Supplementary Information

Construction of 6*H*-benzo[*c*]thiochromenes via a tandem reaction of arynes with thionoesters

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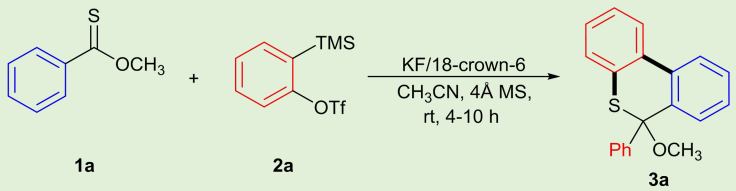
1. General information

All commercially available reagent grade chemicals were purchased from Adamas, Alfa Aesar and Bide Pharmatech and used as received without further purification unless otherwise stated. ^{1}H NMR and ^{13}C NMR were recorded in $CDCl_3$ on a Bruker Avance III 400 MHz spectrometer with TMS as internal standard 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). High resolution mass spectra (HRMS) were obtained on a Thermo Scientific Q Exactive mass spectrometry equipped with an ESI or APCI source. Column chromatography was performed on silica gel (200-300 mesh).

2. General procedure

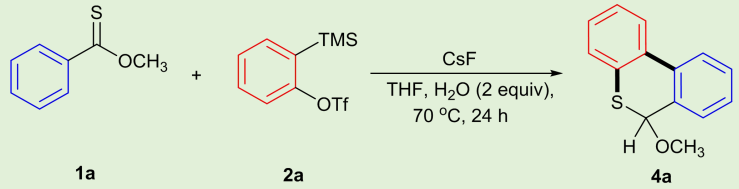
2.1 General procedure for the tandem reaction of thionoester and aryne leading to 6H-benzo[c]thiochromene



1a **2a** **3a**

To a mixture of **1a** (0.10 mmol), KF/18-C-6 (0.90 mmol) and 4Å MS (100 mg) in anhydrous acetonitrile (1.0 mL) was added 2-(trimethylsilyl) aryl triflate **2a** (0.30 mmol) under nitrogen atmosphere. The mixture was stirred at room temperature until full consumption of the thionoester **1a** as indicated by TLC. The reaction mixture was then diluted with ethyl acetate, filtered through a short pad of silica gel, and concentrated. The crude product was purified by flash column chromatography on silica gel (silica gel, PE/EtOAc (v : v) = 50:1-80:1) to afford the desired product **3a.**

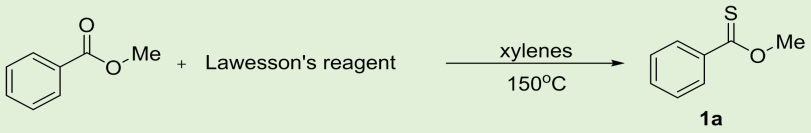
2.2 General procedure for the reaction of thionoester and aryne leading to 6-alkoxyl-6H-benzo[c]thiochromene



1a **2a** **4a**

To a mixture of **1a** (0.10 mmol) and CsF (0.60 mmol) in anhydrous THF (1.0 mL) was added 2-(trimethylsilyl) aryl triflate **2a** (0.20 mmol) and H_2O (0.2 mmol) under nitrogen atmosphere. The mixture was stirred at 68 °C until full consumption of the thionoester **1a** as indicated by TLC. The reaction mixture was then diluted with ethyl acetate, concentrated. The crude product was purified by flash column chromatography on silica gel (silica gel, PE/EtOAc (v: v) = 80:1) to afford the desired product **4a.**

2.3 Typical procedure for the preparation of thionoesters[1]



1a

The mixture of methyl benzoate (10 mmol) and Lawesson's reagent (10 mmol, 4.05 g) in xylenes (15 mL) was refluxed at 150 °C until full consumption of the ester monitored by TLC. Subsequently, the reaction mixture was allowed to room temperature, excess of the Lawesson's reagent precipitated out. The resulting solution was diluted with hexane (10 mL) to precipitate any residual Lawesson's reagent. The resulting solution was filtered through a short pad of silica gel, and concentrated. The residue was purified by flash column chromatography on silica gel (PE as eluent) to get the pure product **1a.**

***O*-methyl benzothioate (1a)**[1] Yellow oil, ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.19-8.16 (m, 2H), 7.52-7.48 (m, 1H), 7.39 – 7.33 (m, 2H), 4.27 (s, 3H).; ^{13}C NMR (101 MHz, Chloroform-*d*) δ 212.2, 138.2, 132.7, 128.8, 128.7, 128.2, 128.1, 59.3.

3. Bioactive study of 6-alkoxy-6-aryl-6H-benzo[c]thiochromenes and 6-alkoxyl-6H-benzo[c]thiochromenes

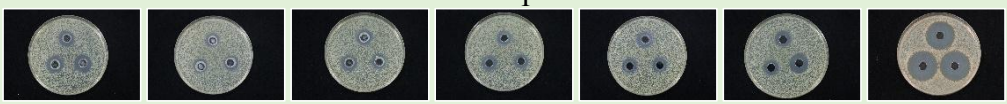
Newly synthesized 6-alkoxy-6-aryl-6H-benzo[c]thiochromenes **3a, 3h, 3j** and 6-alkoxyl-6H-benzo[c]thiochromenes **4a** and **4e**, were selected to screen the antibacterial activity against Gram-negative bacteria *E. coli* and Gram-positive bacteria *Staphylococcus aureus (SA)* using the well diffusion method. Standard drug Norfloxacin and DMSO were used as positive and negative control, respectively. The *in vitro* antifungal activity was performed against *candida Albicans* using well diffusion method. The antifungal drugs Fluconazole was used as reference. All the test solutions were prepared in DMSO at 1000 μg/mL concentration and the wells were filled with 200 μL (200 μg) of the samples. Three parallel experiments were carried out for each compounds. The results of antimicrobial activity in zone of inhibition (mm) have been presented in Table S1 and Table S2. The antimicrobial activity result analysis of **3a, 3h, 3j, 4a and 4e** revealed that, against *E. coli* compound **3a** showed moderate activity, whereas other compounds showed no activity (Table S1). Against *Staphylococcus aureus (SA),* none of tested products showed activity (Table S2).

Table S1 Anti *E. coli* activity in zone of inhibition (mm) of selected products

3a **3h** **3i** **4a** **4e** DMSO Norfloxacin

Product	Parallel experiments of anti E. coli activity in zone of inhibition (mm)			Average (mm)
	1st	2nd	3rd	
3a	17	19	20	**18.7**
3h	12	12	12	12
3j	10	10.5	11	10.5
4a	13	13	13	13
4e	13	13	13	13
DMSO	14	15	17	15.3
Norfloxacin	27	29	29	28.3

Table S2 Anti *SA* activity in zone of inhibition (mm)
of selected products



3a **3h** **3j** **4a** **4e** DMSO Norfloxacin

Product	Parallel experiments of anti SA activity in zone of inhibition (mm)			Average (mm)
	1st	2nd	3rd	
3a	7	8	9	8
3h	5	5	6	5.3
3j	5.5	6	7	6.2
4a	5	5	6	5.3
4e	6	6	7	6.3
DMSO	6	8	11	8.3
Norfloxacin	22	23	23	22.7

The preliminary antifungal activity (Table S3) showed that 6-alkoxy-6-aryl-6H-benzo[c]thiochromenes 3a, 3h, 3j and 6-alkoxyl-6H-benzo[c]thiochromenes 4a and 4e exhibited moderate to good antifungal activity.

Table S3 Antifungal activity in zone of inhibition (mm)

of selected products

3a 3h 3j 4a 4e DMSO Fluconazole

Product	Parallel experiments of anti *candida Albicans* activity in zone of inhibition (mm)			Average (mm)
	1st	2nd	3rd	
3a	6	6	6	**6**
3h	6	6	7	**6.3**
3j	5	5.5	7	5.8
4a	6	**7**	**8**	**7**
4e	5	6	7	**6**
DMSO	5	6	6	5.6
Fluconazole	8	8	8	8

4. Single-crystal X-ray structure analysis

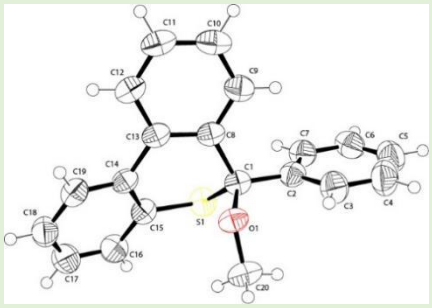


Figure S1 Crystal structure of **3a**

data-3a

Table S1. Crystal data and structure refinement for **3a**

Identification code	**3a**
Empirical formula	$C_{20}H_{16}OS$
Formula weight	304.39
Temperature	305(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 14.5191(13) Å α= 90°. b = 7.2625(5) Å β= 104.832(3)°. c = 15.2169(14) Å γ = 90°.
Volume	1551.1(2) $Å^3$
Z	4
Density (calculated)	1.303 Mg/m^3
Absorption coefficient	0.207 mm^{-1}
F(000)	640
Crystal size	0.190 x 0.170 x 0.160 mm^3
Theta range for data collection	2.769 to 26.966°.
Index ranges	-18<=h<=18, -9<=k<=8, -19<=l<=19
Reflections collected	15306
Independent reflections	3349 [R(int) = 0.0393]
Completeness to theta = 25.242°	99.90%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.7077
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3349 / 0 / 200
Goodness-of-fit on F^2	1.059
Final R indices [I>2sigma(I)]	R_1 = 0.0440, wR_2 = 0.0933
R indices (all data)	R_1 = 0.0619, wR_2 = 0.1048
Extinction coefficient	n/a
Largest diff. peak and hole	0.168 and -0.224 $e.Å^{-3}$

The CCDC number of the product **3a** is 2088155

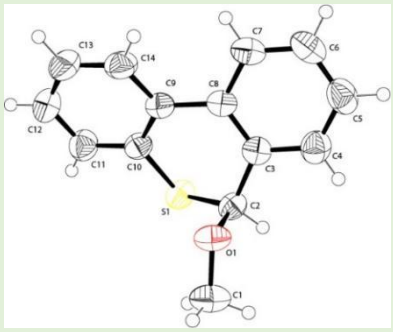


Figure S2 Crystal structure of **4a**

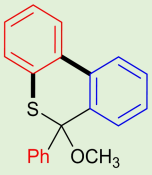
data-4a

Table S2. Crystal data and structure refinement for **4a**

Identification code	**4a**
Empirical formula	$C_{14}H_{12}OS$
Formula weight	228.3
Temperature	305(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$Pna2_1$
Unit cell dimensions	a = 8.8355(6) Å α= 90° b = 15.5836(11) Å β= 90° c = 8.5018(5) Å γ = 90°.
Volume	1170.60(13) $Å^3$
Z	4
Density (calculated)	1.295 Mg/m^3
Absorption coefficient	0.250 mm^{-1}
F(000)	480
Crystal size	0.220 x 0.190 x 0.170 mm^3
Theta range for data collection	2.614 to 26.867°.
Index ranges	-11<=h<=11, -19<=k<=17, -10<=l<=10
Reflections collected	13698
Independent reflections	2518 [R(int) = 0.0330]
Completeness to theta =25.242°	100.00%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.6520
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2518 / 1 / 146
Goodness-of-fit on F^2	1.082
Final R indices [I>2sigma(I)]	R_1 = 0.0272, wR_2 = 0.0734
R indices (all data)	R_1 = 0.0297, wR_2 = 0.0761
Absolute structure parameter	0.07(3)
Extinction coefficient	n/a
Largest diff. peak and hole	0.145 and -0.138 $e.Å^{-3}$

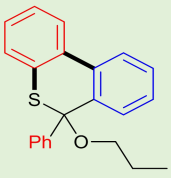
The CCDC number of product **4a** is 2088156.

5.Characterization data of products



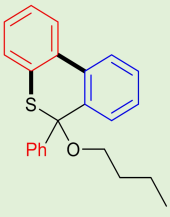
3a

6-methoxy-6-phenyl-6H-benzo[c]thiochromene White solid, 18.8 mg, 62% yield. m.p. 100.1-100.6°C; IR (cm^{-1}) 3056.0, 2934.0, 2820.4, 1484.6, 1474.6, 1441.6, 1427.8, 1224.5, 1177.7, 1064.1 ,941.4, 856.2, 748.0, 700.5, 639.1; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 (dd, *J*= 7.7, 1.0 Hz, 1H)), 7.86 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.67-7.62 (m, 2H), 7.52 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.48-7.43 (m,2H), 7.43-7.37 (m, 2H), 7.37-7.27 (m, 2H), 7.19 (td, *J* = 7.7, 1.3 Hz, 1H), 6.68 (dd, *J* = 7.9, 1.2 Hz, 1H), 3.17 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 139.1, 138.3, 134.2, 133.5, 130.5, 128.5, 128.4, 128.3, 128.0, 127.9, 127.7, 126.5, 126.4, 125.6, 125.5, 90.6, 53.0; HRMS (EI) m/z calcd for $C_{20}H_{16}OS^+$ [M] $^+$ 304.0916, found 304.0919.



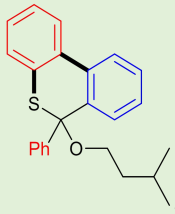
3b

6-phenyl-6-propoxy-6H-benzo[c]thiochromene White solid, 14.6 mg, 44% yield. m.p. 80.1-80.6 °C; IR (cm^{-1}) 3056.0, 2967.0, 2877.2, 1602.0, 1583.6, 1484.6, 1474.6, 1177.7, 1068.8, 1026.6, 956.0, 856.2, 748.0, 695.9, 616.1; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.83 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.68-7.60 (m, 2H), 7.49 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.47-7.32 (m, 4H), 7.32-7.25 (m, 2H), 7.19 (td, *J* = 7.6, 1.3 Hz, 1H), 6.71 (dd, *J* = 7.9, 1.3 Hz, 1H), 3.41-3.36 (m, 1H), 3.31-3.25 (m, 1H), 1.39-1.23 (m, 2H), 0.56 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 139.9, 138.9, 134.6, 133.8, 130.9, 128.4, 128.3, 128.2, 128.1, 127.9, 127.8, 127.6, 126.4, 126.3, 125.3, 90.0, 66.7, 22.6, 10.2; HRMS (EI) m/z calcd for $C_{22}H_{20}OS^+$ [M] $^+$ 332.1229, found 332.1232.



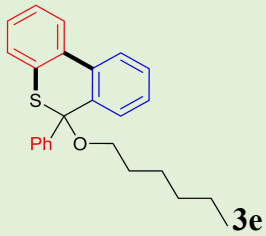
3c

6-butoxy-6-phenyl-6H-benzo[c]thiochromene White solid, 18.3 mg, 53% yield. m.p. 80.1-80.6 °C; IR (cm^{-1}) 3061.3, 2961.6, 2919.4, 2848.8, 1730.1, 1574.4,1470.0, 1441.6, 1173.1, 1064.1, 866.2, 748.0, 695.9, 974.4, 375.1; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.85-7.80 (m, 1H), 7.66-7.61 (m, 2H), 7.49-7.47 (m, 1H), 7.49-7.43 (m, 3H), 7.41-27 (m, 2H),7.27-7.25 (m,1H), 7.21-7.19 (m, 1H), 6.71 (dd, *J* = 7.9, 1.1 Hz, 1H), 3.46-3.41 (m, 1H), 3.33-3.27 (m, 1H), 1.33-1.27 (m, 2H), 1.07-0.92 (m, 2H), 0.66 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-d) δ 139.9, 138.8, 134.5, 133.8, 130.9, 128.4, 128.3, 128.2, 128.1, 127.9, 127.8, 127.6, 126.4, 126.3, 125.3, 90.0, 64.8, 31.5, 18.9, 13.6; HRMS (EI) m/z calcd for $C_{23}H_{22}OS^+$ [M] $^+$ 346.1391, found 346.1389.



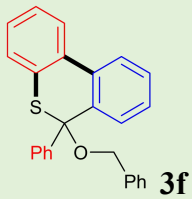
3d

6-(isopentyloxy)-6-phenyl-6H-benzo[c]thiochromene White solid, 23.0 mg, 64% yield. m.p. 80.1-80.6 °C; IR (cm^{-1}) 3363.3, 3060.3, 2957.2, 2871.6, 2400.7, 2279.9, 1471.5, 1445.1, 1177.0, 1070.2, 1041.8, 972.0, 861.0, 744.7, .701.6; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 (dd, J = 7.7, 1.6 Hz, 1H), 7.83 (dd, J = 8.0, 1.3 Hz, 1H), 7.67-7.60 (m, 2H), 7.52-7.47 (m, 1H), 7.47-7.35 (m, 4H), 7.35-7.26 (m, 2H), 7.17-7.21 (m,1H), 6.71 (dd, J = 7.9, 1.3 Hz, 1H), 3.46-3.40 (m, 1H), 3.33-3.28 (m, 1H), 1.40-1.14 (m, 3H), 1.05-0.88 (m, 3H), 0.66 (t, J = 6.6 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 139.9, 138.8, 134.5, 133.8, 131.0, 128.4, 128.3, 128.2, 128.1, 127.9, 127.8, 127.6, 126.4, 126.3, 125.4, 125.3, 90.1, 63.4, 38.2, 24.6, 22.6, 22.0; HRMS (EI) m/z calcd for $C_{24}H_{25}OS^+$ $[M+H]^+$ 361.72214, found 361.72253. HRMS (EI) m/z calcd for $C_{23}H_{22}OS^+$ $[M]^+$ 360.1542, found 360.1543.



3e

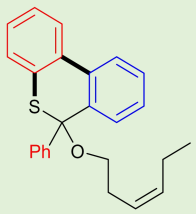
6-(hexyloxy)-6-phenyl-6H-benzo[c]thiochromene White solid, 19.4 mg, 53% yield. m.p. 59.9-60.4 °C; IR (cm^{-1}) 3061.3, 3032.9 ,2952.4, 2872.6, 1597.4, 1470.0, 1380.3, 1272.1, 1182.3, 1064.1, 856.2, 748.0, 695.9, 643.7, 516.3; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.90 (dd, J = 7.7, 1.3 Hz, 1H), 7.82 (d, J = 7.7, 1H), 7.64-7.62 (m, 2H) 7.49 (dd, J = 7.5, 1.4 Hz, 1H), 7.46-7.36 (m, 4H),7.35-7.27(m, 1H), 7.25-7.17 (m, 1H), 6.70 (dd, J = 7.8, 1.0 Hz, 1H), 3.46-3.27 (m, 2H), 1.33-1.28 (m, 2H), 1.15-1.07 (m, 2H), 1.05-0.90 (m, 4H), 0.77 (t, J = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 139.8, 138.9, 134.6, 133.8, 130.9, 128.4, 128.3, 128.2, 128.1, 127.9, 127.8, 127.6, 126.4, 126.3, 90.1, 65.0, 31.4, 29.4, 25.4, 22.5, 14.0; HRMS (EI) m/z calcd for $C_{25}H_{26}OS^+$ $[M]^+$ 374.1699, found 374.1701.



3f

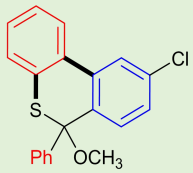
6-(benzyloxy)-6-phenyl-6H-benzo[c]thiochromene White solid, 15.2 mg, 40% yield. m.p. 63.1-63.6 °C; IR (cm^{-1}) 3056.0, 2967.0, 2877.2, 1663.4, 1583.6, 1493.8, 1371.1, 1309.7, 1219.9, 1177.7, 1068.8, 974.4, 757.2, 634.5, 408.1; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.94 (dd, J = 7.9, 1.1 Hz, 1H), 7.84 (dd, J = 7.9, 1.0 Hz, 1H), 7.75-7.69 (m, 2H), 7.51-7.41 (m, 4H), 7.41-7.34 (m, 2H), 7.27 (dd, J = 7.5, 1.3 Hz, 1H), 7.18 (td, J = 7.8, 1.2 Hz, 1H), 7.12-7.00 (m, 3H), 6.82-6..79 (m, 2H), 6.70 (dd, J = 7.9, 1.1 Hz, 1H), 4.61 (d, J = 11.4 Hz, 1H), 4.33 (d, J = 11.4 Hz, 1H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 139.3, 138.7, 137.7, 134.7, 133.8, 130.4, 128.7, 128.5, 128.4, 128.3, 128.1, 128.0, 127.9, 127.6, 127.5, 127.1, 126.53,

126.50, 125.5, 125.5, 90.5, 67.0; HRMS (ESI) m/z calcd for $C_{26}H_{20}OSNa^+$ [M+Na] $^+$ 403.1127, found 403.1128.



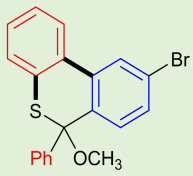
3g

(Z)-6-(hex-3-en-1-yloxy)-6-phenyl-6H-benzo[c]thiochromene White solid, 16.8 mg, 45% yield. m.p. 60.2-60.7 °C; IR (cm^{-1}) 3358.3, 3061.3, 2961.6, 2872.6, 1654.2, 1474.6, 1427.8, 1177.7, 1050.3, 969.2, 860.8, 743.4, 677.4, 639.1, 520.9; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.92 (dd, J = 7.7, 1.5 Hz, 1H), 7.86-7.81 (m, 1H), 7.65-7.63 (m, 2H), 7.50 (dd, J = 7.5, 1.5 Hz, 1H), 7.46-7.37 (m, 4H), 7.35-7.26 (m, 2H), 7.19 (td, J = 7.8, 1.3 Hz, 1H), 6.72-6,69 (m, 1H), 5.28-5.21 (m, 1H), 5.07-5.00 (m, 1H), 3.49-3.35 (m, 1H), 3.35-3.29 (m, 1H), 2.03-1.95 (m, 2H), 1.93-1.81 (m, 2H), 0.86 (t, J = 7.5 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 139.8, 138.7, 134.5, 133.8, 133.7, 130.9, 128.4, 128.3, 128.27, 128.2, 128.0, 127.8, 127.6, 126.5, 126.4, 125.5, 125.4, 124.9, 90.2, 65.1, 32.6, 25.5, 20.5, 13.7; HRMS (ESI) m/z calcd for $C_{25}H_{24}OSNa^+$ [M+Na] $^+$ 395.1440, found 395.1441.



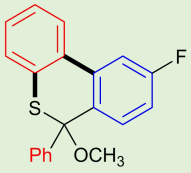
3h

9-chloro-6-methoxy-6-phenyl-6H-benzo[c]thiochromene White solid, 17.6 mg, 52% yield. m.p. 112.7-113.2 °C; IR (cm^{-1}) 3056.0, 2957.0, 2829.6, 1592.8, 1474.6, 1390.2, 1173.1, 1101.7, 1059.5, 960.6, 941.4, 870.8, 818.6, 738.1, 695.9, 596.9; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.93-7.86 (m, 1H), 7.83 (d, J = 2.1 Hz, 1H), 7.62 (d, J = 7.0 Hz, 2H), 7.52 (dd, J = 7.3, 1.7 Hz, 1H), 7.50-7.36 (m, 4H), 7.36-7.29 (m, 2H),7.15 (dd, J = 8.4, 2.1 Hz, 1H), 6.61 (d, J = 8.4 Hz, 1H), 3.15 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 138.6, 136.9, 135.3, 133.1, 130.8, 128.6, 128.4, 127.9, 127.4, 127.2, 126.6, 126.3, 125.6, 90.2, 53.0. HRMS (ESI) m/z calcd for $C_{20}H_{15}ClOSNa^+$ [M+Na] $^+$ 361.0424, found 361.0420.



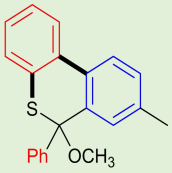
3i

9-bromo-6-methoxy-6-phenyl-6H-benzo[c]thiochromene White solid, 20.2 mg, 50% yield. m.p. 112.7-113.2 °C; IR (cm^{-1}) 3061.3, 2934.0, 2820.4, 1583.6, 1474.6, 1432.4, 1390.2, 1173.1,1064.1, 946.0, 866.2, 761.8, 743.4, 705.1, 587.7; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 (d, J= 1.6 Hz, 1H), 7.92-7.87 (m, 1H), 7.61 (d, J = 7.2 Hz, 2H), 7.54-7.40 (m, 4H), 7.38-7.28 (m, 3H), 6.55 (d, J = 8.4 Hz, 1H), 3.15 (s, 3H);^{13}C NMR (101 MHz, Chloroform-*d*) δ 138.5, 137.3, 135.5, 133.0, 130.8, 130.4, 129.2, 128.6, 128.4, 127.9, 127.4, 126.6, 125.6, 122.5, 90.3, 53.0; HRMS (ESI) m/z calcd for $C_{20}H_{15}BrOSNa^+$ [M+Na] $^+$ 404.9919, found 404.9921.



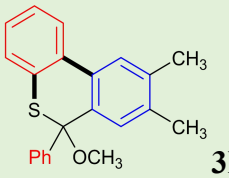
3j

9-fluoro-6-methoxy-6-phenyl-6H-benzo[c]thiochromene White solid, 55%, 17.8 mg, 55% yield. m.p. 116-117 °C; IR (cm^{-1}) 3061.3, 2961.6, 2825.0, 1607.4, 1588.2, 1493.8, 1432.4, 1272.1, 1191.5, 960.6, 908.4, 870.8, 738.1, 695.9, 587.7; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 (dd, J = 7.6, 1.6 Hz, 1H), 7.66-7.60 (m, 2H), 7.57-7.51 (m, 2H), 7.50-7.41 (m, 3H), 7.37-7.30 (m, 2H), 6.90-6.84 (m, 1H), 6.65 (dd, J = 8.7, 5.8 Hz, 1H), 3.15 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.5 (d, J = 247.4 Hz, 1C), 138.8, 135.8 (d, J =7.1 Hz, 1C), 134.5(d, J = 3.0 Hz, 1C),, 133.3 (d, J = 3.0 Hz, 1C), 130.9, 128.6, 128.56, 128.52, 128.4, 127.9, 127.8 (d, J = 7.1 Hz, 1C), 126.64, 125.66, 114.27, 114.06, 113.13, 112.90, 90.34, 53.06; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -137.9; HRMS (ESI) m/z calcd for $C_{20}H_{15}FOSNa^{+}$ $[M+Na]^{+}$ 345.0719, found 345.0721.



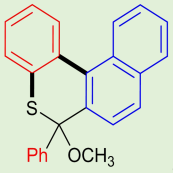
3k

6-methoxy-8-methyl-6-phenyl-6H-benzo[c]thiochromene White solid, 17.5 mg, 55% yield. m.p. 146.2-146.7°C; IR (cm^{-1}) 3056.0, 2957.0, 2829.6, 1630.4, 1588.2, 1489.2, 1243.7, 1173.1, 1064.1, 946.0, 866.2, 733.5, 705.1, 653.7, 502.5; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.77 (dd, J = 7.8, 1.6 Hz, 1H), 7.63-7.55 (m, 3H), 7.49-7.37 (m, 3H), 7.36-7.24 (m, 3H), 7.06 (t, J = 7.7 Hz, 1H), 6.47 (dd, J = 7.8, 1.3 Hz, 1H), 3.08 (s, 3H), 2.60 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 142.0, 138.8, 135.4, 134.7, 133.3, 1318, 131.3, 129.6, 129.5, 128.5, 128.3, 127.9, 127.2, 126.9, 125.3, 122.6, 92.1, 53.2, 23.2; HRMS (ESI) m/z calcd for $C_{21}H_{18}OSNa^{+}$ $[M+Na]^{+}$ 341.0970, found 341.0972.



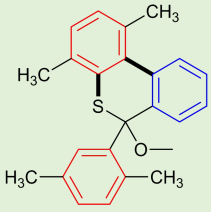
3l

6-methoxy-8,9-dimethyl-6-phenyl-6H-benzo[c]thiochromene White solid, 17.3 mg, 52% yield. m.p. 119.6-120.1°C IR (cm^{-1}) 3056.01, 2957.03, 2820.46, 1951.92, 1890.54, 1612.02, 1441.69, 1262.15 1173.15, 1083.38, 941.43, 851.66, 733.50, 653.71, 511.76. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 (dd, J = 7.8, 1.4 Hz, 1H), 7.61-7.55 (m, 3H), 7.47-7.37 (m, 3H), 7.34 -7.26 (m, 1H), 7.24-7,21 (m, 1H), 7.08 (s, 1H), 6.29 (s, 1H), 3.08 (s, 3H), 2.56 (s, 3H), 2.17 (s, 3H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 141.9, 138.9, 136.7, 135.3, 134.8, 132.5, 131.1, 130.7, 129.4, 129.3, 128.4, 128.2, 127.9, 126.8, 125.2, 123.3, 92.0, 53.2, 23.0, 21.1. HRMS (ESI) m/z calcd for $C_{22}H_{20}OSNa^{+}$ $[M+Na]^{+}$ 355.1127, found 355.1130.



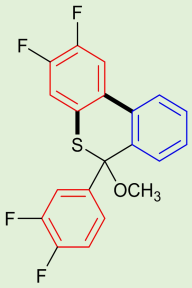
3m

6-methoxy-6-phenyl-6H-naphtho[2,1-c]thiochromene White solid, 24.8 mg, 70%. m.p. 58.4-58.9°C IR (cm^{-1}) 3061.38, 2934.02, 1597.44, 1446.29, 1375.70, 1262.15, 1182.35, 1064.19, 965.22, 866.24, 814.07, 794.88, 700.51, 582.35, 493.35; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.46 (dd, J = 6.3, 3.5 Hz, 1H), 7.96 (dd, J = 7.6, 1.8 Hz, 1H), 7.83-7.81 (m, 1H), 7.71-7.59 (m, 4H), 7.53-7.46 (m, 2H), 7.45-7.29 (m, 5H), 6.90 (s, 1H), 3.16 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 139.5, 138.0, 134.0, 133.3, 131.9, 130.8, 130.2, 129.4, 128.4, 128.3. 128.1, 127.9, 127.7, 127.4, 126.8, 126.2, 125.5, 123.2, 92.0, 53.5; HRMS (ESI) m/z calcd for $C_{24}H_{18}OSNa^{+}$ $[M+Na]^{+}$ 377.0970, found 377.0970.



3n

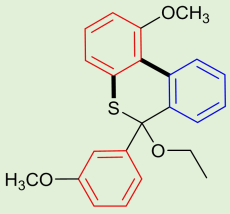
6-(2,5-dimethylphenyl)-6-ethoxy-1,4-dimethyl-6H-benzo[c]thiochromene White solid, 28.8 mg, 80% yield. m.p. 136.2-136.7 °C; IR (cm^{-1}) 3042.2, 2924.0, 2825.0, 1616.6, 1498.4 1375.7 ,1267.5, 1186.9, 1078.0,1989.0, 889.2, 818.6, 757.2, 535.5, 464.9; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.65 (d, J = 6.8 Hz, 1H), 7.48 (s, 1H), 7.30 (t, J = 7.6 Hz, 1H), 7.16-7.05 (m, 5H), 6.77-6.75 (m, 1H), 2.92 (s, 3H), 2.65 (s, 3H), 2.44 (s, 3H), 2.36 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 139.1, 135.7, 135.5, 135.0, 134.4, 133.6, 132.5, 131.7, 131.0, 130.2, 129.7, 129.2, 128.9, 128.4, 126.8, 126.6, 123.6, 92.1, 52.3, 23.0, 22.0, 21.2, 20.6; HRMS (ESI) m/z calcd for $C_{24}H_{24}OSNa^{+}$ $[M+Na]^{+}$ 383.1440, found 383.1439.



3o

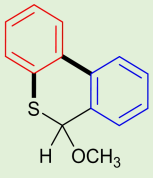
6-(3,4-difluorophenyl)-2,3-difluoro-6-methoxy-6H-benzo[c]thiochromene White solid, 13.9 mg, 37% yield. m.p. 148.3-148.8°C; IR (cm^{-1}) 3065.9, 2938.6, 1730.1, 1612.0, 1574.4, 1493.8, 1394.8, 1285.9, 1206.1, 1167.7, 1064.1, 884.6, 804.8, 766.5, 649.1; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 (q, J = 6.3, 5.6 Hz, 2H), 7.48-7.41 (m, 2H), 7.35-7.27 (m, 3H), 7.21 (d, J = 8.8 Hz, 1H), 6.75 (d, J = 7.8 Hz, 1H), 3.18 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 150.3(dd, J=251.5, 4.0 Hz, 1C), 150.1 (dd, J=251.5, 5.1 Hz, 1C), 149.8 (dd, J=252.5, 13.1 Hz, 1C), 149.2 (dd, J=247.4, 12.0 Hz, 1C), 136.9, 136.2 (t, J=4.2 Hz, 1C), 132.2, 130.8 (dd, J=6.1, 4.0 Hz, 1C), 128.9, 128.4, 126.3, 126.1 (dd, J=6.1, 3.1 Hz, 1C), 125.6, 124.2 (dd, J=6.0, 3.1 Hz, 1C), 117.46, 117.28, 116.8 (d, J=19.3 Hz, 1C), 114.7 (d, J=18.3 Hz, 1C), 89.8, 53.3; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -136.1, -136.2, -137.2, -

137.3, -137.4, -137.4, -139.0, -139.0; HRMS (APCI) m/z calcd for $C_{20}H_{12}F_4OS^-$ [M+e] $^-$ 376.0545, found 376.0544.



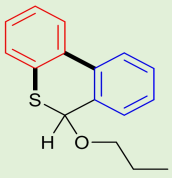
3p

6-ethoxy-1-methoxy-6-(3-methoxyphenyl)-6H-benzo[c]thiochromene White solid, 15.1 mg, 40% yield. m.p. 144.7-145.2 °C; IR (cm^{-1}) 3467.2, 3056.0, 2967.0, 2838.8, 1739.3, 1579.0, 1489.2, 1252.9, 1153.9, 1045.0, 956.0, 785., 695.91,454.99, 384.4; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.27 (d, J = 9.2 Hz, 1H), 7.38-7.28 (m, 2H), 7.22-7.11 (m, 5H), 6.96-6.89 (m, 2H), 6.65 (dd, J = 7.9, 1.3 Hz, 1H), 3.88 (s, 3H), 3.82 (s, 3H), 3.49-3.32 (m, 2H), 0.88 (t, J = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.7, 157.0, 140.9, 140.0, 132.8, 131.1, 129.7, 129.4, 127.8, 127.1, 126.9, 124.6, 124.0, 121.5, 120.3, 114.0, 113.3, 110.1, 90.5, 61.1, 55.9, 55.2, 14.9; HRMS (ESI) m/z calcd for $C_{23}H_{22}O_3SNa^+$ [M+Na] $^+$ 401.1181, found 401.1181.



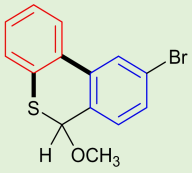
4a

6-methoxy-6H-benzo[c]thiochromene White solid, 17.1 mg, 75% yield. m.p. 76.3-77.8 °C; IR (cm^{-1}) 3060.6, 2926., 2820.01 1718.6, 1697.0, 1589.1, 1473.2, 1446.4, 1427.2, 1285.8, 1183.1, 1067.0, 937.4, 877.9, 742.6. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.94 (dd, J = 7.6, 1.76 Hz,1H), 7.87 (d, J = 7.6 Hz, 1H), 7.46-7.49 (m, 2H) 7.39-7.37 (m, 2H), 7.34-7.26 (m, 2H), 5.40 (s, 1H), 3.39 (s, 3H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 133.0, 132.5, 132.4, 129.3, 129.2, 128.8, 128.0, 127.9, 127.4, 126.4, 126.2, 125.5, 82.5, 55.6. HRMS (APCI) m/z calcd for $C_{14}H_{13}OS^+$ $[M+H]^+$ 229.0691, found 229.0683.



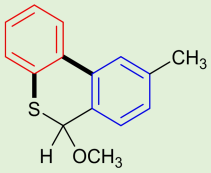
4b

6-propoxy-6H-benzo[c]thiochromene Pale yellow oil, 16.9 mg, 66% yield. IR (cm^{-1}) 3061.2, 2961.4, 2929.1, 2873.2, 2401.7, 2281.5, 1693.8, 1584.4, 1391.1, 1267.5, 1174.1, 1067., 1033.21, 939.2, 742.0; 1H NMR (400 MHz, Chloroform-d) δ 7.91 (dd, J = 7.6, 1.7 Hz, 1H), 7.85 (d, J = 3.8 Hz, 1H), 7.49-7.44 (m, 2H), 7.40-7.36 (m, 2H), 7.32-7.26 (m, 2H), 5.49 (s, 1H), 3.75-3.70 (m, 1H), 3.47 - 3.41 (m, 1H), 1.48 (q, J = 14.2, 7.1 Hz, 2H), 0.74 (t, J = 7.3 Hz, 3H); 13C NMR (101 MHz, Chloroform-d) δ 133.3, 132.9, 132.8, 129.3, 129.1, 129.0, 128.0, 127.9, 127.1, 126.4, 126.3, 126.2, 125.5, 80.8, 69.6, 22.3, 10.4. HRMS (APCI) m/z calcd for $C_{16}H_{17}OS^+$ $[M+H]^+$ 257.1003, found 257.0997.



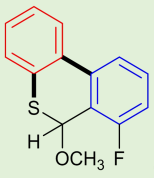
4c

9-bromo-6-methoxy-6H-benzo[c]thiochromene White solid, 21.4 mg, 70% yield. m.p. 109.6-110.1 °C IR (cm^{-1}) 3059.0, 2926.6, 2897.5, 1589.7, 1551.2, 1434, 1471.4, 1391.9, 1264.4, 1183.4, 1065.5, 937.6, 873.0, 750.7, 691.9; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.00 (d, J = 1.9 Hz, 1H), 7.90-7.87 (m, 1H), 7.52-7.47 (m, 2H), 7.33-7.30 (m, 2H), 7.27-7.24 (m, 1H), 5.36 (s, 1H), 3.37 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 134.6, 131.8, 131.2, 130.7, 129.3, 129.2, 129.0, 128.9, 128.7, 126.6, 125.6, 123.1, 81.9, 55.6. HRMS (APCI) m/z calcd for $C_{14}H_{12}OBrS^{+}$ $[M+H]^{+}$ 306.9797, found 306.9789.



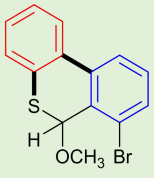
4d

6-methoxy-9-methyl-6H-benzo[c]thiochromene White solid, 15.2 mg, 63%. m.p. 100.9-101.4 °C; IR (cm^{-1}) 3460.8, 2924.9, 2621.1, 2411.7, 2279.9, 1611.4,1502.2, 1433.2, 1314.9, 1182.1, 1066.1, 937.8, 898.3, 815.2, 755.7; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 - 7.91 (m, 1H), 7.68 (s, 1H), 7.48 - 7.45 (m 1H), 7.33-7.25 (m, 3H), 7.21 - 7.19 (m, 1H), 5.38 - 5.37 (m, 3H), 3.38 - 3.37 (s, 3H), 2.45 - 2.44 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 138.9, 133.0, 132.4, 129.8, 129.2, 128.9, 128.6, 127.9, 127.3, 126.7, 126.3, 125.5, 82.3, 55.5, 21.5. HRMS (APCI) m/z calcd for $C_{15}H_{15}OS^{+}$ $[M+H]^{+}$ 243.0847, found 243.0840.



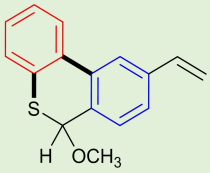
4e

7-fluoro-6-methoxy-6H-benzo[c]thiochromene White solid, 16.0 mg, 60% yield. m.p. 65.9-66.4 °C IR (cm^{-1}) 2924.2, 2854.6, 2402.9, 2289.0, 1609.4, 1582.5, 1454.0, 1321.0, 1238.4, 1184.2, 1077.1, 942.8, 889.4, 799.9, 755.1; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.93-7.91 (m, 1H), 7.66 (d, J = 7.8 Hz, 1H), 7.50-7.40 (m, 2H), 7.32-7.31 (m, 2H), 7.14 (t, J = 8.6 Hz, 1H), 5.84 (s, 1H), 3.40 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 157.5 (d, J = 247.4 Hz, 1C), 134.3 (d, J = 4.0 Hz, 1C), 131.5 (d, J = 3.0 Hz, 1C), 129.2 (d, J = 9 Hz, 1C), 128.9, 128.3, 127.9, 126.0, 125.4, 121.1 (d, J = 3.0 Hz, 1C), 119.6, 114.0 (d, J = 23.1 Hz, 1C), 73.6, 55.1; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -120.83. HRMS (APCI) m/z calcd for $C_{14}H_{12}FOS^{+}$ $[M+H]^{+}$ 247.0596, found 247.0598.



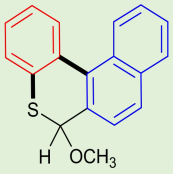
4f

7-bromo-6-methoxy-6H-benzo[c]thiochromene White solid, 16.5 mg, 54% yield. m.p. 115.6-116.1 °C; IR (cm^{-1}) 3063.8, 2993.6, 2820.3, 2362.1, 1573.3, 1439.2, 1328.4, 1257.8, 1183.2, 1065.4, 945.4, 869.8, 754.3, 719.6, 662.2; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.88-7.86 (m, 1H), 7.80 (d, J = 7.9 Hz, 1H), 7.63 (dd, J = 7.9, 1.1 Hz, 1H), 7.50-7.48 (m, 1H), 7.33-7.29 (m, 3H), 5.96 (s, 1H), 3.42 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 135.3, 132.7, 132.2, 132.1, 129.8, 129.3, 128.7, 128.5, 126.5, 126.0, 125.7, 123.2, 80.7, 55.8. HRMS (APCI) m/z calcd for $C_{14}H_{12}BrOS^+$ $[M+H]^+$ 306.9797, found 307.9786.



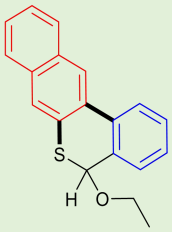
4g

6-methoxy-9-vinyl-6H-benzo[c]thiochromene White solid, 15.0 mg, 59% yield. m.p. 96.7-97.2°C; IR (cm^{-1}) 3061.0, 2926.0, 2360.0, 1723.5, 1689.3, 1473.6, 1388.0, 1263.7, 1183.8, 1064.5, 991.9, 937.6, 836.2, 756.5, 727.1; ^1H NMR (400 MHz, Chloroform-*d*) δ 7.97 (dd, J = 7.6, 1.6 Hz, 1H), 7.87 (d, J = 1.6 Hz, 1H), 7.47 (ddd, J = 9.7, 7.7, 1.7 Hz, 2H), 7.43-7.24 (m, 3H), 6.81 (dd, J = 17.5, 10.9 Hz, 1H), 5.84 (dd, J = 17.6, 0.8 Hz, 1H), 5.40 (s, 1H), 5.33 (dd, J = 10.9, 0.7 Hz, 1H), 3.38 (s, 3H);.^{13}C NMR (101 MHz, Chloroform-*d*) δ 138.5, 136.4, 133.0, 132.8, 131.9, 129.3, 129.0, 128.1, 127.7, 126.5, 125.5, 125.5, 124.4, 114.8. GCMS (ESI) m/z calcd for $C_{16}H_{16}OS^+$ [M] $^+$256.09, found 256.09. HRMS (APCI) m/z calcd for $C_{16}H_{15}OS^+$ $[M+H]^+$ 255.0847, found 255.0835.



4h

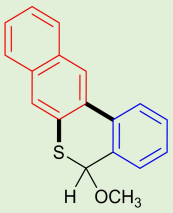
6-methoxy-6H-naphtho[2,1-c]thiochromene White solid, 14.2 mg, 51% yield. m.p. 116.9-117.4 °C; IR (cm^{-1}) 3054.0, 2926.4, 2819.8, 2360, 1595.2, 1464.5, 1384.0, 1266.0, 1184.0, 1078.5, 940.8, 819.2, 778.1, 727.0, 674.2; ^1H NMR (400 MHz, Chloroform-*d*) δ 8.49-8.45 (m, 1H), 8.01 (dd, J = 7.7, 1.6 Hz, 1H), 7.91-7.87 (m, 1H), 7.87 (d, J = 8.2 Hz, 1H), 7.67-7.65 (m, 1H), 7.52-7.48 (m, 3H), 7.40-7.31 (m, 2H), 5.46 (s, 1H), 3.39 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 134.7, 132.9, 132.4, 130.9, 130.8, 130.5, 130.3, 130.2, 128.5, 127.4, 126.5, 126.4, 126.0, 125.5, 124.7, 83.8, 56.0; HRMS (APCI) m/z calcd for $C_{18}H_{15}OS^+$ $[M+H]^+$ 279.0838, found 279.0836.



4i

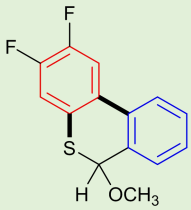
6-ethoxy-6H-naphtho[2,1-c]thiochromene White solid, 19.6 mg, 67% yield. m.p. 116.2-116.7 °C; IR (cm^{-1}) 3056.0, 2967.0, 2858.0, 1730.1, 1678.0, 1588.2, 1498.4, 1267.5, 1059.5, 965.2, 884.6, 766.5, 695.9, 601.5, 469.7. ^1H NMR (400 MHz, Chloroform-*d*) δ 8.38 (s, 1H), 8.01 (d, J = 7.8 Hz, 1H), 7.96 (s, 1H), 7.93-7.86 (m, 1H), 7.79-7.72 (m, 1H), 7.54-7.36 (m,

5H), 5.56 (s, 1H), 3.90-3.82 (m, 1H), 3.56-3.49 (m, 1H), 1.08 (t, J = 7.0 Hz, 3H)^{13}C NMR (101 MHz, Chloroform-*d*) δ 134.3, 133.1, 133.0, 132.3, 131.5, 129.2, 128.3, 127.9, 127.7, 127.5, 127.2, 126.9, 126.6, 126.5, 125.7, 124.6, 81.0, 63.7, 14.7. HRMS (APCI) m/z calcd for $C_{19}H_{15}OS^-$ [M-H]$^-$ 291.0849, found 291.0836.



4j

5-methoxy-5H-dibenzo[c,g]thiochromene White solid, 19.7 mg, 71% yield. m.p. 98.4-99.2 ^{o}C; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.39 (s, 1H), 8.03 (d, J = 7.8 Hz, 1H), 7.99 (s, 1H), 7.92-7.88 (m, 1H), 7.78-7.74 (m, 1H), 7.54-7.44 (m, 3H), 7.44-7.39 (m, 2H), 5.45 (s, 1H), 3.41 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 134.0, 133.0, 133.0, 132.4, 131.3, 129.3, 128.3, 127.9, 127.8, 127.3, 127.1, 126.8, 126.6, 126.5, 125.8, 124.7, 83.0, 55.8. HRMS (APCI) m/z calcd for $C_{18}H_{15}OS^+$ [M+H]$^+$ 279.0845, found 279.0839.



4k

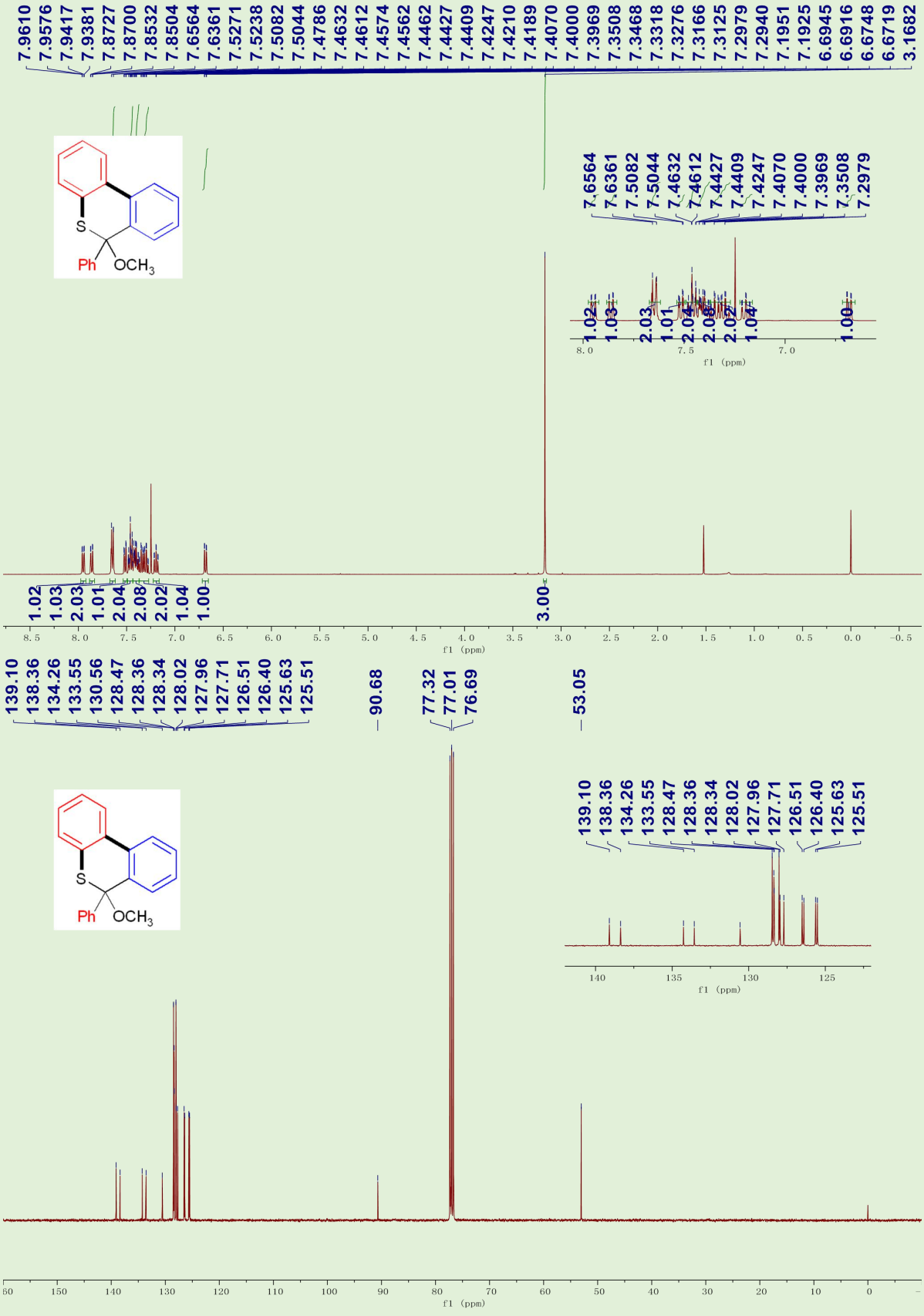
2,3-difluoro-6-methoxy-6H-benzo[c]thiochromene White solid, 16.3 mg, 62% yield. m.p. 92.7-93.2^{o}C; IR (cm^{-1}) 3061.5, 2927.2, 1722.9, 1597.2, 1490.4, 1391.3, 1269.1, 1206.6, 1168.2, 1076.8, 938.6, 880.9, 795.2 ,766.3, 742.5; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.76-7.70 (m, 2H), 7.50 (td, J = 7.5, 1.7 Hz, 1H), 7.44-7.37 (m, 2H), 7.29 (dd, J = 10.1, 7.7 Hz, 1H), 5.39 (s, 1H), 3.40 (s, 3H); ^{13}C NMR (101 MHz, Chloroform-*d*) δ 149.18 (dd, J=252.2, 13.1 Hz, 1C), 148.5 (dd, J=247.5, 13.1Hz, 1C), 131.4, 130.5, 129.4 (dd, J=5.0, 3.0 Hz, 1C), 128.8, 127.8, 126.8, 125.4, 124.2 (dd, J=6.0, 3.0 Hz, 1C), 117.1 (d, J=19.1 Hz, 1C), 113.8(d, J=19.1 Hz, 1C), 82.0, 55.1; ^{19}F NMR (376 MHz, Chloroform-*d*) δ -137.8, -137.90, -139.63, -139.68; HRMS (APCI) m/z calcd for $C_{14}H_{11}F_2OS^+$ [M+H] $^+$ 265.0504, found 265.0499.

Reference

1. J. J. Newton, R. Britton and C. M. Friesen, Base-Catalyzed Transesterification of Thionoesters, *J. Org. Chem.*, 2018, **83**, 12784-12792.

6. Copies of NMR spectra

3a



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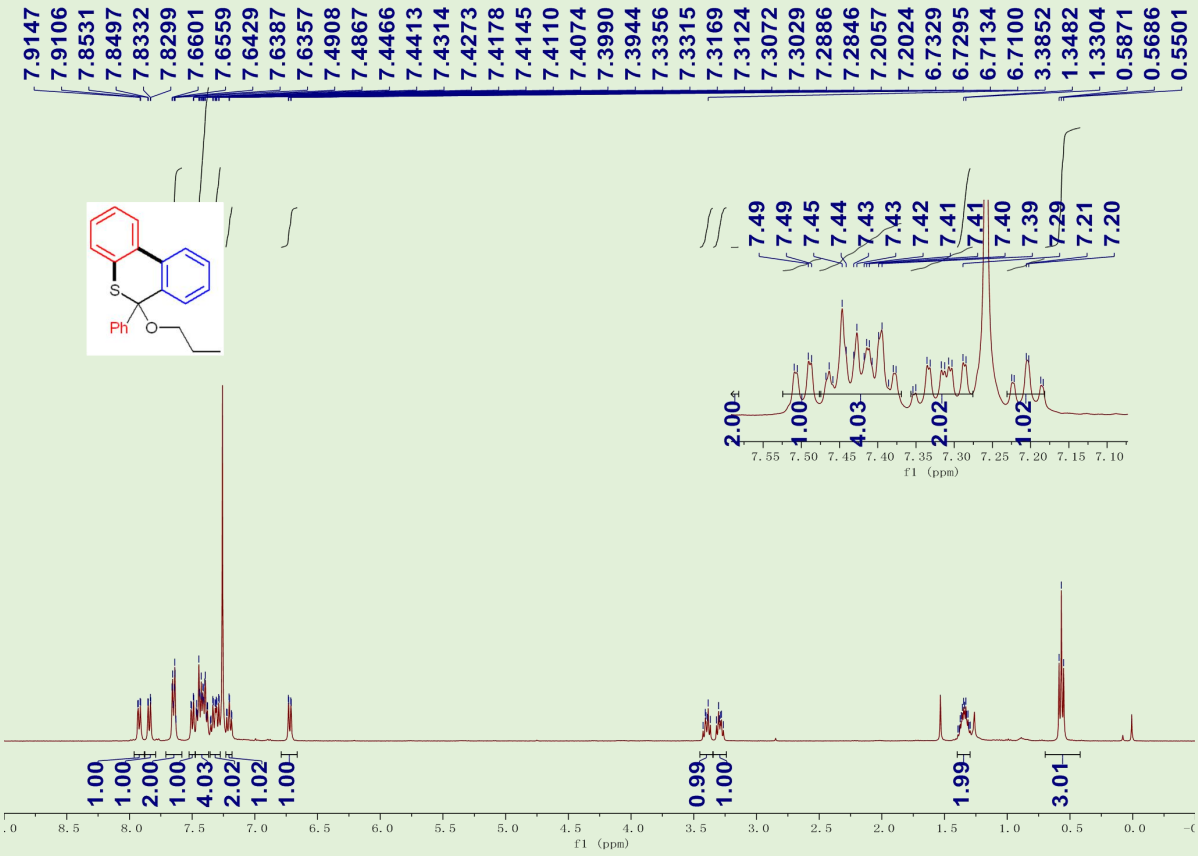
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f1 (ppm)


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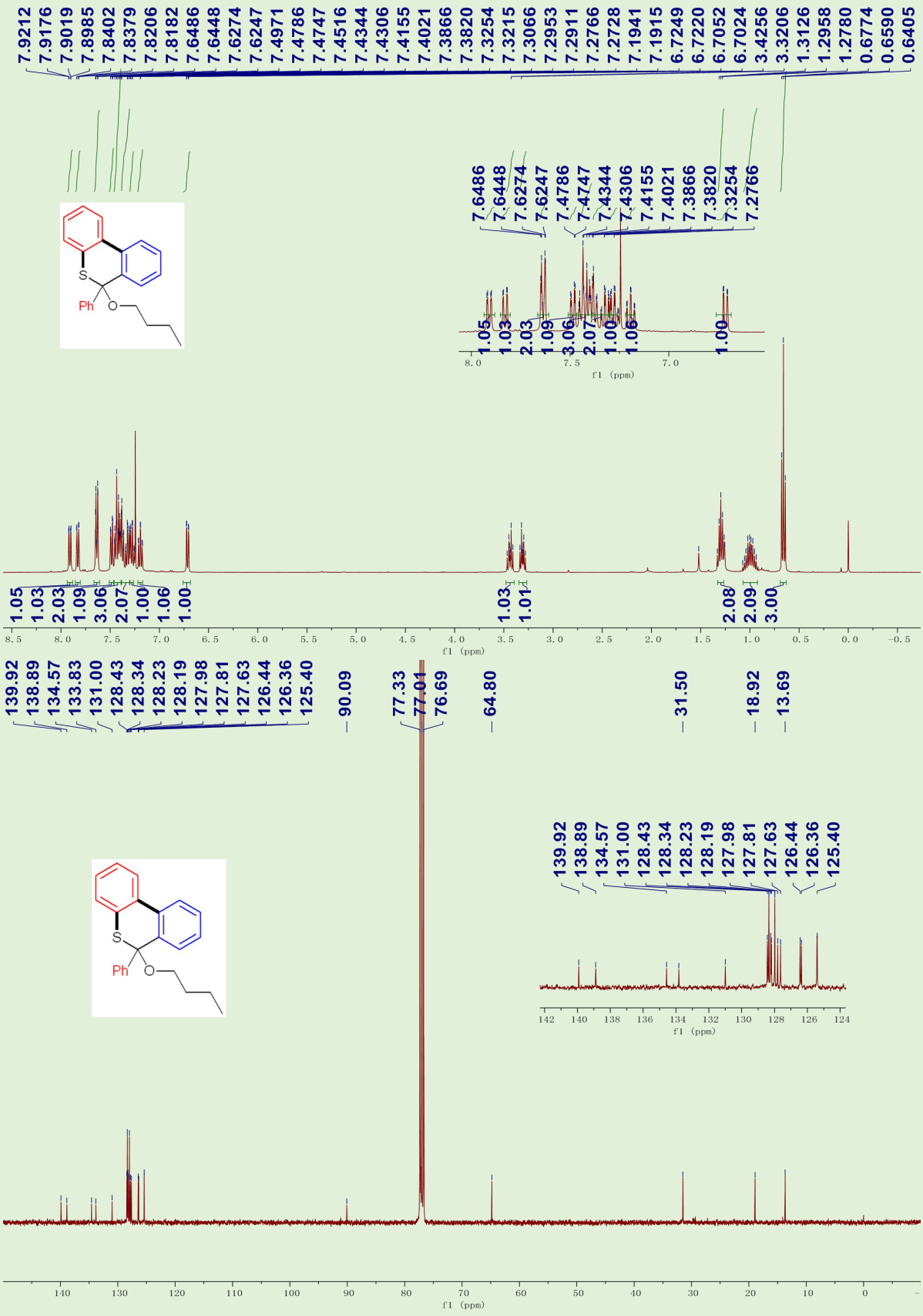
f1 (ppm)
f1 (ppm)

3c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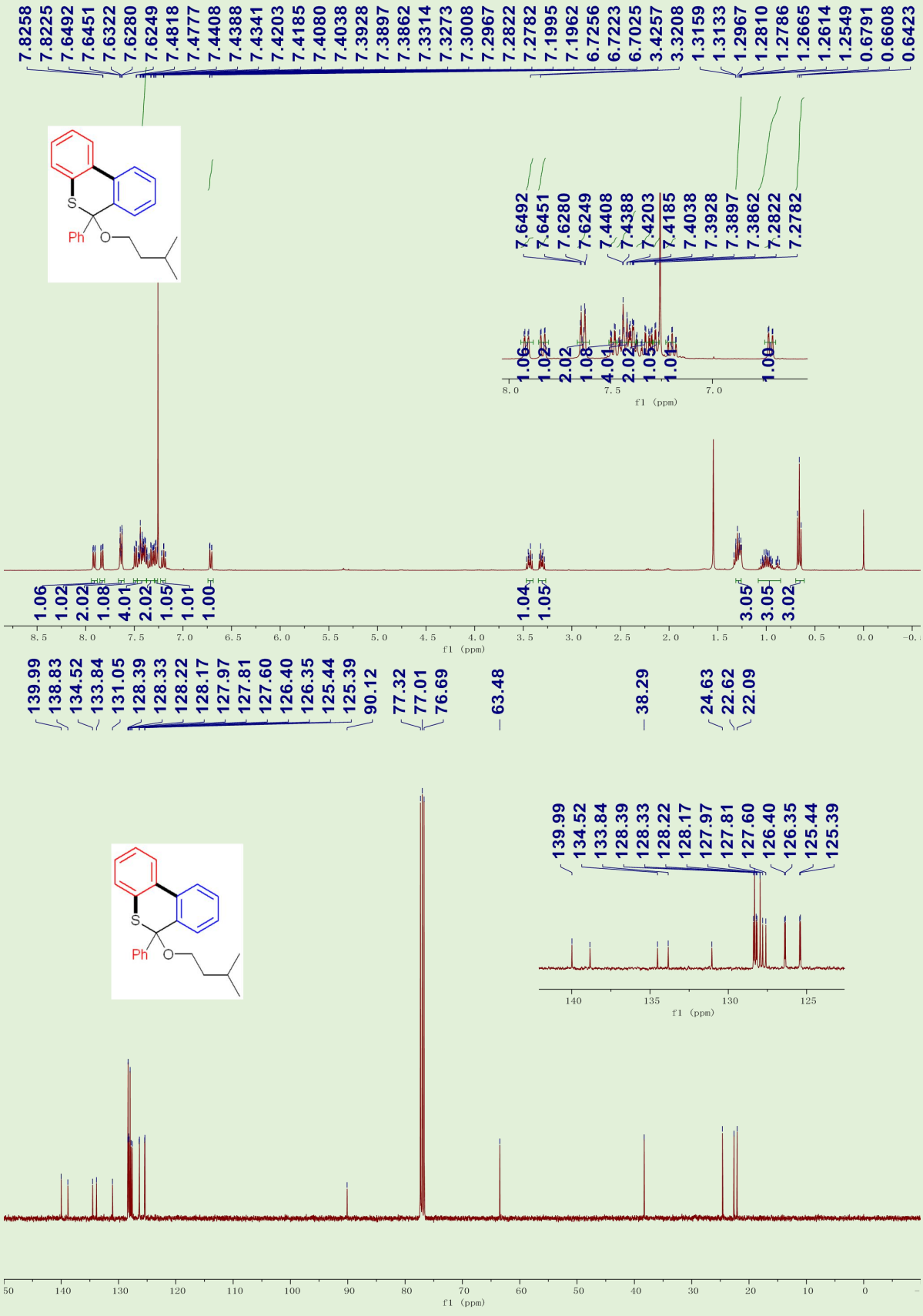
3d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24.63
22.62
22.09

3e


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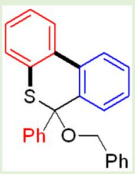
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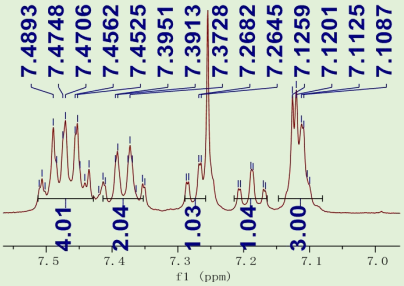
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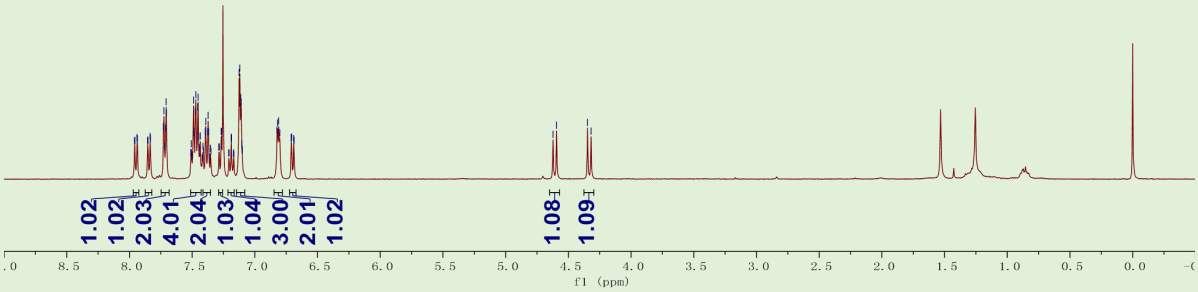
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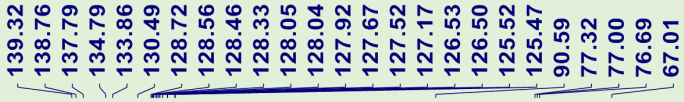
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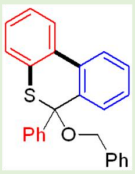
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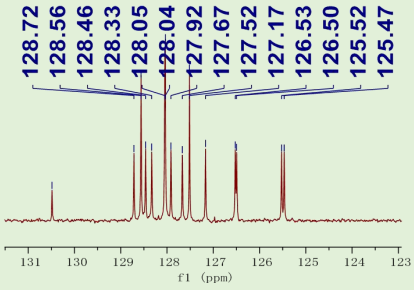
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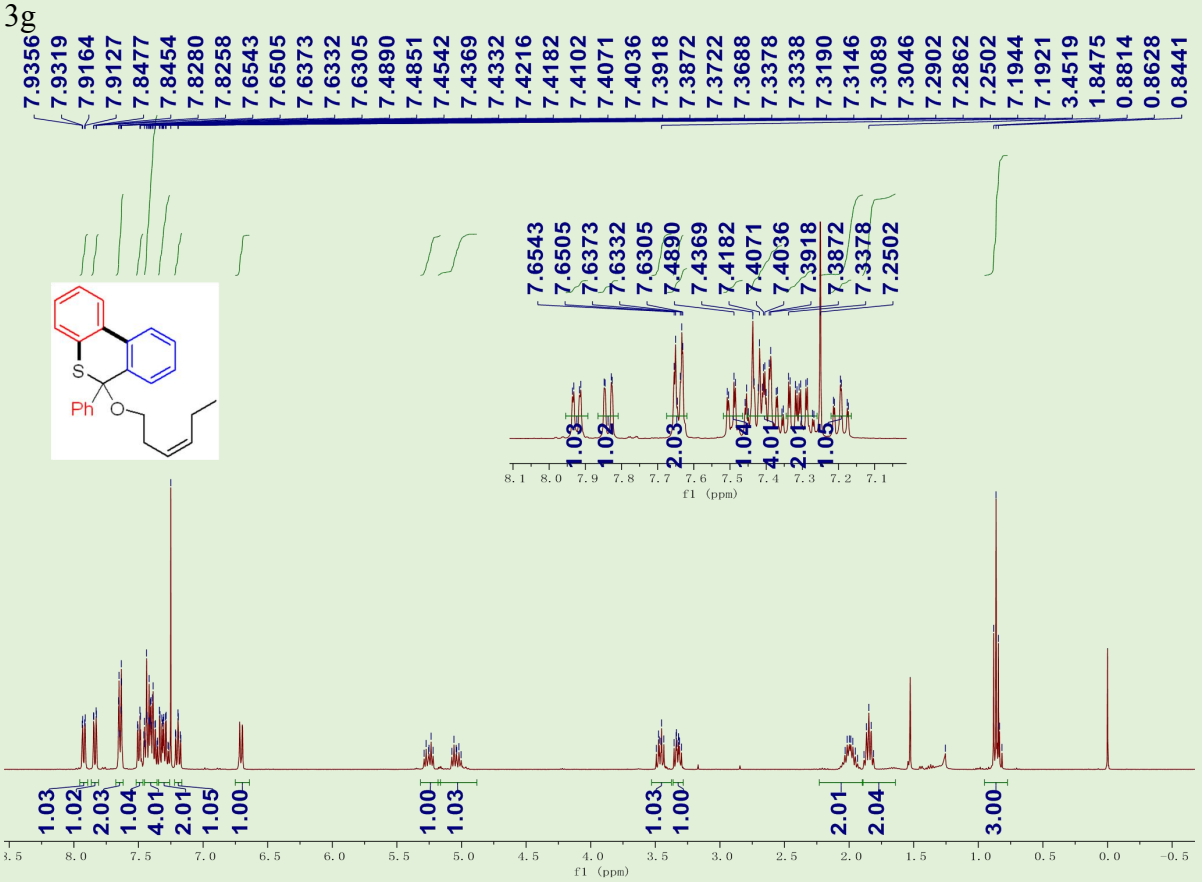
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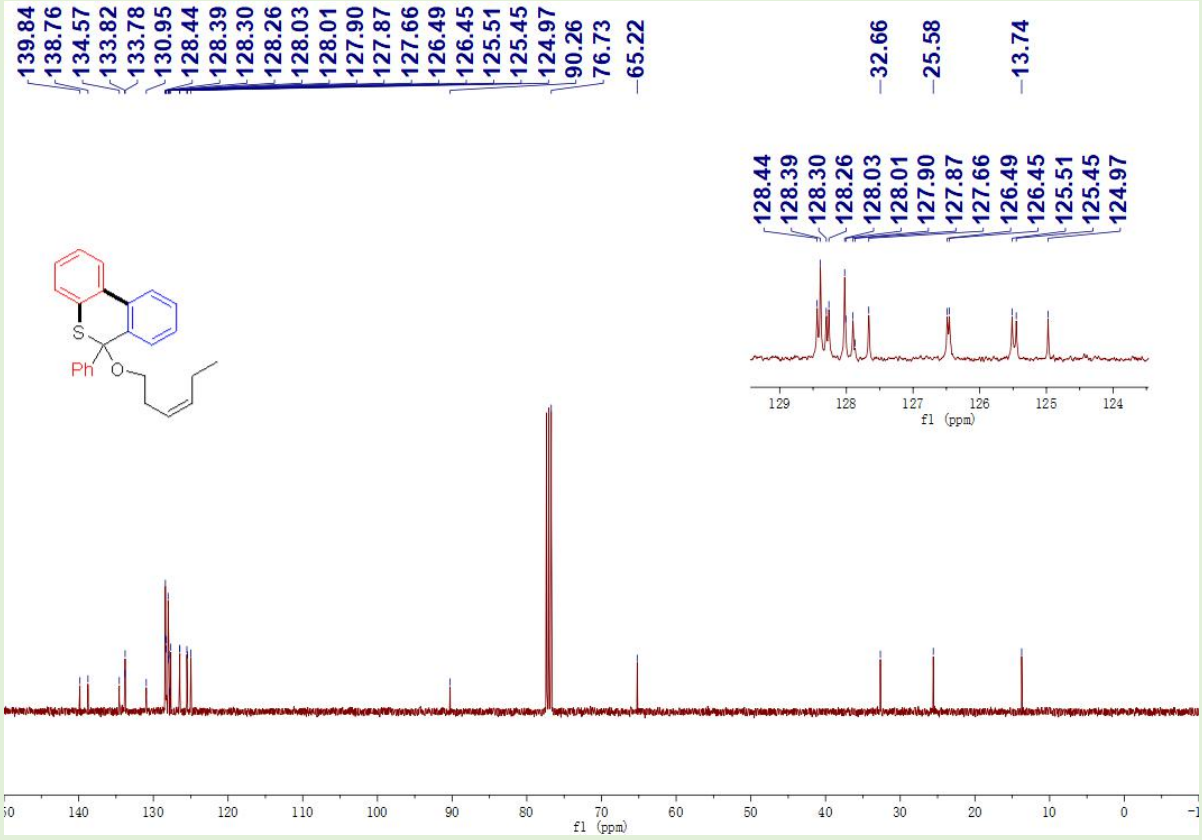
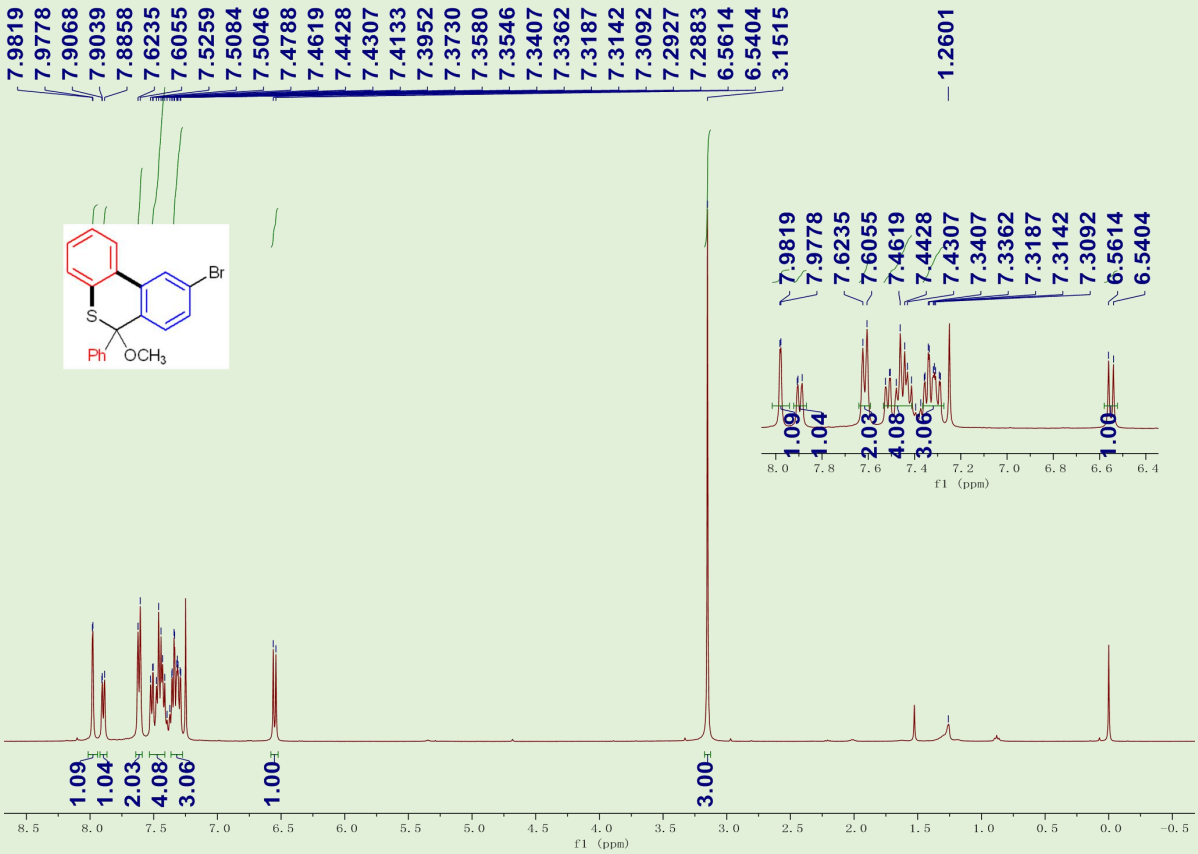
2.03
1.04
4.01
2.01
1.05
1.00
f1 (ppm)


139.84
138.76
134.57
133.82
133.78
130.95
128.44
128.39
128.30
128.26
128.03
128.01
127.90
127.87
127.66
126.49
126.45
125.51
125.45
124.97
90.26
76.73
65.22
32.66
25.58
13.74
S
Ph
O
f1 (ppm)

3h


7.9094
7.9052
7.8869
7.8289
7.8237
7.6275
7.6099
7.5294
7.5255
7.5114
7.5070
7.4804
7.4635
7.4443
7.4310
7.4138
7.3953
7.3777
7.3737
7.3594
7.3553
7.3418
7.3367
7.3235
7.3196
7.3050
7.3015
7.1604
7.1551
7.1393
7.1340
6.6252
6.6041
3.1529
Cl
S
Ph
OCH3
1.02
1.01
2.00
1.00
3.06
2.04
1.02
1.02
3.01
f1 (ppm)
138.60
136.92
135.31
134.30
133.17
130.85
128.60
128.57
128.42
127.92
127.43
127.21
126.68
126.35
125.60
90.28
77.32
77.01
76.69
53.03
f1 (ppm)

3i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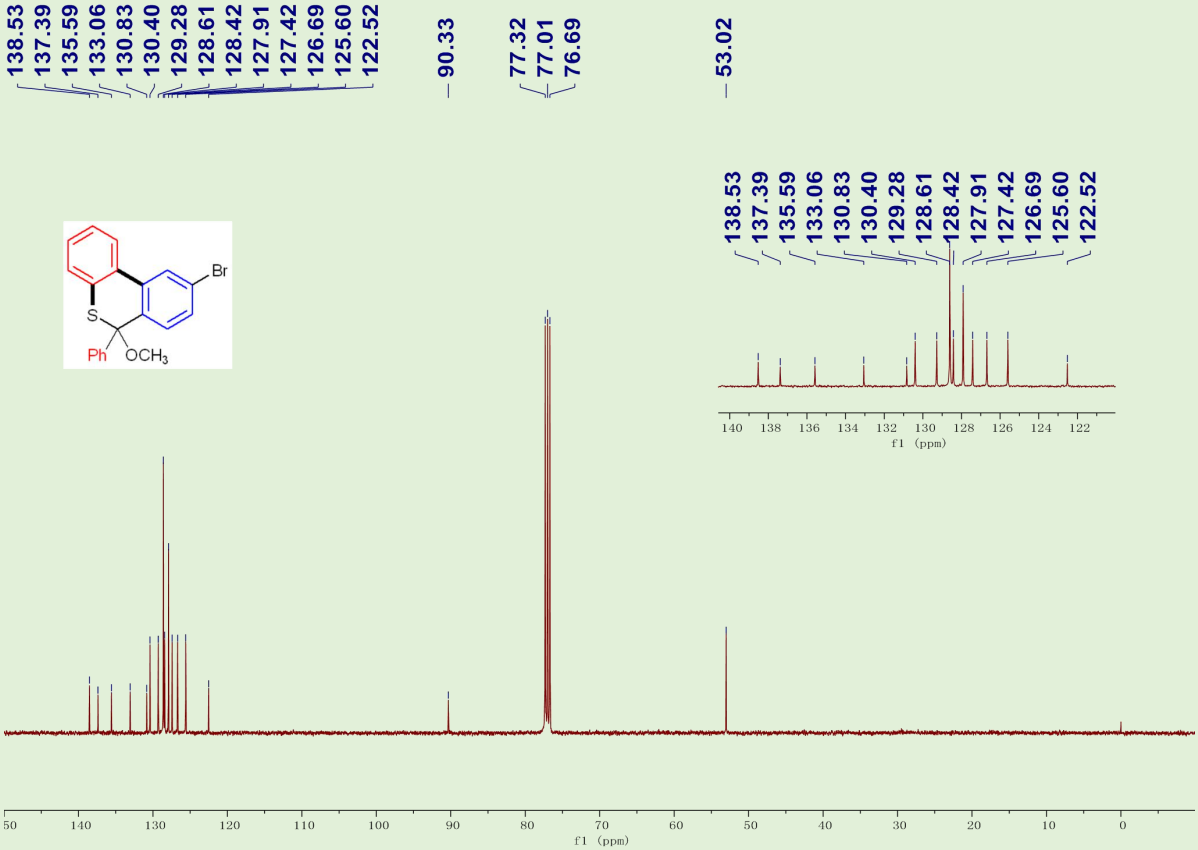
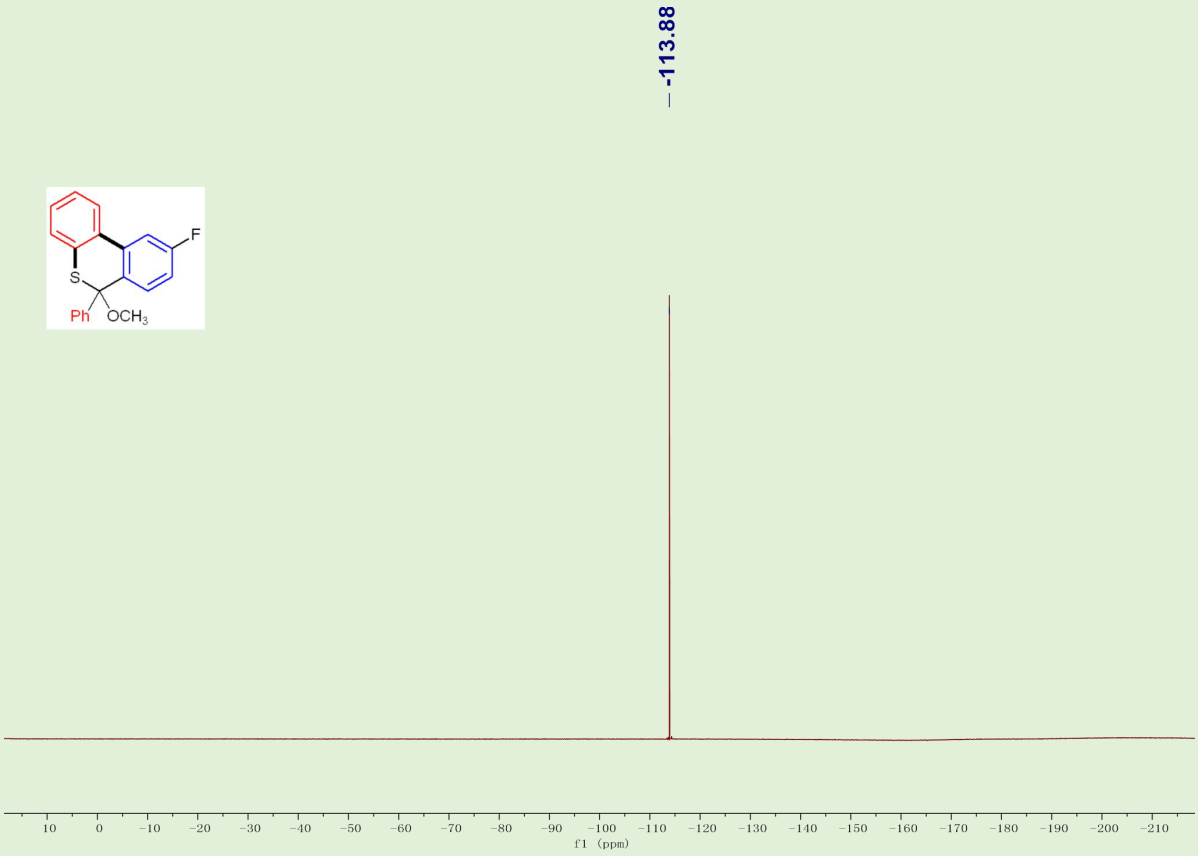
7.8858
7.6235
7.6055
7.5259
7.5084
7.5046
7.4788
7.4619
7.4428
7.4307
7.4133
7.3952
7.3730
7.3580
7.3546
7.3407
7.3362
7.3187
7.3142
7.3092
7.2927
7.2883
6.5614
6.5404
3.1515
1.2601
Br
S
Ph
OCH3
1.09
1.04
2.03
4.08
3.06
1.00
3.00
f1 (ppm)


138.53
137.39
135.59
133.06
130.83
130.40
129.28
128.61
128.42
127.91
127.42
126.69
125.60
122.52
90.33
77.32
77.01
76.69
53.02
Br
S
Ph
OCH3
f1 (ppm)

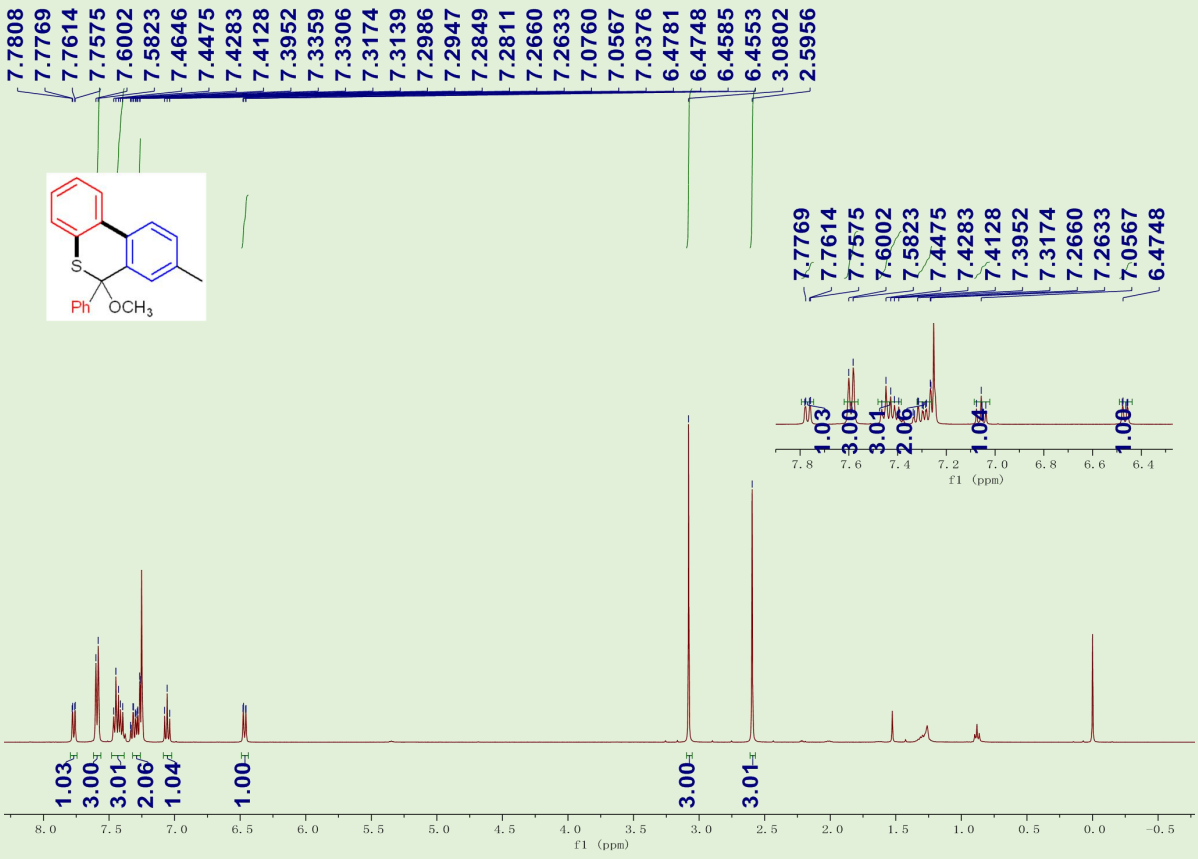
3j


7.8878
7.8833
7.8683
7.8647
7.6461
7.6422
7.6290
7.6249
7.6220
7.5533
7.5466
7.5350
7.5313
7.5286
7.5208
7.5171
7.5125
7.4884
7.4843
7.4670
7.4631
7.4519
7.4484
7.4361
7.4324
7.4288
7.4149
7.3607
7.3563
7.3430
7.3377
7.3246
7.3204
7.2488
6.8917
6.8700
6.8633
6.8501
6.8434
6.6658
6.6513
6.6440
6.6295
F
S
Ph
OCH3
1.01
2.02
2.08
3.00
2.06
1.01
1.00
2.80
f1 (ppm)

163.74
161.29
138.87
135.89
134.60
133.34
130.92
128.58
127.94
127.79
126.64
125.66
114.27
114.06
113.13
112.90
90.34
53.06
F
S
Ph
OCH3
f1 (ppm)


-113.88
F
S
Ph
OCH3
f1 (ppm)

3k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7.7614
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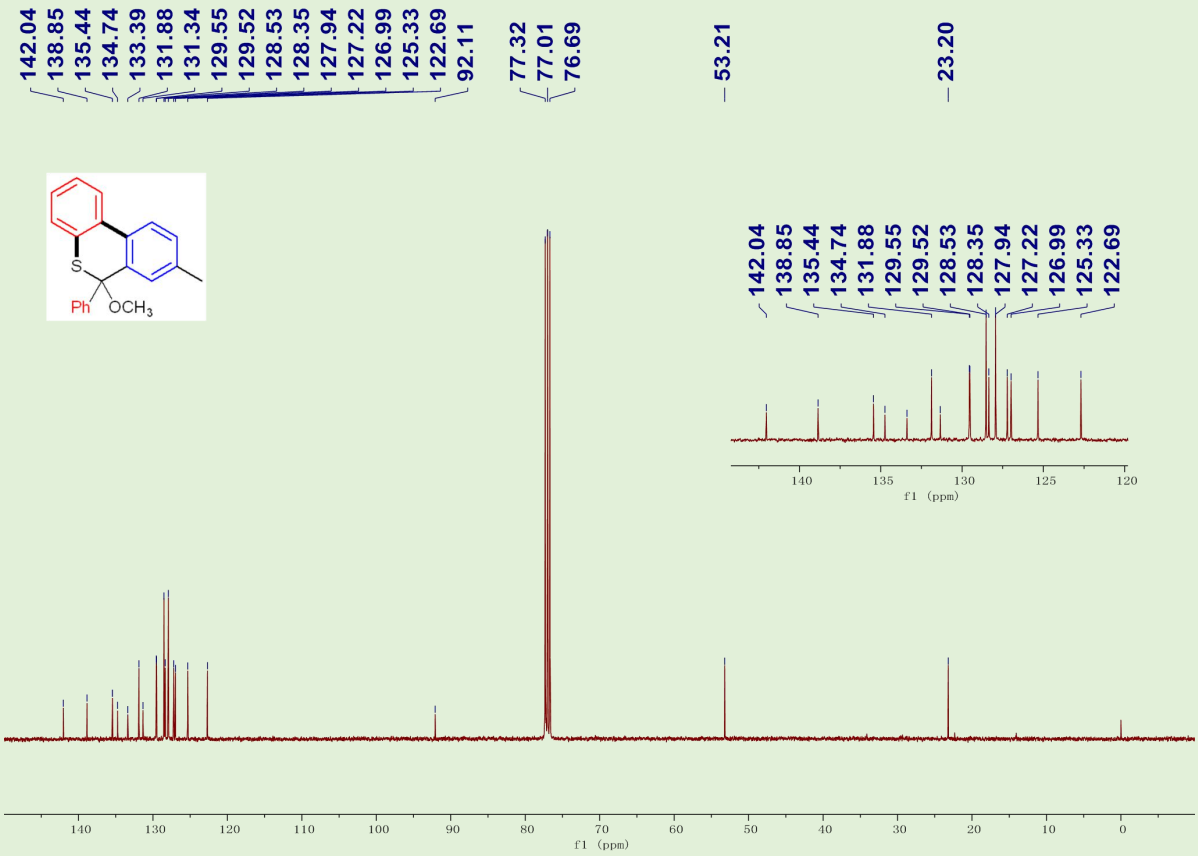
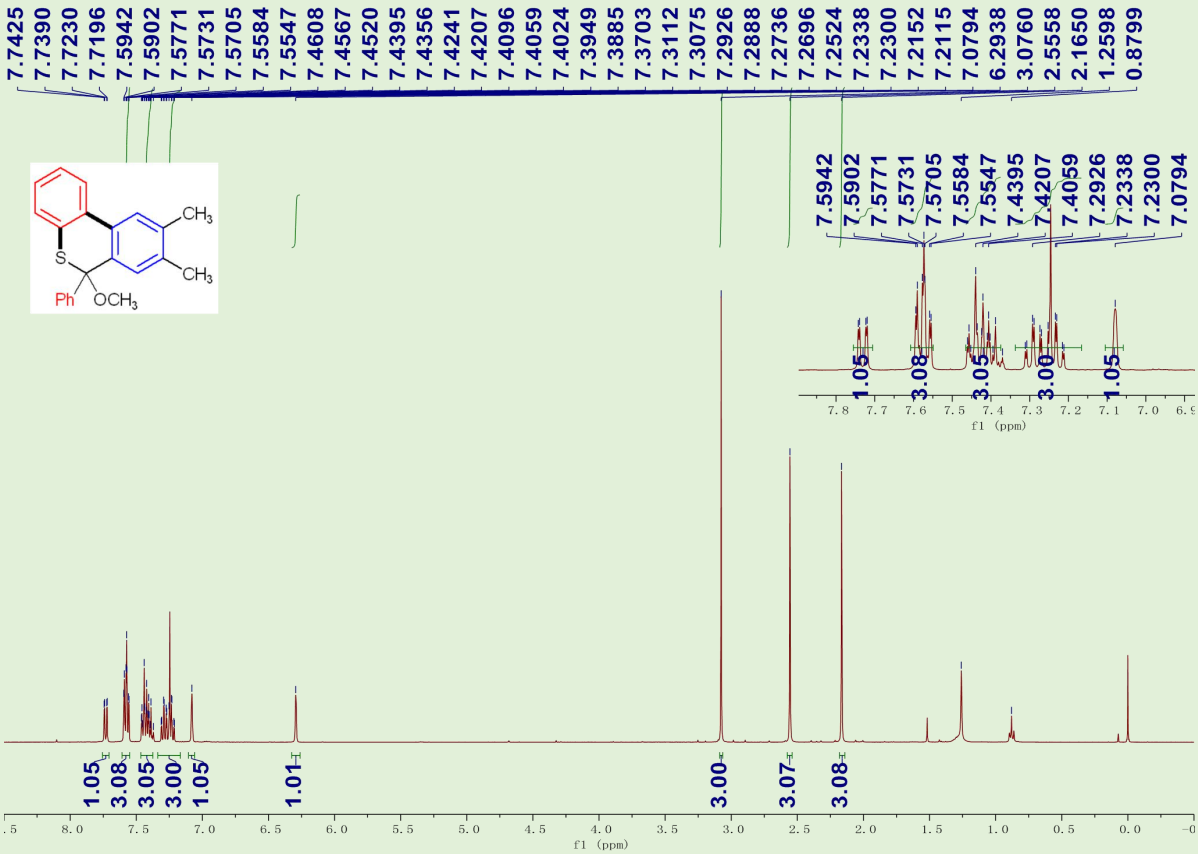
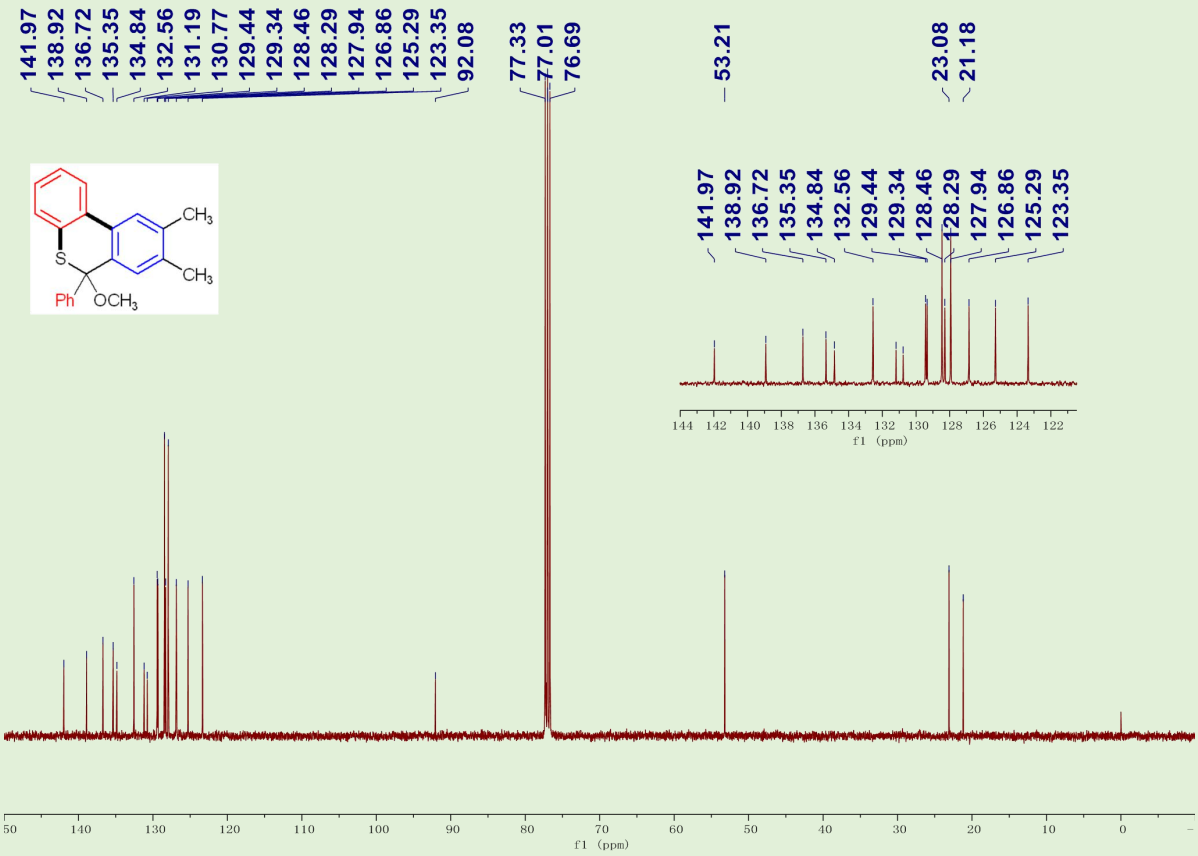
7.6002
7.5823
7.4646
7.4475
7.4283
7.4128
7.3952
7.3359
7.3306
7.3174
7.3139
7.2986
7.2947
7.2849
7.2811
7.2660
7.2633
7.0760
7.0567
7.0376
6.4781
6.4748
6.4585
6.4553
3.0802
2.5956
S
Ph
OCH3
1.03
3.00
3.01
2.06
1.04
1.00
3.00
3.01
f1 (ppm)

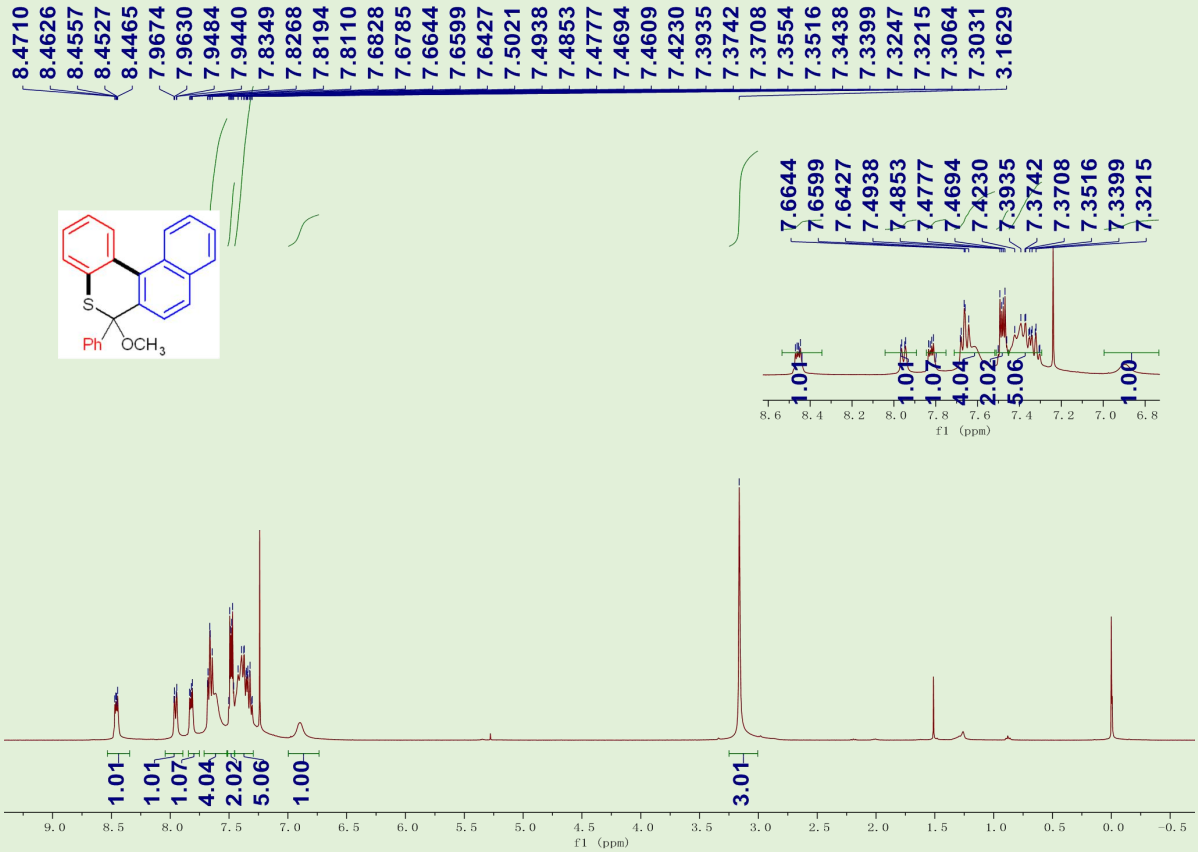

142.04
138.85
135.44
134.74
133.39
131.88
131.34
129.55
129.52
128.53
128.35
127.94
127.22
126.99
125.33
122.69
92.11
77.32
77.01
76.69
53.21
23.20
Ph
OCH3
f1 (ppm)

31


7.7425
7.7390
7.7230
7.7196
7.5942
7.5902
7.5771
7.5731
7.5705
7.5584
7.5547
7.4608
7.4567
7.4520
7.4395
7.4356
7.4241
7.4207
7.4096
7.4059
7.4024
7.3949
7.3885
7.3703
7.3112
7.3075
7.2926
7.2888
7.2736
7.2696
7.2524
7.2338
7.2300
7.2152
7.2115
7.0794
6.2938
3.0760
2.5558
2.1650
1.2598
0.8799
CH3
CH3
S
Ph
OCH3
1.05
3.08
3.05
3.00
1.05
1.01
3.00
3.07
3.08
f1 (ppm)


141.97
138.92
136.72
135.35
134.84
132.56
131.19
130.77
129.44
129.34
128.46
128.29
127.94
126.86
125.29
123.35
92.08
77.33
77.01
76.69
53.21
23.08
21.18
CH3
CH3
S
Ph
OCH3
f1 (ppm)

3m


8.4710
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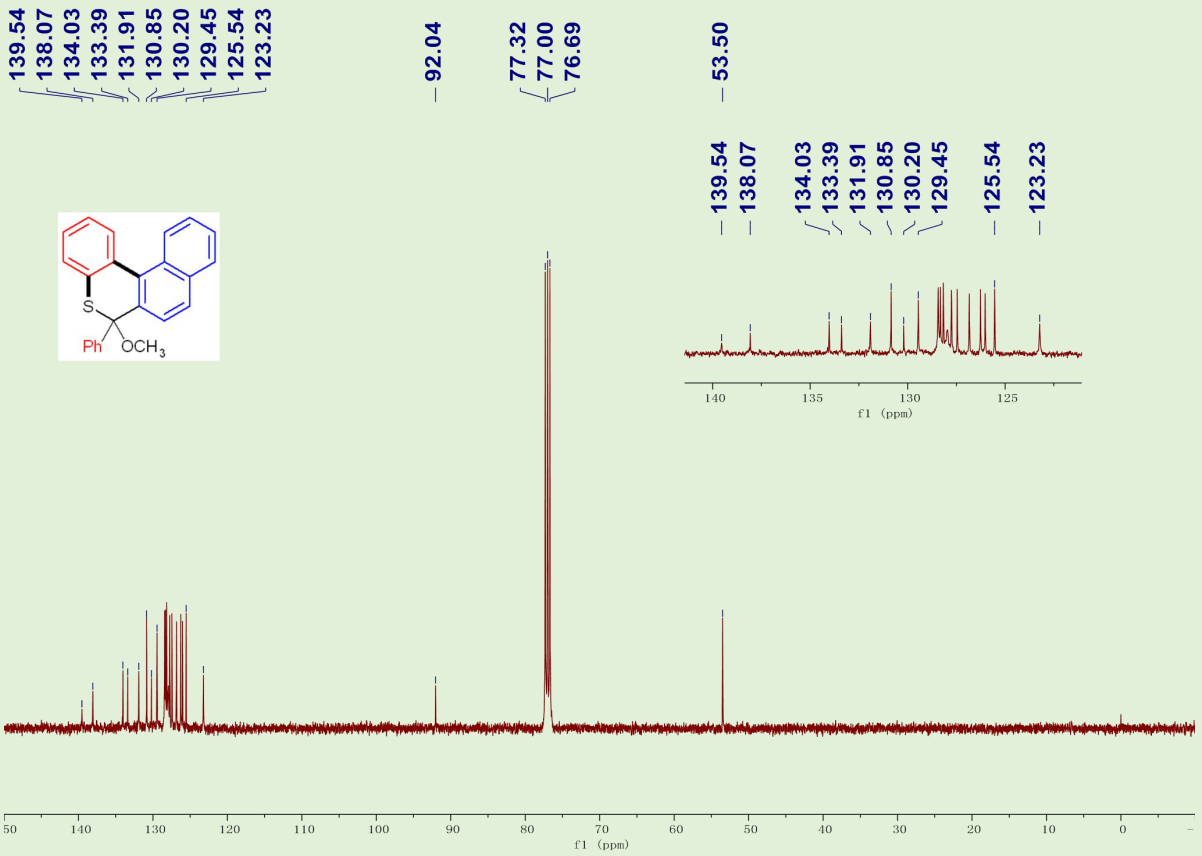
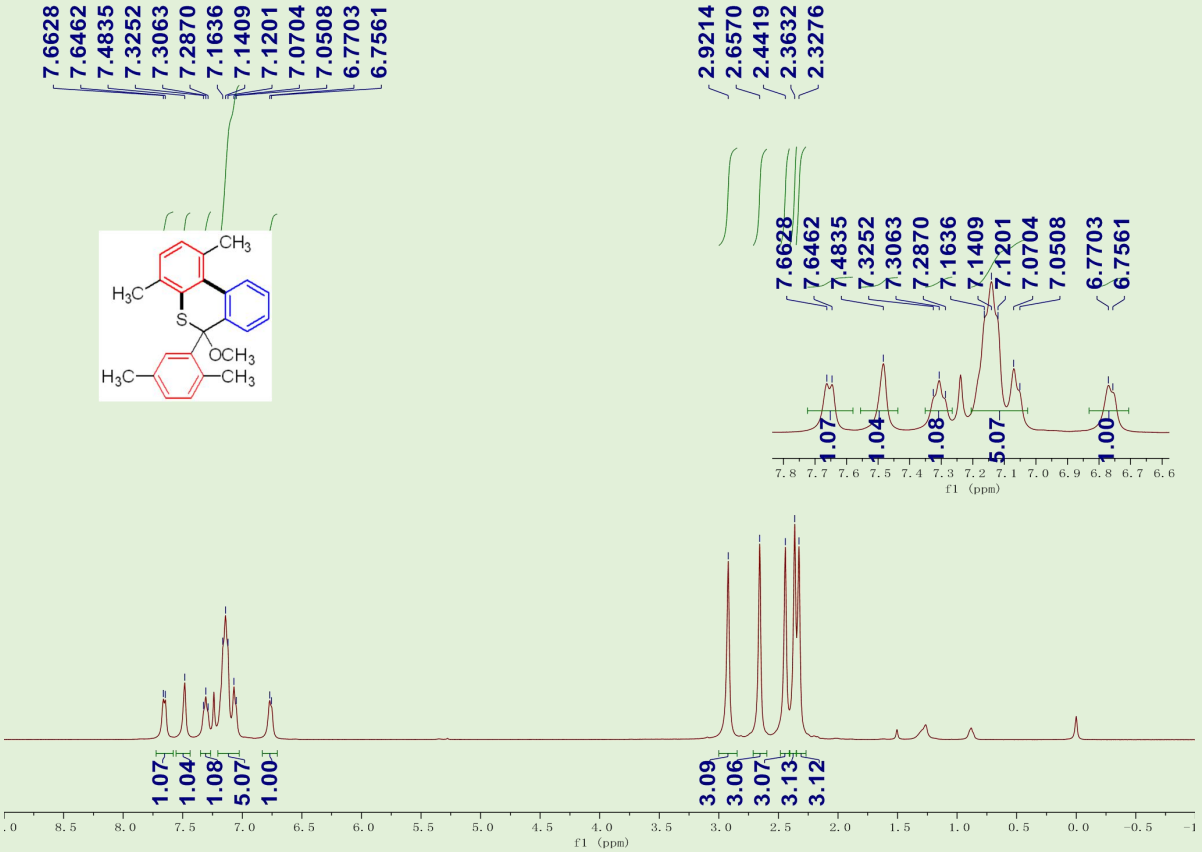
8.4557
8.4527
8.4465
7.9674
7.9630
7.9484
7.9440
7.8349
7.8268
7.8194
7.8110
7.6828
7.6785
7.6644
7.6599
7.6427
7.5021
7.4938
7.4853
7.4777
7.4694
7.4609
7.4230
7.3935
7.3742
7.3708
7.3554
7.3516
7.3438
7.3399
7.3247
7.3215
7.3064
7.3031
3.1629
S
Ph
OCH3
1.01
1.01
1.07
4.04
2.02
5.06
1.00
3.01
f1 (ppm)


139.54
138.07
134.03
133.39
131.91
130.85
130.20
129.45
125.54
123.23
92.04
77.32
77.00
76.69
53.50
Ph
OCH3
f1 (ppm)

3n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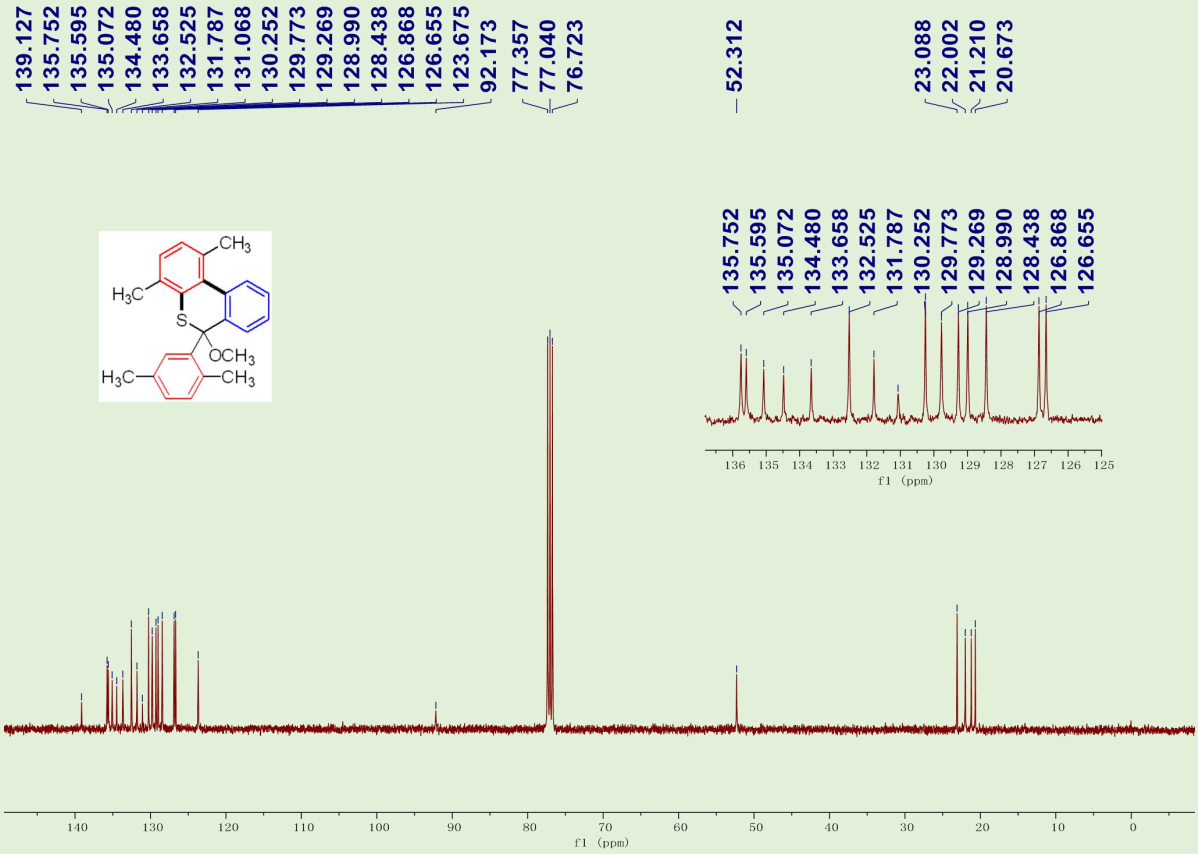
7.6462
7.4835
7.3252
7.3063
7.2870
7.1636
7.1409
7.1201
7.0704
7.0508
6.7703
6.7561
2.9214
2.6570
2.4419
2.3632
2.3276
CH3
H3C
S
OCH3
H3C
CH3
1.07
1.04
1.08
5.07
1.00
3.09
3.06
3.07
3.13
3.12
f1 (ppm)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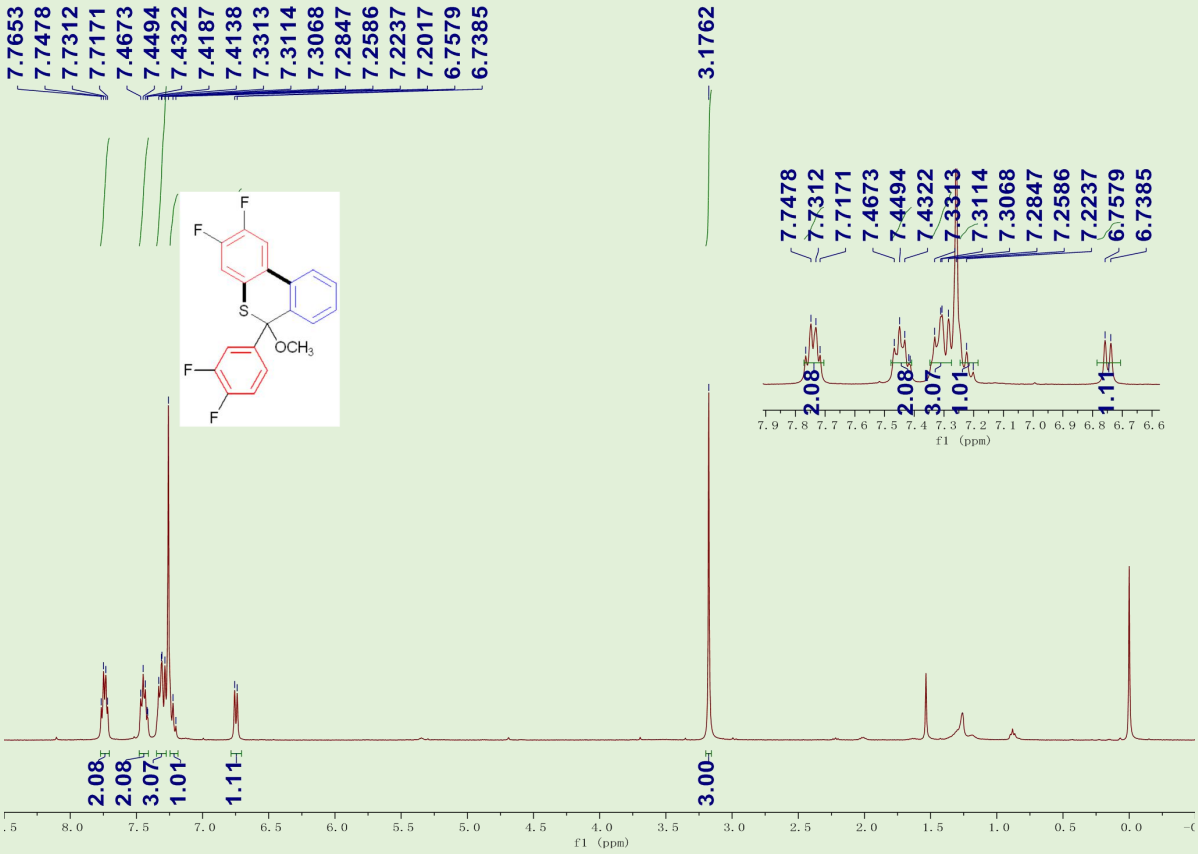
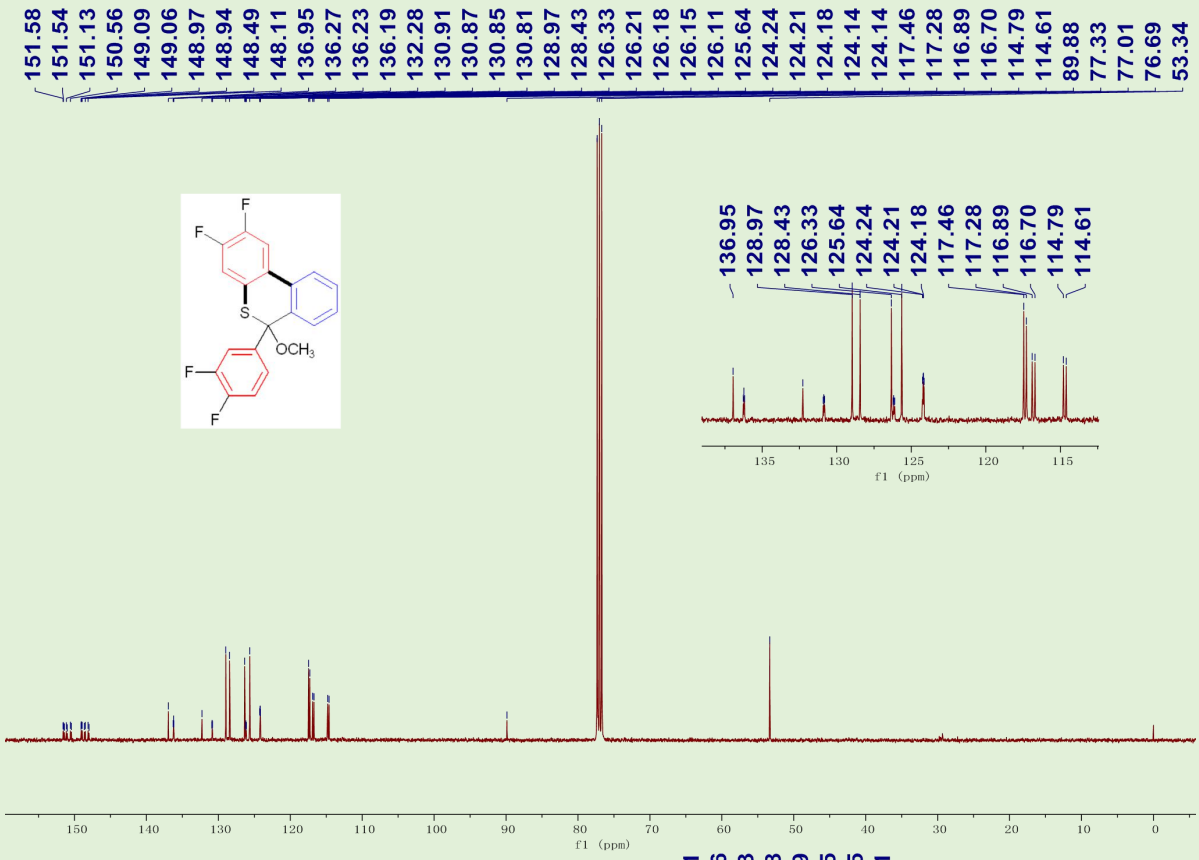
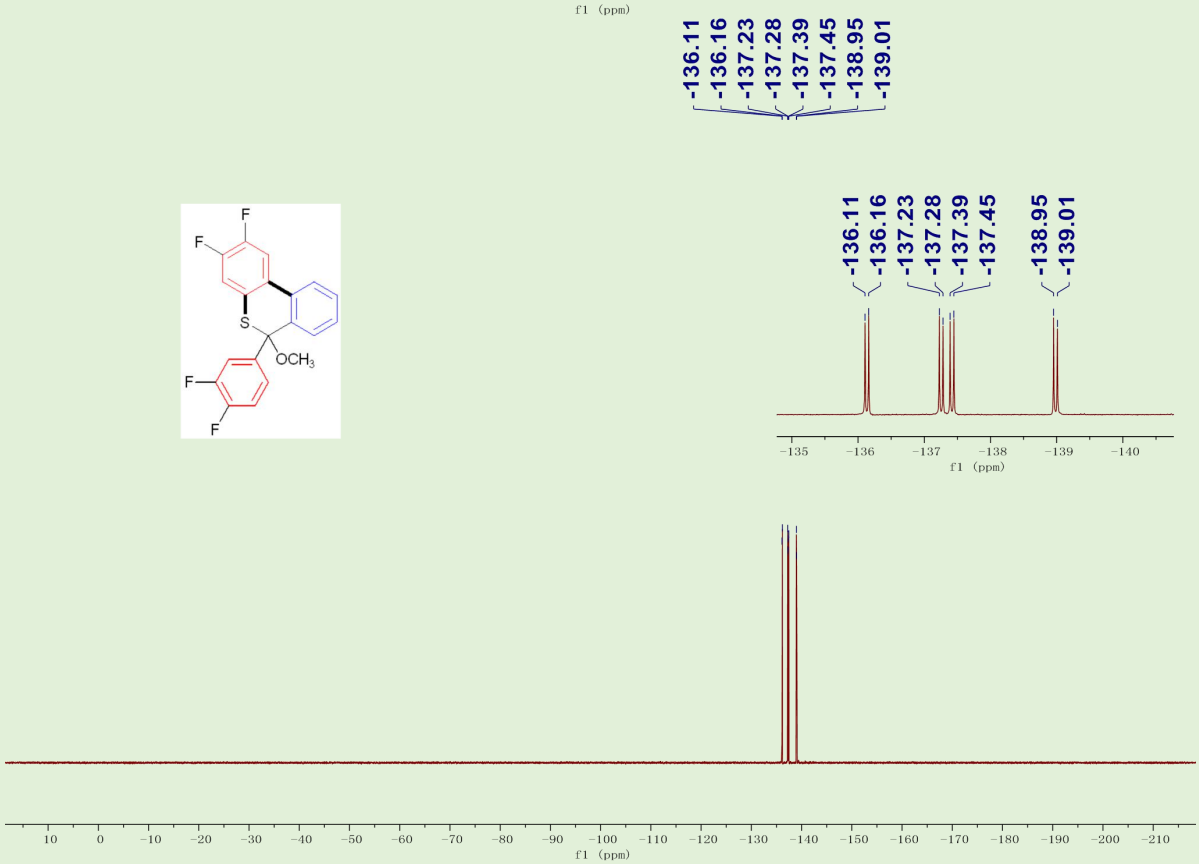
135.752
135.595
135.072
134.480
133.658
132.525
131.787
131.068
130.252
129.773
129.269
128.990
128.438
126.868
126.655
123.675
92.173
77.357
77.040
76.723
52.312
23.088
22.002
21.210
20.673
CH3
H3C
S
OCH3
H3C
CH3
f1 (ppm)

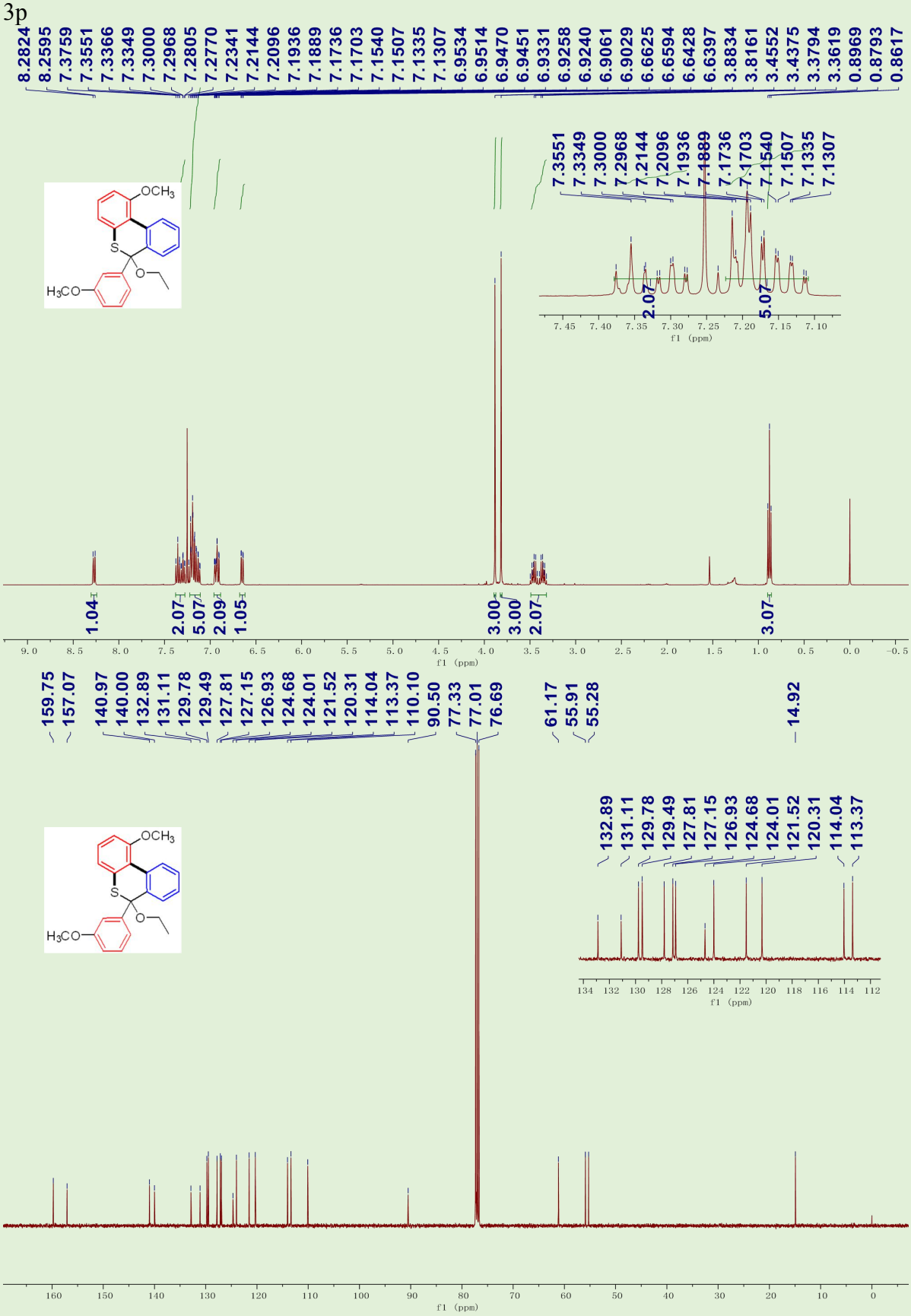
3o


7.7653
7.7478
7.7312
7.7171
7.4673
7.4494
7.4322
7.4187
7.4138
7.3313
7.3114
7.3068
7.2847
7.2586
7.2237
7.2017
6.7579
6.7385
3.1762
F
F
S
OCH3
F
F
2.08
2.08
3.07
1.01
1.11
3.00
f1 (ppm)

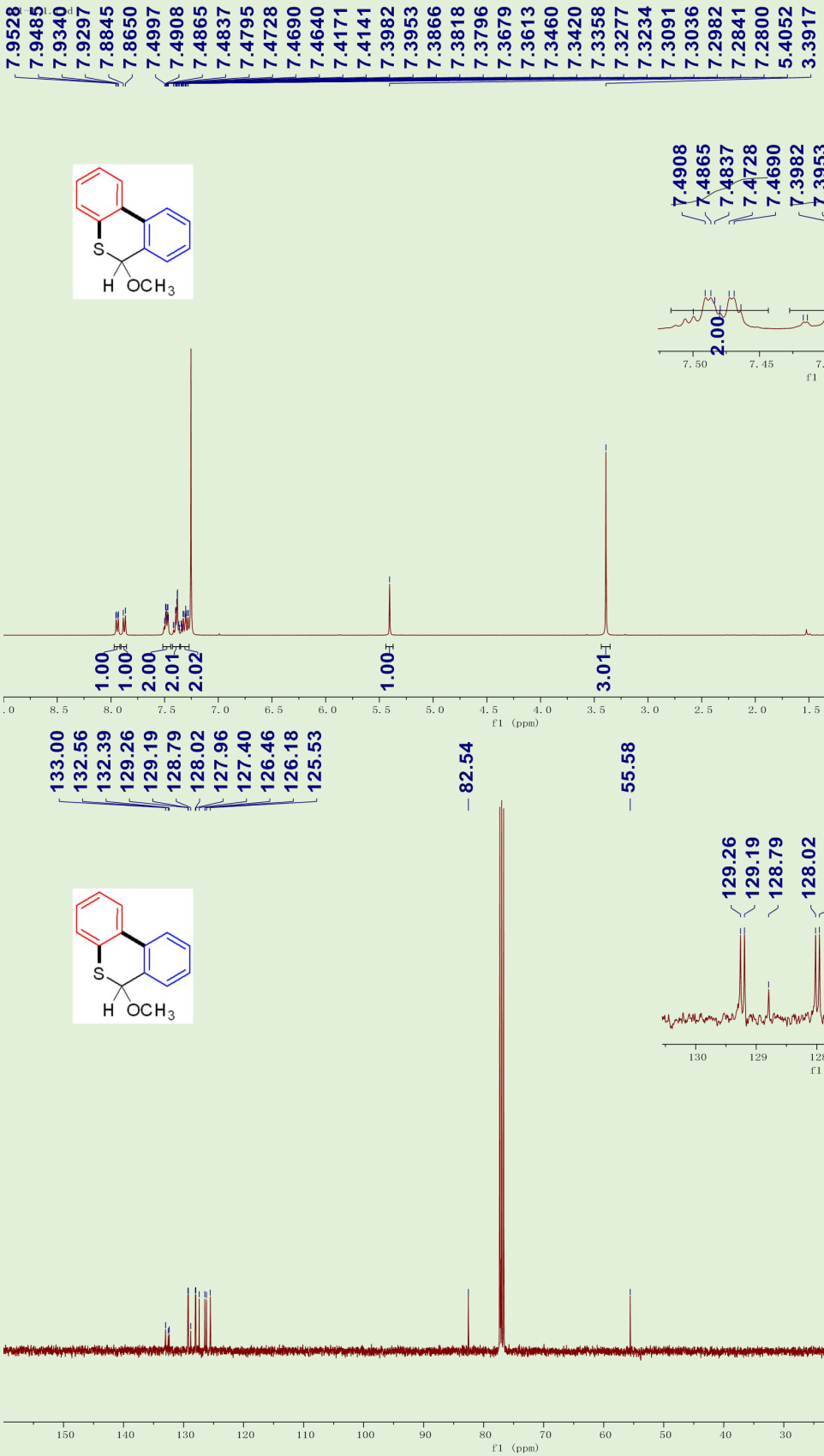

151.58
151.54
151.13
150.56
149.09
149.06
148.97
148.94
148.49
148.11
136.95
136.27
136.23
136.19
132.28
130.91
130.87
130.85
130.81
128.97
128.43
126.33
126.21
126.18
126.15
126.11
125.64
124.24
124.21
124.18
124.14
124.14
117.46
117.28
116.89
116.70
114.79
114.61
89.88
77.33
77.01
76.69
53.34
F
F
S
OCH3
F
F
136.95
128.97
128.43
126.33
125.64
124.24
124.21
124.18
117.46
117.28
116.89
116.70
114.79
114.61
135
130
125
120
115
f1 (ppm)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-136.11
-136.16
-137.23
-137.28
-137.39
-137.45
-138.95
-139.01
F
F
S
OCH3
F
F
-136.11
-136.16
-137.23
-137.28
-137.39
-137.45
-138.95
-139.01
−135
−136
−137
−138
−139
−140
f1 (ppm)
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)

3p


8.2824 8.2595 7.3759 7.3551 7.3366 7.3349 7.3000 7.2968 7.2805 7.2770 7.2341 7.2144 7.2096 7.1936 7.1889 7.1736 7.1703 7.1540 7.1507 7.1335 7.1307 6.9534 6.9514 6.9470 6.9451 6.9331 6.9258 6.9240 6.9061 6.9029 6.6625 6.6594 6.6428 6.6397 3.8834 3.8161 3.4552 3.4375 3.3794 3.3619 0.8969 0.8793 0.8617
OCH3
S
O
H3CO
1.04 2.07 5.07 2.09 1.05 3.00 3.00 2.07 3.07
f1 (ppm)
159.75 157.07 140.97 140.00 132.89 131.11 129.78 129.49 127.81 127.15 126.93 124.68 124.01 121.52 120.31 114.04 113.37 110.10 90.50 77.33 77.01 76.69 61.17 55.91 55.28 14.92
f1 (ppm)

4a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7.9297
7.8845
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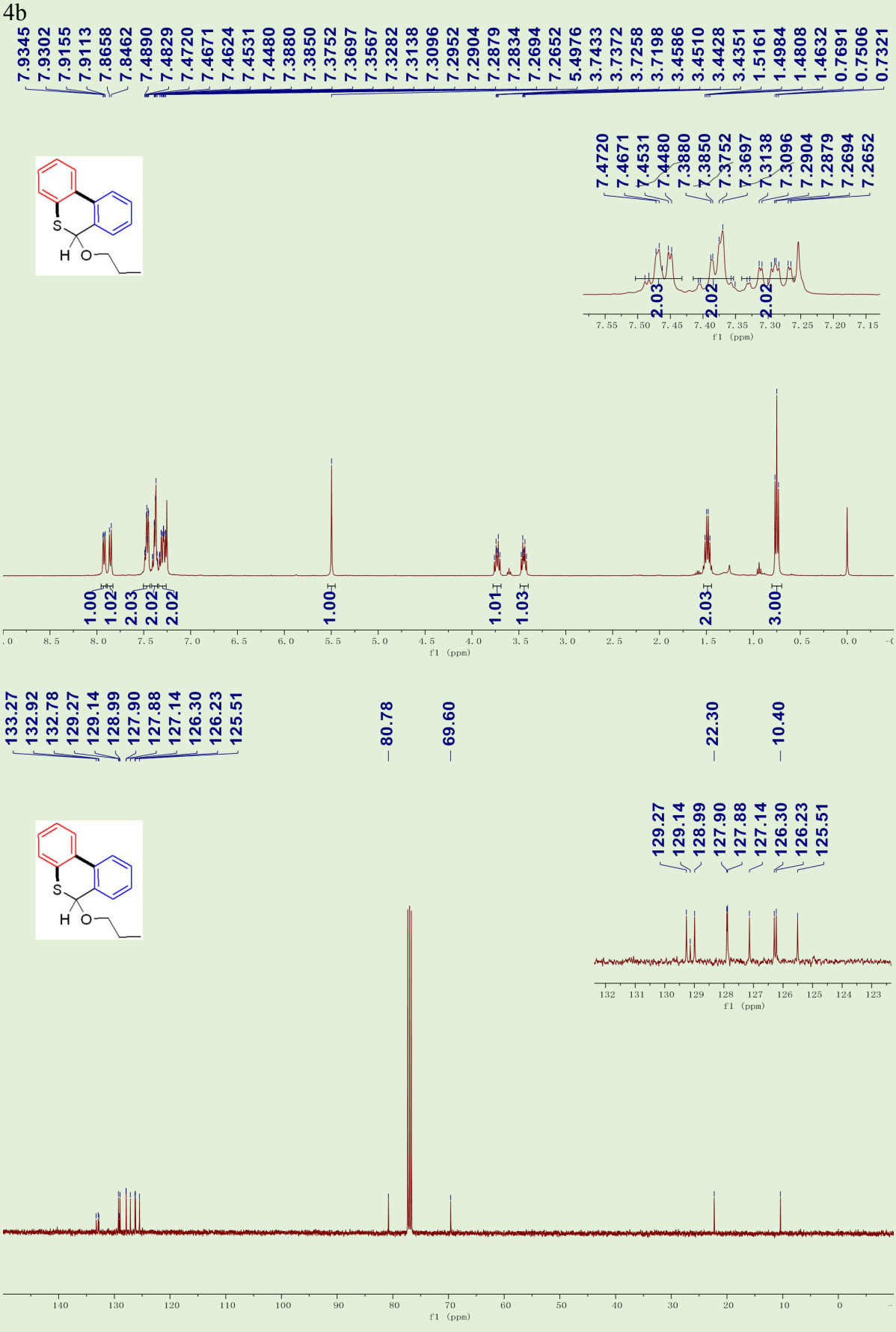
7.4997
7.4908
7.4865
7.4837
7.4795
7.4728
7.4690
7.4640
7.4171
7.4141
7.3982
7.3953
7.3866
7.3818
7.3796
7.3679
7.3613
7.3460
7.3420
7.3358
7.3277
7.3234
7.3091
7.3036
7.2982
7.2841
7.2800
5.4052
3.3917
S
H
OCH3
1.00
1.00
2.00
2.01
2.02
1.00
3.01
f1 (ppm)
2.00
2.01
2.02
f1 (ppm)
133.00
132.56
132.39
129.26
129.19
128.79
128.02
127.96
127.40
126.46
126.18
125.53
82.54
55.58
f1 (ppm)
f1 (ppm)

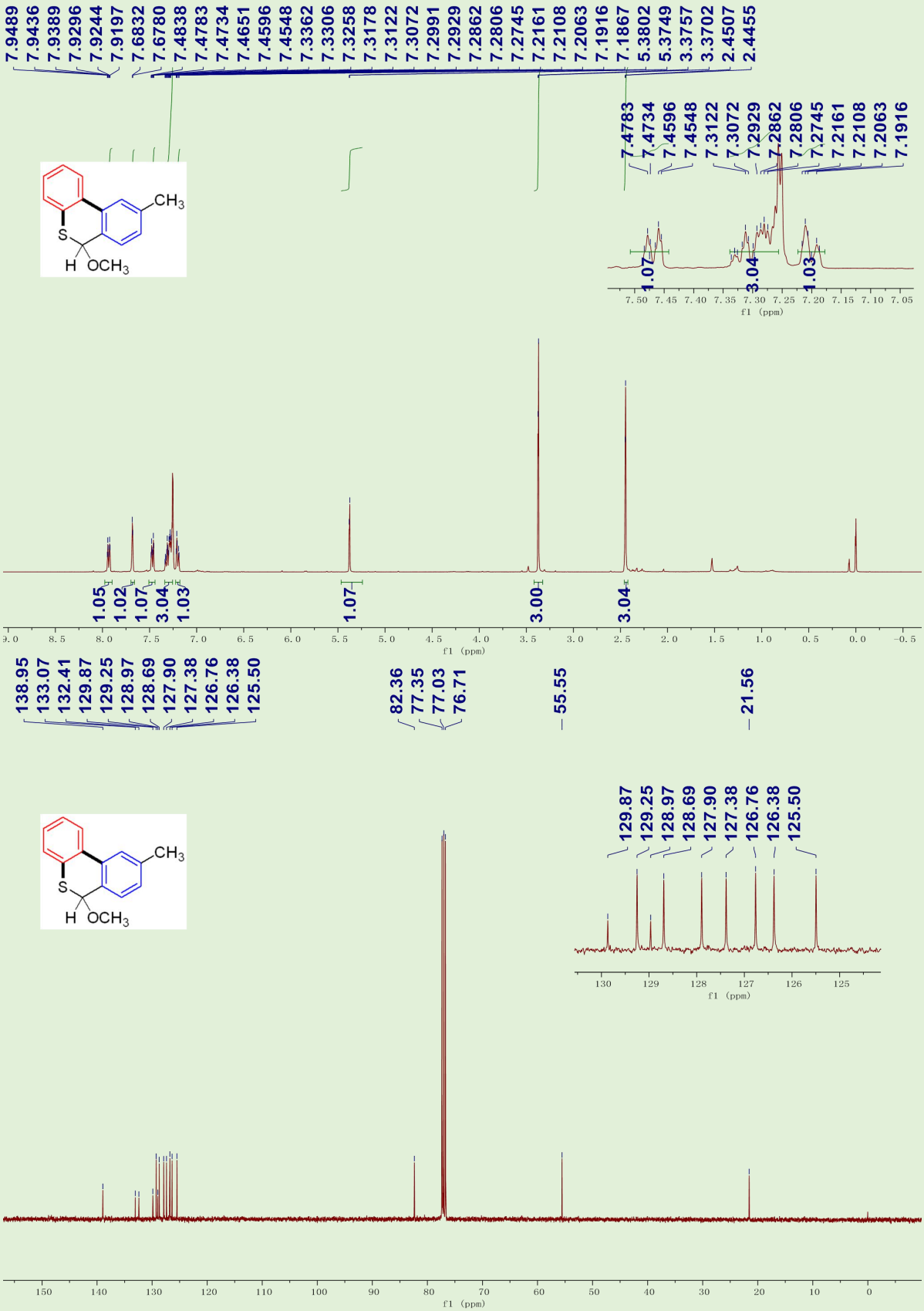
4b


7.9345 7.9302 7.9155 7.9113 7.8658 7.8462 7.4890 7.4829 7.4720 7.4671 7.4624 7.4531 7.4480 7.3880 7.3850 7.3752 7.3697 7.3567 7.3282 7.3138 7.3096 7.2952 7.2904 7.2879 7.2834 7.2694 7.2652 5.4976 3.7433 3.7372 3.7258 3.7198 3.4586 3.4510 3.4428 3.4351 1.5161 1.4984 1.4808 1.4632 0.7691 0.7506 0.7321
7.4720 7.4671 7.4531 7.4480 7.3880 7.3850 7.3752 7.3697 7.3138 7.3096 7.2904 7.2879 7.2694 7.2652
2.03 2.02 2.02
f1 (ppm)
1.00 1.02 2.03 2.02 2.02 1.00 1.01 1.03 2.03 3.00
f1 (ppm)
133.27 132.92 132.78 129.27 129.14 128.99 127.90 127.88 127.14 126.30 126.23 125.51
80.78 69.60 22.30 10.40
129.27 129.14 128.99 127.90 127.88 127.14 126.30 126.23 125.51
f1 (ppm)
f1 (ppm)

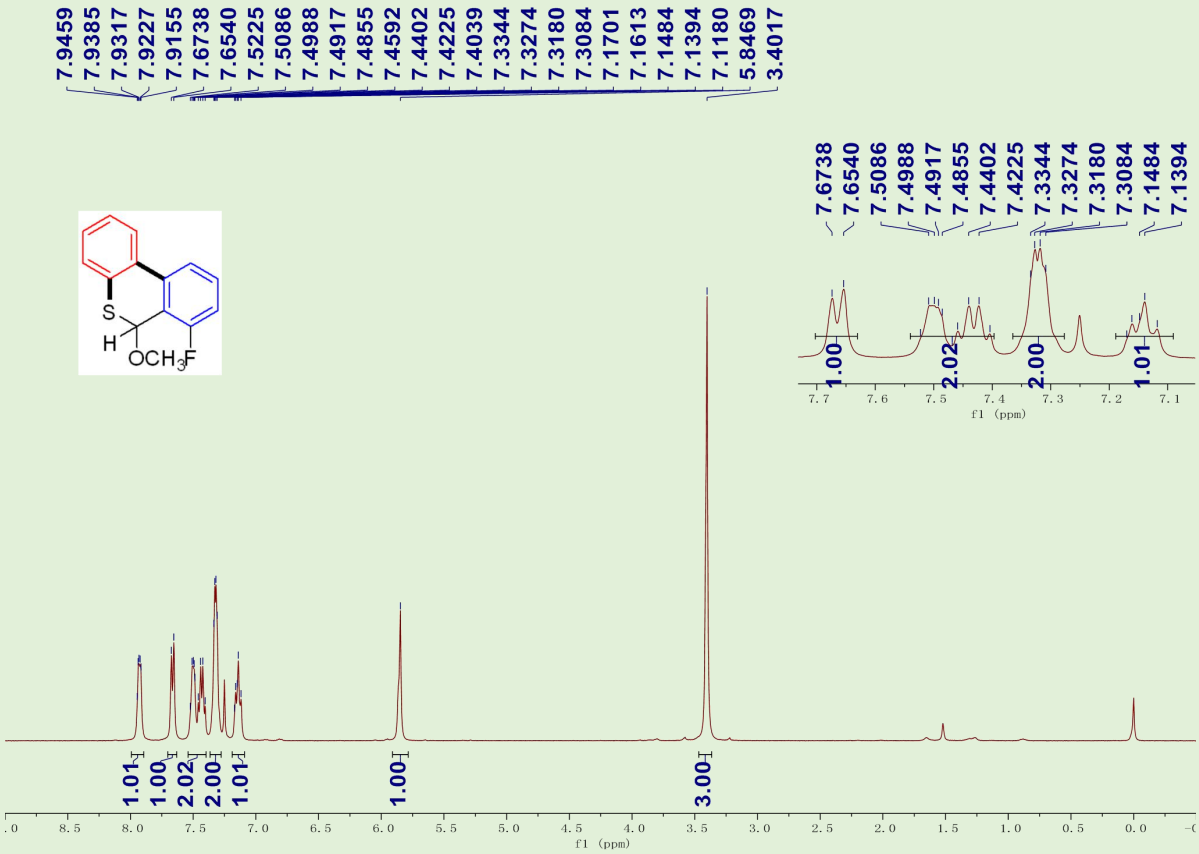
4c


8.0058
8.0010
7.9002
7.8943
7.8847
7.8808
7.8768
7.5264
7.5215
7.5062
7.5012
7.4936
7.4894
7.4857
7.4766
7.4708
7.3386
7.3338
7.3288
7.3221
7.3152
7.3107
7.3060
7.2662
7.2559
7.2459
5.3683
3.3743
Br
S
H
OCH3
1.01
1.04
2.00
2.06
2.04
1.05
3.06
f1 (ppm)
134.63
131.84
131.28
130.75
129.38
129.21
128.99
128.90
128.70
126.67
125.66
123.10
81.91
77.34
77.03
76.71
55.63

4d


7.9489 7.9436 7.9389 7.9296 7.9244 7.9197 7.6832 7.6780 7.4838 7.4783 7.4734 7.4651 7.4596 7.4548 7.3362 7.3306 7.3258 7.3178 7.3122 7.3072 7.2991 7.2929 7.2862 7.2806 7.2745 7.2161 7.2108 7.2063 7.1916 7.1867 5.3802 5.3749 3.3757 3.3702 2.4507 2.4455
CH3
S
H OCH3
1.05 1.02 1.07 3.04 1.03 1.07 3.00 3.04
f1 (ppm)
138.95 133.07 132.41 129.87 129.25 128.97 128.69 127.90 127.38 126.76 126.38 125.50
82.36 77.35 77.03 76.71
55.55
21.56
f1 (ppm)

4e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7.9317
7.9227
7.9155
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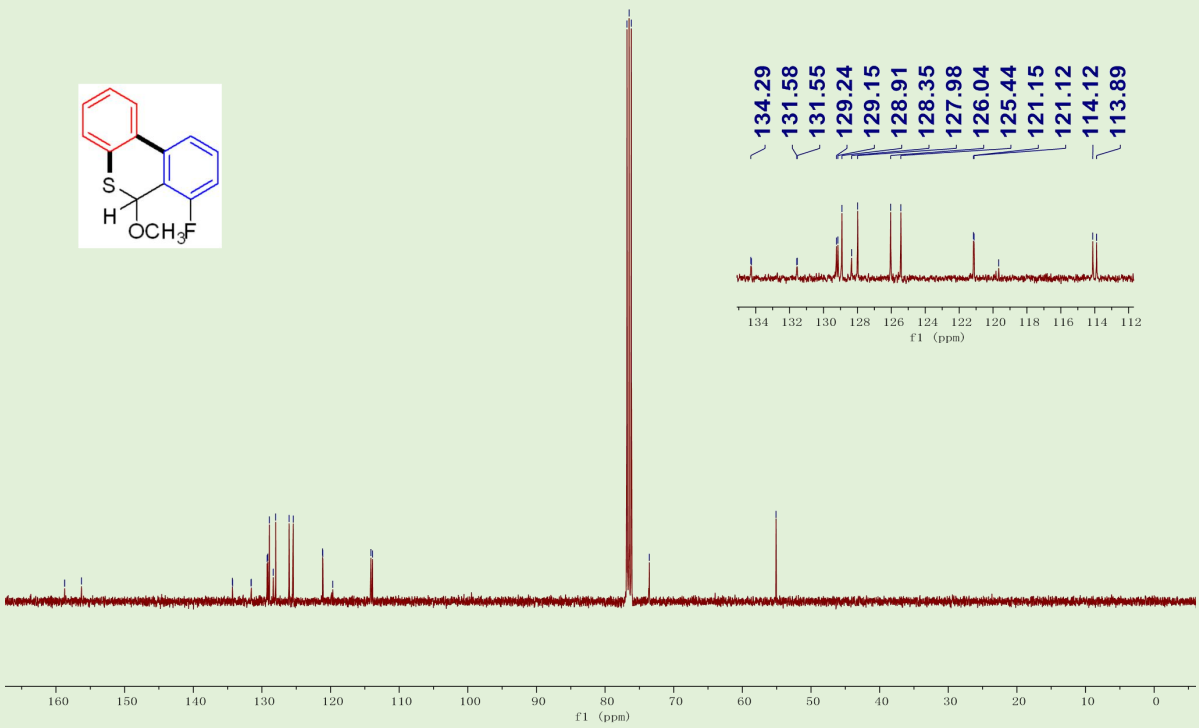
7.6540
7.5225
7.5086
7.4988
7.4917
7.4855
7.4592
7.4402
7.4225
7.4039
7.3344
7.3274
7.3180
7.3084
7.1701
7.1613
7.1484
7.1394
7.1180
5.8469
3.4017
1.01
1.00
2.02
2.00
1.01
1.00
3.00
f1 (ppm)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131.55
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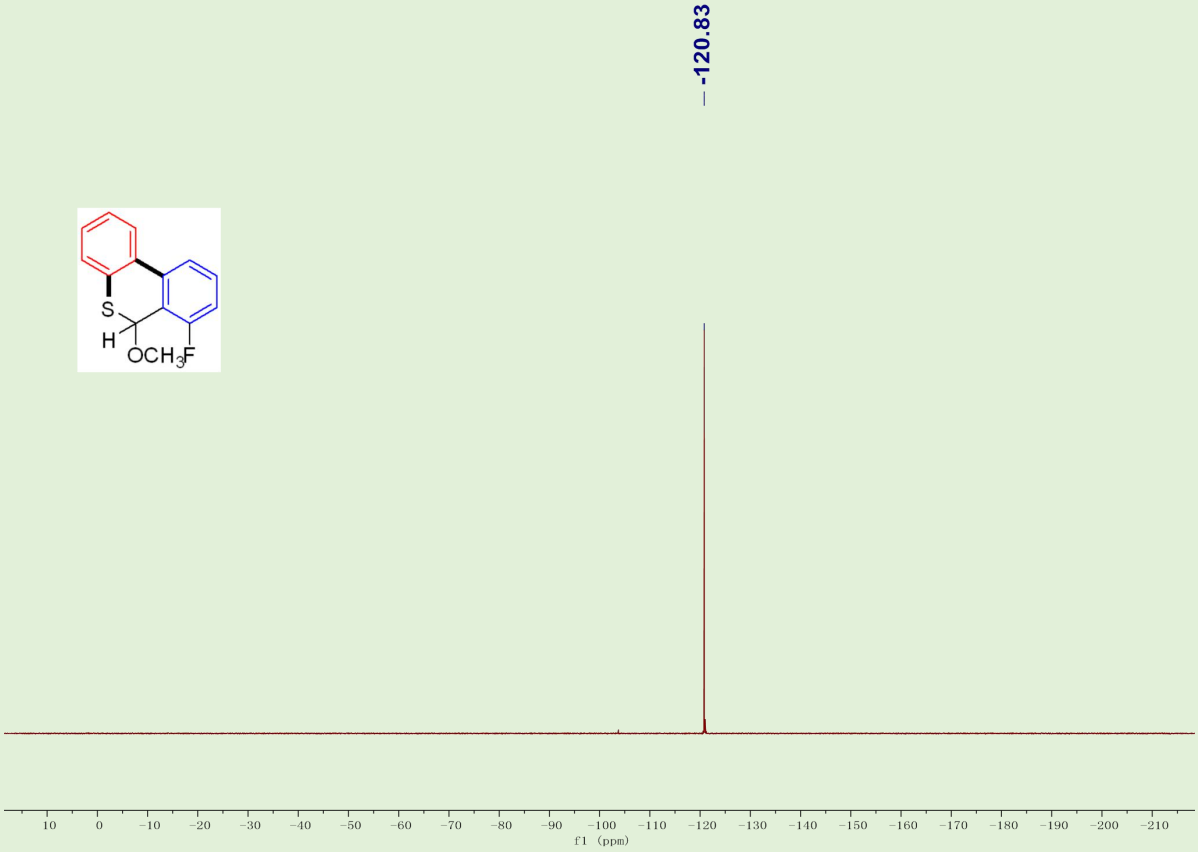
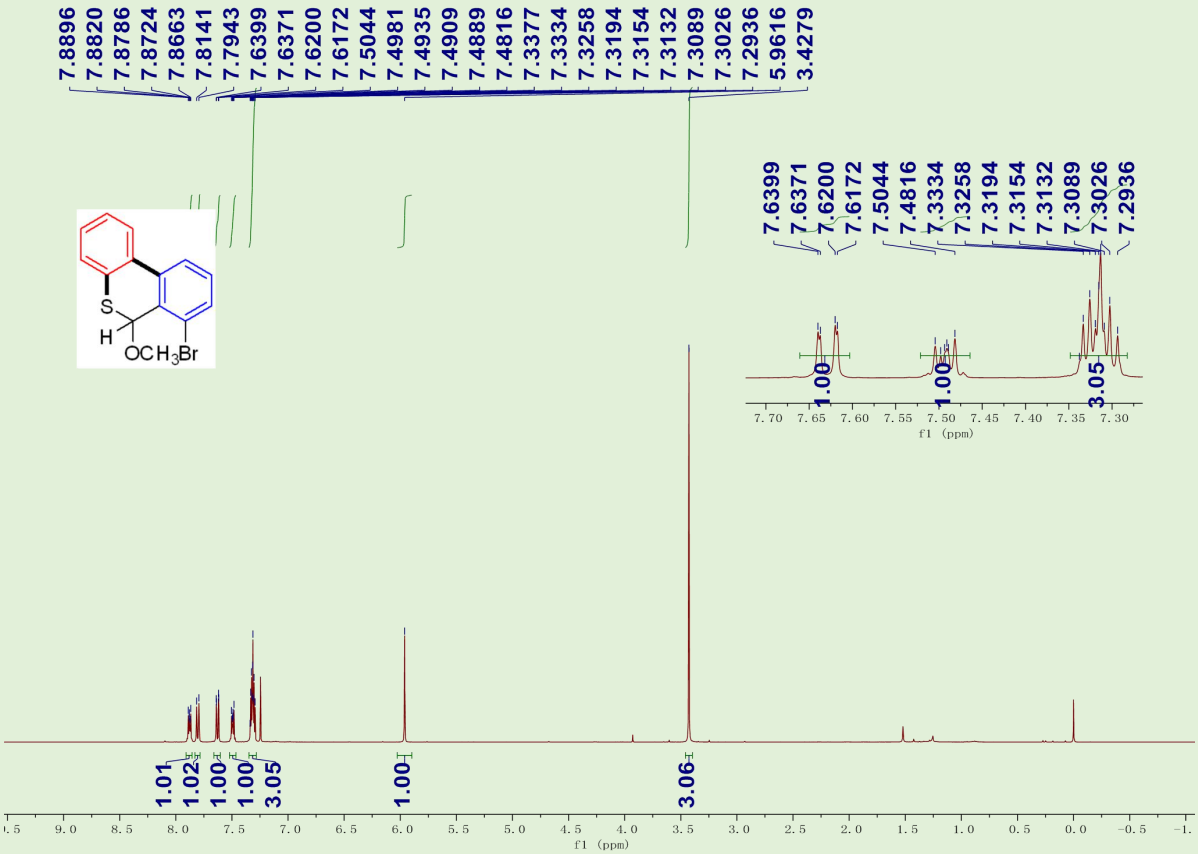
129.15
128.91
128.35
127.98
126.04
125.44
121.15
121.12
119.67
114.12
113.89
76.81
76.49
76.18
73.56
55.09
f1 (ppm)


-120.83
S
H
OCH3F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

4f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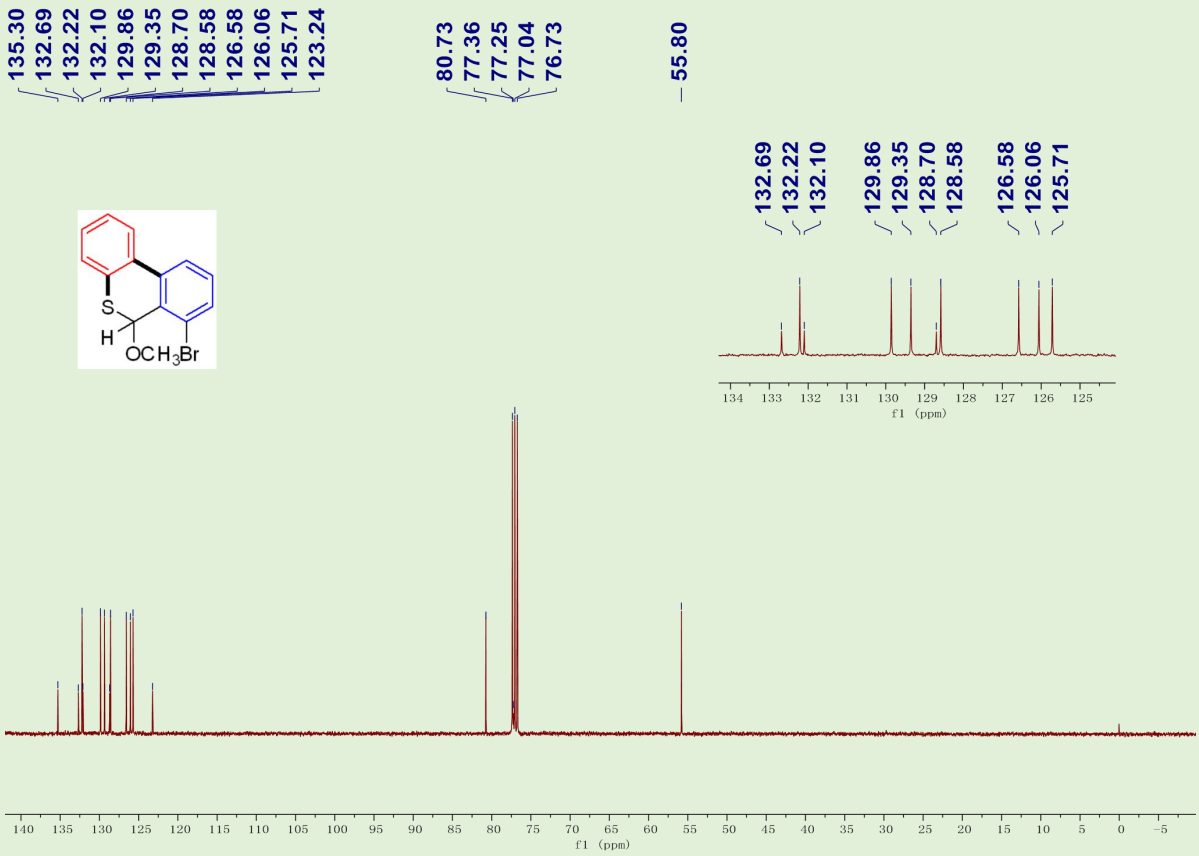
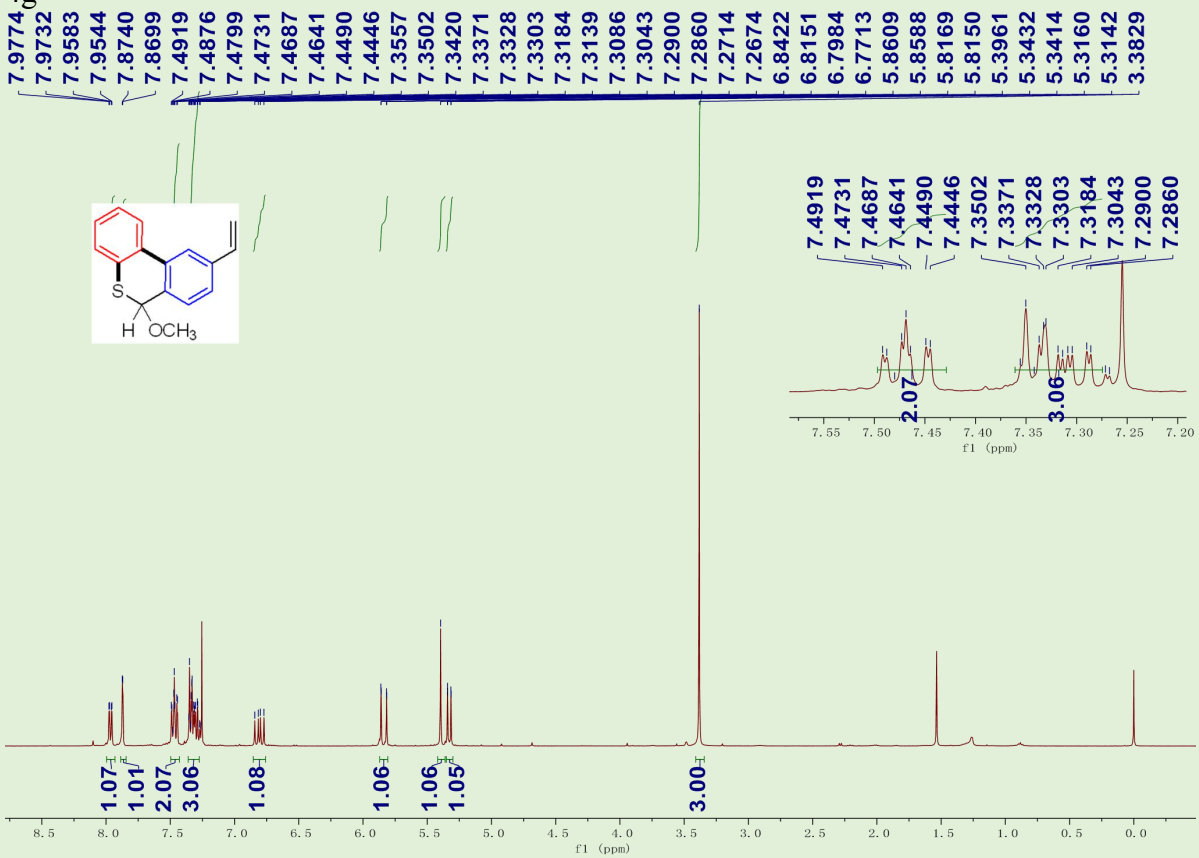
7.8141
7.7943
7.6399
7.6371
7.6200
7.6172
7.5044
7.4981
7.4935
7.4909
7.4889
7.4816
7.3377
7.3334
7.3258
7.3194
7.3154
7.3132
7.3089
7.3026
7.2936
5.9616
3.4279
S
H
OCH3Br
1.01
1.02
1.00
1.00
3.05
1.00
3.06
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)
7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30
f1 (ppm)


135.30
132.69
132.22
132.10
129.86
129.35
128.70
128.58
126.58
126.06
125.71
123.24
80.73
77.36
77.25
77.04
76.73
55.80
S
H
OCH3Br
f1 (ppm)

4g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7.4919
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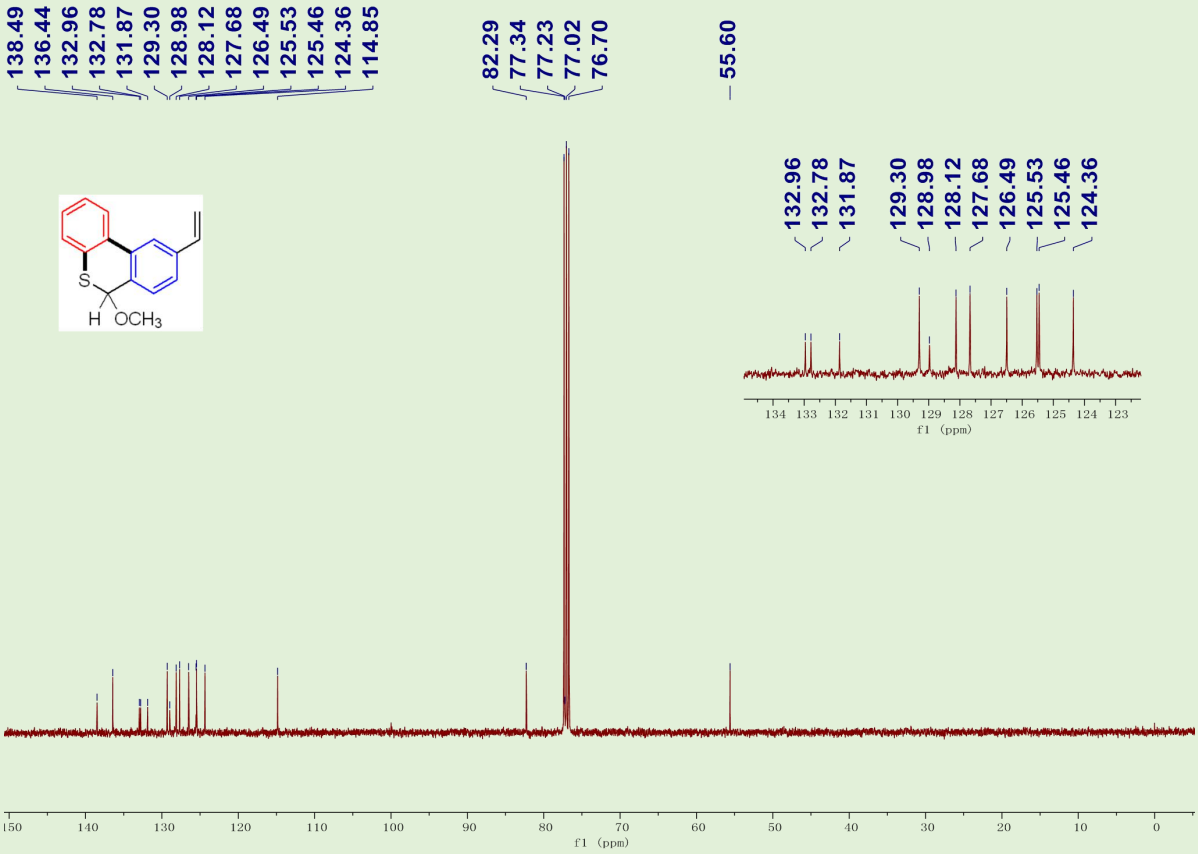
7.4799
7.4731
7.4687
7.4641
7.4490
7.4446
7.3557
7.3502
7.3420
7.3371
7.3328
7.3303
7.3184
7.3139
7.3086
7.3043
7.2900
7.2860
7.2714
7.2674
6.8422
6.8151
6.7984
6.7713
5.8609
5.8588
5.8169
5.8150
5.3961
5.3432
5.3414
5.3160
5.3142
3.3829
S
H
OCH3
2.07
3.06
f1 (ppm)
1.07
1.01
2.07
3.06
1.08
1.06
1.06
1.05
3.00
f1 (ppm)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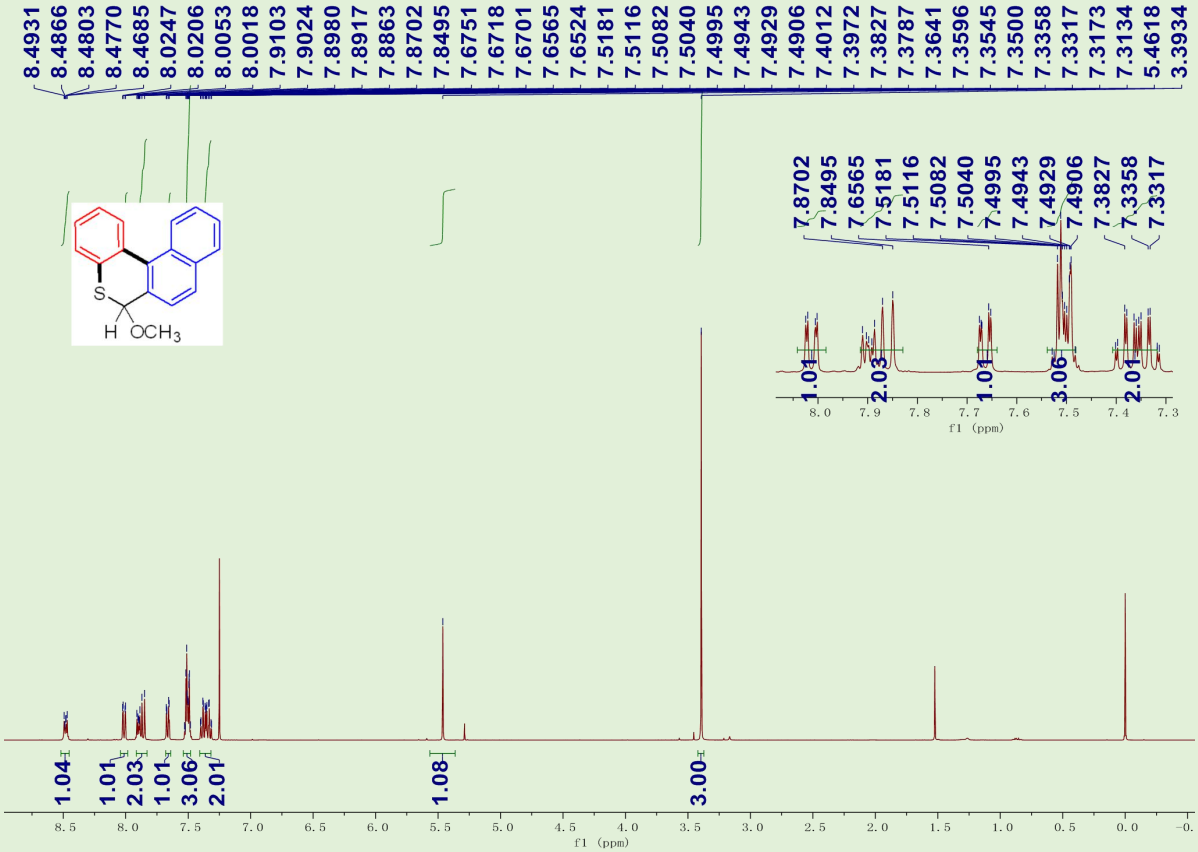
136.44
132.96
132.78
131.87
129.30
128.98
128.12
127.68
126.49
125.53
125.46
124.36
114.85
82.29
77.34
77.23
77.02
76.70
55.60
S
H OCH3
f1 (ppm)

4h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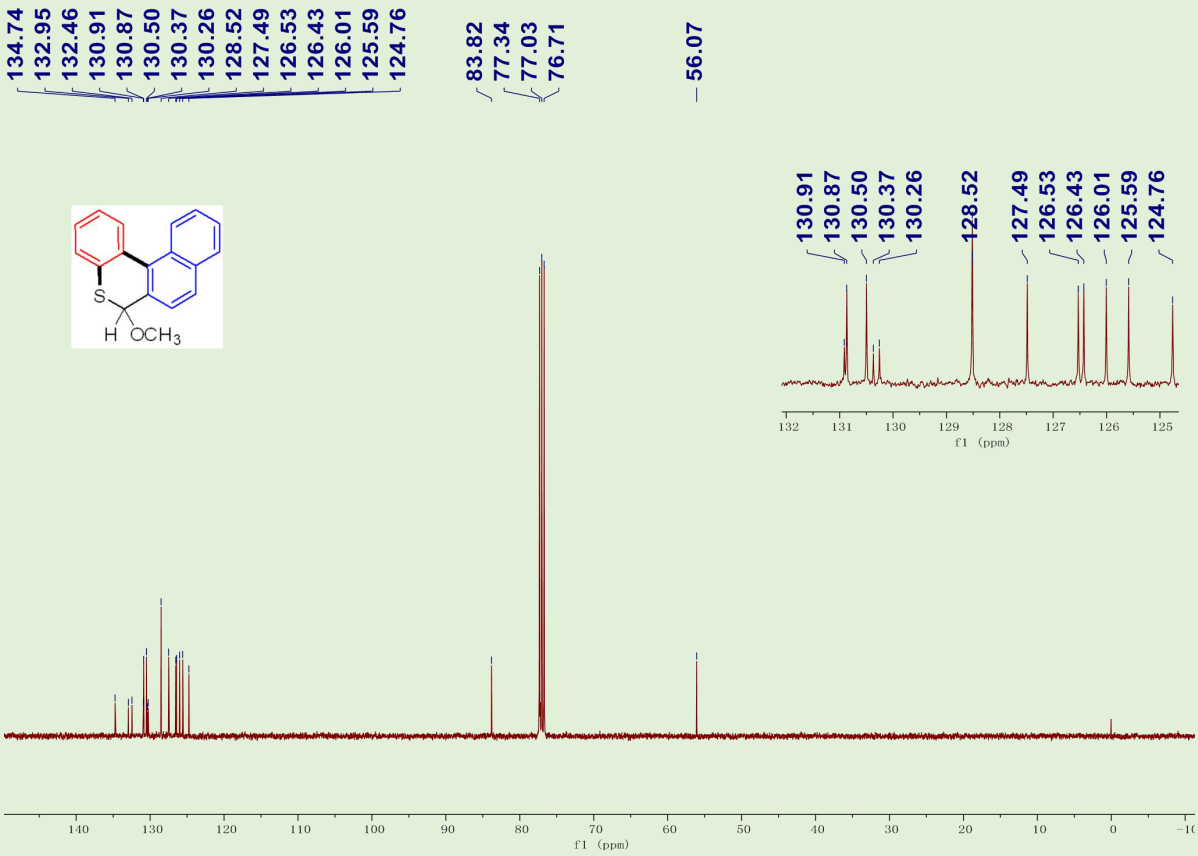
8.4803
8.4770
8.4685
8.0247
8.0206
8.0053
8.0018
7.9103
7.9024
7.8980
7.8917
7.8863
7.8702
7.8495
7.6751
7.6718
7.6701
7.6565
7.6524
7.5181
7.5116
7.5082
7.5040
7.4995
7.4943
7.4929
7.4906
7.4012
7.3972
7.3827
7.3787
7.3641
7.3596
7.3545
7.3500
7.3358
7.3317
7.3173
7.3134
5.4618
3.3934
1.04
1.01
2.03
1.01
3.06
2.01
1.08
3.00
S
H OCH3
f1 (ppm)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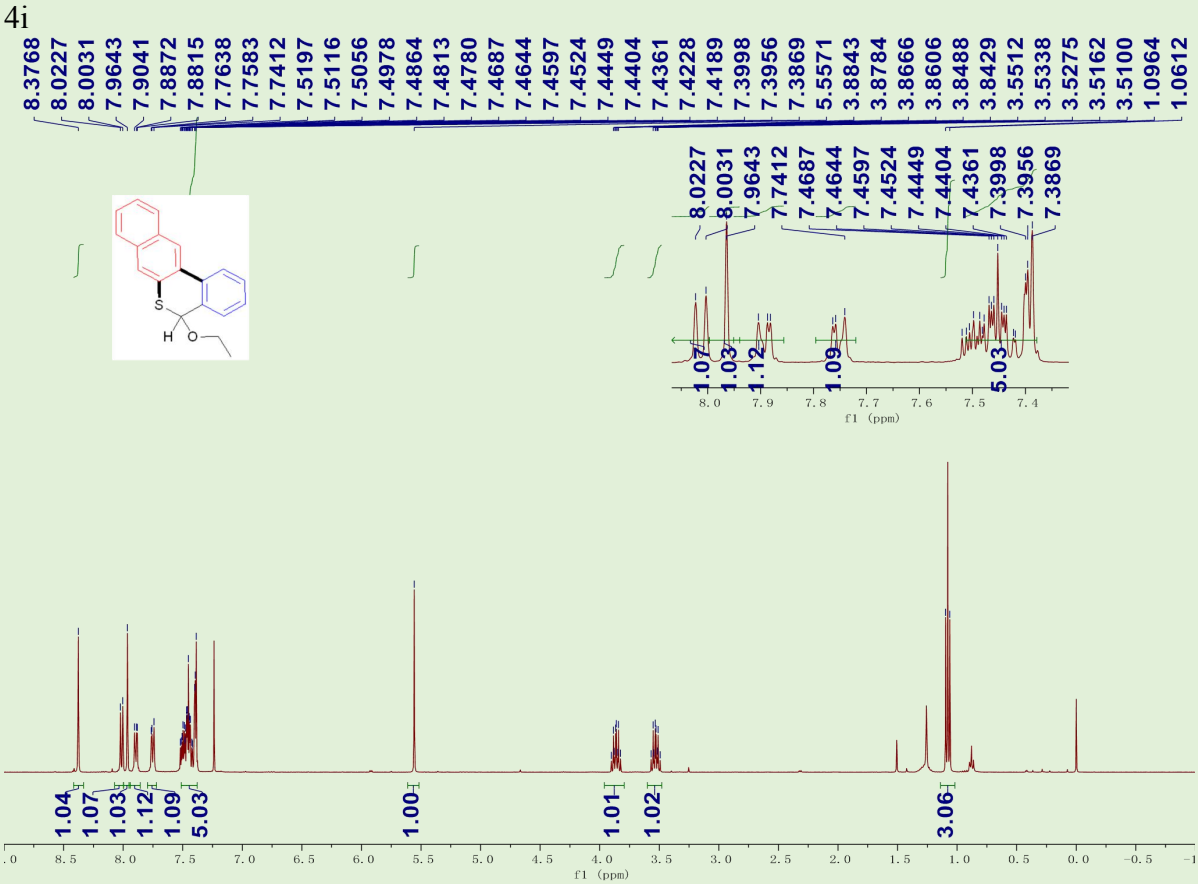
132.95
132.46
130.91
130.87
130.50
130.37
130.26
128.52
127.49
126.53
126.43
126.01
125.59
124.76
83.82
77.34
77.03
76.71
56.07
S
H
OCH3
f1 (ppm)

4i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8.0031
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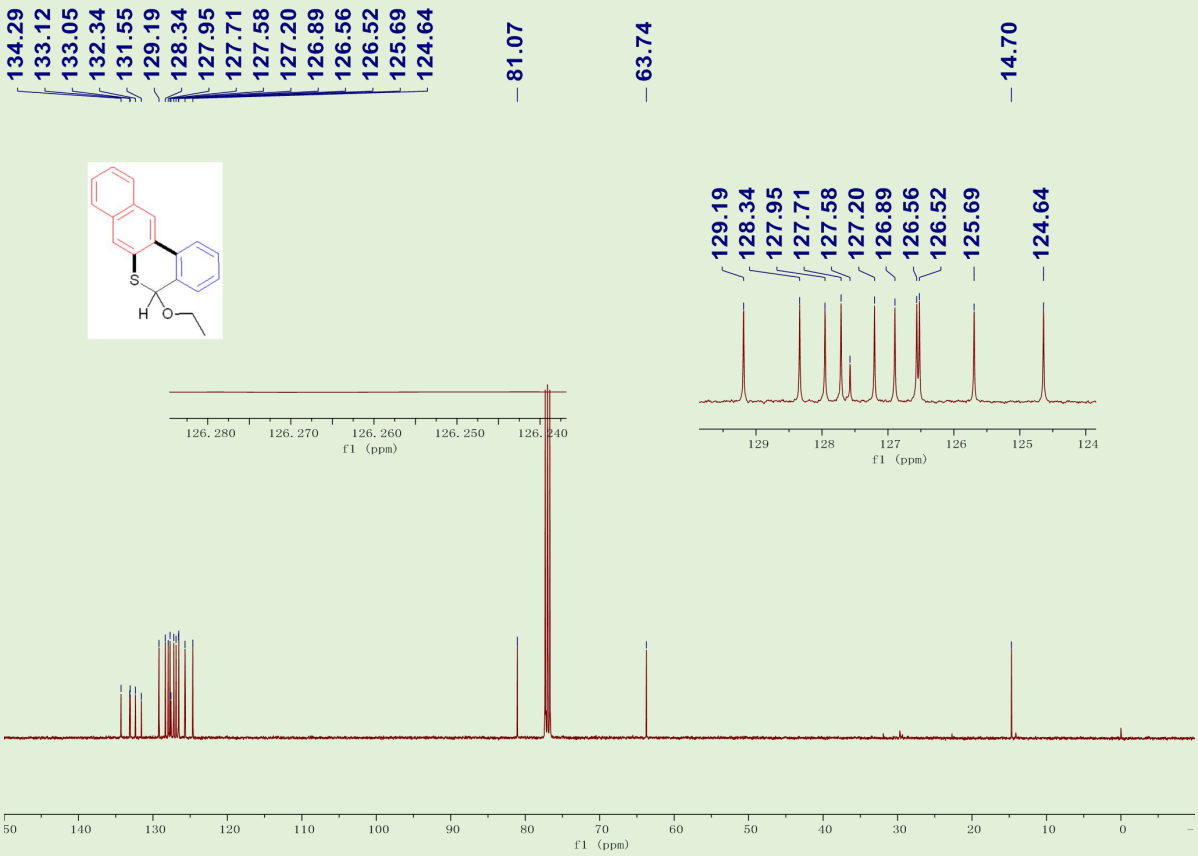
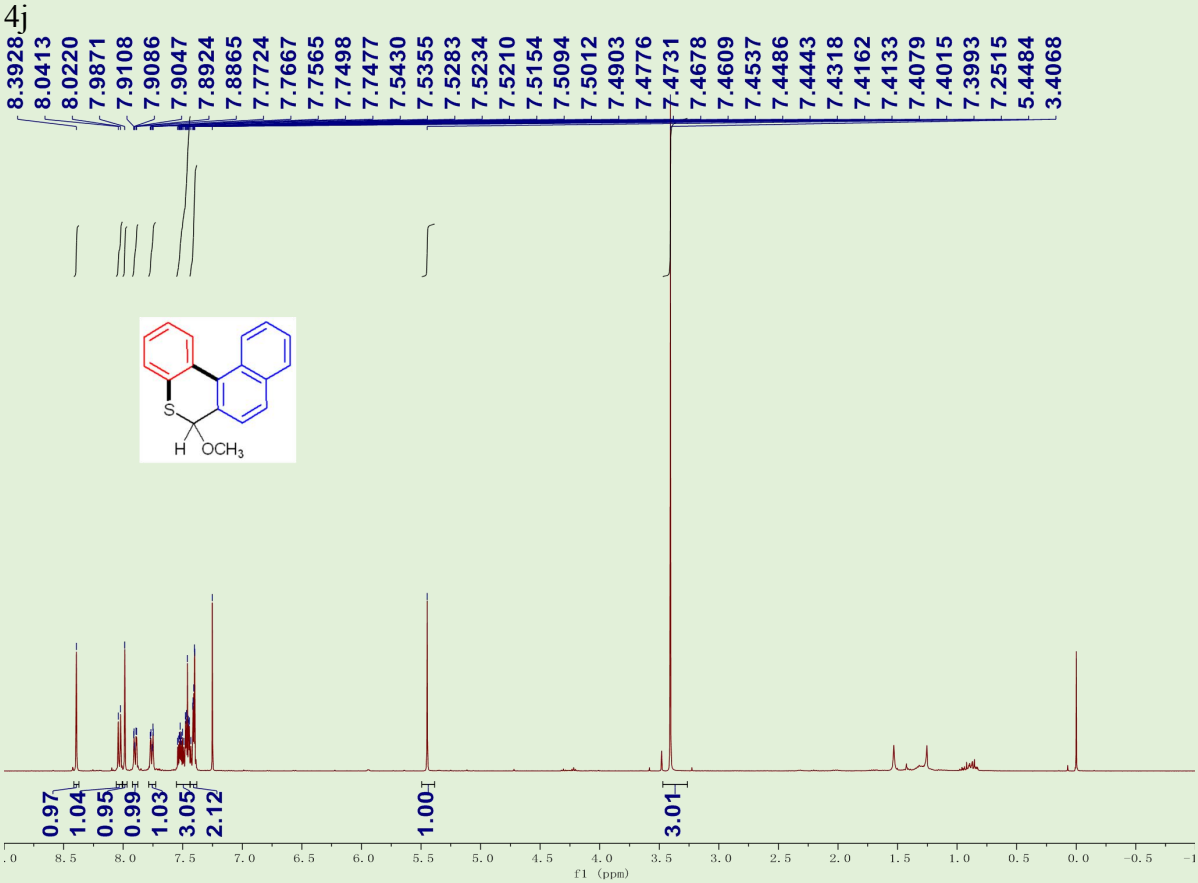
7.9041
7.8872
7.8815
7.7638
7.7583
7.7412
7.5197
7.5116
7.5056
7.4978
7.4864
7.4813
7.4780
7.4687
7.4644
7.4597
7.4524
7.4449
7.4404
7.4361
7.4228
7.4189
7.3998
7.3956
7.3869
5.5571
3.8843
3.8784
3.8666
3.8606
3.8488
3.8429
3.5512
3.5338
3.5275
3.5162
3.5100
1.0964
1.0612
S
H
O
1.04
1.07
1.03
1.12
1.09
5.03
1.00
1.01
1.02
3.06
f1 (ppm)


134.29
133.12
133.05
132.34
131.55
129.19
128.34
127.95
127.71
127.58
127.20
126.89
126.56
126.52
125.69
124.64
81.07
63.74
14.70
S
H
O
126.280
126.270
126.260
126.250
126.240
f1 (ppm)
129
128
127
126
125
124
f1 (ppm)
50
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

4j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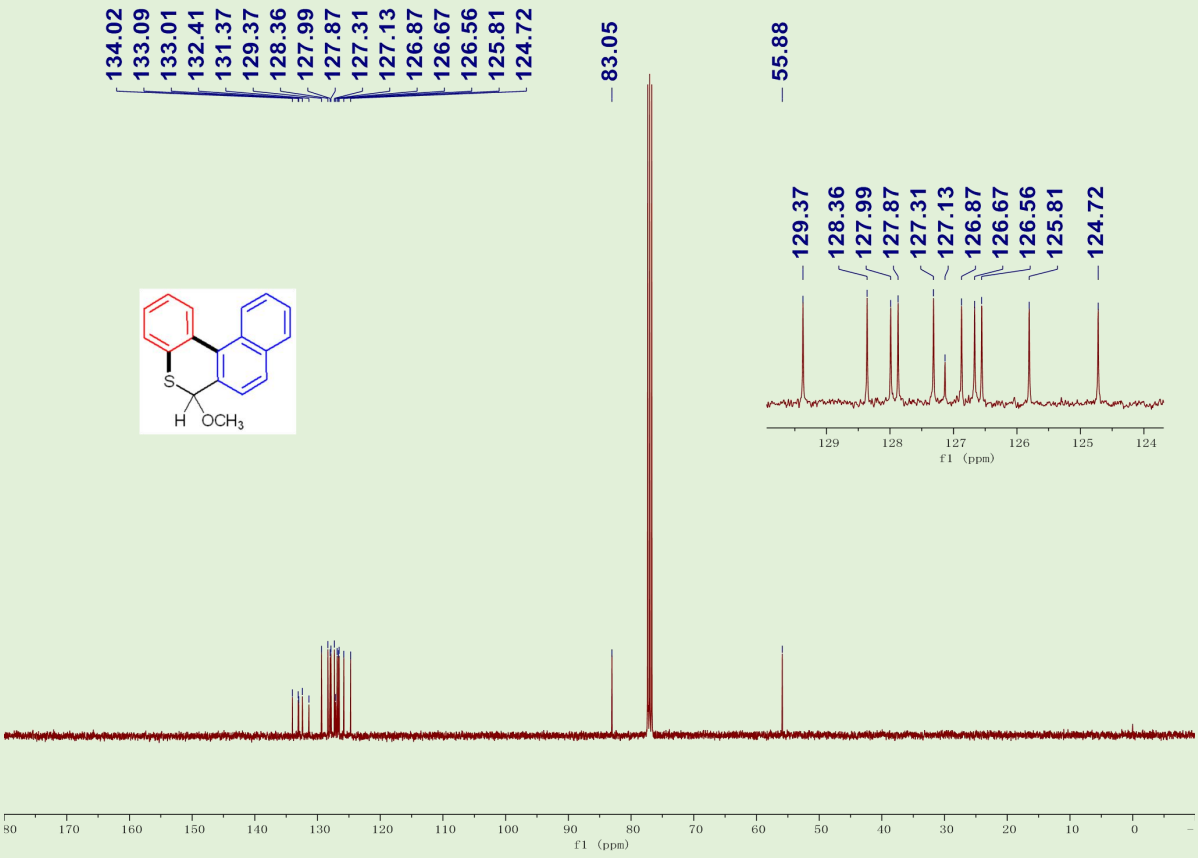
7.9086
7.9047
7.8924
7.8865
7.7724
7.7667
7.7565
7.7498
7.7477
7.5430
7.5355
7.5283
7.5234
7.5210
7.5154
7.5094
7.5012
7.4903
7.4776
7.4731
7.4678
7.4609
7.4537
7.4486
7.4443
7.4318
7.4162
7.4133
7.4079
7.4015
7.3993
7.2515
5.4484
3.4068
S
H
OCH3
0.97
1.04
0.95
0.99
1.03
3.05
2.12
1.00
3.01
f1 (ppm)


134.02
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133.01
132.41
131.37
129.37
128.36
127.99
127.87
127.31
127.13
126.87
126.67
126.56
125.81
124.72
83.05
55.88
S
H
OCH3
129.37
128.36
127.99
127.87
127.31
127.13
126.87
126.67
126.56
125.81
124.72
129
128
127
126
125
124
f1 (ppm)
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)