Supplementary Information

Direct and metal-free arylsulfonylation of alkynes with sulfonylhydrazides for the construction of 3-sulfonated coumarins

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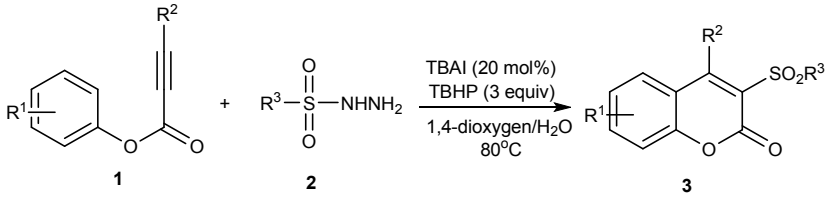
1. General information

All commercially available reagent grade chemicals were purchased from Aldrich, Acros, Alfa Aesar and Beijing Ouhe Chemical Company and used as received without further purification unless otherwise stated. Alkynoates were prepared according to previous literatures.[S1] ^{1}H NMR and ^{13}C NMR were recorded in $CDCl_3$ on a Bruker Avance III 400 spectrometer with TMS as internal standard (400 MHz ^{1}H, 100 MHz ^{13}C) at room temperature, the chemical shifts (δ) were expressed in ppm and J values were given in Hz. The following abbreviations are used to indicate the multiplicity: singlet (s), doublet (d), triplet (t), quartet (q), doublet of doublets (dd), doublet of triplets (dt), and multiplet (m). All first order splitting patterns were assigned on the basis of the appearance of the multiplet. Splitting patterns that could not be easily interpreted were designated as multiplet (m). Mass analyses and HRMS were obtained on a Finnigan-LCQDECA mass spectrometer and a Bruker Daltonics Bio-TOF-Q mass spectrometer by the ESI method, respectively. Column chromatography was performed on silica gel (200-300 mesh).

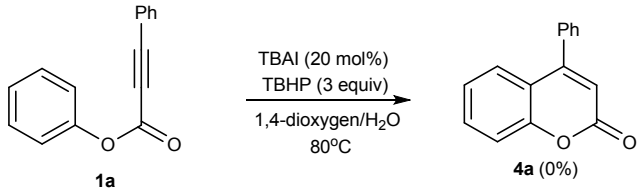
2. General procedure for metal-free direct arylsulfonylation of alkynes with sulfonylhydrazides leading to 3-sulfonated coumarins.



To a mixture of phenyl alkynoate **1a** (0.25 mmol), phenylsulfonohydrazide **2a** (0.75 mmol), and $(n\text{-Bu})_4NI$ (20 mol%), TBHP (0.75 mmol) in a 25 mL round-bottomed flack at room temperature, was added the 1,4-dioxane/H_2O (2.5 mL, 4/1). The reaction vessel was allowed to stir at 80 °C for 12-36 h. After the reaction, the solution was concentrated in vacuum. The resulting mixture purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate as eluent to give the desired product **3**.

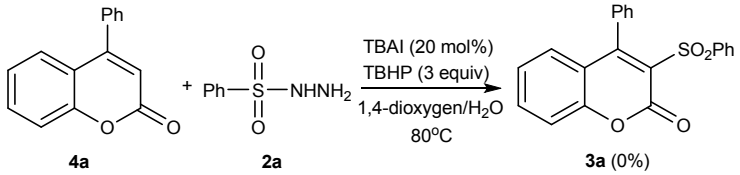
3. Preliminary mechanistic studies.

(1) The reaction of phenyl alkynoate **1a** under standard conditions.



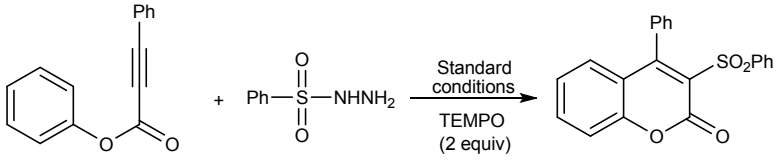
To a mixture of phenyl alkynoate **1a** (0.25 mmol), $(n\text{-Bu})_4NI$ (20 mol%), and TBHP (0.75 mmol) in a 25 mL round-bottomed flack at room temperature, was added the 1,4-dioxane/H_2O (2.5 mL, 4/1). The reaction vessel was allowed to stir at 80 °C for 24 h. After the reaction, the solution was concentrated in vacuum, no desired product **4a** was detected.

(2) The reaction of preformed coumarin **4a**[S2] with phenylsulfonohydrazide **2a** under standard conditions.



To a mixture of coumarin **4a** (0.25 mmol), phenylsulfonohydrazide **2a** (0.75 mmol), (n-Bu)$_4$NI (20 mol%), and TBHP (0.75 mmol) in a 25 mL round-bottomed flack at room temperature, was added the 1,4-dioxane/H_2O (2.5 mL, 4/1). The reaction vessel was allowed to stir at 80 °C for 24 h. After the reaction, the solution was concentrated in vacuum, no desired product **3a** was detected.

(3) The reaction of **1a** and **2a** with TEMPO under the standard conditions.



1a **2a** **3a** (0%)

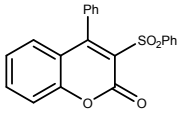
To a mixture of phenyl alkynoate **1a** (0.25 mmol), phenylsulfonohydrazide **2a** (0.75 mmol), (n-Bu)$_4$NI (20 mol%), TBHP (0.75 mmol), and TEMPO (0.5 mmol) in a 25 mL round-bottomed flack at room temperature, was added the 1,4-dioxane/H_2O (2.5 mL, 4/1). The reaction vessel was allowed to stir at 80 °C for 24 h. After the reaction, the solution was concentrated in vacuum, no desired product **3a** was detected.

4. Reference

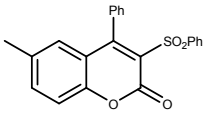
[1] C. E. Song, D-U. Jung, S. Y. Choung, E. J. Roh and S.-G. Lee, *Angew. Chem., Int. Ed.,* 2004, 43, 6183-6185.

[2] (a) M. Khoobi, M. Alipour, S. Zarei, F. Jafarpour and A. Shafiee, *Chem. Commun.*, 2012, 48, 2985-2987; (b) Y. Li, Z. Qi, H. Wang, X.Fu and C. Duan, *J. Org. Chem.* 2012, 77, 2053−2057.

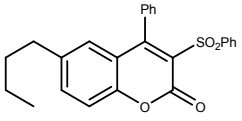
5. Characterization data of sulfonated coumarins (3a-3w)

4-phenyl-3-(phenylsulfonyl)-2H-chromen-2-one (3a) 

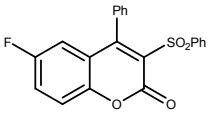
Compound **3a** was obtained in 88% yield according to the general procedure (12h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.03 (t, J = 8.7 Hz, 2H), 7.66-7.60 (m, 5H), 7.53 (t, J = 8.0 Hz, 2H), 7.39-7.35 (m, 3H), 7.22 (t, J = 8.7 Hz, 1H), 7.05 (dd, J_1 = 1.4 Hz, J_2 = 8.1 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm):δ 159.5, 155.6, 153.9, 140.3, 134.7, 133.7, 132.6, 130.0, 129.3, 129.2, 128.6, 128.2, 127.5, 125.9, 124.8, 120.3, 116.8; HRMS calc. for $C_{21}H_{14}O_4SNa$ $(M+Na)^+$, 385.0510; found, 385.0513.

6-methyl-4-phenyl-3-(phenylsulfonyl)-2H-chromen-2-one (3b) 

Compound **3b** was obtained in 84% yield according to the general procedure (12h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.02 (d, J = 7.4 Hz, 2H), 7.63-7.59 (m, 4H), 7.52 (t, J = 7.9 Hz, 2H), 7.37-7.35 (m, 2H), 7.17 (s, 1H), 7.02 (d, J = 8.3 Hz, 1H), 6.91 (d, J = 8.3 Hz, 1H), 2.46 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 159.6, 155.8, 154.1, 146.8, 140.4, 133.6, 132.8, 129.7, 129.2, 129.1, 128.6, 128.1, 127.5, 126.2, 124.7, 117.9, 116.9, 21.9; HRMS calc. for $C_{22}H_{16}O_4SNa$ (M+Na)+, 399.0667; found, 399.0665.

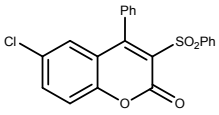
6-butyl-4-phenyl-3-(phenylsulfonyl)-2H-chromen-2-one (3c) 

Compound **3c** was obtained in 89% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.02 (d, J = 7.2 Hz, 2H), 7.61-7.59 (m, 4H), 7.51 (t, J = 7.9 Hz, 2H), 7.37-7.35 (m, 2H), 7.17(d, J = 1.2 Hz, 1H), 7.02 (dd, J_1 = 1.5 Hz, J_2 = 8.4 Hz, 1H), 6.93 (d, J = 8.3 Hz, 1H), 2.70 (t, J = 7.6 Hz, 2H), 1.63-1.59 (m, 2H), 1.38-1.28 (m, 2H), 0.93 (t, J = 7.3 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 159.7, 155.9, 154.1, 151.8, 140.4, 133.6, 132.8, 129.7, 129.2, 129.1, 128.6, 128.1, 127.5, 125.5, 124.7, 118.0, 116.2, 35.7, 32.8, 22.2, 13.8; HRMS calc. for $C_{25}H_{22}O_4SNa$ $(M+Na)^+$, 441.1136; found, 441.1137.



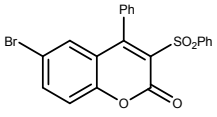
6-fluoro-4-phenyl-3-(phenylsulfonyl)-2H-chromen-2-one (3d)

Compound **3d** was obtained in 94% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.01(d, J = 7.6 Hz, 2H), 7.64-7.60 (m, 4H), 7.52 (t, J = 7.8 Hz, 2H), 7.36 (t, J = 3.4 Hz, 2H), 7.09-7.04 (m, 2H), 6.97-6.92 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ166.1 (d, J = 258.1 Hz), 159.1, 155.3, 155.2 (d, J = 13.4 Hz), 140.1, 133.8, 132.4, 132.3, 129.5, 129.2, 128.7, 128.3, 127.4, 124.9, 117.0 (d, J = 2.6 Hz), 113.3 (d, J = 22.5 Hz), 104.2 (d, J = 25.5 Hz); HRMS calc. for $C_{21}H_{13}FO_4SNa$ $(M+Na)^+$, 403.0416; found, 403.0414.



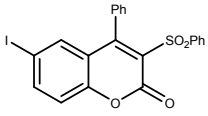
6-chloro-4-phenyl-3-(phenylsulfonyl)-2H-chromen-2-one (3e)

Compound **3e** was obtained in 85% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.02 (d, J = 7.5 Hz, 2H), 7.64-7.61 (m, 4H), 7.54 (t, J = 7.9 Hz, 2H), 7.38-7.34 (m, 3H), 7.18 (dd, J_1 = 2.0 Hz, J_2 = 8.7 Hz, 1H), 6.97 (d, J = 8.7 Hz, 1H); ^{13}C NMR ($CDCl_3$, 150 MHz, ppm): δ 158.8, 155.0, 154.1, 141.1, 140.1, 133.8, 132.2, 130.9, 129.5, 129.2, 128.7, 128.3, 127.4, 125.9, 125.6, 118.9, 117.0; HRMS calc. for $C_{21}H_{13}ClO_4SNa$ $(M+Na)^+$, 419.0121; found, 419.0120.



6-bromo-4-phenyl-3-(phenylsulfonyl)-2H-chromen-2-one (3f)

Compound **3f** was obtained in 74% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.01 (d, J = 7.4 Hz, 2H), 7.63-7.61 (m, 4H), 7.57-7.52 (m, 3H), 7.36-7.32 (m, 3H), 6.89 (d, J = 8.7 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 158.9, 154.9, 153.9, 140.0, 133.8, 132.1, 130.9, 129.5, 129.4, 129.2, 128.7, 128.4, 128.3, 127.4, 126.1, 120.1, 119.3; HRMS calc. for $C_{21}H_{14}BrO_4S$ $(M+H)^+$, 440.9800; found, 440.9796.

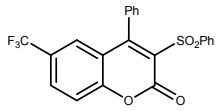


6-iodo-4-phenyl-3-(phenylsulfonyl)-2H-chromen-2-one (3g)

Compound **3g** was obtained in 80% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.01 (d, J = 7.6 Hz, 2H), 7.75 (s, 1H), 7.63-7.60 (m,

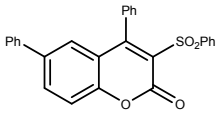
4H), 7.53 (t, J = 8.0 Hz, 3H), 7.36-7.34 (m, 2H), 6.71 (d, J = 8.6 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 159.0, 154.8, 153.4, 140.0, 134.3, 133.8, 132.1, 130.6, 129.5, 129.2, 128.7, 128.3, 127.4, 126.3, 126.0, 119.8, 101.6; HRMS calc. for $C_{21}H_{13}IO_4SNa$ $(M+Na)^+$, 510.9477; found, 510.9475.

4-phenyl-3-(phenylsulfonyl)-6-(trifluoromethyl)-2H-chromen-2-one (3h)



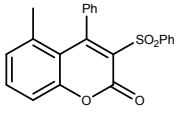
Compound **3h** was obtained in 78% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.02 (d, J = 7.3 Hz, 2H), 7.65-7.62 (m, 5H), 7.55 (t, J = 8.0 Hz, 2H), 7.44 (d, J = 8.5 Hz, 1H), 7.38-7.36 (m, 2H), 7.19 (d, J = 8.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 158.2, 154.7, 153.5, 139.7, 135.8 (d, J = 33.7 Hz), 134.0, 131.8, 130.9, 129.7, 129.0, 128.8, 128.5, 127.4, 124.1, 122.9, 121.2 (d, J = 3.6 Hz), 114.2 (d, J = 4.0 Hz); HRMS calc. for $C_{22}H_{13}F_3O_4SNa$ $(M+Na)^+$, 453.0384; found, 453.0390.

4,6-diphenyl-3-(phenylsulfonyl)-2H-chromen-2-one (3i)



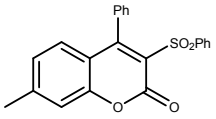
Compound **3i** was obtained in 73% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.05 (d, J = 7.4 Hz, 2H), 7.65-7.61 (m, 5H), 7.58-7.40 (m, 10H), 7.10 (d, J = 8.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 159.4, 155.7, 154.4, 147.9, 140.4, 138.3, 133.6, 132.7, 131.5, 130.9, 130.3, 129.3, 129.2, 128.6, 128.2, 127.5, 127.3, 125.3, 123.6, 119.1, 114.7; HRMS calc. for $C_{27}H_{18}O_4SNa$ $(M+Na)^+$, 461.0823; found, 461.0821.

5-methyl-4-phenyl-3-(phenylsulfonyl)-2H-chromen-2-one (3k)

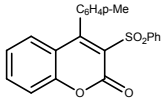


Compound **3k** was obtained in 40% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.03 (d, J = 7.2 Hz, 2H), 7.61-7.58 (m, 4H), 7.54-7.47 (m, 3H), 7.37-7.35 (m, 2H), 7.10 (t, J = 7.9 Hz, 1H), 6.87 (t, J = 8.1 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 159.9, 155.7, 152.3, 140.4, 135.9, 133.6, 132.9, 129.2, 128.6, 128.1, 127.7, 127.5, 126.4, 125.6, 124.3, 120.0, 116.3, 15.4; HRMS calc.

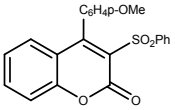
for $C_{22}H_{16}O_4SNa$ $(M+Na)^+$, 399.0667; found, 399.0667.

7-methyl-4-phenyl-3-(phenylsulfonyl)-2H-chromen-2-one (3k') 

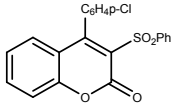
Compound **3k'** was obtained in 44% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.04-8.01 (m, 2H), 7.63-7.60 (m, 4H), 7.52 (t, J = 7.9 Hz, 2H), 7.44 (dd, J_1 = 1.7 Hz, J_2 = 8.4 Hz, 1H), 7.38-7.35 (m, 2H), 7.26 (d, J = 8.4 Hz, 1H), 6.79 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 159.6, 155.8, 152.1, 140.4, 135.9, 134.7, 133.6, 132.6, 129.4, 129.2, 129.1, 128.6, 128.2, 127.5, 125.8, 119.9, 116.6, 20.9; HRMS calc. for $C_{22}H_{16}O_4SNa$ $(M+Na)^+$, 399.0667; found, 399.0666.

3-(phenylsulfonyl)-4-p-tolyl-2H-chromen-2-one (3l) 

Compound **3l** was obtained in 86% yield according to the general procedure (6h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.03 (d, J = 7.6 Hz, 2H), 7.64-7.60 (m, 2H), 7.52 (t, J = 7.8 Hz, 2H), 7.41 (d, J = 7.7 Hz, 2H), 7.38-7.34 (m, 1H), 7.29-7.25 (m, 2H), 7.21 (t, J = 7.7 Hz, 1H), 7.11 (t, J = 6.6 Hz, 1H), 2.52 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 160.0, 155.6, 153.9, 140.4, 139.3, 134.6, 133.6, 130.0, 129.5, 129.1, 128.9, 128.6, 127.5, 125.9, 124.8, 120.4, 116.8, 21.6; HRMS calc. for $C_{22}H_{17}O_4S$ $(M+H)^+$, 377.0848; found, 377.0848.

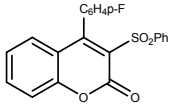
4-(4-methoxyphenyl)-3-(phenylsulfonyl)-2H-chromen-2-one (3m) 

Compound **3m** was obtained in 71% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.01 (d, J = 7.4 Hz, 2H), 7.65-7.59 (m, 2H), 7.52 (t, J = 8.0 Hz, 2H), 7.37-7.35 (m, 1H), 7.31-7.29 (m, 2H), 7.22 (t, J = 8.0 Hz, 1H), 7.17-7.11 (m, 3H), 3.95 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 160.5, 159.7, 155.7, 153.9, 140.5, 134.5, 133.6, 130.9, 130.0, 129.2, 129.1, 128.6, 124.8, 124.3, 120.5, 116.8, 113.7, 55.4; HRMS calc. for $C_{22}H_{16}O_5SNa$ $(M+Na)^+$, 415.0616; found, 415.0619.

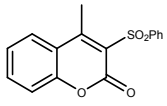
4-(4-chlorophenyl)-3-(phenylsulfonyl)-2H-chromen-2-one (3n) 

Compound **3n** was obtained in 87% yield according to the general procedure (24h). ^{1}H

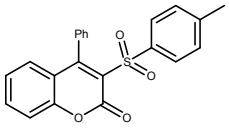
NMR ($CDCl_3$, 400 MHz, ppm): δ 8.02 (d, J = 7.4 Hz, 2H), 7.68-7.58 (m, 4H), 7.54 (t, J = 7.9 Hz, 2H), 7.37 (d, J = 7.8 Hz, 1H), 7.32 (d, J = 8.4 Hz, 2H), 7.24 (t, J = 8.2 Hz, 1H), 7.04 (dd, J_1 = 1.4 Hz, J_2 = 8.1 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 158.3, 155.3, 153.9, 140.0, 135.6, 134.9, 133.8, 130.9, 129.6, 129.2, 128.9, 128.7, 128.6, 126.3, 125.0, 119.9, 117.0; HRMS calc. for $C_{21}H_{13}ClO_4SNa$ $(M+Na)^+$, 419.0121; found, 419.0120.

4-(4-fluorophenyl)-3-(phenylsulfonyl)-2H-chromen-2-one (3o) 

Compound **3o** was obtained in 91% yield according to the general procedure (24h). ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.01 (d, J = 7.3 Hz, 2H), 7.68-7.61 (m, 2H), 7.53 (t, J = 8.0 Hz, 2H), 7.38-7.31 (m, 5H), 7.24 (d, J = 8.1 Hz, 1H), 7.06 (dd, J_1 = 1.4 Hz, J_2 = 8.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 163.3 (d, J = 248.1 Hz), 158.6, 155.4, 153.9, 140.1, 134.8, 133.8, 129.7, 129.5 (d, J = 8.3 Hz), 129.1, 128.7, 128.3 (d, J = 3.7 Hz), 126.4, 125.0, 120.1, 117.0, 115.6 (d, J = 22.0 Hz); HRMS calc. for $C_{21}H_{13}FO_4SNa$ $(M+Na)^+$, 403.0416; found, 403.0416.

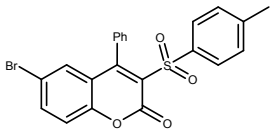
4-methyl-3-(phenylsulfonyl)-2H-chromen-2-one (3p) 

Compound **3p** was obtained in 60% yield according to the general procedure.^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.13 (d, J = 7.3 Hz, 2H), 7.93 (dd, J_1 = 1.3 Hz, J_2 = 8.2 Hz, 1H), 7.69-7.62 (m, 2H), 7.56 (t, J = 7.9 Hz, 2H), 7.43-7.39 (m, 1H), 7.32 (dd, J_1 = 0.9 Hz, J_2 = 8.3 Hz, 1H), 3.19 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 158.3, 155.3, 153.4, 140.8, 134.6, 133.7, 128.7, 128.6, 126.6, 125.0, 119.7, 117.3, 15.3; HRMS calc. for $C_{16}H_{12}O_4SNa$ $(M+Na)^+$, 323.0354; found, 323.0356.

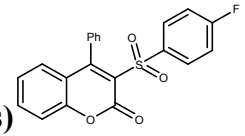
4-phenyl-3-tosyl-2H-chromen-2-one (3q) 

Compound **3q** was obtained in 84% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.91 (d, J = 8.3 Hz, 2H), 7.65-7.59 (m, 4H), 7.38-7.35 (m, 3H), 7.32 (d, J = 8.0 Hz, 2H), 7.23-7.19 (m, 1H), 7.04 (dd, J_1 = 1.4 Hz, J_2 = 8.1 Hz, 1H), 2.44 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 159.2, 155.6, 153.9, 144.8, 137.3,

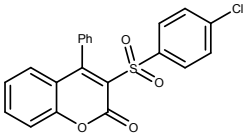
134.6, 132.7, 129.9, 129.3, 129.2, 128.2, 127.5, 126.2, 124.7, 120.3, 116.8, 21.7; HRMS calc. for $C_{22}H_{16}O_4SNa$ $(M+Na)^+$, 399.0667; found, 399.0669.

6-bromo-4-phenyl-3-tosyl-2H-chromen-2-one (3r) 

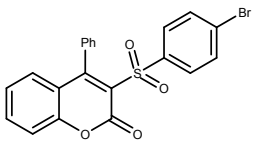
Compound **3r** was obtained in 78% yield according to the general procedure. ^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.89 (d, J = 8.2 Hz, 2H), 7.61 (t, J = 3.2 Hz, 3H), 7.54 (d, J = 1.6 Hz, 1H), 7.35-7.31 (m, 5H), 6.88 (d, J = 8.7 Hz, 1H), 2.44 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 158.5, 155.0, 153.8, 145.0, 137.0, 132.3, 130.8, 129.5, 129.4, 129.3, 129.2, 128.4, 128.3, 127.4, 126.4, 120.0, 119.3, 21.7; HRMS calc. for $C_{22}H_{15}BrO_4SNa$ $(M+Na)^+$, 476.9772; found, 476.9775.

3-(4-fluorophenylsulfonyl)-4-phenyl-2H-chromen-2-one (3s) 

Compound **3s** was obtained in 74% yield according to the general procedure. ^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.07-8.04 (m, 2H), 7.67-7.59 (m, 4H), 7.23-7.17 (m, 3H), 7.25-7.17 (m, 3H), 7.06 (dd, J_1 = 1.4 Hz, J_2 = 8.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 165.9 (d, J = 254.9 Hz), 159.6, 155.6, 153.9, 136.2 (d, J = 3.1 Hz), 134.8, 132.5, 132.3, 132.2, 129.7 (d, J = 62.4 Hz), 128.2, 127.4, 125.8, 124.9, 120.2, 116.9, 115.9 (d, J = 22.6 Hz); HRMS calc. for $C_{21}H_{13}FO_4SNa$ $(M+Na)^+$, 403.0416; found, 403.0418.

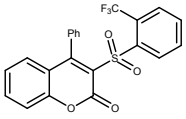
3-(4-chlorophenylsulfonyl)-4-phenyl-2H-chromen-2-one (3t) 

Compound **3t** was obtained in 77% yield according to the general procedure. ^1H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.96 (d, J = 8.7 Hz, 2H), 7.66-7.60 (m, 4H), 7.49 (d, J = 8.7 Hz, 2H), 7.39-7.35 (m, 3H), 7.25-7.21 (m, 1H) 7.06 (dd, J_1 = 1.4 Hz, J_2 = 8.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 159.9, 155.6, 153.9, 140.5, 138.7, 134.9, 132.4, 130.8, 130.0, 129.4, 129.0, 128.3, 127.4, 125.6, 125.0, 120.2, 116.9; HRMS calc. for $C_{21}H_{13}ClO_4SNa$ (M+Na)+, 419.0121; found, 419.0120.

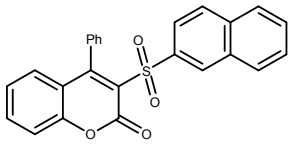
3-(4-bromophenylsulfonyl)-4-phenyl-2H-chromen-2-one (3u) 

Compound **3u** was obtained in 71% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 7.89 (d, J = 8.7 Hz, 2H), 7.68-7.60 (m, 6H), 7.39-7.35(m, 3H), 7.25-7.21 (m, 1H), 7.06 (dd, J_1 = 1.5 Hz, J_2 = 8.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 159.9, 155.6, 153.9, 139.2, 134.9, 132.4, 132.0, 130.8, 130.0, 129.4, 129.2, 128.3, 127.4, 125.6, 125.0, 120.2, 116.9; HRMS calc. for $C_{21}H_{13}BrO_4SNa$ $(M+Na)^+$, 462.9616; found, 462.9613.

4-phenyl-3-(2-(trifluoromethyl)phenylsulfonyl)-2H-chromen-2-one (3v)

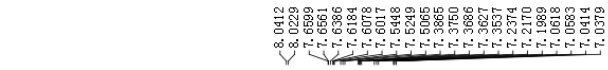


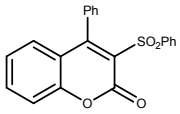
Compound **3v** was obtained in 86% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.54 (d, J = 8.0 Hz, 1H), 7.82-7.79 (m, 2H), 7.72 (t, J = 7.0 Hz, 1H), 7.69-7.64 (m, 1H), 7.60-7.58 (m, 3H), 7.47-7.45 (m, 2H), 7.39 (dd, J_1 = 0.8 Hz, J_2 = 8.3 Hz, 1H), 7.29-7.25 (m, 1H), 7.19 (dd, J_1 = 1.6 Hz, J_2 = 8.2 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 158.8, 155.7, 153.8, 139.8, 134.6, 133.4, 133.2, 132.1, 131.6, 129.7 (d, J = 4.2 Hz), 128.2, 128.1, 127.7 (q, J = 6.4 Hz), 127.5, 126.4, 125.0, 123.0 (d, J = 285 Hz), 120.0, 117.0; HRMS calc. for $C_{22}H_{13}F_3O_4SNa$ (M+Na)+, 453.0384; found, 453.0381.

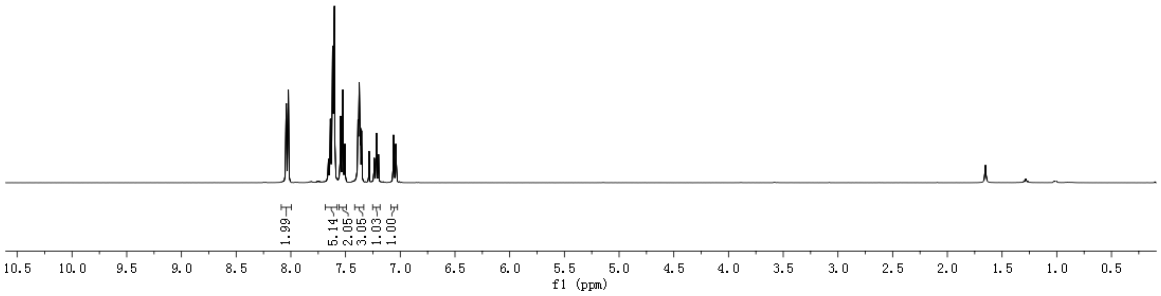
3-(naphthalen-2-ylsulfonyl)-4-phenyl-2H-chromen-2-one (3w) 

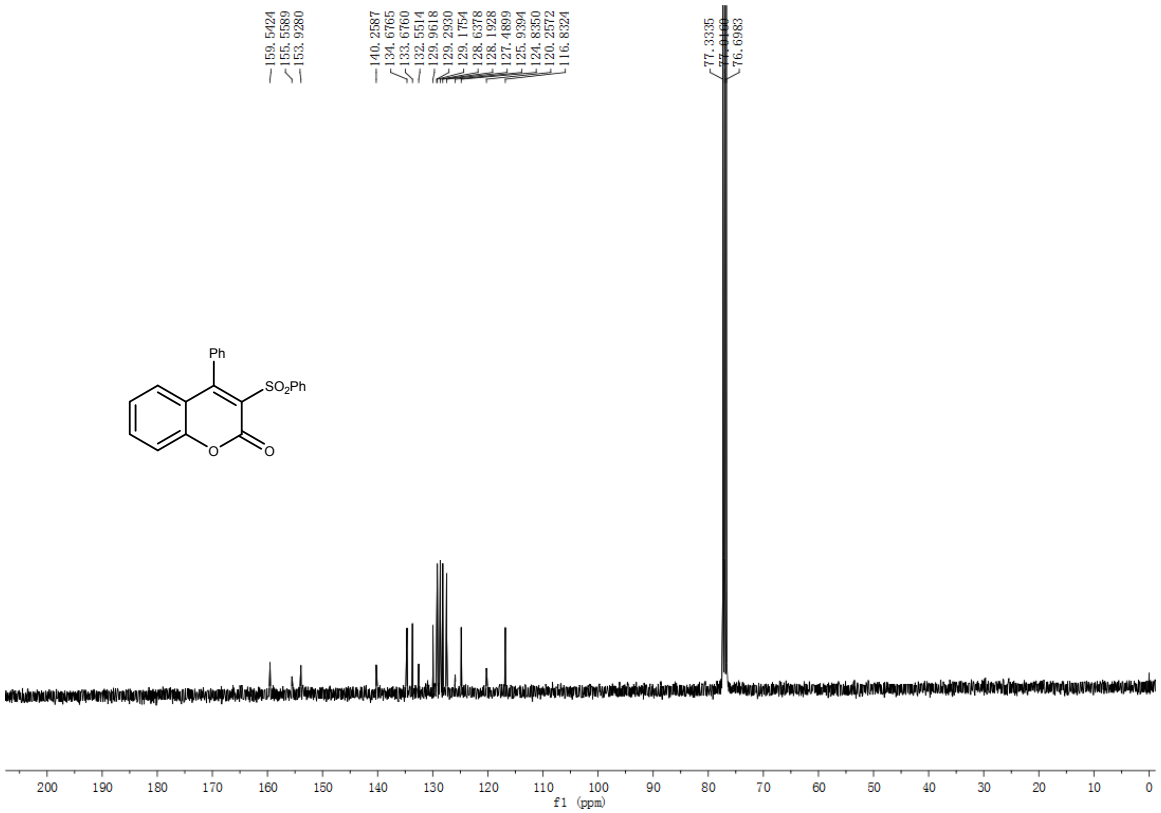
Compound **3w** was obtained in 78% yield according to the general procedure. ^{1}H NMR ($CDCl_3$, 400 MHz, ppm): δ 8.63 (s, 1H), 8.01 (d, J = 7.9 Hz, 1H), 7.95 (s, 2H), 7.91 (d, J = 8.1 Hz, 1H), 7.68-7.60 (m, 6H), 7.43-7.40 (m, 2H), 7.35 (d, J = 8.2 Hz, 1H), 7.22 (t, J = 8.0 Hz, 1H), 7.07 (d, J = 8.1 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz, ppm): δ 159.5, 155.6, 153.9, 137.1, 135.4, 134.7, 132.6, 132.0, 131.4, 129.9, 129.7, 129.4, 129.3, 128.7, 128.2, 127.9, 127.6, 127.4, 126.1, 124.8, 123.6, 120.3, 116.8; HRMS calc. for $C_{25}H_{16}O_4SNa$ (M+Na)+, 435.0667; found, 435.0669.

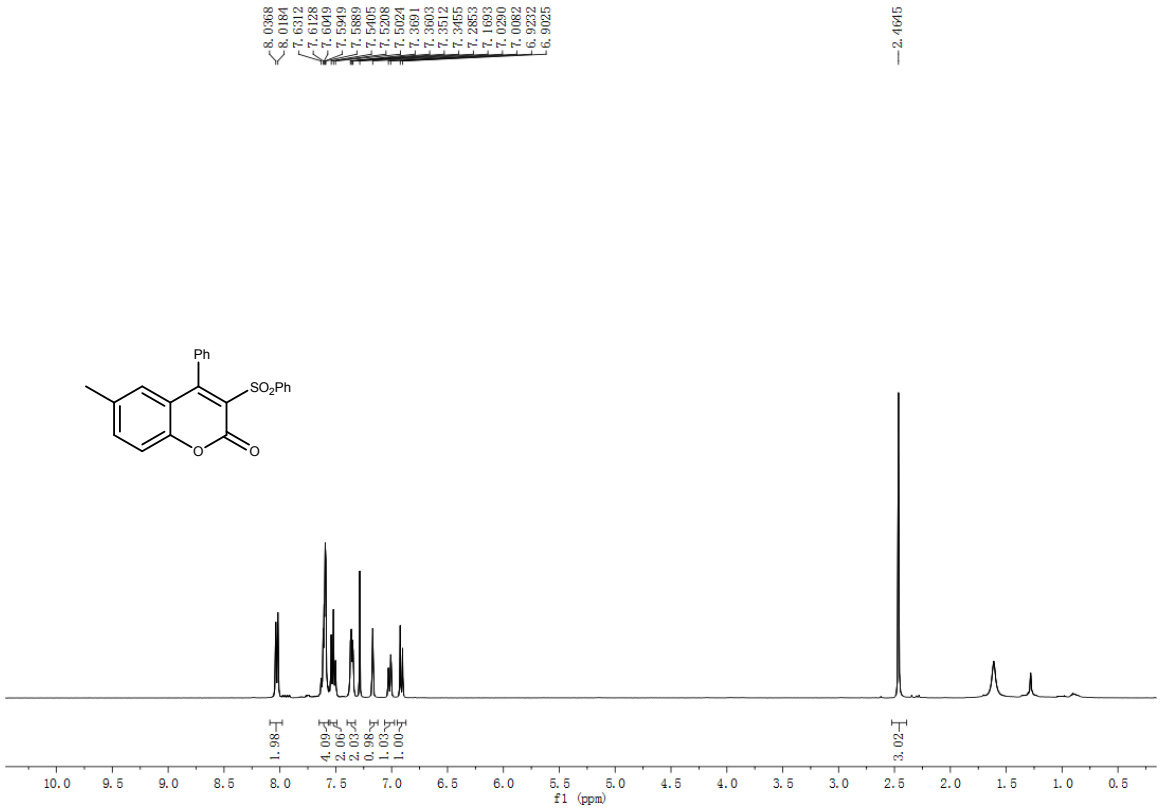
6.Copies of NMR Spectra for 3a-3w







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7.3512
7.3455
7.2853
7.1693
7.0290
7.0082
6.9232
6.9025
2.4645
Ph
SO2Ph
O
O
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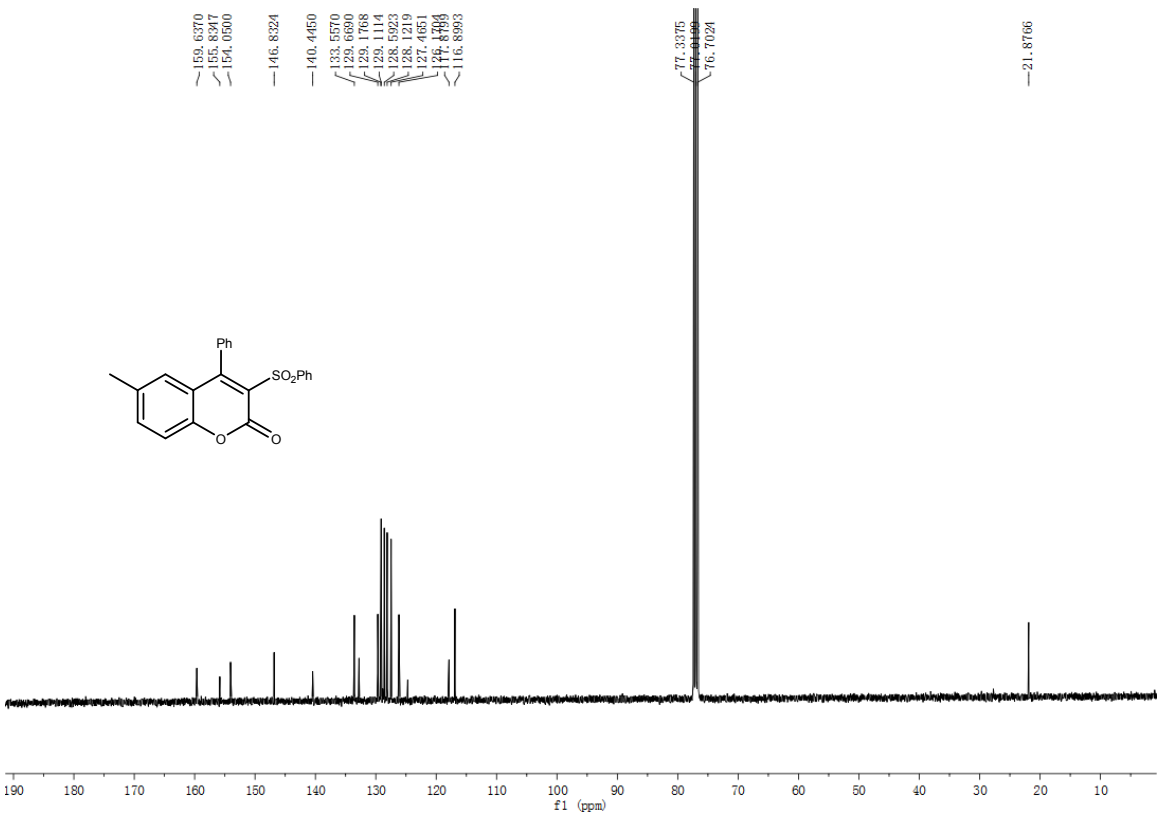
4.09
2.06
2.03
0.98
1.03
1.00
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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127.4651
126.1704
117.8799
116.8993
77.3375
77.0188
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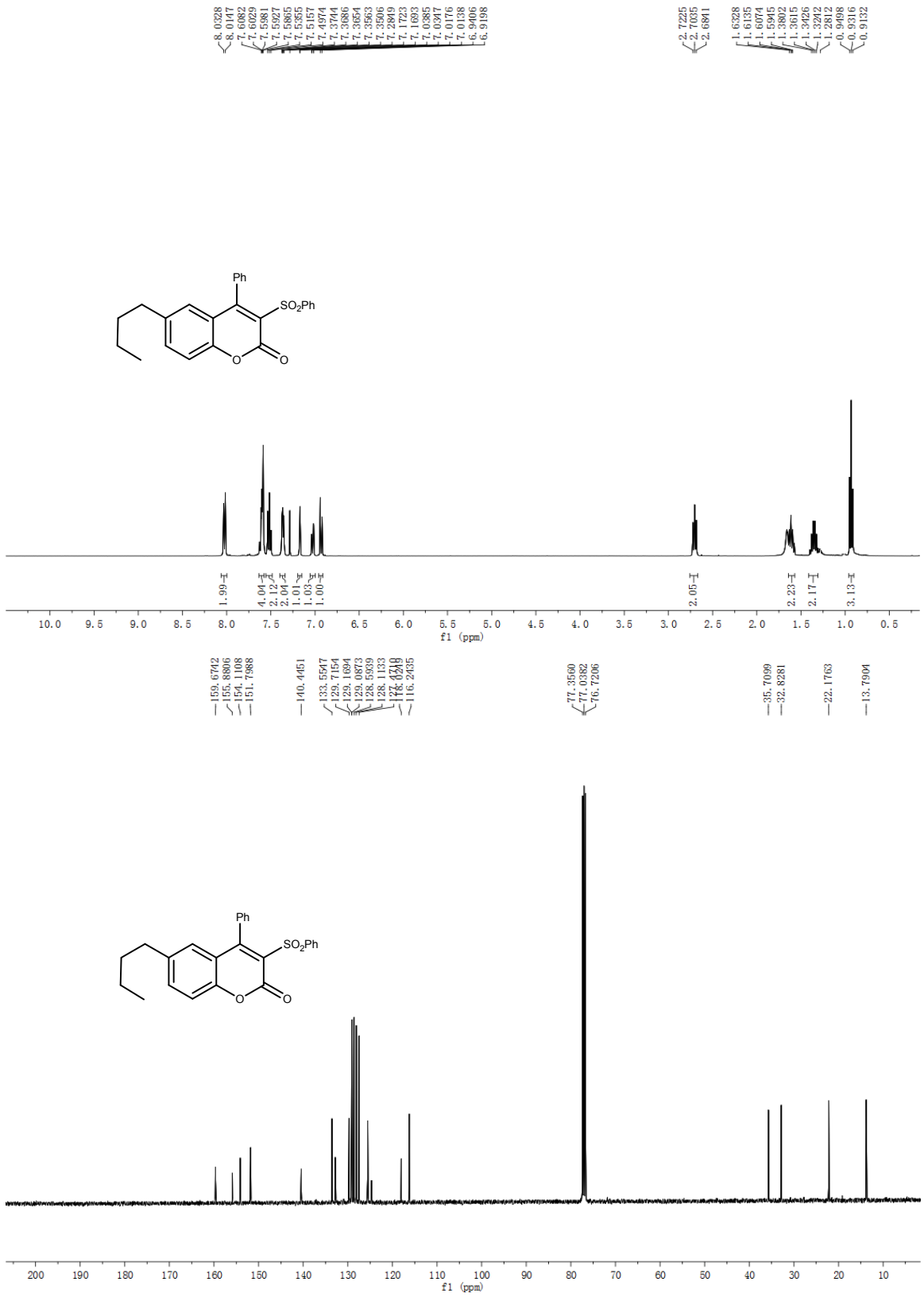
21.8766
Ph
SO2Ph
O
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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7.1723
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7.0176
7.0138
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6.9198
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1.6135
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1.2812
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2.12
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1.01
1.03
1.00
2.05
2.23
2.17
3.13
f1 (ppm)
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151.7988
140.4451
133.5547
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129.1694
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128.5939
128.1133
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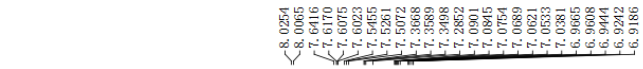
SO2Ph
O
O
f1 (ppm)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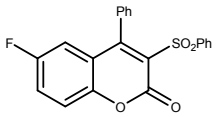
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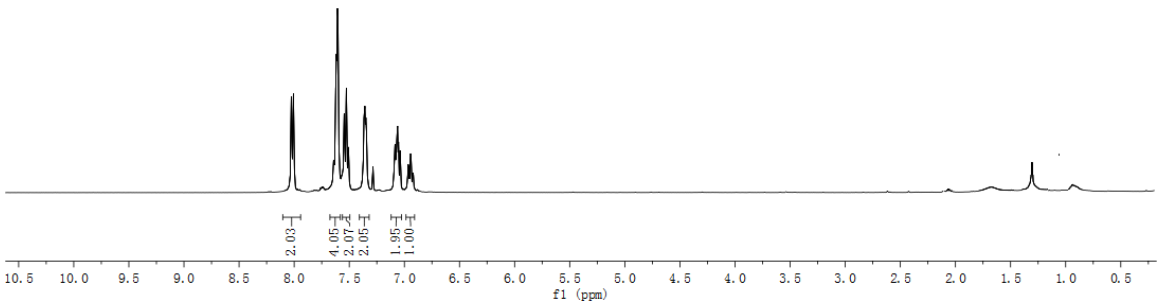
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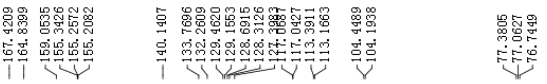
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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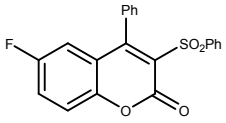
Ph
F
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O

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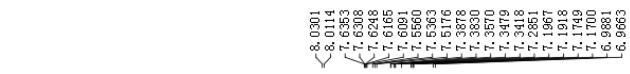
f1 (ppm)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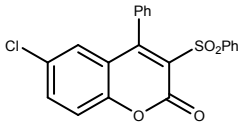
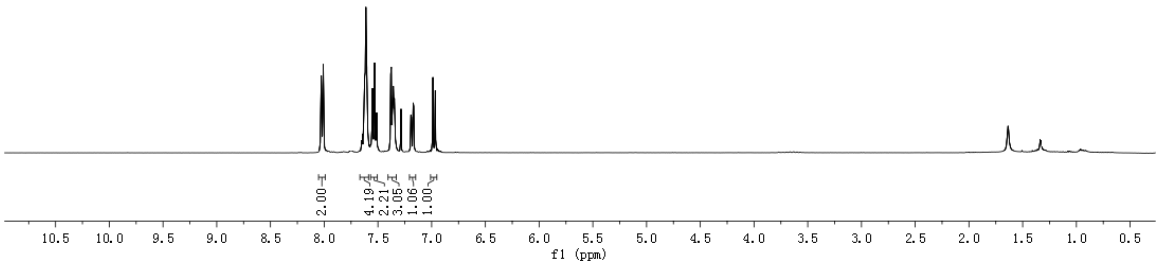
6.9663


Ph
Cl
SO2Ph
O
O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3.86
1.06
1.00
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f1 (ppm)


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154.0528
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140.0508
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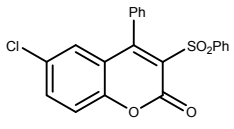
Ph
Cl
SO2Ph
O
O

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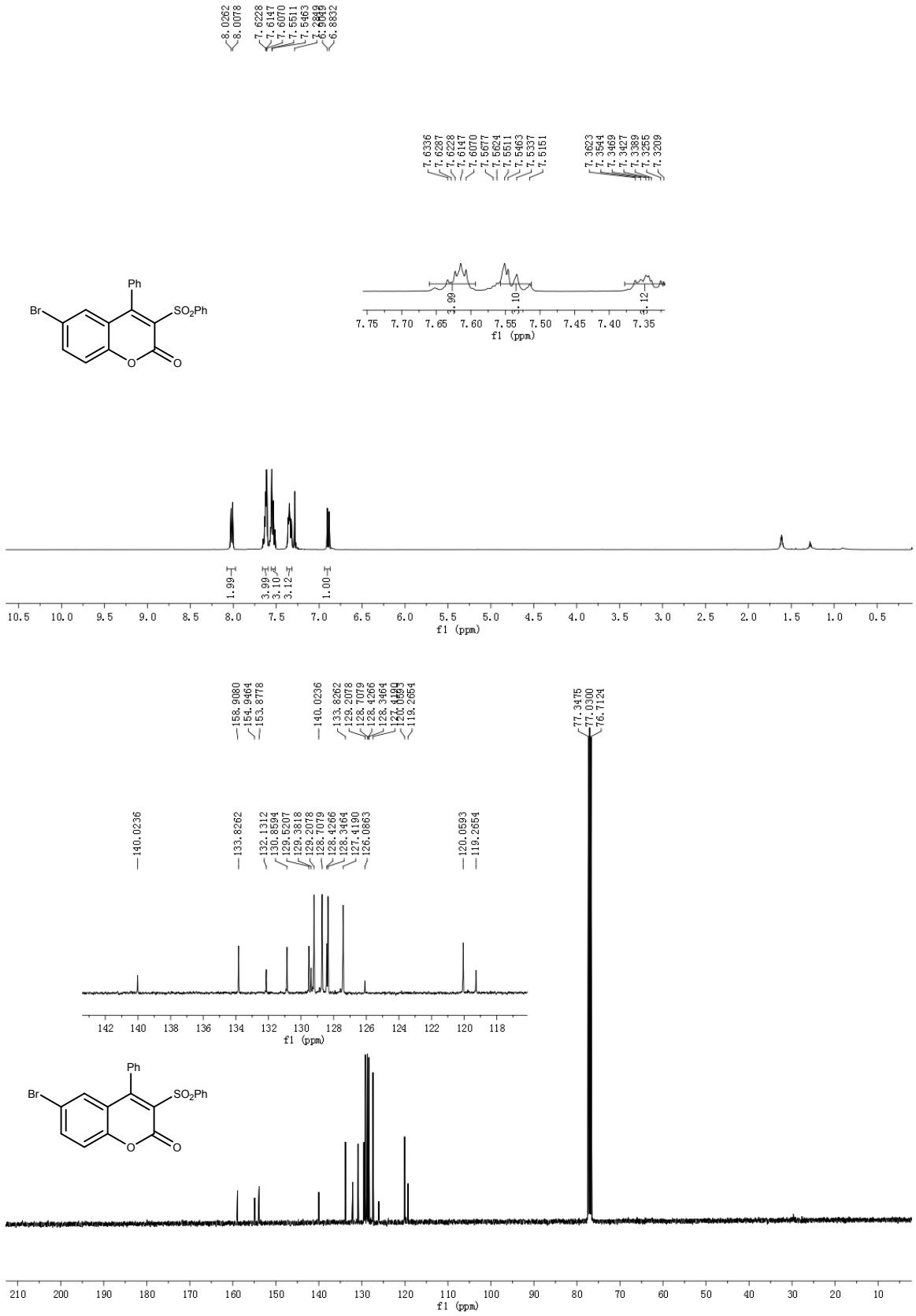
f1 (ppm)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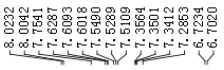
7.5463
6.8832
7.6336
7.6287
7.6228
7.6147
7.6070
7.5677
7.5624
7.5511
7.5463
7.5337
7.5151
7.3623
7.3544
7.3469
7.3427
7.3389
7.3255
7.3209
Ph
Br
SO2Ph
O
O
3.99
3.10
3.12
7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35
f1 (ppm)
1.99
3.99
3.10
3.12
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)
158.9080
154.9464
153.8778
140.0236
133.8262
129.2078
128.7079
128.4266
128.3464
127.4190
126.0863
120.0593
119.2654
77.3475
77.0300
76.7124
140.0236
133.8262
132.1312
130.8594
129.5207
129.3818
129.2078
128.7079
128.4266
128.3464
127.4190
126.0863
120.0593
119.2654
142 140 138 136 134 132 130 128 126 124 122 120 118
f1 (ppm)
Ph
Br
SO2Ph
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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7.7941
7.6287
7.6093
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7.5289
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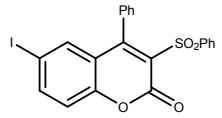
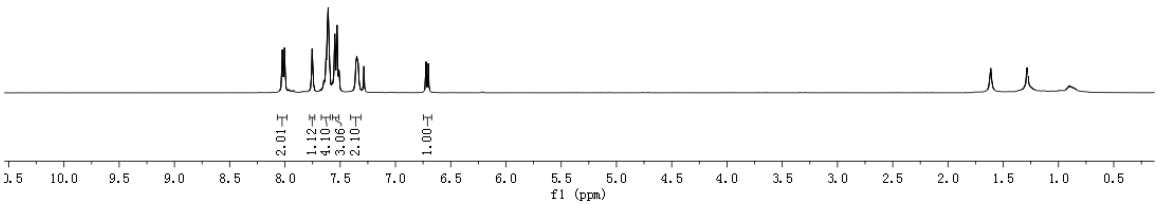
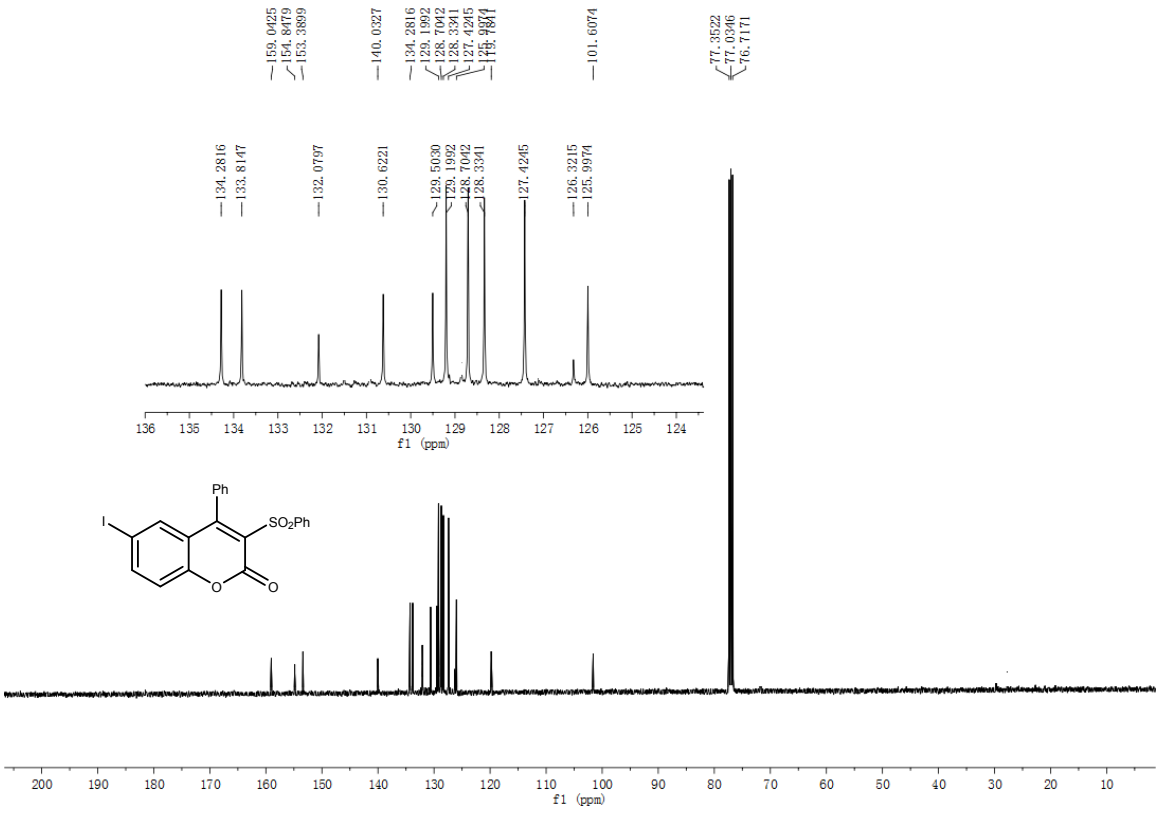
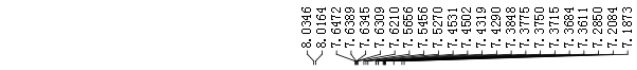
7.3564
7.3501
7.3412
7.2853
6.7234
6.7020


Ph
I
SO2Ph
O
O


2.01
1.12
4.10
3.06
2.10
1.00
f1 (ppm)


159.0425
154.8479
153.3899
140.0327
134.2816
129.1992
128.7042
128.3341
127.4245
101.6074
77.3522
77.0346
76.7171
134.2816
133.8147
132.0797
130.6221
129.5030
129.1992
128.7042
128.3341
127.4245
126.3215
125.9974
f1 (ppm)
Ph
I
SO2Ph
O
O
f1 (ppm)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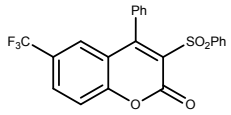
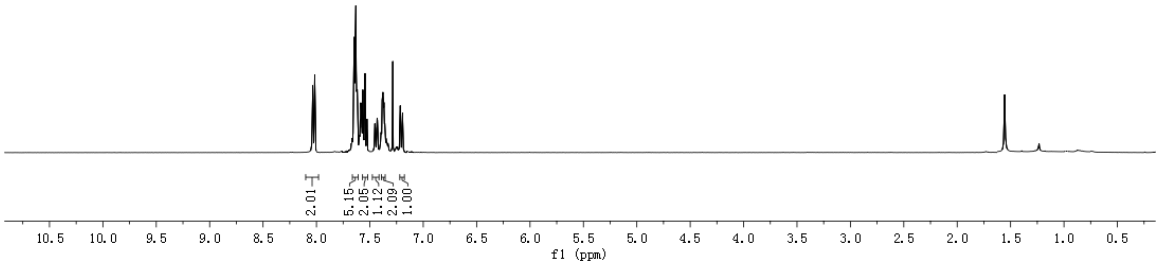
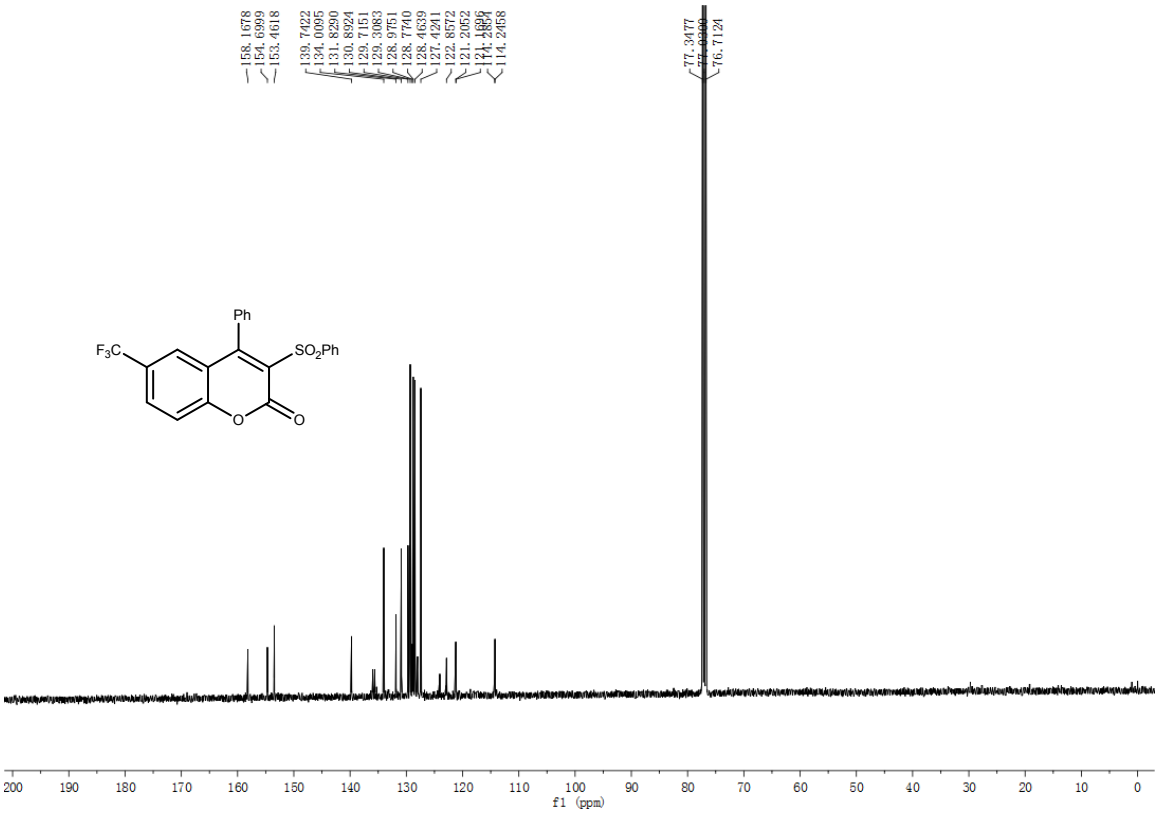
8.0164
7.6472
7.6389
7.6345
7.6309
7.6210
7.5656
7.5456
7.5270
7.4531
7.4502
7.4319
7.4290
7.3848
7.3775
7.3750
7.3715
7.3684
7.3611
7.2850
7.2084
7.1873


Ph
F3C
SO2Ph
O
O


2.01
5.15
2.05
1.12
2.09
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
f1 (ppm)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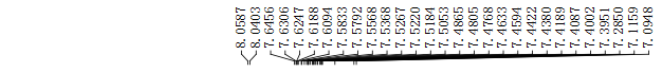
153.4618
139.7422
134.0095
131.8290
130.8924
129.7151
129.3083
128.9751
128.7740
128.4639
127.4241
122.8572
121.2052
114.2458
77.3477
76.7124
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Ph
F3C
SO2Ph
O
O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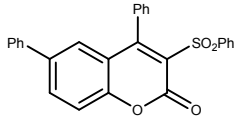
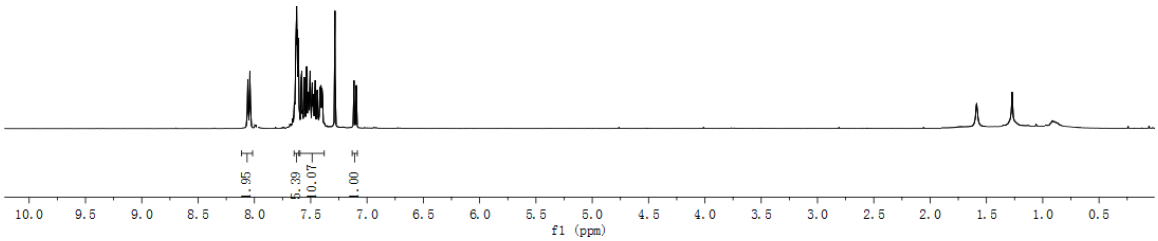
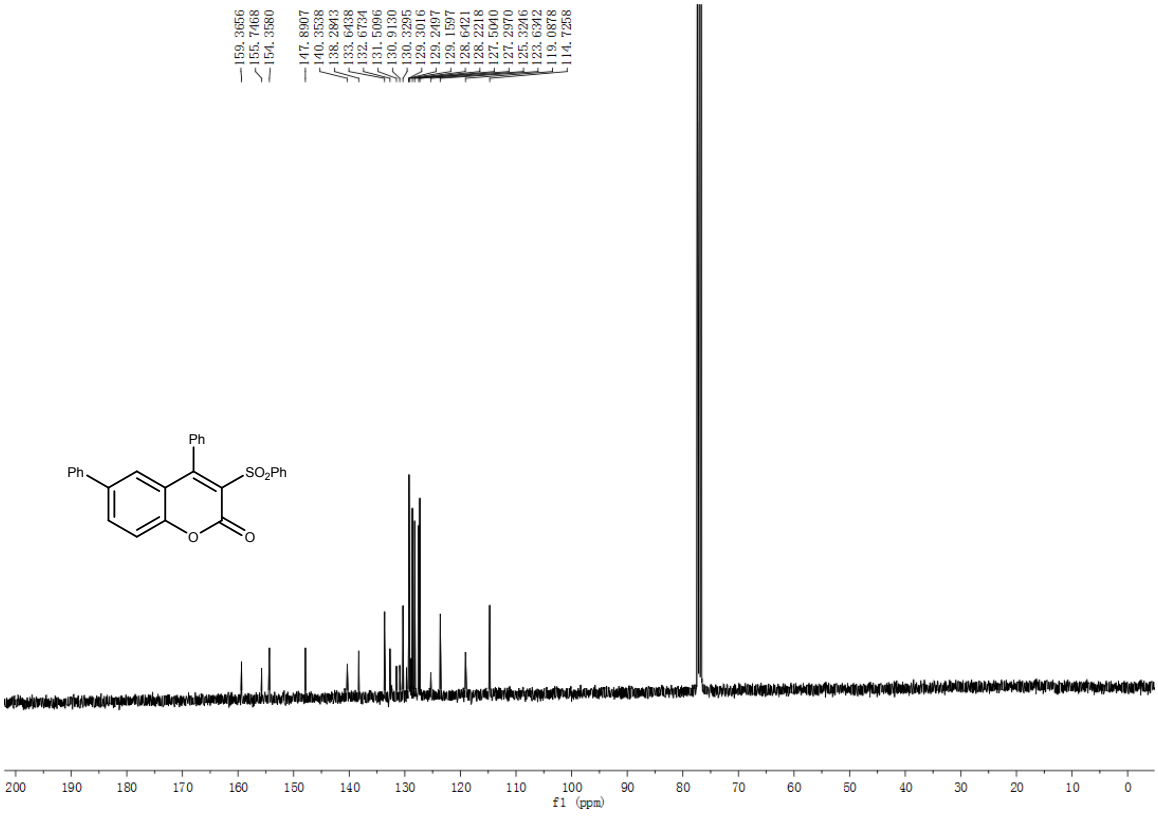
8.0403
7.6456
7.6306
7.6247
7.6188
7.6094
7.5833
7.5792
7.5568
7.5368
7.5267
7.5220
7.5184
7.5053
7.4865
7.4805
7.4768
7.4633
7.4594
7.4422
7.4380
7.4189
7.4087
7.4002
7.3951
7.2850
7.1159
7.0948


Ph
Ph
SO2Ph
O
O


1.95
5.39
10.07
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
f1 (ppm)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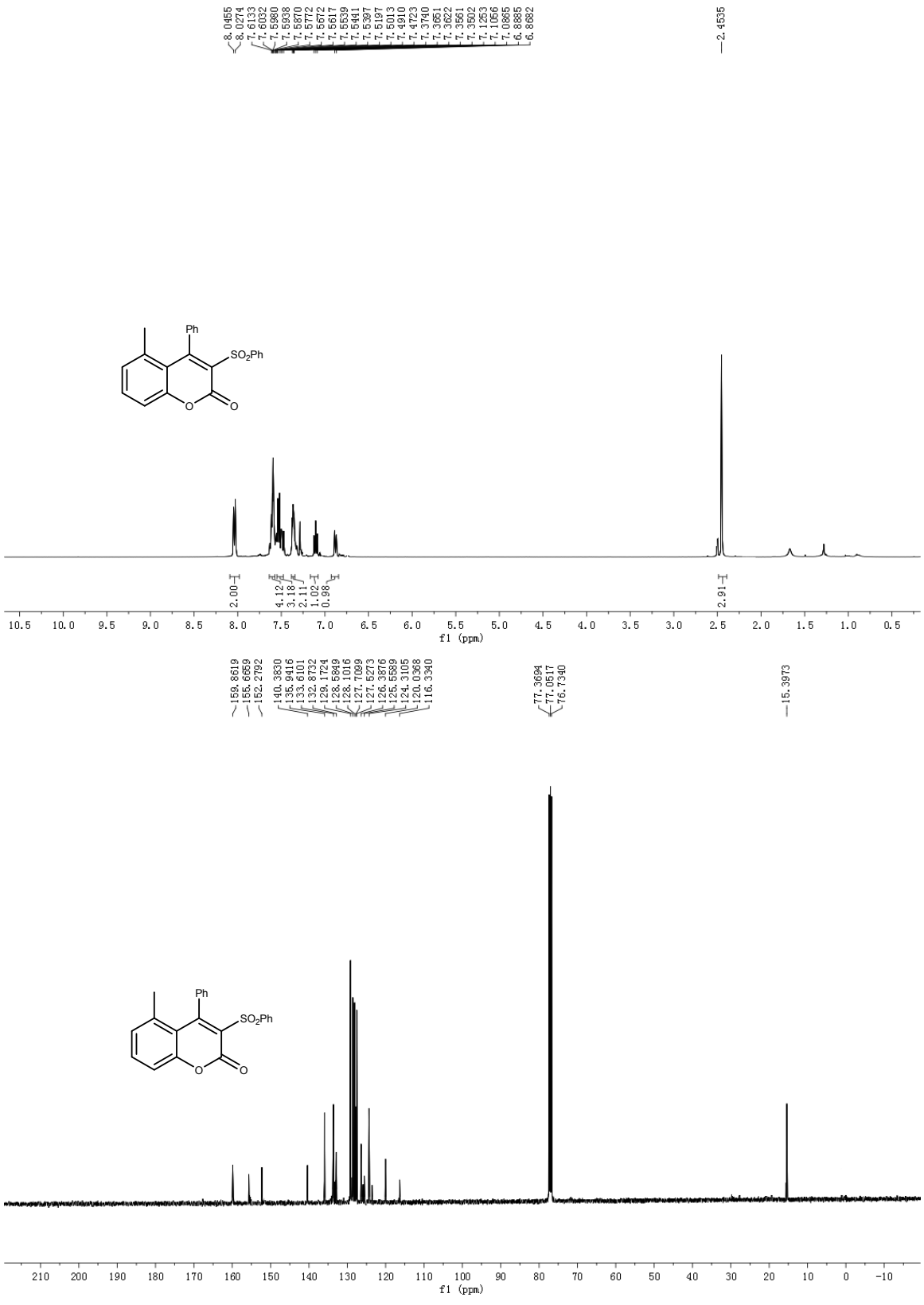
155.7468
154.3580
147.8907
140.3538
138.2843
133.6438
132.6734
131.5096
130.9130
130.3295
129.3016
129.2497
129.1597
128.6421
128.2218
127.5040
127.2970
125.3246
123.6342
119.0878
114.7258
Ph
Ph
SO2Ph
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.6133
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7.5980
7.5938
7.5870
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7.5672
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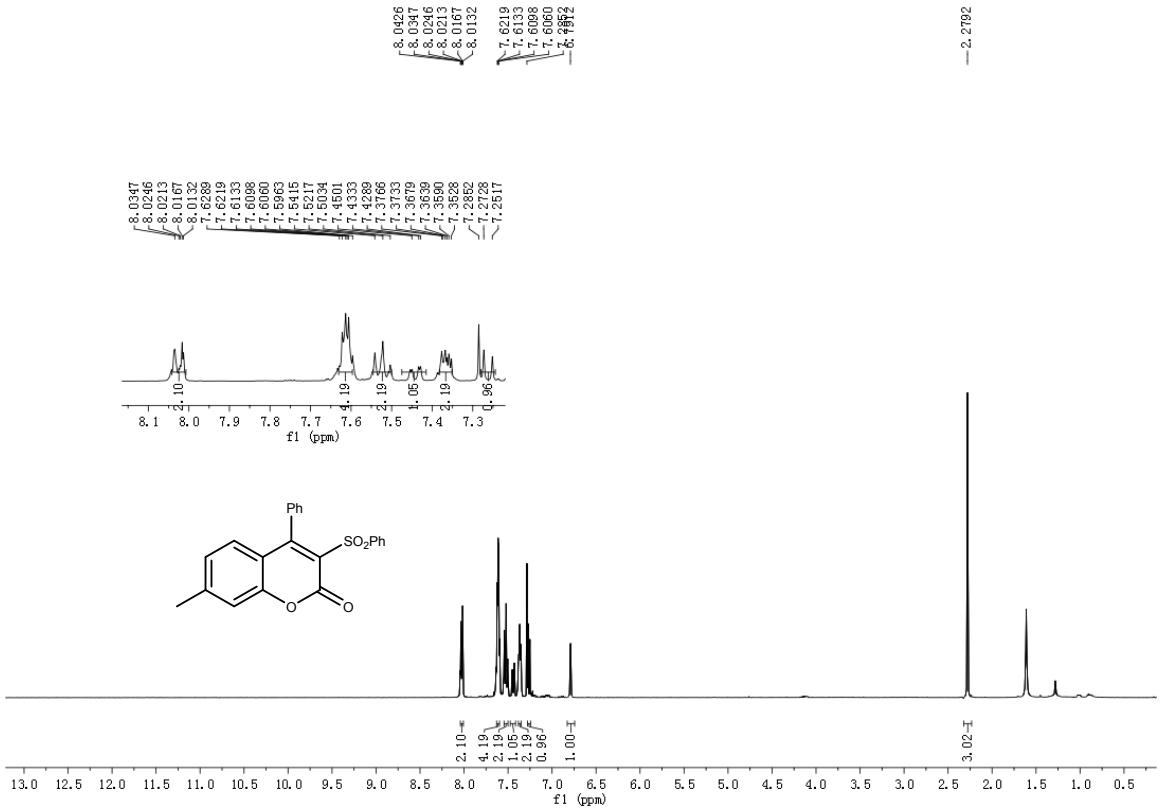
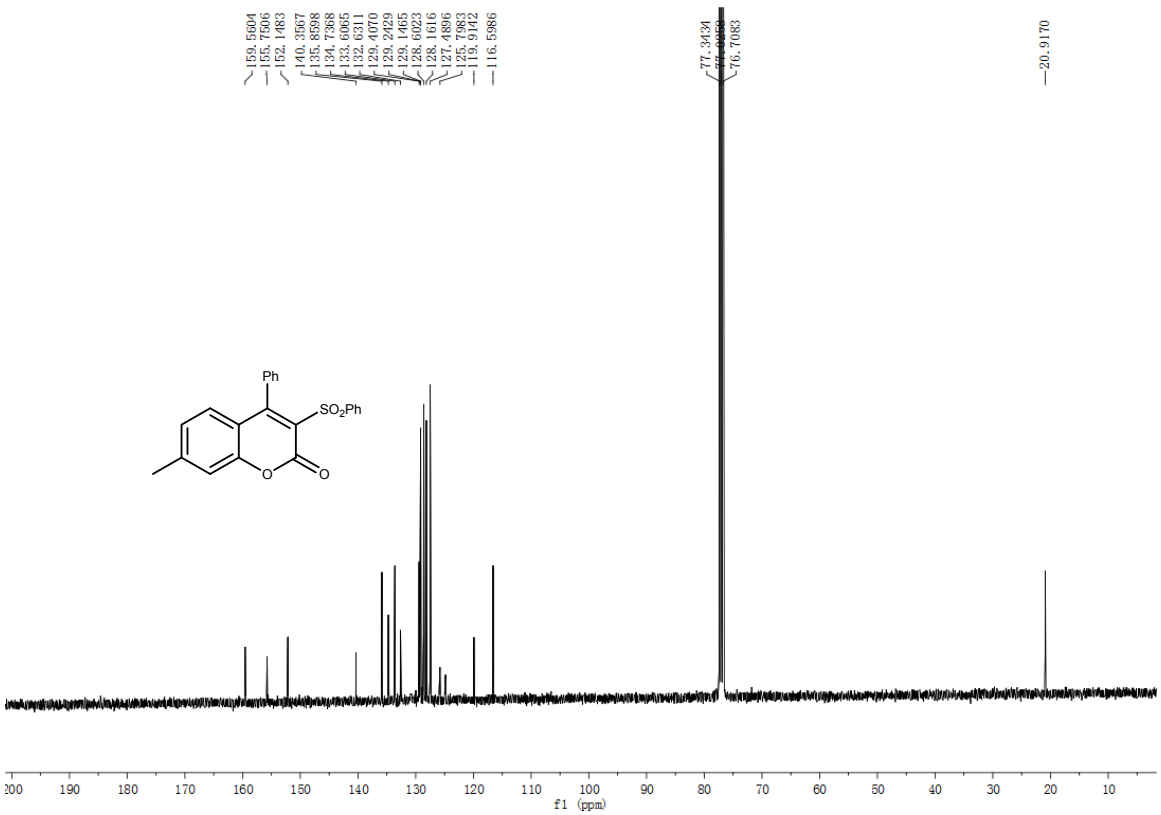
7.5539
7.5441
7.5397
7.5197
7.5013
7.4910
7.4723
7.3740
7.3651
7.3622
7.3561
7.3502
7.1253
7.1056
7.0865
6.8885
6.8682
2.4535
Ph
SO2Ph
O
O
2.00
4.12
3.18
2.11
1.02
0.98
2.91
f1 (ppm)
159.8619
155.6659
152.2792
140.3830
135.9416
133.6101
132.8732
129.1724
128.5849
128.1016
127.7099
127.5273
126.3876
125.5589
124.3105
120.0368
116.3340
77.3694
77.0517
76.7340
15.3973
Ph
SO2Ph
O
O
f1 (ppm)


8.0426
8.0347
8.0246
8.0213
8.0167
8.0132
7.6219
7.6133
7.6098
7.6060
2.2792
8.0347
8.0246
8.0213
8.0167
8.0132
7.6289
7.6219
7.6133
7.6098
7.6060
7.5963
7.5415
7.5217
7.5034
7.4501
7.4333
7.4289
7.3766
7.3733
7.3679
7.3639
7.3590
7.3528
7.2852
7.2728
7.2517
2.10
4.19
2.19
1.05
2.19
0.96
f1 (ppm)
Ph
SO2Ph
O
O
2.10
4.19
2.19
1.05
2.19
0.96
1.00
3.02
f1 (ppm)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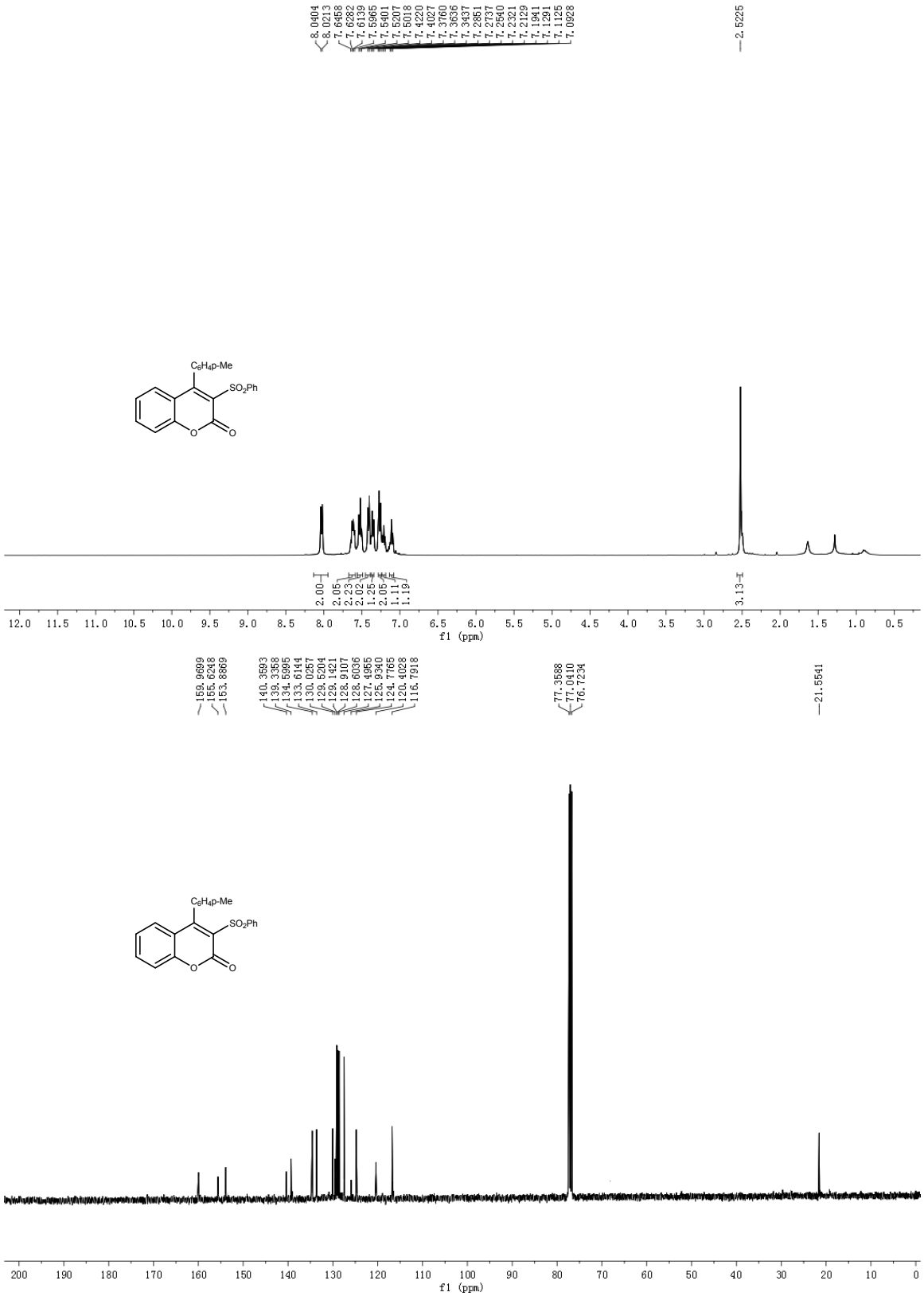
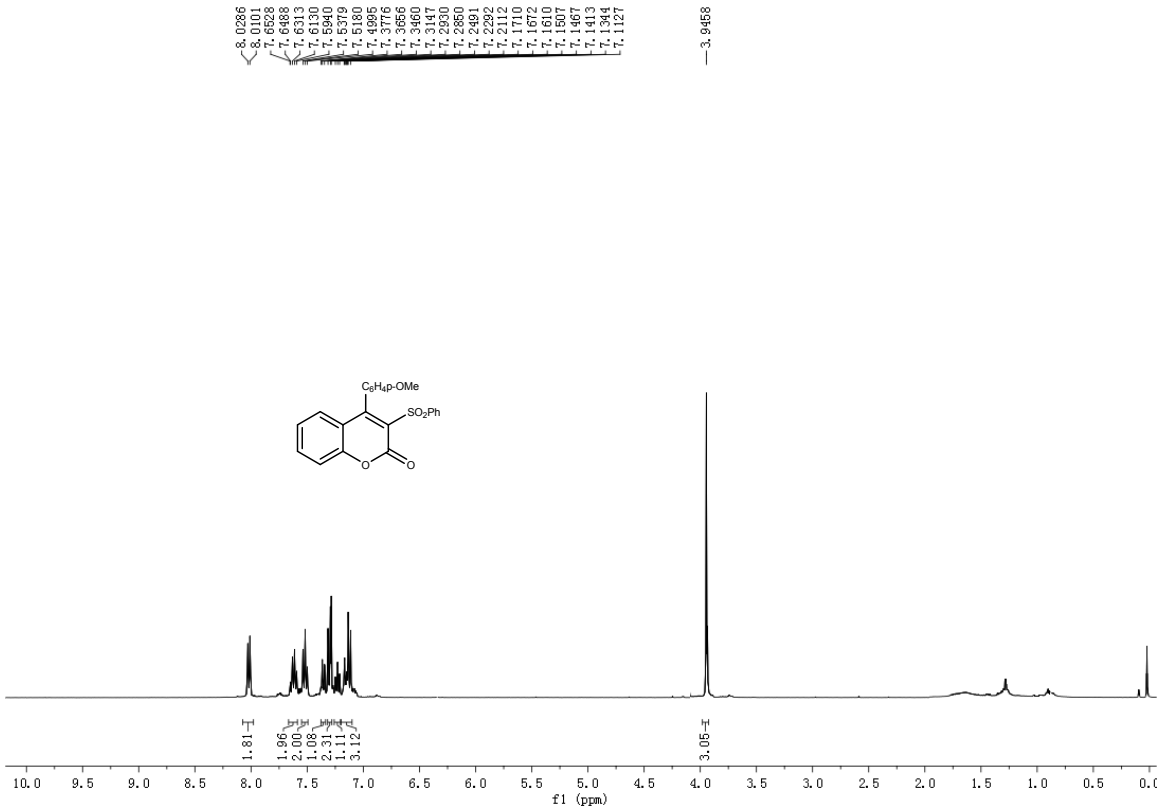
152.1483
140.3567
135.8598
134.7368
133.6065
132.6311
129.4070
129.2429
129.1465
128.6023
128.1616
127.4896
125.7983
119.9142
116.5986
77.3434
77.0959
76.7083
20.9170
Ph
SO2Ph
O
O
f1 (ppm)


8.0404
8.0213
7.6458
7.6282
7.6139
7.5965
7.5401
7.5207
7.5018
7.4220
7.4027
7.3760
7.3636
7.3437
7.2851
7.2737
7.2540
7.2321
7.2129
7.1941
7.1291
7.1125
7.0928
2.5225
C6H4p-Me
SO2Ph
O
O
2.00
2.05
2.23
2.02
1.25
2.05
1.11
1.19
3.13
12.0 11.5 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
f1 (ppm)
159.9699
155.6248
153.8869
140.3693
139.3358
134.5995
133.6144
130.0257
129.5204
129.1421
128.9107
128.6036
127.4955
125.9340
124.7765
120.4028
116.7918
77.3588
77.0410
76.7234
21.5541
C6H4p-Me
SO2Ph
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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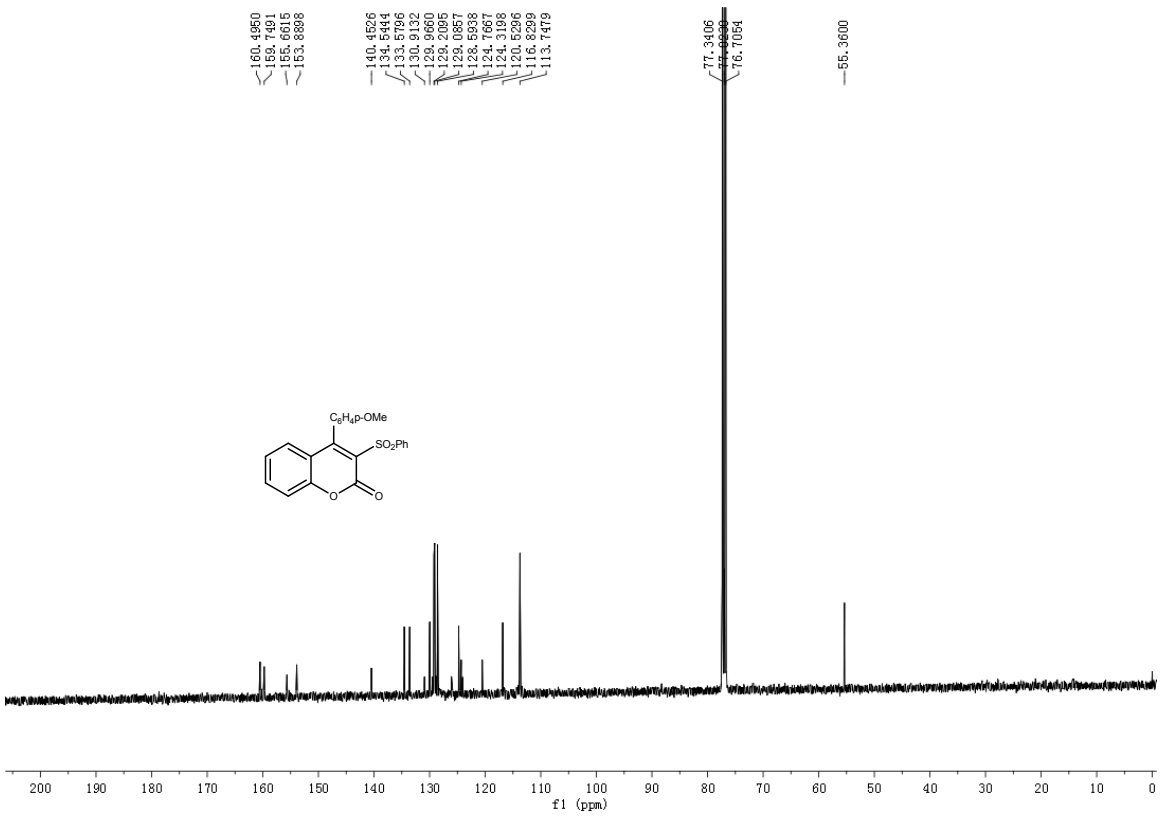
7.3656
7.3460
7.3147
7.2930
7.2850
7.2491
7.2292
7.2112
7.1710
7.1672
7.1610
7.1507
7.1467
7.1413
7.1344
7.1127
3.9458
C6H4p-OMe
SO2Ph
O
O
1.81
1.96
2.00
1.08
2.31
1.11
3.12
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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153.8888
140.4526
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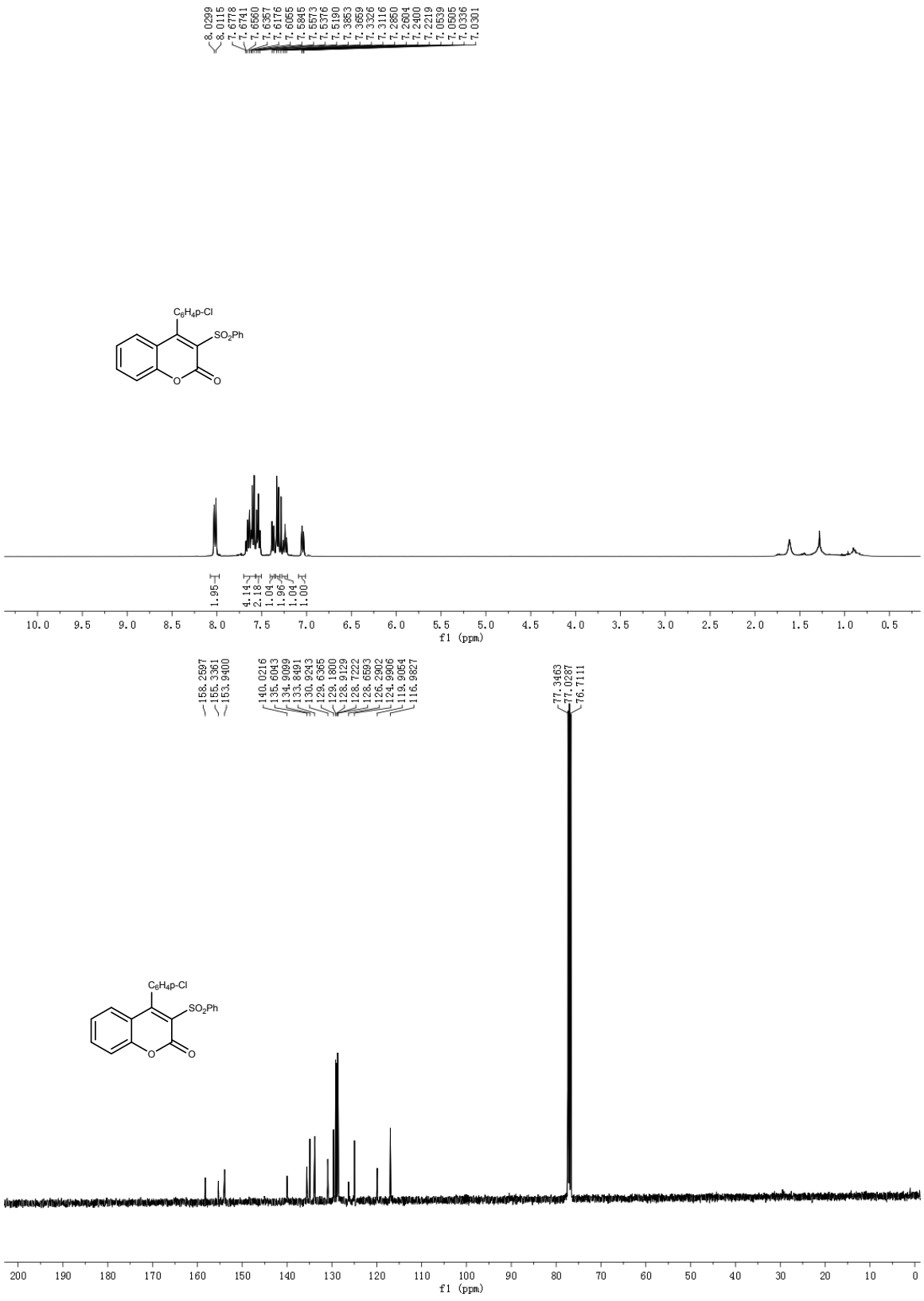
129.0857
128.5938
124.7667
124.3198
120.5296
116.8299
113.7479
77.3406
77.0594
76.7054
55.3600
C6H4p-OMe
SO2Ph
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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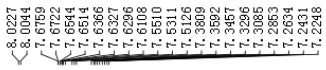
7.5845
7.5573
7.5376
7.5190
7.3853
7.3659
7.3326
7.3116
7.2850
7.2604
7.2400
7.2219
7.0539
7.0505
7.0336
7.0301
C6H4p-Cl
SO2Ph
O
O
1.95
4.14
2.18
1.04
1.96
1.04
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)
158.2597
155.3361
153.9400
140.0216
135.6043
134.9089
133.8491
130.9243
129.6365
129.1800
128.9129
128.7222
128.6593
126.2902
124.9906
119.9054
116.9827
77.3463
77.0287
76.7111
C6H4p-Cl
SO2Ph
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.5311
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7.2853
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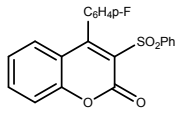
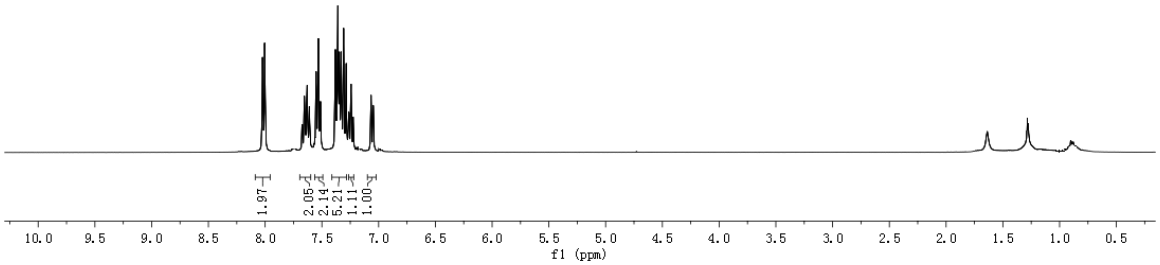
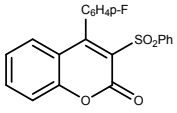
7.2431
7.2248

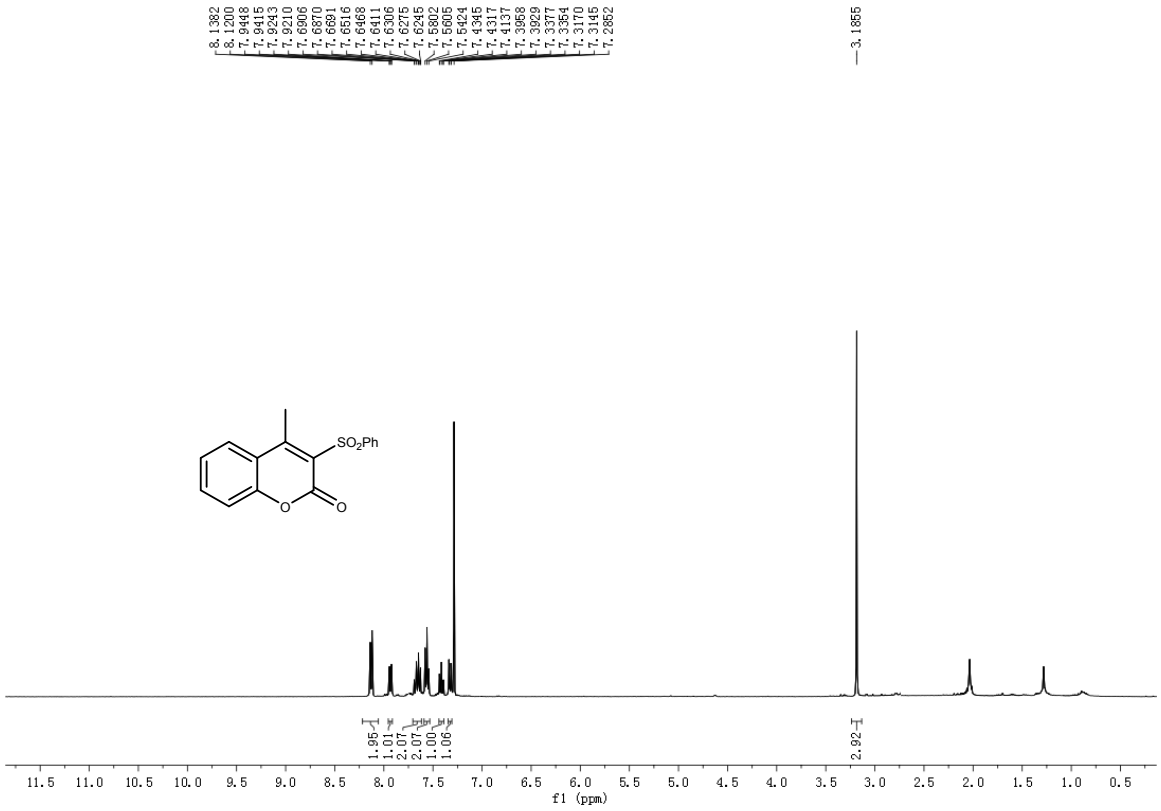

C6H4p-F
SO2Ph
O
O


1.97
2.05
2.14
5.21
1.11
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
f1 (ppm)


164.5176
162.0364
158.5907
155.4047
153.9203
140.1306
134.8587
133.8007
129.6850
129.5670
129.4839
129.1359
128.7027
128.3080
128.2707
126.3850
124.9644
120.1328
116.9545
115.7393
115.5198


C6H4p-F
SO2Ph
O
O

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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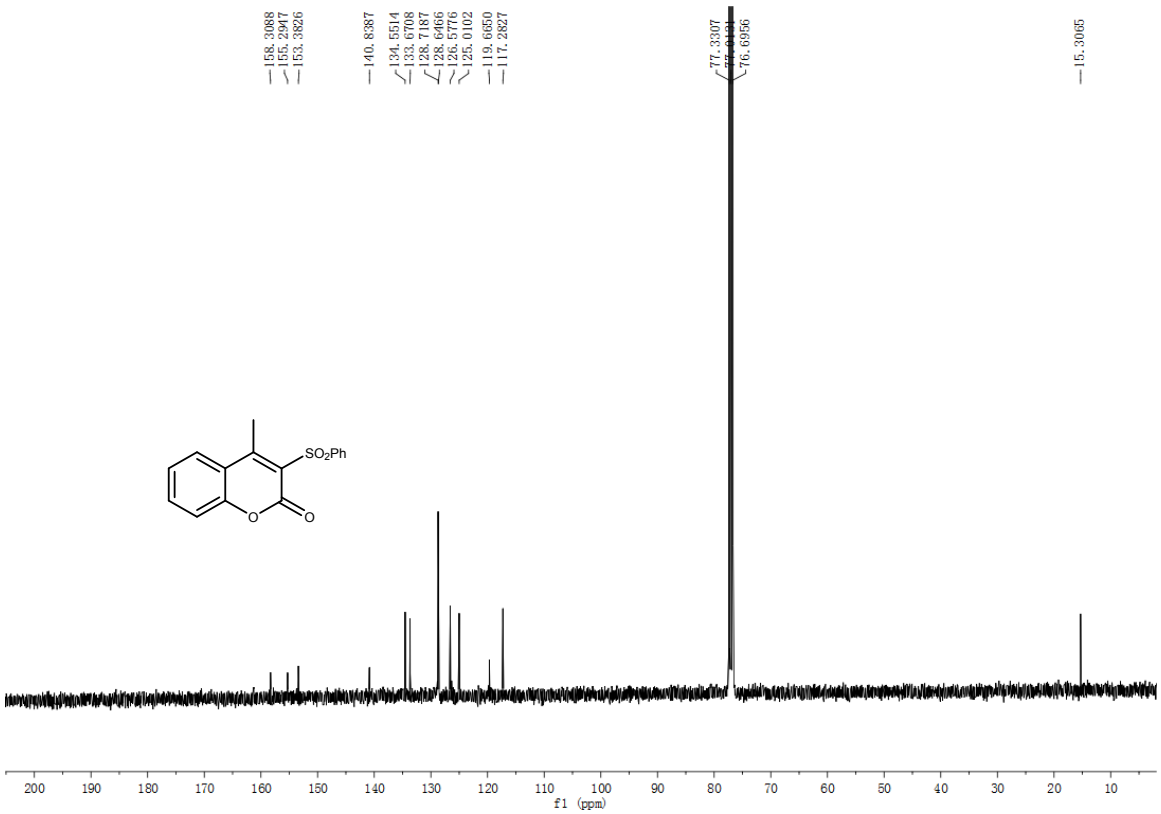
7.5605
7.5424
7.4345
7.4317
7.4137
7.3968
7.3929
7.3377
7.3364
7.3170
7.3145
7.2852
3.1855
SO2Ph
O
O
1.95
1.01
2.07
2.07
1.00
1.06
2.92
f1 (ppm)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153.3826
140.8387
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126.5776
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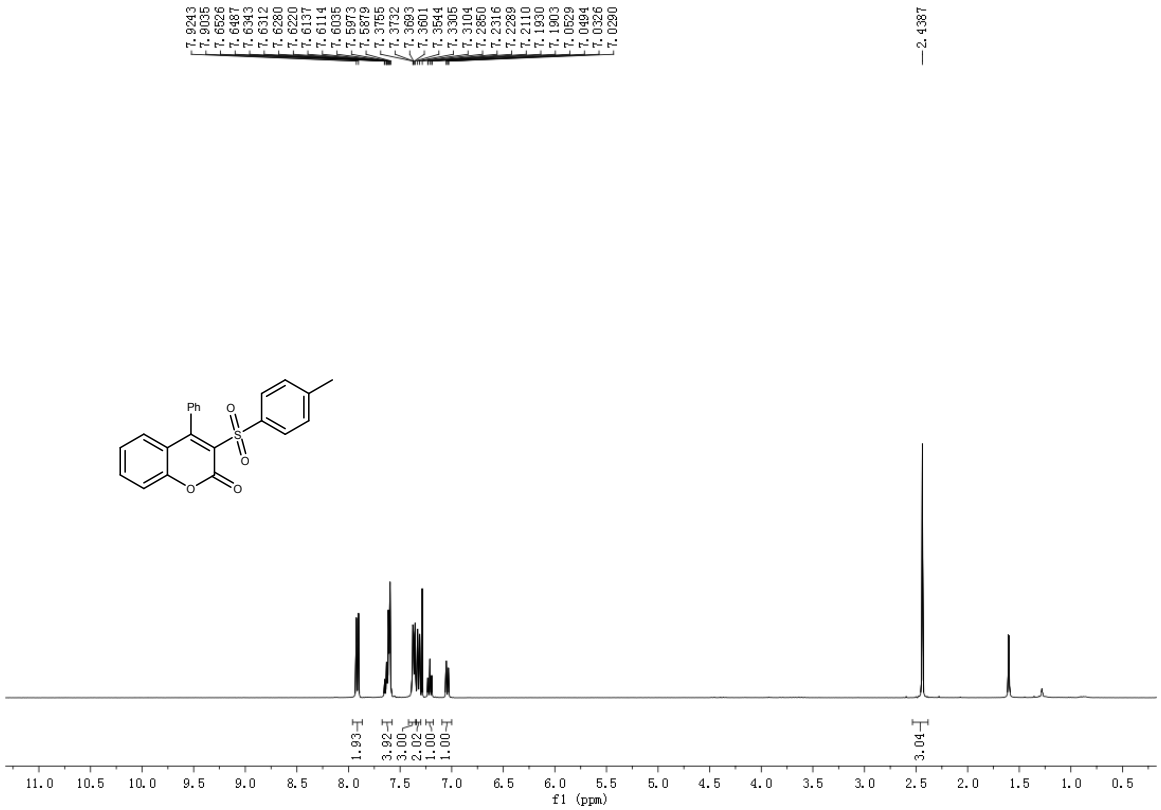
117.2827
77.3307
77.0189
76.6956
15.3065
SO2Ph
O
O
f1 (ppm)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7.6487
7.6343
7.6312
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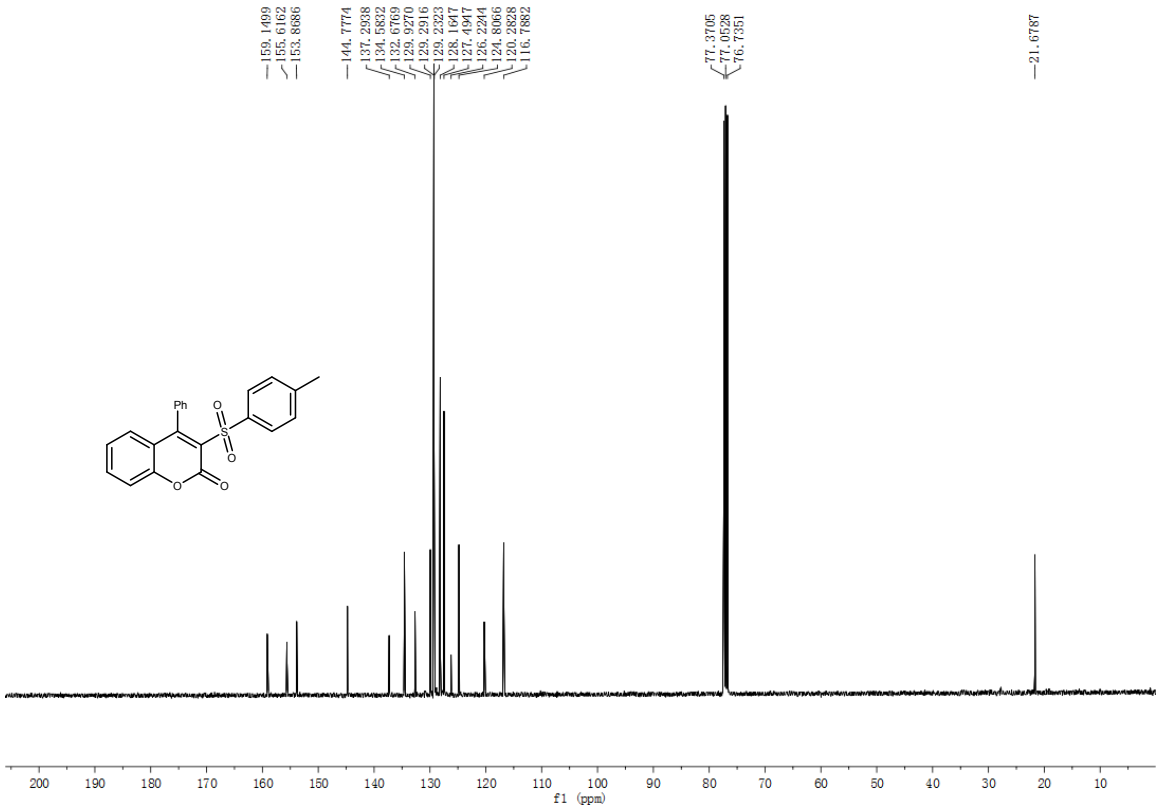
7.6220
7.6137
7.6114
7.6035
7.5973
7.5879
7.3755
7.3732
7.3693
7.3601
7.3544
7.3305
7.3104
7.2850
7.2316
7.2289
7.2110
7.1930
7.1903
7.0629
7.0494
7.0326
7.0290
2.4387
Ph
O
S
O
O
O
1.93
3.82
3.00
2.02
1.00
1.00
3.04
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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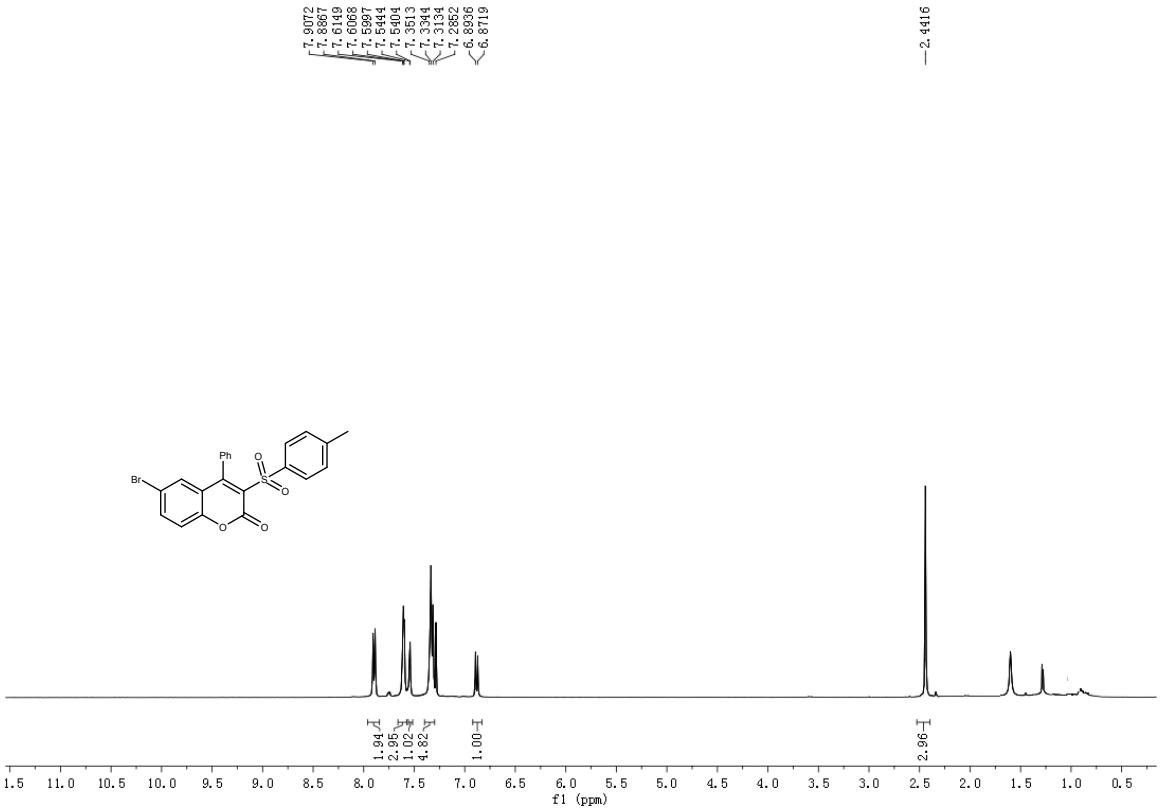
155.6162
153.8686
144.7774
137.2938
134.5832
132.6769
129.9270
129.2916
129.2323
128.1647
127.4947
126.2244
124.8066
120.2828
116.7862
77.3705
77.0528
76.7351
21.6787
Ph
O
S
O
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)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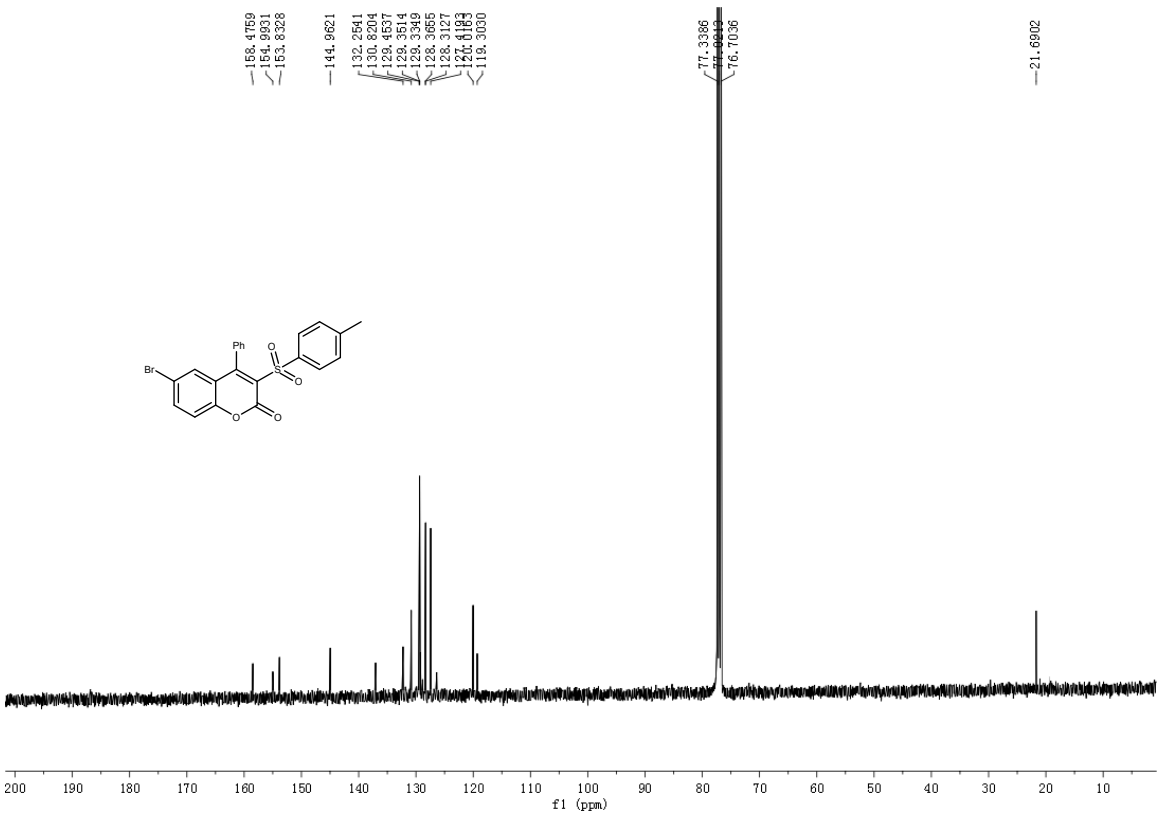
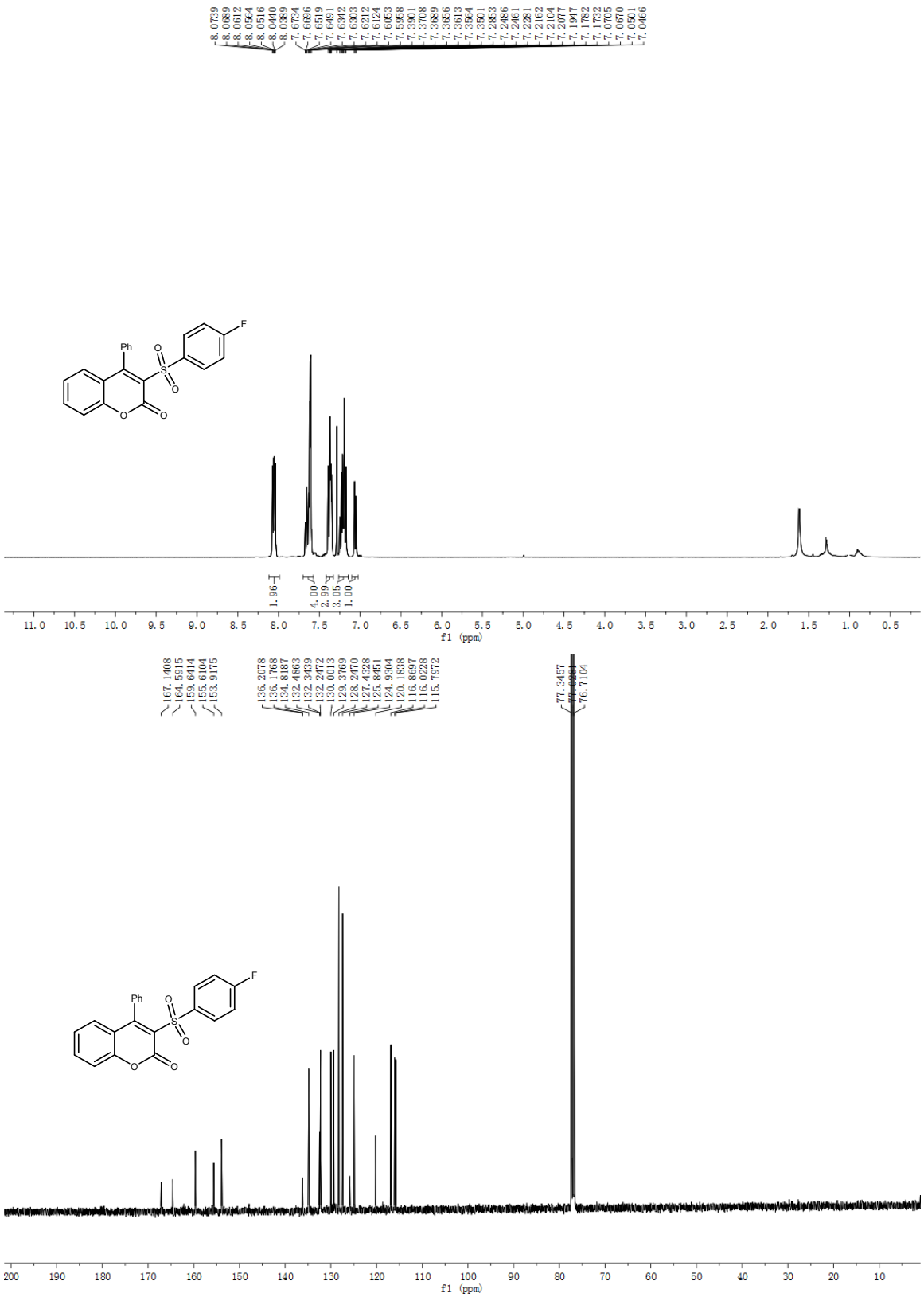
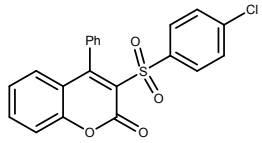
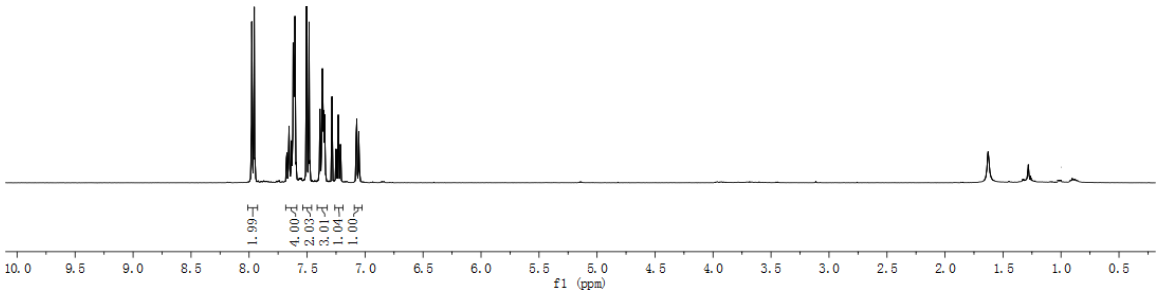
7.8867
7.6149
7.6068
7.5997
7.5444
7.5404
7.3513
7.3344
7.3134
7.2852
6.8936
6.8719
2.4416
Ph
Br
O
S
O
O
O
1.94
2.95
1.02
4.82
1.00
2.96
f1 (ppm)

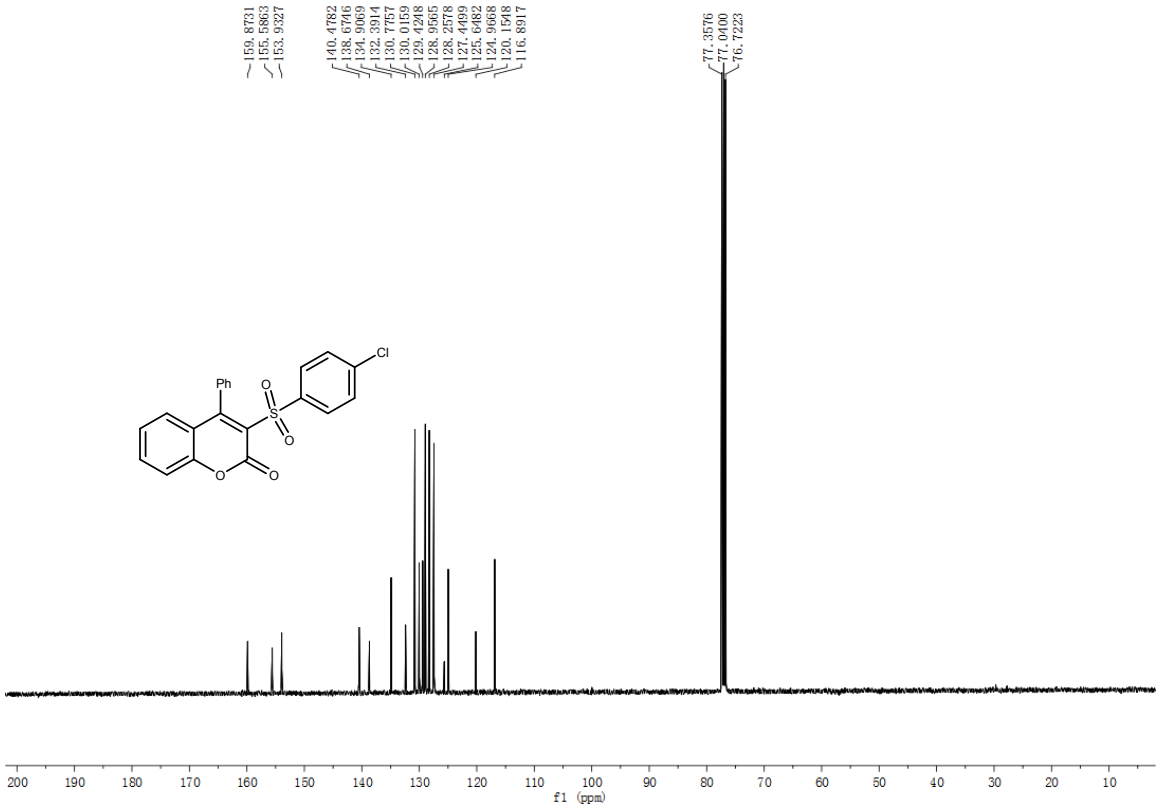

158.4759
154.9931
153.8328
144.9621
132.2541
130.8204
129.4537
129.3514
129.3349
128.3665
128.3127
119.3030
77.3386
76.7036
21.6902
Ph
Br
O
S
O
O
O
f1 (ppm)

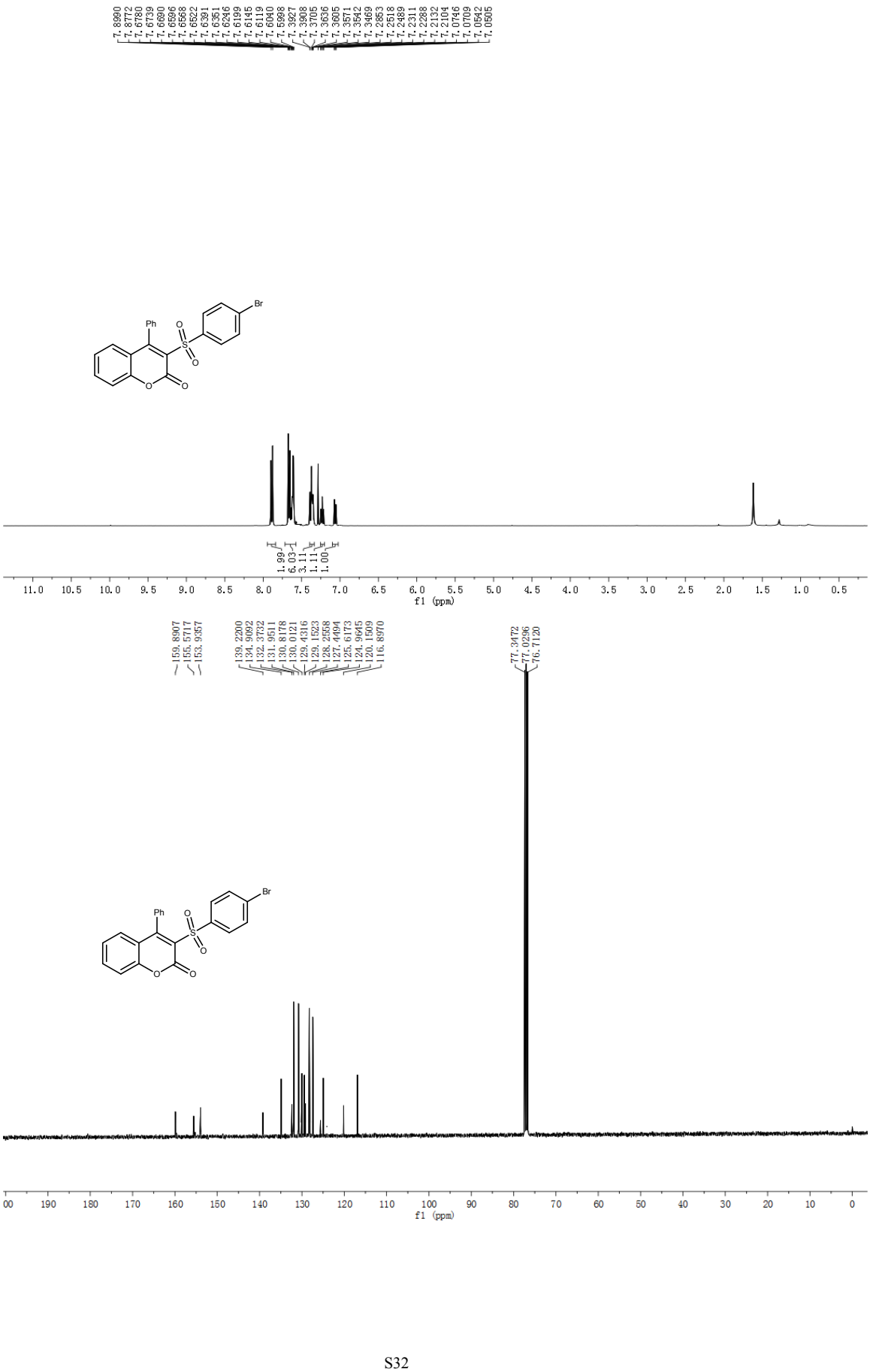

8.0739
8.0689
8.0612
8.0564
8.0516
8.0440
8.0389
7.6734
7.6696
7.6519
7.6491
7.6342
7.6303
7.6212
7.6124
7.6053
7.5958
7.3901
7.3708
7.3689
7.3656
7.3613
7.3564
7.3501
7.2853
7.2486
7.2461
7.2281
7.2162
7.2104
7.2077
7.1947
7.1782
7.1732
7.0705
7.0670
7.0501
7.0466
Ph
O
S
O
O
O
F
1.96
4.00
2.99
3.05
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
f1 (ppm)
167.1408
164.5915
159.6414
155.6104
153.9175
136.2078
136.1768
134.8187
132.4863
132.3439
132.2472
130.0013
129.3769
128.2470
127.4328
125.8451
124.9304
120.1838
116.8697
116.0228
115.7972
77.3457
77.0951
76.7104
Ph
O
S
O
O
O
F
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

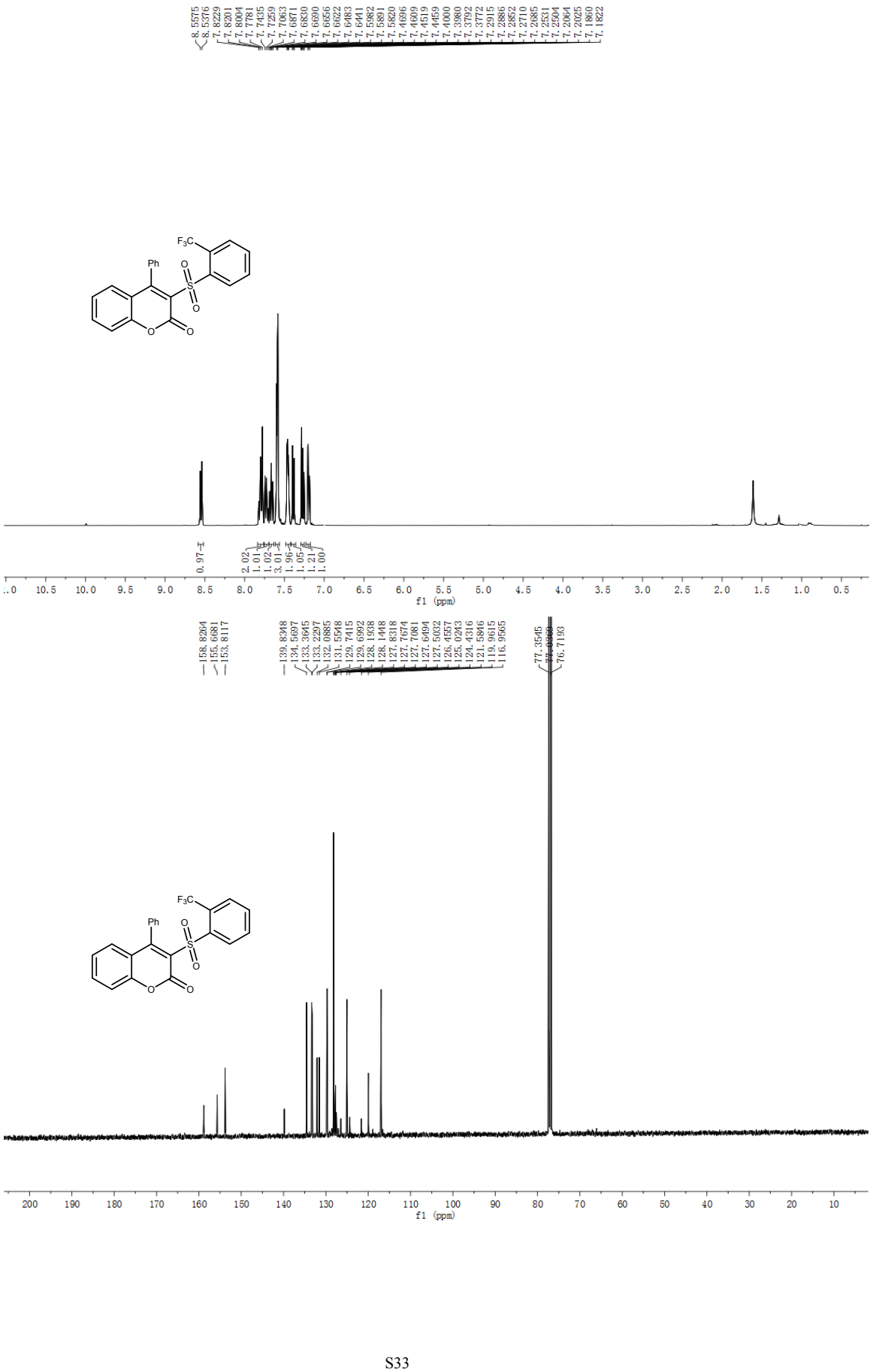

7.9768
7.9550
7.6586
7.6555
7.6524
7.6379
7.6339
7.6204
7.6121
7.6045
7.5094
7.4826
7.3911
7.3891
7.3678
7.3597
7.3560
7.3492
7.2852
7.2515
7.2489
7.2309
7.2130
7.2103
7.0747
7.0711
7.0543
7.0507

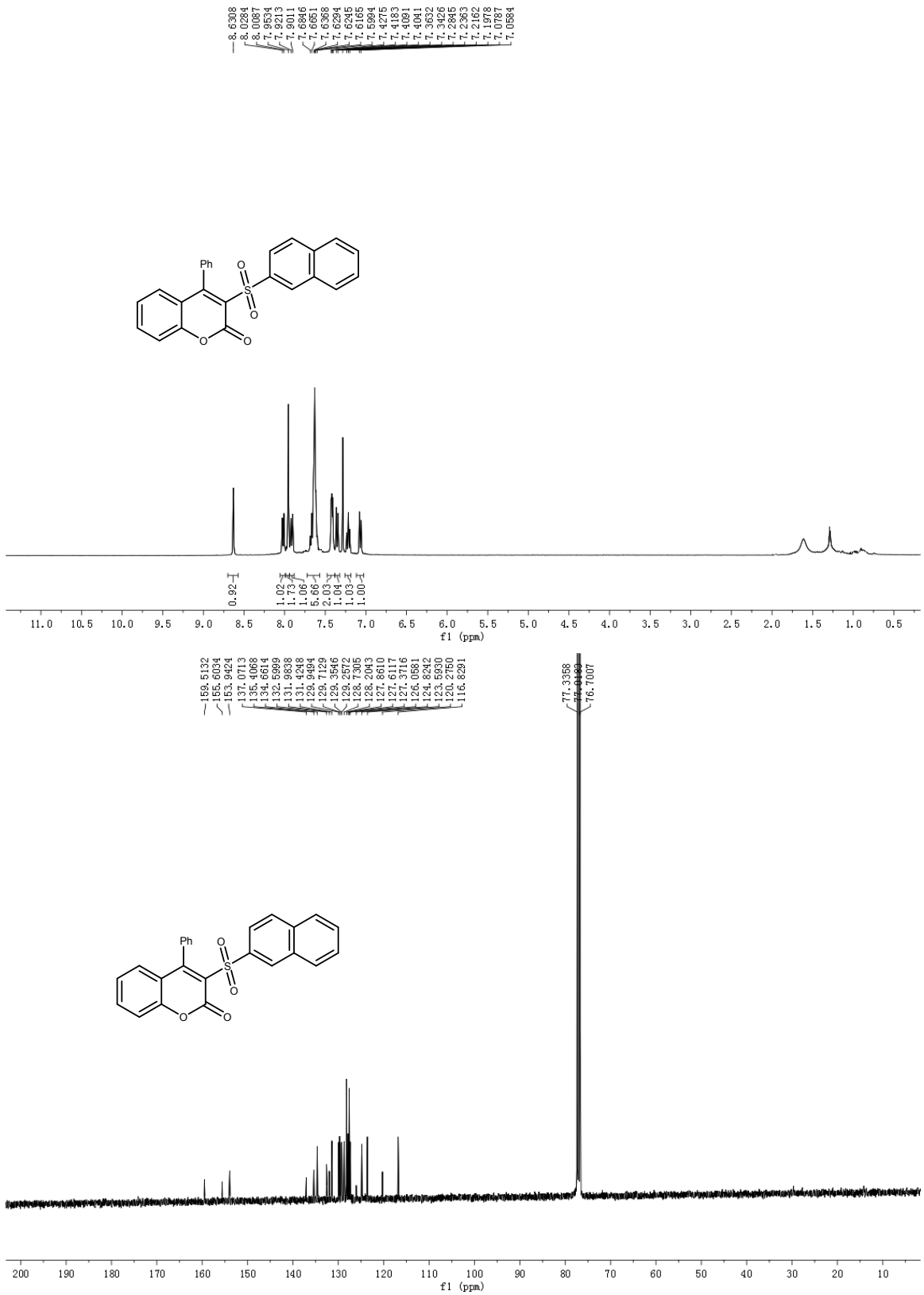

Ph
O
S
O
O
O
Cl


1.99
4.00
2.03
3.01
1.04
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
f1 (ppm)


159.8731
155.5863
153.9327
140.4782
138.6746
134.9069
132.3914
130.7757
130.0159
129.4248
128.9565
128.2578
127.4499
125.6482
124.9668
120.1548
116.8917
77.3576
77.0400
76.7223
Ph
O
S
O
O
O
Cl
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.8990
7.8772
7.6780
7.6739
7.6690
7.6596
7.6568
7.6522
7.6391
7.6351
7.6246
7.6199
7.6145
7.6119
7.6040
7.5898
7.3927
7.3908
7.3705
7.3636
7.3605
7.3571
7.3542
7.3469
7.2853
7.2518
7.2489
7.2311
7.2288
7.2132
7.2104
7.0746
7.0709
7.0642
7.0505
Br
Ph
O
S
O
O
O
1.99
6.03
3.11
1.11
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
f1 (ppm)
159.8907
155.5717
153.9357
139.2200
134.9092
132.3732
131.9511
130.8178
130.0121
129.4316
129.1523
128.2558
127.4494
125.6173
124.9645
120.1509
116.8970
77.3472
77.0296
76.7120
Br
Ph
O
S
O
O
O
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.5575
8.5376
7.8229
7.8201
7.8004
7.7781
7.7435
7.7259
7.7063
7.6871
7.6830
7.6690
7.6656
7.6622
7.6483
7.6441
7.5982
7.5891
7.5820
7.4696
7.4609
7.4519
7.4459
7.4000
7.3980
7.3792
7.3772
7.2915
7.2886
7.2852
7.2710
7.2685
7.2531
7.2504
7.2064
7.2025
7.1860
7.1822
F3C
Ph
O
S
O
O
O
0.97
2.02
1.01
1.02
3.01
1.96
1.05
1.21
1.00
f1 (ppm)
158.8264
155.6681
153.8117
139.8348
134.5697
133.3645
133.2297
132.0885
131.5548
129.7415
129.6992
128.1938
128.1448
127.8318
127.7674
127.7081
127.6494
127.5032
126.4557
125.0243
124.4316
121.5846
119.9615
116.9565
77.3545
76.7193
f1 (ppm)


8.6308
8.0284
8.0087
7.9534
7.9213
7.9011
7.6846
7.6651
7.6368
7.6294
7.6245
7.6165
7.5994
7.4275
7.4183
7.4091
7.4041
7.3652
7.3426
7.2845
7.2363
7.2162
7.1978
7.0787
7.0584
Ph
O
S
O
O
O
0.92
1.02
1.73
1.06
5.66
2.03
1.04
1.03
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
f1 (ppm)
159.5132
155.6034
153.9424
137.0713
135.4068
134.6614
132.5899
131.9838
131.4248
129.9494
129.7129
129.3546
129.2572
128.7305
128.2043
127.8610
127.6117
127.3716
126.0581
124.8242
123.5930
120.2760
116.8291
77.3368
77.0183
76.7007
Ph
O
S
O
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)