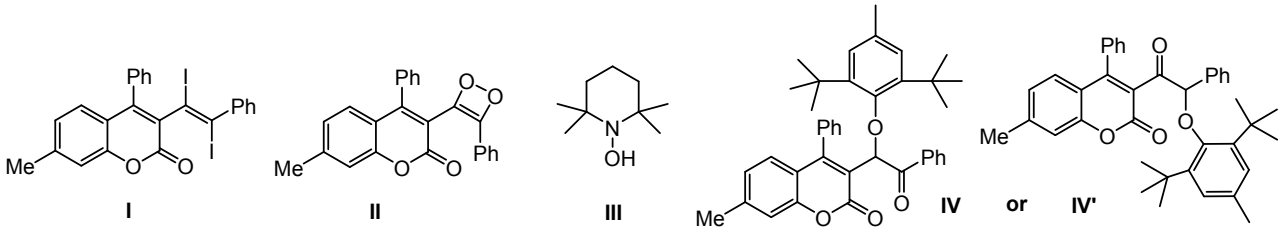
To a reaction tube equipped with a magnetic stirring bar were added 3-arylacetylene coumarins (0.2 mmol), I_2 (2 equiv.), $NaHCO_3$ (3equiv.), DCE:H_2O (2 mL, v/v = 200:3) stirred under 3 W blue LED (E = 5.00-5.15X10^4 lx, λ_{max} = 450-465 nm) under oxygen atmosphere and at room temperature for 24 hours. The solvent was removed under vacuum, and the residue was purified by flash chromatography on silica gel (eluent: petroleum ether/ethyl acetate/dichloromethane = 30:1:1/10:1:1, v/v) to give the desired compound **2**.

3. Control experiments

In order to explore the possible mechanism of the present transformation, a series of control experiments were carried out (Scheme S2, exp 1-6). [2,2,6,6-tetramethylpiperidine]-1-oxyl (TEMPO) or butylated hydroxytoluene (BHT), a radical-trapping reagent was added into the reaction. When added 3-arylacetylene coumarin (0.2 mmol), I_2 (2 equiv.), $NaHCO_3$ (3 equiv.), TEMPO (126.3 mg, 0.8 mmol) (exp 1) or BHT (176.3 mg, 0.8 mmol) (exp 2) DCE:H_2O (2 mL, v/v = 200:3) stirred under 3 W blue LED (E = 5.00-5.15X10^4 lx, λ_{max} = 450-465 nm) under oxygen atmosphere and at room temperature for 24 hours. The oxidation reaction was not completely inhibited. Meanwhile, five strong molecular ion peaks were obtained by ESI-MS and attributed to [**I**+H]$^+$ (exact mass: 590.9314), [**I**+H]$^+$ (exact mass: 590.9316), [**II**+H]$^+$ (exact mass: 369.1122), [**III**+H]$^+$ (exact mass: 158.1536) and [**IV**+H]$^+$ or [**IV'**+H]$^+$ (exact mass: 573.3001) (Fig. S1-S5).



Scheme S2. Control experiments



exp 1: [**I**+H]$^+$ = 590.9314
exp 6: [**I**+H]$^+$ = 590.9316

[**II**+H]$^+$ = 369.1122

[**III**+H]$^+$ = 158.1536

exp 2: [**IV**+H]$^+$ or [**IV'**+H]$^+$ = 573.3001

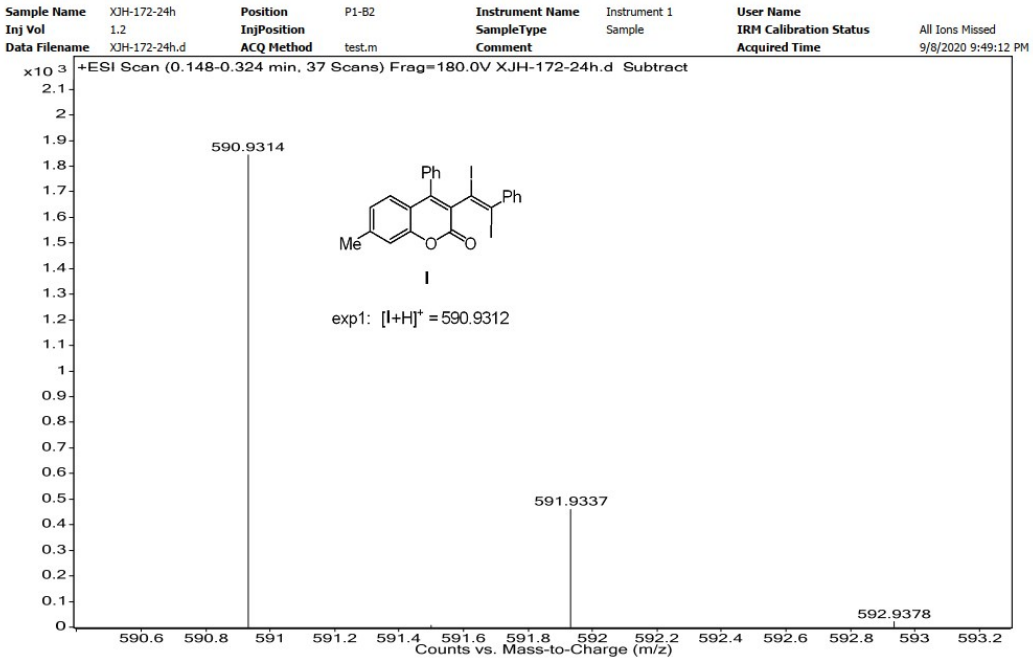


Figure S1. HRMS spectrum of compound [**I**+H]$^+$ for exp 1

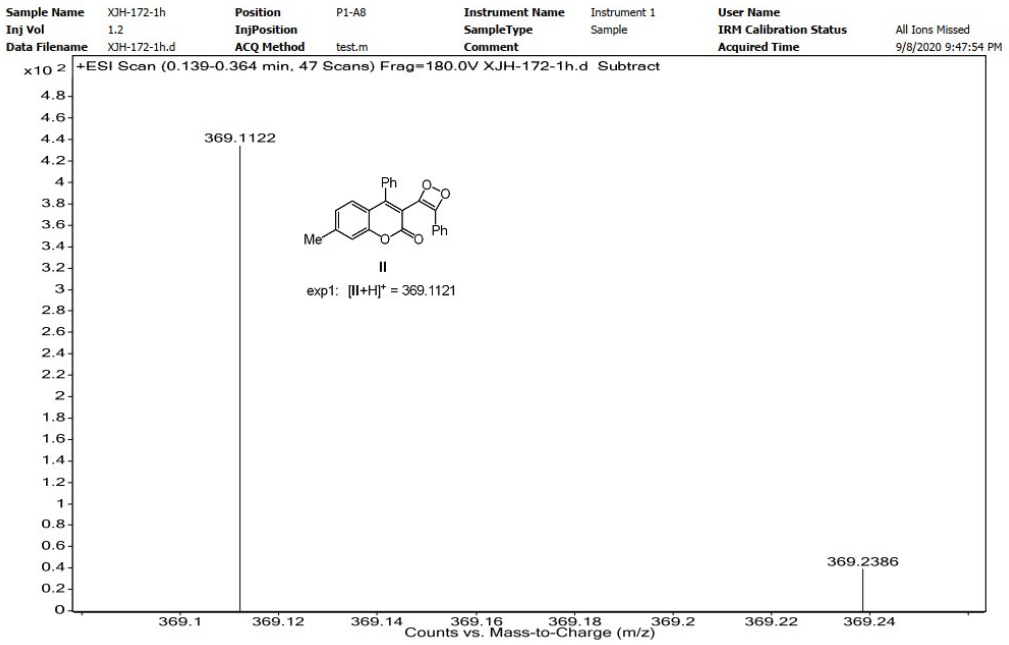


Figure S2. HRMS spectrum of compound [**II**+H]$^+$ for exp 1

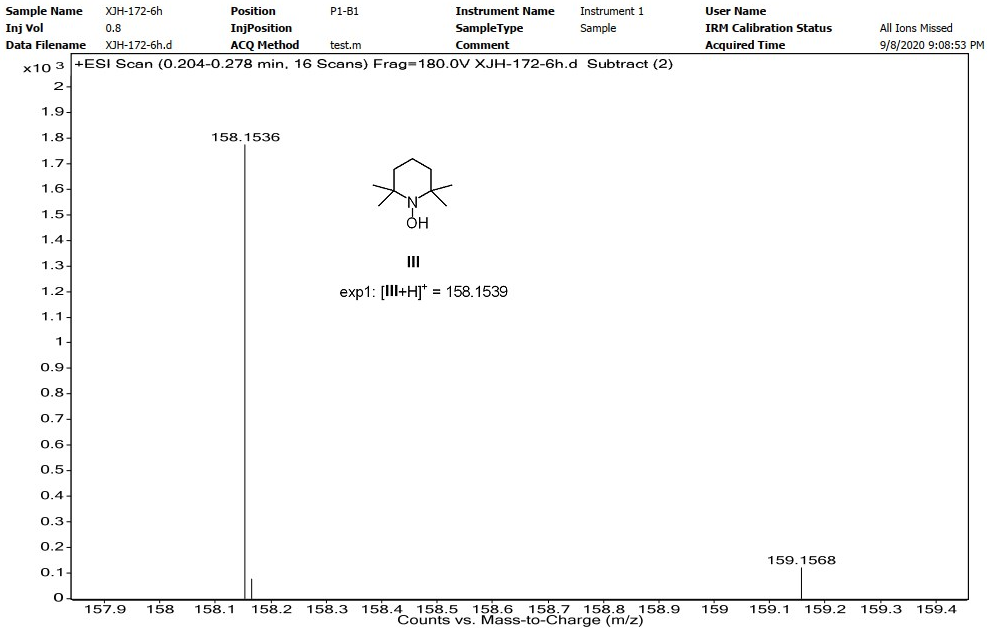


Figure S3. HRMS spectrum of compound [**III**+H]$^+$ for exp 1

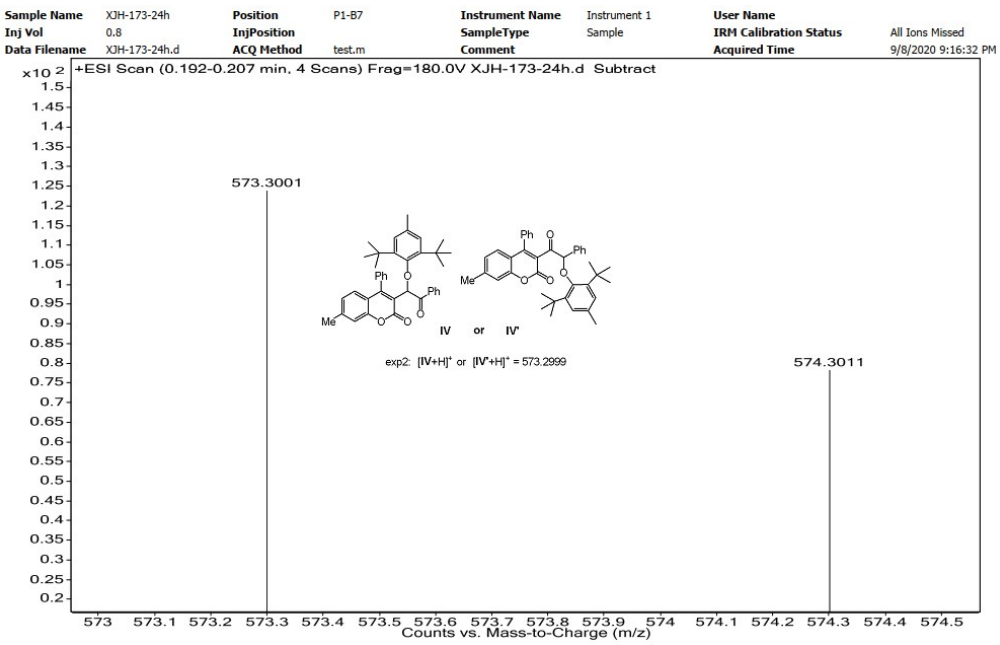


Figure S4. HRMS spectrum of compound [**IV/IV'**+H]$^+$ for exp 2

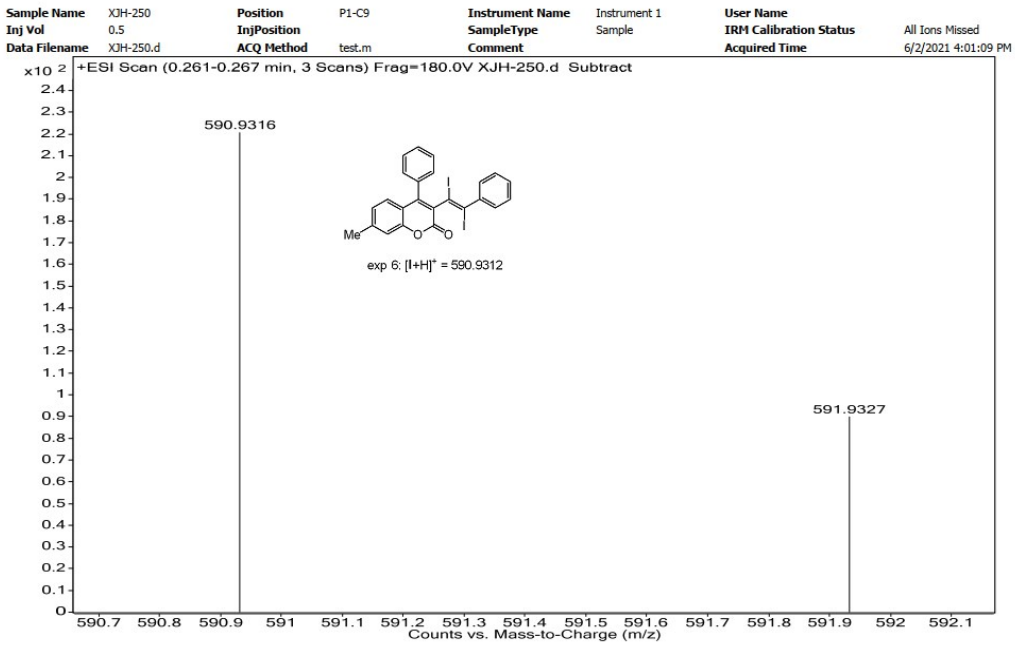
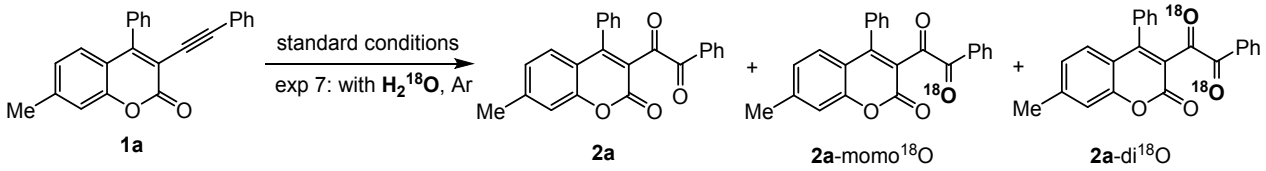


Figure S5. HRMS spectrum of compound [**I**+H]$^+$ for exp 6

4. $H_2{}^{18}O$ isotopic labeling experiments

3-Arylacetylene coumarin (**1a**, 67.9 mg, 0.2 mmol), I_2 (104.7 mg, 2 equiv.), $NaHCO_3$ (50.4 mg, 3 equiv.), DCE:$H_2{}^{18}O$ (2 mL, v/v = 200:3) stirred under 3 W blue LED (E = 5.00-5.15X10^4 lx, λ_{max} = 450-465 nm) under argon atmosphere and at room temperature for 24 hours. After the reaction was

complete, the reaction mixture was concentrated under reduced pressure, and the crude product was purified by silica gel column chromatography and preparative TLC to afford the corresponding product, which was measured HRMS (Fig. S6).



exp 7: **2a** : **2a**-momo^{18}O : **2a**-di^{18}O = 27% : 43% : 30% (total conversion: 40%)

Scheme S3. $H_2{}^{18}O$ isotopic labeling experiments under argon

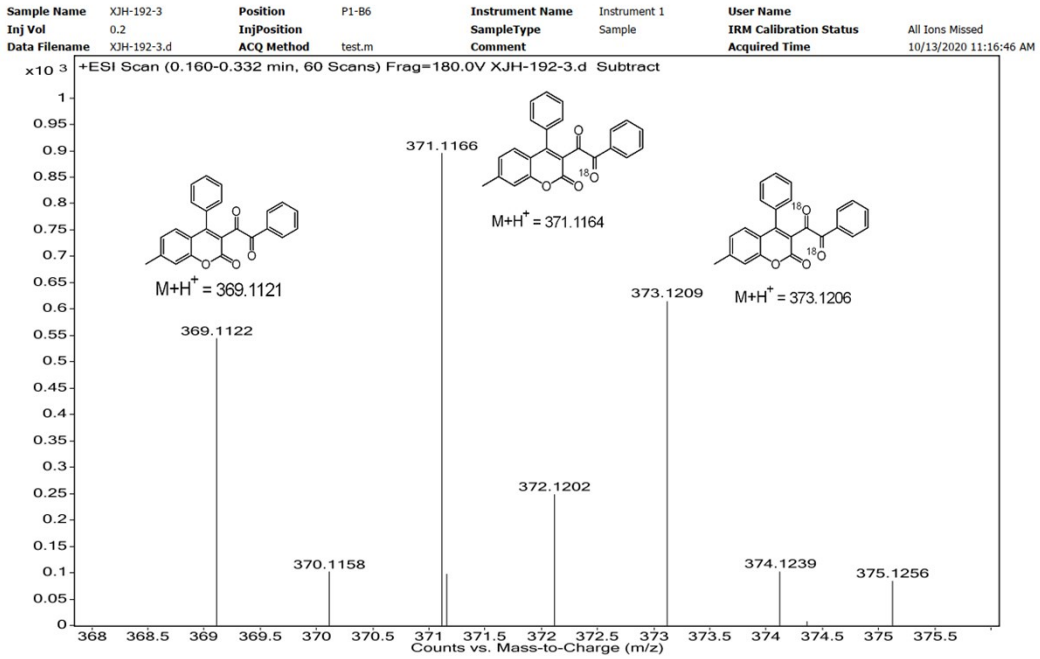
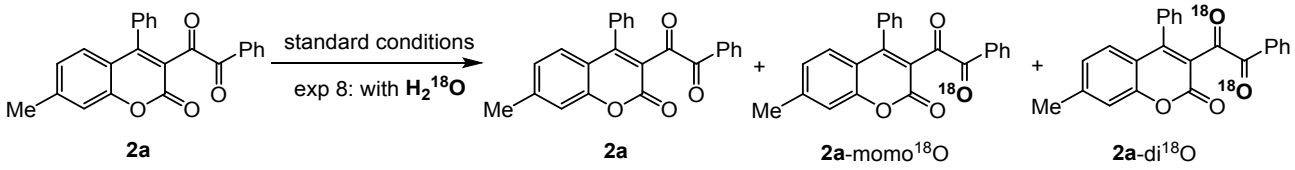


Figure S6. HRMS spectrum of compound [**2a**/**2a**-momo^{18}O/**2a**-di^{18}O+H]$^+$ for exp 7

3-Arylacetylene coumarin (**1a**, 67.9 mg, 0.2 mmol), I_2 (104.7 mg, 2 equiv.), $NaHCO_3$ (50.4 mg, 3 equiv.), DCE:$H_2{}^{18}O$ (2 mL, v/v = 200:3) stirred under 3 W blue LED (E = 5.00-5.15X10^4 lx, λ_{max} = 450-465 nm) under oxgen atmosphere and at room temperature for 24 hours. After the reaction was complete, the reaction mixture was concentrated under reduced pressure, and the crude product was purified by silica gel column chromatography and preparative TLC to afford the corresponding product, which was measured HRMS (Fig. S7-S8).



exp 8: **2a** : **2a**-mono^{18}O : **2a**-di^{18}O = 94% : 6% : 0% (total conversion: 95%)

Scheme S4. $H_2{}^{18}O$ isotopic labeling experiments

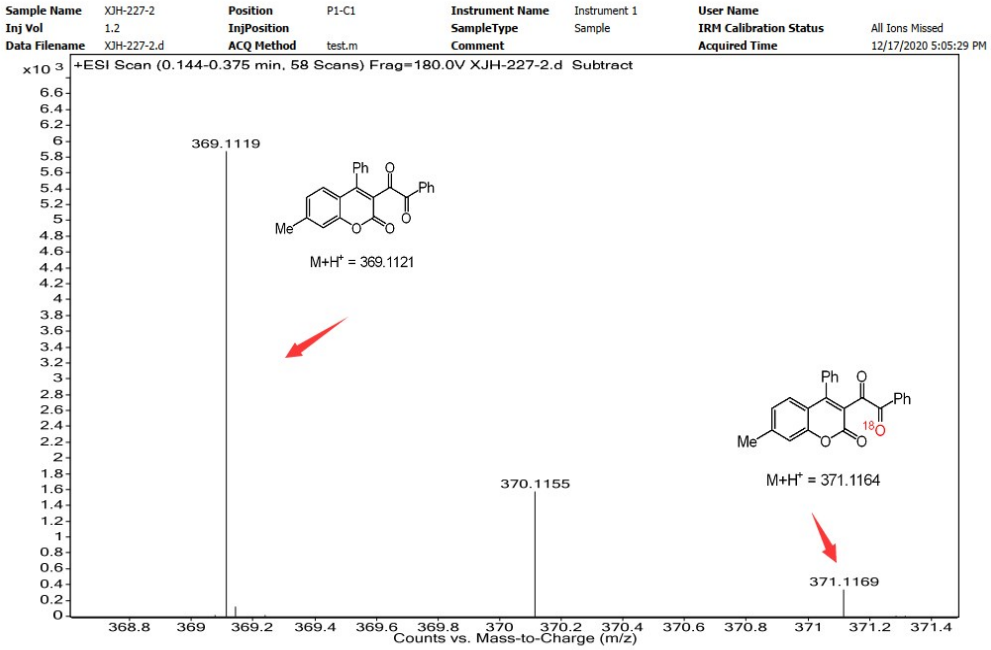


Figure S7. HRMS spectrum of compound [**2a**/**2a**-momo^{18}O+H]$^+$ for exp 8

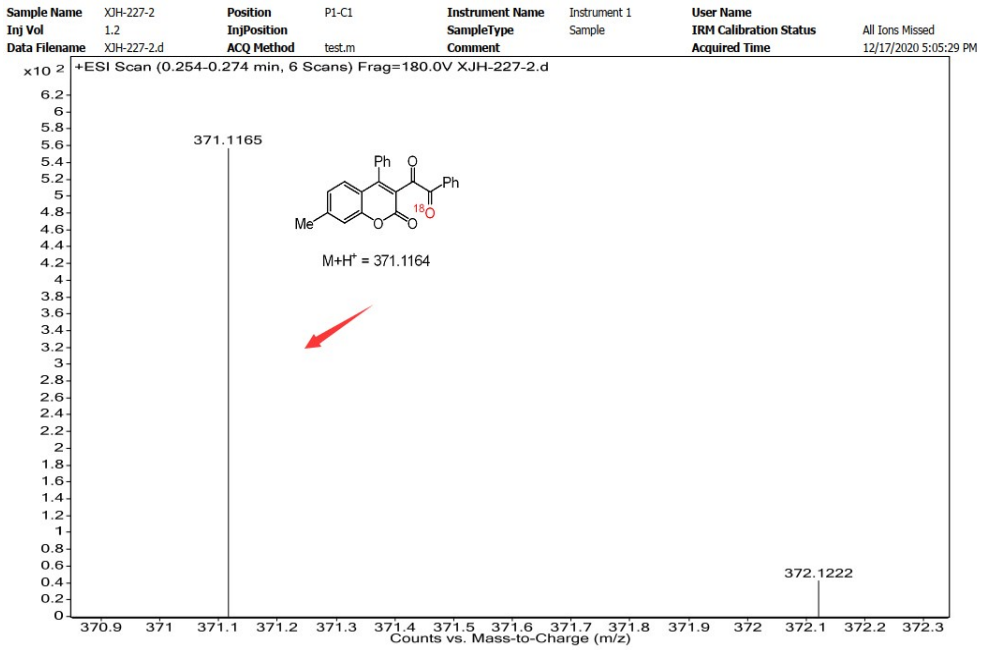


Figure S8. HRMS spectrum of compound [**2a**-momo^{18}O+H]$^+$ for exp 8

5. UV/Vis absorption spectra of 3-arylacetylene coumarin precursors.

The UV/Vis absorption spectra was recorded in MeCN of a 0.05 mM solution in 10 mm path length quartz cuvette on a Perkin Elmer Lambda 35 Spectrometer.

Table S1. UV/Vis absorption spectra of 3-arylacetylene coumarin precursors in acetonitrile solutions.

Compounds	λ_{max} (nm)
1p	356
1q	347
1r	423
1s	343
1t	346
1u	354
1v	342
1w	351
1x	342
1y	422
1z	422
1aa	423
1ab	424

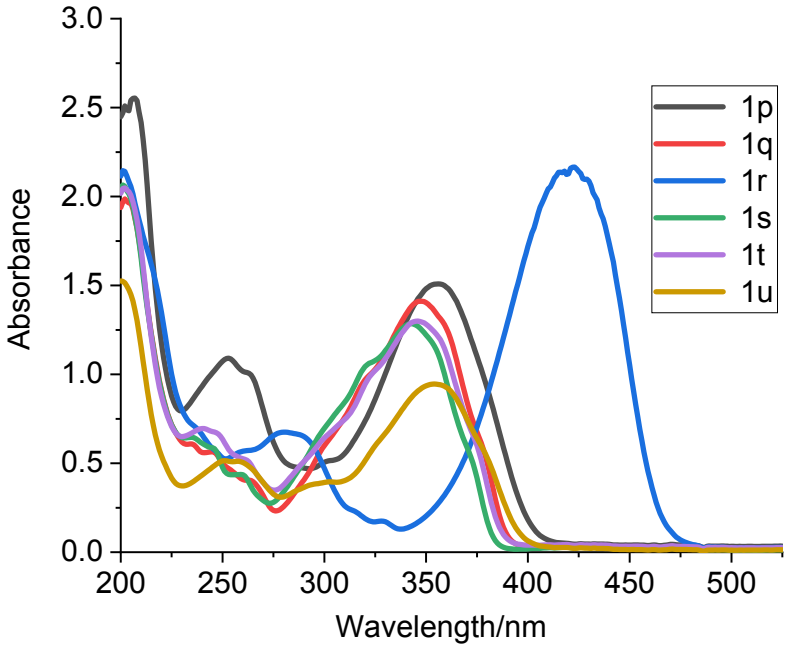


Figure S9. Absorption spectra of **1p-1u** in MeCN

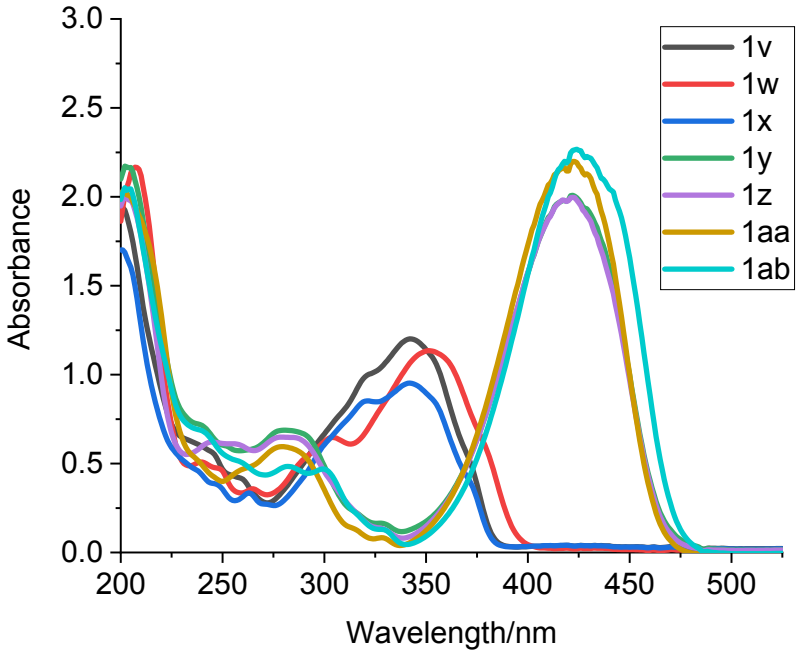
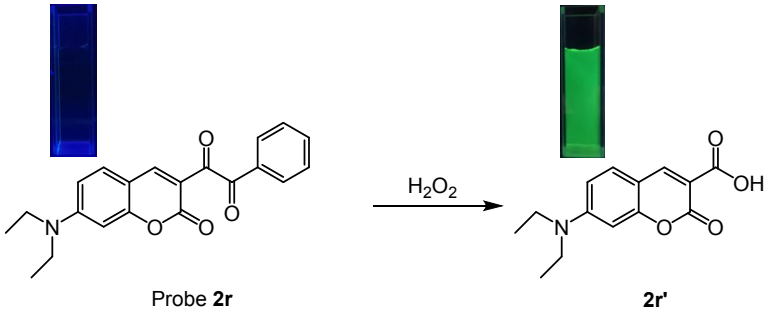


Figure S10. Absorption spectra of **1v-1ab** in MeCN

6. Fluorescent probe for hydrogen peroxide of 2r, 2z and 2ab

Probes **2r**, **2z**, **2ab** were dissolved in DMF for a stock solution (1 mM). H_2O_2 was from dilution of 30% solution in water. Test solutions (10 μM) were prepared by displacing 30 μL of the stock solution into a 3 mL mixture of 0.01 M PBS and CH_3CN (8:2, v/v) at pH 7.4.[4] The detection limit was calculated based on the fluorescence titration. Detection limit = 3σ/k. Where σ is the standard deviation of blank measurement, k is the slope between the fluorescence intensity ratio versus H_2O_2 concentration.

6.1 Fluorescent probe for hydrogen peroxide of 2r



Scheme S5. Fluorescent probe for hydrogen peroxide of **2r**

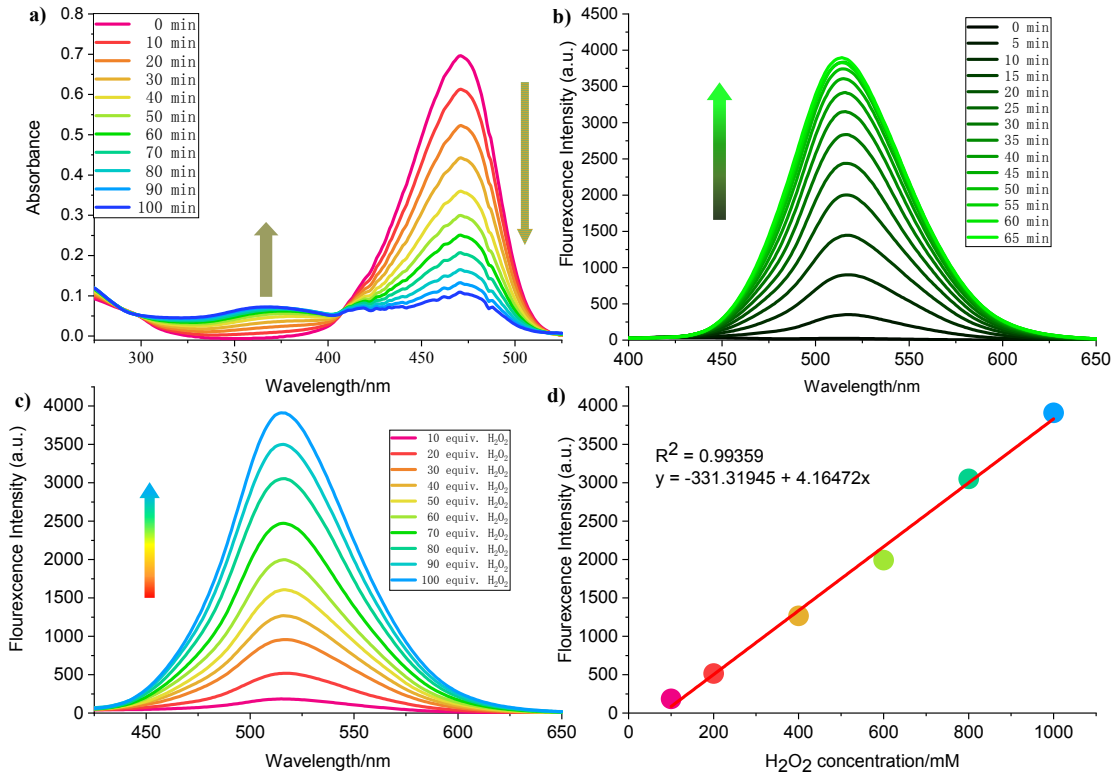


Figure S11. (a) Changes in the absorption spectra of compound **2r** in the presence of 100 equiv. of H_2O_2. (b) Time-dependent fluorescence spectral changes of compound **2r** with 100 equiv. of H_2O_2 (λ_{ex} = 360 nm, steady excitation). (c, d) Fluorescent emission spectra of compound **2r** (10 μM) in the presence of 10-100 equiv. of H_2O_2 (Data were acquired at 515 nm)

The fluorescence emission spectrum of probe **2r** was measured by 15 times and σ (the standard deviation of blank measurement) was achieved. The data were acquired at 515 nm (n = 15), and σ was 0.344621 by calculation. The k was 4.16472. Detection limit = 3σ/k = 0.2482 μM.

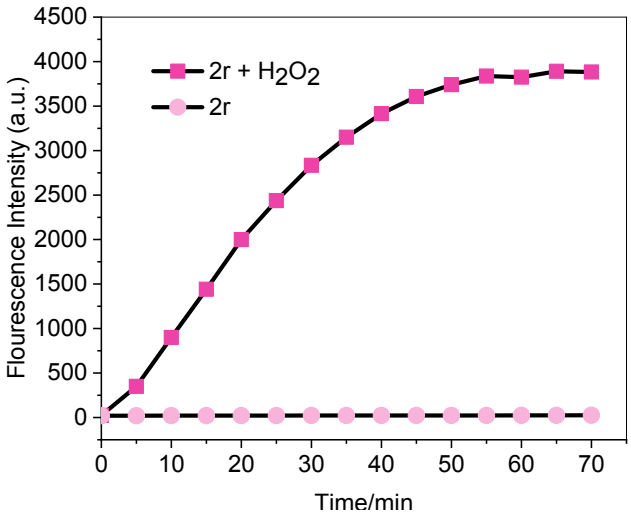
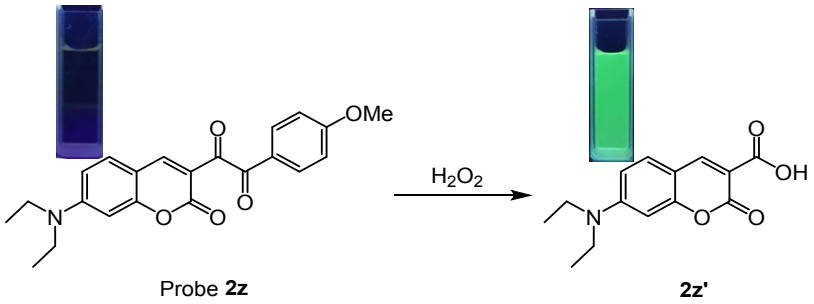


Figure S12. Intensity changes of **2r** in fluorescence at 515 nm (λ_{ex}= 360 nm) over time with or without H_2O_2

6.2 Fluorescent probe for hydrogen peroxide of 2z



Scheme S6. Fluorescent probe for hydrogen peroxide of **2z**

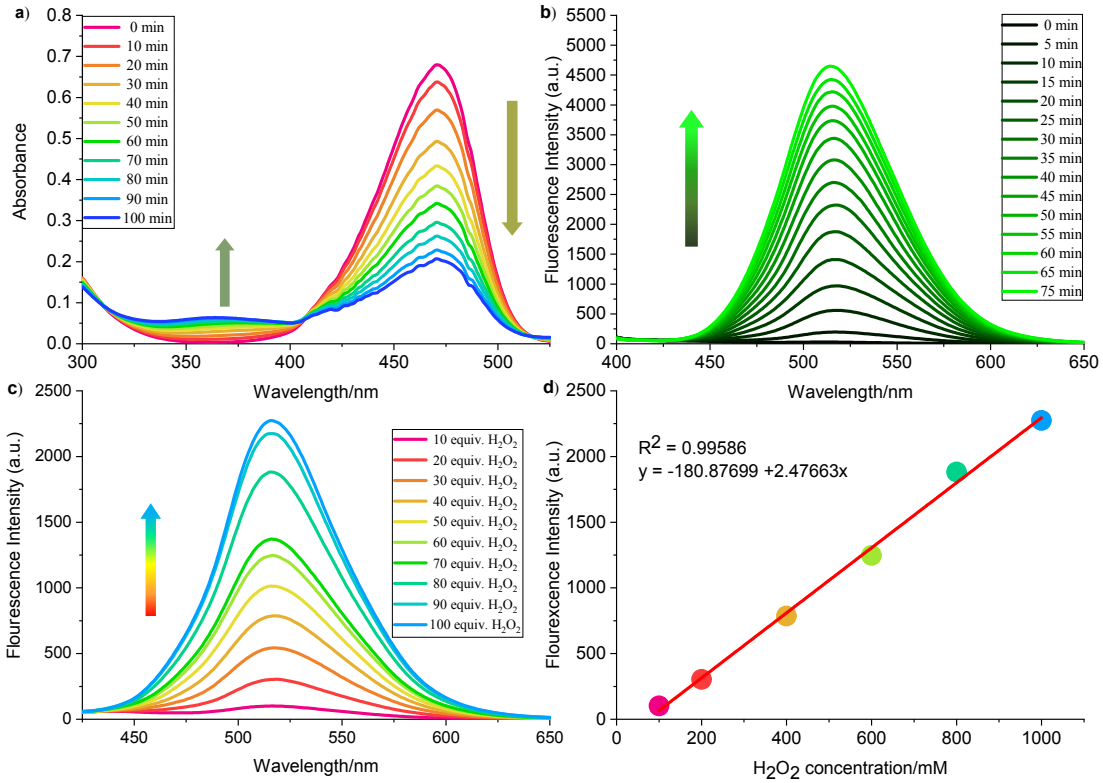


Figure S13. (a) Changes in the absorption spectra of compound **2z** in the presence of 100 equiv. of H_2O_2. (b) Time-dependent fluorescence spectral changes of compound **2z** with 100 equiv. of H_2O_2 (λ_{ex} = 360 nm, steady excitation). (c, d) Fluorescent emission spectra of compound **2z** (10 μM) in the presence of 10-100 equiv. of H_2O_2 (Data were acquired at 516 nm)

The fluorescence emission spectrum of probe **2z** was measured by 15 times and σ (the standard deviation of blank measurement) was achieved. The data were acquired at 516 nm (n = 15), and σ was 0.295761 by calculation. The k was 2.47663. Detection limit = 3σ/k = 0.358 μM.

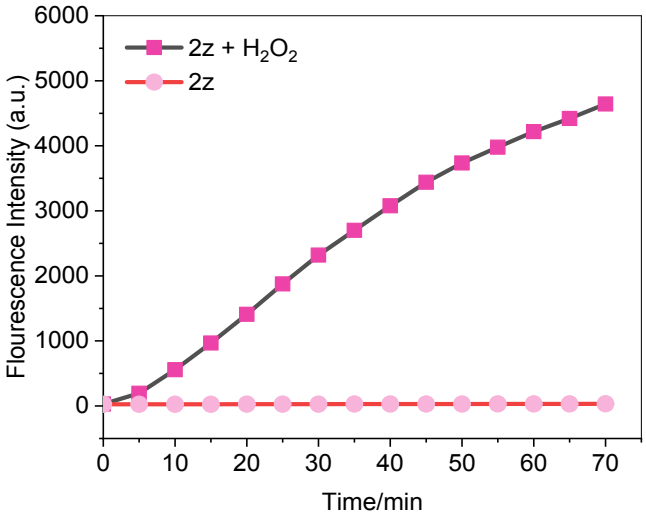
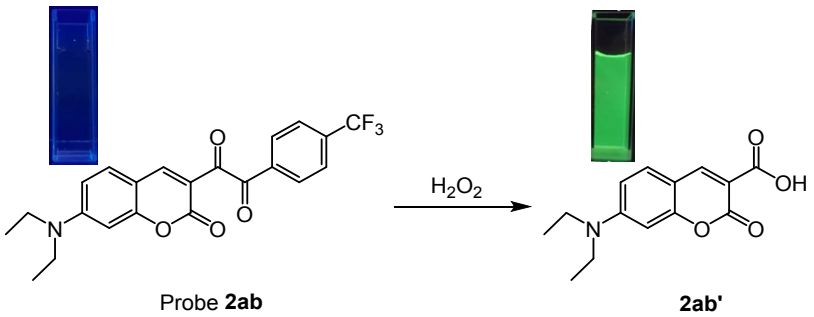


Figure S14. Intensity changes of **2z** in fluorescence at 516 nm (λ_{ex}= 360 nm) over time with or without H_2O_2

6.3 Fluorescent probe for hydrogen peroxide of 2ab



Scheme S7. Fluorescent probe for hydrogen peroxide of **2ab**

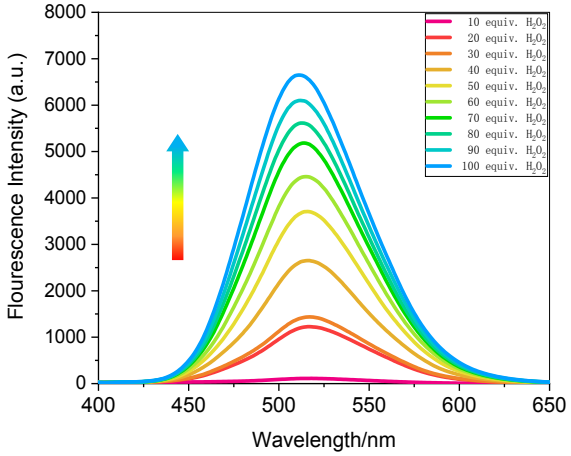


Figure S15. Fluorescent emission spectra of probe **2ab** (10 μM) in the presence of 10-100 equiv. of H_2O_2. Data were acquired at 512 nm

The fluorescence emission spectrum of probe **2ab** was measured by 15 times and σ (the standard deviation of blank measurement) was achieved. The data were acquired at 512 nm (n = 15), and σ was 0.364074 by calculation. The k was 7.29904. Detection limit = 3σ/k = 0.149 μM.

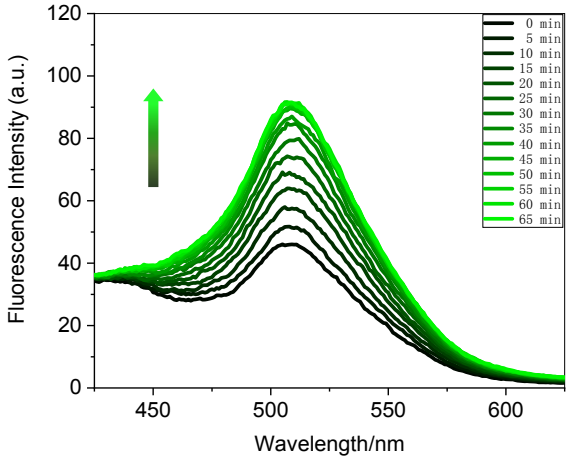


Figure S16. Time-dependent fluorescence spectral changes of probe **2ab** with 10 equiv. of H_2O_2 (λ_{ex} = 360 nm, steady excitation)

7. References

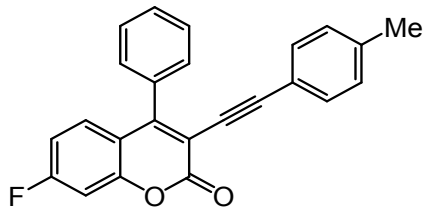
1 X. Wu, M. Jia, M. Huang, J. K. Kim, Z. Zhao, J. Liu, J. Xi, Y. Li and Y. Wu, *Org. Biomol. Chem.,* 2020*,* **18***,* 3346-3353.

2 J. Su, Y. Zhang, M. Chen, W. Li, X. Qin, Y. Xie, L. Qin, S. Huang and M. Zhang, *Synlett,* 2019, **30**, 630-634.

3 A. Wu, J. L. Kolanowski, B. B. Boumelhem, K. Yang, R. Lee, A. Kaur, S. T. Fraser, E. J. New and L. M. Rendina, *Chem. Asian J.,* 2017, **12**, 1704-1708.

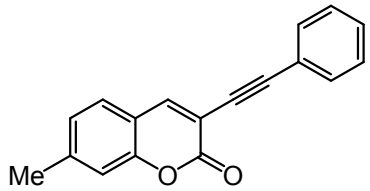
4 K. M. Zhang, W. Dou, P. X. Li, R. Shen, J. X. Ru, W. Liu, Y. M. Cui, C. Y. Chen, W. S. Liu and D. C. Bai, *Biosens. Bioelectron.*, 2015, **64**, 542-546.

8. Characterization data



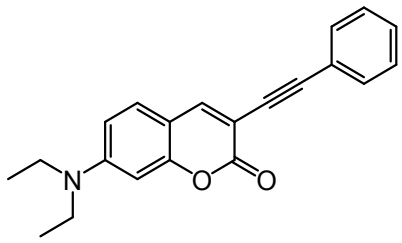
7-fluoro-4-phenyl-3-(*p*-tolylethynyl)-2*H*-chromen-2-one (1p)

Yellow solid (53.0 mg, 75%), mp. 204.9 - 207.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61 - 7.52 (m, 3 H), 7.51 - 7.44 (m, 2 H), 7.30 - 7.23 (m, 1 H), 7.15 - 7.08 (m, 3 H), 7.07 - 7.01 (m, 2 H), 6.94 (td, J = 2.5, 8.4 Hz, 1 H), 2.31 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.4 (d, J = 255.3 Hz), 159.2, 155.2, 153.9 (d, J = 13.2 Hz), 139.2, 134.3, 131.6, 129.5, 129.3 (d, J = 10.3 Hz), 129.1, 129.0, 128.5, 119.3, 116.6 (d, J = 2.9 Hz), 112.6 (d, J = 22.7), 110.3 (d, J = 2.9 Hz), 104.5 (d, J = 25.7 Hz), 99.1, 82.9, 21.6. ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -104.8. HRMS (ESI) calcd. for $C_{24}H_{15}FO_2$ $(M+H)^+$: 355.1129, found: 355.1128.



7-methyl-3-(phenylethynyl)-2*H*-chromen-2-one (1q)

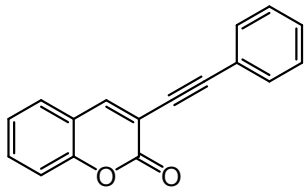
White solid (38.1 mg, 73%). mp. 166.6 - 169.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (s, 1 H), 7.57 (dd, J = 3.0, 6.5 Hz, 2 H), 7.40 - 7.32 (m, 4 H), 7.16 - 7.08 (m, 2 H), 2.46 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.6, 153.5, 144.8, 143.7, 131.9, 129.0, 128.4, 127.4, 126.1, 122.4, 117.0, 116.6, 111.8, 95.3, 83.5, 21.9. HRMS (ESI) calcd. for $C_{18}H_{12}O_2$ $(M+H)^+$: 261.0910, found: 261.0909.



7-(diethylamino)-3-(phenylethynyl)-2*H*-chromen-2-one (1r)

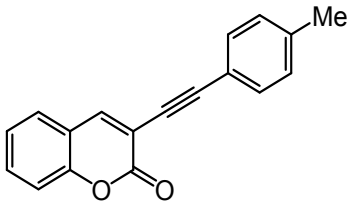
Yellow solid (59.1 mg, 92%), mp. 145.7 - 148.6 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 (s, 1 H), 7.58 - 7.51 (m, 2 H), 7.36 - 7.30 (m, 3 H), 7.27 - 7.22 (m, 1 H), 6.58 (dd, J = 2.4, 8.9 Hz, 1 H), 6.49 (d, J = 2.3 Hz, 1 H), 3.42 (q, J = 7.1 Hz, 4 H), 1.22 (t, J = 7.1 Hz, 6 H). ^{13}C NMR (100 MHz, $CDCl_3$):

δ 161.0, 156.3, 151.1, 145.5, 131.7, 128.9, 128.4, 128.3, 123.1, 109.2, 108.4, 104.7, 97.3, 93.3, 84.6, 45.0, 12.5. HRMS (ESI) calcd. for $C_{21}H_{19}NO_2$ $(M+H)^+$: 318.1489, found: 318.1488.



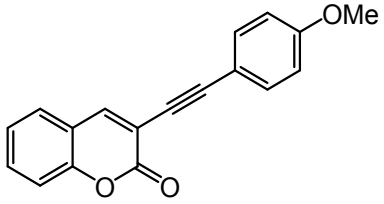
3-(phenylethynyl)-2*H*-chromen-2-one (1s)

Light yellow solid (30.6 mg, 62%), mp. 174.6 - 176.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (s, 1 H), 7.63 - 7.46 (m, 4 H), 7.40 - 7.27 (m, 5 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.3, 153.3, 144.7, 132.1, 132.0, 129.1, 128.4, 127.7, 124.8, 122.2, 118.9, 116.8, 113.1, 95.8, 83.3. HRMS (ESI) calcd. for $C_{17}H_{10}O_2$ $(M+H)^+$: 247.0754, found: 247.0755.



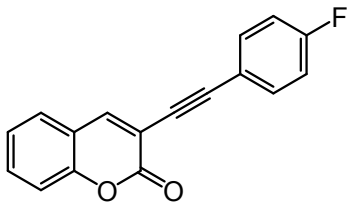
3-(*p*-tolylethynyl)-2*H*-chromen-2-one (1t)

Yellow solid (36.3 mg, 70%), mp. 132.3 - 135.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (s, 1 H), 7.56 - 7.43 (m, 4 H), 7.36 - 7.25 (m, 2 H), 7.16 (d, J = 7.9 Hz, 2 H), 2.37 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.4, 153.2, 144.4, 139.5, 132.0, 131.9, 129.2, 127.7, 124.8, 119.1, 119.0, 116.8, 113.2, 96.2, 82.8, 21.6. HRMS (ESI) calcd. for $C_{18}H_{12}O_2$ $(M+H)^+$: 261.0910, found: 261.0912.



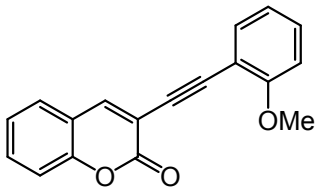
3-((4-methoxyphenyl)ethynyl)-2*H*-chromen-2-one (1u)

Yellow solid (33.1 mg, 60%), mp. 162.1 - 164.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.90 (s, 1 H), 7.55 - 7.46 (m, 4 H), 7.37 - 7.27 (m, 2 H), 6.88 (d, J = 8.8 Hz, 2 H), 3.83 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.3, 159.4, 153.2, 144.0, 133.6, 131.9, 127.6, 124.8, 119.0, 116.8, 114.3, 114.1, 113.4, 96.2, 82.3, 55.3. HRMS (ESI) calcd. for $C_{18}H_{12}O_3$ $(M+H)^+$: 277.0859, found: 277.0856.



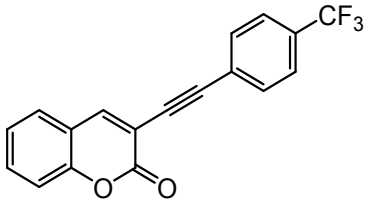
3-((4-fluorophenyl)ethynyl)-2*H*-chromen-2-one (1v)

White solid (37.9 mg, 77%), mp. 61.5 - 61.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.94 (s, 1 H), 7.64 - 7.45 (m, 4 H), 7.40 - 7.27 (m, 2 H), 7.12 - 7.01 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.0 (d, J = 250.9 Hz), 159.3, 153.3, 144.7, 134.0 (d, J = 8.8 Hz), 132.2, 127.7, 124.9, 118.9, 118.3 (d, J = 2.9 Hz), 116.8, 115.9 (d, J = 22.0 Hz), 113.0, 94.7, 83.1. HRMS (ESI) calcd. for $C_{17}H_9FO_2$ $(M+H)^+$: 265.0659, found: 265.0656.



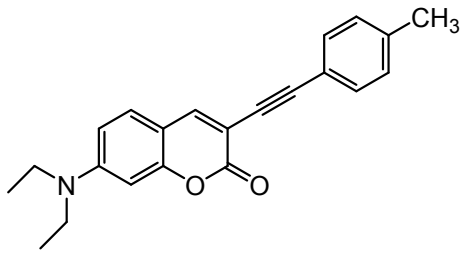
3-((2-methoxyphenyl)ethynyl)-2*H*-chromen-2-one (1w)

Yellow solid (29.0 mg, 53%), mp. 107.3 - 109.6 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (s, 1 H), 7.58 - 7.45 (m, 3 H), 7.38 - 7.25 (m, 3 H), 6.98 - 6.89 (m, 2 H), 3.93 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.3, 159.4, 153.3, 144.4, 134.0, 132.0, 130.8, 127.7, 124.8, 120.5, 119.0, 116.8, 113.4, 111.4, 110.7, 92.5, 87.3, 55.9. HRMS (ESI) calcd. for $C_{18}H_{12}O_3$ $(M+H)^+$: 277.0859, found: 277.0861.



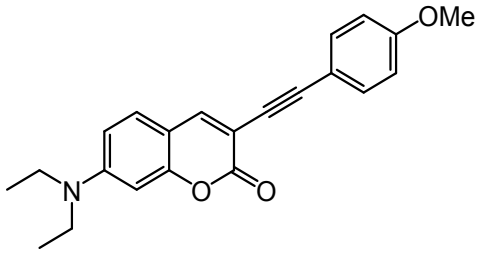
3-((4-(trifluoromethyl)phenyl)ethynyl)-2*H*-chromen-2-one (1x)

Yellow solid (48.5 mg, 77%), mp. 140.3 - 142.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 (s, 1 H), 7.71 - 7.66 (m, J = 8.2 Hz, 2 H), 7.65 - 7.60 (m, J = 8.4 Hz, 2 H), 7.57 (td, J = 1.6, 7.8 Hz, 1 H), 7.51 (dd, J = 1.4, 7.8 Hz, 1 H), 7.39 - 7.29 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.1, 153.5, 145.6, 132.6, 132.2, 130.7 (q, J = 33.0 Hz), 127.9, 126.0 (d, J = 1.47 Hz), 125.4 (q, J = 3.7 Hz), 125.0, 123.8 (d, J = 272.2 Hz), 118.7, 116.9, 112.5, 94.0, 85.5. ^{19}F NMR (376.5 MHz, CDCl3): δ -62.9. HRMS (ESI) calcd. for $C_{18}H_9F_3O_2$ $(M+H)^+$: 315.0627, found: 315.0627.



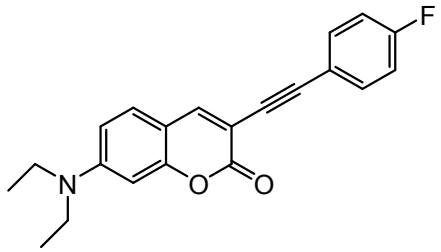
7-(diethylamino)-3-(*p*-tolylethynyl)-2*H*-chromen-2-one (1y)

Yellow solid (58.6 mg, 88%), mp. 182.5 - 184.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 (s, 1 H), 7.47 - 7.41 (m, J = 8.1 Hz, 2 H), 7.24 (d, J = 8.8 Hz, 1 H), 7.17 - 7.10 (m, J = 7.9 Hz, 2 H), 6.58 (dd, J = 2.4, 8.9 Hz, 1 H), 6.52 - 6.45 (m, 1 H), 3.42 (q, J = 7.1 Hz, 4 H), 2.36 (s, 3 H), 1.22 (t, J = 7.1 Hz, 6 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.0, 156.2, 151.0, 145.2, 138.5, 131.6, 129.0, 128.8, 120.0, 109.2, 108.5, 105.0, 97.3, 93.5, 83.9, 44.9, 21.5, 12.5. HRMS (ESI) calcd. for $C_{22}H_{21}NO_2$ $(M+H)^+$: 332.1645, found: 332.1645.



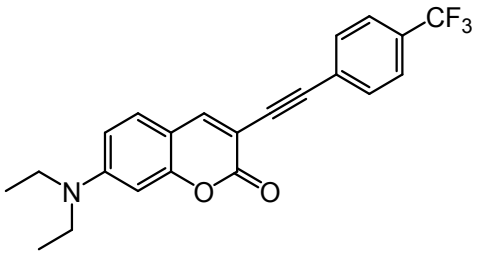
7-(diethylamino)-3-((4-methoxyphenyl)ethynyl)-2*H*-chromen-2-one (1z)

Yellow solid (59.6 mg, 85%), mp. 135.1 - 137.6 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (s, 1 H), 7.51 - 7.45 (m, 2 H), 7.23 (d, J = 8.8 Hz, 1 H), 6.88 - 6.83 (m, 2 H), 6.57 (dd, J = 2.5, 8.9 Hz, 1 H), 6.47 (d, J = 2.3 Hz, 1 H), 3.82 (s, 3 H), 3.41 (q, J = 7.1 Hz, 4 H), 1.21 (t, J = 7.1 Hz, 6 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.1, 159.7, 156.1, 150.9, 145.0, 133.2, 128.8, 115.2, 113.9, 109.2, 108.5, 105.0, 97.3, 93.4, 83.3, 55.3, 44.9, 12.5. HRMS (ESI) calcd. for $C_{22}H_{21}NO_3$ $(M+H)^+$: 348.1594, found: 348.1598.



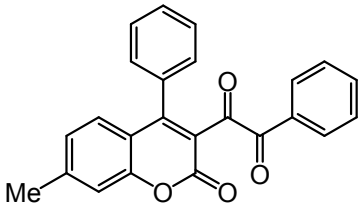
7-(diethylamino)-3-((4-fluorophenyl)ethynyl)-2*H*-chromen-2-one (1aa)

Yellow solid (61.8 mg, 92%), mp. 163.7 - 165.6 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (s, 1 H), 7.56 - 7.49 (m, 2 H), 7.24 (s, 1 H), 7.02 (t, J = 8.7 Hz, 2 H), 6.59 (dd, J = 2.3, 8.8 Hz, 1 H), 6.49 (s, 1 H), 3.43 (d, J = 7.1 Hz, 4 H), 1.22 (t, J = 7.2 Hz, 6 H).^{13}C NMR (100 MHz, $CDCl_3$): δ 162.6 (d, J = 249.2 Hz), 160.9, 156.3, 151.1, 145.5, 133.6, 128.9, 119.2 (d, J = 3.67 Hz), 115.6 (d, J = 22.0 Hz), 109.3, 108.4, 104.5, 97.4, 92.2, 84.3, 45.0, 12.5. ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -110.73. HRMS (ESI) calcd. for $C_{21}H_{18}FNO_2$ $(M+H)^+$: 336.1394, found: 336.1394.



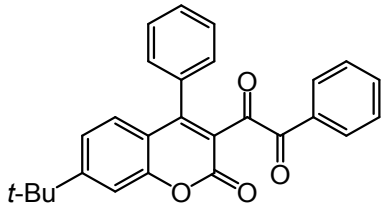
7-(diethylamino)-3-((4-(trifluoromethyl)phenyl)ethynyl)-2*H*-chromen-2-one (1ab)

White solid (68.9 mg, 89%), mp. 184.7 - 186.4 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.83 (s, 1 H), 7.66 - 7.61 (m, J = 8.1 Hz, 2 H), 7.61 - 7.56 (m, J = 8.6 Hz, 2 H), 7.29 - 7.24 (m, 1 H), 6.60 (dd, J = 2.4, 8.9 Hz, 1 H), 6.49 (d, J = 2.3 Hz, 1 H), 3.43 (q, J = 7.1 Hz, 4 H), 1.23 (t, J = 7.1 Hz, 6 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.8, 156.5, 151.4, 146.3, 131.8, 129.8 (q, J = 33.0 Hz), 129.2, 126.9 (d, J = 1.5 Hz), 124.0 (q, J = 272.2 Hz), 125.2 (q, J = 3.7 Hz), 109.4, 108.3, 103.8, 97.3, 91.8, 87.2, 45.0, 12.5. ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -62.8. HRMS (ESI) calcd. for $C_{22}H_{18}F_3NO_3$ $(M+H)^+$: 386.1362, found: 386.1362.



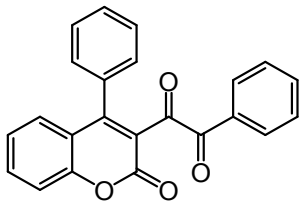
1-(7-methyl-2-oxo-4-phenyl-2*H*-chromen-3-yl)-2-phenylethane-1,2-dione (2a)

Yellow solid (64.0 mg, 87%), mp. 150.1 - 151.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (d, J = 7.5 Hz, 2 H), 7.62 - 7.53 (m, 1 H), 7.50 - 7.35 (m, 7 H), 7.28 - 7.22 (m, 1 H), 7.18 (d, J = 8.2 Hz, 1 H), 7.06 (d, J = 8.1 Hz, 1 H), 2.47 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.3, 190.7, 159.8, 158.9, 154.3, 145.9, 134.2, 132.5, 132.0, 130.4, 130.4, 129.6, 128.8, 128.7, 128.5, 128.3, 126.3, 121.8, 117.5, 117.3, 21.9. HRMS (ESI) calcd. for $C_{24}H_{16}O_4$ $(M+H)^+$: 369.1121, found: 369.1123.



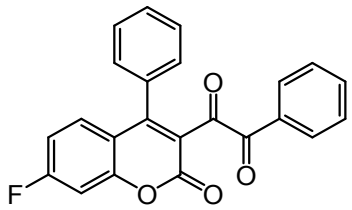
1-(7-(*tert*-butyl)-2-oxo-4-phenyl-2*H*-chromen-3-yl)-2-phenylethane-1,2-dione (2b)

Yellow solid (62.0 mg, 76%), mp. 173.7 - 175.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 - 7.92 (m, 2 H), 7.59 (t, J = 7.5 Hz, 1 H), 7.49 - 7.42 (m, 6 H), 7.42 - 7.37 (m, 2 H), 7.33 - 7.27 (m, 1 H), 7.25 (d, J = 8.4 Hz, 1 H), 1.35 (s, 9 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.3, 190.7, 160.0, 159.0, 158.8, 154.3, 134.2, 132.5, 132.0, 130.4, 129.6, 128.7, 128.7, 128.5, 128.2, 122.6, 122.0, 117.2, 114.1, 35.5, 30.9. HRMS (ESI) calcd. for $C_{27}H_{22}O_4$ $(M+H)^+$: 394.2013, found: 394.2015.



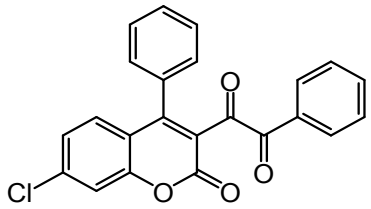
1-(2-oxo-4-phenyl-2*H*-chromen-3-yl)-2-phenylethane-1,2-dione (2c)

Yellow solid (52.5 mg, 74%), mp. 178.1 - 180.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02 - 7.94 (m, 2 H), 7.69 - 7.55 (m, 2 H), 7.52 - 7.38 (m, 8 H), 7.36 - 7.31 (m, 1 H), 7.30 - 7.23 (m, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.0, 190.4, 159.5, 158.5, 154.1, 134.3, 133.9, 132.2, 131.8, 130.5, 129.7, 129.1, 128.7, 128.6, 128.3, 125.0, 123.2, 119.6, 117.3. HRMS (ESI) calcd. for $C_{23}H_{14}O_4$ $(M+H)^+$: 355.0965, found: 355.0967.



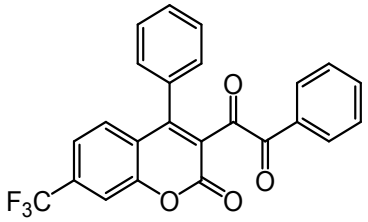
1-(7-fluoro-2-oxo-4-phenyl-2*H*-chromen-3-yl)-2-phenylethane-1,2-dione (2d)

Yellow solid (49.2 mg, 66%), mp. 165.8 - 167.4 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99 - 7.93 (m, 2 H), 7.64 - 7.56 (m, 1 H), 7.51 - 7.42 (m, 5 H), 7.41 - 7.36 (m, 2 H), 7.33 (dd, J = 6.1, 8.9 Hz, 1 H), 7.16 (dd, J = 2.3, 8.7 Hz, 1 H), 7.00 (td, J = 2.4, 8.4 Hz, 1 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.7, 190.4, 165.7 (d, J = 258.23 Hz), 159.2, 158.1, 155.4 (d, J = 13.2 Hz), 134.4, 132.1, 131.8, 131.1 (d, J = 10.3 Hz), 130.4, 129.9, 128.9, 128.6, 128.2, 122.2 (d, J = 2.9 Hz), 116.5 (d, J = 2.9 Hz), 113.3 (d, J = 22.7 Hz), 104.9 (d, J = 25.7 Hz). ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -101.2. HRMS (ESI) calcd. for $C_{23}H_{13}FO_4$ $(M+Na)^+$: 395.0690, found: 395.0693.



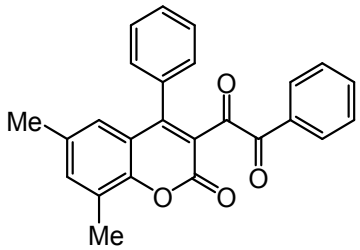
1-(7-chloro-2-oxo-4-phenyl-2*H*-chromen-3-yl)-2-phenylethane-1,2-dione (2e)

Yellow solid (54.3 mg, 70%). mp. 225.8 - 227.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 - 7.91 (m, 2 H), 7.63 - 7.56 (m, 1 H), 7.50 - 7.42 (m, 6 H), 7.41 - 7.34 (m, 2 H), 7.29 - 7.20 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.6, 190.3, 158.9, 157.8, 154.3, 140.1, 134.4, 131.9, 131.7, 130.5, 129.9, 128.9, 128.6, 128.2, 125.6, 123.1, 118.3, 117.6. HRMS (ESI) calcd. for $C_{23}H_{13}ClO_4$ $(M+Na)^+$: 411.0395, found: 411.0396.



1-(2-oxo-4-phenyl-7-(trifluoromethyl)-2*H*-chromen-3-yl)-2-phenylethane-1,2-dione (2f)

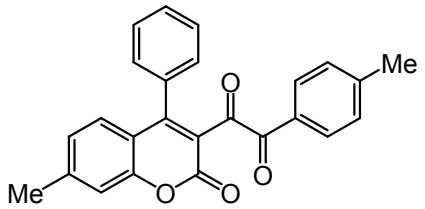
Yellow solid (45.5 mg, 54%), mp. 148.1 - 149.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02 - 7.94 (m, 2 H), 7.71 (s, 1 H), 7.65 - 7.57 (m, 1 H), 7.53 - 7.44 (m, 8 H), 7.41 (dd, J = 3.0, 6.7 Hz, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.1, 189.9, 158.6, 156.7, 153.6, 135.0 (q, J = 33.8 Hz), 134.6, 131.6, 131.4, 130.5, 130.1, 129.8, 129.0, 128.6, 128.3, 125.4, 122.9 (q, J = 272.9 Hz), 122.2, 121.4 (q, J = 3.67 Hz), 114.8 (q, J = 3.7 Hz). ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -63.14. HRMS (ESI) calcd. for $C_{24}H_{13}F_3O_4$ $(M+H)^+$: 423.0839, found: 423.0838.



1-(6,8-dimethyl-2-oxo-4-phenyl-2*H*-chromen-3-yl)-2-phenylethane-1,2-dione (2g)

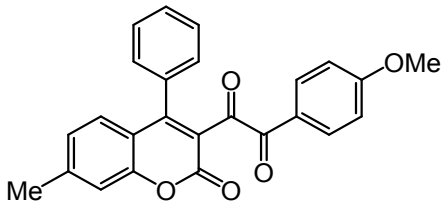
Yellow solid (67.1 mg, 88%), mp. 152.9 - 155.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (d, J = 7.5 Hz, 2 H), 7.61 - 7.53 (m, 1 H), 7.50 - 7.41 (m, 5 H), 7.41 - 7.35 (m, 2 H), 7.30 (s, 1 H), 6.89 (s, 1 H), 2.45 (s, 3 H), 2.26 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.3, 190.6, 159.8, 158.9, 150.7, 136.5,

134.2, 134.1, 132.7, 132.0, 130.4, 129.5, 128.6, 128.5, 128.3, 126.5, 126.4, 122.6, 119.2, 20.9, 15.5. HRMS (ESI) calcd. for $C_{25}H_{18}O_4$ $(M+Na)^+$: 405.1097, found: 405.1098.



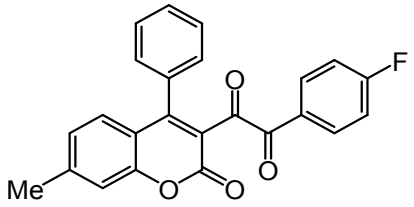
1-(7-methyl-2-oxo-4-phenyl-2*H*-chromen-3-yl)-2-(*p*-tolyl)ethane-1,2-dione (2h)

Yellow solid (64.8 mg, 85%), mp. 63.3 - 65.1 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 (d, J = 8.2 Hz, 2 H), 7.49 - 7.43 (m, 3 H), 7.41 - 7.36 (m, 2 H), 7.25 (d, J = 8.6 Hz, 3 H), 7.18 (d, J = 8.2 Hz, 1 H), 7.06 (dd, J = 1.0, 8.2 Hz, 1 H), 2.47 (s, 3 H), 2.40 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.4, 190.3, 159.8, 158.7, 154.2, 145.8, 145.4, 132.6, 130.5, 129.6, 129.5, 129.3, 128.8, 128.7, 128.3, 126.2, 122.0, 117.4, 117.3, 21.9. HRMS (ESI) calcd. for $C_{25}H_{18}O_4$ $(M+Na)^+$: 405.1097, found: 405.1099.



1-(4-methoxyphenyl)-2-(7-methyl-2-oxo-4-phenyl-2*H*-chromen-3-yl)ethane-1,2-dione (2i)

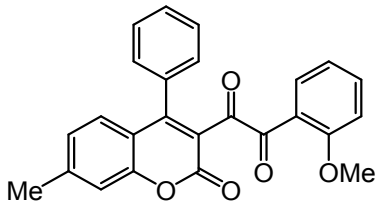
Yellow oil (65.5 mg, 82%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99 - 7.92 (m, 2 H), 7.48 - 7.42 (m, 3 H), 7.42 - 7.35 (m, 2 H), 7.23 (s, 1 H), 7.18 (d, J = 8.2 Hz, 1 H), 7.09 - 7.01 (m, 1 H), 6.95 - 6.87 (m, 2 H), 3.86 (s, 3 H), 2.47 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.5, 189.2, 164.5, 159.7, 158.4, 154.2, 145.7, 132.9, 132.6, 129.5, 128.7, 128.6, 128.3, 126.2, 124.9, 122.3, 117.4, 117.3, 114.0, 55.6, 21.9. HRMS (ESI) calcd. for $C_{25}H_{18}O_5$ $(M+Na)^+$: 421.1046, found: 421.1047.



1-(4-fluorophenyl)-2-(7-methyl-2-oxo-4-phenyl-2*H*-chromen-3-yl)ethane-1,2-dione (2j)

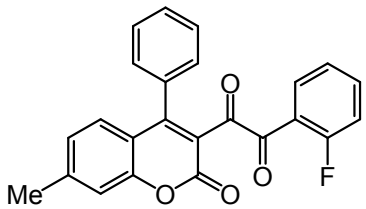
Yellow solid (61.7 mg, 80%), mp. 126.4 - 128.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.04 - 7.97 (m, 2 H), 7.50 - 7.43 (m, 3 H), 7.41 - 7.36 (m, 2 H), 7.26 (d, J = 3.2 Hz, 1 H), 7.20 (d, J = 8.2 Hz, 1 H), 7.16 - 7.05 (m, 3 H), 2.49 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.2, 189.1, 166.5 (d, J = 256.8 Hz), 159.9, 159.0, 154.3, 146.0, 133.2 (d, J = 9.5 Hz), 132.4, 129.7, 128.9, 128.7, 128.4 (d, J = 2.9

Hz), 128.2, 126.3, 121.7, 117.5, 117.3, 115.8 (d, J = 22.0 Hz), 21.9. ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -120.6. HRMS (ESI) calcd. for $C_{24}H_{15}FO_4$ $(M+Na)^+$: 409.0847, found: 409.0849.



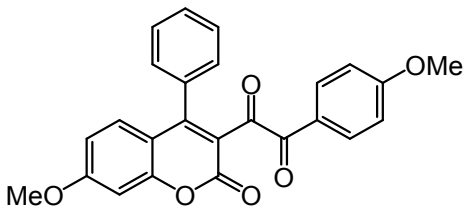
1-(2-methoxyphenyl)-2-(7-methyl-2-oxo-4-phenyl-2*H*-chromen-3-yl)ethane-1,2-dione (2l)

Yellow solid (51.5 mg, 65%). mp. 147.3 - 149.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 (dd, J = 1.7, 7.8 Hz, 1 H), 7.55 - 7.45 (m, 4 H), 7.36 - 7.29 (m, 2 H), 7.23 (s, 1 H), 7.16 - 7.11 (m, 1 H), 7.07 - 7.01 (m, 2 H), 6.93 (d, J = 8.4 Hz, 1 H), 3.74 (s, 3 H), 2.47 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.8, 189.4, 160.8, 160.3, 159.9, 154.5, 146.2, 135.7, 133.3, 131.0, 129.3, 129.1, 128.5, 127.8, 126.1, 122.9, 121.1, 118.8, 117.9, 117.3, 112.5, 56.2, 21.9. HRMS (ESI) calcd. for $C_{25}H_{18}O_5$ $(M+H)^+$: 399.1127, found: 399.1129.



1-(2-fluorophenyl)-2-(7-methyl-2-oxo-4-phenyl-2*H*-chromen-3-yl)ethane-1,2-dione (2m)

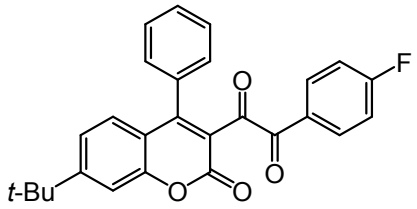
White solid (30.7 mg, 41%), mp. 178.3 - 180.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02 - 7.93 (m, 1 H), 7.63 - 7.54 (m, 1 H), 7.53 - 7.45 (m, 3 H), 7.36 (dd, J = 2.8, 6.4 Hz, 2 H), 7.29 - 7.24 (m, 3 H), 7.18 (d, J = 8.3 Hz, 1 H), 7.14 - 7.04 (m, 2 H), 2.49 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.8, 188.5, 162.8 (d, J = 258.9 Hz), 161.0, 160.3, 154.5, 146.5, 136.0 (d, J = 9.5 Hz), 132.8, 131.2 (d, J = 1.5 Hz), 129.4, 129.3, 128.6, 127.9, 126.3, 124.4 (d, J = 3.7 Hz), 121.4 (d, J = 11.0 Hz), 119.2, 117.7, 117.4, 116.5 (d, J = 22.0 Hz), 22.0. ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -106.7. HRMS (ESI) calcd. for $C_{24}H_{15}FO_4$ $(M+Na)^+$: 409.0847, found: 409.0845.



1-(7-methoxy-2-oxo-4-phenyl-2*H*-chromen-3-yl)-2-(4-methoxyphenyl)ethane-1,2-dione (2n)

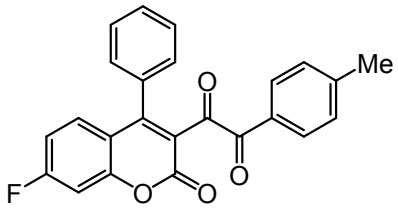
Yellow oil (68.6 mg, 55%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 (d, J = 8.7 Hz, 2 H), 7.43 (s, 3 H), 7.40 - 7.33 (m, 2 H), 7.19 (d, J = 8.8 Hz, 1 H), 6.95 - 6.85 (m, 3 H), 6.79 (dd, J = 2.3, 9.0 Hz, 1 H),

3.88 (s, 3 H), 3.85 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.7, 189.5, 164.6, 164.5, 159.9, 159.1, 156.3, 132.9, 132.8, 130.3, 129.5, 128.6, 128.2, 125.0, 119.7, 113.9, 113.5, 113.3, 100.9, 56.1, 55.6. HRMS (ESI) calcd. for $C_{25}H_{18}O_6$ $(M+Na)^+$: 437.0996, found: 437.0998.



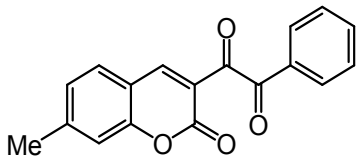
1-(7-(*tert*-butyl)-2-oxo-4-phenyl-2*H*-chromen-3-yl)-2-(4-fluorophenyl)ethane-1,2-dione (2o)

Yellow solid (68.6 mg, 80%). mp. 144.9 - 147.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.04 - 7.97 (m, 2 H), 7.50 - 7.43 (m, 4 H), 7.39 (dd, J = 3.0, 6.8 Hz, 2 H), 7.34 - 7.28 (m, 1 H), 7.27 - 7.23 (m, 1 H), 7.17 - 7.09 (m, 2 H), 1.36 (s, 9 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.1, 189.1, 166.4 (d, J = 256.8 Hz), 160.0, 159.1, 158.9, 154.3, 133.2 (d, J = 9.5 Hz), 132.5, 129.6, 128.7, 128.6, 128.4 (d, J = 2.9 Hz), 128.2, 122.7, 121.9, 117.2, 115.8 (d, J = 22.0 Hz), 114.2, 35.5, 30.9. ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -102.7. HRMS (ESI) calcd. for $C_{27}H_{21}FO_4$ $(M+H)^+$: 429.1497, found: 429.1493.



1-(7-fluoro-2-oxo-4-phenyl-2*H*-chromen-3-yl)-2-(*p*-tolyl)ethane-1,2-dione (2p)

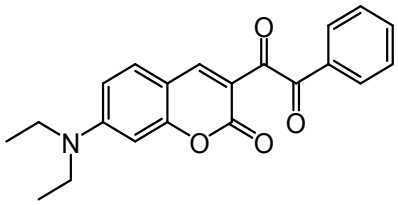
Yellow solid (68.9 mg, 89%), mp. 144.3 - 146.1 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.86 (d, J = 8.3 Hz, 2 H), 7.49 - 7.43 (m, 3 H), 7.42 - 7.36 (m, 2 H), 7.32 (dd, J = 6.0, 8.8 Hz, 1 H), 7.25 (d, J = 7.8 Hz, 2 H), 7.15 (dd, J = 2.5, 8.5 Hz, 1 H), 7.03 - 6.96 (m, 1 H), 2.41 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.8, 190.0, 165.6 (d, J = 258.2 Hz), 159.1, 157.8, 155.4 (d, J = 13.2 Hz), 145.6, 132.2, 131.0 (d, J = 10.3 Hz), 130.6, 129.8, 129.4, 129.3, 128.8, 128.2, 122.3 (d, J = 2.9 Hz), 116.5 (d, J = 2.9 Hz), 113.2 (d, J = 22.0 Hz), 104.8 (d, J = 25.7 Hz), 21.9. ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -101.5. HRMS (ESI) calcd. for $C_{24}H_{15}FO_4$ $(M+H)^+$: 387.1027, found: 387.1029.



1-(7-methyl-2-oxo-2*H*-chromen-3-yl)-2-phenylethane-1,2-dione (2q)

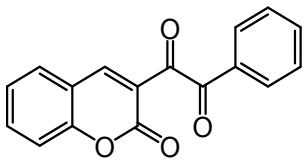
Yellow solid (54.3 mg, 93%), mp. 175.6 - 177.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.64 (s, 1 H), 7.99 - 7.92 (m, 2 H), 7.67 - 7.58 (m, 2 H), 7.55 - 7.46 (m, 2 H), 7.23 - 7.18 (m, 2 H), 2.51 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 192.4, 191.6, 159.3, 156.0, 148.8, 147.8, 134.4, 132.4, 130.4, 129.8, 128.9, 126.8, 121.2, 117.4, 115.9, 22.3. HRMS (ESI) calcd. for $C_{18}H_{12}O_4$ $(M+H)^+$: 293.0808, found: 293.0806.



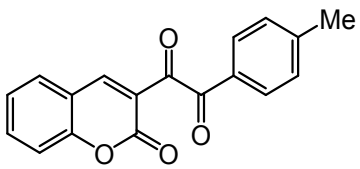
1-(7-(sec-butyl)-2-oxo-2*H*-chromen-3-yl)-2-phenylethane-1,2-dione (2r)

Yellow solid (43.3 mg, 62%), mp. 192.4 - 194.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.53 (s, 1 H), 7.98 - 7.90 (m, 2 H), 7.59 (d, J = 7.5 Hz, 1 H), 7.46 (d, J = 9.0 Hz, 2 H), 7.50 (d, J = 7.8 Hz, 1 H), 6.66 (dd, J = 2.4, 9.0 Hz, 1 H), 6.47 (d, J = 2.3 Hz, 1 H), 3.48 (q, J = 7.2 Hz, 4 H), 1.26 (t, J = 7.2 Hz, 6 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 194.0, 192.2, 160.6, 159.4, 154.0, 148.3, 134.0, 133.0, 132.7, 129.5, 128.8, 112.9, 110.4, 108.6, 97.1, 45.4, 12.5. HRMS (ESI) calcd. for $C_{21}H_{19}NO_4$ $(M+H)^+$: 350.1387, found: 350.1390.



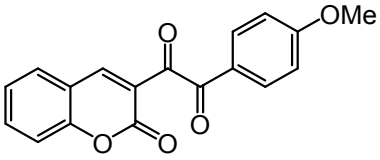
1-(2-oxo-2*H*-chromen-3-yl)-2-phenylethane-1,2-dione (2s)

Yellow solid (44.0 mg, 79%), mp. 152.1 - 154.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.66 (s, 1 H), 8.00 - 7.93 (m, 2 H), 7.75 - 7.62 (m, 3 H), 7.56 - 7.48 (m, 2 H), 7.43 - 7.35 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.2, 191.3, 159.0, 155.7, 148.8, 135.4, 134.5, 132.3, 130.7, 129.8, 128.9, 125.4, 122.5, 118.2, 117.2. HRMS (ESI) calcd. for $C_{17}H_{10}O_4$ $(M+H)^+$: 279.0652, found: 279.0649.



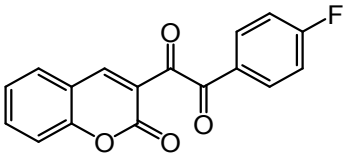
1-(2-oxo-2*H*-chromen-3-yl)-2-(*p*-tolyl)ethane-1,2-dione (2t)

Light yellow (49.8 mg, 85%), mp. 183.4 - 185.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.65 (s, 1 H), 7.90 - 7.83 (m, J = 8.2 Hz, 2 H), 7.76 - 7.67 (m, 2 H), 7.43 - 7.36 (m, 2 H), 7.35 - 7.29 (m, J = 7.9 Hz, 2 H), 2.44 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.9, 191.4, 158.9, 155.7, 148.7, 145.8, 135.3, 130.6, 130.0, 129.8, 129.7, 125.4, 122.7, 118.2, 117.2, 22.0. HRMS (ESI) calcd. for $C_{18}H_{12}O_4$ $(M+H)^+$: 293.0808, found: 293.0808.



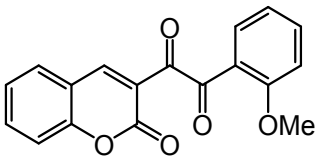
1-(4-methoxyphenyl)-2-(2-oxo-2*H*-chromen-3-yl)ethane-1,2-dione (2u)

Yellow solid (52.4 mg, 85%), mp. 166.7 - 168.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.63 (s, 1 H), 7.98 - 7.92 (m, 2 H), 7.73-7.67 (m, 2 H), 7.41 - 7.35 (m, 2 H), 7.02 - 6.93 (m, 2 H), 3.89 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.3, 190.7, 164.8, 158.8, 155.7, 148.6, 135.2, 132.3, 130.5, 125.3, 125.3, 122.9, 118.2, 117.2, 114.4, 55.6. HRMS (ESI) calcd. for $C_{18}H_{12}O_5$ $(M+H)^+$: 309.0757, found: 309.0756.



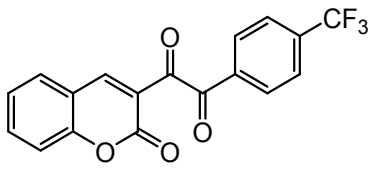
1-(4-fluorophenyl)-2-(2-oxo-2*H*-chromen-3-yl)ethane-1,2-dione (2v)

Light yellow (53.6 mg, 91%), mp. 180.9 - 182.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.65 (s, 1 H), 8.05 - 7.96 (m, 2 H), 7.78 - 7.67 (m, 2 H), 7.46 - 7.37 (m, 2 H), 7.20 (t, J = 8.7 Hz, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.0, 190.5, 166.6 (d, J = 257.5 Hz), 159.0, 155.7, 148.9, 135.5, 132.5 (d, J = 10.27 Hz), 130.7, 128.7 (d, J = 2.9 Hz), 125.5, 122.6, 118.1, 117.3, 116..3 (d, J = 22.0Hz). ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -102.0. HRMS (ESI) calcd. for $C_{17}H_9FO_4$ $(M+H)^+$: 297.0558, found: 297.0555.



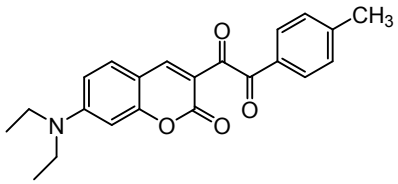
1-(2-methoxyphenyl)-2-(2-oxo-2*H*-chromen-3-yl)ethane-1,2-dione (2w)

Light yellow (26.3 mg, 43%), mp. 187.6 - 189.9 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.72 (s, 1 H), 8.08 (dd, J = 1.7, 7.8 Hz, 1 H), 7.76 - 7.66 (m, 2 H), 7.63 - 7.56 (m, 1 H), 7.43 - 7.35 (m, 2 H), 7.18 - 7.10 (m, 1 H), 6.97 (d, J = 8.3 Hz, 1 H), 3.71 (s, 3 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.8, 189.1, 160.5, 159.0, 155.6, 147.9, 136.3, 135.0, 130.5, 130.4, 125.3, 122.9, 121.8, 121.7, 118.3, 117.1, 112.4, 56.0. HRMS (ESI) calcd. for $C_{18}H_{12}O_5$ $(M+H)^+$: 309.0757, found: 309.0760.



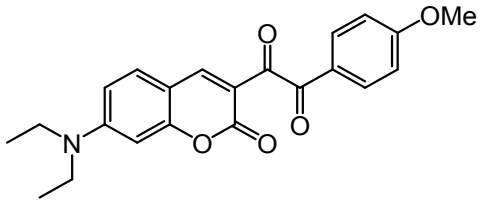
1-(2-oxo-2*H*-chromen-3-yl)-2-(4-(trifluoromethyl)phenyl)ethane-1,2-dione (2x)

Yellow solid (53.5 mg, 77%), mp. 196.1 - 197.2 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.68 (s, 1 H), 8.08 (d, J = 8.2 Hz, 2 H), 7.82 - 7.71 (m, 4 H), 7.45 - 7.38 (m, 2 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.1, 190.8, 159.3, 155.7, 149.0, 135.7, 135.5 (d, J = 33.01 Hz), 135.0, 130.8, 130.0, 126.0 (q, J = 3.7 Hz), 125.6, 123.5(q, J = 272.9 Hz), 122.3, 118.1, 117.3. ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -63.3. HRMS (ESI) calcd. for $C_{18}H_9F_3O_4$ $(M+H)^+$: 347.0526, found: 347.0526.



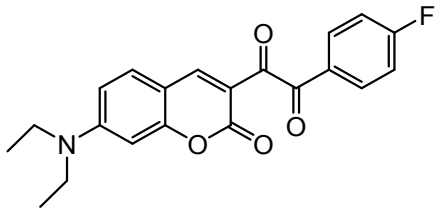
1-(7-(diethylamino)-2-oxo-2*H*-chromen-3-yl)-2-(*p*-tolyl)ethane-1,2-dione (2y)

Yellow solid (44.3 mg, 61%), mp. 180.3 - 182.1 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.51 (s, 1 H), 7.83 (d, J = 8.2 Hz, 2 H), 7.44 (d, J = 9.0 Hz, 1 H), 7.28 (d, J = 7.9 Hz, 2 H), 6.65 (dd, J = 2.4, 9.0 Hz, 1 H), 6.46 (d, J = 2.2 Hz, 1 H), 3.47 (q, J = 7.1 Hz, 4 H), 2.41 (s, 3 H), 1.25 (t, J = 7.2 Hz, 6 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 193.7, 192.3, 160.4, 159.3, 153.9, 148.3, 145.0, 132.6, 130.6, 129.6, 129.5, 113.1, 110.3, 108.5, 97.1, 45.3, 21.9, 12.5. HRMS (ESI) calcd. for $C_{22}H_{21}NO_4$ $(M+Na)^+$: 386.1363, found: 386.1362.



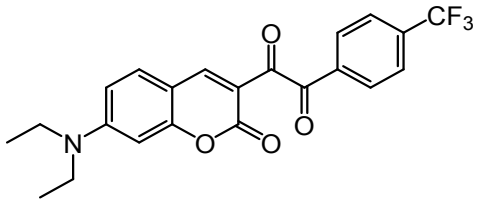
1-(7-(diethylamino)-2-oxo-2*H*-chromen-3-yl)-2-(*p*-tolyl)ethane-1,2-dione (2z)

Yellow solid (50.6 mg, 67%), mp. 187.5 - 189.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.51 (s, 1 H), 7.94 - 7.89 (m, 2 H), 7.44 (d, J = 9.0 Hz, 1 H), 7.00 - 6.93 (m, 2 H), 6.65 (dd, J = 2.4, 9.0 Hz, 1 H), 6.47 (d, J = 2.2 Hz, 1 H), 3.87 (s, 3 H), 3.48 (q, J = 7.1 Hz, 4 H), 1.25 (t, J = 7.1 Hz, 6 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.7, 192.3, 164.3, 160.4, 159.3, 153.9, 148.4, 132.6, 131.9, 126.1, 114.2, 113.1, 110.3, 108.5, 97.1, 55.6, 45.4, 12.5. HRMS (ESI) calcd. for $C_{22}H_{21}NO_5$ $(M+H)^+$: 380.1492, found: 380.1496.



1-(2-oxo-2*H*-chromen-3-yl)-2-(4-(trifluoromethyl)phenyl)ethane-1,2-dione (2aa)

Yellow solid (22.9 mg, 31%), mp. 218.3 - 219.4 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.51 (s, 1 H), 8.01 - 7.93 (m, 2 H), 7.46 (d, J = 9.0 Hz, 1 H), 7.20 - 7.12 (m, 2 H), 6.66 (dd, J = 2.4, 9.0 Hz, 1 H), 6.47 (d, J = 2.3 Hz, 1 H), 3.49 (q, J = 7.1 Hz, 4 H), 1.26 (t, J = 7.2 Hz, 6 H).^{13}C NMR (100 MHz, $CDCl_3$): δ 192.3, 191.9, 166.2 (d, J = 256.0 Hz), 160.6, 159.4, 154.0, 148.3, 132.7 (d, J = 9.54 Hz), 129.5 (d, J = 2.93 Hz), 116.05 (d, J = 22.0 Hz), 112.8, 110.4, 108.6, 97.2, 45.4, 12.5. ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -103.4. HRMS (ESI) calcd. for $C_{21}H_{18}FNO_4$ $(M+Na)^+$: 390.1112, found: 390.1113.



1-(7-(diethylamino)-2-oxo-2*H*-chromen-3-yl)-2-(4-(trifluoromethyl)phenyl)ethane-1,2-dione (2ab)

Yellow solid (28.1 mg, 34%), mp. 191.5 - 193.7 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.53 (s, 1 H), 8.07 - 8.02 (m, J = 8.1 Hz, 2 H), 7.77 - 7.73 (m, J = 8.2 Hz, 2 H), 7.48 (d, J = 9.0 Hz, 1 H), 6.68 (dd, J = 2.4, 9.0 Hz, 1 H), 6.48 (d, J = 2.3 Hz, 1 H), 3.49 (q, J = 7.1 Hz, 4 H), 1.27 (t, J = 7.2 Hz, 6 H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.8, 191.5, 160.9, 159.4, 154.2, 148.3, 135.8, 134.9 (q, J = 33.0 Hz), 132.9, 129.7, 125.8 (q, J = 3.7 Hz), 123.6 (q, J = 272.9 Hz), 112.5, 110.6, 108.7, 97.2, 45.4, 12.5. ^{19}F NMR (376.5 MHz, $CDCl_3$): δ -63.2. HRMS (ESI) calcd. for $C_{22}H_{18}F_3NO_4$ $(M+H)^+$: 418.1261, found: 418.1261.

9. NMR spectra of all compounds

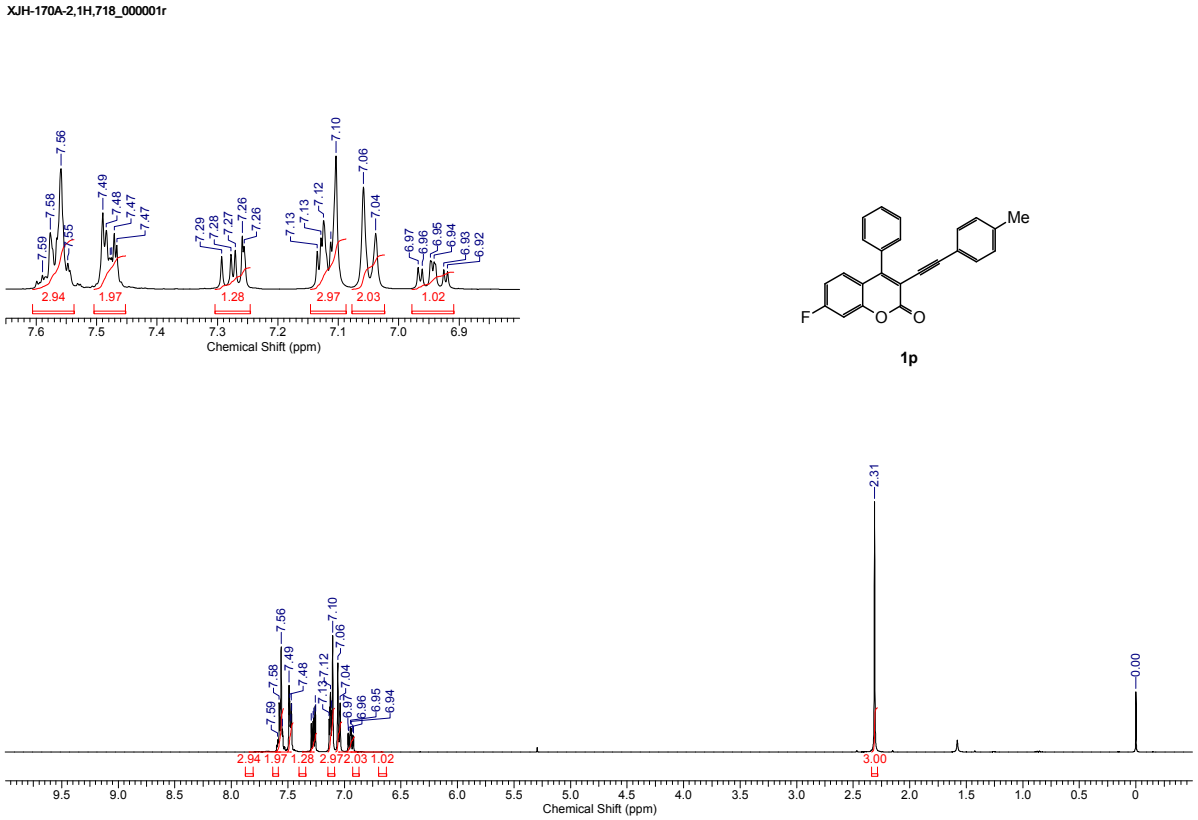


Figure S17. ^{1}H NMR spectrum of compound **1p**

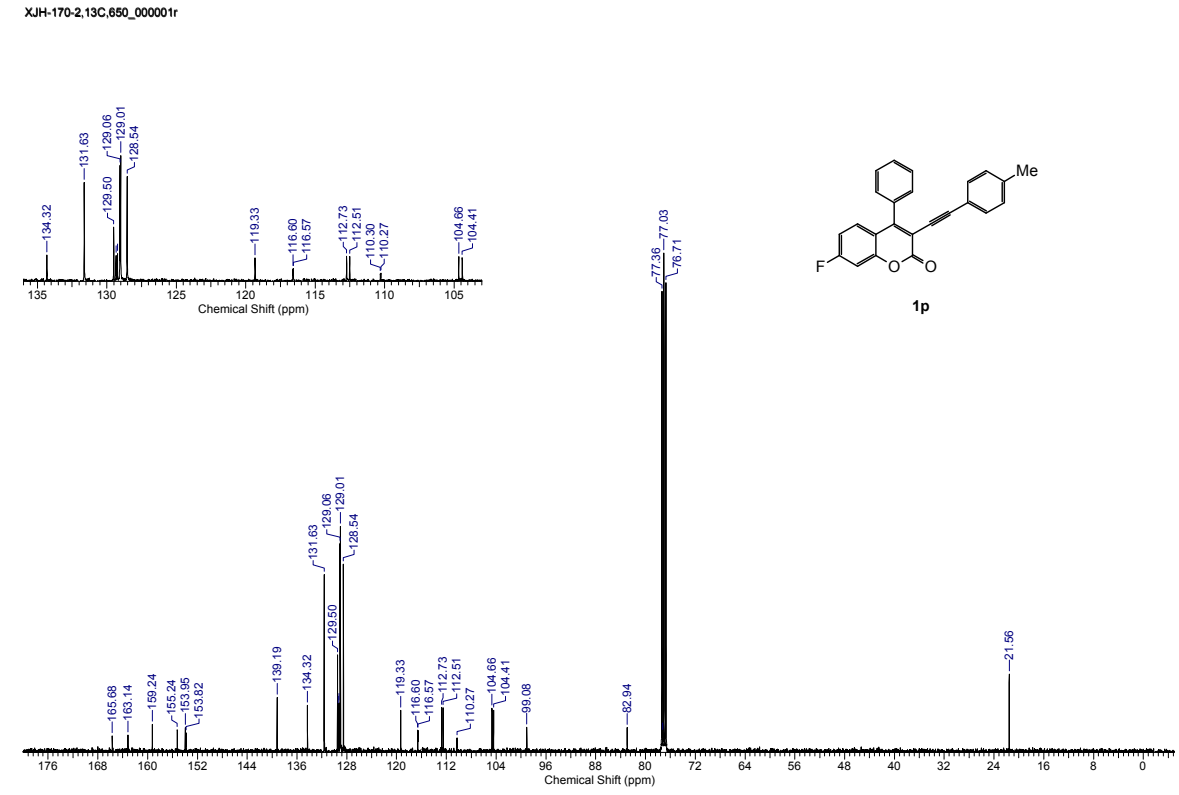


Figure S18. ^{13}C NMR spectrum of compound **1p**

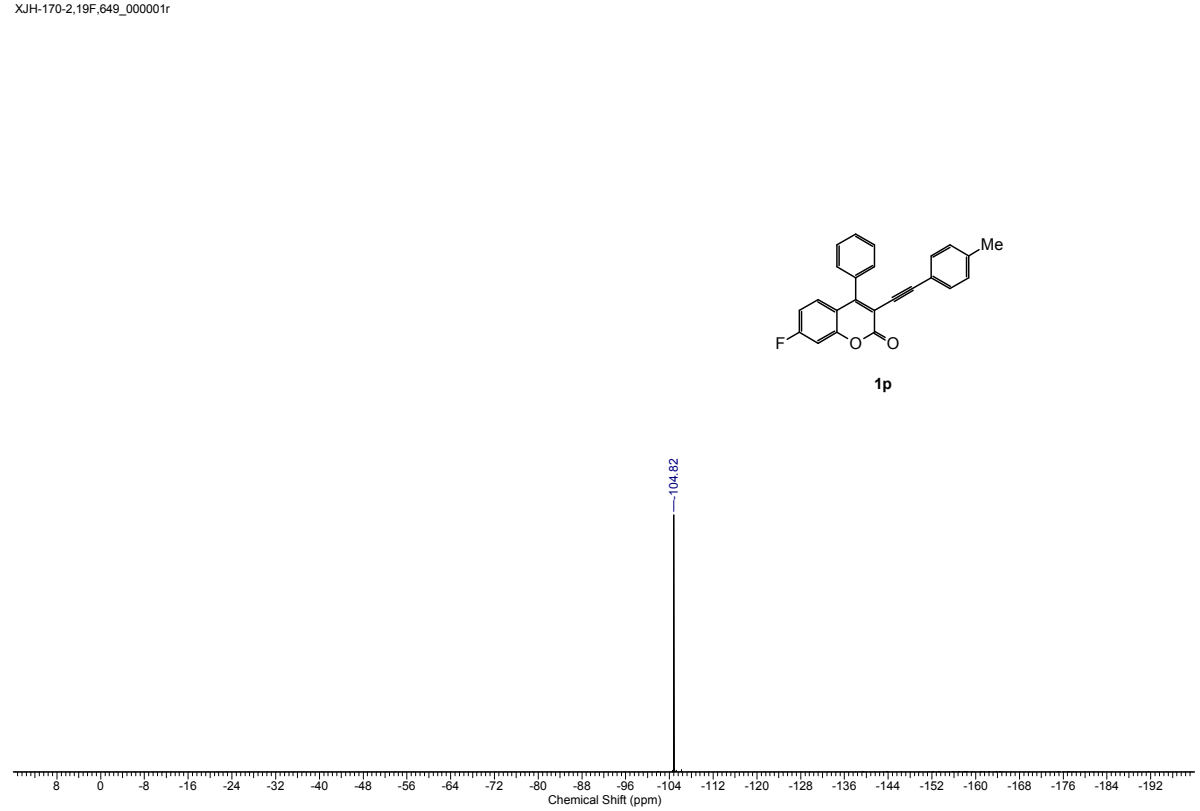


Figure S19. ^{19}F NMR spectrum of compound **1p**

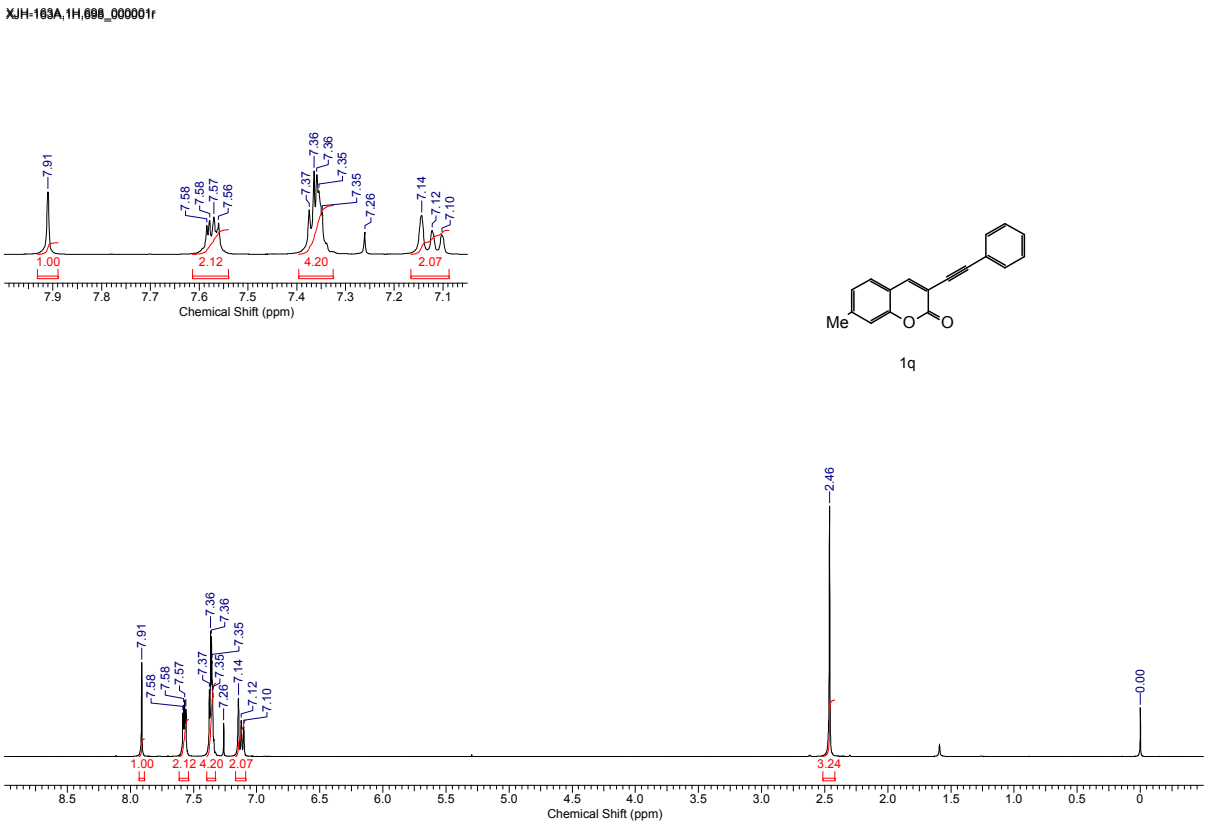


Figure S20. ^{1}H NMR spectrum of compound **1q**

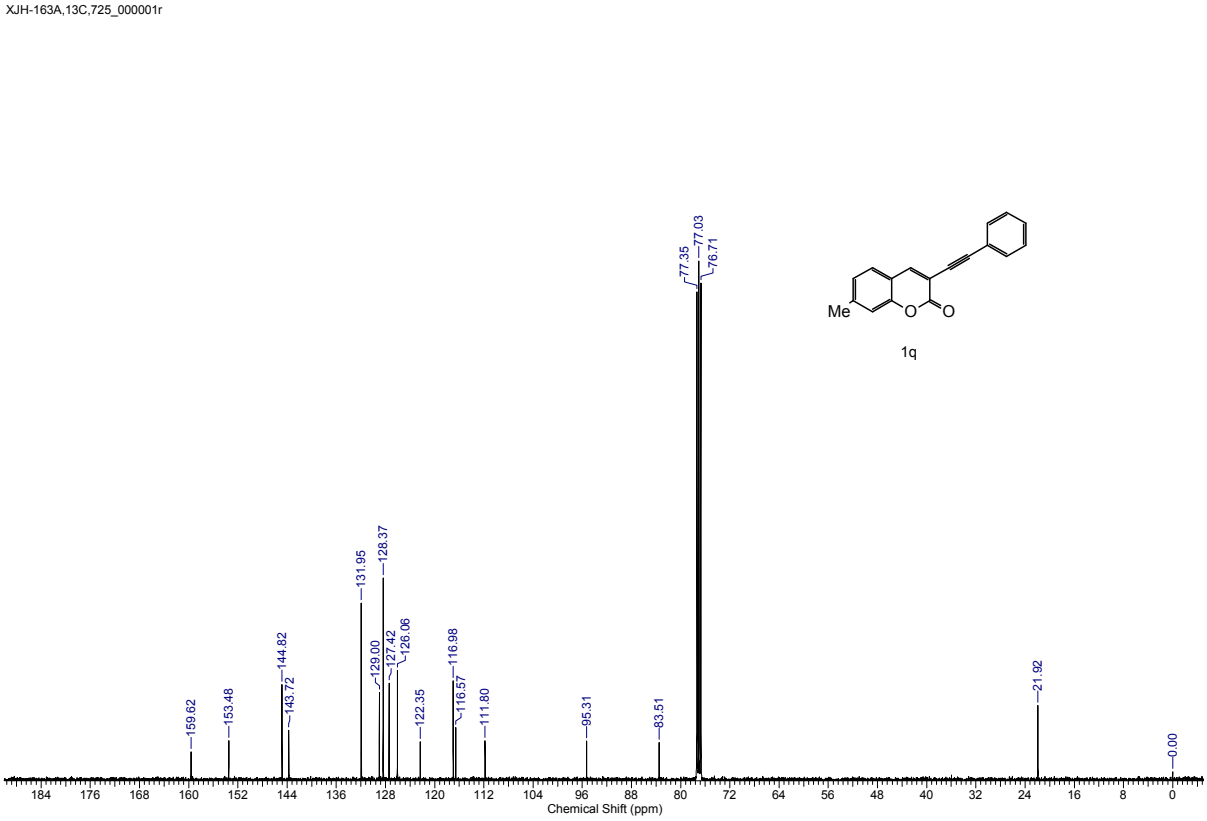


Figure S21. ^{13}C NMR spectrum of compound **1q**

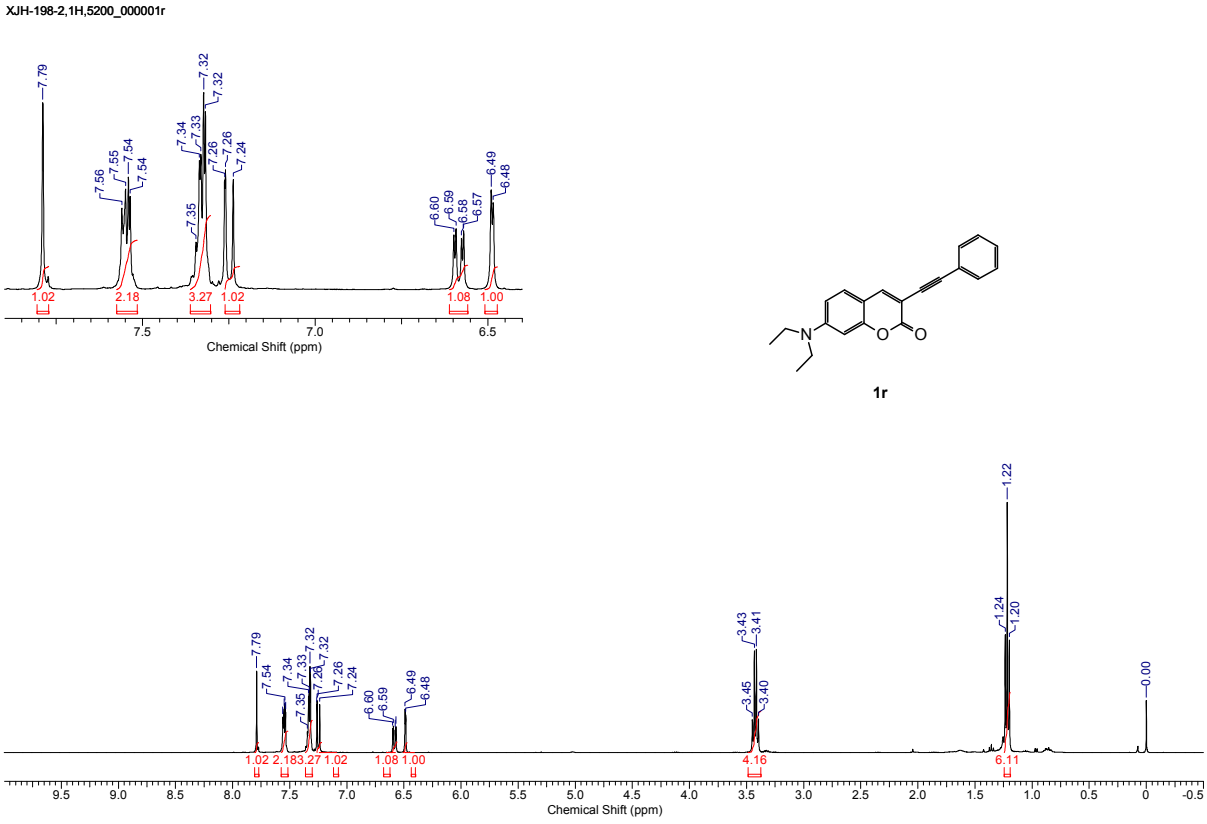


Figure S22. ^{1}H NMR spectrum of compound **1r**

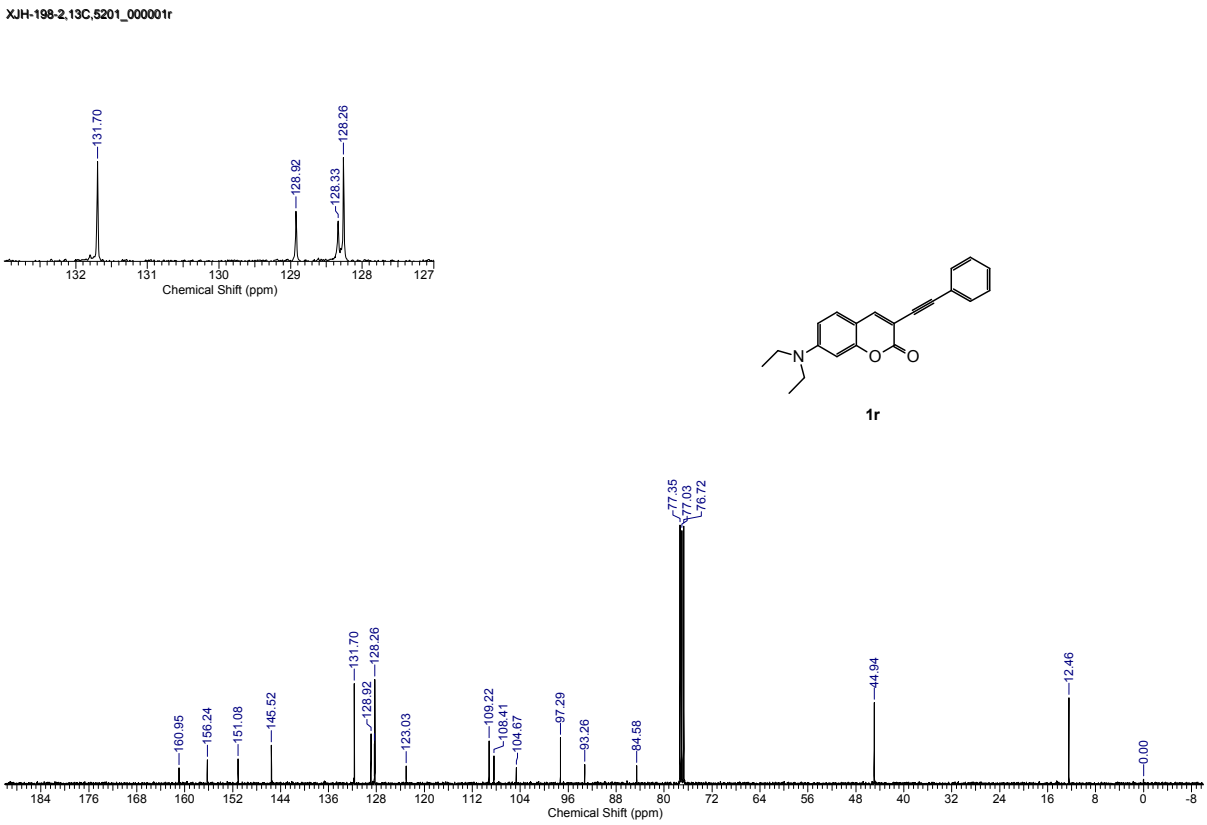


Figure S23. ^{13}CNMR spectrum of compound **1r**

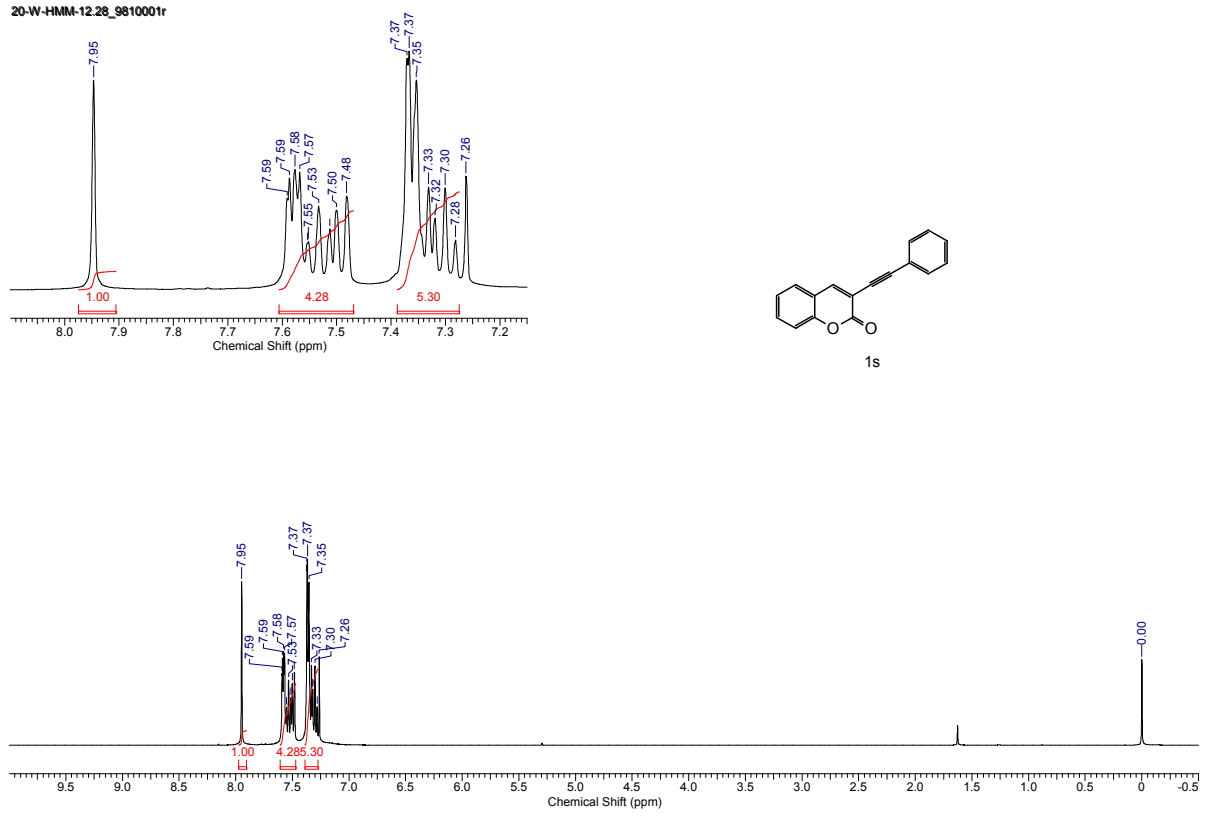


Figure S24. ^{1}H NMR spectrum of compound **1s**

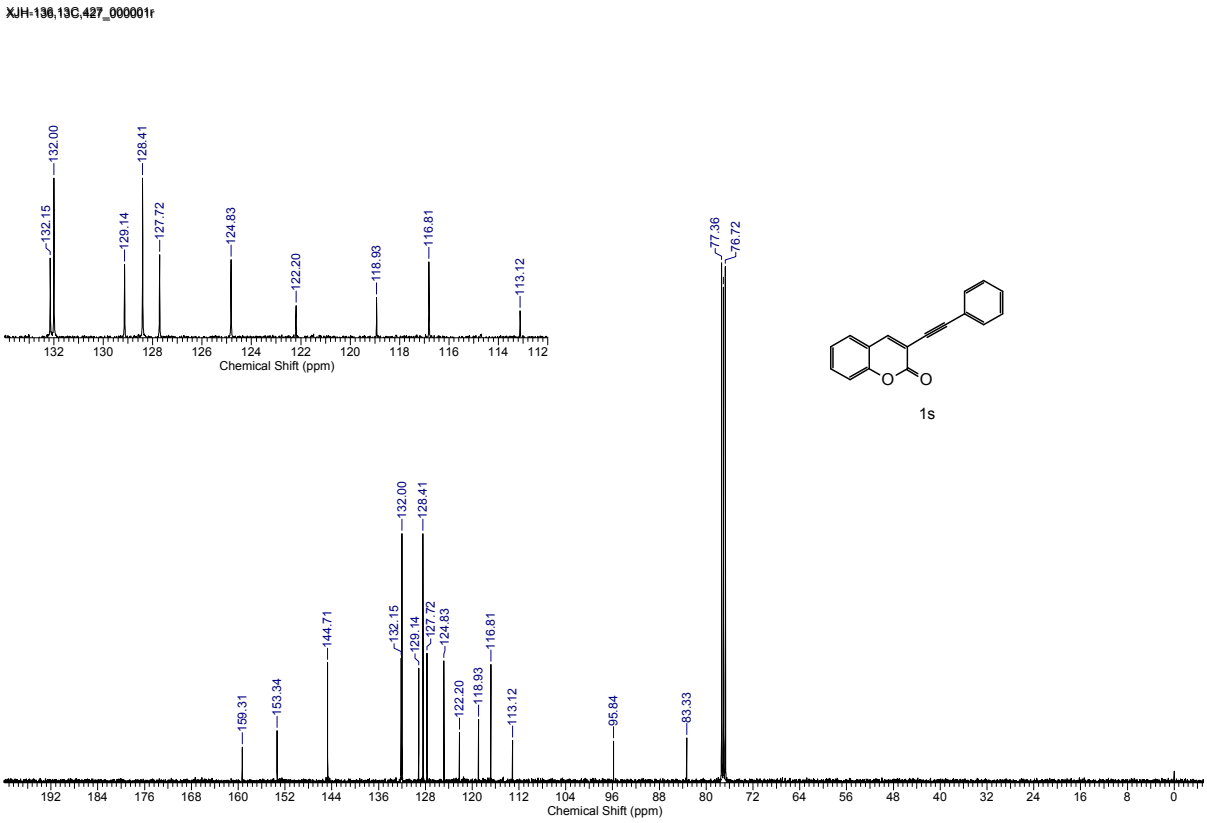


Figure S25. ^{13}C NMR spectrum of compound **1s**

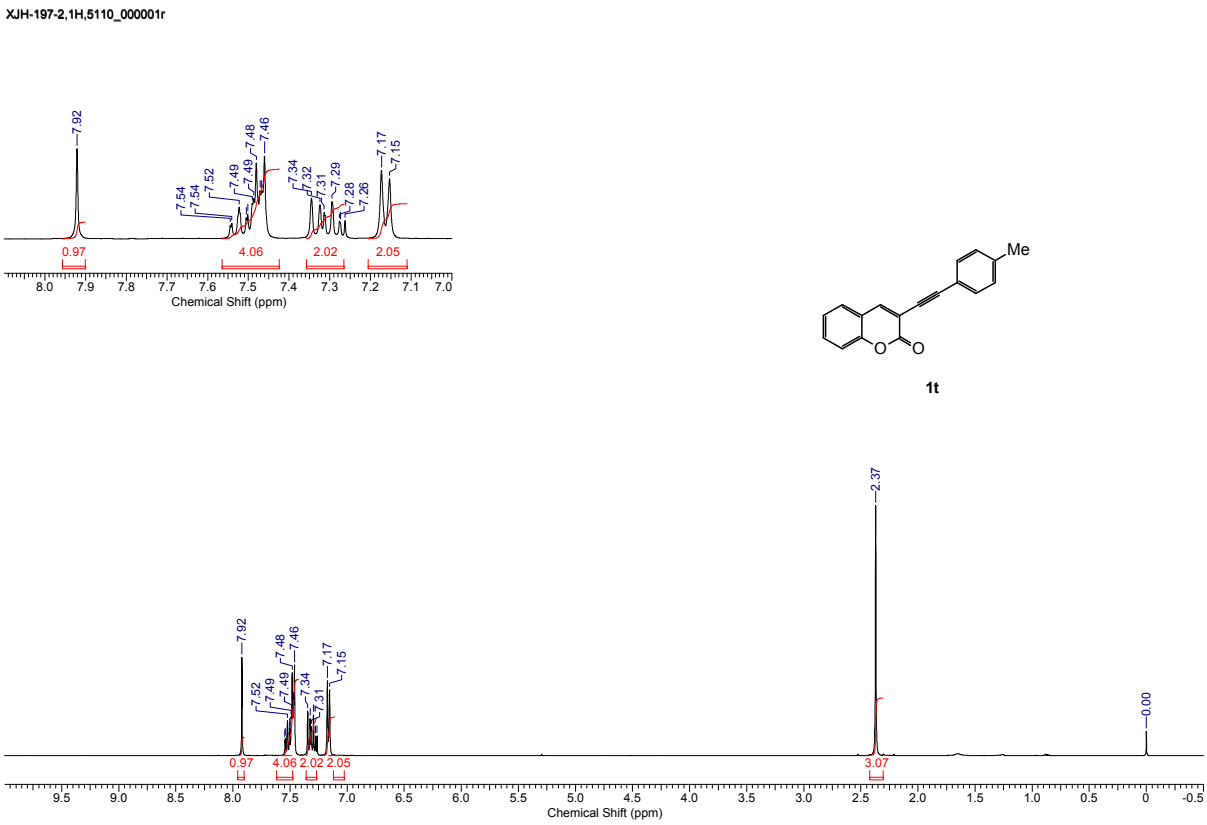


Figure S26. ^{1}H NMR spectrum of compound **1t**

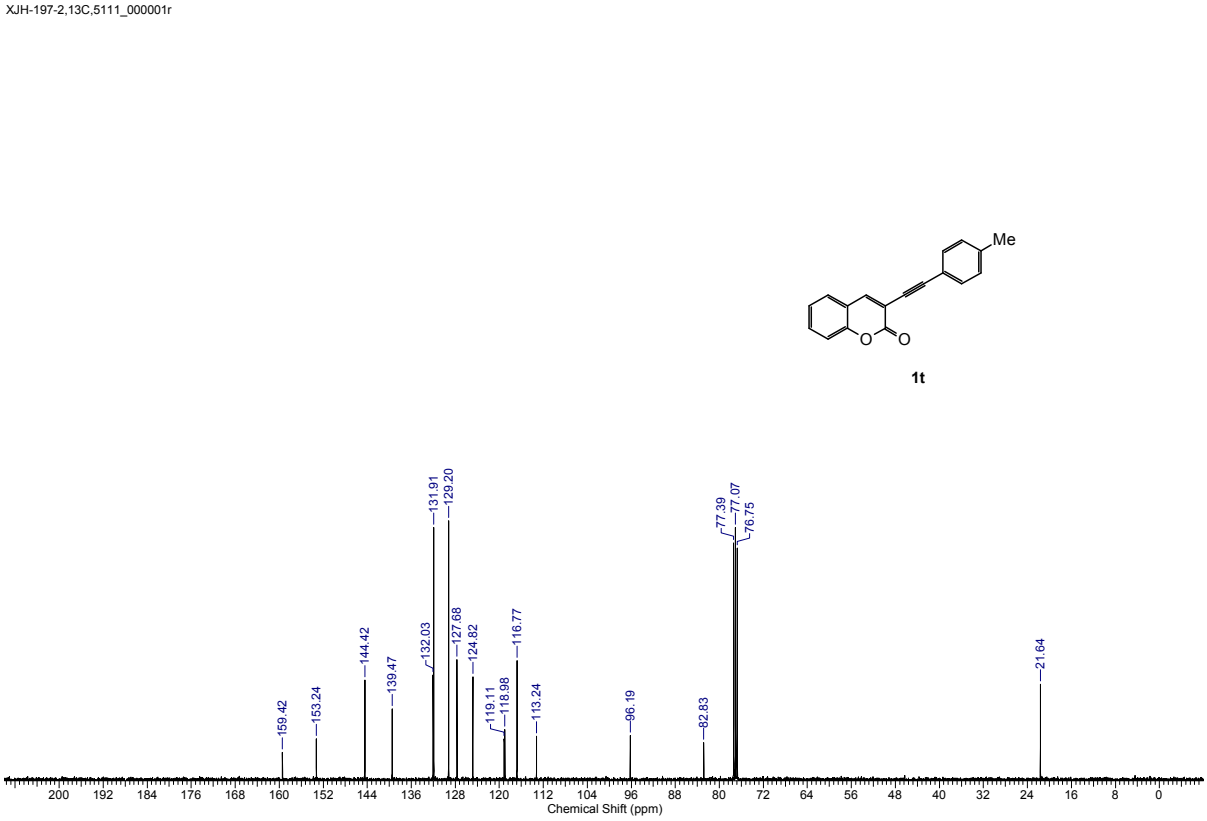


Figure S27. ^{13}C NMR spectrum of compound **1t**

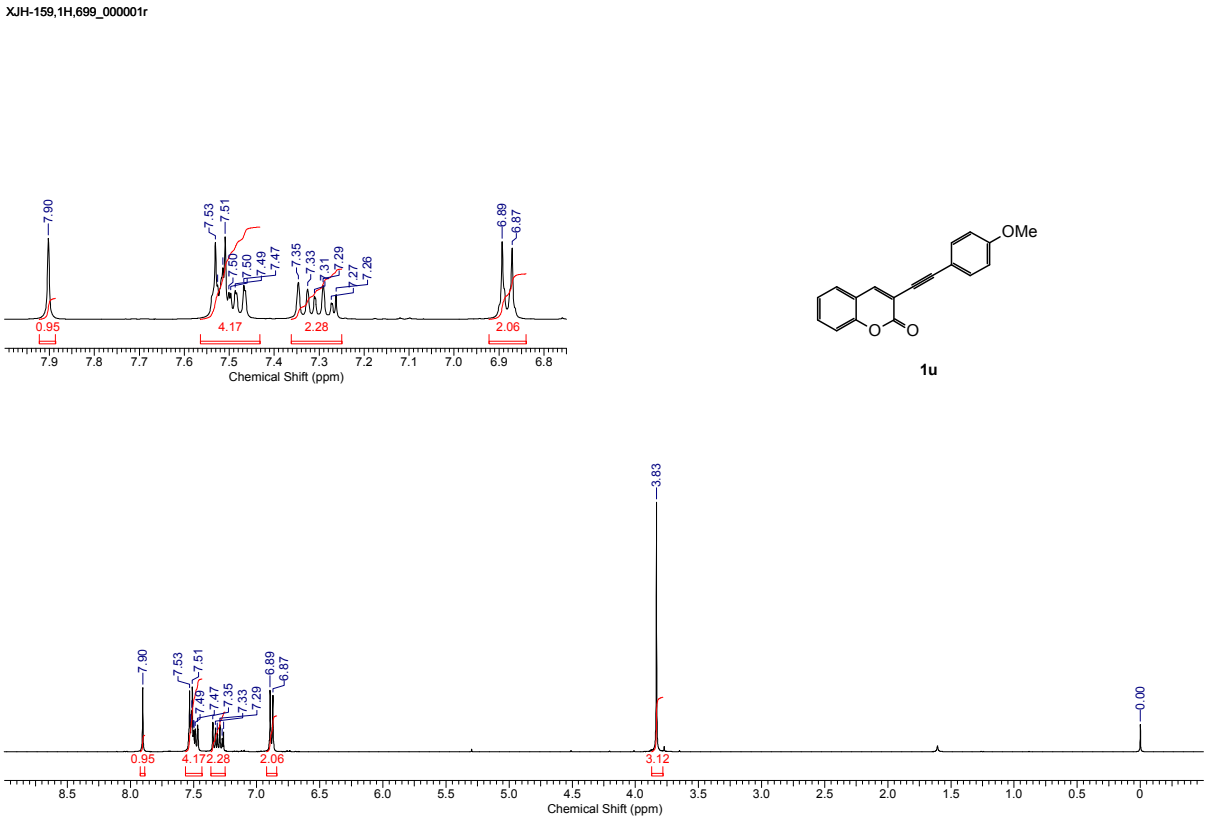


Figure S28. ^{1}H NMR spectrum of compound **1u**

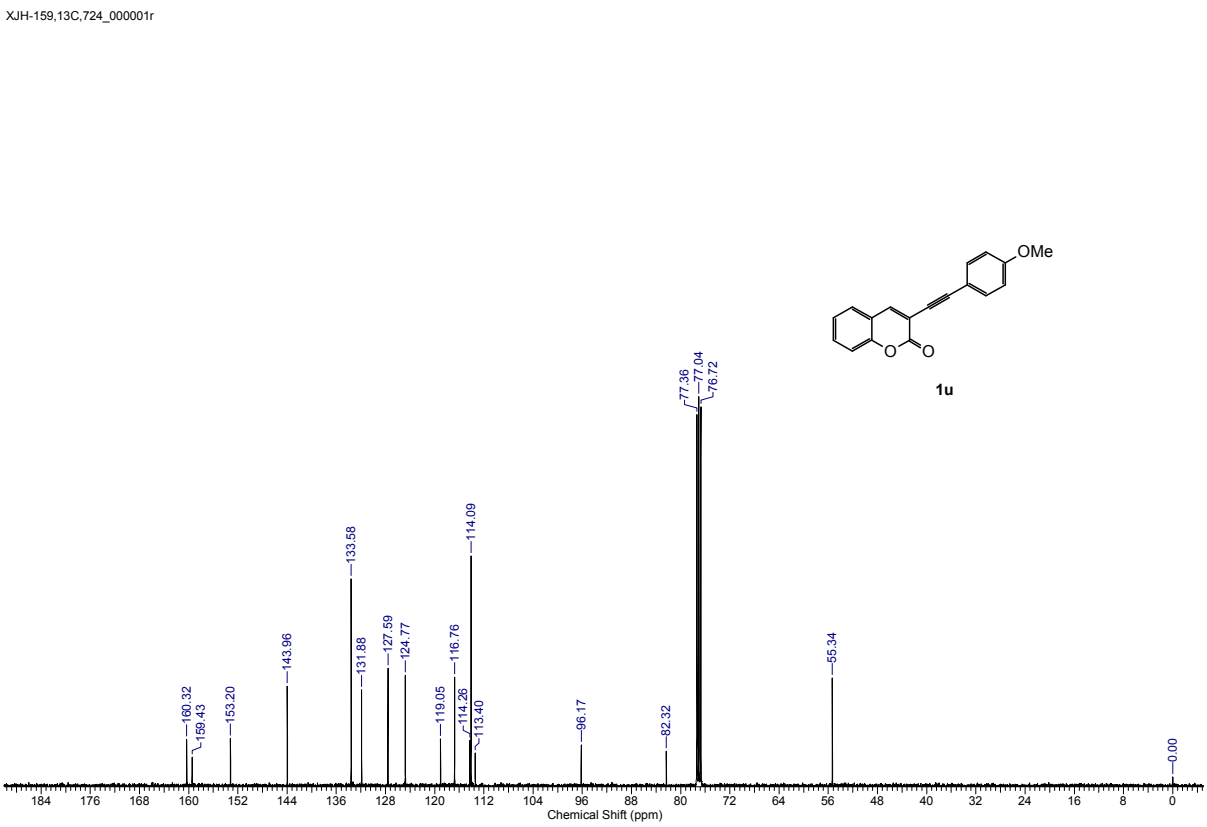


Figure S29. ^{13}C NMR spectrum of compound **1u**

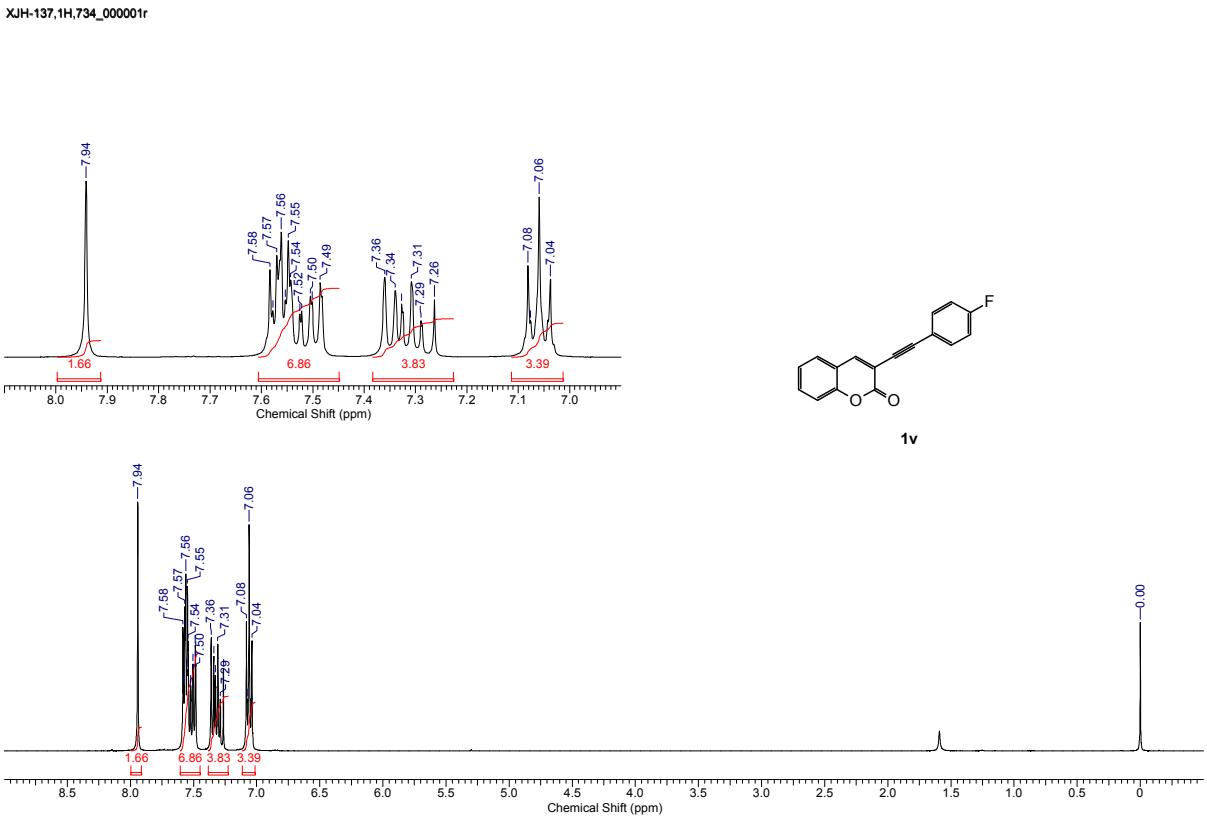


Figure S30. ^{1}H NMR spectrum of compound **1v**

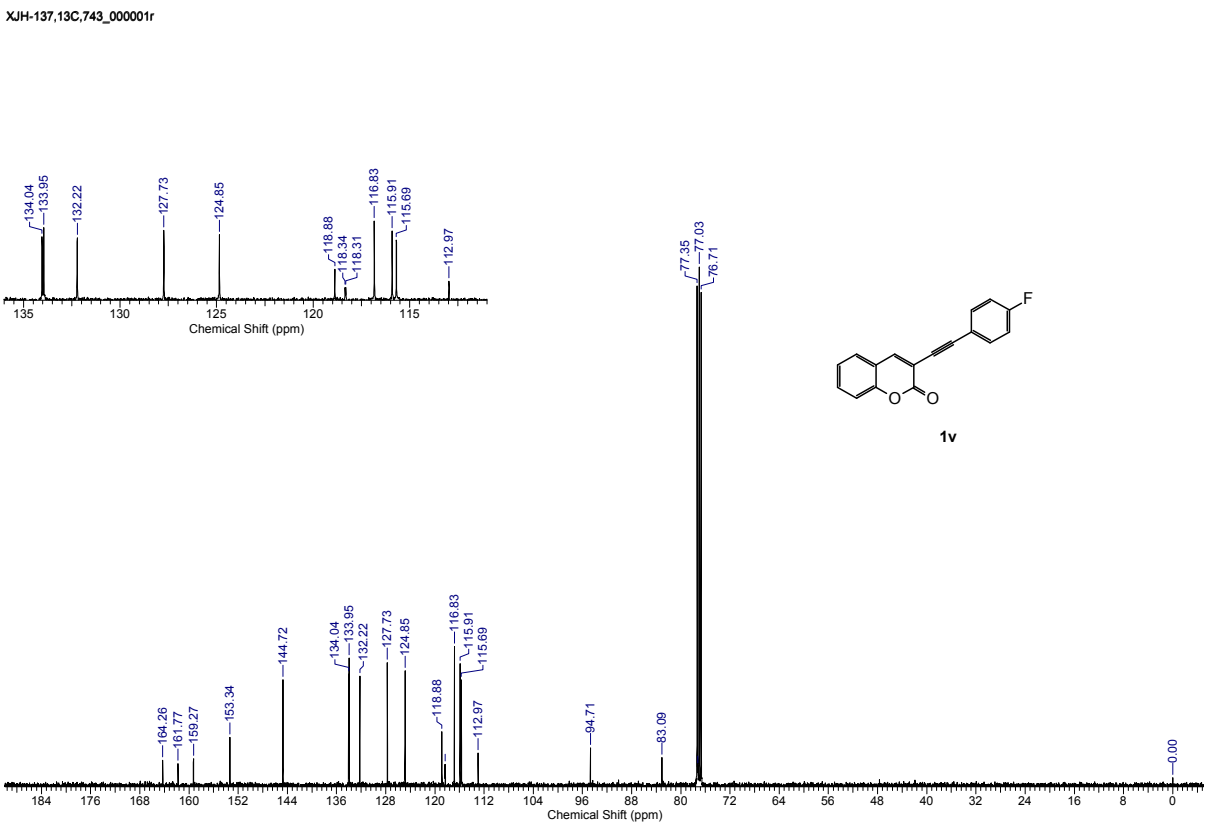


Figure S31. ^{13}C NMR spectrum of compound **1v**

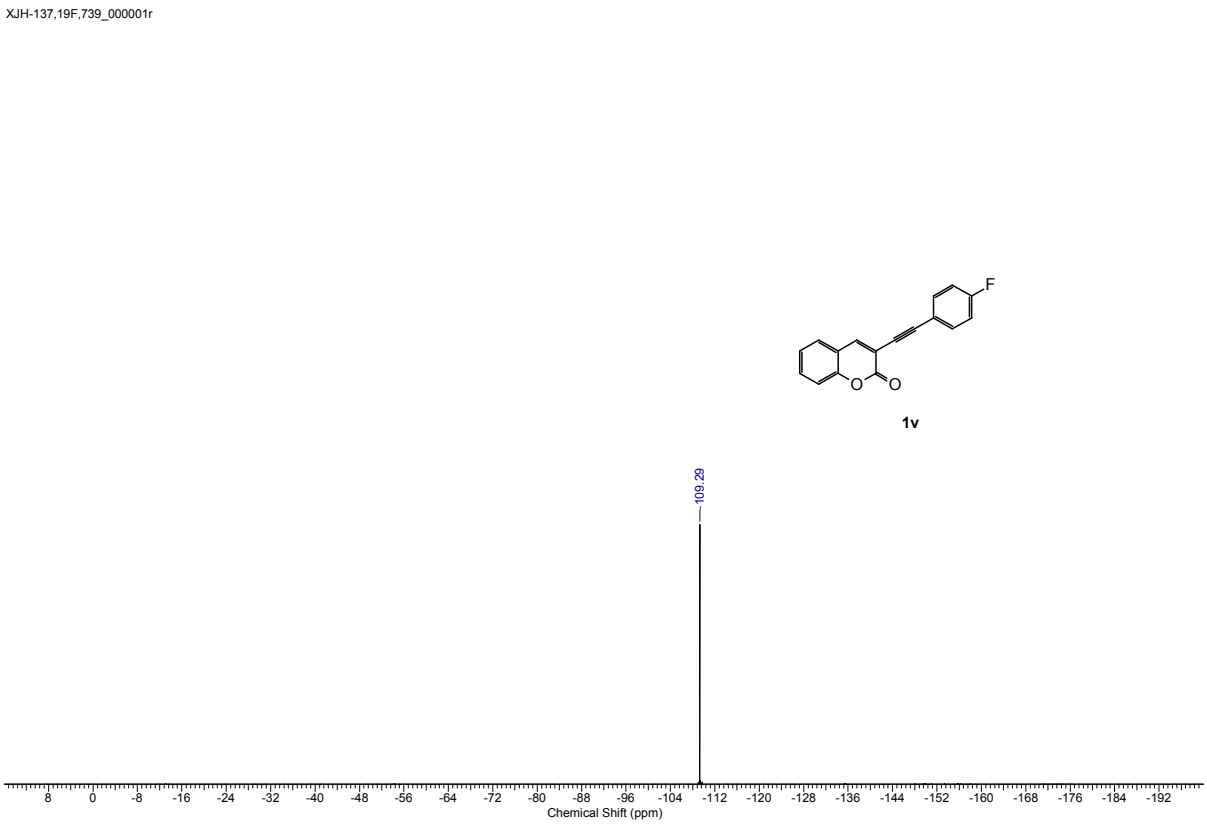


Figure S32. ^{19}F NMR spectrum of compound **1v**

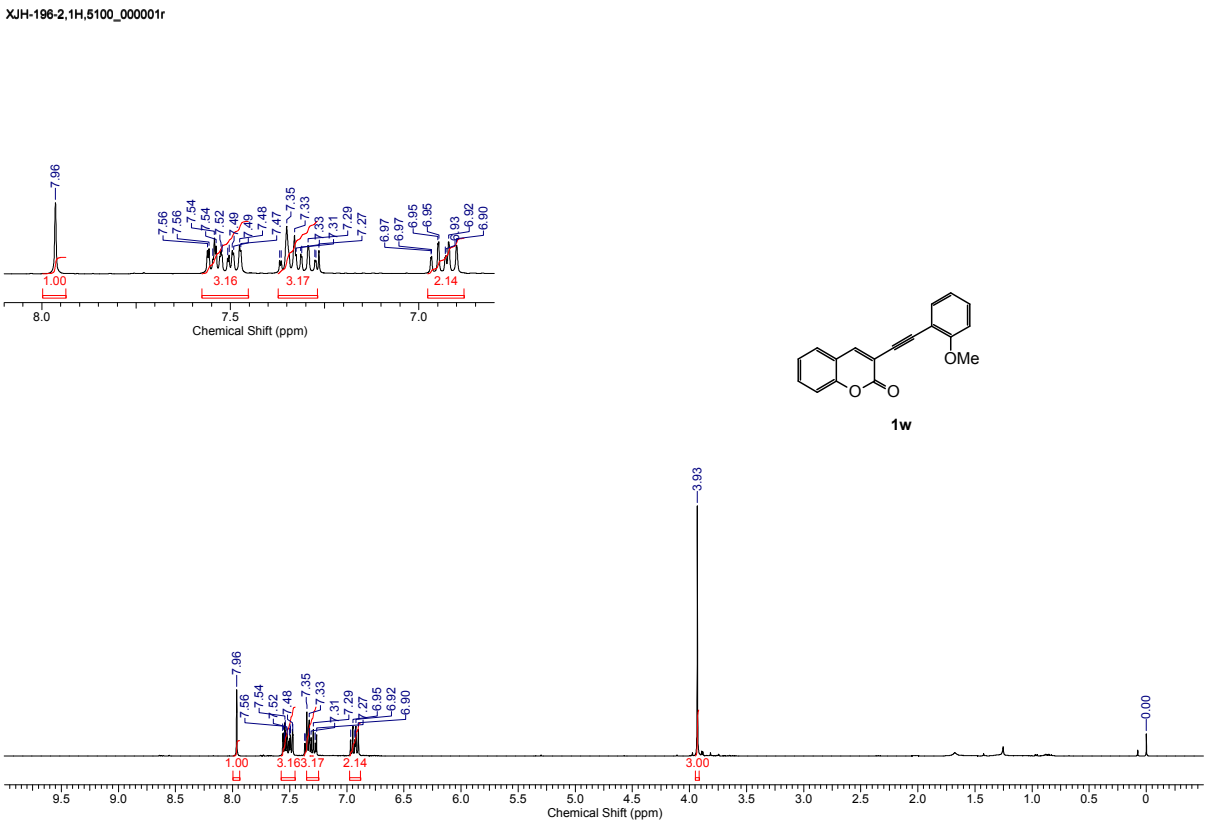


Figure S33. ^{1}H NMR spectrum of compound **1w**

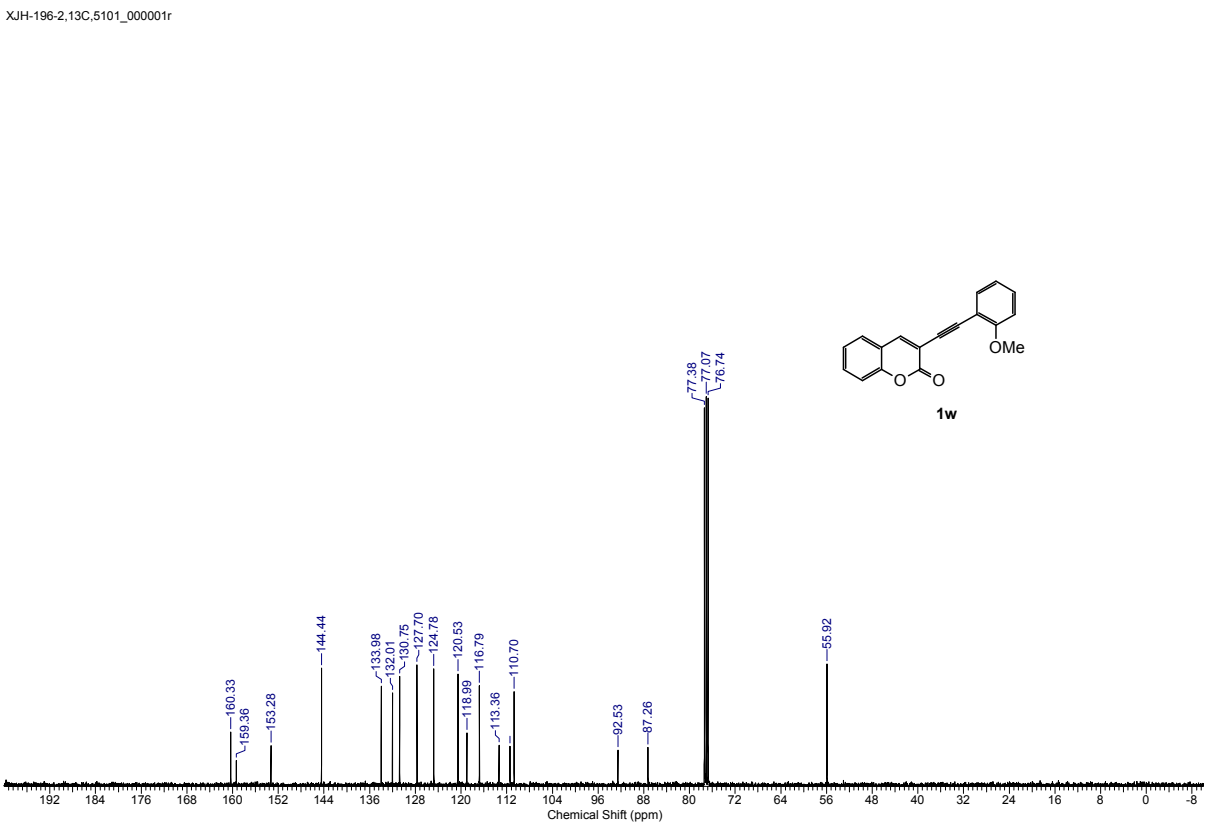


Figure S34. ^{13}C NMR spectrum of compound **1w**

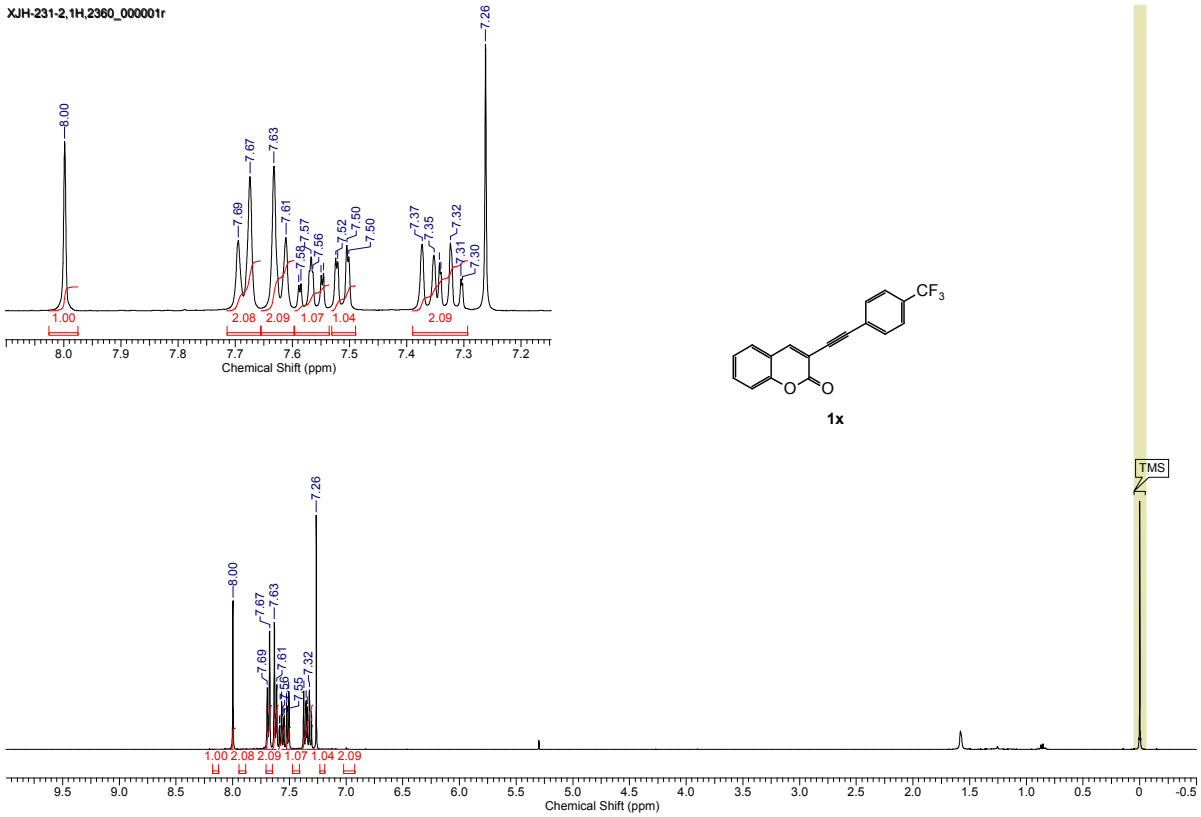


Figure S35. ^{1}H NMR spectrum of compound **1x**

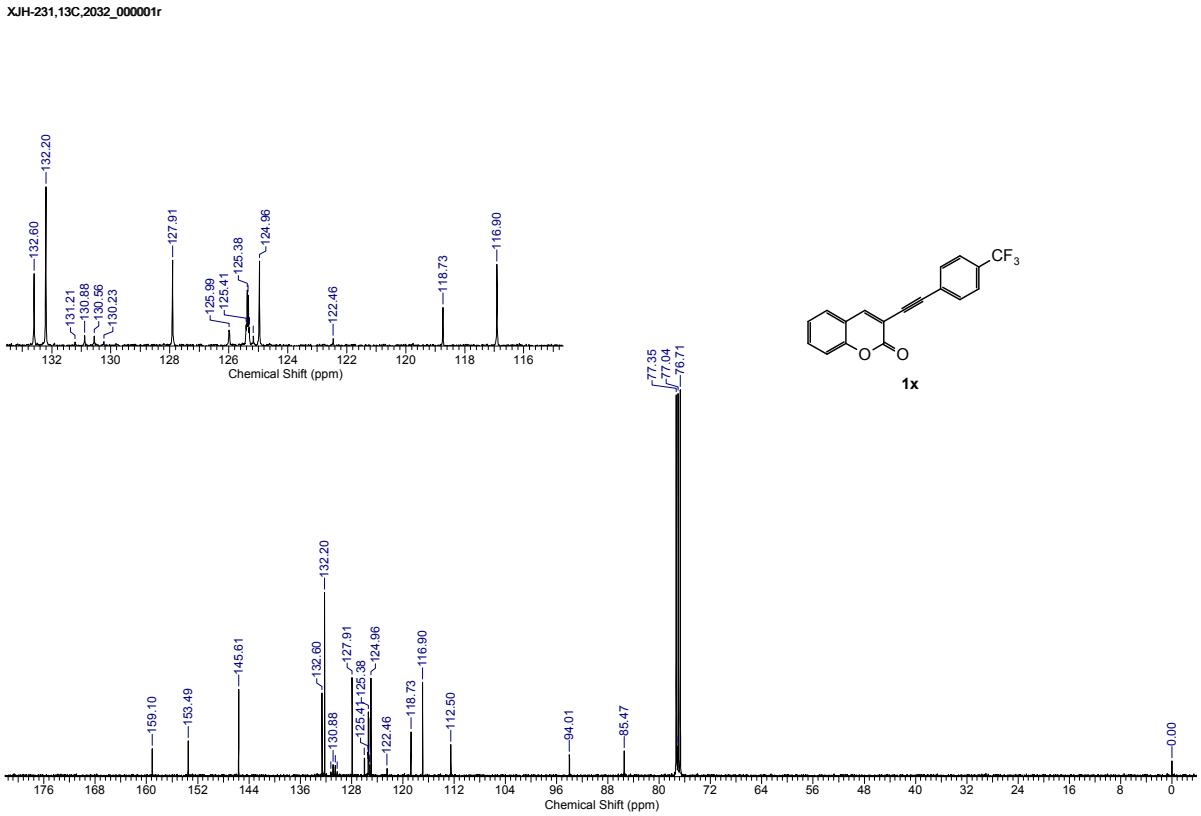


Figure S36. ^{13}C NMR spectrum of compound **1x**

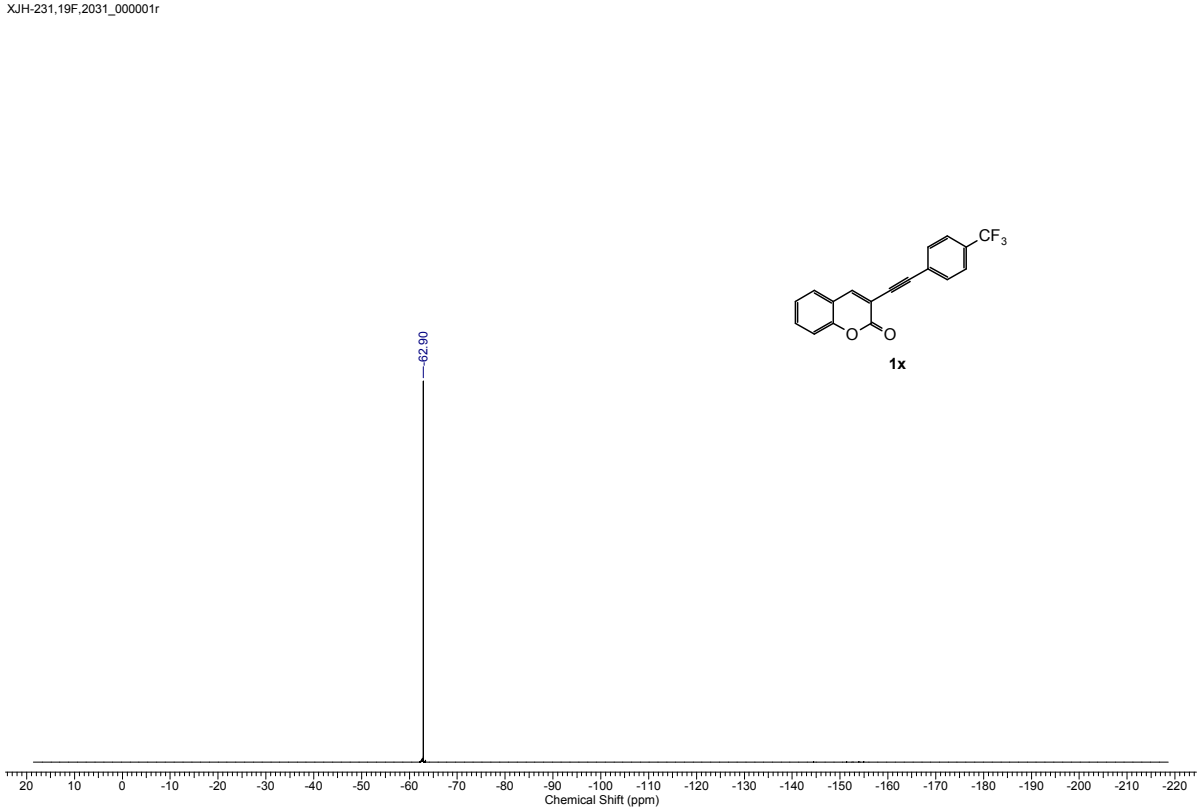


Figure S37. ^{19}F NMR spectrum of compound **1x**

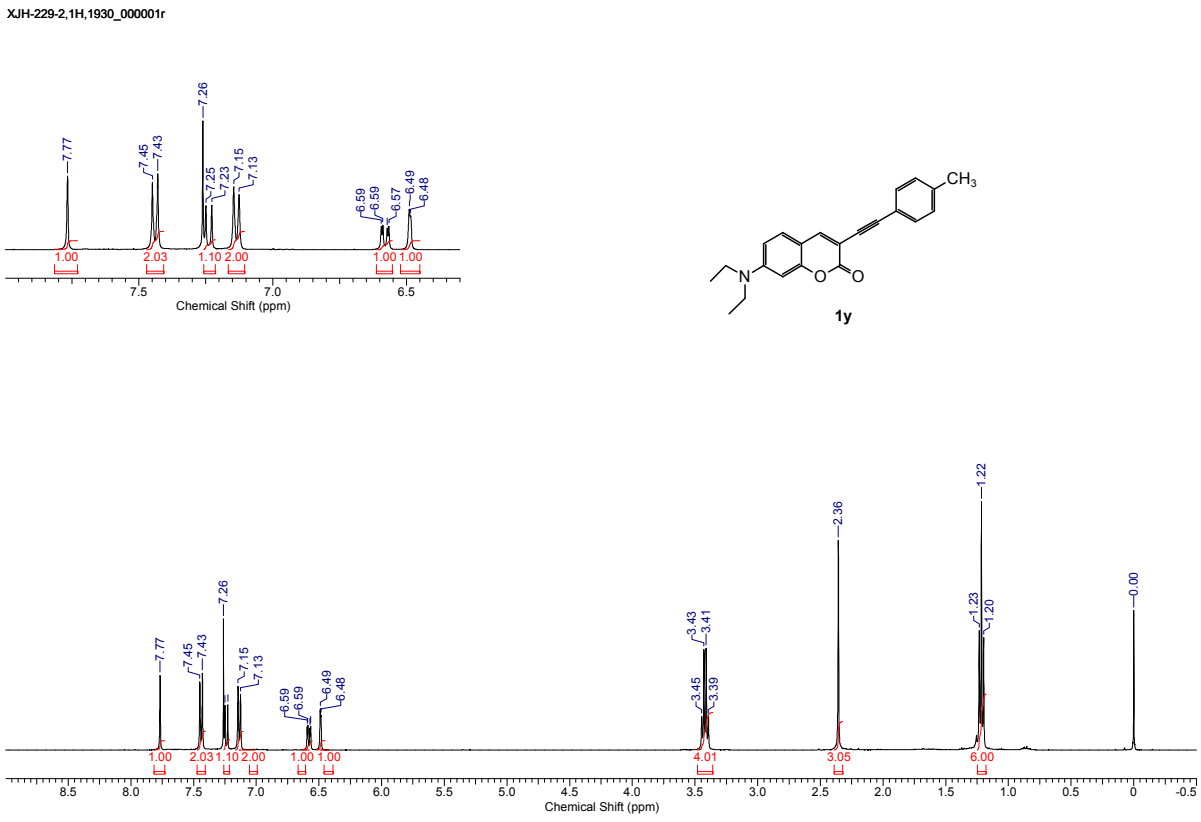


Figure S38. ^{1}H NMR spectrum of compound **1y**

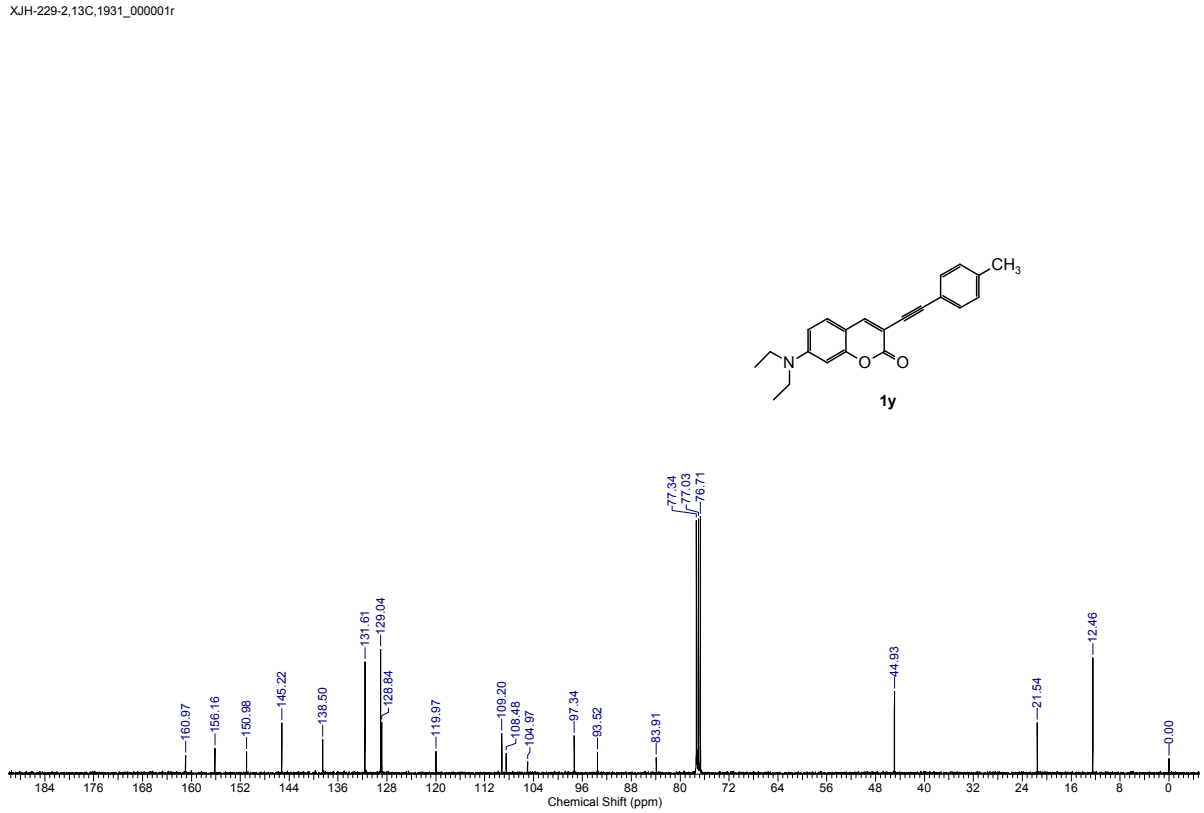


Figure S39. ^{13}C NMR spectrum of compound **1y**

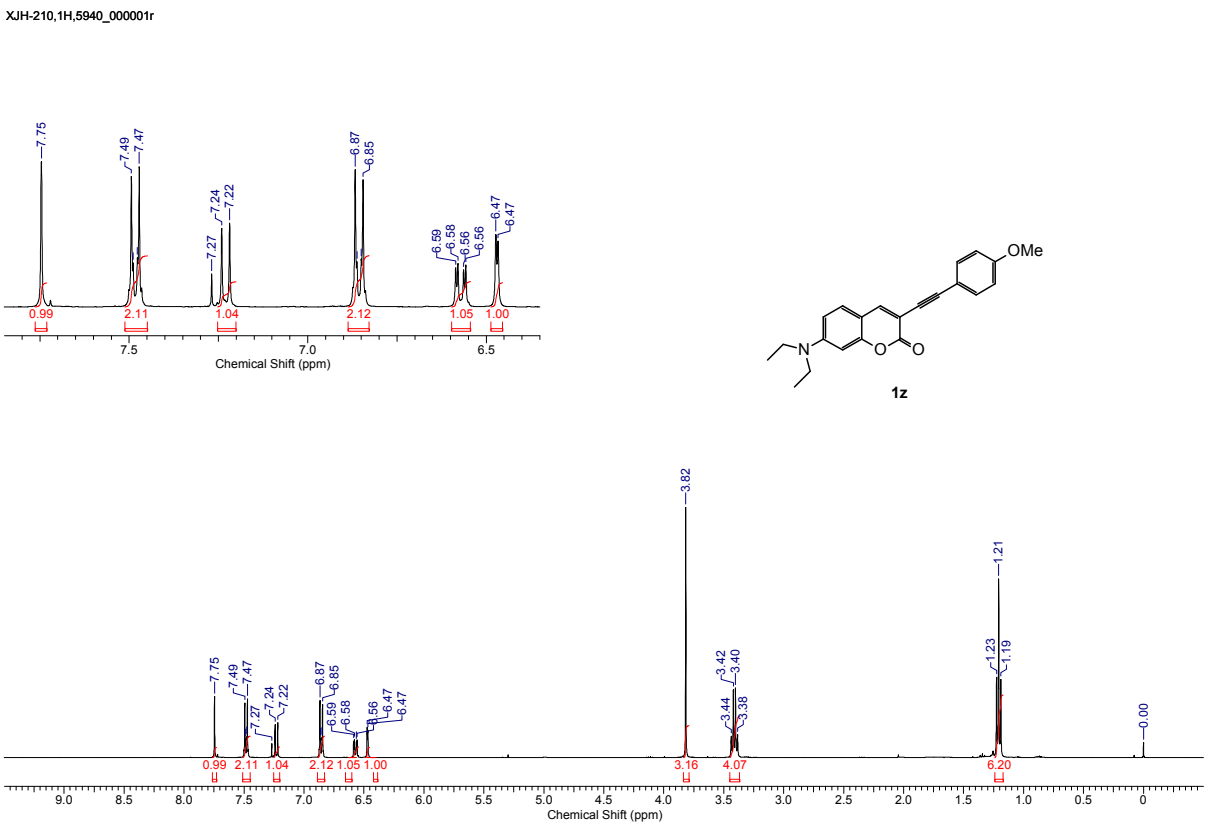


Figure S40. ^{1}H NMR spectrum of compound **1z**

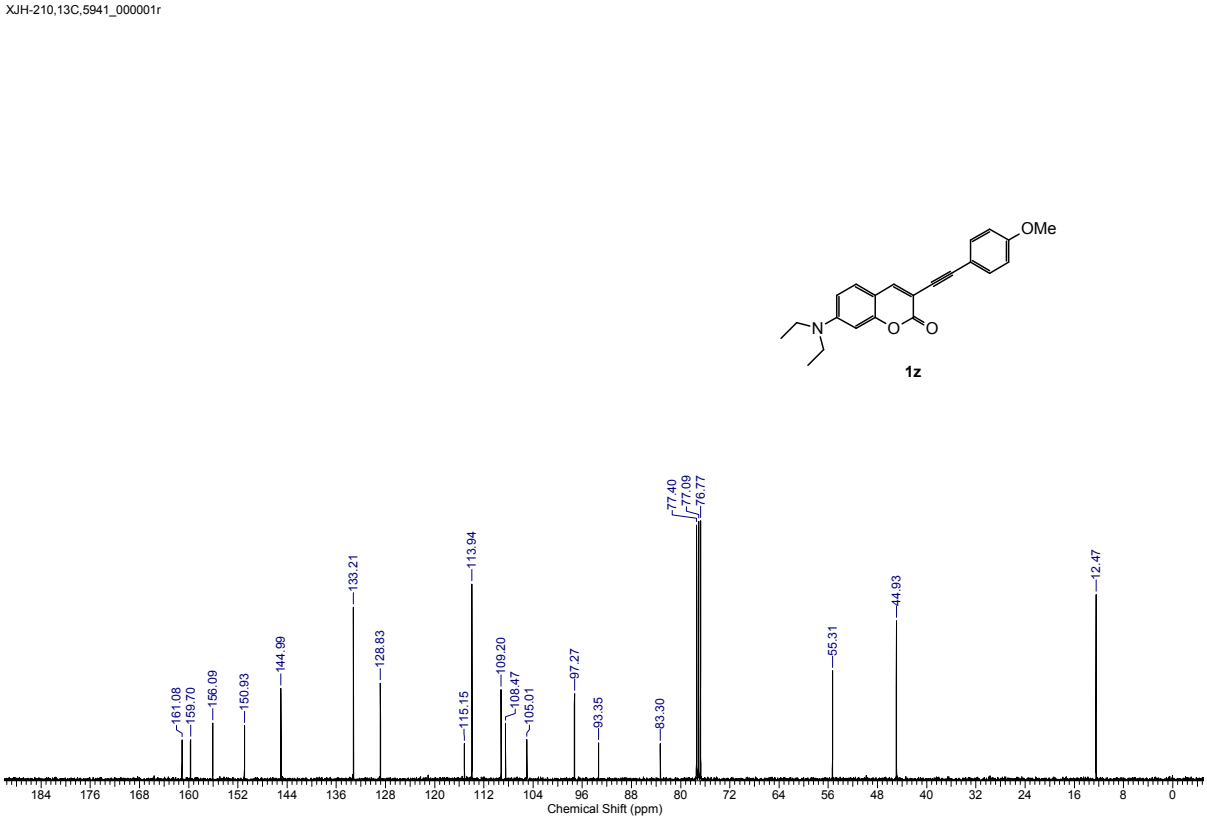


Figure S41. ^{13}C NMR spectrum of compound **1z**

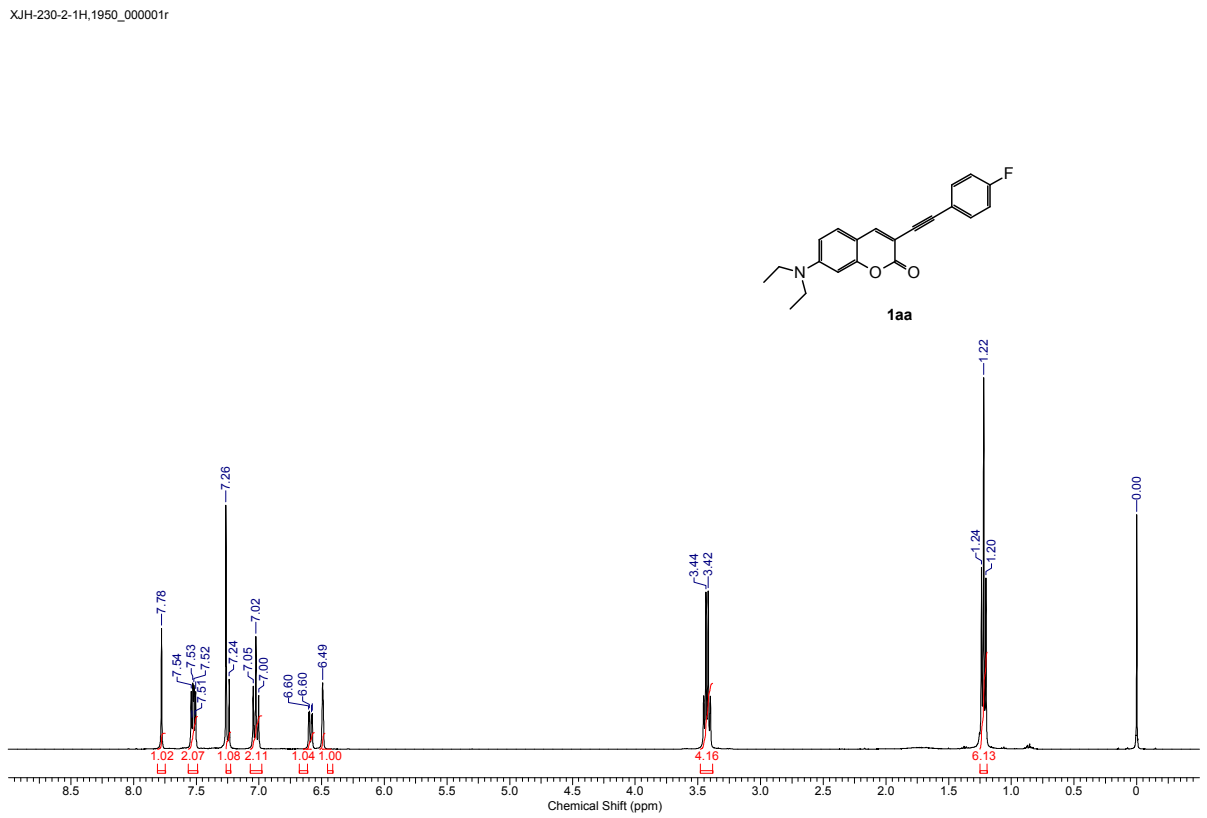


Figure S42. ^{1}H NMR spectrum of compound **1aa**

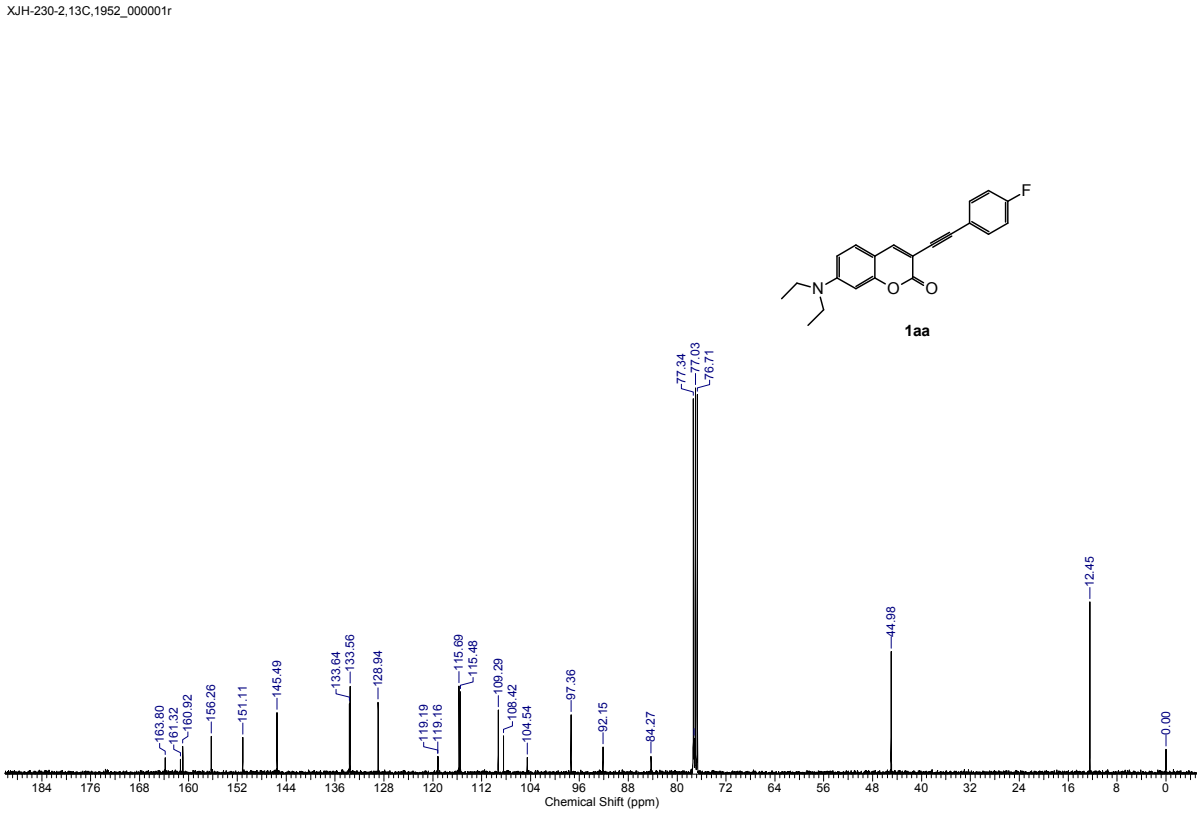


Figure S43. ^{13}C NMR spectrum of compound **1aa**

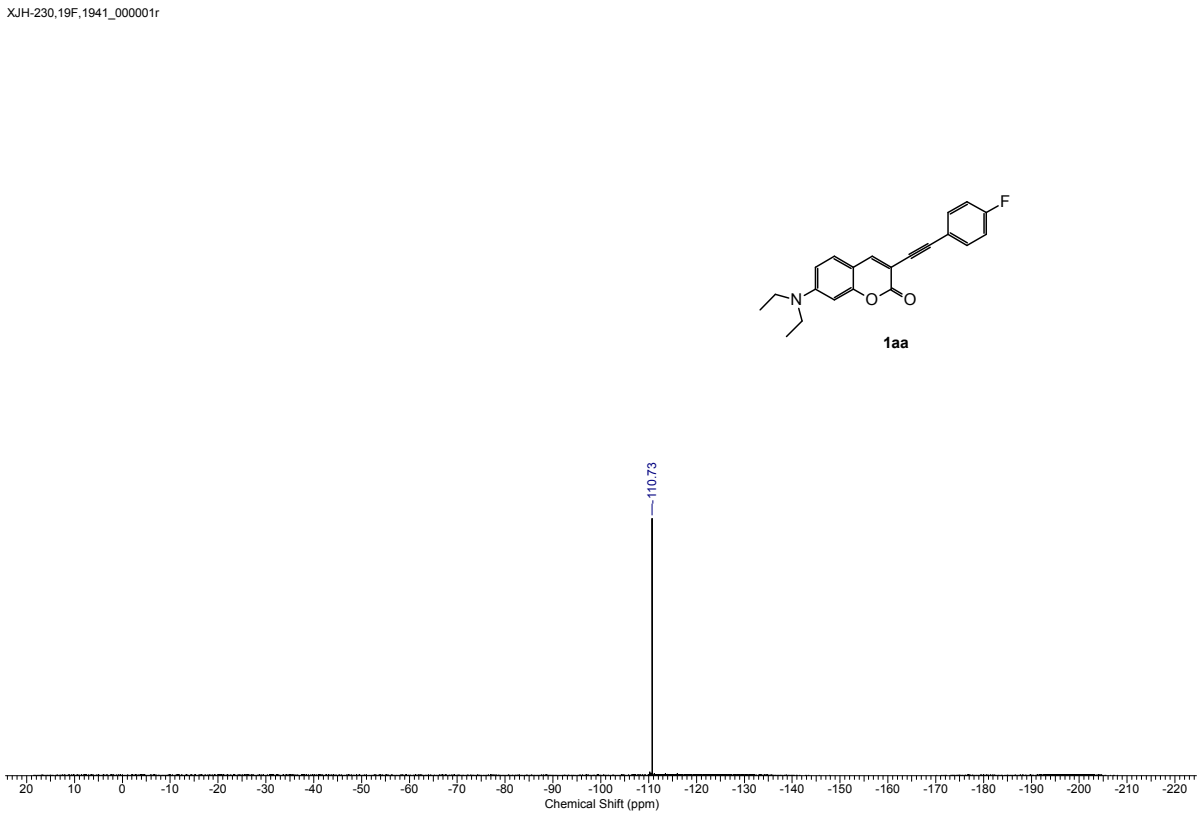


Figure S44. ^{1}H NMR spectrum of compound **1aa**

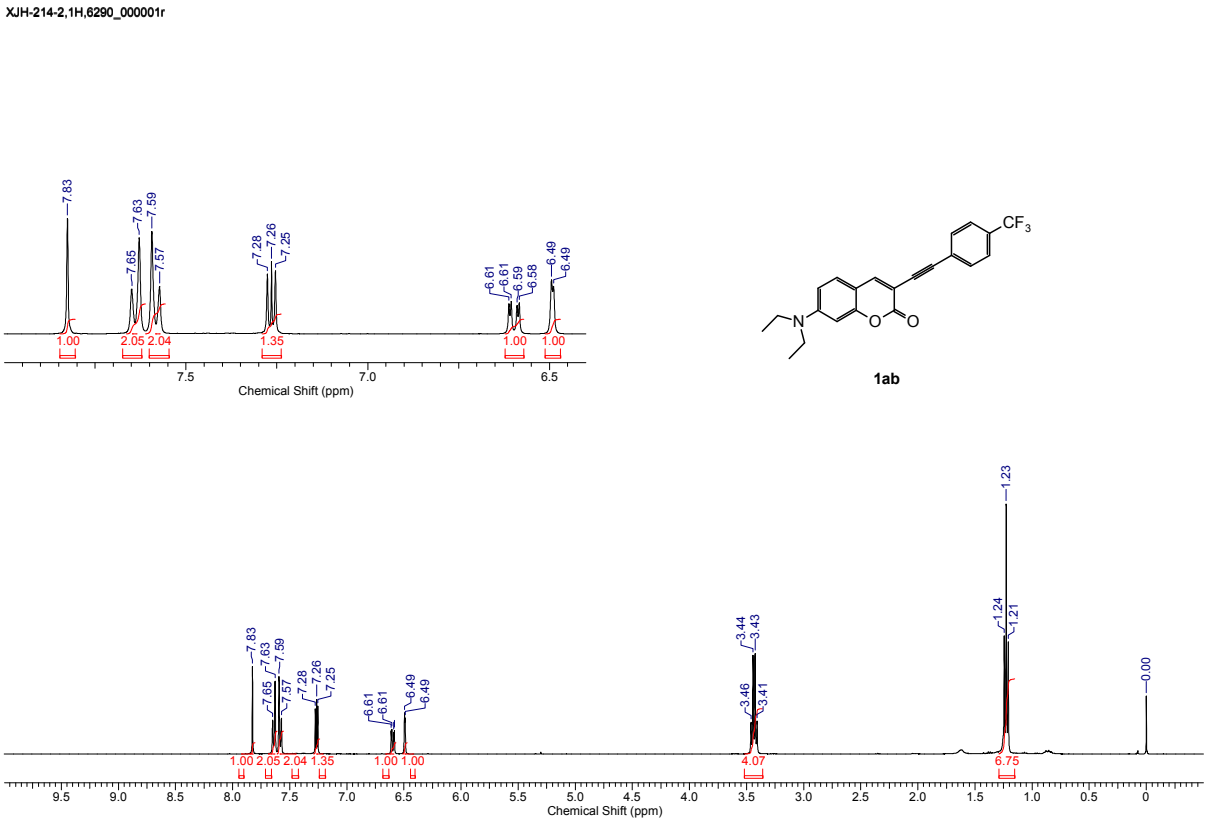


Figure S45. ^{1}H NMR spectrum of compound **1ab**

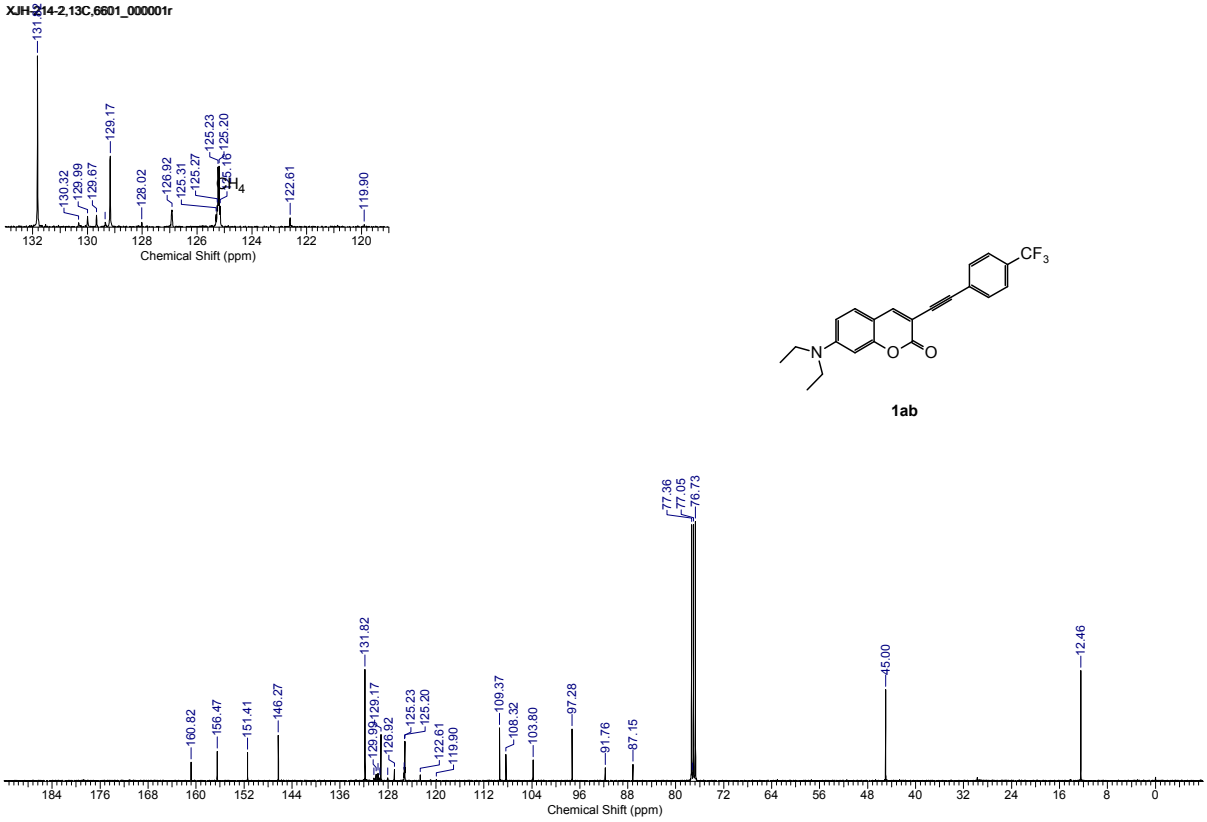


Figure S46. ^{13}C NMR spectrum of compound **1ab**

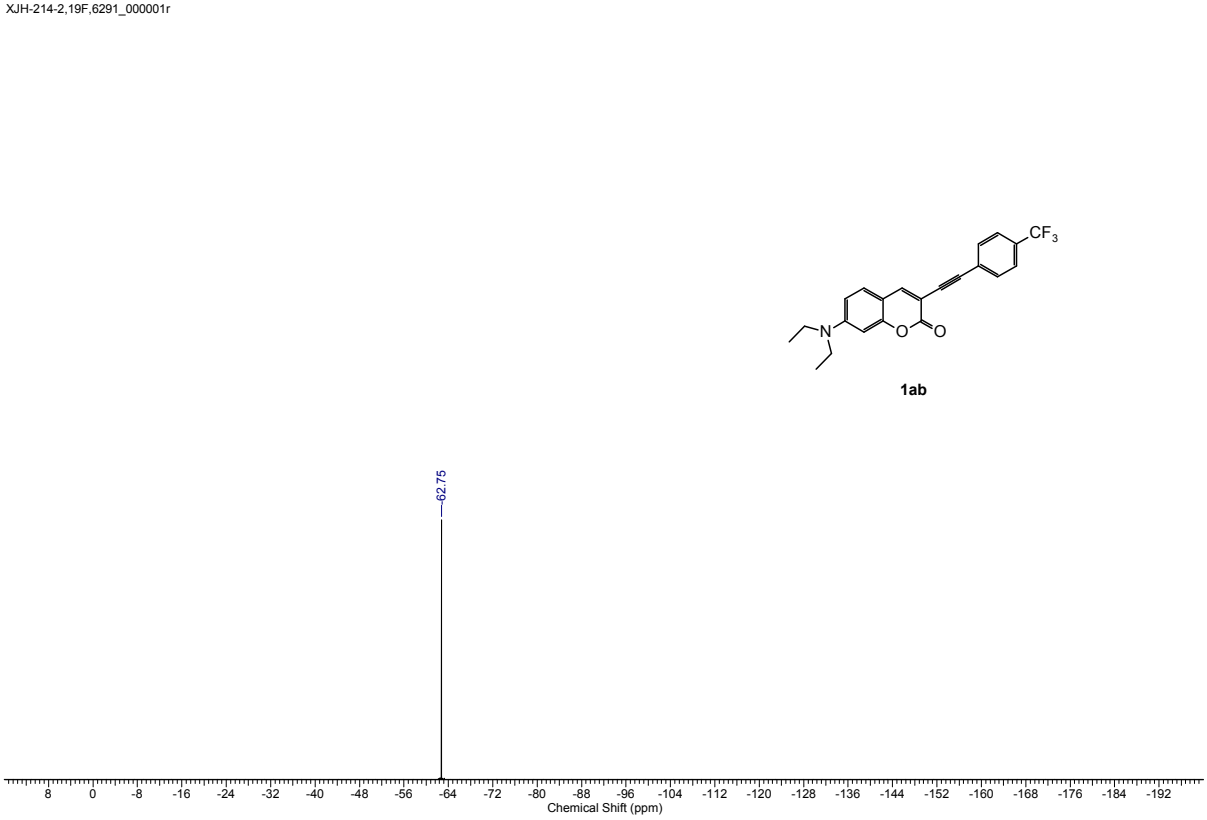


Figure S47. ^{19}F NMR spectrum of compound **1ab**

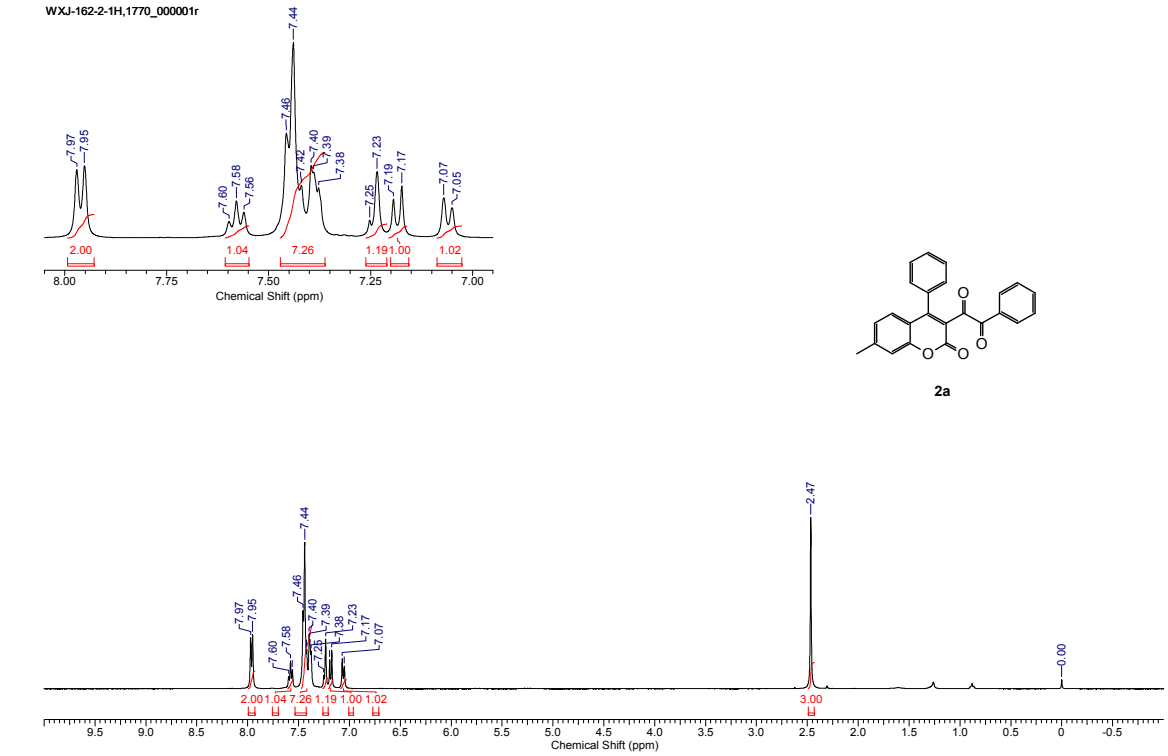


Figure S48. ^{1}H NMR spectrum of compound **2a**

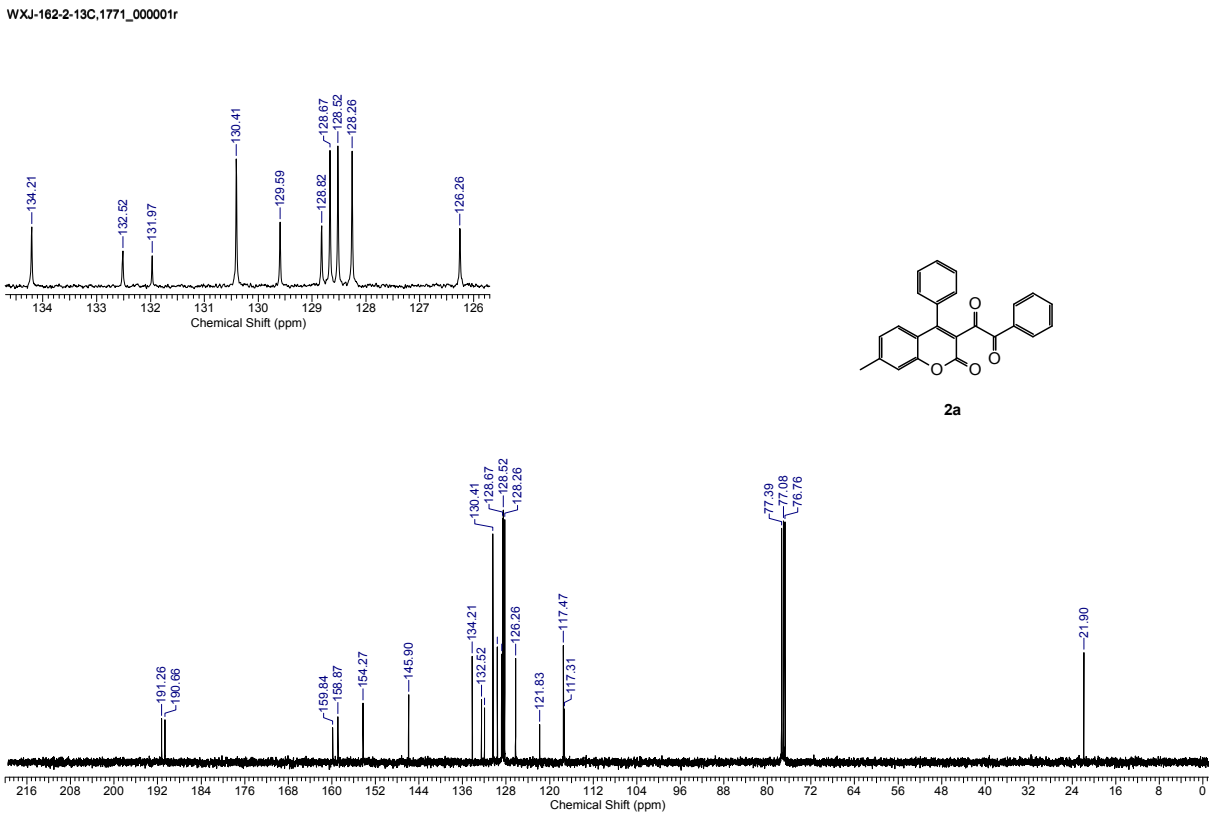


Figure S49. ^{13}C NMR spectrum of compound **2a**

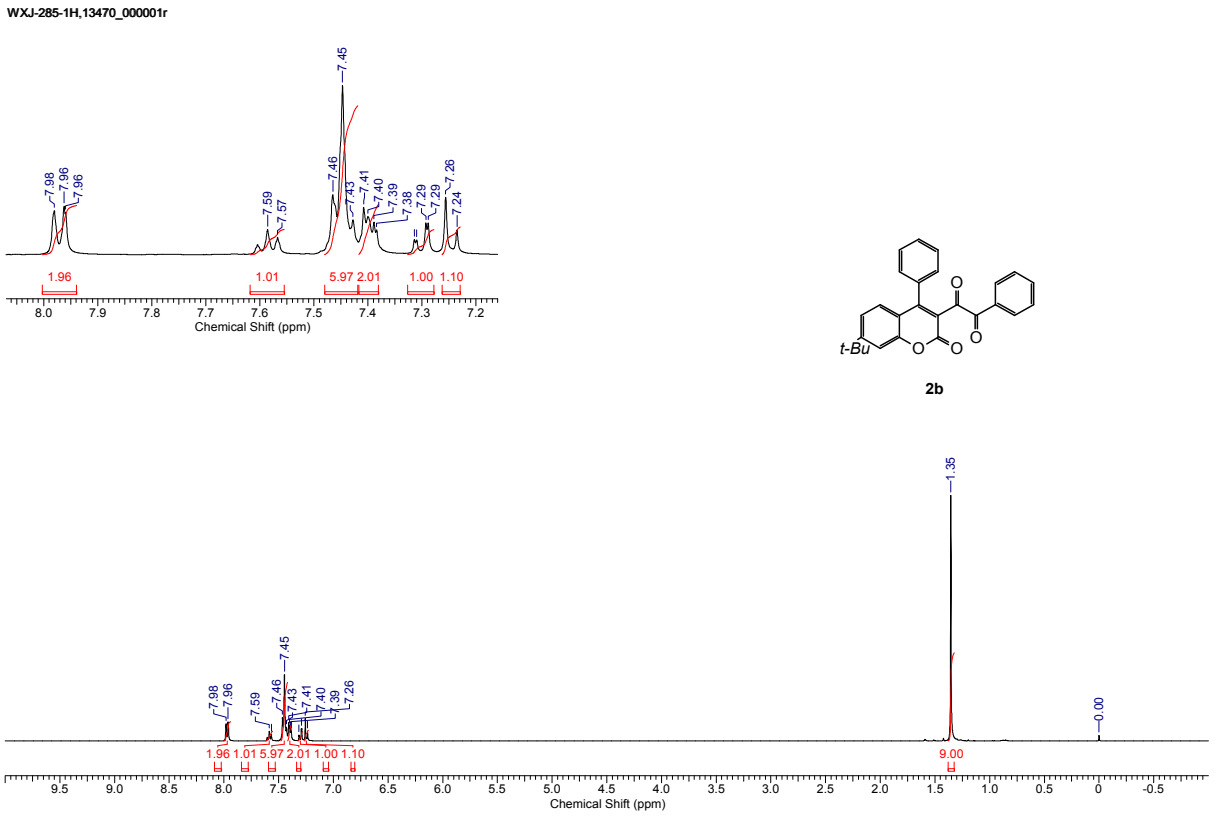


Figure S50. ^{1}H NMR spectrum of compound **2b**

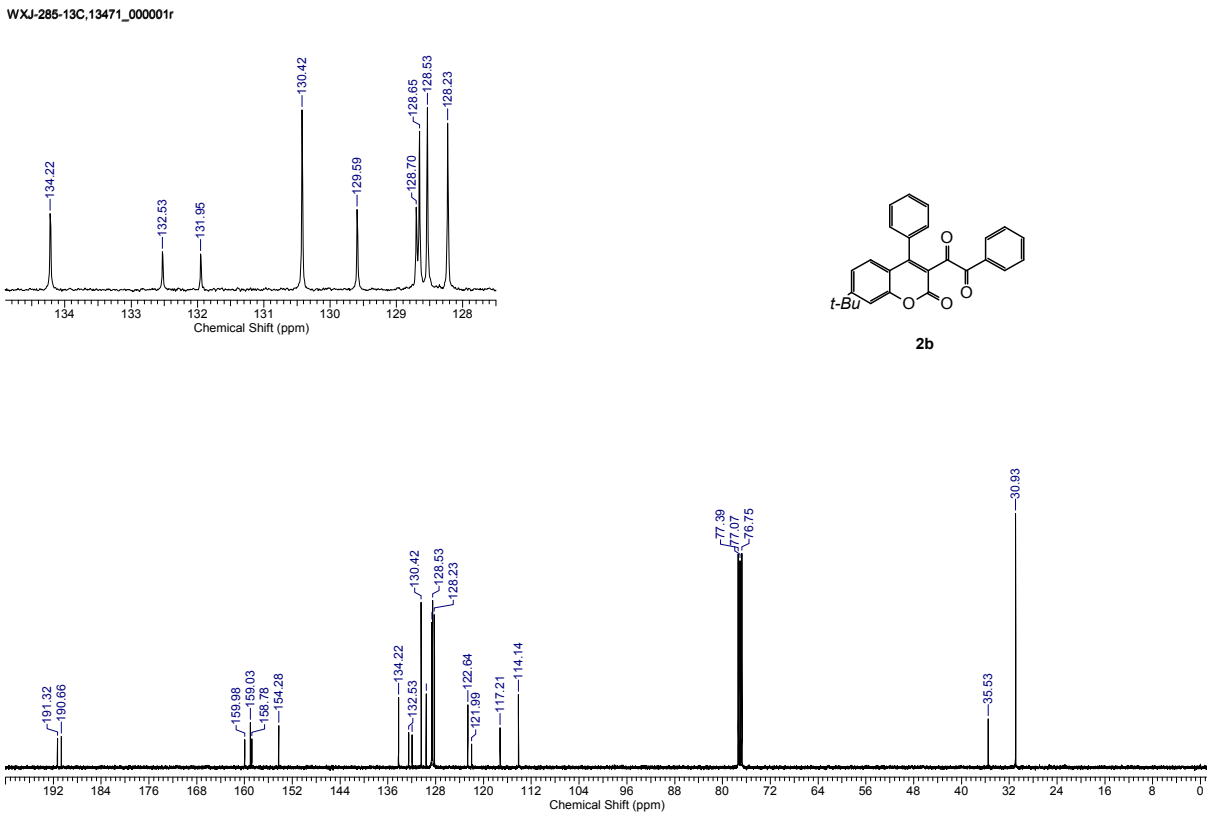


Figure S51. ^{13}C NMR spectrum of compound **2b**

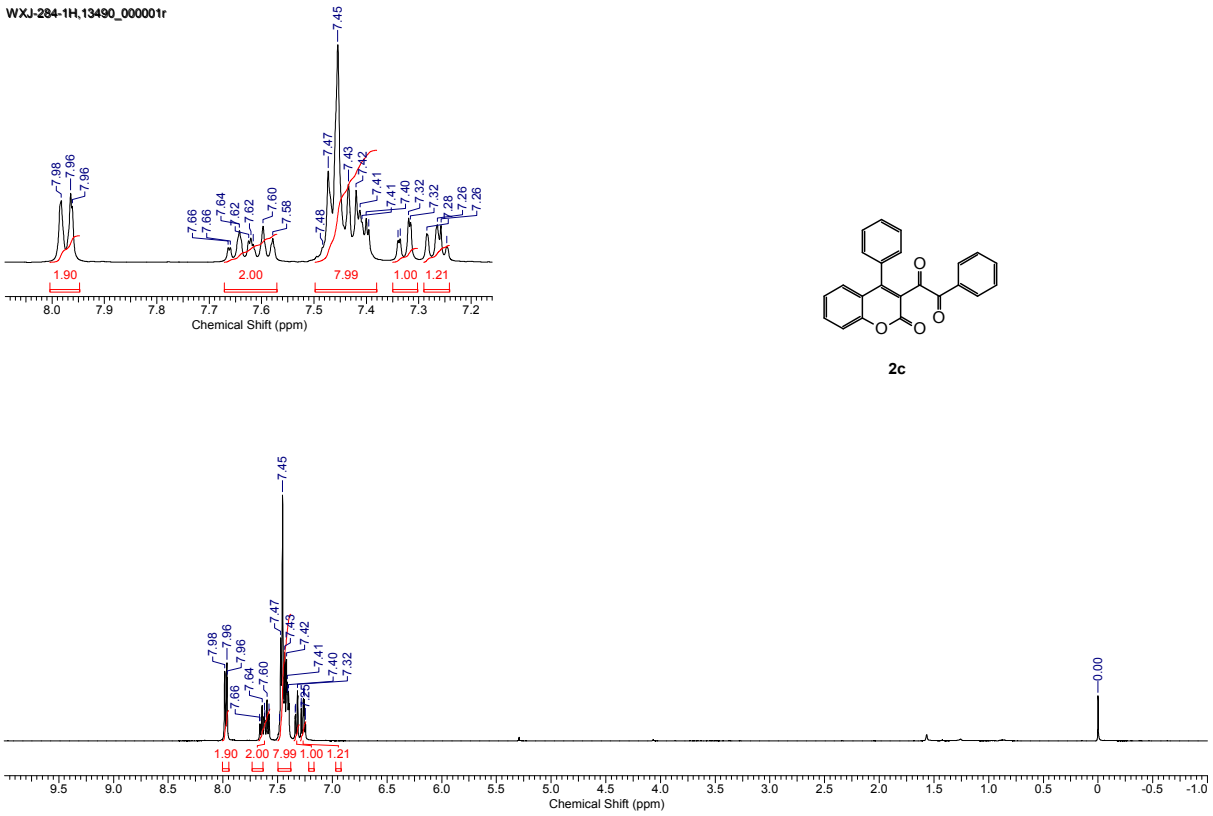


Figure S52. ^{1}H NMR spectrum of compound **2c**

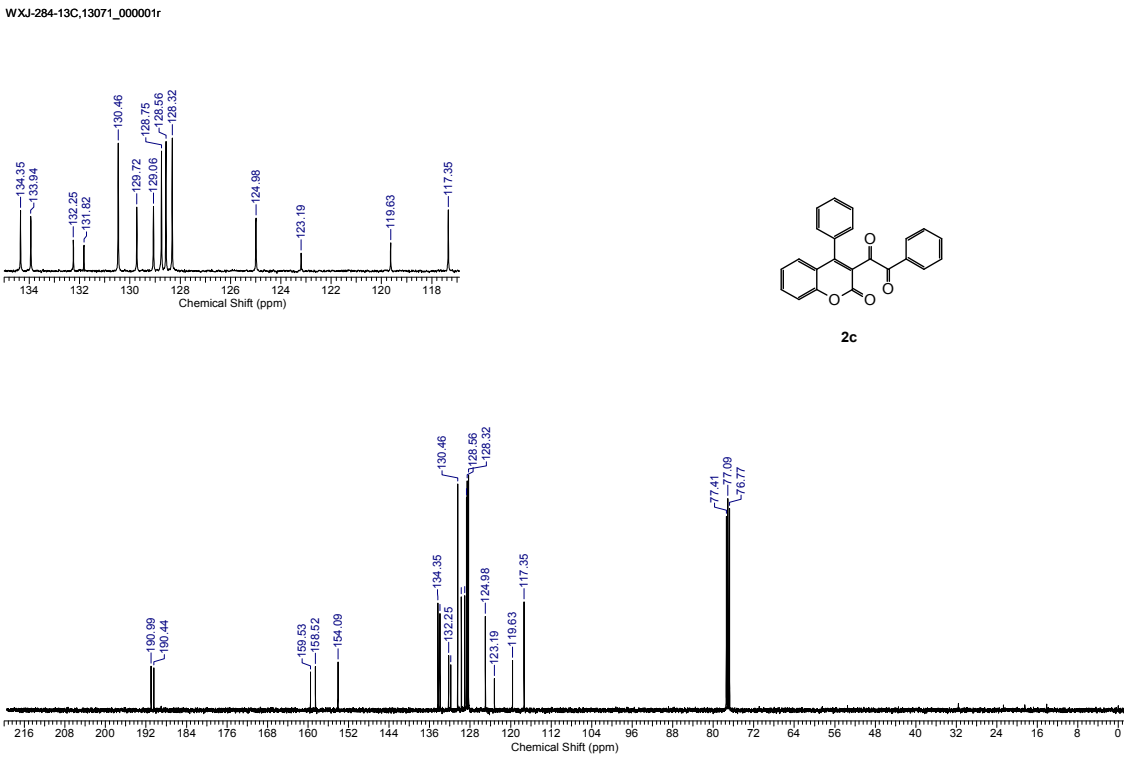


Figure S53. ^{13}C NMR spectrum of compound **2c**

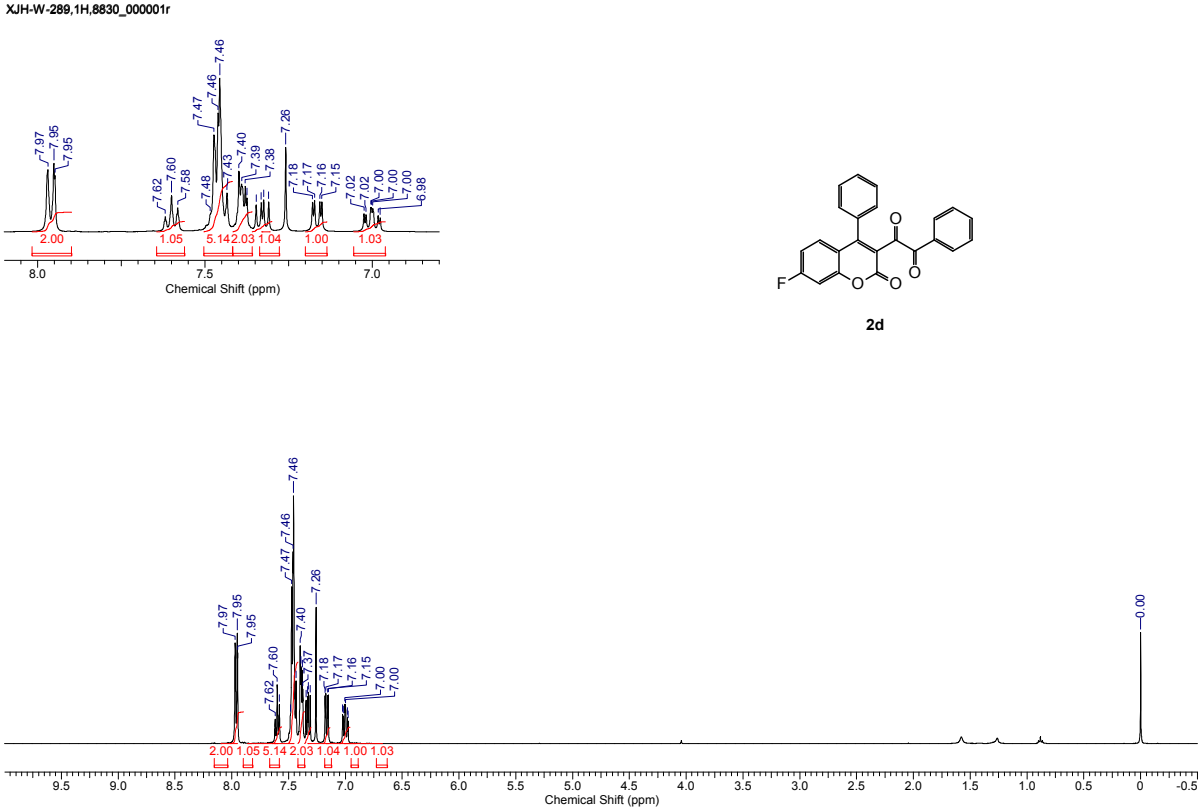


Figure S54. ^{1}H NMR spectrum of compound **2d**

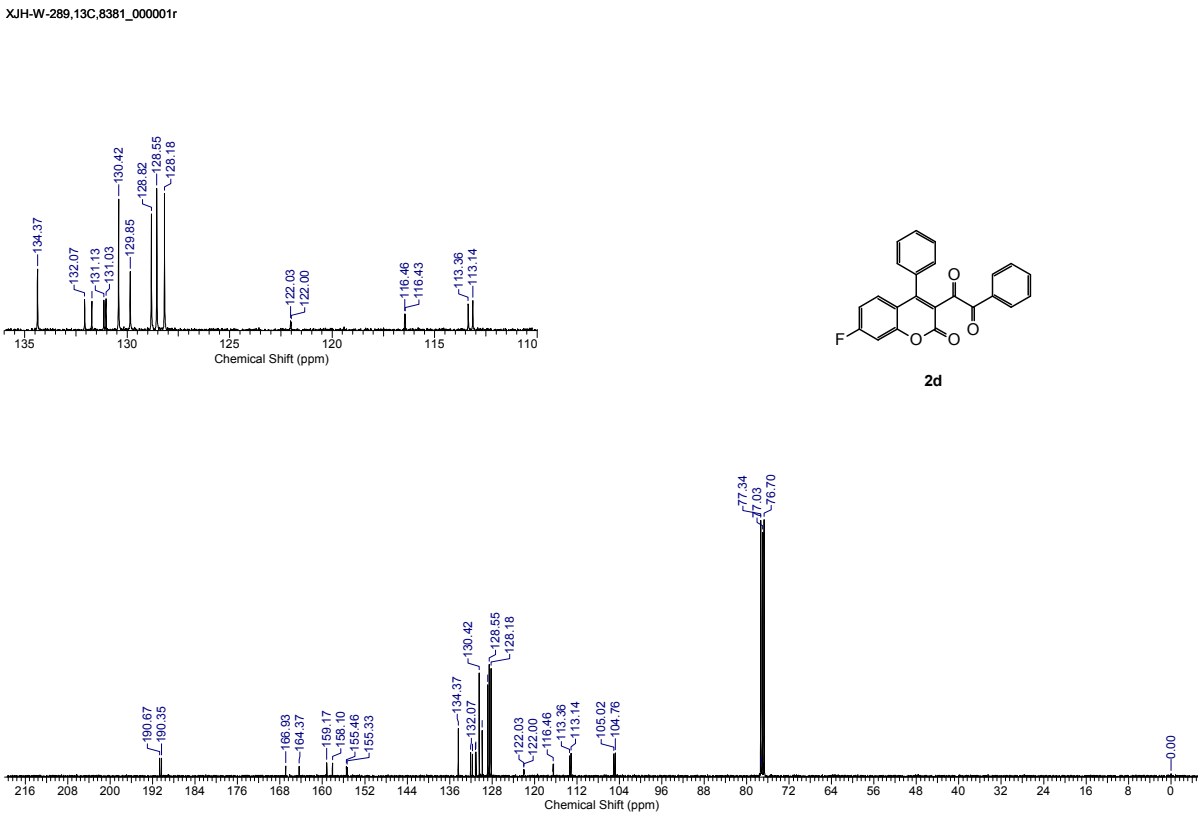


Figure S55. ^{13}C NMR spectrum of compound **2d**

Figure S56. ^{19}F NMR spectrum of compound **2d**

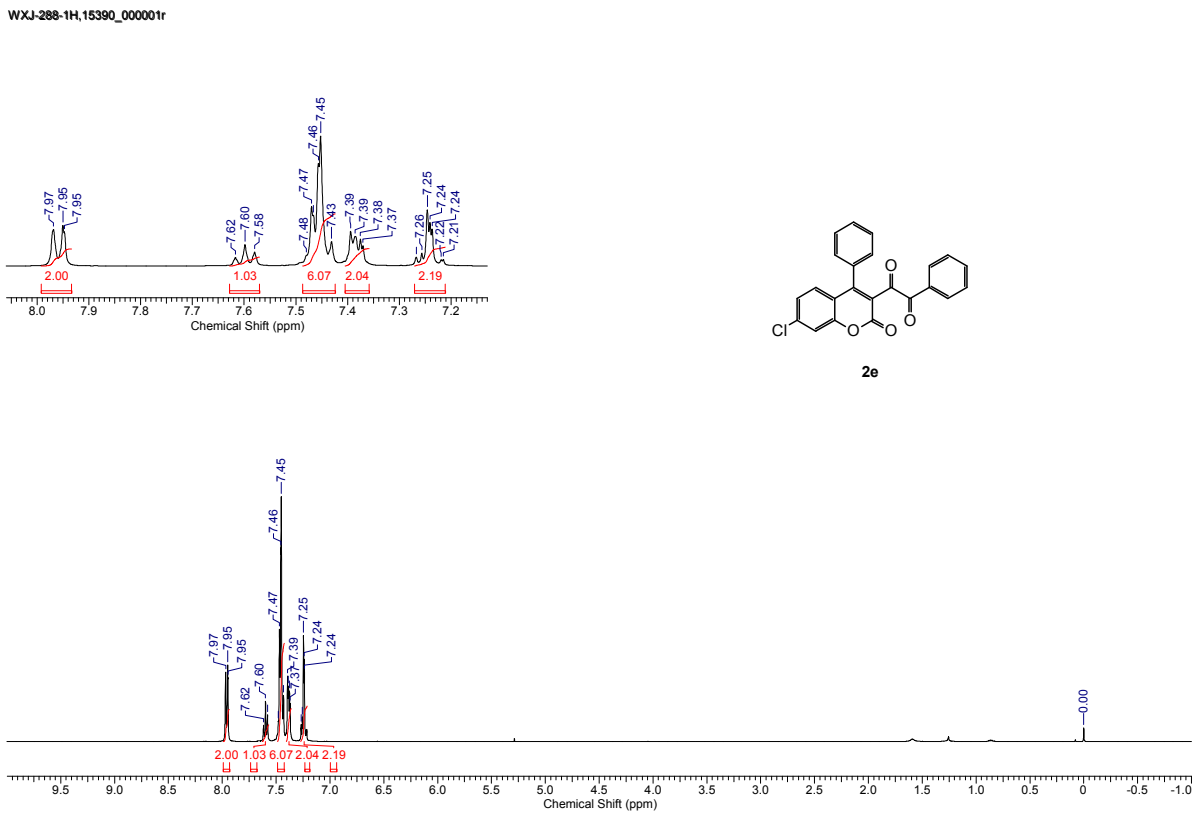


Figure S57. ^{1}H NMR spectrum of compound **2e**

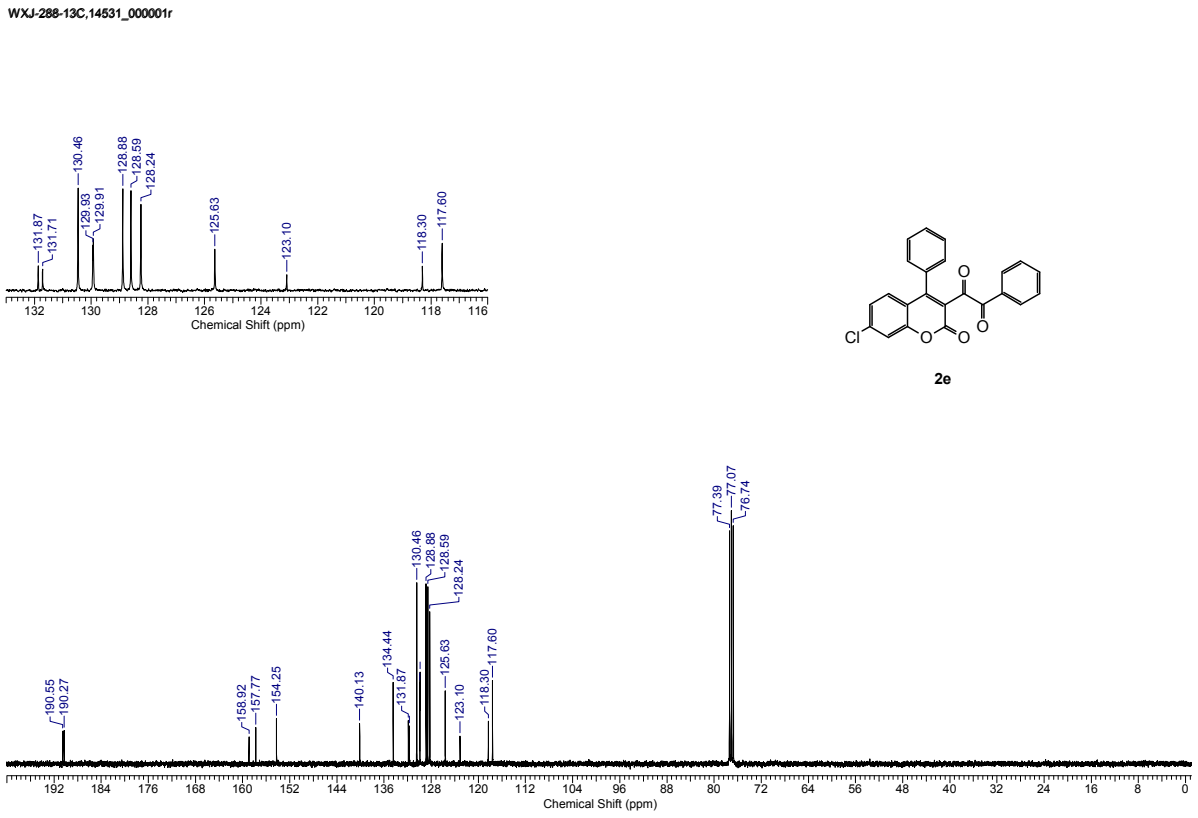


Figure S58. ^{13}C NMR spectrum of compound **2e**

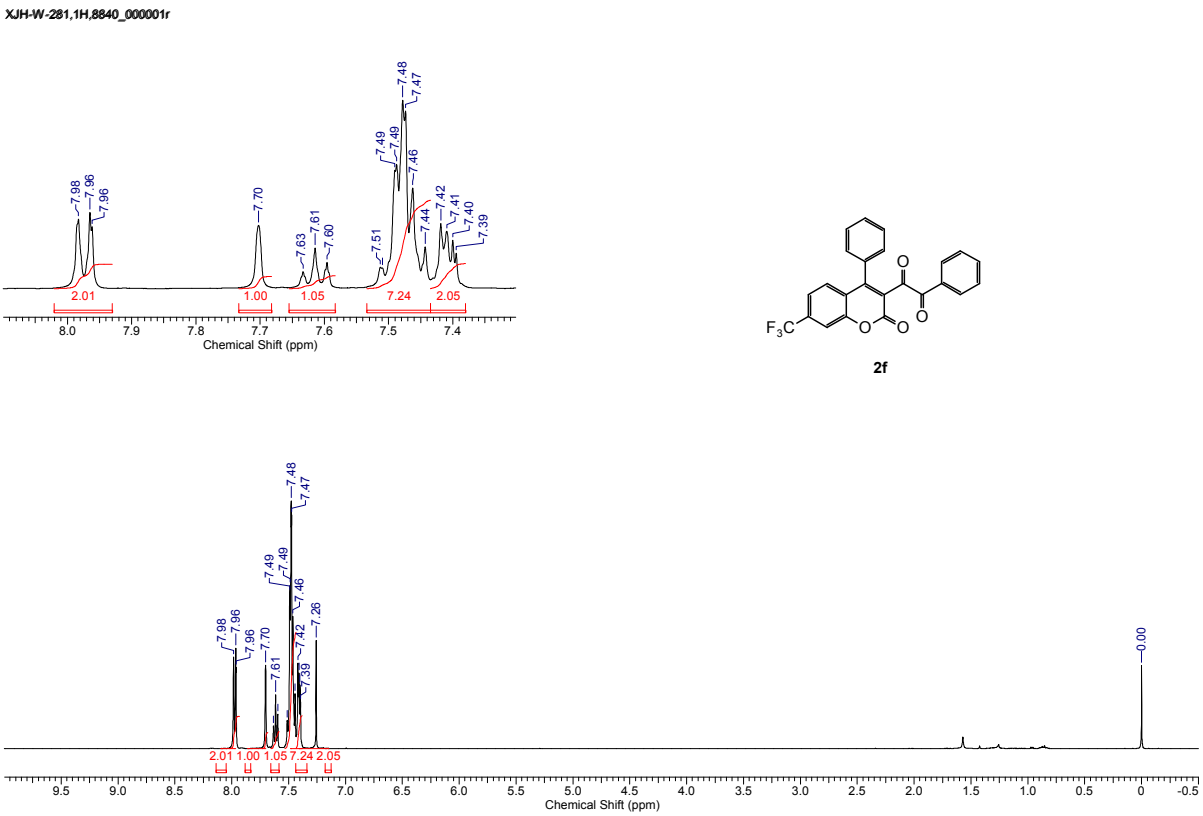


Figure S59. ^{1}H NMR spectrum of compound **2f**

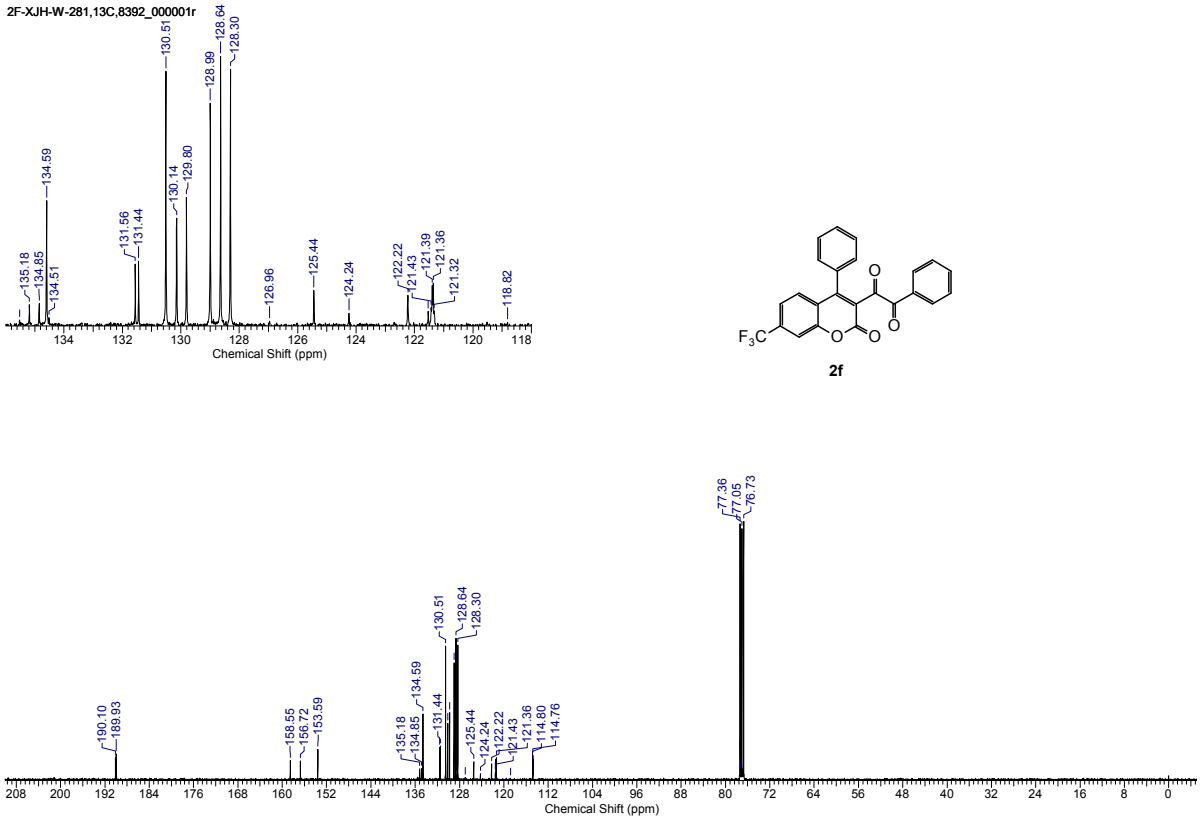
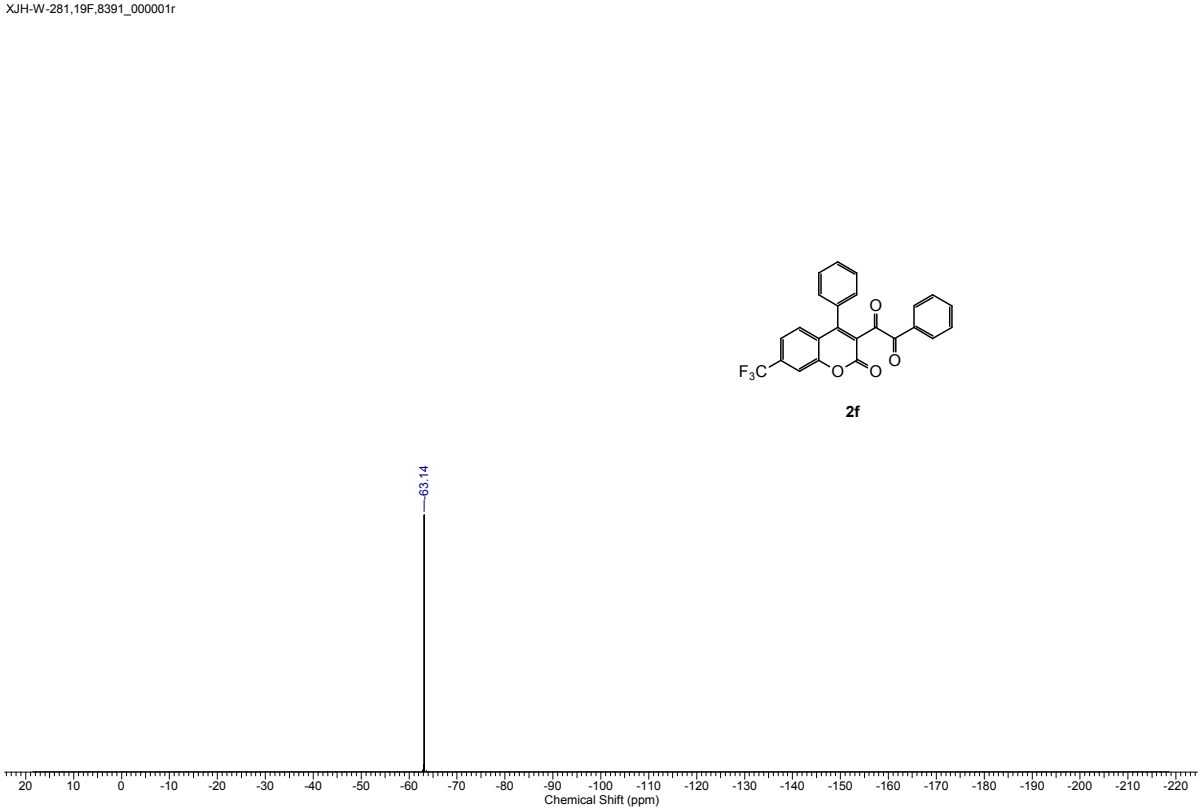
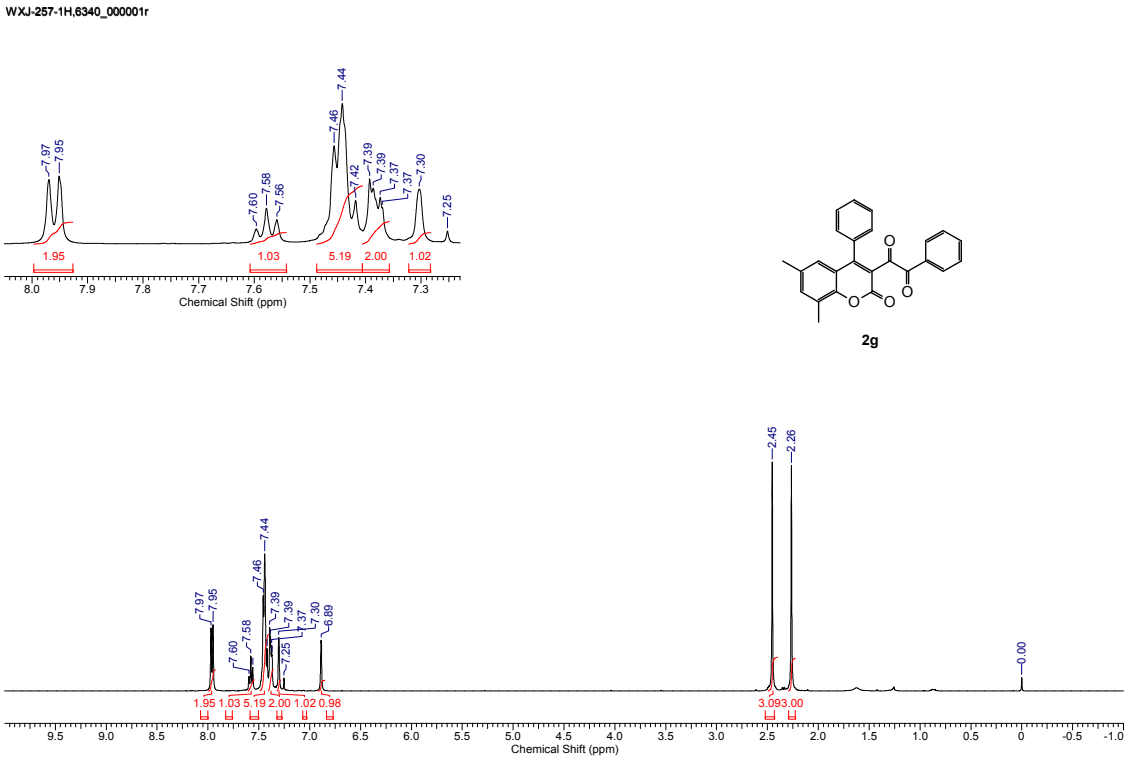


Figure S60. ^{13}C NMR spectrum of compound **2f**



2f

Figure S61. ^{19}F NMR spectrum of compound **2f**



2g

Figure S62. ^{1}H NMR spectrum of compound **2g**

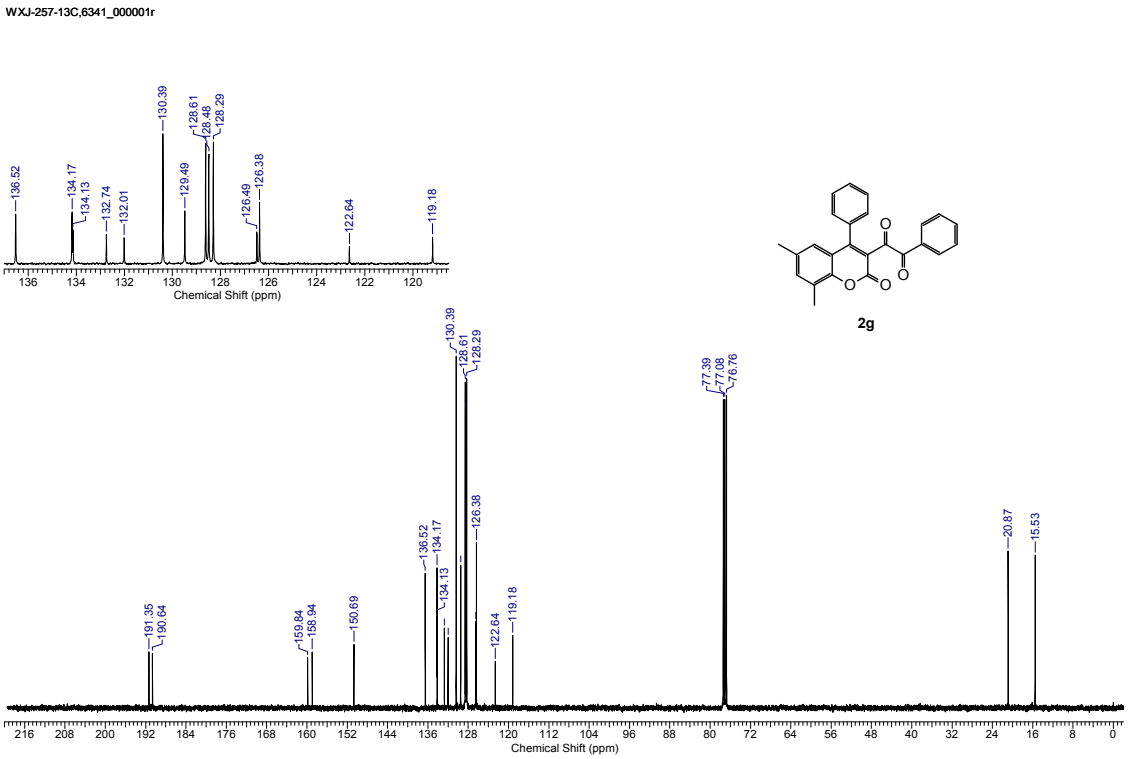


Figure S63. ^{13}C NMR spectrum of compound **2g**

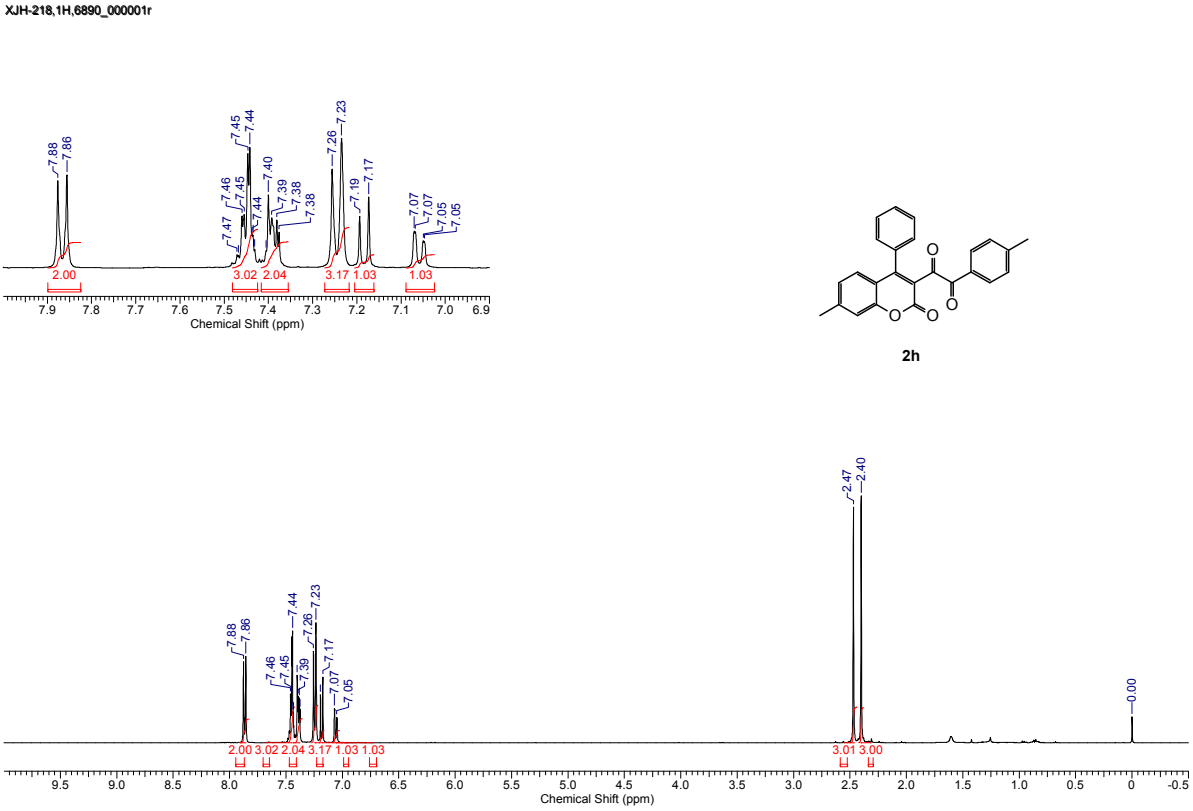


Figure S64. ^{1}H NMR spectrum of compound **2h**

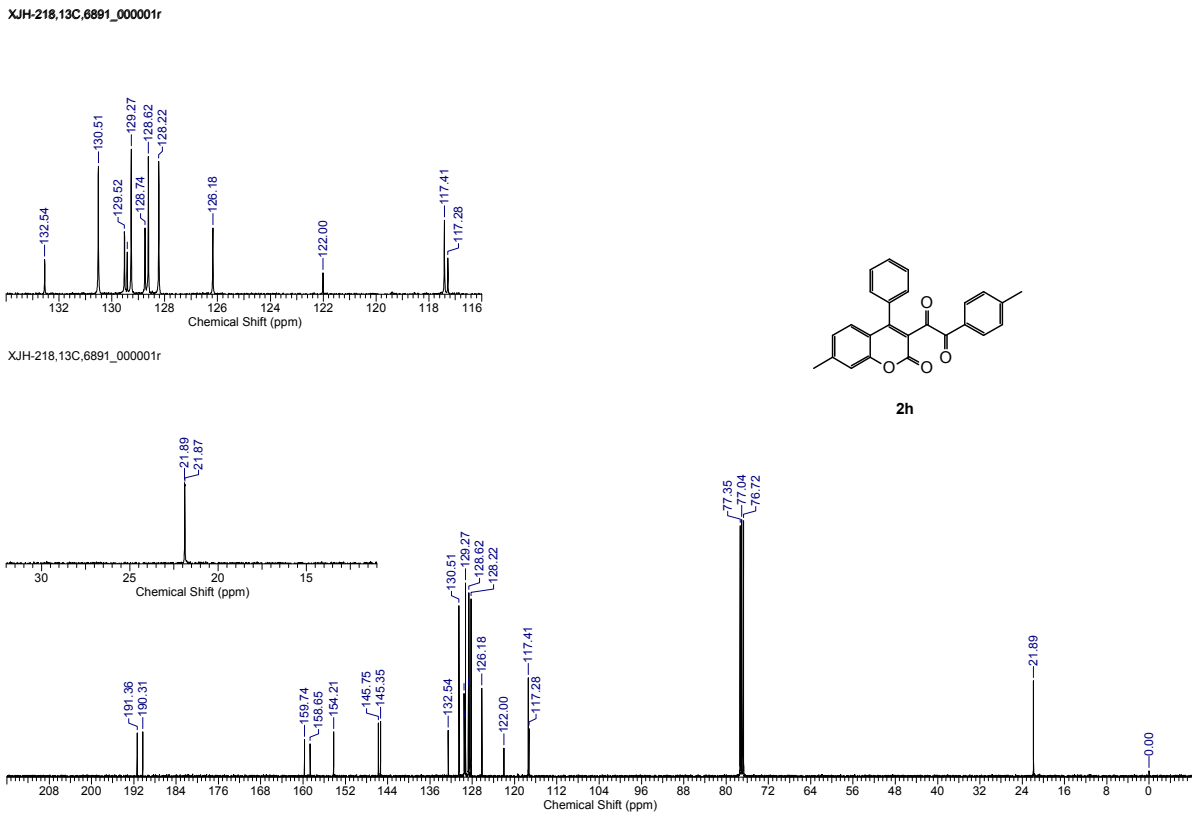


Figure S65. ^{13}C NMR spectrum of compound **2h**

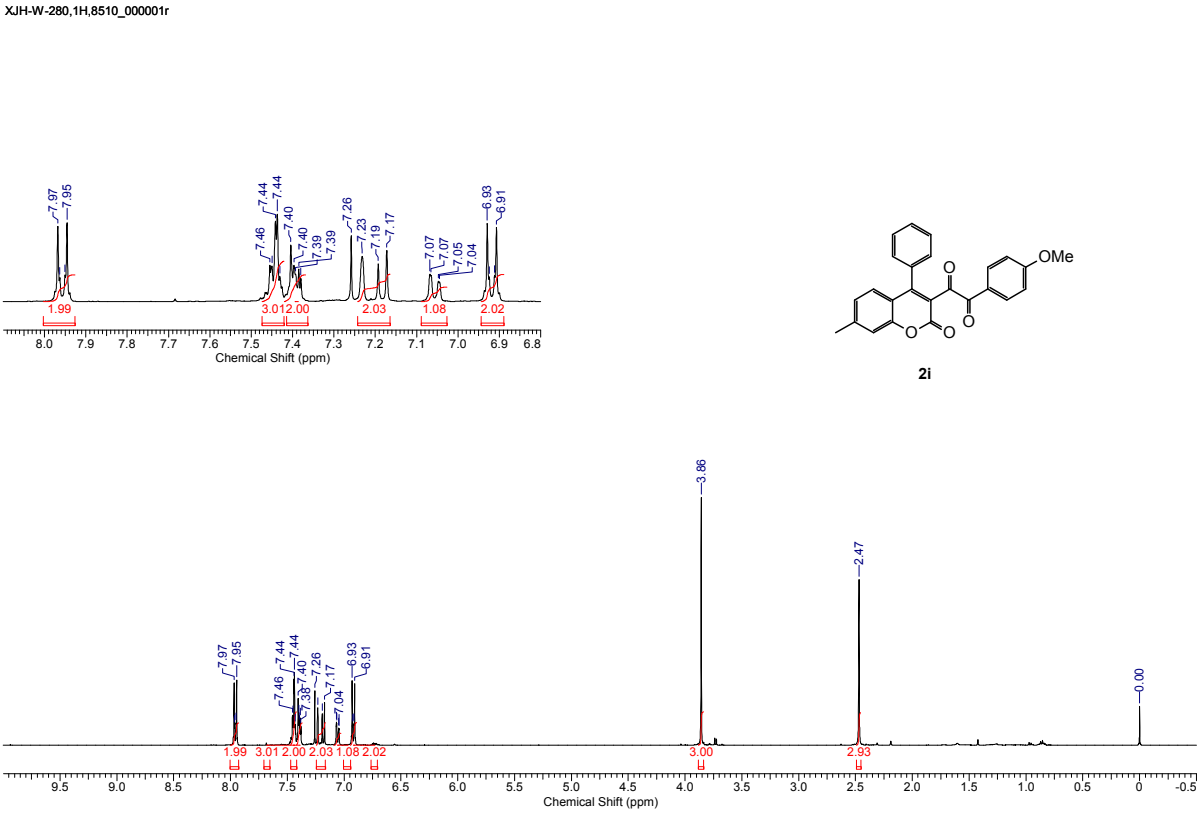


Figure S66. ^{1}H NMR spectrum of compound **2i**

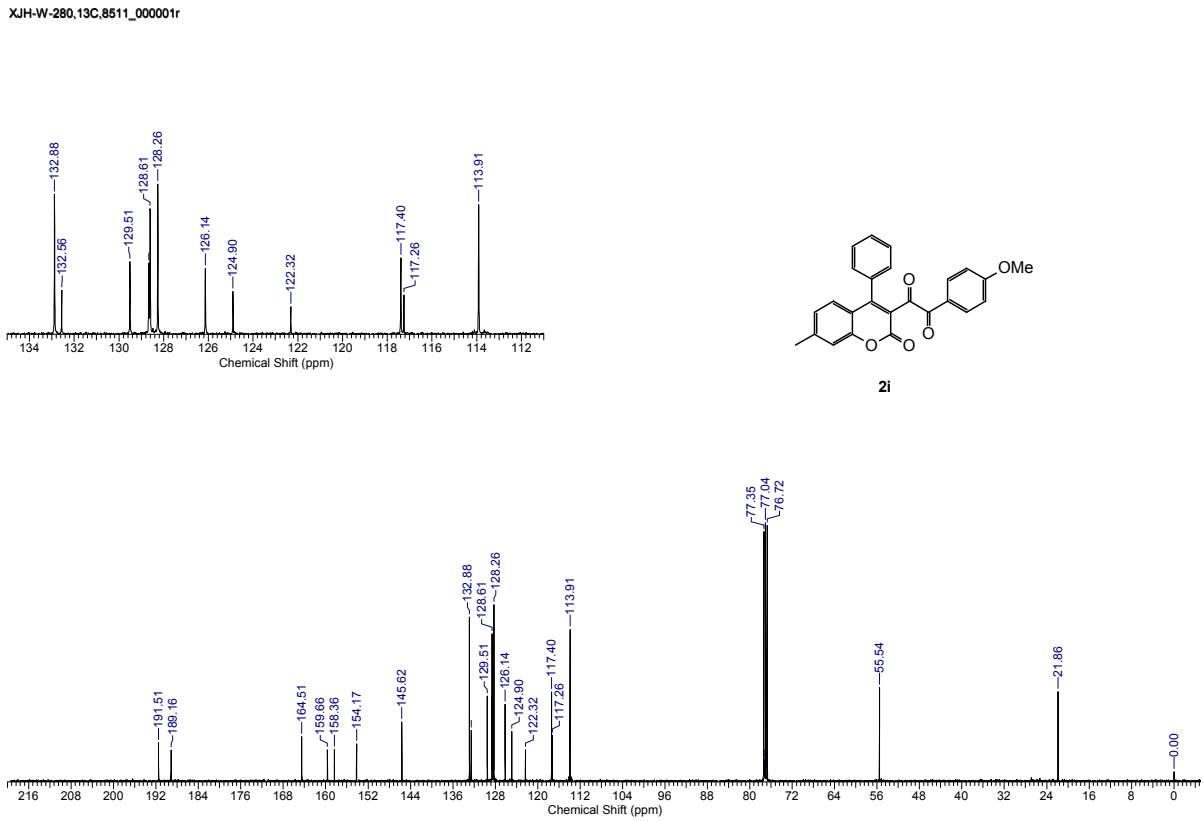


Figure S67. ^{13}C NMR spectrum of compound **2i**

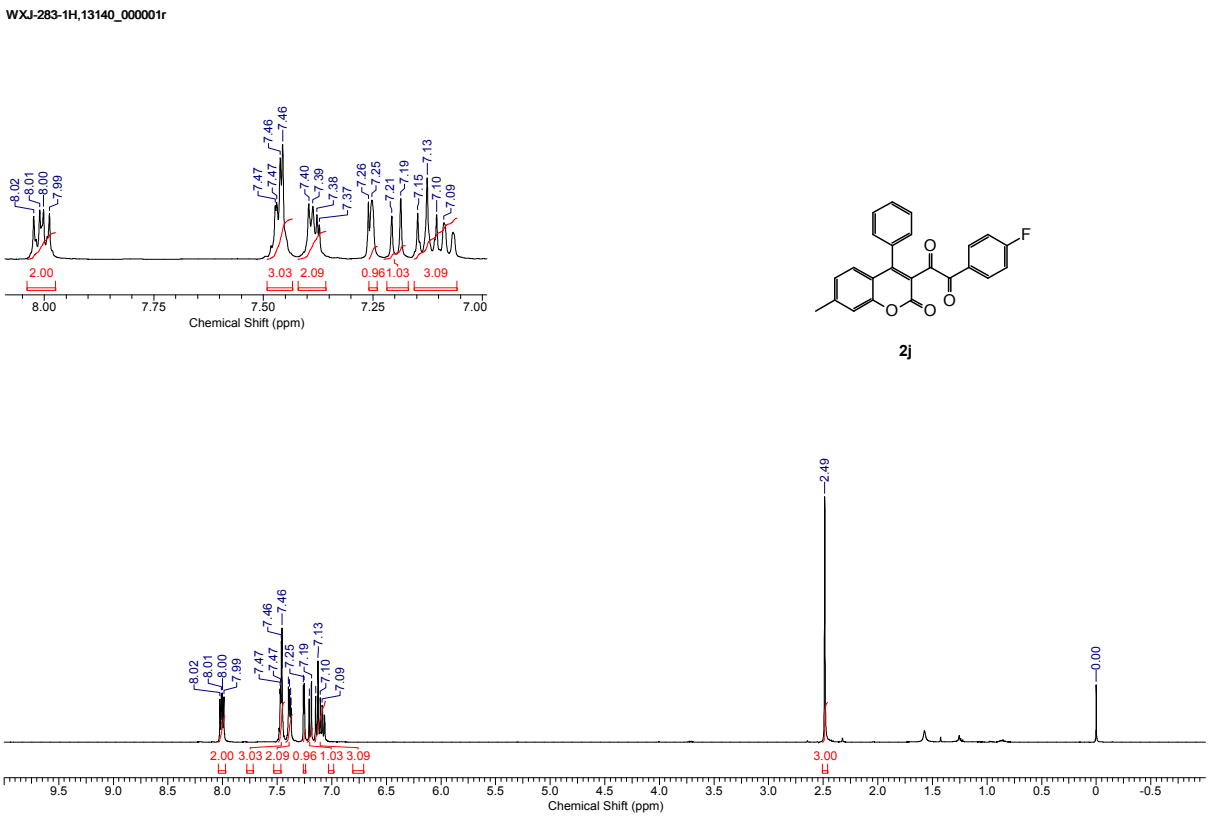


Figure S68. ^{1}H NMR spectrum of compound **2j**

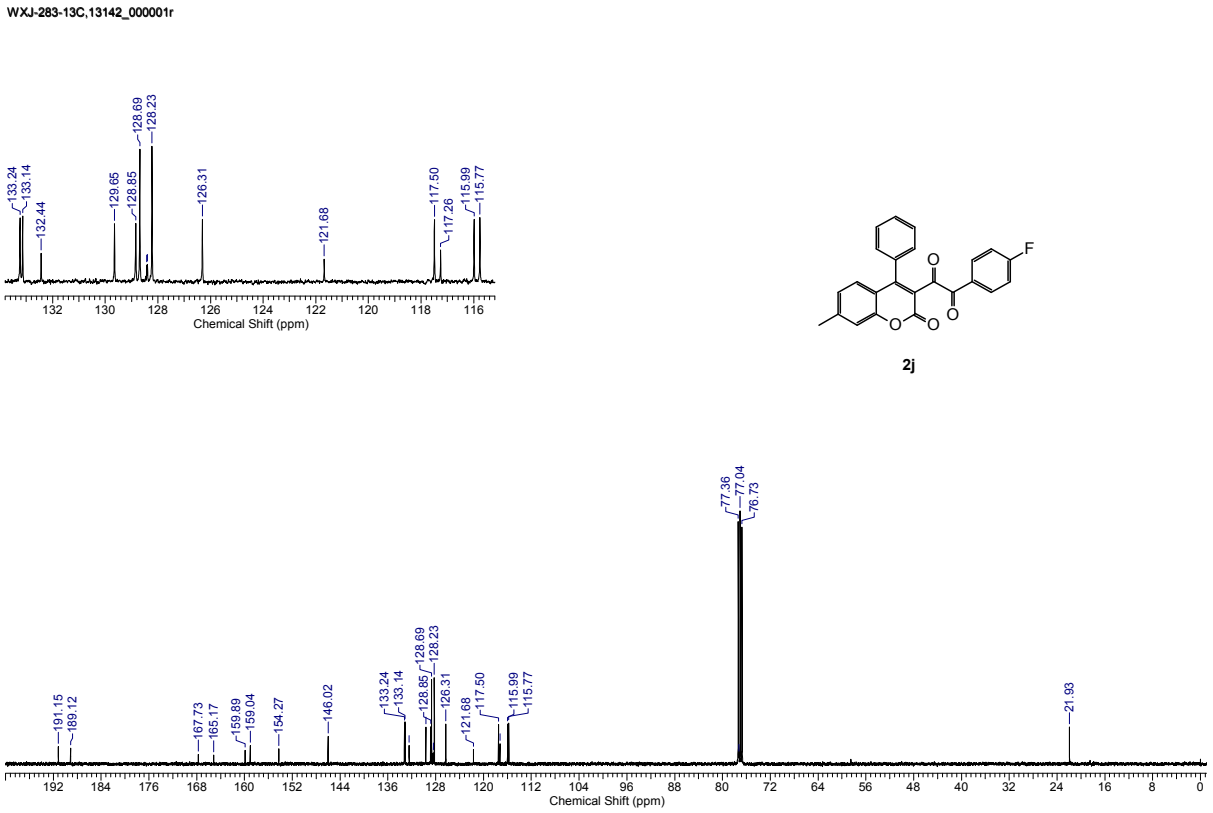


Figure S69. ^{13}C NMR spectrum of compound **2j**

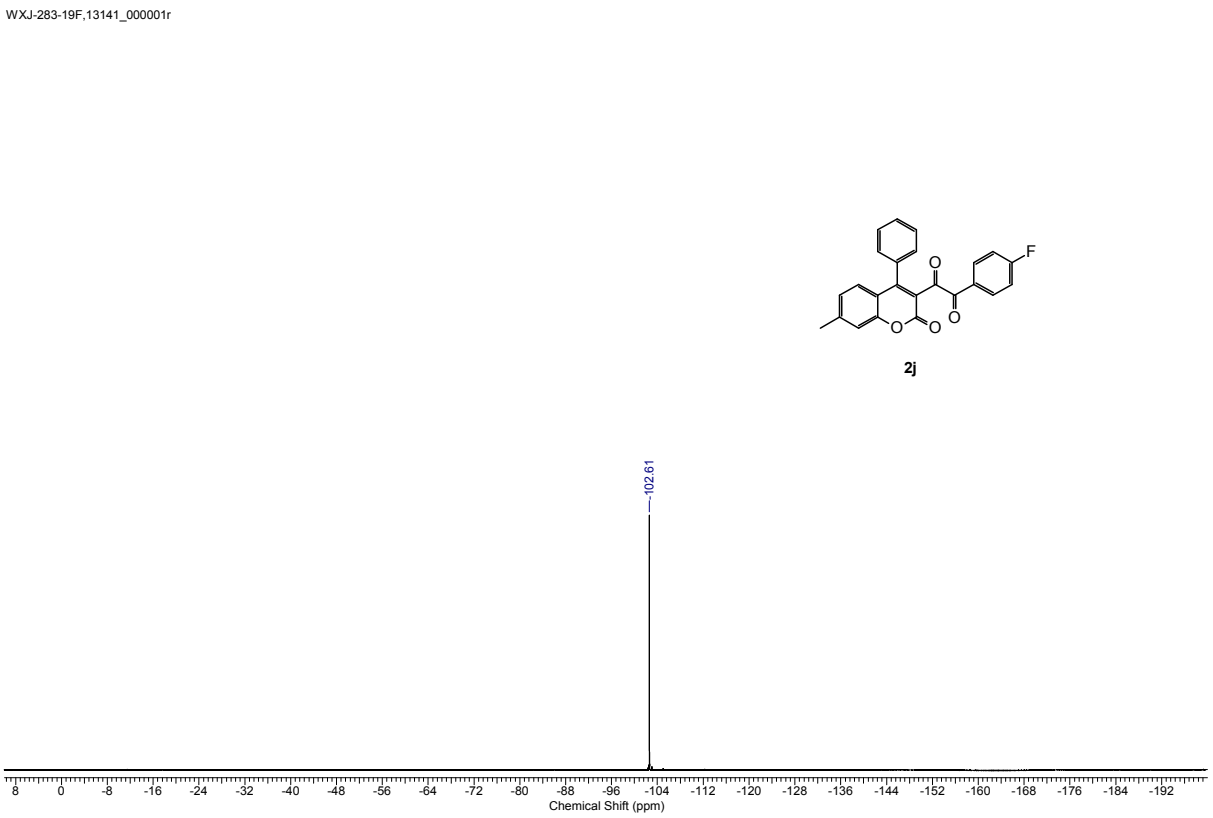


Figure S70. ^{19}F NMR spectrum of compound **2j**

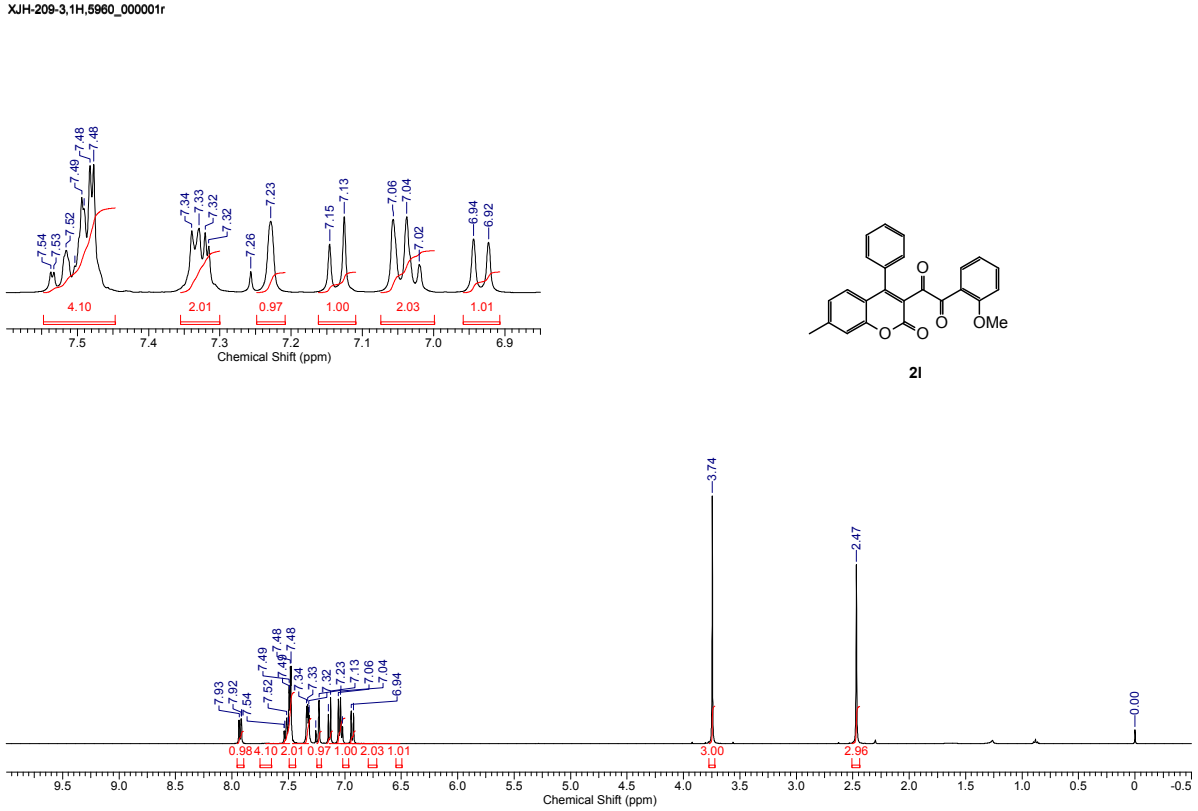


Figure S71. ^{1}H NMR spectrum of compound **2l**

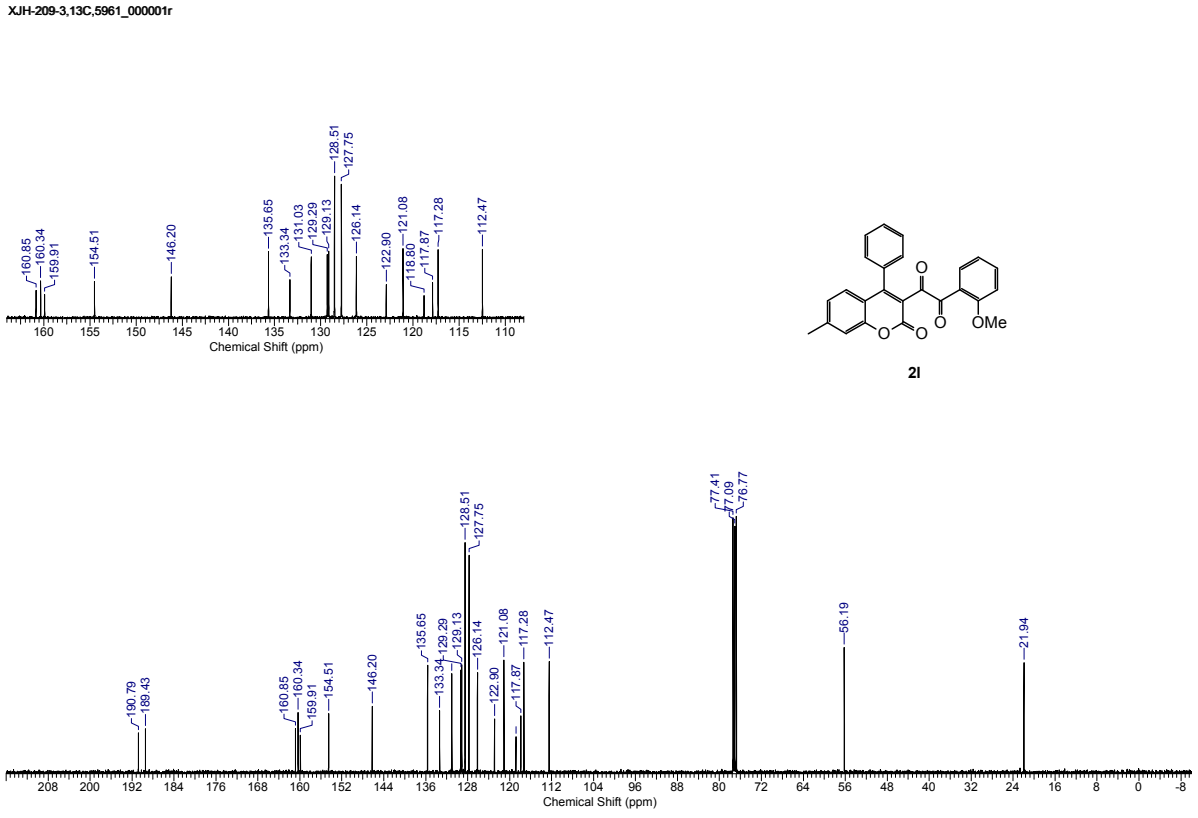


Figure S72. ^{13}C NMR spectrum of compound **2l**

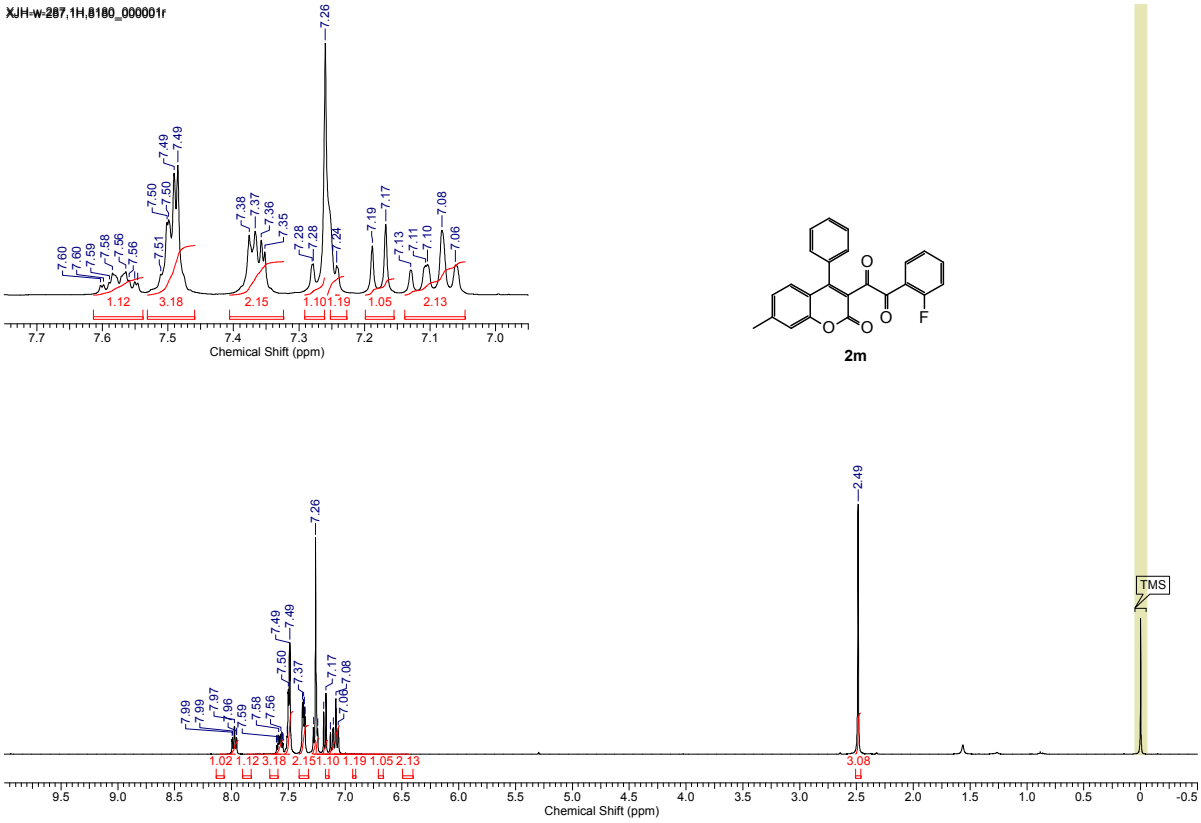


Figure S73. ^{1}H NMR spectrum of compound **2m**

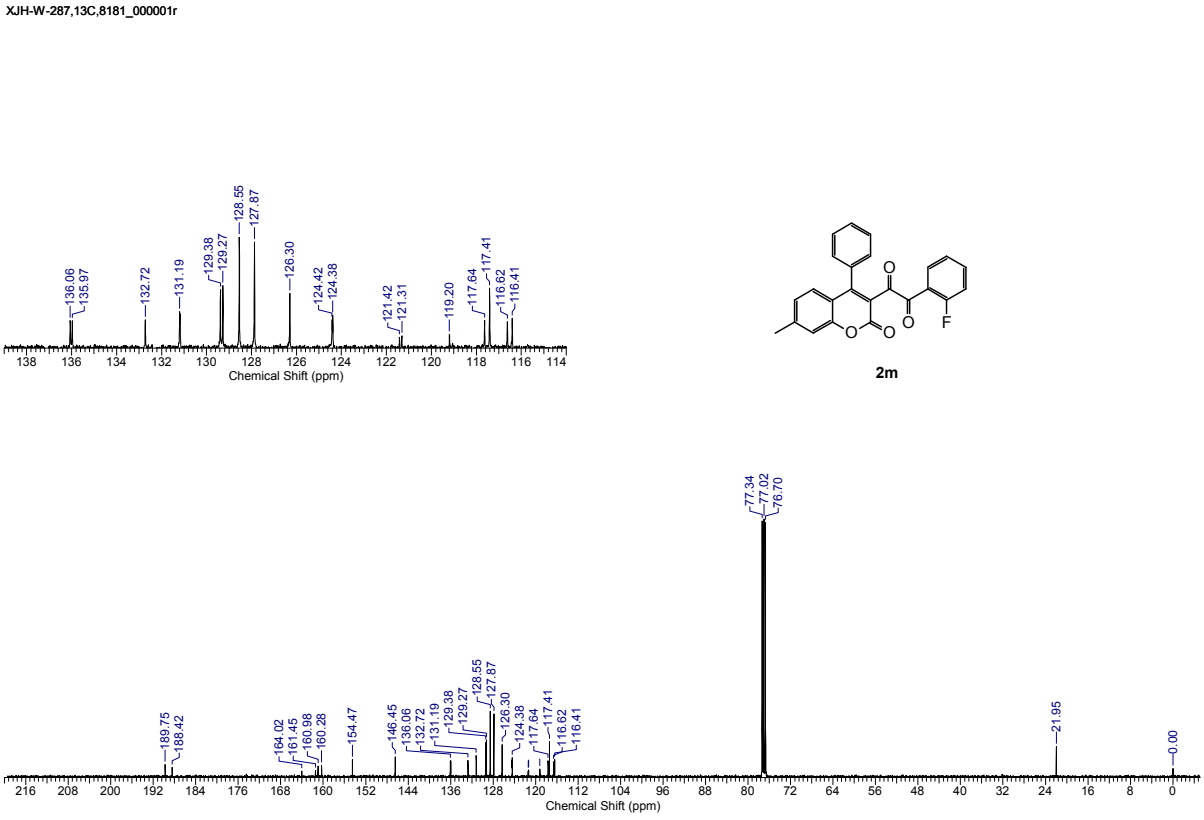


Figure S74. ^{13}C NMR spectrum of compound **2m**

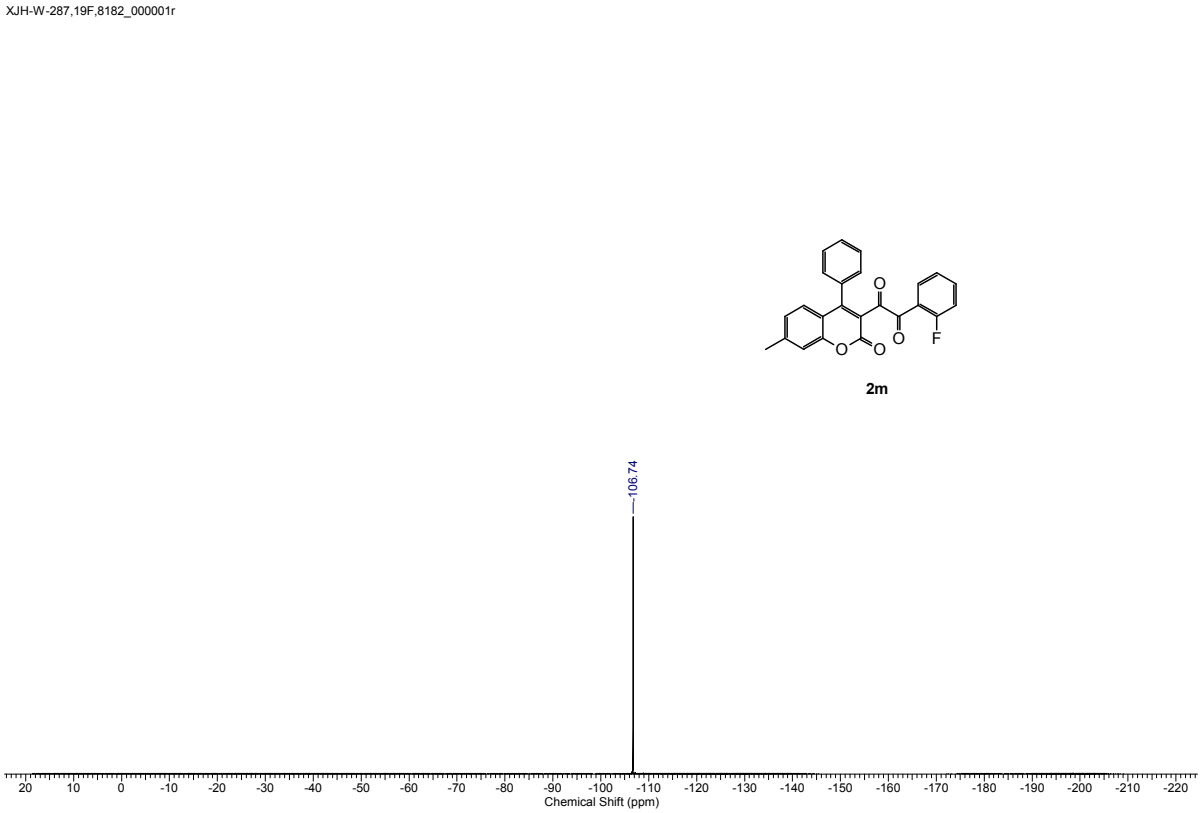


Figure S75. ^{19}F NMR spectrum of compound **2m**

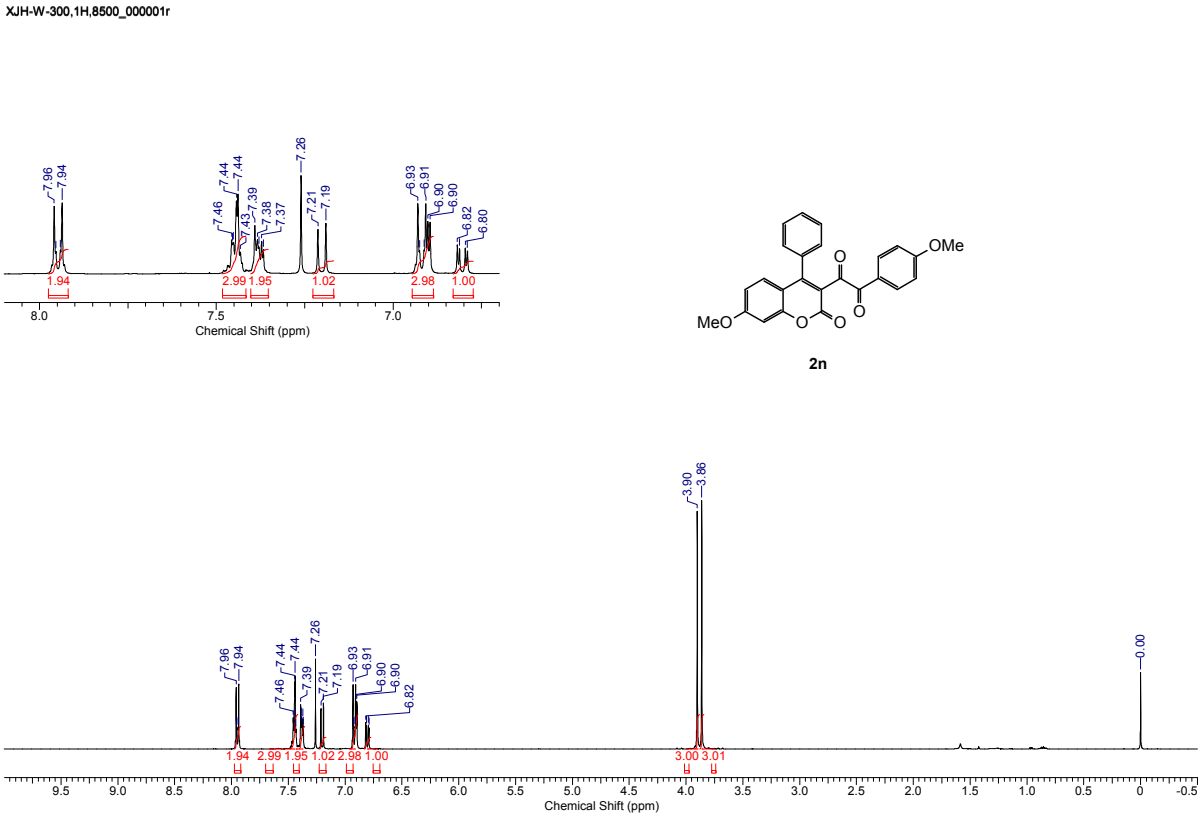


Figure S76. ^{1}H NMR spectrum of compound **2n**

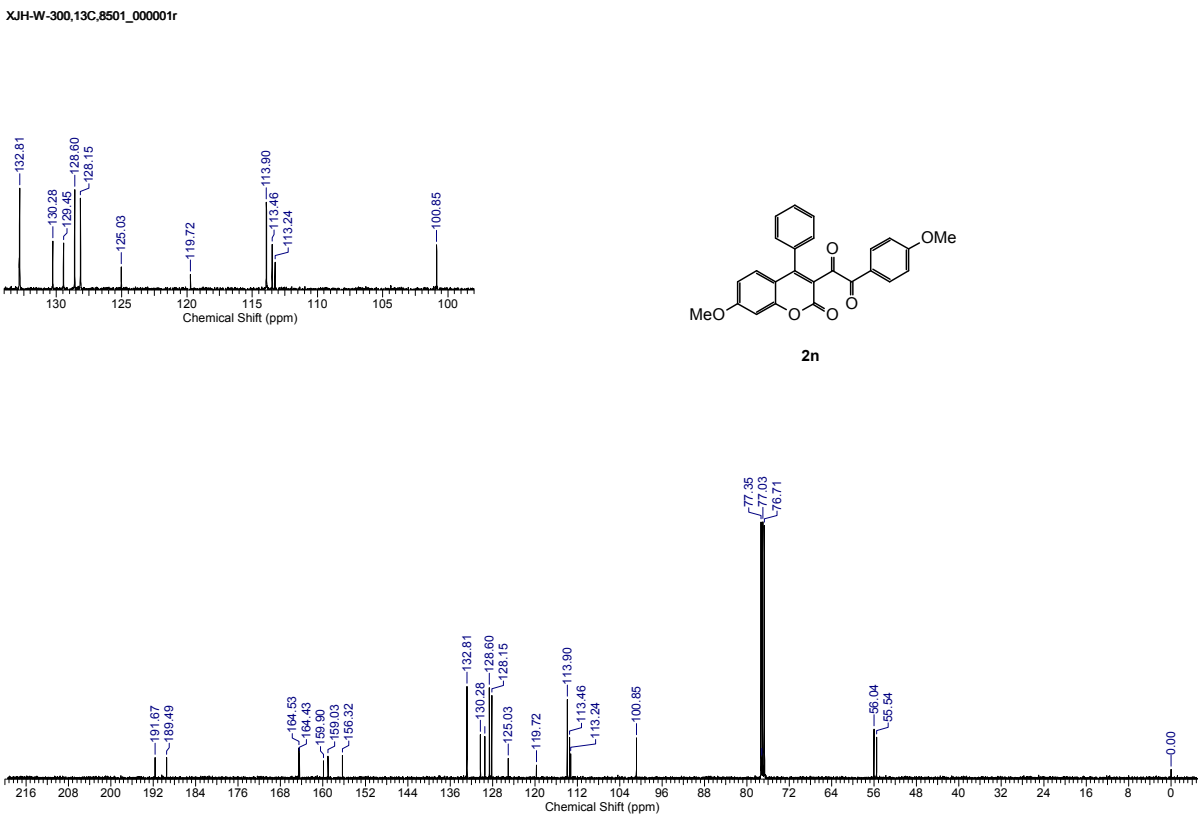


Figure S77. ^{13}C NMR spectrum of compound **2n**

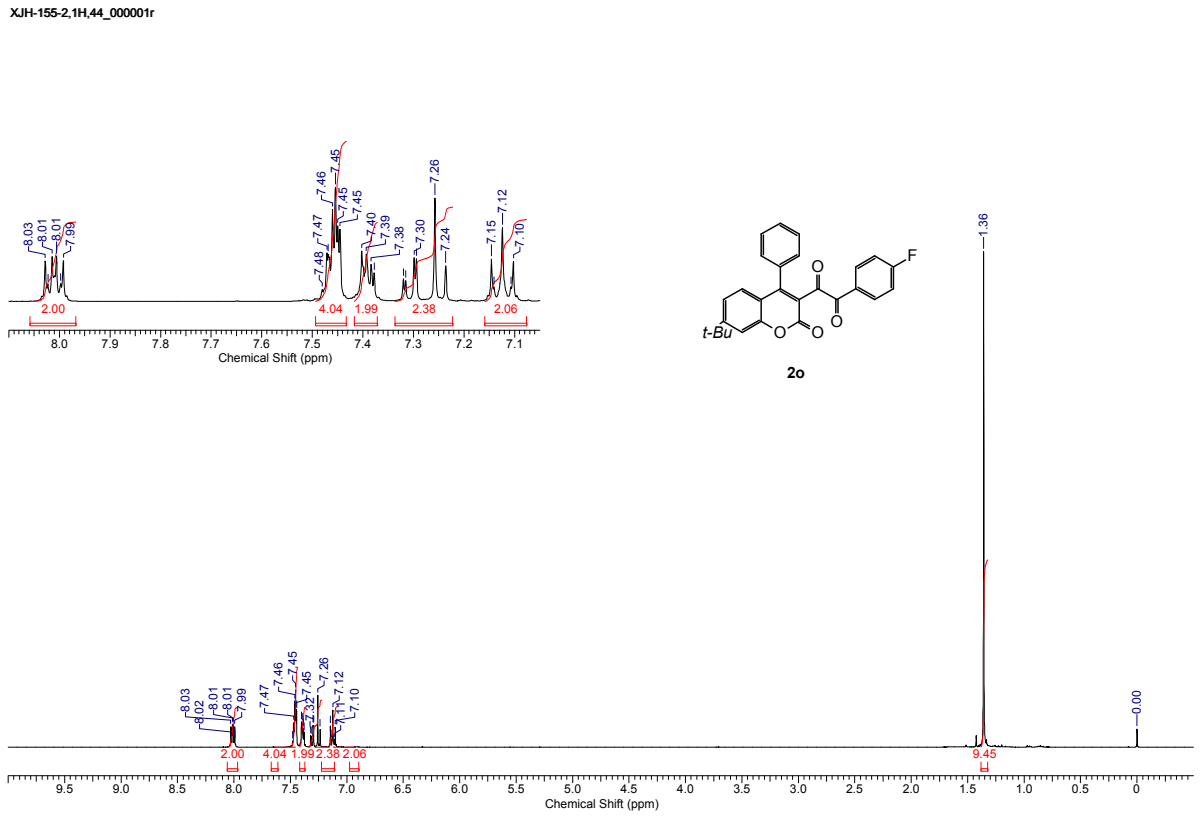


Figure S78. ^{1}H NMR spectrum of compound **2o**

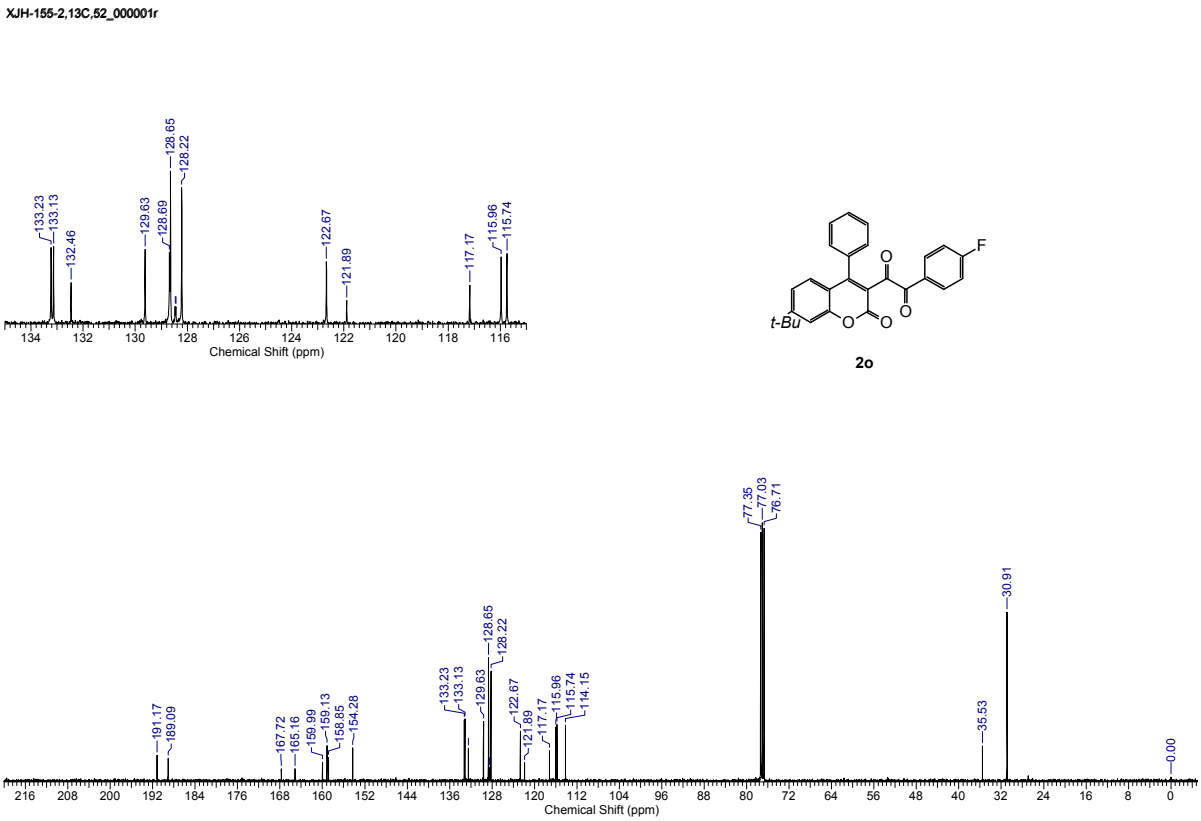


Figure S79. ^{13}C NMR spectrum of compound **2o**

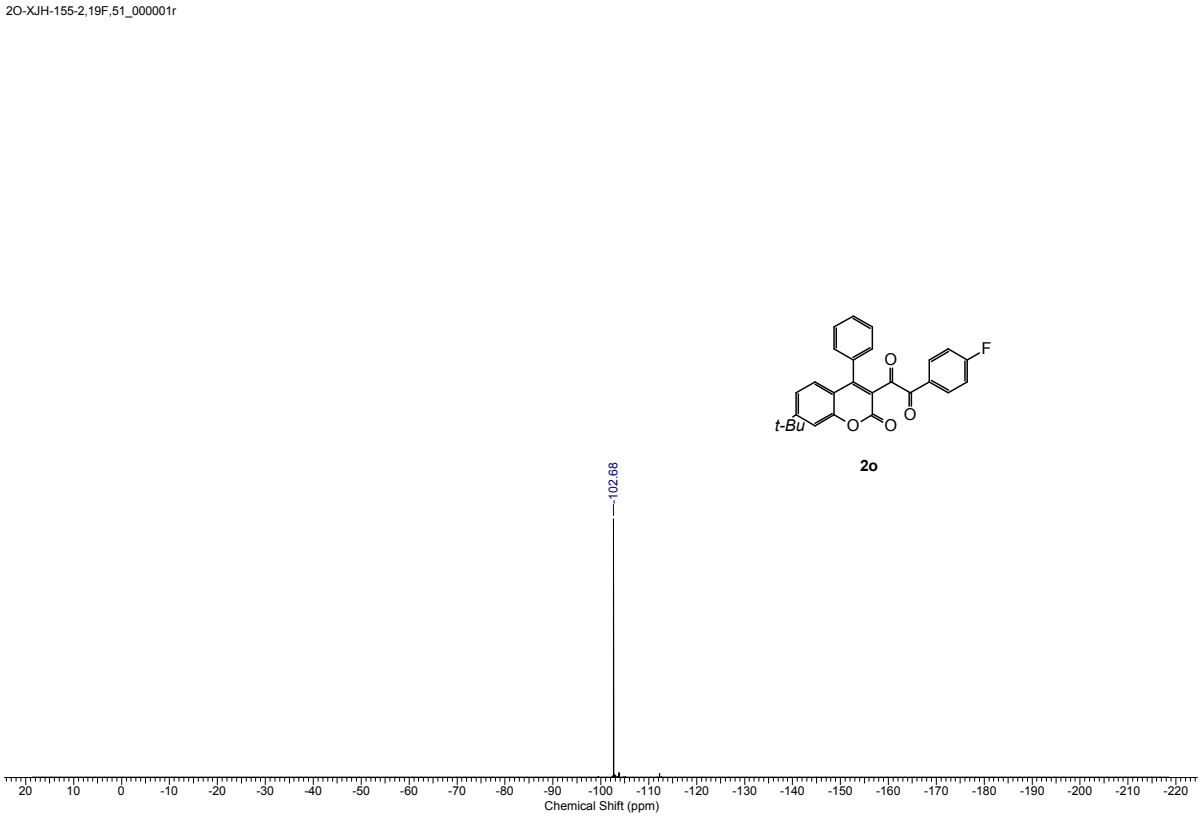


Figure S80. ^{19}F NMR spectrum of compound **2o**

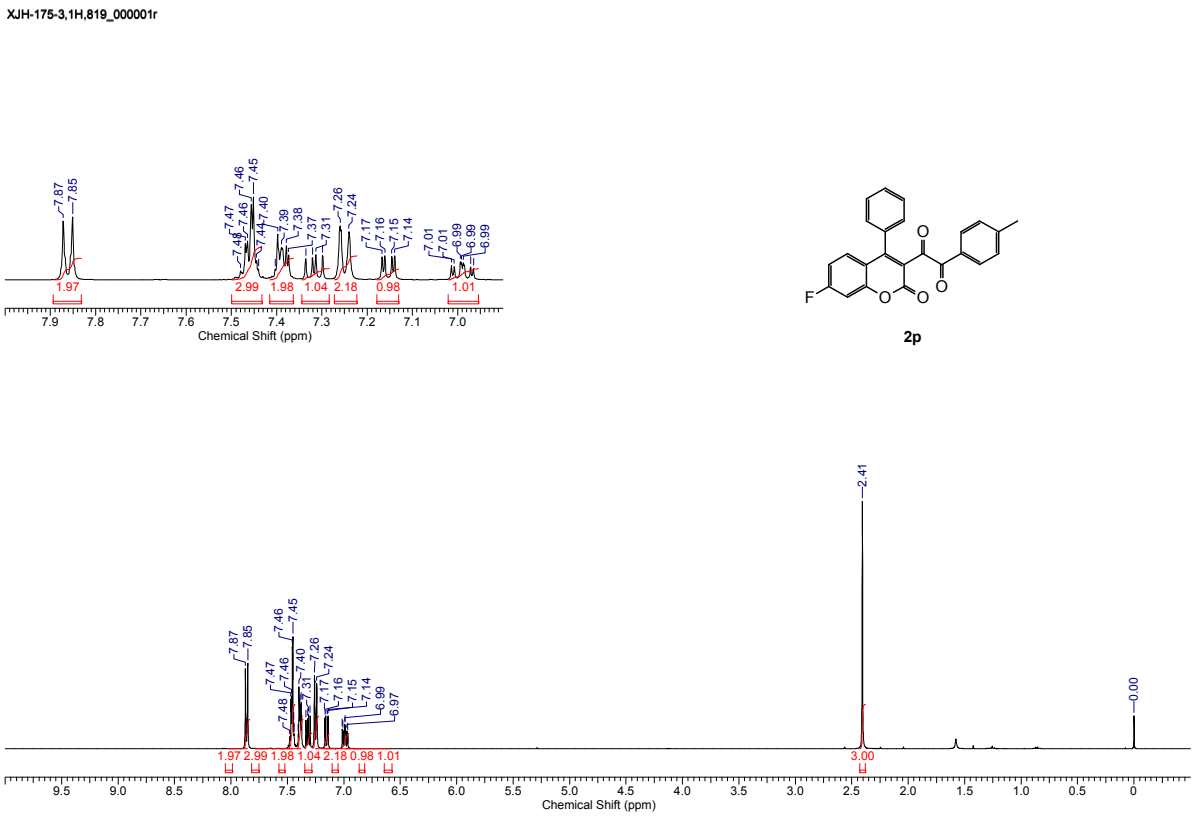


Figure S81. ^{1}H NMR spectrum of compound **2p**

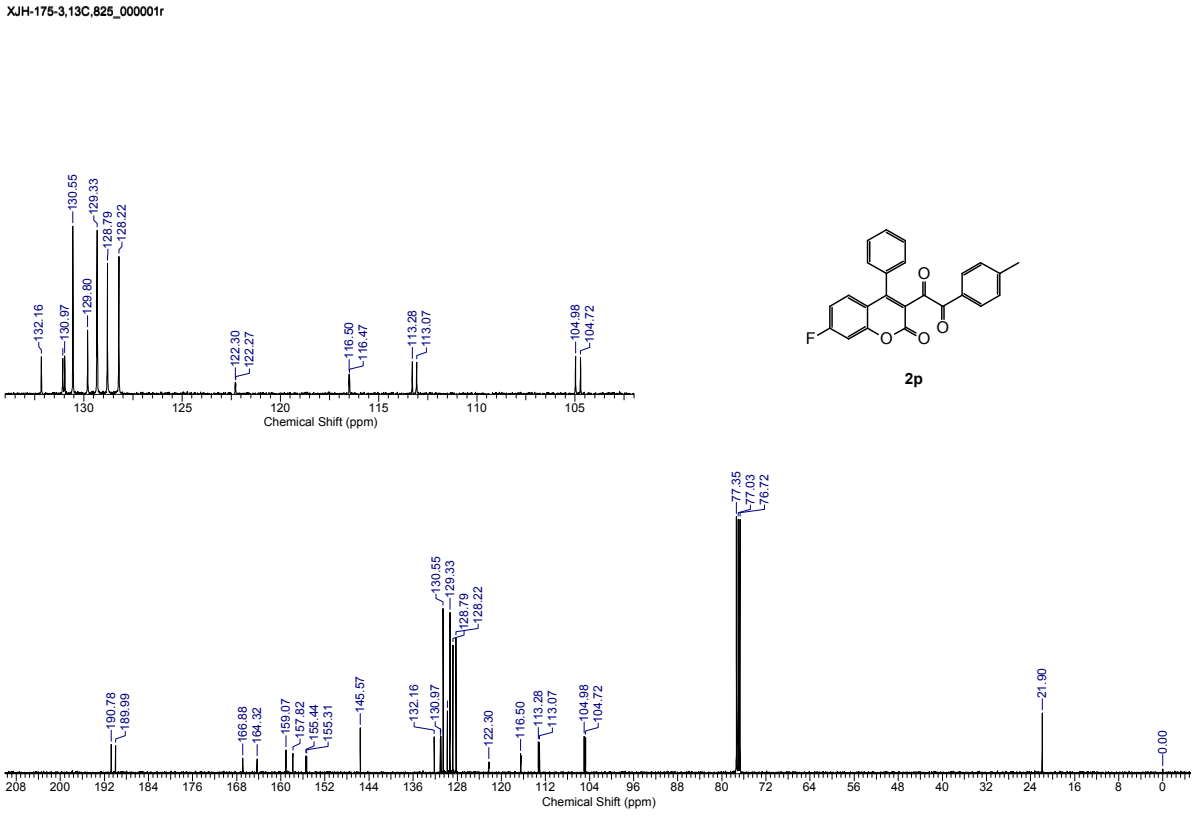


Figure S82. ^{13}C NMR spectrum of compound **2p**

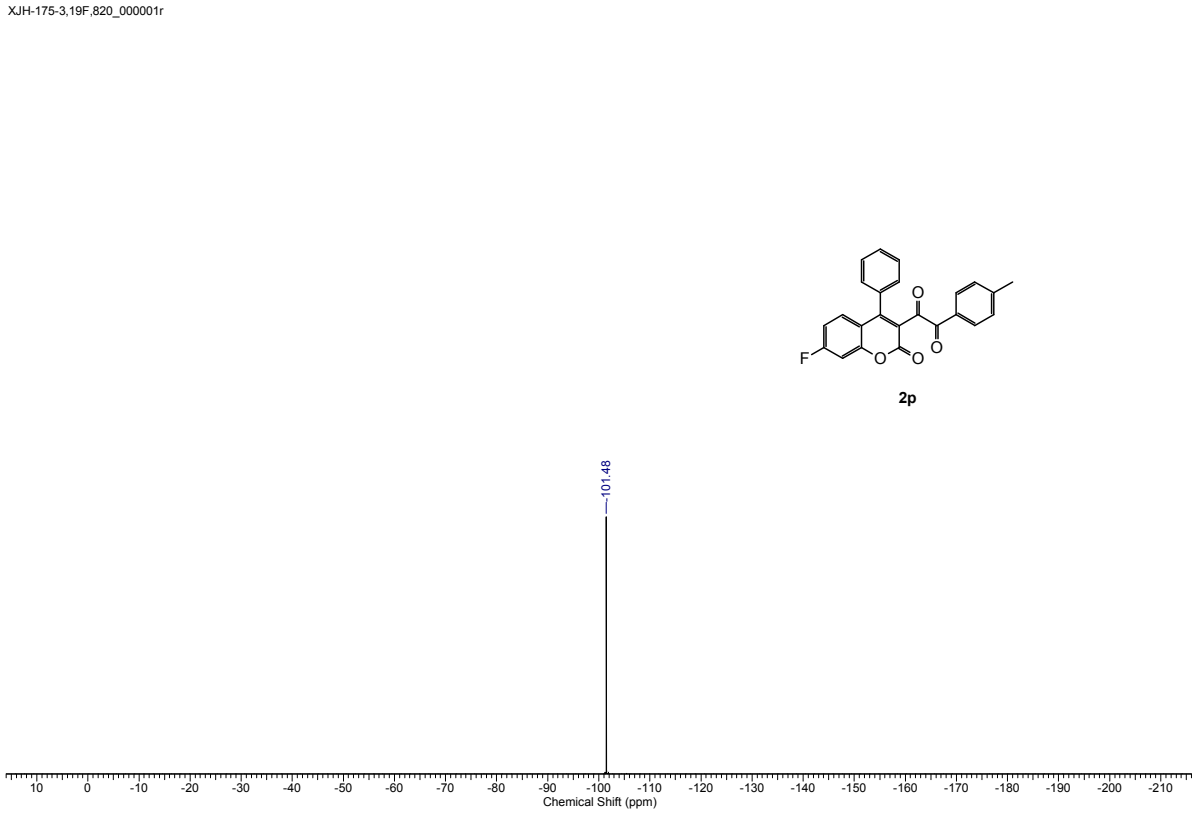


Figure S83. ^{19}F NMR spectrum of compound **2p**

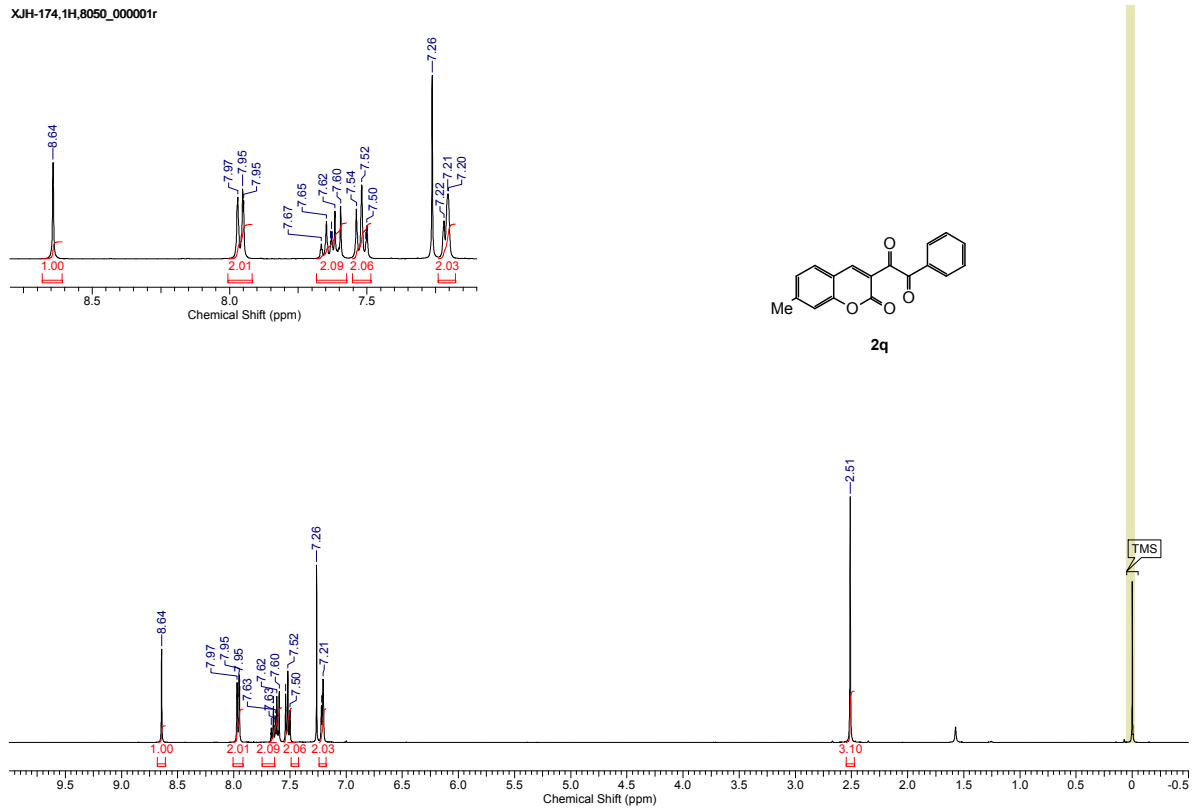


Figure S84. ^{1}H NMR spectrum of compound **2q**

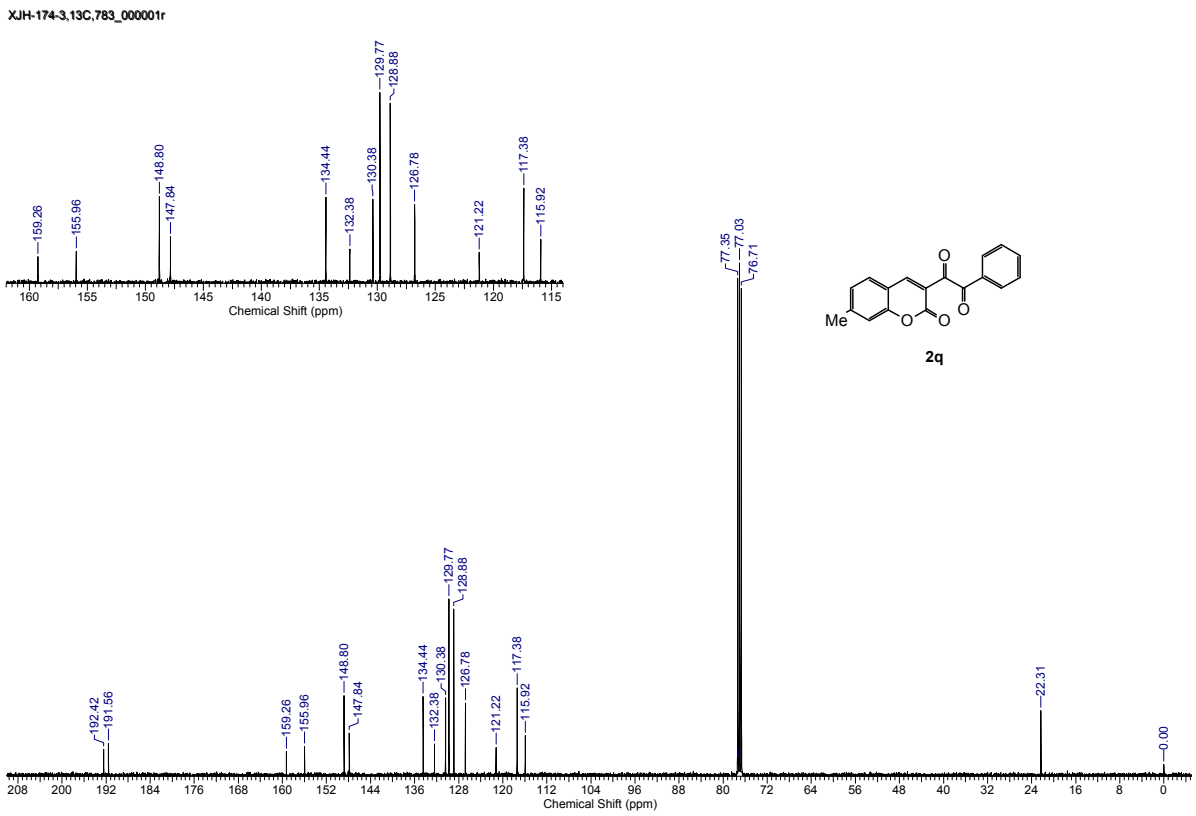


Figure S85. ^{13}C NMR spectrum of compound **2q**

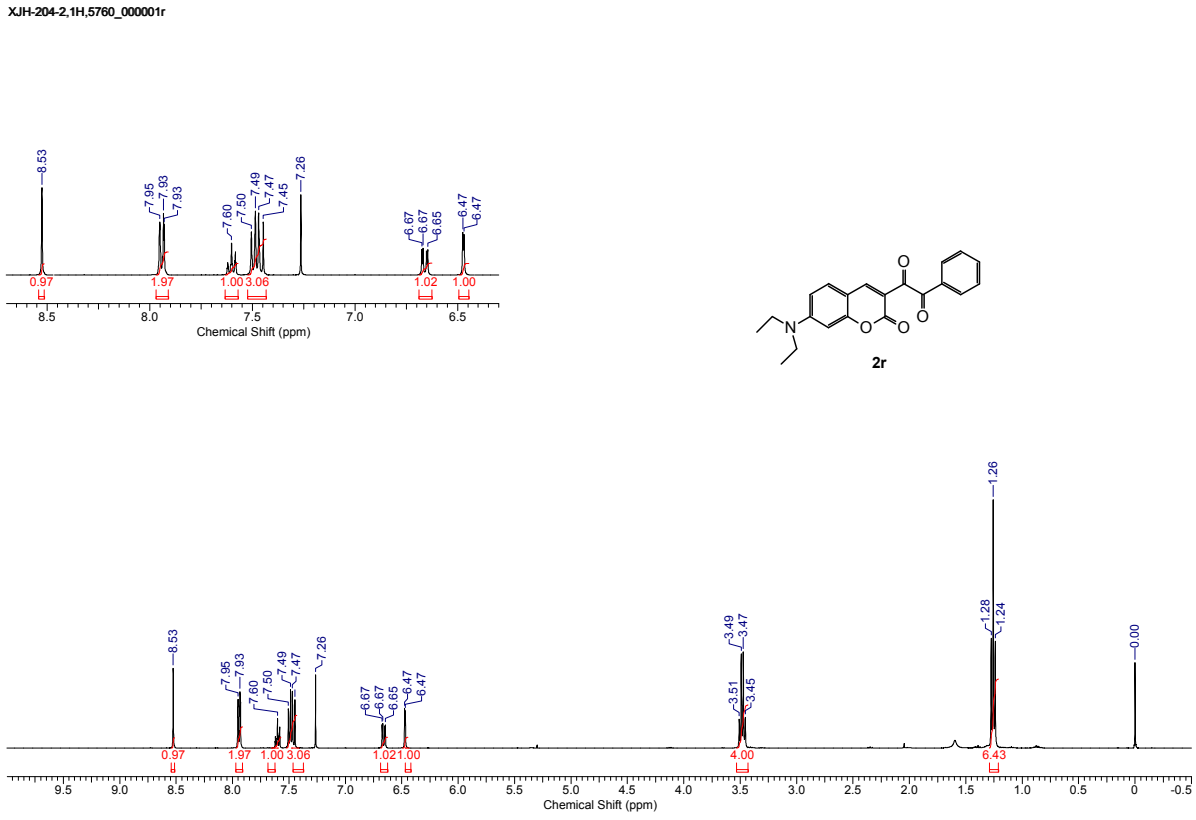


Figure S86. ^{1}H NMR spectrum of compound **2r**

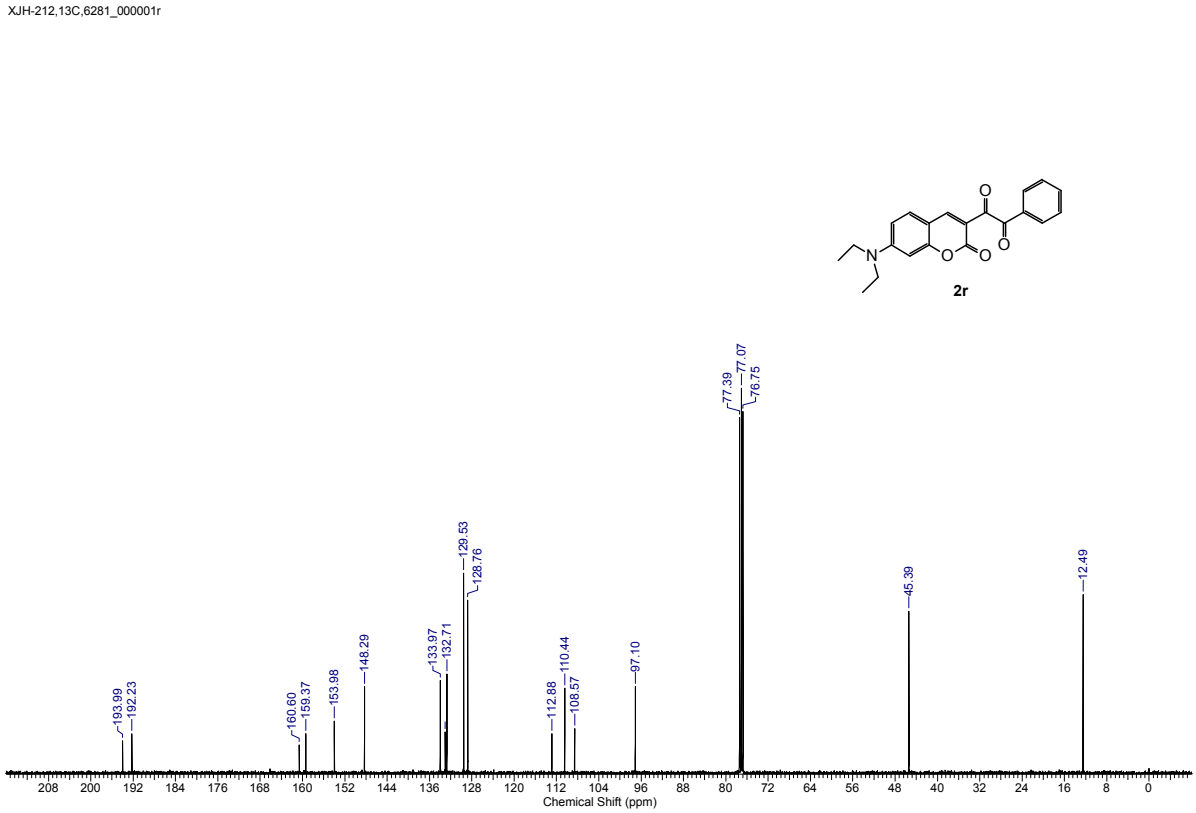


Figure S87. ^{13}C NMR spectrum of compound **2r**

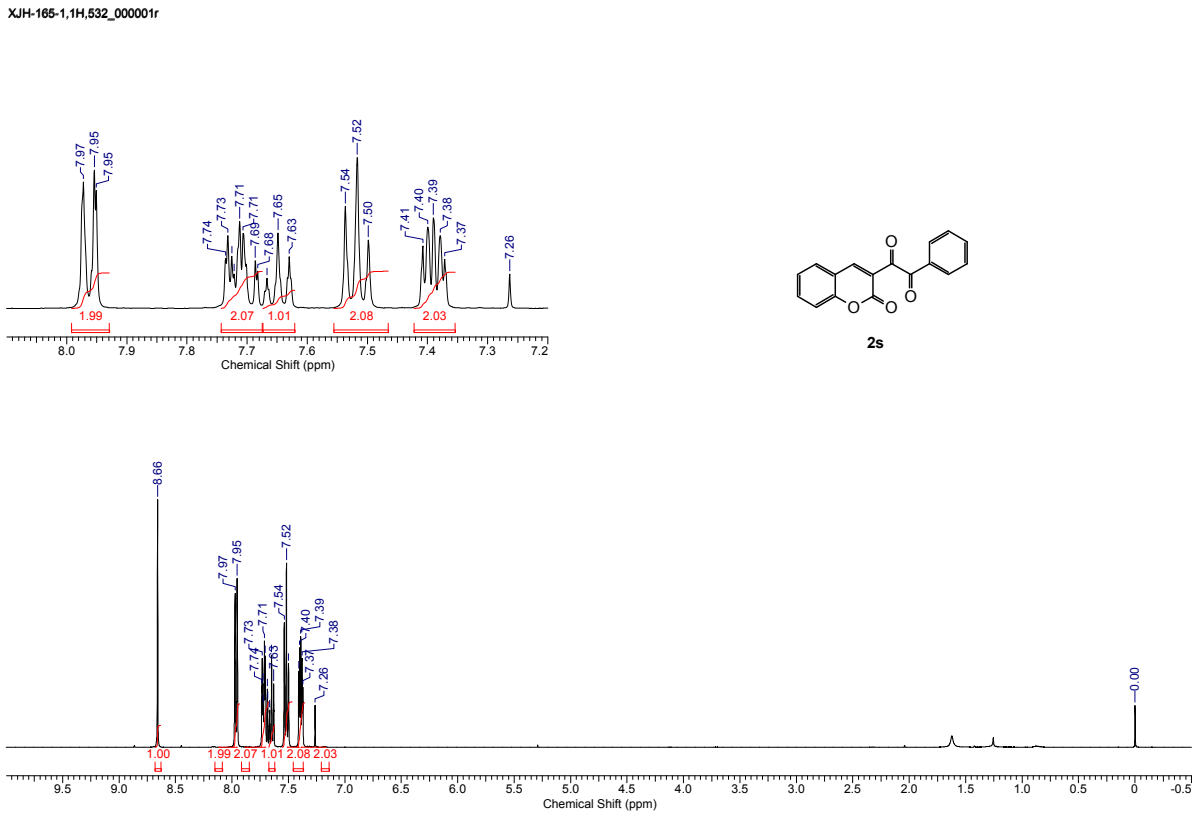


Figure S88. ^{1}H NMR spectrum of compound **2s**

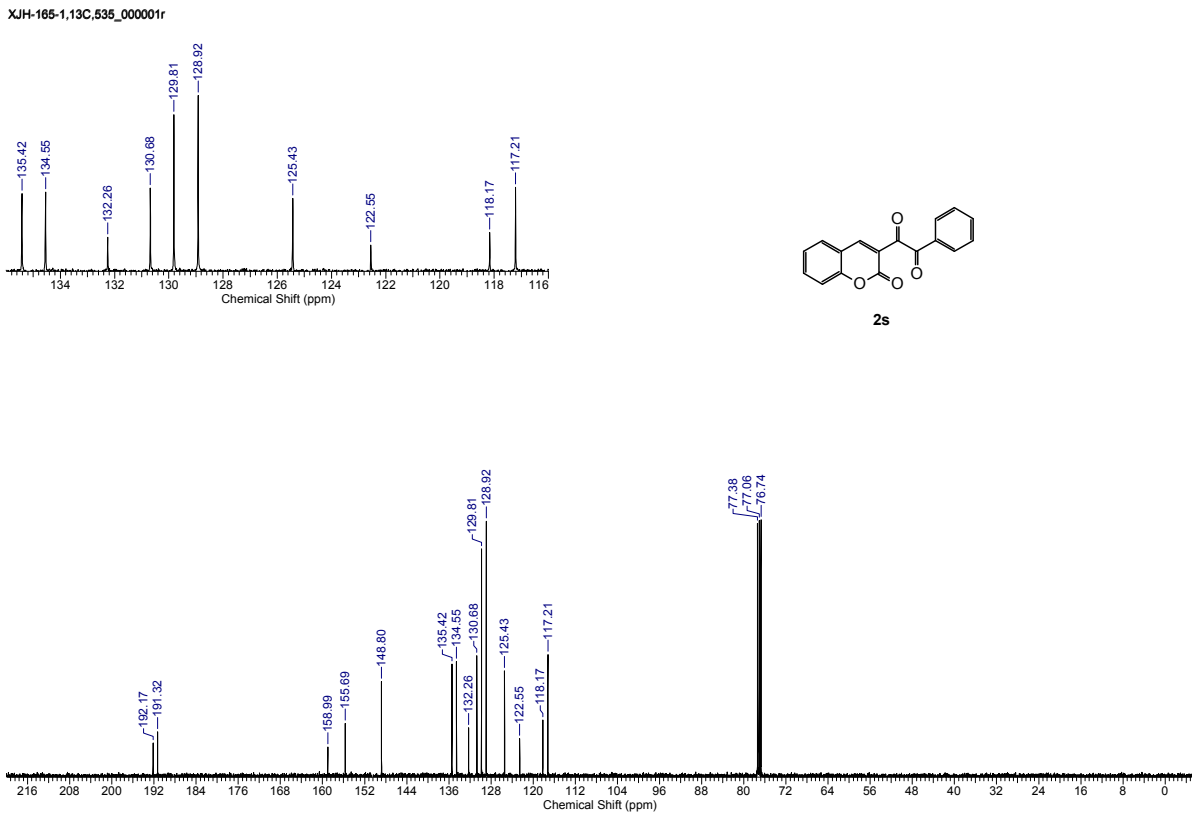


Figure S89. ^{13}C NMR spectrum of compound **2s**

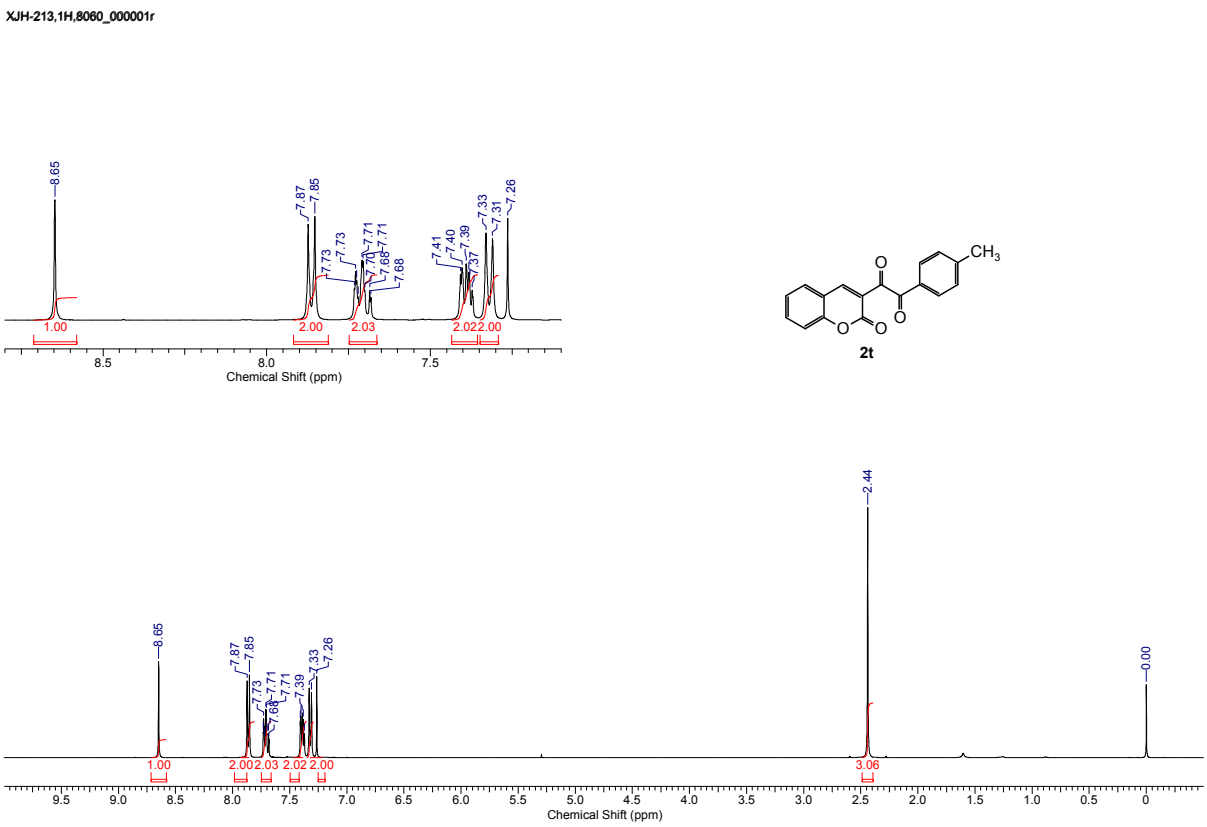


Figure S90. ^{1}H NMR spectrum of compound **2t**

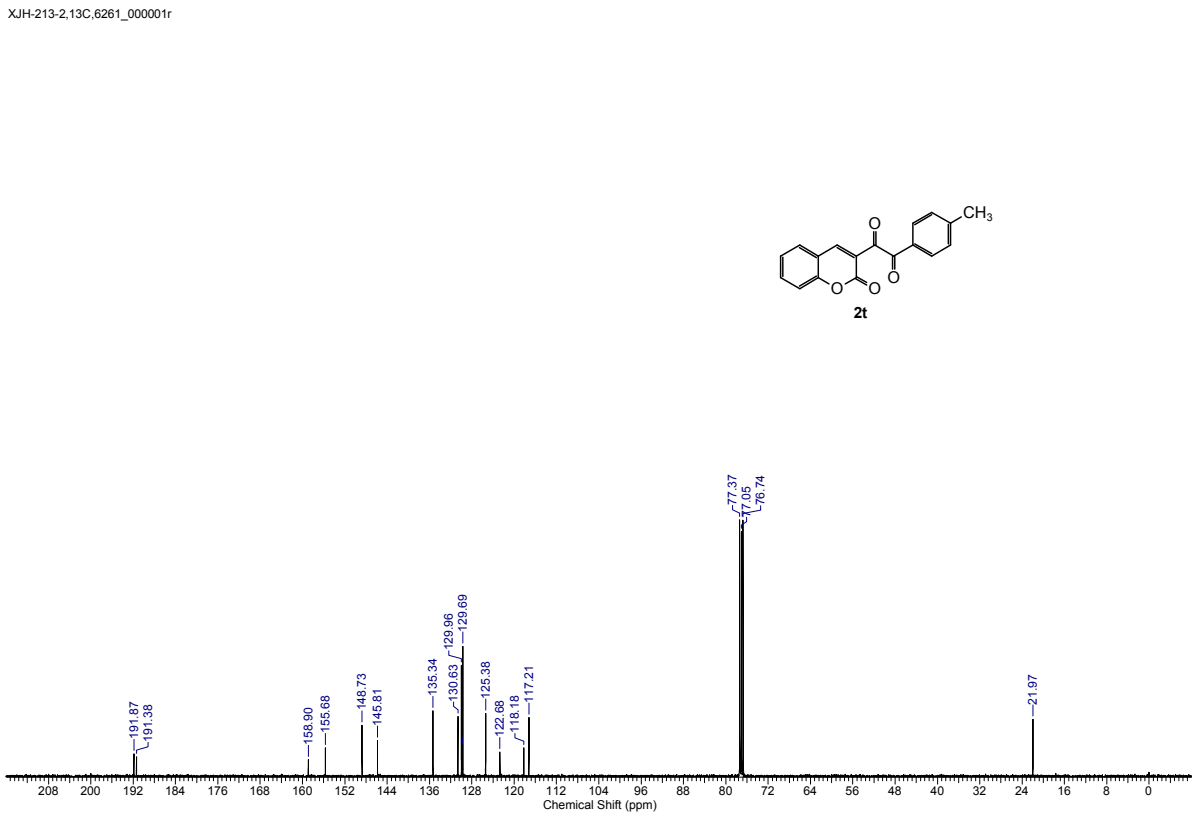


Figure S91. ^{13}C NMR spectrum of compound **2t**

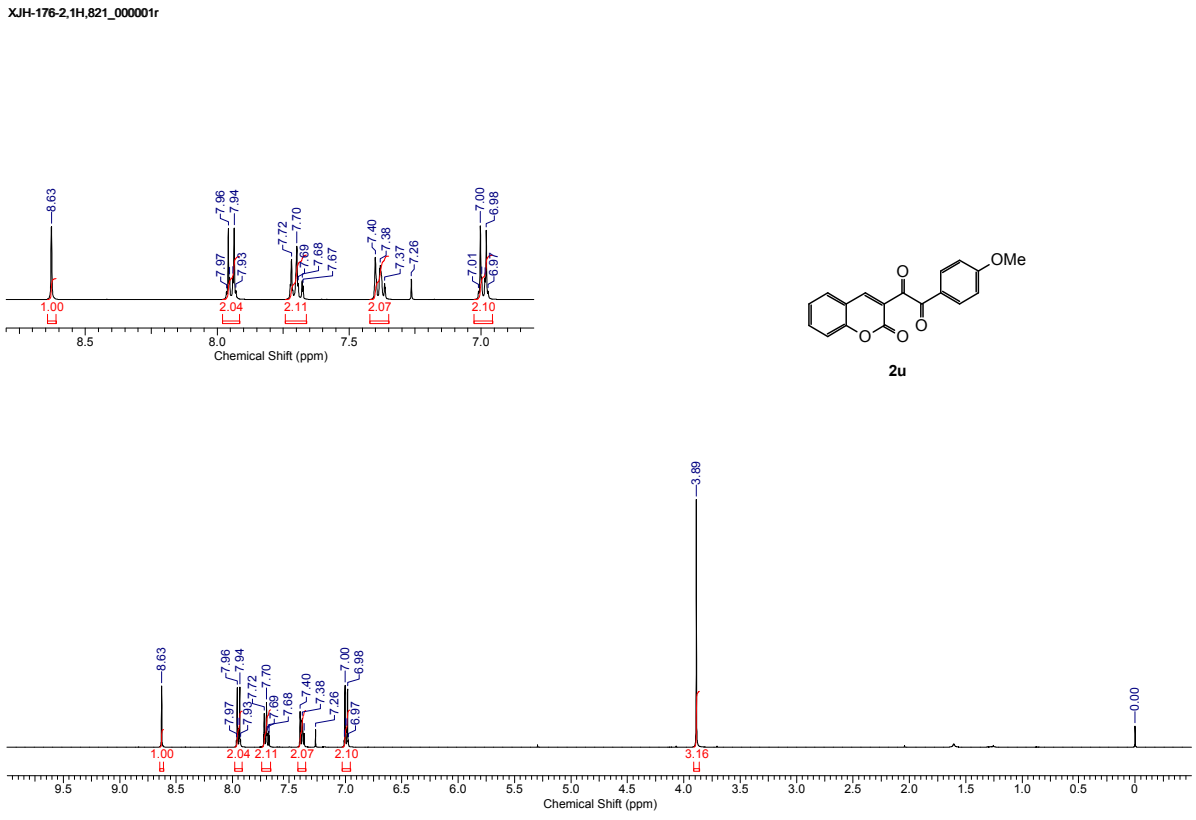


Figure S92. ^{1}H NMR spectrum of compound **2u**

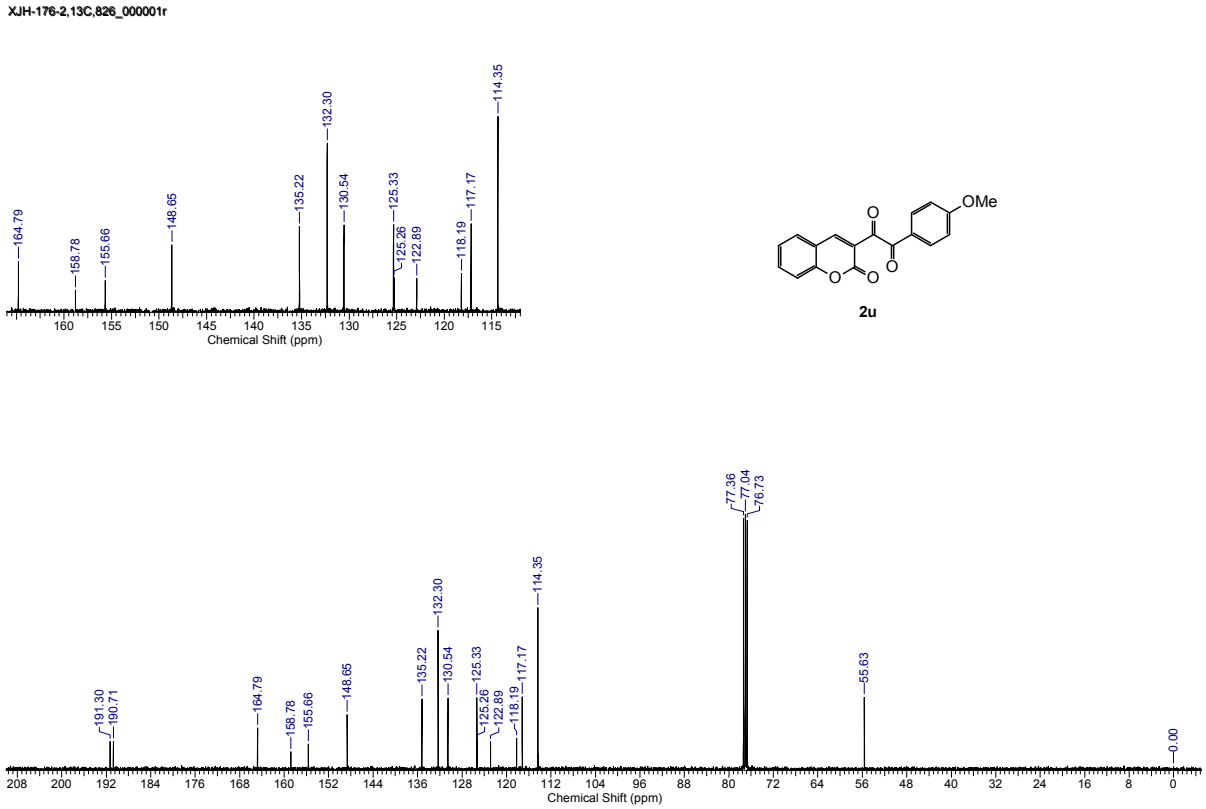


Figure S93. ^{13}C NMR spectrum of compound **2u**

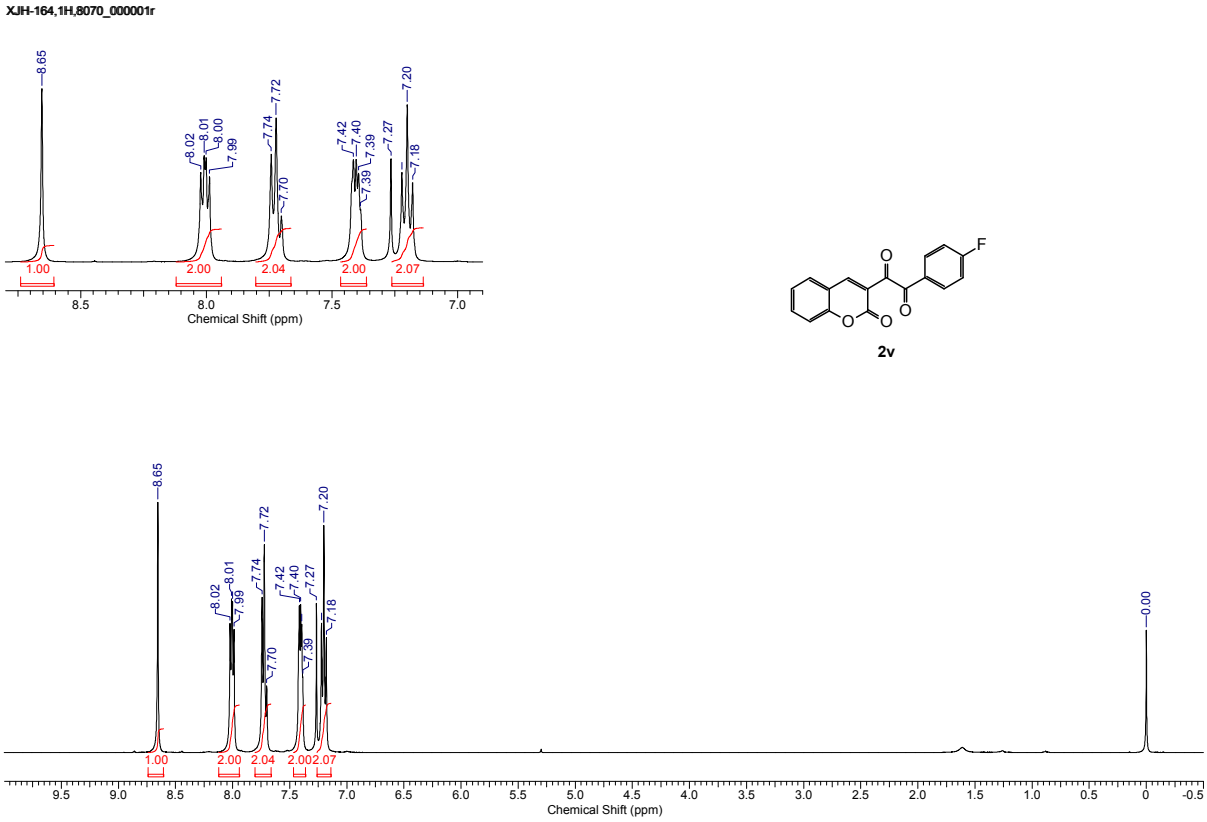


Figure S94. ^{1}H NMR spectrum of compound **2v**

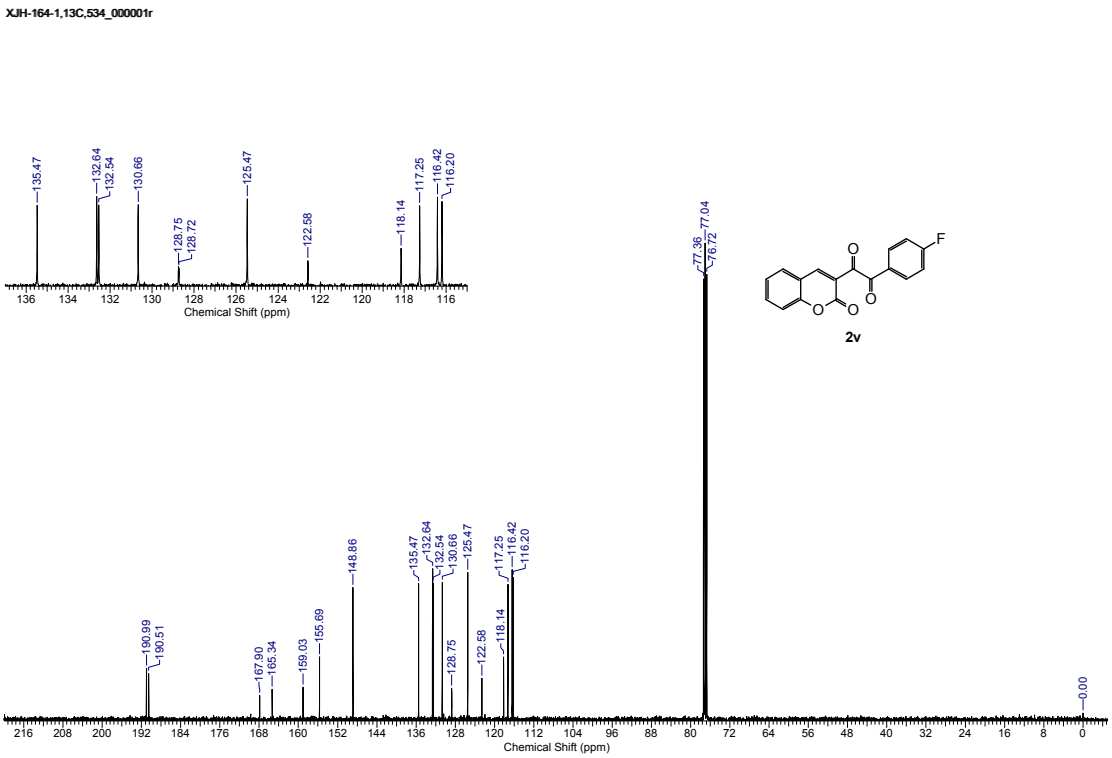


Figure S95. ^{13}C NMR spectrum of compound **2v**

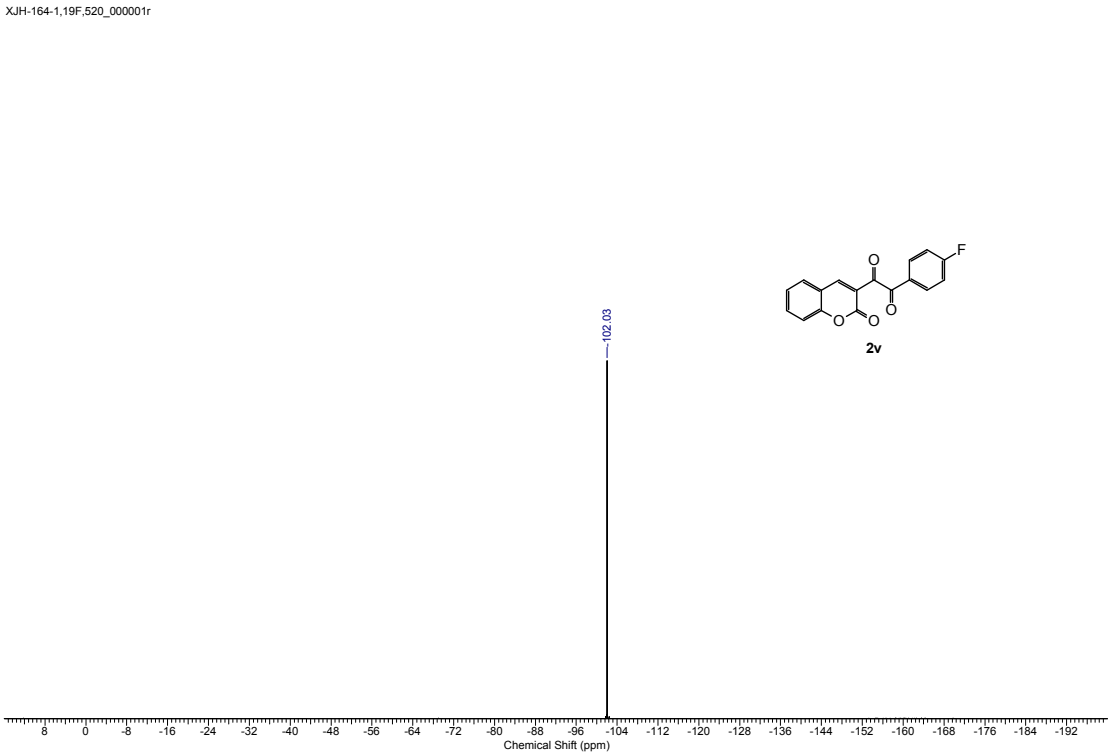


Figure S96. ^{19}F NMR spectrum of compound **2v**

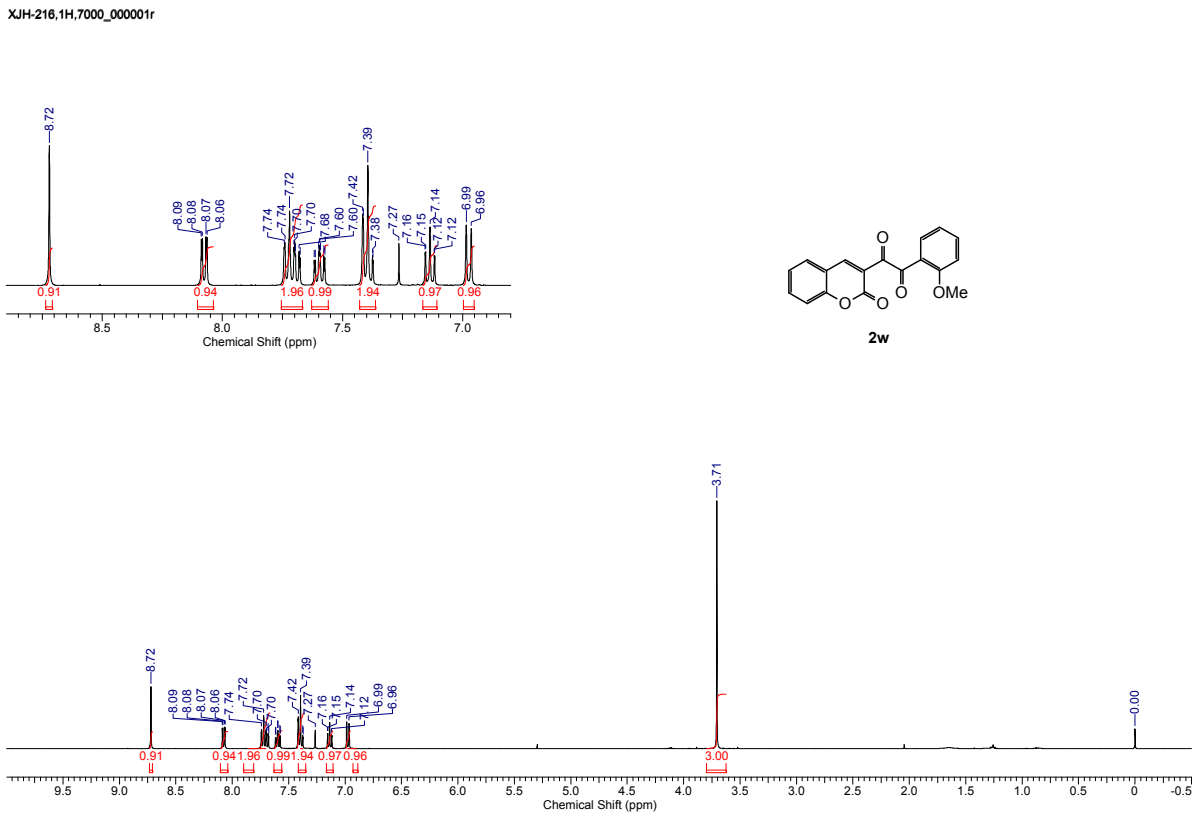


Figure S97. ^{1}H NMR spectrum of compound **2w**

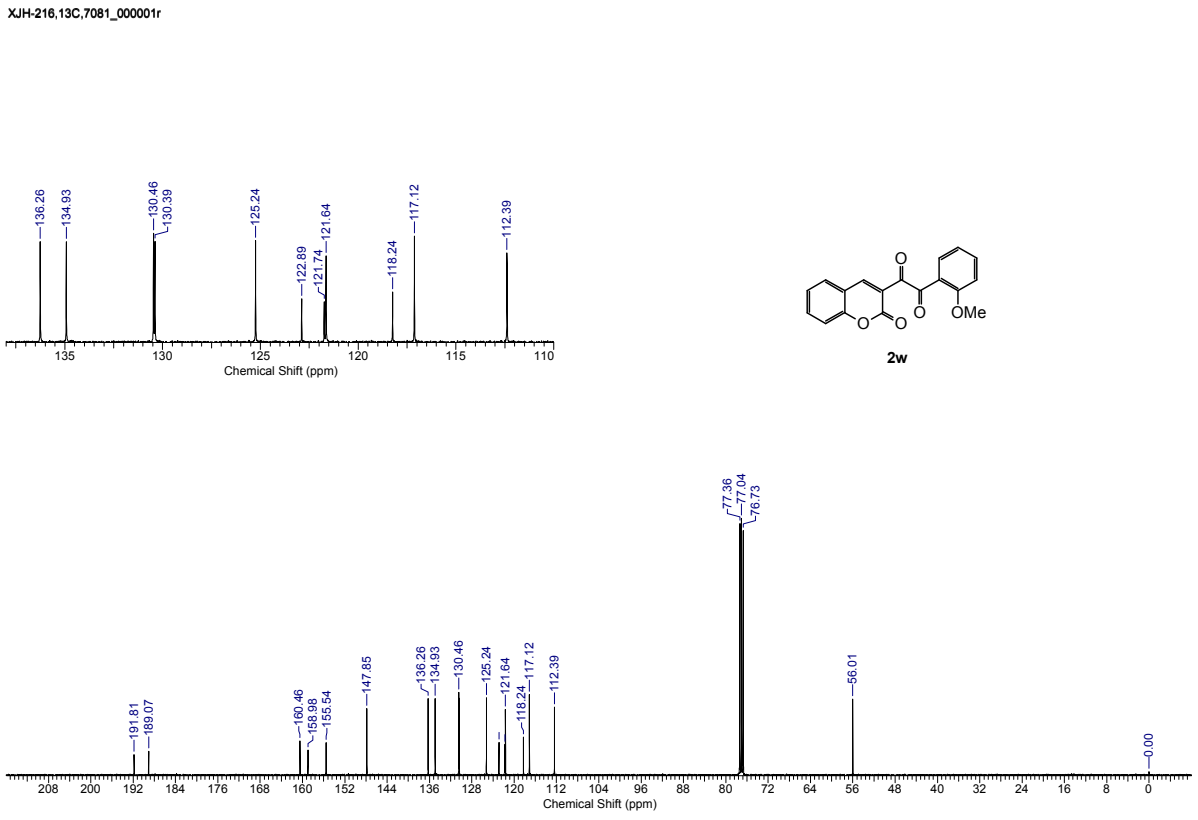


Figure S98. ^{13}C NMR spectrum of compound **2w**

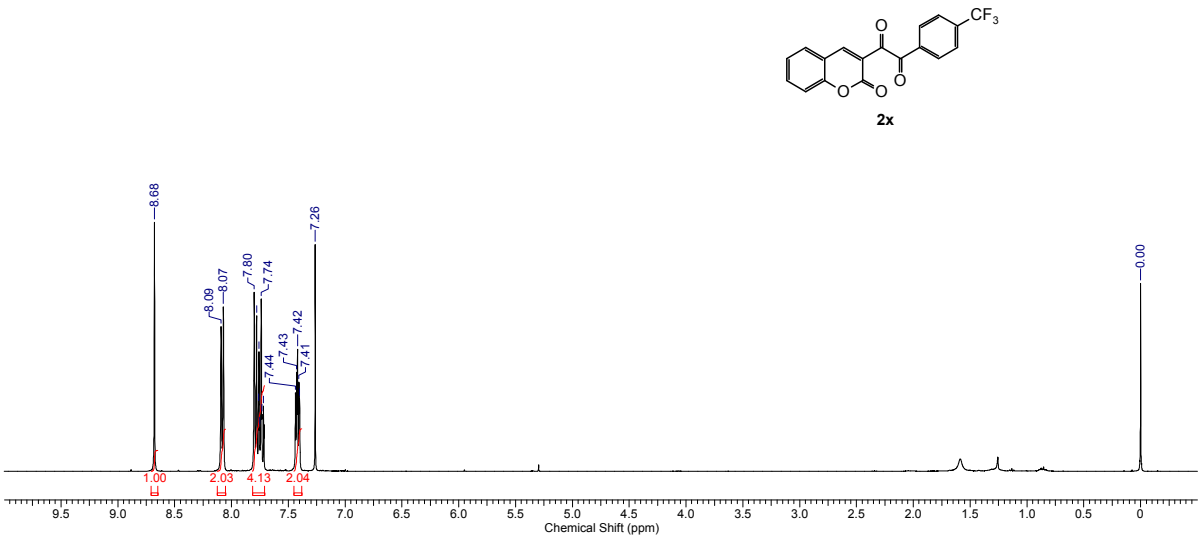


Figure S99. ^{1}H NMR spectrum of compound **2x**

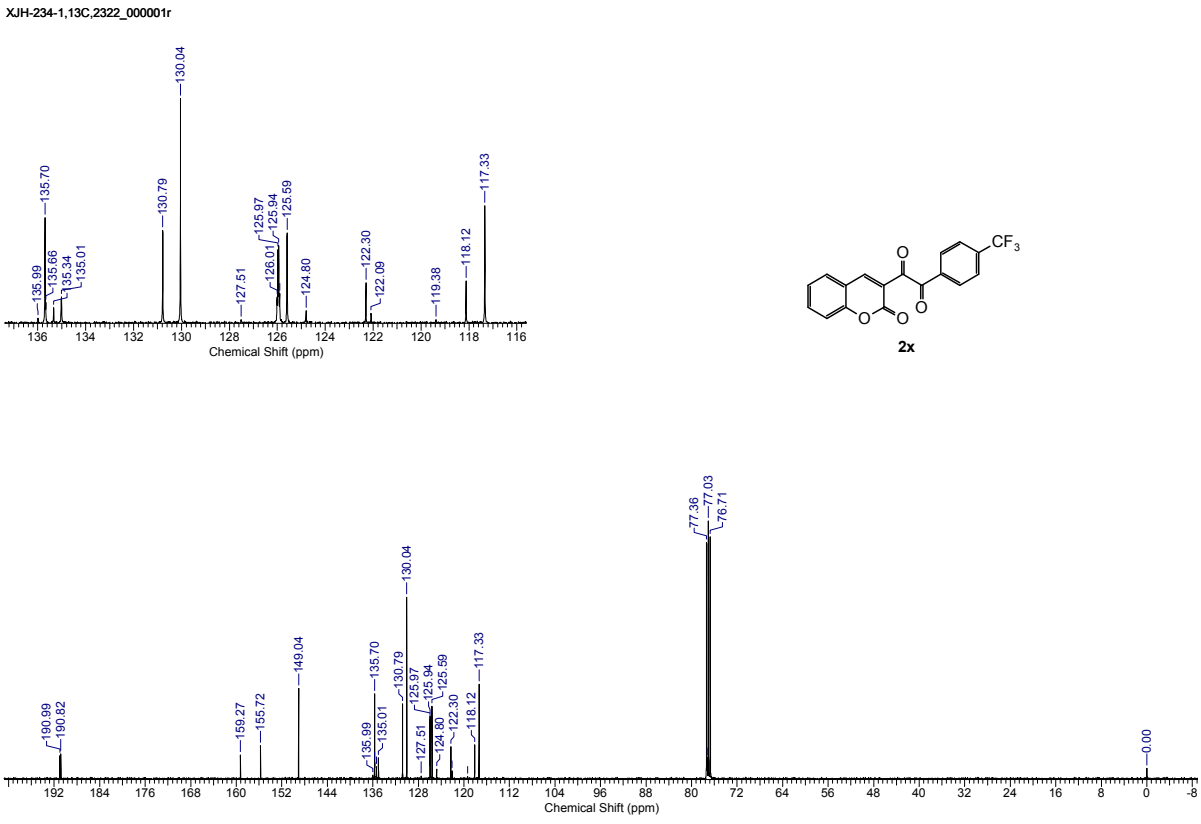


Figure S100. ^{13}C NMR spectrum of compound **2x**

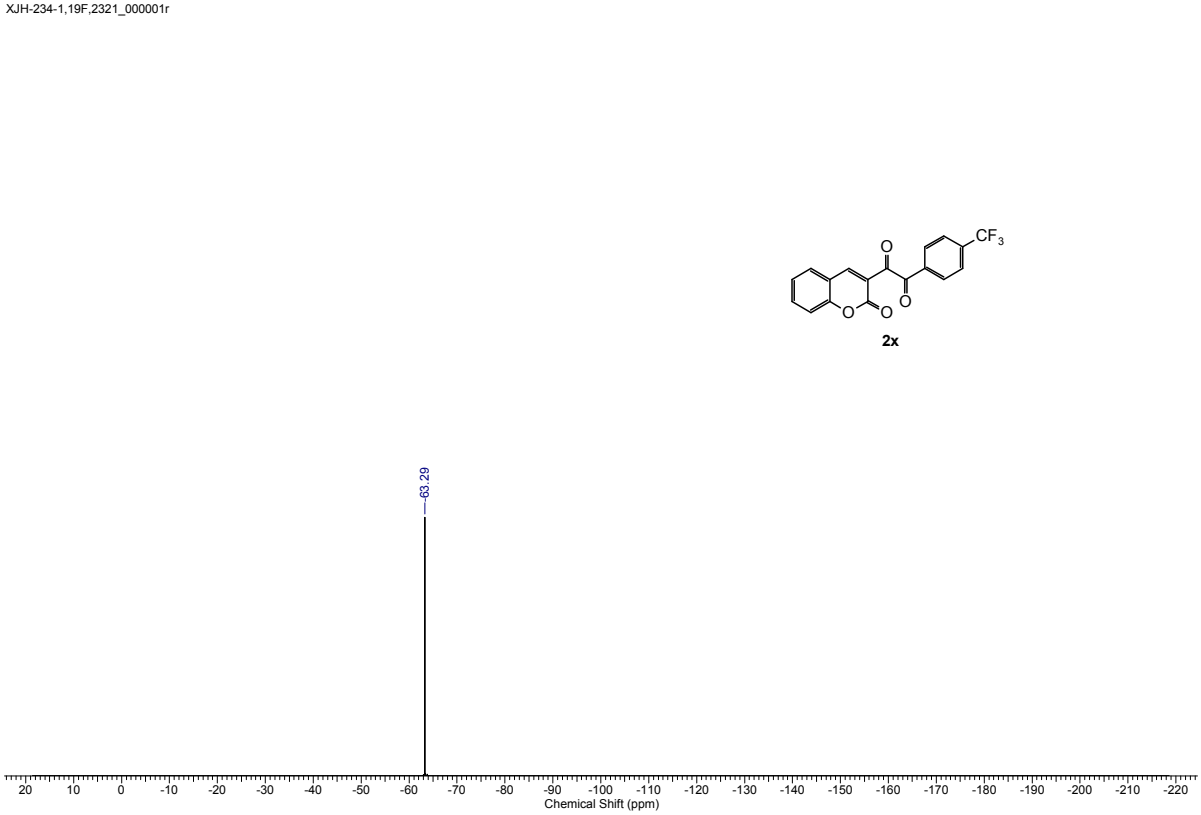


Figure S101. ^{19}F NMR spectrum of compound **2x**

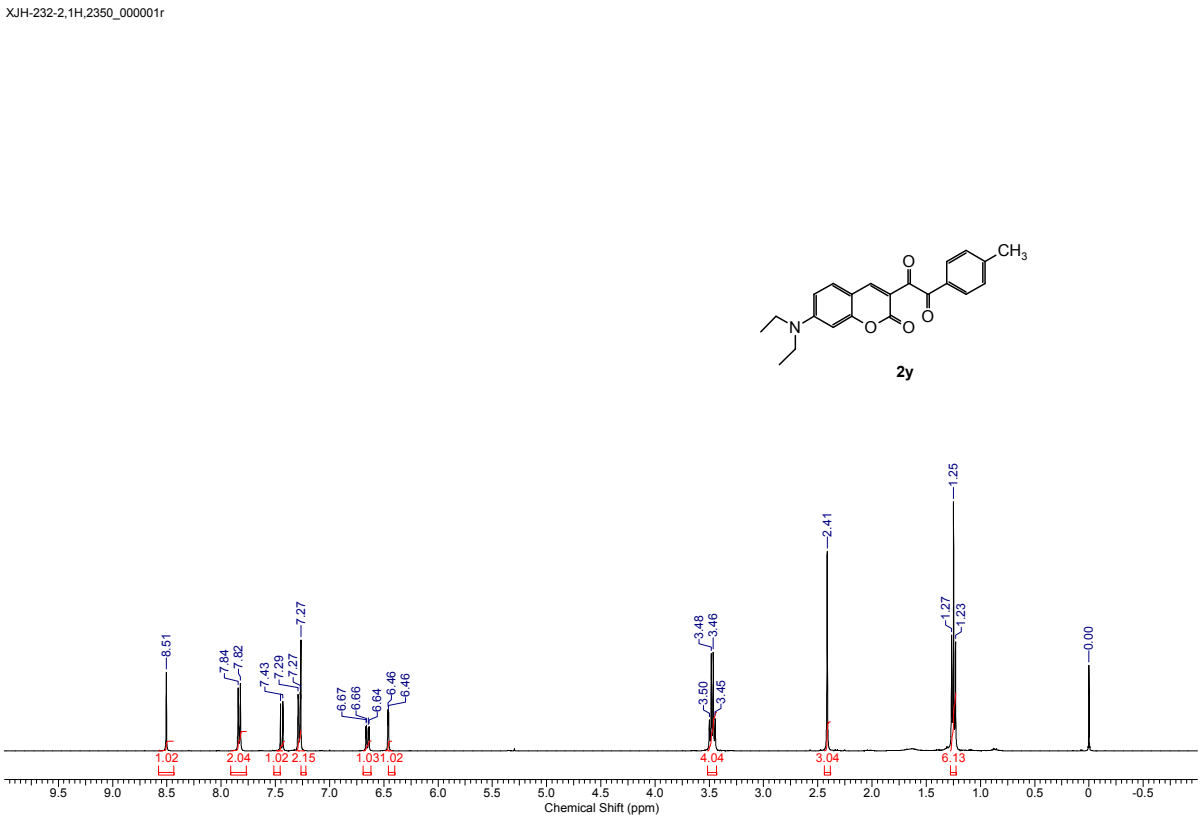


Figure S102. ^{1}H NMR spectrum of compound **2y**

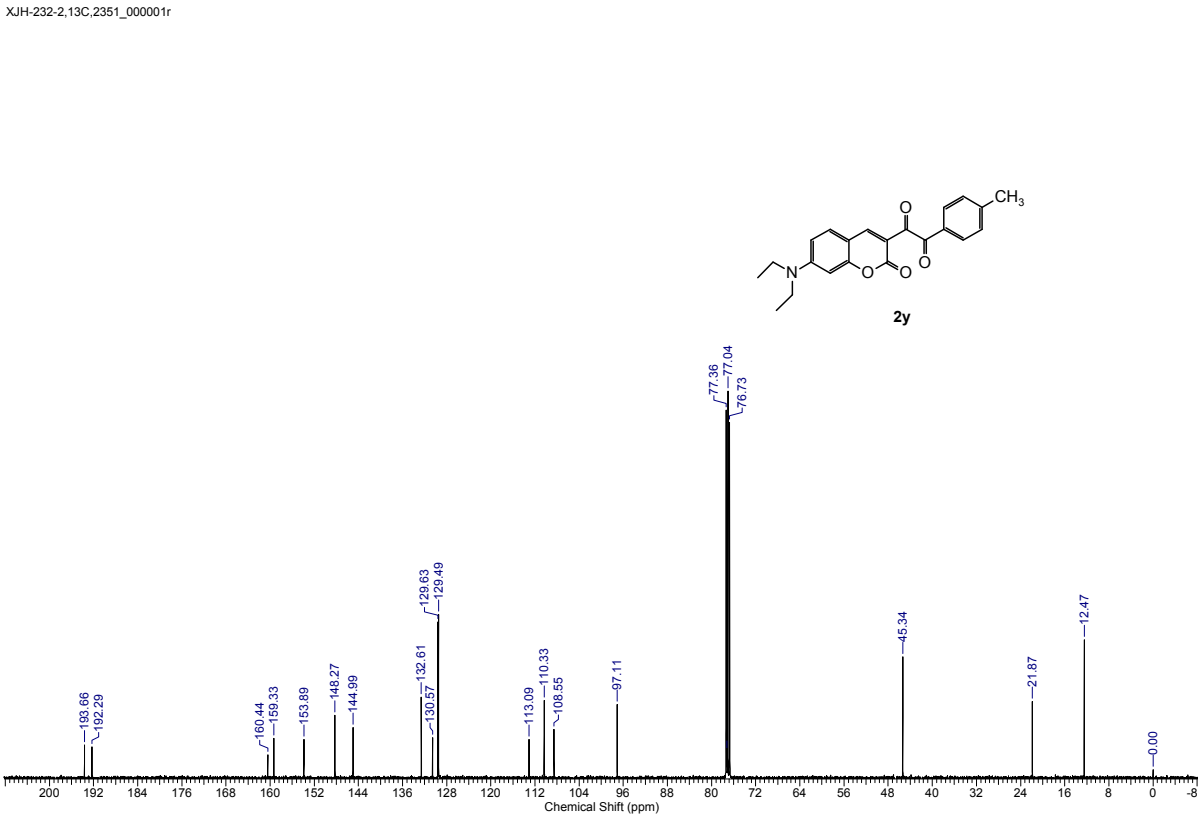


Figure S103. ^{13}C NMR spectrum of compound **2y**

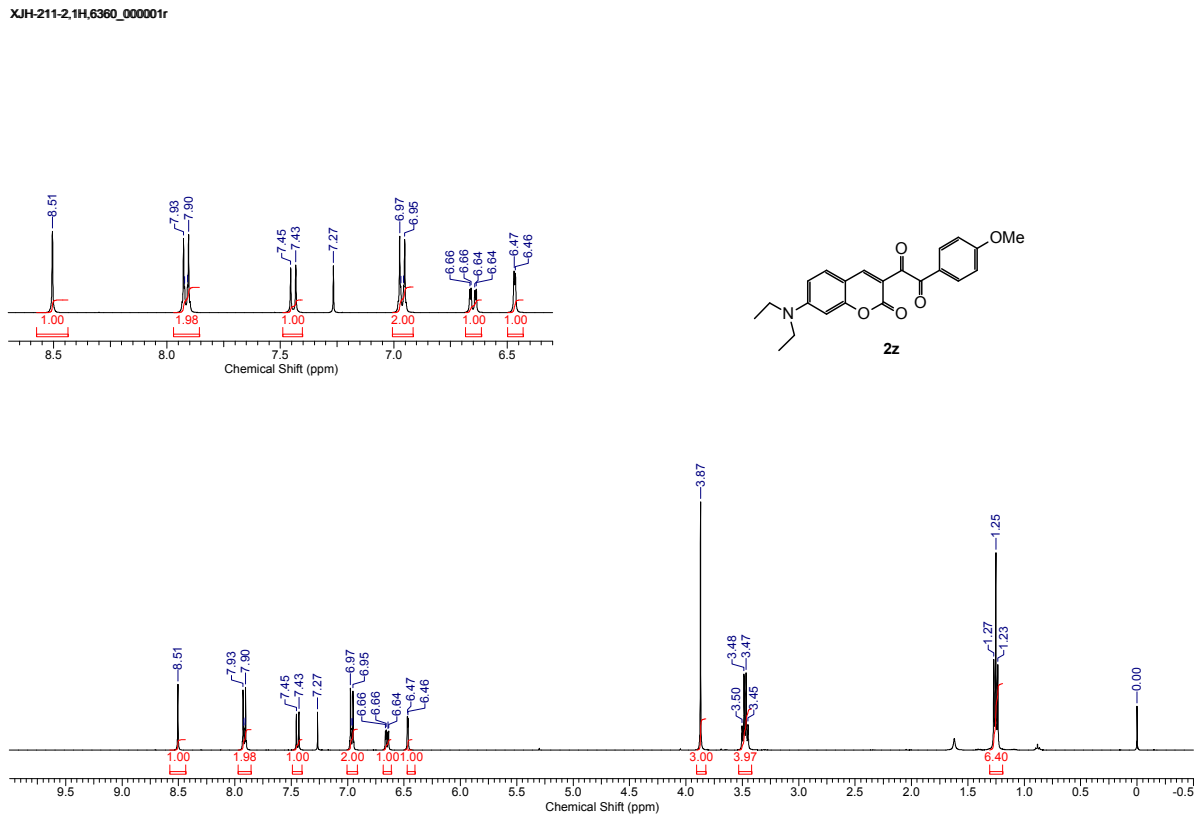


Figure S104. ^{1}H NMR spectrum of compound **2z**

XJH-211-2,13C,6271_000001r

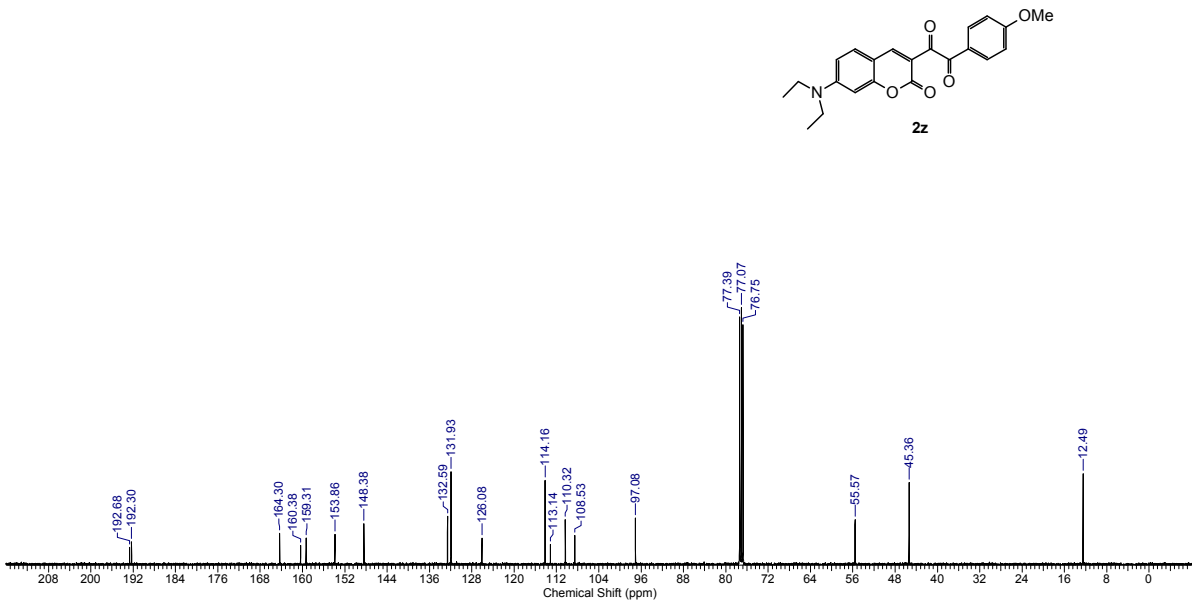


Figure S105. ^{13}C NMR spectrum of compound **2z**

XJH-233-2,1H,2310_000001r

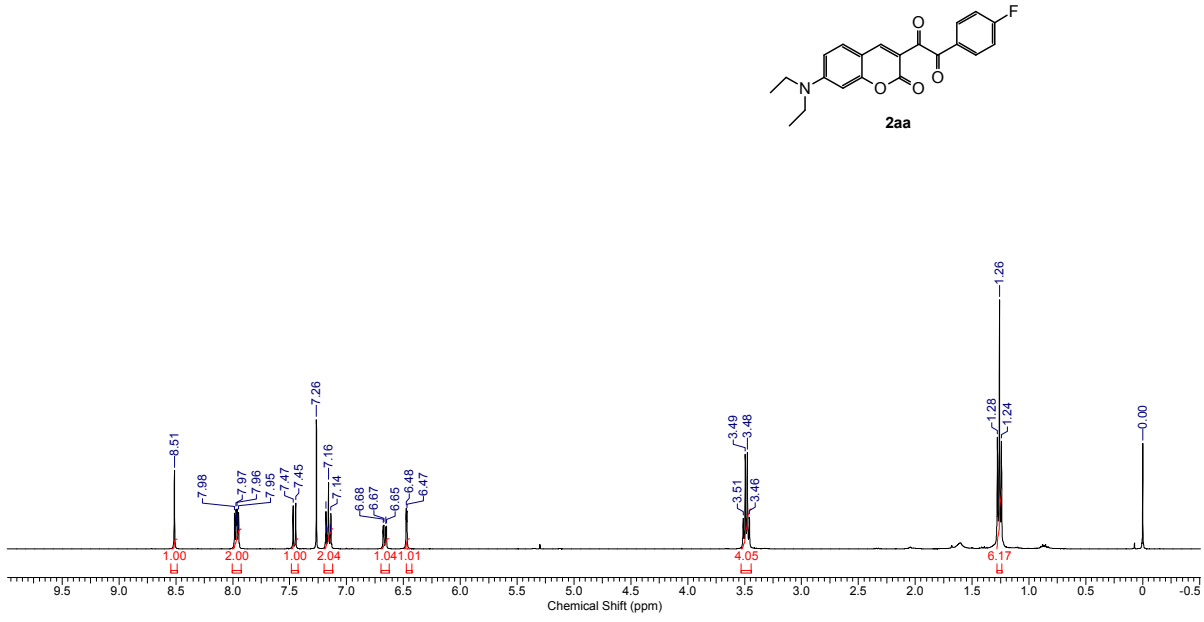


Figure S106. ^{1}H NMR spectrum of compound **2aa**

XJH-233-2,13C,2312_000001r

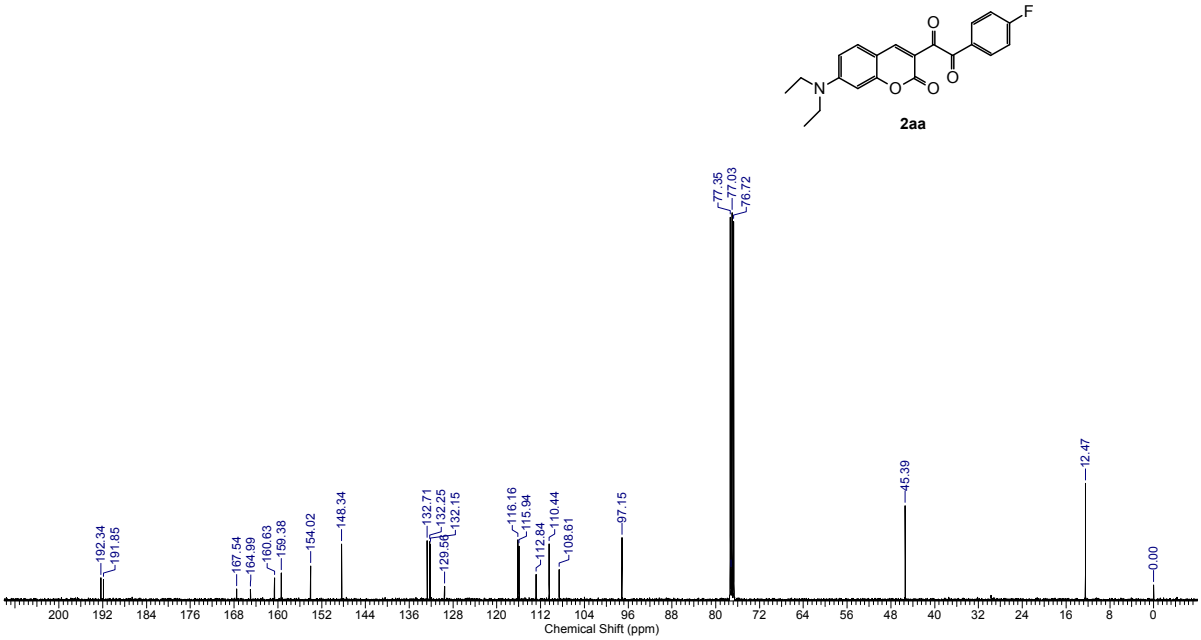


Figure S107. ^{13}C NMR spectrum of compound **2aa**

XJH-233-2,19F,2311_000001r

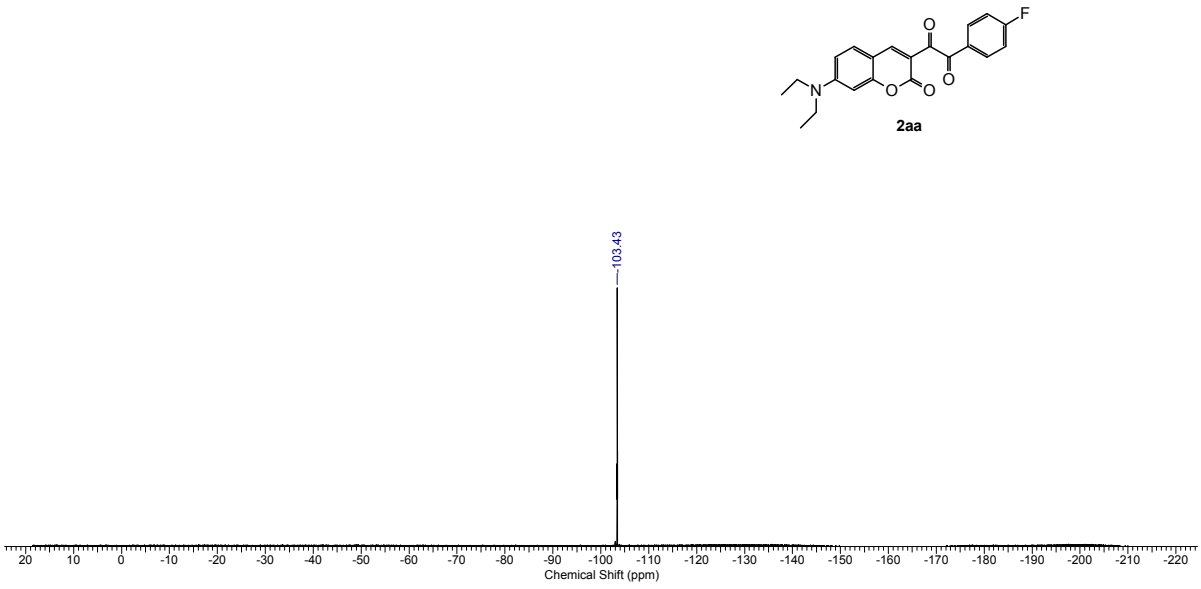


Figure S108. ^{19}F NMR spectrum of compound **2aa**

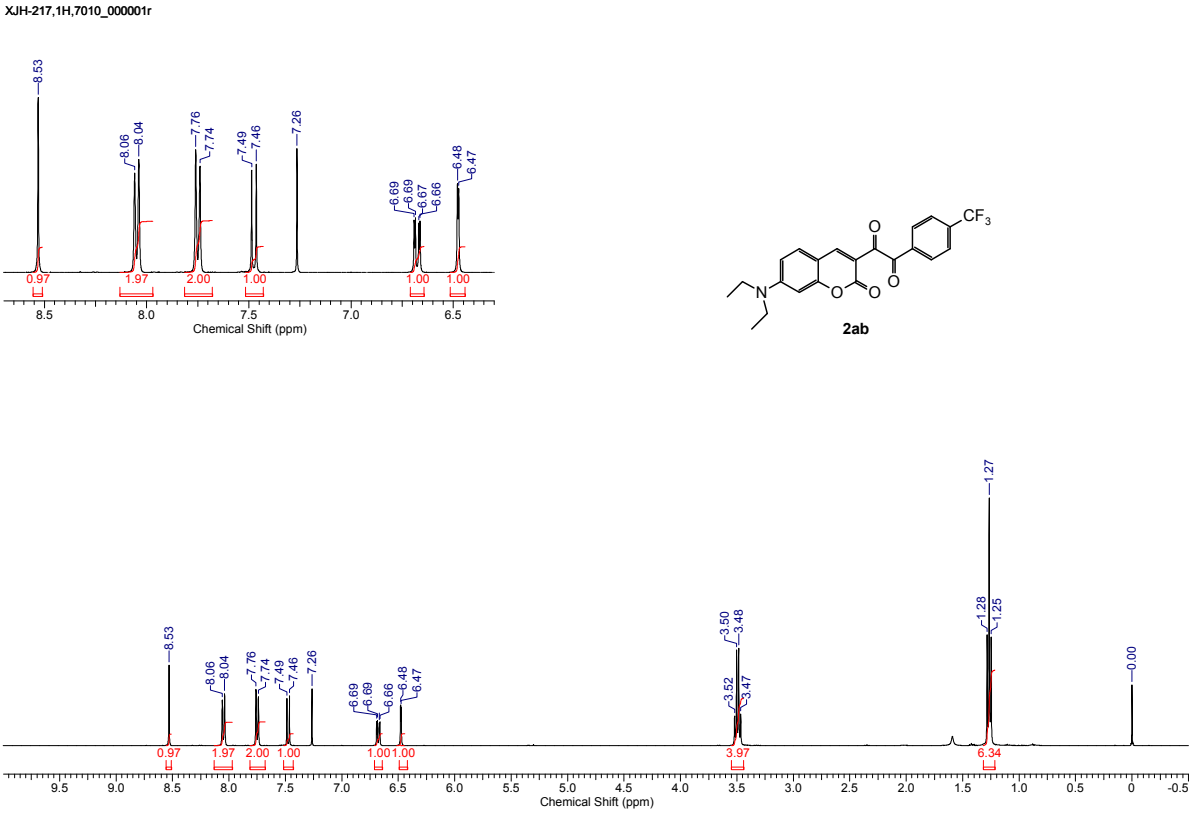


Figure S109. ^{1}H NMR spectrum of compound **2ab**

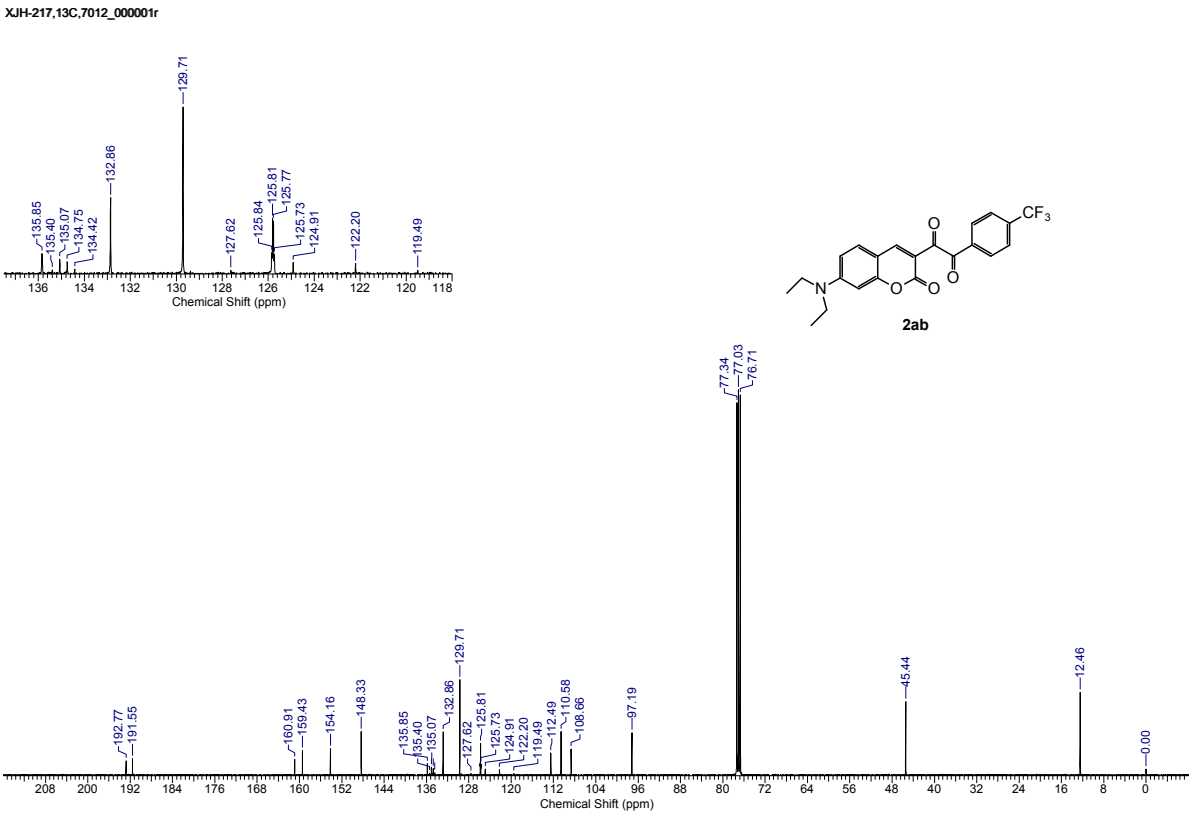


Figure S110. ^{13}C NMR spectrum of compound **2ab**

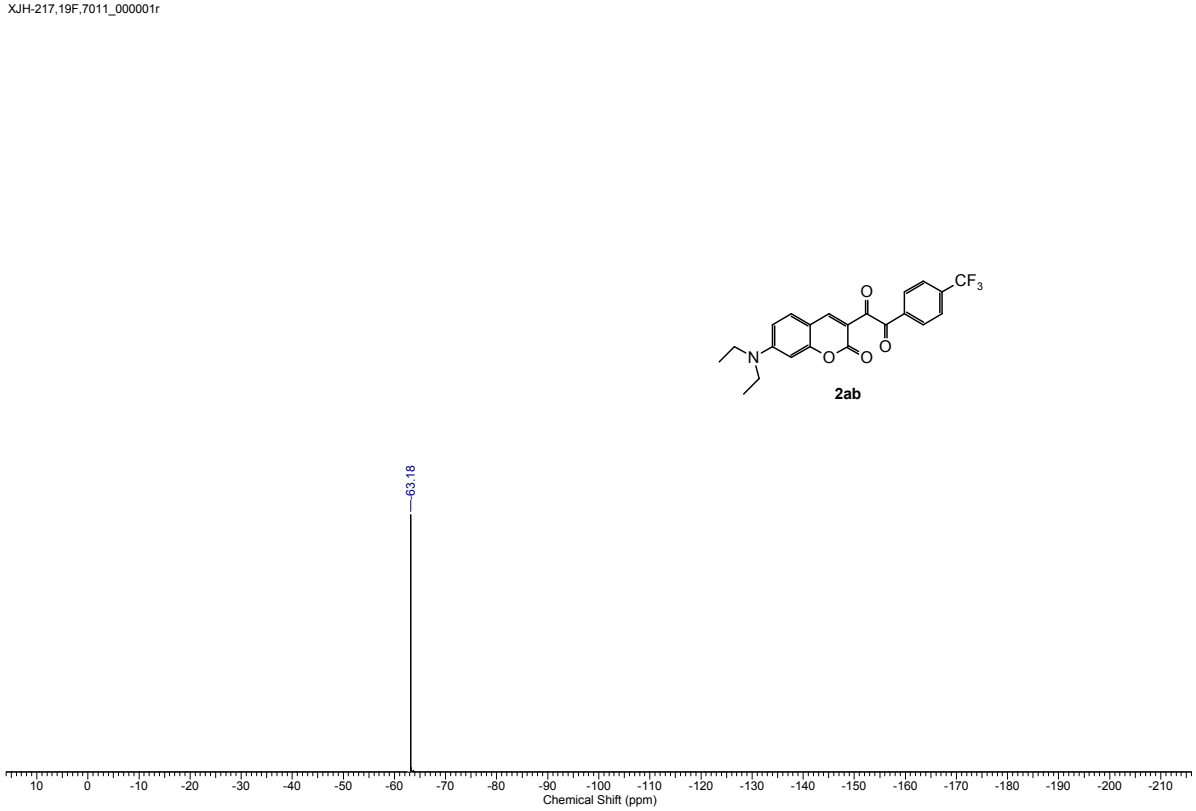


Figure S111. ^{19}F NMR spectrum of compound **2ab**

10. X-ray crystallographic data

1) Structure determination of **2a**

The structure of **2a** was determined by the X-ray diffraction. Recrystallized from EtOH/dichloromethane (v/v = 1/1). Further information can be found in the CIF file. This crystal was deposited in the Cambridge Crystallographic Data Centre and assigned as CCDC 2036909.

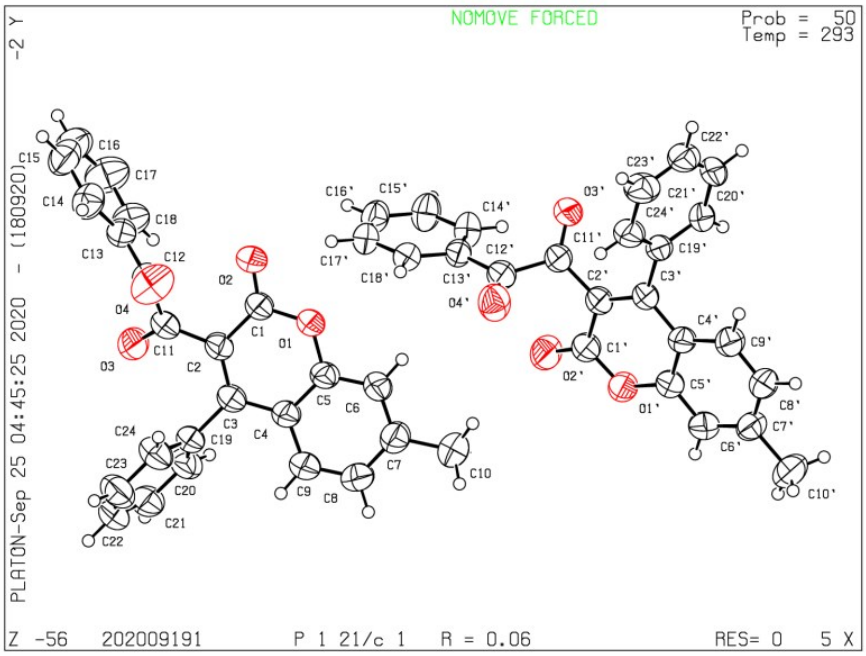


Table S2 Crystal data and structure refinement for 2a.

Identification code	202009191
Empirical formula	$C_{24}H_{16}O_4$
Formula weight	368.37
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	19.224(2)
b/Å	20.020(2)
c/Å	10.0058(12)
α/°	90
β/°	97.418(10)
γ/°	90
Volume/Å^3	3818.6(8)
Z	8
ρ_{calc}g/cm^3	1.281
μ/mm^{-1}	0.709

F(000)	1536.0
Crystal size/mm^3	0.18 × 0.14 × 0.07
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.834 to 134.3
Index ranges	-22 ≤ h ≤ 22, -23 ≤ k ≤ 20, -11 ≤ l ≤ 8
Reflections collected	15425
Independent reflections	6779 [R_{int} = 0.0364, R_{sigma} = 0.0547]
Data/restraints/parameters	6779/0/508
Goodness-of-fit on F^2	1.026
Final R indexes [I>=2σ (I)]	R_1 = 0.0565, wR_2 = 0.1447
Final R indexes [all data]	R_1 = 0.0895, wR_2 = 0.1779
Largest diff. peak/hole / e Å^{-3}	0.20/-0.19

2) Structure determination of **2g**

The structure of **2g** was determined by the X-ray diffraction. Recrystallized from EtOH/dichloromethane (v/v = 1/1). Further information can be found in the CIF file. This crystal was deposited in the Cambridge Crystallographic Data Centre and assigned as CCDC 2026429.

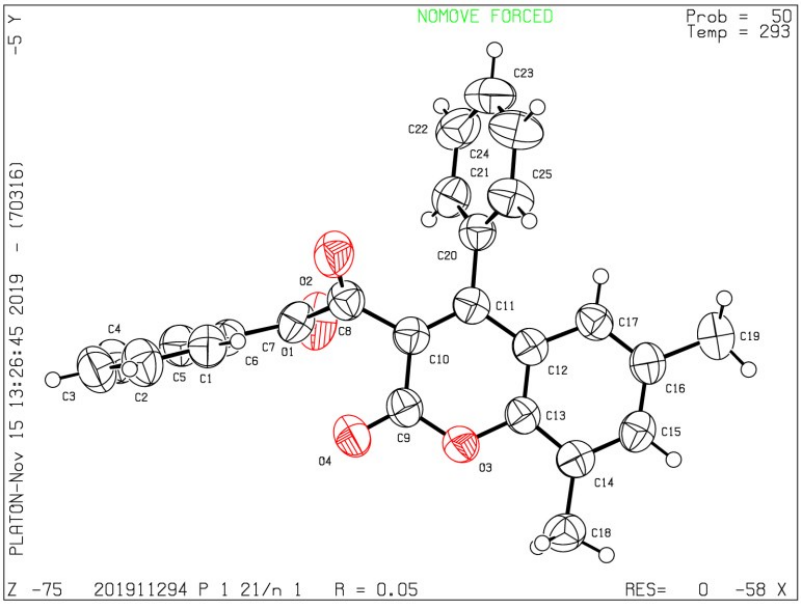


Table S3 Crystal data and structure refinement for 2g.

Identification code	201911294
Empirical formula	$C_{25}H_{18}O_4$
Formula weight	382.39
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	14.5609(6)

b/Å	9.3002(4)
c/Å	14.7714(7)
α/°	90
β/°	94.995(4)
γ/°	90
Volume/Å^3	1992.74(15)
Z	4
ρ_{calc}g/cm^3	1.275
μ/mm^{-1}	0.698
F(000)	800.0
Crystal size/mm^3	0.22 × 0.15 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.178 to 134.16
Index ranges	-17 ≤ h ≤ 16, -8 ≤ k ≤ 11, -17 ≤ l ≤ 16
Reflections collected	7221
Independent reflections	3554 [R_{int} = 0.0250, R_{sigma} = 0.0343]
Data/restraints/parameters	3554/0/264
Goodness-of-fit on F^2	1.028
Final R indexes [I>=2σ (I)]	R_1 = 0.0477, wR_2 = 0.1199
Final R indexes [all data]	R_1 = 0.0667, wR_2 = 0.1383
Largest diff. peak/hole / e Å^{-3}	0.13/-0.17

3) Structure determination of **2s**

The structure of **2s** was determined by the X-ray diffraction. Recrystallized from EtOH/dichloromethane (v/v= 1/1). Further information can be found in the CIF file. This crystal was deposited in the Cambridge Crystallographic Data Centre and assigned as CCDC 2036910.

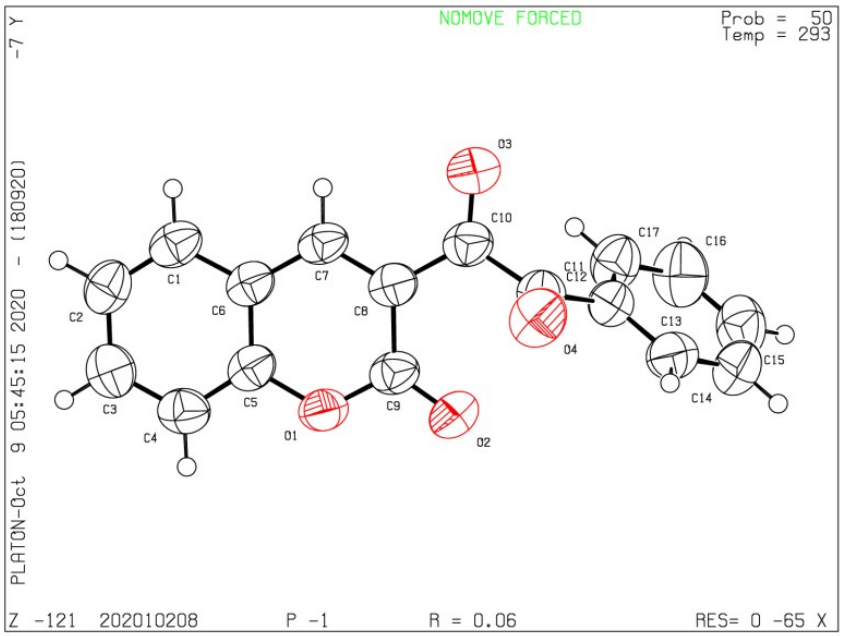


Table S4 rystal data and structure refinement for 2s.

Identification code	202010208
Empirical formula	$C_{17}H_{10}O_4$
Formula weight	278.25
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	7.1288(11)
b/Å	7.3017(9)
c/Å	13.738(2)
α/°	94.814(11)
β/°	90.307(13)
γ/°	112.254(14)
Volume/Å^3	658.95(18)
Z	2
ρ_{calc}g/cm^3	1.402
μ/mm^{-1}	0.835
F(000)	288.0
Crystal size/mm^3	0.22 × 0.1 × 0.04
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	12.944 to 134.118
Index ranges	$-8 \le h \le 5$, $-7 \le k \le 8$, $-16 \le l \le 16$
Reflections collected	4663
Independent reflections	2352 [R_{int} = 0.0339, R_{sigma} = 0.0441]

Data/restraints/parameters	2352/0/190
Goodness-of-fit on F^2	1.035
Final R indexes [I>=2σ (I)]	R_1 = 0.0638, wR_2 = 0.1804
Final R indexes [all data]	R_1 = 0.0994, wR_2 = 0.2205
Largest diff. peak/hole / e $Å^{-3}$	0.22/-0.16