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# High acidity cellulose sulfuric acid from sulfur trioxide: An highly efficient catalyst for the one step synthesis of xanthene and dihydroquinazolinone derivatives

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## General Information

$^{1}H$ NMR and $^{13}C$ NMR spectra were recorded on Bruker 400 ($^{1}H$, 400 MHz; $^{13}C$, 100 MHz) instrument internallyreferenced to tetramethylsilane (TMS) or $CDCl_3$ signals. The NMR data were collected at ambient temperature and Chemical shifts are reported in parts permillion (ppm) relative to the NMR solvent peaks. Data for $^{1}H$-NMR are reported as follows:chemical shift, multiplicity, couplingconstants, and integration. Processing of the NMR data was done using the standard Mestrenova 9.0.1 software.

The powder X-ray diffraction (XRD) patterns were recorded by a Rigaku D/max-2500 X-ray diffractometer using Cu-Karadiation. The fourier transform infrared (FTIR) spectra were recorded in the range of 400-4000 $cm^{-1}$ using a FOSS Fibertec 8000 FT-IR spectrometer employing potassium bromide pellets technique at room temperature. The scanning electron microscopy (SEM) images were obtained on a FEI verous 460 scanning electron microscope. The transmission electron microscope (TEM) images were obtained on a TecnaiG2 F20 S-TWIN scanning electron microscope. The morphology of the materials was obtained on JEOL JEM-2010F High Resolution Transmission Electron Microscope (HRTEM). Thermal gravimetric (TG) analysis was conducted on a TG-DSC instrument (Pyris 103030247) under a $N_2$ atmosphere at a heating rate of 10 ℃/min from 25 to 700℃. The elemental analysis was conducted on a Vario EL cube0303040206 elemental analyzer.

Materials: All reagents were used as received from commercial sources and all of the analytically pure. The benzaldehyde was re-distilled and purified. The $SO_3$ is made in the laboratory.

**The effect of sulfonation time on cellulose.**

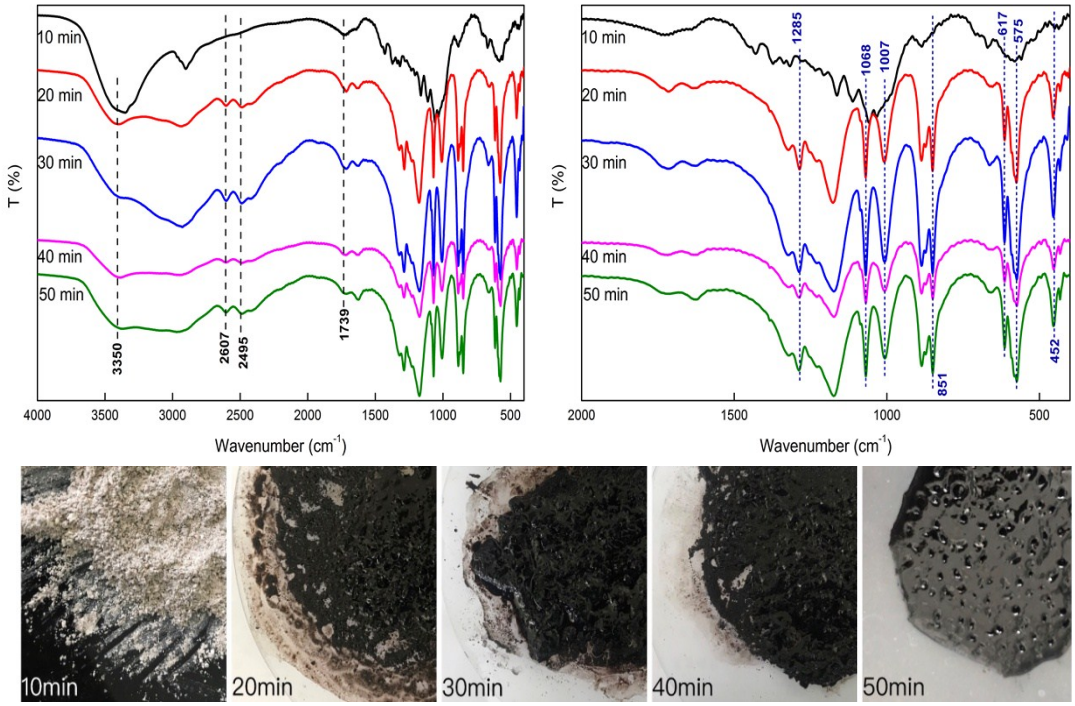



Fig. S1 The IR analysis of the effect of different sulfonation time on cellulose.

By comparing the infrared spectra of CSA in different sulfonation time, we found that OH absorption peak at 3350 $cm^{-1}$ becomes smooth gradually when the sulfonation time more than 20 min; and the peaks corresponding to the O=S=O asymmetric and symmetric stretching vibrations and S-O stretching vibration of the sulfonic acid groups became more incisive and obvious, it was indicated that not only more -O-H groups been substituted by $-SO_3H$ groups, but deeper depolymerization of cellulose with increasing time. In addition, the the new peak at 2600 $cm^{-1}$ appeared in infrared spectra of more than 20 min sulfonation time presumed to be the -S-H.

In summary, longer sulfonation time, means deeper degree of depolymerization of cellulose glucose unit, more complex sulfonated product because formed sulfhydryl groups, and deeper carbonization phenomenon (Fig.S1). Therefore we chosen 10 min as the optimal sulfonation time.

## Optimization of conditions for catalytic synthesis of xanthene compounds.

**Table S1** Optimization of reaction condition between 2-naphthol (1.0 mmol) and benzaldehyde (1.0 mmol) in the presence of HS-cellulose sulphate.

| Entry[a] | Catalyst/mg | Temperature/℃ | Solvent | Yield[b]/% |
|---|---|---|---|---|
| 1 | 10 | 120 | Solvent-free | 90 |
| 2 | 6 | 120 | Solvent-free | 90 |
| 3 | 3 | 120 | Solvent-free | 88 |
| **4** | **10** | **110** | **Solvent-free** | **97** |
| 5 | 6 | 110 | Solvent-free | 93 |
| 6 | 3 | 110 | Solvent-free | 89 |
| 7 | 10 | 100 | Solvent-free | 92 |
| 8 | 6 | 100 | Solvent-free | 91 |
| 9 | 3 | 100 | Solvent-free | 86 |
| 10 | 10 | 90 | Solvent-free | 83 |
| 11 | 6 | 90 | Solvent-free | 81 |
| 12 | 10 | Reflux | Water(2ml) | 21 |
| 13 | 10 | Reflux | Ethyl etate (2ml) | 51 |
| 14 | 10 | Reflux | DCE(2ml) | 52 |
| 15 | 10 | Reflux | Ethanol(2ml) | 56 |

[a]Reaction conditions: 2-naphthol (1.0 mmol); benzaldehyde (1.0 mmol). DCE: Dichloroethane.
[b]Isolated yield.

**Elemental analysis and IR testing of CSA**

Table S2 Element analysis of CSA catalyst before use and after three uses.

| Relative mass of elements | C/% | H/% | N/% | S/% |
|---|---|---|---|---|
| **CSA** | 35.52 | 6.53 | 1.67 | 4.65 |
| **CSA (3 cycles)** | 40.31 | 6.29 | 1.03 | 1.64 |

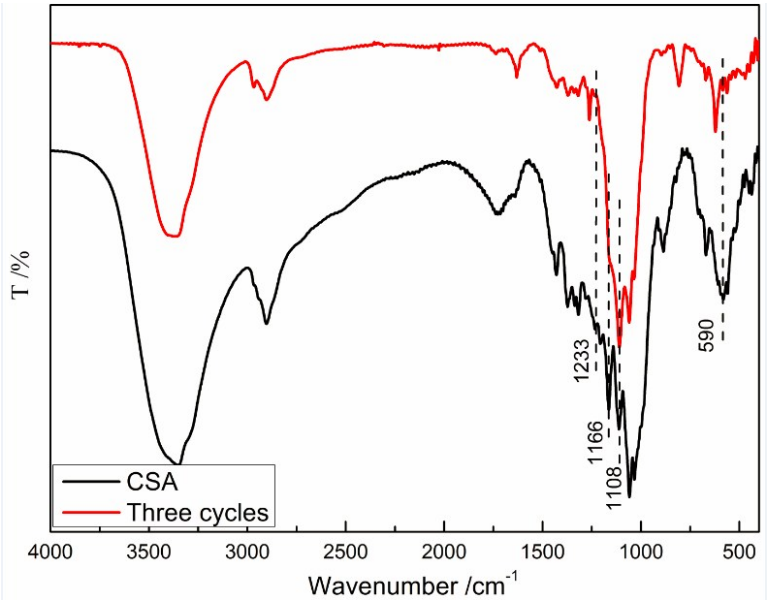
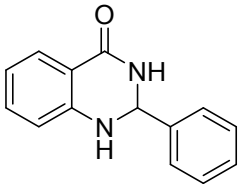
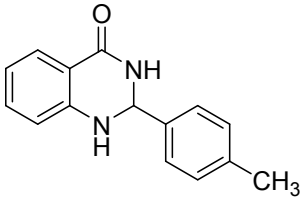



Fig. S2 The IR analysis of HS-cellulose sulfonate catalyst after three uses.

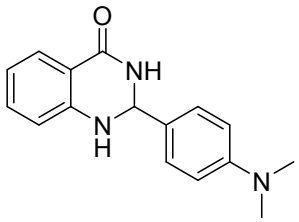
## Compound data of dihydroquinazolinone(3a-3r).



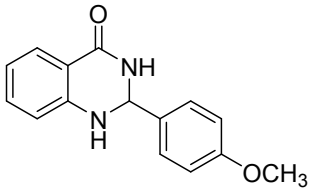
**2-phenyl-2,3-dihydroquinazolin-4(1H)-one (3a):** White powder, 94%.$^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.30 (t, $J$ = 2.0 Hz, 1H), 7.61 (dd, $J$ = 7.8, 1.6 Hz, 1H), 7.50 (d, $J$ = 1.8 Hz, 1H), 7.49 (t, $J$ = 1.5 Hz, 1H), 7.42 – 7.37 (m, 2H), 7.37 – 7.32 (m, 1H), 7.24 (ddd, $J$ = 8.1, 7.2, 1.6 Hz, 1H), 7.12 (d, $J$ = 1.8 Hz, 1H), 6.75 (dd, $J$ = 8.2, 1.0 Hz, 1H), 6.67 (ddd, $J$ = 8.0, 7.2, 1.1 Hz, 1H), 5.75 (t, $J$ = 1.8 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO) δ 163.60, 147.88, 141.61, 133.32, 128.47, 128.33, 127.35, 126.88, 117.11, 114.94, 114.40, 66.55.



**2-(p-tolyl)-2,3-dihydroquinazolin-4(1H)-one (3b):** White powder, 87%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.24 (t, $J$ = 1.9 Hz, 1H), 7.61 (dd, $J$ = 7.8, 1.6 Hz, 1H), 7.37 (d, $J$ = 7.9 Hz, 2H), 7.23 (ddd, $J$ = 8.5, 7.2, 1.7 Hz, 1H), 7.19 (d, $J$ = 7.9 Hz, 2H), 7.06 (s, 1H), 6.77 – 6.72 (m, 1H), 6.70 – 6.64 (m, 1H), 5.71 (t, $J$ = 1.7 Hz, 1H), 2.29 (s, 3H); $^{13}$C NMR (101 MHz, DMSO) δ 163.64, 147.91, 138.64, 137.71, 133.25, 128.80, 127.33, 126.80, 117.05, 114.99, 114.39, 66.37, 20.73.

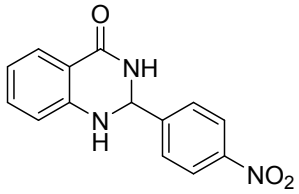


**2-(4-(dimethylamino)phenyl)-2,3-dihydroquinazolin-4(1H)-one (3c):** Light yellow powder, 98%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.09 (t, $J$ = 1.7 Hz, 1H), 7.61 (dd, $J$ = 7.7, 1.6 Hz, 1H), 7.33 – 7.28 (m, 2H), 7.23 (ddd, $J$ = 8.1, 7.2, 1.7 Hz, 1H), 6.93 (s, 1H), 6.75 – 6.70 (m, 3H), 6.66 (ddd, $J$ = 8.0, 7.2, 1.1 Hz, 1H), 5.63 (t, $J$ = 1.4 Hz, 1H), 2.88 (s, 6H); $^{13}$C NMR (101 MHz, DMSO) δ 163.83, 150.70, 148.22, 133.14, 128.62, 127.72, 127.33, 116.94, 115.04, 114.38, 111.93, 66.64.

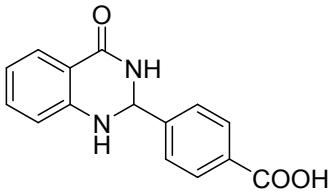


**2-(4-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3d):** White powder, 86%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.20 (d, $J$ = 2.0 Hz, 1H), 7.61 (dd, $J$ = 7.8, 1.6 Hz, 1H), 7.43 (d, $J$ = 2.1 Hz, 1H), 7.41 (d, $J$ = 2.1 Hz, 1H), 7.24 (ddd, $J$ = 8.6, 7.3, 1.6 Hz, 1H), 7.02 (s, 1H), 6.95 (d, $J$ = 2.1 Hz, 1H), 6.94 (d, $J$ = 2.1 Hz, 1H), 6.74 (dd, $J$ = 8.2, 1.0 Hz, 1H), 6.67 (td, $J$ = 7.5, 1.0 Hz, 1H), 5.71 (t, $J$ = 1.6 Hz, 1H), 3.74 (s, 3H); $^{13}$C NMR (101 MHz, DMSO) δ 163.69, 159.41, 148.01, 133.44, 133.23, 128.21,

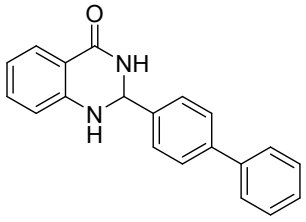
127.34, 117.07, 114.99, 114.40, 113.62, 66.31, 55.18.



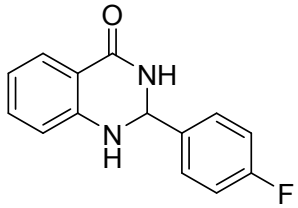

**2-(4-nitrophenyl)-2,3-dihydroquinazolin-4(1H)-one (3e):** White powder, 87%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.54 (dd, $J$ = 3.0, 1.5 Hz, 1H), 8.26 (d, $J$ = 2.0 Hz, 1H), 8.25 (d, $J$ = 2.0 Hz, 1H), 7.75 (d, $J$ = 2.0 Hz, 1H), 7.73 (d, $J$ = 2.0 Hz, 1H), 7.61 (dd, $J$ = 7.7, 1.6 Hz, 1H), 7.34 (d, $J$ = 1.9 Hz, 1H), 7.26 (ddd, $J$ = 8.6, 7.2, 1.7 Hz, 1H), 6.77 (dd, $J$ = 8.2, 1.0 Hz, 1H), 6.69 (td, $J$ = 7.5, 1.1 Hz, 1H), 5.92 (t, $J$ = 2.5 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO) δ 163.27, 149.32, 147.40, 147.23, 133.56, 128.03, 127.40, 123.59, 117.46, 114.89, 114.54, 65.27.




**4-(4-oxo-1,2,3,4-tetrahydroquinazolin-2-yl)benzoic acid (3f):** Light yellow powder, 91%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 13.29 (s, 1H), 8.68 (s, 1H), 8.11 (s, 1H), 8.10 – 8.04 (m, 4H), 7.88 (d, $J$ = 7.7 Hz, 1H), 7.63 (s, 1H), 7.58 – 7.51 (m, 1H), 7.36 (t, $J$ = 7.5 Hz, 1H), 7.25 (d, $J$ = 7.9 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO) δ 167.43, 166.86, 161.52, 149.08, 139.08, 133.61, 131.82, 129.83, 129.68, 129.06, 128.55, 126.29, 119.35.

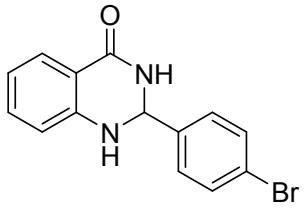



**2-([1,1'-biphenyl]-4-yl)-2,3-dihydroquinazolin-4(1H)-one (3g):** Light yellow powder, 80%.$^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.40 (t, $J$ = 2.0 Hz, 1H), 7.70 (d, $J$ = 1.9 Hz, 1H), 7.69 – 7.63 (m, 4H), 7.59 (d, $J$ = 8.3 Hz, 2H), 7.46 (dd, $J$ = 8.4, 6.9 Hz, 2H), 7.40 – 7.34 (m, 1H), 7.26 (ddd, $J$ = 8.4, 7.2, 1.6 Hz, 1H), 7.21 (d, $J$ = 1.7 Hz, 1H), 6.79 (dd, $J$ = 8.2, 1.0 Hz, 1H), 6.69 (td, $J$ = 7.5, 1.1 Hz, 1H), 5.82 (t, $J$ = 1.8 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO) δ 163.65, 147.86, 140.83, 140.35, 139.72, 133.37, 128.97, 127.59, 127.49, 127.41, 126.72, 126.66, 117.17, 115.00, 114.46, 66.24.

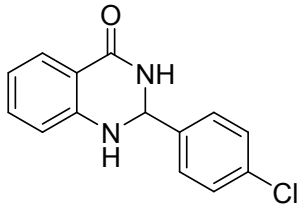



**2-(4-fluorophenyl)-2,3-dihydroquinazolin-4(1H)-one (3h):** White powder, 89%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.29 (d, $J$ = 2.3 Hz, 1H), 7.61 (dd, $J$ = 7.8, 1.5 Hz, 1H), 7.57 – 7.54 (m, 1H), 7.54 – 7.50 (m, 1H), 7.27 – 7.19 (m, 3H), 7.10 (s, 1H), 6.74 (d, $J$ = 8.1 Hz, 1H), 6.71 – 6.66 (m, 1H), 5.77 (t, $J$ =

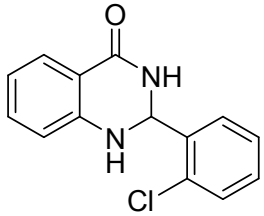
1.7 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO) δ 164.01, 161.35, 148.26, 138.25, 133.82, 129.54, 129.46, 127.82, 117.71, 115.66, 115.45, 115.40, 114.89, 66.38.



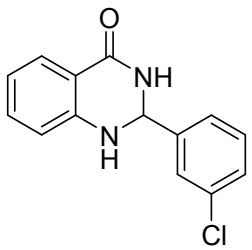

**2-(4-bromophenyl)-2,3-dihydroquinazolin-4(1H)-one (3i):** White powder, 85%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.35 (t, $J$ = 1.9 Hz, 1H), 7.62 – 7.60 (m, 1H), 7.59 (dd, $J$ = 3.0, 1.5 Hz, 1H), 7.58 (s, 1H), 7.45 (d, $J$ = 2.0 Hz, 1H), 7.43 (d, $J$ = 2.0 Hz, 1H), 7.25 (ddd, $J$ = 8.6, 7.2, 1.6 Hz, 1H), 7.15 (d, $J$ = 1.8 Hz, 1H), 6.74 (dd, $J$ = 8.2, 1.0 Hz, 1H), 6.68 (td, $J$ = 7.5, 1.1 Hz, 1H), 5.75 (t, $J$ = 2.0 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO) δ 163.46, 147.62, 141.08, 133.39, 131.22, 129.08, 127.35, 121.56, 117.28, 114.92, 114.45, 65.78.



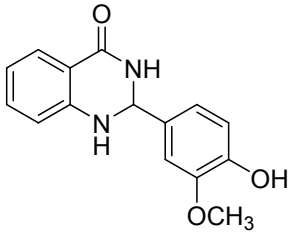

**2-(4-chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one (3j):** White powder, 92%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.35 (t, $J$ = 2.0 Hz, 1H), 7.61 (dd, $J$ = 7.8, 1.6 Hz, 1H), 7.53 – 7.44 (m, 4H), 7.25 (ddd, $J$ = 8.6, 7.2, 1.6 Hz, 1H), 7.15 (d, $J$ = 1.7 Hz, 1H), 6.74 (dd, $J$ = 8.2, 1.0 Hz, 1H), 6.68 (td, $J$ = 7.5, 1.1 Hz, 1H), 5.77 (t, $J$ = 2.0 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO) δ 163.48, 147.64, 140.66, 133.39, 132.95, 128.76, 128.30, 127.35, 117.27, 114.93, 114.45, 65.74.



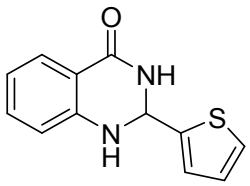

**2-(2-chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one (3k):** White powder, 98%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.23 (t, $J$ = 1.9 Hz, 1H), 7.69 – 7.64 (m, 2H), 7.49 (dt, $J$ = 7.4, 3.7 Hz, 1H), 7.40 (dd, $J$ = 5.9, 3.5 Hz, 2H), 7.26 (ddd, $J$ = 8.5, 7.2, 1.6 Hz, 1H), 7.02 (d, $J$ = 2.0 Hz, 1H), 6.77 (dd, $J$ = 8.2, 1.0 Hz, 1H), 6.72 (td, $J$ = 7.5, 1.0 Hz, 1H), 6.14 (t, $J$ = 1.7 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO) δ 163.63, 147.65, 137.85, 133.43, 131.84, 130.29, 129.57, 128.74, 127.46, 127.37, 117.44, 114.67, 114.56, 63.69.



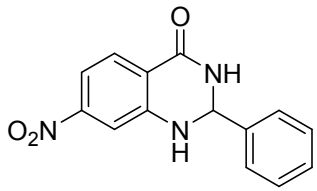
**2-(3-chlorophenyl)-2,3-dihydroquinazolin-4(1H)-one (3l):** White powder, 83%. $^1$H NMR (400 MHz, DMSO-$d_6$) δ 8.41 (t, $J$ = 2.0 Hz, 1H), 7.61 (dd, $J$ = 7.8, 1.5 Hz, 1H), 7.53 (d, $J$ = 1.5 Hz, 1H), 7.47 – 7.43 (m, 1H), 7.43 – 7.38 (m, 2H), 7.26 (ddd, $J$ = 8.5, 7.3, 1.6 Hz, 1H), 7.22 (d, $J$ = 1.8 Hz, 1H), 6.76 (d, $J$ = 8.1 Hz, 1H), 6.71 – 6.66 (m, 1H), 5.78 (t, $J$ = 2.2 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO) δ 163.41, 147.49, 144.37, 133.46, 132.96, 130.30, 128.26, 127.36, 126.75, 125.40, 117.32, 114.89, 114.46, 65.56.



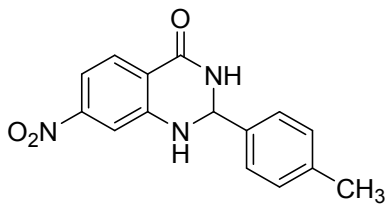

**2-(4-hydroxy-3-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one (3m):** White powder, 95%. $^1$H NMR (400 MHz, DMSO-$d_6$) δ 9.08 (s, 1H), 8.11 (s, 1H), 7.61 (d, $J$ = 7.6 Hz, 1H), 7.27 – 7.21 (m, 1H), 7.09 (d, $J$ = 2.0 Hz, 1H), 6.96 (s, 1H), 6.88 (dd, $J$ = 8.0, 2.0 Hz, 1H), 6.75 (dd, $J$ = 8.1, 5.4 Hz, 2H), 6.67 (t, $J$ = 7.5 Hz, 1H), 5.65 (s, 1H), 3.76 (s, 3H); $^{13}$C NMR (101 MHz, DMSO) δ 163.76, 148.18, 147.39, 146.88, 133.18, 131.89, 127.33, 119.63, 117.08, 115.02, 114.89, 114.40, 111.10, 66.82, 55.58.




**2-(thiophen-2-yl)-2,3-dihydroquinazolin-4(1H)-one (3n):** Light yellow powder, 88%. $^1$H NMR (400 MHz, DMSO-$d_6$) δ 8.46 (s, 1H), 7.62 (d, $J$ = 8.5 Hz, 1H), 7.53 – 7.40 (m, 1H), 7.26 (s, 2H), 7.18 – 7.08 (m, 1H), 6.99 (dt, $J$ = 9.1, 4.5 Hz, 1H), 6.82 – 6.64 (m, 2H), 6.02 (s, 1H); $^{13}$C NMR (101 MHz, DMSO) δ 163.10, 147.23, 146.41, 133.36, 127.30, 126.44, 125.89, 125.70, 117.50, 115.09, 114.68, 62.54.

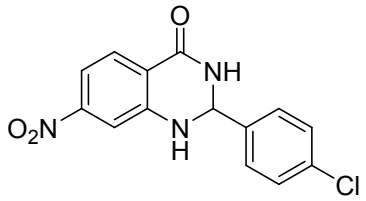



**7-nitro-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3o)**: Yellow powder, 91%. $^1$H NMR (400 MHz, DMSO-$d_6$) δ 8.75 (s, 1H), 7.86 (d, $J$ = 8.5 Hz, 1H), 7.78 (s, 1H), 7.60 (d, $J$ = 2.3 Hz, 1H), 7.56 – 7.50 (m, 2H), 7.47 – 7.32 (m, 4H), 5.94 (t, $J$ = 1.8 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO) δ 161.94, 150.81, 148.23, 141.04, 129.15, 128.82, 128.58, 126.82, 119.26, 111.04, 108.90, 66.50.

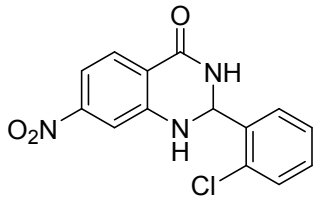



**7-nitro-2-(p-tolyl)-2,3-dihydroquinazolin-4(1*H*)-one (3p)**: Yellow powder, 90%. $^1$H NMR (400 MHz, DMSO-$d_6$) δ 8.69 (d, $J$ = 2.4 Hz, 1H), 7.83 (d, $J$ = 8.5 Hz, 1H), 7.72 (s, 1H), 7.57 (d, $J$ = 2.2 Hz, 1H), 7.42 (dd, $J$ = 8.5, 2.2 Hz, 1H), 7.37 (d, $J$ = 7.9 Hz, 2H), 7.21 (d, $J$ = 7.8 Hz, 2H), 5.87 (t, $J$ = 1.8 Hz,

1H), 2.30 (s, 3H); $^{13}$C NMR (101 MHz, DMSO) δ 161.88, 150.74, 148.20, 138.09, 129.10, 129.01, 126.65, 119.28, 110.95, 108.83, 66.17, 20.72.



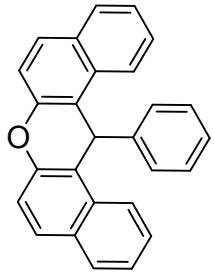

**2-(4-chlorophenyl)-7-nitro-2,3-dihydroquinazolin-4(1*H*)-one (3q)**: Yellow powder, 89%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.78 (t, $J$ = 1.9 Hz, 1H), 7.84 (d, $J$ = 8.5 Hz, 1H), 7.78 (s, 1H), 7.58 (d, $J$ = 2.2 Hz, 1H), 7.50 (q, $J$ = 8.6 Hz, 4H), 7.43 (dd, $J$ = 8.5, 2.2 Hz, 1H), 5.95 (t, $J$ = 1.9 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO) δ 161.81, 150.80, 148.01, 140.04, 133.37, 129.16, 128.68, 128.56, 119.21, 111.19, 108.96, 65.67.



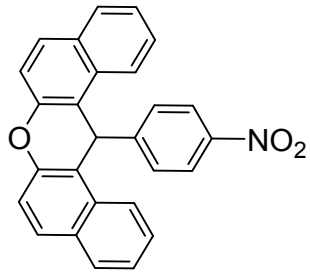

**2-(2-chlorophenyl)-7-nitro-2,3-dihydroquinazolin-4(1*H*)-one (3r)**: Yellow powder, 92%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.65 (d, $J$ = 1.9 Hz, 1H), 7.88 (d, $J$ = 8.5 Hz, 1H), 7.68 (s, 1H), 7.63 (dd, $J$ = 5.9, 3.6 Hz, 1H), 7.60 (d, $J$ = 2.2 Hz, 1H), 7.55 – 7.50 (m, 1H), 7.46 (dd, $J$ = 8.6, 2.3 Hz, 1H), 7.42 (dd, $J$ = 5.9, 3.5 Hz, 2H), 6.29 (t, $J$ = 1.7 Hz, 1H); $^{13}$C NMR (101 MHz, DMSO) δ 161.91, 150.84, 147.89, 137.43, 131.81, 130.63, 129.81, 129.15, 128.66, 127.69, 118.85, 111.24, 109.03, 63.81.

.

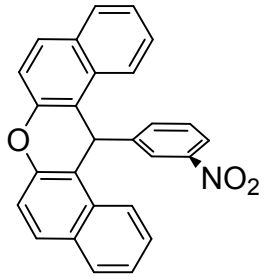
## Compound data of xanthene (5a-5u).



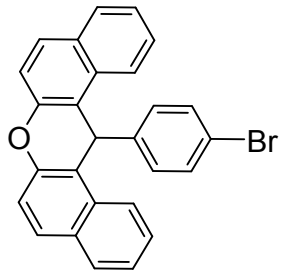
**14-phenyl-14H-dibenzo[a,j]xanthenes (5a):** White powder, 97 %. $^1$H NMR (400 MHz, DMSO-$d_6$) δ 8.69 (d, $J$ = 8.5 Hz, 2H), 7.93 (dd, $J$ = 8.7, 2.1 Hz, 4H), 7.62 (ddd, $J$ = 8.3, 6.5, 1.4 Hz, 4H), 7.56 (d, $J$ = 8.9 Hz, 2H), 7.50 – 7.41 (m, 2H), 7.14 (t, $J$ = 7.7 Hz, 2H), 6.96 (s, 1H), 6.72 (s, 1H). $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 147.94, 145.55, 130.87, 130.62, 129.00, 128.59, 128.37, 127.94, 126.93, 126.24, 124.53, 123.42, 117.68, 117.42, 36.47.



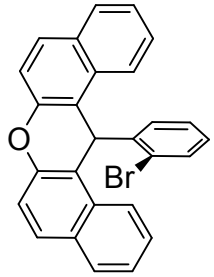
**14-(4-nitrophenyl)-14H-dibenzo[a,j]xanthenes (5b):** Yellow powder, 98%. $^1$H NMR (400 MHz, DMSO-$d_6$) δ 8.69 (d, $J$ = 8.6 Hz, 2H), 7.93 (dt, $J$ = 18.4, 9.2 Hz, 8H), 7.64 (t, $J$ = 7.7 Hz, 2H), 7.58 (d, $J$ = 8.9 Hz, 2H), 7.45 (t, $J$ = 7.6 Hz, 2H), 6.92 (s, 1H). $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 152.64, 147.98, 145.77, 130.73, 130.63, 129.58, 129.03, 128.69, 127.20, 124.72, 123.67, 123.18, 117.75, 116.17, 36.32.



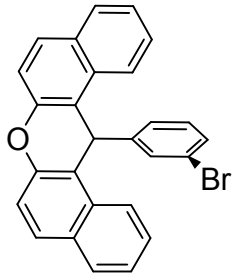
**14-(3-nitrophenyl)-14H-dibenzo[a,j]xanthenes (5c):** Light yellow powder, 97%. $^1$H NMR (400 MHz, DMSO-$d_6$) δ 8.75 (d, $J$ = 8.5 Hz, 2H), 8.48 (t, $J$ = 2.0 Hz, 1H), 8.16 (dt, $J$ = 7.9, 1.3 Hz, 1H), 8.02 – 7.88 (m, 4H), 7.83 (ddd, $J$ = 8.3, 2.3, 1.0 Hz, 1H), 7.71 – 7.55 (m, 4H), 7.46 (t, $J$ = 7.9 Hz, 3H), 6.97 (s, 1H). $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 148.12, 147.84, 147.48, 134.29, 130.68, 130.64, 129.94, 129.61, 128.72, 127.25, 124.77, 123.18, 122.04, 121.58, 117.73, 116.48, 35.92



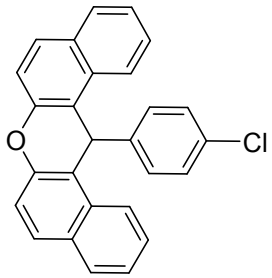
**14-(4-bromophenyl)-14H-dibenzo[a,j]xanthene (5d):** White powder, 97%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.65 (d, $J$ = 8.5 Hz, 2H), 7.92 (d, $J$ = 8.5 Hz, 4H), 7.71 – 7.51 (m, 6H), 7.45 (t, $J$ = 7.5 Hz, 2H), 7.32 (d, $J$ = 8.1 Hz, 2H), 6.73 (s, 1H). $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 147.89, 144.82, 131.24, 130.74, 130.60, 130.02, 129.17, 128.60, 127.00, 124.57, 123.24, 119.41, 117.65, 116.82, 35.89.



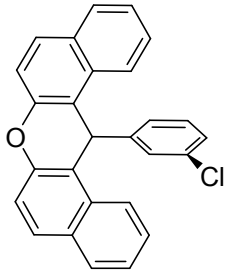

**14-(2-bromophenyl)-14H-dibenzo[a,j]xanthene (5e):** White powder, 94%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.68 (d, $J$ = 8.5 Hz, 2H), 7.91 (dd, $J$ = 8.5, 4.9 Hz, 4H), 7.60 (ddd, $J$ = 8.4, 6.8, 1.4 Hz, 2H), 7.50 (d, $J$ = 8.9 Hz, 2H), 7.48 – 7.41 (m, 3H), 7.40 – 7.32 (m, 1H), 7.14 – 7.00 (m, 1H), 6.88 (td, $J$ = 7.6, 1.7 Hz, 1H), 6.58 (s, 1H). $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 148.19, 144.72, 133.25, 131.76, 130.95, 130.51, 129.43, 128.76, 128.71, 126.86, 124.58, 123.39, 120.53, 117.86, 116.96, 36.65.



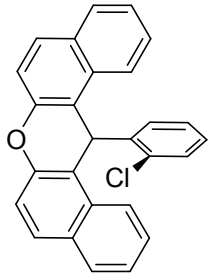

**14-(3-bromophenyl)-14H-dibenzo[a,j]xanthene (5f):** White powder, 95%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.70 (d, $J$ = 8.5 Hz, 2H), 7.92 (d, $J$ = 8.8 Hz, 4H), 7.72 – 7.62 (m, 3H), 7.58 (dd, $J$ = 15.3, 8.4 Hz, 3H), 7.45 (ddd, $J$ = 8.0, 6.8, 1.0 Hz, 2H), 7.16 (t, $J$ = 7.9 Hz, 1H), 7.08 – 6.99 (m, 1H), 6.77 (s, 1H). $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 147.99, 147.78, 133.01, 130.72, 130.60, 130.26, 129.28, 128.63, 127.44, 127.07, 126.57, 126.37, 124.62, 123.22, 117.64, 116.78, 36.03.



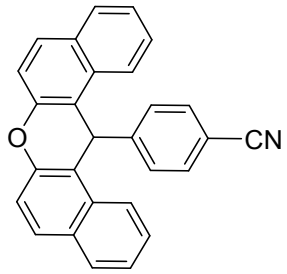

**14-(4-chlorophenyl)-14H-dibenzo[a,j]xanthenes (5g):** White powder, 97%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.66 (d, $J$ = 8.5 Hz, 2H), 7.92 (d, $J$ = 8.6 Hz, 4H), 7.63 (t, $J$ = 7.6 Hz, 4H), 7.55 (d, $J$ = 8.9 Hz, 2H), 7.45 (t, $J$ = 7.5 Hz, 2H), 7.19 (d, $J$ = 8.1 Hz, 2H), 6.75 (s, 1H). $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 147.91, 144.41, 130.89, 130.75, 130.61, 129.64, 129.17, 128.61, 128.33, 127.00, 124.57, 123.26, 117.65, 116.91, 35.81.



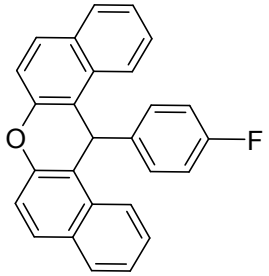

**14-(3-chlorophenyl)-14H-dibenzo[a,j]xanthenes (5h):** White powder, 94%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.70 (d, $J$ = 8.5 Hz, 2H), 7.94 (d, $J$ = 8.8 Hz, 4H), 7.81 (t, $J$ = 1.9 Hz, 1H), 7.65 (ddd, $J$ = 8.2, 6.9, 1.3 Hz, 3H), 7.57 (d, $J$ = 8.9 Hz, 2H), 7.46 (ddd, $J$ = 8.0, 6.8, 1.0 Hz, 2H), 7.22 – 7.06 (m, 2H), 6.76 (s, 1H). $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 148.03, 147.98, 130.71, 130.61, 130.57, 130.28, 129.30, 129.27, 128.64, 127.08, 126.94, 124.64, 123.22, 121.74, 117.65, 116.79, 36.00.



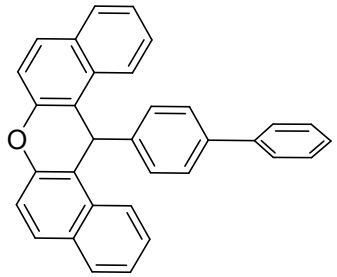

**14-(2-chlorophenyl)-14H-dibenzo[a,j]xanthenes (5i):** White powder, 96%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.58 (d, $J$ = 8.5 Hz, 2H), 8.01 – 7.84 (m, 4H), 7.62 (ddd, $J$ = 8.4, 6.9, 1.4 Hz, 2H), 7.53 (d, $J$ = 8.9 Hz, 2H), 7.50 – 7.39 (m, 3H), 7.31 (dd, $J$ = 7.9, 1.4 Hz, 1H), 7.04 (ddd, $J$ = 20.0, 7.7, 1.7 Hz, 2H), 6.72 (s, 1H). $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 148.25, 142.76, 131.64, 130.95, 130.51, 129.89, 129.85, 129.45, 128.78, 128.52, 128.14, 127.03, 124.59, 122.91, 117.81, 116.48, 34.42.



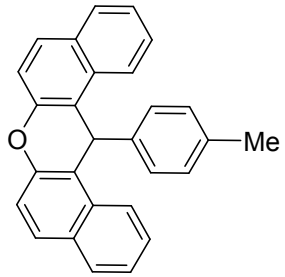

**4-(14H-dibenzo[a,j]xanthen-14-yl)benzonitrile (5j):** White powder, 97%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.68 (d, $J$ = 8.5 Hz, 2H), 7.94 (dd, $J$ = 8.6, 5.0 Hz, 4H), 7.83 (d, $J$ = 8.1 Hz, 2H), 7.70 – 7.53 (m, 6H), 7.46 (t, $J$ = 7.5 Hz, 2H), 6.86 (s, 1H). $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 150.70, 148.01, 132.44, 130.73, 130.62, 129.50, 128.79, 128.69, 127.18, 124.72, 123.18, 118.47, 117.72, 116.34, 109.26, 36.47.



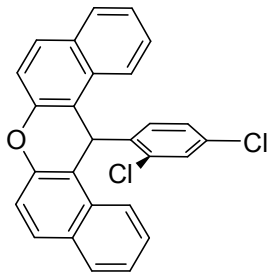
**14-(4-fluorophenyl)-14H-dibenzo[a,j]xanthene (5k):** White powder, 96%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.69 (d, $J$ = 8.5 Hz, 2H), 7.93 (dd, $J$ = 9.2, 2.1 Hz, 4H), 7.72 – 7.59 (m, 4H), 7.56 (d, $J$ = 8.9 Hz, 2H), 7.46 (ddd, $J$ = 7.9, 6.8, 1.0 Hz, 2H), 7.08 – 6.87 (m, 2H), 6.76 (s, 1H). $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 147.93, 141.79, 141.75, 130.78, 130.64, 129.73, 129.65, 129.10, 128.63, 127.00, 124.58, 123.35, 117.69, 117.28, 115.24, 115.03, 35.63.



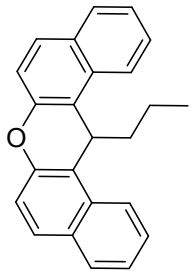

**14-([1,1'-biphenyl]-4-yl)-14H-dibenzo[a,j]xanthene (5l):** White powder, 95%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.74 (d, $J$ = 8.6 Hz, 2H), 7.93 (d, $J$ = 8.5 Hz, 4H), 7.81 – 7.54 (m, 6H), 7.43 (dt, $J$ = 22.4, 8.1 Hz, 6H), 7.35 – 7.10 (m, 3H), 6.78 (s, 1H). $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 147.99, 144.69, 139.59, 138.23, 130.91, 130.66, 129.03, 128.69, 128.61, 128.44, 127.21, 126.99, 126.75, 126.48, 124.55, 123.43, 117.71, 117.31, 36.12.



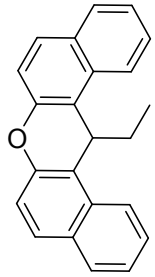

**14-(p-tolyl)-14H-dibenzo[a,j]xanthene (5m):** White powder, 94%.$^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.66 (d, $J$ = 8.5 Hz, 2H), 8.02 – 7.79 (m, 4H), 7.62 (ddd, $J$ = 8.4, 6.8, 1.4 Hz, 2H), 7.55 (d, $J$ = 8.9 Hz, 2H), 7.52 – 7.45 (m, 2H), 7.45 (ddd, $J$ = 8.0, 6.8, 1.0 Hz, 2H), 6.92 (d, $J$ = 7.9 Hz, 2H), 6.66 (s, 1H). $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 147.84, 142.65, 135.34, 130.87, 130.62, 128.88, 128.56, 127.81, 126.86, 124.47, 123.45, 117.65, 117.48, 36.10, 20.37.



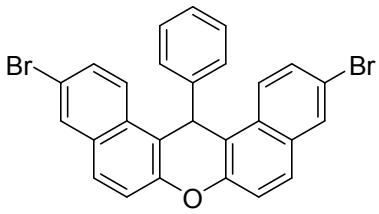

**14-(2,4-dichlorophenyl)-14H-dibenzo[a,j]xanthene (5n):** White powder, 91%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.53 (d, $J$ = 8.5 Hz, 2H), 7.94 (d, $J$ = 8.9 Hz, 4H), 7.62 (ddd, $J$ = 8.4, 6.8, 1.3 Hz, 2H), 7.57 – 7.43 (m, 6H), 7.16 (dt, $J$ = 8.7, 1.8 Hz, 1H), 6.75 (s, 1H). $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 148.27, 141.70, 133.01, 132.17, 130.85, 130.54, 129.68, 129.15, 128.84, 128.37, 127.14, 124.68, 122.80, 117.80, 115.82, 34.18.



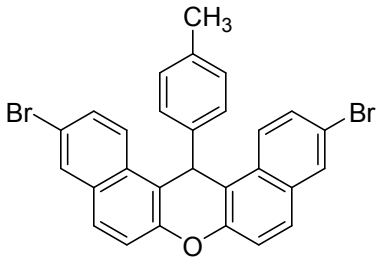
**14-propyl-14H-dibenzo[a,j]xanthene (5o):** White powder, 80%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.44 (d, $J$ = 8.6 Hz, 2H), 7.86 (d, $J$ = 8.1 Hz, 2H), 7.78 (d, $J$ = 8.9 Hz, 2H), 7.62 (t, $J$ = 7.7 Hz, 2H), 7.40 (dd, $J$ = 19.7, 8.2 Hz, 4H), 5.62 (t, $J$ = 4.5 Hz, 1H), 1.83 (dt, $J$ = 12.8, 4.5 Hz, 2H), 0.90 – 0.74 (m, 2H), 0.32 (t, $J$ = 7.3 Hz, 3H). $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 149.24, 130.99, 130.56, 128.52, 128.20, 126.69, 124.15, 122.85, 117.01, 116.41, 37.90, 30.16, 17.54, 13.55.



**14-ethyl-14H-dibenzo[a,j]xanthene (5p):** White powder, 72%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.50 (d, $J$ = 8.5 Hz, 2H), 7.94 (dd, $J$ = 8.3, 1.2 Hz, 2H), 7.87 (d, $J$ = 8.9 Hz, 2H), 7.65 (ddd, $J$ = 8.4, 6.8, 1.4 Hz, 2H), 7.52 – 7.44 (m, 2H), 7.41 (d, $J$ = 8.9 Hz, 2H), 5.69 (t, $J$ = 4.4 Hz, 1H), 1.95 (qd, $J$ = 7.4, 4.3 Hz, 2H), 0.41 (t, $J$ = 7.4 Hz, 3H). $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 149.37, 131.02, 130.61, 128.59, 128.37, 126.77, 124.28, 123.02, 117.01, 115.76, 30.69, 28.03, 27.84, 8.67.

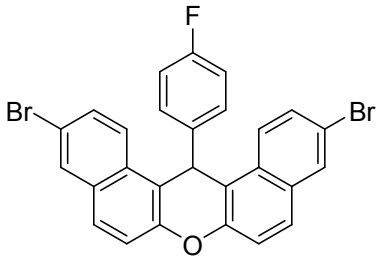


**3,11-dibromo-14-phenyl-14*H*-dibenzo[*a,j*]xanthenes (5q)**: Off-white powder, 80%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.61 (d, $J$ = 9.1 Hz, 2H), 8.18 (d, $J$ = 2.2 Hz, 2H), 7.89 (d, $J$ = 9.0 Hz, 2H), 7.71 (dd, $J$ = 9.0, 2.2 Hz, 2H), 7.61 – 7.53 (m, 4H), 7.14 (t, $J$ = 7.6 Hz, 2H), 6.97 (t, $J$ = 7.4 Hz, 1H), 6.68 (s, 1H); $^{13}$C NMR (101 MHz, DMSO) δ 148.09, 145.12, 132.00, 130.36, 129.68, 129.48, 128.51, 128.34, 127.77, 126.45, 125.80, 118.94, 117.80, 117.56, 36.25.

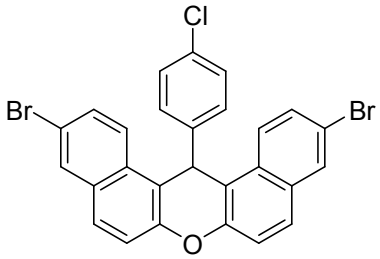


**3,11-dibromo-14-(p-tolyl)-14*H*-dibenzo[*a,j*]xanthenes (5r)**: White powder, 84%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.57 (d, $J$ = 9.2 Hz, 2H), 8.17 (s, 2H), 7.87 (d, $J$ = 9.0 Hz, 2H), 7.70 (d, $J$ = 8.9 Hz, 2H),

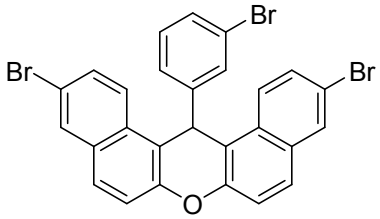
7.56 (d, *J* = 8.9 Hz, 2H), 7.42 (d, *J* = 7.7 Hz, 2H), 6.91 (d, *J* = 7.7 Hz, 2H), 6.61 (s, 1H), 2.01 (s, 3H); $^{13}$C NMR (101 MHz, DMSO) δ 148.00, 142.22, 135.60, 132.00, 130.33, 129.61, 129.47, 129.00, 128.24, 127.63, 125.84, 118.92, 117.74, 117.63, 40.13, 39.92, 39.71, 39.50, 39.29, 39.08, 38.87, 35.87, 20.37.




**3,11-dibromo-14-(4-fluorophenyl)-14*H*-dibenzo[*a,j*]xanthenes (5s)**: White powder, 68%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.61 (d, *J* = 9.1 Hz, 2H), 8.19 (d, *J* = 2.1 Hz, 2H), 7.90 (d, *J* = 9.0 Hz, 2H), 7.73 (dd, *J* = 9.0, 2.2 Hz, 2H), 7.64 – 7.54 (m, 4H), 6.97 (t, *J* = 8.8 Hz, 2H), 6.72 (s, 1H); $^{13}$C NMR (101 MHz, DMSO) δ 161.71, 159.29, 148.08, 141.36, 141.32, 132.02, 130.42, 129.76, 129.61, 129.53, 129.40, 128.46, 125.74, 118.96, 117.86, 117.43, 115.40, 115.19, 35.40.

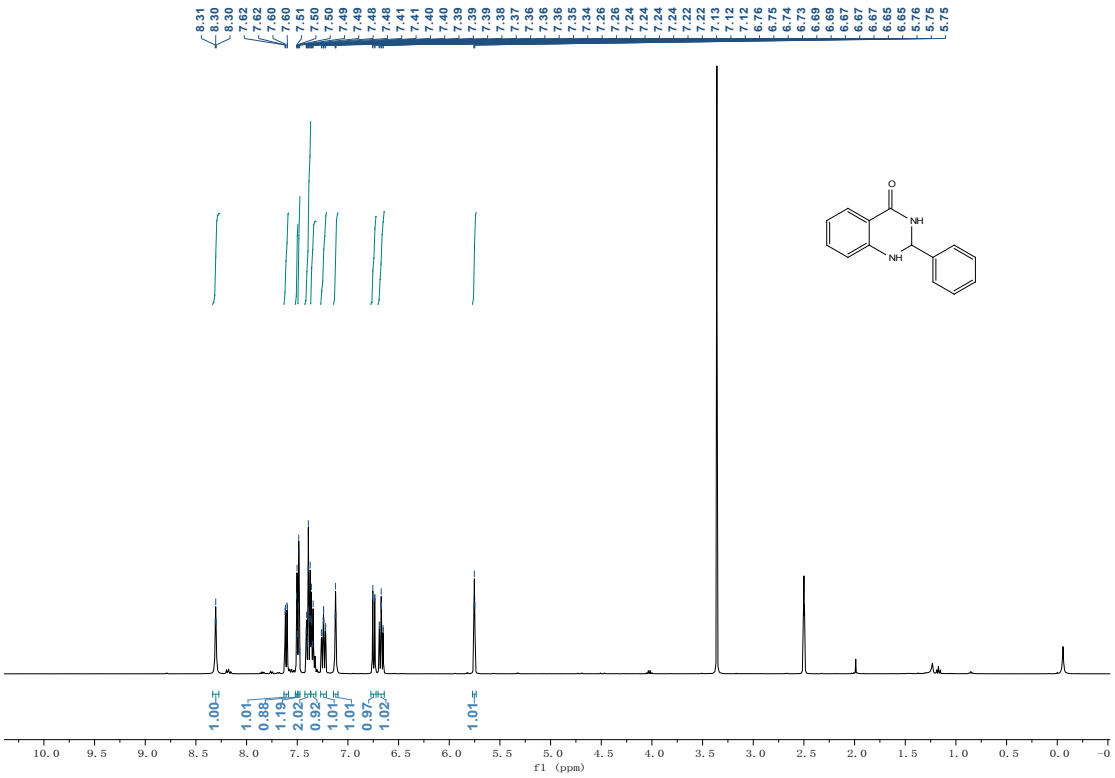


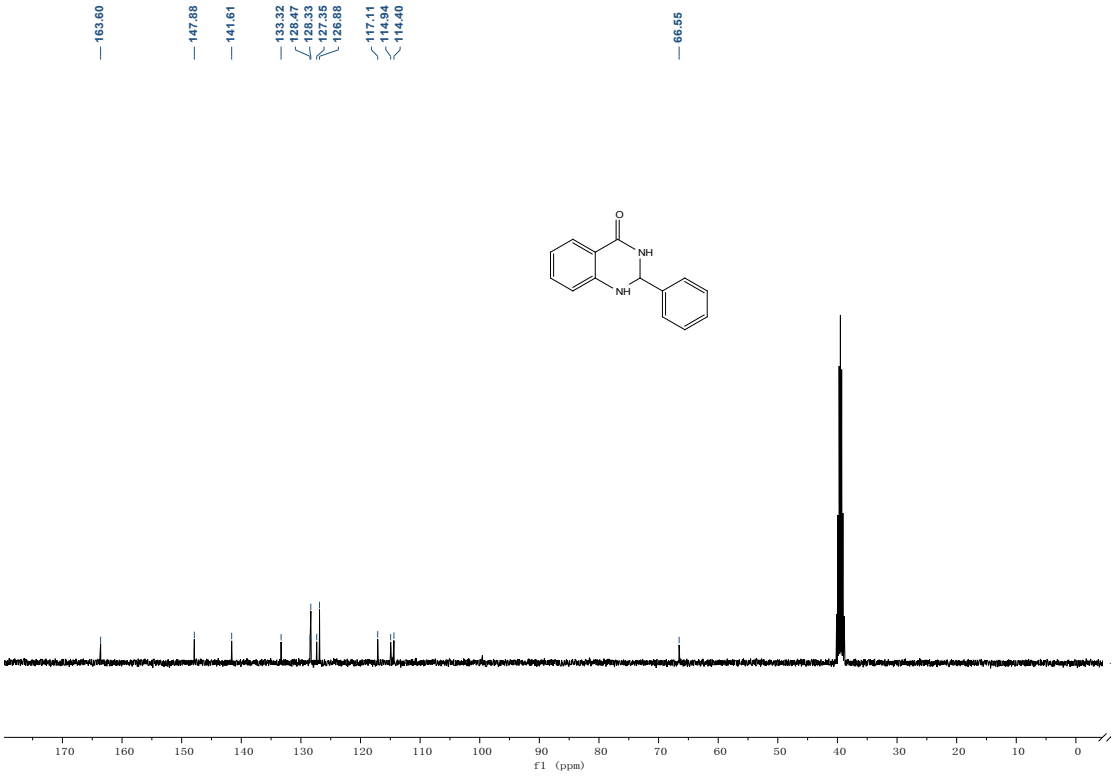

**3,11-dibromo-14-(4-chlorophenyl)-14*H*-dibenzo[*a,j*]xanthenes (5t)**: Light brown powder, 80%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.59 (d, *J* = 9.1 Hz, 2H), 8.19 (d, *J* = 2.2 Hz, 2H), 7.90 (d, *J* = 9.0 Hz, 2H), 7.72 (dd, *J* = 9.1, 2.1 Hz, 2H), 7.57 (dd, *J* = 8.7, 3.7 Hz, 4H), 7.19 (d, *J* = 8.5 Hz, 2H), 6.71 (s, 1H); $^{13}$C NMR (101 MHz, DMSO) δ 148.09, 144.01, 132.02, 131.15, 130.44, 129.81, 129.52, 129.39, 128.56, 128.50, 125.70, 118.97, 117.90, 117.12, 117.10, 35.56.

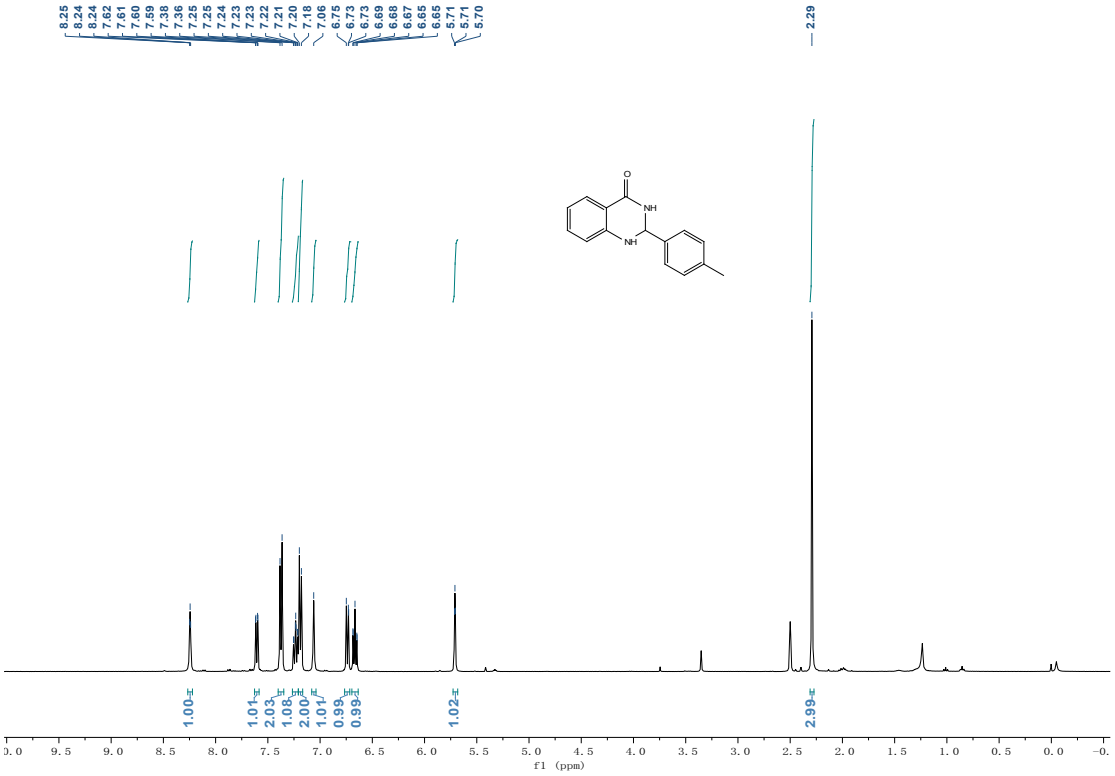



**3,11-dibromo-14-(3-bromophenyl)-14*H*-dibenzo[*a,j*]xanthenes (5u)**: Light yellow powder, 91%. $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 8.62 (d, *J* = 9.1 Hz, 2H), 8.19 (d, *J* = 2.2 Hz, 2H), 7.91 (d, *J* = 9.0 Hz, 2H), 7.81 – 7.72 (m, 3H), 7.58 (dd, *J* = 8.8, 3.2 Hz, 3H), 7.19 (d, *J* = 8.0 Hz, 1H), 7.12 (q, *J* = 7.9, 6.9 Hz, 1H), 6.72 (s, 1H); $^{13}$C NMR (101 MHz, DMSO) δ 148.16, 147.60, 132.02, 130.79, 130.48, 130.12, 129.89, 129.54, 129.35, 128.70, 126.82, 125.64, 121.87, 118.97, 117.98, 116.98, 35.76.

**$^{1}$H-NMR and $^{13}$C-NMR spectrum of compound 3a-3n.**

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6.69
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6.65
5.71
5.71
5.70
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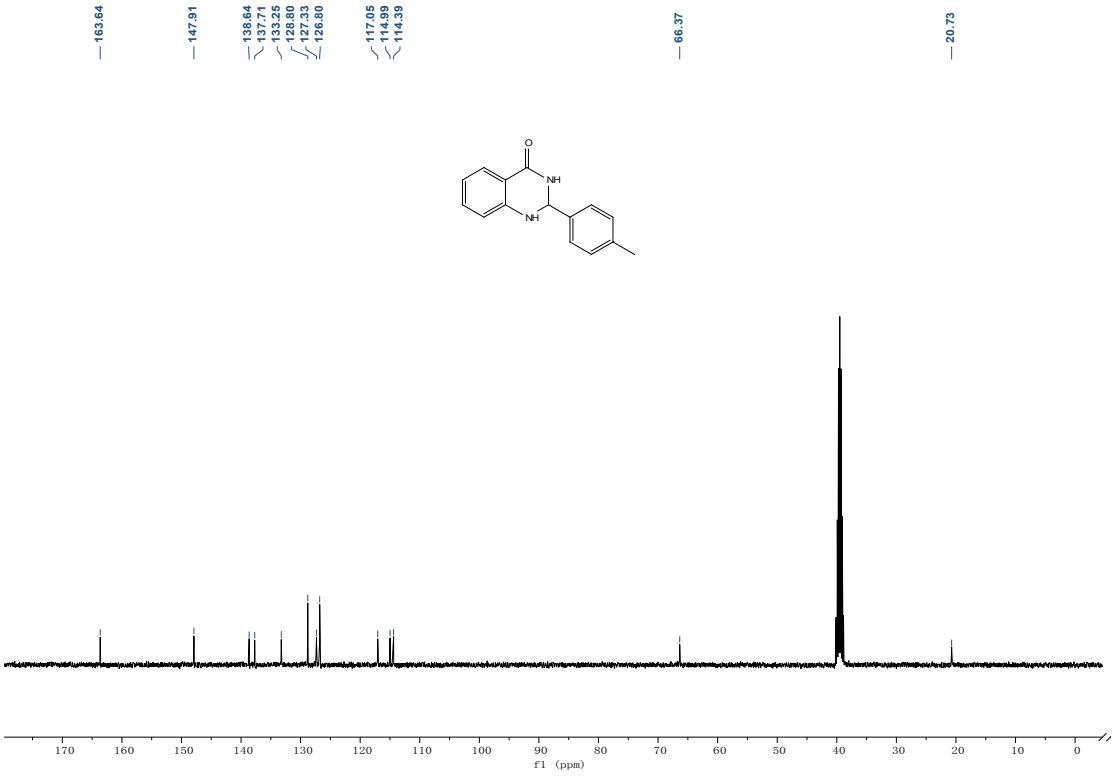
2.99
f1 (ppm)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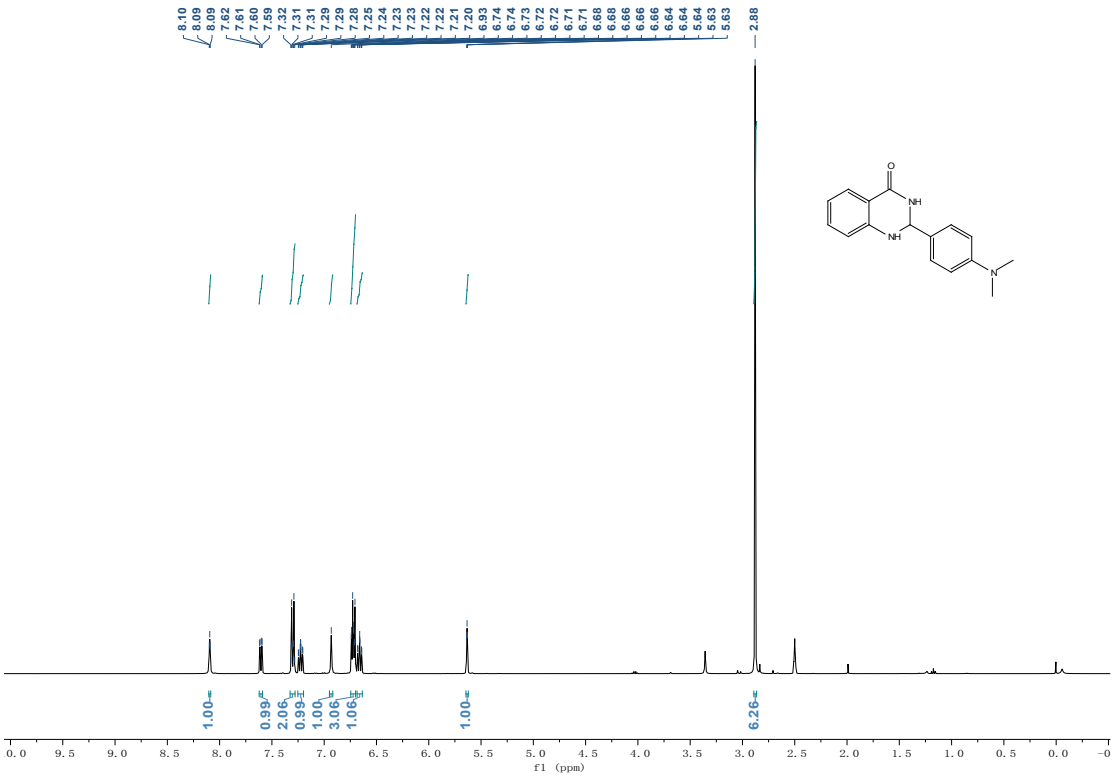
NH
NH
f1 (ppm)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6.73
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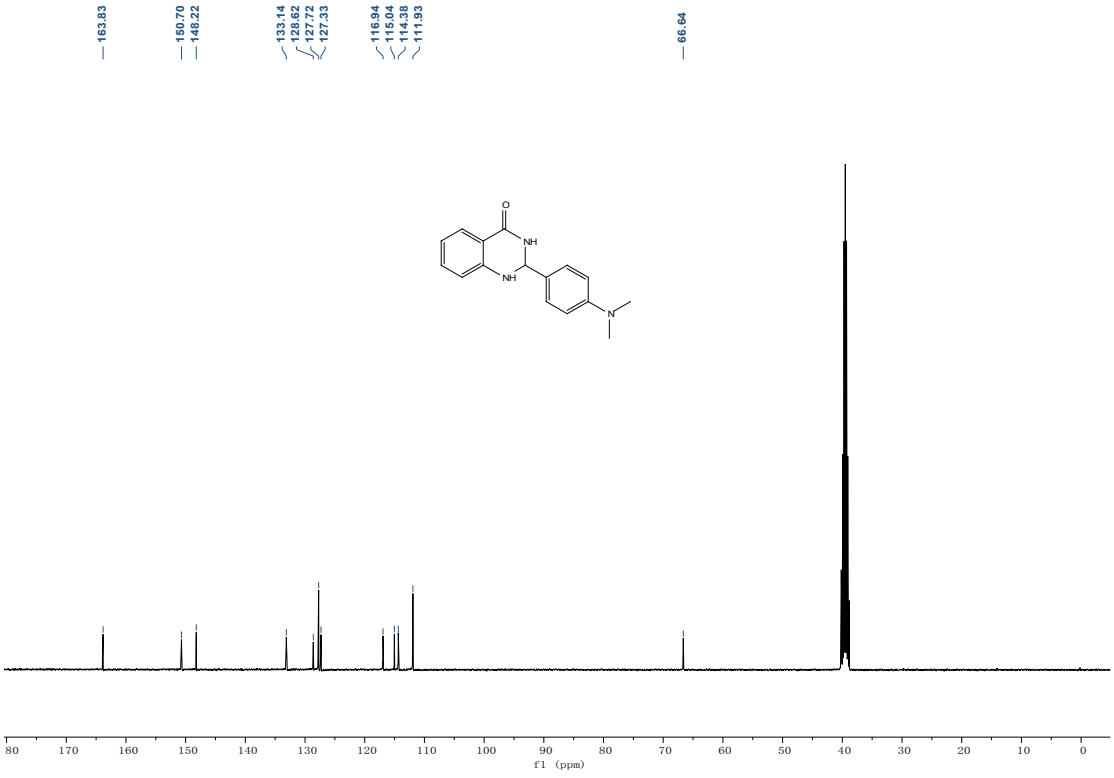
f1 (ppm)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N
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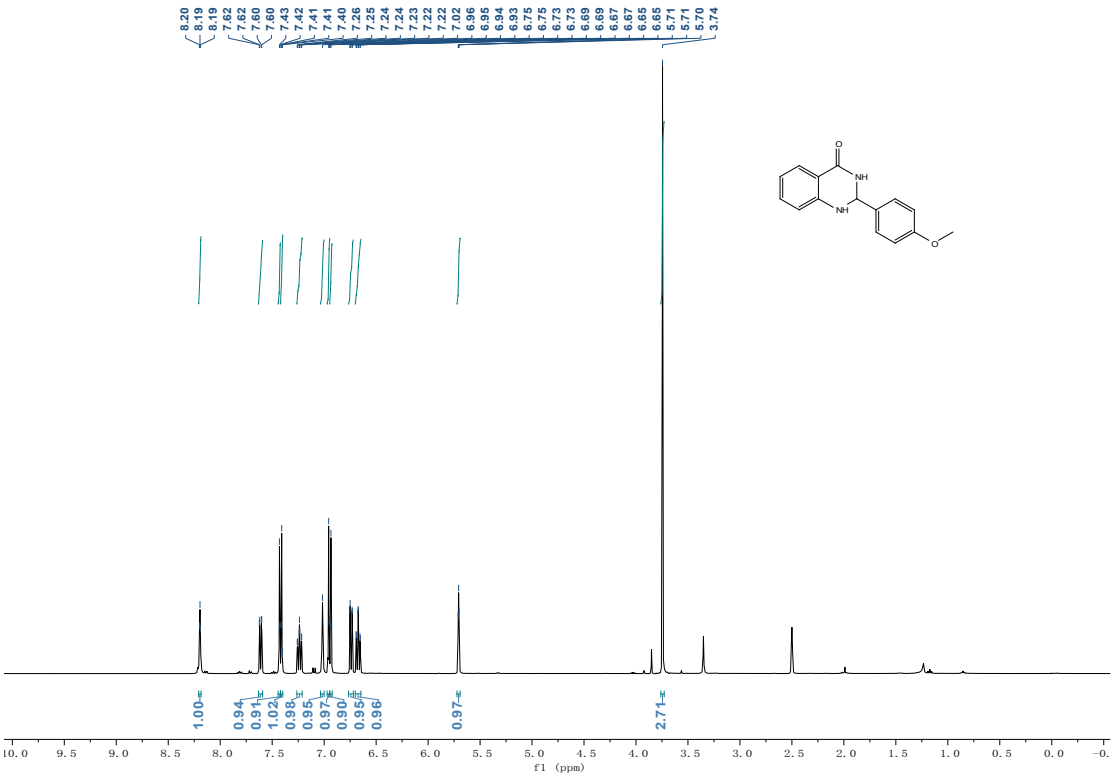
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7.24
7.24
7.23
7.22
7.22
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6.75
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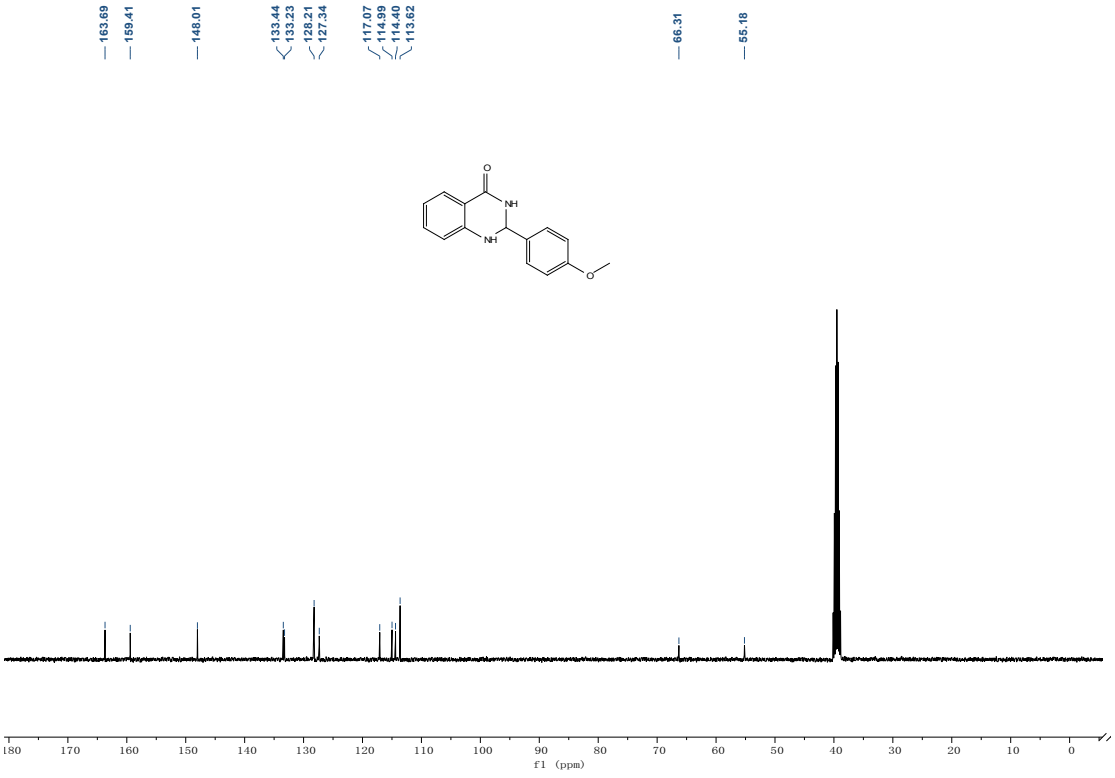
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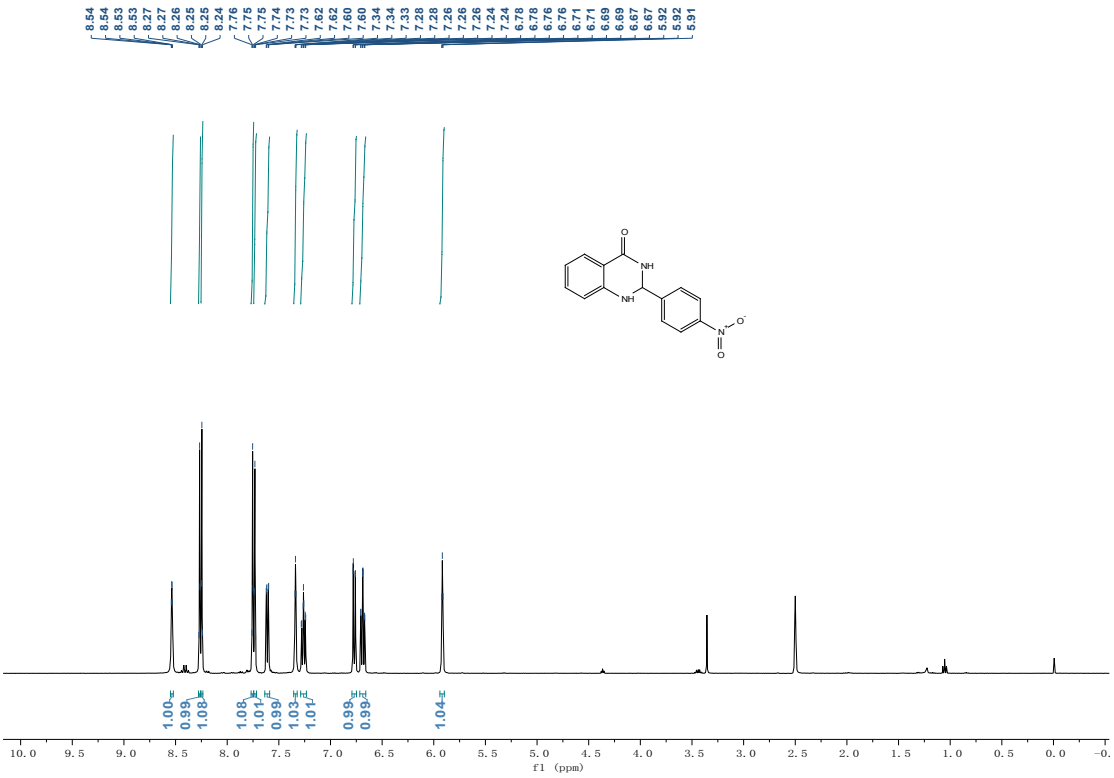
O
f1 (ppm)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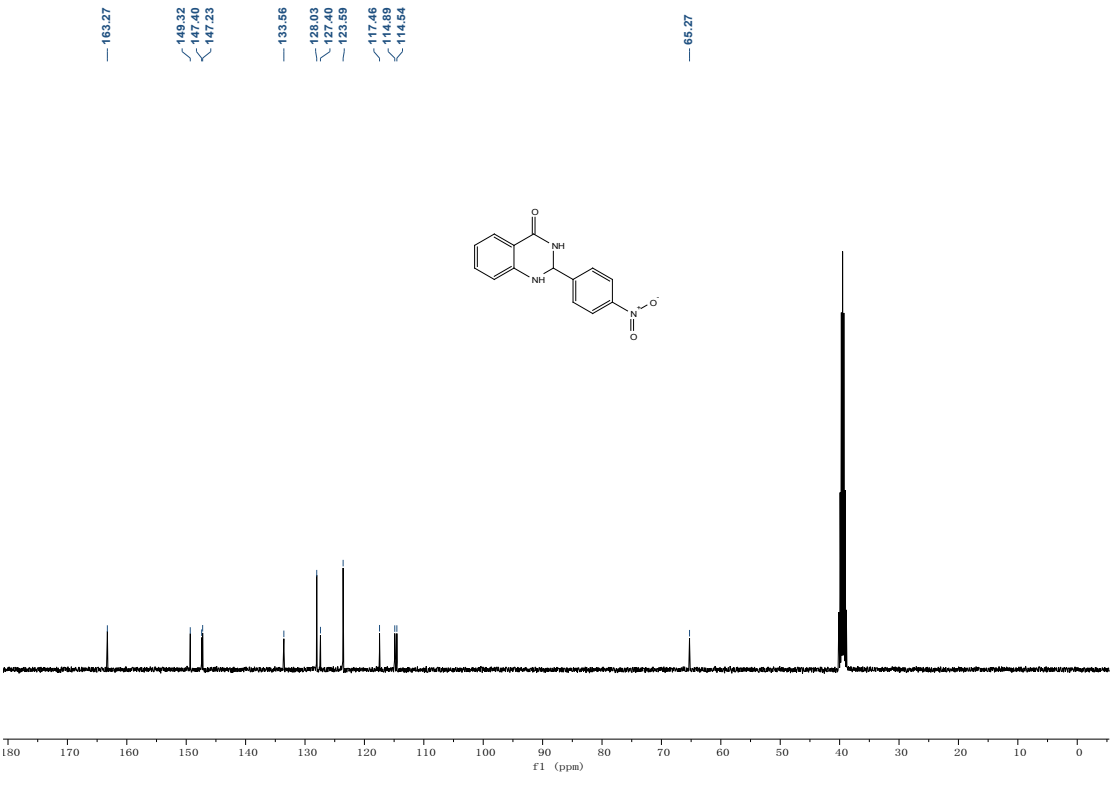
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50
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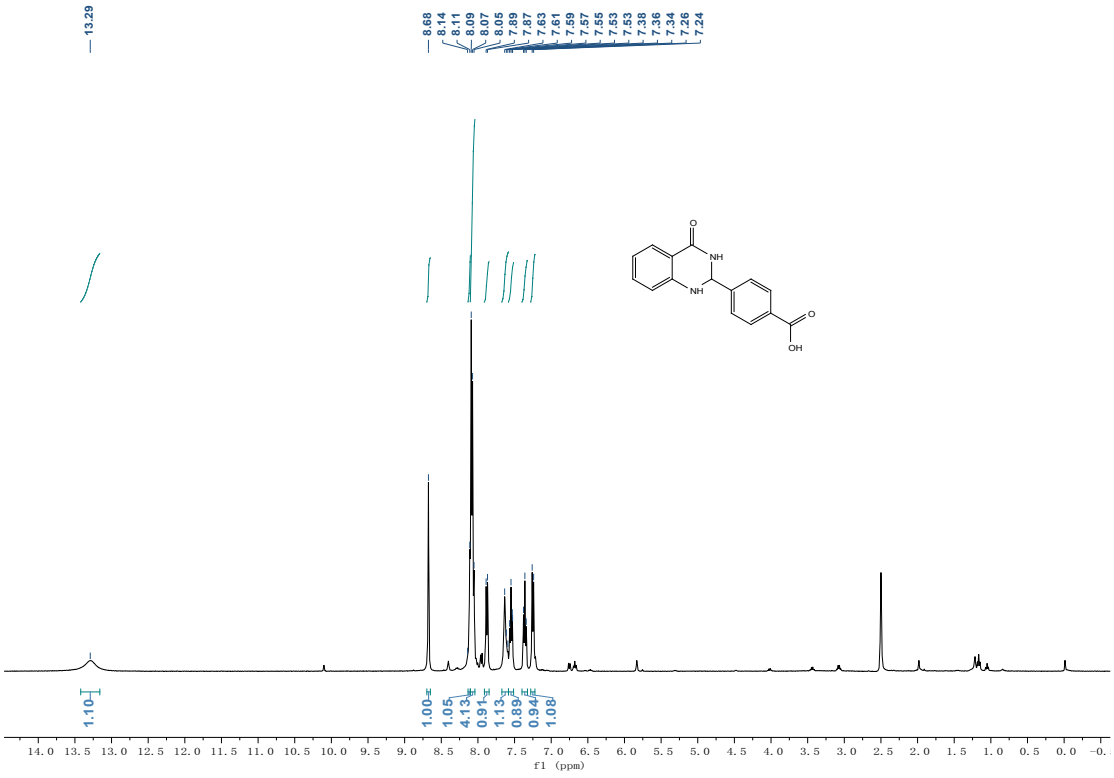
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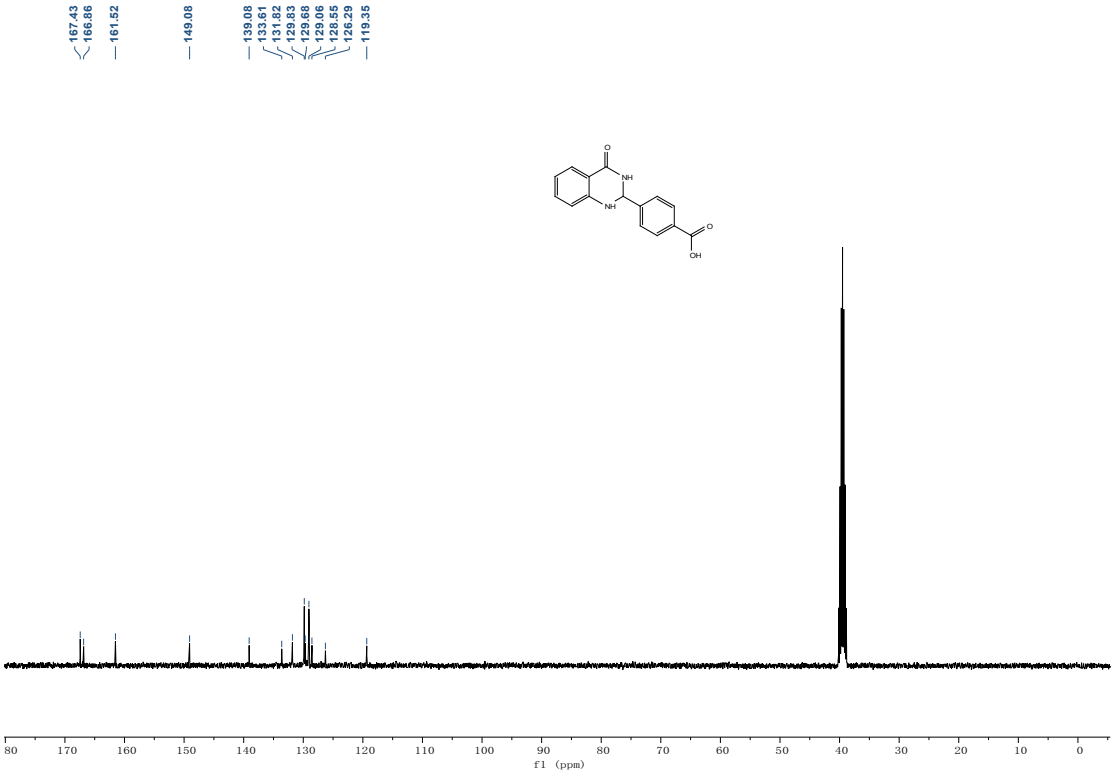
f1 (ppm)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NH
NH
O
OH
f1 (ppm)


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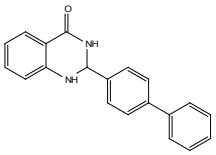
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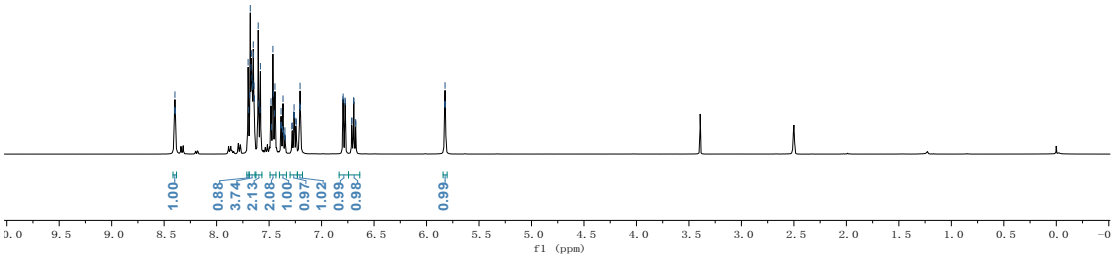
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0.99
0.98
0.99
f1 (ppm)


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140.35
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126.66
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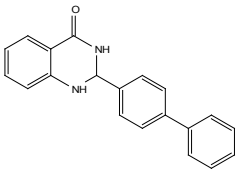
66.24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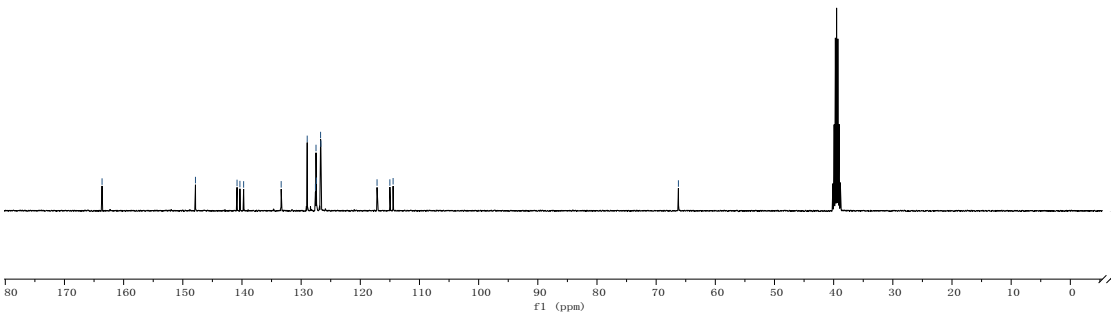
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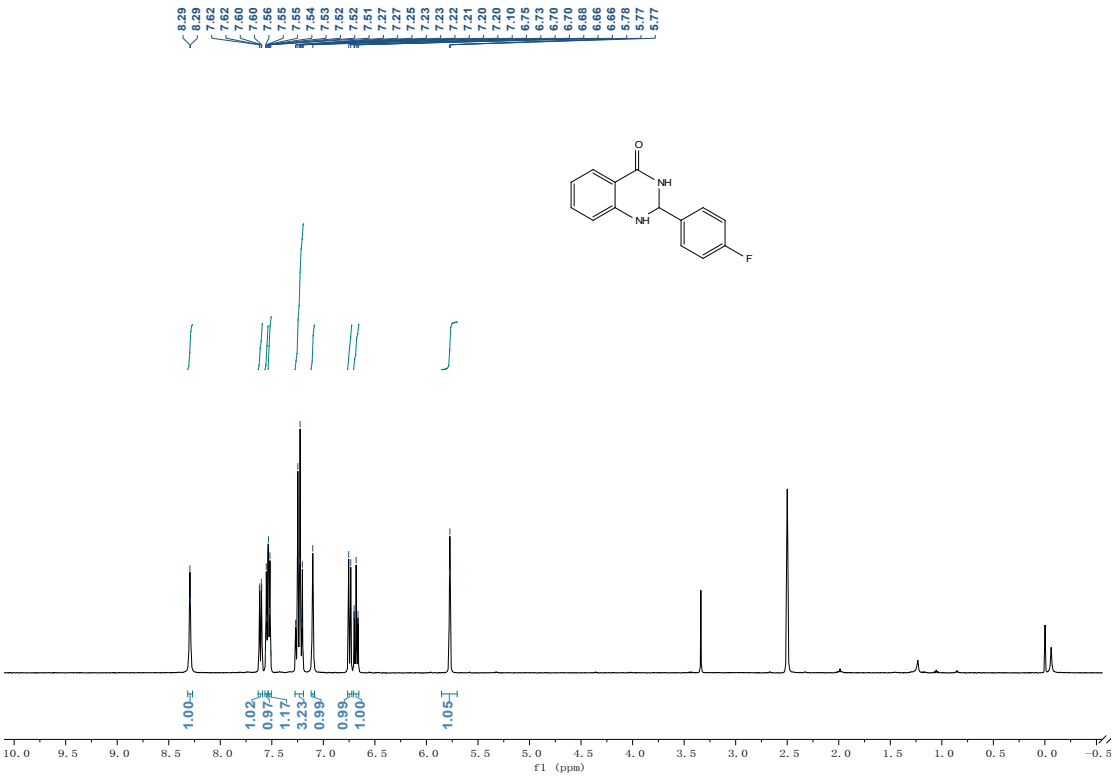
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NH
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1.02
0.97
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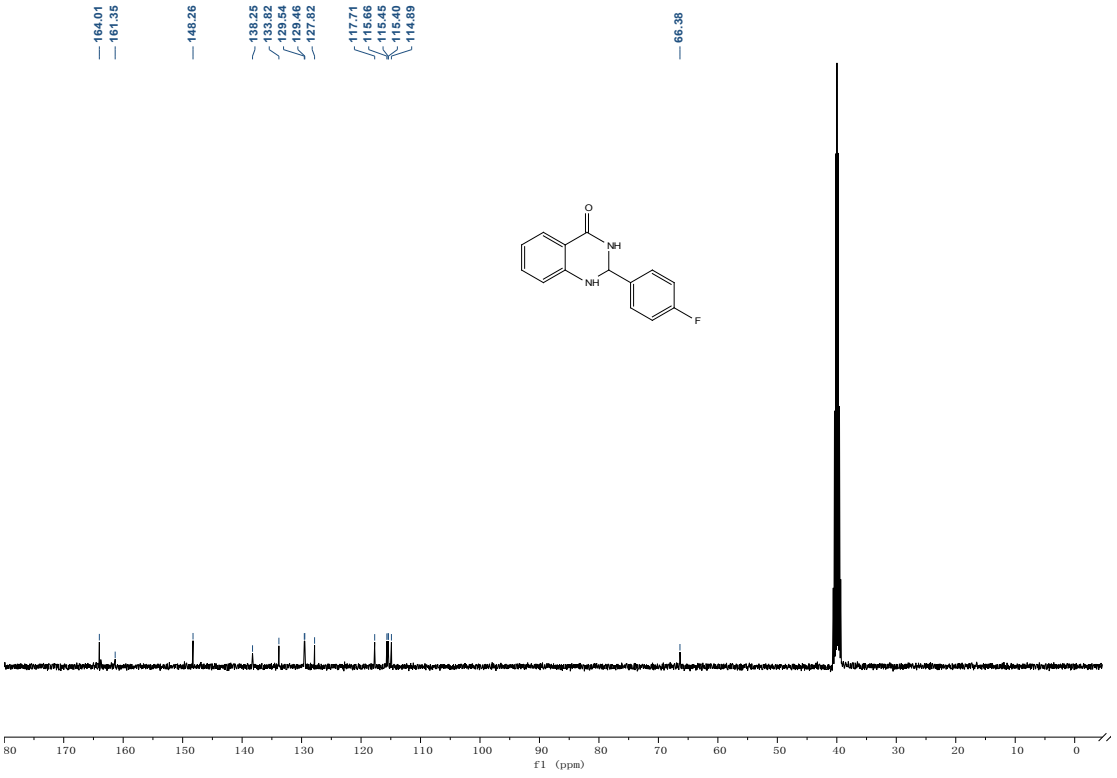
3.23
0.99
0.99
1.00
1.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)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114.89
66.38
O
NH
NH
F
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.35
8.35
8.34
7.62
7.61
7.60
7.60
7.60
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7.59
7.58
7.58
7.46
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7.24
7.23
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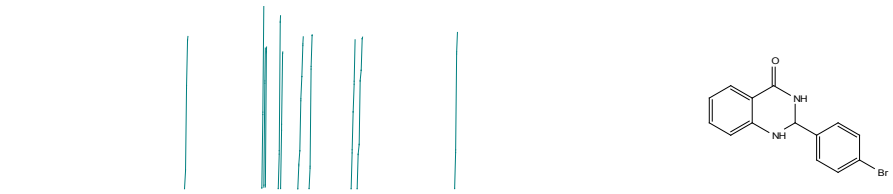
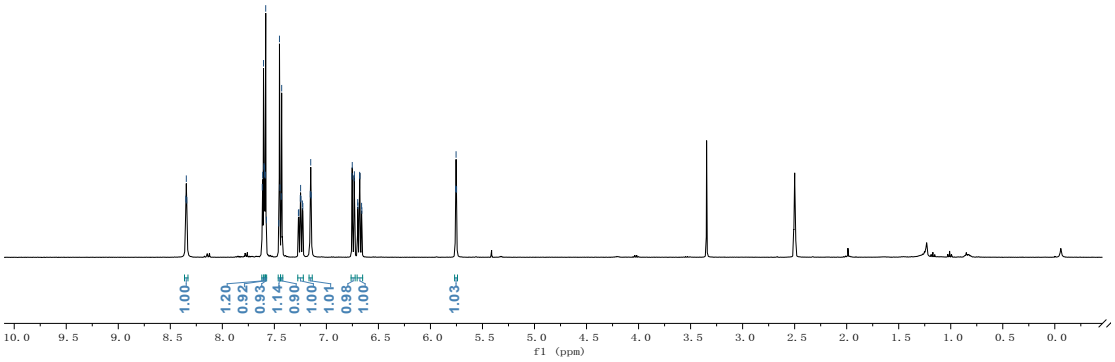

O
NH
NH
Br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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


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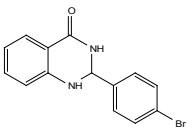
65.78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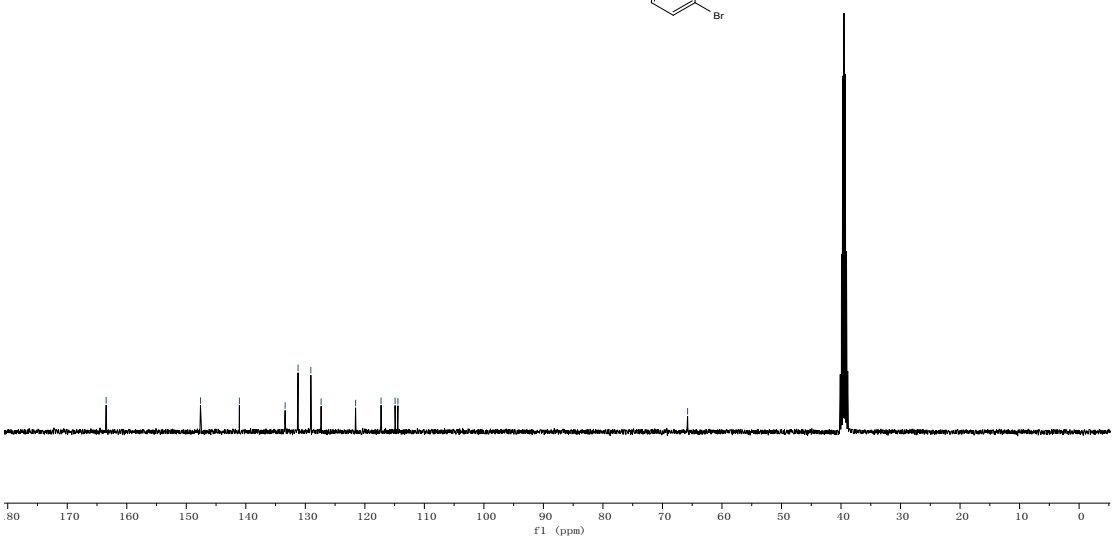
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140
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120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.35
8.35
8.34
7.62
7.61
7.60
7.59
7.52
7.51
7.50
7.50
7.49
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6.70
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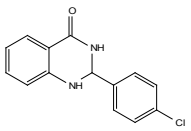
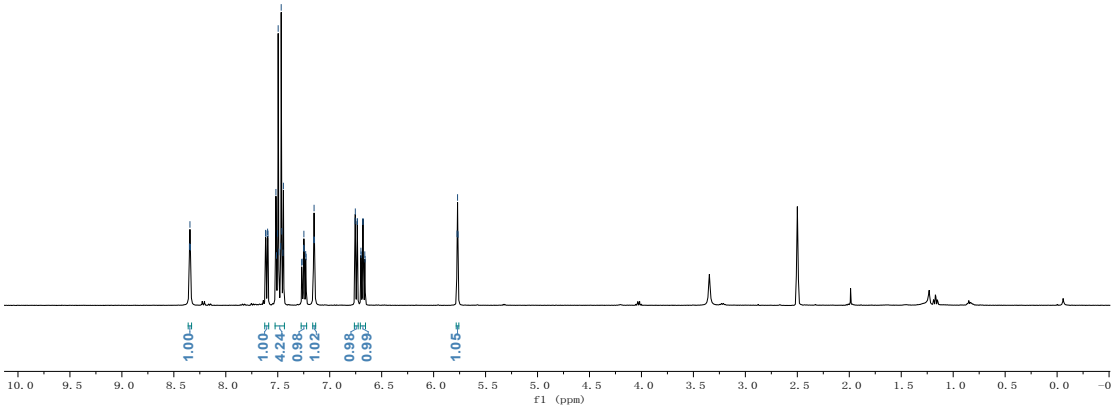
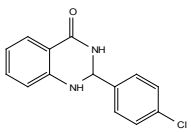
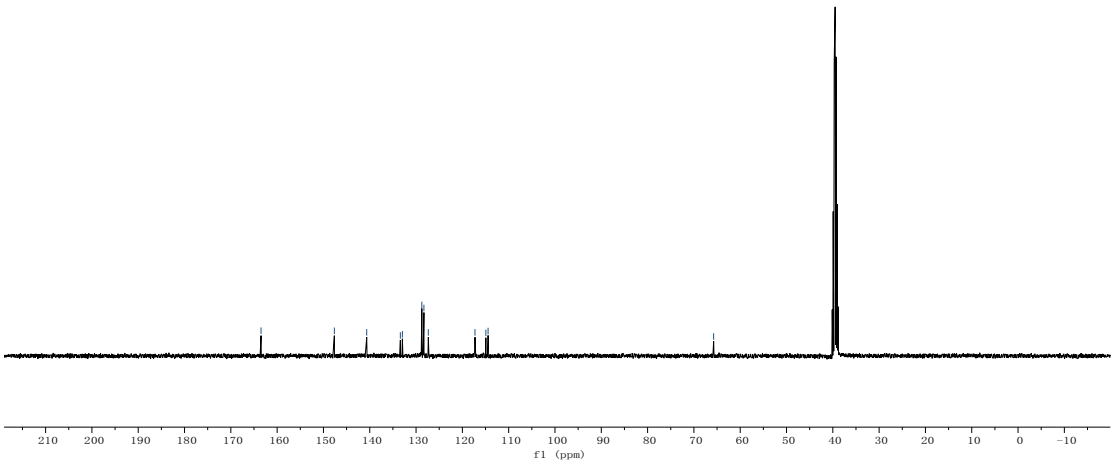
6.68
6.66
6.66
5.77
5.77
5.76

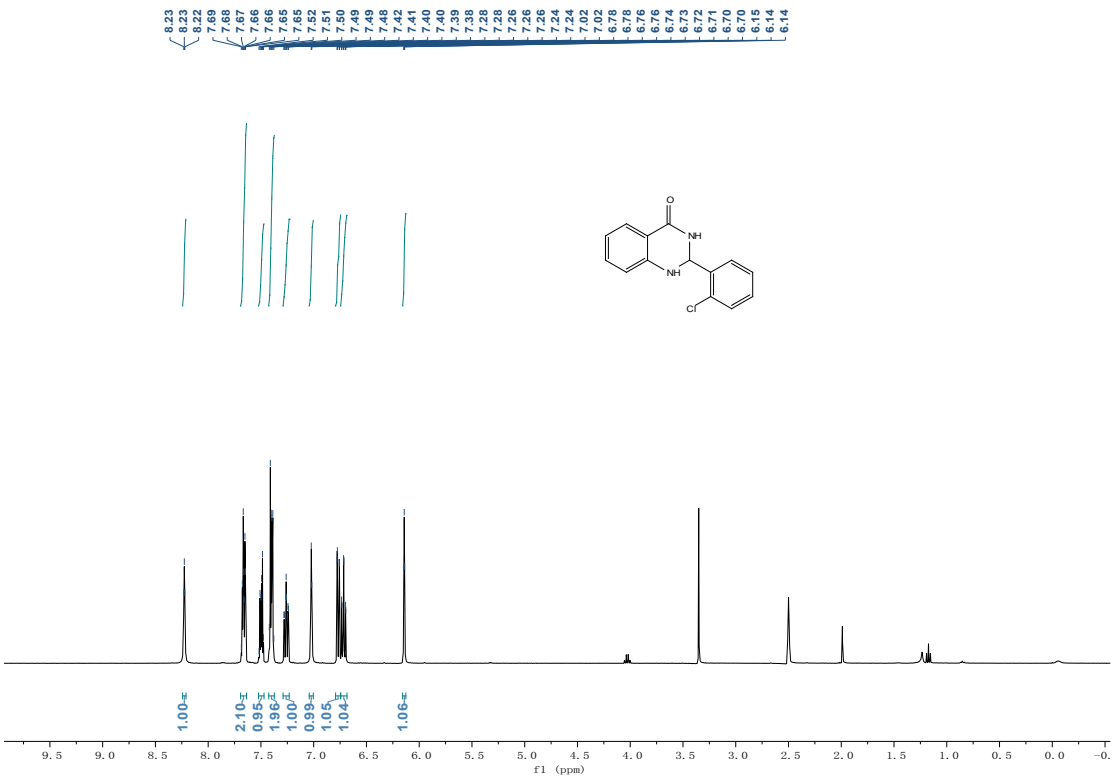

O
NH
NH
Cl

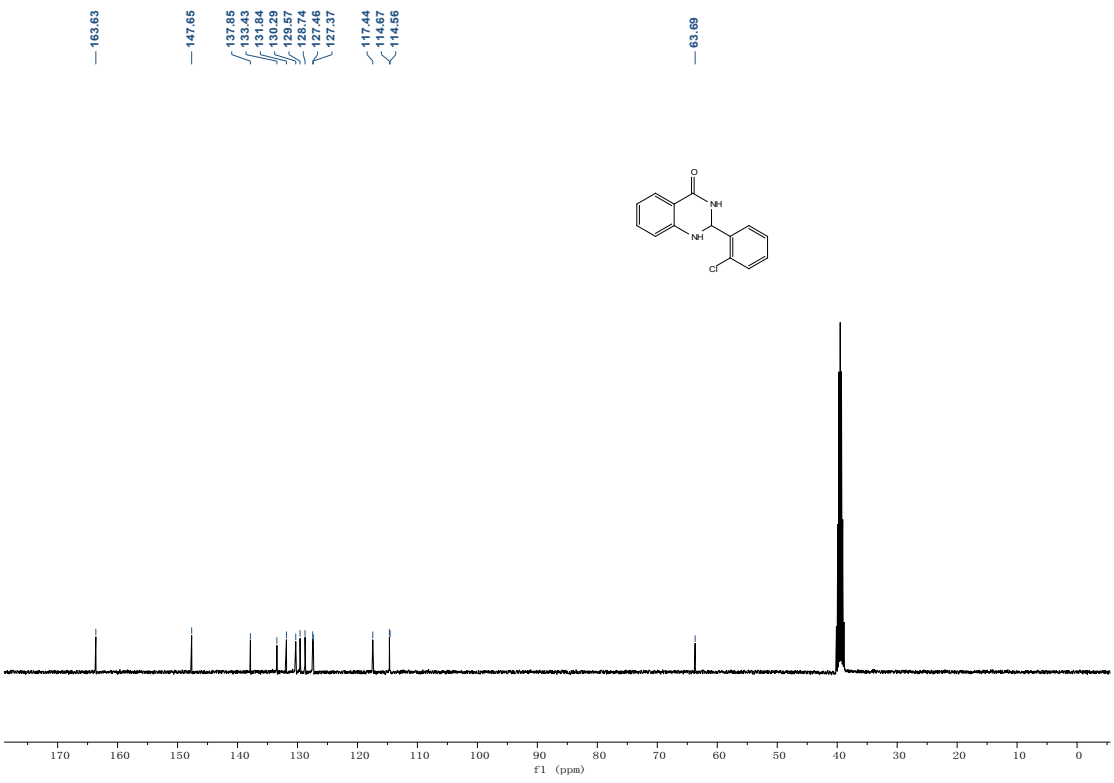

1.00
1.00
4.24
0.98
1.02
0.98
0.99
1.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0
f1 (ppm)


163.48
147.64
140.66
133.39
132.95
128.76
128.30
127.35
117.27
114.93
114.45
65.74

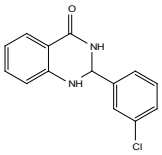

O
NH
NH
Cl

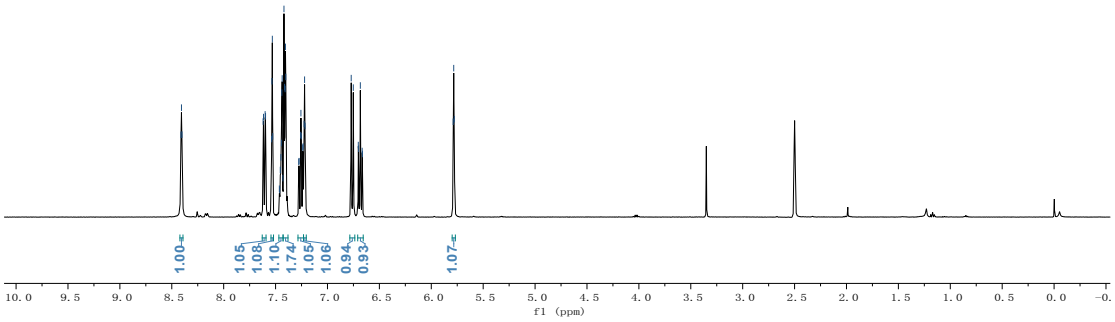

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


8.23
8.23
8.22
7.69
7.68
7.67
7.66
7.66
7.65
7.65
7.52
7.51
7.50
7.49
7.49
7.48
7.42
7.41
7.40
7.40
7.39
7.38
7.28
7.28
7.26
7.26
7.26
7.24
7.24
7.02
7.02
6.78
6.78
6.76
6.76
6.74
6.73
6.72
6.71
6.70
6.70
6.15
6.14
6.14
O
NH
NH
Cl
1.00
2.10
0.95
1.96
1.00
0.99
1.05
1.04
1.06
f1 (ppm)

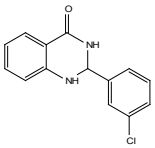

163.63
147.65
137.85
133.43
131.84
130.29
129.57
128.74
127.46
127.37
117.44
114.67
114.56
63.69
O
NH
NH
Cl
f1 (ppm)

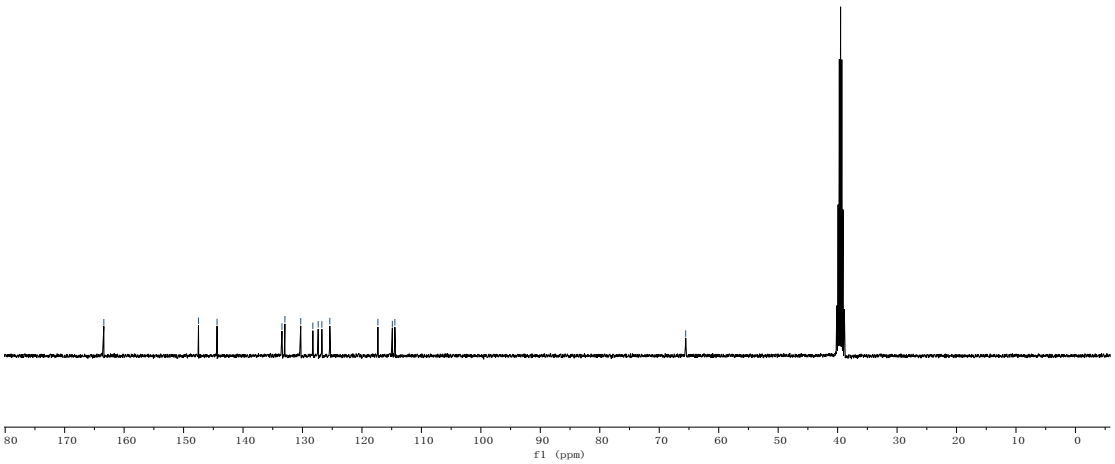

8.41
8.41
8.40
7.62
7.60
7.60
7.54
7.54
7.53
7.53
7.46
7.46
7.45
7.45
7.44
7.44
7.44
7.43
7.42
7.41
7.41
7.40
7.40
7.28
7.27
7.26
7.25
7.24
7.23
7.23
7.22
7.22
6.77
6.75
6.70
6.70
6.68
6.67
6.66
5.79
5.78
5.78

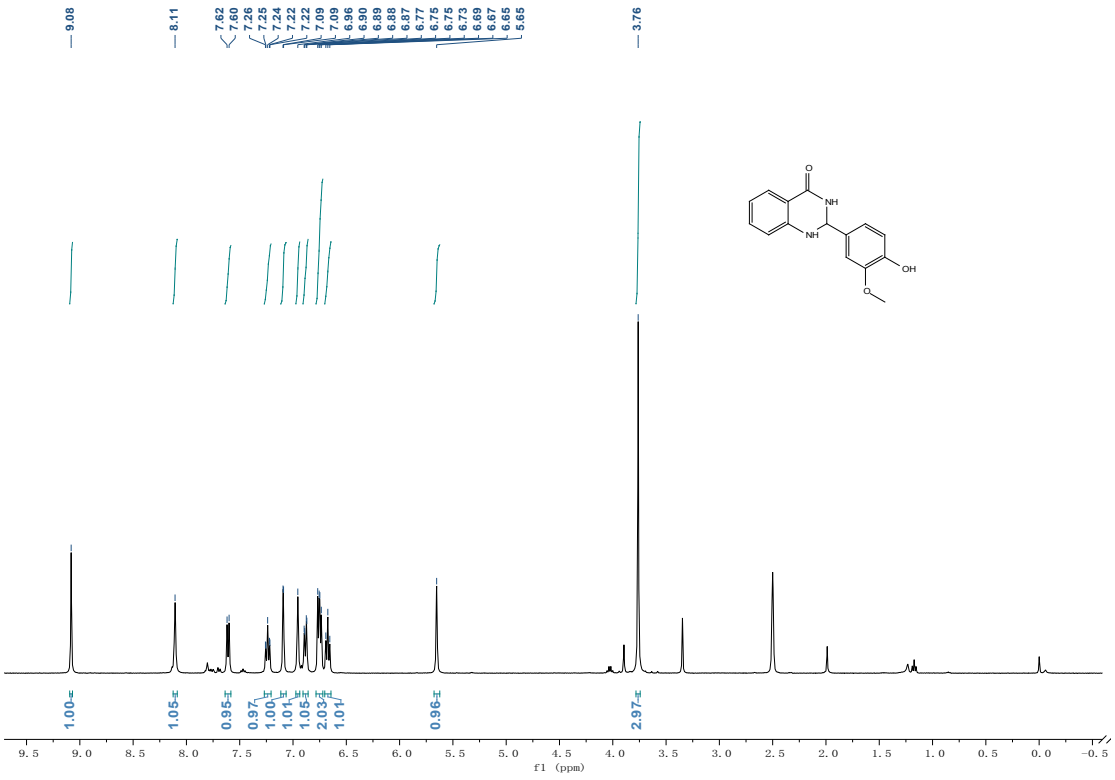

O
NH
NH
Cl

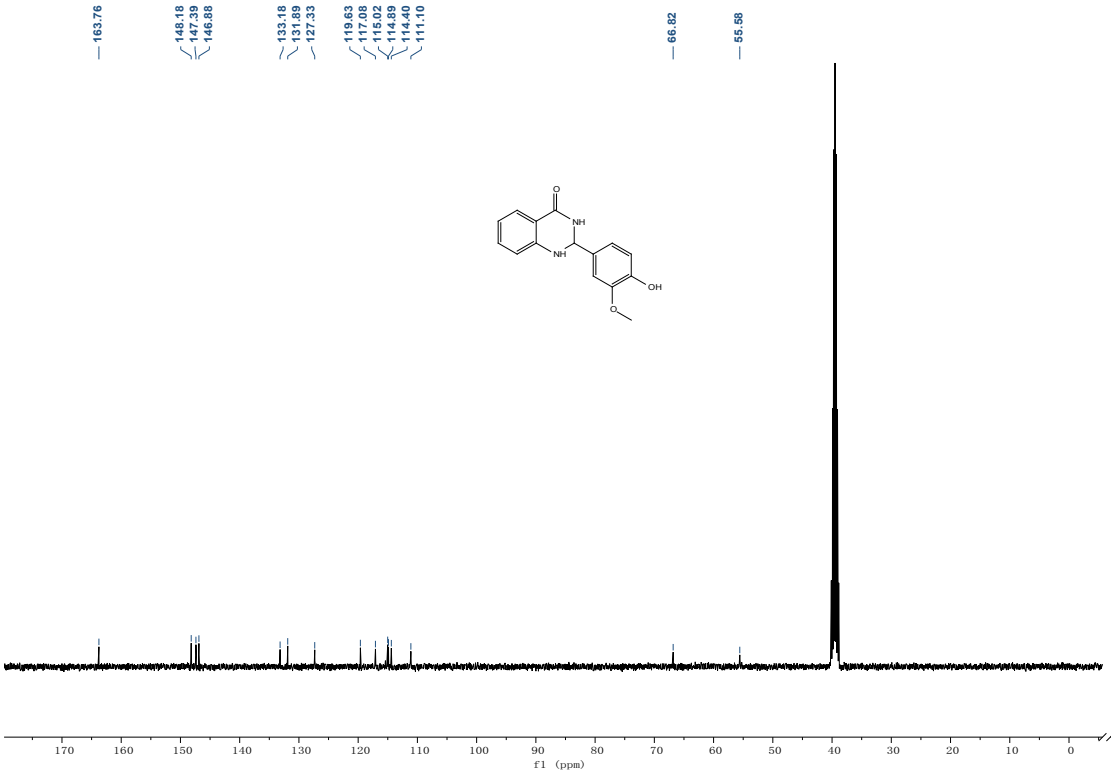

1.00
1.05
1.08
1.10
1.74
1.05
1.06
0.94
0.93
1.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)


163.41
147.49
144.37
133.46
132.96
130.30
128.26
127.36
126.75
125.40
117.32
114.89
114.46
65.56

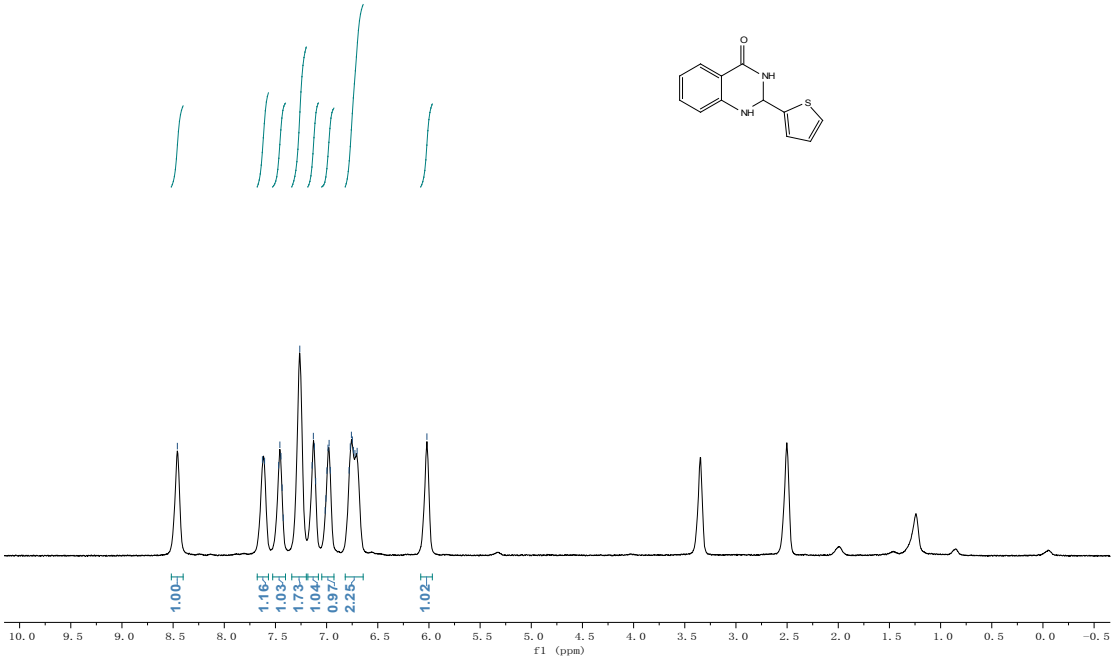

O
NH
NH
Cl

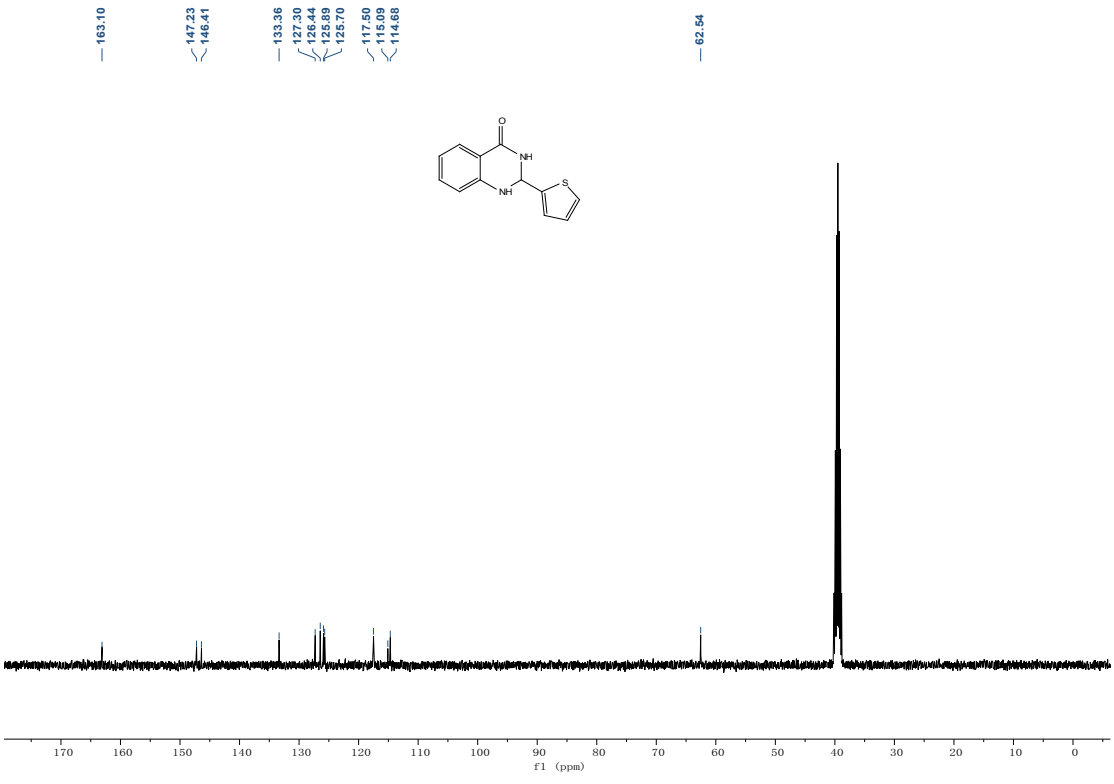

80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.08
8.11
7.62
7.60
7.26
7.25
7.24
7.22
7.22
7.09
7.09
6.96
6.90
6.89
6.88
6.87
6.77
6.75
6.75
6.73
6.69
6.67
6.65
5.65
3.76
O
NH
NH
OH
O
1.00
1.05
0.95
0.97
1.00
1.01
1.05
2.03
1.01
0.96
2.97
f1 (ppm)


163.76
148.18
147.39
146.88
133.18
131.89
127.33
119.63
117.08
115.02
114.89
114.40
111.10
66.82
55.58
O
NH
NH
OH
O
f1 (ppm)


8.46
7.63
7.61
7.47
7.46
7.45
7.43
7.42
7.26
7.14
7.13
7.12
7.11
7.01
7.01
7.00
6.99
6.98
6.96
6.78
6.77
6.76
6.75
6.74
6.72
6.70
6.02


O
NH
NH
S
1.00
1.16
1.03
1.73
1.04
0.97
2.25
1.02
10.0 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)


163.10
147.23
146.41
133.36
127.30
126.44
125.89
125.70
117.50
115.09
114.68
62.54
O
NH
NH
S
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.75
7.87
7.84
7.83
7.78
7.60
7.60
7.53
7.53
7.52
7.52
7.51
7.51
7.50
7.45
7.44
7.44
7.43
7.42
7.41
7.41
7.40
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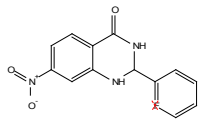
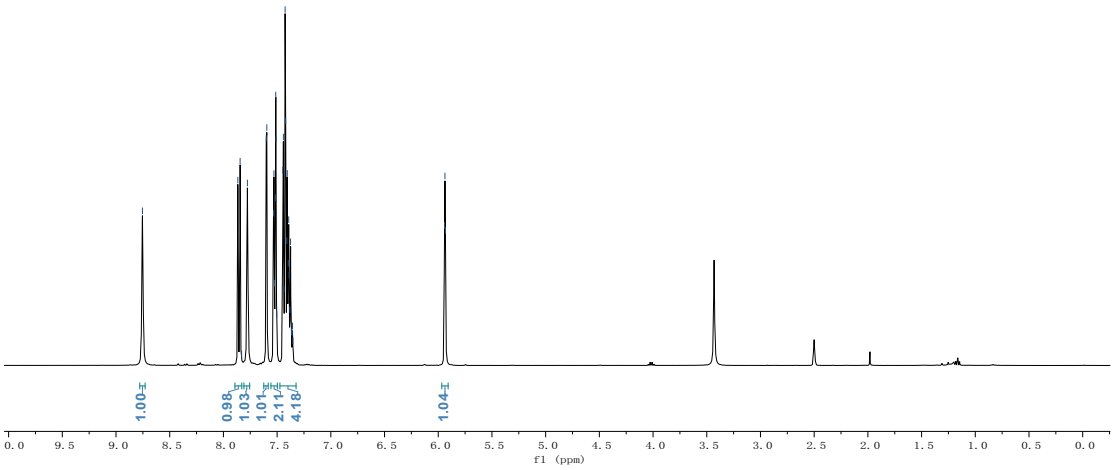
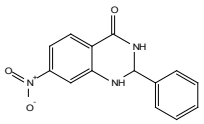
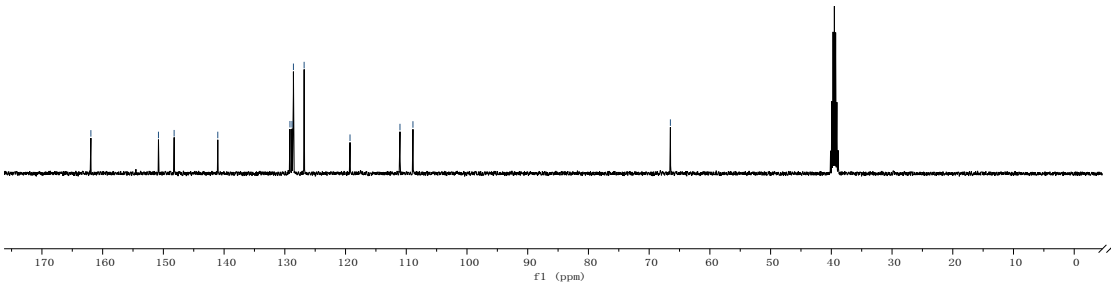
7.38
7.37
7.37
7.36
7.36
7.35
5.94
5.94
5.93

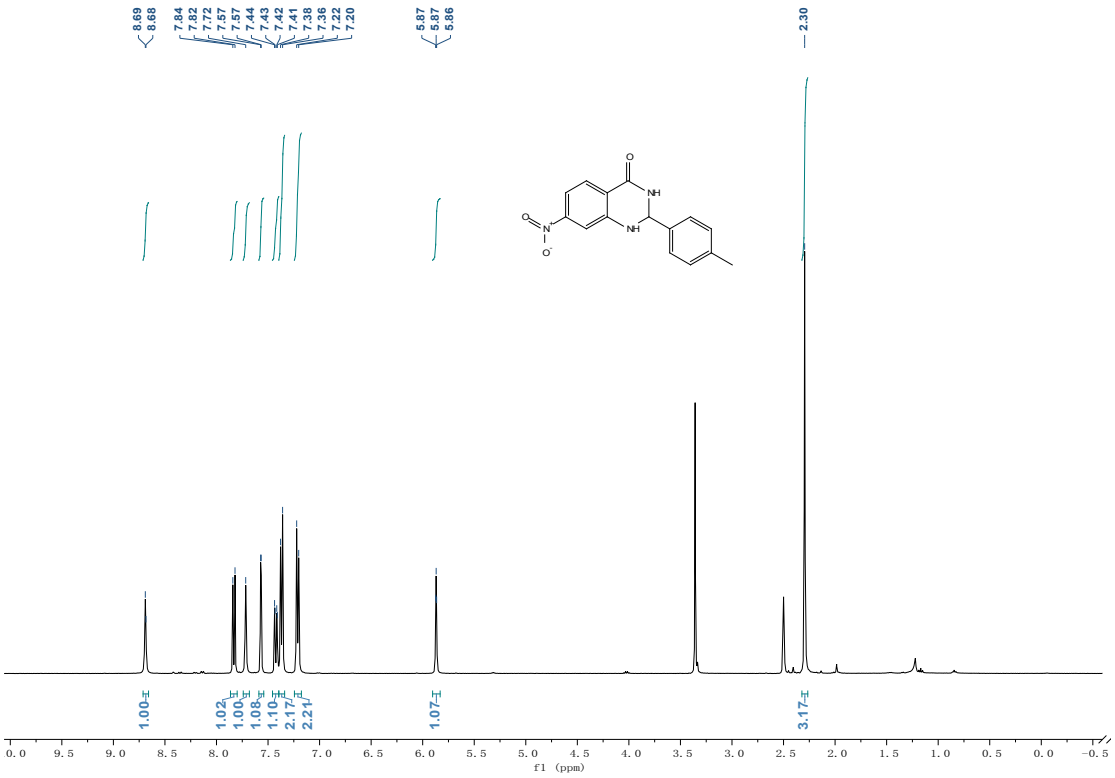

O
NH
NH
N+
O-
F

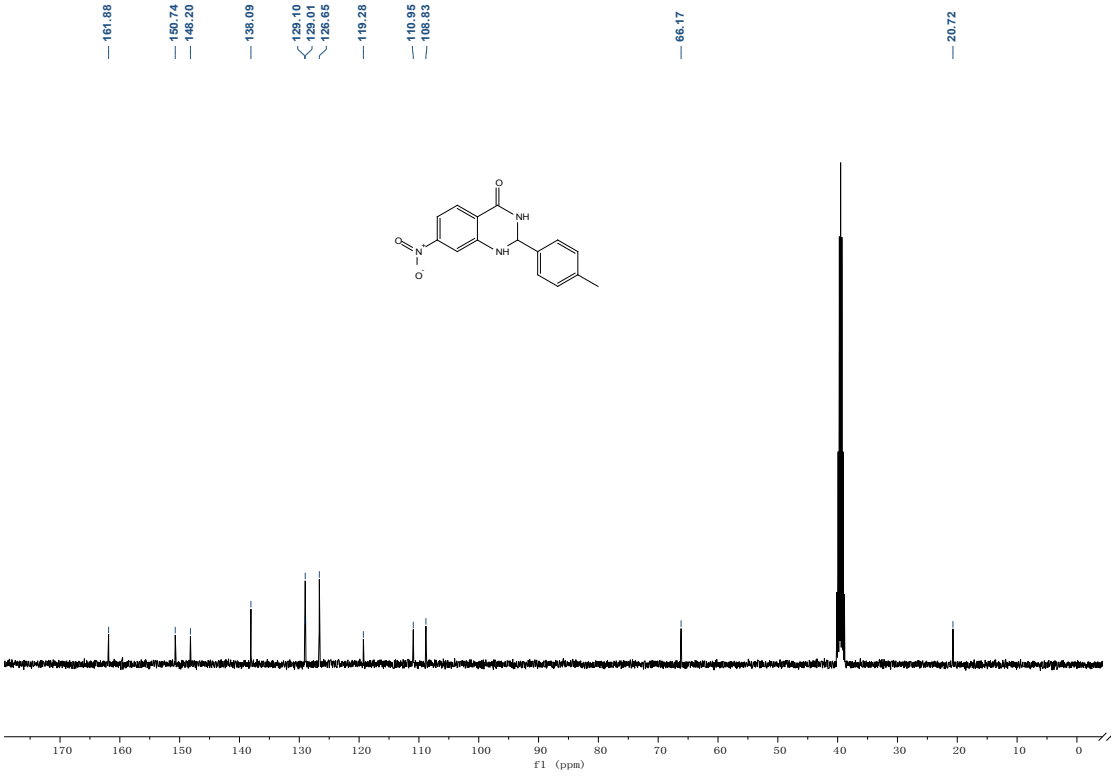

1.00
0.98
1.03
1.01
2.11
4.18
1.04
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

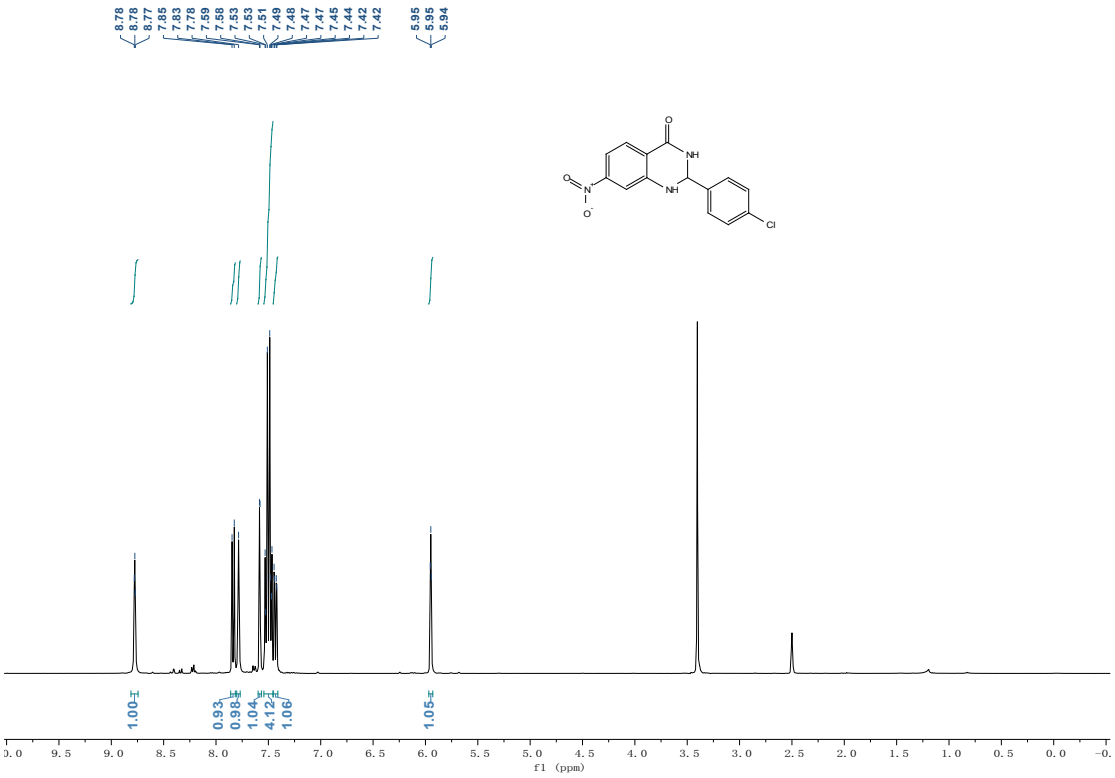

161.94
150.81
148.23
141.04
129.15
128.82
128.58
126.82
119.26
111.04
108.90
66.50

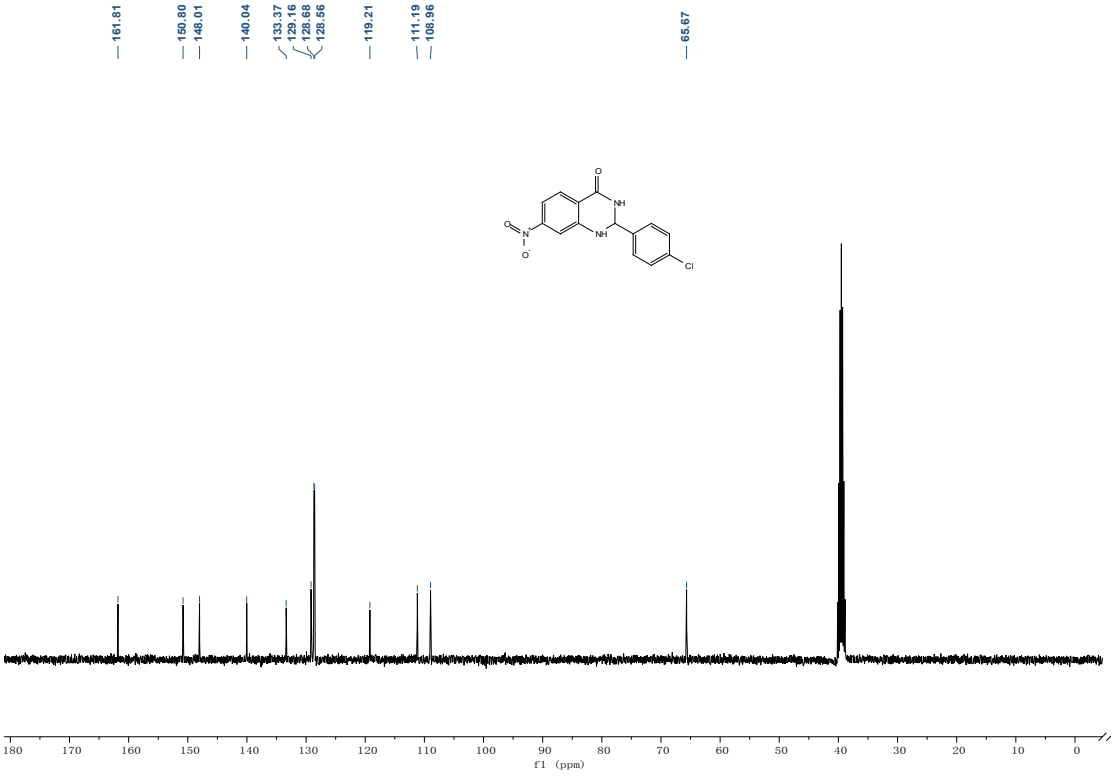

O
NH
NH
N+
O-

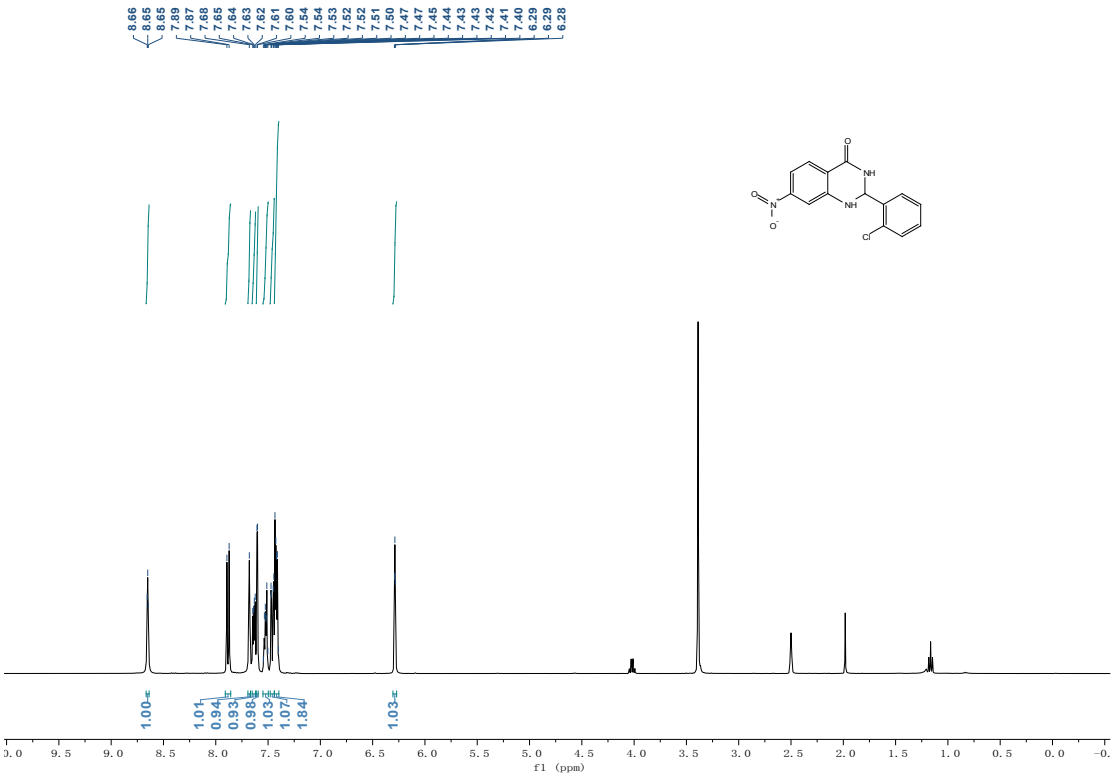

170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

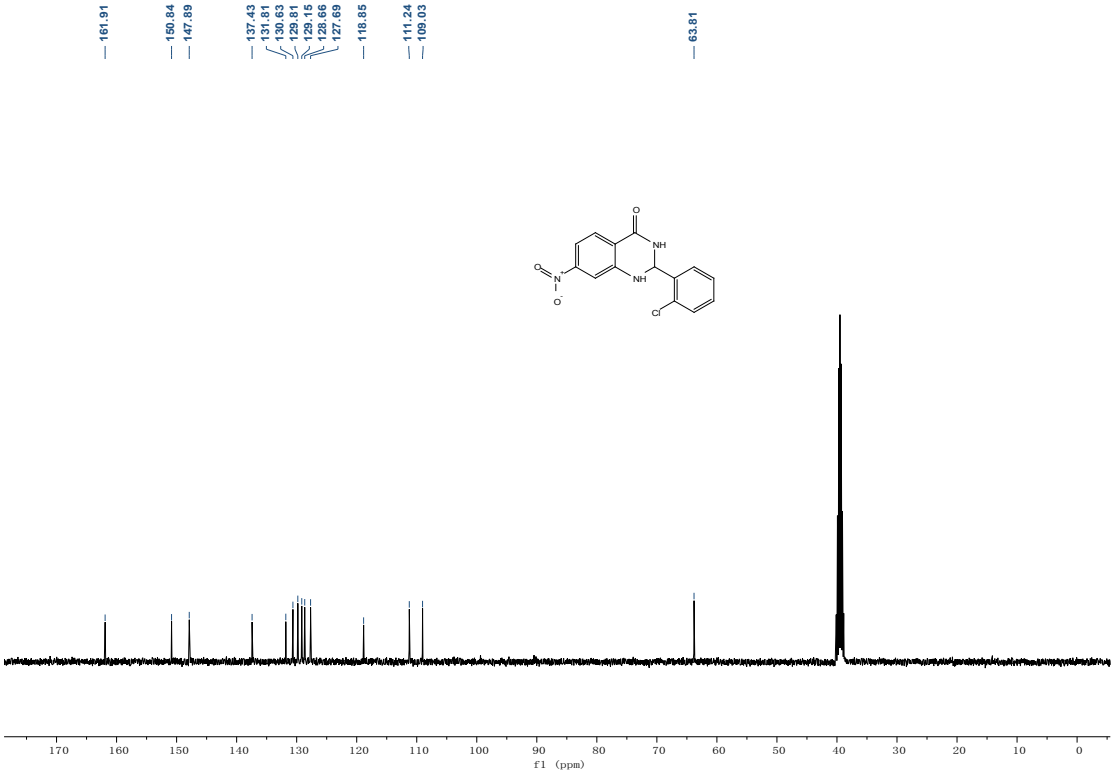

8.69
8.68
7.84
7.82
7.72
7.57
7.57
7.44
7.43
7.42
7.41
7.38
7.36
7.22
7.20
5.87
5.87
5.86
2.30
O
NH
NH
O
N+
O-
1.00
1.02
1.00
1.08
1.10
2.17
2.21
1.07
3.17
f1 (ppm)

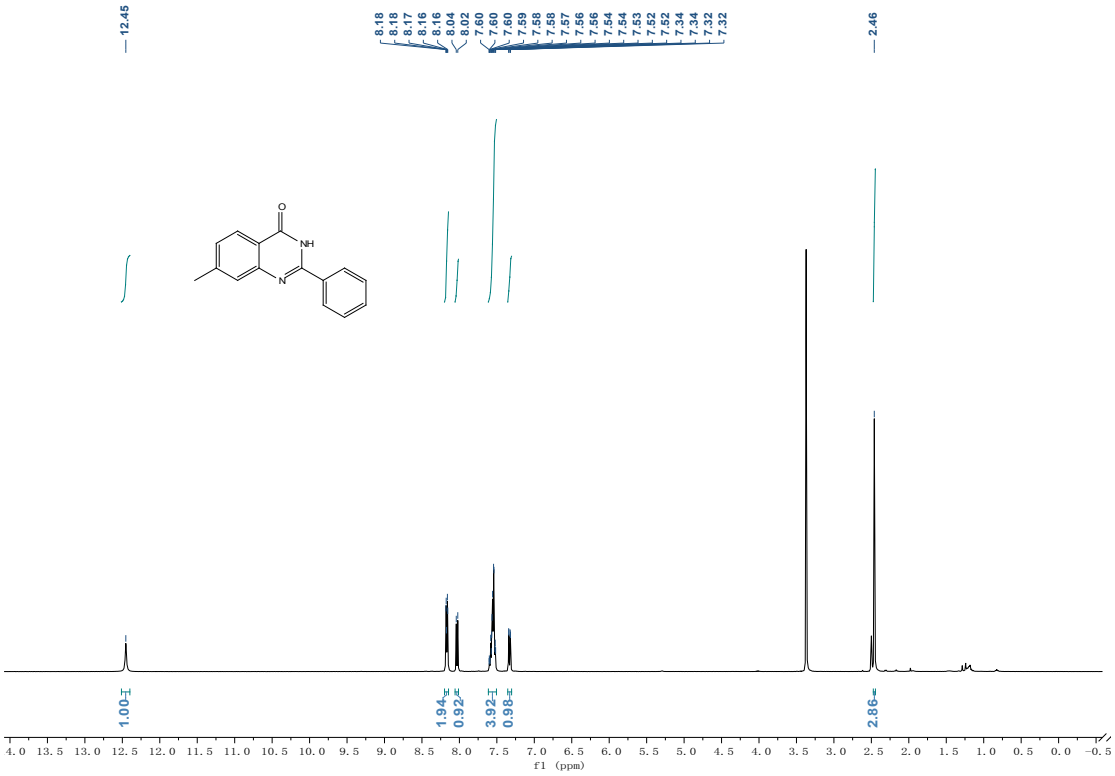

161.88
150.74
148.20
138.09
129.10
129.01
126.65
119.28
110.95
108.83
66.17
20.72
O
NH
NH
O
N+
O-
f1 (ppm)

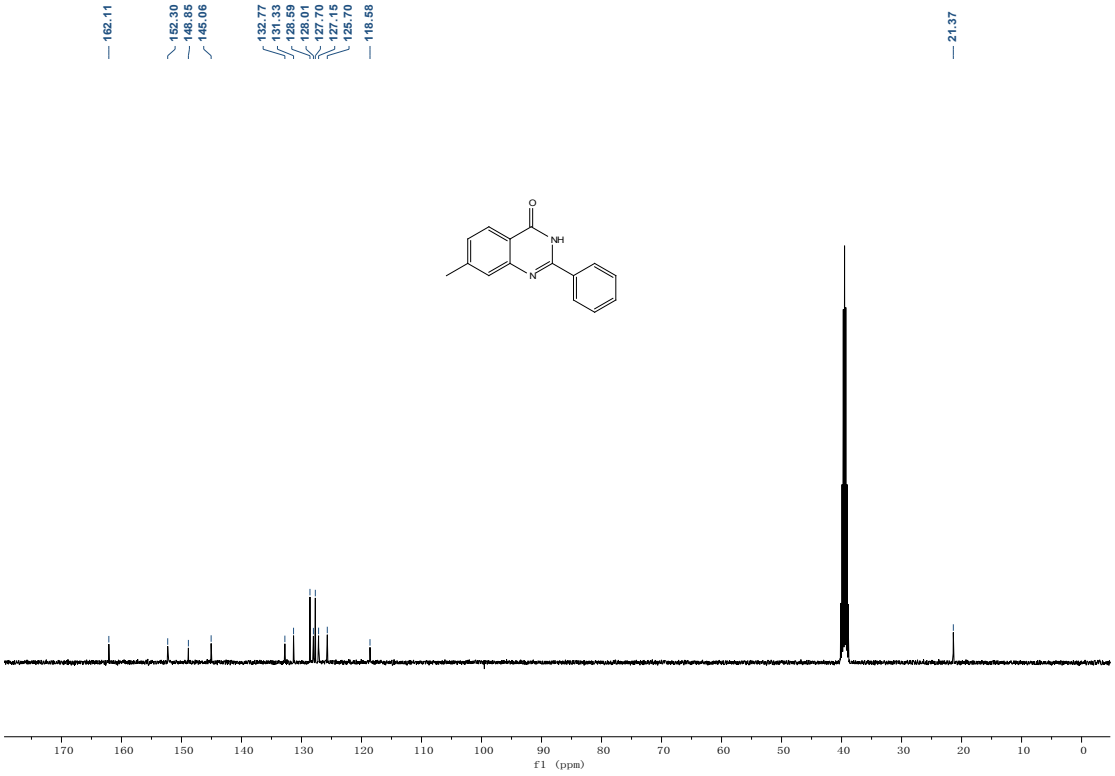

8.78
8.78
8.77
7.85
7.83
7.78
7.59
7.58
7.53
7.53
7.51
7.49
7.48
7.47
7.47
7.45
7.44
7.42
7.42
5.95
5.95
5.94
O
NH
NH
O
N
O
Cl
1.00
0.93
0.98
1.04
4.12
1.06
1.05
f1 (ppm)

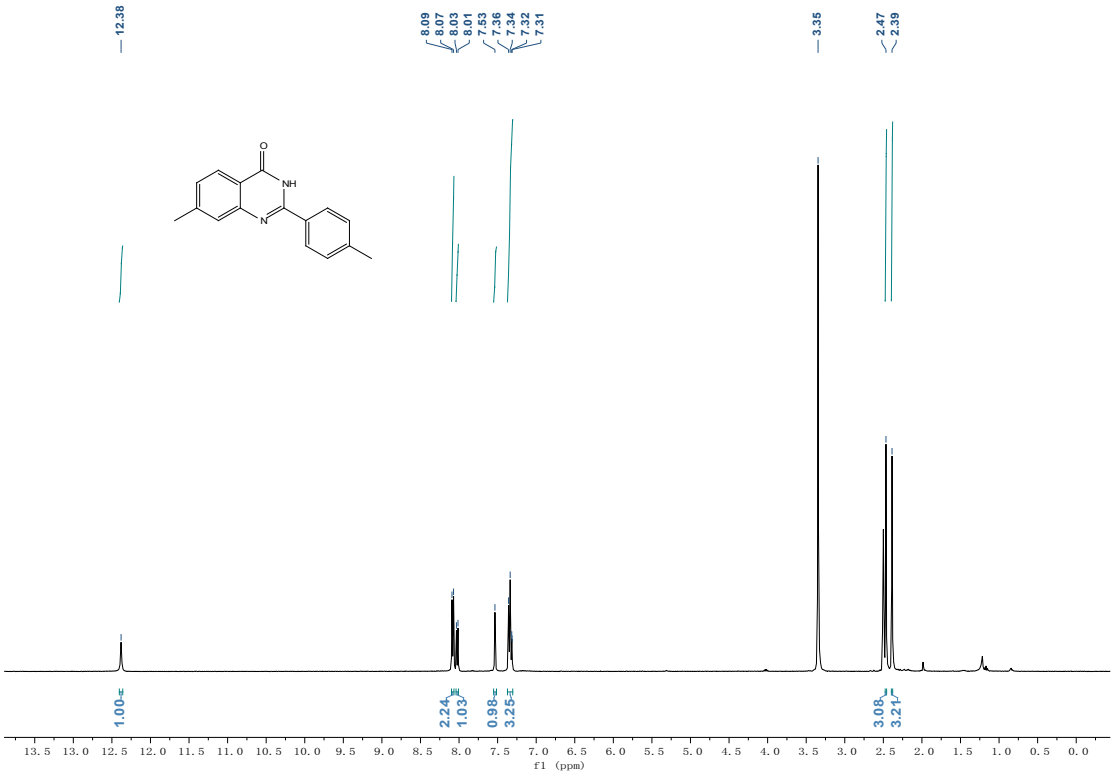

161.81
150.80
148.01
140.04
133.37
129.16
128.68
128.56
119.21
111.19
108.96
65.67
O
NH
NH
O
N
O
Cl
f1 (ppm)

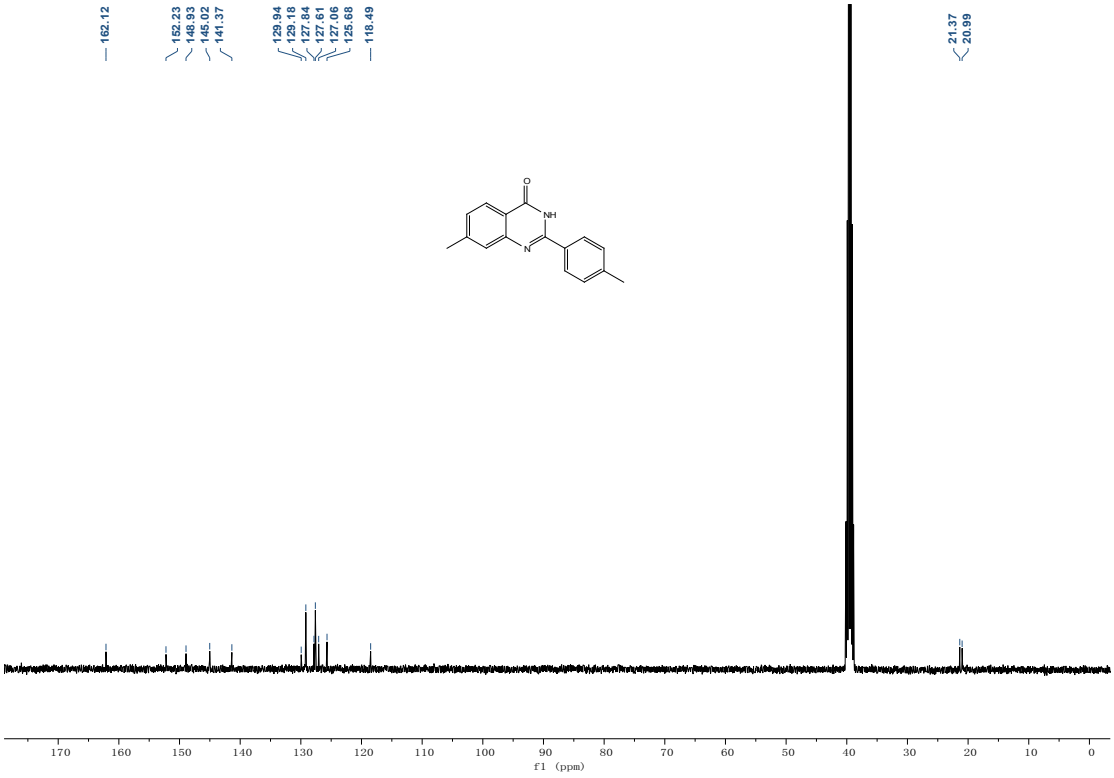

8.66
8.65
8.65
7.89
7.87
7.68
7.65
7.64
7.63
7.62
7.61
7.60
7.54
7.54
7.53
7.52
7.52
7.51
7.50
7.47
7.47
7.45
7.44
7.43
7.43
7.42
7.41
7.40
6.29
6.29
6.28
NH
NH
Cl
1.00
1.01
0.94
0.93
0.98
1.03
1.07
1.84
1.03
f1 (ppm)


161.91
150.84
147.89
137.43
131.81
130.63
129.81
129.15
128.66
127.69
118.85
111.24
109.03
63.81
NH
NH
Cl
f1 (ppm)

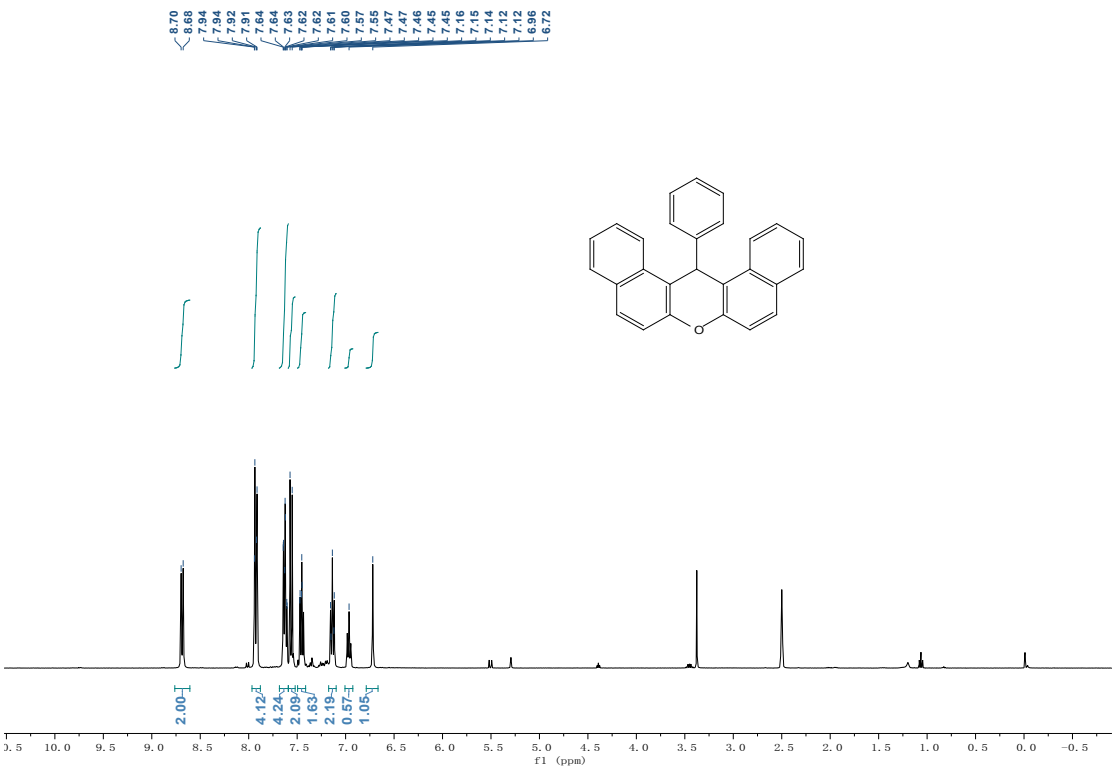

12.45
8.18
8.18
8.17
8.17
8.16
8.16
8.04
8.02
7.60
7.60
7.60
7.59
7.58
7.58
7.57
7.56
7.56
7.54
7.54
7.53
7.52
7.52
7.34
7.34
7.32
7.32
2.46
O
NH
N
1.00
1.94
0.92
3.92
0.98
2.86
f1 (ppm)

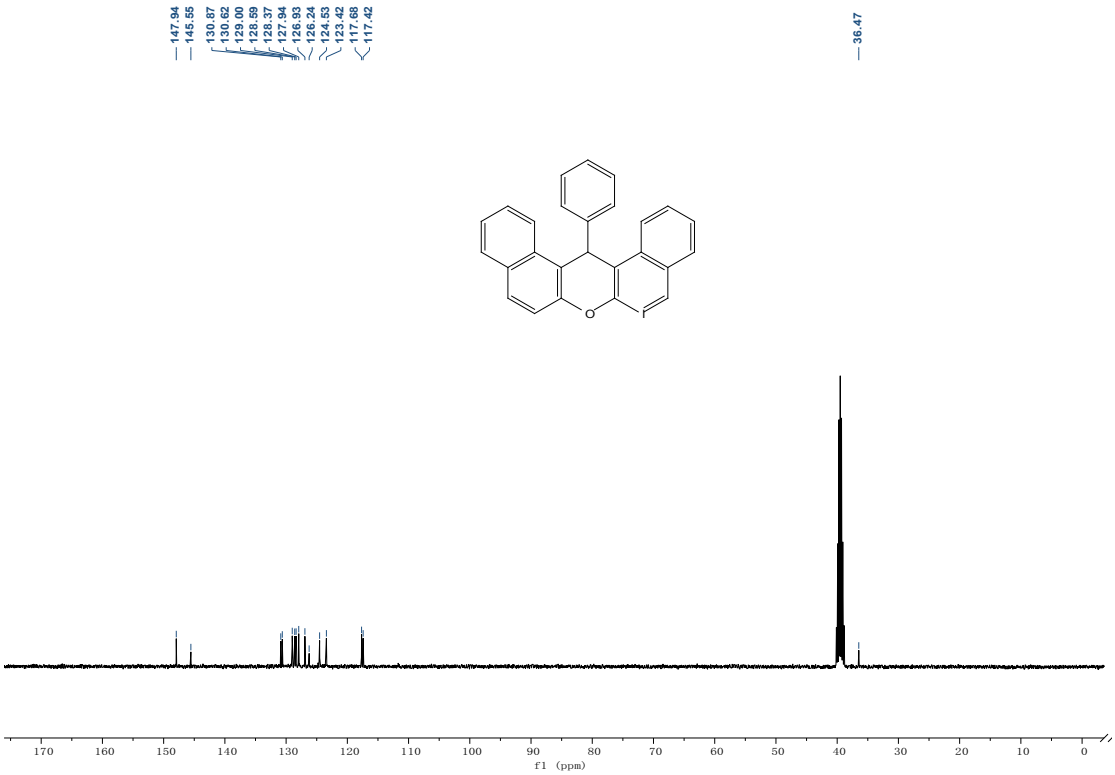

162.11
152.30
148.85
145.06
132.77
131.33
128.59
128.01
127.70
127.15
125.70
118.58
21.37
O
NH
N
f1 (ppm)


12.38
8.09
8.07
8.03
8.01
7.53
7.36
7.34
7.32
7.31
3.35
2.47
2.39
O
NH
N
1.00
2.24
1.03
0.98
3.25
3.08
3.21
f1 (ppm)

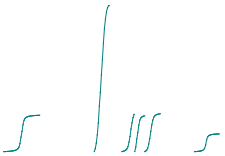

162.12
152.23
148.93
145.02
141.37
129.94
129.18
127.84
127.61
127.06
125.68
118.49
21.37
20.99
O
NH
N
f1 (ppm)

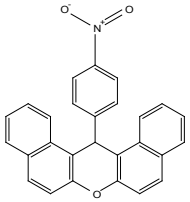
# $^{1}$H-NMR and $^{13}$C-NMR spectrum of compound 5a-5p

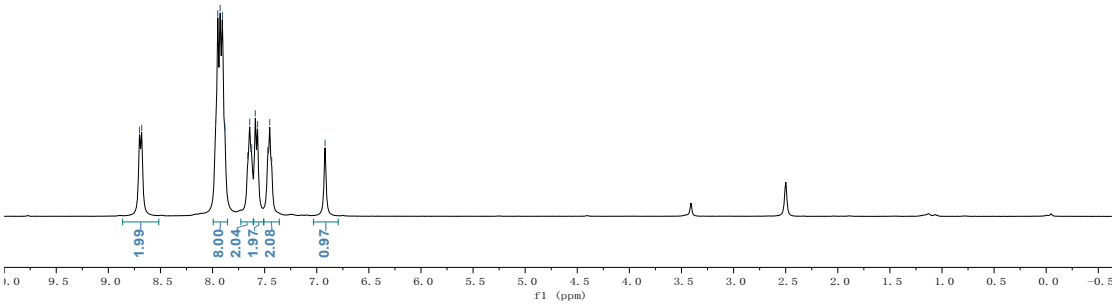


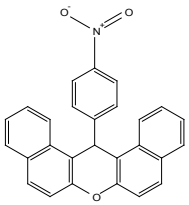

8.70
8.68
7.97
7.95
7.93
7.91
7.88
7.66
7.64
7.62
7.59
7.57
7.47
7.45
7.43
6.92

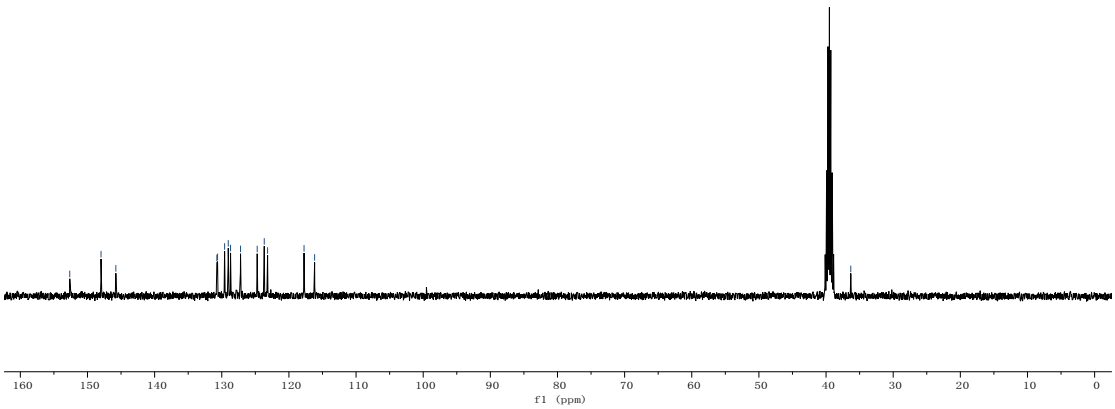


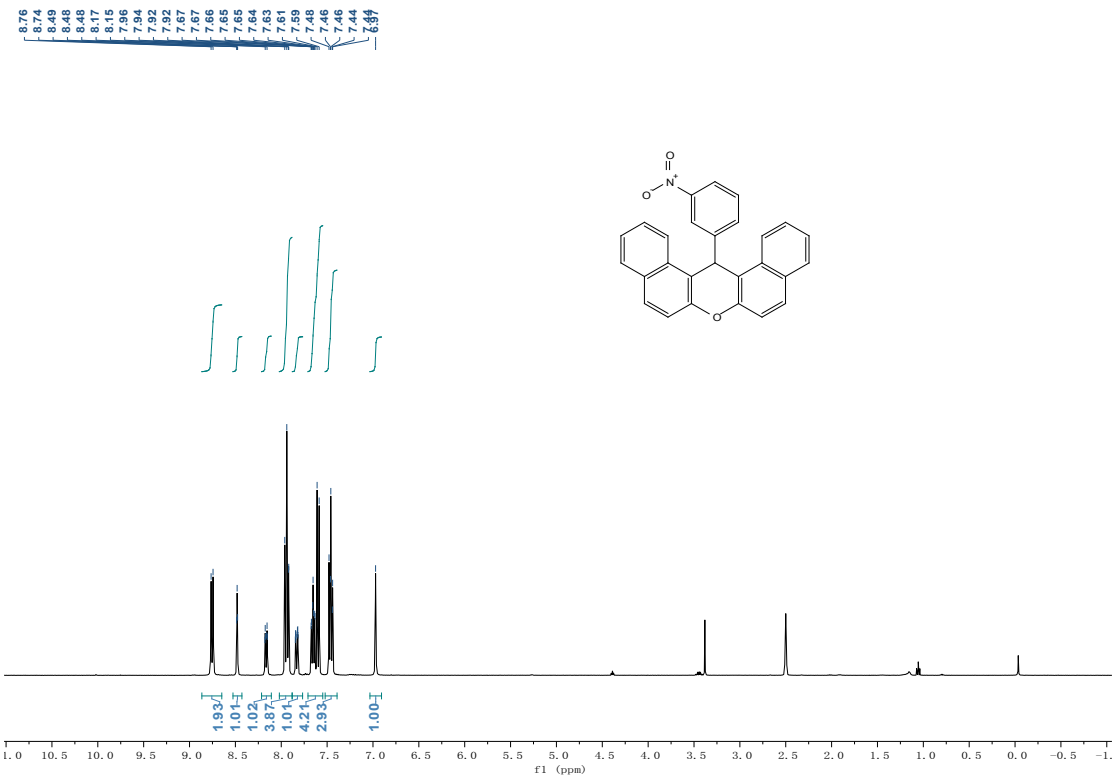



1.99
8.00
2.04
1.97
2.08
0.97
f1 (ppm)


152.64
147.98
145.77
130.73
130.63
129.58
129.03
128.69
127.20
124.72
123.67
123.18
117.75
116.17
36.32




f1 (ppm)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8.17
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7.94
7.92
7.92
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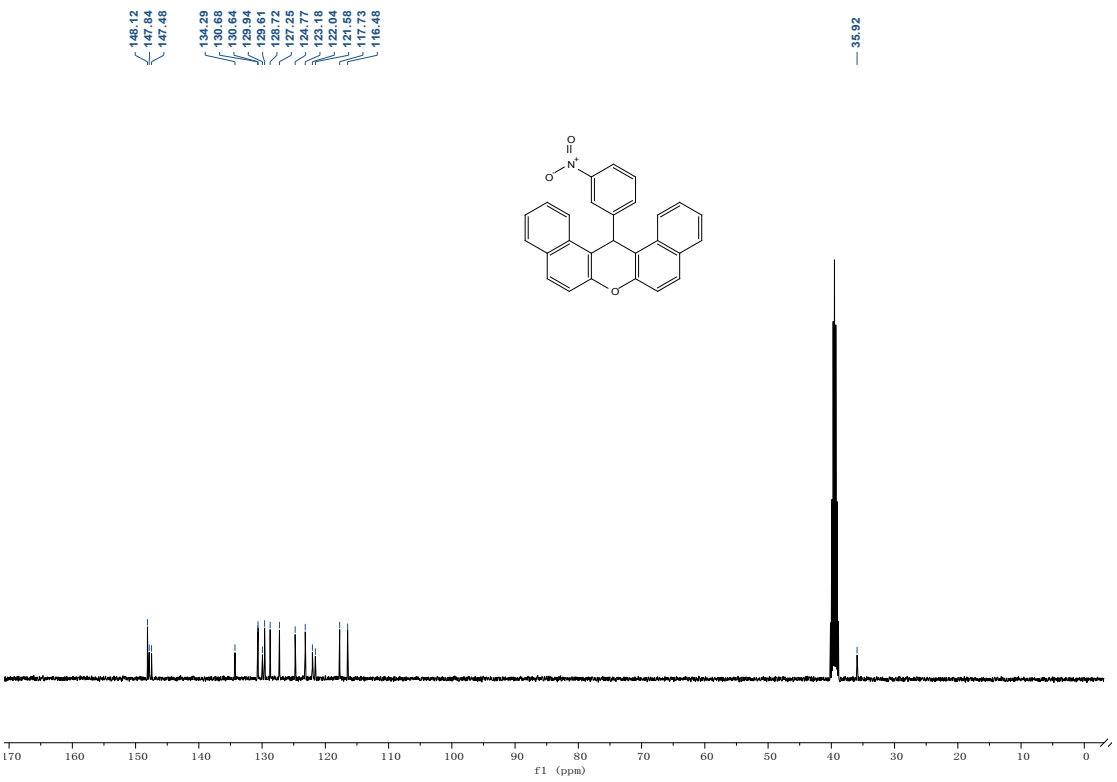
7.67
7.66
7.65
7.65
7.64
7.63
7.61
7.59
7.48
7.46
7.46
7.44
7.44
6.94
1.93
1.01
1.02
3.87
1.01
4.21
2.93
1.00
f1 (ppm)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147.84
147.48
134.29
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130.64
129.94
129.61
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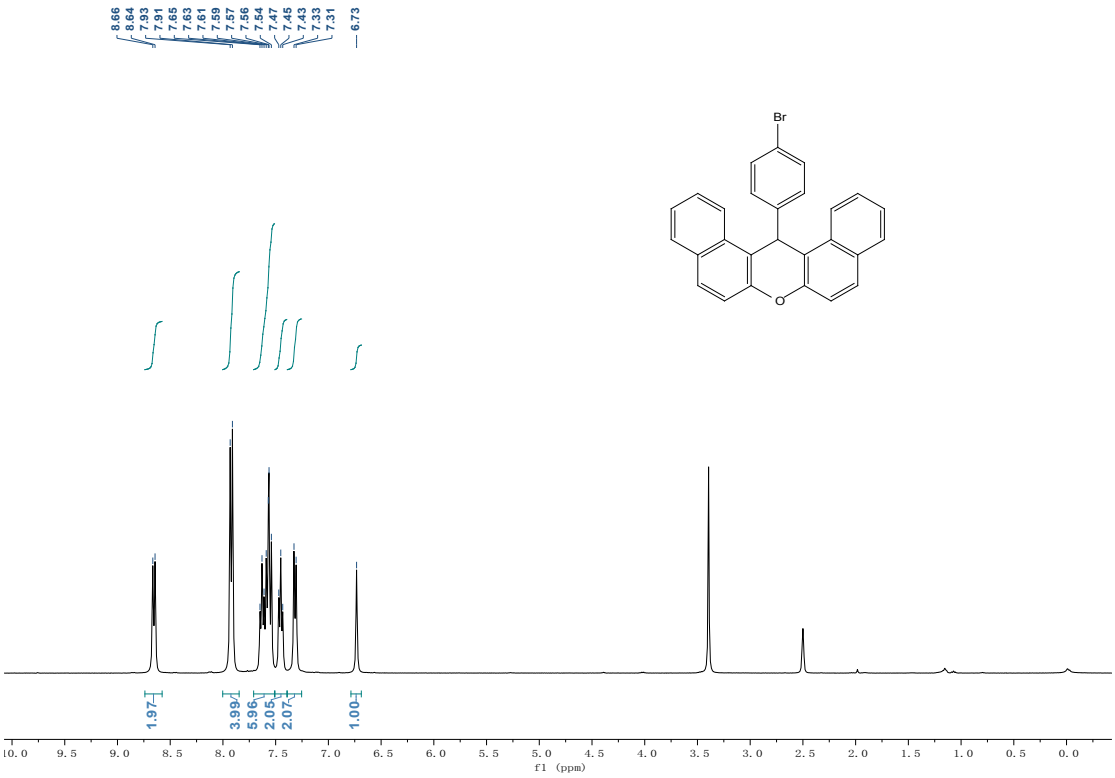
127.25
124.77
123.18
122.04
121.58
117.73
116.48
35.92
f1 (ppm)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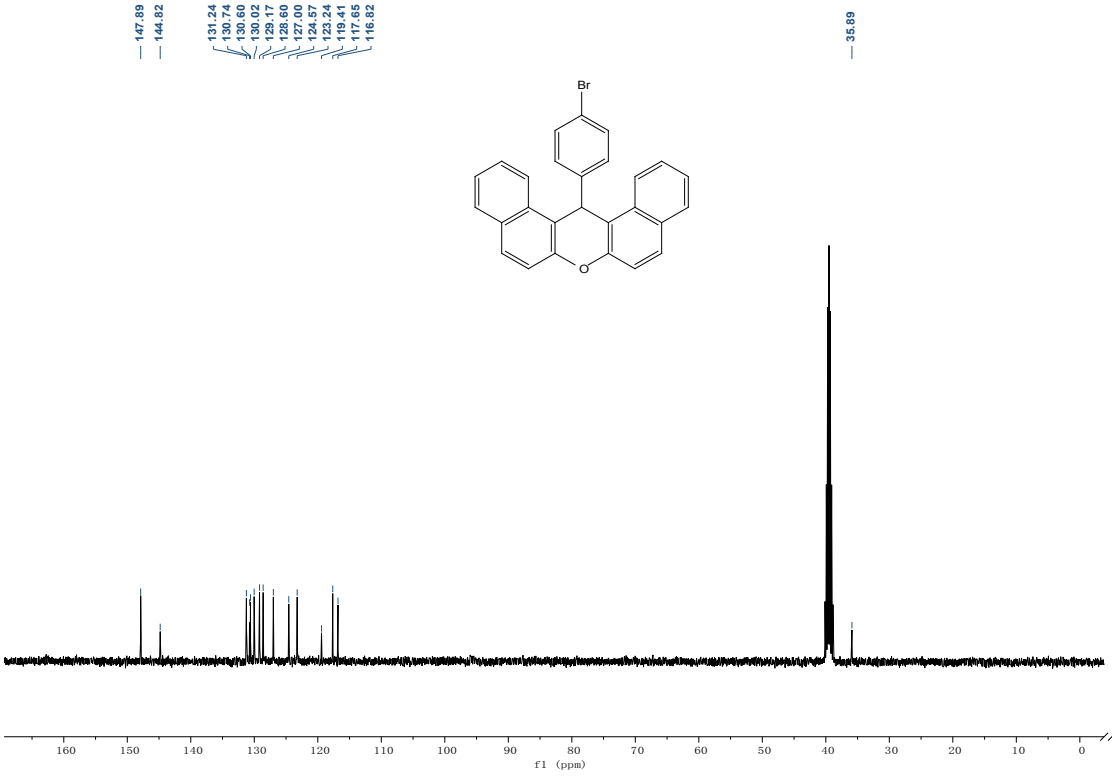
7.63
7.61
7.59
7.57
7.56
7.54
7.47
7.45
7.43
7.33
7.31
6.73
Br
O
1.97
3.99
5.96
2.05
2.07
1.00
f1 (ppm)


147.89
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130.60
130.02
129.17
128.60
127.00
124.57
123.24
119.41
117.65
116.82
35.89
Br
O
f1 (ppm)


8.69
8.67
7.92
7.91
7.90
7.89
7.62
7.62
7.61
7.60
7.60
7.58
7.58
7.52
7.49
7.47
7.46
7.46
7.45
7.44
7.44
7.43
7.38
7.36
7.36
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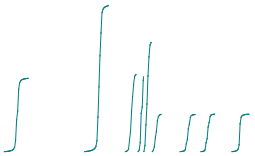
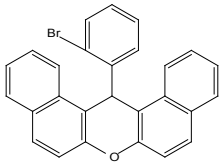
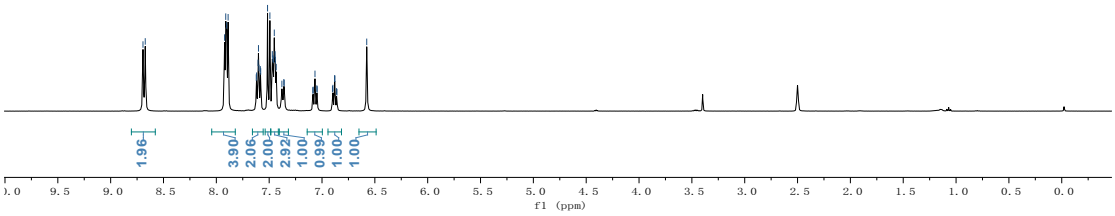
6.90
6.88
6.88
6.86
6.86
6.58




Br
O


1.96
3.90
2.06
2.00
2.92
1.00
0.99
1.00
1.00
f1 (ppm)


148.19
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133.25
131.76
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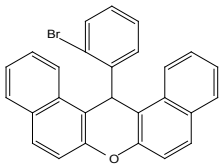
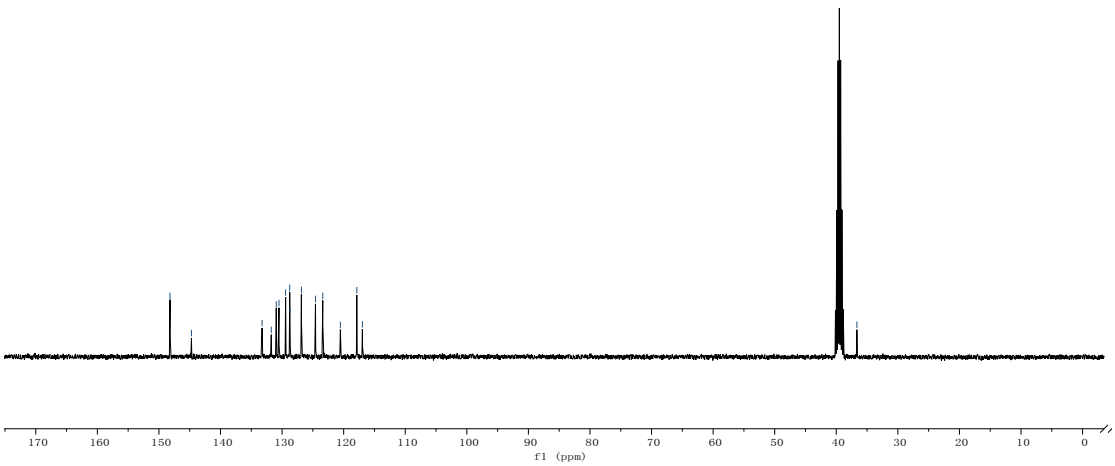
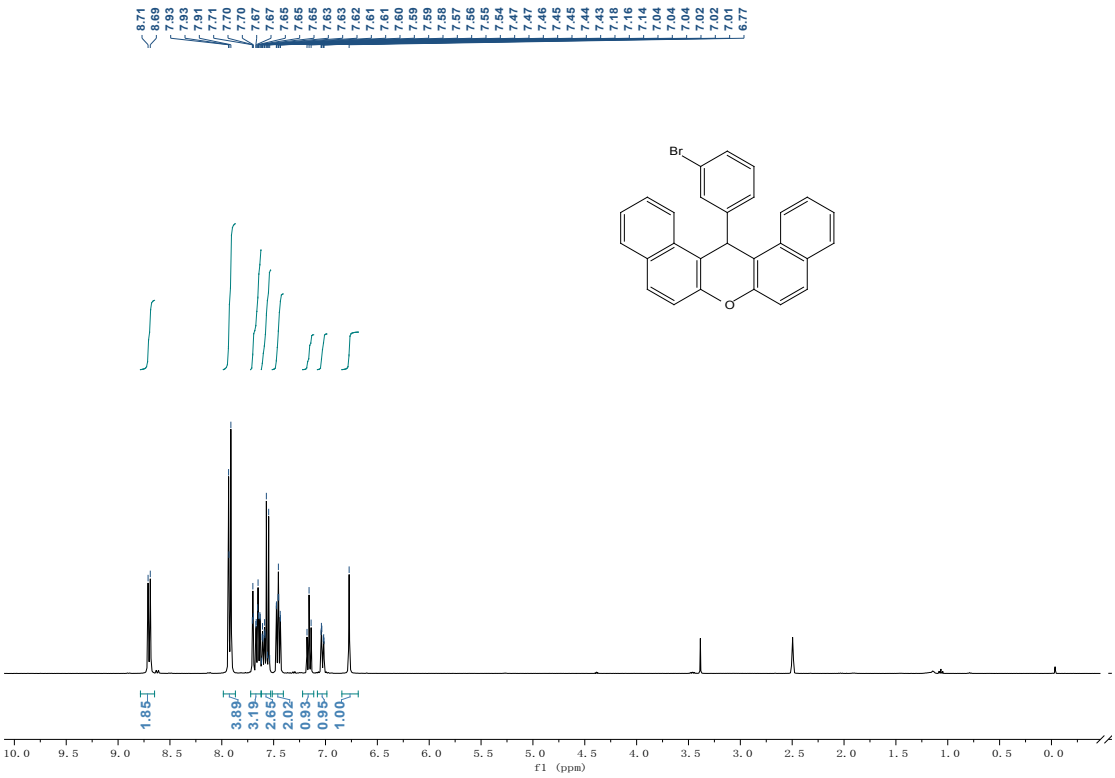
124.58
123.39
120.53
117.86
116.96


36.65


Br
O


f1 (ppm)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7.93
7.93
7.91
7.71
7.70
7.70
7.67
7.67
7.65
7.65
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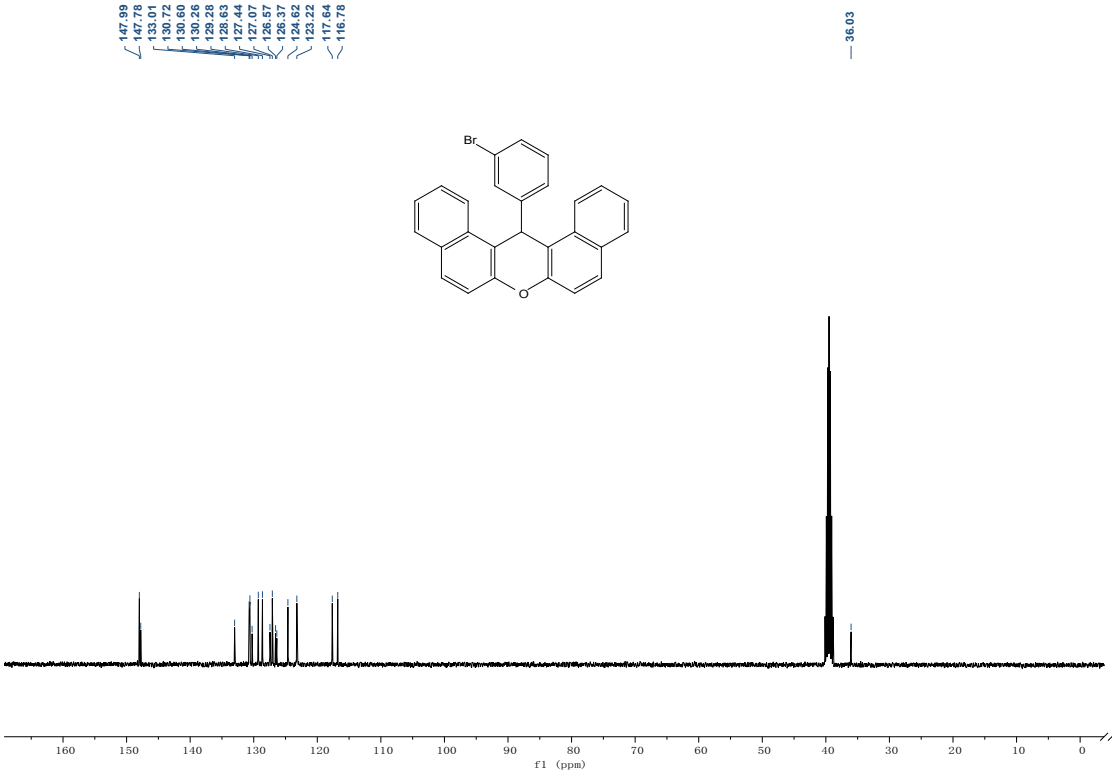
7.63
7.63
7.62
7.61
7.61
7.60
7.59
7.59
7.58
7.57
7.56
7.55
7.54
7.47
7.47
7.46
7.45
7.45
7.44
7.43
7.18
7.16
7.14
7.04
7.04
7.04
7.02
7.02
7.01
6.77
Br
O
1.85
3.89
3.19
2.65
2.02
0.93
0.95
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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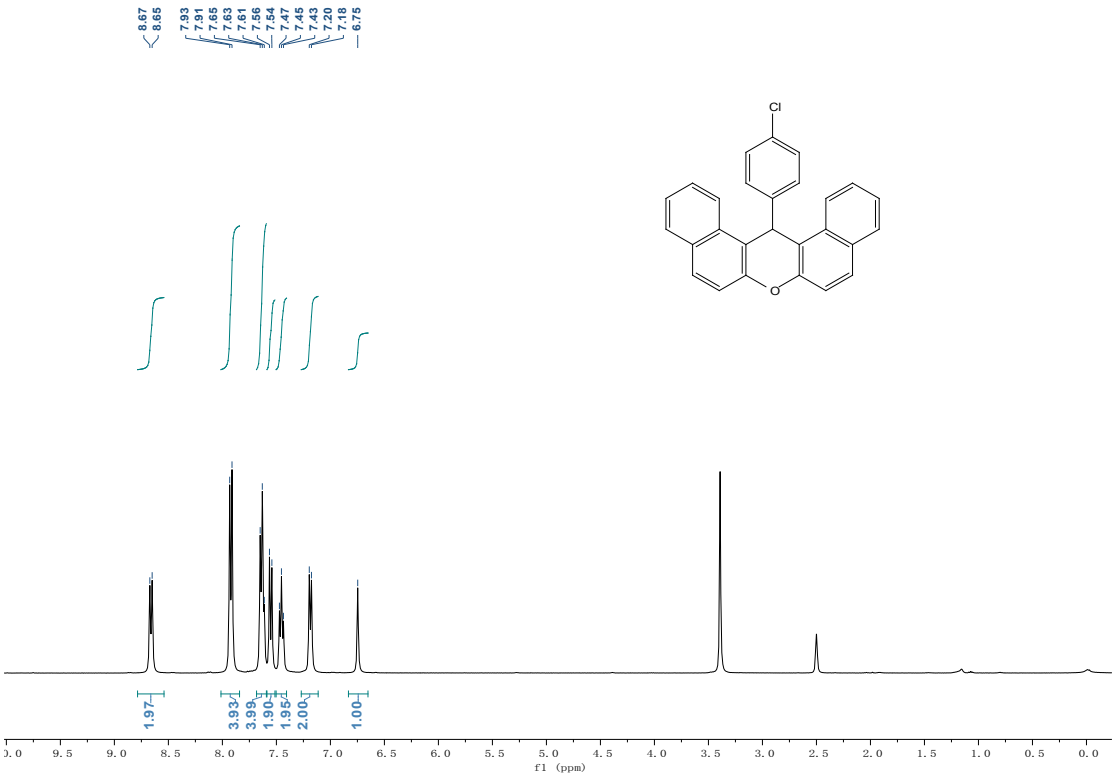
147.78
133.01
130.72
130.60
130.26
129.28
128.63
127.44
127.07
126.57
126.37
124.62
123.22
117.64
116.78
36.03
Br
O
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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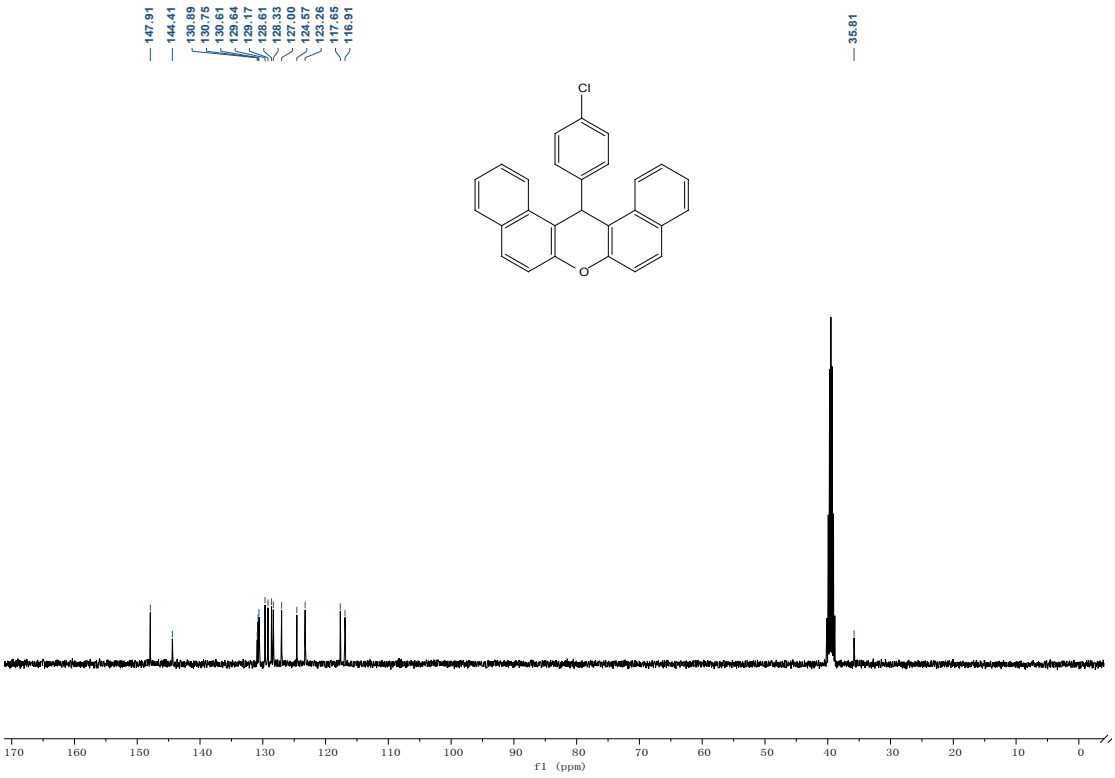
8.65
7.93
7.91
7.65
7.63
7.61
7.56
7.54
7.47
7.45
7.43
7.20
7.18
6.75
Cl
O
1.97
3.93
3.99
1.90
1.95
2.00
1.00
f1 (ppm)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130.89
130.75
130.61
129.64
129.17
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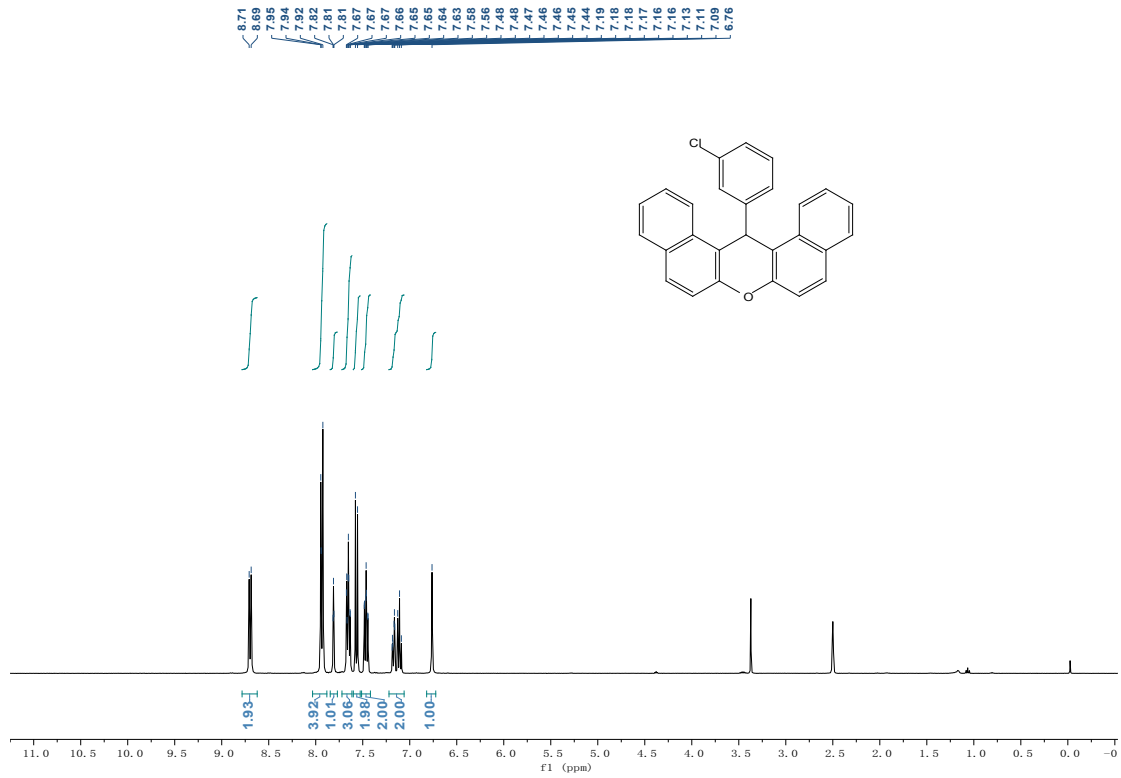
128.33
127.00
124.57
123.26
117.65
116.91
35.81
Cl
O
f1 (ppm)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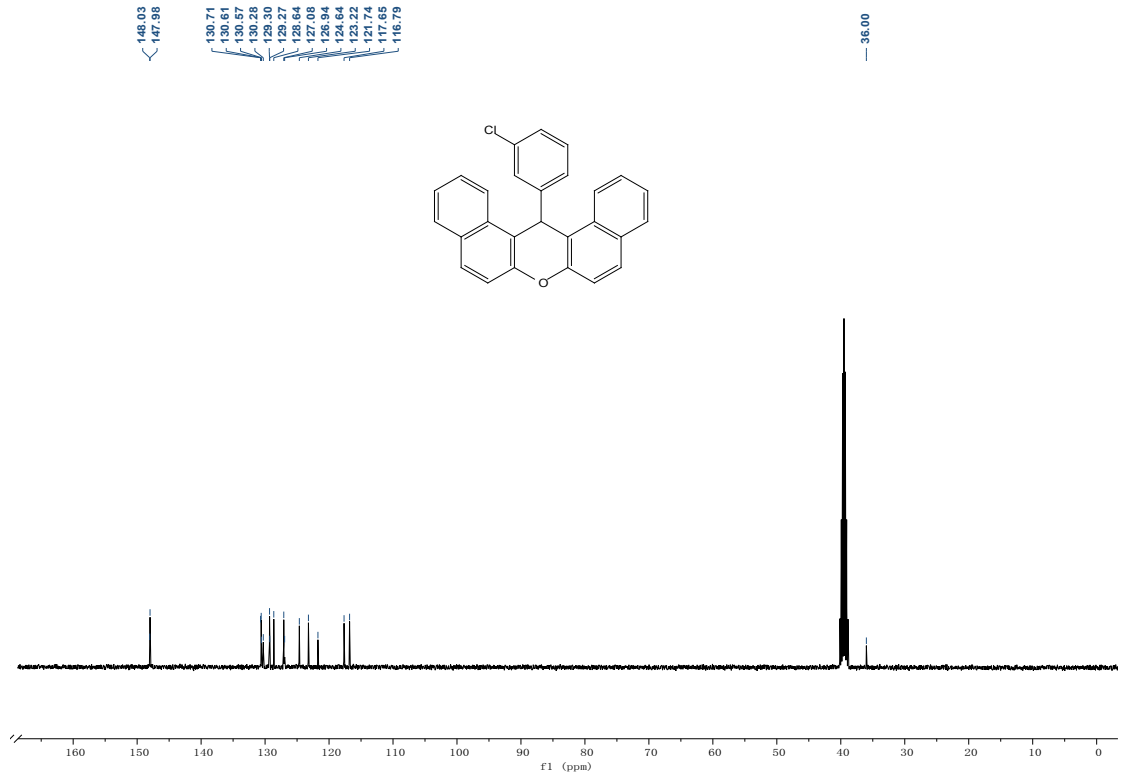
8.69
7.95
7.94
7.92
7.82
7.81
7.81
7.67
7.67
7.67
7.66
7.65
7.65
7.64
7.63
7.58
7.56
7.48
7.48
7.47
7.46
7.46
7.45
7.44
7.19
7.18
7.18
7.17
7.16
7.16
7.13
7.11
7.09
6.76
Cl
O
1.93
3.92
1.01
3.06
1.98
2.00
2.00
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0
f1 (ppm)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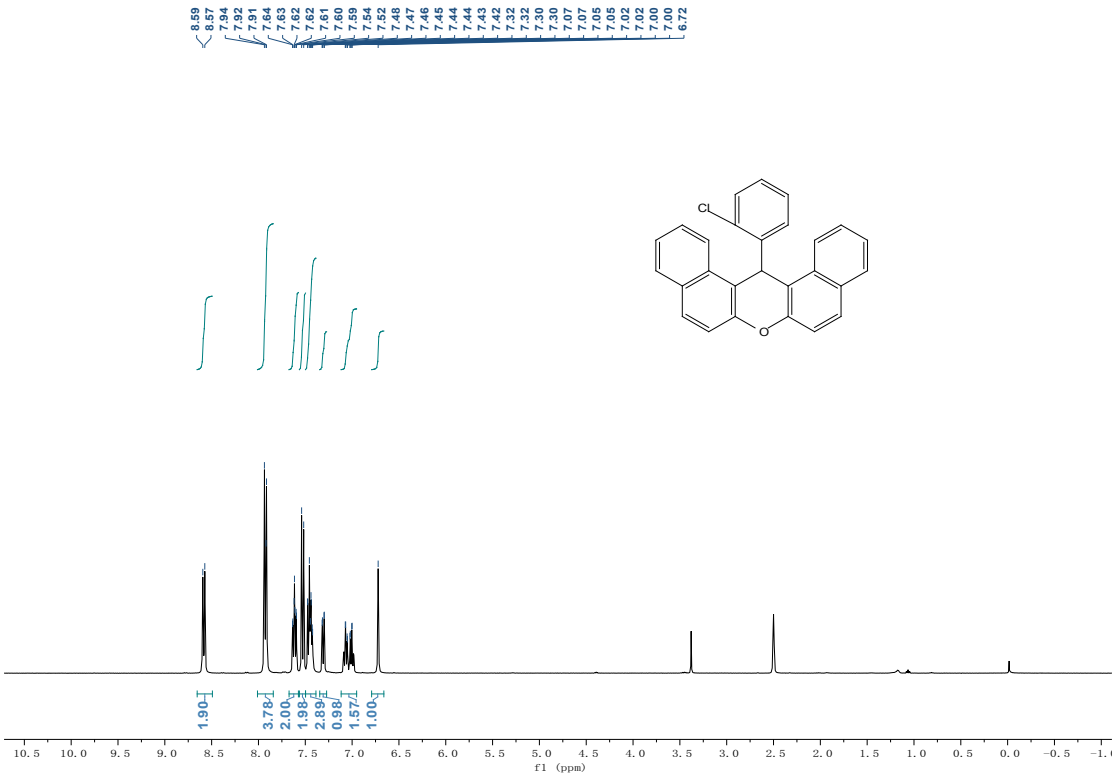
147.98
130.71
130.61
130.57
130.28
129.30
129.27
128.64
127.08
126.94
124.64
123.22
121.74
117.65
116.79
36.00
Cl
O
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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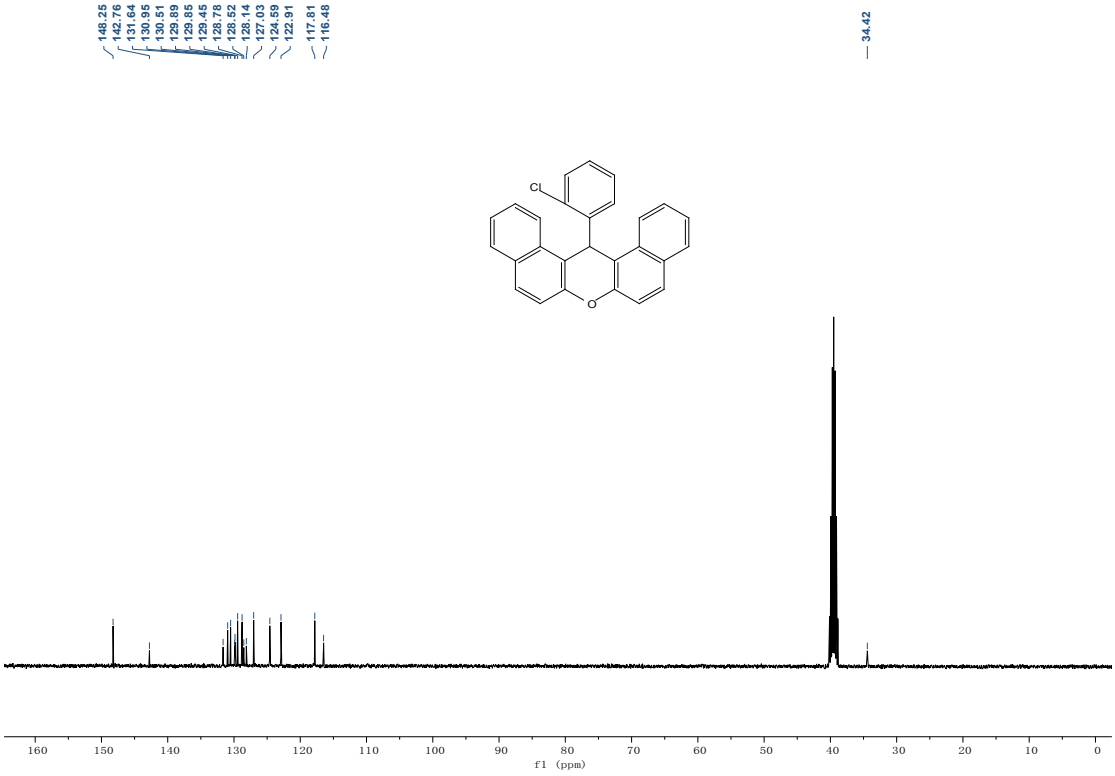
8.57
7.94
7.92
7.91
7.64
7.63
7.62
7.62
7.61
7.60
7.59
7.54
7.52
7.48
7.47
7.46
7.45
7.44
7.44
7.43
7.42
7.32
7.30
7.30
7.07
7.07
7.05
7.05
7.02
7.02
7.00
7.00
6.72
Cl
O
1.90
3.78
2.00
1.98
2.89
0.98
1.57
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)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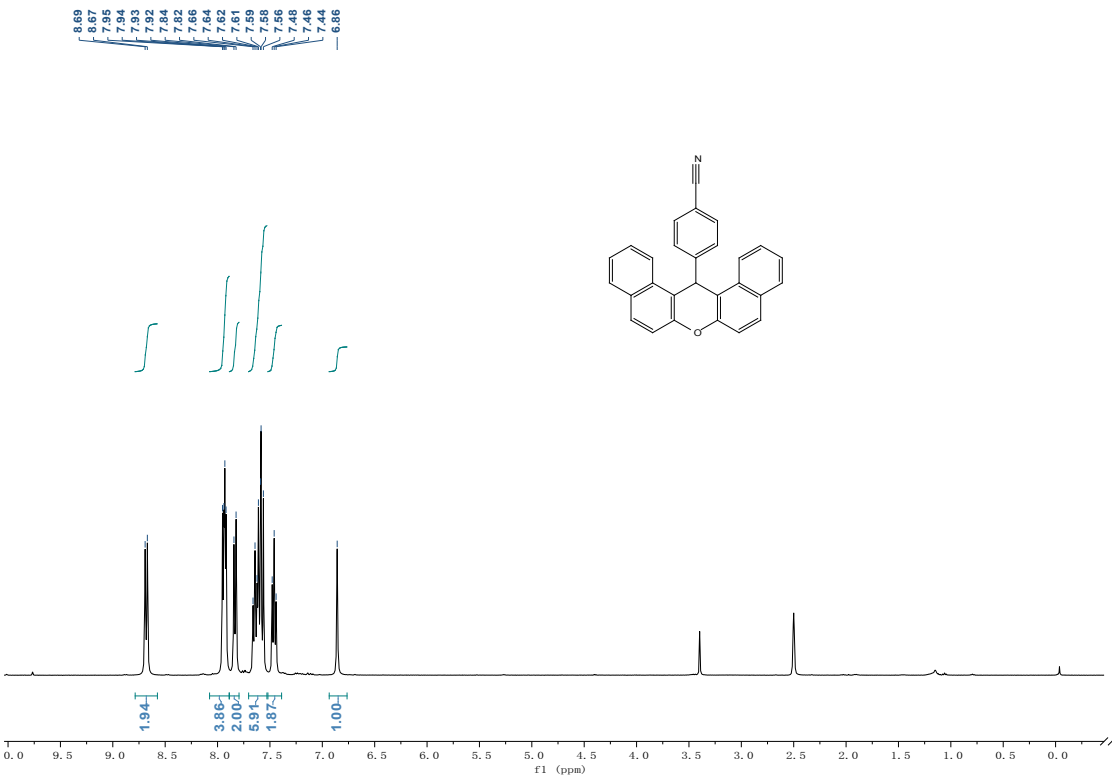
142.76
131.64
130.95
130.51
129.89
129.85
129.45
128.78
128.52
128.14
127.03
124.59
122.91
117.81
116.48
34.42
Cl
O
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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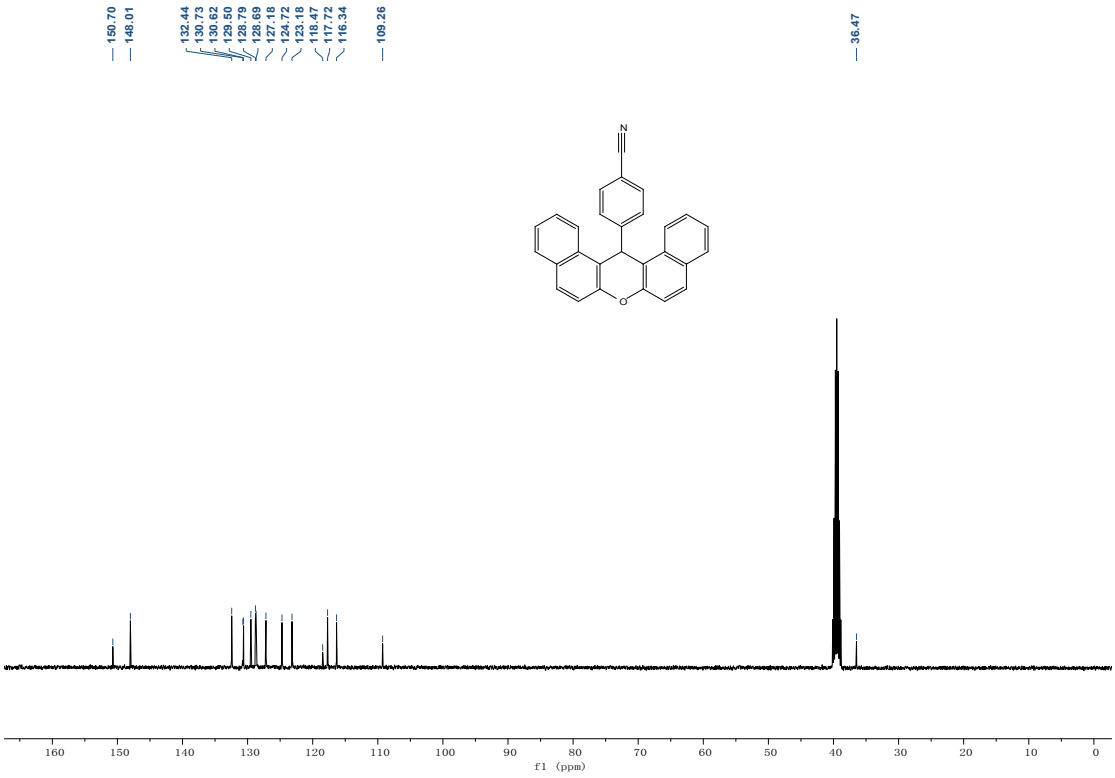
7.95
7.94
7.93
7.92
7.84
7.82
7.66
7.64
7.62
7.61
7.59
7.58
7.56
7.48
7.46
7.44
6.86
N
O
1.94
3.86
2.00
5.91
1.87
1.00
f1 (ppm)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130.62
129.50
128.79
128.69
127.18
124.72
123.18
118.47
117.72
116.34
109.26
36.47
N
O
f1 (ppm)


8.70
8.68
7.94
7.94
7.92
7.92
7.91
7.68
7.68
7.67
7.66
7.66
7.65
7.65
7.64
7.64
7.63
7.62
7.61
7.57
7.55
7.48
7.48
7.46
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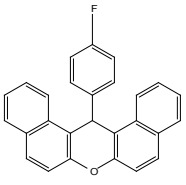
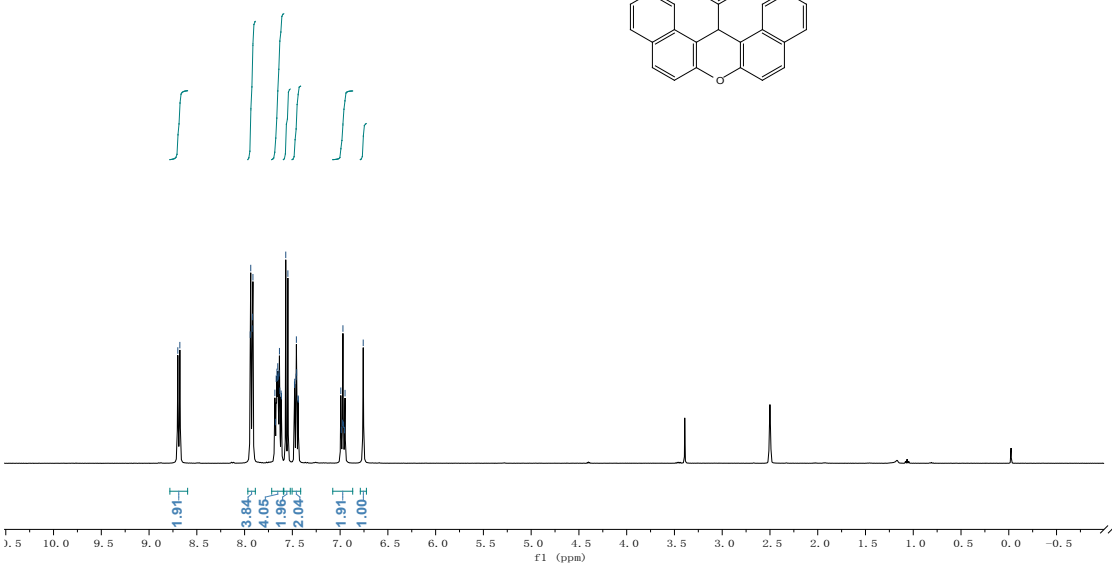
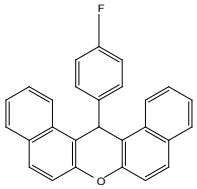
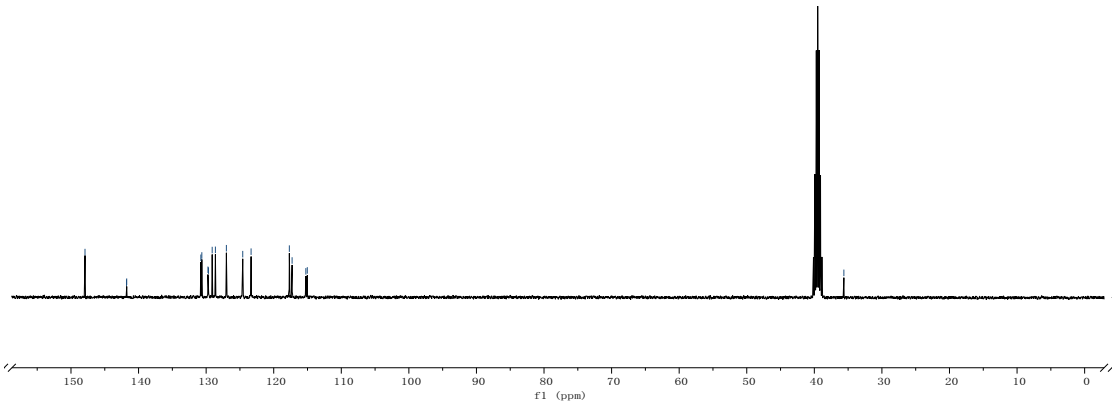
6.98
6.97
6.96
6.95
6.95
6.76

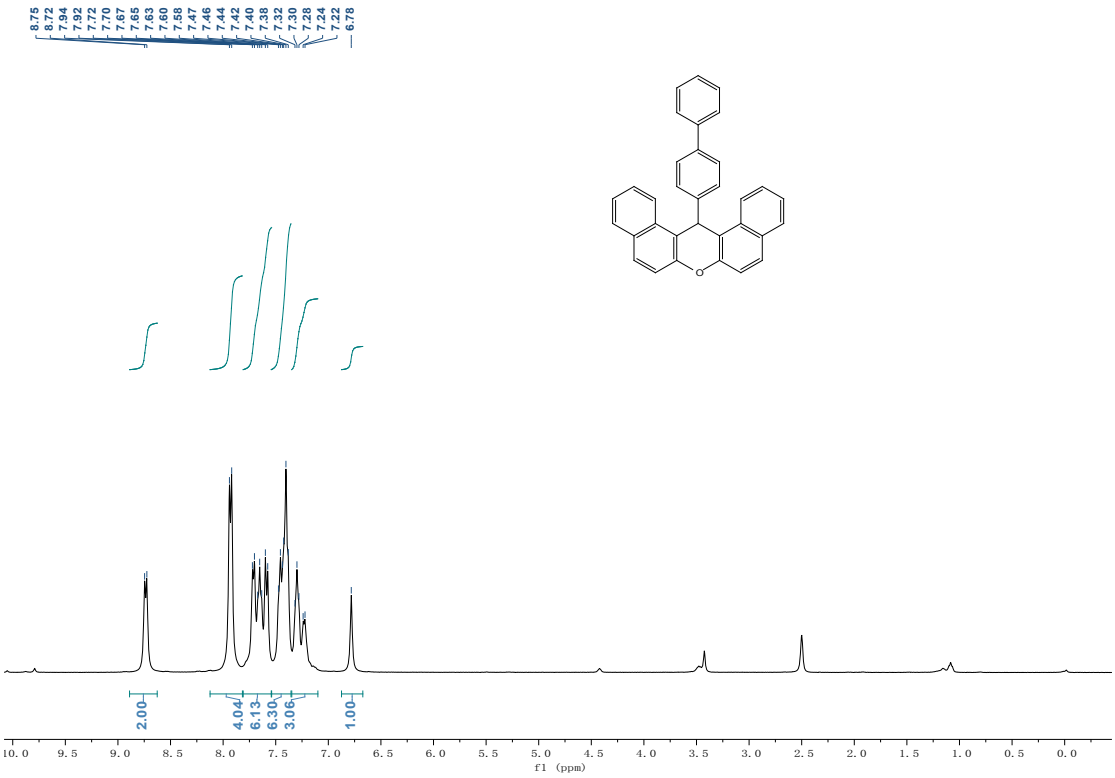

F
O


1.91
3.84
4.05
1.96
2.04
1.91
1.00
f1 (ppm)


147.93
141.79
141.75
130.78
130.64
129.73
129.65
129.10
128.63
127.00
124.58
123.35
117.69
117.28
115.24
115.03
35.63


F
O


f1 (ppm)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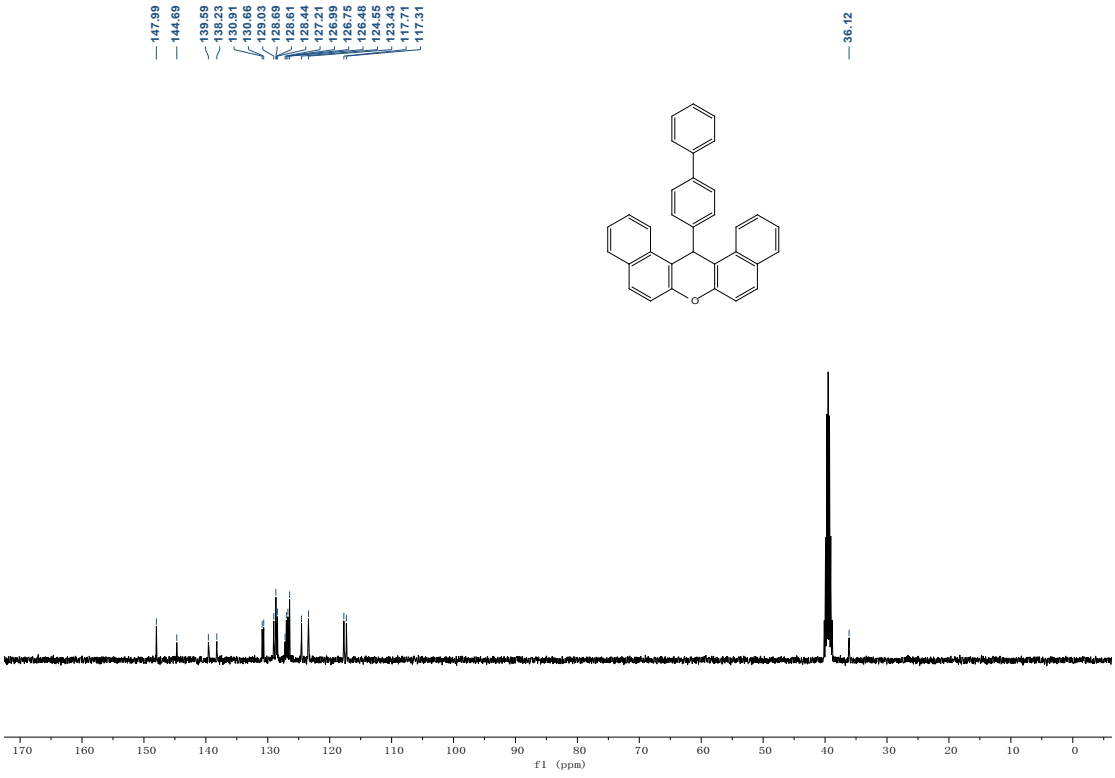
7.94
7.92
7.72
7.70
7.67
7.65
7.63
7.60
7.58
7.47
7.46
7.44
7.42
7.40
7.38
7.32
7.30
7.28
7.24
7.22
6.78
O
2.00
4.04
6.13
6.30
3.06
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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144.69
139.59
138.23
130.91
130.66
129.03
128.69
128.61
128.44
127.21
126.99
126.75
126.48
124.55
123.43
117.71
117.31
36.12
O
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.67
8.65
7.93
7.93
7.92
7.91
7.91
7.90
7.64
7.63
7.62
7.62
7.61
7.60
7.60
7.56
7.54
7.50
7.50
7.48
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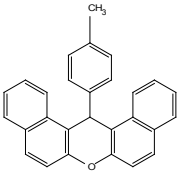
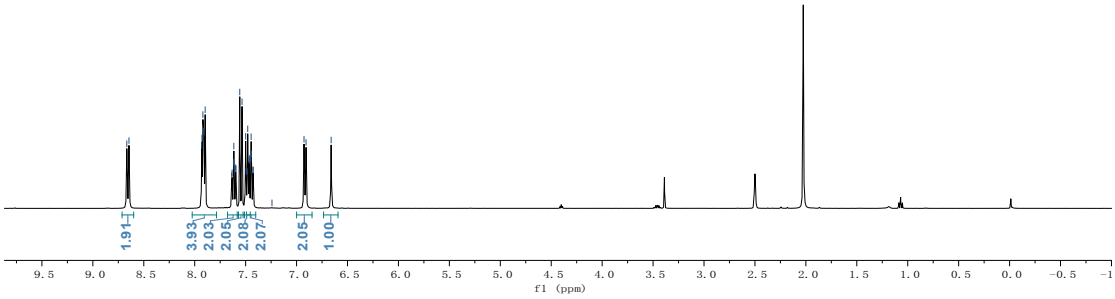
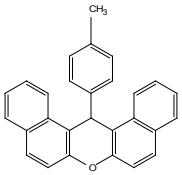
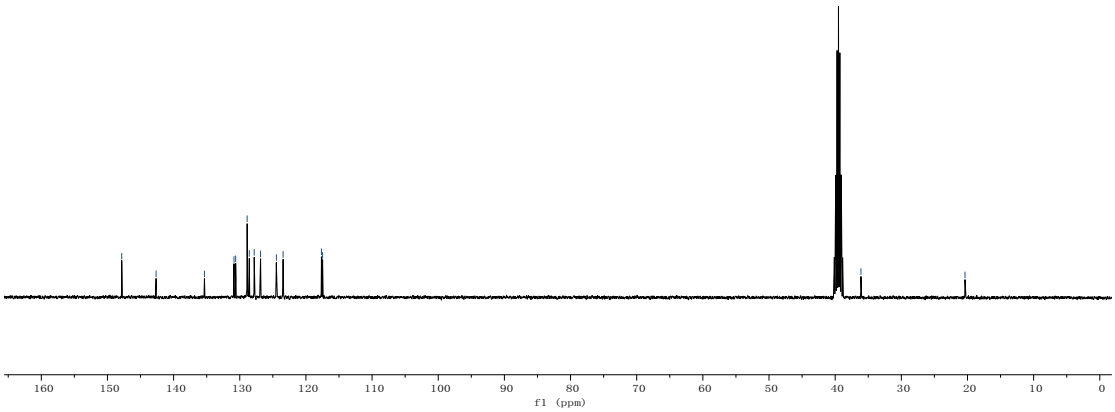
7.43
7.43
7.24
6.93
6.91
6.66


CH3
O


1.91
3.93
2.03
2.05
2.08
2.07
2.05
1.00
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
f1 (ppm)


147.84
142.65
135.34
130.87
130.62
128.88
128.56
127.81
126.86
124.47
123.45
117.65
117.48
36.10
20.37


CH3
O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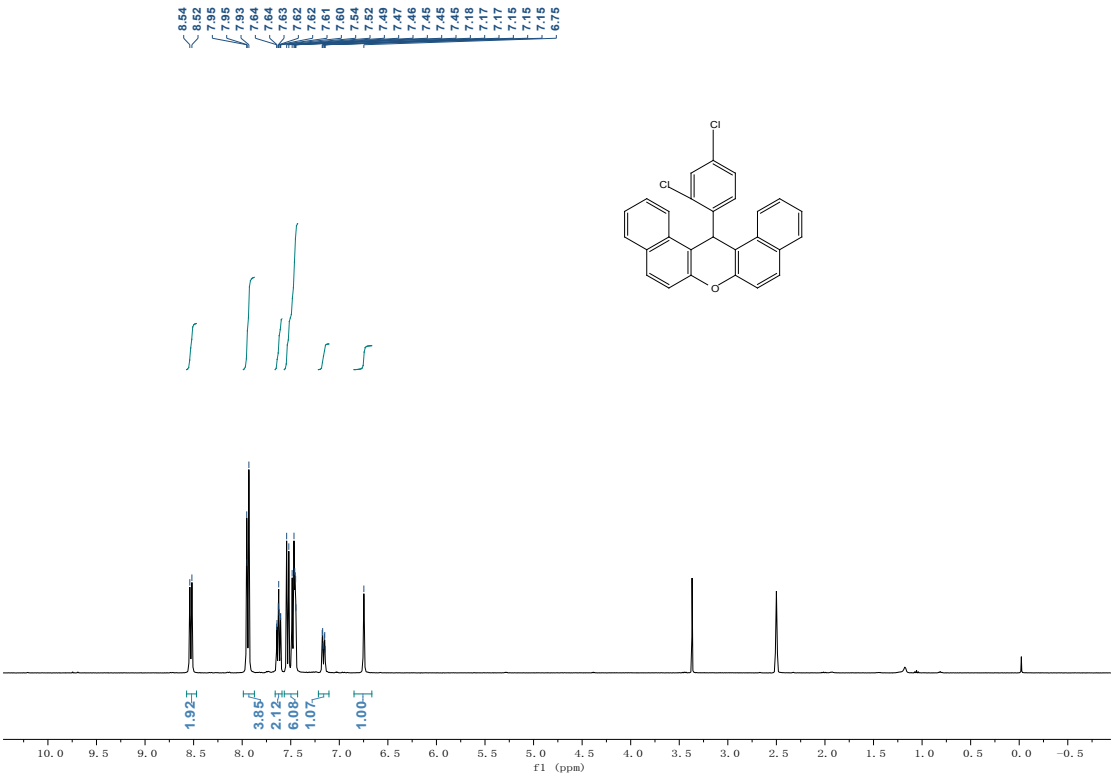
f1 (ppm)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8.52
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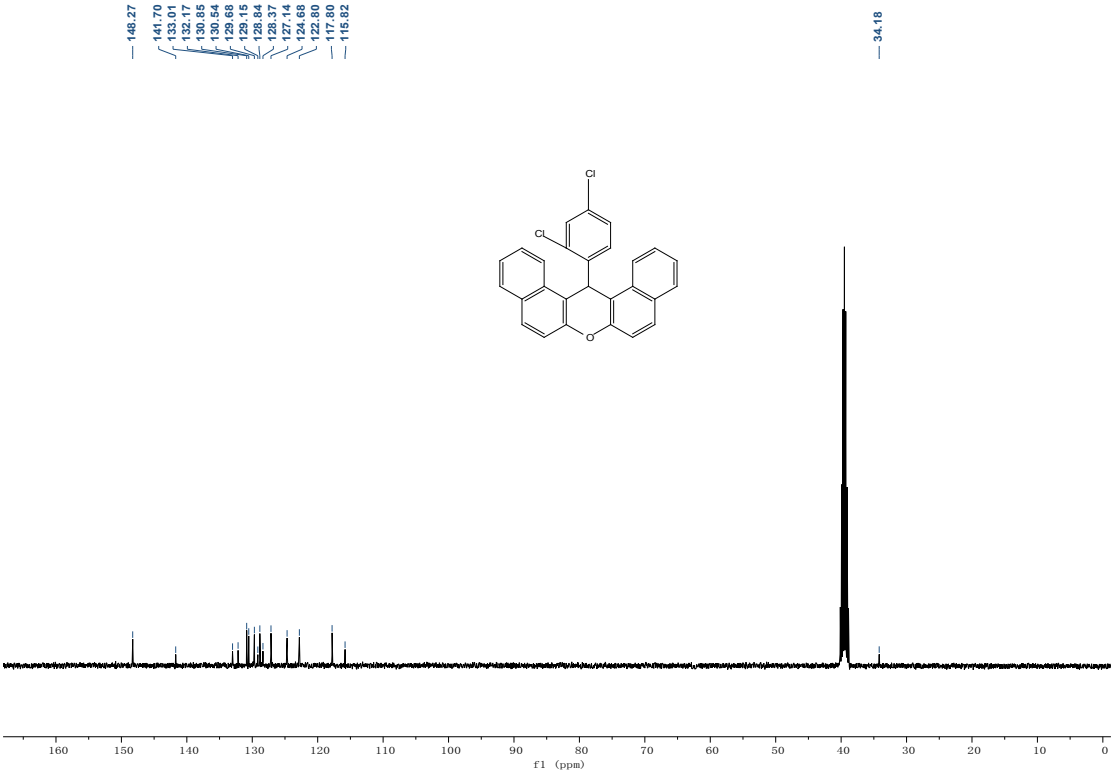
7.95
7.93
7.64
7.64
7.63
7.62
7.62
7.61
7.60
7.54
7.52
7.49
7.47
7.46
7.45
7.45
7.45
7.18
7.17
7.17
7.15
7.15
7.15
6.75
Cl
Cl
O
1.92
3.85
2.12
6.08
1.07
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)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141.70
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132.17
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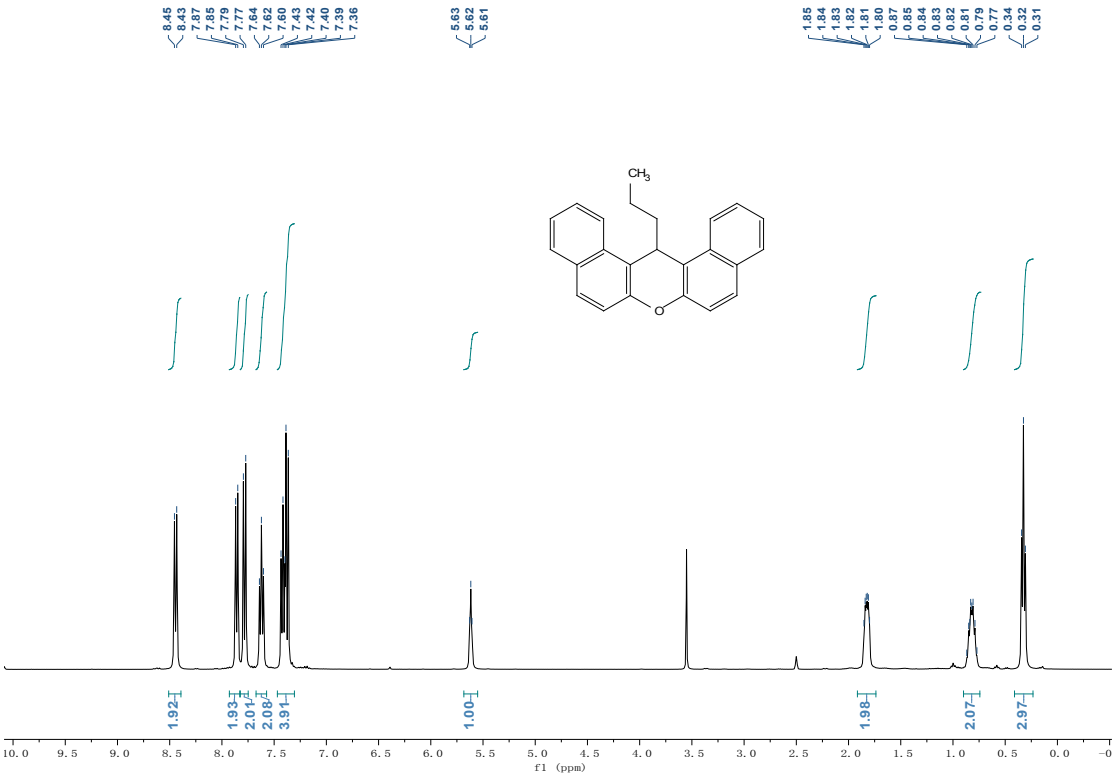
130.54
129.68
129.15
128.84
128.37
127.14
124.68
122.80
117.80
115.82
34.18
Cl
Cl
O
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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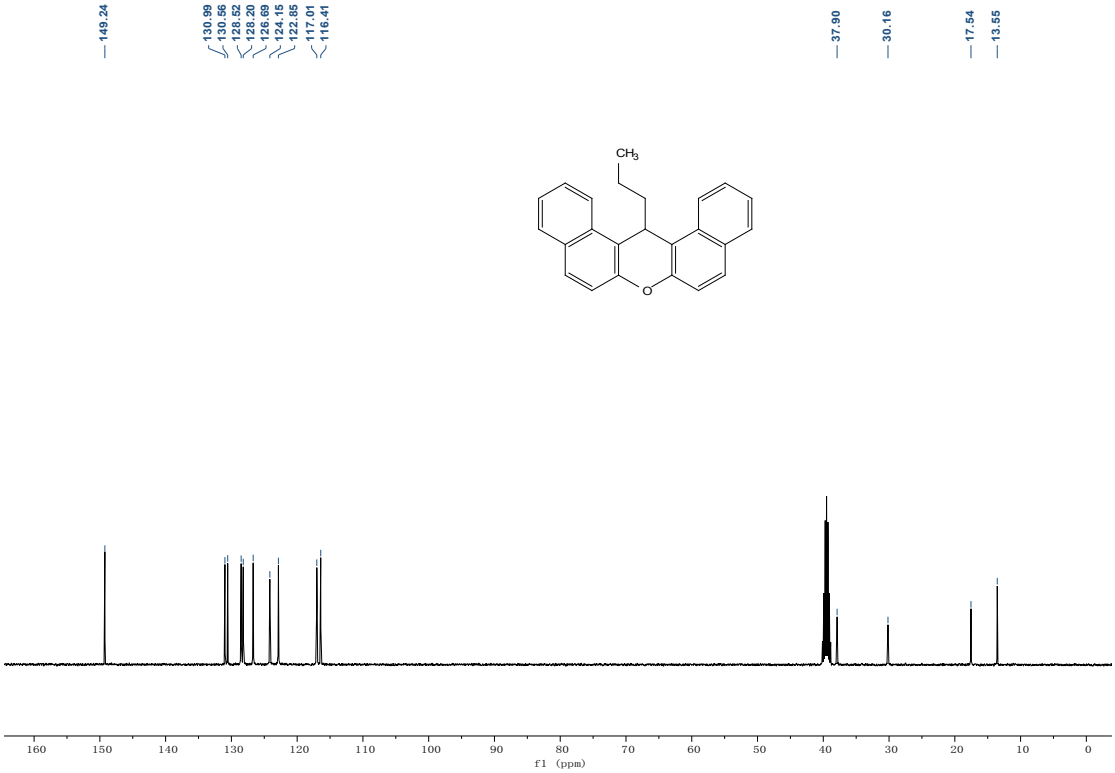
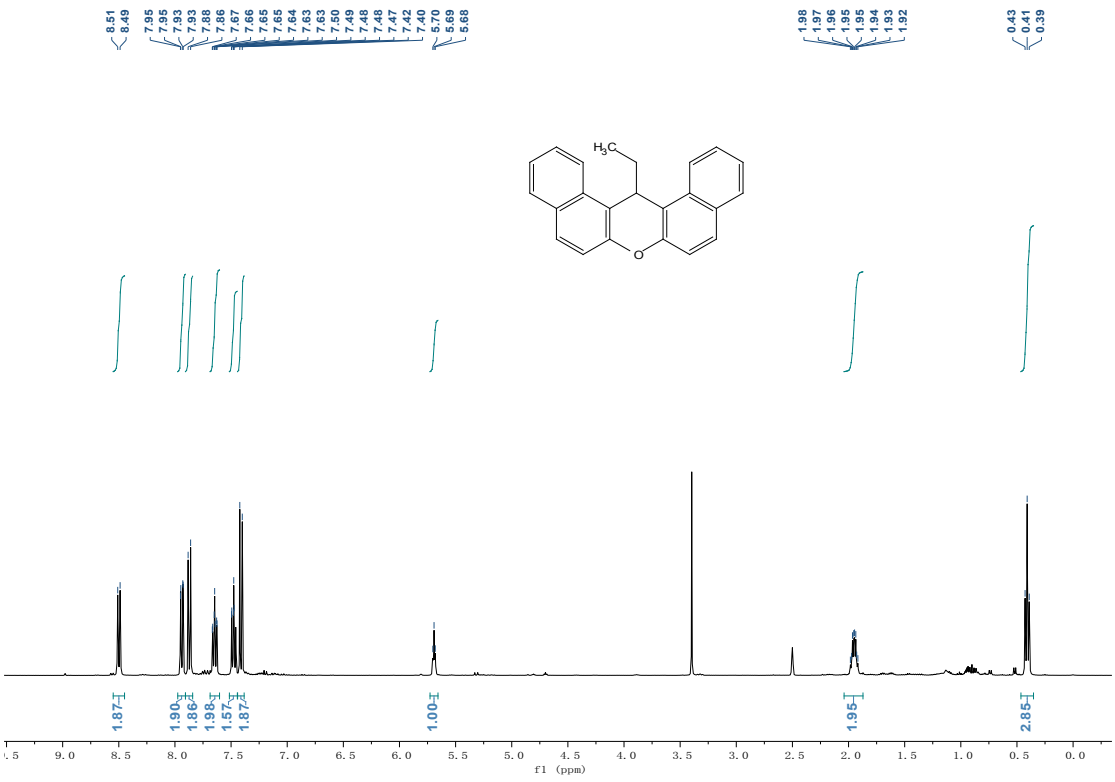
7.85
7.79
7.77
7.64
7.62
7.60
7.43
7.42
7.40
7.39
7.36
5.63
5.62
5.61
1.85
1.84
1.83
1.82
1.81
1.80
0.87
0.85
0.84
0.83
0.82
0.81
0.79
0.77
0.34
0.32
0.31
CH3
O
1.92
1.93
2.01
2.08
3.91
1.00
1.98
2.07
2.97
f1 (ppm)


149.24
130.99
130.56
128.52
128.20
126.69
124.15
122.85
117.01
116.41
37.90
30.16
17.54
13.55
CH3
O
f1 (ppm)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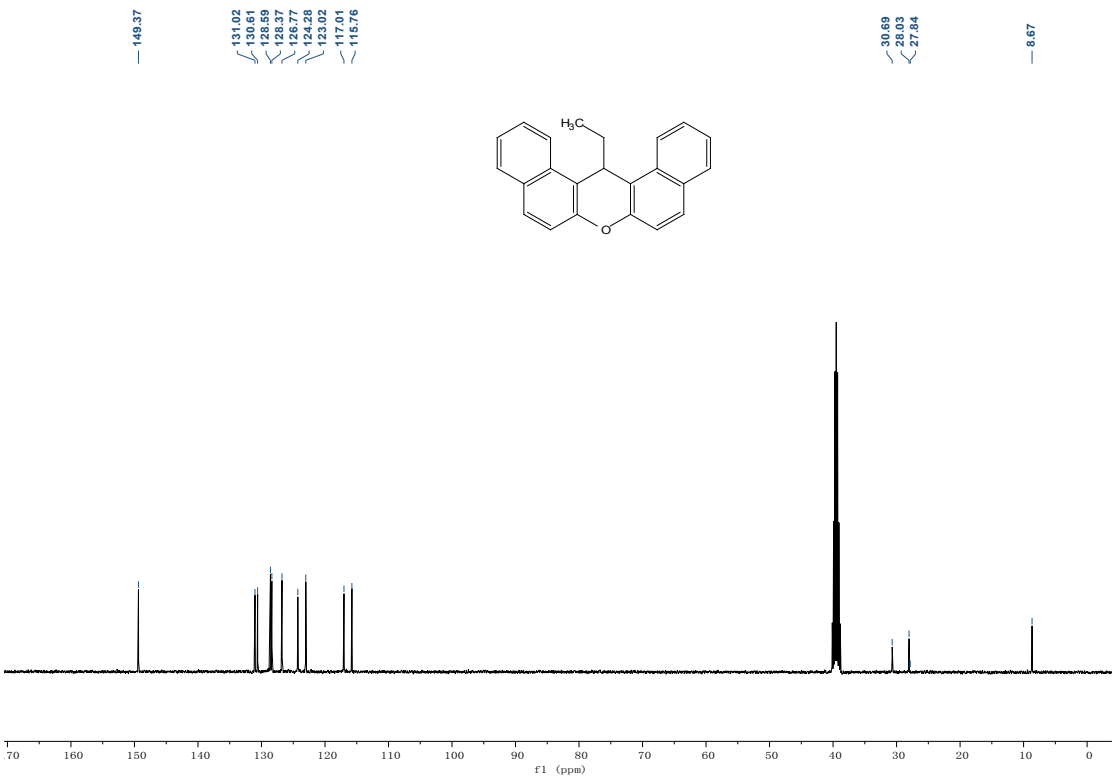
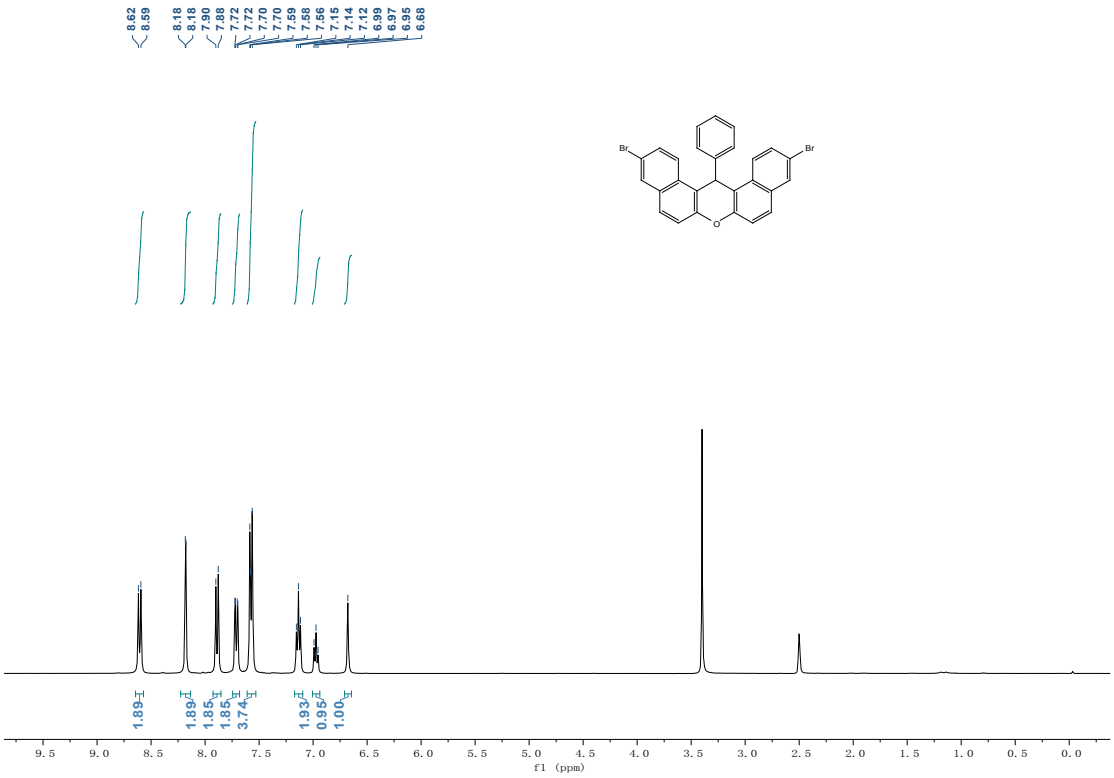
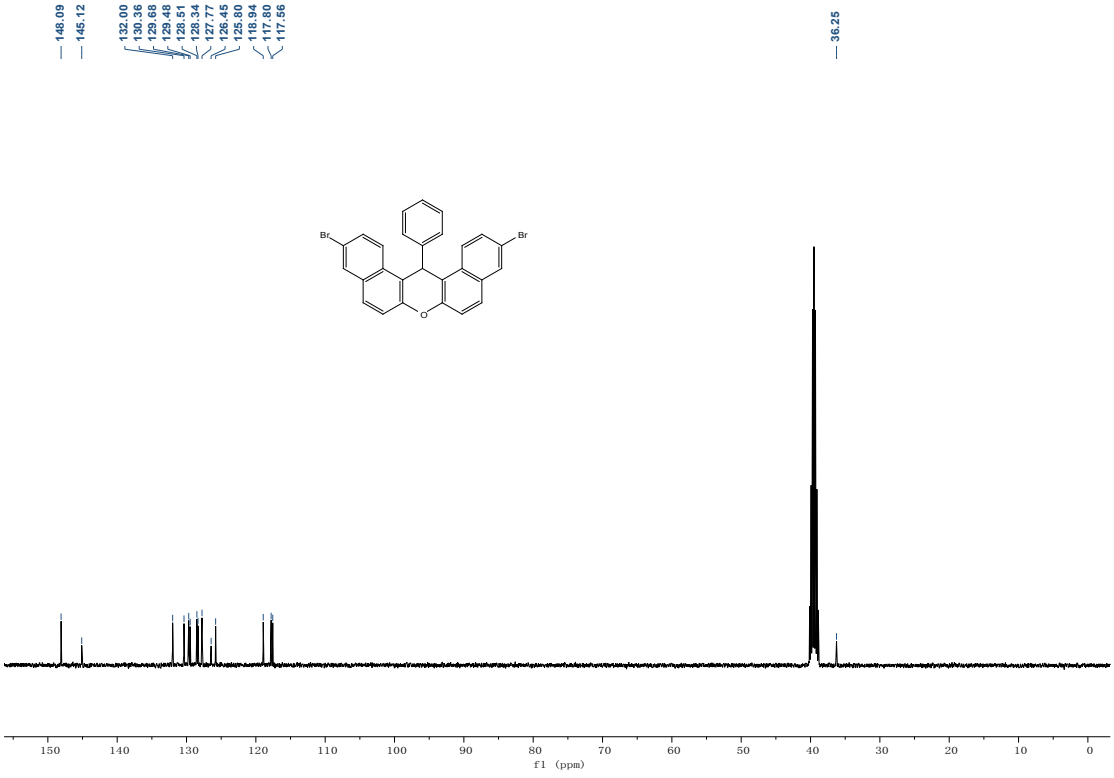
8.49
7.95
7.95
7.93
7.93
7.88
7.86
7.67
7.66
7.65
7.65
7.64
7.63
7.63
7.50
7.49
7.48
7.48
7.47
7.42
7.40
5.70
5.69
5.68
1.98
1.97
1.96
1.95
1.95
1.94
1.93
1.92
0.43
0.41
0.39
H3C
O
1.87
1.90
1.86
1.98
1.57
1.87
1.00
1.95
2.85
f1 (ppm)


149.37
131.02
130.61
128.59
128.37
126.77
124.28
123.02
117.01
115.76
30.69
28.03
27.84
8.67
H3C
O
f1 (ppm)


8.62
8.59
8.18
8.18
7.90
7.88
7.72
7.72
7.70
7.70
7.59
7.58
7.56
7.15
7.14
7.12
6.99
6.97
6.95
6.68
Br
Br
O
1.89
1.89
1.85
1.85
3.74
1.93
0.95
1.00
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
f1 (ppm)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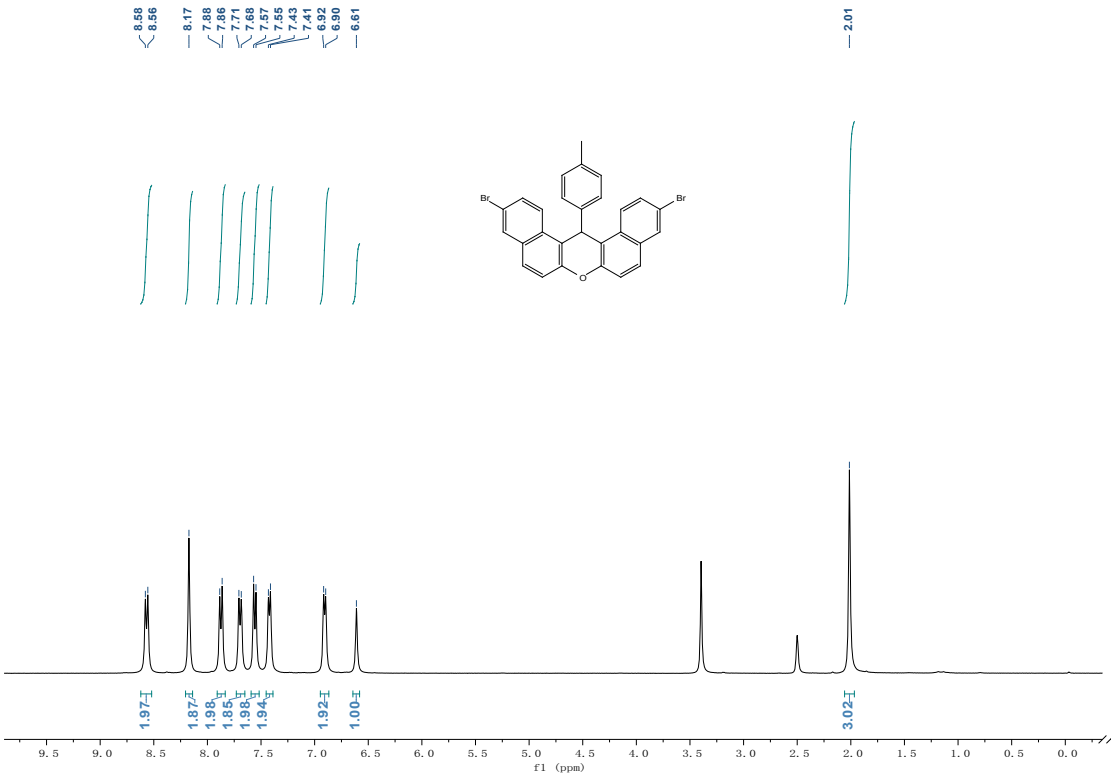
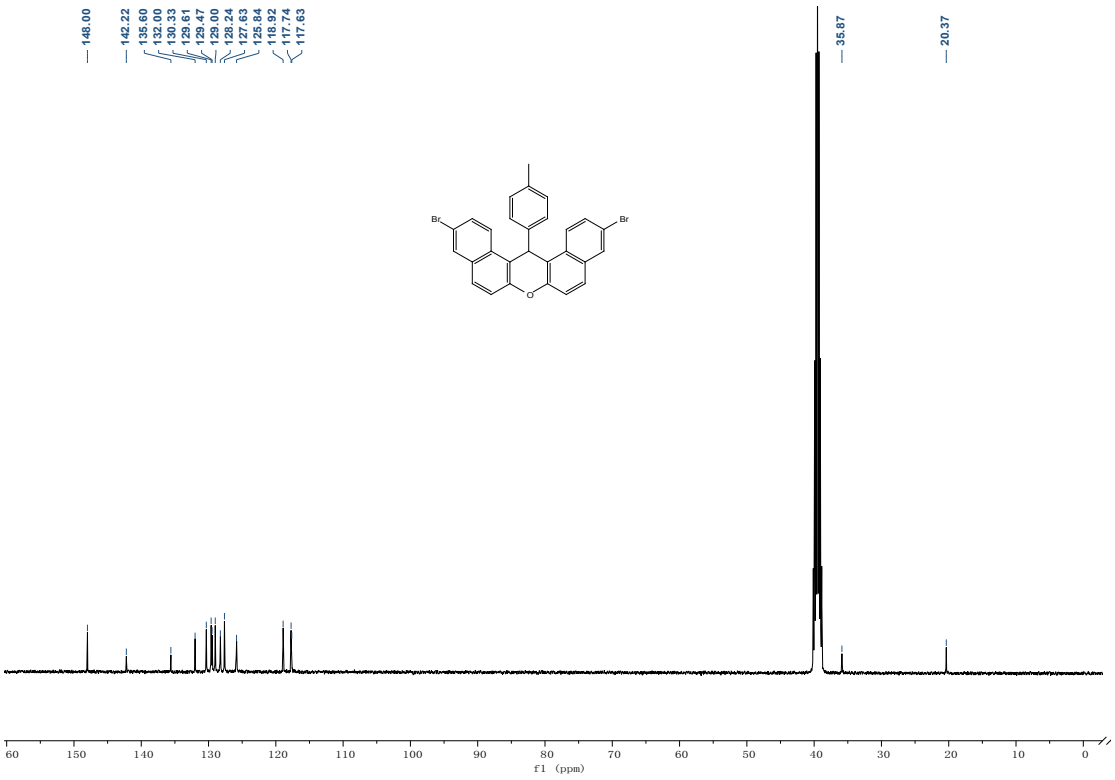
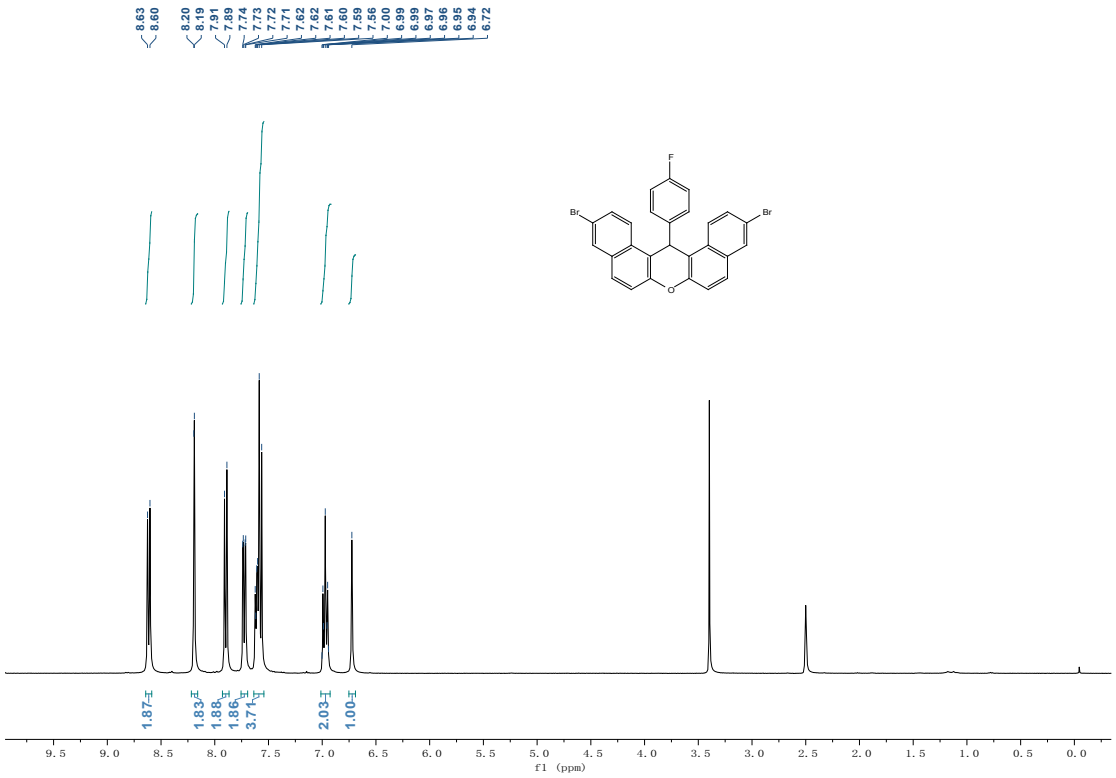
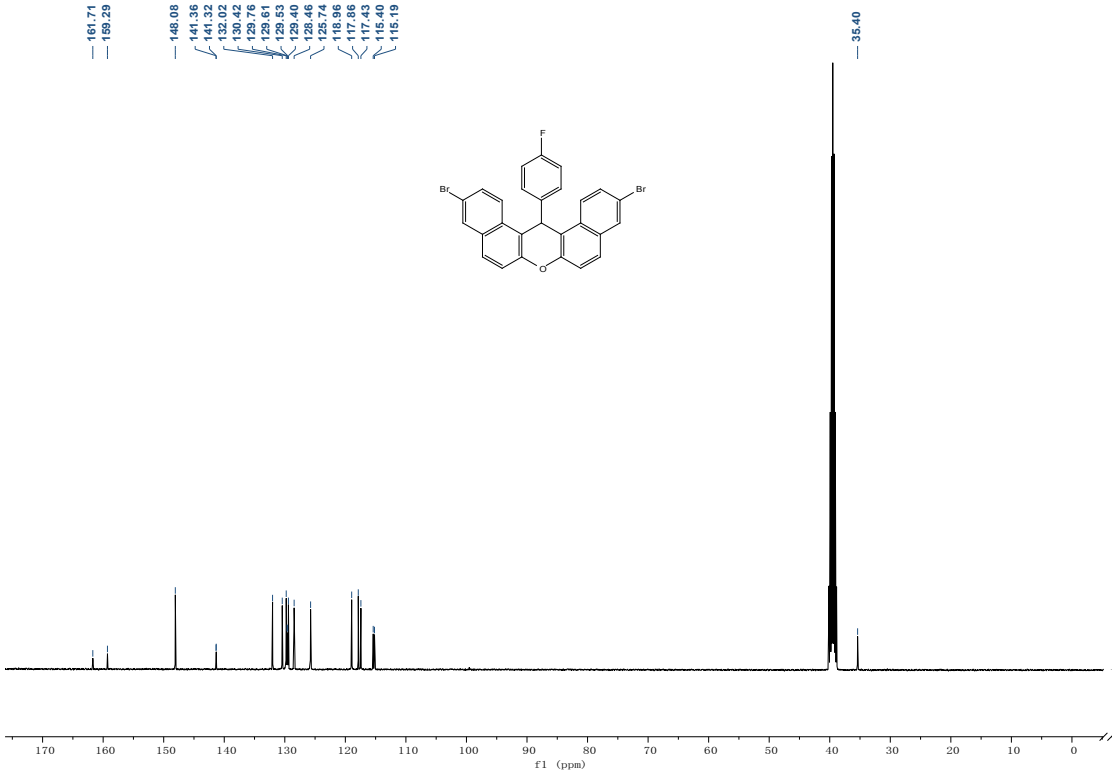
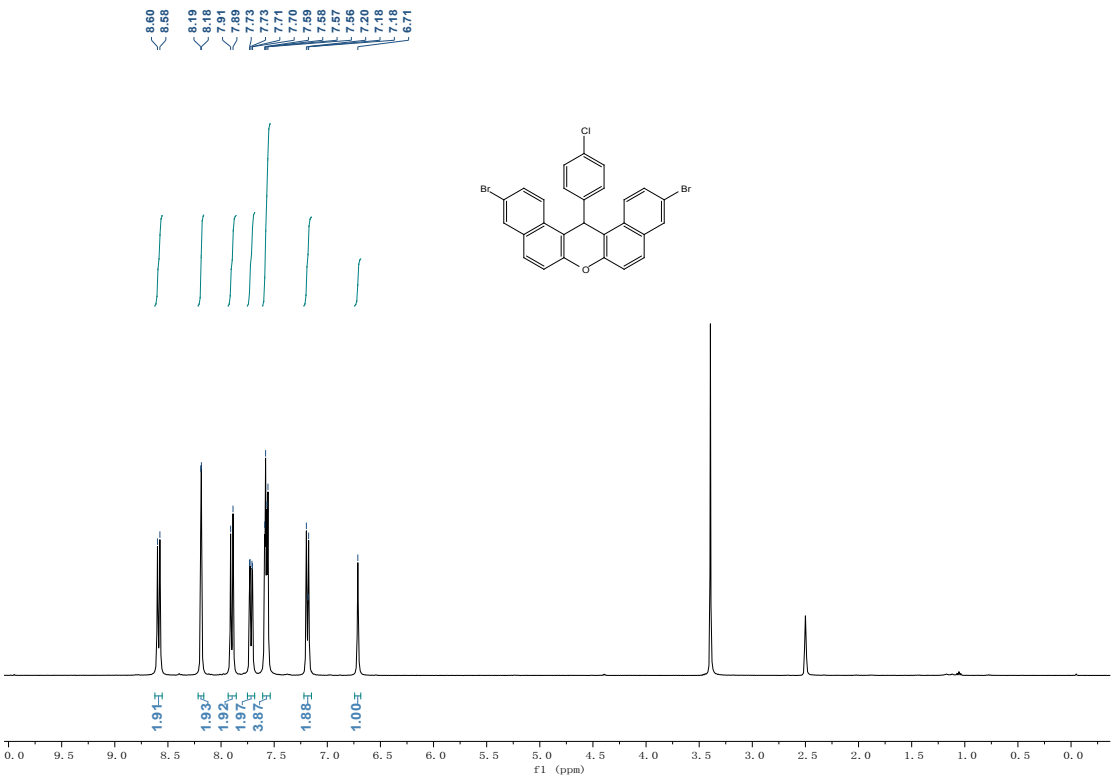
145.12
132.00
130.36
129.68
129.48
128.51
128.34
127.77
126.45
125.80
118.94
117.80
117.56
36.25
Br
Br
O
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

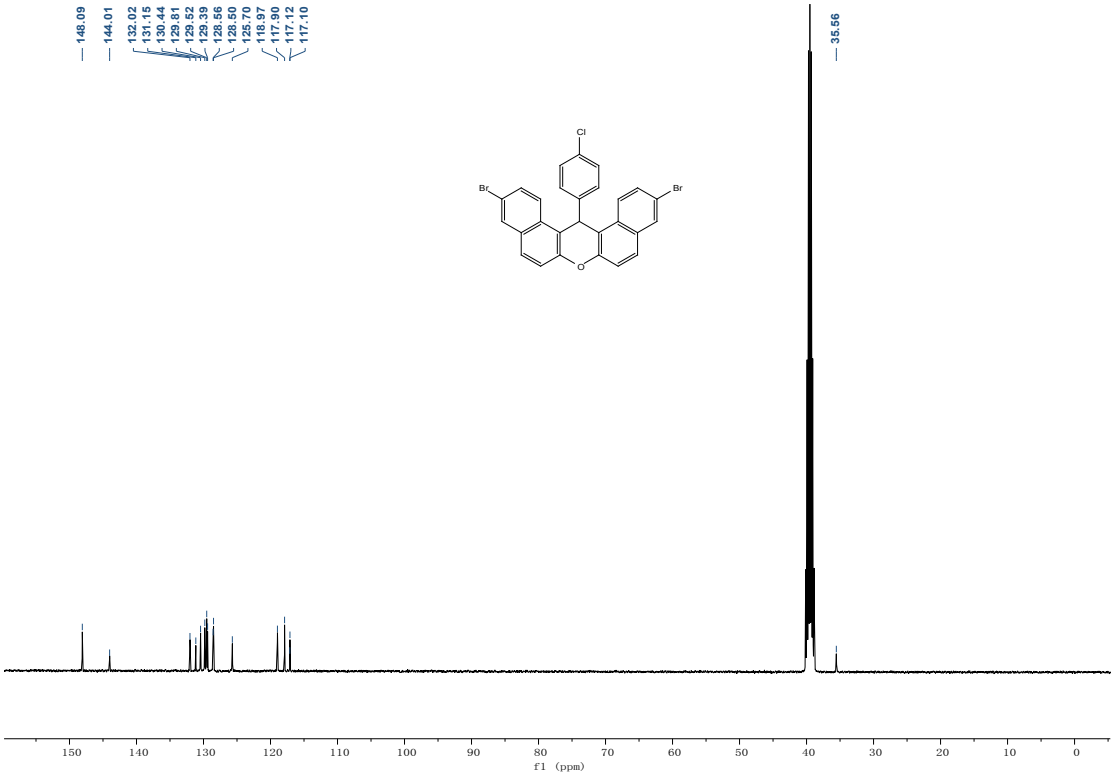

8.58
8.56
8.17
7.88
7.86
7.71
7.68
7.57
7.55
7.43
7.41
6.92
6.90
6.61
2.01
Br
Br
O
1.97
1.87
1.98
1.85
1.98
1.94
1.92
1.00
3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

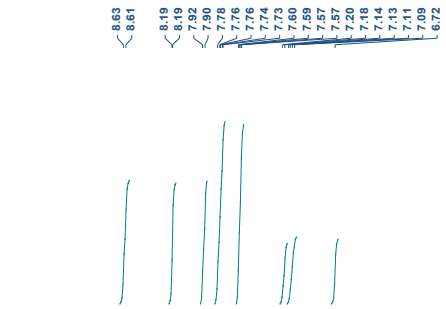

148.00
142.22
135.60
132.00
130.33
129.61
129.47
129.00
128.24
127.63
125.84
118.92
117.74
117.63
35.87
20.37
Br
Br
O
60 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

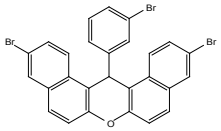

8.63
8.60
8.20
8.19
7.91
7.89
7.74
7.73
7.72
7.71
7.62
7.62
7.61
7.60
7.59
7.56
7.00
6.99
6.99
6.97
6.96
6.95
6.94
6.72
F
Br
Br
O
1.87
1.83
1.88
1.86
3.71
2.03
1.00
f1 (ppm)

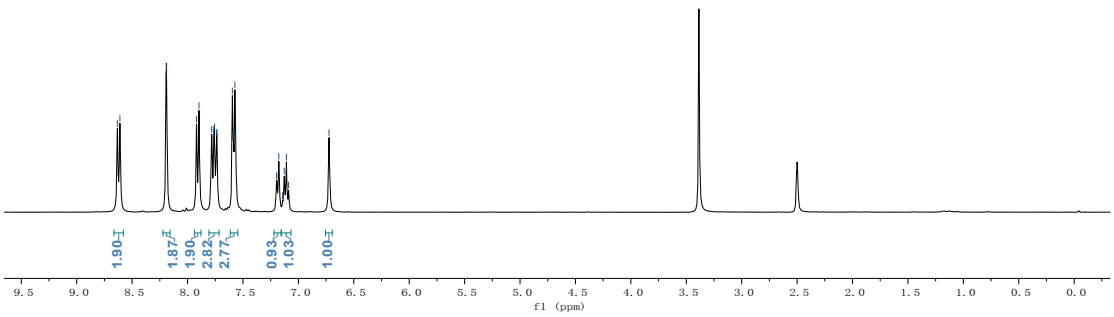

161.71
159.29
148.08
141.36
141.32
132.02
130.42
129.76
129.61
129.53
129.40
128.46
125.74
118.96
117.86
117.43
115.40
115.19
35.40
F
Br
Br
O
f1 (ppm)


8.60
8.58
8.19
8.18
7.91
7.89
7.73
7.73
7.71
7.70
7.59
7.58
7.57
7.56
7.20
7.18
6.71
Cl
Br
Br
O
1.91
1.93
1.92
1.97
3.87
1.88
1.00
f1 (ppm)

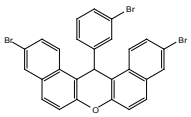

148.09
144.01
132.02
131.15
130.44
129.81
129.52
129.39
128.56
128.50
125.70
118.97
117.90
117.12
117.10
35.56
Cl
Br
Br
O
f1 (ppm)


8.63
8.61
8.19
8.19
7.92
7.90
7.78
7.76
7.76
7.74
7.73
7.60
7.59
7.57
7.57
7.20
7.18
7.14
7.13
7.11
7.09
6.72


Br
Br
Br
O


1.90
1.87
1.90
2.82
2.77
0.93
1.03
1.00
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
f1 (ppm)


148.16
147.60
132.02
130.79
130.48
130.12
129.89
129.54
129.35
128.70
126.82
125.64
121.87
118.97
117.98
116.98


Br
Br
Br
O


35.76
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)