

*(96 pages)*

## Supporting Information For

# CuBr-Mediated Synthesis of 1,4-Naphthoquinones via Ring Expansion of 2-Aryl-1,3-indandiones

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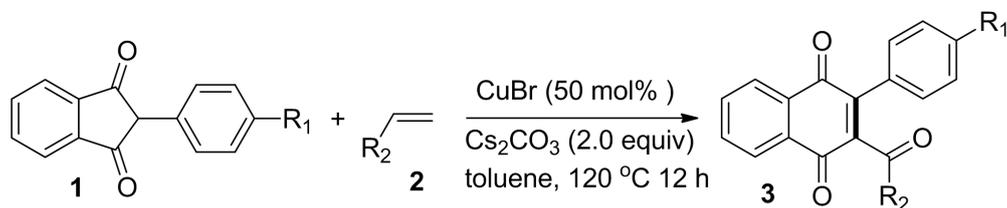
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## General Methods and Materials

CuBr, CuBr<sub>2</sub>, CuI, Cu(OTf)<sub>2</sub>, CuOTf, CuCl<sub>2</sub>, CuBr·SMe<sub>2</sub>, and Cu(OAc)<sub>2</sub> were purchased from Energy Chemical and used without further purification. Other chemicals were purchased from commercial suppliers, further dried and purified if necessary. The water used was re-distilled and ion-free. <sup>1</sup>H and <sup>13</sup>C NMR spectra were achieved on a Bruker AVANCE 400 MHz spectrometer (<sup>1</sup>H 400 MHz; <sup>13</sup>C 100 MHz) in CDCl<sub>3</sub>. Abbreviations for data quoted are *s*-singlet; *brs*-broad singlet; *d*-doublet; *t*-triplet; *dd*-doublet of doublets; *m*-multiplet. High-resolution mass spectra were measured on a Waters Micromass GCT facility. Thin-layer chromatographies were done on pre-coated silica gel 60F254 plates (Merck). Silica gel 60H (200-300 mesh) manufactured by Qingdao Haiyang Chemical Group Co. (China) was used for general chromatography.

## General Catalytic Procedure for CuBr-Mediated Synthesis of 1,4-Naphthoquinones via Ring Expansion of 2-Aryl-1,3-indandiones



A reaction flask (25 mL) was charged with 2-aryl-1,3-indandione **1** (0.2 mmol, 1.0 equiv), alkenes **2** (0.3 mmol, 1.5 equiv), CuBr (14.3 mg, 50 mol%),  $\text{Cs}_2\text{CO}_3$  (0.4 mmol, 130.3 mg, 2.0 equiv), then the toluene (2 mL) was added. The mixture was stirred at  $120\text{ }^\circ\text{C}$  for 12 hours under an atmosphere of air. After the reaction finished, the resulted mixtures were diluted with 20 mL of dichloromethane and washed with 20 mL of  $\text{H}_2\text{O}$ . The aqueous layer was extracted twice with dichloromethane (10 mL) and the combined organic phase was dried over  $\text{Na}_2\text{SO}_4$ . After evaporation of the solvents, the residue was purified by silica gel chromatography (hexane/AcOEt = 10 : 1 ~ 5 : 1) to yield product.

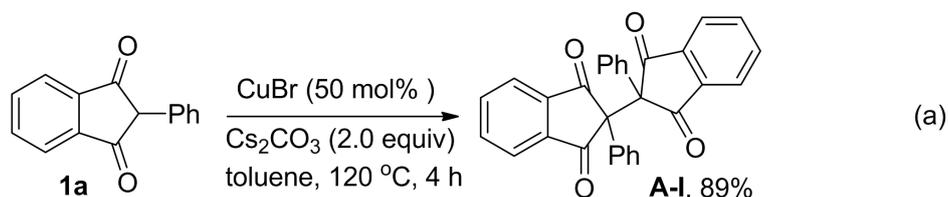
### Procedure Gram-scale for the Synthesis of 3a.

A reaction flask (250 mL) was charged with 2-phenyl-1,3-indandione **1a** (5.0 mmol, 1.0 equiv), styrene **2a** (7.5 mmol, 1.5 equiv), CuBr (357.5 mg, 50 mol%), Cs<sub>2</sub>CO<sub>3</sub> (10.0 mmol, 3258.2 mg, 2.0 equiv), then the toluene (50 mL) was added. The mixture was stirred at 120 °C for 12 hours under an atmosphere of air. After the reaction finished, the resulted mixtures were diluted with 20 mL of dichloromethane and washed with 20 mL of H<sub>2</sub>O. The aqueous layer was extracted twice with dichloromethane (10 mL) and the combined organic phase was dried over Na<sub>2</sub>SO<sub>4</sub>. After evaporation of the solvents, the residue was purified by silica gel chromatography (hexane/AcOEt = 7 : 1) to yield product 1318.2 mg.

### Procedure Gram-scale for the Synthesis of 4a.

A reaction flask (250 mL) was charged with 2-phenyl-1,3-indandione **1a** (5.0 mmol, 1.0 equiv), 4-vinyltoluene **2b** (7.5 mmol, 1.5 equiv), CuBr (357.5 mg, 50 mol%), Cs<sub>2</sub>CO<sub>3</sub> (10.0 mmol, 3258.2 mg, 2.0 equiv), then the toluene (50 mL) was added. The mixture was stirred at 120 °C for 12 hours under an atmosphere of air. After the reaction finished, the resulted mixtures were diluted with 20 mL of dichloromethane and washed with 20 mL of H<sub>2</sub>O. The aqueous layer was extracted twice with dichloromethane (10 mL) and the combined organic phase was dried over Na<sub>2</sub>SO<sub>4</sub>. After evaporation of the solvents, the residue was purified by silica gel chromatography (hexane/AcOEt = 7 : 1) to yield product 1531.2 mg.

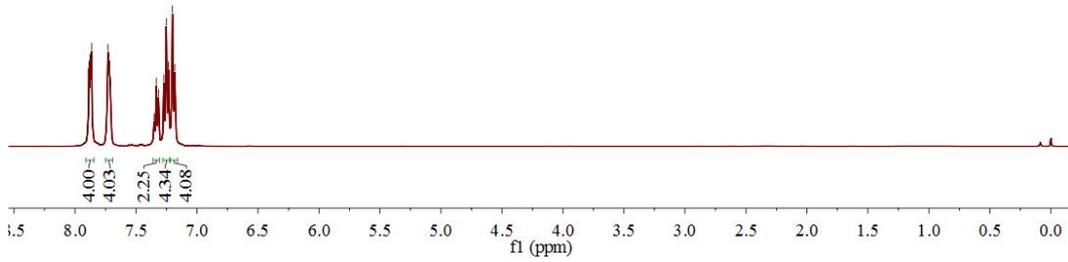
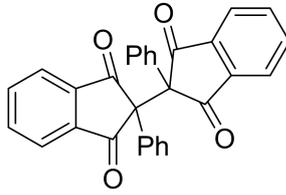
## Control Experiments



A reaction flask (25 mL) was charged with 2-phenyl-1,3-indandione **1a** (0.2 mmol, 1.0 equiv), CuBr (14.3 mg, 50 mol%), Cs<sub>2</sub>CO<sub>3</sub> (0.4 mmol, 130.3 mg, 2.0 equiv), then the toluene (2 mL) was added. The mixture was stirred at 120 °C for 4 hours under an atmosphere of air. After the reaction finished, the resulted mixtures were diluted with 20 mL of dichloromethane and washed with 20 mL of H<sub>2</sub>O. The aqueous layer was extracted twice with dichloromethane (10 mL) and the combined organic phase was dried over Na<sub>2</sub>SO<sub>4</sub>. After evaporation of the solvents, the residue was purified by silica gel chromatography (hexane/AcOEt = 3 : 1) to yield product.

2,2'-diphenyl-1H,1'H-[2,2'-biindene]-1,1',3,3'(2H,2'H)-tetraone (**A-I**): Obtained as a pale yellow solid (84.0 mg, 76% yield), eluting with 20% EtOAc in PE (elution gradient); <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ ppm: 7.86 - 7.89 (m, 4H), 7.71 - 7.73 (m, 4H), 7.32 - 7.35 (t, *J* = 6.8 Hz, 2H), 7.23 - 7.27 (t, *J* = 8.0 Hz, 4H), 7.18 - 7.20 (d, *J* = 8.0 Hz, 4H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ ppm: 197.4, 140.90, 135.6, 130.4, 129.8, 128.7, 127.5, 123.7, 64.3; HRMS (ESI-TOF) *m/z* calcd for C<sub>30</sub>H<sub>19</sub>O<sub>4</sub> [M + H]<sup>+</sup> 443.1278, found 443.1275.

21-308  
7.878  
7.872  
7.864  
7.730  
7.722  
7.731  
7.734  
7.716  
7.272  
7.252  
7.234  
7.202  
7.182

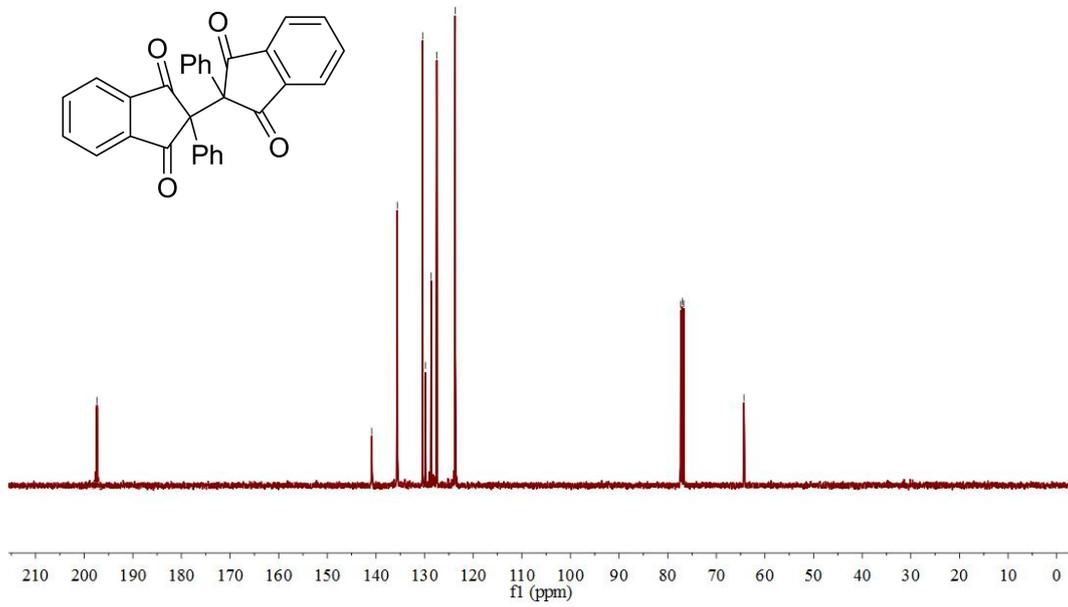
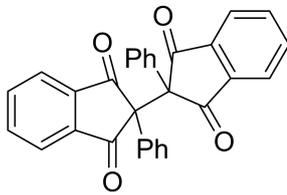


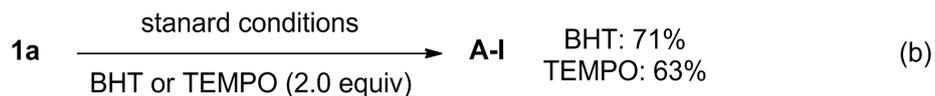
21-302

-197.40

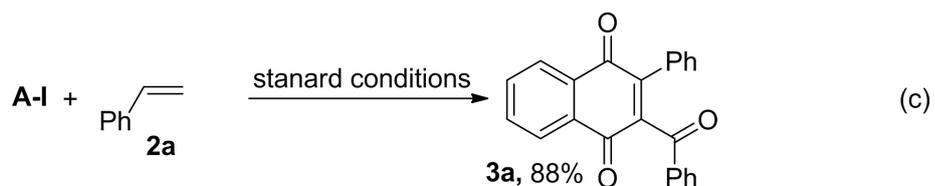
140.87  
135.61  
130.39  
129.81  
128.65  
127.51  
123.70

77.32  
77.00  
76.68  
64.33

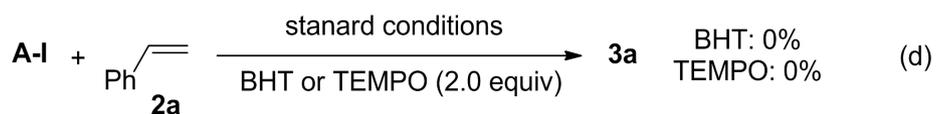




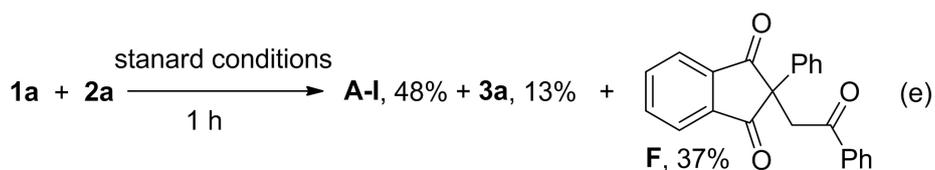
A reaction flask (25 mL) was charged with 2-phenyl-1,3-indandione **1a** (0.2 mmol, 1.0 equiv), CuBr (14.3 mg, 50 mol%), Cs<sub>2</sub>CO<sub>3</sub> (0.4 mmol, 130.3 mg, 2.0 equiv), TEMPO (0.4 mmol, 2.0 equiv) or BHT (0.4 mmol, 2.0 equiv), then the toluene (2 mL) was added. The mixture was stirred at 120 °C for 12 hours under an atmosphere of air. After the reaction finished, the resulted mixtures were diluted with 20 mL of dichloromethane and washed with 20 mL of H<sub>2</sub>O. The aqueous layer was extracted twice with dichloromethane (10 mL) and the combined organic phase was dried over Na<sub>2</sub>SO<sub>4</sub>. After evaporation of the solvents, the residue was purified by silica gel chromatography (hexane/AcOEt = 3 : 1) to yield product **A-I**.



A reaction flask (25 mL) was charged with **A-I** (0.2 mmol, 1.0 equiv), styrene **2a** (0.3 mmol, 1.5 equiv), CuBr (14.3 mg, 50 mol%), Cs<sub>2</sub>CO<sub>3</sub> (0.4 mmol, 130.3 mg, 2.0 equiv), then the toluene (2 mL) was added. The mixture was stirred at 120 °C for 12 hours under an atmosphere of air. After the reaction finished, the resulted mixtures were diluted with 20 mL of dichloromethane and washed with 20 mL of H<sub>2</sub>O. The aqueous layer was extracted twice with dichloromethane (10 mL) and the combined organic phase was dried over Na<sub>2</sub>SO<sub>4</sub>. After evaporation of the solvents, the residue was purified by silica gel chromatography (hexane/AcOEt = 7 : 1) to yield product **3a**.



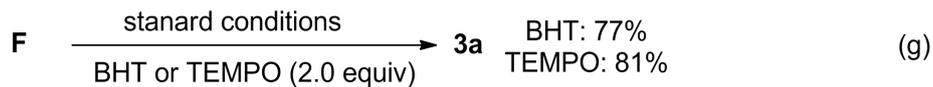
A reaction flask (25 mL) was charged with **A-I** (0.2 mmol, 1.0 equiv), styrene **2a** (0.3 mmol, 1.5 equiv), CuBr (14.3 mg, 50 mol%), Cs<sub>2</sub>CO<sub>3</sub> (0.4 mmol, 130.3 mg, 2.0 equiv), TEMPO (0.4 mmol, 2.0 equiv) or BHT (0.4 mmol, 2.0 equiv), then the toluene (2 mL) was added. The mixture was stirred at 120 °C for 12 hours under an atmosphere of air. No desired product of 3a was detected.



A reaction flask (25 mL) was charged with 2-aryl-1,3-indandione **1** (0.2 mmol, 1.0 equiv), alkenes **2** (0.3 mmol, 1.5 equiv), CuBr (14.3 mg, 50 mol%), Cs<sub>2</sub>CO<sub>3</sub> (0.4 mmol, 130.3 mg, 2.0 equiv), then the toluene (2 mL) was added. The mixture was stirred at 120 °C for 1 hours under an atmosphere of air. After the reaction finished, the resulted mixtures were diluted with 20 mL of dichloromethane and washed with 20 mL of H<sub>2</sub>O. The aqueous layer was extracted twice with dichloromethane (10 mL) and the combined organic phase was dried over Na<sub>2</sub>SO<sub>4</sub>. After evaporation of the solvents, the residue was purified by silica gel chromatography (hexane/AcOEt = 10 : 1 ~ 5 : 1) to yield products **A-1** in 48%, **3a** in 13%, and **F** in 37% yields, respectively.



A reaction flask (25 mL) was charged with **F** (0.2 mmol, 1.0 equiv), CuBr (14.3 mg, 50 mol%), Cs<sub>2</sub>CO<sub>3</sub> (0.4 mmol, 130.3 mg, 2.0 equiv), then the toluene (2 mL) was added. The mixture was stirred at 120 °C for 12 hours under an atmosphere of air. After the reaction finished, the resulted mixtures were diluted with 20 mL of dichloromethane and washed with 20 mL of H<sub>2</sub>O. The aqueous layer was extracted twice with dichloromethane (10 mL) and the combined organic phase was dried over Na<sub>2</sub>SO<sub>4</sub>. After evaporation of the solvents, the residue was purified by silica gel chromatography (hexane/AcOEt = 7 : 1) to yield products **3a** in 91% yield.



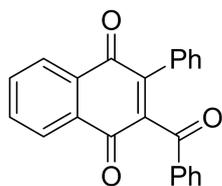
A reaction flask (25 mL) was charged with **F** (0.2 mmol, 1.0 equiv), CuBr (14.3 mg, 50 mol%), Cs<sub>2</sub>CO<sub>3</sub> (0.4 mmol, 130.3 mg, 2.0 equiv), TEMPO (0.4 mmol, 2.0 equiv) or BHT (0.4 mmol, 2.0 equiv), then the toluene (2 mL) was added. The mixture was stirred at 120 °C for 12 hours under an atmosphere of air. After the reaction finished, the resulted mixtures were diluted with 20 mL of dichloromethane and washed with 20 mL of H<sub>2</sub>O. The aqueous layer was extracted twice with dichloromethane (10 mL) and the combined organic phase was dried over Na<sub>2</sub>SO<sub>4</sub>. After evaporation of the solvents, the residue was purified by silica gel chromatography (hexane/AcOEt = 7 : 1) to yield product **3a** in 77%, and 81% yields, respectively.

## X-Ray Crystallographic Data

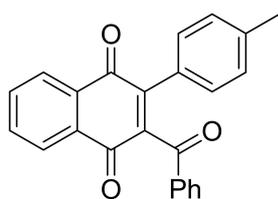
### Crystal structure details for Product 3e (CCDC:2285891)

Identification code	A
Empirical formula	C <sub>27</sub> H <sub>22</sub> O <sub>3</sub>
Formula weight	394.45
Temperature/K	296(2) K
Crystal system	triclinic
Space group	P-1
a/Å	9.6983(19)
b/Å	10.099(2)
c/Å	12.581(3)
α/°	69.766(4)
β/°	70.291(3)
γ/°	65.925(3)
Volume/Å <sup>3</sup>	1027.5(4)
Z	2
ρ <sub>calc</sub> /cm <sup>3</sup>	1.275
μ/mm <sup>-1</sup>	0.082
F(000)	416
Crystal size/mm <sup>3</sup>	0.26 x 0.23 x 0.21
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/	1.77 to 25.00
Index ranges	-11 ≤ h ≤ 9, -12 ≤ k ≤ 10, -14 ≤ l ≤ 9
Reflections collected	5077
Independent reflections	3570 [R(int) = 0.0216]
Data/restraints/parameters	3570/0/271
Goodness-of-fit on F <sup>2</sup>	1.006
Final R indexes [I ≥ 2σ (I)]	R <sub>1</sub> = 0.0504, wR <sub>2</sub> = 0.1408
Final R indexes [all data]	R <sub>1</sub> = 0.0917, wR <sub>2</sub> = 0.1812
Largest diff. peak/hole/eÅ <sup>-3</sup>	0.227 and -0.201

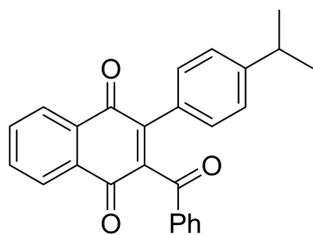
## Characterization data for the products



2-Benzoyl-3-phenylnaphthalene-1,4-dione (**3a**): Obtained as a yellow solid (58.1 mg, 86% yield), eluting with 10% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 - 8.23 (m, 1H), 8.13 - 8.15 (m, 1H), 7.77 - 7.85 (m, 4H), 7.47 - 7.51 (t,  $J = 7.2$  Hz, 1H), 7.33 - 7.37 (t,  $J = 7.6$  Hz, 2H), 7.26 (s, 5H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.9, 184.2, 183.8, 144.6, 143.9, 135.7, 134.4, 134.3, 134.0, 131.8, 131.6, 130.9, 129.7, 129.6, 129.0, 128.7, 128.0, 127.0, 126.4; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{15}\text{O}_3$   $[\text{M} + \text{H}]^+$  339.1016, found 339.1015.

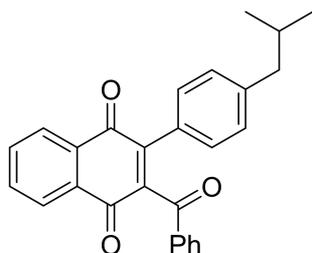


2-Benzoyl-3-(*p*-tolyl)naphthalene-1,4-dione (**3b**): Obtained as a yellow solid (62.4 mg, 91% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.20 - 8.23 (m, 1H), 8.12 - 8.14 (m, 1H), 7.78 - 7.83 (m, 4H), 7.45 - 7.52 (t,  $J = 7.2$  Hz, 1H), 7.34 - 7.38 (t,  $J = 7.6$  Hz, 2H), 7.17 - 7.19 (d,  $J = 8.0$  Hz, 2H), 7.06 - 7.08 (d,  $J = 8.0$  Hz, 2H), 2.26 (s, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  193.1, 184.3, 183.8, 144.8, 143.5, 139.9, 135.9, 134.3, 134.2, 134.0, 131.9, 131.7, 129.8, 129.1, 128.8, 128.7, 128.0, 127.0, 126.4, 21.3; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{24}\text{H}_{17}\text{O}_3$   $[\text{M} + \text{H}]^+$  353.1172, found 353.1173.



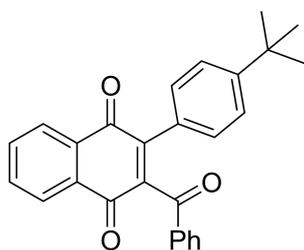
2-Benzoyl-3-(4-isopropylphenyl)naphthalene-1,4-dione (**3c**): Obtained as a yellow solid (122.2 mg, 88% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 - 8.23 (m, 1H), 8.12 - 8.14 (m, 1H), 7.78 - 7.85 (m, 4H), 7.48 - 7.51 (t,  $J = 7.2$  Hz, 1H), 7.34 - 7.38 (t,  $J = 7.6$  Hz,

2H), 7.18 - 7.20 (d,  $J = 8.0$  Hz, 2H), 7.10 - 7.12 (d,  $J = 8.4$  Hz, 2H), 2.76 - 2.86 (m, 1H), 1.16 (s, 3H), 1.15 (s, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  193.3, 184.4, 183.8, 150.6, 144.8, 143.4, 135.9, 134.3, 134.2, 133.9, 131.9, 131.6, 129.9, 129.2, 128.6, 128.3, 127.0, 126.4, 126.2, 33.8, 23.6; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{26}\text{H}_{21}\text{O}_3$  [ $\text{M} + \text{H}$ ] $^+$  381.1485, found 381.1483.



2-Benzoyl-3-(4-isobutylphenyl)naphthalene-1,4-dione (**3d**):

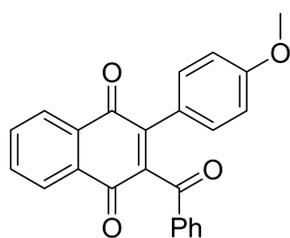
Obtained as a yellow solid (68.6 mg, 87% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 - 8.23 (m, 1H), 8.13 - 8.16 (m, 1H), 7.82 - 7.84 (m, 2H), 7.74 - 7.76 (d,  $J = 7.2$  Hz, 2H), 7.45 - 7.48 (t,  $J = 7.2$  Hz, 1H), 7.31 - 7.34 (t,  $J = 8.0$  Hz, 2H), 7.16 - 7.18 (d,  $J = 8.4$  Hz, 2H), 7.01 - 7.03 (d,  $J = 8.0$  Hz, 2H), 2.36 - 2.38 (d,  $J = 7.2$  Hz, 2H), 1.69 - 1.78 (m, 1H), 0.78 (s, 3H), 0.76 (s, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  193.3, 184.4, 183.7, 144.7, 143.6, 143.4, 135.8, 134.3, 134.2, 133.8, 131.9, 131.7, 129.7, 129.0, 128.8, 128.5, 128.3, 127.0, 126.4, 45.1, 30.0, 22.2; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{27}\text{H}_{23}\text{O}_3$  [ $\text{M} + \text{H}$ ] $^+$  395.1642, found 395.1644.



2-Benzoyl-3-(4-*tert*-butylphenyl)naphthalene-1,4-dione (**3e**):

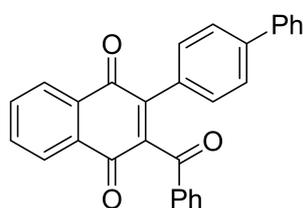
Obtained as a yellow solid (72.5 mg, 92% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.20 - 8.23 (m, 1H), 8.11 - 8.14 (m, 1H), 7.77 - 7.82 (m, 4H), 7.46 - 7.50 (t,  $J = 7.2$  Hz, 1H), 7.33 - 7.37 (t,  $J = 7.6$  Hz, 2H), 7.26 - 7.28 (d,  $J = 8.8$  Hz, 2H), 7.19 - 7.21 (d,  $J = 8.4$  Hz, 2H), 1.22 (s, 9H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  193.2, 184.4, 183.8, 152.8, 144.8, 143.5, 136.1, 134.3,

134.2, 133.8, 131.9, 131.7, 129.6, 129.0, 128.6, 128.0, 127.0, 126.3, 125.0, 34.7, 31.0;  
HRMS (ESI-TOF)  $m/z$  calcd for  $C_{27}H_{23}O_3$   $[M + H]^+$  395.1642, found 395.1640.



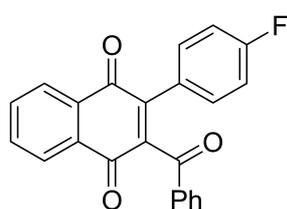
2-Benzoyl-3-(4-methoxyphenyl)naphthalene-1,4-dione (**3f**):

Obtained as a yellow solid (64.0 mg, 87% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.21 - 8.23 (m, 1H), 8.11 - 8.14 (m, 1H), 7.79 - 7.82 (m, 4H), 7.48 - 7.52 (t,  $J = 7.6$  Hz, 1H), 7.34 - 7.38 (t,  $J = 7.2$  Hz, 2H), 7.24 - 7.26 (d,  $J = 9.2$  Hz, 2H), 6.78 - 6.70 (d,  $J = 8.8$  Hz, 2H), 3.73 (s, 3H);  $^{13}C$  NMR (101 MHz,  $CDCl_3$ )  $\delta$  193.4, 184.5, 183.7, 161.0, 144.2, 142.9, 135.7, 134.3, 134.2, 134.0, 131.9, 131.7, 129.0, 128.7, 128.3, 127.0, 126.3, 123.2, 113.6, 55.2; HRMS (ESI-TOF)  $m/z$  calcd for  $C_{24}H_{17}O_4$   $[M + H]^+$  369.1121, found 369.1120.



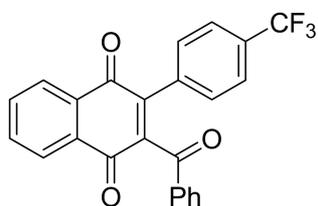
2-([1,1'-Biphenyl]-4-yl)-3-benzoylnaphthalene-1,4-dione (**3g**):

Obtained as a yellow solid (77.8 mg, 94% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.23 - 8.25 (m, 1H), 8.14 - 8.16 (m, 1H), 7.81 - 7.87 (m, 4H), 7.49 - 7.52 (m, 5H), 7.33 - 7.42 (m, 7H);  $^{13}C$  NMR (101 MHz,  $CDCl_3$ )  $\delta$  193.1, 184.2, 183.8, 144.4, 143.7, 142.3, 140.0, 135.8, 134.4, 134.3, 134.1, 131.9, 131.6, 130.3, 129.8, 129.1, 128.8, 128.8, 127.7, 127.1, 127.1, 126.7, 126.4; HRMS (ESI-TOF)  $m/z$  calcd for  $C_{29}H_{19}O_3$   $[M + H]^+$  415.1329, found 415.1327.



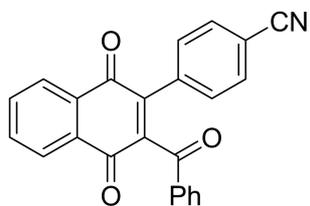
2-Benzoyl-3-(4-fluorophenyl)naphthalene-1,4-dione (**3h**):

Obtained as a yellow solid (57.7 mg, 81% yield), eluting with 15% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.20 - 8.22 (m, 1H), 8.12 - 8.14 (m, 1H), 7.82 - 7.86 (m, 2H), 7.77 - 7.79 (d,  $J = 7.6$  Hz, 2H), 7.50 - 7.53 (t,  $J = 7.6$  Hz, 1H), 7.35 - 7.39 (t,  $J = 7.6$  Hz, 2H), 7.25 - 7.29 (m, 2H), 6.94 - 6.98 (t,  $J = 8.4$  Hz, 2H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.9, 184.0, 183.6, 163.3 (d,  $J = 249.2$  Hz, 1C), 143.9, 143.5, 135.5, 134.5, 134.4, 134.2, 131.9 (d,  $J = 8.5$  Hz, 1C), 131.7, 131.5, 129.0, 128.8, 127.0, 126.8 (d,  $J = 3.4$  Hz, 1C), 126.4, 115.3 (d,  $J = 21.7$  Hz, 1C);  $^{19}\text{F}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  -110.3; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{14}\text{O}_3\text{F}$  [ $\text{M} + \text{H}$ ] $^+$  357.0922, found 357.0920.



2-Benzoyl-3-(4-(trifluoromethyl)phenyl)naphthalene-1,4-dione

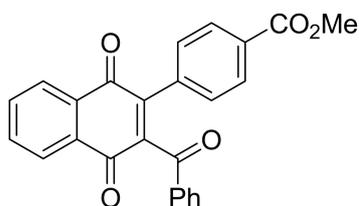
(**3i**): Obtained as a yellow solid (64.3 mg, 79% yield), eluting with 15% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.20 - 8.22 (m, 1H), 8.12 - 8.15 (m, 1H), 7.77 - 7.87 (m, 4H), 7.51 - 7.55 (m, 3H), 7.37 - 7.41 (m, 4H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.5, 183.6, 183.5, 144.6, 143.3, 135.5, 134.6, 134.4 (q,  $J = 3.3, 4.5$  Hz, 1C), 131.8, 131.6, 131.45, 131.3 (q,  $J = 32.4, 64.9$  Hz, 1C), 130.1, 129.0, 128.9, 127.1, 126.5, 125.0 (q,  $J = 3.6, 7.3$  Hz, 1C), 124.3 (q,  $J = 167.6, 270.9$  Hz, 1C);  $^{19}\text{F}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  -63.0; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{24}\text{H}_{14}\text{O}_3\text{F}_3$  [ $\text{M} + \text{H}$ ] $^+$  407.0890, found 407.0878.



4-(3-Benzoyl-1,4-dioxo-1,4-dihydronaphthalen-2-yl)benzonitrile

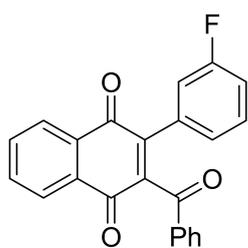
(**3j**): Obtained as a yellow solid (55.2 mg, 76% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.22 - 8.23 (m, 1H), 8.14 - 8.16 (m, 1H), 7.85 - 7.87 (m, 2H), 7.75 - 7.77 (d,  $J = 7.6$  Hz, 2H), 7.53 - 7.57 (m, 3H), 7.37

- 7.41 (m, 4H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.2, 183.4, 183.3, 144.8, 142.8, 135.6, 135.4, 134.8, 134.7, 134.6, 131.7, 131.5, 131.5, 130.5, 129.0, 128.9, 127.2, 126.6, 118.1, 113.3; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{24}\text{H}_{14}\text{NO}_3$   $[\text{M} + \text{H}]^+$  364.0968, found 364.0967.



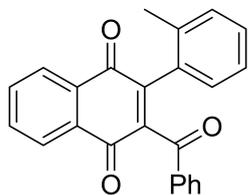
Methyl

4-(3-benzoyl-1,4-dioxo-1,4-dihydronaphthalen-2-yl)benzoate (**3k**): Obtained as a yellow solid (59.4 mg, 75% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 - 8.23 (m, 1H), 8.14 - 8.16 (m, 1H), 7.92 - 7.74 (d,  $J = 8.0$  Hz, 2H), 7.82 - 7.88 (m, 2H), 7.76 - 7.78 (d,  $J = 7.6$  Hz, 2H), 7.50 - 7.53 (t,  $J = 7.2$  Hz, 1H), 7.33 - 7.41 (m, 4H), 3.87 (s, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.5, 183.7, 183.6, 166.3, 144.4, 143.8, 135.6, 135.5, 134.6, 134.5, 134.3, 131.7, 131.6, 130.9, 129.8, 129.2, 129.0, 128.8, 127.1, 126.6, 52.2; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{25}\text{H}_{17}\text{O}_5$   $[\text{M} + \text{H}]^+$  397.1071, found 397.1072.

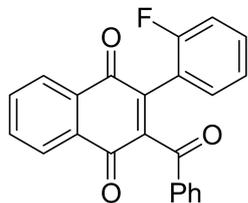


2-Benzoyl-3-(3-fluorophenyl)naphthalene-1,4-dione (**3l**): Obtained as a yellow solid (52.7 mg, 74% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 - 8.23 (m, 1H), 8.13 - 8.15 (m, 1H), 7.83 - 7.87 (m, 2H), 7.77 - 7.79 (d,  $J = 7.6$  Hz, 2H), 7.50 - 7.54 (t,  $J = 7.6$  Hz, 1H), 7.36 - 7.40 (t,  $J = 7.6$  Hz, 2H), 7.20 - 7.24 (t,  $J = 6.4$  Hz, 1H), 6.96 - 7.04 (m, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.6, 183.7, 183.6, 162.0 (d,  $J = 246.0$  Hz, 1C), 144.3, 143.3, 135.6, 134.6, 134.4, 134.3, 132.8 (d,  $J = 8.0$  Hz, 1C), 131.7, 131.5, 129.8 (d,  $J = 8.3$  Hz, 1C), 129.0, 128.8, 127.1, 126.5, 125.6 (d,  $J = 3.2$  Hz, 1C), 117.0 (d,  $J = 22.9$

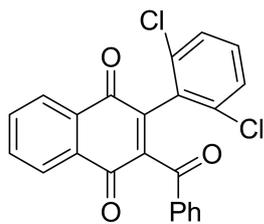
Hz, 1C), 116.7 (d,  $J = 20.9$  Hz, 1C);  $^{19}\text{F}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  -112.4; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{14}\text{O}_3\text{F}$   $[\text{M} + \text{H}]^+$  357.0922, found 357.0923.



2-Benzoyl-3-(*o*-tolyl)naphthalene-1,4-dione (**3m**): Obtained as a yellow solid (54.2 mg, 77% yield), eluting with 10% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.16 - 8.22 (m, 2H), 7.83 - 7.85 (m, 2H), 7.23 - 7.25 (d,  $J = 7.6$  Hz, 2H), 7.50 - 7.53 (t,  $J = 7.2$  Hz, 1H), 7.35 - 7.39 (t,  $J = 7.6$  Hz, 2H), 7.15 - 7.19 (t,  $J = 7.2$  Hz, 1H), 7.09 - 7.11 (d,  $J = 7.2$  Hz, 1H), 7.00 - 7.02 (m, 2H), 2.16 (s, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.4, 183.9, 183.6, 146.5, 145.1, 136.3, 136.0, 134.5, 134.3, 134.0, 131.9, 131.6, 130.8, 130.0, 129.4, 128.8, 128.6, 127.1, 126.5, 125.4, 20.3; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{24}\text{H}_{17}\text{O}_3$   $[\text{M} + \text{H}]^+$  353.1172, found 353.1170.

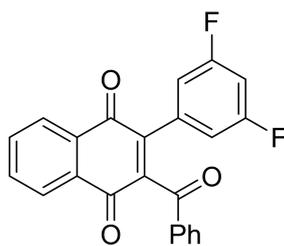


2-Benzoyl-3-(2-fluorophenyl)naphthalene-1,4-dione (**3n**): Obtained as a yellow solid (51.3 mg, 72% yield), eluting with 15% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.23 - 8.24 (m, 1H), 8.14 - 8.17 (m, 1H), 7.79 - 7.87 (m, 4H), 7.50 - 7.53 (t,  $J = 7.6$  Hz, 1H), 7.36 - 7.40 (t,  $J = 8.0$  Hz, 2H), 7.27 - 7.31 (m, 1H), 7.17 - 7.20 (t,  $J = 6.4$  Hz, 1H), 7.03 - 7.07 (t,  $J = 7.2$  Hz, 1H), 6.96 - 7.04 (m, 1H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.1, 183.3, 182.4, 159.4 (d,  $J = 247.1$  Hz, 1C), 145.3, 141.4, 135.3, 134.6, 134.3 (d,  $J = 7.3$  Hz, 1C), 131.8 (d,  $J = 8.2$  Hz, 1C), 131.7, 131.5, 131.0, 130.9, 128.9, 128.7, 127.1, 126.6, 124.0 (d,  $J = 3.4$  Hz, 1C), 119.3 (d,  $J = 16.0$  Hz, 1C), 115.4 (d,  $J = 21.1$  Hz, 1C);  $^{19}\text{F}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  -110.3; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{14}\text{O}_3\text{F}$   $[\text{M} + \text{H}]^+$  357.0922, found 357.0925.



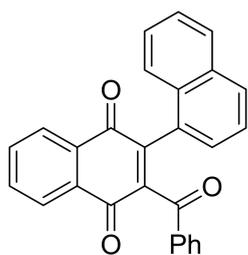
2-Benzoyl-3-(2,6-dichlorophenyl)naphthalene-1,4-dione (**3o**):

Obtained as a yellow solid (52.0 mg, 64% yield), eluting with 15% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.22 - 8.24 (m, 1H), 8.17 - 8.19 (m, 1H), 7.86 - 7.87 (m, 2H), 7.80 - 7.82 (d,  $J = 7.6$  Hz, 2H), 7.53 - 7.56 (t,  $J = 7.6$  Hz, 1H), 7.37 - 7.41 (t,  $J = 7.6$  Hz, 2H), 7.23 - 7.25 (d,  $J = 8.0$  Hz, 2H), 7.16 - 7.20 (t,  $J = 7.2$  Hz, 1H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  191.2, 183.5, 182.0, 145.8, 142.6, 135.2, 134.6, 134.5, 134.4, 134.2, 131.7, 131.6, 130.9, 130.1, 129.3, 128.4, 127.7, 127.2, 126.7; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{13}\text{Cl}_2\text{O}_3$   $[\text{M} + \text{H}]^+$  407.0236, found 407.0237.



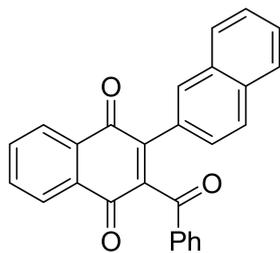
2-Benzoyl-3-(3,5-difluorophenyl)naphthalene-1,4-dione (**3p**):

Obtained as a yellow solid (47.9 mg, 65% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 - 8.23 (m, 1H), 8.14 - 8.16 (m, 1H), 7.82 - 7.88 (m, 2H), 7.77 - 7.79 (d,  $J = 8.0$  Hz, 2H), 7.54 - 7.57 (t,  $J = 7.6$  Hz, 1H), 7.39 - 7.43 (t,  $J = 7.2$  Hz, 2H), 6.79 - 6.81 (d,  $J = 6.4$  Hz, 2H), 6.72 - 6.76 (t,  $J = 9.2$  Hz, 1H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.2, 183.4, 183.3, 162.4 (d,  $J = 248.6$  Hz, 1C), 162.3 (d,  $J = 248.8$  Hz, 1C), 144.7, 142.3, 135.5, 134.7, 134.6, 134.5, 133.7 (t,  $J = 10.1$  Hz, 1C), 131.6, 131.5, 129.0, 128.9, 127.2, 126.6, 113.2 (d,  $J = 19.1$  Hz, 1C), 113.1 (d,  $J = 19.2$  Hz, 1C), 105.1 (t,  $J = 24.9$  Hz, 1C);  $^{19}\text{F}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  -108.8; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{13}\text{O}_3\text{F}_2$   $[\text{M} + \text{H}]^+$  375.0827, found 375.0824.



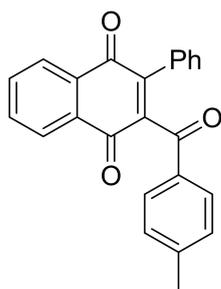
3'-Benzoyl-[1,2'-binaphthalene]-1',4'-dione (**3q**):

Obtained as a yellow solid (39.6 mg, 51% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.20 - 8.22 (m, 2H), 7.84 - 7.87 (m, 2H), 7.74 - 7.76 (d,  $J = 7.6$  Hz, 2H), 7.69 - 7.71 (d,  $J = 7.6$  Hz, 2H), 7.58 - 7.61 (m, 1H), 7.22 - 7.43 (m, 7H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.3, 183.9, 183.7, 146.0, 145.7, 134.5, 134.4, 133.9, 133.1, 132.0, 131.8, 131.2, 130.0, 129.1, 128.9, 128.4, 127.2, 126.6, 126.4, 126.1, 125.7, 124.7; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{27}\text{H}_{17}\text{O}_3$   $[\text{M} + \text{H}]^+$  389.1172, found 389.1175.



3-Benzoyl-[2,2'-binaphthalene]-1,4-dione (**3r**):

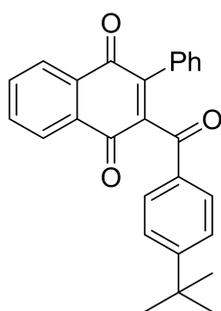
Obtained as a yellow solid (60.5 mg, 78% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.24 - 8.26 (m, 1H), 8.15 - 8.18 (m, 1H), 7.71 - 7.87 (m, 8H), 7.41 - 7.49 (m, 3H), 7.30 - 7.38 (m, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  193.0, 184.4, 183.8, 144.6, 144.1, 135.7, 134.5, 134.3, 134.1, 133.4, 132.5, 131.7, 131.6, 130.2, 129.0, 128.7, 128.6, 128.5, 127.7, 127.6, 127.2, 127.1, 126.6, 126.5, 126.4; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{27}\text{H}_{17}\text{O}_3$   $[\text{M} + \text{H}]^+$  389.1172, found 389.1171.



2-(4-Methylbenzoyl)-3-phenylnaphthalene-1,4-dione (**4a**):

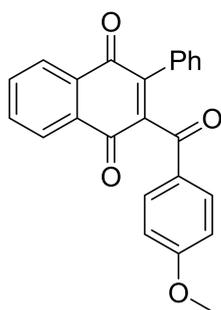
Obtained as a yellow solid (65.5 mg, 93% yield), eluting with 15% EtOAc in PE (elution

gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 - 8.23 (m, 1H), 8.12 - 8.14 (m, 1H), 7.79 - 7.85 (m, 2H), 7.67 - 7.69 (d,  $J = 8.0$  Hz, 2H), 7.26 - 7.27 (m, 5H), 7.14 - 7.16 (d,  $J = 8.0$  Hz, 2H), 2.34 (s, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.5, 184.2, 183.8, 145.2, 144.4, 144.0, 134.4, 134.2, 133.4, 131.9, 131.6, 131.0, 129.7, 129.5, 129.4, 129.2, 128.0, 127.0, 126.4, 21.8; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{24}\text{H}_{17}\text{O}_3$   $[\text{M} + \text{H}]^+$  353.1172, found 353.1174.



2-(4-(*Tert*-butyl)benzoyl)-3-phenylnaphthalene-1,4-dione (**4b**):

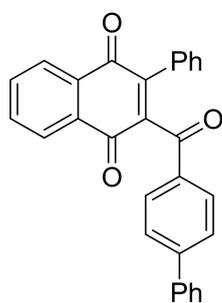
Obtained as a yellow solid (70.1 mg, 89% yield), eluting with 15% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 - 8.23 (m, 1H), 8.12 - 8.14 (m, 1H), 7.79 - 7.86 (m, 2H), 7.71 - 7.73 (d,  $J = 8.0$  Hz, 2H), 7.36 - 7.38 (d,  $J = 8.0$  Hz, 2H), 7.26 - 7.28 (m, 5H), 1.28 (s, 9H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.5, 184.3, 183.9, 157.9, 144.5, 144.1, 134.4, 134.2, 133.3, 131.9, 131.6, 131.0, 129.8, 129.5, 129.0, 128.0, 127.0, 126.4, 125.7, 35.2, 30.9; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{27}\text{H}_{23}\text{O}_3$   $[\text{M} + \text{H}]^+$  395.1642, found 395.1643.



2-(4-Methoxybenzoyl)-3-phenylnaphthalene-1,4-dione (**4c**):

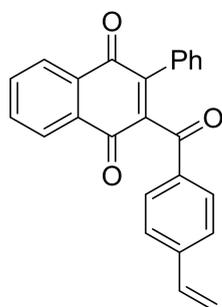
Obtained as a yellow solid (64.0 mg, 87% yield), eluting with 12% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.18 - 8.21 (m, 1H), 8.11 - 8.13 (m, 1H), 7.79 - 7.83 (m, 2H), 7.74 - 7.76 (d,  $J = 8.8$  Hz, 2H), 7.27 (s, 5H), 6.80 - 6.82 (d,  $J = 8.8$  Hz, 2H), 3.78 (s, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  191.2, 184.2, 183.8, 164.2, 144.2, 144.0, 134.3, 134.2, 131.8, 131.6, 131.5, 131.1, 129.7, 129.5, 128.9, 127.9,

126.9, 126.3, 113.9, 55.4; HRMS (ESI-TOF)  $m/z$  calcd for  $C_{24}H_{17}O_4$   $[M + H]^+$  369.1121, found 369.1122.

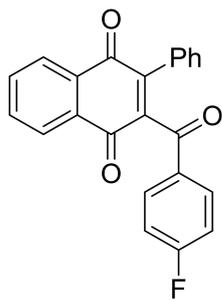


2-([1,1'-Biphenyl]-4-carbonyl)-3-phenylnaphthalene-1,4-dione (**4d**):

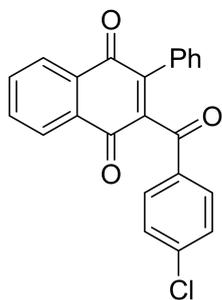
Obtained as a yellow solid (77.0 mg, 93% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.22 - 8.24 (m, 1H), 8.14 - 8.16 (m, 1H), 7.80 - 7.86 (m, 4H), 7.54 - 7.60 (t,  $J = 8.8$  Hz, 4H), 7.34 - 7.45 (m, 3H), 7.27 - 7.30 (m, 5H);  $^{13}C$  NMR (101 MHz,  $CDCl_3$ )  $\delta$  192.5, 184.2, 183.9, 146.7, 144.7, 143.9, 139.5, 134.5, 134.4, 134.3, 131.9, 131.6, 131.0, 129.8, 129.6, 129.0, 128.9, 128.4, 128.1, 127.4, 127.2, 127.1, 126.4; HRMS (ESI-TOF)  $m/z$  calcd for  $C_{29}H_{19}O_3$   $[M + H]^+$  415.1329, found 415.1328.



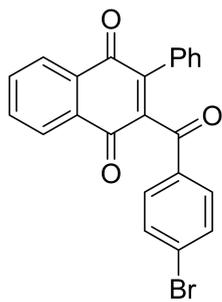
2-Phenyl-3-(4-vinylbenzoyl)naphthalene-1,4-dione (**4e**): Obtained as a yellow solid (64.1 mg, 88% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  8.22 - 8.23 (m, 1H), 8.14 - 8.15 (m, 1H), 7.80 - 7.86 (m, 2H), 7.73 - 7.75 (d,  $J = 7.6$  Hz, 2H), 7.36 - 7.38 (d,  $J = 8.0$  Hz, 2H), 7.25 - 7.28 (m, 5H), 6.64 - 6.71 (q,  $J = 10.8, 17.6$  Hz, 1H), 5.82 - 5.84 (d,  $J = 17.6$  Hz, 1H), 5.37 - 5.39 (d,  $J = 10.8$  Hz, 1H);  $^{13}C$  NMR (101 MHz,  $CDCl_3$ )  $\delta$  192.3, 184.2, 183.8, 144.6, 143.9, 143.0, 135.8, 135.0, 134.4, 134.3, 131.9, 131.7, 131.0, 129.8, 129.6, 129.5, 128.1, 127.1, 126.5, 117.4; HRMS (ESI-TOF)  $m/z$  calcd for  $C_{25}H_{17}O_3$   $[M + H]^+$  365.1172, found 365.1170.



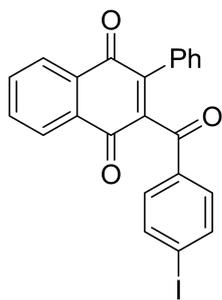
2-(4-Fluorobenzoyl)-3-phenylnaphthalene-1,4-dione (**4f**): Obtained as a yellow solid (59.1 mg, 83% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 - 8.23 (m, 1H), 8.13 - 8.15 (m, 1H), 7.78 - 7.86 (m, 4H), 7.26 - 7.39 (m, 5H), 7.00 - 7.04 (t,  $J = 8.0$  Hz, 2H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  191.3, 184.1, 183.7, 166.1 (d,  $J = 255.4$  Hz, 1C), 144.7, 143.5, 134.5, 134.3, 132.3 (d,  $J = 2.9$  Hz, 1C), 131.8 (d,  $J = 5.0$  Hz, 1C), 131.7, 131.6, 130.9, 129.72, 129.71, 128.1, 127.1, 126.4, 116.0 (d,  $J = 22.2$  Hz, 1C);  $^{19}\text{F}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  -102.8; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{14}\text{O}_3\text{F}$   $[\text{M} + \text{H}]^+$  357.0922, found 357.0920.



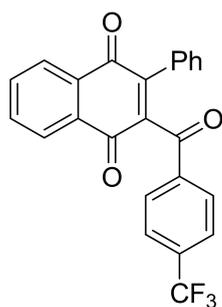
2-(4-Chlorobenzoyl)-3-phenylnaphthalene-1,4-dione (**4g**): Obtained as a yellow solid (62.5 mg, 84% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 - 8.23 (m, 1H), 8.13 - 8.15 (m, 1H), 7.81 - 7.86 (m, 2H), 7.70 - 7.72 (d,  $J = 8.4$  Hz, 2H), 7.24 - 7.34 (m, 7H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  191.8, 184.0, 183.7, 144.8, 143.3, 140.6, 134.5, 134.4, 134.1, 131.8, 131.5, 130.8, 130.3, 129.8, 129.7, 129.1, 128.1, 127.1, 126.4; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{14}\text{ClO}_3$   $[\text{M} + \text{H}]^+$  373.0626, found 373.0625.



2-(4-Bromobenzoyl)-3-phenylnaphthalene-1,4-dione (**4h**): Obtained as a yellow solid (69.9 mg, 84% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 - 8.23 (m, 1H), 8.12 - 8.14 (m, 1H), 7.80 - 7.86 (m, 2H), 7.62 - 7.64 (d,  $J = 8.4$  Hz, 2H), 7.48 - 7.50 (d,  $J = 8.4$  Hz, 2H), 7.24 - 7.30 (m, 5H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.0, 184.0, 183.7, 144.8, 143.3, 134.5, 134.5, 134.4, 132.1, 131.8, 131.5, 130.8, 130.4, 129.8, 129.7, 129.5, 128.1, 127.1, 126.4; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{14}\text{BrO}_3$   $[\text{M} + \text{H}]^+$  417.0121, found 417.0125.

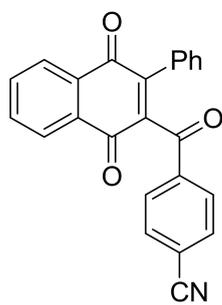


2-(4-Iodobenzoyl)-3-phenylnaphthalene-1,4-dione (**4i**): Obtained as a yellow solid (75.9 mg, 82% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.20 - 8.22 (m, 1H), 8.11 - 8.13 (m, 1H), 7.80 - 7.85 (m, 2H), 7.71 - 7.73 (d,  $J = 8.4$  Hz, 2H), 7.46 - 7.48 (d,  $J = 8.8$  Hz, 2H), 7.23 - 7.30 (m, 5H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.3, 184.0, 183.7, 144.8, 143.2, 138.1, 135.0, 134.5, 134.3, 131.8, 131.5, 130.7, 130.2, 129.8, 129.7, 128.1, 127.1, 126.4, 102.6; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{14}\text{IO}_3$   $[\text{M} + \text{H}]^+$  464.9982, found 464.9987.



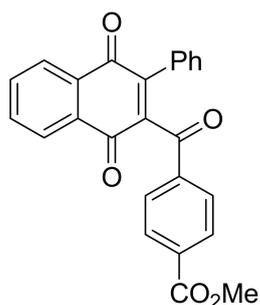
**4j**: 2-Phenyl-3-(4-(trifluoromethyl)benzoyl)naphthalene-1,4-dione (**4j**):

Obtained as a yellow solid (63.3 mg, 78% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.22 - 8.24 (m, 1H), 8.13 - 8.15 (m, 1H), 7.82 - 7.89 (m, 4H), 7.61 - 7.63 (d,  $J = 8.0$  Hz, 2H), 7.24 - 7.30 (m, 5H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.1, 183.9, 183.7, 145.1, 143.1, 138.3, 134.9 (q,  $J = 32.4, 65.1$  Hz, 1C), 134.6, 134.4, 131.8, 131.5, 130.6, 129.9, 129.7, 129.2, 128.2, 127.2, 126.5, 125.8 (q,  $J = 3.7, 7.4$  Hz, 1C), 123.3 (q,  $J = 271.3$  Hz, 1C);  $^{19}\text{F}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  -63.3; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{24}\text{H}_{14}\text{O}_3\text{F}_3$  [ $\text{M} + \text{H}$ ] $^+$  407.0890, found 407.0893.



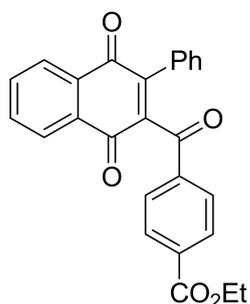
**4k**: 4-(1,4-Dioxo-3-phenyl-1,4-dihydronaphthalene-2-carbonyl)benzonitrile (**4k**):

Obtained as a yellow solid (53.0 mg, 73% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.22 - 8.24 (m, 1H), 8.13 - 8.15 (m, 1H), 7.83 - 7.88 (m, 4H), 7.63 - 7.65 (t,  $J = 8.0$  Hz, 2H), 7.26 - 7.33 (m, 3H), 7.21 - 7.23 (d,  $J = 6.8$  Hz, 2H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  191.8, 183.7, 183.6, 145.3, 142.7, 138.5, 134.7, 134.5, 132.5, 131.8, 131.5, 130.5, 130.0, 129.7, 129.2, 128.2, 127.2, 126.5, 117.6, 117.0; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{24}\text{H}_{14}\text{O}_3$  [ $\text{M} + \text{H}$ ] $^+$  364.0968, found 364.0971.



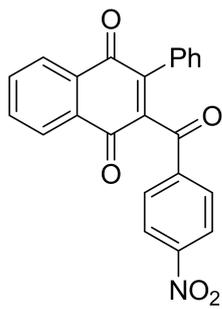
Methyl

4-(1,4-dioxo-3-phenyl-1,4-dihydronaphthalene-2-carbonyl)benzoate (**4l**): Obtained as a yellow solid (60.2 mg, 76% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.20 - 8.22 (m, 1H), 8.13 - 8.14 (m, 1H), 7.92 - 7.94 (d,  $J = 8.0$  Hz, 2H), 7.80 - 7.86 (m, 2H), 7.76 - 7.78 (d,  $J = 8.0$  Hz, 2H), 7.49 - 7.52 (t,  $J = 7.2$  Hz, 1H), 7.33 - 7.38 (m, 4H), 3.86 (s, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.5, 183.7, 183.5, 166.3, 144.4, 143.7, 135.5, 135.4, 134.6, 134.4, 134.3, 131.7, 131.5, 130.9, 129.8, 129.1, 129.0, 128.8, 127.1, 126.5, 52.2; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{25}\text{H}_{17}\text{O}_5$   $[\text{M} + \text{H}]^+$  397.1071, found 397.1074.

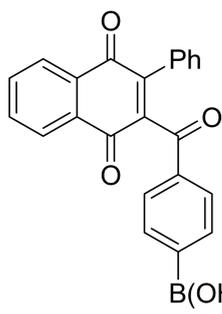


Ethyl

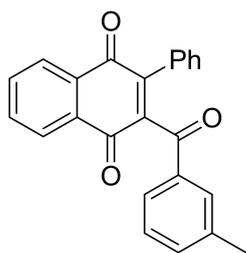
4-(1,4-dioxo-3-phenyl-1,4-dihydronaphthalene-2-carbonyl)benzoate (**4m**): Obtained as a yellow solid (63.1 mg, 77% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.15 - 8.17 (m, 1H), 8.07 - 8.09 (m, 1H), 7.93 - 7.95 (d,  $J = 8.0$  Hz, 2H), 7.74 - 7.80 (m, 4H), 7.17 - 7.20 (m, 5H), 4.27 - 4.32 (q,  $J = 6.8, 14.0$  Hz, 2H), 1.29 - 1.32 (t,  $J = 7.2$  Hz, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.6, 184.0, 183.7, 165.4, 144.9, 143.4, 138.7, 134.9, 134.6, 134.4, 131.9, 131.6, 130.7, 129.8, 129.8, 128.8, 128.1, 127.1, 126.5, 61.5, 14.2; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{26}\text{H}_{19}\text{O}_5$   $[\text{M} + \text{H}]^+$  411.1227, found 411.1225.



2-(4-Nitrobenzoyl)-3-phenylnaphthalene-1,4-dione (**4n**): Obtained as a yellow solid (54.4 mg, 71% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.22 - 8.24 (m, 1H), 8.17 - 8.19 (d,  $J = 8.4$  Hz, 2H), 8.13 - 8.15 (m, 1H), 7.90 - 7.92 (d,  $J = 8.4$  Hz, 2H), 7.83 - 7.88 (m, 2H), 7.23 - 7.29 (m, 5H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  191.6, 183.7, 183.5, 150.5, 145.3, 142.6, 139.9, 134.7, 134.5, 131.8, 131.5, 130.5, 130.1, 129.8, 129.8, 128.3, 127.2, 126.5, 123.9; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{14}\text{NO}_5$   $[\text{M} + \text{H}]^+$  384.0867, found 384.0868.

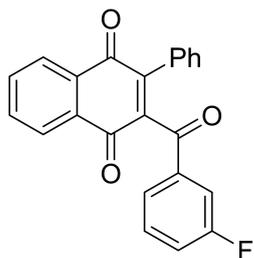


4-(1,4-Dioxo-3-phenyl-1,4-dihydronaphthalene-2-carbonyl)phenylboronic acid (**4o**): Obtained as a yellow solid (66.5 mg, 87% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 - 8.23 (m, 1H), 8.13 - 8.15 (m, 1H), 7.82 - 7.86 (m, 2H), 7.77 - 7.79 (d,  $J = 8.0$  Hz, 2H), 7.47 - 7.51 (t,  $J = 7.2$  Hz, 1H), 7.34 - 7.37 (t,  $J = 7.6$  Hz, 2H), 7.25 - 7.27 (m, 4H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  193.0, 184.2, 183.8, 144.7, 143.9, 135.8, 134.4, 134.3, 134.0, 131.9, 131.6, 131.0, 129.8, 129.6, 129.0, 128.7, 128.0, 127.1, 126.4; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{16}\text{BO}_5$   $[\text{M} + \text{H}]^+$  383.1085, found 383.1086.



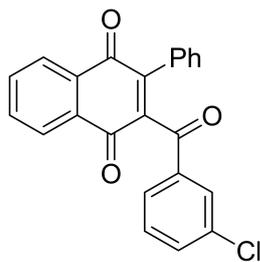
2-(3-Methylbenzoyl)-3-phenylnaphthalene-1,4-dione (**4p**):

Obtained as a yellow solid (66.2 mg, 94% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 - 8.22 (m, 1H), 8.12 - 8.14 (m, 1H), 7.79 - 7.85 (m, 2H), 7.60 (s, 1H), 7.55 - 7.57 (d,  $J = 7.6$  Hz, 1H), 7.21 - 7.31 (m, 7H), 2.31 (s, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  193.1, 184.2, 183.8, 144.5, 144.0, 138.5, 135.7, 134.9, 134.4, 134.2, 131.8, 131.6, 131.0, 129.7, 129.5, 129.3, 128.5, 128.0, 127.0, 126.5, 126.4, 21.2; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{24}\text{H}_{17}\text{O}_3$   $[\text{M} + \text{H}]^+$  353.1172, found 353.1174.



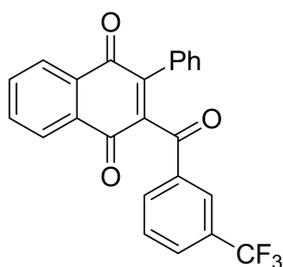
2-(3-Fluorobenzoyl)-3-phenylnaphthalene-1,4-dione (**4q**):

Obtained as a yellow solid (56.2 mg, 79% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 - 8.23 (m, 1H), 8.13 - 8.15 (m, 1H), 7.81 - 7.86 (m, 2H), 7.51 - 7.53 (d,  $J = 7.6$  Hz, 1H), 7.45 - 7.47 (d,  $J = 9.2$  Hz, 1H), 7.26 - 7.35 (m, 6H), 7.17 - 7.21 (t,  $J = 8.4$  Hz, 1H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  191.8, 184.0, 183.6, 162.7 (d,  $J = 247.4$  Hz, 1C), 144.9, 143.3, 137.7 (d,  $J = 6.4$  Hz, 1C), 134.5, 134.4, 131.8, 131.5, 130.7, 130.4 (d,  $J = 7.7$  Hz, 1C), 129.8, 129.7, 128.1, 127.1, 126.4, 125.0 (d,  $J = 2.9$  Hz, 1C), 121.2 (d,  $J = 21.5$  Hz, 1C), 115.3 (d,  $J = 22.5$  Hz, 1C);  $^{19}\text{F}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  -110.3; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{14}\text{O}_3\text{F}$   $[\text{M} + \text{H}]^+$  357.0922, found 357.0925.



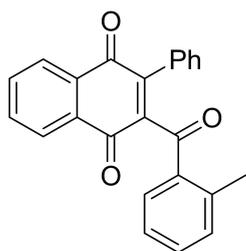
2-(3-Chlorobenzoyl)-3-phenylnaphthalene-1,4-dione (**4r**):

Obtained as a yellow solid (60.3 mg, 81% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 - 8.23 (m, 1H), 8.13 - 8.15 (m, 1H), 7.81 - 7.86 (m, 2H), 7.74 (s, 1H), 7.62 - 7.64 (d,  $J = 7.6$  Hz, 1H), 7.44 - 7.46 (d,  $J = 8.0$  Hz, 1H), 7.24 - 7.32 (m, 6H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  191.7, 184.0, 183.6, 144.9, 143.1, 137.2, 135.0, 134.5, 134.4, 133.9, 131.8, 131.5, 130.7, 130.0, 129.8, 129.7, 128.7, 128.1, 127.2, 127.1, 126.5; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{14}\text{ClO}_3$   $[\text{M} + \text{H}]^+$  373.0626, found 373.0628.



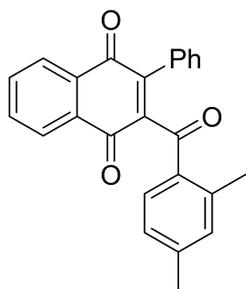
2-Phenyl-3-(3-(trifluoromethyl)benzoyl)naphthalene-1,4-dione

(**4s**): Obtained as a yellow solid (56.8 mg, 70% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.22 - 8.24 (m, 1H), 8.14 - 8.16 (m, 1H), 7.99 (s, 1H), 7.92 - 7.94 (d,  $J = 7.6$  Hz, 1H), 7.82 - 7.87 (m, 2H), 7.71 - 7.73 (d,  $J = 7.6$  Hz, 1H), 7.47 - 7.50 (t,  $J = 8.0$  Hz, 1H), 7.24 - 7.28 (m, 5H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  191.7, 183.9, 183.6, 145.1, 142.8, 136.1, 134.6, 134.4, 132.0, 131.5 (q,  $J = 26.0, 36.0$  Hz, 1C), 130.7, 130.3 (q,  $J = 3.8, 7.3$  Hz, 1C), 129.9, 129.7, 129.4, 128.7 (d,  $J = 168.4$  Hz, 1C), 128.2, 127.2, 126.5, 125.7 (q,  $J = 3.5, 7.2$  Hz, 1C), 123.4 (q,  $J = 160.2, 271.2$  Hz, 1C);  $^{19}\text{F}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  -62.9; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{24}\text{H}_{14}\text{O}_3\text{F}_3$   $[\text{M} + \text{H}]^+$  407.0890, found 407.0893.



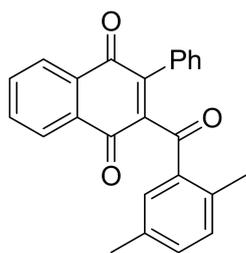
2-(2-Methylbenzoyl)-3-phenylnaphthalene-1,4-dione (**4t**):

Obtained as a yellow solid (59.1 mg, 84% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.11 - 8.14 (m, 1H), 8.06 - 8.08 (m, 1H), 7.72 - 7.77 (m, 2H), 7.41 - 7.43 (d,  $J = 7.6$  Hz, 1H), 7.13 - 7.24 (m, 6H), 7.02 - 7.07 (m, 2H), 2.40 (s, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  194.5, 184.5, 184.0, 145.1, 143.9, 140.4, 135.1, 134.4, 134.2, 132.7, 132.1, 131.8, 131.6, 131.4, 131.1, 129.5, 129.4, 127.9, 127.0, 126.4, 125.6, 21.5; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{24}\text{H}_{17}\text{O}_3$  [ $\text{M} + \text{H}$ ] $^+$  353.1172, found 353.1170.



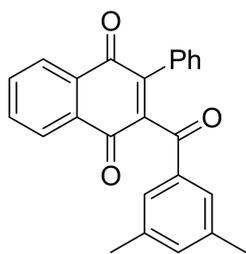
2-(2,4-Dimethylbenzoyl)-3-phenylnaphthalene-1,4-dione (**4u**):

Obtained as a yellow solid (65.9 mg, 90% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.19 - 8.21 (m, 1H), 8.13 - 8.15 (m, 1H), 7.79 - 7.84 (m, 2H), 7.40 - 7.42 (d,  $J = 8.0$  Hz, 1H), 7.23 - 7.28 (m, 5H), 6.96 (s, 1H), 6.90 - 6.92 (d,  $J = 7.6$  Hz, 1H), 2.46 (s, 3H), 2.27 (s, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  194.0, 184.6, 184.1, 145.2, 143.7, 143.7, 140.6, 134.3, 134.2, 133.1, 132.4, 132.0, 131.9, 131.6, 131.2, 129.6, 129.3, 127.9, 126.9, 126.4, 126.3, 21.6, 21.5; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{25}\text{H}_{19}\text{O}_3$  [ $\text{M} + \text{H}$ ] $^+$  367.1329, found 367.1327.



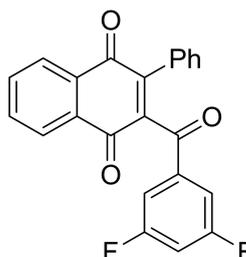
2-(2,5-Dimethylbenzoyl)-3-phenylnaphthalene-1,4-dione (**4v**):

Obtained as a yellow solid (63.7 mg, 87% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 - 8.22 (m, 1H), 8.15 - 8.17 (m, 1H), 7.82 - 7.84 (m, 2H), 7.26 - 7.28 (m, 4H), 7.20 - 7.22 (m, 2H), 7.10 - 7.12 (d,  $J = 7.6$  Hz, 1H), 7.01 - 7.03 (d,  $J = 7.6$  Hz, 1H), 2.41 (s, 3H), 2.22 (s, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  194.6, 184.6, 184.1, 145.2, 143.8, 137.3, 135.1, 135.0, 134.3, 134.2, 133.6, 132.0, 131.9, 131.8, 131.7, 131.2, 129.5, 129.4, 127.9, 127.0, 126.5, 21.0, 20.8.; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{25}\text{H}_{19}\text{O}_3$   $[\text{M} + \text{H}]^+$  367.1329, found 367.1327.



2-(3,5-Dimethylbenzoyl)-3-phenylnaphthalene-1,4-dione (**4w**):

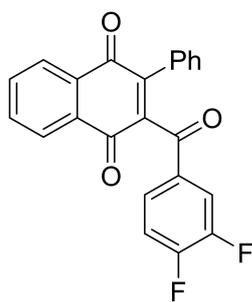
Obtained as a yellow solid (70.3 mg, 96% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.22 - 8.23 (m, 1H), 8.13 - 8.15 (m, 1H), 7.79 - 7.85 (m, 2H), 7.38 (s, 2H), 7.25 - 7.29 (m, 5H), 7.12 (s, 1H), 2.27 (s, 6H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  193.3, 184.3, 183.9, 144.4, 144.1, 138.4, 135.89, 135.85, 134.3, 134.2, 131.9, 131.7, 131.1, 129.7, 129.5, 128.0, 127.0, 126.8, 126.4, 21.1; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{25}\text{H}_{19}\text{O}_3$   $[\text{M} + \text{H}]^+$  367.1329, found 367.1328.



2-(3,5-Difluorobenzoyl)-3-phenylnaphthalene-1,4-dione (**4x**):

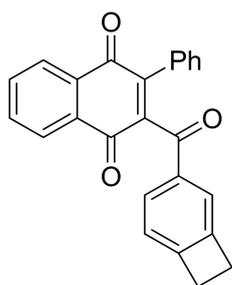
Obtained as a yellow solid (53.1 mg, 71% yield), eluting with 20% EtOAc in PE

(elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 - 8.23 (m, 1H), 8.13 - 8.15 (m, 1H), 7.82 - 7.87 (m, 2H), 7.25 - 7.32 (m, 7H), 6.91 - 6.95 (m, 1H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  190.6, 183.8, 183.5, 163.0 (d,  $J = 250.4$  Hz, 1C), 162.8 (d,  $J = 250.4$  Hz, 1C), 145.2, 142.6, 138.5 (t,  $J = 7.8$  Hz, 1C), 134.7, 134.4, 131.8, 131.5, 130.6, 130.0, 129.7, 128.2, 127.2, 126.5, 111.9 (d,  $J = 7.4$  Hz, 1C), 111.7 (d,  $J = 7.5$  Hz, 1C), 109.3 (t,  $J = 25.4$  Hz, 1C);  $^{19}\text{F}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  -107.4; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{13}\text{O}_3\text{F}_2$   $[\text{M} + \text{H}]^+$  375.0827, found 375.0828.



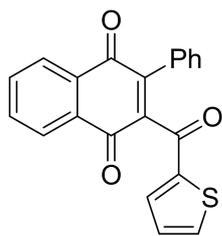
2-(3,4-Difluorobenzoyl)-3-phenylnaphthalene-1,4-dione (**4y**):

Obtained as a yellow solid (53.1 mg, 71% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.21 - 8.23 (m, 1H), 8.13 - 8.15 (m, 1H), 7.81 - 7.87 (m, 2H), 7.60 - 7.64 (t,  $J = 9.6$  Hz, 1H), 7.52 - 7.53 (m, 1H), 7.23 - 7.31 (m, 5H), 7.09 - 7.16 (q,  $J = 8.4, 16.8$  Hz, 1H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  190.5, 183.8, 183.6, 154.1 (dd,  $J = 12.9, 257.5$  Hz, 1C), 150.4 (dd,  $J = 13.0, 250.6$  Hz, 1C), 145.0, 142.8, 134.6, 134.4, 132.8 (t,  $J = 3.9$  Hz, 1C), 131.8, 131.5, 130.7, 129.9, 129.7, 128.2, 127.1, 126.5, 126.3 (dd,  $J = 3.5, 7.7$  Hz, 1C), 117.9 (dd,  $J = 1.6, 18.0$  Hz, 1C), 117.7 (d,  $J = 18.0$  Hz, 1C);  $^{19}\text{F}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  -127.3 (d,  $J = 22.0$  Hz, 1F), -135.3 (d,  $J = 22.1$  Hz, 1F); HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{23}\text{H}_{13}\text{O}_3\text{F}_2$   $[\text{M} + \text{H}]^+$  375.0827, found 375.0826.



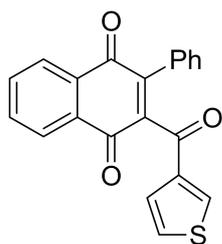
2-(Bicyclo[4.2.0]octa-1,3,5-triene-3-carbonyl)-3-phenylnaphthalene-1,4-dione (**4z**): Obtained as a yellow solid (64.1 mg, 88% yield), eluting with 20%

EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.20 - 8.22 (m, 1H), 8.12 - 8.14 (m, 1H), 7.79 - 7.84 (m, 2H), 7.66 - 7.68 (d,  $J = 7.6$  Hz, 1H), 7.49 (s, 1H), 7.27 - 7.31 (m, 5H), 7.02 - 7.04 (d,  $J = 7.6$  Hz, 1H), 3.14 (s, 4H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  193.1, 184.3, 183.9, 153.5, 146.3, 144.4, 135.0, 134.3, 134.2, 131.9, 131.6, 131.1, 129.7, 129.5, 129.0, 128.0, 127.0, 126.4, 122.9, 122.7, 30.0, 29.3; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{25}\text{H}_{17}\text{O}_3$   $[\text{M} + \text{H}]^+$  365.1172, found 365.1173.



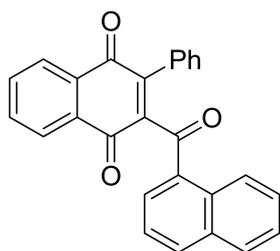
2-Phenyl-3-(thiophene-2-carbonyl)naphthalene-1,4-dione (**4aa**):

Obtained as a yellow solid (59.9 mg, 87% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.20 - 8.22 (m, 1H), 8.14 - 8.16 (m, 1H), 7.82 - 7.84 (m, 2H), 7.59 - 7.61 (d,  $J = 4.8$  Hz, 1H), 7.45 - 7.47 (d,  $J = 3.6$  Hz, 1H), 7.29 - 7.34 (m, 5H), 6.97 - 6.99 (m, 1H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  184.5, 184.2, 183.2, 144.5, 143.2, 142.9, 135.6, 134.5, 134.4, 134.3, 131.8, 131.6, 130.9, 129.9, 129.7, 128.2, 128.1, 127.0, 126.5; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{21}\text{H}_{13}\text{O}_3\text{S}$   $[\text{M} + \text{H}]^+$  345.0580, found 345.0578.



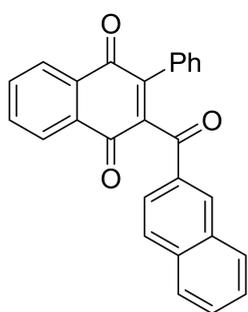
2-Phenyl-3-(thiophene-3-carbonyl)naphthalene-1,4-dione (**4ab**):

Obtained as a yellow solid (61.2 mg, 89% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.20 - 8.22 (m, 1H), 8.14 - 8.16 (m, 1H), 7.80 - 7.86 (m, 3H), 7.39 - 7.41 (d,  $J = 5.2$  Hz, 1H), 7.28 - 7.32 (m, 5H), 7.20 - 7.22 (m, 1H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  186.2, 184.3, 183.5, 144.1, 143.9, 141.2, 134.8, 134.4, 134.3, 131.8, 131.6, 131.0, 129.8, 129.7, 128.1, 127.0, 126.8, 126.7, 126.4; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{21}\text{H}_{13}\text{O}_3\text{S}$   $[\text{M} + \text{H}]^+$  345.0580, found 345.0581.



2-(1-Naphthoyl)-3-phenylnaphthalene-1,4-dione (**4ac**):

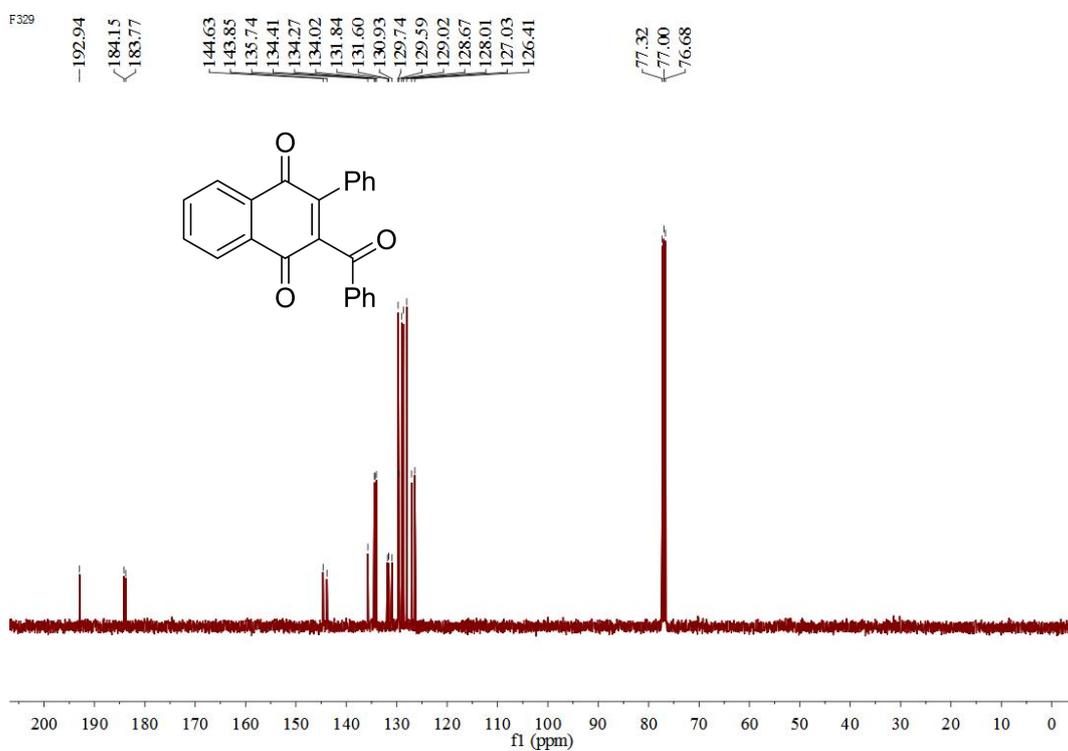
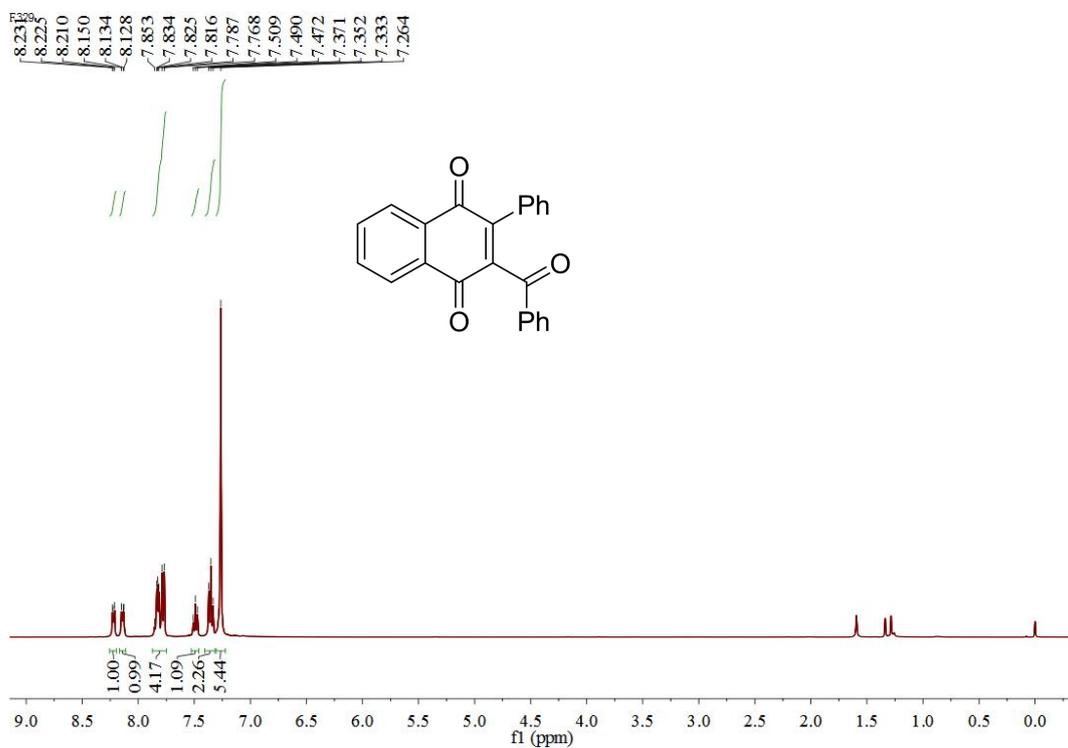
Obtained as a yellow solid (63.6 mg, 82% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.98 - 9.00 (d,  $J = 8.8$  Hz, 1H), 8.21 - 8.23 (m, 1H), 8.14 - 8.16 (m, 1H), 7.92 - 7.94 (d,  $J = 8.4$  Hz, 1H), 7.79 - 7.85 (m, 4H), 7.59 - 7.63 (t,  $J = 7.6$  Hz, 1H), 7.50 - 7.53 (t,  $J = 7.6$  Hz, 1H), 7.32 - 7.36 (t,  $J = 7.6$  Hz, 1H), 7.27 - 7.29 (d,  $J = 7.2$  Hz, 2H), 7.13 - 7.19 (m, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  194.5, 184.5, 184.1, 145.0, 144.1, 134.9, 134.4, 134.3, 133.8, 132.4, 131.9, 131.7, 131.1, 130.4, 129.6, 129.3, 128.8, 128.3, 128.0, 127.0, 126.7, 126.5, 125.9, 124.1; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{27}\text{H}_{17}\text{O}_3$   $[\text{M} + \text{H}]^+$  389.1172, found 389.1173.



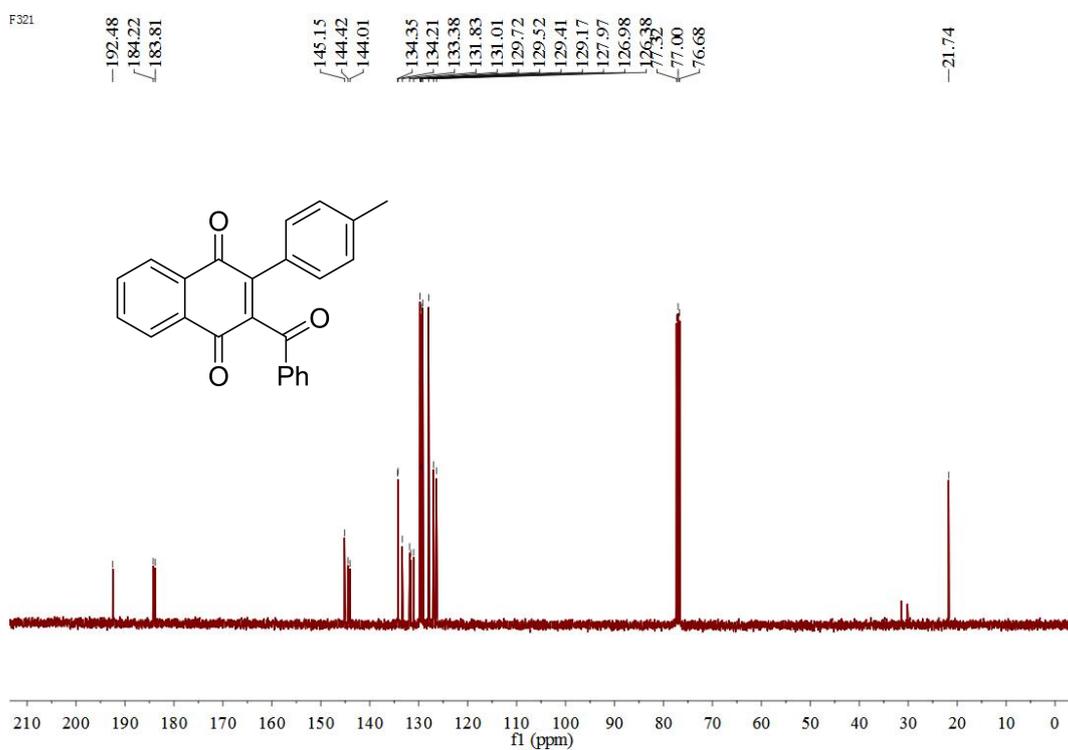
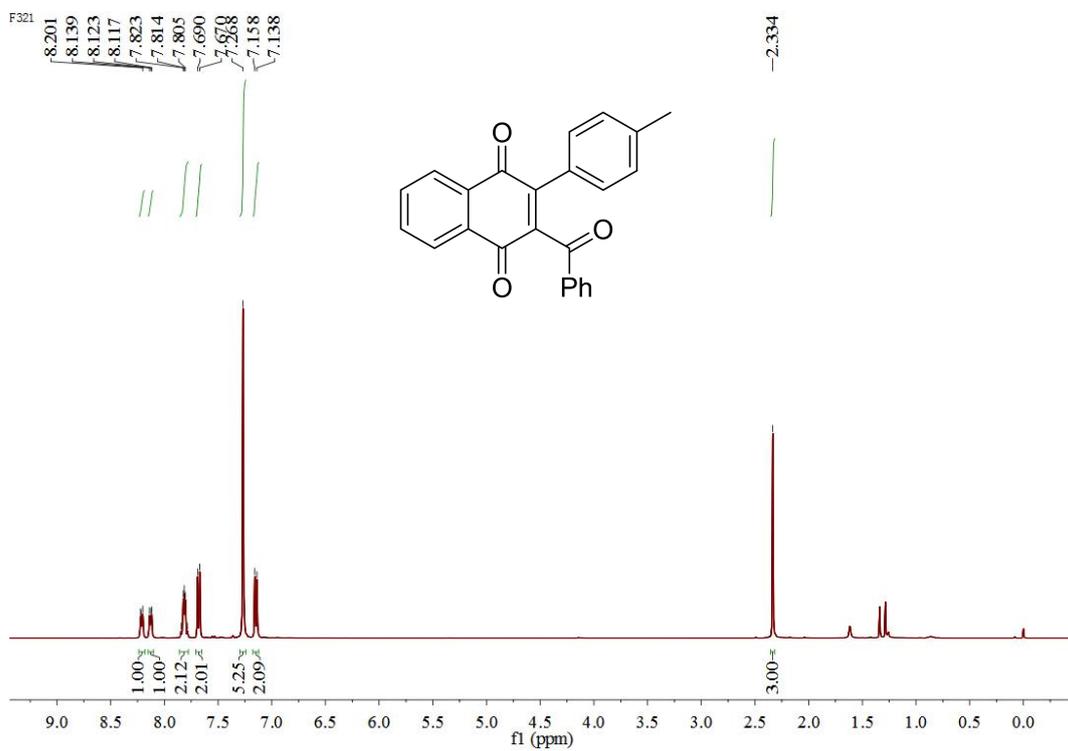
2-(2-Naphthoyl)-3-phenylnaphthalene-1,4-dione (**4ad**): Obtained as a yellow solid (69.8 mg, 90% yield), eluting with 20% EtOAc in PE (elution gradient);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.15 - 8.16 (m, 2H), 8.05 - 8.07 (m, 1H), 7.70 - 7.81 (m, 6H), 7.46 - 7.49 (t,  $J = 7.2$  Hz, 1H), 7.38 - 7.42 (t,  $J = 7.6$  Hz, 1H), 7.21 - 7.43 (m, 2H), 7.13 - 7.16 (m, 3H);  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  192.9, 184.2, 183.9, 144.7, 143.9, 135.9, 134.4, 134.3, 133.2, 132.3, 131.9, 131.8, 131.6, 131.0, 129.7, 129.6, 129.0, 128.8, 128.0, 127.8, 127.0, 126.9, 126.4, 123.7; HRMS (ESI-TOF)  $m/z$  calcd for  $\text{C}_{27}\text{H}_{17}\text{O}_3$   $[\text{M} + \text{H}]^+$  389.1172, found 389.1170.

# Copies of $^1\text{H}$ and $^{13}\text{C}$ NMR spectra of products

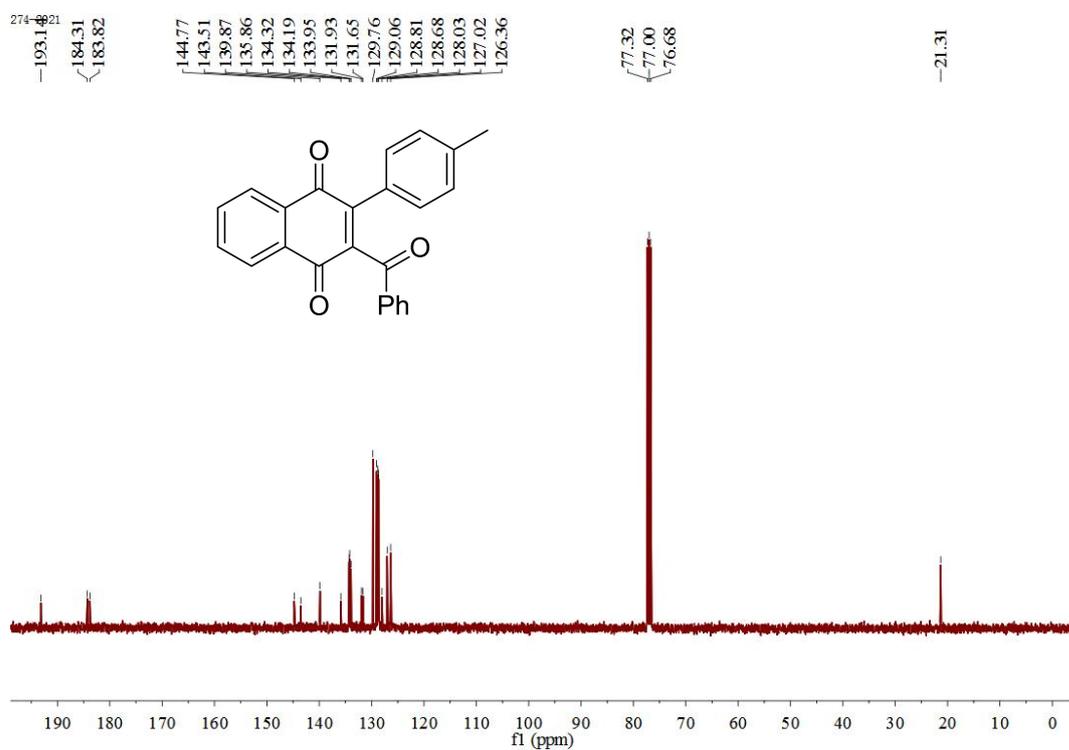
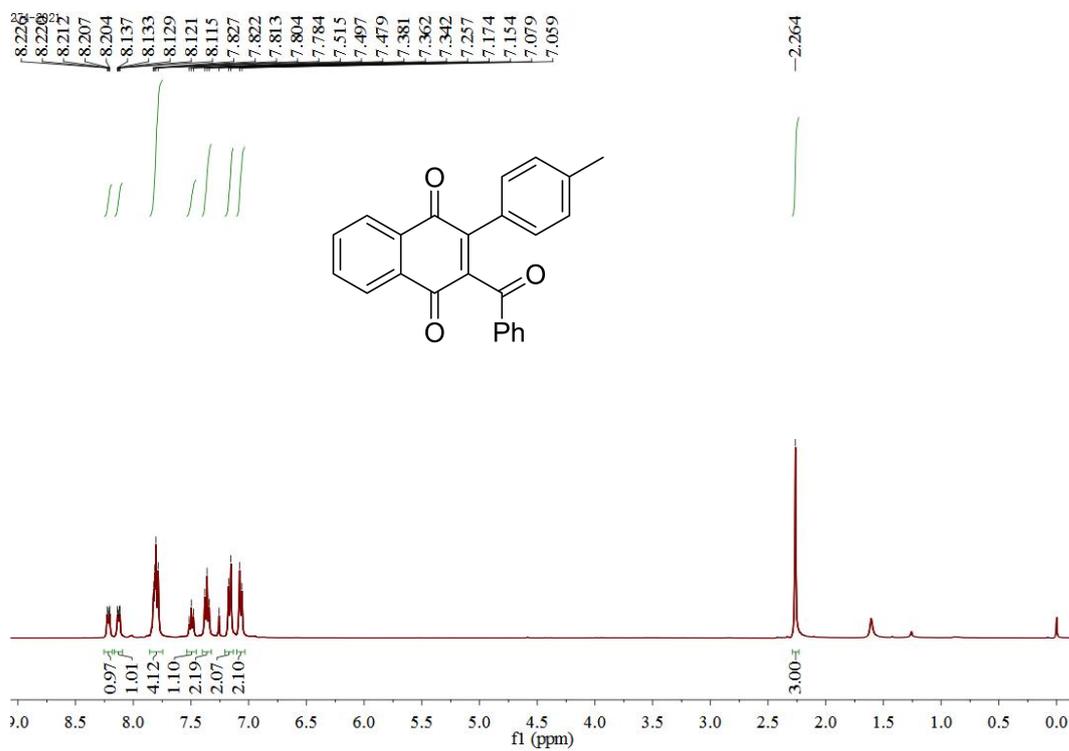
## $^1\text{H}$ NMR and $^{13}\text{C}$ NMR of 3a



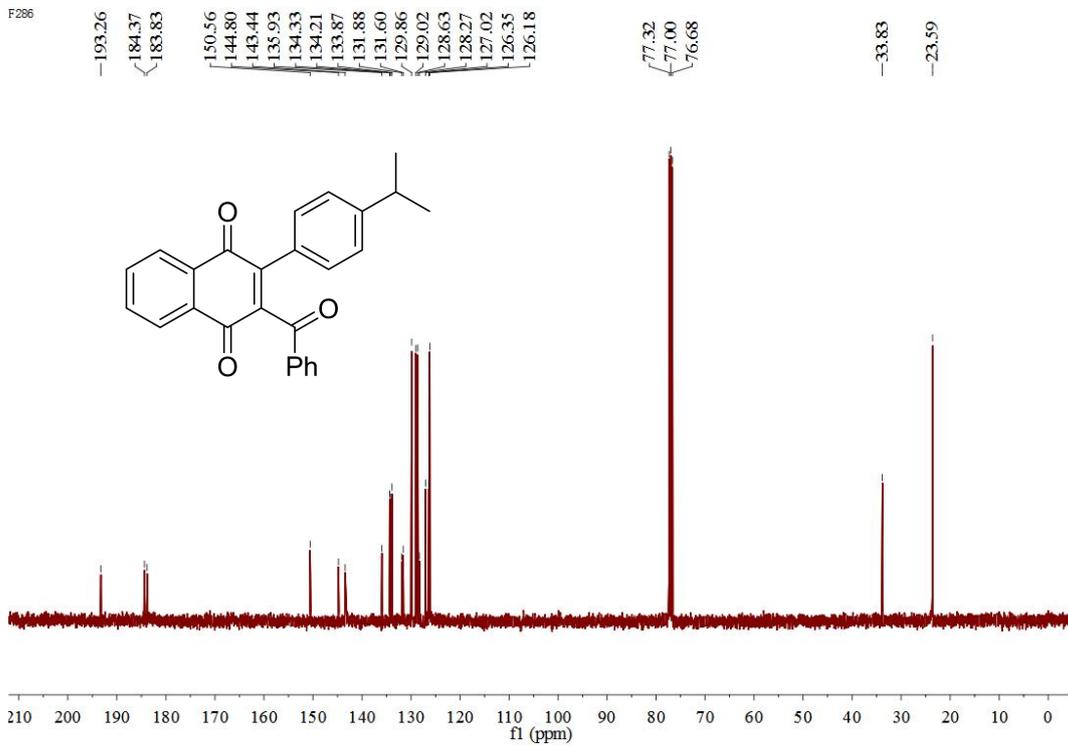
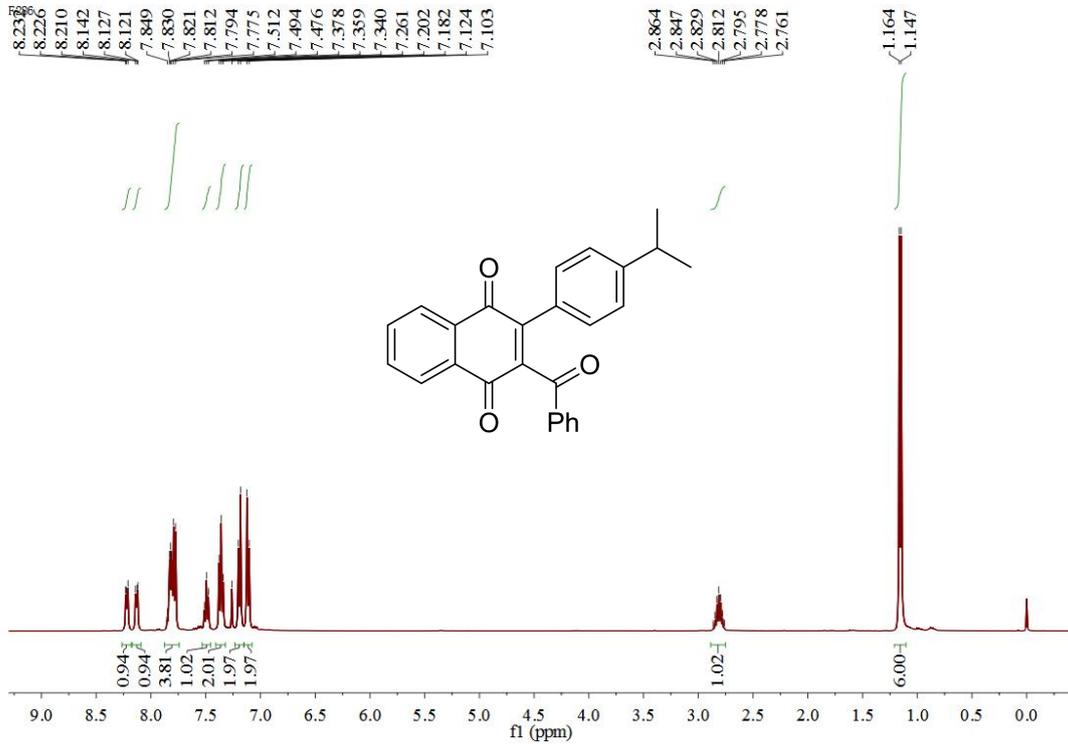
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 3b



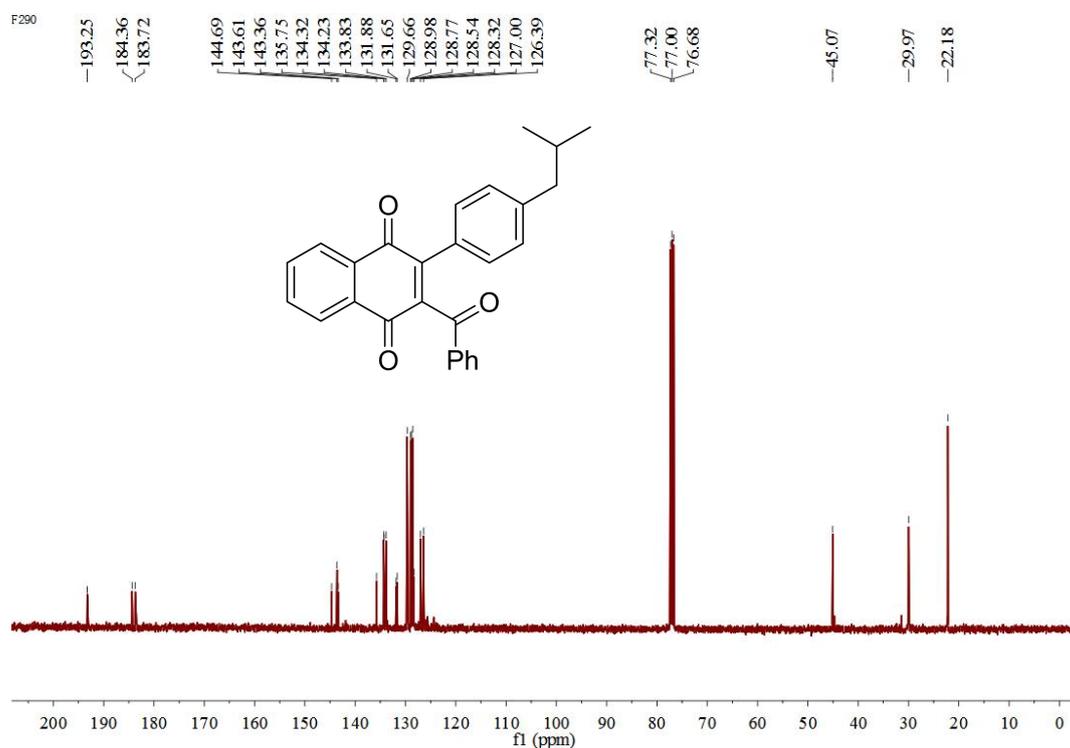
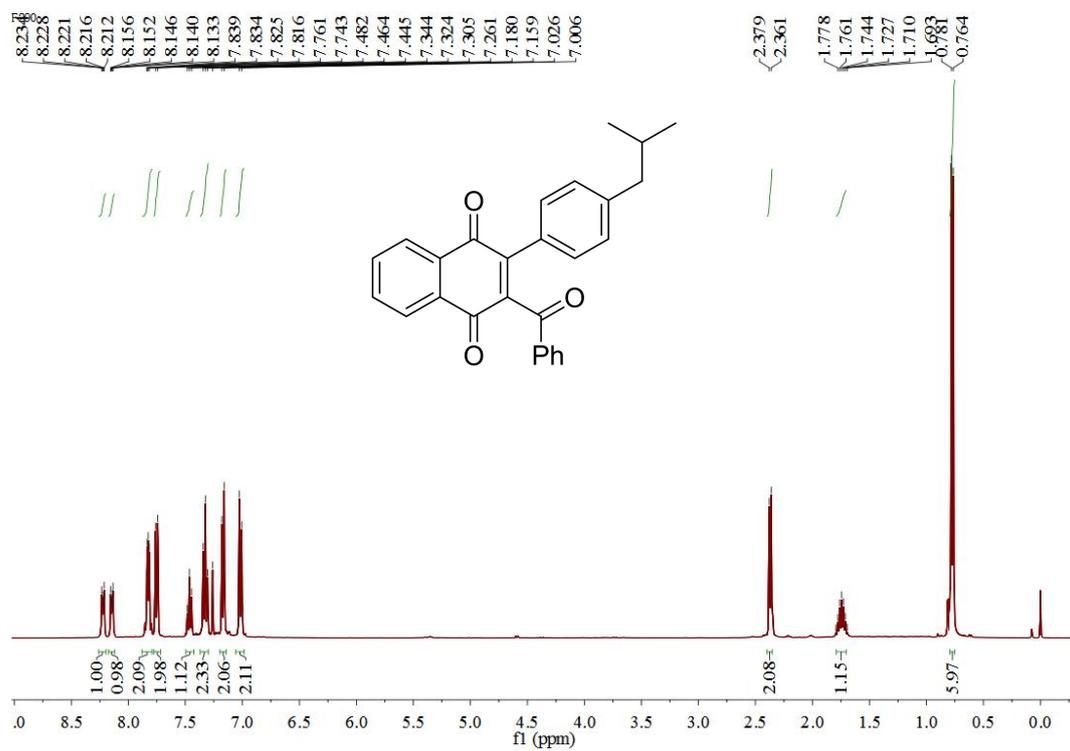
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 3b



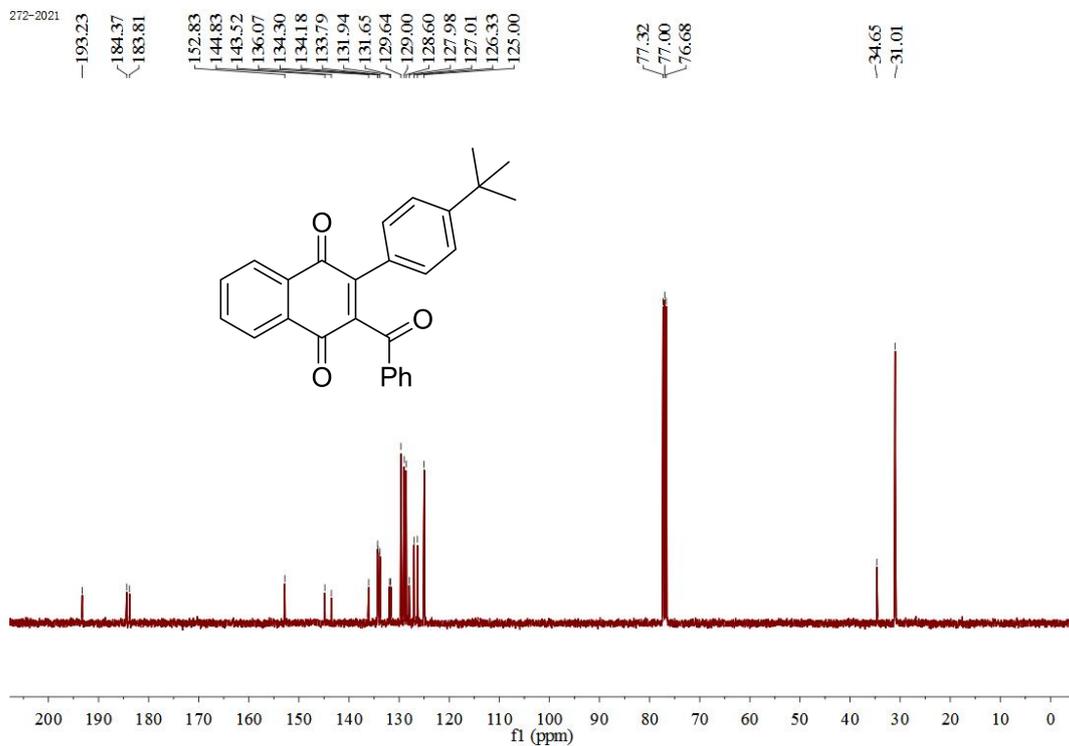
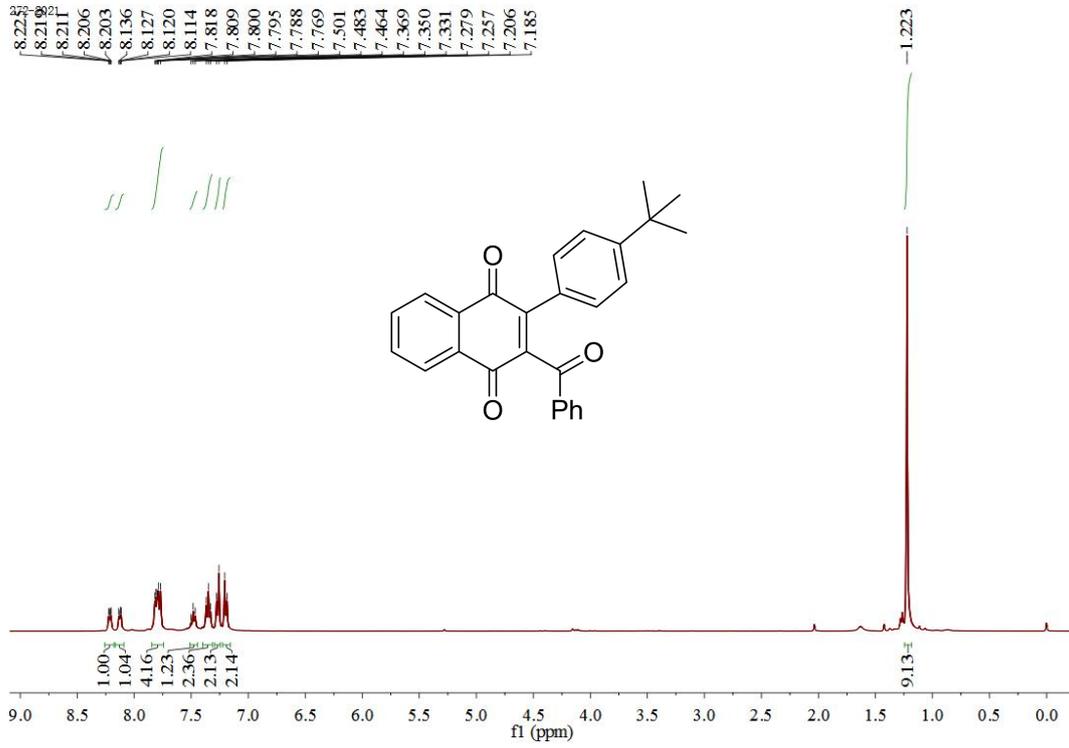
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 3c



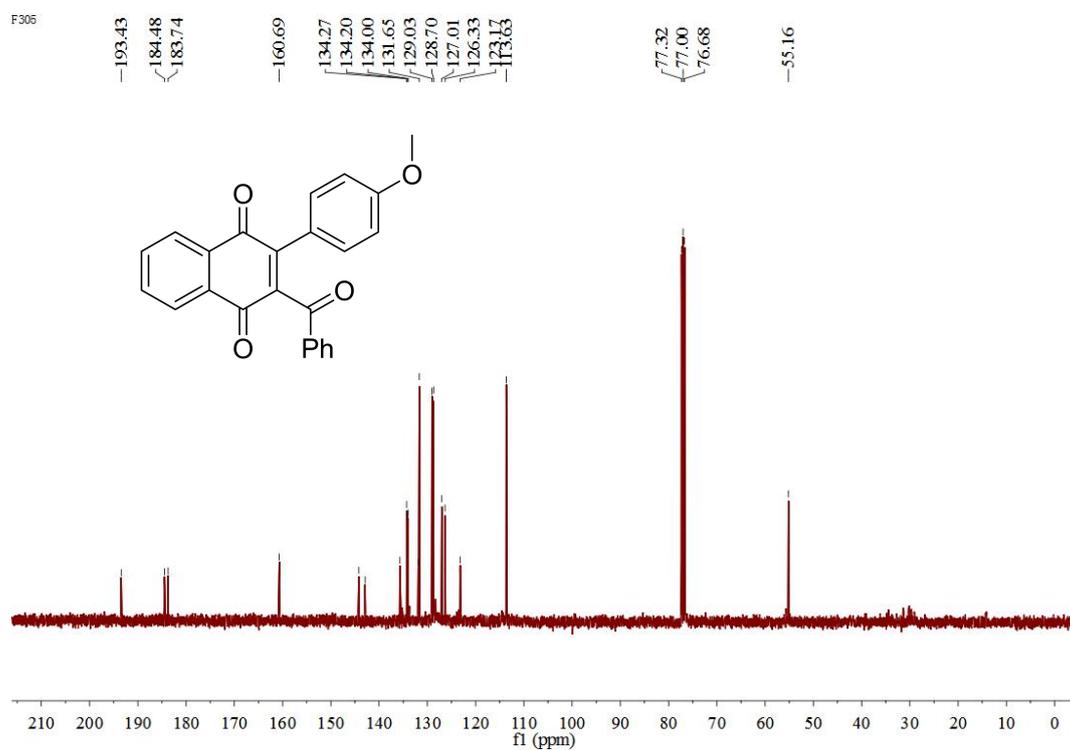
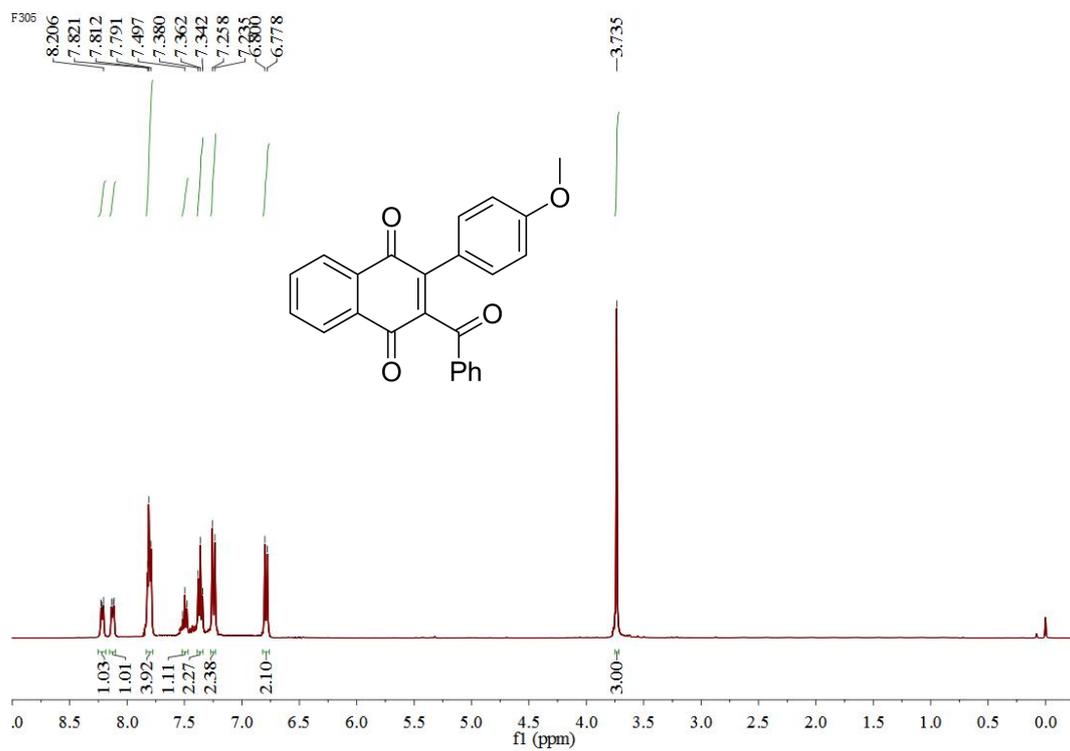
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 3d



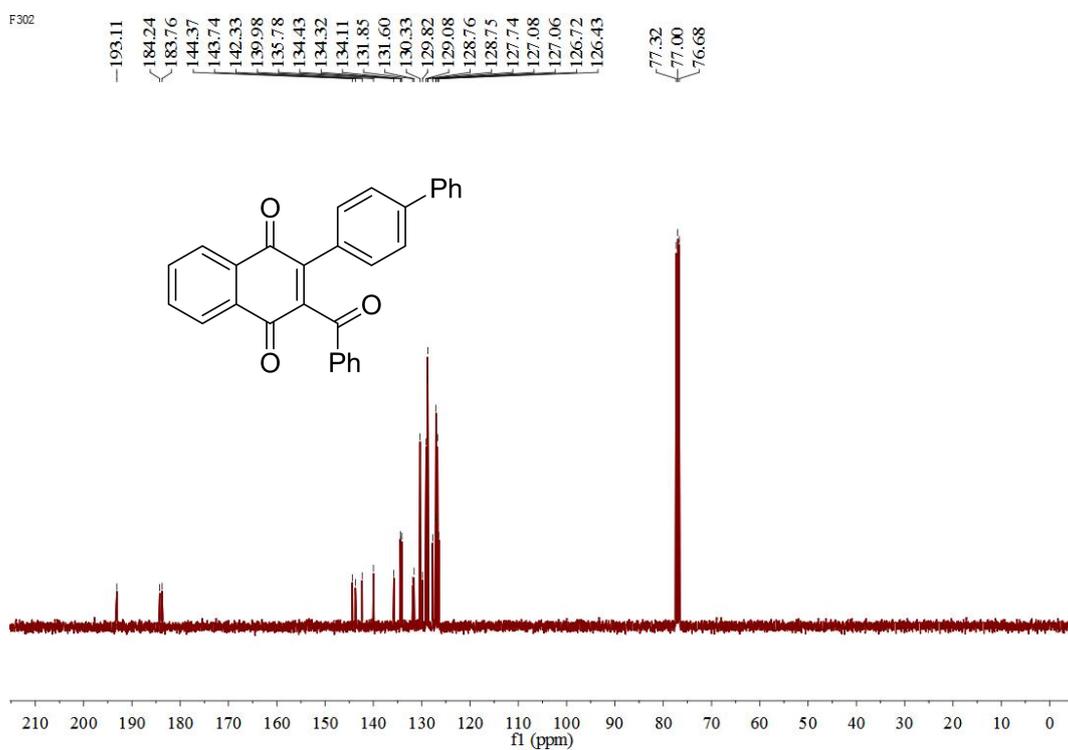
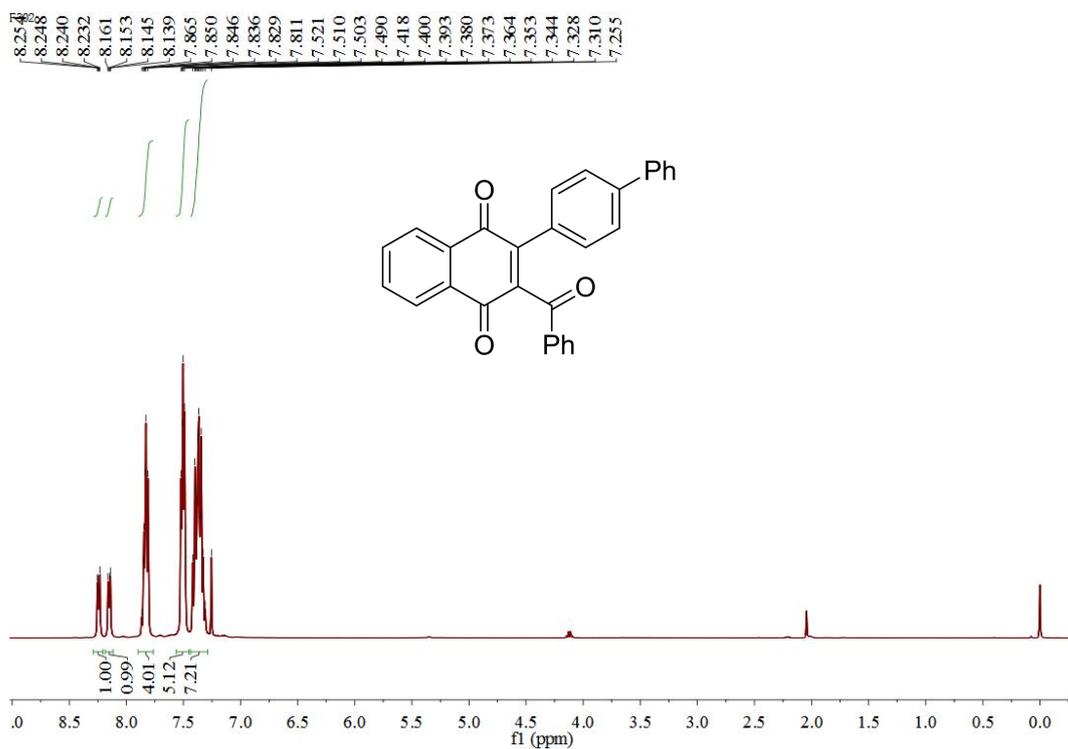
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 3e



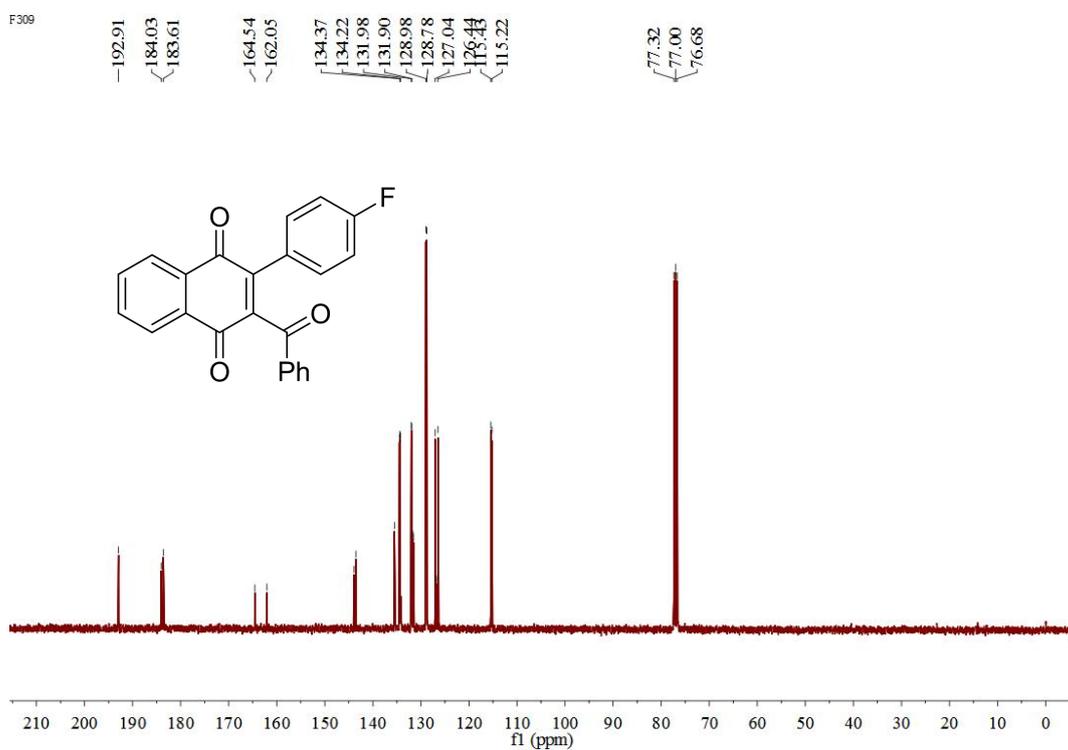
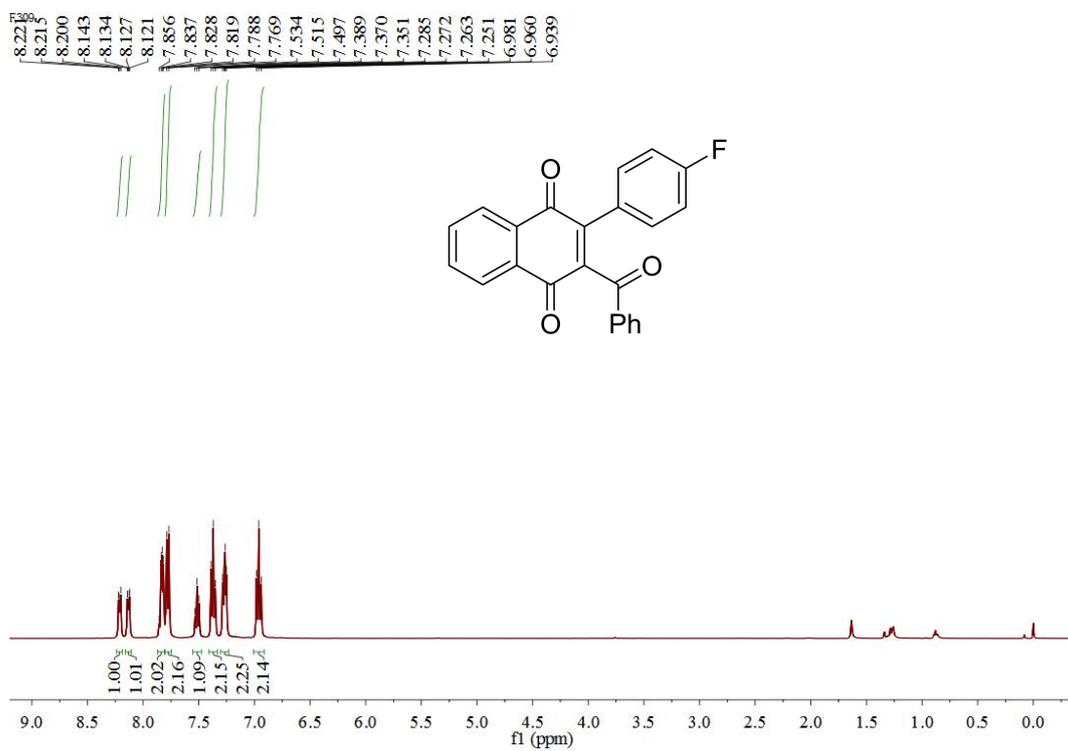
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 3f



# <sup>1</sup>H NMR, <sup>13</sup>C NMR and <sup>19</sup>F NMR of 3g

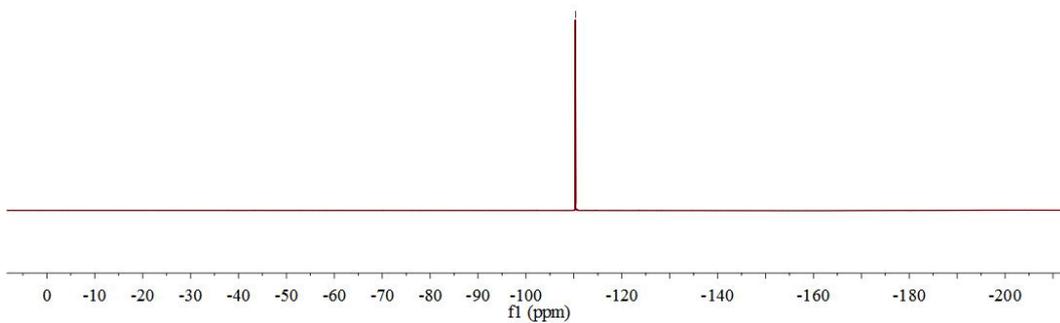
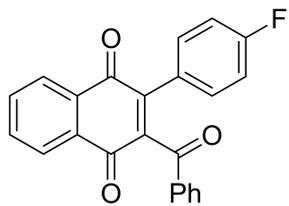


# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 3h

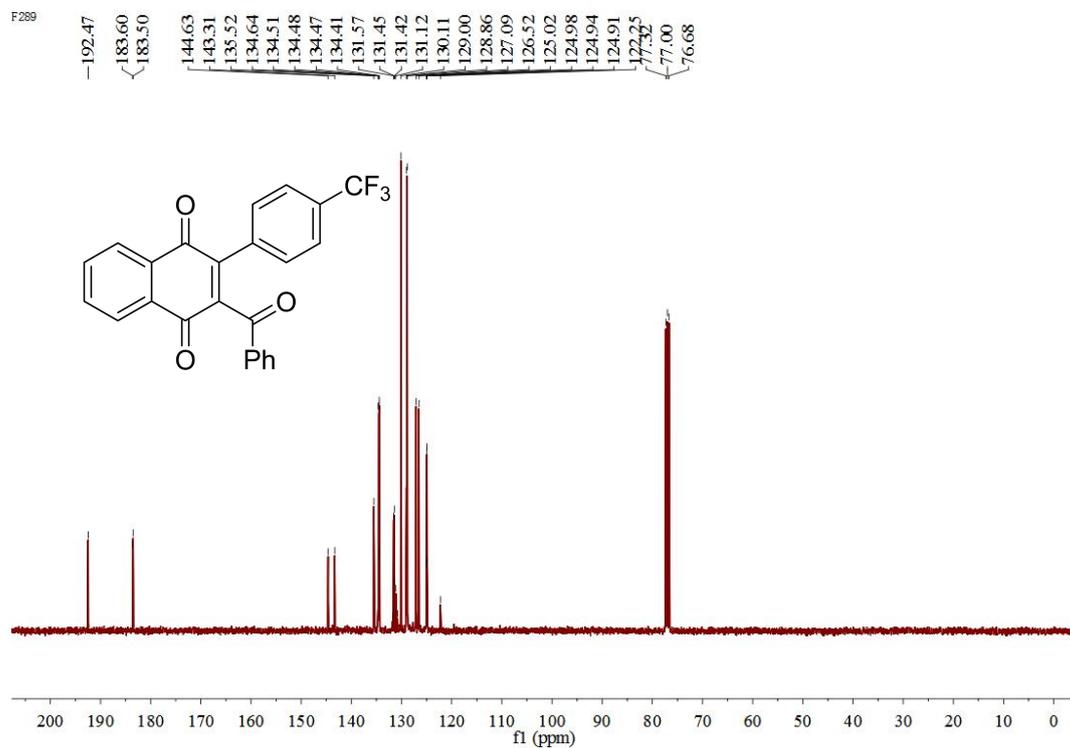
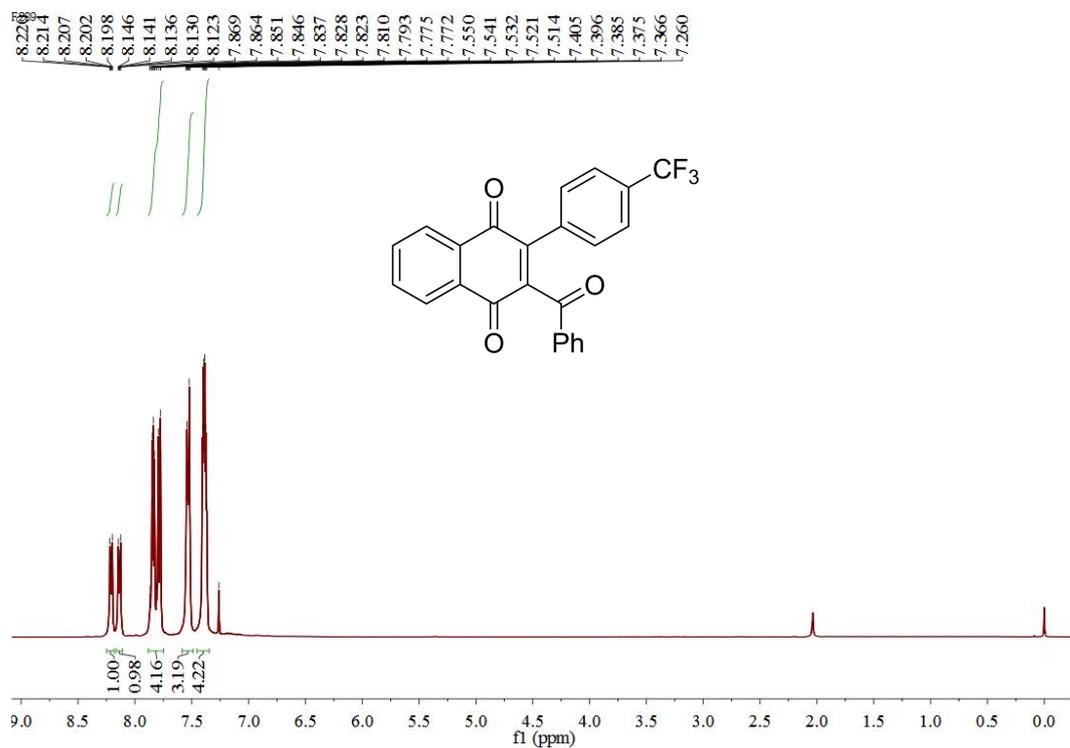


F309

--110.34

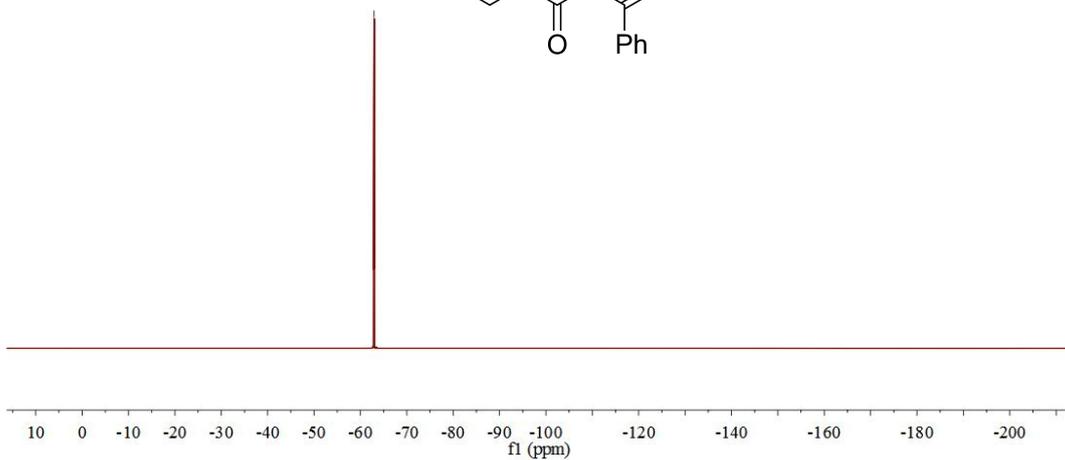
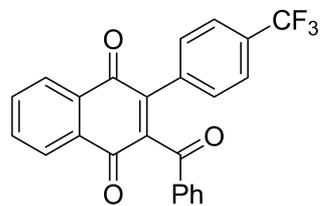


# <sup>1</sup>H NMR, <sup>13</sup>C NMR and <sup>19</sup>F NMR of 3i

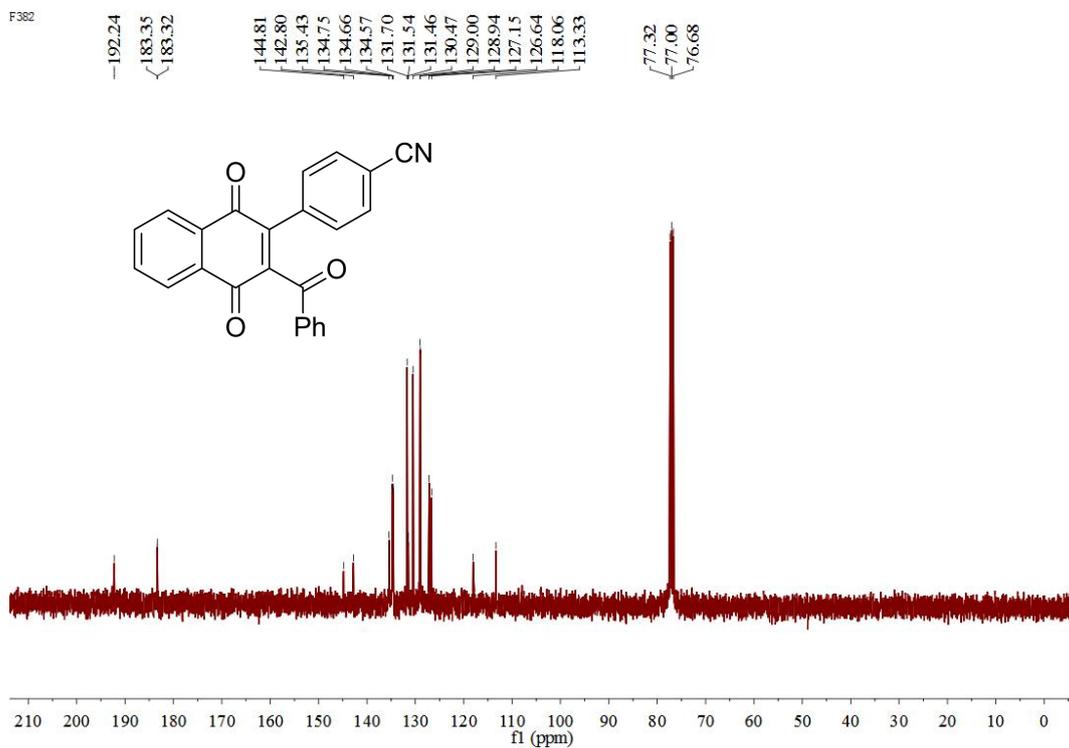
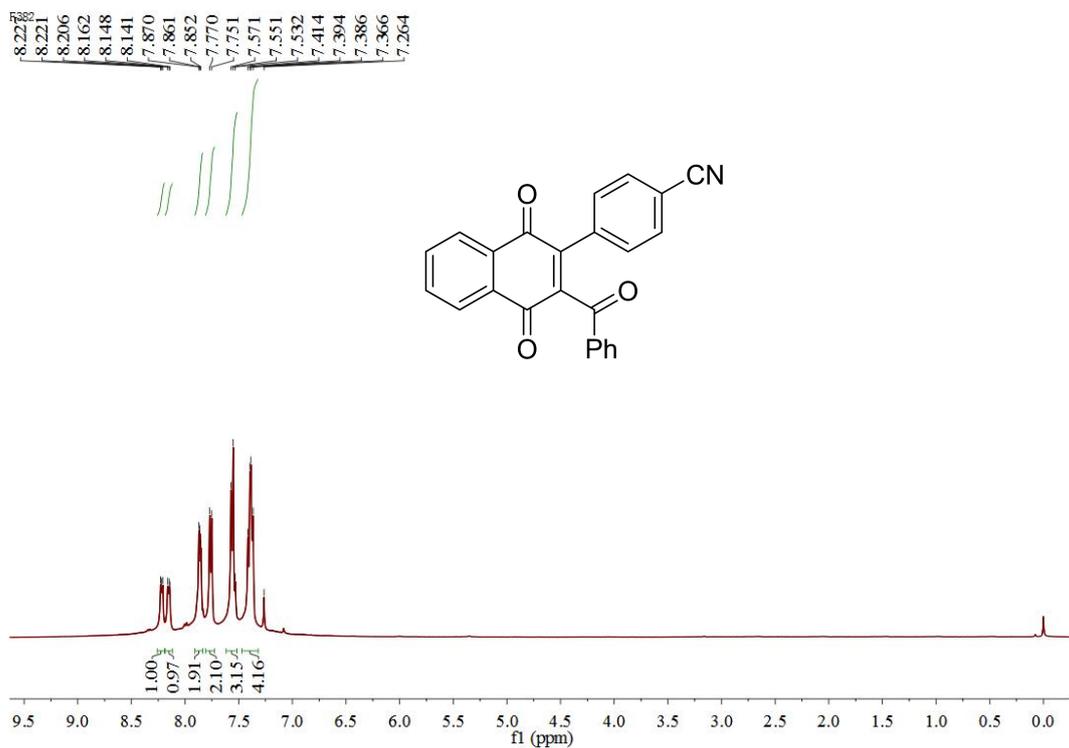


F289

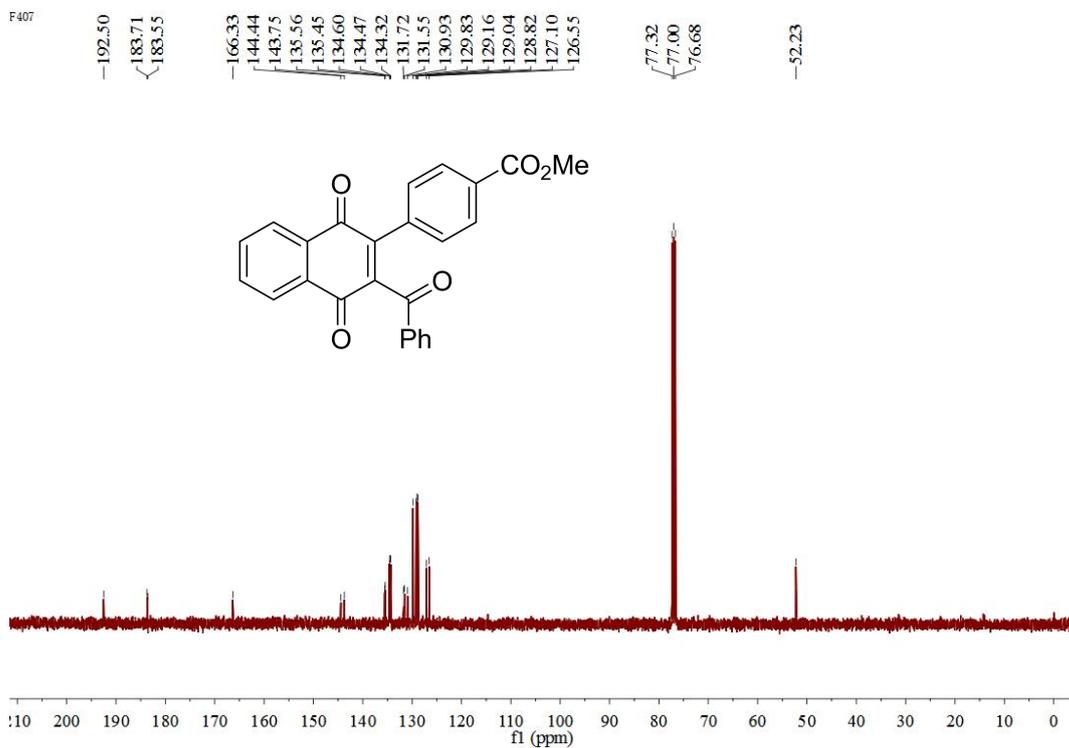
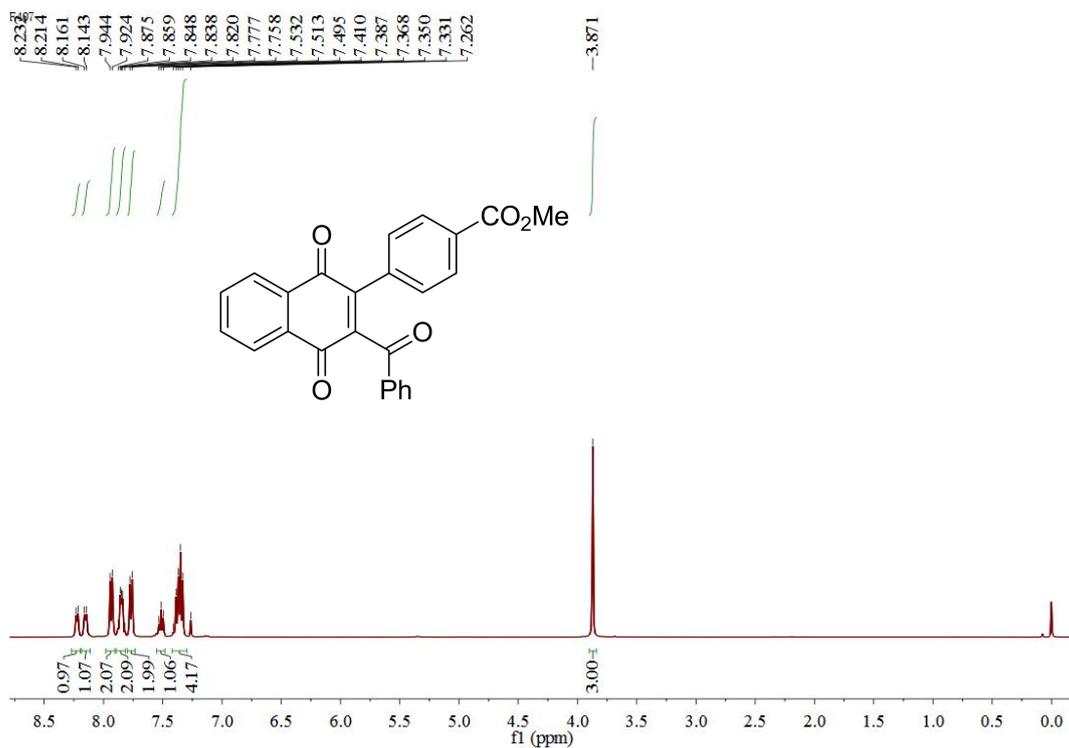
-62.96



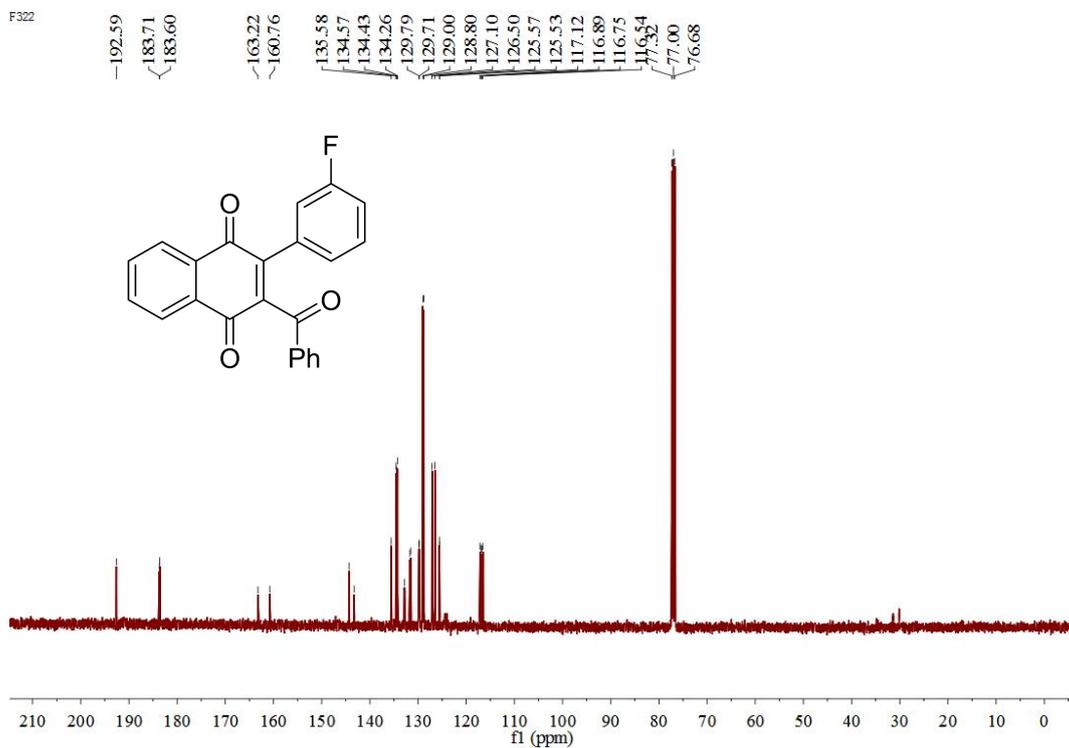
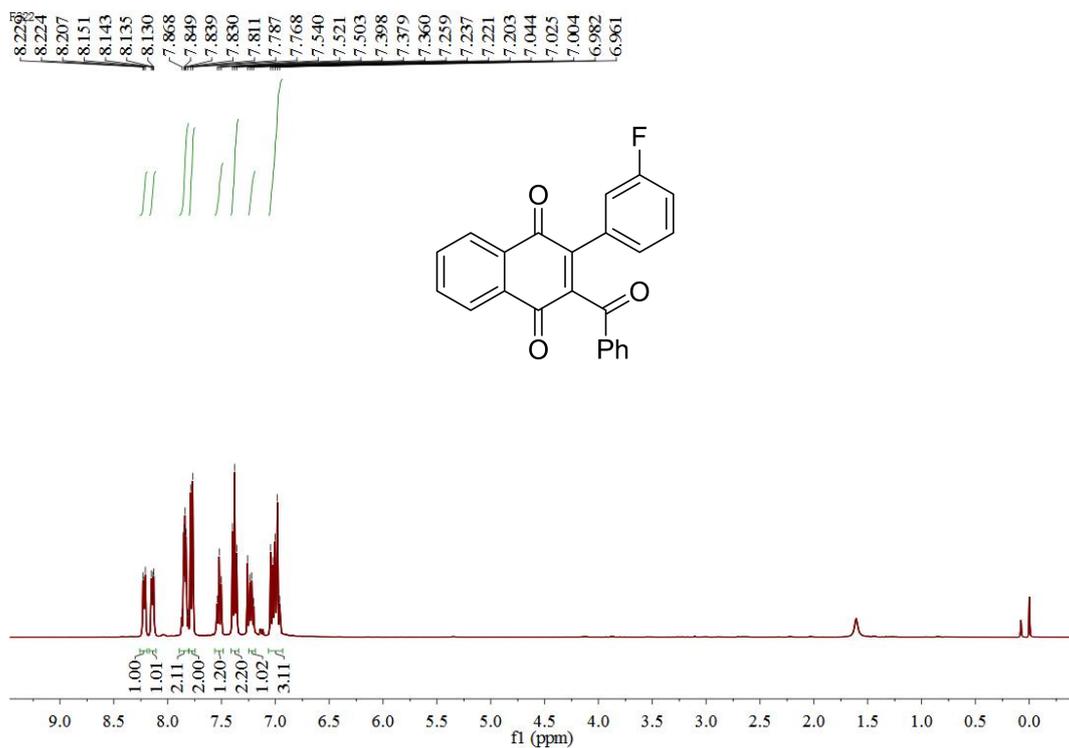
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 3j



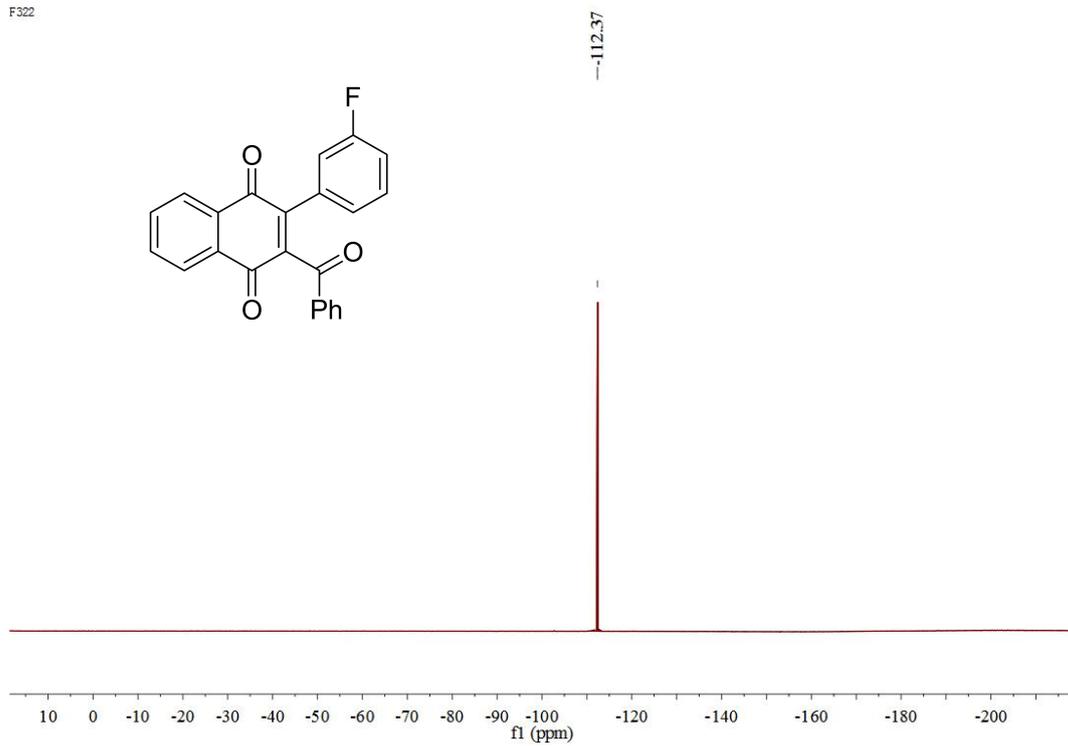
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 3k



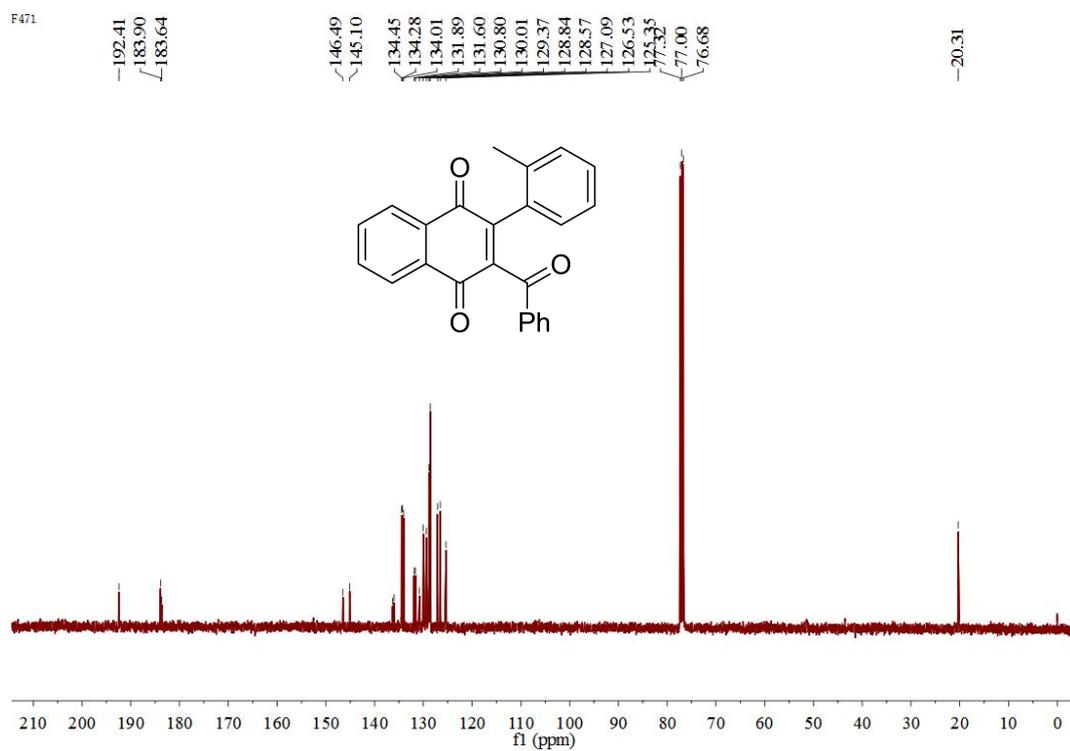
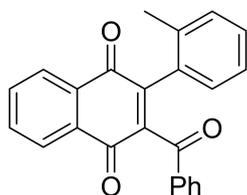
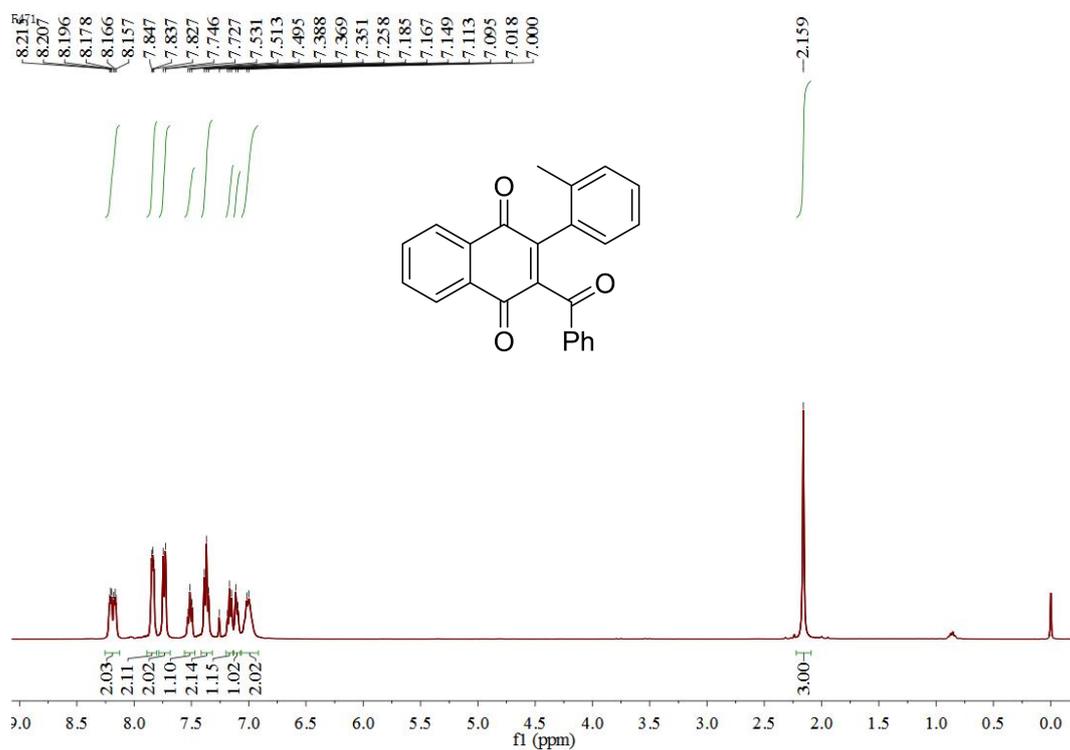
# <sup>1</sup>H NMR, <sup>13</sup>C NMR and <sup>19</sup>F NMR of 3l



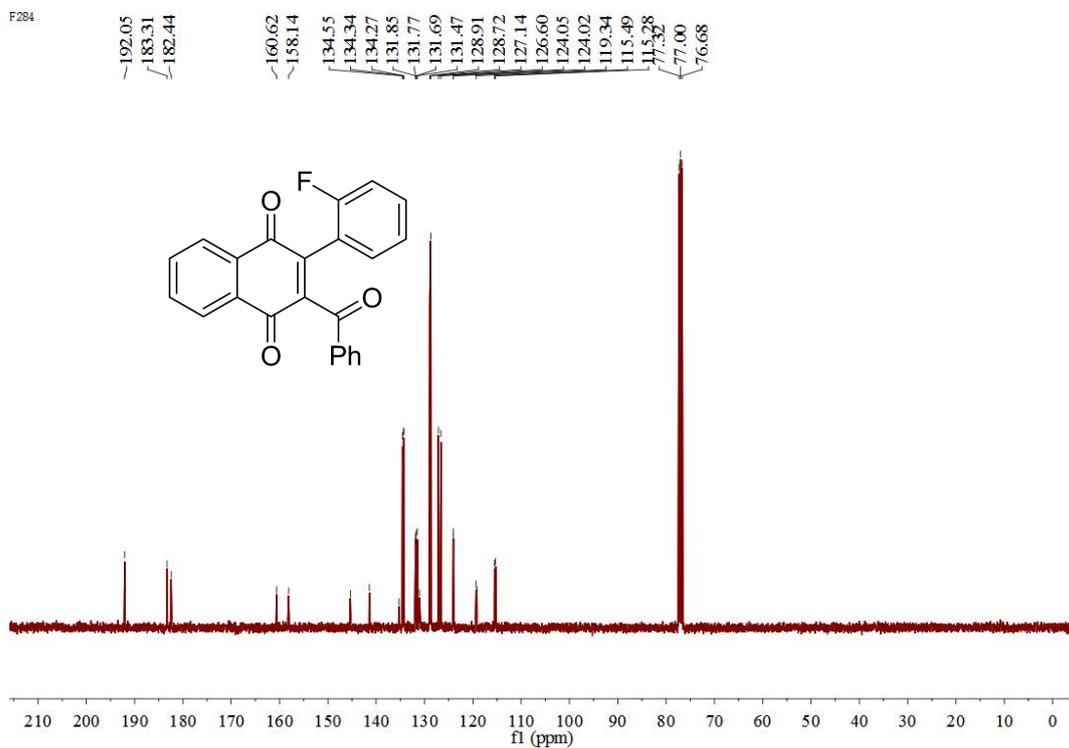
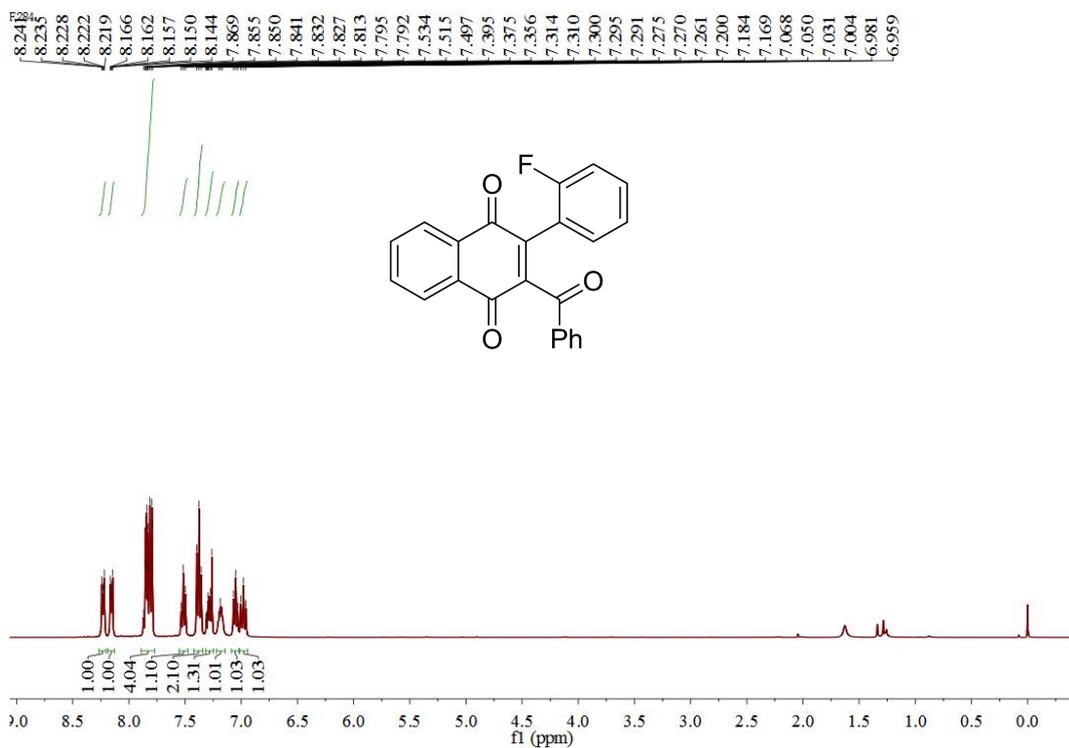
F322



# <sup>1</sup>H NMR, <sup>13</sup>C NMR and <sup>19</sup>F NMR of 3m

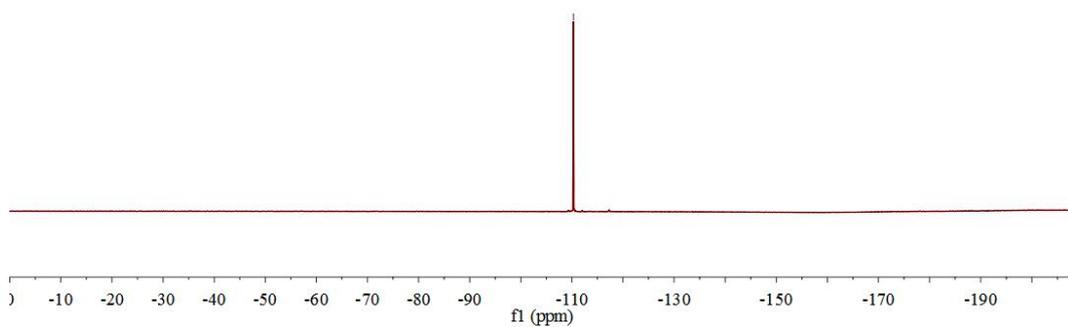
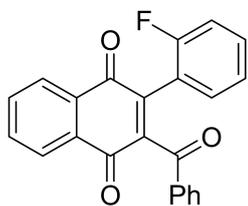


# <sup>1</sup>H NMR, <sup>13</sup>C NMR and <sup>19</sup>F NMR of 3n



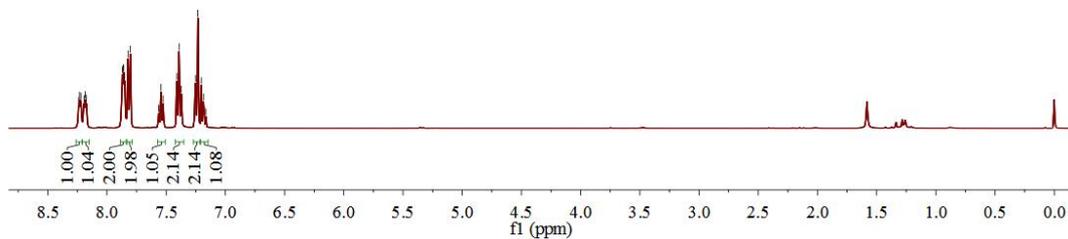
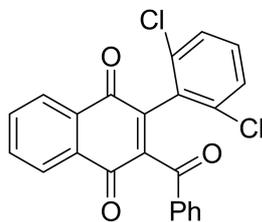
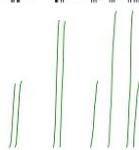
F284

--110.30



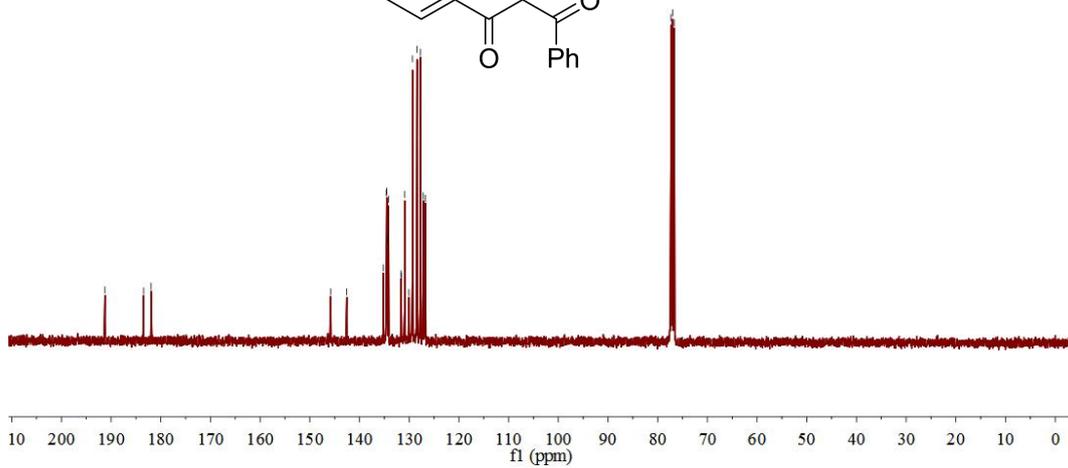
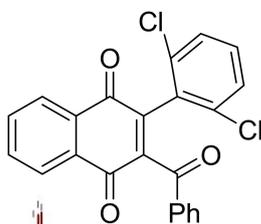
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 3o

8.236  
8.231  
8.220  
8.194  
8.183  
8.174  
7.869  
7.861  
7.859  
7.851  
7.822  
7.803  
7.563  
7.544  
7.526  
7.410  
7.391  
7.372  
7.252  
7.232  
7.203  
7.185  
7.164

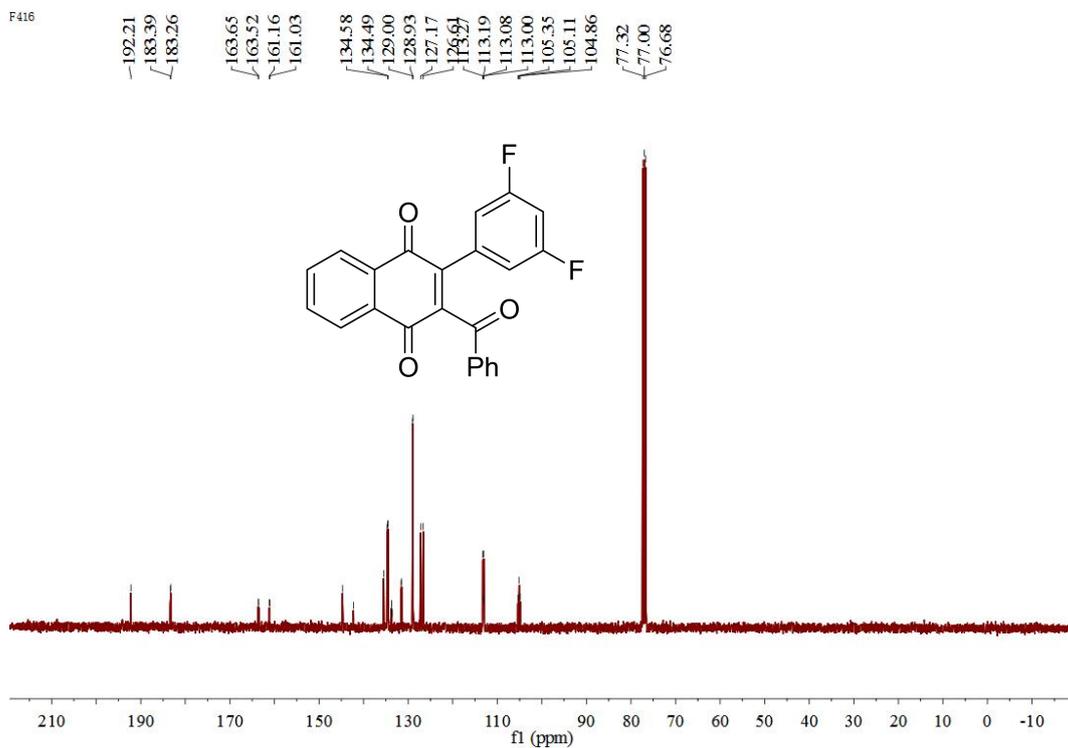
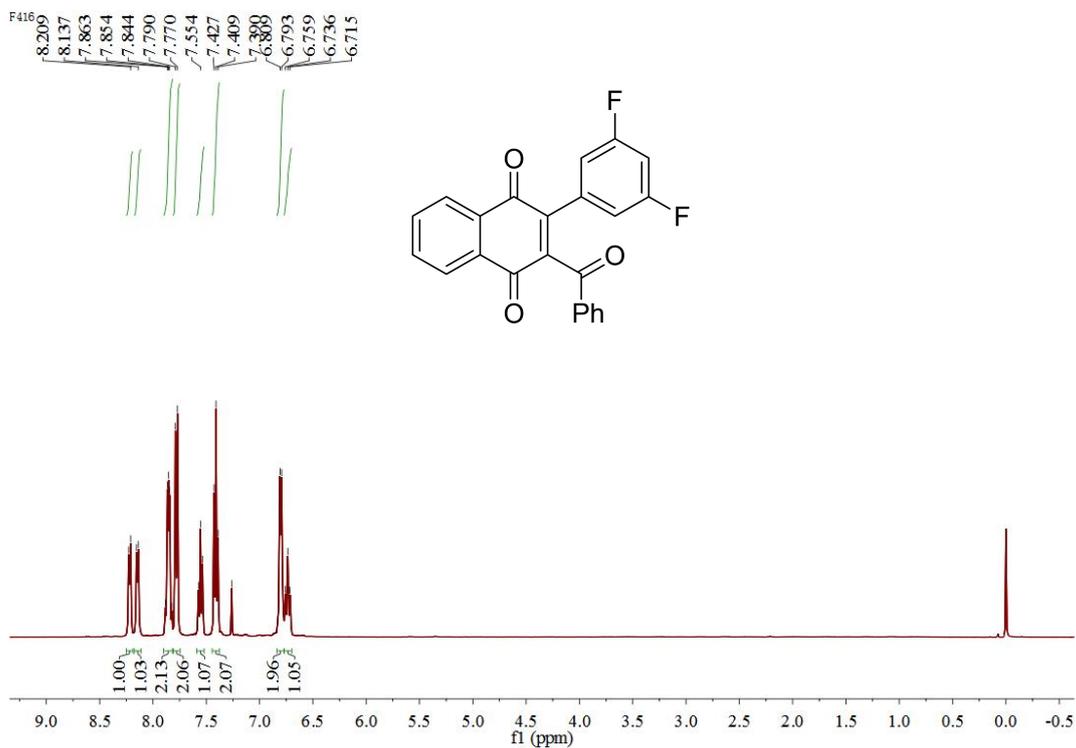


F417

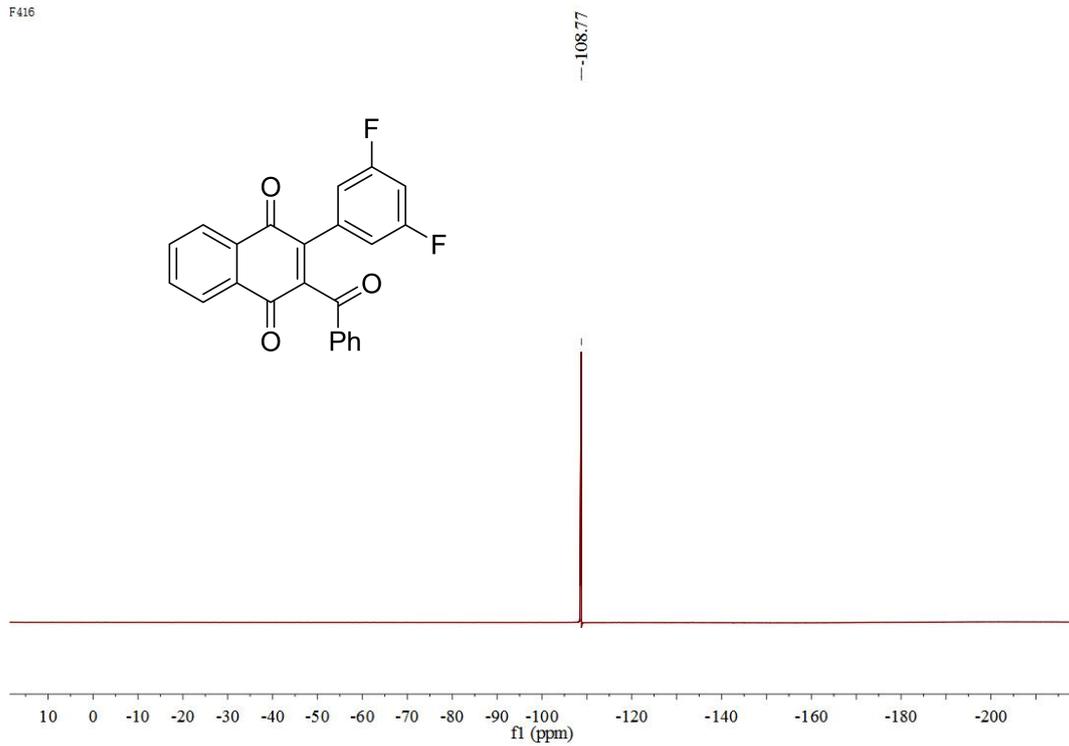
191.23  
183.46  
181.95  
145.81  
142.57  
135.21  
134.61  
134.50  
134.38  
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131.65  
131.59  
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127.73  
127.17  
126.74  
77.32  
77.00  
76.68



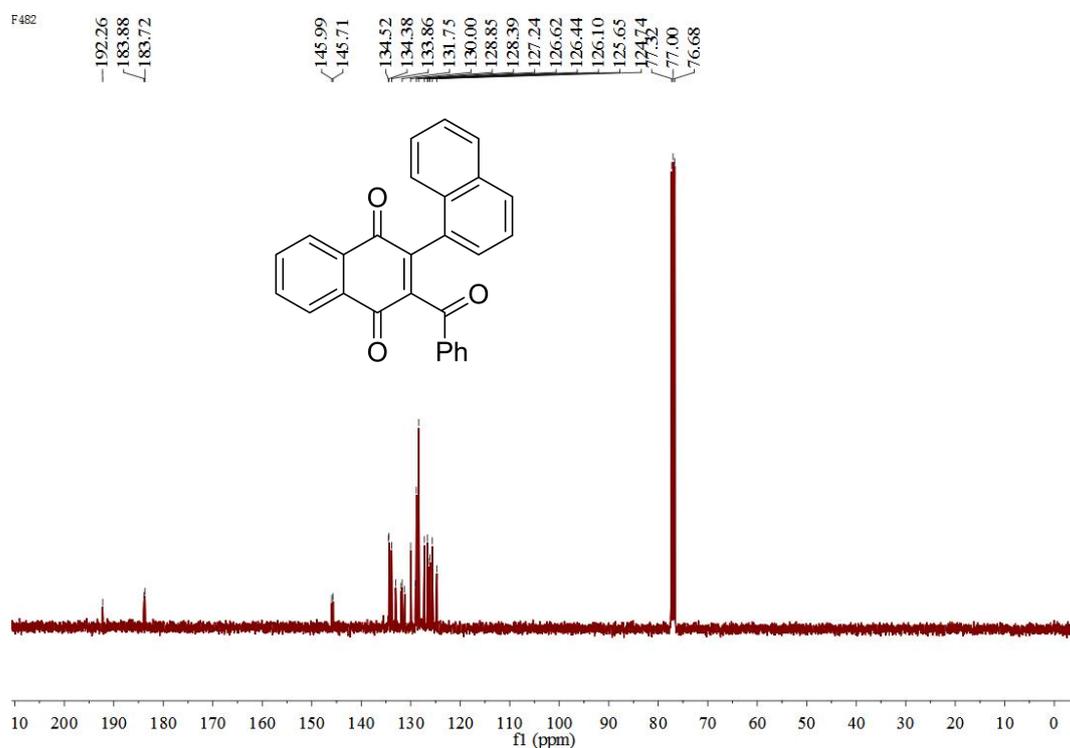
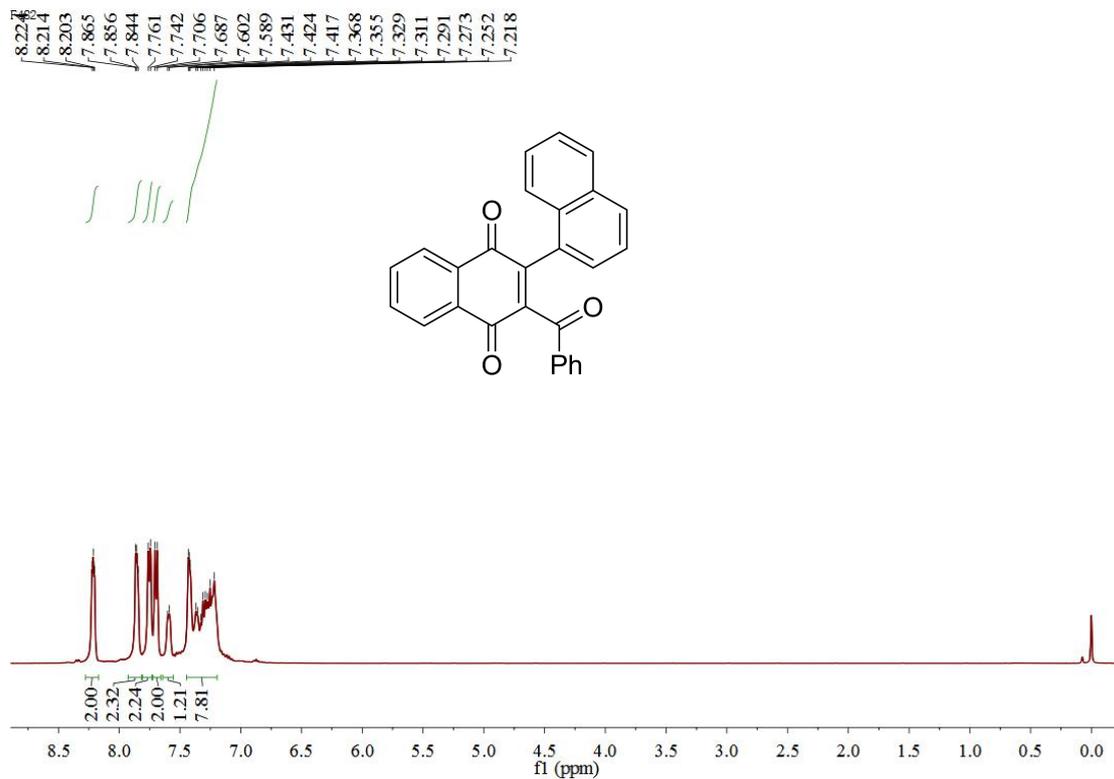
# <sup>1</sup>H NMR, <sup>13</sup>C NMR and <sup>19</sup>F NMR of 3p



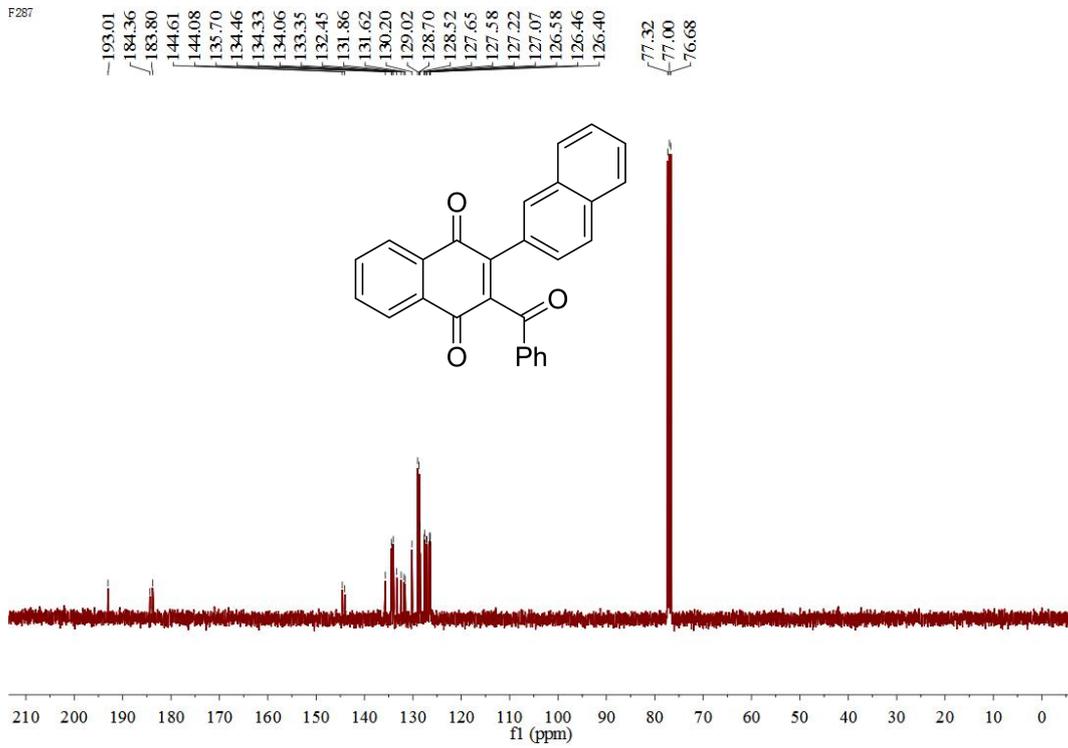
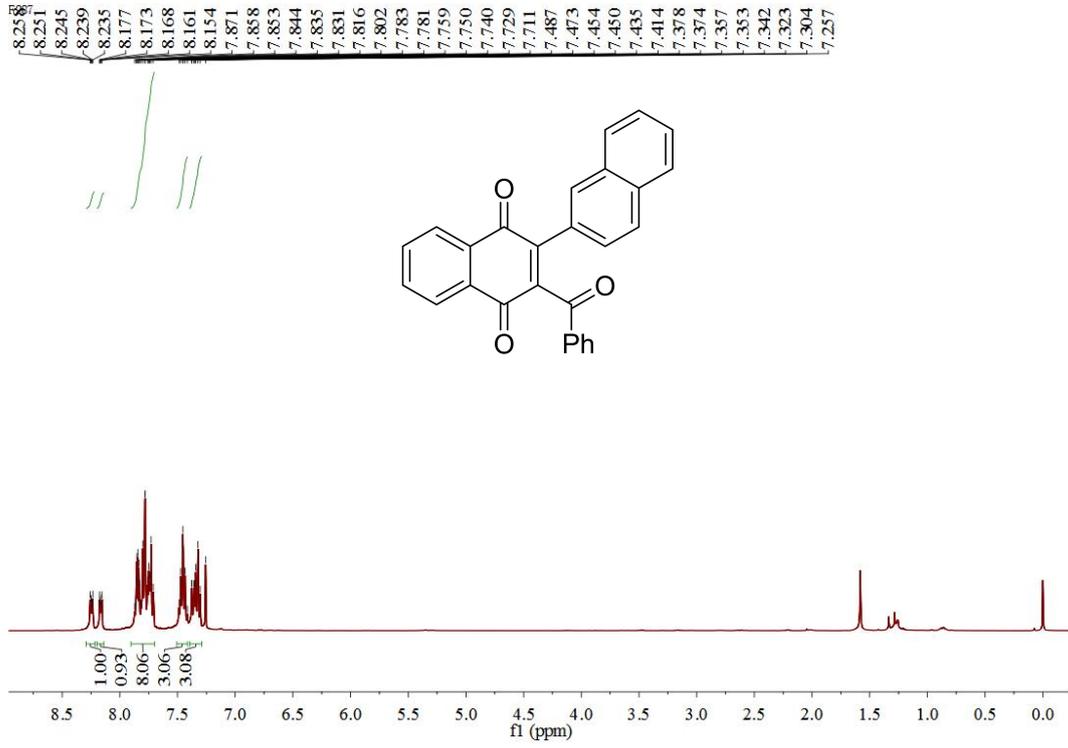
F416



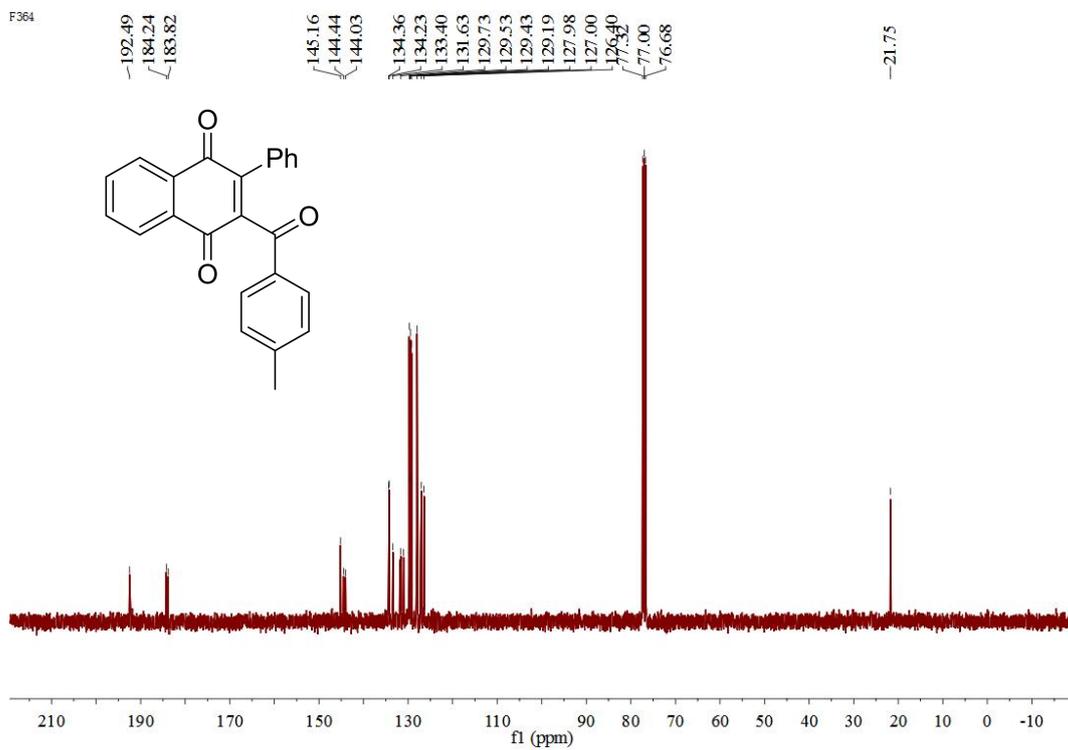
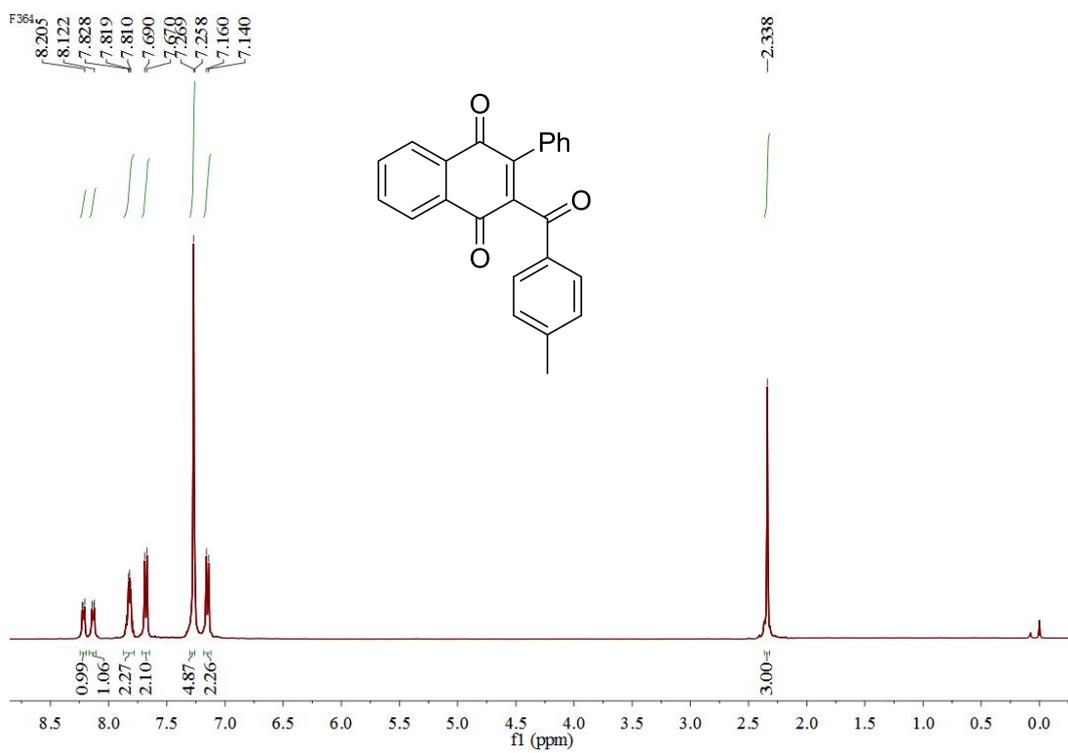
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 3q



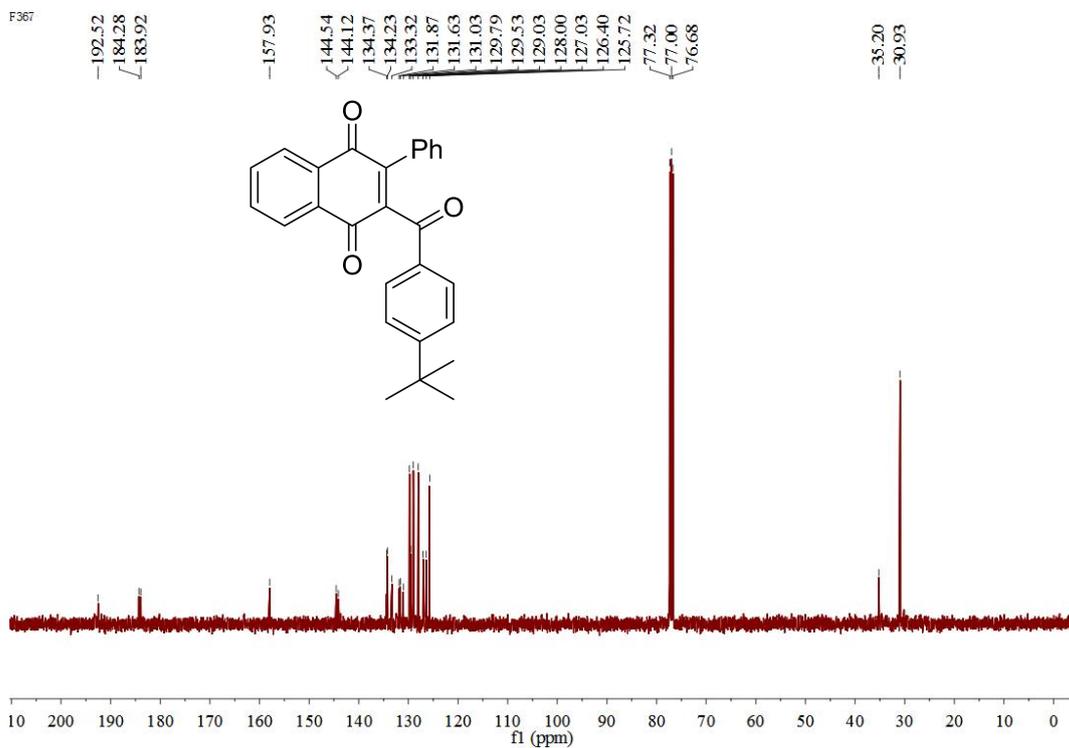
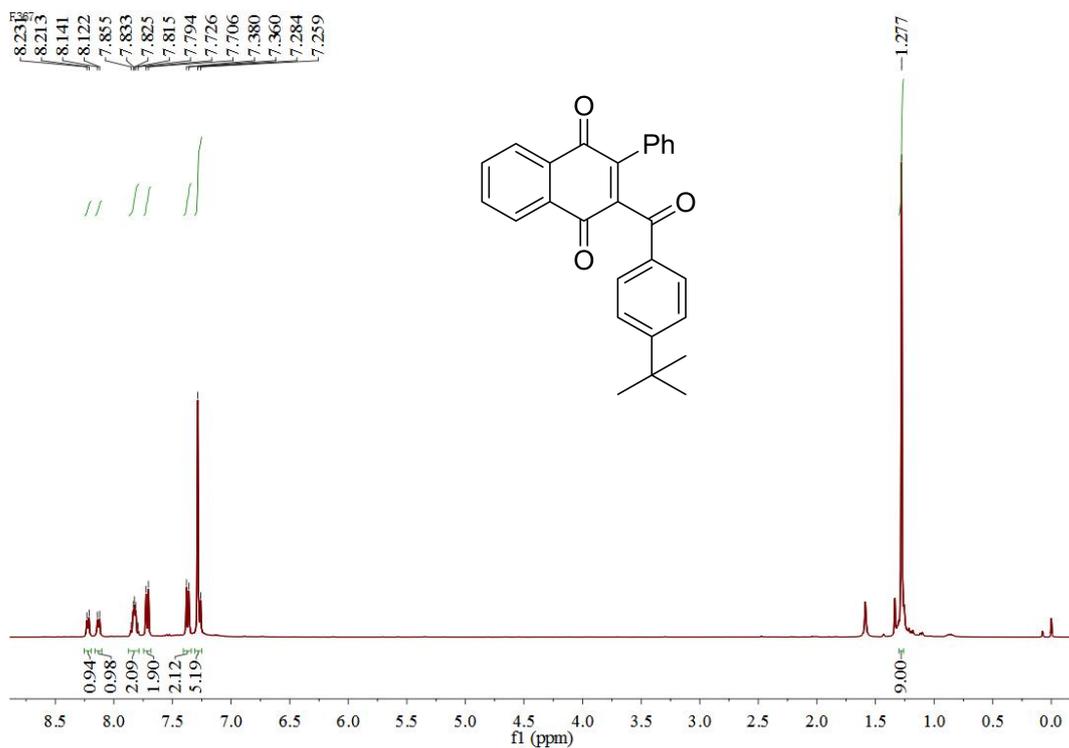
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 3r



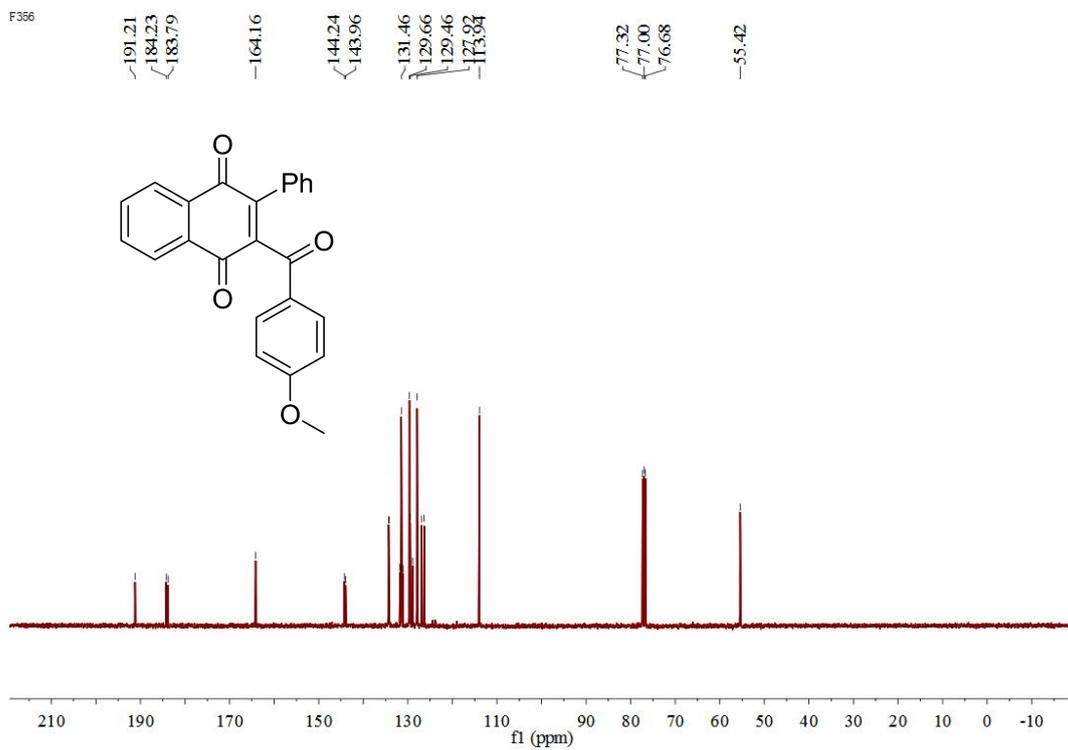
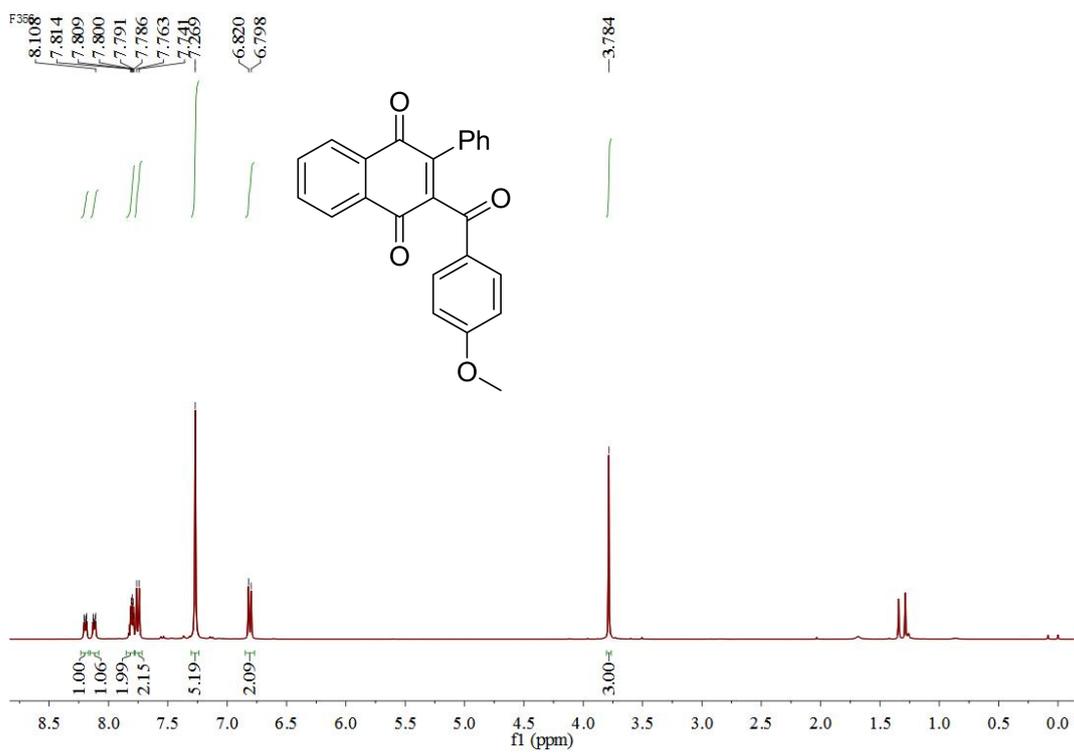
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4a



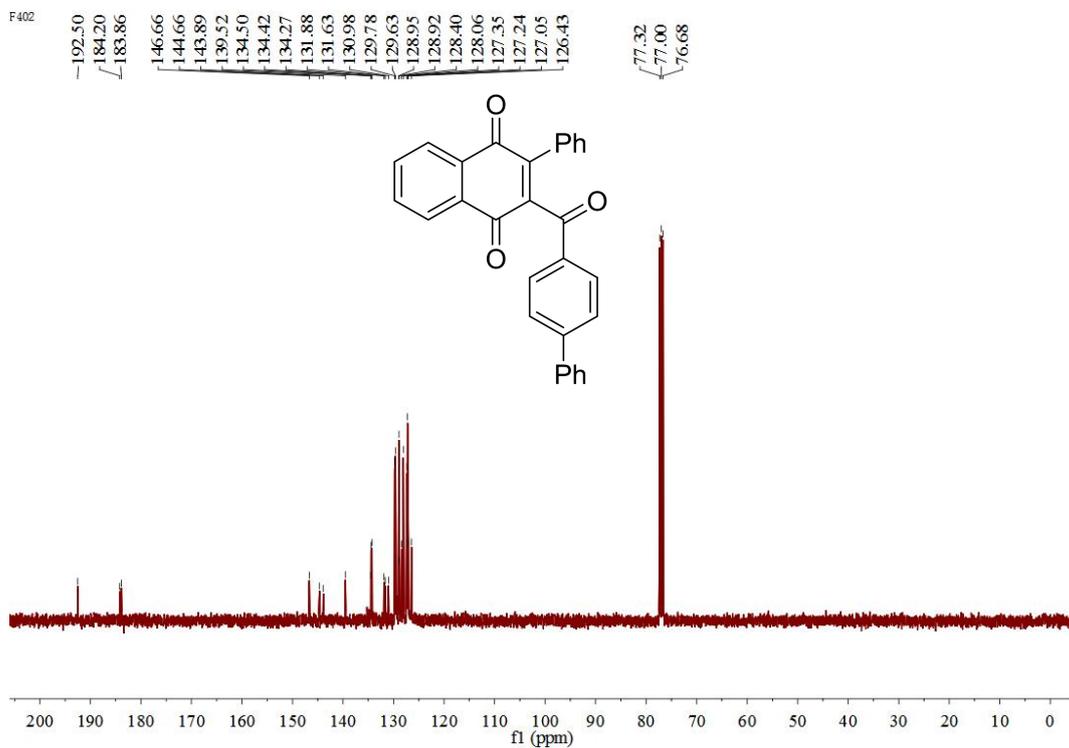
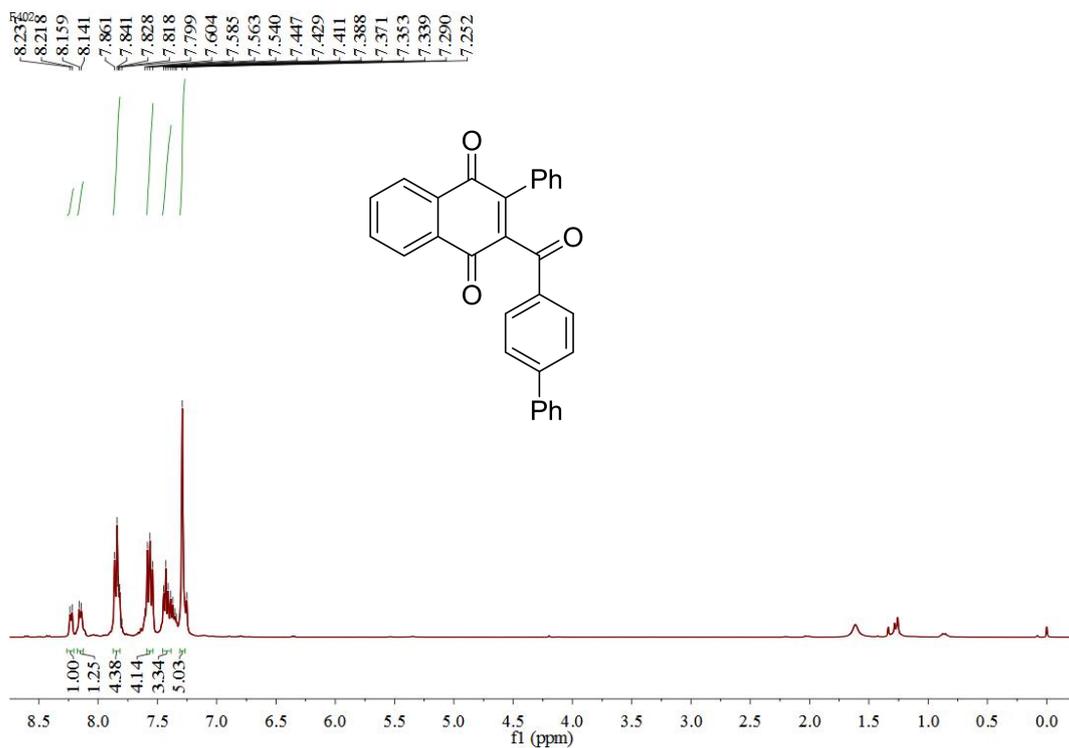
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4b



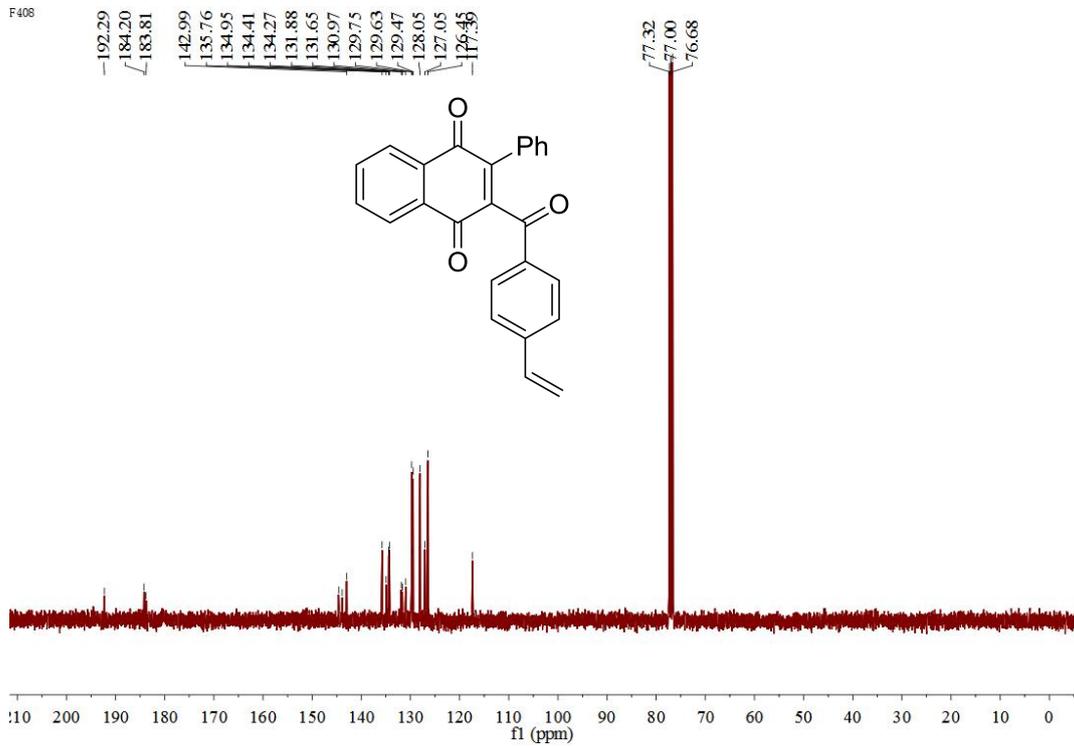
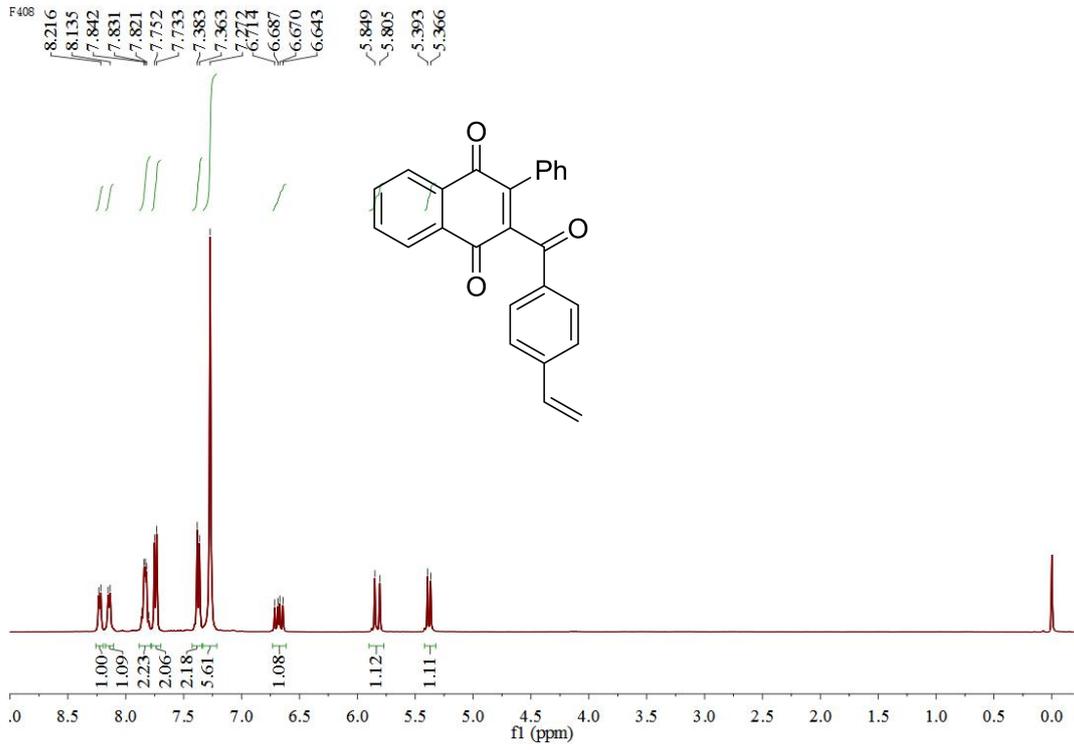
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4c



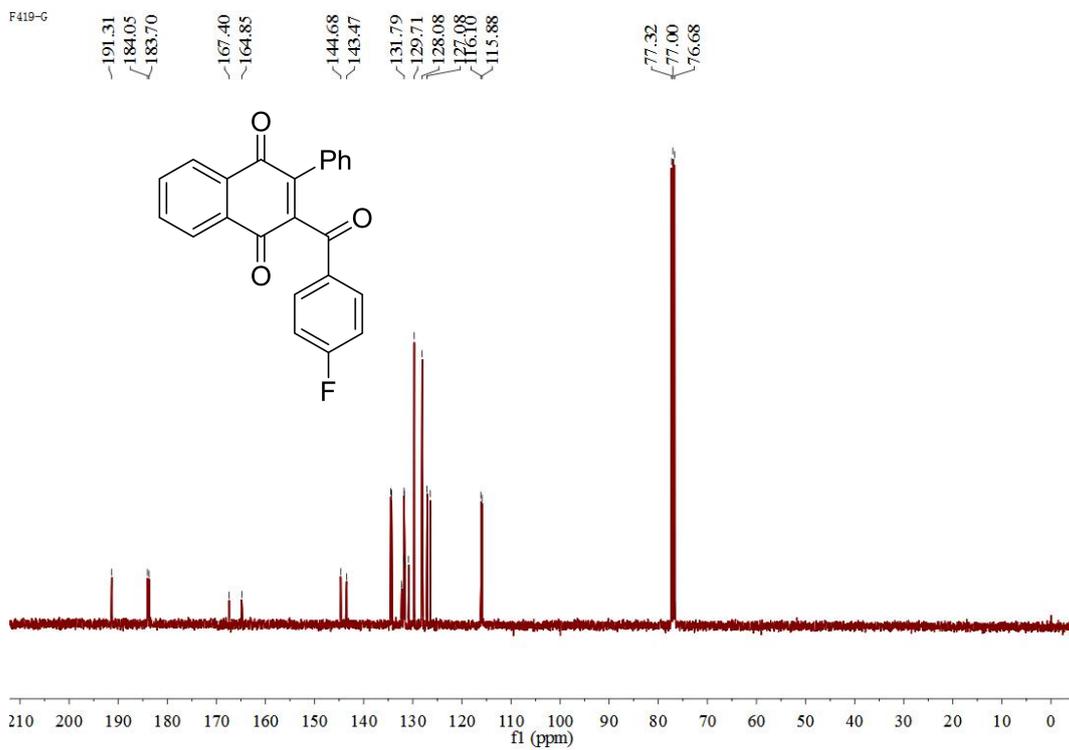
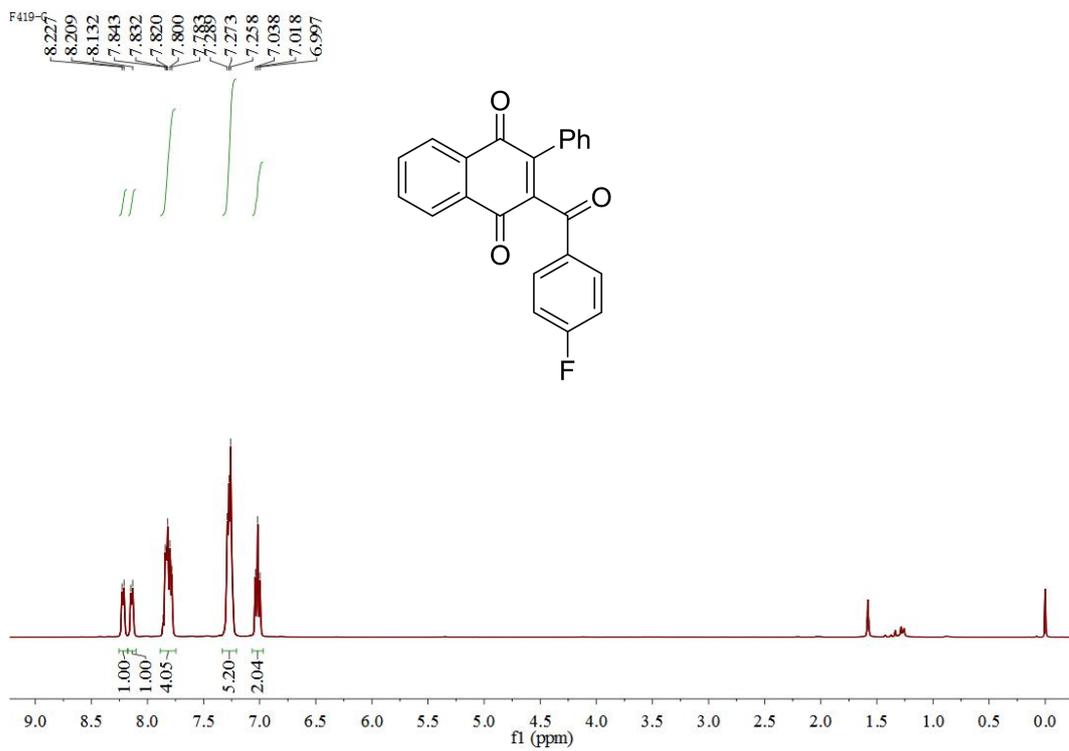
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4d



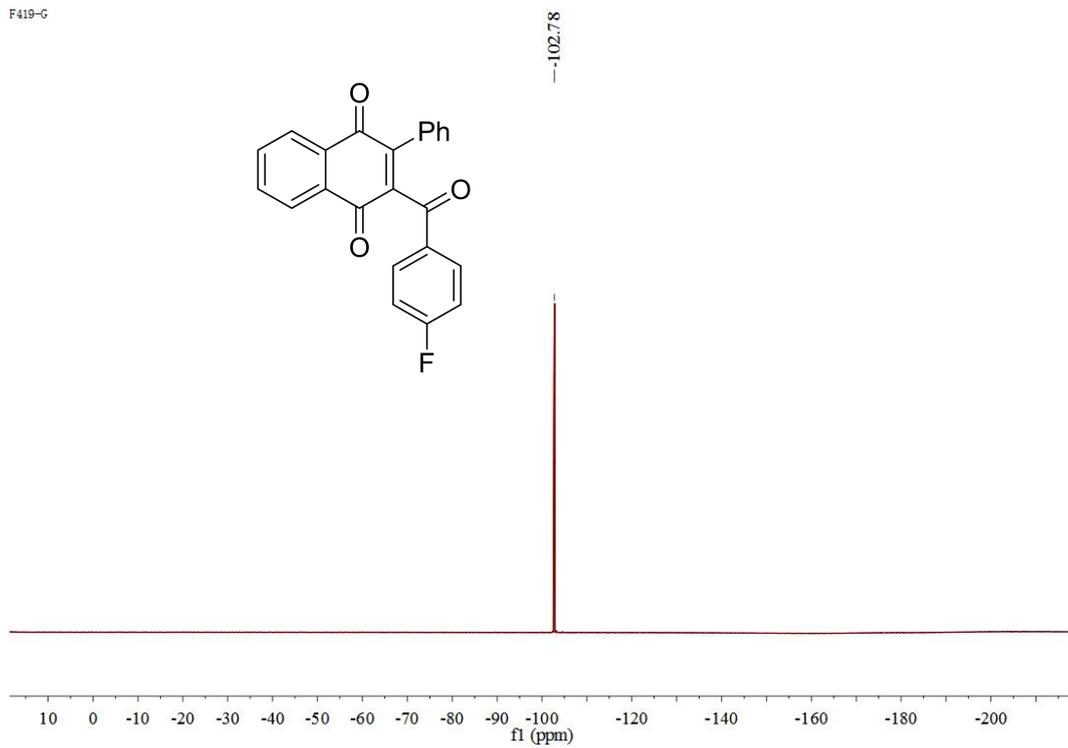
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4e



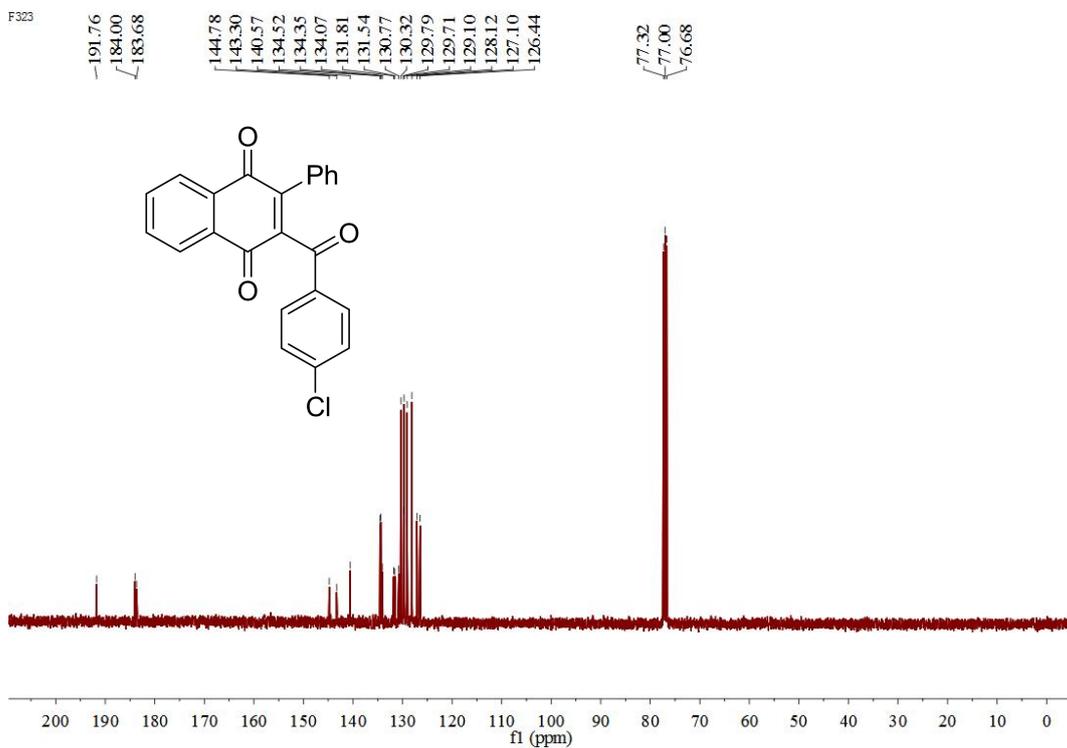
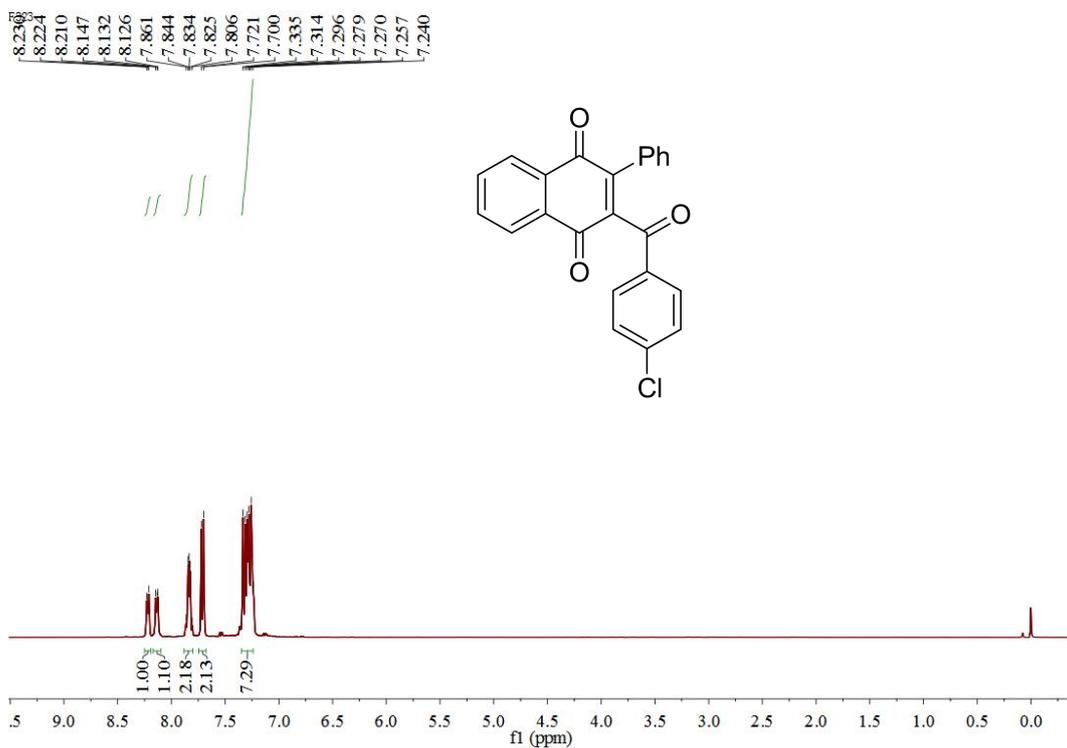
# <sup>1</sup>H NMR, <sup>13</sup>C NMR and <sup>19</sup>F NMR of 4f



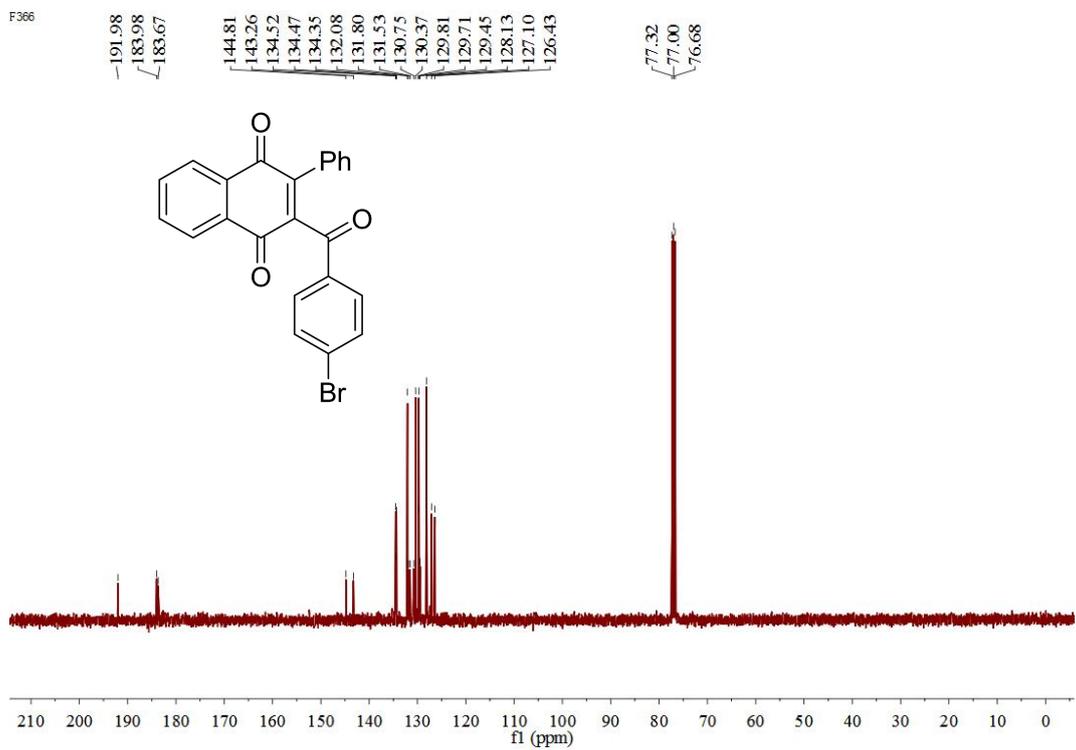
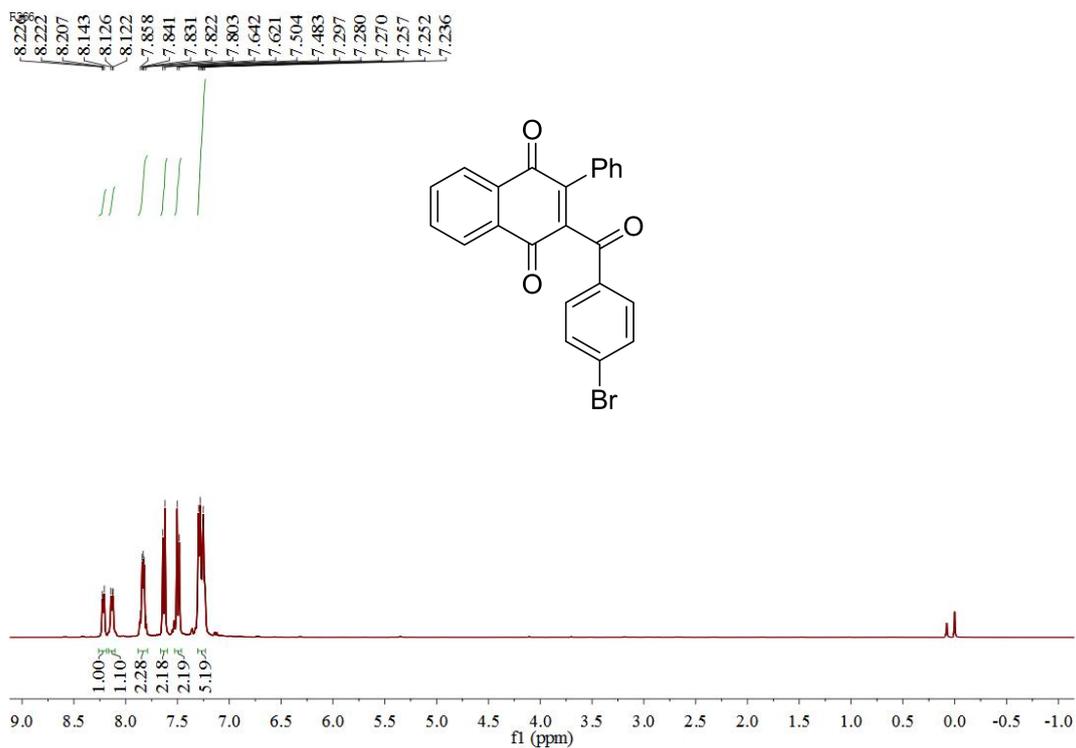
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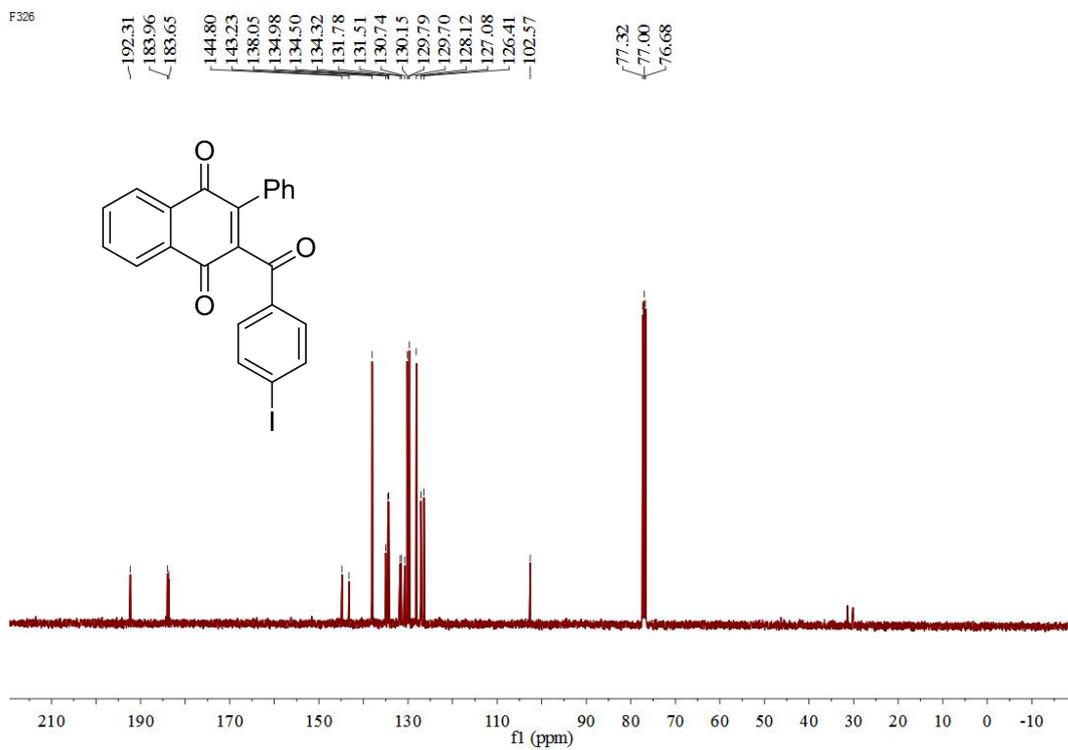
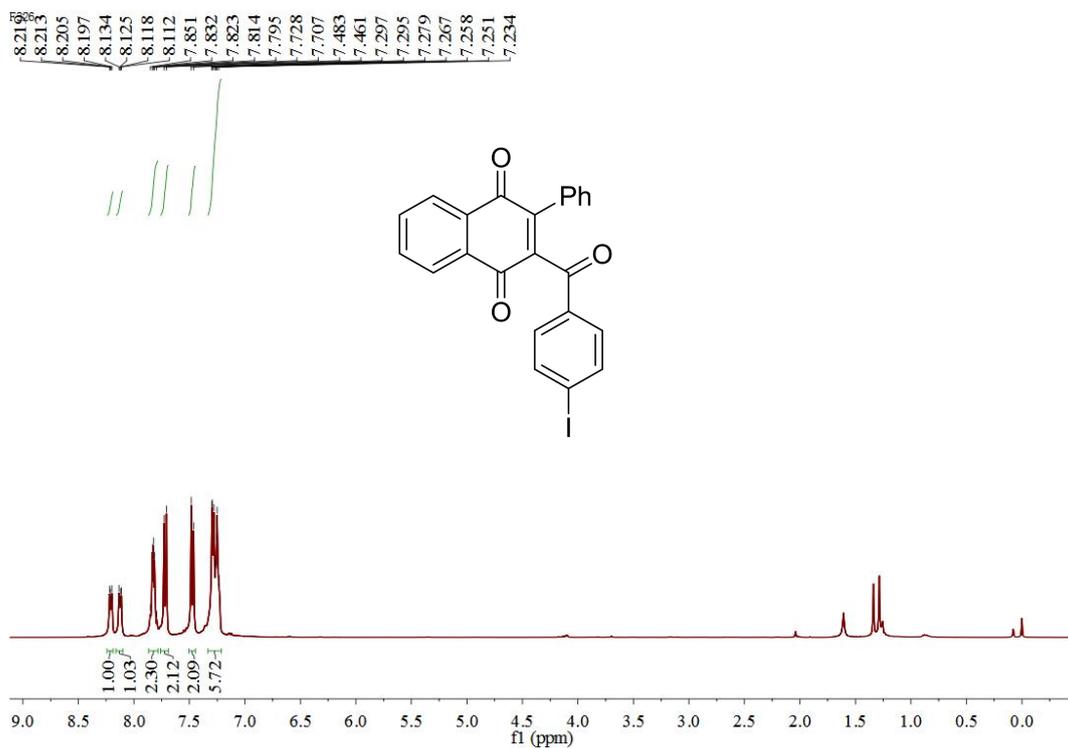
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4g



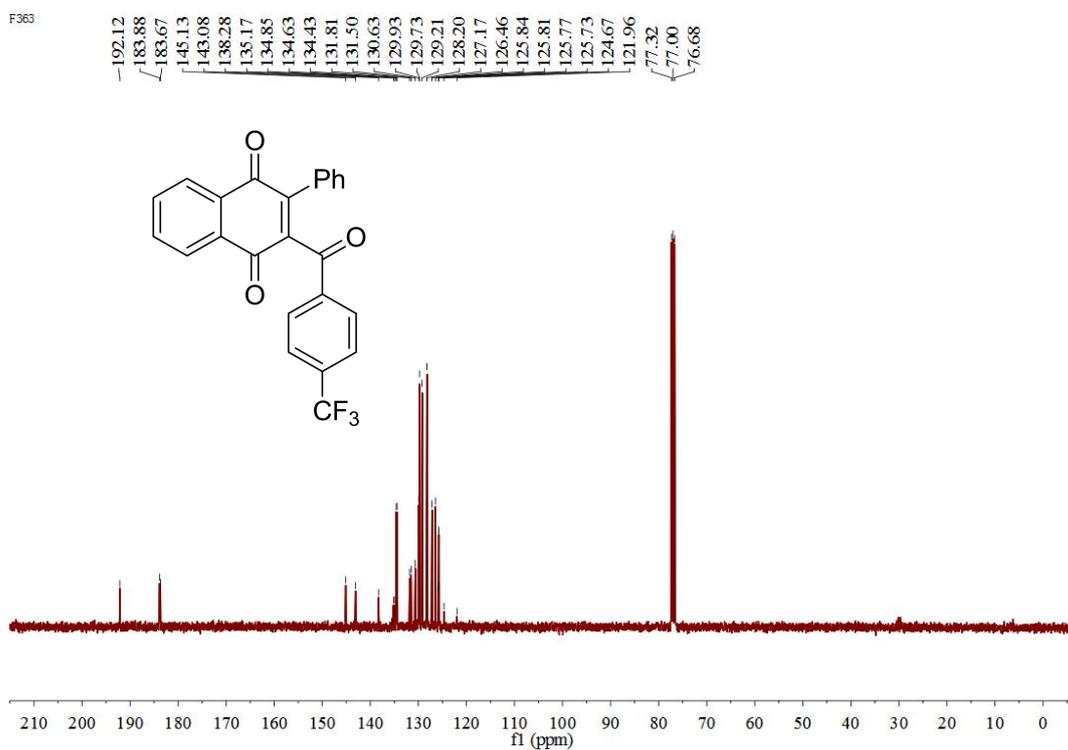
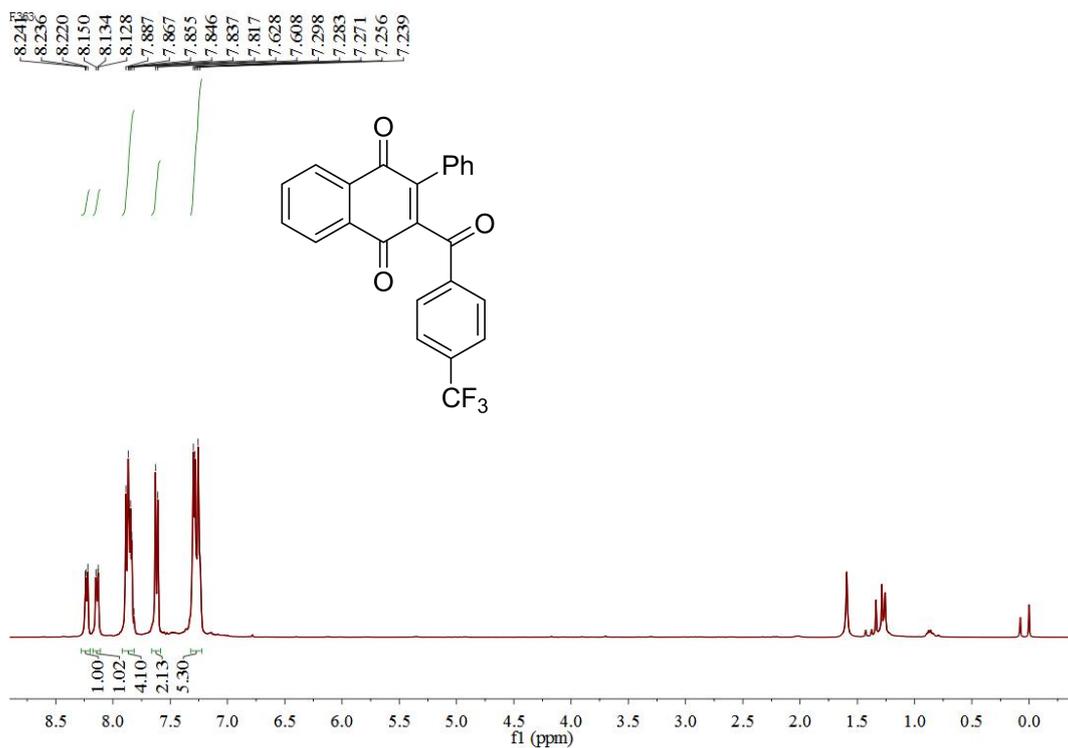
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4h



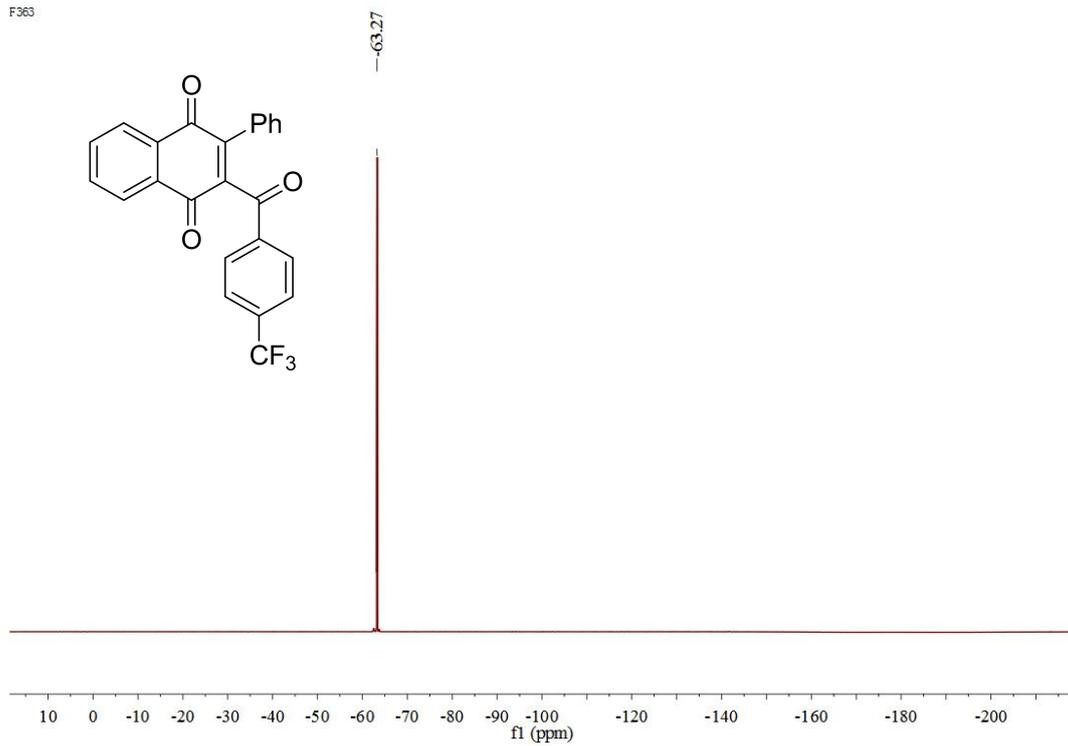
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4i



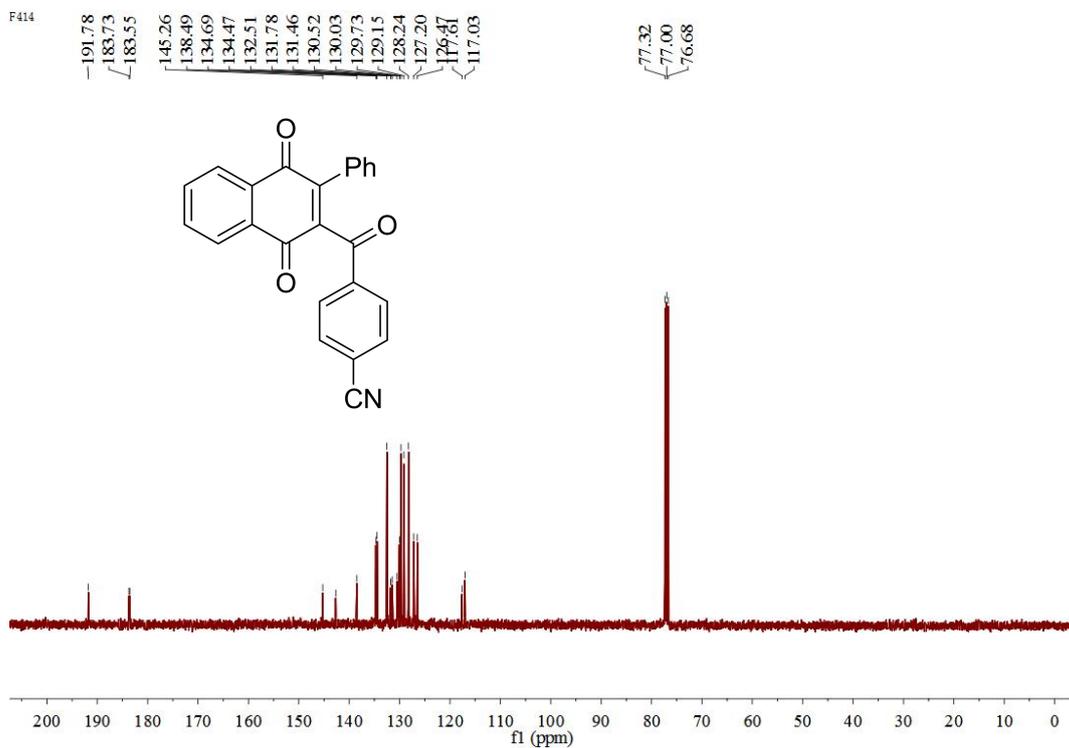
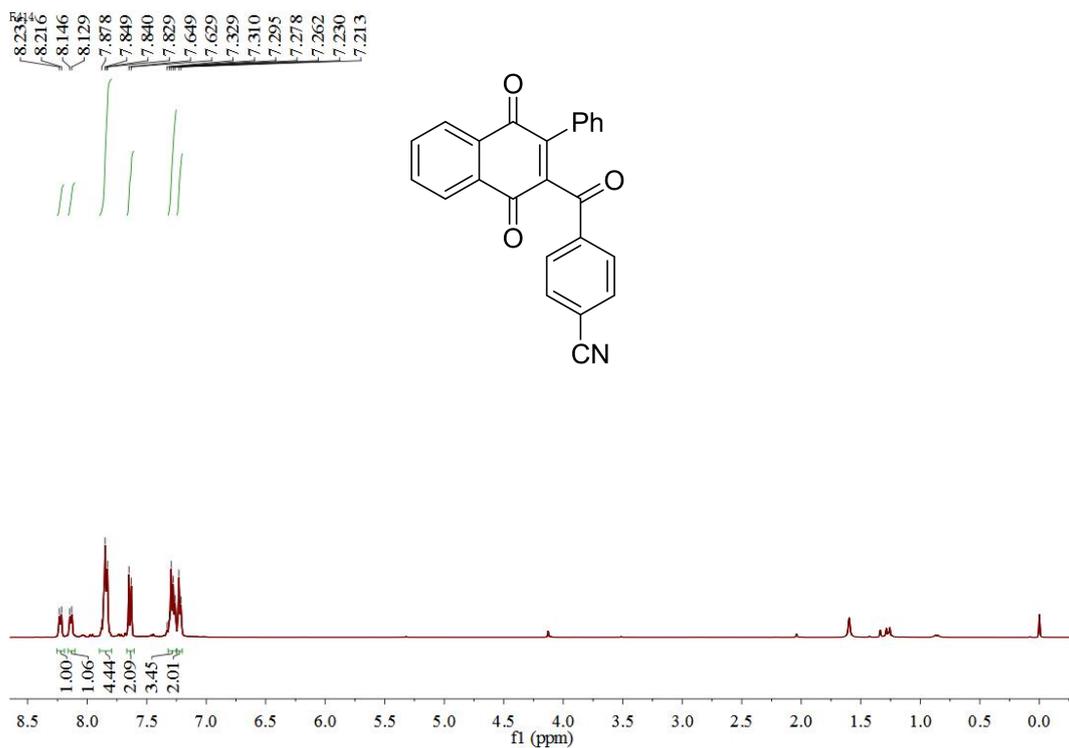
# <sup>1</sup>H NMR, <sup>13</sup>C NMR and <sup>19</sup>F NMR of 4j



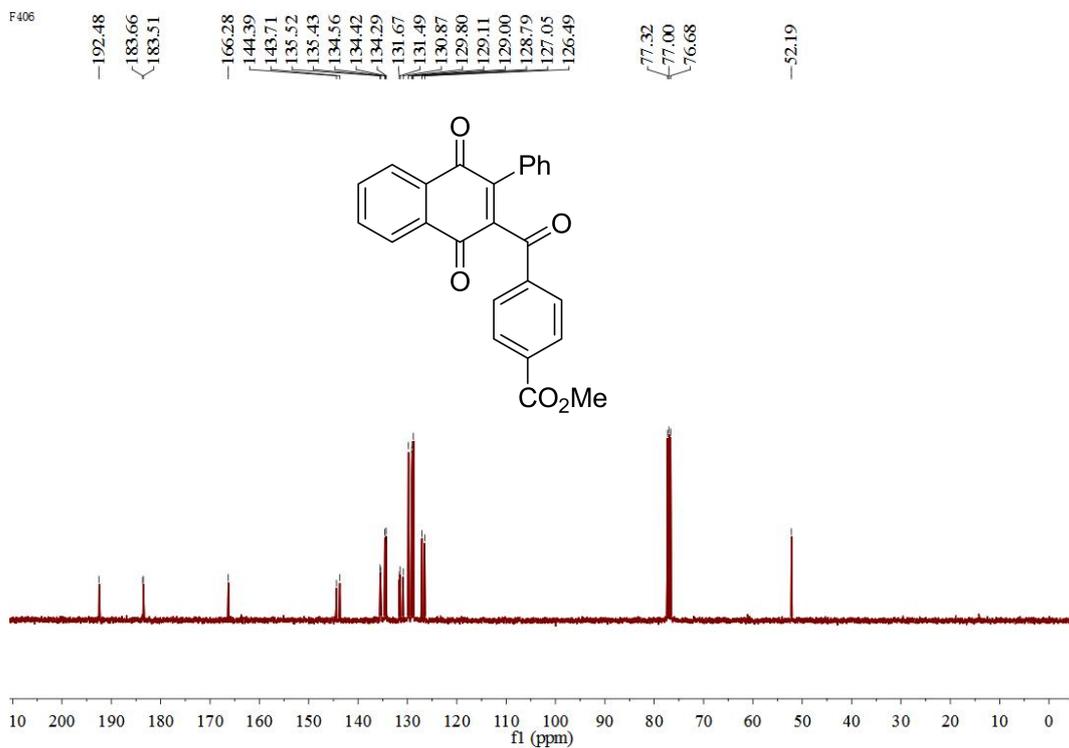
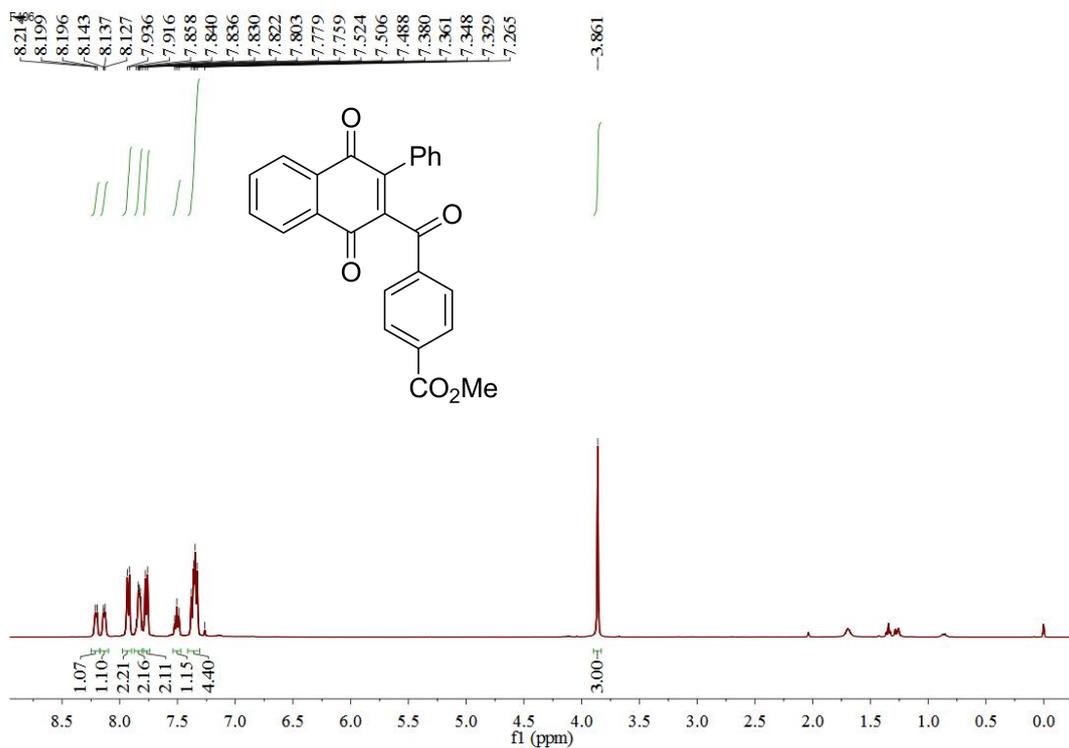
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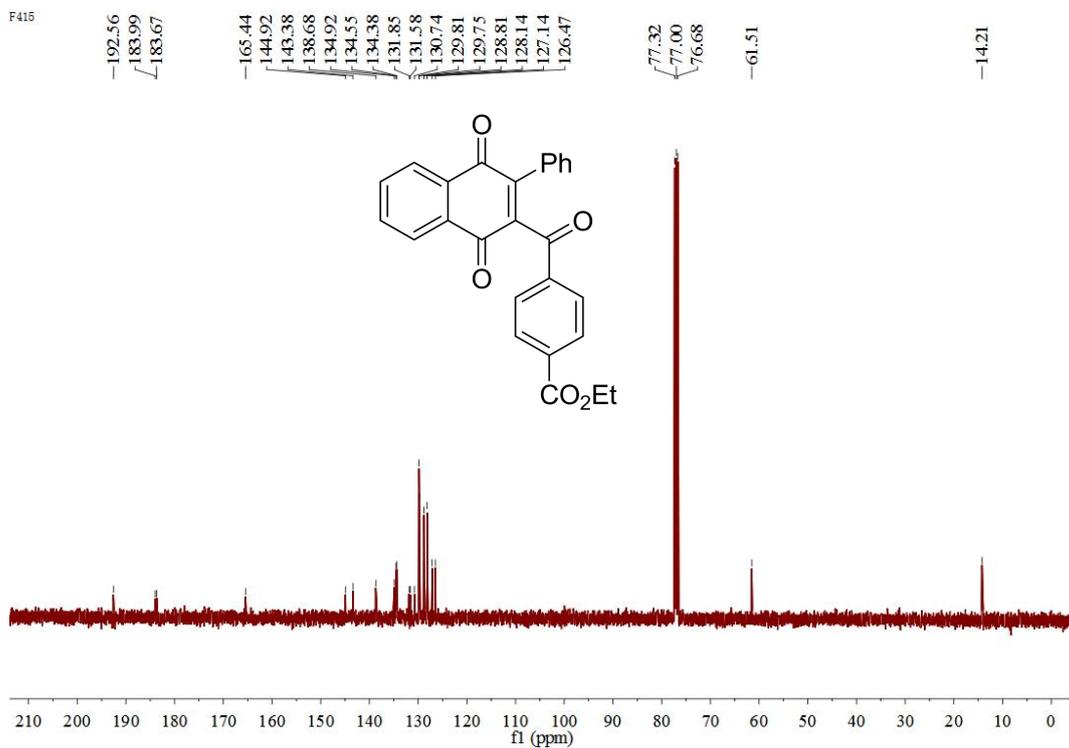
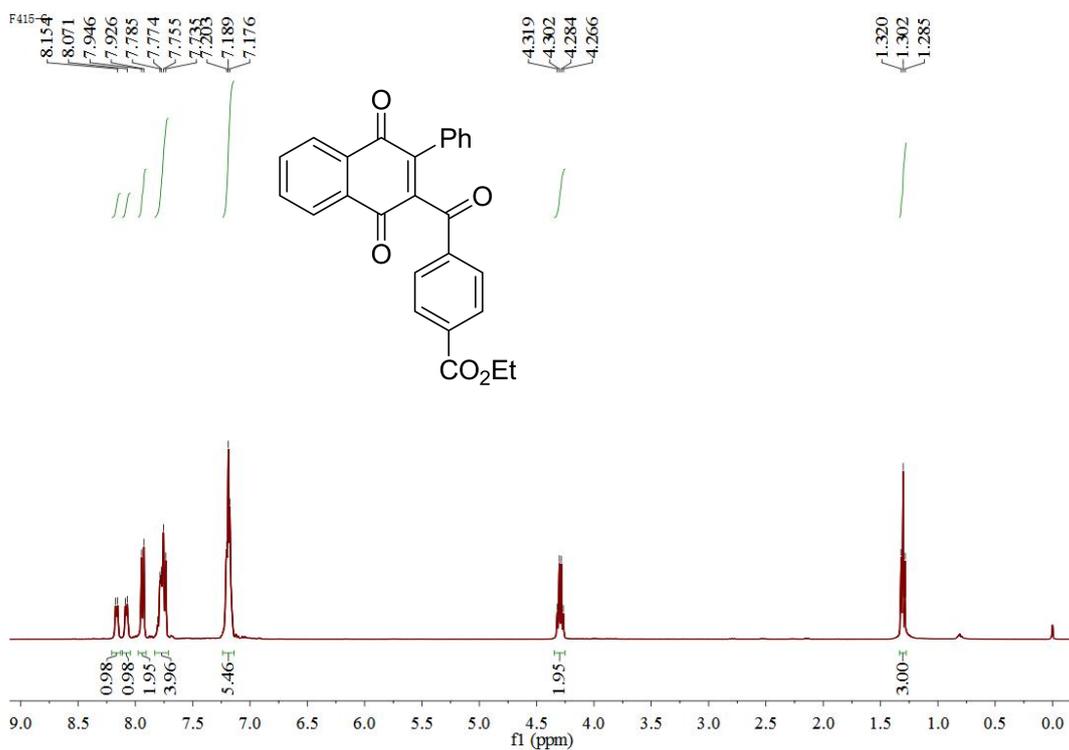
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4k



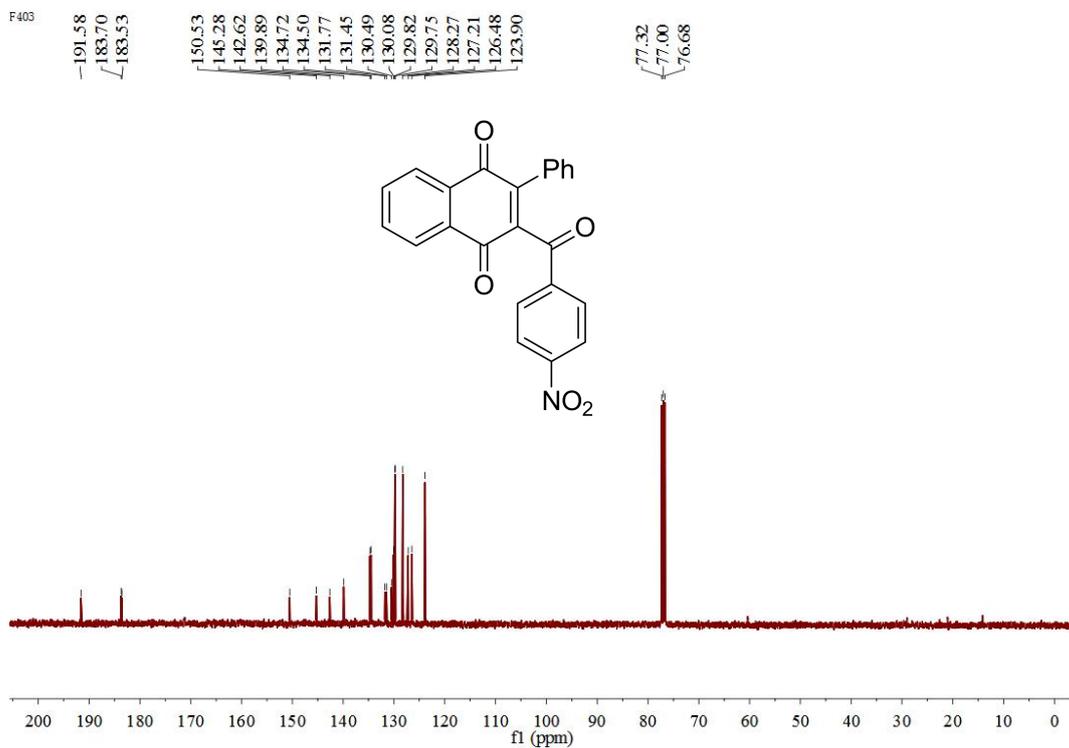
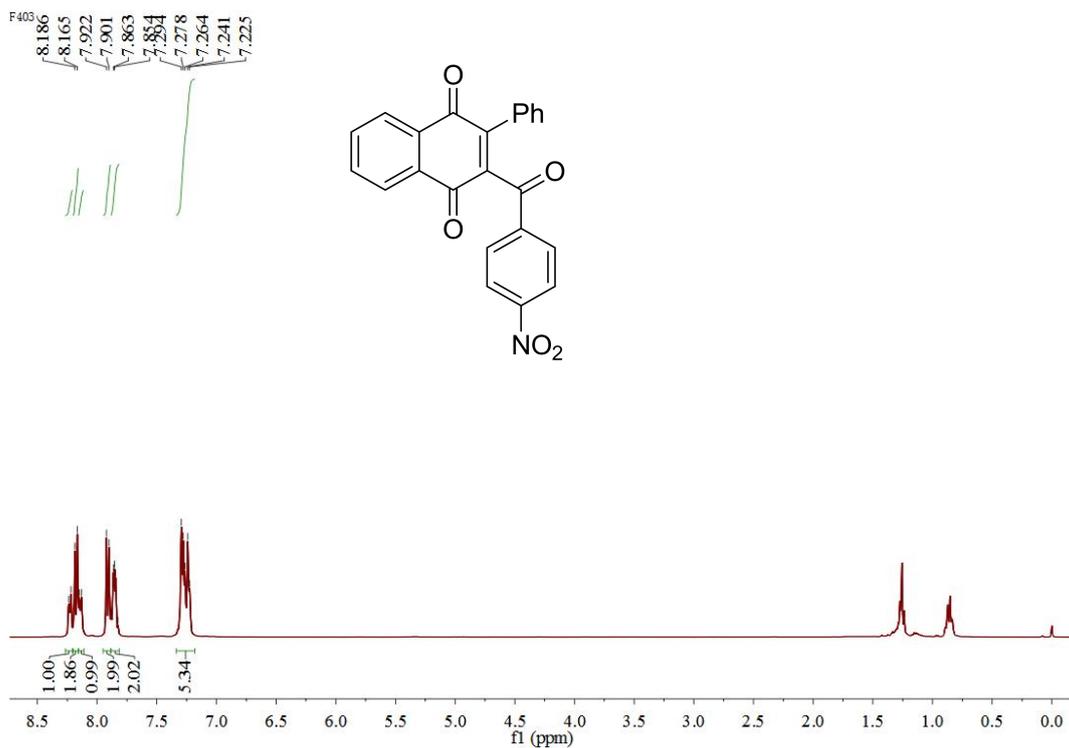
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4l



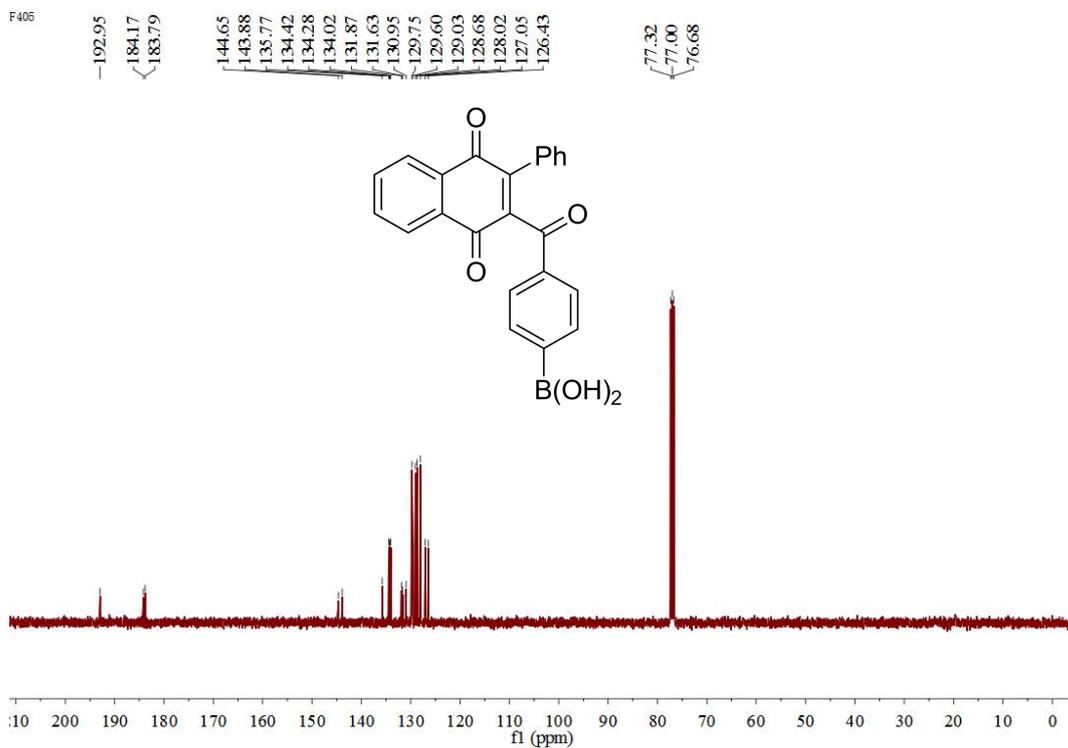
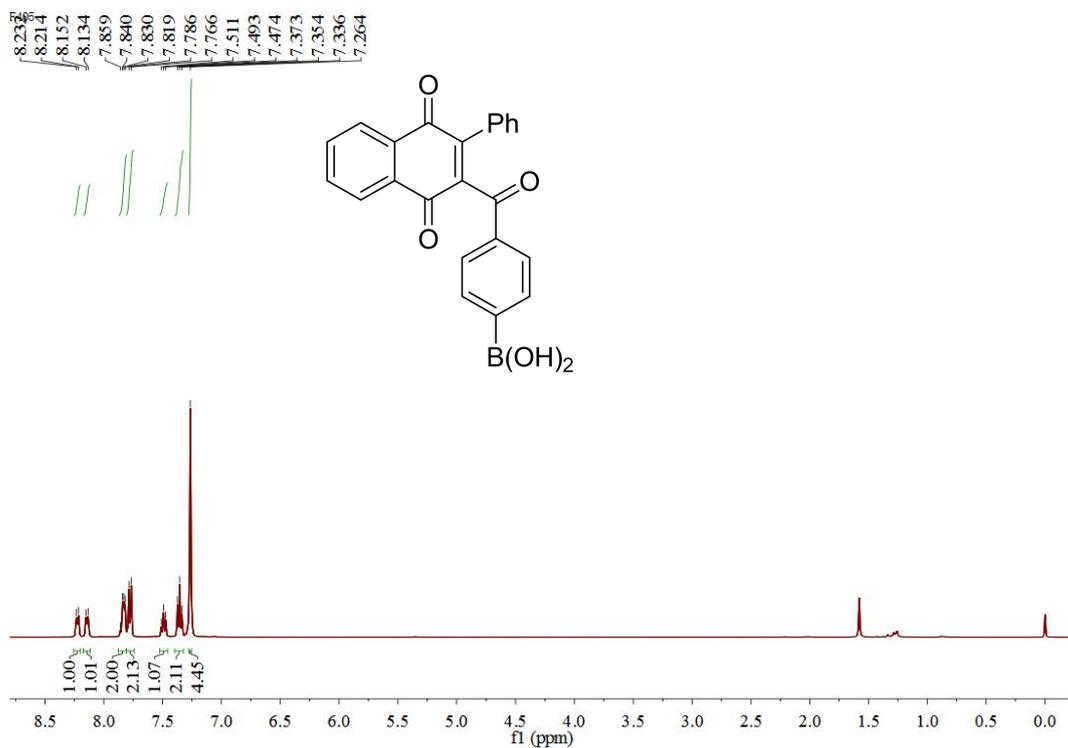
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4m



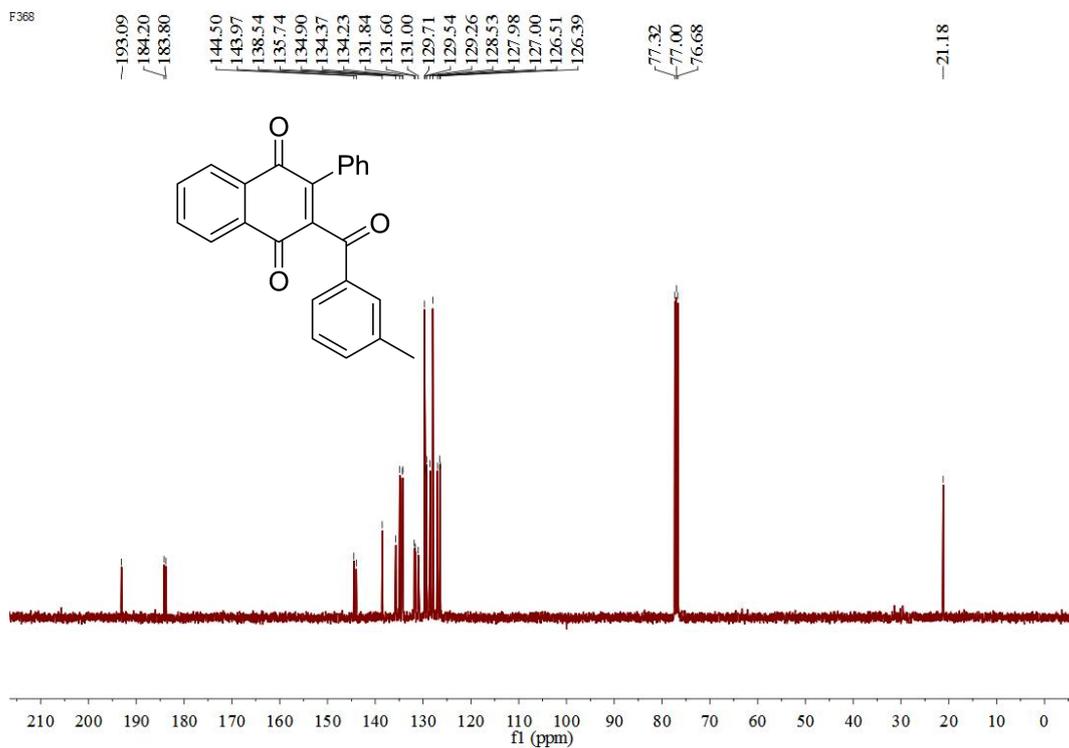
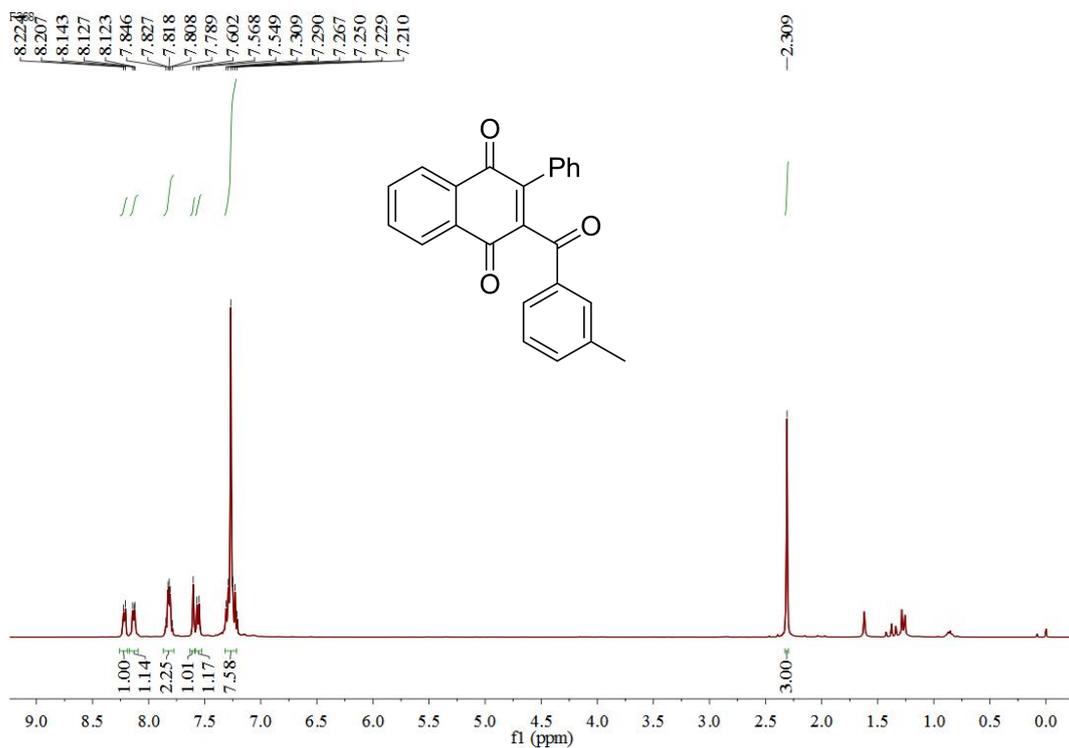
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4n



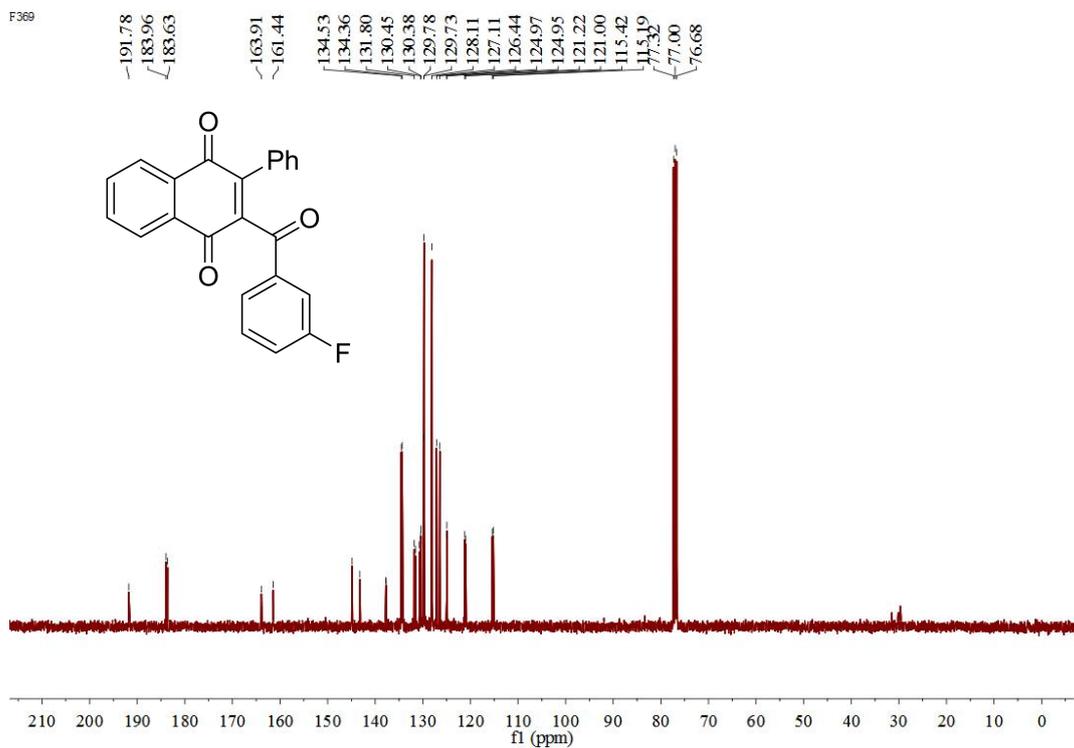
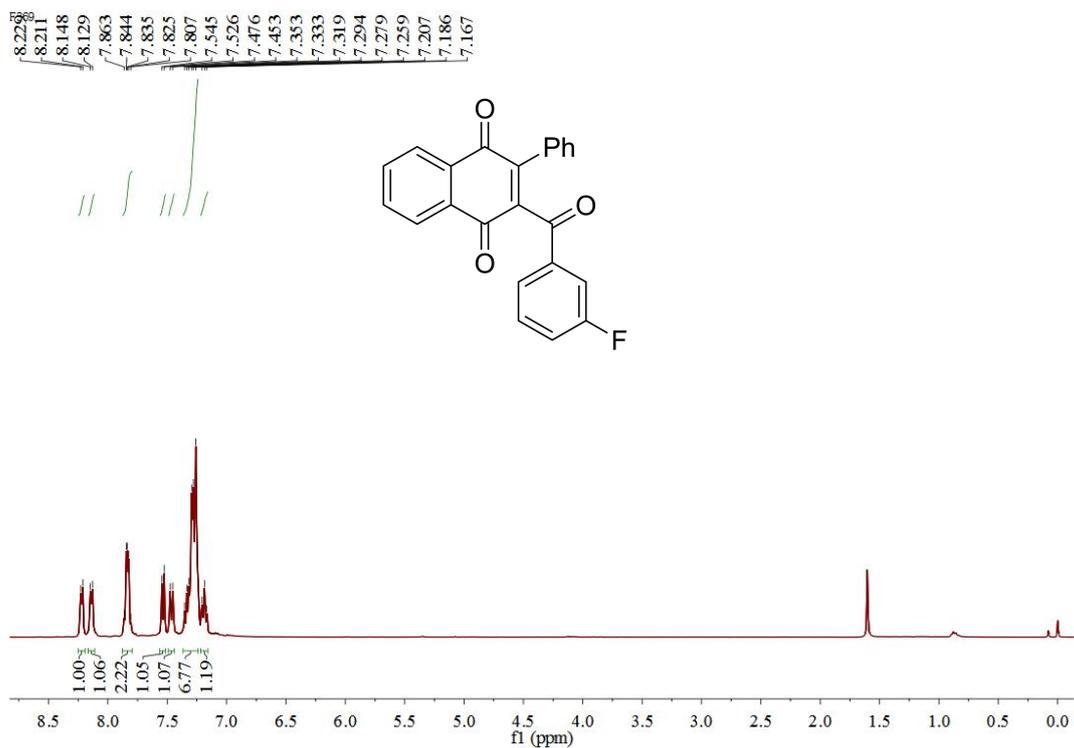
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4o



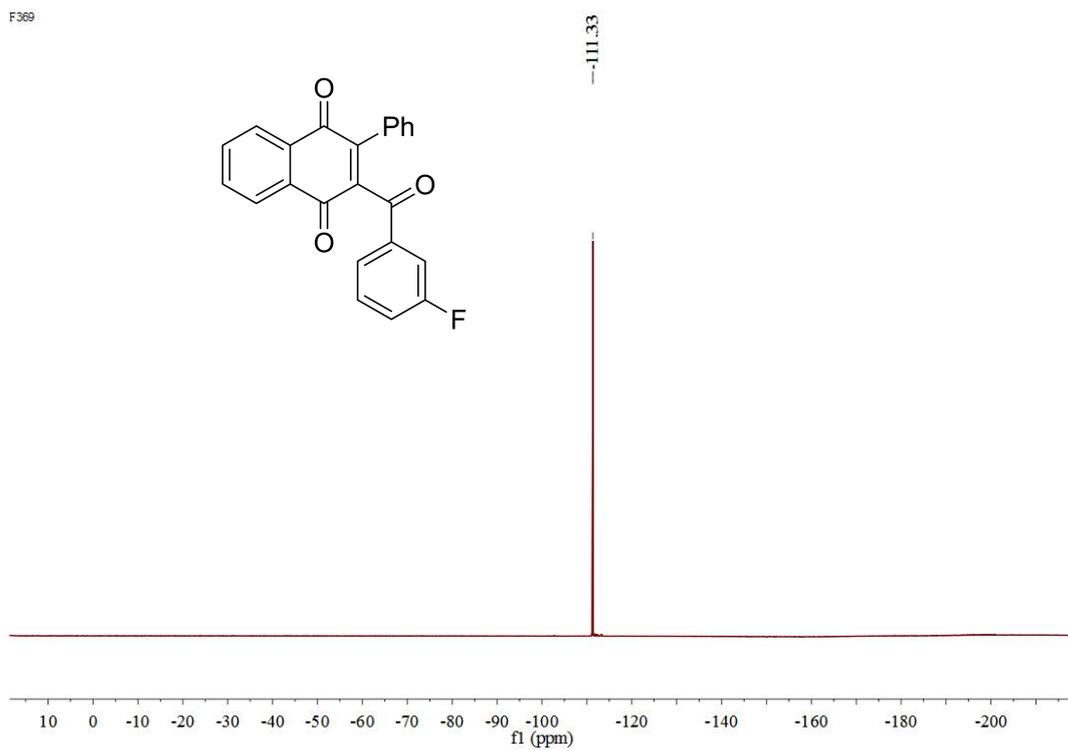
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4p



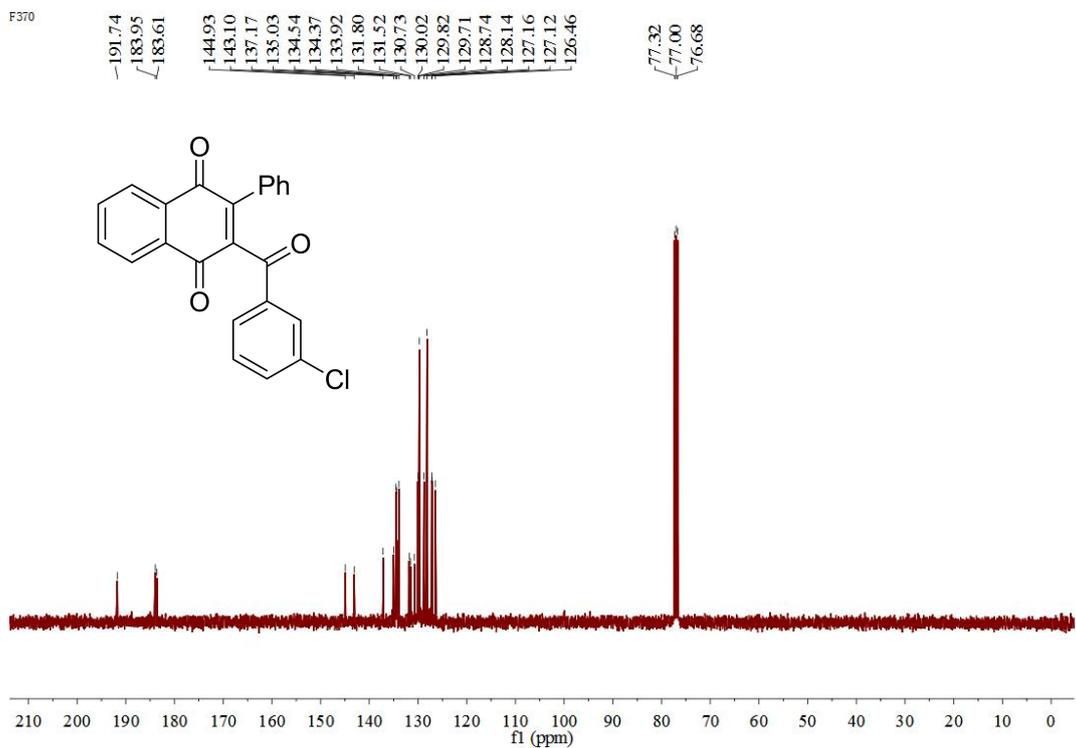
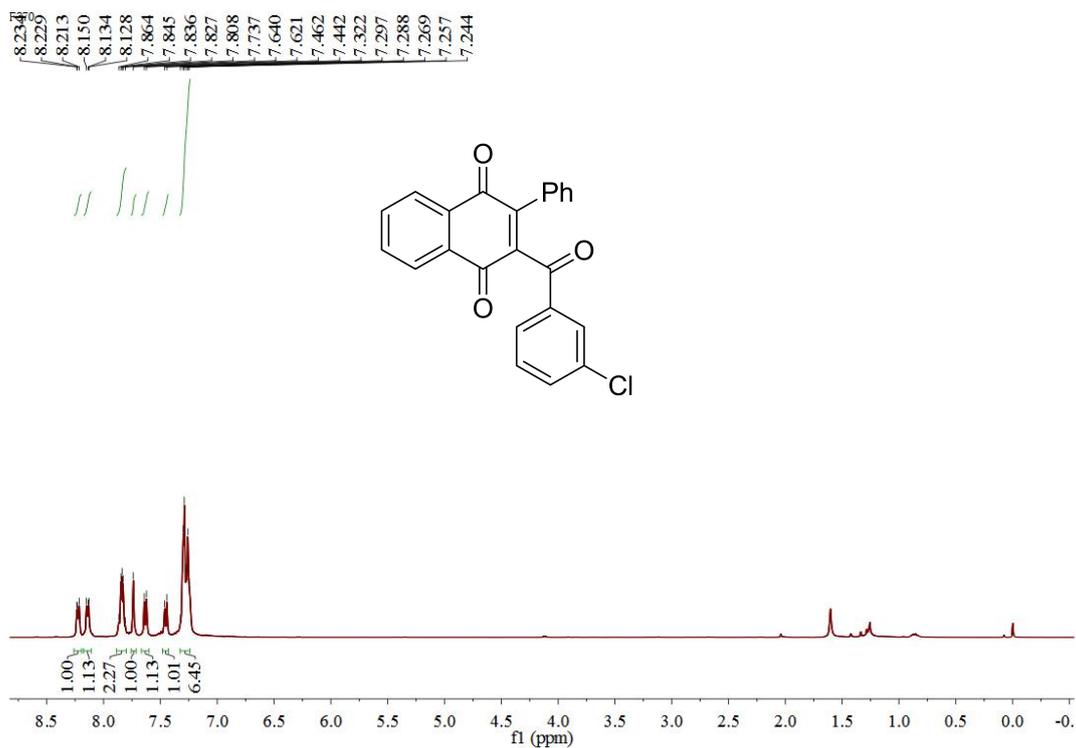
# <sup>1</sup>H NMR, <sup>13</sup>C NMR and <sup>19</sup>F NMR of 4q



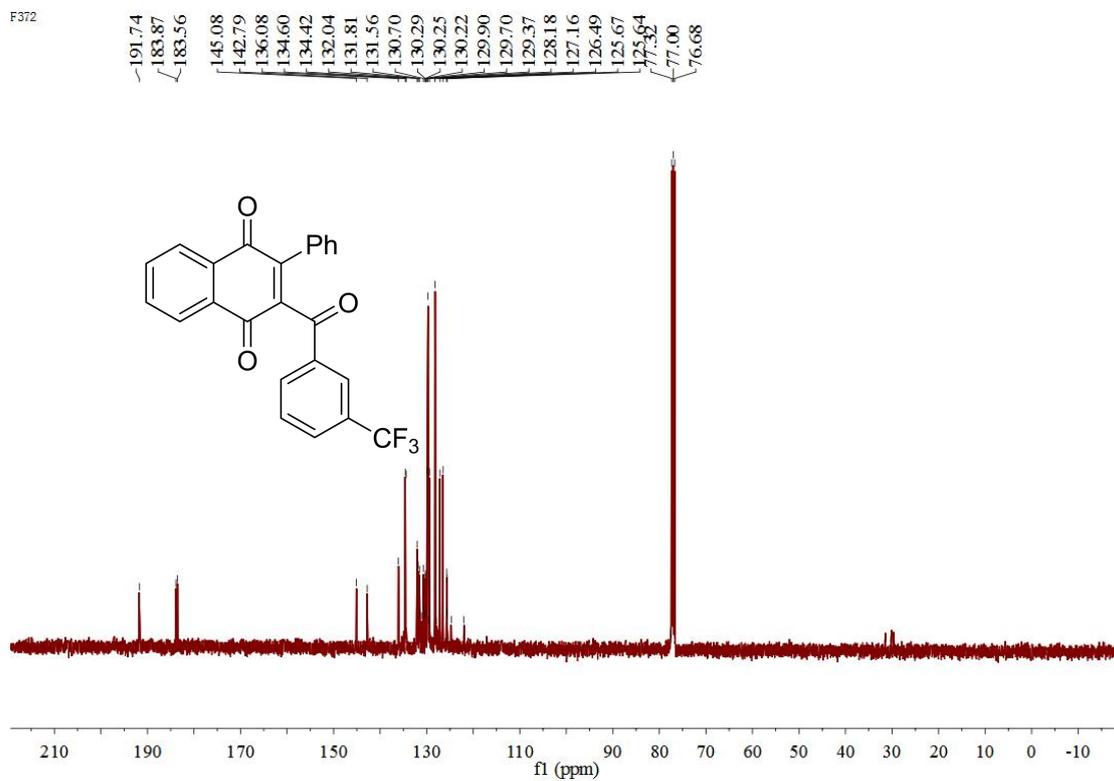
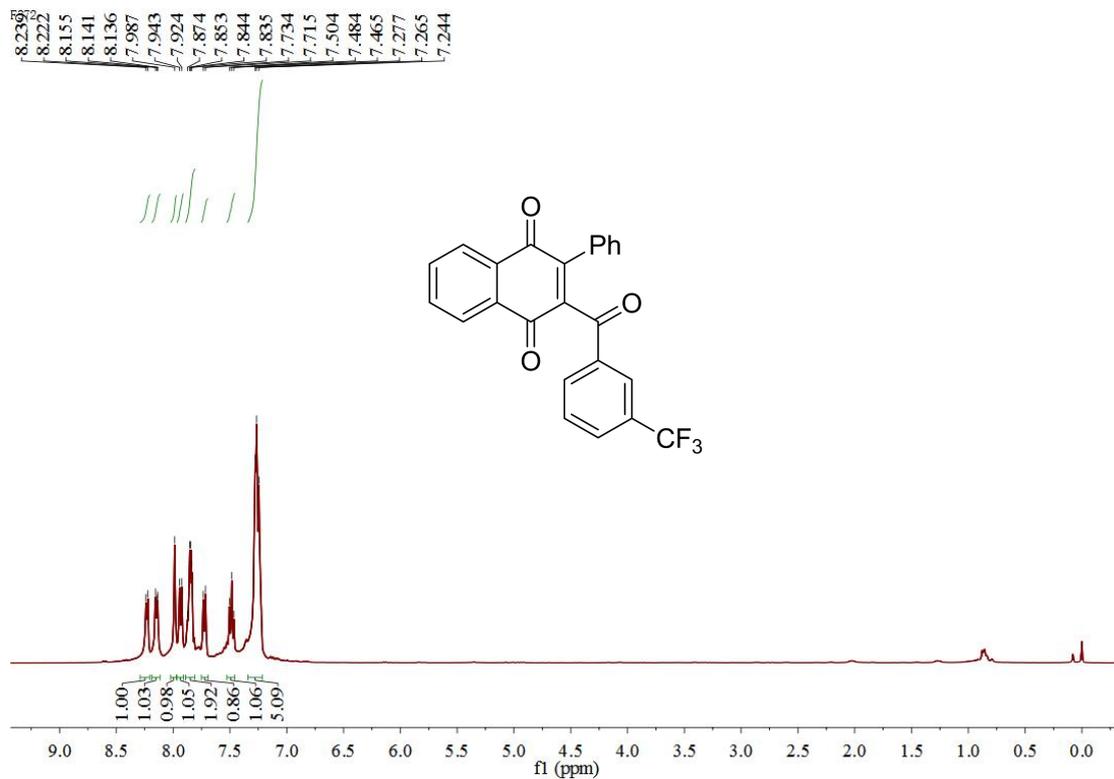
F369



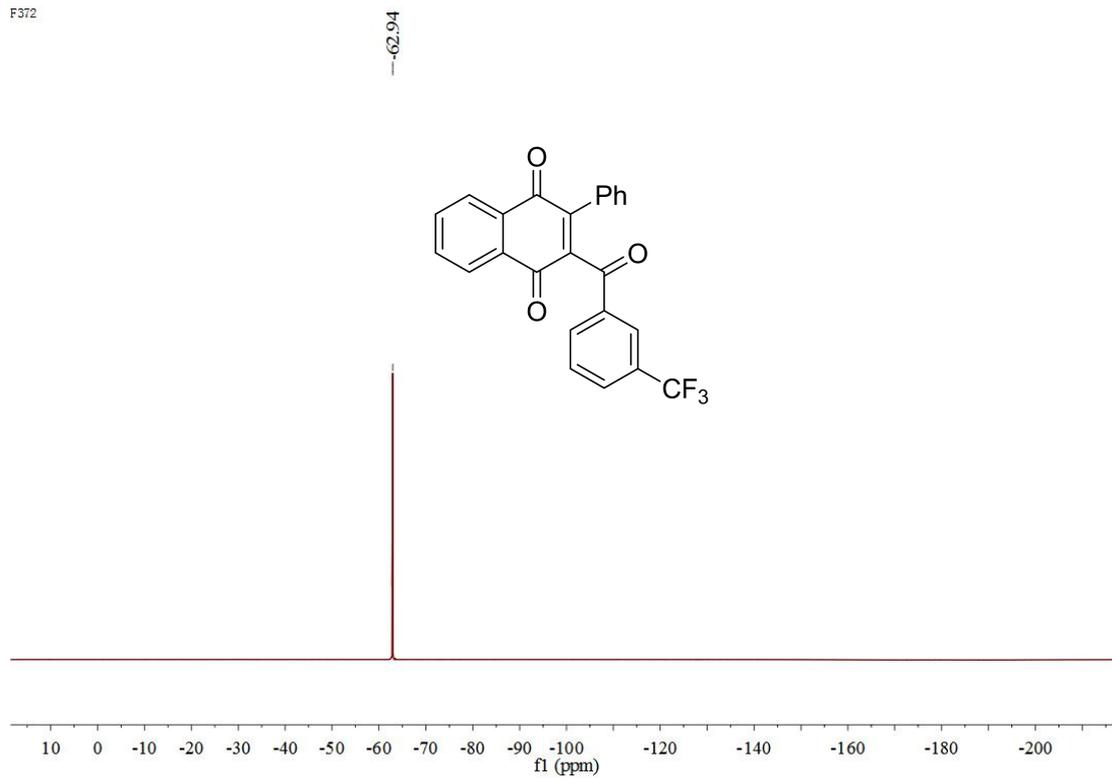
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4r



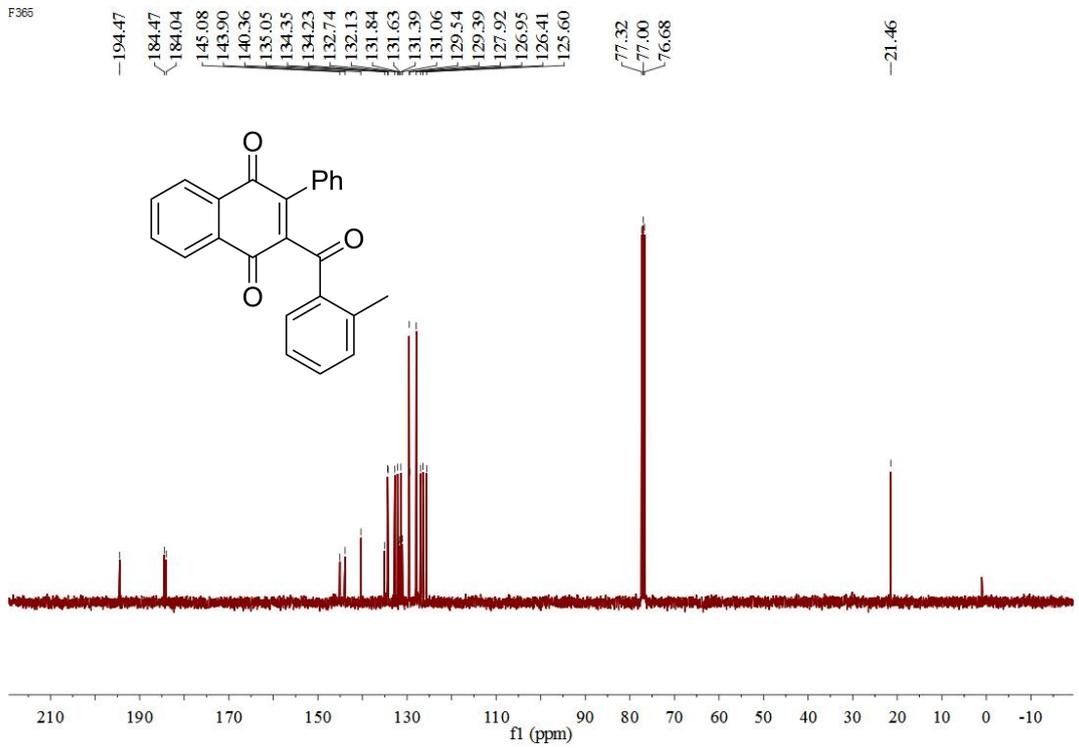
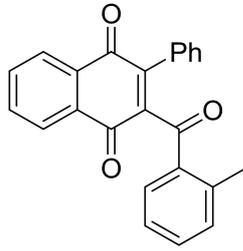
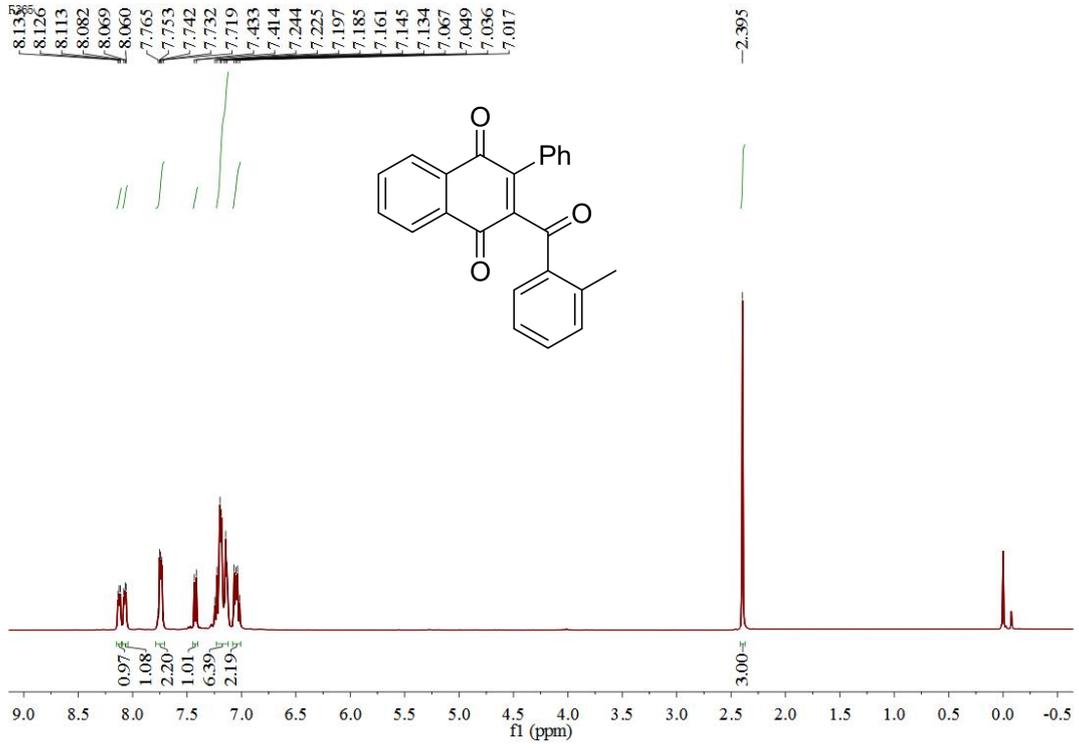
# <sup>1</sup>H NMR, <sup>13</sup>C NMR and <sup>19</sup>F NMR of 4s



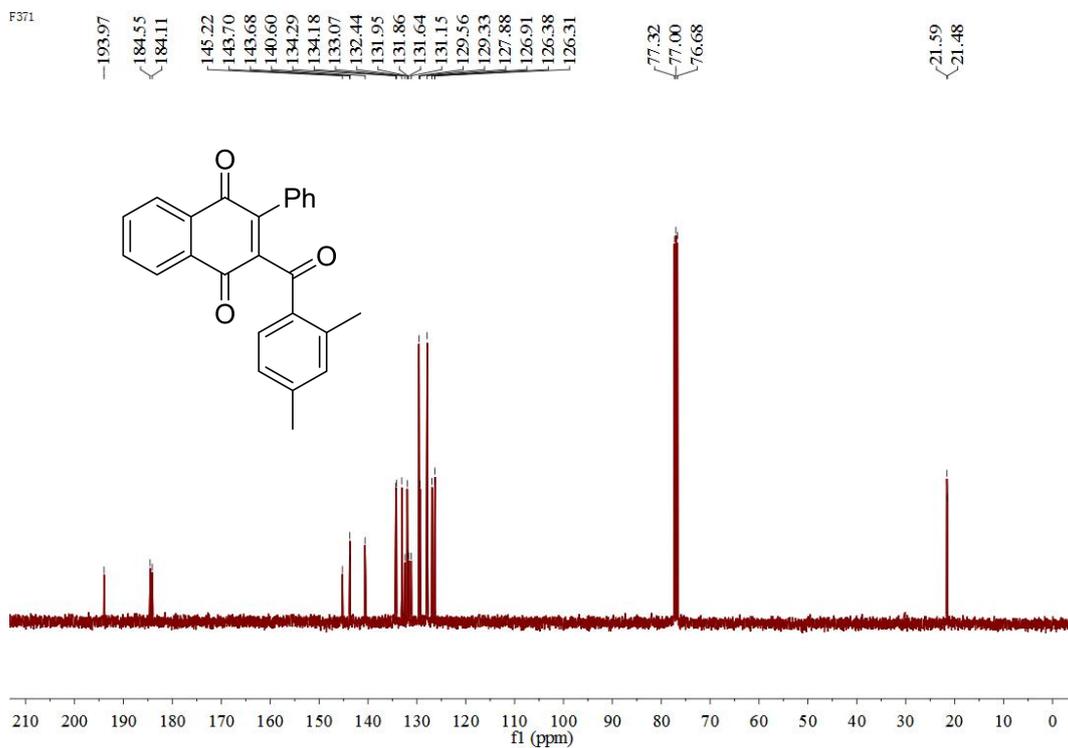
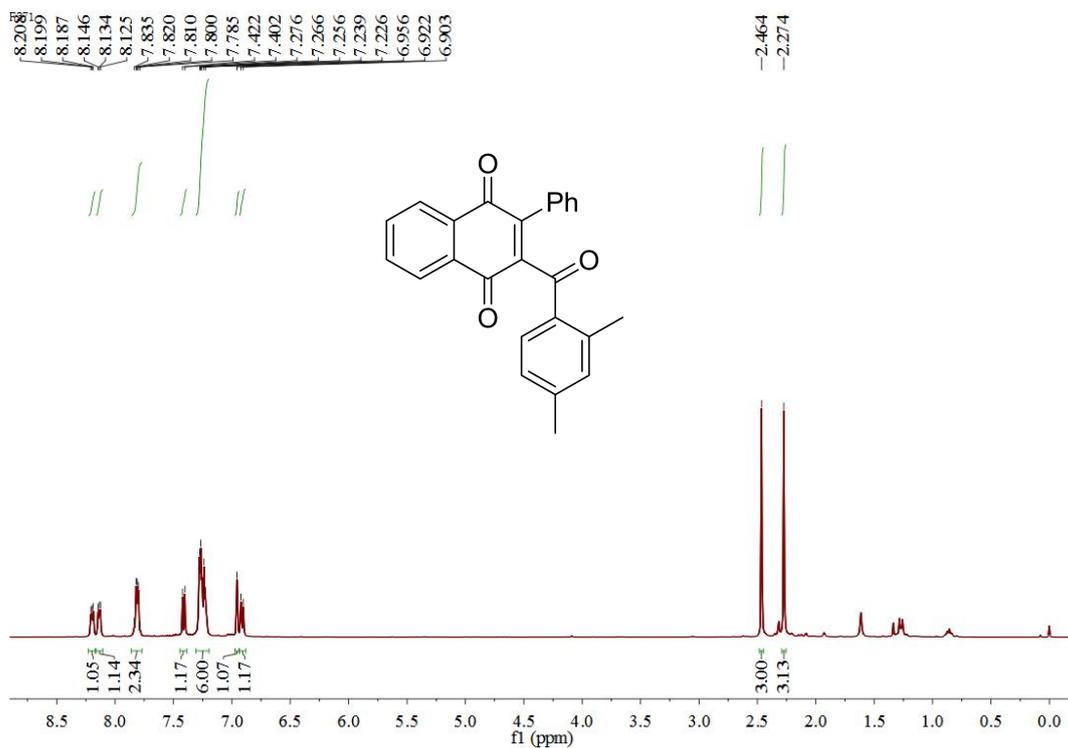
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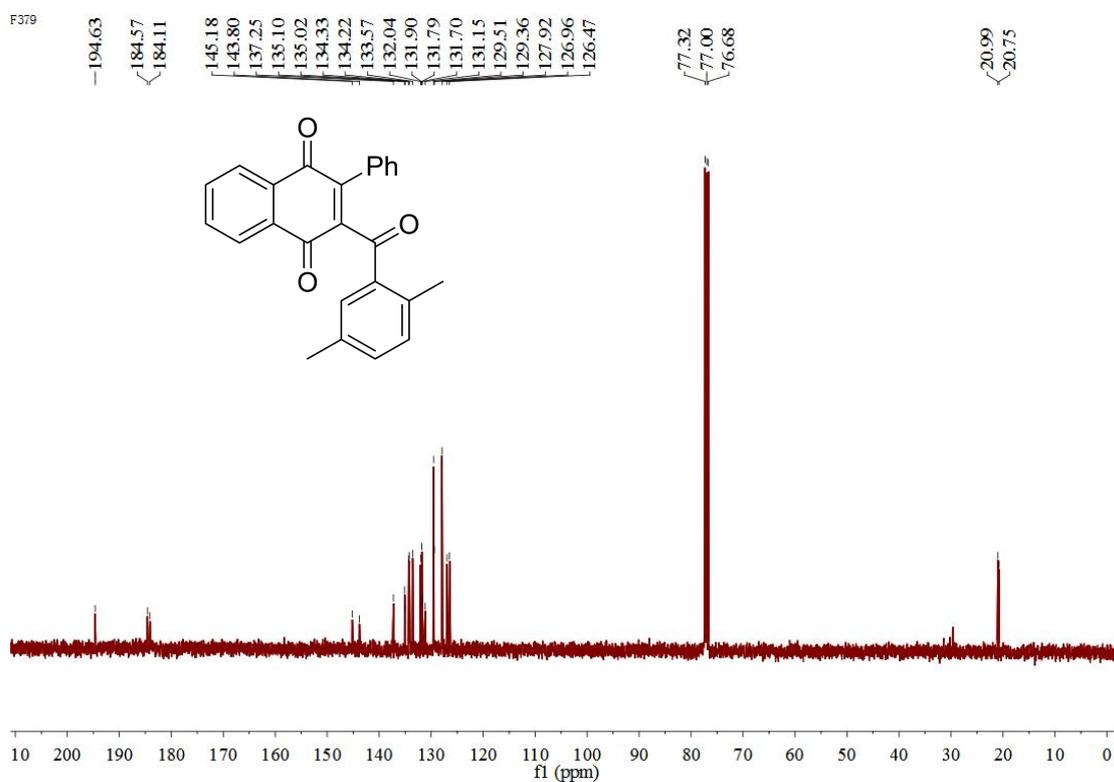
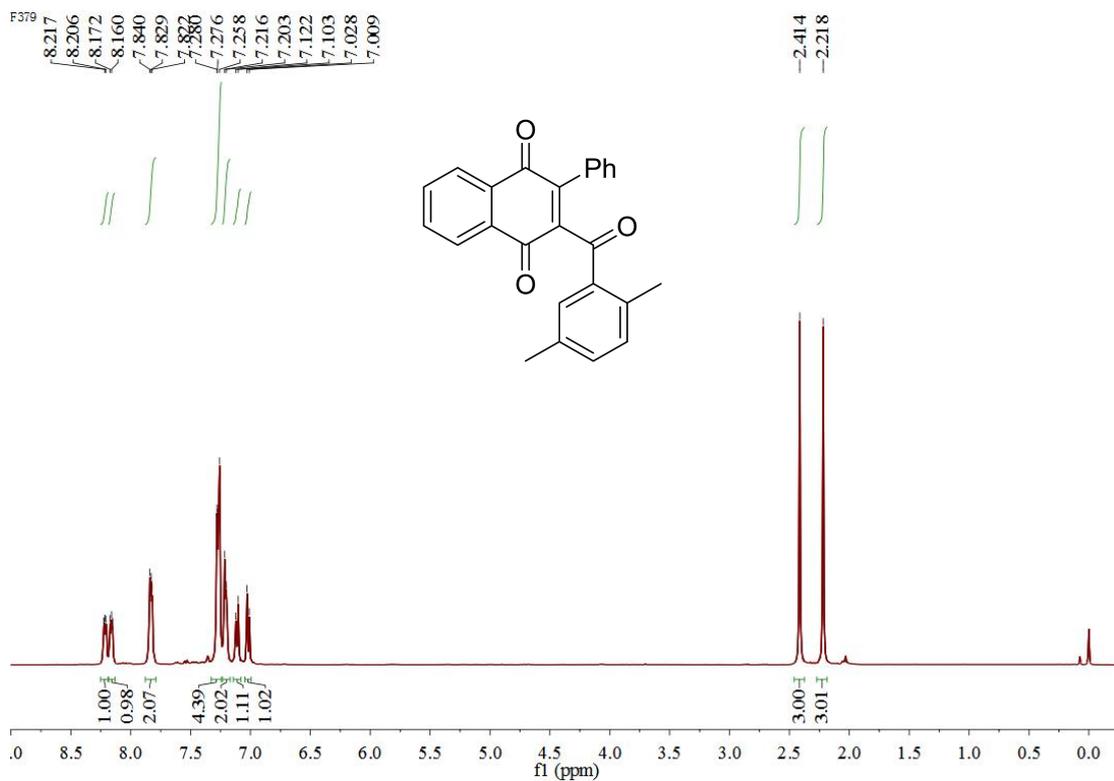
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4t



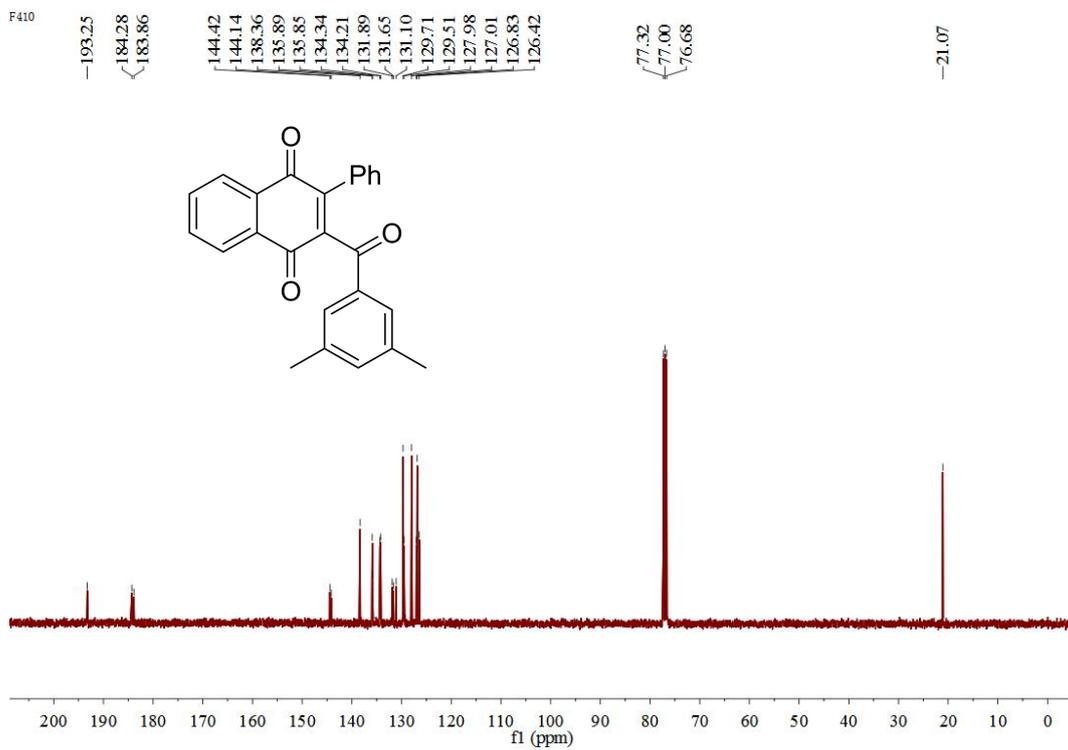
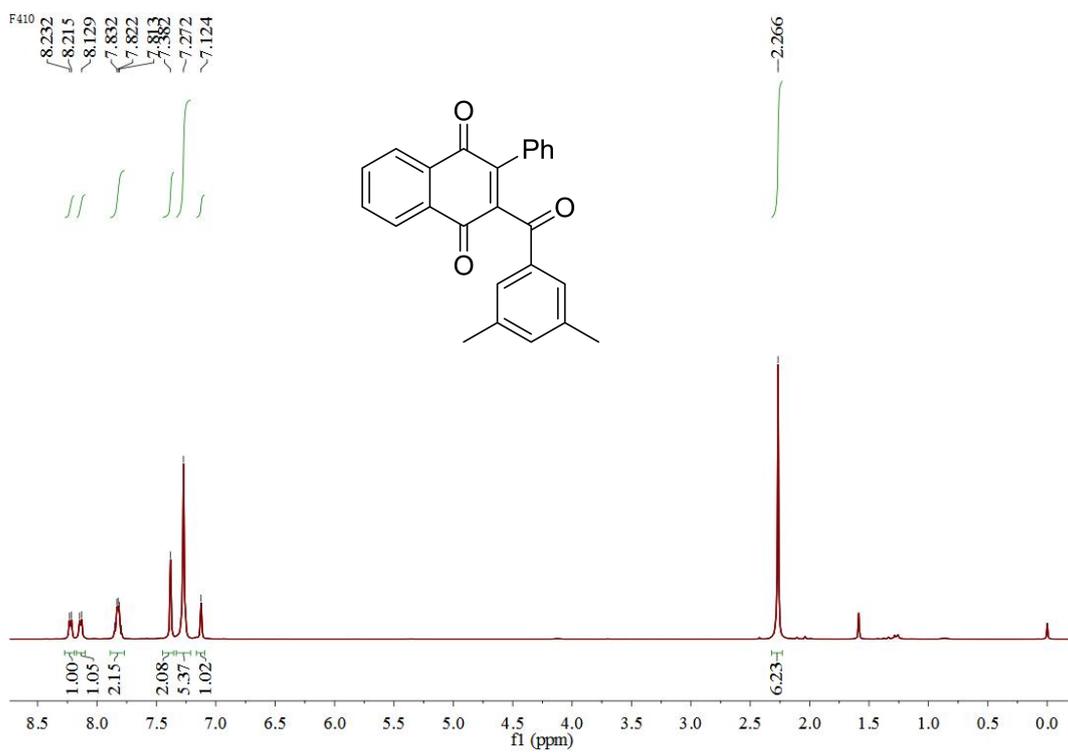
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4u



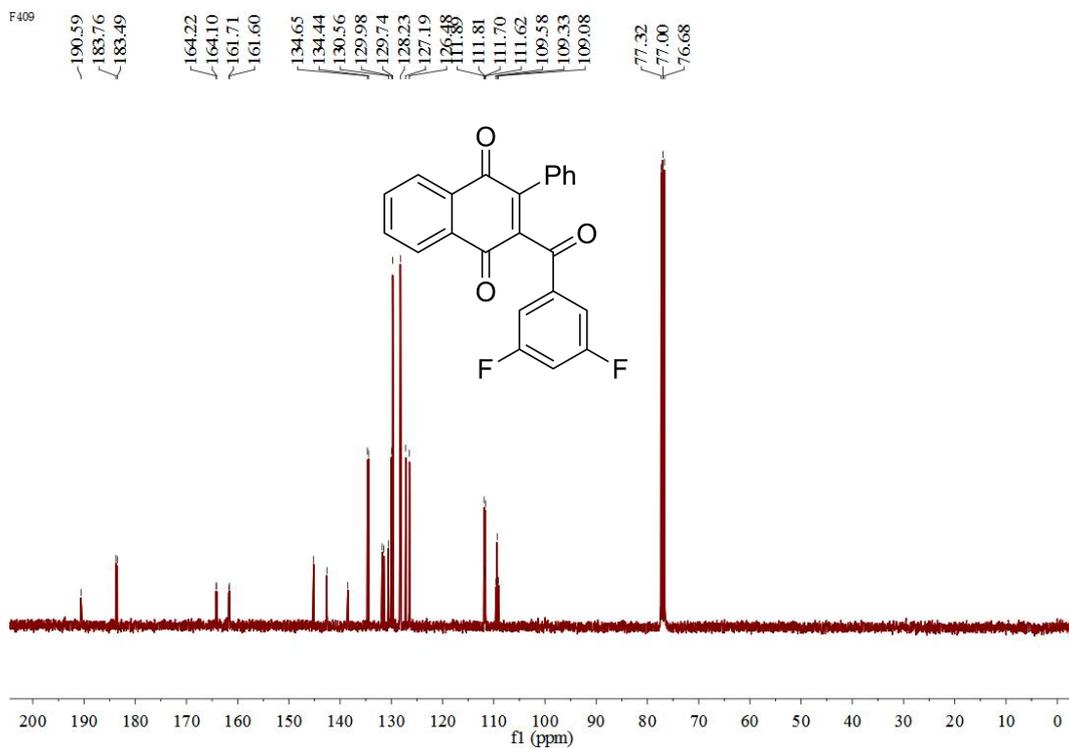
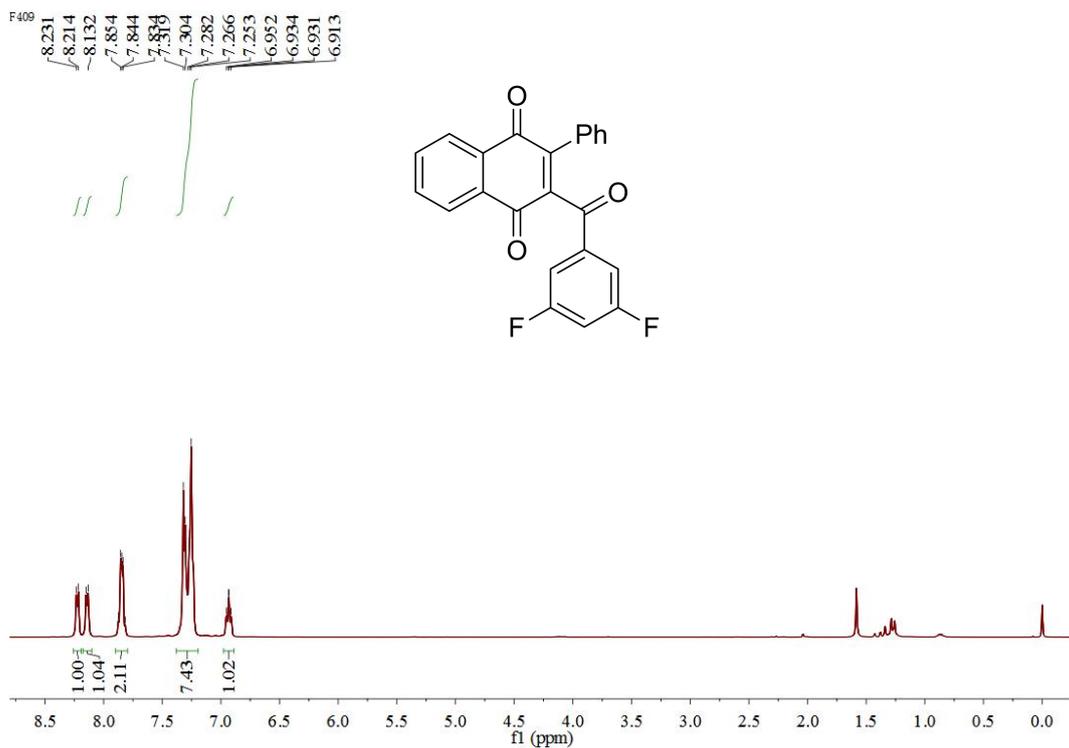
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4v



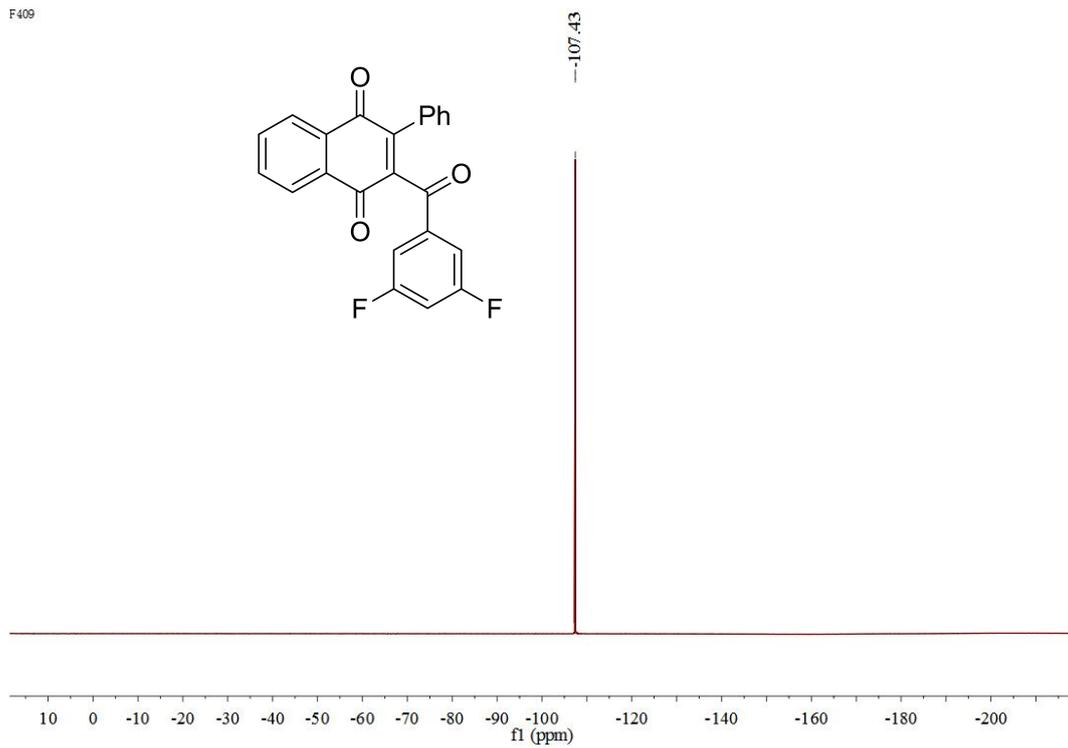
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4w



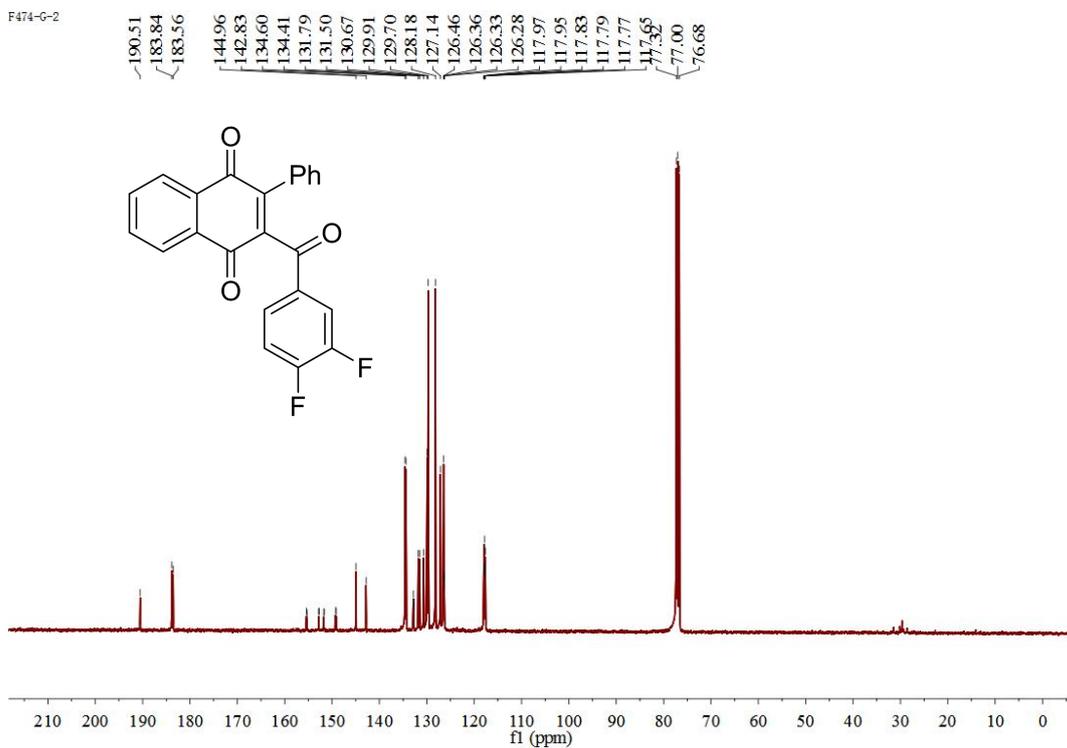
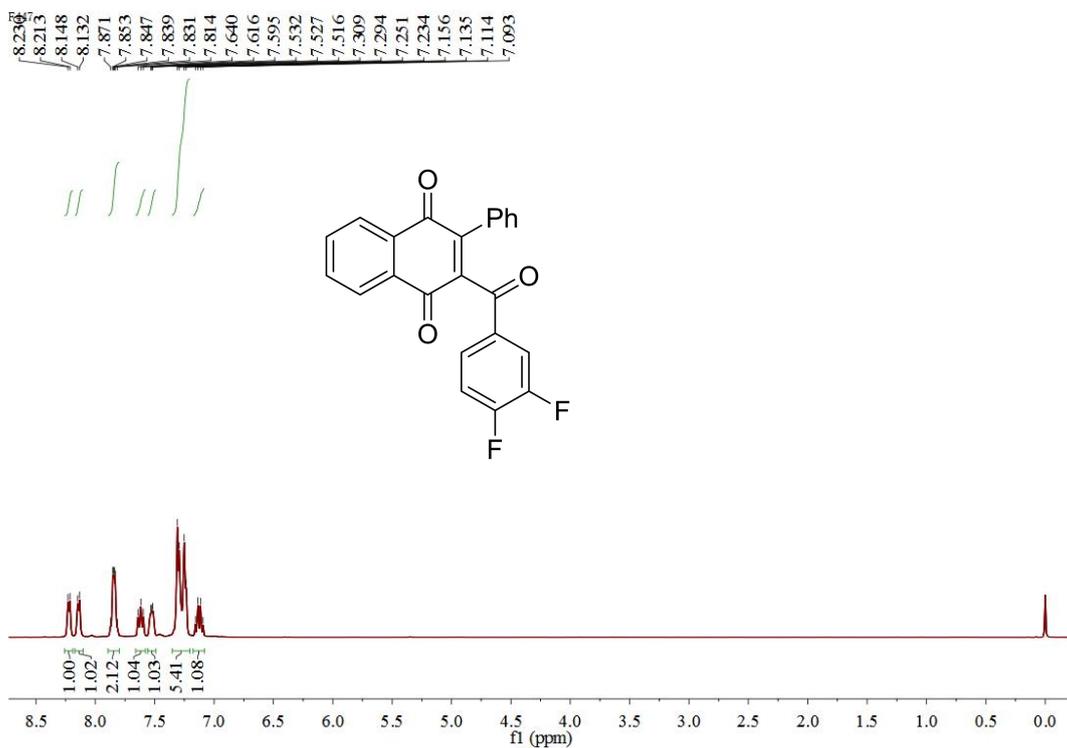
# <sup>1</sup>H NMR, <sup>13</sup>C NMR and <sup>19</sup>F NMR of 4x



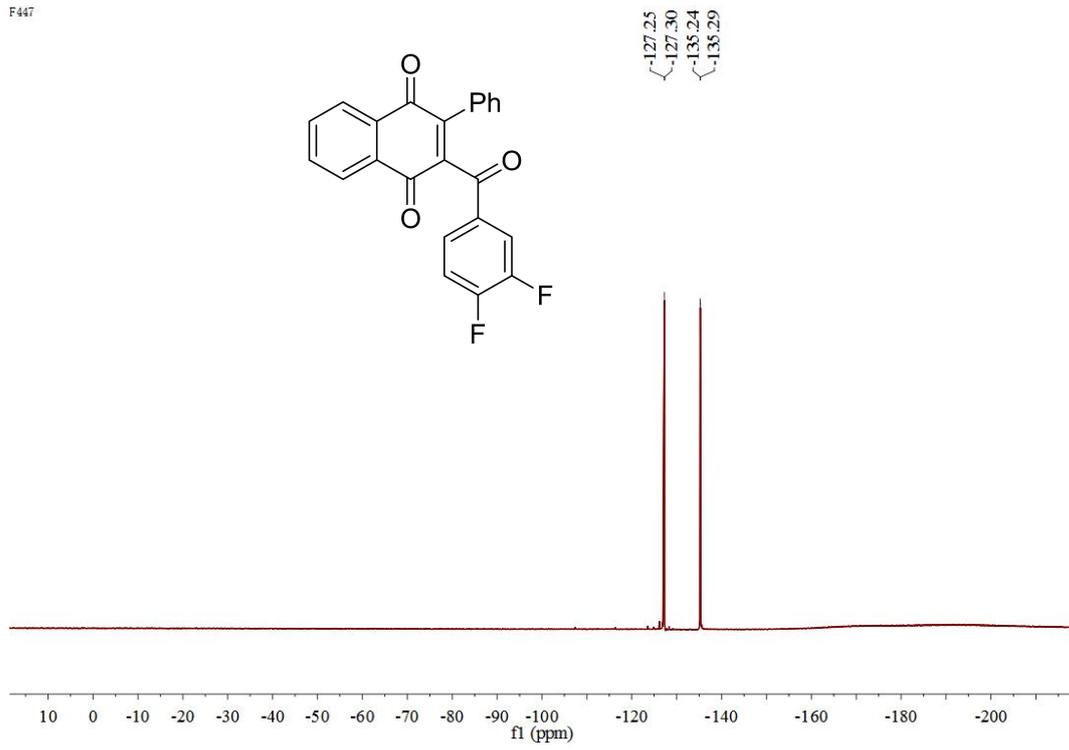
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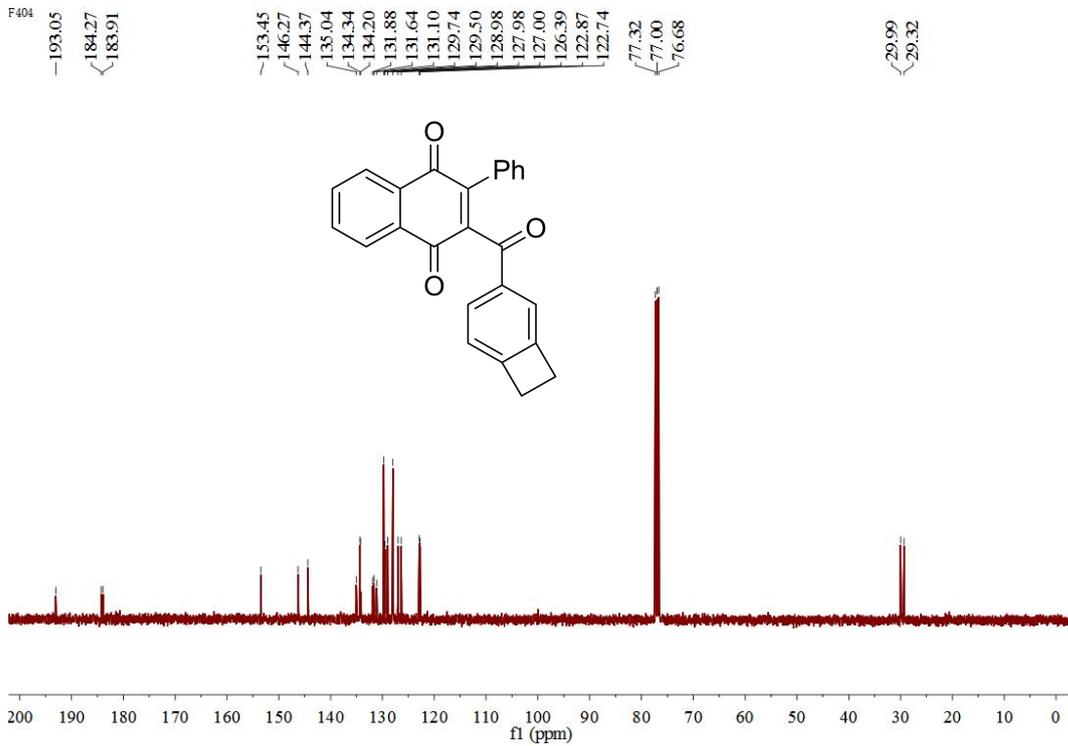
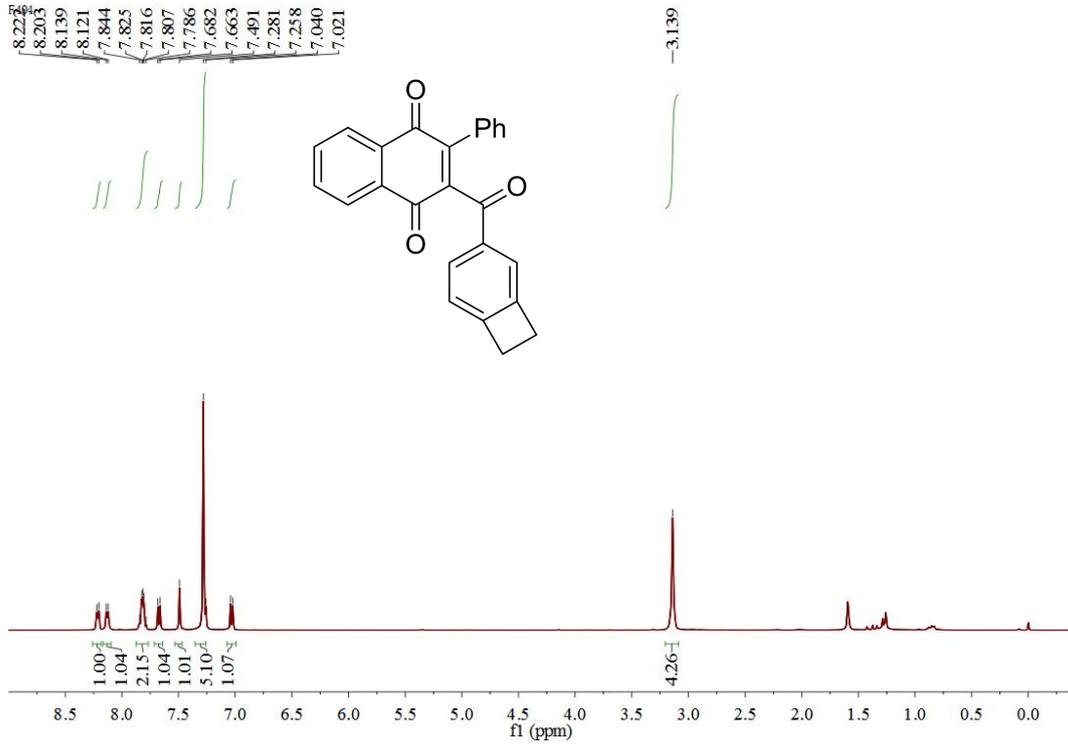
# <sup>1</sup>H NMR, <sup>13</sup>C NMR and <sup>19</sup>F NMR of 4y



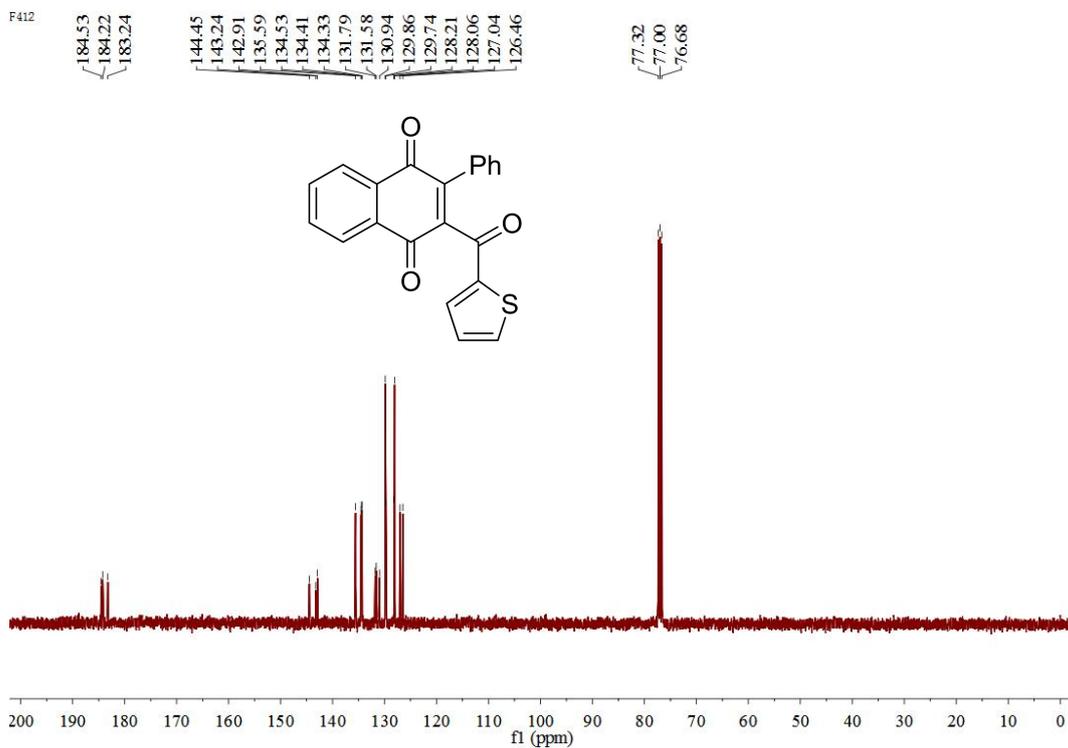
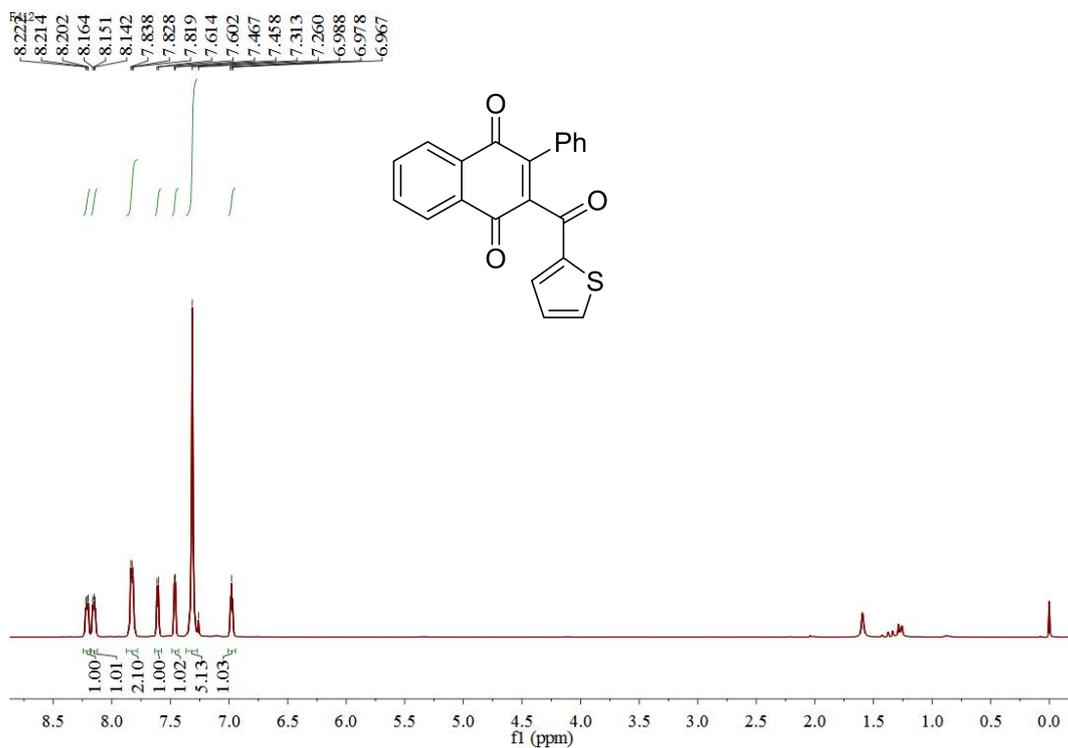
F447



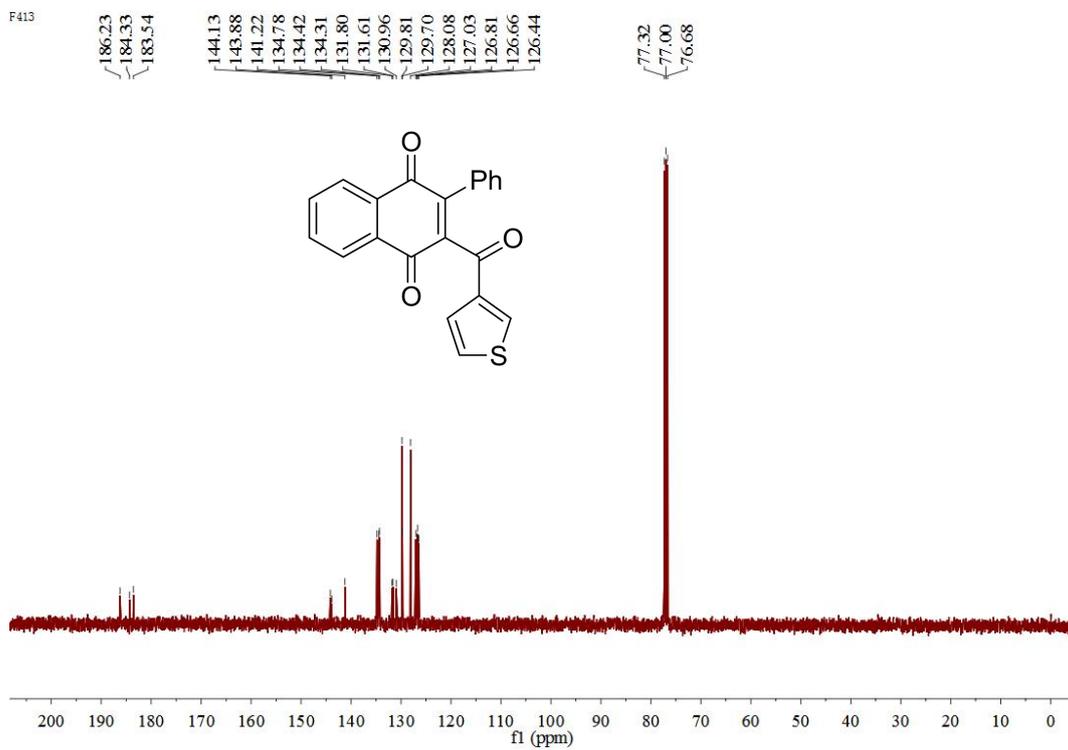
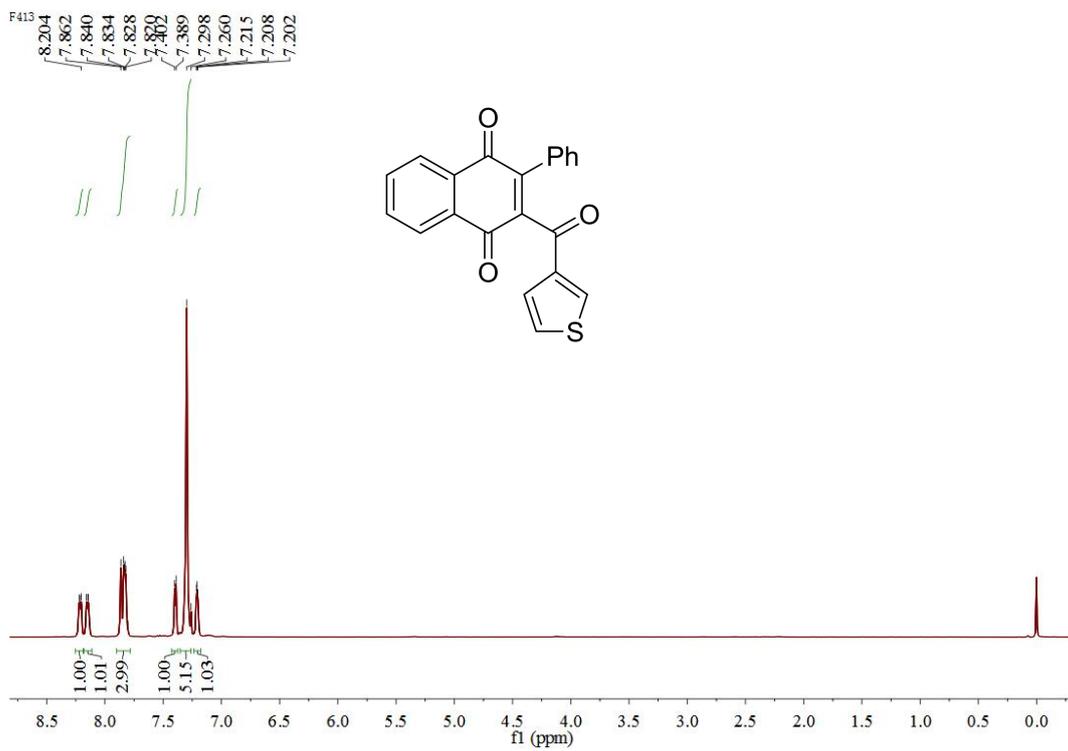
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4z



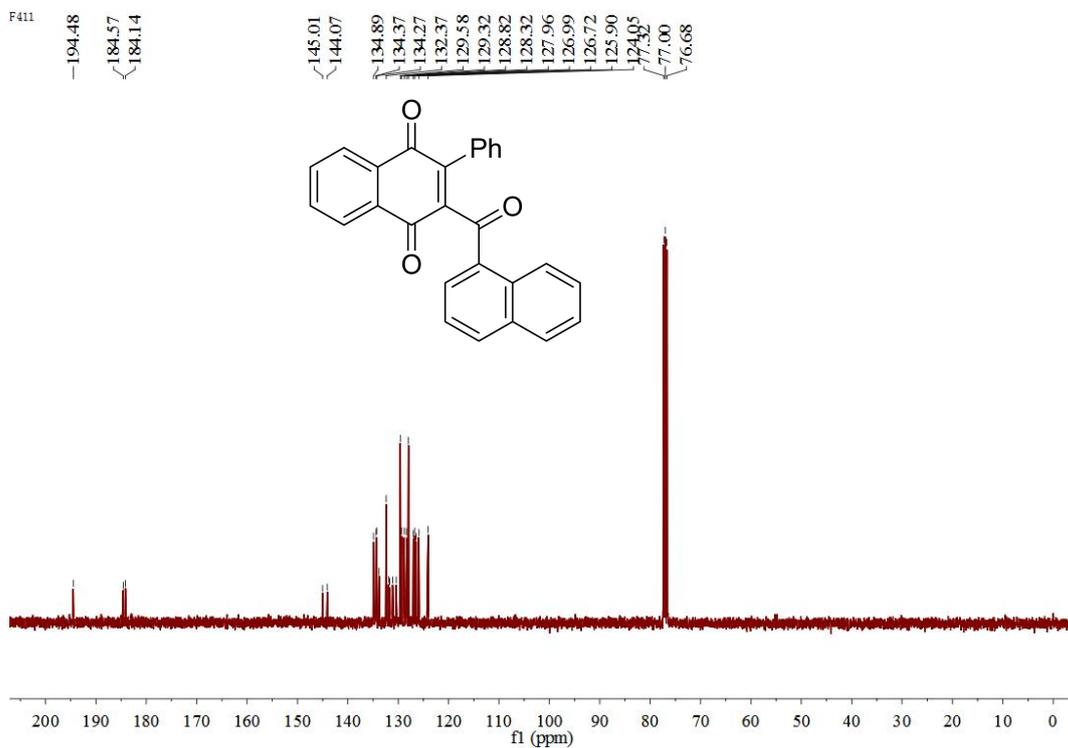
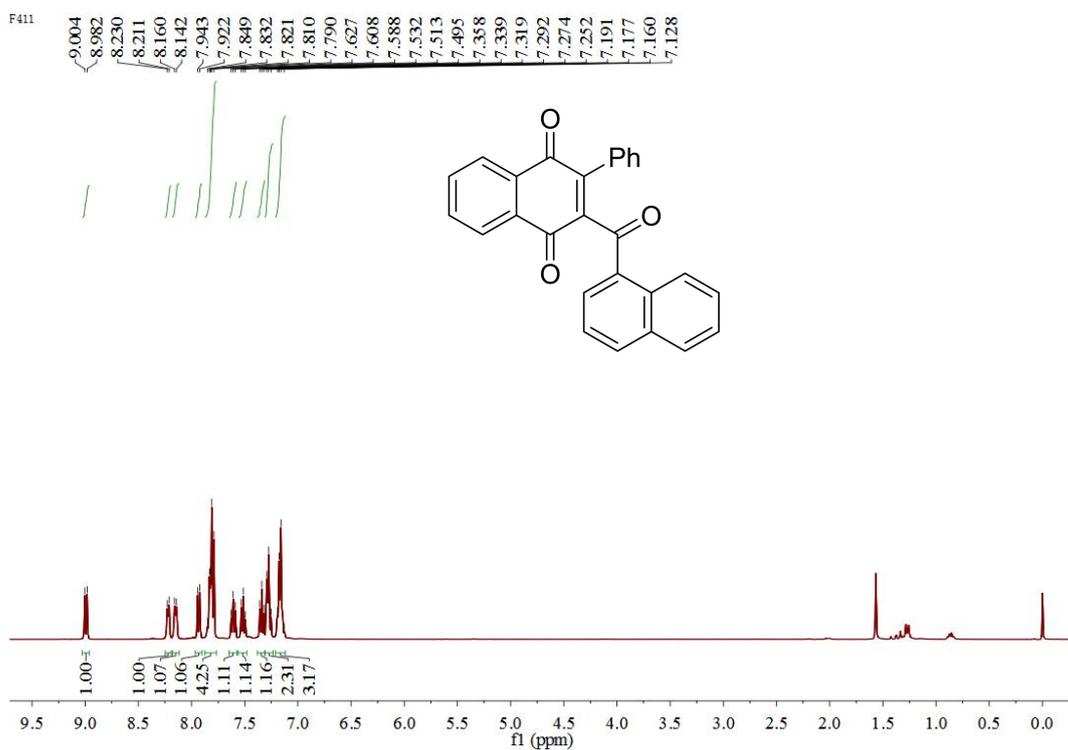
# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4aa



# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4ab



# $^1\text{H}$ NMR and $^{13}\text{C}$ NMR of 4ac



# <sup>1</sup>H NMR and <sup>13</sup>C NMR of 4ad

