Electronic Supplementary Material (ESI) for Chemical Science.

Supplementary Information

For

Enantiodivergent Steglich Rearrangement of *O*-Carboxylazlactones Catalyzed by a Chirality Switchable Helicene Containing a 4-Aminopyridine Unit

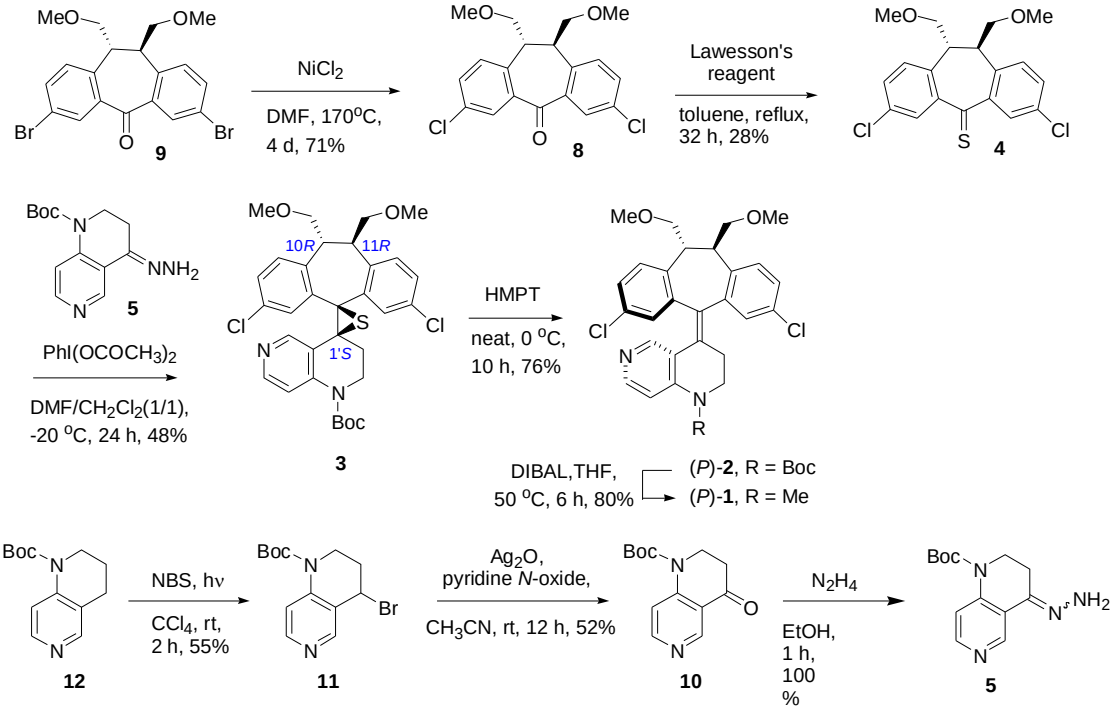
Chien-Tien Chen,* Cheng-Che Tsai, Pei-Kang Tsou, Gou-Tao Huang, and Chin-Hui Yu*

Department of Chemistry, National Tsing Hua University, No. 101, Section 2, Kuang-Fu Road, Hsinchu 30013, Taiwan. E-mail: ctchen@mx.nthu.edu.tw; chyu@mx.nthu.edu.tw; Fax and Tel: +886-3-5739240

General. ^{1}H NMR and ^{13}C NMR were recorded on Bruker Avance 400 (400 MHz ^{1}H, 100 MHz ^{13}C) spectrometers in deuterochloroform and were reference to TMS using the residual solvent as an internal standard. Chemical shifts are reported in ppm (δ). Coupling constants, *J*, are reported in Hz. Infrared spectra were recorded on a Bruker ALPHA FTIR spectrometer. Peaks are reported in units of cm^{-1}. High-resolution mass (Electrospray ionization, ESI) spectra were recorded on a Bruker Impact HD, EVOQ spectrometer. Melting points were determined on a Fargo MP-2D melting point apparatus and are uncorrected. Optical rotation were obtained on a Jasco P-2000 Digital Polarimeter at room temperature and reported as follows: $[\alpha]_D$, concentration (c = g/100 mL), and solvent. Analytical TLC was performed on Merck silica gel plates with QF-254 indicator. Visualization was accomplished with UV light, PMA, and KMnO4. Column (flash) chromatography was performed using 32-63 μm

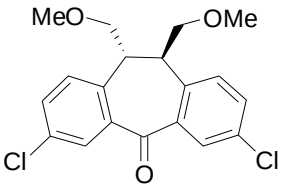
silicagel. UV-vis spectra were measured on a Metertech SP-8001 spectrometer in CH_2Cl_2. CD spectra were recorded on a AVIV model 410 spectropolarimeter in CH_2Cl_2. Analytical high-pressure liquid chromatography (HPLC) was performed on a Jasco Liquid Chromatograph equipped with PU-980 pumps, UV-975 detector, and 807-IT integrator. The column used was Dicel chiralpak AD or OD-H column with the detector wavelength at 254 or 310 nm. The flow rate and solvent systems were as denoted. Photoirradiation in solution were performed by irradiation of a sample (10^{-4} M in CH_2Cl_2) in a sealed 1 cm path-length quartz cuvette with an 300 W Oriel 66901 Xe-lamp attached to an Oriel 74100 CornerstoneTM 260 1/4M monochromator. Photostationary states were ensured by monitoring composition changes in time by taking UV-vis or CD spectra at distinct intervals until no changes were observed. Ratios of the different isomers of the optical switches were determined by HPLC with the detection wavelength at a given isosbestic point. All reagents were purchased from Acros, Aldrich, and TCI with purification before use unless otherwise stated. Solvents for extraction and chromatography were reagent grade. Dichloromethane, carbontetrachloride, acetonitrile, toluene, and DMF were dried over CaH_2 before use. THF was dried over Na with benzophenone-ketyl intermediate as indicator before use. $NiCl_2$ and Ag_2O were flamed-dried under high vacuum before use. NBS was purified by recrystallization from water at 90–95 °C. $PhI(OCOCH_3)_2$ was purified by recrystallization from toluene. HMPT was purified by distillation under reduced pressure. DIBAL and pyridine-*N*-oxide were carefully stored in desiccators at -4 ℃.

Preparation procedures for the synthesis of 1



Experimental section and characterization:

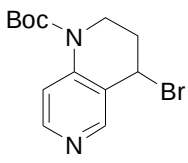
(10*R*,11*R*)-3,7-Dichloro-10,11-dimethoxymethyl-10,11-dihydro-5*H*-dibenzo[*a*,*d*]-cyclohepten-5-one (8).



In a 10-mL, round-bottomed, flask was placed dibromo **9** [1](519 mg, 1.15 mmol), $NiCl_2$ (595 mg, 4.6 mmol) in anhydrous DMF (3.2 mL). The vessel was sealed with a Teflon screw cap, immersed in a preheated oil bath. The reaction mixture was heated to 170 °C and stirred for 4 days. The reaction mixture was cooled to room temperature and then poured into water (30 mL). The aqueous layer was separated and extracted with CH_2Cl_2 (2 × 40 mL). The combined organic extracts were washed with H_2O (20 mL), dried ($MgSO_4$), and evaporated. The residue was purified by column chromatography (EtOAc/hexanes, 1/5) to give 298 mg (71 %) of dichloro **8** as a pale yellowish solid.: m. p. 78-79℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ

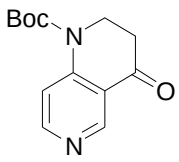
8.03 (d, J = 2.3 Hz, 2H), 7.43 (dd, J = 8.2 Hz, 2.3, 2H), 7.24 (d, J = 8.2 Hz, 2H), 3.63-3.58 (m, 2H), 3.34 (dd, J = 9.5, 5.5 Hz, 2H), 3.21 (t, J = 9.0 Hz, 2H), 3.11 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.7, 138.5, 137.1, 133.6, 133.4, 132.8, 130.8, 75.2, 58.8, 46.0; IR(neat) ν_{max} 2927, 2875, 2825, 1648, 1587, 1476, 1410, 1380, 1300, 1260, 1222, 1194, 1113 cm^{-1}; HRMS-ESI $[M+Na]^+$ calcd. For $C_{19}H_{18}Cl_2NaO_3$: 387.0531, found: 387.0523.; R_f = 0.30 (EtOAc/hexanes, 1/5); $[\alpha]_D^{25}$ = 275 (c 0.1, $CHCl_3$)

tert-Butyl 4-bromo-1,2,3,4-tetrahydro-1,6-naphthyridine-1-carboxylate (11).



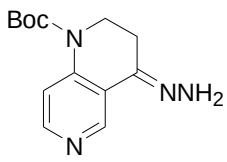
In a 10-mL, round-bottomed, flask was placed *tert*-butyl 1,2,3,4-tetrahydro-1,6-naphthyridine-1-carboxylate **12**[2] (100 mg, 0.43 mmol), NBS (91 mg, 0.51 mmol) in anhydrous CCl_4 (25 mL). The reaction mixture was stirred and irradiated using 40W incandescent light bulb for 2h. The solution was filtered and evaporated under reduced pressure. The residue was purified by column chromatography (EtOAc/hexanes, 1/2) to give 73 mg (55 %) of bromo **11** as a yellowish oil.: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (s, 1H), 8.27 (d, J = 6.0 Hz, 1H), 7.98 (d, J = 6.0 Hz, 1H), 5.43 (t, J = 3.4 Hz, 1H), 4.26 (ddt, J = 13.2, 3.7, 1.2 Hz, 1H), 3.83 (dt, J = 13.0, 3.4 Hz, 1H), 2.39 (dq, J = 13.4, 3.0 Hz, 1H), 2.27-2.19 (m, 1H), 1.53 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 151.3, 149.7, 141.2, 122.6, 115.4, 82.8, 44.3, 40.9, 31.2, 28.1; IR(neat) ν_{max} 2978, 2931, 1716, 1593, 1558, 1490, 1369, 1327, 1232, 1154, 1057, 1028, 909, 850, 836 cm^{-1}; HRMS-ESI $[M+H]^+$ calcd. For $C_{13}H_{18}BrN_2O_2$: 313.0552, found: 313.0539.; R_f = 0.30 (EtOAc/hexanes, 1/2)

***tert*-Butyl 4-oxo-1,2,3,4-tetrahydro-1,6-naphthyridine-1-carboxylate (10)**



In a 10-mL, round-bottomed, flask was placed bromo **11** (63 mg, 0.20 mmol), pyridine *N*-oxide (38 mg, 0.40 mmol), and Ag_2O (23 mg, 0.10 mmol) in anhydrous CH_3CN (5.0 mL). The reaction mixture was stirred at room temperature for 2h. The solution was filtered and evaporated under reduced pressure. The residue was purified by column chromatography (EtOAc/hexanes, 1/2) to give 26 mg (52 %) of ketone **10** as a white solid.: m. p. 138-139℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.01 (s, 1H), 8.48 (d, J = 6.0 Hz, 1H), 7.84 (d, J = 6.0 Hz, 1H), 4.13 (t, J = 6.4 Hz, 2H), 2.73 (t, J = 6.4 Hz, 2H), 1.53 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.9, 153.7, 151.8, 150.1, 149.9, 118.3, 115.7, 83.6, 43.8, 37.9, 28.0; IR(neat) v_{max} 2976, 2931, 1717, 1696, 1592, 1556, 1483, 1462, 1352, 1252, 1226, 1148, 1090, 1058 cm^{-1}; HRMS-ESI $[M+H]^+$ calcd. For $C_{13}H_{17}N_2O_3$: 249.1239, found : 249.1224.; R_f = 0.30 (EtOAc/hexanes, 1/2)

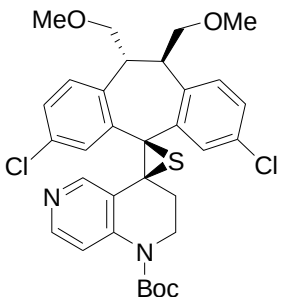
***tert*-Butyl 4-hydrazono-1,2,3,4-tetrahydro-1,6-naphthyridine-1-carboxylate (5).**



In a 10-mL, two-necked, round-bottomed, flask fitted with a Dean-stark and condenser was placed ketone **10** (28 mg, 0.11 mmol) in EtOH (3.0 mL). Hydrazine hydrate (0.1 mL, 2.03 mmol) was added to the reaction. The reaction mixture was heated to reflux for 2 h. After cooling, the mixture was concentrated under reduced pressure to yield 30 mg (100%) of hydrazone **5** as a white solid.: m. p. 139-140℃; ^{1}HNMR (400 MHz, CD_3Cl) Major: δ 9.08 (s, 1H), 8.29 (d, J = 5.8 Hz, 1H), 7.46 (d, J = 5.8 Hz, 1H), 5.48 (brs, 2H), 3.86 (t, J = 6.3 Hz, 2H), 2.59 (t, J = 6.3 Hz, 2H), 1.49 (s, 9H); Minor: δ 8.81 (s, 1H), 7.98 (d, J = 5.7 Hz, 1H), 6.38 (d, J = 5.7 Hz, 1H), 4.84 (brs, 2H), 3.34 (t, J = 6.2 Hz, 2H), 2.55 (t, J = 6.2 Hz, 2H), 1.49 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) Major: δ 152.2,

148.0, 146.5, 144.8, 140.5, 121.6, 116.9, 82.3, 41.4, 28.1, 24.4; Minor: δ 150.8, 148.3, 145.8, 144.7, 142.0, 115.5, 109.3, 82.3, 39.2, 28.1, 22.0; IR(neat) ν_{max} 3395, 3193, 2976, 2930, 1704, 1605, 1558, 1484, 1458, 1425, 1369, 1327, 1232, 1155, 1076, 1061 cm^{-1}; HRMS-ESI $[M+H]^+$ calcd. For $C_{13}H_{19}N_4O_2$: 263.1508, found : 263.1498.; R_f = 0.10 (EtOAc/hexanes, 1/1)

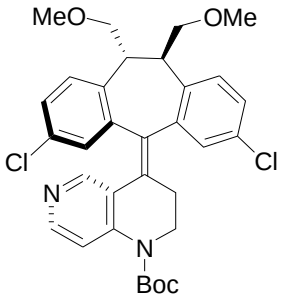
(10*R*,11*R*,1'*S*)-5-(4'-*tert*-Butoxycarbonyl-1',2',3',4'-tetrahydro-4',7'-naphthyridin-2'-thirrane)-3,7-dichloro-10,11-dimethoxymethyl-10,11-dihydro-5*H*-dibenzo[*a*,*d*]-cycloheptene (3).



In a 10-mL, round-bottomed, flask was placed hydrazone **5** (30 mg, 0.11 mmol) in anhydrous DMF (0.3 mL). The solution was cooled to -40 °C, whereupon a solution of thione **4** (74 mg, 0.23 mmol) in anhydrous CH_2Cl_2 (0.6 mL) and a solution of $PhI(OCOCH_3)_2$ in anhydrous DMF (0.3 mL) were slowly added. After having been stirred for 20 min, the reaction mixture was warmed -20 °C and stirred for 24 h. The reaction mixture was poured into water (10 mL). The aqueous layer was separated and extracted with CH_2Cl_2 (2 × 20 mL). The combined organic extracts were washed with H_2O (10 mL), dried ($MgSO_4$), and evaporated. The residue was purified by column chromatography (EtOAc/hexanes, 1/3) to give 30 mg (48 %) of episulfide **3** as a colorless oil.: ^1H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 5.8 Hz, 1H), 8.09 (s, 1H), 7.91 (d, *J* = 2.2 Hz, 1H), 7.70 (d, *J* = 5.8 Hz, 1H), 7.39 (d, *J* = 2.2 Hz, 1H), 7.37 (d, *J* = 8.3 Hz, 1H), 7.22 (dd, *J* = 8.3, 2.2 Hz, 1H), 7.14 (dd, *J* = 8.3, 2.2 Hz, 1H), 6.96 (d, *J* = 8.3 Hz, 1H), 4.32(dt, *J* = 13.1, 4.0 Hz, 1H), 3.86-3.85 (m, 2H), 3.46-3.42 (m, 1H), 3.39 (s, 3H), 3.36-3.34 (m, 1H), 3.11 (dd, *J* = 9.6, 4.2 Hz, 1H), 2.94 (dt, *J* = 11.9, 4.4 Hz, 1H), 2.90 (s, 3H), 2.80 (dd, *J* = 9.5, 4.6 Hz, 1H),

2.45-2.37 (m, 1H), 1.93 (dt, J = 15.2, 3.2 Hz, 1H) , 1.55 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 150.5, 147.8, 147.7, 144.9, 138.2, 137.6, 135.6, 134.0, 132.5, 132.3, 131.5, 128.7, 128.4, 128.3, 127.8, 123.0, 116.6, 82.4, 78.5, 71.9, 68.2, 58.9, 58.7, 54.4, 45.2, 43.3, 40.3, 38.9, 28.2; IR(neat) ν_{max} 2983, 2928, 2888, 1712, 1588, 1555, 1477, 1370, 1339, 1263, 1222, 1153, 1111, 1032 cm^{-1};HRMS-ESI $[M+H]^+$ calcd. For $C_{32}H_{35}Cl_2N_2O_4S$: 613.1695, found : 613.1689.; R_f = 0.30 (EtOAc/hexanes, 1/3); $[\alpha]_D^{25}$ = -59 (c 0.1, $CHCl_3$)

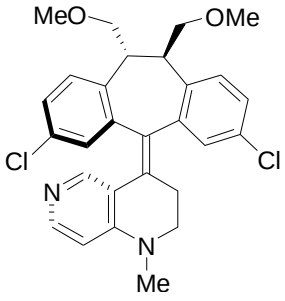
(10*R*,11*R*,*P*)-5-(4'-*tert*-Butoxycarbonyl-1',2',3',4'-tetrahydro-4',7'-naphthyriden) -3,7-dichloro-10,11-dimethoxymethyl-10,11-dihydro-5*H*-dibenzo[*a*,*d*] cycloheptene ((*P*)-2).



In a 5-mL, round-bottomed flask was placed episulfide **3** (18 mg, 0.03 mmol). The reaction flask was cooled to 0 °C, and fresh HMPT (0.3 mL) was slowly added. The reaction mixture was stirred at 0 °C for 10 hours. The reaction mixture was poured into water (5 mL). The aqueous layer was separated and extracted with CH_2Cl_2 (2 × 10 mL). The combined organic extracts were washed with H_2O (5 mL), dried ($MgSO_4$), and evaporated. The residue was purified by column chromatography (EtOAc/hexanes, 1/2) to give 13 mg (76 %) of helicene **2** as a colorless oil.: ^{1}H NMR (400 MHz, $CDCl_3$) Major: δ 8.58 (s, 1H), 8.25 (d, J = 5.9 Hz, 1H), 8.06 (d, J = 5.9 Hz, 1H), 7.48 (d, J = 8.3 Hz, 1H), 7.22-7.00 (m, 4H), 6.86 (s, 1H), 4.15-3.59 (m, 7H), 3.46 (s, 3H), 3.44-3.40 (m, 1H), 3.34 (s, 3H), 3.04-2.96 (m, 1H), 2.29-2.19 (m, 1H), 1.63 (s, 9H); Minor: δ 8.22 (d, J = 5.4 Hz, 1H), 7.99 (d, J = 5.4 Hz, 1H), 7.77 (s, 1H), 7.31 (d, J = 8.5 Hz, 1H), 7.22-7.00 (m, 4H), 6.94 (s, 1H), 4.15-3.59 (m, 7H), 3.38 (s, 3H), 3.26-3.21 (m, 1H), 3.18 (s, 3H), 3.04-2.96 (m, 1H),

2.29-2.19 (m, 1H), 1.63 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) Major: δ 153.0, 148.8, 147.9, 146.0, 144.6, 141.5, 138.6, 138.2, 135.2, 132.9, 131.9, 131.6, 128.6, 128.5, 127.8×2, 125.2, 122.5, 115.8, 82.8, 77.2, 72.5, 59.2, 58.9, 46.7, 45.6, 38.8, 28.3; Minor: δ 153.0, 148.4, 147.9, 145.7, 142.0, 141.6, 136.9, 136.2, 134.9, 133.2, 132.3, 131.1, 128.1, 128.0×2, 127.1, 127.0, 122.8, 116.3, 82.7, 75.9, 74.3, 59.1, 58.7, 46.5, 45.0, 41.8, 28.3; IR(neat) ν_{max} 2976, 2926, 1716, 1587, 1551, 1487, 1416, 1369, 1330, 1255, 1230, 1154, 1111, 1043, 1026 cm^{-1}; HRMS-ESI $[M+H]^+$ calcd. For $C_{32}H_{35}Cl_2N_2O_4$: 581.1974, found : 581.1964.; R_f = 0.13 (EtOAc/hexanes, 1/2); $[\alpha]_D^{25}$ = -158 (c 0.1, $CHCl_3$)

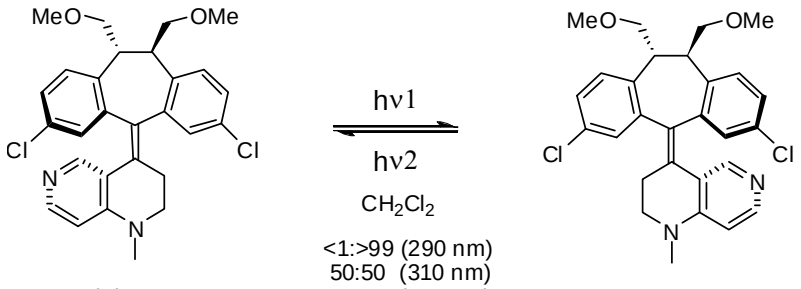
(10*R*,11*R*,*P*)-3,7-Dichloro-10,11-dimethoxymethyl-5-(4'-methyl-1',2',3',4'-tetrahy -dro-4',7'-naphthyriden)-10,11-dihydro-5*H*- dibenzo[*a*,*d*]cycloheptene ((*P*)-1).



In a 5-mL, round-bottomed flask was placed *N*-Boc **2** (13 mg, 0.02 mmol) in anhydrous THF (2.0 mL). The reaction mixture was cooled to 0 °C, and fresh DIBAL (1.2 M in toluene) (0.37 mL, 0.45 mmol) was added over 20 min. Having been stirred for 30 min, the reaction mixture was heated to 50 °C and stirred for 6 hours. After cooling to 0 °C, NaF (19 mg, 0.45 mmol) and water (0.5 mL) were added in small portions, and the mixture was allowed to warm to room temperature over 3 h. The solution was filtered through a plug of Celite and was evaporated under reduced pressure. The residue was purified by column chromatography (CH_2Cl_2/MeOH/NEt_3, 20/1/0.1) to give 9 mg (80 %) of *N*-Me **1** as a colorless oil.: ^{1}H NMR (400 MHz, $CDCl_3$) Major: δ 8.32 (s, 1H), 8.01 (d, *J* = 7.0 Hz, 1H), 7.47 (d, *J* = 8.4 Hz, 1H), 7.20-7.06 (m, 3H), 6.85 (d, *J* = 2.1 Hz, 1H), 6.75 (d, *J* = 1.9 Hz, 1H), 6.65 (d, *J* = 7.0 Hz, 1H), 3.97-3.49 (m, 7H), 3.49-3.35 (m, 1H), 3.45 (s, 3H), 3.40 (s, 3H), 3.22 (s, 3H), 3.12-2.98 (m, 1H), 2.38-2.28 (m, 1H); Minor: δ 7.97

(d, J = 6.7 Hz, 1H), 7.36 (d, J = 8.3 Hz, 1H), 7.29 (s, 1H), 7.20-7.06 (m, 3H), 6.94 (d, J = 2.3 Hz, 1H), 6.85 (d, J = 2.1 Hz, 1H), 6.57 (d, J = 6.8 Hz, 1H), , 3.97-3.49 (m, 7H), 3.49-3.35 (m, 1H), 3.45 (s, 3H), 3.40 (s, 3H), 3.16 (s, 3H), 3.12-2.98 (m, 1H), 2.38-2.28 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) Major: δ 151.5, 147.8, 146.7, 145.1, 141.9, 138.6, 137.3, 133.0, 132.6, 131.8, 131.5, 128.5, 128.3, 127.6, 127.5, 127.0, 126.8, 125.1, 115.9, 105.4, 77.2, 72.5, 59.2, 58.9, 51.5, 45.6, 39.0, 37.9, 26.8.; Minor: δ 151.0, 148.2, 147.6, 142.7, 142.6, 138.4, 136.3, 133.6, 133.2, 132.1, 131.7, 130.7, 128.4, 127.6, 127.4, 127.2, 126.9, 116.0, 105.5, 76.3, 75.1, 59.0, 58.6, 51.3, 45.0, 41.6, 37.8, 26.5.; IR(neat) ν_{max} 2920, 2872, 2812, 1645, 1591, 1558, 1474, 1458, 1415, 1387, 1349, 1324, 1296, 1267, 1249, 1212, 1177, 1106, 1028, 1006, 913, 873, 824, 803 cm^{-1}; HRMS-ESI $[M+H]^+$ calcd. For $C_{28}H_{29}Cl_2N_2O_2$: 495.1606, found: 495.1623.; R_f = 0.3 (CH_2Cl_2/MeOH/NEt_3, 20/1/0.1); $[\alpha]_D^{25}$ = -304 (c 0.1, $CHCl_3$)

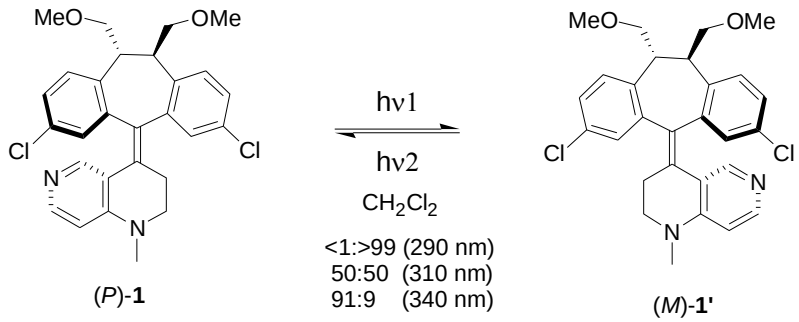
General procedure photoisomerization of helicene 1



(*P*)-**1** (*M*)-**1'**

A solution of helicene **1** (85 μg, 2.0 μmol) in degassed CH_2Cl_2 (2.0 mL) was irradiated with a 300 W Xe-lamp equipped with a monochromator. The irradiation wavelength was set at 290, 310, or 340 nm with a slit size equivalent to 8 nm bandwidth. The experiment was carried out for 1 hour until a constant composition was observed by HPLC analysis on a Chiralpak AD column.

HPLC data of photoisomerization of helicene 1



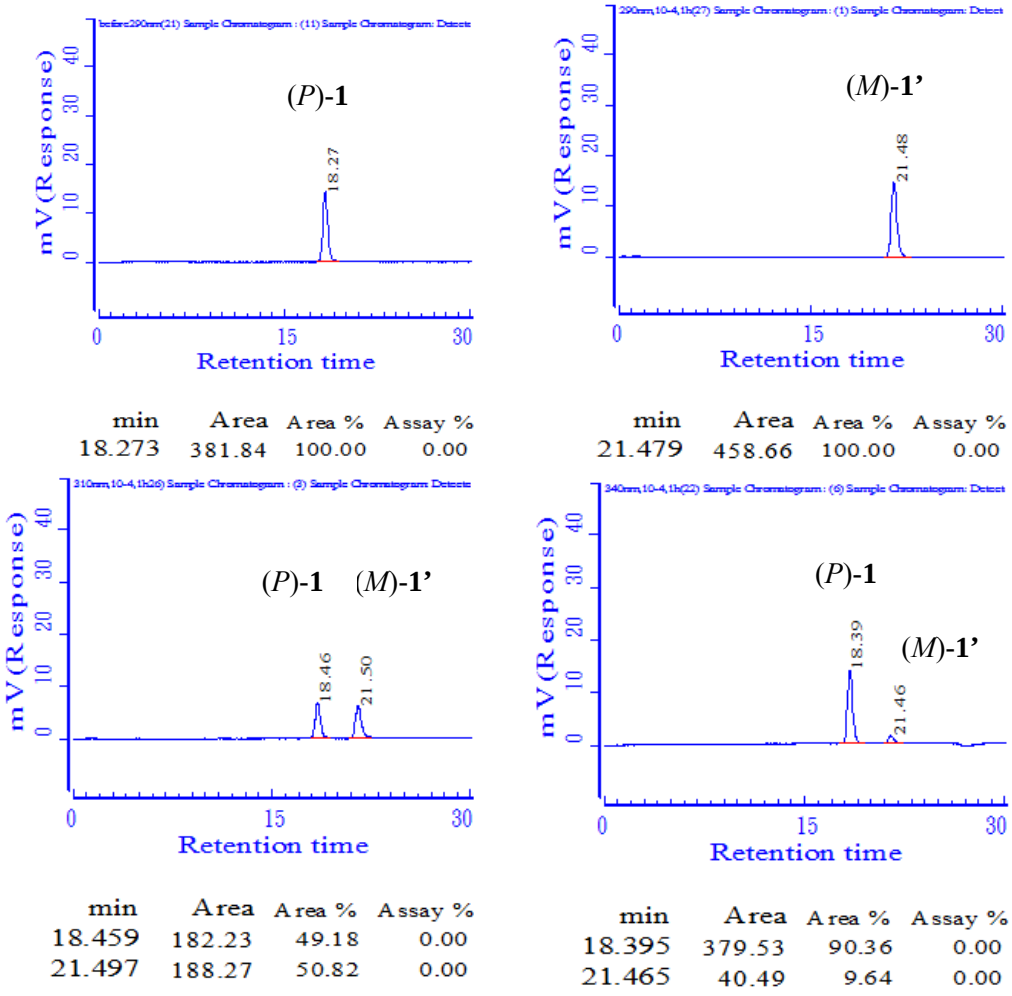
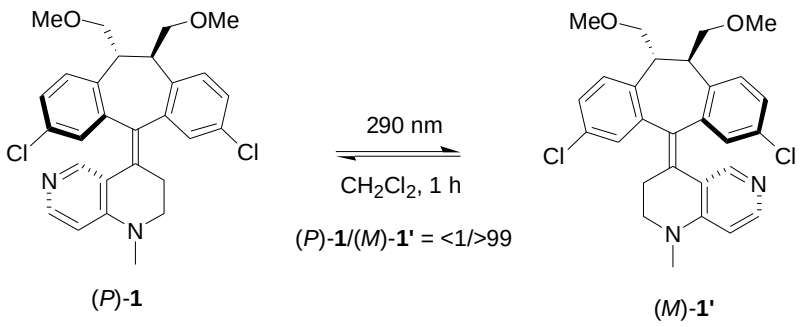


Figure S1. Ratios of the (10*R*,11*R*,*P*)-**1** and (10*R*,11*R*,*M*)-**1'** in solution (CH_2Cl_2, 10^{-4} M) after photoisomerization at 290 nm (top right), 310 nm (bottom left), and 340 nm (bottom right) as monitored by HPLC on a Chiralpak AD column by using a mixture of hexanes/*i*-PA (75/25) as eluent at 1.0 mL/min flow rate and at 310 nm (which is an isosbestic point in their stacked UV plots) detection wavelength.

HPLC tracing data of photoisomerization of helicene (*P*)-1



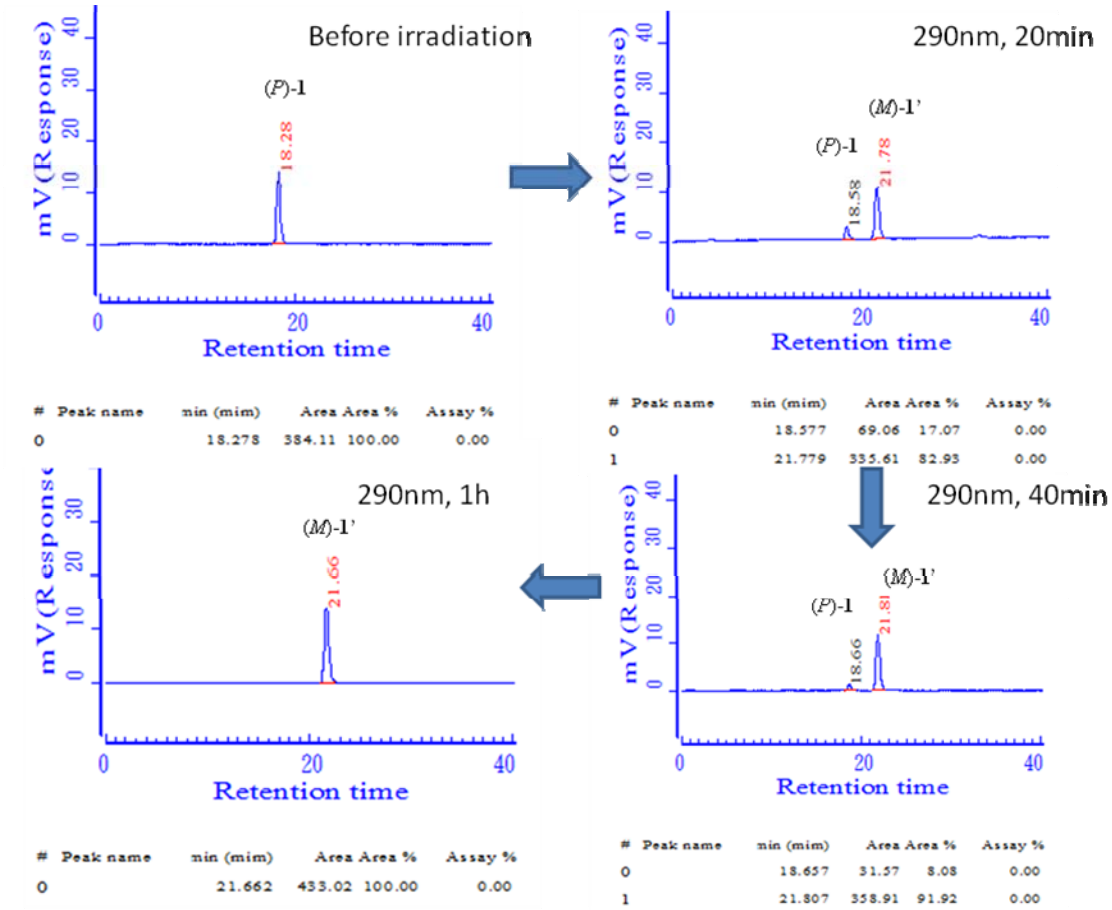


Figure S2. Ratios of the (10*R*,11*R*,*P*)-**1** and (10*R*,11*R*,*M*)-**1'** in solution (CH_2Cl_2, 10^{-4} M) during the period of photoisomerization at 290 nm as monitored by HPLC on a Chiralpak AD column by using a mixture of hexanes/*i*-PA (75/25) as eluent at 1.0 mL/min flow rate and at 310 nm (which is an isosbestic point in their stacked UV plots) detection wavelength.

HPLC tracing data of photoisomerization of helicene (*M*)-1'

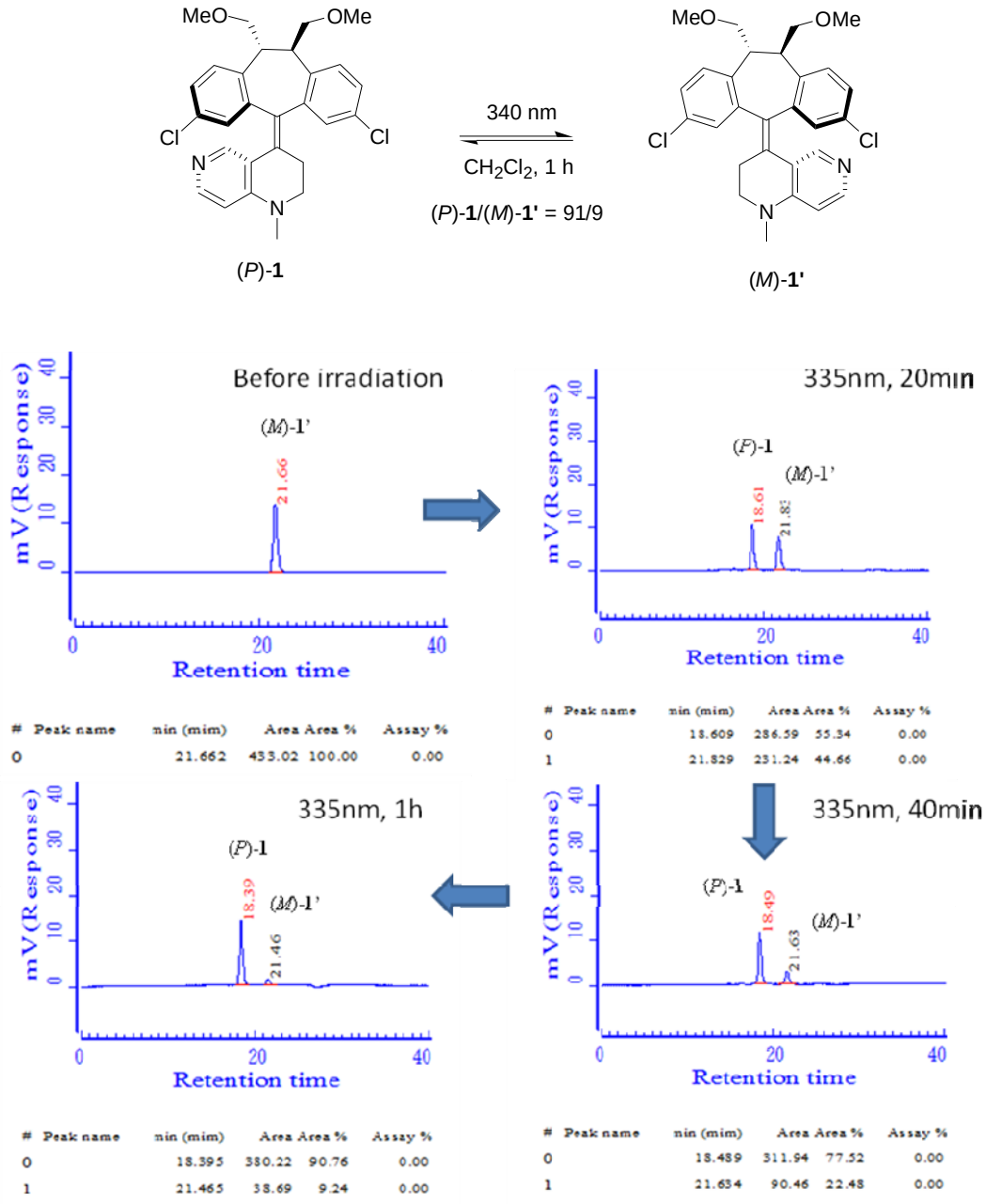


Figure S3. Ratios of the (10*R*,11*R*,*P*)-**1** and (10*R*,11*R*,*M*)-**1'** in solution (CH_2Cl_2, 10^{-4} M) during the period of photoisomerization at 340 nm as monitored by HPLC on a Chiralpak AD column by using a mixture of hexanes/*i*-PA (75/25) as eluent at 1.0 mL/min flow rate and at 310 nm (which is an isosbestic point in their stacked UV plots) detection wavelength.

HPLC tracing data of thermoisomerization of helicene (*M*)-1'

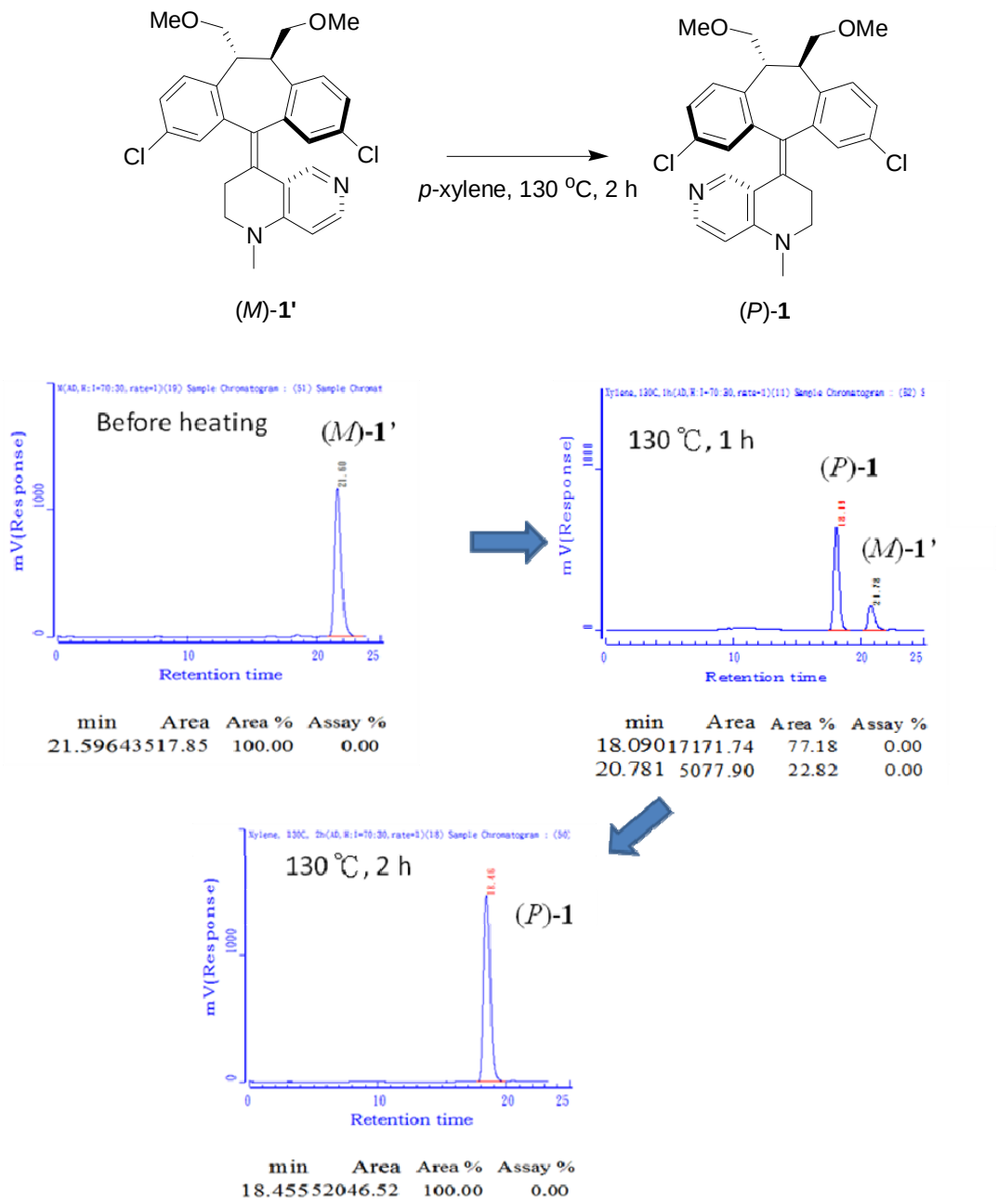
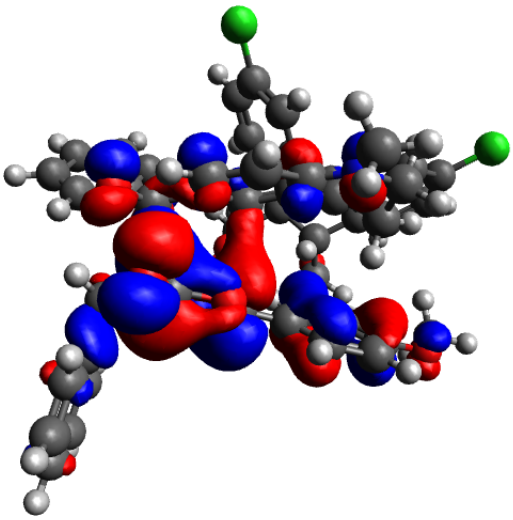


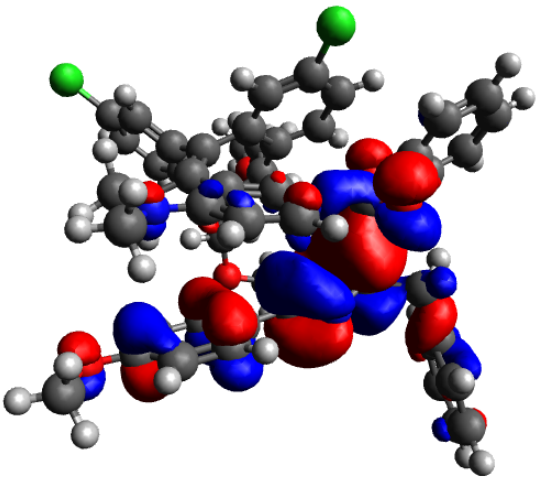
Figure S4. Ratios of the (10*R*,11*R*,*P*)-**1** and (10*R*,11*R*,*M*)-**1'** in *p*-xylene during the period of thermoisomerization at 130 ℃ as monitored by HPLC on a Chiralpak AD column by using a mixture of hexanes/*i*-PA (75/25) as eluent at 1.0 mL/min flow rate and at 310 nm (which is an isosbestic point in their stacked UV plots) detection wavelength.

Orbital interactions in the transition states of the C–C formation during the Steglich rearrangement using (*P*)-1 and (*M*)-1'

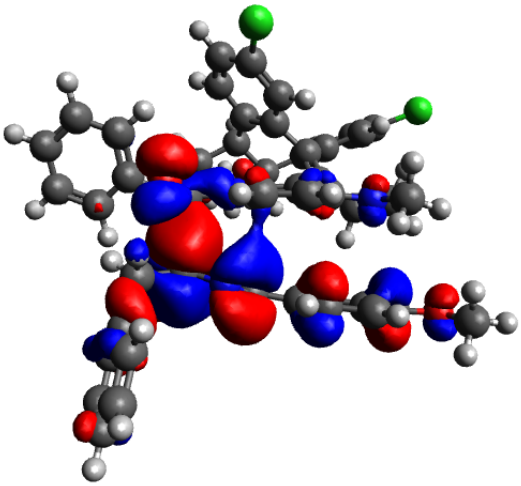
(*P*)-**1**, favoring *Re* face attack



(*M*)-**1'**, favoring *Si* face attack



(*P*)-**1**, disfavoring *Si* face attack



(*M*)-**1'**, disfavoring *Re* face attack

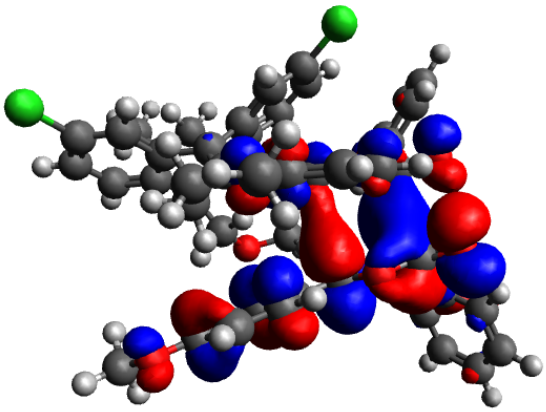


Figure S5. Orbital interactions in the transition states of the Steglich rearrangement using (*P*)-**1** and (*M*)-**1'** for illusrtration orbital interactions in the transition states.

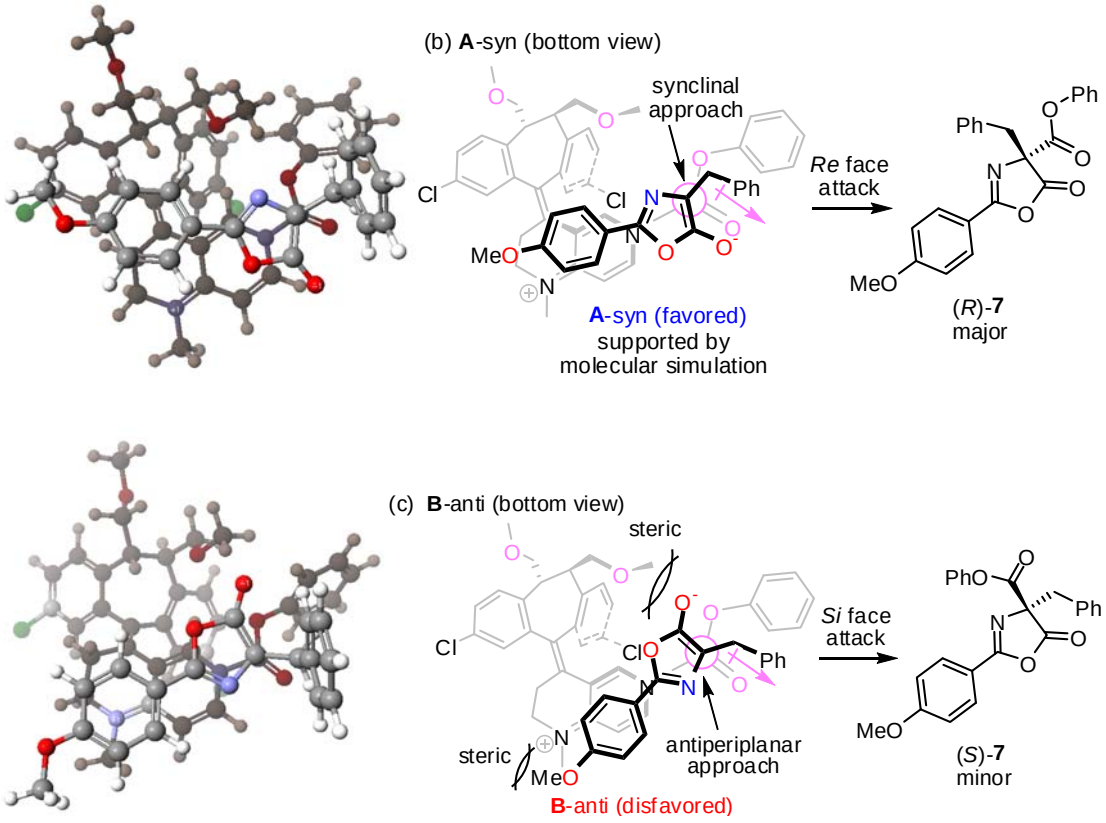


Figure S6. Chem 3D and Chem Draw presentations of the transition state assemblies in the ion pairs: preferred **A**-syn (top) and diafavored **B**-anti (bottom) assembly mode by catalyst (*P*)-**1**.

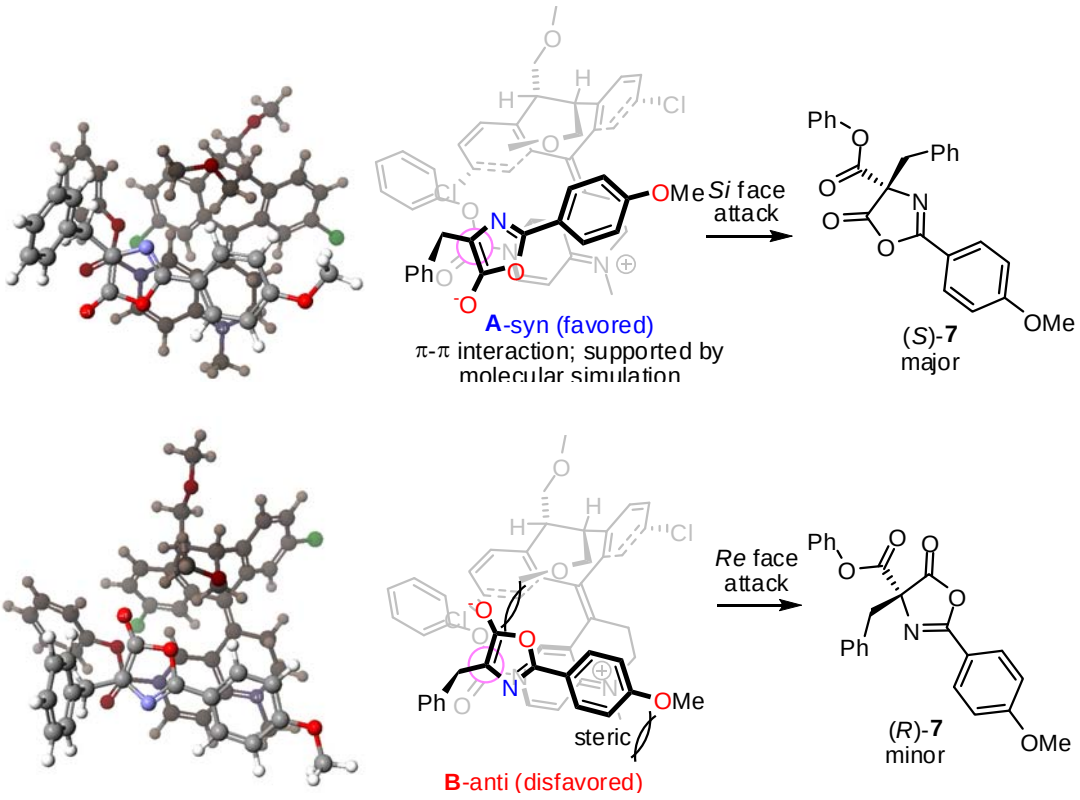


Figure S7. Chem 3D and Chem Draw presentations of the transition state assemblies in the ion pairs: favored **A**-syn (top) and disfavored **B**-syn (bottom) assembly mode by catalyst (*M*)-**1'**.

All transition states were optimized at the M06-2X/6-31+G(d) level.[3] During the optimization, the solvent effect was included with the integral equation formalism polarizable continuum model (IEFPCM) with DME as solvent.[4] Frequency calculations are done to verify the saddle-point structures characterized by one and only one imaginary value. All the calculations were performed with *Gaussian 09* program suit.[5] As shown in **Figures S2** and **S3**, the dibenzosuberane in the helicene has two possible conformations, leading to (*R*)- and (*S*)-products. **Figure S2** shows that the enolate attacks the carbon atom of the carbamate from the *Re*-face while **Figure S3** shows the attack from the *Si*-face. The activation energies listed in **Figures S2** and **S3** are relative to **R-TS1**. In both cases, the rotation of the carboxylic group (–CO_2Ph) and the flip of the seven-membered ring (X1 and X2) can yield four transitions states. Calculations show that for the *Re*-face attack, **R-TS1** is the lowest-energy transition state (**Figure S2**). **S-TS3** is the lowest-energy transition state for *Si*-face attack (**Figure S3**). The two transition states, **R-TS1** and **S-TS3**, were hence chosen to explore the stereoselectivity in the reaction. The difference of the barrier of 2.35 kcal mol^{-1} (**R-TS1** vs **S-TS3**) allows us to conclude that the *Re*-face attack leading to the (*R*)-product is more kinetically favorable than the *Si*-face attack, in agreement with our experimental results (entry 7 in **Table 7**). The frontier orbitals in the two TSs were further analyzed. For the clear illustration of the orbital interactions, the single-point calculations were done on the two separated moieties in **R-TS1**/**S-TS3**. Three major overlaps between HOMO and LUMO, represented by arrows in **Figure S4**, are observed for the *Re*-face attack while only two interactions occur during the *si*-face attack. The difference of the orbital interactions might be one of the factors leading to the preference of the *Re*-face attack.

To study solvent effect on the reaction, the two transition states of **R-TS1** and **S-TS3** were computed by the IEFPCM model, which is based on the implicit surrounding subjected to a dielectric field. The influence of the implicit solvent model on the optimized structures was negligible; therefore, single-point calculations were done on the two TSs optimized in DME. **Table S1** lists the difference of the barriers in **R-TS1** and **S-TS3** in five solvents of DME, Et_2O, toluene, CH_2Cl_2, and THF. The fact that the energy of **R-TS1** is lower than that of **S-TS3** in all five solvents indicates the preference of the enantioselectivity remains unchanged with various solvents. The implicit solvent model yields the values of $\Delta E^{\ddagger}$ ranging between 3.78 and 4.16 kcal

mol^{-1}. The small variation of ca. 0.5 kcal mol^{-1} might not be decisive to predict ee values. In fact, solutes are surrounded by real solvent molecules, namely an explicit environment. The differences in barrier may further decrease if the solvent molecules are included into calculations explicitly with the solution dynamics considered. Table S2 lists the difference in barrier between **R-TS1** and **S-TS3** with different functional groups, where the calculations are preformed in the IEFPCM model with solvent CH_2Cl_2. It is also observed that the change of the difference in barrier ($\Delta G^{\ddagger}$ = 2.42 to 2.92 kcal mol^{-1}) is small.

solvent	$\Delta E^{\ddagger}$ (kcal mol^{-1})
DME (OPT) 7.2	3.78
Et_2O (SP) 4.24	4.14
Toluene (SP) 2.37	3.93
CH_2Cl_2 (SP) 8.93	4.15
THF (SP) 7.42	4.16

Table S1. Differences of the electronic energies between **R-TS1** and **S-TS3** ($\Delta E^{\ddagger}$ = $E_{S\text{-}TS3} - E_{R\text{-}TS1}$) with R=Ph in various solvents.

R	$\Delta G^{\ddagger}$ (kcal mol^{-1})
CMe_2CCl_3 (OPT)	2.42
Bn (OPT)	2.92
Ph (SP)	2.65

Table S2. Differences of the free energies between **R-TS1** and **S-TS3** ($\Delta G^{\ddagger}$ = $G_{S\text{-}TS3} - G_{R\text{-}TS1}$) with three R groups in CH_2Cl_2.

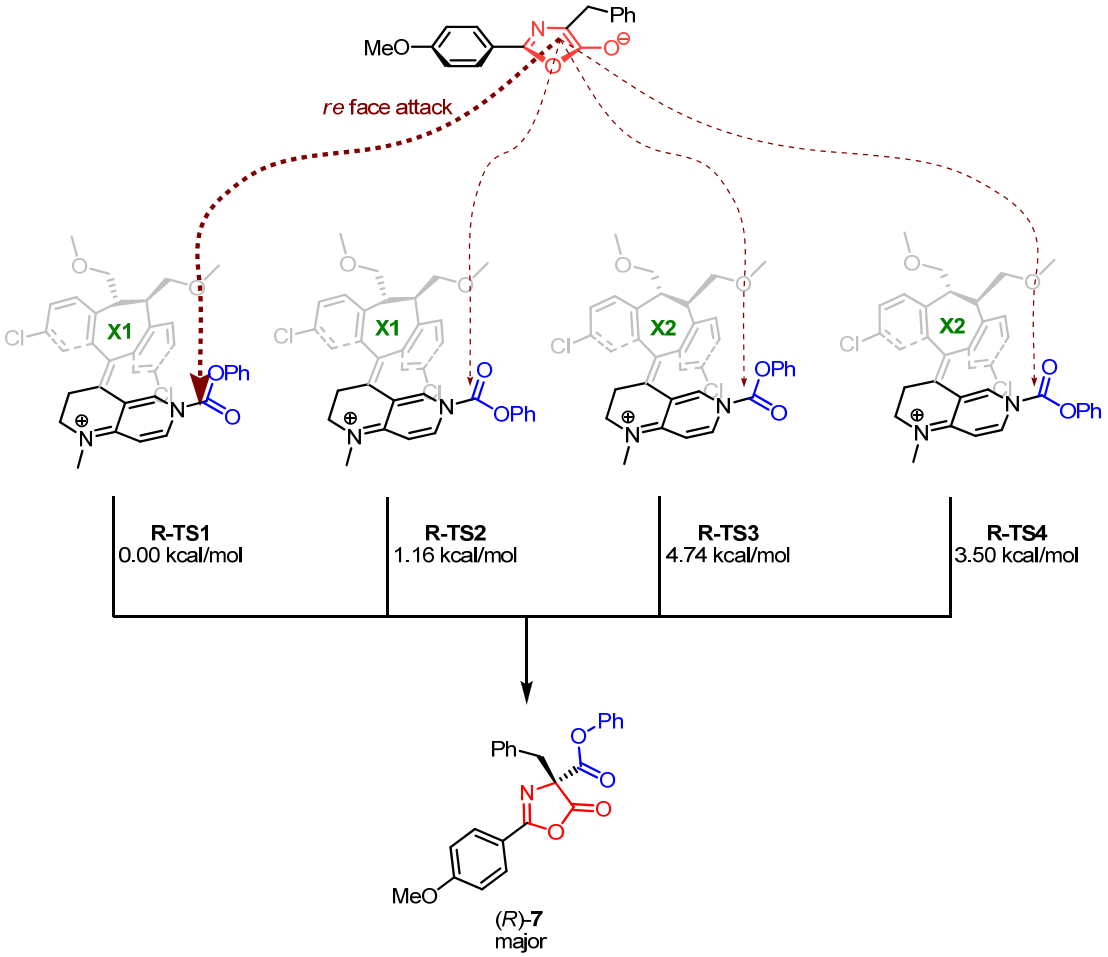


Figure S8. Four pathways for the *re*-face attack. The listed energies ($\Delta G^{\ddagger}$ in kcal mol^{-1}) are relative to **R-TS1**.

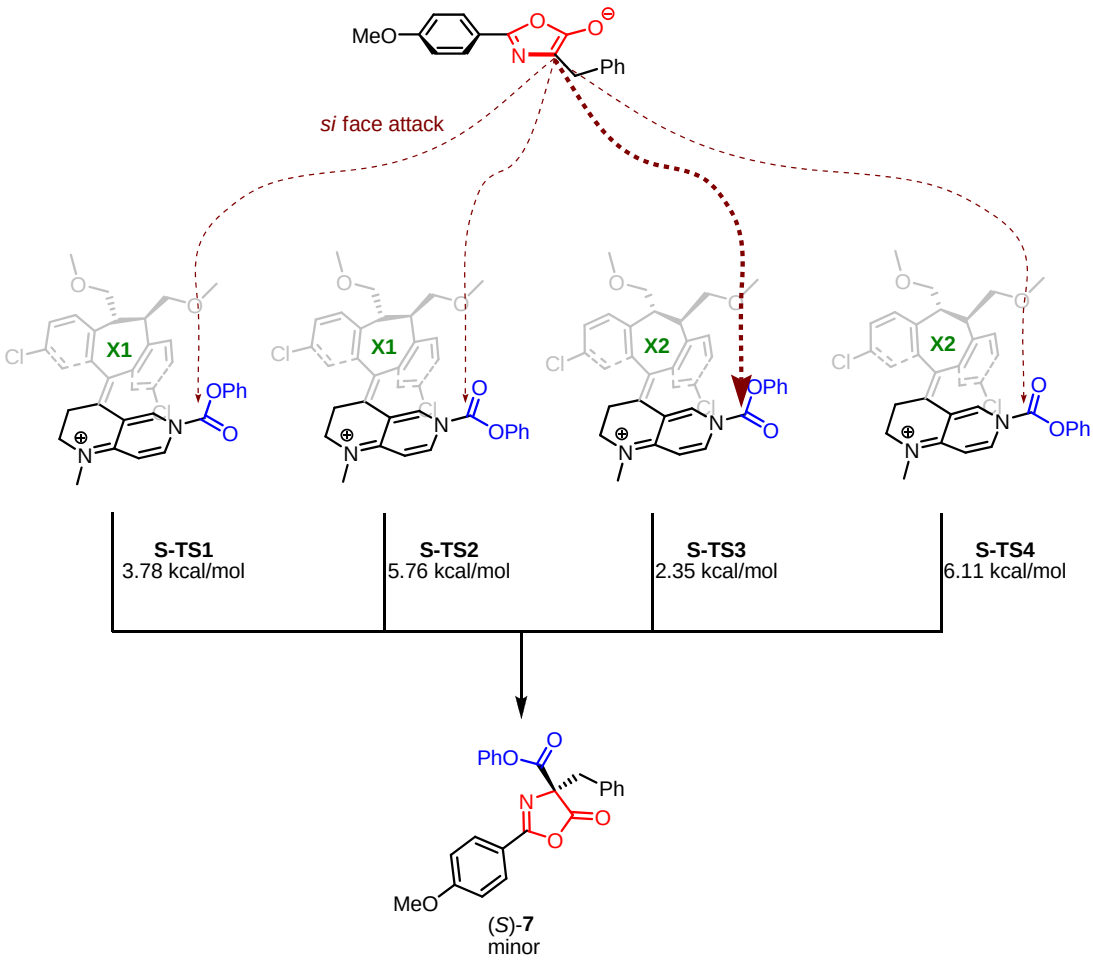


Figure S9. Four pathways for the *si*-face attack. The listed energies ($\Delta G^{\ddagger}$ in kcal mol^{-1}) are relative to **R-TS1**.

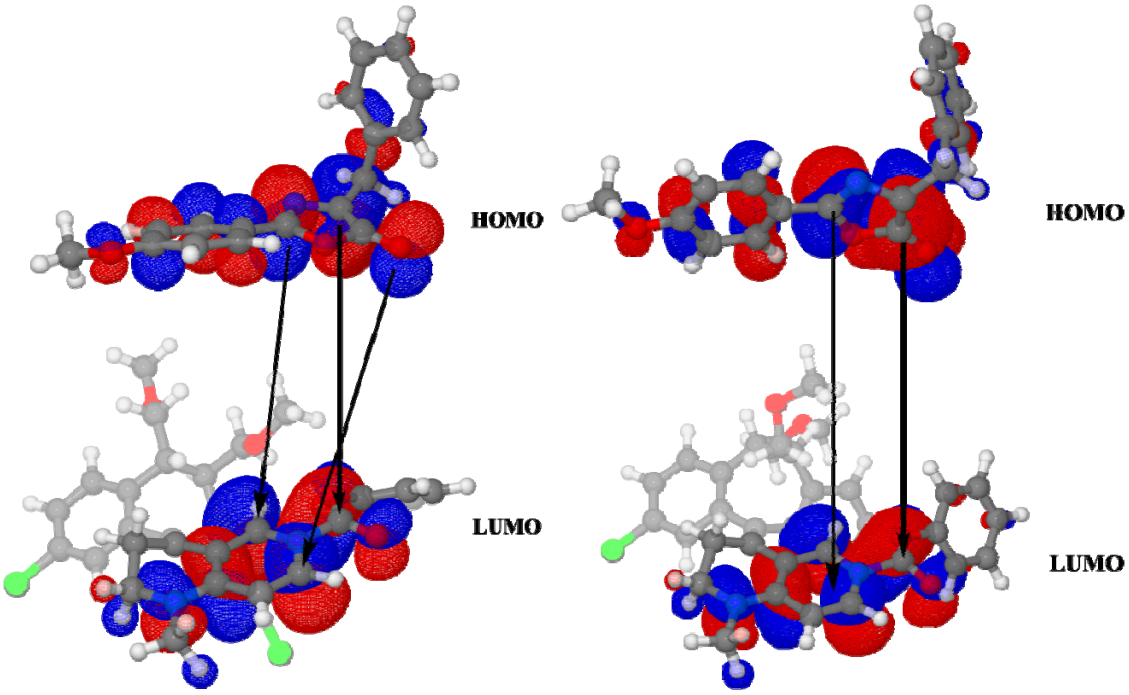
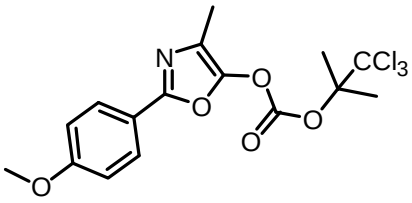


Figure S10. Comparison of the HOMO-LUMO interactions in the lowest-energy transition states of **R-TS1** and **S-TS3** from *Re*- and *Si*-face attacks, respectively.

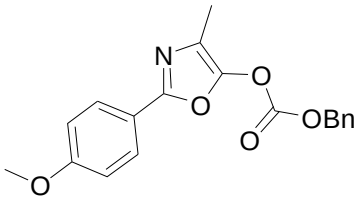
Characterization of *O*-Carboxylazlactones:

5-(2,2,2-Trichloroethoxycarboxyl)-4-methyl-2-(4-methoxyphenyl)-oxazole (6a).[8]



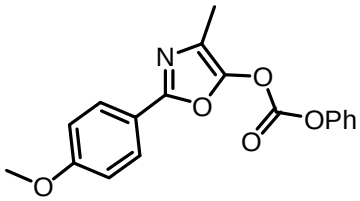
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 9.0 Hz, 2H), 6.92 (d, *J* = 9.0 Hz, 2H), 3.82 (s, 3H), 2.13 (s, 3H), 2.00 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3, 155.0, 148.4, 145.2, 127.5, 120.0, 119.7, 114.1, 104.4, 92.2, 55.3, 20.9, 10.2; HRMS-ESI $[M+H]^+$ calcd. For $C_{16}H_{17}Cl_3NO_5$: 408.0172, found: 408.0181.; R_f = 0.23 (EtOAc/hexanes, 1/10)

5-Benzyloxycarboxyl-4-methyl-2-(4-methoxyphenyl)-oxazole (6b).[6]



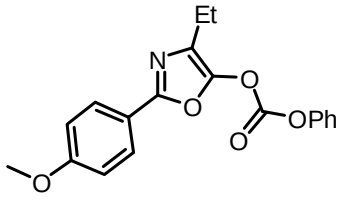
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.8 Hz, 2H), 7.45-7.40 (m, 5H), 6.93 (d, *J* = 8.8 Hz, 2H), 5.32 (s, 2H), 3.84 (s, 3H), 2.12 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3, 154.9, 151.6, 145.6, 133.8, 129.1, 128.8, 128.6, 127.5, 120.0, 119.9, 114.1, 71.7, 55.3, 10.2; HRMS-ESI $[M+H]^+$ calcd. For $C_{19}H_{18}NO_5$: 340.1185, found: 340.1177.; R_f = 0.15 (EtOAc/hexanes, 1/10).

5-Phenoxycarboxyl-4-methyl-2-(4-methoxyphenyl)-oxazole (6c).[7]



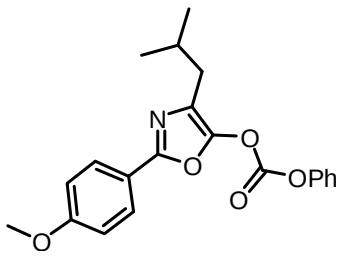
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.8 Hz, 2H), 7.46-7.42 (m, 2H), 7.33-7.29 (m, 3H), 6.95 (d, *J* = 8.8 Hz, 2H), 3.85 (s, 3H), 2.19 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3, 155.1, 150.7, 150.1, 145.3, 129.7, 127.5, 126.8, 120.5, 120.2, 119.8, 114.1, 55.3, 10.3; HRMS-ESI $[M+H]^+$ calcd. For $C_{18}H_{16}NO_5$: 326.1028, found: 326.1031.; R_f = 0.18 (EtOAc/hexanes, 1/10).

5-Phenoxycarboxyl-4-ethyl-2-(4-methoxyphenyl)-oxazole (6d).[11]



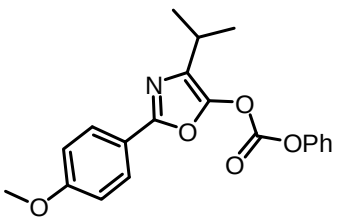
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.8 Hz, 2H), 7.46-7.42 (m, 2H), 7.33-7.29 (m, 3H), 6.95 (d, *J* = 8.8 Hz, 2H), 3.85 (s, 3H), 2.57 (q, *J* = 7.6 Hz, 2H), 1.29 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3, 155.2, 150.8, 150.3, 144.7, 129.7, 127.7, 126.8, 125.5, 120.5, 119.9, 114.1, 55.3, 18.5, 10.3; HRMS-ESI $[M+H]^+$ calcd. For $C_{19}H_{18}NO_5$: 340.1185, found: 340.1180.; R_f = 0.25 (EtOAc/hexanes, 1/10).

5-Phenoxycarboxyl-4-*iso*-butyl-2-(4-methoxyphenyl)-oxazole (6e).[7]



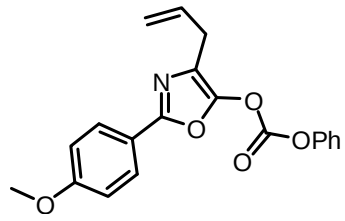
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.8 Hz, 2H), 7.46-7.42 (m, 2H), 7.33-7.29 (m, 3H), 6.95 (d, *J* = 8.8 Hz, 2H), 3.85 (s, 3H), 2.40 (d, *J* = 6.8 Hz, 2H), 2.13-2.05 (m, 1H), 0.99 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3, 155.2, 150.8, 150.3, 145.8, 129.7, 127.7, 126.8, 123.7, 120.5, 120.0, 114.1, 55.3, 33.9, 27.6, 22.3; HRMS-ESI $[M+H]^+$ calcd. For $C_{21}H_{22}NO_5$: 368.1498, found: 368.1499.; R_f = 0.30 (EtOAc/hexanes, 1/10).

5-Phenoxycarboxyl-4-*iso*-propyl-2-(4-methoxyphenyl)-oxazole (6f).[9]



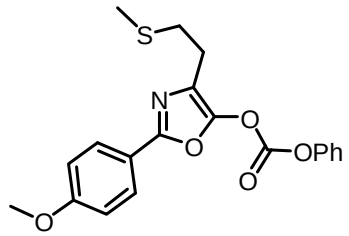
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.9 Hz, 2H), 7.46-7.42 (m, 2H), 7.33-7.29 (m, 3H), 6.95 (d, *J* = 8.9 Hz, 2H), 3.84 (s, 3H), 2.95 (sept, *J* = 7.0 Hz, 1H), 1.33 (d, *J* = 7.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3, 155.1, 150.7, 150.5, 143.8, 129.7, 129.4, 127.6, 126.8, 120.5, 120.0, 114.1, 55.3, 25.5, 21.0; HRMS-ESI $[M+H]^+$ calcd. For $C_{20}H_{20}NO_5$: 354.1336, found: 354.1342; R_f 0.28 (EtOAc/hexanes, 1/10).

5-Phenoxycarboxyl-4-allyl-2-(4-methoxyphenyl)-oxazole (6g).[7]



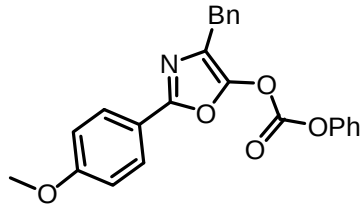
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.8 Hz, 2H), 7.46-7.42 (m, 2H), 7.33-7.27 (m, 3H), 6.95 (d, *J* = 8.8 Hz, 2H), 6.06-5.96 (m, 1H), 5.24(dd, *J* = 17.2, 1.6 Hz, 1H), 5.17(dd, *J* = 10.1, 1.4 Hz, 1H), 3.85 (s, 3H), 3.34 (dt, *J*= 6.6, 1.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.4, 155.4, 150.7, 150.1, 145.5, 133.4, 129.7, 127.7, 126.8, 122.3, 120.5, 119.7, 117.1, 114.2, 55.4, 29.7; HRMS-ESI $[M+H]^+$ calcd. For $C_{20}H_{18}NO_5$: 352.1185, found: 352.1182.; R_f = 0.25 (EtOAc/hexanes, 1/10).

5-Phenoxycarboxyl-4-((2-methylthio)ethyl)-2-(4-methoxyphenyl)-oxazole (6h).[9]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.8 Hz, 2H), 7.46-7.42 (m, 2H), 7.33-7.29 (m, 3H), 6.95 (d, *J* = 8.8 Hz, 2H), 3.85 (s, 3H), 2.86-2.84 (m, 4H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ161.4, 155.4, 150.7, 150.1, 145.6, 129.7, 127.7, 126.8, 122.7, 120.5, 119.7, 114.1, 55.3, 32.3, 25.3, 15.5; HRMS-ESI $[M+H]^+$ calcd. For $C_{20}H_{20}NO_5S$: 386.1062, found : 386.1069.; R_f = 0.20 (EtOAc/hexanes, 1/10).

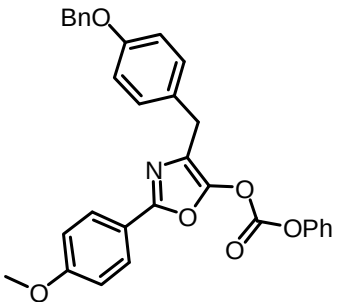
5-Phenoxycarboxyl-4-benzyl-2-(4-methoxyphenyl)-oxazole (6i).[7]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.8 Hz, 2H), 7.42-7.38 (m, 2H), 7.34-7.22 (m, 6H), 7.18-7.15 (m, 2H), 6.92 (d, *J* = 8.8 Hz, 2H), 3.82 (s, 2H), 3.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.4, 155.4,

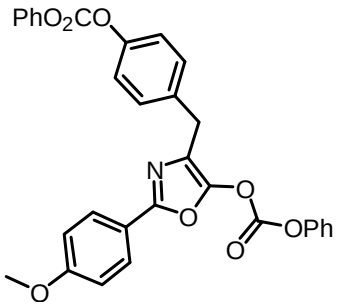
150.6, 149.9, 145.6, 137.3, 129.7, 128.9, 128.5, 127.7, 126.8, 126.6, 123.3, 120.5, 119.7, 114.1, 55.4, 31.7.; HRMS-ESI $[M+H]^+$ calcd. For $C_{24}H_{20}NO_5$: 402.1341, found: 402.1350.; R_f = 0.23 (EtOAc/hexanes, 1/10).

5-Phenoxycarboxyl-4-((4-benzyloxy)benzyl)-2-(4-methoxyphenyl)-oxazole (6j).[10]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.6 Hz, 2H), 7.41-7.17 (m, 12H), 6.93 (d, *J* = 8.6 Hz, 4H), 5.01 (s, 2H), 3.87 (s, 2H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.4, 157.5, 155.4, 150.6, 149.9, 145.5, 137.0, 130.0, 129.6, 128.5, 127.9, 127.7, 127.4, 126.7, 123.6, 120.4, 119.7, 114.9, 114.1, 69.9, 55.3, 30.9; HRMS-ESI $[M+H]^+$ calcd. For $C_{31}H_{26}NO_6$: 508.1755, found: 508.1760.; R_f = 0.28 (EtOAc/hexanes, 1/5).

5-Phenoxycarboxyl-4-((4-phenoxycarbonyloxy)benzyl)-2-(4-methoxyphenyl)-oxazole (6k).[10]

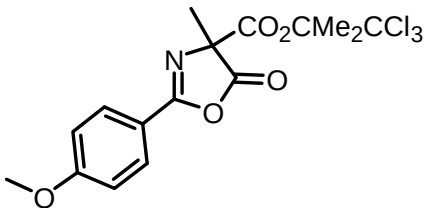


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 9.0 Hz, 2H), 7.45-7.38 (m, 6H), 7.32-7.27 (m, 5H), 7.24-7.22 (m, 3H), 6.95 (d, *J* = 9.0 Hz, 2H), 3.95 (s, 2H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.4, 155.5, 152.0, 151.0, 150.6, 150.0, 149.7, 145.7, 135.6, 130.0, 129.7, 129.5, 127.7, 126.8, 126.2, 122.8, 120.9, 120.4, 119.6, 114.1, 55.3, 30.8; HRMS-ESI $[M+H]^+$ calcd. For $C_{31}H_{24}NO_8$: 538.1496, found: 538.1484; R_f 0.23 (EtOAc/hexanes, 1/5).

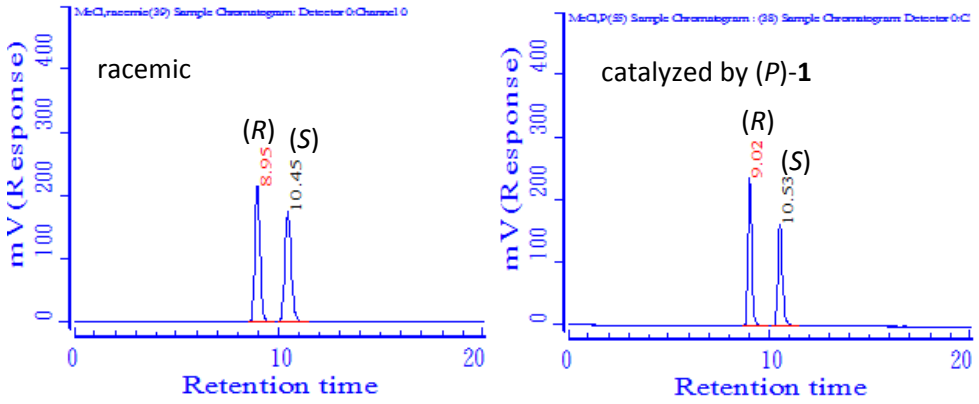
Representative procedure for catalytic asymmetric Steglich rearrangement. A 5-mL test tube was placed (*P*)-**1** (1 mg, 2.34 μmol) in a anhydrous 1/1 mixture of dimethoxyethane/*t*-amyl alcohol (0.25 mL) at -40 °C. The resulting solution was

cannulated to a precooled (-40 °C) solution of *O*-carboxyazlactone **6c** (15 mg, 0.05 mmol) in anhydrous 1/1 mixture of dimethoxyethane/*t*-amyl alcohol (0.25 mL). Upon reaction completion, iodomethane (0.25 mL) was added, and the solvent was evaporated under reduced pressure. The residue was purified by column chromatography (EtOAc/hexanes, 1/4) to give 13 mg (84 %) of *C*-carboxyazlactone **7c** as colorless oil.

4-Methyl-5-oxo-2-(4-methoxyphenyl)-4,5-dihydrooxazole-4-carboxylic acid 2,2,2-trichloroethyl ester (7a).[8]



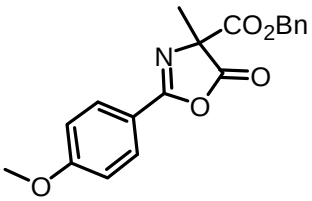
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.2 Hz, 2H), 6.97 (d, *J* = 8.2 Hz, 2H), 3.88 (s, 3H), 1.91 (s, 3H) , 1.88 (s, 3H) , 1.74 (s, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.0, 163.7, 163.6, 163.5, 130.1, 117.5, 114.3, 105.1, 90.7, 73.6, 55.5, 21.1, 19.3.; HRMS-ESI $[M+H]^+$ calcd. For $C_{16}H_{17}Cl_3NO_5$: 408.0172, found: 408.0168.; R_f = 0.3 (EtOAc/hexanes, 1/5); HPLC t_R 8.95 min (*R*), 10.45 min (*S*) (Chiralpak OD-H column, *i*-PrOH/hexanes, 1/99, 1.0 mL/min, λ = 254 nm). Reaction catalyzed by (*P*)-**1**: 9.02 min (major, 55.2 %), 10.53 min (minor, 44.8 %); $[\alpha]_D^{25}$ = +3.0 (c 0.5, $CHCl_3$) for 10 % ee (lit.[8] $[\alpha]_D^{22}$ = +18.0 (c 1.0, $CHCl_3$ for 76 % ee)); the absolute configuration of the major enantiomer was deduced to be (*R*).



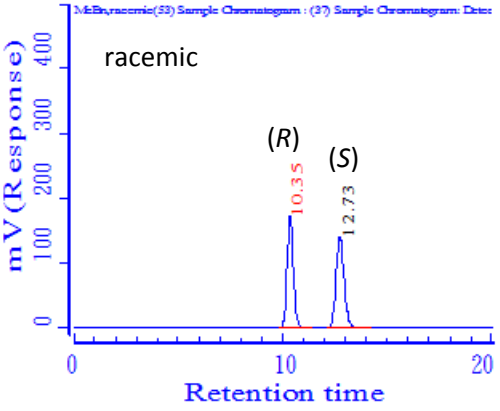
min	Area	Area %	Assay %
8.953	3876.09	50.33	0.00
10.453	3825.16	49.67	0.00

min	Area	Area %	Assay %
9.020	3155.98	55.24	0.00
10.534	2556.86	44.76	0.00

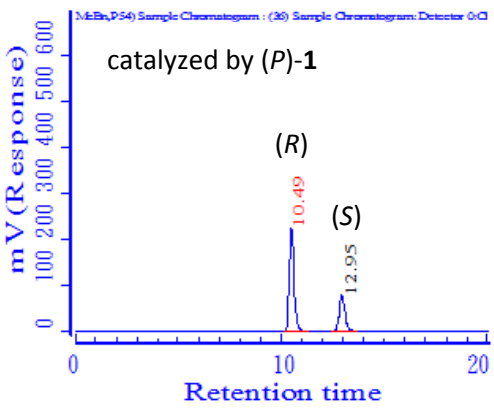
4-Methyl-5-oxo-2-(4-methoxyphenyl)-4,5-dihydrooxazole-4-carboxylic acid benzyl ester (7b).[6]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 9.0 Hz, 2H), 7.35-7.27 (m, 5H), 6.98 (d, *J* = 9.0 Hz, 2H), 5.22 (ABq, *J* = 12.4 Hz, 2H), 3.88 (s, 3H), 1.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.2, 166.1, 163.7, 163.0, 134.8, 130.2, 128.6, 128.4, 127.8, 117.4, 114.3, 72.8, 68.1, 55.5, 20.5.; HRMS-ESI $[M+H]^+$ calcd. For $C_{19}H_{18}NO_5$: 340.1185, found: 340.1181; R_f = 0.23 (EtOAc/hexanes, 1/5); HPLC t_R 10.35 min (*R*), 12.73 min (*S*) (Chiralpak OD-H column, *i*-PrOH/hexanes, 5/95, 1.0 mL/min, λ = 254 nm). Reaction catalyzed by (*P*)-**1**: 10.49 min (major, 70.6 %), 12.95 min (minor, 29.4 %); $[\alpha]_D^{25}$ = +28 (c 0.1, $CHCl_3$) for 41 % ee (lit.[6] ent $[\alpha]_D^{20}$ = -55.0 (c 0.95, $CHCl_3$ for 91 % ee)); the absolute configuration of the major enantiomer was deduced to be (*R*).

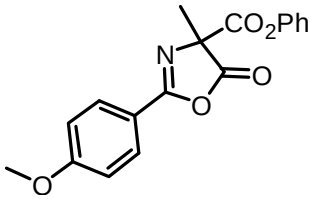


min	Area	Area %	Assay %
10.352	3613.73	48.60	0.00
12.733	3822.13	51.40	0.00

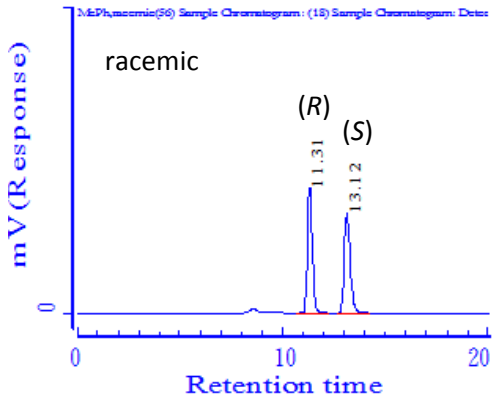


min	Area	Area %	Assay %
10.491	3618.92	70.60	0.00
12.947	1507.05	29.40	0.00

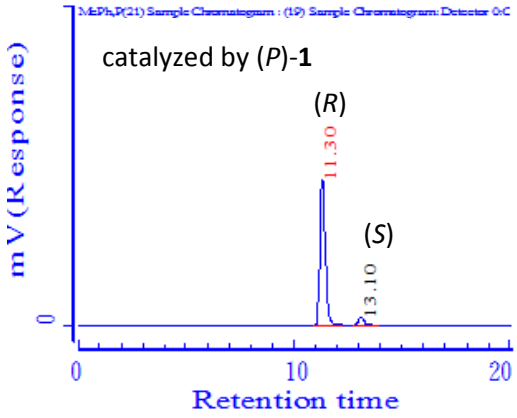
4-Methyl-5-oxo-2-(4-methoxyphenyl)-4,5-dihydrooxazole-4-carboxylic acid phenyl ester (7c).[11]



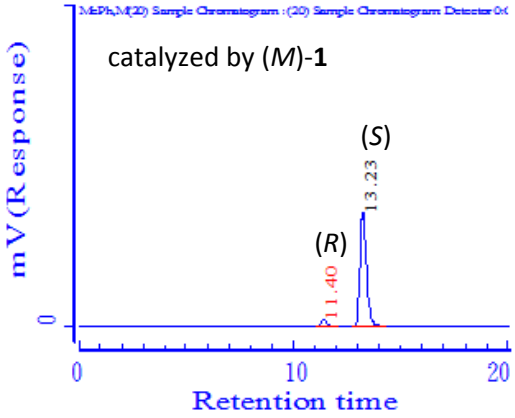
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, J = 9.0 Hz, 2H), 7.39-7.35 (m, 2H), 7.26-7.22 (m, 1H), 7.11-7.09 (m, 2H), 7.01 (d, J = 9.0 Hz, 2H), 3.89 (s, 3H), 1.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.0, 164.8, 163.8, 163.4, 150.3, 130.3, 129.5, 126.5, 121.0, 117.4, 114.4, 72.8, 55.5, 20.5.; HRMS-ESI $[M+H]^+$ calcd. For $C_{18}H_{16}NO_5$: 326.1028, found: 326.1026; R_f = 0.25 (EtOAc/hexanes, 1/5); HPLC t_R 11.31 min (*R*), 13.12 min (*S*) (Chiralpak OD-H column, *i*-PrOH/hexanes, 2/98, 1.0 mL/min, λ = 254 nm). Reaction catalyzed by (*P*)-**1**: 11.30 min (major, 93.9 %), 13.10 min (minor, 6.1 %); $[\alpha]_D^{25}$ = +94 (c 0.5, $CHCl_3$) for 88 % ee (lit.[11] $[\alpha]_D^{20}$ = +88.9 (c 0.4, $CHCl_3$ for 94 % ee)); the absolute configuration of the major enantiomer was deduced to be (*R*). Reaction catalyzed by (*M*)-**1'** : 11.40 min (minor, 4.8 %), 13.23 min (major, 95.2 %); $[\alpha]_D^{25}$ = -98 (c 0.5, $CHCl_3$) for 90 % ee; the absolute configuration of the major enantiomer was deduced to be (*S*).



min	Area	Area %	Assay %
11.308	6895.10	50.77	0.00
13.122	6686.00	49.23	0.00

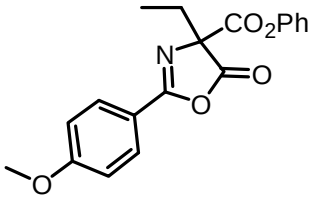


min	Area	Area %	Assay %
11.303	7973.18	93.87	0.00
13.098	520.34	6.13	0.00



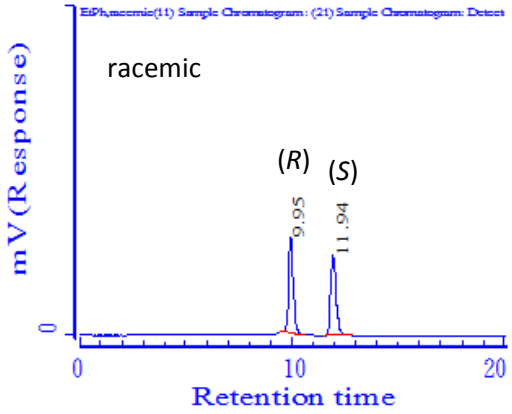
min	Area	Area %	Assay %
11.401	380.54	4.83	0.00
13.229	7495.91	95.17	0.00

4-Ethyl-5-oxo-2-(4-methoxyphenyl)-4,5-dihydrooxazole-4-carboxylic acid phenyl ester (7d).[11]

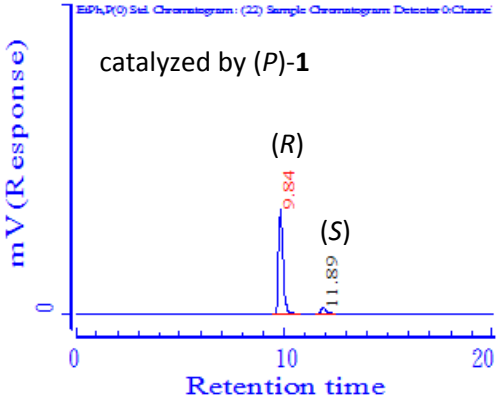


^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, J = 9.0 Hz, 2H), 7.39-7.35 (m, 2H), 7.26-7.22 (m, 1H), 7.12-7.09 (m, 2H), 7.01 (d, J = 9.0 Hz, 2H), 3.89 (s, 3H), 2.48-2.31 (m, 2H), 1.00 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.2, 164.6, 163.8, 163.3, 150.2, 130.3, 129.5, 126.4, 121.1, 117.3, 114.3, 77.2, 55.5, 27.9, 7.7; HRMS-ESI $[M+H]^+$ calcd. For $C_{19}H_{18}NO_5$: 340.1185, found: 340.1182; R_f

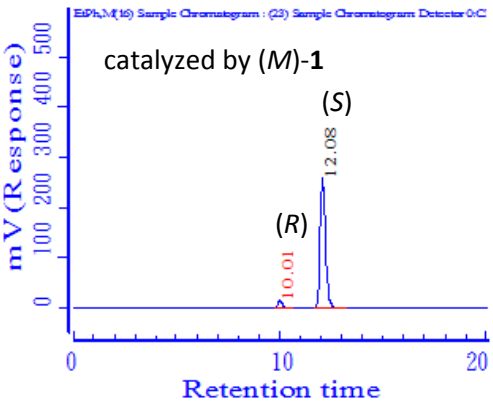
= 0.25 (EtOAc/hexanes, 1/2); HPLC t_R 9.95 min (*R*), 11.94 min (*S*) (Chiralpak OD-H column, *i*-PrOH/hexanes, 4/96, 1.0 mL/min, λ = 254 nm). Reaction catalyzed by (*P*)-**1**: 9.84 min (major, 93.9 %), 11.89 min (minor, 6.1 %); $[\alpha]_D^{25}$ = +82 (c 0.5, $CHCl_3$) for 88 % ee ; the absolute configuration of the major enantiomer was deduced to be (*R*). Reaction catalyzed by (*M*)-**1'** : 10.01 min (minor, 4.6 %), 12.08 min (major, 95.4 %); $[\alpha]_D^{25}$ = -84 (c 0.5, $CHCl_3$) for 91 % ee (lit.[11] $[\alpha]_D^{20}$ = -74.8 (c 0.29, $CHCl_3$ for 92 % ee)); the absolute configuration of the major enantiomer was deduced to be (*S*).



min	Area	Area %	Assay %
9.947	4345.48	50.16	0.00
11.939	4318.00	49.84	0.00

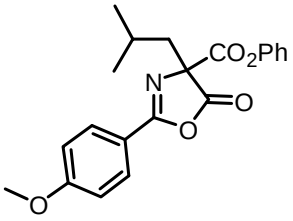


min	Area	Area %	Assay %
9.840	4999.06	93.89	0.00
11.893	325.18	6.11	0.00

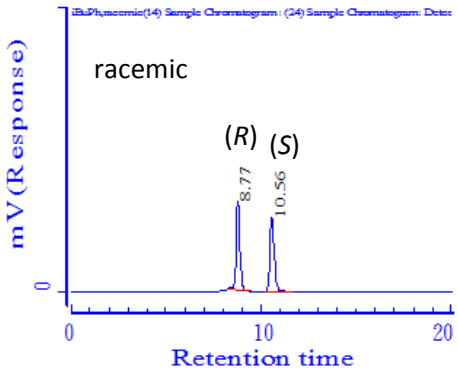


min	Area	Area %	Assay %
10.014	229.10	4.62	0.00
12.076	4725.22	95.38	0.00

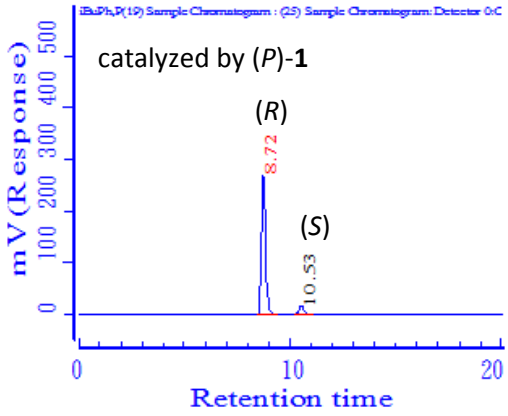
4-*iso*-Butyl-5-oxo-2-(4-methoxyphenyl)-4,5-dihydrooxazole-4-carboxylic acid phenyl ester (7e).[7]



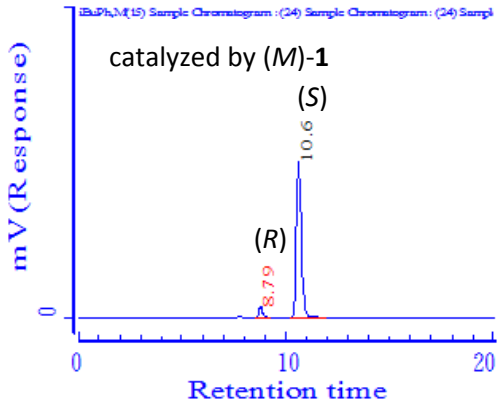
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.9 Hz, 2H), 7.38-7.34 (m, 2H), 7.25-7.22 (m, 1H), 7.11-7.08 (m, 2H), 7.01 (d, *J* = 8.9 Hz, 2H), 3.88 (s, 3H), 2.50 (dd, *J* = 14.3, 5.8 Hz, 1H), 2.17 (dd, *J* = 14.3, 7.2 Hz, 1H), 1.86-1.77 (m, 1H), 1.00 (d, *J*= 6.7 Hz, 3H), 0.96 (d, *J*= 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.8, 164.8, 163.7, 162.8, 150.3, 130.3, 129.5, 126.4, 121.1, 117.4, 114.3, 76.3, 55.5, 42.7, 24.7, 23.8, 23.1; HRMS-ESI $[M+H]^+$ calcd. For $C_{21}H_{22}NO_5$: 368.1498, found : 368.1497; R_f = 0.28 (EtOAc/hexanes, 1/5); HPLC t_R 8.77 min (*R*), 10.56 min (*S*) (Chiralpak OD-H column, *i*-PrOH/hexanes, 2/98, 1.0 mL/min, λ = 254 nm). Reaction catalyzed by (*P*)-**1**: 8.72 min (major, 93.6 %), 10.53 min (minor, 6.4 %); $[\alpha]_D^{25}$ = +118 (c 0.5, $CHCl_3$) for 88 % ee; the absolute configuration of the major enantiomer was deduced to be (*R*). Reaction catalyzed by (*M*)-**1'** : 8.79 min (minor, 5.0 %), 10.61 min (major, 95.0 %); $[\alpha]_D^{25}$ = -126 (c 0.5, $CHCl_3$) for 90 % ee; the absolute configuration of the major enantiomer was deduced to be (*S*).



min	Area	Area %	Assay %
8.767	4146.73	49.71	0.00
10.563	4194.27	50.29	0.00

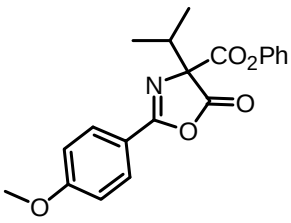


min	Area	Area %	Assay %
8.724	3614.34	93.63	0.00
10.529	245.96	6.37	0.00

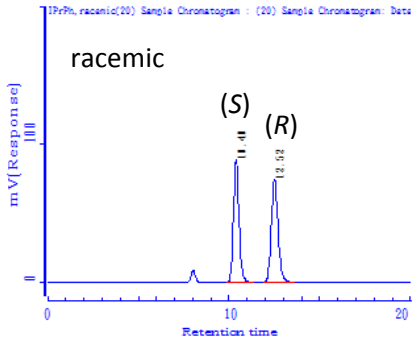


min	Area	Area %	Assay %
8.785	439.72	4.95	0.00
10.609	8438.75	95.05	0.00

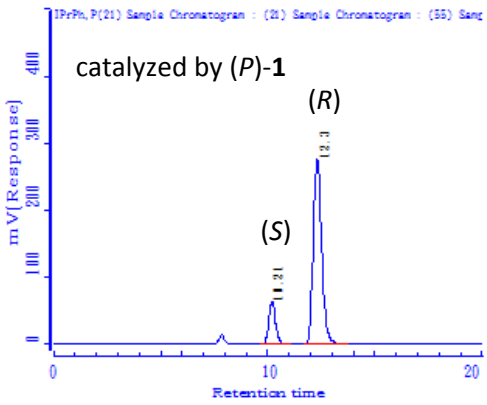
4-*iso*-Propyl-5-oxo-2-(4-methoxyphenyl)-4,5-dihydrooxazole-4-carboxylic acid phenyl ester (7f).[11]



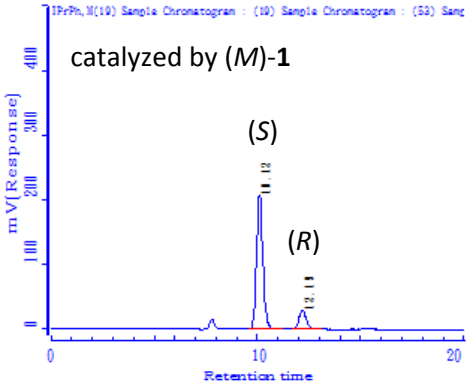
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, J = 9.0 Hz, 2H), 7.40-7.36 (m, 2H), 7.26-7.24 (m, 1H), 7.13-7.09 (m, 2H), 7.00 (d, J = 9.0 Hz, 2H), 3.89 (s, 3H), 2.97 (sept, J = 6.8 Hz, 1H), 1.18 (d, J = 6.8 Hz, 3H), 1.08 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.4, 164.5, 163.7, 162.8, 150.3, 130.3, 129.5, 126.4, 121.1, 117.4, 114.3, 80.4, 55.5, 34.7, 17.2, 16.4.; HRMS-ESI $[M+H]^+$ calcd. For $C_{20}H_{20}NO_5$: 354.1336, found: 354.1339; R_f 0.25 (EtOAc/hexanes, 1/10); HPLC t_R 10.40 min (*S*), 12.52 min (*R*) (Chiralpak AD-H column, *i*-PrOH/hexanes, 5/95, 1.0 mL/min, λ = 254 nm). Reaction catalyzed by (*P*)-**1**: 10.21 min (minor, 15.5 %), 13.32 min (major, 84.5 %); $[\alpha]_D^{25}$ = +62 (c 0.5, $CHCl_3$) for 69 % ee; the absolute configuration of the major enantiomer was deduced to be (*R*). Reaction catalyzed by (*M*)-**1'** : 11.12 min (major, 85.8 %), 12.19 min (minor, 14.2 %); $[\alpha]_D^{25}$ = -65 (c 0.5, $CHCl_3$) for 72 % ee; the absolute configuration of the major enantiomer was deduced to be (*S*).



min	Area	Area %	Assay %
10.398	1872.01	49.26	0.00
12.516	1928.42	50.74	0.00

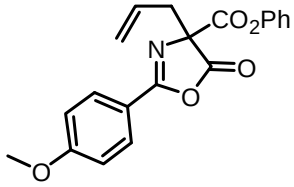


min	Area	Area %	Assay %
10.210	1394.75	15.53	0.00
12.324	7583.42	84.47	0.00



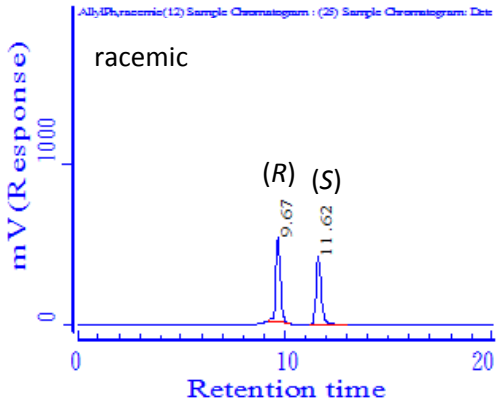
min	Area	Area %	Assay %
10.117	4402.70	85.79	0.00
12.193	729.15	14.21	0.00

4-Allyl-5-oxo-2-(4-methoxyphenyl)-4,5-dihydrooxazole-4-carboxylic acid phenyl ester (7g).[11]

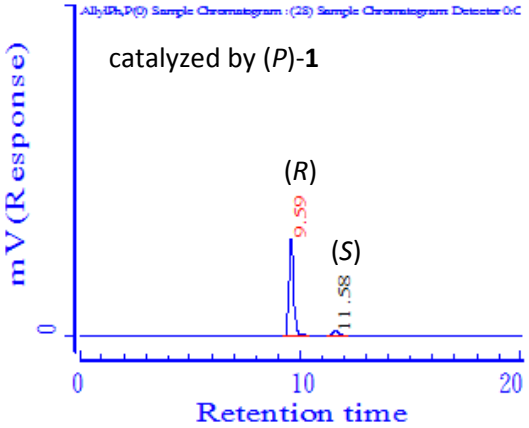


^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 9.0 Hz, 2H), 7.39-7.35 (m, 2H), 7.24-7.23 (m, 1H), 7.12-7.09 (m, 2H), 7.00 (d, *J* = 9.0 Hz, 2H), 5.76-5.66 (m, 1H), 5.33-5.20 (m, 2H), 3.89 (s, 3H), 3.16 (dd, *J* = 13.9, 6.6 Hz, 1H), 3.02 (dd, *J* = 13.9, 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.7, 164.3, 163.8, 163.3, 150.2, 130.4, 129.5, 129.2, 126.5, 121.8, 121.1, 117.3, 114.3, 76.6, 55.6, 38.4; HRMS-ESI $[M+H]^+$ calcd. For $C_{20}H_{18}NO_5$: 352.1185, found: 352.1180; R_f = 0.28 (EtOAc/hexanes, 1/5); HPLC t_R 9.67 min (*R*), 11.62 min (*S*) (Chiralpak OD-H column,

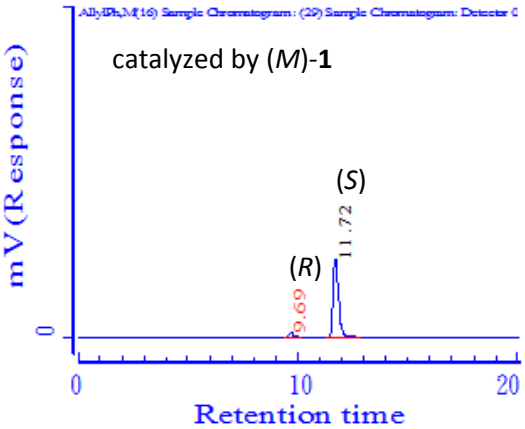
i-PrOH/hexanes, 4/96, 1.0 mL/min, λ = 254 nm). Reaction catalyzed by (*P*)-**1**: 9.59 min (major, 94.0 %), 11.58 min (minor, 6.0 %); $[\alpha]_D^{25}$ = +97 (c 0.5, $CHCl_3$) for 88 % ee (lit.[11] $[\alpha]_D^{20}$ = +107.7 (c 0.79, $CHCl_3$ for 89 % ee)); the absolute configuration of the major enantiomer was deduced to be (*R*). Reaction catalyzed by (*M*)-**1'** : 9.69 min (minor, 4.5 %), 11.72 min (major, 95.5 %); $[\alpha]_D^{25}$ = -103 (c 0.5, $CHCl_3$) for 91 % ee; the absolute configuration of the major enantiomer was deduced to be (*S*).



min	Area	Area %	Assay %
9.674	8005.38	50.62	0.00
11.615	7809.10	49.38	0.00

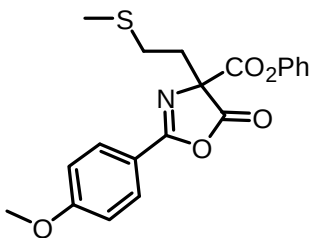


min	Area	Area %	Assay %
9.587	4239.90	93.98	0.00
11.579	271.63	6.02	0.00

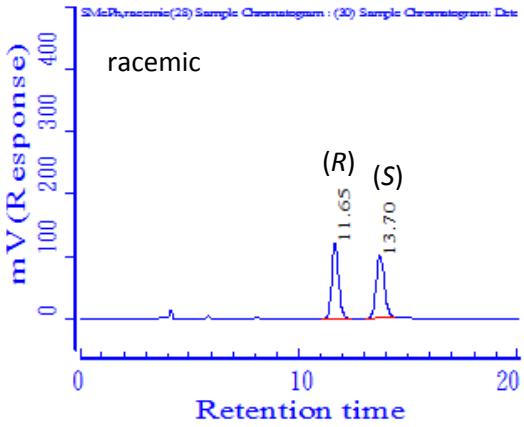


min	Area	Area %	Assay %
9.690	199.46	4.48	0.00
11.720	4254.25	95.52	0.00

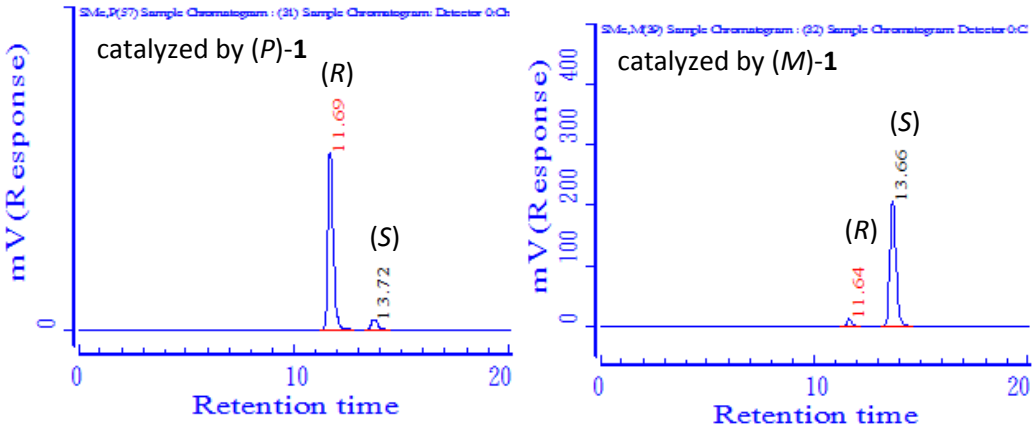
4-((2-Methylthio)ethyl)-5-oxo-2-(4-methoxyphenyl)-4,5-dihydrooxazole-4-carboxylic acid phenyl ester (7h).[11]



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, J = 8.9 Hz, 2H), 7.39-7.35 (m, 2H), 7.24-7.22 (m, 1H), 7.11-7.09 (m, 2H), 7.01 (d, J = 8.9 Hz, 2H), 3.89 (s, 3H), 2.79-2.54 (m, 4H), 2.10 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.3, 164.4, 163.9x2, 150.2, 130.4, 129.5, 126.5, 121.0, 117.3, 114.4, 75.6, 55.6, 33.2, 28.3, 15.1; HRMS-ESI $[M+H]^+$ calcd. For $C_{20}H_{20}NO_5S$: 386.1062, found: 386.1054; R_f = 0.25 (EtOAc/hexanes, 1/2); HPLC t_R 11.65 min (*R*), 13.70 min (*S*) (Chiralpak OD-H column, *i*-PrOH/hexanes, 4/96, 1.0 mL/min, λ = 254 nm). Reaction catalyzed by (*P*)-**1**: 11.69 min (major, 93.7 %), 13.72 min (minor, 6.3 %); $[\alpha]_D^{25}$ = +183 (c 0.5, $CHCl_3$) for 87 % ee (lit.[11] $[\alpha]_D^{20}$ = +111.0 (c 0.68, $CHCl_3$ for 90 % ee)); the absolute configuration of the major enantiomer was deduced to be (*R*). Reaction catalyzed by (*M*)-**1'** : 11.64 min (minor, 4.7 %), 13.66 min (major, 95.3%); $[\alpha]_D^{25}$ = -191 (c 0.5, $CHCl_3$) for 91 % ee; the absolute configuration of the major enantiomer was deduced to be (*S*).



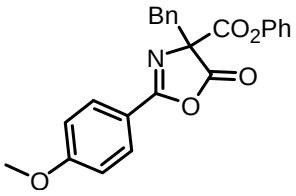
min	Area	Area %	Assay %
11.650	2725.70	50.83	0.00
13.703	2636.75	49.17	0.00



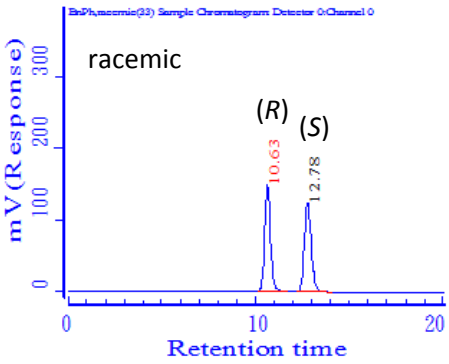
min	Area	Area %	Assay %
11.687	9942.89	93.66	0.00
13.717	672.61	6.34	0.00

min	Area	Area %	Assay %
11.643	207.51	4.70	0.00
13.658	4209.54	95.30	0.00

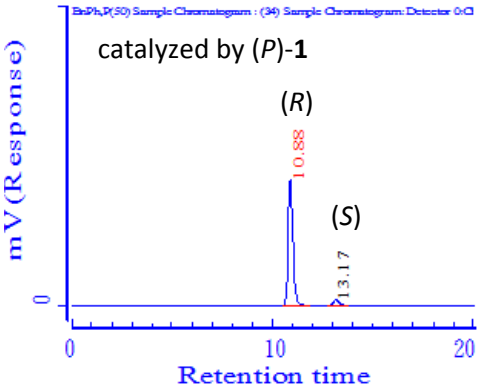
4-Benzyl-5-oxo-2-(4-methoxyphenyl)-4,5-dihydrooxazole-4-carboxylic acid phenyl ester (7i).[11]



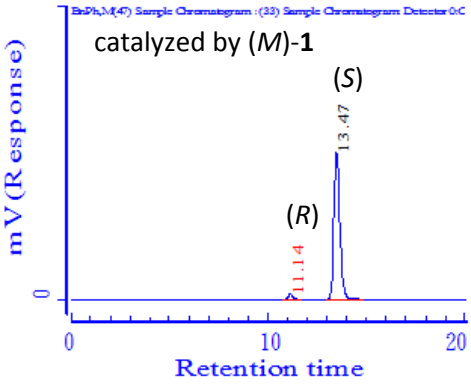
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 9.0 Hz, 2H), 7.40-7.36 (m, 2H), 7.27-7.18 (m, 6H), 7.11-7.10 (m, 2H), 6.94 (d, J = 9.0 Hz, 2H), 3.86 (s, 3H), 3.72 (ABq, J = 13.7 Hz, 1H), 3.60 (ABq, J = 13.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.6, 164.5, 163.7, 163.1, 150.3, 132.8, 130.5, 130.2, 129.5, 128.3, 127.6, 126.5, 121.1, 117.2, 114.2, 77.5, 55.5, 40.2; HRMS-ESI $[M+Na]^+$ calcd. For $C_{24}H_{20}NO_5$: 402.1341, found: 402.1339; R_f = 0.3 (EtOAc/hexanes, 1/5); HPLC t_R 10.63 min (*R*), 12.78 min (*S*) (Chiralpak OD-H column, *i*-PrOH/hexanes, 6/94, 1.0 mL/min, λ = 254 nm). Reaction catalyzed by (*P*)-**1**: 10.88 min (major, 94.8 %), 13.17 min (minor, 5.2 %); $[\alpha]_D^{25}$ = +116 (c 0.5, $CHCl_3$) for 90 % ee (lit.[11] $[\alpha]_D^{20}$ = +195 (c 0.61, $CHCl_3$ for 91 % ee)); the absolute configuration of the major enantiomer was deduced to be (*R*). Reaction catalyzed by (*M*)-**1'** : 11.14 min (minor, 2.9 %), 13.47 min (major, 97.1 %); $[\alpha]_D^{25}$ = -125 (c 0.1, $CHCl_3$) for 94 % ee; the absolute configuration of the major enantiomer was deduced to be (*S*).



min	Area	Area %	Assay %
10.629	3142.14	49.39	0.00
12.776	3220.00	50.61	0.00

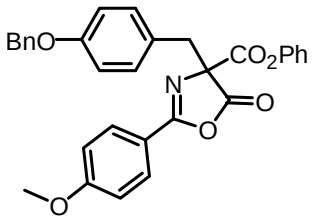


min	Area	Area %	Assay %
10.881	6927.99	94.82	0.00
13.169	378.58	5.18	0.00



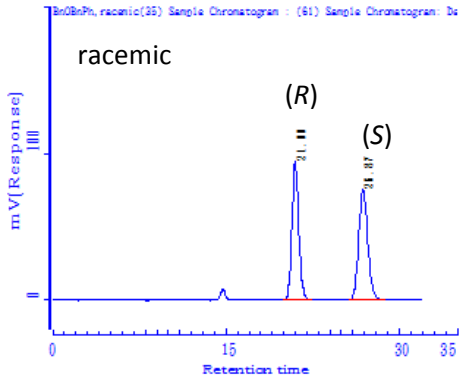
min	Area	Area %	Assay %
11.138	317.37	2.91	0.00
13.472	10597.60	97.09	0.00

4-((4-Benzyloxy)benzyl)-5-oxo-2-(4-methoxyphenyl)-4,5-dihydrooxazole-4-carboxylic acid phenyl ester (7j).[11]

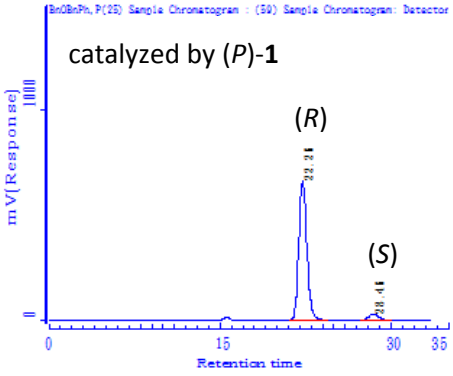


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, J = 9.0 Hz, 2H), 7.40-7.11 (m, 12H), 6.96 (d, J = 9.0 Hz, 2H), 6.83 (d, J = 8.7 Hz, 2H), 4.97 (s, 2H), 3.87 (s, 3H), 3.68 (ABq, J = 13.9 Hz, 1H), 3.57 (ABq, J = 13.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.6, 164.5, 163.6, 163.1, 158.2, 150.2, 136.8, 131.6, 130.2, 129.5, 128.5, 127.9, 127.4, 126.5, 125.0, 121.1, 117.2, 114.6, 114.2, 77.6, 69.8, 55.5,

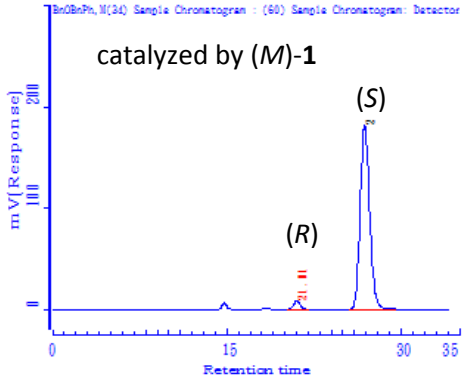
39.4.; HRMS-ESI $[M+H]^+$ calcd. For $C_{31}H_{26}NO_6$: 508.1755, found: 508.1798; R_f 0.25 (EtOAc/hexanes, 1/5); HPLC t_R 21.00 min (*R*), 26.87 min (*S*) (Chiralpak OD-H column, *i*-PrOH/hexanes, 10/90, 1.0 mL/min, λ = 254 nm). Reaction catalyzed by (*P*)-**1**: 22.26 min (major, 95.3 %), 28.46 min (minor, 4.7 %); $[\alpha]_D^{25}$ = +150 (c 0.5, $CHCl_3$) for 91 % ee (lit.[11] $[\alpha]_D^{20}$ = +154.1 (c 0.54, $CHCl_3$ for 91 % ee)); the absolute configuration of the major enantiomer was deduced to be (*R*). Reaction catalyzed by (*M*)-**1'** : 20.01 min (minor, 3.3 %), 26.87 min (major, 96.7 %); $[\alpha]_D^{25}$ = -156 (c 0.5, $CHCl_3$) for 93 % ee; the absolute configuration of the major enantiomer was deduced to be (*S*).



min	Area	Area %	Assay %
20.996	4057.09	49.67	0.00
26.874	4110.21	50.33	0.00

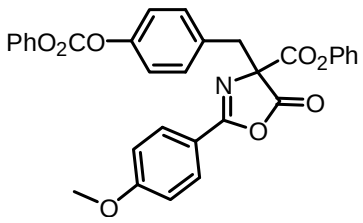


min	Area	Area %	Assay %
22.256	32310.30	95.27	0.00
28.458	1604.64	4.73	0.00

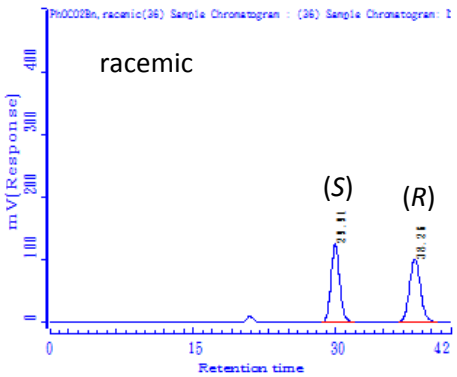


min	Area	Area %	Assay %
21.010	347.96	3.28	0.00
26.869	10259.22	96.72	0.00

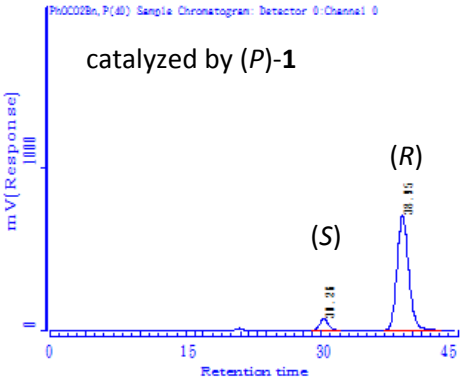
4-((4-Phenoxycarbonyloxy)benzyl)-5-oxo-2-(4-methoxyphenyl)-4,5-dihydrooxazole-4-carboxylic acid phenyl ester (7k).[11]



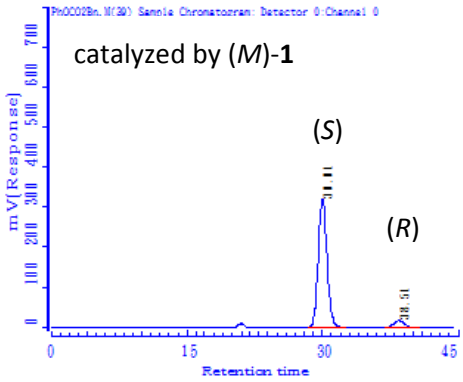
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, J = 9.0 Hz, 2H), 7.40-7.07 (m, 14H), 6.92 (d, J = 9.0 Hz, 2H), 3.84 (s, 3H), 3.72 (ABq, J = 13.8 Hz, 1H), 3.58 (ABq, J = 13.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.5, 164.3, 163.8, 163.4, 151.7, 150.9, 150.5, 150.2, 131.7, 131.0, 130.2, 129.5, 126.5, 126.3, 121.1, 120.8, 120.7, 117.0, 114.3, 77.3, 55.5, 39.4.; HRMS-ESI $[M+H]^+$ calcd. For $C_{31}H_{24}NO_8$: 538.1496, found: 538.1489; R_f 0.20 (EtOAc/hexanes, 1/5); HPLC t_R 29.91 min (*S*), 38.26 min (*R*) (Chiralpak AD-H column, *i*-PrOH/hexanes, 20/80, 1.0 mL/min, λ = 254 nm). Reaction catalyzed by (*P*)-**1**: 30.26 min (minor, 6.4 %), 38.95 min (major, 93.6 %); $[\alpha]_D^{25}$ = +118 (c 0.5, $CHCl_3$) for 87 % ee (lit.[11] $[\alpha]_D^{20}$ = +125.4 (c 0.52, $CHCl_3$ for 89.9 % ee)); the absolute configuration of the major enantiomer was deduced to be (*R*). Reaction catalyzed by (*M*)-**1'** : 30.01 min (major, 94.8 %), 38.51 min (minor, 5.2 %); $[\alpha]_D^{25}$ = -123 (c 0.5, $CHCl_3$) for 90 % ee; the absolute configuration of the major enantiomer was deduced to be (*S*).



min	Area	Area %	Assay %
29.911	8162.25	49.98	0.00
38.259	8167.77	50.02	0.00



min	Area	Area %	Assay %
30.264	4306.69	6.44	0.00
38.949	62562.41	93.56	0.00



min	Area	Area %	Assay %
30.006	21578.73	94.80	0.00
38.509	1182.71	5.20	0.00

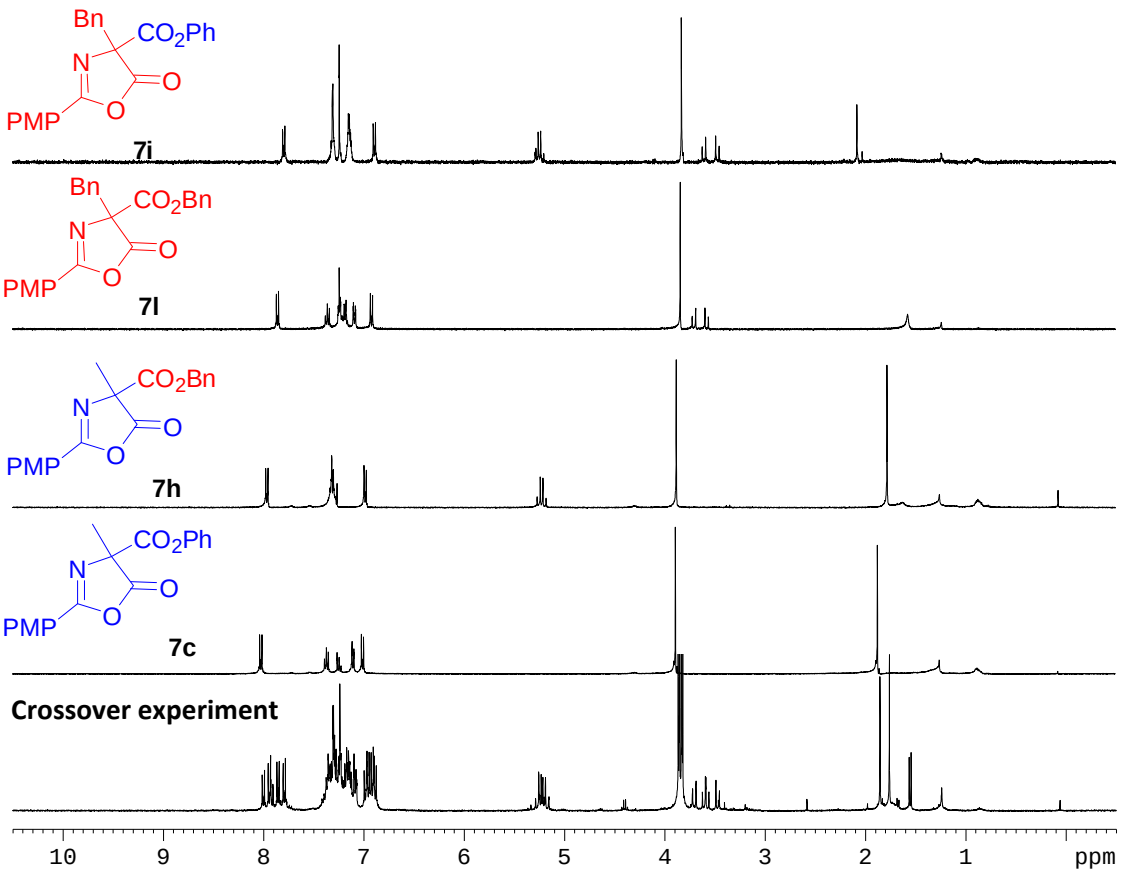


Figure S11. Stacked ^{1}H NMR spectra of crossover experiments of *O*-carboxylazlactones 6c and 6l under optimal reaction conditions.

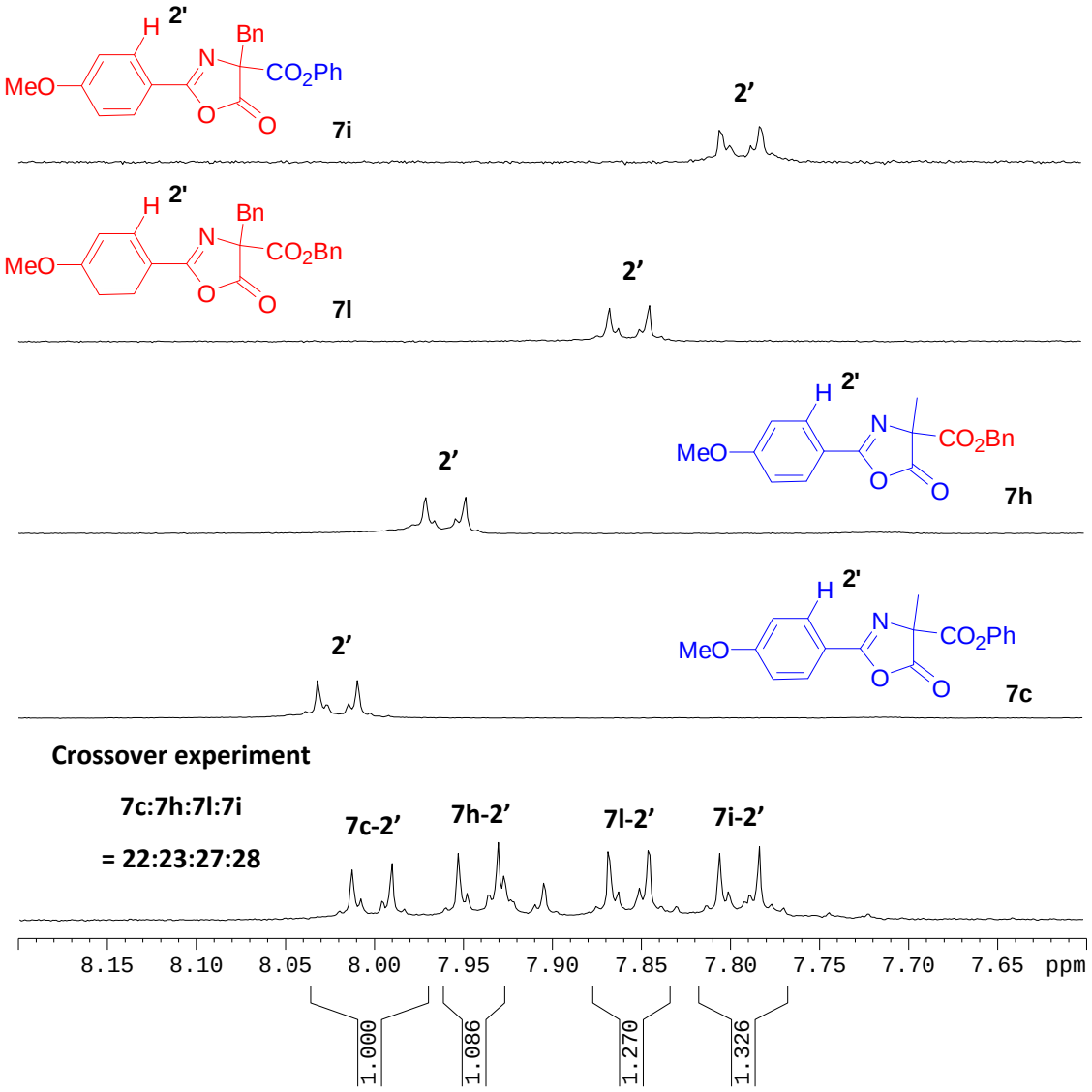


Figure S12. Expanded Stacked ^{1}H NMR spectra of crossover experiments of *O*-carboxylazlactones 6c and 6l under optimal reaction condition.

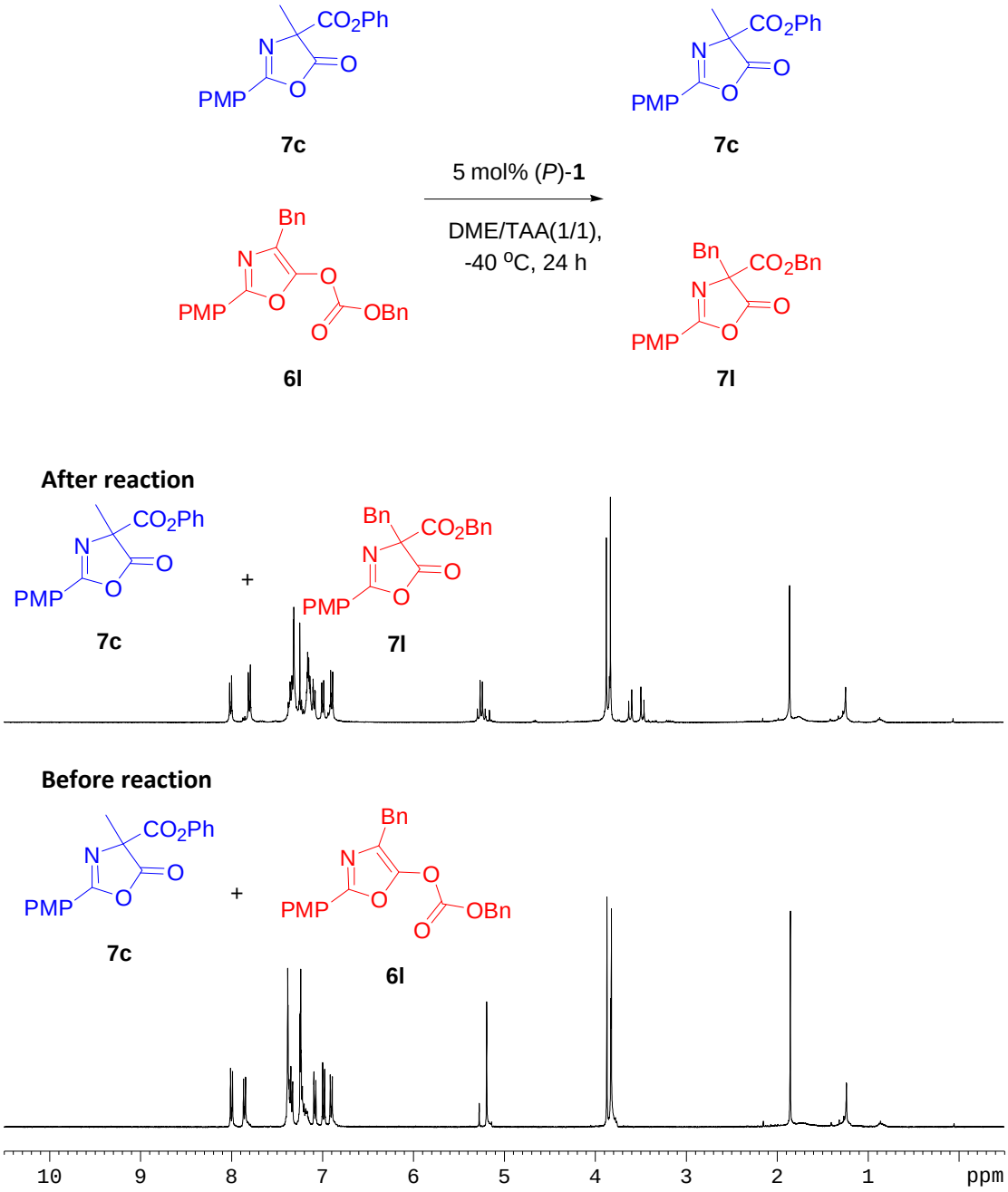


Figure S13. Stacked ^{1}H NMR spectra of control experiment performed by reaction of a mixture of *C*-carboxyl 7c and *O*-carboxyl 6l under optimal reaction conditions.

References

1. C.-T. Chen, C.-H. Chen and T.-G. Ong, *J. Am. Chem. Soc.,* 2013, **135**, 5294−5297.

2. M. R. Heinrich, H. S. Klisa, H. Mayr, W.Steglich and H. Zipse, *Angew. Chem. Int. Ed., 2003*, **42**, 4826−4828.

3. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-41.

4. E. Cancès and B. Mennucci, J. Chem. Phys., **2001**, *114*, 4744-45.

5. Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

6. J. C. Ruble and G. C. Fu, *J. Am.Chem. Soc.*, 1998, **120**, 11532−11533.

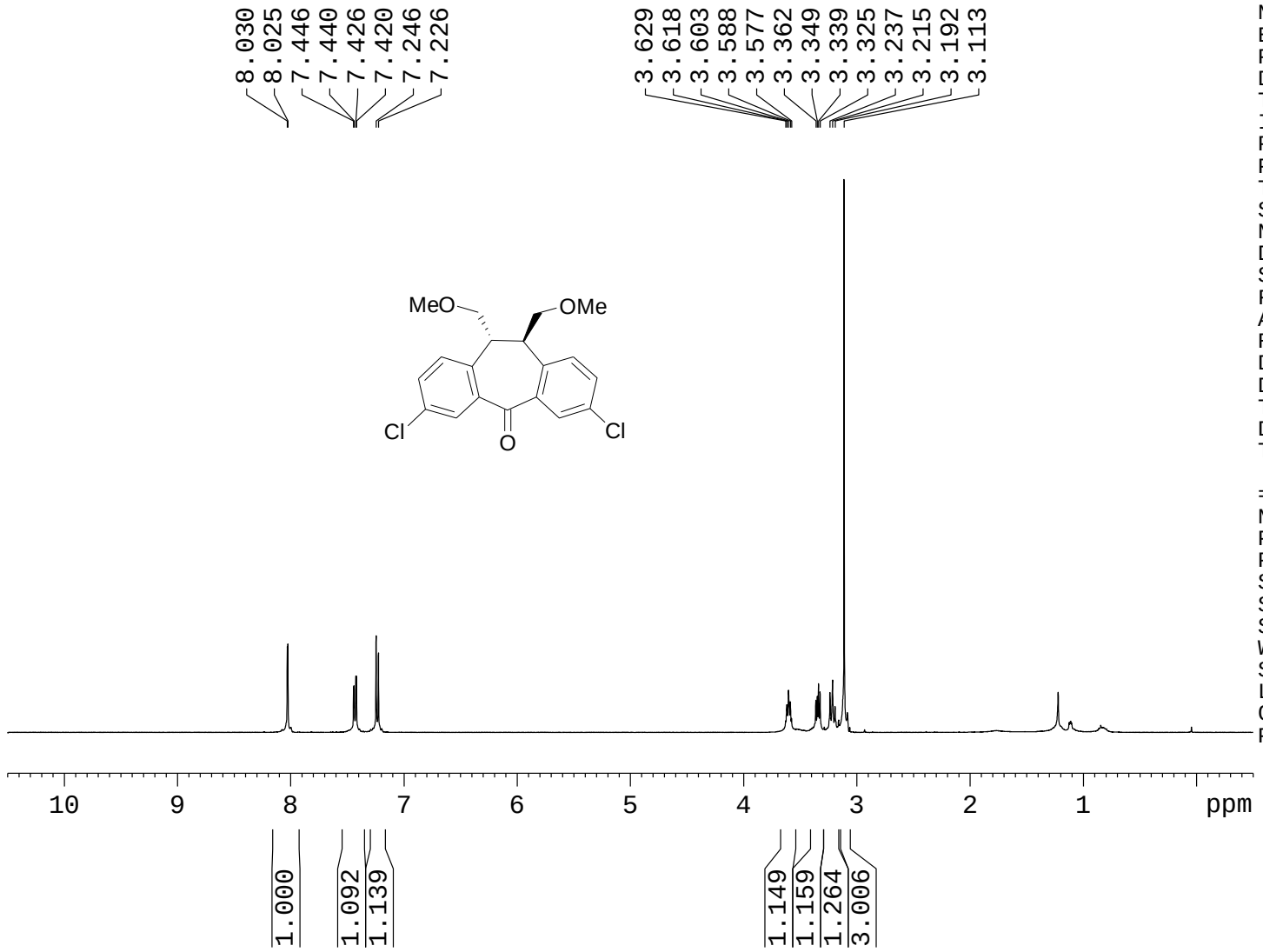
7. S. A. Shaw, P. Aleman and E. Vedejs, *J. Am.Chem. Soc.*, 2003, **125**, 13368−13369.

8. H. V. Nguyen, D. C. D. Butler and C. J. Richards, *Org. Lett*., 2006, **8**, 769-772.

9. J. E. Thomson, C. D. Campbell, C. Concellon, N. Duguet, K. Rix, A. M. Z. Slawin and A. D. Smith, *J. Org. Chem*., 2008, **73**, 2784-2791.

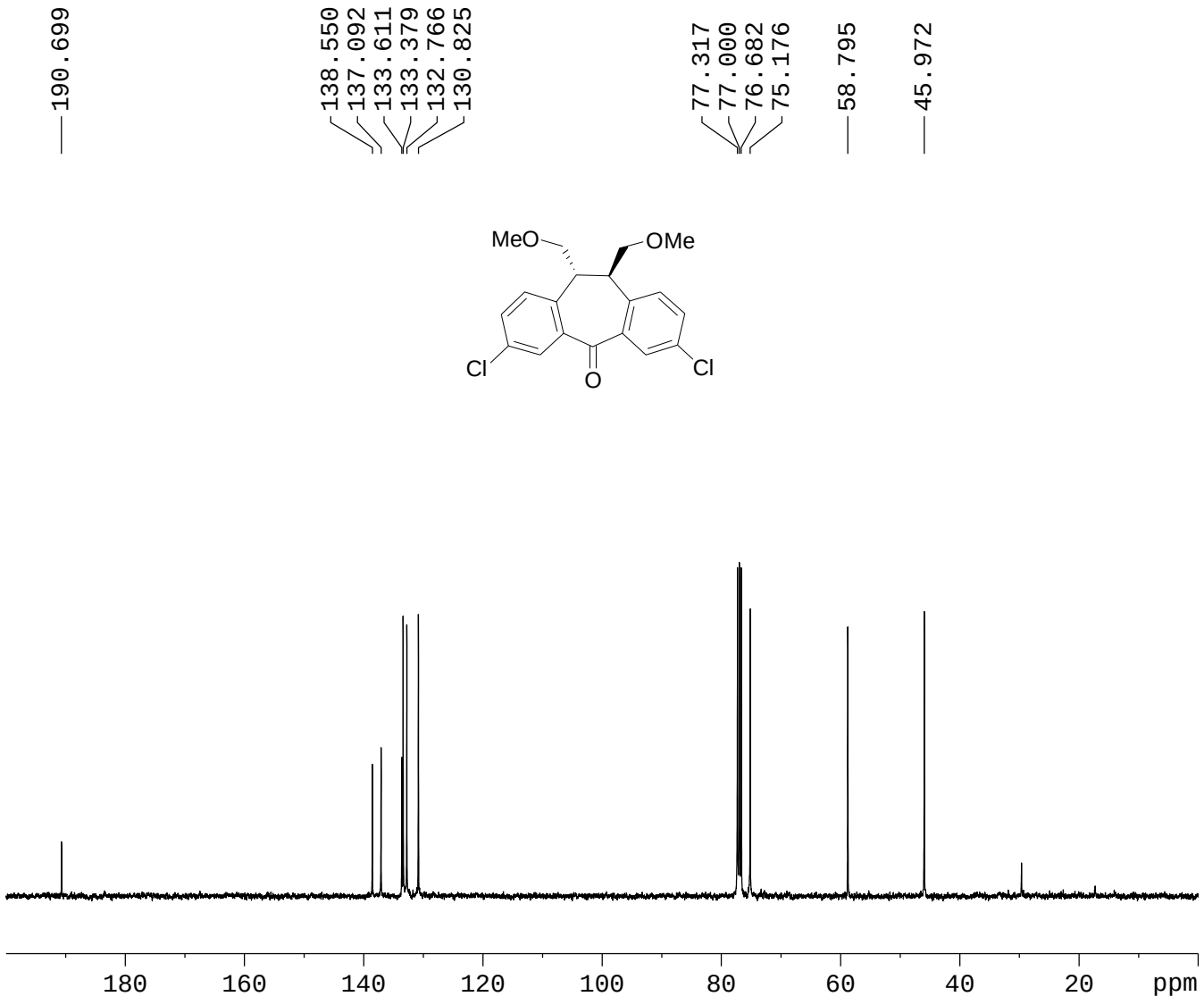
10. C. Joannesse, C. Simal, C. Concellon, J. E. Thomson, C. D. Campbell, A. M. Z. Slawin, A. D. Smith, *Org. Biomol. Chem.,* 2008, **6**, 2900-2907.

11. C. Joannesse, C. P. Johnston, C. Concellon, C. Simal, D. Philp and A. D. Smith, *Angew. Chem., Int. Ed.*, 2009, **48**, 8914−8918.

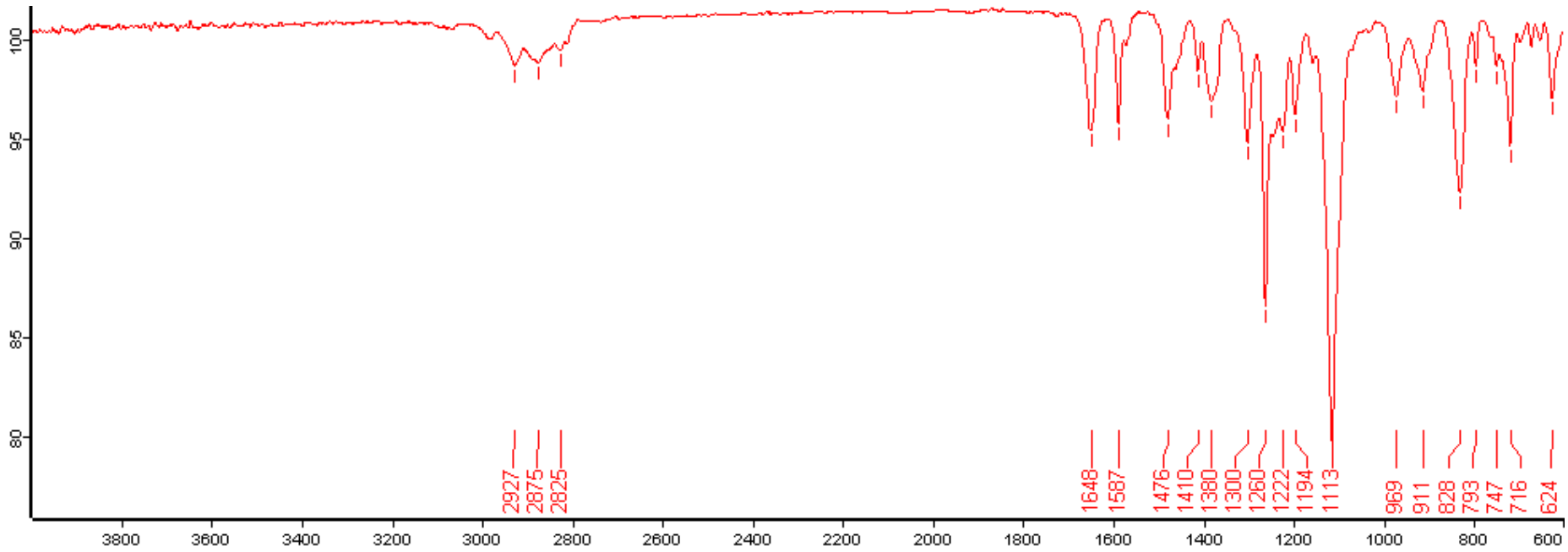


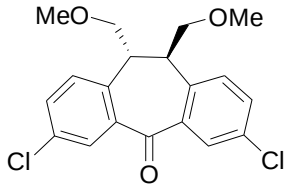
NAME	140222MOMdiCl
EXPNO	1
PROCNO	1
Date_	20140222
Time	12.46
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500168 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	140222MOMdiCl
EXPNO	13
PROCNO	1
Date_	20140222
Time	12.47
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	590
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6178027 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00


100
95
90
85
80
2927
2875
2825
1648
1587
1476
1410
1380
1300
1260
1222
1194
1113
969
911
828
793
747
716
624
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600


MeO
OMe
Cl
Cl
O

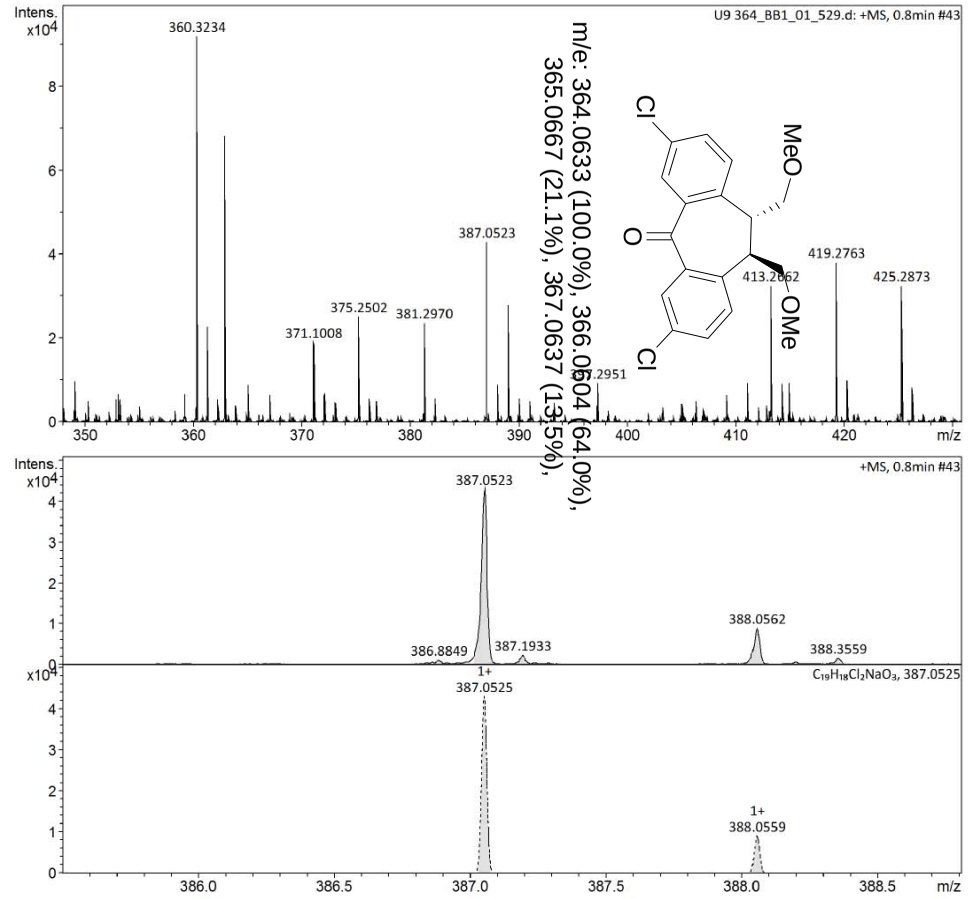
Display Report

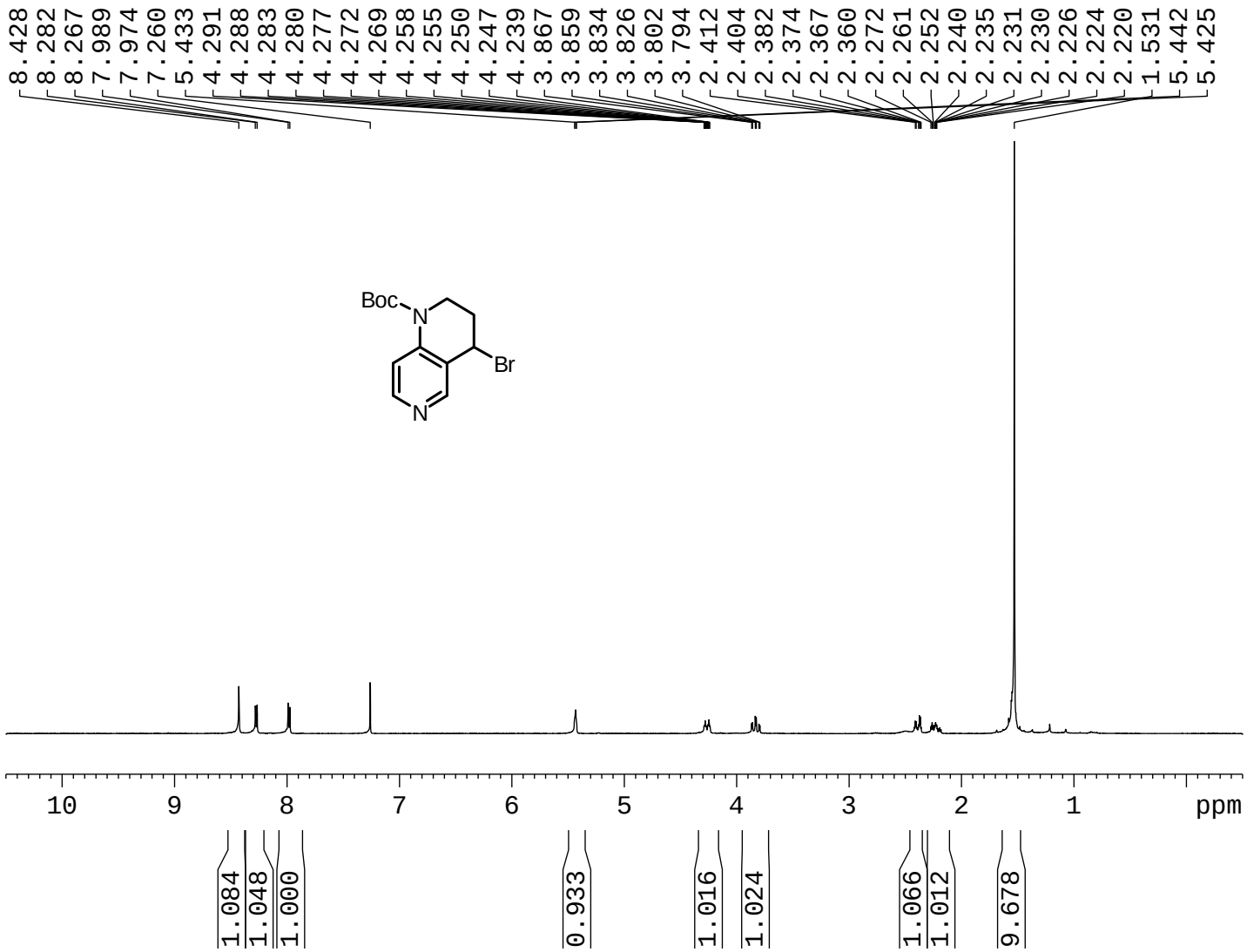
Analysis Info

Analysis Name	D:\Data\NCTU SERVICE\Data\20140303\U9 364_BB1_01_529.d	Acquisition Date	3/3/2014 3:38:38 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	U9 364	Instrument	impact HD 1819696.00164
Comment			

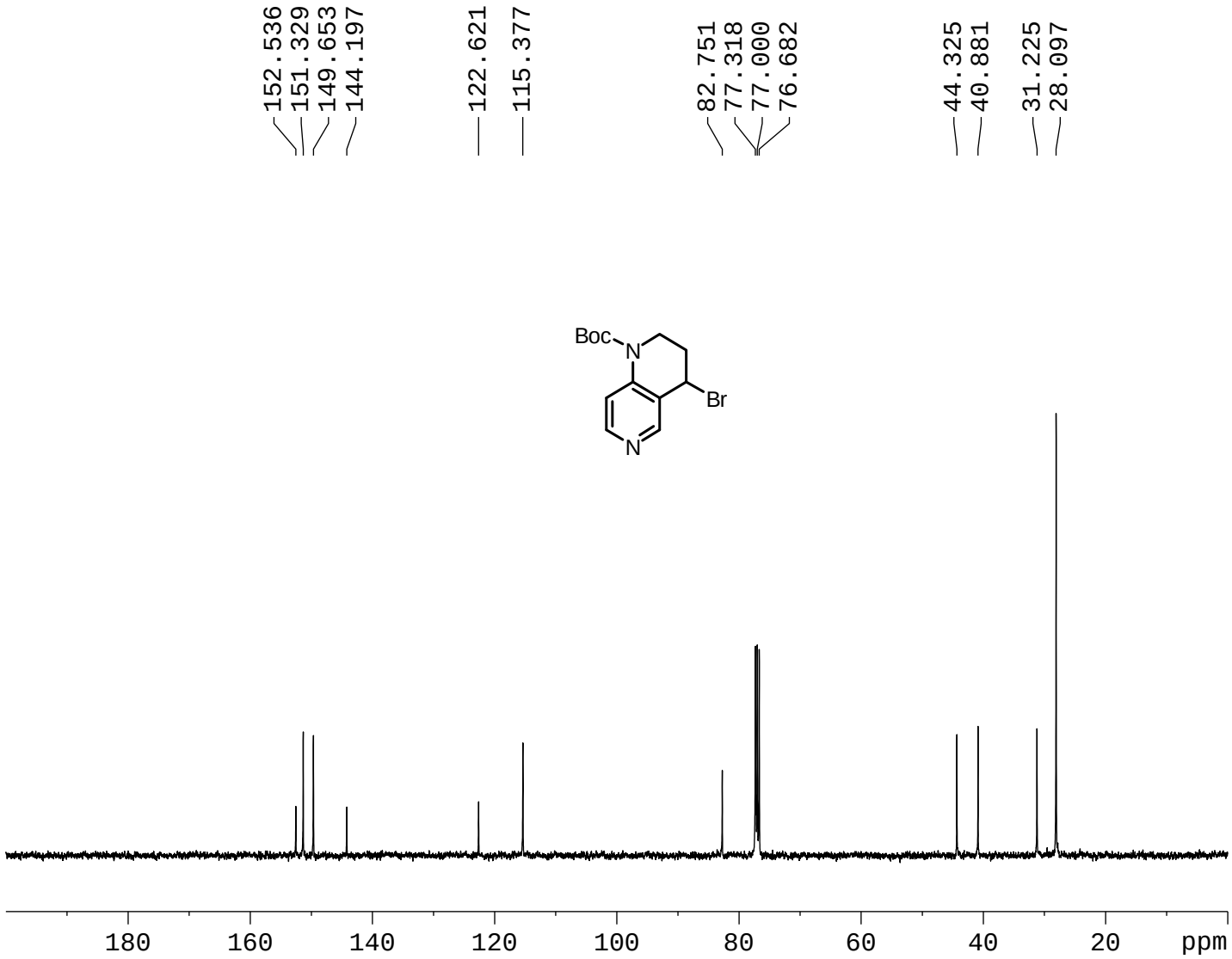
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



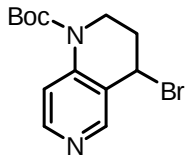


NAME	141011Br	
EXPNO	2	
PROCNO	1	
Date_	20141013	
Time	15.21	
INSTRUM	spect	
PROBHD	5 mm DUL 13C-1	
PULPROG	zg30	
TD	32768	
SOLVENT	CDCl3	
NS	8	
DS	0	
SWH	6410.256	Hz
FIDRES	0.195625	Hz
AQ	2.5559540	sec
RG	4	
DW	78.000	usec
DE	6.00	usec
TE	300.0	K
D1	2.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	usec
PL1	-2.40	dB
SFO1	400.1528010	MHz
SI	16384	
SF	400.1500094	MHz
WDW	EM	
SSB	0	
LB	0.00	Hz
GB	0	
PC	1.00	



NAME	141011Br
EXPNO	14
PROCNO	1
Date_	20141013
Time	15.22
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	120
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6178084 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00


100
95
90
85
80
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
2978
2931
1716
1593
1558
1490
1369
1327
1232
1154
1057
1028
909
850
836
768
733


Boc
N
Br
N

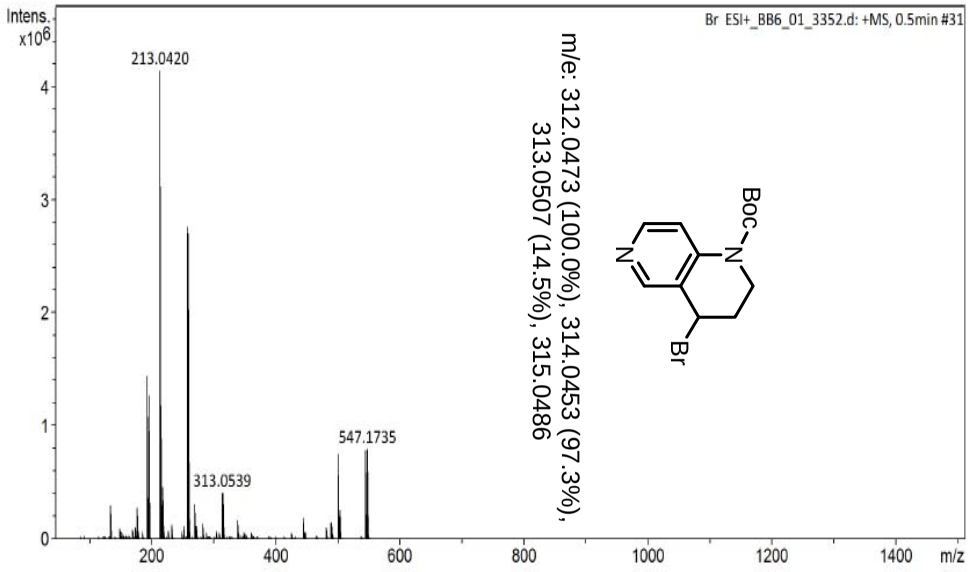
Display Report

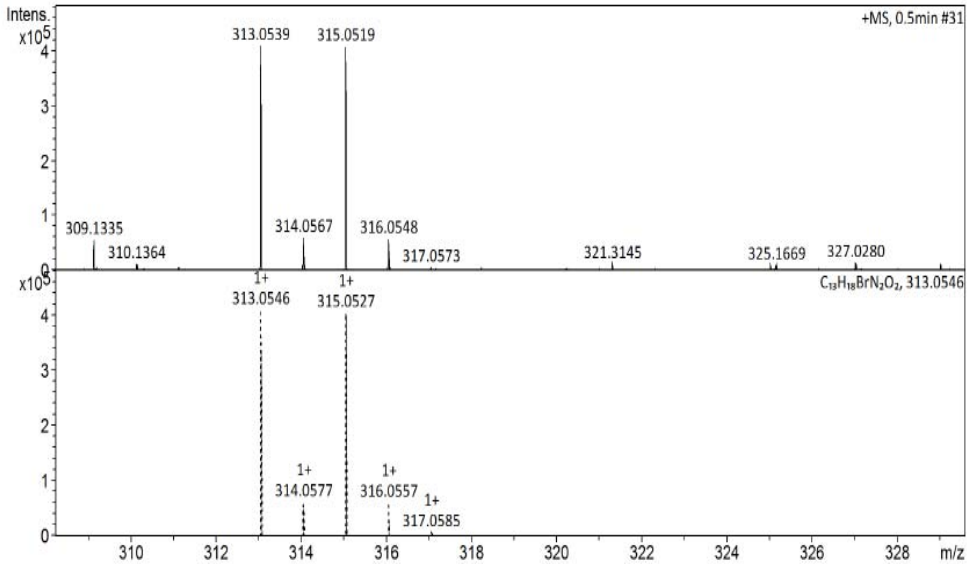
Analysis Info

Acquisition Date	10/6/2014 6:47:09 PM		
Analysis Name	D:\Data\NCTU SERVICE\Data\20141006\Br ESI+_BB6_01_3352.d		
Method	Small molecule.m	Operator	NCTU
Sample Name	Br ESI+	Instrument	impact HD 1819696.00164
Comment			

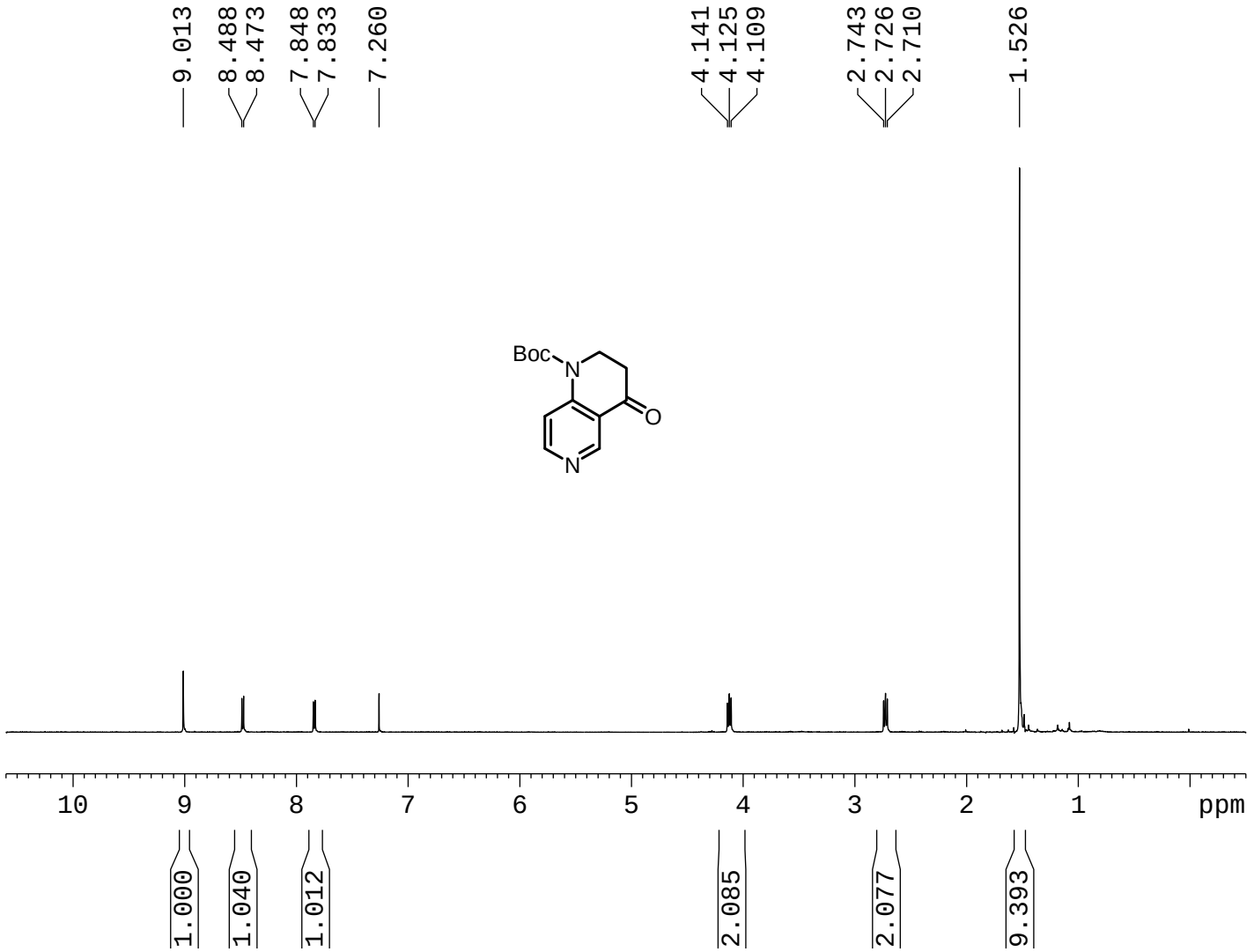
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

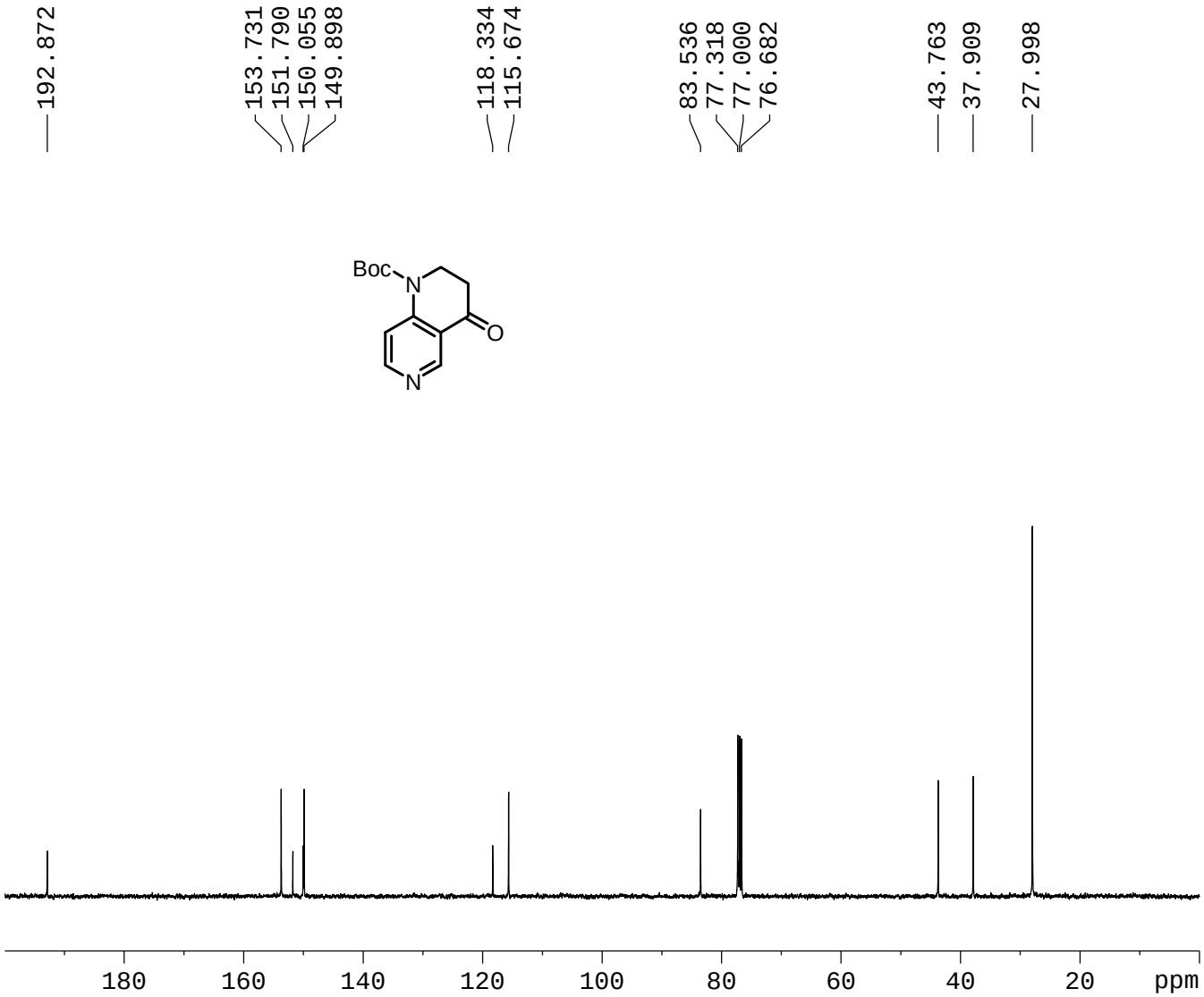




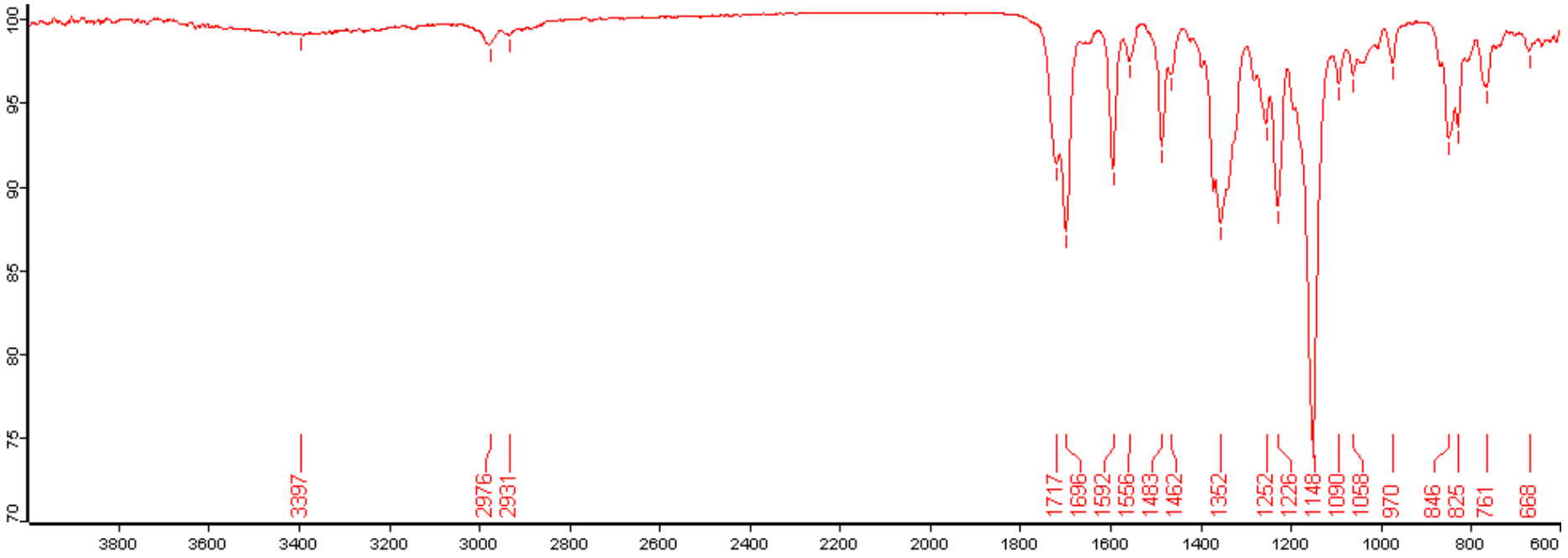
Br ESI+_BB6_01_3352.d

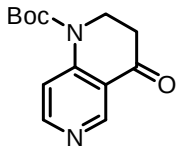


NAME	140219ketoneBoc
EXPNO	1
PROCNO	1
Date_	20140219
Time	19.21
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500090 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	140219ketoneBoc
EXPNO	13
PROCNO	1
Date_	20140219
Time	19.22
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	106
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6178116 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00


100
95
90
85
80
75
70
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
3397
2976
2931
1717
1696
1592
1556
1483
1462
1352
1252
1226
1148
1090
1058
970
846
825
761
668


Boc
N
O
N

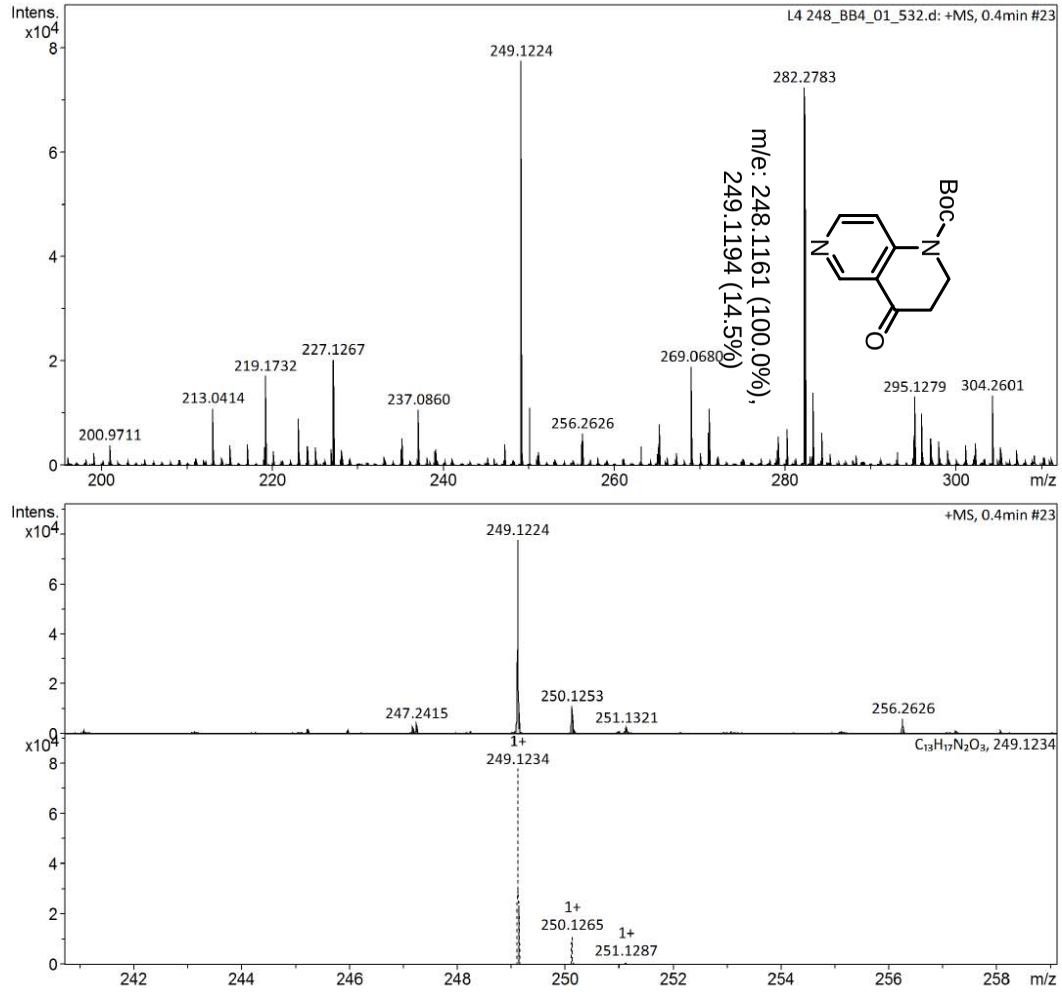
Display Report

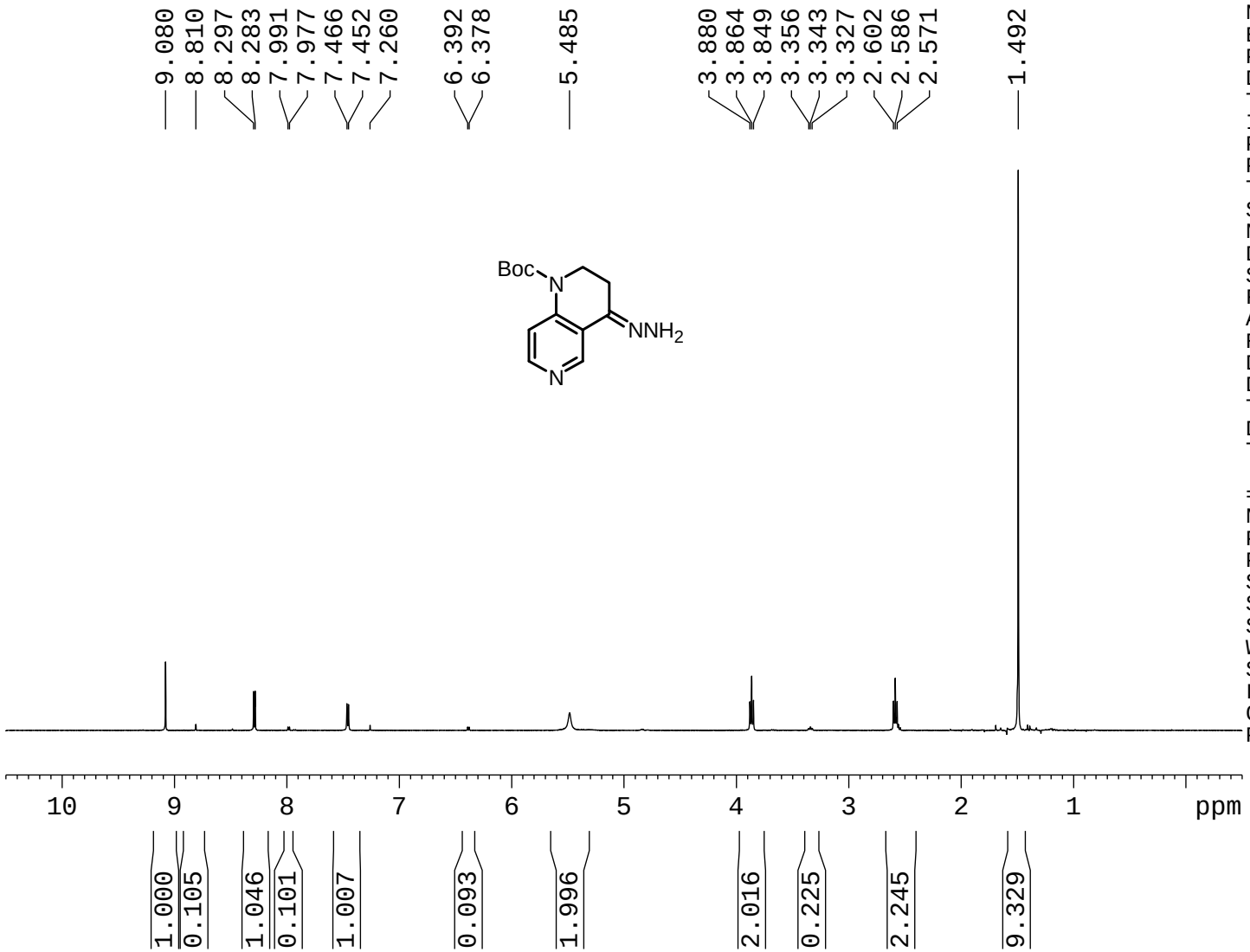
Analysis Info

Analysis Name	D:\Data\NCTU SERVICE\Data\20140303\L4 248_BB4_01_532.d	Acquisition Date	3/3/2014 3:51:44 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	L4 248	Instrument	impact HD 1819696.00164
Comment			

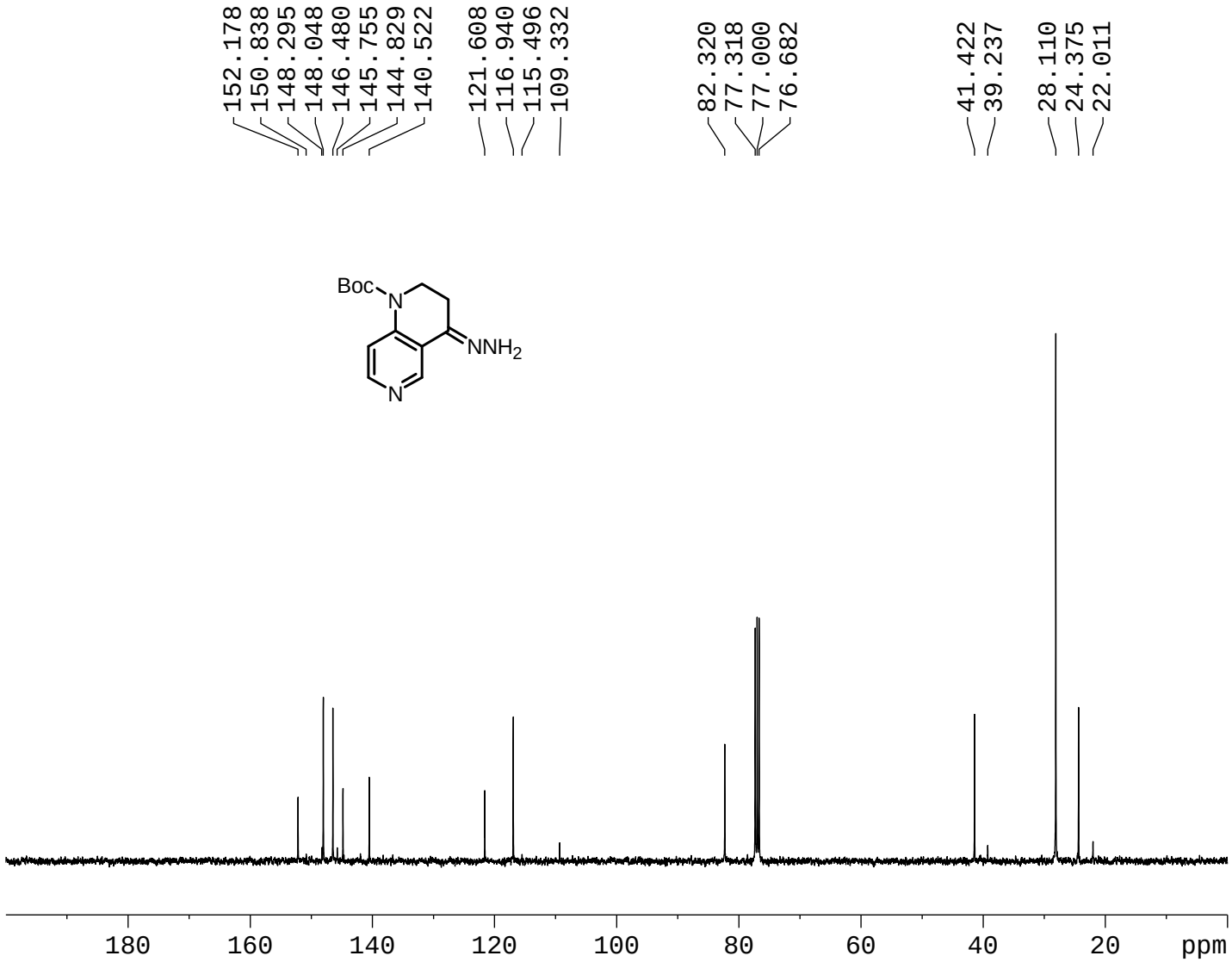
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

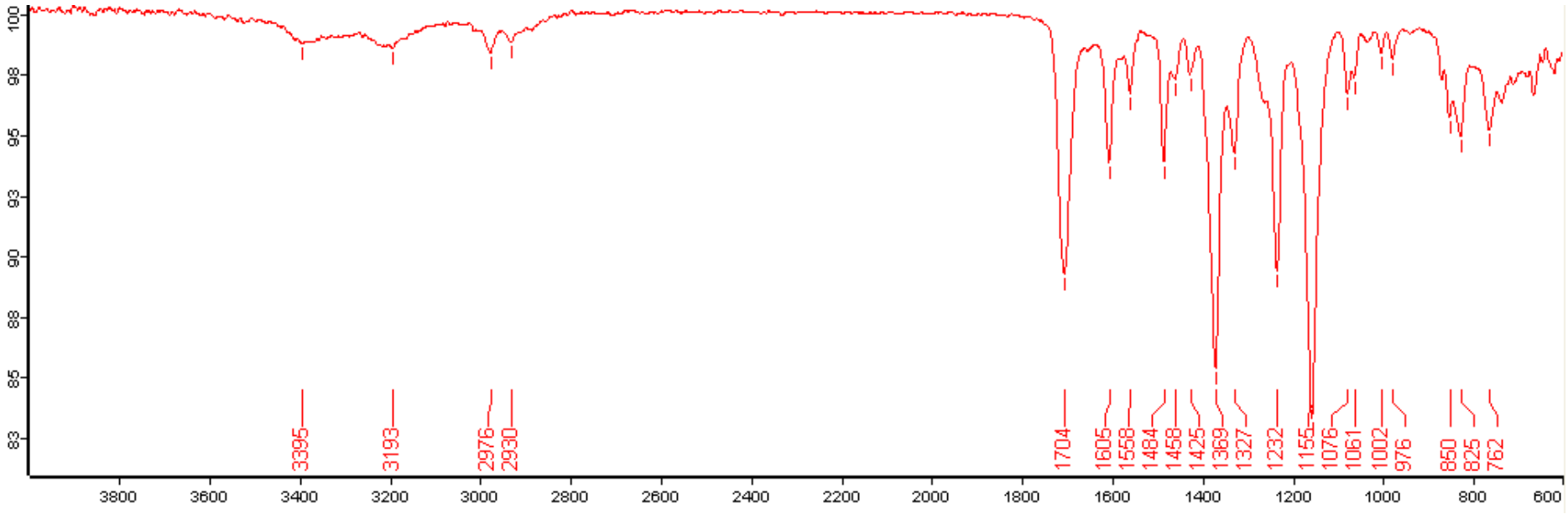


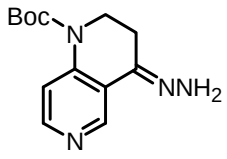


NAME	141225NBocNNH2
EXPNO	2
PROCNO	1
Date_	20150101
Time	13.10
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500093 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	141225NBocNNH2
EXPNO	14
PROCNO	1
Date_	20150101
Time	13.13
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	101
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6178099 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00


100
98
95
93
90
88
85
83
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
3395
3193
2976
2930
1704
1605
1558
1484
1458
1425
1369
1327
1232
1155
1076
1061
1002
976
850
825
762


Boc
N
NNH2
N

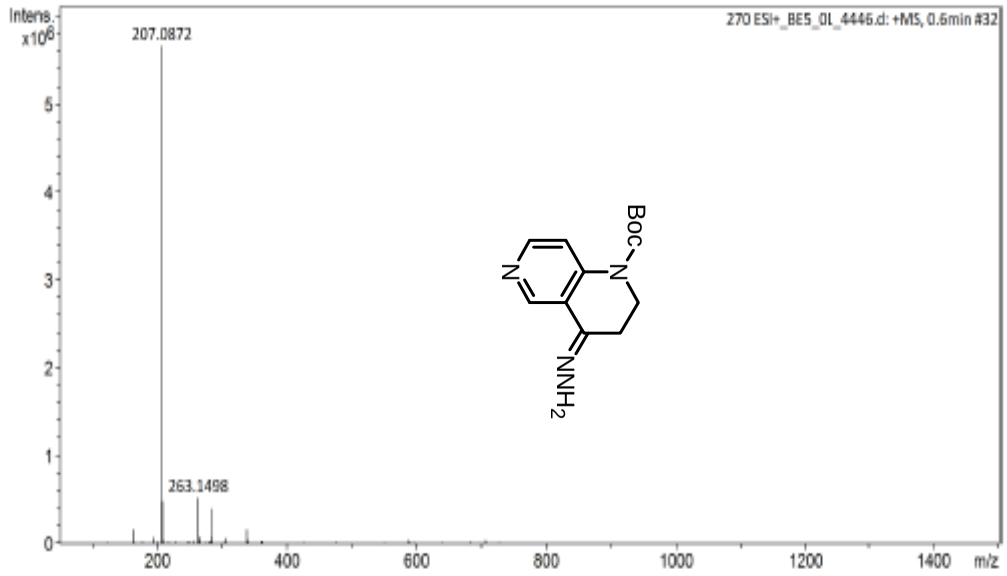
Display Report

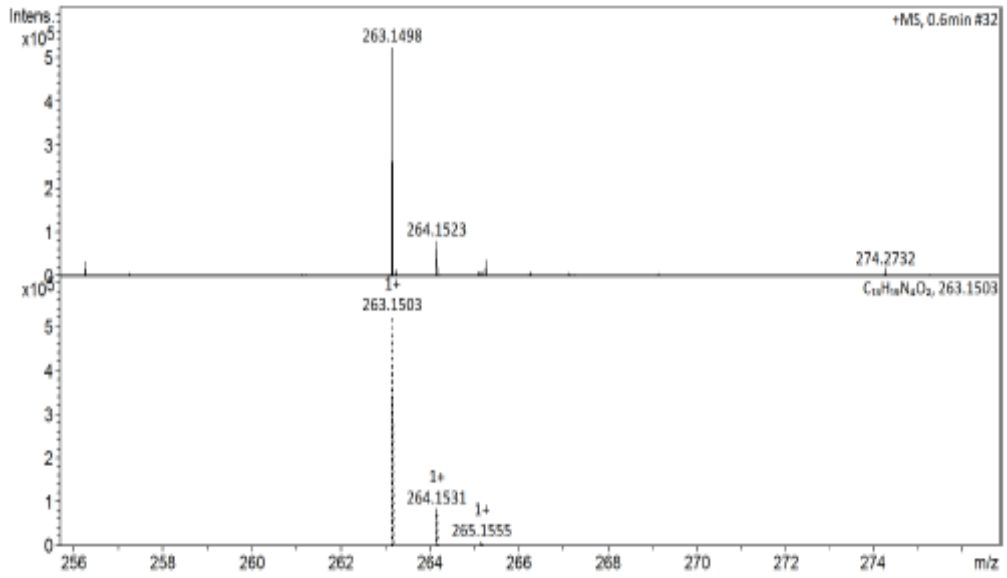
Analysis Info

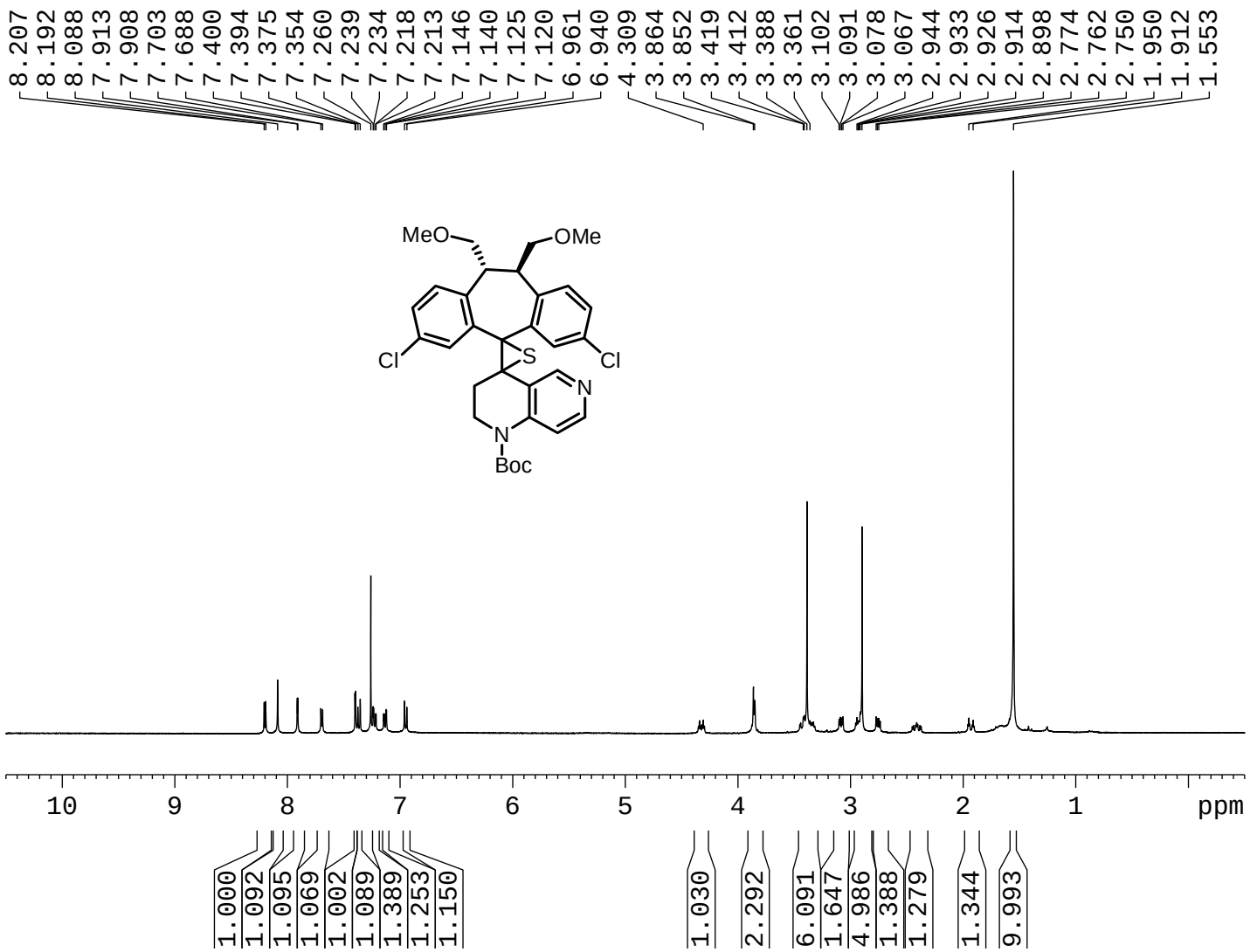
Acquisition Date	1/12/2015 9:53:12 AM		
Analysis Name	D:\Data\nctu service\data\2015\20150112\270 ESI+_BE5_01_4446.d		
Method	Small molecule.m	Operator	NCTU
Sample Name	270 ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

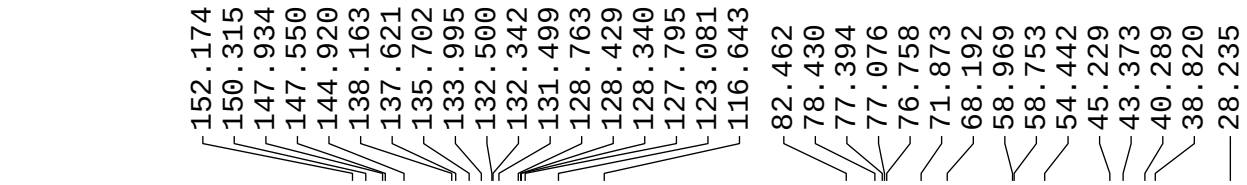
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

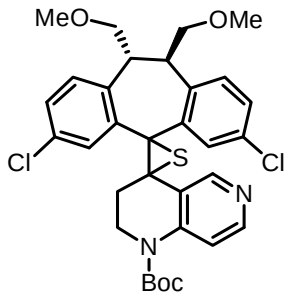


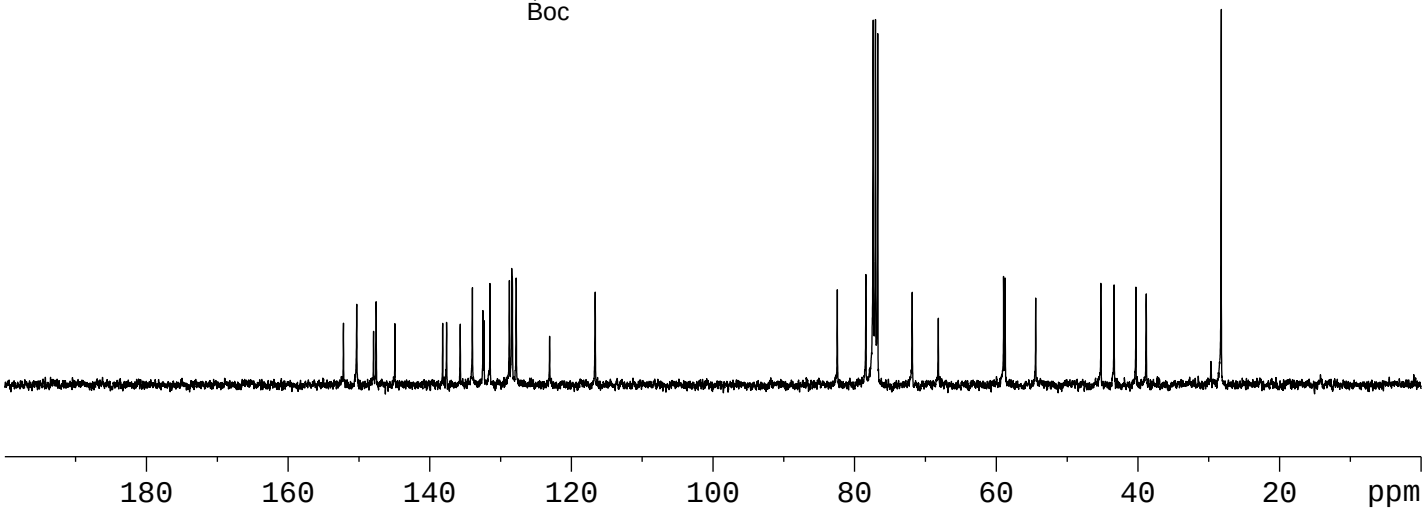




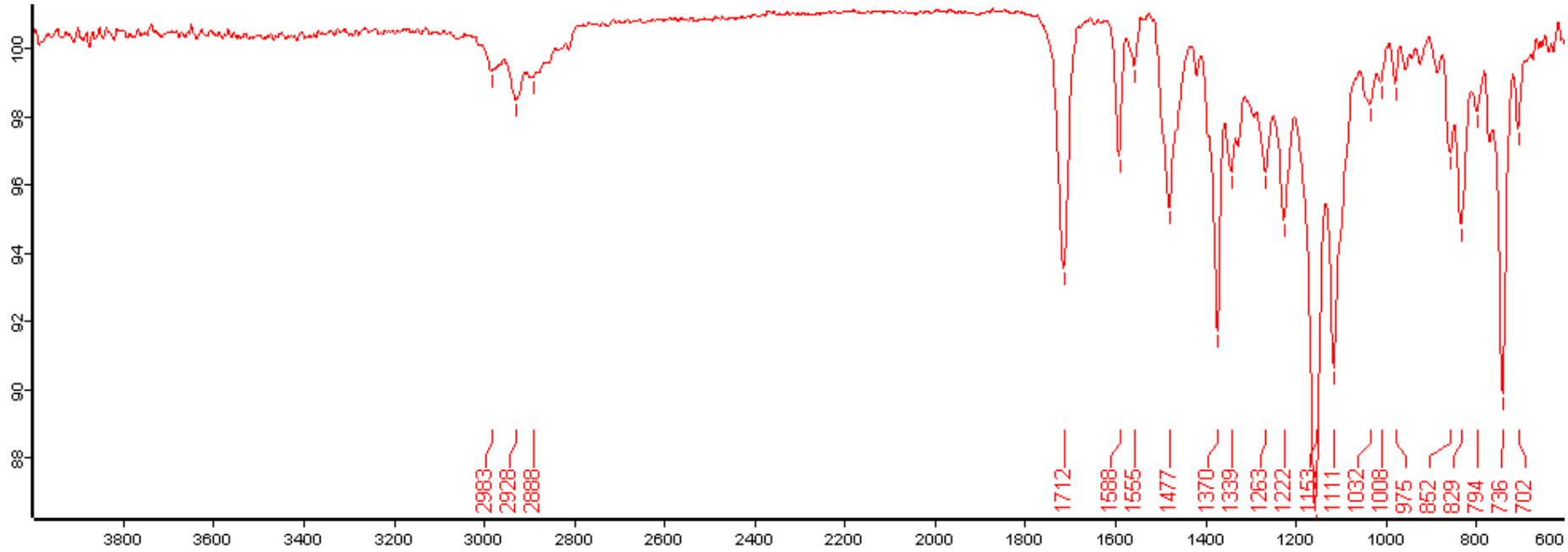
NAME	140502-EMCNB
EXPNO	5
PROCNO	1
Date_	20150113
Time	15.44
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500088 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

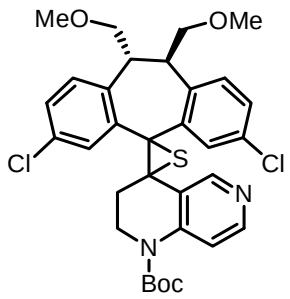






NAME	140502-EMCNB	
EXPNO	14	
PROCNO	1	
Date_	20140703	
Time	19.23	
INSTRUM	spect	
PROBHD	5 mm DUL 13C-1	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	260	
DS	0	
SWH	22727.273	Hz
FIDRES	0.346791	Hz
AQ	1.4418420	sec
RG	57	
DW	22.000	usec
DE	6.00	usec
TE	300.0	K
D1	2.00000000	sec
d11	0.03000000	sec
DELTA	1.89999998	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.70	usec
PL1	-0.50	dB
SFO1	100.6288660	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	90.00	usec
PL2	-2.40	dB
PL12	15.10	dB
PL13	18.10	dB
SFO2	400.1516010	MHz
SI	32768	
SF	100.6177980	MHz
WDW	EM	
SSB	0	
LB	3.00	Hz
GB	0	
PC	1.00	


100
98
96
94
92
90
88
2983
2928
2888
1712
1588
1555
1477
1370
1339
1263
1222
1153
1111
1032
1008
975
852
829
794
736
702
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600


MeO
OMe
Cl
Cl
S
N
N
Boc

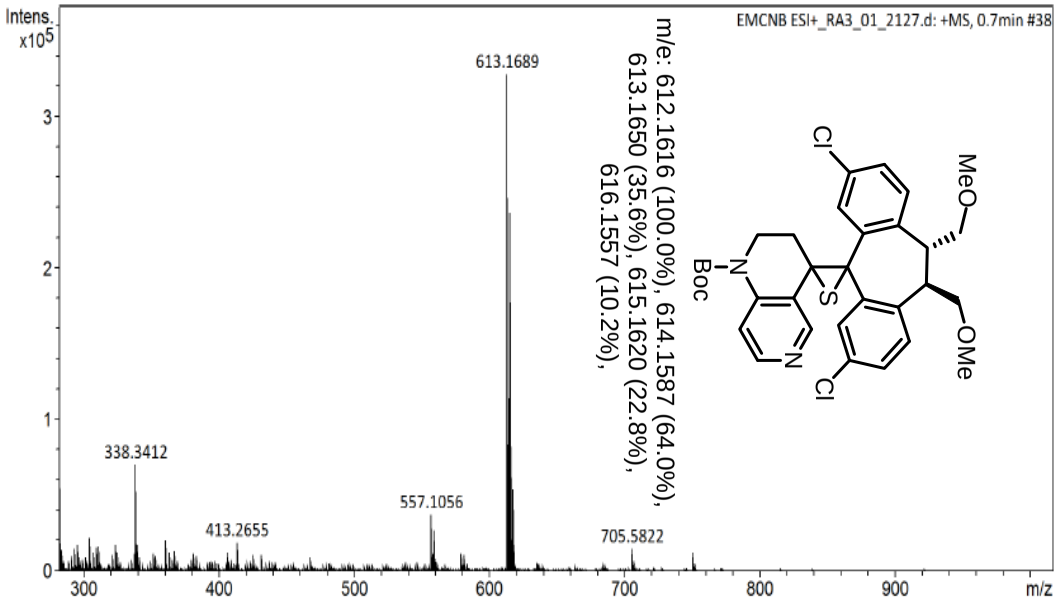
Display Report

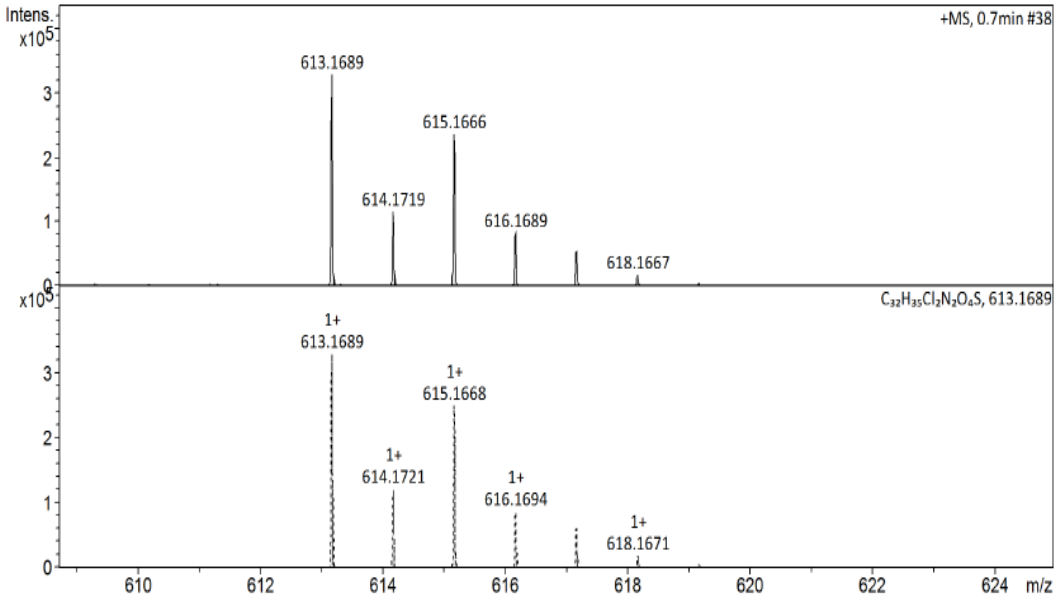
Analysis Info

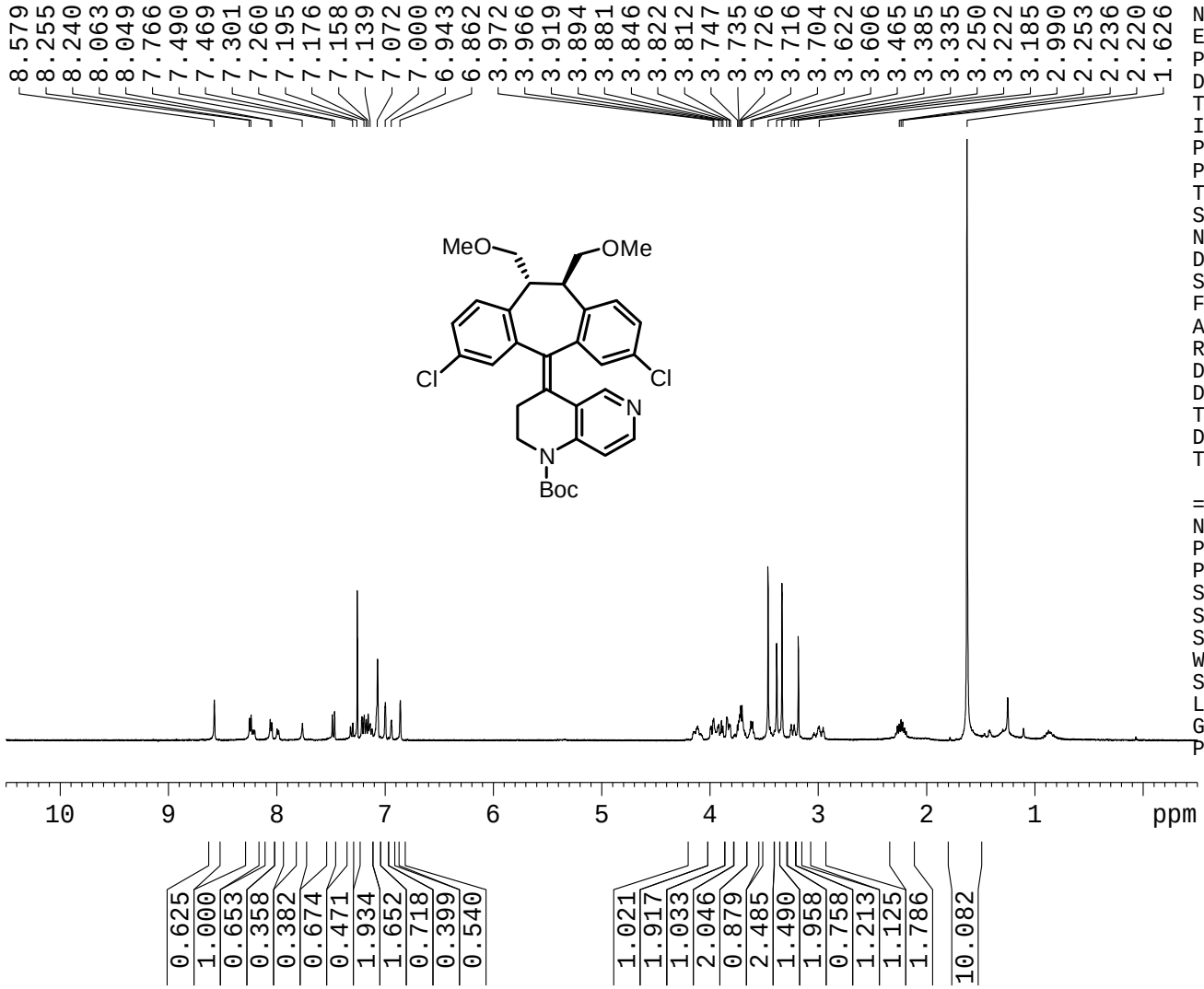
Analysis Name	D:\Data\NCTU SERVICE\Data\20140704\EMCNB ESI+_RA3_01_2127.d	Acquisition Date	7/4/2014 8:57:33 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	EMCNB ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

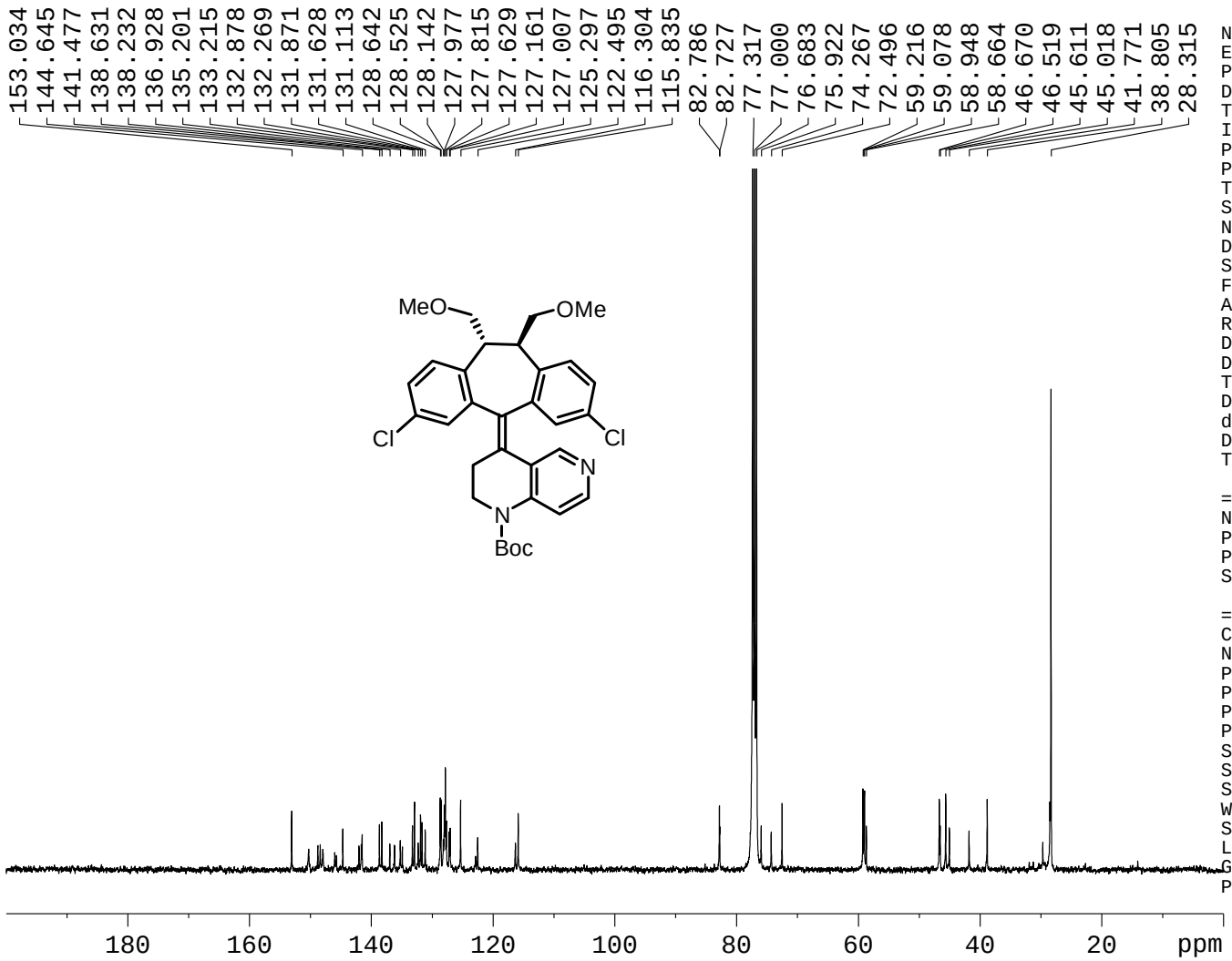
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C







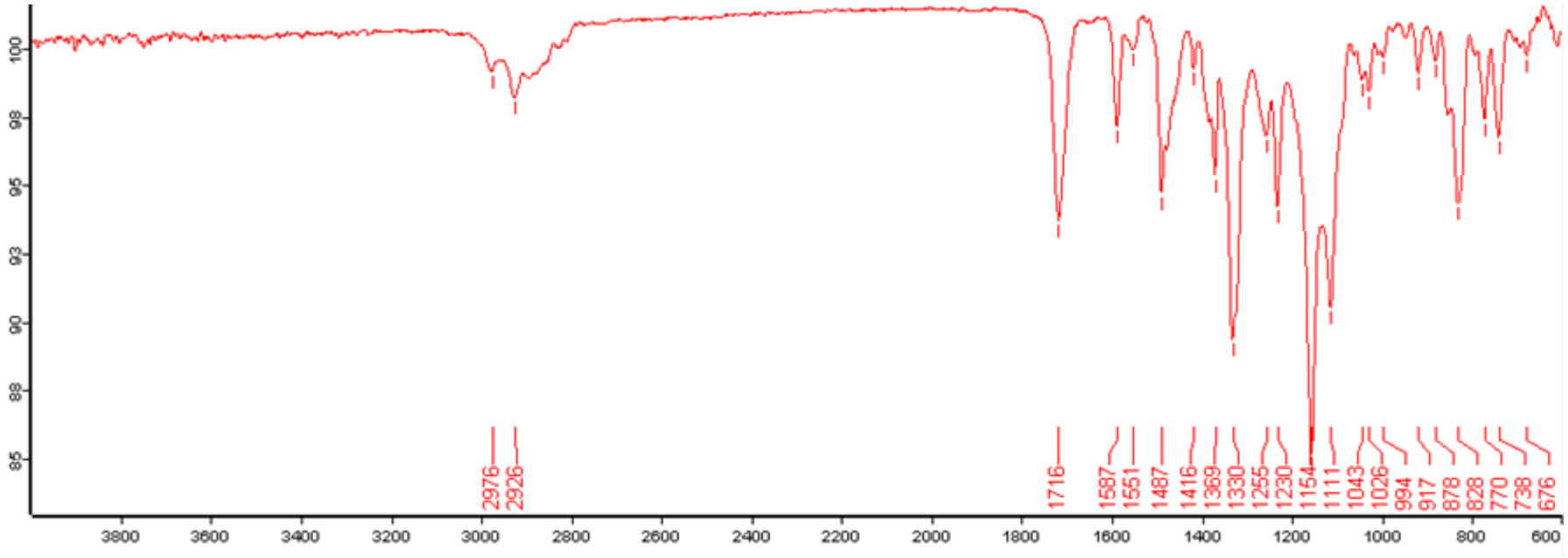
NAME	140715-helicene-MOMdiCl-DMAP-NBoc
EXPNO	3
PROCNO	1
Date_	20140718
Time	18.59
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	4
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500099 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

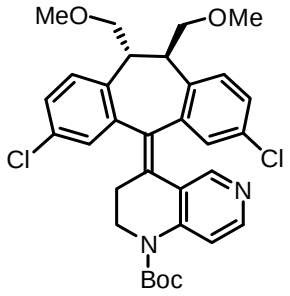



```
NAME      140715-helicene-MOMdiCl-DMAP-NBoc
EXPNO                 14
PROCNO                 1
Date_           20140719
Time                0.03
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  8265
DS                     0
SWH           22727.273 Hz
FIDRES         0.346791 Hz
AQ             1.4418420 sec
RG                    57
DW                22.000 usec
DE                 6.00 usec
TE                300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.70 usec
PL1                -0.50 dB
SFO1         100.6288660 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                -2.40 dB
PL12               15.10 dB
PL13               18.10 dB
SFO2         400.1516010 MHz
SI                 32768
SF           100.6178006 MHz
WDW                  EM
SSB                   0
LB                 3.00 Hz
GB                    0
PC                 1.00
```


100
98
95
93
90
88
85
2976
2926
1716
1587
1551
1487
1416
1369
1330
1255
1230
1154
1111
1043
1026
994
917
878
828
770
738
676
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600


MeO
OMe
Cl
Cl
N
N
Boc

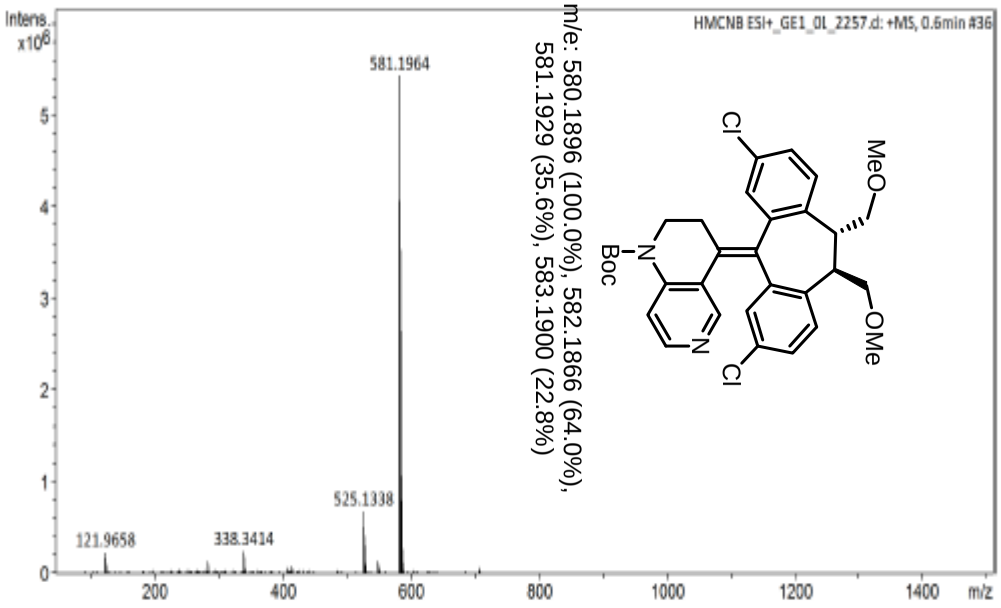
Display Report

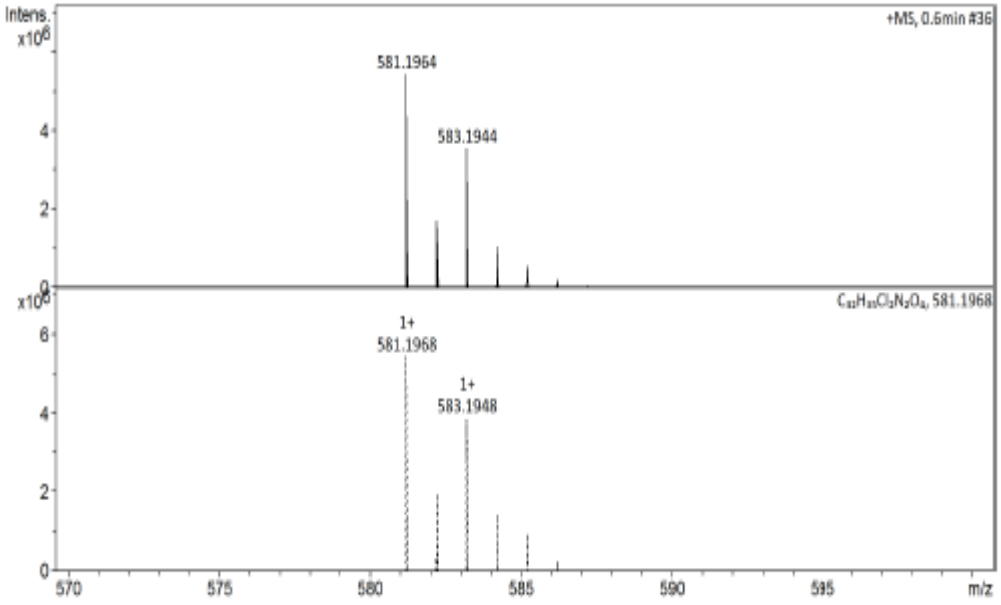
Analysis Info

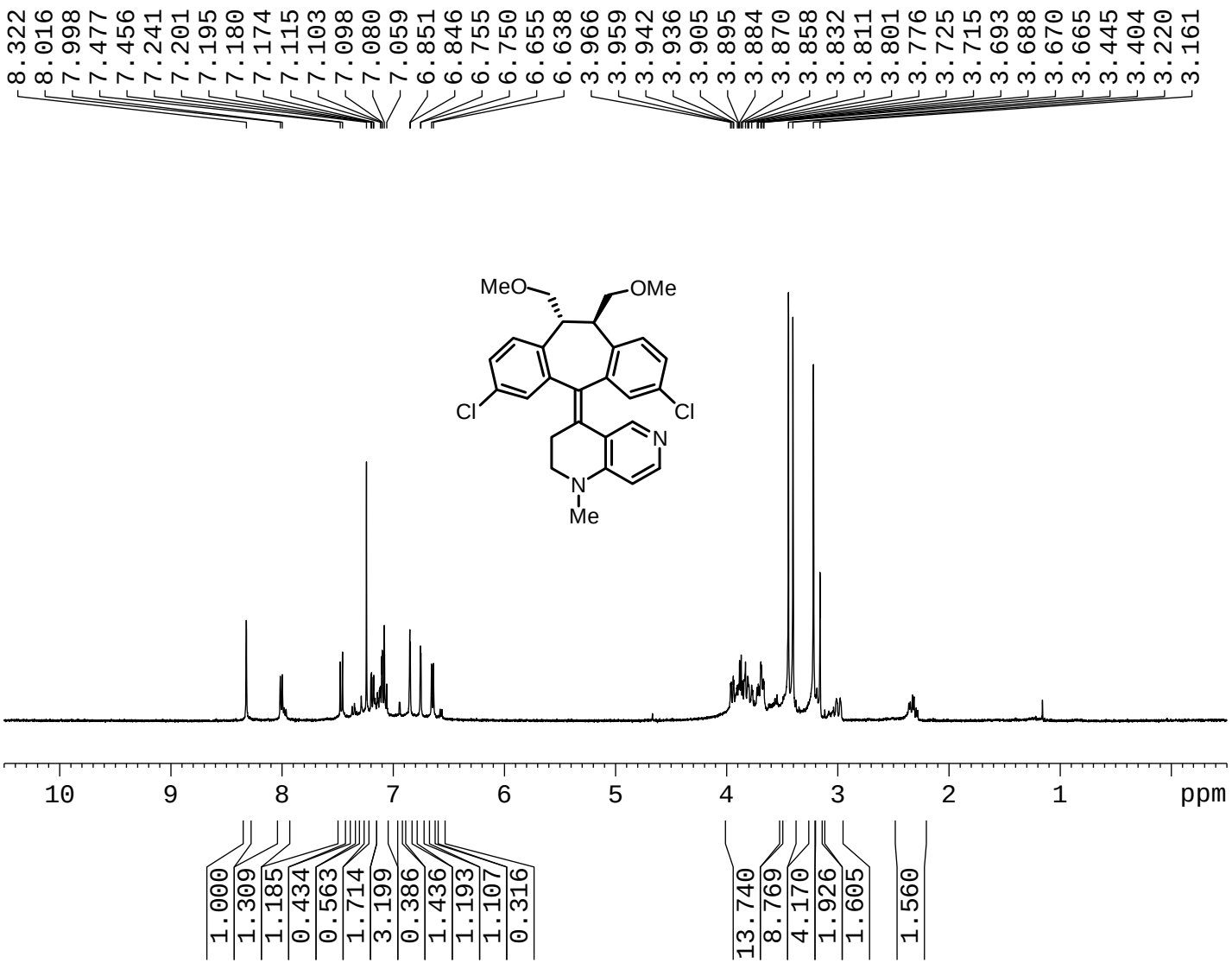
Analysis Name	D:\Data\NCTU SERVICE\Data\20140718\HMCNB ESI+_GE1_01_2257.d	Acquisition Date	7/18/2014 9:02:30 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	HMCNB ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

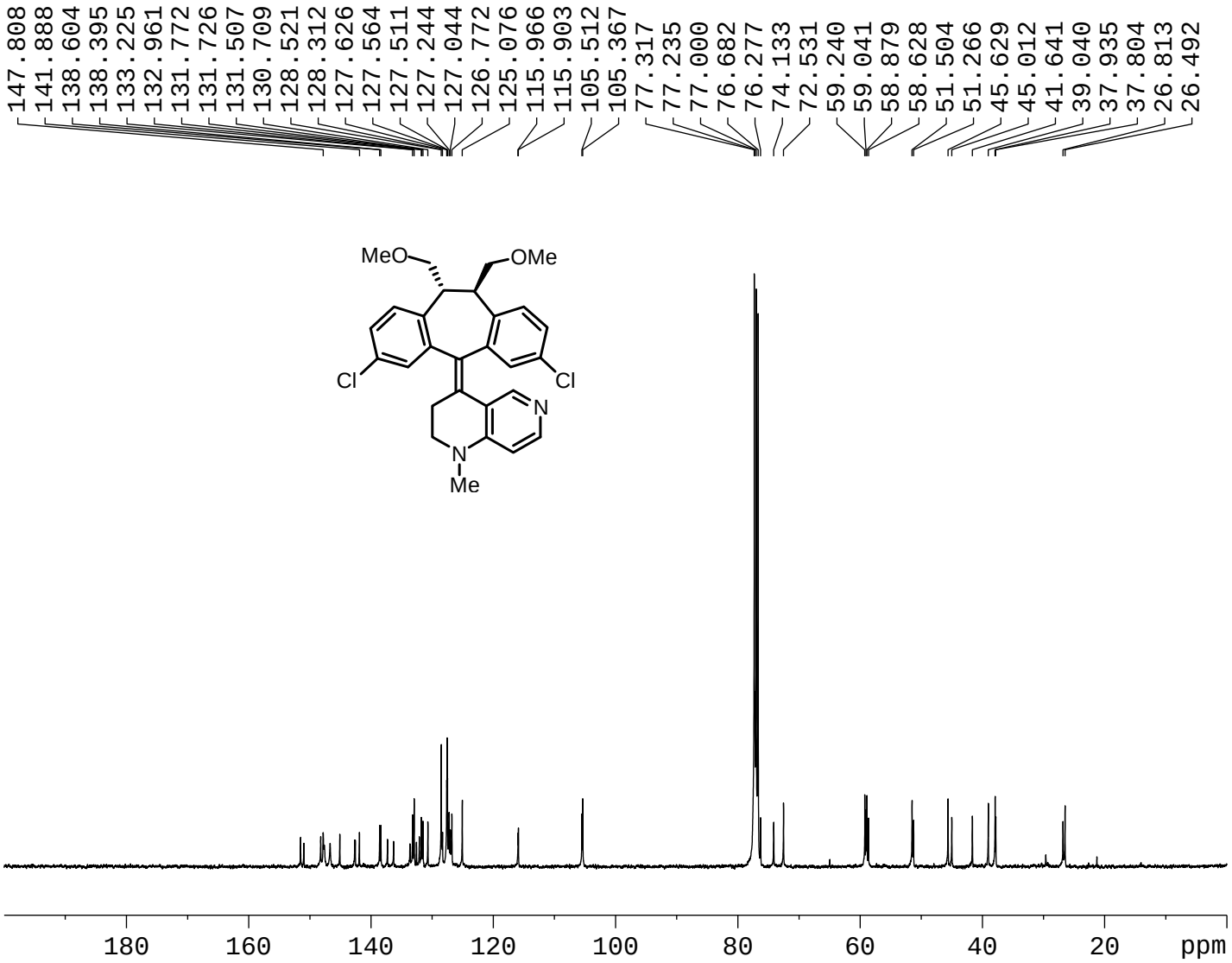
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C





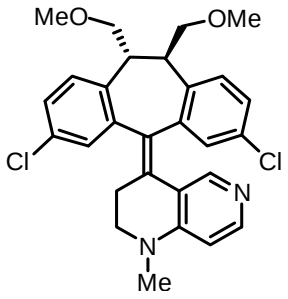


NAME	150313HMCNM
EXPNO	6
PROCNO	1
Date_	20150319
Time	9.17
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500168 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	150313HMCNM	
EXPNO	13	
PROCNO	1	
Date_	20150315	
Time	0.00	
INSTRUM	spect	
PROBHD	5 mm DUL 13C-1	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	7783	
DS	0	
SWH	22727.273	Hz
FIDRES	0.346791	Hz
AQ	1.4418420	sec
RG	57	
DW	22.000	usec
DE	6.00	usec
TE	300.0	K
D1	2.00000000	sec
d11	0.03000000	sec
DELTA	1.89999998	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.70	usec
PL1	-0.50	dB
SFO1	100.6288660	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	90.00	usec
PL2	-2.40	dB
PL12	15.10	dB
PL13	18.10	dB
SFO2	400.1516010	MHz
SI	32768	
SF	100.6178030	MHz
WDW	EM	
SSB	0	
LB	3.00	Hz
GB	0	
PC	1.00	


100.000
98.000
96.000
94.000
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
3399
2920
2872
2812
1645
1591
1558
1474
1458
1415
1387
1349
1324
1296
1267
1249
1212
1177
1105
1028
1006
913
873
824
803
730
641


MeO
OMe
Cl
Cl
N
N
Me

Display Report

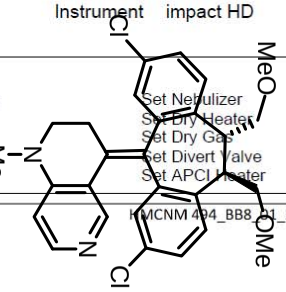
Analysis Info

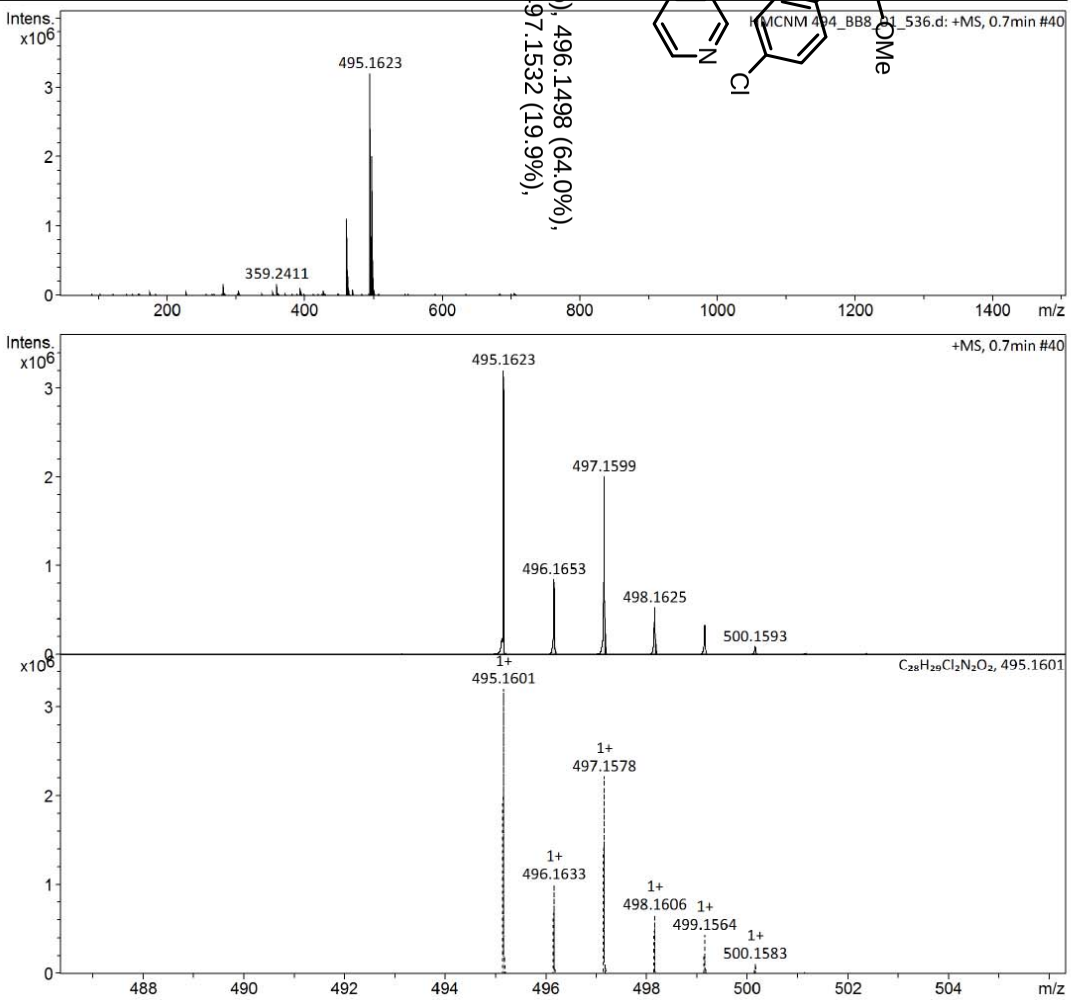
Analysis Name	D:\Data\NCTU SERVICE\Data\20140303\HMCNM 494_BB8_01_536.d	Acquisition Date	3/3/2014 4:09:05 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	HMCNM 494	Instrument	impact HD 1819696.00164
Comment			

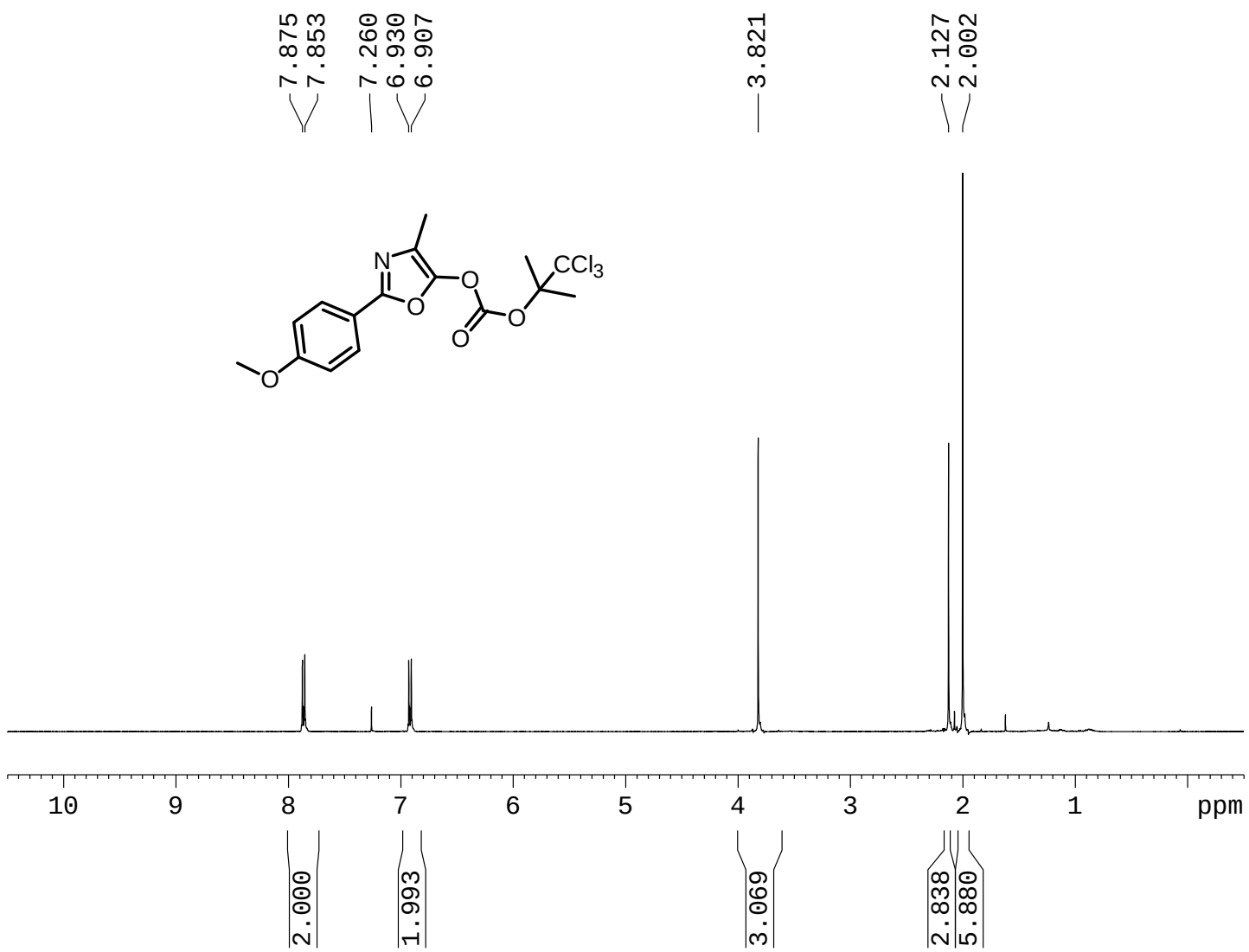
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

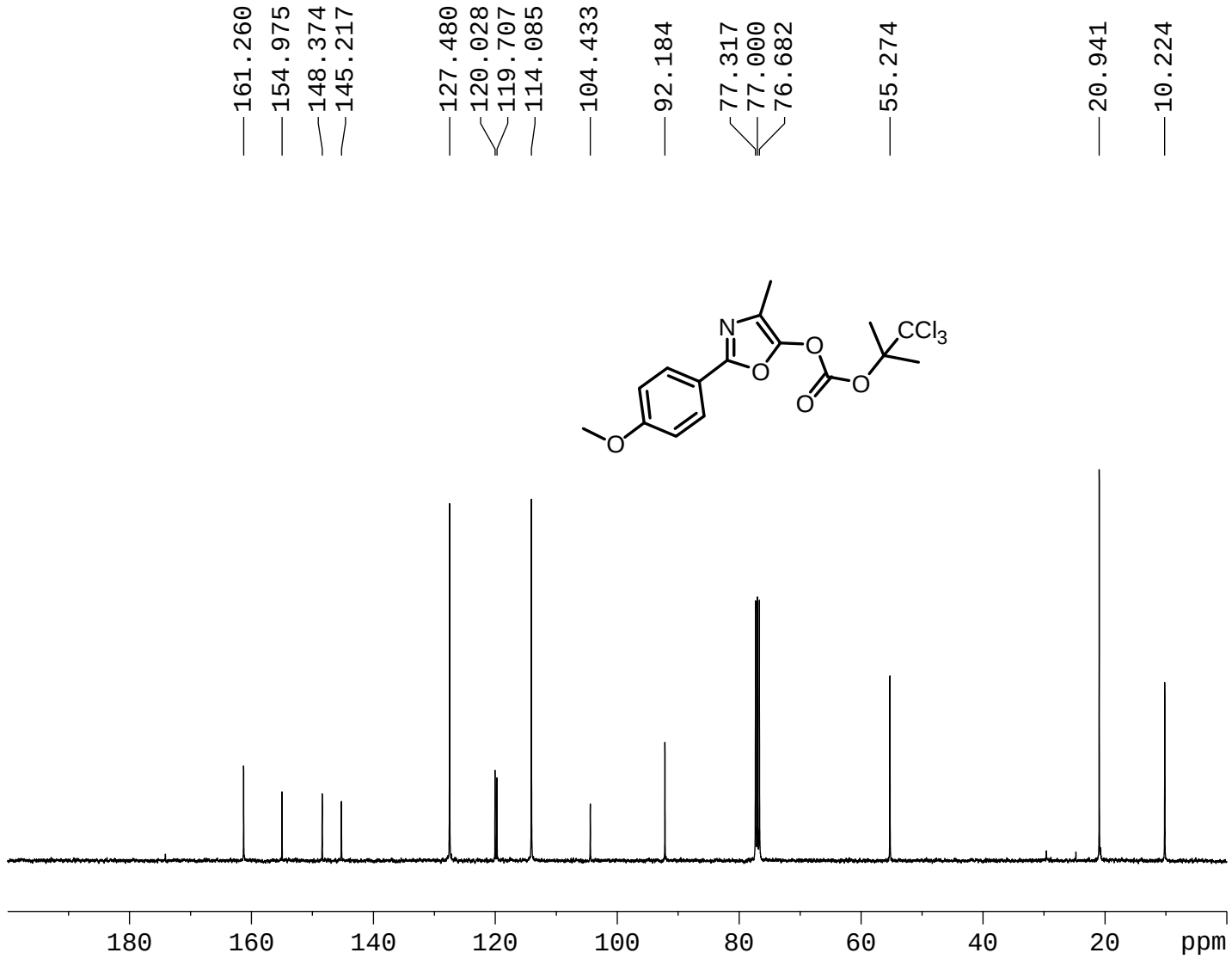
m/z: 494.1528 (100.0%), 496.1498 (64.0%), 495.1561 (31.1%), 497.1532 (19.9%),







NAME	140223MeCMe2CCl3
EXPNO	2
PROCNO	1
Date_	20140224
Time	18.30
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500093 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	140223MeCMe2CCl3
EXPNO	13
PROCNO	1
Date_	20140224
Time	18.32
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	471
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6178055 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

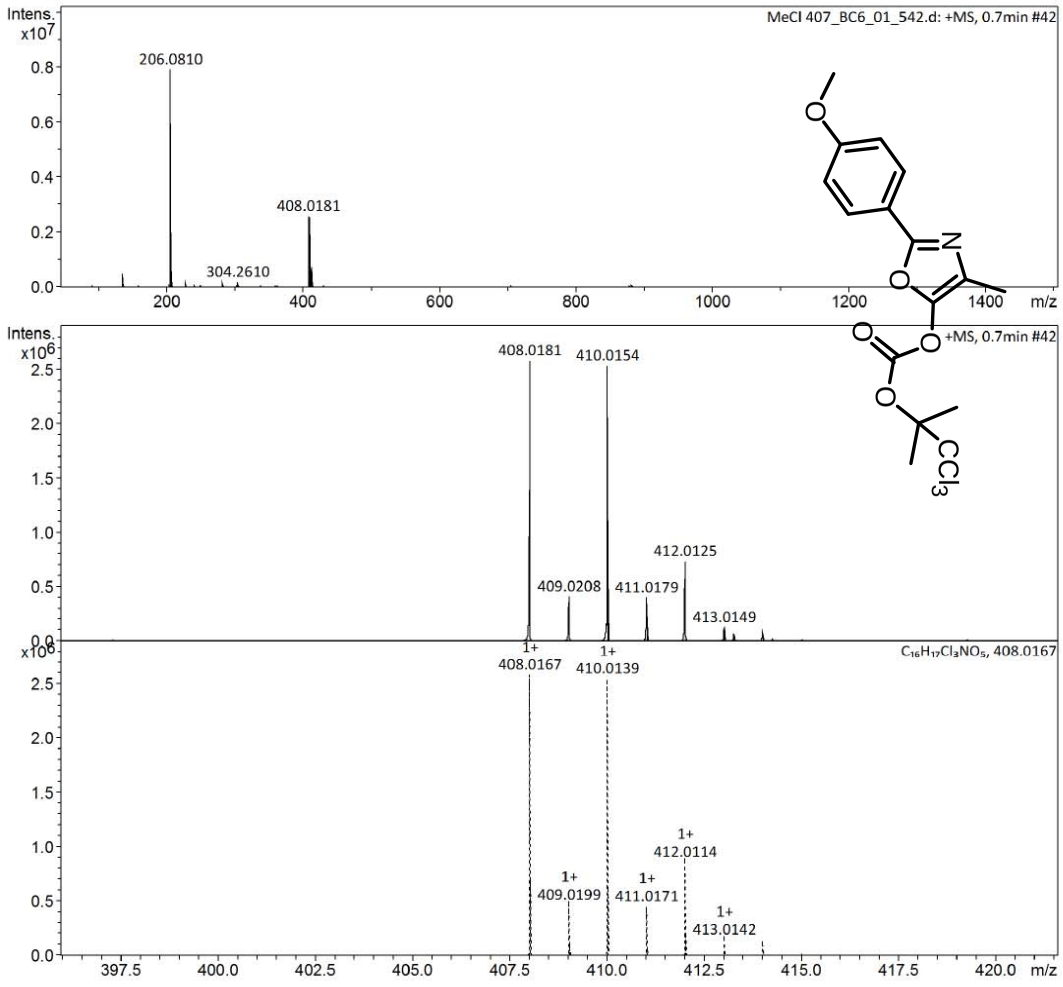
Display Report

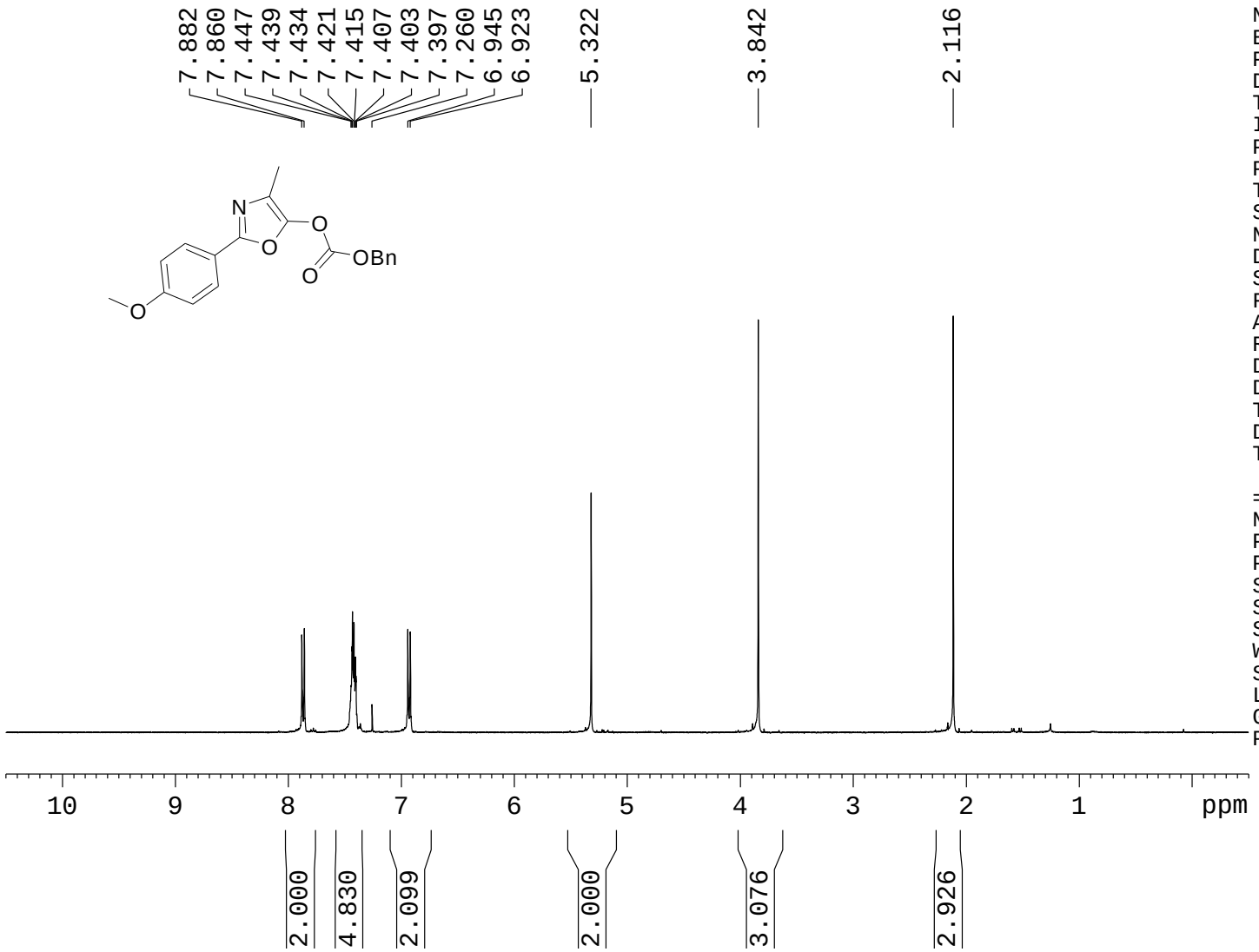
Analysis Info

Analysis Name	D:\Data\NCTU SERVICE\Data\20140303\MeCl 407_BC6_01_542.d	Acquisition Date	3/3/2014 4:35:15 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	MeCl 407	Instrument	impact HD 1819696.00164
Comment			

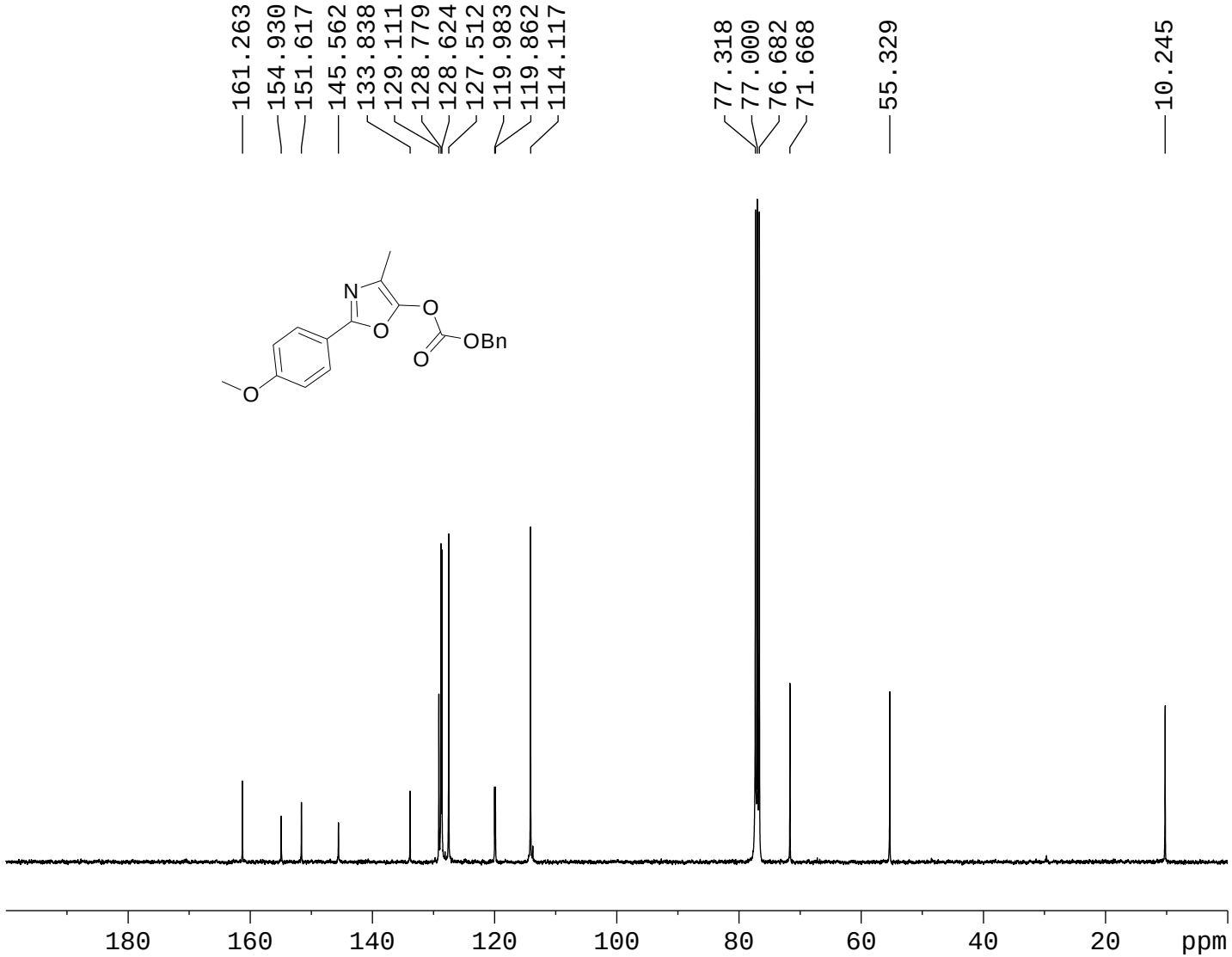
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C





NAME	140223MeBn
EXPNO	1
PROCNO	1
Date_	20140223
Time	11.38
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	8
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500095 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	140223MeBn
EXPNO	15
PROCNO	1
Date_	20140228
Time	0.03
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	7804
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6178023 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

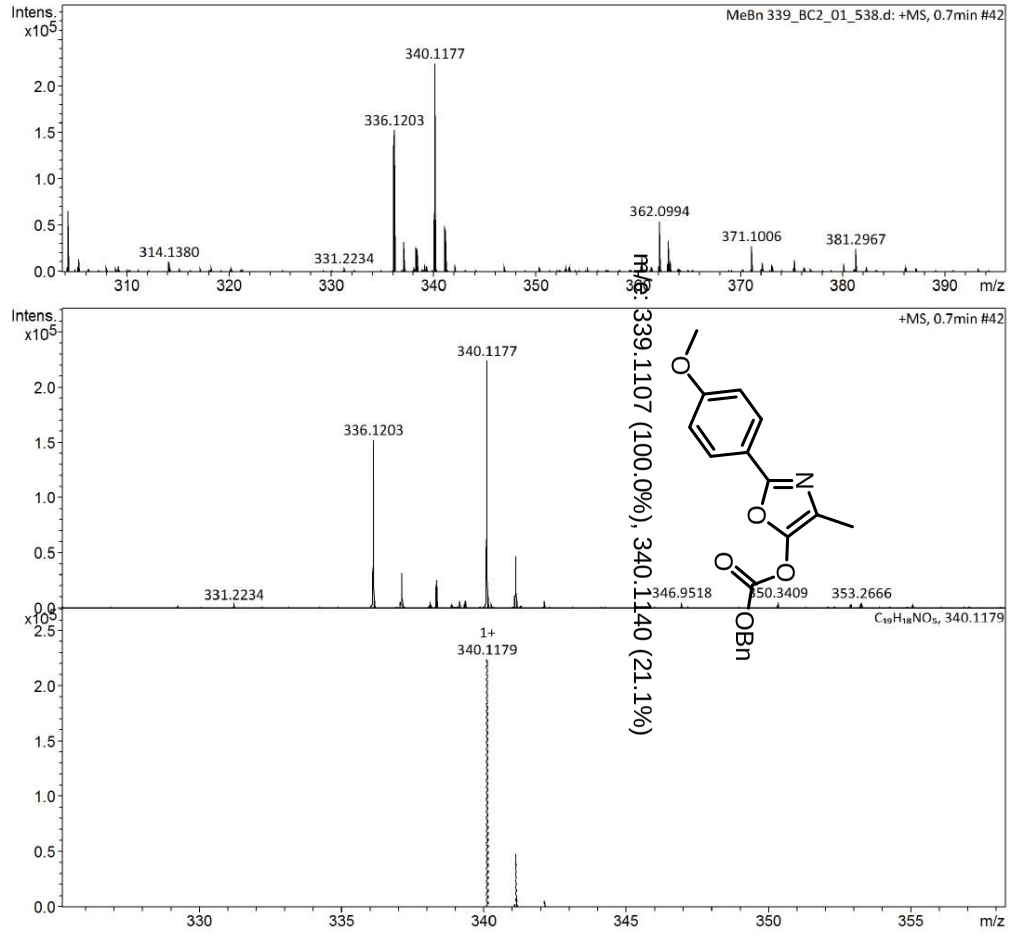
Display Report

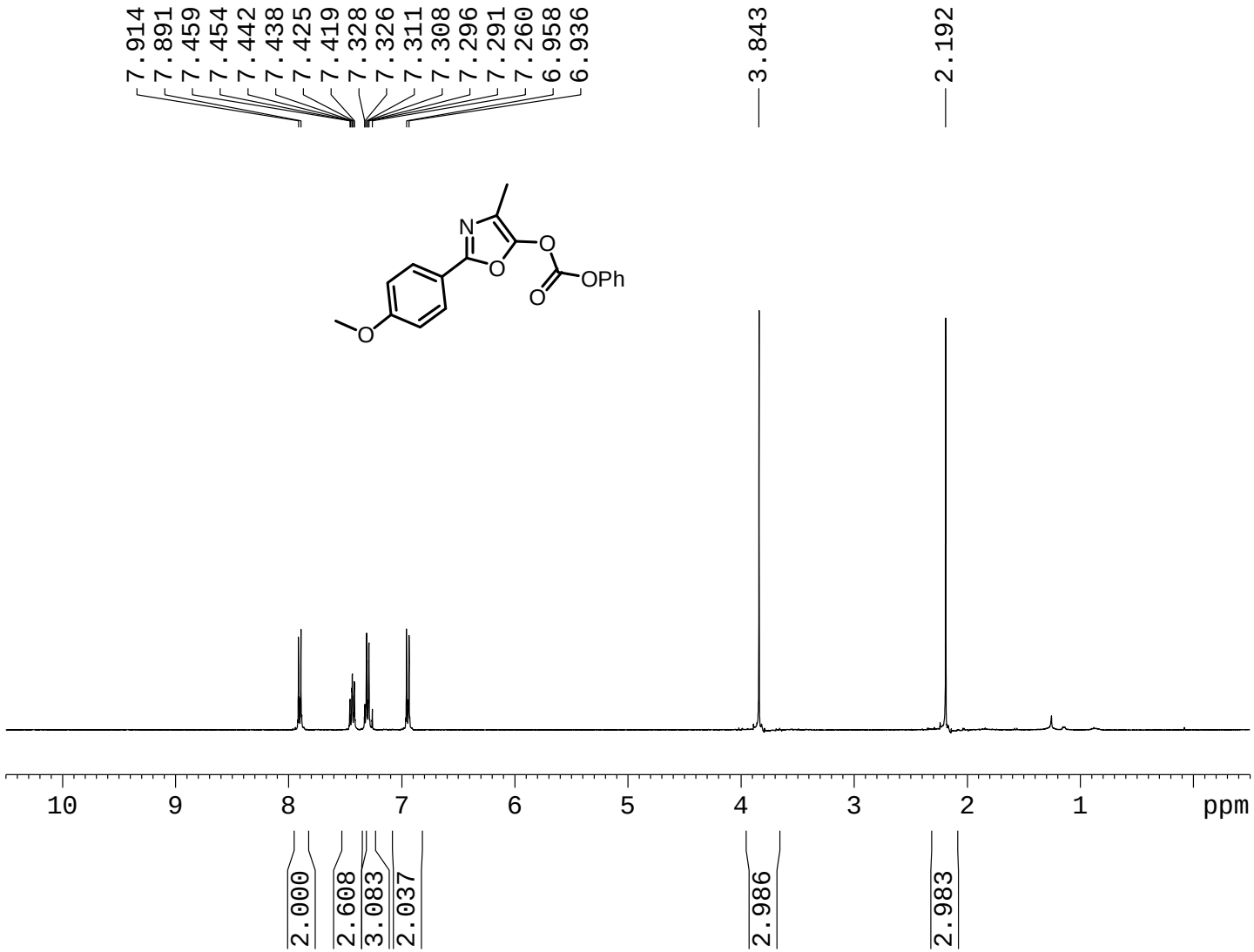
Analysis Info

Analysis Name	D:\Data\NCTU SERVICE\Data\20140303\MeBn 339_BC2_01_538.d	Acquisition Date	3/3/2014 4:17:49 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	MeBn 339	Instrument	impact HD 1819696.00164
Comment			

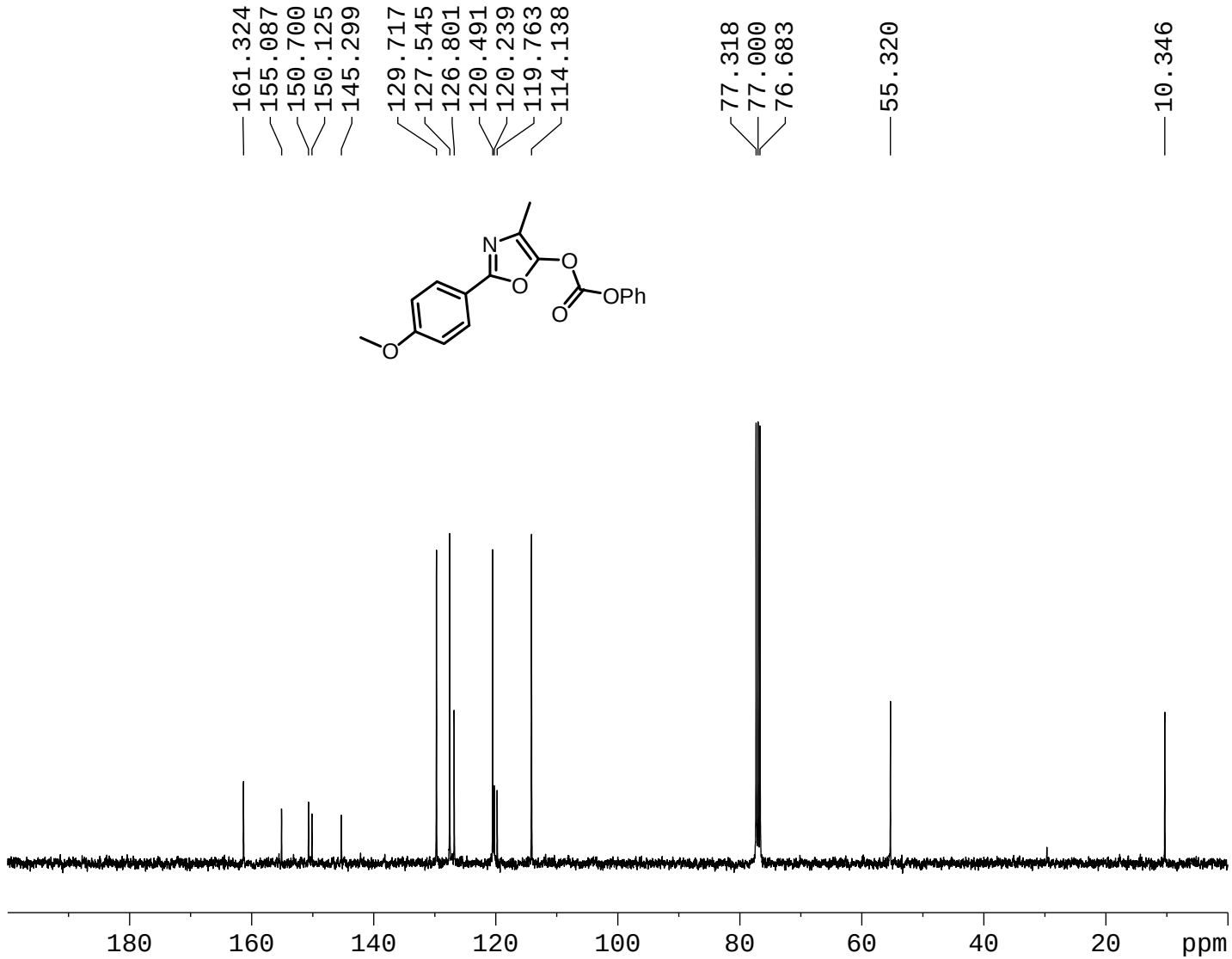
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C





NAME	140223MePh
EXPNO	2
PROCNO	1
Date_	20140224
Time	19.42
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500092 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	140223MePh
EXPNO	13
PROCNO	1
Date_	20140224
Time	19.43
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	216
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6178038 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

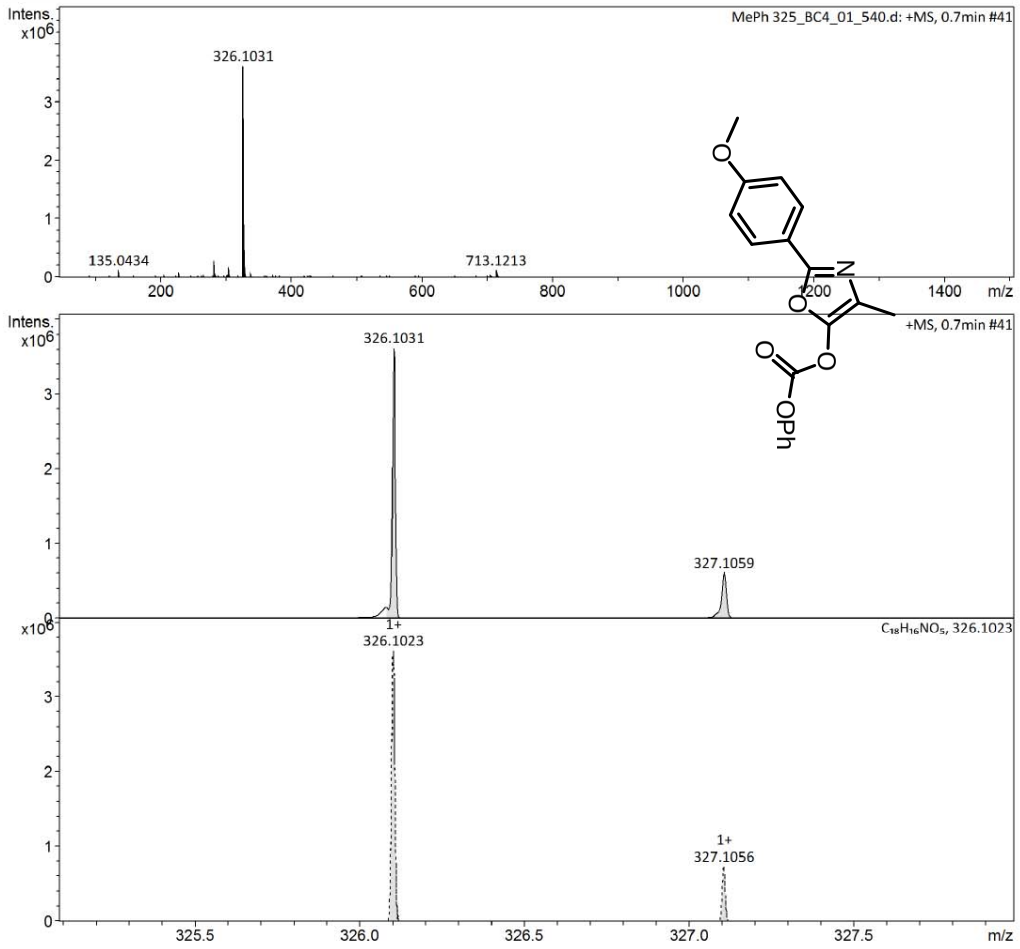
Display Report

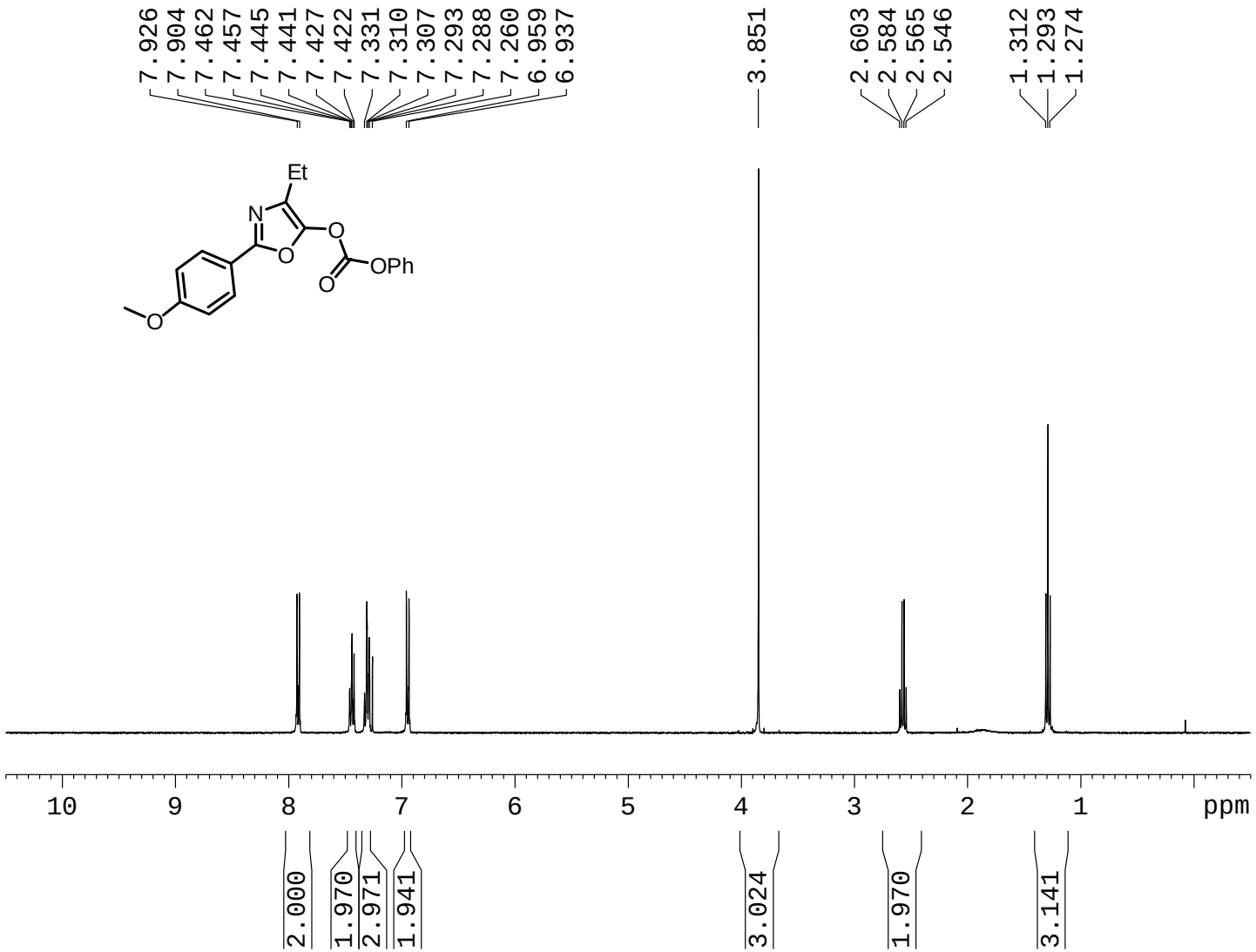
Analysis Info

Analysis Name	D:\Data\NCTU SERVICE\Data\20140303\MePh 325_BC4_01_540.d	Acquisition Date	3/3/2014 4:26:32 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	MePh 325	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

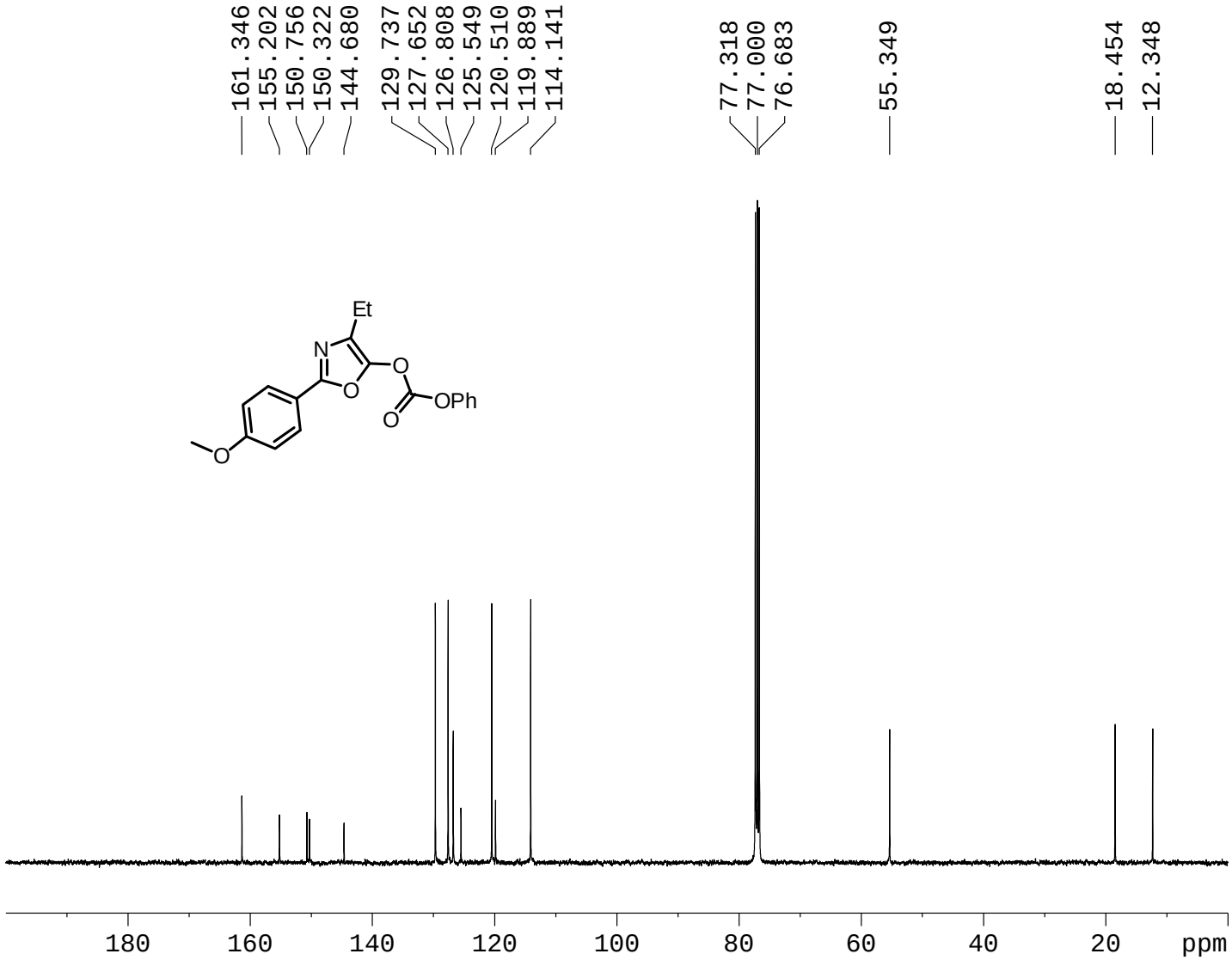
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C





NAME	140627EtPh
EXPNO	3
PROCNO	1
Date_	20140629
Time	8.25
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1

======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500090 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	140627EtPh
EXPNO	14
PROCNO	1
Date_	20140629
Time	8.26
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1612
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6178008 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

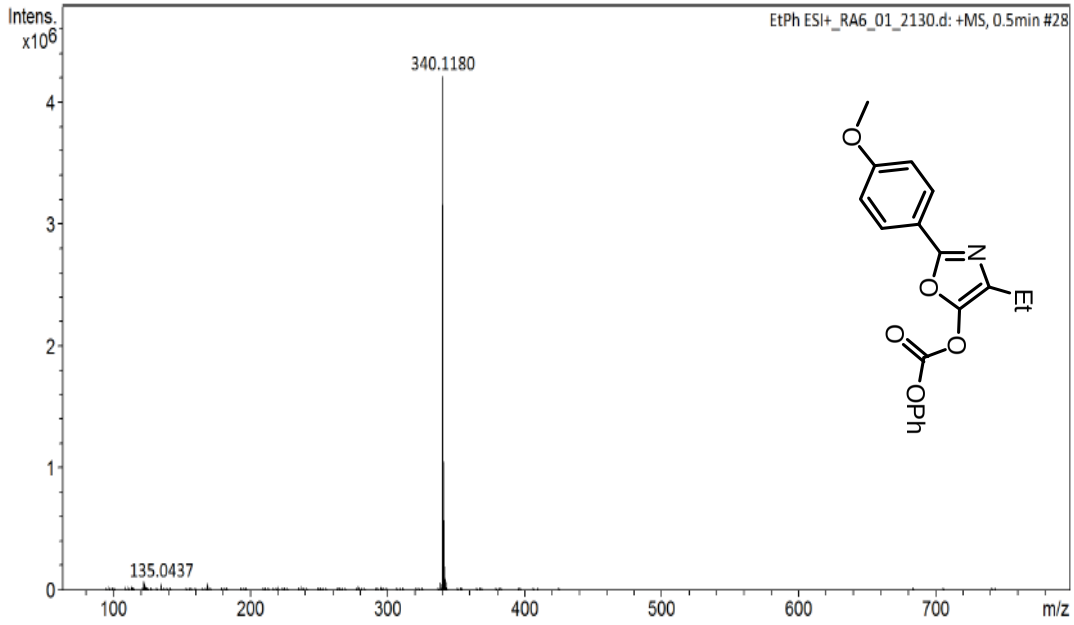
Display Report

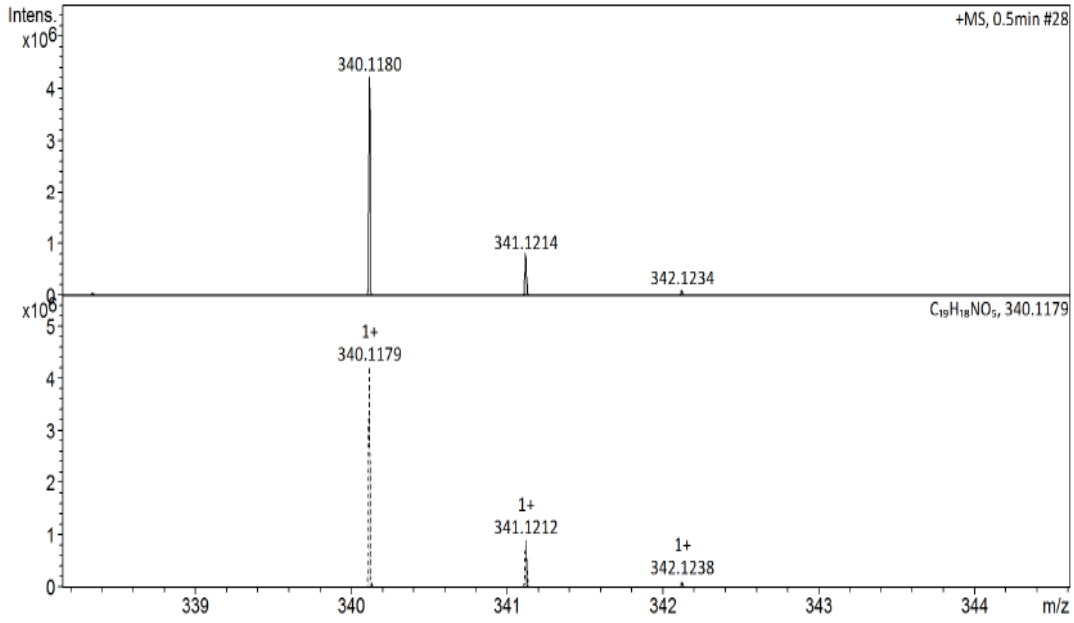
Analysis Info

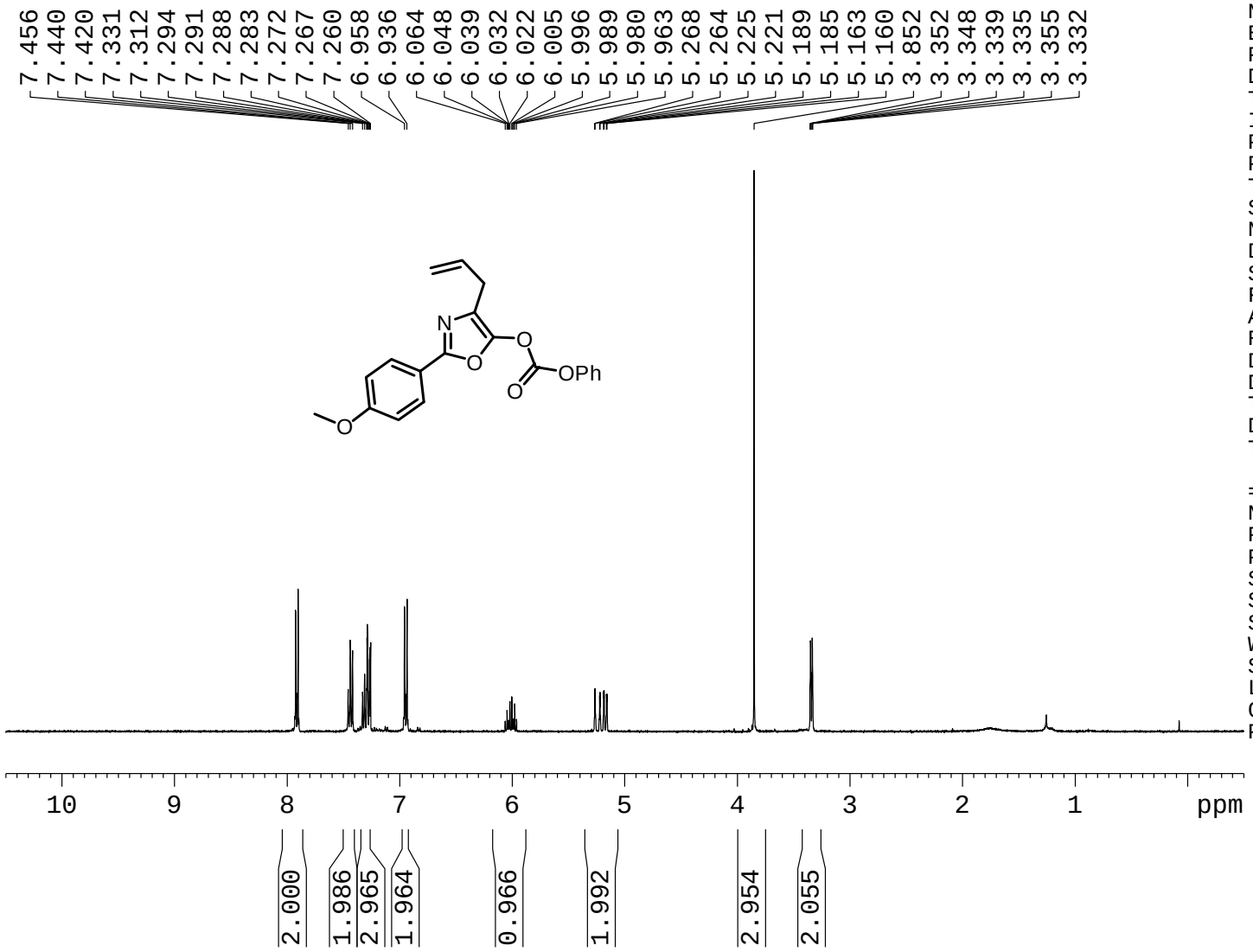
Analysis Name	D:\Data\NCTU SERVICE\Data\20140704\EtPh ESI+_RA6_01_2130.d	Acquisition Date	7/4/2014 9:23:38 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	EtPh ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

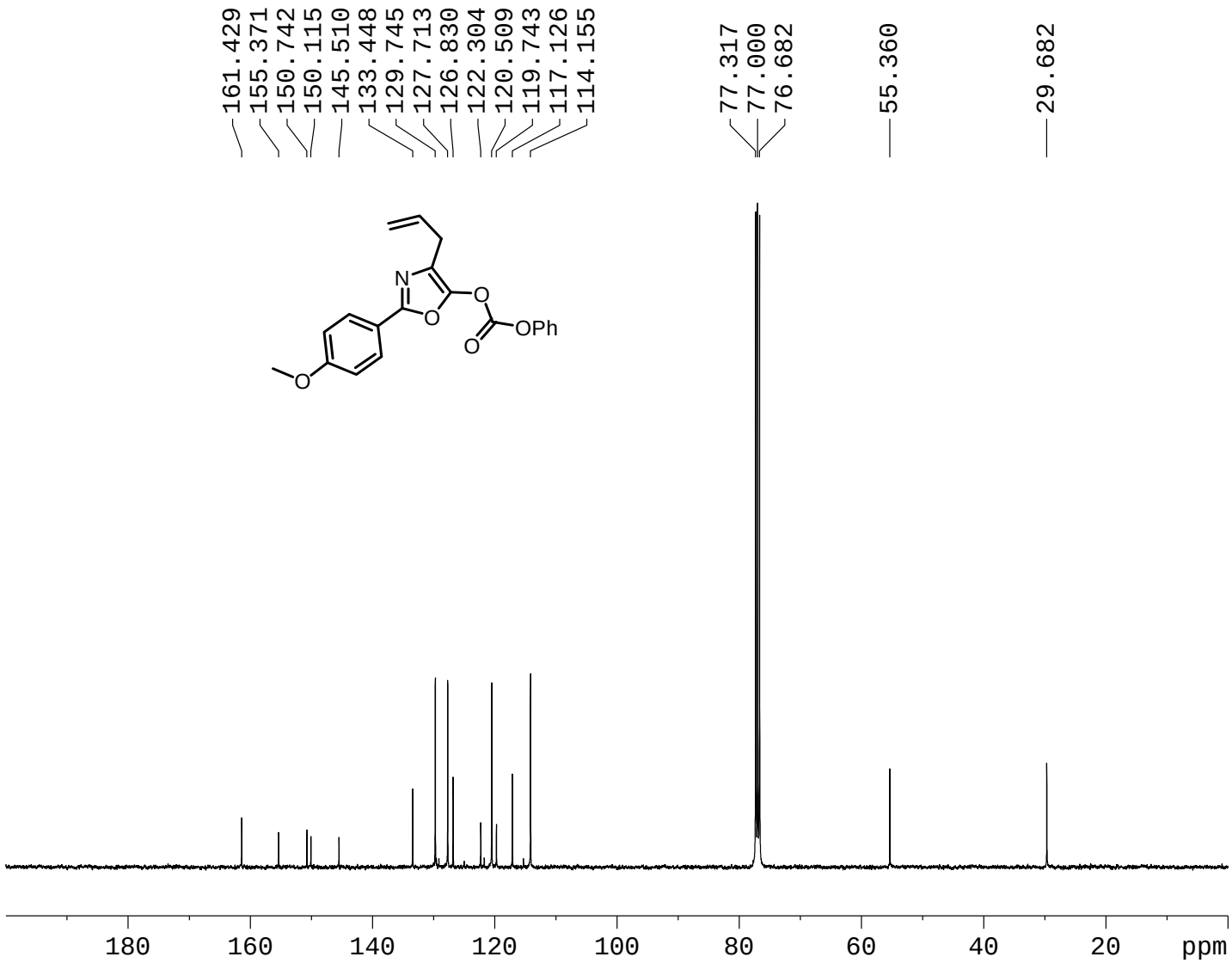
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C







NAME	140628allyPh
EXPNO	1
PROCNO	1
Date_	20140629
Time	5.28
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500092 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	140628allyPh	
EXPNO	13	
PROCNO	1	
Date_	20140629	
Time	5.29	
INSTRUM	spect	
PROBHD	5 mm DUL 13C-1	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	2660	
DS	0	
SWH	22727.273	Hz
FIDRES	0.346791	Hz
AQ	1.4418420	sec
RG	57	
DW	22.000	usec
DE	6.00	usec
TE	300.0	K
D1	2.00000000	sec
d11	0.03000000	sec
DELTA	1.89999998	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.70	usec
PL1	-0.50	dB
SFO1	100.6288660	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	90.00	usec
PL2	-2.40	dB
PL12	15.10	dB
PL13	18.10	dB
SFO2	400.1516010	MHz
SI	32768	
SF	100.6178004	MHz
WDW	EM	
SSB	0	
LB	3.00	Hz
GB	0	
PC	1.00	

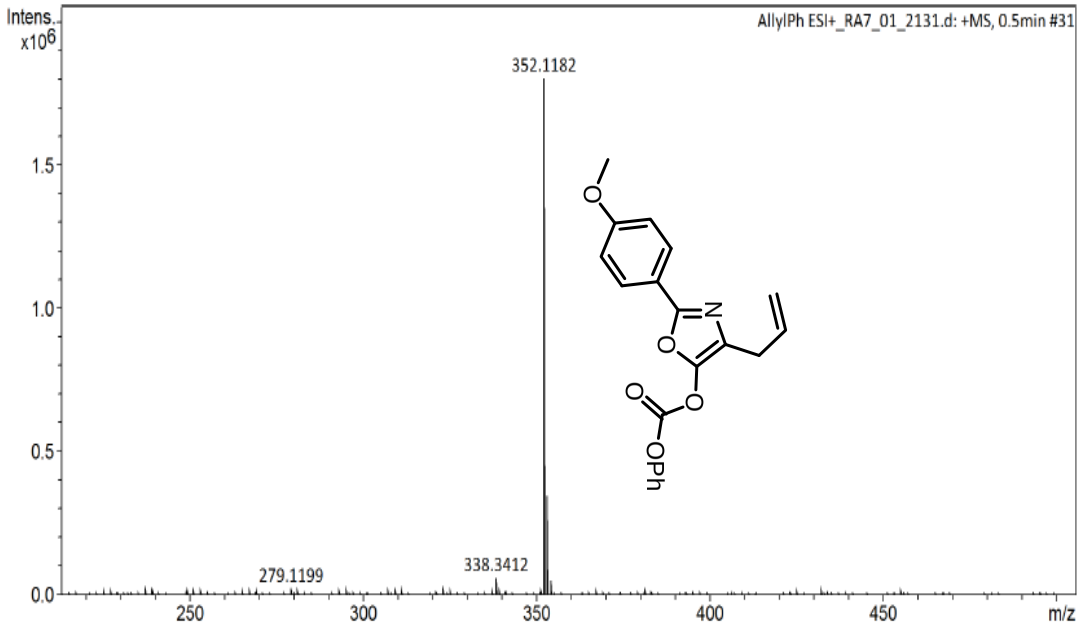
Display Report

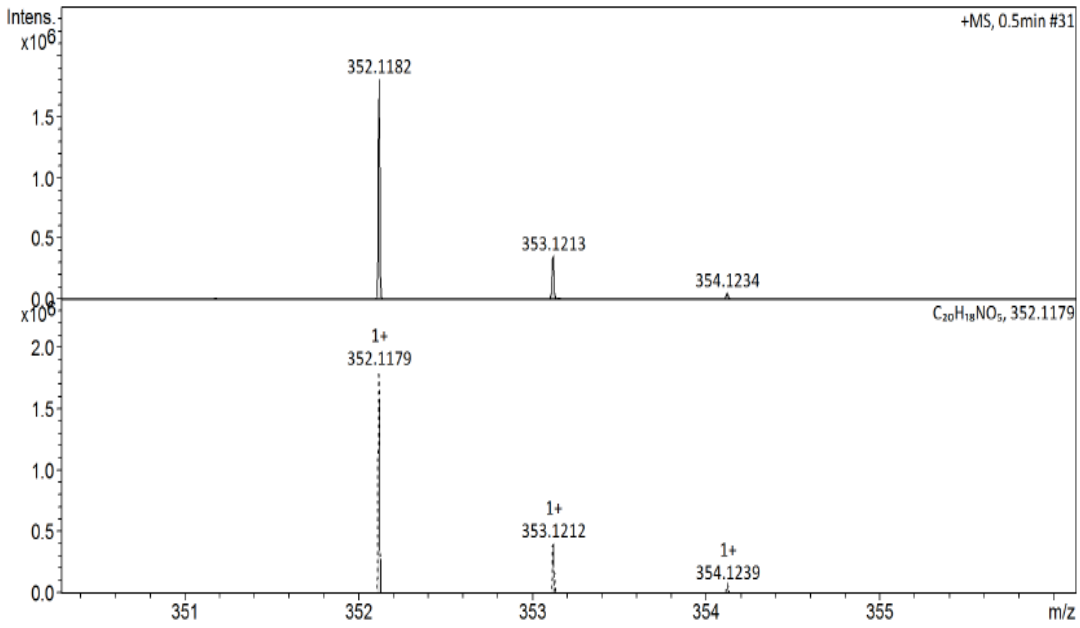
Analysis Info

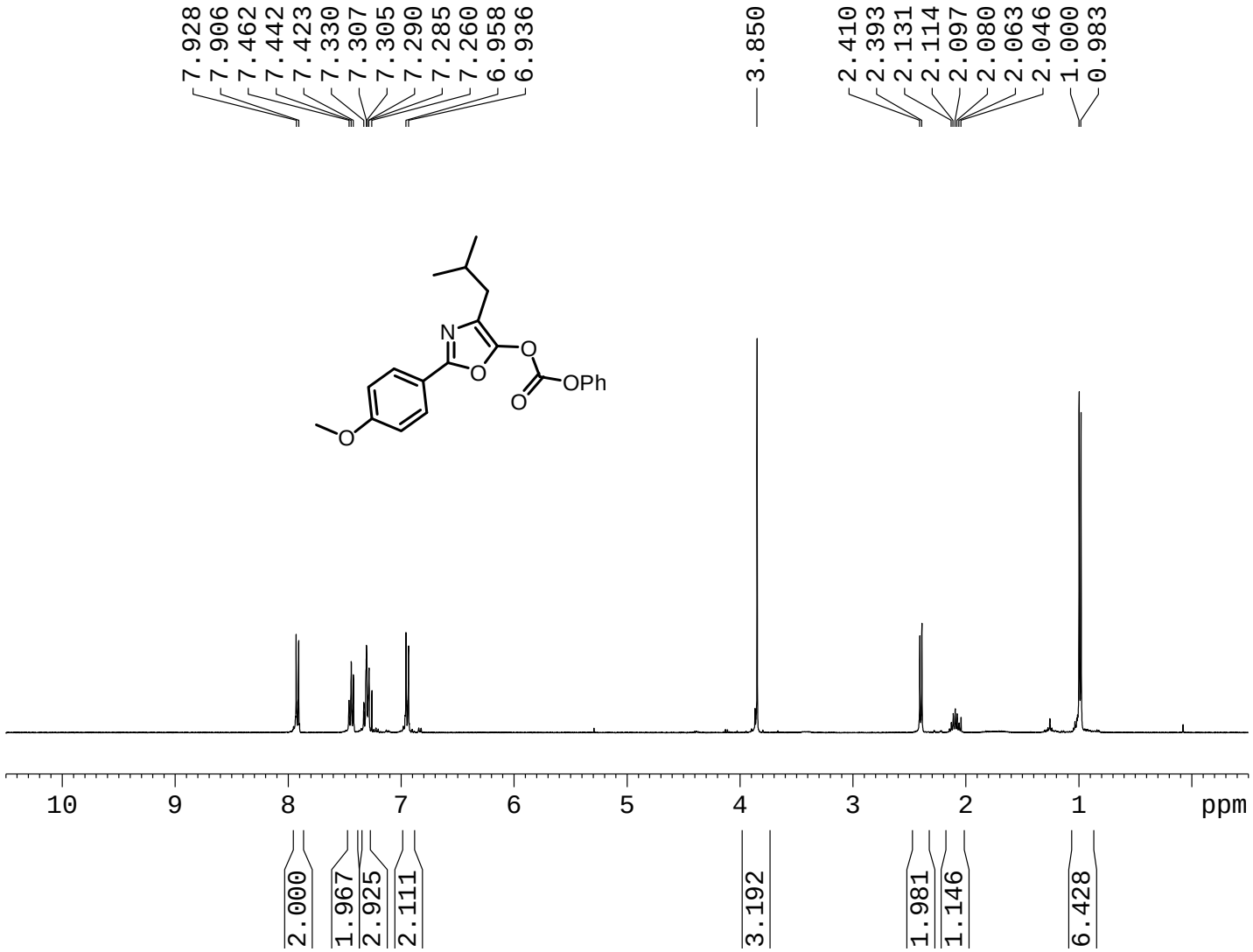
Analysis Name	D:\Data\NCTU SERVICE\Data\20140704\AllylPh ESI+_RA7_01_2131.d	Acquisition Date	7/4/2014 9:28:00 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	AllylPh ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

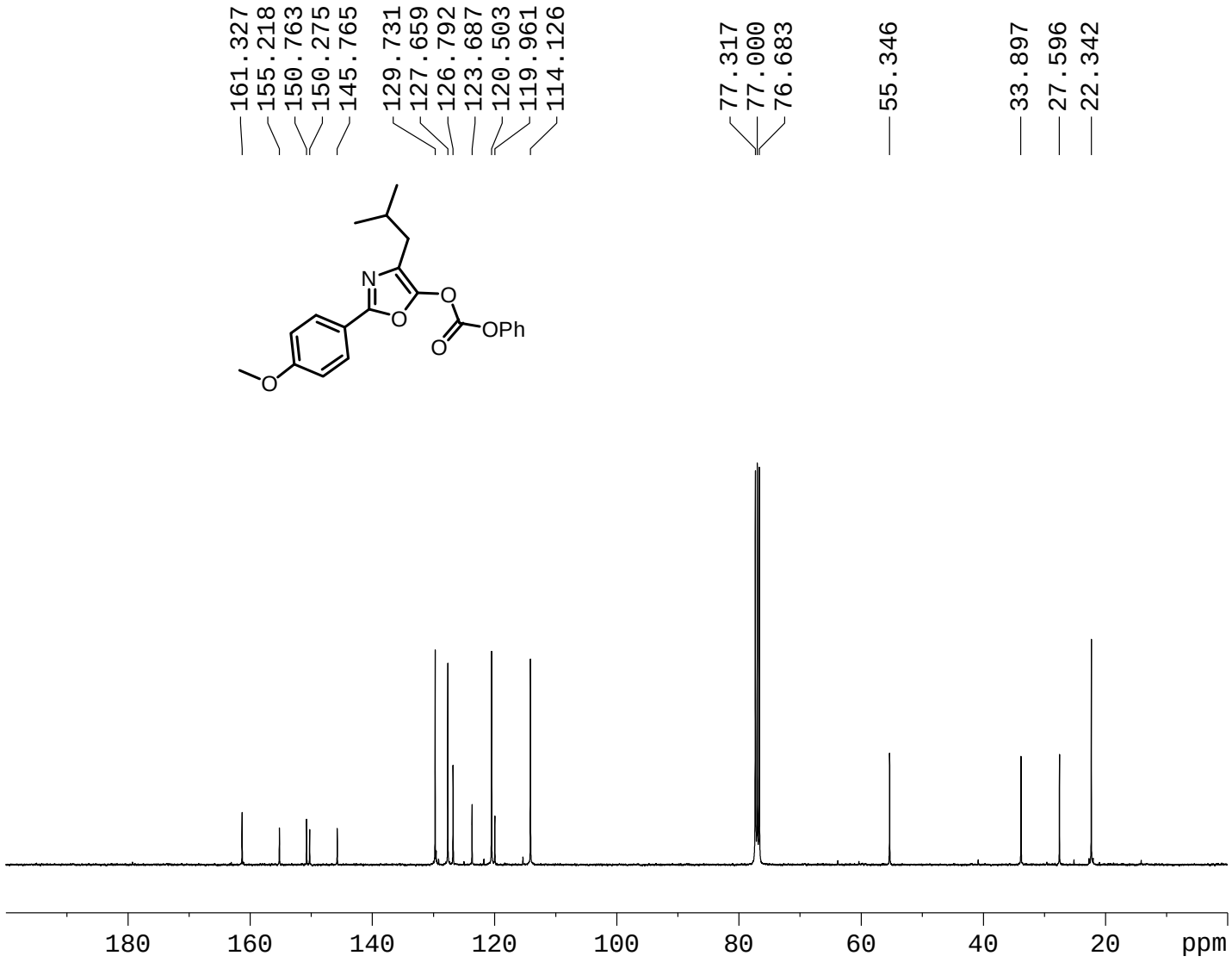
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C







NAME	140705-iBuPh	
EXPNO	1	
PROCNO	1	
Date_	20140705	
Time	0.09	
INSTRUM	spect	
PROBHD	5 mm DUL 13C-1	
PULPROG	zg30	
TD	32768	
SOLVENT	CDCl3	
NS	4	
DS	0	
SWH	6410.256	Hz
FIDRES	0.195625	Hz
AQ	2.5559540	sec
RG	4	
DW	78.000	usec
DE	6.00	usec
TE	300.0	K
D1	2.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	usec
PL1	-2.40	dB
SFO1	400.1528010	MHz
SI	16384	
SF	400.1500089	MHz
WDW	EM	
SSB	0	
LB	0.00	Hz
GB	0	
PC	1.00	



NAME	140705-iBuPh	
EXPNO	13	
PROCNO	1	
Date_	20140705	
Time	0.11	
INSTRUM	spect	
PROBHD	5 mm DUL 13C-1	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	6278	
DS	0	
SWH	22727.273	Hz
FIDRES	0.346791	Hz
AQ	1.4418420	sec
RG	57	
DW	22.000	usec
DE	6.00	usec
TE	300.0	K
D1	2.00000000	sec
d11	0.03000000	sec
DELTA	1.89999998	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.70	usec
PL1	-0.50	dB
SFO1	100.6288660	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	90.00	usec
PL2	-2.40	dB
PL12	15.10	dB
PL13	18.10	dB
SFO2	400.1516010	MHz
SI	32768	
SF	100.6178008	MHz
WDW	EM	
SSB	0	
LB	3.00	Hz
GB	0	
PC	1.00	

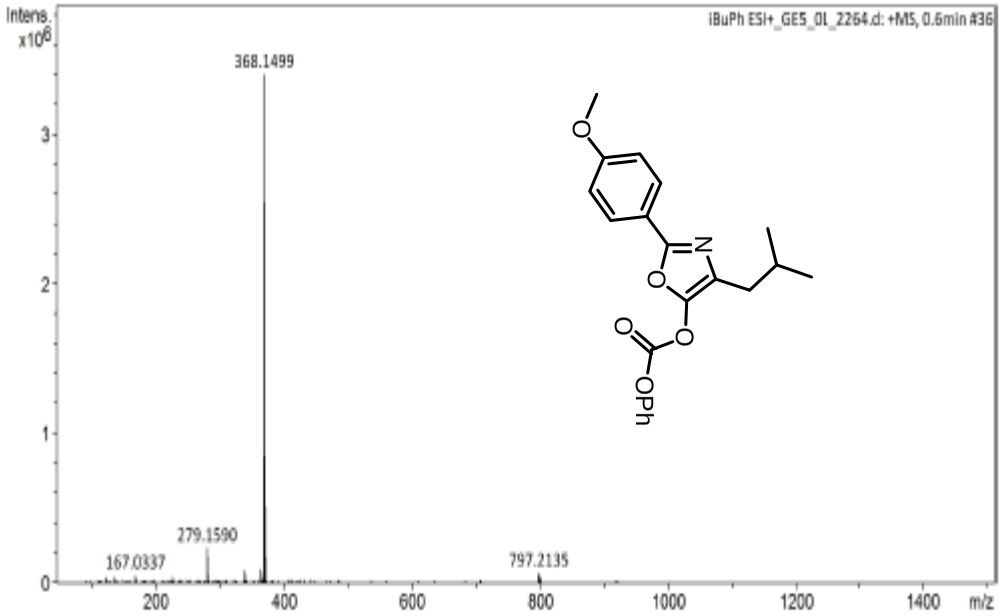
Display Report

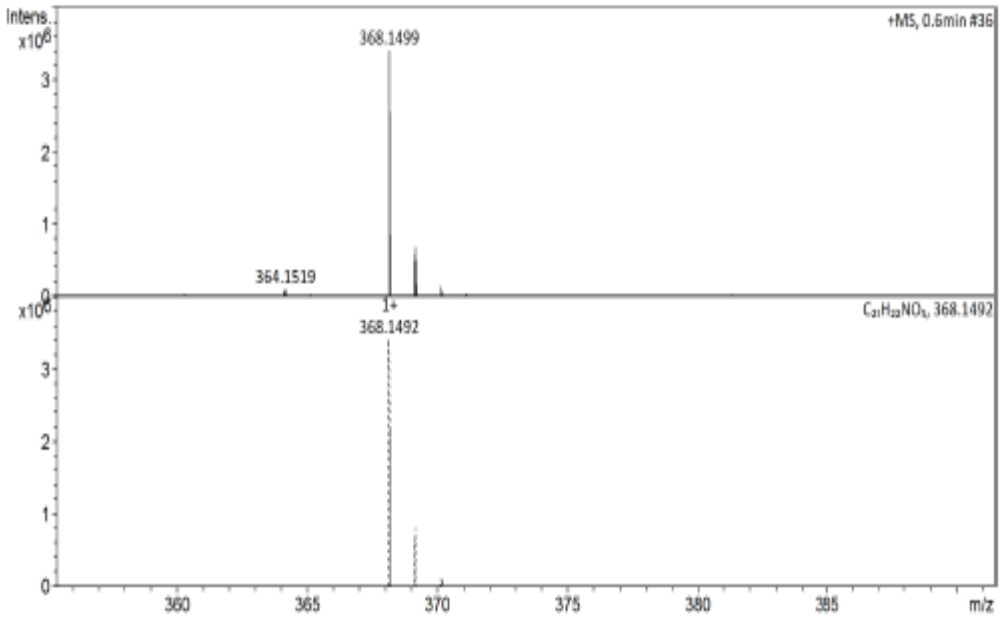
Analysis Info

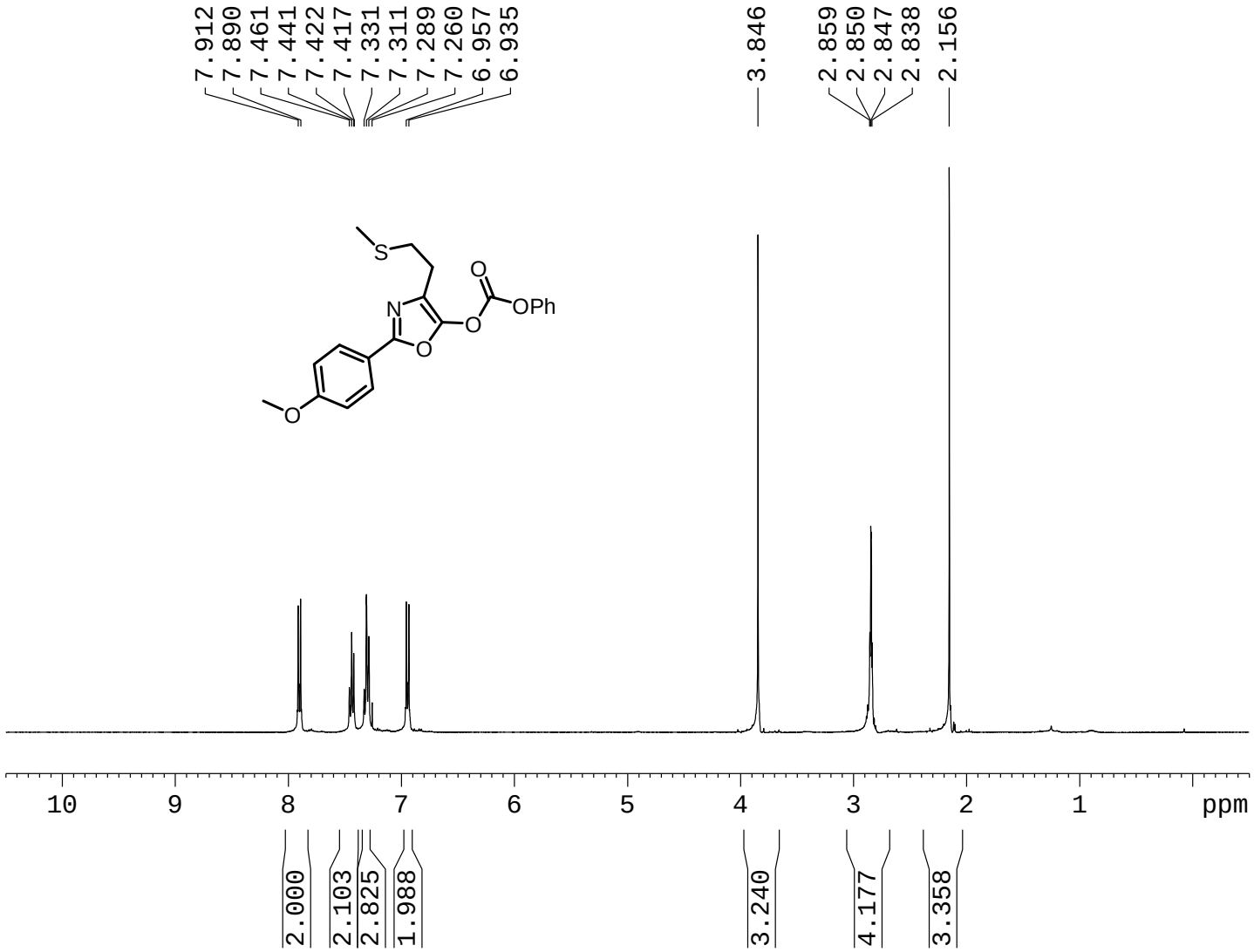
Analysis Name	D:\Data\NCTU SERVICE\Data\20140718\iBuPh ESI+_GE5_01_2264.d	Acquisition Date	7/18/2014 9:55:57 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	iBuPh ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

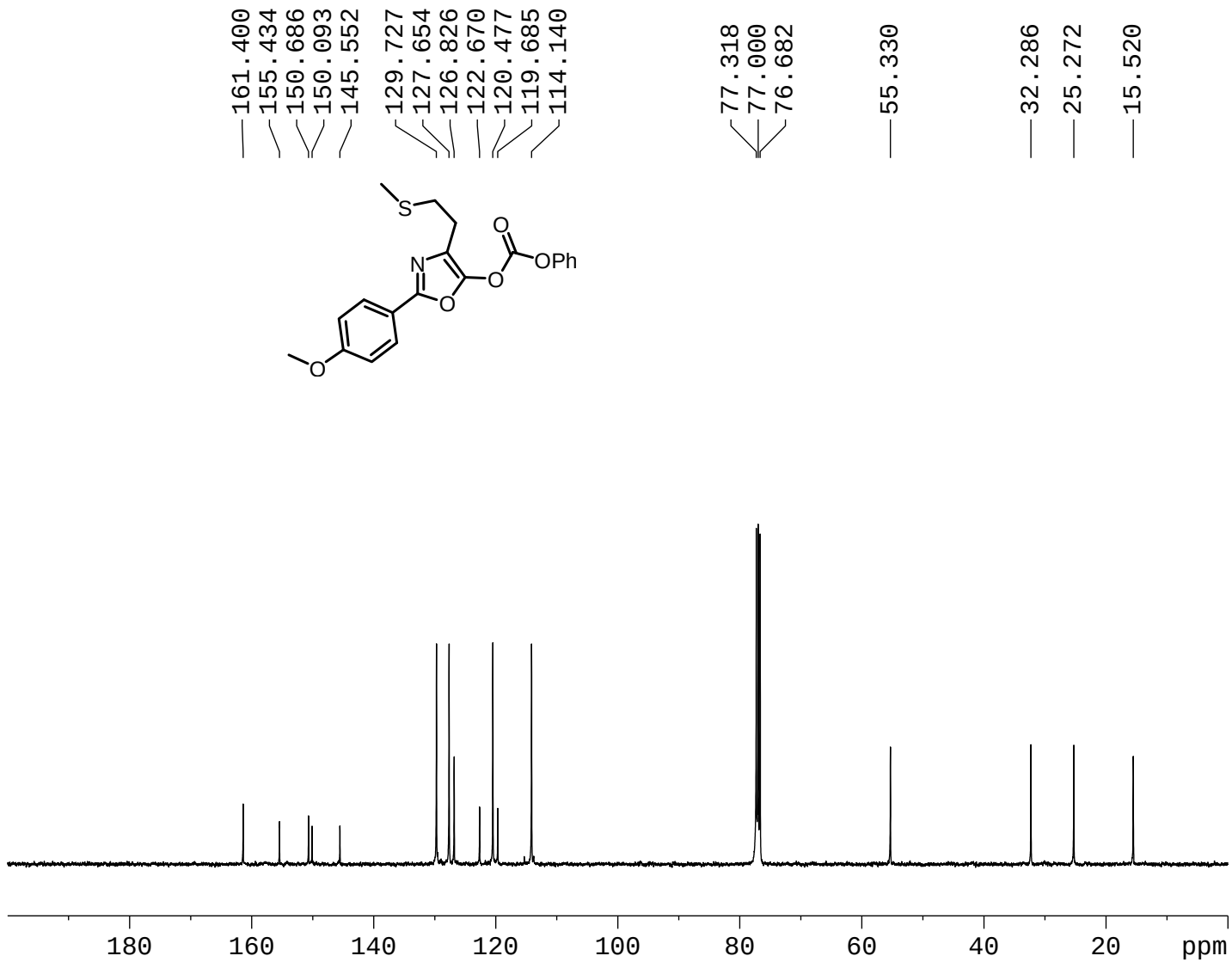
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C







NAME	140225SMePh	
EXPNO	1	
PROCNO	1	
Date_	20140227	
Time	9.06	
INSTRUM	spect	
PROBHD	5 mm DUL 13C-1	
PULPROG	zg30	
TD	32768	
SOLVENT	CDCl3	
NS	16	
DS	0	
SWH	6410.256	Hz
FIDRES	0.195625	Hz
AQ	2.5559540	sec
RG	4	
DW	78.000	usec
DE	6.00	usec
TE	300.0	K
D1	2.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	usec
PL1	-2.40	dB
SFO1	400.1528010	MHz
SI	16384	
SF	400.1500092	MHz
WDW	EM	
SSB	0	
LB	0.00	Hz
GB	0	
PC	1.00	



NAME	140225SMePh
EXPNO	15
PROCNO	1
Date_	20140228
Time	23.57
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	9248
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6178043 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

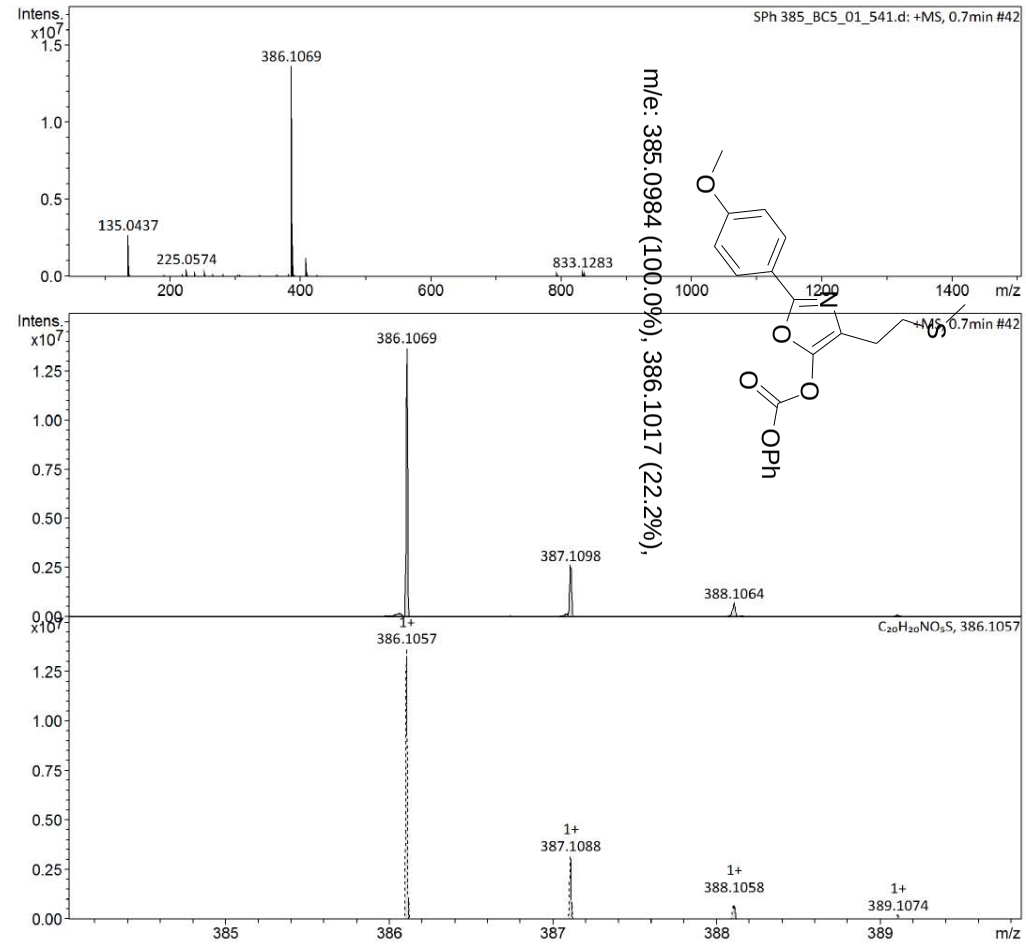
Display Report

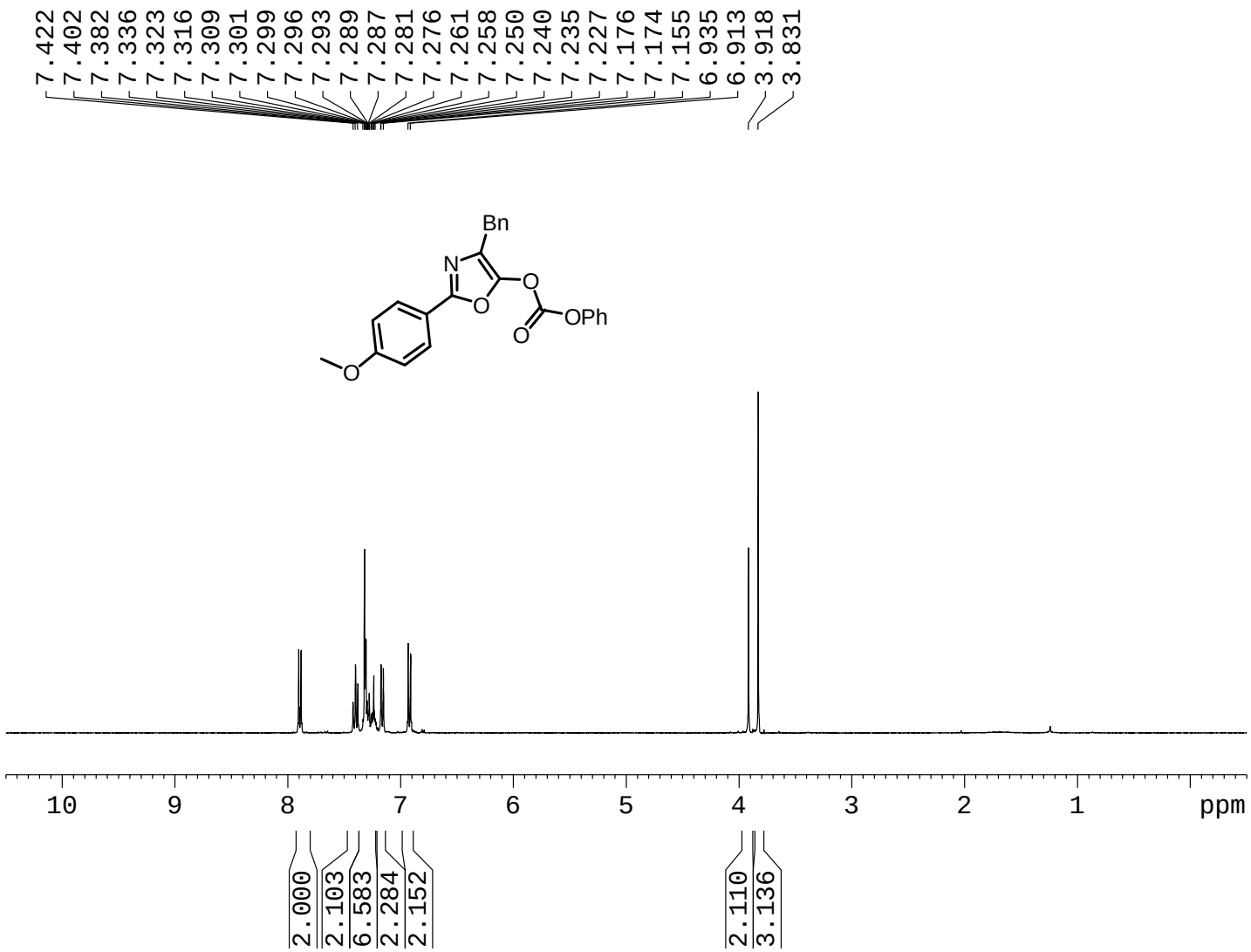
Analysis Info

Analysis Name	D:\Data\NCTU SERVICE\Data\20140303\SPh 385_BC5_01_541.d	Acquisition Date	3/3/2014 4:30:54 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	SPh 385	Instrument	impact HD 1819696.00164
Comment			

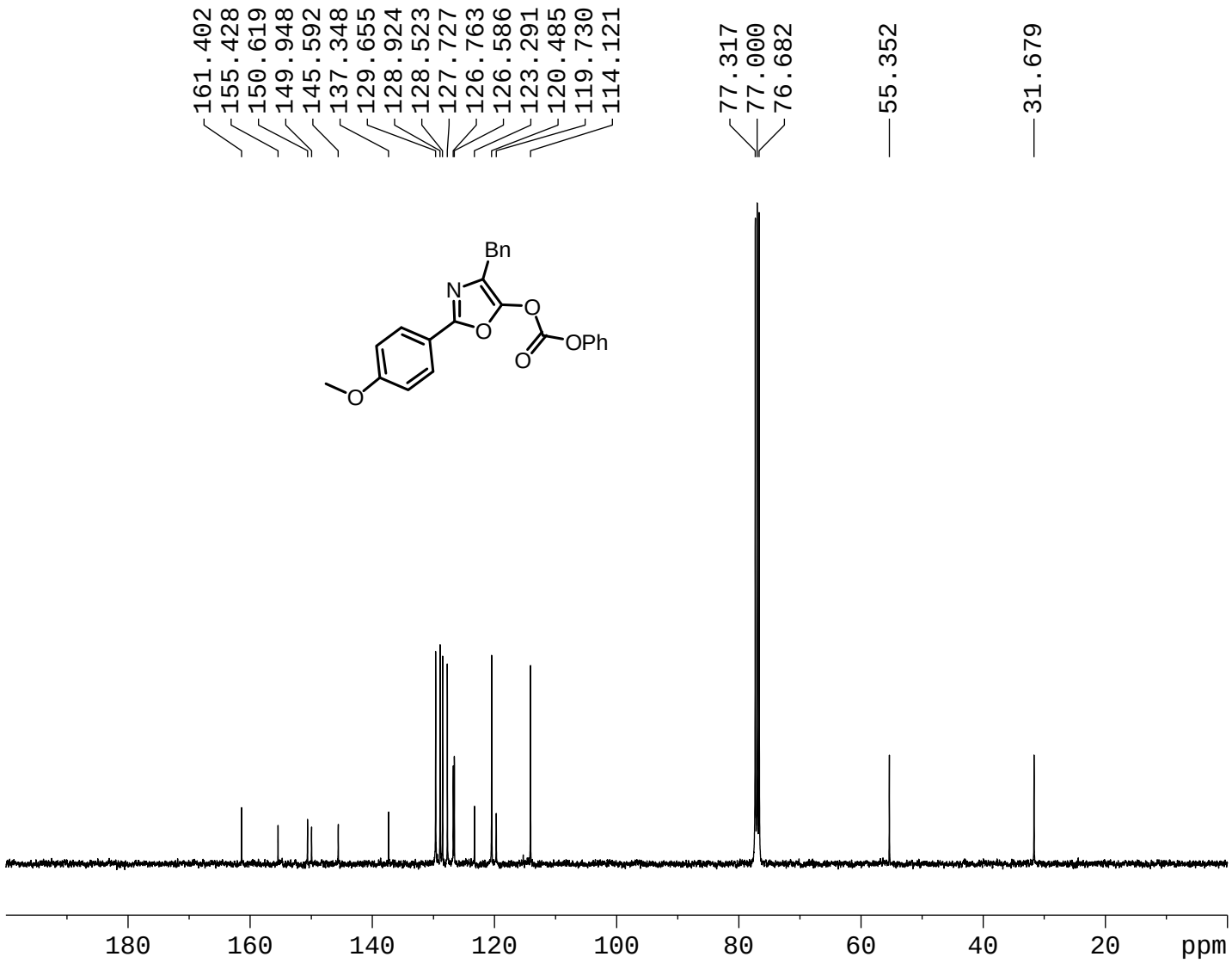
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C





NAME	140225BnPh
EXPNO	1
PROCNO	1
Date_	20140225
Time	18.32
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	32
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	2
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500168 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	140225BnPh
EXPNO	13
PROCNO	1
Date_	20140225
Time	18.34
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1253
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6178023 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

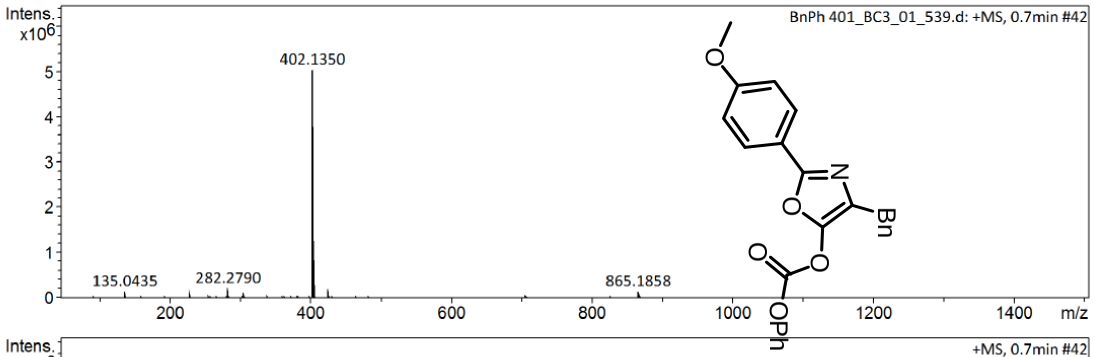
Display Report

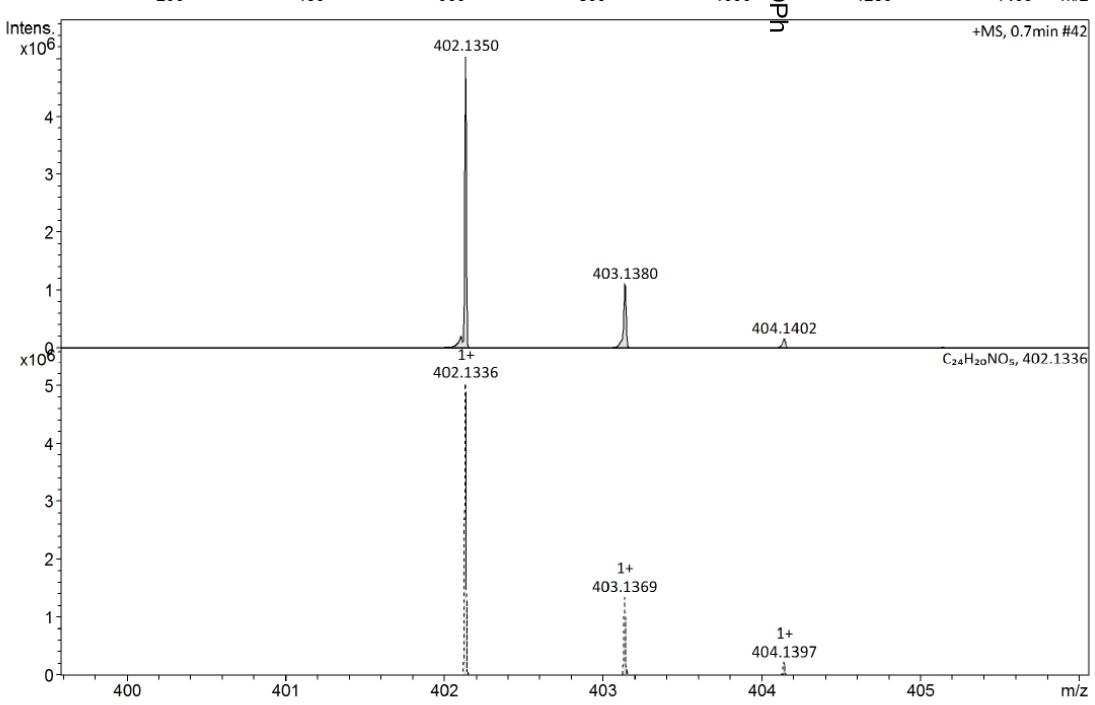
Analysis Info

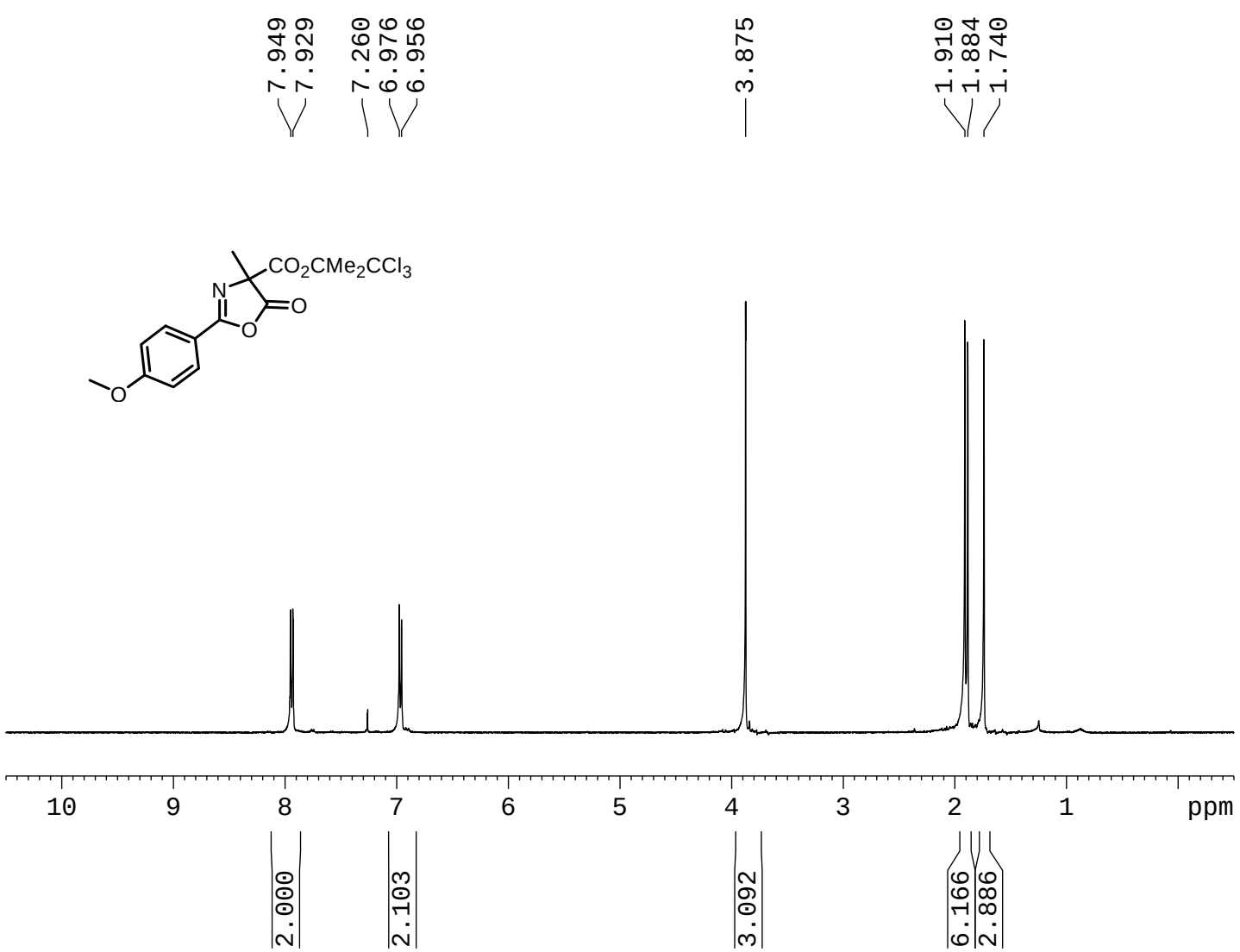
Acquisition Date	3/3/2014 4:22:08 PM		
Analysis Name	D:\Data\NCTU SERVICE\Data\20140303\BnPh 401_BC3_01_539.d		
Method	Small molecule.m	Operator	NCTU
Sample Name	BnPh 401	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

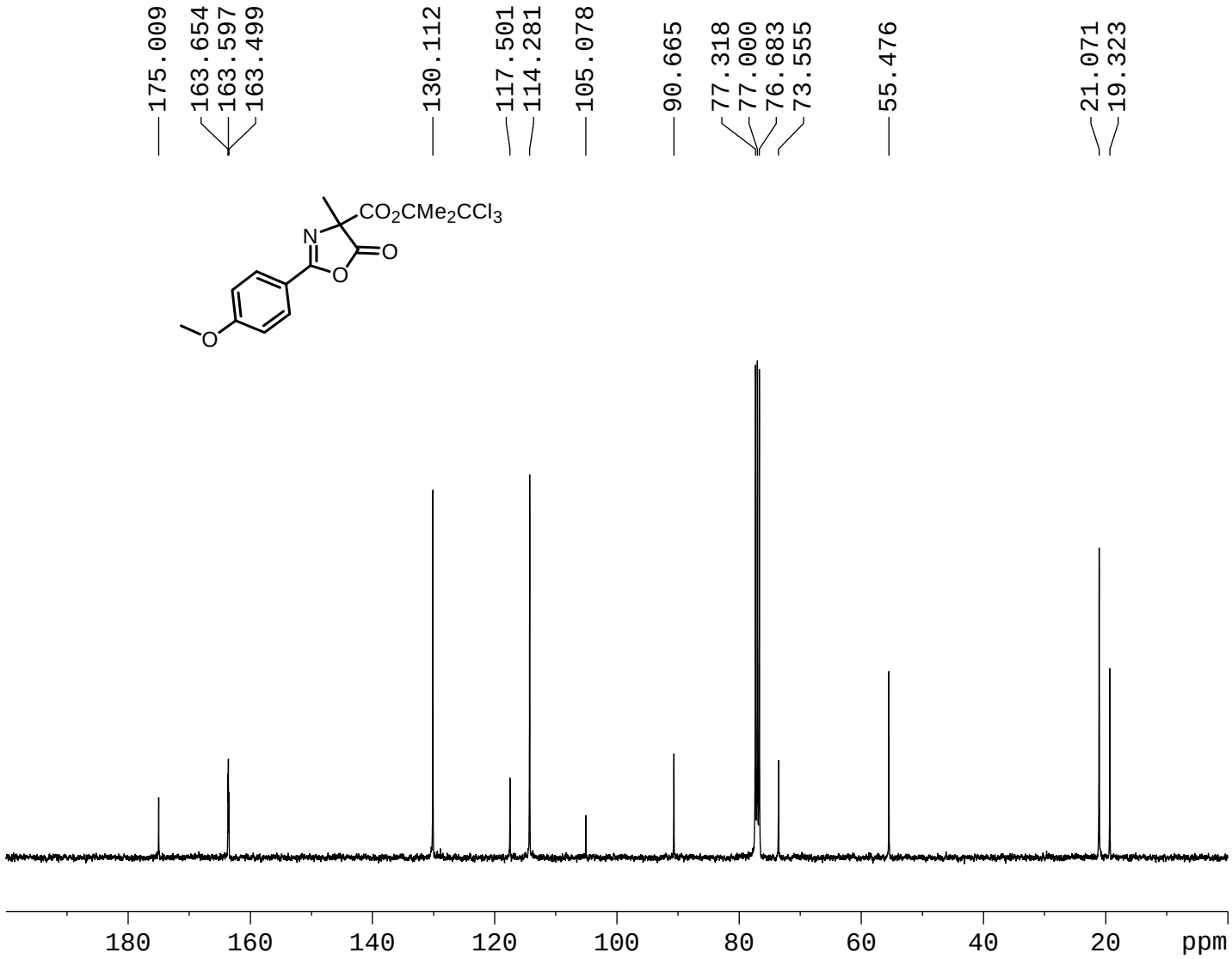
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C







NAME	150314MeCl-P
EXPNO	1
PROCNO	1
Date_	20150314
Time	10.25
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500085 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	150314MeCl-P
EXPNO	13
PROCNO	1
Date_	20150314
Time	10.26
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	842
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6178004 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

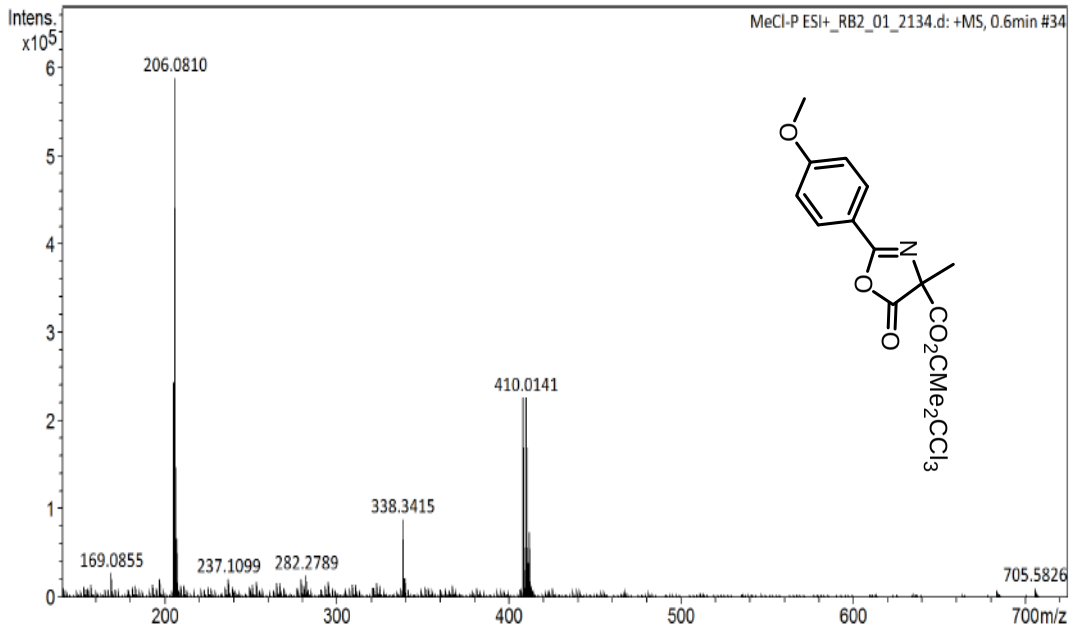
Display Report

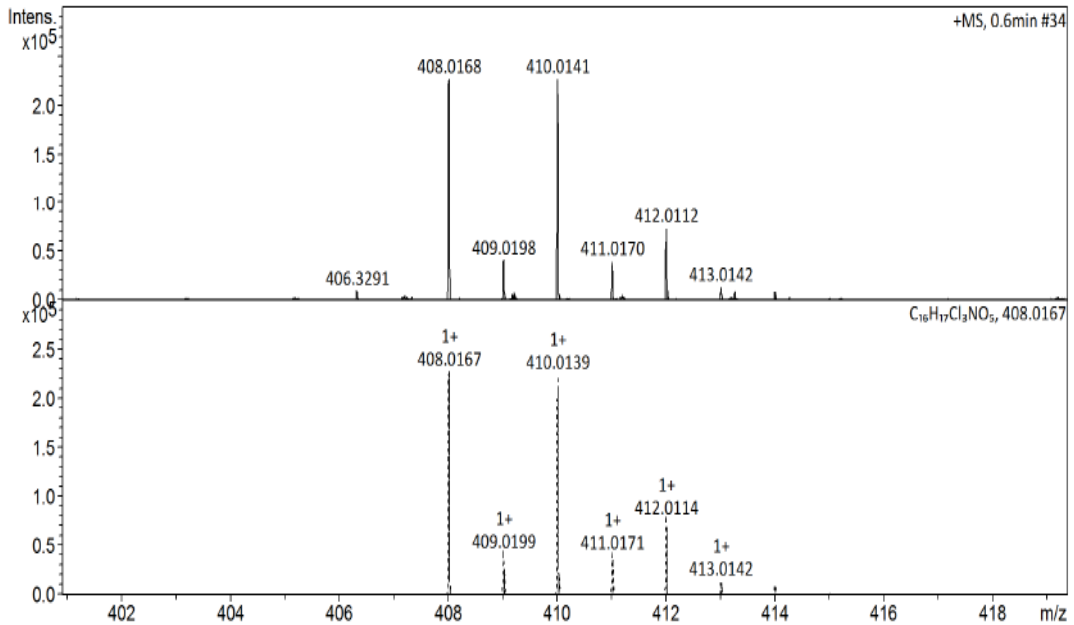
Analysis Info

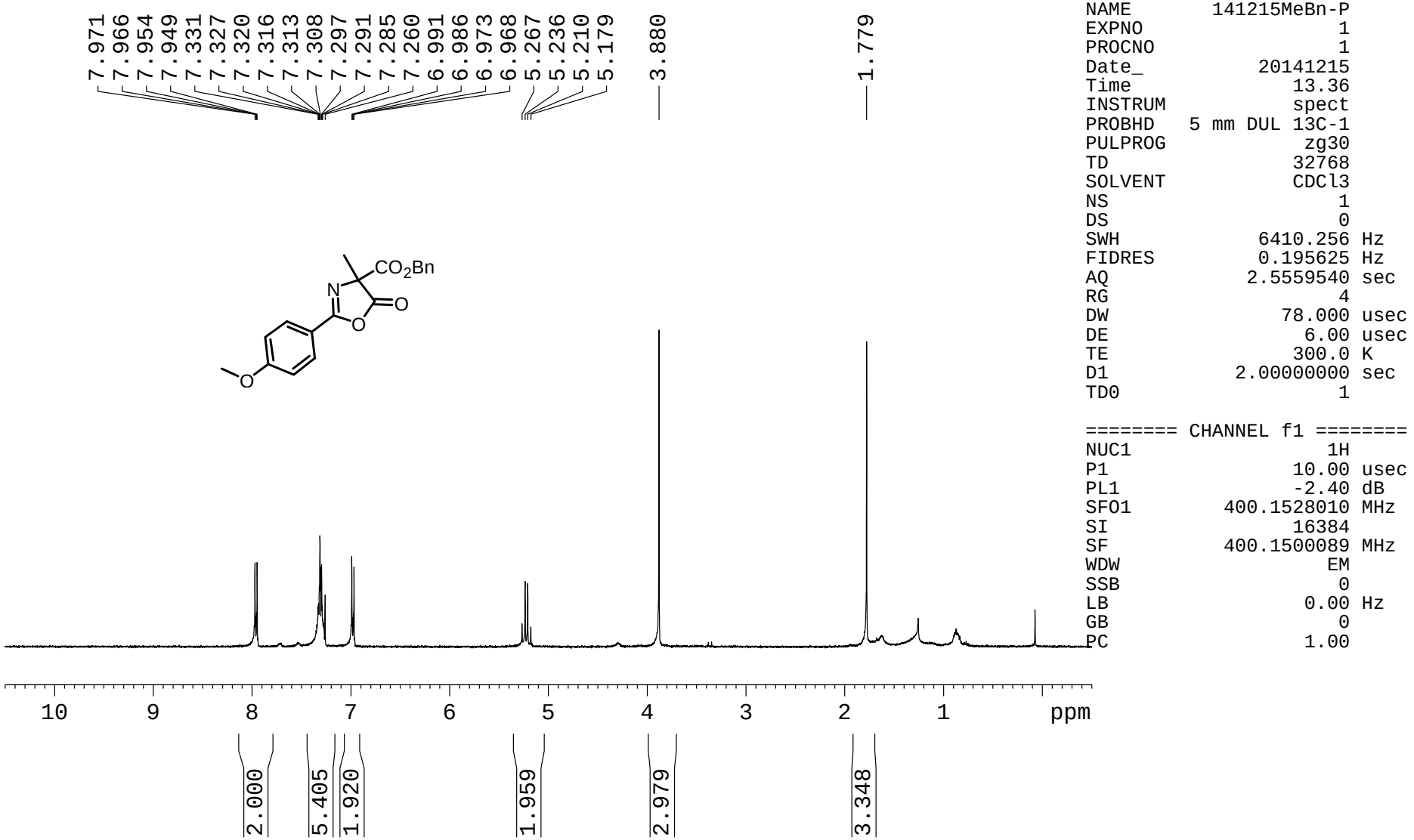
Analysis Name	D:\Data\NCTU SERVICE\Data\20140704\MeCl-P ESI+_RB2_01_2134.d	Acquisition Date	7/4/2014 9:40:56 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	MeCl-P ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

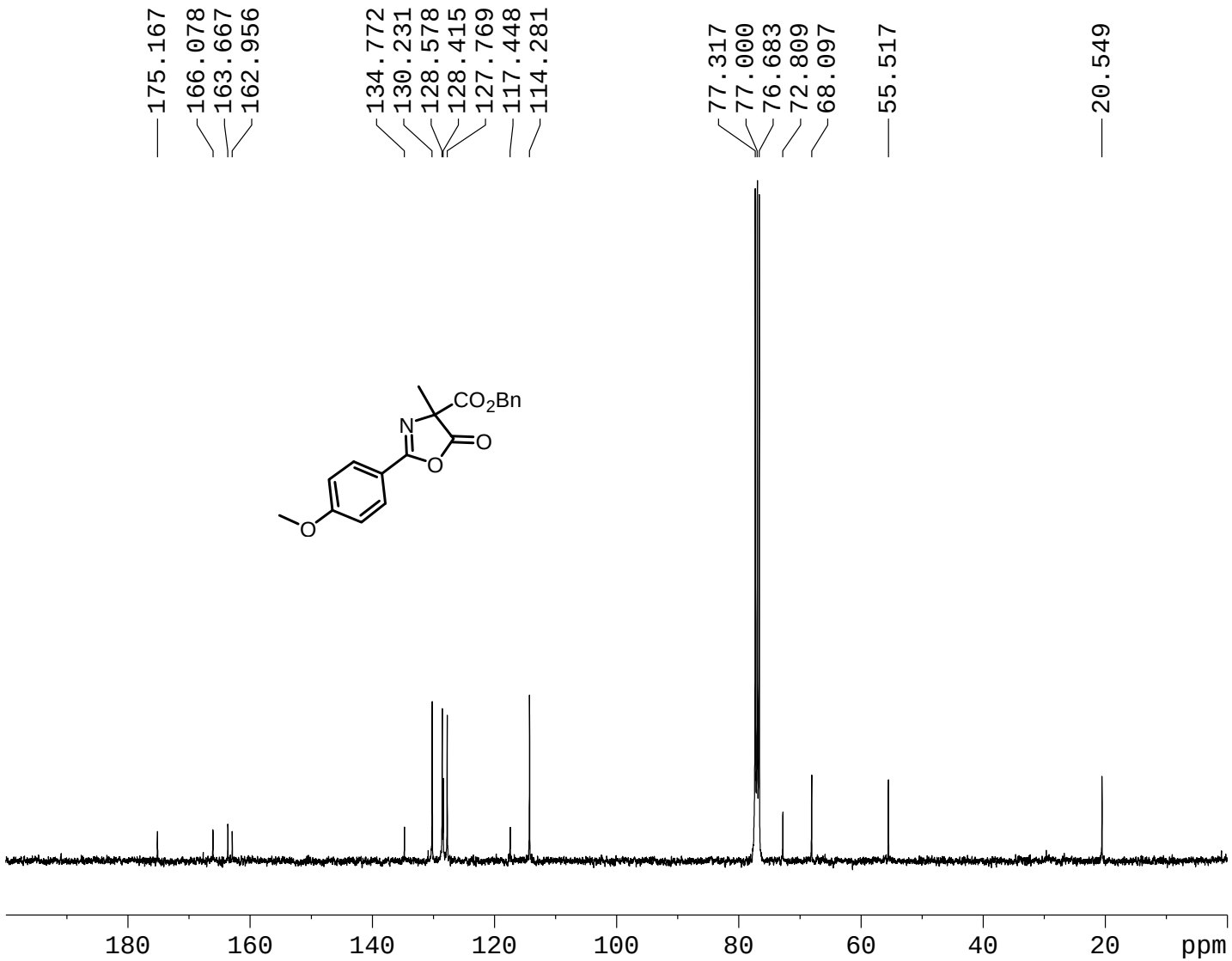
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C







NAME	141215MeBn-P
EXPNO	1
PROCNO	1
Date_	20141215
Time	13.36
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500089 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00




```
NAME        141215MeBn-P
EXPNO                 14
PROCNO                 1
Date_           20141215
Time               13.39
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1008
DS                    0
SWH           22727.273 Hz
FIDRES         0.346791 Hz
AQ             1.4418420 sec
RG                   57
DW                22.000 usec
DE                 6.00 usec
TE                300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.70 usec
PL1                -0.50 dB
SFO1         100.6288660 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                -2.40 dB
PL12               15.10 dB
PL13               18.10 dB
SFO2         400.1516010 MHz
SI                 32768
SF           100.6178001 MHz
WDW                  EM
SSB                   0
LB                 3.00 Hz
GB                    0
PC                 1.00
```

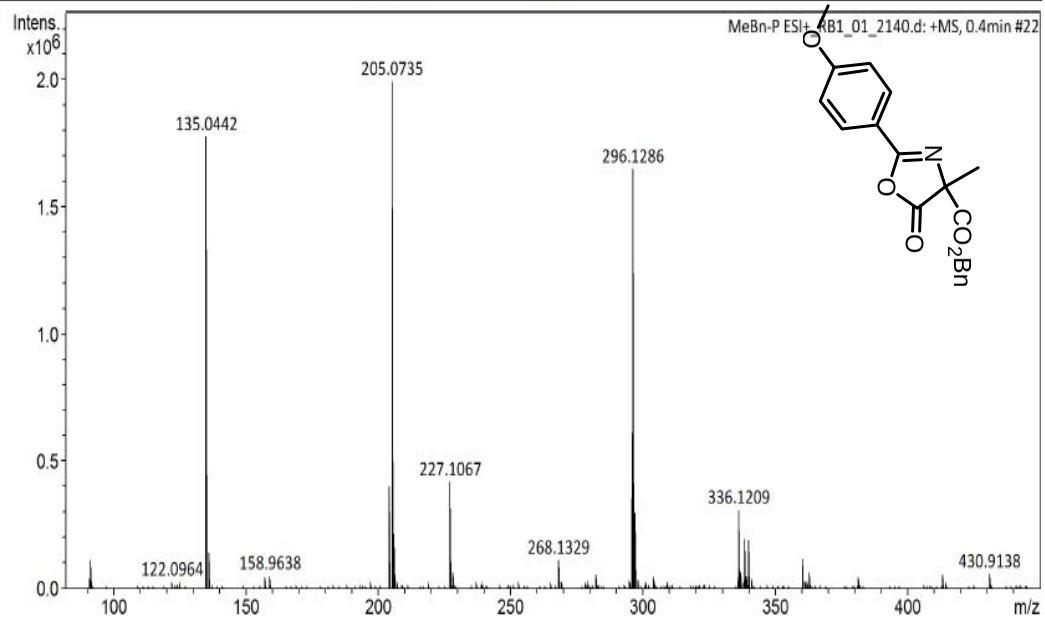
Display Report

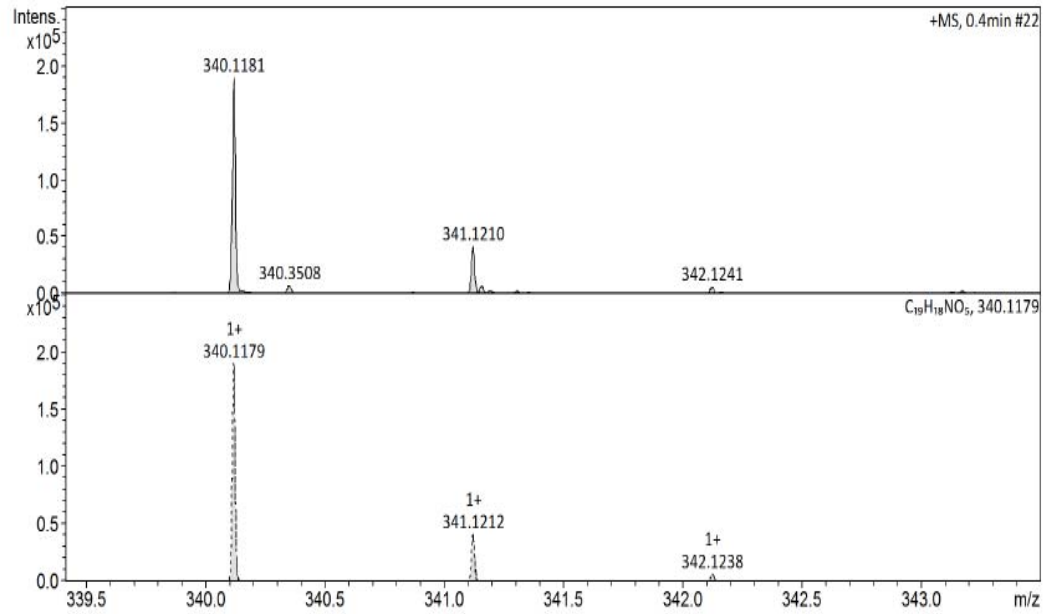
Analysis Info

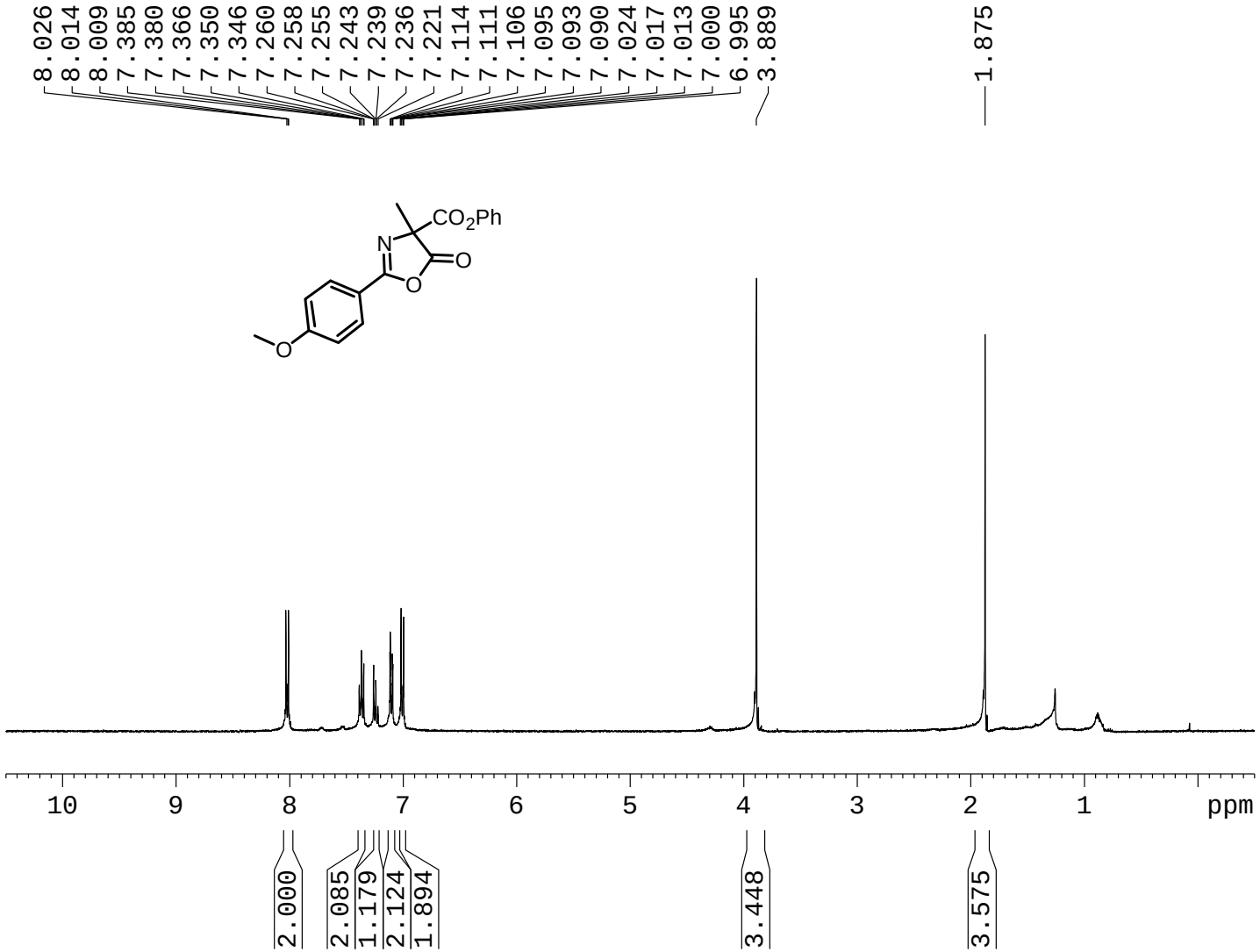
		Acquisition Date	7/4/2014 10:34:49 AM
Analysis Name	D:\Data\nctu service\data\20140704\MeBn-P ESI+_RB1_01_2140.d		
Method	Small molecule.m	Operator	NCTU
Sample Name	MeBn-P ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

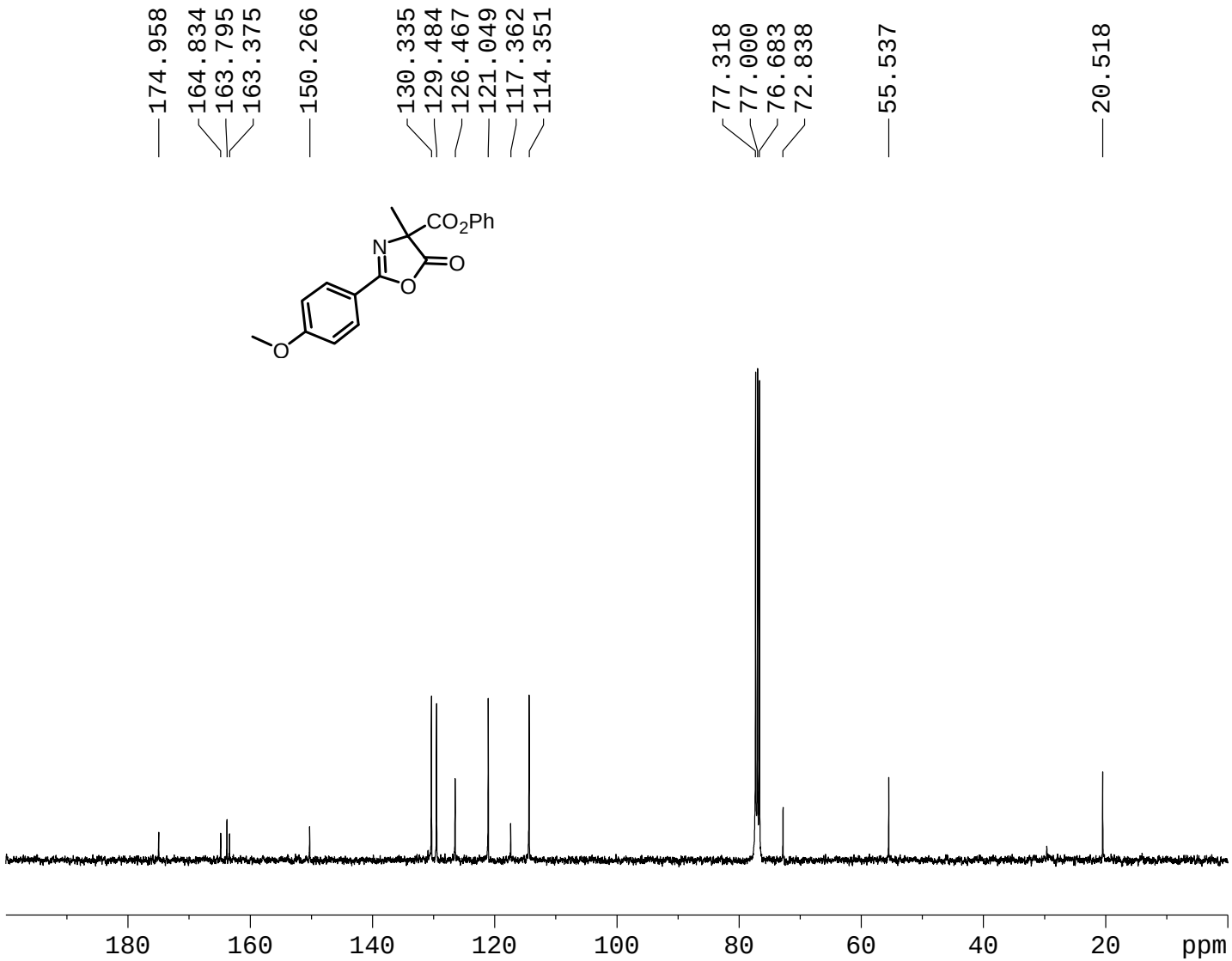
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C







NAME	141216MePh-P
EXPNO	2
PROCNO	1
Date_	20141216
Time	16.51
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500089 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00




```
NAME          141216MePh-P
EXPNO                   13
PROCNO                   1
Date_             20141216
Time                  9.39
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     501
DS                       0
SWH             22727.273 Hz
FIDRES           0.346791 Hz
AQ               1.4418420 sec
RG                      57
DW                 22.000 usec
DE                  6.00 usec
TE                 300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.70 usec
PL1                  -0.50 dB
SFO1           100.6288660 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2                90.00 usec
PL2                  -2.40 dB
PL12                 15.10 dB
PL13                 18.10 dB
SFO2           400.1516010 MHz
SI                   32768
SF             100.6178006 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.00
```

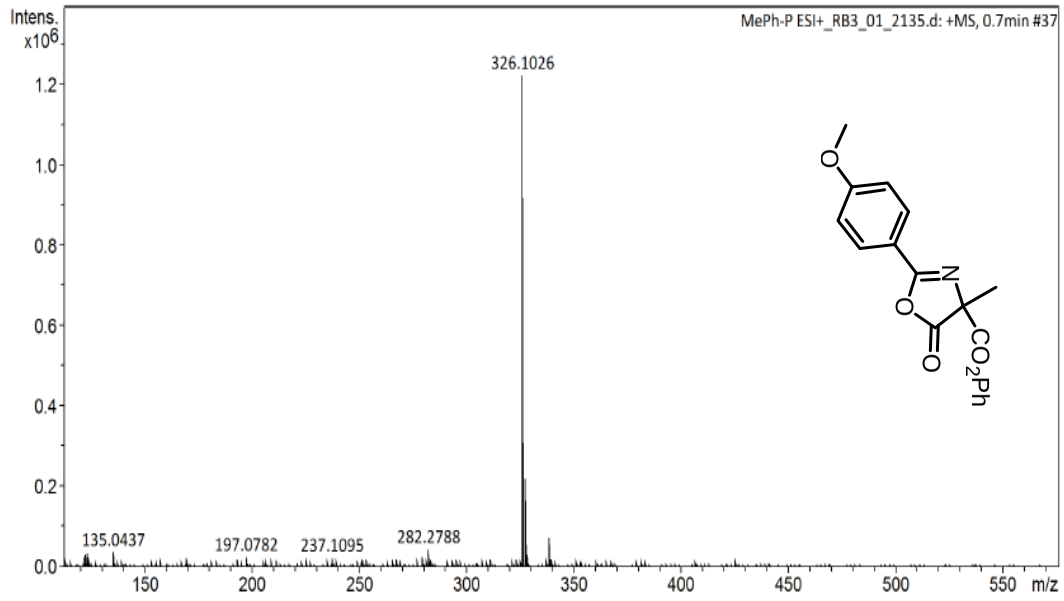
Display Report

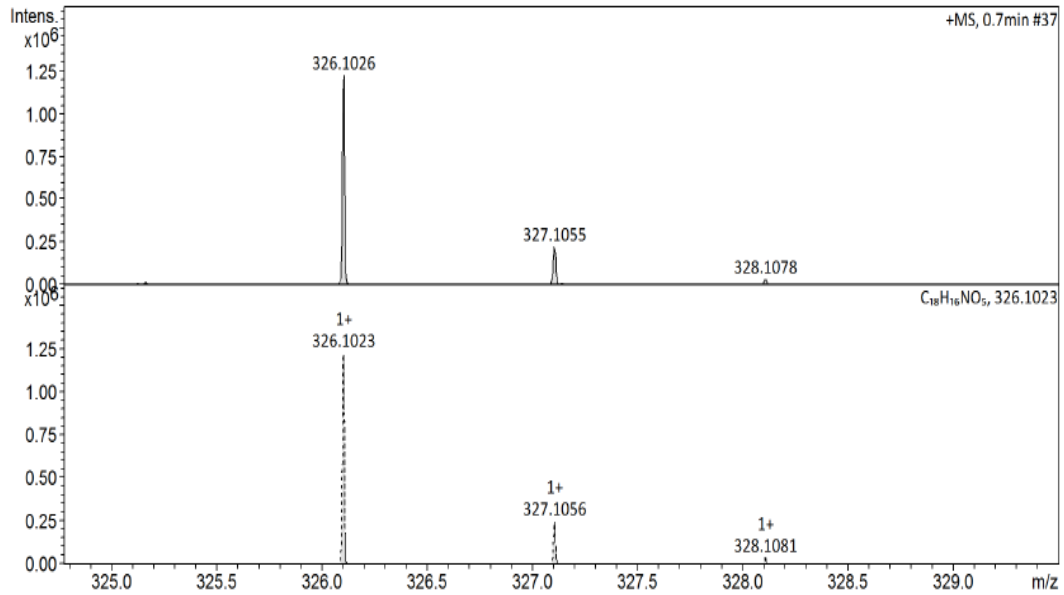
Analysis Info

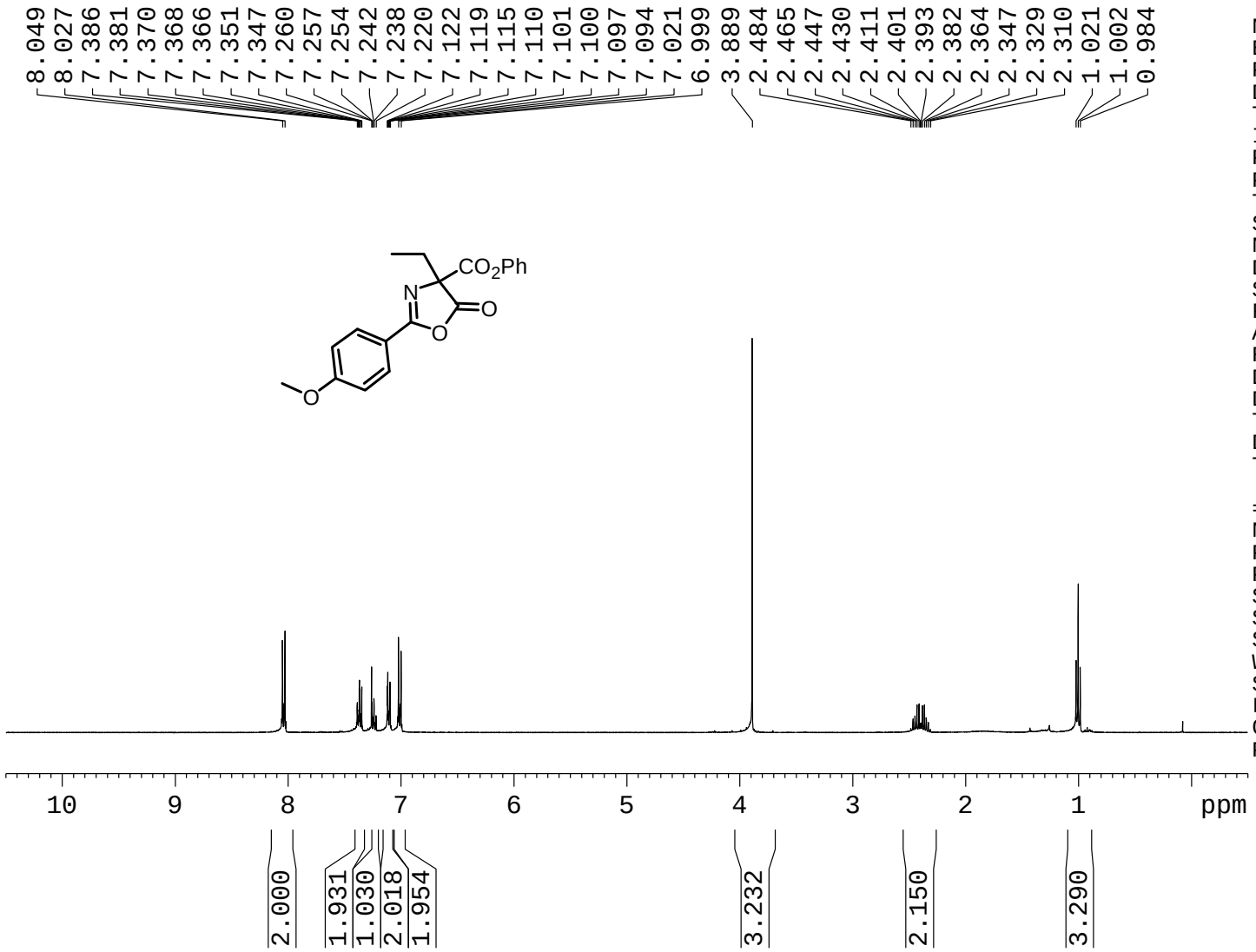
Analysis Name	D:\Data\NCTU SERVICE\Data\20140704\MePh-P ESI+_RB3_01_2135.d	Acquisition Date	7/4/2014 9:45:14 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	MePh-P ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

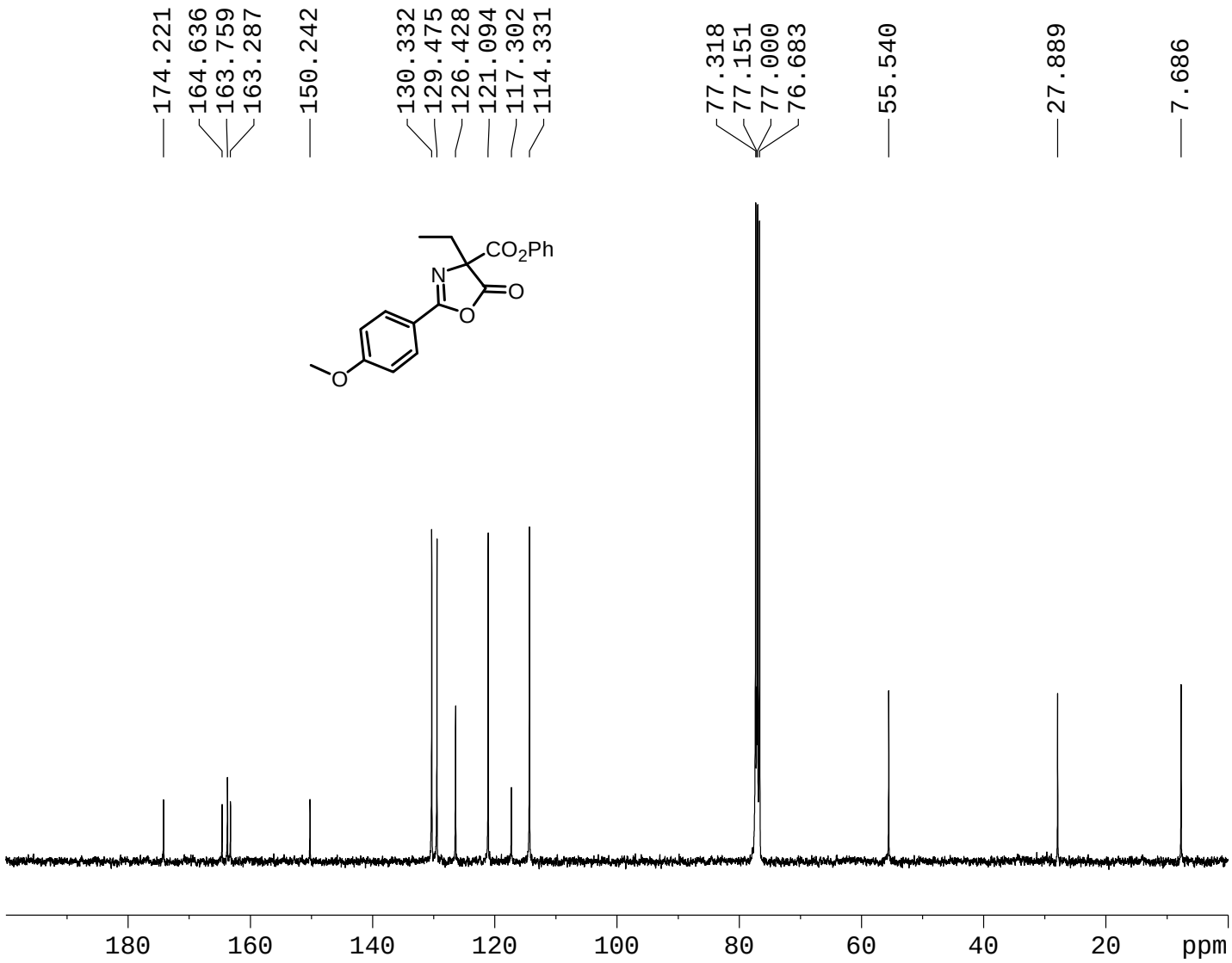
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C







NAME	140629EtPh-P
EXPNO	1
PROCNO	1
Date_	20140629
Time	10.04
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	4
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500088 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	140629EtPh-P
EXPNO	13
PROCNO	1
Date_	20140629
Time	10.06
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	928
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6178015 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

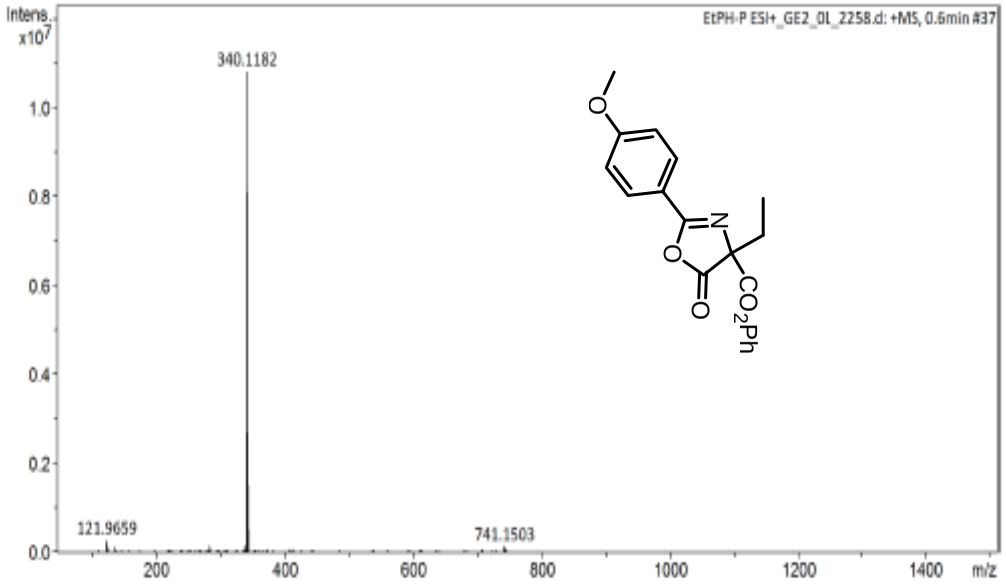
Display Report

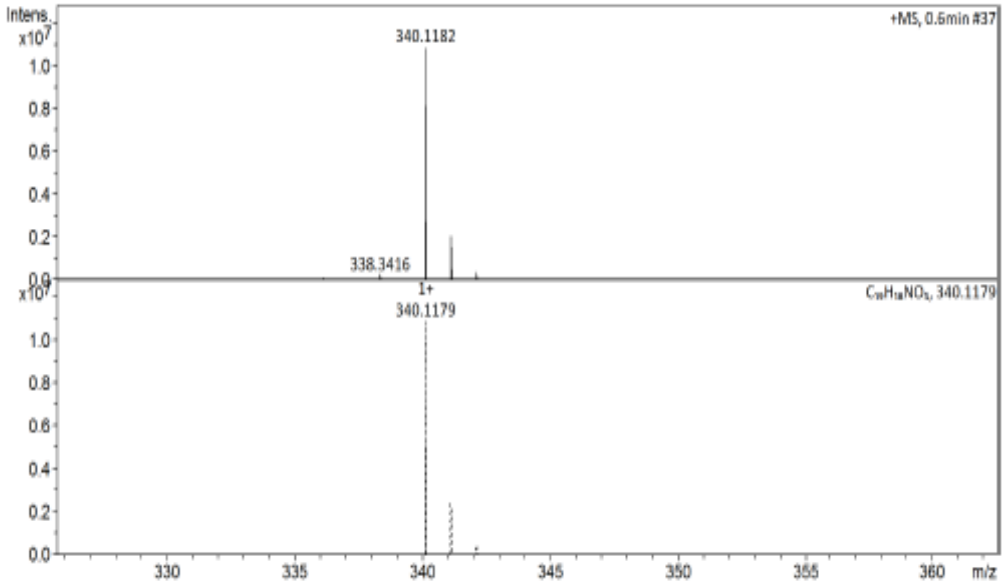
Analysis Info

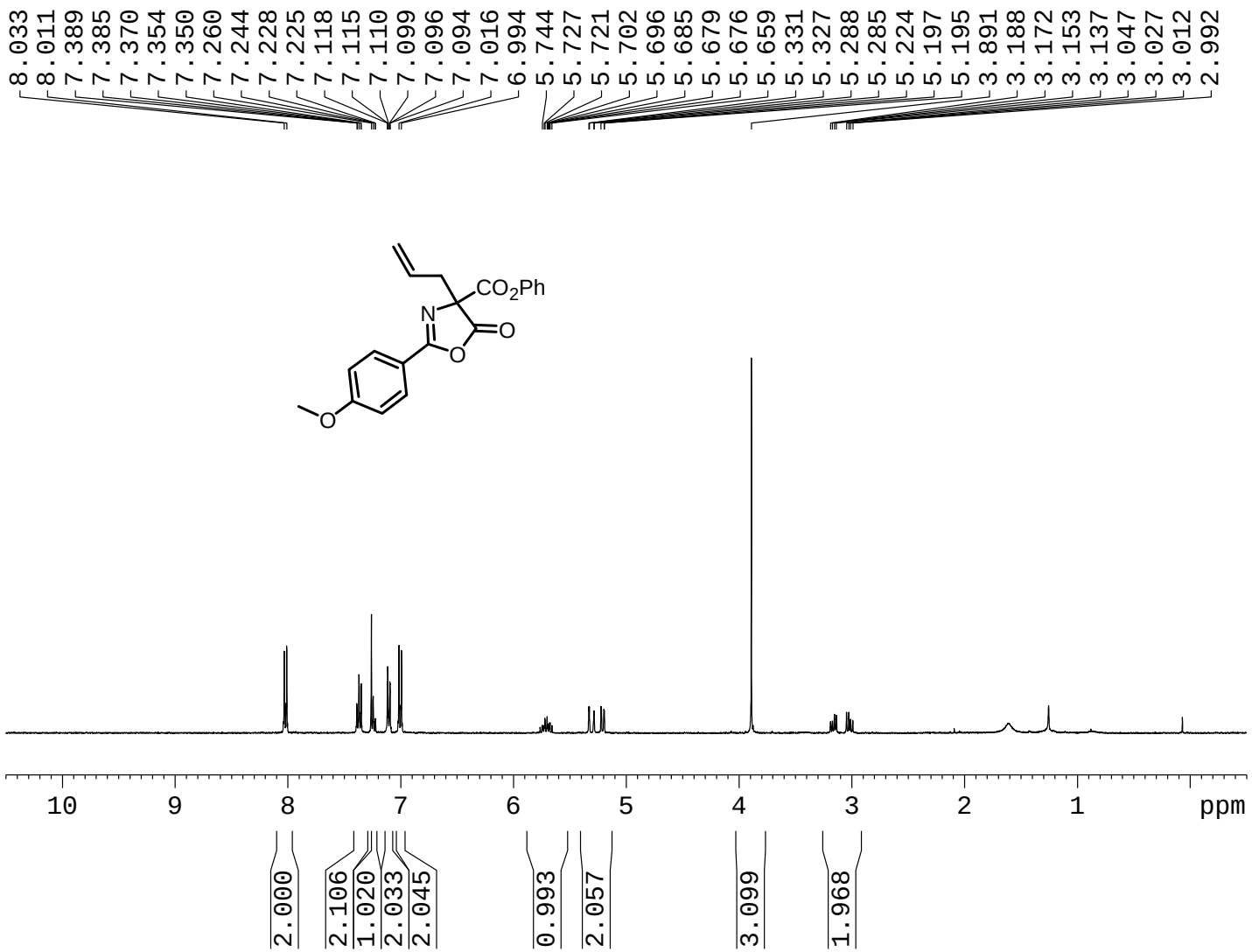
Analysis Name	D:\Data\NCTU SERVICE\Data\20140718\EtPH-P ESI+_GE2_01_2258.d	Acquisition Date	7/18/2014 9:06:49 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	EtPH-P ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

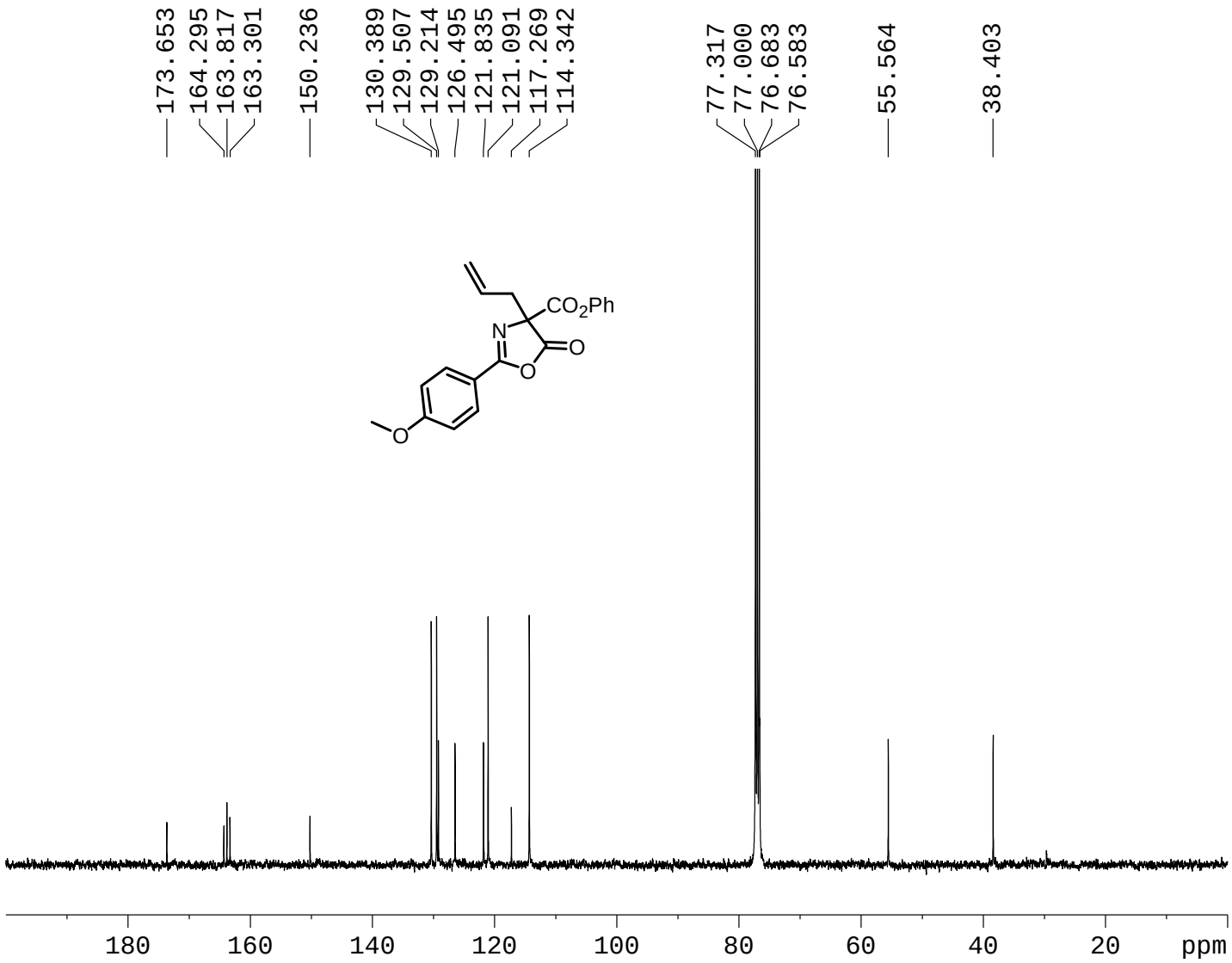
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C







NAME	140629allylPh-P	
EXPNO	1	
PROCNO	1	
Date_	20140629	
Time	11.05	
INSTRUM	spect	
PROBHD	5 mm DUL 13C-1	
PULPROG	zg30	
TD	32768	
SOLVENT	CDCl3	
NS	4	
DS	0	
SWH	6410.256	Hz
FIDRES	0.195625	Hz
AQ	2.5559540	sec
RG	4	
DW	78.000	usec
DE	6.00	usec
TE	300.0	K
D1	2.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	usec
PL1	-2.40	dB
SFO1	400.1528010	MHz
SI	16384	
SF	400.1500092	MHz
WDW	EM	
SSB	0	
LB	0.00	Hz
GB	0	
PC	1.00	



NAME	140629allylPh-P
EXPNO	13
PROCNO	1
Date_	20140629
Time	11.06
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	2743
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6177993 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

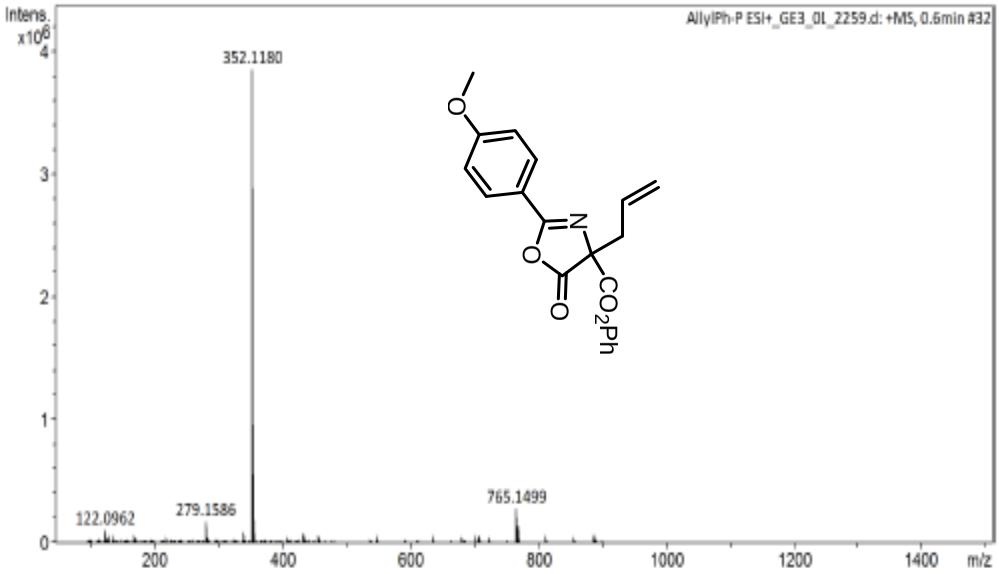
Display Report

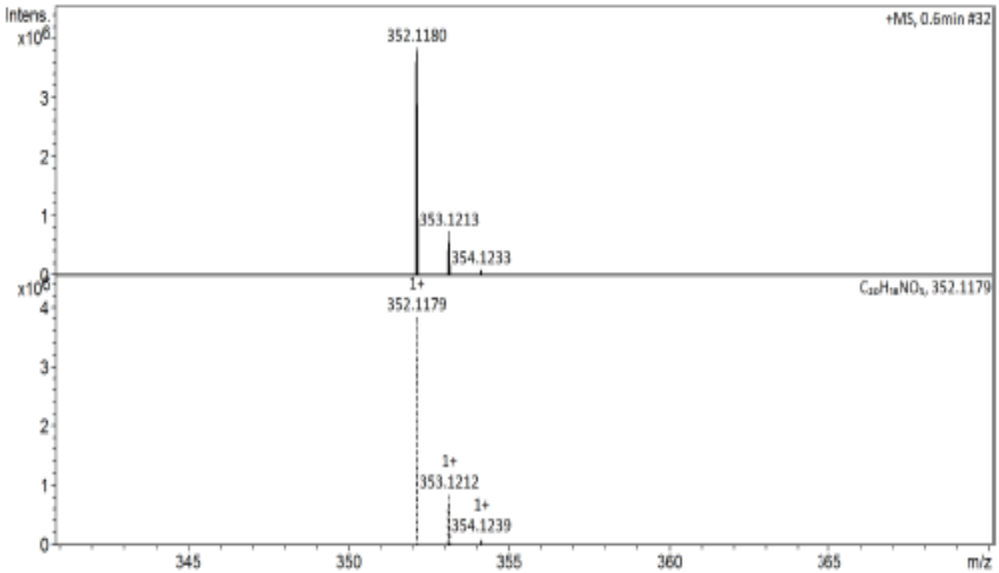
Analysis Info

Analysis Name	D:\Data\NCTU SERVICE\Data\20140718\AllylPh-P ESI+_GE3_01_2259.d	Acquisition Date	7/18/2014 9:11:08 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	AllylPh-P ESI+	Instrument	impact HD 1819696.00164
Comment			

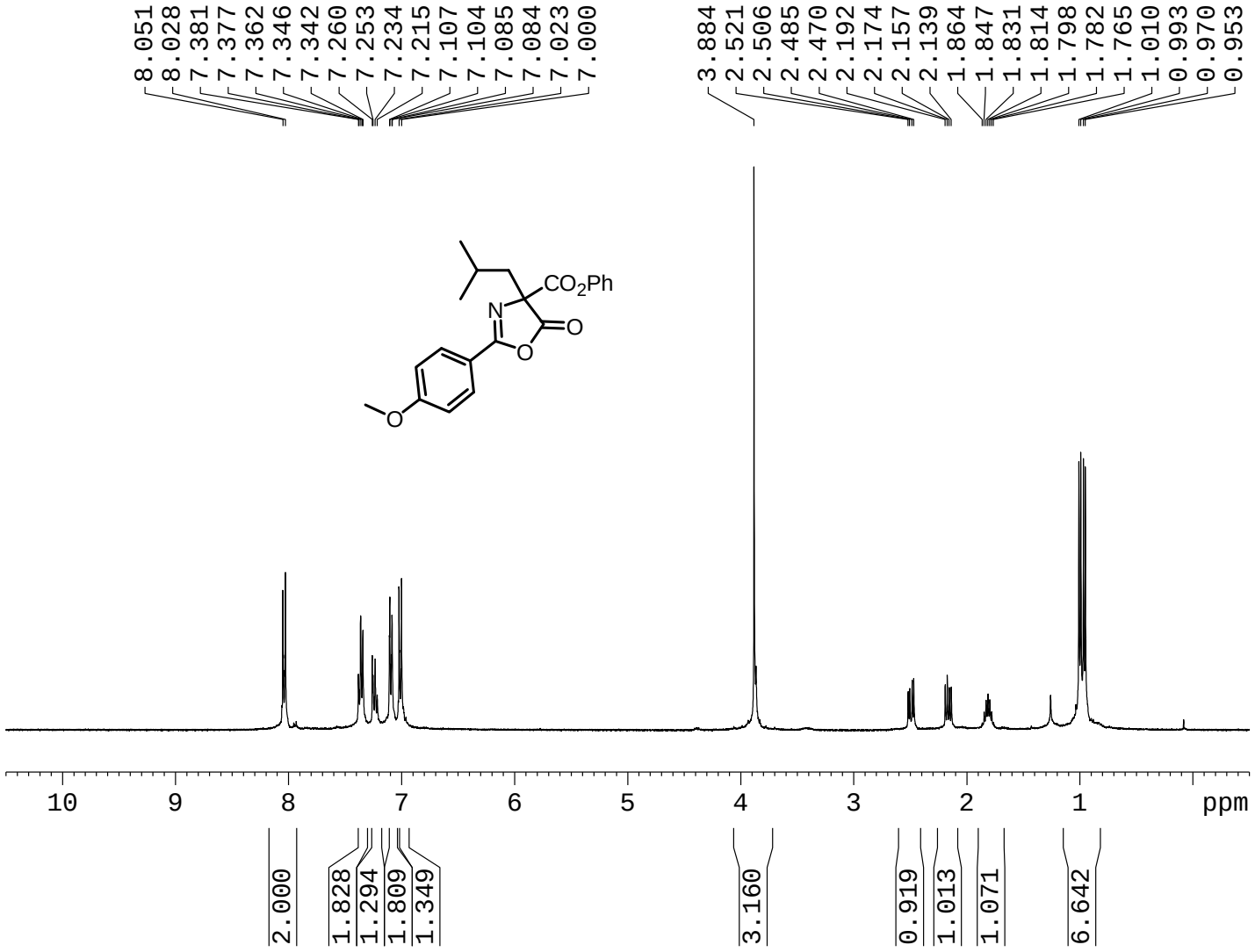
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

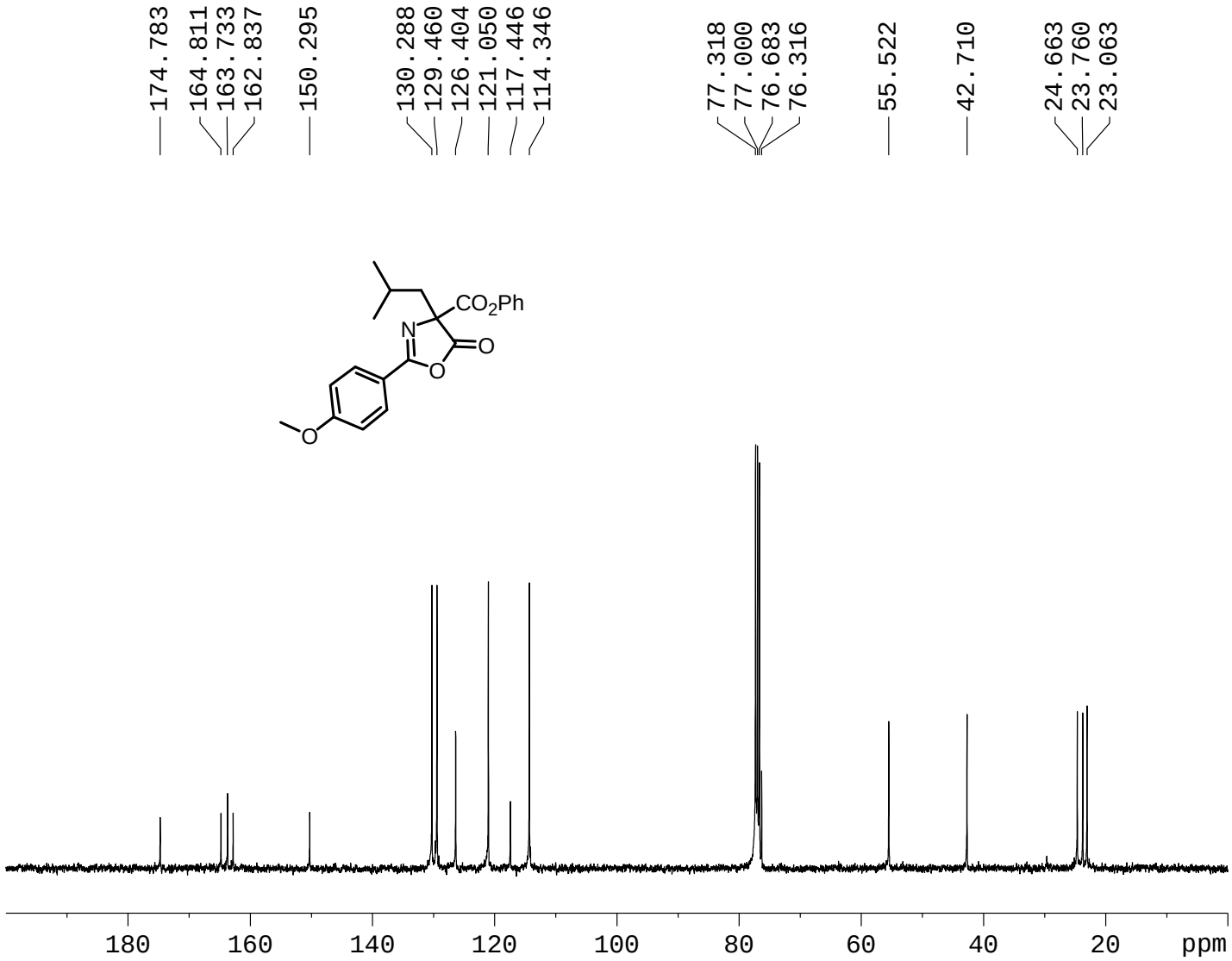




AllylPh-P ESI+_GE3_01_2259.d



NAME	140707-iBuPh-P
EXPNO	49
PROCNO	1
Date_	20140707
Time	19.11
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500094 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00




```
NAME      140707-iBuPh-P
EXPNO                13
PROCNO                1
Date_          20140707
Time              19.12
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                  564
DS                    0
SWH           22727.273 Hz
FIDRES         0.346791 Hz
AQ             1.4418420 sec
RG                   57
DW                22.000 usec
DE                 6.00 usec
TE                300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.70 usec
PL1                -0.50 dB
SFO1         100.6288660 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                -2.40 dB
PL12               15.10 dB
PL13               18.10 dB
SFO2         400.1516010 MHz
SI                 32768
SF           100.6178026 MHz
WDW                  EM
SSB                   0
LB                 3.00 Hz
GB                    0
PC                 1.00
```

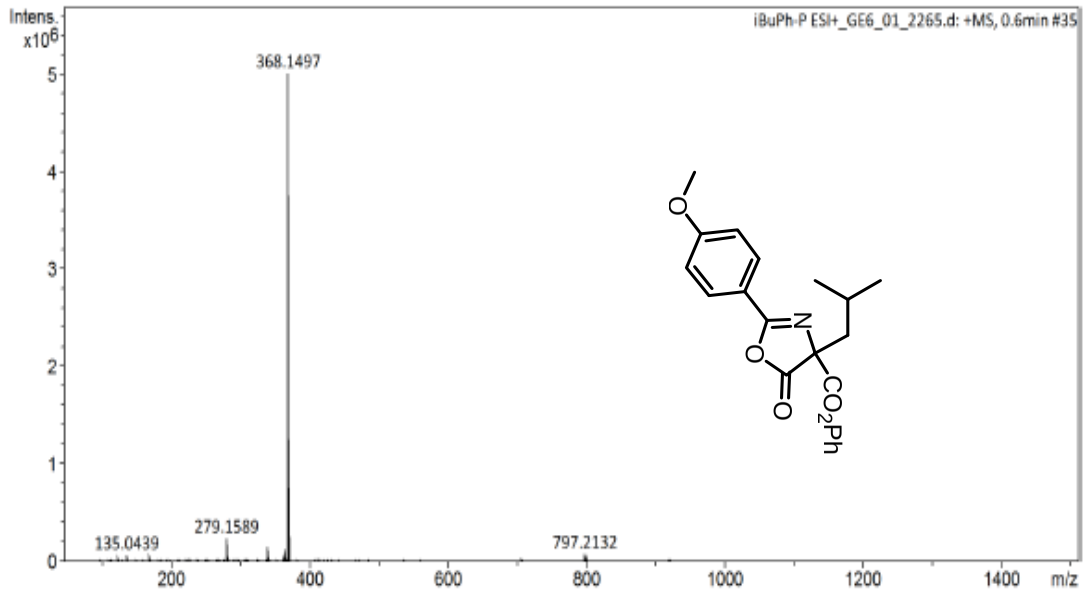
Display Report

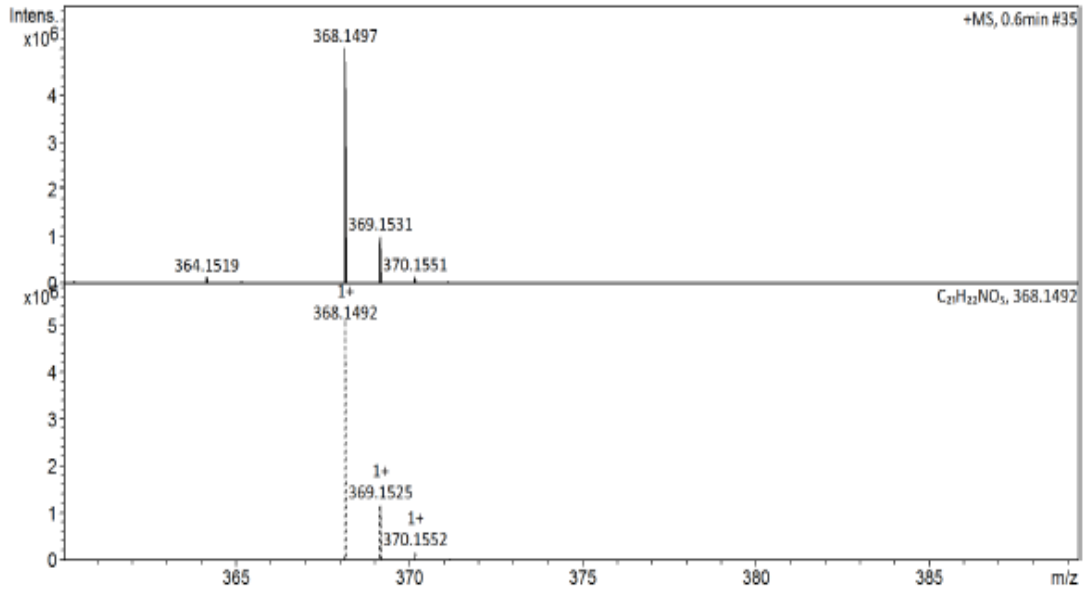
Analysis Info

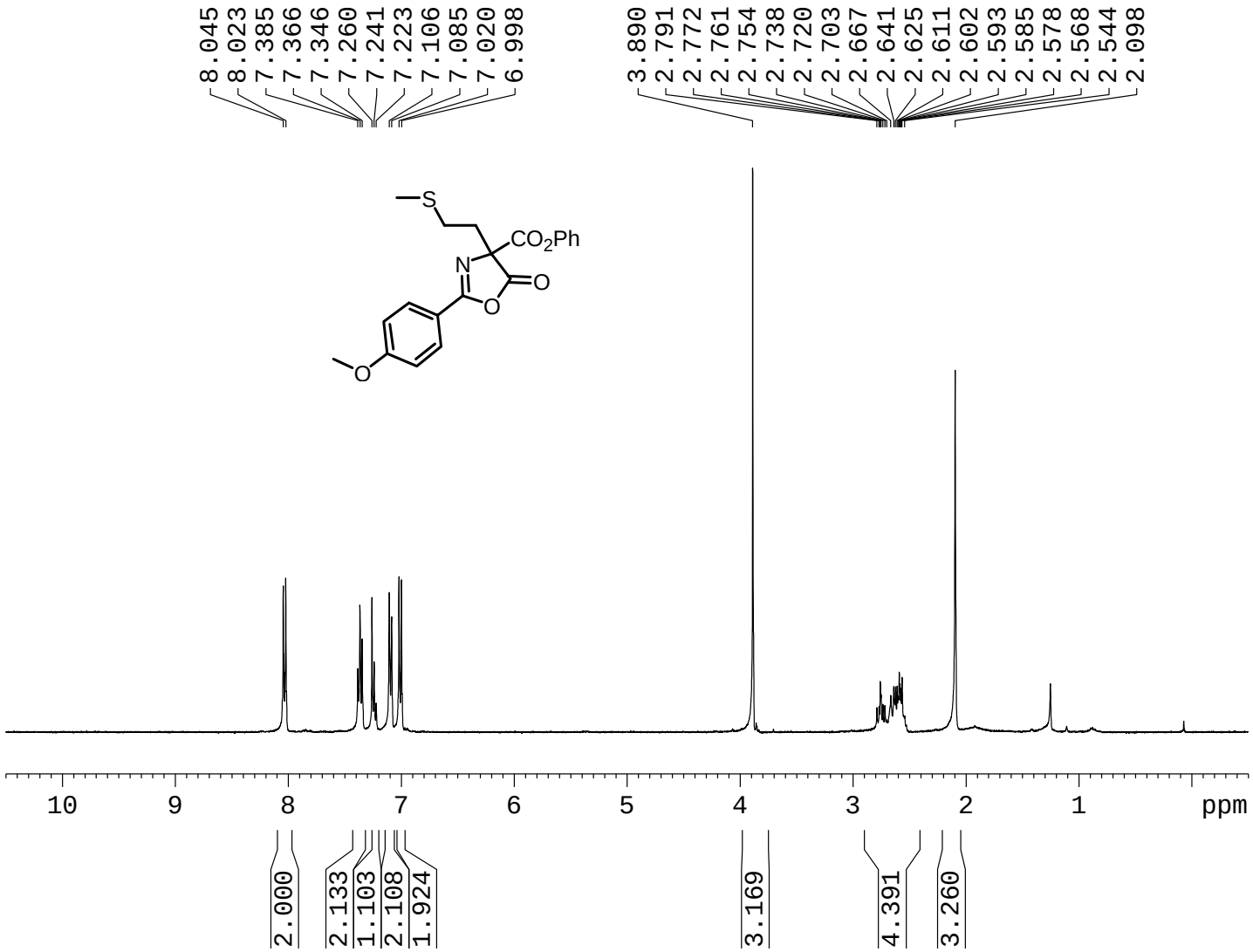
Analysis Name	D:\Data\NCTU SERVICE\Data\20140718\iBuPh-P ESI+_GE6_01_2265.d	Acquisition Date	7/18/2014 10:00:19 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	iBuPh-P ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

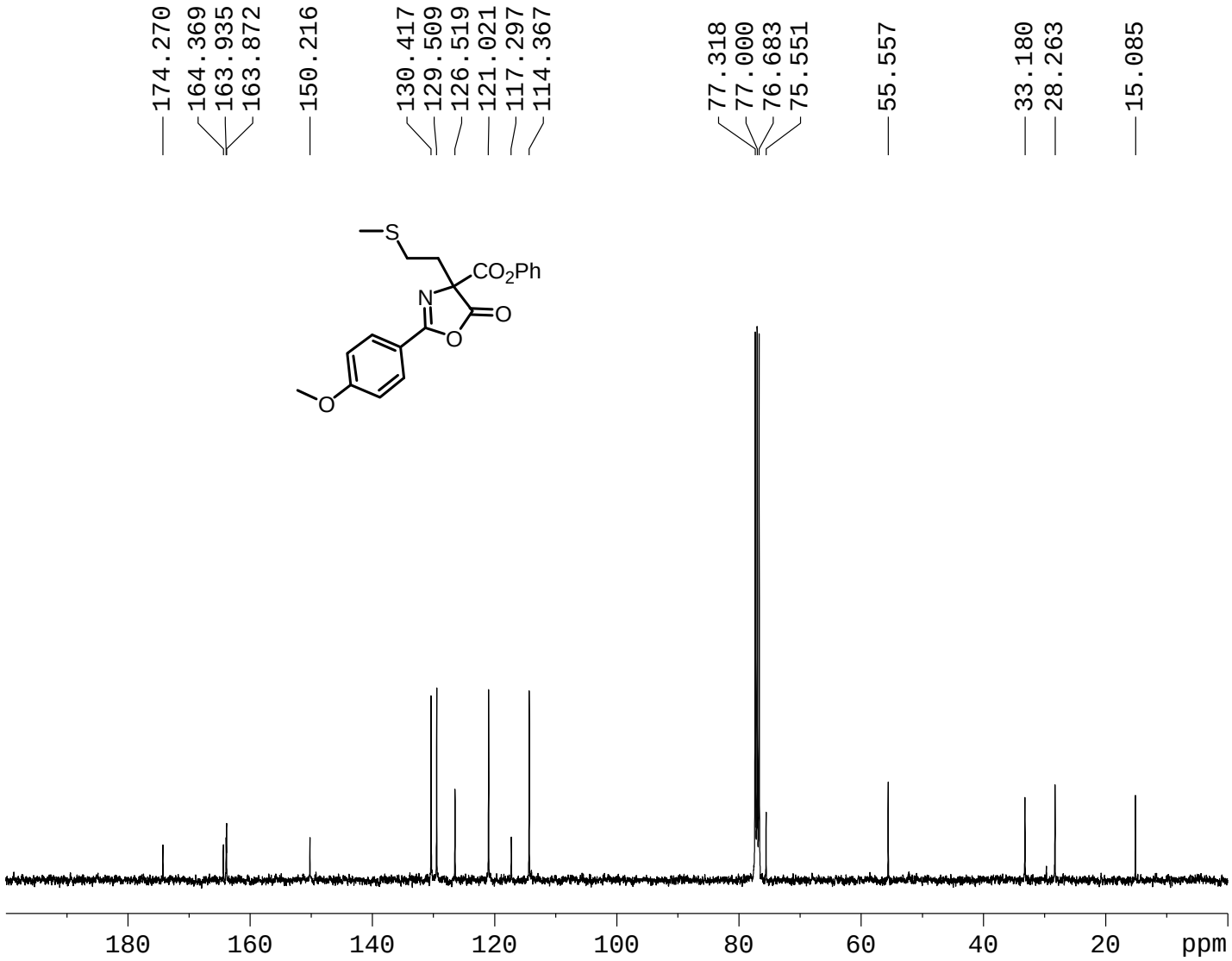
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C







NAME	140714-SMePh-P	
EXPNO	1	
PROCNO	1	
Date_	20140714	
Time	20.16	
INSTRUM	spect	
PROBHD	5 mm DUL 13C-1	
PULPROG	zg30	
TD	32768	
SOLVENT	CDCl3	
NS	4	
DS	0	
SWH	6410.256	Hz
FIDRES	0.195625	Hz
AQ	2.5559540	sec
RG	4	
DW	78.000	usec
DE	6.00	usec
TE	300.0	K
D1	2.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	usec
PL1	-2.40	dB
SFO1	400.1528010	MHz
SI	16384	
SF	400.1500096	MHz
WDW	EM	
SSB	0	
LB	0.00	Hz
GB	0	
PC	1.00	




```
NAME        140714-SMePh-P
EXPNO                   13
PROCNO                   1
Date_             20140714
Time                 20.17
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     508
DS                       0
SWH              22727.273 Hz
FIDRES            0.346791 Hz
AQ                1.4418420 sec
RG                      57
DW                  22.000 usec
DE                   6.00 usec
TE                  300.0 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    13C
P1                    9.70 usec
PL1                  -0.50 dB
SFO1           100.6288660 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  -2.40 dB
PL12                 15.10 dB
PL13                 18.10 dB
SFO2           400.1516010 MHz
SI                   32768
SF             100.6178010 MHz
WDW                     EM
SSB                      0
LB                    3.00 Hz
GB                       0
PC                    1.00
```

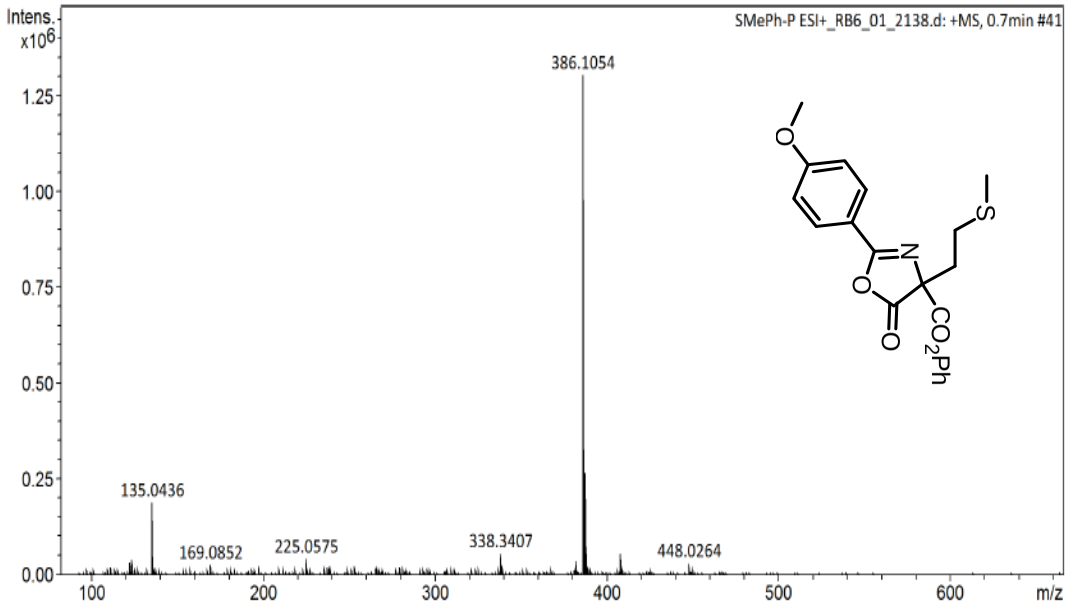
Display Report

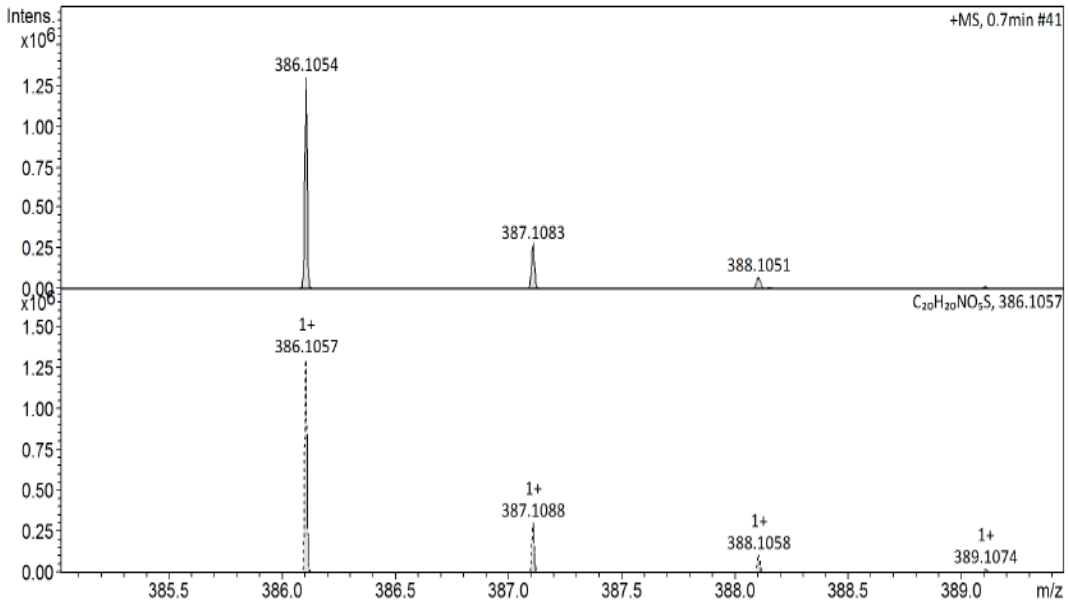
Analysis Info

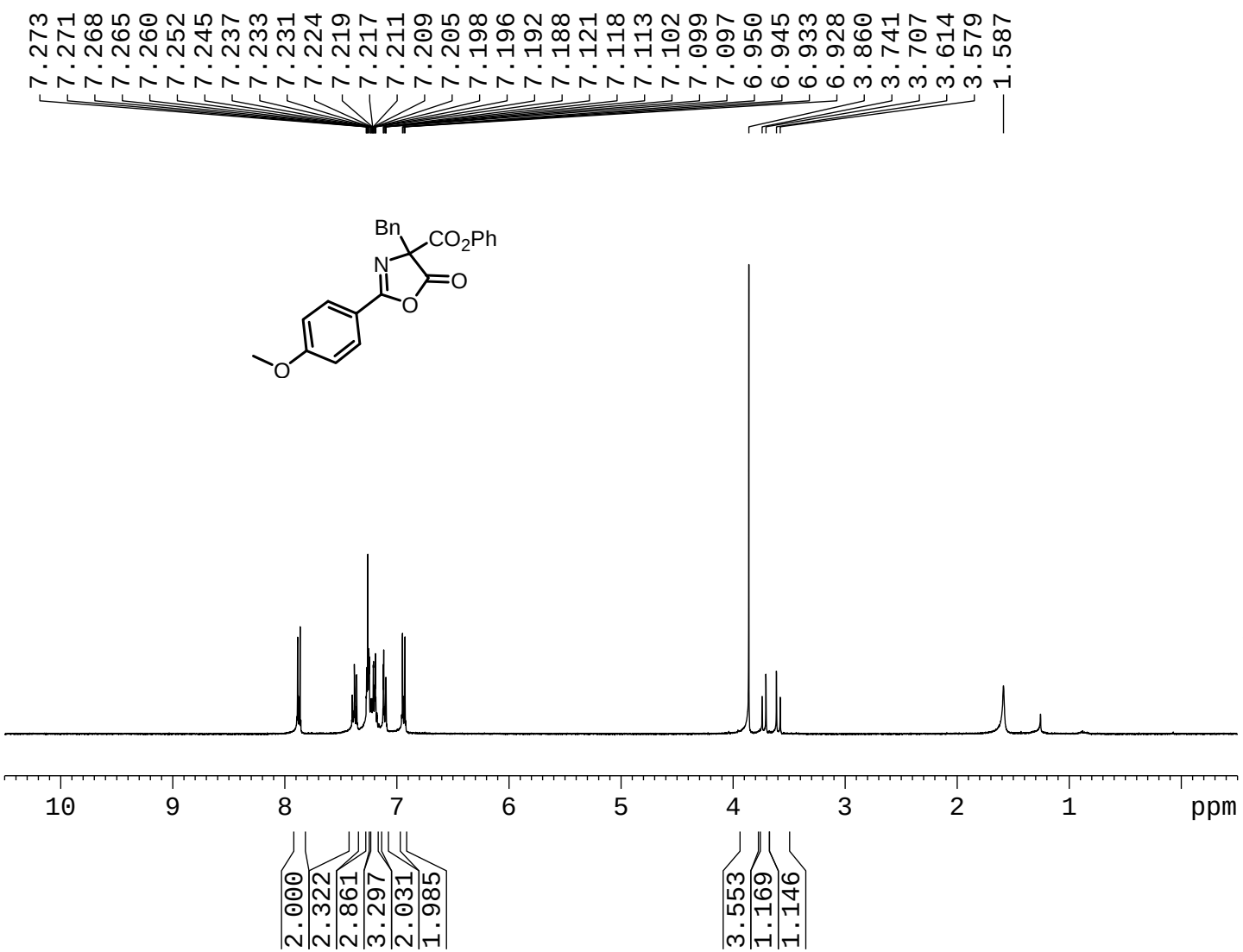
Analysis Name	D:\Data\NCTU SERVICE\Data\20140704\SMePh-P ESI+_RB6_01_2138.d	Acquisition Date	7/4/2014 9:58:14 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	SMePh-P ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

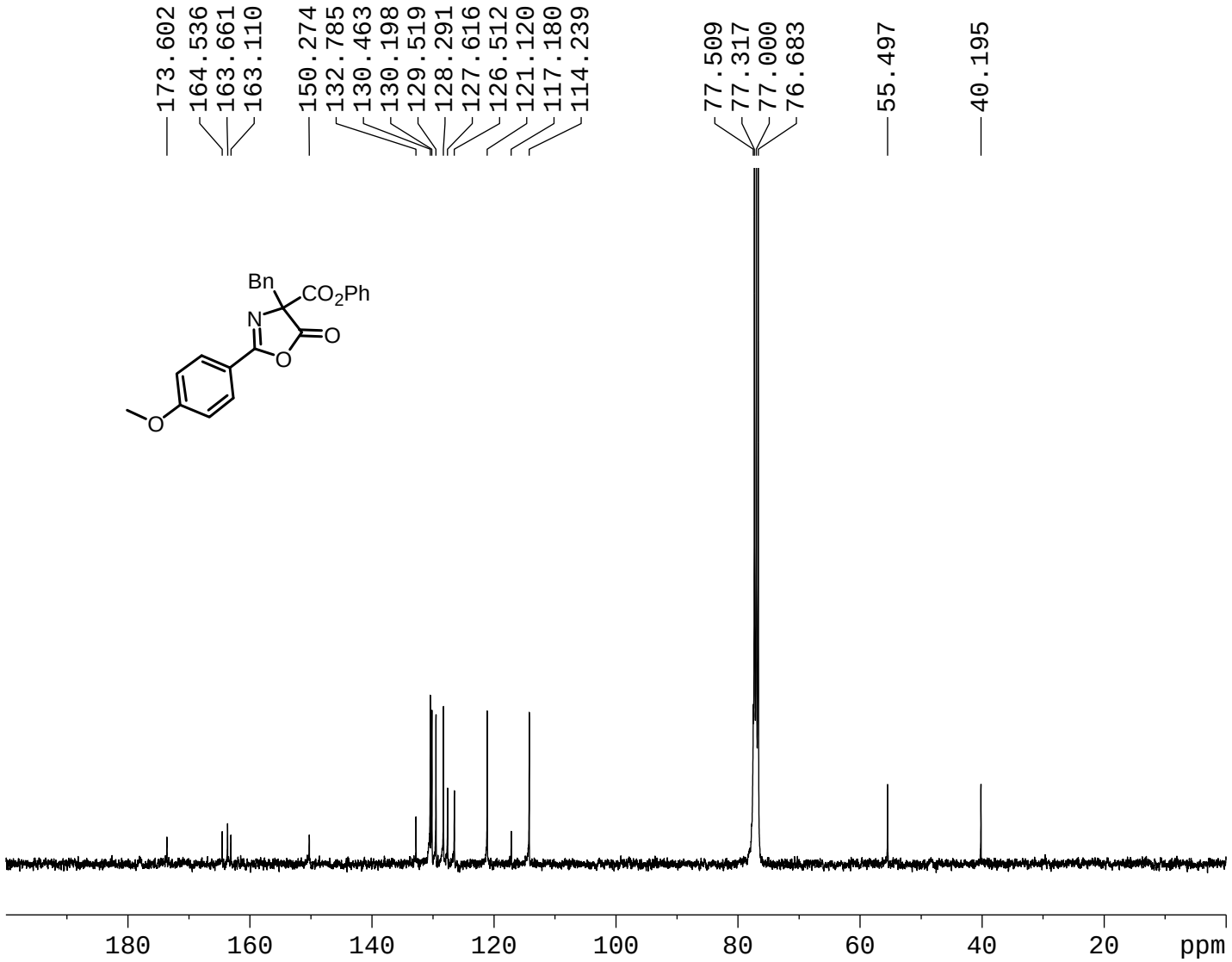
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C







NAME	150331BnPh-P	
EXPNO	1	
PROCNO	1	
Date_	20150331	
Time	13.27	
INSTRUM	spect	
PROBHD	5 mm DUL 13C-1	
PULPROG	zg30	
TD	32768	
SOLVENT	CDCl3	
NS	8	
DS	0	
SWH	6410.256	Hz
FIDRES	0.195625	Hz
AQ	2.5559540	sec
RG	4	
DW	78.000	usec
DE	6.00	usec
TE	300.0	K
D1	2.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	10.00	usec
PL1	-2.40	dB
SFO1	400.1528010	MHz
SI	16384	
SF	400.1500088	MHz
WDW	EM	
SSB	0	
LB	0.00	Hz
GB	0	
PC	1.00	



NAME	150331BnPh-P
EXPNO	13
PROCNO	1
Date_	20150331
Time	13.28
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	2634
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6177995 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

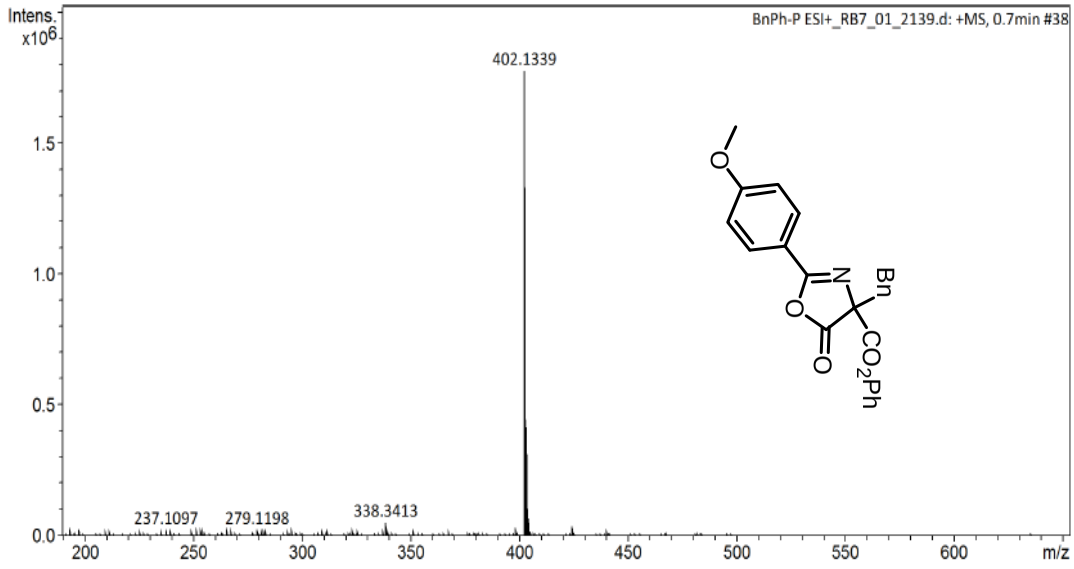
Display Report

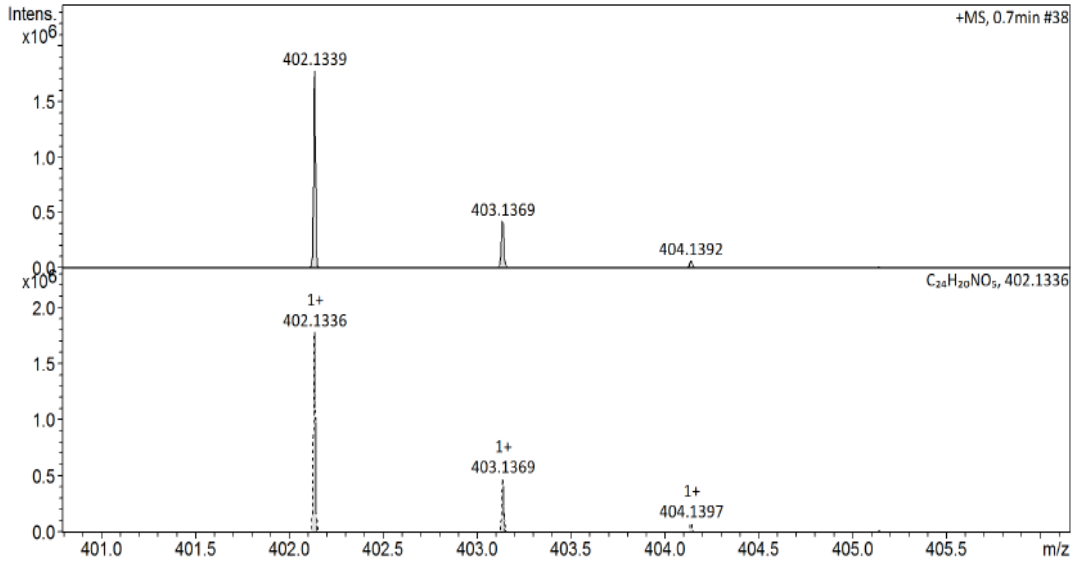
Analysis Info

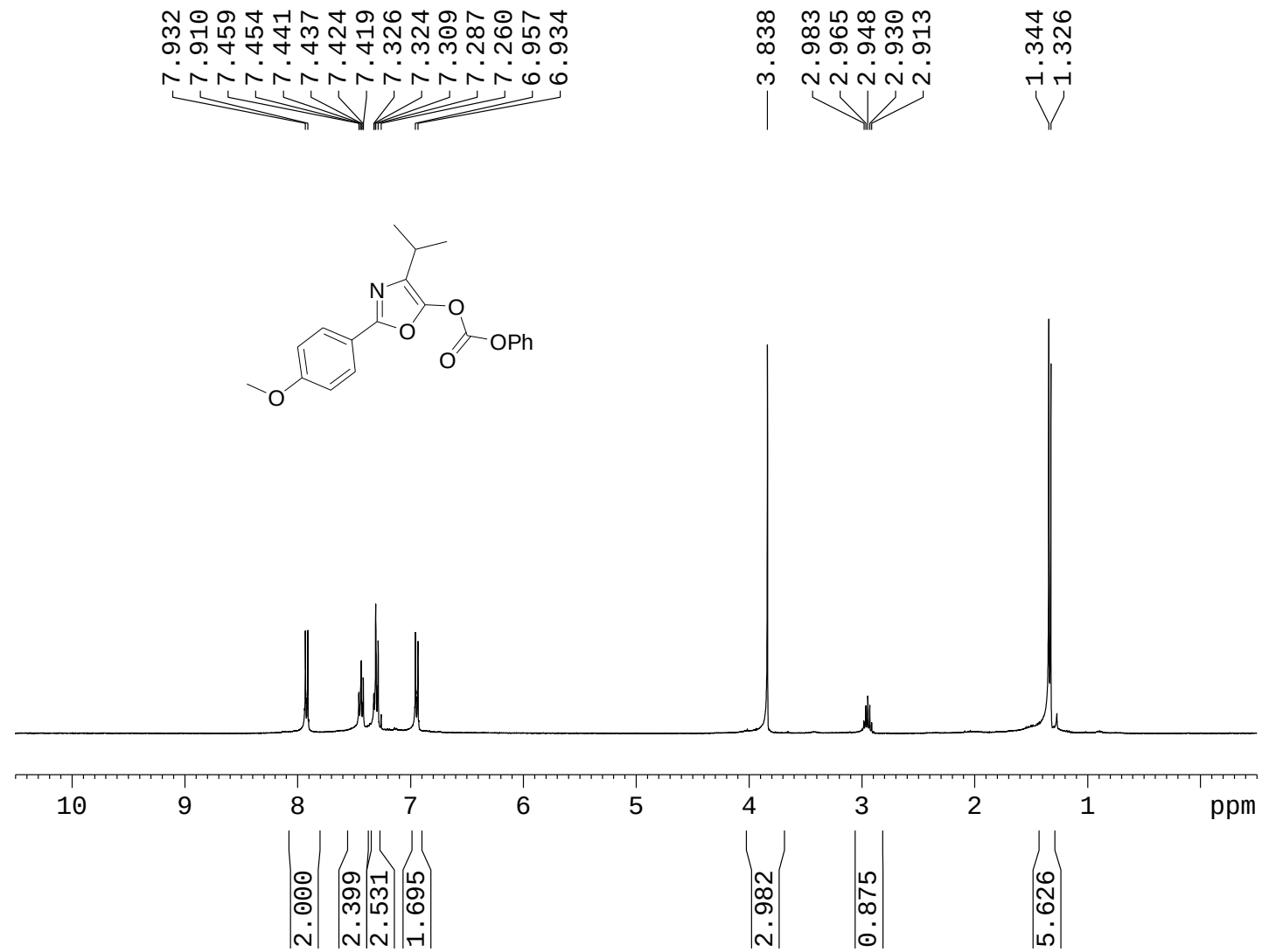
Analysis Name	D:\Data\NCTU SERVICE\Data\20140704\BnPh-P ESI+_RB7_01_2139.d	Acquisition Date	7/4/2014 10:02:36 AM
Method	Small molecule.m	Operator	NCTU
Sample Name	BnPh-P ESI+	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

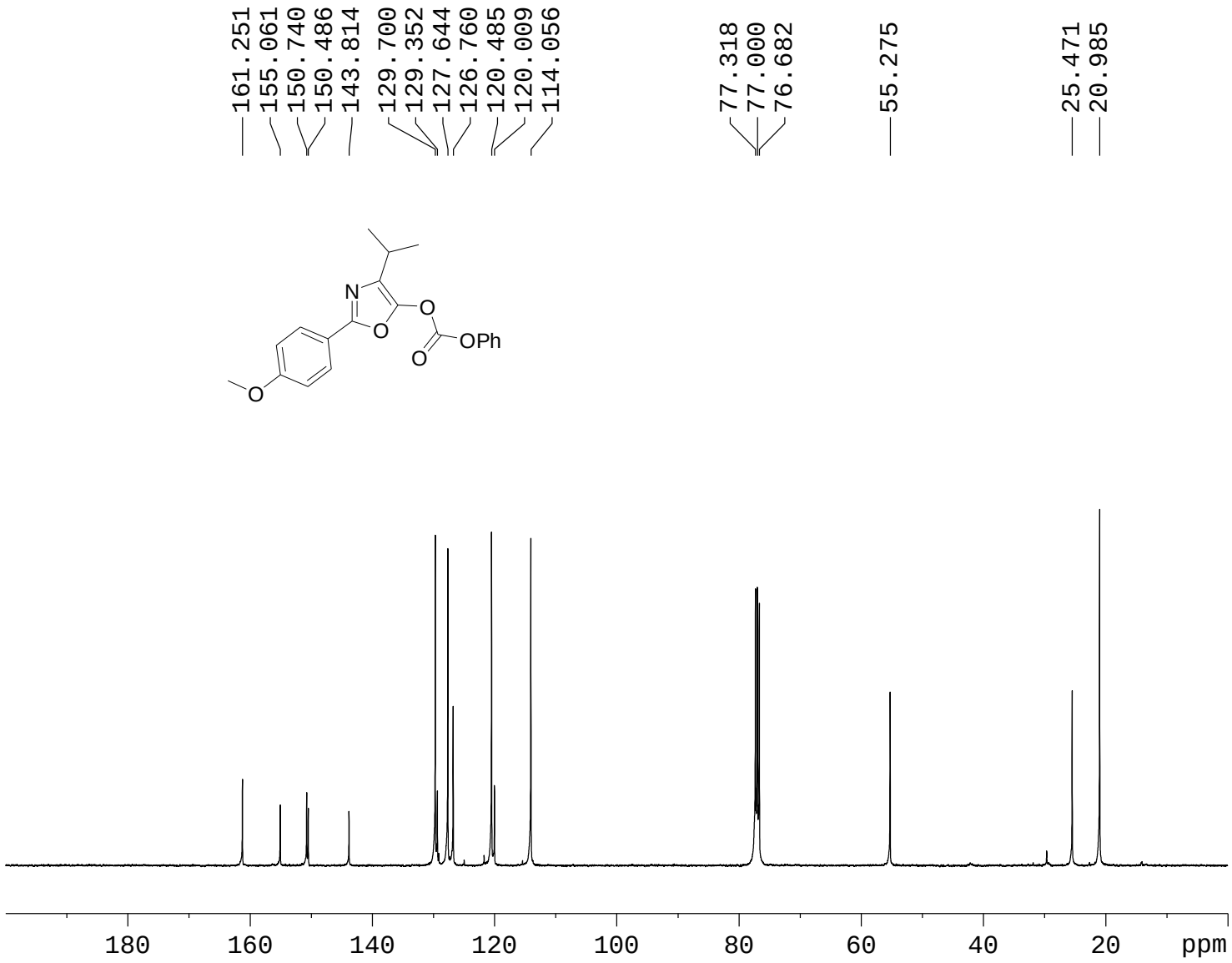
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C







NAME	160710-IPrPh
EXPNO	2
PROCNO	1
Date_	20160712
Time	1.02
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500085 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	160710-IPrPh	
EXPNO	14	
PROCNO	1	
Date_	20160712	
Time	1.03	
INSTRUM	spect	
PROBHD	5 mm DUL 13C-1	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	6864	
DS	0	
SWH	22727.273	Hz
FIDRES	0.346791	Hz
AQ	1.4418420	sec
RG	57	
DW	22.000	usec
DE	6.00	usec
TE	300.0	K
D1	2.00000000	sec
d11	0.03000000	sec
DELTA	1.89999998	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.70	usec
PL1	-0.50	dB
SFO1	100.6288660	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	90.00	usec
PL2	-2.40	dB
PL12	15.10	dB
PL13	18.10	dB
SFO2	400.1516010	MHz
SI	32768	
SF	100.6178052	MHz
WDW	EM	
SSB	0	
LB	3.00	Hz
GB	0	
PC	1.00	

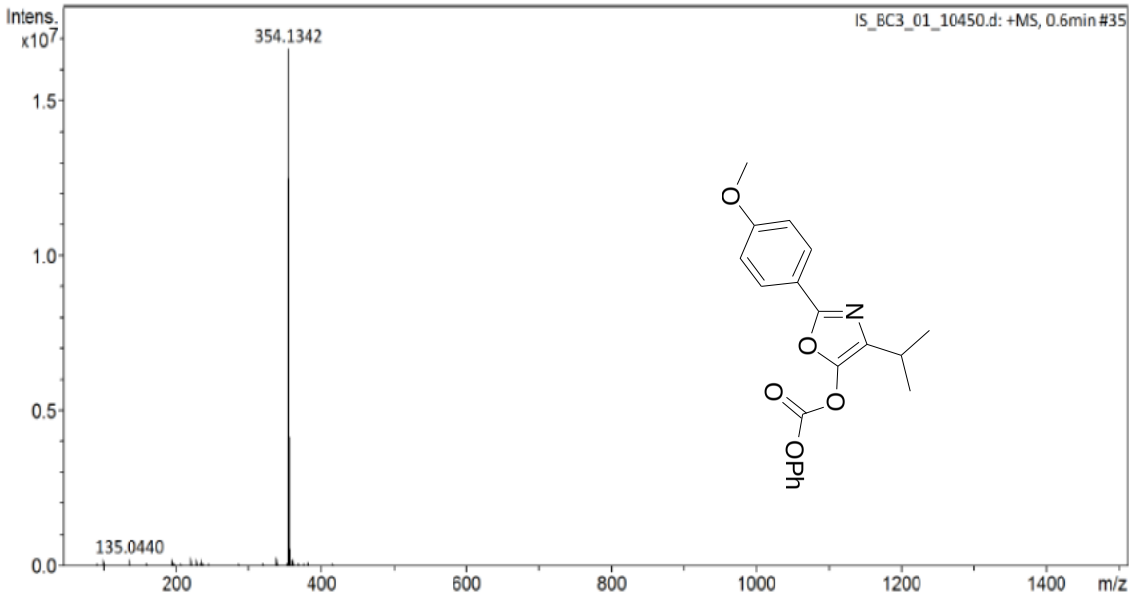
Display Report

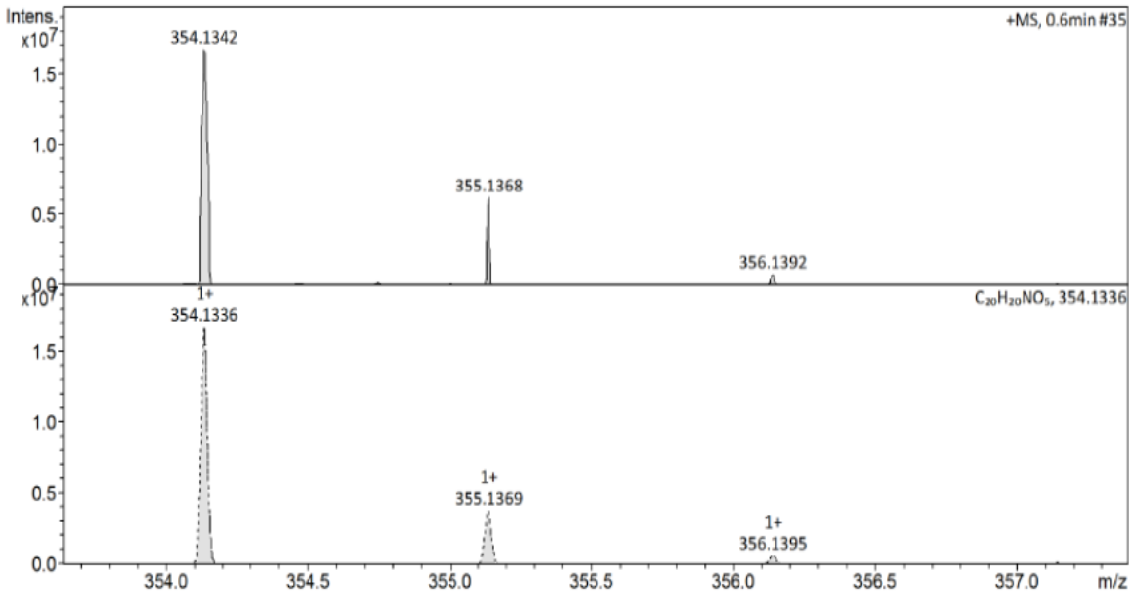
Analysis Info

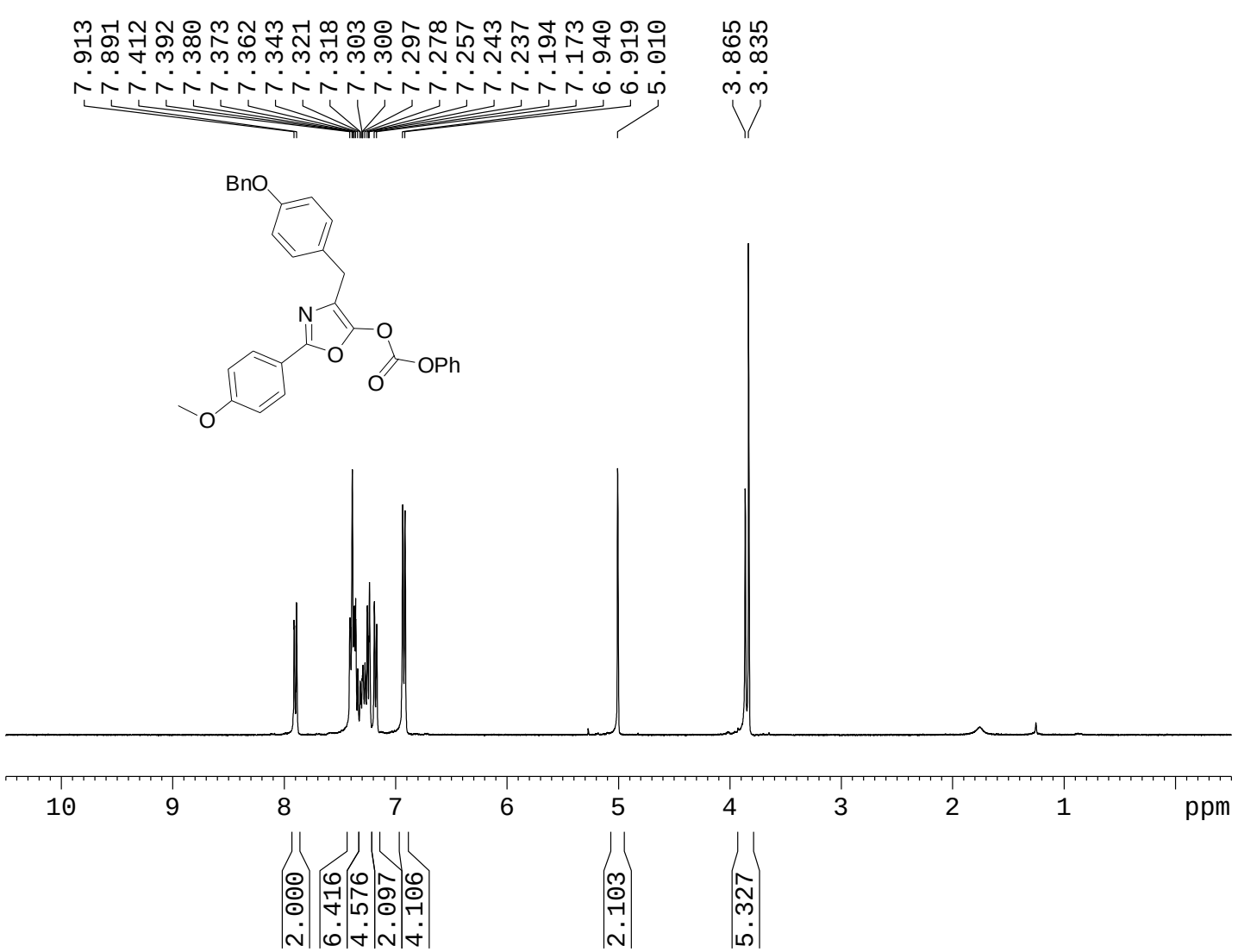
Analysis Name	D:\Data\nctu service\data\2016\20160712\IS_BC3_01_10450.d	Acquisition Date	7/12/2016 12:08:55 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	IS	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

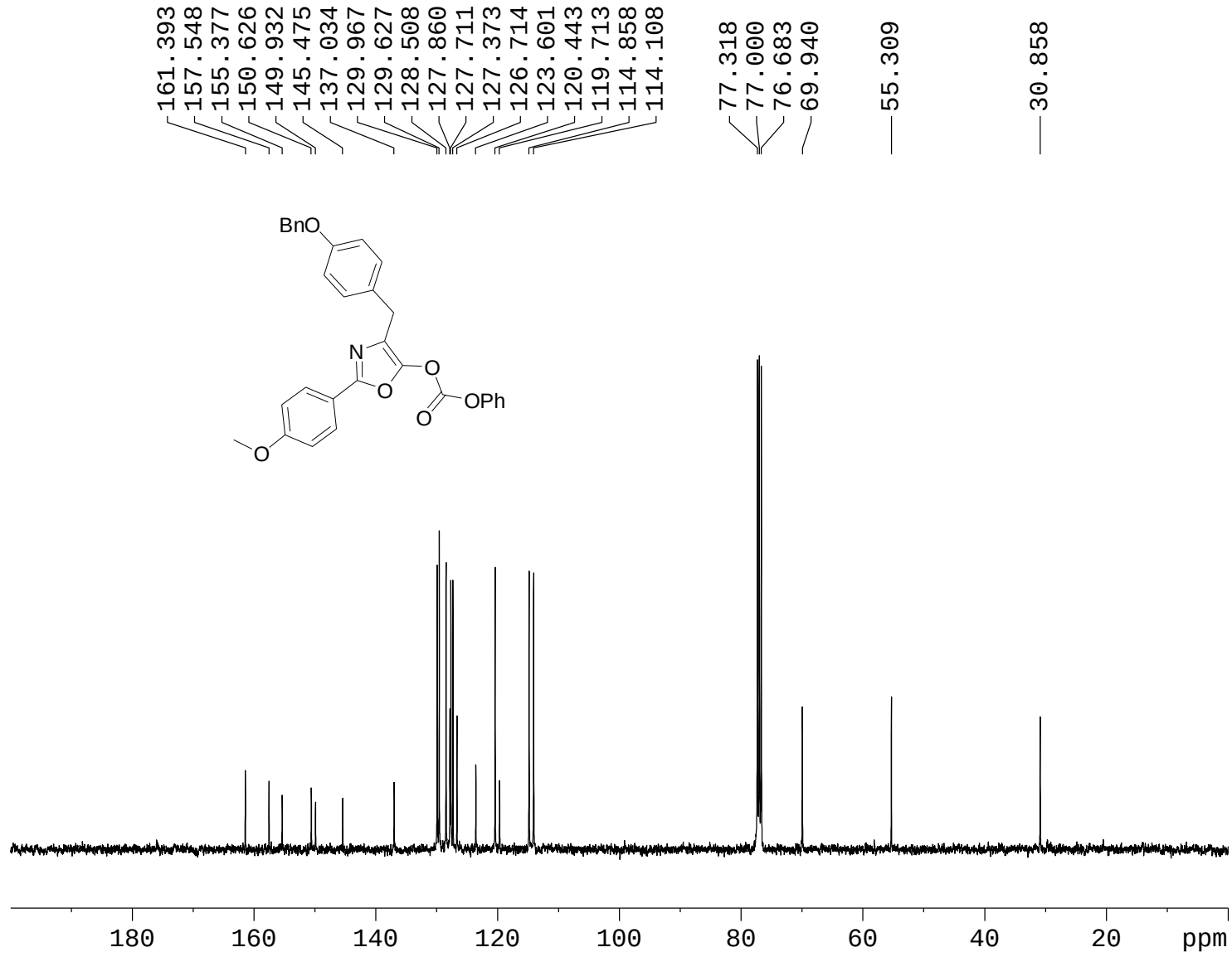
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C







NAME	160717-BnOBnPh
EXPNO	2
PROCNO	1
Date_	20160718
Time	1.24
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	4
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500168 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	160717-BnOBnPh
EXPNO	13
PROCNO	1
Date_	20160717
Time	0.28
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	245
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6178062 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

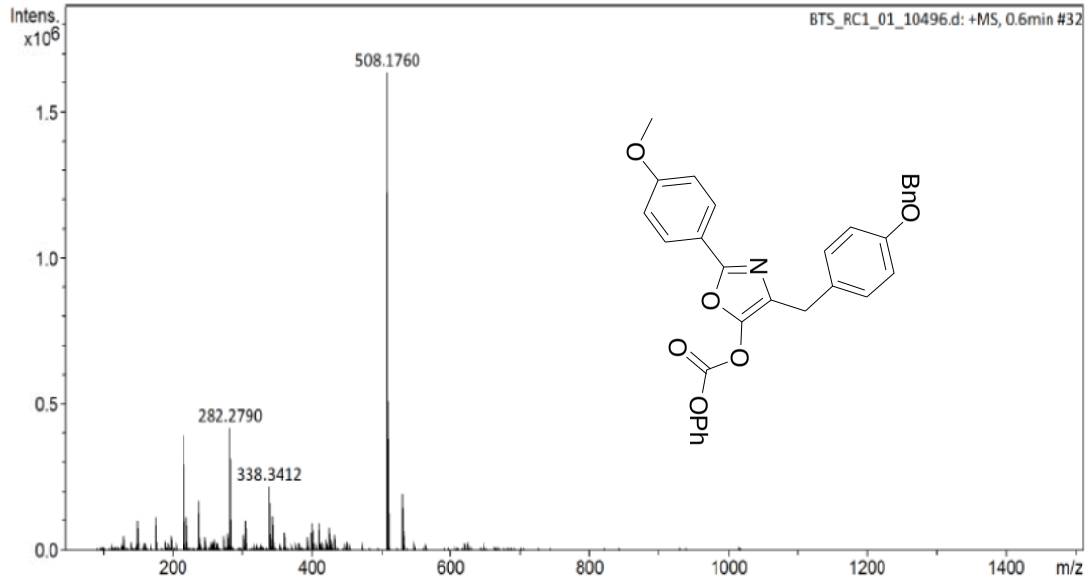
Display Report

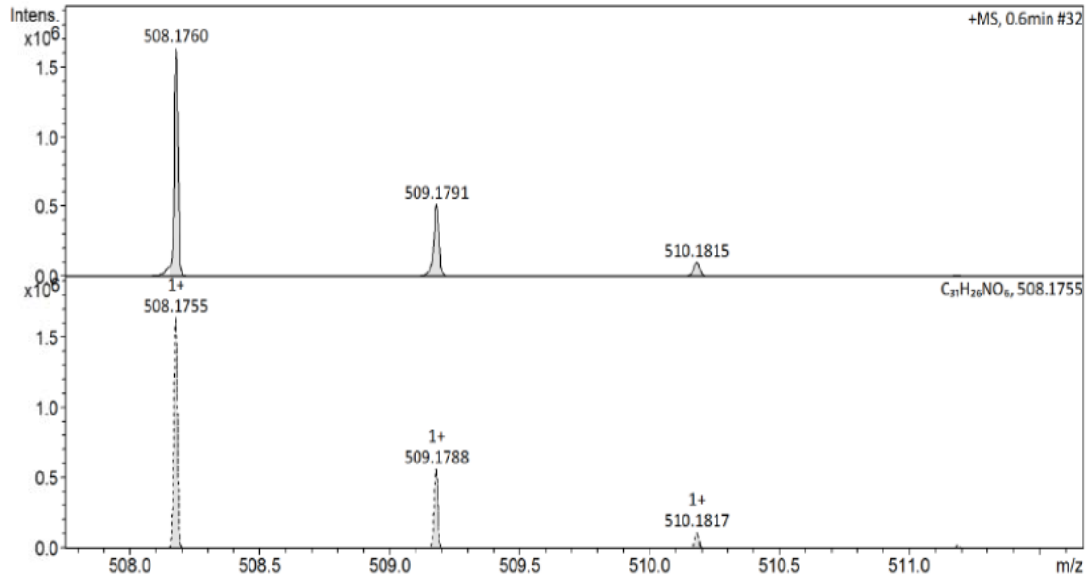
Analysis Info

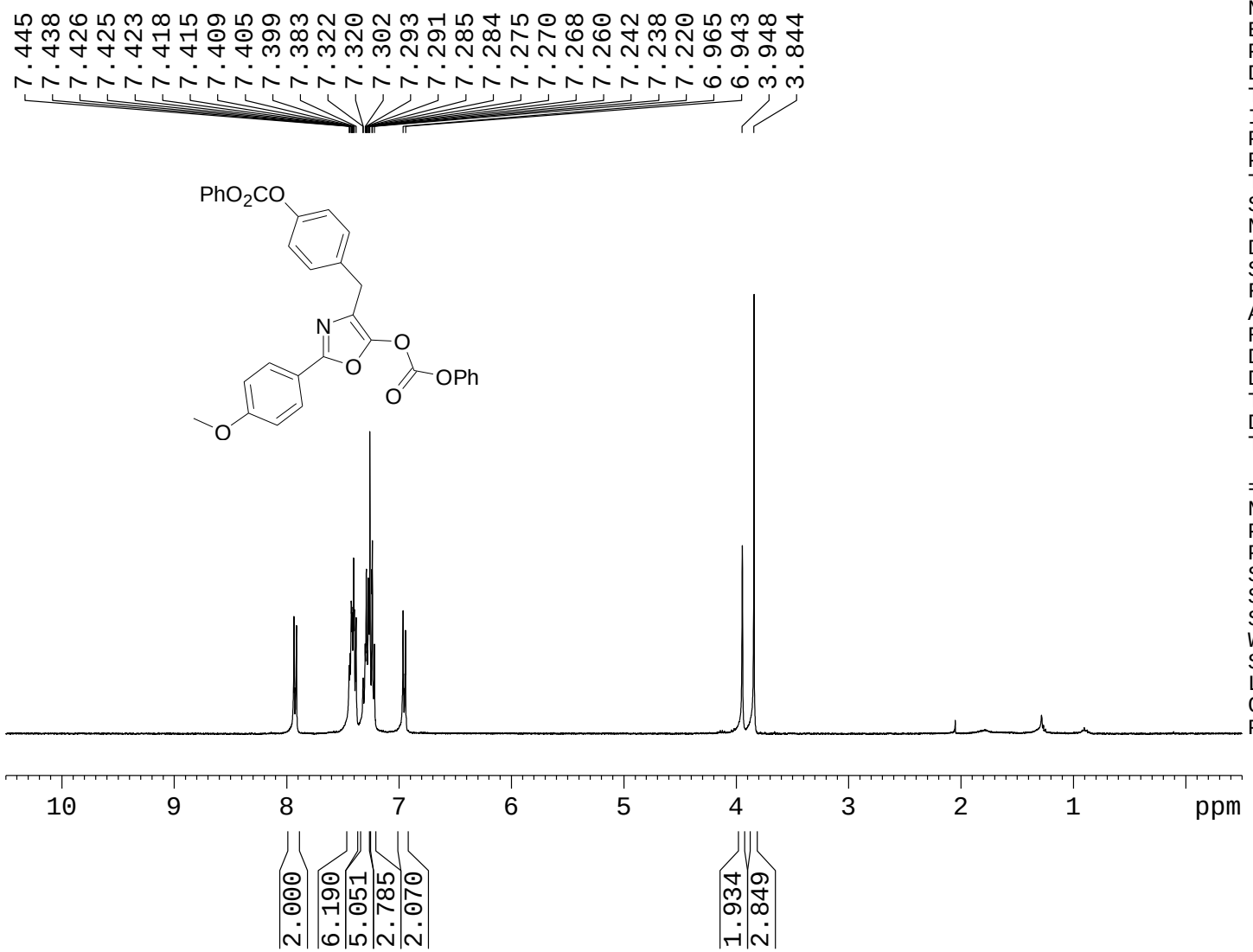
Analysis Name	D:\Data\nctu service\data\2016\20160719\BTS_RC1_01_10496.d	Acquisition Date	7/19/2016 12:04:47 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	BTS	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

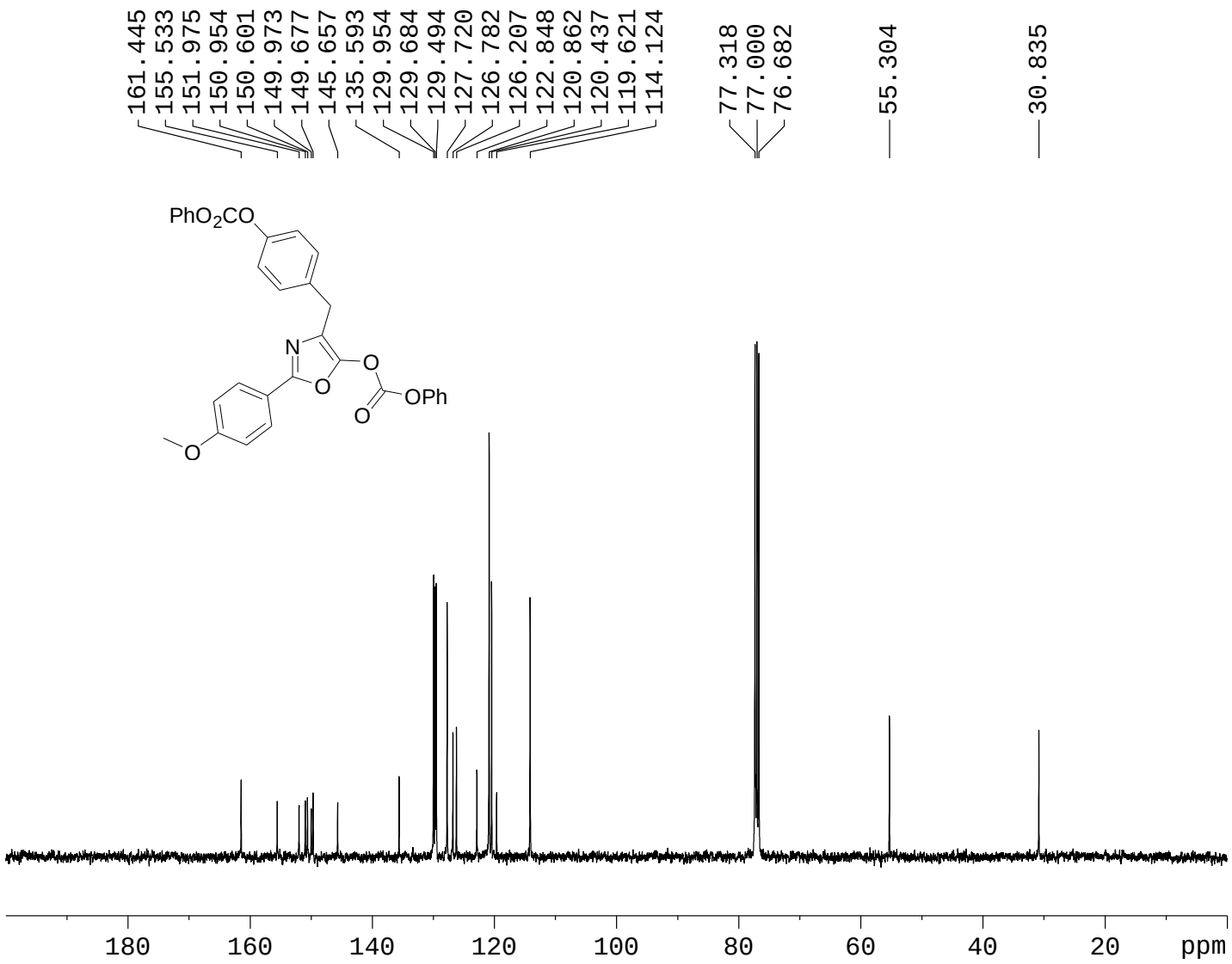
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C







NAME	160713-PhOCO2BnPh
EXPNO	2
PROCNO	1
Date_	20160713
Time	7.48
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500084 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	160713-PhOCO2BnPh	
EXPNO	14	
PROCNO	1	
Date_	20160713	
Time	7.49	
INSTRUM	spect	
PROBHD	5 mm DUL 13C-1	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	217	
DS	0	
SWH	22727.273	Hz
FIDRES	0.346791	Hz
AQ	1.4418420	sec
RG	57	
DW	22.000	usec
DE	6.00	usec
TE	300.0	K
D1	2.00000000	sec
d11	0.03000000	sec
DELTA	1.89999998	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.70	usec
PL1	-0.50	dB
SFO1	100.6288660	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	90.00	usec
PL2	-2.40	dB
PL12	15.10	dB
PL13	18.10	dB
SFO2	400.1516010	MHz
SI	32768	
SF	100.6178067	MHz
WDW	EM	
SSB	0	
LB	3.00	Hz
GB	0	
PC	1.00	

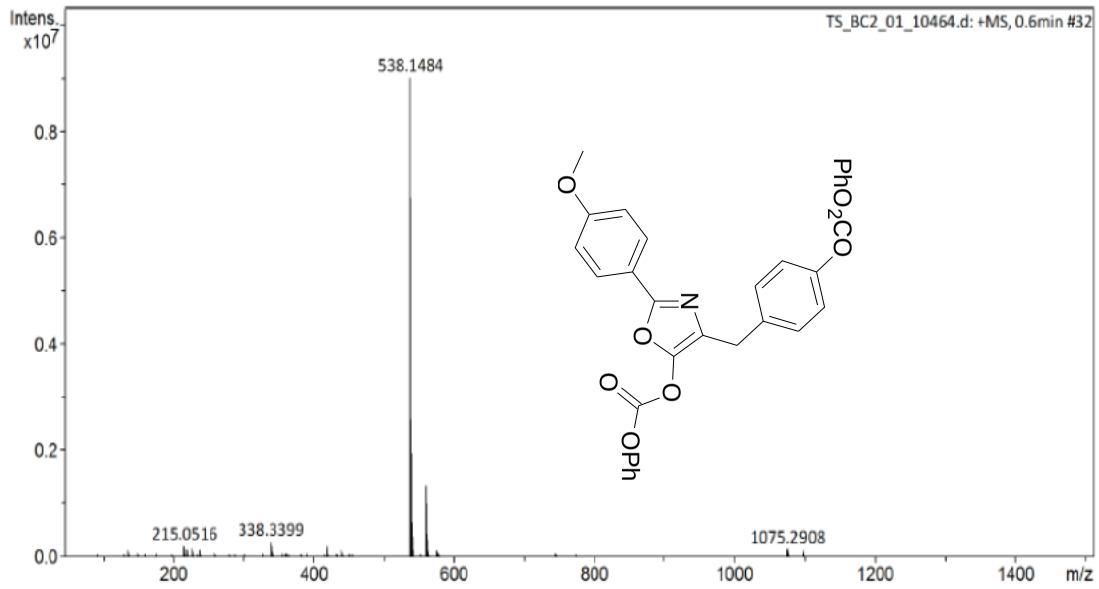
Display Report

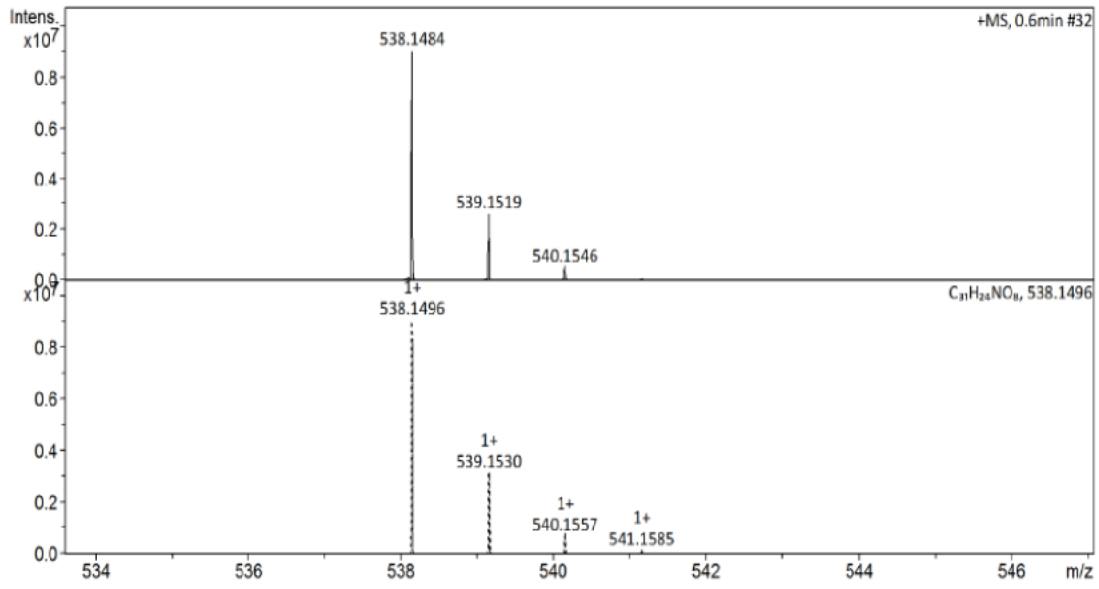
Analysis Info

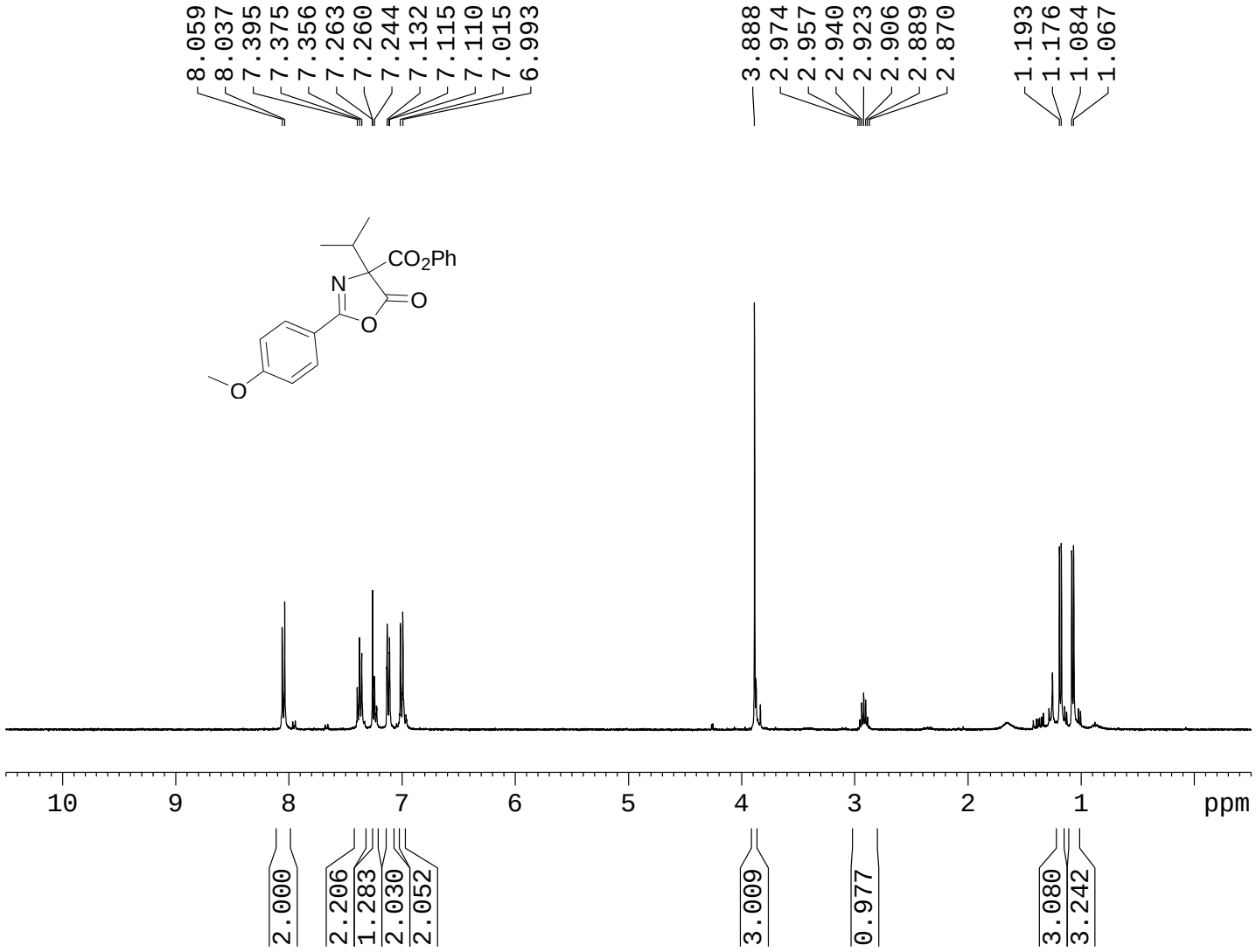
Acquisition Date	7/15/2016 11:51:59 AM		
Analysis Name	D:\Data\nctu service\data\2016\20160715\TS_BC2_01_10464.d		
Method	Small molecule.m	Operator	NCTU
Sample Name	TS	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

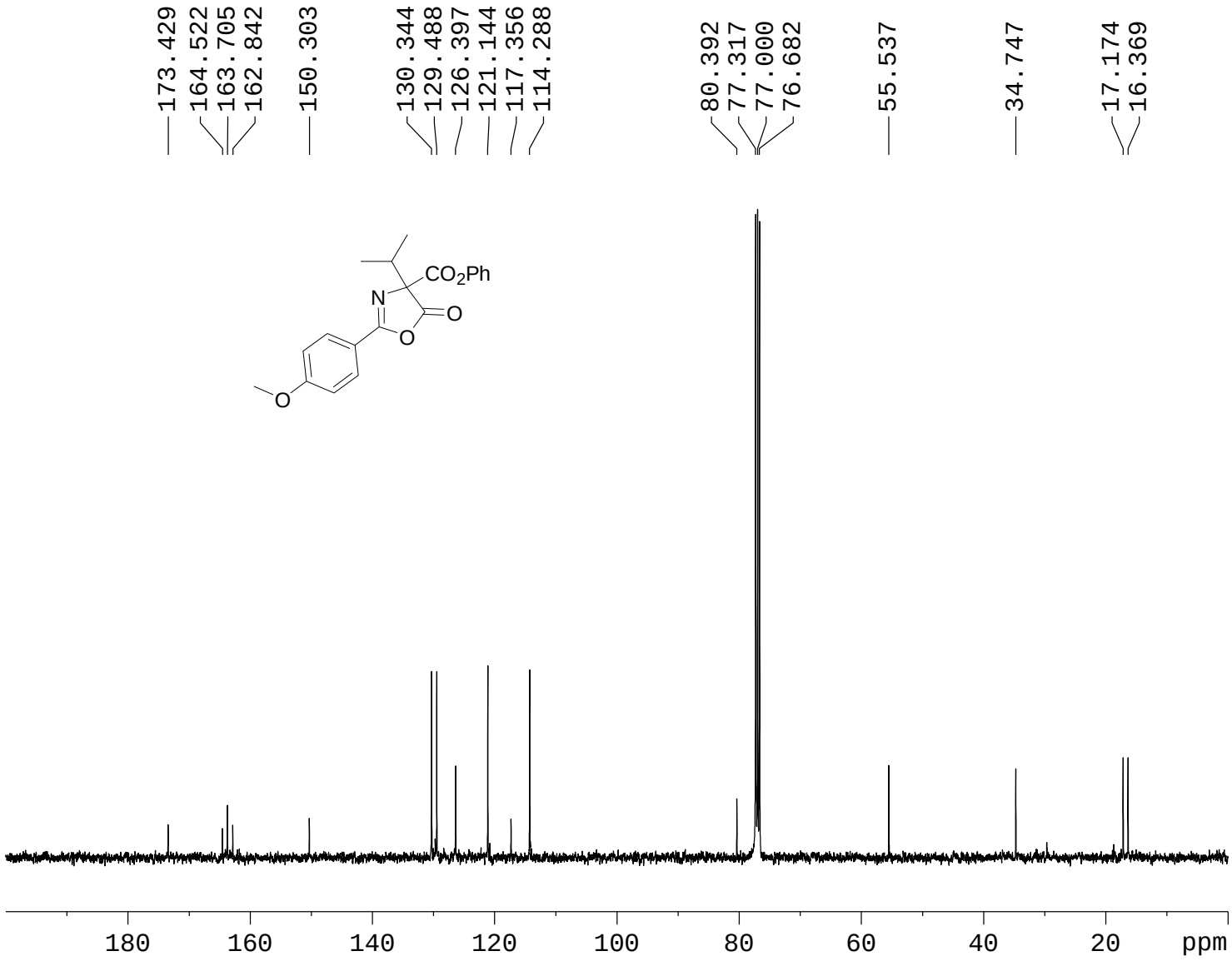
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C







NAME	160712-IPrPh-P
EXPNO	5
PROCNO	1
Date_	20160719
Time	2.36
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500096 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	160712-IPrPh-P
EXPNO	15
PROCNO	1
Date_	20160719
Time	2.38
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	340
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6178007 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

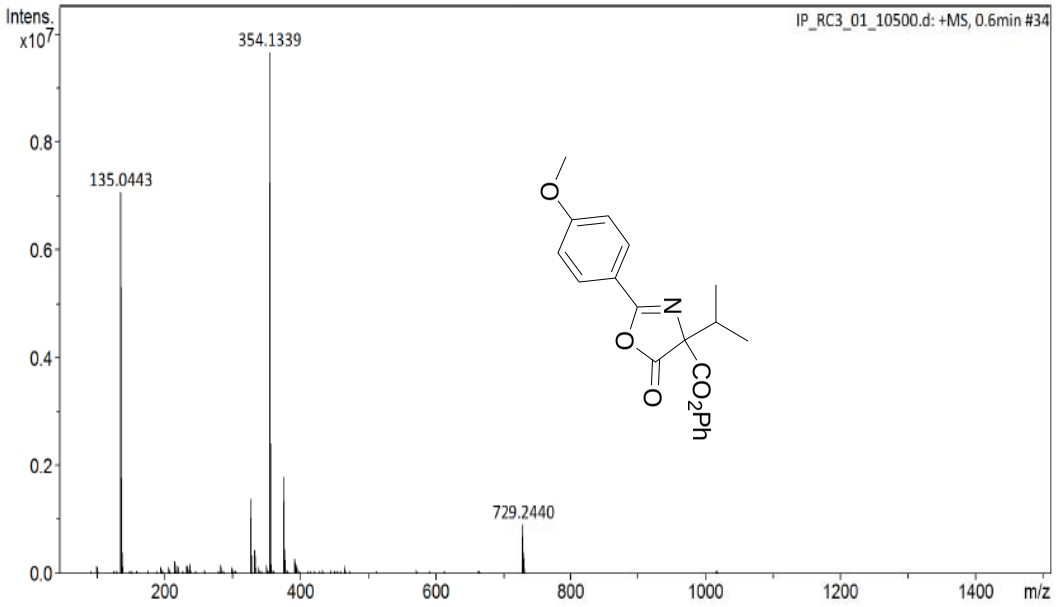
Display Report

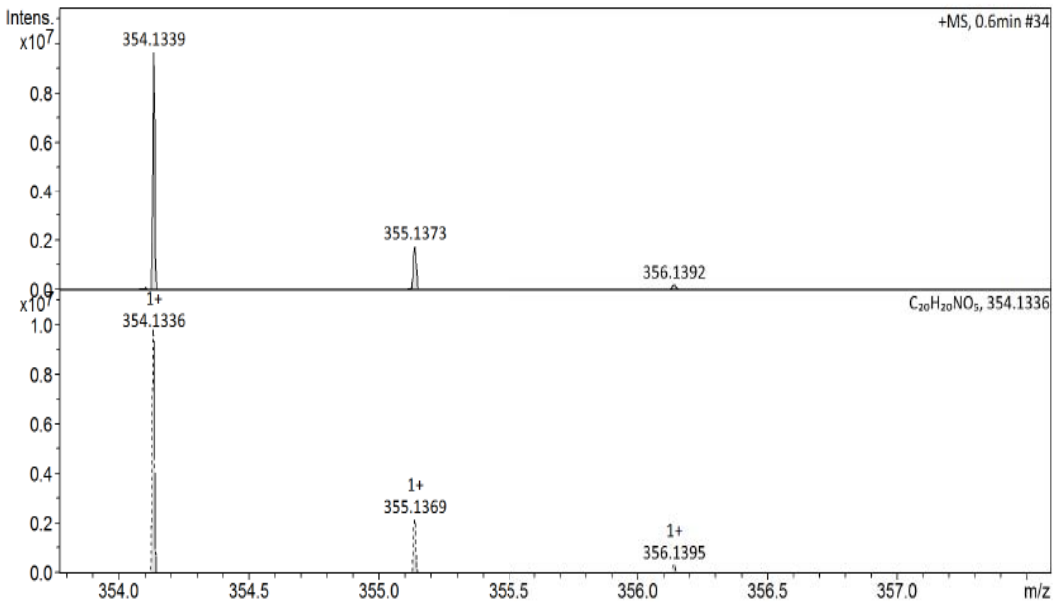
Analysis Info

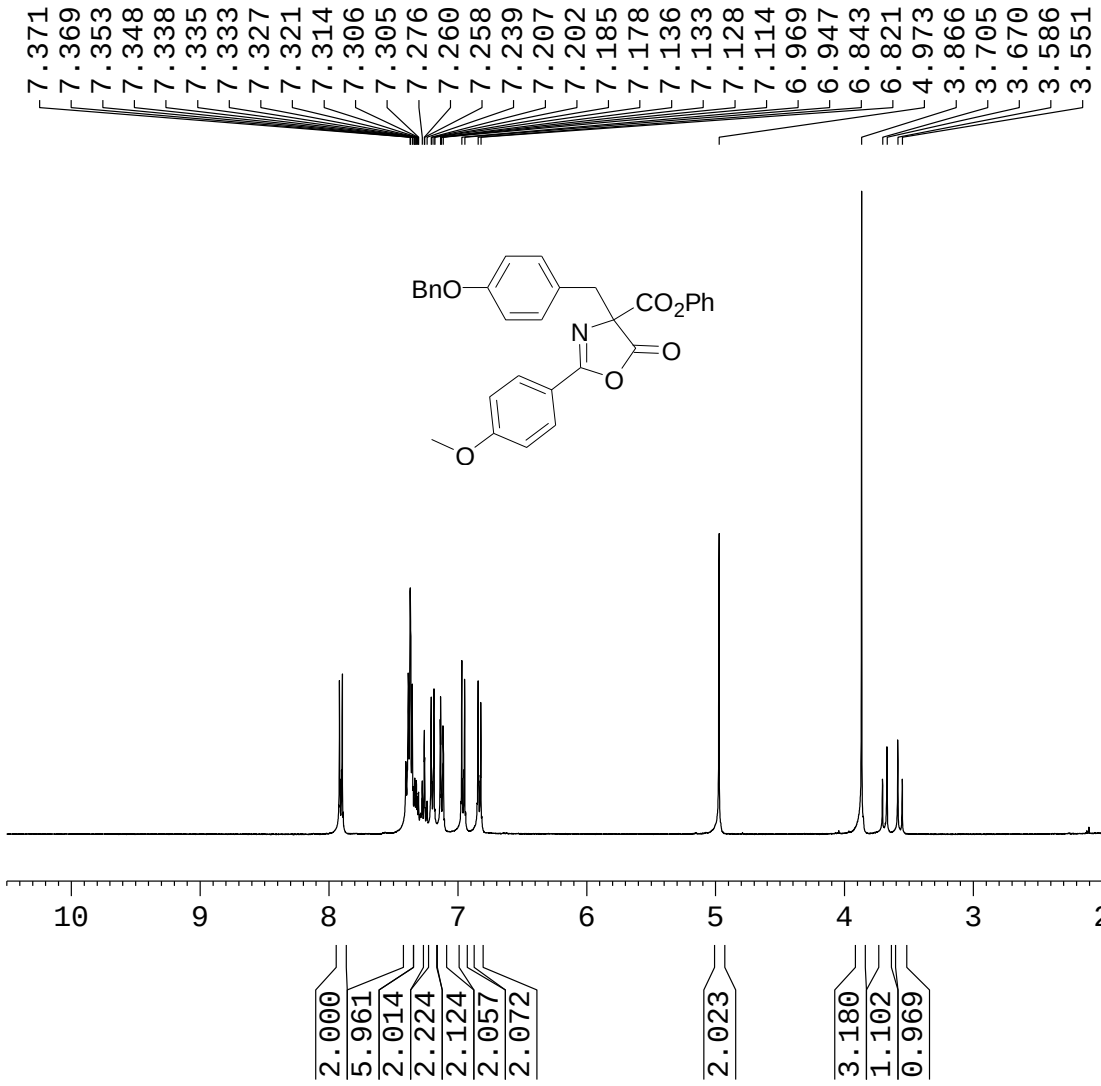
Analysis Name	D:\Data\nctu service\data\2016\20160719\IP_RC3_01_10500.d	Acquisition Date	7/19/2016 2:34:35 PM
Method	Small molecule.m	Operator	NCTU
Sample Name	IP	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

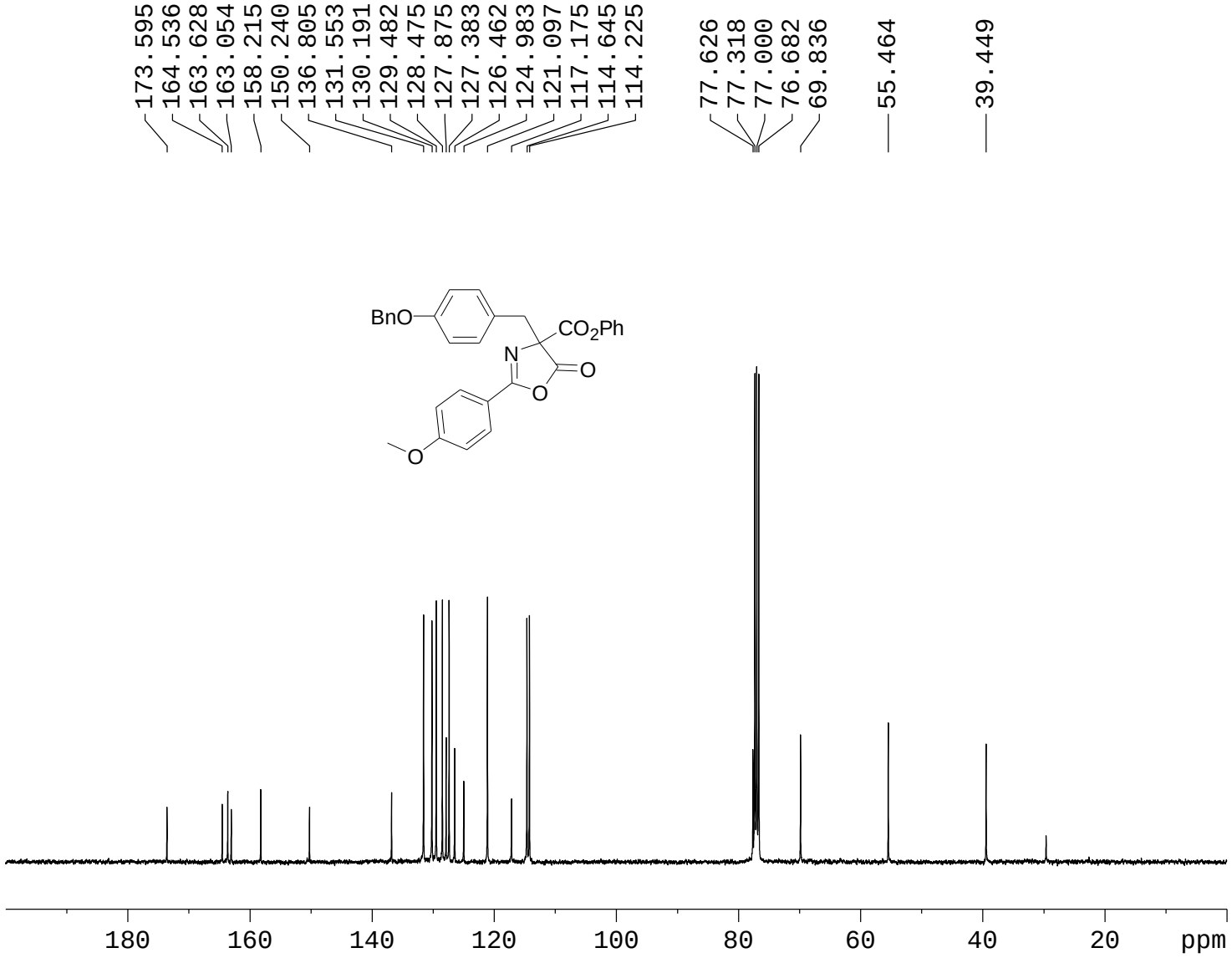
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C







NAME	160718-BnOBnPh-P
EXPNO	1
PROCNO	1
Date_	20160718
Time	0.05
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	4
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500085 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	160718-BnOBnPh-P
EXPNO	13
PROCNO	1
Date_	20160718
Time	0.06
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1223
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6178049 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

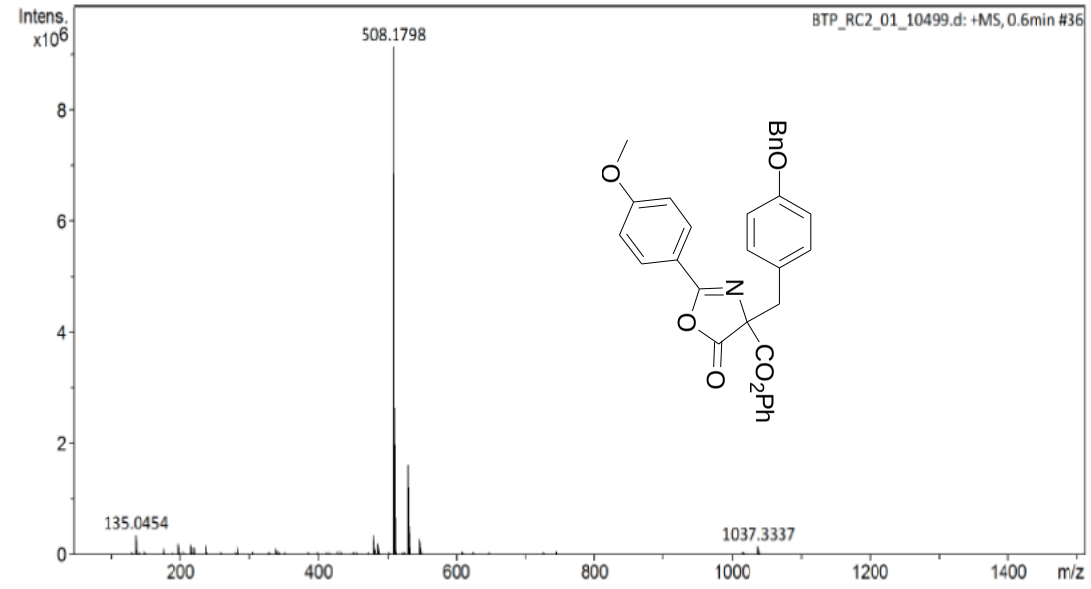
Display Report

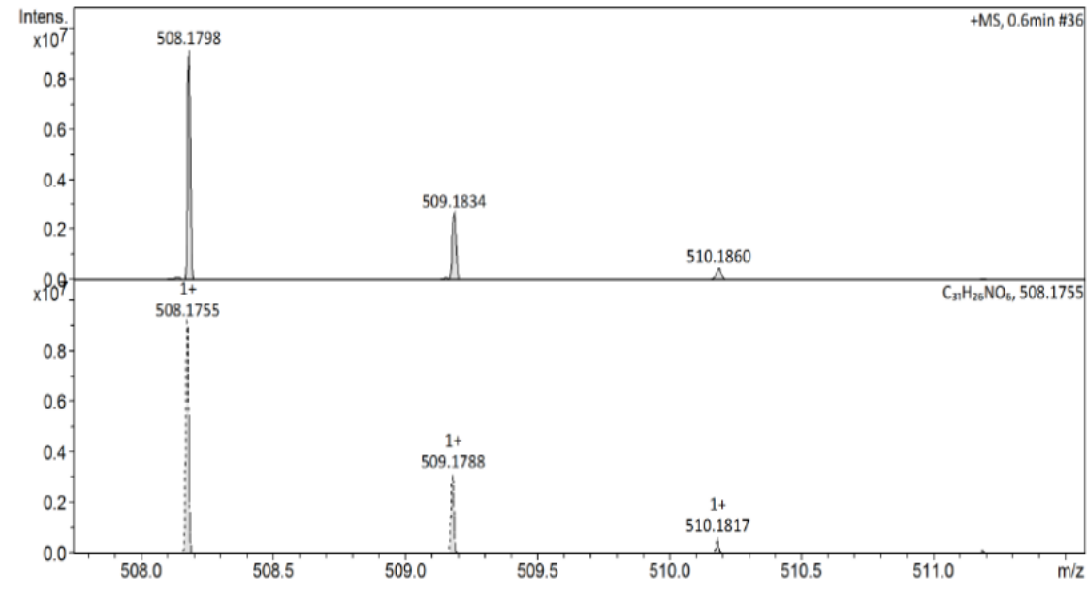
Analysis Info

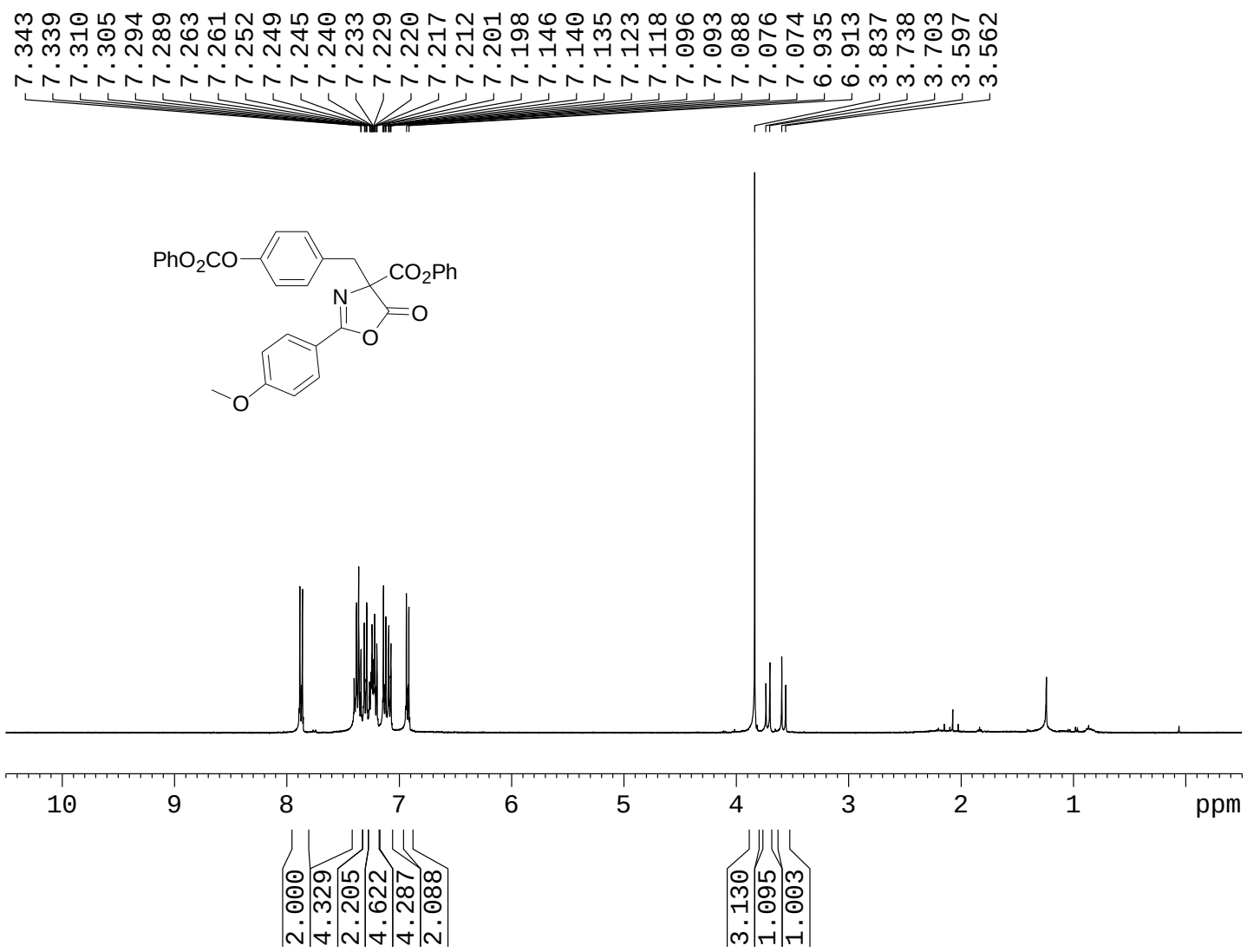
Acquisition Date	7/19/2016 2:30:19 PM		
Analysis Name	D:\Data\nctu service\data\2016\20160719\BTP_RC2_01_10499.d		
Method	Small molecule.m	Operator	NCTU
Sample Name	BTP	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

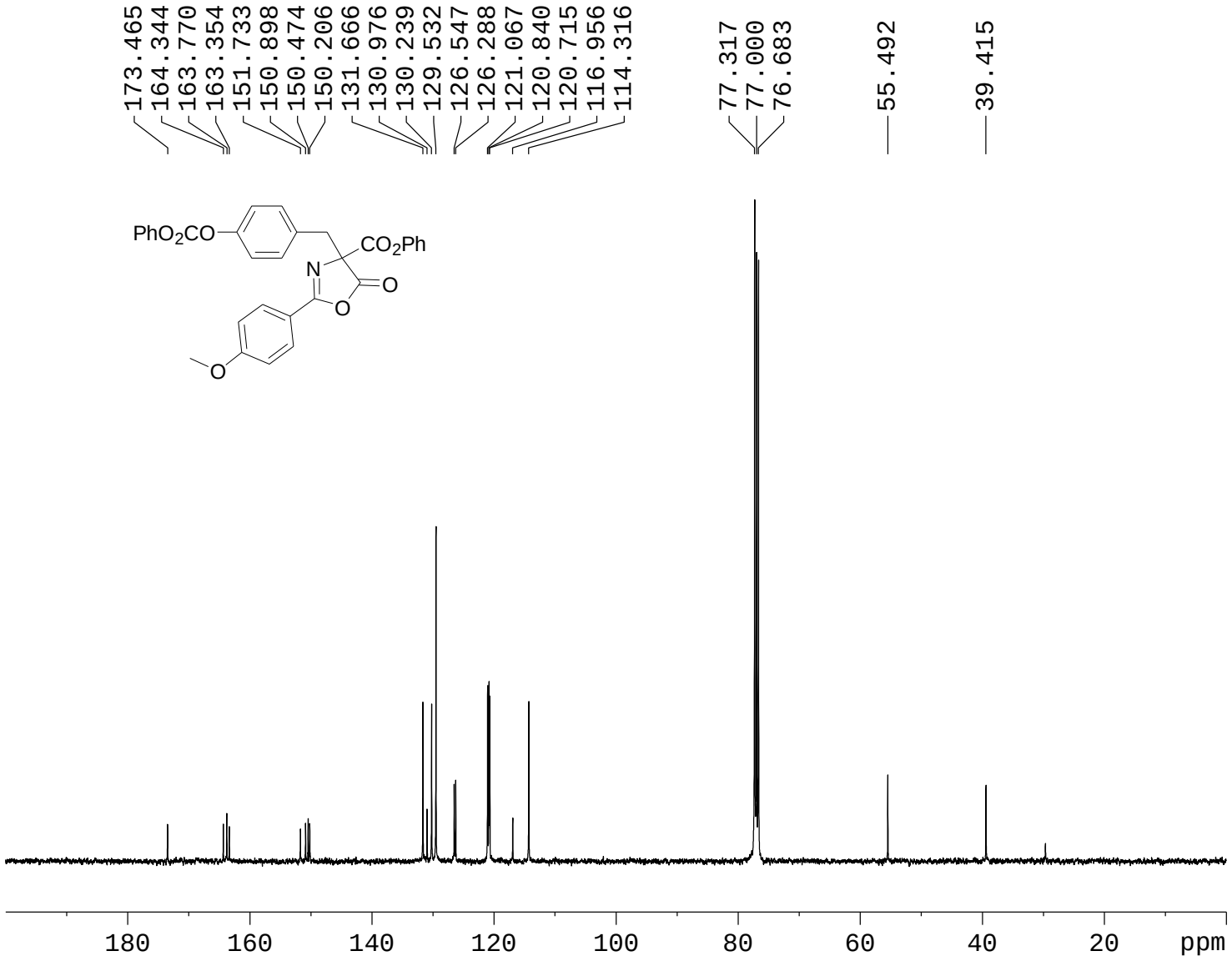
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C







NAME	160714-PhOCO2BnPh-P
EXPNO	1
PROCNO	1
Date_	20160714
Time	8.34
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	4
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500168 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	160714-PhOCO2BnPh-P
EXPNO	13
PROCNO	1
Date_	20160714
Time	8.35
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1280
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6178017 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

Display Report

Analysis Info

Acquisition Date	7/15/2016 11:47:40 AM		
Analysis Name	D:\Data\nctu service\data\2016\20160715\TP_BC1_01_10463.d		
Method	Small molecule.m	Operator	NCTU
Sample Name	TP	Instrument	impact HD 1819696.00164
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C