Electronic Supporting Information

Synergistic catalysis-induced ring-opening reactions of 2-substituted 3,4-dihydropyrans with α-oxoketene dithioacetals

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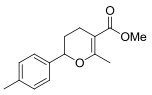
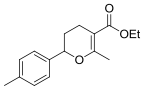
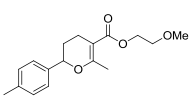
1. General remarks.

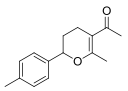
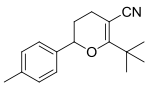
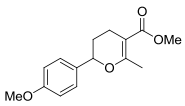
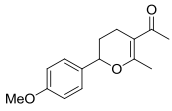
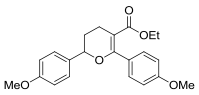
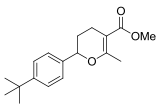
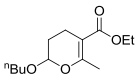
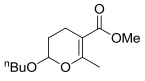
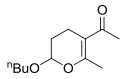
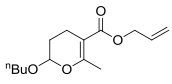
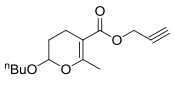
Unless otherwise noted, all reagents were purchased from commercial suppliers and used without purification. Acetophenone, 1-(4-nitrophenyl)ethanone, methyl 3-oxobutanoate, pentane-2,4-dione, ethyl 3-oxobutanoate, carbon disulfide, 1,2-dibromoethane, iodomethane, formalin were purchased from Sinopharm Chemical Reagent Co., Ltd. 1-(4-Chlorophenyl)ethanone, potassium 2-methylpropan-2-olate were purchased from Accela ChemBio Co., Ltd. 1-(4-Fluorophenyl)ethanone, 1-(*p*-tolyl)ethanone were purchased from Aladdin Industrial Corporation. 1-(4-Iodophenyl)ethanone, methyl 4-acetylbenzoate, 4,4-dimethyl-3-oxopentanenitrile were purchased from Energy Chemical Company. 1-methyl-4-vinylbenzene, 1-(*tert*-butyl)-4-vinylbenzene, 2-methoxyethyl 3-oxobutanoate, ethyl 3-(4-methoxyphenyl)-3-oxopropanoate were purchased from Alfa Aesar Chemical Company. 1-Methoxy-4-vinylbenzene was purchased from Tokyo Industry Co., Ltd. 1-(4-Methoxyphenyl)ethanone was purchased from Shanghai Feixiang Chemistry Company. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AV-400. Chemical shifts are expressed in ppm relative to Me_4Si in $CDCl_3$. IR spectra were recorded on a FT-IR Bruker (EQUINOX 55) using KBr technology. High-resolution mass spectra (HRMS) were obtained on Brüker Bruker Compass DataAnalysis 4.0.

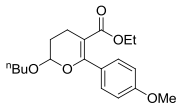
2. General procedure for the synthesis of 2-substituted 3,4-dihydropyrans[1].

The reactions were conducted in a 250 mL of round bottomed flask equipped with magnetic stirring. In the reaction, styrene derivative or 1-(vinyloxy)butane (20.0 mmol) was mixed with methyl 1,3-dicarbonyl compound (40.0 mmol) and formalin (4.05 g, 50.0 mmol, 37%). The mixture was stirred for 6 to 12 hours at 80 ^{o}C. After reaction, the mixture was cooled to room temperature and then water (20 mL) was added. The reaction liquid was extracted with ethyl acetate (3×20 mL). The organic extracts were combined then washed with brine (1×40 mL), After drying with anhydrous sodium sulfate, the organic solution was concentrated under vacuum to obtain the crude product, which was finally purified by silica gel column chromatography (eluting solution: petroleum ether / ethyl acetate = 20 / 1 (v/v)) . The yields of dihydropyrans were listed in Table **S1**.

Table S1. The yield of different dihydropyans.

Entry	Molecular structure		Yield/%
1		**1a**	85
2		**1b**	80
3		**1c**	82

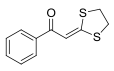
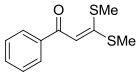
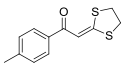
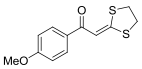
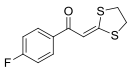
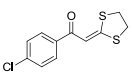
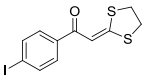
4		**1d**	76
5		**1e**	55
6		**1f**	88
7		**1g**	84
8		**1h**	85
9		**1i**	66
10		**4a**	75
11		**4b**	77
12		**4c**	76
13		**4d**	77
14		**4e**	76

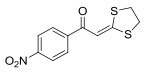
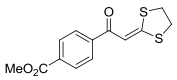
15		**4f**	75

3. General procedure for the synthesis of ketene dithioacetals[2]

All reactions were conducted in a 250 mL of three-necked round bottomed flask equipped with magnetic stirring. To a stirred suspension of potassium *tert*-butoxide (4.48 g, 40 mmol) in dry THF (10 mL) at 0 ℃, a dry THF solution (10 mL) of ketone (10 mmol) and carbon disulfide (12 mmol, 0.913 g, 0.73 mL) was dropwise added. The reaction mixture was vigorously stirred at 0 ℃ for 90 minutes. To this suspension, a dry THF solution (5 mL) of methyl iodide or 1,2-dibromoethane (22 mmol) was added dropwise within 10 minutes at 0 ℃. The reaction mixture was stirred for 3 hours. After completion of the reaction (monitored by TLC), the mixture was poured into saturated aqueous solution of ammonium chloride with crushed ice. Then, the aqueous solution was extracted with ethyl acetate (3 × 25 mL). The combined organic extracts were washed with brine (1×25 mL), dried, and then concentrated under vacuum to obtain the crude product. Pure product was obtained by silica gel column chromatography (eluting solution: petroleum ether / ethyl acetate = 10 / 1 (v/v)). The yields of ketene dithioacetals were listed in Table **S2**.

Table S2. The yield of different ketene dithioacetals.

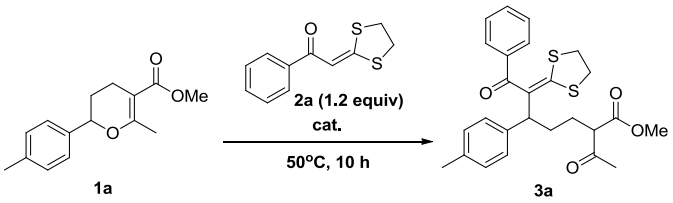
Entry	Molecular structure		Yield/%
1		**2a**	55
2		**2b**	68
3		**2c**	75
4		**2d**	65
5		**2e**	68
6		**2f**	57
7		**2g**	48

8		**2h**	20
9		**2i**	66

4. A typical procedure for ring-opening reaction of 2-aryl-3,4-dihydropyrans

All reactions were conducted in a 10 mL of V-type flask equipped with triangle magnetic stirring. In a typical reaction, ketene dithioacetal (0.24 mmol) was mixed with dihydropyran (0.20 mmol), $CuBr_2$ (5 mol %) and $MnCl_2$ $4H_2O$ (15 mol %) in nitromethane (1.0 mL). The mixture was then stirred at 50 ^oC for 10 hours. After reaction, the mixture was cooled to room temperature, and the product was obtained by isolation with preparative TLC (eluting solution: petroleum ether / ethyl acetate = 5 / 1 (v/v)). Tests for substrate scope were all performed with an analogous procedure.

Table S3. Ring-opening Reaction of **1a** with **2a** under different catalysts



entry [a]	catalyst	time (h)	Yield (%)
1	$Zn(OTf)_2$	10	nr
2	$In(OTf)_3$	2.5	mess
3	I_2	2.5	mess
4	$Sc(OTf)_2$	2.5	mess
5	$FeCl_3$	10	35
6	$FeBr_3$	10	trace
7	TsOH H_2O	10	15
8	LiBr H_2O	10	NR
9	HBr	10	NR

[a] The reaction was performed in 0.20 mmol scale in 1.0 ml of nitromethane at 50 ^oC , catalyst loading is 20 mol %.

5. A typical procedure for ring-opening reaction of 2-butoxy-3,4-dihydropyrans

All reactions were conducted in a 10 mL of V-type flask equipped with triangle magnetic stirring. In a typical reaction, ketene dithioacetal (0.24 mmol) was mixed with dihydropyran (0.20 mmol), $CuBr_2$ (5 mol %) and $MnCl_2$ $4H_2O$ (15 mol %) in nitromethane (1.0 mL). The mixture was then stirred at 80 ^oC for 1 h. After reaction, the mixture was cooled to room temperature, and the product was obtained by isolation with preparative TLC (eluting solution: petroleum ether / ethyl acetate = 3 / 1 (v/v)). Tests for substrate scope were all performed with an analogous procedure.

6. Catalytic mechanism analysis

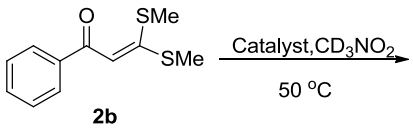
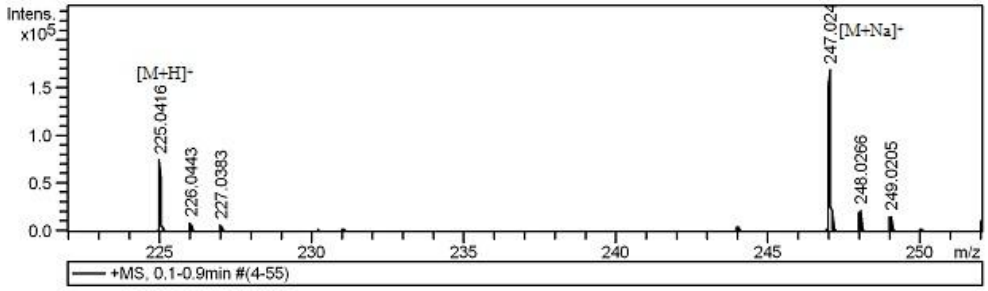
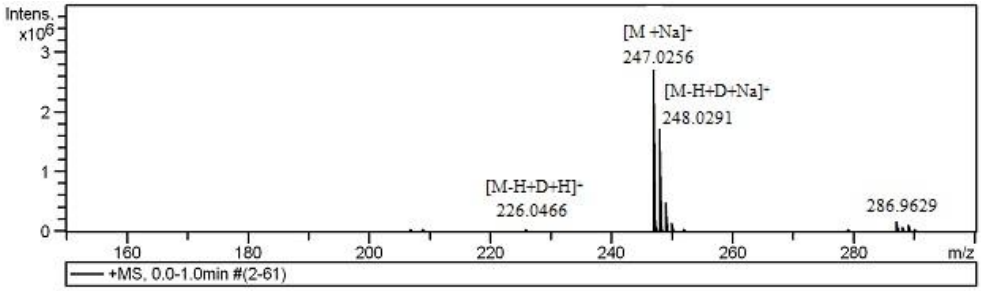


Figure S1. HRMS analysis of a nitromethane-d_3 solution of **2b** treated with $CuBr_2$ (the reaction was conducted at 50 °C, 0.5 h).



(1)



(2)

Figure S2. HRMS spectra of **2b**. (1) without catalyst; (2) with $CuBr_2$.

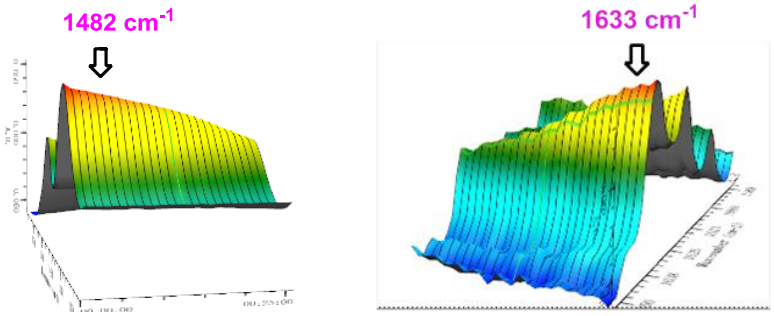


Figure S3 *In-situ* FTIR analysis of **2b** (treated **2b** with $CuBr_2$ in DCE under 50 °C for 30 minutes).

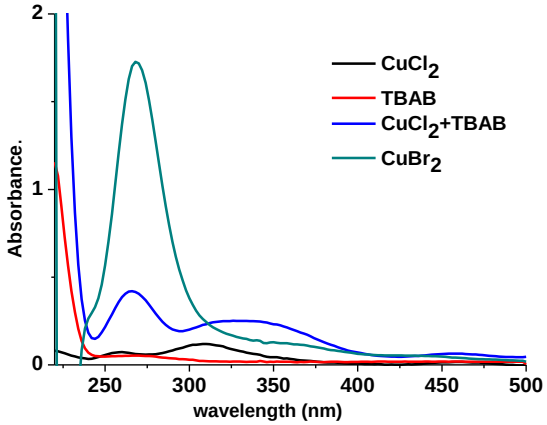
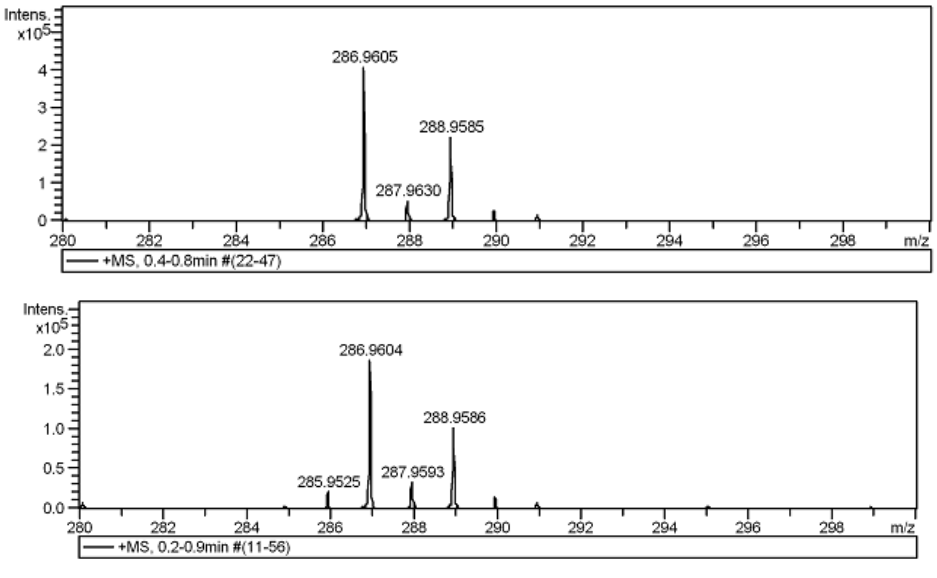


Figure S4. UV-Vis spectra of Cu(II) salts and TBAB.



(**1**)

(**2**)

Figure S5. HRMS spectra of **2b**. (1) **2b** + $CuBr_2$; (2) **2b** + $Cu(OTf)_2$ (peak of 285.9525 can be ascribed to the formation of $[(\mathbf{I}) - H]^+$)

7. Characterization data of new compounds

2-Methoxyethyl 6-methyl-2-(*p*-tolyl)-3,4-dihydro-2H-pyran-5-carboxylate (**1c**): Colorless oil, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C): δ = 7.21 (d, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 2H), 4.82 (d, *J* = 10.2 Hz, 1H), 4.28 – 4.24 (m, 2H), 3.64 – 3.60 (m, 2H), 3.38 (s, 3H), 2.53 – 2.39 (m, 2H), 2.34 (s, 3H), 2.32 (s, 3H), 2.07 (ddd, *J* = 10.5, 5.5, 2.7 Hz, 1H), 1.91 – 1.79 ppm (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 ^{o}C): *δ* = 168.4, 165.4, 137.8, 137.7, 129.2, 125.9, 101.2, 78.1, 70.8, 62.8, 58.9, 29.1, 21.9, 21.1, 20.4 ppm. IR (KBr) *v*: 2925, 2884, 1705, 1623, 1516, 1380, 1269, 1206, 1133, 1079, 1017, 813, 760 cm^{-1}. HRMS-ESI (m/z) calcd for $C_{17}H_{22}NaO_4$, $[M+Na]^+$ 313.1416, found 313.1424.

6-(*tert*-Butyl)-2-(*p*-tolyl)-3,4-dihydro-2H-pyran-5-carbonitrile (**1e**): Colorless oil, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 ^{o}C): *δ* = 7.19 (s, 4H), 4.82 (dd, *J* = 10.4, 2.1 Hz, 1H), 2.36 (s, 3H), 1.37 (s,

2H), 1.34 (s, 9H), 1.16 ppm (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) δ = 175.5, 137.9, 137.3, 129.3, 125.5, 120.8, 79.5, 78.3, 38.3, 28.7, 26.3, 25.1, 21.2 ppm. IR (KBr) *v*: 2965, 2876, 2202, 1705, 1608, 1516, 1479, 1398, 1368, 1274, 1188, 1079, 1041, 814 cm^{-1}. HRMS-ESI (m/z) calcd for $C_{17}H_{21}NNaO$, $[M+Na]^+$ 278.1521, found 278.1523.

Methyl-2-(4-(tert-butyl)phenyl)-6-methyl-3,4-dihydro-2H-pyran-5-carboxylate (**1i**): Colorless oil, ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C): δ = 7.40 (d, *J* = 8.3 Hz, 2H), 7.27 (d, *J* = 8.3 Hz, 2H), 4.85 (dd, *J* = 10.3, 2.1 Hz, 1H), 3.71 (s, 3H), 2.50 – 2.37 (m, 2H), 2.31 (s, 3H), 2.14 – 2.07 (m, 1H), 1.93 – 1.81 (m, 1H), 1.32 ppm (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ = 169.0, 165.3, 151.0, 137.7, 125.7, 125.5, 101.2, 78.1, 51.0, 34.6, 31.3, 29.0, 21.9, 20.4. IR (KBr) *v*: 2956, 2867, 1709, 1624, 1513, 1434, 1381, 1272, 1209, 1186, 1083, 1017, 956, 834, 765, 576 cm^{-1}. HRMS-ESI (m/z) calcd for $C_{18}H_{24}NaO_3$, $[M+Na]^+$ 311.1623, found 311.1633.

2-(1,3-dithiolan-2-ylidene)-1-(4-iodophenyl)ethanone (**2g**): Light yellow solid, mp = 165-167 ℃; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C): δ = 7.80 (d, *J* = 8.3 Hz, 2H), 7.66 (d, *J* = 8.3 Hz, 2H), 7.28 (s, 1H), 3.49 (t, *J* = 6.1 Hz, 2H), 3.42 – 3.37 ppm (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ = 185.1, 169.3, 137.8, 129.4, 107.8, 99.6, 39.0, 35.5 ppm. IR (KBr) *v*: 2917, 1608, 1578, 1549, 1488, 1224, 1053, 999, 965, 778 cm^{-1}. HRMS-ESI (m/z) calcd for $C_{11}H_{10}IOS_2$, $[M+H]^+$ 348.9218, found 348.9223.

Methyl-4-(2-(1,3-dithiolan-2-ylidene)acetyl)benzoate (**2i**): Light yellow solid, mp = 148-150 ℃; ^{1}H NMR (400 MHz, $CDCl_3$, TMS, 25 °C): δ = 8.11 (d, *J* = 8.3 Hz, 2H), 8.00 (d, *J* = 8.3 Hz, 2H), 7.36 (s, 1H), 3.94 (s, 3H), 3.54 – 3.49 (m, 2H), 3.45 – 3.39 ppm (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$, 25 °C): δ = 185.2, 169.9, 166.5, 141.8, 129.8, 127.8, 108.2, 52.4, 39.0, 35.6 ppm. IR (KBr) *v*: 2922, 1718, 1596, 1560, 1507, 1477, 1438, 1280, 1222, 1108, 969, 772 cm^{-1}. HRMS-ESI (m/z) calcd for $C_{13}H_{13}O_3S_2$, $[M+H]^+$ 281.0306, found 281.0310.

Allyl 2-butoxy-6-methyl-3,4-dihydro-2H-pyran-5-carboxylate (**4d**): Colorless oil, ^{1}H NMR (600 MHz, $CDCl_3$, TMS, 25 ℃): δ = 6.03 – 5.89 (m, 1H), 5.32 (dd, *J* = 17.2, 1.4, 1H), 5.25 – 5.18 (m, 1H), 5.07 – 4.99 (m, 1H), 4.65 – 4.58 (m, 2H), 3.86 – 3.75 (m, 1H), 3.58 – 3.48 (m, 1H), 2.46 – 2.30 (m, 2H), 2.25 (d, *J* = 1.2 Hz, 3H), 1.91 – 1.82 (m, 1H), 1.81 – 1.72 (m, 1H), 1.61 – 1.49 (m, 2H), 1.40 – 1.31 (m, 2H), 0.95 – 0.87 ppm (m, 3H).^{13}C NMR (151 MHz, $CDCl_3$, 25 ℃): δ = 167.9, 162.2, 133.0, 117.2, 101.8, 98.0, 68.5, 64.4, 31.7, 26.1, 20.0, 19.2, 17.8, 13.8 ppm. IR (KBr) *v*: 2959, 2935, 2873, 1709, 1629, 1456, 1380, 1337, 1270, 1119, 1059, 1011, 933, 769 cm^{-1}. HRMS-ESI (m/z) calcd for $C_{13}H_{20}NaO_4$, $[M+Na]^+$ 277.1416, found 277.1422.

Prop-2-yn-1-yl 2-butoxy-6-methyl-3,4-dihydro-2H-pyran-5-carboxylate (**4e**): Colorless oil, ^{1}H NMR (600 MHz, $CDCl_3$, TMS, 25 ℃): δ = 5.04 (d, *J* = 2.7 Hz, 1H), 4.71 (d, *J* = 1.0 Hz, 1H), 3.89 – 3.77 (m, 1H), 3.70 (s, 1H), 3.53 (dt, *J* = 10.9, 4.1 Hz, 1H), 2.45 (t, *J* = 2.2 Hz, 1H), 2.44 – 2.30 (m, 2H), 2.25 (d, *J* = 11.3 Hz, 3H), 1.94 – 1.82 (m, 1H), 1.76 (dt, *J* = 10.6, 6.9 Hz, 1H), 1.56 (dd, *J* = 13.8, 7.0 Hz, 2H), 1.36 (dt, *J* = 14.7, 7.3 Hz, 2H), 0.91 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$, 25 ℃): δ = 167.3, 163.2, 101.8, 101.2, 98.1, 97.9, 78.5, 74.1, 68.5, 68.4, 51.2, 51.0, 31.7, 31.6, 26.1, 26.0, 20.1, 19.9, 19.2, 17.8, 17.7, 13.9 ppm. IR (KBr) *v*: 3293, 2959, 2936, 2873, 1711, 1628, 1435, 1380, 1339,. 1273, 1119, 1061, 1011, 860, 769 cm^{-1}. HRMS-ESI (m/z) calcd for $C_{13}H_{18}NaO_4$, $[M+Na]^+$ 275.1529, found 275.2755.

8. Molecular calculation of 2b

The molecular structure of **2b** was optimized by minimizing the energy of its structure without any symmetry constraints. To achieve the most stable structure, the study was implemented over GAUSSIAN 98 code using the hybrid density functional approach (DFT) with B3LYP**,** PBEPBE and ab inito theory with HF methods, employed 6-311++g**, 6-31+g* and 3-21+g basis sets, **Figure S6**. The structural optimization of **2b** showed that all of the carbon, oxygen and sulfur atoms as well as hydrogen in the aromatic ring are in the same surface, indicating the existence of a conjugated system (**Figure S7**). Vibrational frequency calculation at B3LYP/6-31+g* level of the geometry optimization has verified the electron delocalization of the conjugate system of **2b** (contour plat at HOMO orbital of **2b**, **Figure S8**). It was also found that there are strong hydrogen bond interactions around H9, which include CH9-O and CH9-S4 and the pseudo-bond lengths are 2.152 and 2.379 Å respectively. The van-der Waals radiuses of Hydrogen, Oxygen and Sulfur atoms are 1.20, 1.52 and 1.80 Å respectively. Both of the pseudo-bond lengths are less than the sum of van-der Waals radiuses of each atom pair (2.72 Å for H + O, and 3.00 Å for H + S). Additionally, the molecular structure was also affected by hydrogen bond between CH20 and S5, which has a pseudo-bond length of 2.809 Å. It should be noted however that H9 rotated to out of the plate, and the torsion angel of O6-C1-C2-H9 is 33.81^{o}. In the molecule, the distance between O6 and S4 is 4.294 Å. Considering the fact that the sum of van-der Waals radius of Hydrogen, Oxygen and Sulfur atoms is 5.72 Å, we therefore deduced that the molecule of **2b** was characterized by a heavy space hindrance, which is responsible for the orientation of the H9. To scrutinize the effects of molecular configuration on its energy, the torsion angle of S5-C3-C2-C1 is changed to eleven different values, then the optimal structure, **S1-S11**, was computed with B3LYP/6-31+g* level of theory, **Figure S9**. The obtained results manifested that the conjugated system played a critical role to stabilize the structure of **2b**.

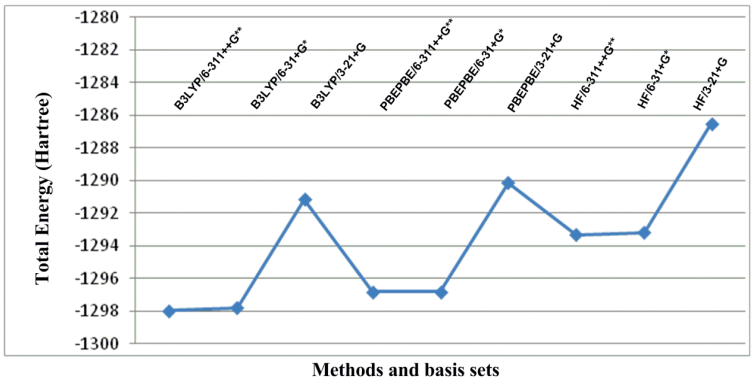


Figure S6. Energy surfaces (Hartree) of **2b** optimized at B3LYP, PBEPBE and HF methods of theories, employed 6-311++g**, 6-31+g* and 3-21+g basis sets

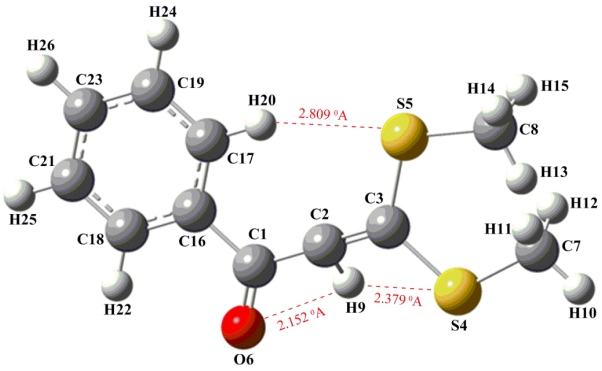


Figure S7. Numbering of **2b** structure optimized by B3LYP/6-311++g** level of theory and H-bond interactions, CH/o and CH/s

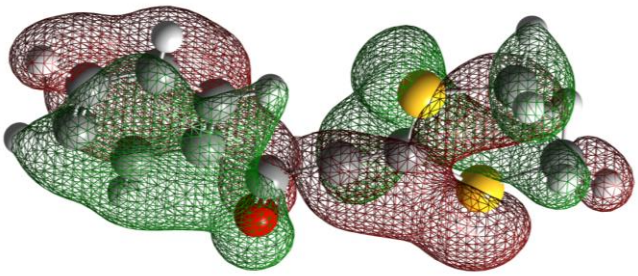


Figure S8. HOMO orbital contour plots of **2b** shows electron delocalization of conjugate system, green the negative and red the positive interaction

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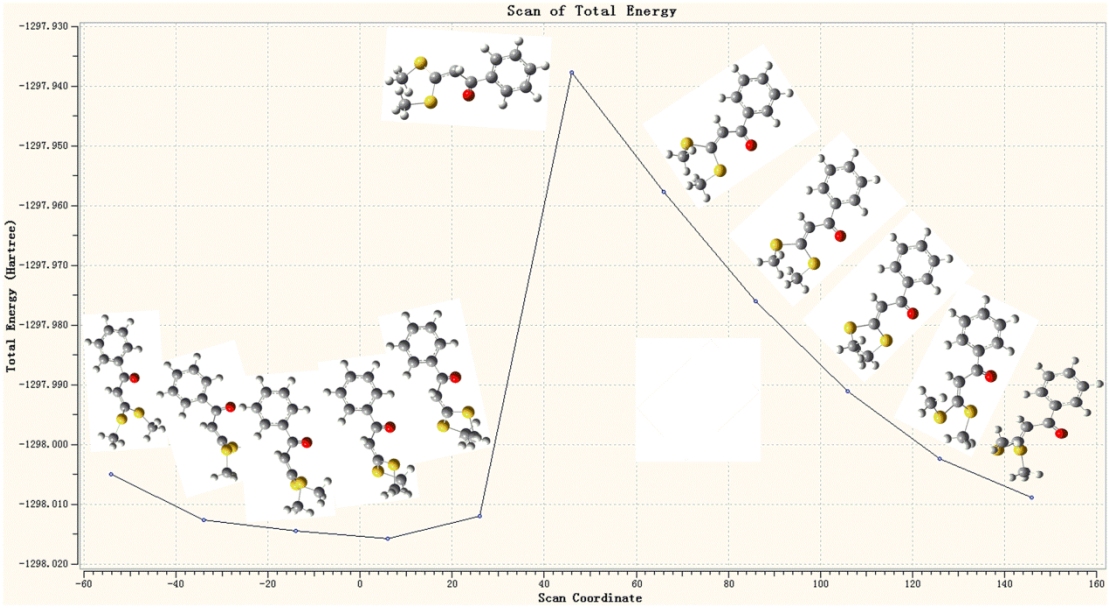

Figure S9. Energy surfaces (Hartree) of **S1-S11** conformations by changing torsion angle of **S5-C3-C2-C1** to 11 different values (optimized at B3LYP/6-31+g* level)

……

xyz coordinates calculated according to the methods and basis sets of the DFT and ab inito theories for the structure of **S** studied in this work .

B3LYP/6-311++G**

****

S *(C1)*

Hf= -1297.9632966

C	1.04947200	-1.34979100	-0.00772700
C	-0.28146300	-0.77454800	-0.00642000
C	-1.48342600	-0.25409900	-0.00581800
S	-2.92001700	-1.32136300	-0.01599900
S	-1.68935300	1.52386700	0.00538300
O	1.19041100	-2.56230100	-0.01059400
C	-4.40539300	-0.32296800	-0.01219600
C	-3.43374600	1.92216000	0.00431300
H	-0.63460400	-1.59187800	0.58701100
H	-5.26416400	-0.96122800	-0.01828400
H	-4.41826000	0.30056500	-0.88164400
H	-4.42179300	0.28865300	0.86561400
H	-4.00601400	1.01808000	-0.00280800
H	-3.66734800	2.49900600	-0.86607600
H	-3.67103000	2.48757200	0.88118500
C	2.28587000	-0.43168700	-0.00554800
C	2.12553600	0.95422700	-0.00227100
C	3.56598700	-0.98562400	-0.00674000
C	3.24512300	1.78593800	-0.00086800
H	1.11618300	1.39063000	-0.00210900
C	4.68601900	-0.15380000	-0.00434200
H	3.69253700	-2.07791900	-0.00914300
C	4.52580100	1.23179000	-0.00154400
H	3.11882500	2.87834000	0.00108200
H	5.69521200	-0.59084000	-0.00486700
H	5.40840600	1.88776600	-0.00037900

B3LYP/6-31+G*

****

S *(C1)*

HF= -1297.7874751

C	1.04947200	-1.34979100	-0.00772700
C	-0.28146300	-0.77454800	-0.00642000
C	-1.48342600	-0.25409900	-0.00581800
S	-2.92001700	-1.32136300	-0.01599900
S	-1.68935300	1.52386700	0.00538300
O	1.19041100	-2.56230100	-0.01059400
C	-4.40539300	-0.32296800	-0.01219600
C	-3.43374600	1.92216000	0.00431300

H	-0.63460400	-1.59187800	0.58701100
H	-5.26416400	-0.96122800	-0.01828400
H	-4.41826000	0.30056500	-0.88164400
H	-4.42179300	0.28865300	0.86561400
H	-4.00601400	1.01808000	-0.00280800
H	-3.66734800	2.49900600	-0.86607600
H	-3.67103000	2.48757200	0.88118500
C	2.28587000	-0.43168700	-0.00554800
C	2.12553600	0.95422700	-0.00227100
C	3.56598700	-0.98562400	-0.00674000
C	3.24512300	1.78593800	-0.00086800
H	1.11618300	1.39063000	-0.00210900
C	4.68601900	-0.15380000	-0.00434200
H	3.69253700	-2.07791900	-0.00914300
C	4.52580100	1.23179000	-0.00154400
H	3.11882500	2.87834000	0.00108200
H	5.69521200	-0.59084000	-0.00486700
H	5.40840600	1.88776600	-0.00037900

B3LYP/3-21+G

****

S *(C1)*

Hf= -1291.1453931

C	1.04947200	-1.34979100	-0.00772700
C	-0.28146300	-0.77454800	-0.00642000
C	-1.48342600	-0.25409900	-0.00581800
S	-2.92001700	-1.32136300	-0.01599900
S	-1.68935300	1.52386700	0.00538300
O	1.19041100	-2.56230100	-0.01059400
C	-4.40539300	-0.32296800	-0.01219600
C	-3.43374600	1.92216000	0.00431300
H	-0.63460400	-1.59187800	0.58701100
H	-5.26416400	-0.96122800	-0.01828400
H	-4.41826000	0.30056500	-0.88164400
H	-4.42179300	0.28865300	0.86561400
H	-4.00601400	1.01808000	-0.00280800
H	-3.66734800	2.49900600	-0.86607600
H	-3.67103000	2.48757200	0.88118500
C	2.28587000	-0.43168700	-0.00554800
C	2.12553600	0.95422700	-0.00227100
C	3.56598700	-0.98562400	-0.00674000
C	3.24512300	1.78593800	-0.00086800
H	1.11618300	1.39063000	-0.00210900
C	4.68601900	-0.15380000	-0.00434200

H	3.69253700	-2.07791900	-0.00914300
C	4.52580100	1.23179000	-0.00154400
H	3.11882500	2.87834000	0.00108200
H	5.69521200	-0.59084000	-0.00486700
H	5.40840600	1.88776600	-0.00037900

PBEPBE/6-311++G**

****

S*(C1)*

Hf= -1296.8141875

C	1.04947200	-1.34979100	-0.00772700
C	-0.28146300	-0.77454800	-0.00642000
C	-1.48342600	-0.25409900	-0.00581800
S	-2.92001700	-1.32136300	-0.01599900
S	-1.68935300	1.52386700	0.00538300
O	1.19041100	-2.56230100	-0.01059400
C	-4.40539300	-0.32296800	-0.01219600
C	-3.43374600	1.92216000	0.00431300
H	-0.63460400	-1.59187800	0.58701100
H	-5.26416400	-0.96122800	-0.01828400
H	-4.41826000	0.30056500	-0.88164400
H	-4.42179300	0.28865300	0.86561400
H	-4.00601400	1.01808000	-0.00280800
H	-3.66734800	2.49900600	-0.86607600
H	-3.67103000	2.48757200	0.88118500
C	2.28587000	-0.43168700	-0.00554800
C	2.12553600	0.95422700	-0.00227100
C	3.56598700	-0.98562400	-0.00674000
C	3.24512300	1.78593800	-0.00086800
H	1.11618300	1.39063000	-0.00210900
C	4.68601900	-0.15380000	-0.00434200
H	3.69253700	-2.07791900	-0.00914300
C	4.52580100	1.23179000	-0.00154400
H	3.11882500	2.87834000	0.00108200
H	5.69521200	-0.59084000	-0.00486700
H	5.40840600	1.88776600	-0.00037900

PBEPBE/6-31+G*

****

S *(C1)*

Hf= -1296.7912315

C	1.04947200	-1.34979100	-0.00772700
C	-0.28146300	-0.77454800	-0.00642000
C	-1.48342600	-0.25409900	-0.00581800

S	-2.92001700	-1.32136300	-0.01599900
S	-1.68935300	1.52386700	0.00538300
O	1.19041100	-2.56230100	-0.01059400
C	-4.40539300	-0.32296800	-0.01219600
C	-3.43374600	1.92216000	0.00431300
H	-0.63460400	-1.59187800	0.58701100
H	-5.26416400	-0.96122800	-0.01828400
H	-4.41826000	0.30056500	-0.88164400
H	-4.42179300	0.28865300	0.86561400
H	-4.00601400	1.01808000	-0.00280800
H	-3.66734800	2.49900600	-0.86607600
H	-3.67103000	2.48757200	0.88118500
C	2.28587000	-0.43168700	-0.00554800
C	2.12553600	0.95422700	-0.00227100
C	3.56598700	-0.98562400	-0.00674000
C	3.24512300	1.78593800	-0.00086800
H	1.11618300	1.39063000	-0.00210900
C	4.68601900	-0.15380000	-0.00434200
H	3.69253700	-2.07791900	-0.00914300
C	4.52580100	1.23179000	-0.00154400
H	3.11882500	2.87834000	0.00108200
H	5.69521200	-0.59084000	-0.00486700
H	5.40840600	1.88776600	-0.00037900

PBEPBE/3-21+G

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S *(C1)*

Hf= -1290.1464107

C	1.04947200	-1.34979100	-0.00772700
C	-0.28146300	-0.77454800	-0.00642000
C	-1.48342600	-0.25409900	-0.00581800
S	-2.92001700	-1.32136300	-0.01599900
S	-1.68935300	1.52386700	0.00538300
O	1.19041100	-2.56230100	-0.01059400
C	-4.40539300	-0.32296800	-0.01219600
C	-3.43374600	1.92216000	0.00431300
H	-0.63460400	-1.59187800	0.58701100
H	-5.26416400	-0.96122800	-0.01828400
H	-4.41826000	0.30056500	-0.88164400
H	-4.42179300	0.28865300	0.86561400
H	-4.00601400	1.01808000	-0.00280800
H	-3.66734800	2.49900600	-0.86607600
H	-3.67103000	2.48757200	0.88118500
C	2.28587000	-0.43168700	-0.00554800

C	2.12553600	0.95422700	-0.00227100
C	3.56598700	-0.98562400	-0.00674000
C	3.24512300	1.78593800	-0.00086800
H	1.11618300	1.39063000	-0.00210900
C	4.68601900	-0.15380000	-0.00434200
H	3.69253700	-2.07791900	-0.00914300
C	4.52580100	1.23179000	-0.00154400
H	3.11882500	2.87834000	0.00108200
H	5.69521200	-0.59084000	-0.00486700
H	5.40840600	1.88776600	-0.00037900

HF/6-311++G**

****

S *(C1)*

HF= -1293.3252412

C	1.04947200	-1.34979100	-0.00772700
C	-0.28146300	-0.77454800	-0.00642000
C	-1.48342600	-0.25409900	-0.00581800
S	-2.92001700	-1.32136300	-0.01599900
S	-1.68935300	1.52386700	0.00538300
O	1.19041100	-2.56230100	-0.01059400
C	-4.40539300	-0.32296800	-0.01219600
C	-3.43374600	1.92216000	0.00431300
H	-0.63460400	-1.59187800	0.58701100
H	-5.26416400	-0.96122800	-0.01828400
H	-4.41826000	0.30056500	-0.88164400
H	-4.42179300	0.28865300	0.86561400
H	-4.00601400	1.01808000	-0.00280800
H	-3.66734800	2.49900600	-0.86607600
H	-3.67103000	2.48757200	0.88118500
C	2.28587000	-0.43168700	-0.00554800
C	2.12553600	0.95422700	-0.00227100
C	3.56598700	-0.98562400	-0.00674000
C	3.24512300	1.78593800	-0.00086800
H	1.11618300	1.39063000	-0.00210900
C	4.68601900	-0.15380000	-0.00434200
H	3.69253700	-2.07791900	-0.00914300
C	4.52580100	1.23179000	-0.00154400
H	3.11882500	2.87834000	0.00108200
H	5.69521200	-0.59084000	-0.00486700
H	5.40840600	1.88776600	-0.00037900

HF/6-31+G*

****

S *(C1)*

Hf= -1293.1656756

C	1.04947200	-1.34979100	-0.00772700
C	-0.28146300	-0.77454800	-0.00642000
C	-1.48342600	-0.25409900	-0.00581800
S	-2.92001700	-1.32136300	-0.01599900
S	-1.68935300	1.52386700	0.00538300
O	1.19041100	-2.56230100	-0.01059400
C	-4.40539300	-0.32296800	-0.01219600
C	-3.43374600	1.92216000	0.00431300
H	-0.63460400	-1.59187800	0.58701100
H	-5.26416400	-0.96122800	-0.01828400
H	-4.41826000	0.30056500	-0.88164400
H	-4.42179300	0.28865300	0.86561400
H	-4.00601400	1.01808000	-0.00280800
H	-3.66734800	2.49900600	-0.86607600
H	-3.67103000	2.48757200	0.88118500
C	2.28587000	-0.43168700	-0.00554800
C	2.12553600	0.95422700	-0.00227100
C	3.56598700	-0.98562400	-0.00674000
C	3.24512300	1.78593800	-0.00086800
H	1.11618300	1.39063000	-0.00210900
C	4.68601900	-0.15380000	-0.00434200
H	3.69253700	-2.07791900	-0.00914300
C	4.52580100	1.23179000	-0.00154400
H	3.11882500	2.87834000	0.00108200
H	5.69521200	-0.59084000	-0.00486700
H	5.40840600	1.88776600	-0.00037900

HF/3-21+G

****

S *(C1)*

Hf= -1286.5189913

C	1.04947200	-1.34979100	-0.00772700
C	-0.28146300	-0.77454800	-0.00642000
C	-1.48342600	-0.25409900	-0.00581800
S	-2.92001700	-1.32136300	-0.01599900
S	-1.68935300	1.52386700	0.00538300
O	1.19041100	-2.56230100	-0.01059400
C	-4.40539300	-0.32296800	-0.01219600
C	-3.43374600	1.92216000	0.00431300
H	-0.63460400	-1.59187800	0.58701100
H	-5.26416400	-0.96122800	-0.01828400
H	-4.41826000	0.30056500	-0.88164400

H	-4.42179300	0.28865300	0.86561400
H	-4.00601400	1.01808000	-0.00280800
H	-3.66734800	2.49900600	-0.86607600
H	-3.67103000	2.48757200	0.88118500
C	2.28587000	-0.43168700	-0.00554800
C	2.12553600	0.95422700	-0.00227100
C	3.56598700	-0.98562400	-0.00674000
C	3.24512300	1.78593800	-0.00086800
H	1.11618300	1.39063000	-0.00210900
C	4.68601900	-0.15380000	-0.00434200
H	3.69253700	-2.07791900	-0.00914300
C	4.52580100	1.23179000	-0.00154400
H	3.11882500	2.87834000	0.00108200
H	5.69521200	-0.59084000	-0.00486700
H	5.40840600	1.88776600	-0.00037900

****

Dihedral angel scan of C1-C2-C3-S5 in eleven conformations calculated with the B3LYP/6-31+G* method and basis set

S1 *(C1)*

Hf= -1298.00887574

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.47343500
C	1.11290100	0.00000000	2.27050000
S	0.99526200	0.89319900	3.81237300
S	2.66274000	-0.62394600	1.70067700
O	0.97115100	-0.36921800	-0.66302300
C	1.43916500	-0.37275900	5.06910400
C	3.91916400	0.33032300	2.63063000
H	-0.91140600	0.31976100	1.96426700
H	0.65855600	-1.13303200	5.13013900
H	1.50988500	0.15581400	6.02262000
H	2.39709600	-0.84508400	4.84747700
H	3.95910000	0.07983700	3.69178500
H	3.76271300	1.40228900	2.50526400
H	4.86722200	0.04712400	2.16583200
C	-1.22450800	0.52984600	-0.70353500
C	-2.48617200	0.64838900	-0.09719700
C	-1.08770100	0.88932400	-2.05536800
C	-3.58265400	1.11529300	-0.82592200
H	-2.63594900	0.35640700	0.93660200
C	-2.17767900	1.37016300	-2.77749800
H	-0.11334000	0.77898800	-2.51922600

C	-3.43060700	1.48445600	-2.16457000
H	-4.55424100	1.19016600	-0.34623400
H	-2.05391100	1.65211300	-3.81913200
H	-4.28230700	1.85481500	-2.72797200

S2 *(C1)*

HF= -129800230790

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.49346500
C	1.09994700	0.00000000	2.30105100
S	1.23417900	1.25911900	3.53266800
S	2.44386300	-1.09485700	1.92384100
O	0.99779200	0.30216500	-0.64856000
C	1.98984800	0.43356400	4.98648500
C	3.90259600	0.00880800	1.81055900
H	-0.89974100	0.44417900	1.92004900
H	1.23556500	-0.12345800	5.54588500
H	2.40183700	1.22484600	5.61663300
H	2.78968500	-0.23980300	4.67467300
H	4.09670900	0.53507800	2.74605400
H	3.75965100	0.71786300	0.99364300
H	4.74835300	-0.64520400	1.58472200
C	-1.30840600	-0.26088800	-0.68703400
C	-2.38883500	-0.86601100	-0.02644500
C	-1.43879200	0.08414400	-2.04216200
C	-3.58075100	-1.11901600	-0.70806300
H	-2.29408700	-1.15784600	1.01514600
C	-2.63123200	-0.15994400	-2.72016400
H	-0.59129800	0.54109100	-2.54244900
C	-3.70537000	-0.76177000	-2.05427100
H	-4.40896000	-1.59489500	-0.19103500
H	-2.72609400	0.11569900	-3.76649300
H	-4.63465700	-0.95350700	-2.58335100

S3 *(C1)*

HF= -1297.99103460

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.48743100
C	1.12267200	0.00000000	2.28409500
S	1.56498200	1.47955100	3.11667700
S	2.24551500	-1.34453300	2.08413600
O	1.03183200	0.00269800	-0.66828400
C	2.35758700	0.95377800	4.69203000
C	3.90057800	-0.57977100	1.89136900

H	-0.81844200	0.60528000	1.88161300
H	1.66914300	1.11950200	5.52281000
H	3.26358200	1.54500800	4.84069900
H	2.61380600	-0.10596500	4.63517000
H	4.26097100	-0.12166500	2.81336300
H	3.87222700	0.15208100	1.08304000
H	4.56668100	-1.40106300	1.61619800
C	-1.33903600	0.11716800	-0.67412800
C	-2.53245300	-0.25274800	-0.03565500
C	-1.38436100	0.56991800	-2.00213600
C	-3.75067900	-0.17130500	-0.71318400
H	-2.50895000	-0.62595200	0.98386400
C	-2.60192600	0.66370000	-2.67407700
H	-0.45252000	0.83872200	-2.48869400
C	-3.78828500	0.29279200	-2.03095500
H	-4.66779400	-0.47091000	-0.21427900
H	-2.62826500	1.02197100	-3.69920500
H	-4.73690400	0.36214600	-2.55586000

S4 *(C1)*

HF= -1297.97597856

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.48234100
C	1.15414200	0.00000000	2.25781100
S	1.91576900	1.51911200	2.64016100
S	2.02305300	-1.52538100	2.26648200
O	1.02067900	-0.13751200	-0.67455200
C	2.82945100	1.26870100	4.22158200
C	3.79861100	-1.13559400	2.02958100
H	-0.72944300	0.73493800	1.83646200
H	2.47028700	1.99739600	4.95064200
H	3.89981200	1.41007900	4.05772200
H	2.64050600	0.25981300	4.59300800
H	4.26984000	-0.76564900	2.94134900
H	3.91010500	-0.41582400	1.21712500
H	4.26658200	-2.08094200	1.74507500
C	-1.31589700	0.29115100	-0.67014400
C	-2.54524100	0.06120200	-0.03506100
C	-1.30440800	0.76512300	-1.99086300
C	-3.74418100	0.30186900	-0.70911400
H	-2.56525900	-0.32734400	0.97883700
C	-2.50160200	1.01851700	-2.65921000
H	-0.34653200	0.92291700	-2.47548800
C	-3.72457500	0.78732300	-2.01982200

H	-4.69124800	0.10919500	-0.21331000
H	-2.48339700	1.39205600	-3.67910800
H	-4.65741700	0.98075600	-2.54199900

S5 *(C1)*

HF= -1297.95764958

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.47750800
C	1.17675100	0.00000000	2.24638400
S	2.21907900	1.38102100	2.19142800
S	1.76926100	-1.61919400	2.55431900
O	1.00565700	-0.22480500	-0.67757900
C	3.22802800	1.37049800	3.73652200
C	3.58931500	-1.61946300	2.32958400
H	-0.63797900	0.84186200	1.77902000
H	3.15791000	2.36061500	4.19078500
H	4.27153200	1.14615600	3.50678700
H	2.82879500	0.62618400	4.42766600
H	4.11801000	-1.25661700	3.21229300
H	3.84828400	-1.02465600	1.45126200
H	3.86108700	-2.66326300	2.15588800
C	-1.29327400	0.38304200	-0.67002400
C	-2.53416700	0.24930600	-0.03085900
C	-1.24935900	0.84543400	-1.99369600
C	-3.71338800	0.57583100	-0.70343900
H	-2.57757800	-0.13185900	0.98517300
C	-2.42647000	1.18288200	-2.66146300
H	-0.28370700	0.92712600	-2.48166800
C	-3.66143700	1.04901700	-2.01795300
H	-4.67091700	0.45783100	-0.20419700
H	-2.38290500	1.54631300	-3.68431000
H	-4.57868800	1.30748200	-2.53968100

S6 *(C1)*

HF= -1297.93768765

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.46802900
C	1.20723200	0.00000000	2.23205200
S	2.46088000	1.08632300	1.78205600
S	1.45072100	-1.51370200	3.04916100
O	0.97954800	-0.30515600	-0.69292300
C	3.60278800	1.30685000	3.21623400
C	3.24548100	-1.90161300	3.11866600
H	-0.54636800	0.92221700	1.72721900

H	3.89848600	2.35789400	3.21582400
H	4.49041900	0.68019600	3.11912000
H	3.07869400	1.08212200	4.14658200
H	3.74777900	-1.41035700	3.95298900
H	3.71609700	-1.63539200	2.16945700
H	3.29922600	-2.98392100	3.25802200
C	-1.27952300	0.44156800	-0.66598200
C	-2.51903100	0.40242600	-0.01186000
C	-1.22246500	0.87100500	-1.99988300
C	-3.68158800	0.79741100	-0.67690400
H	-2.57323200	0.03843800	1.00983100
C	-2.38300700	1.27327200	-2.66197500
H	-0.25963700	0.87733800	-2.50002300
C	-3.61573100	1.23871100	-2.00216100
H	-4.63854300	0.75331900	-0.16436800
H	-2.32750500	1.61054900	-3.69333000
H	-4.52029200	1.54681200	-2.51923800

S7 *(C1)*

HF= -1298.01197885

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.47583600
C	1.11858700	0.00000000	2.25787600
S	2.65795500	0.65406000	1.69464700
S	0.91211600	-0.52740500	3.95990400
O	0.91610900	0.51025800	-0.64839900
C	3.90459100	-0.21750900	2.71835200
C	1.33581500	0.98529300	4.90927300
H	-0.93314200	-0.23331800	1.97591900
H	4.86585700	0.07957000	2.29156900
H	3.79186400	-1.29870500	2.62748200
H	3.87742400	0.07039500	3.76977900
H	2.36237400	1.30927400	4.73280500
H	1.21953100	0.71615400	5.96200400
H	0.64418800	1.79274100	4.66201700
C	-1.16168600	-0.63683700	-0.71423400
C	-2.08362700	-1.49371400	-0.08981700
C	-1.30578400	-0.36948900	-2.08667000
C	-3.12797700	-2.06445800	-0.82092000
H	-1.98236000	-1.74127300	0.96138000
C	-2.35211200	-0.93275100	-2.81356500
H	-0.58241400	0.28512400	-2.56107300
C	-3.26751000	-1.78229600	-2.18194000
H	-3.82862100	-2.73189200	-0.32767700

H	-2.45599000	-0.71140500	-3.87190100
H	-4.08260700	-2.22362100	-2.74844800

S8 *(C1)*

HF= -1298.01577836

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.46943000
C	1.12529200	0.00000000	2.24013600
S	2.74621200	0.15517600	1.54750900
S	0.88842200	-0.16473600	4.01263800
O	1.01544100	0.30722500	-0.63320900
C	3.84319600	-0.49868400	2.86325000
C	1.42815500	1.48466000	4.61171600
H	-0.95000100	-0.02913500	1.98924900
H	4.82653900	-0.54665200	2.38786300
H	3.54235600	-1.50142600	3.16864400
H	3.90541100	0.15179200	3.73637400
H	2.47352500	1.68632400	4.37200700
H	1.30682100	1.46131800	5.69747800
H	0.79293700	2.26682200	4.19187700
C	-1.26347100	-0.35962500	-0.72858000
C	-2.35631500	-0.98983600	-0.11018600
C	-1.33474000	-0.06837100	-2.10157900
C	-3.49613900	-1.31608500	-0.84824100
H	-2.31898100	-1.25109400	0.94207000
C	-2.47521200	-0.38666400	-2.83558200
H	-0.48085200	0.40869600	-2.57092000
C	-3.56026000	-1.01135800	-2.21017400
H	-4.33078800	-1.81087000	-0.36020300
H	-2.52047000	-0.14979600	-3.89466900
H	-4.44907800	-1.26179400	-2.78234000

S9 *(C1)*

HF= -1298.01436372

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.46865500
C	1.13185100	0.00000000	2.23068000
S	2.72514400	-0.36483600	1.54511400
S	0.91258900	0.19284100	4.00438900
O	1.06020700	0.05855400	-0.63261600
C	3.72652700	-0.84732500	3.00266300
C	1.67926200	1.84108700	4.26219800
H	-0.93306800	0.19891600	1.98237200
H	4.66282900	-1.20705800	2.56709100

H	3.25602900	-1.65434900	3.56502700
H	3.94789500	-0.01116000	3.66721100
H	2.72744200	1.85293700	3.95790100
H	1.61433700	2.03739900	5.33514800
H	1.12475000	2.60780500	3.71783600
C	-1.31275100	-0.03774300	-0.72737100
C	-2.51529800	-0.42878200	-0.11554500
C	-1.32249300	0.30527900	-2.08985800
C	-3.70179300	-0.47268200	-0.85051800
H	-2.53126200	-0.72373400	0.92853200
C	-2.50860000	0.27211600	-2.81999400
H	-0.38545500	0.59310600	-2.55486700
C	-3.70234700	-0.11724500	-2.20177800
H	-4.62325100	-0.78635300	-0.36871700
H	-2.50482400	0.54690300	-3.87085100
H	-4.62688100	-0.14622000	-2.77138200

S10 *(C1)*

HF= -1298.01258845

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.46340800
C	1.14682400	0.00000000	2.21874500
S	2.59018600	-0.85147600	1.66031800
S	1.19484300	0.59123300	3.89061200
O	1.00881200	-0.27050400	-0.66159800
C	3.78857400	-0.66623600	3.03328200
C	-0.38317100	1.48064200	4.08977600
H	-0.89722400	0.37785000	1.93523000
H	4.68702600	-1.16950500	2.66767300
H	3.45452800	-1.15964900	3.94841000
H	4.02704700	0.38059200	3.23085900
H	-0.50931000	2.23200900	3.30736500
H	-0.30660700	1.97711700	5.05999700
H	-1.23475700	0.79725400	4.10689300
C	-1.27526200	0.37383100	-0.71104200
C	-2.54671500	0.26183300	-0.12574400
C	-1.17743000	0.81701500	-2.04000800
C	-3.69375900	0.58985400	-0.85205600
H	-2.65435600	-0.11077500	0.88807600
C	-2.32070700	1.16017400	-2.75978000
H	-0.19196400	0.88009700	-2.48947700
C	-3.58339800	1.04733700	-2.16783100
H	-4.67216400	0.48453200	-0.39198500
H	-2.22966500	1.51073100	-3.78392000

H	-4.47537400	1.30883900	-2.73004100

S11*(C1)*

HF= -1298.00493802

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.48524400
C	1.11763700	0.00000000	2.27260900
S	2.34466700	-1.24926900	2.02856300
S	1.22486200	0.83465600	3.82976600
O	1.01622400	0.18372800	-0.66730500
C	3.94866400	-0.37596100	2.20922800
C	0.09277600	2.25599600	3.62435400
H	-0.90514500	0.42116700	1.91780100
H	4.71281100	-1.15505500	2.15661900
H	4.02415200	0.13824000	3.16754100
H	4.08687600	0.32400700	1.38342200
H	0.24915600	2.72536400	2.65062800
H	0.34881800	2.96331100	4.41657900
H	-0.95199400	1.95978600	3.73643300
C	-1.33385500	-0.14576300	-0.68069400
C	-2.44644200	-0.71232800	-0.03921400
C	-1.45176800	0.26503200	-2.01814900
C	-3.65542400	-0.86406500	-0.72175800
H	-2.36398200	-1.06002400	0.98625700
C	-2.66152500	0.12489600	-2.69572500
H	-0.57967400	0.68687900	-2.50692200
C	-3.76661200	-0.44022800	-2.04877000
H	-4.50677800	-1.31515900	-0.22028900
H	-2.74495000	0.45175700	-3.72826300
H	-4.70842800	-0.55314700	-2.57831100

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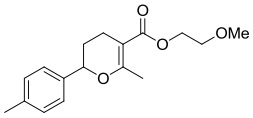
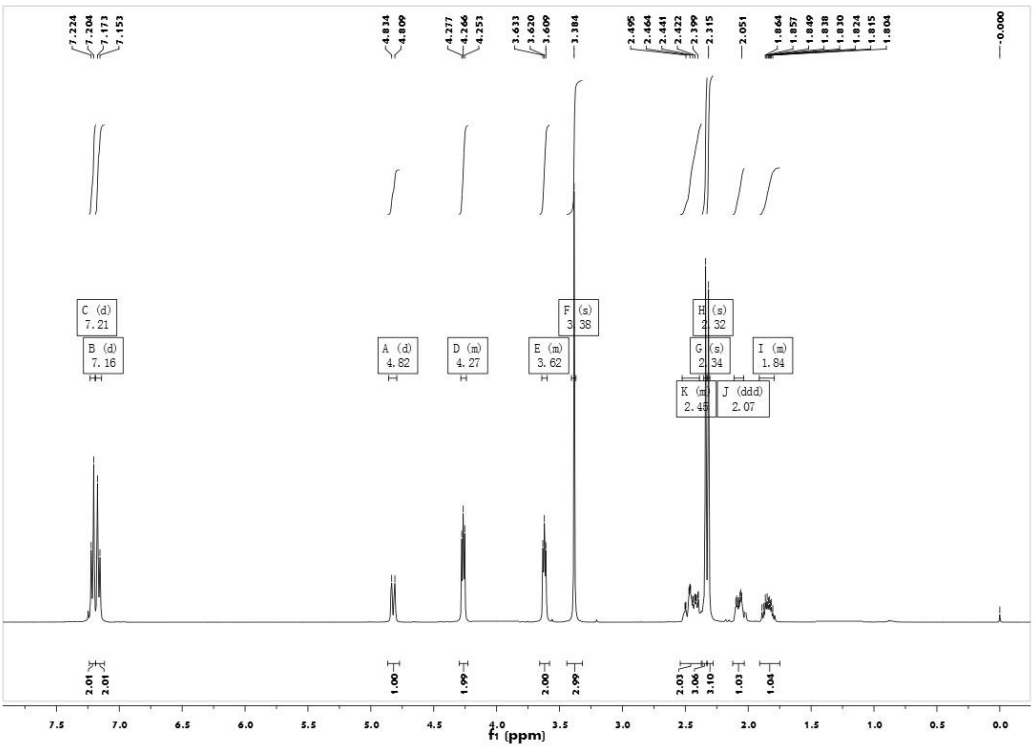
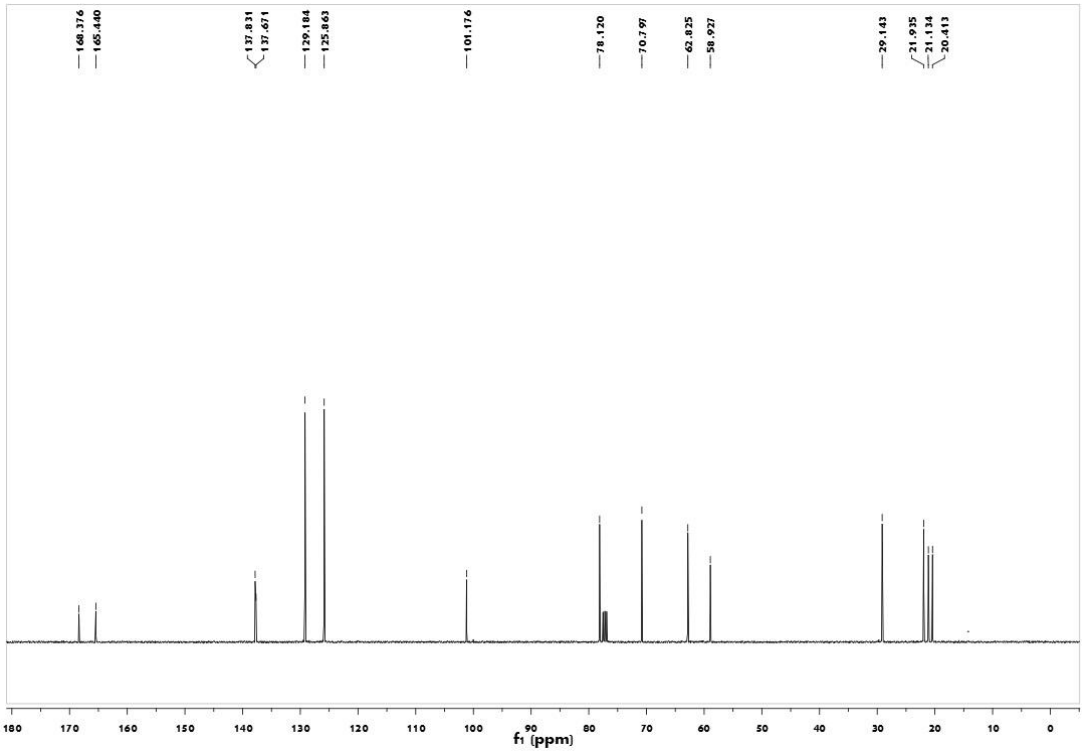
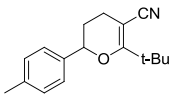
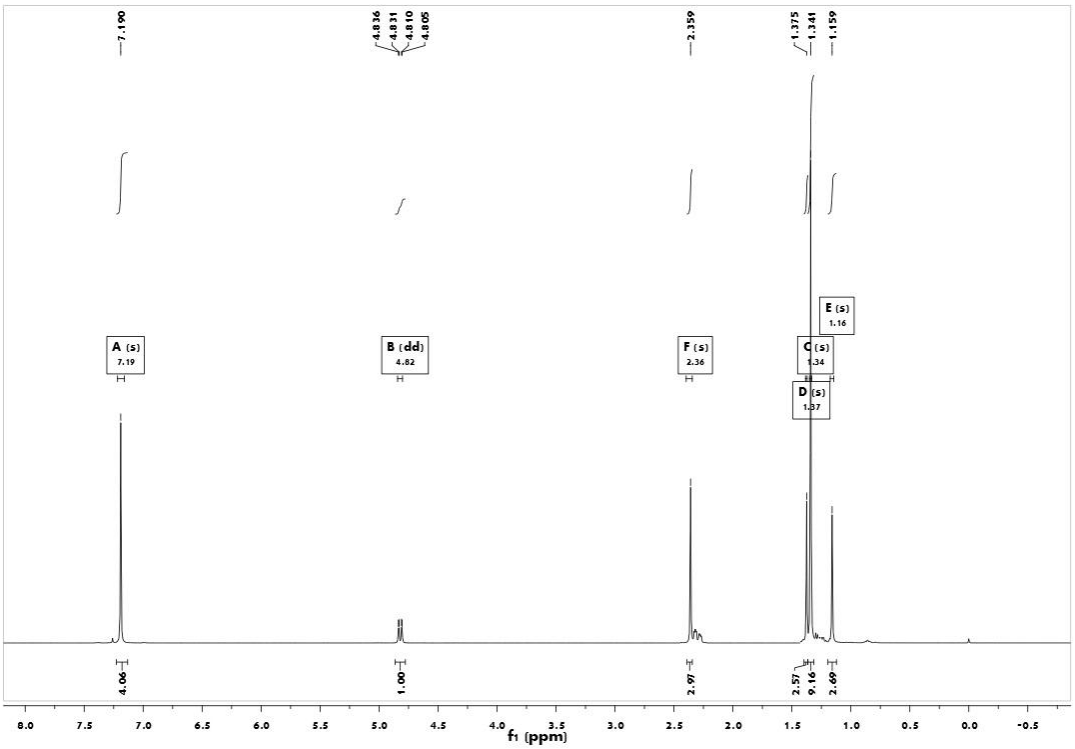
9. ^{1}H NMR and ^{13}C NMR spectra

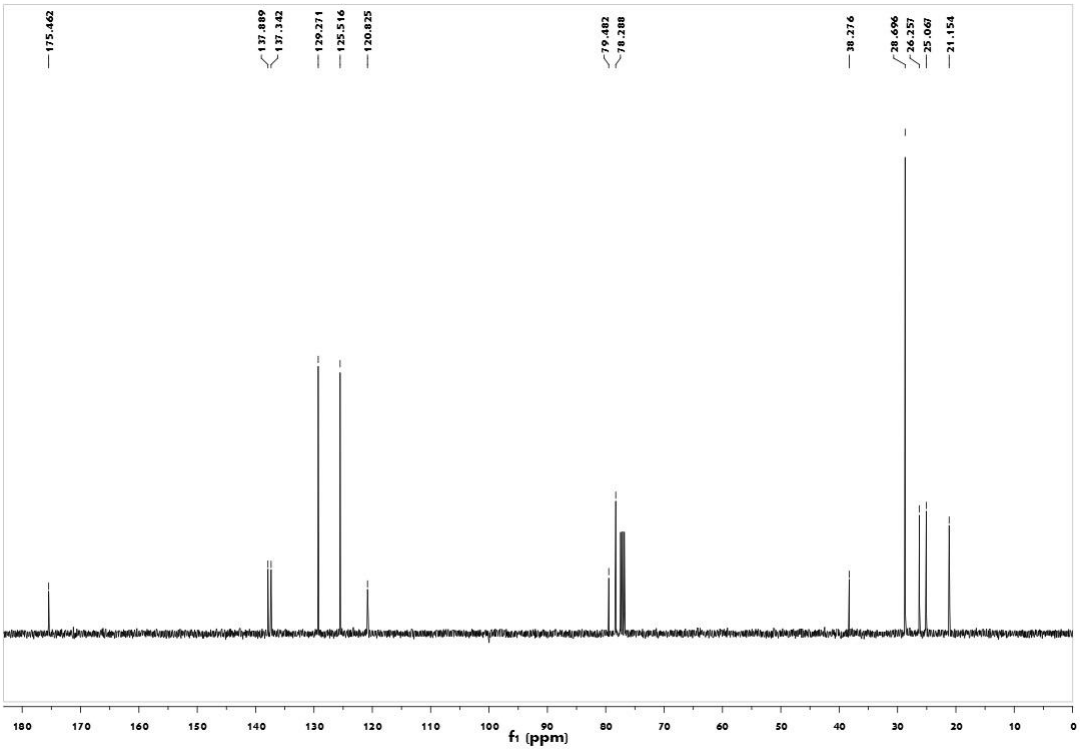


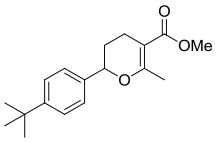


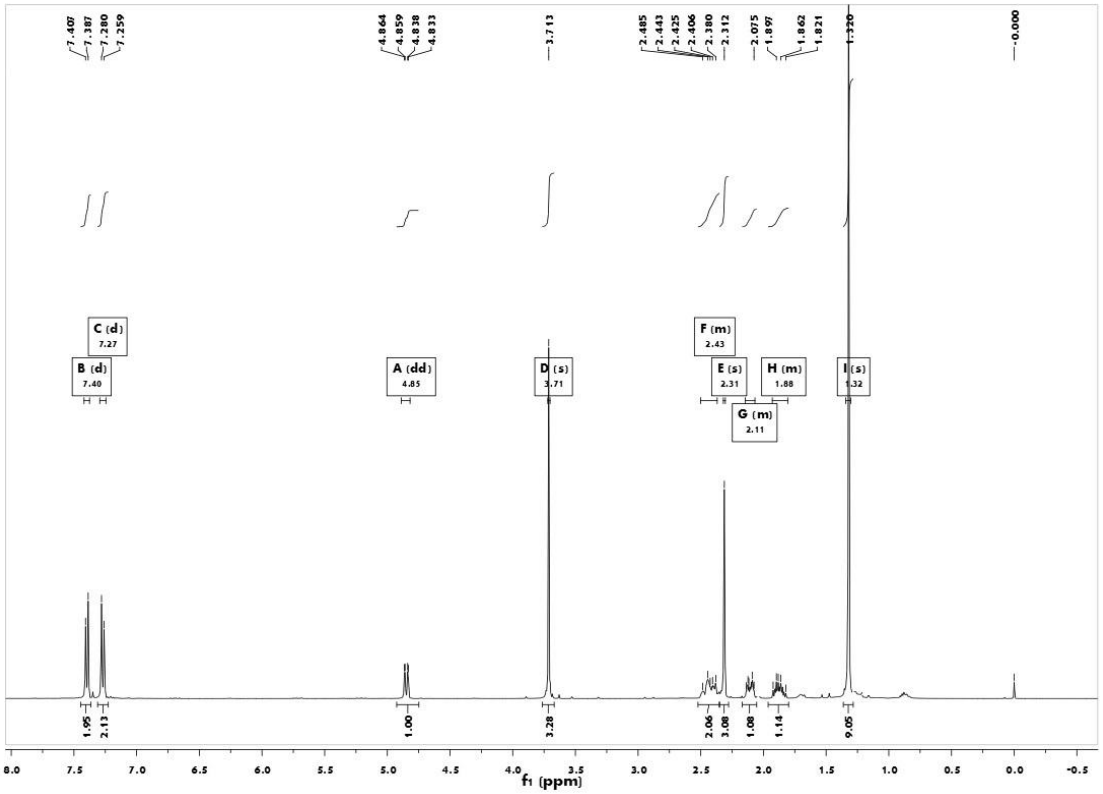


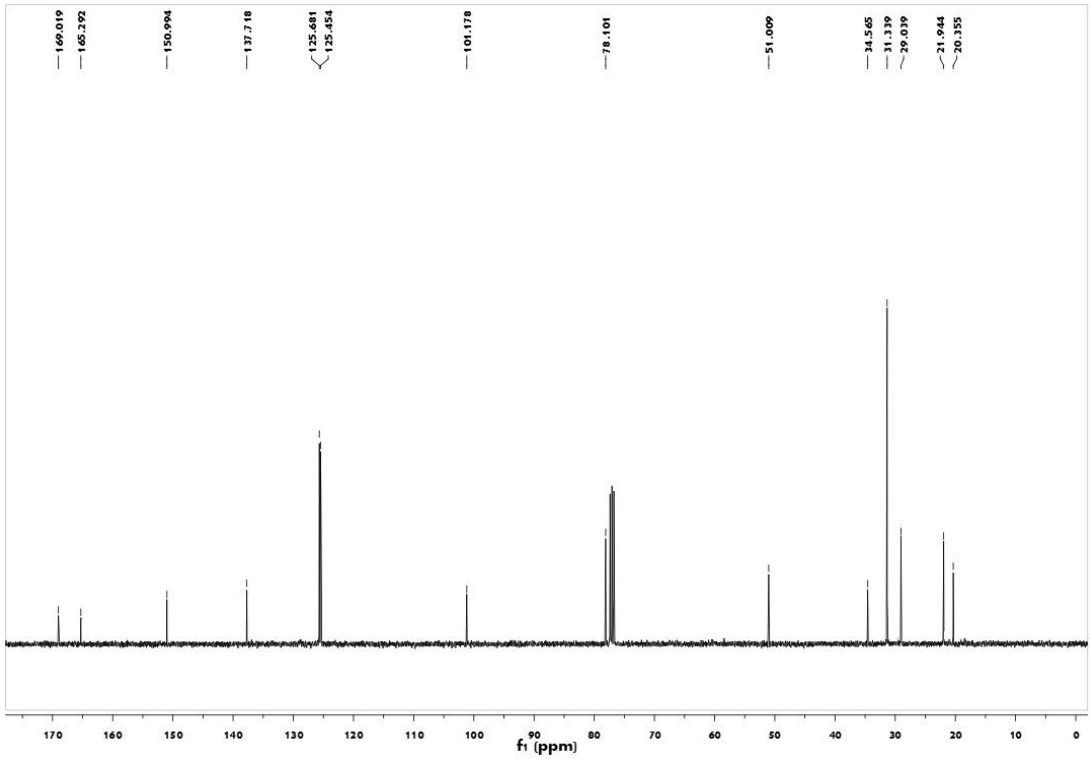

CN
O
t-Bu

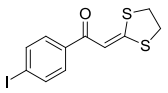

7.190
4.836
4.831
4.810
4.805
2.359
1.375
1.341
1.159
A (s)
7.19
B (dd)
4.82
F (s)
2.36
C (s)
1.34
D (s)
1.37
E (s)
1.16
4.06
1.00
2.97
2.57
9.16
2.69
f1 (ppm)

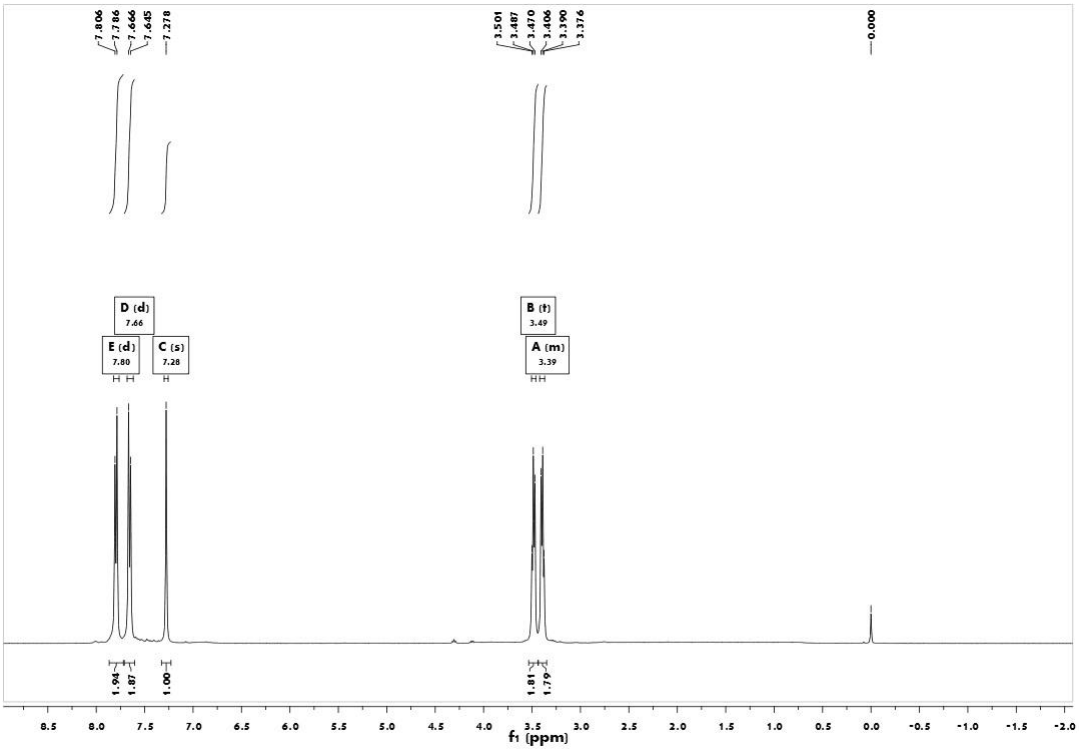

175.462
137.889
137.342
129.271
125.516
120.825
79.482
78.280
38.276
28.696
26.257
25.067
21.154
f1 (ppm)

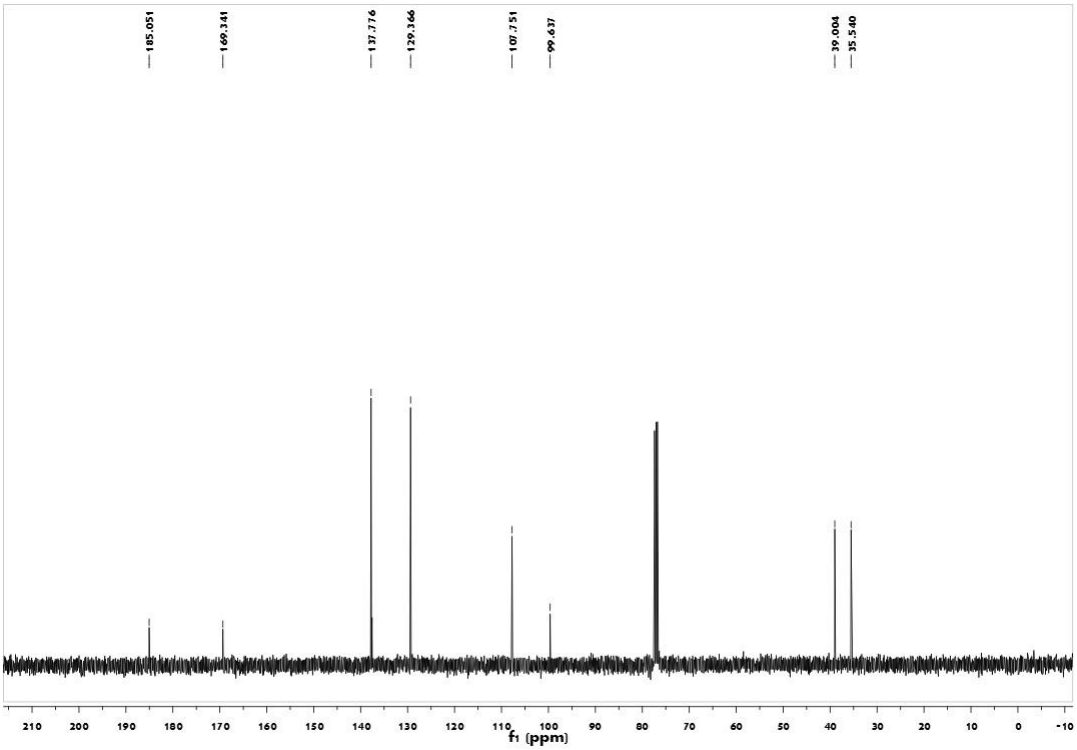

O
OMe
O

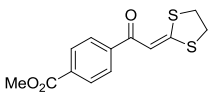

7.407
7.387
7.280
7.259
4.864
4.859
4.838
4.833
3.713
2.485
2.443
2.425
2.406
2.380
2.312
2.075
1.897
1.862
1.821
1.320
0.000
C (d) 7.27
B (d) 7.40
A (dd) 4.85
D (s) 3.71
F (m) 2.43
E (s) 2.31
H (m) 1.88
G (m) 2.11
I (s) 1.32
1.95
2.13
1.00
3.28
2.06
3.08
1.08
1.14
9.05
f1 (ppm)

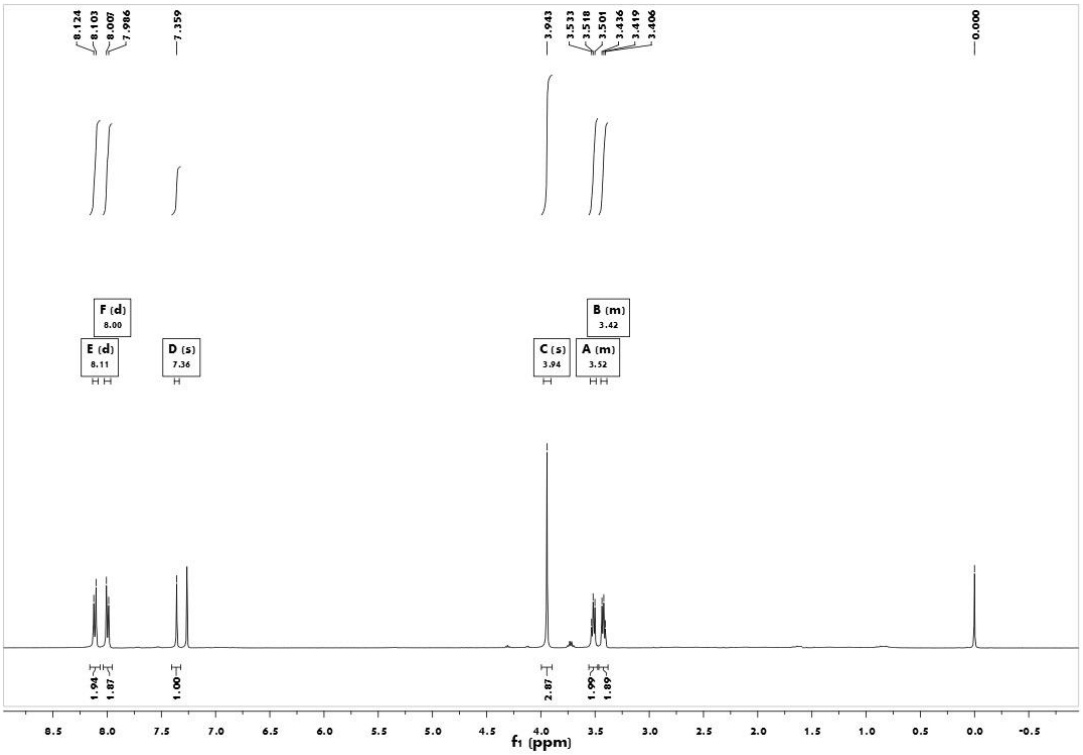

169.019
165.292
150.994
137.718
125.681
125.454
101.178
78.101
51.009
34.565
31.339
29.039
21.944
20.355
f1 (ppm)

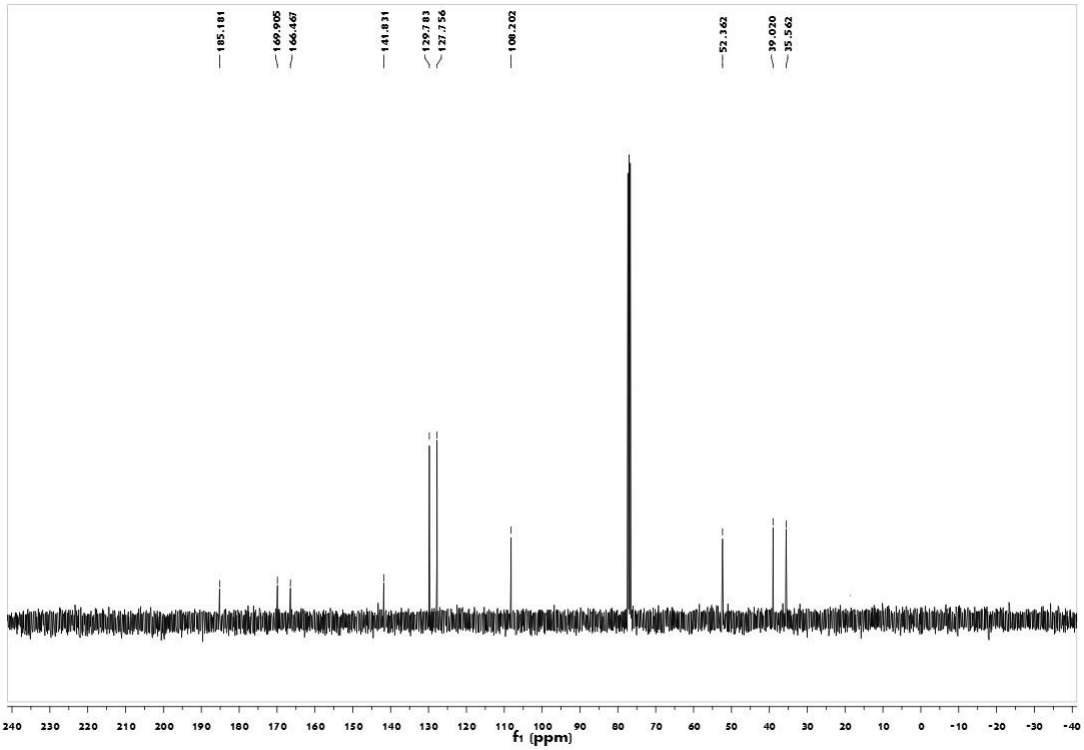


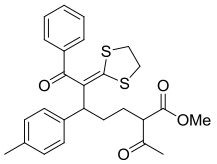

7.806
7.786
7.666
7.645
7.278
3.501
3.487
3.470
3.406
3.390
3.376
0.000
D (d)
7.66
E (d)
7.80
C (s)
7.28
B (t)
3.49
A (m)
3.39
1.94
1.87
1.00
1.81
1.79
f1 (ppm)

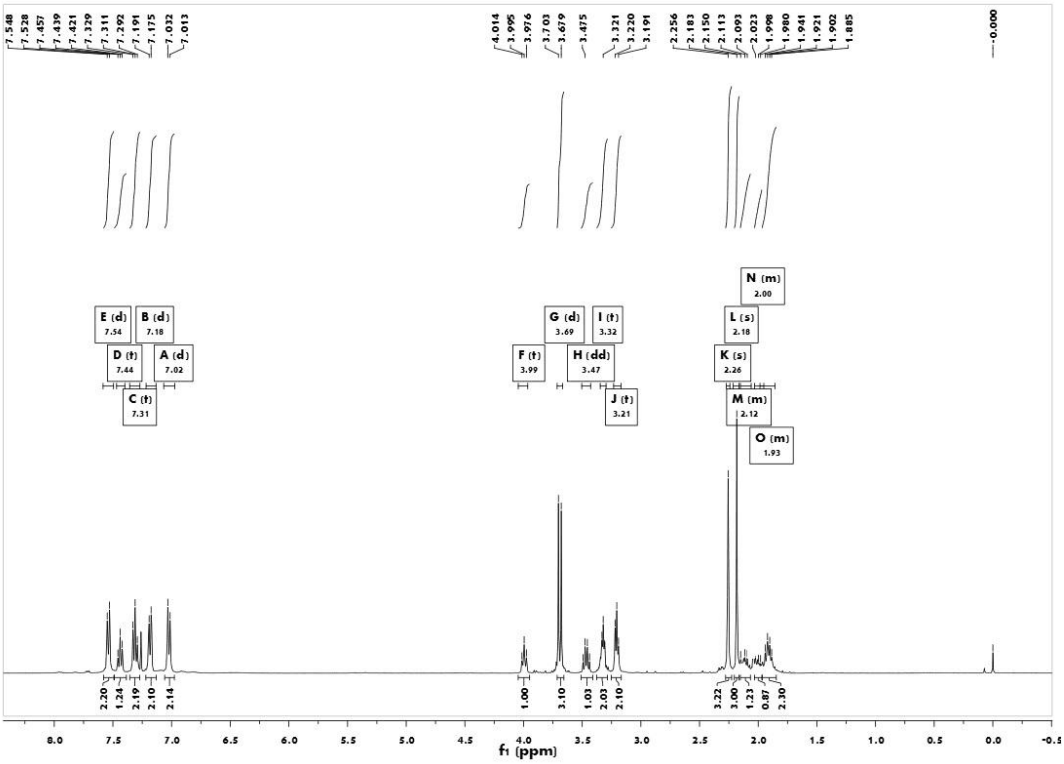

185.051
169.341
137.776
129.366
107.751
99.637
39.004
35.540
f1 (ppm)

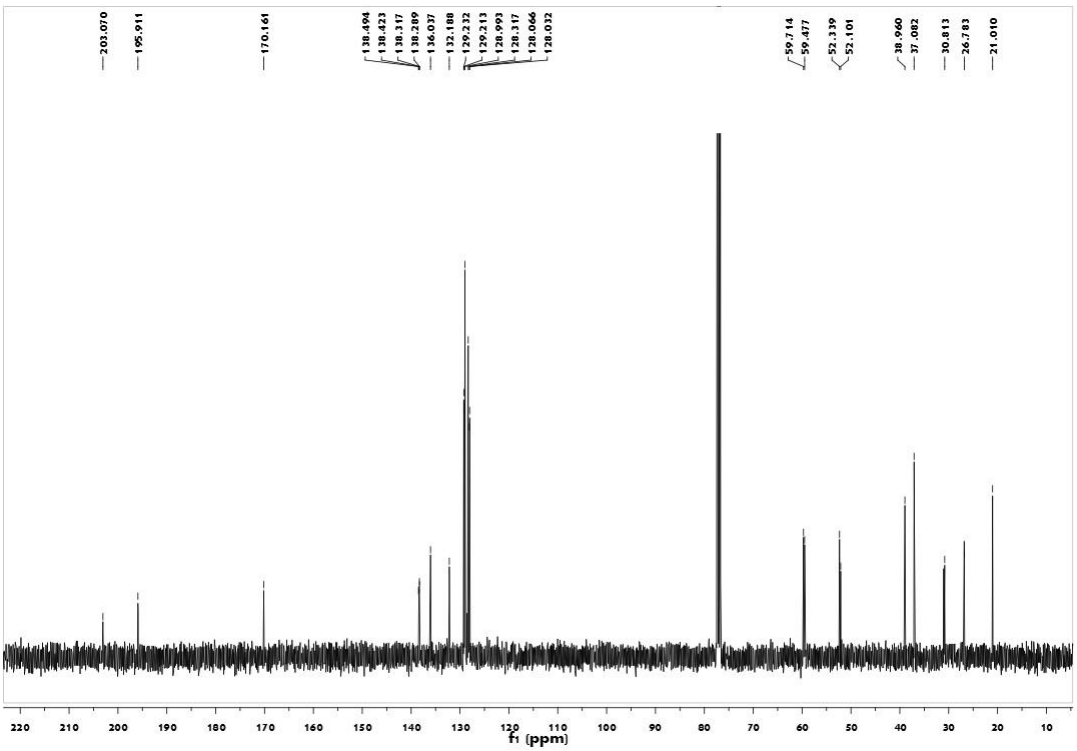

O
S
S
MeO2C

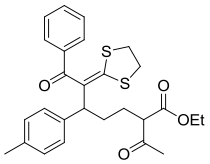

8.124
8.103
8.007
7.986
7.359
3.943
3.533
3.518
3.501
3.436
3.419
3.406
0.000
F (d) 8.00
E (d) 8.11
D (s) 7.36
C (s) 3.94
B (m) 3.42
A (m) 3.52
1.94
1.87
1.00
2.87
1.99
1.89
f1 (ppm)

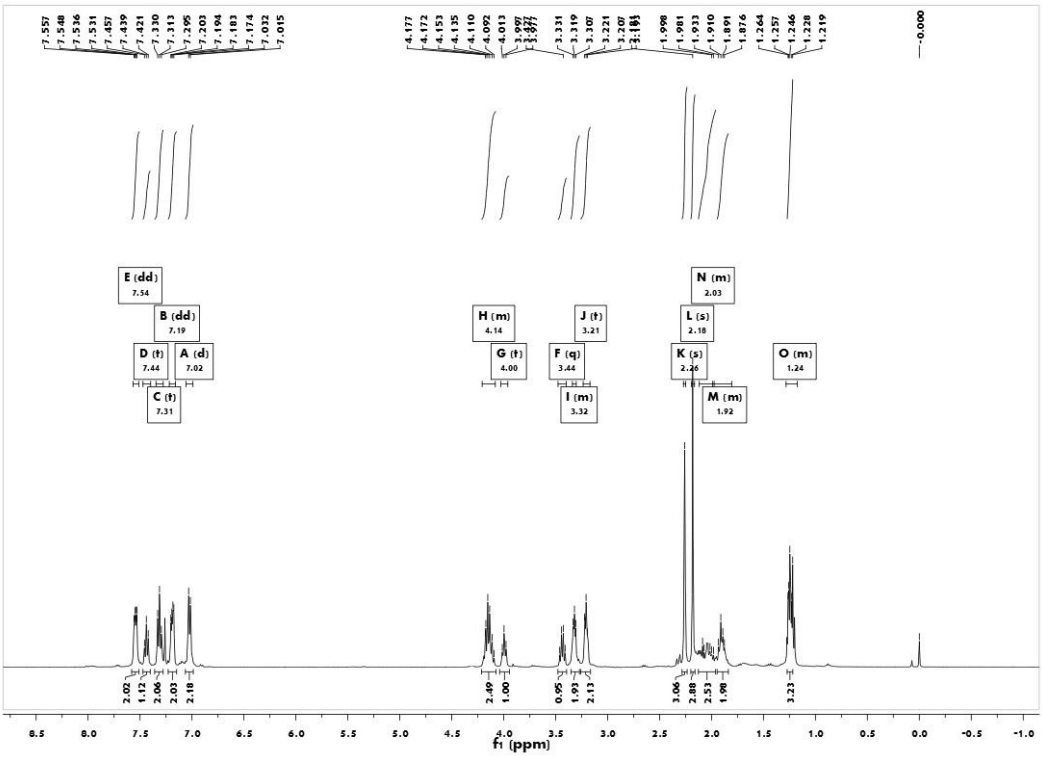

185.181
169.905
166.467
141.831
129.783
127.756
108.202
52.362
39.020
35.562
f1 (ppm)

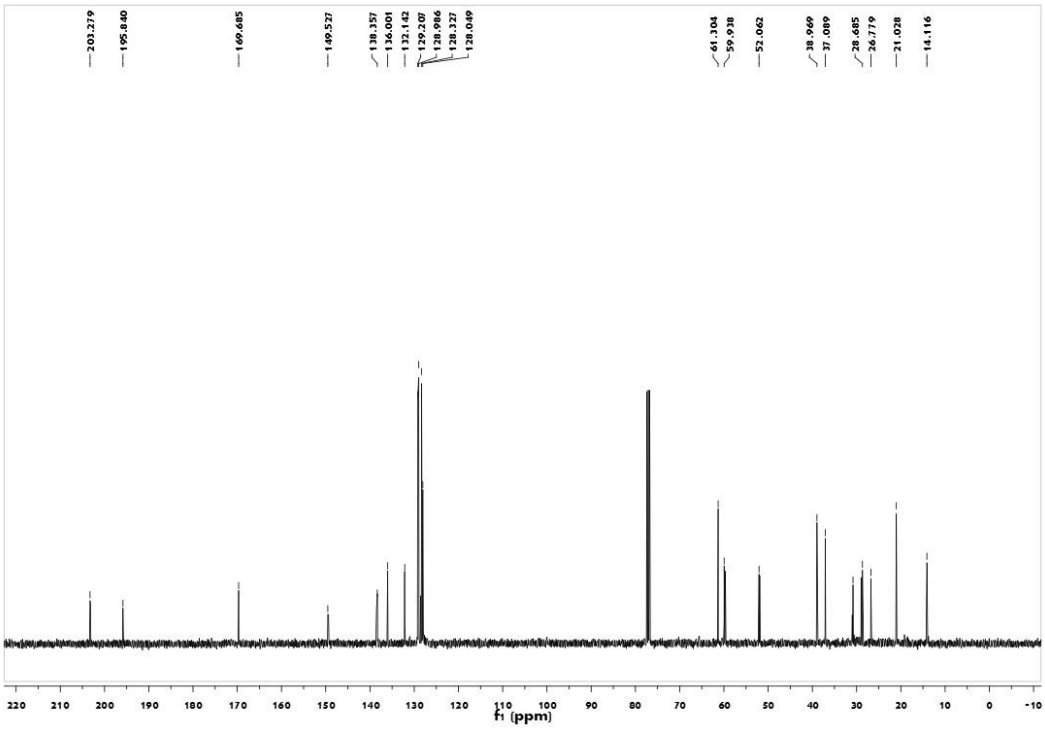

S
S
O
O
OMe
O

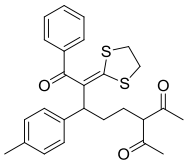

E (d) 7.54
B (d) 7.18
D (t) 7.44
A (d) 7.02
C (t) 7.31
G (d) 3.69
I (t) 3.32
F (t) 3.99
H (dd) 3.47
J (t) 3.21
N (m) 2.00
L (s) 2.18
K (s) 2.26
M (m) 2.12
O (m) 1.93
f1 (ppm)

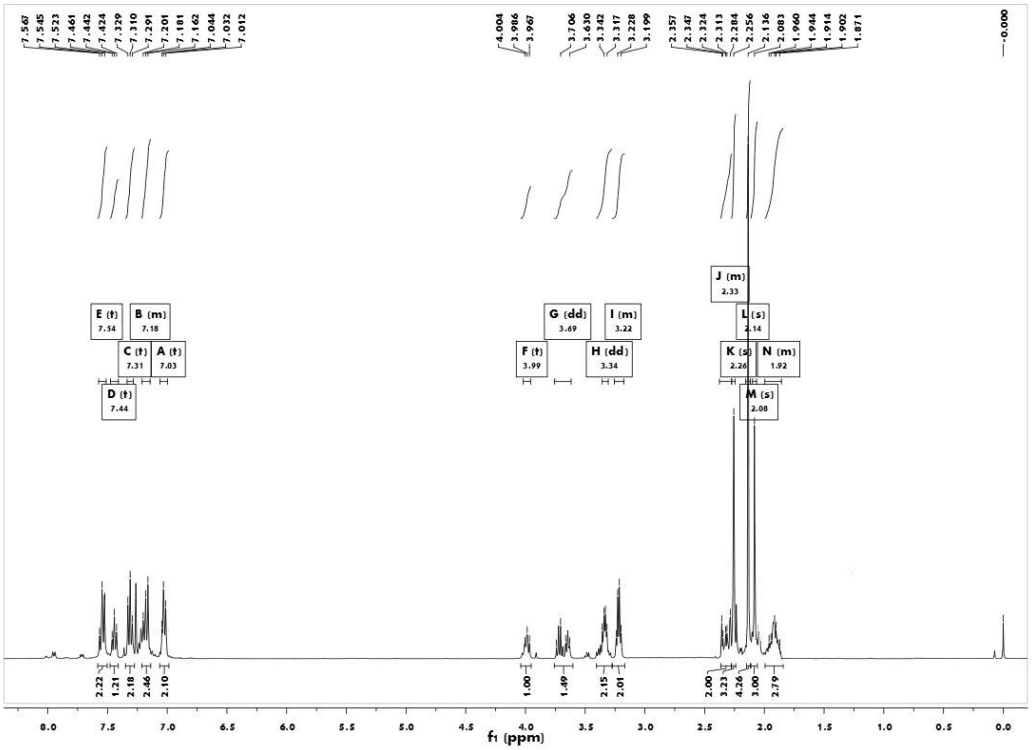

f1 (ppm)

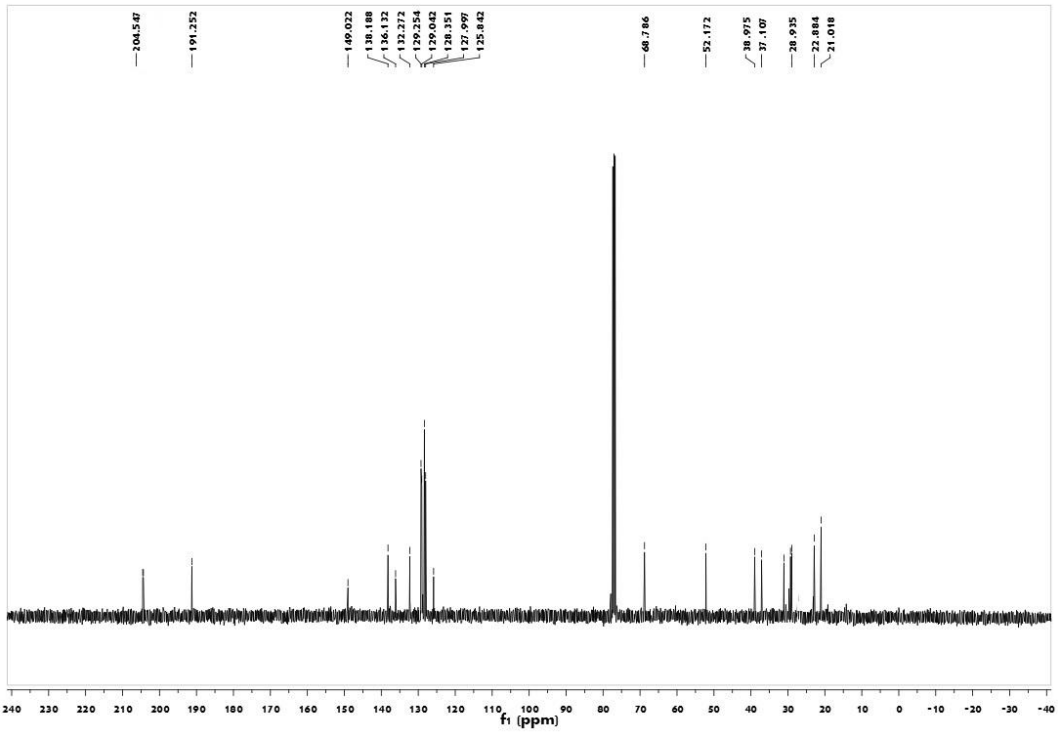

S
S
O
O
OEt
O

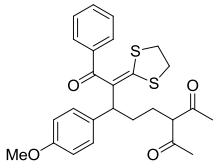

E (dd) 7.54
B (dd) 7.19
D (t) 7.44
A (d) 7.02
C (t) 7.31
H (m) 4.14
G (t) 4.00
J (t) 3.21
F (q) 3.44
I (m) 3.32
N (m) 2.03
L (s) 2.18
K (s) 2.26
M (m) 1.92
O (m) 1.24
f1 (ppm)

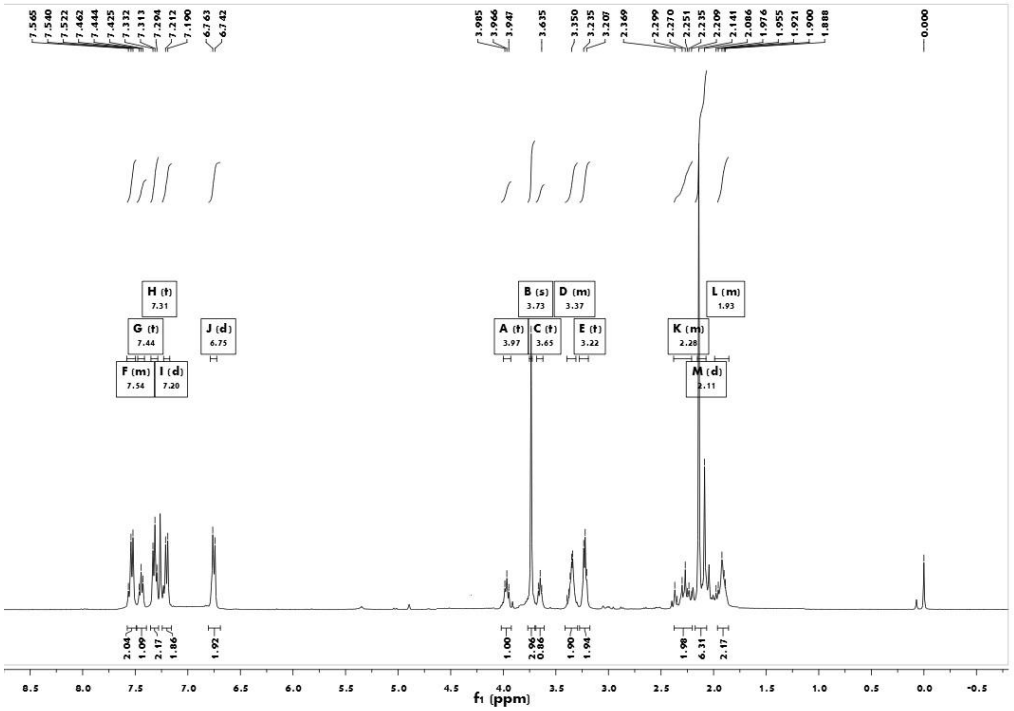

f1 (ppm)

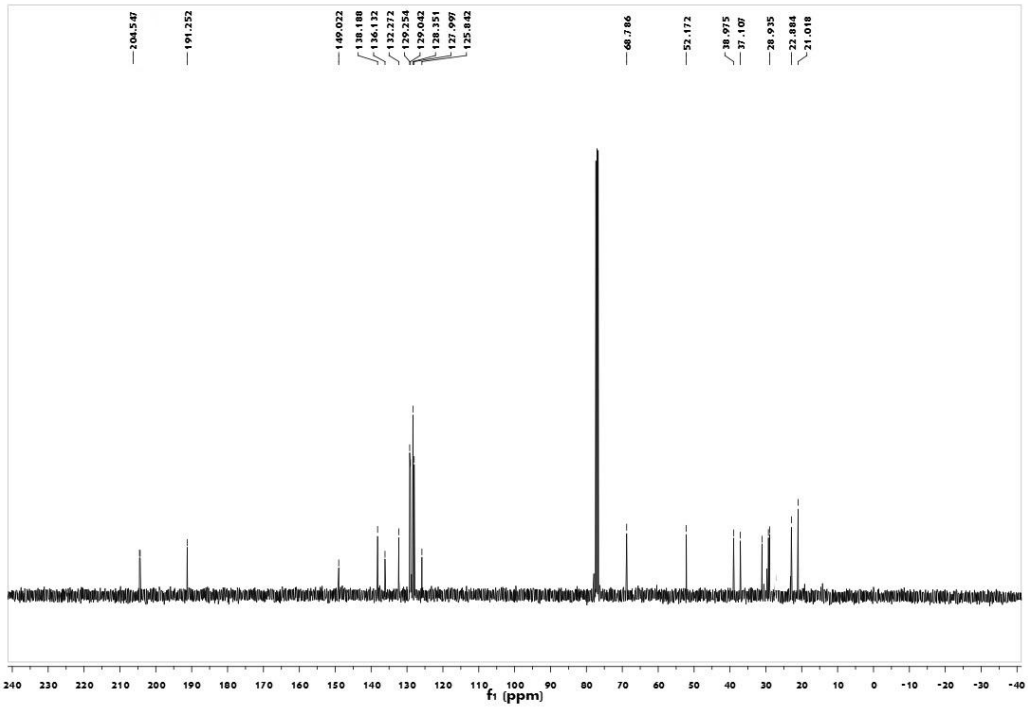


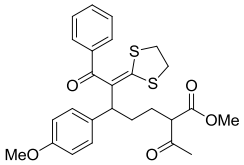

E (t) 7.54
B (m) 7.18
C (t) 7.31
A (t) 7.03
D (t) 7.44
G (dd) 3.69
I (m) 3.22
F (t) 3.99
H (dd) 3.34
J (m) 2.33
L (s) 2.14
K (s) 2.26
N (m) 1.92
M (s) 2.08
f1 (ppm)

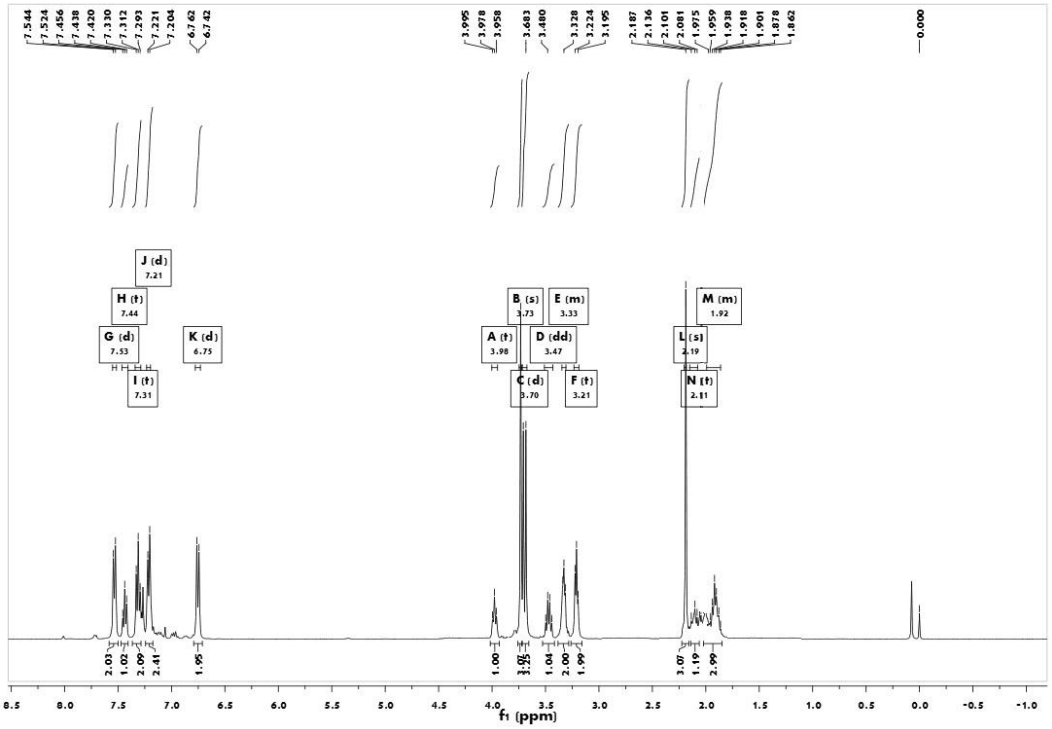

204.547
191.252
149.022
138.188
136.132
132.272
129.254
129.042
128.351
127.997
125.842
68.786
52.172
38.975
37.107
28.935
22.884
21.018
f1 (ppm)

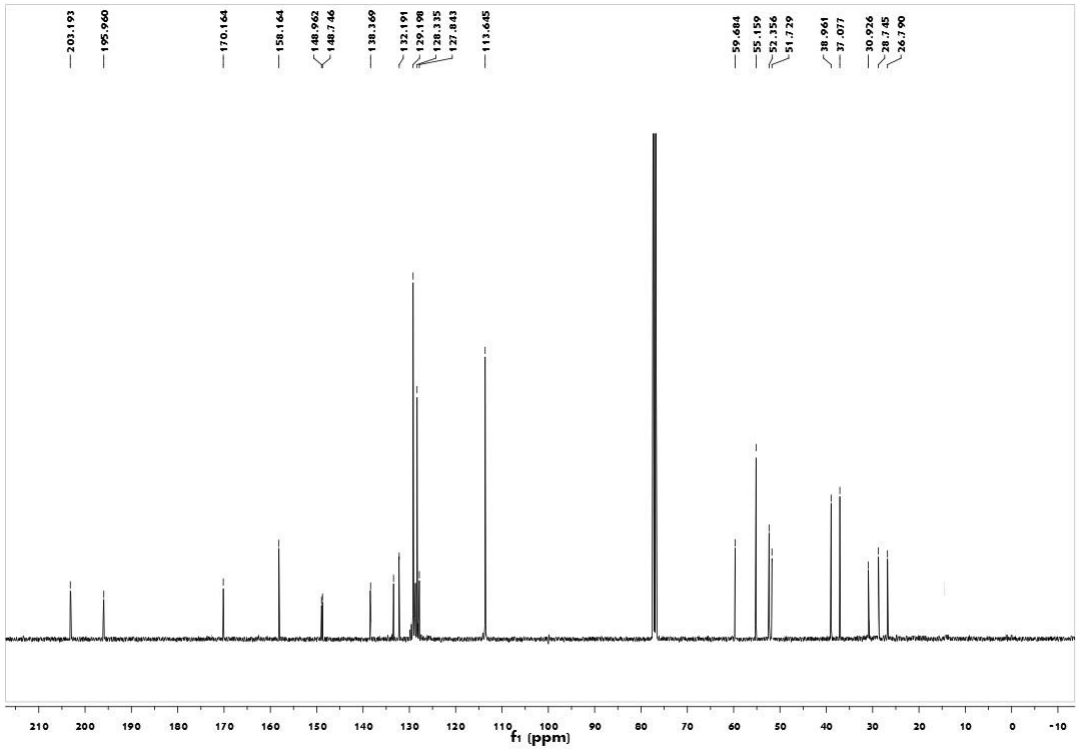

S
S
O
O
O
MeO

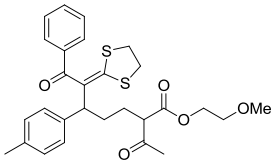

f1 (ppm)

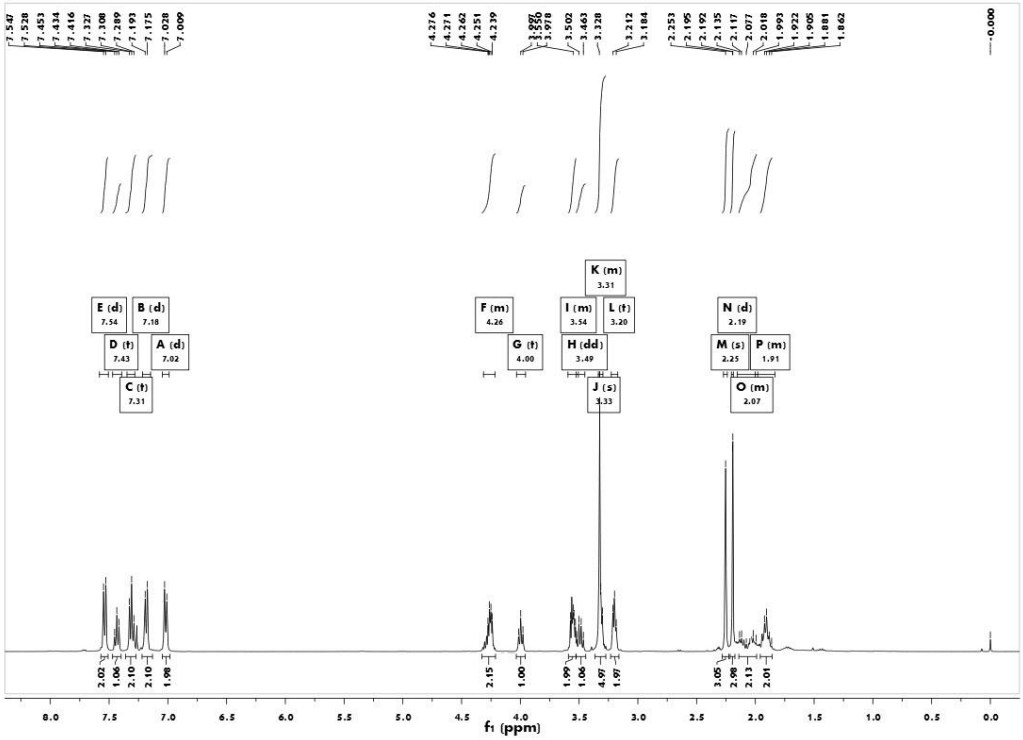

f1 (ppm)

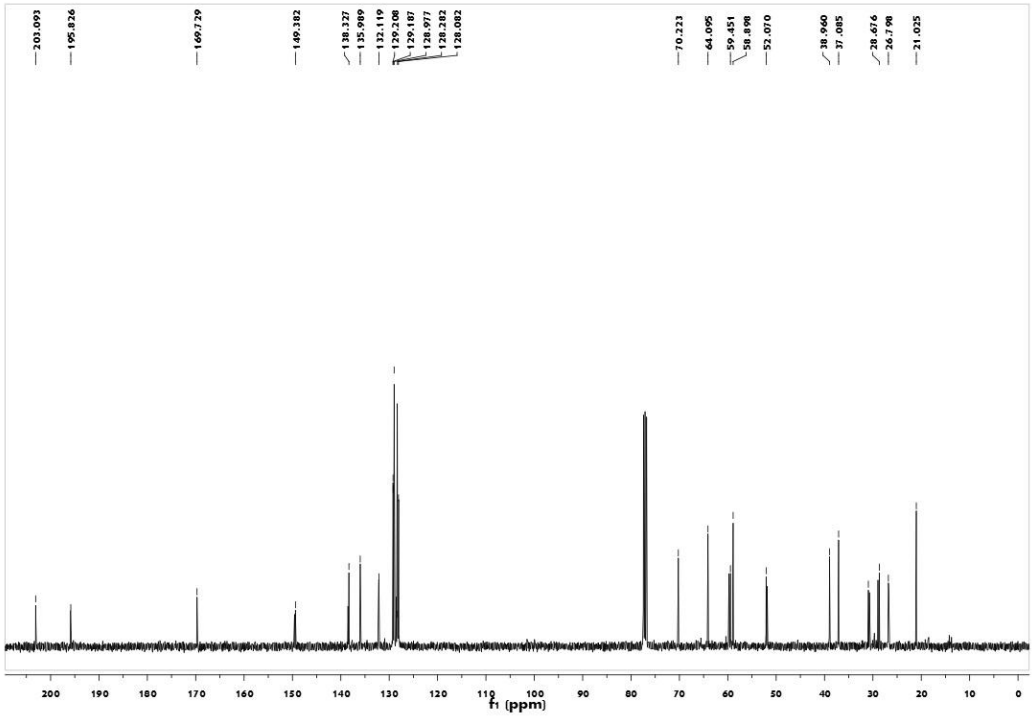

S
S
O
O
OMe
MeO
O

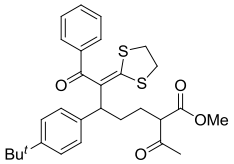

7.544
7.524
7.456
7.438
7.420
7.330
7.312
7.293
7.221
7.204
6.762
6.742
3.995
3.978
3.958
3.683
3.480
3.328
3.224
3.195
2.187
2.136
2.101
2.081
1.975
1.959
1.938
1.918
1.901
1.878
1.862
0.000
J (d) 7.21
H (t) 7.44
G (d) 7.53
I (t) 7.31
K (d) 6.75
B (s) 3.73
E (m) 3.33
A (t) 3.98
D (dd) 3.47
C (d) 3.70
F (t) 3.21
M (m) 1.92
L (s) 2.19
N (t) 2.11
2.03
1.02
2.09
2.41
1.95
1.00
3.05
1.04
2.00
1.99
3.07
1.19
2.99
f1 (ppm)

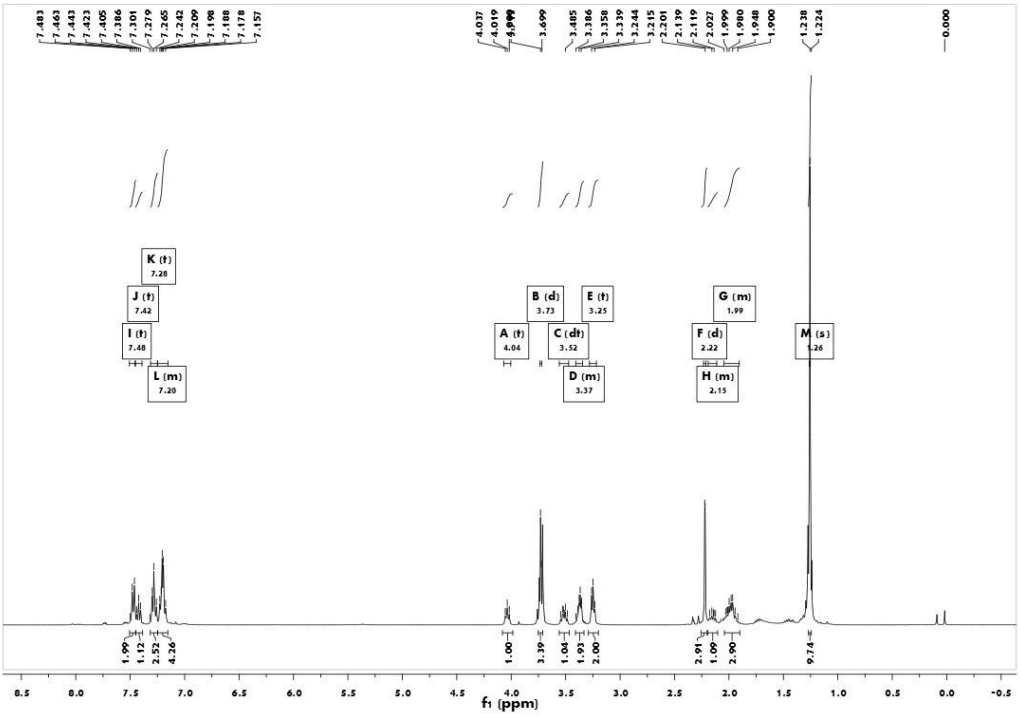

203.193
195.960
170.164
158.164
148.962
148.746
138.369
132.191
129.198
128.335
127.843
113.645
59.684
55.159
52.356
51.729
38.961
37.077
30.926
28.745
26.790
f1 (ppm)

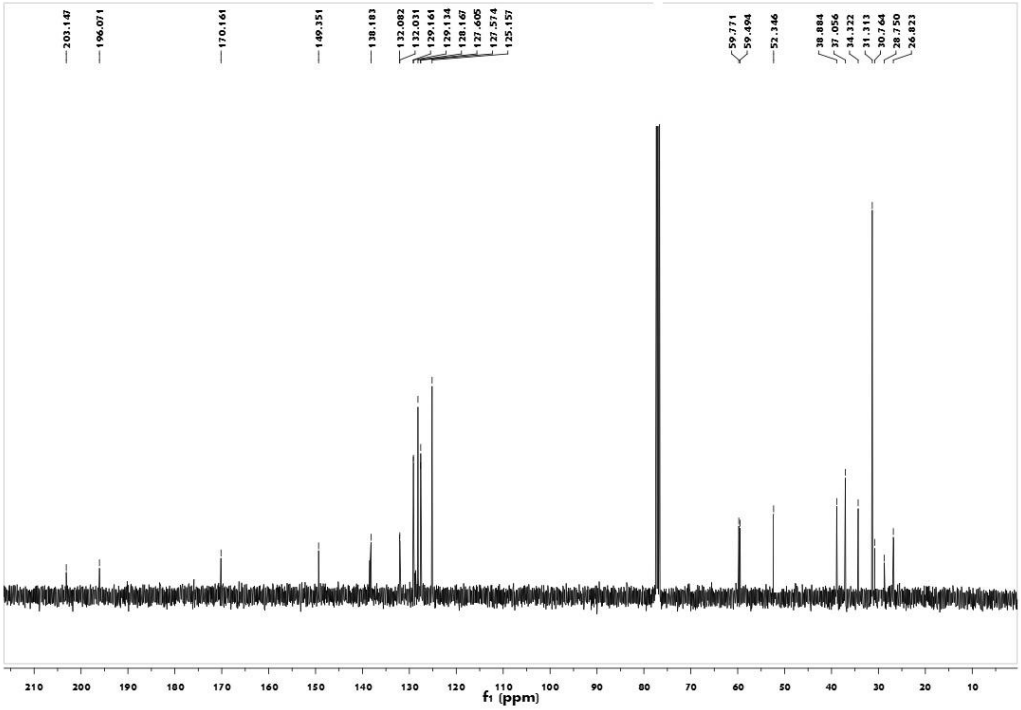

S
S
O
O
O
O
OMe

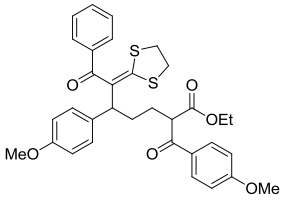

E (d) 7.54
B (d) 7.18
D (t) 7.43
A (d) 7.02
C (t) 7.31
F (m) 4.26
G (t) 4.00
K (m) 3.31
I (m) 3.54
L (t) 3.20
H (dd) 3.49
J (s) 3.33
N (d) 2.19
M (s) 2.25
P (m) 1.91
O (m) 2.07
f1 (ppm)

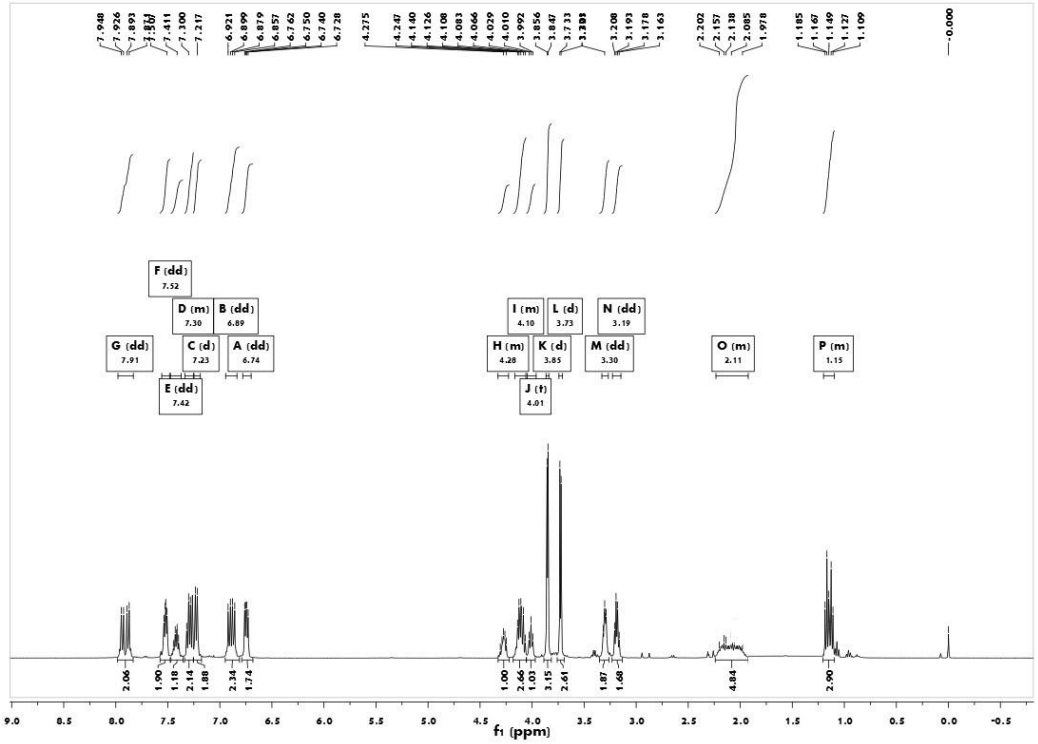

203.093
195.826
169.729
149.382
138.327
135.989
132.119
129.208
129.187
128.977
128.282
128.082
70.223
64.095
59.451
58.898
52.070
38.960
37.085
28.676
26.790
21.025
f1 (ppm)

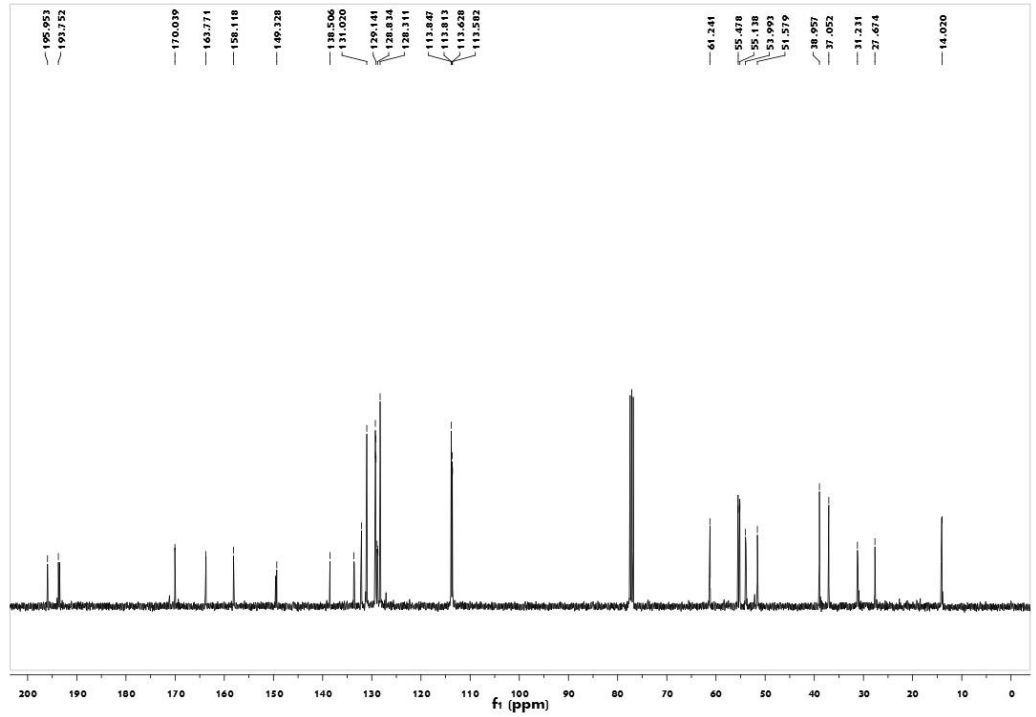

S
S
O
O
OMe
O
Bu^t

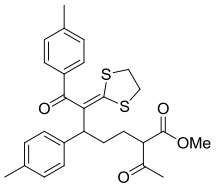

K (t) 7.28
J (t) 7.42
I (t) 7.48
L (m) 7.20
B (d) 3.73
E (t) 3.25
A (t) 4.04
C (dt) 3.52
D (m) 3.37
G (m) 1.99
F (d) 2.22
H (m) 2.15
M (s) 1.26
f1 (ppm)

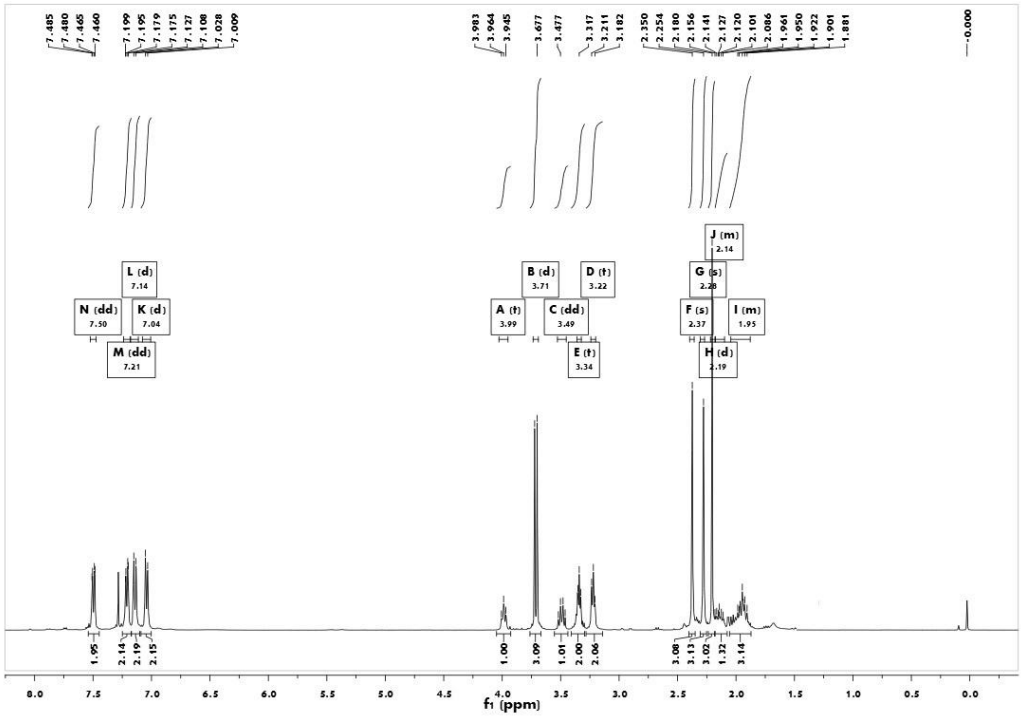

f1 (ppm)

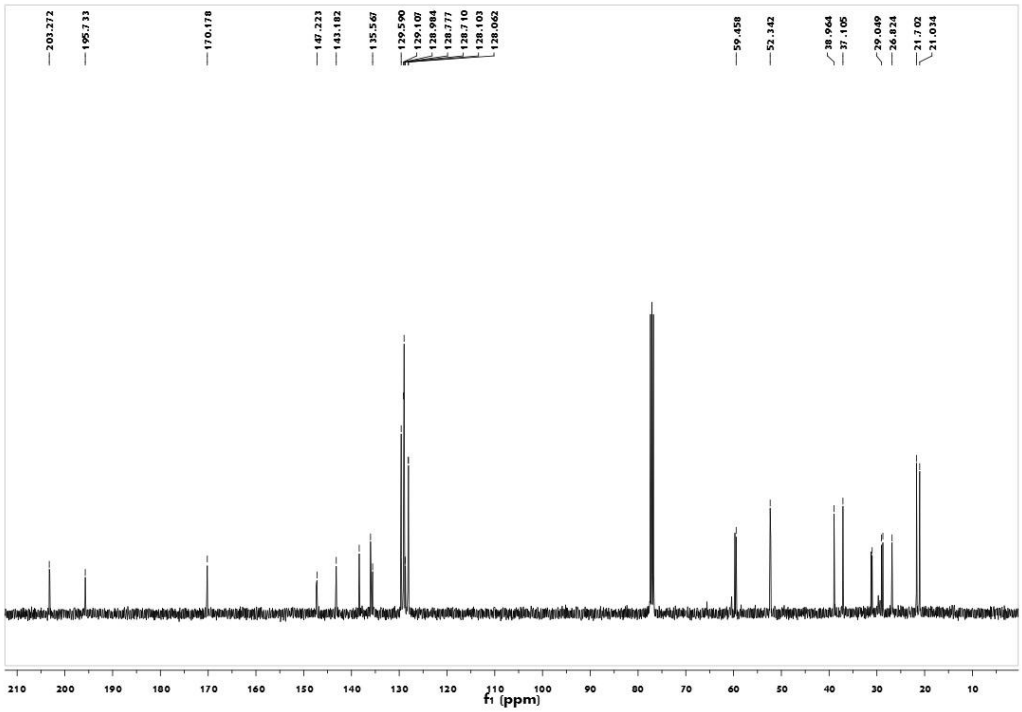

S
S
O
O
OEt
MeO
O
OMe

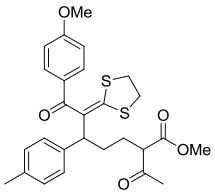

F (dd) 7.52
D (m) 7.30
B (dd) 6.89
G (dd) 7.91
C (d) 7.23
A (dd) 6.74
E (dd) 7.42
I (m) 4.10
L (d) 3.73
N (dd) 3.19
H (m) 4.28
K (d) 3.85
M (dd) 3.30
J (t) 4.01
O (m) 2.11
P (m) 1.15
f1 (ppm)

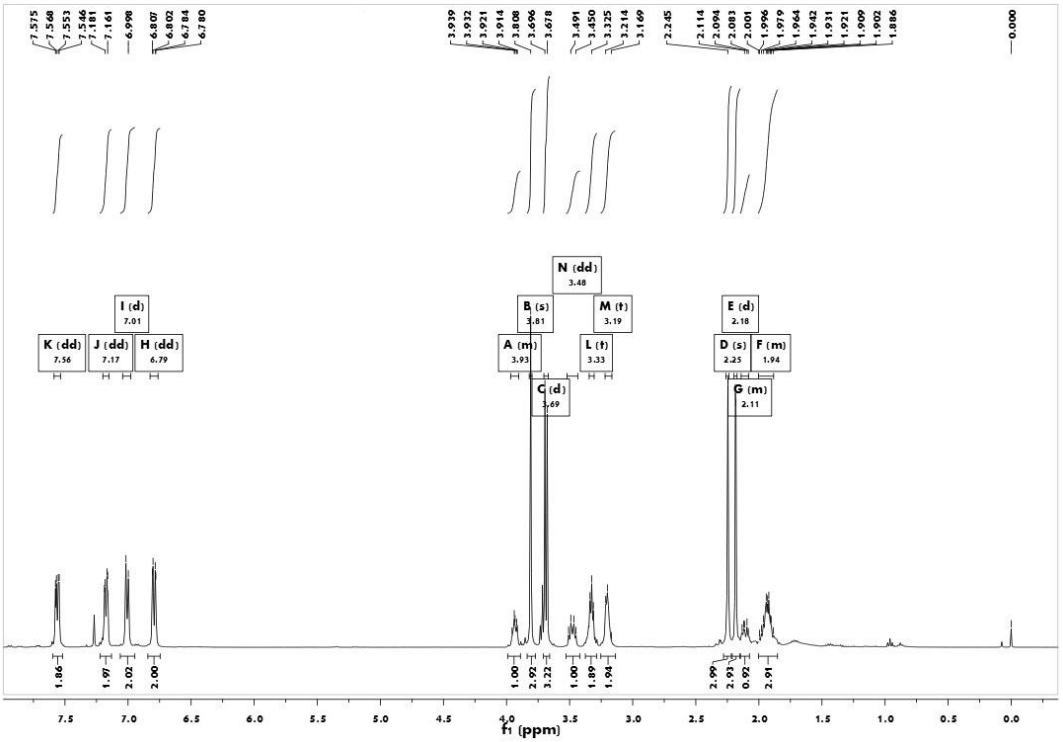

f1 (ppm)

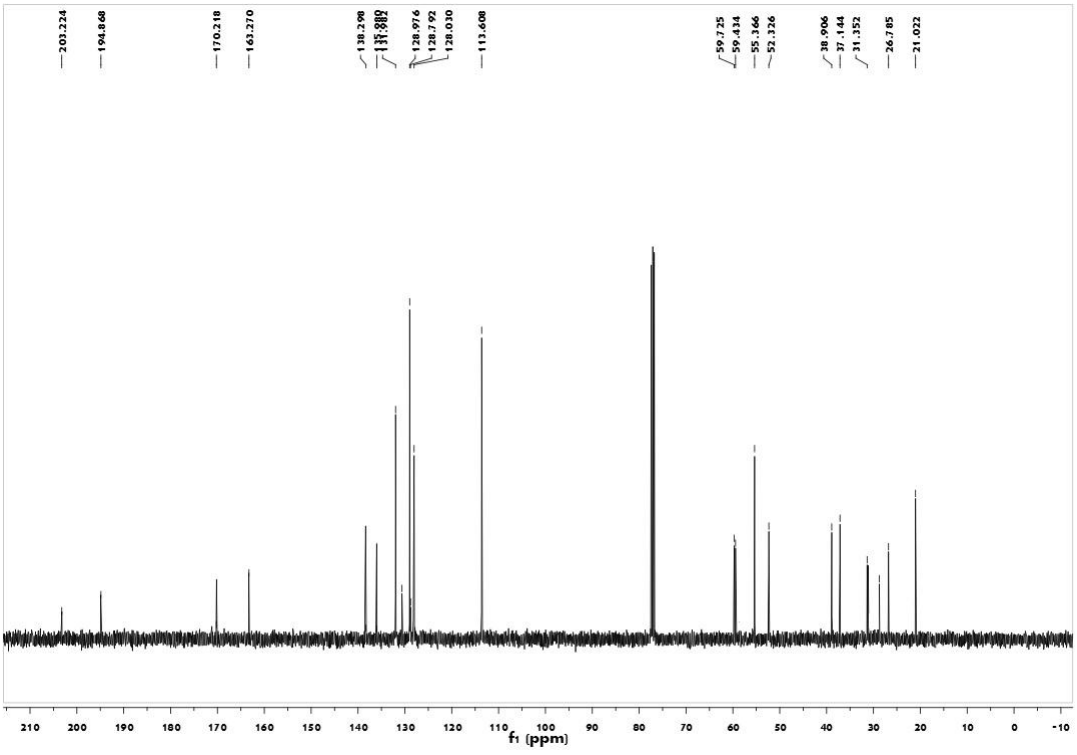

S
S
O
O
OMe
O

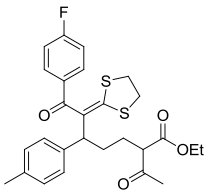

7.485
7.480
7.465
7.460
7.199
7.195
7.179
7.175
7.127
7.108
7.028
7.009
3.983
3.964
3.945
3.677
3.477
3.317
3.211
3.182
2.350
2.254
2.180
2.156
2.141
2.127
2.120
2.101
2.086
1.961
1.950
1.922
1.901
1.881
0.000
L (d) 7.14
N (dd) 7.50
K (d) 7.04
M (dd) 7.21
B (d) 3.71
D (t) 3.22
A (t) 3.99
C (dd) 3.49
E (t) 3.34
J (m) 2.14
G (s) 2.28
F (s) 2.37
I (m) 1.95
H (d) 2.19
1.95
2.14
2.19
2.15
1.00
3.09
1.01
2.00
2.06
3.08
3.13
3.02
1.32
3.14
f1 (ppm)

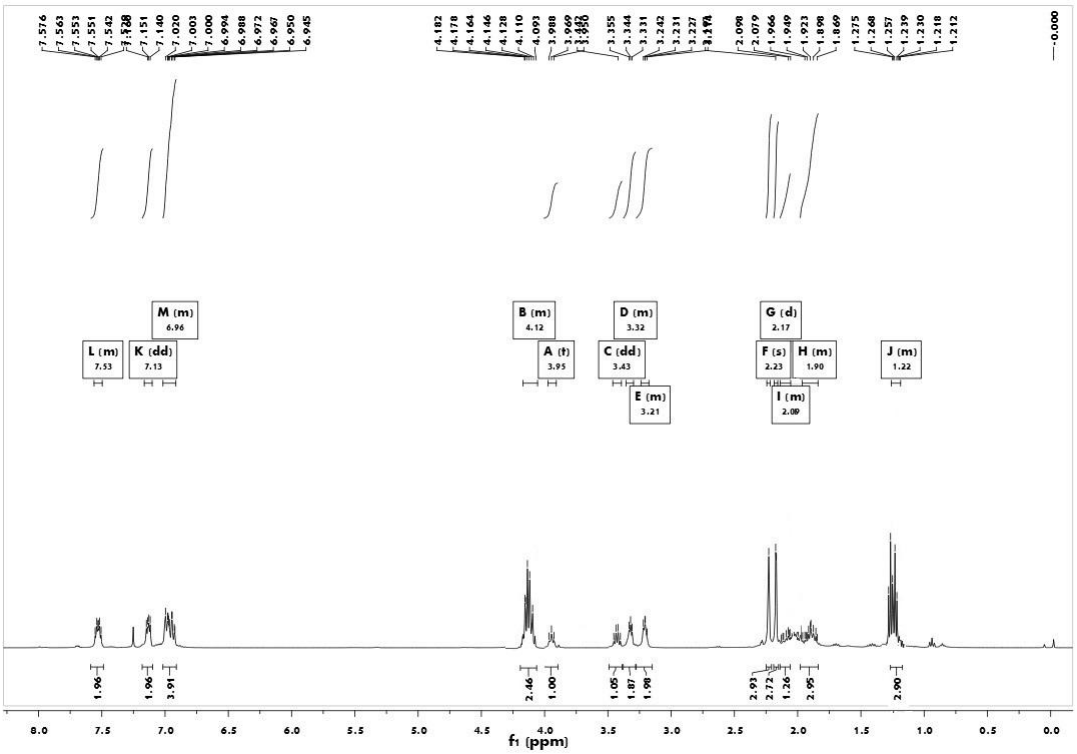

203.272
195.733
170.178
147.223
143.182
135.567
129.590
129.107
128.984
128.777
128.710
128.103
128.062
59.458
52.342
38.964
37.105
29.049
26.824
21.702
21.034
f1 (ppm)

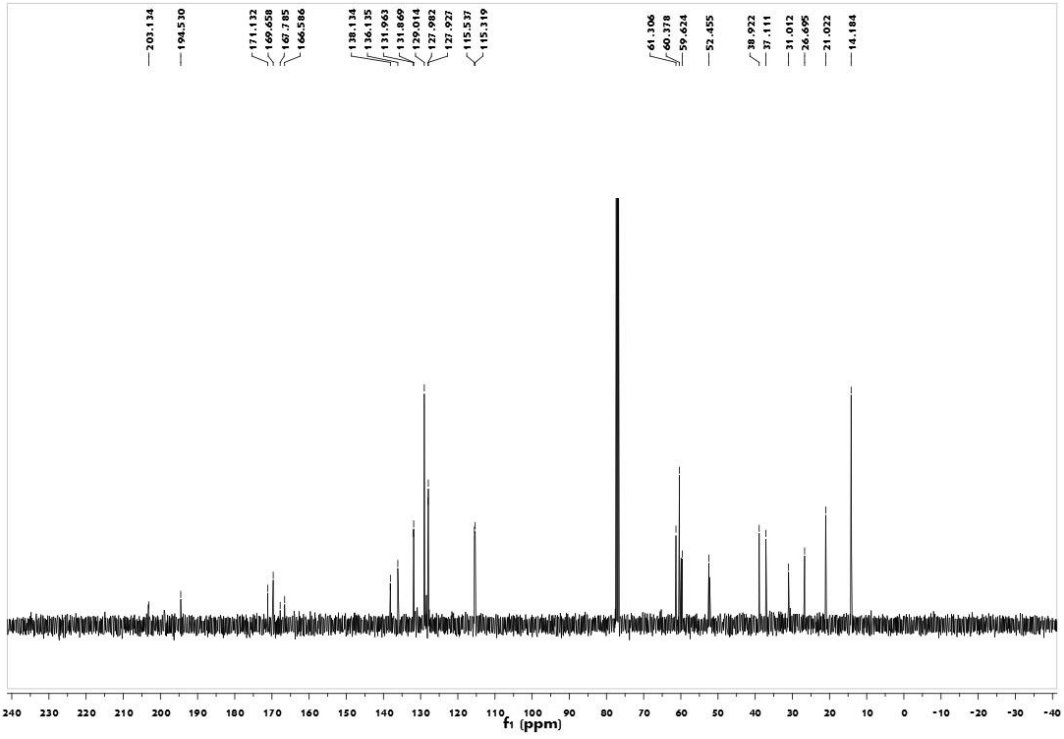

OMe
S
S
O
O
OMe
O

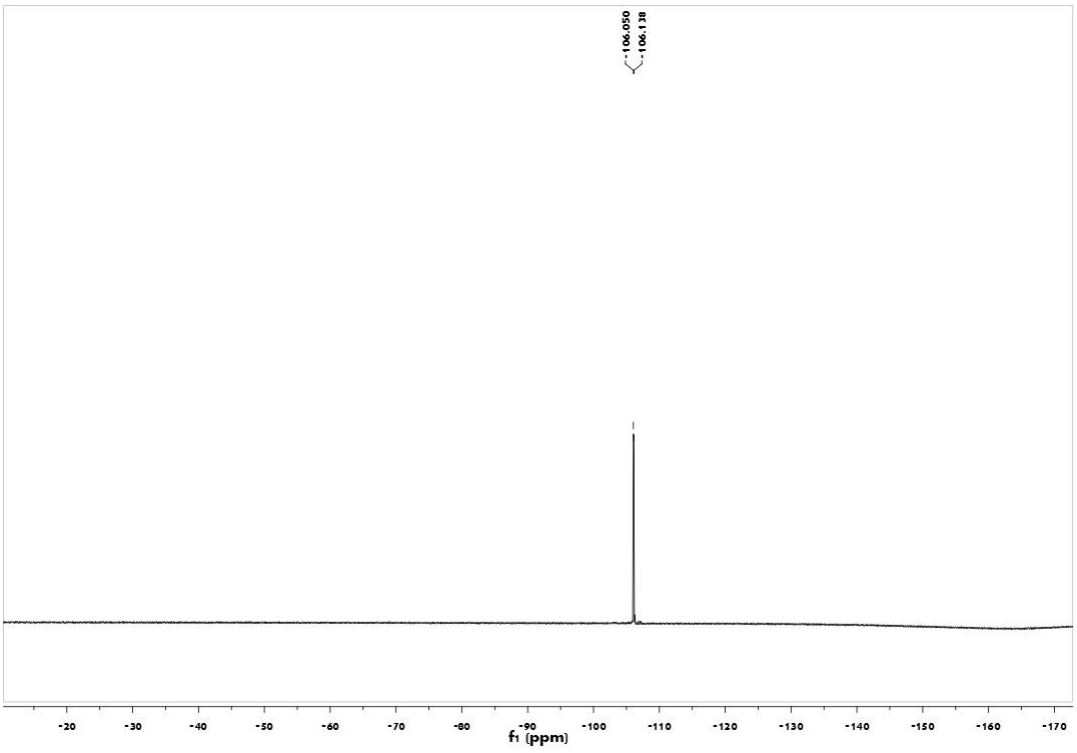

N (dd) 3.48
B (s) 3.61
M (t) 3.19
I (d) 7.01
K (dd) 7.56
J (dd) 7.17
H (dd) 6.79
A (m) 3.93
L (t) 3.33
C (d) 3.69
E (d) 2.18
D (s) 2.25
F (m) 1.94
G (m) 2.11
f1 (ppm)

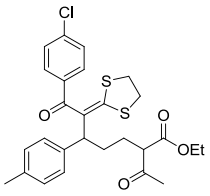

f1 (ppm)

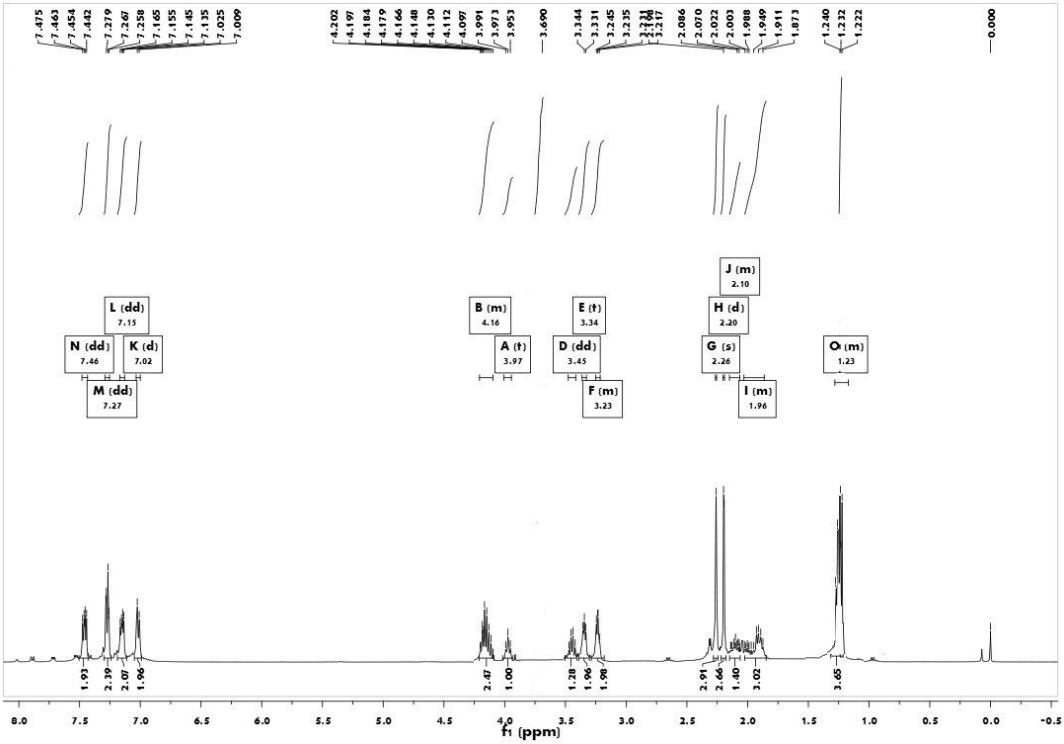

F
S
S
O
O
OEt
O

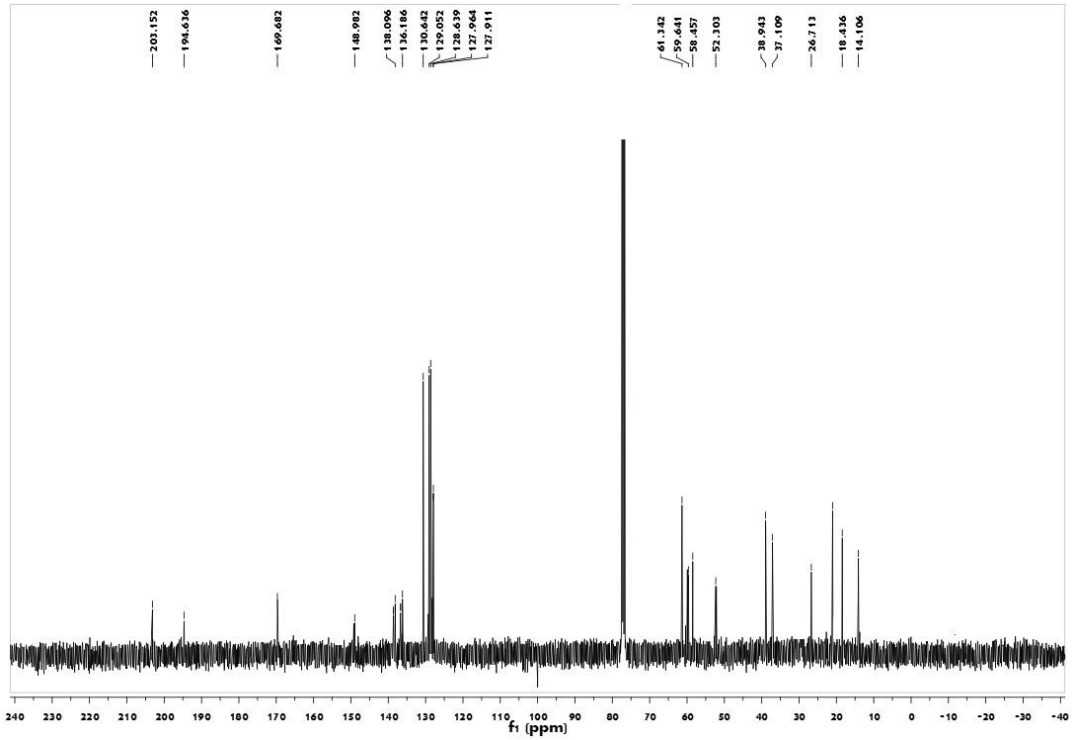

M (m) 6.96
L (m) 7.53
K (dd) 7.13
B (m) 4.12
A (t) 3.95
D (m) 3.32
C (dd) 3.43
E (m) 3.21
G (d) 2.17
F (s) 2.23
H (m) 1.90
I (m) 2.09
J (m) 1.22
f1 (ppm)

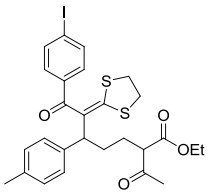

f1 (ppm)

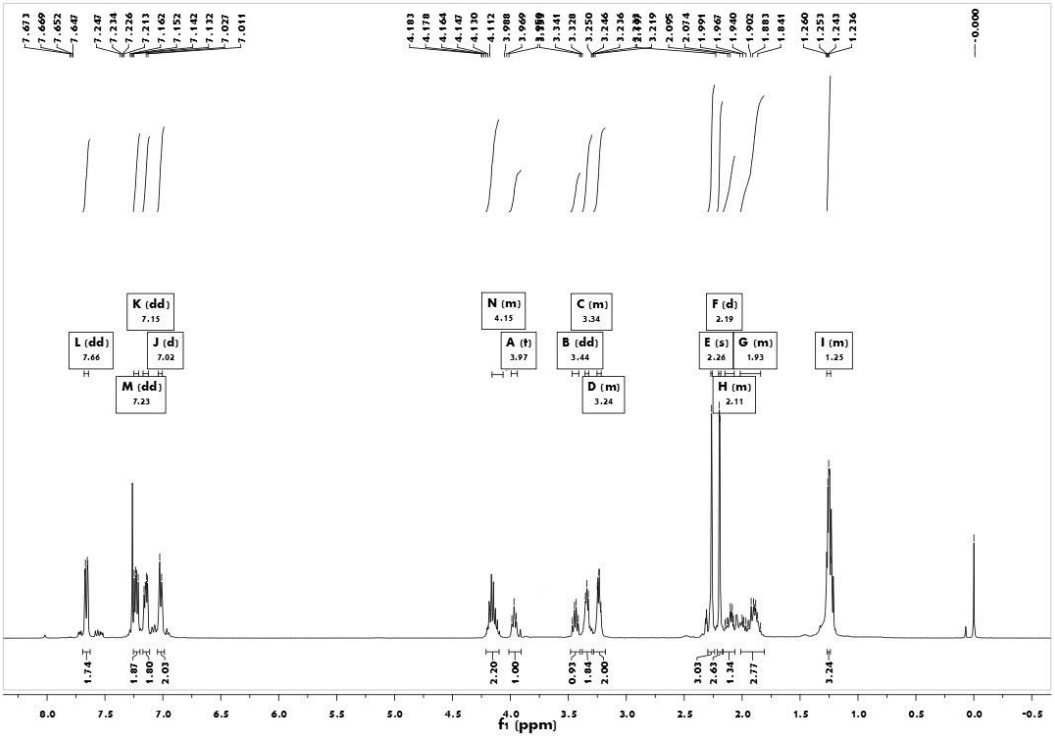

-106.050
-106.138
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
f1 (ppm)

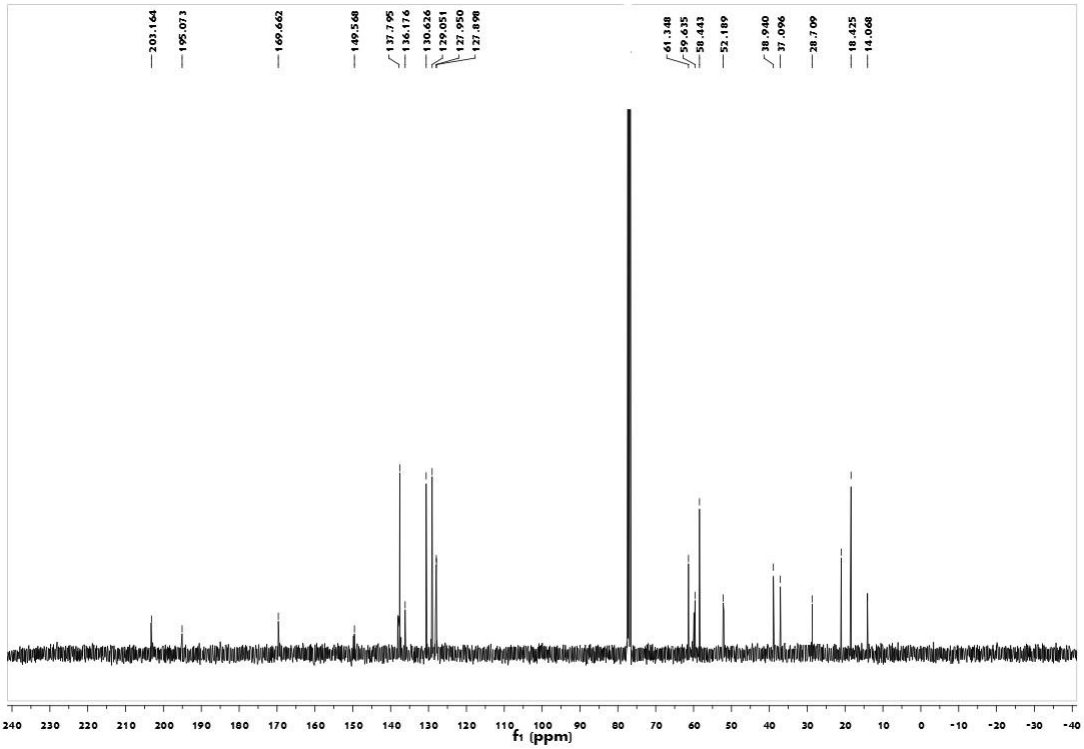

Cl
O
S
S
O
OEt
O

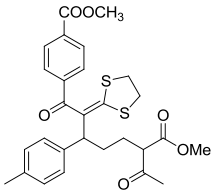

L (dd) 7.15
N (dd) 7.46
K (d) 7.02
M (dd) 7.27
B (m) 4.16
A (t) 3.97
E (t) 3.34
D (dd) 3.45
F (m) 3.23
J (m) 2.10
H (d) 2.20
G (s) 2.26
I (m) 1.96
O (m) 1.23
f1 (ppm)

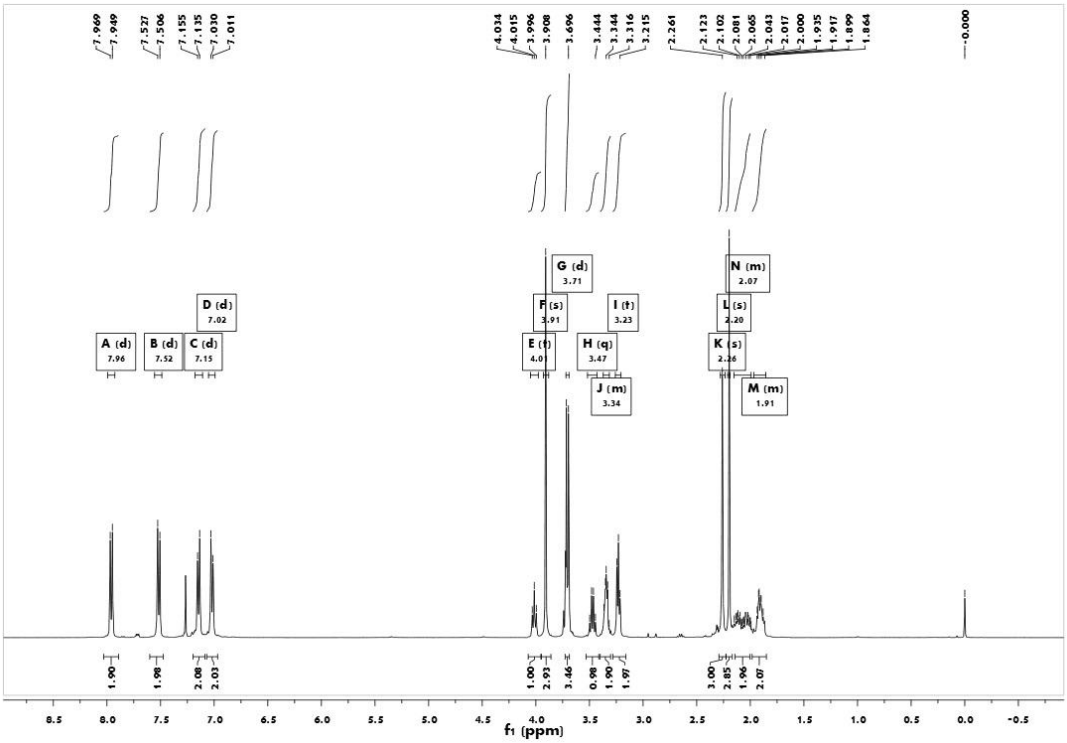

f1 (ppm)

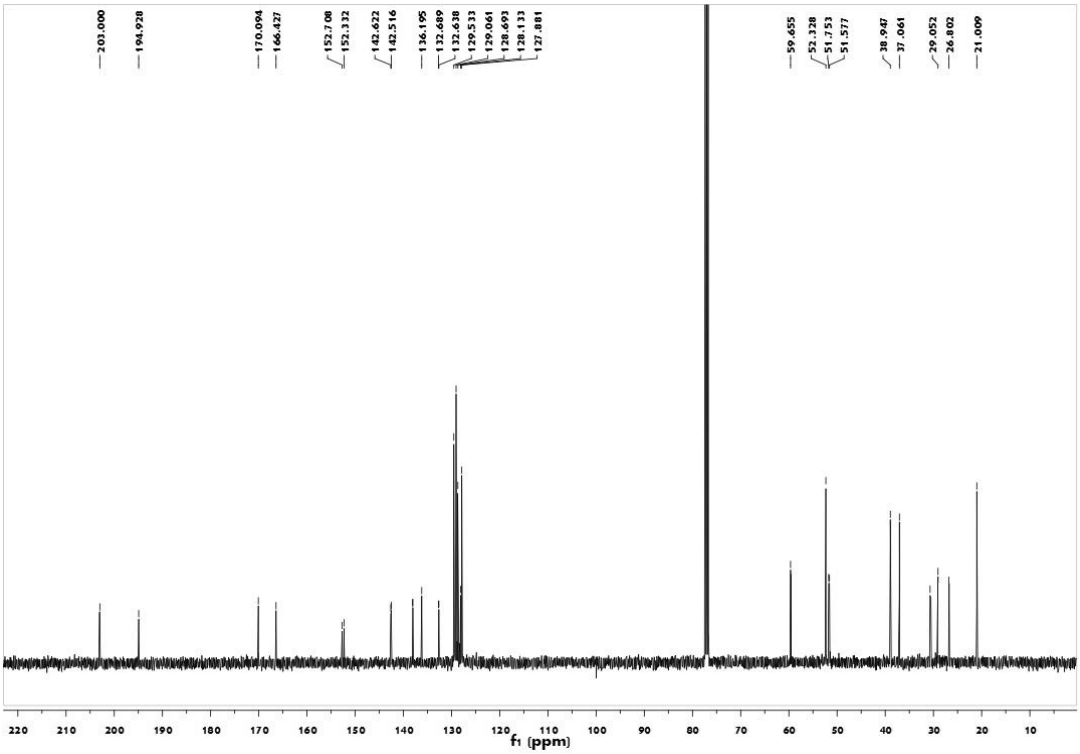

I
S
S
O
O
OEt
O

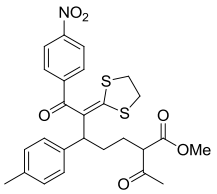

K (dd) 7.15
L (dd) 7.66
J (d) 7.02
M (dd) 7.23
N (m) 4.15
A (t) 3.97
C (m) 3.34
B (dd) 3.44
D (m) 3.24
F (d) 2.19
E (s) 2.26
G (m) 1.93
H (m) 2.11
I (m) 1.25
f1 (ppm)

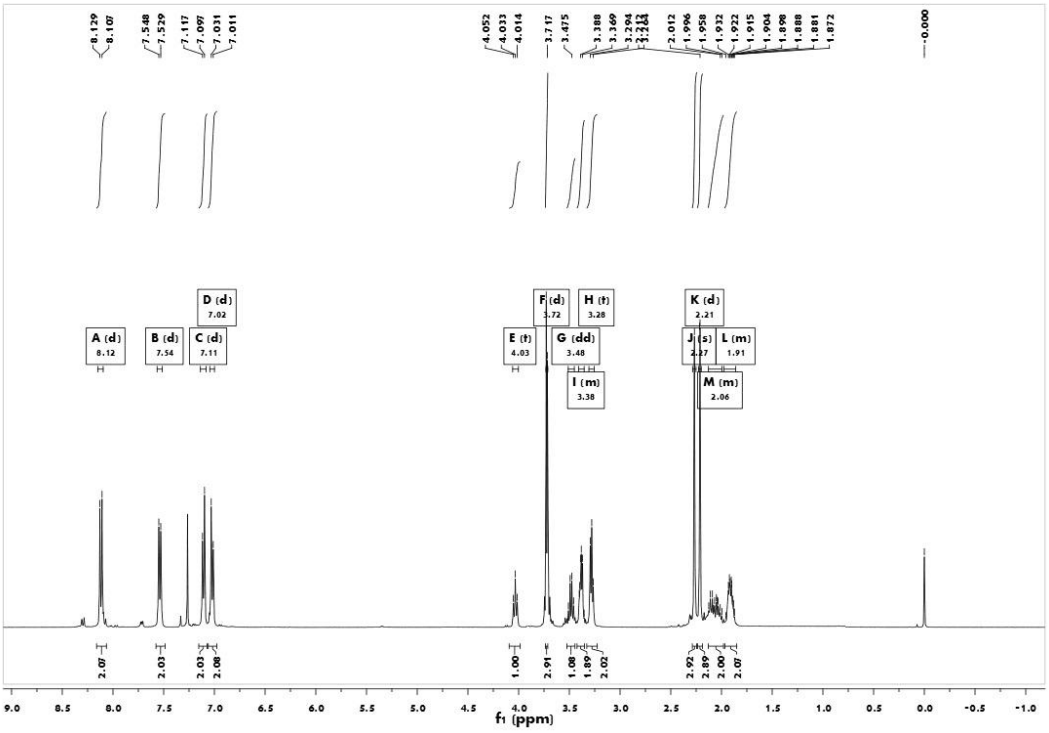

f1 (ppm)

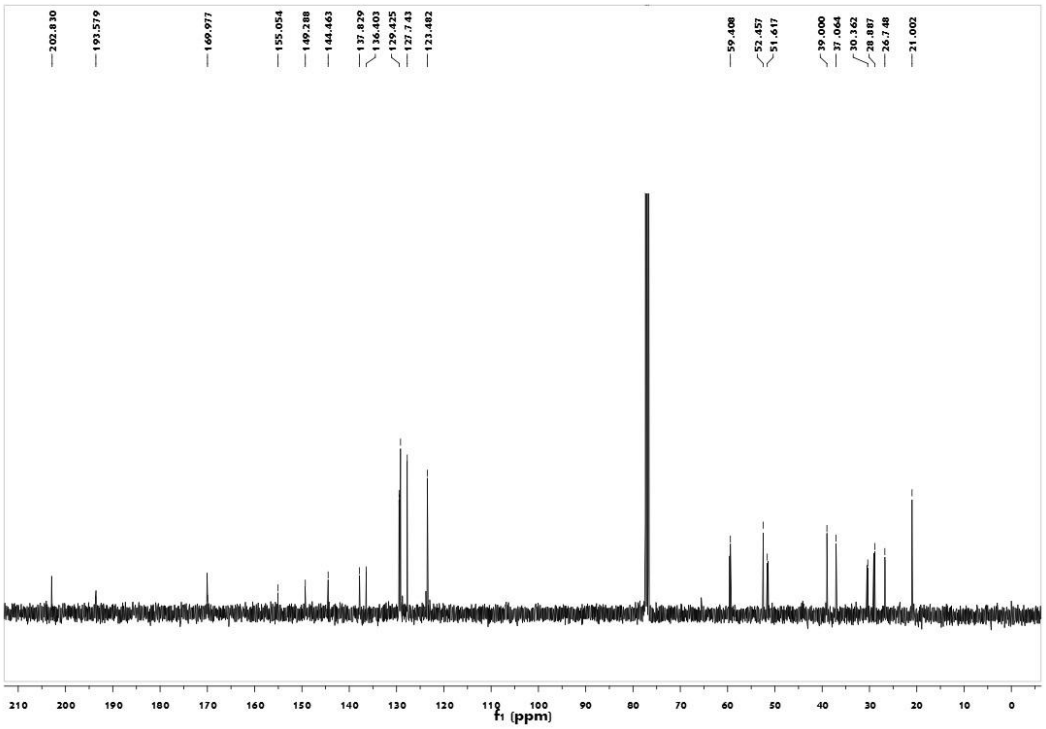

COOCH3
S
S
O
O
OMe
O

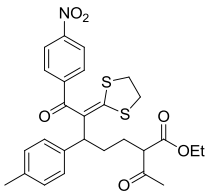

A (d) 7.96
B (d) 7.52
C (d) 7.15
D (d) 7.02
E (t) 4.01
F (s) 3.91
G (d) 3.71
H (q) 3.47
I (t) 3.23
J (m) 3.34
K (s) 2.26
L (s) 2.20
M (m) 1.91
N (m) 2.07
f1 (ppm)

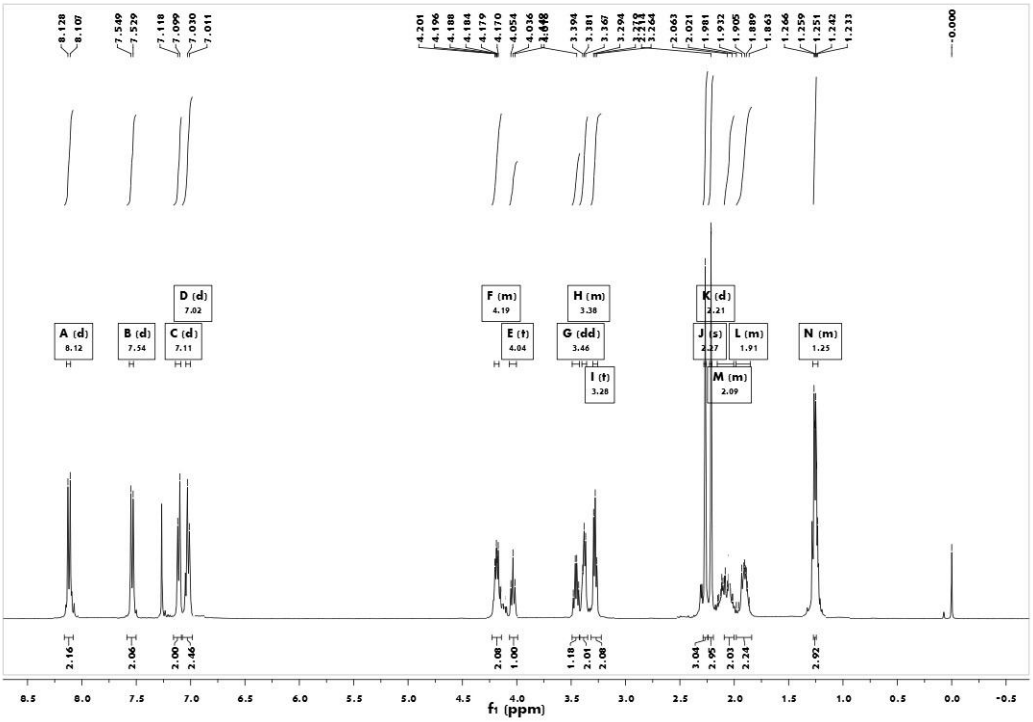

f1 (ppm)

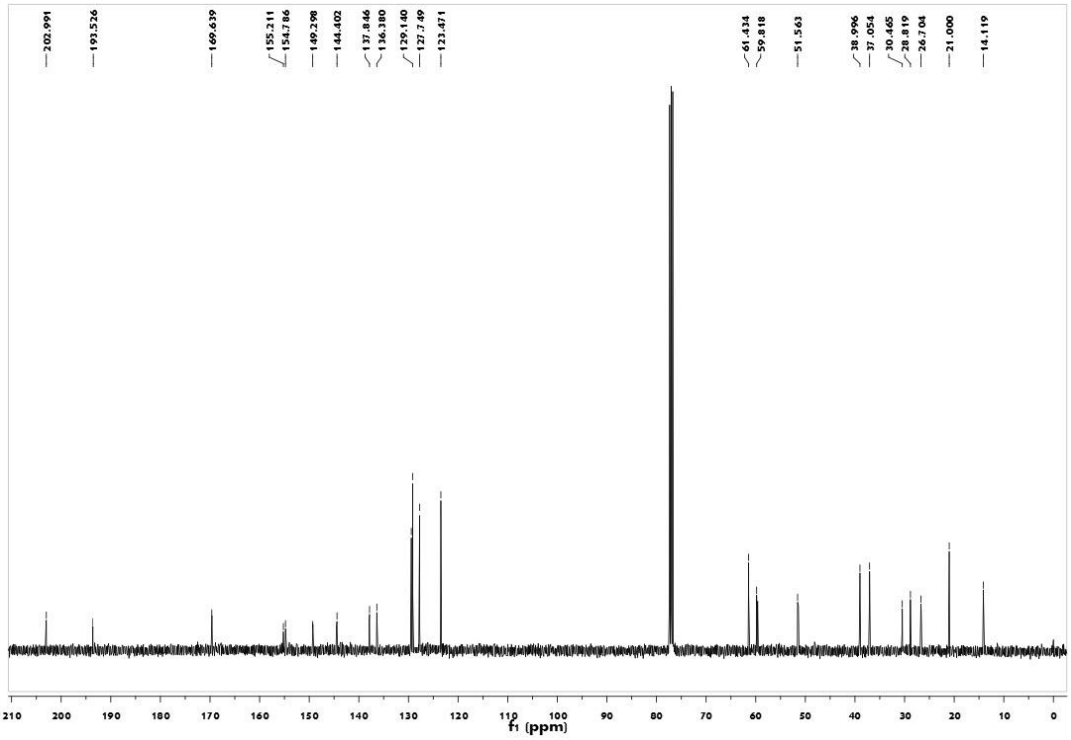

NO2
S
S
O
O
OMe
O

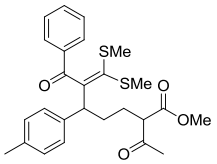

A (d) 8.12
B (d) 7.54
C (d) 7.11
D (d) 7.02
E (t) 4.03
F (d) 3.72
G (dd) 3.48
H (t) 3.28
I (m) 3.38
J (s) 2.27
K (d) 2.21
L (m) 1.91
M (m) 2.06
f1 (ppm)

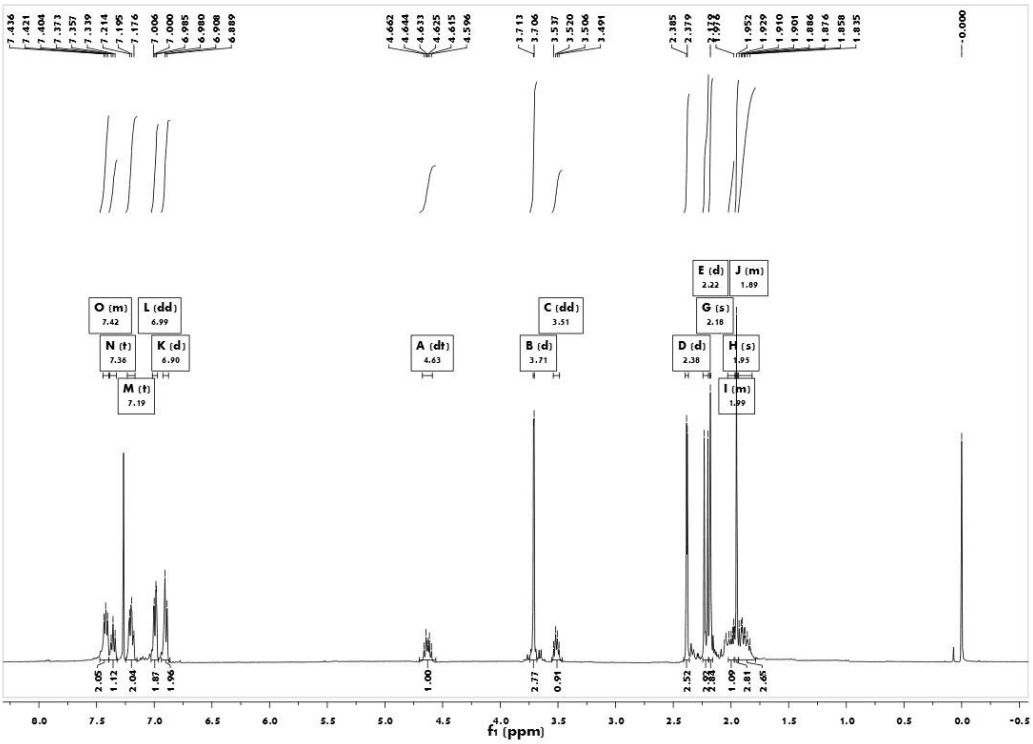

202.830
193.579
169.977
155.054
149.288
144.463
137.829
136.403
129.425
127.743
123.482
59.408
52.457
51.617
39.000
37.064
30.362
28.887
26.748
21.002
f1 (ppm)

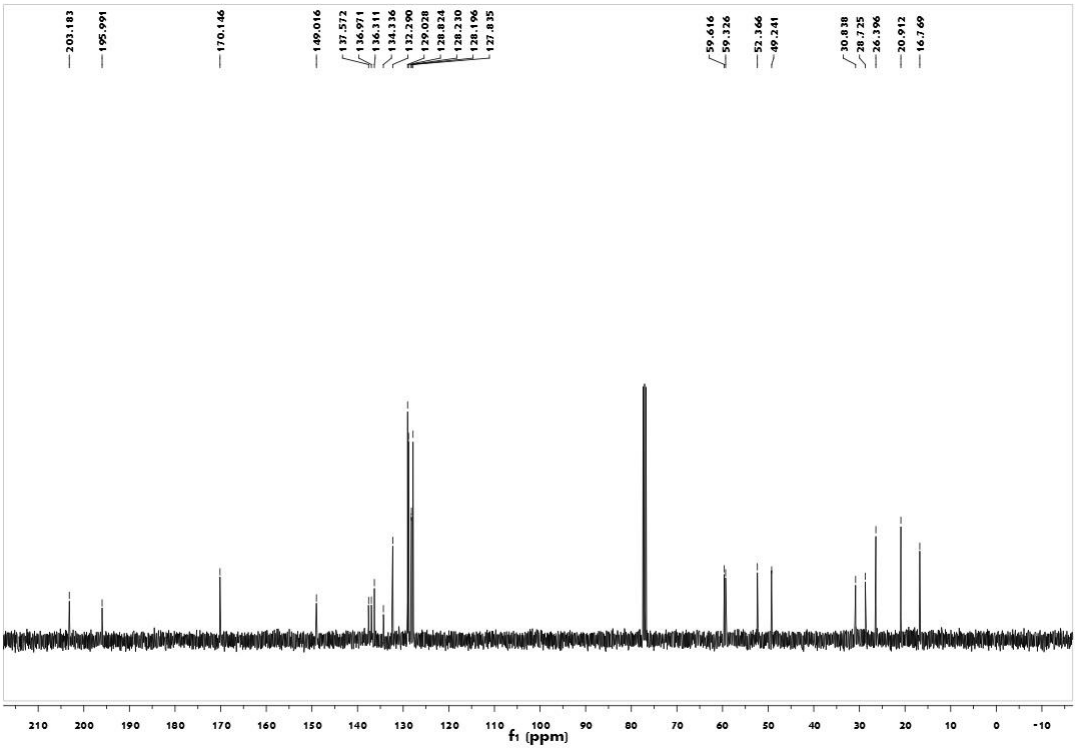

NO2
S
S
O
O
OEt
O

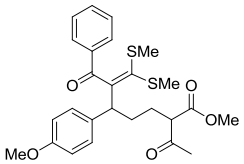

A (d) 8.12
B (d) 7.54
C (d) 7.11
D (d) 7.02
E (t) 4.04
F (m) 4.19
G (dd) 3.46
H (m) 3.38
I (t) 3.28
J (s) 2.37
K (d) 2.21
L (m) 1.91
M (m) 2.09
N (m) 1.25
f1 (ppm)

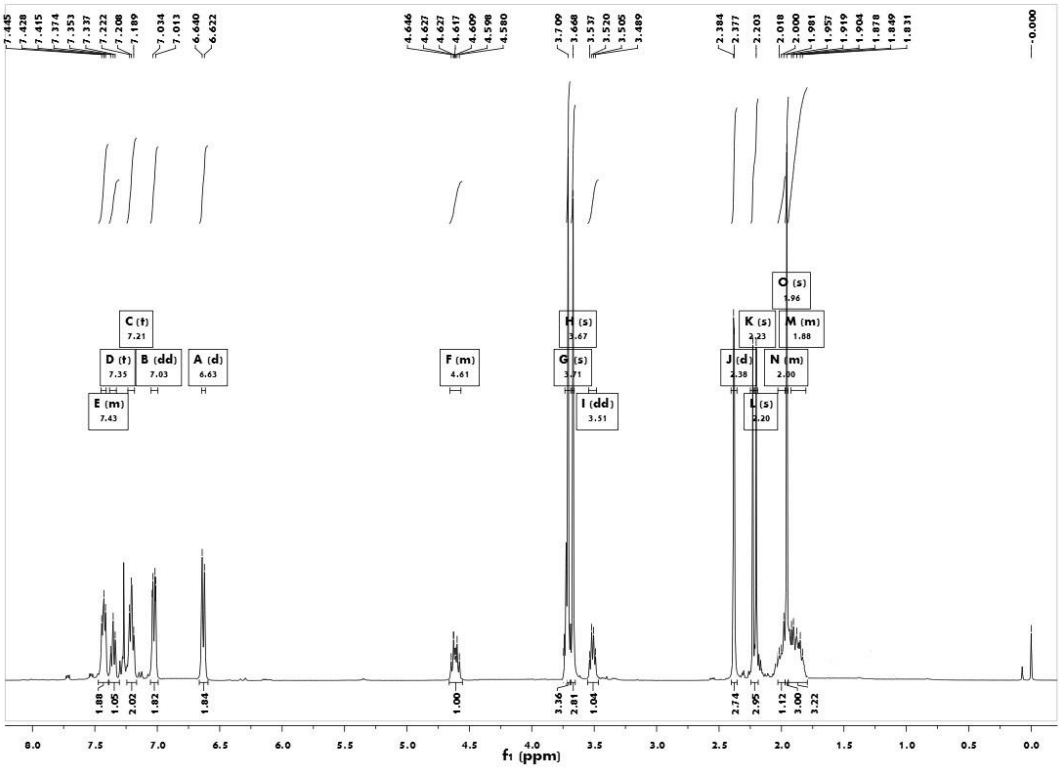

202.991
193.526
169.639
155.211
154.786
149.298
144.402
137.846
136.380
129.140
127.749
123.471
61.434
59.818
51.563
38.996
37.054
30.465
28.819
26.704
21.000
14.119
f1 (ppm)

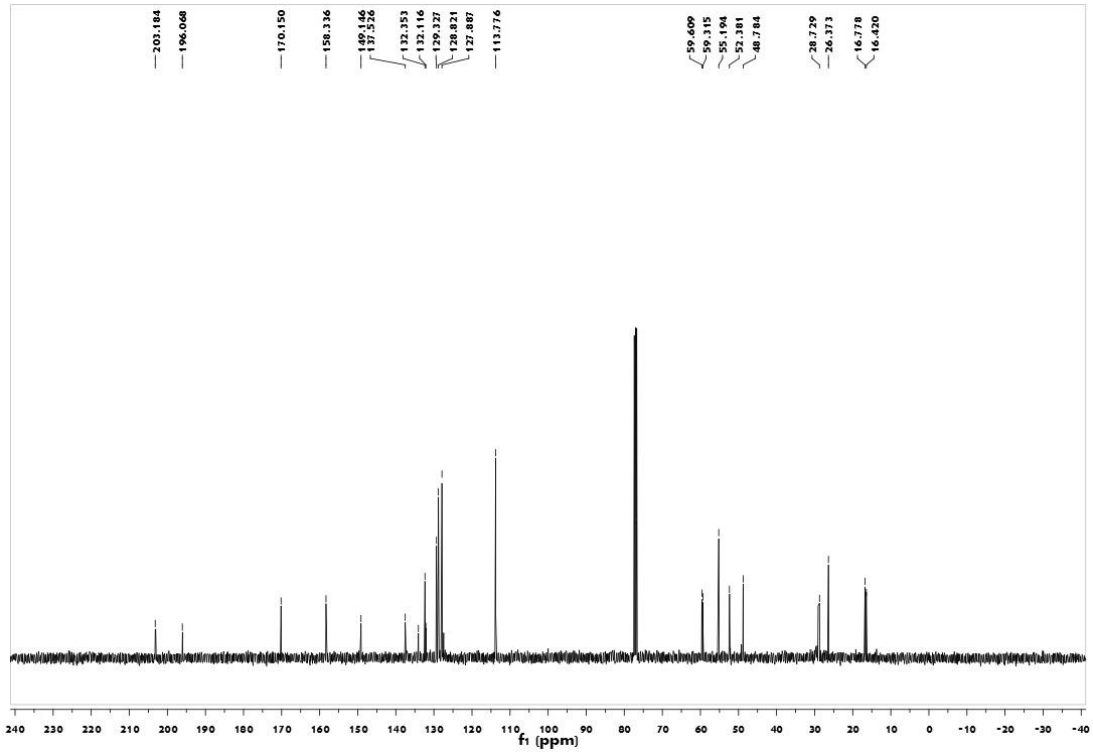

SMe
SMe
O
O
O
OMe
O


O (m) 7.42
L (dd) 6.99
N (t) 7.36
K (d) 6.90
M (t) 7.19
A (dt) 4.63
C (dd) 3.51
B (d) 3.71
E (d) 2.22
J (m) 1.89
G (s) 2.18
D (d) 2.38
H (s) 1.95
I (m) 1.99
f1 (ppm)


203.183
195.991
170.146
149.016
137.572
136.971
136.311
134.336
132.290
129.028
128.824
128.230
128.196
127.835
59.616
59.326
52.366
49.241
30.838
28.725
26.396
20.912
16.769
f1 (ppm)


SMe
SMe
O
O
O
OMe
MeO
O


C (t) 7.21
D (t) 7.35
B (dd) 7.03
A (d) 6.63
E (m) 7.43
F (m) 4.61
H (s) 3.67
G (s) 3.71
I (dd) 3.51
O (s) 1.96
K (s) 2.23
M (m) 1.88
J (d) 2.38
N (m) 2.00
L (s) 2.20
f1 (ppm)


203.184
196.068
170.150
158.336
149.146
137.526
132.353
132.116
129.327
128.821
127.887
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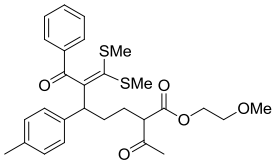
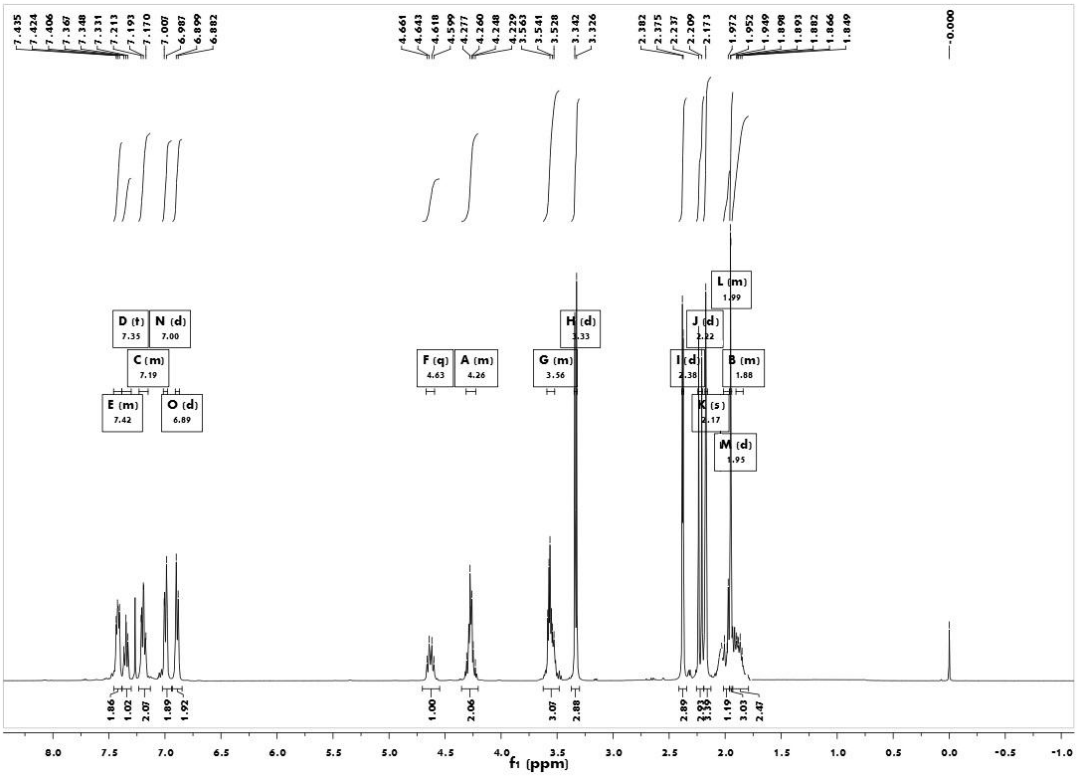
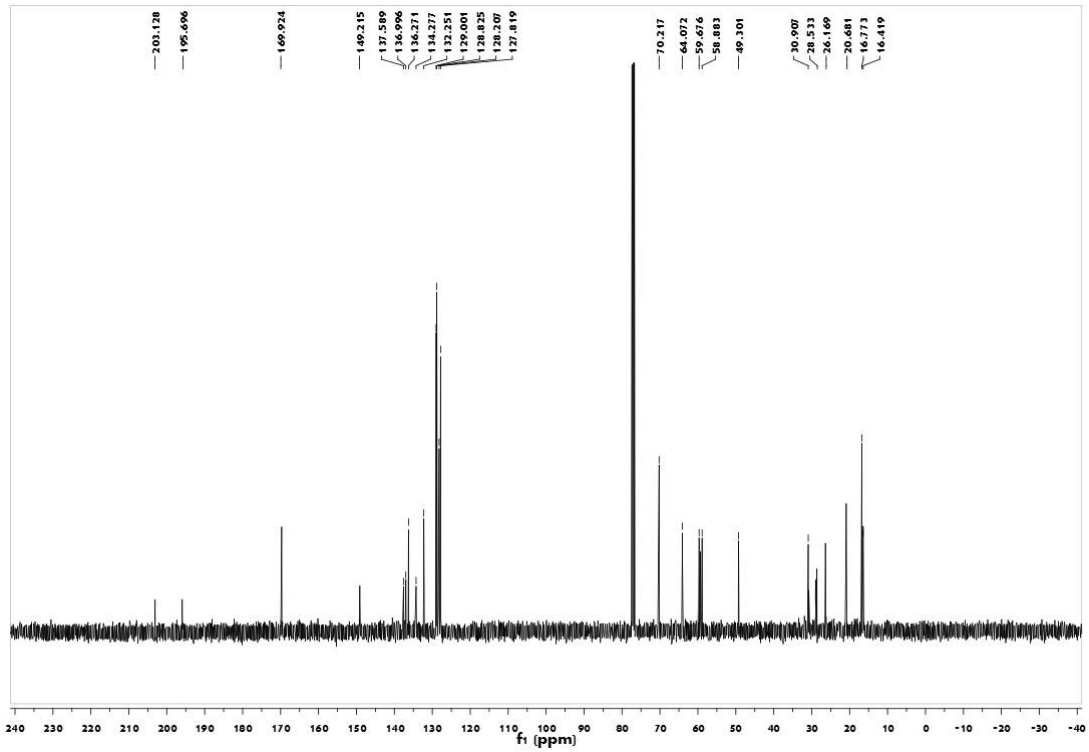
28.729
26.373
16.778
16.420
f1 (ppm)


SMe
SMe
O
O
O
O
OMe
O


D (t) 7.35
N (d) 7.00
C (m) 7.19
E (m) 7.42
O (d) 6.89
F (q) 4.63
A (m) 4.26
G (m) 3.56
H (d) 3.33
I (d) 2.38
J (d) 2.22
L (m) 1.99
B (m) 1.88
K (s) 2.17
M (d) 1.95
f1 (ppm)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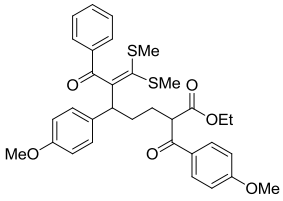
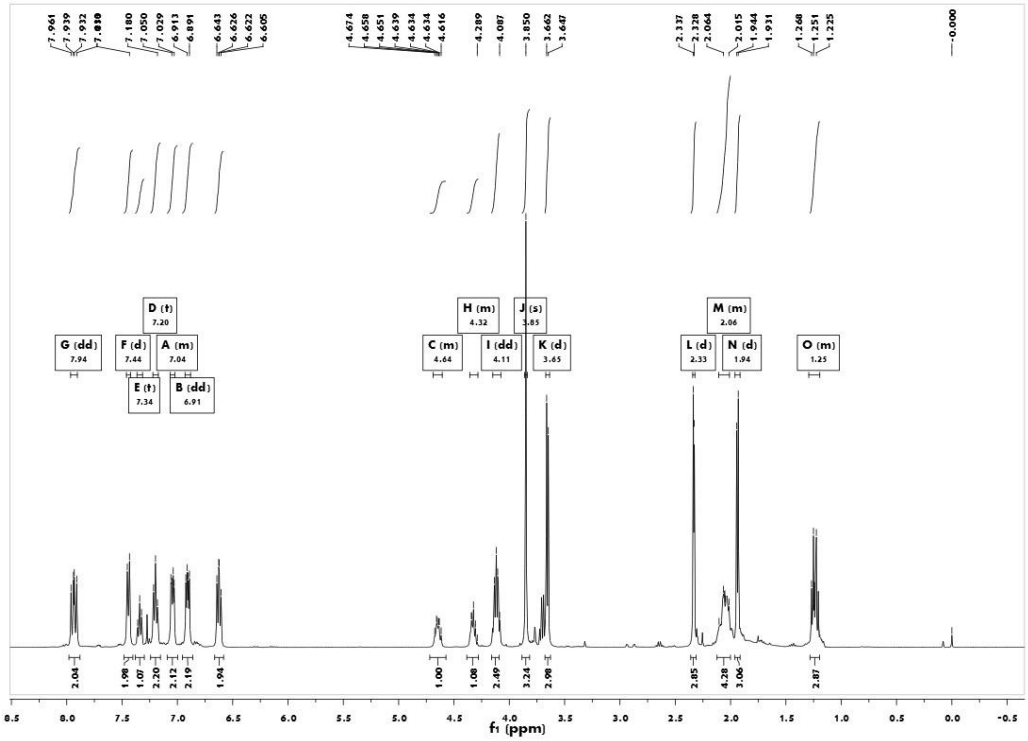
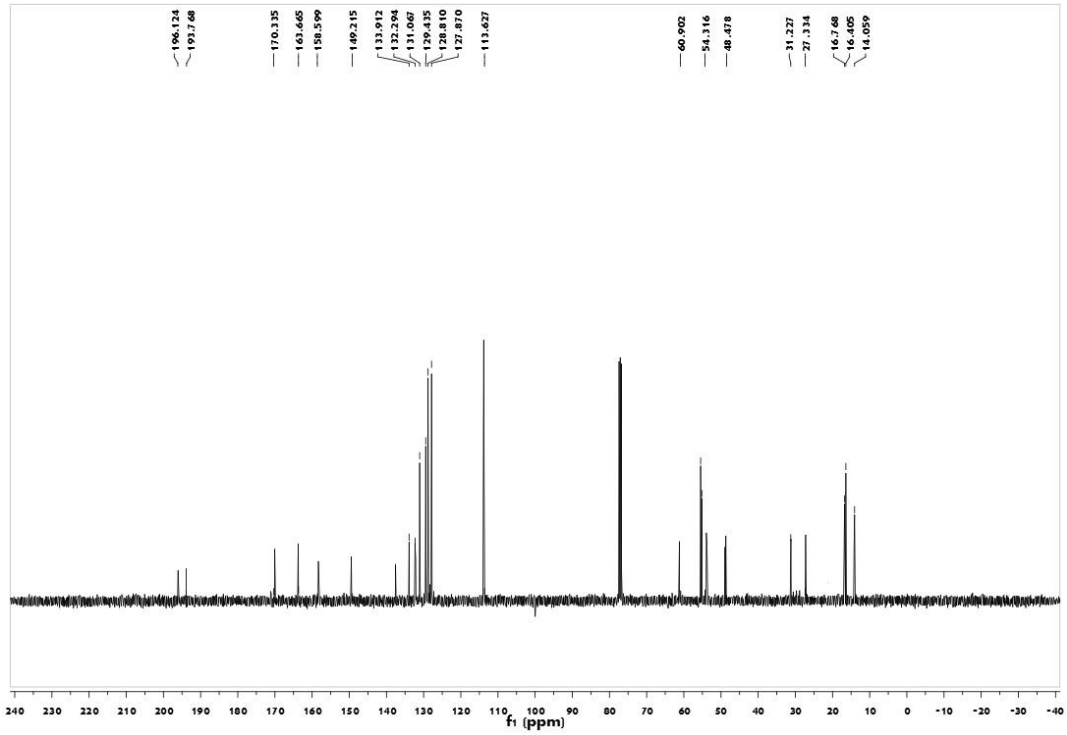
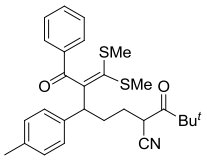
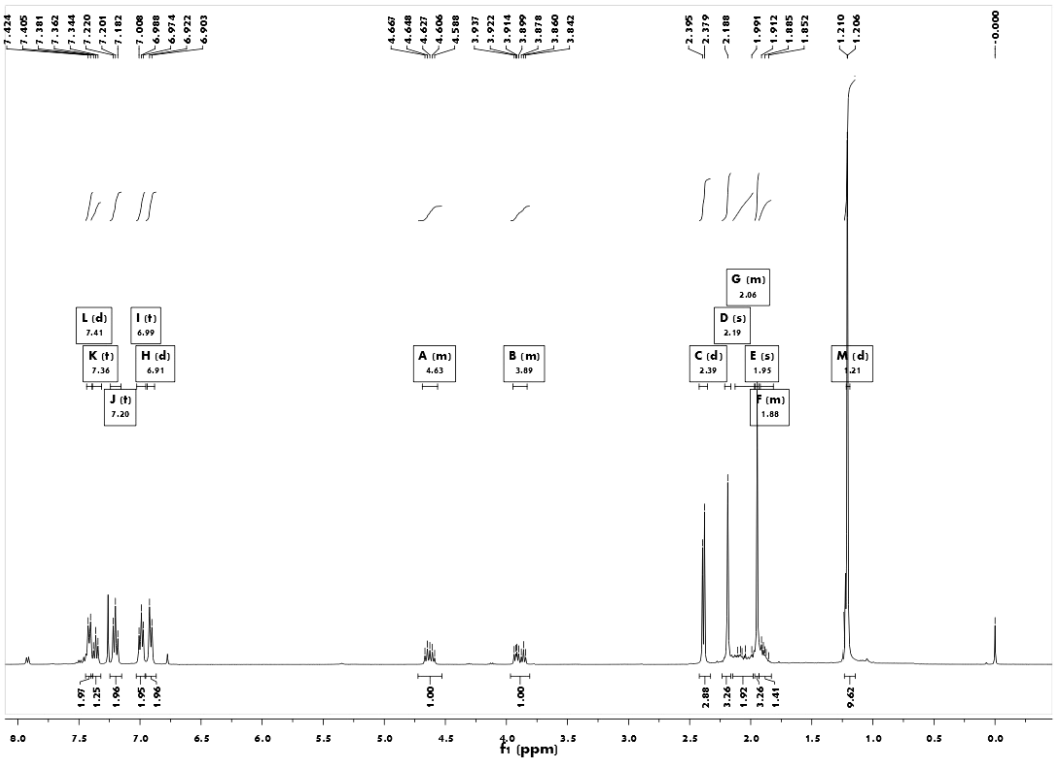
169.924
149.215
137.589
136.996
136.271
134.277
132.251
129.001
128.825
128.207
127.819
70.217
64.072
59.676
58.883
49.301
30.907
28.533
26.169
20.681
16.773
16.419
f1 (ppm)

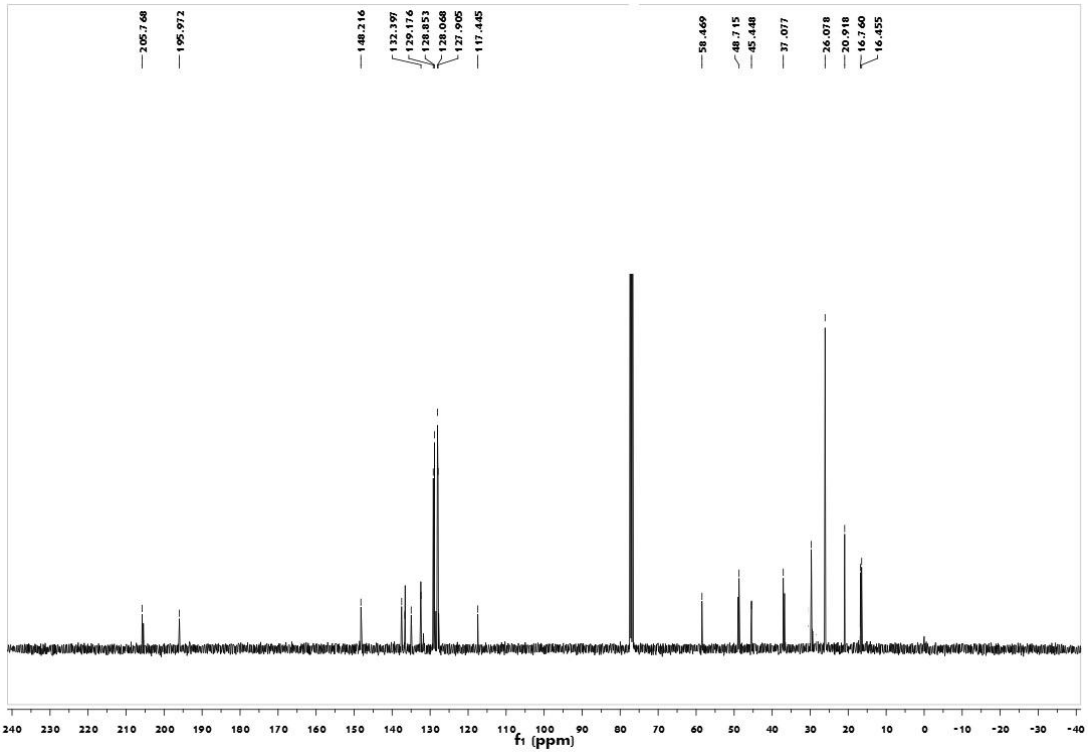

SMe
SMe
O
O
OEt
O
MeO
OMe


f1 (ppm)


f1 (ppm)


SMe
SMe
O
O
O
Bu^t
CN


L (d) 7.41
I (t) 6.99
K (t) 7.36
H (d) 6.91
J (t) 7.20
A (m) 4.63
B (m) 3.89
G (m) 2.06
D (s) 2.19
C (d) 2.39
E (s) 1.95
F (m) 1.88
M (d) 1.21
f1 (ppm)


205.760
195.972
140.216
132.397
129.176
128.853
128.068
127.905
117.445
58.469
48.715
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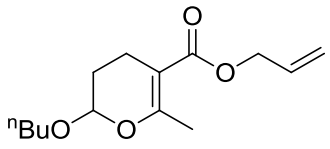
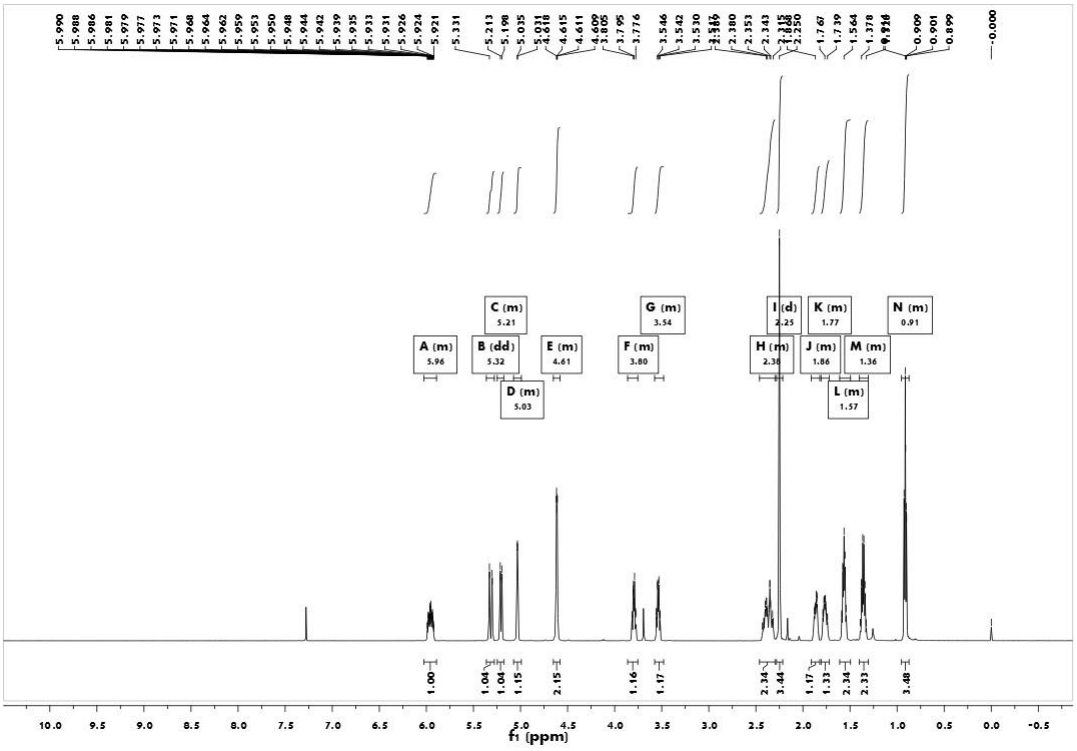
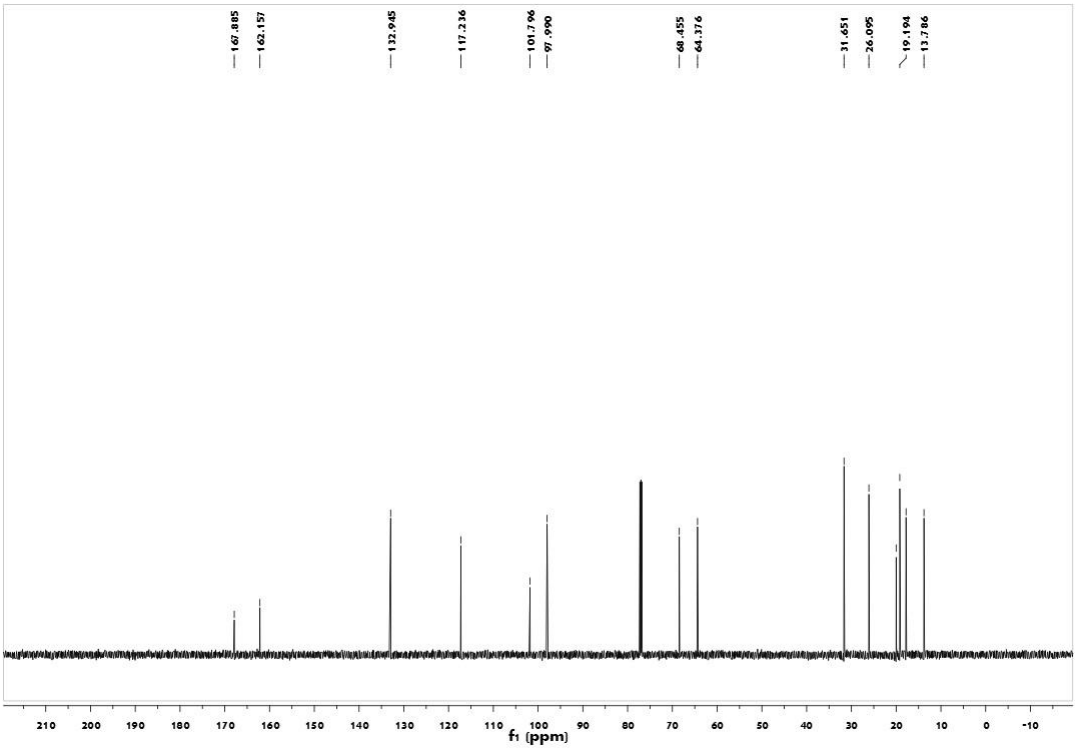
37.077
26.078
20.918
16.760
16.455
f1 (ppm)


O
O
nBuO
O


A (m) 5.96
B (dd) 5.32
C (m) 5.21
D (m) 5.03
E (m) 4.61
F (m) 3.80
G (m) 3.54
H (m) 2.36
I (d) 2.25
J (m) 1.86
K (m) 1.77
L (m) 1.57
M (m) 1.36
N (m) 0.91
f1 (ppm)


167.885
162.157
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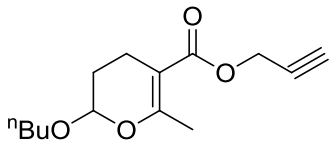
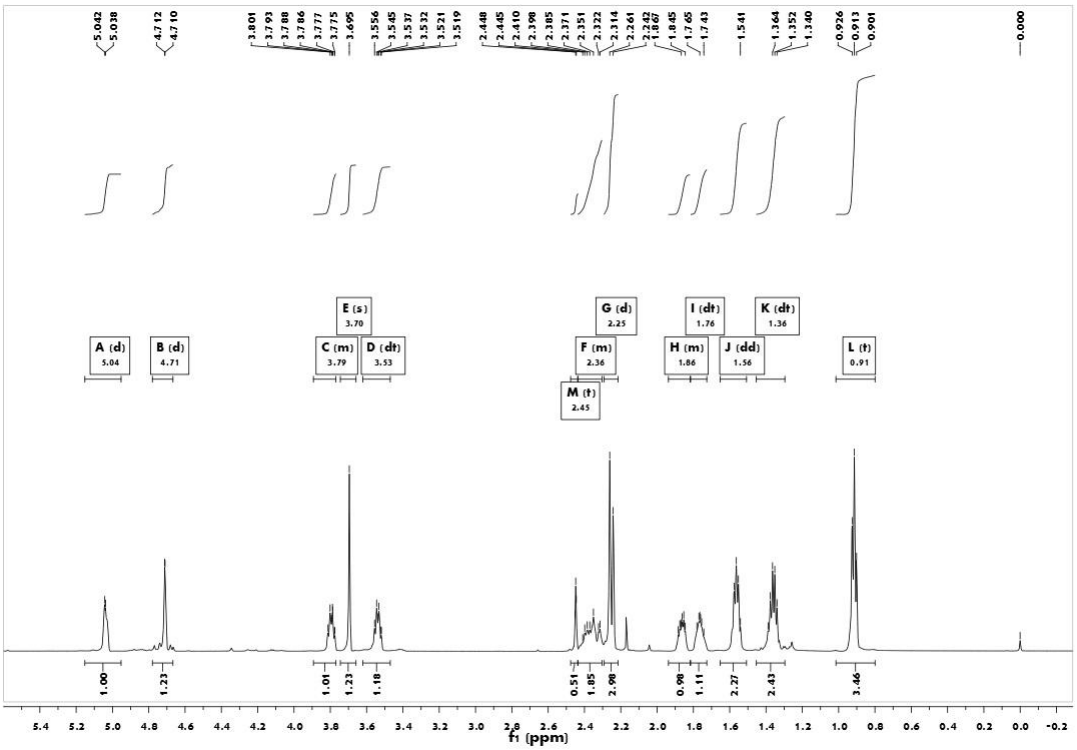
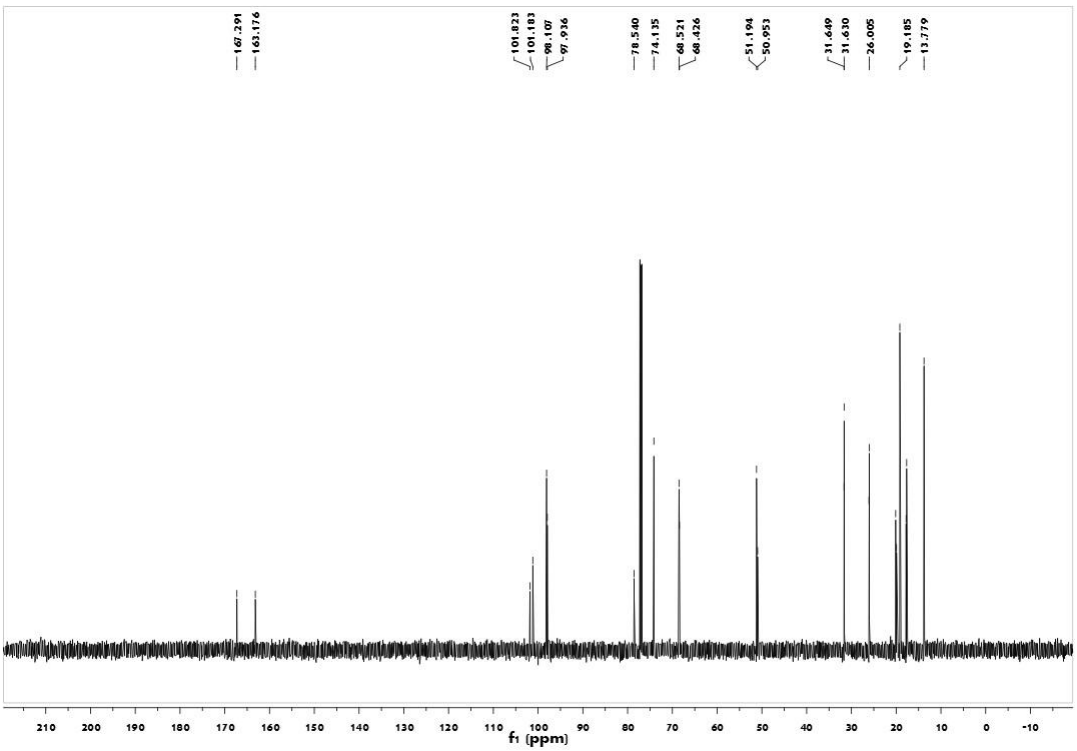
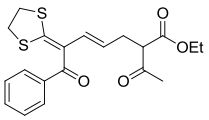
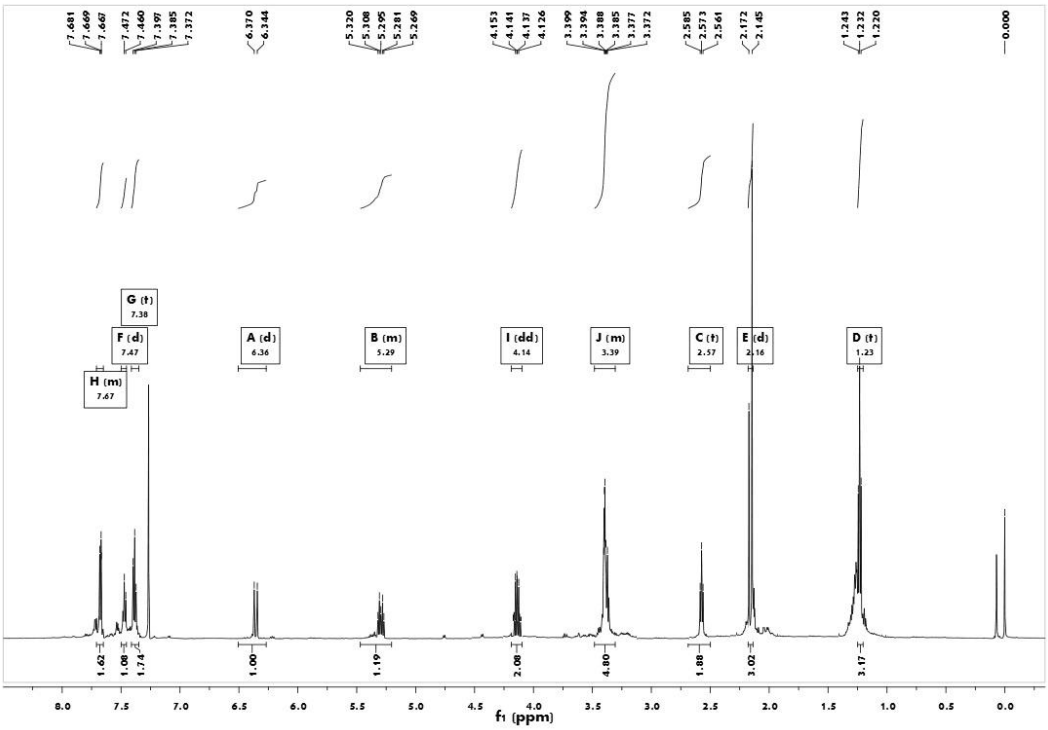
117.236
101.796
97.990
68.455
64.376
31.651
26.095
19.194
13.786
f1 (ppm)

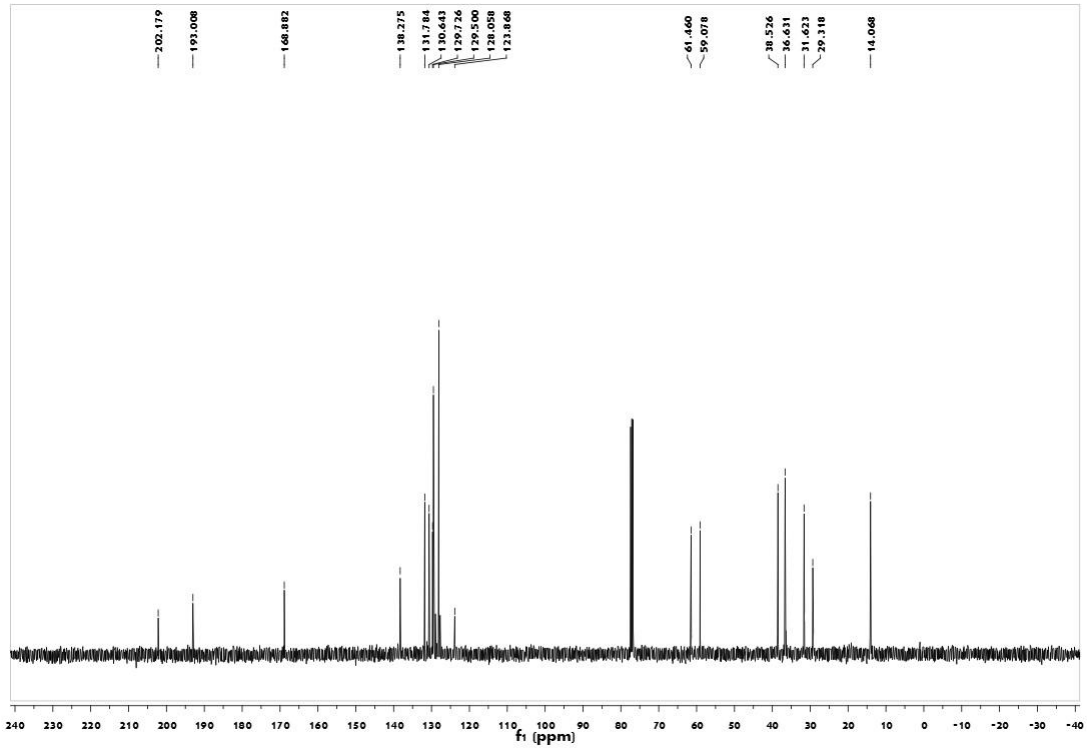

O
O
nBuO
O


A (d) 5.04
B (d) 4.71
C (m) 3.79
D (dt) 3.53
E (s) 3.70
F (m) 2.36
G (d) 2.25
H (m) 1.86
I (dt) 1.76
J (dd) 1.56
K (dt) 1.36
L (t) 0.91
M (t) 2.45
f1 (ppm)


f1 (ppm)


S
S
O
OEt
O
O


7.681
7.669
7.662
7.472
7.460
7.397
7.385
7.372
6.370
6.344
5.320
5.308
5.295
5.281
5.269
4.153
4.141
4.137
4.126
3.399
3.394
3.388
3.385
3.377
3.372
2.585
2.573
2.561
2.172
2.145
1.243
1.232
1.220
0.000
G (t) 7.38
F (d) 7.47
H (m) 7.67
A (d) 6.36
B (m) 5.29
I (dd) 4.14
J (m) 3.39
C (t) 2.57
E (d) 2.16
D (t) 1.23
1.62
1.08
1.74
1.00
1.19
2.08
4.80
1.88
3.02
3.17
f1 (ppm)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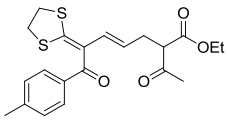
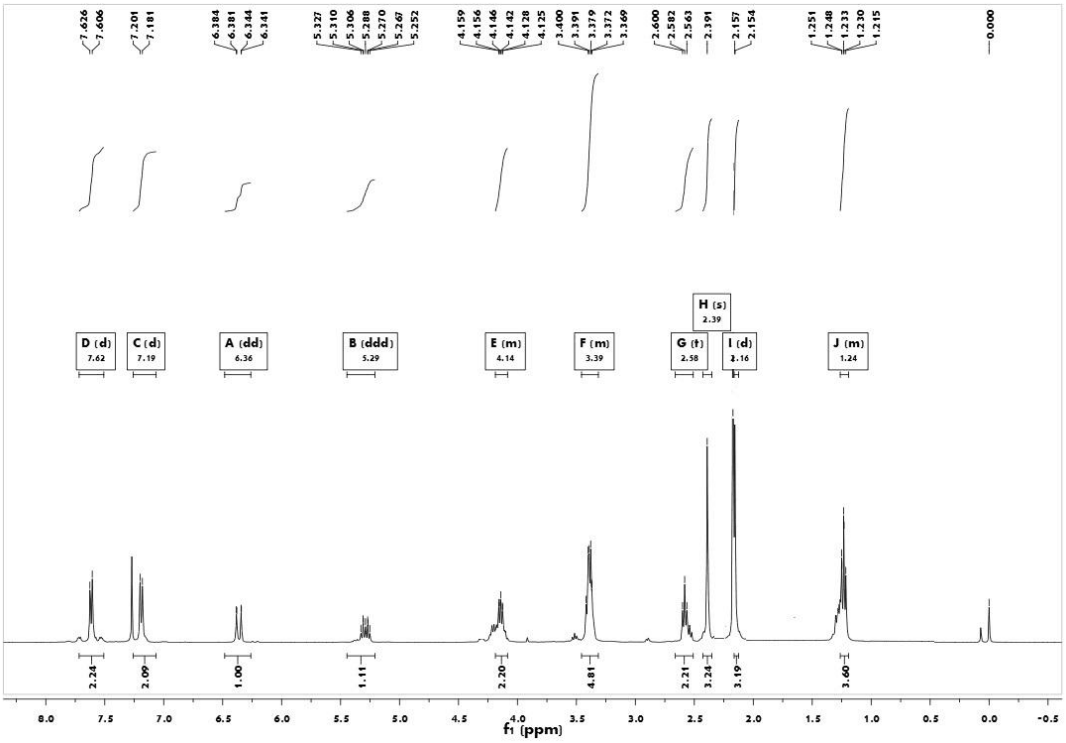
193.008
168.882
138.275
131.784
130.643
129.726
129.500
128.058
123.868
61.460
59.078
38.526
36.631
31.623
29.318
14.068
f1 (ppm)


S
S
O
OEt
O
O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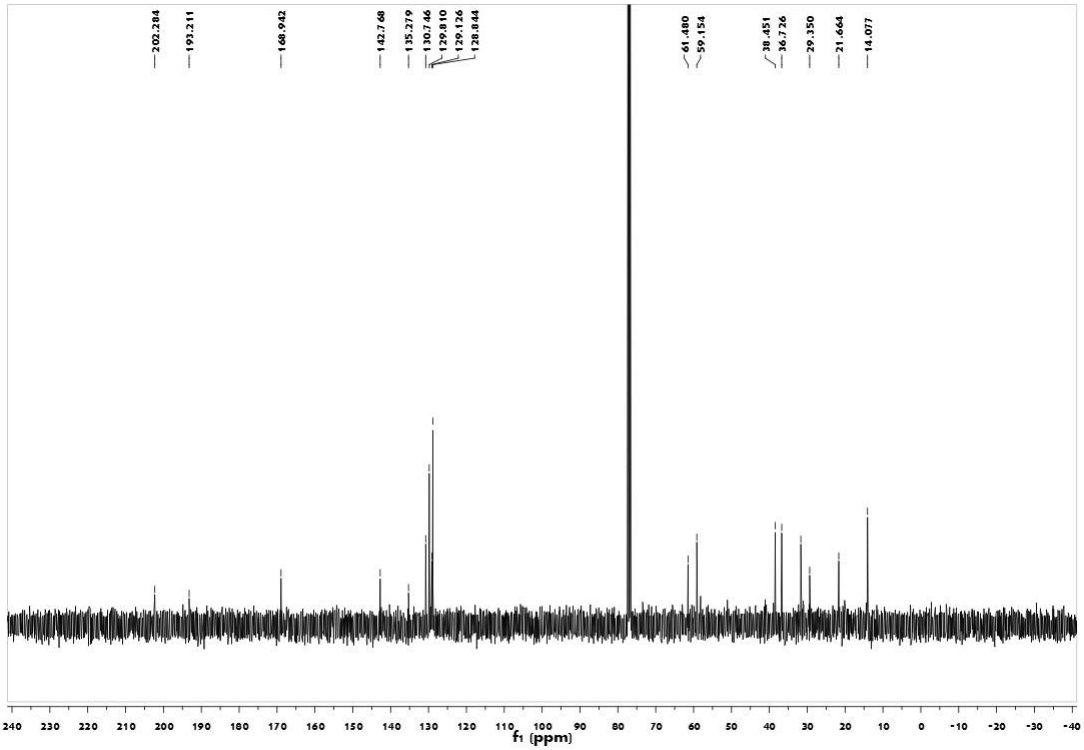
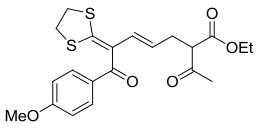
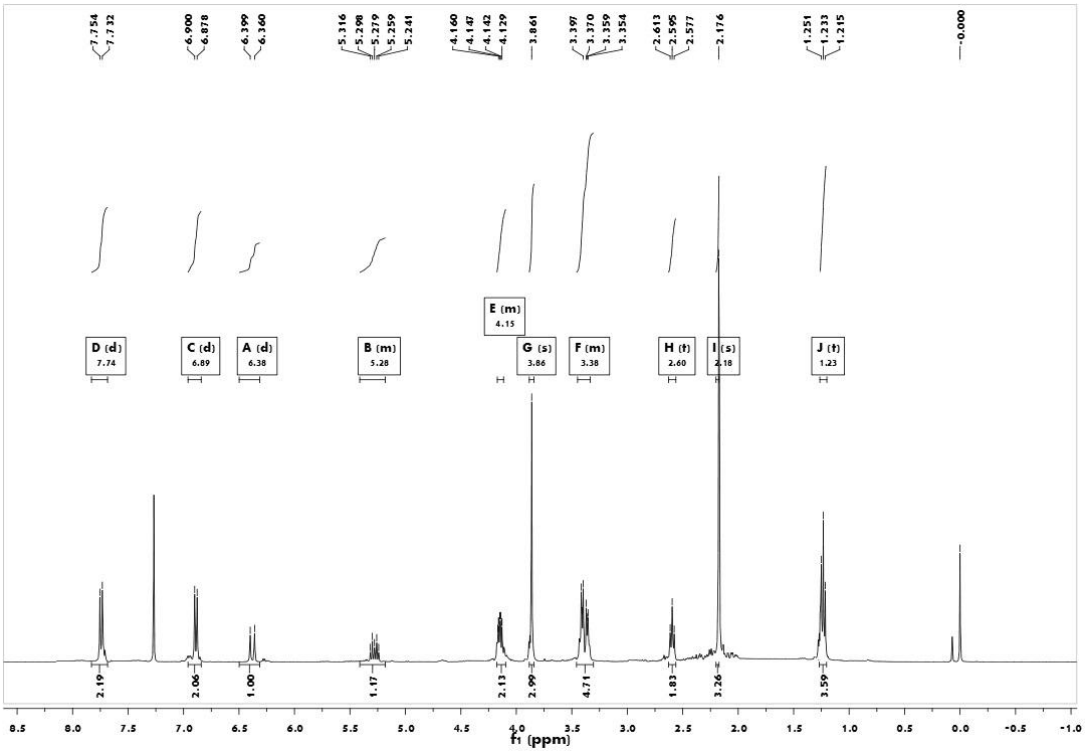
7.606
7.201
7.181
6.384
6.381
6.344
6.341
5.327
5.310
5.306
5.288
5.270
5.267
5.252
4.159
4.156
4.146
4.142
4.128
4.125
3.400
3.391
3.379
3.372
3.369
2.600
2.582
2.563
2.391
2.157
2.154
1.251
1.248
1.233
1.230
1.215
0.000
H (s) 2.39
D (d) 7.62
C (d) 7.19
A (dd) 6.36
B (ddd) 5.29
E (m) 4.14
F (m) 3.39
G (t) 2.58
I (d) 2.16
J (m) 1.24
2.24
2.09
1.00
1.11
2.20
4.81
2.21
3.24
3.19
3.60
f1 (ppm)


202.284
193.211
168.942
142.768
135.279
130.746
129.810
129.126
128.844
61.480
59.154
38.451
36.726
29.350
21.664
14.077
f1 (ppm)


S
S
O
OEt
O
O
MeO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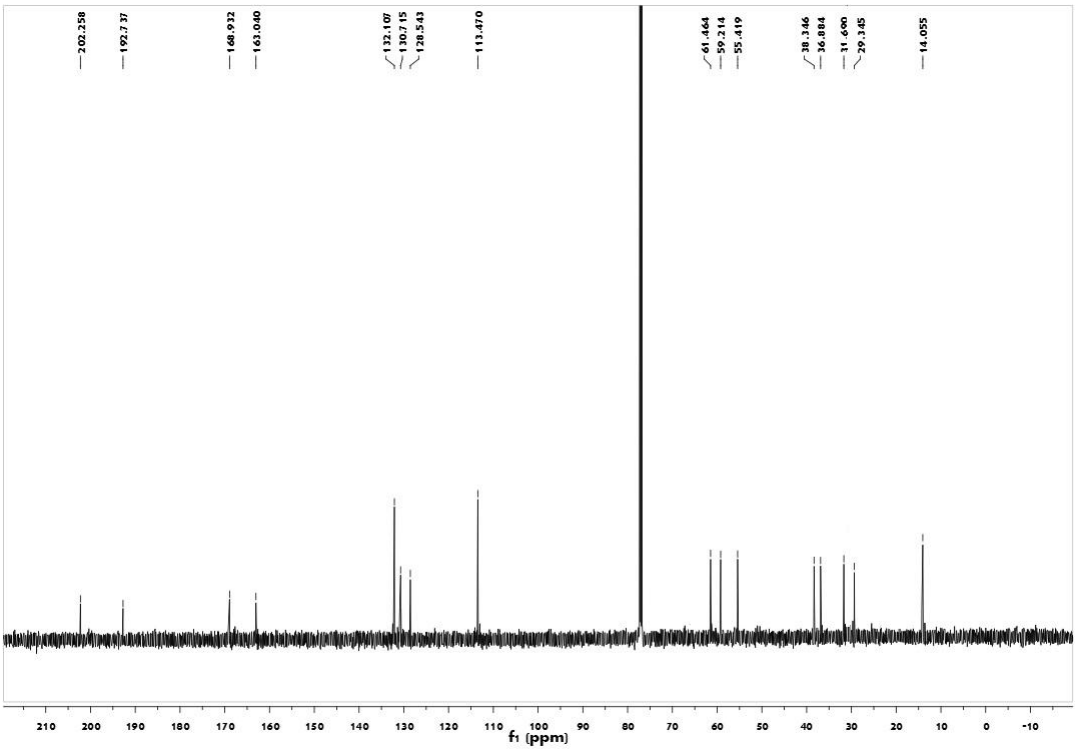
7.732
6.900
6.878
6.399
6.360
5.316
5.298
5.279
5.259
5.241
4.160
4.147
4.142
4.129
3.861
3.397
3.370
3.359
3.354
2.613
2.595
2.577
2.176
1.251
1.233
1.215
0.000
D (d) 7.74
C (d) 6.89
A (d) 6.38
B (m) 5.28
E (m) 4.15
G (s) 3.86
F (m) 3.38
H (t) 2.60
I (s) 2.18
J (t) 1.23
2.19
2.06
1.00
1.17
2.13
2.99
4.71
1.83
3.26
3.59
f1 (ppm)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168.932
163.040
132.107
130.715
128.543
113.470
61.464
59.214
55.419
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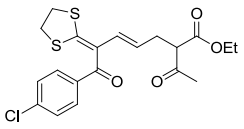
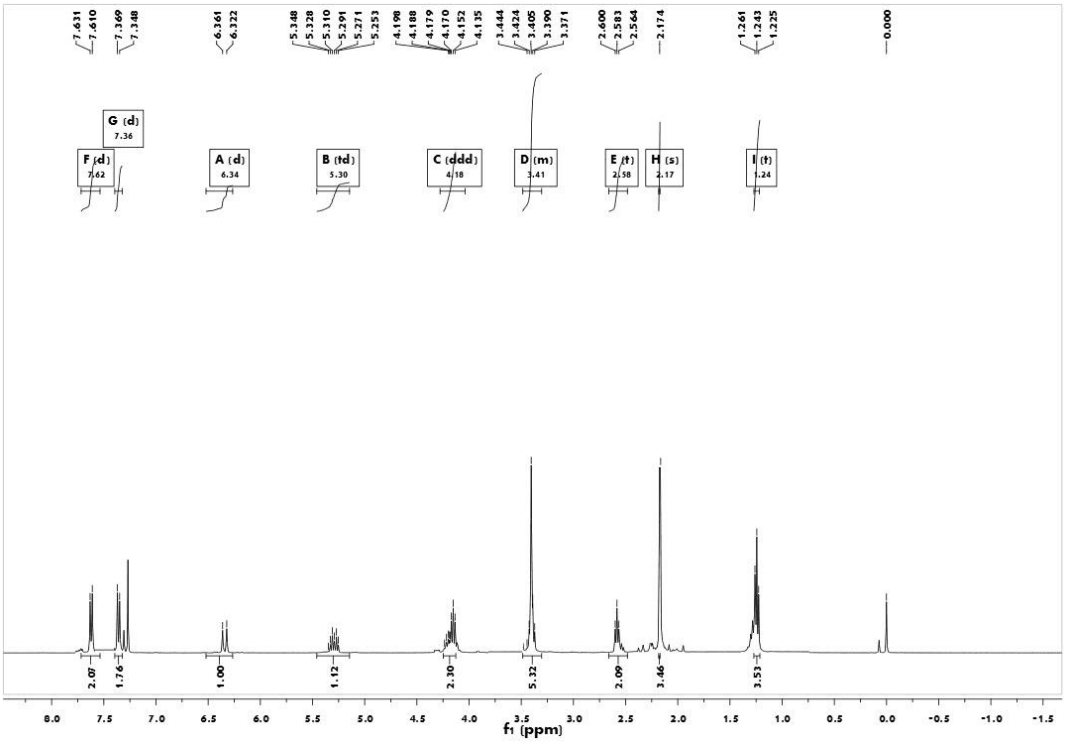
36.884
31.690
29.345
14.055
f1 (ppm)


S
S
O
OEt
O
O
Cl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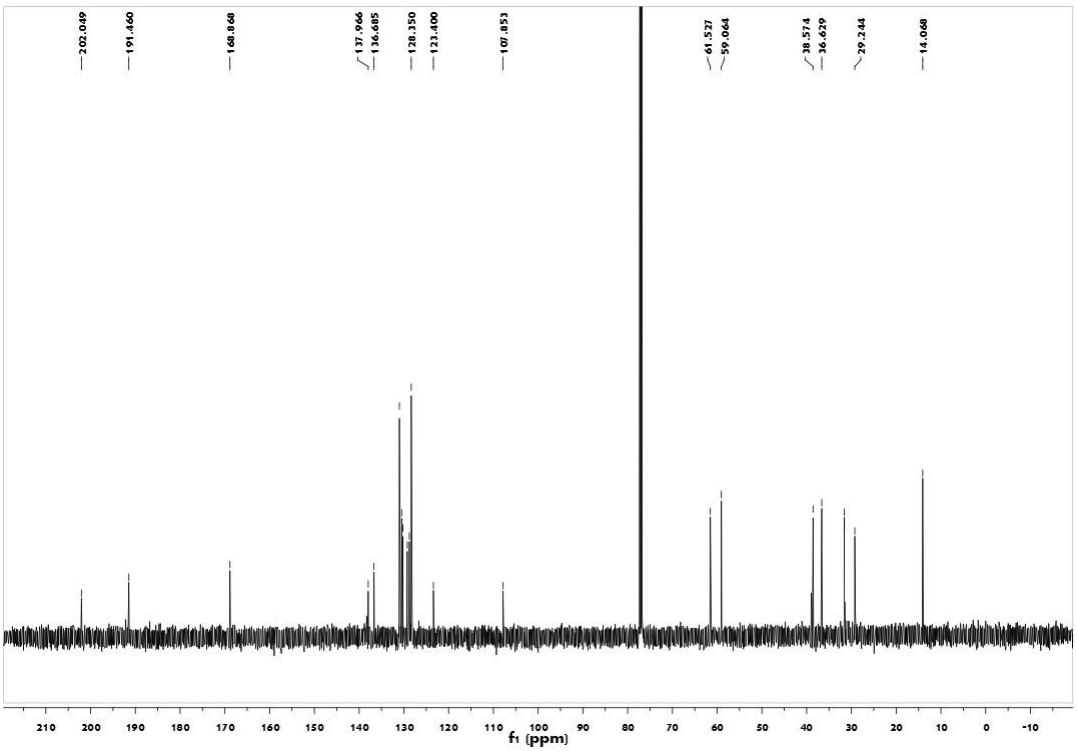
7.369
7.348
6.361
6.322
5.348
5.328
5.310
5.291
5.271
5.253
4.198
4.188
4.179
4.170
4.152
4.135
3.444
3.424
3.405
3.390
3.371
2.600
2.583
2.564
2.174
1.261
1.243
1.225
0.000
G (d) 7.36
F (d) 7.62
A (d) 6.34
B (td) 5.30
C (ddd) 4.18
D (m) 3.41
E (t) 2.58
H (s) 2.17
I (t) 1.24
2.07
1.76
1.00
1.12
2.30
5.32
2.09
3.46
3.53
f1 (ppm)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168.868
137.966
136.685
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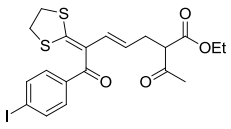
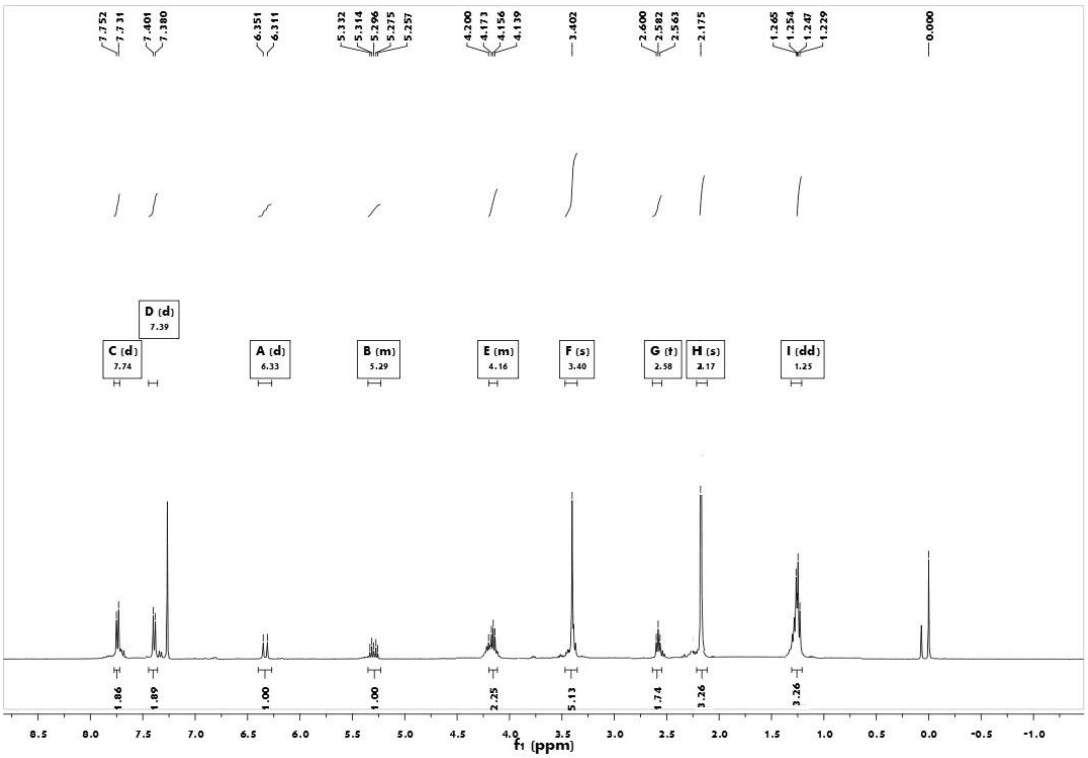
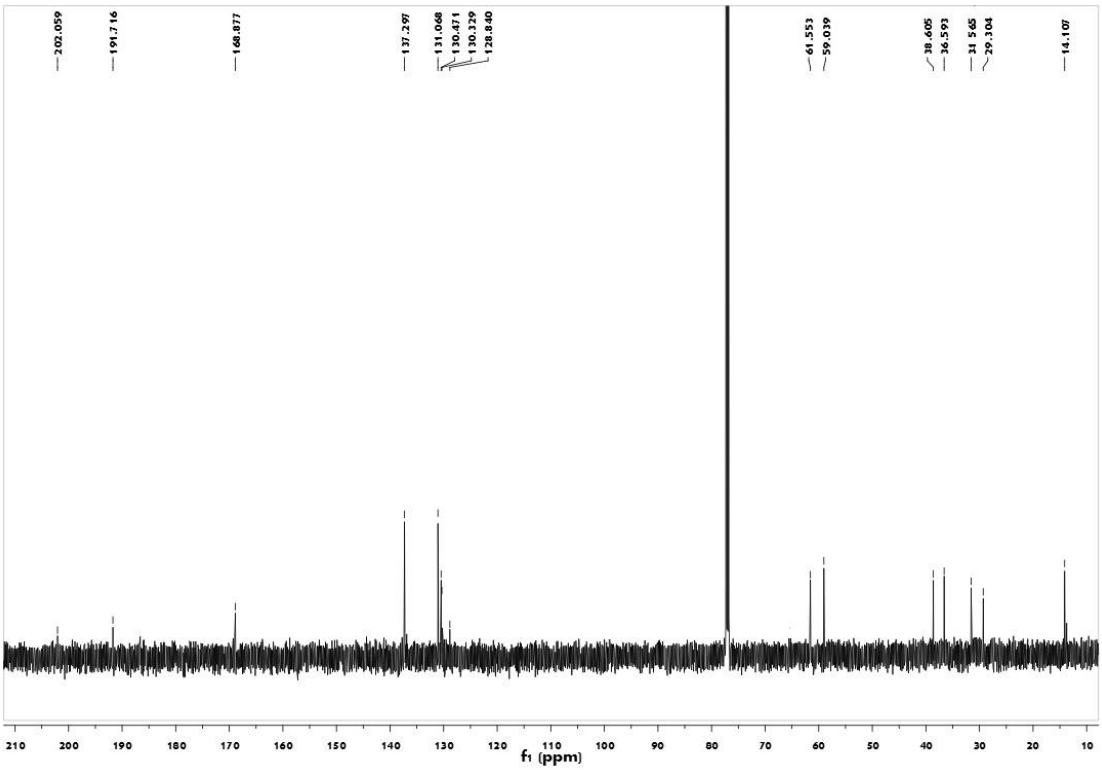
123.400
107.853
61.527
59.064
38.574
36.629
29.244
14.068
f1 (ppm)


S
S
O
OEt
O
O
I


7.752
7.731
7.401
7.380
6.351
6.311
5.332
5.314
5.296
5.275
5.257
4.200
4.173
4.156
4.139
3.402
2.600
2.582
2.563
2.175
1.265
1.254
1.247
1.229
0.000
D (d) 7.39
C (d) 7.74
A (d) 6.33
B (m) 5.29
E (m) 4.16
F (s) 3.40
G (t) 2.58
H (s) 2.17
I (dd) 1.25
1.86
1.89
1.00
1.00
2.25
5.13
1.74
3.26
3.26
f1 (ppm)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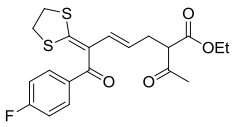
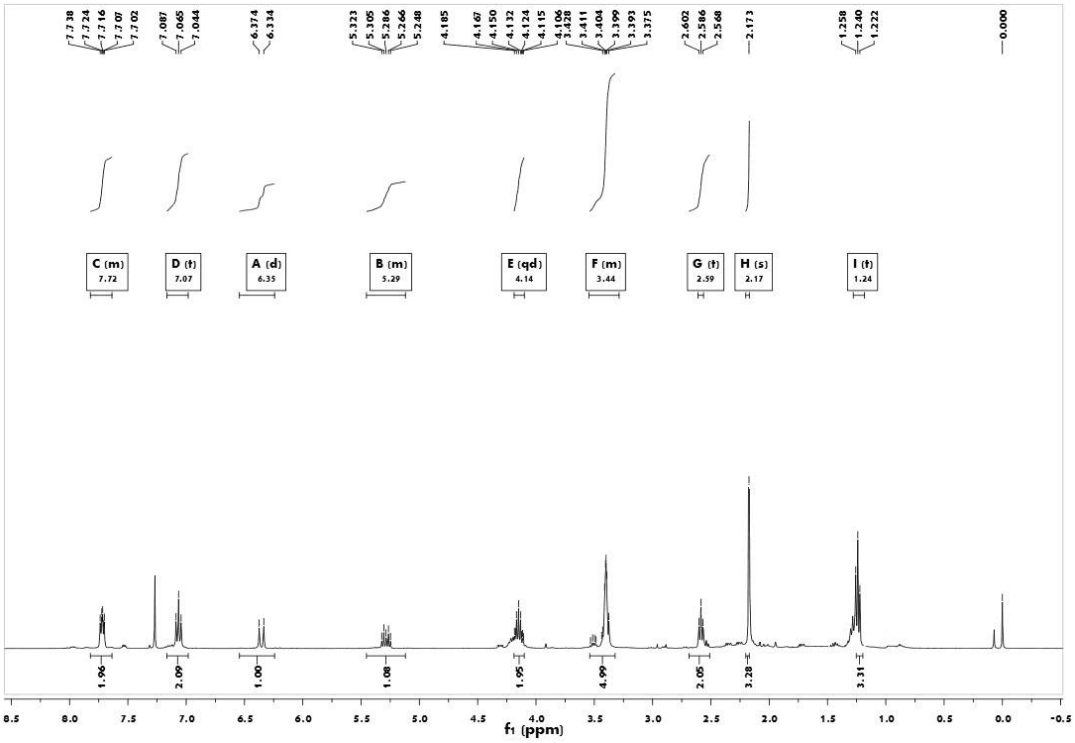
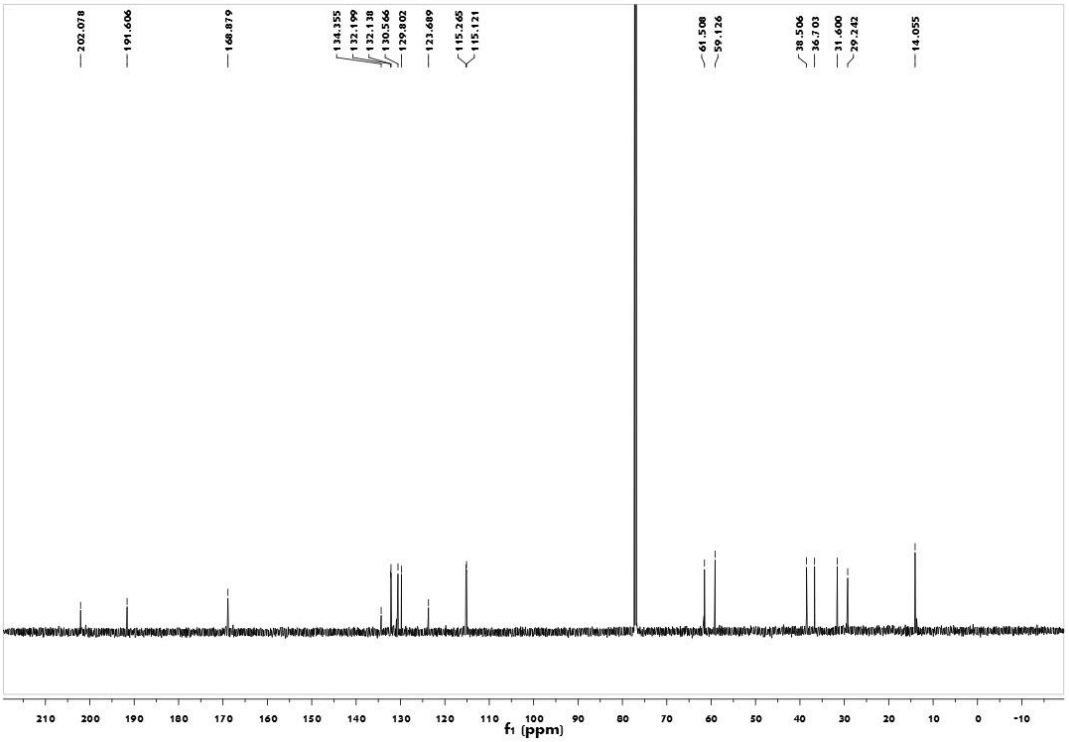
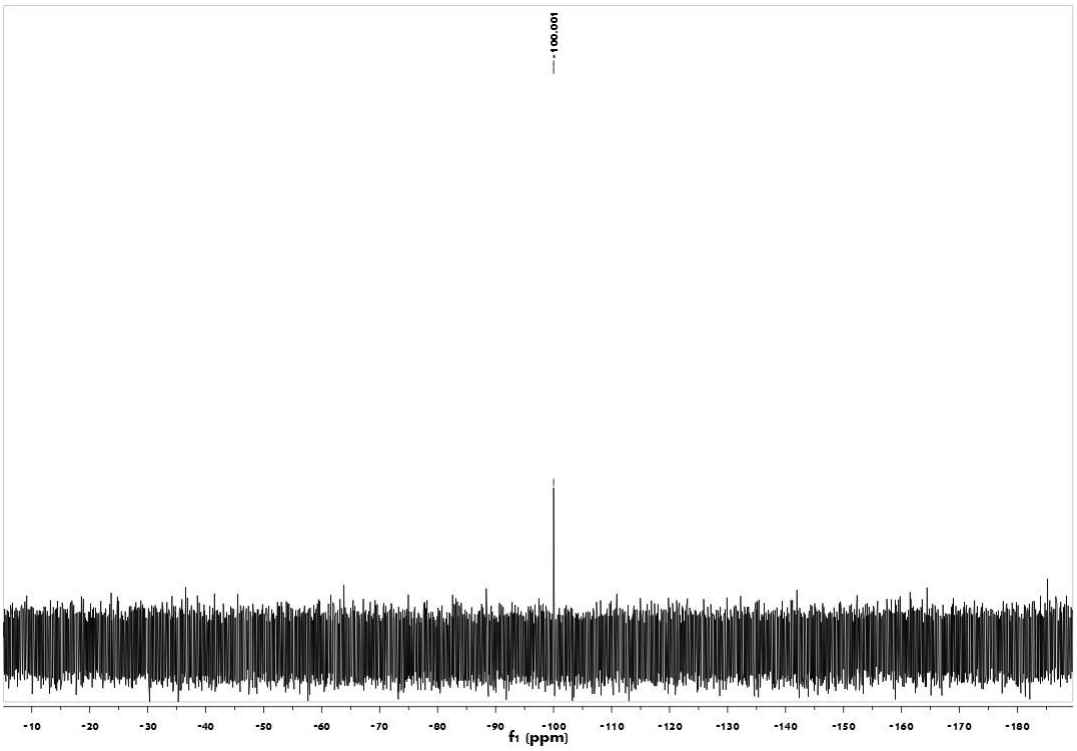
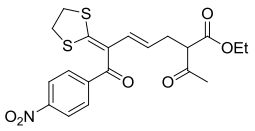
168.877
137.297
131.068
130.471
130.329
128.840
61.553
59.039
38.605
36.593
31.565
29.304
14.107
f1 (ppm)

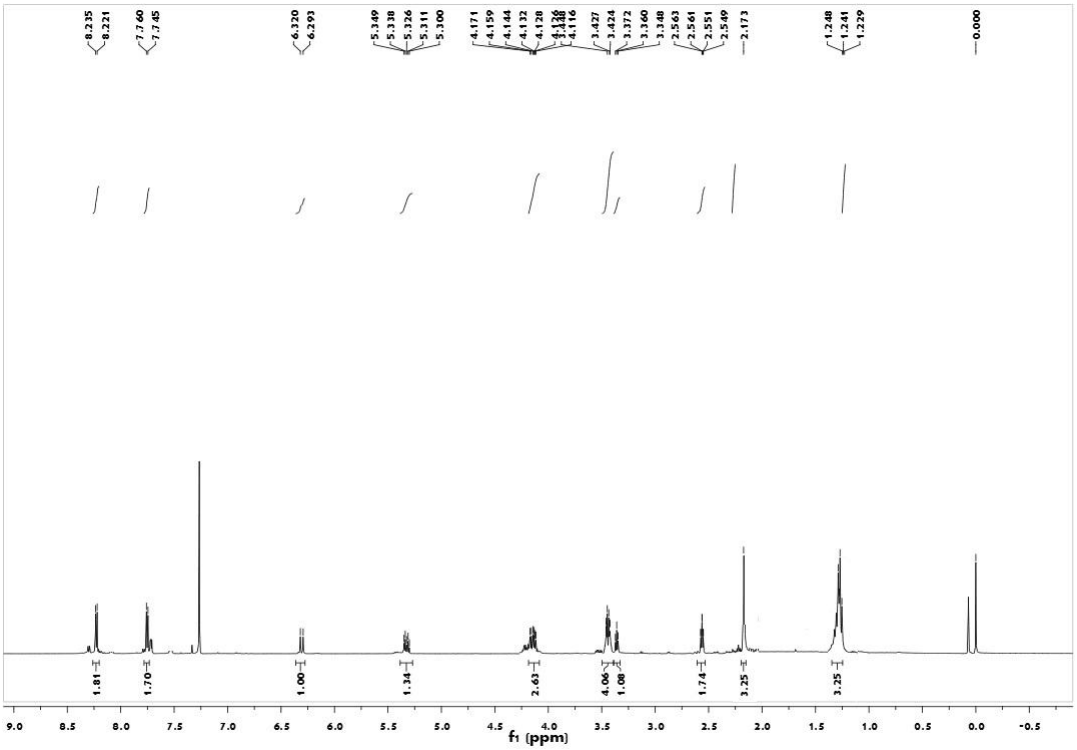

S
S
O
OEt
O
O
F


C (m) 7.72
D (t) 7.07
A (d) 6.35
B (m) 5.29
E (qd) 4.14
F (m) 3.44
G (t) 2.59
H (s) 2.17
I (t) 1.24
f1 (ppm)


f1 (ppm)


-100.001
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
f1 (ppm)


S
S
O
OEt
O
O
O_2N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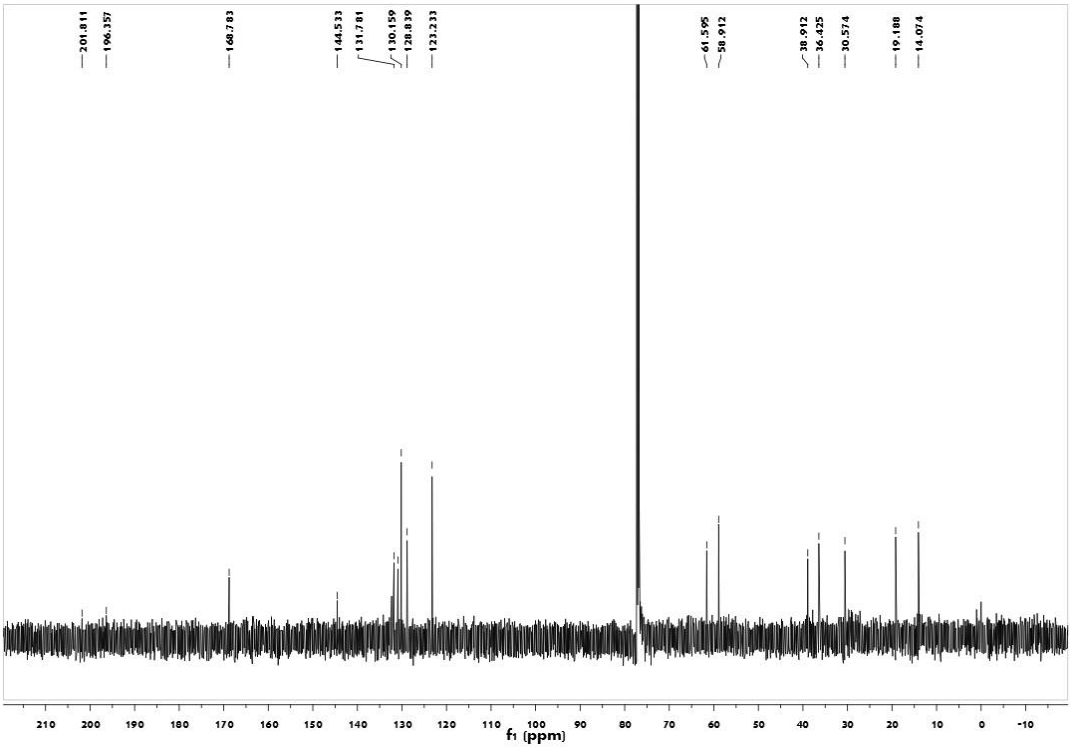
8.221
7.760
7.745
6.320
6.293
5.349
5.338
5.326
5.311
5.300
4.171
4.159
4.144
4.132
4.128
4.116
3.427
3.424
3.372
3.360
3.348
2.563
2.561
2.551
2.549
2.173
1.248
1.241
1.229
0.000
1.81
1.70
1.00
1.34
2.63
4.06
1.08
1.74
3.25
3.25
f1 (ppm)


201.811
196.357
168.783
144.533
131.781
130.159
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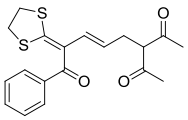
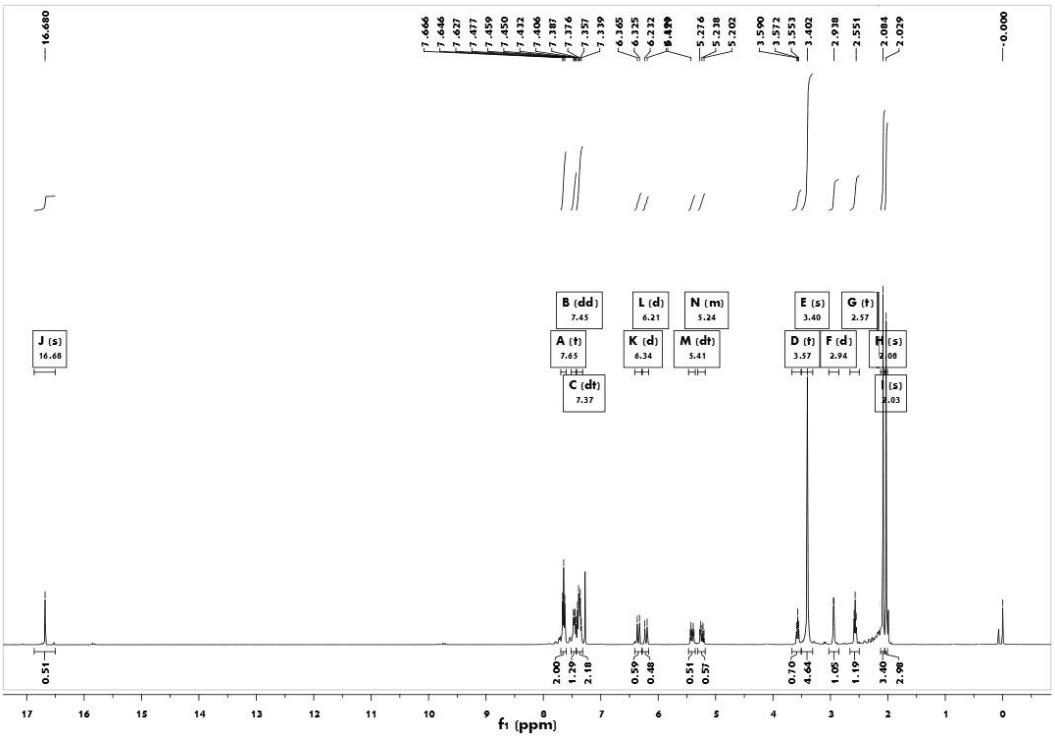
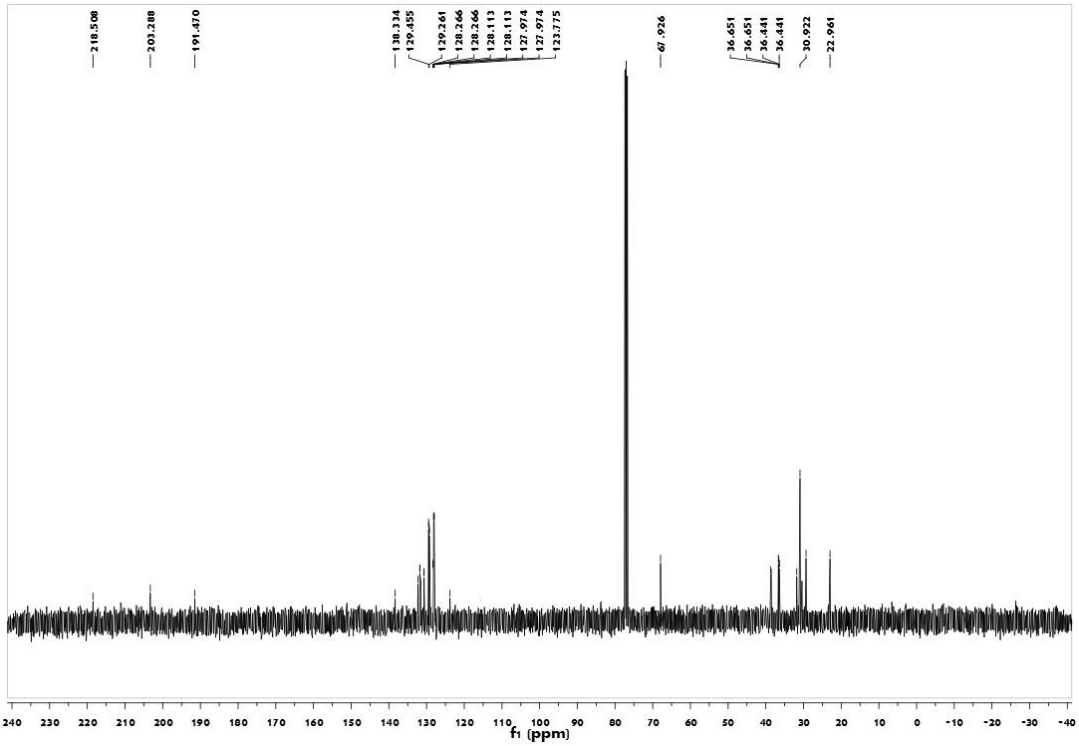
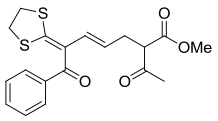
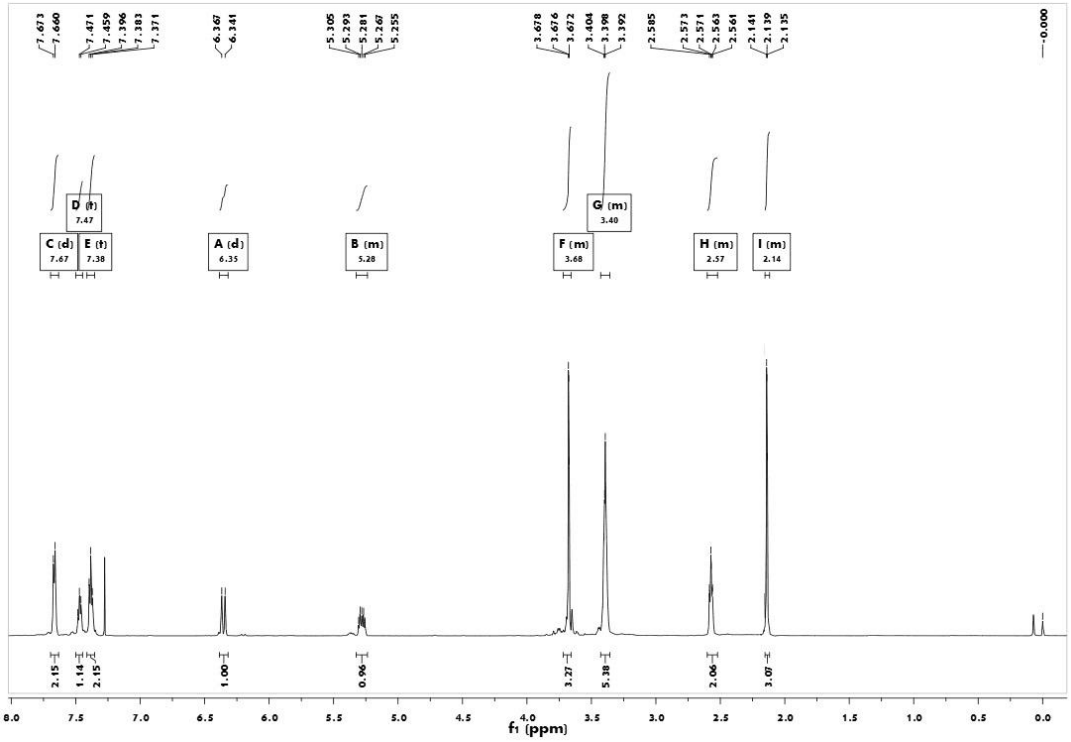
123.233
61.595
58.912
38.912
36.425
30.574
19.188
14.074
f1 (ppm)

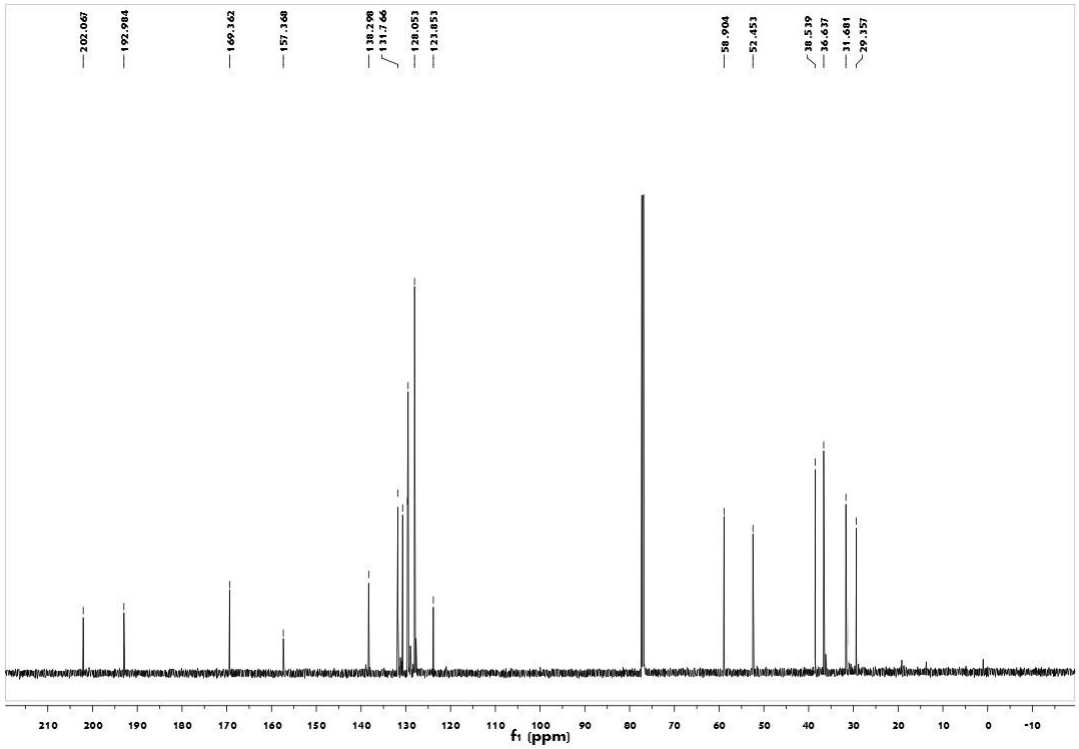


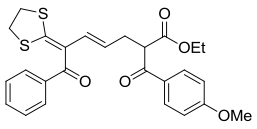

f1 (ppm)

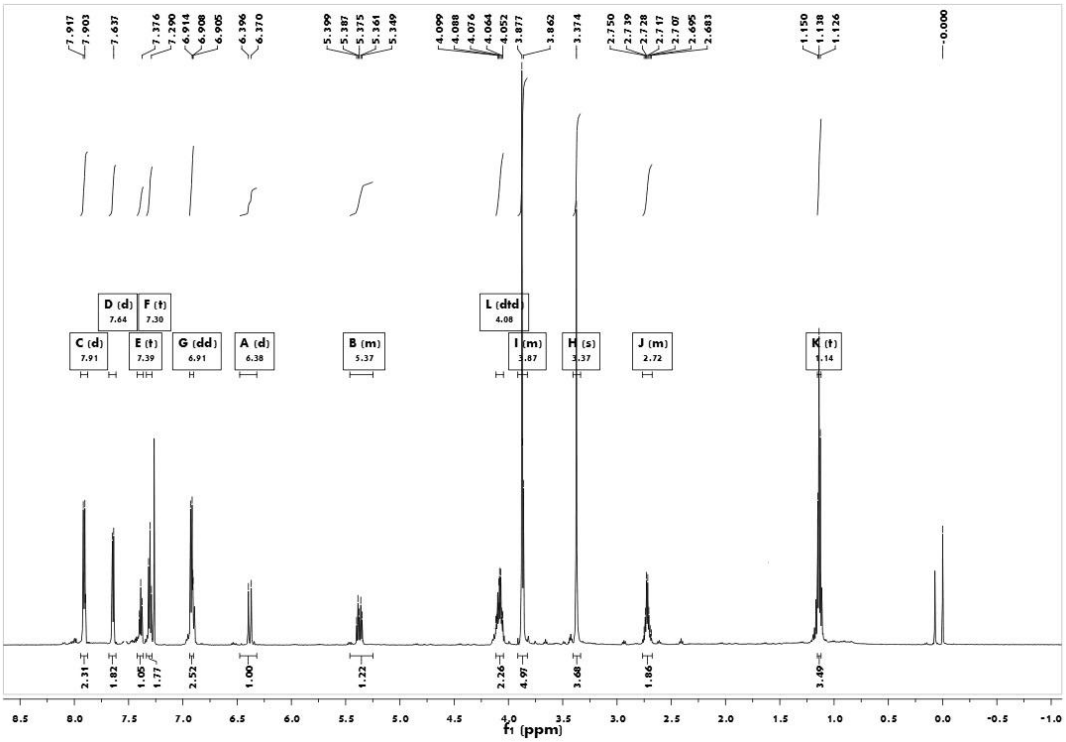

f1 (ppm)


S
S
O
OMe
O
O


D (t) 7.47
C (d) 7.67
E (t) 7.38
A (d) 6.35
B (m) 5.28
F (m) 3.68
G (m) 3.40
H (m) 2.57
I (m) 2.14
f1 (ppm)


202.067
192.984
169.362
157.368
138.298
131.766
128.053
123.853
58.904
52.453
38.539
36.637
31.681
29.357
f1 (ppm)


S
S
O
OEt
O
O
OMe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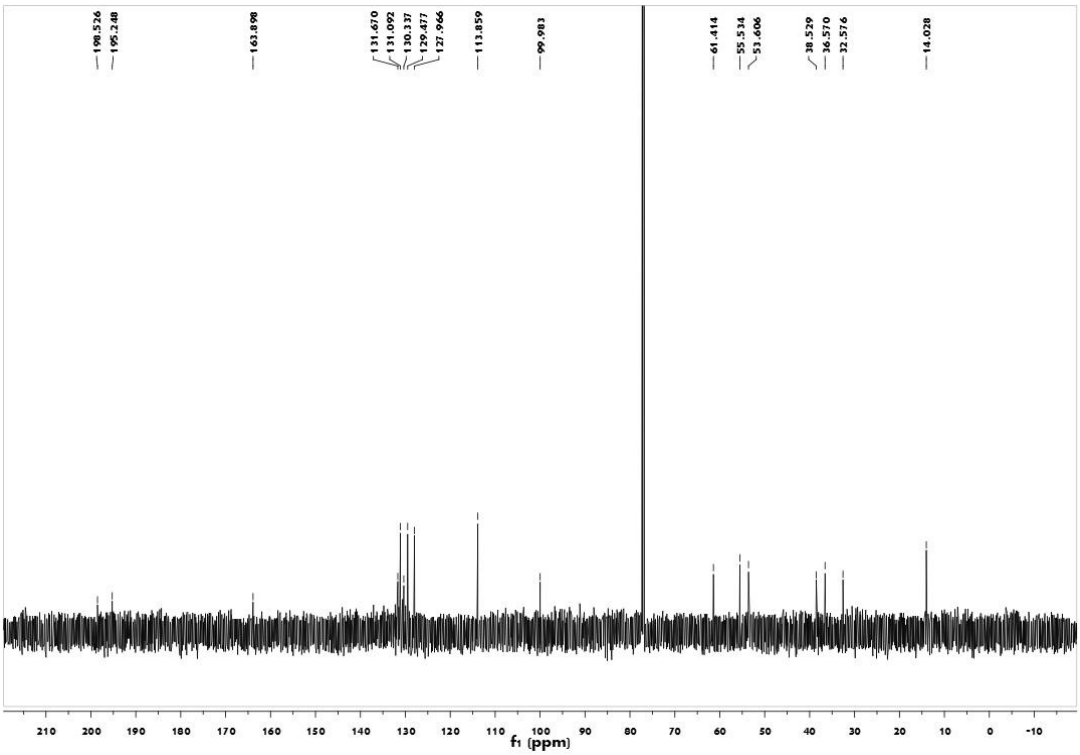
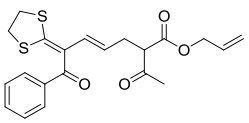
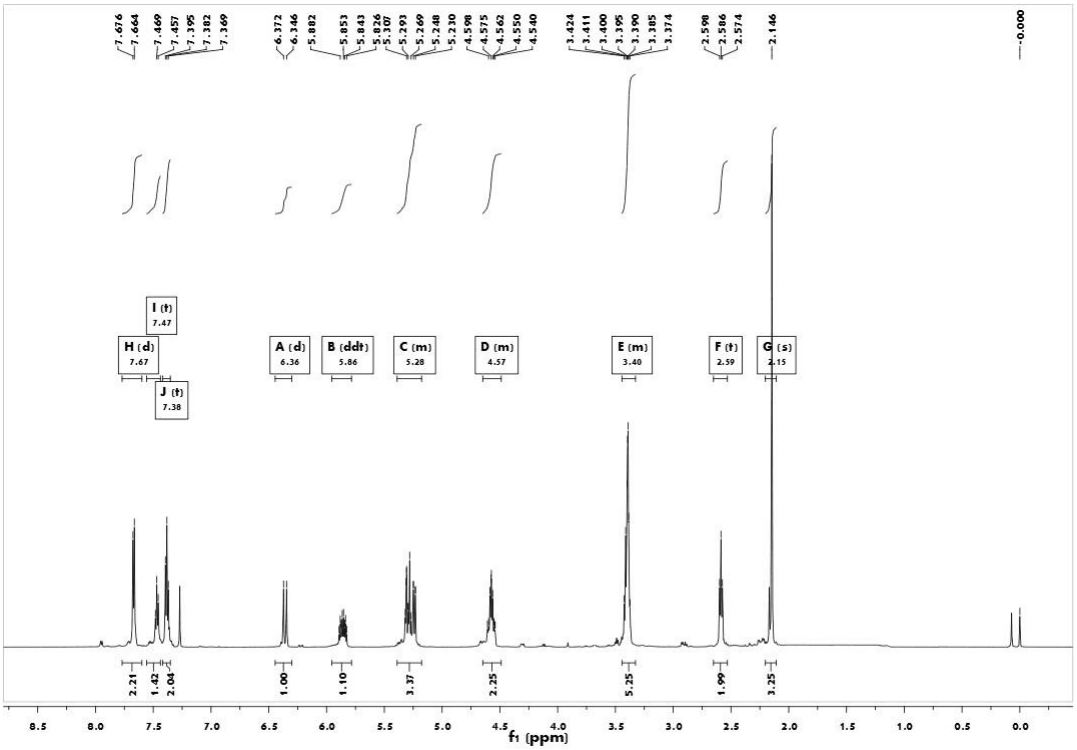
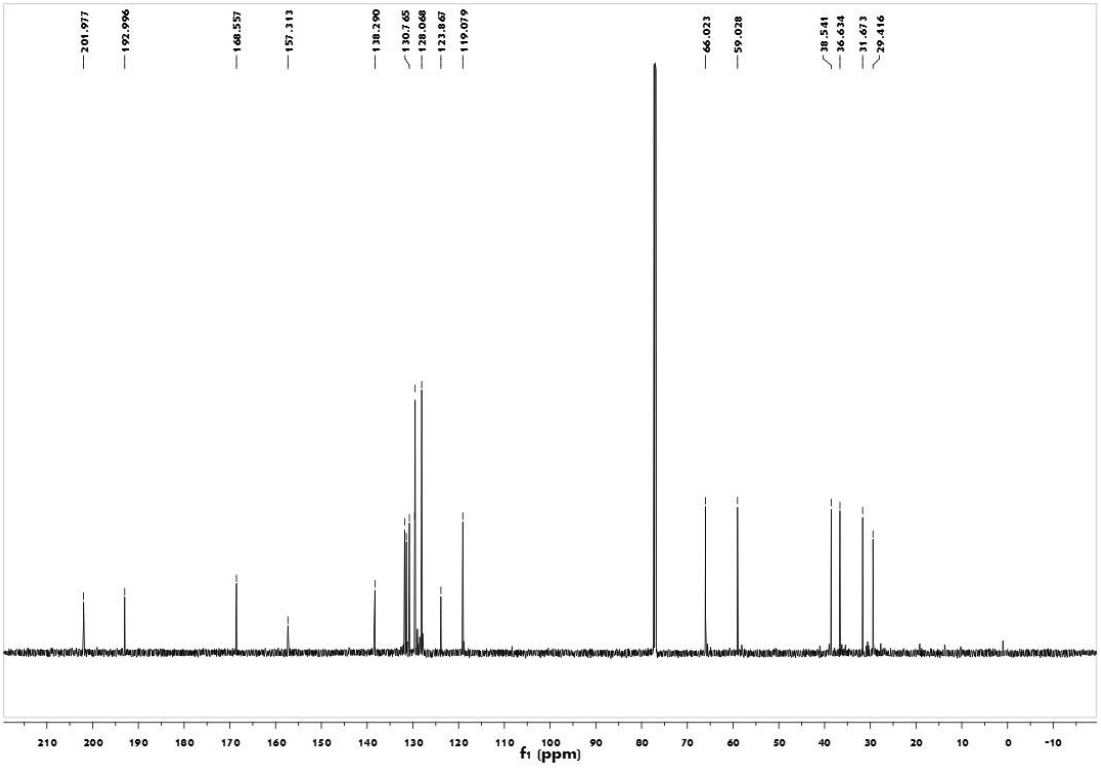
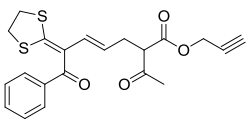
7.376
7.290
6.914
6.908
6.905
6.396
6.370
5.399
5.387
5.375
5.361
5.349
4.099
4.088
4.076
4.064
4.052
3.877
3.862
3.374
2.750
2.739
2.728
2.717
2.707
2.695
2.683
1.150
1.138
1.126
-0.000
D (d) 7.64
F (t) 7.30
C (d) 7.91
E (t) 7.39
G (dd) 6.91
A (d) 6.38
B (m) 5.37
L (dtd) 4.08
I (m) 3.87
H (s) 3.37
J (m) 2.72
K (t) 1.14
2.31
1.82
1.05
1.77
2.52
1.00
1.22
2.26
4.97
3.68
1.86
3.49
f1 (ppm)

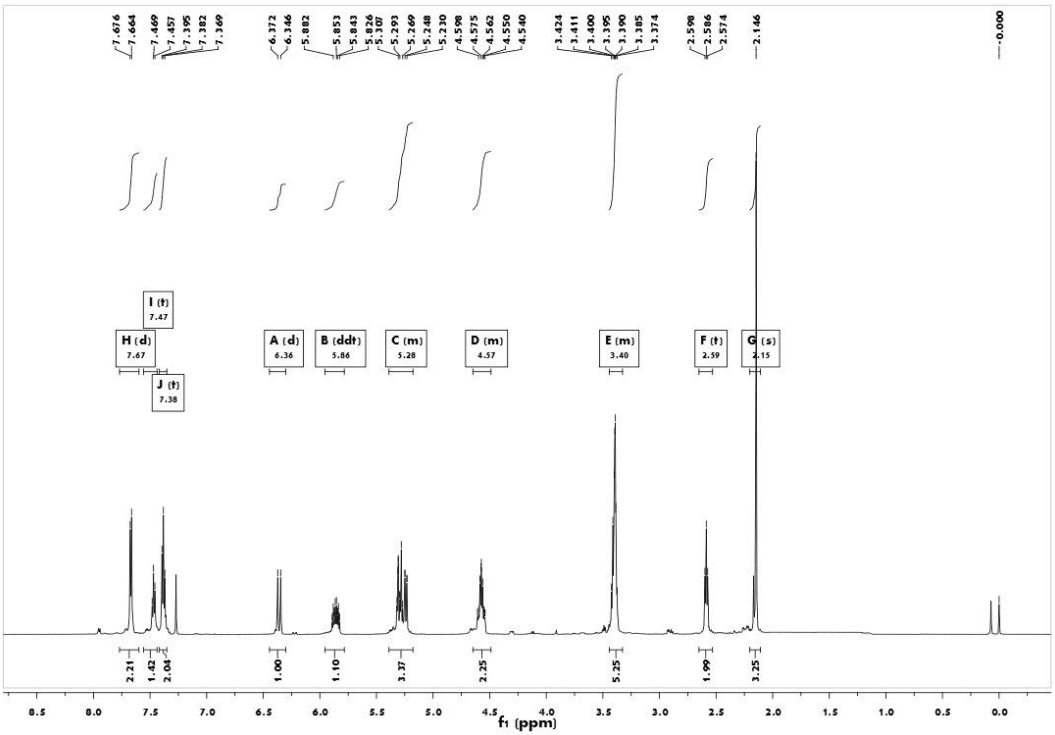

198.526
195.248
163.898
131.670
131.092
130.337
129.477
127.966
113.859
99.983
61.414
55.534
53.606
38.529
36.570
32.576
14.028
f1 (ppm)

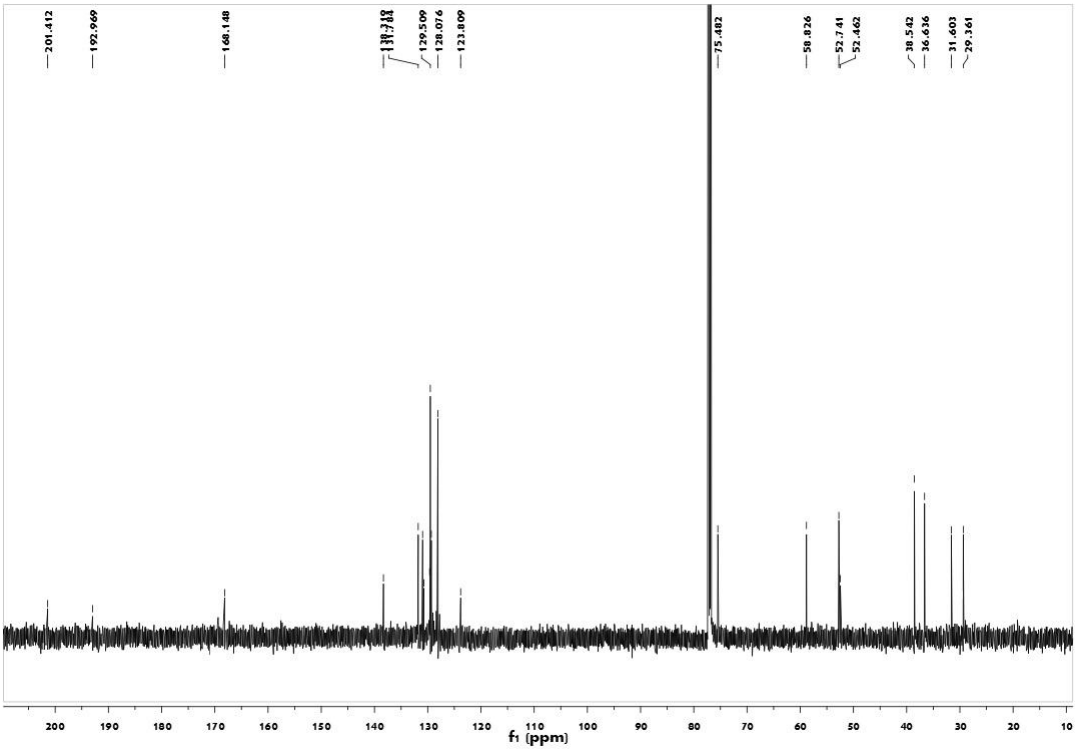


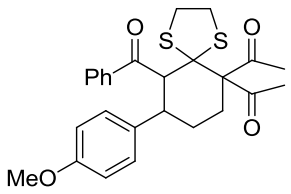

7.676
7.664
7.469
7.457
7.395
7.382
7.369
6.372
6.346
5.882
5.853
5.843
5.826
5.307
5.293
5.269
5.248
5.230
4.598
4.575
4.562
4.550
4.540
3.424
3.411
3.400
3.395
3.390
3.385
3.374
2.598
2.586
2.574
2.146
-0.000
I (t) 7.47
H (d) 7.67
J (t) 7.38
A (d) 6.36
B (ddt) 5.86
C (m) 5.28
D (m) 4.57
E (m) 3.40
F (t) 2.59
G (s) 2.15
2.21
1.42
2.04
1.00
1.10
3.37
2.25
5.25
1.99
3.25
f1 (ppm)

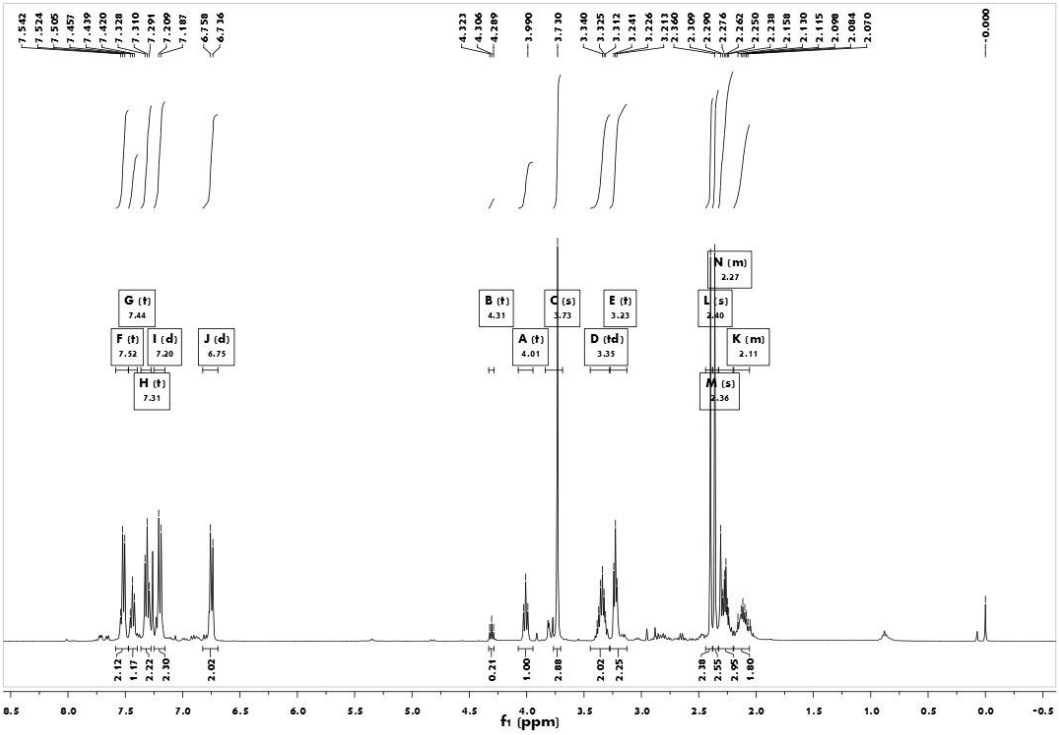

201.977
192.996
168.557
157.313
138.290
130.765
128.068
123.867
119.079
66.023
59.028
38.541
36.634
31.673
29.416
f1 (ppm)

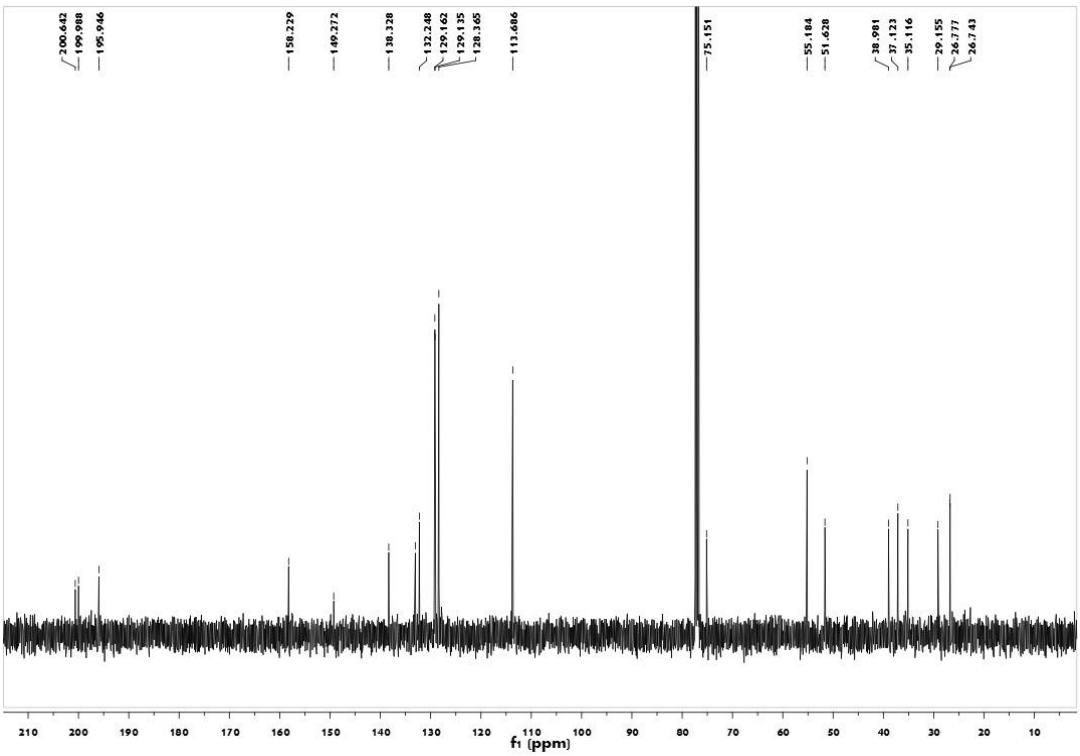



7.676
7.664
7.469
7.457
7.395
7.382
7.369
6.372
6.346
5.882
5.853
5.843
5.826
5.107
5.293
5.269
5.248
5.230
4.598
4.575
4.562
4.550
4.540
3.424
3.411
3.400
3.395
3.390
3.385
3.374
2.598
2.586
2.574
2.146
0.000
I (t) 7.47
H (d) 7.67
J (t) 7.38
A (d) 6.36
B (ddt) 5.86
C (m) 5.28
D (m) 4.57
E (m) 3.40
F (t) 2.59
G (s) 2.15
2.21
1.42
2.04
1.00
1.10
3.37
2.25
5.25
1.99
3.25
f1 (ppm)

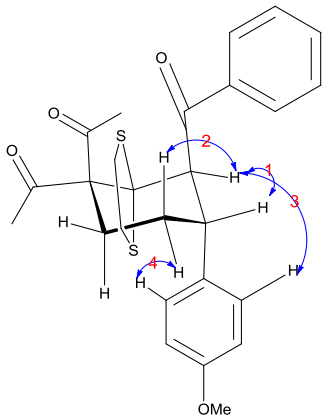

201.412
192.969
168.148
137.718
137.484
129.509
128.076
123.809
75.482
58.826
52.741
52.462
38.542
36.636
31.603
29.361
f1 (ppm)

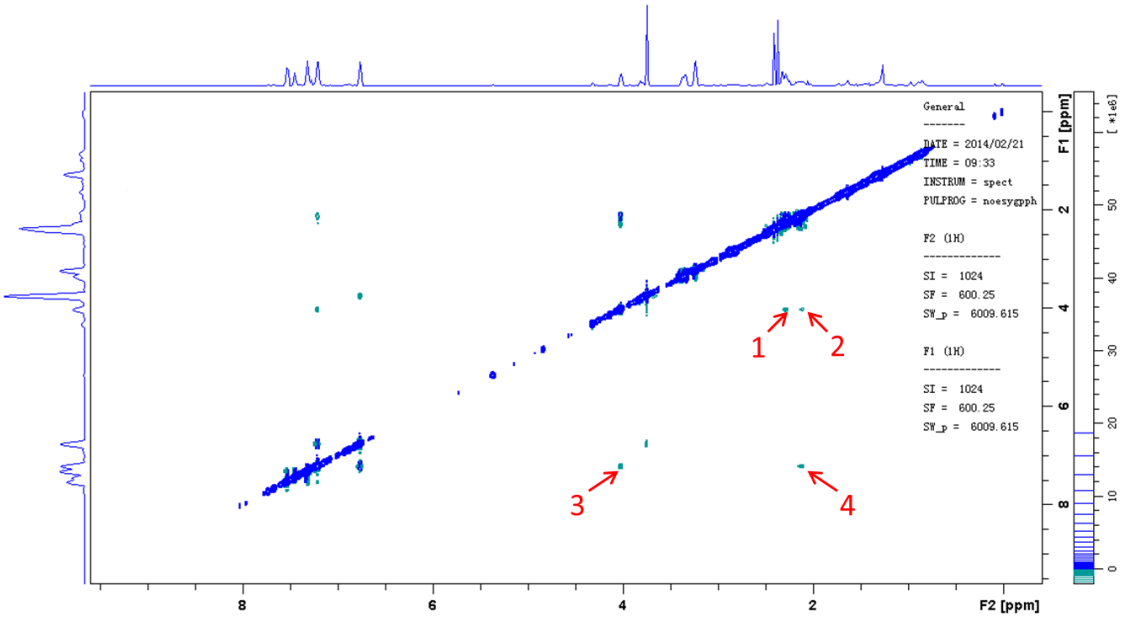

O
S
S
O
Ph
O
MeO


f1 (ppm)


f1 (ppm)

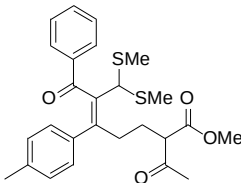
H-H NOESY of **6a**

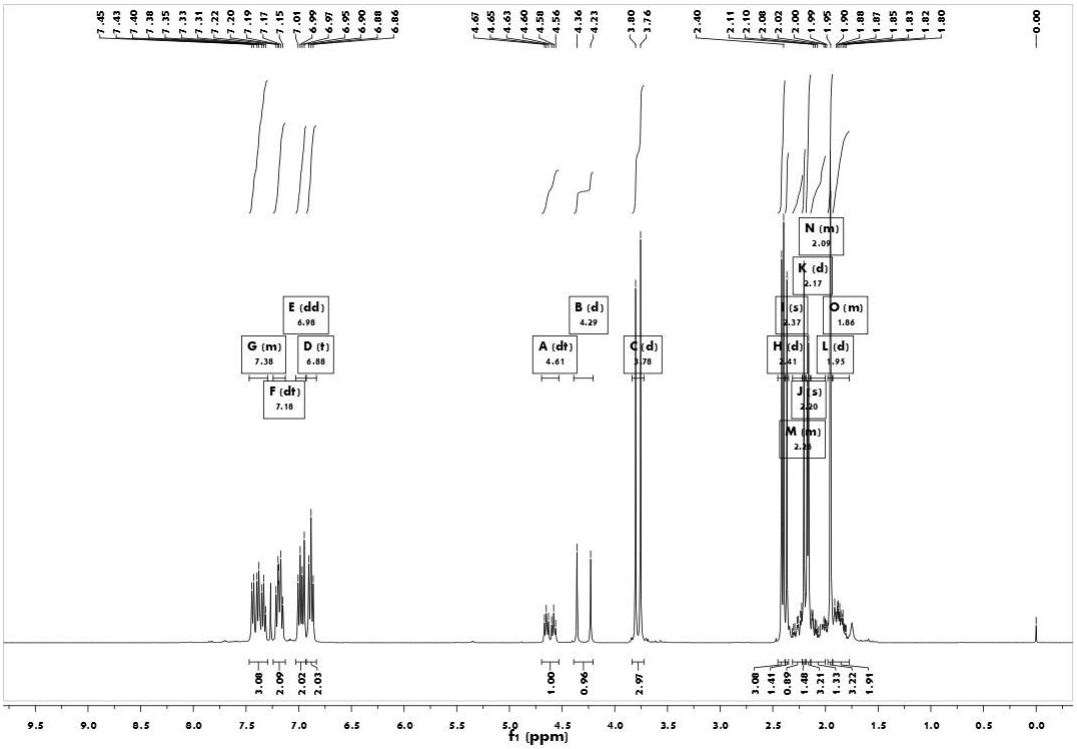


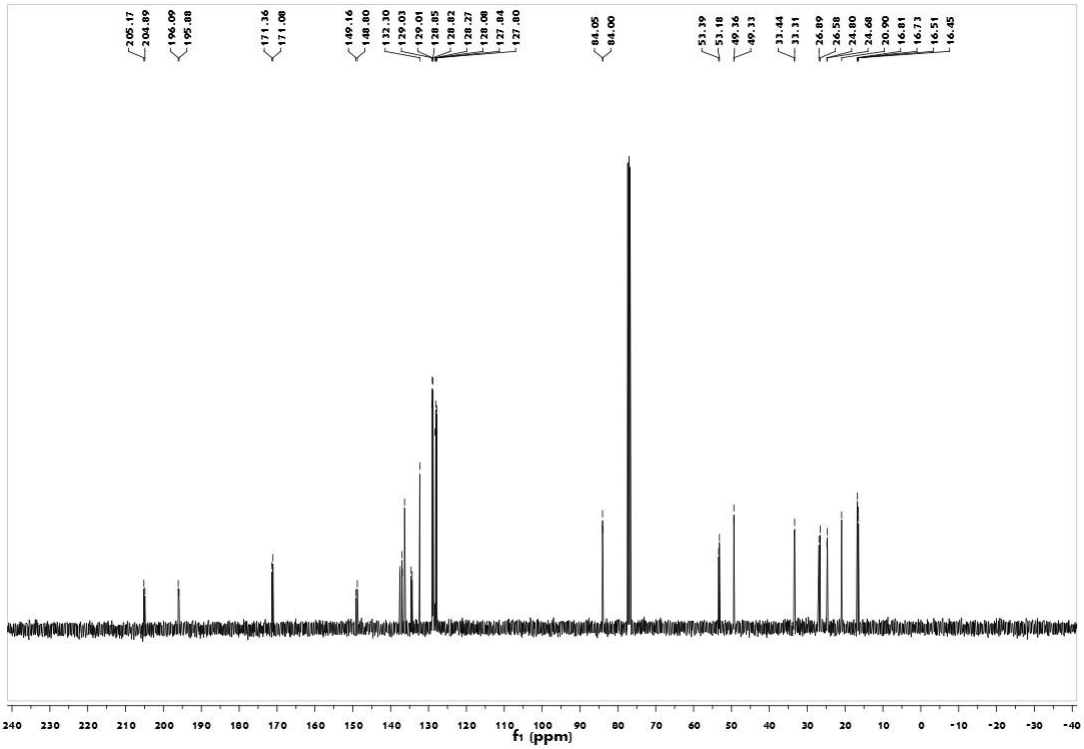


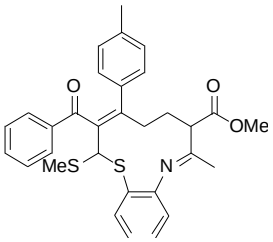
1（2.27，4.01） **3** (4.01, 7.20)

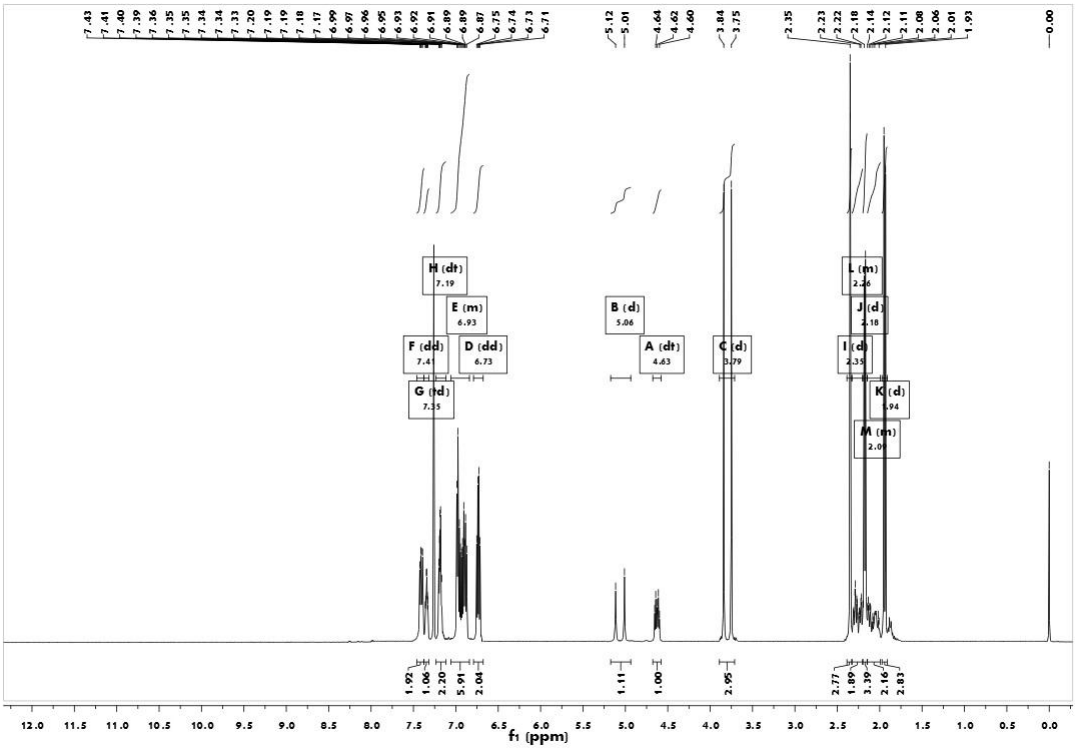
2（ 2.11，4.01） **4**（2.11，7.20）

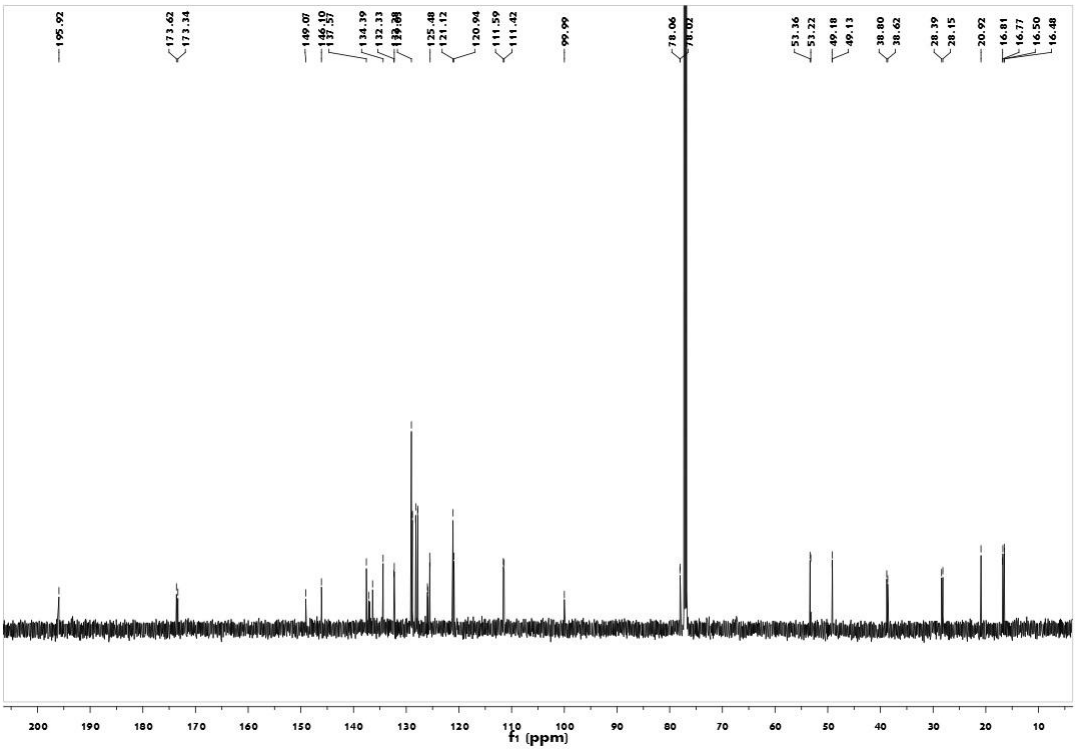

SMe
O
SMe
O
OMe
O


E (dd) 6.98
G (m) 7.38
D (t) 6.88
F (dt) 7.18
B (d) 4.29
A (dt) 4.61
C (d) 3.78
N (m) 2.09
K (d) 2.17
I (s) 2.37
O (m) 1.86
H (d) 2.41
L (d) 1.95
J (s) 2.20
M (m) 2.28
f1 (ppm)


f1 (ppm)


O
O
OMe
MeS
S
N


H (dt)
7.19
E (m)
6.93
F (dd)
7.41
D (dd)
6.73
G (td)
7.35
B (d)
5.06
A (dt)
4.63
C (d)
3.79
L (m)
2.26
J (d)
2.18
I (d)
2.35
K (d)
1.94
M (m)
2.09
f1 (ppm)


f1 (ppm)