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Supporting Information

Photoredox-catalyzed Chemoselective Aerobic Cα-H Oxidation of Propargylamine: Synthesis of Substituted 2-Ynamide and Oxazolo[2,3-a]isoquinolinone derivatives

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1. General Experimental Details:

The ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ on Bruker spectrometers 300, 400MHz NMR spectrometer spectrometer (300, 400 MHz for ^{1}H NMR and 75, 100MHz for ^{13}C NMR) respectively with TMS as an internal standard. Mass spectra were recorded on Xevo G2S Q-TOF spectrometer. TLC was performed on using Merck pre-coated TLC plates (Merck 60 F254) and detected under UV light. Column chromatography was carried out with silica gel (100-200 mesh). Reagents and solvents were purified as per standard procedures.

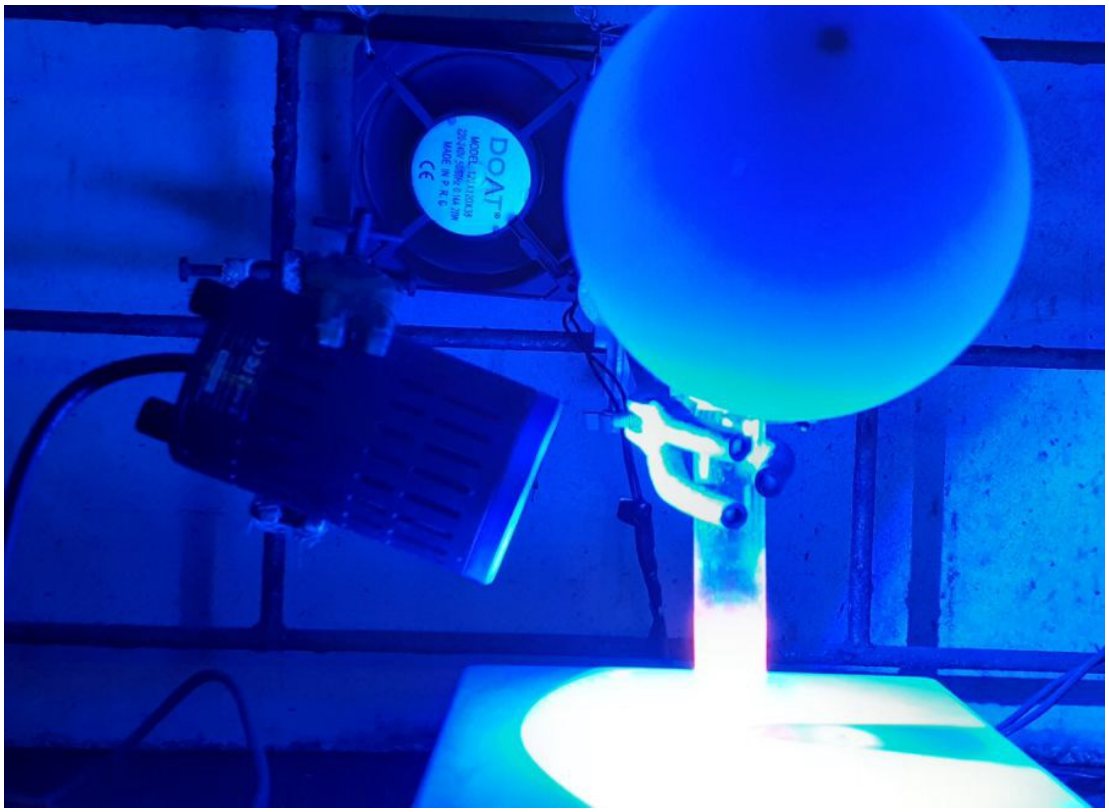


Fig 1: Reaction setup for synthesis of 2-ynamides and Oxazolo[2,3-a]isoquinolinone.

2. General procedure A for synthesis of propargylamine

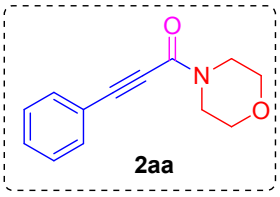
Propargylamine were synthesized using the modified literature procedure.[1]

Reaction tube was charged with amine (0.57 mmol), paraformaldehyde (0.62 mmol), alkyne (0.62 mmol) and CuI (5 mol%) in ACN. The reaction mixture was stirred at 70 °C for 6 hours. After the reaction completion, solvent was evaporated under reduced pressure. The crude product was purified by column chromatography using EtOAc/Hexane as eluent to furnish the corresponding Propargylamine compounds.

3. General procedure B for synthesis of 2-ynamides

Reaction tube was charged with 2-propynyl-tertiary amines (0.5 mmol), DBU (0.5 mmol) and rose bengal (2 mol%) in ACN (4 mL). The reaction mixture was stirred in the presence of O_2 (balloon) under blue light for 3 hours. After the reaction completion, solvent was evaporated under reduced pressure. The crude product was purified by column chromatography using EtOAc/Hexane as eluent to furnish the corresponding 2-ynamide compounds.

1-morpholino-3-phenylprop-2-yn-1-one 2aa[2]

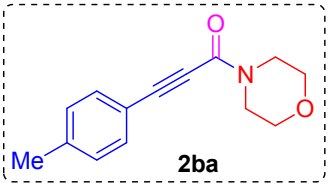


2aa

2aa (102 mg) was obtained from **1aa** (101 mg) following general procedure **B**; colorless oily liquid; 94% yield (eluent: EtOAc/Hexanes= 3:7);

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 3.69 (s, 4H), 3.72-3.75 (m, 2H), 3.81-3.84 (m, 2H), 7.33-7.41 (m, 3H), 7.51-7.55 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ_C 42.0, 47.3, 66.4, 66.8, 80.8, 91.0, 120.4, 128.5, 130.0, 132.3, 153.1.

1-morpholino-3-(p-tolyl)prop-2-yn-1-one 2ba[3]

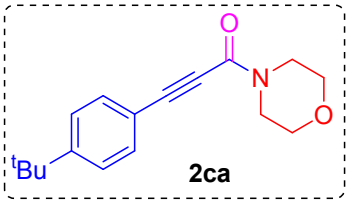


2ba

2ba (105 mg) was obtained from **1ba** (108 mg) following general procedure **B**; white solid; 91% yield (eluent: EtOAc/Hexanes= 3:7); mp: 87-89 °C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 2.36 (s, 3H), 3.68 (s, 4H), 3.71-3.74 (m, 2H), 3.81-3.84 (m, 2H), 7.16 (d, *J*= 7.8 Hz,2H), 7.42 (d, *J*= 8.1 Hz, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C 21.5, 42.0, 47.3, 66.4, 66.8, 80.4, 91.5, 117.3, 129.2, 132.3, 140.6, 153.3.

3-(4-(tert-butyl)phenyl)-1-morpholinoprop-2-yn-1-one 2ca[2]

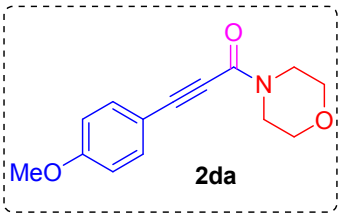


2ca

2ca (123 mg) was obtained from **1ca** (129 mg) following general procedure **B**; yellow solid; 91% yield (eluent: EtOAc/Hexanes= 3:7); mp: 149-151 °C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 1.31 (s, 9H), 3.68 (s, 4H), 3.71-3.74 (m, 2H), 3.81-3.84 (m, 2H), 7.38 (d, *J*= 8.1 Hz, 2H), 7.47 (d, *J*= 8.4 Hz, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C 31.0, 34.9, 42.0, 47.3, 66.4, 66.8, 80.4, 91.4, 117.2, 125.5, 132.1, 153.3, 153.8.

3-(4-methoxyphenyl)-1-morpholinoprop-2-yn-1-one 2da

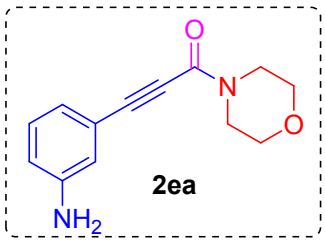


2da

2da (108 mg) was obtained from **1da** (116 mg) following general procedure **B**; colorless oily liquid; 88% yield (eluent: EtOAc/Hexanes= 3:7);

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 3.68 (s, 4H), 3.71-3.74 (m, 2H), 3.80-3.86 (s, 5H), 6.87 (d, *J*= 8.7 Hz, 2H), 7.47 (d, *J*= 9.0 Hz, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C41.9, 47.3, 55.3, 66.5, 66.8, 80.1, 91.7, 112.2, 114.3, 134.1, 153.5, 161.2; **IR (KBr) ν:** 2973, 2224, 1616, 1556, 1113, 1046; **HRMS:** $(M+H)^+$ calculated for $C_{14}H_{16}NO_3$: 246.1130, Found: 246.1088.

3-(3-aminophenyl)-1-morpholinoprop-2-yn-1-one 2ea

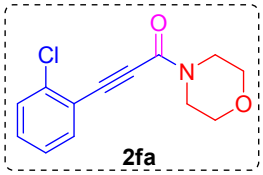


2ea

2ea (86 mg) was obtained from **1ea** (108 mg) following general procedure **B**; yellow oily liquid; 75% yield (eluent: EtOAc/Hexanes= 1:1);

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 3.68 (s, 4H), 3.70-3.74 (m, 2H), 3.79-3.82 (m, 2H), 6.69-6.73 (m, 1H), 6.82 (s, 1H), 6.91 (d, *J*= 7.8Hz, 2H), 7.09-7.14 (m, 1H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C42.0, 47.3, 66.4, 66.8, 80.2, 91.5, 117.0, 118.2, 120.9, 122.5, 129.4, 146.5, 153.3; **IR (KBr) ν:** 3546, 2989, 2211, 1621, 1570, 1117, 1050; **HRMS:** $(M+H)^+$ calculated for $C_{13}H_{14}N_2O_2$: 231.1133, Found: 231.1135.

3-(2-chlorophenyl)-1-morpholinoprop-2-yn-1-one 2fa

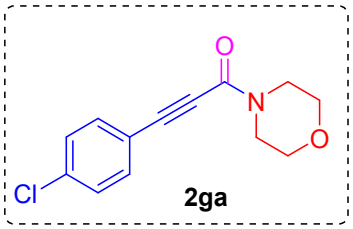


2fa

2fa (100 mg) was obtained from **1fa** (118 mg) following general procedure **B**; colorless oily liquid; 80% yield (eluent: EtOAc/Hexanes= 3:7);

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 3.69 (s, 4H), 3.73-3.76 (m, 2H), 3.89-3.93 (m, 2H), 7.24-7.29 (m, 1H), 7.33 (dt, *J*= 1.8, 6.8 Hz, 1H), 7.43 (d, *J*= 7.5 Hz, 1H), 7.60 (dd, *J*= 1.2, 6.3 Hz, 1H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C42.0, 47.3, 66.4, 66.8, 85.4, 87.1, 120.6, 126.7, 129.4, 131.1, 134.4, 136.7, 152.8; **HRMS:** $(M+H)^+$ calculated for $C_{13}H_{13}ClNO_2$: 250.0635, Found: 250.0593.

3-(4-chlorophenyl)-1-morpholinoprop-2-yn-1-one 2ga[2]

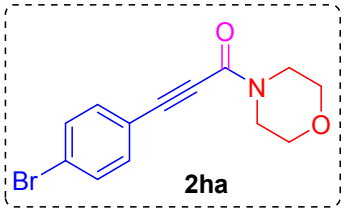


2ga

2ga (112 mg) was obtained from **1ga** (118 mg) following general procedure **B**; white solid; 90% yield (eluent: EtOAc/Hexanes= 3:7); mp: 110-112 ^{o}C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 3.68 (s, 4H), 3.71-3.74 (m, 2H), 3.79-3.81 (m, 2H), 7.34 (d, *J*= 8.4 Hz, 2H), 7.46 (m, *J*= 8.4 Hz, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C42.0, 47.2, 66.4, 66.8, 81.7, 89.7, 118.8, 128.9, 133.5, 136.5, 152.8.

3-(4-bromophenyl)-1-morpholinoprop-2-yn-1-one 2ha

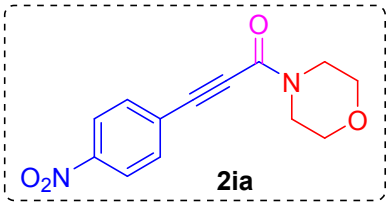


2ha

2ha (129 mg) was obtained from **1ha** (140 mg) following general procedure **B**; pale yellow solid; 88% yield (eluent: EtOAc/Hexanes= 3:7); mp: 110-112 ^{o}C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H3.69 (s, 4H), 3.71-3.75 (m, 2H), 3.79-3.82 (m, 2H), 7.39 (d, *J*= 8.4 Hz, 2H), 7.51 (m, *J*= 6.3 Hz, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C42.0, 47.3, 66.4, 66.8, 81.8, 89.8, 119.3, 124.8, 131.9, 133.6, 152.9; **HRMS:** $(M+H)^+$ calculated for $C_{13}H_{13}BrNO_2$: 294.0129, Found: 294.0097.

1-morpholino-3-(4-nitrophenyl)prop-2-yn-1-one 2ia

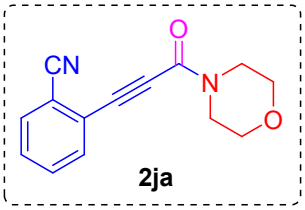


2ia

2ia (108 mg) was obtained from **1ia** (123 mg) following general procedure **B**; yellow solid; 83% yield (eluent: EtOAc/Hexanes= 4:6); mp: 194-196 ^{o}C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 3.71 (s, 4H), 3.74-3.77 (m, 2H), 3.80-3.83 (m, 2H), 7.69 (d, *J*= 8.7Hz, 2H), 8.22 (d, *J*= 9Hz, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C42.1, 47.3, 66.4, 66.8, 84.6, 88.1, 123.6, 126.9, 133.0, 148.3, 152.2; **IR (KBr) ν:** 2978, 2225, 1620, 1569, 1113, 1050; **HRMS:** $(M+H)^+$ calculated for $C_{13}H_{13}N_2O_4$: 261.0875, Found: 261.0835.

2-(3-morpholino-3-oxoprop-1-yn-1-yl)benzonitrile 2ja[2]

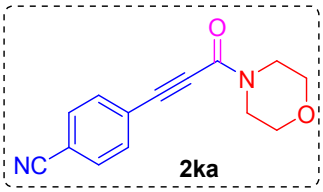


2ja

2ja (98 mg) was obtained from **1ja** (113 mg) following general procedure **B**; pale yellow solid; 82% yield (eluent: EtOAc/Hexanes= 4:6); mp: 108-110 ^{o}C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 3.71 (s, 4H), 3.75-3.79 (m, 2H), 3.96-3.99 (m, 2H), 7.51-7.55 (m, 1H), 7.60-7.66 (m, 1H), 7.69-7.75 (m, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C40.0, 47.3, 66.1, 66.7, 85.5, 85.9, 115.7, 116.9, 124.3, 130.0, 132.4, 133.5, 151.9.

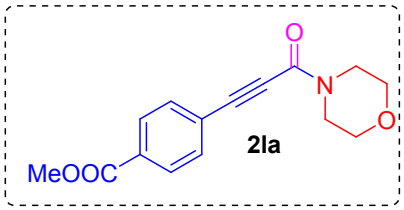
4-(3-morpholino-3-oxoprop-1-yn-1-yl)benzonitrile 2ka[3]



2ka (102 mg) was obtained from **1ka** (113 mg) following general procedure **B**; white solid; 85% yield (eluent: EtOAc/Hexanes= 4:6); mp: 197-199 ^{o}C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H3.70 (s, 4H), 3.72-3.75 (m, 2H), 3.78-3.81 (m, 2H), 7.60-7.67 (m, 4H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C42.1, 47.3, 66.4, 66.7, 84.1, 88.5, 113.7, 117.7, 125.1, 132.1, 132.7, 152.3.

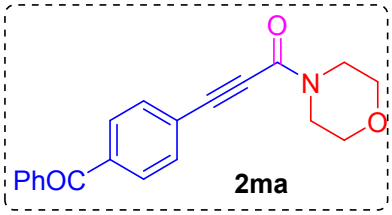
Methyl 4-(3-morpholino-3-oxoprop-1-yn-1-yl)benzoate 2la[3]



2la (109 mg) was obtained from **1la** (130 mg) following general procedure **B**; white solid; 80% yield (eluent: EtOAc/Hexanes= 4:6); mp: 124-126 ^{o}C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 3.69 (s, 4H), 3.73-3.76 (m, 2H), 3.81-3.84 (m, 2H), 3.92(s, 3H), 7.59 (d, *J*= 8.4Hz, 2H), 8.02 (d, *J*= 8.4Hz, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C42.0, 47.3, 52.3, 66.4, 66.8, 82.9, 89.7, 124.8, 129.5, 131.4, 132.1, 152.7, 165.9.

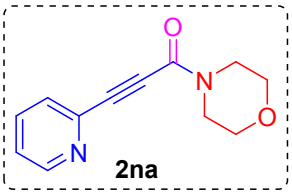
3-(4-benzoylphenyl)-1-morpholinoprop-2-yn-1-one 2ma



2ma (135 mg) was obtained from **1ma** (153 mg) following general procedure **B**; pale yellow oily liquid; 85% yield (eluent: EtOAc/Hexanes= 4:6);

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 3.70 (s, 4H), 3.73-3.77 (m, 2H), 3.82-3.85 (m, 2H), 6.45-6.50 (m, 2H), 7.58 (d, *J*= 7.5Hz, 1H), 7.64 (d, *J*= 8.4Hz, 2H), 7.75-7.80 (m, 4H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C42.0, 47.3, 66.4, 66.8, 83.0, 89.8, 124.2, 128.4, 129.8, 132.1, 132.7, 137.0, 138.6, 152.7, 195.3; **HRMS:** $(M+H)^+$ calculated for $C_{20}H_{17}NO_3$: 320.1287, Found: 320.1295.

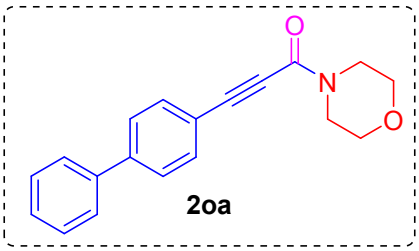
1-morpholino-3-(pyridin-2-yl)prop-2-yn-1-one 2na



2na (76 mg) was obtained from **1na** (101 mg) following general procedure **B**; brown solid; 70% yield (eluent: EtOAc/Hexanes= 1:1); mp: 59-61 ^{o}C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 3.69 (s, 4H), 3.71-3.75 (m, 2H), 3.85-3.88 (m, 2H), 7.31-7.35 (m, 1H), 6.59 (d, *J*= 7.8Hz, 1H), 7.69-7.75 (m, 1H), 8.63 (d, *J*= 4.2Hz, 1H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C42.0, 47.3, 66.3, 66.8, 79.4, 89.1, 124.2, 128.3, 136.2, 141.0, 150.2, 152.4; **HRMS:** $(M+H)^+$ calculated for $C_{12}H_{13}N_2O_2$: 217.0977, Found: 217.0983.

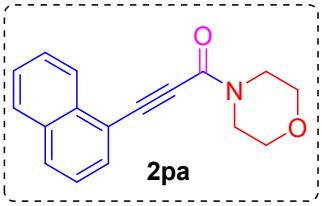
3-([1,1'-biphenyl]-4-yl)-1-morpholinoprop-2-yn-1-one 2oa[3]



2oa (131 mg) was obtained from **1oa** (139 mg) following general procedure B; white solid; 90% yield (eluent: EtOAc/Hexanes= 3:7); mp: 128-130 ^{o}C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 3.69 (s, 4H), 3.72-3.75 (m, 2H), 3.83-3.85 (m, 2H), 7.36-7.46 (m, 3H), 7.56-7.59 (m, 6h); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C42.0, 47.3, 66.4, 66.8, 81.4, 91.0, 119.1, 127.0, 127.1, 128.0, 128.9, 132.8, 139.8, 143.0, 153.2.

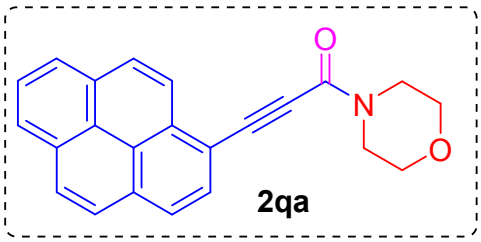
1-morpholino-3-(naphthalen-1-yl)prop-2-yn-1-one 2pa[2]



2pa (114 mg) was obtained from **1pa** (126 mg) following general procedure B; yellow solid; 86% yield (eluent: EtOAc/Hexanes= 3:7); mp: 133-135 ^{o}C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H3.72 (s, 4H), 3.75-3.78 (m, 2H), 3.91-3.94 (m, 2H), 7.40-7.46 (m, 1H), 7.50-7.61 (m, 2H), 7.78 (d, *J*= 7.2Hz, 1H), 7.84-7.91 (m, 2H), 8.27 (d, *J*= 8.1Hz, 1H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C42.1, 47.4, 66.5, 66.8, 85.5, 89.5, 118.0, 125.0, 125.6, 126.7, 127.4, 128.4, 130.7, 132.0, 133.1, 133.3, 153.2.

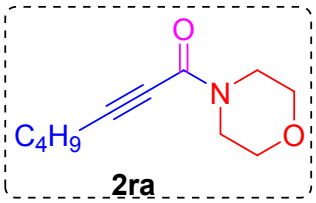
1-morpholino-3-(pyren-1-yl)prop-2-yn-1-one 2qa



2qa (121 mg) was obtained from **1qa** (164 mg) following general procedure B; brown solid; 71% yield (eluent: EtOAc/Hexanes= 3:7); mp: 138-140 ^{o}C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H3.67 (s, 4H), 3.68-3.75 (m, 2H), 3.90-3.93 (m, 2H), 7.88-7.97 (m, 4H), 8.01-7.12 (m, 4H), 8.37 (d, *J*= 9Hz, 1H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C42.1, 47.5, 66.5, 66.9, 86.2, 90.7, 114.2, 124.0, 124.3, 124.4, 124.8, 126.1, 126.2, 126.4, 127.0, 129.1, 129.2, 130.2, 130.8, 131.1, 132.6, 132.9, 153.4; **HRMS:** $(M+H)^+$ calculated for $C_{23}H_{18}NO_2$: 340.1337, Found: 340.1389.

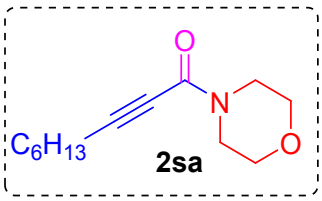
1-morpholinohept-2-yn-1-one 2ra



2ra (74 mg) was obtained from **1ra** (91 mg) following general procedure B; colorless oily liquid; 76% yield (eluent: EtOAc/Hexanes= 3:7);

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 0.95 (t, *J*= 7.2Hz, 3H), 1.42-1.44 (m, 2H), 1.54-1.57 (m, 2H), 2.35 (t, *J*= 6.9Hz, 2H), 3.63 (s, 4H), 3.67-3.69 (m, 2H), 3.72-3.74 (m, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C13.3, 18.5, 21.9, 29.80, 41.8, 47.1, 66.4, 66.8, 73.3, 94.0, 153.3; **HRMS:** $(M+H)^+$ calculated for $C_{11}H_{18}NO_2$: 196.1337, Found: 196.1290.

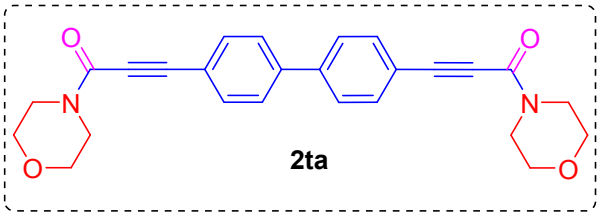
1-morpholinonon-2-yn-1-one 2sa



2sa (84 mg) was obtained from **1sa** (105 mg) following general procedure B; colorless oily liquid; 76% yield (eluent: EtOAc/Hexanes= 3:7);

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 0.96 (t, *J*= 7.2Hz, 3H),1.28-1.31 (m, 4H), 1.35-1.43 (m, 2H), 1.53-1.60 (m, 2H), 2.35 (t, *J*= 6.9Hz, 2H), 3.63 (s, 4H), 3.66-3.68 (m, 2H), 3.69-3.73 (m, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C13.8, 18.8, 22.3, 27.7, 28.4, 31.1, 41.8, 47.1, 66.4, 66.8, 73.3, 94.0, 153.3; **HRMS:** $(M+H)^+$ calculated for $C_{13}H_{22}NO_2$: 224.1650, Found: 224.1604.

3,3'-([1,1'-biphenyl]-4,4'-diyl)bis(1-morpholinoprop-2-yn-1-one) 2ta

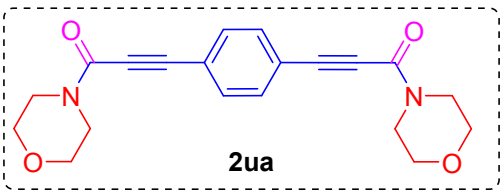


2ta

2ta (91 mg) was obtained from **1ta** (100 mg) following general procedure B; pale yellow solid; 85% yield (eluent: EtOAc/Hexanes= 1:1); mp: 231-233 ^oC;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 3.70 (s, 8H), 3.73-3.76 (m, 4H), 3.83-3.86 (m, 4H), 7.61 (s, 8H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C42.1, 47.4, 66.5, 66.9, 81.9, 90.7, 120.1, 127.2, 133.0, 141.6, 153.1; **IR (KBr) v:** 2876, 2218, 1621, 1562, 1113, 1039; **HRMS:** $(M+H)^+$ calculated for $C_{26}H_{24}N_2O_4$: 429.1814, Found: 429.1829.

3,3'-(1,4-phenylene)bis(1-morpholinoprop-2-yn-1-one) 2ua

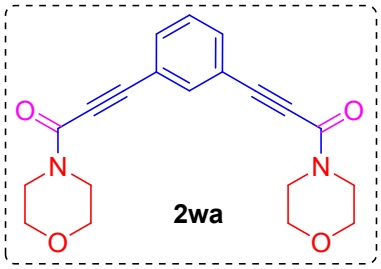


2ua

2ua (137 mg) was obtained from **1ua** (162 mg) following general procedure B; brown solid; 78% yield (eluent: EtOAc/Hexanes= 1:1); mp: 238-240 ^oC;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 3.69 (s, 8H), 3.72-3.75 (m, 4H), 3.79-3.82 (m, 4H), 7.53 (s, 4H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C42.0, 47.3, 66.4, 66.8, 83.0, 89.7, 122.0, 132.3, 152.7; **HRMS:** $(M+H)^+$ calculated for $C_{20}H_{20}N_2O_4$: 353.1501, Found: 353.1509.

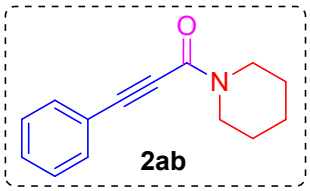
3,3'-(1,3-phenylene)bis(1-morpholinoprop-2-yn-1-one) 2va



2va (123 mg) was obtained from **1va** (162 mg) following general procedure B; colorless oily liquid; 75% yield (eluent: EtOAc/Hexanes= 1:1);

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 3.62 (s, 8H), 3.66-3.69 (m, 4H), 3.73-3.76 (m, 4H), 7.29-7.34 (m, 1H), 7.51 (d, *J*= 7.8Hz, 2H), 7.63 (s, 1H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C 42.0, 47.3, 66.4, 66.8, 81.75, 89.25, 121.1, 128.9, 133.5, 135.8, 152.7; **HRMS:** $(M+H)^+$ calculated for $C_{20}H_{20}N_2O_4$: 353.1501, Found: 353.1510.

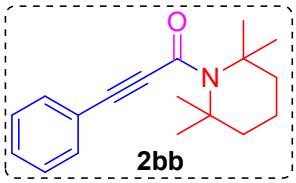
3-phenyl-1-(piperidin-1-yl)prop-2-yn-1-one 2ab[2]



2ab (97 mg) was obtained from **1ab** (100 mg) following general procedure B; white solid; 91% yield (eluent: EtOAc/Hexanes= 2:8); mp: 96-98 ^oC;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 1.57-1.66 (m, 6H), 3.60-3.64 (m, 2H), 3.75-3.78 (m, 2H), 7.34-7.39 (m, 3H), 7.52-7.54 (m, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C24.5, 25.3, 26.4, 42.3, 48.1, 81.6, 90.1, 120.8, 128.4, 129.7, 132.2, 152.9.

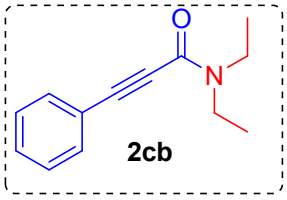
3-phenyl-1-(2,2,6,6-tetramethylpiperidin-1-yl)prop-2-yn-1-one 2bb



2bb (112 mg) was obtained from **1bb** (128 mg) following general procedure B; yellow liquid; 83% yield (eluent: EtOAc/Hexanes= 1:9);

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 1.68 (s, 12H), 1.74-1.79 (m, 6H), 7.37-7.39 (m, 3H), 7.54-7.56 (m, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C15.0, 29.8, 39.3, 57.0, 87.2, 88.5, 121.6, 128.2, 129.2, 131.6, 155.9; **HRMS:** $(M+H)^+$ calculated for $C_{18}H_{24}NO$: 270.1859, Found: 270.1819.

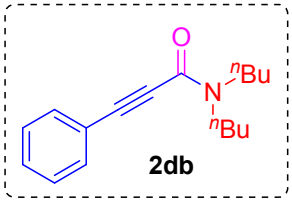
***N,N*-diethyl-3-phenylpropiolamide 2cb[2]**



2cb (60 mg) was obtained from **1cb** (94 mg) following general procedure B; yellow liquid; 60% yield (eluent: EtOAc/Hexanes= 1:9);

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 1.10 (t, *J*= 6.9Hz, 3H), 1.21 (t, *J*= 6.9Hz, 3H), 3.37-3.44 (m, 2H), 3.55-3.62 (m, 2H), 7.25-7.33 (m, 3H), 7.44-7.47 (m, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C12.7, 14.3, 39.3, 43.5, 82.0, 88.9, 120.9, 128.4, 129.7, 132.2, 153.9.

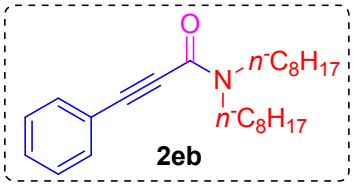
***N,N*-dibutyl-3-phenylpropiolamide 2db[4]**



2db (83 mg) was obtained from **1db** (122 mg) following general procedure B; yellow liquid; 65% yield (eluent: EtOAc/Hexanes= 1:9);

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 0.84-0.92 (m, 6H), 1.19-1.36 (m, 4H), 1.44-1.60 (m, 4H), 3.30-3.35 (m, 2H), 3.49-3.54 (m, 2H), 7.25-7.32 (m, 3H), 7.43-7.45 (m, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C13.7, 19.9, 20.1, 29.6, 31.0, 44.6, 48.9, 82.3, 89.1, 120.9, 128.4, 129.7, 132.2, 154.4.

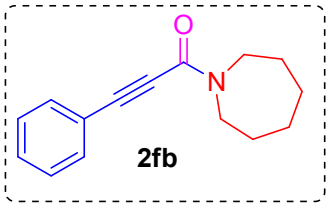
N,N-dinonyl-3-phenylpropiolamide 2eb



2eb (102 mg) was obtained from **1eb** (179 mg) following general procedure B; colorless oily liquid; 55% yield (eluent: EtOAc/Hexanes= 1:9);

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 0.76-0.82 (m, 6H), 1.14-1.31 (m, 20H), 1.48-1.61 (m, 4H), 3.29-3.34 (m, 2H), 3.48-3.53 (m, 2H), 7.24-7.32 (m, 3H), 7.43-7.45 (m, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C13.9, 22.5, 22.6, 26.7, 26.9, 27.5, 28.9, 29.1, 29.2, 29.3, 31.7, 31.8, 44.9, 49.1, 82.3, 89.1, 121.0, 128.4, 129.7, 132.2, 154.3; **HRMS:** $(M+H)^+$ calculated for $C_{25}H_{40}NO$: 370.3109, Found: 370.3081.

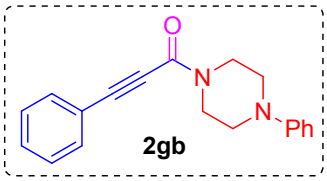
1-(azepan-1-yl)-3-phenylprop-2-yn-1-one 2fb[3]



2fb (100 mg) was obtained from **1fb** (107 mg) following general procedure B; colorless oily liquid; 88% yield (eluent: EtOAc/Hexanes= 1:9);

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 1.90 (s, 4H), 2.06-2.11 (m, 4H), 3.86-3.90 (m, 2H), 4.04-4.08 (m, 2H), 7.63-7.68 (m, 3H), 7.80-7.8.3 (m, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C26.9, 27.1, 27.2, 29.2, 45.3, 49.1, 82.1, 89.5, 120.9, 128.4, 129.7, 132.2, 154.4.

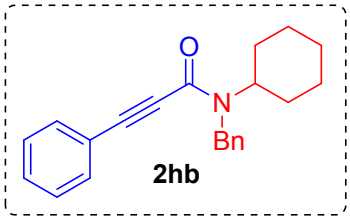
3-phenyl-1-(4-phenylpiperazin-1-yl)prop-2-yn-1-one 2gb



2gb (134 mg) was obtained from **1gb** (138 mg) following general procedure B; pale yellow solid; 93% yield (eluent: EtOAc/Hexanes= 2:8); mp: 95-97 ^{o}C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 3.18 (t, *J*= 5.1Hz, 2H), 3.24 (t, *J*= 4.8Hz, 2H), 3.82-3.85 (m, 2H), 3.95-3.99 (m, 2H), 6.90-6.94 (m, 3H), 7.25-7.41 (m, 5H), 7.55 (d, *J*= 7.2Hz,2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C41.5, 46.9, 49.3, 50.0, 81.1, 90.8, 116.9, 120.5, 120.7, 128.5, 129.2, 130.0, 132.3, 150.9, 153.0; **HRMS:** $(M+H)^+$ calculated for $C_{19}H_{18}N_2O$: 291.1497, Found: 291.1501.

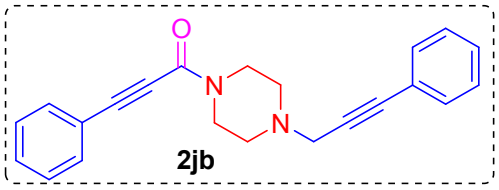
***N*-benzyl-*N*-cyclohexyl-3-phenylpropiolamide 2hb**



2hb (103 mg) was obtained from **1hb** (151 mg) following general procedure B; white solid; 65% yield (eluent: EtOAc/Hexanes= 1:9); mp: 88-90 ^{o}C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 1.26-1.45 (m, 5H), 1.57-1.82 (m, 5H), 4.34-4.35 (m, 1H), 4.65 (s, 1H), 4.83 (s, 1H),7.24-7.41 (m, 9H), 7.53-7.56 (m, 1H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C25.3, 25.5, 25.9, 26.2, 29.7, 30.7, 32.2, 44.8, 49.5, 54.8, 59.8, 82.2, 82.9, 89.5, 90.4, 115.9, 120.8, 121.0, 126.8, 126.9, 127.3, 127.4, 128.4, 128.5, 128.6, 129.8, 130.0, 132.3, 132.4, 138.7, 138.8, 155.2, 155.4; **HRMS:** $(M+H)^+$ calculated for $C_{22}H_{24}NO$: 318.1857, Found: 318.1824.

3-phenyl-1-(4-(3-phenylprop-2-yn-1-yl)piperazin-1-yl)prop-2-yn-1-one 2jb

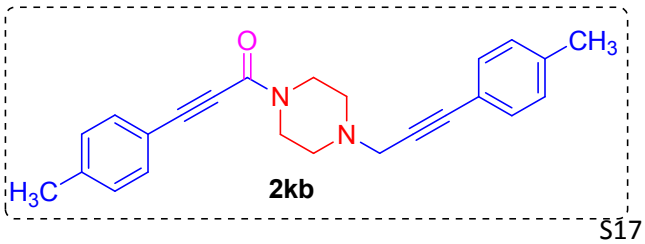


2jb

2jb (116 mg) was obtained from **1jb** (157 mg) following general procedure B; white solid; 71% yield (eluent: EtOAc/Hexanes= 2:8); mp: 86-88 ^{o}C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 2.58 (t, *J*= 5.1Hz, 2H), 2.64 (t, *J*= 5.1Hz, 2H), 3.50 (s, 2H), 3.67-3.71 (m, 2H), 3.81-3.84 (m, 2H), 7.18-7.24 (m, 3H), 7.27-7.36 (m, 5H),, 7.44-7.47 (m, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C41.3, 46.8, 47.6, 51.3, 52.1, 81.1, 83.4, 85.9, 90.7, 120.5, 122.8, 128.2, 128.4, 129.9, 131.7, 132.3, 153.0; **IR (KBr) ν:** 2999, 2876, 2220, 1616, 1125, 1056; **HRMS:** $(M+H)^+$ calculated for $C_{22}H_{21}N_2O$: 329.1653, Found: 329.1619.

3-(p-tolyl)-1-(4-(3-(p-tolyl)prop-2-yn-1-yl)piperazin-1-yl)prop-2-yn-1-one 2kb



2kb

2kb (133 mg) was obtained from **1kb** (171 mg) following general procedure B; white

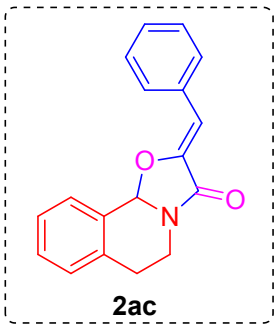
solid; 75% yield (eluent: EtOAc/Hexanes= 2:8); mp: 87-89 ^{o}C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 2.36 (s, 3H), 2.37 (s, 3H), 2.65 (t, *J*= 5.1Hz, 2H), 2.70 (t, *J*= 5.1Hz, 2H), 3.56 (s, 2H), 3.74-3.78 (m, 2H), 3.88-3.92 (m, 2H), 7.09 (d, *J*= 7.8Hz, 2H), 7.14-7.18 (m, 2H),7.30 (d, *J*= 8.1HZ, 2H), 7.41-7.45 (m, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C21.3, 21.5, 41.2, 48.8, 47.7, 51.4, 52.1, 80.7, 82.6, 88.1, 91.1, 117.4, 119.7, 128.9, 129.2, 131.5, 132.2, 138.3, 140.4, 153.1; **HRMS:** $(M+H)^+$ calculated for $C_{24}H_{25}N_2O$: 357.1966, Found: 357.1962.

4. General procedure C for synthesis of Oxazolo[2,3-a]isoquinolinone

Reaction tube was charged with phenylpropynyltetrahydroisoquinoline (0.3 mmol), DBU (0.3 mmol), Rose bengal (2 mol%) and Ag(OTf) (10 mol%) in ACN 4 mL. The reaction mixture was stirred in the presence of O_2 (balloon) under blue light for 2 hours. After the reaction completion, solvent was evaporated under reduced pressure. The crude product was purified by column chromatography using EtOAc/Hexane as eluent to furnish the corresponding Oxazolo[2,3-a]isoquinolinone compounds.

(*Z*)-2-benzylidene-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2ac

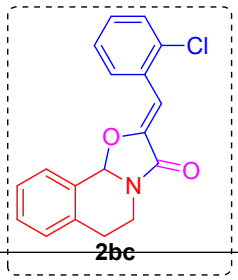


2ac

2ac (51 mg) was obtained from **1ac** (74 mg) following general procedure C; yellow liquid; 61% yield (eluent: EtOAc/Hexanes= 3:7);

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 2.81-2.88 (m, 1H), 3.09-3.16 (m, 1H), 3.44-3.52 (m, 1H), 4.37-4.45 (m, 1H), 6.32 (s, 1H), 6.55 (s, 1H), 7.20 (d, *J*= 6.6Hz, 1H), 7.27-7.29 (m, 1H), 7.34-7.41 (m, 4H), 7.63-7.65 (m, 1H), 7.74 (d, *J*= 7.2Hz, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C 27.5, 37.7, 87.1, 103.7, 125.8, 127.2, 127.4, 128.4, 128.8, 129.1, 129.2, 133.2, 133.8, 133.9, 144.1, 161.8; **IR (KBr) v:** 2935, 1562, 1158, 967; **HRMS:** $(M+H)^+$ calculated for $C_{18}H_{16}NO_2$: 278.1181, Found: 278.1184.

(*Z*)-2-(2-chlorobenzylidene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2bc

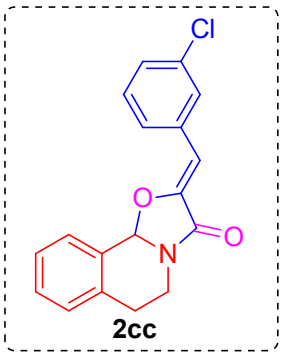


2bc

2bc (52 mg) was obtained from **1bc** (85 mg) following general procedure C; white solid; 55% yield (eluent: EtOAc/Hexanes= 3:7); mp: 128-130 ^{o}C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 2.79-2.86 (m, 1H), 3.00-3.17 (m, 1H), 3.43-3.52 (m, 1H), 4.39-4.46 (m, 1H), 6.55 (s, 1H), 6.74 (s, 1H), 7.15-7.20 (m, 2H), 7.27-7.40 (m, 4H), 7.57-760 (m, 1H), 8.17 (d, *J*= 6Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ_C 27.6, 37.9, 87.3, 99.0, 125.9, 126.7, 127.3, 128.4, 129.0, 129.3, 129.6, 130.1, 131.7, 132.8, 133.6, 133.9, 145.5, 161.4; **IR (KBr) v:** 2932, 2876, 1562, 1153, 973; **HRMS:** $(M+H)^+$ calculated for $C_{18}H_{15}ClNO_2$: 312.0791, Found: 312.0795.

(*Z*)-2-(3-chlorobenzylidene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2cc

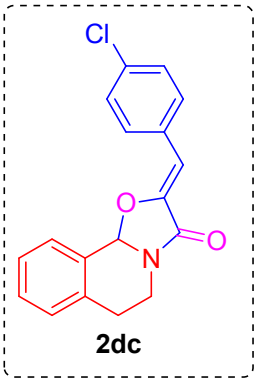


2cc

2cc (42 mg) was obtained from **1cc** (85 mg) following general procedure C; white solid; 45% yield (eluent: EtOAc/Hexanes= 3:7); mp: 123-125 ^{o}C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 2.83-2.88 (m, 1H), 3.12-3.19 (m, 1H), 3.46-3.55 (m, 1H), 4.42-4.44 (m, 1H), 6.25 (s, 1H), 6.57 (s, 1H), 7.20-7.30 (m, 3H), 7.33-7.40 (m, 2H), 7.56 (d, *J*= 6.9Hz, 1H), 7.64 (d, *J*= 6.6Hz, 1H), 7.77 (s, 1H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C 27.6, 37.8, 87.4, 102.2, 125.8, 127.3, 127.4, 127.5, 128.9, 129.3, 129.6, 132.9, 133.9, 134.4, 134.6, 135.7, 145.1, 161.4; **HRMS:** $(M+H)^+$ calculated for $C_{18}H_{15}ClNO_2$: 312.0791, Found: 312.0784.

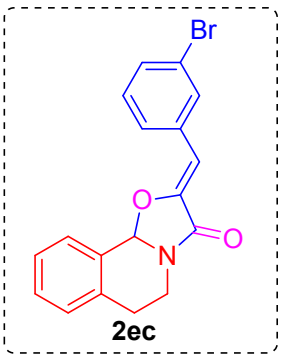
(*Z*)-2-(4-chlorobenzylidene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2dc



2dc (61 mg) was obtained from **1dc** (85 mg) following general procedure C; white solid; 65% yield (eluent: EtOAc/Hexanes= 3:7); mp: 118-120 ^{o}C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 2.80-2.88 (m, 1H), 3.07-3.18 (m, 1H), 3.44-3.53 (m, 1H), 4.38-4.45 (m, 1H), 6.26 (s, 1H), 6.55 (s, 1H), 7.21 (d, *J*= 6.6Hz, 1H), 7.28-7.41 (m, 4H), 7.60-7.67 (m, 3H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C 27.6, 37.8, 87.3, 1024, 125.8, 127.3, 128.7, 128.9, 129.3, 130.3, 132.4, 133.0, 133.1, 133.9, 144.6, 161.5; **HRMS:** $(M+H)^+$ calculated for $C_{18}H_{15}ClNO_2$: 312.0791, Found: 312.0789.

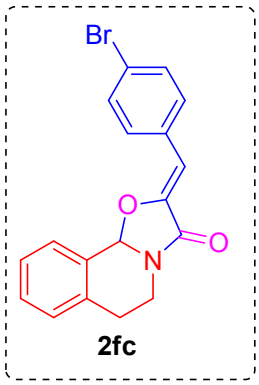
(*Z*)-2-(3-bromobenzylidene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2ec



2ec (55 mg) was obtained from **1ec** (98 mg) following general procedure C; brown solid; 52% yield (eluent: EtOAc/Hexanes= 3:7); mp: 130-132 ^{o}C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 2.93-2.77 (m, 1H), 3.06-3.17 (m, 1H), 3.44-3.54 (m, 1H), 4.38-4.45 (m, 1H), 6.21 (s, 1H), 6.57 (s, 1H), 7.16-7.266 (m, 2H), 7.31-7.46 (m, 3H), 7.60 (d, *J*= 7.4Hz, 2H), 7.90 (s, 1H); **^{13}C NMR (75 MHz, $CDCl_3$):** 27.6, 37.9, 87.4, 102.1, 122.6, 125.9, 127.3, 127.7, 129.9, 129.4, 130.0, 130.3, 131.8, 132.7, 133.8, 135.9, 145.1, 161.4; **HRMS:** $(M+H)^+$ calculated for $C_{18}H_{15}BrNO_2$: 356.0286, Found: 356.0287.

(*Z*)-2-(4-bromobenzylidene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2fc

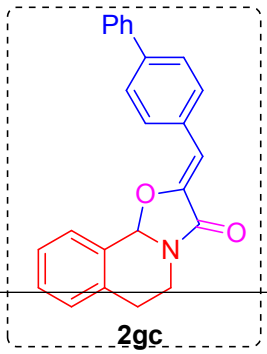


2fc

2fc (62 mg) was obtained from **1fc** (98 mg) following general procedure C; brown solid; 58% yield (eluent: EtOAc/Hexanes= 3:7); mp: 185-187 ^oC;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 2.80-2.86 (m, 1H), 3.07-3.15 (m, 1H), 3.44-3.51 (m, 1H), 4.38-4.44 (m, 1H), 6.22 (s, 1H), 6.55 (s, 1H), 7.19 (d, *J* = 7.0Hz, 1H), 7.32-7.41 (m, 2H), 7.46-7.52 (m, 2H), 7.55-7.63 (m, 3H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C 27.6, 37.8, 87.3, 102.4, 121.2, 125.9, 127.3, 129.0, 129.3, 130.6, 131.7, 132.7, 132.8, 133.9, 144.7, 161.6; **HRMS:** $(M+H)^+$ calculated for $C_{18}H_{15}BrNO_2$: 356.0286, Found: 356.0286.

(*Z*)-2-([1,1'-biphenyl]-4-ylmethylene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2gc

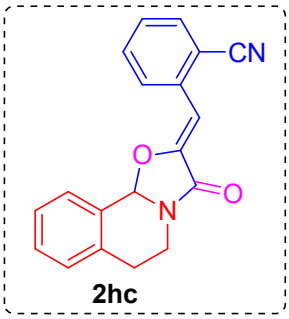


2gc

2gc (51 mg) was obtained from **1gc** (97 mg) following general procedure C; white solid; 48% yield (eluent: EtOAc/Hexanes= 3:7); mp: 212-214 ^{o}C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 2.81-2.86 (m, 1H), 3.00-3.17 (m, 1H), 3.43-3.53 (m, 1H), 4.38-4.43 (m, 1H), 6.34 (s, 1H), 6.57 (s, 1H), 7.19 (d, *J*= 6.7Hz, 1H), 7.32-7.36 (m, 2H), 7.47-7.47 (m, 3H), 7.57-7.63 (m, 5H), 7.80 (d, *J*= 8Hz, 2H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ_C 27.6, 37.8, 87.2, 103.3, 125.9, 127.0, 127.2, 127.3, 127.4, 128.8, 128.9, 129.2, 129.6, 132.8, 133.0, 133.9, 140.1, 140.7, 144.3, 161.8; **HRMS:** $(M+H)^+$ calculated for $C_{24}H_{20}NO_2$: 354.1494, Found: 354.1496.

(*Z*)-2-((3-oxo-3,5,6,10b-tetrahydro-2H-oxazolo[2,3-a]isoquinolin-2-ylidene)methyl)benzonitrile 2hc



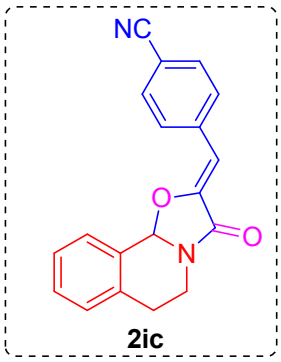
2hc

2hc (56 mg) was obtained from **1hc** (82 mg) following general procedure C; white solid; 62% yield (eluent: EtOAc/Hexanes= 3:7); mp: 155-157 ^{o}C;

^{1}H NMR (400 MHz, $CDCl_3$): δ_H 2.74-2.79 (m, 1H), 3.00-3.07 (m, 1H), 3.37-3.45 (m, 1H), 4.30-4.40 (m, 1H), 6.52 (s, 1H), 6.58 (s, 1H), 7.13 (d, *J*= 4.8Hz, 1H), 7.18-7.29 (m, 3H), 7.50-7.56 (m,

3H), 8.18 (d, *J*= 6Hz, 1H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ_C 27.6, 37.9, 87.7, 98.7, 111.7, 117.7, 125.9, 127.2, 127.3, 129.1, 129.2, 129.5, 132.3, 132.6, 133.1, 134.0, 136.9, 147.1, 160.7; **IR (KBr) v:** 2932, 2343, 1562, 1155, 961; **HRMS:** $(M+H)^+$ calculated for $C_{19}H_{15}N_2O_2$: 303.1133, Found: 303.1097.

(*Z*)-4-((3-oxo-3,5,6,10b-tetrahydro-2H-oxazolo[2,3-a]isoquinolin-2-ylidene)methyl)benzonitrile 2ic

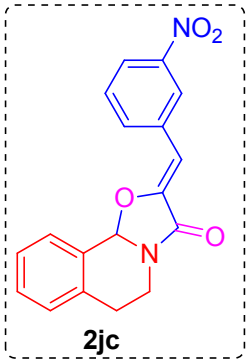


2ic

2ic (62 mg) was obtained from **1ic** (82 mg) following general procedure C; white solid; 69% yield (eluent: EtOAc/Hexanes= 3:7); mp: 195-197 ^oC;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 2.83-2.91 (m, 1H), 3.09-3.20 (m, 1H), 3.47-3.57 (m, 1H), 4.41-4.48 (m, 1H), 6.30 (s, 1H), 6.61 (s, 1H), 7.23 (d, *J*= 6.6Hz, 1H), 7.35-7.43 (m, 2H), 7.63 (T, *J*= 7.2Hz, 3H), 7.79 (d, *J*= 6Hz, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C 27.2, 37.6, 87.4, 101.3, 110.0, 118.5, 125.5, 127.0, 128.7, 129.0, 129.1, 131.8, 132.1, 133.5, 138.2, 146.3, 160.6; HRMS: (M+H)+ calculated for $C_{19}H_{15}N_2O_2$: 303.1133, Found: 303.1098.

(*Z*)-2-(3-nitrobenzylidene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2jc

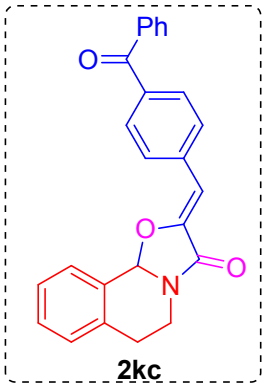


2jc

2jc (62 mg) was obtained from **1jc** (88 mg) following general procedure C; yellow liquid; 65% yield (eluent: EtOAc/Hexanes= 4:6);

^{1}H NMR (400 MHz, $CDCl_3$): δ_H 2.84-2.91 (m, 1H), 3.09-3.20 (m, 1H), 3.47-3.53 (m, 1H), 4.41-4.48 (m, 1H), 6.34 (s, 1H), 6.62 (s, 1H), 7.22 (d, *J*= 7.2Hz, 1H), 7.34-7.44 (m, 2H), 7.52 (t, *J*= 7.8Hz, 1H), 7.66 (d, *J*= 7.5Hz, 1H), 7.90 (d, *J*= 7.5Hz, 1H), 8.09 (d, *J*= 7.5Hz, 1H), 8.70 (s, 1H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ_C 27.6, 37.9, 87.7, 101.1, 121.8, 123.4, 125.9, 127.5, 129.0, 129.3, 129.5, 132.6, 133.8, 134.6, 135.6, 146.3, 148.7, 160.9; **HRMS:** $(M+H)^+$ calculated for $C_{18}H_{15}N_2O_4$: 323.1031, Found: 323.0996.

(*Z*)-2-(4-benzoylbenzylidene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2kc

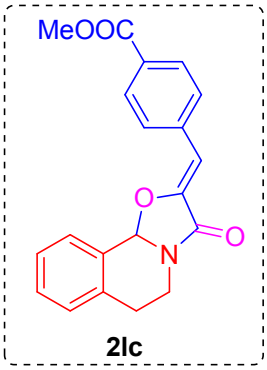


2kc

2kc (58 mg) was obtained from **1kc** (105 mg) following general procedure C; yellow liquid; 51% yield (eluent: EtOAc/Hexanes= 4:6);

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 2.85-2.90 (m, 1H), 3.13-3.20 (m, 1H), 3.48-3.56 (m, 1H), 4.41-4.48 (m, 1H), 6.37 (s, 1H), 6.60 (s, 1H), 7.23 (d, *J*= 6.6Hz, 1H), 7.37-7.39 (m, 2H), 7.47-7.52 (m, 2H), 7.57-7.64 (m, 2H), 7.80-7.84 (m, 6H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C 27.6, 37.9, 87.5, 102.5, 125.8, 127.3, 128.2, 128.8, 128.9, 129.3, 129.8, 130.3, 132.1, 132.8, 133.9, 136.0, 137.9, 138.1, 145.9, 161.3, 195.9; **HRMS:** $(M+H)^+$ calculated for $C_{25}H_{20}NO_3$: 382.1443, Found: 382.1412.

(*Z*)-methyl 4-((3-oxo-3,5,6,10b-tetrahydro-2H-oxazolo[2,3-a]isoquinolin-2-ylidene)methyl)benzoate 2lc

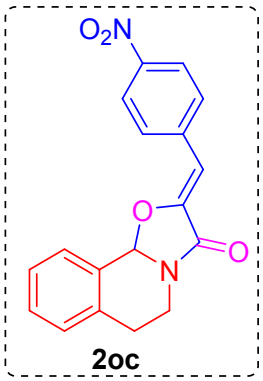


2lc

2lc (67 mg) was obtained from **1lc** (91 mg) following general procedure C; white solid; 67% yield (eluent: EtOAc/Hexanes= 4:6); mp: 202-204 ^{o}C;

^{1}H NMR (400 MHz, $CDCl_3$): δ_H 2.75-2.78 (m, 1H), 3.00-3.07 (m, 1H), 3.38-3.44 (m, 1H), 4.32-4.36 (m, 1H), 6.23 (s, 1H), 6.50 (s, 1H), 7.10 (d, *J*= 6.6Hz, 1H), 7.26-7.32 (m, 2H), 7.54 (d, *J*= 3Hz, 1H), 7.68 (d, *J*= 6Hz, 2H), 7.95 (d, *J*= 6Hz, 2H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ_C 27.6, 37.9, 52.1, 87.5, 102.4, 125.9, 127.3, 128.5, 128.9, 129.0, 129.4, 129.7, 132.6, 133.8, 138.4, 145.8, 161.3, 166.8; **IR (KBr) ν:** 2847, 1712, 1556, 1153, 954; **HRMS:** $(M+H)^+$ calculated for $C_{20}H_{18}NO_4$: 336.1236, Found: 336.1234.

(*Z*)-2-(4-nitrobenzylidene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2oc



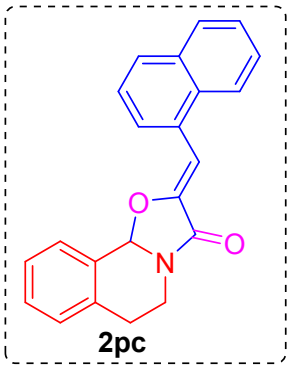
2oc

2oc (68 mg) was obtained from **1oc** (88 mg) following general procedure B; yellow solid; 71% yield (eluent: EtOAc/Hexanes= 4:6); mp: 220-222 ^{o}C;

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 2.85-2.90 (m, 1H), 3.10-3.25 (m, 1H), 3.52-3.56 (m, 1H), 4.43-4.49 (m, 1H), 6.35 (s, 1H), 6.63 (s, 1H), 7.23 (d, *J*= 6.6Hz, 1H), 7.36-7.41 (m, 2H), 7.62-7.65 (m, 1H), 7.85 (d, *J*= 8.7Hz, 2H), 8.23 (d, *J*= 8.7Hz, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C 27.6, 38.0, 87.8, 101.2, 123.8, 125.8, 127.4, 129.0, 129.4, 129.5, 132.4, 133.9, 140.5, 146.4, 147.1, 160.8; **HRMS:** $(M+H)^+$ calculated for $C_{18}H_{15}N_2O_4$: 323.1031, Found: 323.1031.

(Z)-2-(naphthalen-1-ylmethylene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one

2pc



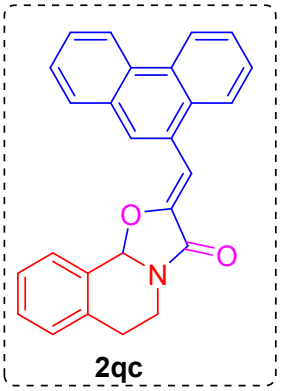
2pc

2pc (51 mg) was obtained from **1pc** (89 mg) following general procedure C; yellow liquid; 52% yield (eluent: EtOAc/Hexanes= 3:7);

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 2.82-2.91 (m, 1H), 3.11-3.22 (m, 1H), 3.47-3.57 (m, 1H), 4.42-4.50 (m, 1H), 6.58 (s, 1H), 7.08 (s, 1H), 7.20-7.23 (m, 1H), 7.35-7.41 (m, 2H), 7.50-7.58 (m, 3H), 7.62-7.65 (m, 1H), 7.79-7.88 (m, 2H), 8.26 (d, *J*= 7.2Hz, 2H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C 27.6, 37.8, 87.1, 99.3, 123.8, 125.4, 125.7, 125.9, 126.2, 127.2, 127.3, 128.0, 128.6, 128.9, 129.2, 129.8, 131.6, 133.2, 133.8, 133.9, 145.1, 161.8; **HRMS:** $(M+H)^+$ calculated for $C_{22}H_{18}NO_2$: 328.1337, Found: 328.1335.

(*Z*)-2-(phenanthren-9-ylmethylene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one

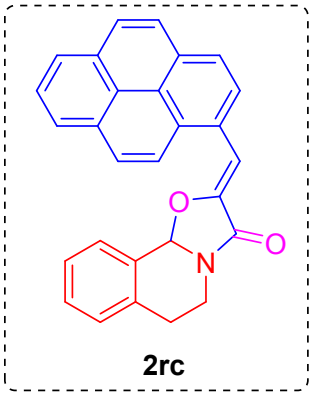
2qc



2qc (57 mg) was obtained from **1qc** (104 mg) following general procedure C; yellow liquid; 50% yield (eluent: EtOAc/Hexanes= 3:7);

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 2.85-2.91 (m, 1H), 3.16-3.24 (m, 1H), 3.49-3.59 (m, 1H), 4.44-4.51 (m, 1H), 6.62 (s, 1H), 7.07 (s, 1H), 7.21-7.39 (m, 3H), 7.60-7.68 (m, 5H), 7.95 (d, *J*= 6.9Hz, 1H), 8.31 (d, *J*= 7.2Hz, 1H), 8.49 (s, 1H), 8.68 (d, *J*= 7.5Hz, 1H), 8.75 (d, *J*= 8.4Hz, 1H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C 27.6, 37.9, 87.2, 99.5, 122.5, 123.08, 124.5, 125.9, 126.4, 126.6, 126.7, 126.8, 127.3, 128.2, 128.4, 128.7, 128.9, 129.2, 130.2, 130.6, 130.1, 131.7, 133.3, 134.0, 145.6, 161.7; **HRMS:** $(M+H)^+$ calculated for $C_{26}H_{20}NO_2$: 378.1494, Found: 378.1466.

(*Z*)-2-(pyren-1-ylmethylene)-6,10b-dihydro-5H-oxazolo[2,3-a]isoquinolin-3(2H)-one 2rc

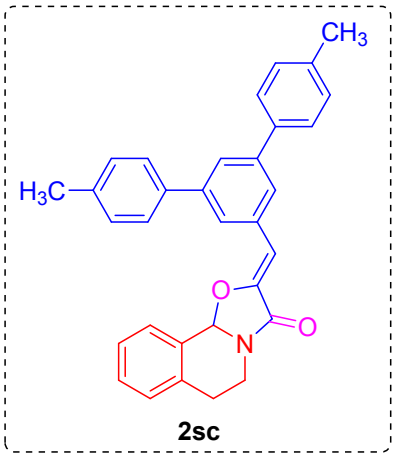


2rc

2rc (61 mg) was obtained from **1rc** (111 mg) following general procedure C; brown semi solid; 49% yield (eluent: EtOAc/Hexanes= 3:7);

^{1}H NMR (400 MHz, $CDCl_3$): δ_H 2.77-2.96 (m, 1H), 3.13-3.22 (m, 1H), 3.50-3.57 (m, 1H), 4.37-4.55 (m, 1H), 6.64 (s, 1H), 7.21 (d, *J*= 7.3Hz, 1H), 7.30-7.44 (m, 3H), 7.69 (d, *J*= 7.3Hz, 1H), 7.96-8.07 (m, 3H), 8.10-8.23 (m, 4H), 8.51 (d, *J*= 9.3 Hz, 1H), 8.78 (d, *J*= 8.2Hz, 1H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ_C 27.7, 37.9, 87.2, 99.9, 123.2, 124.8, 124.9, 125.2, 125.3, 126.0, 126.9, 127.3, 127.4, 127.5, 127.6, 127.7, 128.9, 129.3, 130.7, 130.9, 131.4, 133.1, 134.0, 145.1, 161.9; **HRMS:** $(M+H)^+$ calculated for $C_{28}H_{20}NO_2$: 402.1494, Found: 402.1486

(*Z*)-2-((4,4''-dimethyl-[1,1':3',1''-terphenyl]-5'-yl)methylene)-5,6-dihydro-2H-oxazolo[2,3-a]isoquinolin-3(10bH)-one 2sc

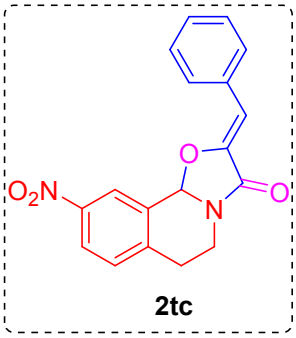


2sc

2sc (61 mg) was obtained from **1sc** (128 mg) following general procedure B; yellow liquid; 45% yield (eluent: EtOAc/Hexanes= 3:7);

^{1}H NMR (400 MHz, $CDCl_3$): δ_H 2.45 (s, 6H), 2.83-2.90 (m, 1H), 3.10-3.19 (m, 1H), 3.47-3.56 (m, 1H), 4.39-4.47 (m, 1H), 6.44 (s, 1H), 6.58 (S, 1H), 7.21 (d, *J*= 7.2Hz, 1H), 7.28-7.38 (m, 6H), 7.59-7.61 (m, 5H), 7.69 (s, 1H), 7.94 (d, *J*= 1.2Hz, 2H); **^{13}C NMR (101 MHz, $CDCl_3$):** δ_C 21.1, 27.6, 37.8, 87.2, 103.8, 125.0, 125.7, 126.6, 127.1, 127.3, 128.9, 129.2, 129.5, 133.3, 134.0, 134.6, 137.2, 138.4, 141.9, 144.6, 161.8; **HRMS:** $(M+H)^+$ calculated for $C_{32}H_{28}NO_2$: 458.2120, Found: 458.2101.

(*Z*)-2-benzylidene-9-nitro-6,10b-dihydro-5H-oxazolo[2,3-a]isoquinolin-3(2H)-one 2tc

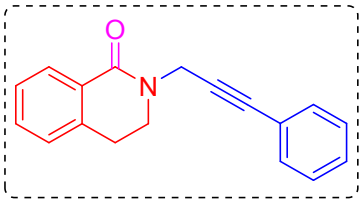


2tc

2tc (56 mg) was obtained from **1tc** (88 mg) following general procedure B; yellow liquid; 59% yield (eluent: EtOAc/Hexanes= 3:7);

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 2.94-3.00 (m, 1H), 3.15-3.26 (m, 1H), 3.47-3.57 (m, 1H), 4.45-4.51 (m, 1H), 6.37 (s, 1H), 6.58 (S, 1H), 7.32 (d, *J*= 7.5Hz, 1H), 7.38-7.44 (m, 3H), 7.73 (d, *J*= 1.2Hz, 2H), 8.21 (d, J= 8.4Hz, 1H), 8.50 (s, 1H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C 27.7, 37.1, 86.1, 105.1, 121.5, 124.0, 128.0, 128.7, 129.4, 130.2, 133.2, 134.8, 141.3, 143.2, 147.4, 161.6; **HRMS:** $(M+H)^+$ calculated for $C_{18}H_{15}N_2O_4$: 323.1032, Found: 323.1039.

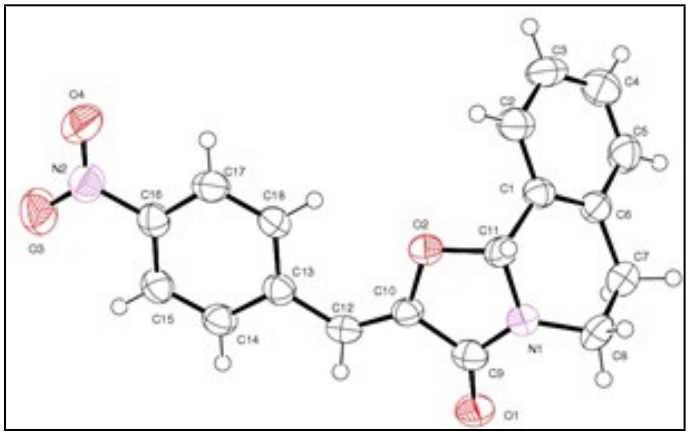
2-(3-phenylprop-2-yn-1-yl)-3,4-dihydroisoquinolin-1(2H)-one 2ad



2ad (20 mg) was obtained from **1ad** (74 mg) following general procedure B; yellow liquid; 25% yield (eluent: EtOAc/Hexanes= 1:9);

^{1}H NMR (300 MHz, $CDCl_3$): δ_H 3.04 (t, *J*= 6.6Hz, 2H), 3.74 (t, *J*= 6.6Hz, 2H), 4.65 (s, 2H), 7.17 (d, *J*= 6.6Hz, 1H), 7.24-7.38 (m, 4H), 7.40-7.43 (m, 3H), 8.11 (d, *J*= 7.8Hz, 1H); **^{13}C NMR (75 MHz, $CDCl_3$):** δ_C 28.0, 36.6, 45.1, 83.8, 84.0, 122.8, 126.9, 127.0, 128.2, 128.3, 128.5, 129.2, 129.8, 131.7, 138.1, 164.1; **HRMS:** $(M+H)^+$ calculated for $C_{18}H_{16}NO$: 262.1231, Found: 262.1248.

5. X-Ray Crystallographic Studies of compound 2oc



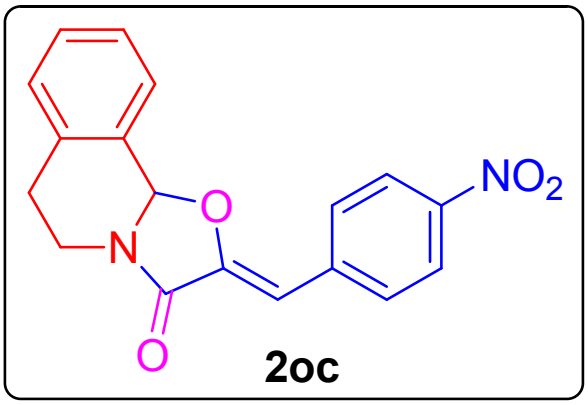


Figure 2. ORTEP structure of compound **2oc (CCDC 1988860)**.

Table 1. Crystal data and structure refinement for Compound **2oc**.

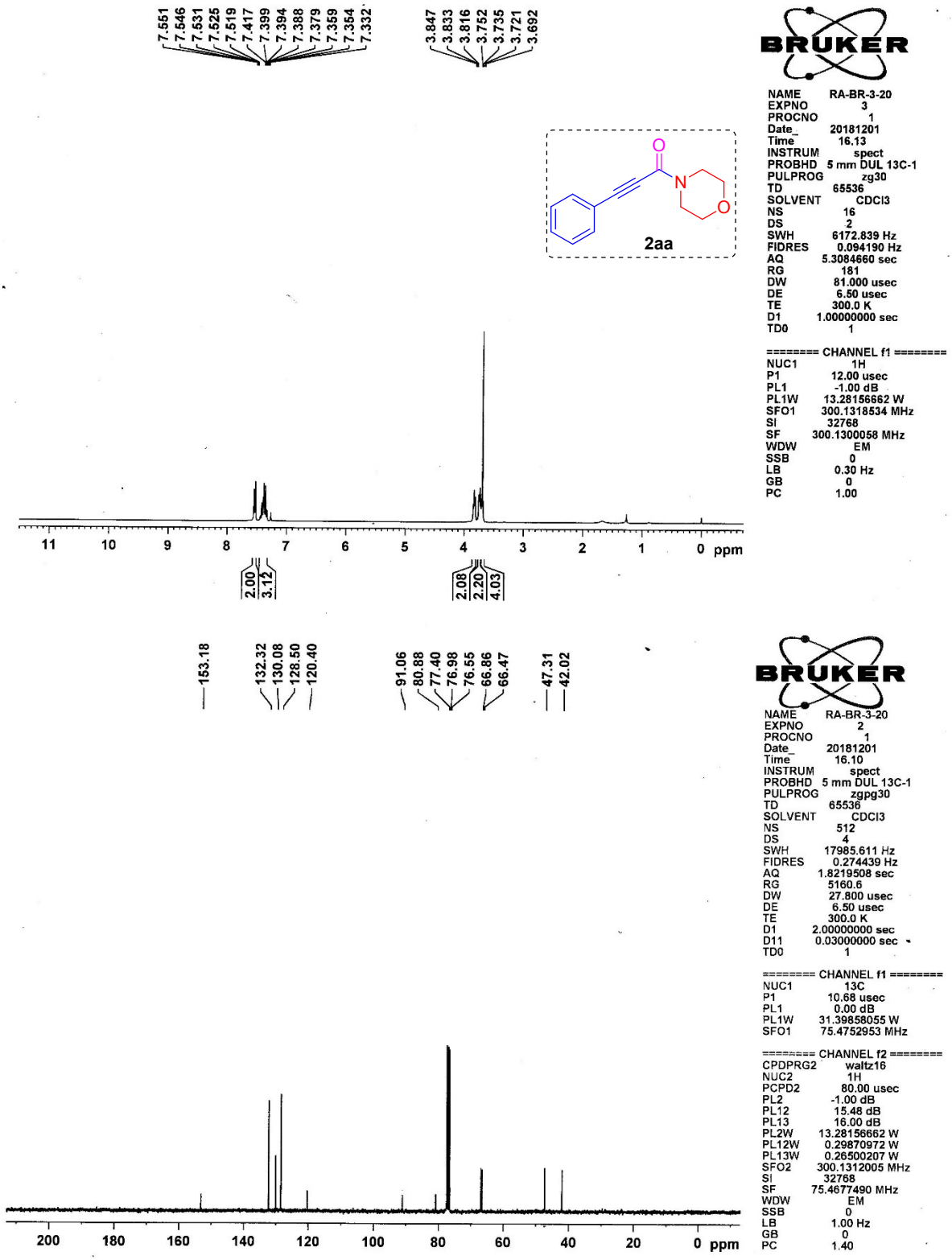
Identification code	2oc	
Chemical formula	$C_{18}H_{14}N_2O_4$	
Formula weight	322.31 g/mol	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal size	0.100 x 0.110 x 0.150 mm	
Crystal habit	clear light yellow Block	
Crystal system	Monoclinic	
Space group	P 1 n 1	
Unit cell dimensions	a = 6.3537(8) Å	α = 90°
	b = 5.0200(6) Å	β = 90.173(4)°
	c = 23.596(3) Å	γ = 90°
Volume	752.60(16) $Å^3$	
Z	2	
Density (calculated)	1.422 g/cm^3	
Absorption coefficient	0.102 mm^{-1}	
F(000)	336	

Theta range for data collection	3.32 to 24.70°
Index ranges	-5<=h<=7, -5<=k<=5, -27<=l<=27
Reflections collected	3980
Independent reflections	2005 [R(int) = 0.0421]
Coverage of independent reflections	99.8%
Absorption correction	multi-scan
Max. and min. transmission	0.9900 and 0.9850
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	2005 / 2 / 218
Goodness-of-fit on F^2	1.032
Final R indices	1414 data; $I>2\sigma(I)$ R1 = 0.0420, wR2 = 0.0778
	all data R1 = 0.0730, wR2 = 0.0913
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0305P)^2+0.0216P]$ where $P=(F_o^2+2F_c^2)/3$
Absolute structure parameter	-0.8(10)
Extinction coefficient	0.0310(40)
Largest diff. peak and hole	0.161 and -0.164 $eÅ^{-3}$
R.M.S. deviation from mean	0.039 $eÅ^{-3}$

6. References:

1. L. W. Bieber and M. F. da silva, Mild and efficient synthesis of propargylamines by copper-catalyzed Mannich reaction, *Tetrahedron Lett.,* 2004, **45**, 8281-8283.
2. Y. Dong, S. Sun, F. Yang, Y. Zhu, W. Zhu, H. Qiao, Y. Wu and Y. Wu, Pd-catalyzed aminocarbonylation of alkynes with amines using $Co_2(CO)_8$ as a carbonyl source, *Org. Chem. Front.,* 2016**, 3**, 720-724.
3. J. Hwang, J. Choi, K. Park, W. Kim, K. H. Song and S. Lee, Palladium-Catalyzed Oxidative Aminocarbonylation by Decarboxylative Coupling: Synthesis of Alkynyl Amides, *Eur. J. Org. Chem.,* 2015**, 2015**, 2235-2243.
4. R. S. Mane and B. M. Bhanage, Palladium-Catalyzed Oxidative N-Dealkylation/Carbonylation of Tertiary Amines with Alkynes to α,β-Alkynylamides, *J. Org. Chem.,* 2016**, 81**, 4974-4980.

7. Spectral data:



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SOLVENT	CDCl3
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DS	2
SWH	6172.839 Hz
FIDRES	0.094190 Hz
AQ	5.3084660 sec
RG	181
DW	81.000 usec
DE	6.50 usec
TE	300.0 K
D1	1.00000000 sec
TD0	1
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NUC1	1H
P1	12.00 usec
PL1	-1.00 dB
PL1W	13.28156662 W
SFO1	300.1318534 MHz
SI	32768
SF	300.1300058 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

BRUKER

NAME	RA-BR-3-20
EXPNO	2
PROCNO	1
Date_	20181201
Time	16.10
INSTRUM	spect
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PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	4
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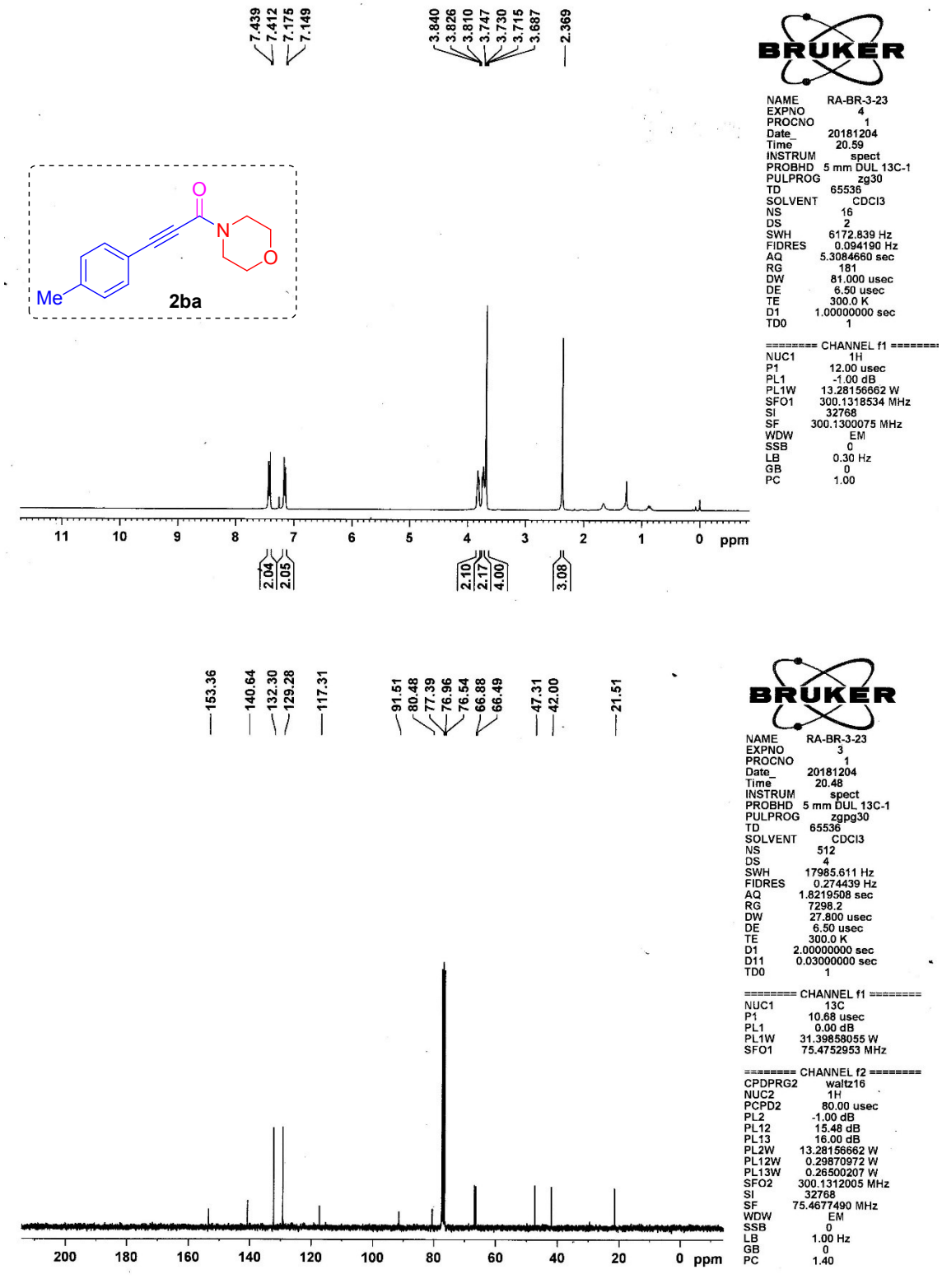
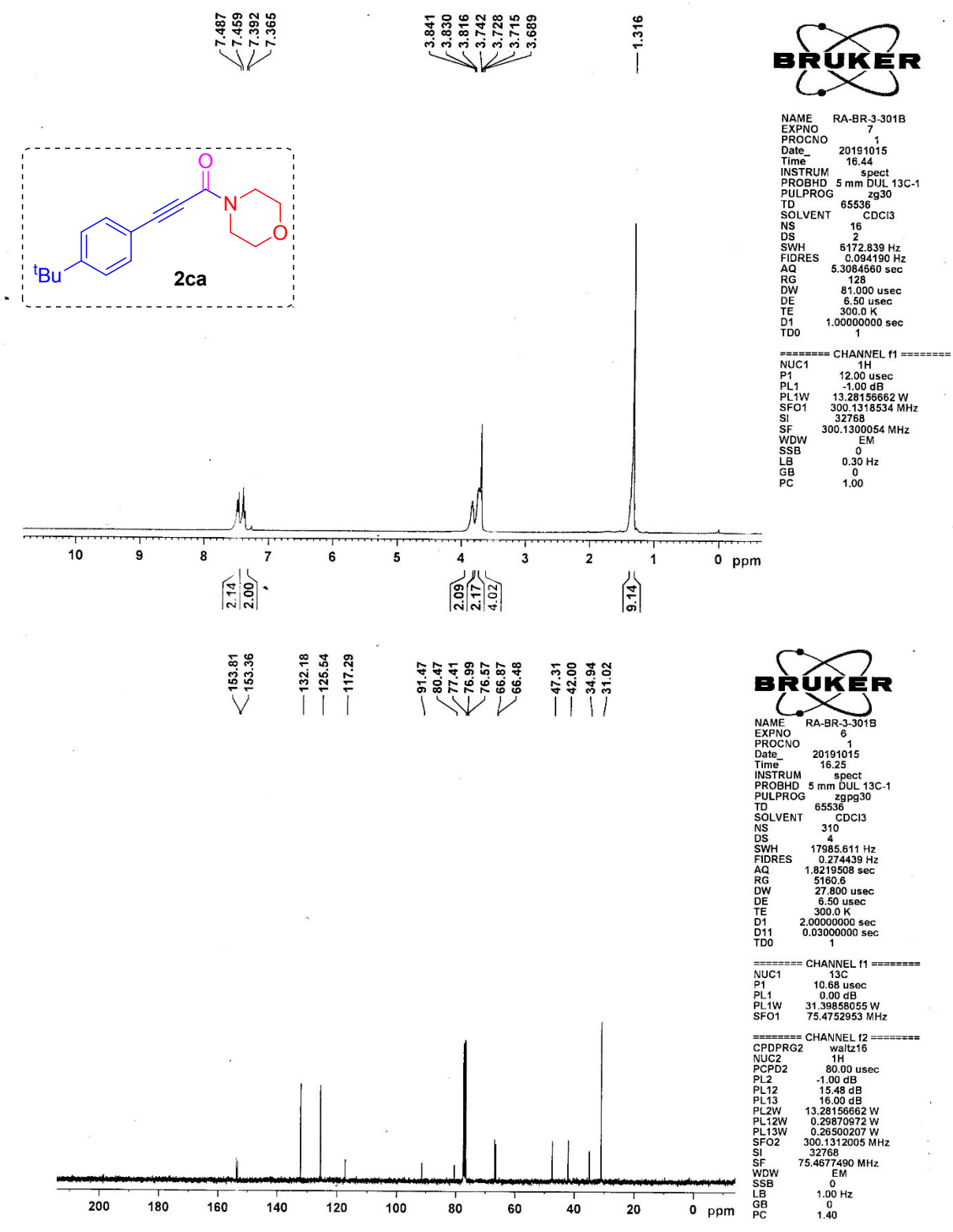
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	5160.6
DW	27.800 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.68 usec
PL1	0.00 dB
PL1W	31.39858055 W
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-1.00 dB
PL12	15.48 dB
PL13	16.00 dB
PL2W	13.28156662 W
PL12W	0.29870972 W
PL13W	0.26500207 W
SFO2	300.1312005 MHz
SI	32768
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

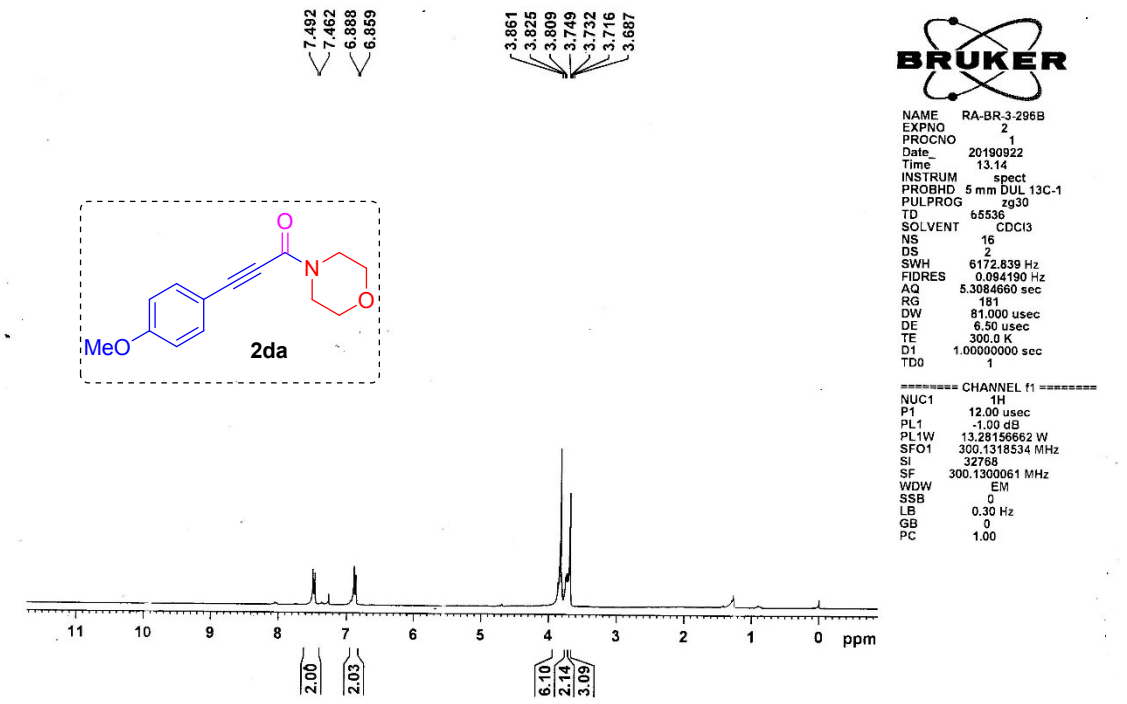
^{1}H&^{13}C spectra of compound 2aa

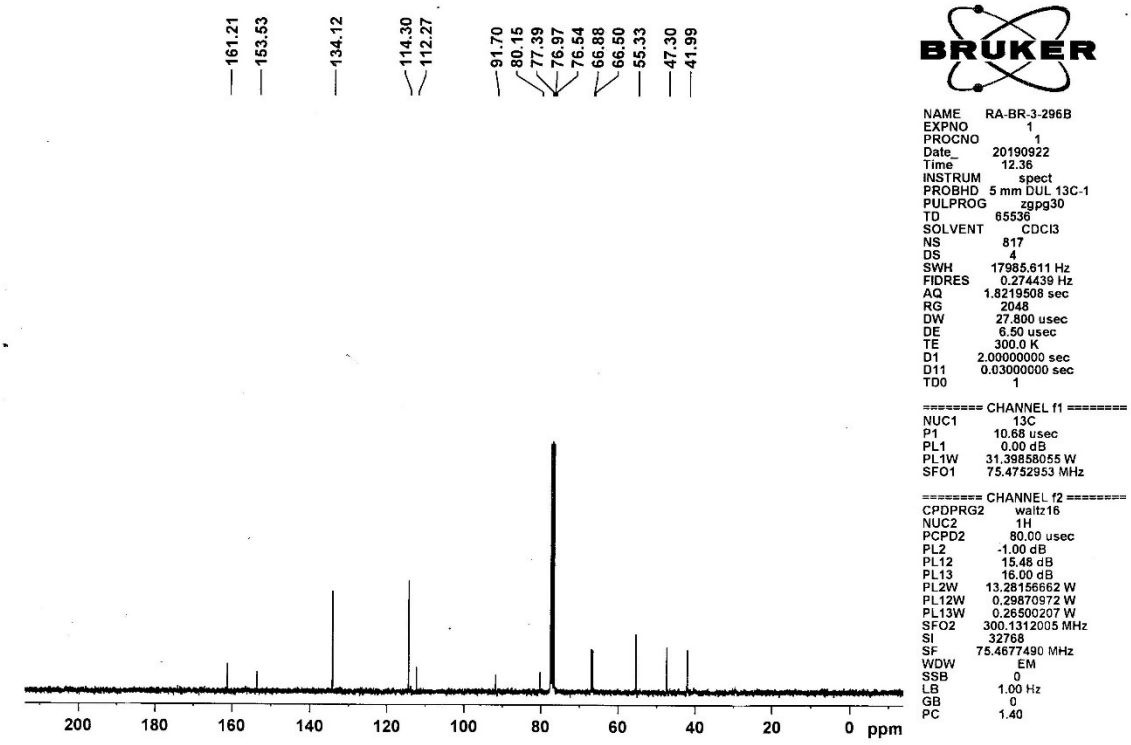


^{1}H&^{13}C spectra of compound 2ba

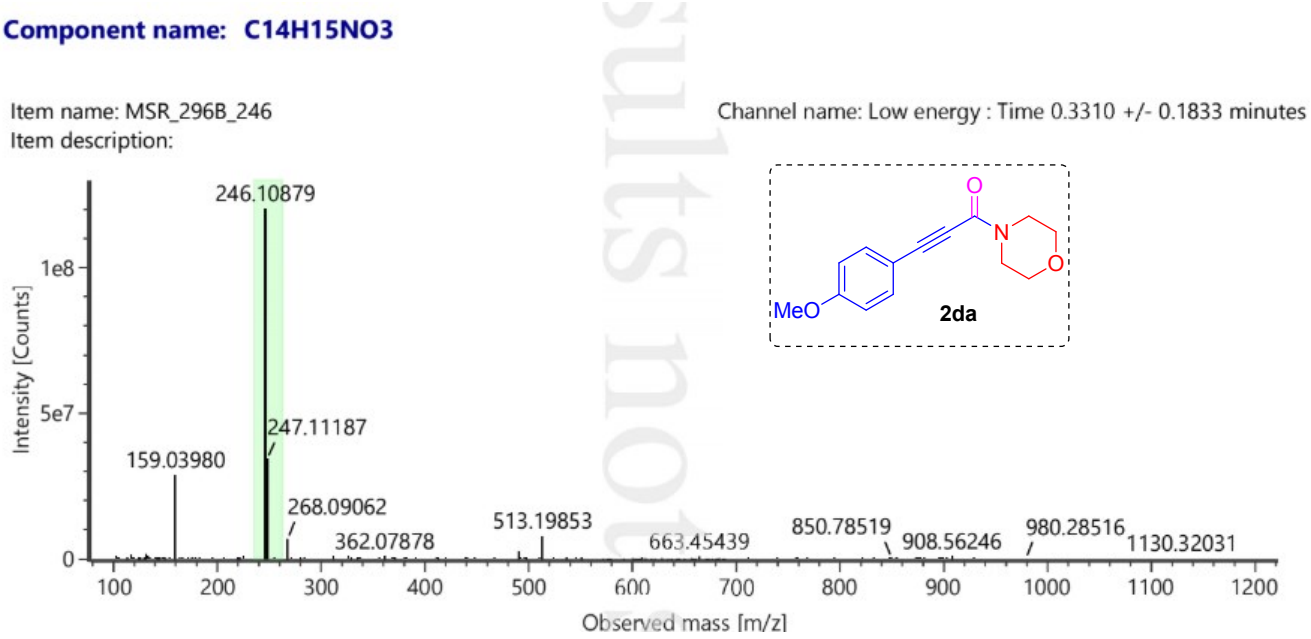


^{1}H&^{13}C spectra of compound 2ca

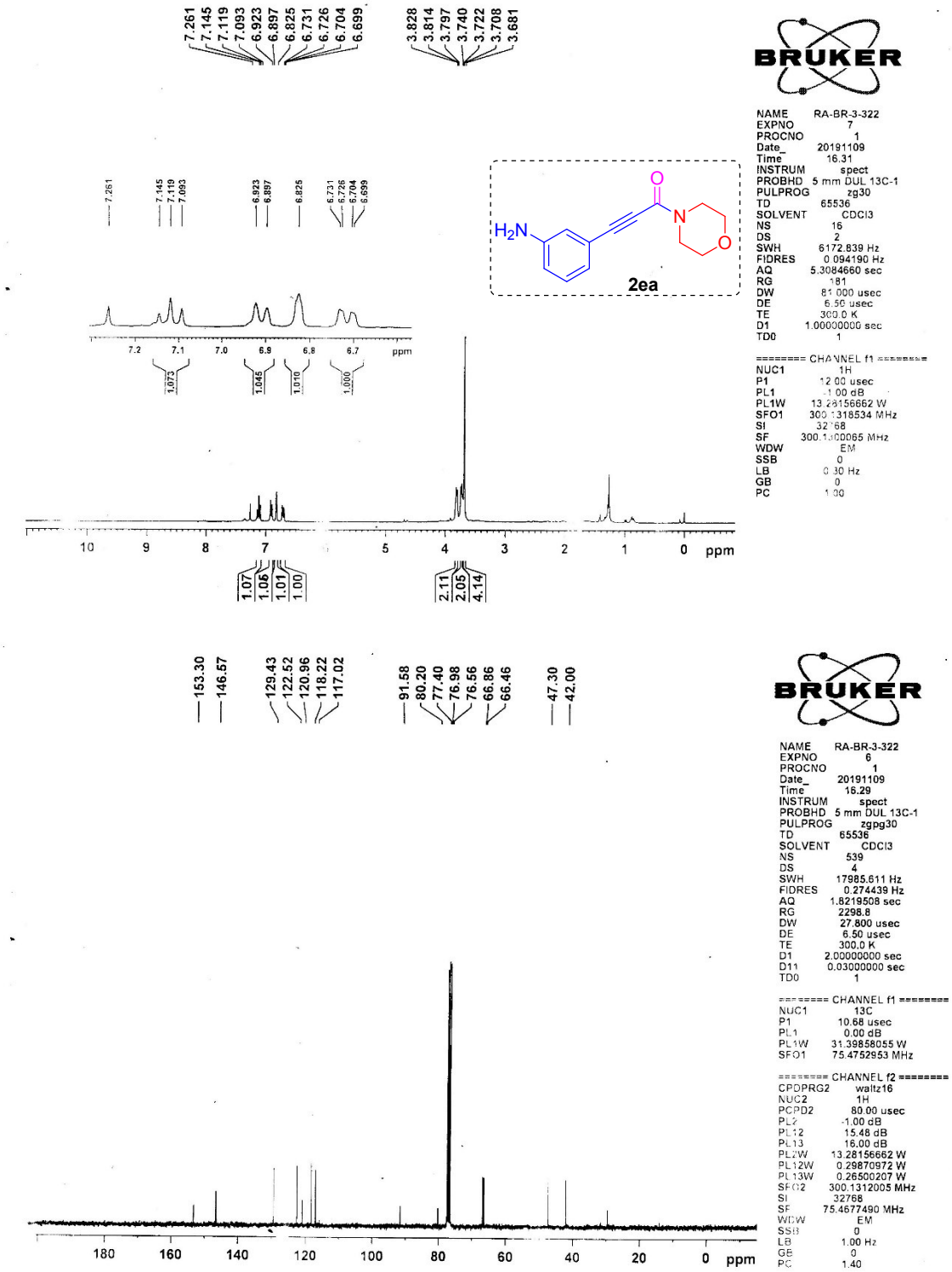




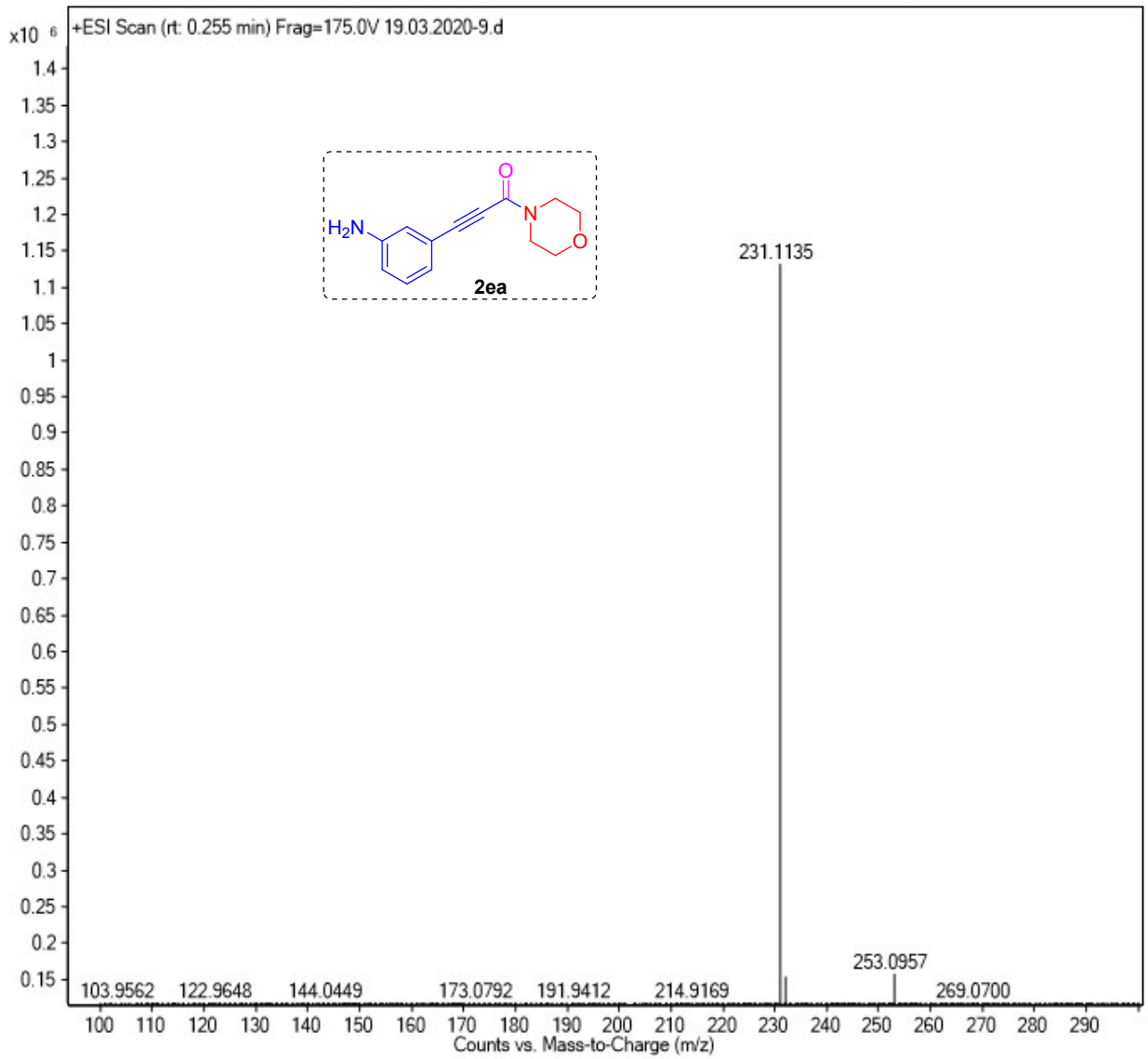
^{1}H&^{13}C spectra of compound 2da



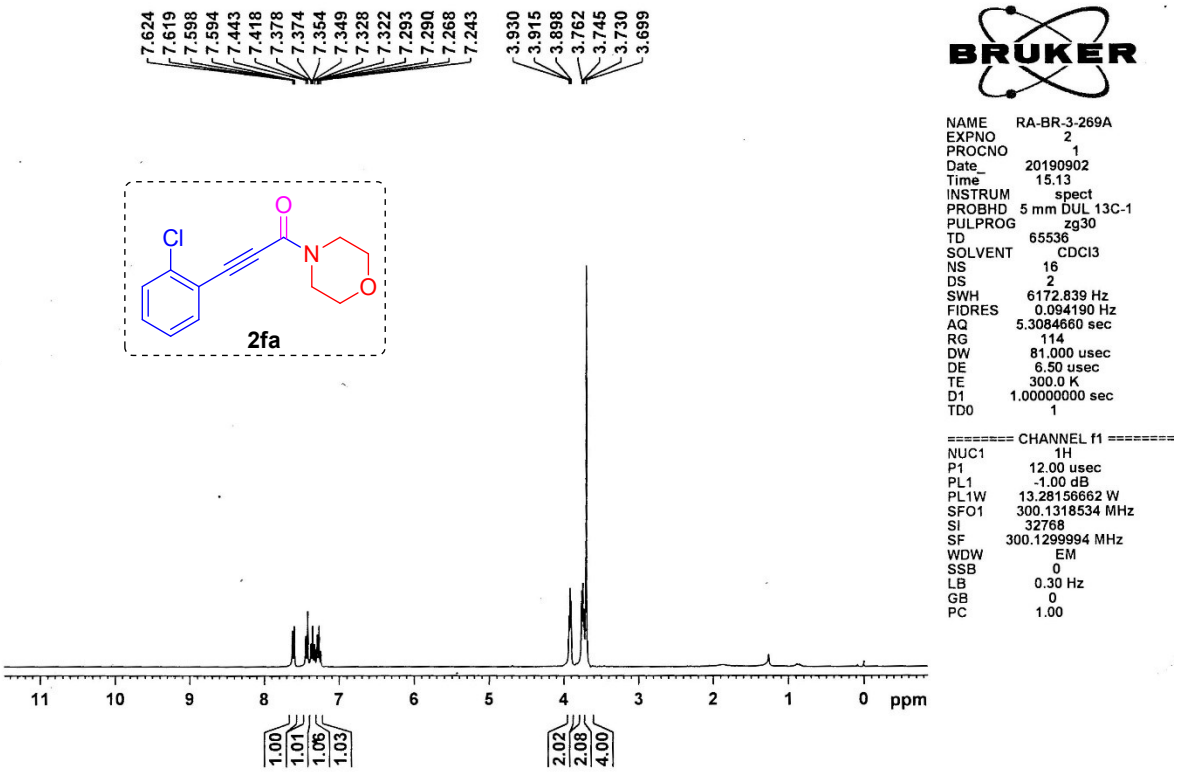
HRMS Spectrum of Compound 2da

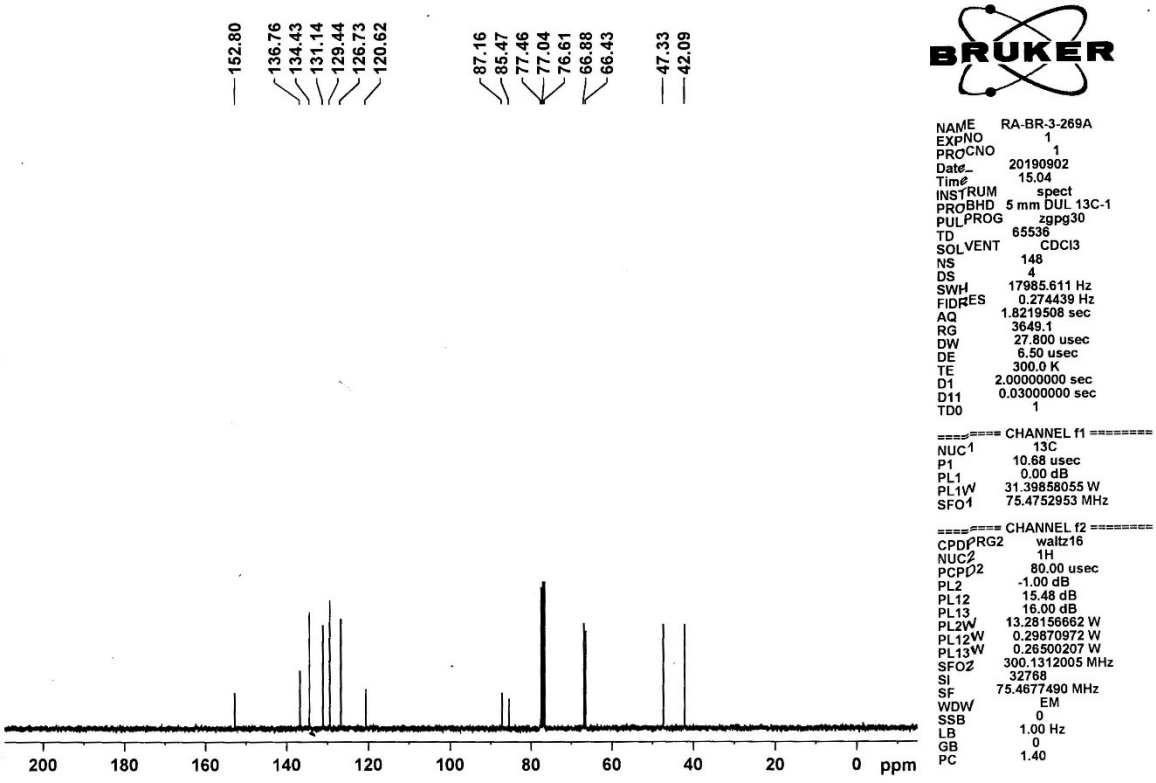


^{1}H&^{13}C spectra of compound 2ea

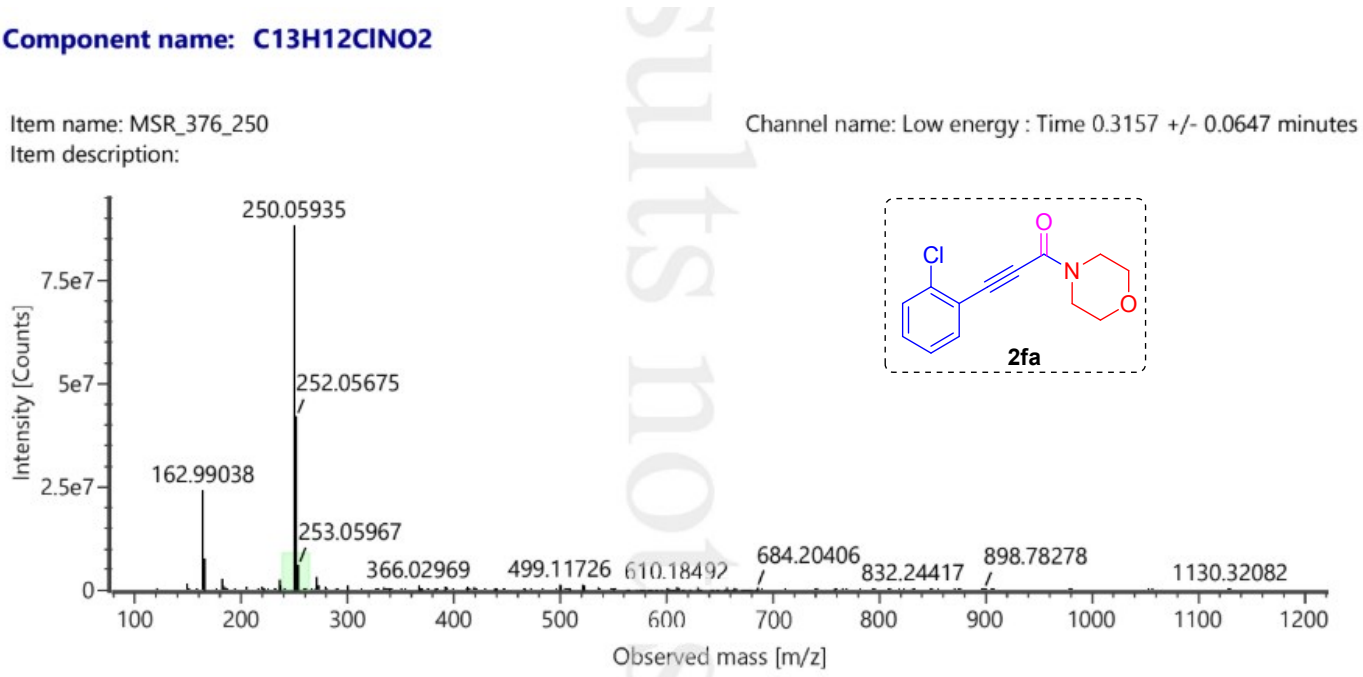


HRMS spectrum of compound 2ea

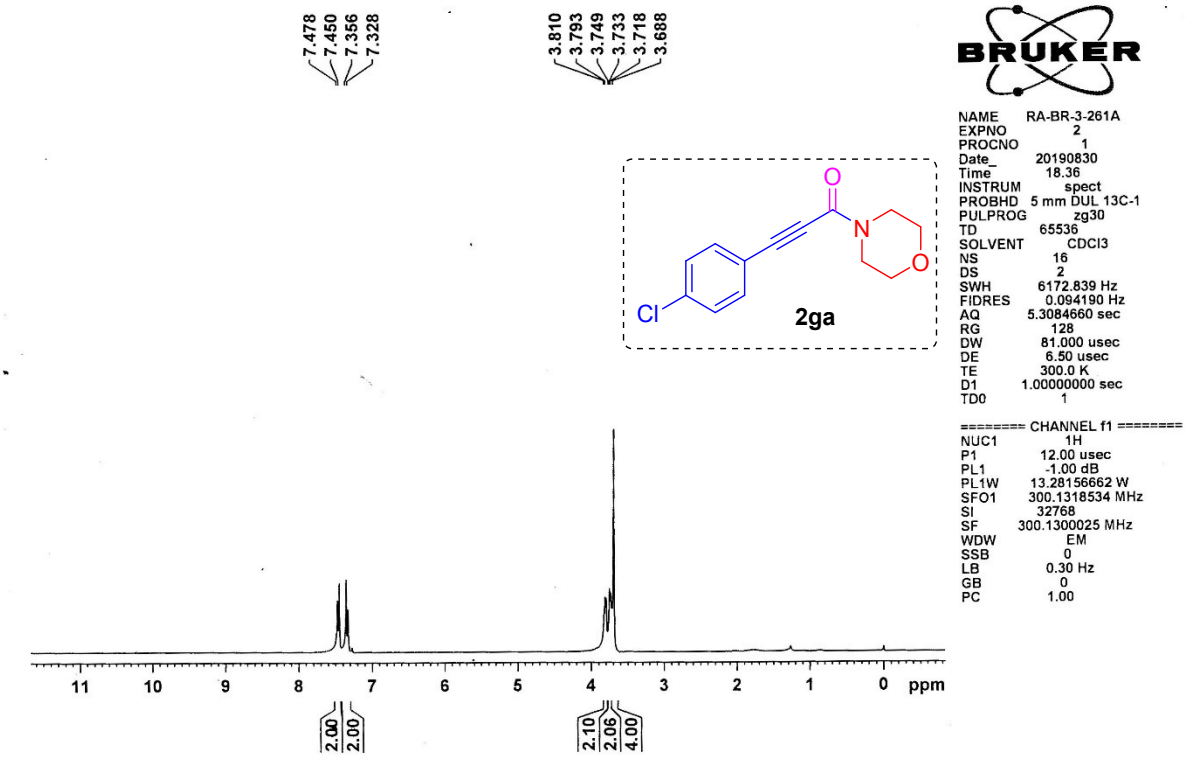




^{1}H&^{13}C spectra of compound 2fa



HRMS Spectrum of Compound 2fa



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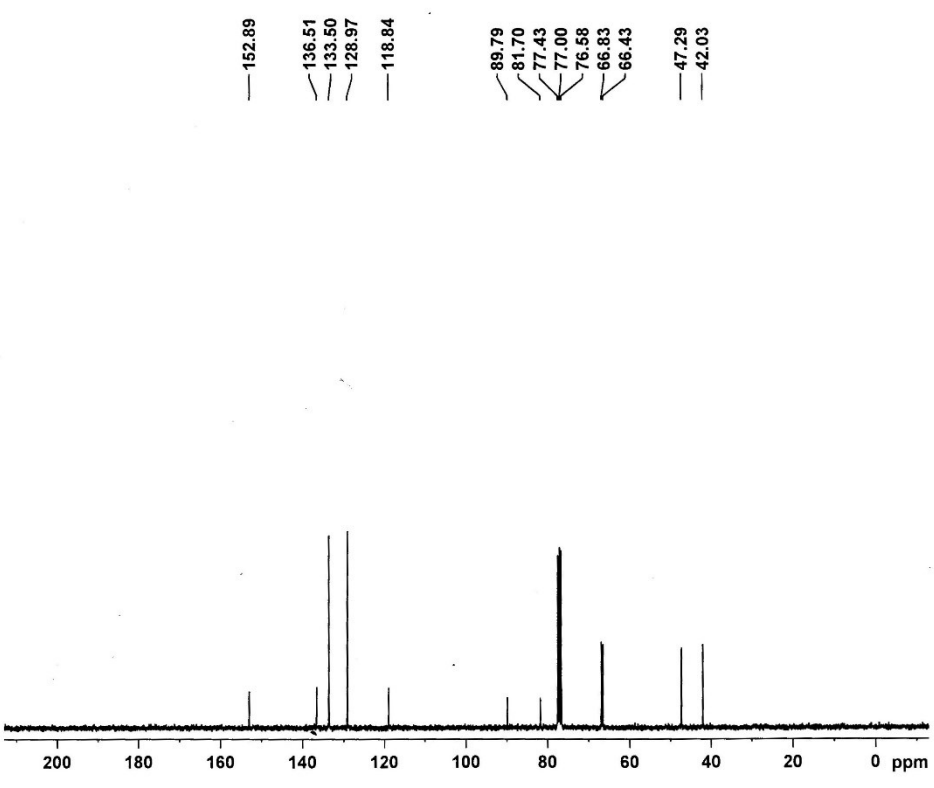
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 128
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -1.00 dB
PL1W 13.28156662 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300025 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

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SOLVENT CDCl3
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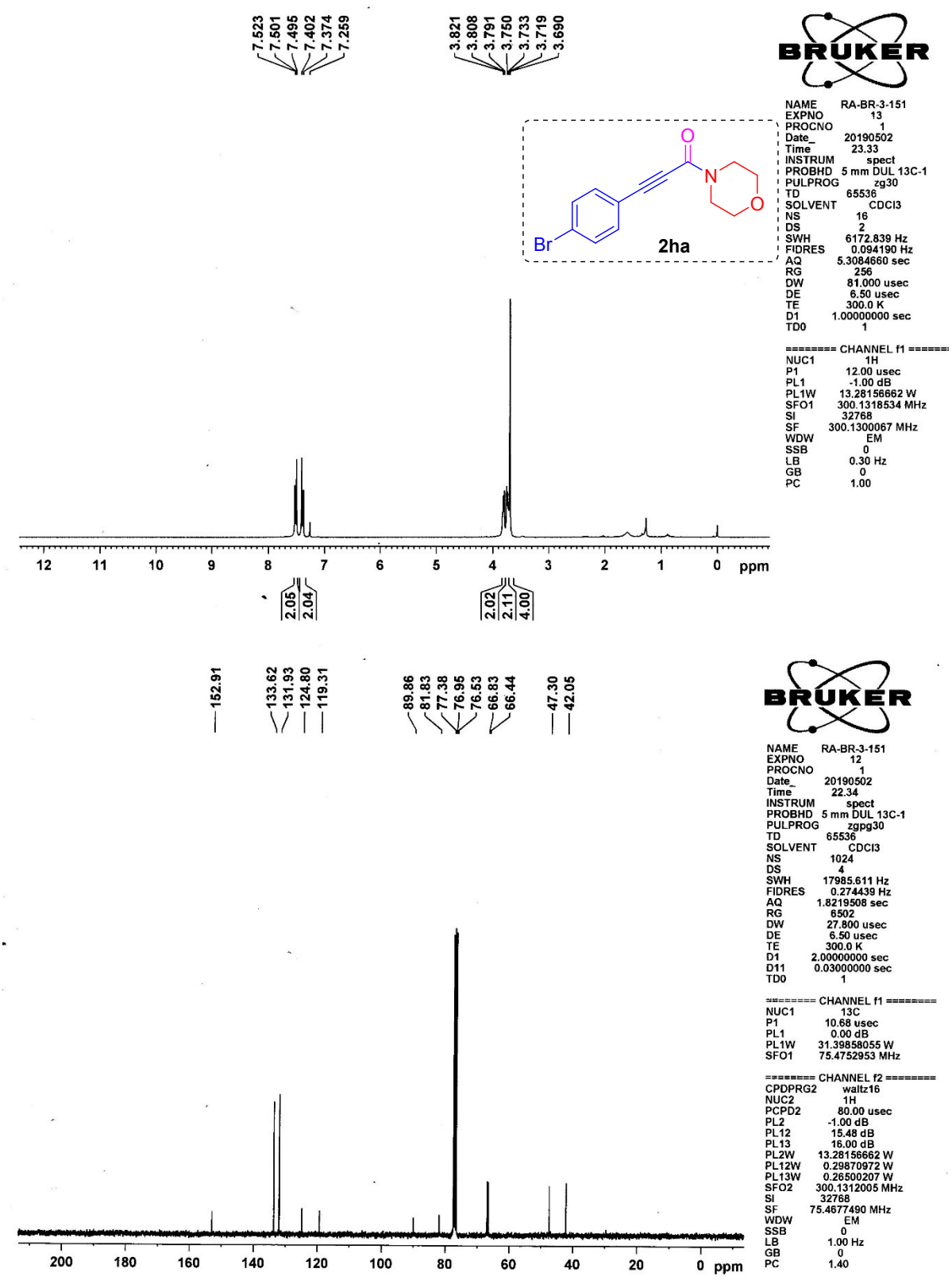
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2580.3
DW 27.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

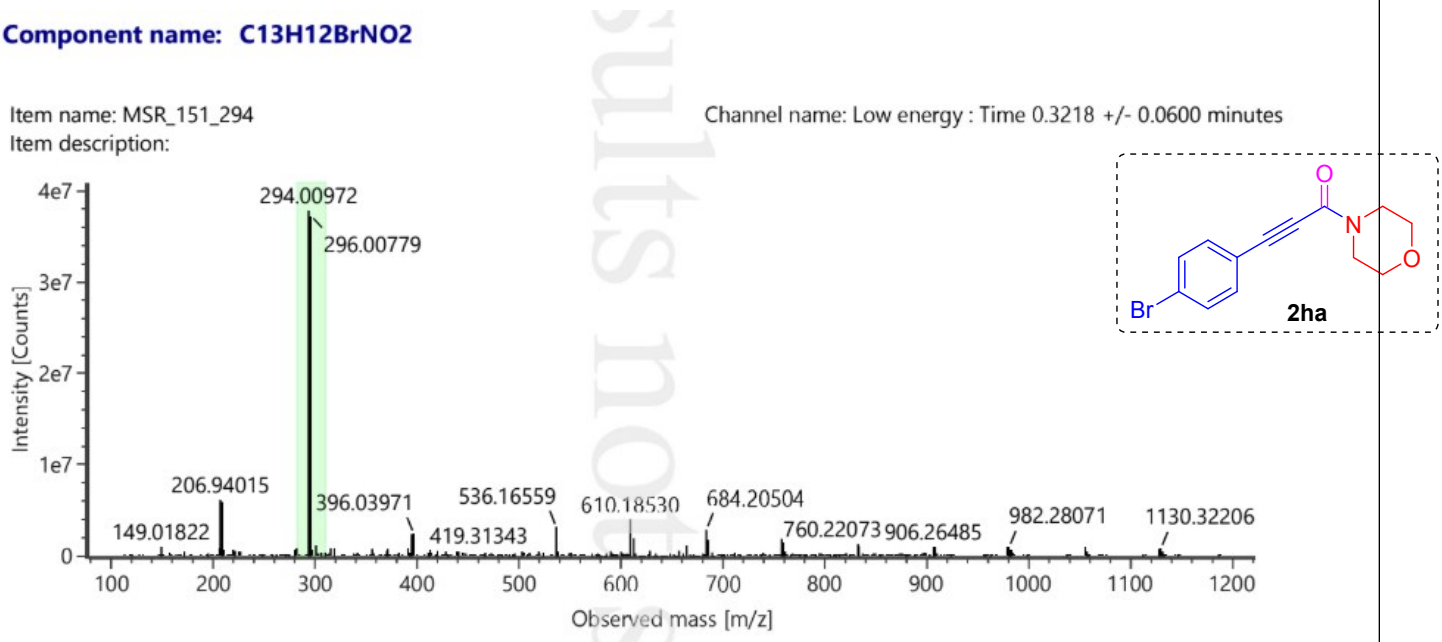
======== CHANNEL f1 ========
NUC1 13C
P1 10.68 usec
PL1 0.00 dB
PL1W 31.39858055 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 15.48 dB
PL13 16.00 dB
PL2W 13.28156662 W
PL12W 0.29870972 W
PL13W 0.26500207 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

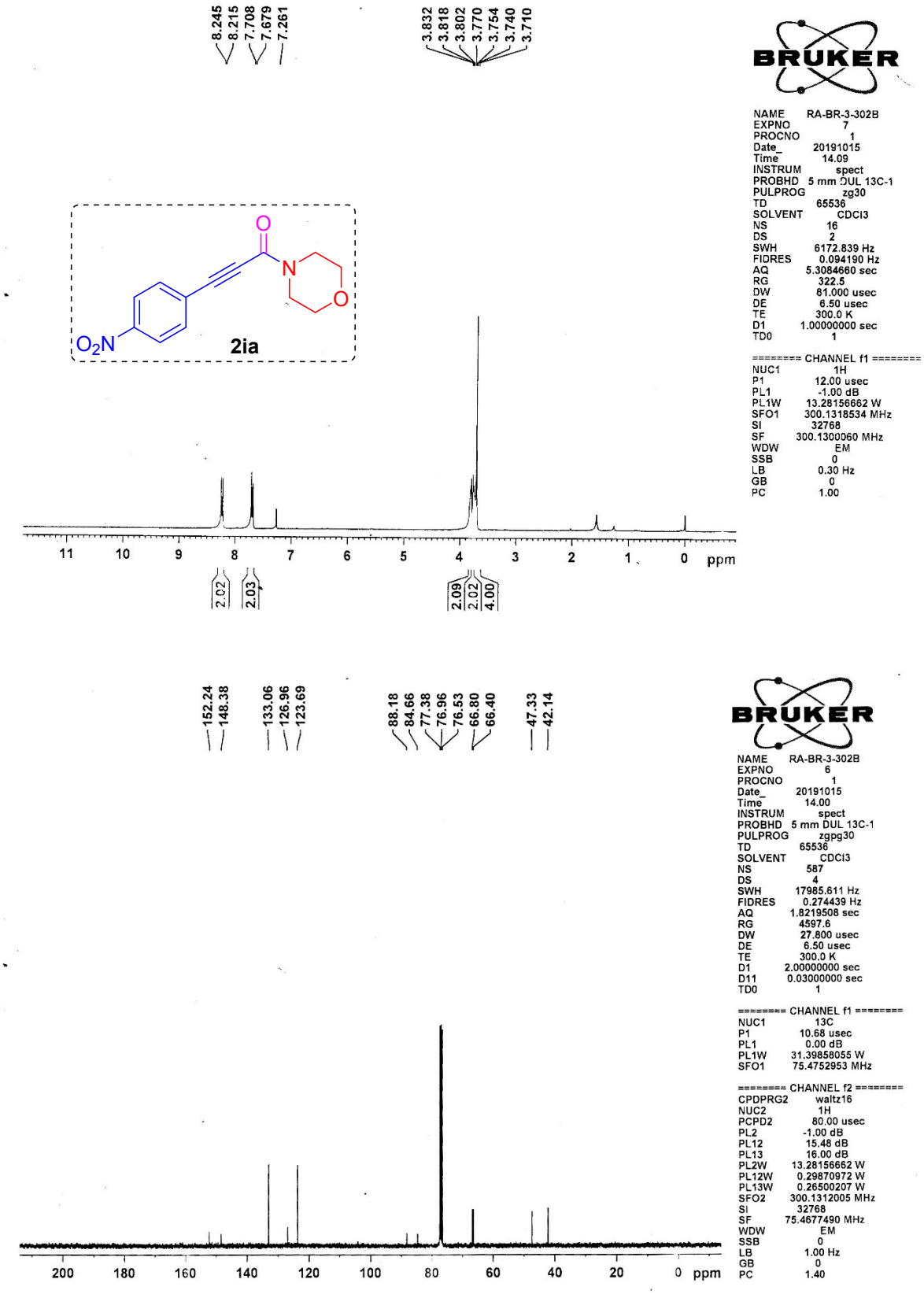
^{1}H&^{13}C spectra of compound 2ga



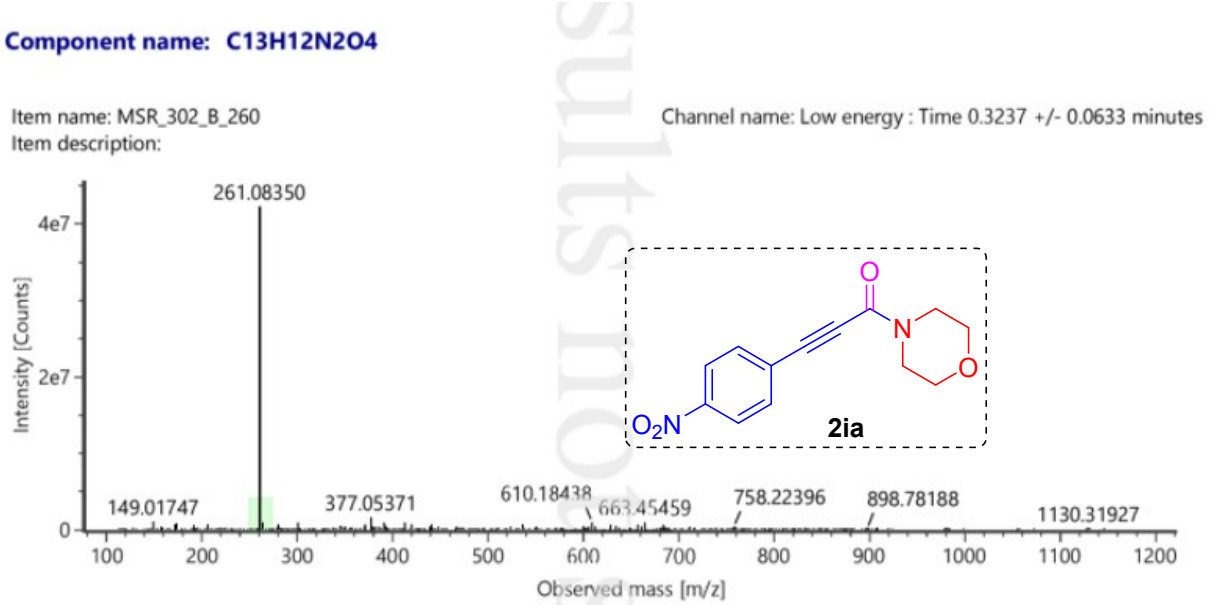
^{1}H&^{13}C spectra of compound 2ha



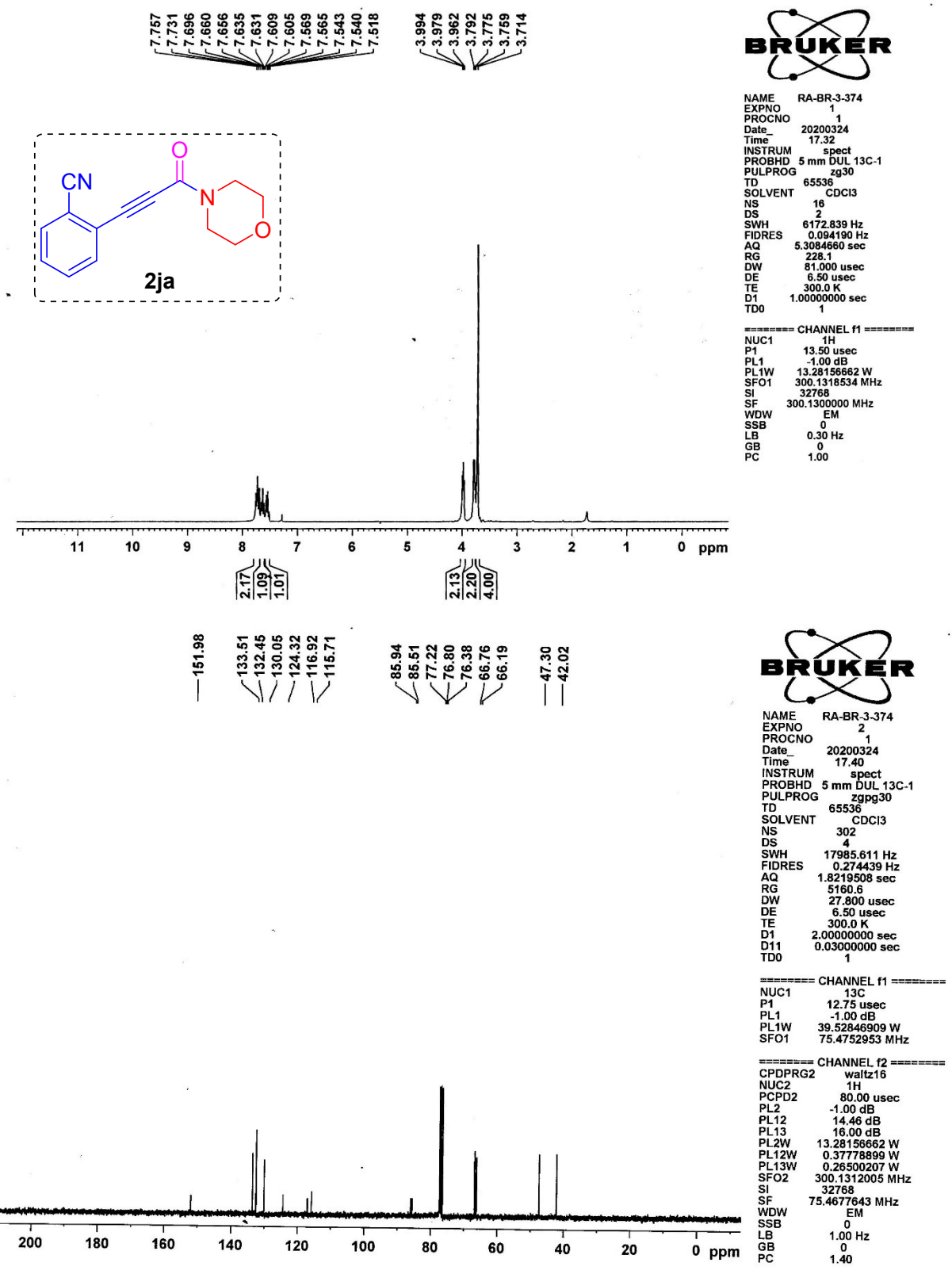
HRMS Spectrum of Compound 2ha



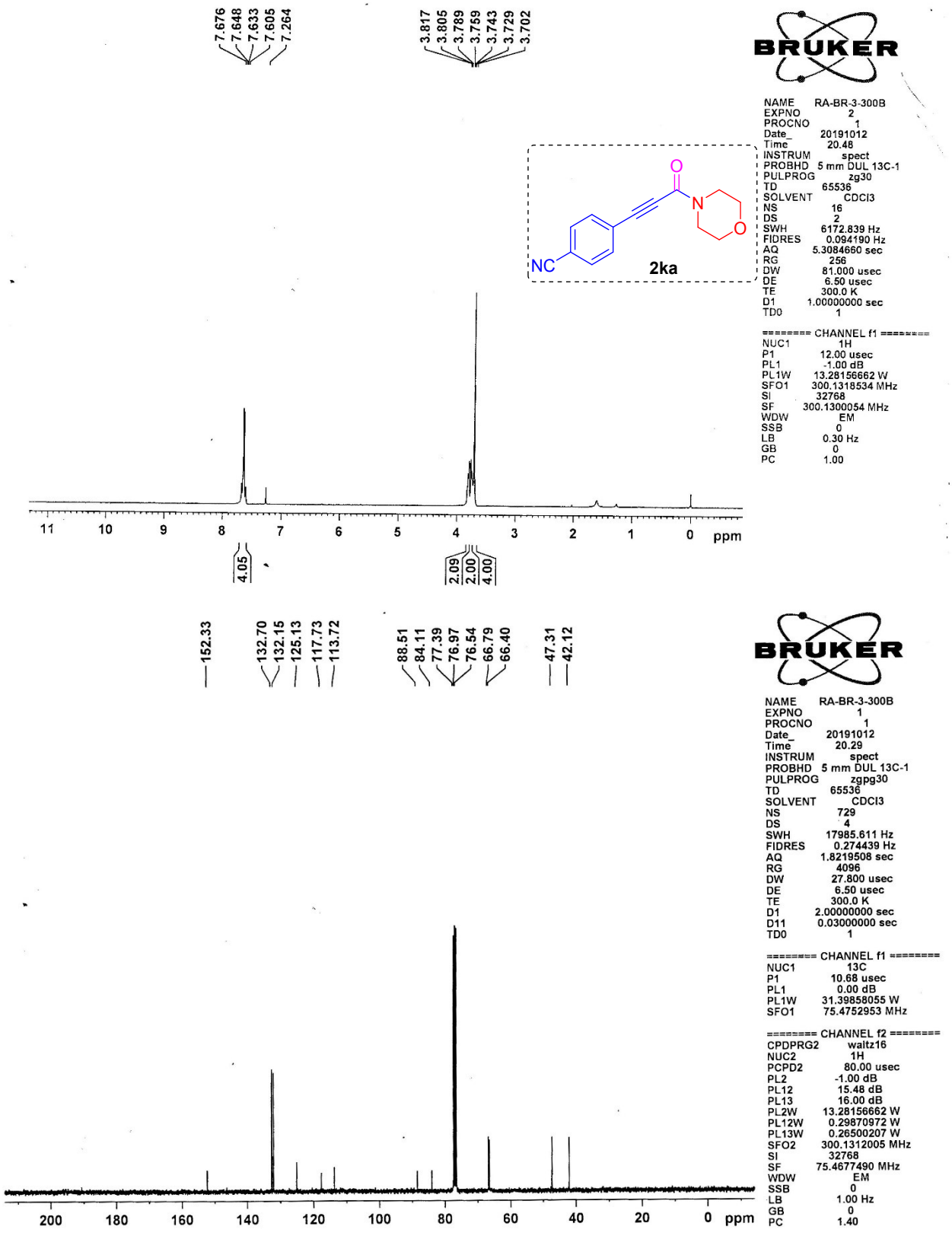
^{1}H&^{13}C spectra of compound 2ia



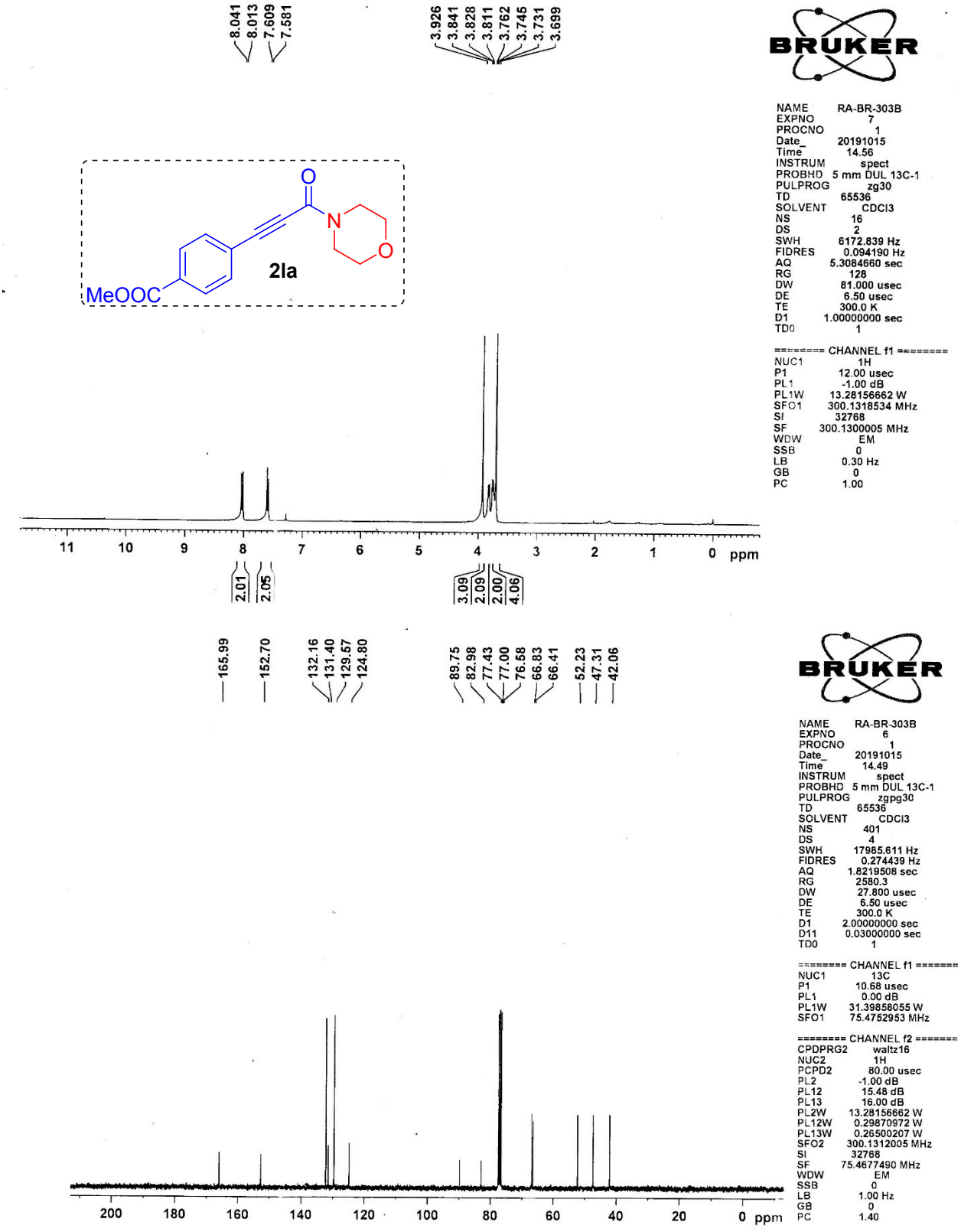
HRMS spectrum of compound 2ia



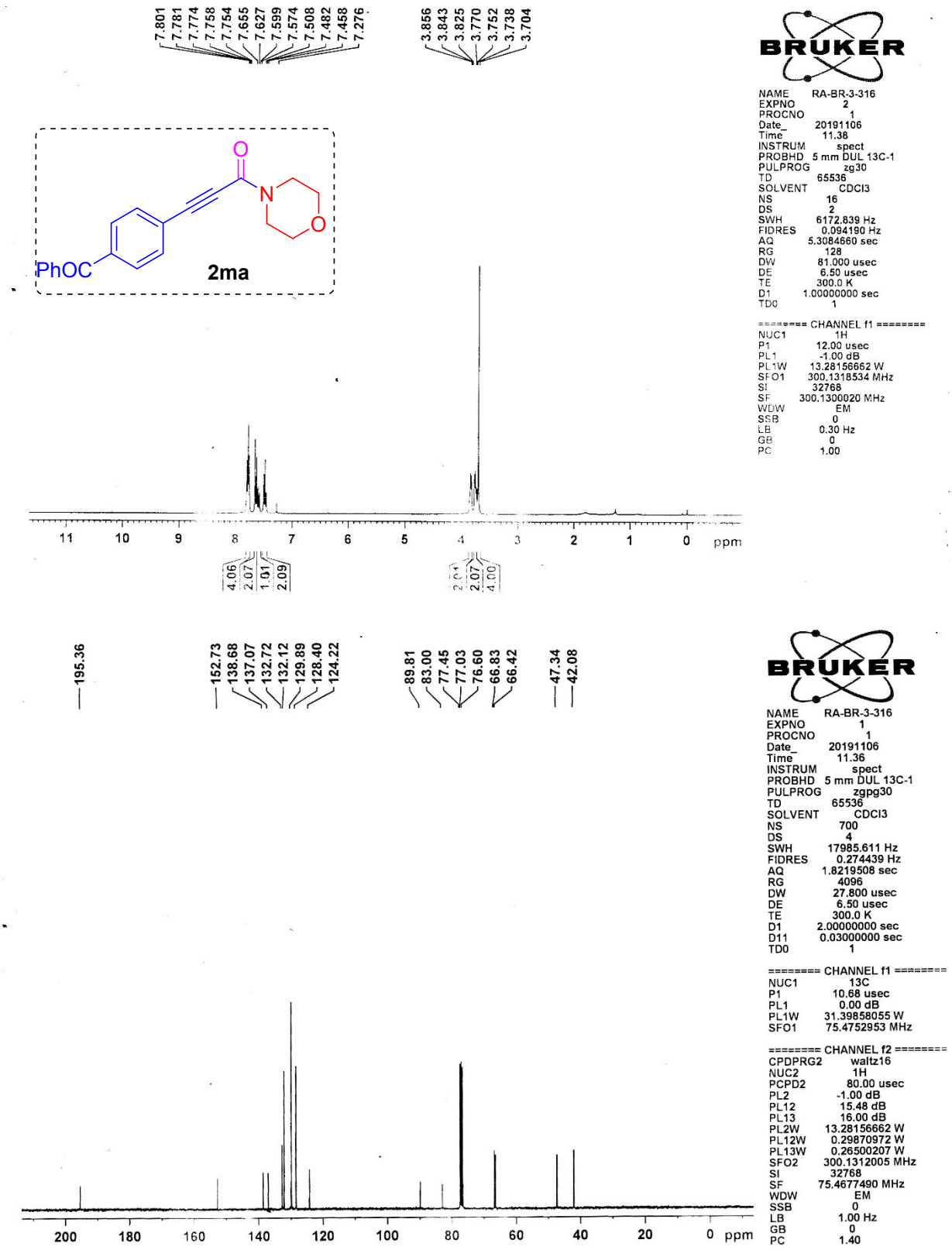
^{1}H&^{13}C spectra of compound 2ja



^{1}H&^{13}C spectra of compound 2ka



^{1}H &^{13}C spectra of compound 2la



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SOLVENT CDCl3
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FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 128
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -1.00 dB
PL1W 13.28156662 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300020 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

BRUKER

NAME RA-BR-3-316
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PROCNO 1
Date_ 20191106
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SOLVENT CDCl3
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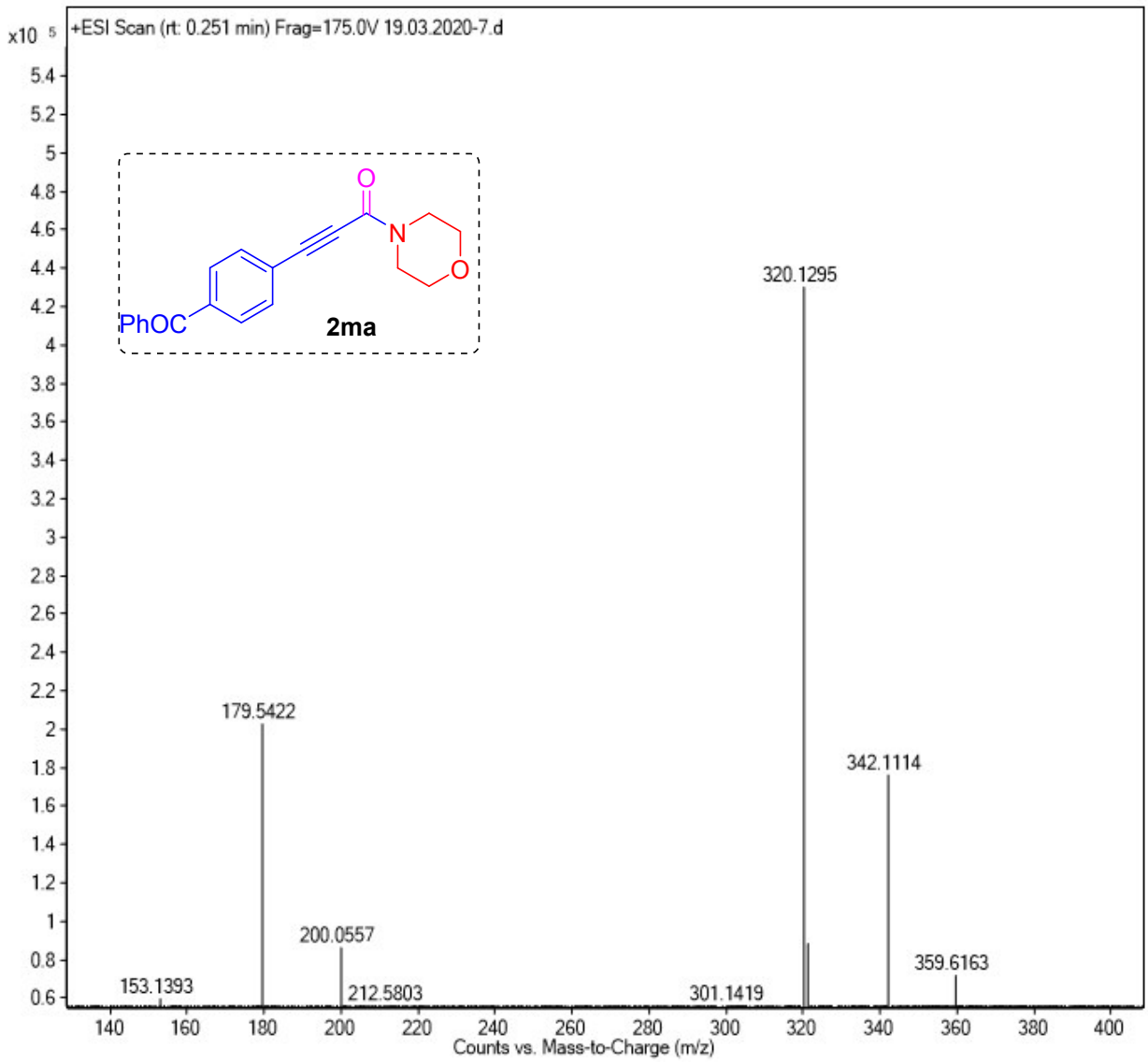
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4096
DW 27.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

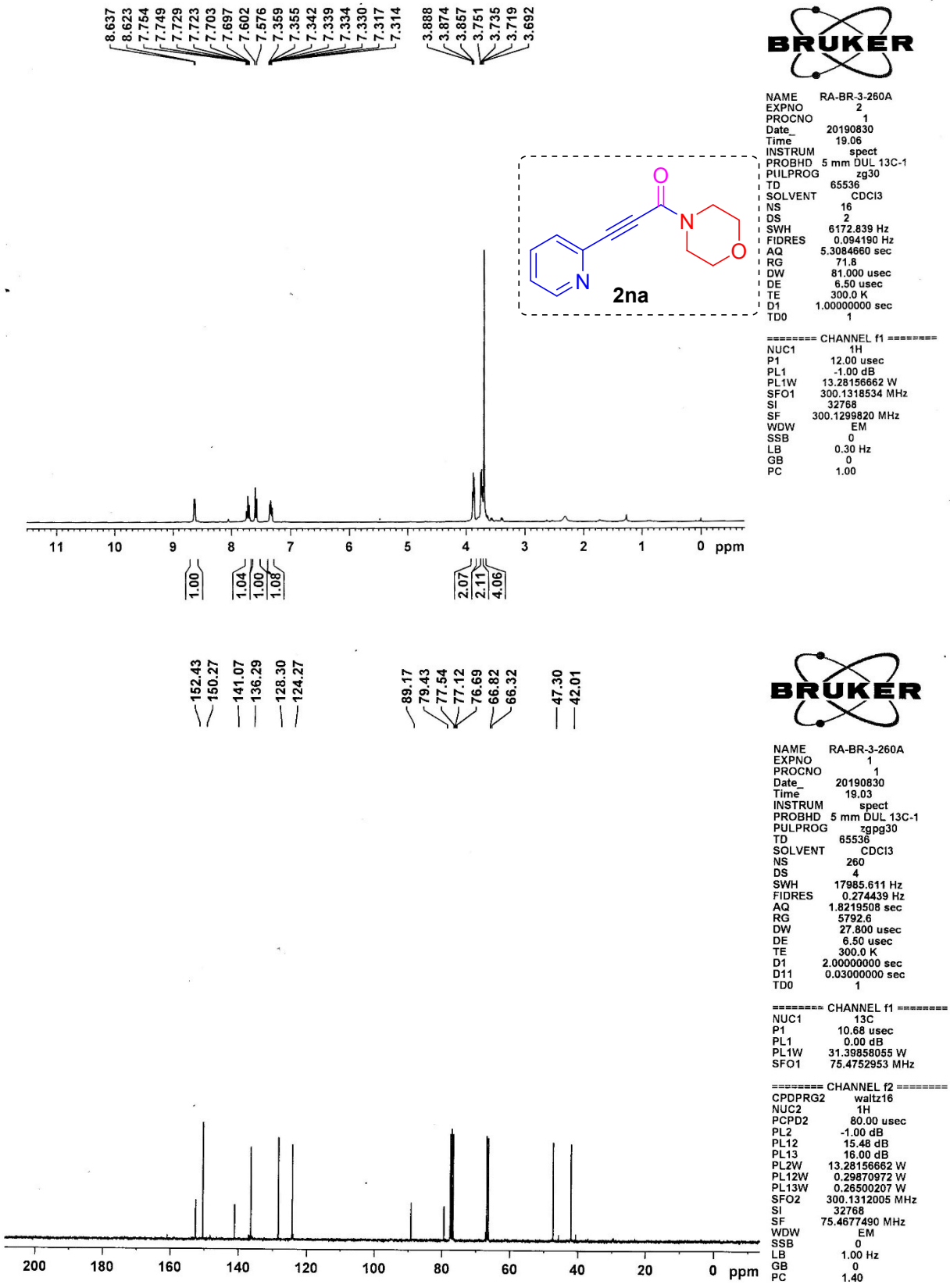
======== CHANNEL f1 ========
NUC1 13C
P1 10.68 usec
PL1 0.00 dB
PL1W 31.39858055 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 15.48 dB
PL13 16.00 dB
PL2W 13.28156662 W
PL12W 0.29870972 W
PL13W 0.26500207 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{1}H&^{13}C spectra of compound 2ma



HRMS spectrum of compound 2ma



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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 71.8
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -1.00 dB
PL1W 13.28156662 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1299820 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

BRUKER

NAME RA-BR-3-260A
EXPNO 1
PROCNO 1
Date_ 20190830
Time 19.03
INSTRUM spect
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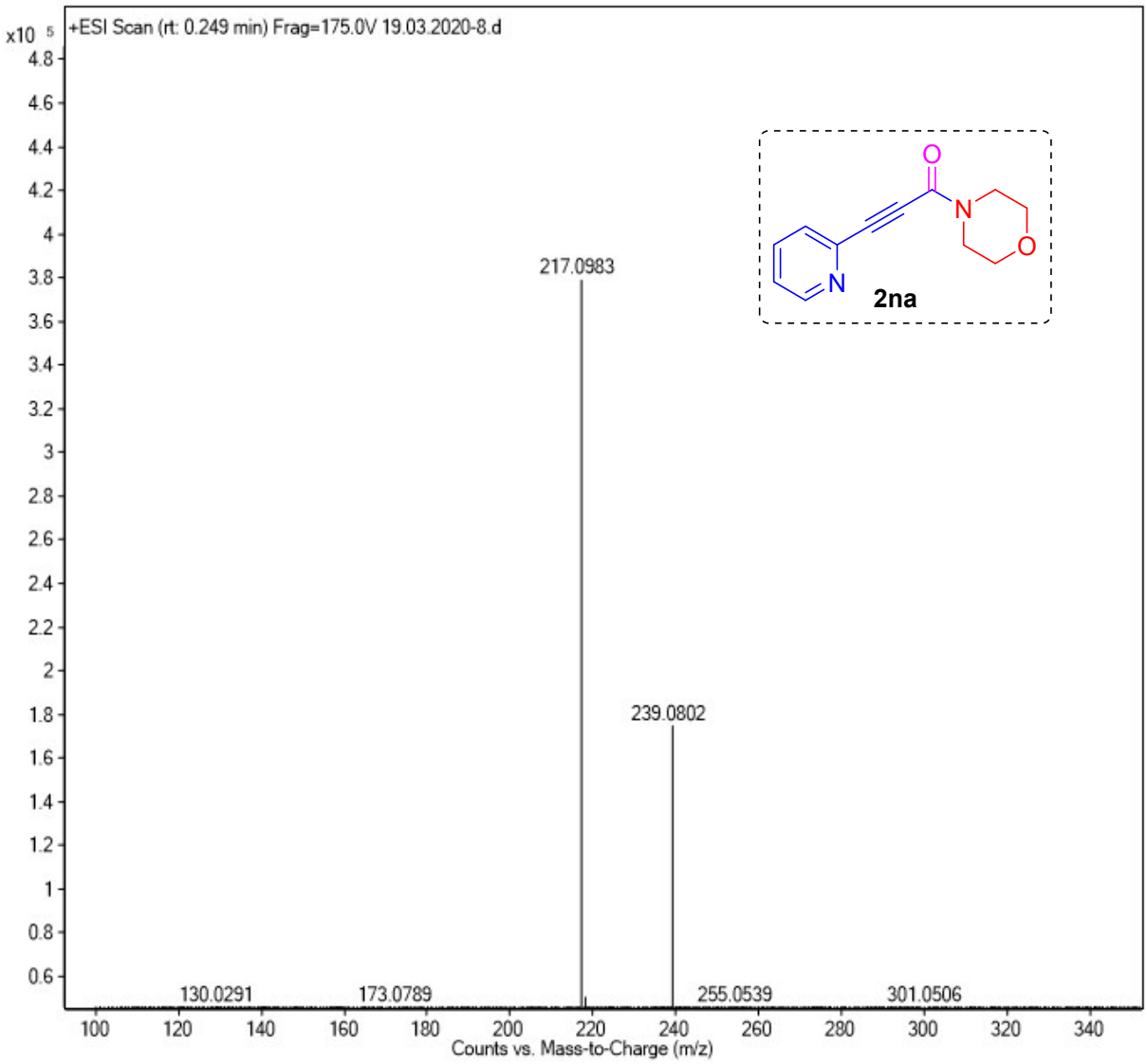
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 260
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 5792.6
DW 27.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

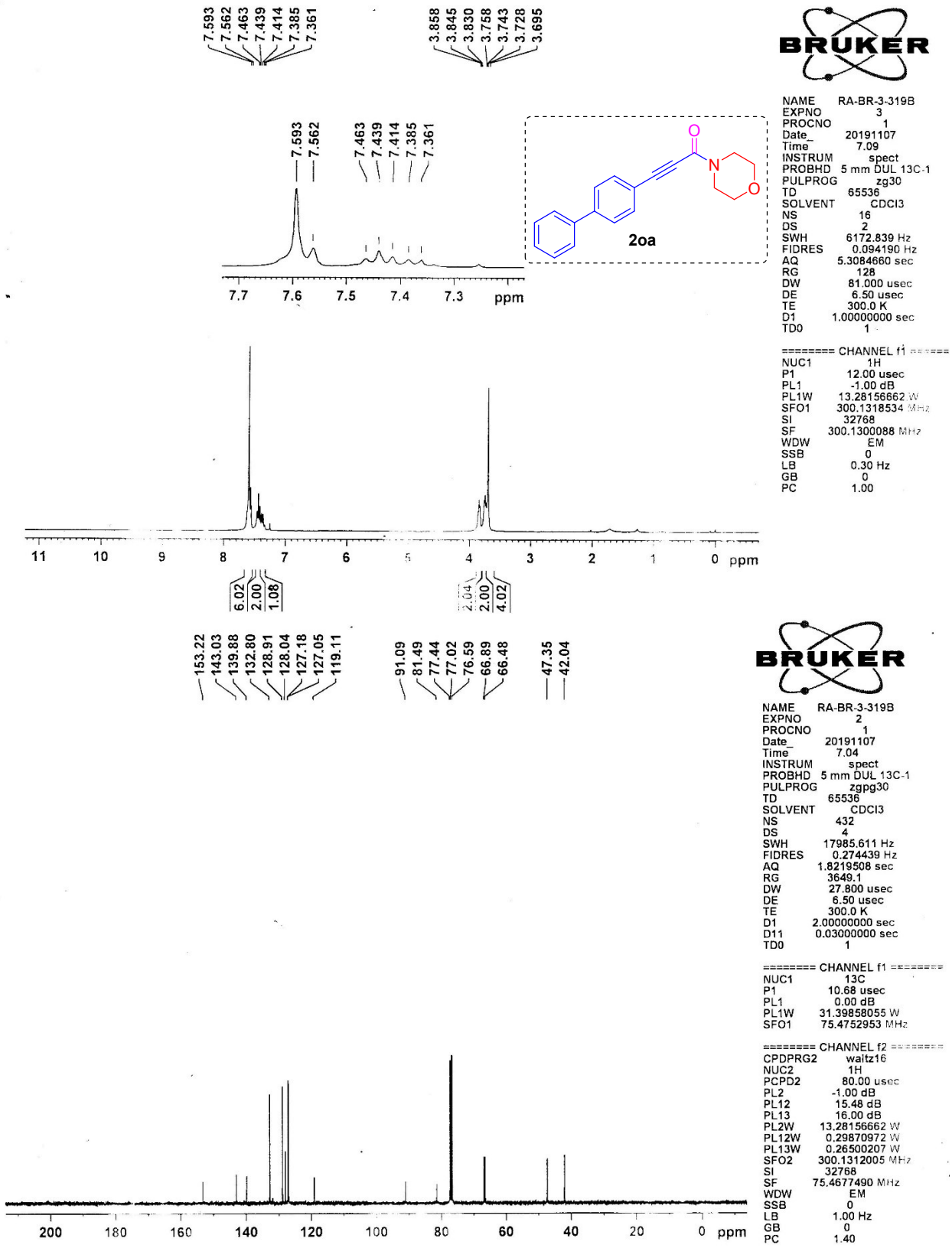
======== CHANNEL f1 ========
NUC1 13C
P1 10.68 usec
PL1 0.00 dB
PL1W 31.39858055 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 15.48 dB
PL13 16.00 dB
PL2W 13.28156662 W
PL12W 0.29870972 W
PL13W 0.26500207 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

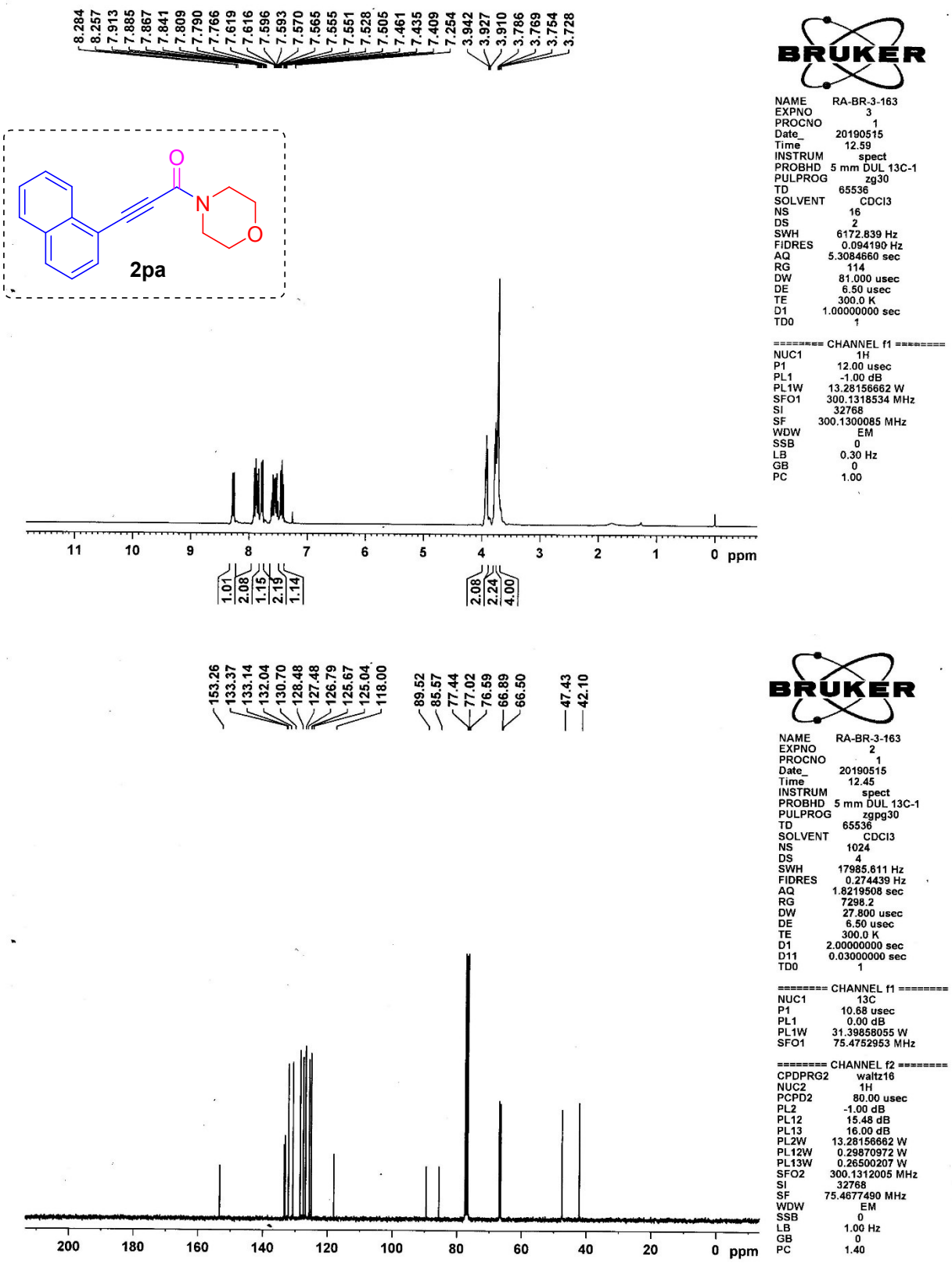
^{1}H&^{13}C spectra of compound 2na



HRMS spectrum of compound 2na



^{1}H&^{13}C spectra of compound 2oa



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PULPROG zg30
TD 65536
SOLVENT CDCl3
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DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 114
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -1.00 dB
PL1W 13.28156662 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300085 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

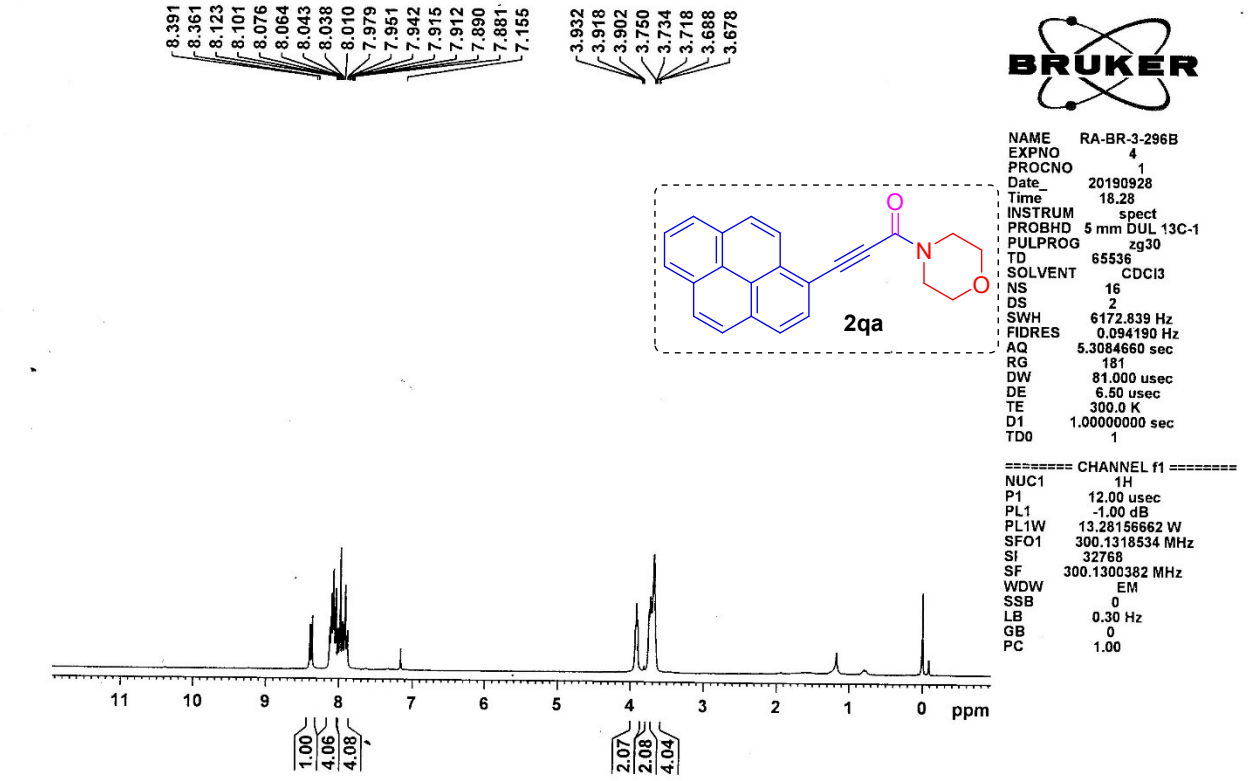
BRUKER

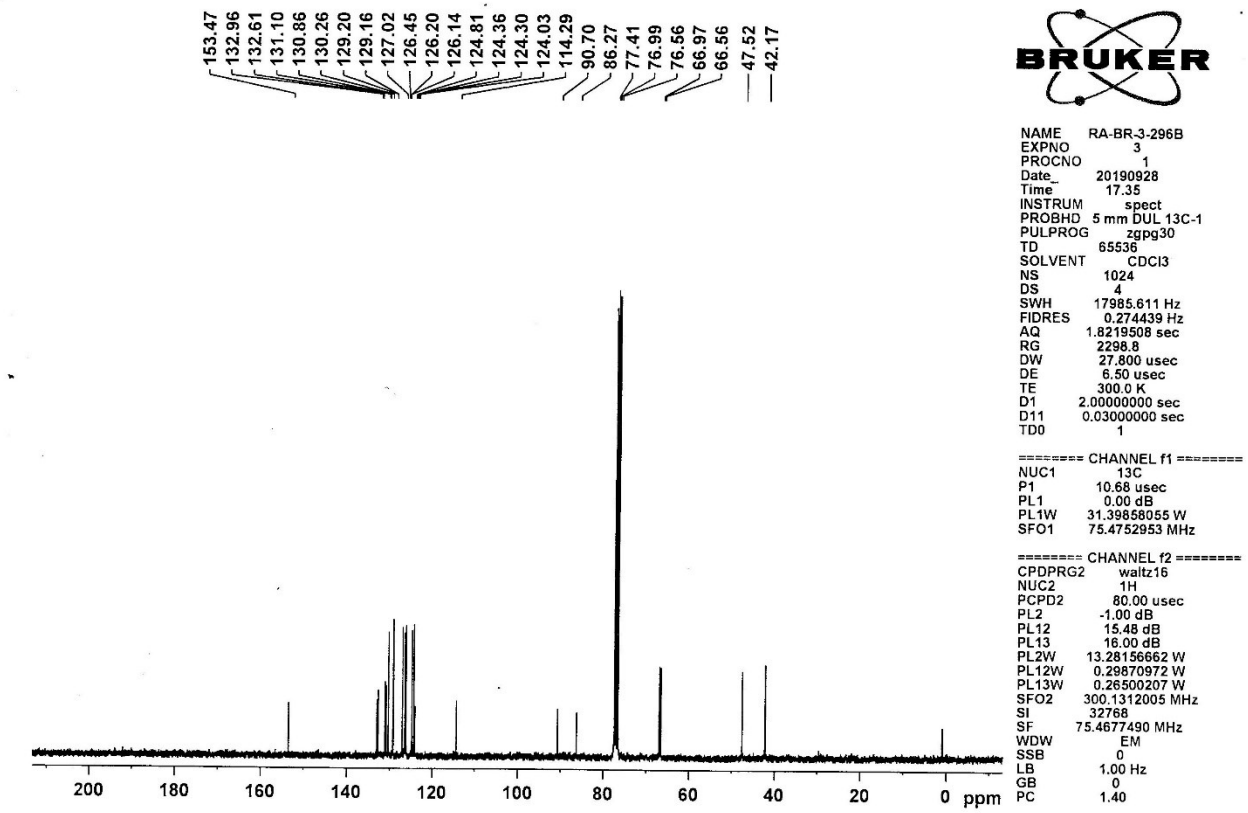
NAME RA-BR-3-163
EXPNO 2
PROCNO 1
Date_ 20190515
Time 12.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 7298.2
DW 27.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.68 usec
PL1 0.00 dB
PL1W 31.39858055 W
SFO1 75.4752953 MHz

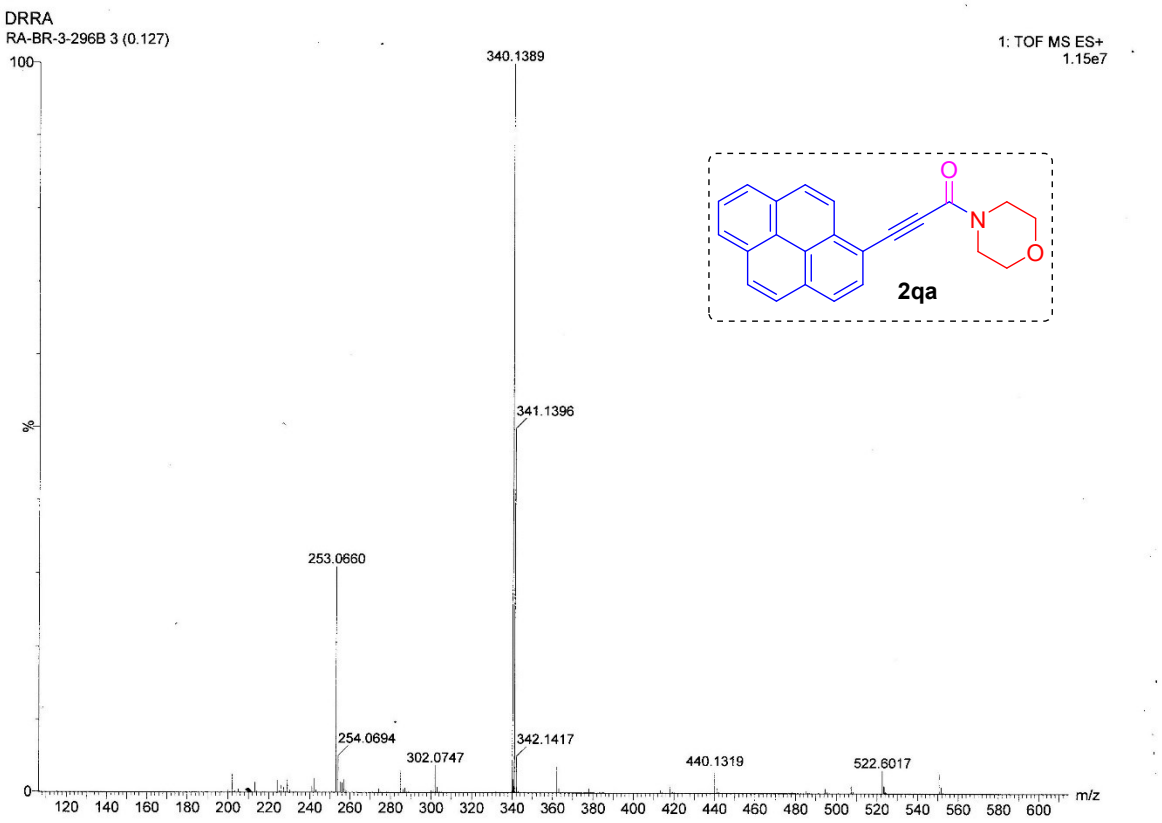
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 15.48 dB
PL13 16.00 dB
PL2W 13.28156662 W
PL12W 0.29870972 W
PL13W 0.26500207 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{1}H&^{13}C spectra of compound 2pa

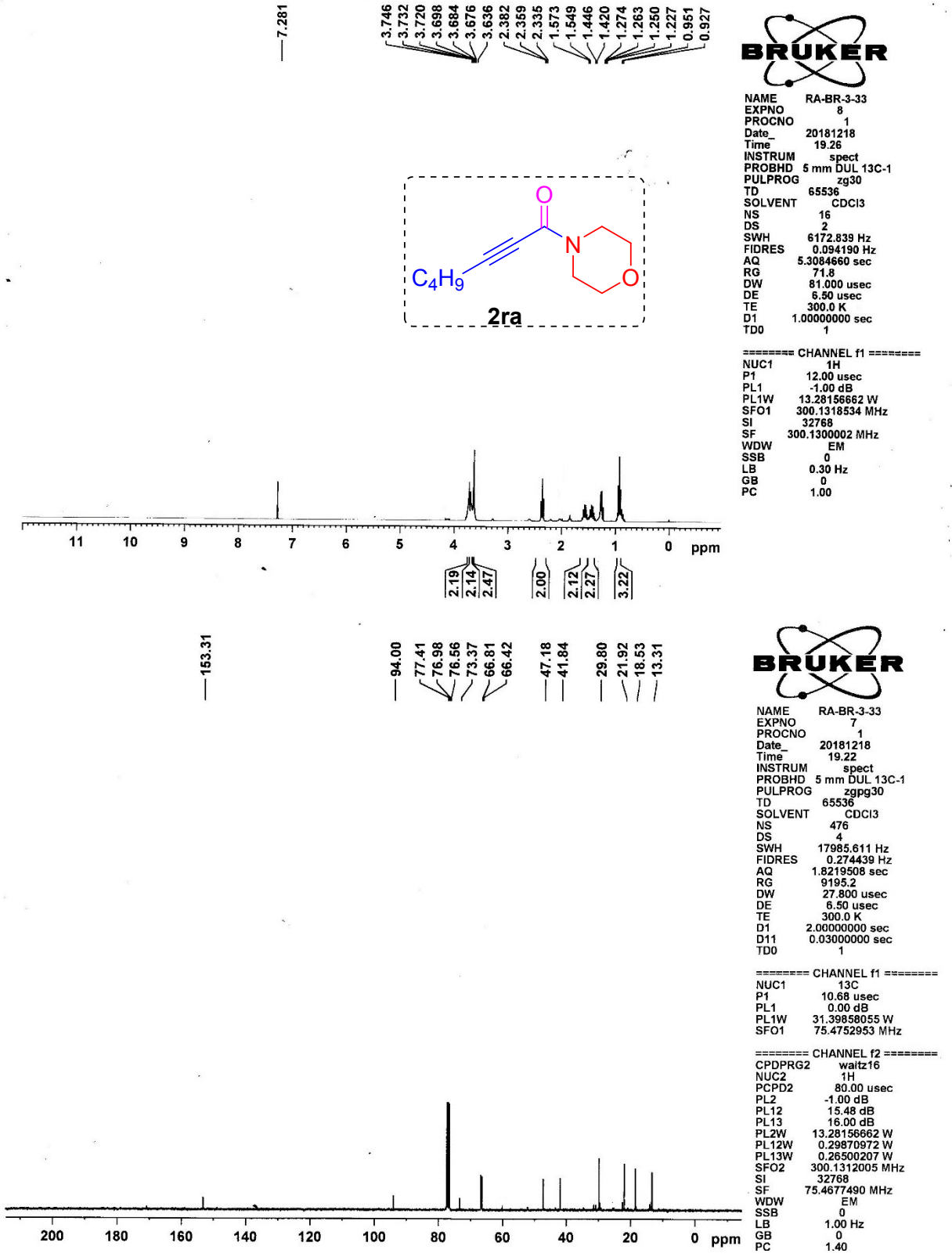




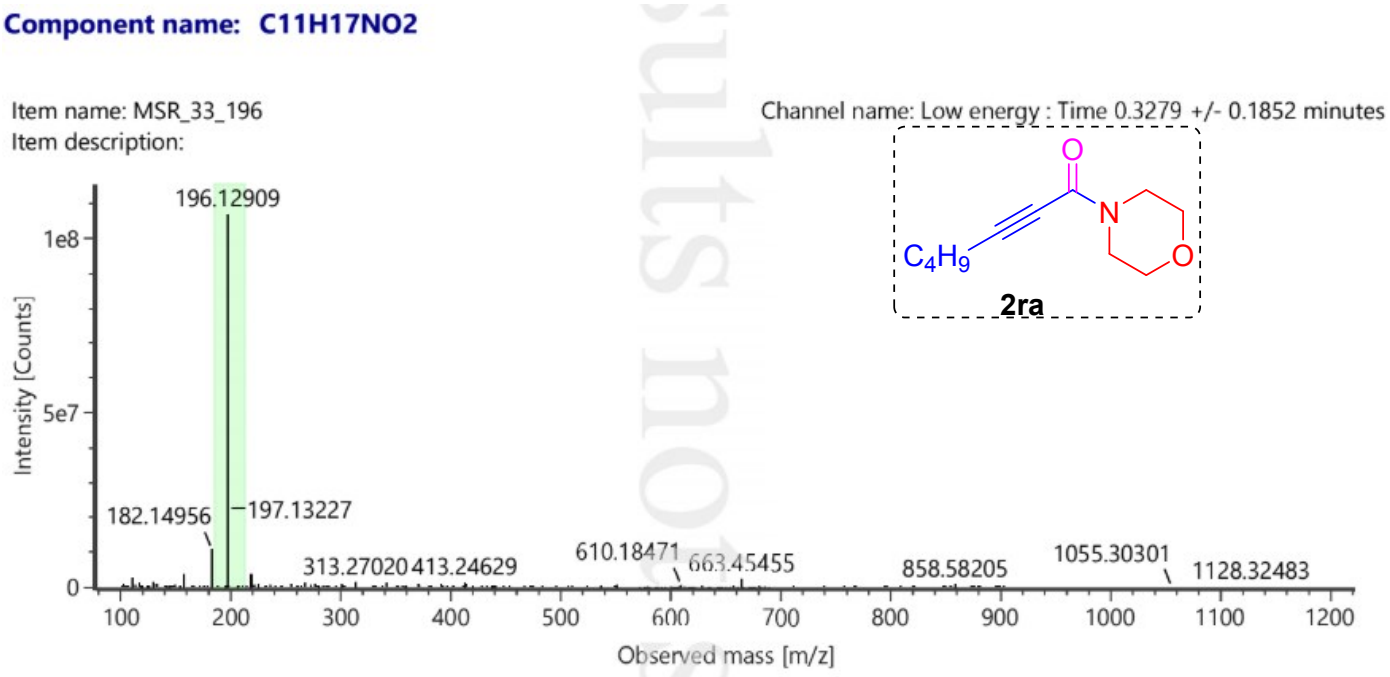
^{1}H&^{13}C spectra of compound 2qa



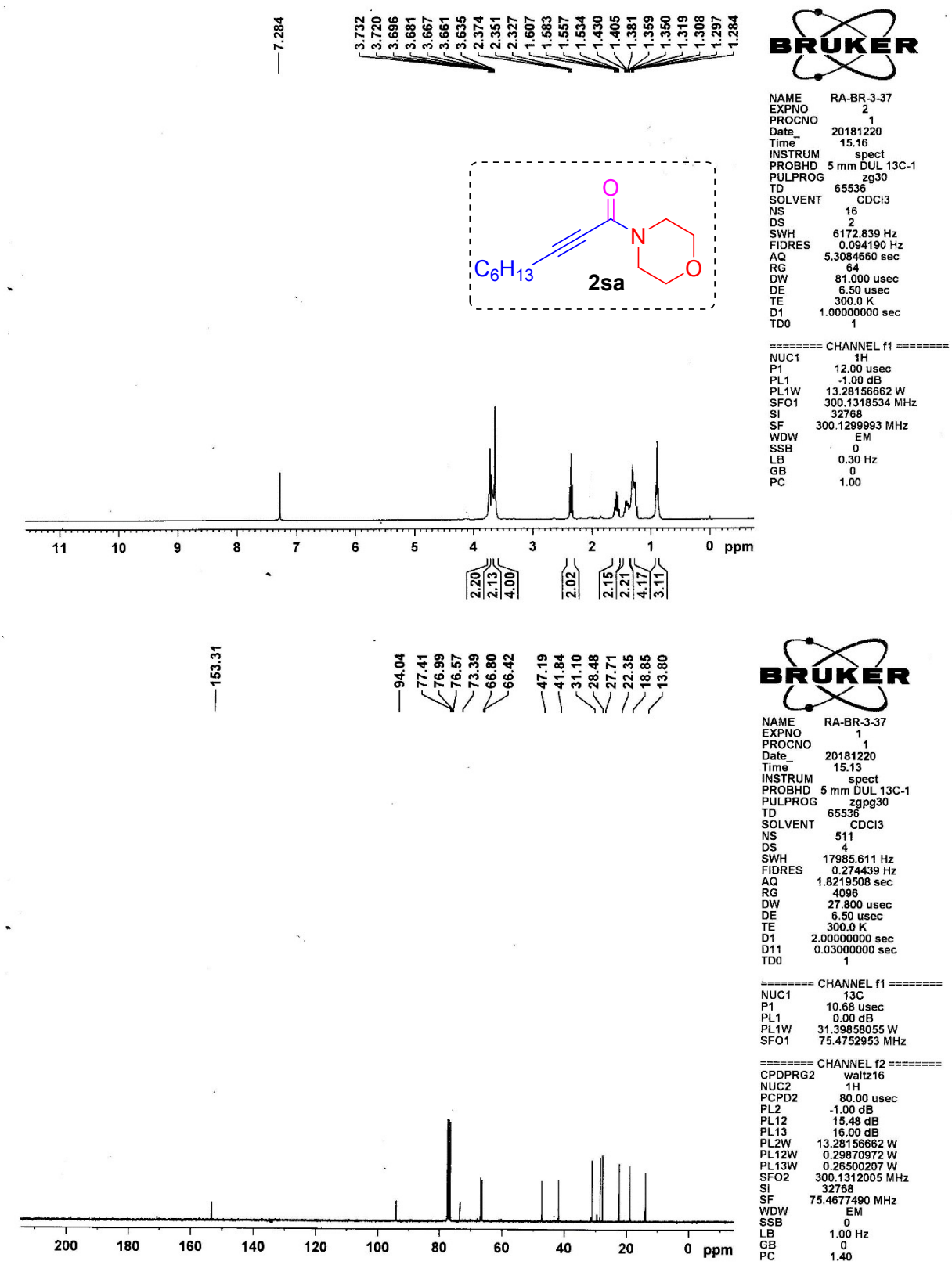
HRMS spectrum of compound 2qa



^{1}H&^{13}C spectra of compound 2ra



HRMS Spectrum of Copmpound 2ra



BRUKER

NAME RA-BR-3-37
EXPNO 2
PROCNO 1
Date_ 20181220
Time 15.16
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 64
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -1.00 dB
PL1W 13.28156662 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1299993 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

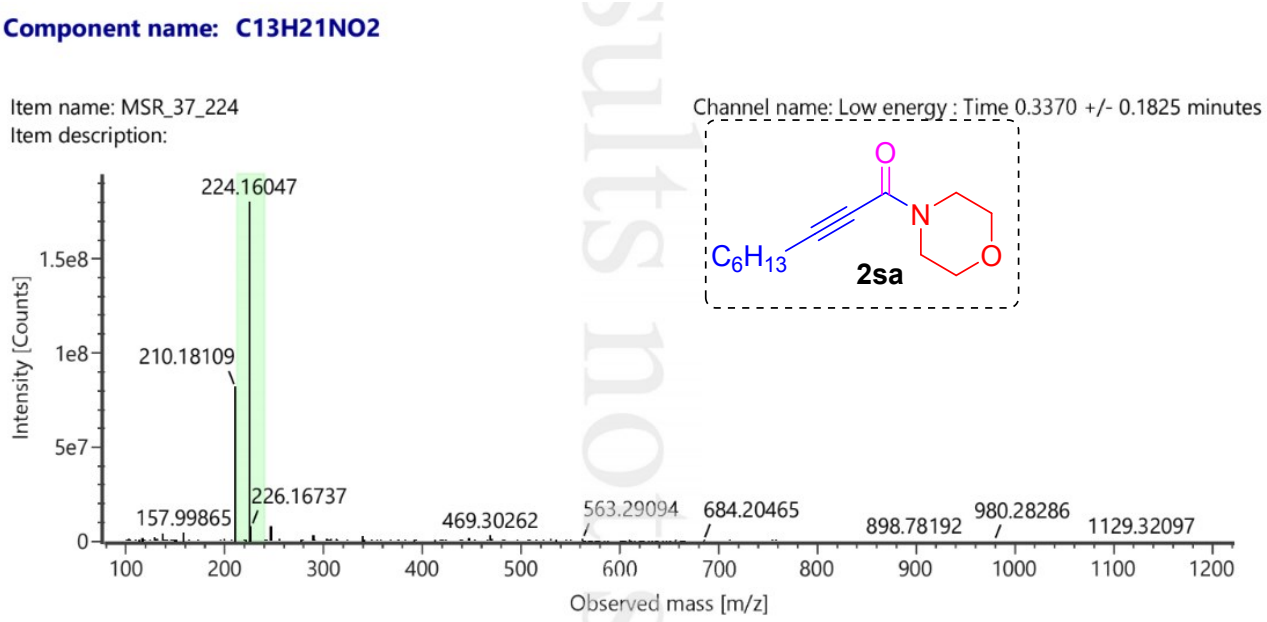
BRUKER

NAME RA-BR-3-37
EXPNO 1
PROCNO 1
Date_ 20181220
Time 15.13
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 511
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4096
DW 27.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

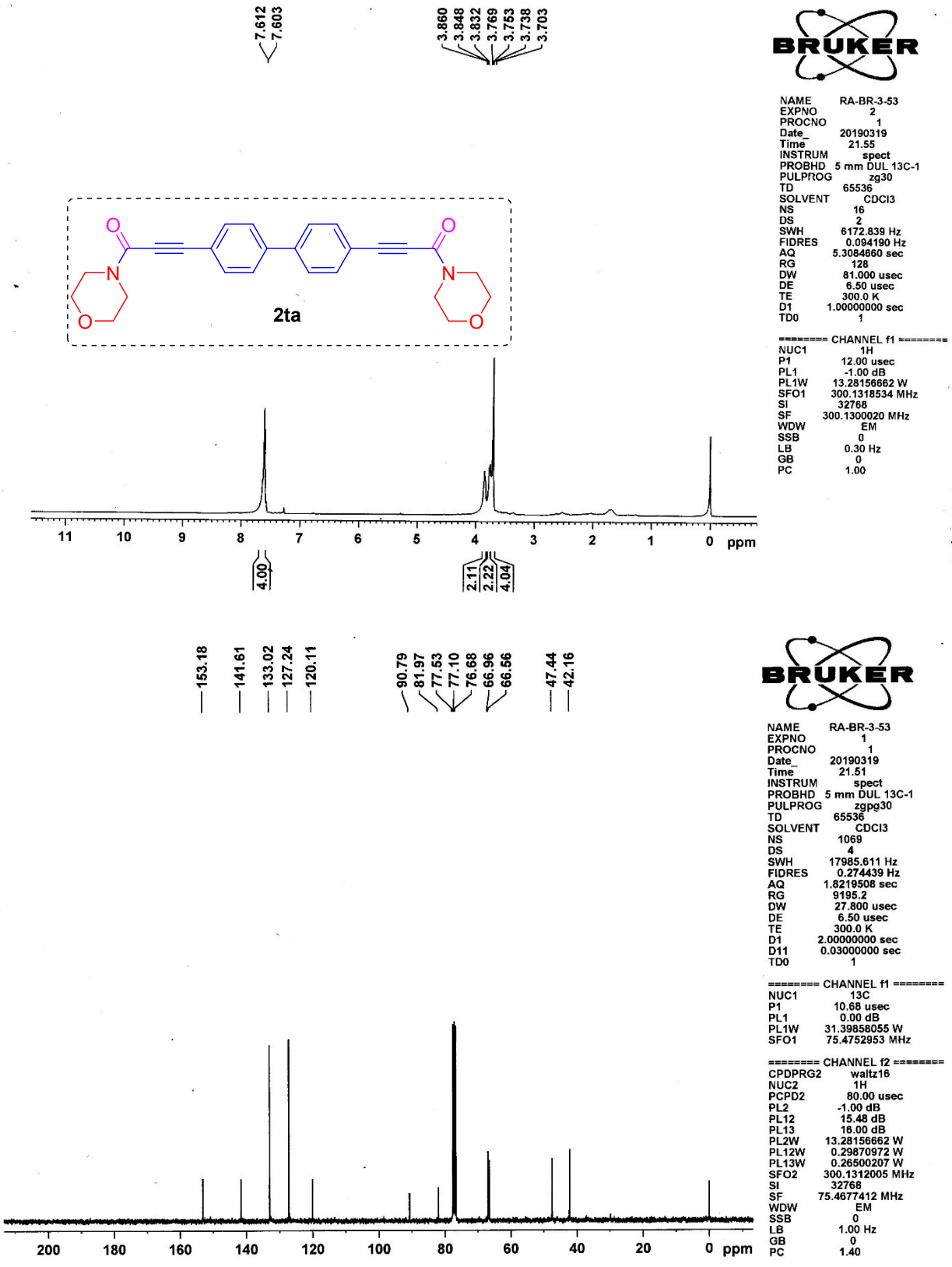
======== CHANNEL f1 ========
NUC1 13C
P1 10.68 usec
PL1 0.00 dB
PL1W 31.39858055 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 15.48 dB
PL13 16.00 dB
PL2W 13.28156662 W
PL12W 0.29870972 W
PL13W 0.26500207 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{1}H&^{13}C spectra of compound 2sa



HRMS Spectrum of Compound 2sa



BRUKER

NAME RA-BR-3-53
EXPNO 2
PROCNO 1
Date_ 20190319
Time 21.55
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 128
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -1.00 dB
PL1W 13.28156662 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300020 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

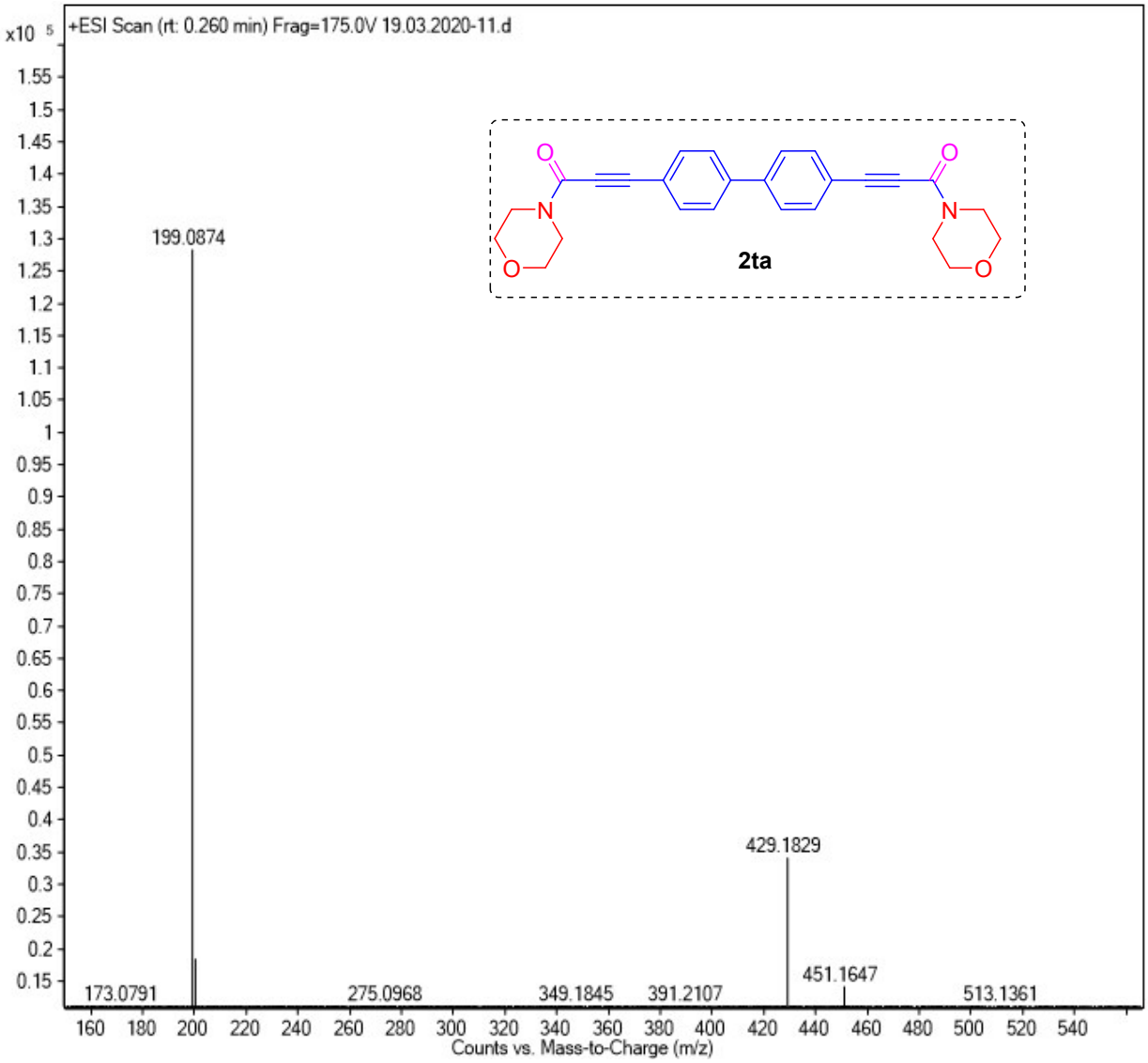
BRUKER

NAME RA-BR-3-53
EXPNO 1
PROCNO 1
Date_ 20190319
Time 21.51
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1069
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 9195.2
DW 27.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

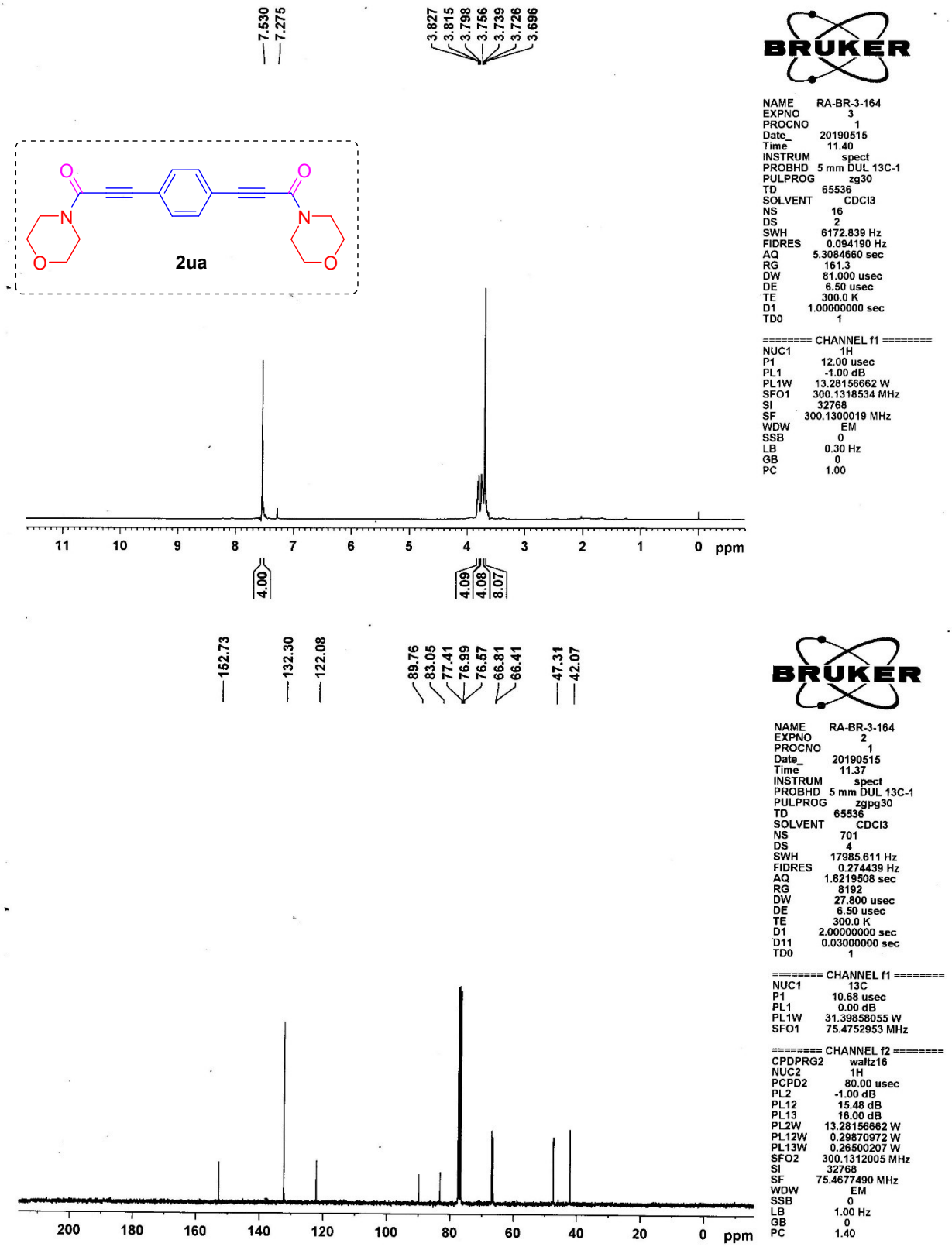
======== CHANNEL f1 ========
NUC1 13C
P1 10.68 usec
PL1 0.00 dB
PL1W 31.39858055 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 15.48 dB
PL13 16.00 dB
PL2W 13.28156662 W
PL12W 0.29870972 W
PL13W 0.26500207 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677412 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

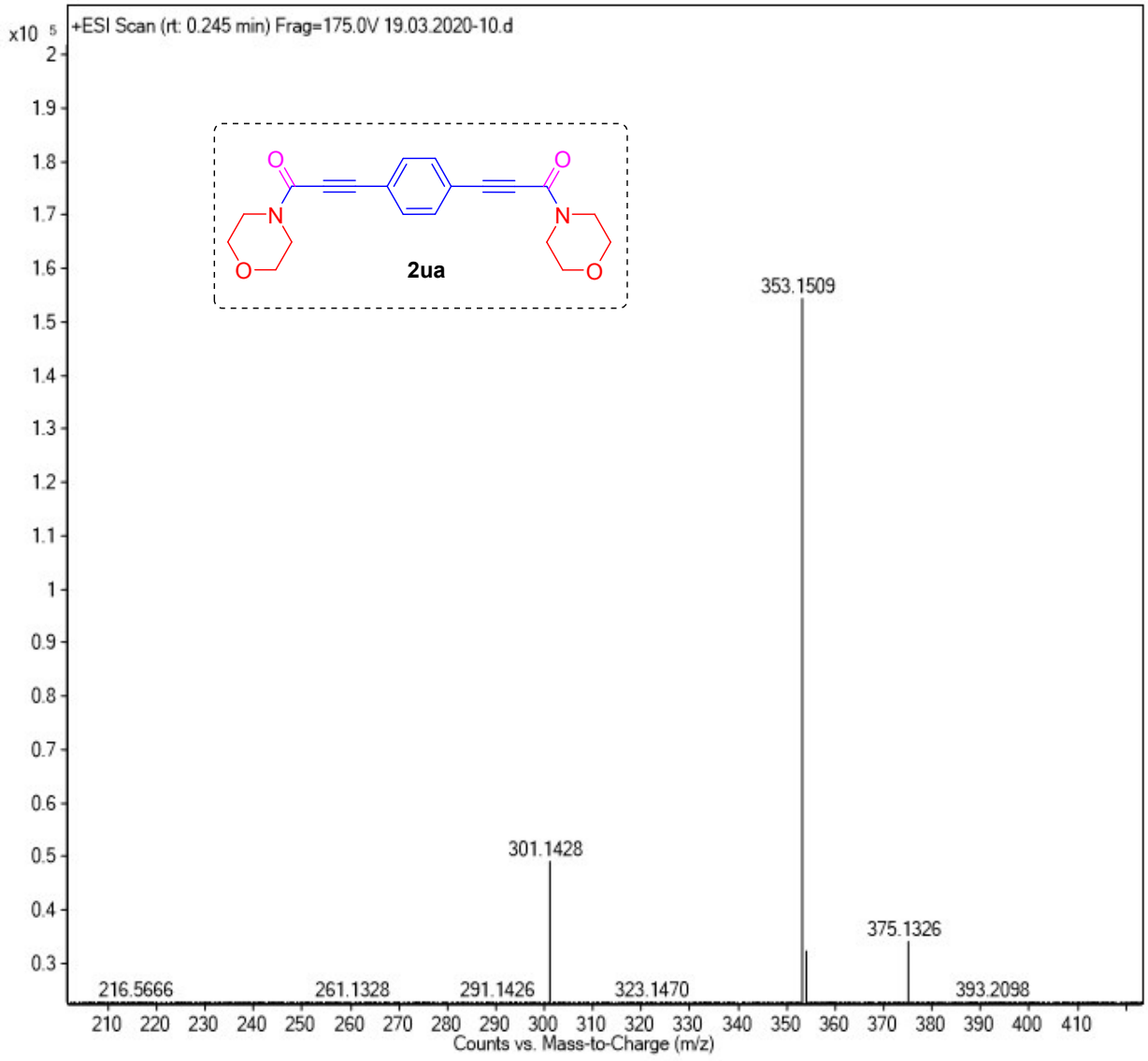
^{1}H & ^{13}C spectra of compound 2ta



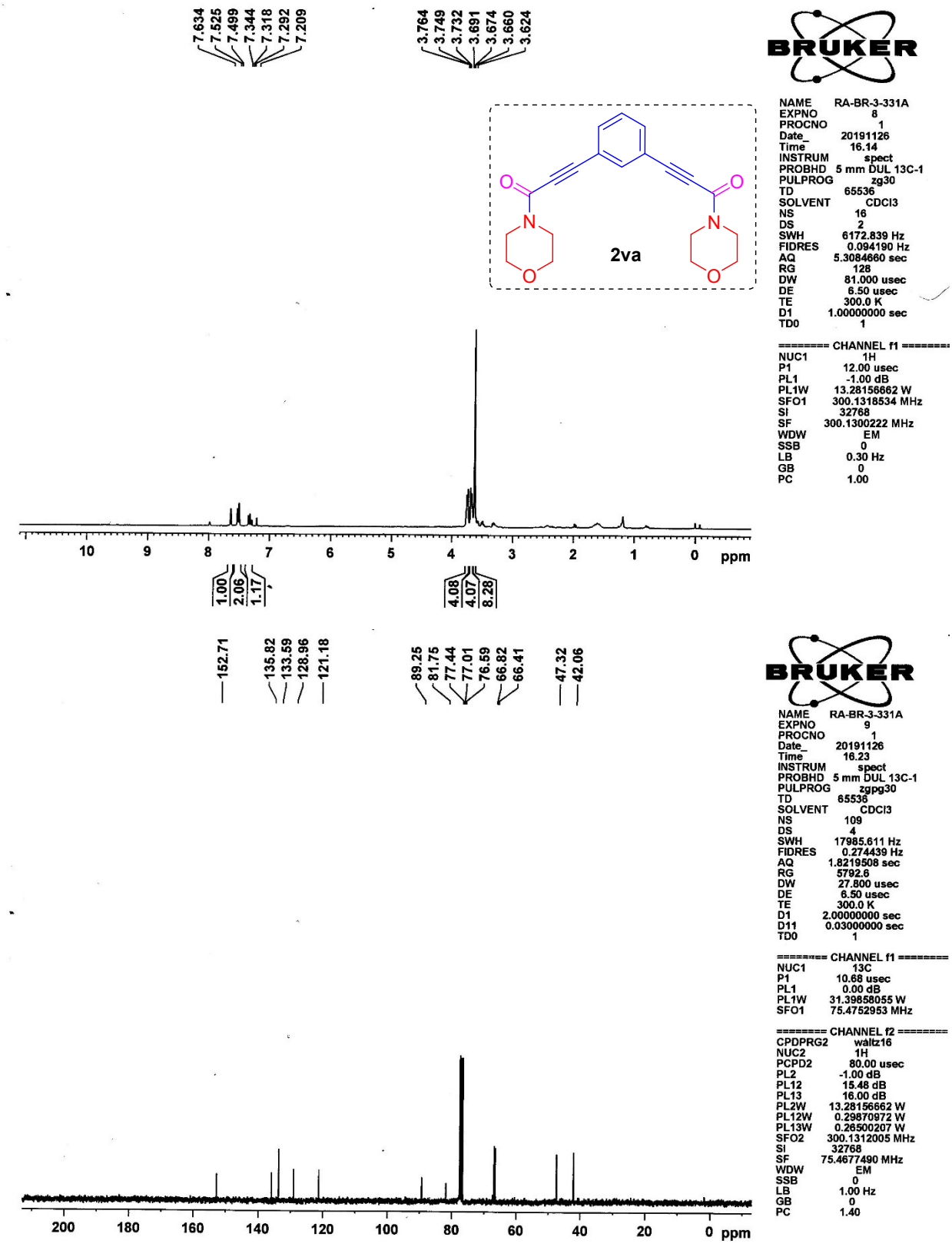
HRMS spectrum of compound 2ua



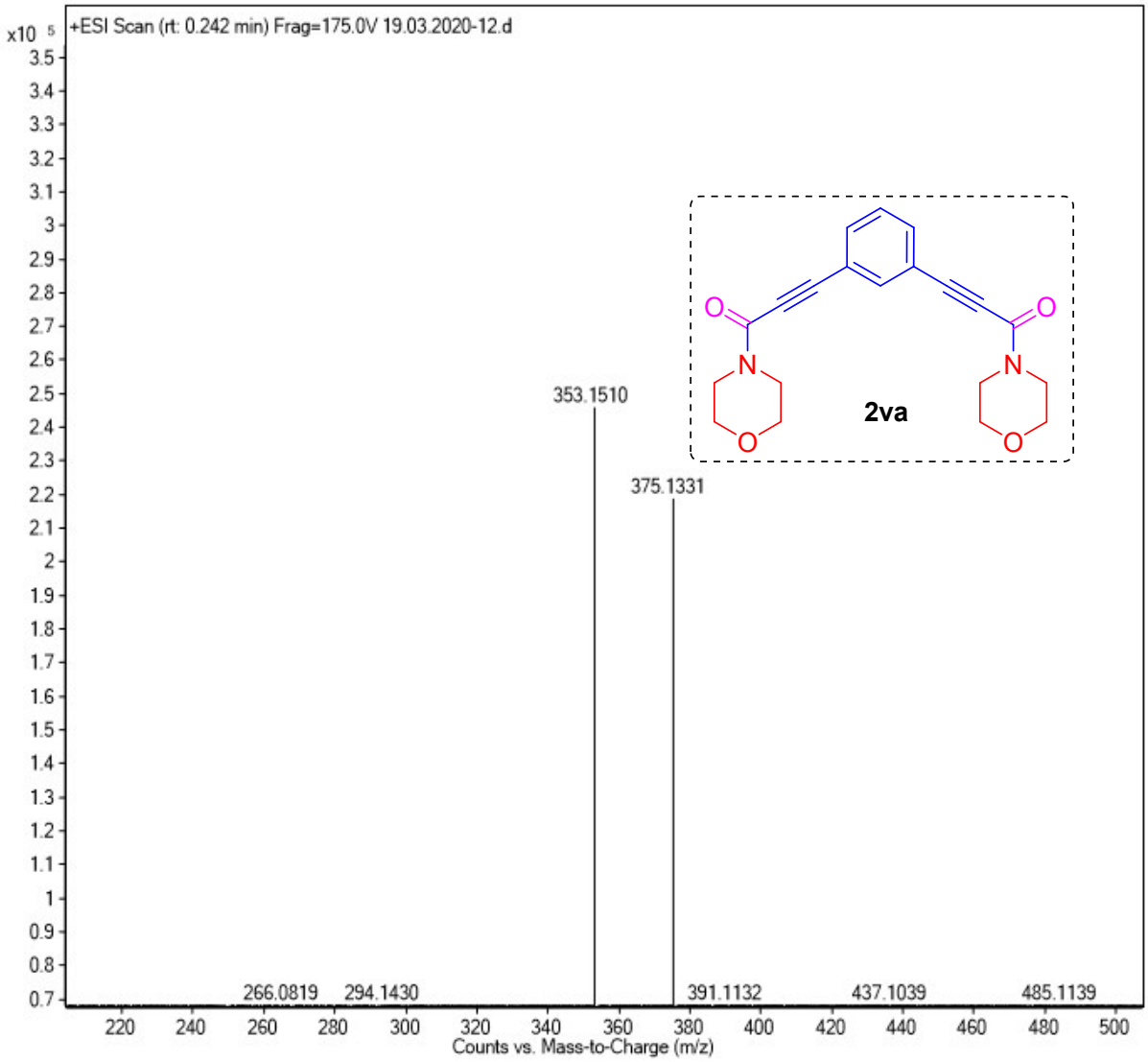
^{1}H & ^{13}C spectra of compound 2ua



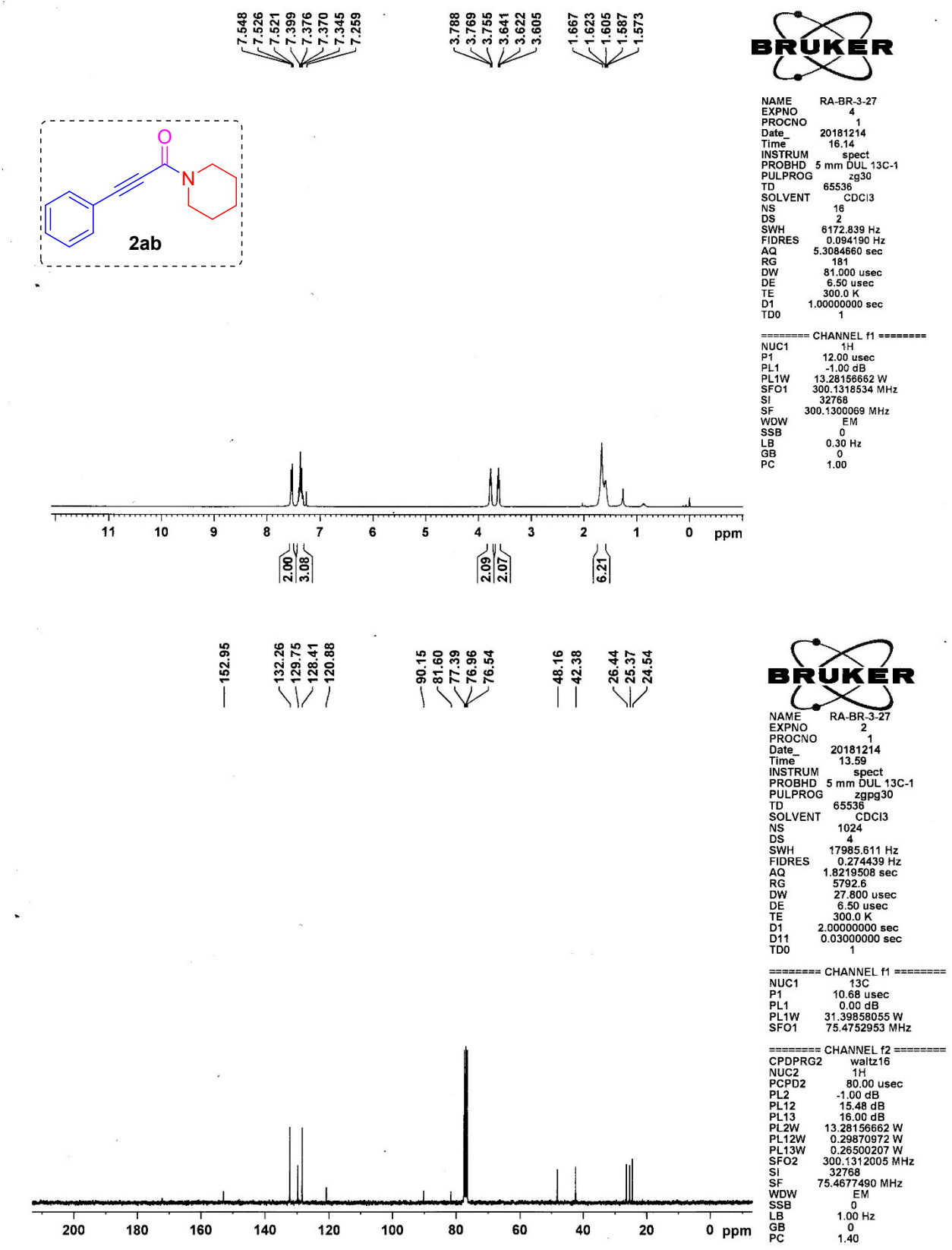
HRMS spectrum of compound 2ua



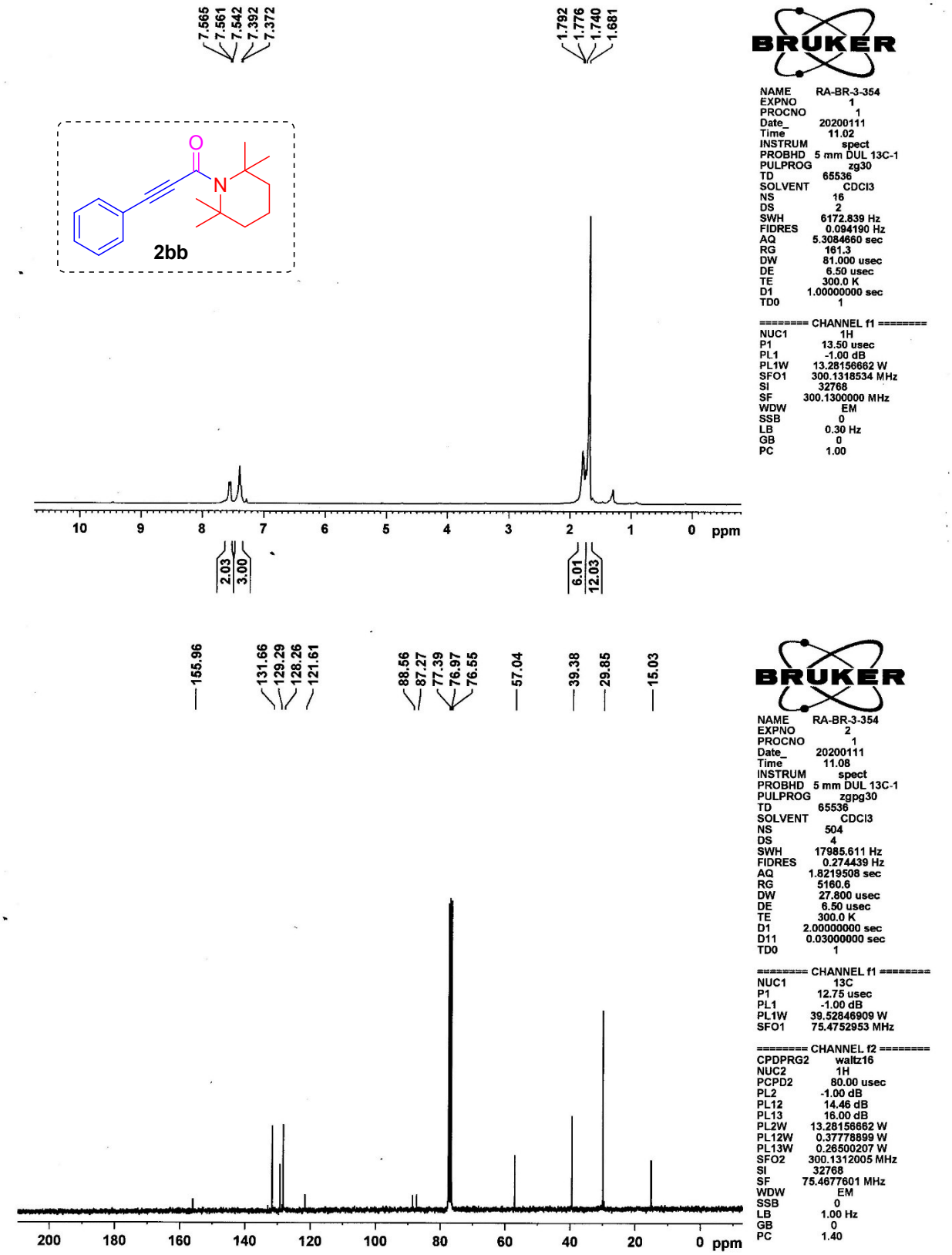
^{1}H & ^{13}C spectra of compound 2va



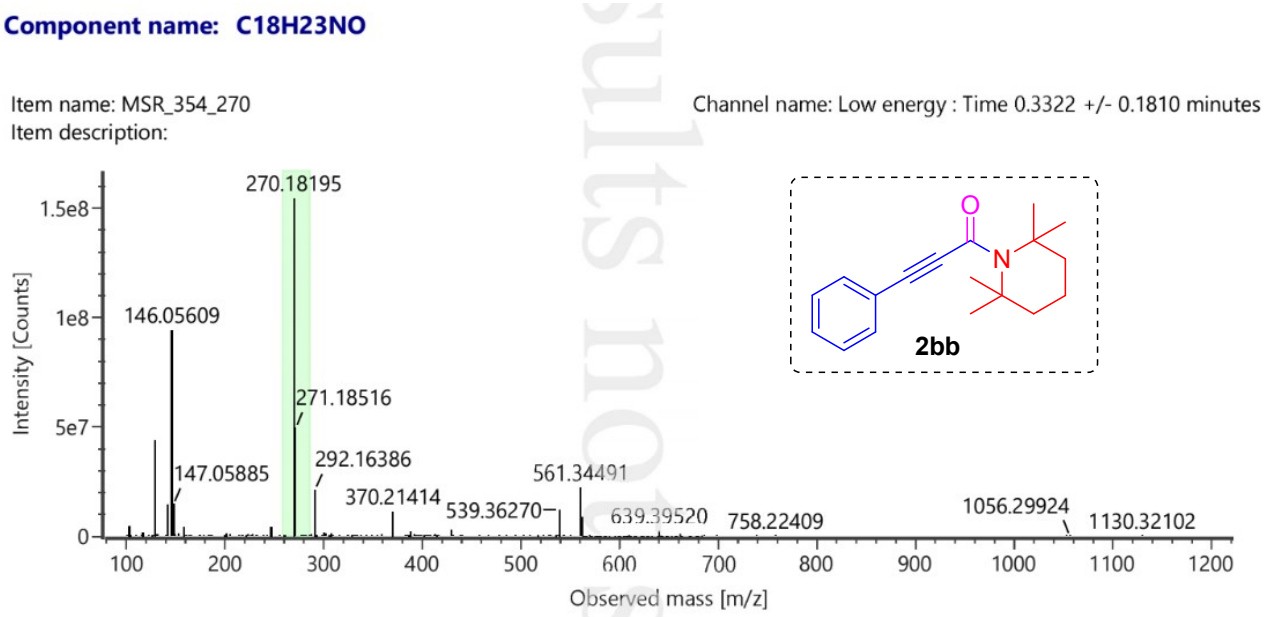
HRMS spectrum of compound 2va



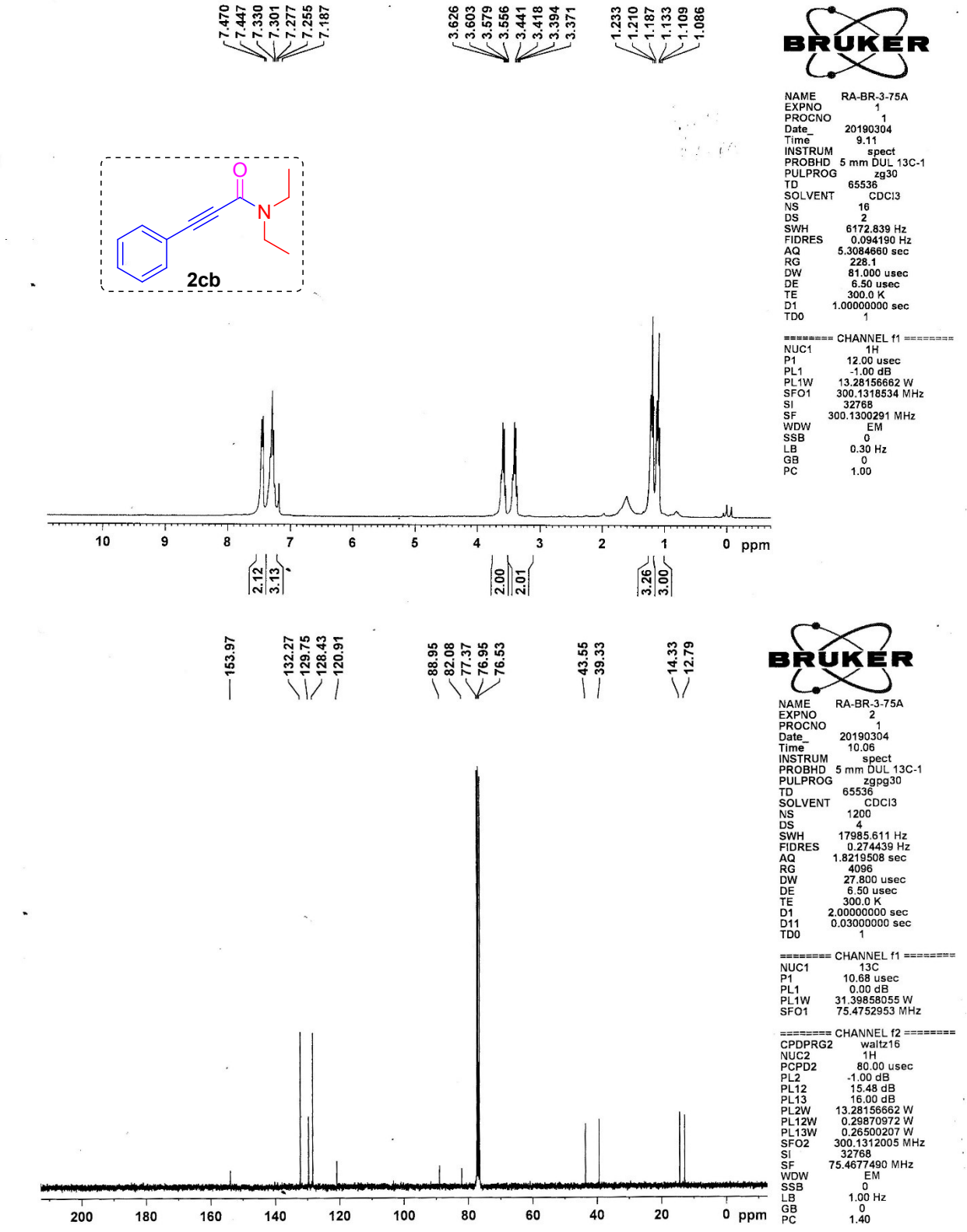
^{1}H & ^{13}C spectra of compound 2ab



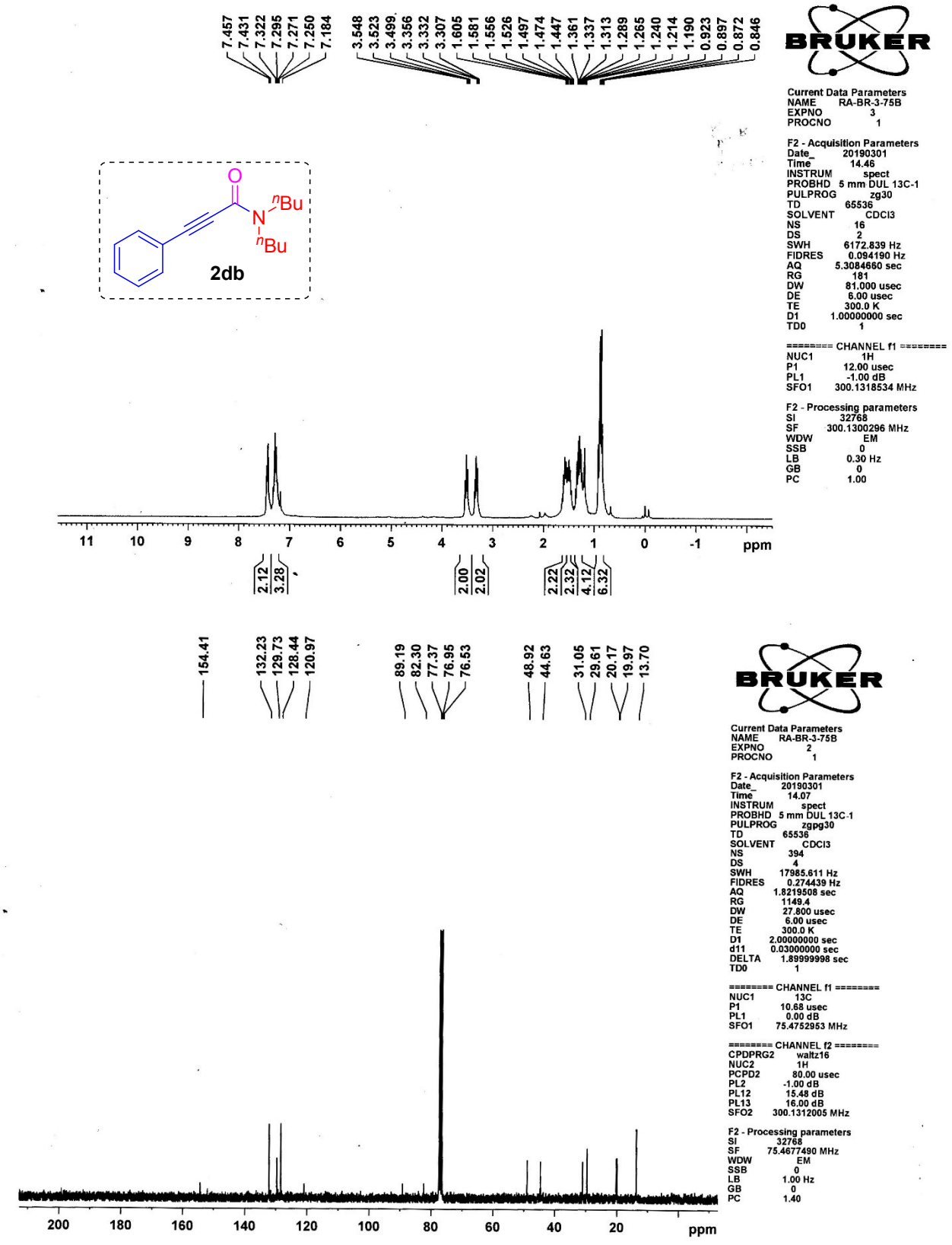
^{1}H & ^{13}C spectra of compound2bb



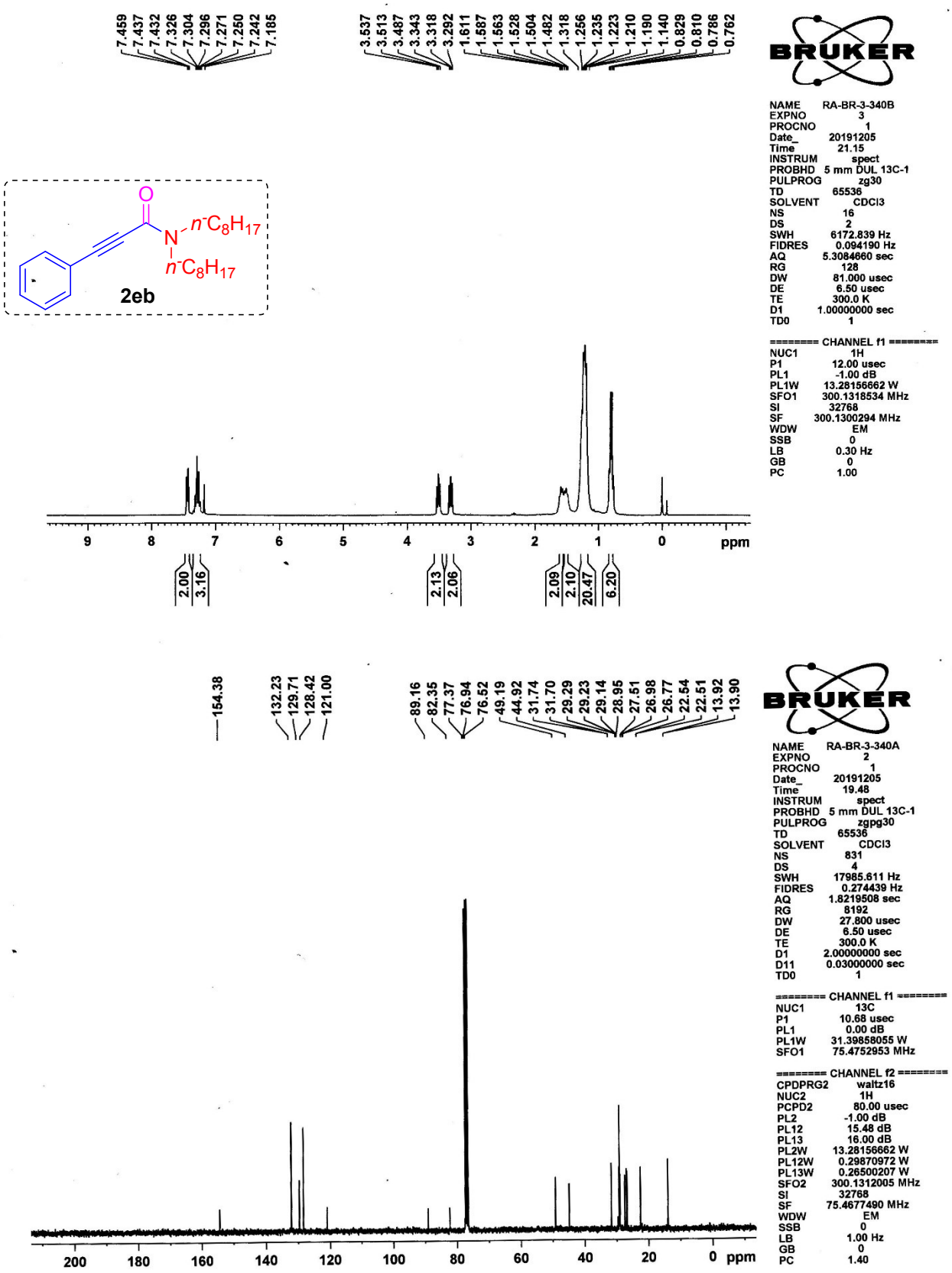
HRMS Spectrum of compound 2bb



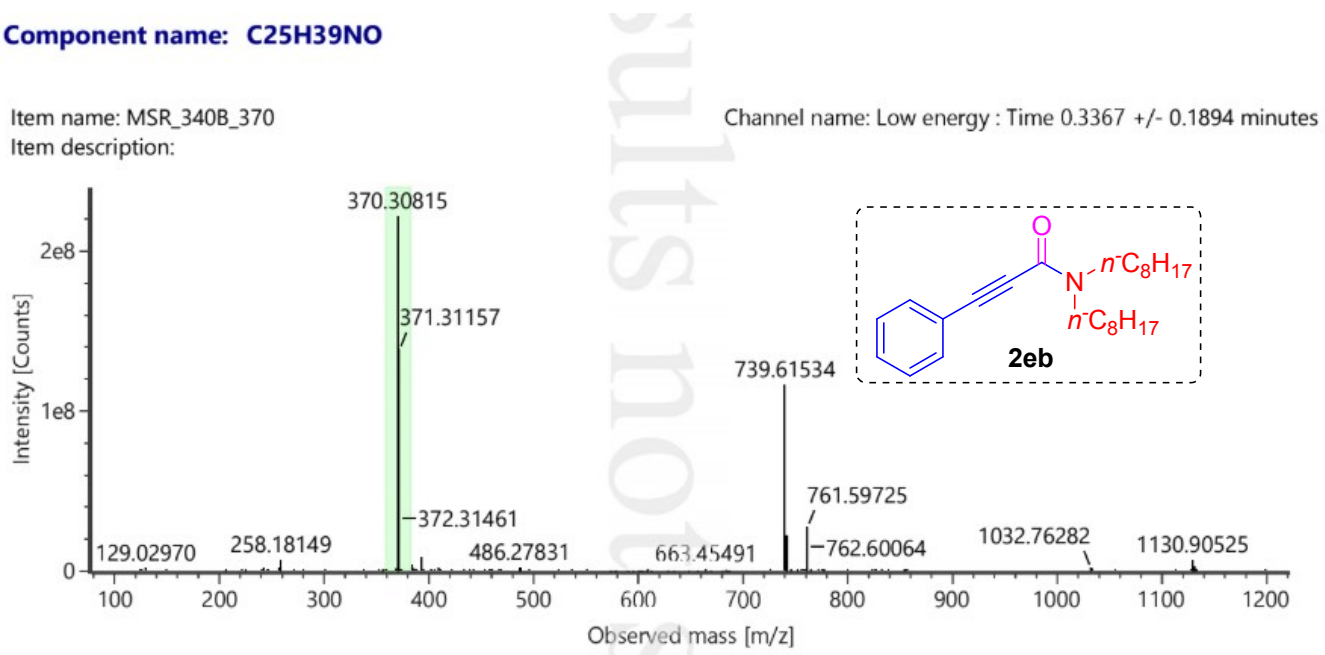
^{1}H&^{13}C spectra of compound 2cb



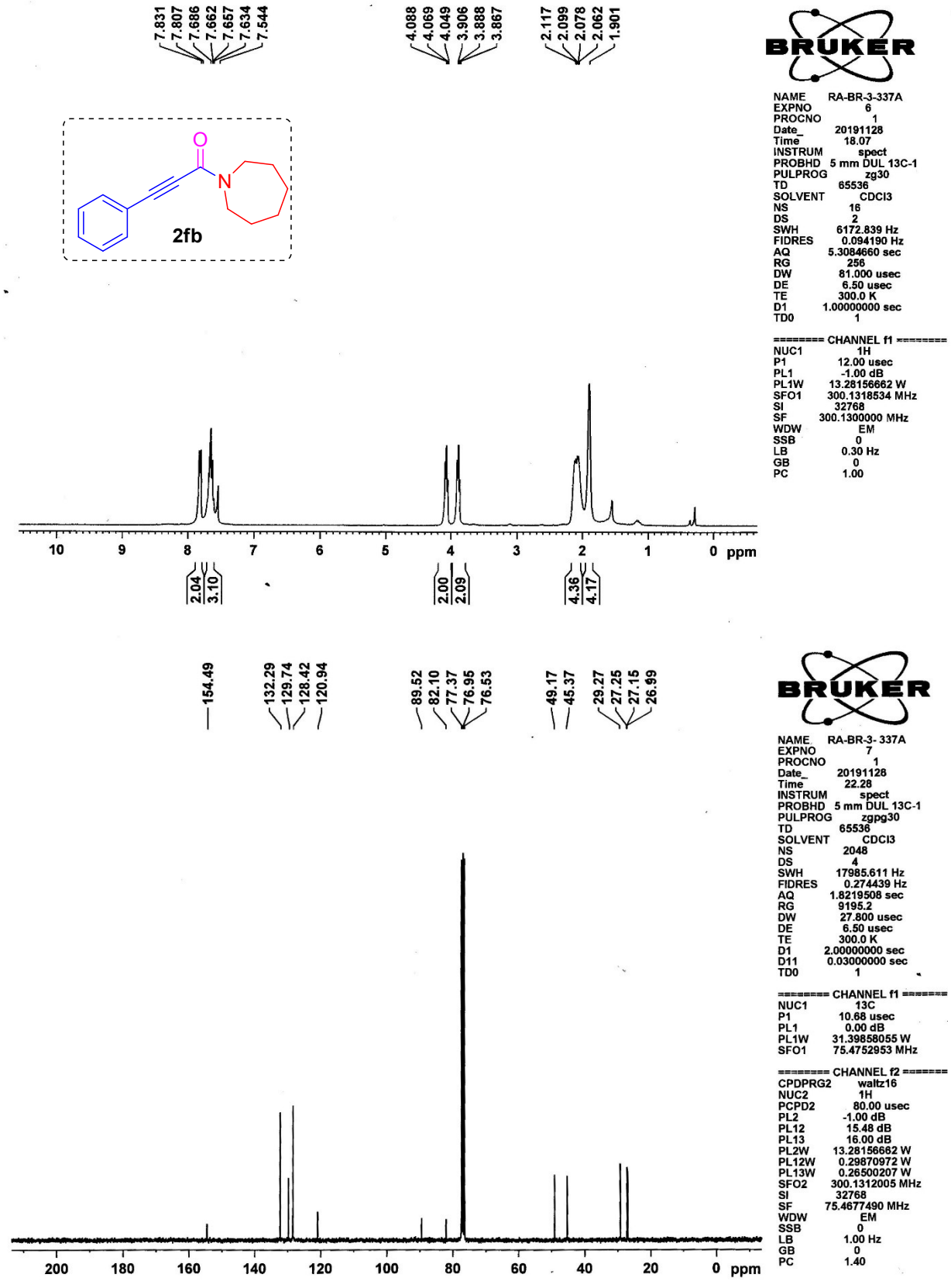
^{1}H&^{13}C spectra of compound 2db



^{1}H & ^{13}C spectra of compound 2eb



HRMS spectrum of compound 2eb



BRUKER

NAME RA-BR-3-337A
EXPNO 6
PROCNO 1
Date_ 20191128
Time 18.07
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 256
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -1.00 dB
PL1W 13.28156662 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

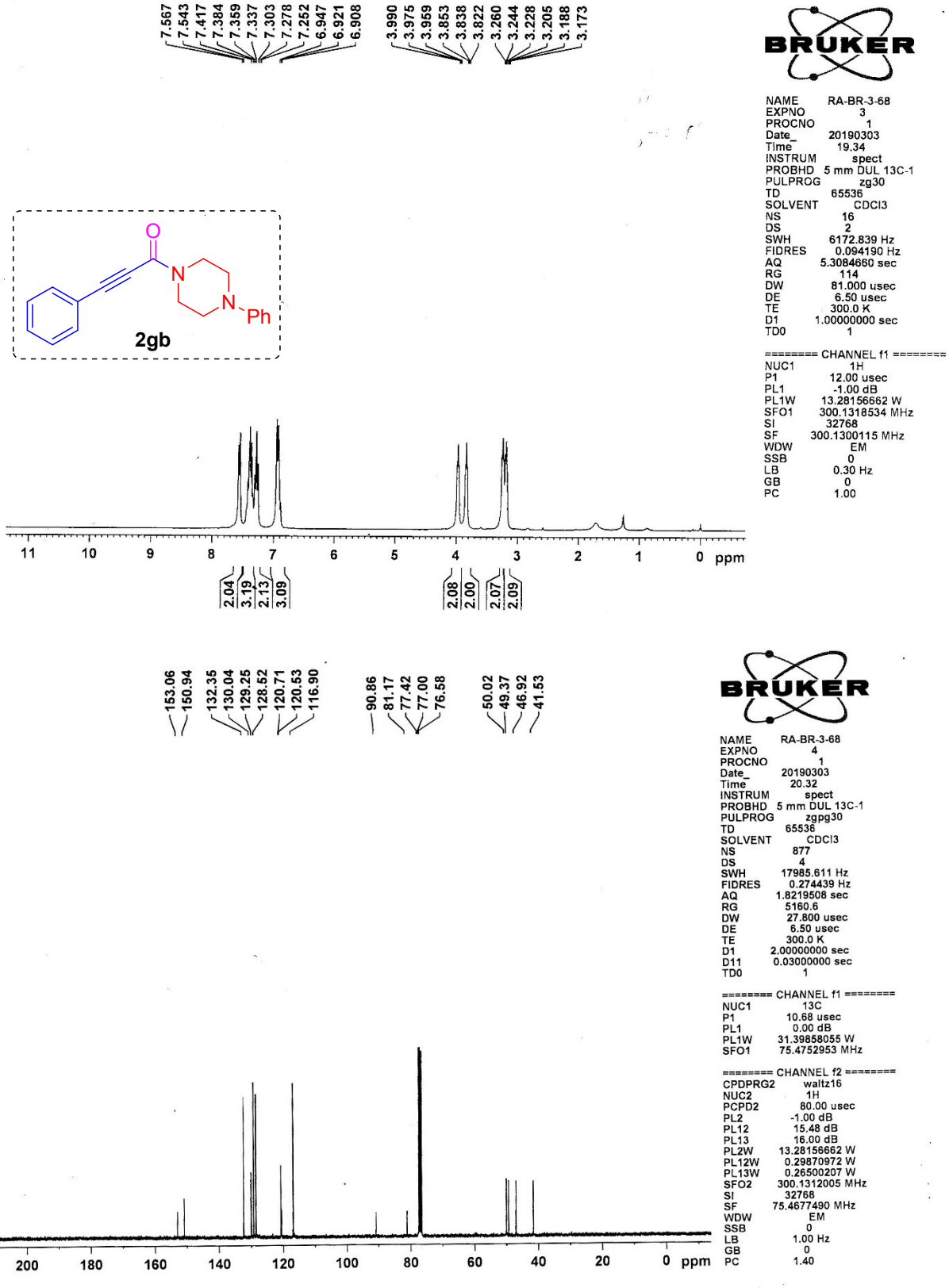
BRUKER

NAME RA-BR-3- 337A
EXPNO 7
PROCNO 1
Date_ 20191128
Time 22.28
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 9195.2
DW 27.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

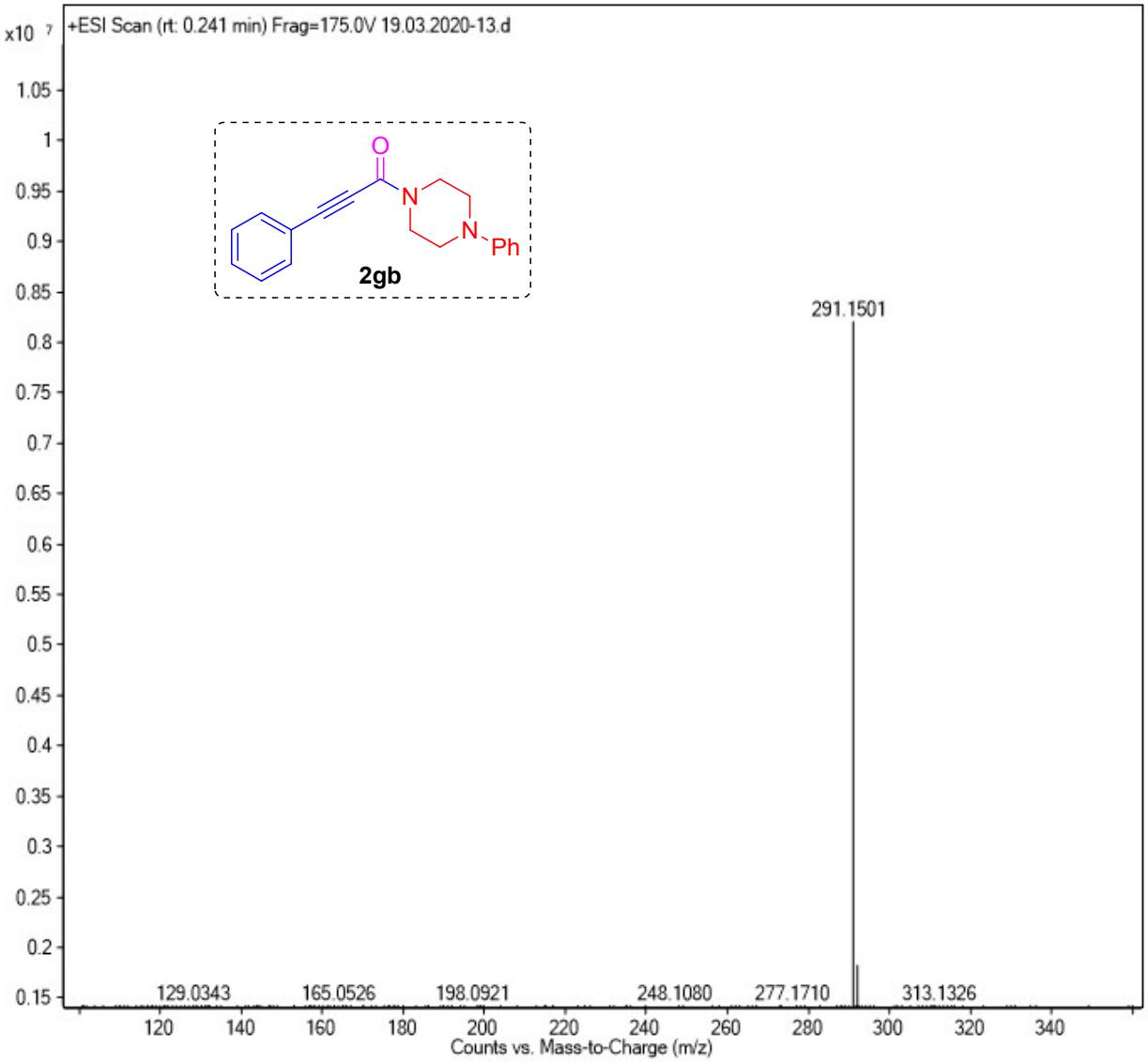
======== CHANNEL f1 ========
NUC1 13C
P1 10.68 usec
PL1 0.00 dB
PL1W 31.39858055 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 15.48 dB
PL13 16.00 dB
PL2W 13.28156662 W
PL12W 0.29870972 W
PL13W 0.26500207 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

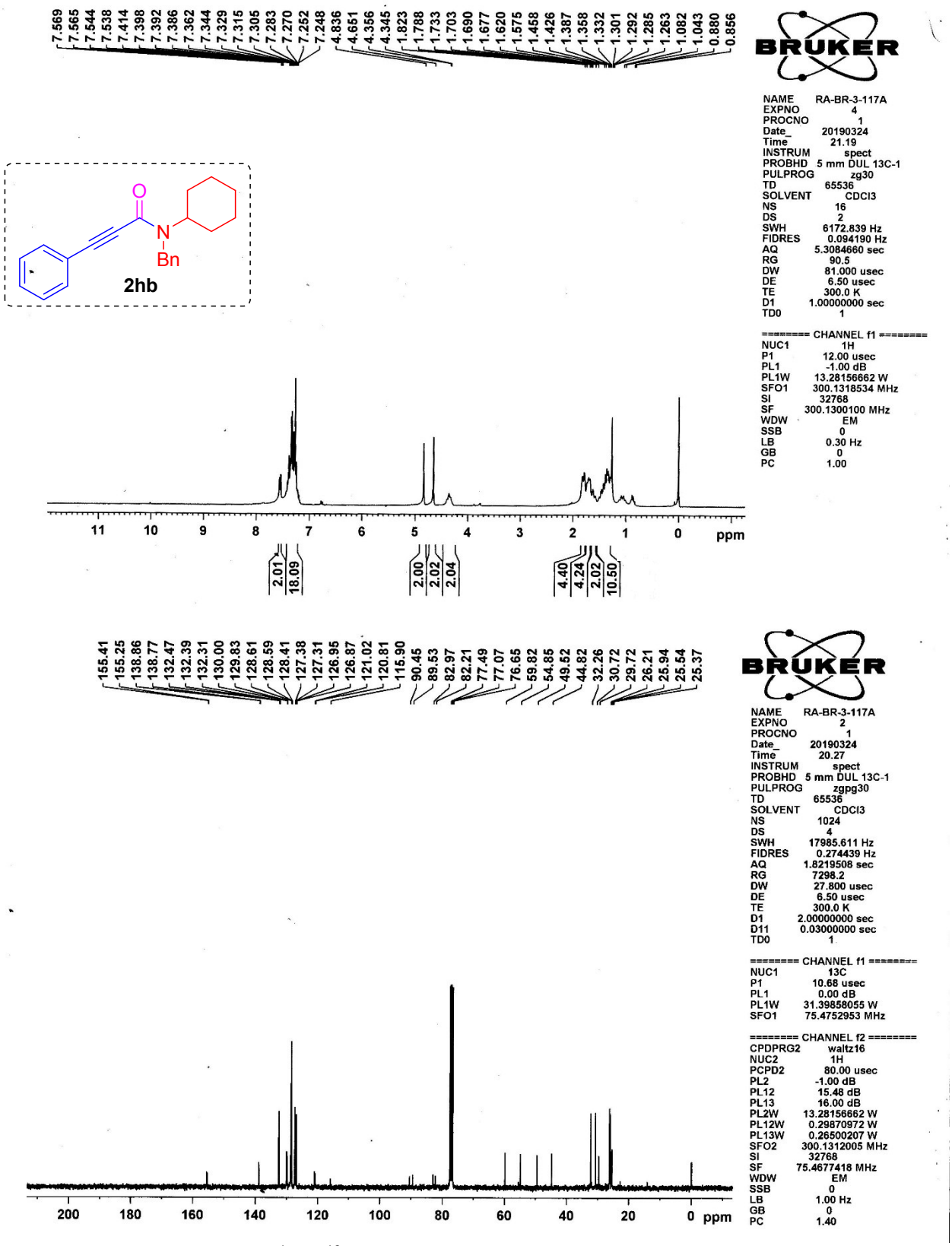
^{1}H & ^{13}C spectra of compound 2fb



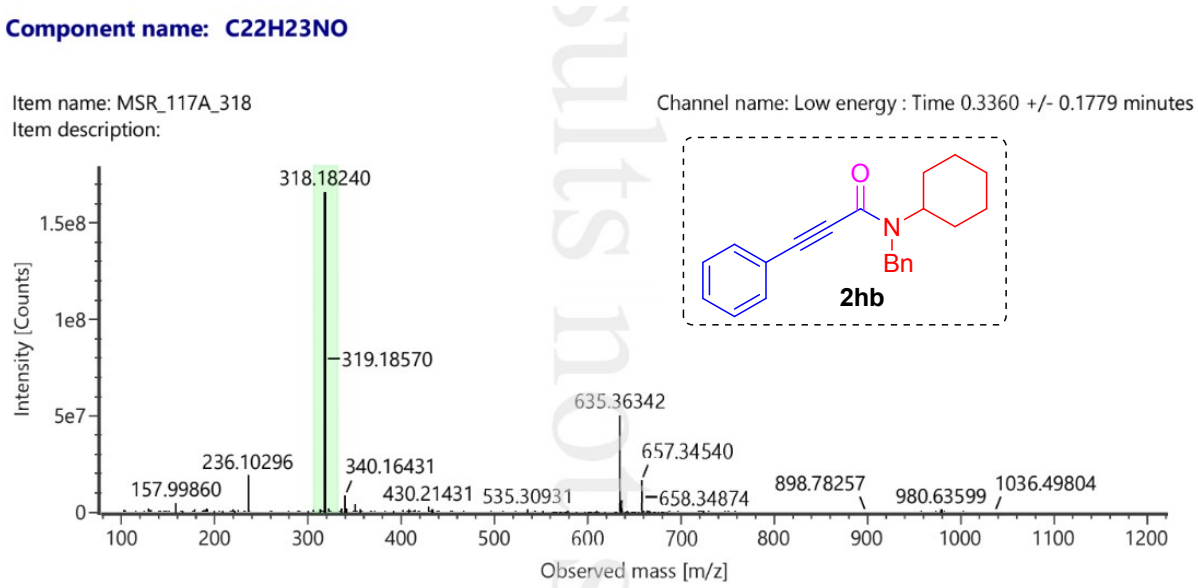
^{1}H & ^{13}C spectra of compound 2gb



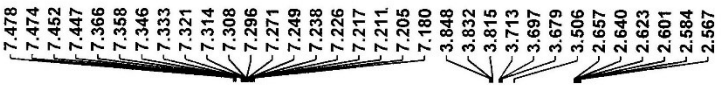
HRMS spectrum of compound 2gb

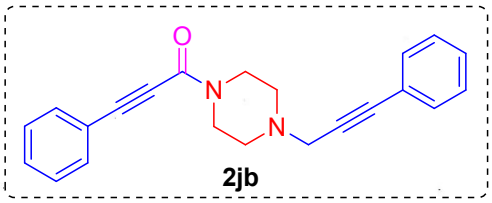


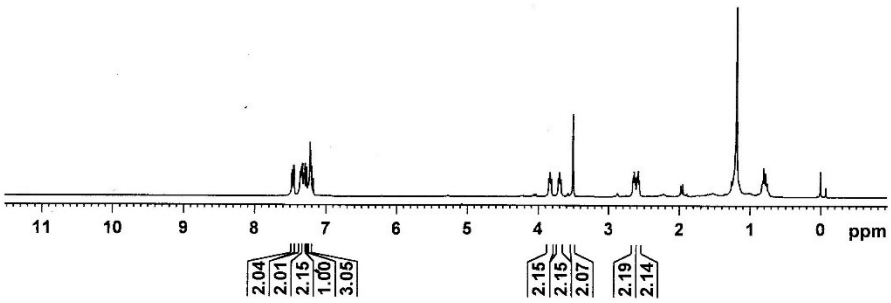
^{1}H&^{13}C spectra of compound 2hb



HRMS Spectrum of compound 2hb

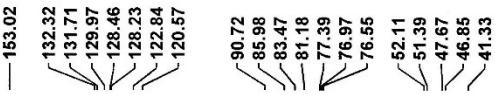


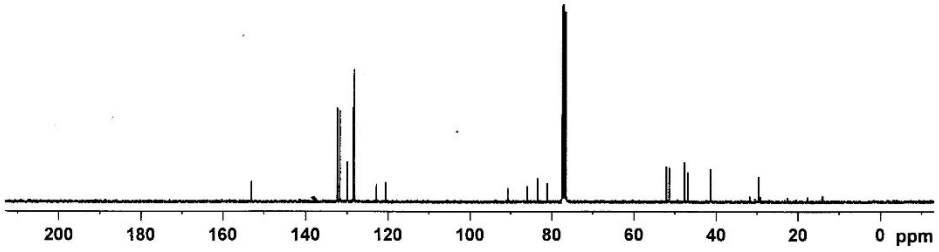




NAME RA-BR-3-26
EXPNO 3
PROCNO 1
Date_ 20181213
Time 13.40
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 114
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -1.00 dB
PL1W 13.28156662 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300304 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



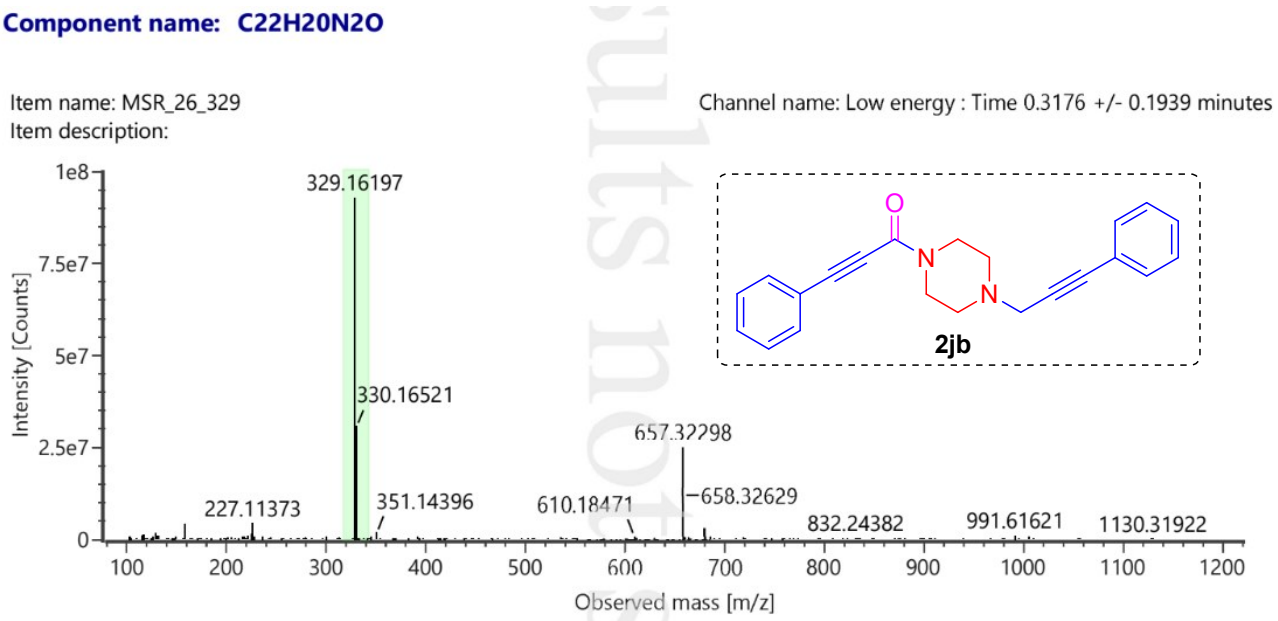


NAME RA-BR-3-26
EXPNO 4
PROCNO 1
Date_ 20181214
Time 15.51
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 8192
DW 27.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

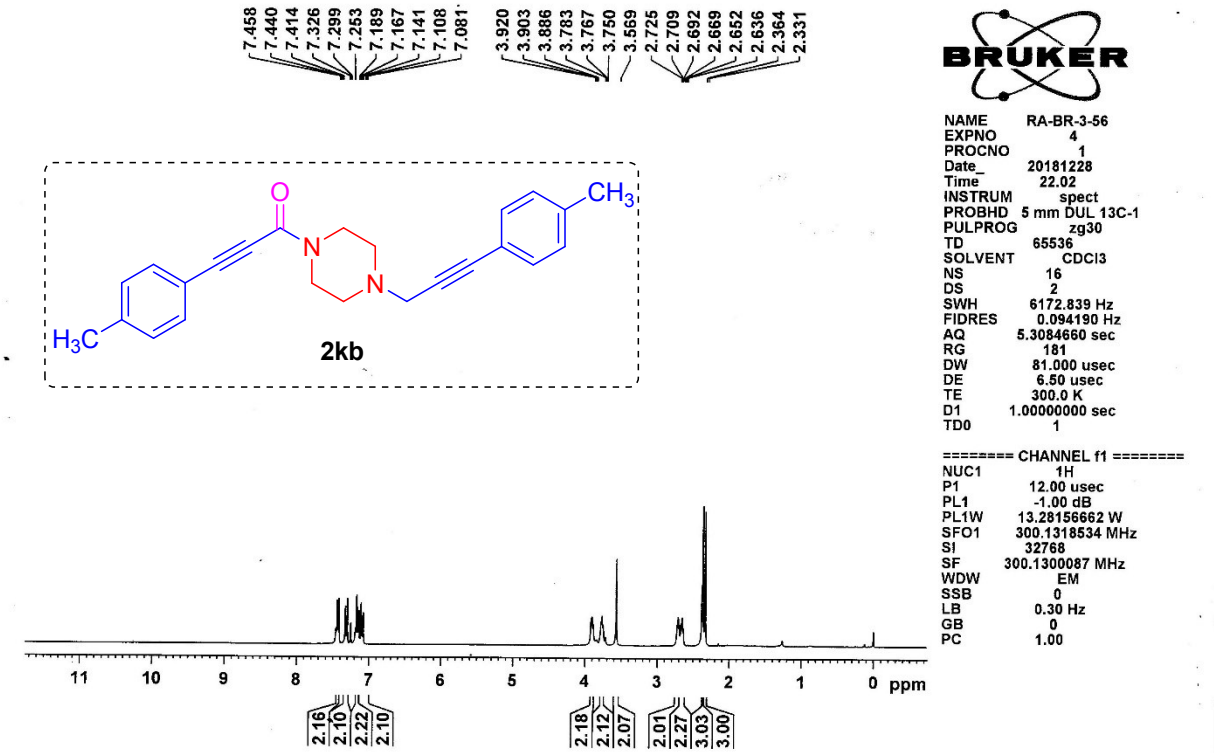
======== CHANNEL f1 ========
NUC1 13C
P1 10.68 usec
PL1 0.00 dB
PL1W 31.39858055 W
SFO1 75.4752953 MHz

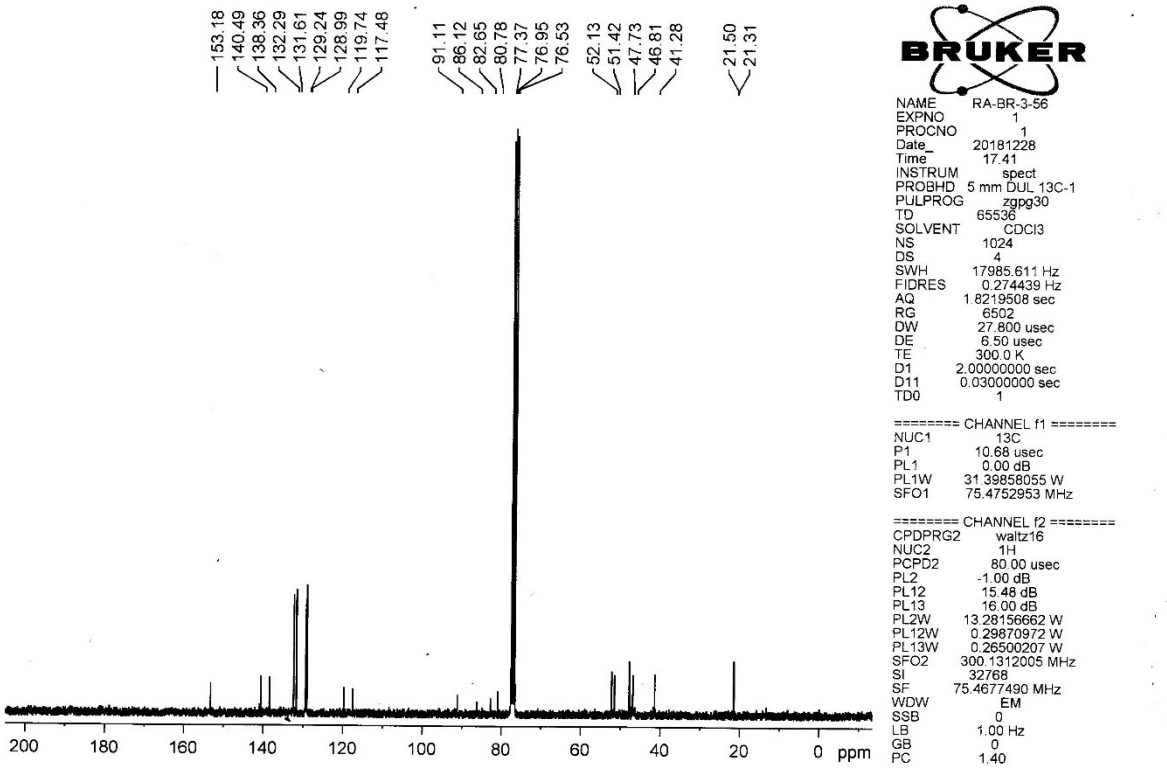
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 15.48 dB
PL13 16.00 dB
PL2W 13.28156662 W
PL12W 0.29870972 W
PL13W 0.26500207 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{1}H & ^{13}C spectra of compound 2jb

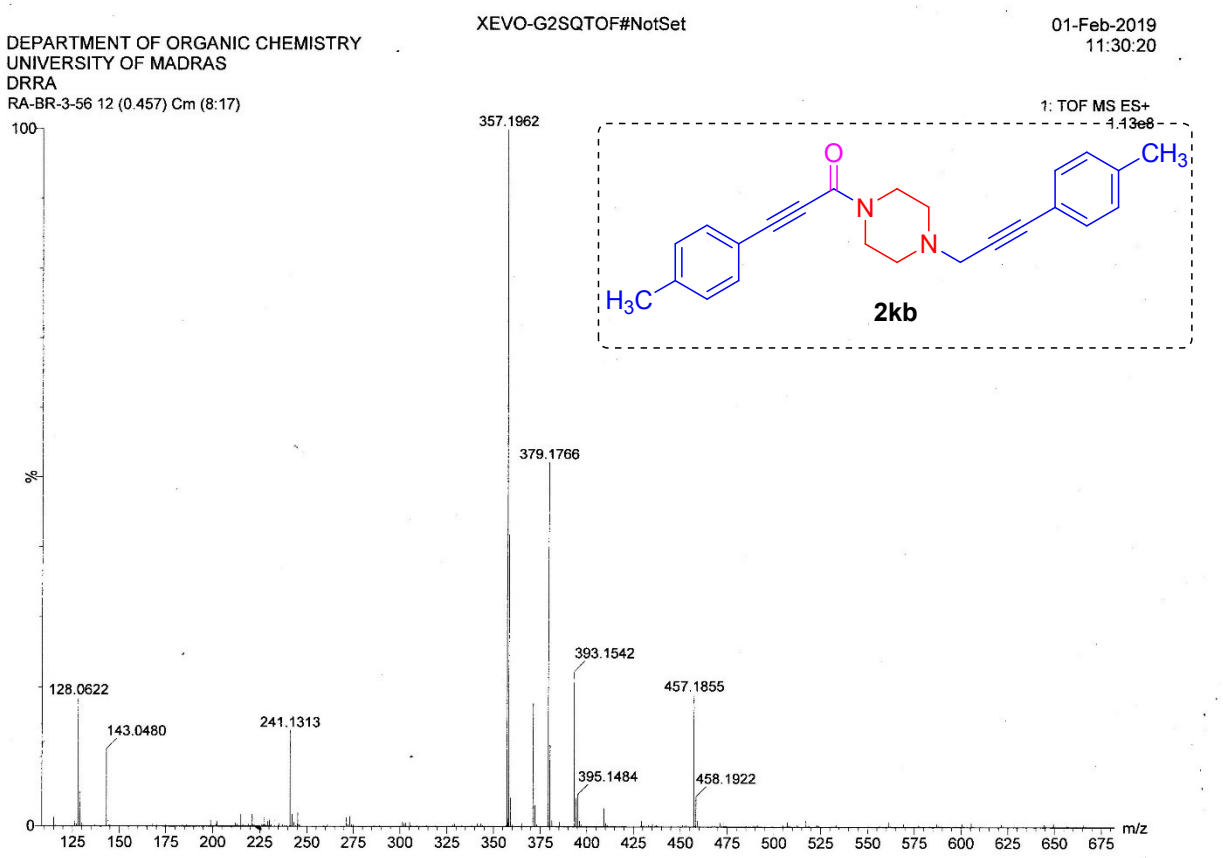


HRMS Spectrum of compound 2jb

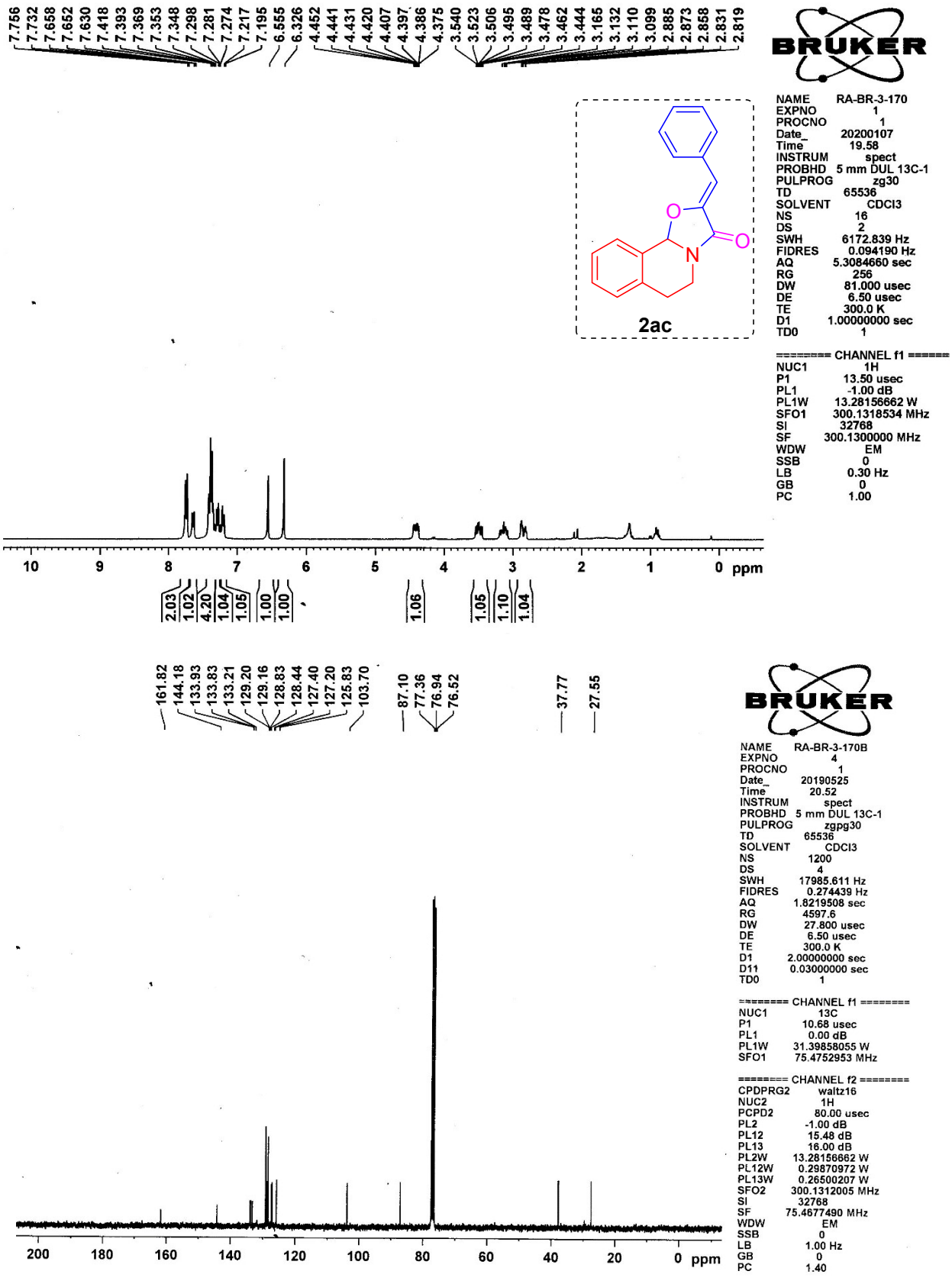




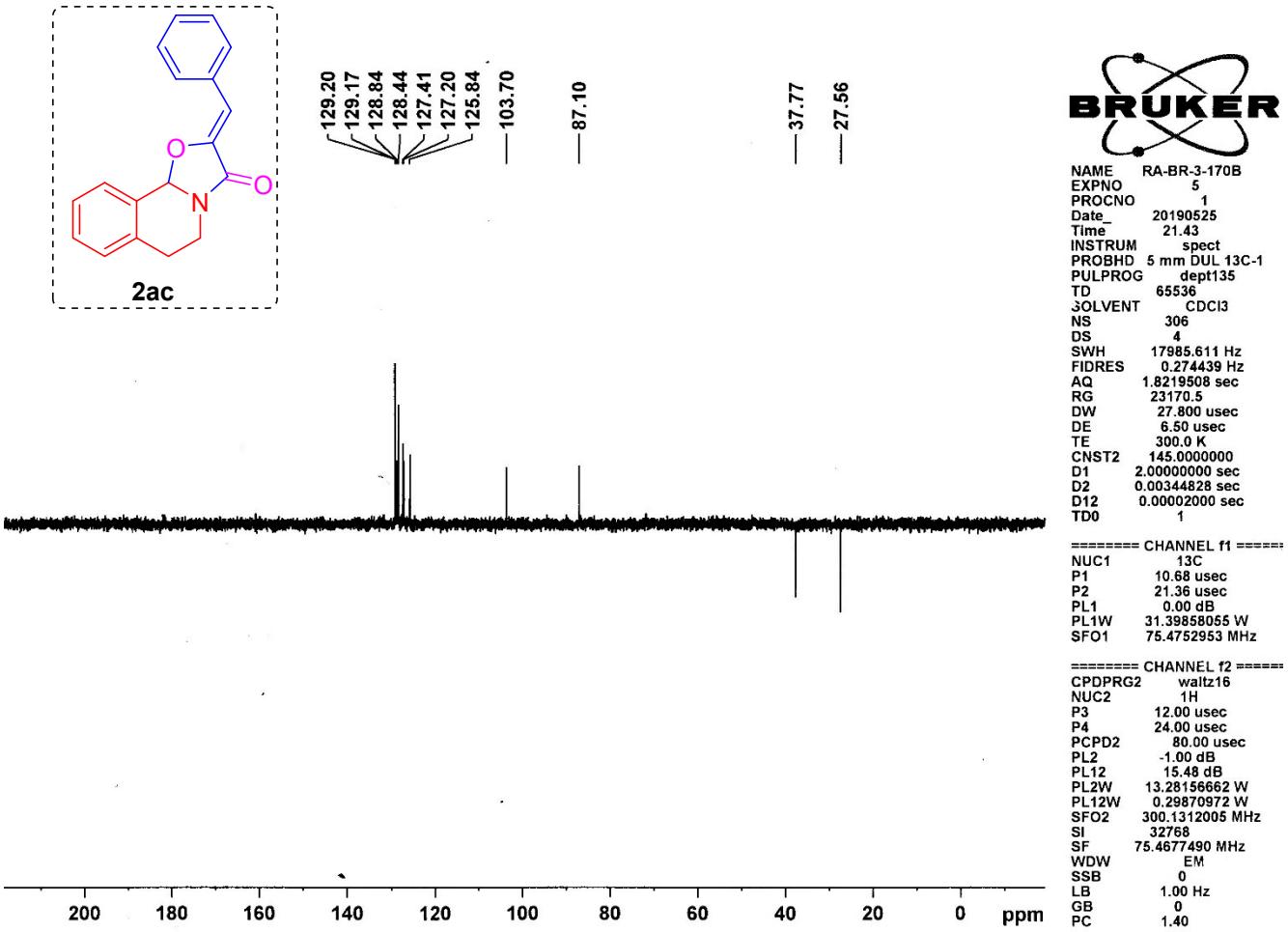
^{1}H & ^{13}C spectra of compound 2kb



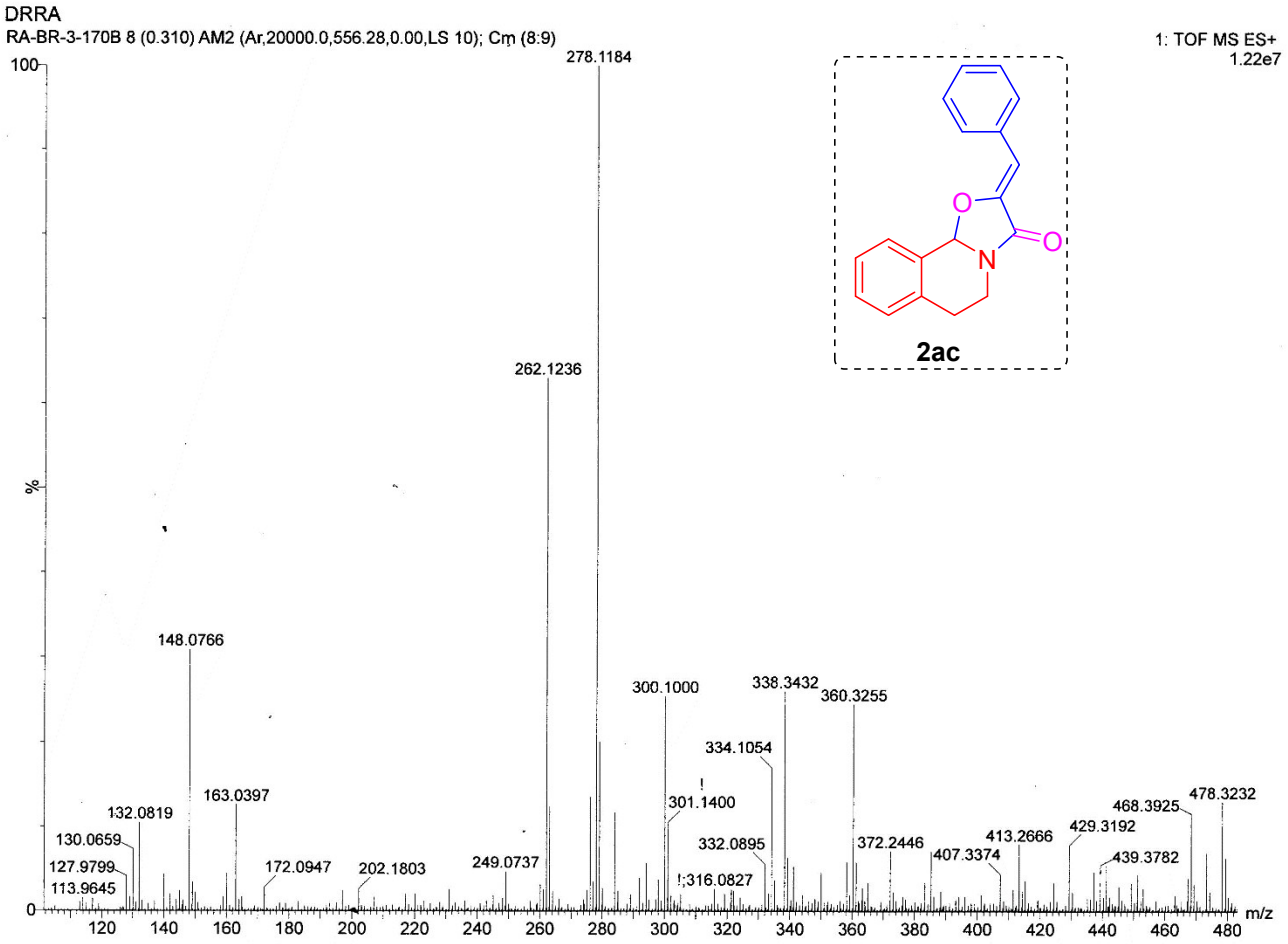
HRMS spectrum of compound 2kb



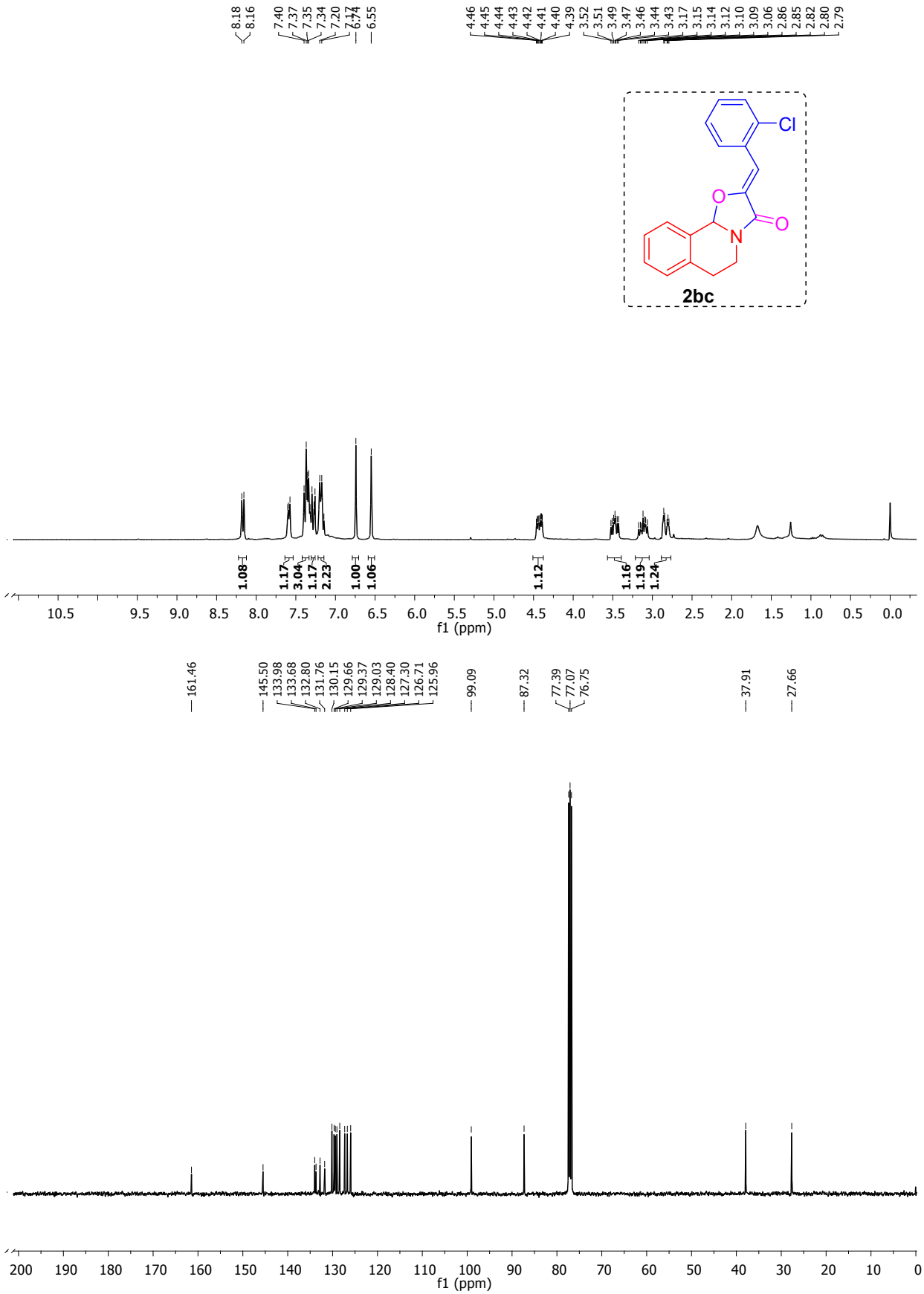
^{1}H & ^{13}C spectra of compound 2ac



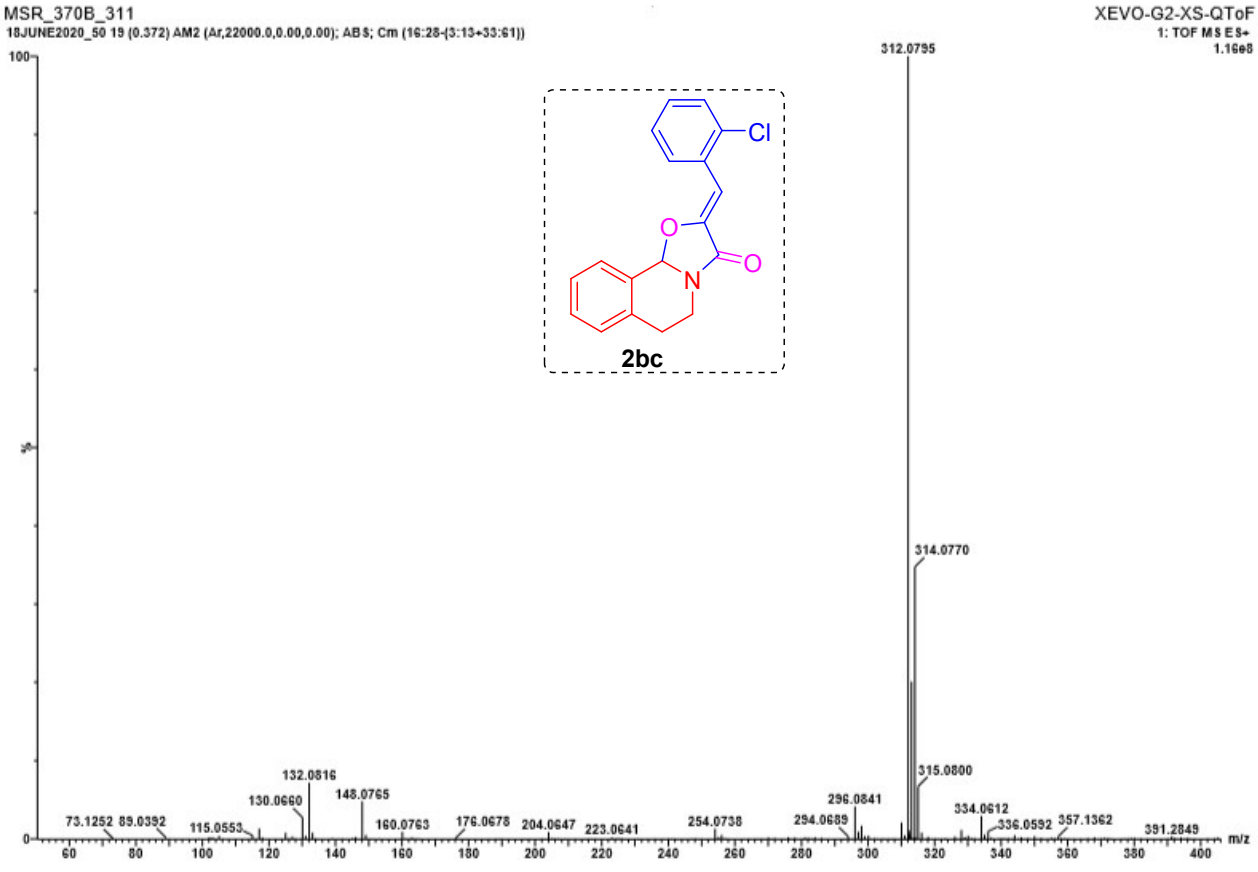
DEPT-135 spectra of compound 2ac



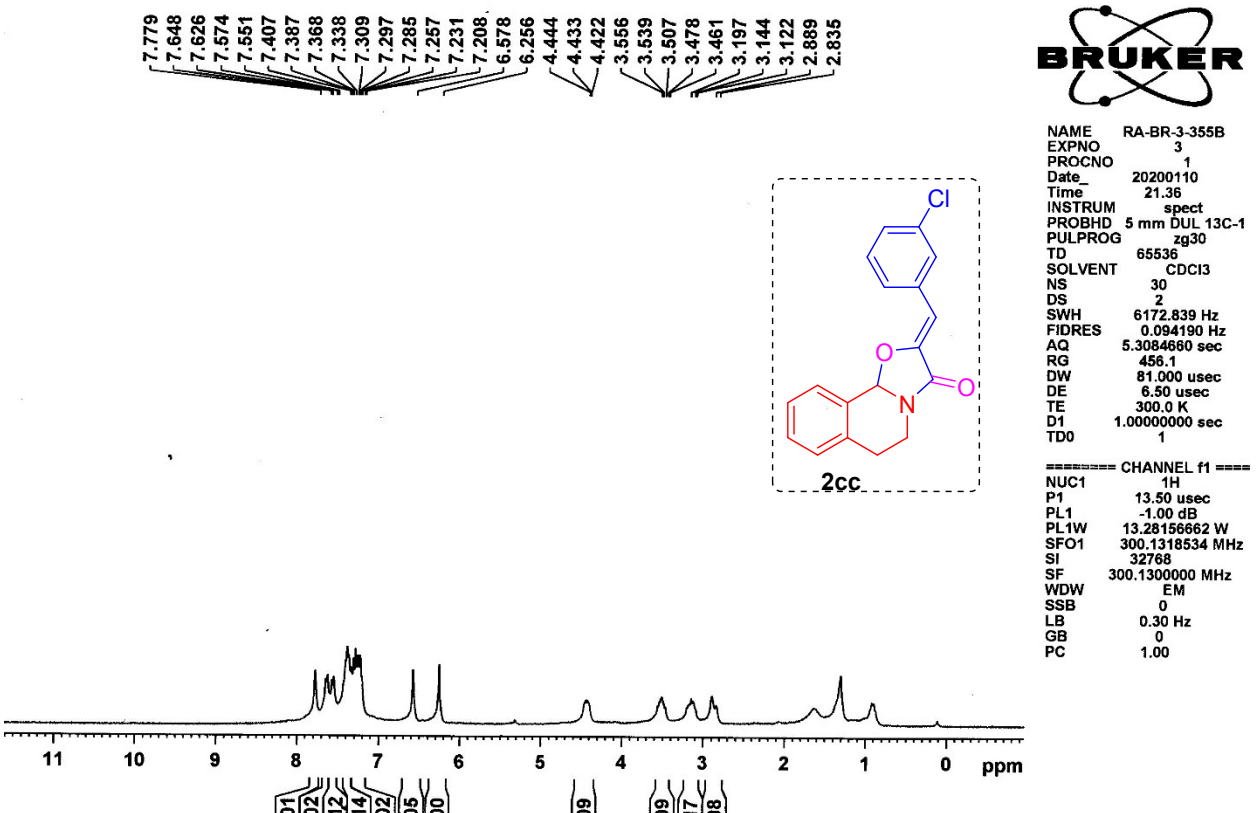
HRMS spectrum of compound 2ac



^{1}H & ^{13}C spectra of compound 2bc



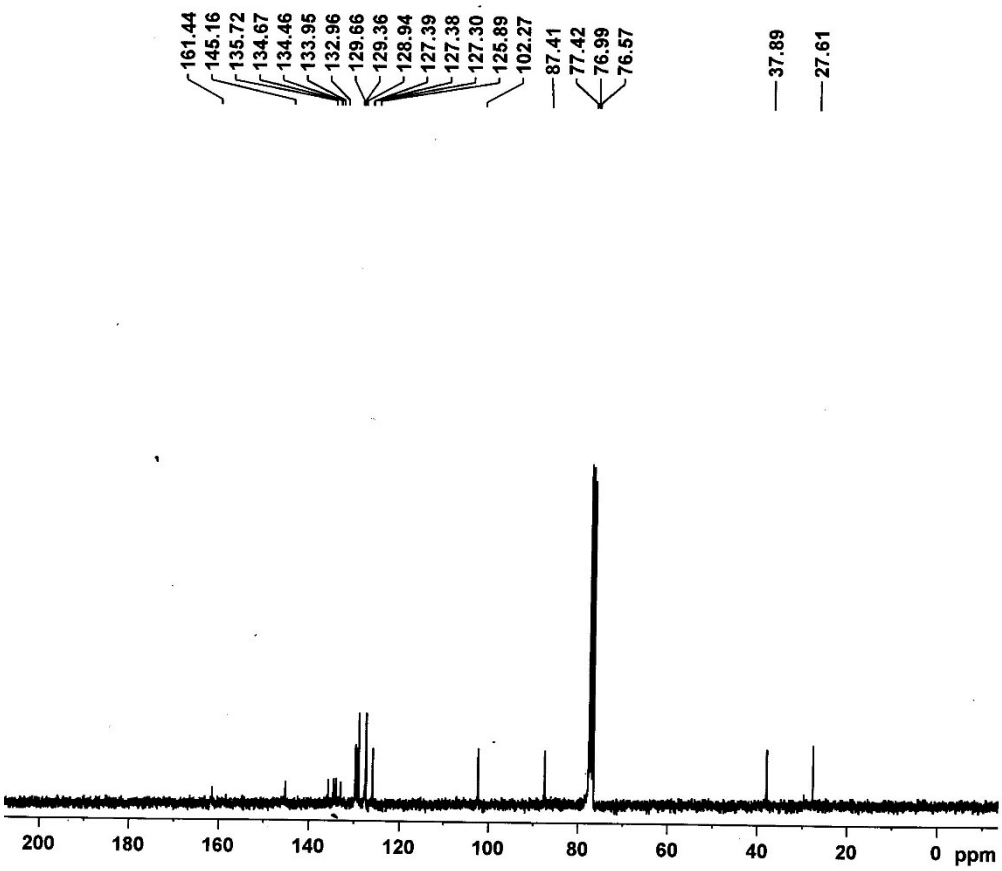
HRMS spectrum of compound 2bc



BRUKER

NAME RA-BR-3-355B
EXPNO 3
PROCNO 1
Date_ 20200110
Time 21.36
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 30
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 456.1
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ====
NUC1 1H
P1 13.50 usec
PL1 -1.00 dB
PL1W 13.28156662 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



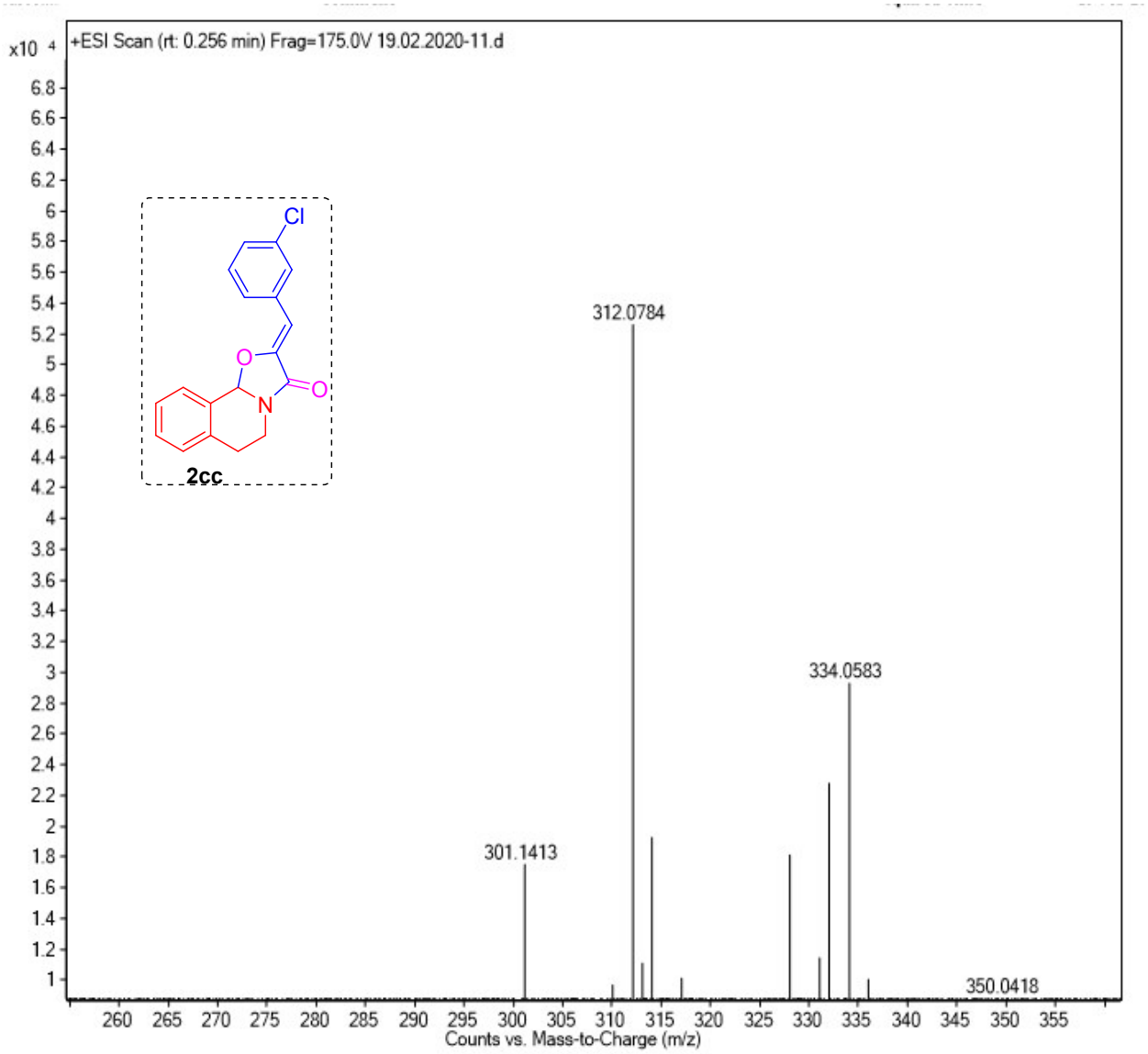
BRUKER

NAME RA-BR-3-355B
EXPNO 2
PROCNO 1
Date_ 20200110
Time 19.23
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 5160.6
DW 27.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

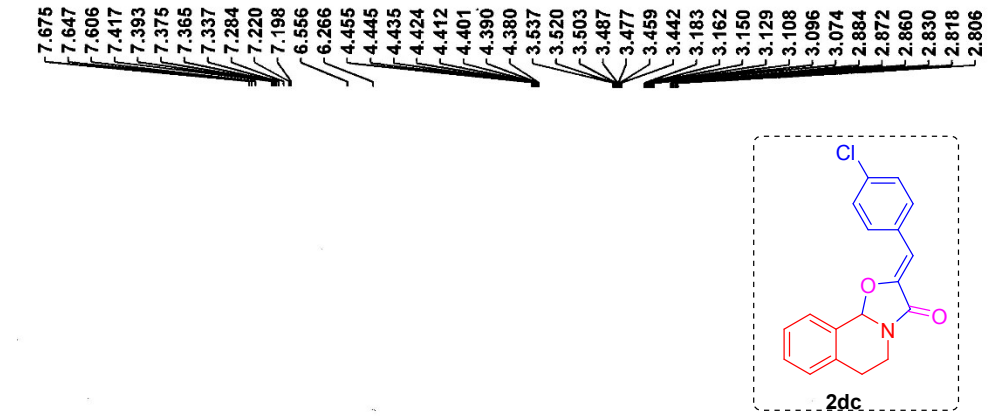
======== CHANNEL f1 ========
NUC1 13C
P1 12.75 usec
PL1 -1.00 dB
PL1W 39.52846909 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.46 dB
PL13 16.00 dB
PL2W 13.28156662 W
PL12W 0.37778899 W
PL13W 0.26500207 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677447 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{1}H & ^{13}C spectra of compound 2cc



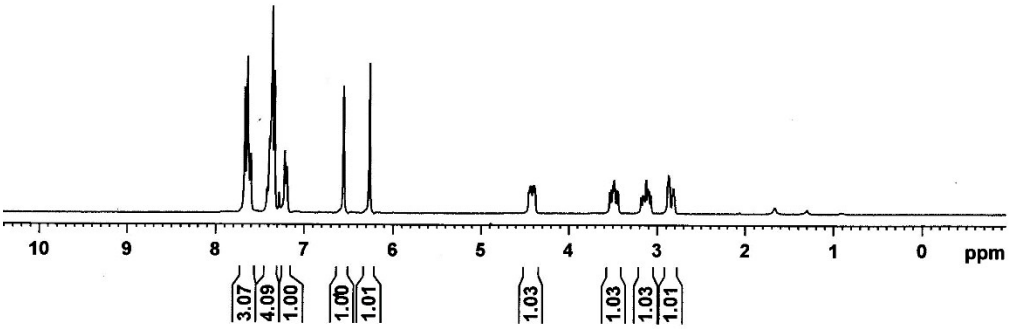
HRMS spectrum of compound 2cc

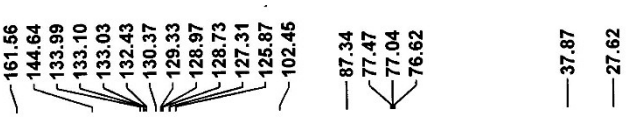


2dc

NAME RA-BR-3-353B
EXPNO 1
PROCNO 1
Date_ 20200109
Time 19.05
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 181
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ======
NUC1 1H
P1 13.50 usec
PL1 -1.00 dB
PL1W 13.28156662 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

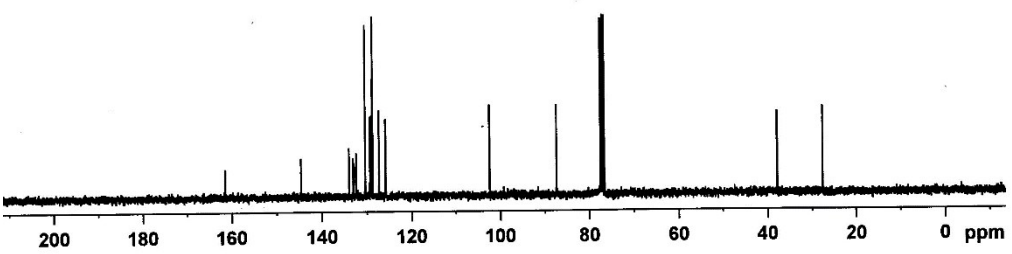




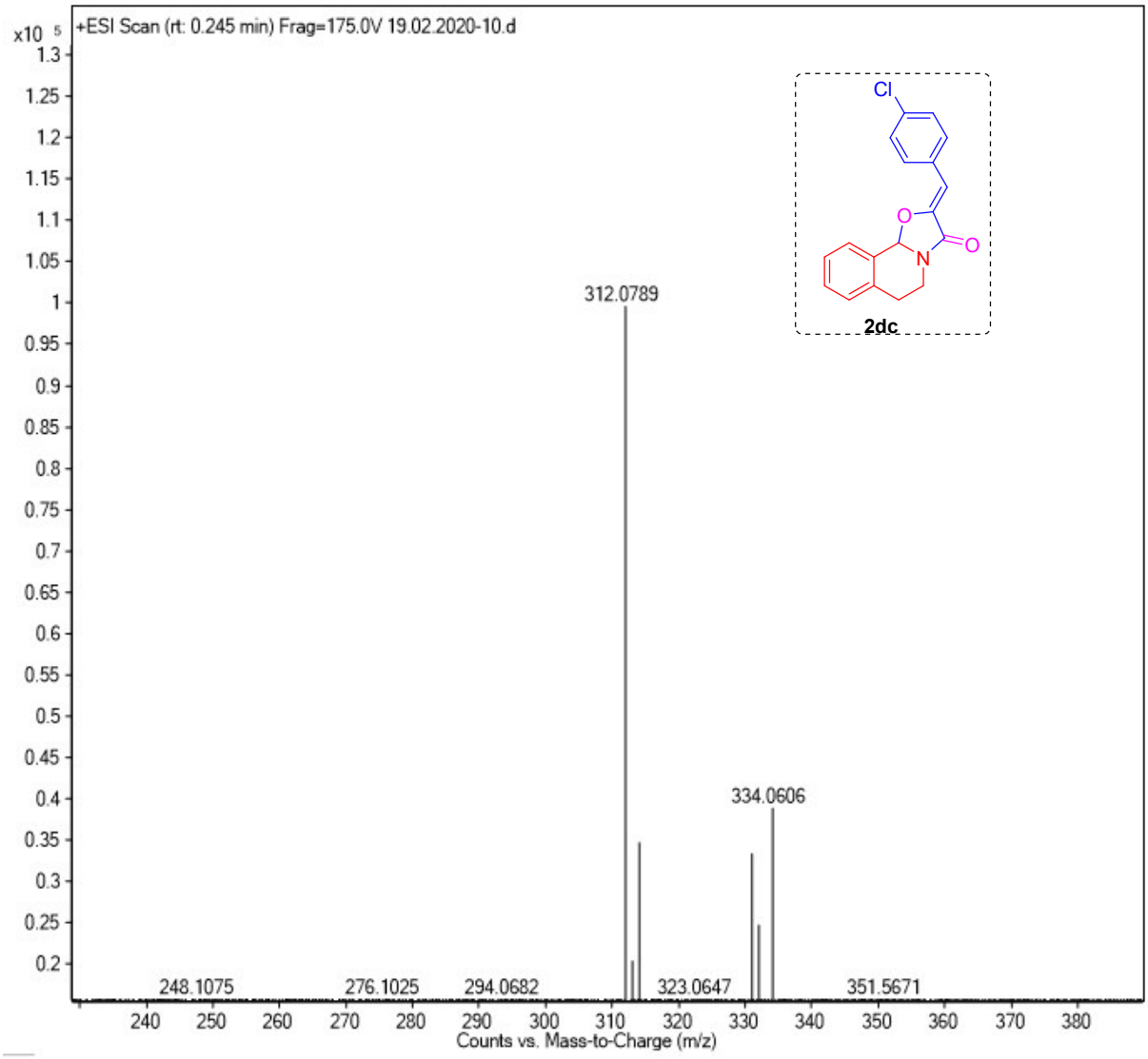
NAME RA-BR-3-353B
EXPNO 2
PROCNO 1
Date_ 20200109
Time 19.14
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 150
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 12.75 usec
PL1 -1.00 dB
PL1W 39.52846909 W
SFO1 75.4752953 MHz

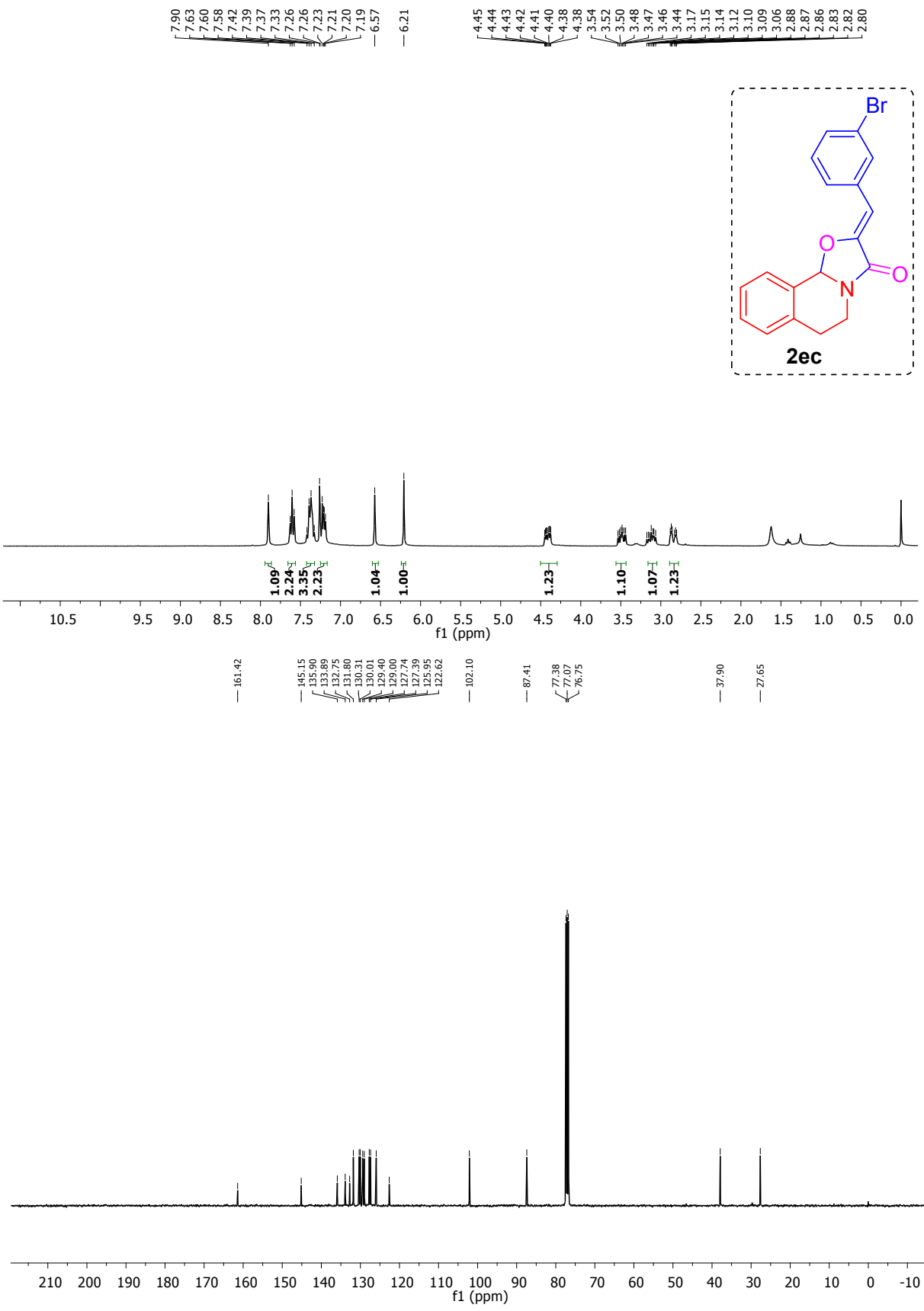
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.46 dB
PL13 16.00 dB
PL2W 13.28156662 W
PL12W 0.37778899 W
PL13W 0.26500207 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677447 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



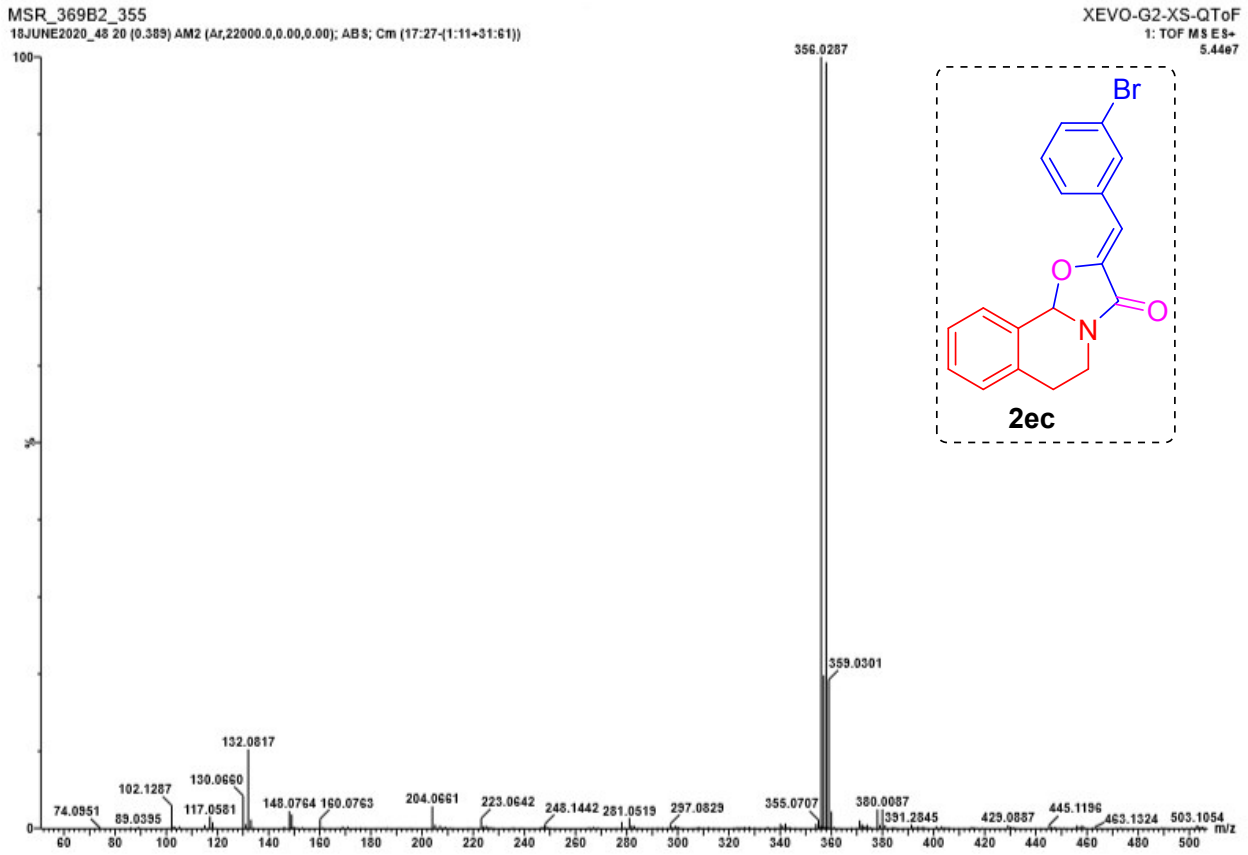
^{1}H & ^{13}C spectra of compound 2dc



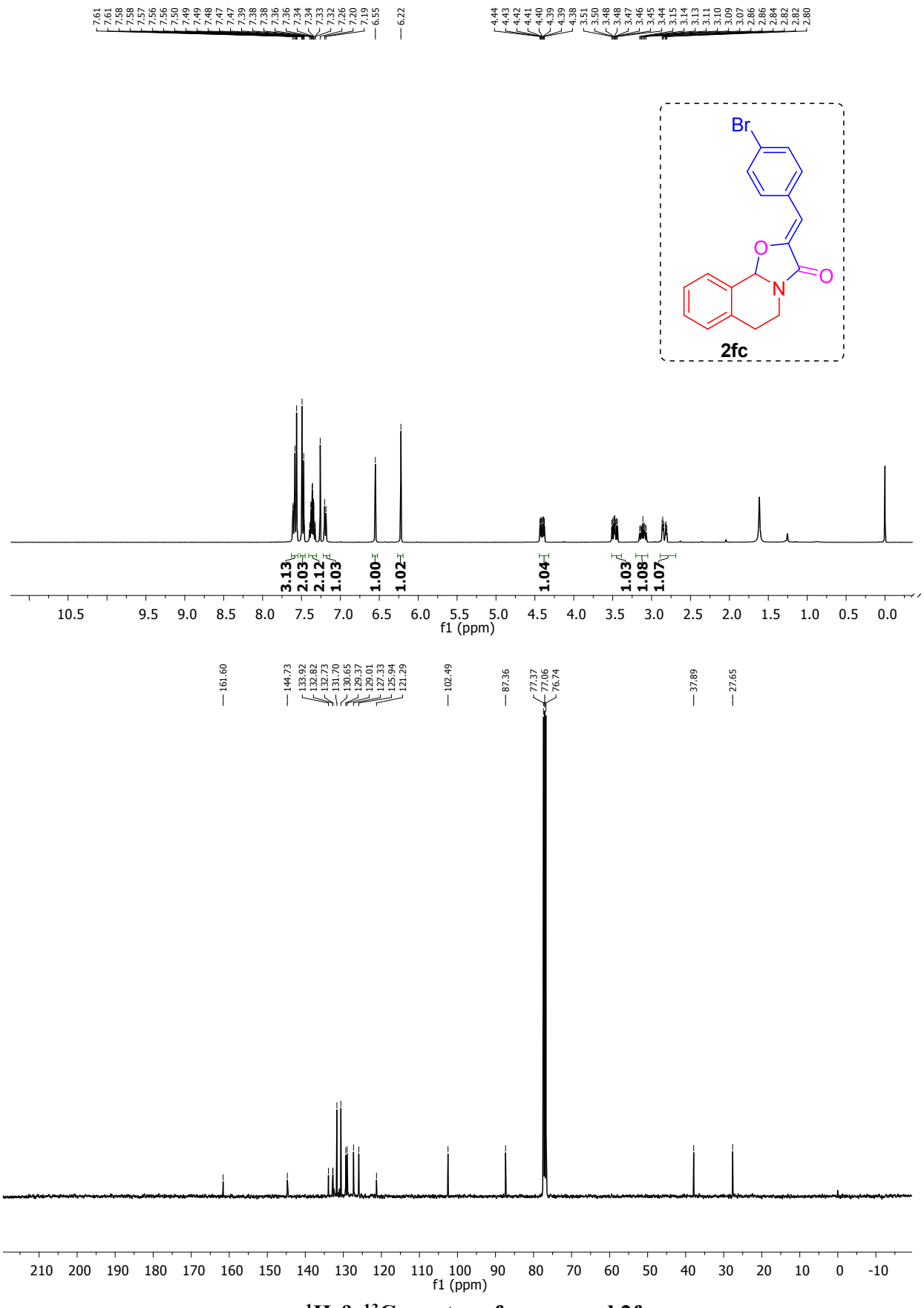
HRMS spectrum of compound 2dc



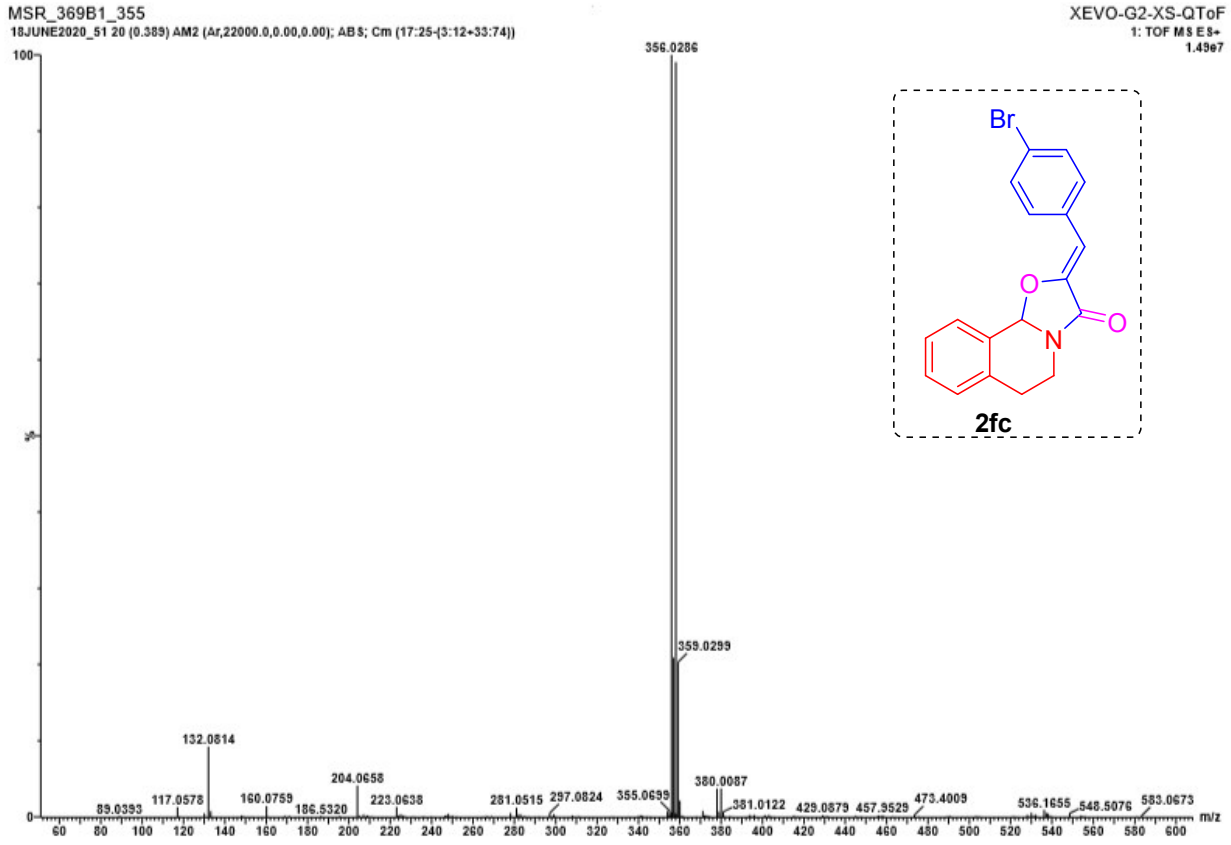
^{1}H & ^{13}C spectra of compound 2ec



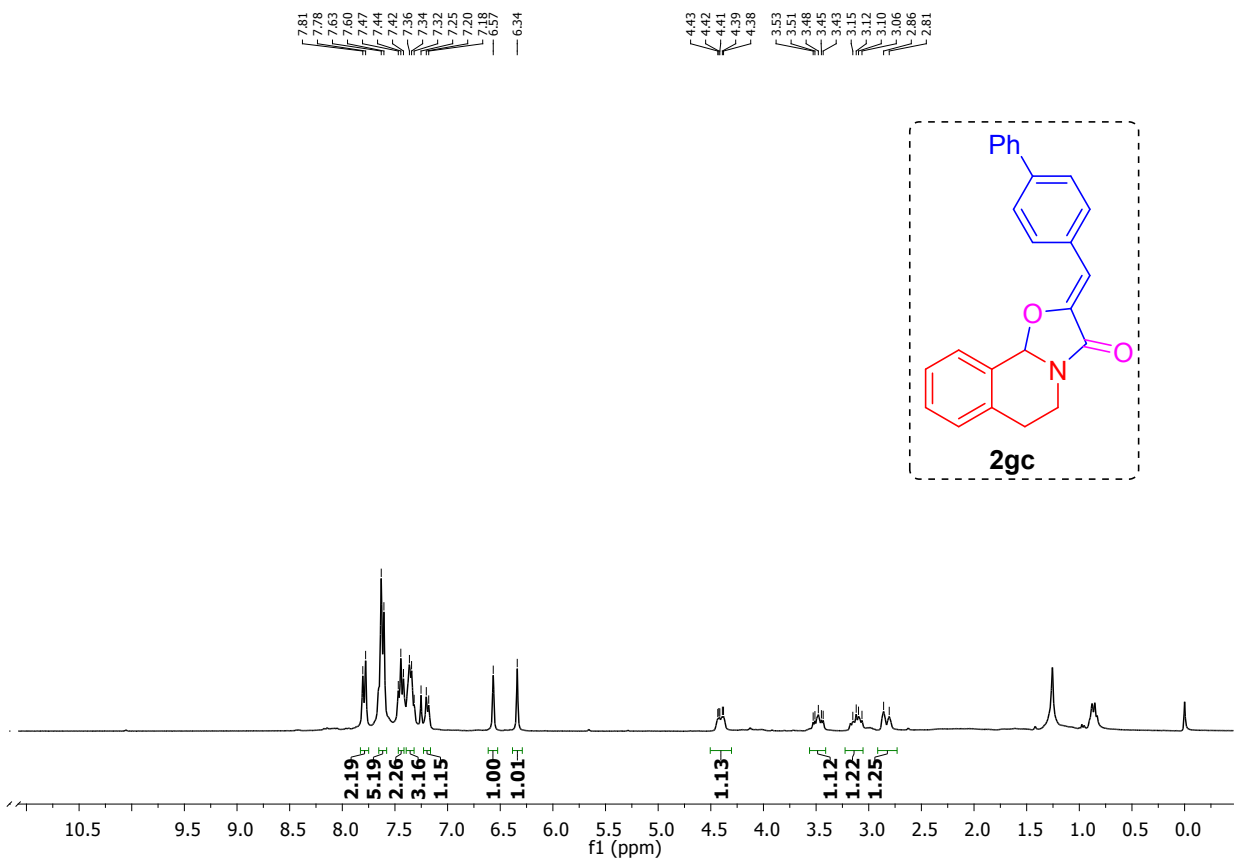
HRMS spectrum of compound 2ec

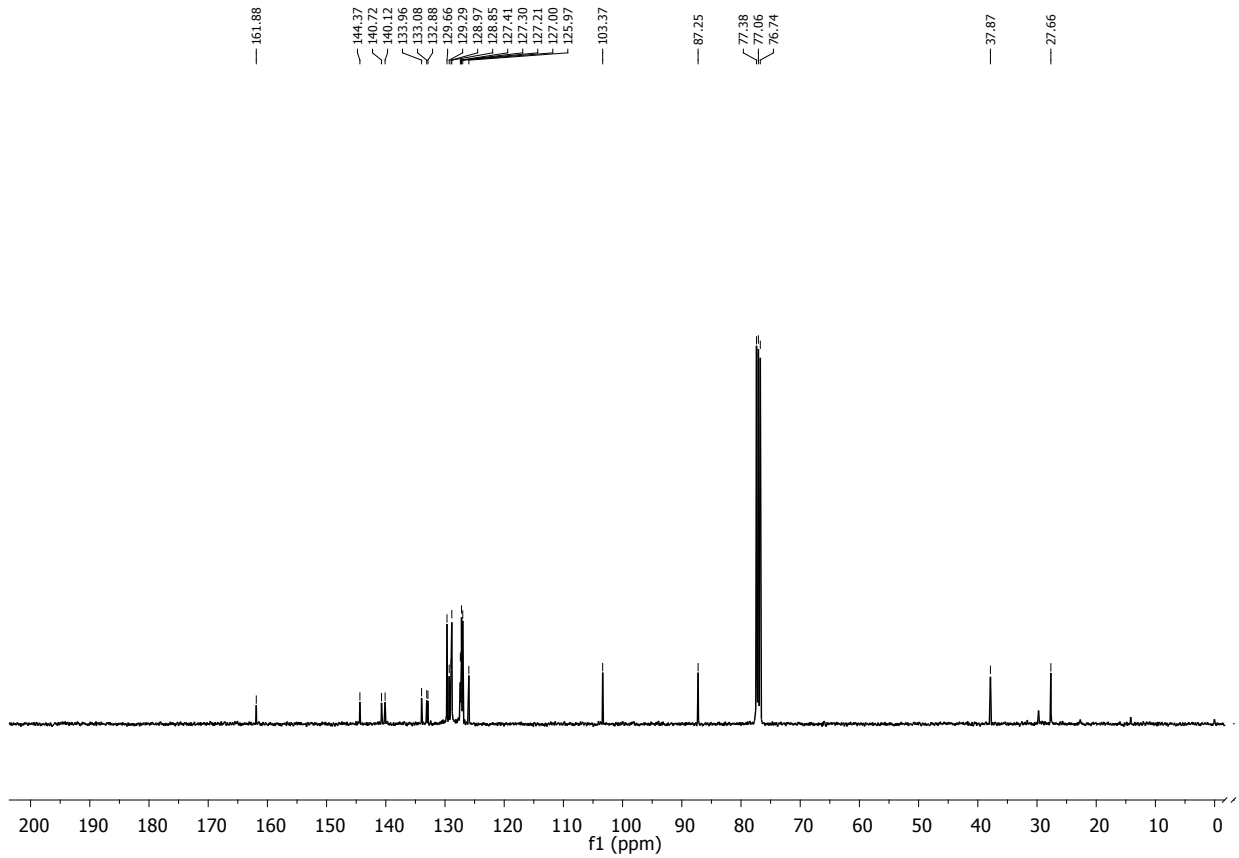


^{1}H & ^{13}C spectra of compound 2fc

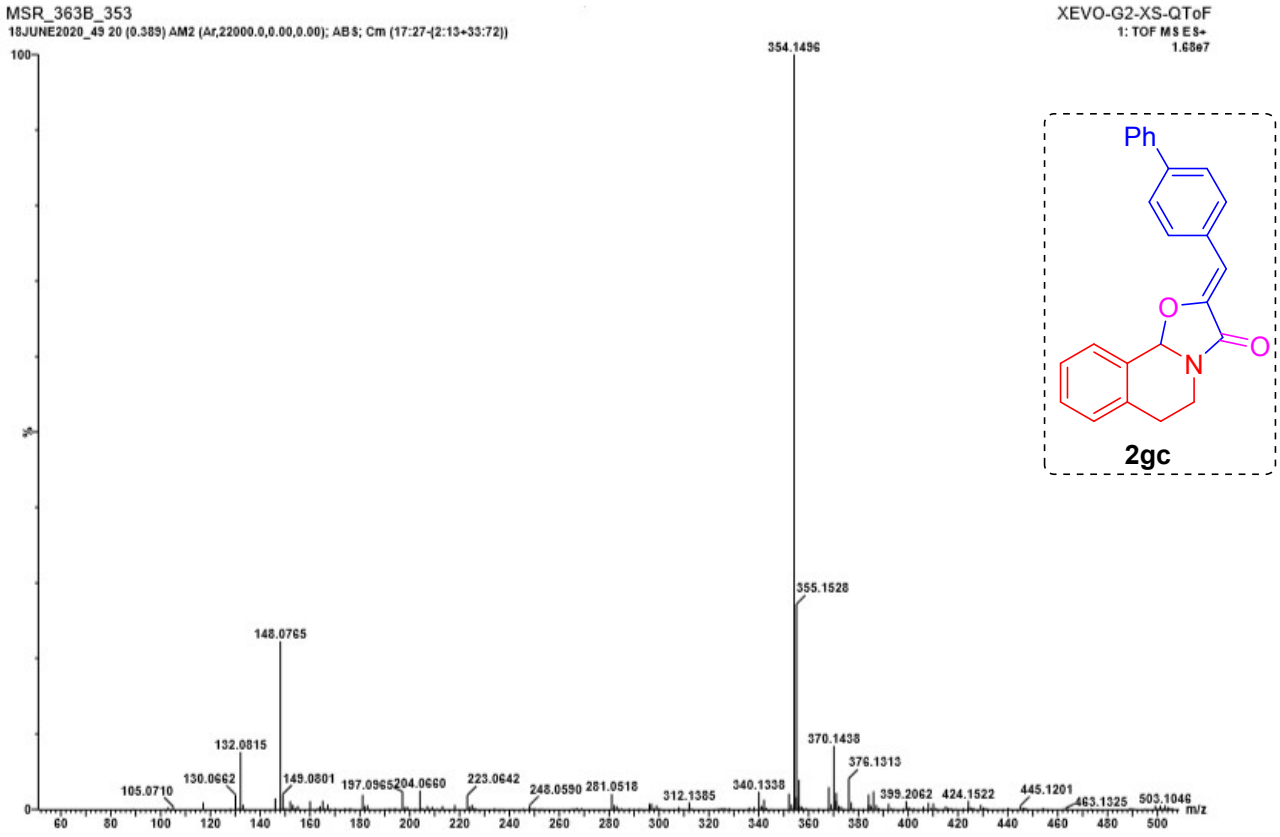


HRMS spectrum of compound 2fc

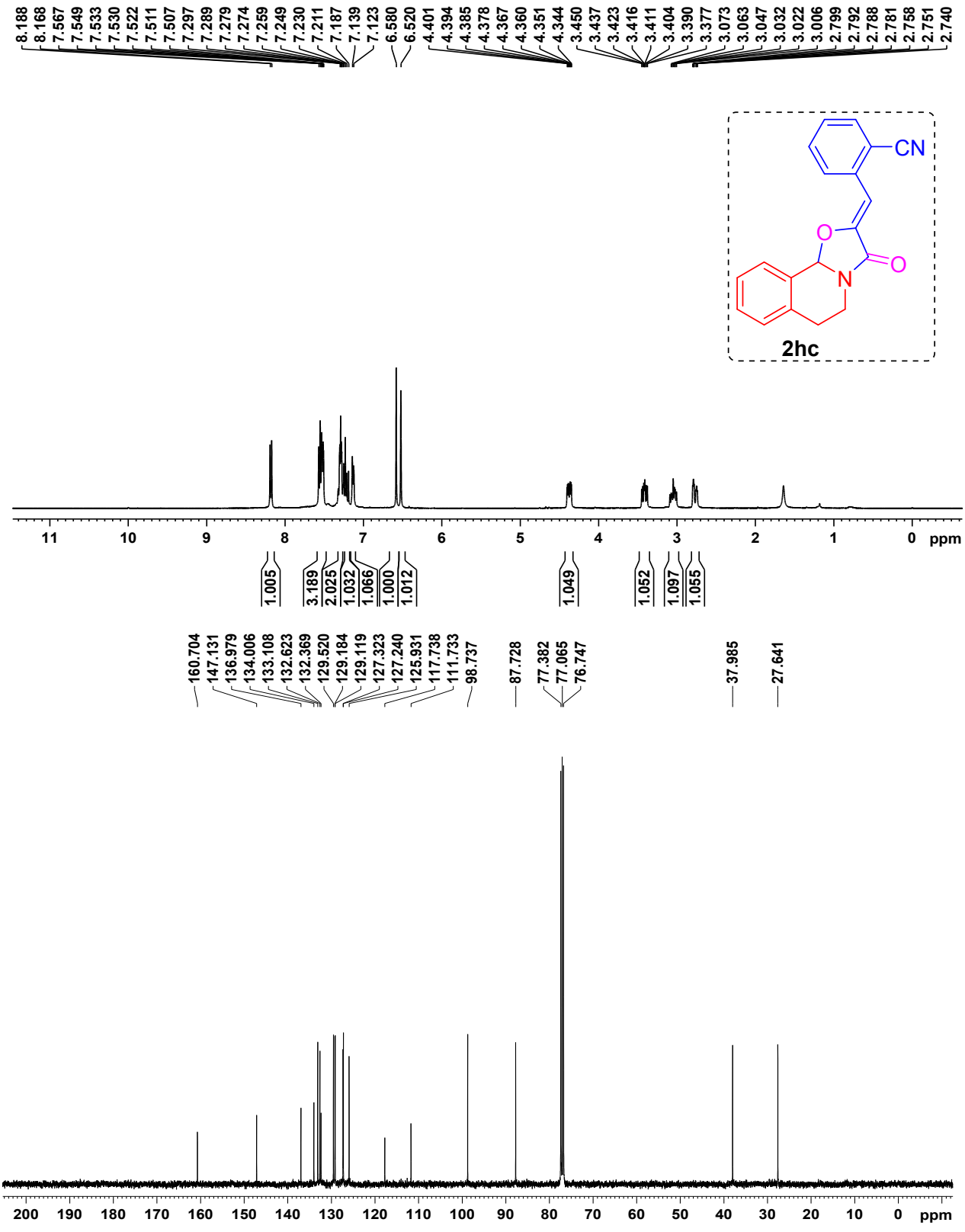




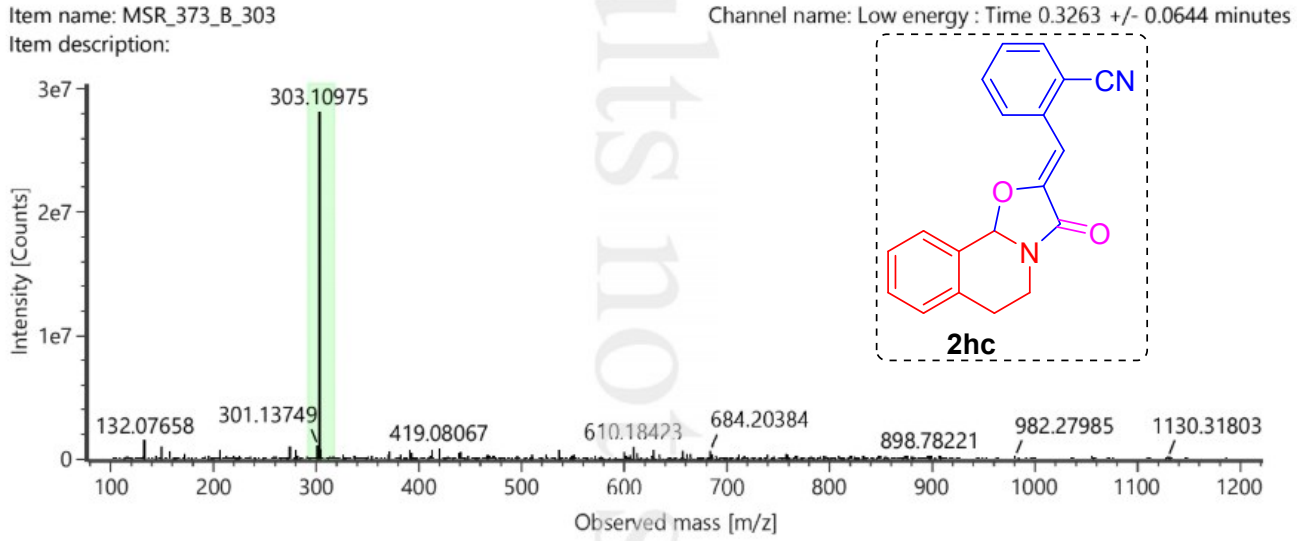
^{1}H & ^{13}C spectra of compound 2gc



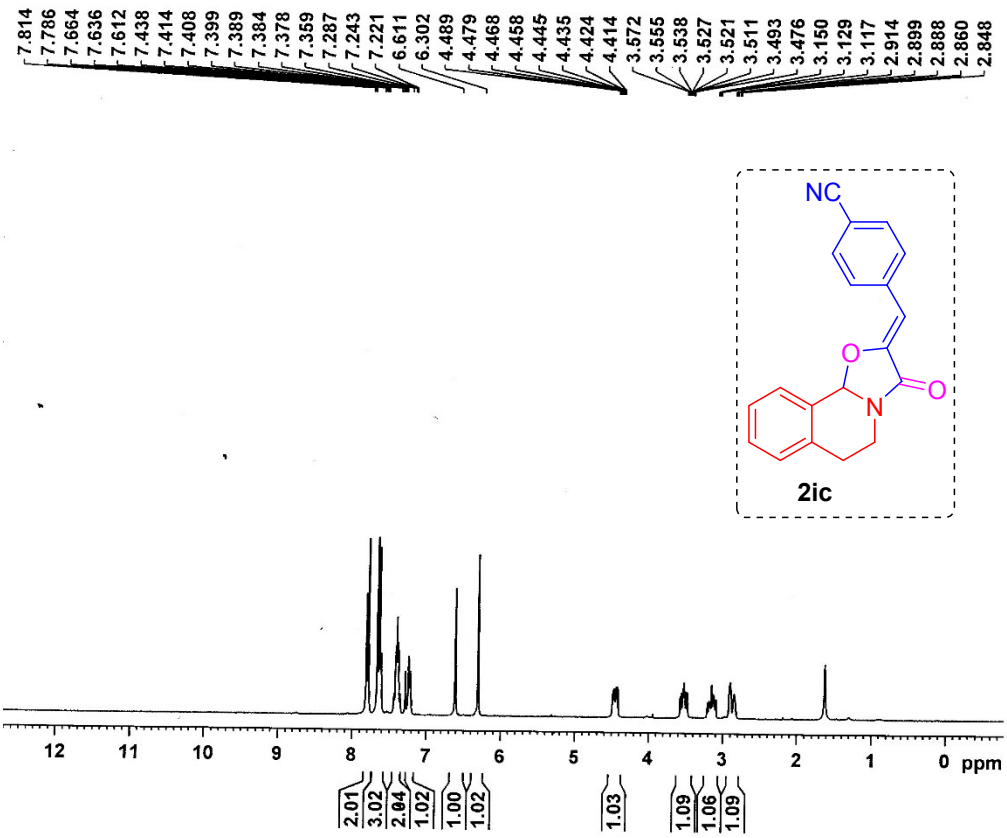
HRMS spectrum of compound 2gc



^{1}H & ^{13}C spectra of compound 2hc



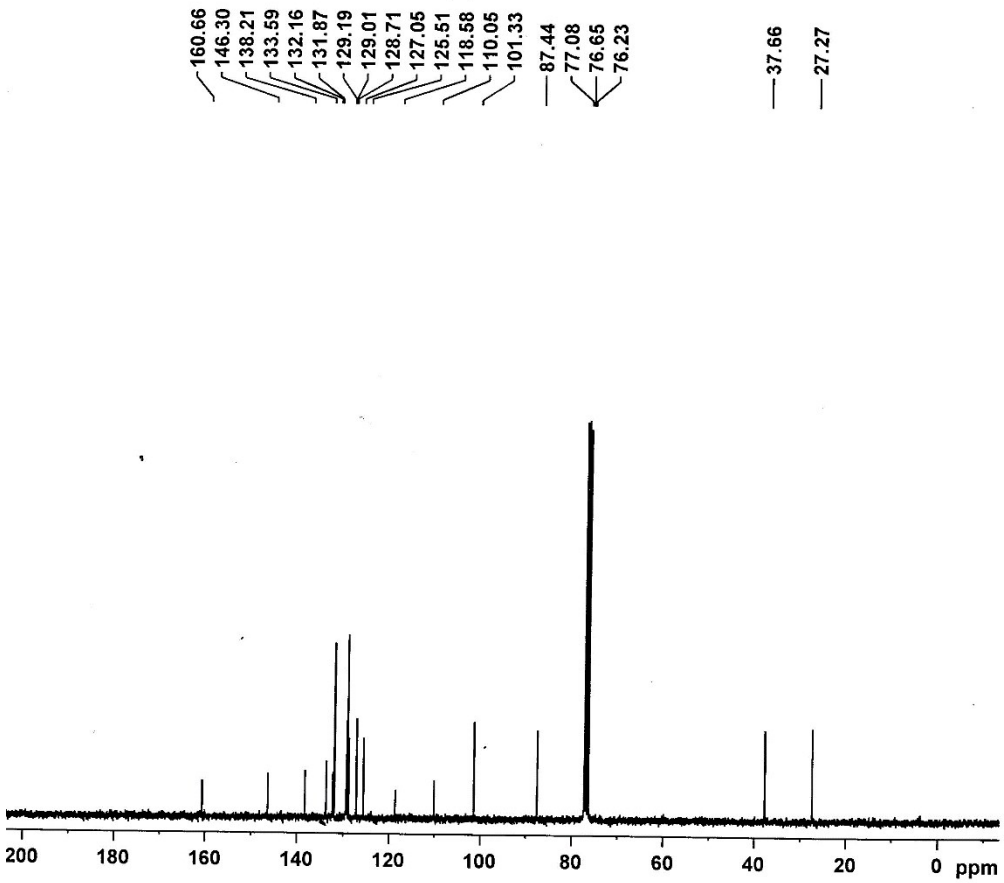
HRMS Spectrum of compound 2hc



BRUKER

NAME PROTON_UOM
EXPNO 1
PROCNO 1
Date_ 20200320
Time 15.51
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 362
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =======
NUC1 1H
P1 13.50 usec
PL1 -1.00 dB
PL1W 13.28156662 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



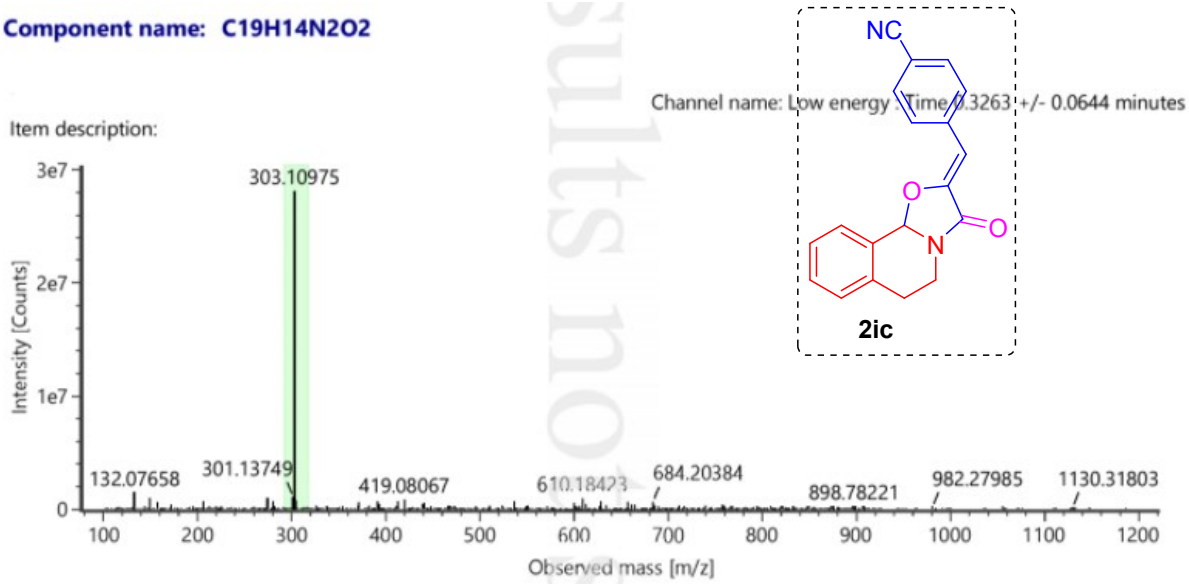
BRUKER

NAME RA-BR-3-373 B
EXPNO 1
PROCNO 1
Date_ 20200320
Time 15.43
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 737
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 5160.6
DW 27.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

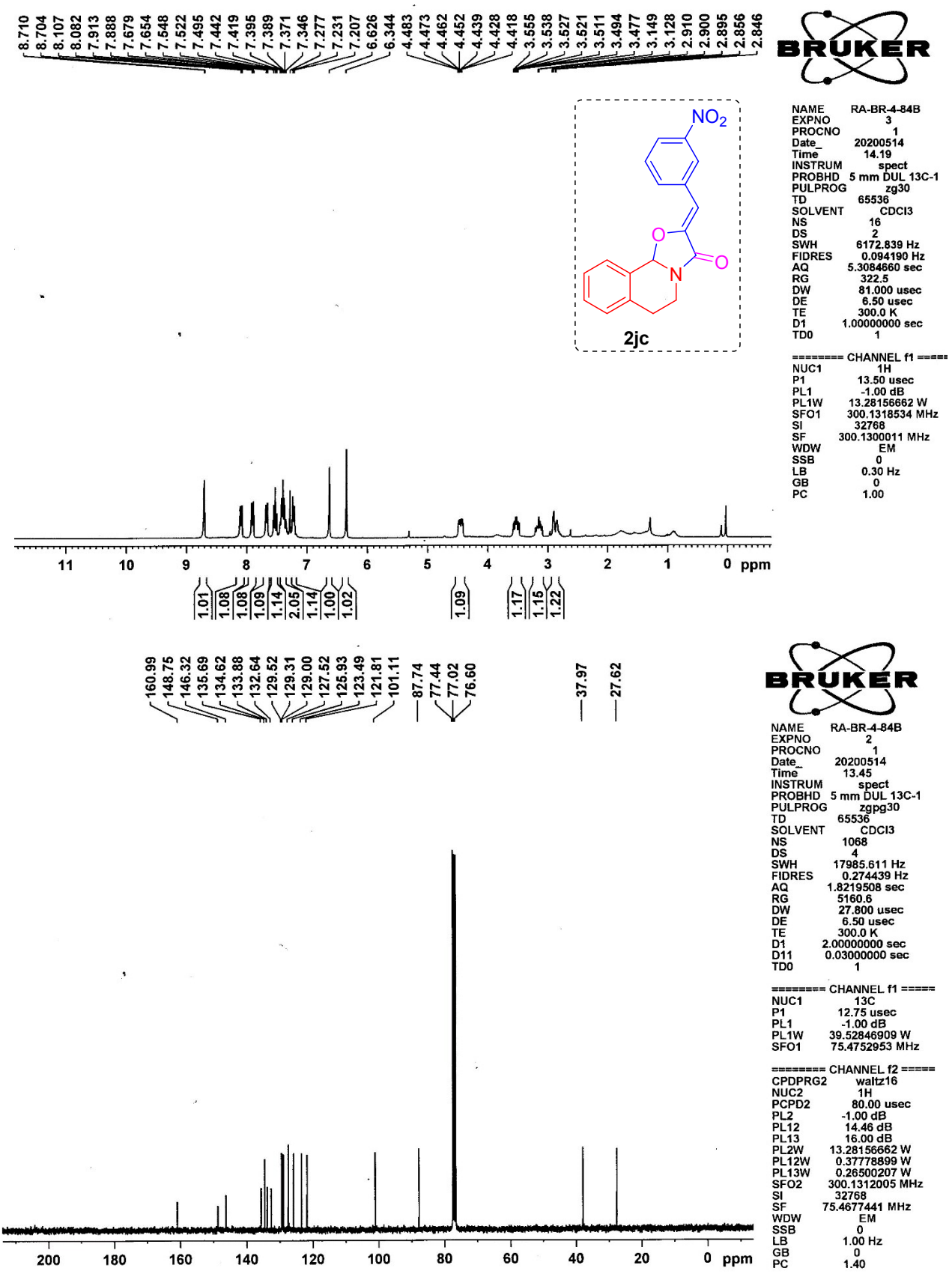
======== CHANNEL f1 ======
NUC1 13C
P1 12.75 usec
PL1 -1.00 dB
PL1W 39.52846909 W
SFO1 75.4752953 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.46 dB
PL13 16.00 dB
PL2W 13.28156662 W
PL12W 0.37778899 W
PL13W 0.26500207 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677728 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

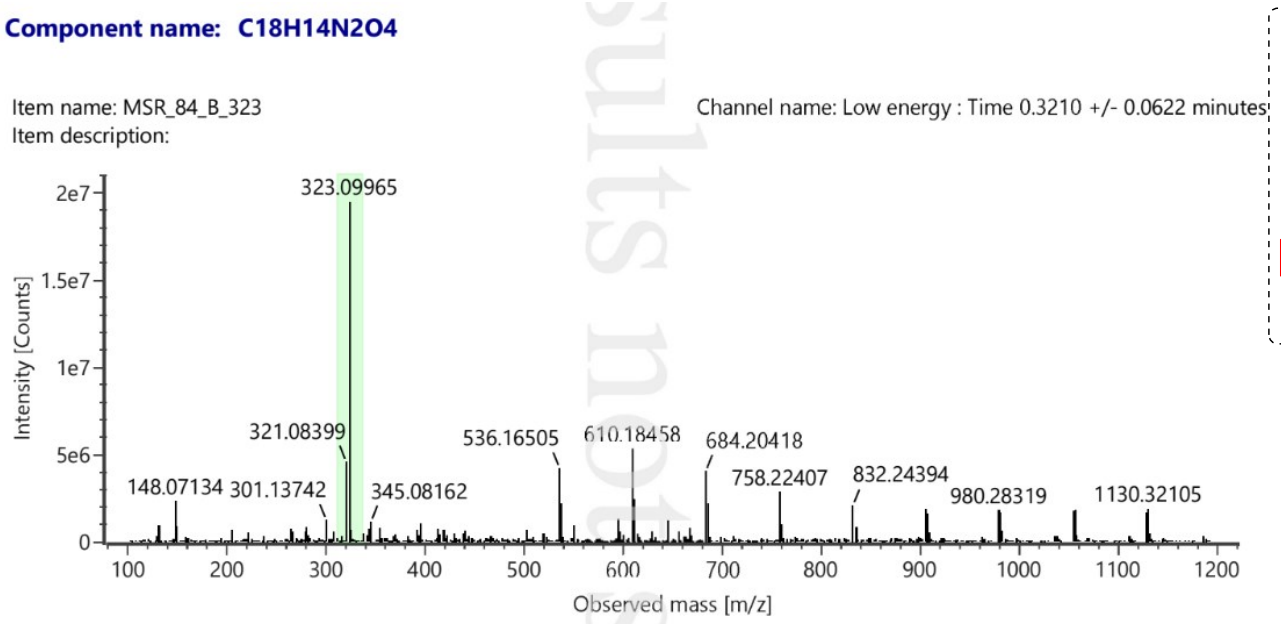
^{1}H & ^{13}C spectra of compound 2ic



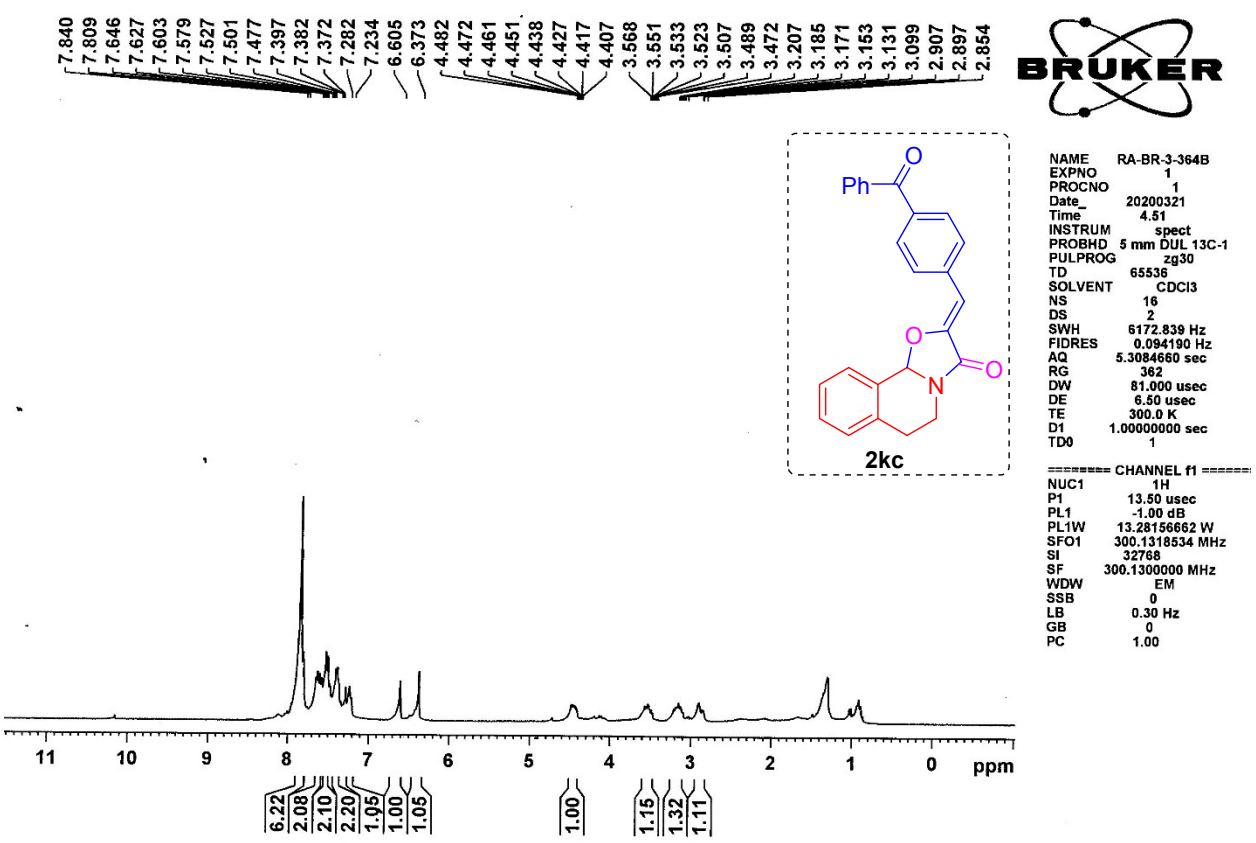
MS Spectrum of Compound 2ic

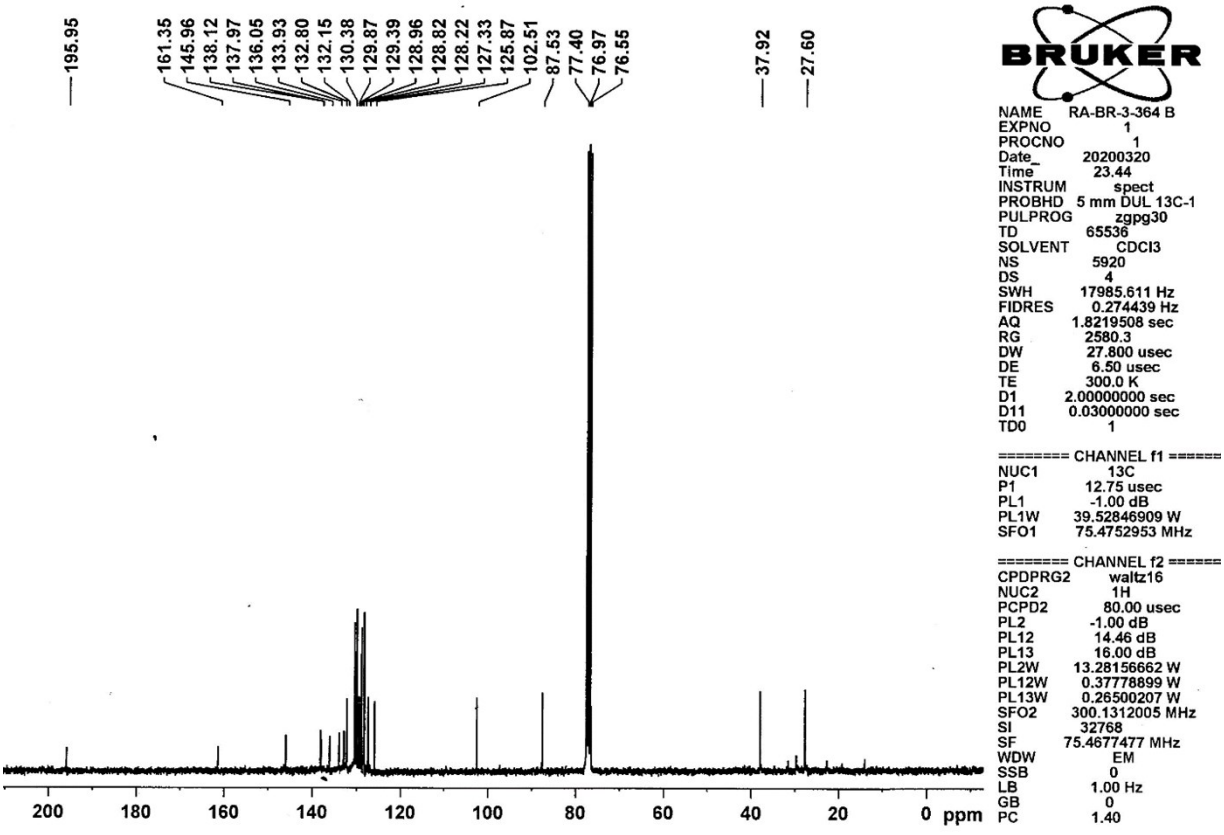


^{1}H & ^{13}C spectra of compound 2jc

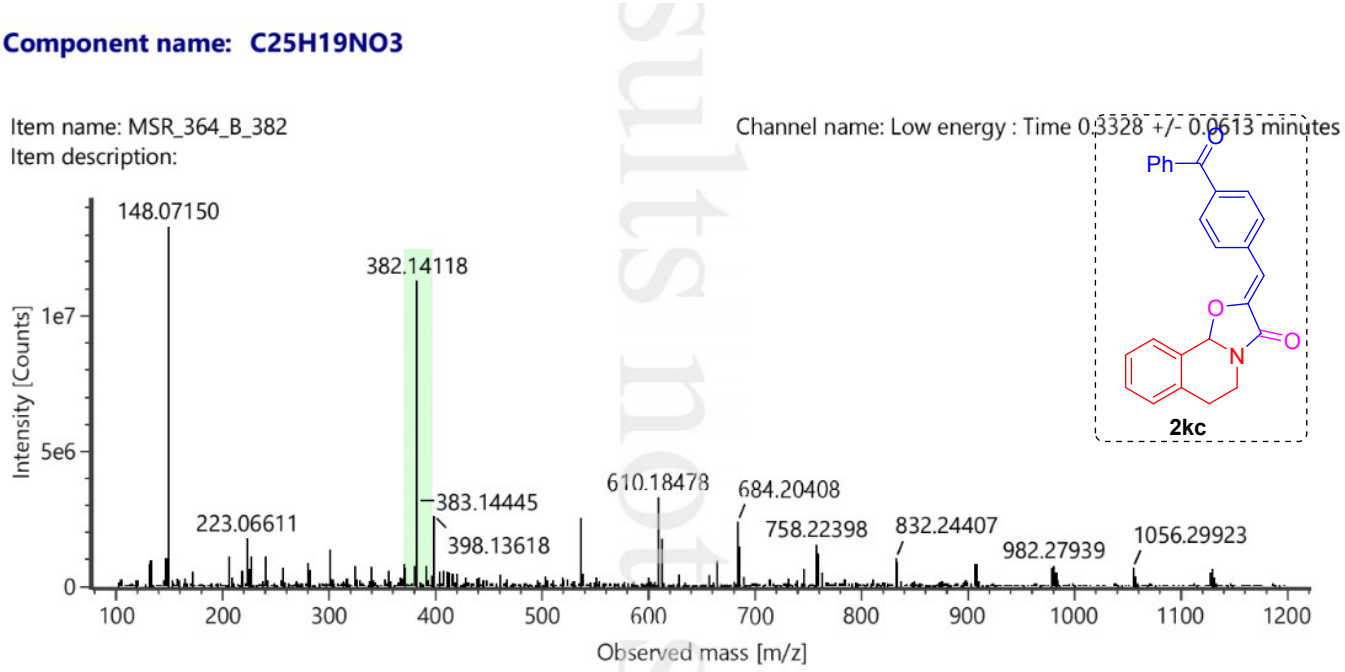


HRMS Spectrum of Compound 2jc

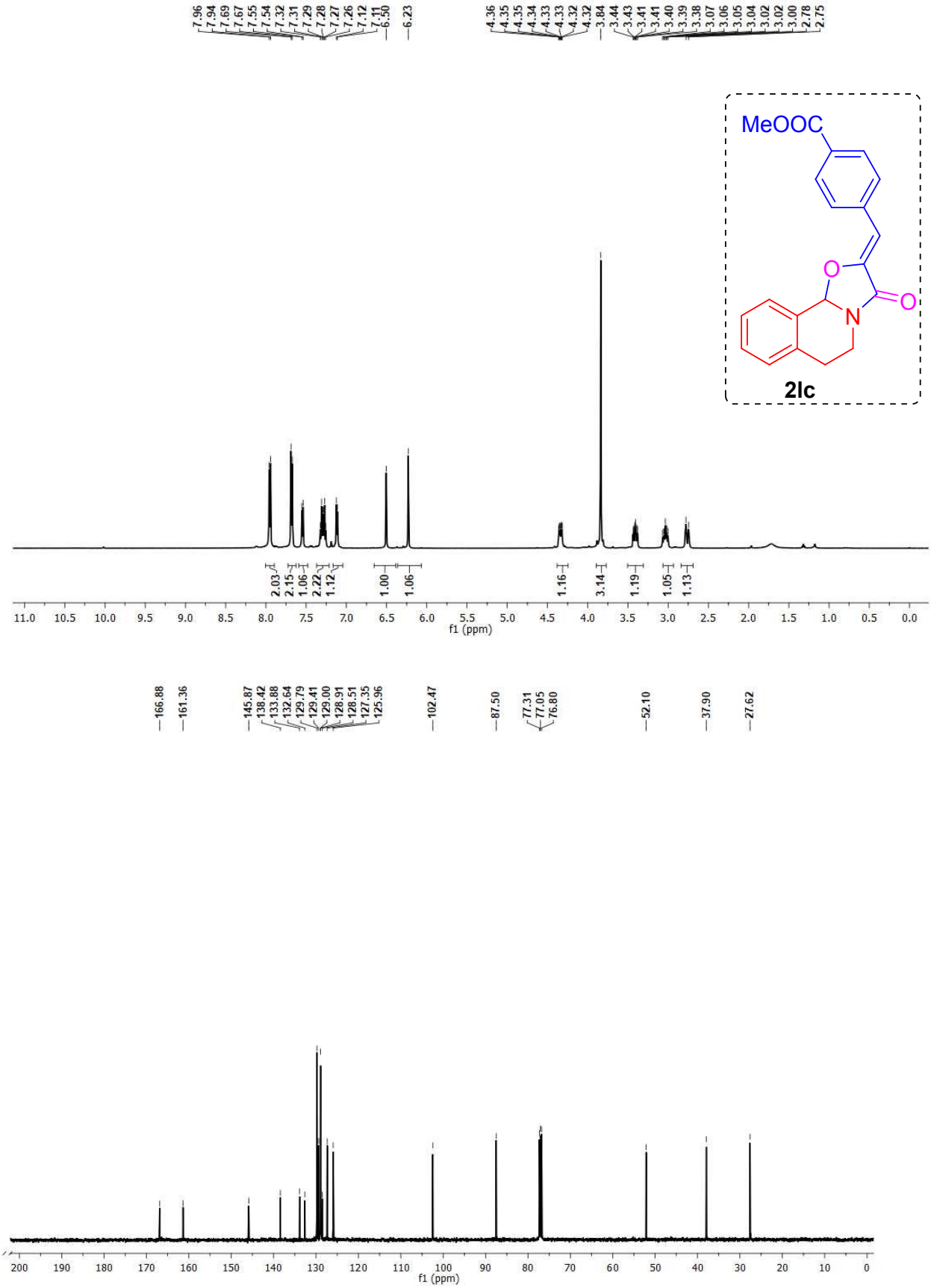




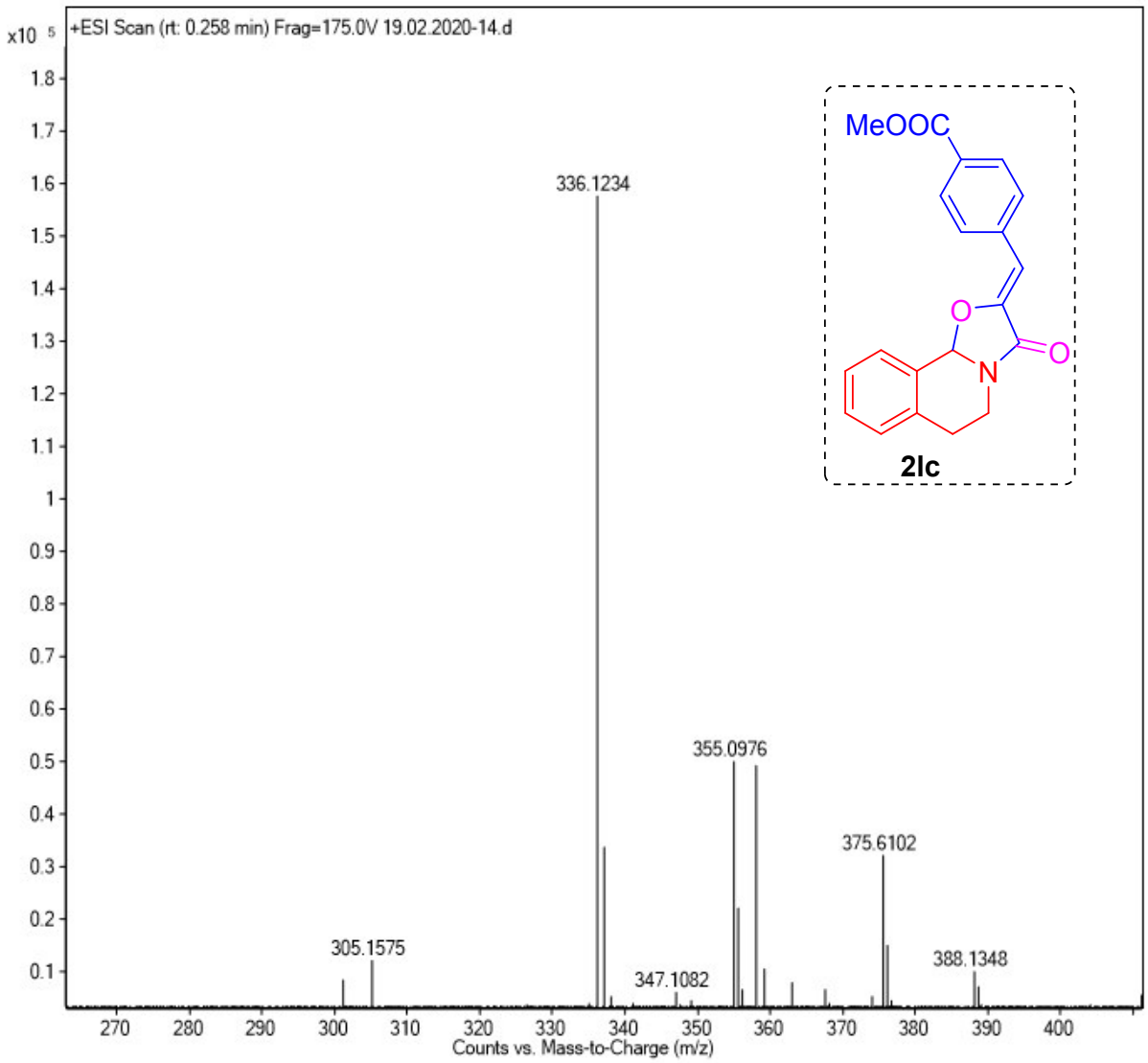
1H & 13C spectra of compound 2kc



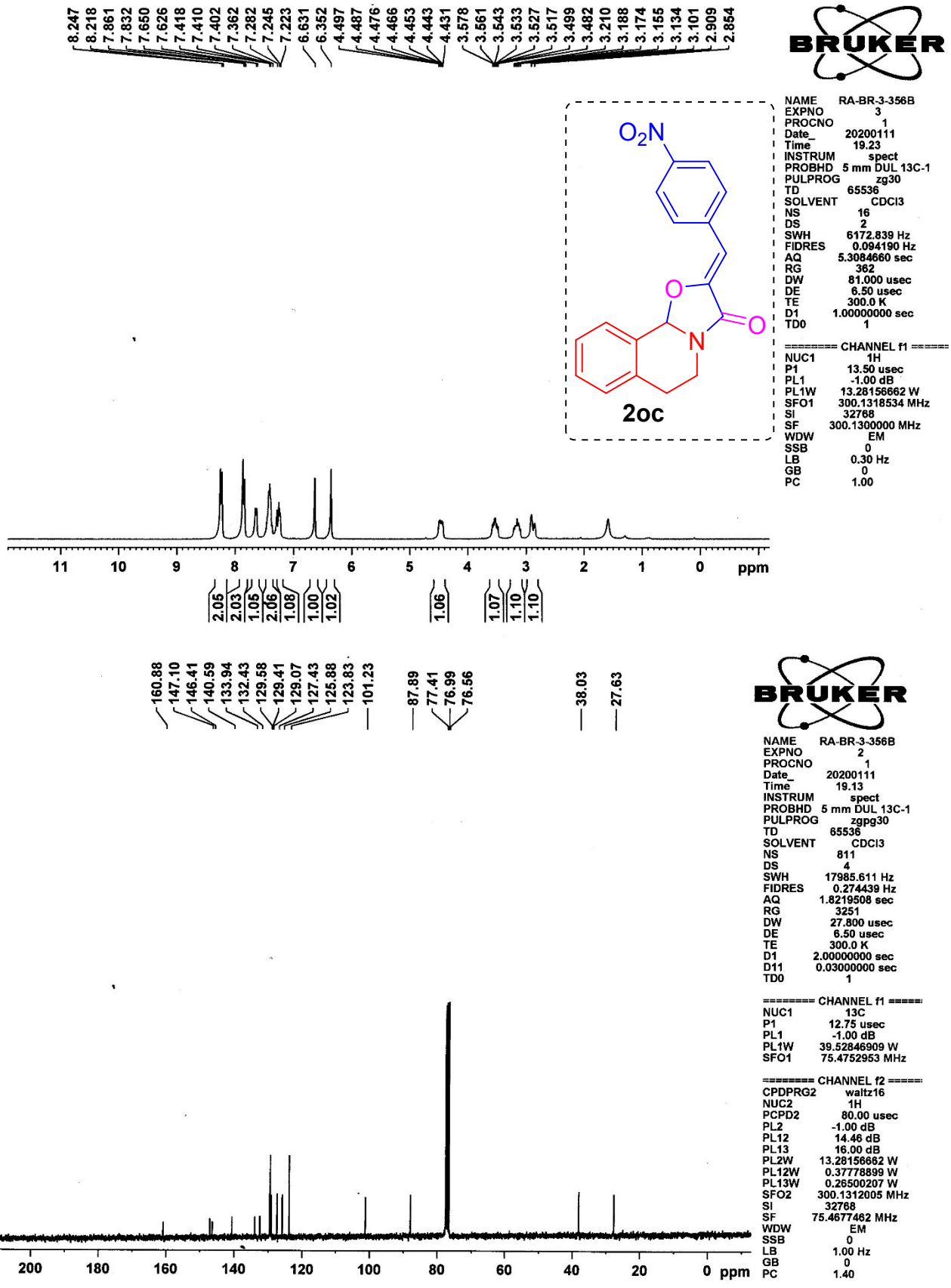
HRMS Spectrum of Copmound 2kc



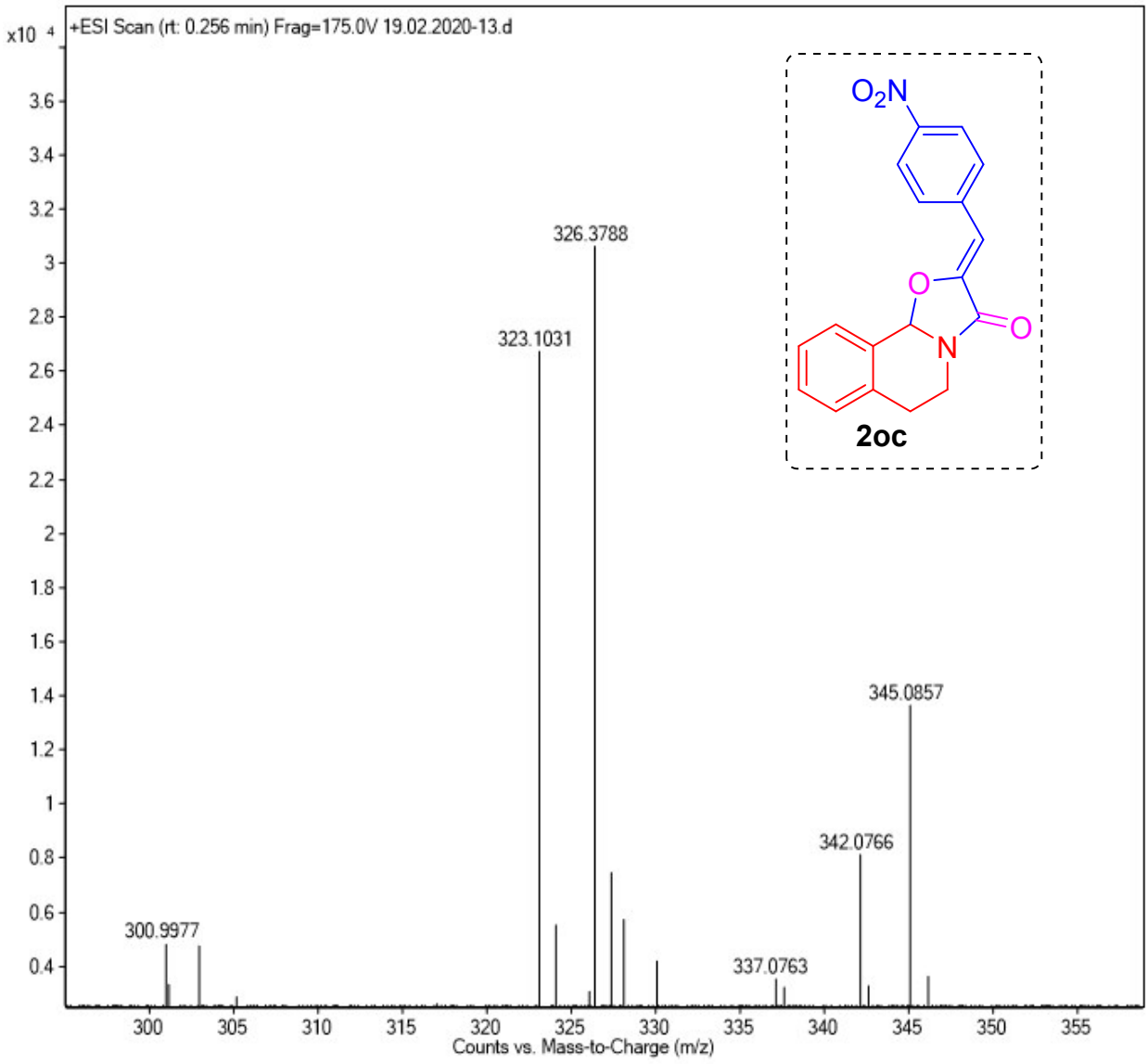
^{1}H & ^{13}C spectra of compound 2lc



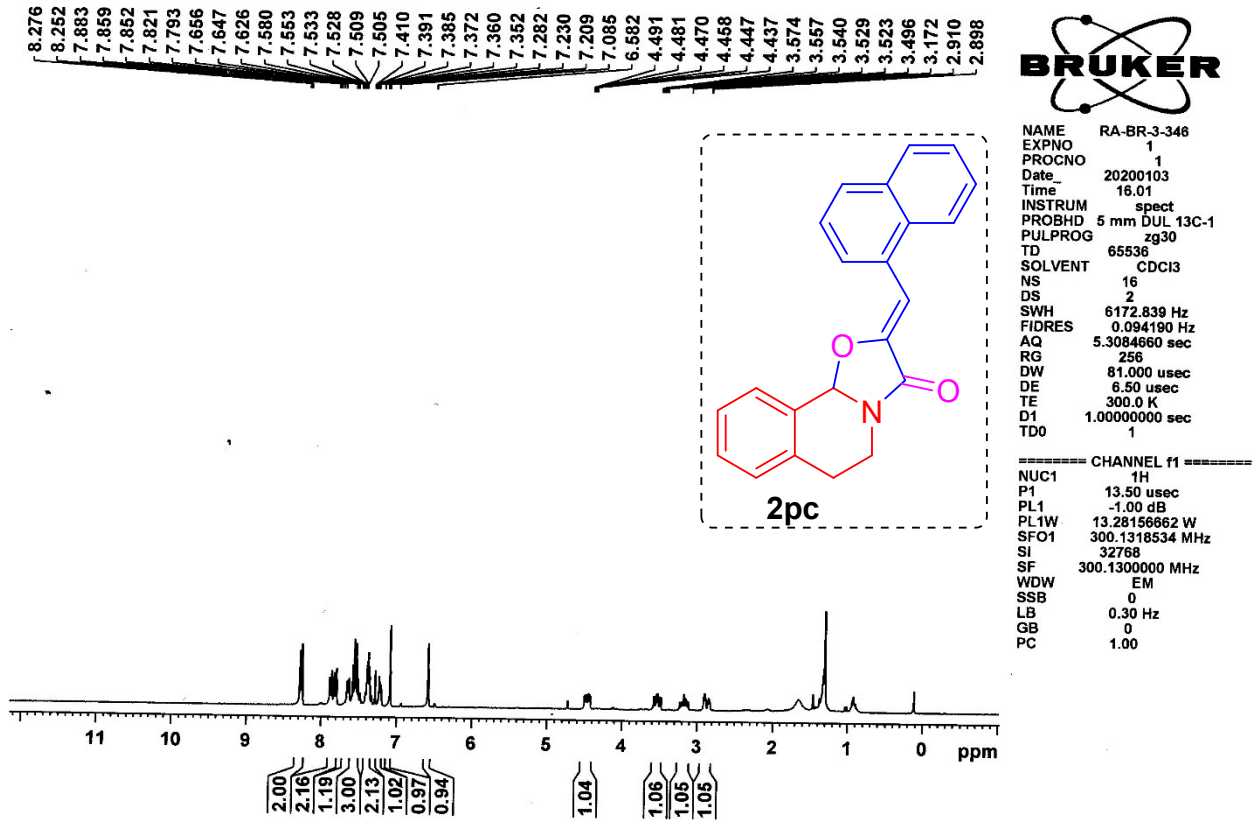
HRMS spectrum of compound 2lc



^{1}H & ^{13}C spectra of compound 2oc



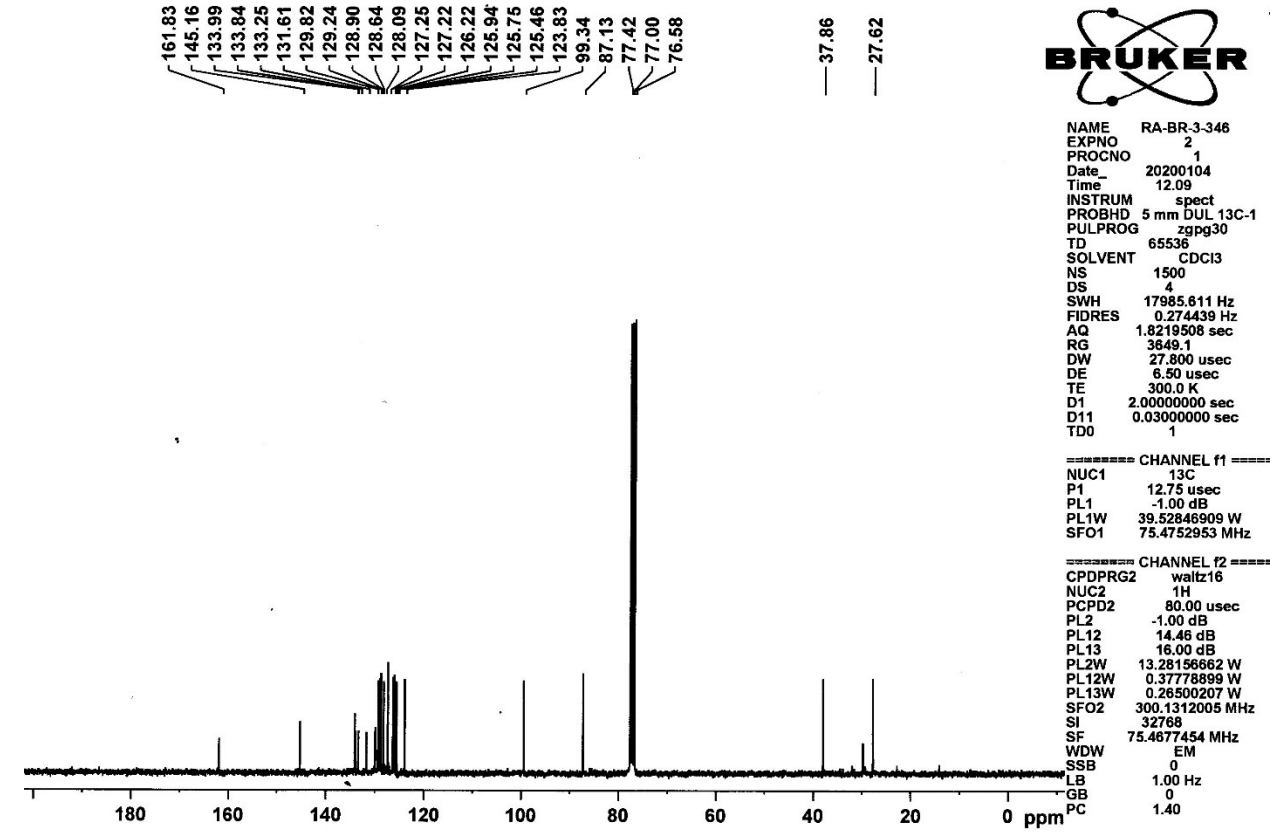
HRMS spectrum of compound 2oc



BRUKER

NAME RA-BR-3-346
EXPNO 1
PROCNO 1
Date_ 20200103
Time 16.01
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 256
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.50 usec
PL1 -1.00 dB
PL1W 13.28156662 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



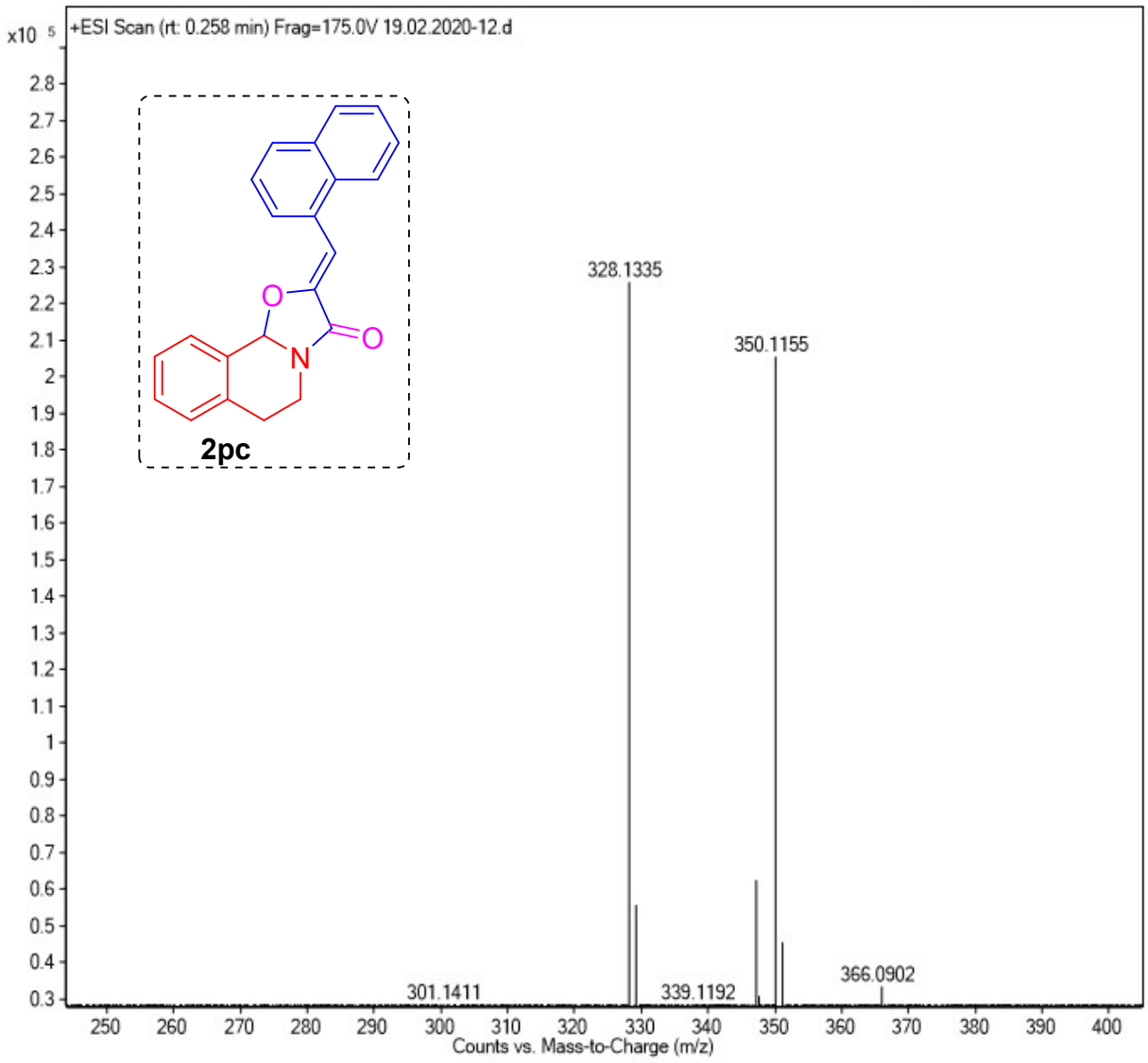
BRUKER

NAME RA-BR-3-346
EXPNO 2
PROCNO 1
Date_ 20200104
Time 12.09
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1500
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 3649.1
DW 27.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

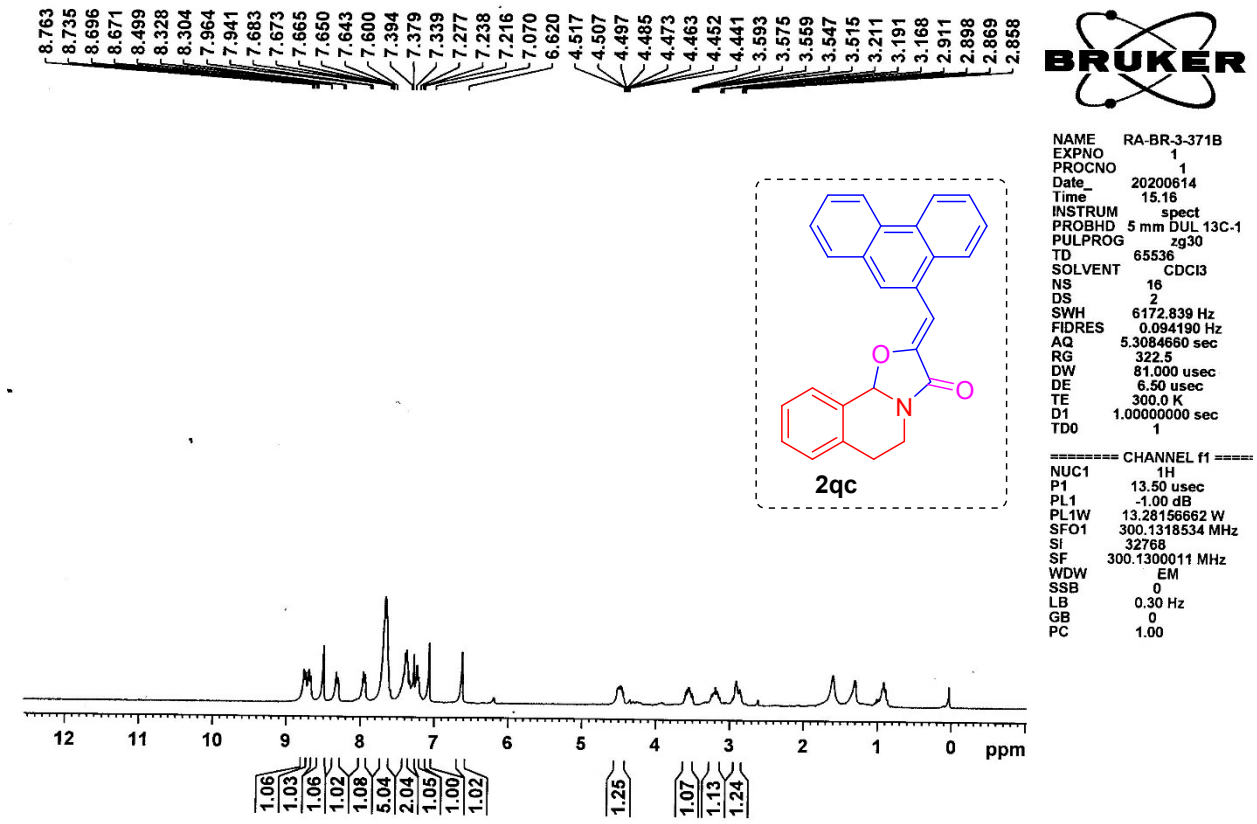
======== CHANNEL f1 ========
NUC1 13C
P1 12.75 usec
PL1 -1.00 dB
PL1W 39.52846909 W
SFO1 75.4752953 MHz

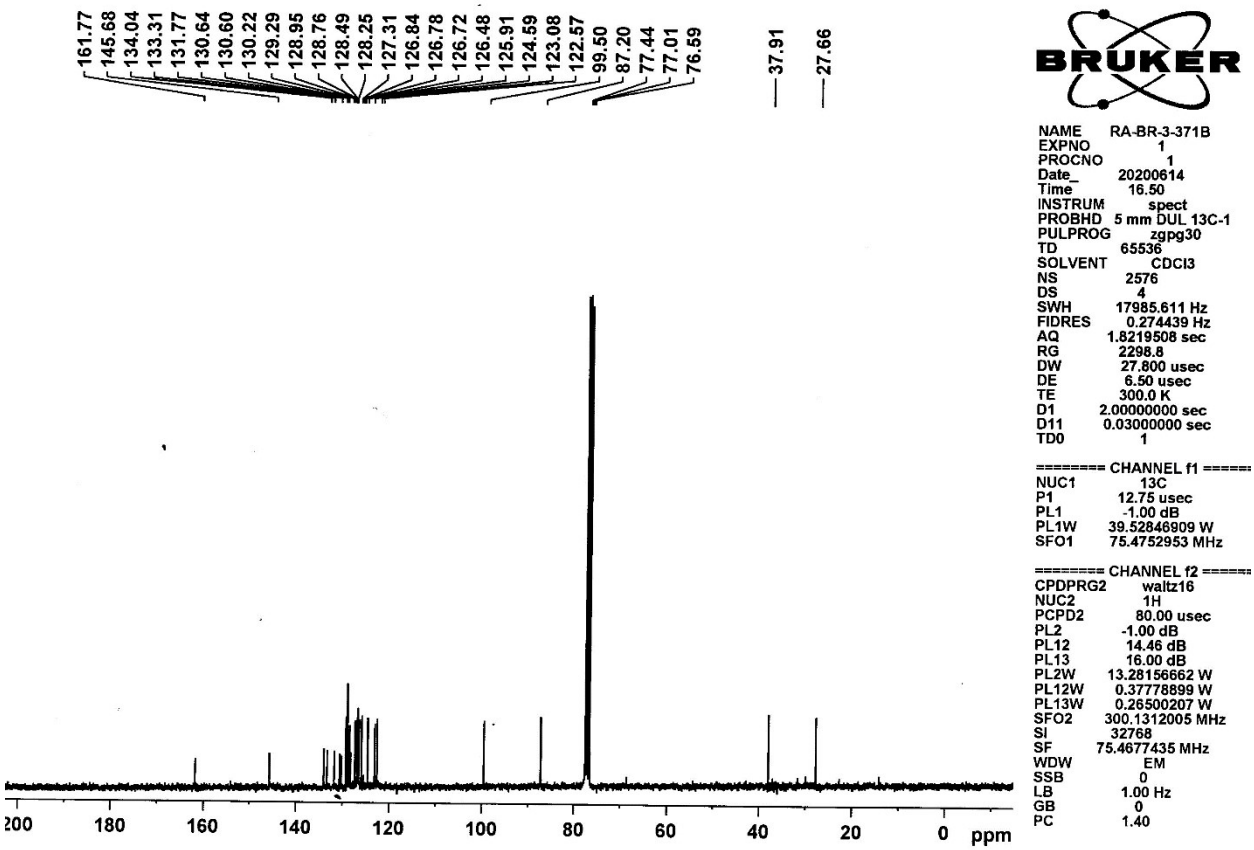
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.46 dB
PL13 16.00 dB
PL2W 13.28156662 W
PL12W 0.37778899 W
PL13W 0.26500207 W
SFO2 300.1312005 MHz
SI 32768
SF 75.4677454 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{1}H & ^{13}C spectra of compound 2pc

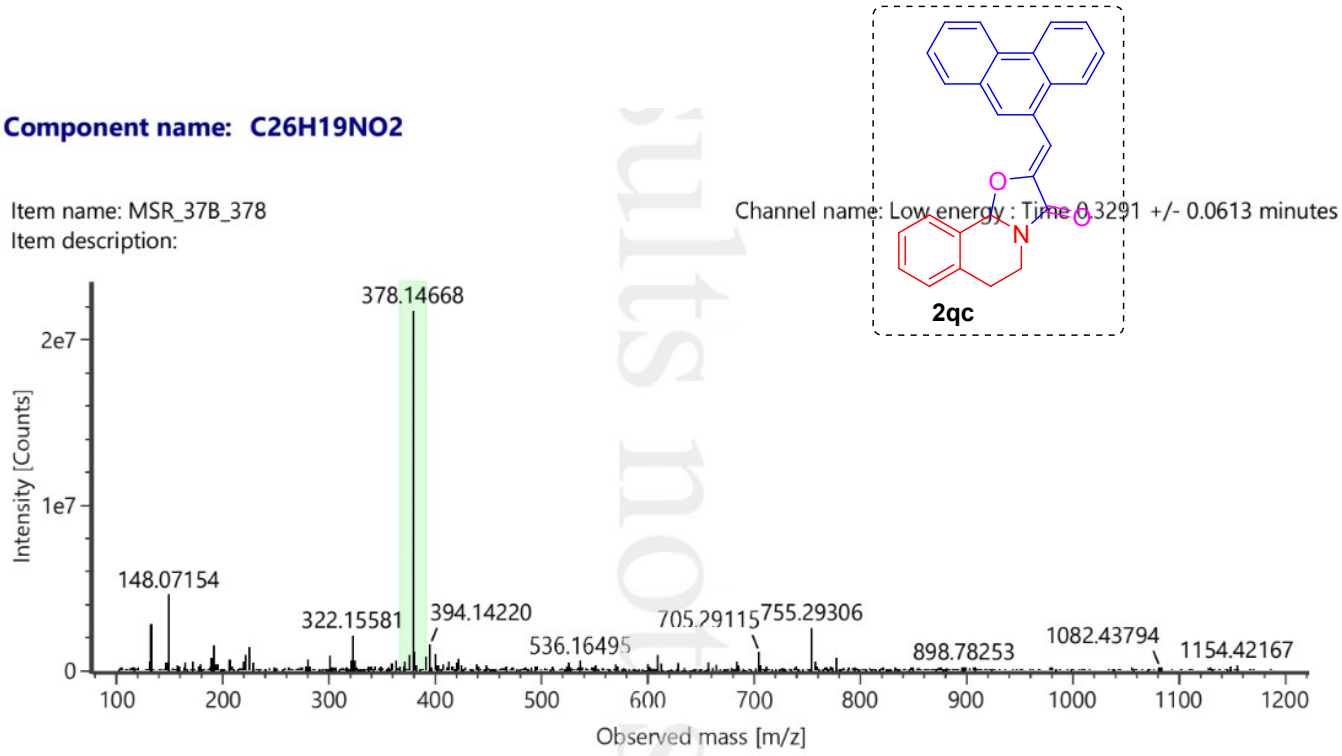


HRMS spectrum of compound 2pc

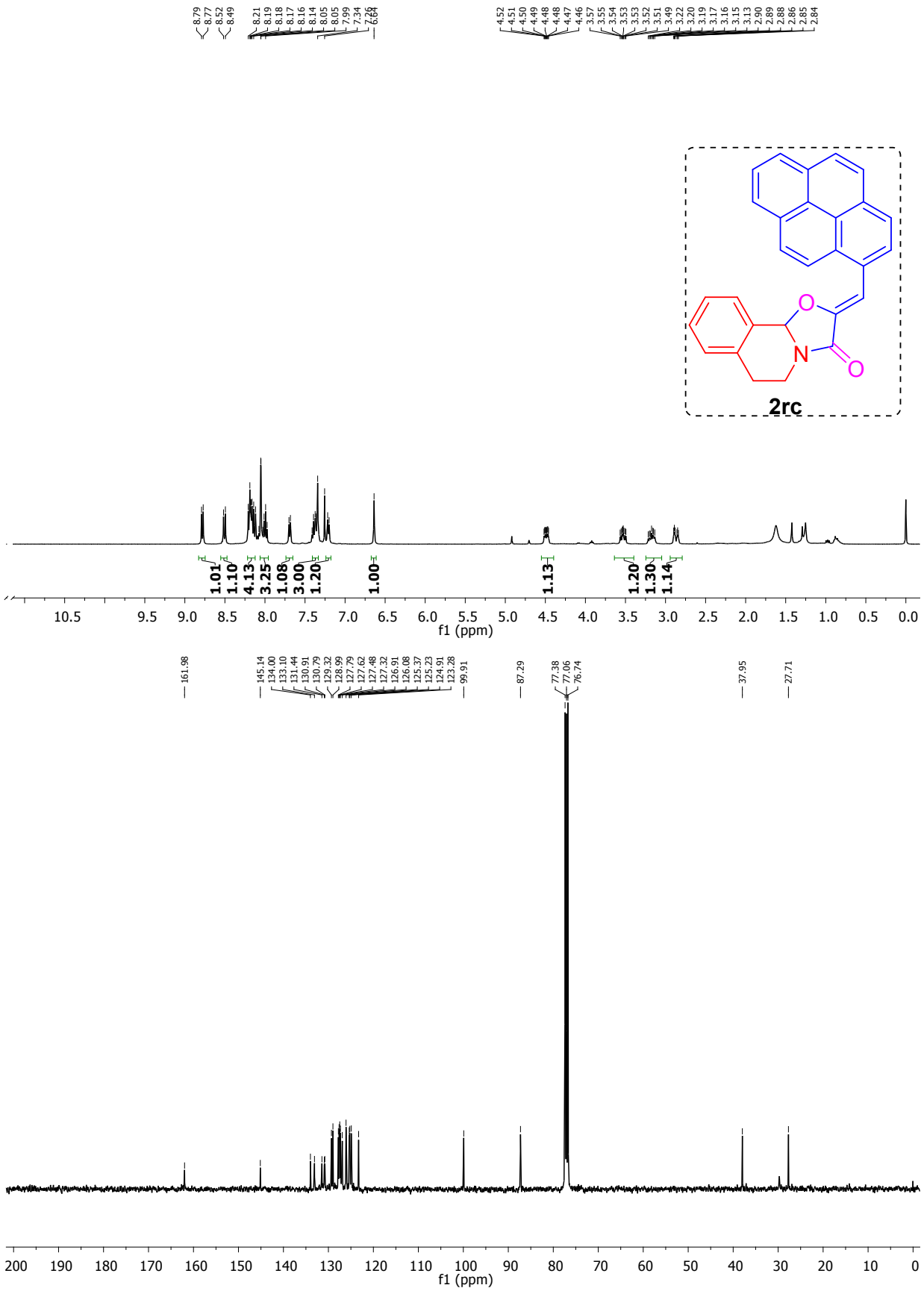




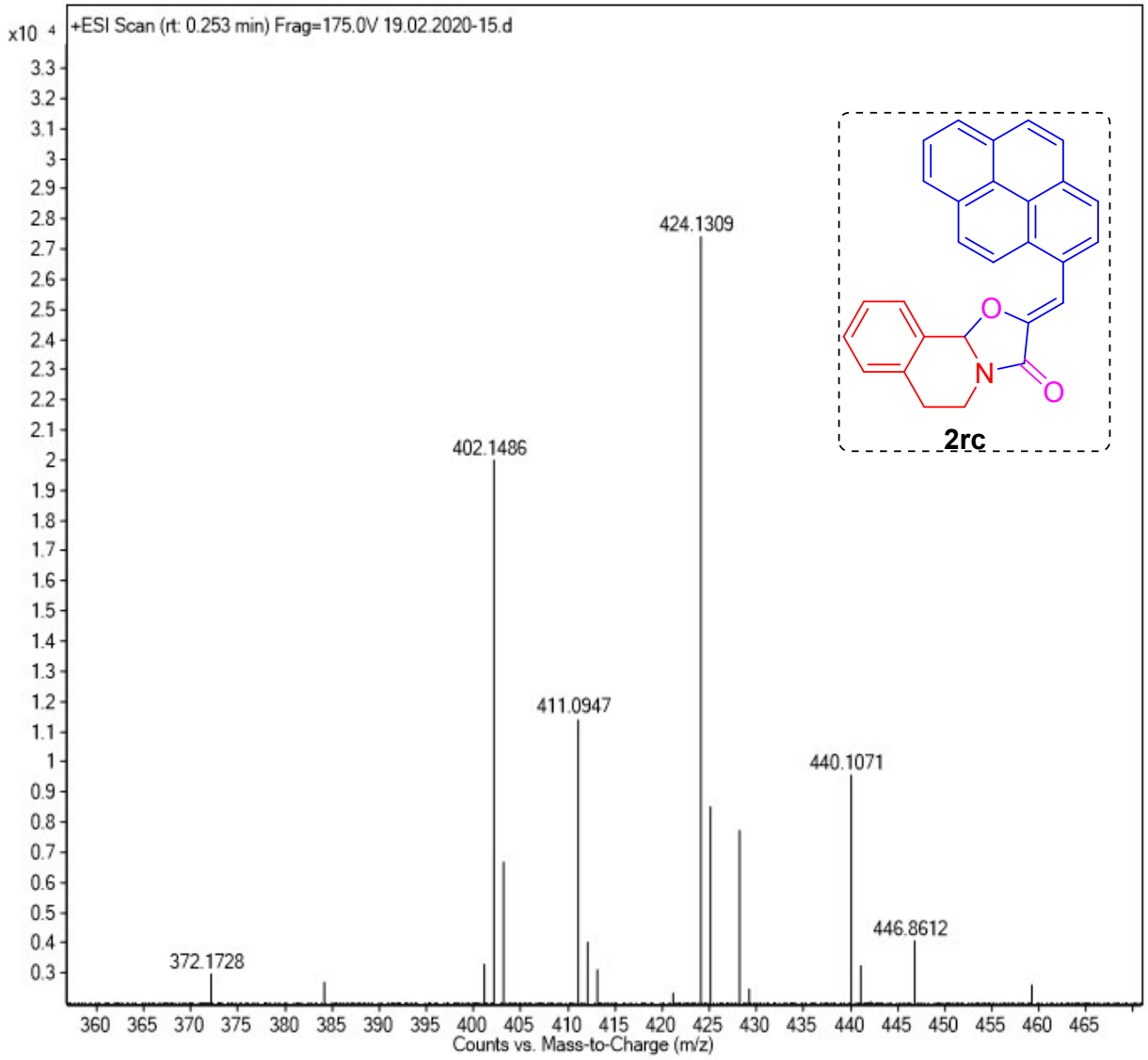
^{1}H & ^{13}C spectra of compound 2qc



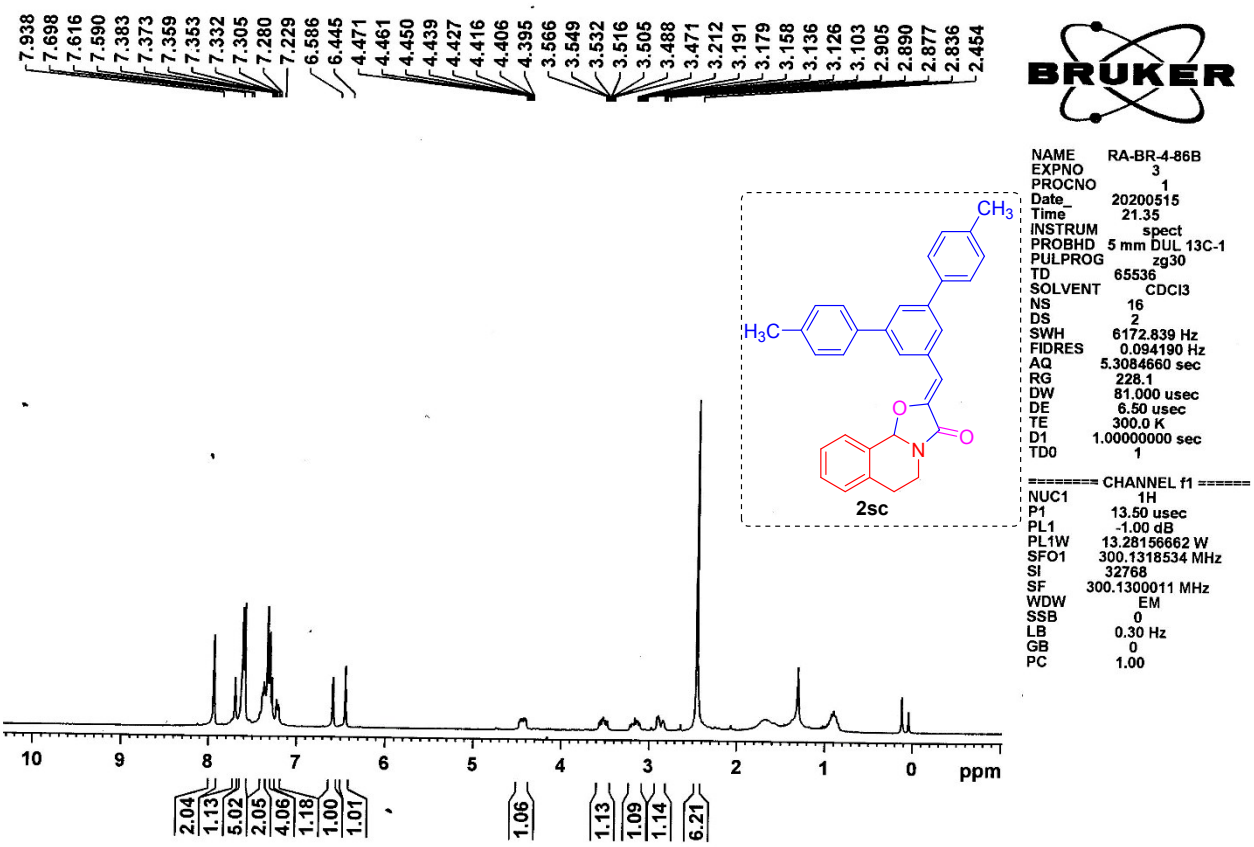
HRMS Spectrum of copound 2qc

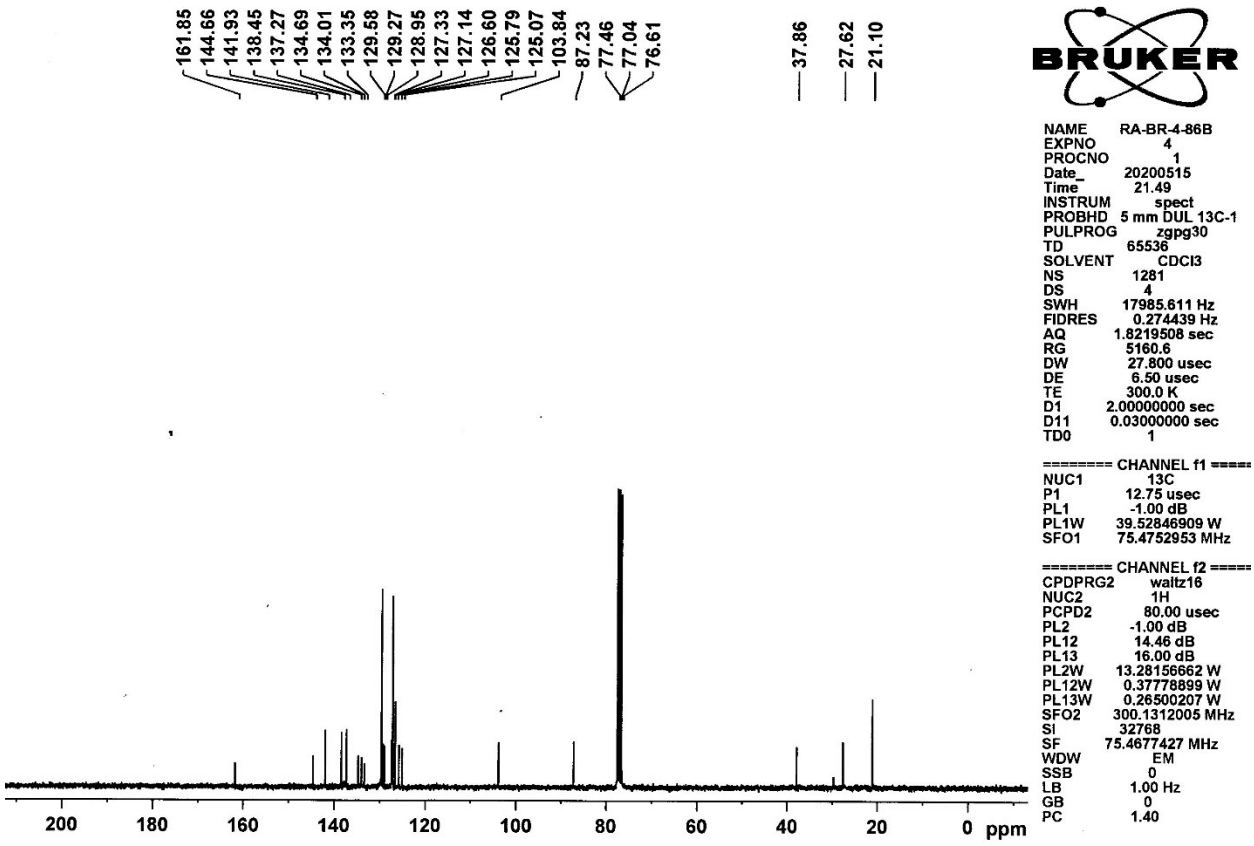


^{1}H & ^{13}C spectra of compound 2rc

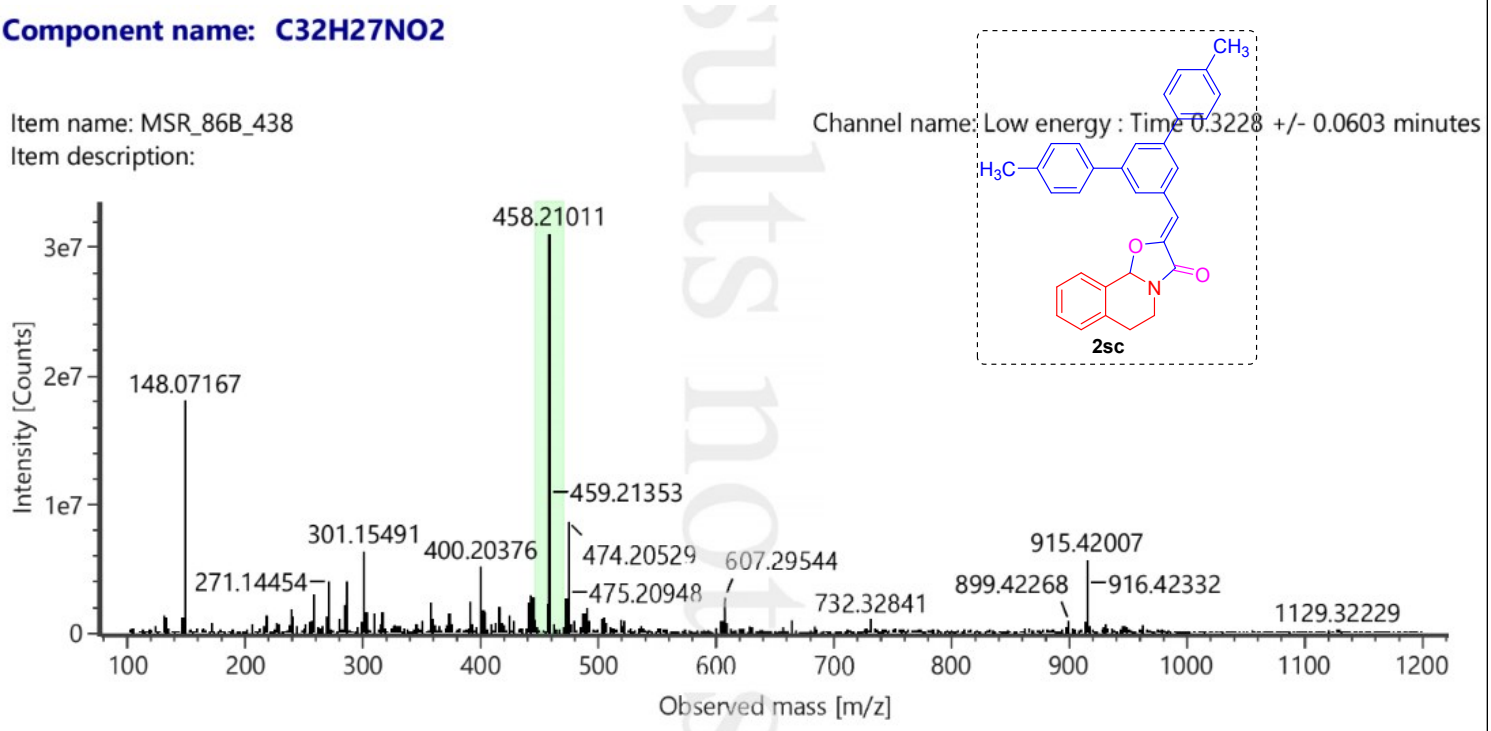


HRMS spectrum of compound 2rc

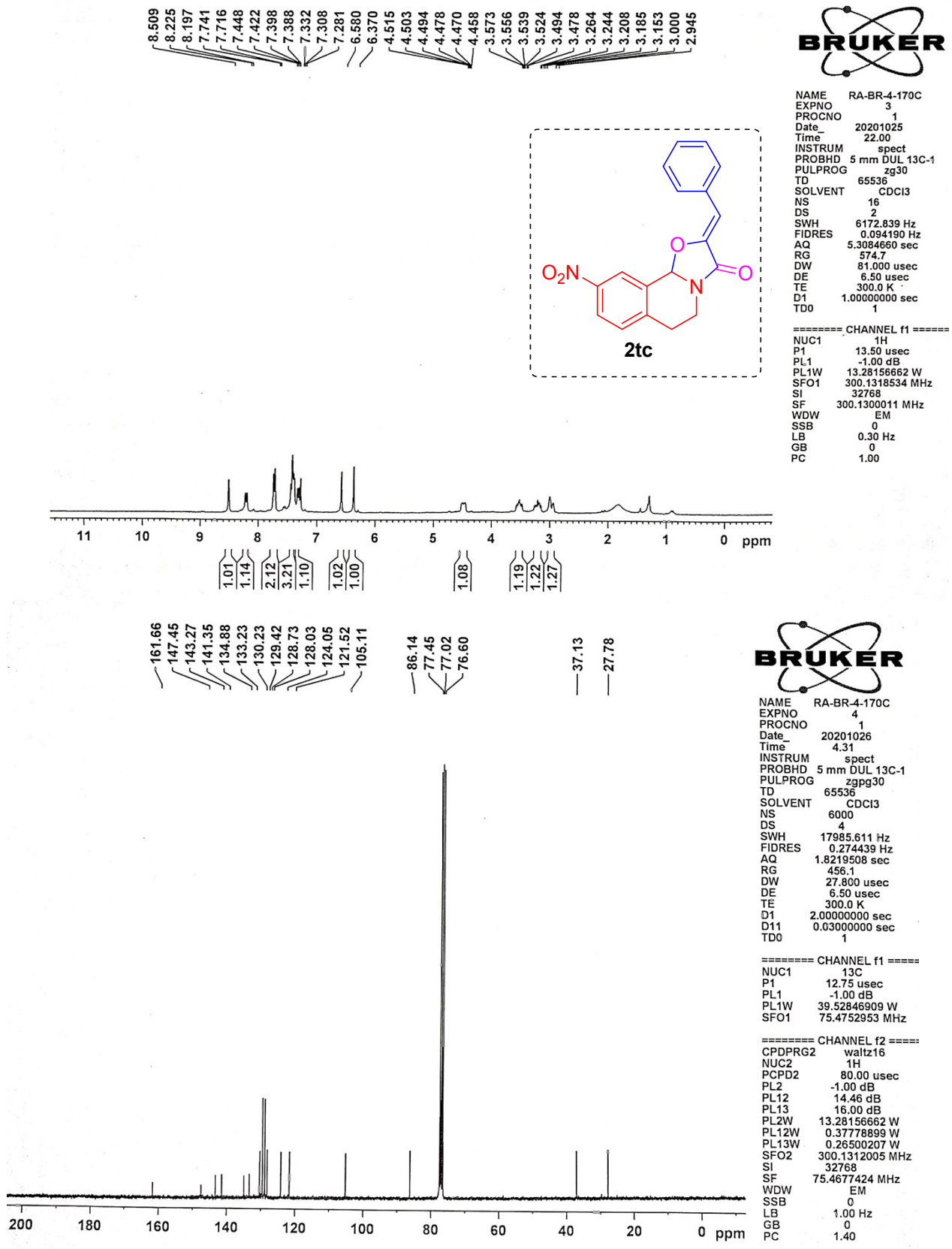




^{1}H & ^{13}C spectra of compound 2sc



HRMS Spectrum of Compound 2sc

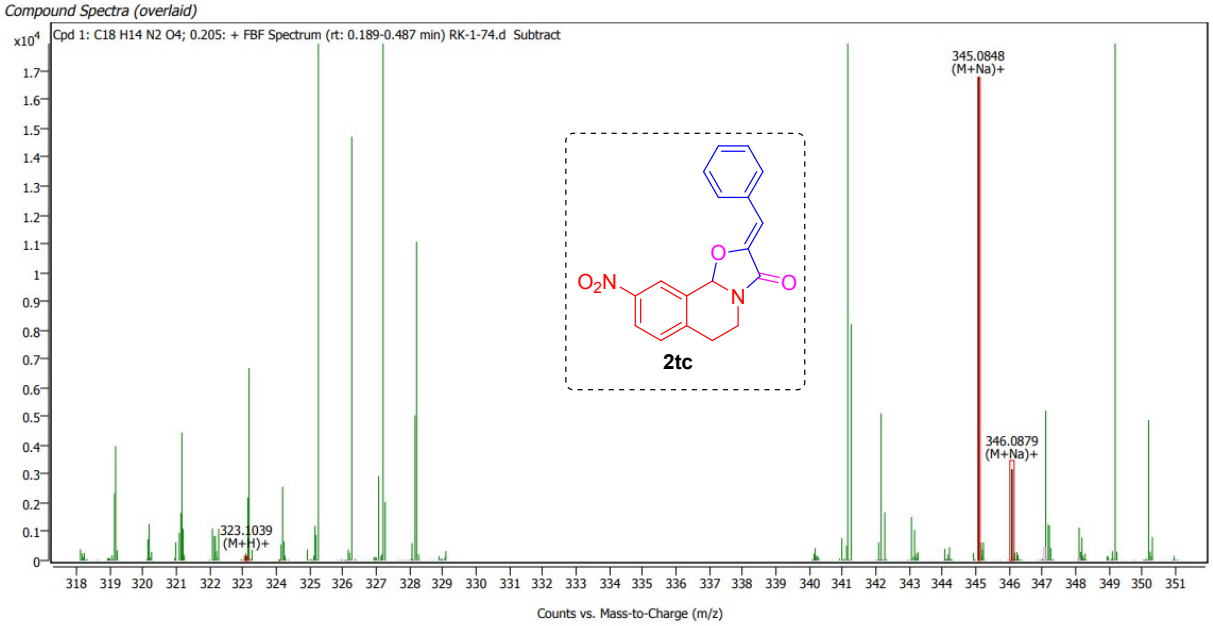


^{1}H & ^{13}C spectra of compound 2tc

Compound Details

Cpd. 1: C18 H14 N2 O4

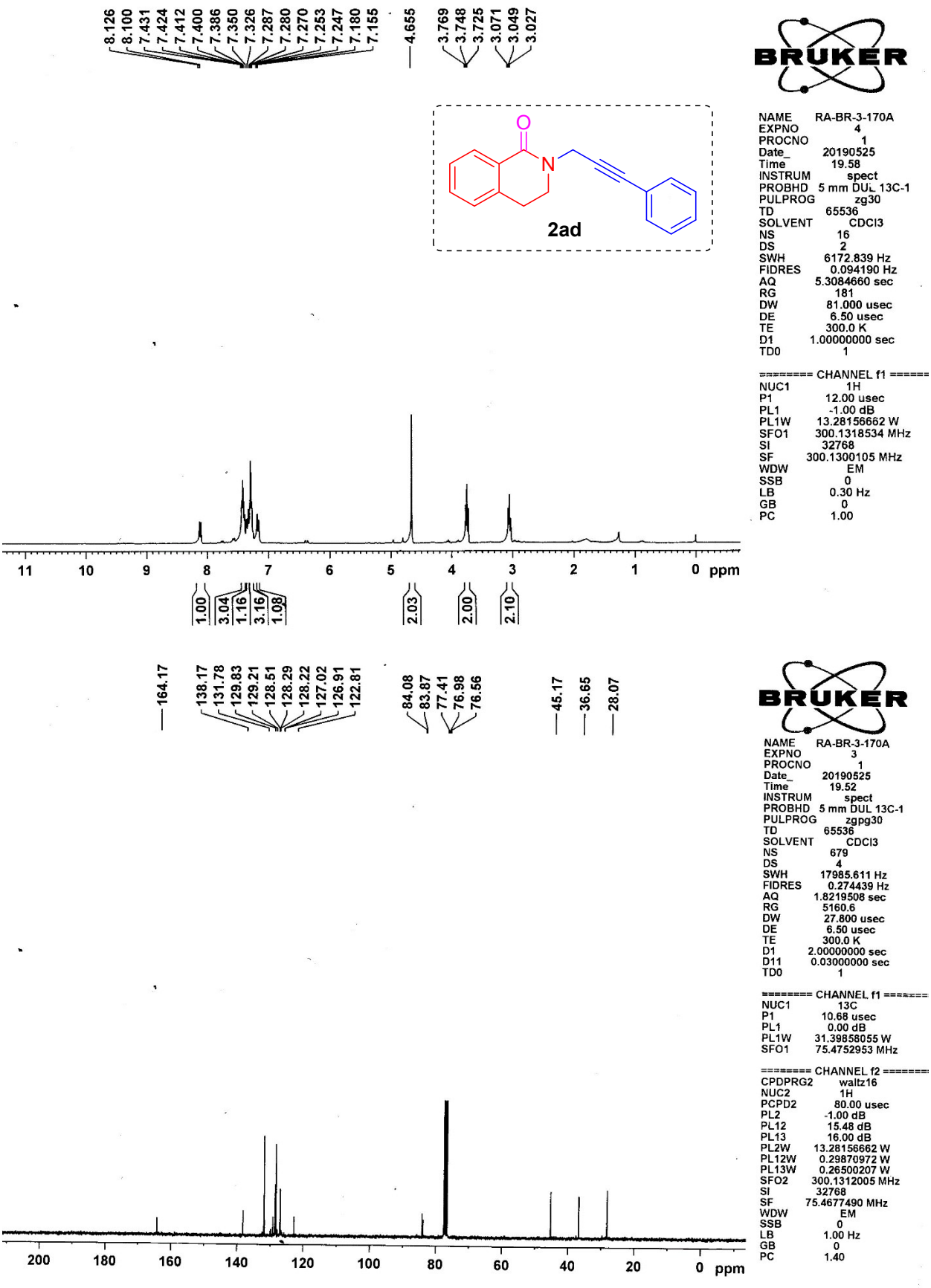
Compound Spectra (overlaid)



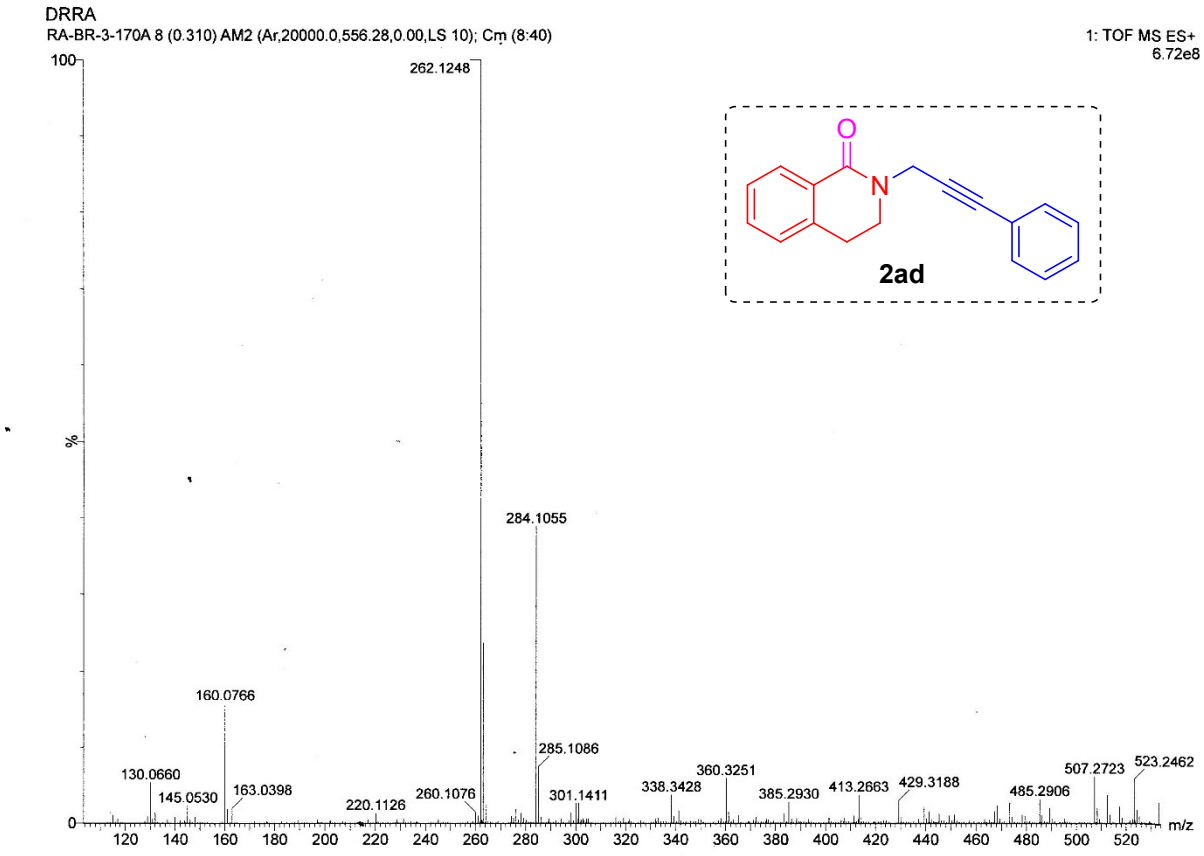
Compound ID Table

Cpd	Formula	Mass (Tgt)	Calc. Mass	Mass	Species	Diff(Tgt.ppm)	mDa
1	C18 H14 N2 O4	322.0954	322.0956	323.1039 345.0848	(M+H)+ (M+Na)+	0.79	0.25

HRMS Spectrum of Compound 2tc



^{1}H & ^{13}C spectra of compound 2ad



HRMS spectrum of compound 2ad