Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

For

Tetra-n-Butylammonium Bromide (TBAB)-Initiated Carbonylation-Peroxidation of Alkenes with Aldehydes and Hydroperoxides

Yao Yao, Zhen Wang and Bin Wang*

*E-mail: wangbin@nankai.edu.cn

State Key Laboratory of Medicinal Chemical Biology, College of Pharmacy and Tianjin Key Laboratory of Molecular Drug Research, Nankai University, Haihe Education Park, 38 Tongyan Road, Tianjin 300353, People's Republic of China.

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1. Experimental Section

(i) General Remarks

^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker AVANCE AV400 (400 MHz for H and 101 MHz for C). Signal positions were recorded in ppm with the abbreviations s, d, t, q, and m denoting singlet, doublet, triplet, quartet, and multiplet respectively. All NMR chemical shifts were referenced to residual solvent peaks or to $Si(CH_3)_4$ as an internal standard. NMR Spectra recorded in $CDCl_3$ were referenced to residual $CHCl_3$ at 7.26 ppm for ^{1}H or 77.0 ppm for ^{13}C. NMR spectra recorded in DMSO-d_6 were referenced to residual DMSO at 2.49 ppm and 3.33 ppm for ^{1}H or 39.6 ppm for ^{13}C. All coupling constants *J* were quoted in Hz. Data were reported as follows: chemical shift, multiplicity, coupling constant and integration. HRMS were measured using Q-TOF LC−MS and the ESI-FTICR technique. Reactions were monitored by thin-layer chromatography (TLC) on 0.25mm silica gel glass plates coated with 60 F254. Column chromatography was performed on silica gel (200-300 mesh) using a mixture of petroleum ether (60-90°C) and ethyl acetate as eluant. Commercially available reagents were used as received without further purification.

(ii) General Procedure for the Preparation of Products **3aa-4aa**

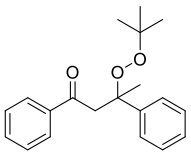
Toluene (10 mL) was added to a mixture of prop-1-en-2-ylbenzene **1a** (5 mmol, 0.66 mL), benzaldehyde **2a** (15 mmol, 1.53 mL), and TBAB (0.5 mmol, 0.16 g) under air at room temperature, then *tert*-butyl hydroperoxide (TBHP, 70% aq, 15 mmol, 2.07 mL) and acetonitrile (10 mL) were added. After the mixture was stirred at 90°C for 3 h, the residue was mixed with silica gel and concentrated. The resulting mixture was purified by silica gel column chromatography on silica gel with petroleum ether: ethyl acetate (100:1) as eluent to give the desired product 3-(*tert*-butylperoxy)-1,3-diphenylbutan-1-one **3aa** (1.23 g, 79%).

(iii) One-pot procedure for synthesis of epoxide **5**

Toluene (1.0 mL) was added to a mixture of prop-1-en-2-ylbenzene **1a** (0.5 mmol, 65.7 μL), benzaldehyde **2a** (1.5 mmol, 153.2 μL), and TBAB (0.05 mmol, 16.1 mg) under air at room temperature, then *tert*-butyl hydroperoxide (TBHP, 70% aq, 1.5 mmol, 206.9 μL) and acetonitrile (1.0 mL) were added. After the mixture was stirred at 90°C for 3 h, then K_2CO_3 (0.5 mmol, 69.1 mg) was directly added to the reaction solution without cooling. After the resulting mixture was stirred at 90°C for 2 h, the residue was mixed with silica gel and concentrated. The resulting mixture was purified by silica gel column chromatography on silica gel with petroleum ether: ethyl acetate (30:1) as eluent to give the desired product (3-methyl-3-phenyloxiran-2-yl)(phenyl)methanone **5** (103.7 mg, 87%).

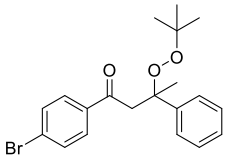
2. The Characterization of Products

3-(*tert*-butylperoxy)-1,3-diphenylbutan-1-one (3aa)



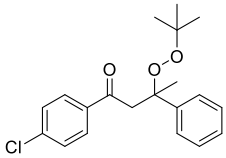
Colorless oil (133.7 mg, 86%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, J = 7.7 Hz, 2H), 7.53 – 7.47 (m, 3H), 7.40 (t, J = 7.3 Hz, 2H), 7.32 (t, J = 7.3 Hz, 2H), 7.23 (t, J = 6.9 Hz, 1H), 3.66 (d, J = 14.4 Hz, 1H), 3.32 (d, J = 14.4 Hz, 1H), 1.84 (s, 3H), 1.09 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.88, 144.56, 138.15, 132.78, 128.61, 128.61, 128.28, 128.01, 127.17, 125.81, 83.07, 79.38, 48.31, 26.55, 23.64. HRMS(ESI) calcd for $C_{20}H_{24}O_3(M+Na)^+$: 335.1618; found: 335.1624.

1-(4-bromophenyl)-3-(*tert*-butylperoxy)-3-phenylbutan-1-one (3ab)



Colorless oil (156.5 mg, 80%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, J = 8.4 Hz, 2H), 7.54 (d, J = 8.4 Hz, 2H), 7.45 (d, J = 7.5 Hz, 2H), 7.32 (t, J = 7.5 Hz, 2H), 7.24 (t, J = 7.0 Hz, 1H), 3.59 (d, J = 14.3 Hz, 1H), 3.28 (d, J = 14.3 Hz, 1H), 1.83 (s, 3H), 1.09 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.88, 144.33, 136.90, 131.50, 130.18, 128.04, 127.88, 127.23, 125.68, 83.08, 79.49, 48.25, 26.55, 23.77. HRMS(ESI) calcd for $C_{20}H_{23}BrO_3(M+Na)^+$: 413.0723; found: 413.0726.

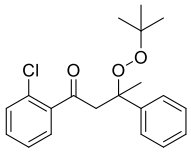
3-(*tert*-butylperoxy)-1-(4-chlorophenyl)-3-phenylbutan-1-one (3ac)



Colorless oil (128.3 mg, 74%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, J = 8.3 Hz, 2H), 7.46 (d, J = 7.9 Hz, 2H), 7.37 (d, J = 8.4 Hz, 2H), 7.32 (t, J = 7.5 Hz, 2H), 7.24 (t, J = 7.2 Hz, 1H), 3.60 (d, J = 14.3 Hz, 1H), 3.28 (d, J = 14.3 Hz, 1H), 1.83 (s, 3H), 1.09 (s,

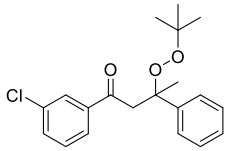
9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.68, 144.35, 139.14, 136.50, 130.06, 128.50, 128.03, 127.22, 125.68, 83.09, 79.48, 48.29, 26.54, 23.75. HRMS(ESI) calcd for $C_{20}H_{23}ClO_3(M+Na)^+$: 369.1228; found: 369.1225.

3-(*tert*-butylperoxy)-1-(2-chlorophenyl)-3-phenylbutan-1-one (3ad)



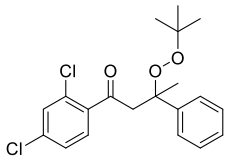
Colorless oil (126.7 mg，55%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, J = 8.8 Hz, 2H), 7.32 – 7.25 (m, 4H), 7.24 – 7.18 (m, 3H), 3.64 (d, J = 14.7 Hz, 1H), 3.54 (d, J = 14.7 Hz, 1H), 1.83 (s, 3H), 1.12 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.66, 143.65, 140.42, 131.22, 130.70, 130.22, 129.23, 127.91, 127.23, 126.52, 125.90, 82.90, 79.33, 52.38, 26.57, 24.08. HRMS(ESI) calcd for $C_{20}H_{23}ClO_3(M+NH_4)^+$: 364.1674; found: 364.1670.

3-(*tert*-butylperoxy)-1-(3-chlorophenyl)-3-phenylbutan-1-one (3ae)



Colorless oil (129.7 mg，75%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, J = 1.7 Hz, 1H), 7.79 (d, J = 7.8 Hz, 1H), 7.51 – 7.43 (m, 3H), 7.36 – 7.30 (m, 3H), 7.28 – 7.23 (m, 1H), 3.60 (d, J = 14.2 Hz, 1H), 3.29 (d, J = 14.2 Hz, 1H), 1.82 (s, 3H), 1.10 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.67, 144.26, 139.70, 134.51, 132.59, 129.54, 128.86, 128.03, 127.25, 126.65, 125.66, 83.06, 79.53, 48.41, 26.51, 23.83. HRMS(ESI) calcd for $C_{20}H_{23}ClO_3(M+Na)^+$: 369.1228; found: 369.1231.

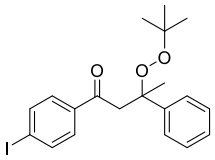
3-(*tert*-butylperoxy)-1-(2,4-dichlorophenyl)-3-phenylbutan-1-one (3af)



Colorless oil (126.7 mg，55%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.37 (m, 2H), 7.33 (d, J = 1.6 Hz, 1H), 7.30 – 7.14 (m, 5H), 3.59 (d, J = 14.6 Hz, 1H), 3.52 (d, J = 14.6 Hz,

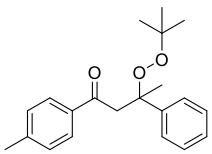
1H), 1.81 (s, 3H), 1.13 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.52, 143.44, 138.64, 136.72, 131.80, 130.38, 130.03, 127.98, 127.31, 126.86, 125.80, 82.93, 79.45,52.30, 26.57, 24.31. HRMS(ESI) calcd for $C_{20}H_{22}Cl_2O_3(M+Na)^+$: 403.0838; found: 403.0835.

3-(*tert*-butylperoxy)-1-(4-iodophenyl)-3-phenylbutan-1-one (3ag)



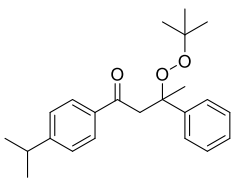
Colorless oil (109.2 mg，50%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 8.4 Hz, 2H), 7.63 (d, J = 8.4 Hz, 2H), 7.45 (d, J = 7.5 Hz, 2H), 7.32 (t, J = 7.5 Hz, 2H), 7.28 – 7.23 (m, 1H), 3.59 (d, J = 14.3 Hz, 1H), 3.27 (d, J = 14.3 Hz, 1H), 1.82 (s, 3H), 1.09 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.21, 144.32, 137.53, 137.42, 130.08, 128.05, 127.24, 125.68, 100.70, 83.07, 79.50, 48.19, 26.56, 23.77. HRMS(ESI) calcd for $C_{20}H_{23}IO_3(M+Na)^+$: 461.0584; found: 461.0576.

3-(*tert*-butylperoxy)-3-phenyl-1-(p-tolyl)butan-1-one (3ah)



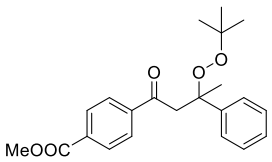
Colorless oil (136.1 mg, 83%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, J = 8.2 Hz, 2H), 7.48 (d, J = 7.4 Hz, 2H), 7.30 (t, J = 7.6 Hz, 2H), 7.20 (dd, J = 16.9, 7.7 Hz, 3H), 3.62 (d, J = 14.5 Hz, 1H), 3.29 (d, J = 14.5 Hz, 1H), 2.36 (s, 3H), 1.84 (s, 3H), 1.10 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.39, 144.68, 143.45, 135.78, 128.96, 128.75, 127.97, 127.11, 125.85, 83.09, 79.33, 48.19, 26.59, 23.65, 21.63. HRMS(ESI) calcd for $C_{21}H_{26}O_3$ $(M+Na)^+$: 349.1774; found: 349.1767.

3-(*tert*-butylperoxy)-1-(4-isopropylphenyl)-3-phenylbutan-1-one (3ai)



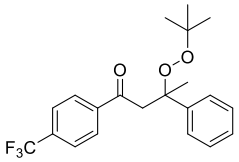
Colorless oil (134.5 mg, 76%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, J = 7.9 Hz, 2H), 7.48 (d, J = 7.8 Hz, 2H), 7.31 (t, J = 7.5 Hz, 2H), 7.25 (d, J = 13.2 Hz, 3H), 3.64 (d, J = 14.5 Hz, 1H), 3.30 (d, J = 14.5 Hz, 1H), 2.99 – 2.89 (m, 1H), 1.83 (s, 3H), 1.25 (d, J = 6.8 Hz, 6H), 1.09 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.52, 154.19, 144.60, 136.12, 128.82, 127.93, 127.07, 126.30, 125.84, 83.01, 79.29, 48.33, 34.21, 26.51, 23.70, 23.51. HRMS(ESI) calcd for $C_{23}H_{30}O_3(M+Na)^+$: 377.2087; found: 377.2081.

4-(3-(*tert*-butylperoxy)-3-phenylbutanoyl)phenyl acetate (3aj)



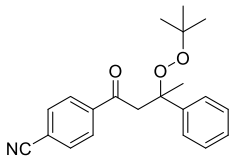
Colorless oil (59.4 mg，32%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, J = 8.3 Hz, 2H), 7.97 (d, J = 8.3 Hz, 2H), 7.46 (d, J = 7.6 Hz, 2H), 7.33 (t, J = 7.6 Hz, 2H), 7.25 (d, J = 5.7 Hz, 1H), 3.95 (s, 3H), 3.67 (d, J = 14.3 Hz, 1H), 3.33 (d, J = 14.3 Hz, 1H), 1.84 (s, 3H), 1.07 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.52, 166.35, 144.28, 141.38, 133.42, 129.47, 128.48, 128.05, 127.26, 125.65, 83.12, 79.52, 52.44, 48.55, 26.51, 23.81. HRMS(ESI) calcd for $C_{22}H_{26}O_5(M+Na)^+$: 393.1672; found: 393.1669.

3-(*tert*-butylperoxy)-3-phenyl-1-(4-(trifluoromethyl)phenyl)butan-1-one (3ak)



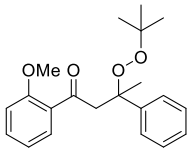
Colorless oil (108.4 mg，57%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 8.1 Hz, 2H), 7.67 (d, J = 8.3 Hz, 2H), 7.48 – 7.44 (m, 2H), 7.33 (t, J = 15.0 Hz, 2H), 7.28 – 7.24 (m, 1H), 3.66 (d, J = 14.3 Hz, 1H), 3.35 (d, J = 14.3 Hz, 1H), 1.84 (s, 3H), 1.08 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.10, 144.14, 140.83, 133.94 (q, J = 32.8 Hz), 128.88, 128.08, 127.31, 125.62, 125.26 (q, J = 3.6 Hz), 83.10, 79.57, 48.56, 26.48, 23.85. HRMS(ESI) calcd for $C_{21}H_{23}F_3O_3(M+Na)^+$: 403.1492; found: 403.1486.

4-(3-(*tert*-butylperoxy)-3-phenylbutanoyl)benzonitrile (3al)



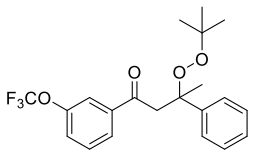
Colorless oil (56.6 mg，33%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 8.4 Hz, 2H), 7.70 (d, J = 8.4 Hz, 2H), 7.44 (d, J = 7.4 Hz, 2H), 7.32 (t, J = 7.5 Hz, 2H), 7.28 – 7.24 (m, 1H), 3.63 (d, J = 14.1 Hz, 1H), 3.33 (d, J = 14.1 Hz, 1H), 1.82 (s, 3H), 1.07 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.75, 143.99, 141.10, 132.11, 128.99, 128.13, 127.40, 125.55, 118.11, 115.85, 83.17, 79.66, 48.52, 26.50, 23.95. HRMS(ESI) calcd for $C_{21}H_{23}NO_3(M+Na)^+$:360.1570; found:360.1572.

3-(*tert*-butylperoxy)-1-(2-methoxyphenyl)-3-phenylbutan-1-one (3am)



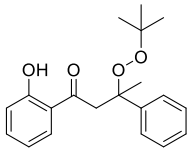
Colorless oil (98.5 mg，58%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.40 (m, 3H), 7.34 (t, J = 7.1 Hz, 1H), 7.26 (t, J = 7.5 Hz, 2H), 7.18 (t, J = 7.2 Hz, 1H), 6.89 (t, J = 7.5 Hz, 1H), 6.84 (d, J = 8.3 Hz, 1H), 3.81 (s, 3H), 3.71 (d, J = 15.1 Hz, 1H), 3.56 (d, J = 15.1 Hz, 1H), 1.81 (s, 3H), 1.12 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.43, 157.93, 144.32, 132.83, 130.18, 130.07, 127.73, 126.98, 126.08, 120.47, 111.29, 83.00, 79.07, 55.43, 53.17, 26.62, 23.69. HRMS(ESI) calcd for $C_{21}H_{26}O_4(M+H)^+$: 343.1904; found: 343.1901.

3-(*tert*-butylperoxy)-3-phenyl-1-(3-(trifluoromethoxy)phenyl)butan-1-one (3an)



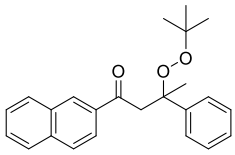
Colorless oil (126.7 mg，64%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, J = 7.7 Hz, 1H), 7.76 (s, 1H), 7.48 – 7.42 (m, 3H), 7.32 (t, J = 7.6 Hz, 3H), 7.27 – 7.22 (m, 1H), 3.62 (d, J = 14.2 Hz, 1H), 3.30 (d, J = 14.2 Hz, 1H), 1.83 (s, 3H), 1.08 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.47, 149.32, 144.22, 140.10, 129.70, 128.05, 127.27, 126.92, 125.63, 124.92, 120.93, 83.10, 79.54, 48.42, 26.43, 23.78. HRMS(ESI) calcd for $C_{21}H_{23}F_3O_4(M+Na)^+$: 419.1441; found: 419.1444.

3-(*tert*-butylperoxy)-1-(2-hydroxyphenyl)-3-phenylbutan-1-one (3ao)



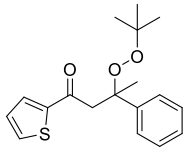
Colorless oil (37.8 mg，23%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.34 (s, 1H), 7.83 (dd, J = 8.1, 1.4 Hz, 1H), 7.50 – 7.42 (m, 3H), 7.34 (t, J = 7.5 Hz, 2H), 7.28 – 7.25 (m, 1H), 6.96 – 6.92 (m, 1H), 6.85 (t, J = 8.1 Hz, 1H), 3.66 (d, J = 14.3 Hz, 1H), 3.33 (d, J = 14.3 Hz, 1H), 1.84 (s, 3H), 1.10 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 204.12, 162.61, 144.24, 136.20, 131.43, 128.06, 127.28, 125.63, 120.63, 118.51, 118.19, 83.05, 79.55, 47.92, 26.49, 24.01. HRMS(ESI) calcd for $C_{20}H_{24}O_4(M+Na)^+$: 351.1567; found: 351.1562.

3-(*tert*-butylperoxy)-1-(naphthalen-2-yl)-3-phenylbutan-1-one (3ap)



Colorless oil (115.9 mg, 64%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (s, 1H), 7.99 (d, J = 8.5 Hz, 1H), 7.89 (d, J = 7.9 Hz, 1H), 7.81 (d, J = 8.3 Hz, 2H), 7.51 (t, J = 7.9 Hz, 4H), 7.32 (t, J = 7.5 Hz, 2H), 7.22 (t, J = 7.4 Hz, 1H), 3.78 (d, J = 14.4 Hz, 1H), 3.44 (d, J = 14.4 Hz, 1H), 1.89 (s, 3H), 1.07 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.78, 144.69, 135.52, 135.45, 132.46, 130.57, 129.67, 128.35, 128.09, 128.07, 127.74, 127.22, 126.64, 125.87, 124.34, 83.21, 79.44, 48.40, 26.60, 23.86. HRMS(ESI) calcd for $C_{24}H_{26}O_3(M+H)^+$: 363.1955; found: 363.1954.

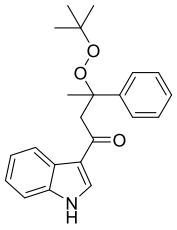
3-(*tert*-butylperoxy)-3-phenyl-1-(thiophen-2-yl)butan-1-one (3aq)



Colorless oil (116.1 mg, 73%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (dd, J = 3.8, 0.9 Hz, 1H), 7.57 (dd, J = 4.9, 1.0 Hz, 1H), 7.50 – 7.45 (m, 2H), 7.32 (t, J = 7.6 Hz, 2H), 7.27 – 7.22 (m, 1H), 7.06 (dd, J = 4.9, 3.9 Hz, 1H), 3.56 (d, J = 13.9 Hz, 1H), 3.23 (d, J = 13.9 Hz, 1H), 1.84 (s, 3H), 1.12 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.44, 145.89,

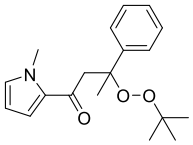
144.54, 133.74, 132.80, 128.02, 127.86, 127.19, 125.71, 82.88, 79.43,49.40, 26.54, 23.65. HRMS(ESI) calcd for $C_{18}H_{22}O_3S(M+H)^+$: 319.1362; found: 319.1358.

3-(*tert*-butylperoxy)-1-(1H-indol-3-yl)-3-phenylbutan-1-one (3ar)



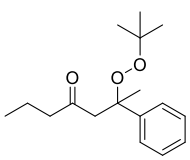
Yellow oil (95.0 mg，54%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.62 (s, 1H), 8.42 – 8.36 (m, 1H), 7.67 (d, J = 2.7 Hz, 1H), 7.50 (d, J = 7.6 Hz, 2H), 7.36 – 7.31 (m, 1H), 7.30 – 7.19 (m, 5H), 3.49 (d, J = 13.8 Hz, 1H), 3.28 (d, J = 13.8 Hz, 1H), 1.90 (s, 3H), 1.13 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.65, 144.79, 136.48, 133.62, 128.03, 127.17, 125.97, 125.66, 123.54, 122.61, 122.28, 119.00, 111.81, 83.02, 79.46, 50.43, 26.71, 23.81. HRMS(ESI) calcd for $C_{22}H_{25}NO_3(M+H)^+$: 352.1907; found: 352.1906.

3-(*tert*-butylperoxy)-1-(1-methyl-1H-pyrrol-2-yl)-3-phenylbutan-1-one (3as)



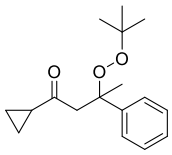
Colorless oil (133.7 mg，85%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, J = 7.3 Hz, 2H), 7.31 (t, J = 7.6 Hz, 2H), 7.25 – 7.21 (m, 1H), 6.92 (dd, J = 4.1, 1.6 Hz, 1H), 6.76 – 6.71 (m, 1H), 6.06 (dd, J = 4.1, 2.5 Hz, 1H), 3.85 (s, 3H), 3.42 (d, J = 14.0 Hz, 1H), 3.15 (d, J = 14.0 Hz, 1H), 1.83 (s, 3H), 1.14 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 188.05, 144.82, 132.06, 130.93, 127.86, 126.97, 125.87, 120.33, 107.60, 82.84, 79.19, 49.19, 37.76, 26.57, 23.71. HRMS(ESI) calcd for $C_{19}H_{25}NO_3(M+H)^+$: 316.1907; found:316.1902.

2-(*tert*-butylperoxy)-2-phenylheptan-4-one (3at)



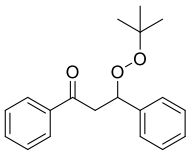
Colorless oil (100.1 mg, 72%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, J = 7.8 Hz, 2H), 7.32 (t, J = 7.5 Hz, 2H), 7.24 (t, J = 7.1 Hz, 1H), 2.99 (d, J = 13.9 Hz, 1H), 2.90 (d, J = 13.9 Hz, 1H), 2.43 – 2.34 (m, 1H), 2.24 – 2.16 (m, 1H), 1.73 (s, 3H), 1.47 (q, J = 7.3 Hz, 2H), 1.24 (s, 9H), 0.80 (t, J = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.71, 144.08, 127.98, 127.17, 125.68, 82.55, 79.35, 52.49, 46.51, 26.69, 24.09, 16.87, 13.64. HRMS(ESI) calcd for $C_{17}H_{26}O_3(M+NH4)^+$: 296.2220; found: 296.2221.

3-(*tert*-butylperoxy)-1-cyclopropyl-3-phenylbutan-1-one (3au)



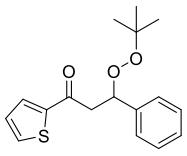
Colorless oil (117.6 mg, 85%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, J = 7.7 Hz, 2H), 7.32 (t, J = 7.5 Hz, 2H), 7.24 (t, J = 7.0 Hz, 1H), 3.14 (d, J = 13.6 Hz, 1H), 3.03 (d, J = 13.5 Hz, 1H), 1.95 – 1.86 (m, 1H), 1.74 (s, 3H), 1.24 (s, 9H), 1.02 – 0.95 (m, 1H), 0.86 – 0.67 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.66, 144.25, 127.93, 127.14, 125.79, 82.66, 79.32, 54.04, 26.71, 23.94, 21.92, 11.71, 11.23. HRMS(ESI) calcd for $C_{17}H_{24}O_3(M+Na)^+$: 299.1618; found: 299.1618.

3-(*tert*-butylperoxy)-1,3-diphenylpropan-1-one (3ba)



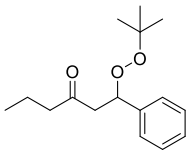
Colorless oil (116.4 mg, 78%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, J = 7.8 Hz, 2H), 7.53 (d, J = 6.4 Hz, 1H), 7.44 (t, J = 7.4 Hz, 4H), 7.38 – 7.28 (m, 3H), 5.60 (t, J = 6.5 Hz, 1H), 3.77 (dd, J = 16.2, 7.1 Hz, 1H), 3.21 (dd, J = 16.2, 5.9 Hz, 1H), 1.16 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.46, 140.04, 137.20, 133.08, 128.54, 128.41, 128.26, 128.11, 127.12, 82.34, 80.78, 44.04, 26.37. HRMS(ESI) calcd for $C_{19}H_{22}O_3(M+Na)^+$: 321.1461; found: 321.1461.

3-(*tert*-butylperoxy)-3-phenyl-1-(thiophen-2-yl)propan-1-one (3bq)



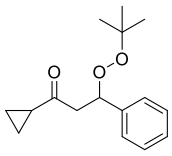
Colorless oil (99.8 mg, 66%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 3.7 Hz, 1H), 7.60 (d, J = 4.9 Hz, 1H), 7.42 (d, J = 7.7 Hz, 2H), 7.34 (t, J = 7.4 Hz, 2H), 7.29 (d, J = 7.4 Hz, 1H), 7.09 (t, J = 4.3 Hz, 1H), 5.57 (t, J = 6.5 Hz, 1H), 3.66 (dd, J = 15.6, 7.5 Hz, 1H), 3.13 (dd, J = 15.6, 5.6 Hz, 1H), 1.16 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.10, 144.59, 139.84, 133.93, 132.32, 128.45, 128.18, 128.10, 127.03, 82.29, 80.87, 44.98, 26.36. HRMS(ESI) calcd for $C_{17}H_{20}O_3S$ $(M+Na)^+$: 327.1025; found: 327.1024.

1-(*tert*-butylperoxy)-1-phenylhexan-3-one (3bt)



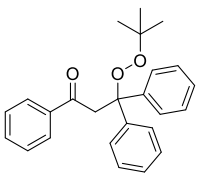
Colorless oil (81.9 mg, 62%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.26 (m, 5H), 5.46 – 5.36 (m, 1H), 3.09 (dd, J = 15.8, 7.9 Hz, 1H), 2.65 (dd, J = 15.8, 5.3 Hz, 1H), 2.45 (dt, J = 14.8, 7.3 Hz, 1H), 2.39 – 2.30 (m, 1H), 1.61 – 1.52 (m, 2H), 1.19 (s, 9H), 0.87 (t, J = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 207.96, 139.94, 128.36, 128.06, 126.97, 81.98, 80.66, 48.07, 45.76, 26.37, 16.92, 13.66. HRMS(ESI) calcd for $C_{16}H_{24}O_3(M+NH_4)^+$: 282.2064; found: 282.2058.

3-(*tert*-butylperoxy)-1-cyclopropyl-3-phenylpropan-1-one (3bu)



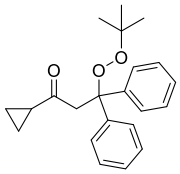
Colorless oil (93.2 mg, 71%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.24 (m, 5H), 5.42 (dd, J = 7.6, 5.7 Hz, 1H), 3.23 (dd, J = 15.7, 7.7 Hz, 1H), 2.81 (dd, J = 15.7, 5.6 Hz, 1H), 1.94 (ddd, J = 12.4, 7.9, 4.6 Hz, 1H), 1.21 (s, 9H), 1.06 – 0.94 (m, 2H), 0.89 – 0.79 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 207.81, 140.05, 128.34, 128.01, 126.97, 81.96, 80.64, 48.63, 26.43, 21.32, 11.05, 10.98. HRMS(ESI) calcd for $C1_6H_{22}O_3(M+Na)^+$: 285.1461; found: 285.1460.

3-(*tert*-butylperoxy)-1,3,3-triphenylpropan-1-one (3ca)



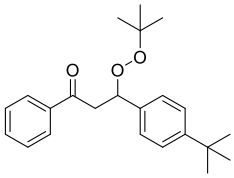
Colorless oil (150.9 mg, 81%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, J = 7.8 Hz, 2H), 7.49 (t, J = 7.2 Hz, 1H), 7.42 – 7.35 (m, 6H), 7.26 (dt, J = 14.8, 7.1 Hz, 6H), 4.17 (s, 2H), 1.03 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.13, 143.74, 138.48, 132.55, 128.44, 128.20, 127.59, 127.41, 127.14, 86.38, 79.79, 44.88, 26.50. HRMS(ESI) calcd for $C_{25}H_{26}O_3(M+Na)^+$: 397.1774; found: 397.1779.

3-(*tert*-butylperoxy)-1-cyclopropyl-3,3-diphenylpropan-1-one (3cu)



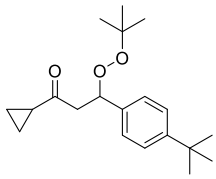
Colorless oil (153.7 mg, 91%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, J = 7.8 Hz, 4H), 7.23 (dt, J = 21.0, 7.0 Hz, 6H), 3.73 (s, 2H), 2.03 (tt, J = 8.1, 4.6 Hz, 1H), 1.13 (s, 9H), 0.83 – 0.79 (m, 2H), 0.68 – 0.64 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.51, 143.56, 127.60, 127.38, 127.22, 85.91, 79.77, 51.12, 26.64, 21.53, 11.54. HRMS(ESI) calcd for $C_{22}H_{26}O_3(M+Na)^+$: 361.1774; found: 361.1778.

3-(4-(*tert*-butyl)phenyl)-3-(tert-butylperoxy)-1-phenylpropan-1-one (3da)



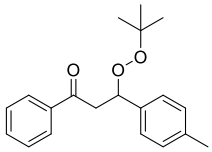
Colorless oil (145.2 mg, 82%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, J = 7.4 Hz, 2H), 7.54 (d, J = 7.3 Hz, 1H), 7.44 (t, J = 7.6 Hz, 2H), 7.36 (s, 4H), 5.59 (t, J = 6.4 Hz, 1H), 3.81 (dd, J = 16.2, 7.0 Hz, 1H), 3.22 (dd, J = 16.2, 5.9 Hz, 1H), 1.30 (s, 9H), 1.17 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.72, 150.98, 137.26, 136.75, 133.01, 128.51, 128.27, 126.81, 125.36, 82.25, 80.80, 44.04, 34.56, 31.35, 26.38. HRMS(ESI) calcd for $C_{23}H_{30}O_3(M+Na)^+$: 377.2087; found: 377.2081.

3-(4-(*tert*-butyl)phenyl)-3-(tert-butylperoxy)-1-cyclopropylpropan-1-one (3du)



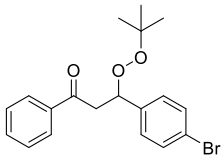
Colorless oil (124.2 mg, 78%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, J = 8.4 Hz, 2H), 7.29 (d, J = 8.3 Hz, 2H), 5.42 (dd, J = 7.5, 5.6 Hz, 1H), 3.25 (dd, J = 15.7, 7.6 Hz, 1H), 2.81 (dd, J = 15.7, 5.5 Hz, 1H), 1.95 (tt, J = 7.9, 4.6 Hz, 1H), 1.30 (s, 9H), 1.21 (s, 9H), 1.03 – 0.97 (m, 2H), 0.86 – 0.80 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.00, 150.83, 136.81, 126.68, 125.26, 81.83, 80.64, 48.66, 34.53, 31.37, 26.43, 21.30, 11.01, 10.92. HRMS(ESI) calcd for $C_{20}H_{30}O_3(M+Na)^+$: 341.2087; found: 341.2084.

3-(*tert*-butylperoxy)-1-phenyl-3-(p-tolyl)propan-1-one (3ea)



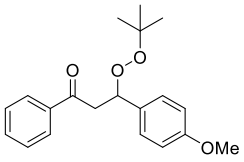
Colorless oil (121.9 mg, 78%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, J = 7.5 Hz, 2H), 7.55 (t, J = 7.2 Hz, 1H), 7.45 (t, J = 7.5 Hz, 2H), 7.32 (d, J = 7.7 Hz, 2H), 7.16 (d, J = 7.6 Hz, 2H), 5.56 (t, J = 6.4 Hz, 1H), 3.79 (dd, J = 16.2, 6.9 Hz, 1H), 3.21 (dd, J = 16.2, 6.1 Hz, 1H), 2.33 (s, 3H), 1.16 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.64, 137.91, 137.20, 136.82, 133.05, 129.13, 128.52, 128.26, 127.14, 82.29, 80.76, 43.93, 26.37, 21.23. HRMS(ESI) calcd for $C_{20}H_{24}O_3(M+Na)^+$: 335.1618; found: 335.1618.

3-(4-bromophenyl)-3-(*tert*-butylperoxy)-1-phenylpropan-1-one (3fa)



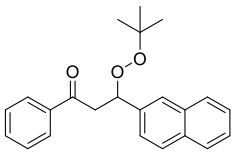
Colorless oil (116.6 mg, 62%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, J = 7.2 Hz, 2H), 7.56 (t, J = 6.8 Hz, 1H), 7.47 (dd, J = 8.1, 4.6 Hz, 4H), 7.31 (d, J = 8.4 Hz, 2H), 5.55 (t, J = 6.5 Hz, 1H), 3.72 (dd, J = 16.4, 6.9 Hz, 1H), 3.17 (dd, J = 16.4, 6.2 Hz, 1H), 1.16 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.97, 139.28, 136.98, 133.25, 131.53, 128.82, 128.60, 128.21, 121.98, 81.54, 80.89, 43.78, 26.35. HRMS(ESI) calcd for $C_{19}H_{21}BrO_3(M+Na)^+$: 399.0566; found: 3399.0563.

3-(*tert*-butylperoxy)-3-(4-methoxyphenyl)-1-phenylpropan-1-one (3ga)



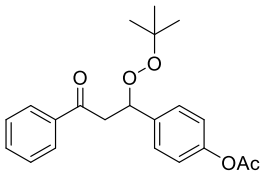
Colorless oil (95.1 mg, 58%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.93 (m, 2H), 7.54 (t, J = 7.4 Hz, 1H), 7.44 (t, J = 7.6 Hz, 2H), 7.39 – 7.33 (m, 2H), 6.90 – 6.85 (m, 2H), 5.55 (t, J = 6.5 Hz, 1H), 3.85 – 3.76 (m, 4H), 3.24 (dd, J = 16.2, 6.4 Hz, 1H), 1.17 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.69, 159.50, 137.18, 133.09, 131.77, 128.59, 128.55, 128.25, 113.82, 82.08, 80.73, 55.23, 43.77, 26.39. HRMS(ESI) calcd for $C_{20}H_{24}O_4(M+Na)^+$: 351.1567; found: 351.1564.

3-(*tert*-butylperoxy)-3-(naphthalen-2-yl)-1-phenylpropan-1-one (3ha)



Colorless oil (90.6 mg, 52%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, J = 7.7 Hz, 2H), 7.88 – 7.81 (m, 4H), 7.59 – 7.53 (m, 2H), 7.47 – 7.43 (m, 4H), 5.77 (t, J = 6.3 Hz, 1H), 3.85 (dd, J = 16.3, 7.0 Hz, 1H), 3.29 (dd, J = 16.2, 5.7 Hz, 1H), 1.18 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.38, 137.56, 137.16, 133.27, 133.22, 133.13, 128.56, 128.27, 128.22, 128.13, 127.68, 126.30, 126.08, 126.02, 124.87, 82.46, 80.88,44.07, 26.40. HRMS(ESI) calcd for $C_{23}H_{24}O_3(M+Na)^+$: 371.1618; found: 371.1618.

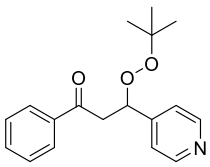
4-(1-*(tert*-butylperoxy)-3-oxo-3-phenylpropyl)phenyl acetate (3ia)



Colorless oil (110.4 mg, 62%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.92 (m, 2H), 7.55 (t, J = 7.4 Hz, 1H), 7.48 – 7.43 (m, 4H), 7.07 (d, J = 8.5 Hz, 2H), 5.61 (t, J = 6.5 Hz, 1H), 3.75 (dd, J = 16.4, 7.2 Hz, 1H), 3.17 (dd, J = 16.4, 5.7 Hz, 1H), 2.28 (s, 3H), 1.16

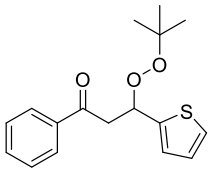
(s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.21, 169.41, 150.37, 137.74, 137.08, 133.17, 128.57, 128.24, 128.16, 121.48, 81.65, 80.85, 44.06, 26.35, 21.15. HRMS(ESI) calcd for $C_{21}H_{24}O_5$(M+Na)$^+$: 379.1516; found: 379.1520.

3-(*tert*-butylperoxy)-1-phenyl-3-(pyridin-4-yl)propan-1-one (3ja)



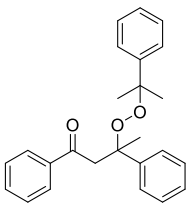
Colorless oil (58.3 mg, 39%) ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.57 (d, J = 4.3 Hz, 2H), 8.00 (d, J = 7.5 Hz, 2H), 7.66 – 7.60 (m, 1H), 7.53 (t, J = 7.4 Hz, 2H), 7.48 (d, J = 4.5 Hz, 2H), 5.48(dd, J = 8.0, 4.8 Hz, 1H), 3.67 (dd, J = 16.9, 8.4 Hz, 1H), 3.38 (dd, J = 4.5 Hz, 1H), 1.09 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 196.88, 151.14, 149.98, 136.99, 133.89, 129.17, 128.67, 122.56, 80.95, 80.90, 43.14, 26.50. HRMS(ESI) calcd for $C_{18}H_{21}NO_3$(M+H)$^+$: 300.1594; found: 300.1598.

3-(*tert*-butylperoxy)-1-phenyl-3-(thiophen-2-yl)propan-1-one (3ka)



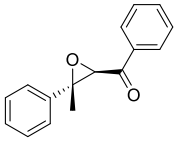
Colorless oil (112.6 mg, 74%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, J = 7.9 Hz, 2H), 7.56 (t, J = 7.0 Hz, 1H), 7.46 (t, J = 7.6 Hz, 2H), 7.27 (d, J = 5.0 Hz, 1H), 7.09 (d, J = 3.0 Hz, 1H), 6.96 (t, J = 4.1 Hz, 1H), 5.84 (t, J = 6.5 Hz, 1H), 3.88 (dd, J = 16.4, 6.4 Hz, 1H), 3.39 (dd, J = 16.4, 6.6 Hz, 1H), 1.18 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.01, 142.35, 137.02, 133.19, 128.59, 128.25, 126.56, 125.98, 125.49, 80.93, 77.64 , 43.92, 26.34. HRMS(ESI) calcd for $C_{17}H_{20}O_3S$ (M+Na)$^+$: 327.1025; found: 327.1028.

1,3-diphenyl-3-((2-phenylpropan-2-yl)peroxy)butan-1-one (4aa)



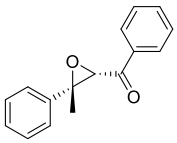
Colorless oil (89.7 mg，48%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, J = 8.2 Hz, 2H), 7.44 (d, J = 7.5 Hz, 3H), 7.33 – 7.20 (m, 10H), 3.54 (d, J = 14.6 Hz, 1H), 3.22 (d, J = 14.6 Hz, 1H), 1.88 (s, 3H), 1.42 (d, J = 6.5 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.64, 145.54, 144.27, 137.95, 132.76, 128.58, 128.29, 128.03, 127.91, 127.29, 126.97, 125.99, 125.71, 83.51, 82.23,48.72, 27.07, 26.38, 23.34. HRMS(ESI) calcd for $C_{25}H_{26}O_3(M+NH_4)^+$: 392.2220; found: 392.2219.

trans-(3-Methyl-3-phenyloxiran-2-yl)(phenyl)methanone (5)



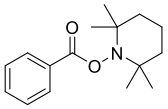
white solid (67.9 mg, 57%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, J = 7.4 Hz, 2H), 7.62 (t, J = 7.4 Hz, 1H), 7.50 (dd, J = 7.4, 4.8 Hz, 4H), 7.43 (t, J = 7.4 Hz, 2H), 7.37 (t, J = 7.1 Hz, 1H), 4.15 (s, 1H), 1.63 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.99, 140.45, 135.63, 133.97, 128.94, 128.77, 128.25, 125.14, 66.88, 62.83, 17.00.

cis-(3-Methyl-3-phenyloxiran-2-yl)(phenyl)methanone (5’)



white solid (35.8 mg, 30%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, J = 7.6 Hz, 2H), 7.53 (t, J = 7.4 Hz, 1H), 7.41 (t, J = 7.7 Hz, 2H), 7.31 (d, J = 8.1 Hz, 2H), 7.21 – 7.15 (m, 3H), 4.34 (s, 1H), 1.93 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.48, 136.66, 135.52, 133.54, 128.63, 128.06, 128.01, 127.87, 126.27, 66.12, 64.54, 24.45. HRMS(ESI) calcd for $C_{16}H_{14}O_2(M+H)^+$:239.1067; found: 239.1067.

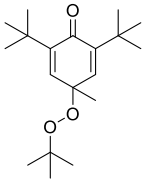
2,2,6,6-tetramethylpiperidin-1-yl benzoate (6)



Colorless solid (372.5 mg，95%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, J = 7.3 Hz, 2H), 7.56 (t, J = 7.4 Hz, 1H), 7.45 (t, J = 7.6 Hz, 2H), 1.83 – 1.55 (m, 5H), 1.49 – 1.41 (m, 1H), 1.27 (s, 6H), 1.13 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.31, 132.85,

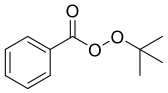
129.51, 128.44,60.35, 39.03, 31.96, 20.84, 16.99. HRMS(ESI) calcd for $C_{16}H_{23}NO_2(M+H)^+$: 262.1802; found: 262.1796.

2,6-di-*tert*-butyl-4-(tert-butylperoxy)-4-methylcyclohexa-2,5-dien-1-one (7)



Yellow solid (457.8 mg，99%).^{1}H NMR (400 MHz, $CDCl_3$) δ 6.57 (s, 2H), 1.33 (s, 3H), 1.23 (s, 18H), 1.19 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 186.57, 146.57, 141.78, 79.32, ,76.14, 34.67, 29.43, 26.45, 24.21. HRMS(ESI) calcd for $C_{19}H_{32}O_3(M+Na)^+$: 331.2244; found: 331.2245.

tert-butyl benzoperoxoate (8)



Colorless oil ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, J = 7.6 Hz, 2H), 7.59 (t, J = 7.4 Hz, 1H), 7.46 (t, J = 7.6 Hz, 2H), 1.42 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.42, 133.35, 130.57, 129.13, 128.63, 83.99, 26.27. HRMS (EI) m/z $[M]^+$ Calcd for $C_{11}H_{14}O_3$: 194.0943, found: 194.0940.

3. References

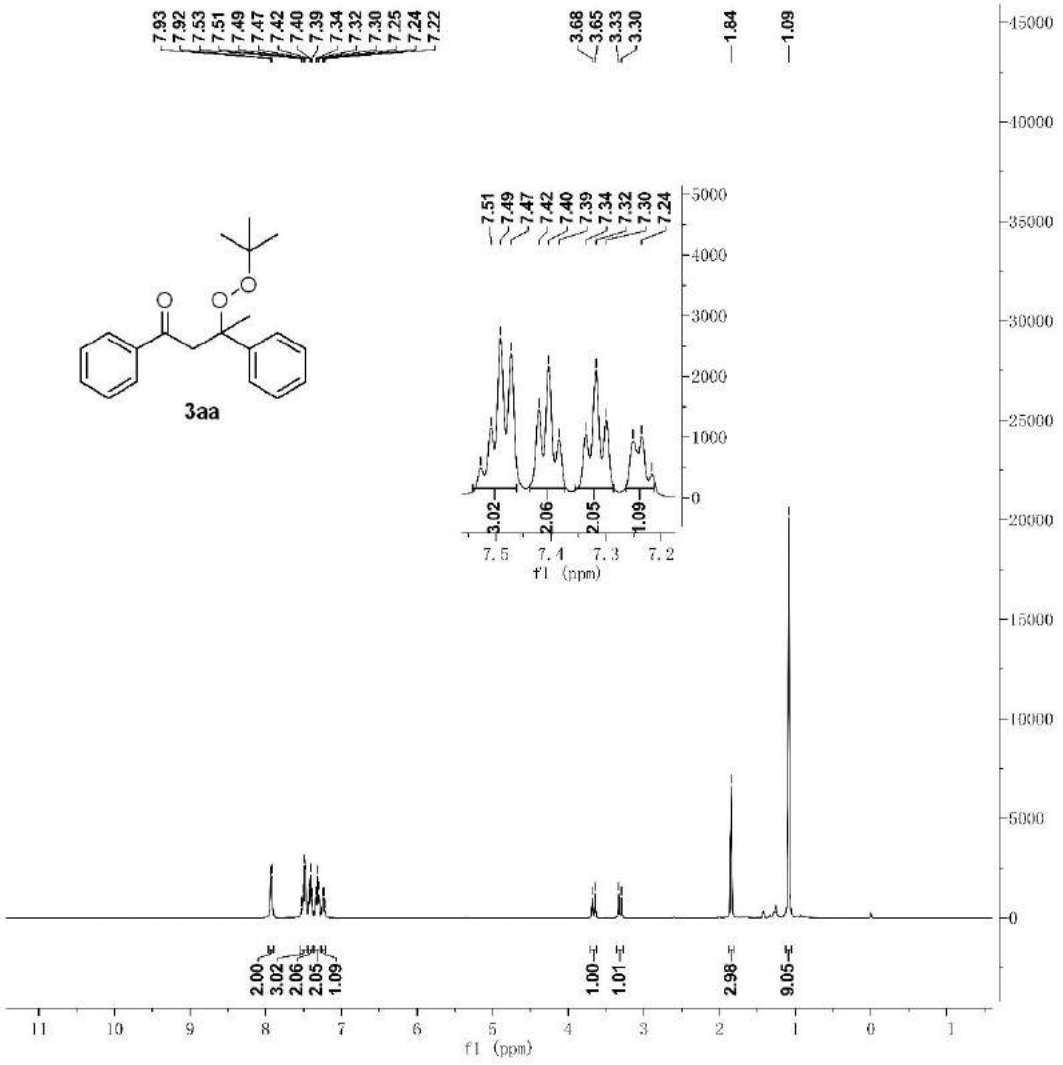
(1) Liu, W.; Li, Y.; Liu, K.; Li, Z. *Journal of the American Chemical Society* **2011,** *133, 10756.*

(2) Yang, W. C.; Weng, S. S.; Ramasamy, A.; Rajeshwaren, G.; Liao, Y. Y.; Chen, C. T. *Organic & Biomolecular Chemistry* **2015**, *13, 2385.*

(3) Wei, W.; Zhang, C.; Xu, Y.; Wan, X. *Chem. Commun*. **2011**, *47, 10827*.

4. NMR and HRMS Spectra

^{1}H，^{13}C NMR and HRMS spectra for all compounds.



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5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.7
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	5 mm PADDO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
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15	Receiver Gain	61
16	Relaxation Delay	1.0000
17	Pulse Width	14.4000
18	Presaturation Frequency	
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20	Acquisition Date	2018-01-11T12:06:00
21	Modification Date	2018-01-11T12:05:00
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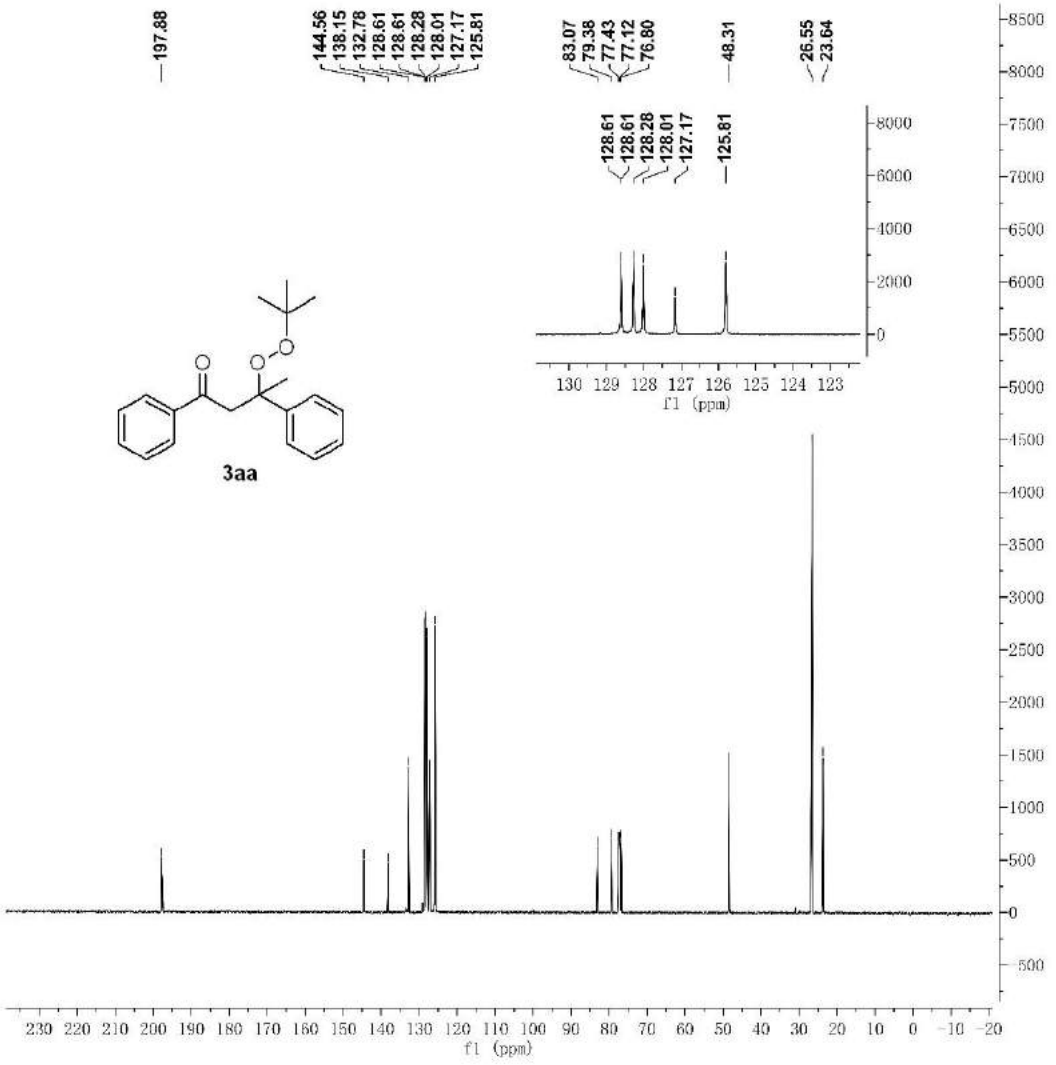
25	Lowest Frequency	-1551.8
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536



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7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
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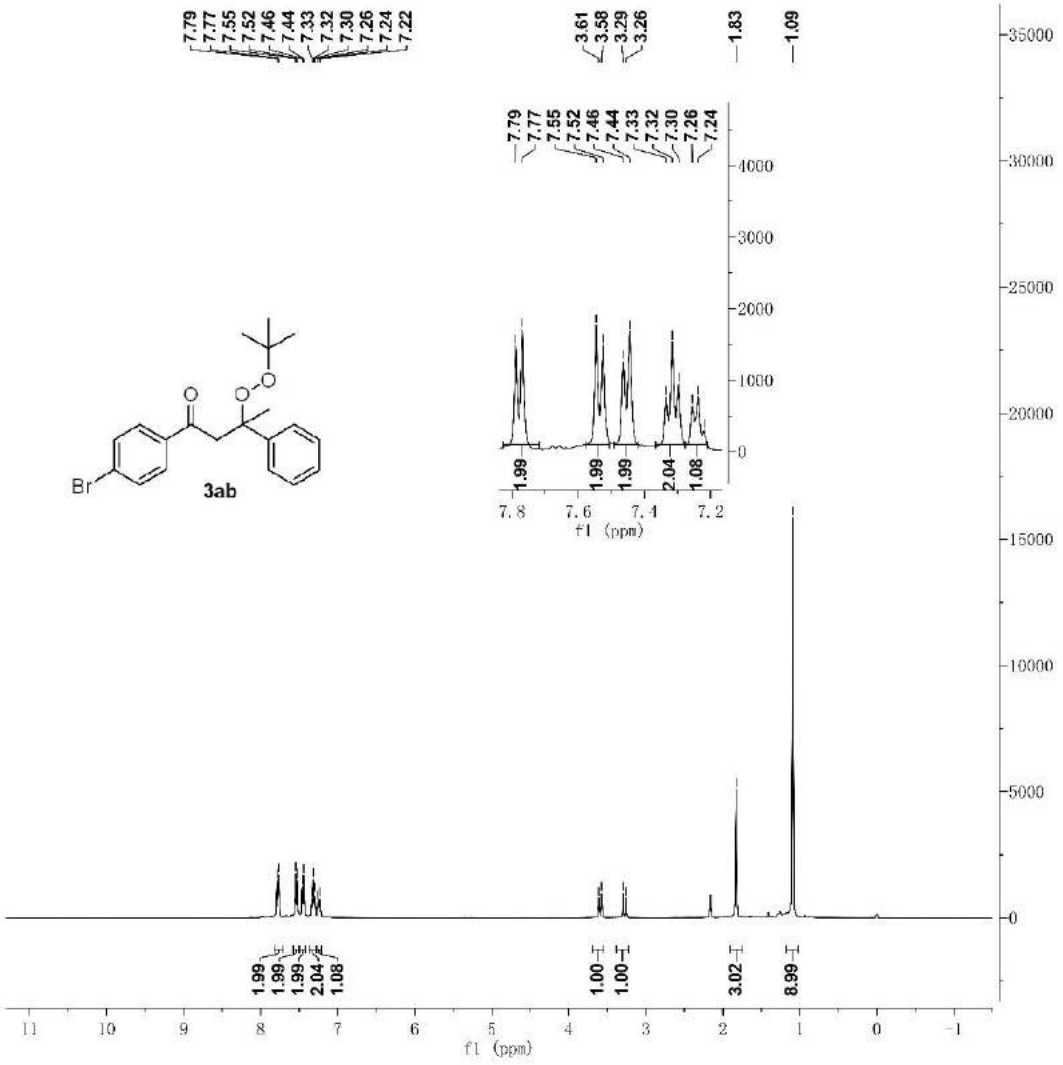
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	65536



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8 Author	
9 Solvent	CDCl3
10 Temperature	297.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PADDO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
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18 Presaturation Frequency	
19 Acquisition Time	4.0894
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21 Modification Date	2018-03-21T03:30:00
22 Class	
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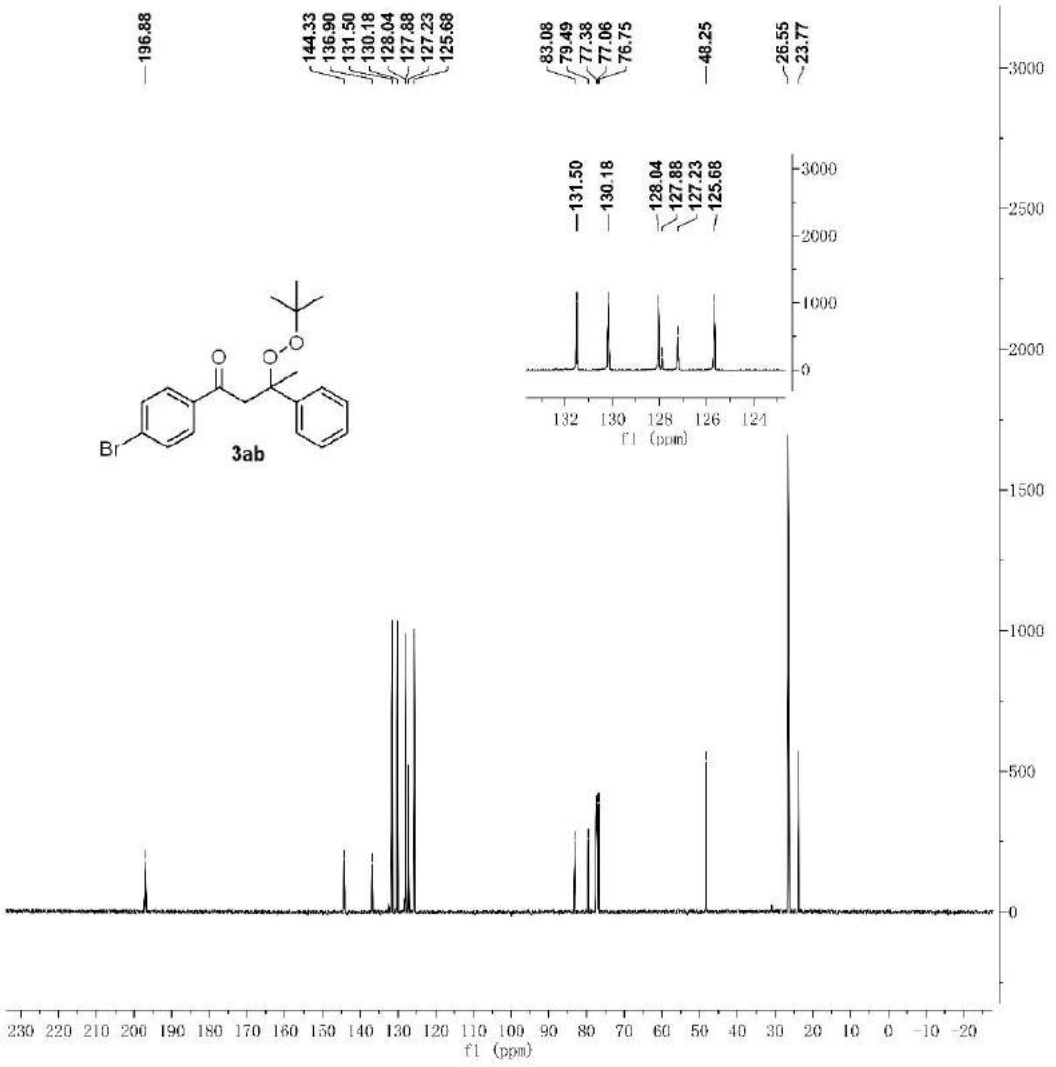
25 Lowest Frequency	-1551.3
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



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6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.2
11	Pulse Sequence	zgpg30
12	Experiment	1D
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14	Number of Scans	500
15	Receiver Gain	78
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
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21	Modification Date	2018-03-21T03:44:00
22	Class	
23	Spectrometer Frequency	100.62
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	65536

Sample Name	Sample2	**Position**	P1-A4	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
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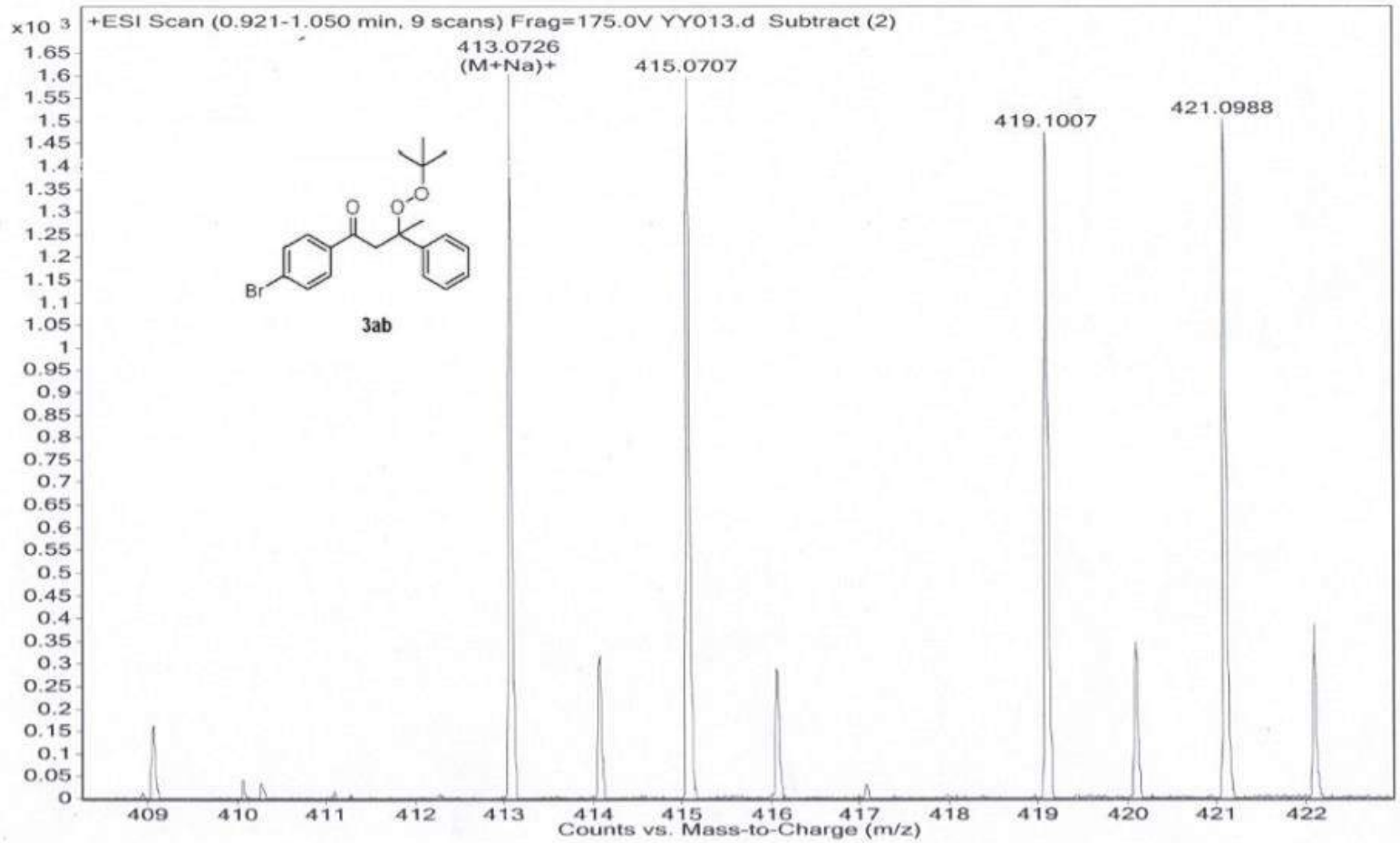

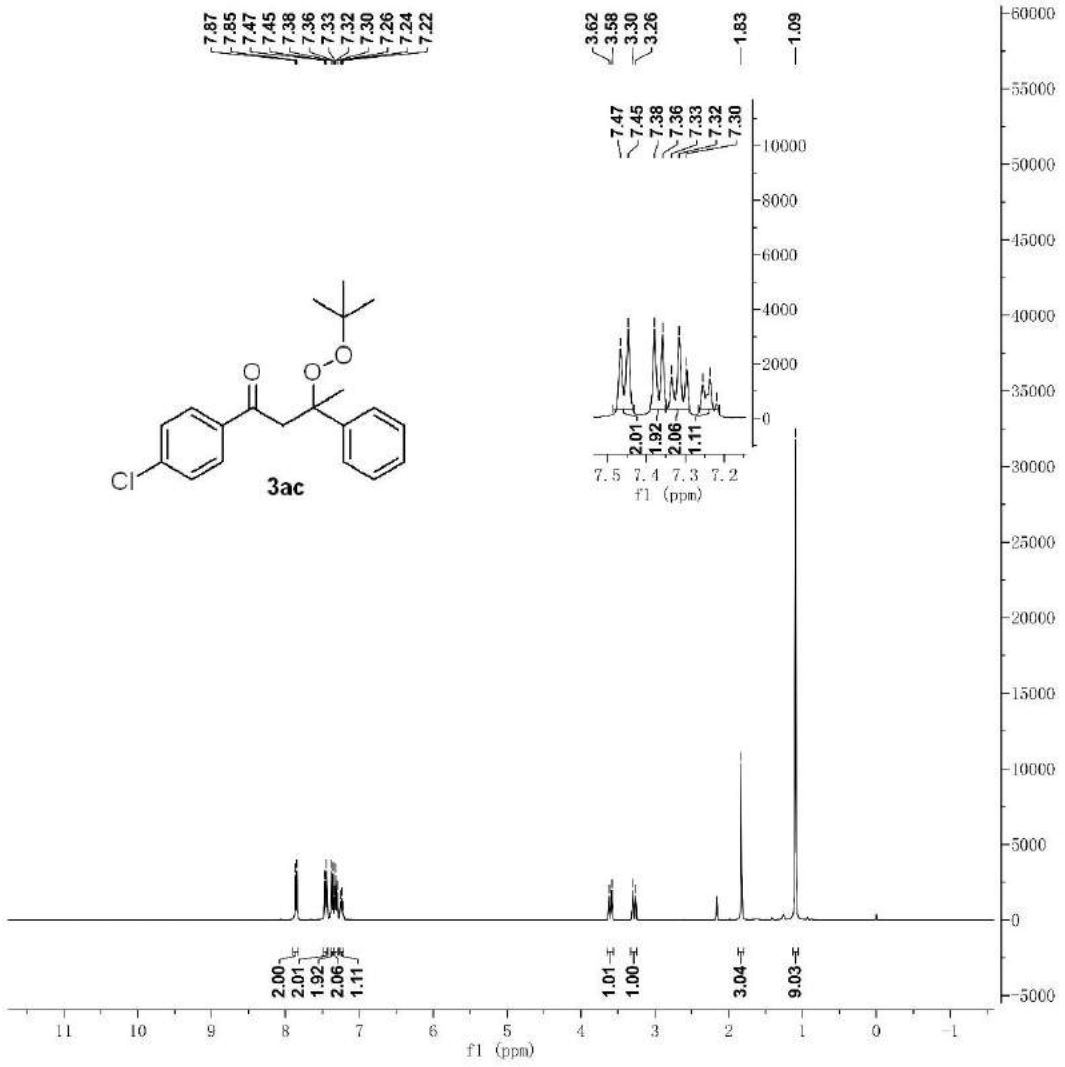

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6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.3
11 Pulse Sequence	zg30
12 Experiment	1D
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21 Modification Date	2018 03 21T03:49:00
22 Class	
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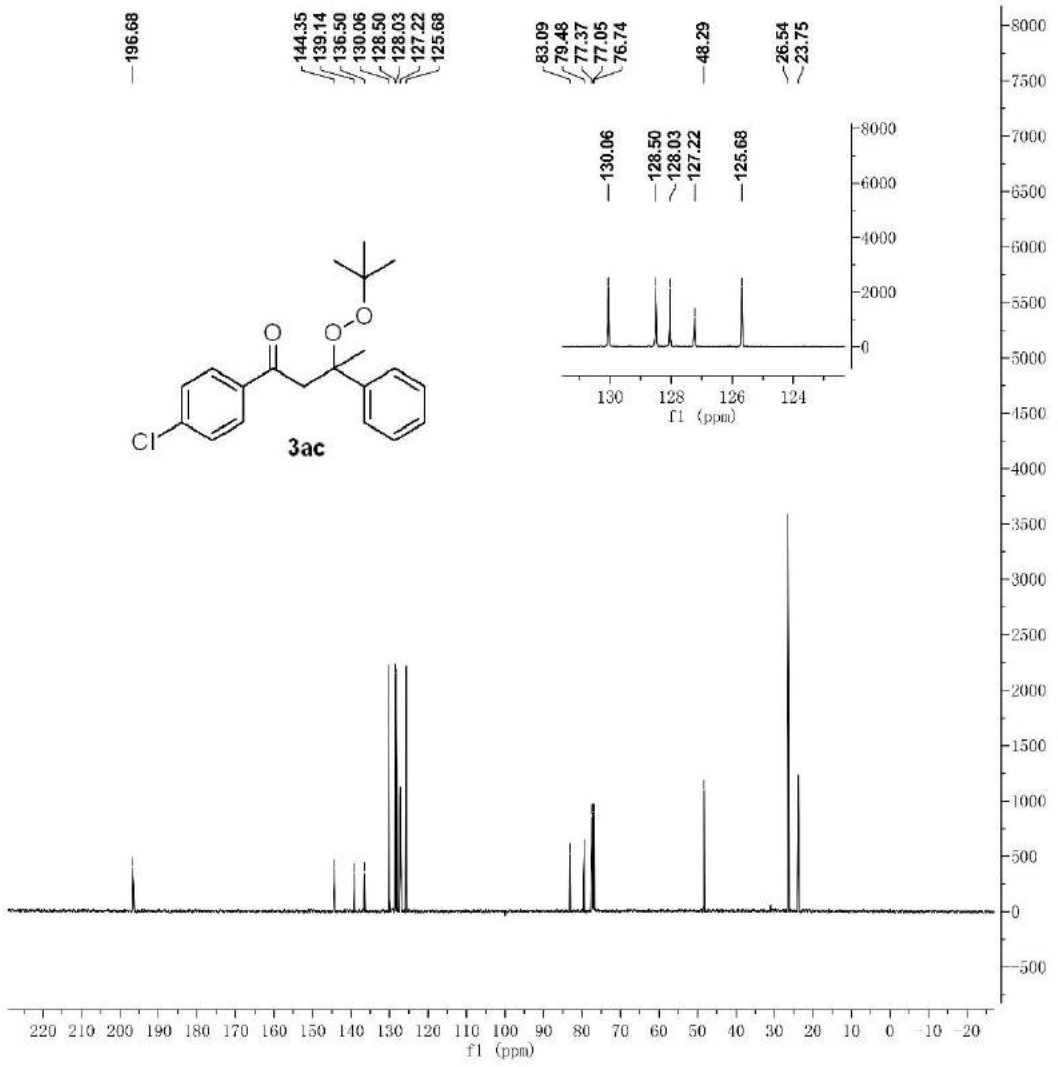
24 Spectral Width	8012.8
25 Lowest Frequency	-1551.4
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



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26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample9	**Position**	P1-A9	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
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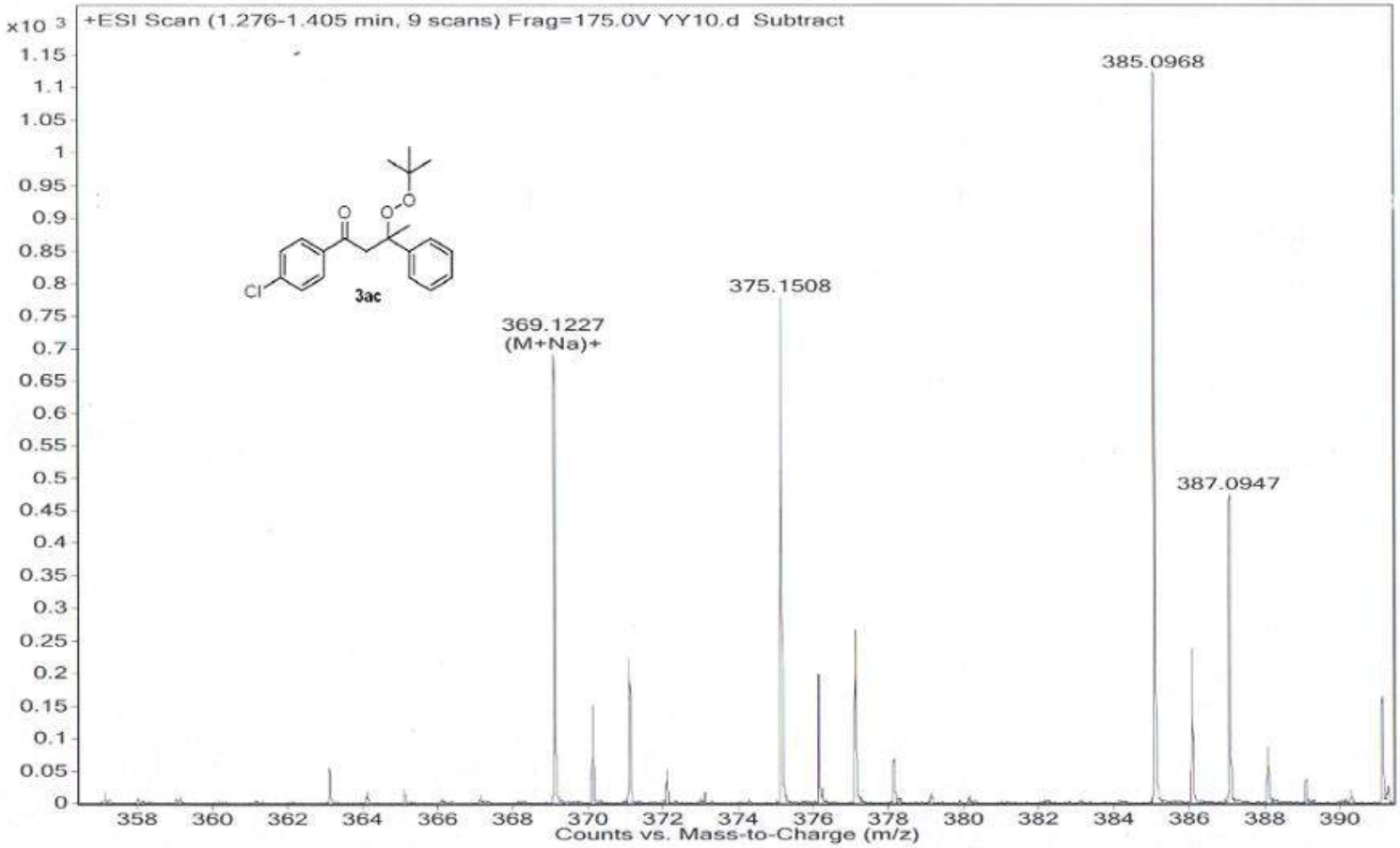

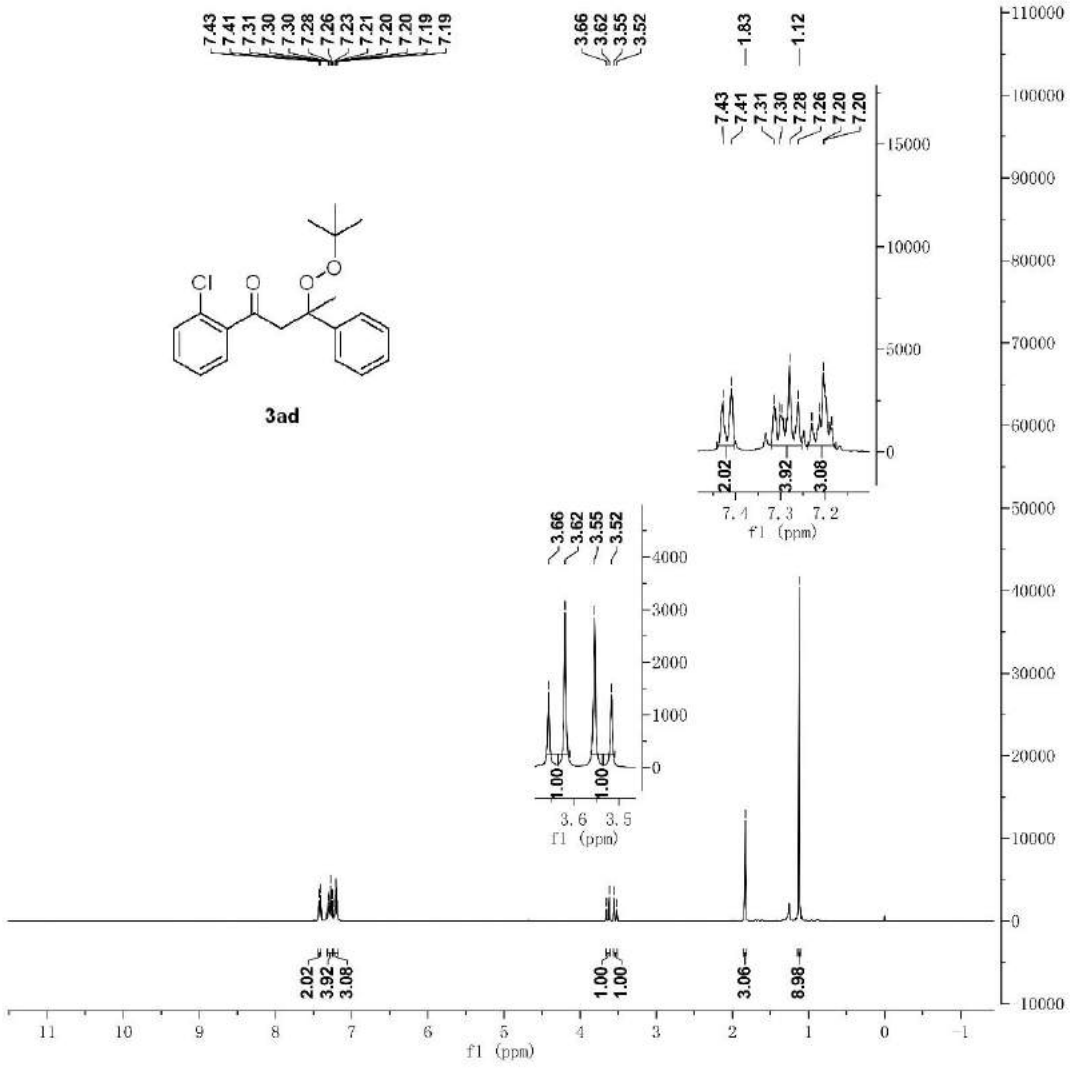

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7 Spectrometer	spect
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17 Pulse Width	14.4000
18 Presaturation Frequency	
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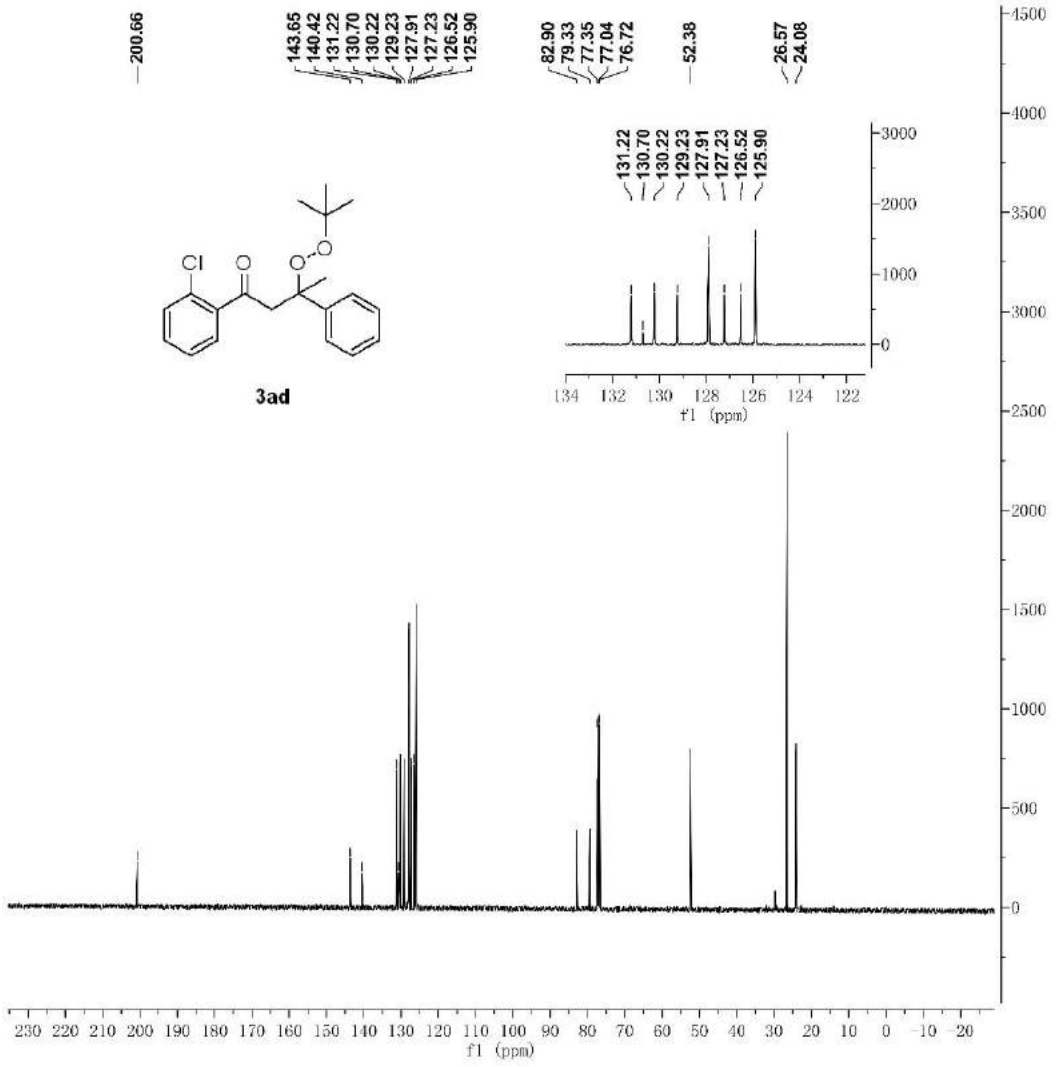
27 Acquired Size	32768
28 Spectral Size	65536



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7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	299.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
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14 Number of Scans	500
15 Receiver Gain	133
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
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22 Class	
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25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample21	**Position**	P1-C3	**Instrument Name**	Instrument 1	**User Name**	
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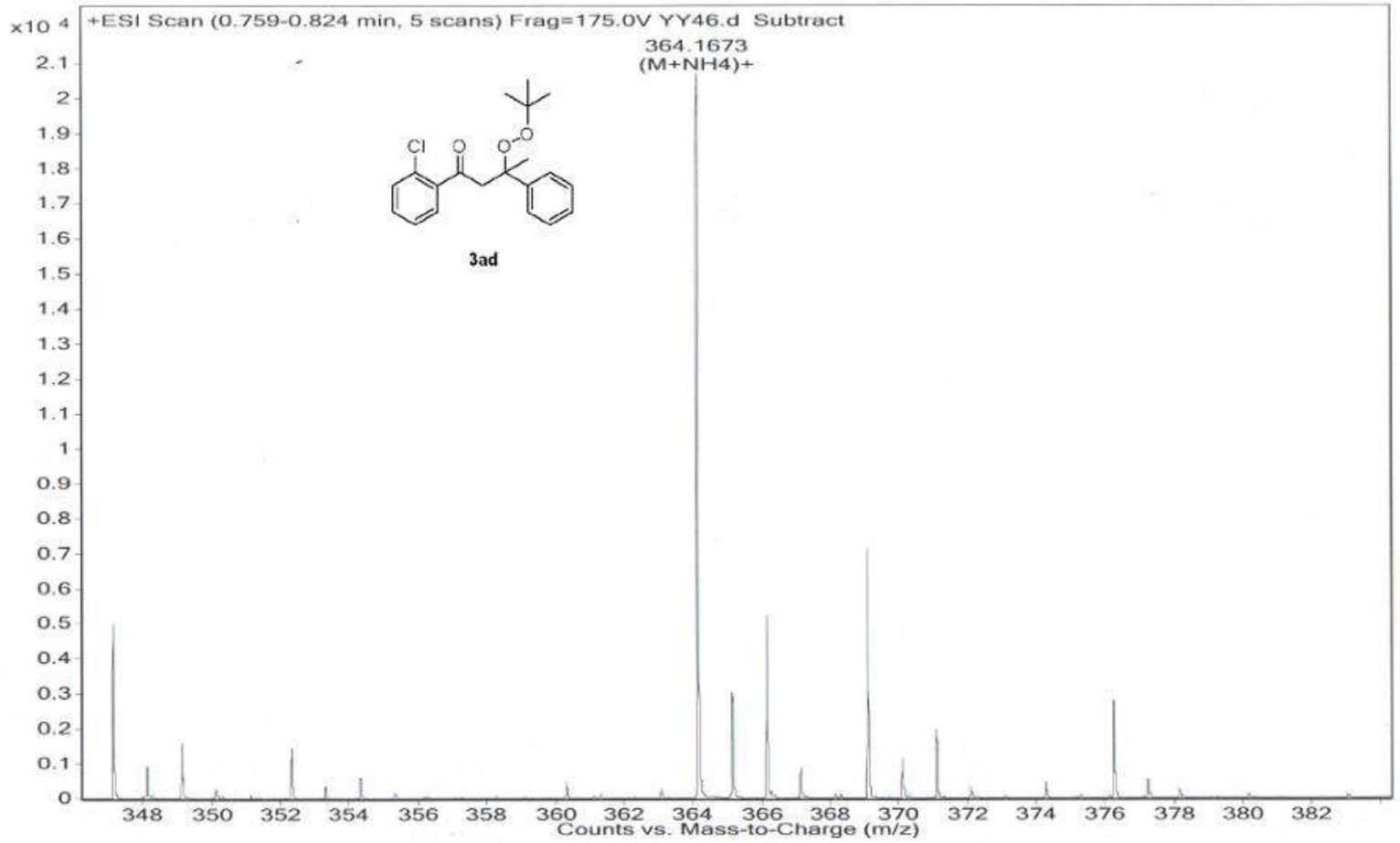

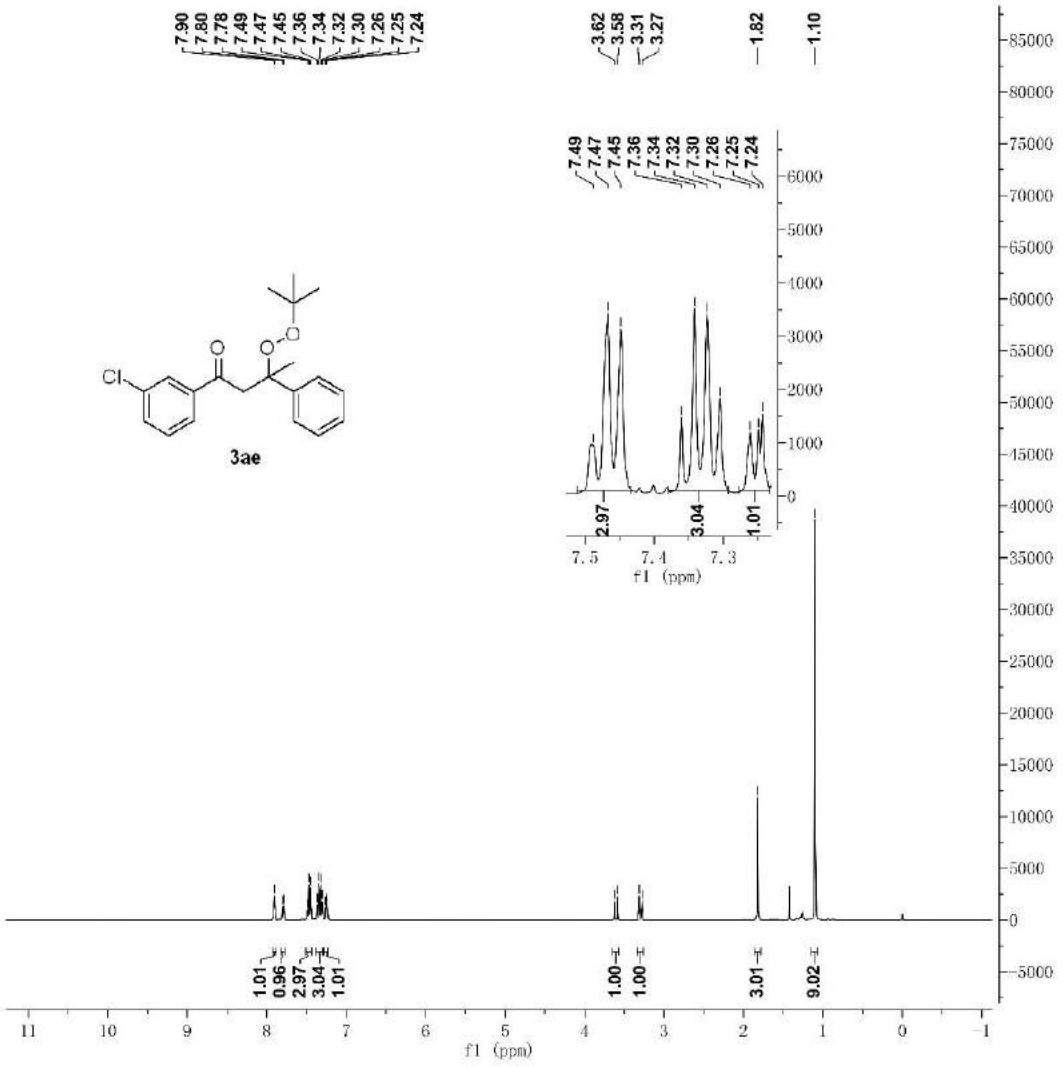

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17 Pulse Width	14.4000
18 Presaturation Frequency	
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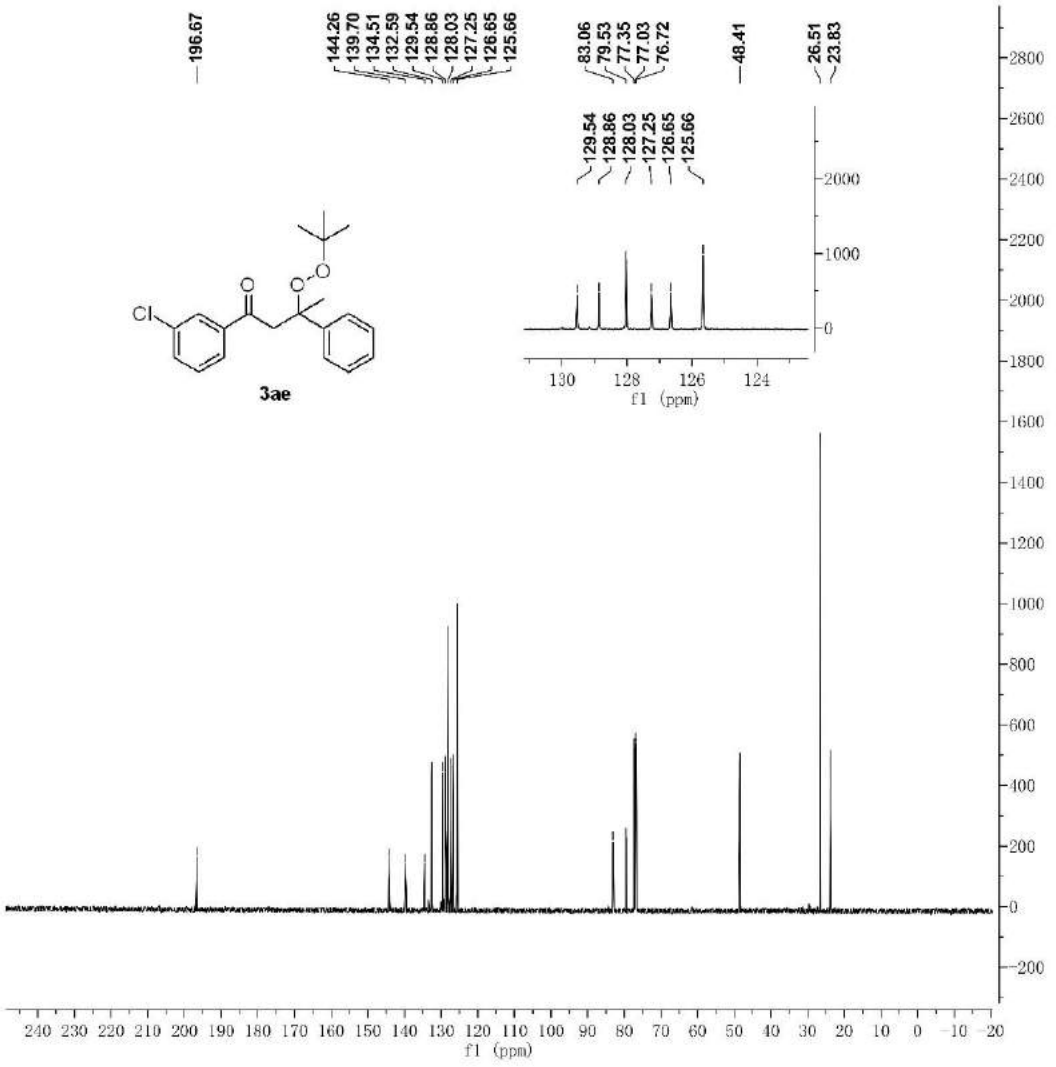
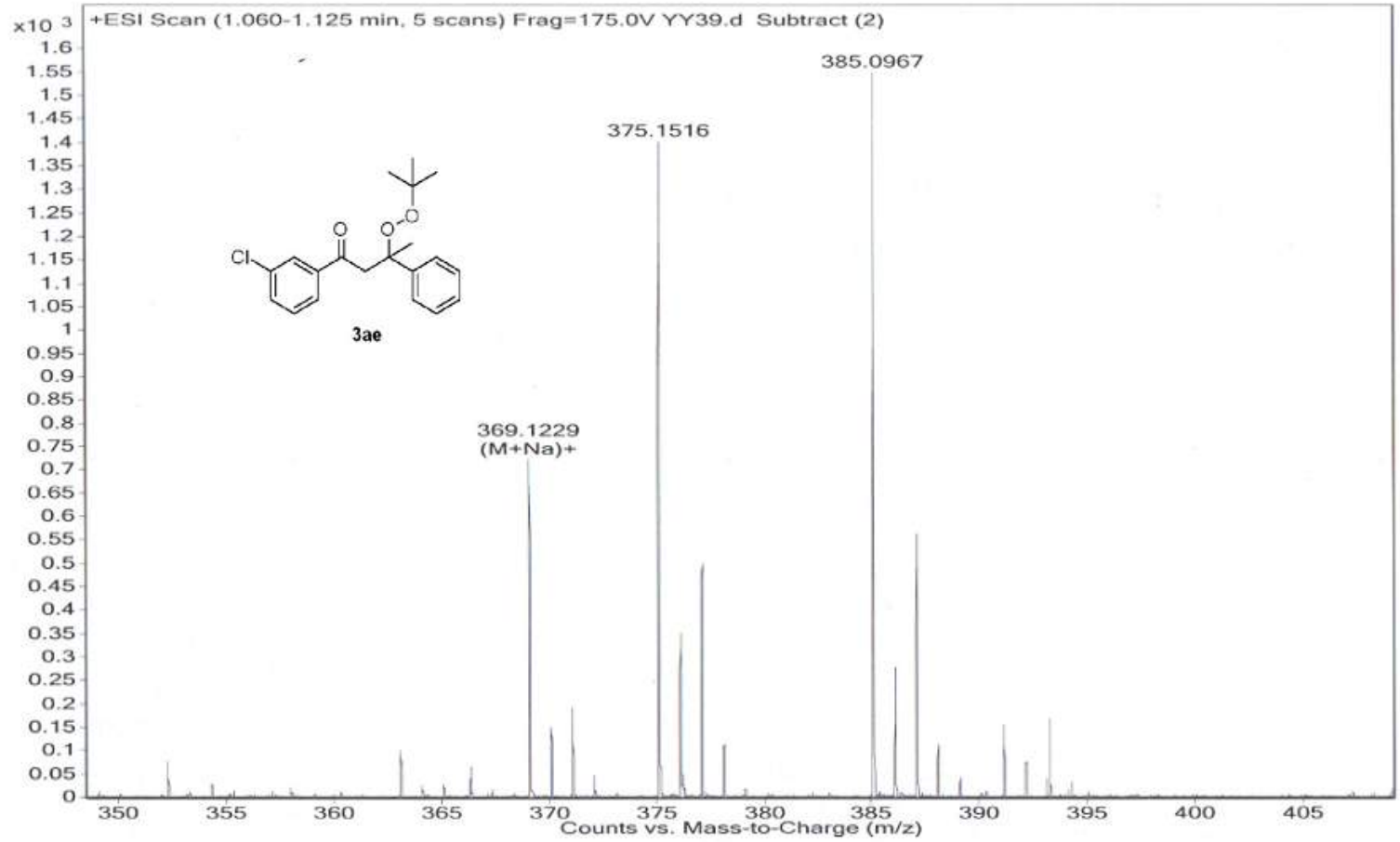
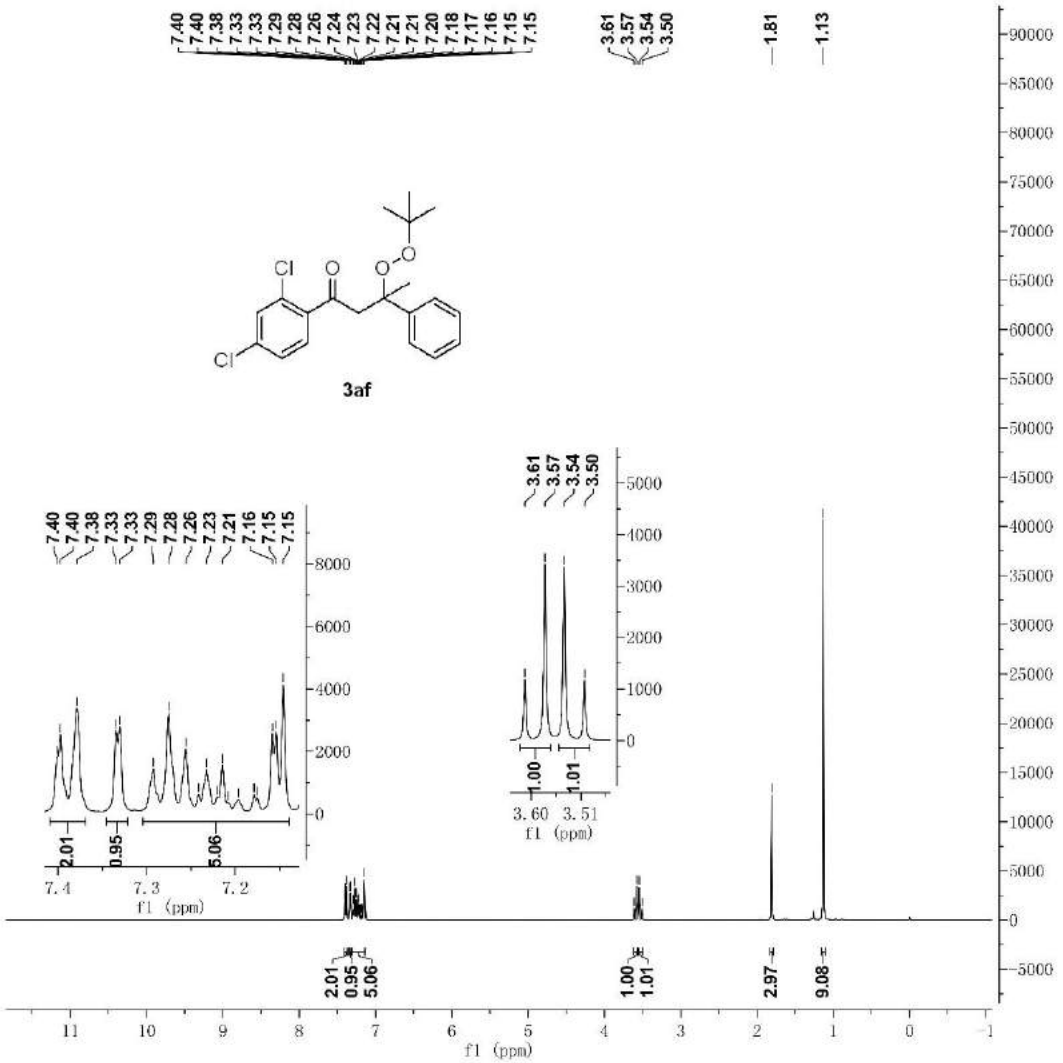
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



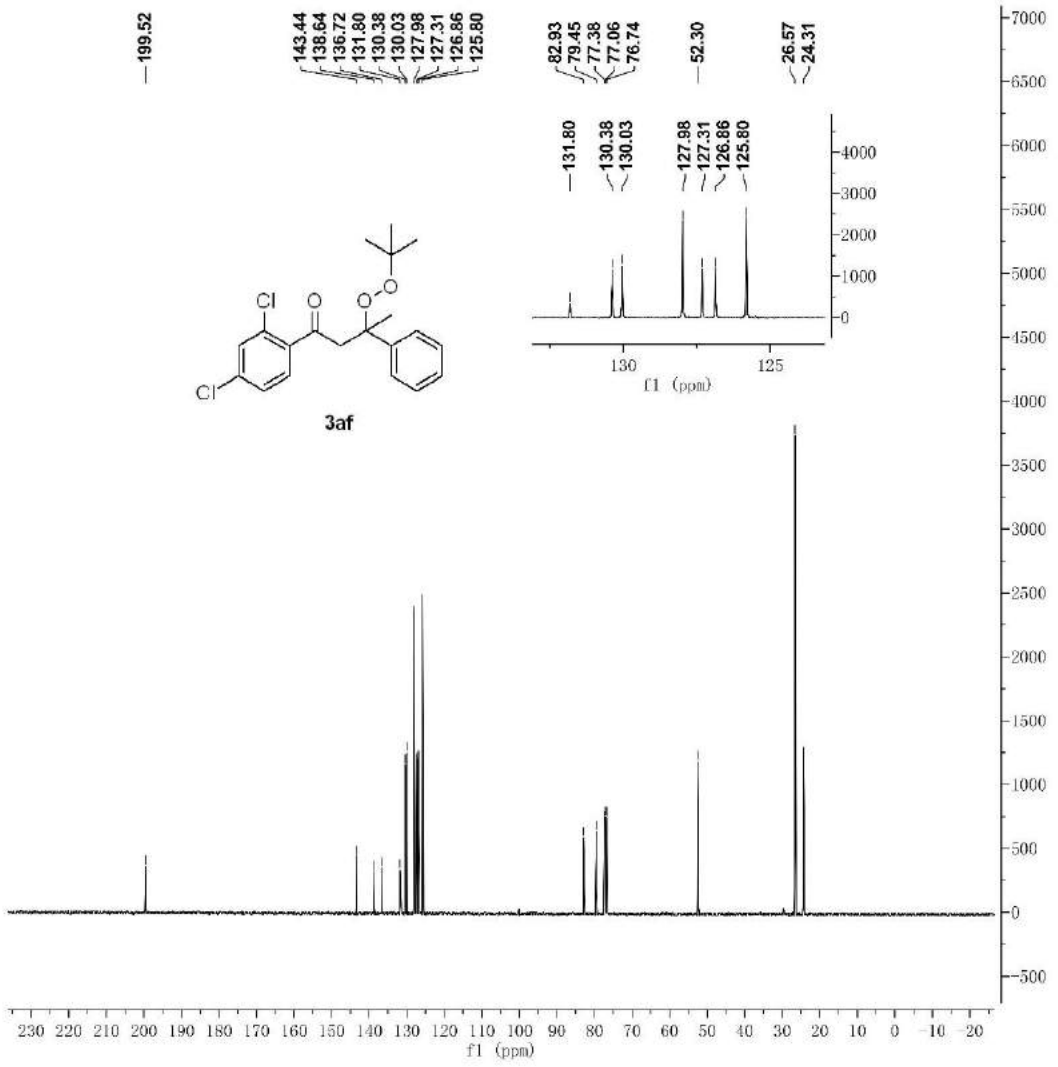
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy39/ 2/ fid
2 Title	yy39.2.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 19
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	299.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	500
15 Receiver Gain	88
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-03-30T01:39:00
21 Modification Date	2018 03 30T01:39:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample18	**Position**	P1-B9	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY39.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/4/2018 11:10:46 AM



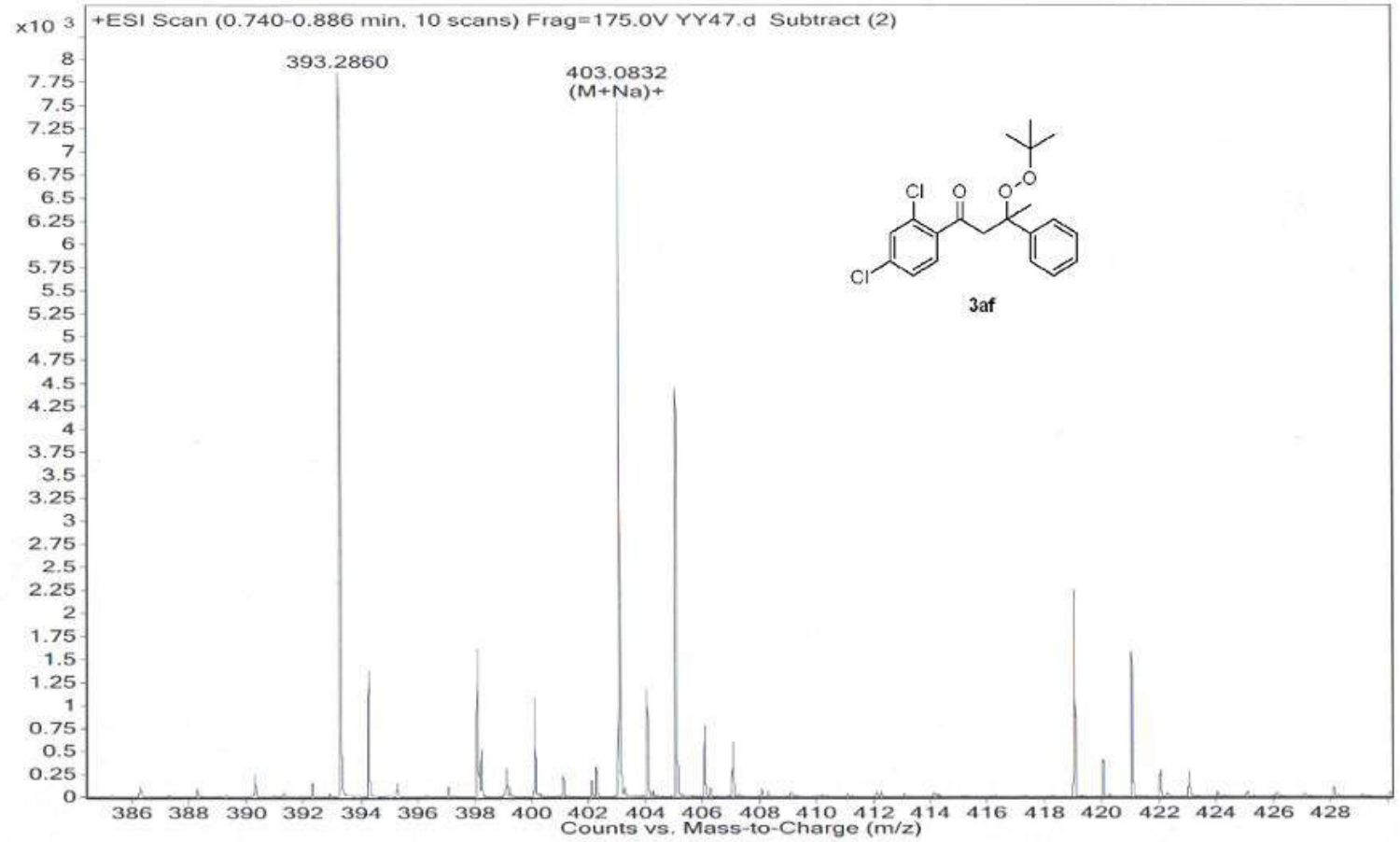


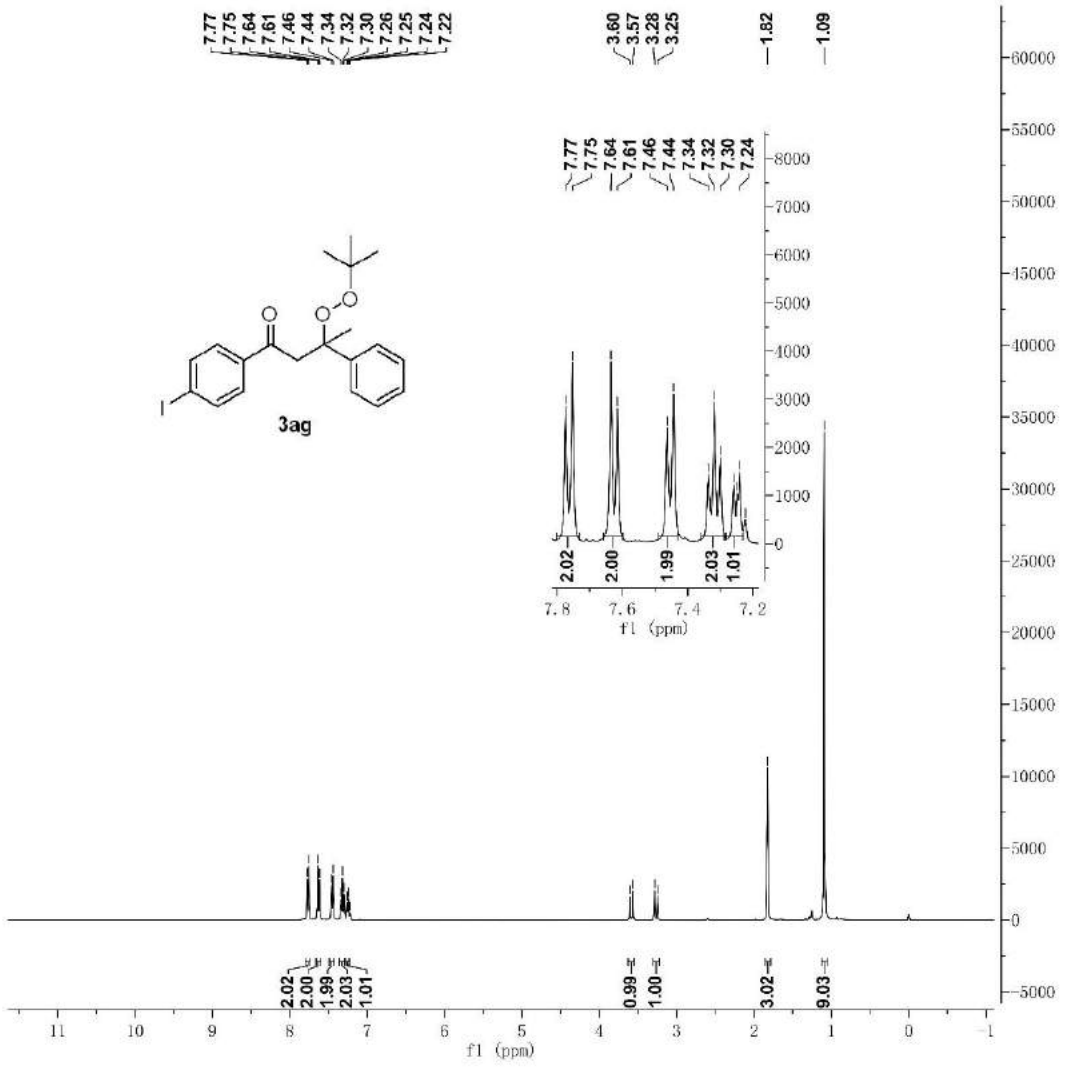
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy47/ 1/ fid
2 Title	yy47.1.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 17
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	33
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-03-30T01:09:00
21 Modification Date	2018-03-30T01:08:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1553.0
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



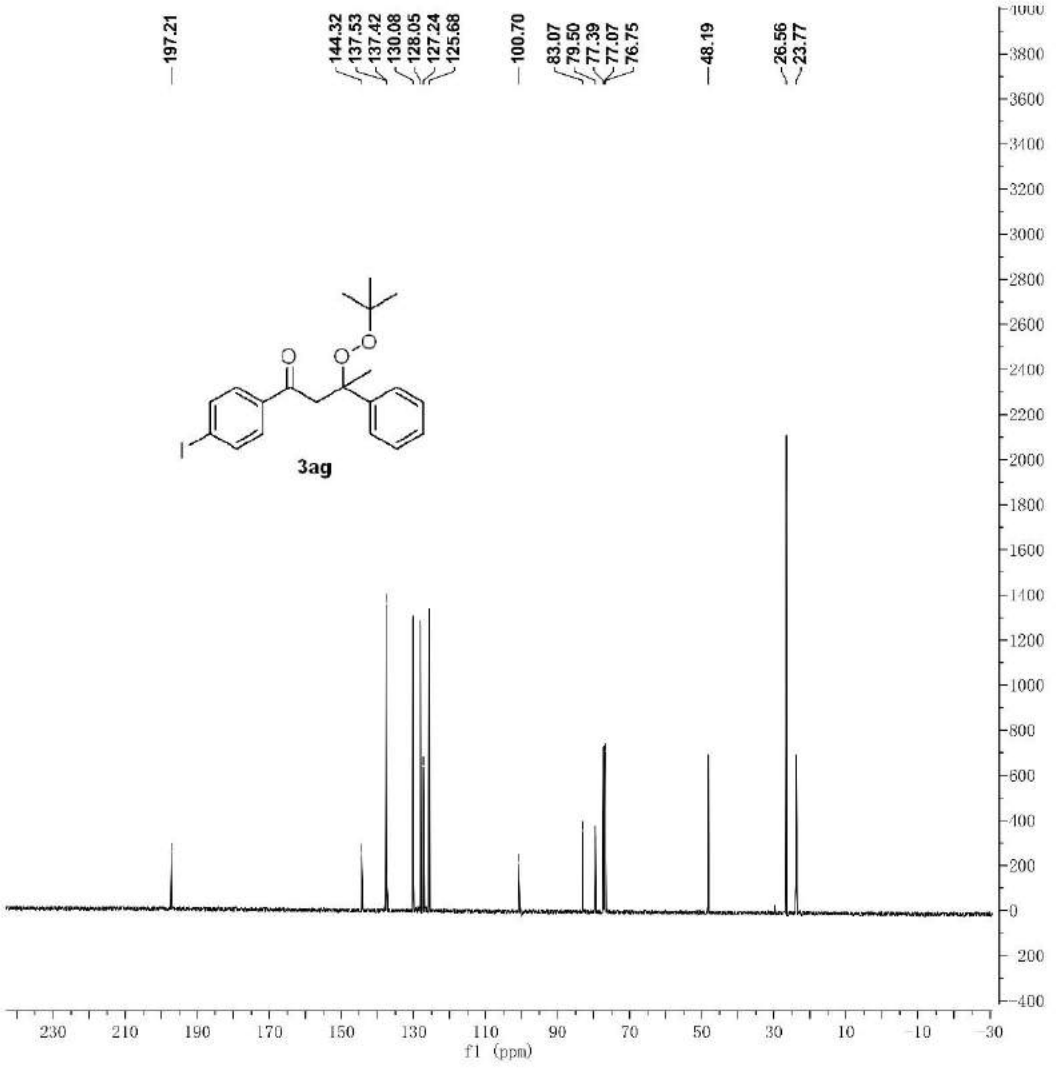
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy47/ 2/ fid
2 Title	yy47.2.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 17
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	299.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	400
15 Receiver Gain	133
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-03-30T01:20:00
21 Modification Date	2018 03 30T01:19:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample22	**Position**	P1-C4	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY47.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/4/2018 11:34:01 AM



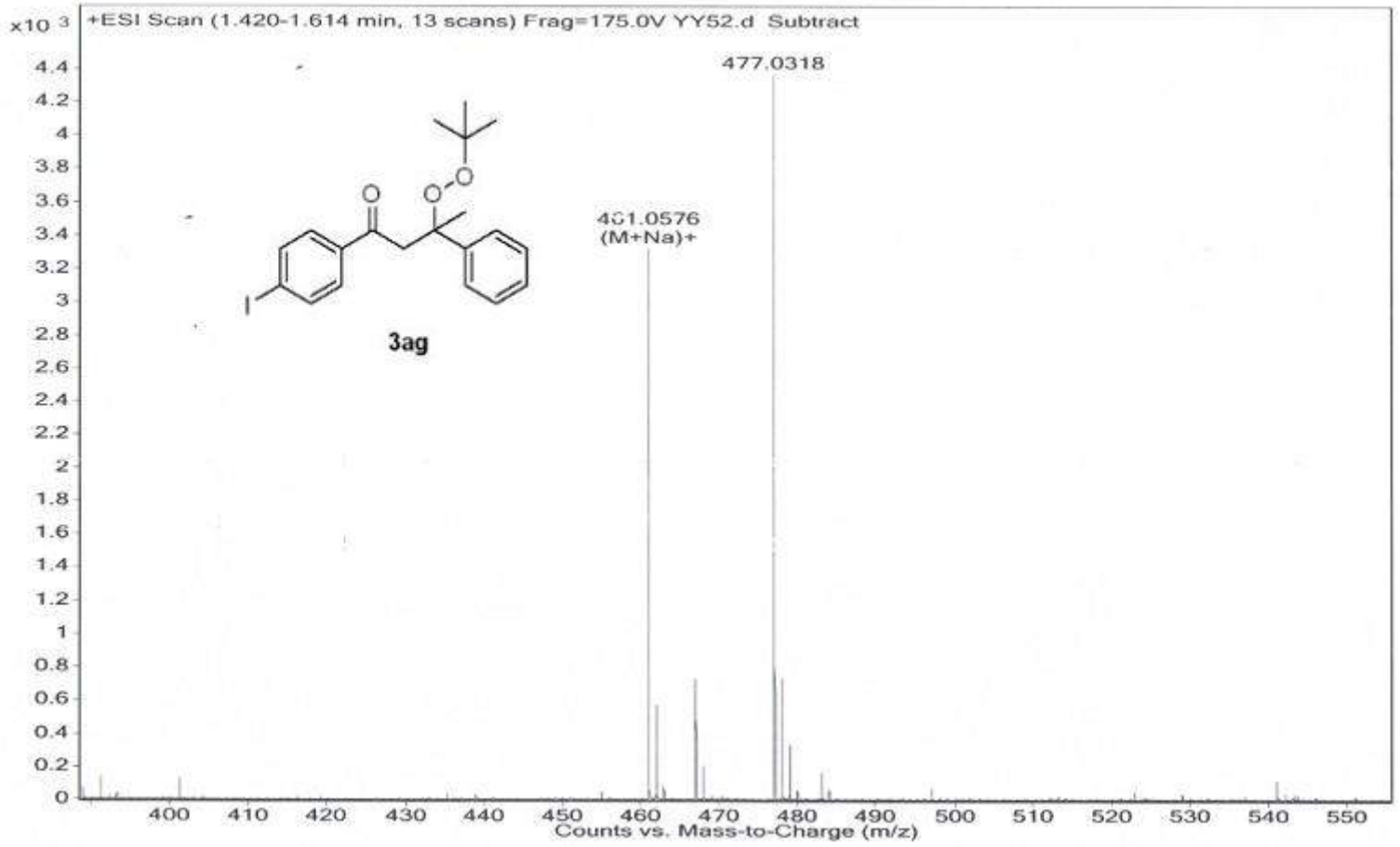


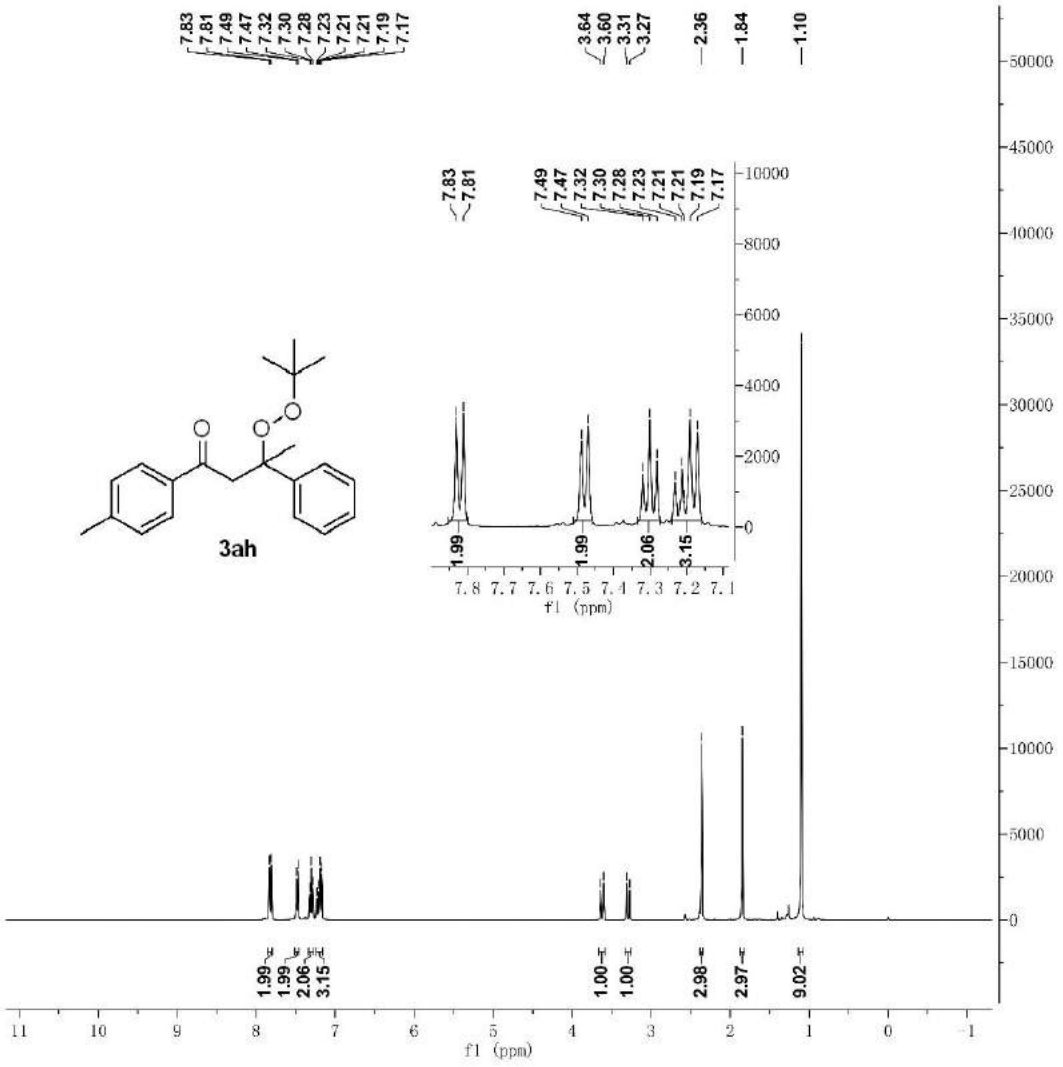
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy52/ 1/ fid
2 Title	yy52.1.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 13
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	56
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-04-06T15:18:00
21 Modification Date	2018-04-06T15:18:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1550.4
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



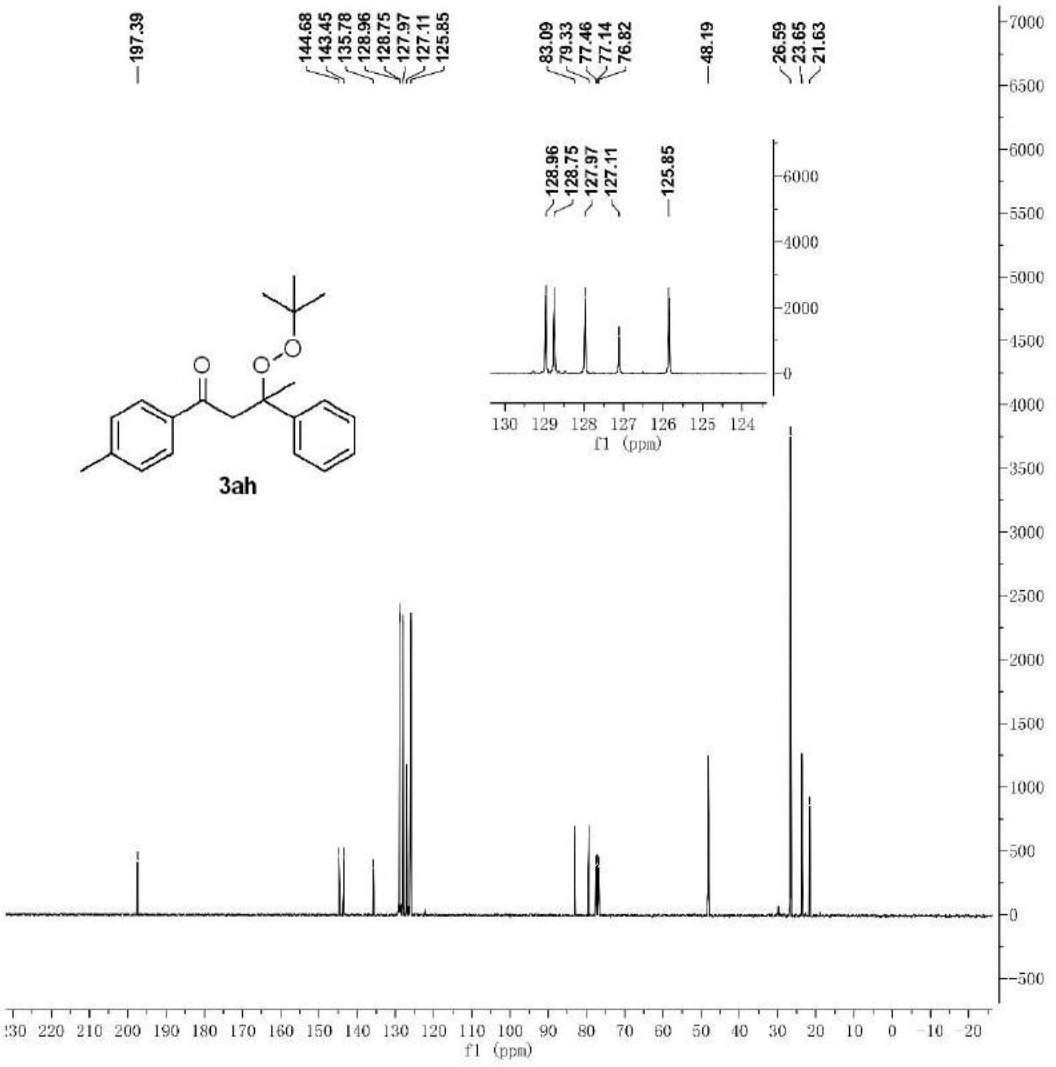
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy52/ 2/ fid
2 Title	yy52. 2. fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 13
4 Origin	Bruker BioSpin GmbH
5 Owner	rool
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	295. 8
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	600
15 Receiver Gain	78
16 Relaxation Delay	1. 0000
17 Pulse Width	10. 0000
18 Presaturation Frequency	
19 Acquisition Time	0. 4999
20 Acquisition Date	2018-04-06T15:35:00
21 Modification Date	2018-04-06T15:34:00
22 Class	
23 Spectrometer Frequency	100. 62
24 Spectral Width	35714. 3
25 Lowest Frequency	-7796. 8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	SampleS	**Position**	P1-A5	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY52.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/10/2018 3:38:45 PM

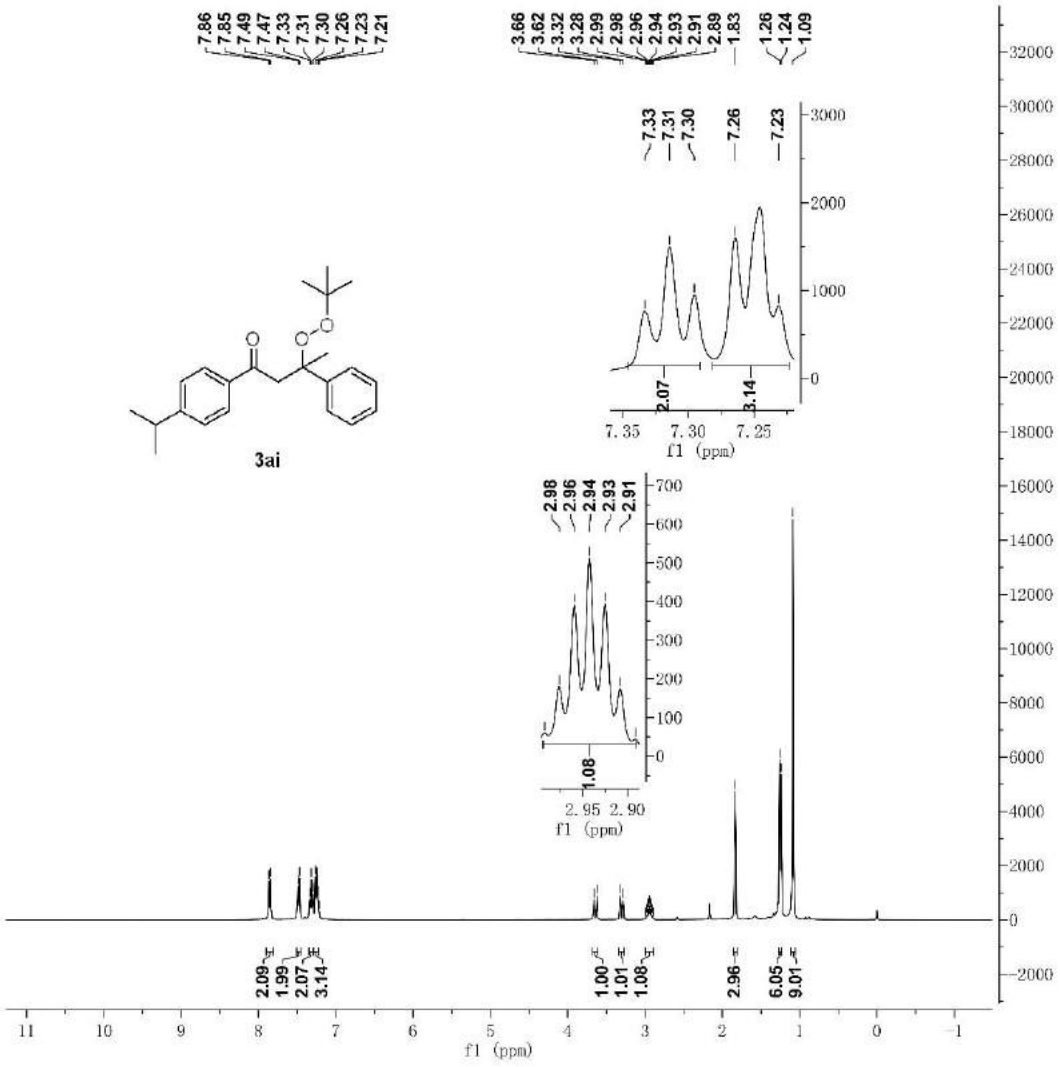




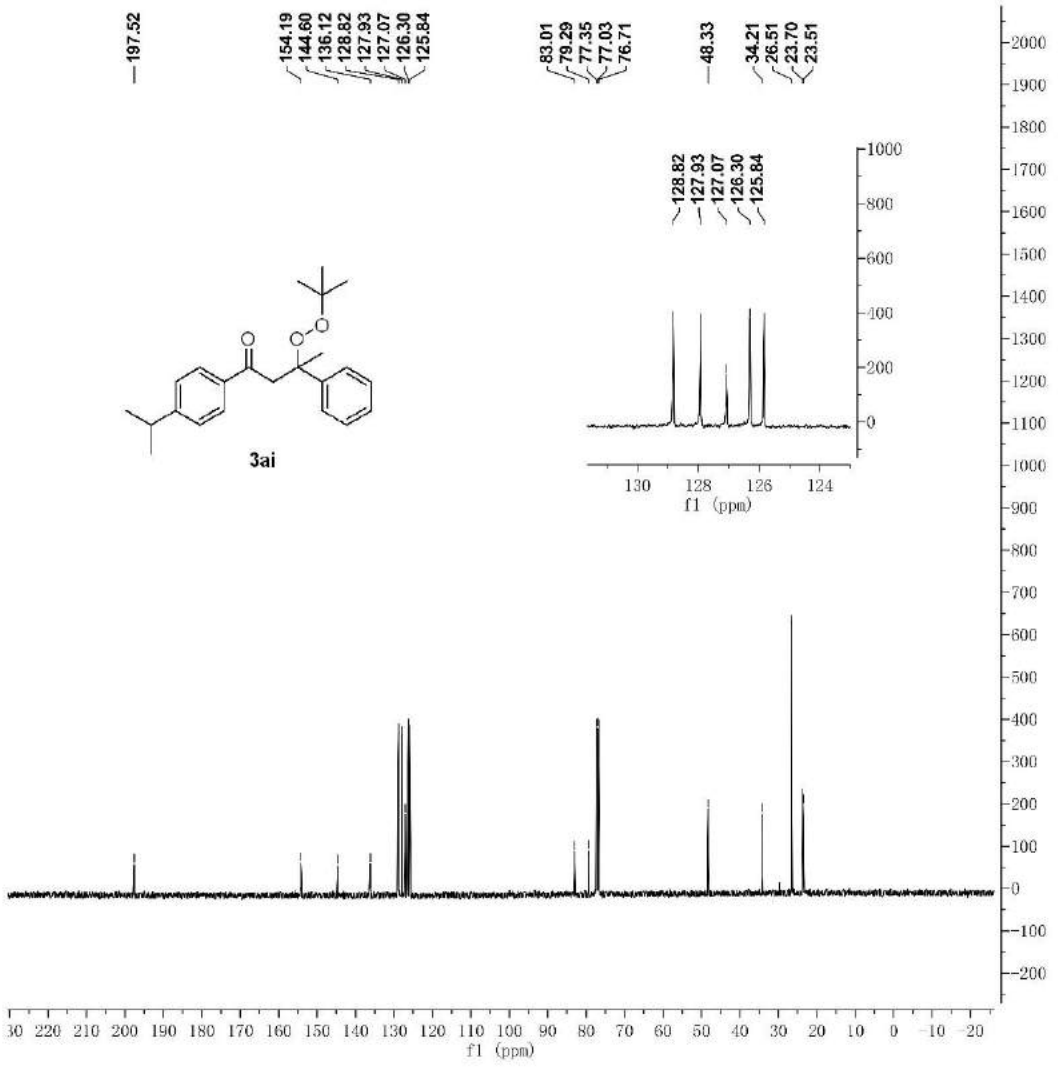
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy34/ 1/ fid
2 Title	yy34.1.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 2
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	19
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-03-30T03:53:00
21 Modification Date	2018 03 30T03:53:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1566.6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy34/ 2/ fid
2 Title	yy34. 2. fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 2
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	299. 0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	200
15 Receiver Gain	159
16 Relaxation Delay	1. 0000
17 Pulse Width	10. 0000
18 Presaturation Frequency	
19 Acquisition Time	0. 4999
20 Acquisition Date	2018-03-30T03:59:00
21 Modification Date	2018 03 30T03:59:00
22 Class	
23 Spectrometer Frequency	100. 62
24 Spectral Width	35711. 3
25 Lowest Frequency	-7796. 8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

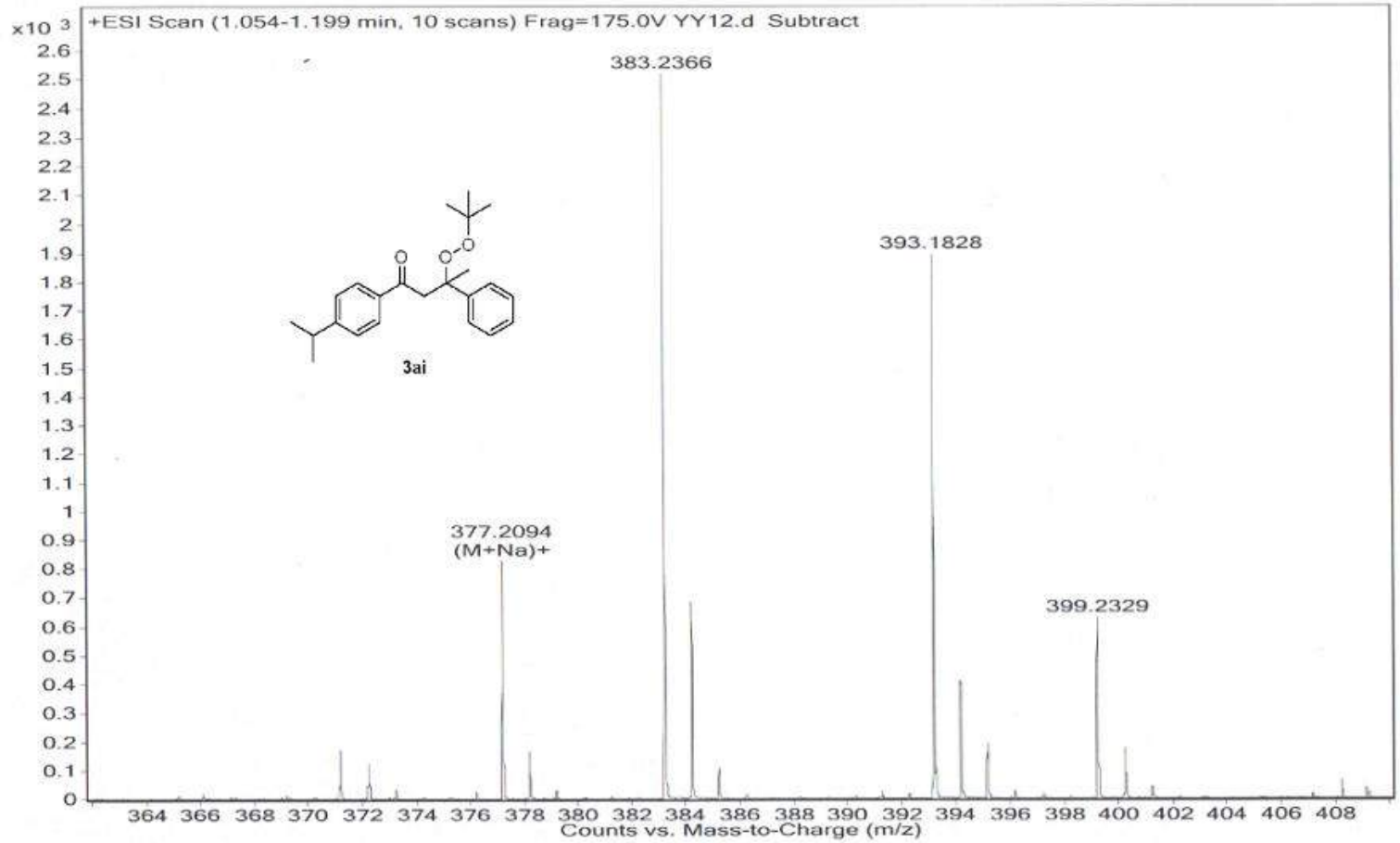


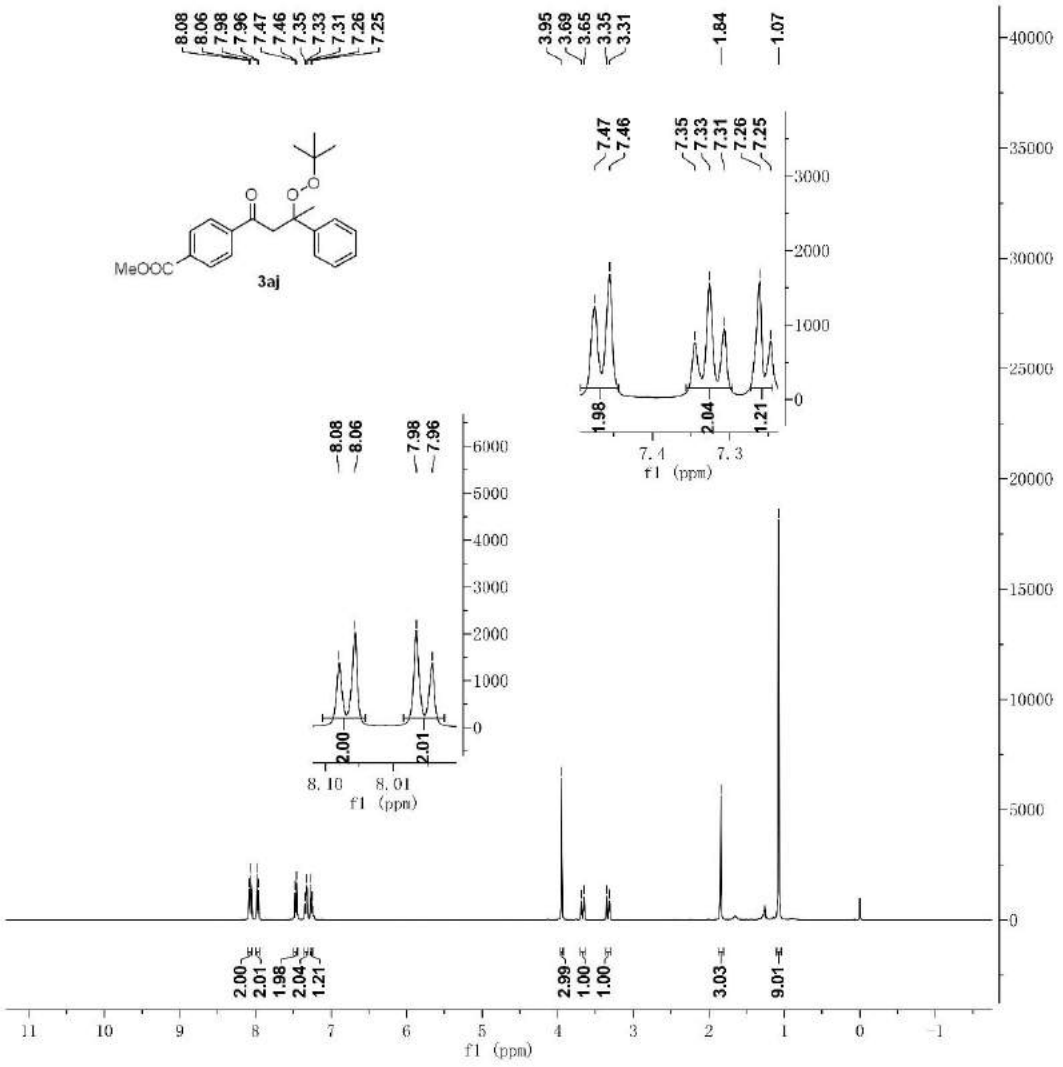
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ YYD/ 3/ fid
2 Title	YYD.3.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 14
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	78
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-03-21T01:45:00
21 Modification Date	2018-03-21T01:45:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1549.3
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



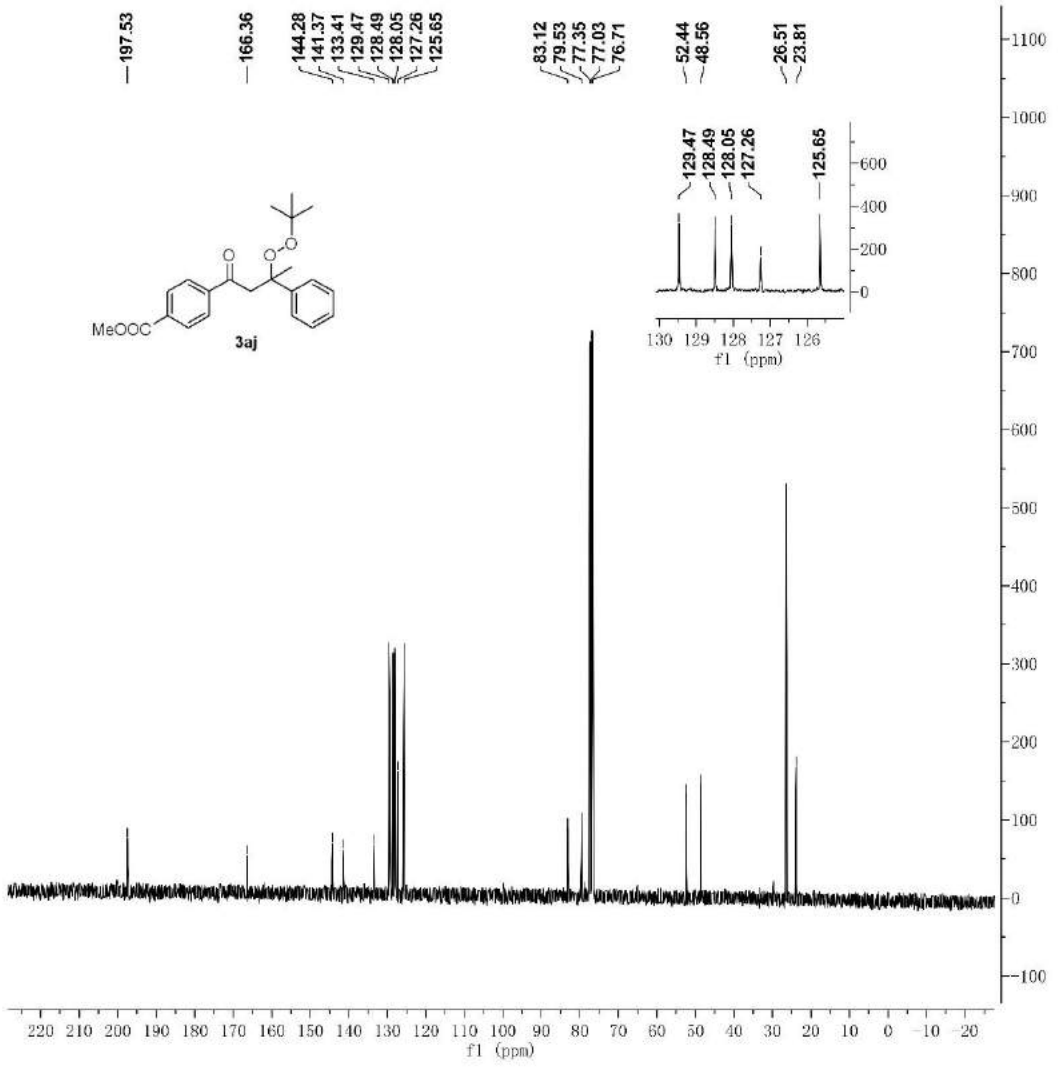
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ YYO/ 4/ fid
2 Title	YYO.4.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 14
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	500
15 Receiver Gain	78
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-03-21T01:59:00
21 Modification Date	2018 03 21T01:59:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample11	**Position**	P1-B2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY12.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/4/2018 10:30:03 AM



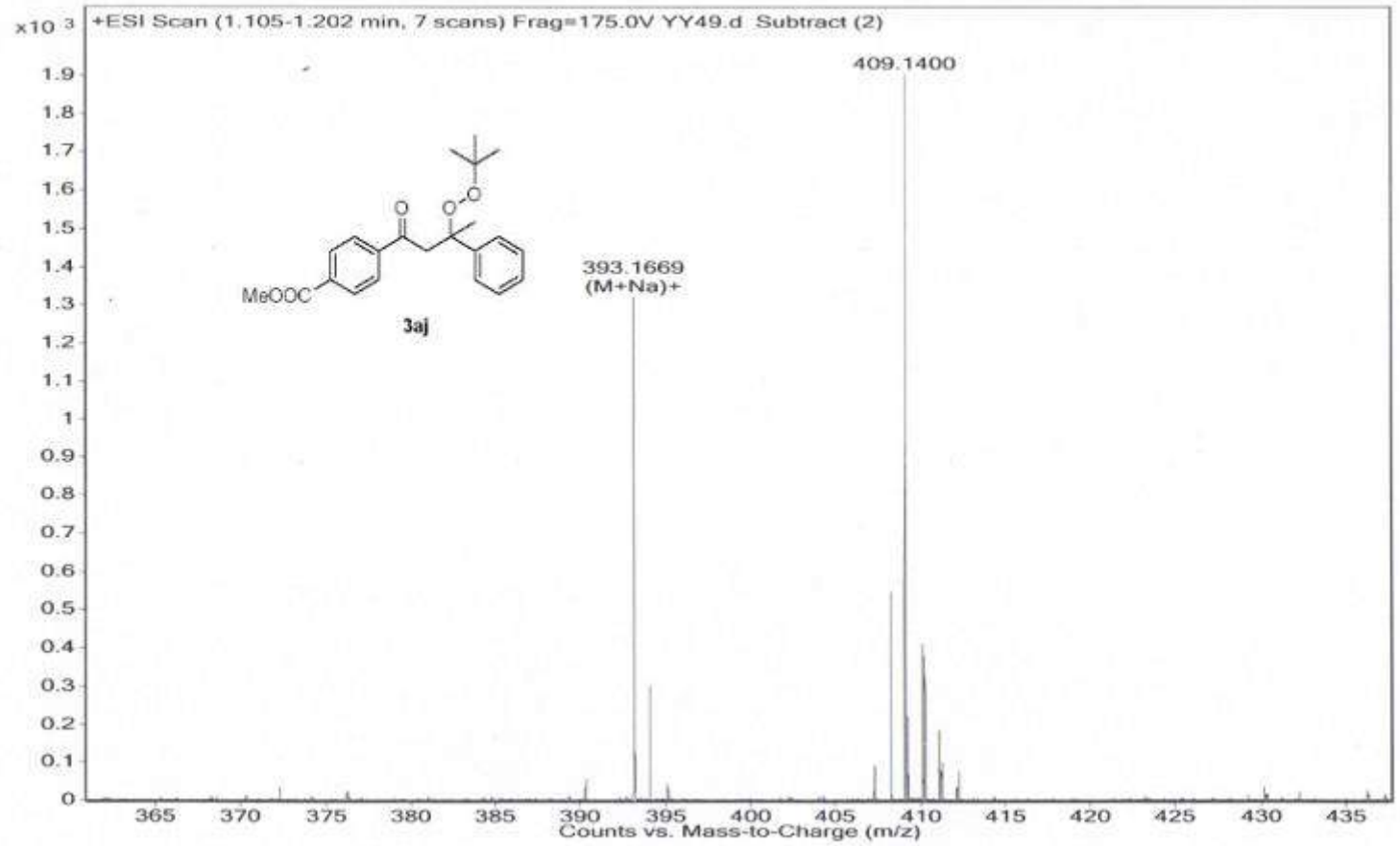


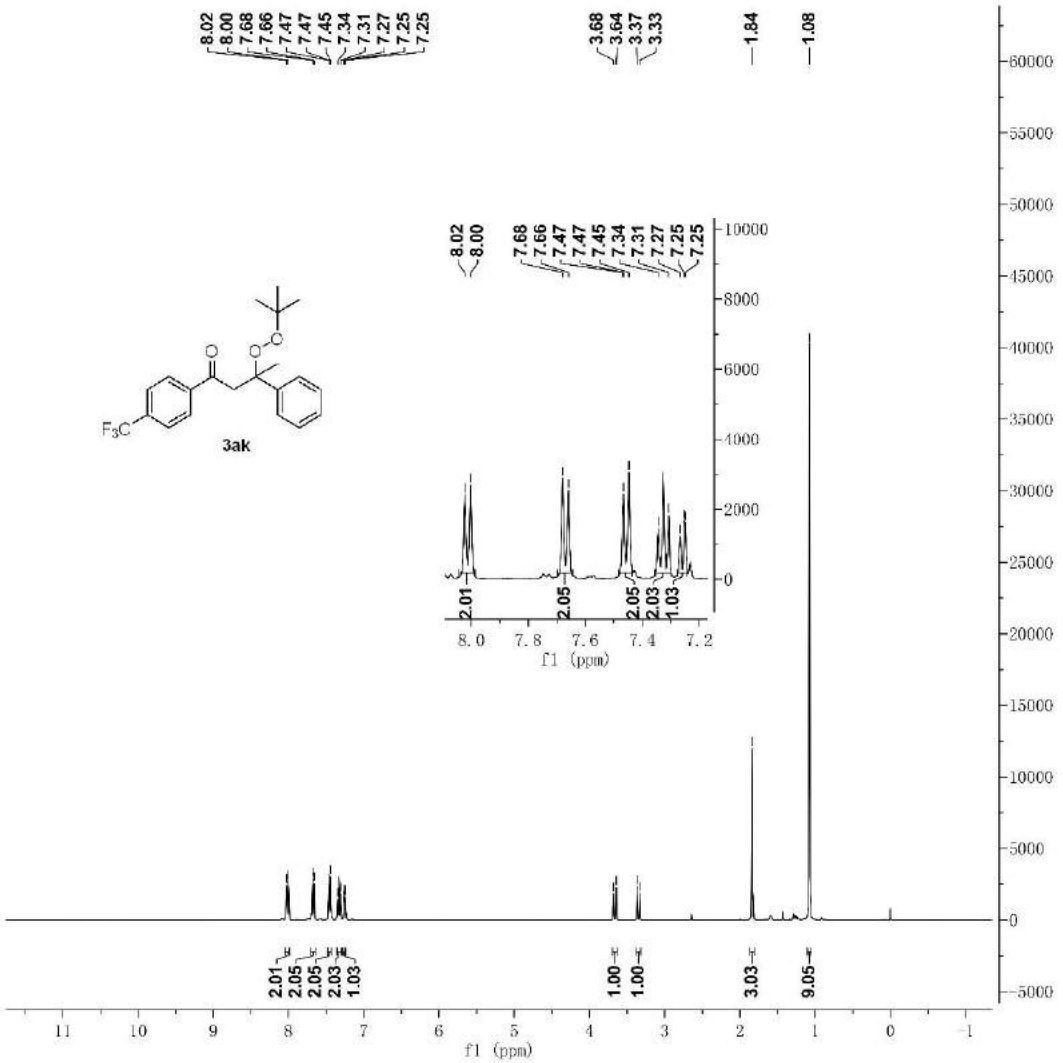
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy49/ 9/ fid
2 Title	yy49.9.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 1D
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	293.4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	119
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-04-24T20:14:00
21 Modification Date	2018-04-24T20:14:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1545.5
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



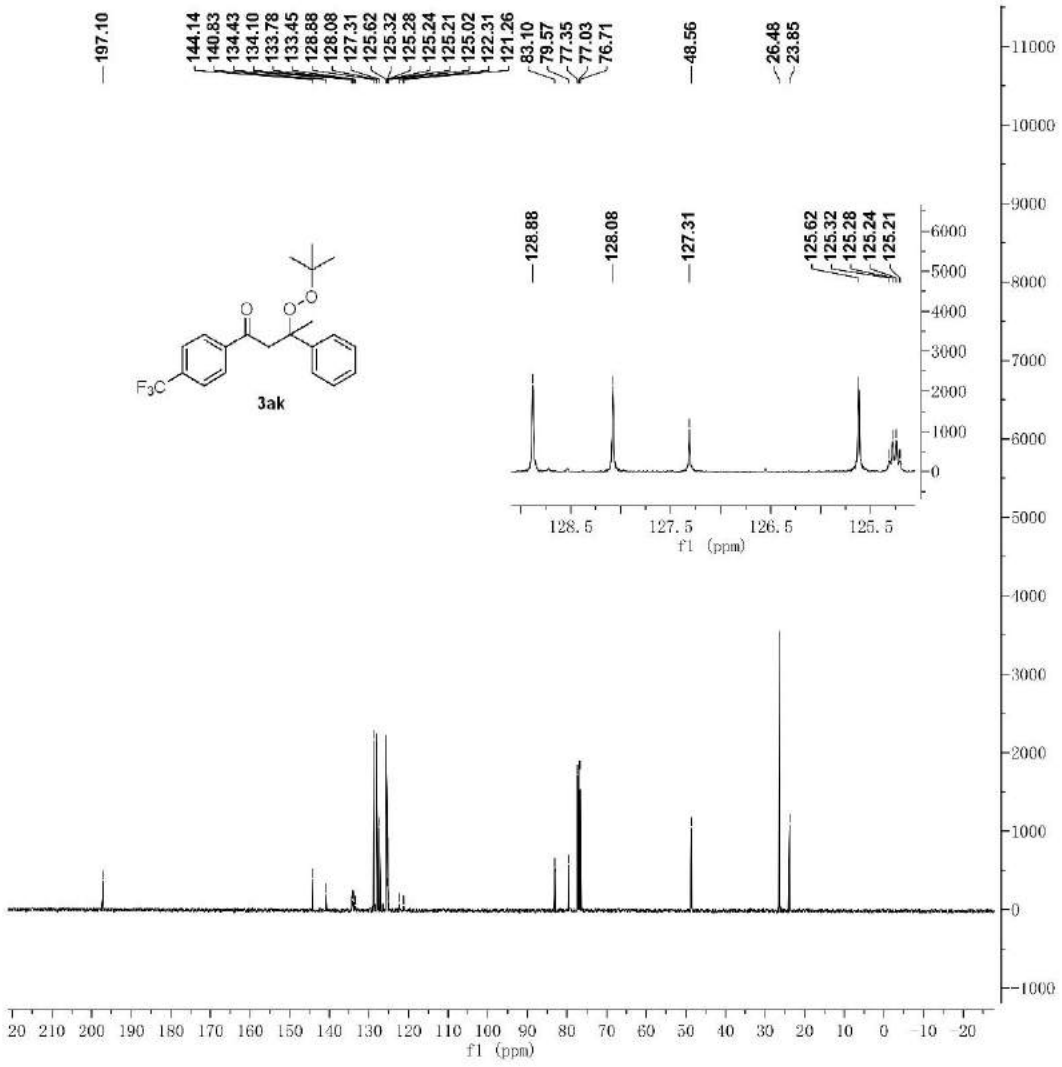
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy49/ 10/ fid
2 Title	yy49.10.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 1D
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.3
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	400
15 Receiver Gain	113
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-04-24T20:26:00
21 Modification Date	2018-04-24T20:25:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample2	**Position**	P1-A2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY49.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/10/2018 3:21:18 PM



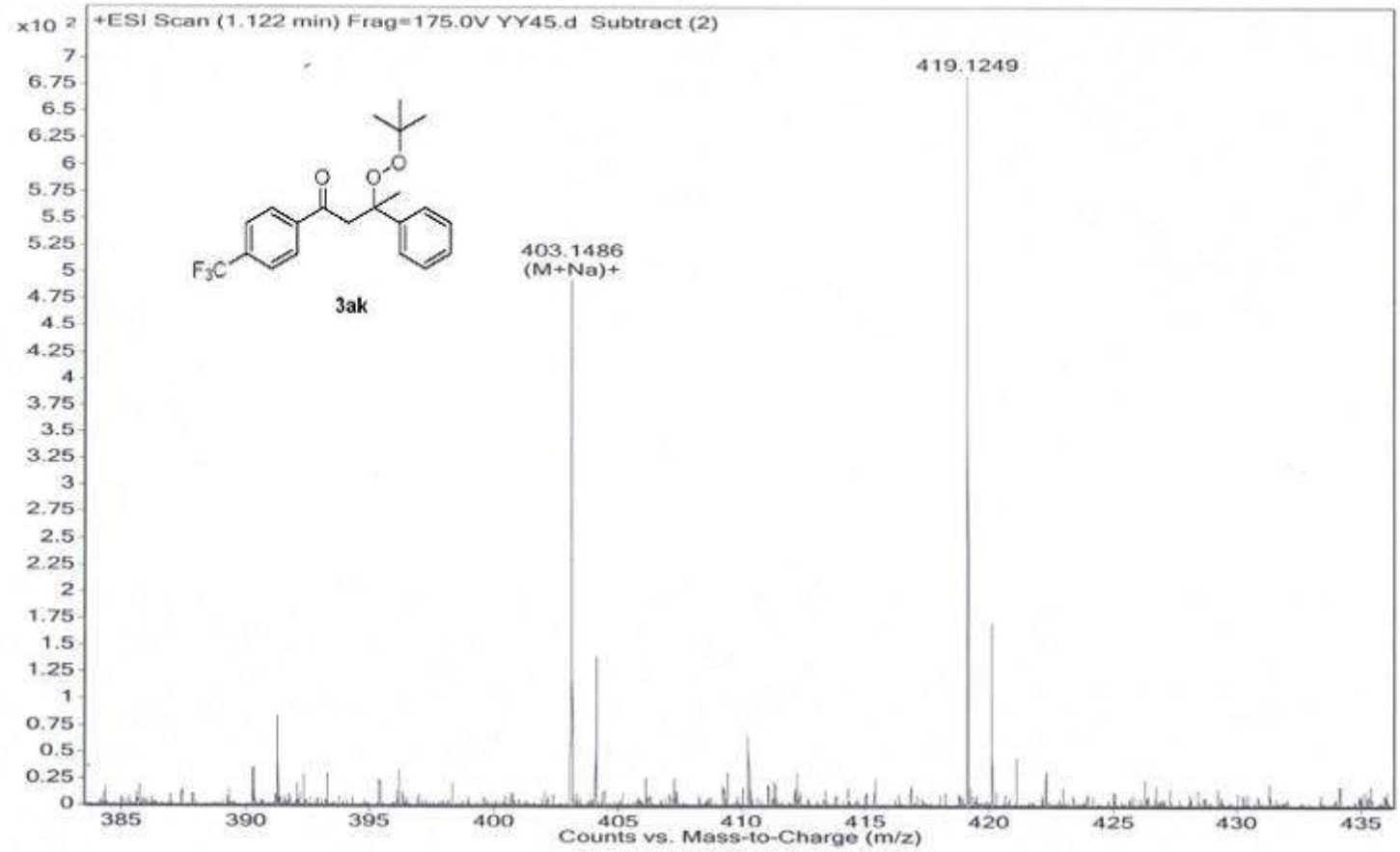


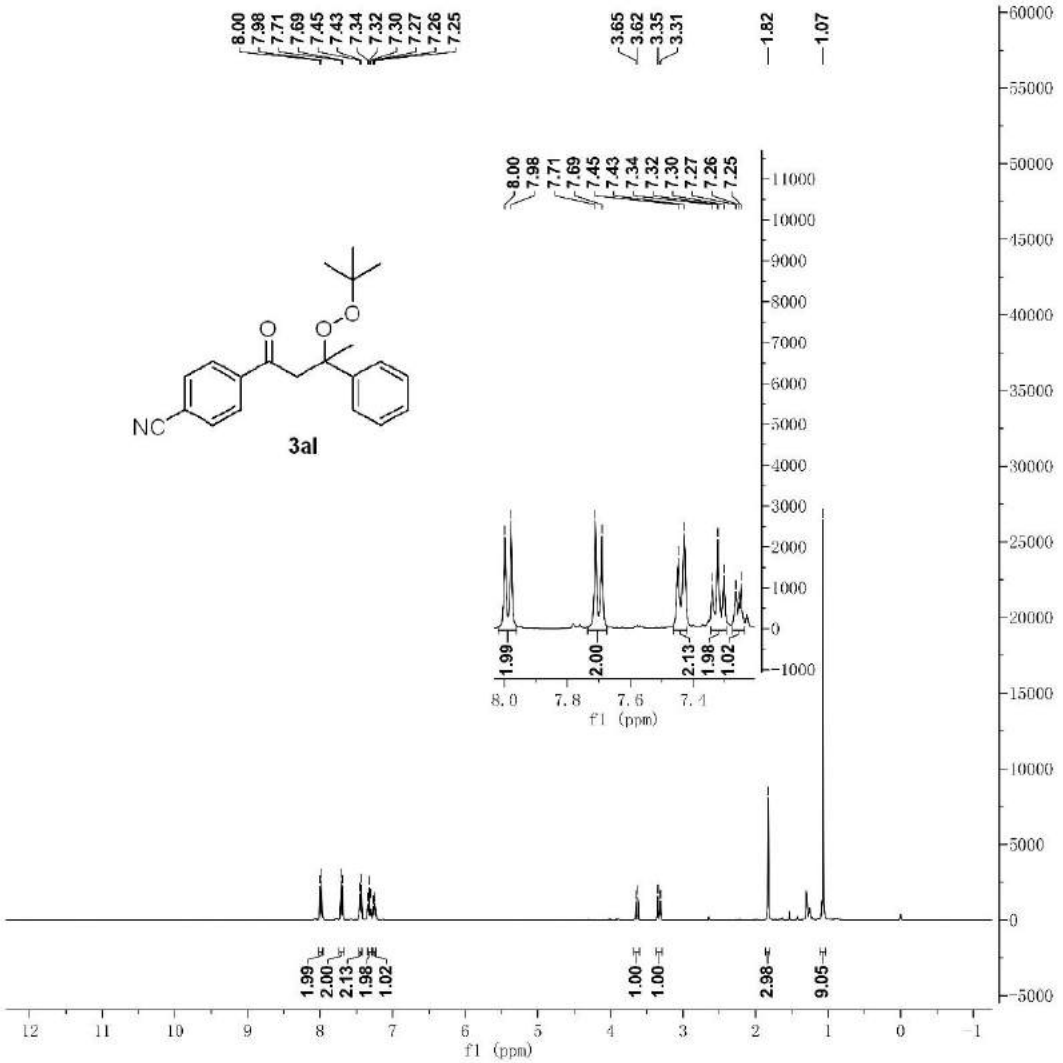
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy45/ 7/ fid
2 Title	yy45.7.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 15
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	293.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	78
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-04-21T15:45:00
21 Modification Date	2018-04-21T15:44:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1548.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



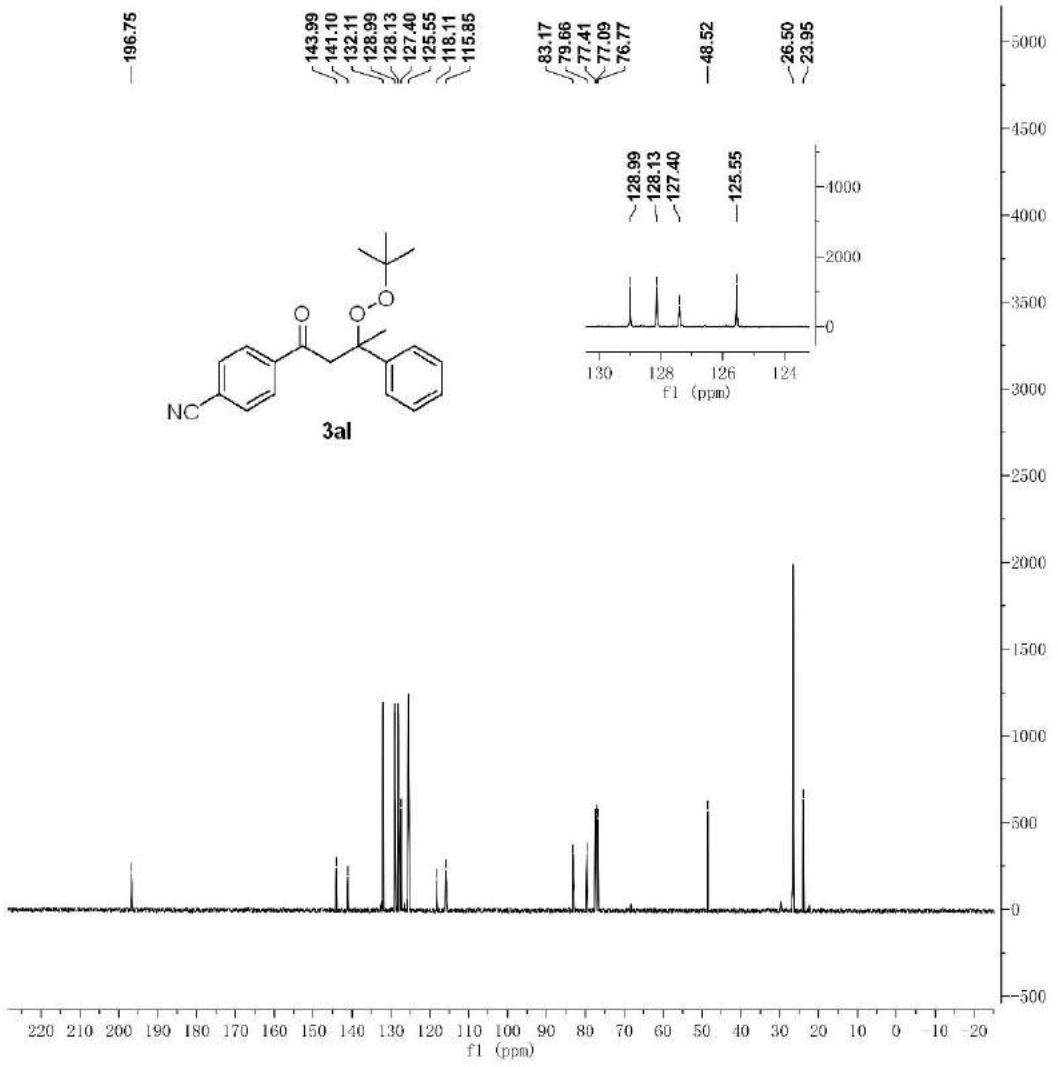
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy45/ 8/ fid
2 Title	yy45.8.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 15
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.6
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	600
15 Receiver Gain	200
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-04-21T16:05:00
21 Modification Date	2018 04 21T16:04:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample3	**Position**	P1-A3	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY45.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/10/2018 3:27:07 PM

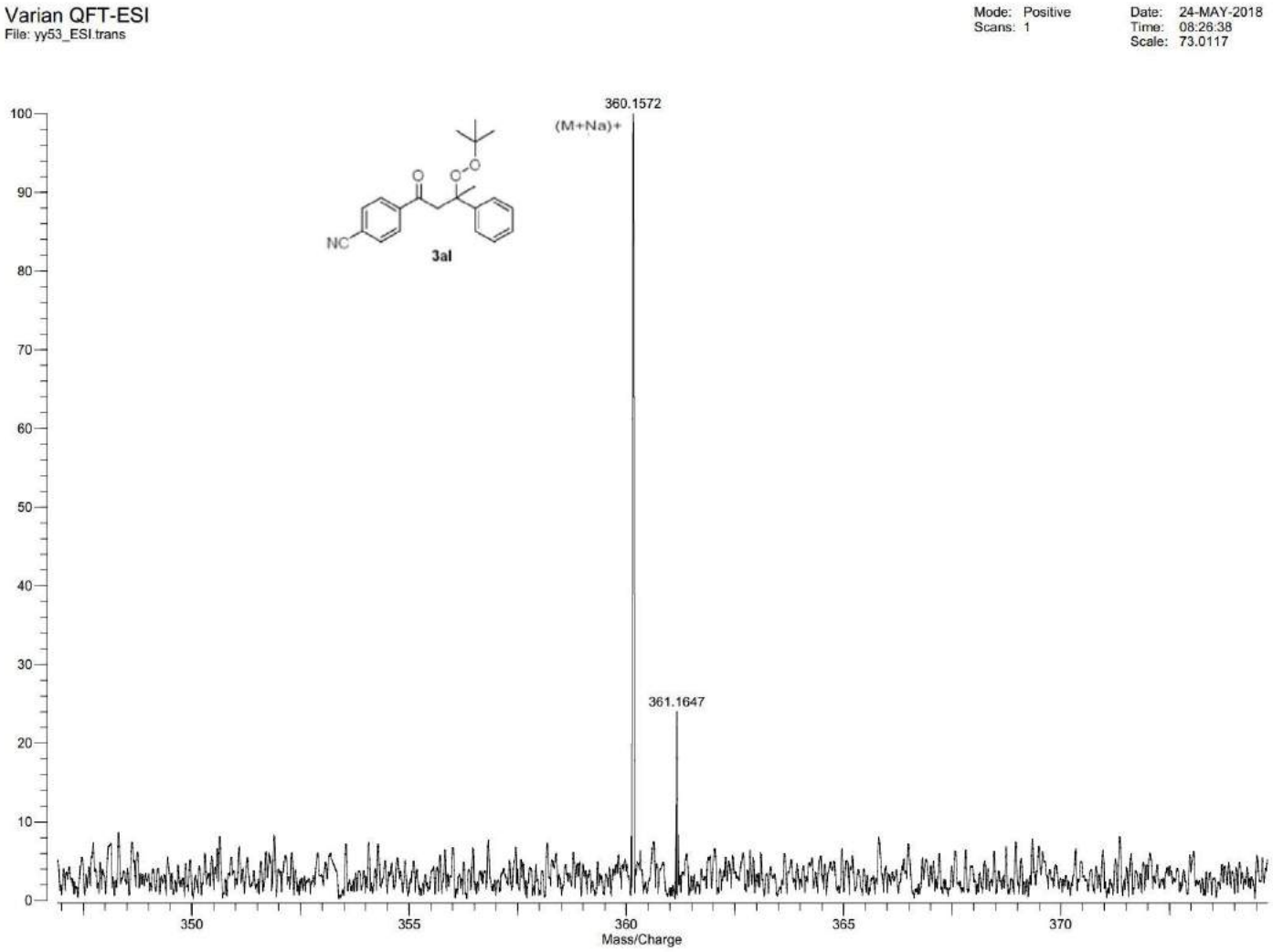


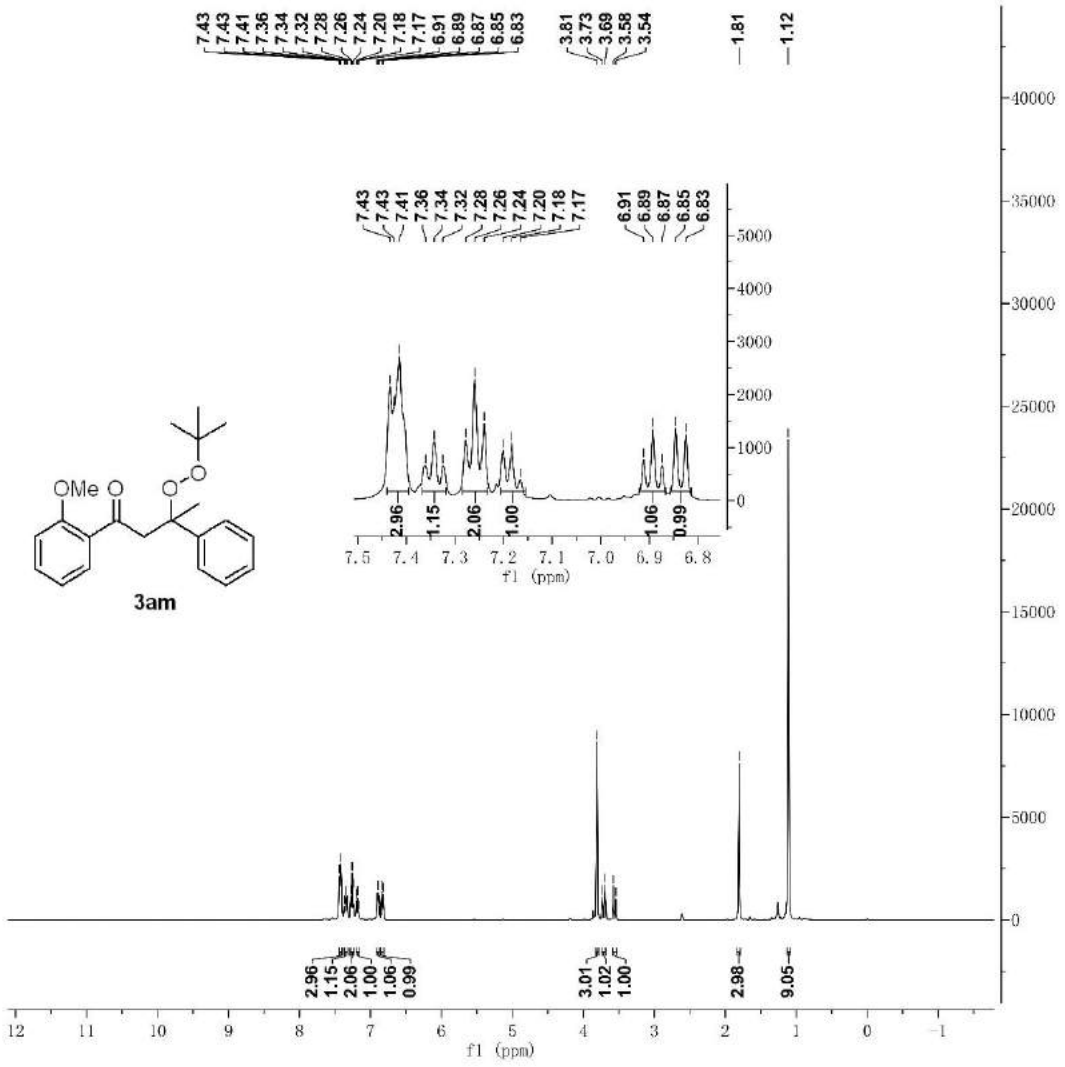


Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy53/ yy53/ 9/ fid
2 Title	yy53.9.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 6
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	293.5
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	33
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-04-24T19:19:00
21 Modification Date	2018-04-24T19:19:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1547.7
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

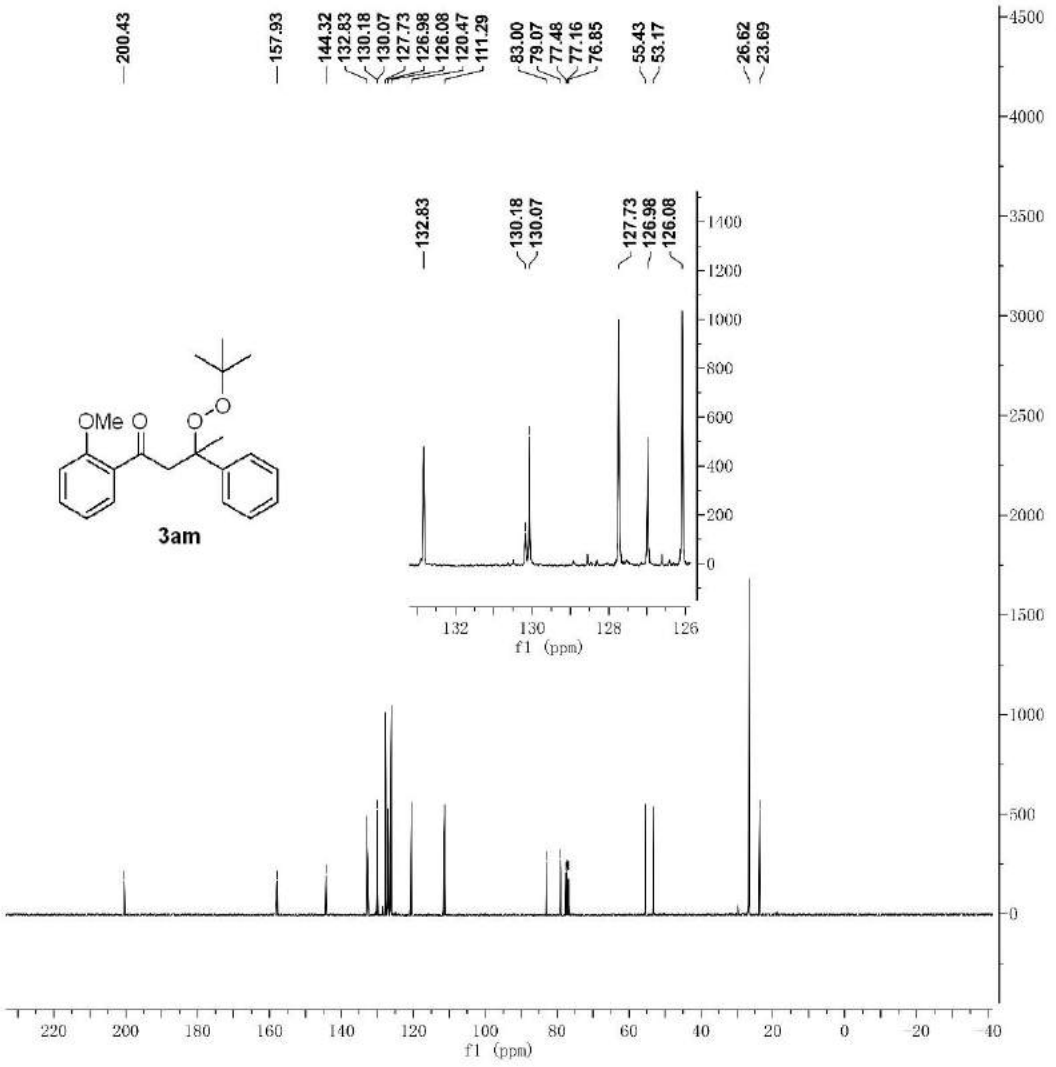


Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy53/ yy53/ 10/ fid
2 Title	yy53.10.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 6
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.3
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-[H/ D Z-GRD Z108618/ 0525
14 Number of Scans	200
15 Receiver Gain	200
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-04-24T19:25:00
21 Modification Date	2018 04 24T19:25:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536


Varian QFT-ESI
File: yy53_ESI.trans
Mode: Positive
Scans: 1
Date: 24-MAY-2018
Time: 08:26:38
Scale: 73.0117
360.1572
(M+Na)+
361.1647
3al
NC
O
O-O
100
90
80
70
60
50
40
30
20
10
0
350
355
360
365
370
Mass/Charge

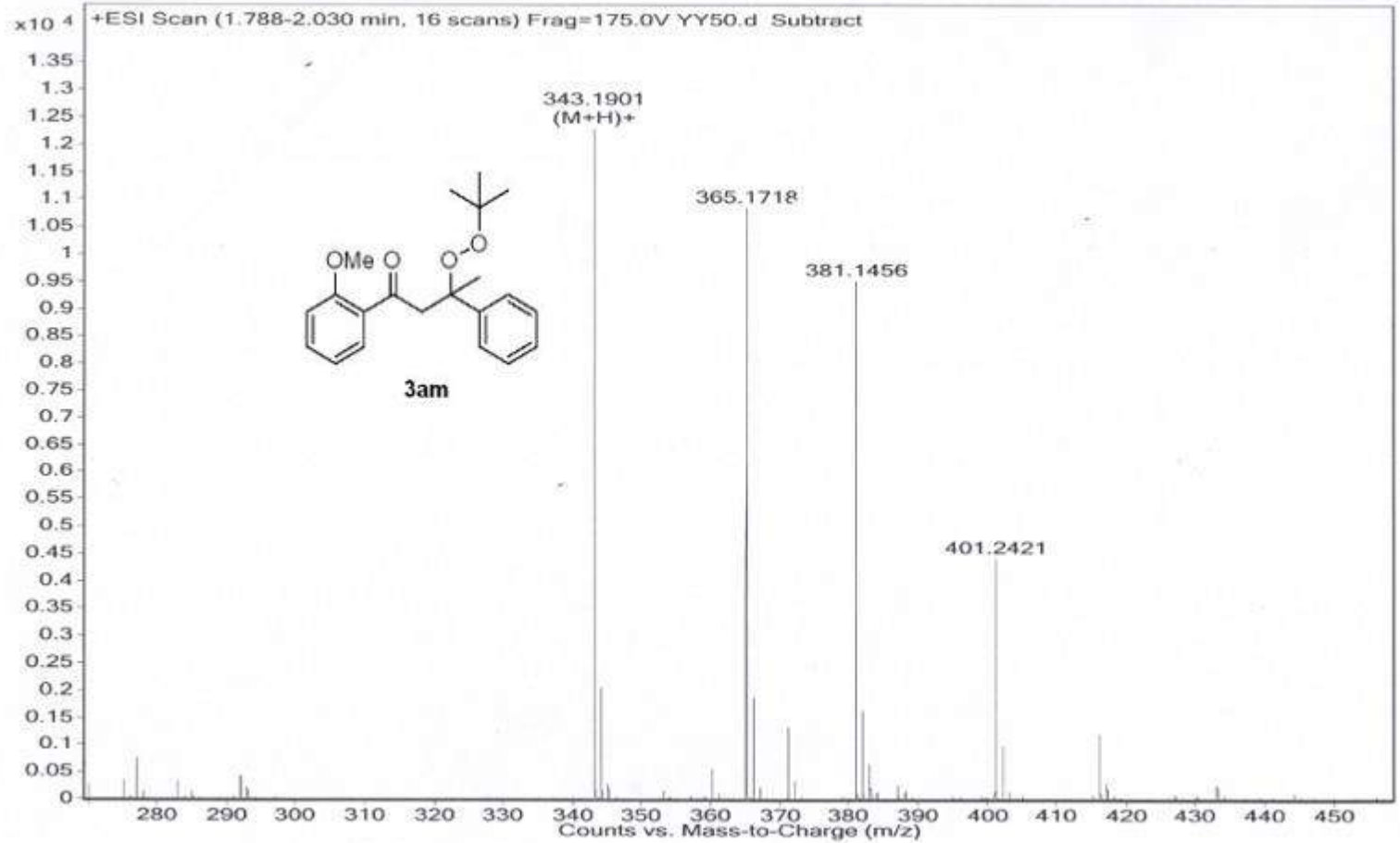


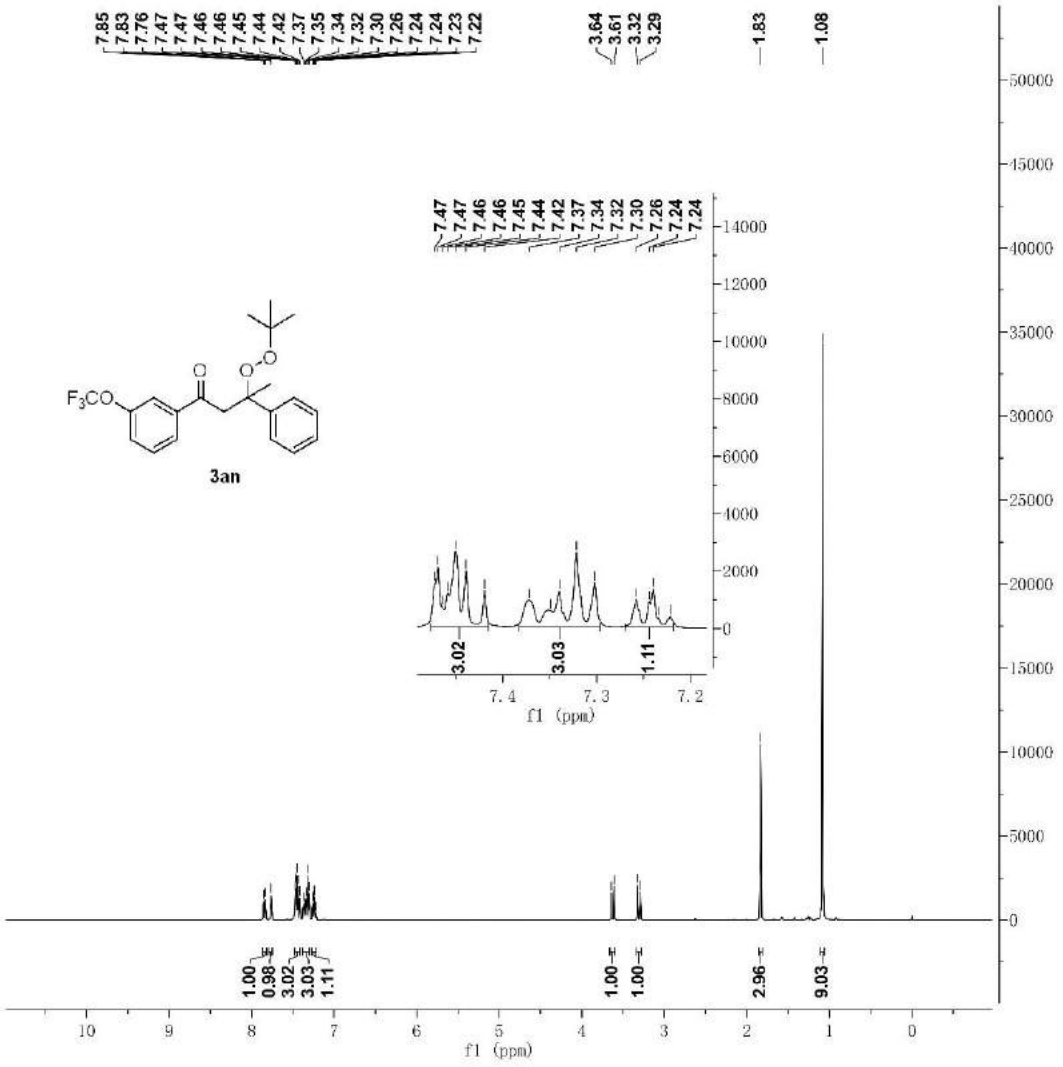
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy50/ 1/ fid
2 Title	yy50.1.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 14
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	19
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-01-04T21:56:00
21 Modification Date	2018 04 04T21:55:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1563.7
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



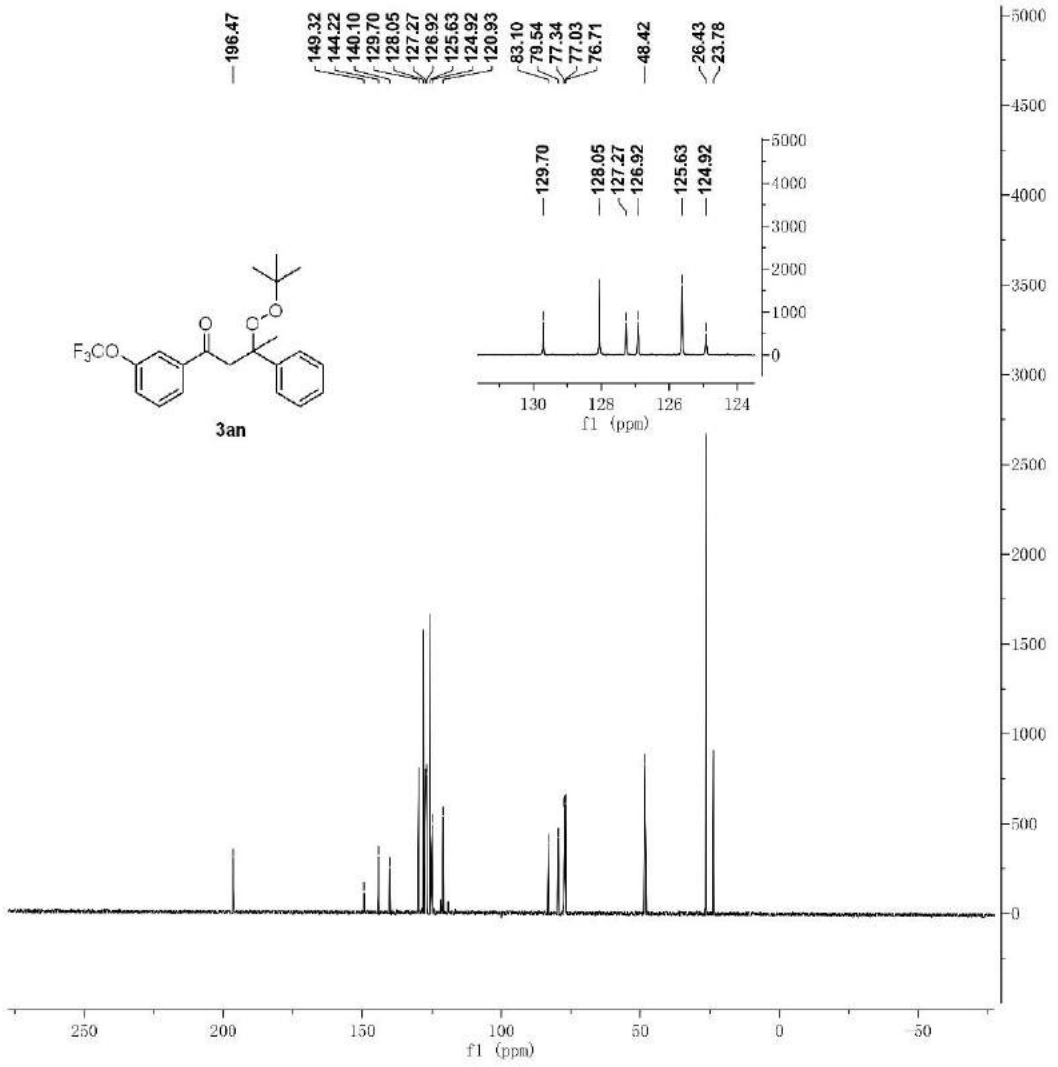
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy50/ 2/ fid
2 Title	yy50.2.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 14
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	295.6
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	200
15 Receiver Gain	78
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-04-04T22:02:00
21 Modification Date	2018 04 04T22:01:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample4	**Position**	P1-A4	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY50.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/10/2018 3:32:56 PM



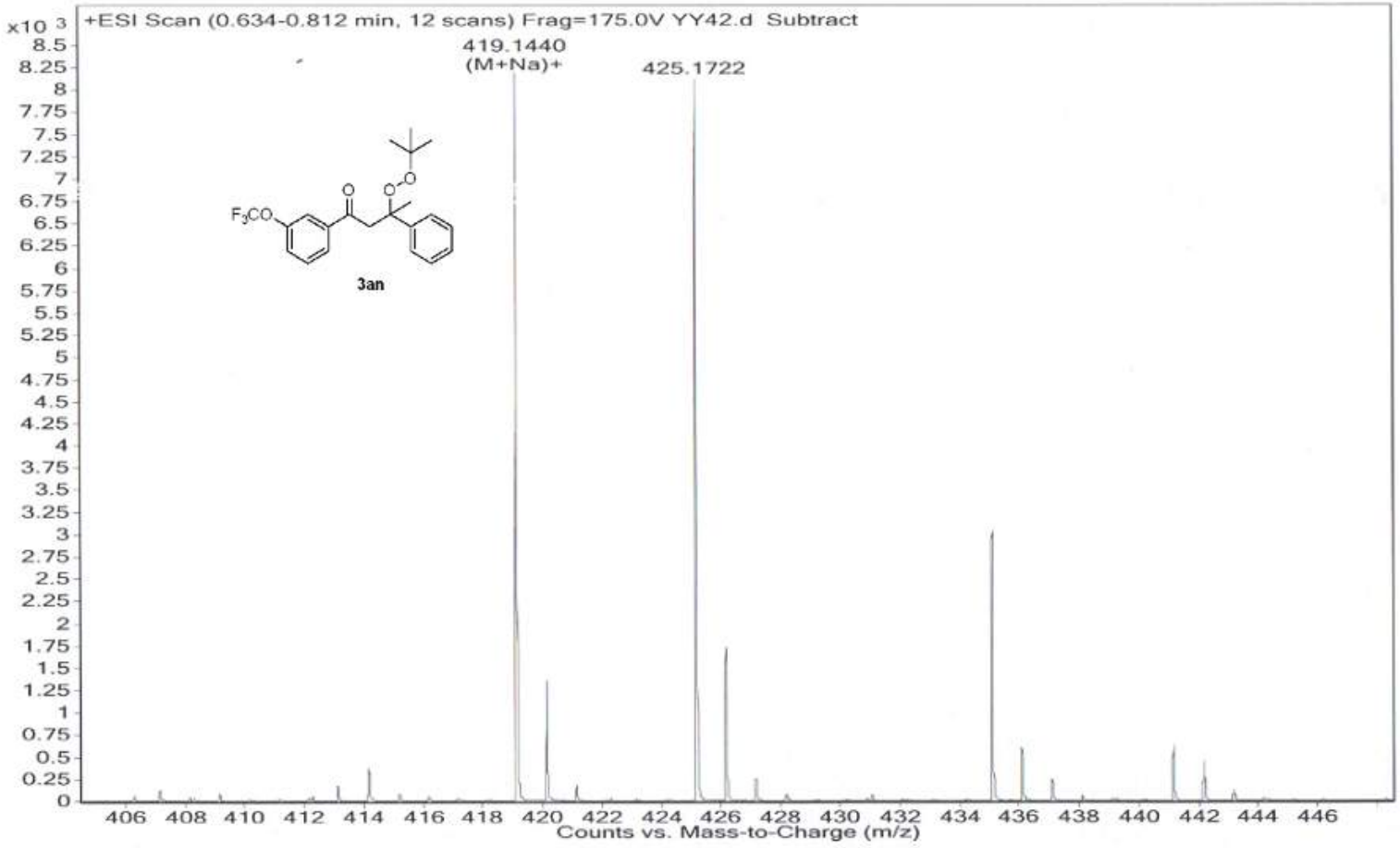


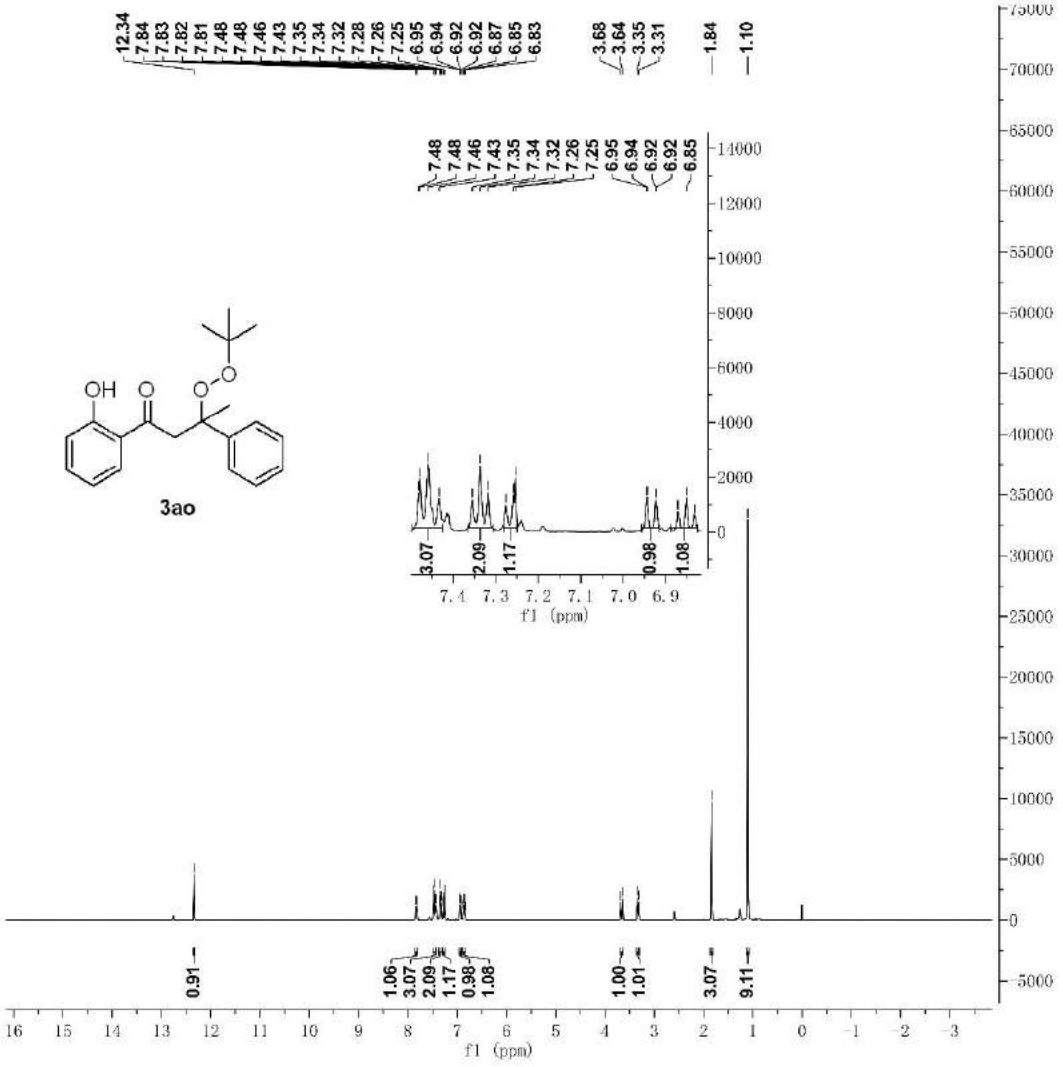
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy42/ 1/ fid
2 Title	yy42.1.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 21
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.3
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	33
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-03-30T02:09:00
21 Modification Date	2018-03-30T02:09:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1552.0
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



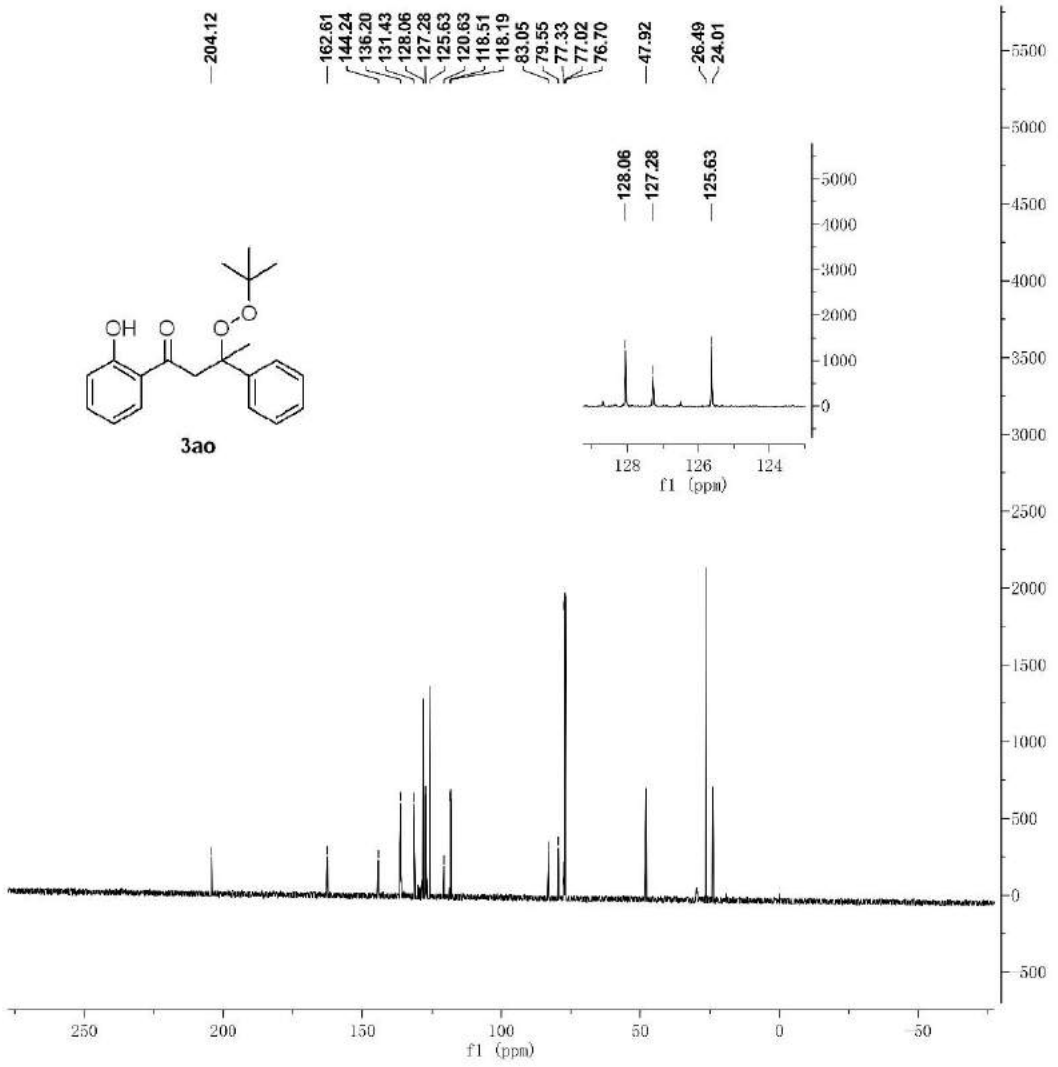
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy42/ 2/ fid
2 Title	yy42.2.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 21
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	299.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	400
15 Receiver Gain	113
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-03-30T02:21:00
21 Modification Date	2018 03 30T02:20:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample20	**Position**	P1-C2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY42.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/4/2018 11:22:23 AM



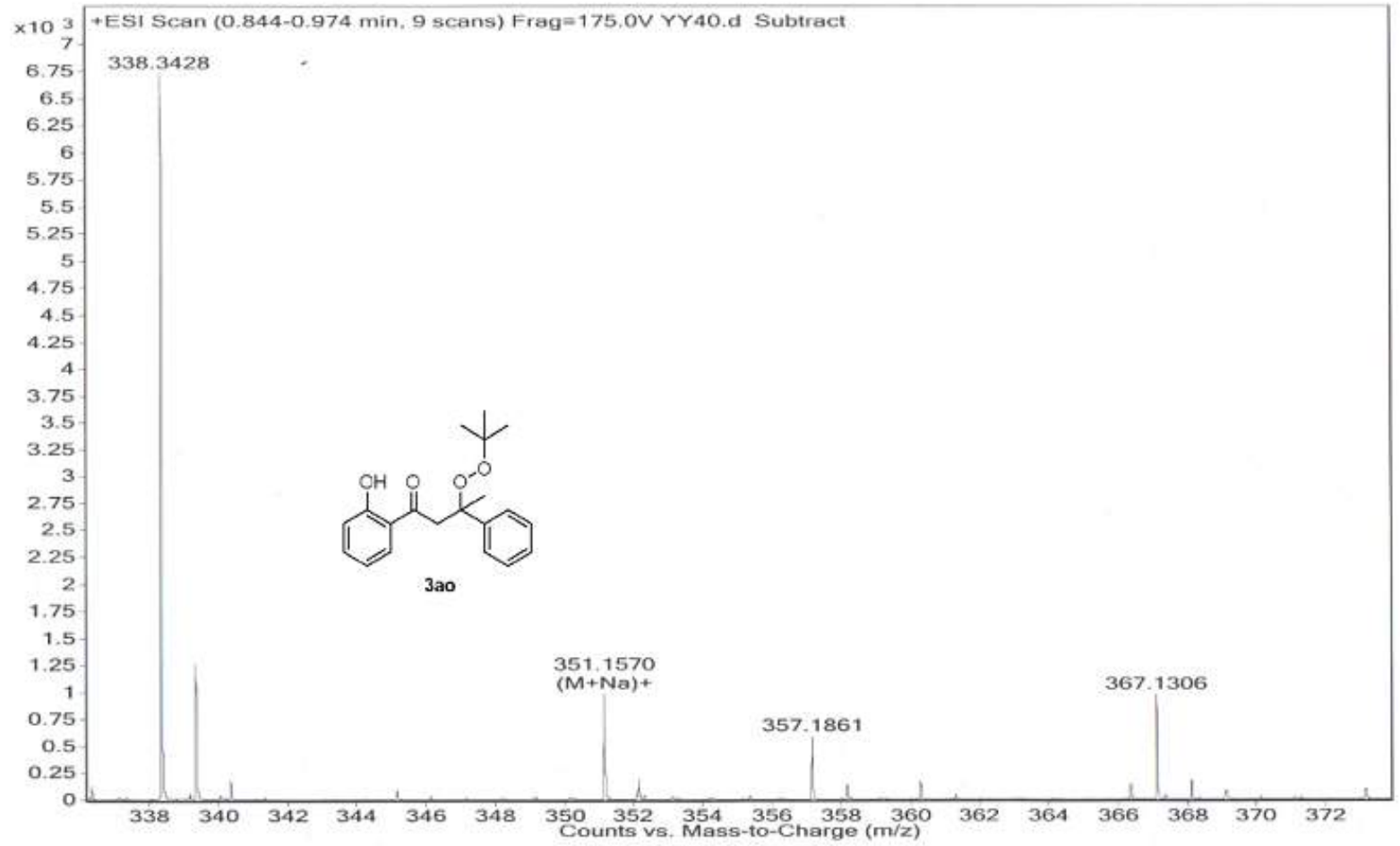


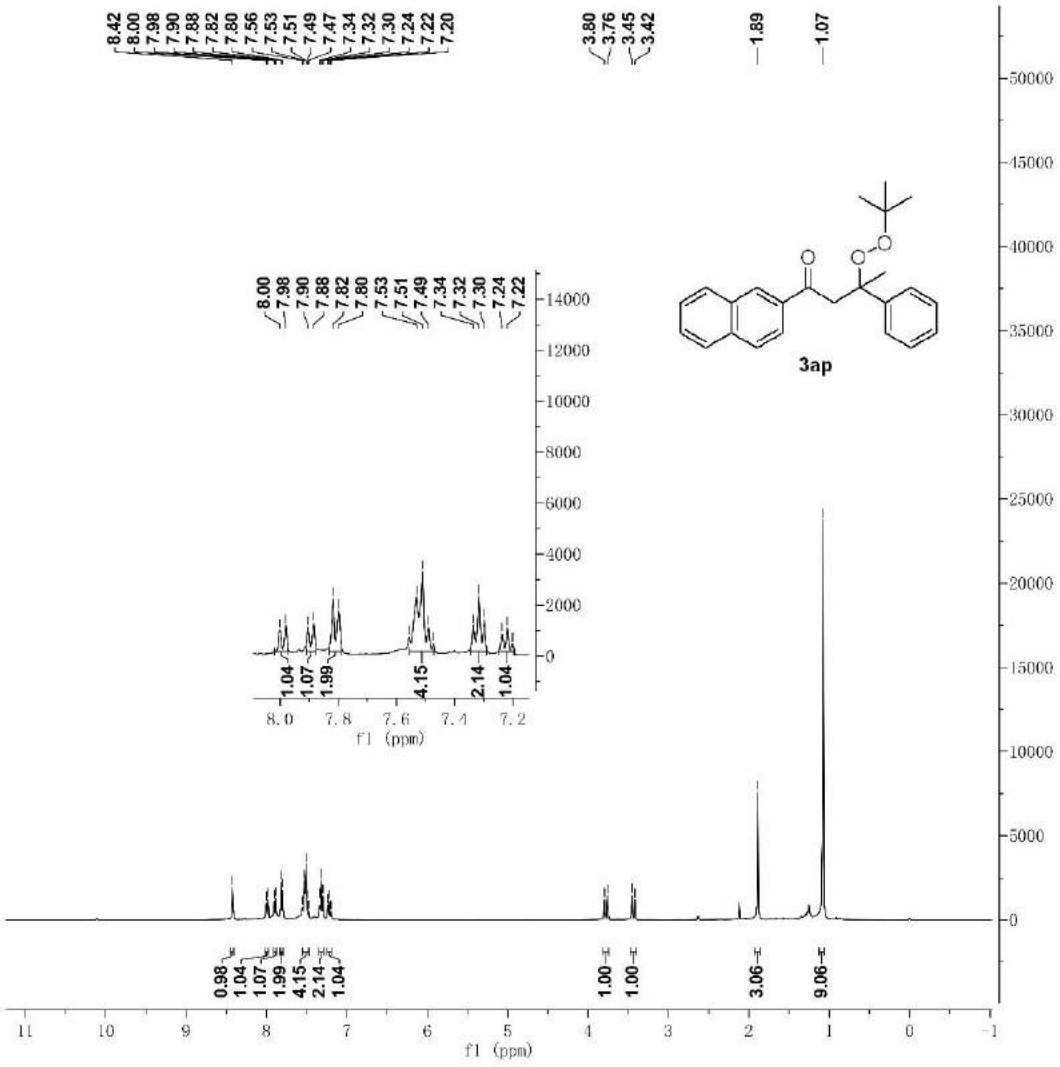
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy40/ 1/ fid
2 Title	yy40.1.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 22
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.3
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	113
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-03-30T02:26:00
21 Modification Date	2018 03 30T02:26:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1548.3
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



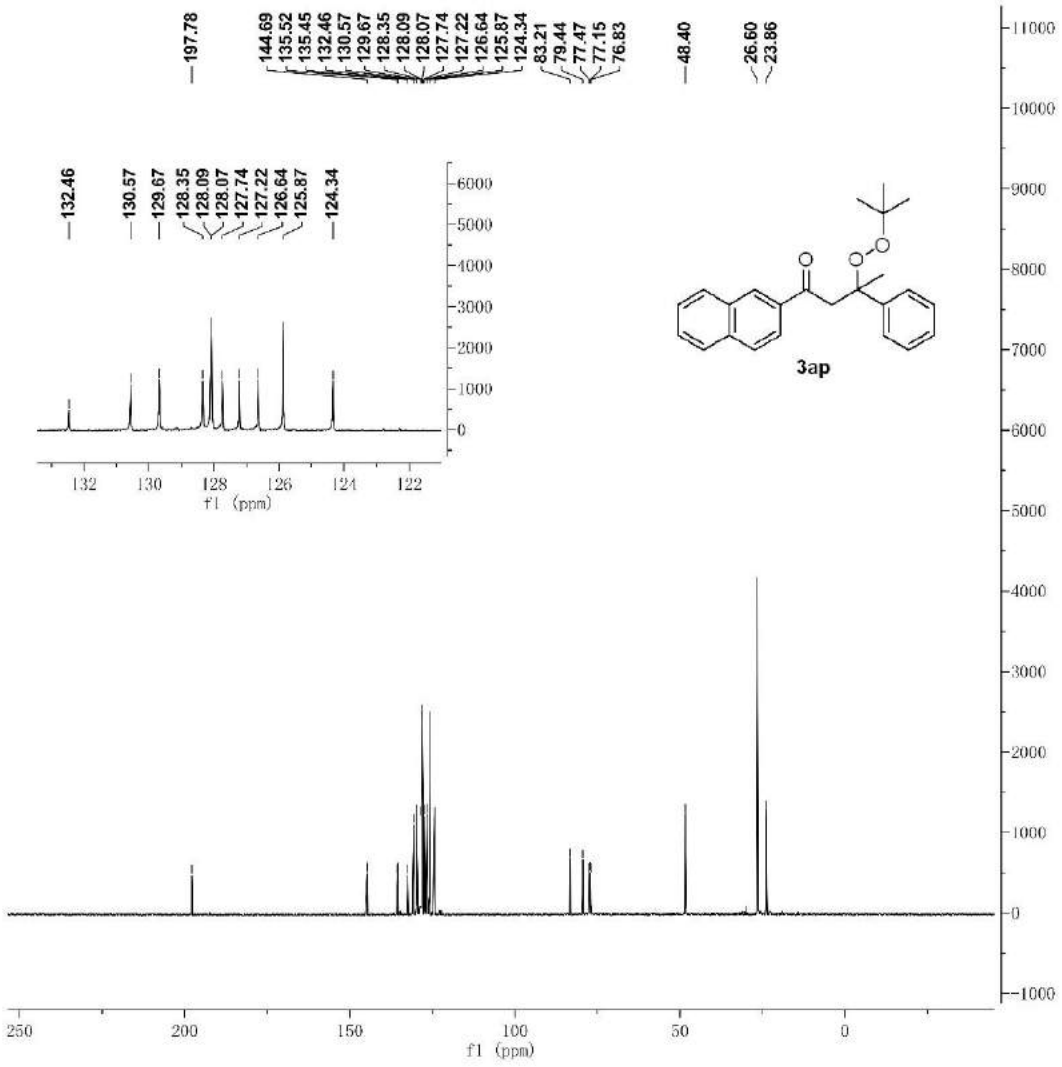
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy40/ 2/ fid
2 Title	yy40.2.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 22
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	299.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	1024
15 Receiver Gain	133
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-03-30T02:54:00
21 Modification Date	2018 03 30T02:53:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample19	**Position**	P1-C1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY40.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/4/2018 11:16:34 AM



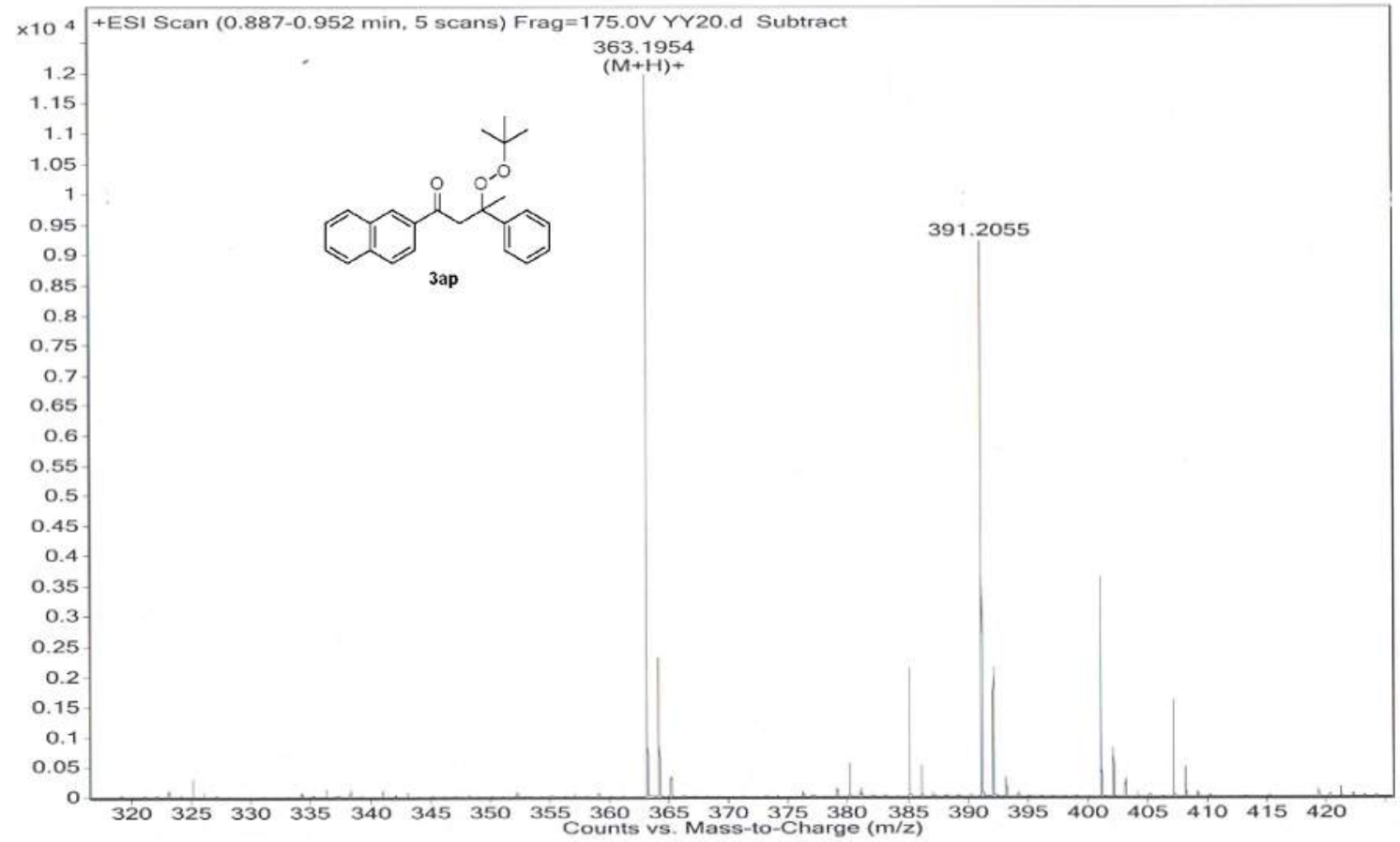


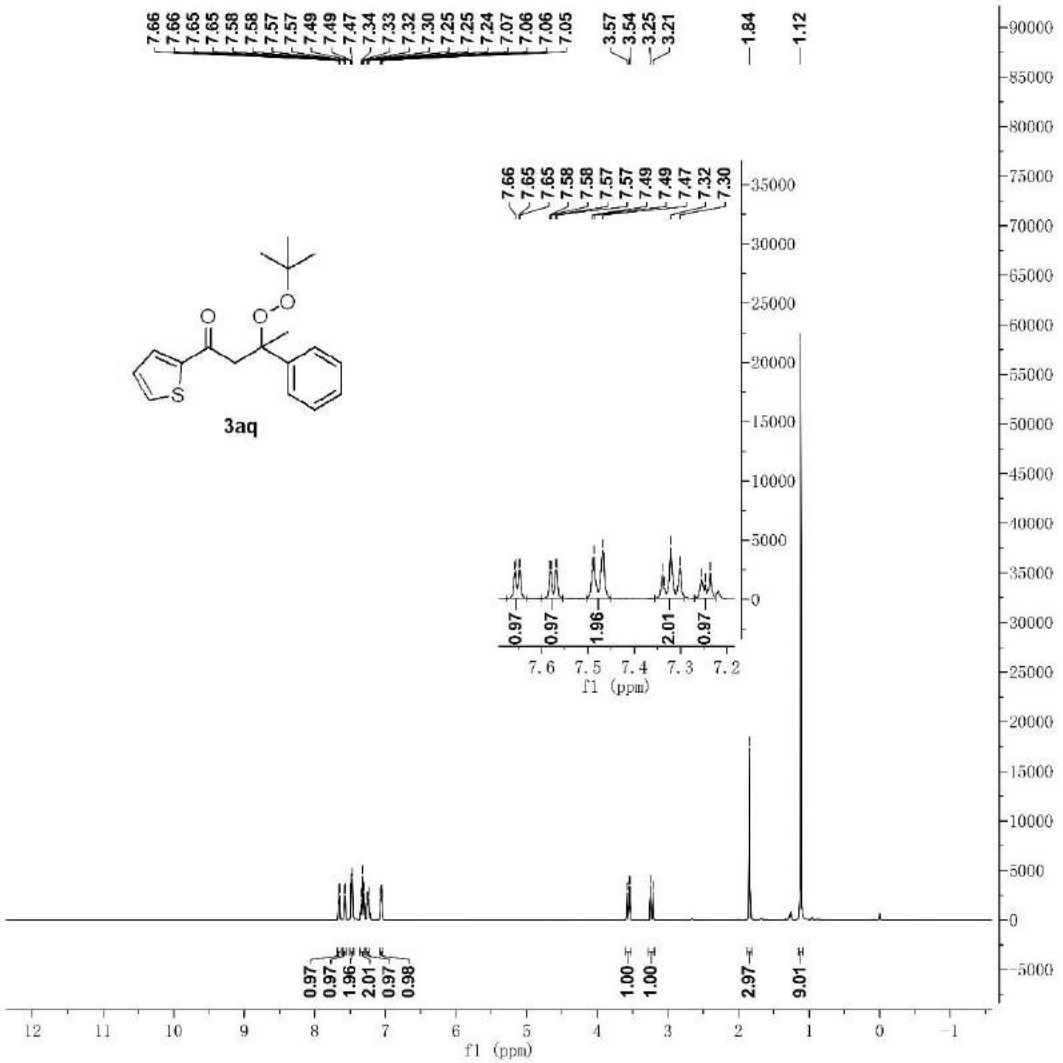
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy20-2/ 1/ fid
2 Title	yy20 2.1.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 24
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	33
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-03-21T05:28:00
21 Modification Date	2018-03-21T05:27:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1570.1
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



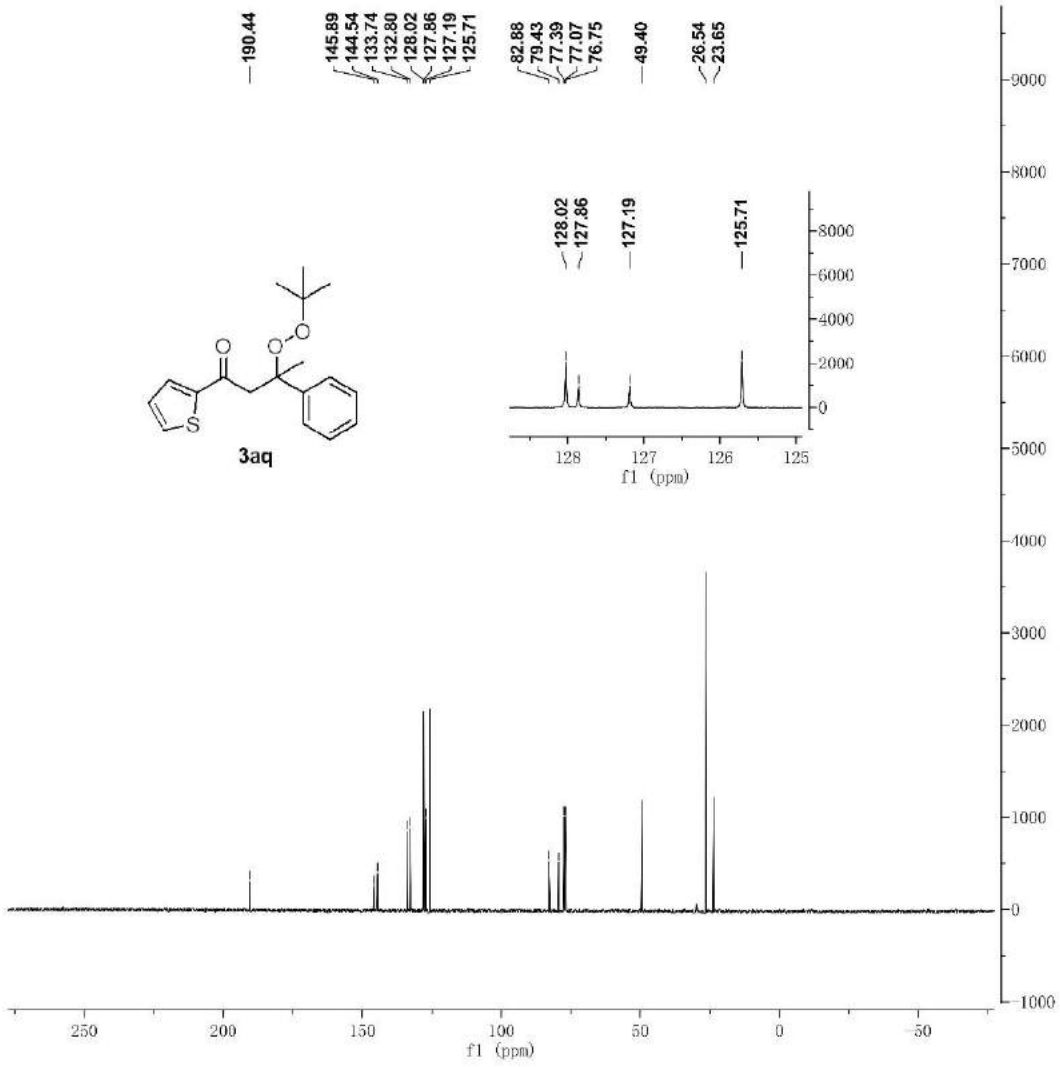
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy20-2/ 2/ fid
2 Title	yy20 2.2.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 24
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	500
15 Receiver Gain	133
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-03-21T05:42:00
21 Modification Date	2018 03 21T05:41:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample16	**Position**	P1-B7	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY20.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/4/2018 10:59:08 AM



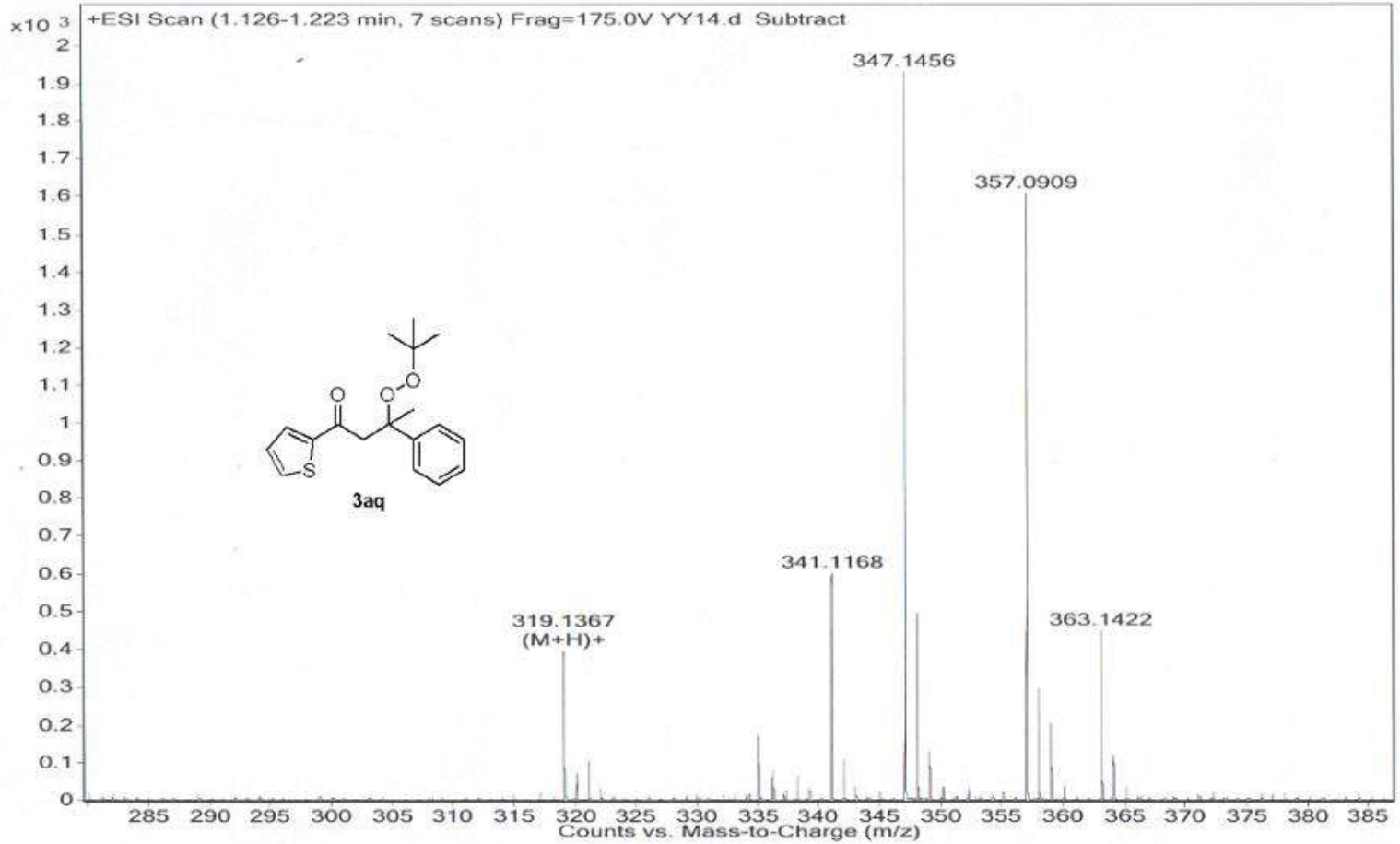


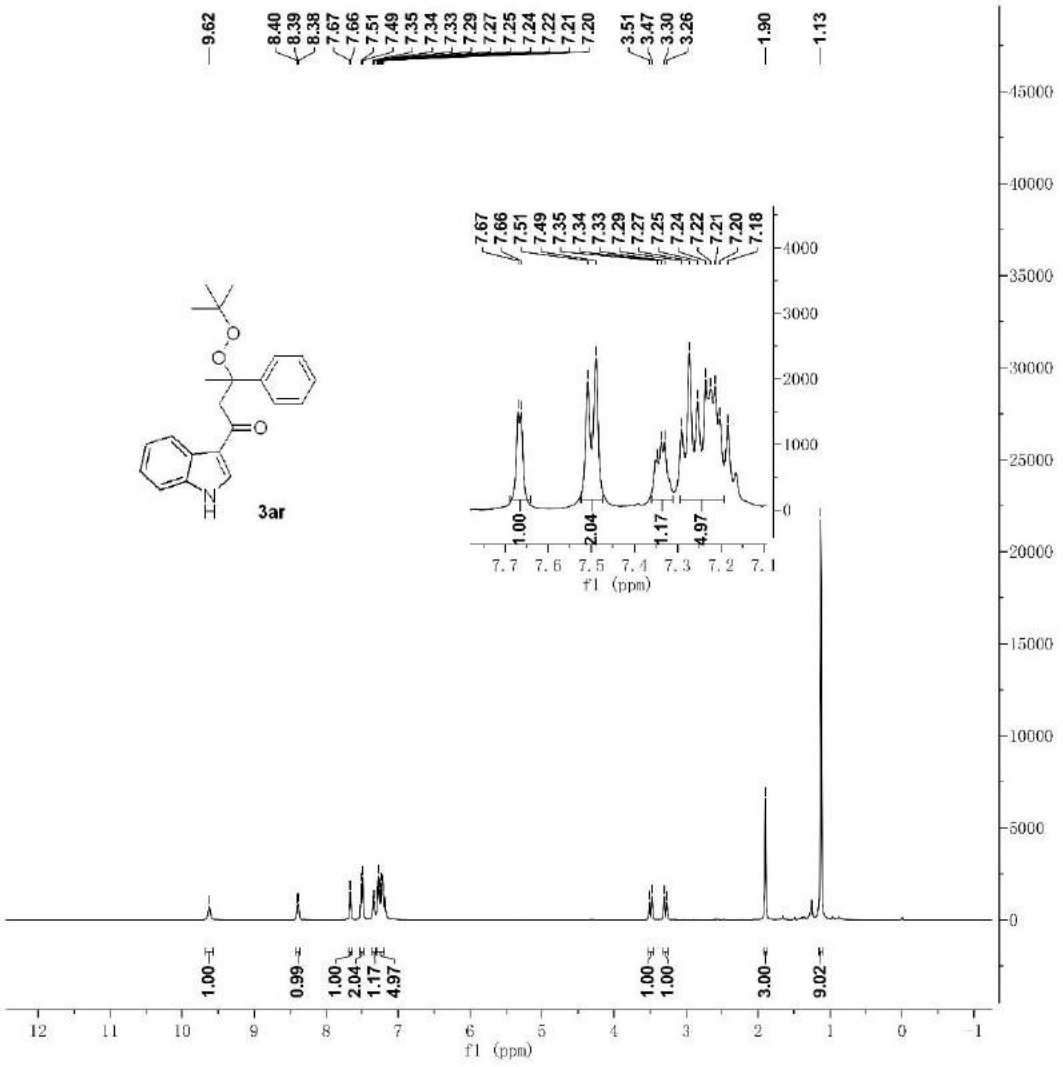
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy14/ 1/ fid
2 Title	yy14.1.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 3
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	293.8
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	56
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-04-12T11:56:00
21 Modification Date	2018-04-12T11:56:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1550.9
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



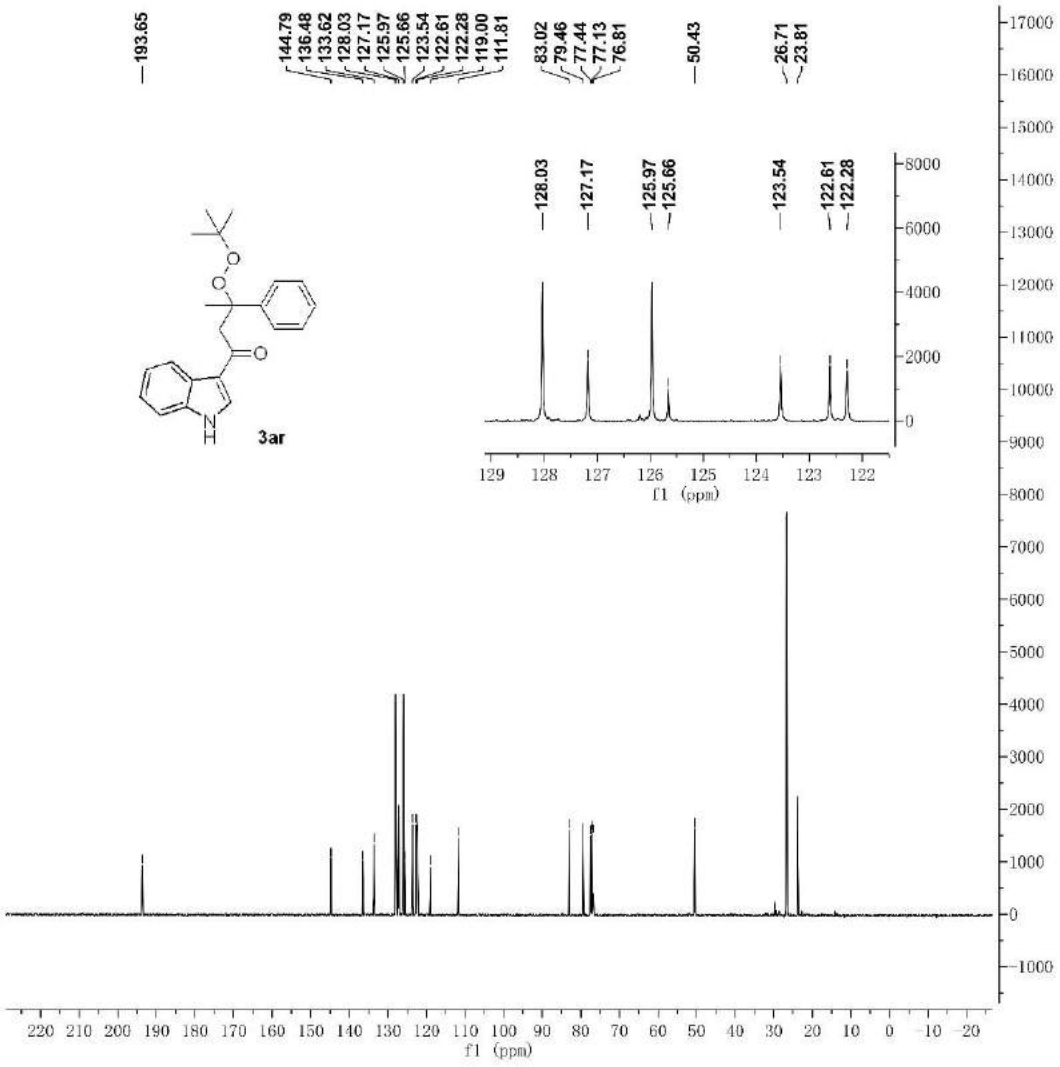
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy14/ 2/ fid
2 Title	yy14.2.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 3
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	300
15 Receiver Gain	200
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-04-12T12:05:00
21 Modification Date	2018-04-12T12:05:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample12	**Position**	P1-B3	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY14.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/4/2018 10:35:53 AM



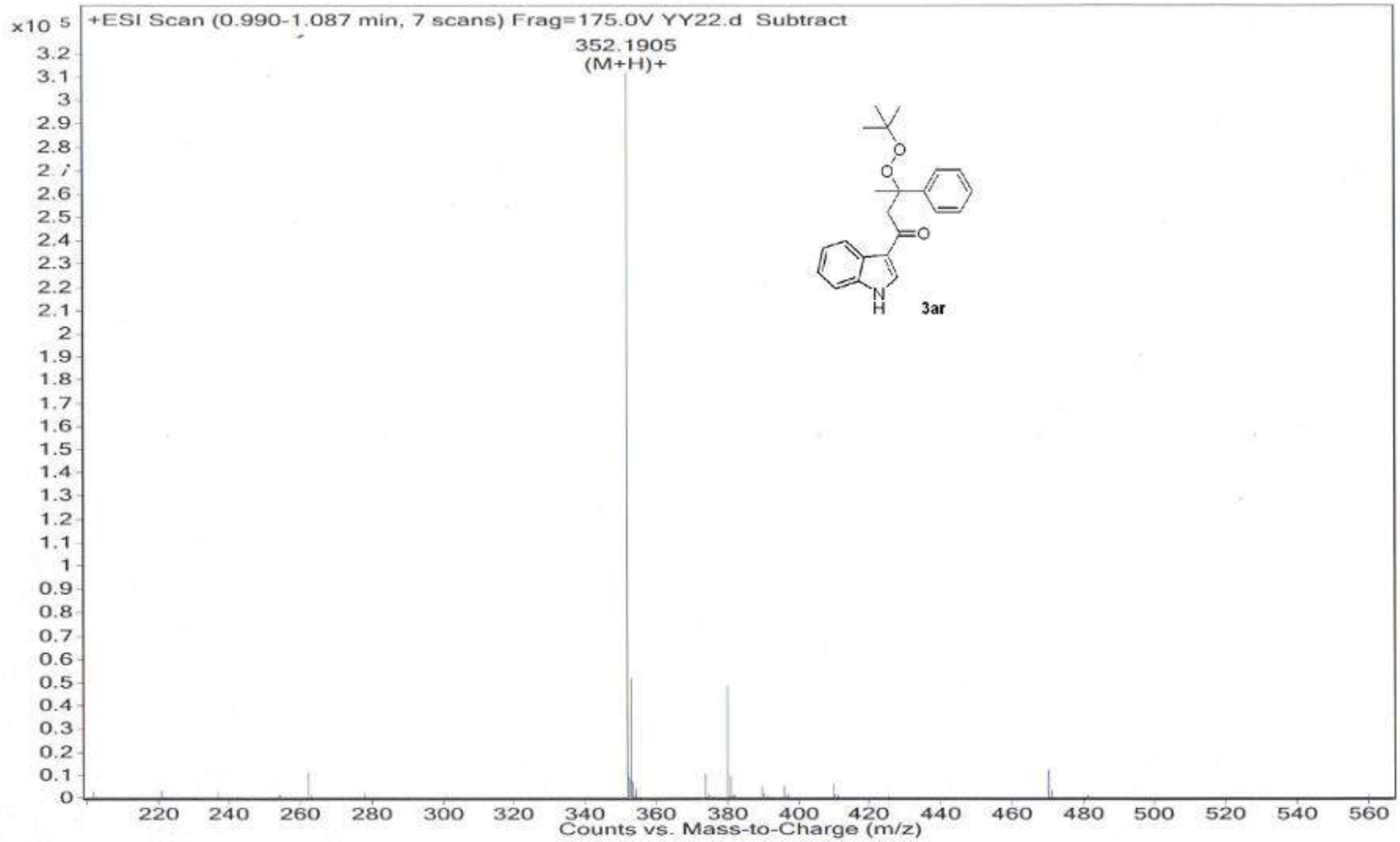


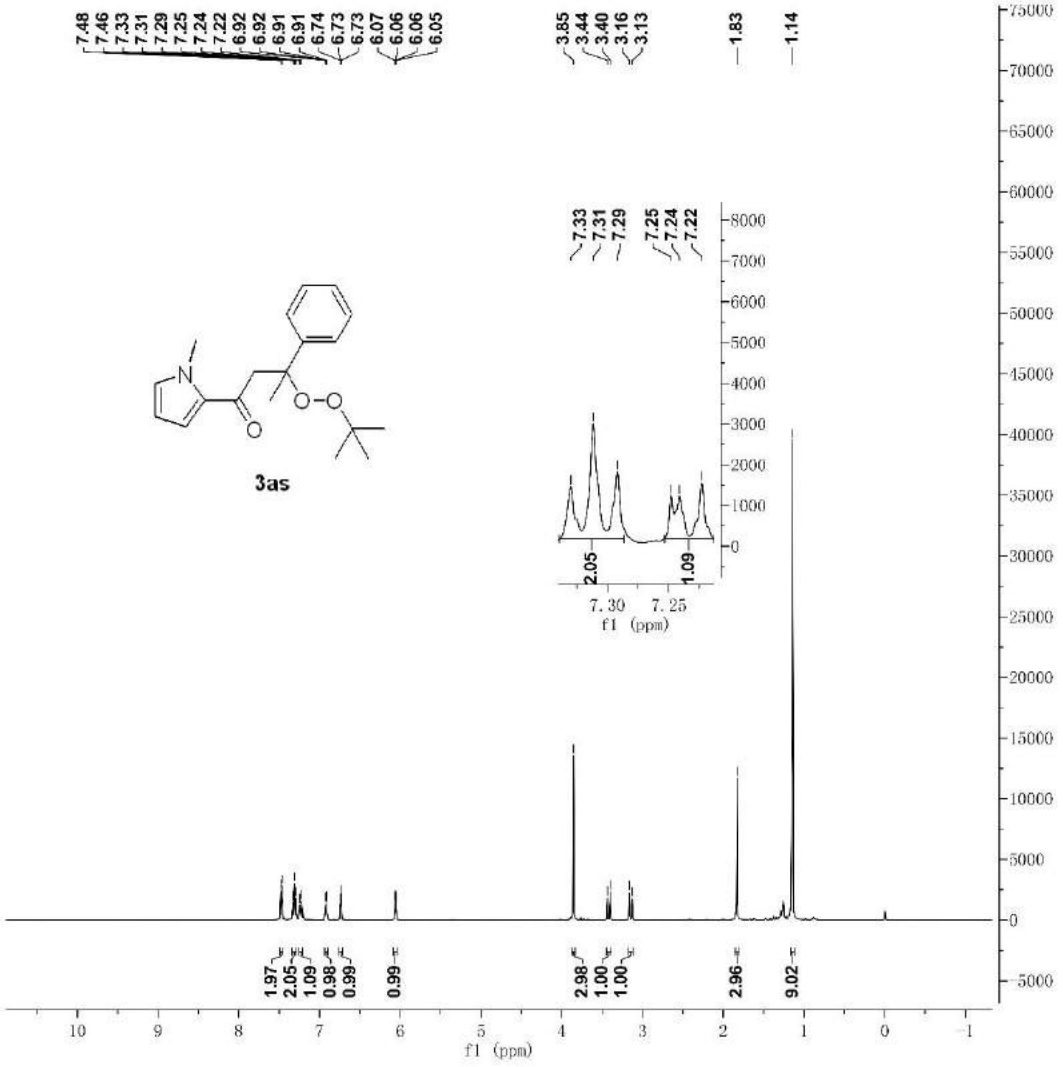
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy22/ 1/ fid
2 Title	yy22.1.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 4
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	293.8
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	33
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-04-12T12:11:00
21 Modification Date	2018-04-12T12:11:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1565.9
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



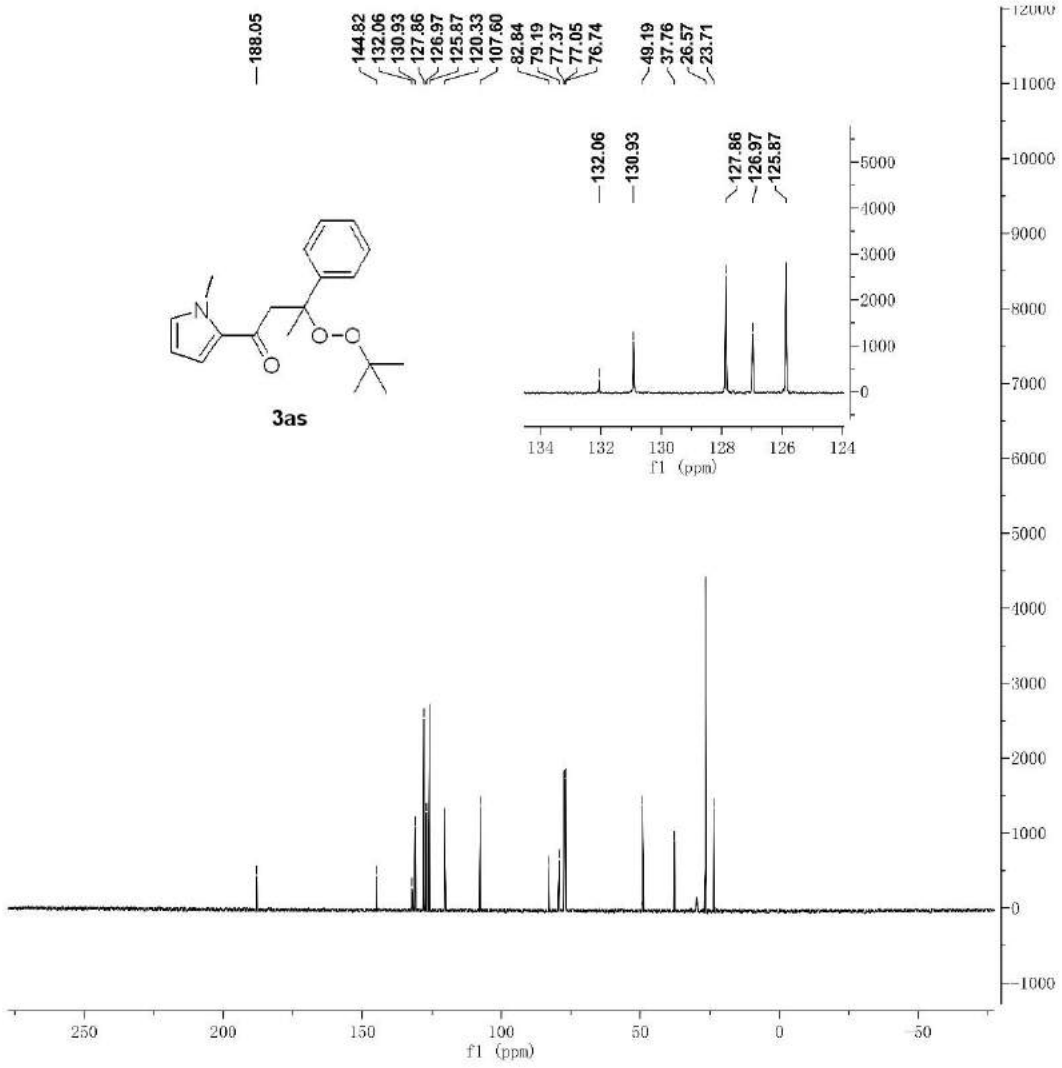
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy22/ 2/ fid
2 Title	yy22.2.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 4
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	600
15 Receiver Gain	200
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-04-12T12:28:00
21 Modification Date	2018 04 12T12:28:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample1	**Position**	P1-A1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY22.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/20/2018 11:20:31 AM



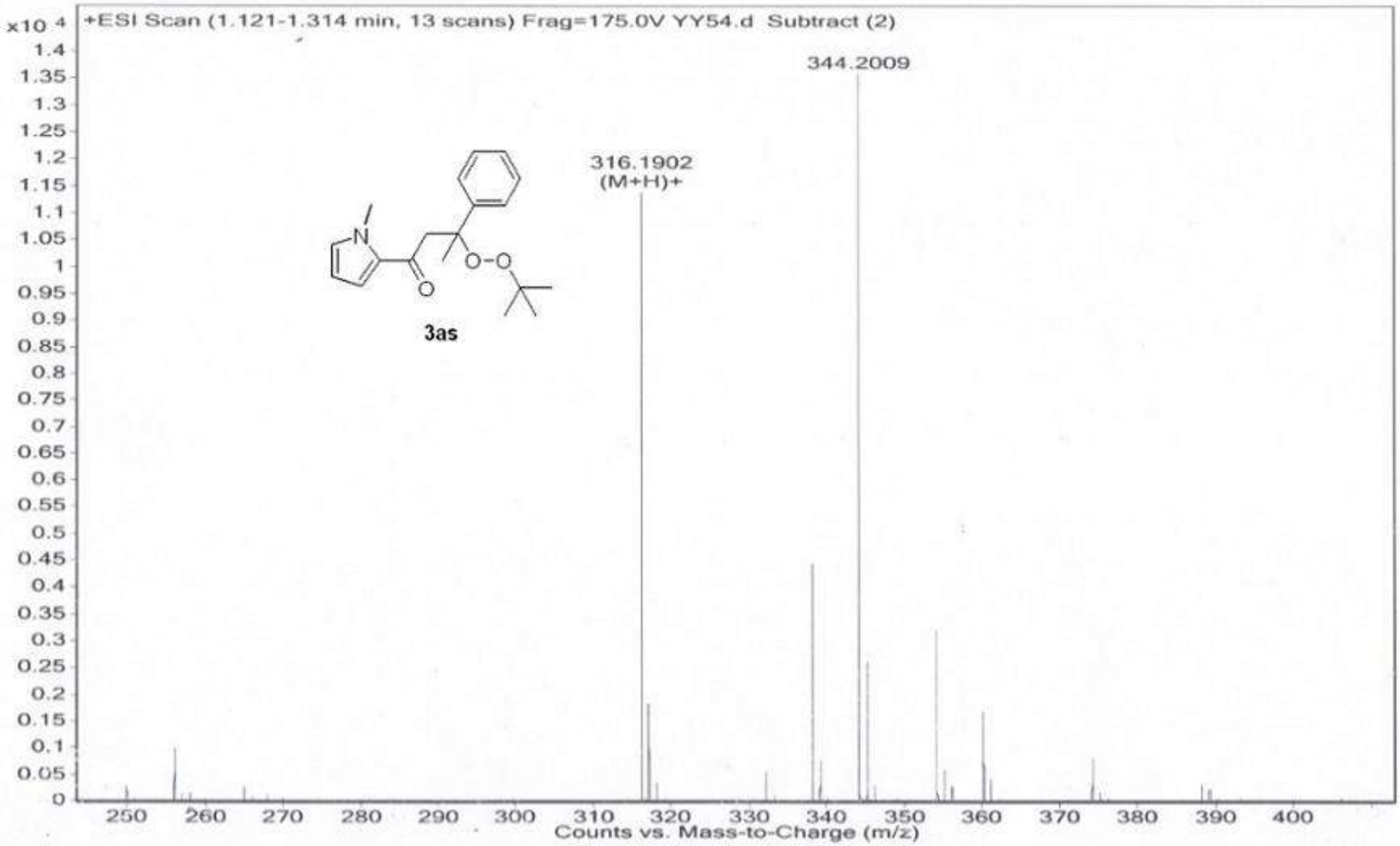


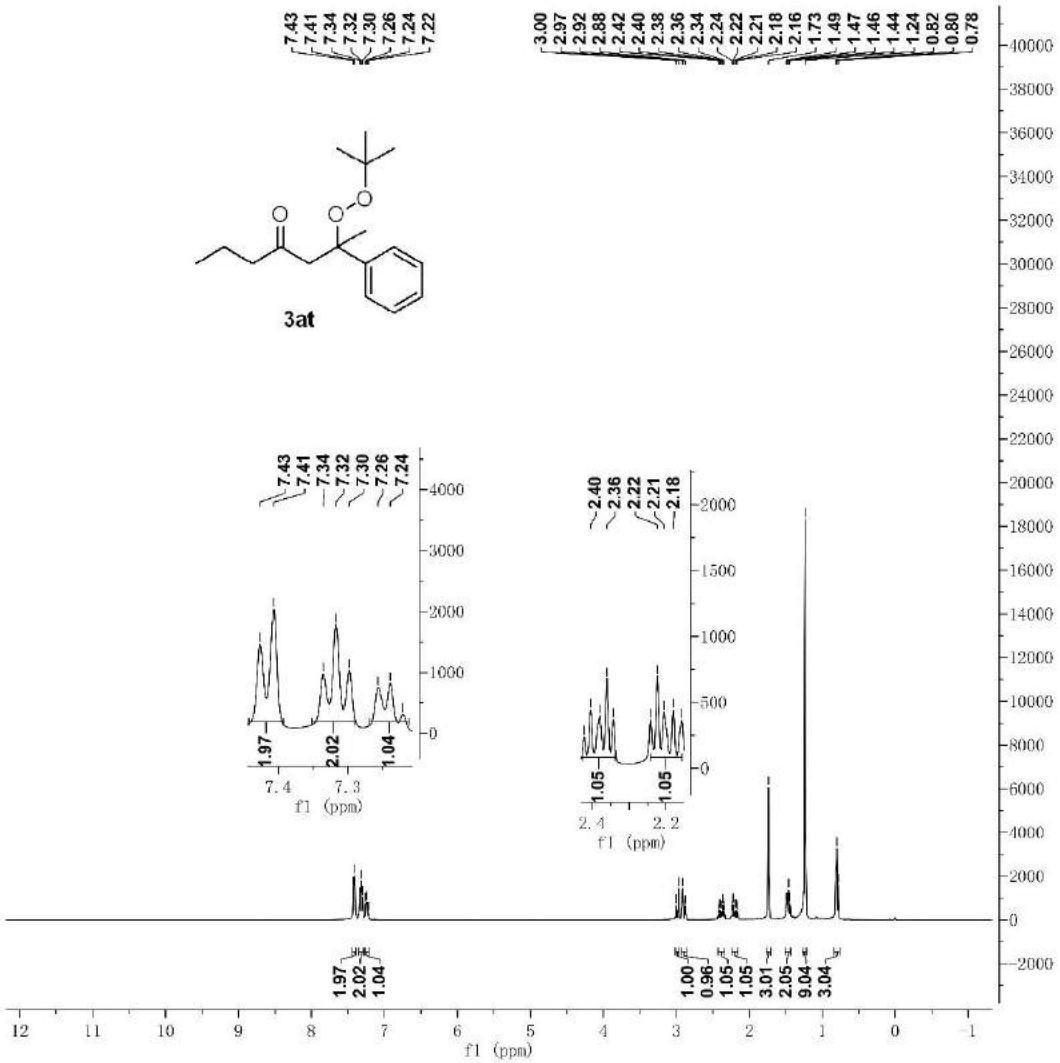
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy54/ 1/ fid
2 Title	yy54.1.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 2
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	293.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	61
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-04-12T11:34:00
21 Modification Date	2018-04-12T11:33:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1550.4
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



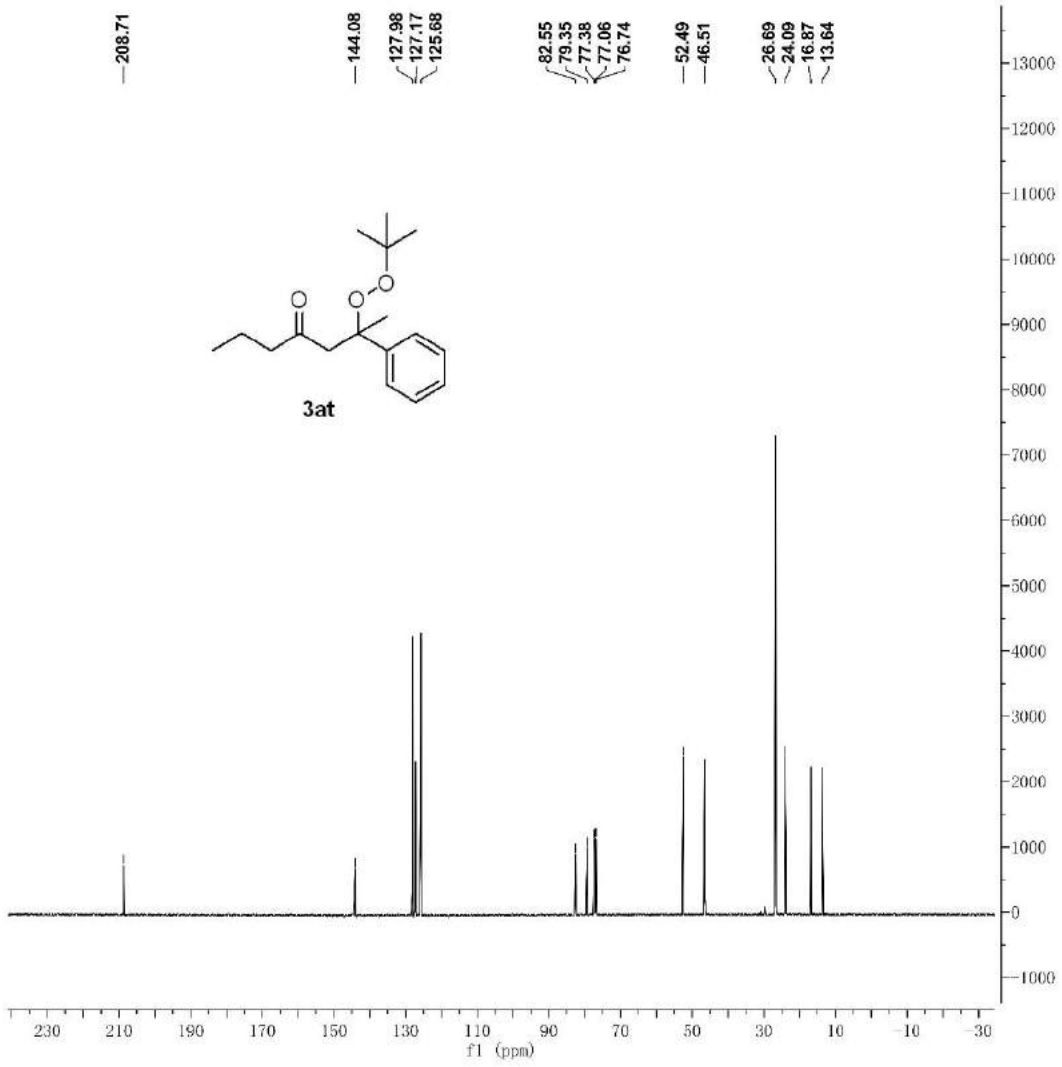
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy54/ 2/ fid
2 Title	yy54.2.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 2
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	600
15 Receiver Gain	200
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-04-12T11:50:00
21 Modification Date	2018-04-12T11:50:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample1	**Position**	P1-A2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY54.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/20/2018 11:26:17 AM



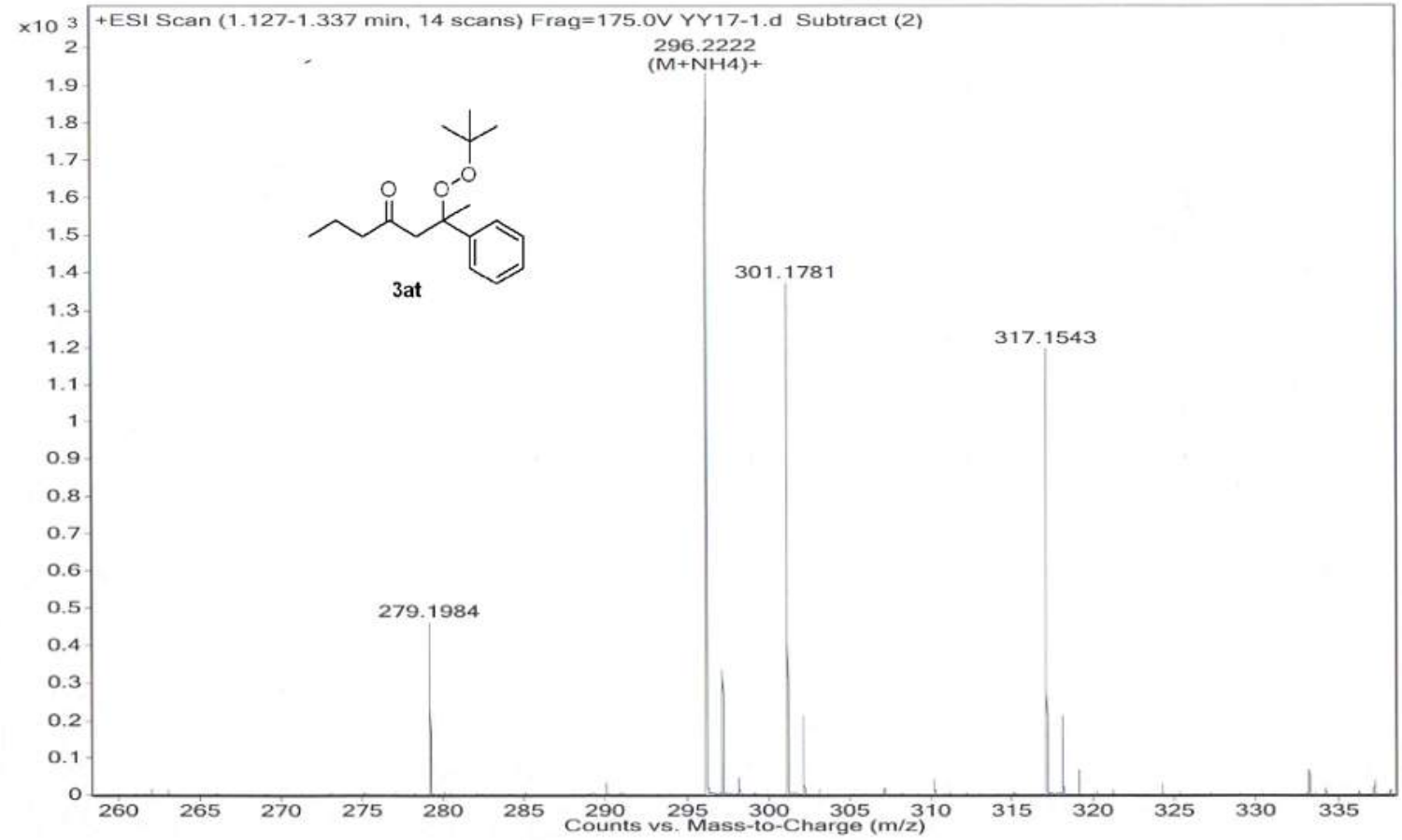


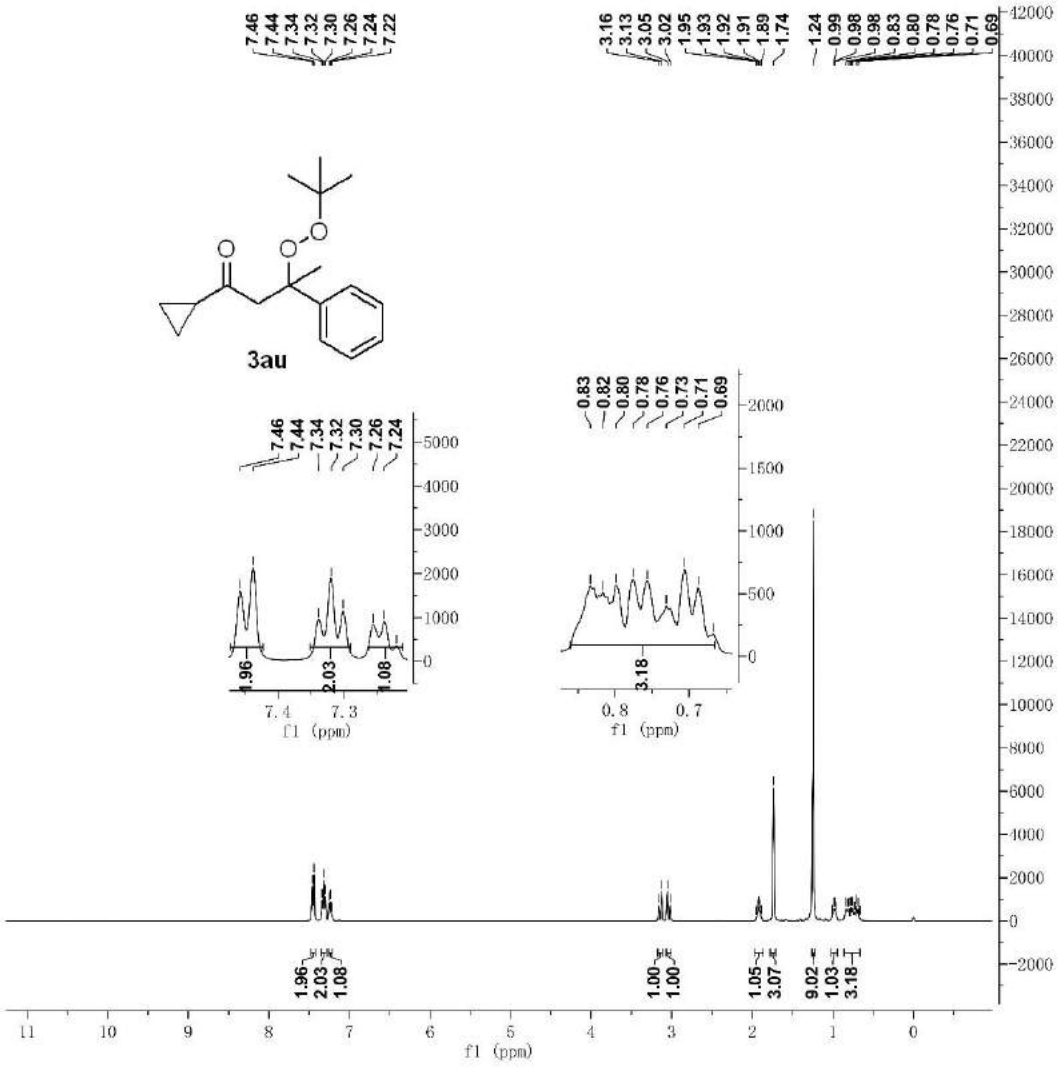
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yyX/ 1/ fid
2 Title	yyX. 1. fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 17
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	33
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-03-21T02:57:00
21 Modification Date	2018 03 21T02:56:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1549.7
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



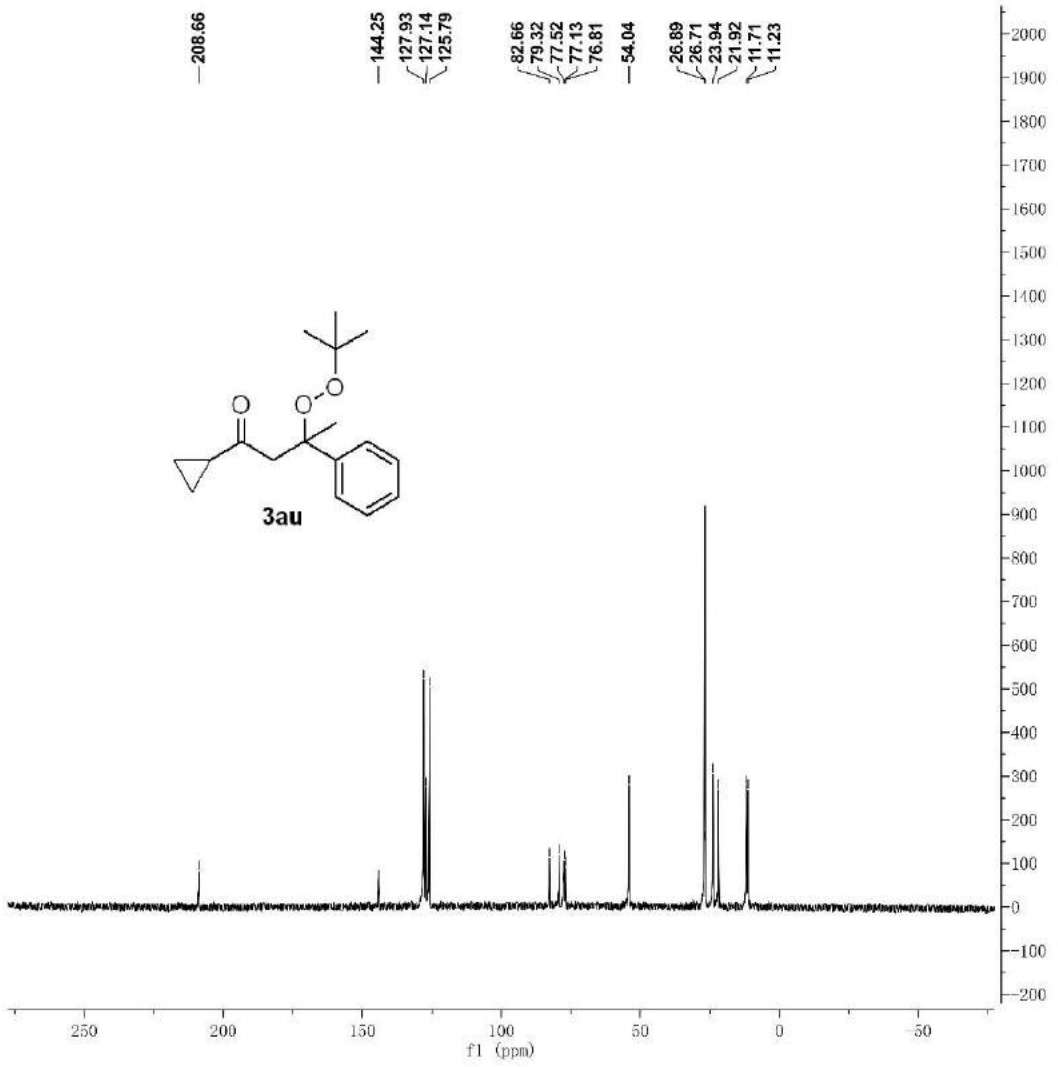
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yyX/ 2/ fid
2 Title	yyX. 2. fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 17
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	1024
15 Receiver Gain	133
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-03-21T03:21:00
21 Modification Date	2018 03 21T03:23:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample14	**Position**	P1-B5	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY17-1.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/4/2018 10:47:31 AM

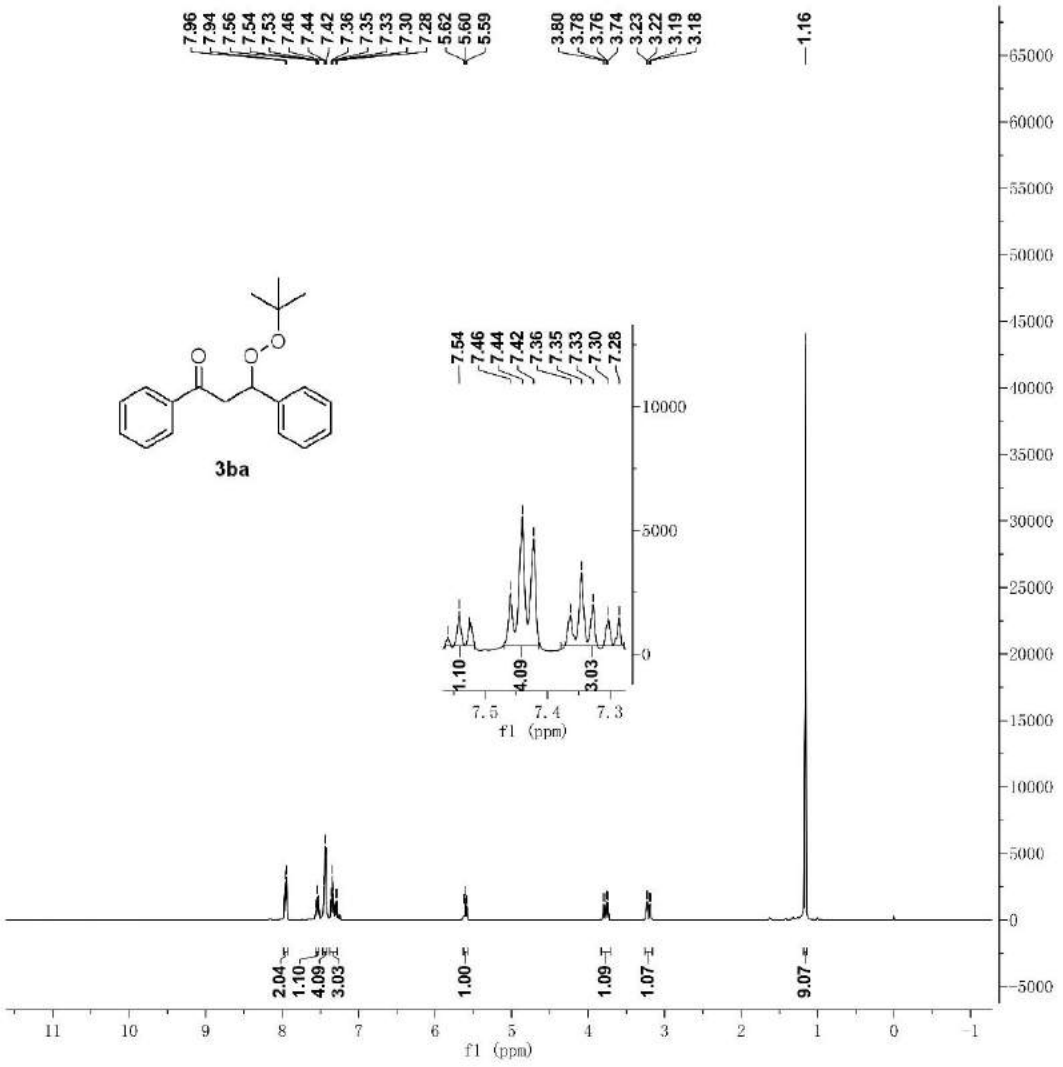




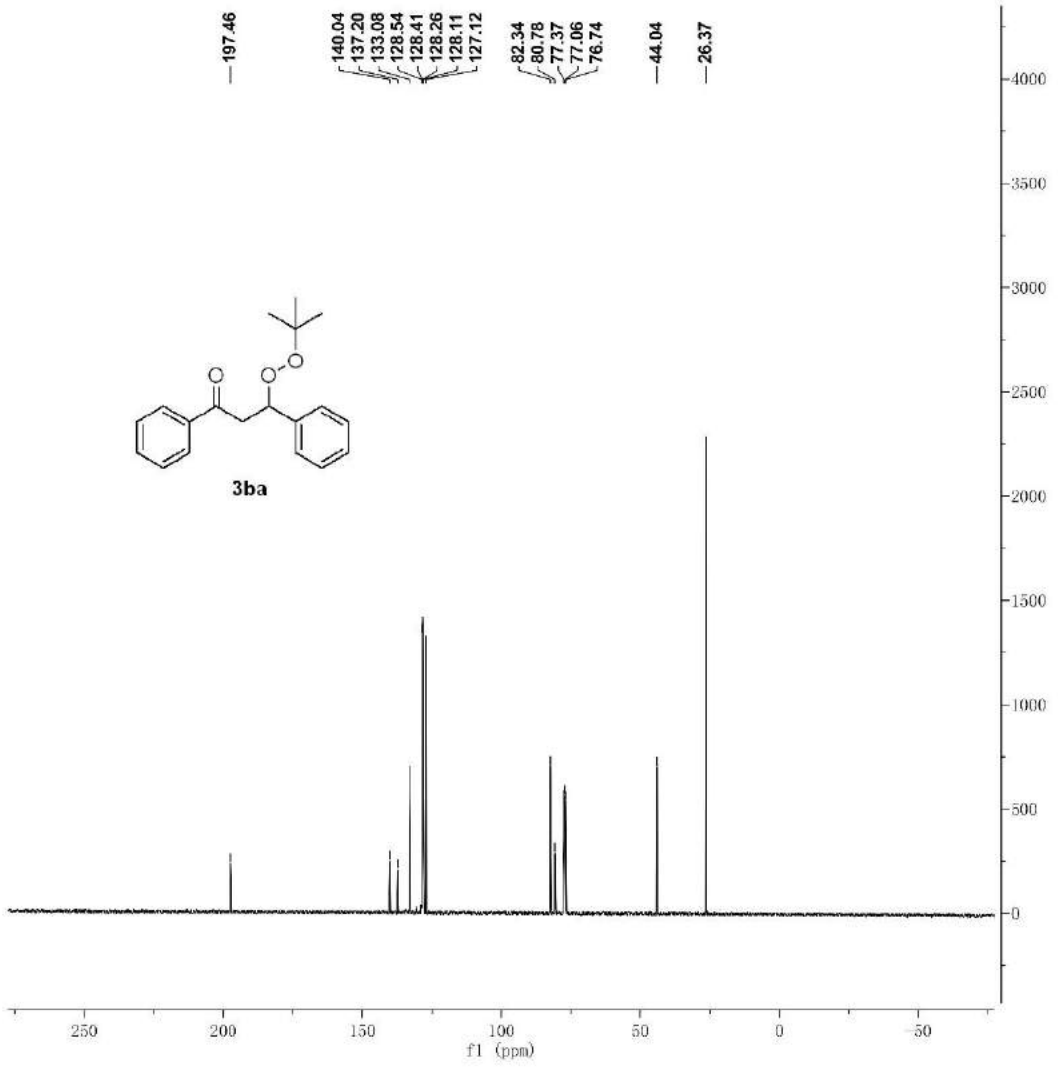
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy18+/ 1/ fid
2 Title	yy18+. 1. fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 5
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.6
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	33
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-03-20T23:14:00
21 Modification Date	2018 03 20T23:13:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1550.3
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



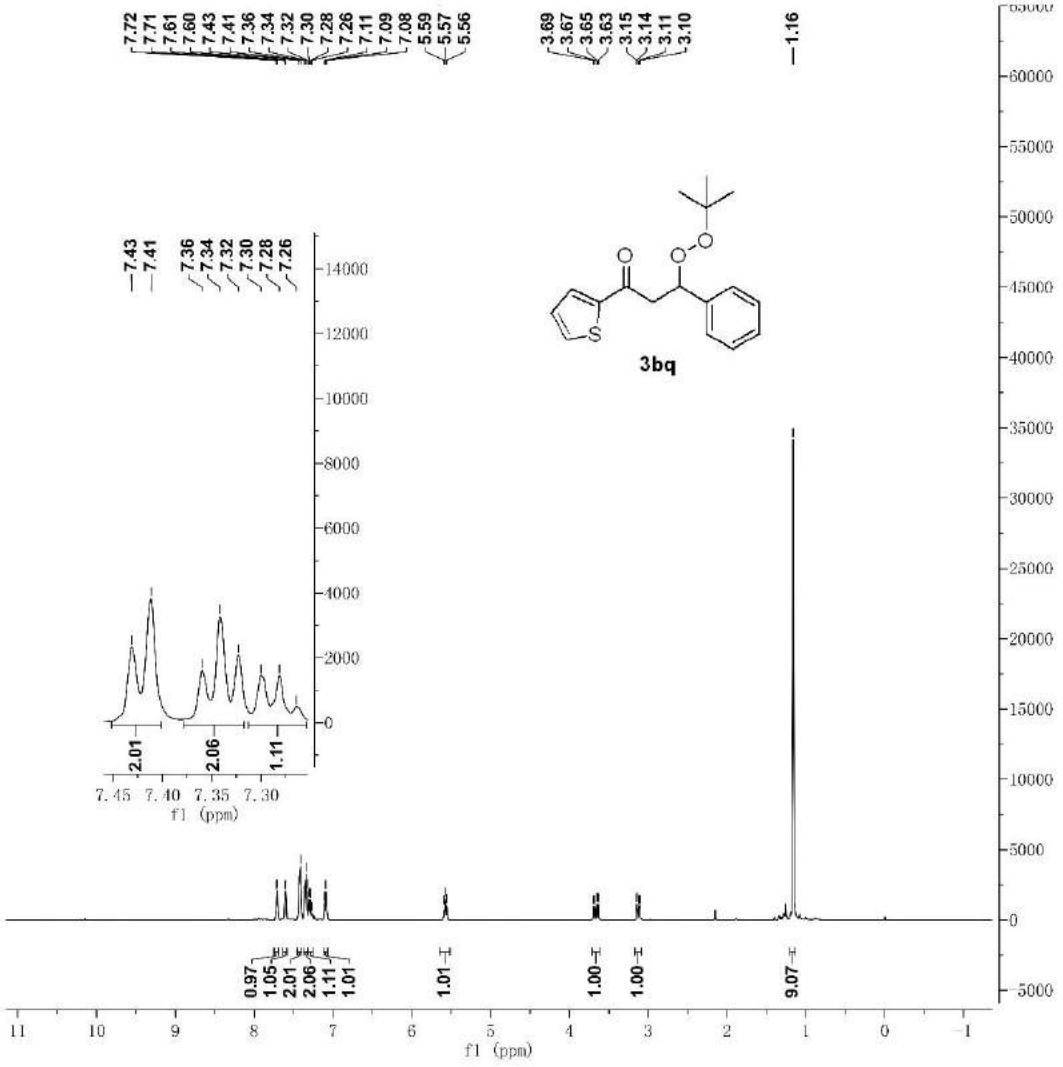
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy18/ 4/ fid
2 Title	yy18.4.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 4
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	300
15 Receiver Gain	113
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-03-20T18:45:00
21 Modification Date	2018 03 20T18:44:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536



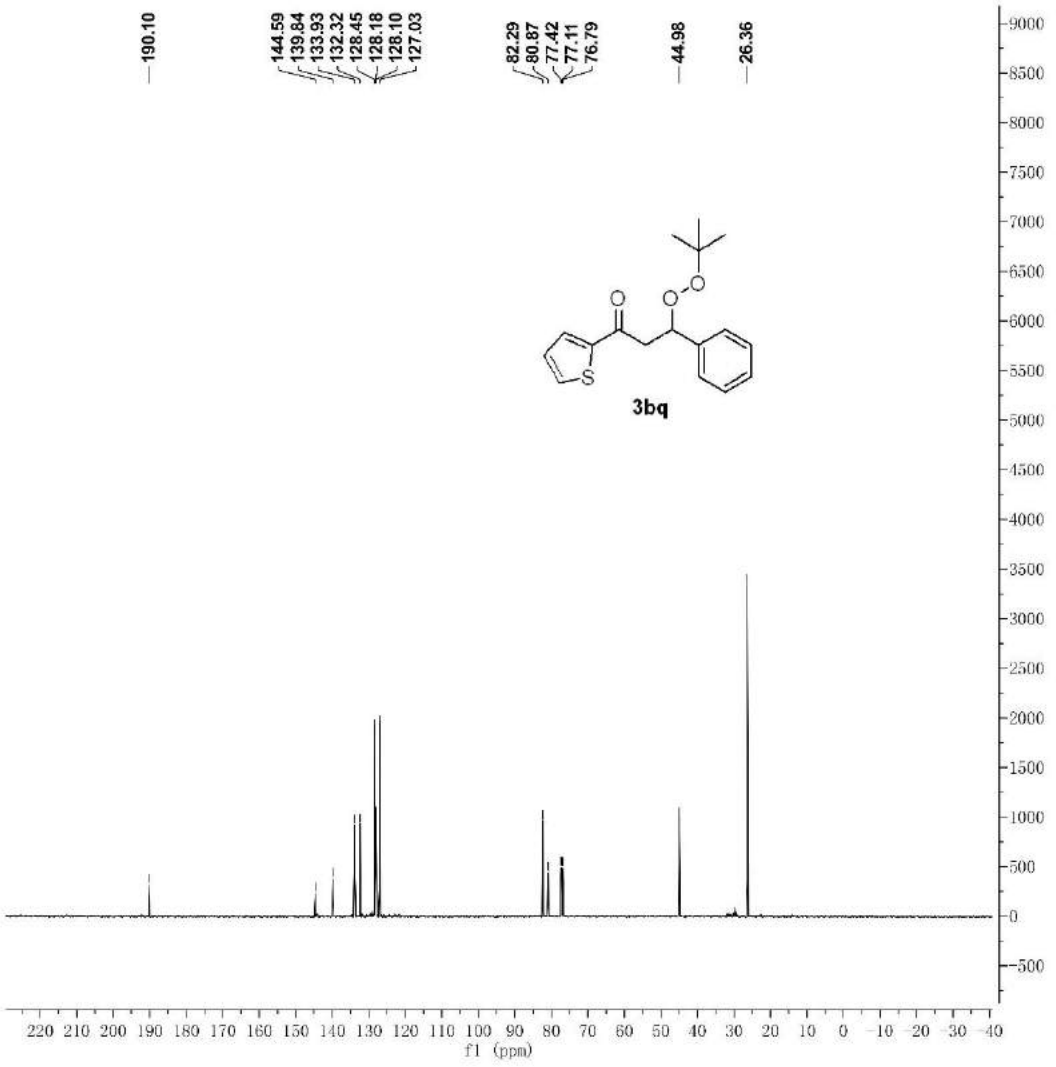
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ 核NMR/ yy3/ 1/ fid
2 Title	yy3.1.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 18
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	299.3
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	53
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-03-15T01:03:00
21 Modification Date	2018 03 15T01:02:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1552.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



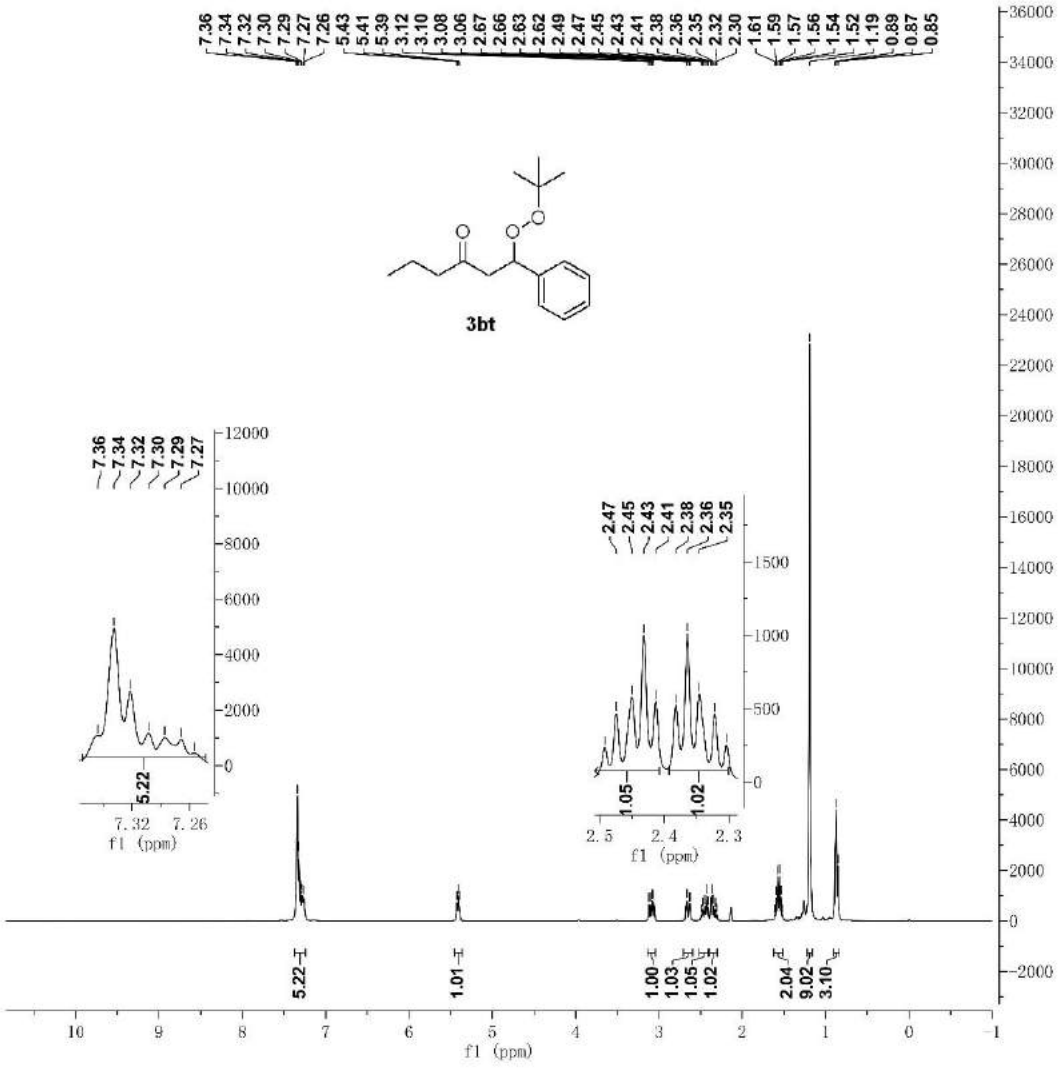
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ 核NMR/ yy3/ 2/ fid
2 Title	yy3.2.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 18
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	500
15 Receiver Gain	88
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-03-15T01:17:00
21 Modification Date	2018 03 15T01:16:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536



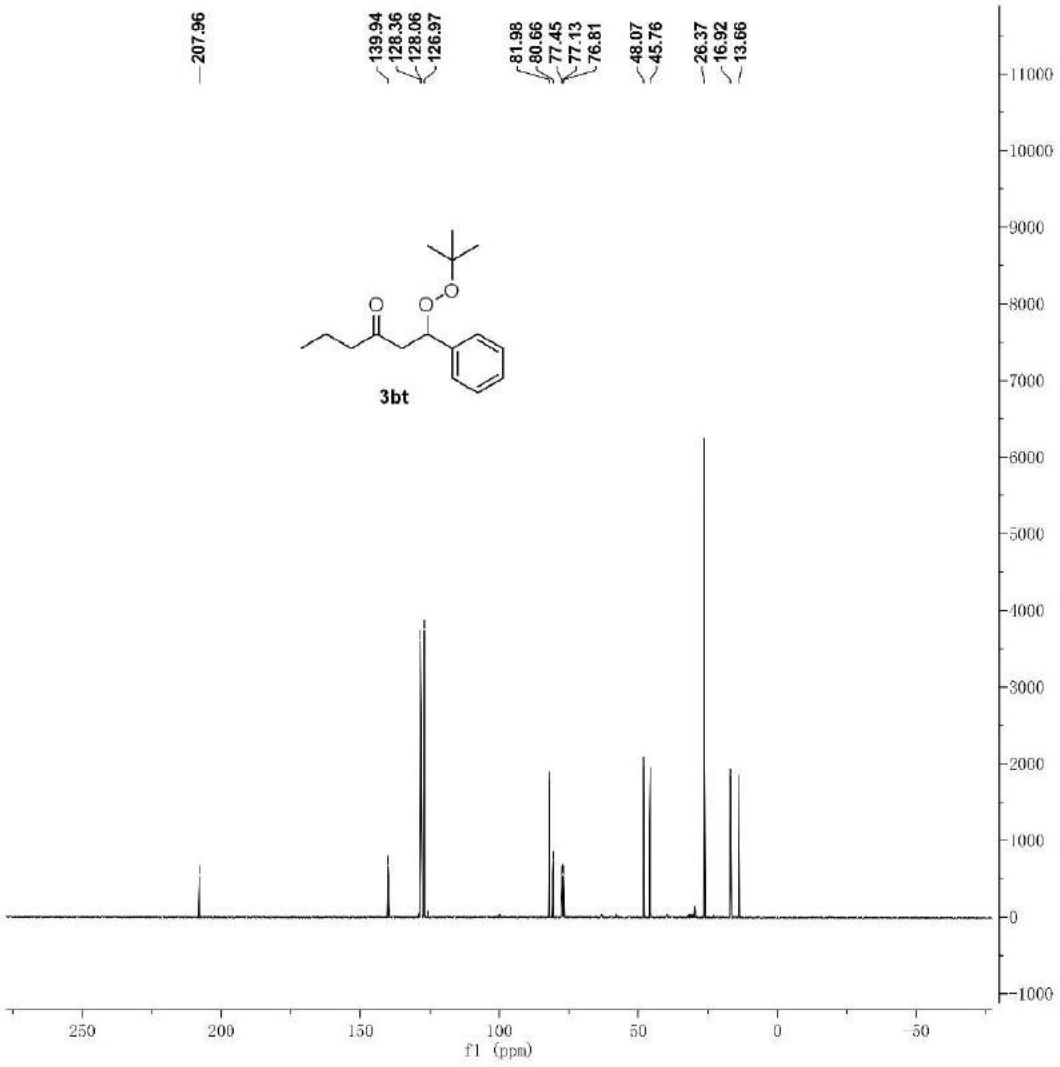
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy14-1/ 1/ fid
2 Title	yy14 1.1.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 21
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	33
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-03-21T04:27:00
21 Modification Date	2018 03 21T04:26:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1552.8
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy14-1/ 2/ fid
2 Title	yy14 1.2.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 21
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.0
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	500
15 Receiver Gain	78
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-03-21T04:41:00
21 Modification Date	2018 03 21T04:40:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35714.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

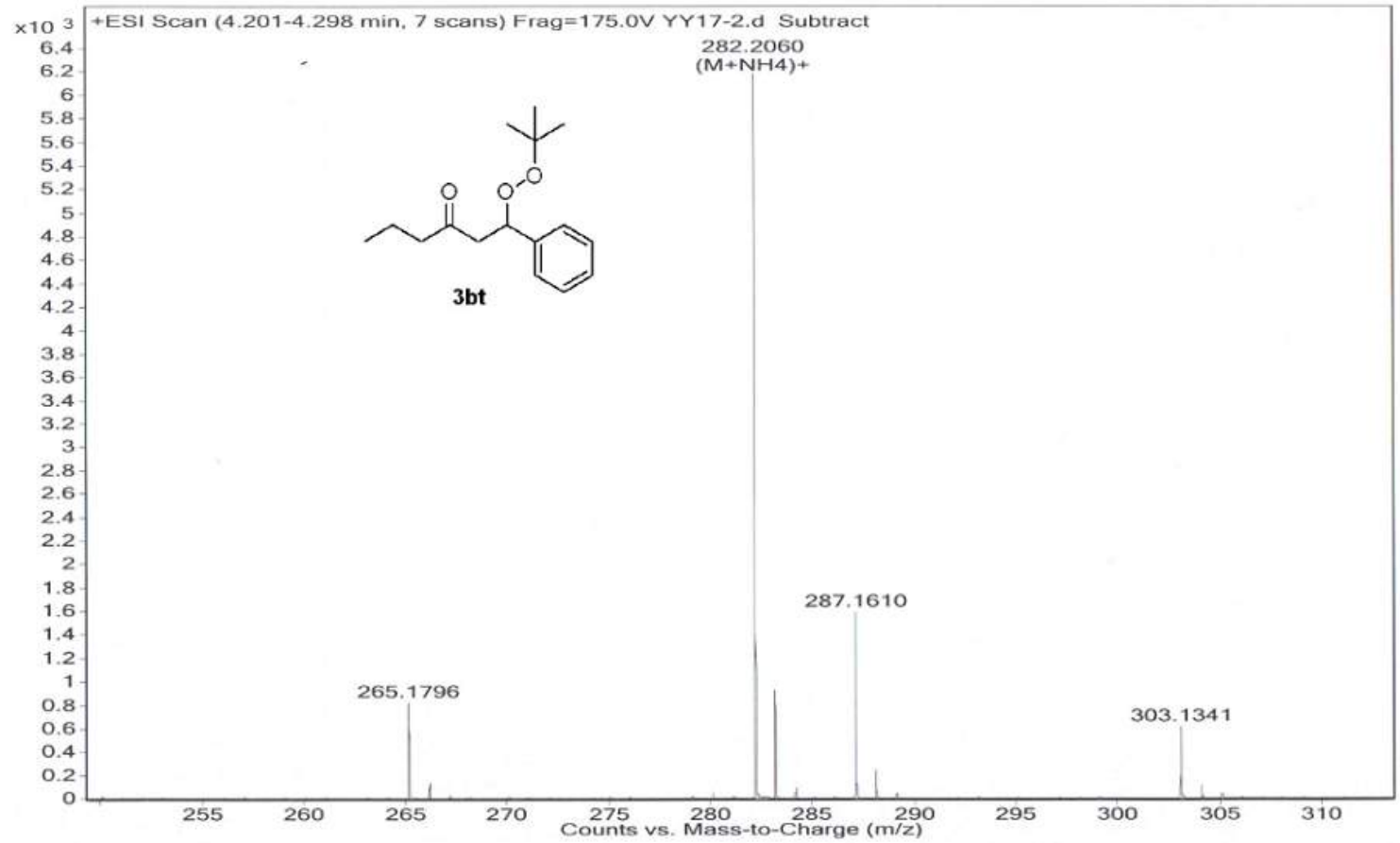


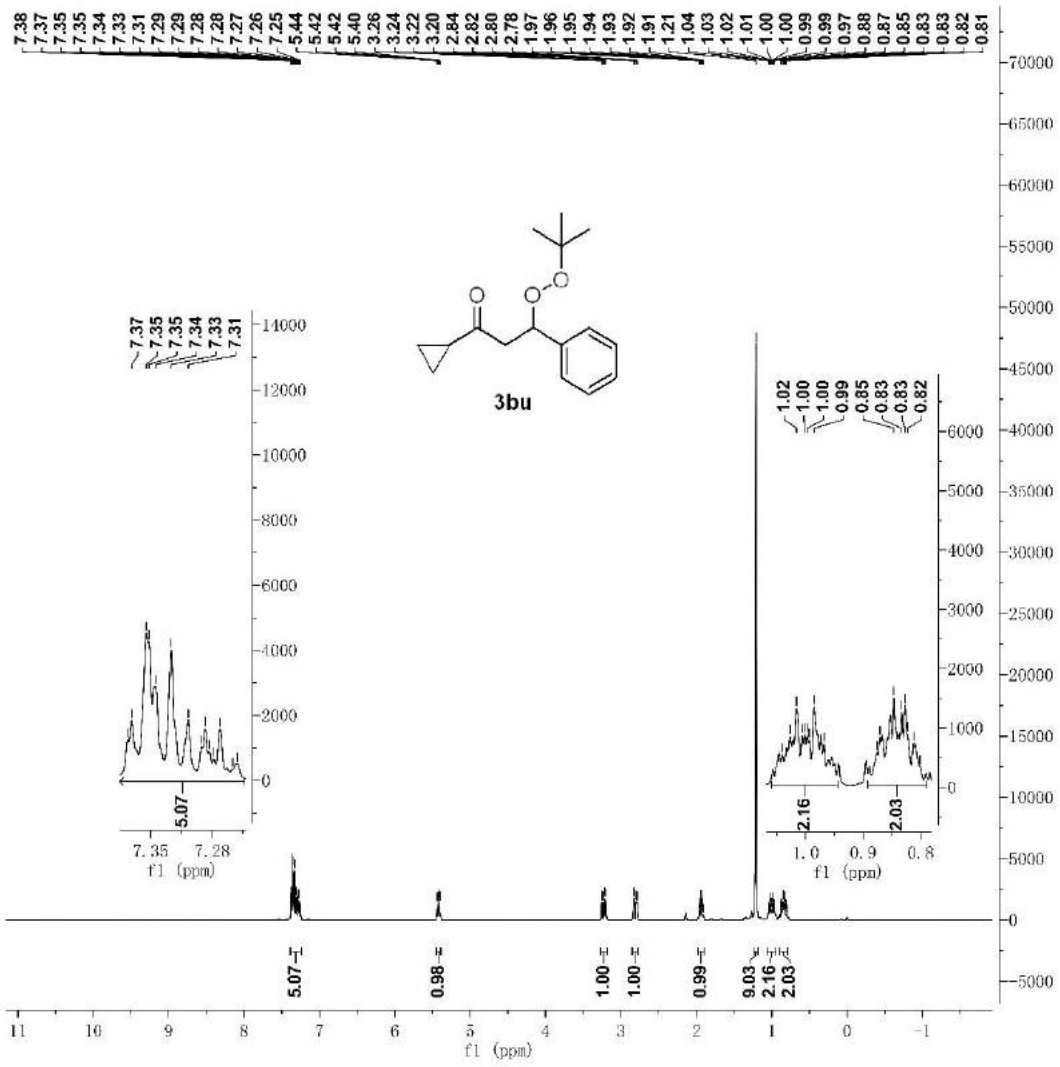
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ 17-2/ 1/ fid
2 Title	17-2.1.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 2
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.8
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	16
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-03-20T18:07:00
21 Modification Date	2018-03-20T18:06:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1547.4
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



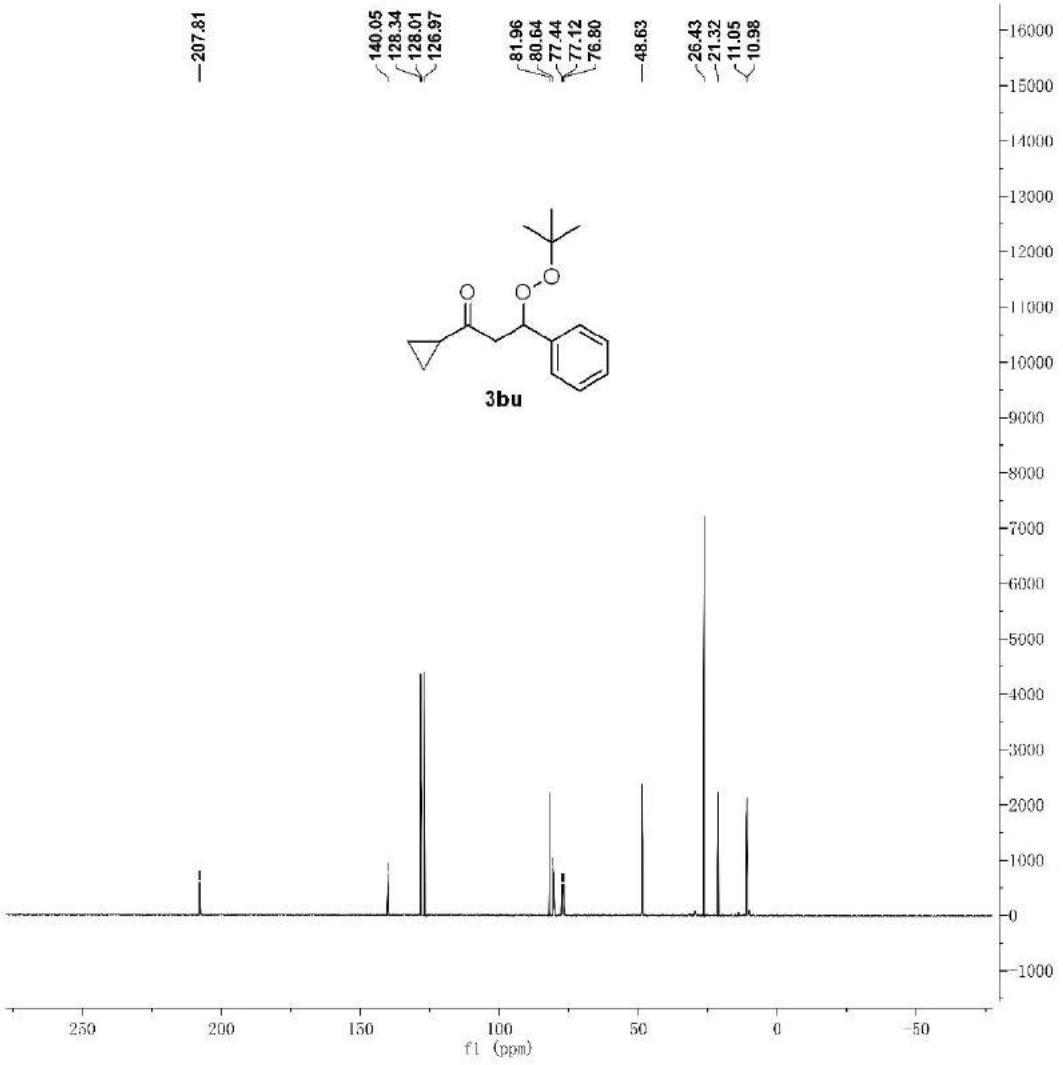
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ 17-2/ 2/ fid
2 Title	17-2.2.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 2
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.8
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	300
15 Receiver Gain	133
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-03-20T18:15:00
21 Modification Date	2018-03-20T18:15:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample15	**Position**	P1-B6	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY17-2.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/4/2018 10:53:20 AM

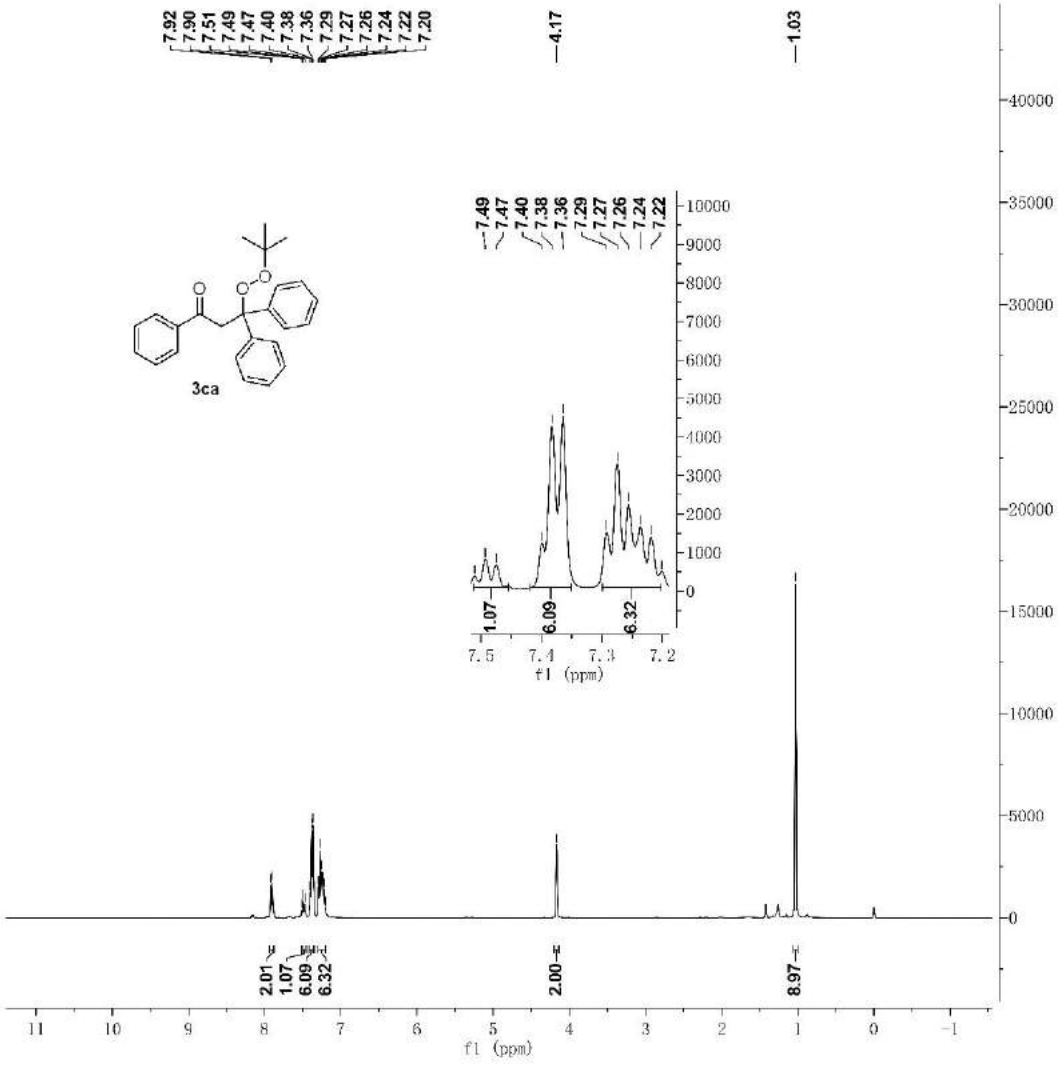




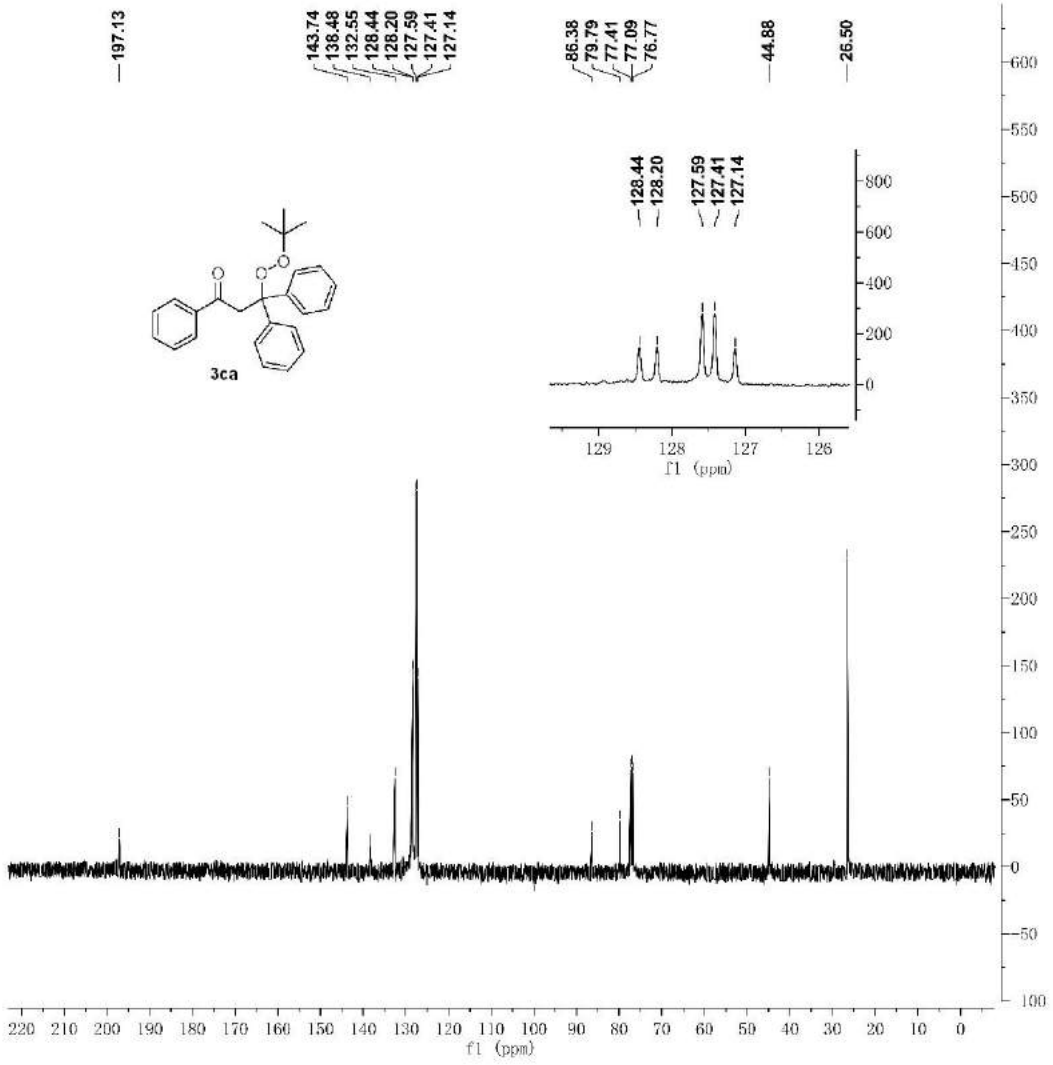
	Parameter	Value
1	Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy29/ 1/ fid
2	Title	yy29.1.fid
3	Comment	PROTON CDCl3 [D:\ NMR_DATA\ Wangbin\ Wangbin 24
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.2
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	5 mm PADDO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	16
15	Receiver Gain	19
16	Relaxation Delay	1.0000
17	Pulse Width	14.4000
18	Presaturation Frequency	
19	Acquisition Time	4.0894
20	Acquisition Date	2018 03 30T03:17:00
21	Modification Date	2018-03-30T03:17:00
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8012.8
25	Lowest Frequency	-1549.1
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536



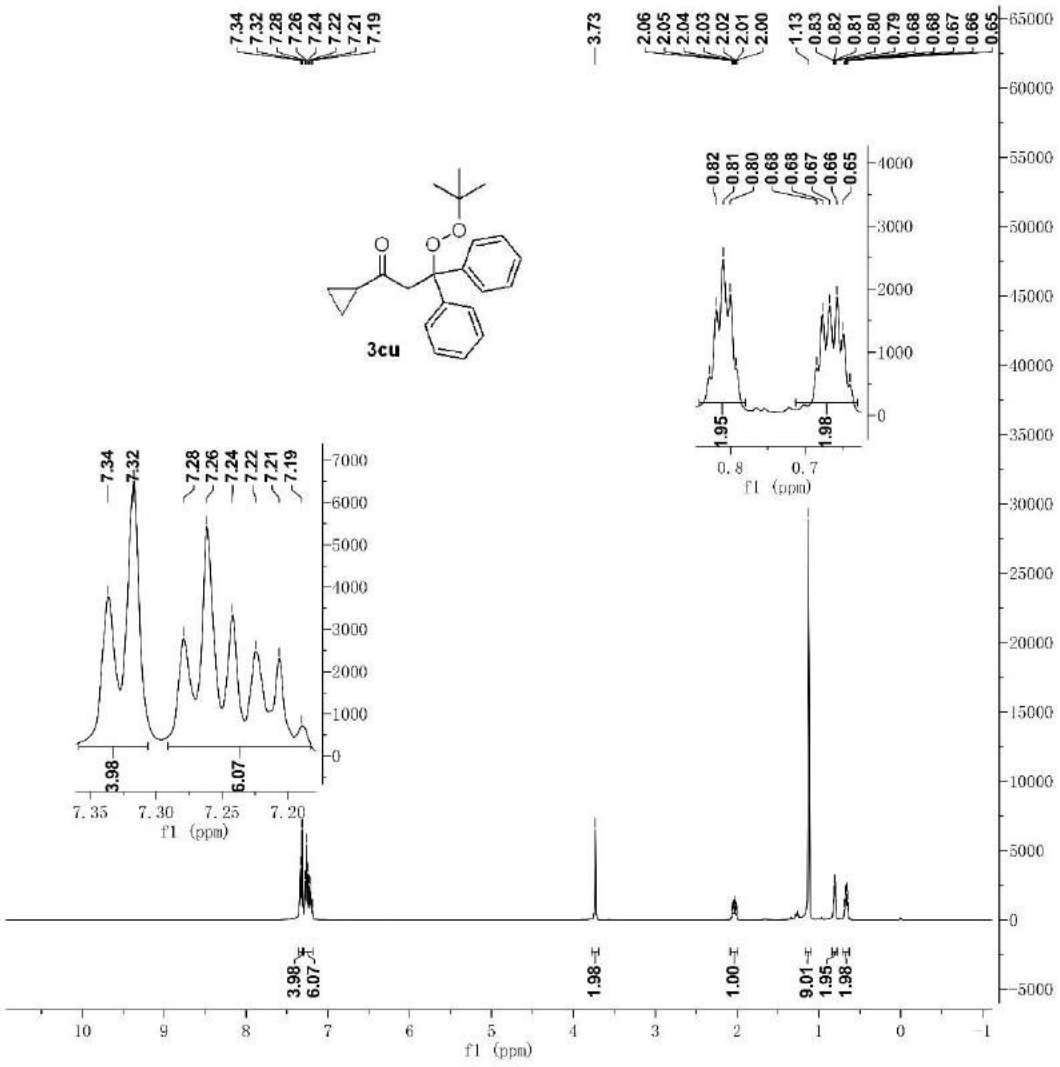
	Parameter	Value
1	Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy29/ 2/ fid
2	Title	yy29.2.fid
3	Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin\ Wangbin 24
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	299.1
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PADDO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	400
15	Receiver Gain	113
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2018 03 30T03:28:00
21	Modification Date	2018-03-30T03:28:00
22	Class	
23	Spectrometer Frequency	100.62
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	65536



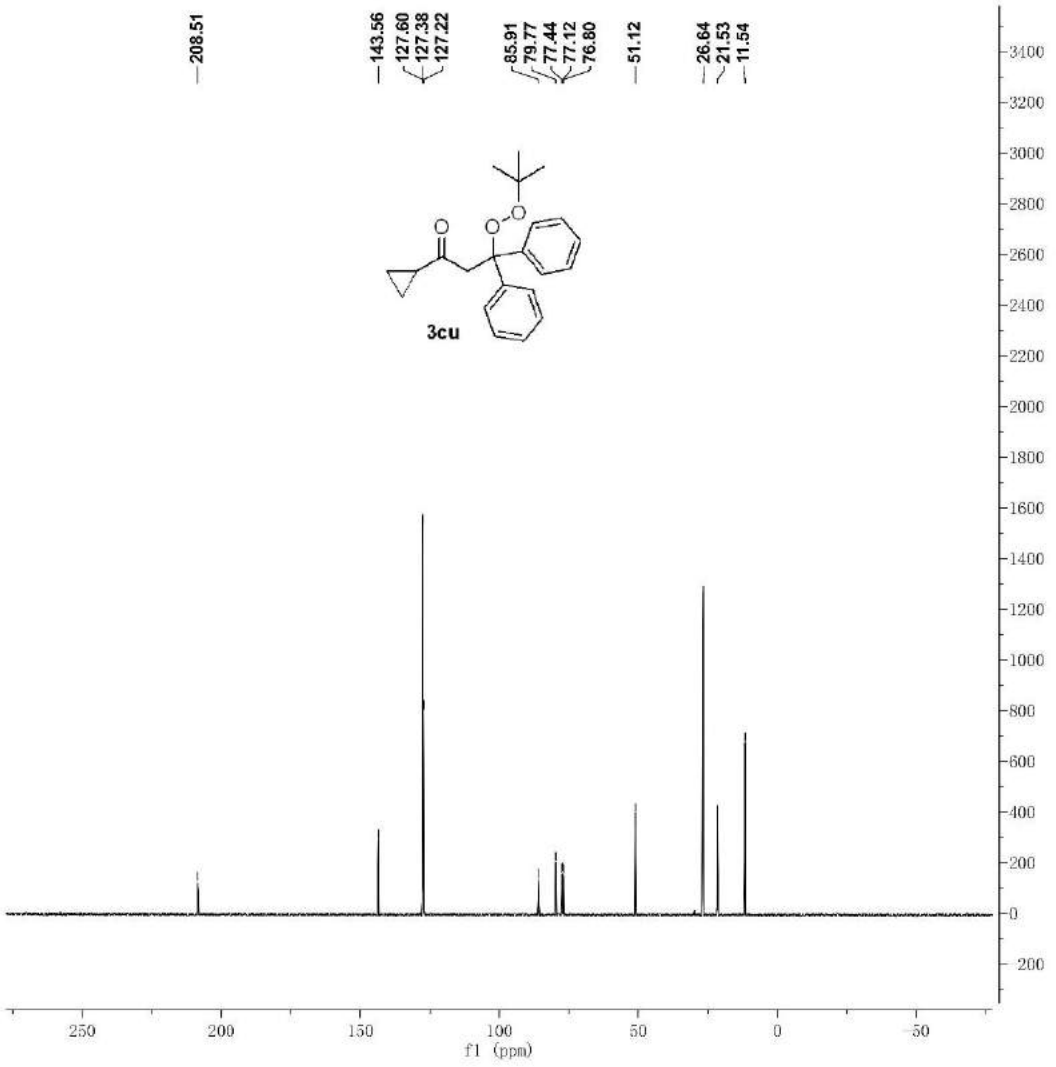
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy4/ 7/ fid
2 Title	yy4.7.fid
3 Comment	PROTON CDCl3 \D:\ NMR_DATA\ Wangbin\ Wangbin 3
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PADDO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	88
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018 03 20T23:04:00
21 Modification Date	2018-03-20T23:03:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1551.8
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



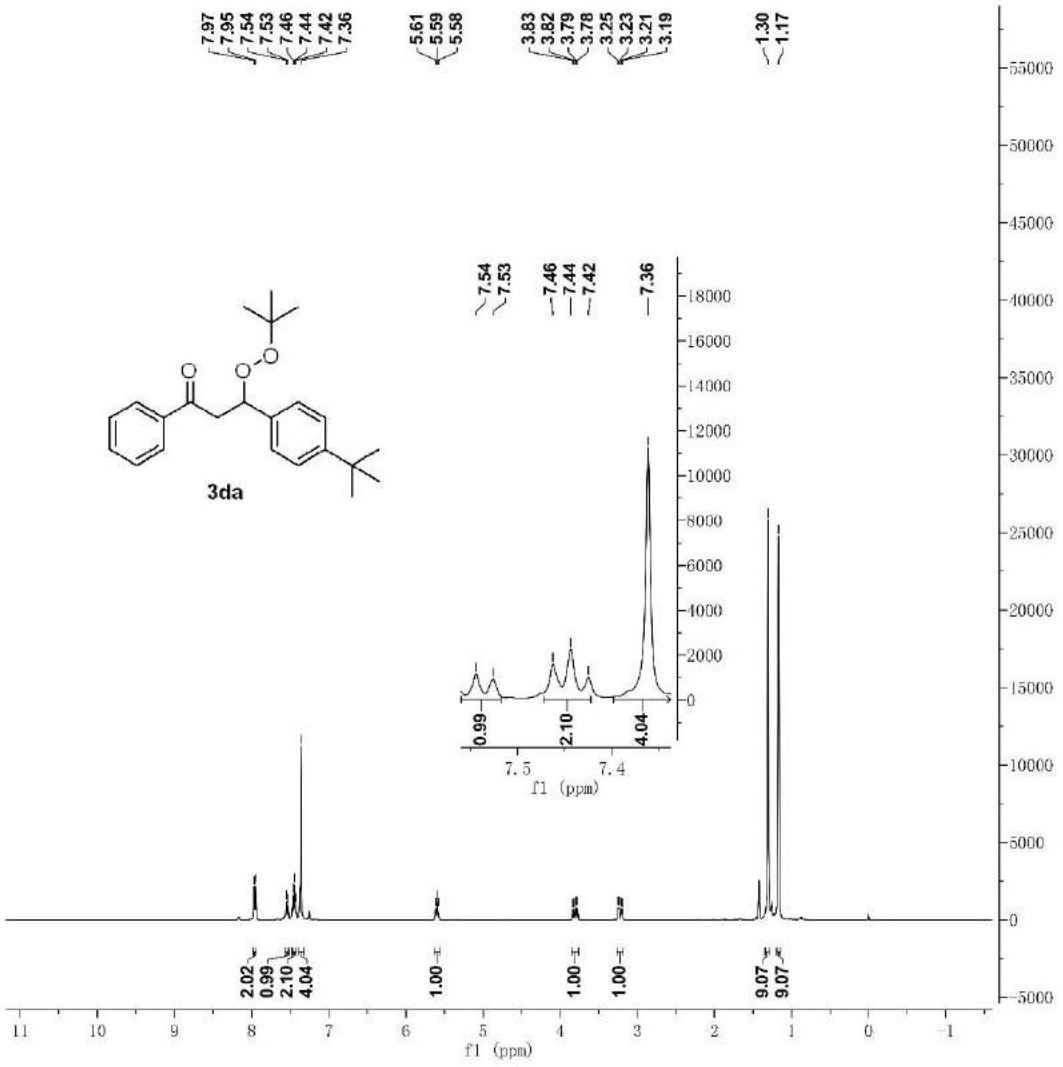
	Parameter	Value
1	Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy4/ 6/ fid
2	Title	yy4.6.fid
3	Comment	C13CPD CDCl3 3D:\ NMR_DATA\ Wangbin\ Wangbin 23
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.3
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PADDO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	150
15	Receiver Gain	119
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2018 03 20T16:47:00
21	Modification Date	2018-03-20T16:46:00
22	Class	
23	Spectrometer Frequency	100.62
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	65536



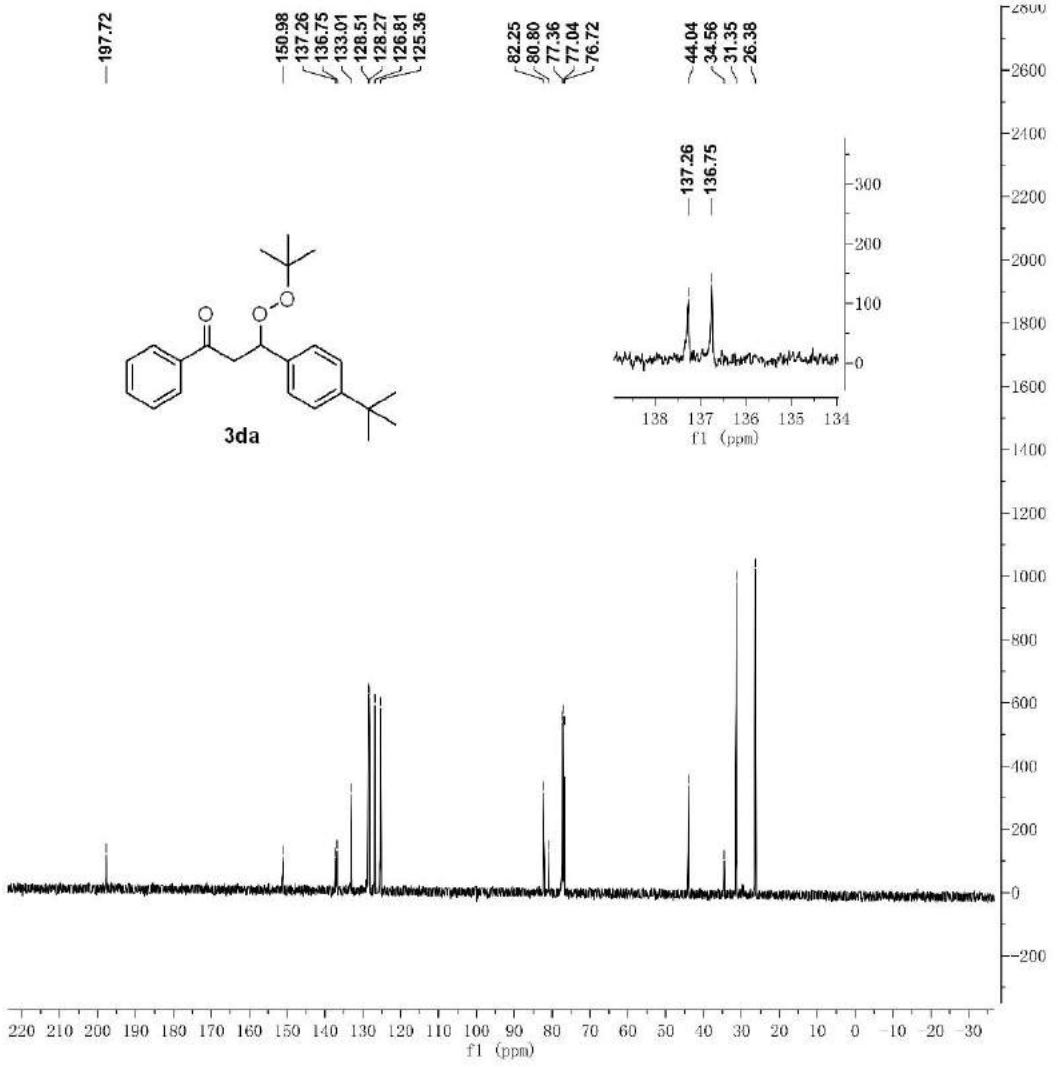
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy31/ 1/ fid
2 Title	yy31.1.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin\ Wangbin 11
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	33
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-03-29T23:07:00
21 Modification Date	2018-03-29T23:06:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1562.6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy31/ 2/ fid
2 Title	yy31.2.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 11
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	200
15 Receiver Gain	88
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-03-29T23:13:00
21 Modification Date	2018 03 29T23:13:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

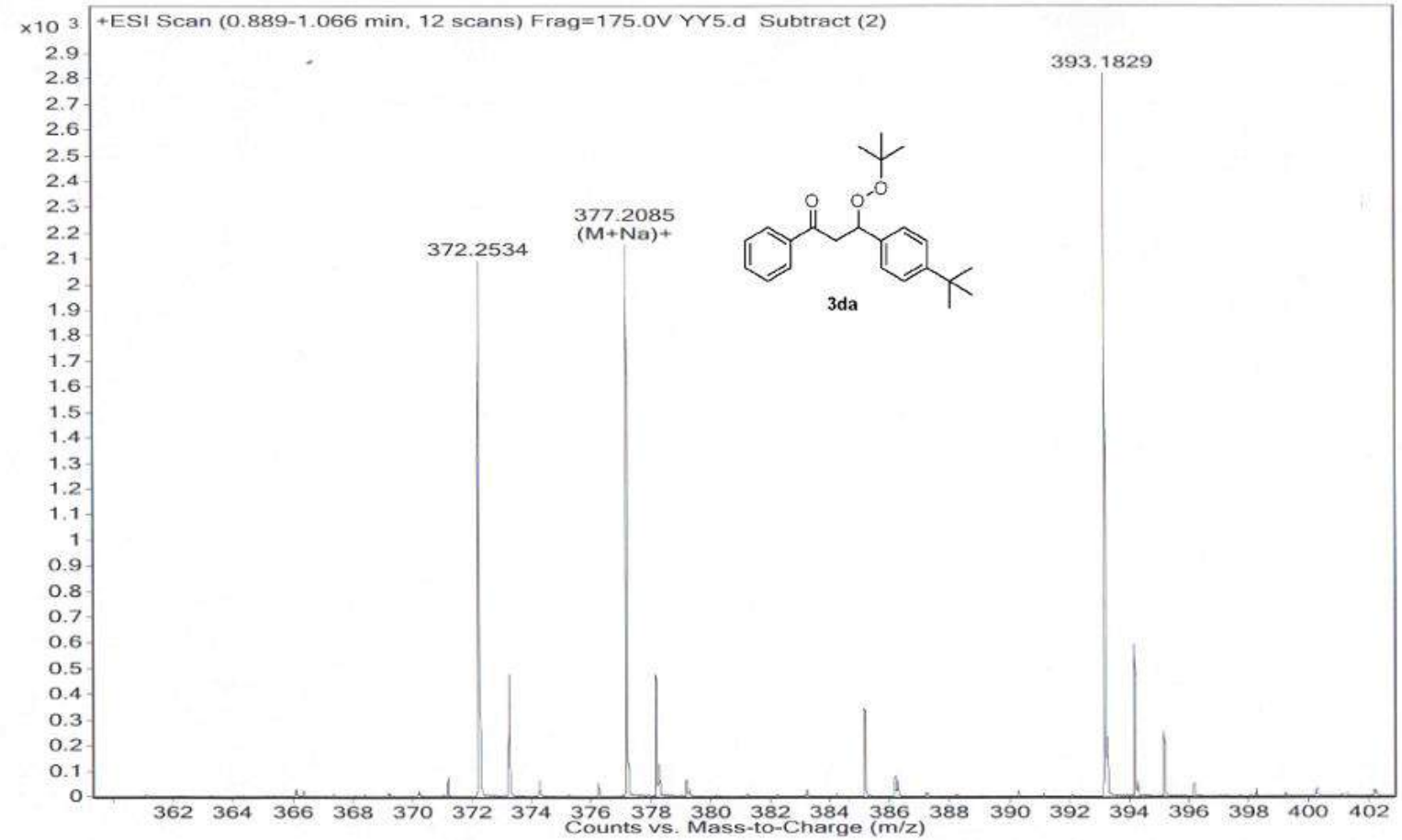


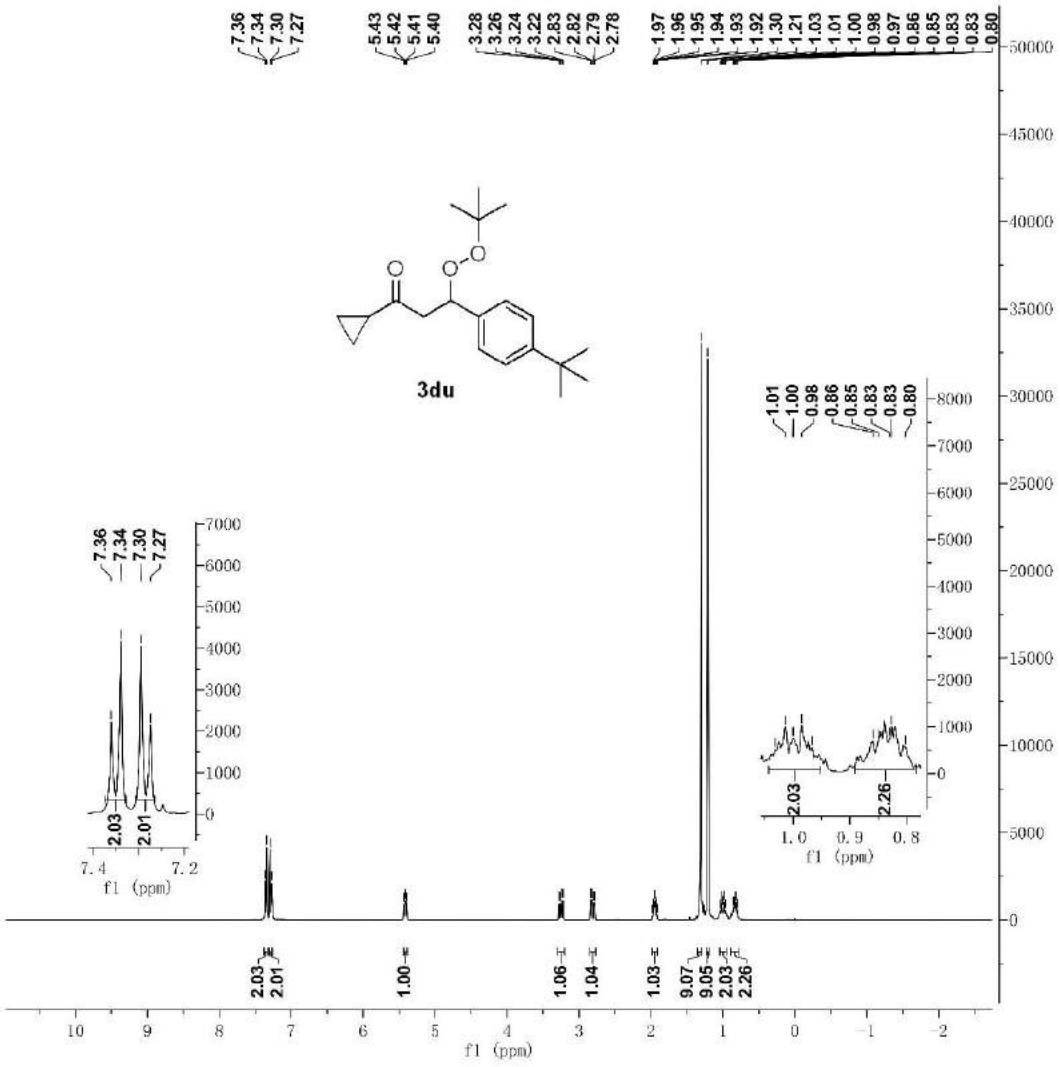
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy5/ 3/ fid
2 Title	yy5.3.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 2
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	295.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	53
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-04-05T19:45:00
21 Modification Date	2018 04 05T19:45:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1549.4
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



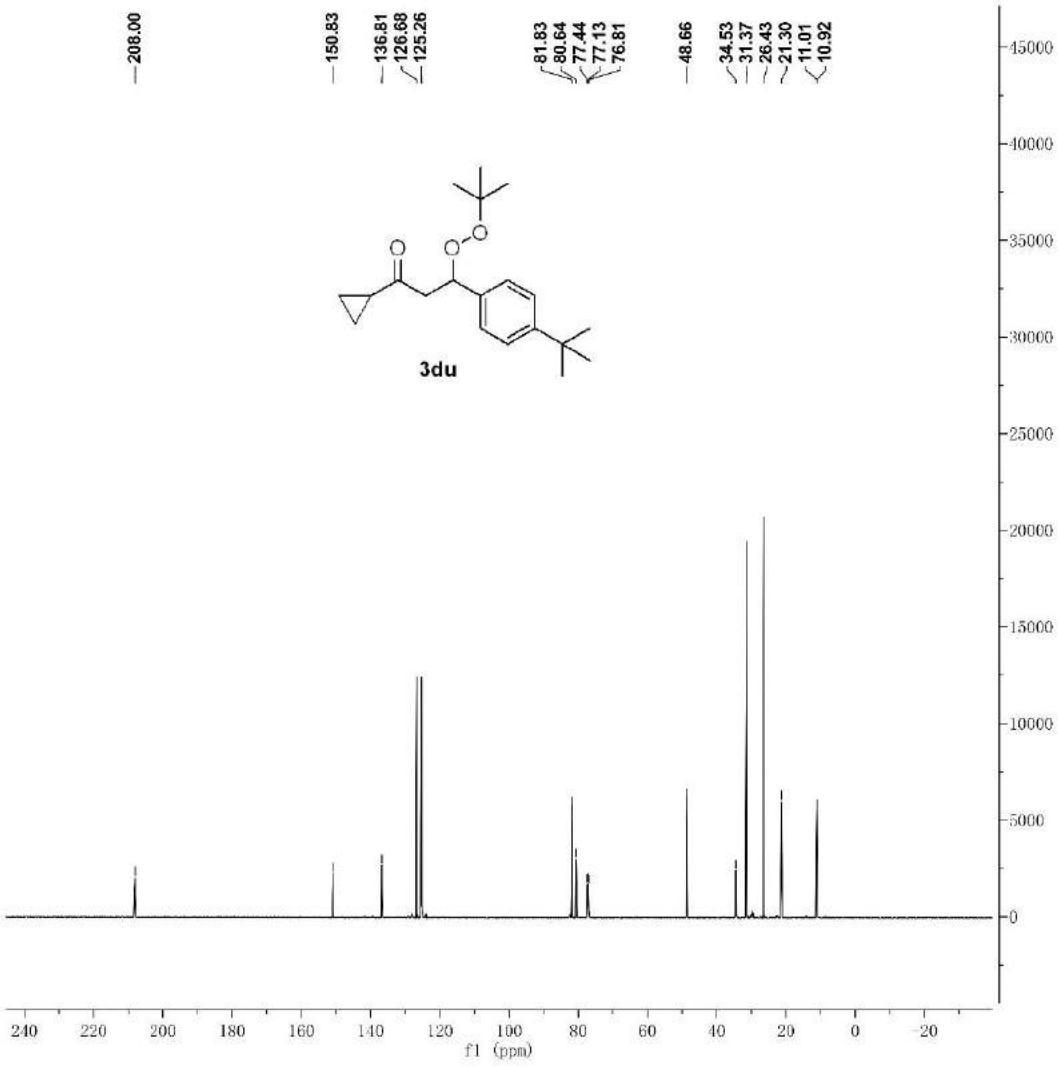
	Parameter	Value
1	Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy5/ 2/ fid
2	Title	yy5.2.fid
3	Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 19
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.3
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	500
15	Receiver Gain	159
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2018-03-15T01:35:00
21	Modification Date	2018 03 15T01:35:00
22	Class	
23	Spectrometer Frequency	100.62
24	Spectral Width	35711.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	65536

Sample Name	Sample10	**Position**	P1-B1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY5.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/4/2018 10:24:15 AM



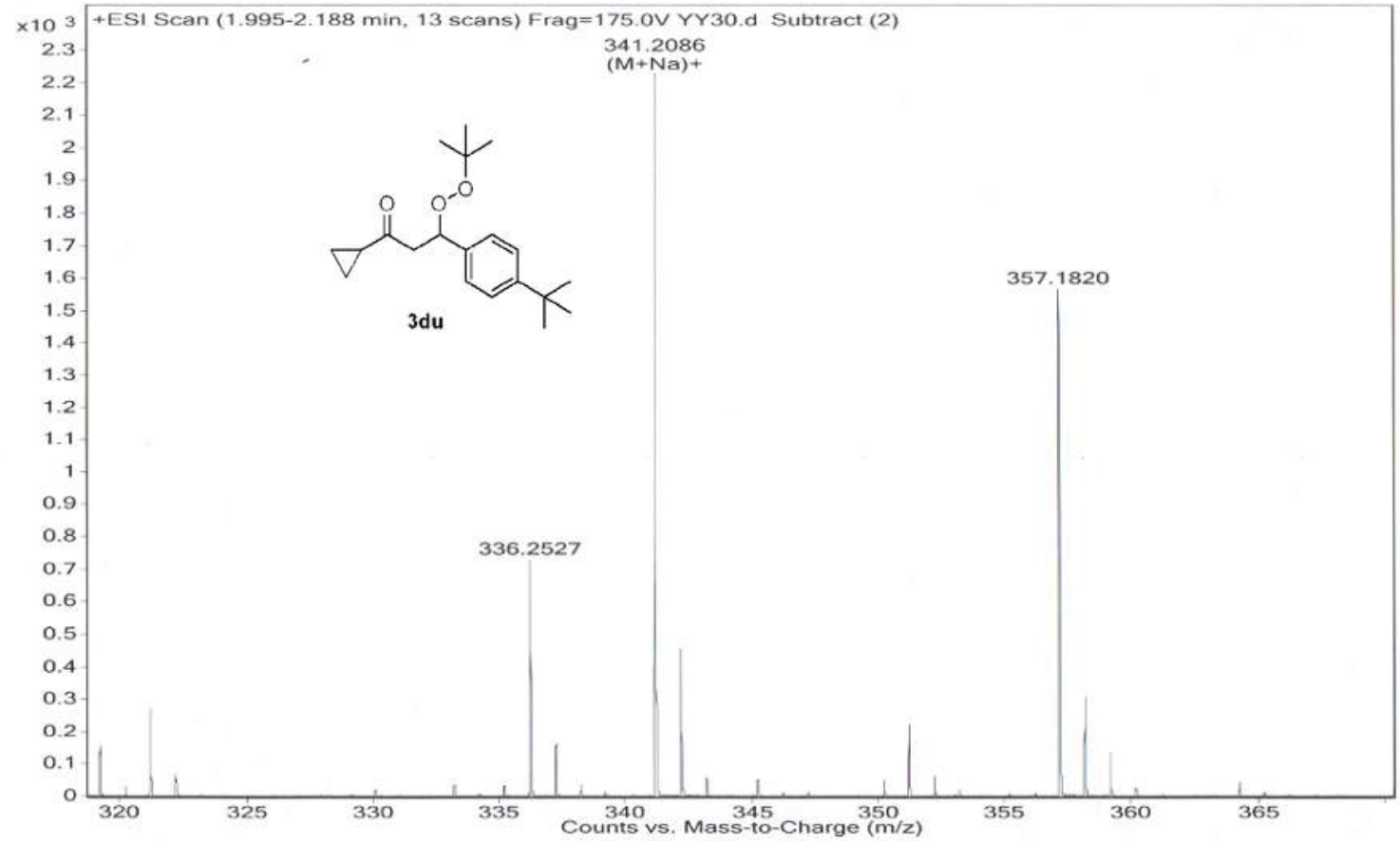


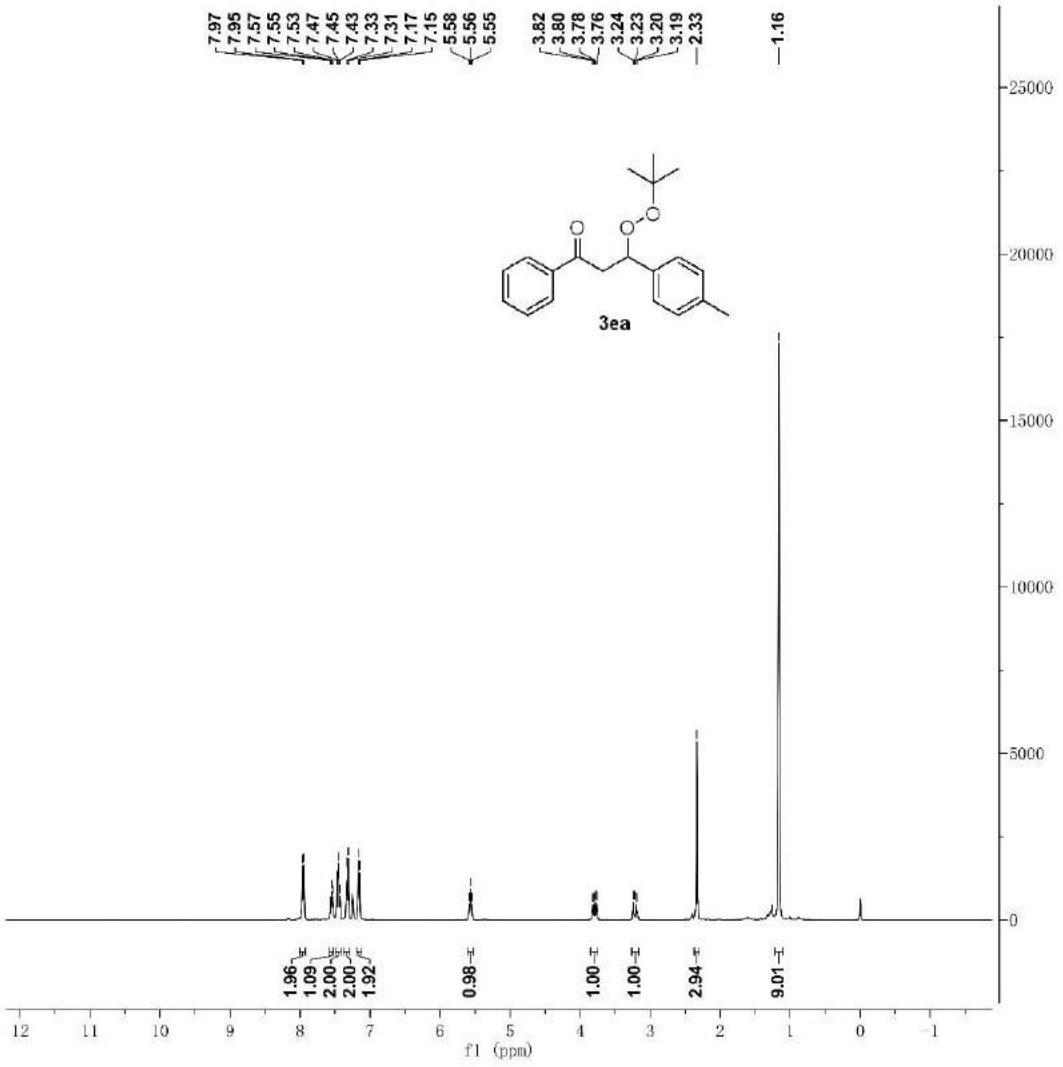
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy30/ 1/ fid
2 Title	yy30.1.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 13
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.5
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	14
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-03-30T08:16:00
21 Modification Date	2018-03-30T08:16:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1550.3
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



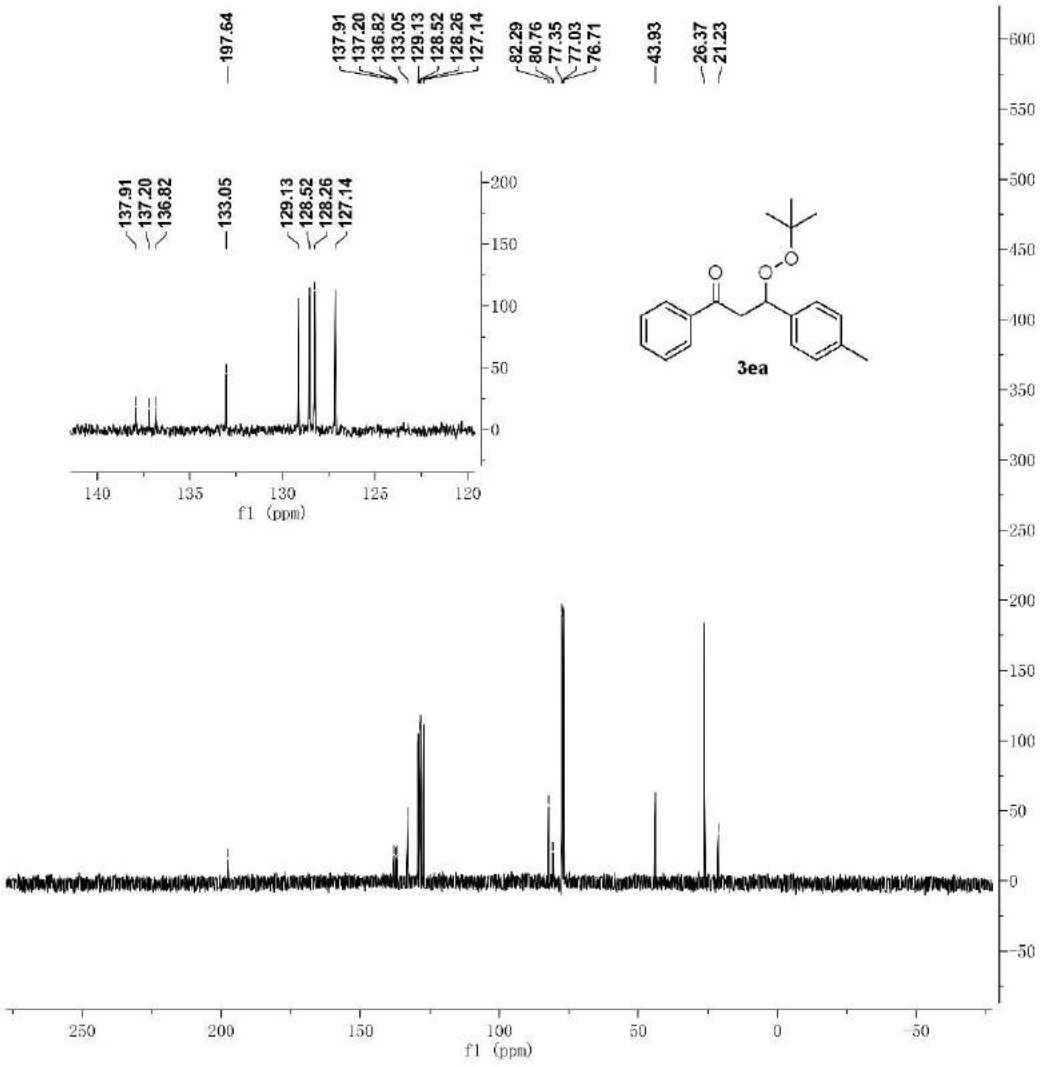
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy30/ 2/ fid
2 Title	yy30.2.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 13
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	299.3
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	800
15 Receiver Gain	159
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-03-30T08:38:00
21 Modification Date	2018 03 30T08:38:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample17	**Position**	P1-B8	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY30.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/4/2018 11:04:57 AM



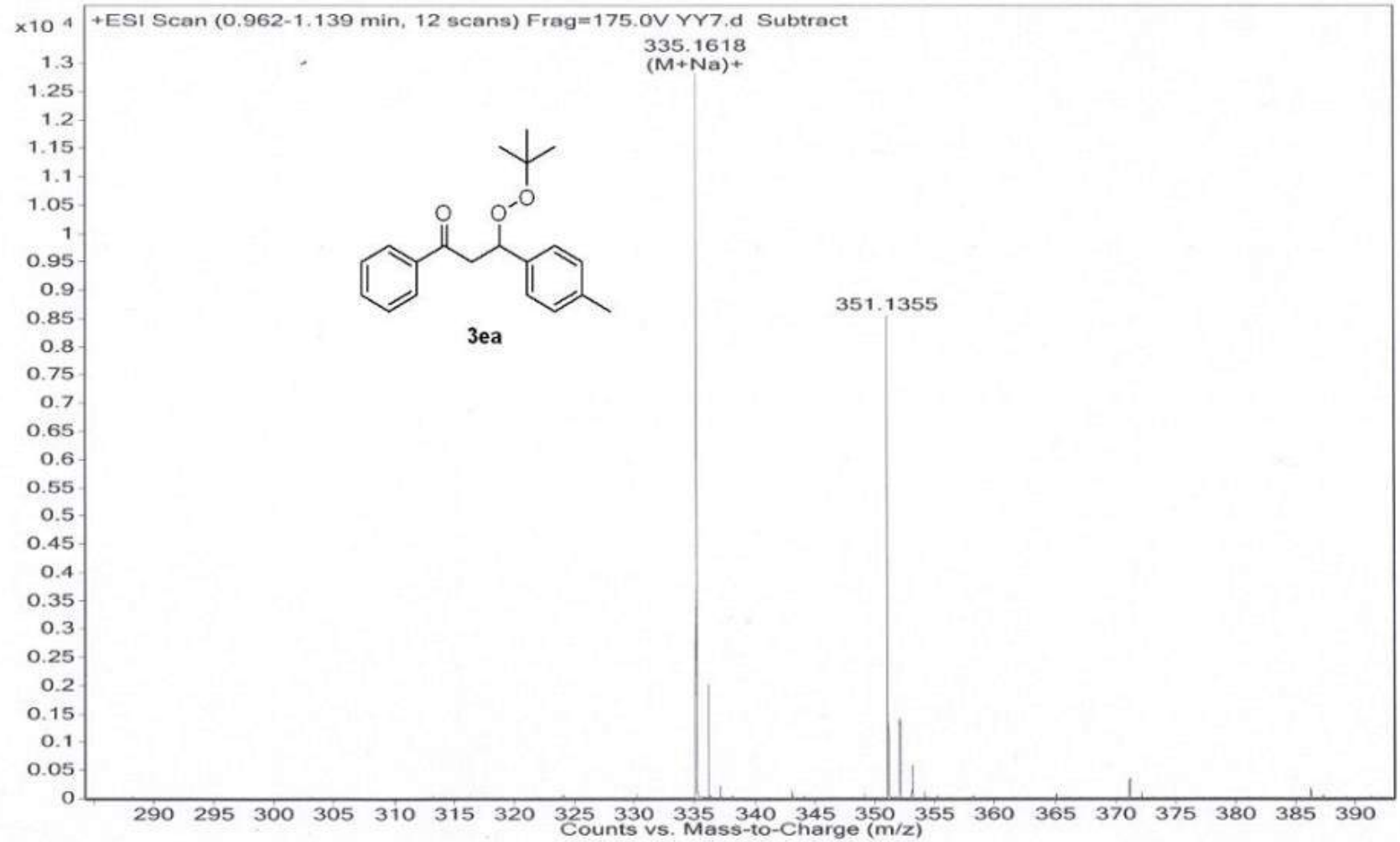


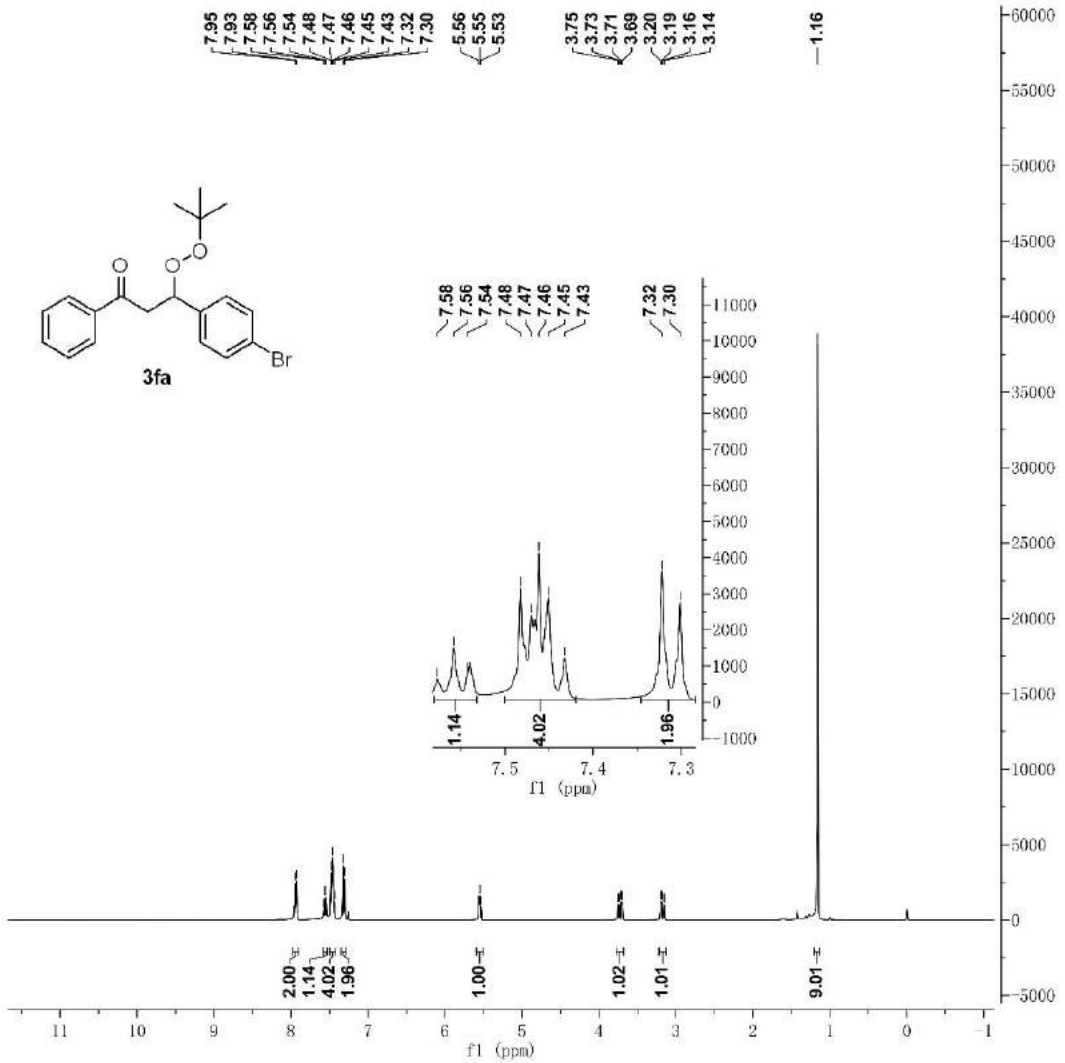
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy7/ 3/ fid
2 Title	yy7.3.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 7
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	113
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-03-20T23:27:00
21 Modification Date	2018 03 20T23:26:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	−1547.9
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



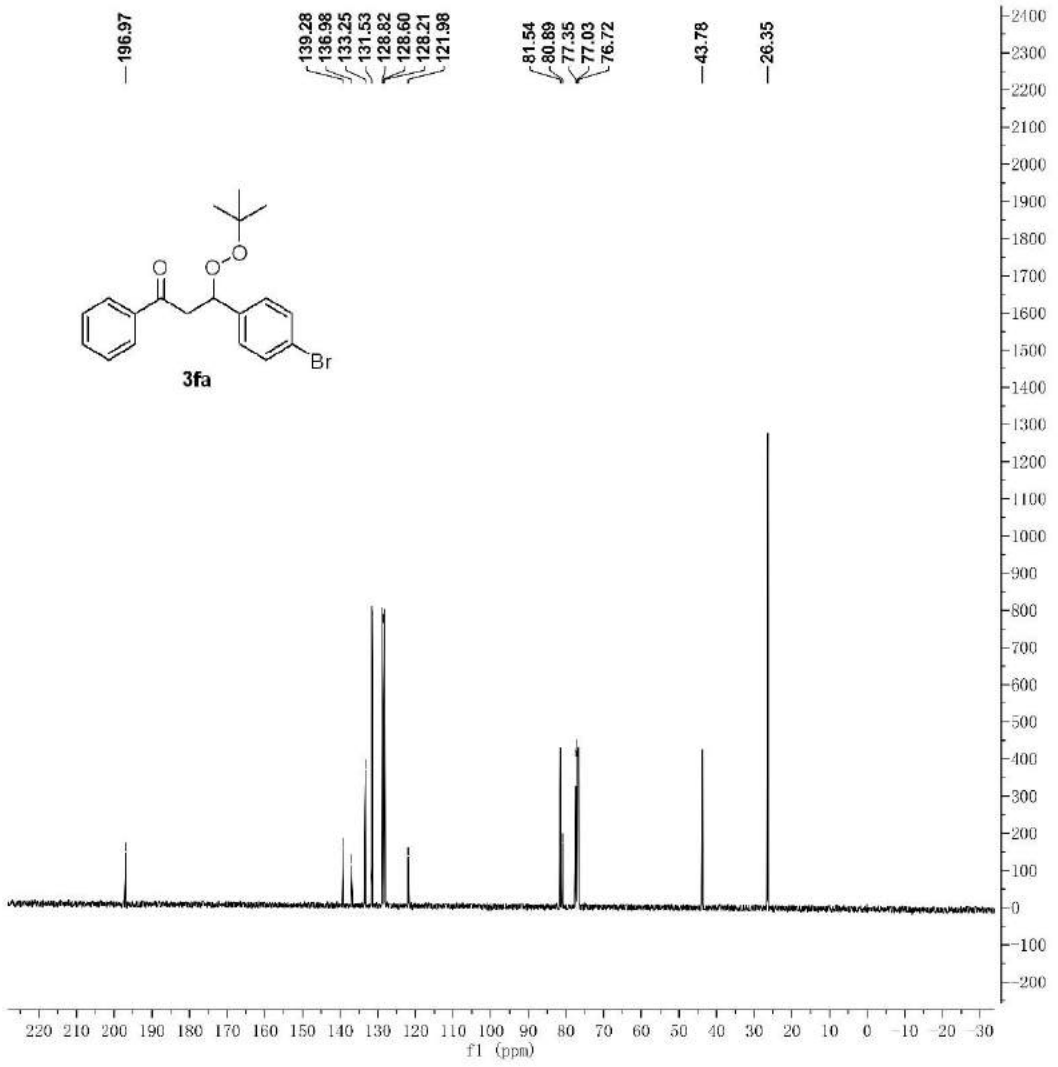
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy7/ 4/ fid
2 Title	yy7.4.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 7
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.5
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	100
15 Receiver Gain	119
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-03-20T23:30:00
21 Modification Date	2018 03 20T23:30:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample2	**Position**	P1-A2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY7.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/24/2018 2:43:37 PM



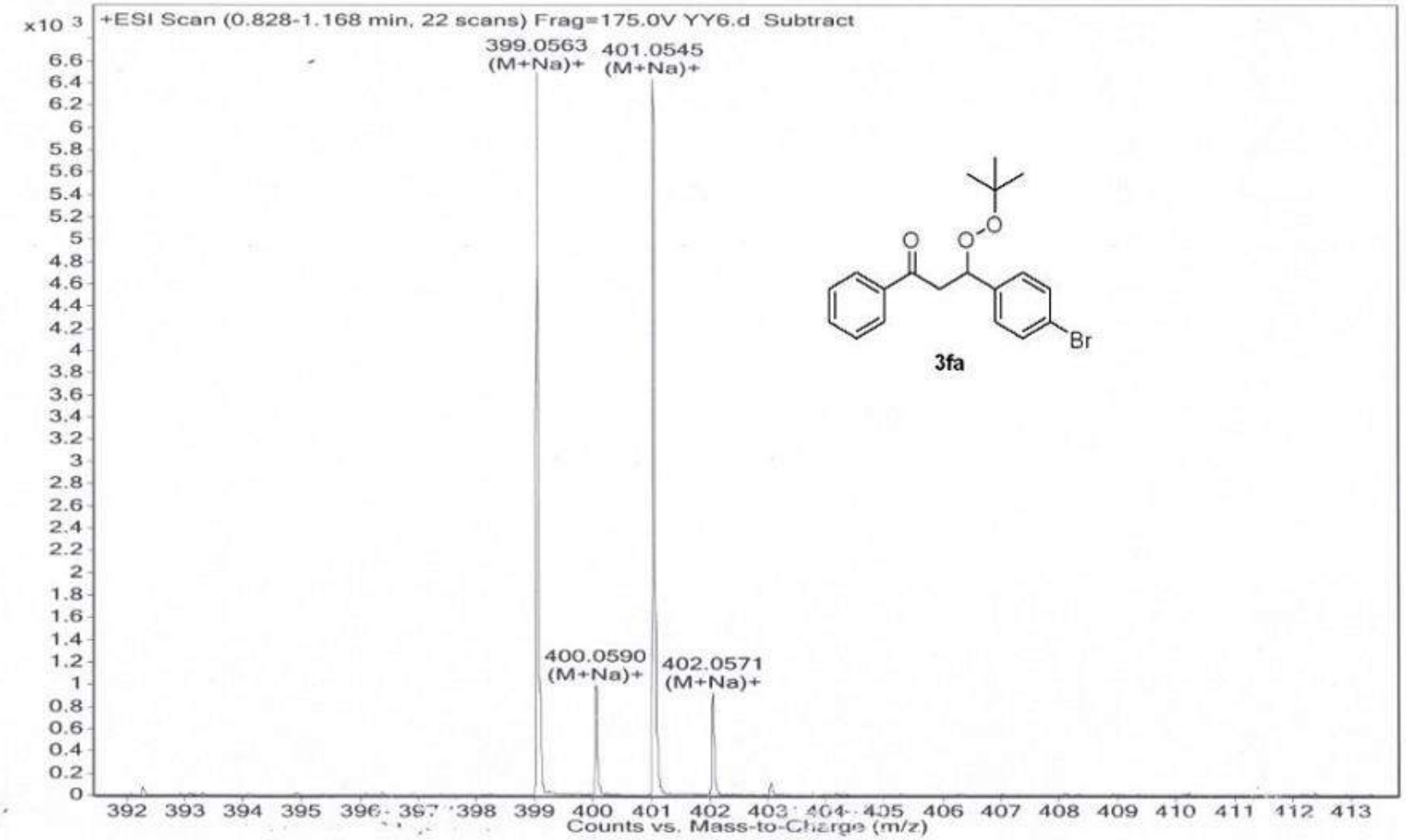


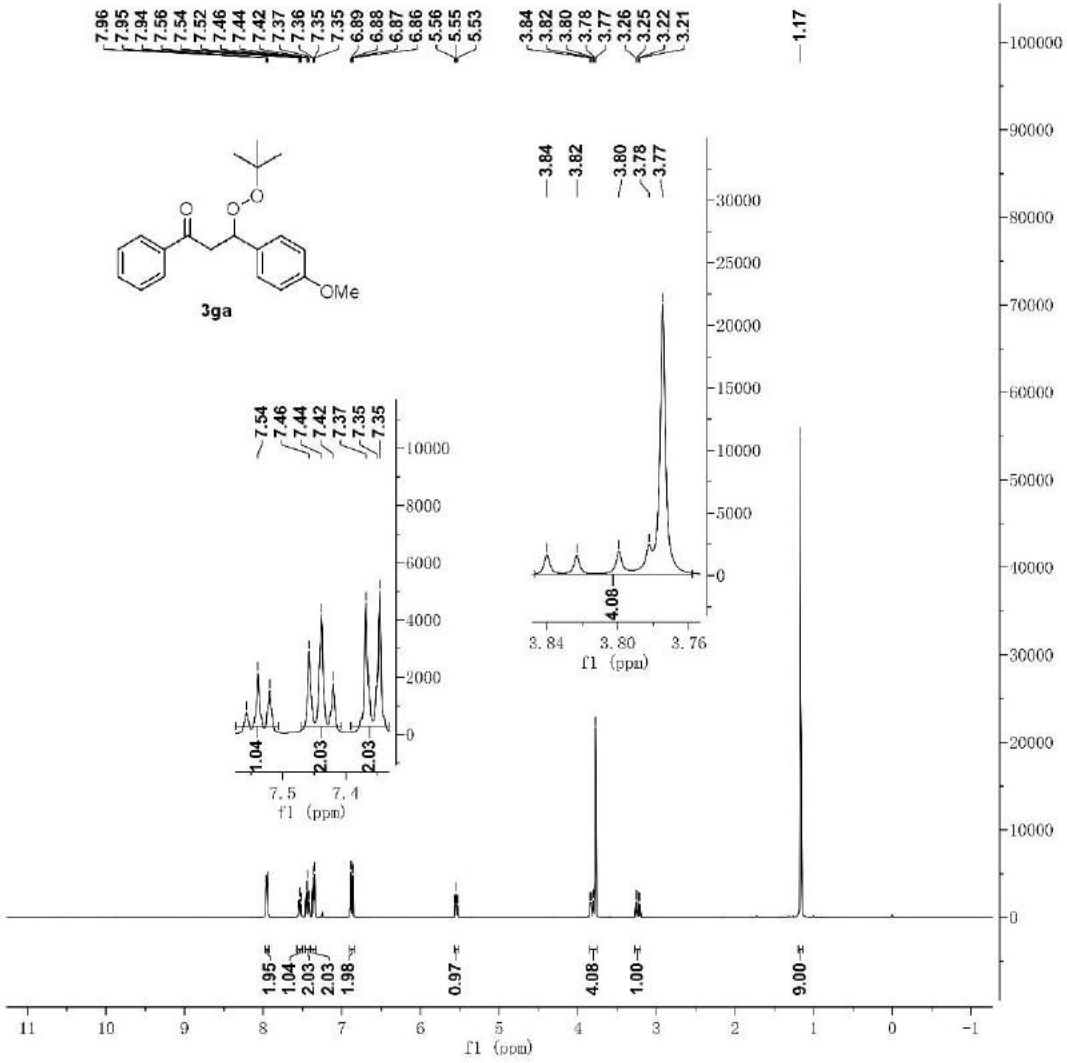
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ 核NMR/ yy6/ 1/ fid
2 Title	yy6.1.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 24
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	299.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	71
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-03-15T02:42:00
21 Modification Date	2018-03-15T02:42:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1547.8
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



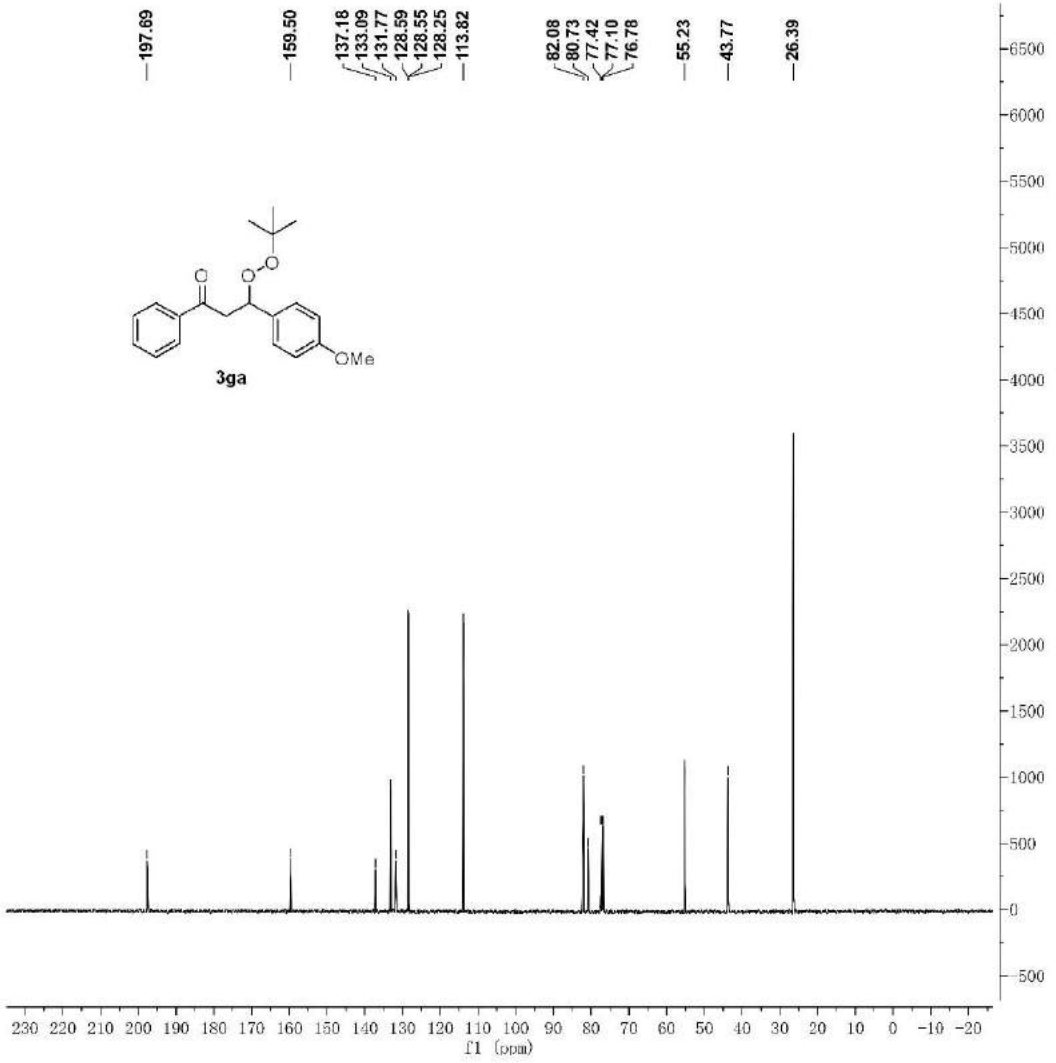
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ 核磁NMR/ yy6/ 2/ fid
2 Title	yy6.2.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 24
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	500
15 Receiver Gain	88
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-03-15T02:56:00
21 Modification Date	2018 03 15T02:56:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample1	**Position**	P1-A1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY6.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/24/2018 2:37:47 PM

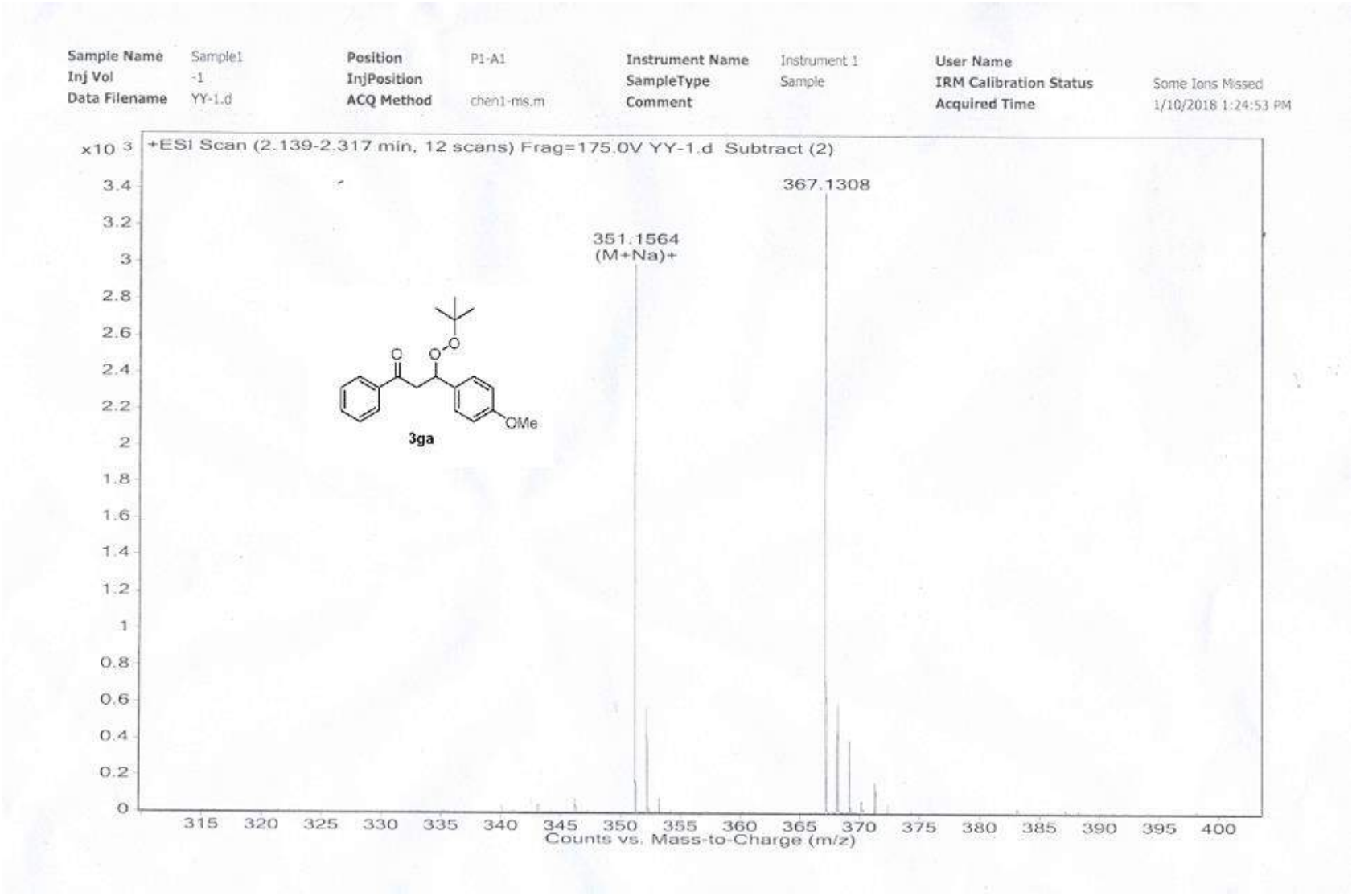


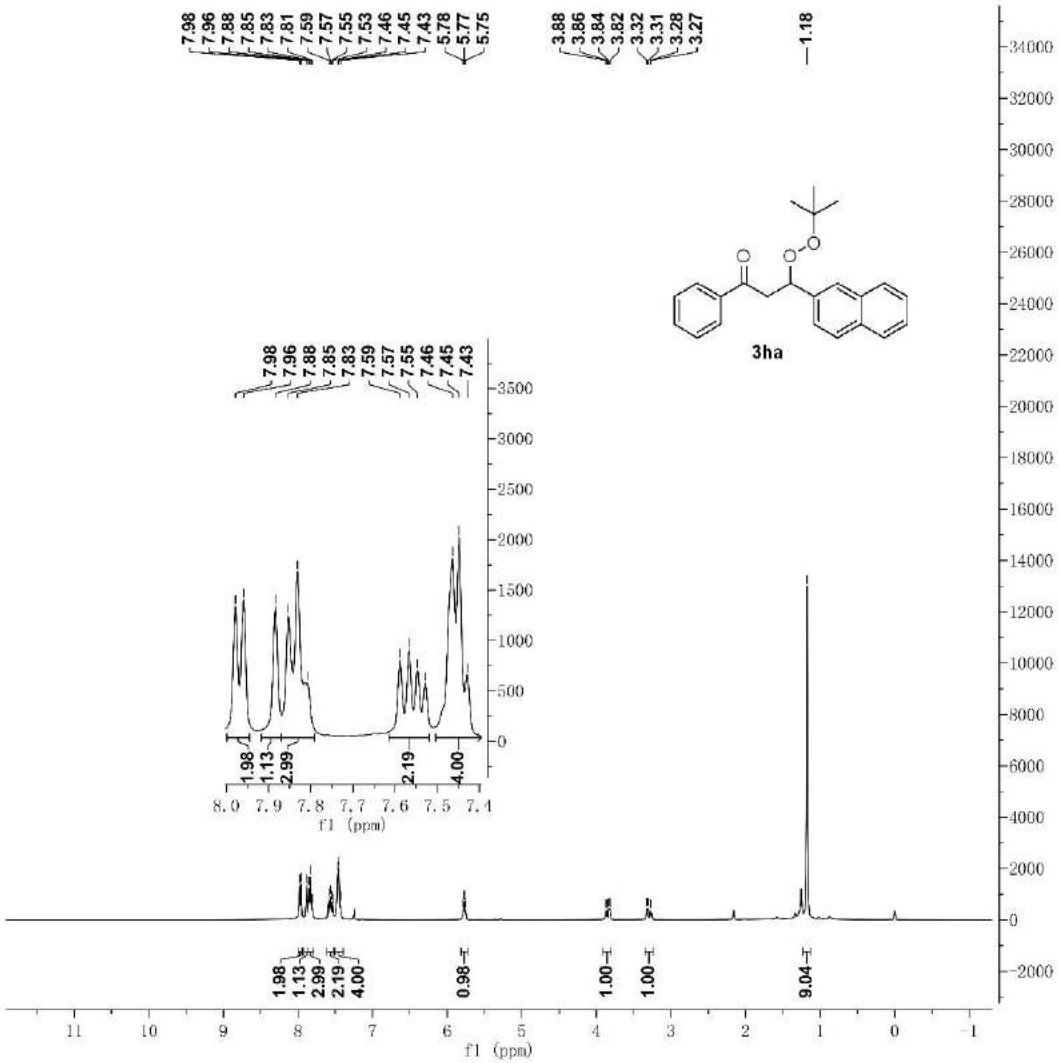


Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ YY1/ 5/ fid
2 Title	YY1.5.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 16
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	293.6
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	33
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-04-11T22:28:00
21 Modification Date	2018-04-11T22:28:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1550.9
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

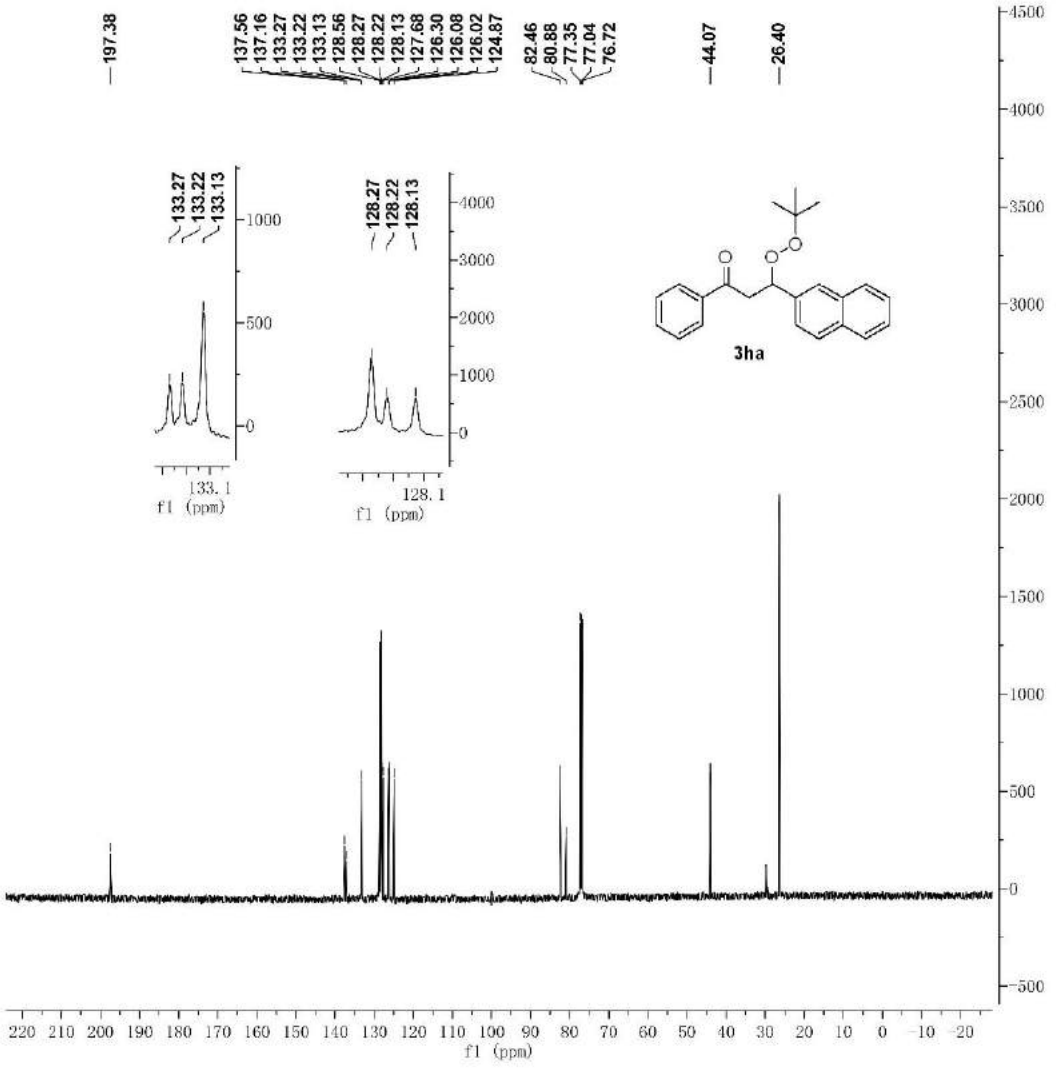


Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ YY1/ 6/ fid
2 Title	YY1.6.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 16
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.5
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	200
15 Receiver Gain	200
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-04-11T22:34:00
21 Modification Date	2018 04 11T22:34:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

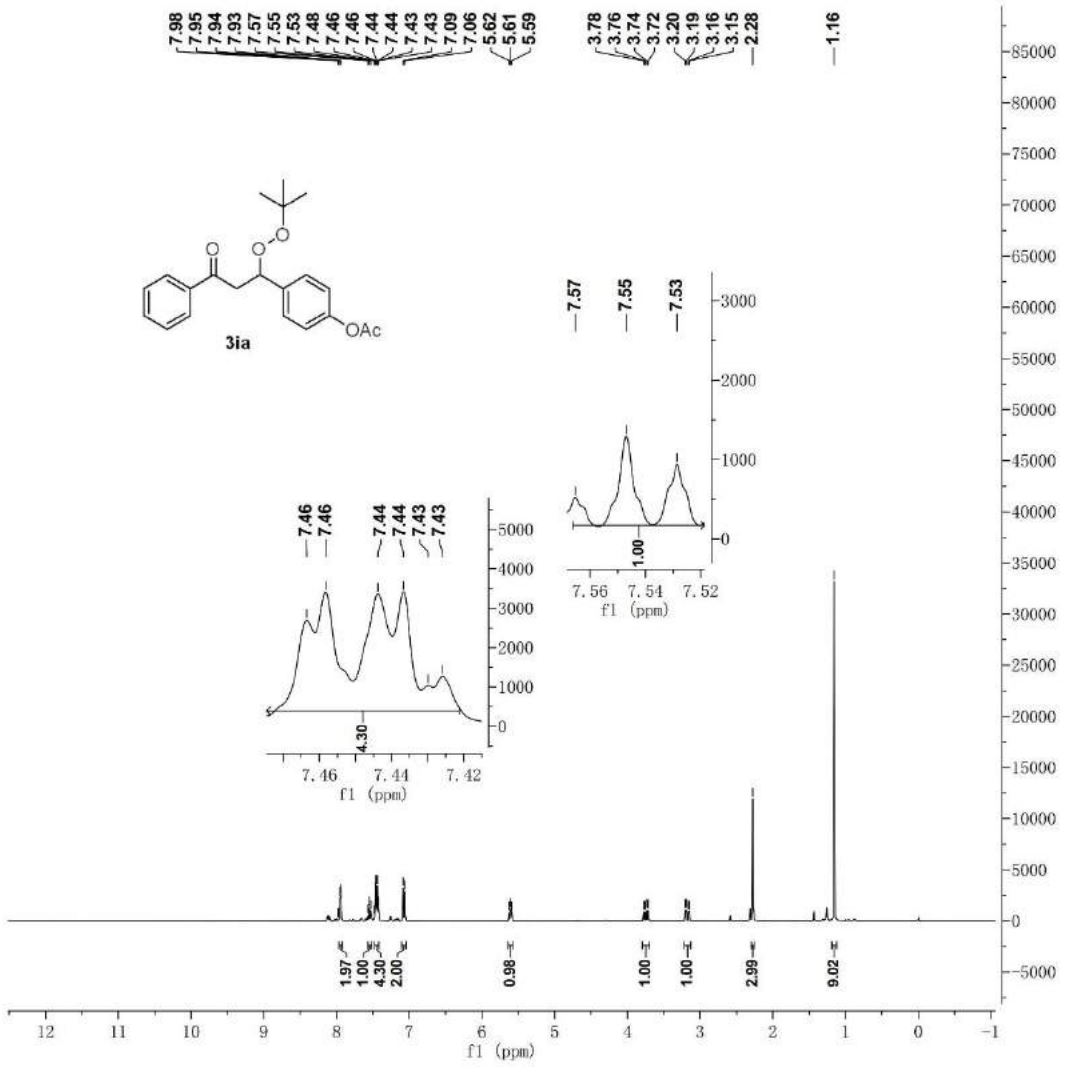

Sample Name Sample1
Inj Vol -1
Data Filename YY-1.d
Position P1-A1
InjPosition
ACQ Method chen1-ms.m
Instrument Name Instrument 1
SampleType Sample
Comment
User Name
IRM Calibration Status Some Ions Missed
Acquired Time 1/10/2018 1:24:53 PM
+ESI Scan (2.139-2.317 min, 12 scans) Frag=175.0V YY-1.d Subtract (2)
x10 3
367.1308
351.1564
(M+Na)+
OMe
3ga
Counts vs. Mass-to-Charge (m/z)



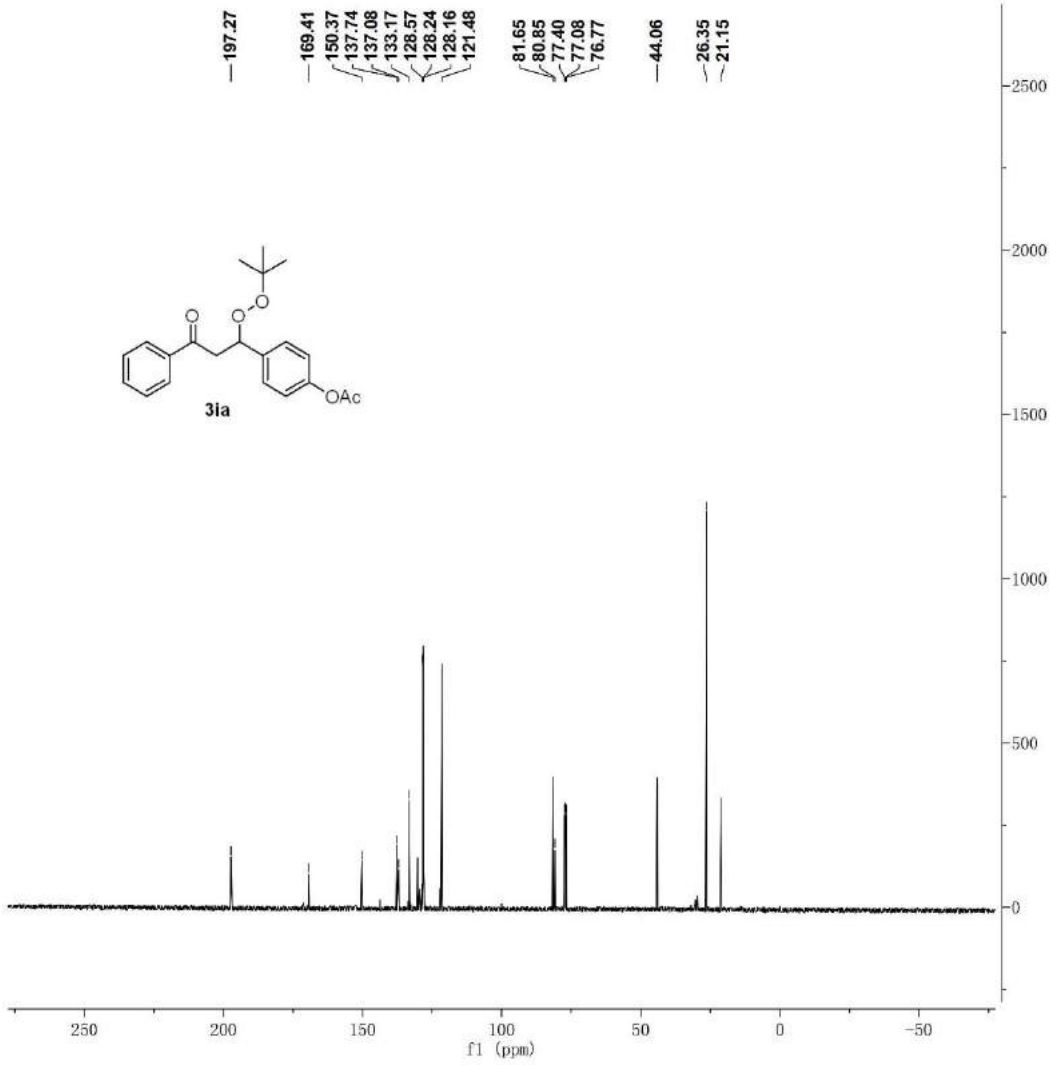
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy8-1/ 3/ fid
2 Title	yy8 1.3.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 13
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	297.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	88
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-03-21T01:11:00
21 Modification Date	2018 03 21T01:10:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1550.8
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy8-1/ 4/ fid
2 Title	yy8 1.4.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 13
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	1024
15 Receiver Gain	133
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-03-21T01:38:00
21 Modification Date	2018-03-21T01:38:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536



Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy57/ 1/ fid
2 Title	yy57.1.fid
3 Comment	PROTON CDCl3 (D:\ NMR_DATA\ Wangbin\ Wangbin 11
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	0.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	33
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-06-29T10:18:00
21 Modification Date	2018-06-29T10:15:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1547.9
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

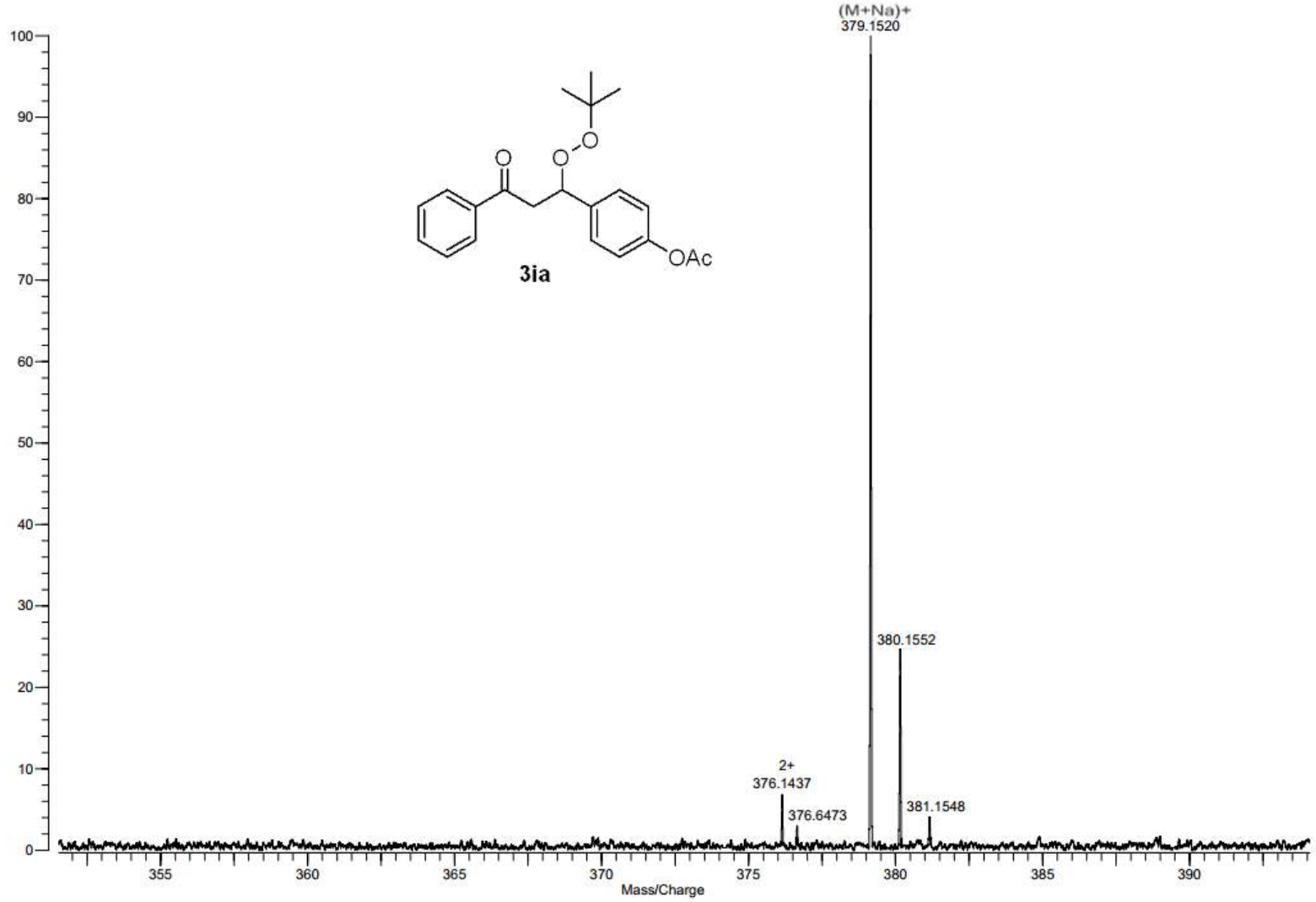


	Parameter	Value
1	Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy57/ 2/ fid
2	Title	yy57.2.fid
3	Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 11
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	0.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	200
15	Receiver Gain	113
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2018-06-29T10:24:00
21	Modification Date	2018-06-29T10:21:00
22	Class	
23	Spectrometer Frequency	100.62
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	65536

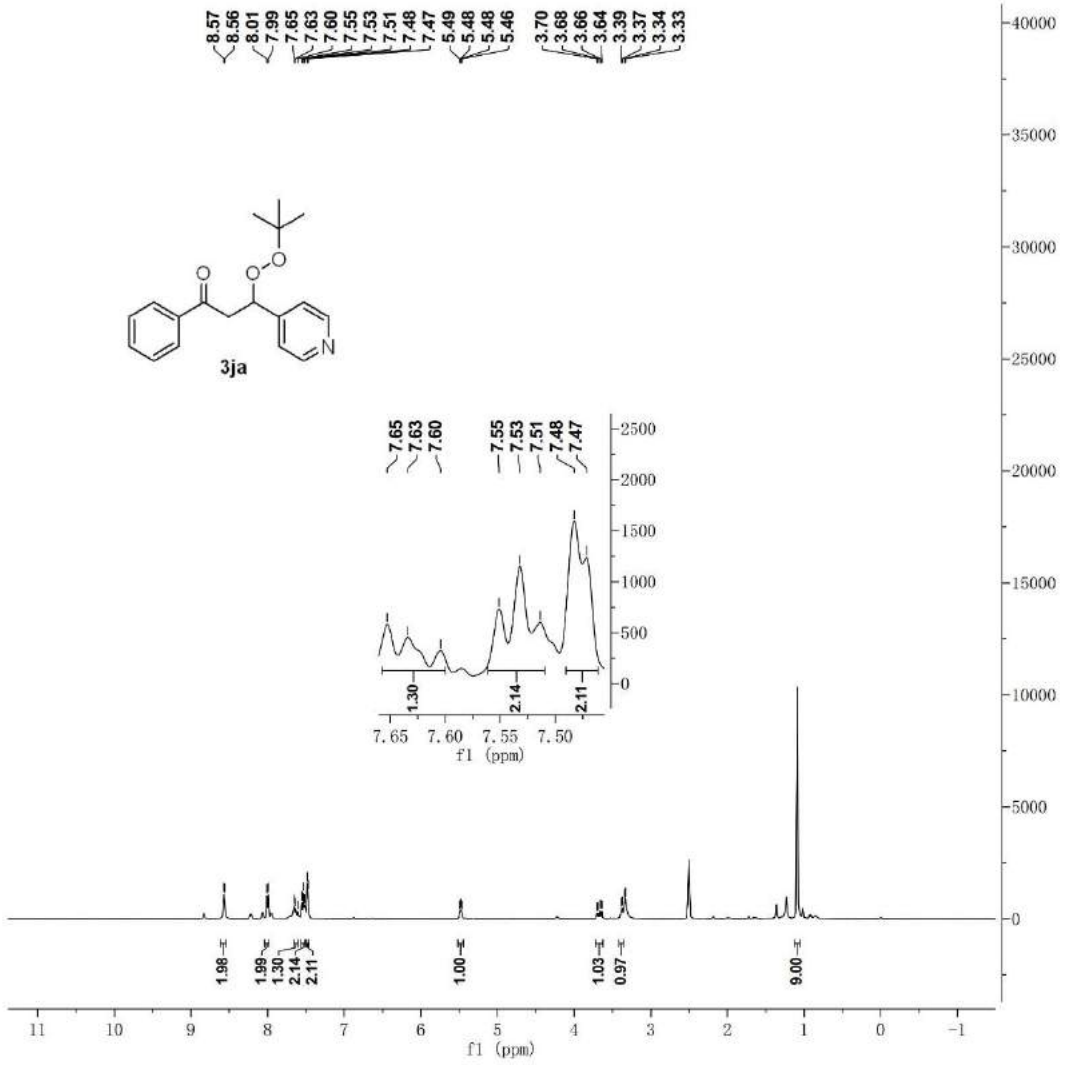
Varian QFT-ESI
File: yy57_ESI.trans

Mode: Positive
Scans: 1

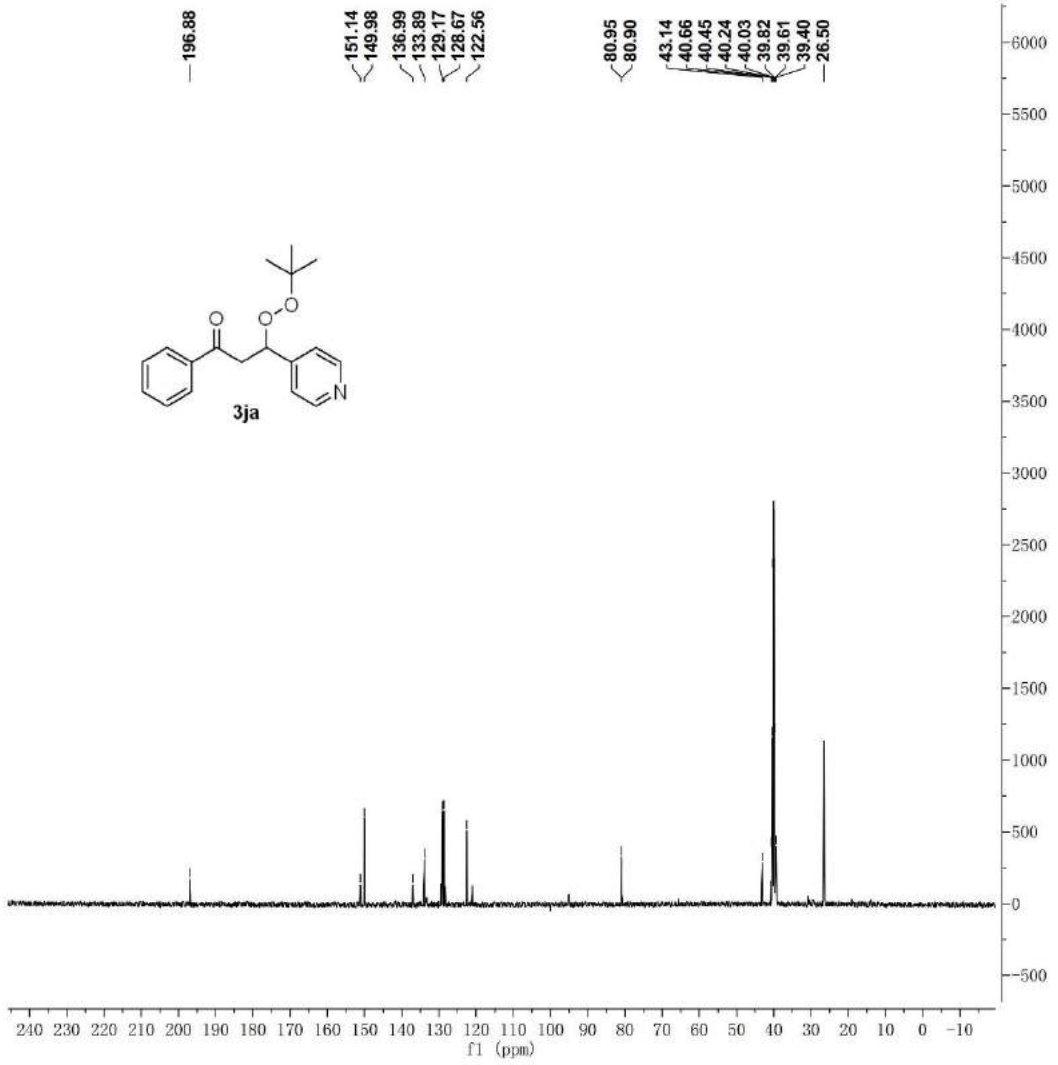
Date: 02-JUL-2018
Time: 15:54:04
Scale: 12.5906



3ia



Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyy/ Desktop/ yy55/ 1/ fid
2 Title	yy55.1.fid
3 Comment	PROTON DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 16
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	0.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	113
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-06-29T13:09:00
21 Modification Date	2018-06-29T13:06:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1538.4
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

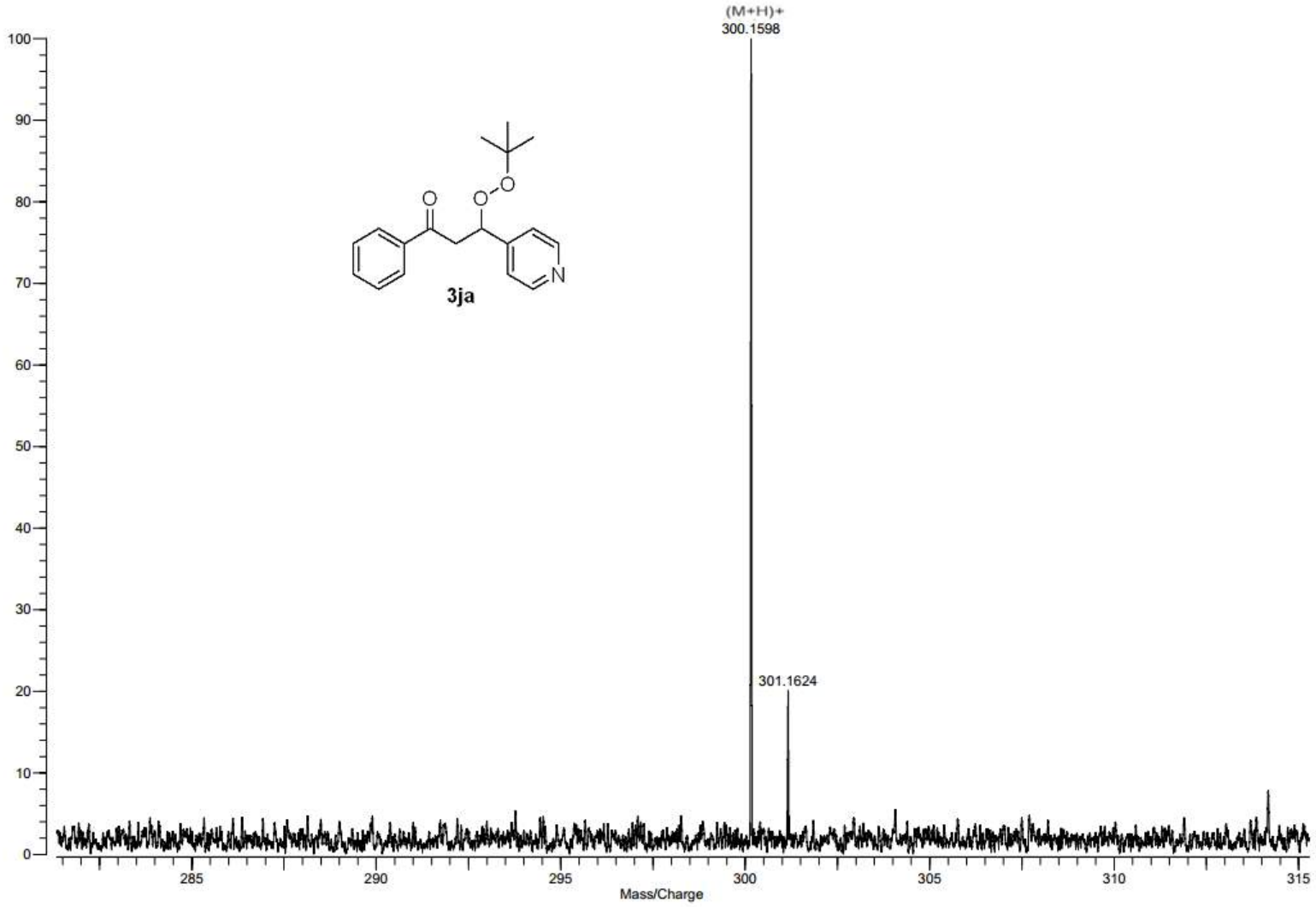


	Parameter	Value
1	Data File Name	C:/ Users/ yyyyyyyyyyy/ Desktop/ yy55/ 2/ fid
2	Title	yy55.2.fid
3	Comment	C13CPD DMSO {D:\ NMR_DATA\ Wangbin} Wangbin 16
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	0.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	600
15	Receiver Gain	176
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2018-06-29T13:25:00
21	Modification Date	2018-06-29T13:22:00
22	Class	
23	Spectrometer Frequency	100.62
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	65536

Varian QFT-ESI
File: yy55_ESI.trans

Mode: Positive
Scans: 1

Date: 02-JUL-2018
Time: 15:49:20
Scale: 46.0160



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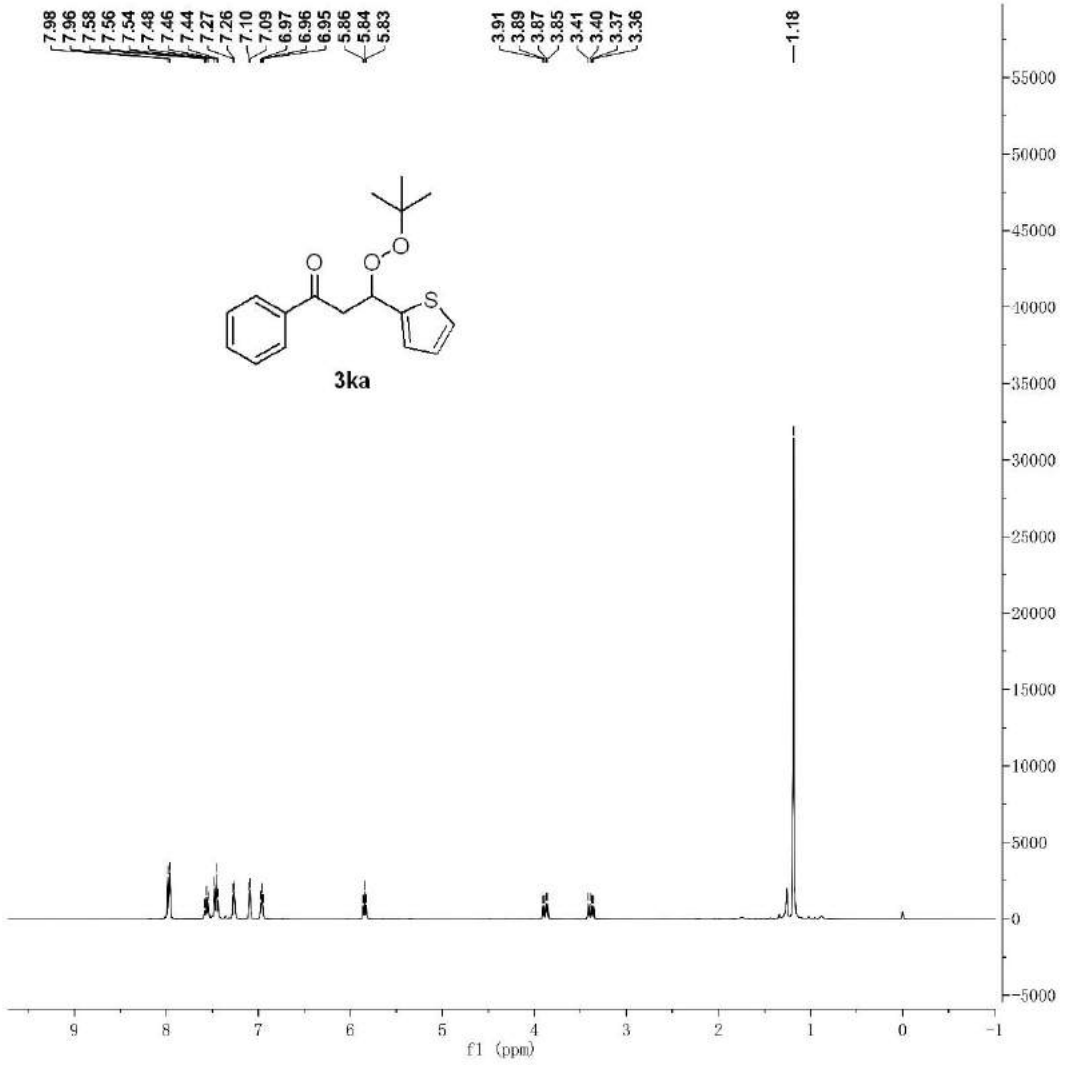
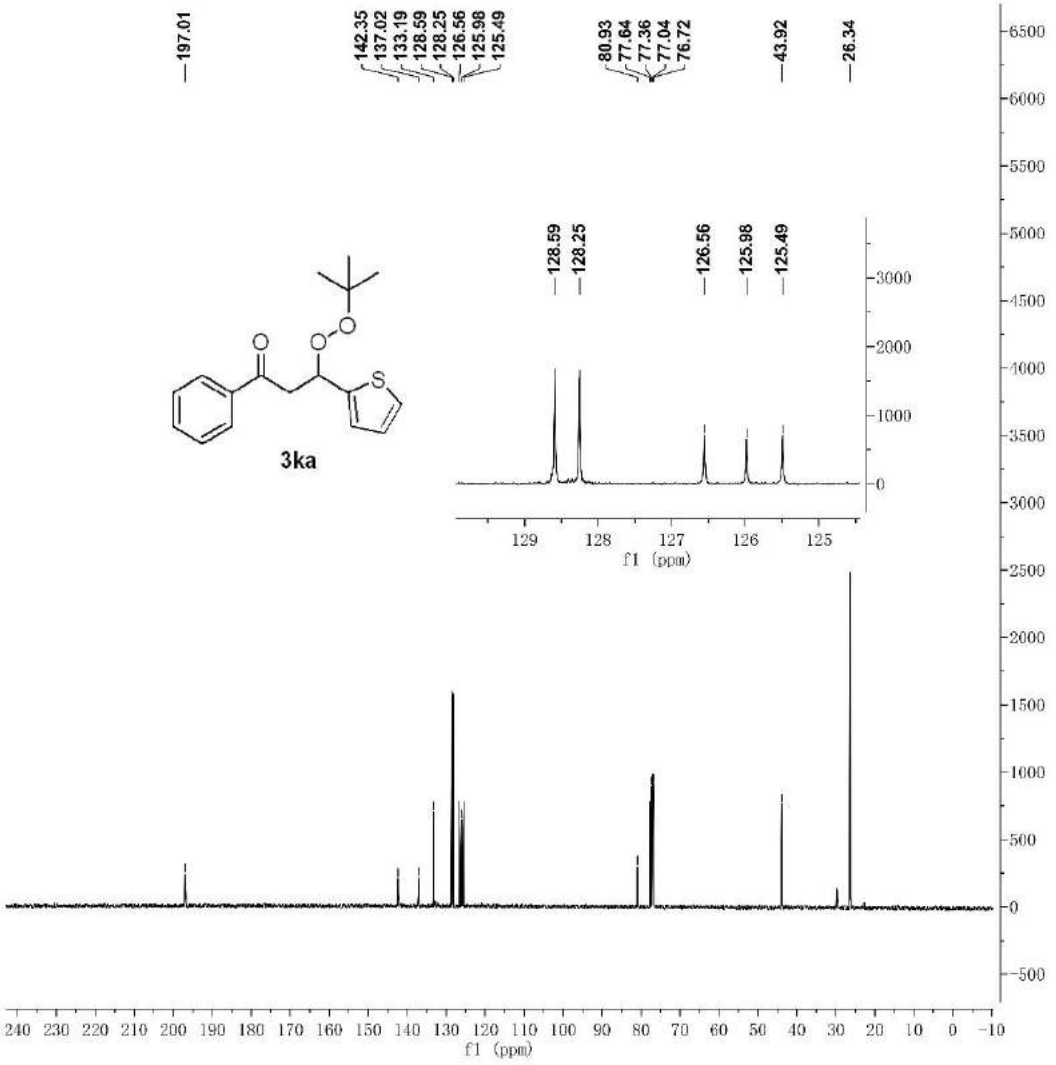


	Parameter	Value
1	Data File Name	C:/ Users/ yyyyyyyyyyy/ Desktop/ yy58-2/ 1/ fid
2	Title	yy58-2.1.fid
3	Comment	PROTON CDCl3 (D:\ NMR_DATA\ Wangbin) Wangbin 6
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	0.0
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	16
15	Receiver Gain	71
16	Relaxation Delay	1.0000
17	Pulse Width	14.4000
18	Presaturation Frequency	
19	Acquisition Time	4.0894
20	Acquisition Date	2018-07-01T13:34:00
21	Modification Date	2018-07-01T13:31:00
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8012.8
25	Lowest Frequency	-1549.0
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536



	Parameter	Value
1	Data File Name	C:/ Users/ yyyyyyyyyyy/ Desktop/ yy58-2/ 2/ fid
2	Title	yy58-2.2.fid
3	Comment	C13CPD CDCl3 (D:\ NMR_DATA\ Wangbin) Wangbin 6
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	0.0
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	400
15	Receiver Gain	159
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2018-07-01T13:46:00
21	Modification Date	2018-07-01T13:43:00
22	Class	
23	Spectrometer Frequency	100.62
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17856
28	Spectral Size	65536

Varian QFT-ESI
File: yy58_ESI.trans

Mode: Positive
Scans: 1

Date: 02-JUL-2018
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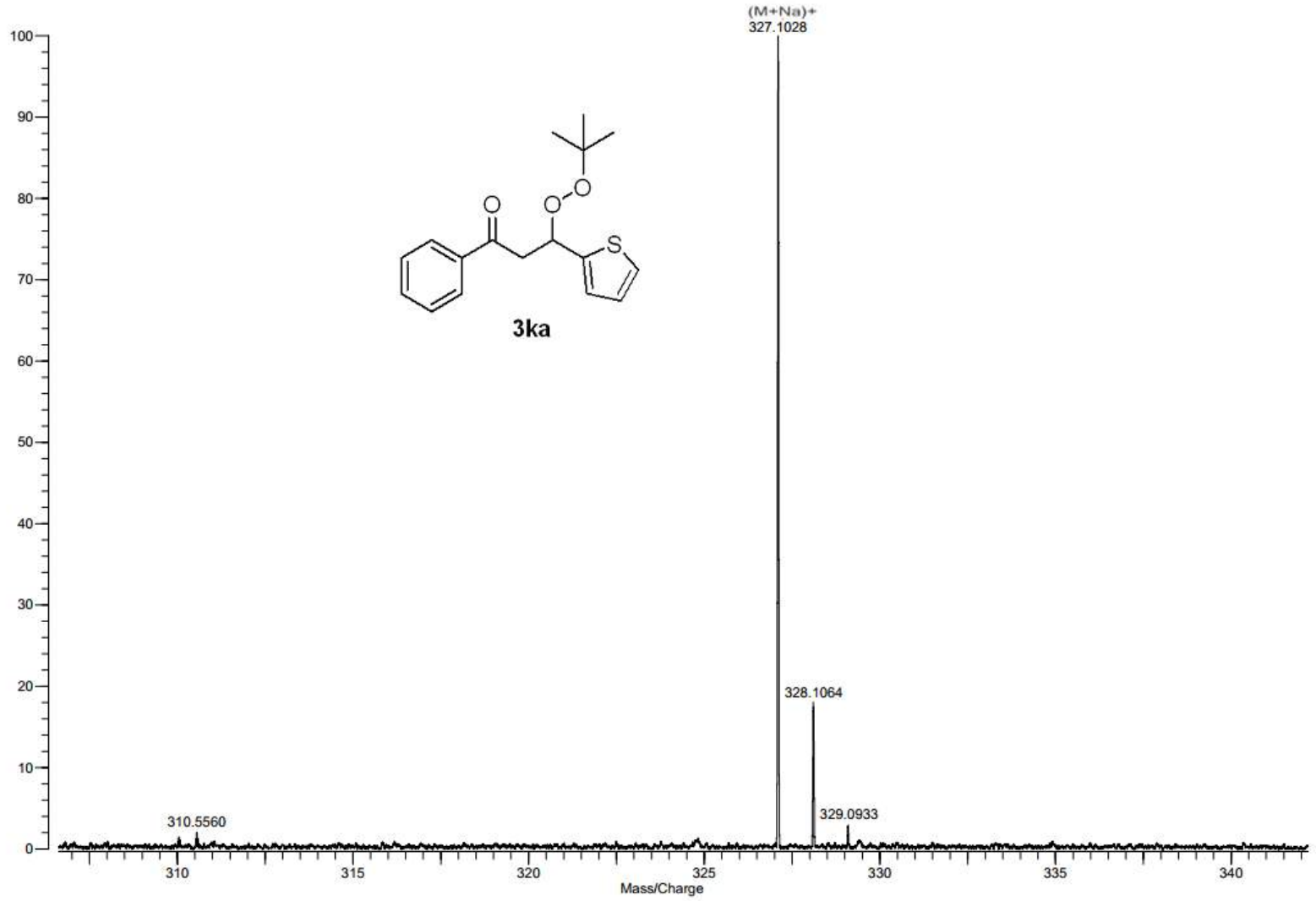

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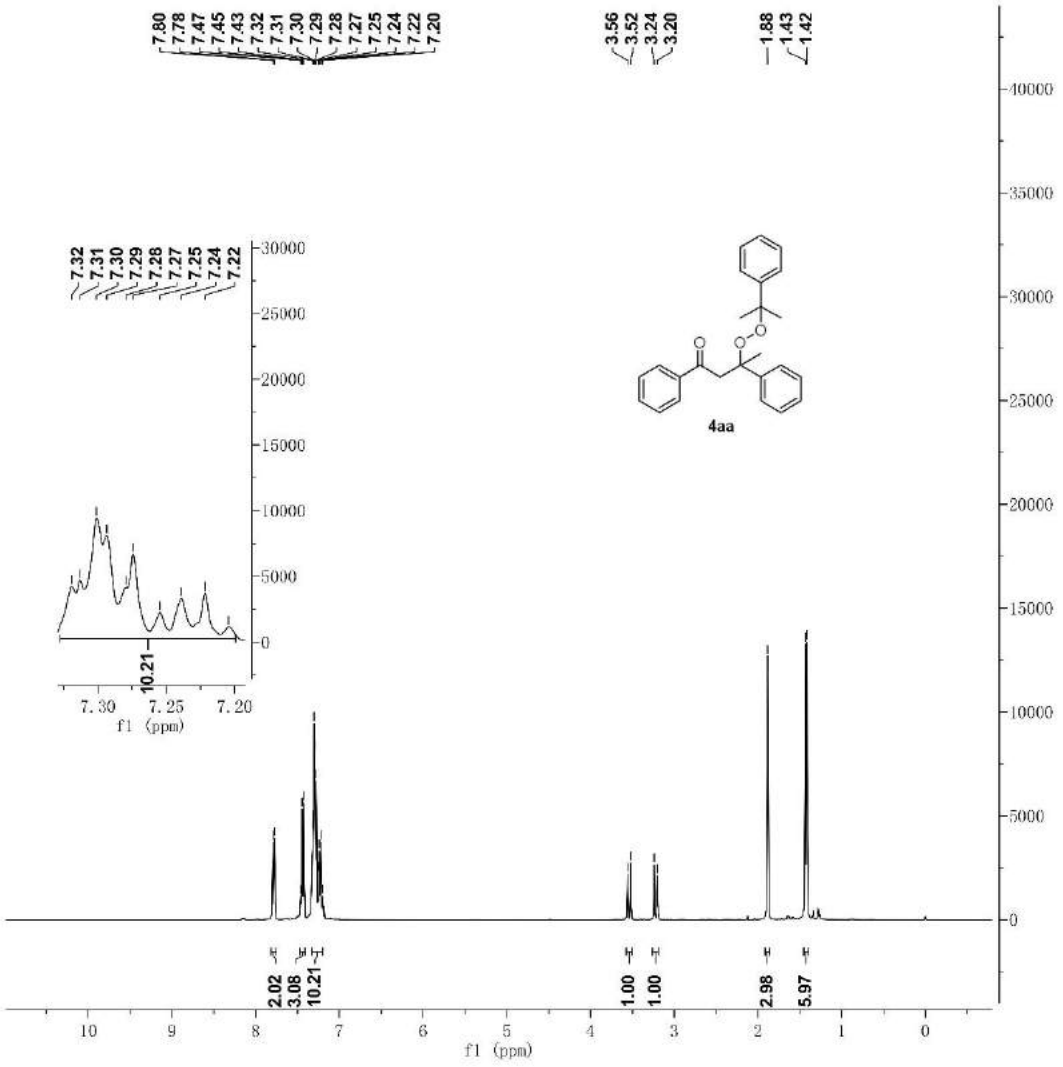
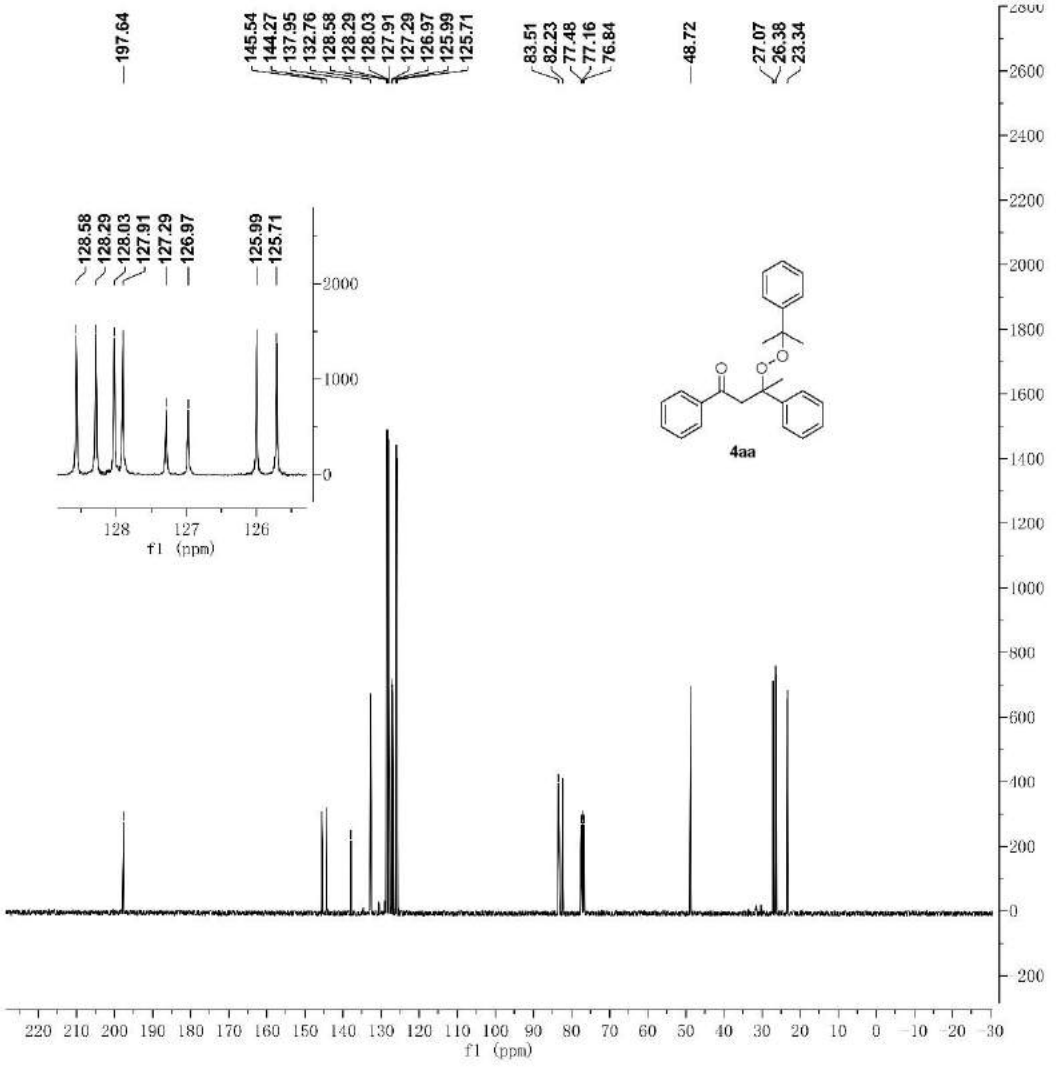
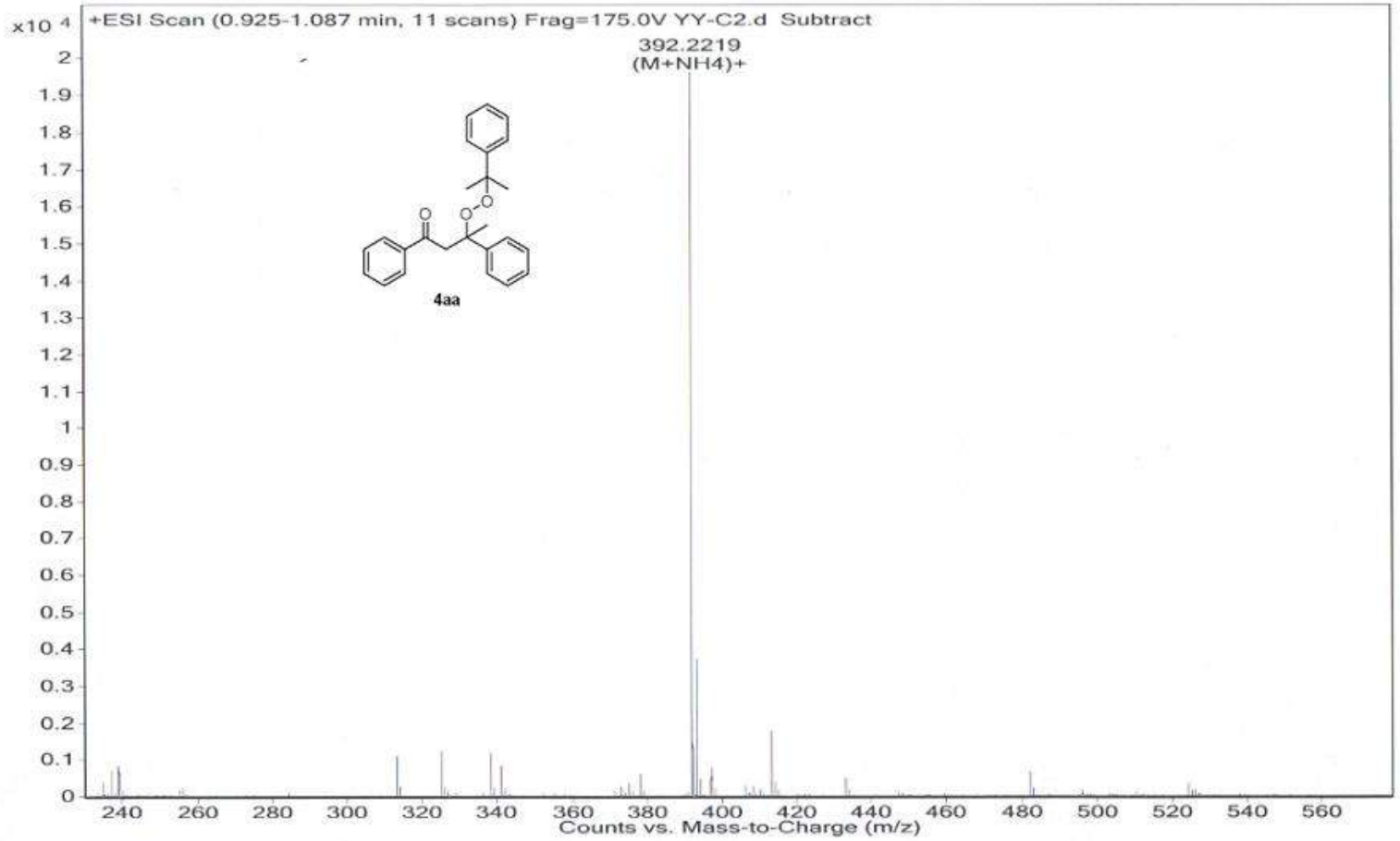


Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy53/ yyC2/ 5/ fid
2 Title	yyC2.5.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 2D
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	293.8
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	33
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-04-12T09:52:00
21 Modification Date	2018-04-12T09:51:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1575.7
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy53/ yyC2/ 6/ fid
2 Title	yyC2.6.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 2D
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	200
15 Receiver Gain	113
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-04-12T09:58:00
21 Modification Date	2018-04-12T09:58:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample23	**Position**	P1-C5	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY-C2.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/4/2018 11:39:51 AM



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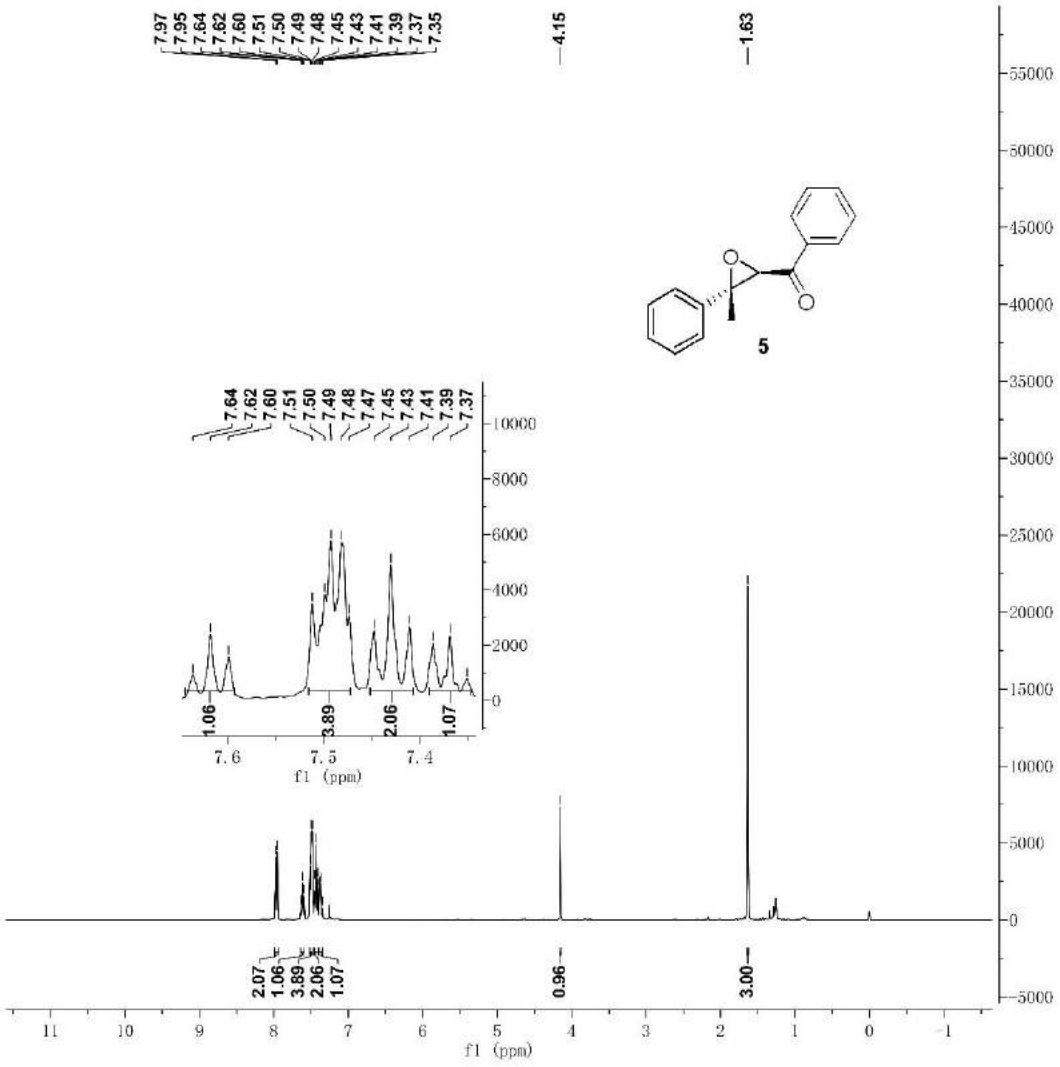
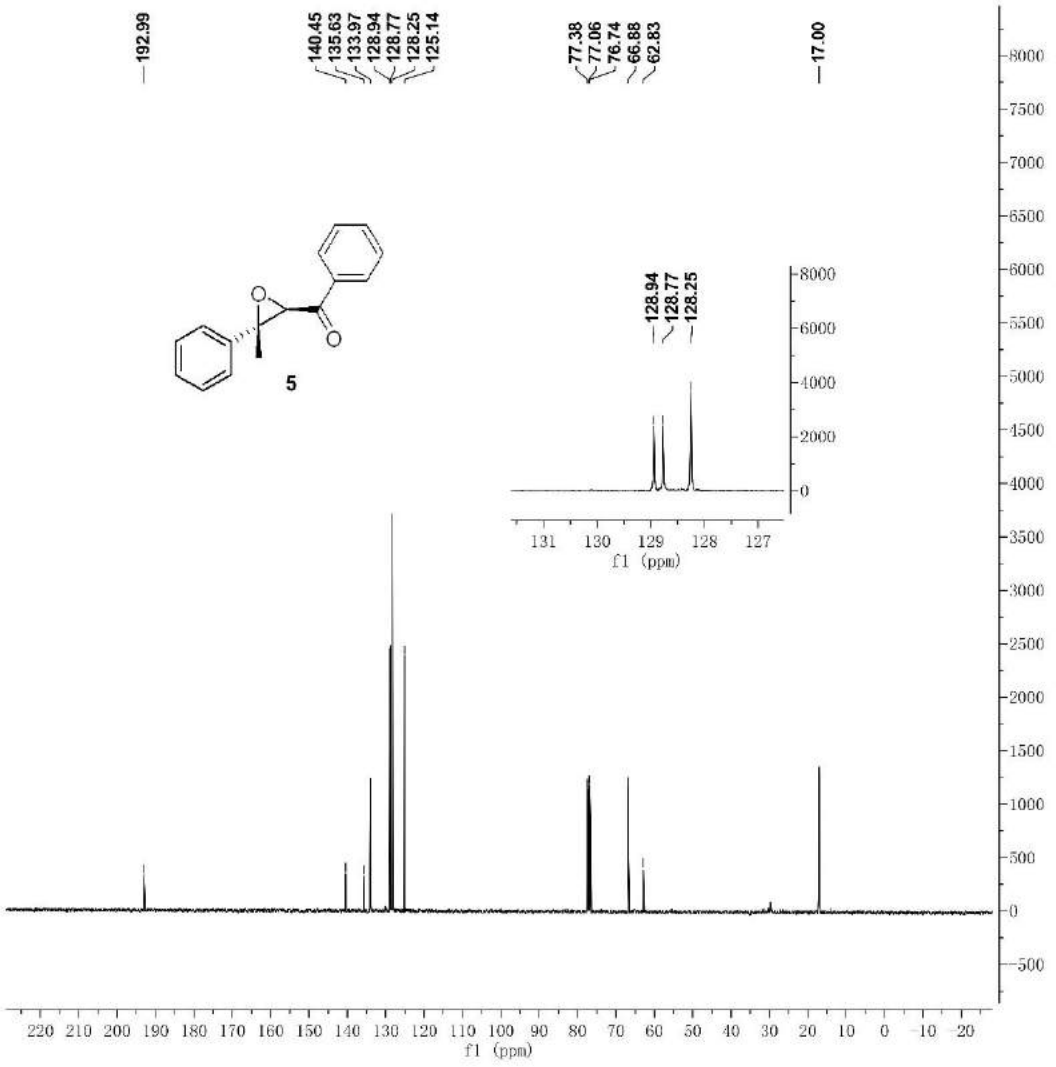
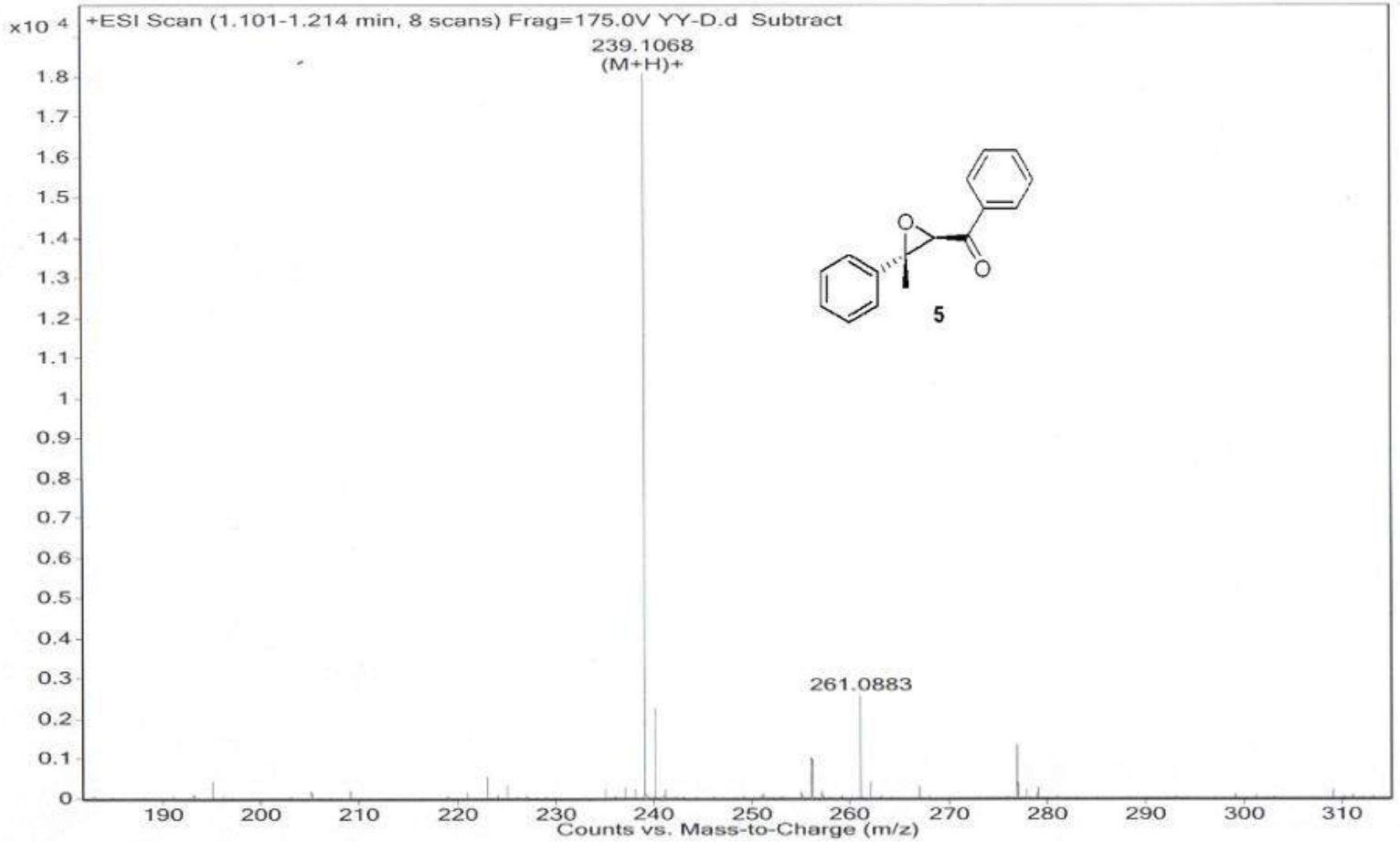


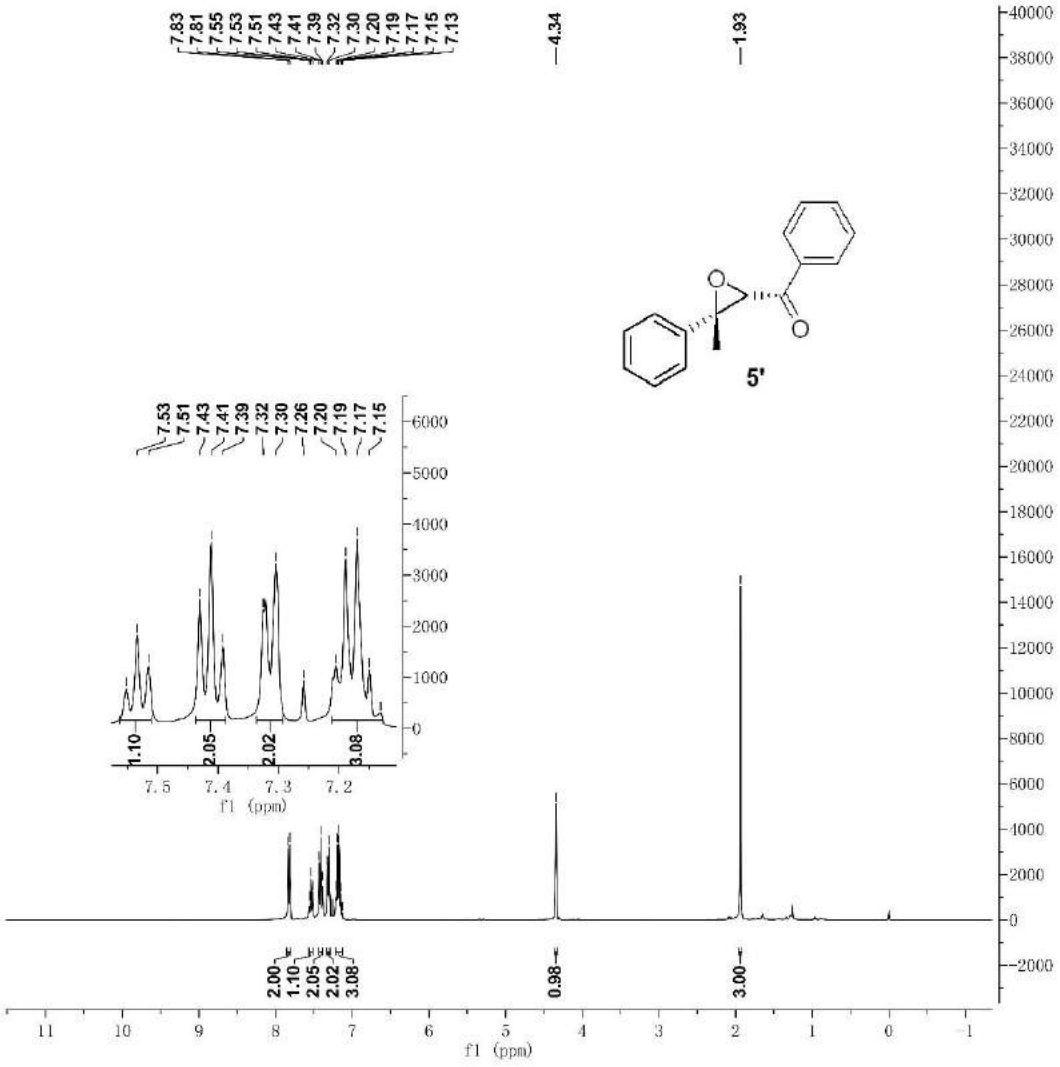
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yyzhong/ 1/ fid
2 Title	yyzhong.1.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 16
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	71
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-03-30T00:50:00
21 Modification Date	2018 03 30T00:49:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1546.9
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



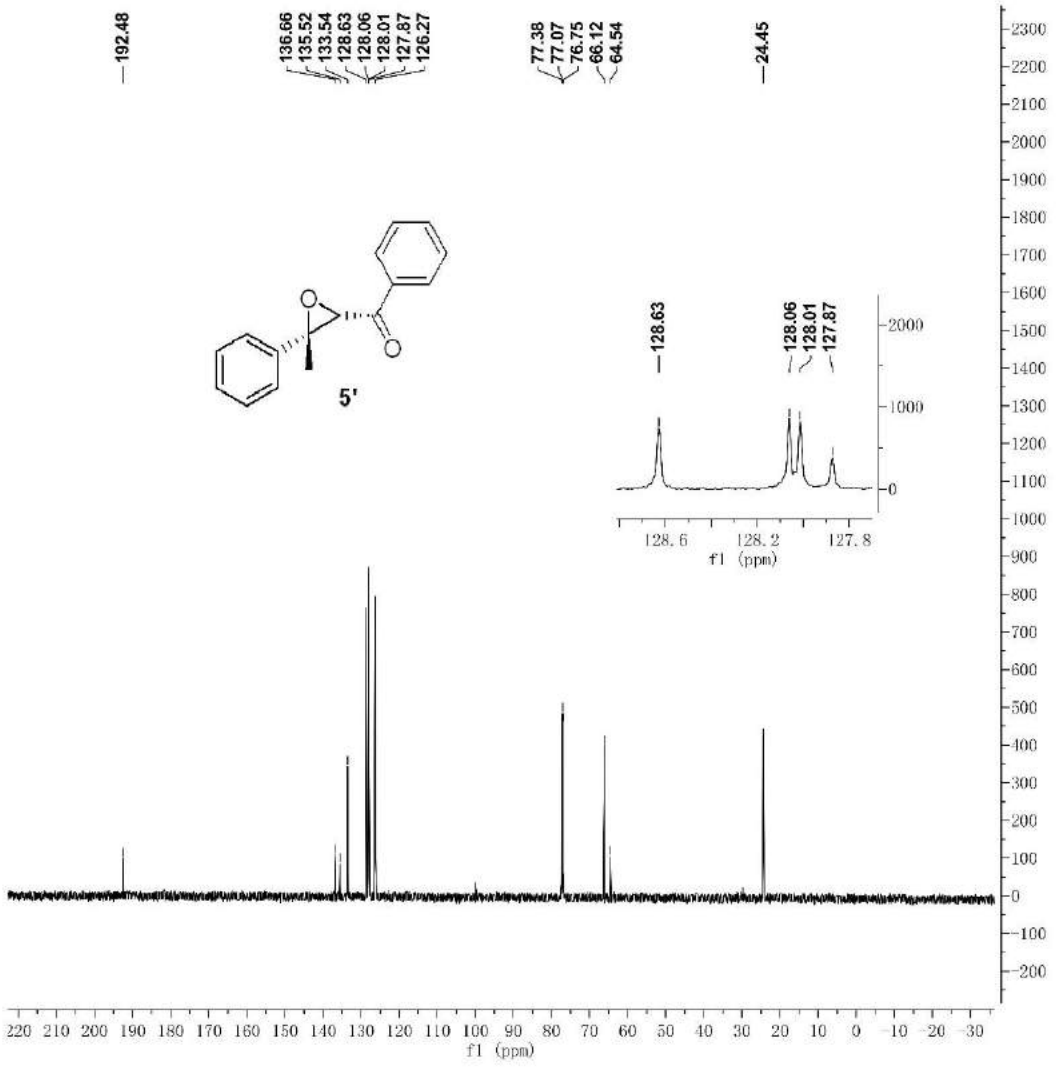
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yyzhong/ 2/ fid
2 Title	yyzhong.2.fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 16
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	299.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	500
15 Receiver Gain	159
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-03-30T01:04:00
21 Modification Date	2018 03 30T01:03:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35711.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536

Sample Name	Sample24	**Position**	P1-C6	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	YY-D.d	**ACQ Method**	Default-TEST.m	**Comment**		**Acquired Time**	4/4/2018 11:45:39 AM

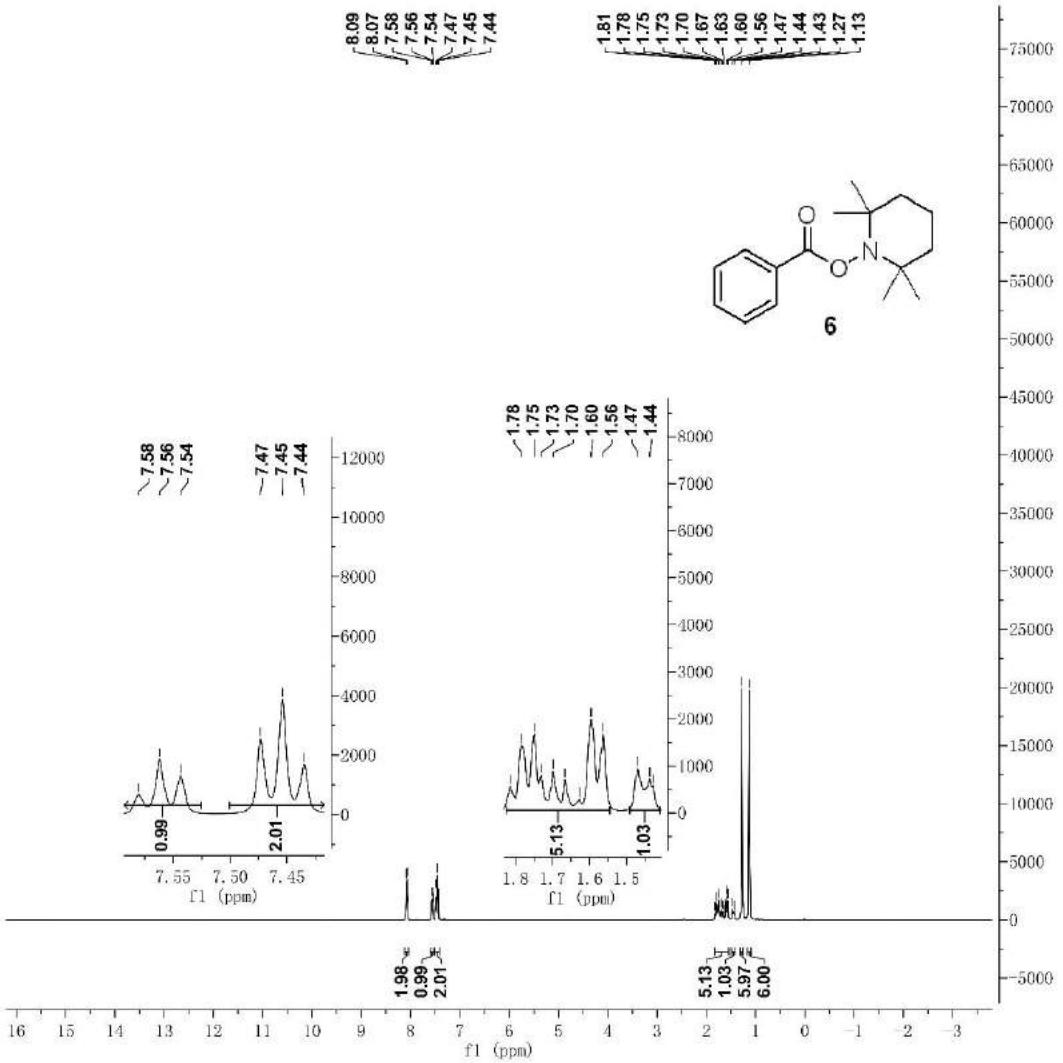




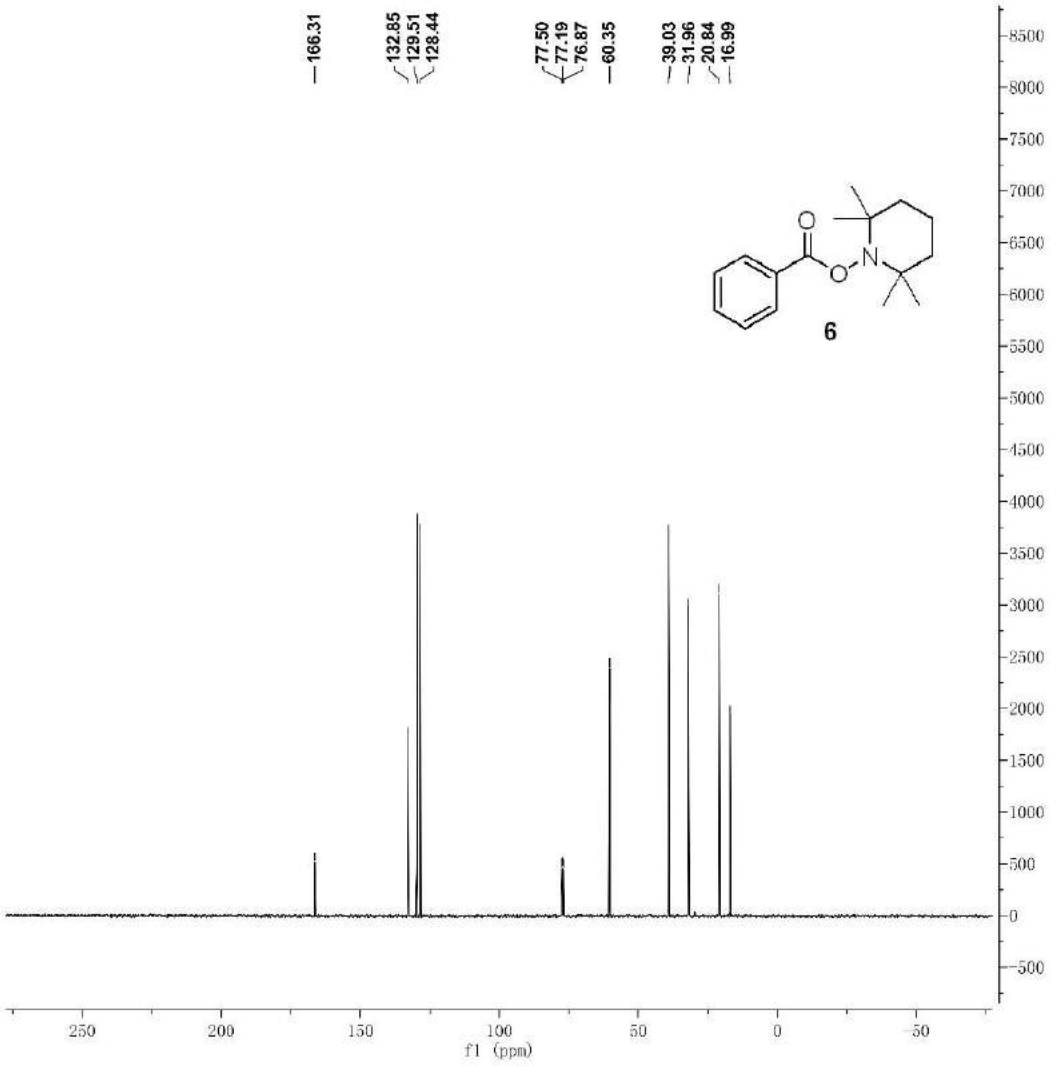
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yyDxia/ 1/ fid
2 Title	yyDxia. 1. fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 11
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	293. 4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	88
16 Relaxation Delay	1. 0000
17 Pulse Width	14. 4000
18 Presaturation Frequency	
19 Acquisition Time	4. 0894
20 Acquisition Date	2018-04-24T20:31:00
21 Modification Date	2018 04 24T20:30:00
22 Class	
23 Spectrometer Frequency	400. 13
24 Spectral Width	8012. 8
25 Lowest Frequency	-1546. 5
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



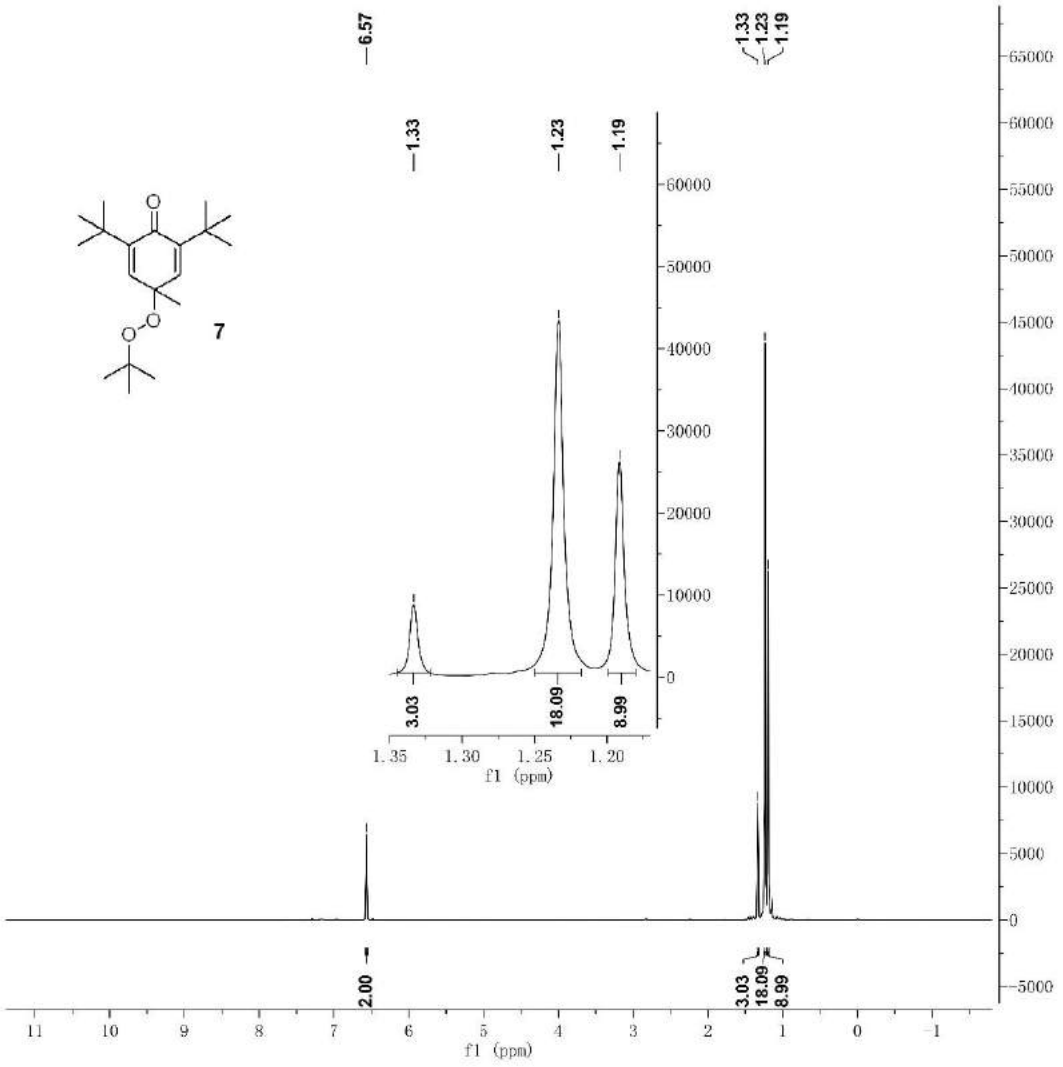
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yyDxia/ 2/ fid
2 Title	yyDxia. 2. fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 11
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294. 3
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	200
15 Receiver Gain	200
16 Relaxation Delay	1. 0000
17 Pulse Width	10. 0000
18 Presaturation Frequency	
19 Acquisition Time	0. 4999
20 Acquisition Date	2018-01-24T20:37:00
21 Modification Date	2018 04 24T20:36:00
22 Class	
23 Spectrometer Frequency	100. 62
24 Spectral Width	35711. 3
25 Lowest Frequency	-7796. 8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536



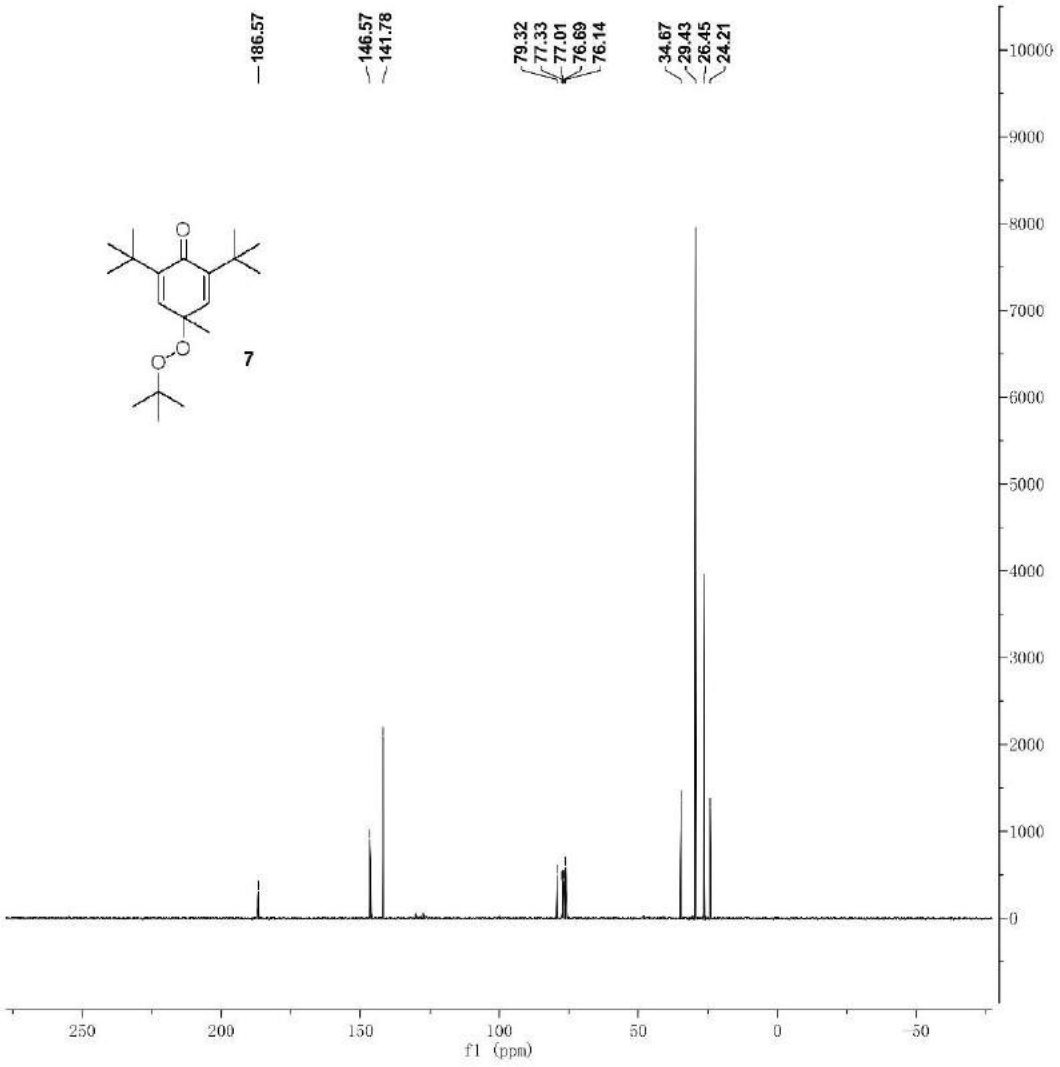
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yyM1/ 1/ fid
2 Title	yyM1. 1. fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 16
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	293.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	16
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-04-21T16:11:00
21 Modification Date	2018 04 21T16:10:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1526.4
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



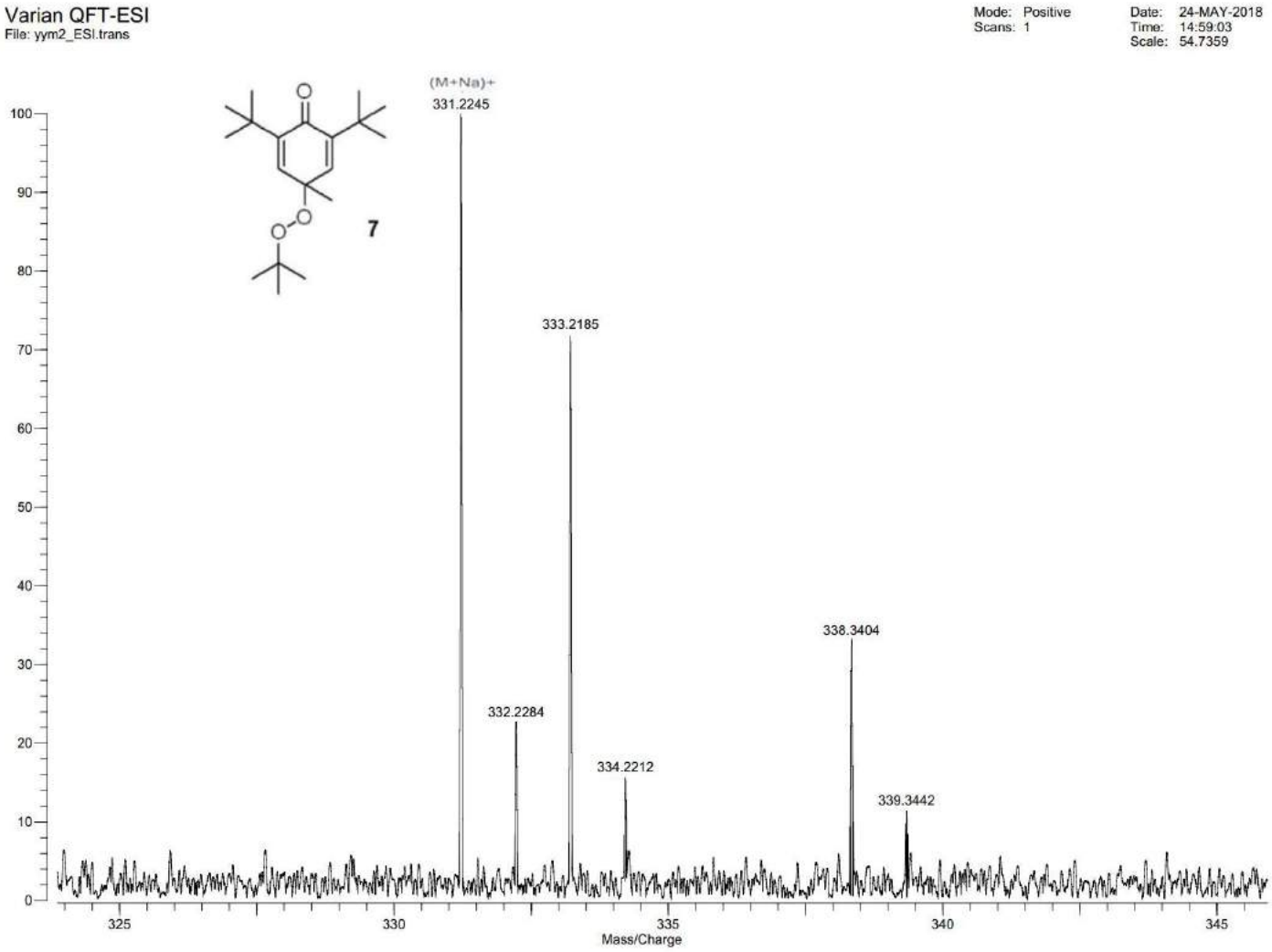
Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yyM1/ 2/ fid
2 Title	yyM1.2.fid
3 Comment	C13CPD CDCl3 (D:\ NMR_DATA\ Wangbin\ Wangbin 16
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294.4
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	150
15 Receiver Gain	200
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4999
20 Acquisition Date	2018-04-21T16:16:00
21 Modification Date	2018-04-21T16:15:00
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	35714.3
25 Lowest Frequency	-7796.8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536



Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yyM2/ 1/ fid
2 Title	yyM2.1.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 18
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	293.5
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	16
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-04-21T16:44:00
21 Modification Date	2018 04 21T16:43:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1533.1
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yyM2/ 2/ fid
2 Title	yyM2. 2. fid
3 Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 18
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	294. 3
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	150
15 Receiver Gain	200
16 Relaxation Delay	1. 0000
17 Pulse Width	10. 0000
18 Presaturation Frequency	
19 Acquisition Time	0. 4999
20 Acquisition Date	2018-04-21T16:48:00
21 Modification Date	2018 04 21T16:47:00
22 Class	
23 Spectrometer Frequency	100. 62
24 Spectral Width	35711. 3
25 Lowest Frequency	-7796. 8
26 Nucleus	13C
27 Acquired Size	17855
28 Spectral Size	65536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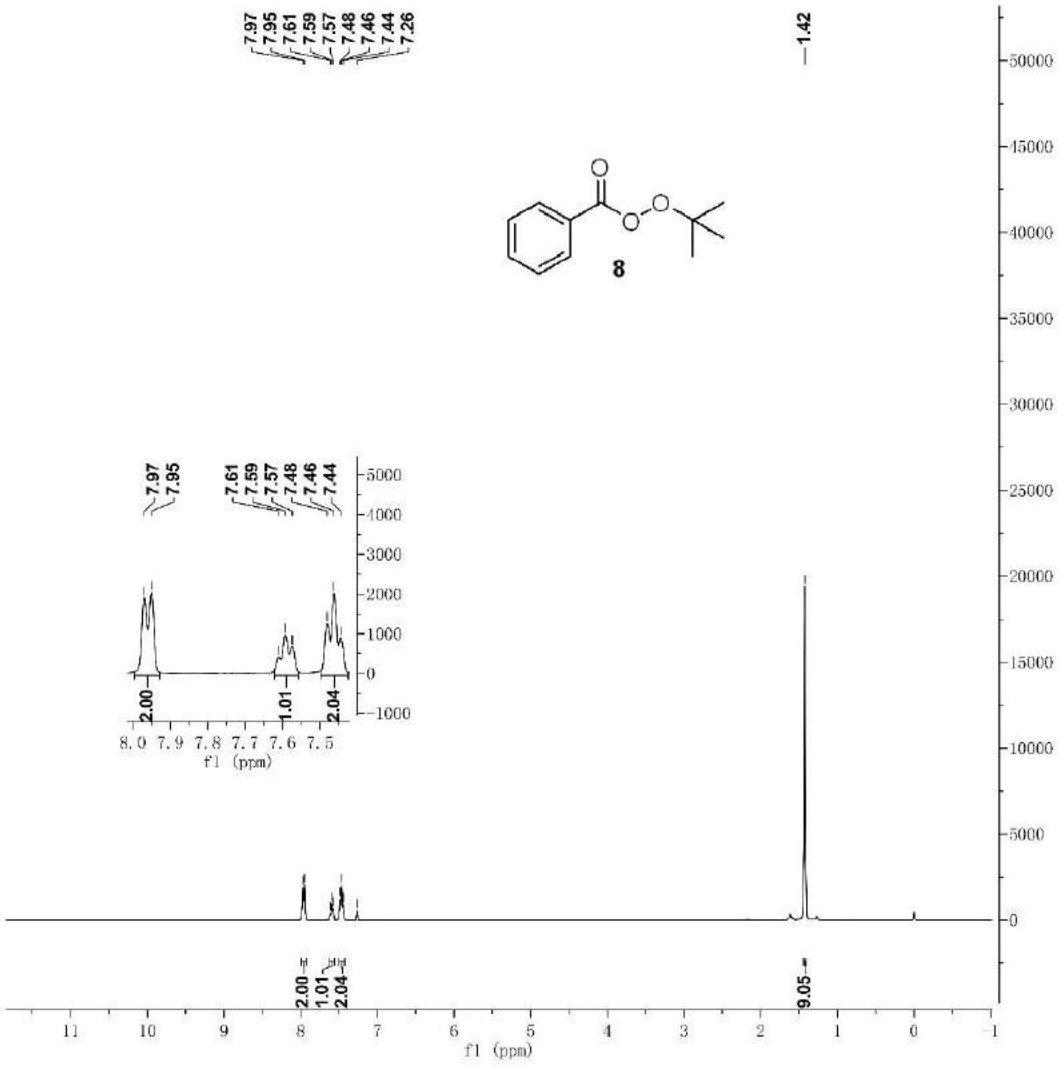
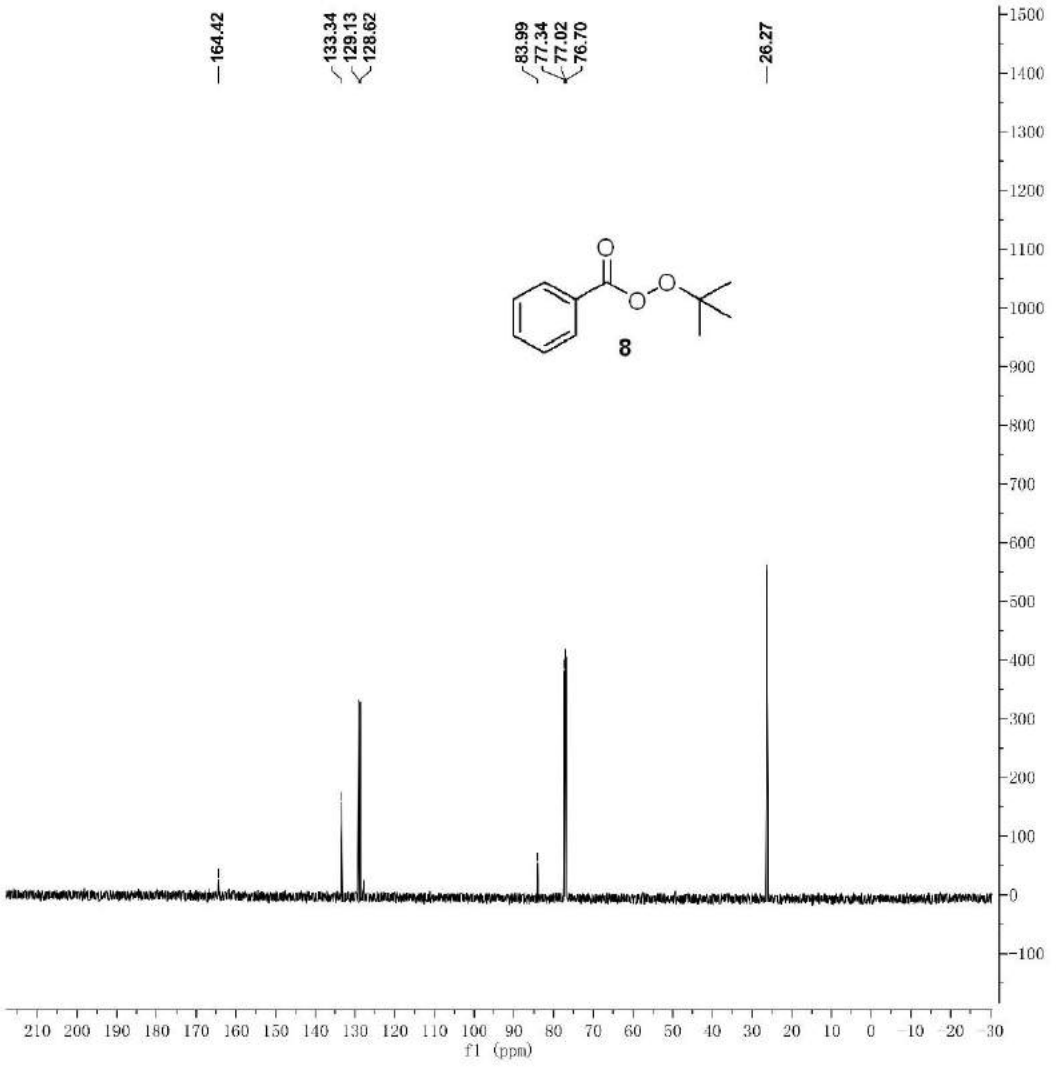
File: yym2_ESI.trans
Mode: Positive
Scans: 1
Date: 24-MAY-2018
Time: 14:59:03
Scale: 54.7359
(M+Na)+
331.2245
333.2185
332.2284
334.2212
338.3404
339.3442
7
100
90
80
70
60
50
40
30
20
10
0
325
330
335
340
345
Mass/Charge



Parameter	Value
1 Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy28/ 1/ fid
2 Title	yy28.1.fid
3 Comment	PROTON CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 6
4 Origin	Bruker BioSpin GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.6
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14 Number of Scans	16
15 Receiver Gain	71
16 Relaxation Delay	1.0000
17 Pulse Width	14.4000
18 Presaturation Frequency	
19 Acquisition Time	4.0894
20 Acquisition Date	2018-03-20T23:18:00
21 Modification Date	2018 03 20T23:18:00
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8012.8
25 Lowest Frequency	-1543.1
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



	Parameter	Value
1	Data File Name	C:/ Users/ yyyyyyyyyyyy/ Desktop/ yy28/ 2/ fid
2	Title	yy28.2.fid
3	Comment	C13CPD CDCl3 {D:\ NMR_DATA\ Wangbin} Wangbin 6
4	Origin	Bruker BioSpin GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.4
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z108618/ 0525
14	Number of Scans	100
15	Receiver Gain	133
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	0.4999
20	Acquisition Date	2018-03-20T23:22:00
21	Modification Date	2018-03-20T23:21:00
22	Class	
23	Spectrometer Frequency	100.62
24	Spectral Width	35714.3
25	Lowest Frequency	-7796.8
26	Nucleus	13C
27	Acquired Size	17855
28	Spectral Size	65536