# Supporting Information

# Synthesis of Dibenzofurans via Palladium-Catalyzed Phenol-Directed C-H Activation/C-O Cyclization

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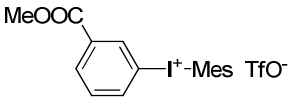
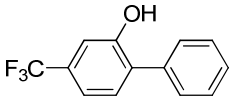
**General Remark:**

Mesitylene (>99%) was purchased from commercial source and used without further treatment. MS 3A (Acros, <50 μM) was used after drying under vacuum at 120 $^{o}$C for 12h. Analytical TLC was done on pre-coated silica gel plates. Column chromatography was conducted with 300-400 mesh silica gel. $^{1}$H NMR spectra were recorded on 400 MHz spectrometers. Chemical shifts of $^{1}$H NMR spectra were reported in parts per million relative to tetramethylsilane ($\delta$ = 0). $^{13}$C NMR spectra were recorded on 100 MHz spectrometers. Chemical shifts were reported in parts per million relative to the solvent resonance as the internal standard ($CDCl_3$, δ 77.16 ppm). High-resolution mass spectra (HRMS) were recorded on a BRUKER VPEXII spectrometer with EI mode unless otherwise stated.

**Table S1**:

| Reagent | Literature or Commercial Source |
|---|---|
| $Pd(OAc)_2$<br>4,5-Diazafluoren-9-one | Aldrich |
| $Pd(OPiv)_2$ | Bancroft, D. P.; Cotton, F. A.; Falvello, L. R.; Schwotzer, W. *Polyhedron* **1988**, *7*, 615. |
| IPr<br>$PhI(OAc)_2$<br>Biphenyl-2-ol<br>Estrone | TCI |
| MesCOOH<br>HOTf | Alfa Aesar |
| Ms 3A<br>Mesitylene | Acros |
|  | Phipps, R. J.; Gaunt, M. J. *Science* **2009**, *323*, 1593. |
| 2-Hydroxyphenylboronic acid | Frontier Scientific |
|  | Xiao, B.; Fu, Y.; Xu, J.; Gong, T.-J.; Dai, J.-J.; Yi, J.; Liu, L. *J. Am. Chem. Soc.* **2010**, *132*, 468. |

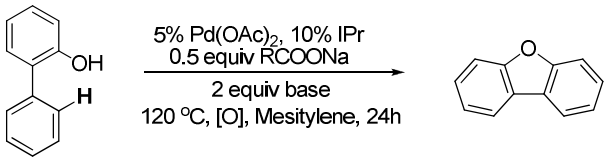
**General Procedure for The Synthesis of 1a':**

To a 10 mL vial was sequentially added biphenyl-2-ol (17.0 mg, 0.1 mmol), $Pd(OPiv)_2$ (32.3 mg, 0.105 mmol), IPr (40.7 mg, 0.105 mmol), $K_2CO_3$ (41.4 mg, 0.3 mmol) and toluene (0.5 mL). The vial was stirred at 90 $^{o}$C for 15 minutes then the

reaction mixture was purified by flash chromatography using $CH_2Cl_2$ to remove the unreacted biphenyl-2-ol(8.4 mg, 49%). $CH_2Cl_2$ and MeOH(20:1) were then used to give the desired Palladecycle as a white solid(35.4 mg, 41%).

Evaporation of the chloroform solution of **1a'** gave colourless crystals for X-ray analysis.

**Table S2:** Optimization of Reaction Conditions [a]




| Entry | RCOOM | base | [O] | Yield %[b] |
|---|---|---|---|---|
| 1 | - | $K_2CO_3$ | air | 23 |
| 2 | - | $K_2CO_3$ | $Cu(OAc)_2$ | 0 |
| 3 | - | $K_2CO_3$ | AgOAc | 0 |
| 4 | - | $K_2CO_3$ | BQ | 0 |
| 5 | AcONa | $K_2CO_3$ | air | 15 |
| 6 | PivONa | $K_2CO_3$ | air | 47 |
| 7 | 1-AdCOONa | $K_2CO_3$ | air | 27 |
| 8 | PhCOONa | $K_2CO_3$ | air | 30 |
| 9 | MesCOONa | $K_2CO_3$ | air | 59 |
| 10 | 2,4,6-$OMeC_6H_2COONa$ | $K_2CO_3$ | air | 24 |
| 11 | 2,4,6-$iPrC_6H_2COONa$ | $K_2CO_3$ | air | 11 |
| 12 | 2-Ph-$C_6H_4COONa$ | $K_2CO_3$ | air | 26 |
| 13 | 2-OPh-$C_6H_4COONa$ | $K_2CO_3$ | air | 38 |
| 14 | MesCOONa | - | air | 0 |
| 15 | MesCOONa | CsOPiv | air | 0 |
| 16 | MesCOONa | $Na_2CO_3$ | air | 0 |
| 17 | MesCOONa | $Rb_2CO_3$ | air | 36 |
| 18 | MesCOONa | $Cs_2CO_3$ | air | trace |
| 19 | MesCOONa | NaO*t*Bu | air | 0 |
| 20 | MesCOONa | KO*t*Bu | air | 0 |
| 21 [c] | MesCOONa | $K_2CO_3$ | air | 67 |
| 22 [c,d] | **MesCOONa** | **$K_2CO_3$** | **air** | **90(85)** |
| 23 [c,d] | MesCOONa | $K_2CO_3$ | $O_2$ | 81 |
| 24 [c,d,e] | MesCOONa | $K_2CO_3$ | air | 0 |
| 25 [c,d,f] | MesCOONa | $K_2CO_3$ | air | 0 |

[a] All the reactions were carried out in 0.2 mmol scale, 1 mL Mesitylene. [b] GC yields with *n*-decane as an internal standard and isolated yield in parentheses. [c] MS 3A(200 mg) was added. [d] 10% 4,5-Diazafluoren-9-one was added. [e] IPr NOT used. [f] biphenyl-2,2'-diol as starting material.

**Synthesis of MesCOONa:**

A solution of *t*BuONa and 1.05 equiv MesCOOH in MeOH was stirred at room temperature for 2h. The solvent was removed in vacuum. $Et_2O$ was added and the reaction was violently stirred over night. The white solid was filtered out, washed with $Et_2O$, dried under vacuum. >95% yield.

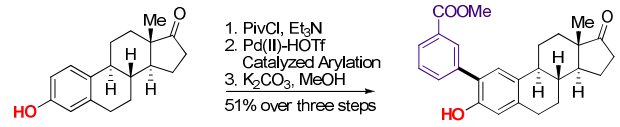
**General Procedure for The Intramolecular C-O Crosscoupling:**

To a diameter of 17 mm, 100 mm long vial was sequentially added substrate (0.2 mmol), $Pd(OAc)_2$ (2.3 mg, 0.01 mmol), IPr (7.8 mg, 0.02 mmol), 4,5-diazafluoren-9-one (3.7 mg, 0.02 mmol), MesCOONa (18.6 mg, 0.1 mmol), $K_2CO_3$ (55 mg, 0.4

mmol), MS 3A (200 mg) and 1 mL Mesitylene. The vial was stirred at room temperature for 1 minutes and then stirred at the 120 °C under air (caution: The reaction must be put on the center of the magnetic stirrer. 750 r/min with a 7~9 mm long magnetic stirring bar was recommended). The reaction was monitored with TLC (EtOAc/petroleum ether, or $CH_2Cl_2$/petroleum Ether), then the mixture was diluted with 5 ml EtOAc and filtered. The solid was washed with 10 ml EtOAc and the combined filtrate was concentrated under vacuum. The crude product was purified by flash chromatography (Petroleum Ether, or EtOAc/Petroleum Ether, or $CH_2Cl_2$/Petroleum Ether) to give the desired product as white solid.

For the catalyst loading was doubled, after reaction for 12h, another 5% $Pd(OAc)_2$ and 10% IPr was added and kept stirring for the 12 more hours.

**Alyation of estrone:**

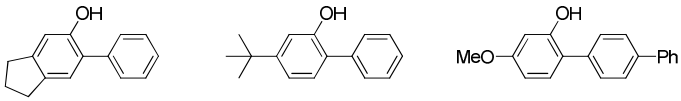



The Piv-ester of estrone was obtained by the reaction of estrone and PivCl in a mixed solvent of $CHCl_3$ and $Et_3N$ (1:1) in quantitative yield.

To a 10 mL vial was sequentially added Estrone ester (355 mg, 1 mmol), $Pd(OAc)_2$ (22.4 mg, 0.1 mmol), mesityl(3-(methoxycarbonyl)phenyl)iodonium trifluoromethane -sulfonate (636 mg, 1.2 mmol), $Piv_2O$ (93.2 mg, 0.5 mmol) and DCE (4 mL). The vial was stirred at room temperature for 5 minutes then HOTf (15 mg, 0.1 mmol) was added. The vial was sealed and stirred at the 25 °C for 24 h. The reaction mixture was purified by flash chromatography (EtOAc/Petroleum Ether 1:10) to give the desired product as a white solid (260 mg, 53%).

The arylation product of the Piv-ester was dissolved in 10 ml MeOH, $K_2CO_3$ (276 mg, 2 mmol) was added, and the mixture was stirred at room temperature for 2h and then diluted with water (40 ml), acided by HCl and extracted with $Et_2O$ (3 x 10 mL). The organic layer was dried with $MgSO_4$, concentrated, and the mixture was purified by flash chromatography (EtOAc/Petroleum Ether 1: 5) to give arylation product of estrone as a white solid (207 mg, 51% yield over three steps).

The following substrates were prepared by the same process:

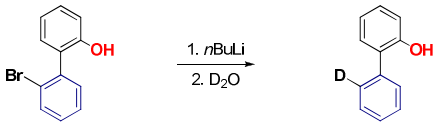



**Synthesis of Other Substrates via Suzuki Coupling:**

Ary-Br or Ary-I (1 mmol), 2-Hydroxyphenylboronic acid (1.1 mmol, 152 mg), $Pd(Ph_3P)_4$ (0.05 mmol, 57.8 mg) and $K_2CO_3$ (2 mmol, 276 mg) was placed in a vial under Ar, then a mixed solvent of 1 mL toluene, 1 mL EtOH and 1 mL $H_2O$ was added. The mixture was violently stirred at 80 °C for 4~8 h and cooled to room

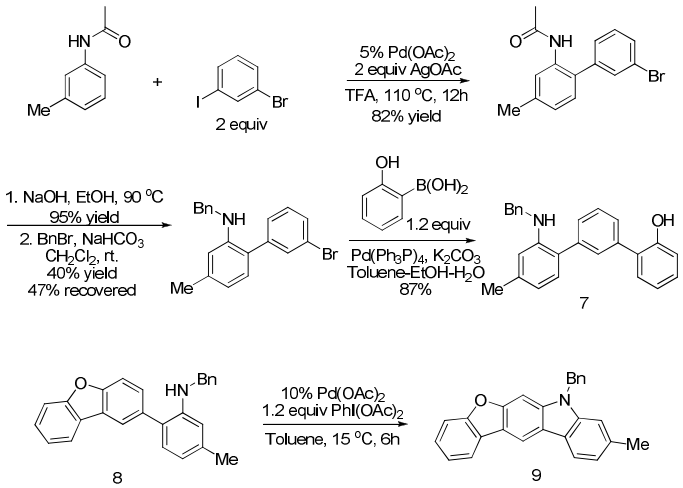
temperature. The organic phase was purified by flash chromatography to give the 2-Arylphenol product as white solid or thick oil.

**Synthesis of 2'- deuterio -biphenyl-2-ol:**

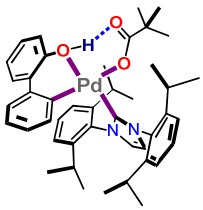



A solution of 2'-bromobiphenyl-2-ol (249 mg, 1 mmol, produced from Suzuki coupling of 2-Hydroxyphenylboronic acid and excess 1,2-dibromobenzene) in 1 mL toluene was slowly added to excess *n*BuLi (3 mL, 1.6 M in THF) at -20 $^{o}$C under Ar. The temperature was allowed to rise to 10 $^{o}$C and stirred for 2h, then 2 mL $D_2O$ was carefully added. After violently stirred, the mixture was extracted with $Et_2O$ (3 x 10 mL), organic layer was dried with $MgSO_4$, concentrated, and the mixture was purified by flash chromatography to give 2'- deuterio -biphenyl-2-ol as a white solid(158 mg, 91%).

**Synthesis of compound 9:**



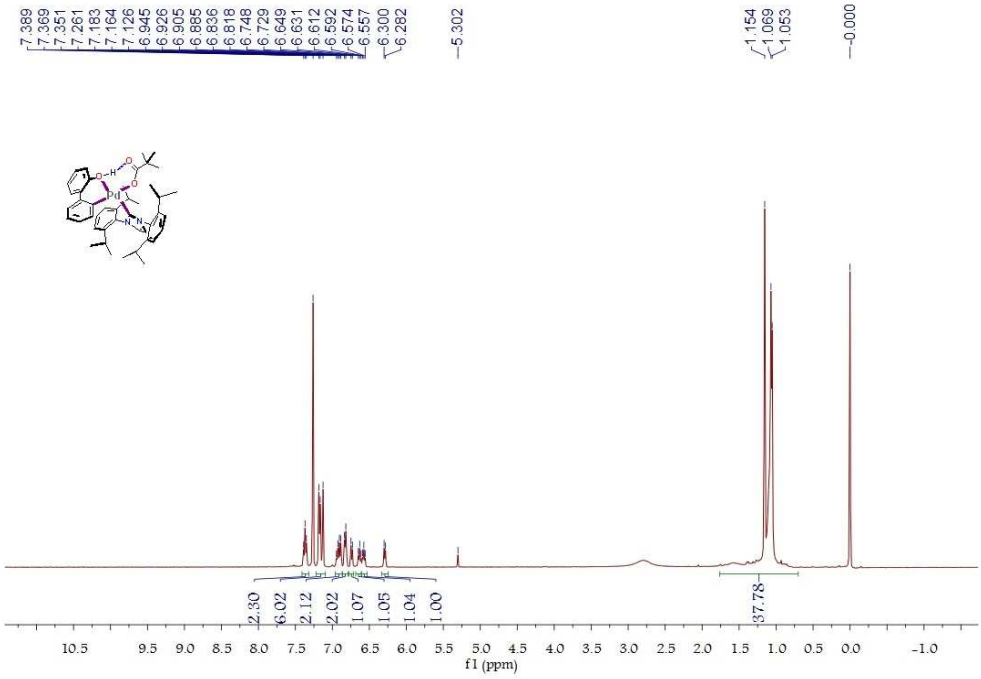

**8** (47.2 mg, 0.13 mmol, 65% yield from **7**), $PhI(OAc)_2$ (51.5 mg, 0.16 mmol, 1.2 equiv), and $Pd(OAc)_2$ (2.9 mg, 0.013 mmol, 0.1 equiv) was stirred in 2.6 mL toluene at 15 $^{o}$C for 6 hours. The solvent was removed under reduced pressure and the resulting residue absorbed onto silica and purified by flash column chromatography. **9** was obtained as a thick oil (36.5 mg, 78% yield).

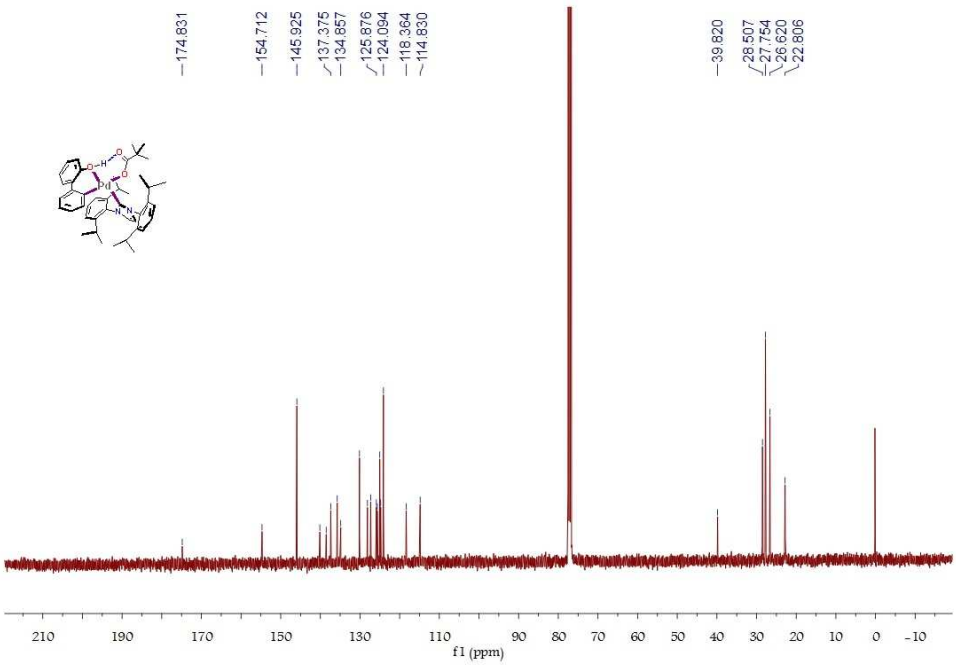


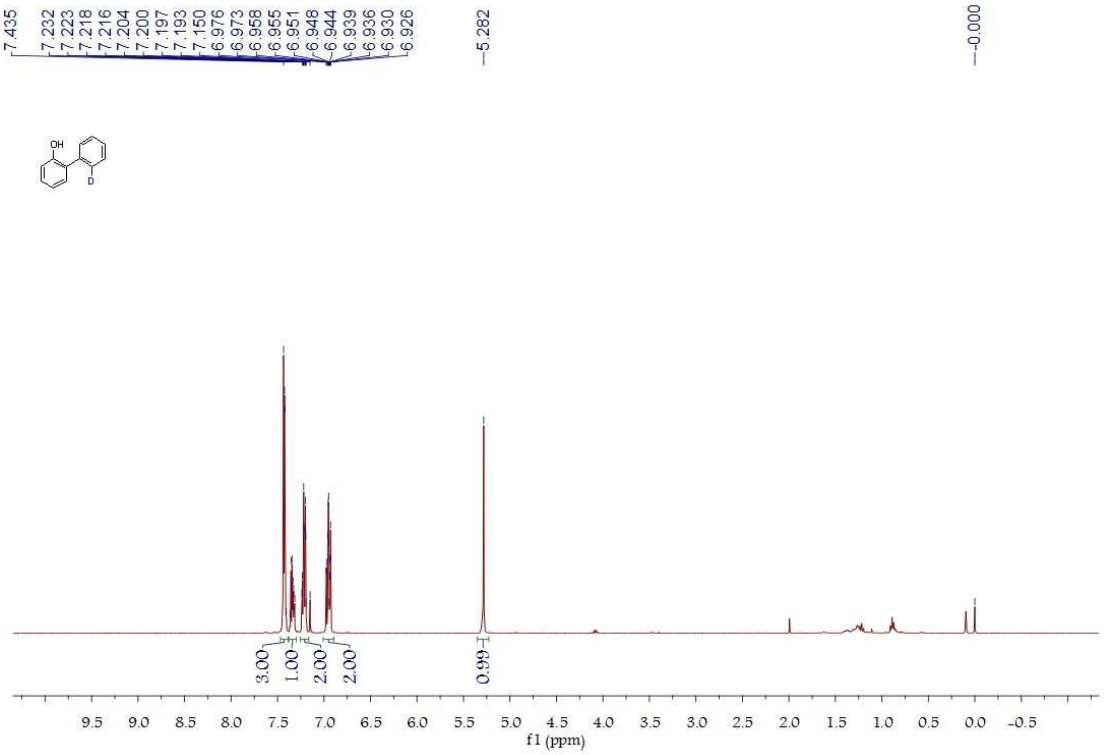
White solid.

$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.39-7.35 (m, 2H), 7.18-7.13 (m, 6H), 6.94-6.88 (m, 2H), 6.84-6.80 (m, 2H), 6.75-6.73 (m, 1H), 6.65-6.56 (m, 2H), 6.30-6.28 (m, 1), 1.15-1.05 (m, 37H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 174.83, 154.71, 145.92, 140.13, 138.53, 137.38, 135.75, 134.86, 130.13, 128.12, 127.31, 125.88, 125.64, 125.02, 124.79, 124.09, 118.36, 114.83, 39.82, 28.51, 27.75, 26.62, 22.81.

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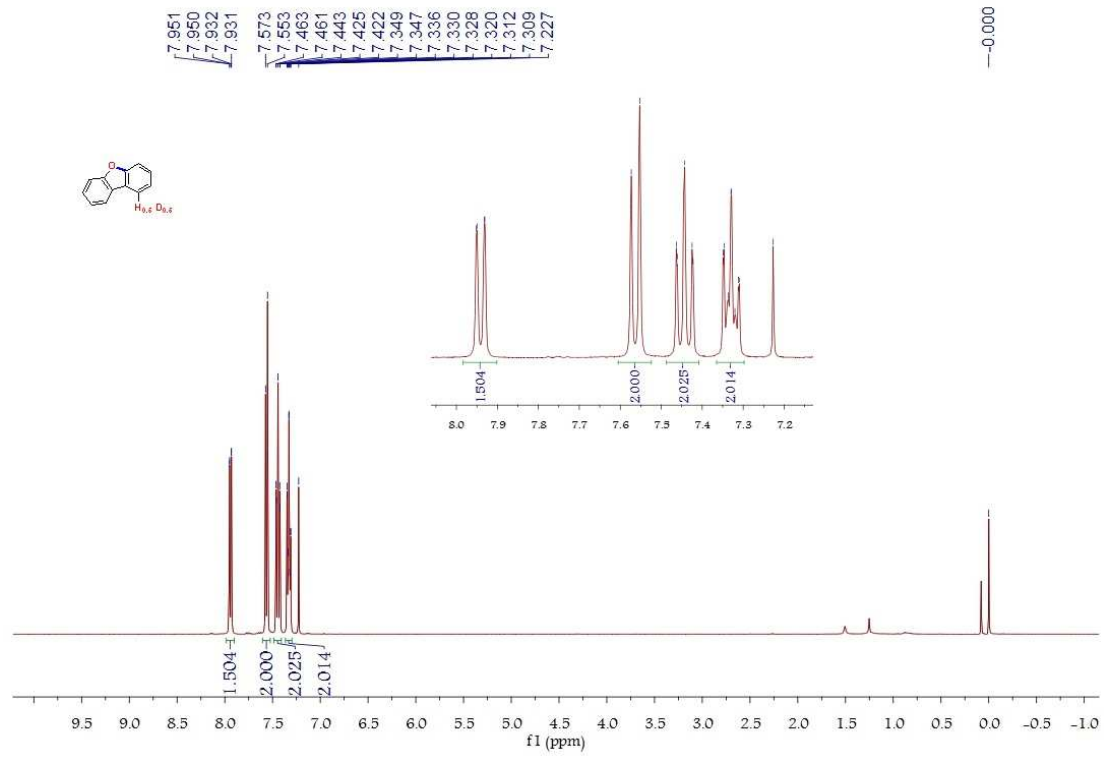
7.232
7.223
7.218
7.216
7.204
7.200
7.197
7.193
7.150
6.976
6.973
6.958
6.955
6.951
6.948
6.944
6.939
6.936
6.930
6.926
5.282
0.000
OH
D
3.00
1.00
2.00
2.00
0.99
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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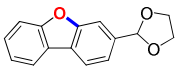
7.950
7.932
7.931
7.573
7.553
7.463
7.461
7.443
7.425
7.422
7.349
7.347
7.336
7.330
7.328
7.320
7.312
7.309
7.227
0.000
O
H0.6 D0.6
1.504
2.000
2.025
2.014
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

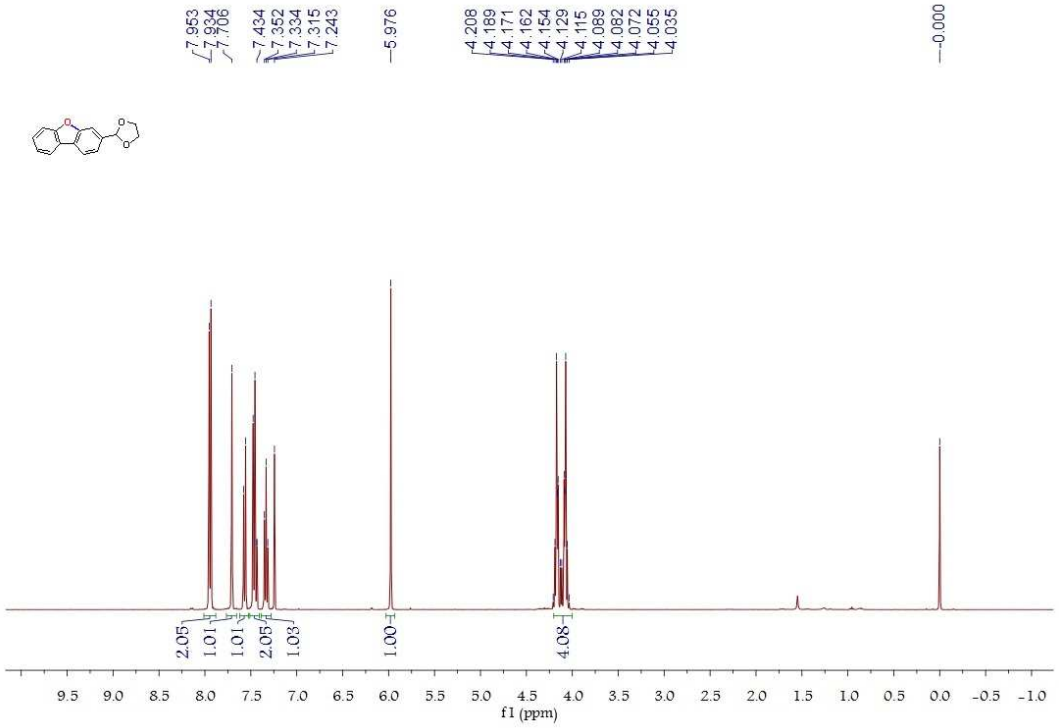


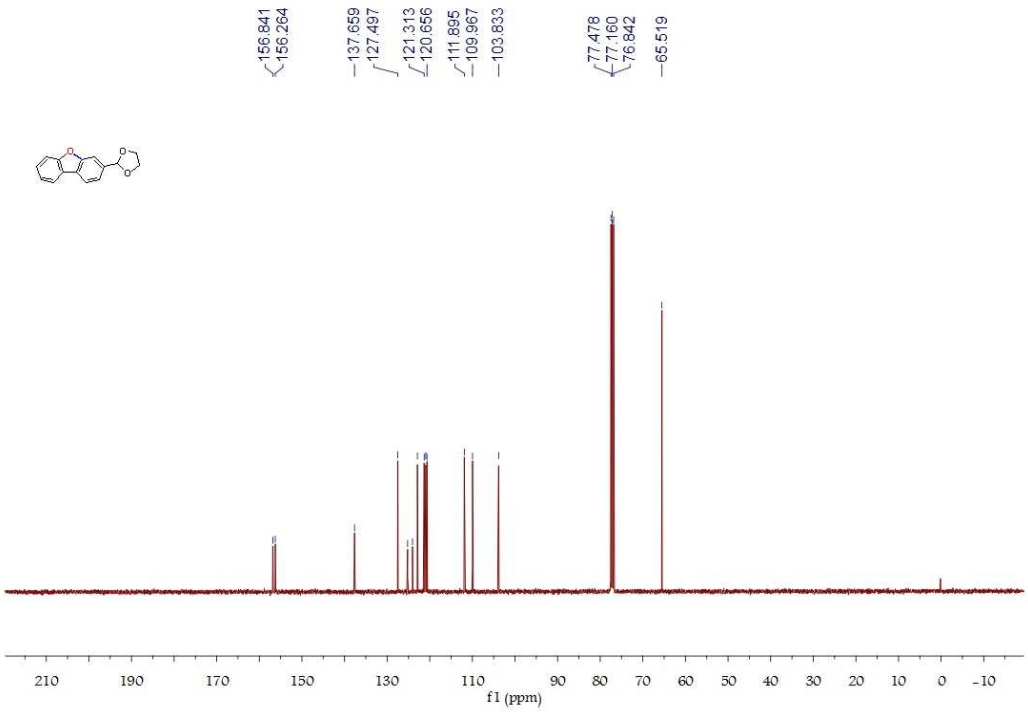
**3-(1,3-dioxolan-2-yl)dibenzo[b,d]furan.**

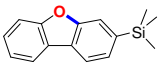
White solid.

$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.95-7.93 (m, 2H), 7.71 (s, 1H), 7.58-7.56 (m, 1H), 7.47-7.43 (m, 2H), 7.35-7.32 (m, 1H), 5.98 (s, 1H), 4.21-4.04 (m,4H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 156.84, 156.26, 137.66, 127.50, 125.20, 124.05, 122.90, 121.31, 120.94, 120.66, 111.90, 109.97, 103.83, 65.52. HRMS calcd for C15H12O3: 240.0786; found: 240.0787.



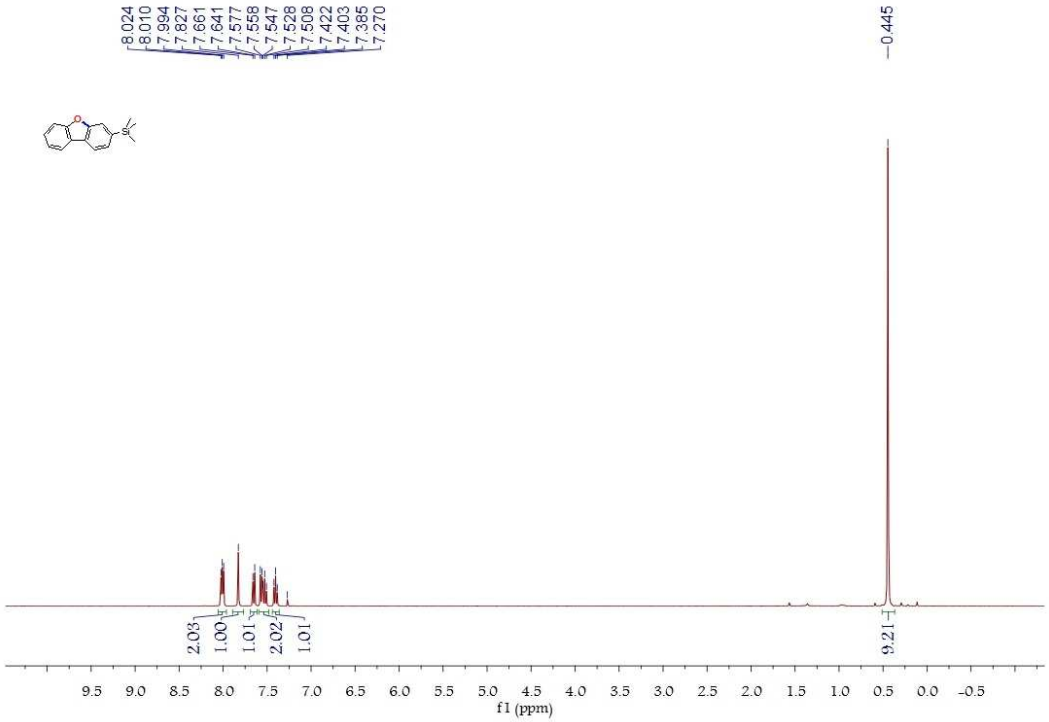


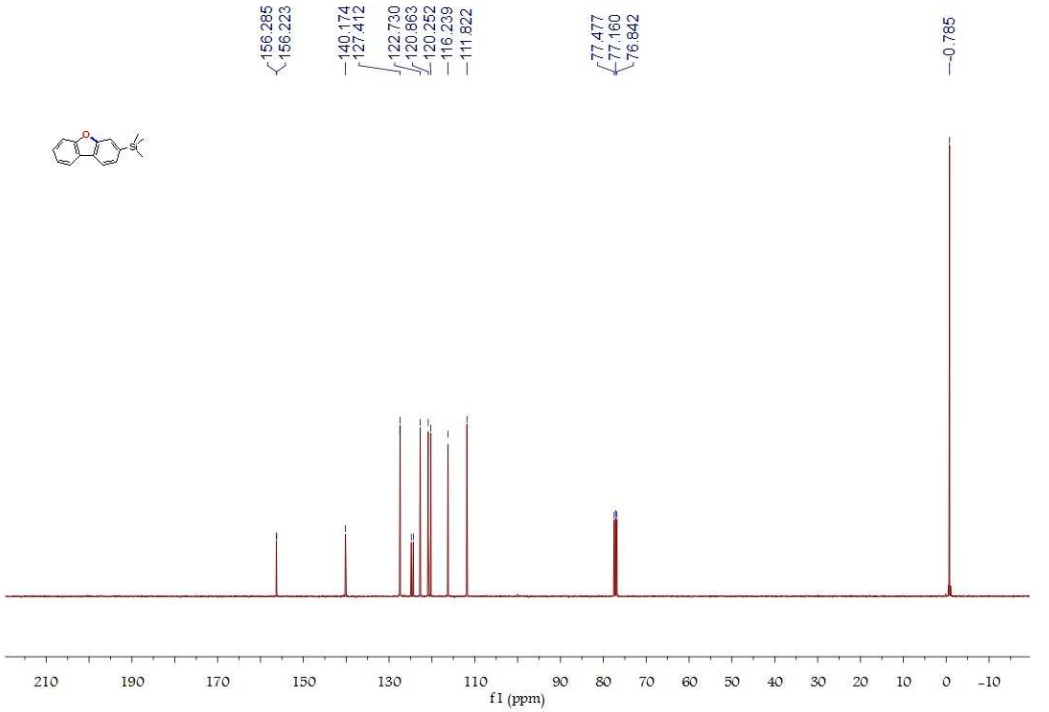
**Dibenzofuran-3-yl-trimethyl-silane.**

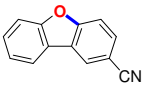
White solid.

$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.02-7.99 (m, 2H), 7.83 (s, 1H), 7.66-7.64 (m, 1H), 7.58-7.51 (m, 2H), 7.42-7.38 (m, 1H), 0.44 (s, 9H); $^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 156.28, 156.22, 140.17, 127.49, 127.41, 124.81, 124.33, 122.73, 120.86, 120.25, 116.24, 111.82, -0.78.

HRMS calcd for C15H16OSi: 240.0970; found: 240.0973.





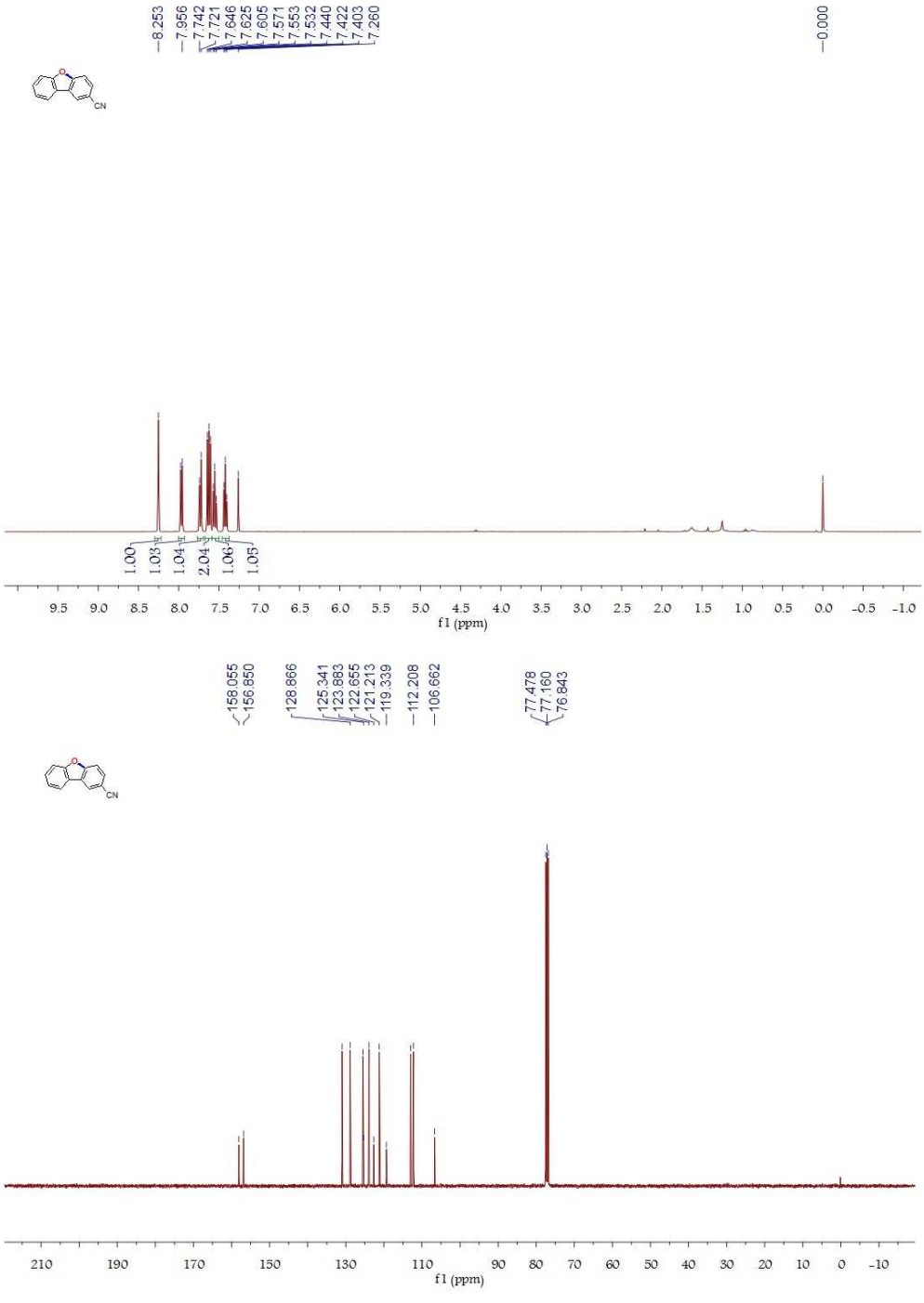
**Dibenzofuran-2-carbonitrile.**

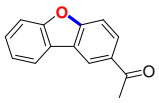
Known compound (Reference: Xu, H.; Fan, L.-L. *Chem. Pharm. Bull.* **2008**, *56*, 1496.)

White solid.

$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.25 (s, 1H), 7.97 (d, $J$ = 8.0 Hz, 1H), 7.73 (d, $J$ = 8.0 Hz, 1H), 7.65-7.60 (m, 2H), 7.57-7.53 (m, 1H), 7.44-7.40 (m, 1H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 158.06, 156.85, 130.97, 128.87, 125.50, 125.34, 123.88, 122.66, 121.21, 119.34, 112.96, 112.21, 106.66.





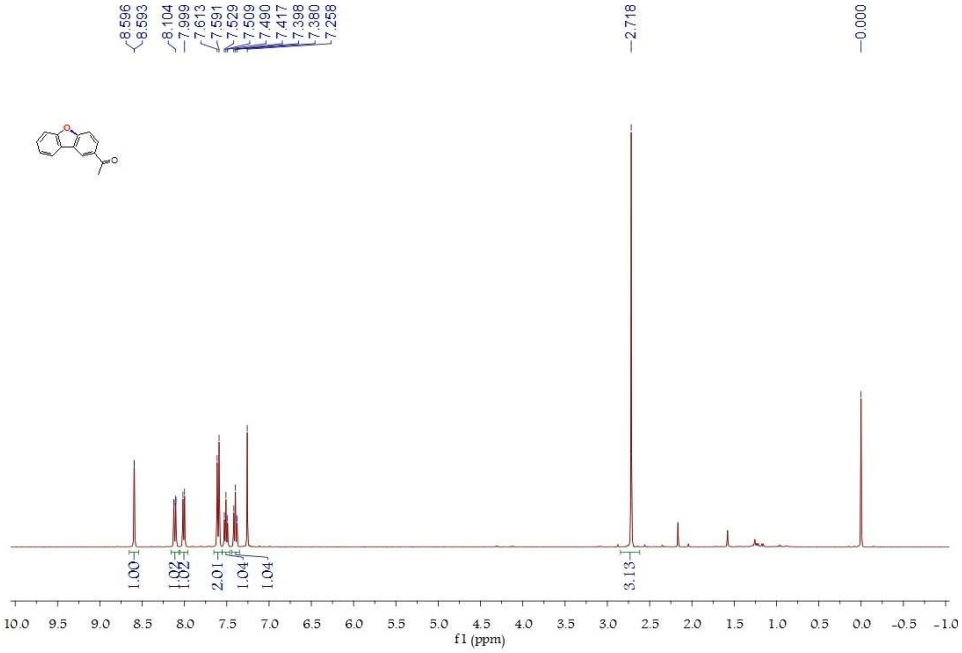
**1-Dibenzofuran-2-yl-ethanone.**

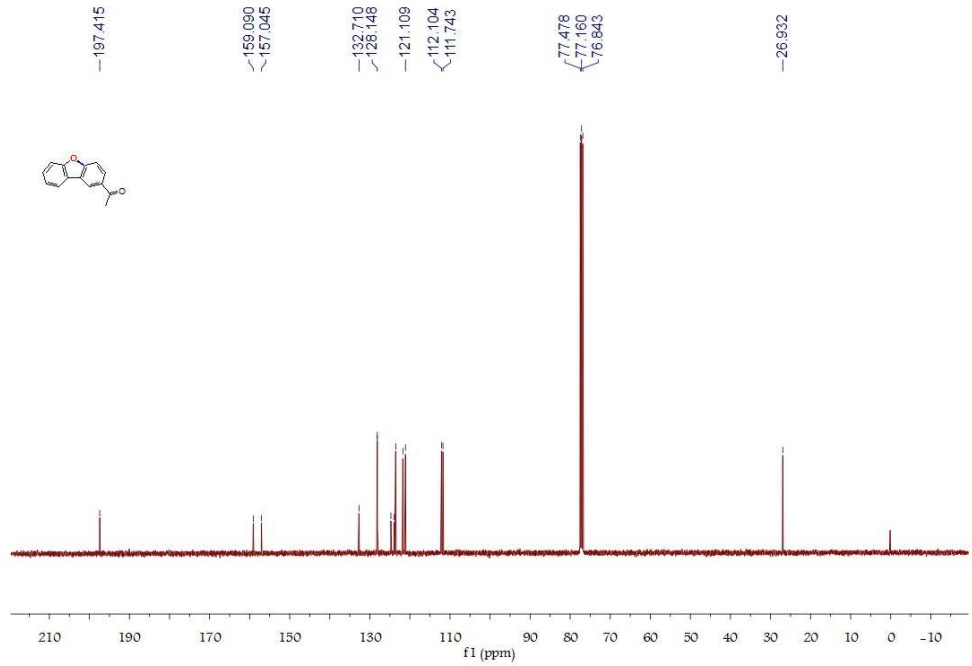
Known compound (Reference: Liu, Z.; Larock, R. C. *Tetrahedron.* **2007**, *63*, 347.)

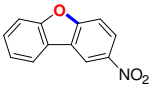
White solid.

$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.60 (s, 1H), 8.12-8.10 (m, 1H), 8.02-8.00 (m, 1H), 7.61-7.59 (m, 2H), 7.53-7.49 (m, 1H), 7.42-7.38 (m, 1H), 2.72 (s, 3H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 197.42, 159.09, 157.04, 132.71, 128.15, 128.13, 124.75, 123.91, 123.54, 121.76, 121.11, 112.10, 111.74, 26.93.





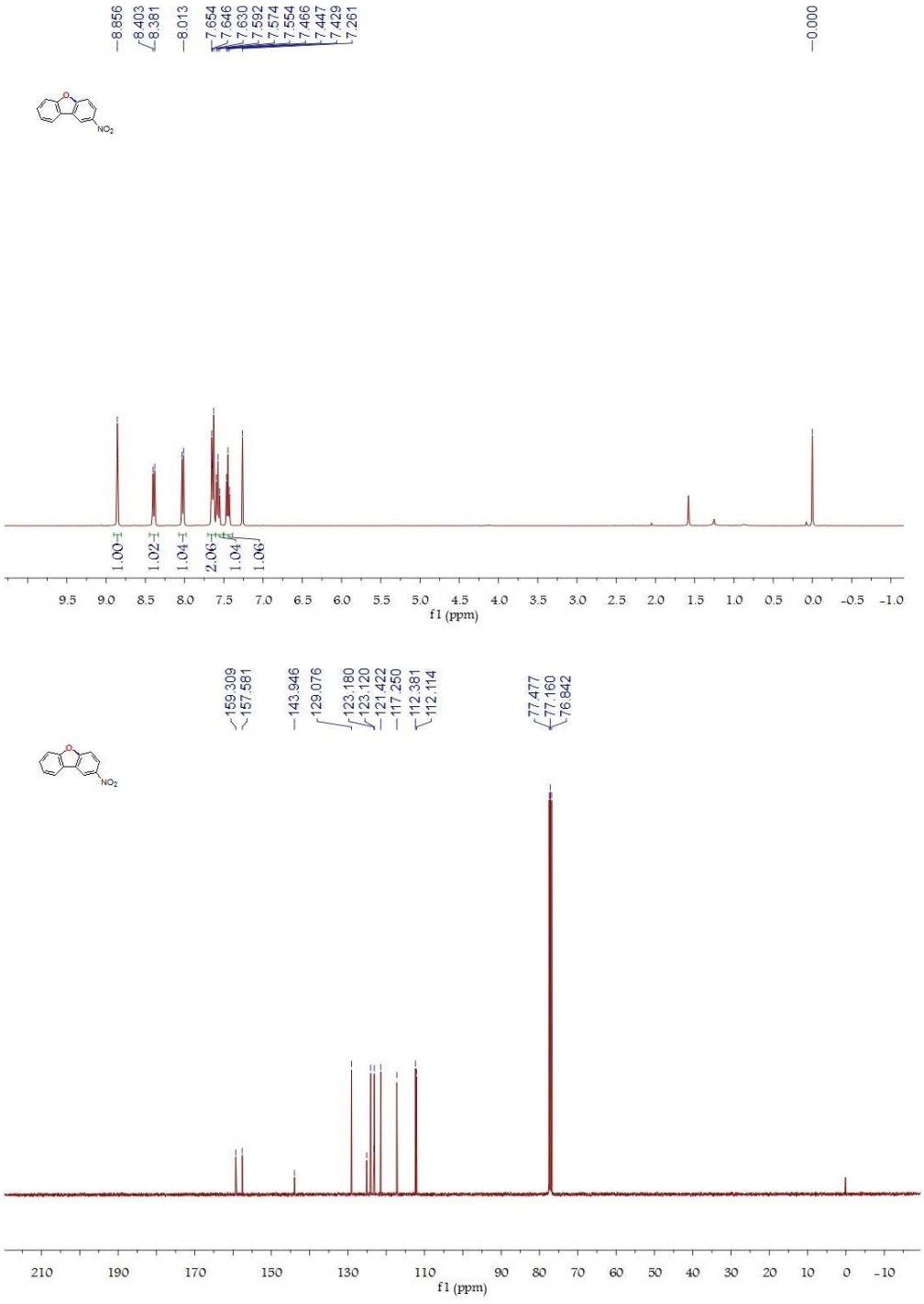
**2-Nitro-dibenzofuran.**

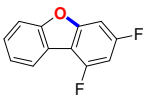
Known compound (Reference: Xu, H.; Fan, L.-L. *Chem. Pharm. Bull.* **2008**, *56*, 1496.)

White solid.

$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.86 (s, 1H), 8.39 (d, $J$ = 8.4 Hz, 1H), 8.02 (d, $J$ = 8.4 Hz, 1H), 7.65-7.63 (m, 2H), 7.59-7.55 (m, 1H), 7.47-7.43 (m, 1H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 159.31, 157.58, 143.95, 129.08, 125.13, 124.06, 123.18, 123.12, 121.42, 117.25, 112.38, 112.11.





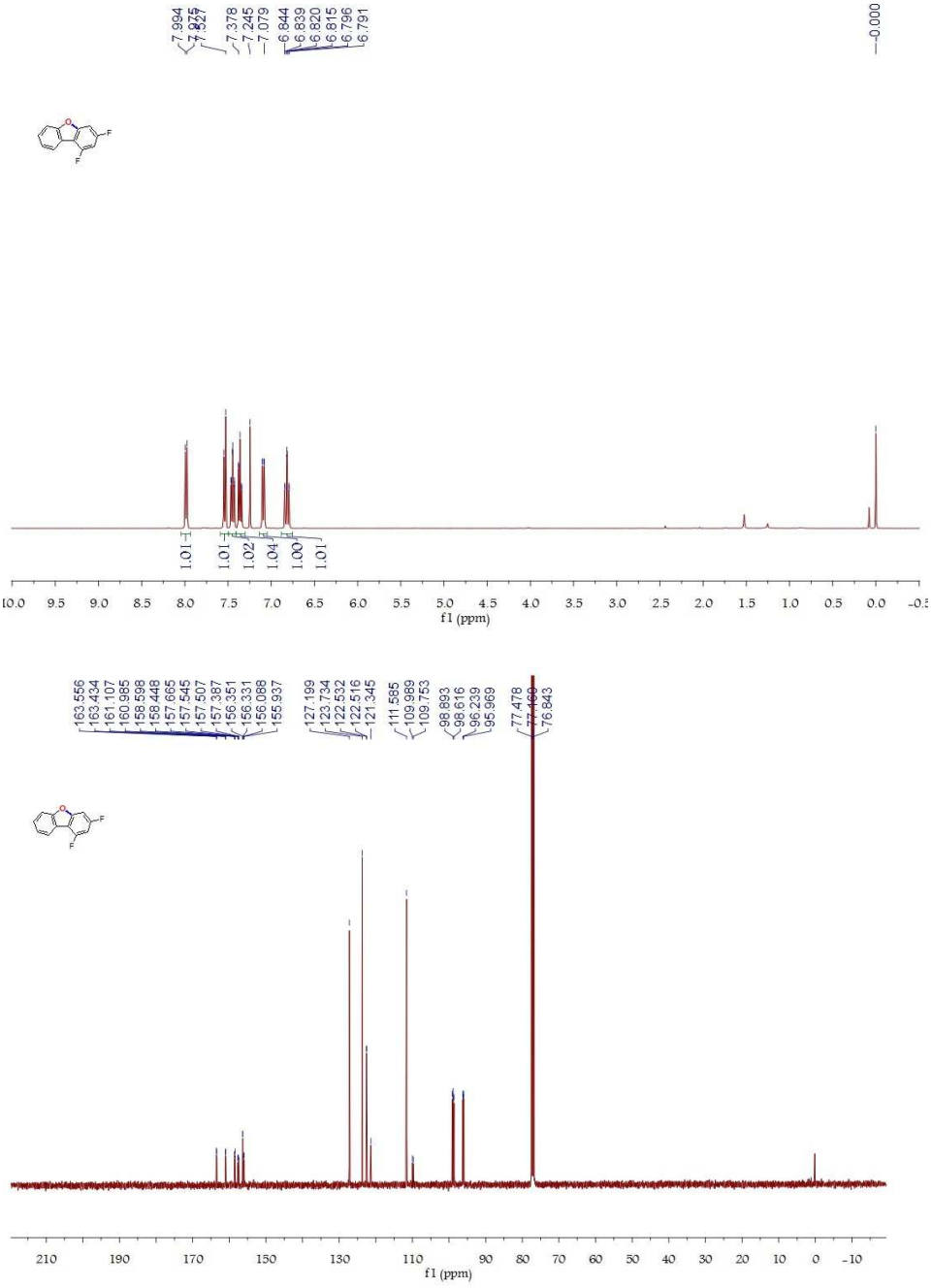
**1,3-Difluoro-dibenzofuran.**

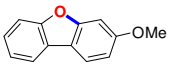
White solid.

$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.98 (d, $J$ = 8.0 Hz, 1H), 7.54 (d, $J$ = 8.0 Hz, 1H), 7.47-7.42 (m, 1H), 7.38-7.34 (m, 1H), 7.10-7.08 (m, 1H), 6.84-6.79 (m, 1H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 163.56, 163.43, 161.11, 160.98, 158.60, 158.45, 157.66, 157.54, 157.51, 157.39, 156.35, 156.33, 156.09, 155.94, 127.20, 123.73, 122.53, 122.52, 121.34, 111.58, 109.99, 109.75, 99.12, 98.89, 98.85, 98.62, 96.29, 96.24, 96.02, 95.97.

HRMS calcd for C12H6F2O: 204.0387; found: 204.0384.





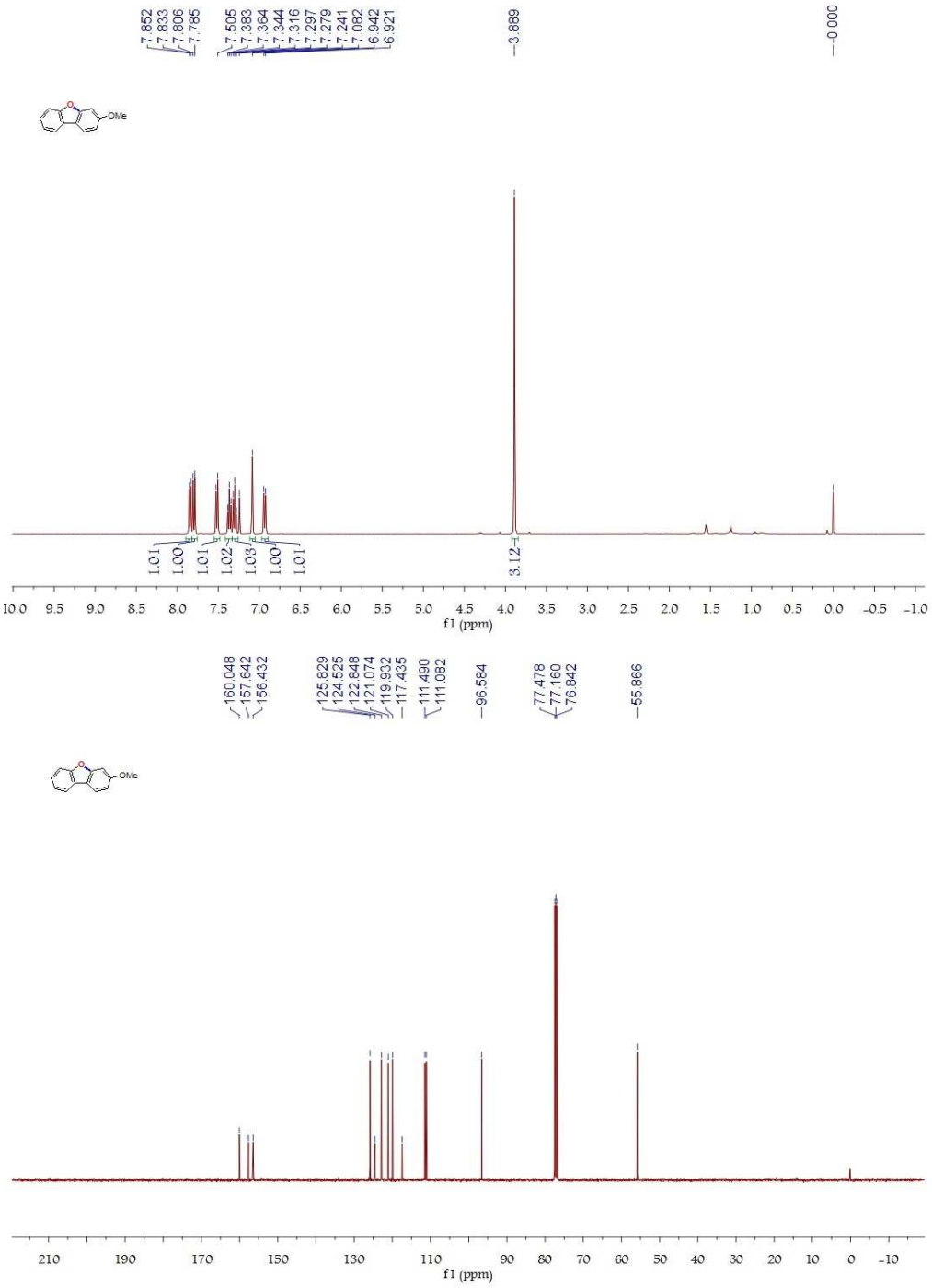

**3-Methoxy-dibenzofuran.**

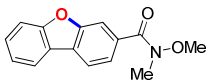
White solid.

Known compound (Reference: Oliveira, A. M. A. G.; Raposo, M. M. M.; Oliveira-Campos, A. M. F.; Griffiths, J.; Machado, A. E. H. *Helv. Chim. Acta.* **2003**, *86*, 2900.)

$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.84 (d, $J$ = 8.0 Hz, 1H), 7.80 (d, $J$ = 8.0 Hz, 1H), 7.51 (d, $J$ = 8.0 Hz, 1H), 7.38-7.34 (m, 1H), 7.32-7.28 (m, 1H), 7.08 (s, 1H), 6.93 (m, 1H), 3.89 (s, 3H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 160.05, 157.64, 156.43, 125.83, 124.52, 122.85, 121.07, 119.93, 117.44, 111.49, 111.08, 96.58, 55.87.





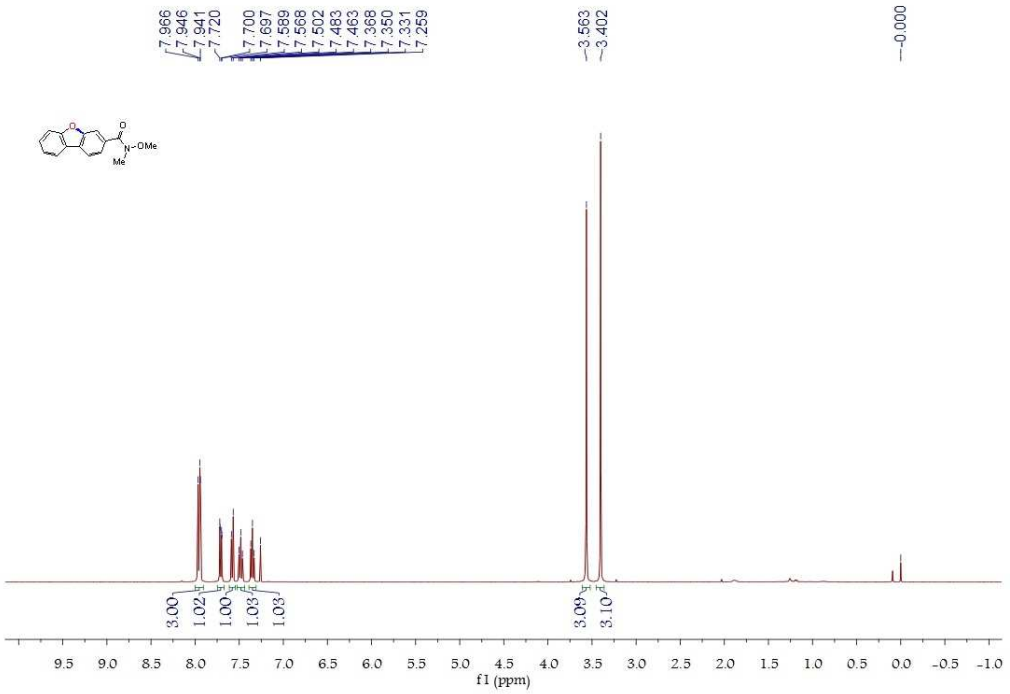
**N-methoxy-N-methyldibenzo[b,d]furan-3-carboxamide.**

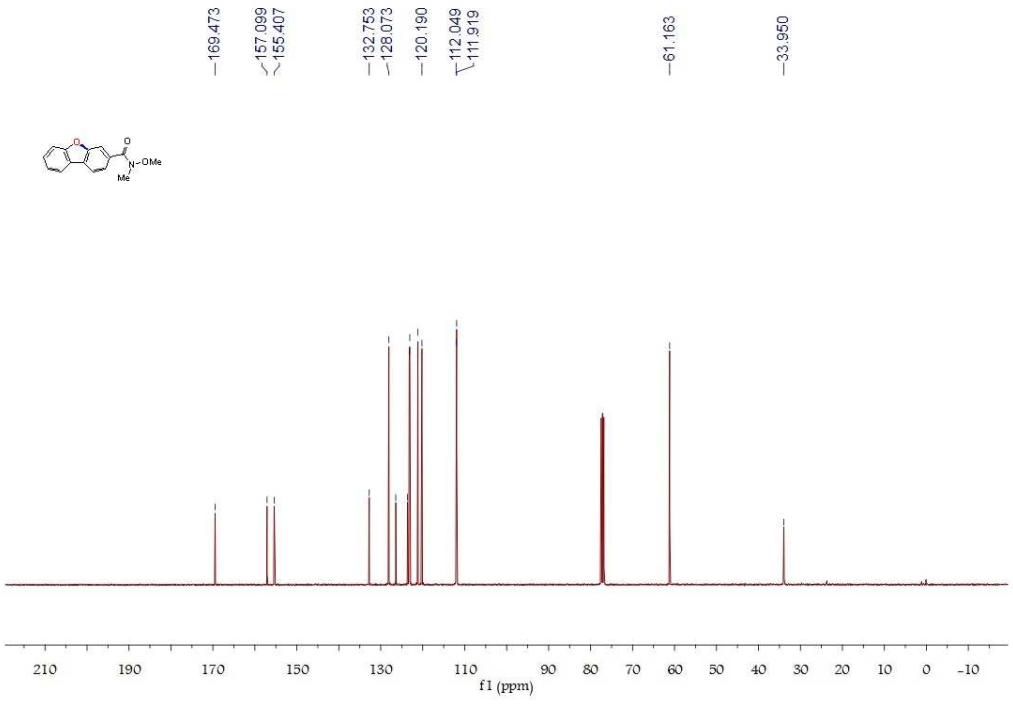
White solid.

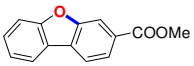
$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.97-7.94 (m, 3H), 7.72-7.70 (m, 1H), 7.59-7.57 (m, 1H), 7.50-7.46 (m, 1H), 7.37-7.33 (m, 1H), 3.56 (s, 3H), 3.40 (s, 3H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 169.47, 157.10, 155.41, 132.75, 128.07, 126.42, 123.62, 123.22, 123.09, 121.15, 120.19, 112.05, 111.92, 61.16, 33.95.

HRMS calcd for C15H13NO3: 255.0895; found: 255.0897.





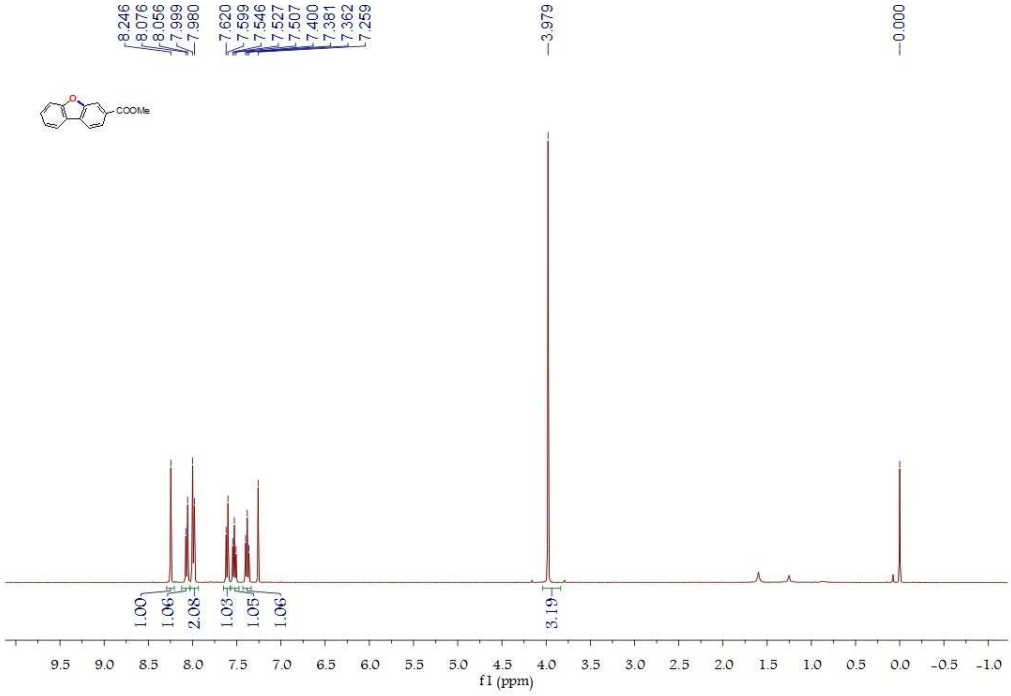

**Dibenzofuran-3-carboxylic acid methyl ester.**

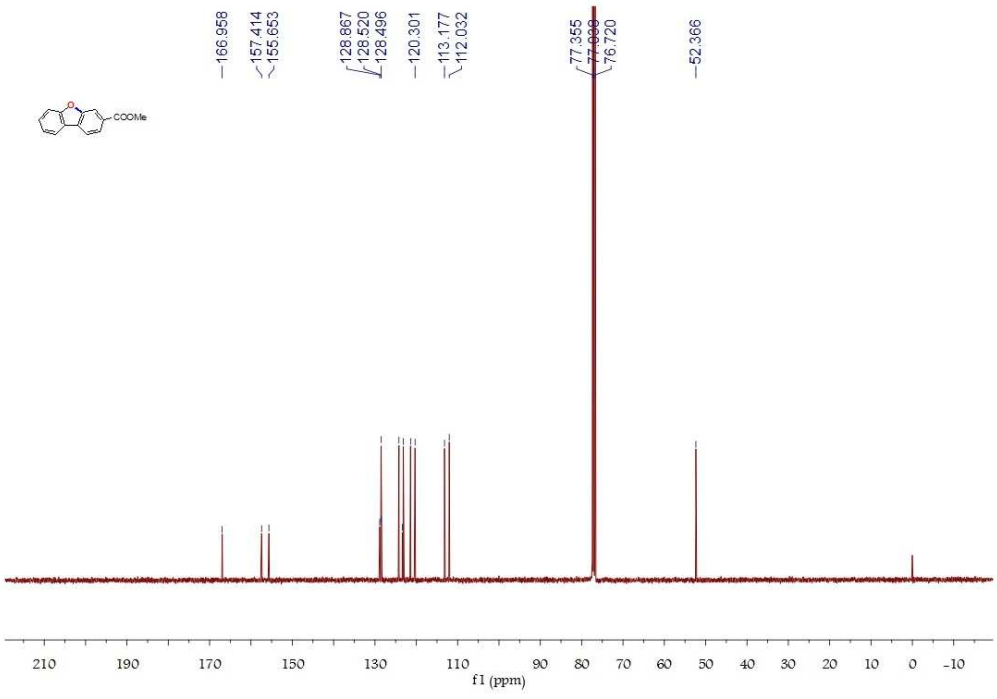
White solid.

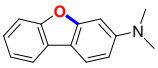
$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.25 (s, 1H), 8.08-8.06 (m, 1H), 8.00-7.98 (m, 2H), 7.62-7.60 (m, 1H), 7.55-7.51 (m, 1H), 7.40-7.36 (m, 1H), 3.98 (s, 3H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 167.08, 157.54, 155.78, 128.99, 128.64, 128.62, 124.32, 123.50, 123.27, 121.51, 120.42, 113.30, 112.15, 52.49.

HRMS calcd for C14H10O3: 226.0630; found: 226.0635.





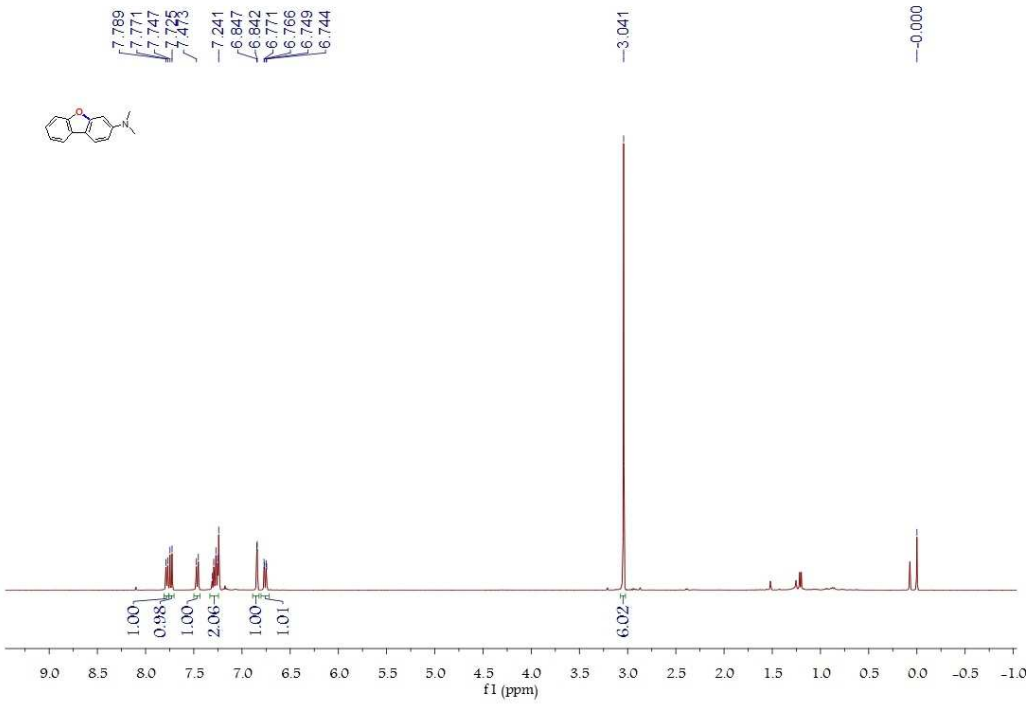
**Dibenzofuran-3-yl-dimethyl-amine.**

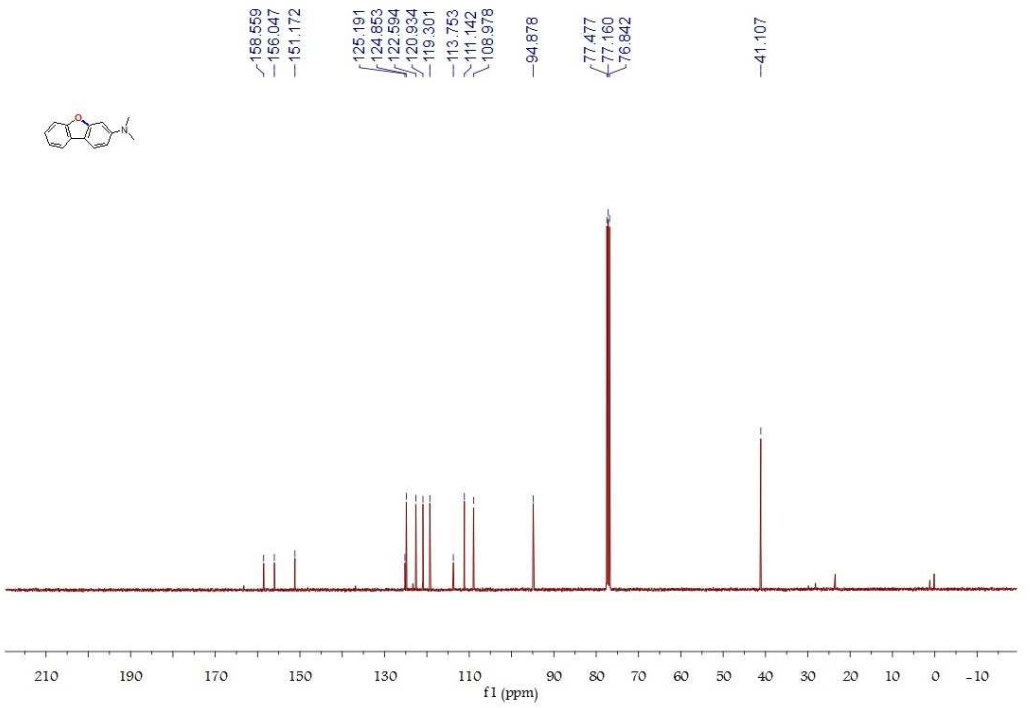
White solid.

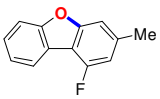
$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.70 (d, $J$ = 7.2 Hz, 1H), 7.74 (d, $J$ = 7.6 Hz, 1H), 7.46 (d, $J$ = 7.6 Hz, 1H), 7.31-7.24 (m, 2H), 6.84-6.84 (m, 1H), 6.77, 6.74 (m, 1H), 3.04 (s, 6H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 158.56, 156.05, 151.17, 125.19, 124.85, 122.59, 120.93, 119.30, 113.75, 111.14, 108.98, 94.88, 41.11.

HRMS calcd for C14H13NO: 211.0997; found: 211.0999.





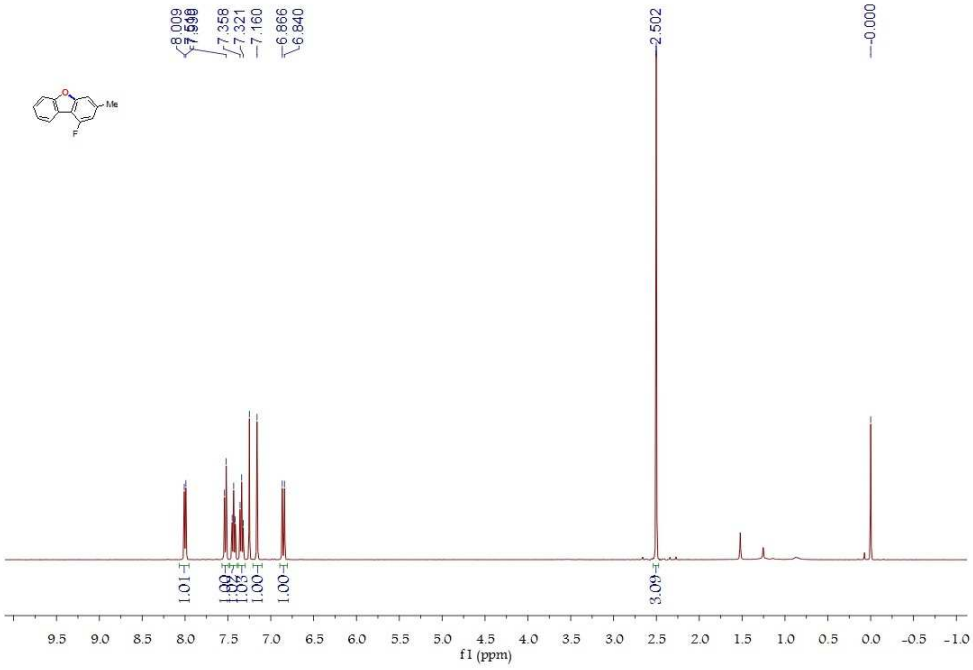

**1-Fluoro-3-methyl-dibenzofuran.**

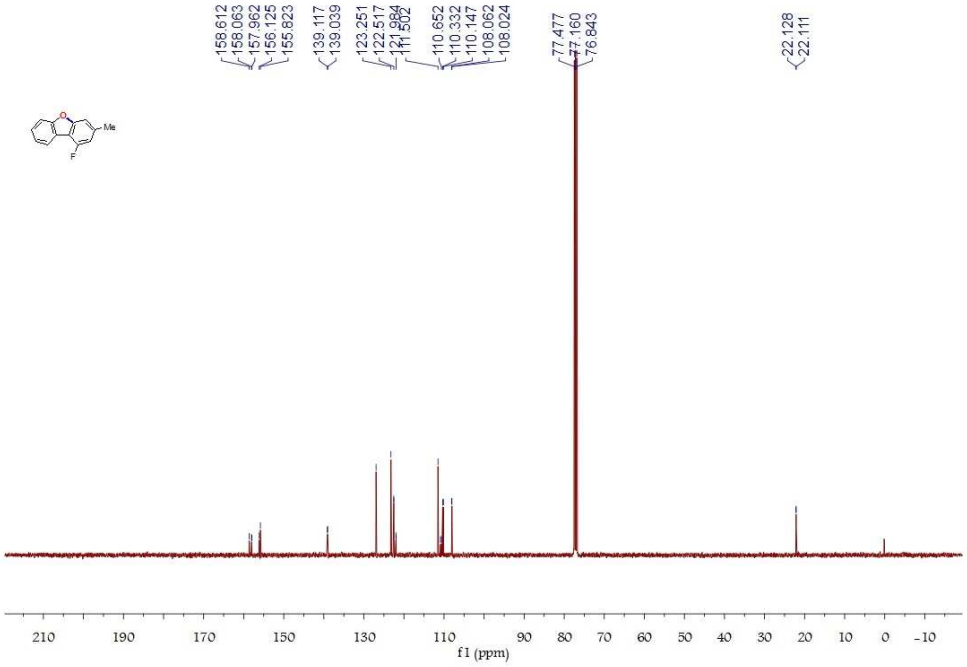
White solid.

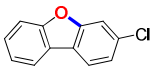
$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.00 (d, $J$ = 8.0 Hz, 1H), 7.53 (d, $J$ = 8.0 Hz, 1H), 7.45-7.41 (m, 1H), 7.36-7.32 (m, 1H), 7.16 (s, 1H), 6.87-6.84 (m, 1H), 2.50 (s, 3H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 158.61, 158.06, 157.96, 156.12, 155.82, 139.12, 139.04, 126.96, 123.25, 122.54, 122.52, 122.01, 121.98, 111.50, 110.86, 110.65, 110.33, 110.15, 108.06, 108.02, 22.13, 22.11.

HRMS calcd for C13H9FO: 200.0637; found: 200.0633.





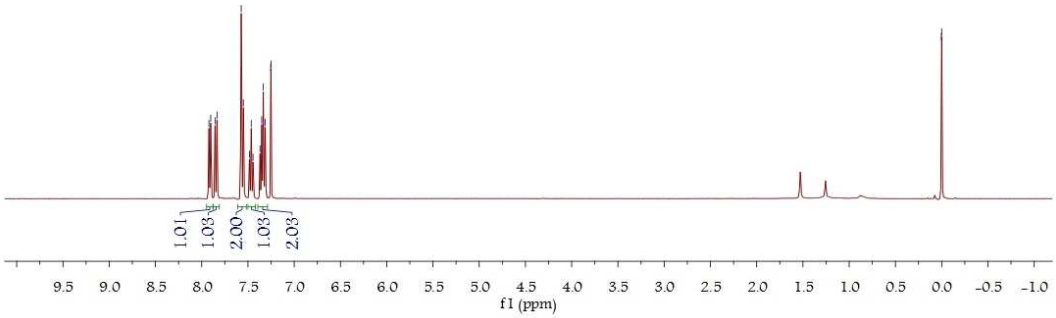
**3-chlorodibenzo[b,d]furan.**

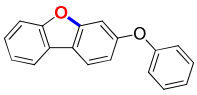
White solid.

$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 9.91 (d, $J$ = 8 Hz, 1H), 7.84 (d, $J$ = 8 Hz, 1H), 7.57-7.55 (m,2H), 7.48-7.44 (m,1H), 7.37-7.31 (m, 2H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 156.68, 156.50, 132.81, 127.58, 123.66, 123.51, 123.25, 123.13, 121.31, 120.76, 112.47, 111.96.

HRMS calcd for C12H7ClO: 202.0185; found: 202.0188.

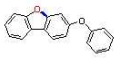
**3-phenoxydibenzo[b,d]furan.**

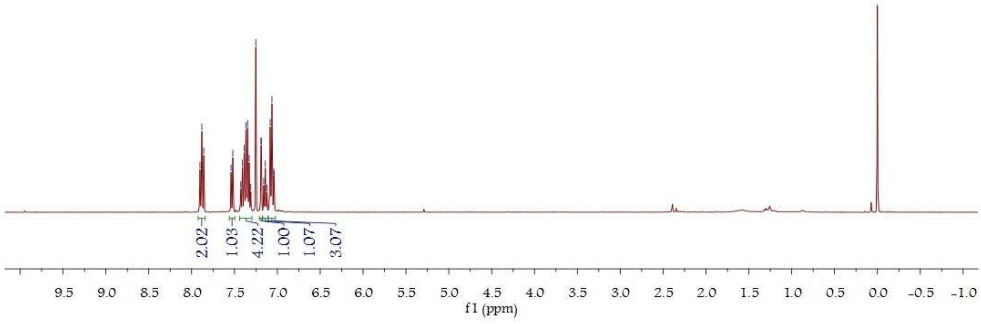
White solid.

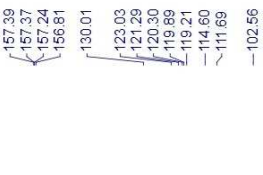
$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.90-7.86 (m, 2H), 7.54-7.52 (m, 1H), 7.43-7.31 (m, 4H), 7.19 (s, 1H), 7.16-7.12 (m, 1H), 7.08-7.04 (m, 3H);

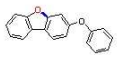
$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 157.39, 157.37, 157.24, 156.81, 130.01, 126.55, 124.20, 123.74, 123.03, 121.29, 120.30, 119.89, 119.21, 114.60, 111.69, 102.56.

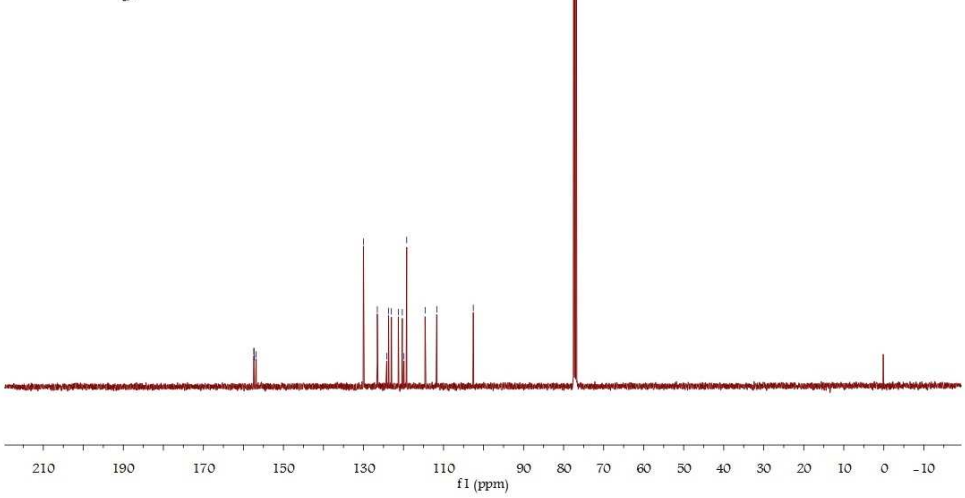
HRMS calcd for C18H12O2: 260.0837; found: 260.0838.

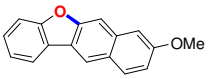









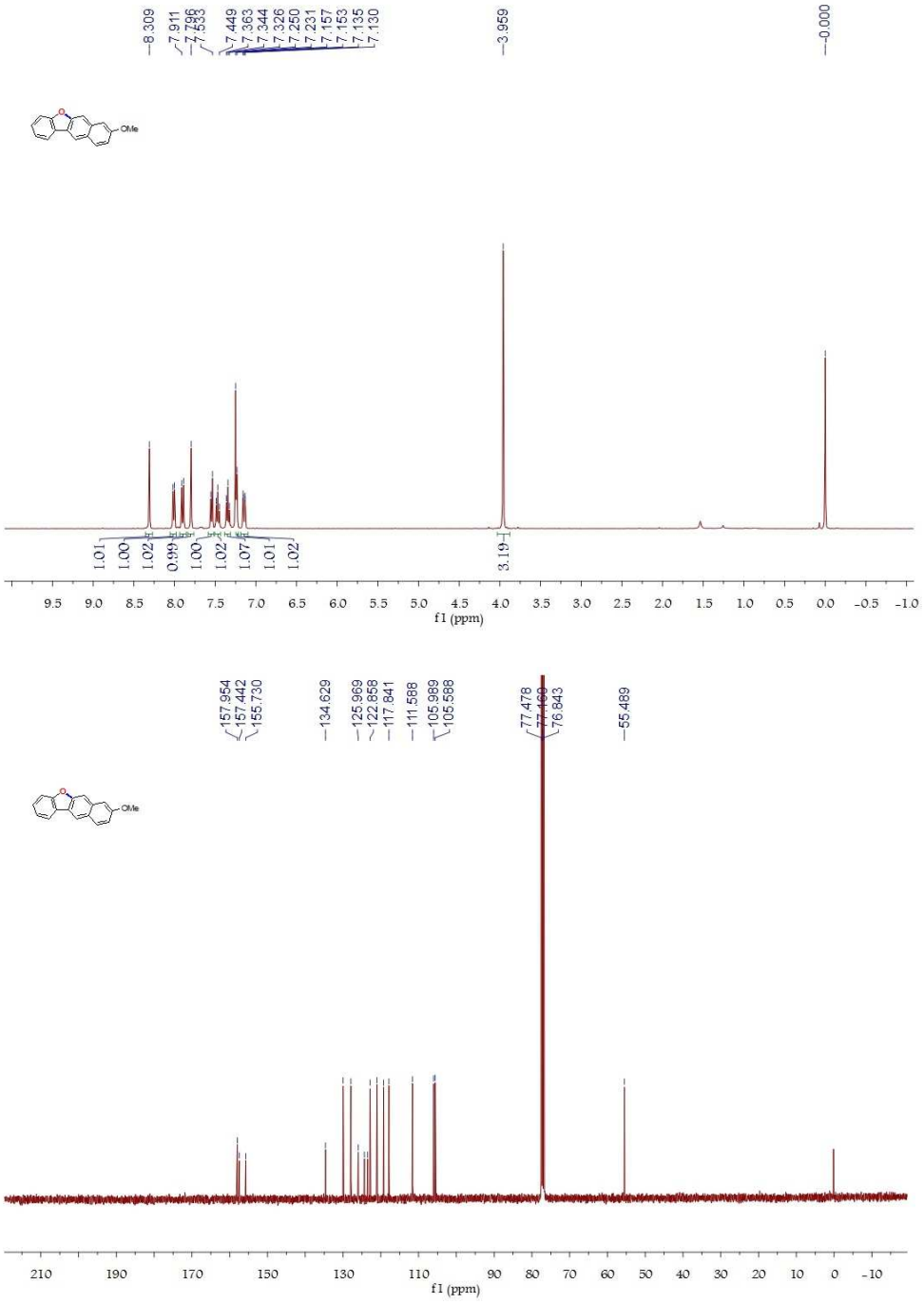

**8-Methoxy-benzo[b]naphtho[2,3-d]furan.**

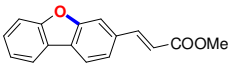
White solid.

Known compound (Reference:Martínez, A.; Fernández, M.; Estévez, J. C.; Estévez, R. J.; Castedo, L. *Tetrahedron* **2005**, *61*, 1353.)

$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.31 (s, 1H), 8.01 (d, $J$ = 8.0 Hz, 1H), 7.90 (d, $J$ = 8.0 Hz, 1H), 7.80 (s, 1H), 7.54 (d, $J$ = 8.0 Hz, 1H), 7.49-7.45 (m, 1H), 7.36-7.33 (m, 1H), 7.23 (s, 1H), 7.16-7.13 (m, 1H), 3.96 (s, 3H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 157.95, 157.44, 155.73, 134.63, 129.97, 127.91, 125.97, 124.33, 123.46, 122.86, 121.03, 119.25, 117.84, 111.59, 105.99, 105.59, 55.49.





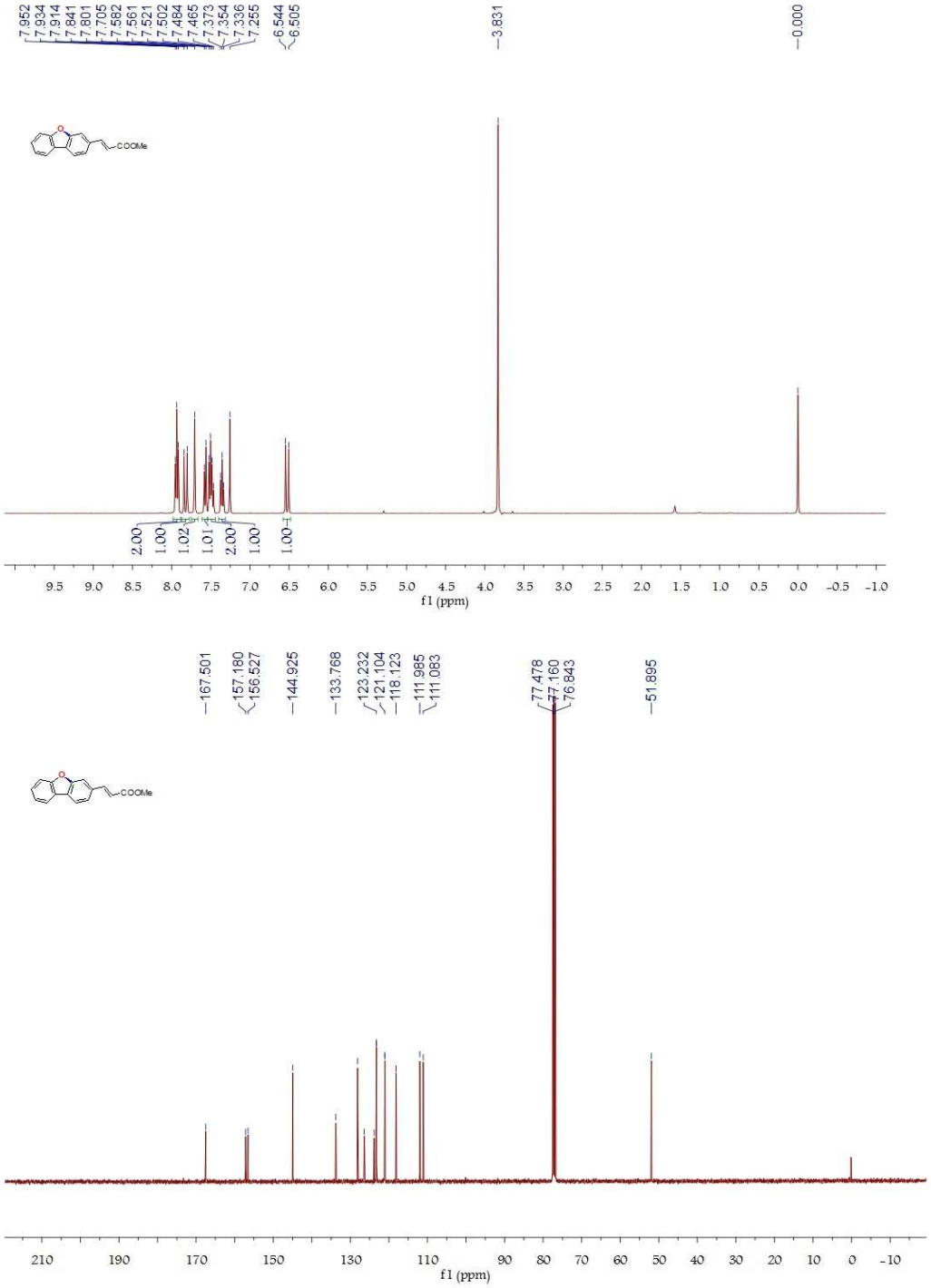

**3-Dibenzofuran-3-yl-acrylic acid methyl ester.**

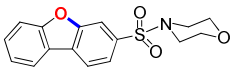
White solid.

$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.95-7.91 (m, 2H), 7.82 (d, $J$ = 16.0 Hz, 1H), 7.70 (s, 1H), 7.57 (d, $J$ = 8.0 Hz, 1H), 7.52-7.46 (m, 2H), 7.37-7.34 (m, 1H), 6.52 (d, $J$ = 16.0 Hz, 1H), 3.83 (s, 3H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 167.50, 157.18, 156.53, 144.92, 133.77, 128.11, 126.38, 123.23, 123.21, 121.10, 121.02, 118.12, 111.98, 111.08, 51.90.

HRMS calcd for C16H12O3: 252.0786; found: 252.0790.





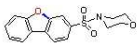
**4-(dibenzo[b,d]furan-3-ylsulfonyl)morpholine.**

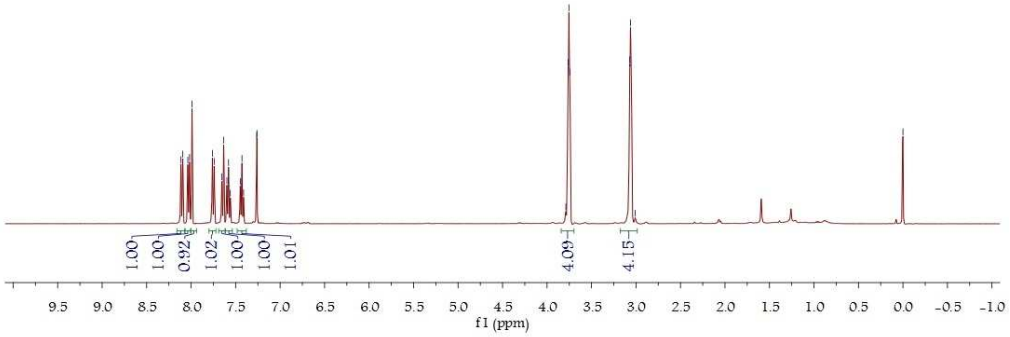
White solid.

$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.10 (d, $J$ = 8.0 Hz, 1H), 8.03 (d, $J$ = 8.0 Hz, 1H), 7.99 (s, 1H), 7.75 (d, $J$ = 8.0 Hz, 1H), 7.64 (d, $J$ = 8.0 Hz, 1H), 7.60-7.56 (m, 1H), 7.44-7.41 (m,1H), 3.79-3.74 (m, 4H), 3.07-3.01 (m, 4H);

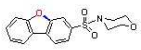
$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 157.66, 155.49, 133.64, 129.30, 128.86, 123.74, 122.86, 122.34, 121.66, 121.23, 112.32, 111.89, 66.25, 46.24.

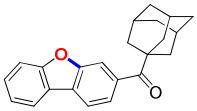
HRMS calcd for C16H15NO4S: 317.0722; found: 317.0727.









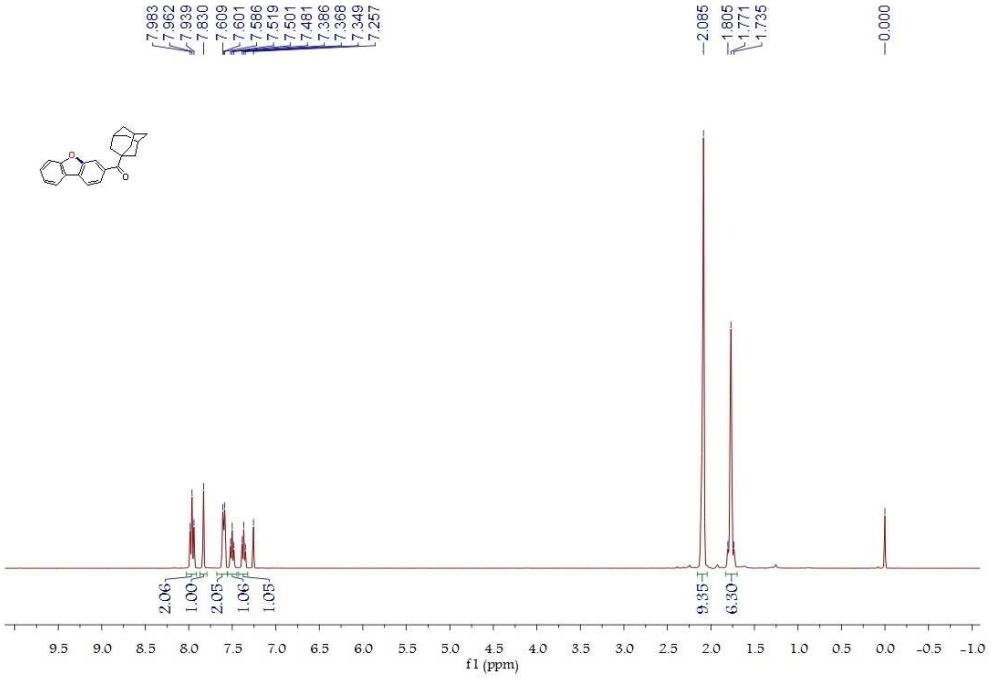
**Adamantan-1-yl-dibenzofuran-3-yl-methanone.**

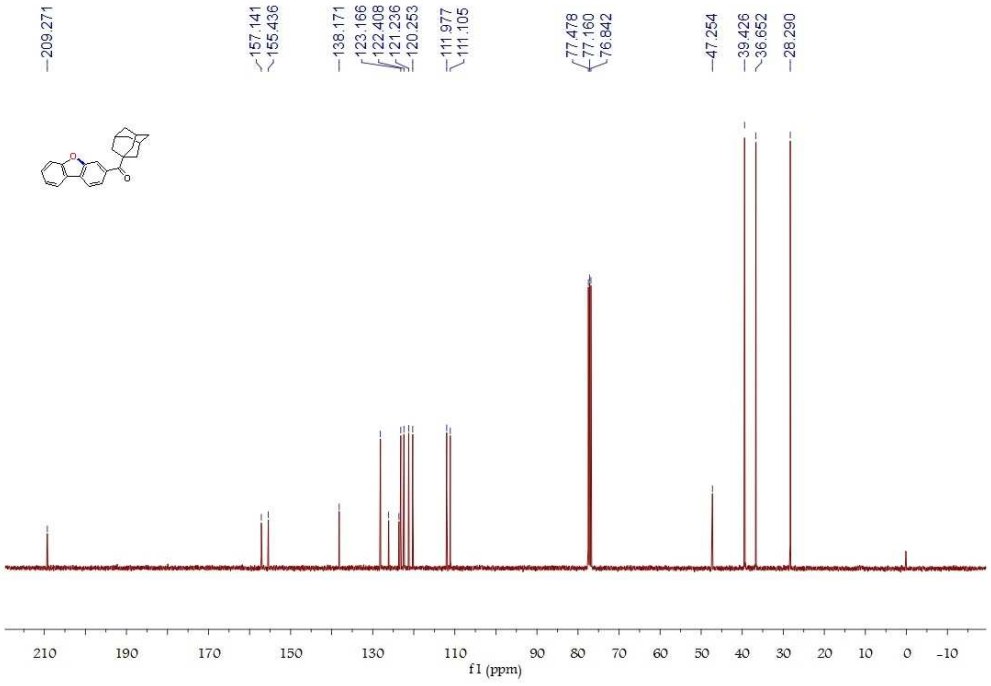
White solid.

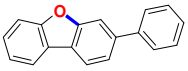
$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.98-7.94 (m, 2H), 7.83 (m, 1H), 7.61-7.59 (m, 2H), 7.52-7.48 (m, 1H), 7.39-7.35 (m, 1H), 2.08 (m, 9H), 1.80-1.74 (m, 6H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 209.27, 157.14, 155.44, 138.17, 128.13, 126.12, 123.63, 123.17, 122.41, 121.24, 120.25, 111.98, 111.10, 47.25, 39.43, 36.65, 28.29.

HRMS calcd for C23H22O2: 330.1620; found: 330.1626.





**3-Phenyl-dibenzofuran.**

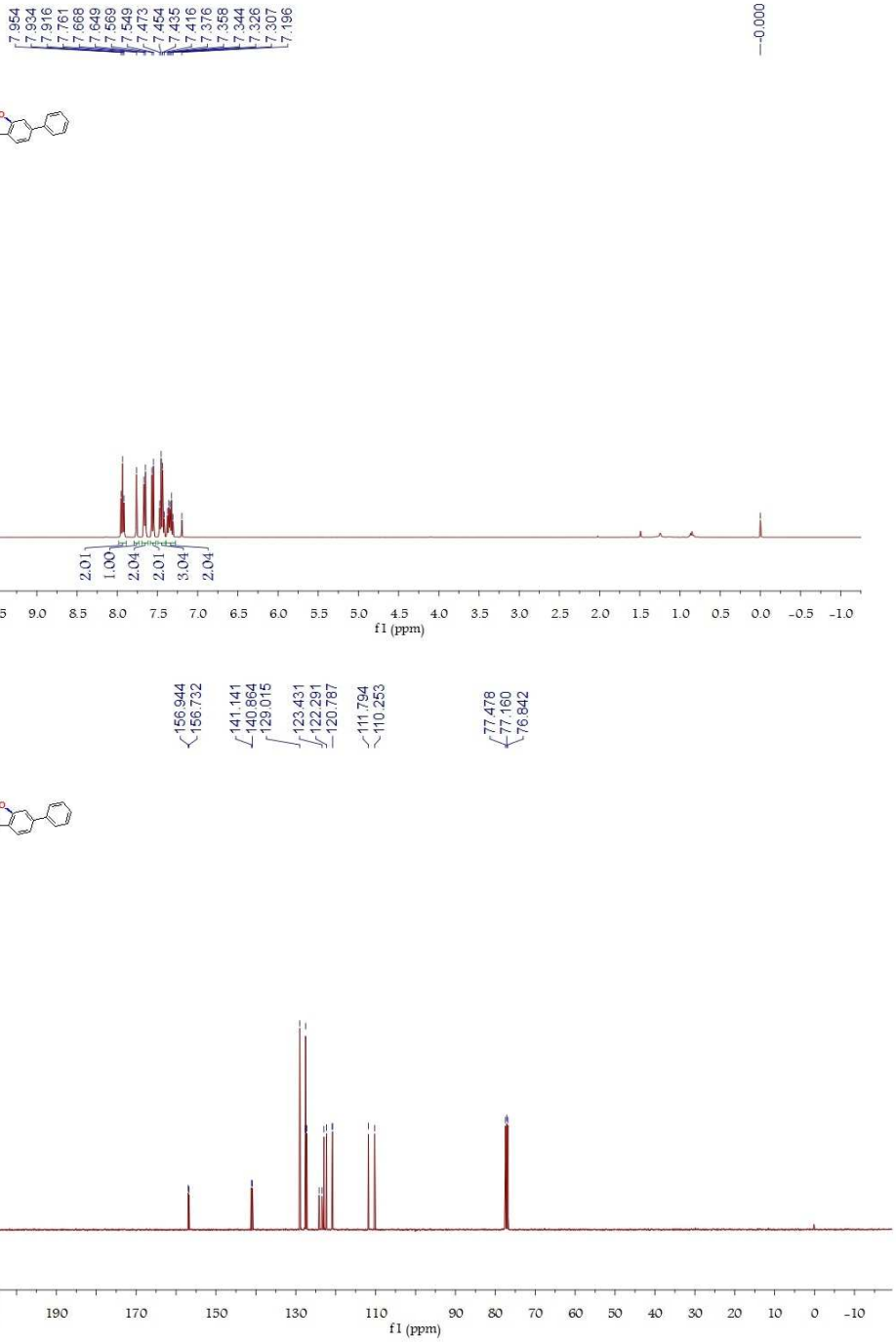
White solid.

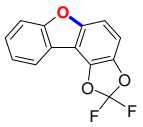
Known compound (Reference: Liu, Z.; Larock, R. C. *Tetrahedron.* **2007**, *63*, 347.)

$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.95-7.92 (m, 2H), 7.76 (s, 1H), 7.66 (d, $J$ = 8.0 Hz, 2H), 7.56 (d, $J$ = 8.0 Hz, 2H), 7.47-7.42 (m, 3H), 7.38-7.31 (m, 2H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 156.94, 156.73, 141.14, 140.86, 129.02, 127.61, 127.54, 127.24, 124.16, 123.43, 122.93, 122.29, 120.87, 120.79, 111.79, 110.25.

HRMS calcd for C18H12O: 244.0888; found: 244.0893.





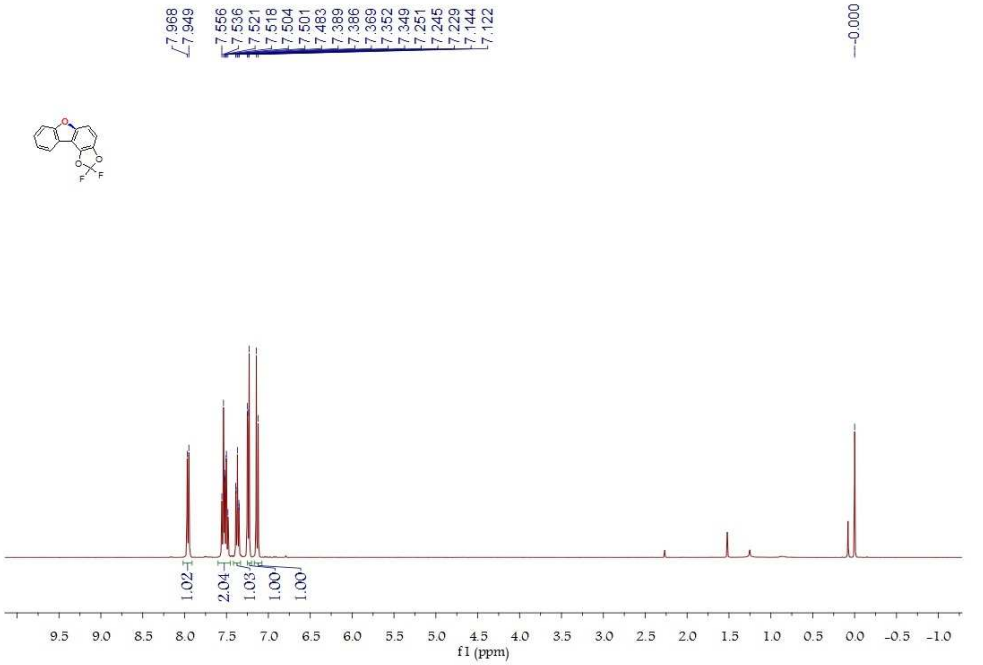
**2,2-Difluoro-1,3,6-trioxa-cyclopenta[c]fluorene.**

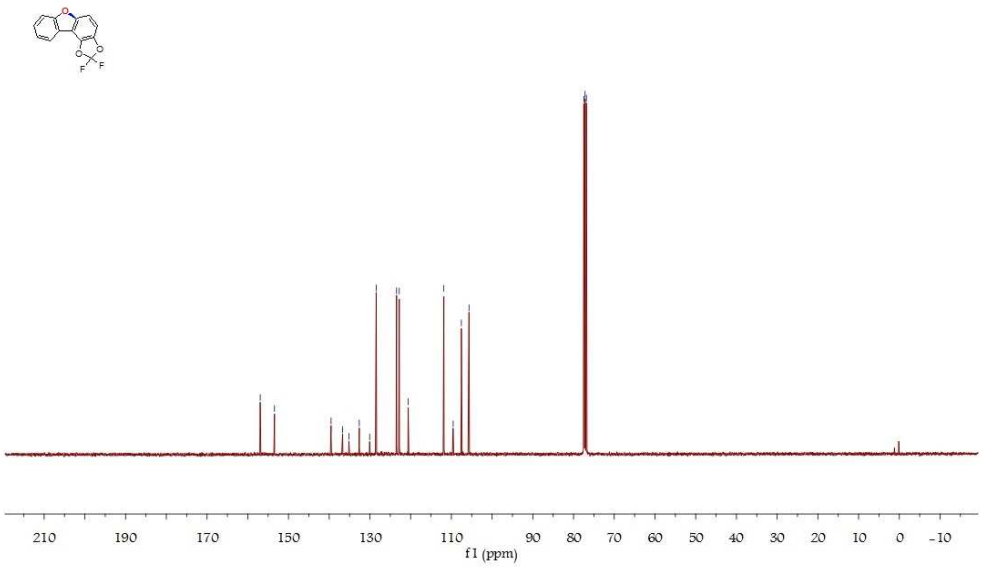
White solid.

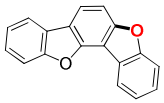
$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.96 (d, $J$ = 8.0 Hz, 1H), 7.56-7.48 (m, 2H), 7.39-7.35 (m, 1H), 7.25-7.22 (m, 1H), 7.14-7.12 (m, 1H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 156.94, 153.43, 139.54, 136.72, 132.61 (t, $J$ = 254 Hz), 128.46, 123.46, 122.80, 120.61, 111.85, 109.56, 107.54, 105.67.

HRMS calcd for C13H6F2O3: 248.0285; found: 248.0288.





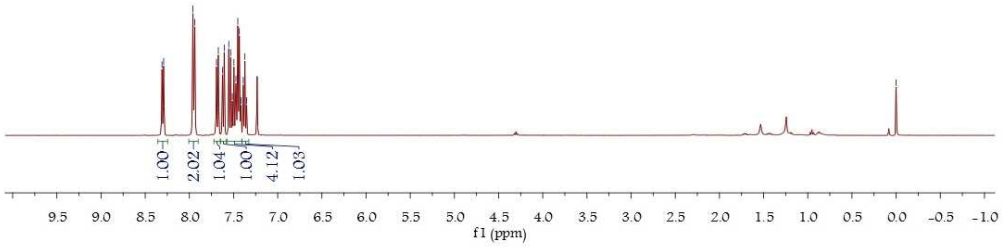
**7,12-Dioxa-indeno[1,2-a]fluorene.**

White solid.

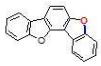
$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.30 (d, $J$ = 8.0 Hz, 1H), 7.96-7.94 (m, 2H), 7.68 (d, $J$ = 8.0 Hz, 1H), 7.61 (d, $J$ = 8.0 Hz, 1H), 7.55-7.42 (m, 4H), 7.39-7.35 (m, 1H);

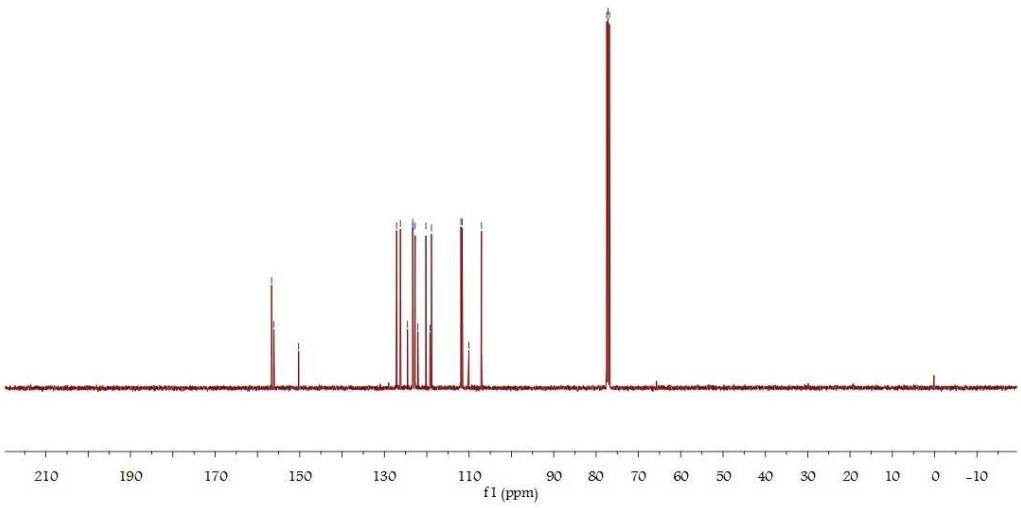
$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 156.66, 156.11, 150.26, 127.13, 126.24, 124.54, 123.33, 123.22, 122.74, 122.10, 120.21, 119.23, 118.89, 111.94, 111.64, 110.04, 107.07.

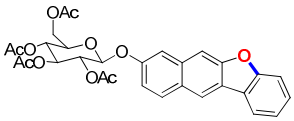
HRMS calcd for C18H10O2: 258.0681; found: 258.0685.









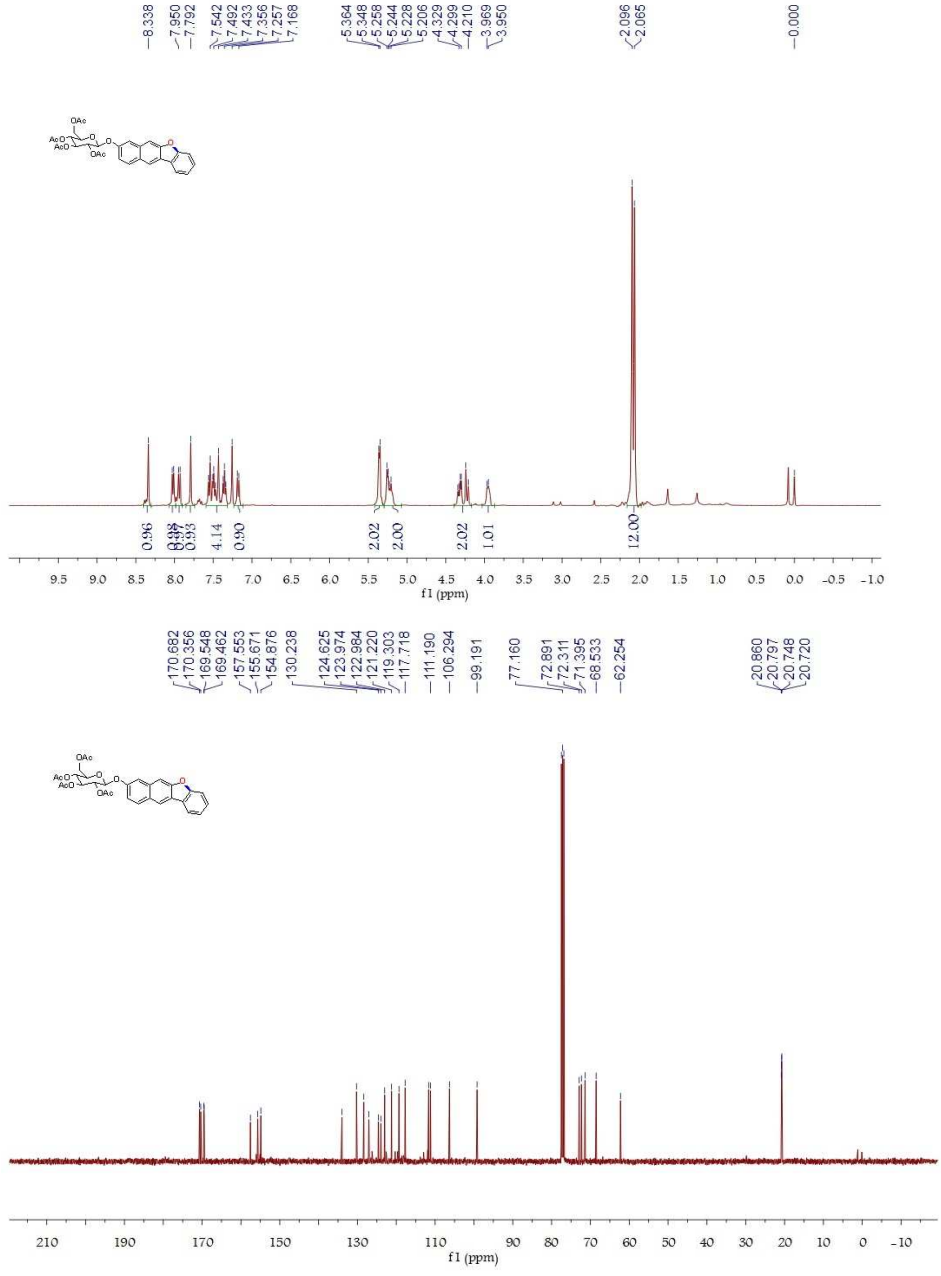
**(2R,3R,4S,5R,6S)-2-(acetoxymethyl)-6-(benzo[d]naphtho[2,3-b]furan-8-yloxy)tetrahydro-2H-pyran-3,4,5-triyl triacetate.**

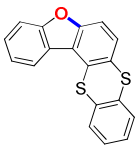
White solid.

$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.33 (s, 1H), 8.02 (d, $J$ = 8.0 Hz, 1H), 7.94 (d, $J$ = 8.0 Hz, 1H), 7.79 (s, 1H), 7.56-7.34 (m, 4H), 7.18 (d, $J$ = 8.0 Hz, 1H), 5.36-5.35 (m, 2H), 5.26-5.21 (m, 2H), 4.34-4.21 (m, 2H), 3.97-3.95 (m, 1H), 2.10-2.06 (m, 12H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 170.68, 170.36, 169.55, 169.46, 157.55, 155.67, 154.88, 133.98, 130.24, 128.36, 127.05, 124.62, 123.97, 122.98, 121.22, 119.30, 117.72, 111.66, 111.19, 106.29, 99.19, 72.89, 72.31, 71.40, 68.53, 62.25, 20.86, 20.80, 20.75, 20.72.

HRMS calcd for C30H28O11: 564.1632; found: 587.1533(ESI, +Na).





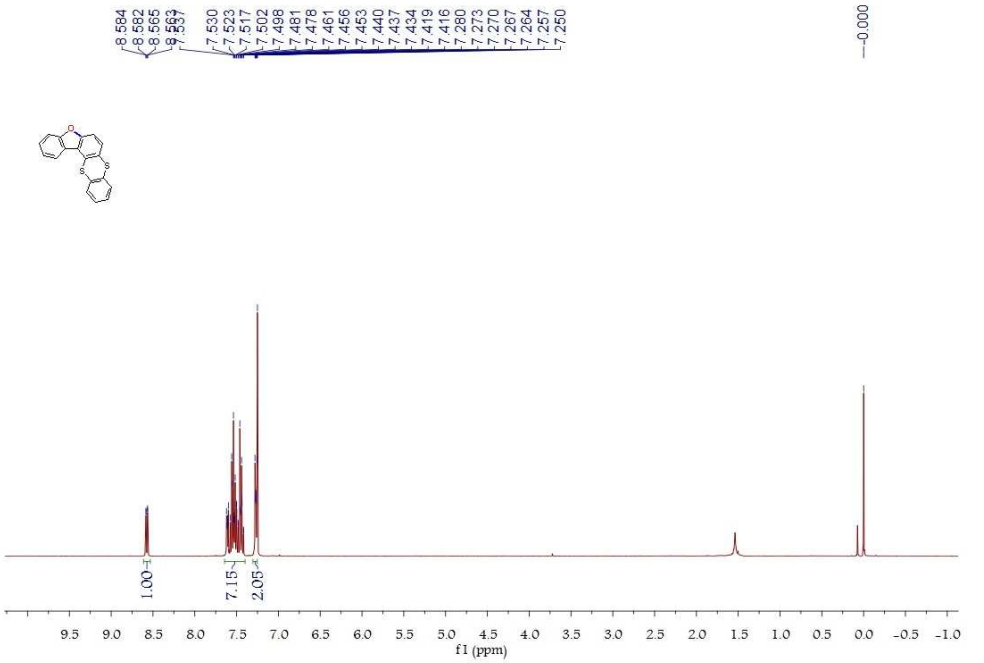
**benzo[d]thianthreno[2,1-b]furan.**

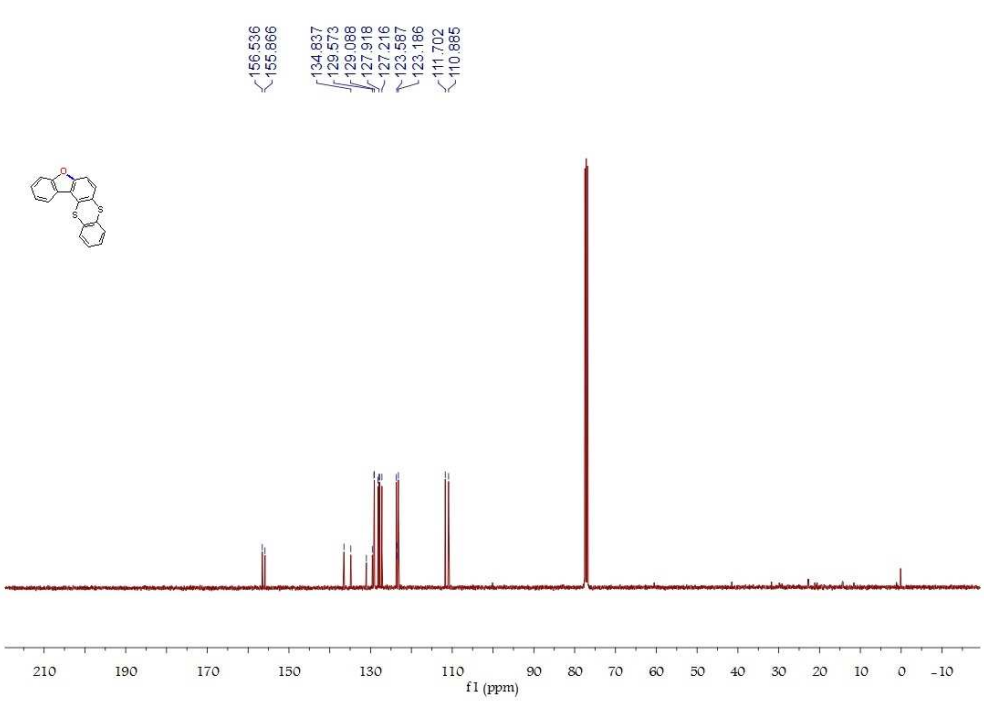
White solid.

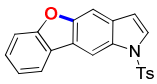
$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.58-8.56 (m, 1H), 7.54-7.42 (m, 7H), 7.28-7.26 (m, 2H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 156.54, 155.87, 136.52, 134.84, 131.02, 129.57, 129.18, 129.09, 128.17, 127.92, 127.79, 127.22, 123.69, 123.59, 123.57, 123.19, 111.70, 110.88.

HRMS calcd for C18H10OS2: 306.0173; found: 306.0177.





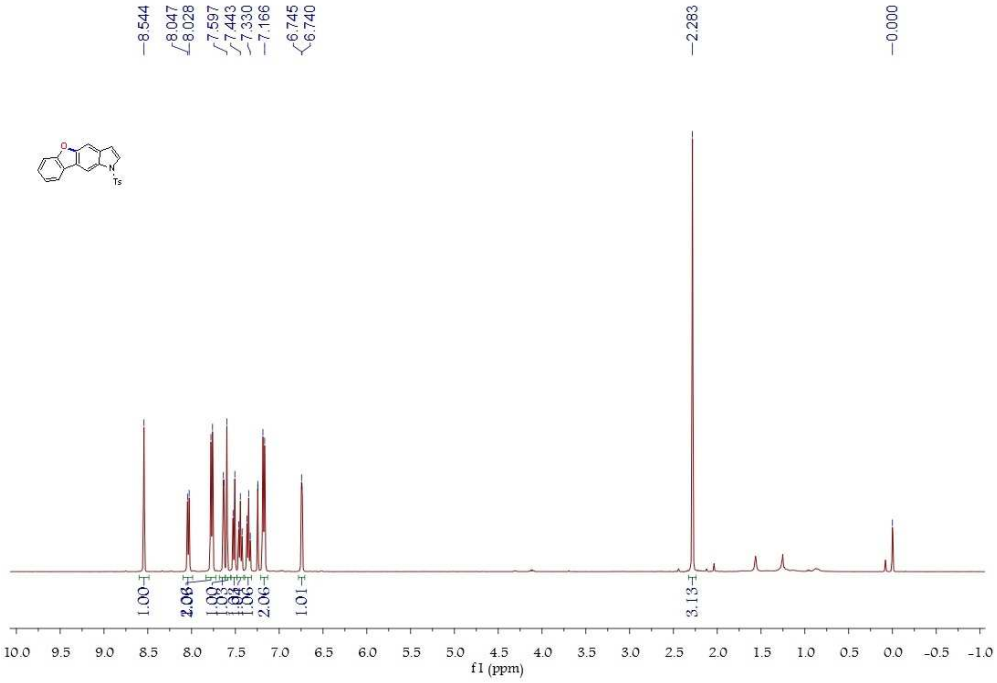
**1-tosyl-1H-benzofuro[2,3-f]indole.**

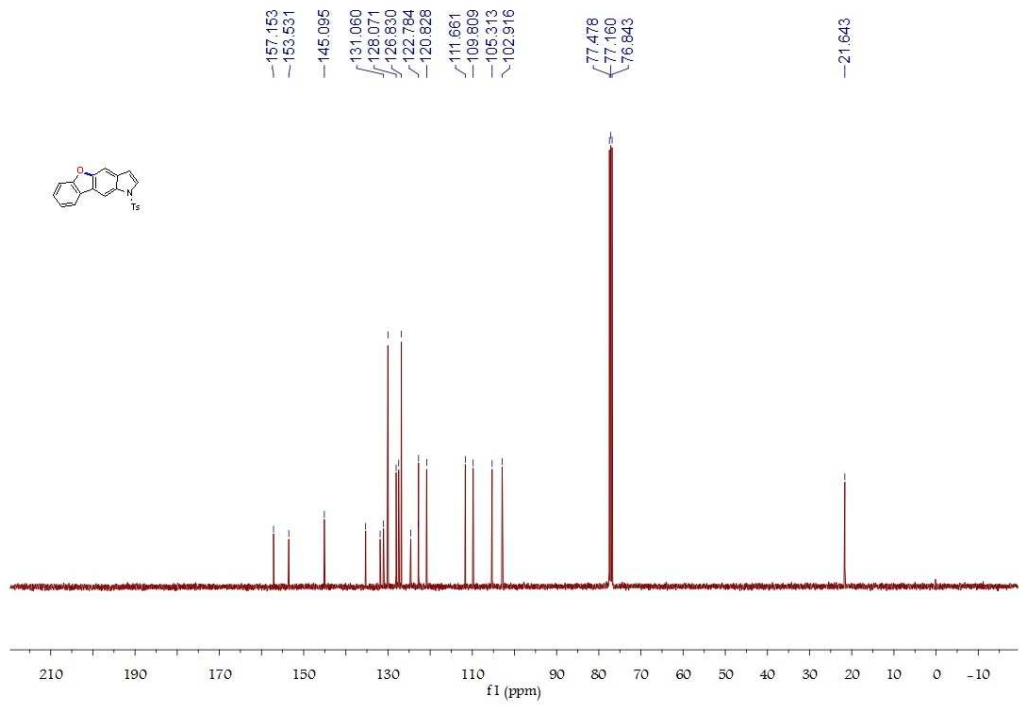
White solid.

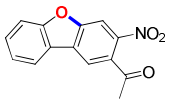
$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.54 (s, 1H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.77 (d, *J* = 8.0 Hz, 2H), 7.64-7.63 (m, 1H), 7.60 (s, 1H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.46-7.42 (m, 1H), 7.37-7.33 (m, 1H), 7.18 (d, *J* = 8.0 Hz, 2H), 6.75-6.74 (m, 1H), 2.28 (s, 3H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 157.15, 153.53, 145.10, 135.31, 131.87, 131.06, 130.02, 128.07, 127.46, 126.83, 124.61, 122.78, 122.75, 120.83, 111.66, 109.81, 105.31, 102.92, 21.64.

HRMS calcd for C21H15NO3S: 361.0773; found: 361.0778.





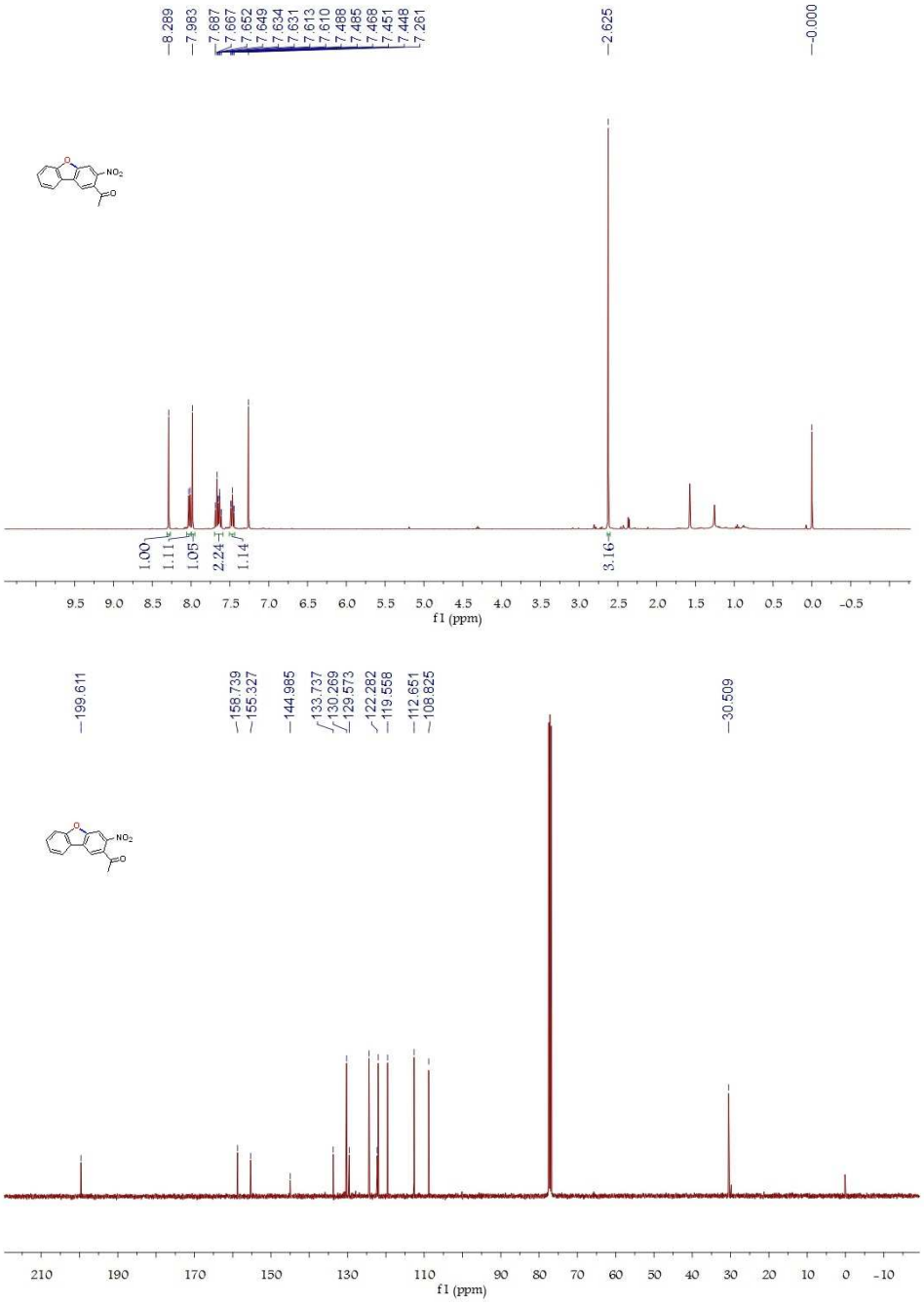
**1-(3-nitrodibenzo[b,d]furan-2-yl)ethanone.**

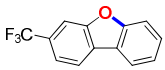
Known compound (Reference: Momotake, A.; Lindegger, N.; Niggli, E.; Barsotti, R. J.; Ellis-Davies, G. C. R. *Nat. Methods* **2006**, *3*, 35.)

White solid.

$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.29 (s, 1H), 8.03-8.01 (m, 1H), 7.98 (s, 1H), 7.66-7.61 (m, 2H), 7.49-7.45 (m, 1H), 2.62 (s, 3H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 199.61, 158.74, 155.33, 144.98, 133.74, 130.27, 129.57, 124.40, 122.28, 122.02, 119.56, 112.65, 108.83, 30.51.





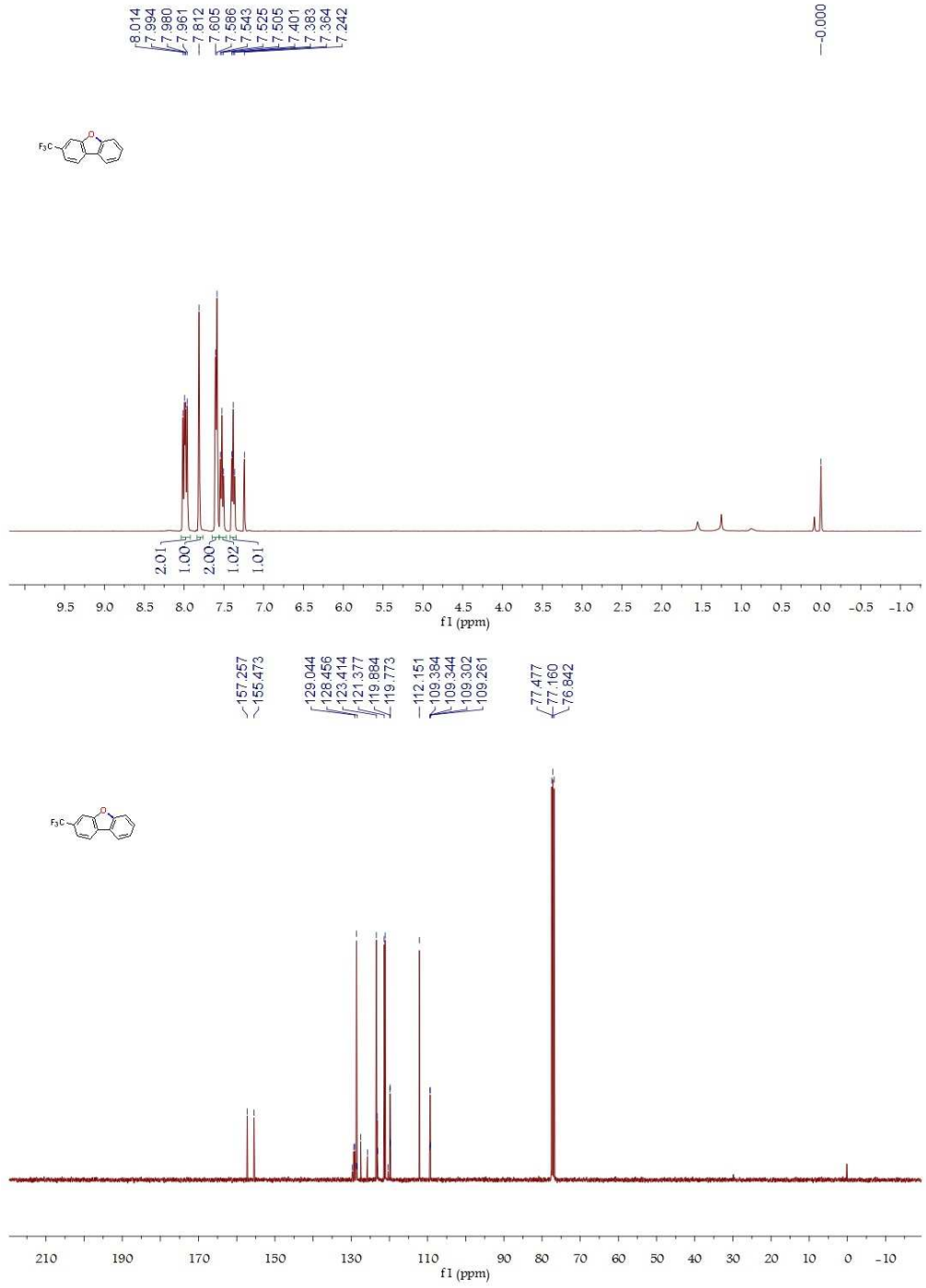
**3-(trifluoromethyl)dibenzo[b,d]furan.**

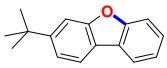
Known compound (Reference: Tobisu, M.; Kita, Y.; Ano, Y.; Chatani, N. *J. Am. Chem. Soc.* **2008**, *130*, 15982.)

White solid.

$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.01-7.96 (m, 2H), 7.81 (s, 1H), 7.60-7.59 (m, 2H), 7.54-7.50 (m, 1H), 7.40-7.36 (m, 1H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 157.26, 155.47, 129.21 (q, $J$ = 32 Hz ), 128.63, 127.51, 124.40 (q, $J$ = 270 Hz ), 123.41, 123.18, 121.38, 121.12, 119.83 (q, $J$ = 4 Hz ), 112.15, 109.32 (q, $J$ = 4 Hz ).





**3-tert-Butyl-dibenzofuran.**

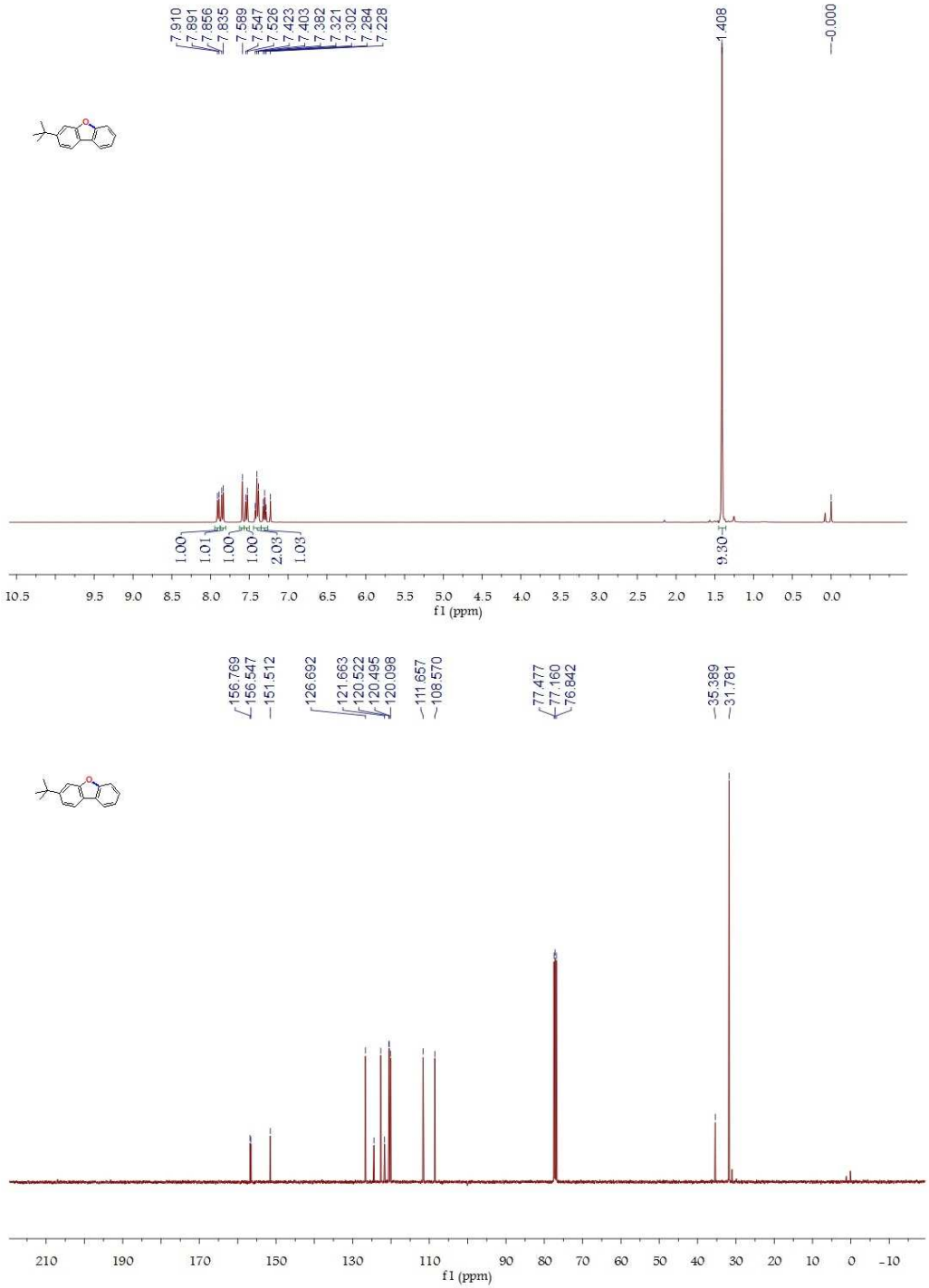
Known compound (Reference: Wang, C.; Piel, I.; Glorius, F. *J. Am. Chem. Soc.* **2009**, *131*, 4195.)

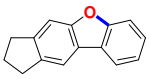
White solid.

$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.90 (d, $J$ = 8.0 Hz, 1H), 7.85 (d, $J$ = 8.0 Hz, 1H), 7.59 (s, 1H), 7.54 (d, $J$ = 8.0 Hz, 1H), 7.42-7.38 (m, 2H), 7.32-7.28 (m, 1H)1.41 (s, 9H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 156.77, 156.55, 151.51, 126.69, 124.46, 122.68, 121.66, 120.52, 120.50, 120.10, 111.66, 108.57, 35.39, 31.78.

HRMS calcd for C16H16O: 224.1201; found: 224.1207.





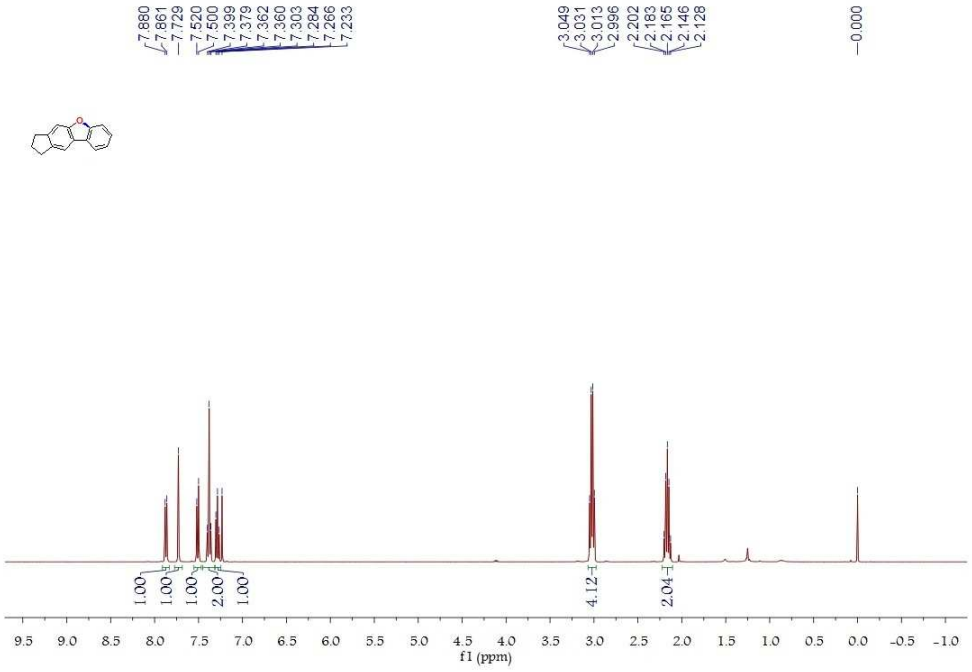
**2,3-Dihydro-1H-9-oxa-cyclopenta[b]fluorene.**

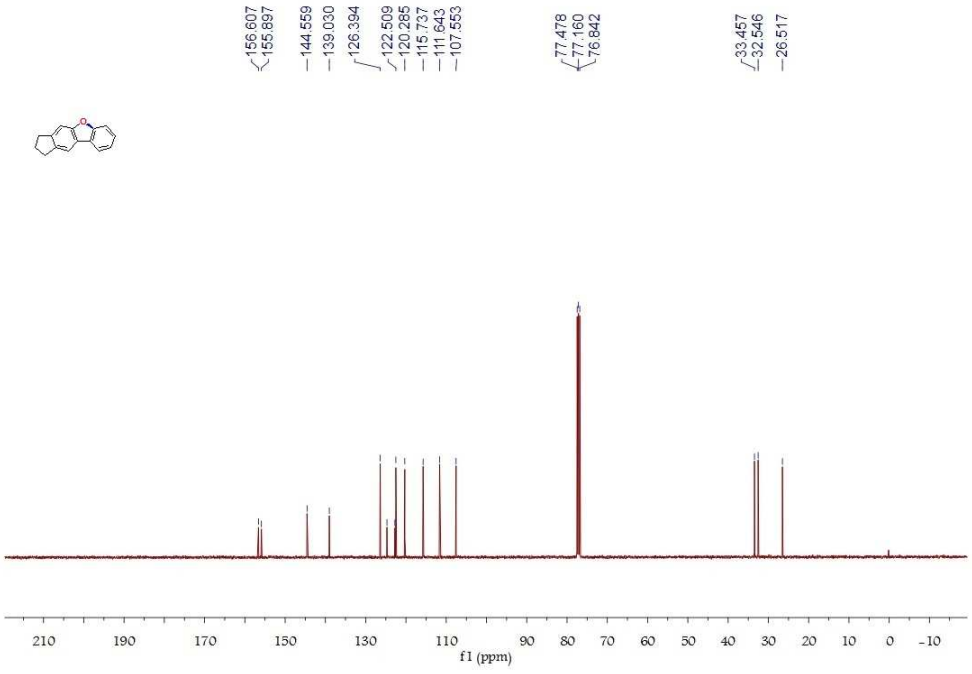
White solid.

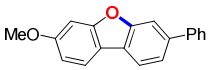
$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.87 (d, $J$ = 7.6 Hz, 1H), 7.73 (s, 1H), 7.51 (d, $J$ = 7.6 Hz, 1H), 7.40-7.36 (m, 2H), 7.30-7.26 (m, 1H), 3.05-3.00 (m, 4H), 2.20-2.13 (m, 2H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 156.61, 155.90, 144.56, 139.03, 126.39, 124.72, 122.51, 120.29, 115.74, 111.64, 107.55, 33.46, 32.55, 26.52.

HRMS calcd for C15H12O: 208.0888; found: 208.0886.





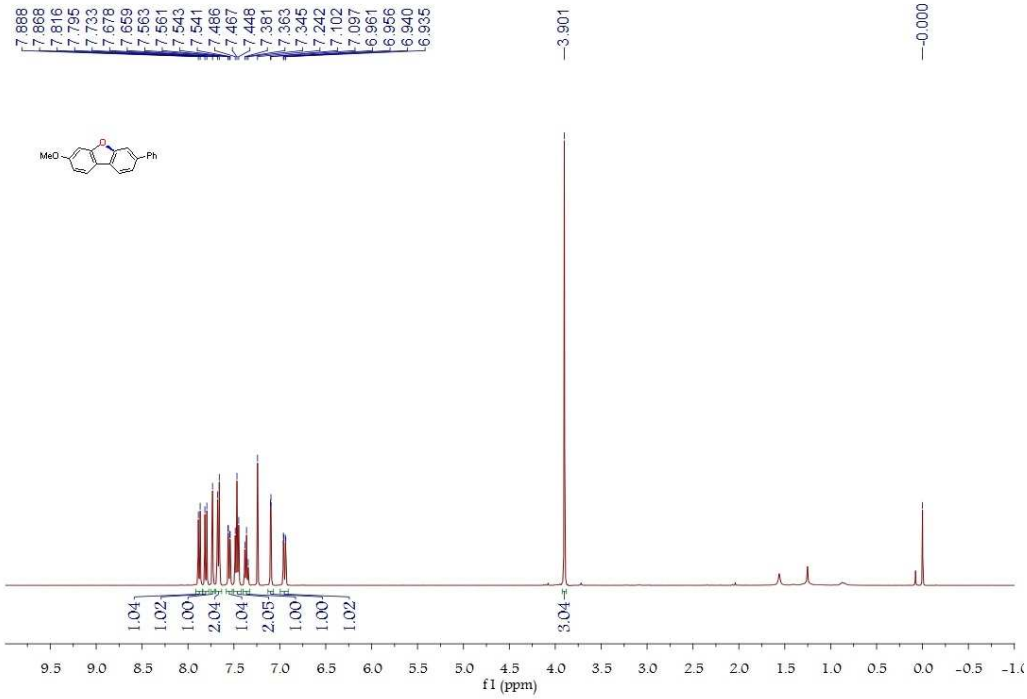

**3-methoxy-7-phenyldibenzo[b,d]furan.**

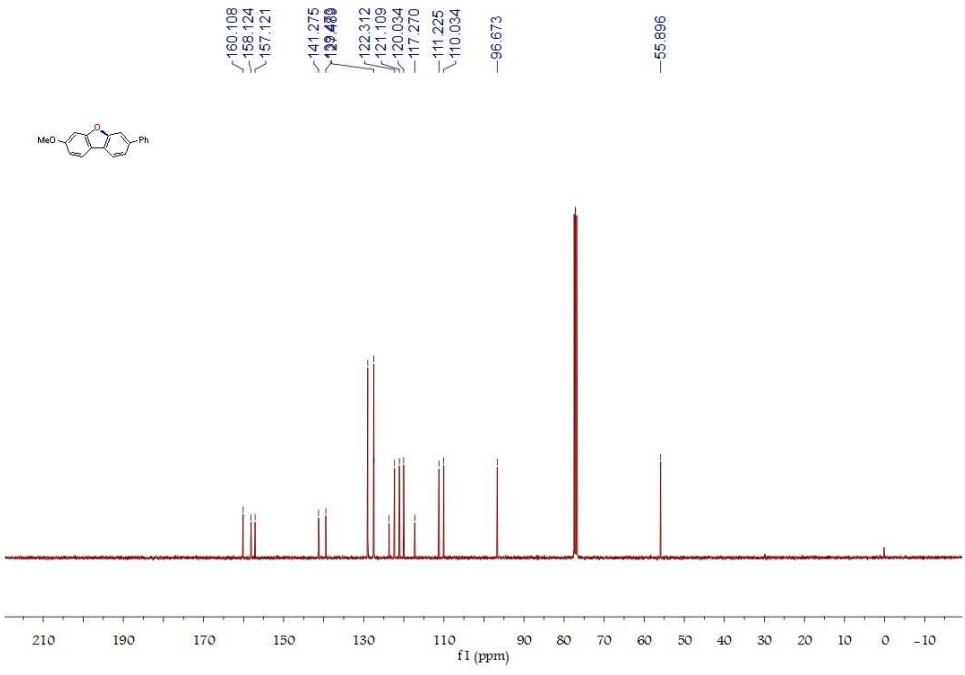
White solid.

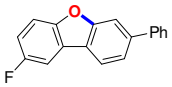
$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.87 (d, $J$ = 8.0 Hz, 1H), 7.80 (d, $J$ = 8.0 Hz, 1H), 7.73 (s, 1H), 7.68-7.66 (m, 2H), 7.56-7.54 (m, 1H), 7.49-7.45 (m, 2H), 7.38-7.34 (m, 1H), 7.10 (m, 1H), 6.96-6.94 (m, 1H), 3.90 (s, 3H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 160.11, 158.12, 157.12, 141.28, 139.47, 129.01, 127.49, 127.46, 123.67, 122.31, 121.11, 120.03, 117.27, 111.22, 110.03, 96.67, 55.90.

HRMS calcd for C19H14O2: 274.0994; found: 274.0998.





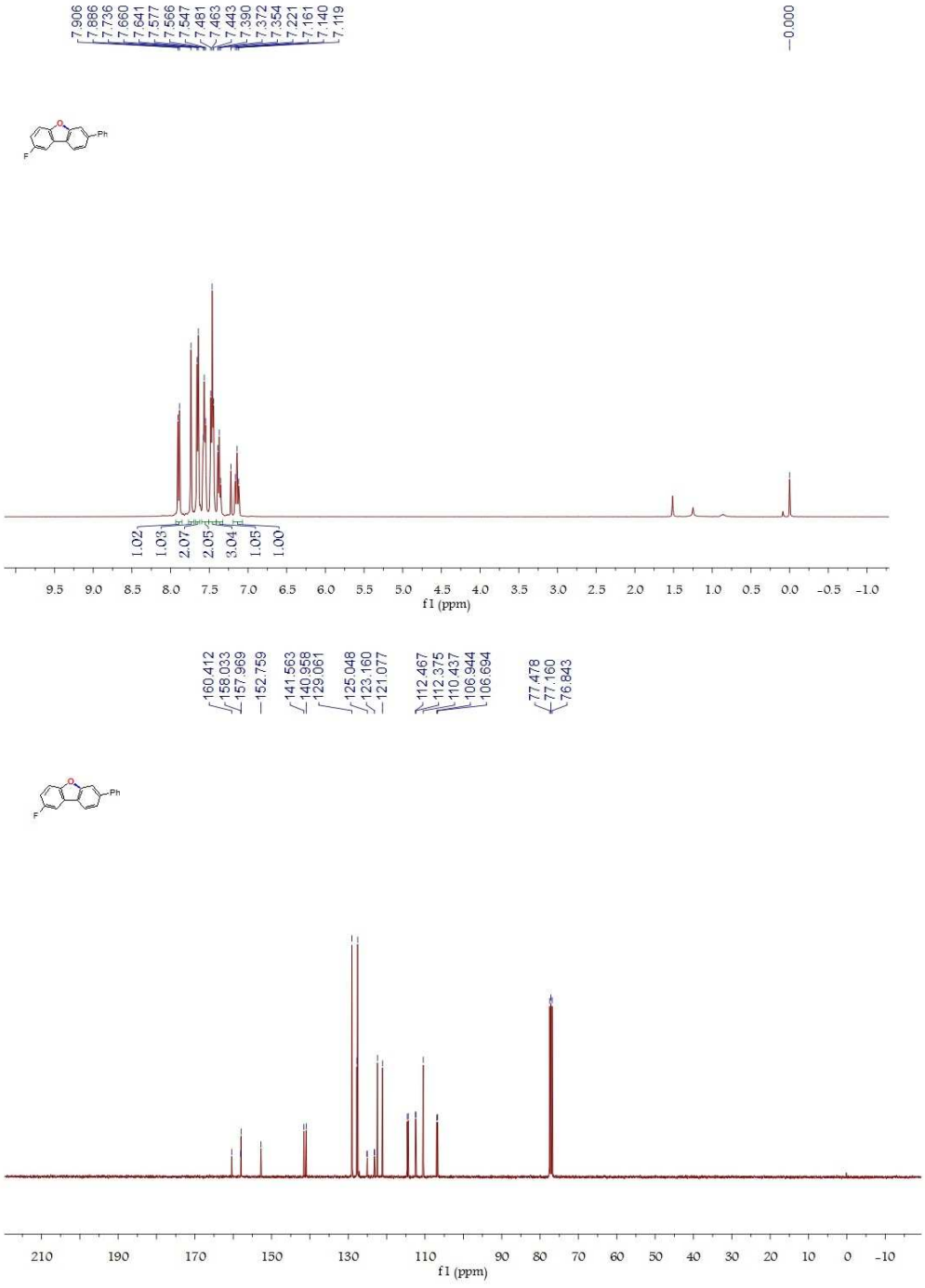

**2-Fluoro-7-phenyl-dibenzofuran.**

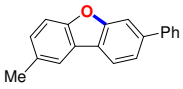
White solid.

$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.89 (d, $J$ = 8.0 Hz, 1H), 7.74 (s, 1H), 7.66-7.64 (m, 2H), 7.58-7.55 (m, 2H), 7.48-7.44 (m, 3H), 7.39-7.35 (m, 1H), 7.16-7.12 (m, 1H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 160.41, 158.03, 157.97, 152.76, 141.56, 140.96, 129.06, 127.79, 127.56, 125.15, 125.05, 123.20, 123.16, 122.40, 121.08, 114.64, 114.38, 112.47, 112.38, 110.44, 106.94, 106.69.

HRMS calcd for C18H11FO: 262.0794; found: 262.0796.





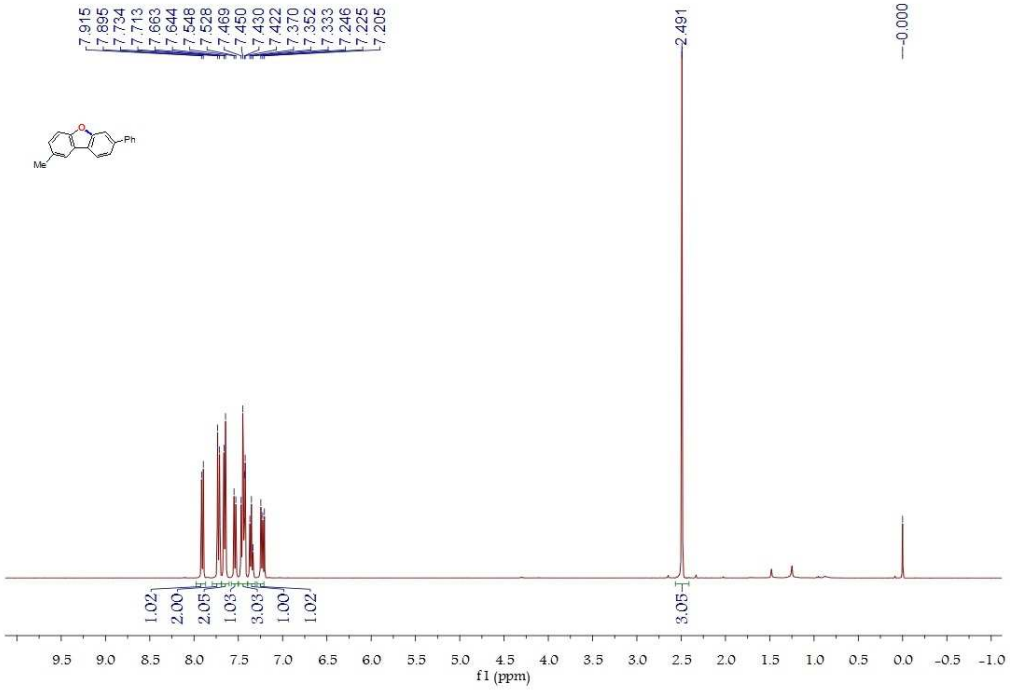

**2-Methyl-7-phenyl-dibenzofuran.**

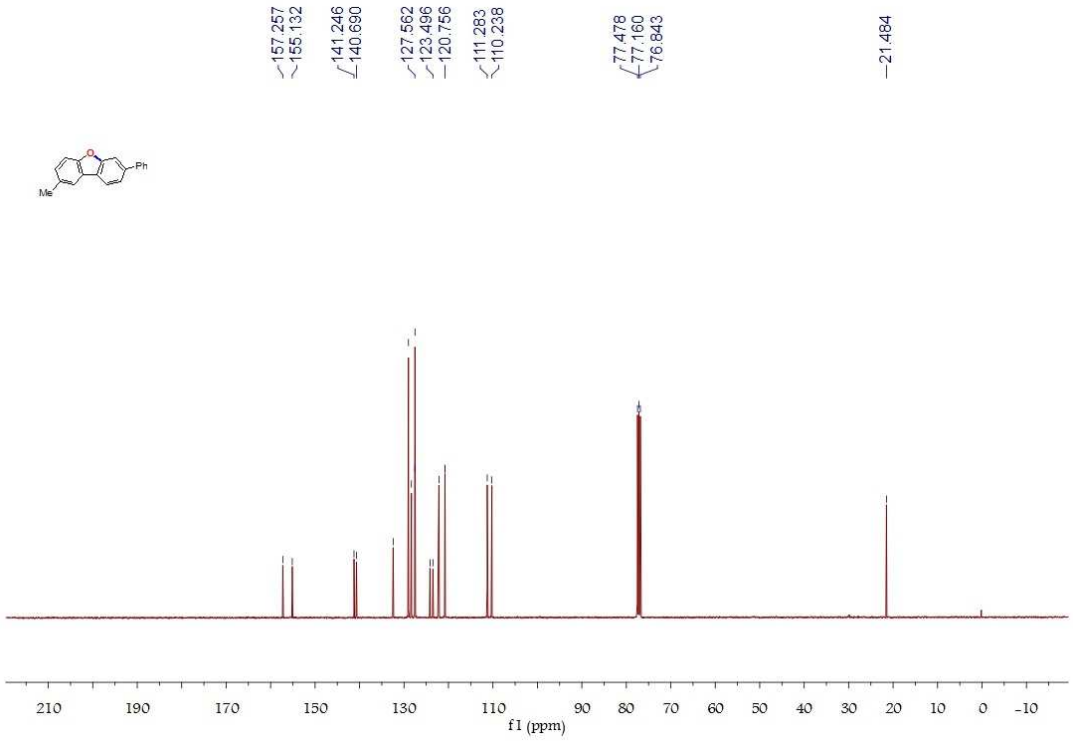
White solid.

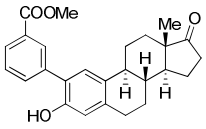
$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.91 (d, $J$ = 8.0 Hz, 1H), 7.72 (d, $J$ = 8.0 Hz, 2H), 7.65 (d, $J$ = 8.0 Hz, 2H), 7.54 (d, $J$ = 8.0 Hz, 1H), 7.47-7.42 (m, 3H), 7.37-7.33 (m, 1H), 7.24 (d, $J$ = 8.0 Hz, 1H), 2.49 (s, 3H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 157.26, 155.13, 141.25, 140.69, 132.44, 129.01, 128.34, 127.56, 127.54, 124.16, 123.50, 122.14, 120.78, 120.76, 111.28, 110.24, 21.48.

HRMS calcd for C19H14O: 258.1045; found: 258.1047.





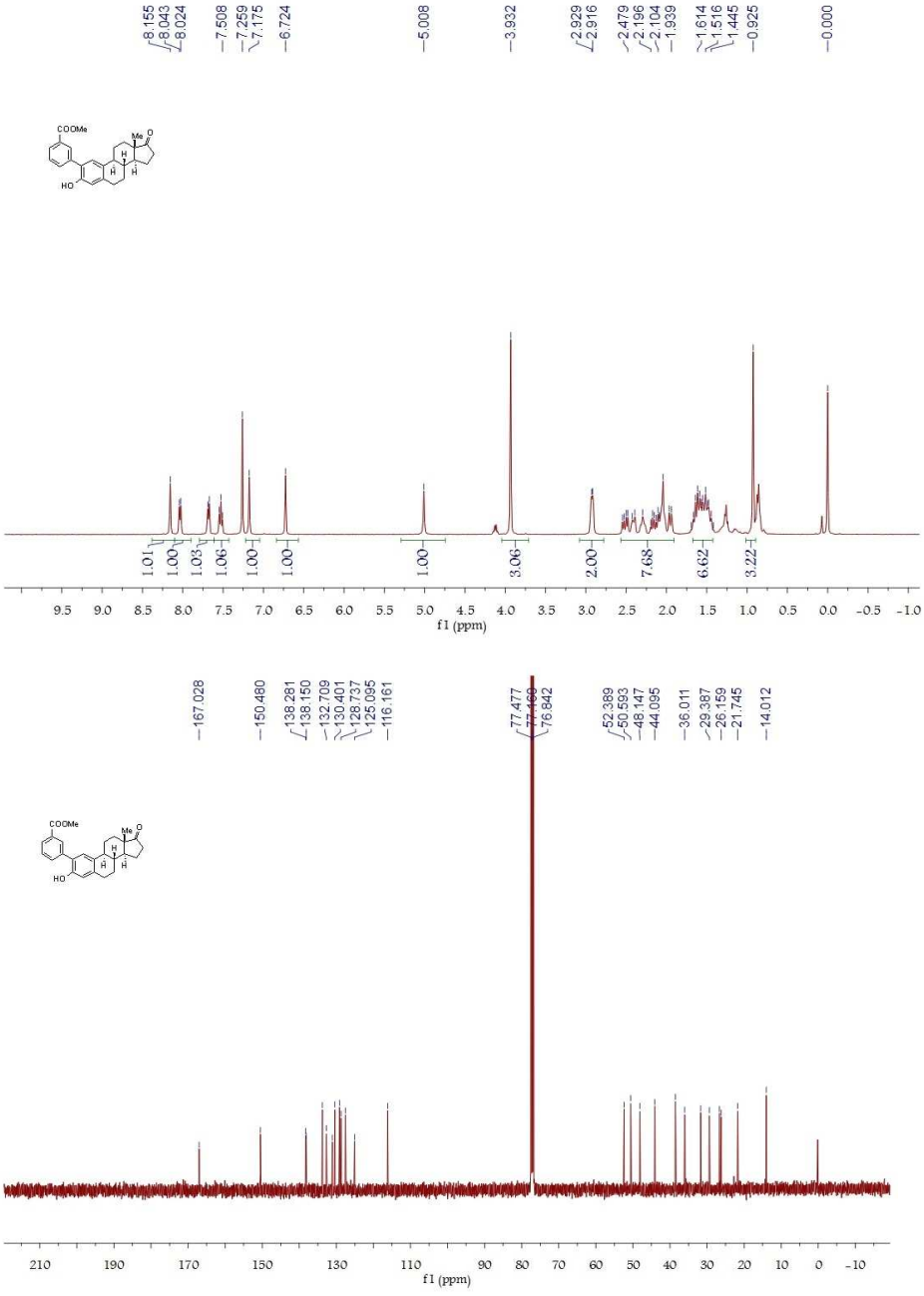

**methyl 3-((8R,9S,13S,14S)-3-hydroxy-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-2-yl)benzoate.**

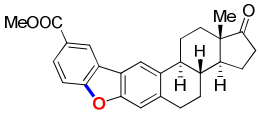
White solid.

$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.16 (m, 1H), 8.03 (d, $J$ = 8.0 Hz, 1H), 7.68 (d, $J$ = 8.0 Hz, 1H), 7.55-7.51 (m, 1H), 7.18 (s, 1H), 6.72 (s, 1H), 5.01 (s, 1H), 3.93 (s, 3H), 2.93-2.92 (m, 2H), 2.55-1.94 (m, 7H), 1.67-1.44 (m, 6H), 0.92 (s, 3H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 167.03, 150.48, 138.28, 138.15, 133.75, 132.71, 131.05, 130.40, 129.15, 128.74, 127.56, 125.10, 116.16, 52.39, 50.59, 48.15, 44.10, 38.52, 36.01, 31.70, 29.39, 26.64, 26.16, 21.74, 14.01.

HRMS calcd for C26H28O4: 404.1988; found: 404.1989.



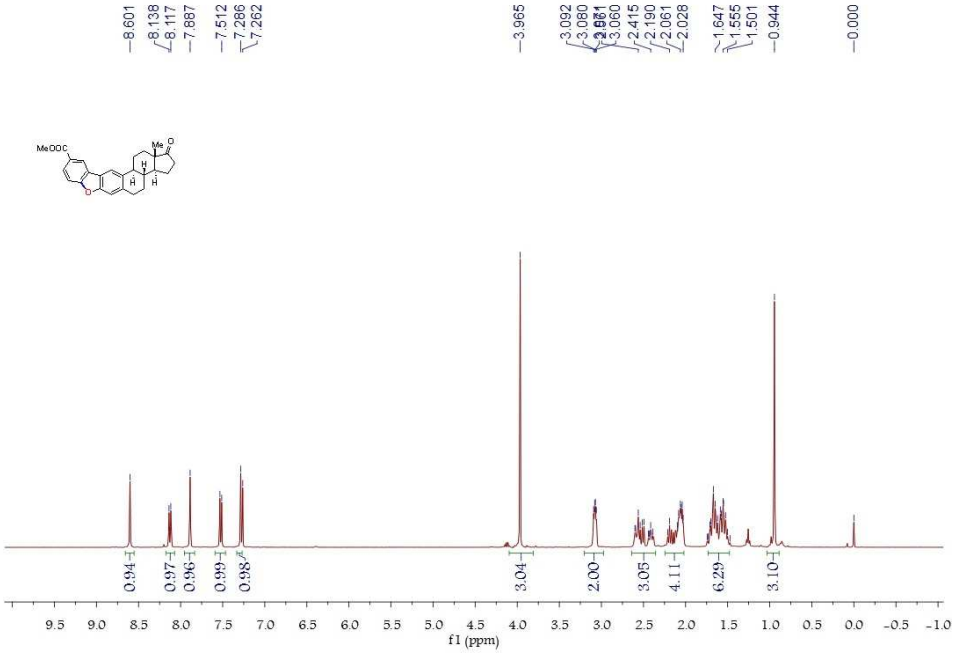


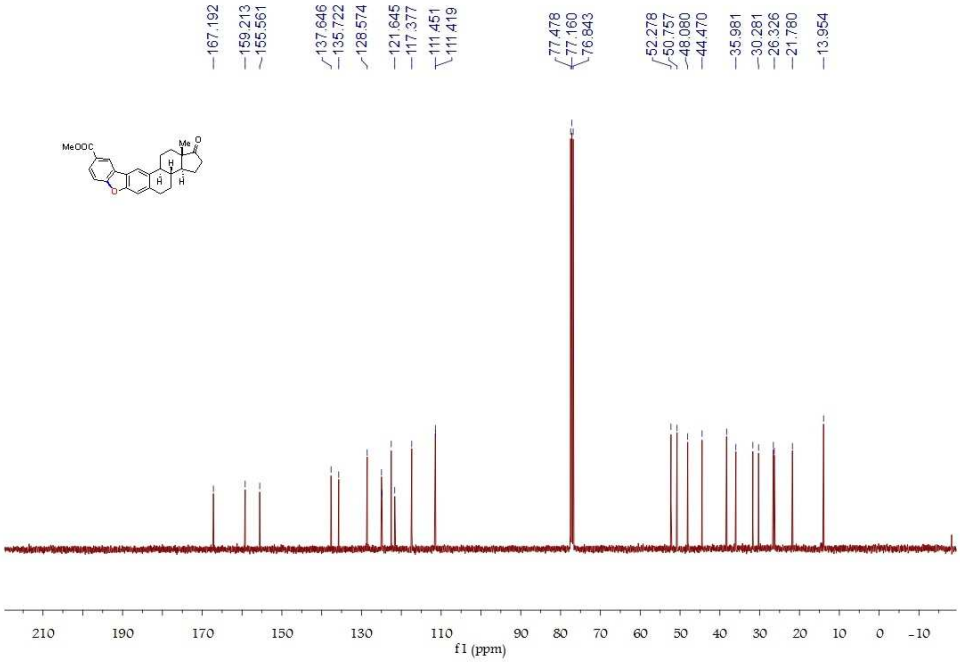

White solid.

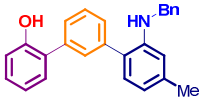
$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.60 (s, 1H), 8.13 (d, $J$ = 8.0 Hz, 1H), 7.89 (s, 1H), 7.53 (d, $J$ = 8.0 Hz, 1H), 7.29 (s, 1H), 3.96 (s, 3H), 3.09-3.06 (m, 2H), 2.60-2.39 (m, 3H), 2.21-2.03 (m, 4H), 1.74-1.47 (m, 6H), 0.94 (s, 3H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 167.19, 159.21, 155.56, 137.65, 135.72, 128.57, 124.98, 124.86, 122.53, 121.65, 117.38, 111.45, 111.42, 52.28, 50.76, 48.08, 44.47, 38.31, 35.98, 31.71, 30.28, 26.56, 26.33, 21.78, 13.95.

HRMS calcd for C26H26O4: 402.1831; found: 402.1837.





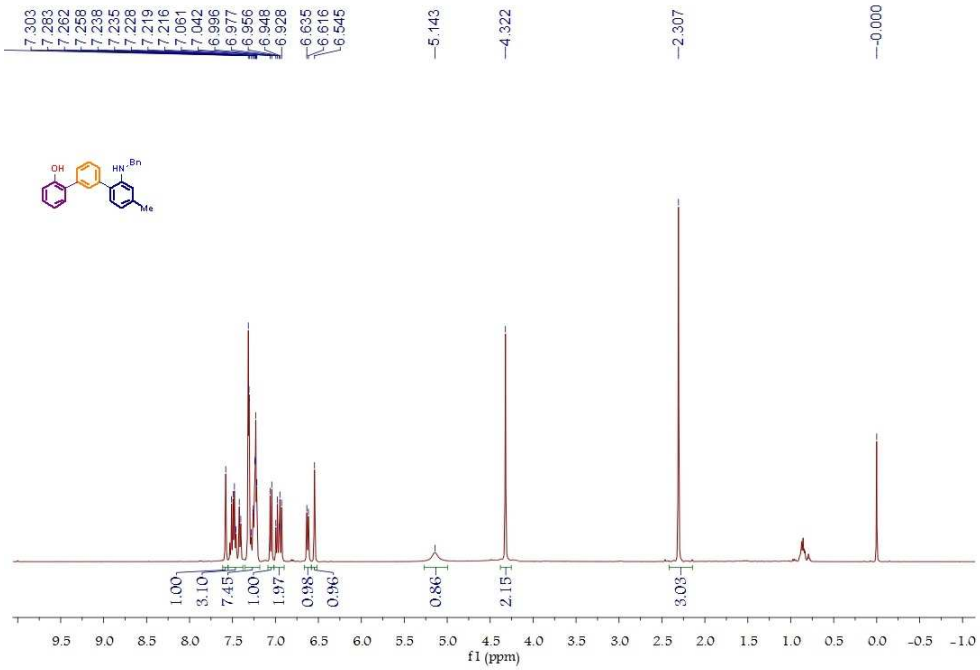

**2-Benzylamino-4-methyl-[1,1';3',1'']terphenyl-2''-ol.**

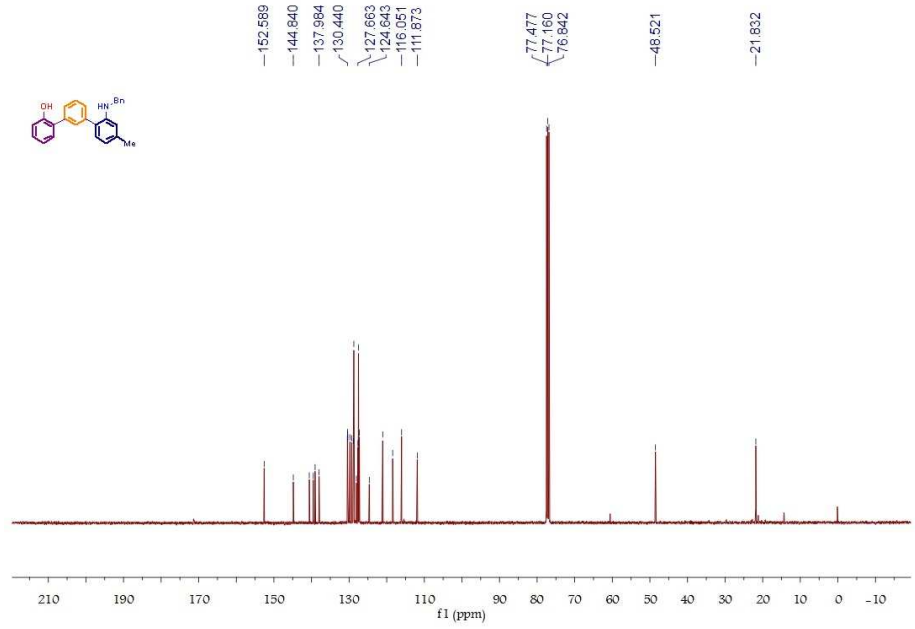
yellow solid.

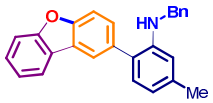
$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.58 (s, 1H), 7.53-7.46 (m, 2H), 7.42-7.40 (m, 1H), 7.32-7.22 (m, 7H), 7.06-7.04 (m, 1H), 7.00-6.93 (m, 2H), 6.64-6.62 (m, 1H), 6.54 (s, 1H), 5.14 (s, 1H), 4.32 (s, 2H), 2.31 (s, 3H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 152.59, 144.84, 140.59, 139.53, 139.05, 137.98, 130.44, 130.38, 130.34, 129.79, 129.30, 128.88, 128.75, 128.07, 127.66, 127.51, 127.28, 124.64, 121.06, 118.42, 116.05, 111.87, 48.52, 21.83.

HRMS calcd for C26H23NO: 365.1780; found: 365.1783.





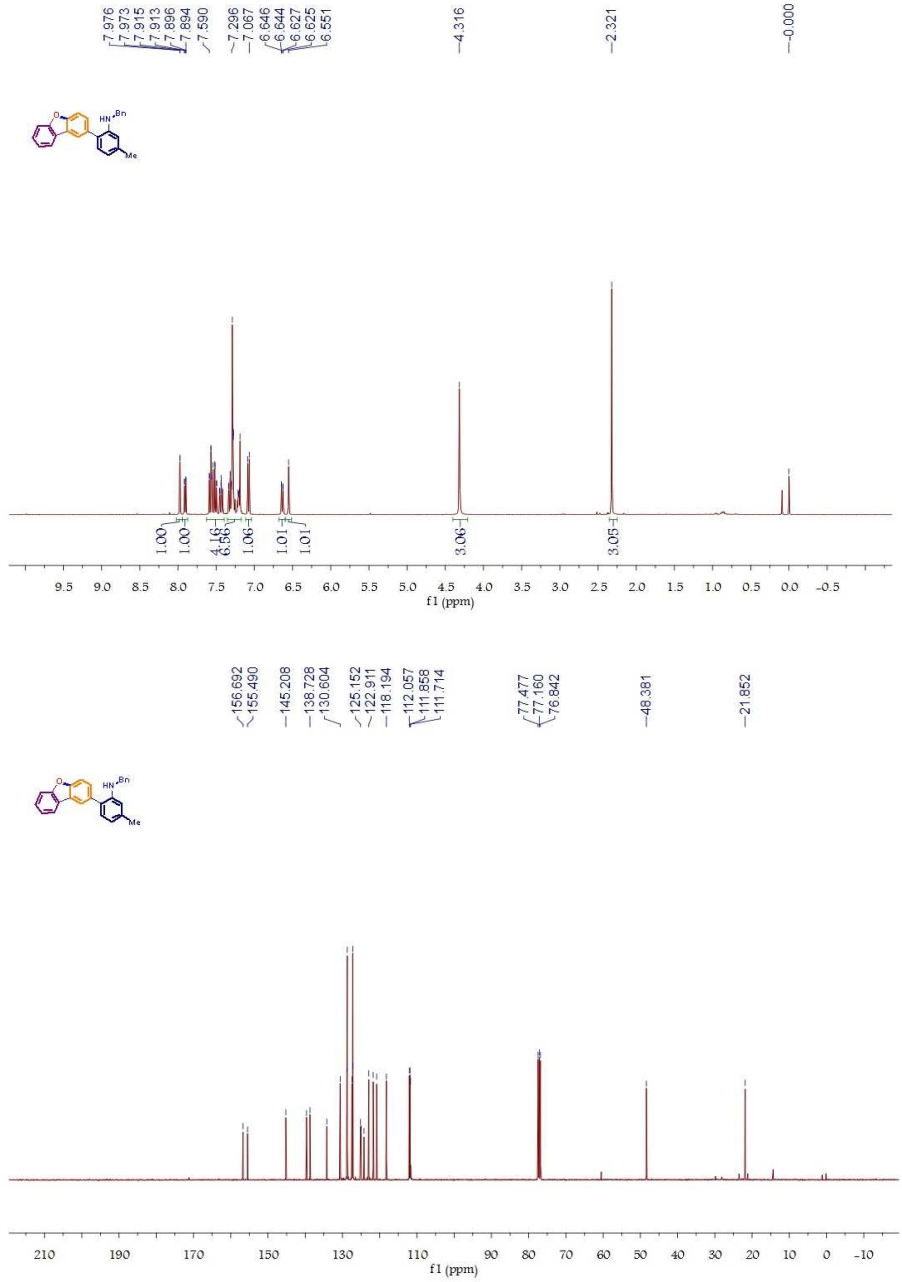

**N-benzyl-2-(dibenzo[b,d]furan-2-yl)-5-methylaniline.**

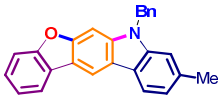
thick oil.

$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 7.98-7.97 (m, 1H),7.92-7.89 (m, 1), 7.59-7.49 (m, 3), 7.45-7.41 (m, 1H), 7.34-7.18 (m, 6H), 7.08-7.07 (m, 1H), 6.65-6.62 (m, 1H), 6.55 (s, 1H), 4.32 (s+brs, 3H) C$H_2$+N$H$, 2.32 (s, 3H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 156.69, 155.49, 145.21, 139.65, 138.73, 134.20, 130.60, 128.75, 128.71, 127.45, 127.24, 127.17, 125.15, 124.98, 124.21, 122.91, 121.74, 120.81, 118.19, 112.06, 111.86, 111.71, 48.38, 21.85.

HRMS calcd for C26H21NO: 363.1623; found: 363.1627.





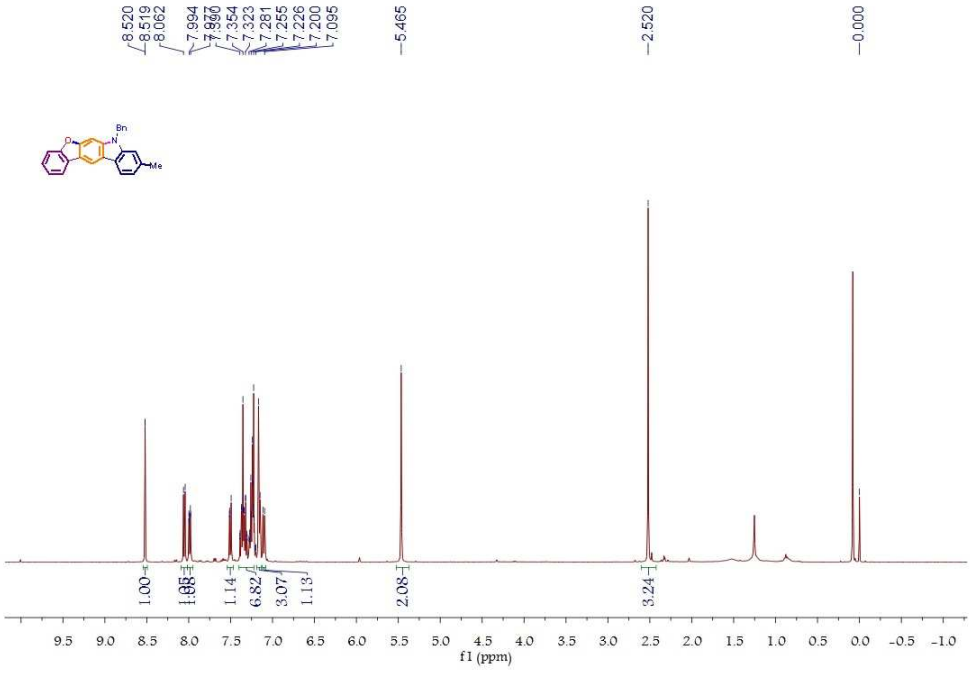

**2-Benzylamino-4-methyl-[1,1';3',1'']terphenyl-2''-ol.**

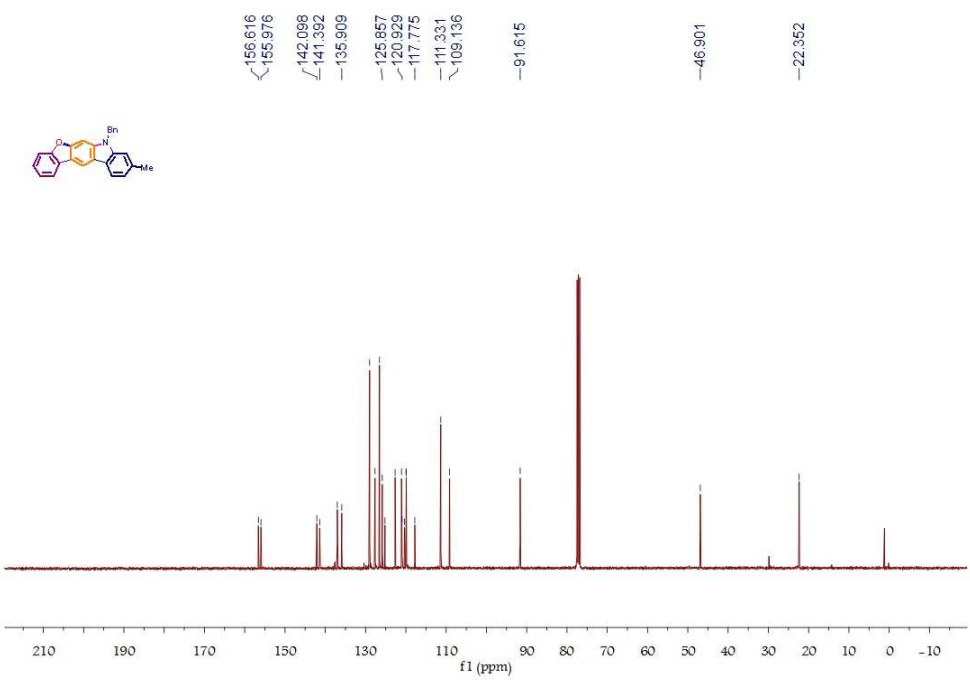
thick oil.

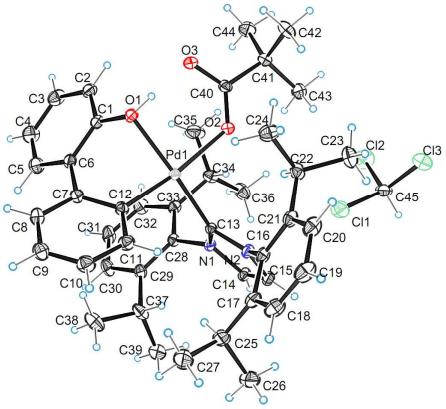
$^{1}$H NMR ($CDCl_3$, 400 MHz) $\delta$ 8.52 (s, 1H), 8.06-8.04 (m, 1H), 8.00-7.98 (m, 1H), 7.51-7.49 (m, 1H), 7.39-7.20 (m, 6H), 7.17-7.15 (m, 3H), 7.12-7.10 (m, 1H), 5.46 (s, 2H), 2.52 (s, 3H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) $\delta$ 156.62, 155.98, 142.10, 141.39, 137.02, 135.91, 128.99, 127.66, 126.55, 125.86, 125.18, 122.67, 121.08, 120.93, 120.33, 119.97, 119.89, 117.77, 111.33, 109.14, 91.62, 46.90, 22.35.

HRMS calcd for C26H19NO: 361.1467; found: 361.1469.



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C18 C 0.8132(3) 0.0424(2) -0.08520(14) 0.0674(9) Uani 1 1 d . . .
H18 H 0.8322 0.0456 -0.1232 0.081 Uiso 1 1 calc R . .
C39 C 0.8793(4) 0.4029(3) -0.01997(17) 0.0959(14) Uani 1 1 d . . .
H39A H 0.8734 0.4546 -0.0170 0.144 Uiso 1 1 calc R . .
H39B H 0.9052 0.3901 -0.0572 0.144 Uiso 1 1 calc R . .
H39C H 0.9444 0.3851 0.0078 0.144 Uiso 1 1 calc R . .
C32 C 0.6488(3) 0.42017(19) 0.16090(13) 0.0658(8) Uani 1 1 d . . .
H32 H 0.6306 0.4330 0.1978 0.079 Uiso 1 1 calc R . .
C44 C 0.4847(4) 0.1232(2) 0.30427(14) 0.0752(10) Uani 1 1 d . . .
H44A H 0.5202 0.1010 0.3386 0.113 Uiso 1 1 calc R . .
H44B H 0.3898 0.1171 0.3014 0.113 Uiso 1 1 calc R . .
H44C H 0.5057 0.1739 0.3049 0.113 Uiso 1 1 calc R . .
C23 C 0.7921(4) -0.0369(2) 0.12061(17) 0.0803(11) Uani 1 1 d . . .
H23A H 0.7804 -0.0828 0.1020 0.120 Uiso 1 1 calc R . .
H23B H 0.7625 -0.0403 0.1585 0.120 Uiso 1 1 calc R . .
H23C H 0.8846 -0.0239 0.1220 0.120 Uiso 1 1 calc R . .
C45 C 1.1010(3) 0.0934(2) 0.23670(13) 0.0694(10) Uani 1 1 d . . .
H42 H 1.1949 0.1043 0.2314 0.083 Uiso 1 1 calc R . .
C31 C 0.6278(4) 0.46991(18) 0.11841(15) 0.0717(9) Uani 1 1 d . . .
H31 H 0.5941 0.5153 0.1266 0.086 Uiso 1 1 calc R . .

C4 C 0.2083(4) 0.41179(19) 0.12028(18) 0.0820(11) Uani 1 1 d . . .
H4 H 0.1857 0.4603 0.1240 0.098 Uiso 1 1 calc R . .
C9 C 0.3156(3) 0.2854(2) -0.09368(14) 0.0757(11) Uani 1 1 d . . .
H9 H 0.2735 0.3024 -0.1271 0.091 Uiso 1 1 calc R . .
C36 C 0.8587(4) 0.3115(2) 0.22780(16) 0.0797(11) Uani 1 1 d . . .
H36A H 0.9249 0.3118 0.2000 0.120 Uiso 1 1 calc R . .
H36B H 0.8784 0.2737 0.2549 0.120 Uiso 1 1 calc R . .
H36C H 0.8589 0.3573 0.2469 0.120 Uiso 1 1 calc R . .
C38 C 0.6411(4) 0.3950(2) -0.05413(15) 0.0835(12) Uani 1 1 d . . .
H38A H 0.5560 0.3746 -0.0467 0.125 Uiso 1 1 calc R . .
H38B H 0.6665 0.3798 -0.0909 0.125 Uiso 1 1 calc R . .
H38C H 0.6356 0.4468 -0.0530 0.125 Uiso 1 1 calc R . .
C27 C 0.7545(5) 0.1860(3) -0.13779(17) 0.0996(15) Uani 1 1 d . . .
H27A H 0.7957 0.1581 -0.1663 0.149 Uiso 1 1 calc R . .
H27B H 0.7529 0.2361 -0.1486 0.149 Uiso 1 1 calc R . .
H27C H 0.6651 0.1693 -0.1340 0.149 Uiso 1 1 calc R . .
H1 H 0.334(4) 0.177(2) 0.1362(10) 0.085(13) Uiso 1 1 d D . .

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Cl3 0.1162(9) 0.0976(9) 0.1349(10) 0.0450(8) 0.0383(7) 0.0040(7)
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O2 0.0382(9) 0.0448(10) 0.0442(9) 0.0072(7) 0.0075(7) 0.0021(7)
N1 0.0354(10) 0.0324(10) 0.0386(10) 0.0001(8) 0.0035(7) 0.0019(8)
O3 0.0397(10) 0.0721(15) 0.0655(12) 0.0269(11) 0.0136(8) 0.0029(9)
N2 0.0337(10) 0.0340(10) 0.0454(10) -0.0025(8) 0.0060(8) 0.0040(8)
C28 0.0381(12) 0.0311(11) 0.0448(12) -0.0030(10) 0.0011(9) -0.0001(10)
C1 0.0333(12) 0.0367(13) 0.0554(14) -0.0025(11) 0.0035(10) 0.0008(10)
C13 0.0390(12) 0.0300(11) 0.0317(10) 0.0007(8) 0.0039(8) 0.0038(9)
C33 0.0469(14) 0.0406(14) 0.0479(14) -0.0064(11) 0.0052(10) 0.0008(11)
C6 0.0393(13) 0.0414(14) 0.0618(16) 0.0065(12) 0.0056(11) 0.0060(11)
C16 0.0430(13) 0.0376(13) 0.0514(14) -0.0117(11) 0.0061(10) 0.0074(11)
C41 0.0515(15) 0.0549(17) 0.0516(15) 0.0139(13) 0.0087(11) 0.0032(13)
C15 0.0355(12) 0.0427(14) 0.0530(14) -0.0001(11) 0.0054(10) 0.0061(10)
C29 0.0528(15) 0.0360(13) 0.0494(14) -0.0011(11) -0.0019(11) 0.0030(11)

C17 0.0473(14) 0.0575(18) 0.0552(15) -0.0103(13) 0.0125(11) 0.0090(13)
C7 0.0424(14) 0.0477(15) 0.0515(14) 0.0098(12) 0.0014(11) 0.0015(11)
C21 0.0430(14) 0.0400(14) 0.0652(17) -0.0114(12) 0.0039(12) 0.0040(11)
C14 0.0316(11) 0.0446(14) 0.0495(13) -0.0007(11) 0.0010(9) -0.0003(10)
C12 0.0391(12) 0.0404(13) 0.0424(12) 0.0040(10) 0.0005(9) -0.0025(10)
C40 0.0478(14) 0.0351(13) 0.0465(13) 0.0047(10) 0.0087(10) -0.0009(10)
C2 0.0457(14) 0.0513(16) 0.0627(17) -0.0008(13) 0.0124(12) 0.0020(12)
C34 0.0699(18) 0.0453(15) 0.0416(13) -0.0046(11) 0.0096(12) -0.0057(13)
C20 0.0605(18) 0.0426(16) 0.086(2) -0.0206(15) 0.0102(15) -0.0015(14)
C37 0.101(3) 0.0432(16) 0.0462(15) 0.0060(12) 0.0044(15) 0.0093(16)
C25 0.084(2) 0.068(2) 0.0541(17) 0.0003(15) 0.0247(15) 0.0199(18)
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C22 0.0577(16) 0.0368(14) 0.0621(17) -0.0008(12) 0.0023(13) 0.0025(12)
C5 0.074(2) 0.0445(17) 0.092(2) 0.0128(16) 0.0186(18) 0.0151(16)
C19 0.069(2) 0.063(2) 0.089(2) -0.0373(19) 0.0158(17) -0.0022(17)
C11 0.0499(15) 0.0580(17) 0.0442(14) -0.0019(12) 0.0025(11) -0.0019(13)
C43 0.0573(18) 0.096(3) 0.0655(19) 0.0263(19) 0.0009(14) 0.0113(18)
C30 0.092(2) 0.0377(15) 0.0627(18) 0.0037(13) -0.0051(16) 0.0139(15)
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C10 0.0646(19) 0.090(3) 0.0436(15) -0.0008(16) 0.0002(13) -0.0052(18)
C3 0.071(2) 0.062(2) 0.085(2) -0.0213(18) 0.0244(17) 0.0076(17)
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C45 0.0543(17) 0.096(3) 0.0588(18) 0.0235(18) 0.0088(13) -0.0079(17)
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C9 0.063(2) 0.112(3) 0.0507(17) 0.0213(19) -0.0100(14) 0.007(2)
C36 0.090(3) 0.080(3) 0.066(2) 0.0123(18) -0.0193(19) -0.008(2)
C38 0.120(3) 0.073(2) 0.0550(19) 0.0105(17) -0.0174(19) -0.015(2)
C27 0.105(3) 0.131(4) 0.064(2) 0.017(2) 0.018(2) 0.038(3)

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;
All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)

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  treatment of cell esds is used for estimating esds involving l.s. planes.
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O3 C40 1.275(3) . ?
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N2 C15 1.385(3) . ?
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H42B C42 H42C 109.5 . . ?
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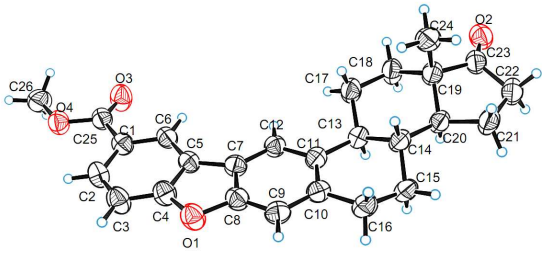


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 (compiled Oct 25 2010,18:11:34)
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C12 0.0567(14) 0.0634(15) 0.0615(14) -0.0041(12) 0.0022(11) -0.0009(13)
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C11 0.0546(14) 0.0650(15) 0.0646(15) 0.0003(13) -0.0017(12) -0.0007(13)
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C6 0.0682(16) 0.0530(14) 0.0604(14) -0.0027(12) -0.0047(12) -0.0003(13)
C17 0.0609(16) 0.0764(18) 0.094(2) -0.0163(16) 0.0143(15) -0.0128(16)
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C7 0.0638(15) 0.0598(14) 0.0603(14) 0.0016(12) -0.0004(12) 0.0026(13)
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C10 0.0572(14) 0.0659(16) 0.0662(15) 0.0038(13) 0.0009(12) 0.0051(14)
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C18 0.0678(17) 0.0762(19) 0.0842(19) -0.0158(16) 0.0146(14) -0.0185(15)
C22 0.0723(18) 0.0774(19) 0.089(2) 0.0128(17) -0.0123(16) -0.0173(17)
C15 0.0483(14) 0.0786(18) 0.0904(19) 0.0034(16) 0.0040(13) 0.0031(13)

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  All esds (except the esd in the dihedral angle between two l.s. planes)
  are estimated using the full covariance matrix. The cell esds are taken
  into account individually in the estimation of esds in distances, angles
  and torsion angles correlations between esds in cell parameters are only
  used when they are defined by crystal symmetry. An approximate (isotropic)
  treatment of cell esds is used for estimating esds involving l.s. planes.
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  C16 H16A 0.9700 . ?
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H24C C24 H24B 109.5 . . ?
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