Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Construction of 5-Methyleneoxazolidine-2,4-diones Bearing Modifiable Halogen Groups through a Halopalladation Strategy

Huilin Zhan,[1] Bin Chen,[1] Biao Zhu,[1] Xiang Li,[1] Zhengyu Han,[1] Jianwei Sun,[2] Hai Huang[1,*]

[1] *Jiangsu Key Laboratory of Advanced Catalytic Materials & Technology, School of Petrochemical Engineering, Changzhou University, Changzhou (China)*

[2] *Department of Chemistry, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong SAR (China)*

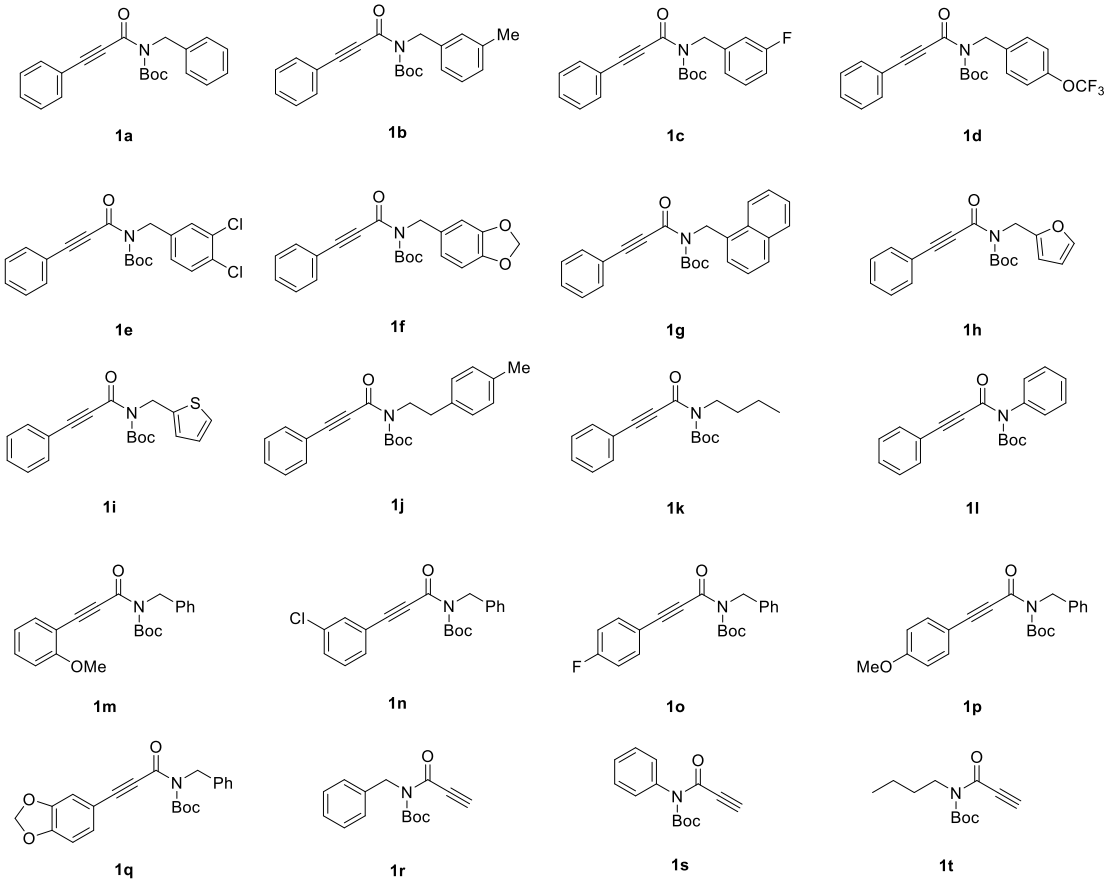
Table of contents

I. General Information

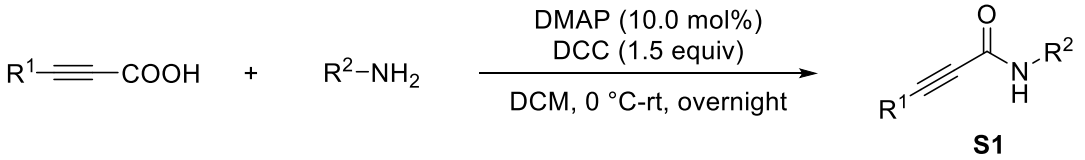
Flash column chromatography was performed over silica gel (200-300 mesh) purchased from Qindao Puke Co. Lit., China. All air or moisture sensitive reactions were conducted in oven-dried glassware under nitrogen atmosphere using anhydrous solvents. Anhydrous toluene, acetonitrile, dichloromethane, chloroform, dimethyl sulfoxide and tetrahydrofuran were purified by the Innovative® solvent purification system. Other anhydrous solvents were purchased from J&K Scientific. ^{1}H, ^{13}C, and ^{19}F NMR spectra were collected on a Bruker AV 400 MHz NMR spectrometer using residue solvent peaks as an internal standard (^{1}H NMR: $CDCl_3$ at 7.26 ppm, d_6-Acetone at 2.05 ppm; ^{13}C NMR: $CDCl_3$ at 77.15 ppm, d_6-Acetone at 206.00 ppm). Mass spectra were collected on an Agilent GC/MS 5975C system, a MALDI Micro MX mass spectrometer, or an API QSTAR XL System. The X-ray data was collected by Xcalibur, Sapphire3, Gemini ultra diffractometer and SuperNova, Dual, Cu at home/near, Atlas diffractometer.

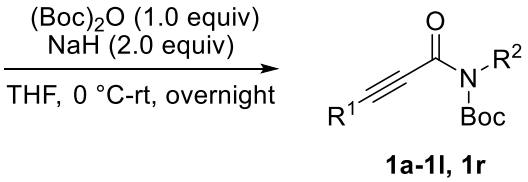
II. Preparation of Substrates 1

Substrates **1a-1r** were synthesized according to the literature procedure.[1]



General Procedure A: Preparation of *N*-Boc amides 1a-1l, 1r



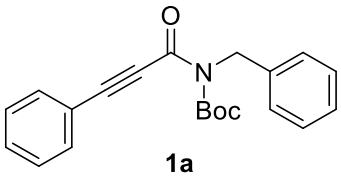


To a solution of amines (10.0 mmol, 1.0 equiv), propiolic acids (12.0 mmol,

[1] S. Azeez, P. Sureshbabu, S. Sabiah and J. kandasamy, *Org. Biomol. Chem.*, 2022, **20**, 2048-2053.

1.2 equiv) in CH_2Cl_2 (20 mL) was dropwise added a solution of DCC (3.09 g, 15.0 mmol, 1.5 equiv) and DMAP (0.12 g, 1.0 mmol, 0.1 equiv) in CH_2Cl_2 (20 mL). The resulting mixture was stirred at room temperature for overnight. Then the crude mixture was filtered and washed with CH_2Cl_2. The combined organic phase was concentrated under reduced pressure to give a residue which was purified by a silica gel column chromatography (petroleum ether / EtOAc = 10:1) to give product amines **S1**.

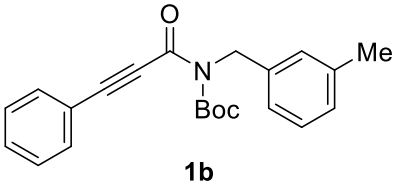
Under N_2 at 0 °C, to a round-bottom flask charged with the amines (5.0 mmol, 1.0 equiv.) and THF (20 mL) was added with NaH (0.40 g, 10.0 mmol, 2.0 equiv.). The mixture was allowed to stir at 0 °C for 30 min before it was added $(Boc)_2O$ (2.18 g, 10.0 mmol, 2.0 equiv.). The resulting mixture was warmed up to room temperature and kept stirring for overnight. Then the reaction was quenched with aqueous NH_4Cl solution (20 mL) and extracted with ethyl acetate (10 mL × 3). The combined organic layers were washed with brine water (20 mL), dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum ether/EtOAc = 50:1) to afford the desired propargylic amides **1a-1l, 1r**.



1a

***tert*-Butyl benzyl(3-phenylpropioloyl)carbamate (1a)** was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 50:1) in 49% yield (0.82 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61-7.55 (m, 2H), 7.45-7.22 (m, 8H), 4.96 (s, 2H), 1.46 (s, 9H) ppm.



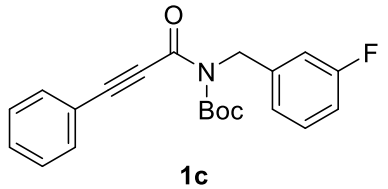
1b

***tert*-Butyl (3-methylbenzyl)(3-phenylpropioloyl)carbamate (1b)** was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 50:1) in 64% yield (1.20 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63-7.55 (m, 2H), 7.47-7.33 (m, 3H), 7.21 (t, *J* = 7.5 Hz, 1H), 7.16-7.10 (m, 2H), 7.07 (d, *J* = 7.4 Hz, 1H), 4.93 (s, 2H), 2.33 (s, 3H), 1.48 (s, 9H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.9, 151.8, 138.0, 137.2, 132.6, 130.2, 128.6, 128.5, 128.2, 128.1, 124.9, 120.6, 93.1, 84.1, 83.4, 47.2, 27.9, 21.4 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{22}H_{24}NO_3$: 350.1756; found: 350.1757.



1c

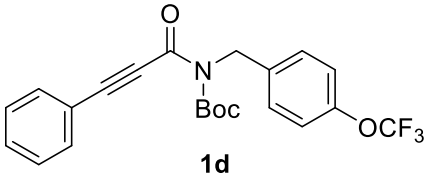
***tert*-Butyl (3-fluorobenzyl)(3-phenylpropioloyl)carbamate (1c)** was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 50:1) in 40% yield (0.70 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62-7.55 (m, 2H), 7.46-7.35 (m, 3H), 7.32-7.24 (m, 1H), 7.14-7.08 (m, 1H), 7.04 (d, *J* = 9.7, Hz, 1H), 6.96 (td, J_1 = 2.3 Hz, J_2 = 8.4 Hz, 1H), 4.95 (s, 2H), 1.49 (s, 9H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 162.7 (d, *J* = 245.0 Hz), 153.8, 151.5, 139.7 (d, *J* = 8.0 Hz) 132.5, 130.3, 129.9 (d, *J* = 8.0 Hz), 128.5, 123.4 (d, *J* = 3.0 Hz), 120.4, 114.7(d, *J* = 21.0 Hz), 114.3 (d, *J* = 21.0 Hz), 93.5, 84.4, 83.2, 46.7 (d, *J* = 2.0 Hz), 27.9 ppm.

^{19}F NMR (300 MHz, $CDCl_3$) δ -113.07 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{21}H_{21}FNO_3$: 354.1505; found 354.1496.



1d

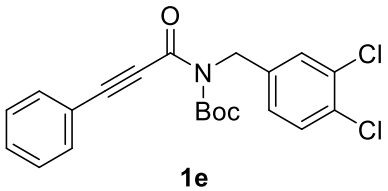
***tert*-Butyl (3-phenylpropioloyl)(4-(trifluoromethoxy)benzyl)carbamate (1d)** was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 50:1) in 69% yield (1.40 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62-7.55 (m, 2H), 7.46-7.34 (m, 5H), 7.16 (d, *J* =8.1 Hz, 2H), 4.95 (s, 2H), 1.49 (s, 9H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.8, 151.6, 148.5, 136.0, 132.6, 130.4, 129.5, 128.5, 120.9, 120.5 (q, *J* = 225.4 Hz), 119.1, 93.5, 84.5, 83.3, 46.5, 27.9 ppm.

^{19}F NMR (300 MHz, $CDCl_3$) δ -57.88 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{22}H_{21}F_3NO_4$: 420.1422; found: 420.1417.



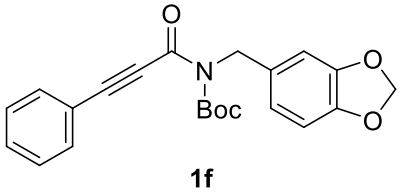
1e

***tert*-Butyl (3,4-dichlorobenzyl)(3-phenylpropioloyl)carbamate (1e)** was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 50:1) in 42% yield (0.85 g)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62-7.55 (m, 2H), 7.48-7.41 (m, 2H), 7.41-7.35 (m, 3H), 7.19 (dd, J_1 = 2.0 Hz, J_2 = 8.2 Hz, 1H), 4.89 (s, 2H), 1.51 (s, 9H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.7, 151.4, 137.4, 132.5, 132.4, 131.5, 130.4, 130.3, 130.1, 128.5, 127.5, 120.4, 93.8, 84.7, 83.1, 46.1, 27.9 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{21}H_{20}Cl_2NO_3$: 404.0820; found: 404.0826.



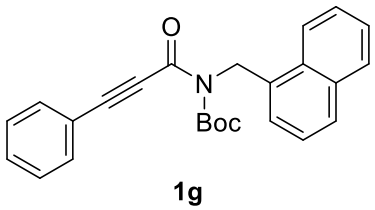
1f

***tert*-Butyl (benzo[d][1,3]dioxol-5-ylmethyl)(3-phenylpropioloyl)carbamate (1f)** was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 50:1) in 39% yield (0.73 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61-7.54 (m, 2H), 7.46-7.33 (m, 3H), 6.90-6.80 (m, 2H), 6.74 (d, *J* = 8.0 Hz, 1H), 5.93 (s, 2H), 4.85 (s, 2H), 41.51 (s, 9H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.8, 151.7, 147.6, 146.9, 132.5, 131.0, 130.2, 128.5, 121.7, 120.6, 108.8, 108.0, 100.9, 93.1, 84.2, 83.4, 47.0, 28.0 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{22}H_{21}NNaO_5$: 402.1318.; found: 402.1309.



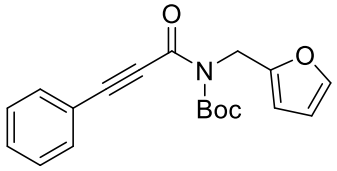
1g

***tert*-Butyl (naphthalen-1-ylmethyl)(3-phenylpropioloyl)carbamate (1g)** was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 50:1) in 50% yield (0.97 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10-8.03 (d, *J* = 8.3 Hz, 1H), 7.88 (d, *J* = 7.9 Hz , 1H), 7.77 (d, *J* = 8.2 Hz, 1H), 7.64-7.48 (m, 4H), 7.47-7.34 (m, 4H), 7.31 (d, *J* = 7.1 Hz, 1H), 5.49 (s, 2H), 1.40 (s, 9H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.9, 151.9, 133.6, 132.6, 132.3, 130.8, 130.3, 128.7, 128.5, 127.7, 126.2, 125.7, 125.2, 123.3, 122.8, 120.5, 93.1, 84.2, 83.3, 44.9, 27.8 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{25}H_{23}NNaO_3$: 408..1576.; found: 408.1571.



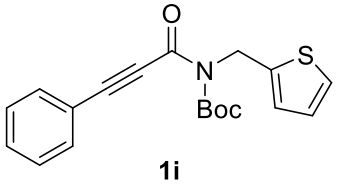
1h

***tert*-Butyl (furan-2-ylmethyl)(3-phenylpropioloyl)carbamate (1h)** was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 50:1) in 88% yield (1.60 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61-7.55 (m, 2H), 7.46-7.32 (m, 4H), 6.34-6.26 (m, 2H), 4.96 (s, 2H), 1.55 (s, 9H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.4, 151.4, 150.5, 141.9, 132.6, 130.3, 128.5, 120.6, 110.3, 108.5, 93.2, 84.3, 83.3, 40.3, 27.9 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{19}H_{19}NNaO_4$: 348.1212; found 348.1204.



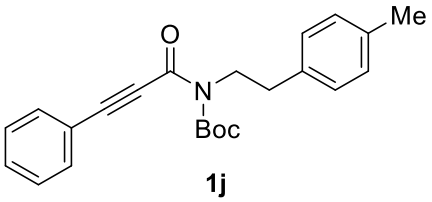
1i

***tert*-Butyl (3-phenylpropioloyl)(thiophen-2-ylmethyl)carbamate** was prepared according to the General Procedure A as a white solid (chromatography eluent: petroleum ether/EtOAc = 50:1) in 34% yield (0.60 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62-7.54 (m, 2H), 7.46-7.32 (m, 3H), 7.22 (dd, J_1 = 1.1 Hz, J_2 = 5.1 Hz, 1H), 7.11 (d, J = 3.3 Hz, 1H), 6.98-6.91 (m, 1H), 5.10 (s, 2H), 1.58 (s, 9H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.5, 151.3, 138.8, 132.6, 130.3, 128.5, 127.9, 126.5, 125.6, 120.6, 93.4, 84.6, 83.4, 41.9, 28.2 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{19}H_{19}NNaO_3S$: 364.0984; found: 364.0974.



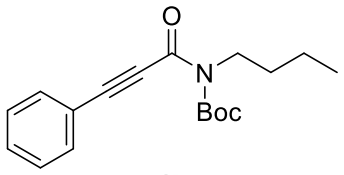
1j

***tert*-Butyl (4-methylphenethyl)(3-phenylpropioloyl)carbamate (1j)** was prepared according to the General Procedure A as a white soild (chromatography eluent: petroleum ether/ EtOAc = 50:1) in 44% total yield (0.79 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62-7.56 (m, 2H), 7.47-7.34 (m, 3H), 7.18-7.08 (m, 4H), 4.00-3.91 (m, 2H), 2.91-2.82 (m, 2H), 2.32 (s, 3H), 1.52 (s, 9H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.7, 151.7, 135.9, 135.3, 132.5, 130.2, 129.2, 128.9, 128.5, 120.7, 92.6, 83.8, 83.6, 46.0, 34.2, 27.9, 21.0 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{23}H_{25}NNaO_3$: 386.1732; found: 386.1728.



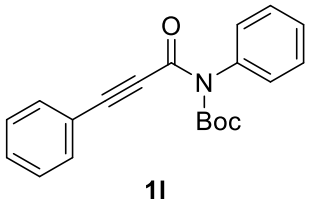
1k

***tert*-Butyl butyl(3-phenylpropioloyl)carbamate (1k)** was prepared according to the General Procedure A as a white oil (chromatography eluent: petroleum ether/ EtOAc = 50:1) in 83% total yield (1.50 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.1 Hz, 2H), 7.41-7.27 (m, 3H), 3.70 (t, *J* = 7.5 Hz, 2H), 1.51 (s, 9H), 1.48-1.45 (m, 2H), 1.36-1.24 (m, 2H), 0.89 (t, *J* = 7.3 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.5, 151.8, 132.3, 123.0, 128.3, 120.5, 92.1, 83.5, 44.0, 30.3, 27.8, 27.2, 19.9, 13.6 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{25}H_{23}NNaO_3$: 324.1576; found: 324.1569.



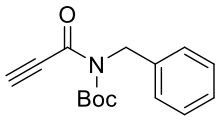
1l

***tert*-Butyl phenyl(3-phenylpropioloyl)carbamate (1l)** was prepared according to the General Procedure A as a white oil (chromatography eluent: petroleum ether/ EtOAc = 50:1) in 61% total yield (0.98 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50-7.29 (m, 8H), 7.28-7.20 (m, 2H), 1.46 (s, 9H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.6, 151.2, 138.0, 132.8, 130.5, 129.1, 128.6, 128.5, 128.4, 120.1, 93.8, 84.0, 83.1, 27.8 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{20}H_{19}NNaO_3$: 324.1263; found: 344.1257.



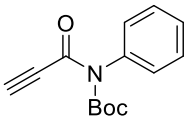
1r

***tert*-Butyl benzyl(propioloyl)carbamate (1l)** was prepared according to the General Procedure A as a white oil (chromatography eluent: petroleum ether/ EtOAc = 50:1) in 20% total yield (0.26 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.22 (m, 5H), 4.90 (s, 2H), 3.41 (s, 1H), 1.47 (s, 9H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 152.9, 151.5, 136.8, 128.4, 127.8(2C), 127.5, 84.8, 82.3, 47.1, 27.8 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{15}H_{17}NNaO_3$: 282.1106; found: 282.1101.



1s

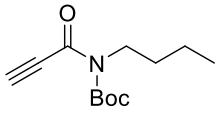
***tert*-Butyl phenyl(propioloyl)carbamate (1s)** was prepared according to

the General Procedure C as a white solid (chromatography eluent: petroleum ether/ EtOAc = 50:1) in 32% total yield (0.62 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45-7.34 (m, 3H), 7.19-7.12 (m, 2H), 3.35 (s, 1H), 1.44 (s, 9H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 152.6, 151.2, 137.0, 129.1 (2C), 128.6, 128.2, 84.6, 82.5, 27.7 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{14}H_{15}NNaO_3$: 268.0950; found: 268.0951.



1t

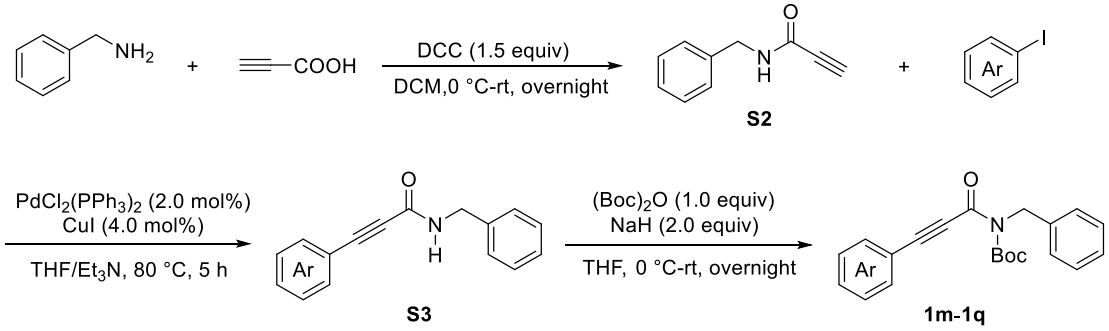
***tert*-Butyl butyl(propioloyl)carbamate (1t)** was prepared according to the General Procedure C as a white oil (chromatography eluent: petroleum ether/ EtOAc = 50:1) in 39% total yield (0.71 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.63 (t, *J* = 7.2 Hz, 2H), 3.34 (s, 1H), 1.50 (s, 9H) 1.49-1.43 (m, 2H), 1.31-1.15 (m, 2H), 0.86 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 152.6, 151.6, 84.3, 81.5, 43.9, 30.2, 28.3, 27.7, 19.8, 13.6 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{12}H_{19}NNaO_3$: 248.1263; found: 248.1260.

General Procedure B: Preparation of *N*-Boc amides 1m-1q.

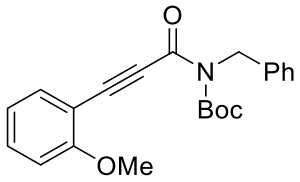


To a solution of phenylmethanamine (1.07 g, 10.0 mmol, 1.0 equiv), propiolic acid (0.84 g, 12.0 mmol, 1.2 equiv) in CH_2Cl_2 (20 mL) was dropwise added a solution of DCC (3.09 g, 15.0 mmol, 1.5 equiv) and DMAP (0.12 g, 1.0 mmol, 0.1 equiv) in CH_2Cl_2 (20 mL). The resulting mixture was stirred at room temperature for overnight. Then the crude mixture was filtered and washed with CH_2Cl_2. The combined organic phase was concentrated under reduced pressure to give a residue which was purified by a silica gel column chromatography (petroleum ether / EtOAc = 10:1) to give product **S2** as a white solid (1.30 g, 82%).

To a solution of *N*-benzylpropiolamide **S2** (1.27 g, 8.0 mmol, 1.2 equiv), CuI (60.8 mg, 0.32 mmol, 4 mol %) and $Pd(PPh_3)_4$ (184.89 mg, 0.16 mmol, 2.0 mol %) were mixed in THF/Et_3N (v/v = 1:1, 20 mL) was added aryl iodides (9.6 mmol, 1.2 equiv). The mixture was stirred at room temperature overnight. The reaction mixture was diluted with H_2O and extracted with EtOAc (10 mL × 3）.The combined organic layers were dried with anhydrous Na_2SO_4 and filtered, and the solvent was removed under reduced pressure. The resulting crude product was purified by column chromatography on silica gel to provide the desired product *N*-benzyl-3-arylpropiolamides **S3**.

Under N_2 at 0 °C, to a solution of *N*-benzyl-3-arylpropiolamide **S3** (3.0 mmol, 1.0 equiv.) in THF (9.0 mL) was added NaH (0.24 g, 6.0 mmol, 2.0 equiv). The mixture was allowed to stir at 0 °C for 30 min before it was added $(Boc)_2O$ (1.31 g, 6.0 mmol, 1.0 equiv.). Then, the resulting mixture was warm

up to room temperature and kept stirring for overnight. Then the reaction was quenched with aqueous NH_4Cl solution (10 mL) and extracted with ethyl acetate (10 mL × 3). The combined organic layers were washed with water (10 mL × 2), dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum ether/EtOAc = 50:1) to afford the desired *N*-Boc amides **1m**-**1q**.



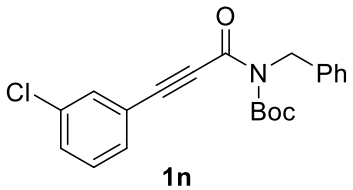
1m

***tert*-Butyl benzyl(3-(2-methoxyphenyl)propioloyl)carbamate (1m)** was prepared according to the General Procedure B as a yellow soild (chromatography eluent: petroleum ether/EtOAc = 80:1) in 57% total yield (0.58 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.4 Hz, 1H), 7.42-7.22 (m, 6H), 6.97-6.85 (m, 2H), 4.97 (s, 2H), 3.85 (s, 3H), 1.46 (s, 9H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 161.1, 154.0, 151.7, 137.3, 134.5, 131.9, 128.2, 127.8, 127.2, 120.4, 110.7, 109.7, 90.3, 87.1, 83.9, 55.6, 47.2, 27.7 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{22}H_{23}NNaO_4$: 388.1515; found: 388.1515.



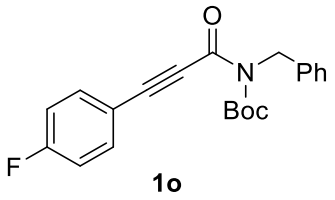
1n

***tert*-Butyl benzyl(3-(3-chlorophenyl)propioloyl)carbamate (1n)** was prepared according to the General Procedure B as a yellow soild (chromatography eluent: petroleum ether/EtOAc = 80:1) in 58% total yield (0.65 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (s, 1H), 7.50-7.43 (m, 1H), 7.42-7.36 (m, 1H), 7.35-7.22 (m, 6H), 4.95 (s, 2H), 1.47 (s, 9H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.6, 151.6, 137.1, 134.4, 132.1, 130.6, 130.5, 129.8, 128.4, 127.8, 127.4, 122.3, 91.4, 84.3, 84.0, 47.2, 27.9 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{21}H_{20}ClNNaO_3$: 392.1020; found: 392.1022.



1o

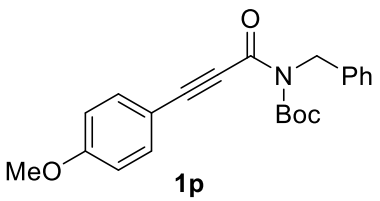
***tert*-Butyl benzyl(3-(4-fluorophenyl)propioloyl)carbamate (1o)** was prepared according to the General Procedure B as a yellow soild (chromatography eluent: petroleum ether/EtOAc = 80:1) in 57% total yield (0.98 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63-7.54 (m, 2H), 7.34-7.23 (m, 5H), 7.07 (t, *J* = 8.6 Hz, 2H), 4.95 (s, 2H), 1.46 (s, 9H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.7 (d, *J* = 252.0 Hz), 153.8, 151.7, 137.2, 134.9 (d, *J* = 8.0 Hz), 128.4, 127.8, 127.4, 116.7 (d, *J* = 4.0 Hz), 116.0 (d, *J* = 22.2 Hz), 92.2, 84.1, 83.3, 47.2, 27.9 ppm.

^{19}F NMR (300 MHz, $CDCl_3$) δ -107.08 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{21}H_{20}FNNaO_3$: 282.1106; found: 282.1101.



1p

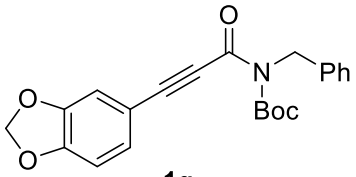
***tert*-Butyl benzyl(3-(4-methoxyphenyl)propioloyl)carbamate (1p)** was

prepared according to the General Procedure B as a yellow soild (chromatography eluent: petroleum ether/EtOAc = 80:1) in 38% total yield (0.38 g).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.8 Hz, 2H), 7.36-7.22 (m, 5H), 6.88 (d, *J* = 8.8 Hz 2H), 4.96 (s, 2H), 3.83 (s, 3H), 1.47 (s, 9H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3, 154.2, 151.8, 137.4, 134.6, 128.3, 127.8, 127.3, 114.2, 112.4, 94.1, 83.9, 83.0, 55.3, 47.2, 27.9 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{22}H_{23}NNaO_4$: 388.1515; found: 388.1516.



1q

***tert*-Butyl (3-(benzo[d][1,3]dioxol-5-yl)propioloyl)(benzyl)carbamate (1q)** was prepared according to the General Procedure B as a white soild (chromatography eluent: petroleum ether/EtOAc = 80:1) in 47% total yield (0.54 g).

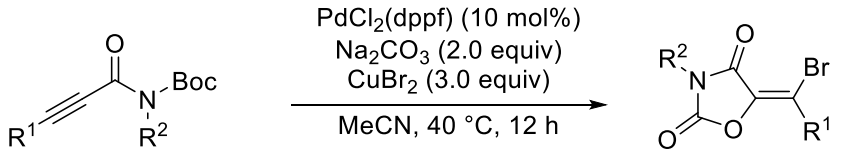
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.21 (m, 5H), 7.16 (dd, J_1 = 1.4 Hz, J_2 = 8.0 Hz 1H), 7.01 (d, *J* = 1.3 Hz, 1H), 6.79 (d, *J* = 8.1 Hz, 1H), 6.01 (s, 2H), 4.95 (s, 2H), 1.46 (s, 9H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 154.0, 151.8, 149.7, 147.5, 137.3, 128.5, 128.3, 127.7, 127.3, 113.6, 112.3, 108.7, 101.6, 93.7, 84.0, 82.4, 47.2, 27.9 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{22}H_{21}NNaO_5$: 402.1318; found: 402.1312.

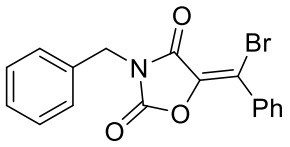
III. Synthesis of Oxazolidin-2,4-Diones Compounds 2-3

General Procedure C: The Synthesis of Oxazolidin-2,4-Diones 2a-2r.



1 **2a-2r**

Under N_2 atmosphere, to a solution of *N*-Boc amides (0.3 mmol, 1.2 equiv), $CuBr_2$ (201.0 mg, 0.9 mmol, 3.0 equiv), Na_2CO_3 (63.4 mg, 0.6 mmol, 2.0 equiv) and) in MeCN (3 mL) was added $PdCl_2$(dppf) (21.9 mg, 0.03 mmol, 10 mol%). Then the reaction mixture was heated to 40 °C on an oil bath and stirred at 40 °C for 12 h. The reaction mixture was diluted with H_2O (10 mL) and extracted with EtOAc (5 mL × 3). The combined organic layers were washed with water, birne, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum ether/ethyl acetate = 20: 1) to afford the desired oxazolidin-2,4-diones **2a**-**2r**.



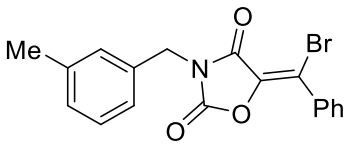
2a

(*E*)-3-Benzyl-5-(bromo(phenyl)methylene)oxazolidine-2,4-dione (2a) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 87% yield (93.0 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73-7.67 (m, 2H), 7.50-7.46 (m, 2H), 7.45-7.41 (m, 3H), 7.40-7.34 (m, 3H), 4.79 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 150.3, 135.3, 134.2, 134.1, 130.9, 129.9, 129.1, 128.9, 128.7, 128.5, 114.6, 44.1 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{17}H_{12}BrNNaO_3$: 379.9899; found: 379.9908.



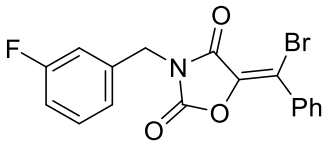
2b

(*E*)-5-(Bromo(phenyl)methylene)-3-(3-methylbenzyl)oxazolidine-2,4-dione (2b) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 81% yield (90.2 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74-7.66 (m, 2H), 7.47-7.39 (m, 3H), 7.30-7.21 (m, 3H), 7.18-7.11 (m, 1H), 4.75 (s, 2H), 2.35 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 150.3, 138.7, 135.3, 134.1, 130.9, 129.8 (2C), 129.7, 129.4, 128.8, 128.4, 126.1, 114.5, 44.1, 21.3 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{18}H_{15}BrNO_3$: 372.0235; found: 388.0226.



2c

(*E*)-5-(Bromo(phenyl)methylene)-3-(3-fluorobenzyl)oxazolidine-2,4-dione (2c) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 80% yield (87.9 mg).

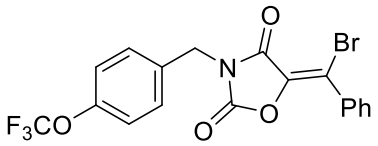
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75-7.65 (m, 2H), 7.50-7.39 (m, 3H), 7.37-7.29 (m, 1H), 7.28-7.21 (m, 1H), 7.21-7.14 (m, 1H), 7.04 (td, J_1 = 2.2 Hz, J_2 = 8.4 Hz, 1H),

4.77 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 162.8 (d, *J* = 245.0 Hz), 159.8, 150.2, 136.3 (d, *J* = 7.0 Hz), 135.2, 134.0, 131.0, 130.5 (d, *J* = 8.0 Hz), 129.9, 128.6, 124.6 (d, *J* = 3.0 Hz), 116.0 (d, *J* = 2.2 Hz), 115.7 (d, *J* = 2.0 Hz), 115.1, 43.5 (d, *J* = 14.7 Hz) ppm.

^{19}F NMR (300 MHz, $CDCl_3$) δ -111.81 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{17}H_{12}BrFNO_3$: 375.9984; found: 375.9989.



2d

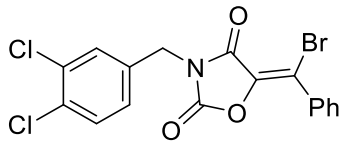
(*E*)-5-(Bromo(phenyl)methylene)-3-(4-(trifluoromethoxy)benzyl)oxazoli -dine-2,4-dione (2d) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 86% yield (114.2 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76-7.66 (m, 2H), 7.55-7.48 (m, 2H), 7.43-7.38 (m, 3H), 7.24-7.16 (m, 2H), 4.79 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 150.1, 149.3, 135.2, 134.0, 132.8, 131.1, 130.8, 129.8, 128.5, 121.4, 120.3 (q, *J* = 256.0 Hz), 115.1, 43.2 ppm.

^{19}F NMR (100 MHz, $CDCl_3$) δ -57.84 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{18}H_{12}BrF_3NO_4$: 441.9902; found: 441.9894.



2e

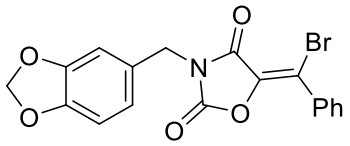
(*E*)-5-(Bromo(phenyl)methylene)-3-(3,4-dichlorobenzyl)oxazolidine-2,4-dione (2e) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 82% yield

(104.7 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75-7.67 (m, 2H), 7.56 (d, J = 2.0 Hz, 1H), 7.48-7.39 (m, 4H), 7.31 (d, J_1 = 2.0 Hz, J_2 = 8.2 Hz, 1H), 4.74 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.6, 150.0, 135.1, 134.0, 133.9, 133.0, 132.9, 131.0, 131.0, 130.8, 129.8, 128.4 (2C), 115.3, 42.8 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{15}H_{11}BrCl_2NO_3$: 425.9299; found: 425.9290.



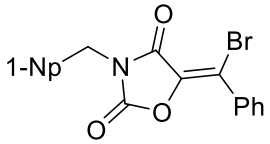
2f

(*E*)-3-(Benzo[*d*][1,3]dioxol-5-ylmethyl)-5-(bromo(phenyl)methylene)oxazolidine-2,4-dione （2f） was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 83% yield (99.3 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74-7.65 (m, 2H), 7.47-7.39 (m, 3H), 6.99-6.92 (m, 2H), 6.81-6.74 (m, 1H), 5.95 (s, 2H), 4.69 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 160.4, 151.3, 147.9, 147.7, 136.8, 133.0, 130.3, 129.8, 128.8, 127.8, 123.5, 122.5, 109.2, 108.4, 101.2, 43.6 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{17}H_{12}BrNNaO_3$: 423.9797; found: 423.9788.



2g

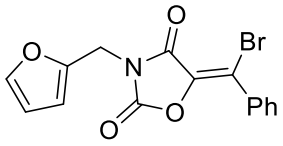
(*E*)-5-(Bromo(phenyl)methylene)-3-(naphthalen-1-ylmethyl)oxazolidine-2,4-dione (2g) was prepared according to the General Procedure C at 0.2

mmol as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 63% yield (50.2 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 8.8 Hz, 1H), 7.88 (t, *J* = 8.4 Hz, 2H), 7.73 (d, *J* = 7.2 Hz, 1H), 7.72-7.65 (m, 2H), 7.64-7.58 (m, 1H), 7.57-7.44 (m, 2H), 7.44-7.36 (m, 3H), 5.26 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 160.6, 151.3, 136.8, 133.7, 132.9, 131.0, 130.3, 129.8, 129.3, 129.1, 128.8, 128.7, 128.2, 126.8, 126.0, 125.2, 123.6, 123.1, 41.7 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{21}H_{14}BrNNaO_3$: 429.9961; found: 430.0063.



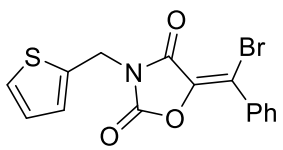
2h

(*E*)-5-(Bromo(phenyl)methylene)-3-(furan-2-ylmethyl)oxazolidine-2,4-d-ione (2h) was prepared according to the General Procedure C at 0.2 mmol as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 71% yield (49.0 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78-7.65 (m, 2H), 7.49-7.35 (m, 4H), 6.46 (d, *J* = 3.2 Hz, 1H), 6.37-6.32 (m, 1H), 4.82 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 149.9, 147.0, 143.2, 135.2, 134.1, 130.9, 129.9, 128.5, 114.9, 110.7, 110.3, 36.6 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{15}H_{10}BrNNaO_3$: 379.9691; found: 369.9697.



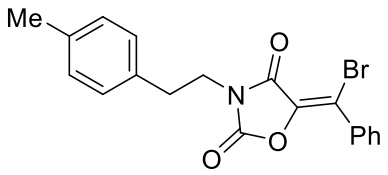
2i

(*E*)-5-(Bromo(phenyl)methylene)-3-(thiophen-2-ylmethyl)oxazolidine-2, 4-dione (2i) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 79% yield (86.2 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75-7.65 (m, 2H), 7.46-7.38 (m, 3H), 7.29 (dd, J_1 = 1.2 Hz, J_2 = 5.2 Hz, 1H), 7.21 (d, J = 3.2 Hz, 1H), 7.01-6.97 (m, 1H), 4.97 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 149.9, 135.2, 134.0, 130.9, 129.9 (2C), 129.0, 128.5, 127.1, 126.9, 114.9, 38.0 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{15}H_{10}BrNNaO_3S$: 385.9463; found: 385.9469.



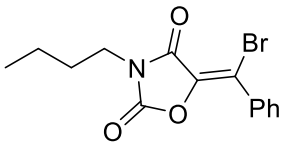
2j

(*E*)-5-(Bromo(phenyl)methylene)-3-(4-methylphenethyl)oxazolidine-2,4 -dione (2j) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 86% yield (95.6 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77-7.68 (m, 2H), 7.49-7.41 (m, 3H), 7.16-7.10 (m, 4H), 3.92-3.82 (m, 2H), 3.03-2.95 (m, 2H), 2.33 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 149.3, 135.6, 134.2, 133.1, 132.6, 129.9, 128.9, 128.4, 127.6, 127.4, 113.2, 40.7, 32.0, 20.0 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{19}H_{17}BrNO_3$: 388.0392; found: 386.0387.



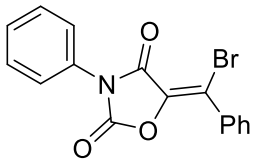
2k

(*E*)-5-(Bromo(phenyl)methylene)-3-butyloxazolidine-2,4-dione (**2k)** was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 76% yield (74.0 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76-7.68 (m, 2H), 7.49-7.40 (m, 3H), 3.66 (t, *J* = 7.2 Hz, 2H), 1.75-1.63 (m, 2H), 1.45-1.32 (m, 2H), 0.96 (t, *J* = 7.6 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 150.6, 135.4, 134.2, 130.8, 129.9, 128.4, 114.1, 40.4, 29.53, 19.8, 13.5 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{14}H_{15}BrNO_3$: 323.0235; found: 323.0225.



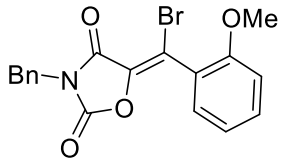
2l

(*E*)-5-(Bromo(phenyl)methylene)-3-phenyloxazolidine-2,4-dione (2l) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 84% yield (87.2 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82-7.76 (m, 2H), 7.57-7.40 (m, 8H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 149.3, 135.0, 134.2, 131.0, 130.4, 129.9, 129.2, 128.5, 127.7, 125.5, 115.5 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{16}H_{10}BrNNaO_3$: 365.9732; found: 365.9733.



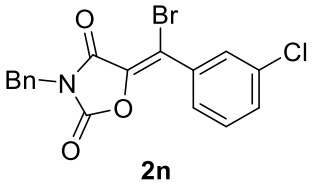
2m

(*E*)-3-Benzyl-5-(bromo(2-methoxyphenyl)methylene)oxazolidine-2,4-dione (2m) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 85% yield (99.3 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50-7.44 (m, 2H), 7.42-7.31 (m, 4H), 7.28-7.23 (m, 1H), 7.03-6.91 (m, 2H), 4.76 (s, 2H), 3.84 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 156.2, 150.4, 136.6, 134.3, 132.1, 130.2, 129.1, 128.9, 128.6, 123.5, 120.5, 111.5, 110.7, 55.7, 44.0 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{18}H_{15}BrNO_4$: 388.0184; found: 388.0174.



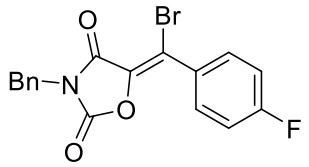
2n

(*E*)-3-Benzyl-5-(bromo(3-chlorophenyl)methylene)oxazolidine-2,4-dione (2n) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 83% yield (99.3 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (s, 1H), 7.63-7.53 (m, 1H), 7.52-7.43 (m, 2H), 7.42-7.30 (m, 5H), 4.78 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.6, 150.0, 135.9, 135.7, 134.5, 134.0, 130.8, 129.7, 129.7, 129.1, 128.9, 128.7, 127.9, 112.2, 44.2 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{17}H_{12}BrClNO_3$: 391.9689; found: 391.9698.



2o

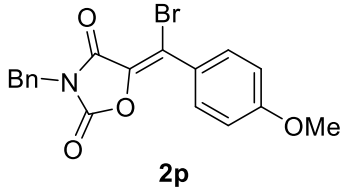
(*E*)-3-Benzyl-5-(bromo(4-fluorophenyl)methylene)oxazolidine-2,4-dion e (**2o**) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 79% yield (89.1 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78-7.69 (m, 2H), 7.52-7.43 (m, 2H), 7.41-7.30 (m, 3H), 7.19-7.08 (m, 2H), 4.79 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8 (d, *J* = 253.0 Hz), 159.8, 150.2, 135.3, 134.1, 132.24, 132.15, 130.1 (d, *J* = 3.0 Hz), 129.1, 128.9, 128.7, 115.7 (d, *J* = 8.8 Hz), 44.2 ppm.

^{1}H NMR (300 MHz, $CDCl_3$) δ -107.74 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{17}H_{12}BrFNO_3$: 375.9984; found: 375.9978.



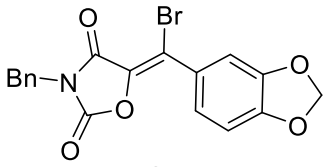
2p

(*E*)-3-Benzyl-5-(bromo(4-methoxyphenyl)methylene)oxazolidine-2,4-di-one (2p) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 91% yield (106.5 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78-7.69 (m, 2H), 7.52-7.43 (m, 2H), 7.41– 7.31 (m, 3H), 6.96-6.89 (m, 2H), 4.79 (s, 2H), 3.86 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 161.6, 160.1, 150.4, 134.3, 134.2, 132.0, 129.1, 128.9, 128.6, 126.2, 115.1, 113.8, 55.5, 44.0 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{18}H_{15}BrNO_4$: 388.0184; found: 388.0175.



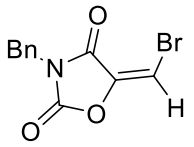
2q

(*E*)-5-(Benzo[*d*][1,3]dioxol-5-ylbromomethylene)-3-benzyloxazolidine-2, 4-dione (2q) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 81% yield (96.9 mg).

H NMR (400 MHz, $CDCl_3$) δ 7.50-7.42 (m, 2H), 7.41-7.27 (m, 5H), 7.23 (s, 1H), 6.84 (d, *J* = 8.4 Hz, 1H), 6.03 (s, 2H), 4.78 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 156.0, 150.4, 149.9, 147.8, 134,7, 134.3, 129.1, 129.0, 128.7, 127.8, 125.7, 114.5, 110.2, 108.2, 102.0, 44.1 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{18}H_{12}BrNNaO_3$: 364.0717; found: 364.0714.



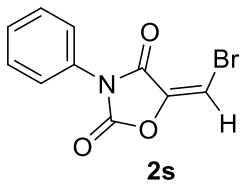
2r

(*E*)-3-Benzyl-5-(bromomethylene)oxazolidine-2,4-dione (2r) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 79% yield (66.8 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47-7.40 (m, 2H), 7.39-7.30 (m, 3H), 6.76 (s, 1H), 4.74 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 150.3, 140.5, 133.9, 129.0, 128.9, 128.7, 97.8, 44.0 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{11}H_8BrNNaO_3$: 303.9586; found: 303.9577.



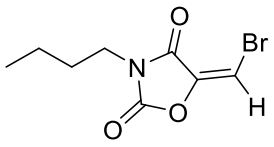
2s

(*E*)-5-(Bromomethylene)-3-phenyloxazolidine-2,4-dione (2s) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 67% yield (53.4 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55-7.48 (m, 2H), 7.47-7.42 (m, 3H), 6.89 (s, 1H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 149.3, 140.2, 130.1, 129.4 (2C), 129.2, 98.6 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{10}H_6BrNNaO_3$: 289.9429; found: 289.9432.



2t

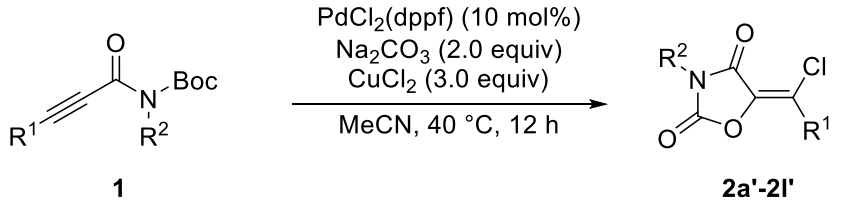
(*E*)-5-(Bromomethylene)-3-butyloxazolidine-2,4-dione (2t) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 63% yield (46.8 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.75 (s, 1H), 3.61 (t, *J* = 7.2 Hz, 2H), 1.70-1.60 (m, 2H), 1.40-1.28 (m, 2H), 0.94 (t, *J* = 7.6 Hz, 3H)ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.6, 150.6, 140.6, 97.2, 40.2, 29.4, 19.7, 13.4 ppm.

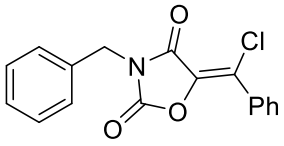
HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_8H_{10}BrNNaO_3$: 269.9742; found: 269.9746.

General Procedure D: The Synthesis of Oxazolidin-2,4-Diones 2a′-2l′.



1 **2a'-2l'**

Under N_2 atmosphere, to a solution of *N*-Boc amides **1** (0.3 mmol, 1.2 equiv), $CuCl_2$ (121.0 mg, 0.9 mmol, 3.0 equiv), Na_2CO_3 (63.4 mg, 0.6 mmol, 2.0 equiv) and) in MeCN (3.0 mL) was added $PdCl_2$(dppf) (21.9 mg, 0.03 mmol, 10 mol%). Then the reaction mixture was heated to 40 °C on an oil bath and stirred at 40 °C for 12 h. The reaction mixture was diluted with H_2O (10 mL) and extracted with EtOAc (5 mL × 3). The combined organic layers were washed with water, birne, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum ether/ethyl acetate = 10: 1) to afford the desired oxazolidin-2,4-diones **2a′-2l′**.



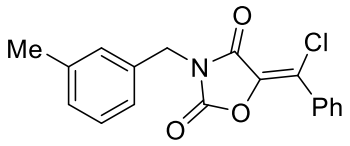
2a'

(*E*)-3-Benzyl-5-(chloro(phenyl)methylene)oxazolidine-2,4-dione (2a′) was prepared according to the General Procedure D as a white solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 73% yield (68.1 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85-7.77 (m, 2H), δ 7.52-7.42 (m, 5H), 7.41-7.29 (m, 3H), 4.79 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 150.5, 134.8, 134.2, 132.5, 131.1, 129.2, 129.0, 128.9, 128.6, 128.5, 125.2, 43.9 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{17}H_{13}ClNO_3$: 314.0652; found: 314.0574.



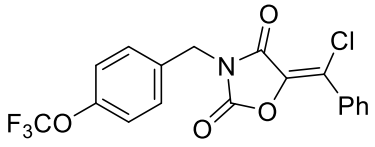
2b'

(*E*)-5-(Chloro(phenyl)methylene)-3-(3-methylbenzyl)oxazolidine-2,4-dione (2b') was prepared according to the General Procedure D as a white solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 90% yield (89.2 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85-7.77 (m, 2H), 7.49-7.41 (m, 3H), 7.30-7.21 (m, 3H), 7.15 (d, *J* = 6.8 Hz, 1H), 4.75 (s, 2H), 2.35 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.6, 150.5, 138.7, 134.9, 134.1, 132.5, 131.1, 129.6, 129.4, 129.2, 128.8, 128.5, 126.1, 125.2, 44.0, 21.3 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{18}H_{15}ClNO_3$: 328.0740; found: 328.0732.



2c'

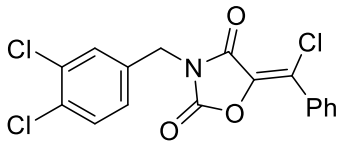
(*E*)-5-(Chloro(phenyl)methylene)-3-(4-(trifluoromethoxy)benzyl)oxazoli-dine-2,4-dione (2c') was prepared according to the General Procedure D as a white solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 89% yield (116.0 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88-7.77 (m, 2H), 7.56-7.42 (m, 5H), 7.21 (d, *J* = 8.2 Hz, 2H), 4.79 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 150.4, 149.4, 134.7, 132.8, 132.4, 131.3, 130.8, 129.3, 128.6, 125.8, 121.4, 120.3 (d, *J* = 255.9 Hz), 43.2 ppm.

^{19}F NMR (300 MHz, $CDCl_3$) δ -57.86 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{18}H_{12}ClF_3NO_4$: 398.0407; found: 398.0403.



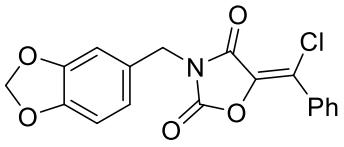
2d'

(*E*)-5-(Chloro(phenyl)methylene)-3-(3,4-dichlorobenzyl)oxazolidine-2,4-dione（2d'） was prepared according to the General Procedure D as a white solid (chromatography eulent: petroleum ether/EtOAc = 10:1) in 82% yield (92.9 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86-7.77 (m, 2H), 7.55 (d, J = 1.8 Hz, 1H), 7.51-7.40 (m, 4H), 7.30 (dd, J_1 = 1.8 Hz, J_2 = 8.2 Hz 1H), 4.73 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.3, 150.2, 134.6, 134.1, 133.0, 132.9, 131.3, 130.9, 130.9, 129.2, 128.5, 128.4, 126.0, 42.7, 28.0 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{17}H_{11}Cl_3NO_3$: 381.9804; found: 381.9795.



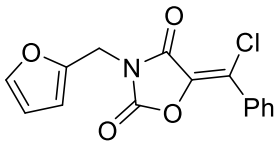
2e'

(*E*)-3-(Benzo[*d*][1,3]dioxol-5-ylmethyl)-5-(chloro(phenyl)methylene)oxazoli- dine-2,4-dione (2e') was prepared according to the General Procedure D as a white solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 83% yield (103.9 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85-7.76 (m, 2H), 7.49-7.40 (m, 3H), 6.99-6.91 (m, 2H), 7.75 (d, J = 8.2 Hz, 1H), 5.93 (s, 2H), 4.67 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 150.4, 147.8, 147.8, 134.8, 132.5, 131.1, 129.2, 128.5, 127.8, 125.1, 122.9, 109.5, 108.4, 101.2, 43.8 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{18}H_{13}ClNO_5$: 358.0482; found: 358.0477.



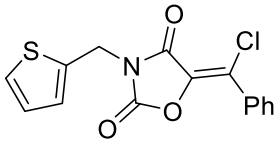
2f'

(*E*)-5-(Chloro(phenyl)methylene)-3-(furan-2-ylmethyl)oxazolidine-2,4-d-ione (2f') was prepared according to the General Procedure D as a white solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 88% yield (79.9 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86-7.77 (m, 2H), 7.49-7.43 (m, 3H), 7.38 (d, *J* = 0.9 Hz, 1H), 7.21 (d, *J* = 3.0 Hz, 1H), 6.38-6.31 (m, 1H), 4.82 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 150.1, 147.0, 143.1, 134.7, 132.5, 131.2, 129.3, 128.5, 125. 5, 110.7, 110.2, 36.5 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{15}H_{11}ClNO_4$: 304.0376; found: 358.0368.



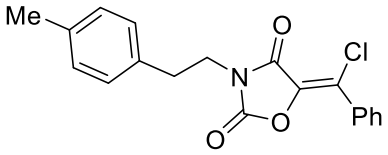
2g'

(*E*)-5-(Chloro(phenyl)methylene)-3-(thiophen-2-ylmethyl)oxazolidine-2,4-dione (2g') was prepared according to the General Procedure D as a white solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 91% yield (88.2 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86-7.77 (m, 2H), 7.49-7.41 (m, 3H), 7.29 (d, *J* = 5.1 Hz, 1H), 7.21 (d, *J* = 3.2 Hz, 1H), 7.02-6.95 (m, 1H), 4.97 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 150.0, 135.2, 134.7, 132.4, 131.1, 129.2, 128.9, 128.5, 127.1, 126.8, 125.4, 37.8 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{15}H_{11}ClNO_3S$: 320.0148; found: 320.0138.



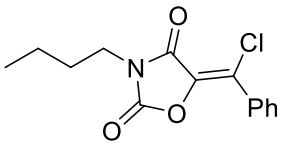
2h'

(*E*)-5-(Chloro(phenyl)methylene)-3-(4-methylphenethyl)oxazolidine-2,4-dione (2h') was prepared according to the General Procedure D as a white solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 74% yield (91.0 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87-7.80 (m, 2H), 7.50-7.44 (m, 3H), 7.19-7.10 (m, 4H), 3.93-3.91 (m, 2H), 2.98 (t, J = 7.2 Hz, 2H), 2.33 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.7, 150.5, 136.6, 134.8, 133.6, 132.5, 131.1, 129.4, 129.2, 128.6, 128.5, 124.9, 41.6, 33.0, 21.0 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{19}H_{16}ClNNaO_3$: 364.0717; found: 364.0714.



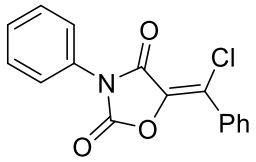
2i'

(*E*)-3-Butyl-5-(chloro(phenyl)methylene)oxazolidine-2,4-dione (2i') was prepared according to the General Procedure D as a white solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 76% yield (74.0 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86-7.81 (m, 2H), 7.50-7.44 (m, 3H), 3.66 (t, J = 7.2 Hz, 2H), 1.75-1.63 (m, 2H), 1.38 (dq, J_1 = 7.2 Hz, J_2 = 14.6 Hz, 2H), 0.96 (t, J = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 150.8, 134.9, 132.6, 131.1, 129.3, 128.5, 124.8, 40.2, 29.5, 19.8, 13.5 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{14}H_{14}ClNNaO_3$: 302.0560; found: 328.0555.



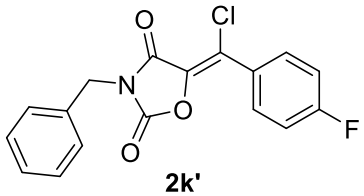
2j'

(*E*)-5-(Chloro(phenyl)methylene)-3-phenyloxazolidine-2,4-dione (2j') was prepared according to the General Procedure D as a white solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 84% yield (87.0 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93-7.86 (m, 2H), 7.57-7.43 (m, 8H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 149.5, 134.5, 132.6, 131.3, 130.4, 129.4, 129.3, 129.2, 128.6, 126.1, 125.5 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{16}H_{11}ClNO_3$: 300.0427; found: 300.0424.



2k'

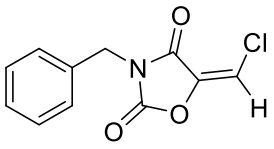
(*E*)-3-Benzyl-5-(chloro(4-fluorophenyl)methylene)oxazolidine-2,4-dione (2k') was prepared according to the General Procedure D as a white solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 57% yield (56.0 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88-7.81 (m, 2H), 7.49-7.43 (m, 2H), 7.40-7.30 (m, 3H), 7.19-7.11 (m, 2H), 3.79 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 164.0 (d, J = 252.5 Hz), 159.5, 150.4, 134.7, 134.1, 131.6 (d, J = 8.8 Hz), 129.1, 128.9, 128.7, 128.6 (d, J = 36.5 Hz), 124.1, 115.8 (d, J = 22.0 Hz), 44.1 ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ -107.13 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{17}H_{12}ClFNO_3$: 332.0489; found: 332.0495.



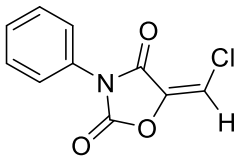
2l'

(*E*)-3-Benzyl-5-(chloromethylene)oxazolidine-2,4-dione (2l') was prepared according to the General Procedure D as a white solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 79% yield (66.8 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46-7.39 (m, 2H), 7.39-7.30 (m, 3H), 6.64 (s, 1H), 4.73 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 150.4, 140.2, 133.9, 129.0, 128.9, 128.7, 111.4, 43.9 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{11}H_9ClNO_3$: 238.0272; found: 238.0269.



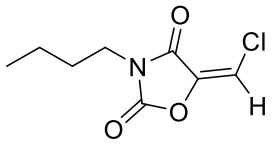
2m'

(*E*)-5-(Chloromethylene)-3-phenyloxazolidine-2,4-dione (2m') was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 72% yield (48.7 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55-7.48 (m, 2H), 7.48-7.42 (m, 3H), 6.79 (s, 1H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 149.4, 139.9, 130.0, 129.4, 129.2, 125.3, 112.2 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{10}H_6ClNNaO_3$: 245.9934; found: 245.9925.



2n'

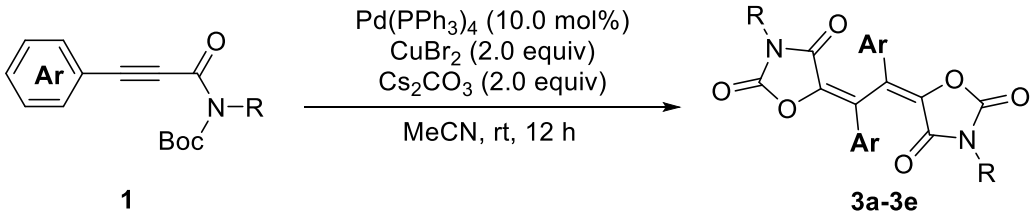
(*E*)-3-Butyl-5-(chloromethylene)oxazolidine-2,4-dione (2n′) was prepared according to the General Procedure C as a white solid (chromatography eluent: petroleum ether/EtOAc = 20:1) in 70% yield (42.8 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.65 (s, 1H), 3.61 (t, *J* = 7.2 Hz, 2H), 1.70-1.60 (m, 2H), 1.40-1.28 (m, 2H), 0.94 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 150.8, 140.3, 111.0, 40.1, 29.4, 19.7, 13.4 ppm

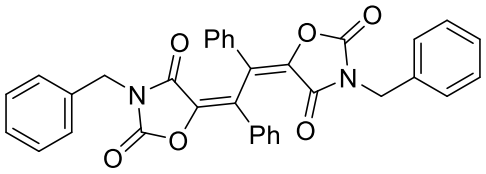
HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_8H_{10}ClNNaO_3$: 226.0244; found: 226.0246.

General Procedure E: The Synthesis of dimeric oxazolidine-2,4-diketones 3a-3e.



1 **3a-3e**

Under N_2 atmosphere, to a solution of *N*-Boc amides **1** (0.5 mmol, 1.2 equiv), $CuBr_2$ (223.4 mg, 1.0 mmol, 2.0 equiv), Cs_2CO_3 (325.8 mg,1.0 mmol, 2.0 equiv) and) in MeCN (5 mL) was added $Pd(PPh_3)_4$ (57.8 mg, 0.05 mmol, 10 mol%). Then the reaction mixture was heated to 40 °C on an oil bath and stirred at 40 °C for 12 h. The reaction mixture was diluted with H_2O (10 mL) and extracted with EtOAc (5 mL × 3). The combined organic layers were washed with water, birne, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum ether/ethyl acetate = 10:1) to afford the desired products dimeric oxazolidin-2,4-diones **3a**-**3e**.



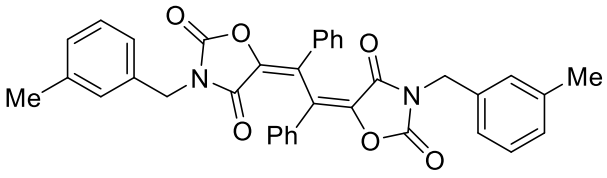
3a

(5*E*,5'*E*)-5,5'-(1,2-Diphenylethane-1,2-diylidene)bis(3-benzyloxazolidine -2,4-dione) (3a) was prepared according to the General Procedure E as a white solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 59% yield (164.1 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74-7.67 (m, 4H), 7.42-7.35 (m, 6H), 7.35-7.28 (m, 10H), 7.41-4.60 (m, 4H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 160.4, 151.3, 136.8, 134.1, 133.0, 130.3, 129.9, 128.9, 128.8, 128.7, 128.5, 123.6, 43.7 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{34}H_{24}N_2NaO_6$: 579.1532; found: 579.1542.



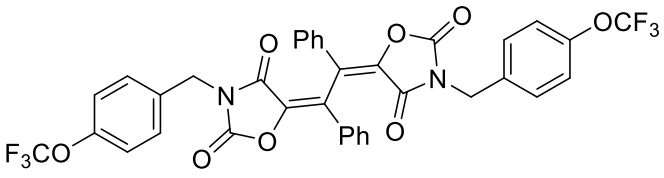
3b

(5*E*,5'*E*)-5,5'-(1,2-diphenylethane-1,2-diylidene)bis(3-(3-methylbenzyl)oxazolidine-2,4-dione) (3b) was prepared according to the General Procedure E as a white solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 49% yield (72.3mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74-7.68 (m, 4H), 7.44-7.35 (m, 6H), 7.22-7.17 (m, 2H), 7.2216-7.09 (m, 6H), 4.63 (s, 4H), 2.30 (s, 6H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 160.4, 151.4, 138.6, 136.8, 134.0, 133.0, 132.8, 130.2, 129.9, 129.2, 128.7,128.4, 125.6, 123.3, 43.7, 21.3 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{36}H_{28}N_2NaO_6$: 607.1845; found: 607.1844.



3c

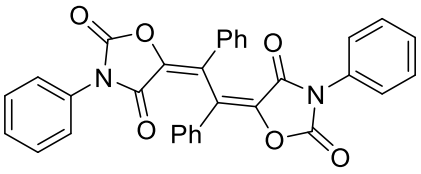
(5*E*,5'*E*)-5,5'-(1,2-Diphenylethane-1,2-diylidene)bis(3-(4-(trifluorometho-xy)benzyl)oxazolidine-2,4-dione) (3c) was prepared according to the General Procedure E as a white solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 52% yield (118.9 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80-7.65 (m, 4H), 7.46 – 7.31 (m, 10H), 7.20-7.05 (m, 4H), 4.65 (s, 4H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 1512, 149.3, 136.6, 132.9, 132.7, 130.5, 130.4, 129.9, 128.8, 124.0, 121.5 (d, J = 255.9 Hz), 121.3, 42.9 ppm.

^{19}F NMR (300 MHz, $CDCl_3$) δ -57.90 ppm.

HRMS (ESI) m/z: [M + Na]$^+$ calcd for $C_{36}H_{22}N_2NaO_6$: 747.1178; found: 747.1168.



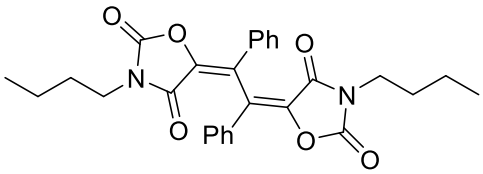
3d

(5*E*,5'*E*)-5,5'-(1,2-Diphenylethane-1,2-diylidene)bis(3-phenyloxazolidine-2,4-dione) (3d) was prepared according to the General Procedure E as a white solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 47% yield (124.1 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89-7.80 (m, 4H), .50-7.36 (m, 16H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 159.6, 150.2, 136.0, 133.1, 130.6, 130.2, 130.0, 129.3, 129.0, 128.9, 125.4, 124.6 ppm.

HRMS (ESI) m/z: [M + Na]$^+$ calcd for $C_{32}H_{20}N_2NaO_6$: 551.1219; found: 551.1210.



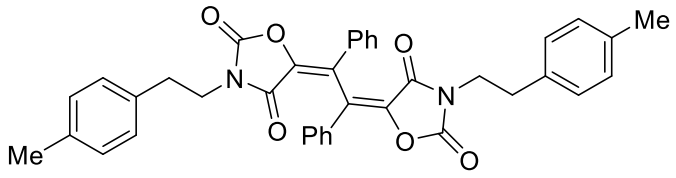
3e

(5*E*,5'*E*)-5,5'-(1,2-Diphenylethane-1,2-diylidene)bis(3-butyloxazolidine-2,4-dione) (3e) was prepared according to the General Procedure E as a white solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 36% yield (88.1 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80-7.65 (m, 4H), 7.50-7.30 (m, 6H), 3.65-3.45 (m, 4H), 1.72-1.52 (m, 4H), 1.35-1.20 (m, 4H), 1.02-0.82 (m, 6H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 160.8, 151.6, 136.8, 133.1, 130.2, 129.8, 128.7, 123.2, 40.4, 29.5, 19.7, 13.4 ppm.

HRMS (ESI) m/z: [M + Na]$^+$ calcd for $C_{28}H_{28}N_2NaO_6$: 511.1845; found: 511.1844.



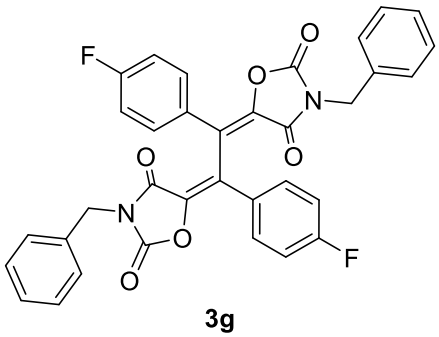
3f

(5*E*,5′*E*)-5,5'-(1,2-diphenylethane-1,2-diylidene)bis(3-(4-methylphenethyl)oxazolidine-2,4-dione) (3f) was prepared according to the General Procedure E as a white solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 40% yield (42.0 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72-7.66 (m, 4H), 7.44-7.35 (m, 6H), 7.12-6.99 (m, 8H), 3.80-3.70(m, 4H), 2.89 (t, *J* = 8.0 Hz, 4H), 2.29 (s, 6H)ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 160.5, 151.4, 136.5, 136.4, 133.6, 133.1, 130.2, 129.8, 129.4, 128.8, 128.6, 123.3, 41.5, 32.9, 21.1ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{38}H_{32}N_2NaO_6$: 635.2158; found: 635.2155.



3g

(5*E*,5'*E*)-5,5'-(1,2-Bis(4-fluorophenyl)ethane-1,2-diylidene)bis(3-benzylo-xyloxazolidine-2,4-dione) (3g) was prepared according to the General Procedure E as a white solid (chromatography eluent: petroleum ether/EtOAc = 10:1) in 40% yield (118.9 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74-7.66 (m, 4H), 7.34-7.28 (m, 10H), 7.12-7.03 (m, 4H), 4.70-4.60 (m, 4H) ppm.

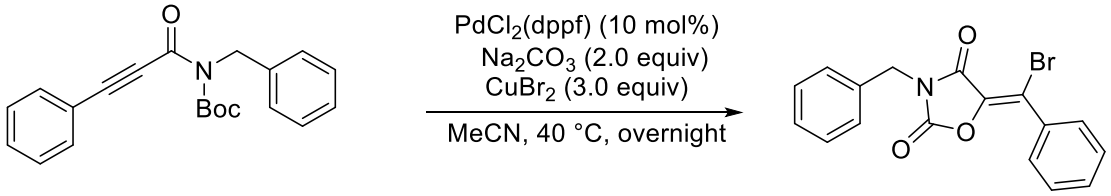
^{13}C NMR (100 MHz, $CDCl_3$) δ 163,5 (d, *J* = 252.0 Hz), 160.3, 151.1, 136.6, 134.0, 132.1 (d, *J* = 9.0 Hz), 129.0 (d, *J* = 3.1 Hz), 128.9, 128.8, 128.6, 122.2, 116.1 (d, *J* = 2.2 Hz), 43.8 ppm.

^{19}F NMR (300 MHz, $CDCl_3$) δ -108.14 ppm.

HRMS (ESI) m/z: $[M + Na]^+$ calcd for $C_{34}H_{22}F_2N_2NaO_6$: 615.1344; found: 615.1345.

IV. Synthetic Transformation of Oxazolidine-2,4-diones

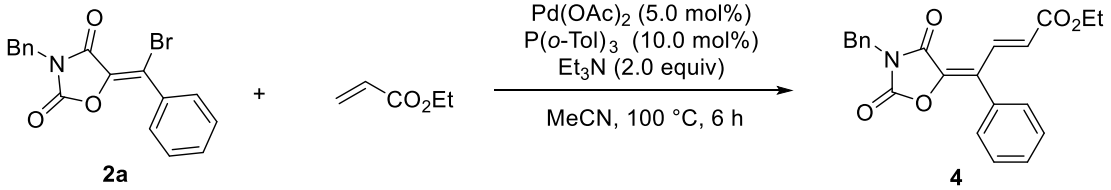
Scale-up reaction



1a **2a**

Under N_2 atmosphere, to a solution of *N*-Boc amides **1a** (1.67 g, 5.0 mmol, 1.2 equiv), $CuBr_2$ (3.35 g, 15.0 mmol, 3.0 equiv), Na_2CO_3 (1.01 g, 10.0 mmol, 2.0 equiv) in MeCN (50 mL) was added $PdCl_2$(dppf) (0.36 g, 0.5 mmol, 10 mol%). Then the reaction mixture was heated to 40 °C on an oil bath and stirred at 40 °C for 12 h. The reaction mixture was diluted with H_2O (50 mL) and extracted with EtOAc (30 mL × 3). The combined organic layers were washed with water, birne, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum ether/ethyl acetate = 20:1) to afford the desired oxazolidin-2,4-dione **2a** as a white solid in 82% yield (1.47 g).

Heck coupling of 2a.



2a **4**

Ethyl (2*E*, 4*Z*)-4-(3-benzyl-2,4-dioxooxazolidin-5-ylidene)-4-phenylbut-2-enoate (4): Under N_2 atmosphere, to a solution of $Pd(OAc)_2$ (2.2 mg, 0.01 mmol, 5.0 mol%), P(*o*-tol)$_3$ (6.0 mg, 0.02 mmol, 10 mol %) and **2a** (72.0 mg, 0.2 mmol, 1.0 equiv) in MeCN (2 mL) was added ethyl acrylate (45.0 mg, 0.4 mmol, 2.0 equiv) and Et_3N (101.1 mg, 2.0 mmol, 10.0 equiv). Then the

reaction mixture was heated to 100 °C on an oil bath and stirred at 100 °C for 6 h. The reaction mixture was diluted with H_2O (10 mL) and extracted with EtOAc (5.0 mL × 3). The combined organic layers were washed with water, birne, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum ether/ethyl acetate = 30:1) to afford the desired products **4** as a yellow soild in 53% yield (40.0 mg).

Major isomer:

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.73 (d, *J* = 15.8 Hz, 1H), 7.51 – 7.40 (m, 4H), 7.40-7.29 (m, 4H), 7.28-7.18 (m, 2H), 5.92 (d, *J* = 15.8 Hz, 1H), 4.78 (s, 2H), 4.28-4.18 (m, 2H), 1.34-1.27(m, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) 165.8, 160.4, 151.1, 137.6, 137.5, 134.2, 131.0, 129.6, 129.5, 129.4, 129.2, 129.0, 128.9, 128.6, 128.5, 61.0, 43.8, 29.7 ppm.

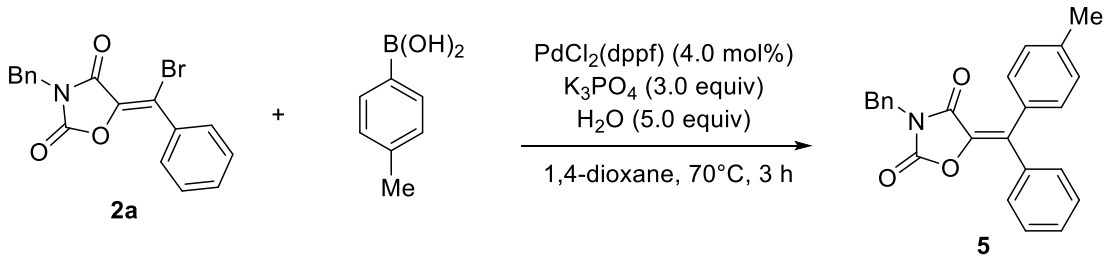
Minor isomer:

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.94 (d, *J* = 15.7 Hz, 1H), 7.51 – 7.40 (m, 4H), 7.40-7.29 (m, 4H), 7.28-7.18 (m, 2H), 5.80 (d, *J* = 15.7 Hz, 1H), 4.78 (s, 2H), 4.28-4.18 (m, 2H), 1.34-1.27(m, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) 165.6, 159.5, 150.9, 137.8, 137.5, 134.2, 130.3, 129.6, 129.34, 129.31, 129.1, 129.0, 128.8, 128.6, 127.4, 60.9, 43.8, 14.2 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{22}H_{20}NO_5$: 378.1441; found: 378.1336.

Suzuki-Miyaura Cross-Coupling of 2a



(*E*)-3-Benzyl-5-(phenyl(p-tolyl)methylene)oxazolidine-2,4-dione (5): Under N_2 atmosphere, to a solution of Pd(dppf)Cl_2 (7.3 mg, 0.008 mmol, 4.0

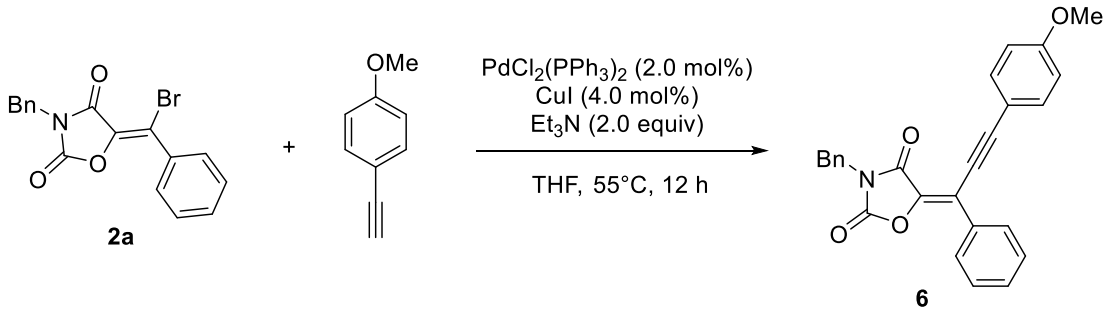
mol%), **2a** (72.0 mg, 0.2 mmol,1.0 equiv), and *p*-tolylboronic acid (54.4 mg, 0.6 mmol, 2.0 equiv), K_3PO_4 (127.0 mg, 0.6 mmol, 3.0 equiv) in 1,4-dioxane (2.0 mL) was added H_2O (18 μL, 1.0 mmol, 5.0 equiv).Then the reaction mixture was heated to 70 °C on an oil bath and stirred at 70 °C for 3 h. The reaction mixture was diluted with H_2O (10 mL) and extracted with EtOAc (5.0 mL × 3). The combined organic layers were washed with water, birne, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum ether/ethyl acetate = 30: 1) to afford the desired products **5** as a white soild in 92% yield (65.9 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47-7.29 (m, 10 H), 7.25 - 7.20 (m, 2H), 7.20-7.14 (m, 2H), 4.72 (s, 2H), 2.41 (s, 3H)ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 160.6, 151.9, 139.5, 136.0, 134.6, 134.5, 133.6, 131.8, 130.8, 130.3, 129.8, 129.3, 128.9, 128.8, 128.4, 128.2, 43.6, 21.5 ppm.

HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{24}H_{20}NO_3$: 370.1443; found: 370.1435.

Sonogashira coupling of 2a.



(*E*)-3-Benzyl-5-(3-(4-methoxyphenyl)-1-phenylprop-2-yn-1-ylidene)oxazolidine-2,4-dione (6): Under N_2 atmosphere, to a solution of $PdCl_2(PPh_3)_2$ (4.2 mg, 12.0 mg, 2.0 mol%), CuI (2.3 mg, 0.006 mmol, 4.0 mol%), and 2a (107.5 mg, 0.3 mmol, 1.0 equiv) in THF (2.0 mL) was added1-ethynyl-4-methoxybenzene (48.0 mg, 0.36 mmol, 1.2 equiv) and Et_3N (60.7 mg, 0.6 mmol, 2.0 equiv).Then the reaction mixture was heated to 55 °C on an oil bath and stirred at 55 °C for

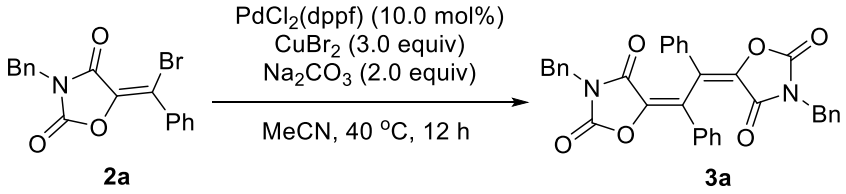
12 h. The reaction mixture was diluted with H_2O (10 mL) and extracted with EtOAc (5.0 mL × 3). The combined organic layers were washed with water, birne, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum ether/ethyl acetate = 12:1) to afford the desired products **6** as a white soild in 58% yield (70.1 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.92 (m, 2H), 7.62 (d, *J* = 8.8 Hz, 2H), 7.52 - 7.39 (m, 5H), 7.40-7.30 (m, 3H), 6.91 (d, *J* = 8.2 Hz, 2H), 4.82 (s, 2H), 3.85 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 160.6, 160.1, 151.0, 140.1, 134.5, 133.9, 132.5, 130.2, 129.7, 128.8 (2C), 128.52, 128.45, 114.3, 114.2, 113.2, 101.5, 83.7, 55.3, 43.7 ppm.

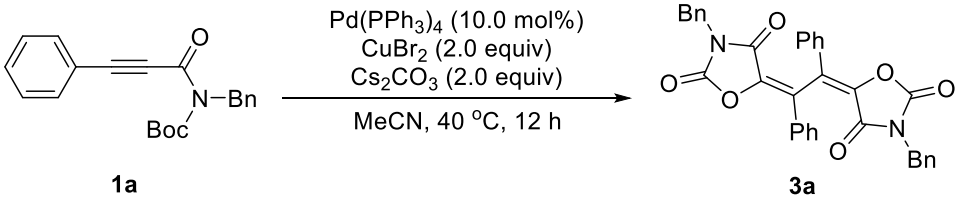
HRMS (ESI) m/z: $[M + H]^+$ calcd for $C_{26}H_{20}NO_4$: 410.1392; found: 410.1396.

V. Controlled Experiments for Mechanism



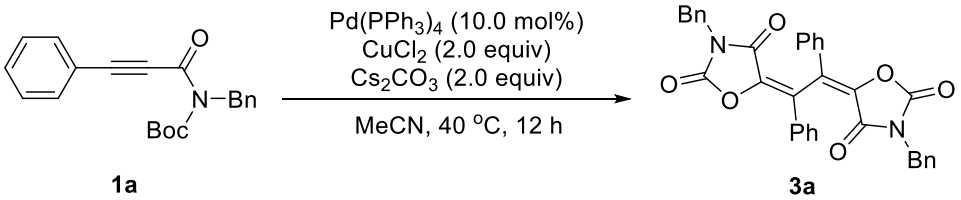
2a **3a**

Under N_2 atmosphere, to a solution of **2a** (35.8 mg, 0.1 mmol, 1.0 equiv), $CuBr_2$ (66.9 mg, 0.3 mmol, 3.0 equiv), Na_2CO_3 (21.2 g, 0.2 mmol, 2.0 equiv) in MeCN (1.0 mL)was added $Pd(PPh_3)_4$ (7.3 mg, 0.01 mmol, 10.0 mol%). Then the reaction mixture was heated to 40 °C on an oil bath and stirred at 40 °C for 12 h. **3a** cannot be obtained from this reaction.



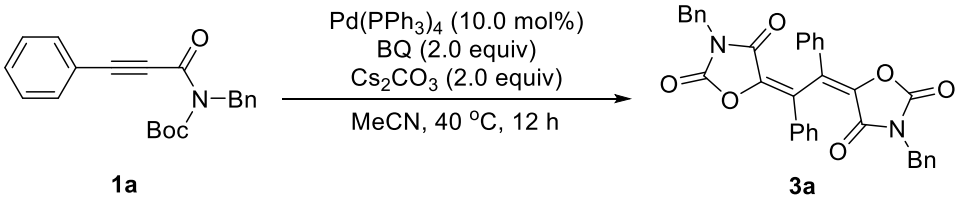
1a **3a**

Under N_2 atmosphere, to a solution of **1a** (33.5 mg, 0.1 mmol, 1.0 equiv), $CuBr_2$ (44.6 mg, 0.2 mmol, 2.0 equiv), Cs_2CO_3 (65.0 g, 0.2 mmol, 2.0 equiv) in MeCN (1.0 mL)was added $Pd(PPh_3)_4$ (11.6 mg, 0.01 mmol, 10.0 mol%). Then the reaction mixture was heated to 40 °C on an oil bath and stirred at 40 °C for 12 h. The yield of 69% was determined by ^1H NMR on the crude reaction mixture using CH_2Br_2 as an internal standard.



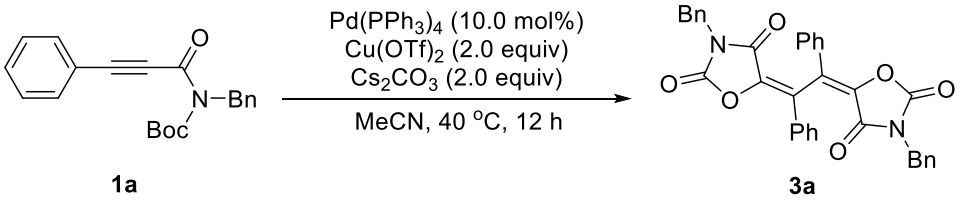
1a **3a**

Under N_2 atmosphere, to a solution of **1a** (33.5 mg, 0.1 mmol, 1.0 equiv), $CuCl_2$ (26.8 mg, 0.2 mmol, 2.0 equiv), Cs_2CO_3 (65.0 g, 0.2 mmol, 2.0 equiv) in MeCN (1.0 mL)was added $Pd(PPh_3)_4$ (11.6 mg, 0.01 mmol, 10.0 mol%). Then the reaction mixture was heated to 40 °C on an oil bath and stirred at 40 °C for 12 h. The yield of 51% was determined by ^1H NMR on the crude reaction mixture using CH_2Br_2 as an internal standard.



1a **3a**

Under N_2 atmosphere, to a solution of **1a** (33.5 mg, 0.1 mmol, 1.0 equiv), 1,4-Benzoquinone (21.6 mg, 0.2 mmol, 2.0 equiv), Cs_2CO_3 (65.0 g, 0.2 mmol, 2.0 equiv) in MeCN (1.0 mL)was added $Pd(PPh_3)_4$ (11.6 mg, 0.01 mmol, 10.0 mol%). Then the reaction mixture was heated to 40 °C on an oil bath and stirred at 40 °C for 12 h. The yield of 28% was determined by ^1H NMR on the crude reaction mixture using CH_2Br_2 as an internal standard.



1a **3a**

Under N_2 atmosphere, to a solution of **1a** (33.5 mg, 0.1 mmol, 1.0 equiv), $Cu(OTf)_2$ (72.3 mg, 0.2 mmol, 2.0 equiv), Cs_2CO_3 (65.0 g, 0.2 mmol, 2.0 equiv) in MeCN (1.0 mL)was added $Pd(PPh_3)_4$ (11.6 mg, 0.01 mmol, 10.0 mol%). Then the reaction mixture was heated to 40 ^oC on an oil bath and stirred at 40 ^oC for 12 h. The yield of 25% was determined by ^1H NMR on the crude reaction mixture using CH_2Br_2 as an internal standard.

VI. Determination of Product Structure

The structure of product **2a′** was determined by X-ray diffraction. The X-ray data have been deposited at the Cambridge Crystallographic Data Center (CCDC 2289407). The data can be obtained free of charge via the internet at https://www.ccdc.cam.ac.uk/structures/. The measurements were taken in a Bruker D8 Venture CCD diffractometer. The data were integrated by Bruker D8 Venture with \f and \w scans absorption corrections. The structure solution and refinement were processed by ShelXL (Sheldrick, 2015).

Method of crystallization: A solution of **2a′** in EA and petroleum ether was evaporated the solvent slowly at room temperature.

Crystal data and structure for 2a′

Table S1 Crystal data and structure refinement for 2a'

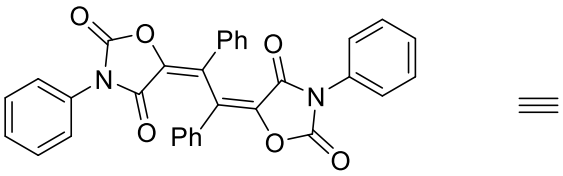
Identification code	**2a'**
Empirical formula	$C_{17}H_{12}ClNO_3$
Formula weight	313.73
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.33774(13)
b/Å	12.11111(16)
c/Å	12.88123(17)
α/°	90
β/°	106.4445(14)
γ/°	90

Volume/Å^3	1397.15(3)
Z	4
ρ_{calc}g/cm^3	1.491
μ/mm^{-1}	2.537
F(000)	648.0
Crystal size/mm^3	0.28 × 0.24 × 0.07
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	9.876 to 148.204
Index ranges	-10 ≤ h ≤ 11, -14 ≤ k ≤ 14, -14 ≤ l ≤ 16
Reflections collected	8023
Independent reflections	2780 [R_{int} = 0.0162, R_{sigma} = 0.0161]
Data/restraints/parameters	2780/0/199
Goodness-of-fit on F^2	1.039
Final R indexes [I>=2σ (I)]	R_1 = 0.0273, wR_2 = 0.0726
Final R indexes [all data]	R_1 = 0.0293, wR_2 = 0.0738
Largest diff. peak/hole / e Å^{-3}	0.30/-0.28

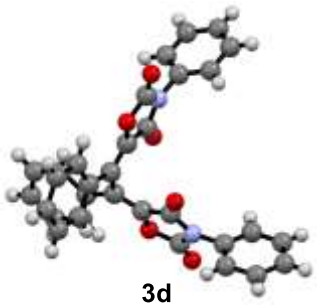
The structure of product **3d** was determined by X-ray diffraction. The X-ray data have been deposited at the Cambridge Crystallographic Data Center (CCDC 2289645). The data can be obtained free of charge via the internet at https://www.ccdc.cam.ac.uk/structures/. The measurements were taken in a Bruker D8 Venture CCD diffractometer. The data were integrated by Bruker D8 Venture with \f and \w scans absorption corrections. The structure solution and refinement were processed by ShelXL (Sheldrick, 2015).

Method of crystallization: A solution of **3c** in EA and petroleum ether was evaporated the solvent slowly at room temperature.

Crystal data and structure for 3c



3d



3d
CCDC 2289645
ORTEP at 50% probability

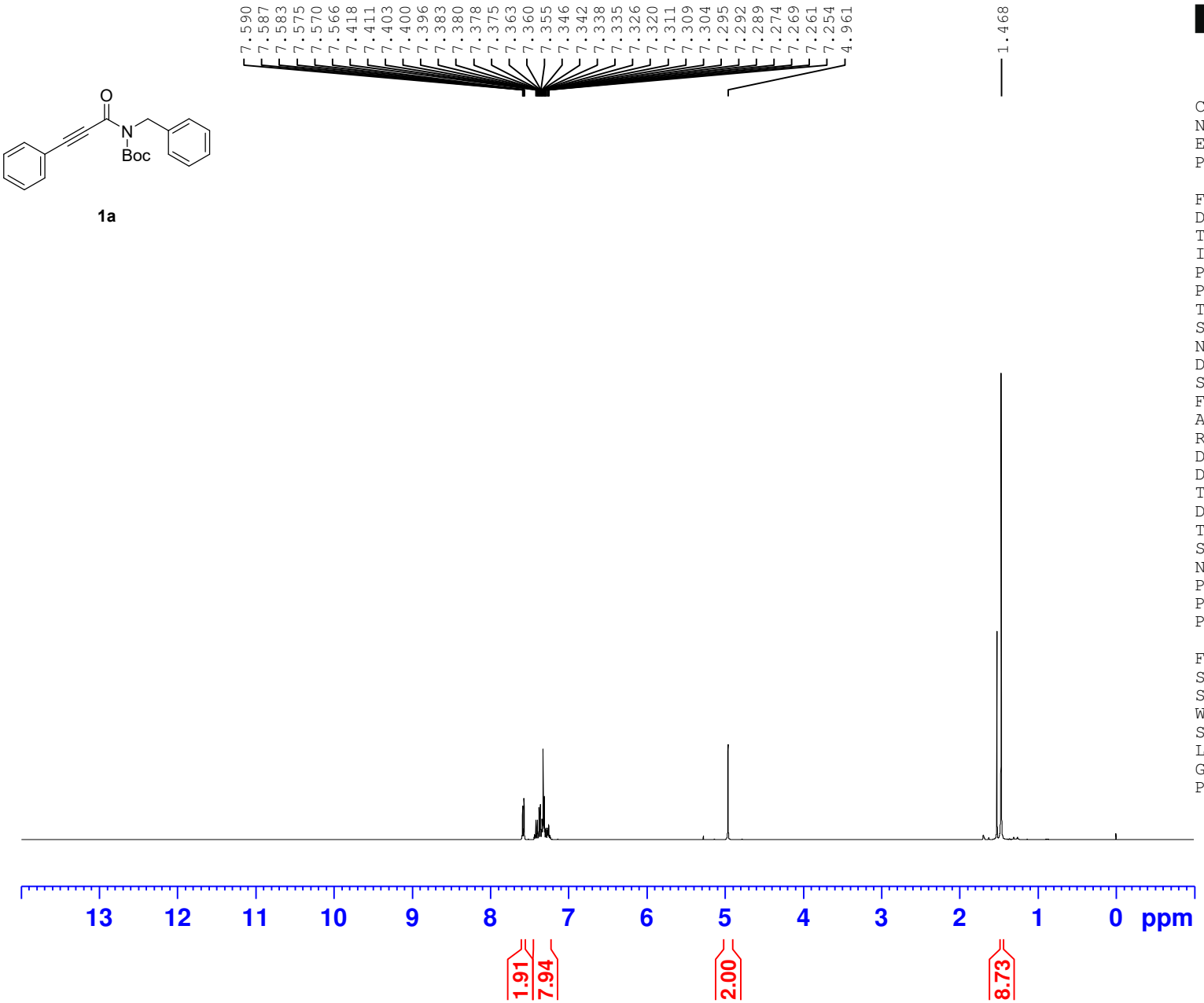
Table S2 Crystal data and structure refinement for 3d

Identification code	**3d**
Empirical formula	$C_{32}H_{20}N_2O_6$
Formula weight	528.50
Temperature/K	100
Crystal system	monoclinic
Space group	C 2/c
a/Å	19.868(1)
b/Å	8.3809(4)
c/Å	16.6626(9)
α/°	90
β/°	116.2585(14)
γ/°	90
Volume/Å^3	2488.2(2)
Z	4

ρ_{calc}g/cm^3	1.411
μ/mm^{-1}	2.286
F(000)	1096
Crystal size/mm^3	0.27 × 0.25 × 0.19
Radiation	MoK\a (λ = 0.71073)
Reflections collected	8557
Independent reflections	2189 [R_{int} = 0.0394, R_{sigma} = 0.0456]
Data/restraints/parameters	2189/0/181
Goodness-of-fit on F^2	1.031
Final R indexes [I>=2σ (I)]	R_1 = 0.0367, wR_2 = 0.0895
Final R indexes [all data]	R_1 = 0.0450, wR_2 = 0.0951
Largest diff. peak/hole / e Å^{-3}	0.165/-0.225

NMR spectra

1a



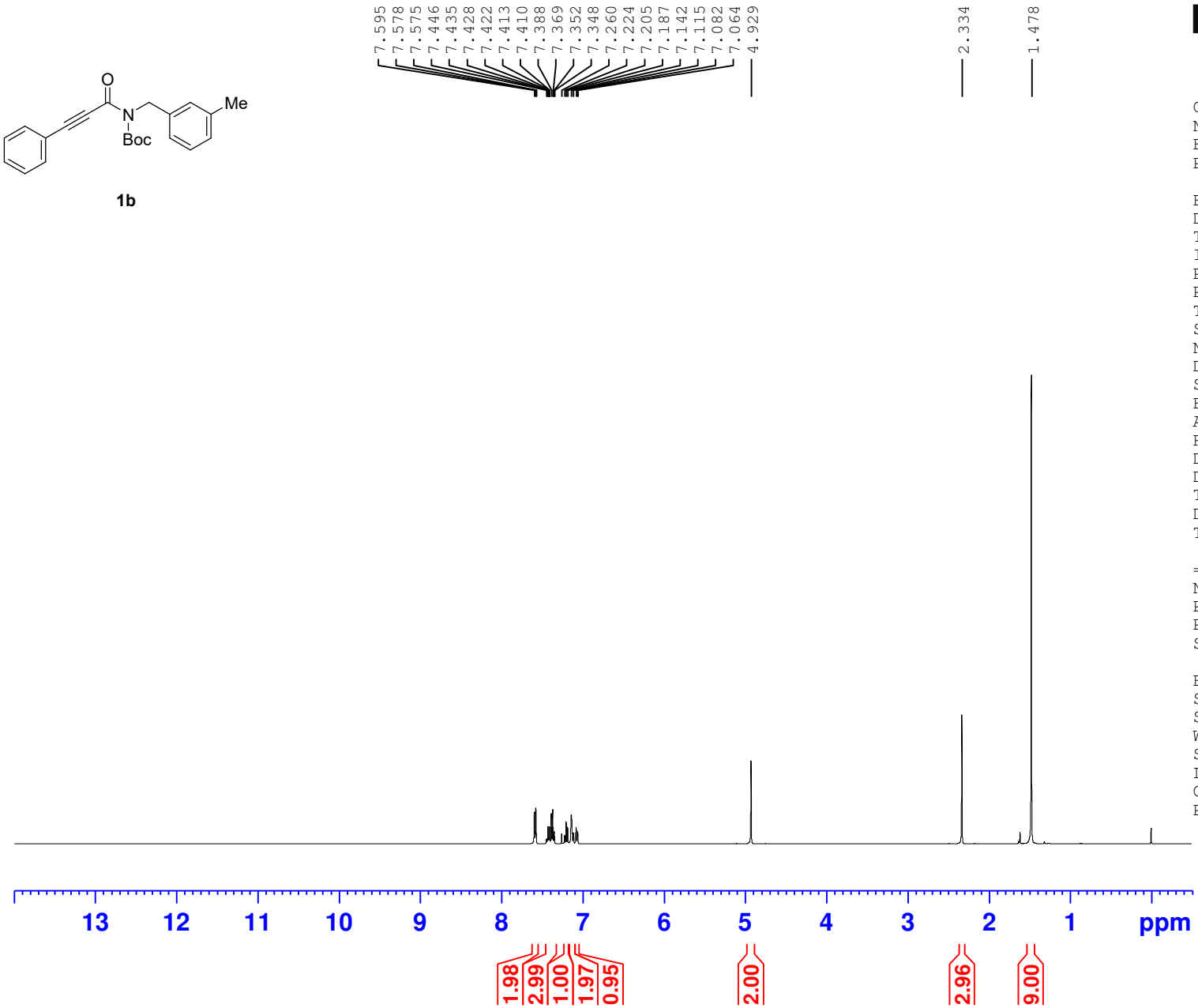
Current Data Parameters
NAME ZHL-2-24-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221102
Time 13.44 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 45.4545
DW 61.000 usec
DE 13.54 usec
TE 294.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.73200035 W

F2 - Processing parameters
SI 65536
SF 400.1300121 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZHL-3-18

1b



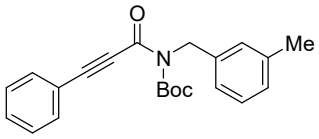
Current Data Parameters
NAME 20230308-400M
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230307
Time 22.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 113.67
DW 60.800 usec
DE 6.50 usec
TE 292.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

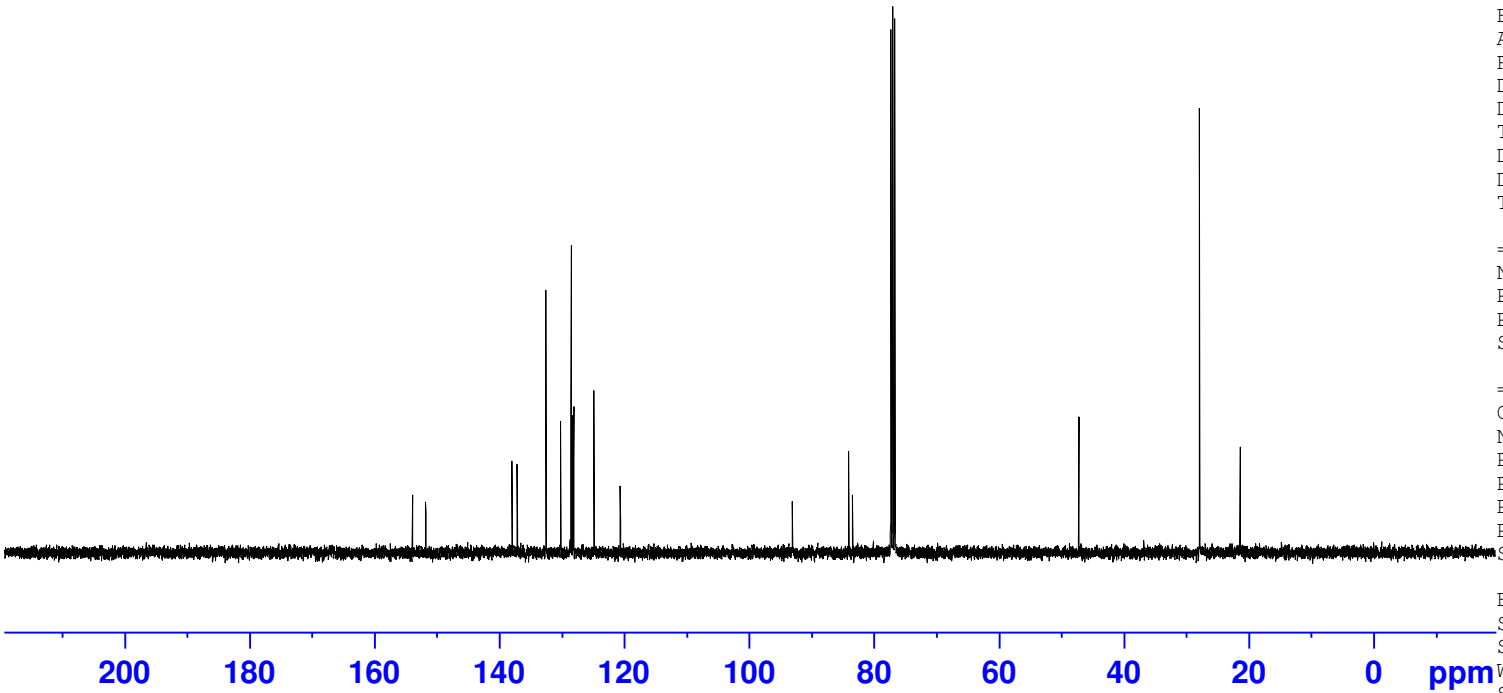
F2 - Processing parameters
SI 65536
SF 400.1900161 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-18



1b

153.92
151.80
137.98
137.15
132.57
130.22
128.55
128.47
128.24
128.11
124.86
120.64
93.11
84.05
83.43
77.31
77.00
76.68
47.19
27.89
21.36



Current Data Parameters
NAME 20230310-400M
EXPNO 58
PROCNO 1

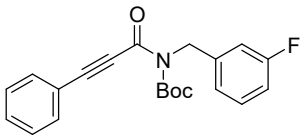
F2 - Acquisition Parameters
Date_ 20230309
Time 14.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 110
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 295.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

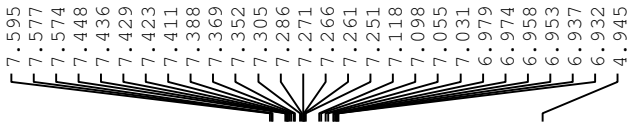
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

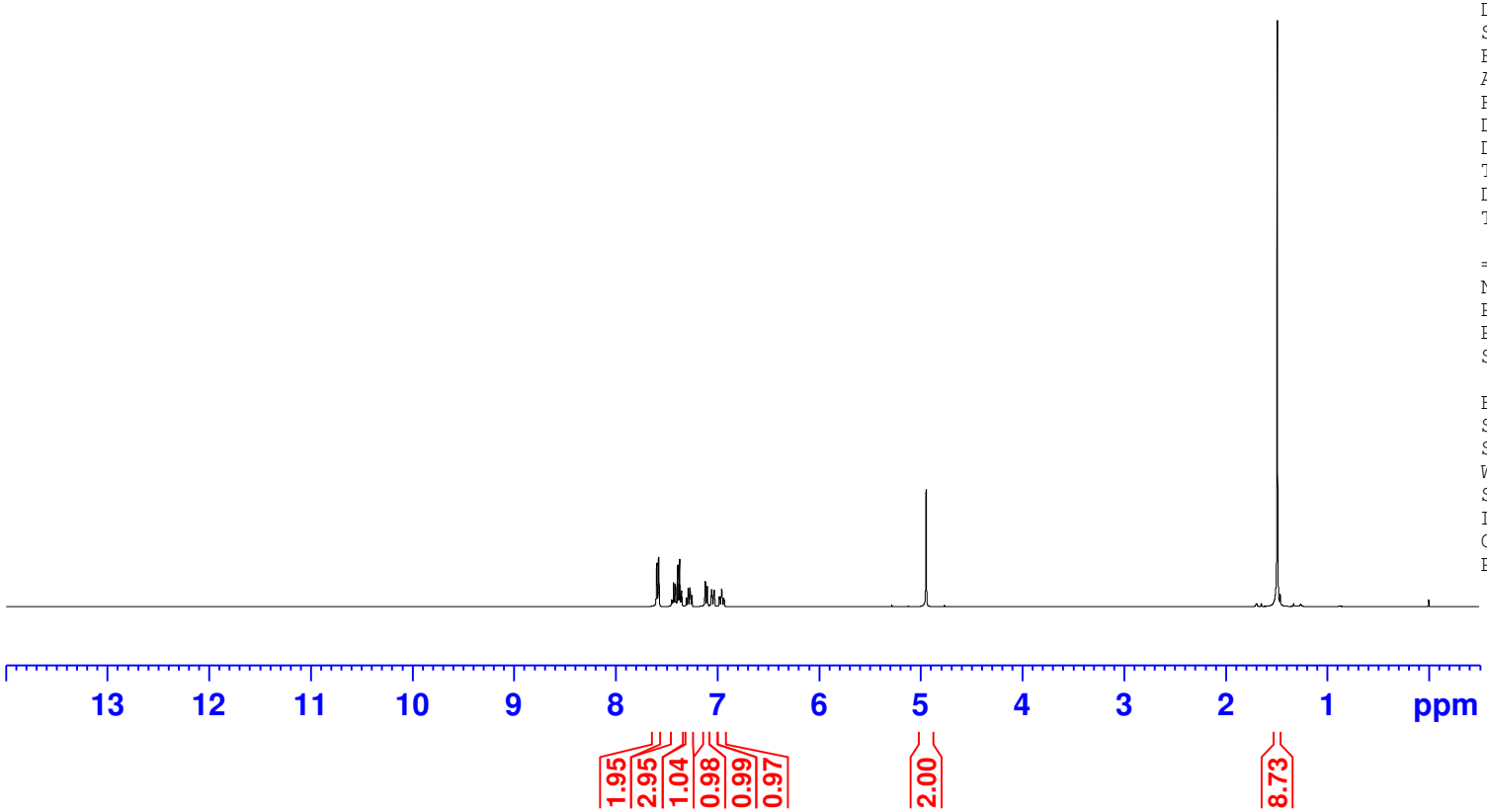
F2 - Processing parameters
SI 32768
SF 100.6278630 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZHL-3-23



1c





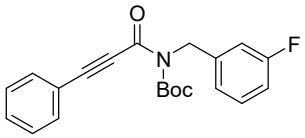
Current Data Parameters
NAME 20230308-400M
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230307
Time 23.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 61.19
DW 60.800 usec
DE 6.50 usec
TE 292.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

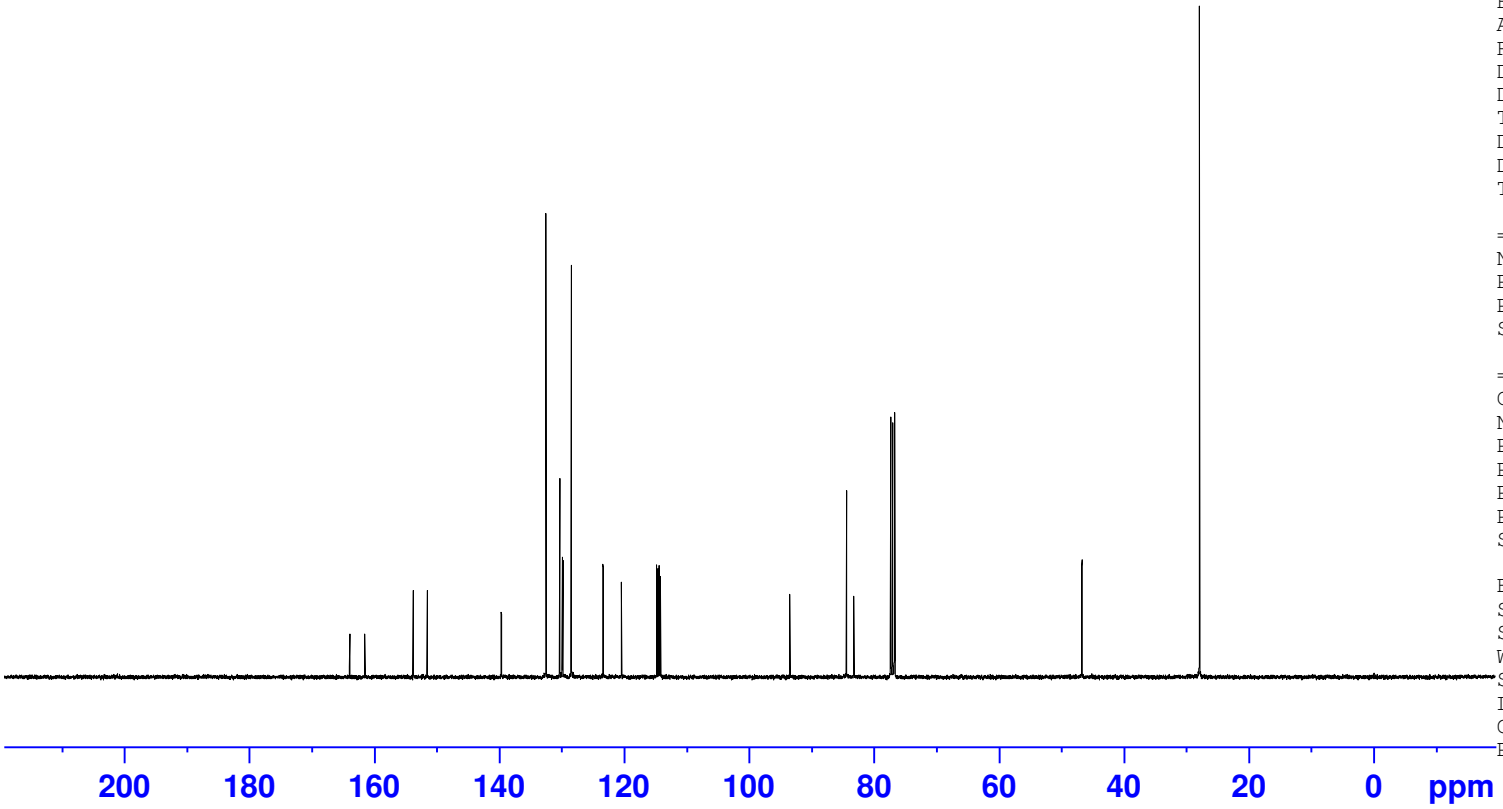
F2 - Processing parameters
SI 65536
SF 400.1900157 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-23



1c

163.97
161.52
153.78
151.53
139.73
139.65
132.53
130.31
129.91
129.83
128.48
123.38
123.35
120.44
114.81
114.60
114.40
114.19
93.47
84.38
83.22
77.31
77.00
76.68
46.70
46.69
27.86



Current Data Parameters
NAME 20230310-400M
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230310
Time 8.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 294.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

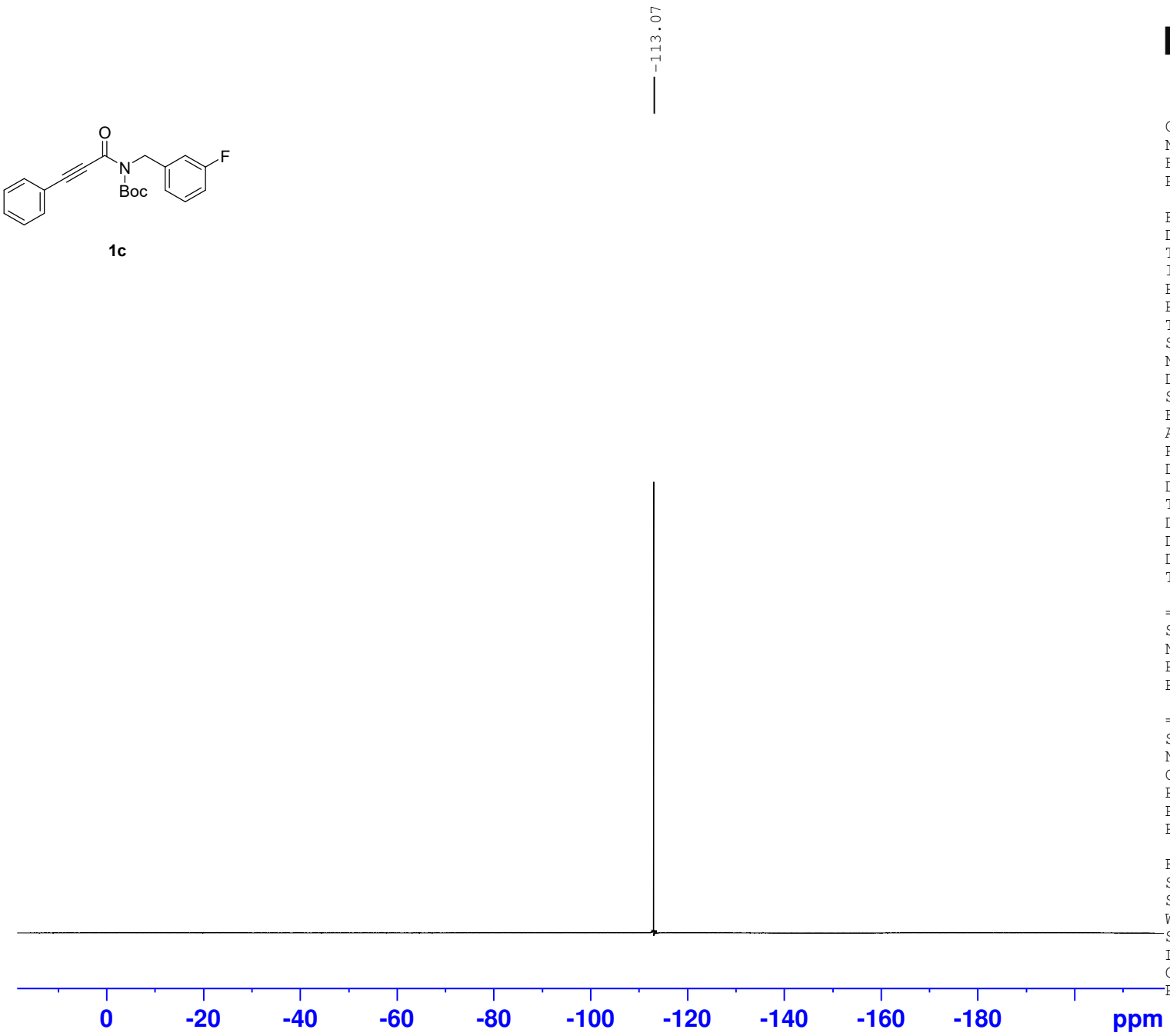
======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278664 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

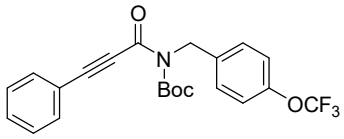
hh-zhl-3-23

1c

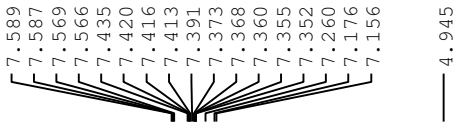


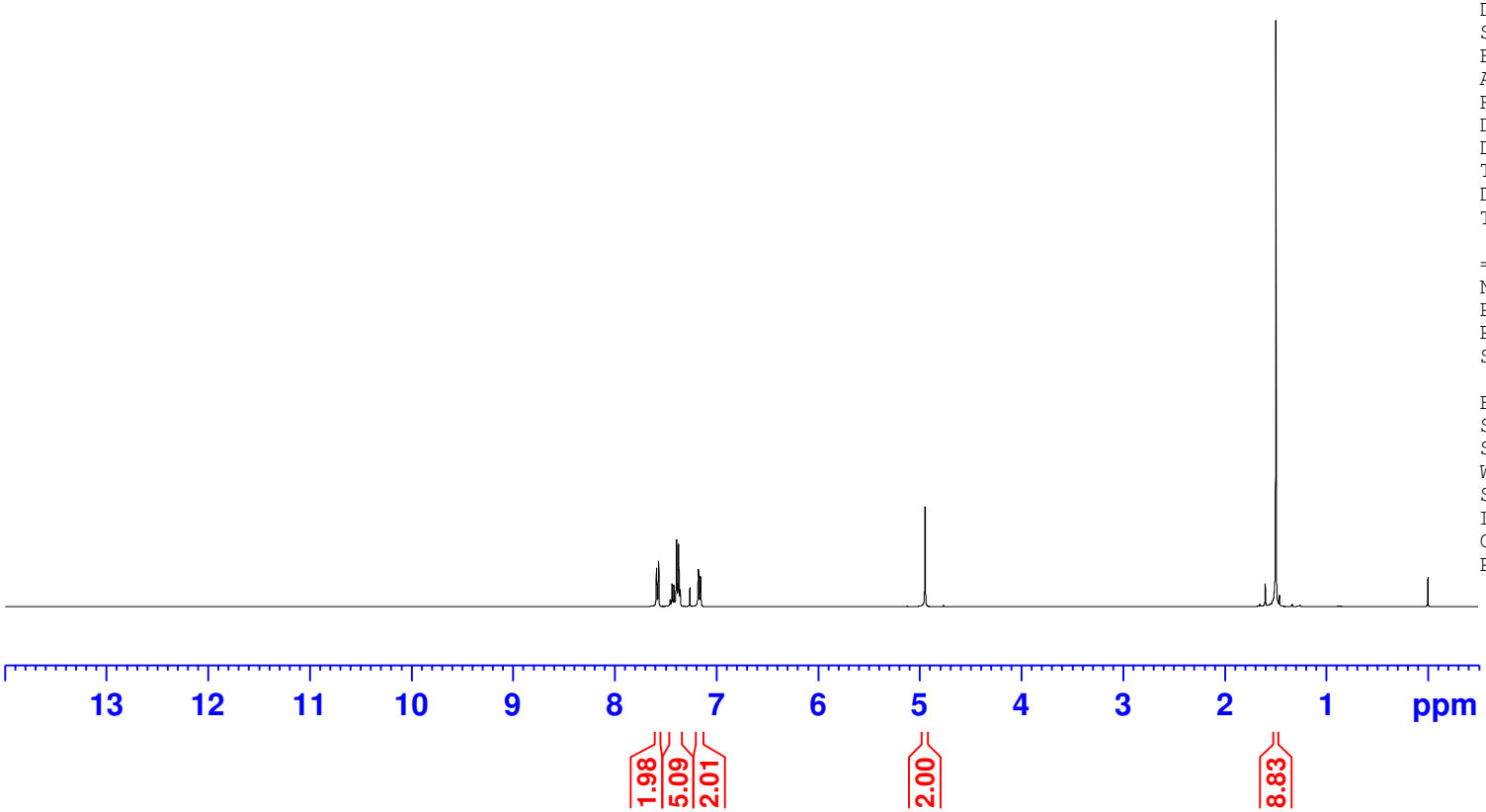

```
Current Data Parameters
NAME      20230320-300M
EXPNO                18
PROCNO                1

F2 - Acquisition Parameters
Date_          20230320
Time               14.36
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG      zgfhigqn.2
TD              131072
SOLVENT            CDCl3
NS                    16
DS                     4
SWH           66964.289 Hz
FIDRES         0.510897 Hz
AQ            0.9786710 sec
RG                   203
DW                 7.467 usec
DE                 6.50 usec
TE                 289.7 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        282.3761148 MHz
NUC1                19F
P1                14.50 usec
PLW1        10.39999962 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.17284000 W

F2 - Processing parameters
SI                 65536
SF          282.4043552 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

ZHL-3-19



1d





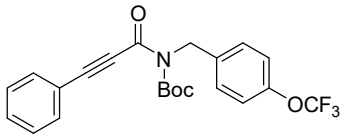
Current Data Parameters
NAME 20230308-400M
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230307
Time 23.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 140.02
DW 60.800 usec
DE 6.50 usec
TE 292.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

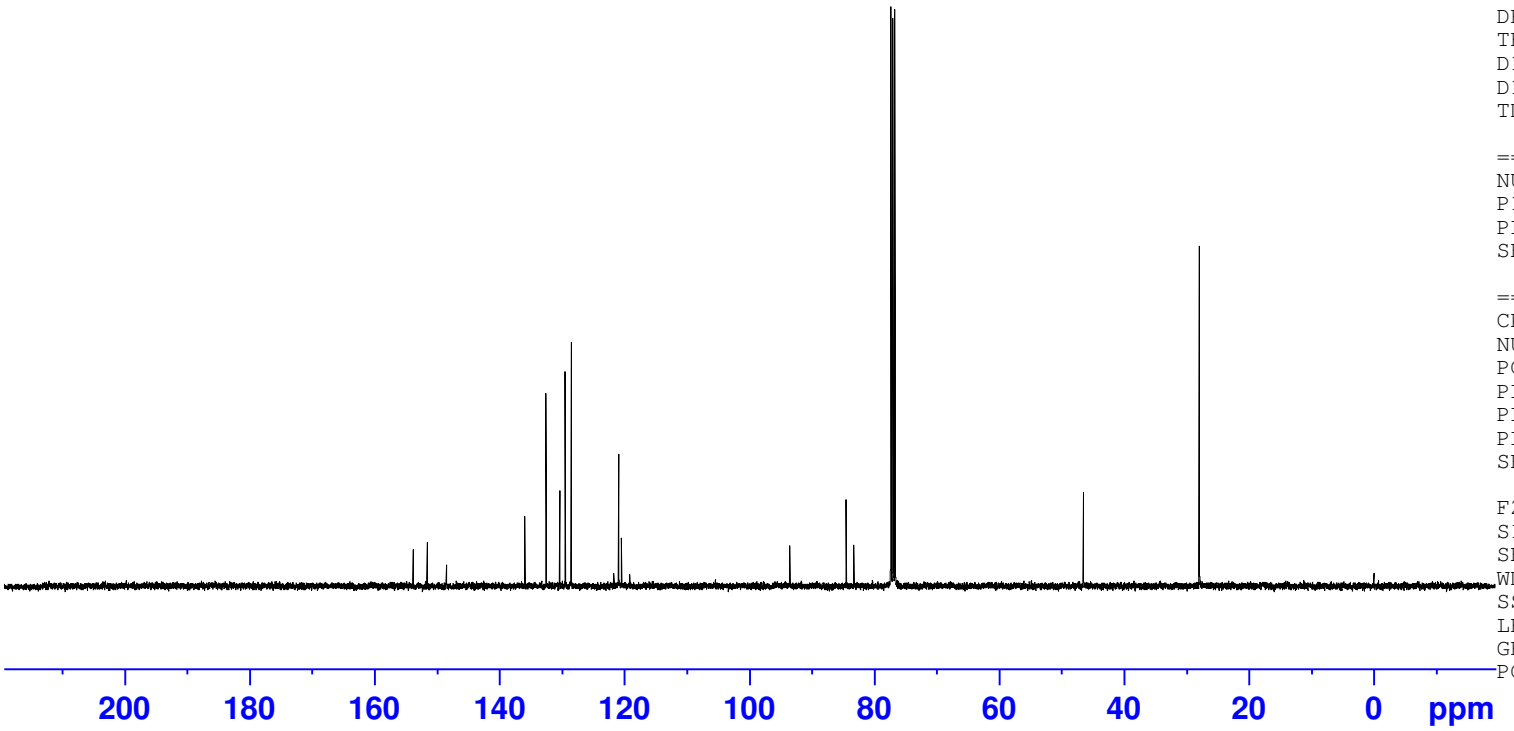
F2 - Processing parameters
SI 65536
SF 400.1900160 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-19



1d

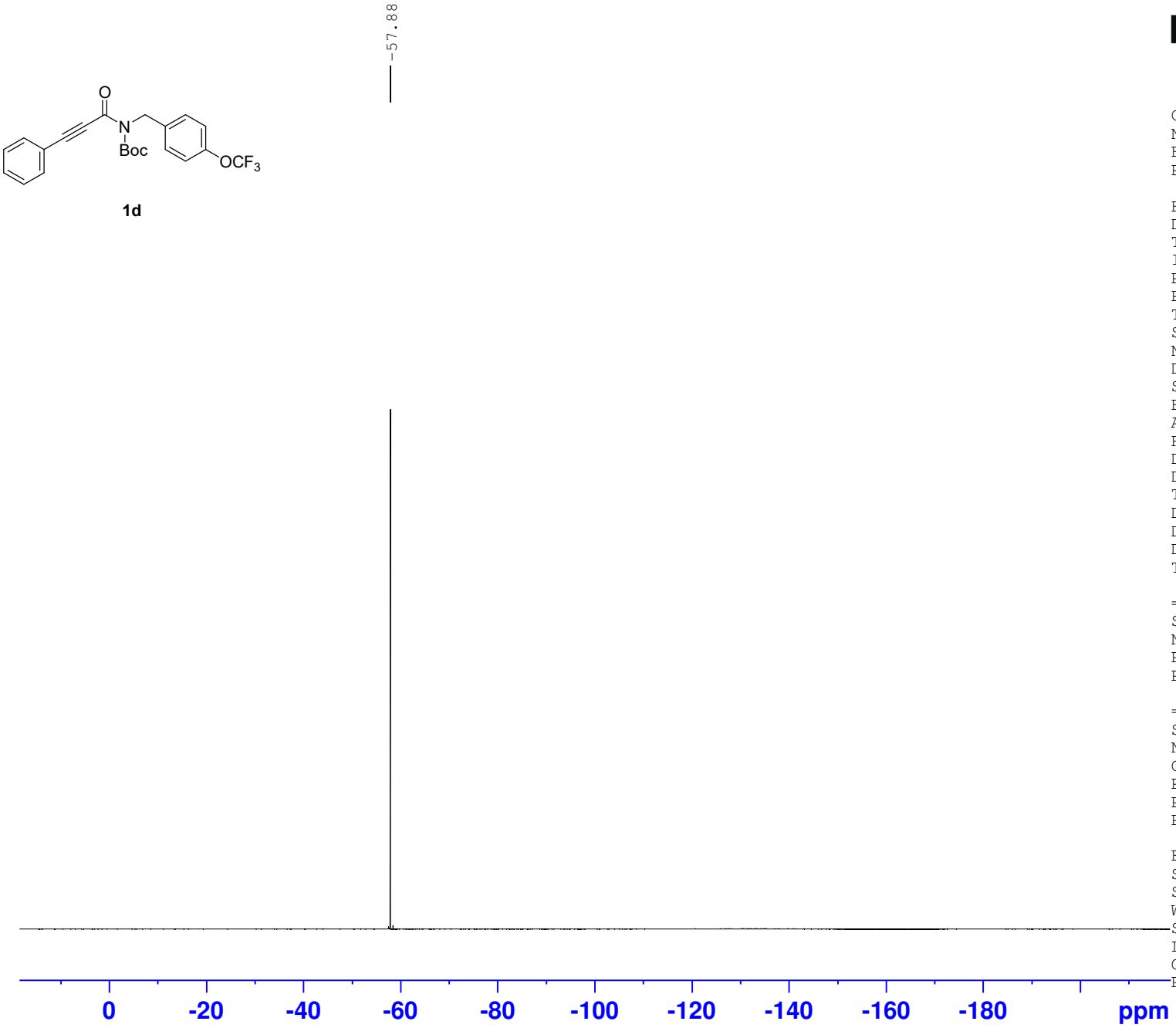
153.84
151.60
148.51
135.97
132.55
130.35
129.51
128.53
123.77
121.69
120.91
120.48
119.14
116.94
93.52
84.50
83.26
77.32
77.00
76.68
46.50
27.93




```
Current Data Parameters
NAME      20230310-400M
EXPNO                22
PROCNO                1

F2 - Acquisition Parameters
Date_          20230310
Time               9.07
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE                294.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                12.00 usec
PLW1         53.00000000 W
SFO1        100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2         14.00000000 W
PLW12         0.37246999 W
PLW13         0.30170000 W
SFO2        400.1916008 MHz

F2 - Processing parameters
SI                32768
SF          100.6278609 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

hh-zhl-3-19

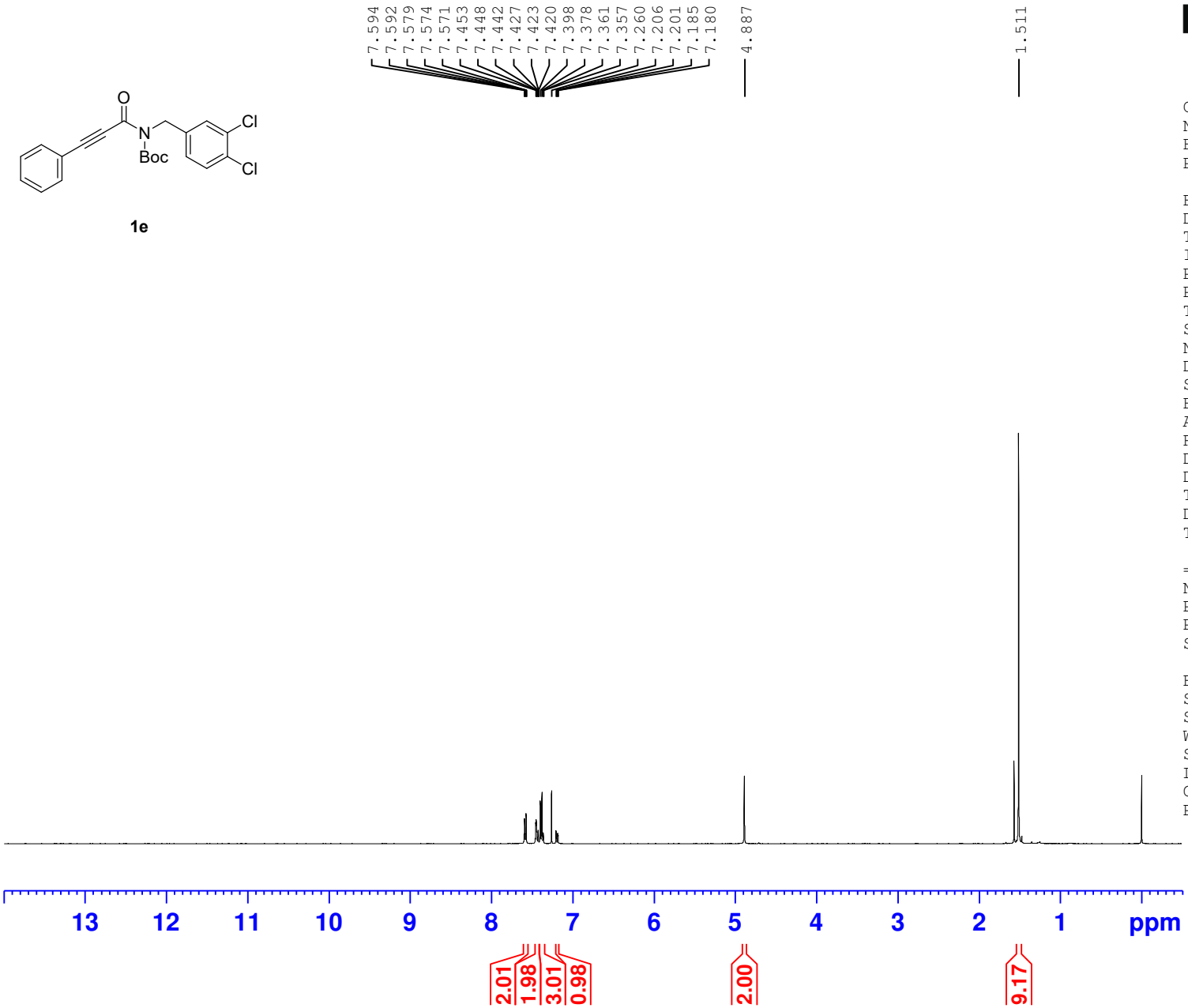
1d




```
Current Data Parameters
NAME      20230320-300M
EXPNO                17
PROCNO                1

F2 - Acquisition Parameters
Date_          20230320
Time               14.32
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG      zgfhigqn.2
TD              131072
SOLVENT            CDCl3
NS                    16
DS                     4
SWH           66964.289 Hz
FIDRES         0.510897 Hz
AQ            0.9786710 sec
RG                   203
DW                 7.467 usec
DE                 6.50 usec
TE                 289.7 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        282.3761148 MHz
NUC1                19F
P1                14.50 usec
PLW1        10.39999962 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.17284000 W

F2 - Processing parameters
SI                 65536
SF          282.4043552 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

CB-1-19

1e



Current Data Parameters
NAME 20230310-400M
EXPNO 41
PROCNO 1

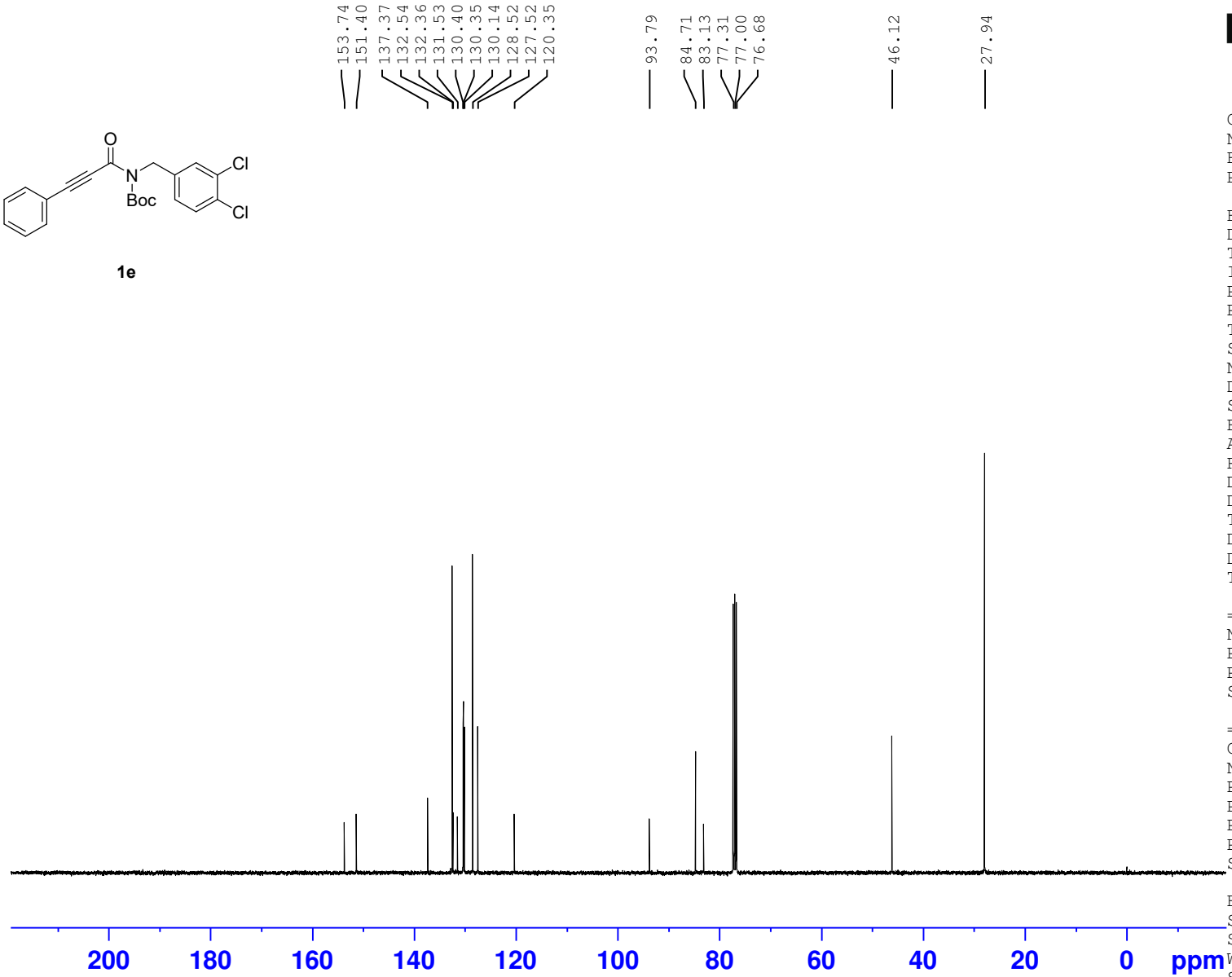
F2 - Acquisition Parameters
Date_ 20230306
Time 23.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 193.13
DW 60.800 usec
DE 6.50 usec
TE 292.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900161 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

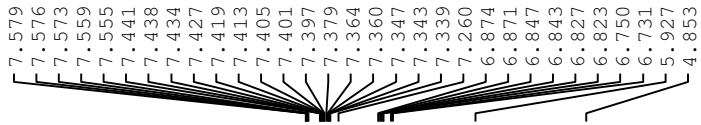
cb-1-19

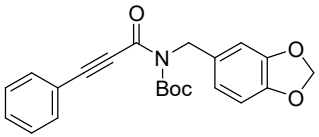
1e



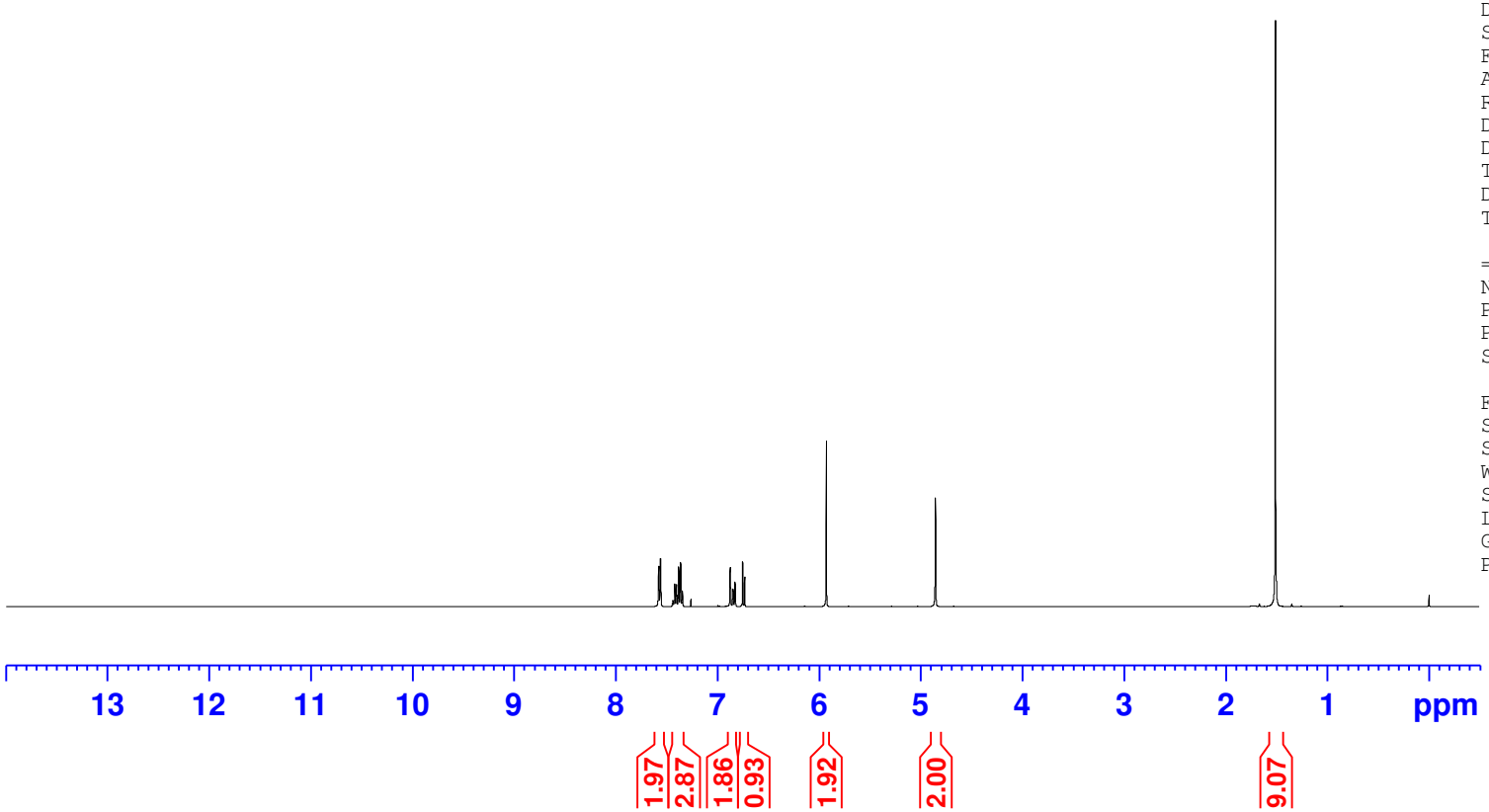

```
Current Data Parameters
NAME            zh1-400m
EXPNO                 27
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230514
Time               19.32
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  600
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE               291.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                12.00 usec
PLW1         53.00000000 W
SFO1        100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2         14.00000000 W
PLW12         0.37246999 W
PLW13         0.30170000 W
SFO2        400.1916008 MHz

F2 - Processing parameters
SI                32768
SF          100.6278646 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

ZHL-3-14





1f



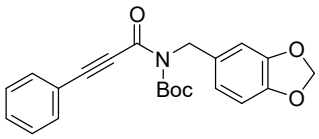
Current Data Parameters
NAME 20230308-400M
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230307
Time 23.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 75.43
DW 60.800 usec
DE 6.50 usec
TE 292.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

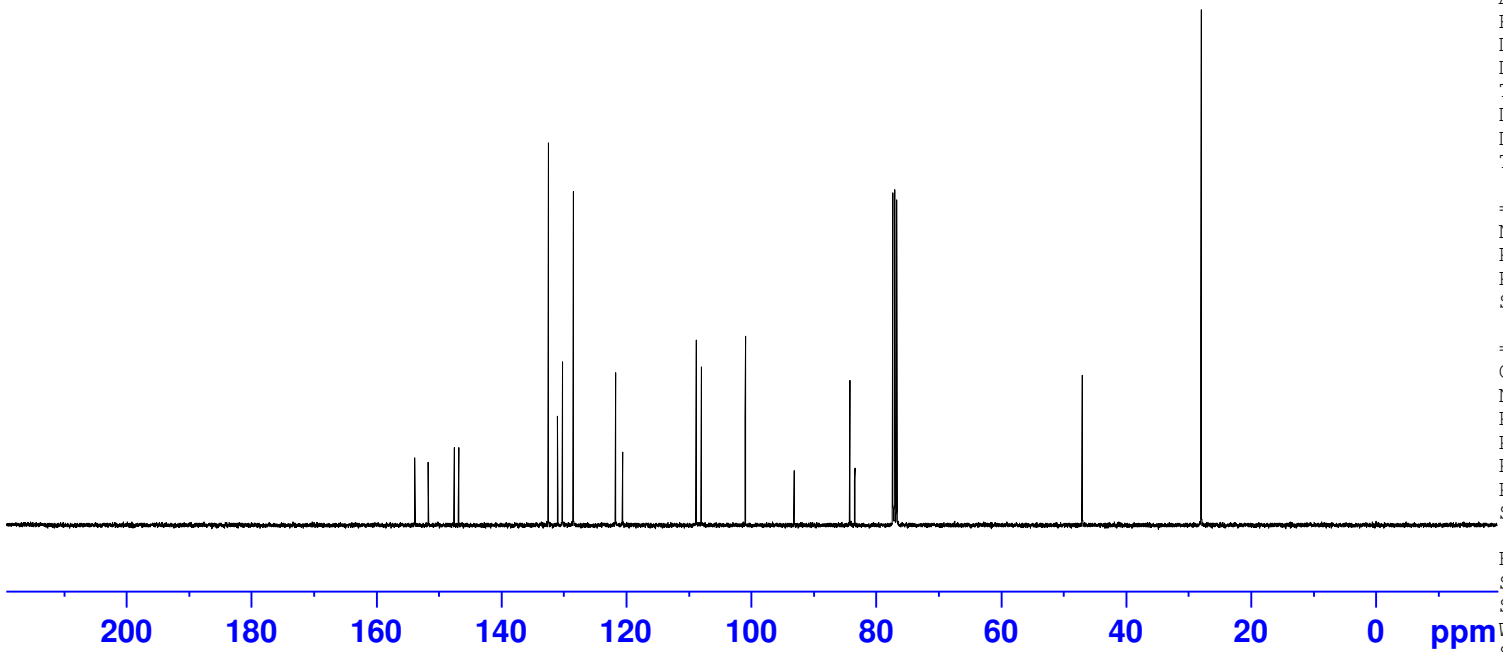
F2 - Processing parameters
SI 65536
SF 400.1900161 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-14



1f

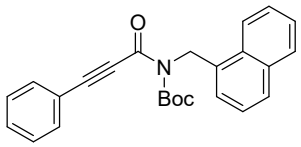
153.84
151.73
147.56
146.85
132.48
130.98
130.21
128.47
121.71
120.57
108.78
107.99
100.94
93.09
84.19
83.41
77.32
77.00
76.68
46.98
27.95



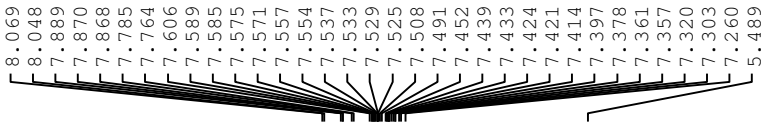
BRUKER

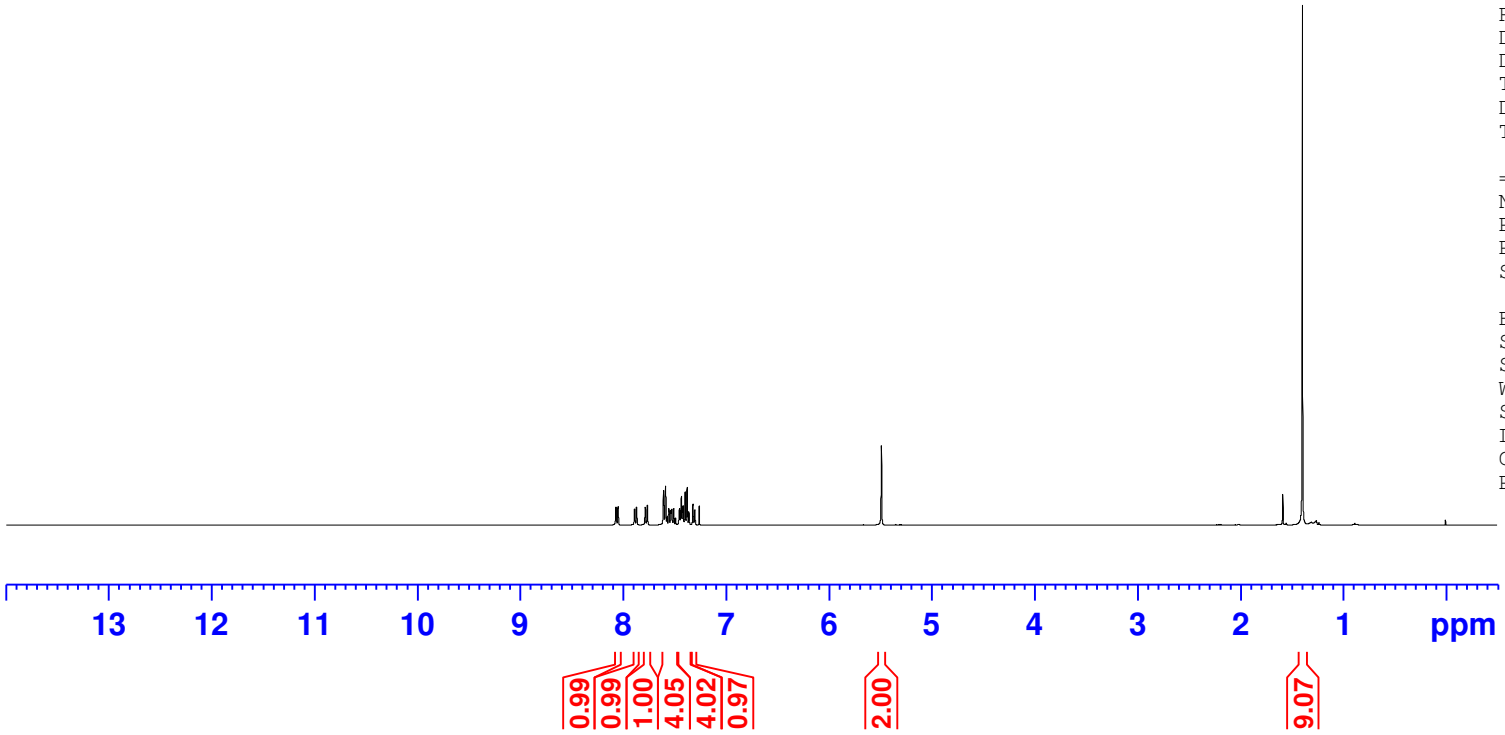
```
Current Data Parameters
NAME      20230310-400M
EXPNO               19
PROCNO               1

F2 - Acquisition Parameters
Date_          20230310
Time               7.45
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE                294.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                12.00 usec
PLW1        53.00000000 W
SFO1       100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2                1H
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.37246999 W
PLW13        0.30170000 W
SFO2       400.1916008 MHz

F2 - Processing parameters
SI                 32768
SF         100.6278645 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

CB-1-18



1g





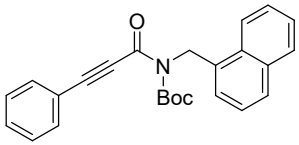
Current Data Parameters
NAME cb-1-18
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230302
Time 9.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 154.68
DW 60.800 usec
DE 6.50 usec
TE 294.3 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

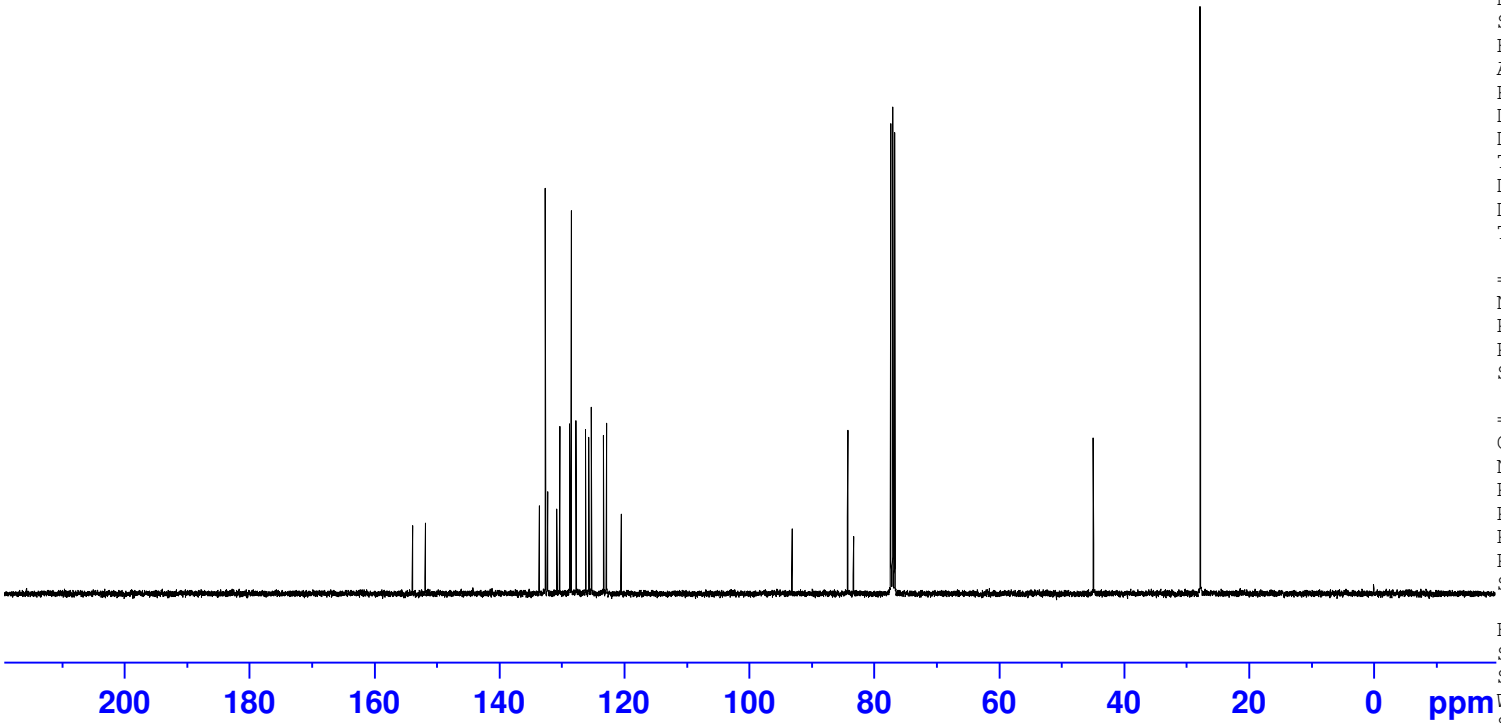
F2 - Processing parameters
SI 65536
SF 400.1900151 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

cb-1-18



1g

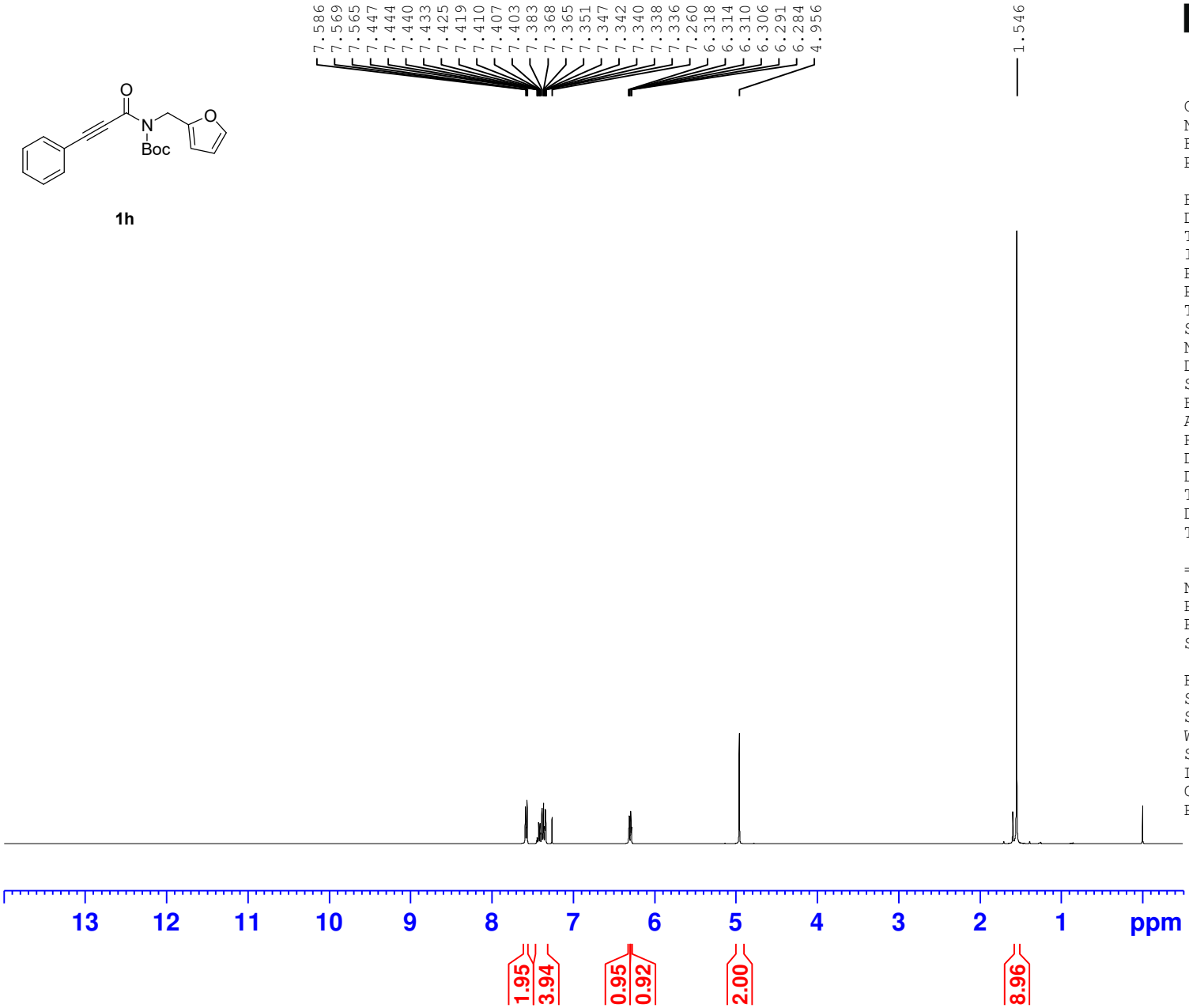
153.90
151.86
133.60
132.62
132.26
130.81
130.31
128.73
128.49
127.72
126.18
125.68
125.24
123.31
122.82
120.50
93.13
84.22
83.29
77.31
77.00
76.68
44.88
27.76




```
Current Data Parameters
NAME            zhl-400m
EXPNO                 26
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230514
Time               18.54
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   600
DS                     4
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ           1.3631488 sec
RG                193.13
DW               20.800 usec
DE                6.50 usec
TE                291.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                12.00 usec
PLW1         53.00000000 W
SFO1        100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2         14.00000000 W
PLW12         0.37246999 W
PLW13         0.30170000 W
SFO2        400.1916008 MHz

F2 - Processing parameters
SI                 32768
SF          100.6278653 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

ZHL-3-10

1h



Current Data Parameters
NAME 20230308-400M
EXPNO 15
PROCNO 1

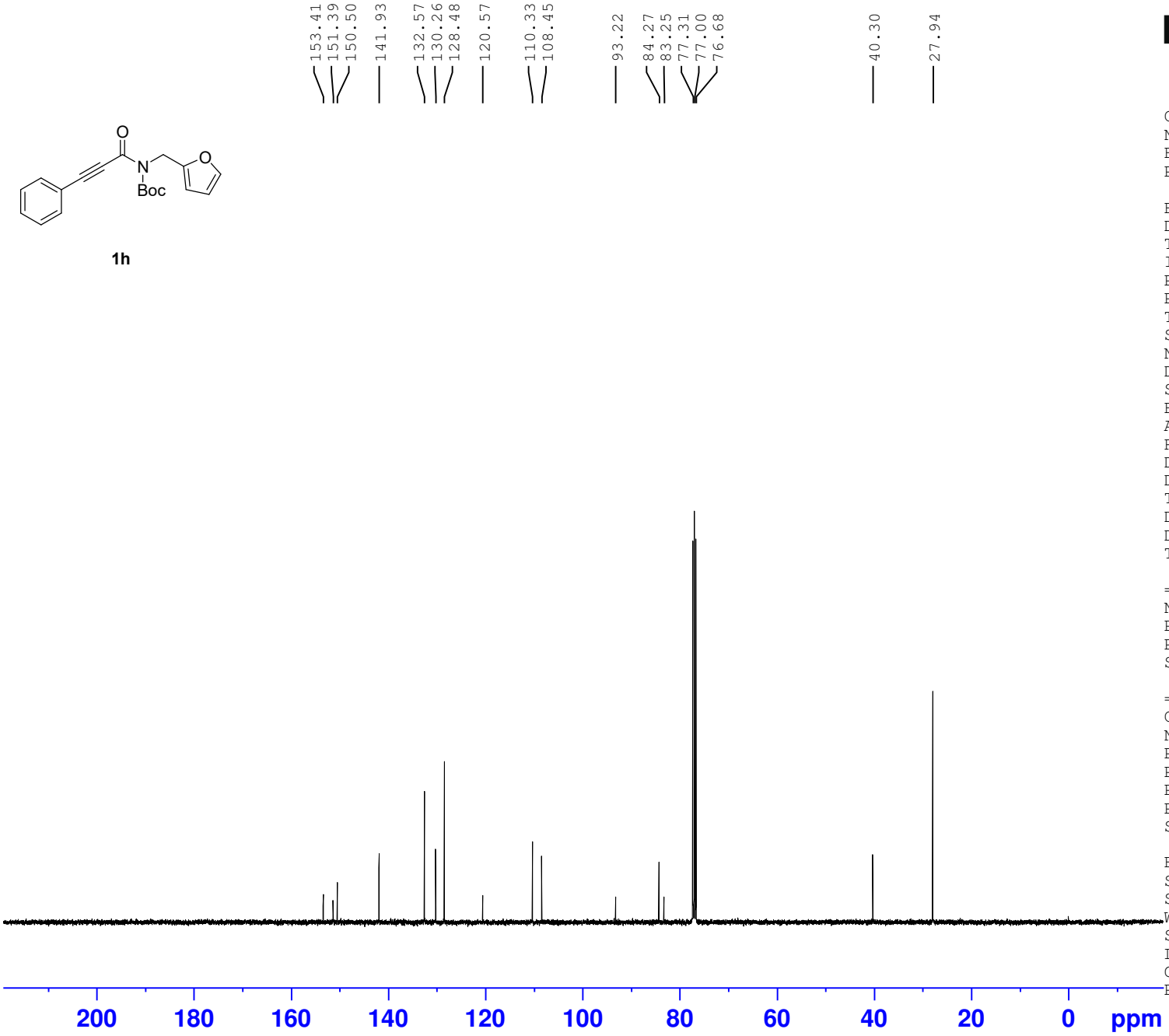
F2 - Acquisition Parameters
Date_ 20230307
Time 23.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 181.41
DW 60.800 usec
DE 6.50 usec
TE 292.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900161 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-10

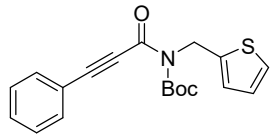
1h



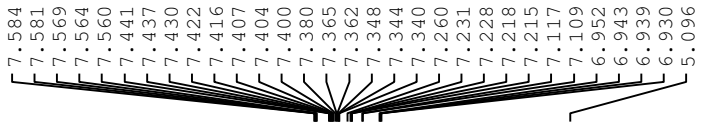
BRUKER

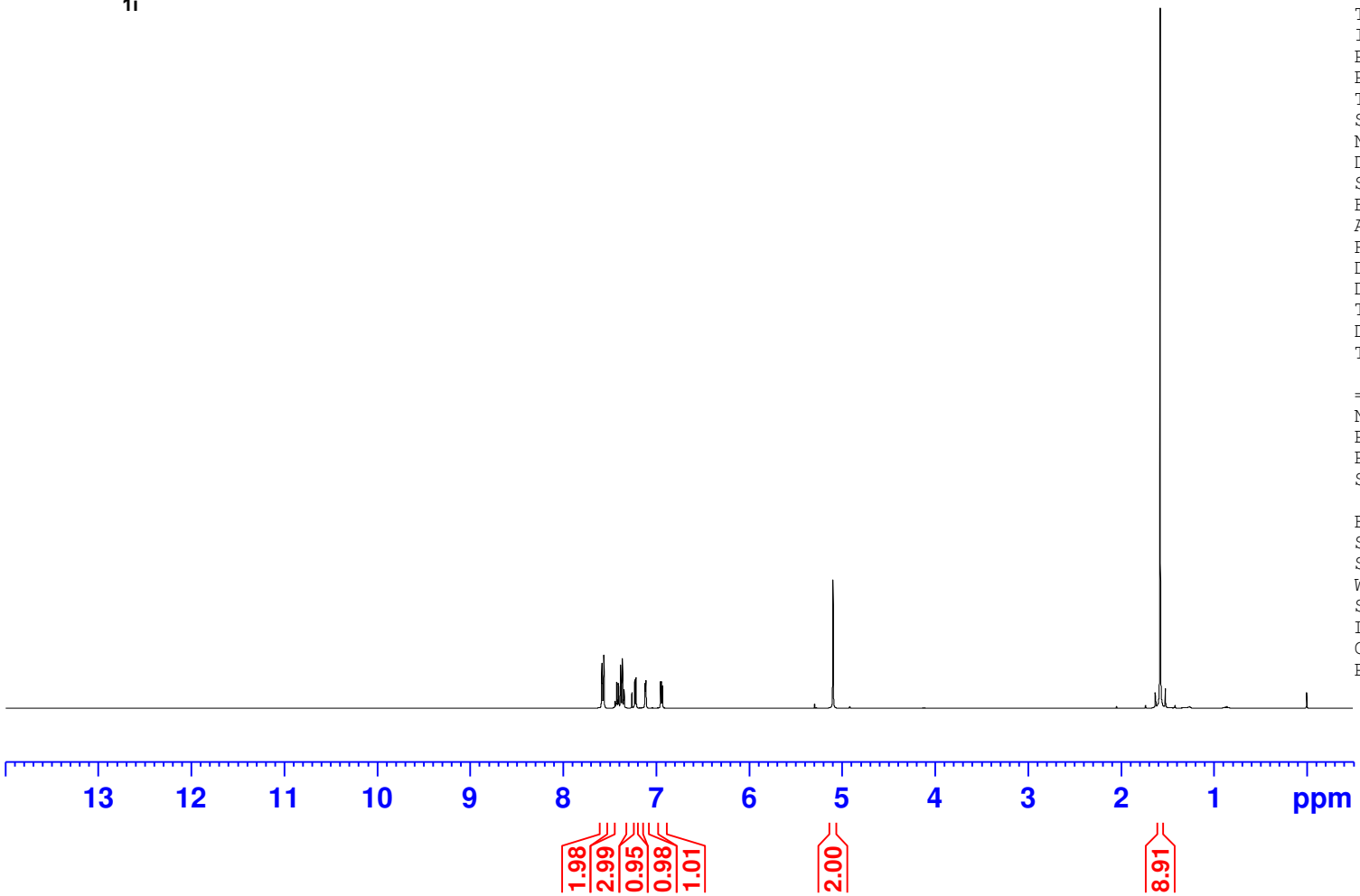
```
Current Data Parameters
NAME      20230310-400M
EXPNO               20
PROCNO               1

F2 - Acquisition Parameters
Date_          20230310
Time               8.13
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE               294.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1               12.00 usec
PLW1        53.00000000 W
SFO1       100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2                1H
PCPD2            90.00 usec
PLW2        14.00000000 W
PLW12        0.37246999 W
PLW13        0.30170000 W
SFO2       400.1916008 MHz

F2 - Processing parameters
SI                32768
SF          100.6278616 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC                1.40
```

ZHL-3-3U



1i





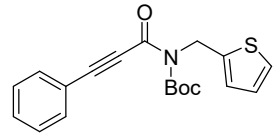
Current Data Parameters
NAME 20230308-400M
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230307
Time 23.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 113.67
DW 60.800 usec
DE 6.50 usec
TE 292.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

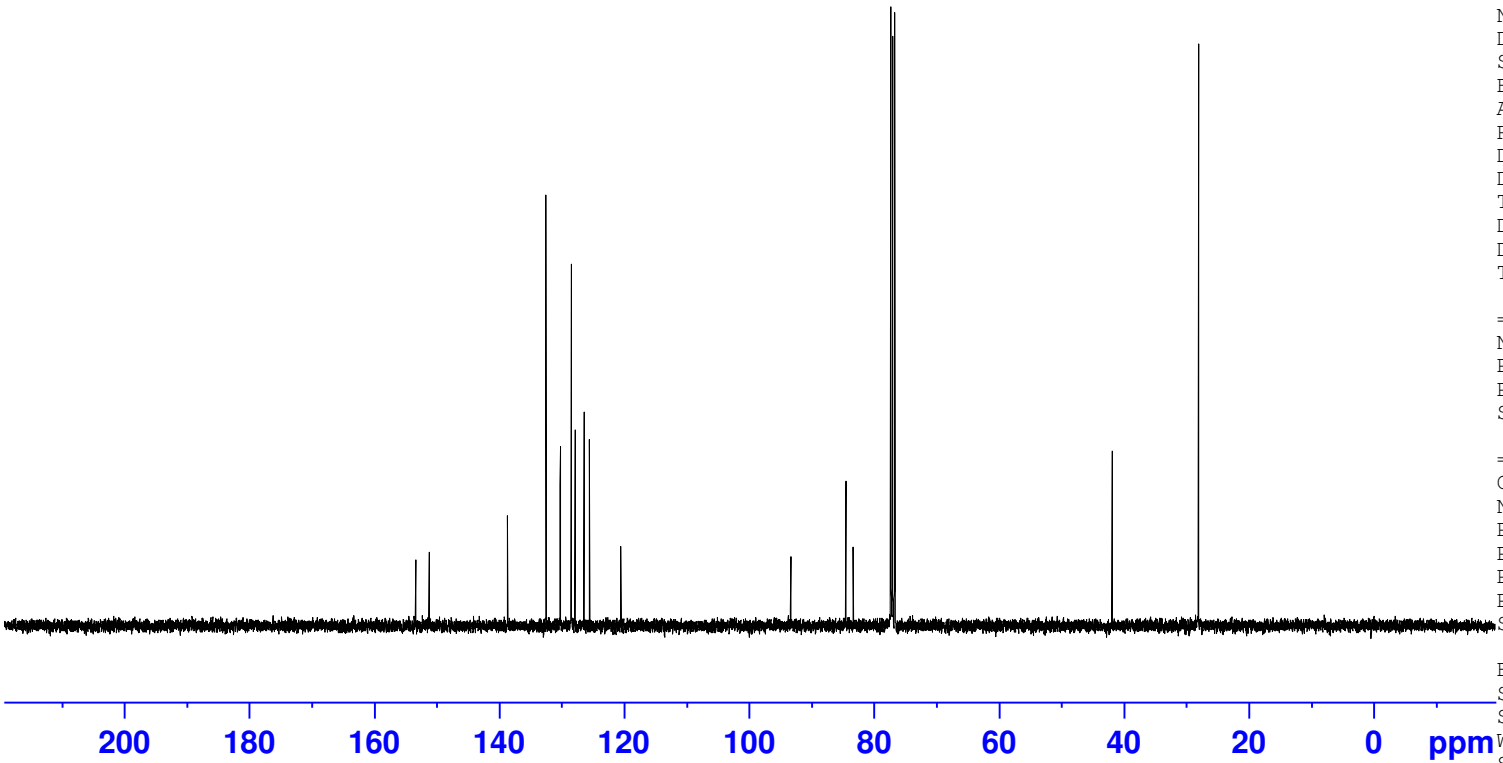
F2 - Processing parameters
SI 65536
SF 400.1900162 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-2-30



1i

153.41
151.25
138.68
132.54
130.25
128.47
127.87
126.44
125.57
120.55
93.34
84.51
83.34
77.32
77.00
76.68
41.84
28.02

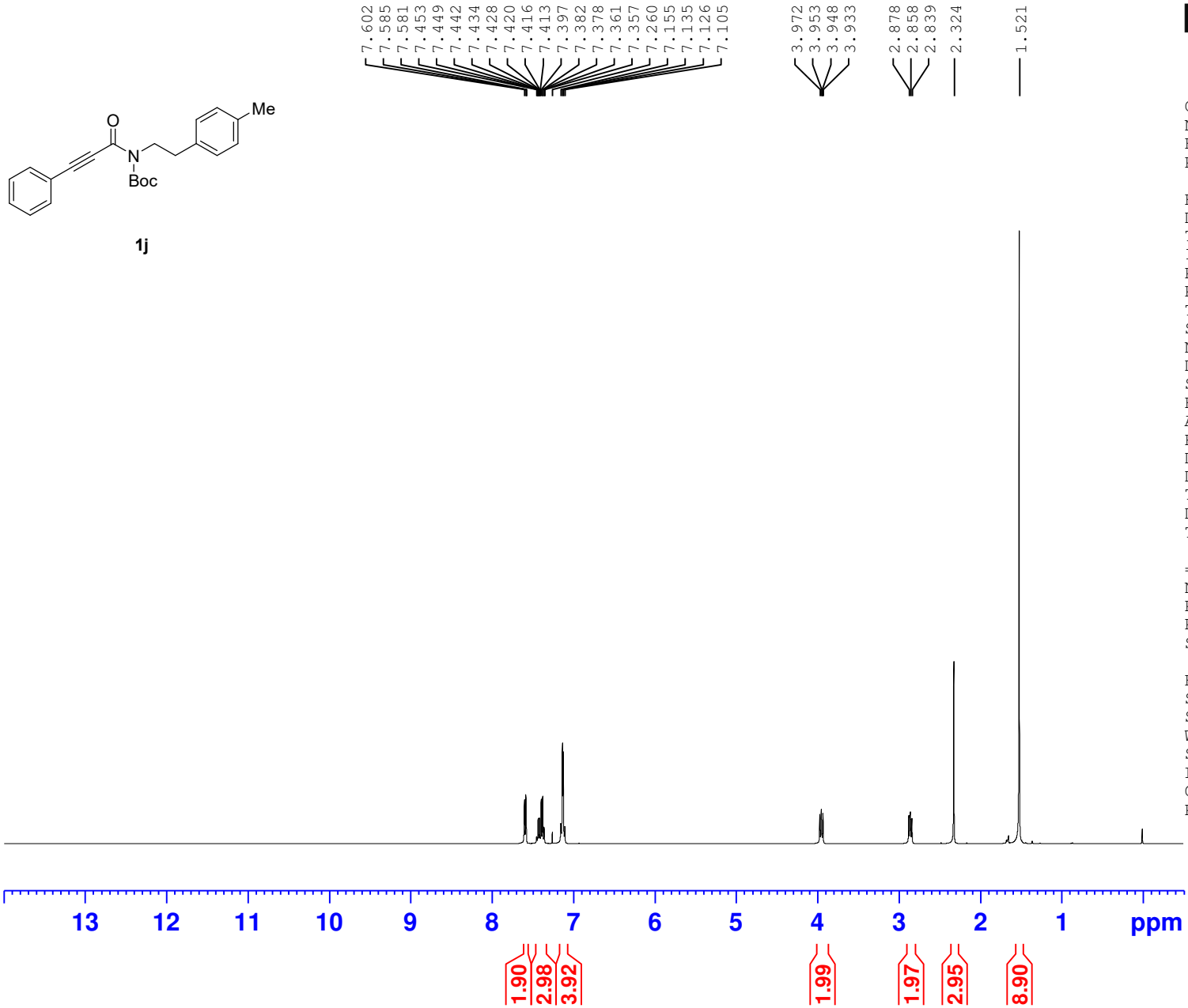


BRUKER

```
Current Data Parameters
NAME      20230310-400M
EXPNO                26
PROCNO                1

F2 - Acquisition Parameters
Date_          20230310
Time               9.40
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  154
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE               294.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                12.00 usec
PLW1         53.00000000 W
SFO1        100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2         14.00000000 W
PLW12         0.37246999 W
PLW13         0.30170000 W
SFO2        400.1916008 MHz

F2 - Processing parameters
SI                32768
SF          100.6278631 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

ZHL-3-31

1j



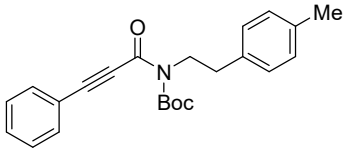
Current Data Parameters
NAME 20230308-400M
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230307
Time 23.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 75.43
DW 60.800 usec
DE 6.50 usec
TE 292.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

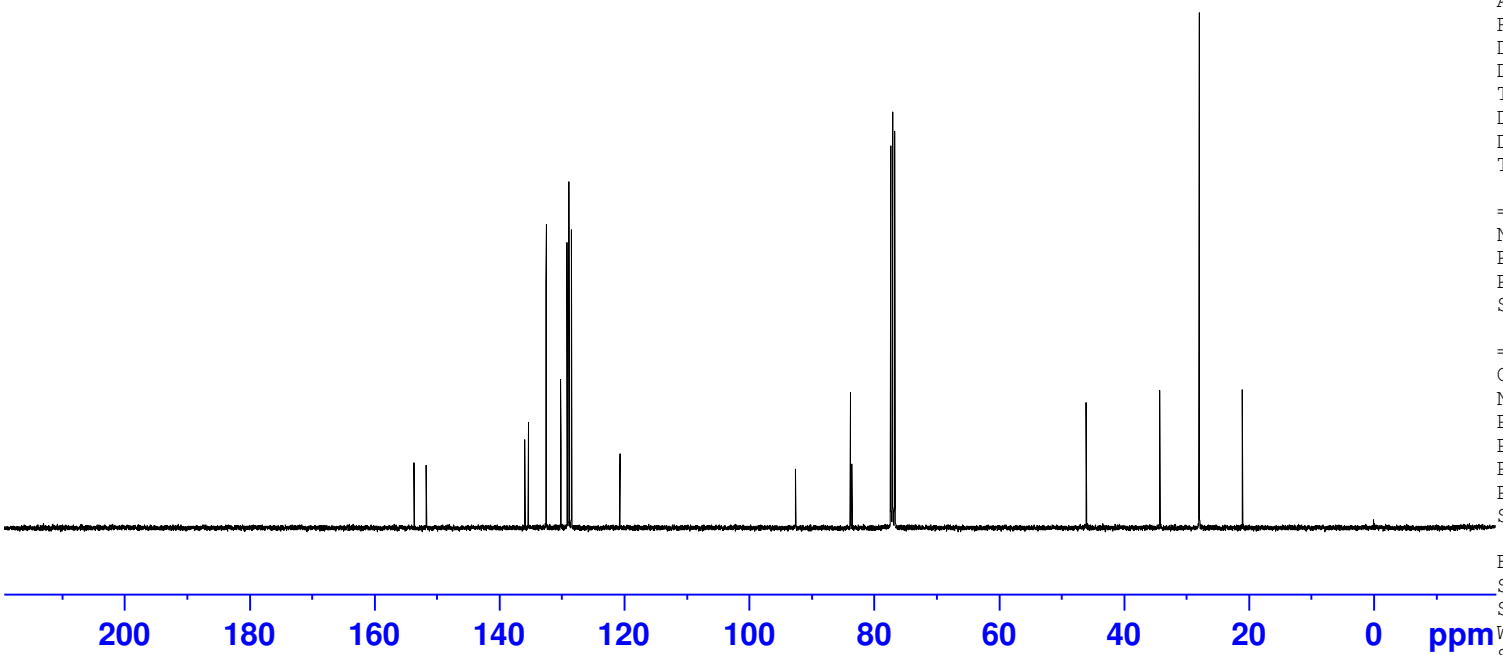
F2 - Processing parameters
SI 65536
SF 400.1900161 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-31



1j

153.67
151.70
135.94
135.34
132.51
130.16
129.16
128.85
128.46
120.67
92.55
83.78
83.55
77.31
77.00
76.68
46.00
34.23
27.90
20.99



BRUKER

Current Data Parameters
NAME zhl-3-1,31
EXPNO 28
PROCNO 1

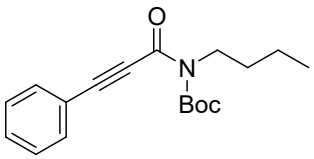
F2 - Acquisition Parameters
Date_ 20230309
Time 8.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 294.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

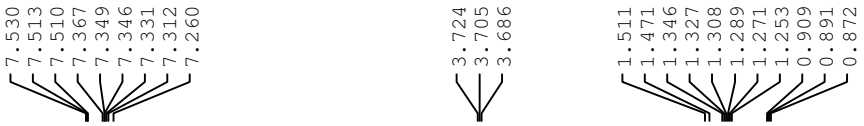
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

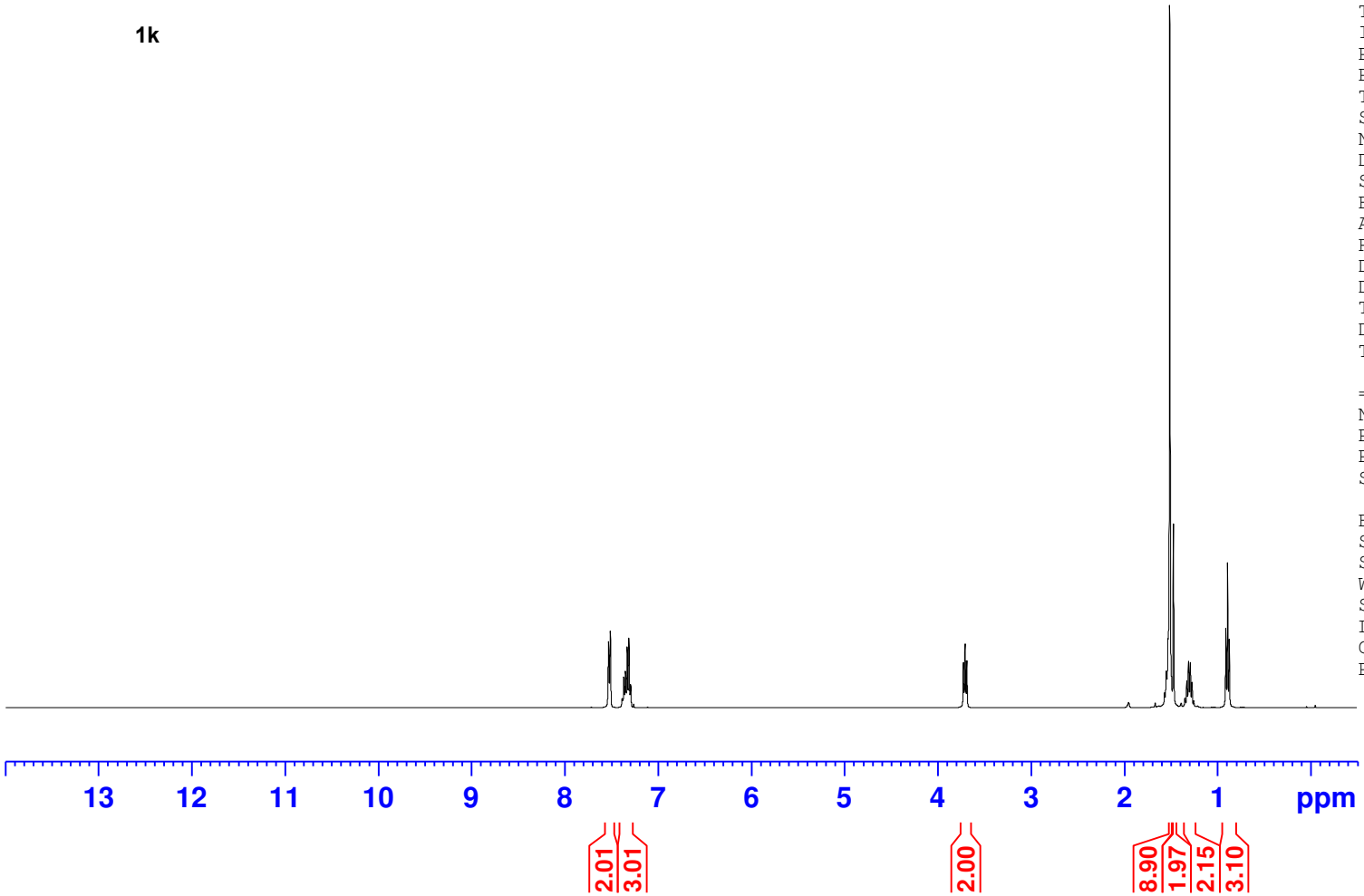
F2 - Processing parameters
SI 32768
SF 100.6278646 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZHL-3-8



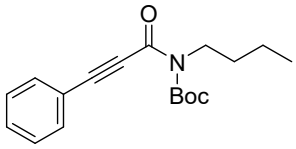
1k



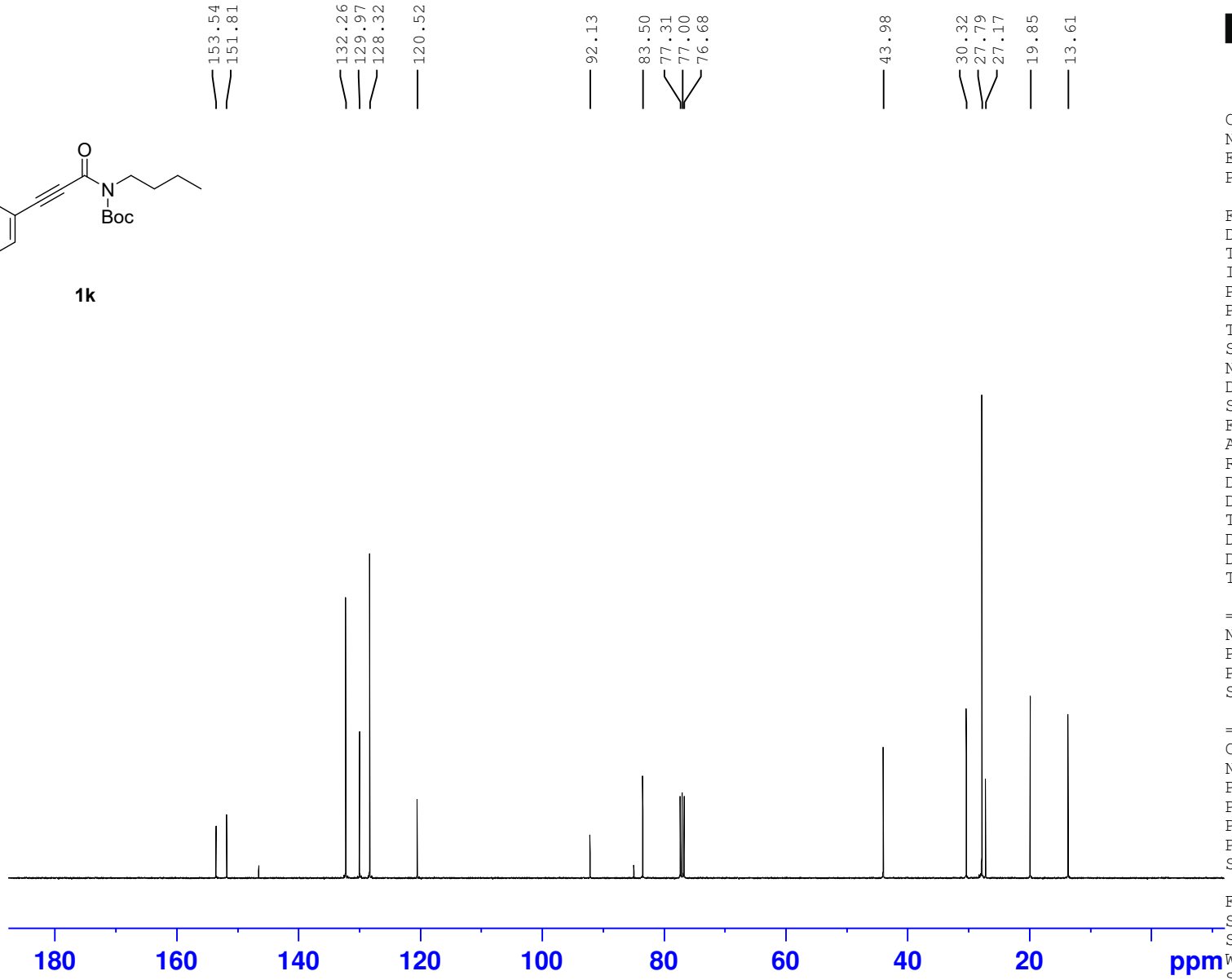



```
Current Data Parameters
NAME       20230423-400m
EXPNO                 23
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230422
Time               15.10
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     6
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9845889 sec
RG                 17.43
DW                60.800 usec
DE                 6.50 usec
TE                290.5 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.68 usec
PLW1        14.00000000 W
SFO1        400.1924713 MHz

F2 - Processing parameters
SI                 65536
SF          400.1900168 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```

ZHL-3-8



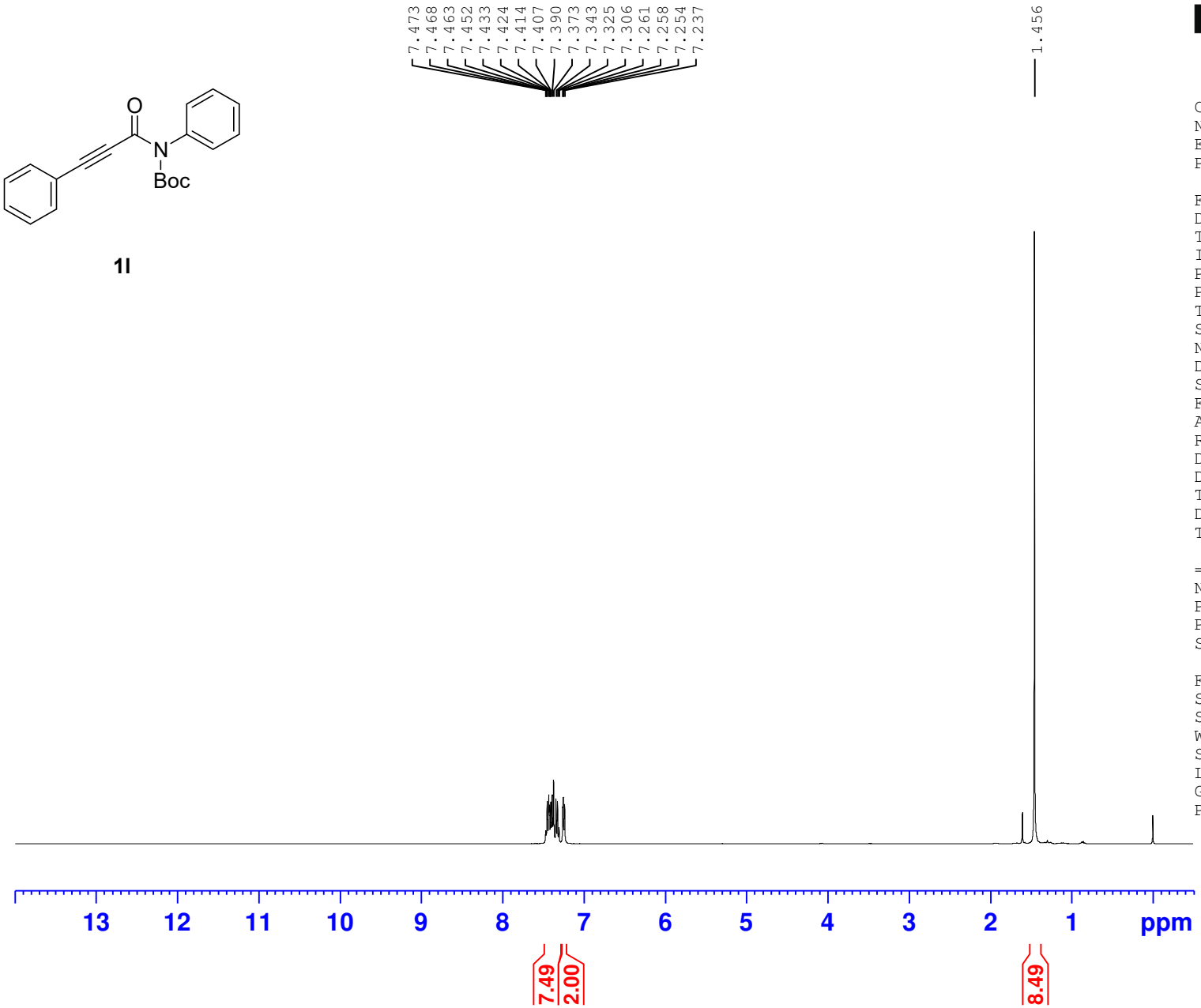
1k




```
Current Data Parameters
NAME       20230423-400m
EXPNO                 24
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230422
Time               15.29
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  300
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE                291.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                12.00 usec
PLW1        53.00000000 W
SFO1       100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.37246999 W
PLW13        0.30170000 W
SFO2       400.1916008 MHz

F2 - Processing parameters
SI                32768
SF         100.6278756 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

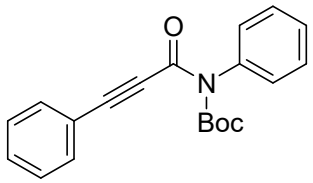
ZHL-3-1

1l



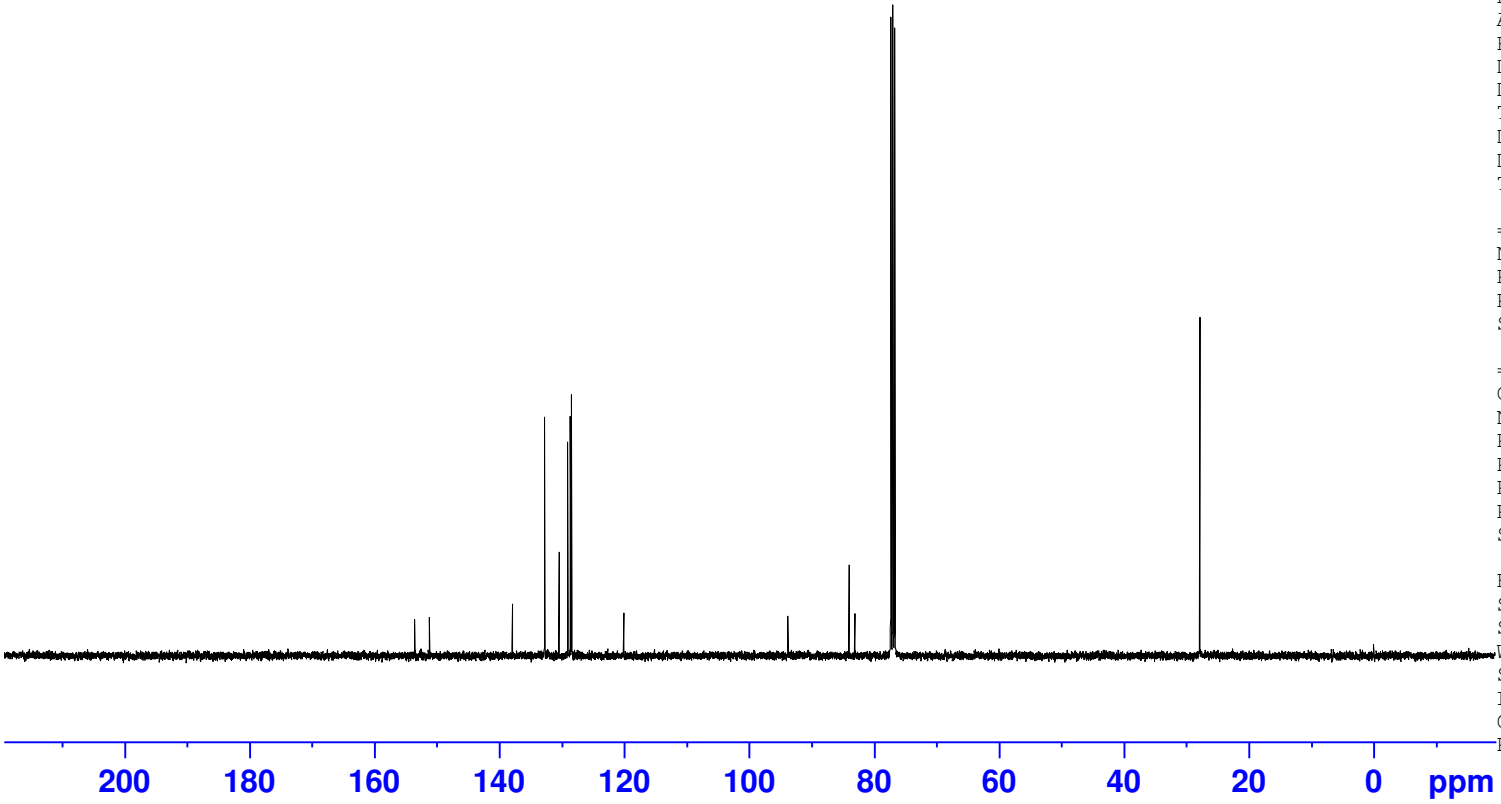

```
Current Data Parameters
NAME       20230308-400M
EXPNO                 19
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230307
Time               23.42
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     6
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9845889 sec
RG                 154.68
DW                 60.800 usec
DE                  6.50 usec
TE                 292.7 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.68 usec
PLW1         14.00000000 W
SFO1         400.1924713 MHz

F2 - Processing parameters
SI                 65536
SF           400.1900160 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

zhl-3-1



1l

153.60
151.22
137.96
132.78
130.46
129.06
128.64
128.47
128.44
120.11
93.79
83.99
83.10
77.32
77.00
76.68
27.82



Current Data Parameters
NAME zhl-3-1,31
EXPNO 27
PROCNO 1

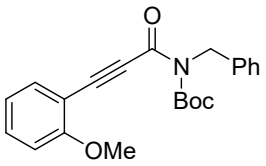
F2 - Acquisition Parameters
Date_ 20230309
Time 7.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 293.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

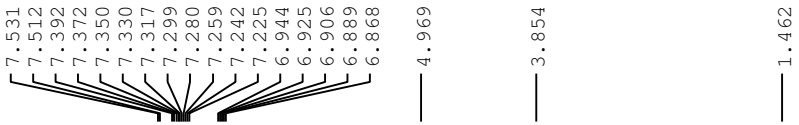
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

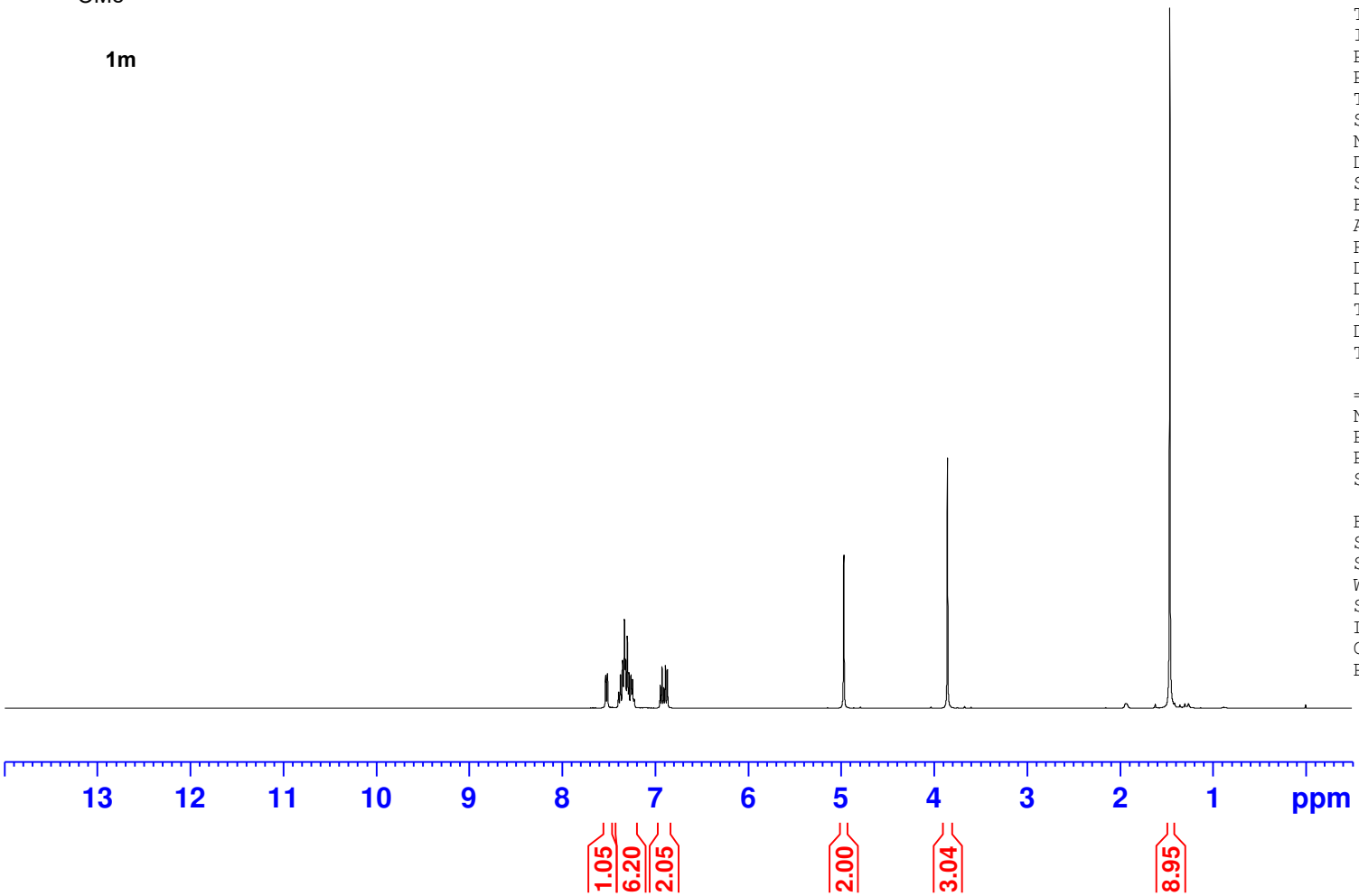
F2 - Processing parameters
SI 32768
SF 100.6278624 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-3-33



1m

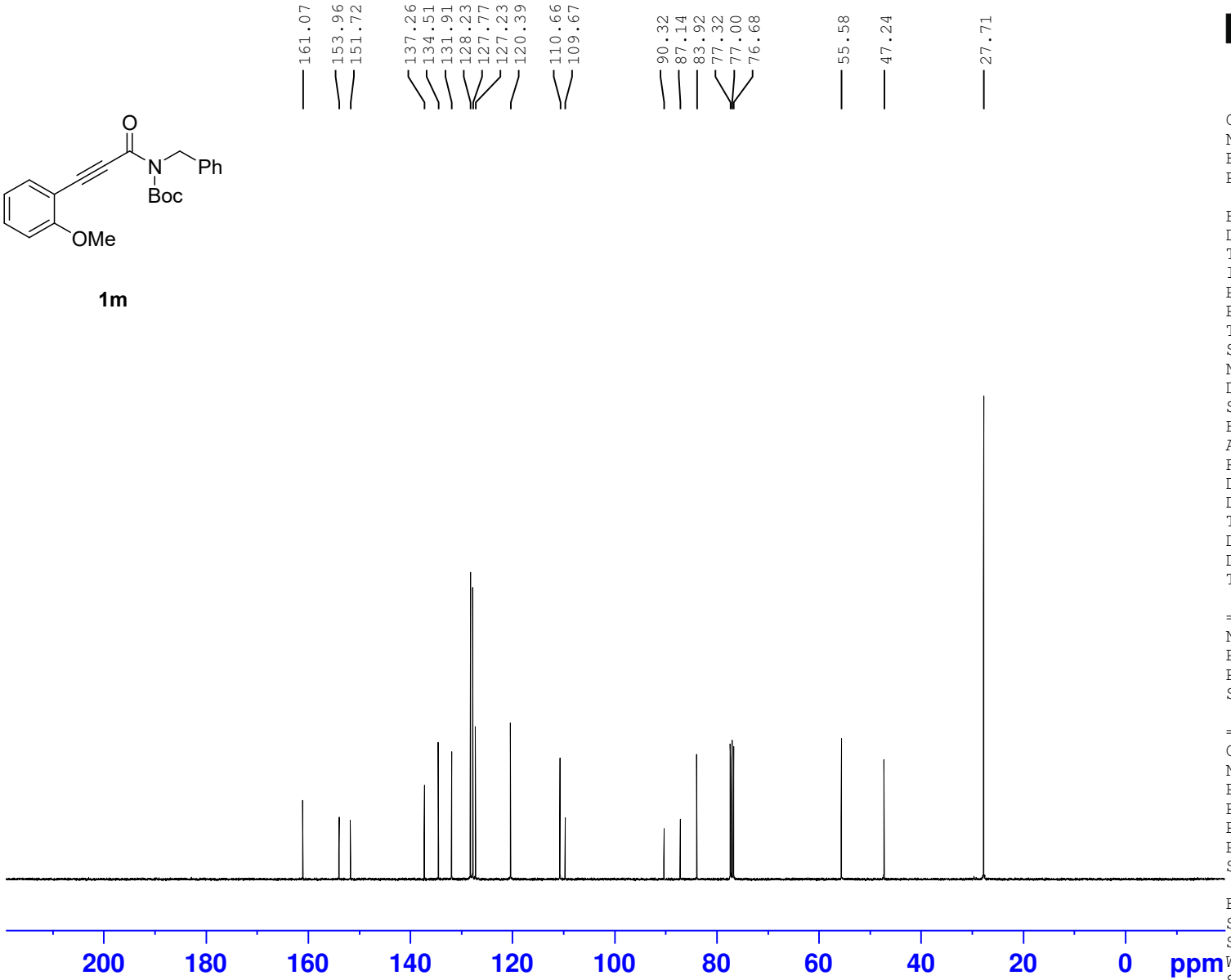





```
Current Data Parameters
NAME       20230418-400M
EXPNO                 18
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230418
Time                6.04
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     6
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9845889 sec
RG                 29.75
DW                60.800 usec
DE                 6.50 usec
TE                291.7 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.68 usec
PLW1        14.00000000 W
SFO1        400.1924713 MHz

F2 - Processing parameters
SI                 65536
SF          400.1900180 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

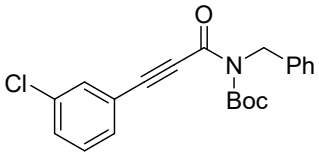
zhl-3-33

1m

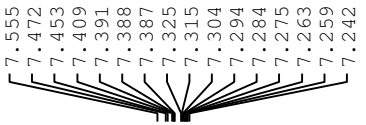


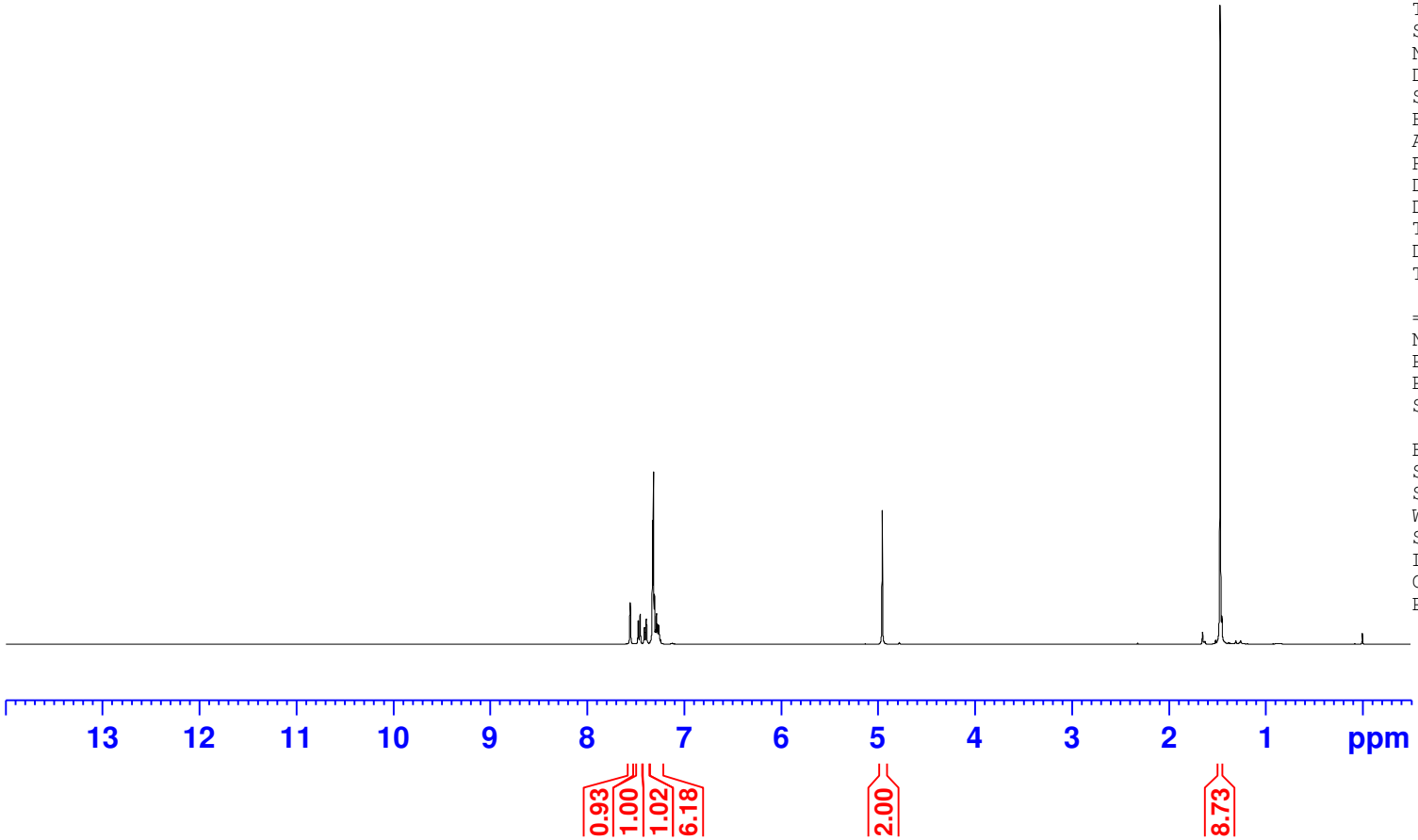

```
Current Data Parameters
NAME       20230418-400M
EXPNO                 19
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230418
Time                6.28
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   400
DS                     4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE                292.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                12.00 usec
PLW1        53.00000000 W
SFO1       100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                  1H
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.37246999 W
PLW13        0.30170000 W
SFO2       400.1916008 MHz

F2 - Processing parameters
SI                 32768
SF          100.6278734 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

zhl-3-41



1n





Current Data Parameters
NAME zhl-400m
EXPNO 28
PROCNO 1

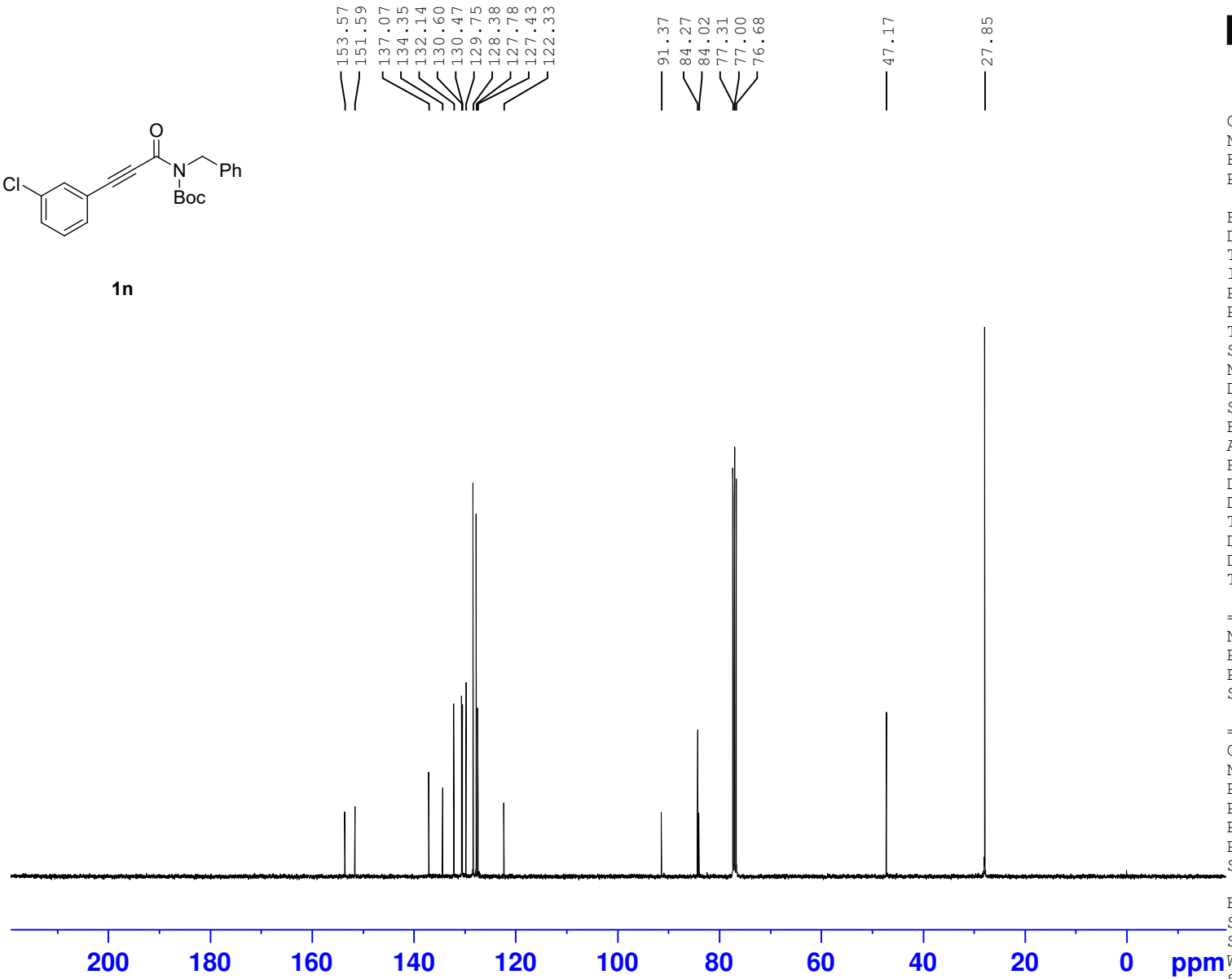
F2 - Acquisition Parameters
Date_ 20230514
Time 19.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 75.43
DW 60.800 usec
DE 6.50 usec
TE 291.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900167 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-41

1n



Current Data Parameters
NAME zhl-400m
EXPNO 29
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230514
Time 20.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 600
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 291.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

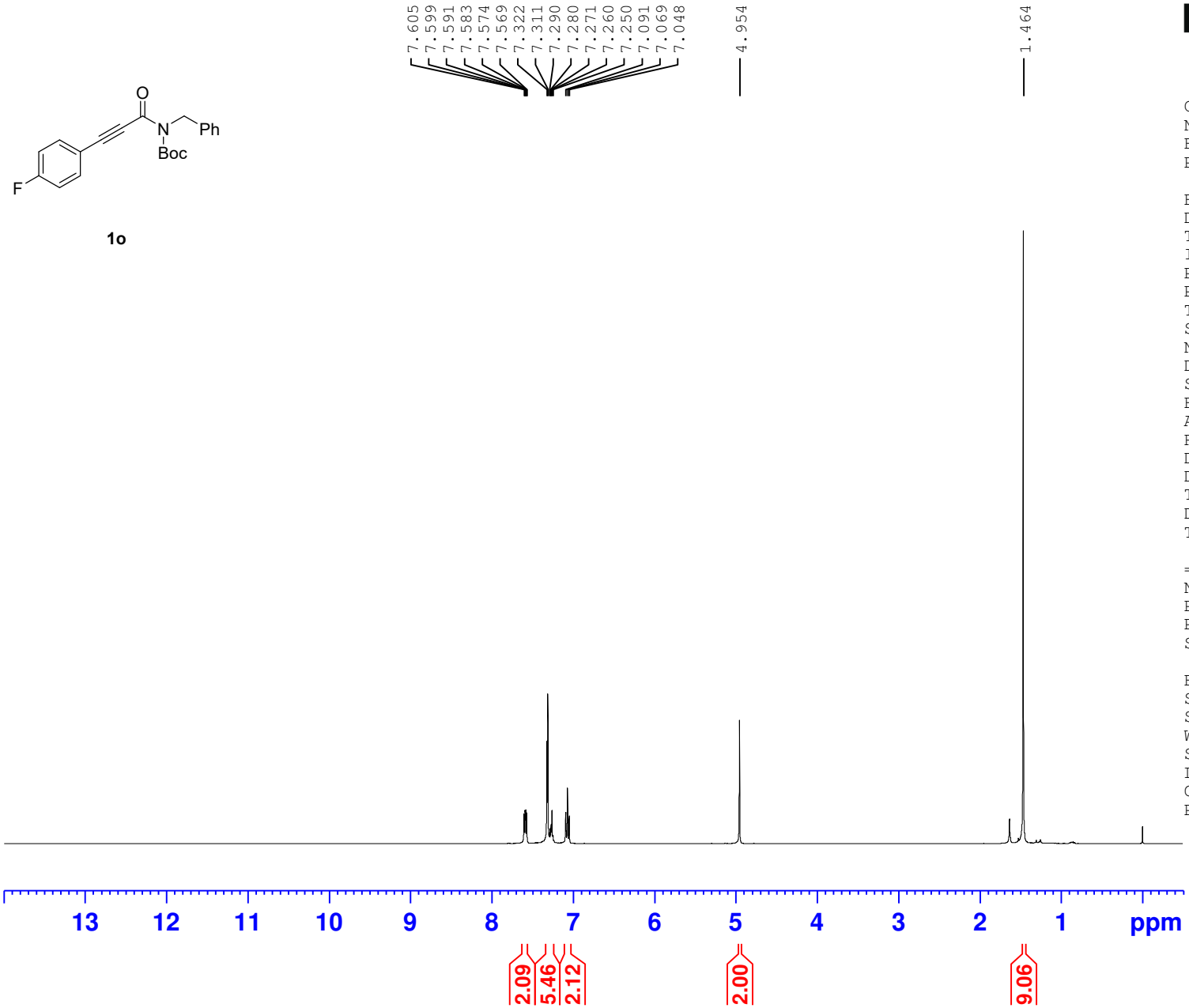
======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278653 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZHL-3-25

1o



Current Data Parameters
NAME 20230423-400m
EXPNO 19
PROCNO 1

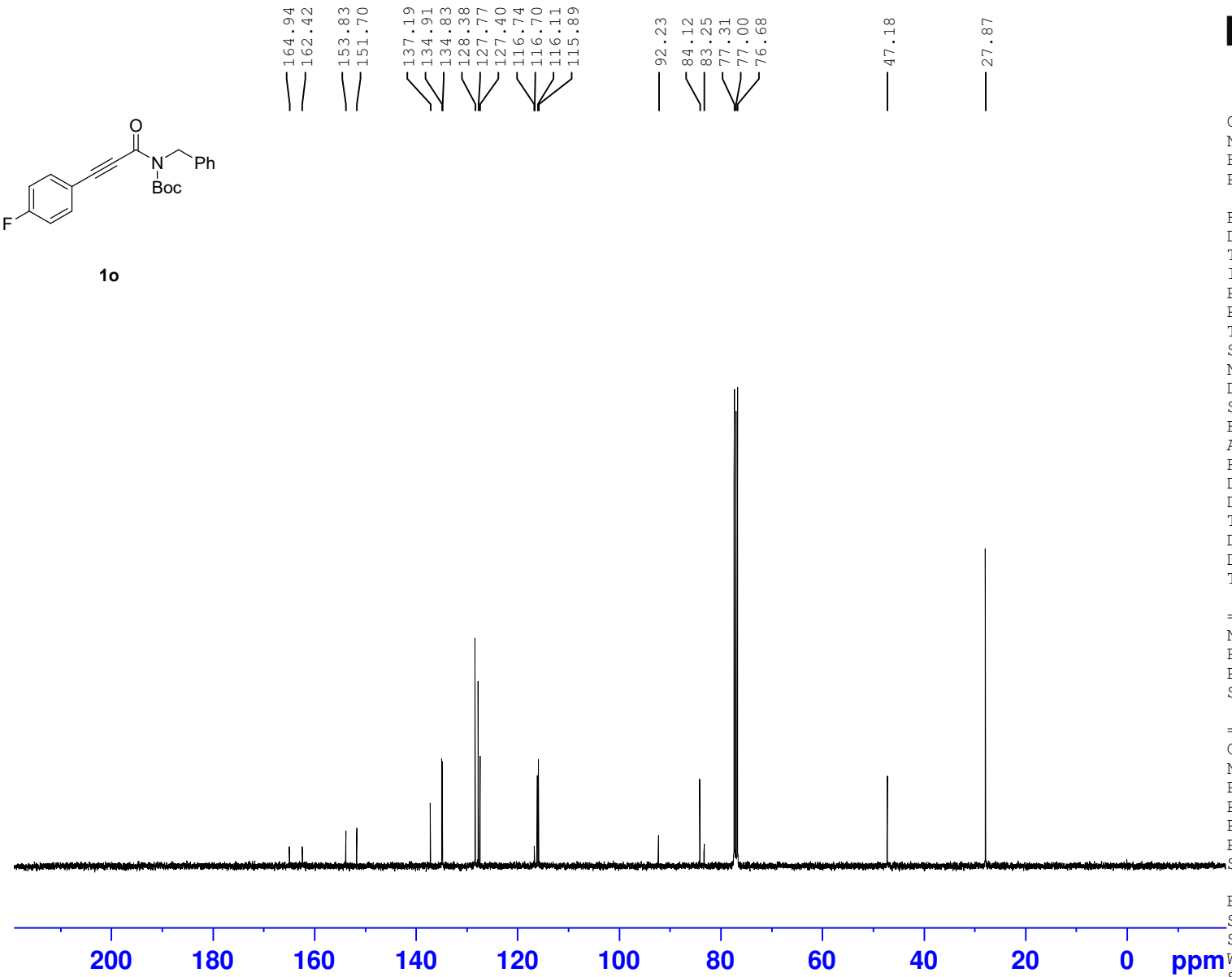
F2 - Acquisition Parameters
Date_ 20230422
Time 14.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 125.76
DW 60.800 usec
DE 6.50 usec
TE 290.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900161 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZHL-3-25

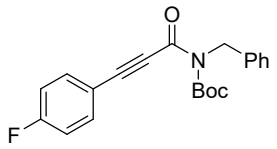
1o



BRUKER

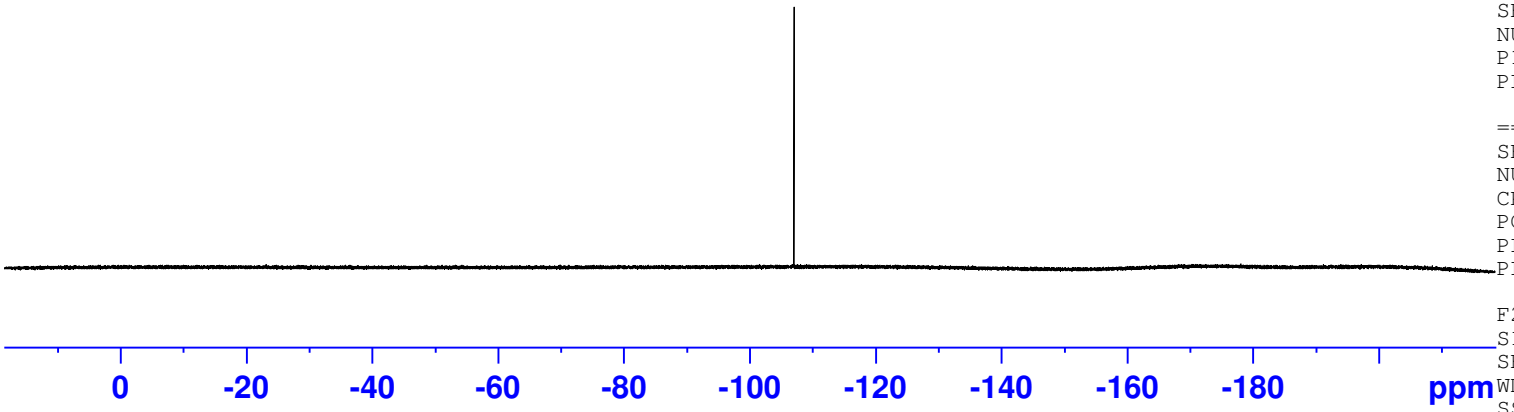
```
Current Data Parameters
NAME      20230423-400m
EXPNO               20
PROCNO               1

F2 - Acquisition Parameters
Date_          20230422
Time              14.43
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 300
DS                   4
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE                291.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                12.00 usec
PLW1        53.00000000 W
SFO1       100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2                1H
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.37246999 W
PLW13        0.30170000 W
SFO2       400.1916008 MHz

F2 - Processing parameters
SI                 32768
SF         100.6278636 MHz
WDW                   EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

zhl-3-25



1o

-107.08



Current Data Parameters
NAME 20230627-300M
EXPNO 204
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230627
Time 12.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn.2
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 0.510897 Hz
AQ 0.9786710 sec
RG 203
DW 7.467 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

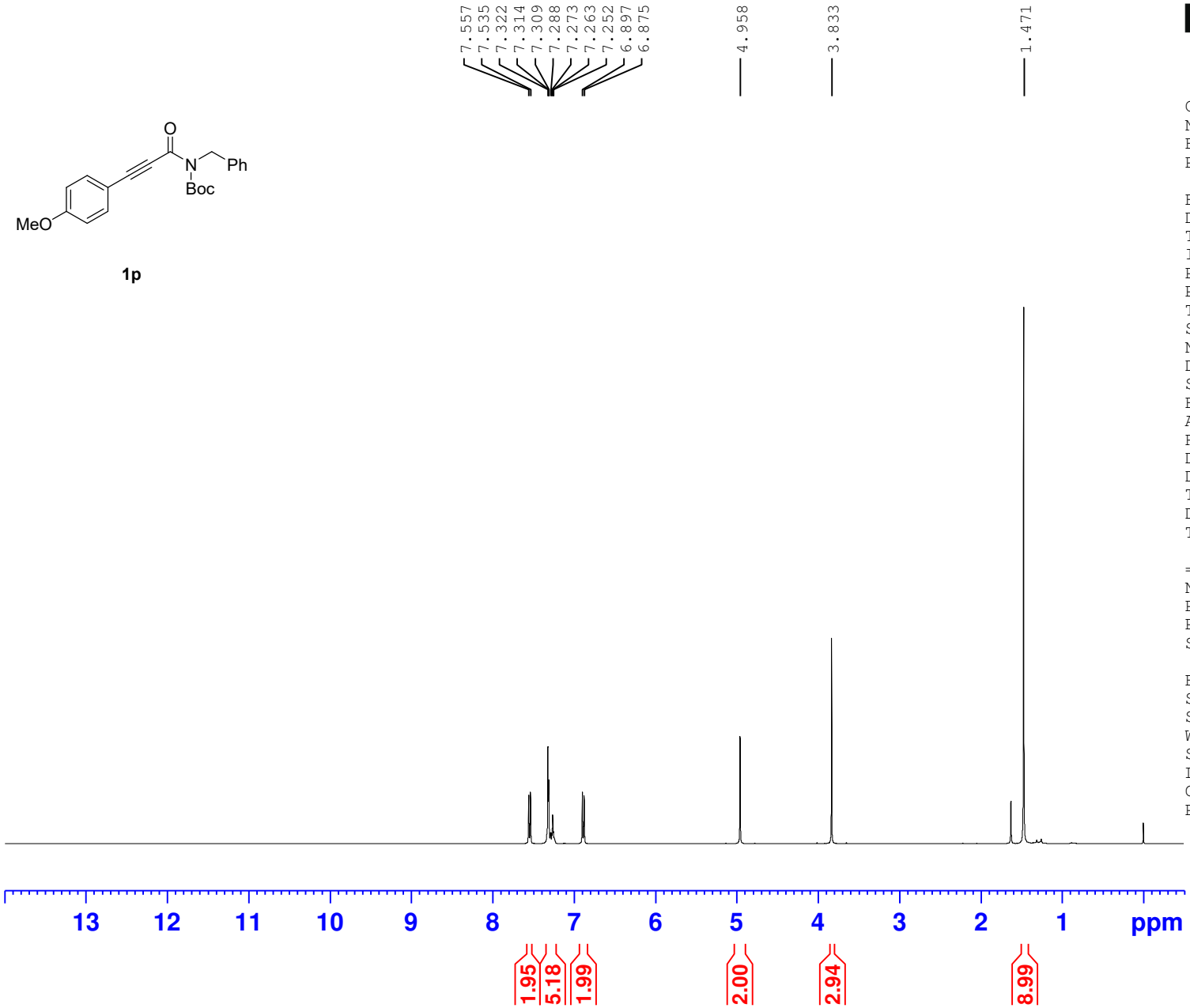
======== CHANNEL f1 ========
SFO1 282.3761148 MHz
NUC1 19F
P1 14.50 usec
PLW1 10.39999962 W

======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W

F2 - Processing parameters
SI 65536
SF 282.4043552 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZHL-3-50

1p



Current Data Parameters
NAME 20230423-400m
EXPNO 29
PROCNO 1

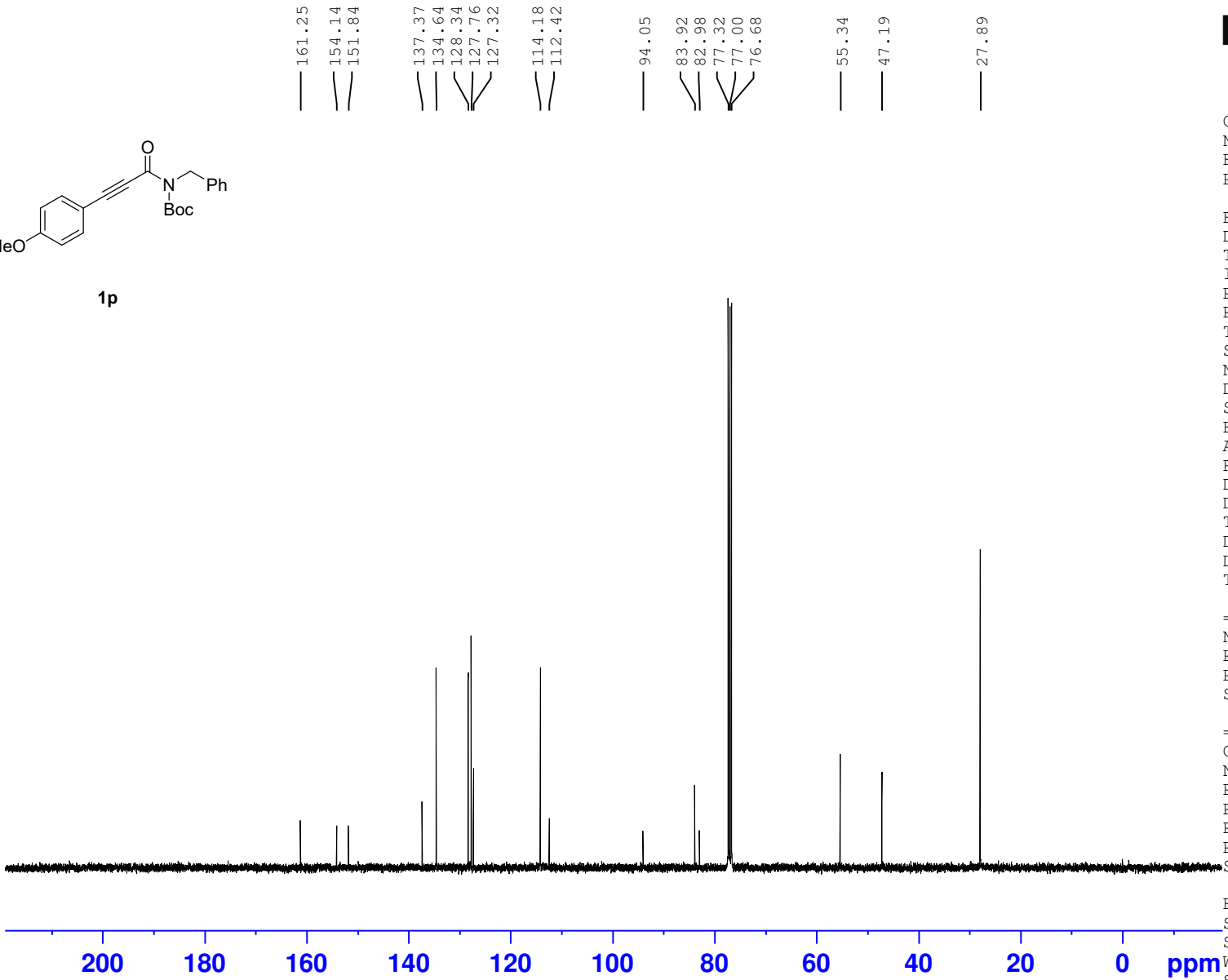
F2 - Acquisition Parameters
Date_ 20230422
Time 16.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 140.02
DW 60.800 usec
DE 6.50 usec
TE 290.6 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900153 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZHL-3-50

1p



Current Data Parameters
NAME 20230423-400m
EXPNO 30
PROCNO 1

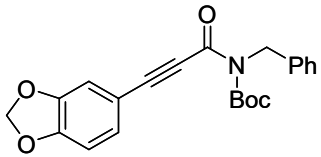
F2 - Acquisition Parameters
Date_ 20230422
Time 16.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 291.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

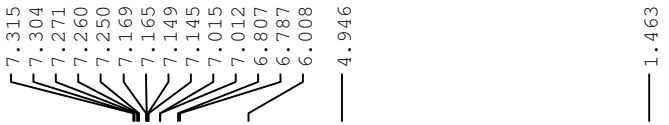
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

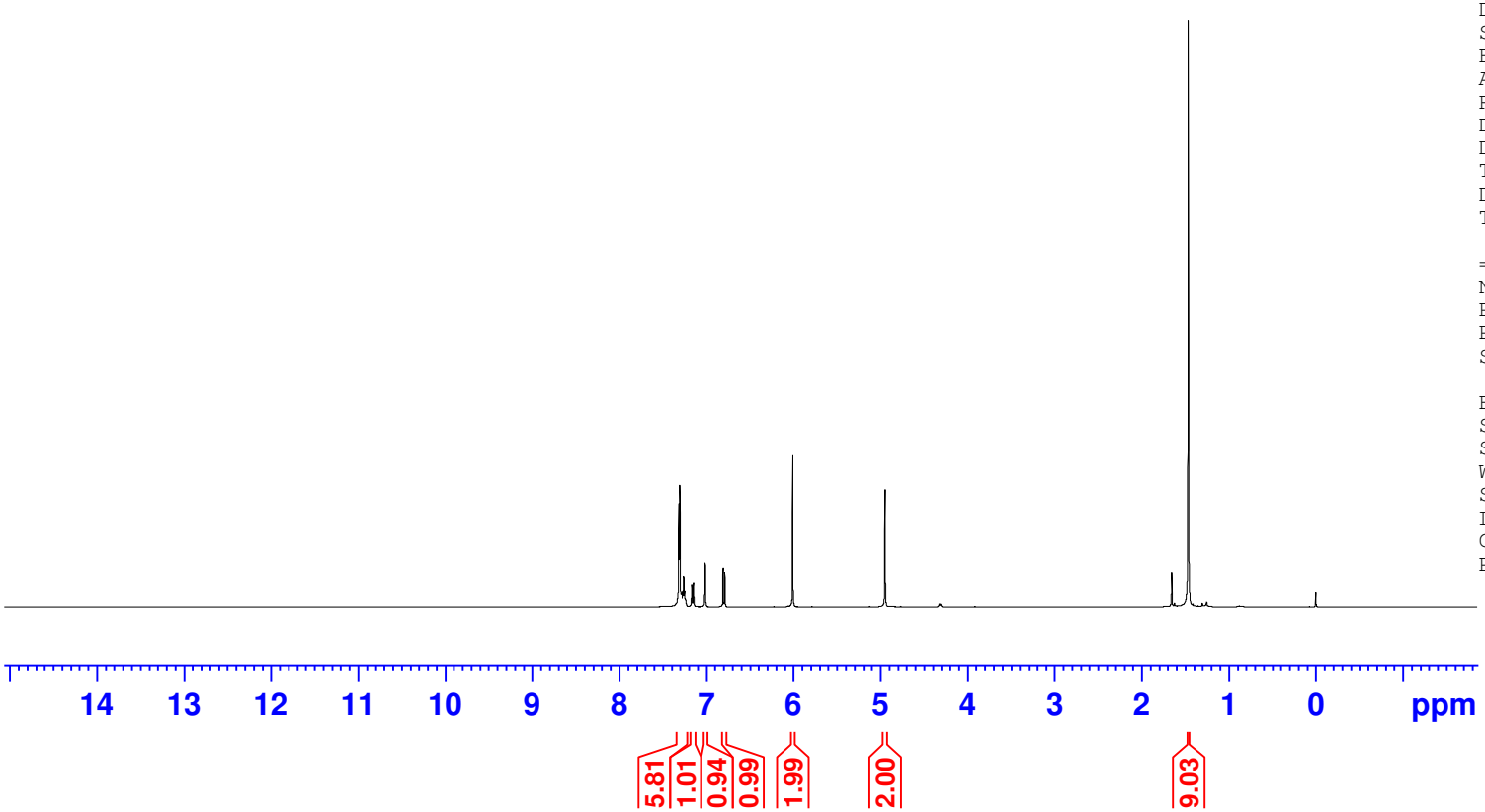
F2 - Processing parameters
SI 32768
SF 100.6278631 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZHL-3-42



1q





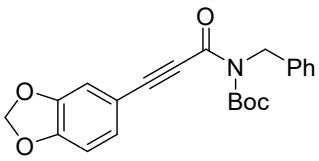
Current Data Parameters
NAME 20230423-400m
EXPNO 25
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230422
Time 15.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 100.49
DW 60.800 usec
DE 6.50 usec
TE 290.5 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

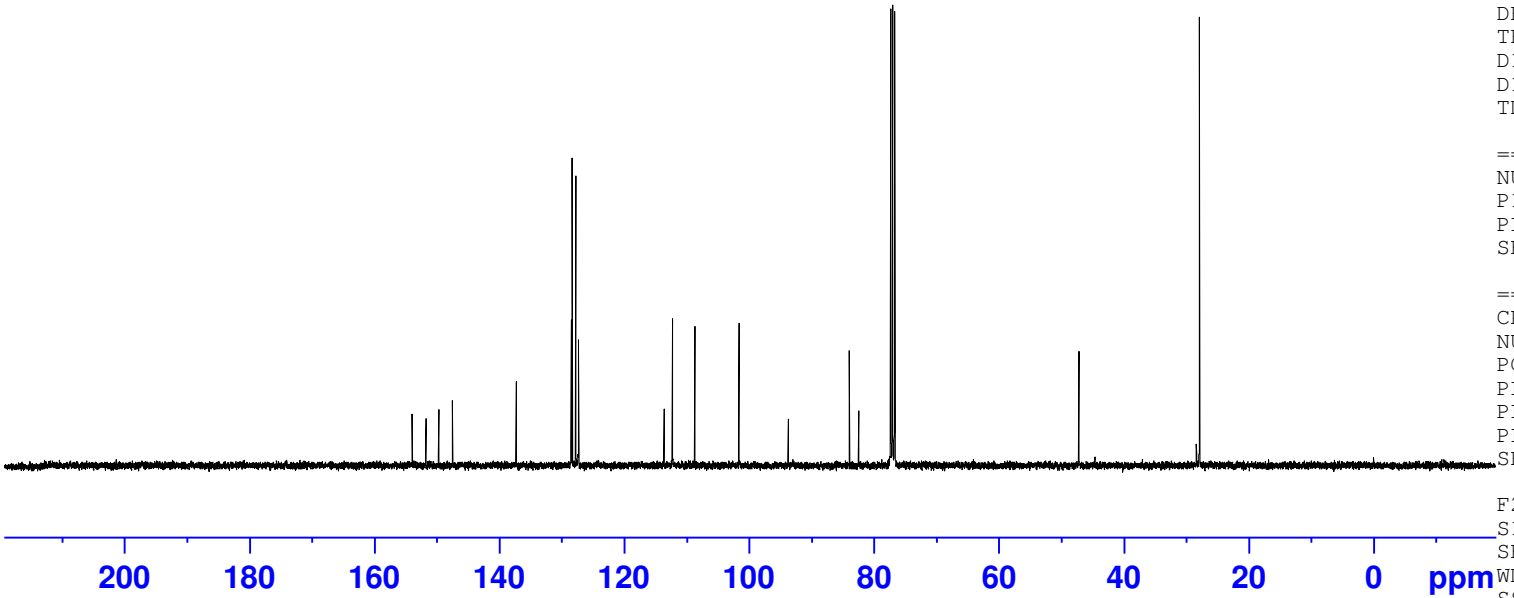
F2 - Processing parameters
SI 65536
SF 400.1900170 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZHL-3-42



1q

153.97
151.76
149.72
147.52
137.30
128.49
128.34
127.74
127.33
113.61
112.29
108.67
101.63
93.70
83.96
82.44
77.32
77.00
76.68
47.15
27.87



Current Data Parameters
NAME 20230423-400m
EXPNO 26
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230422
Time 15.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 291.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

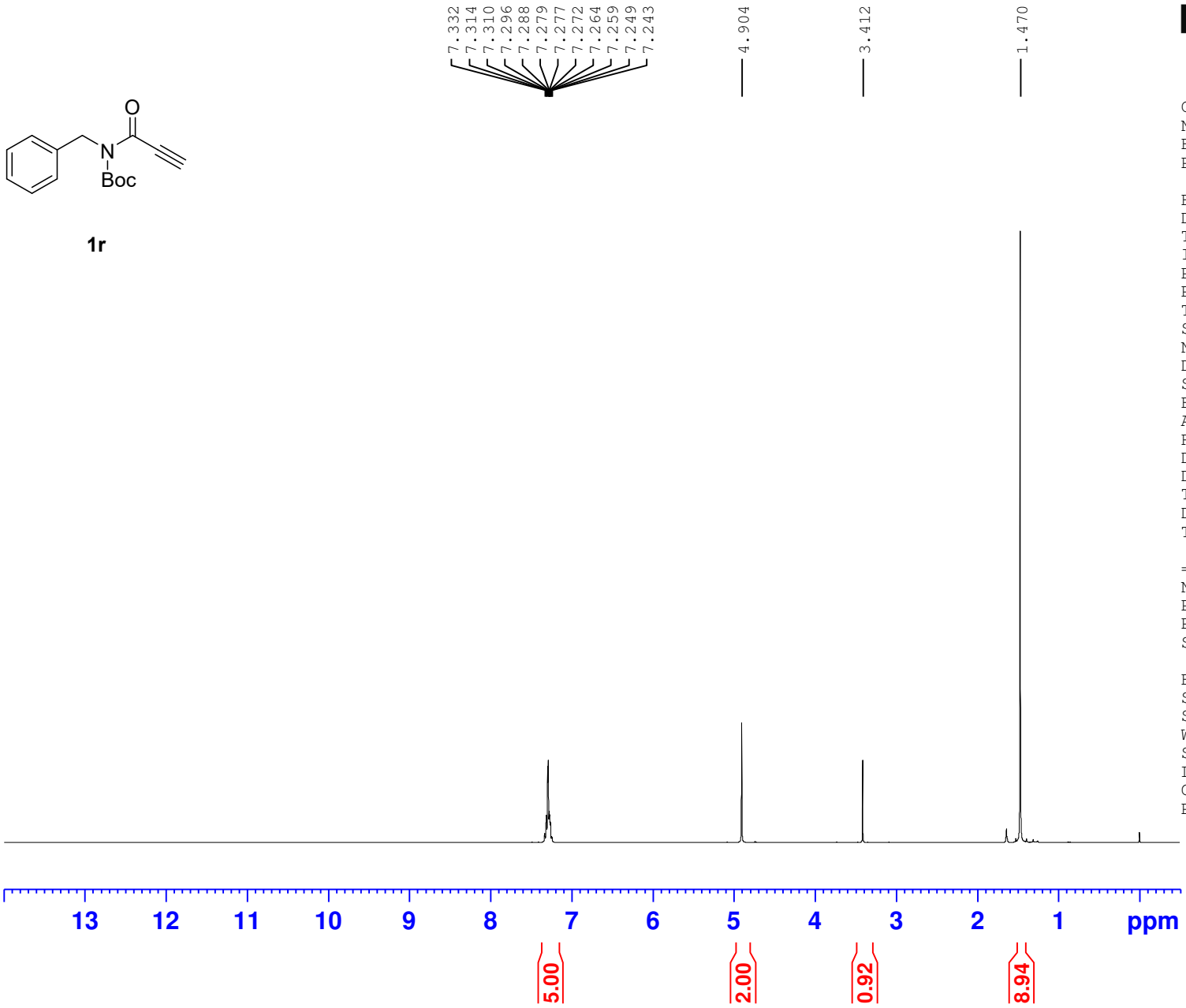
======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278645 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-2-100

1r



Current Data Parameters
NAME 20230418-400M
EXPNO 22
PROCNO 1

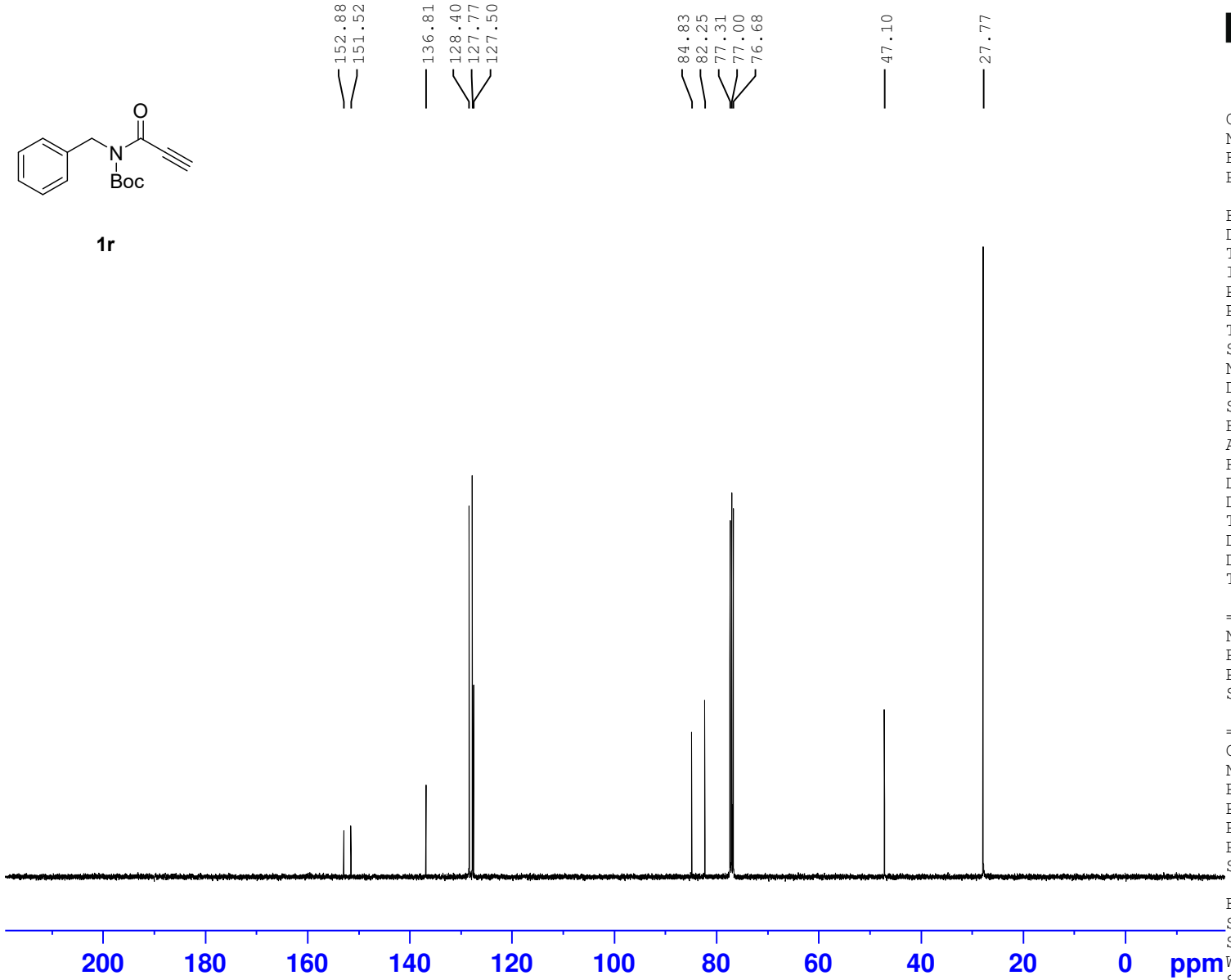
F2 - Acquisition Parameters
Date_ 20230418
Time 7.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 100.49
DW 60.800 usec
DE 6.50 usec
TE 291.6 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900151 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

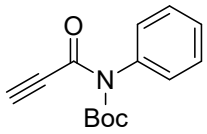
zhl-2-100

1r

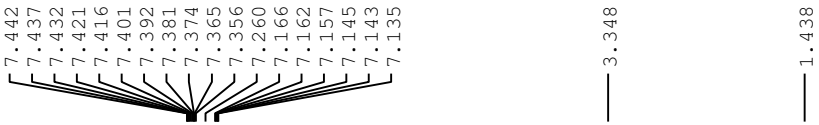


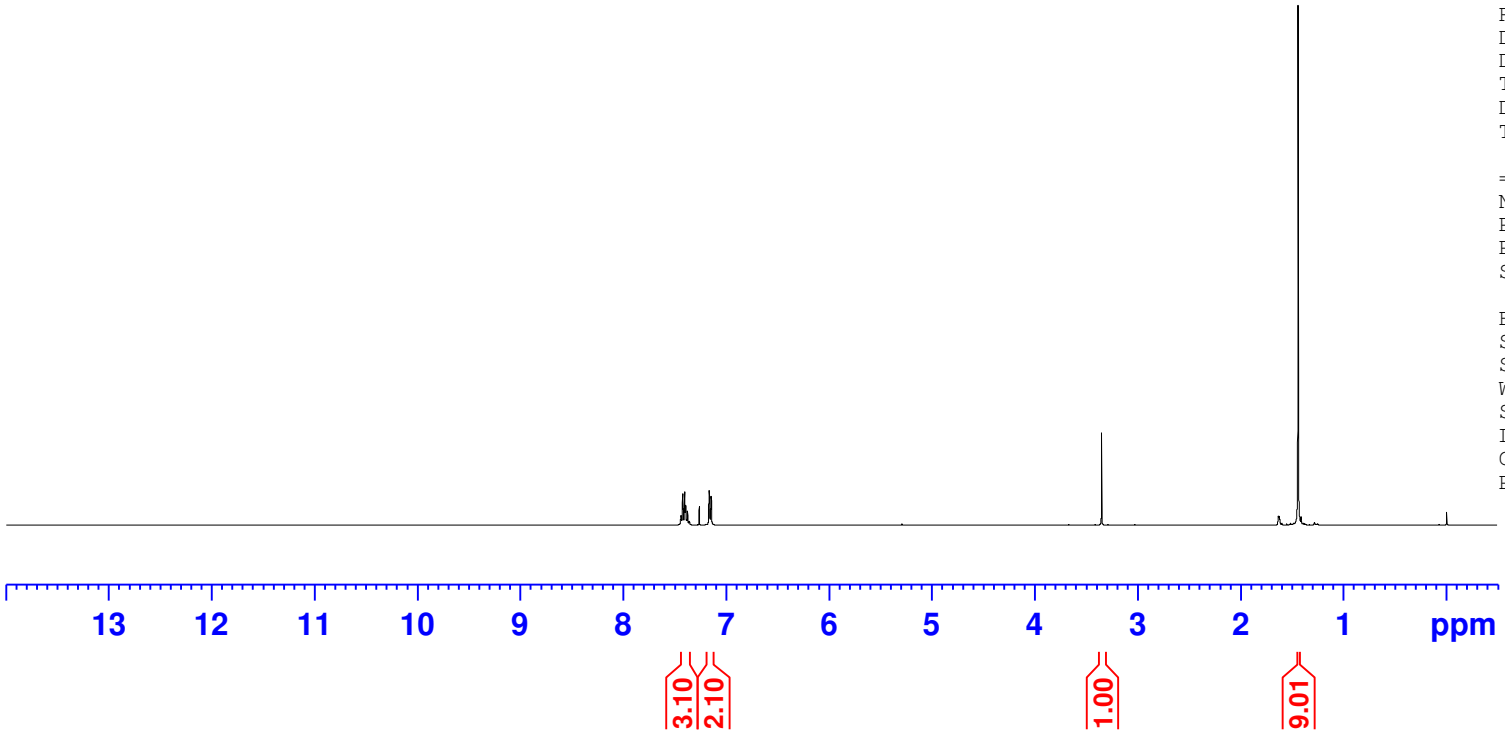

```
Current Data Parameters
NAME      20230418-400M
EXPNO                23
PROCNO                1

F2 - Acquisition Parameters
Date_          20230418
Time               7.24
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE               292.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                12.00 usec
PLW1         53.00000000 W
SFO1        100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2         14.00000000 W
PLW12         0.37246999 W
PLW13         0.30170000 W
SFO2        400.1916008 MHz

F2 - Processing parameters
SI                32768
SF          100.6278645 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

zhl-5-68



1s

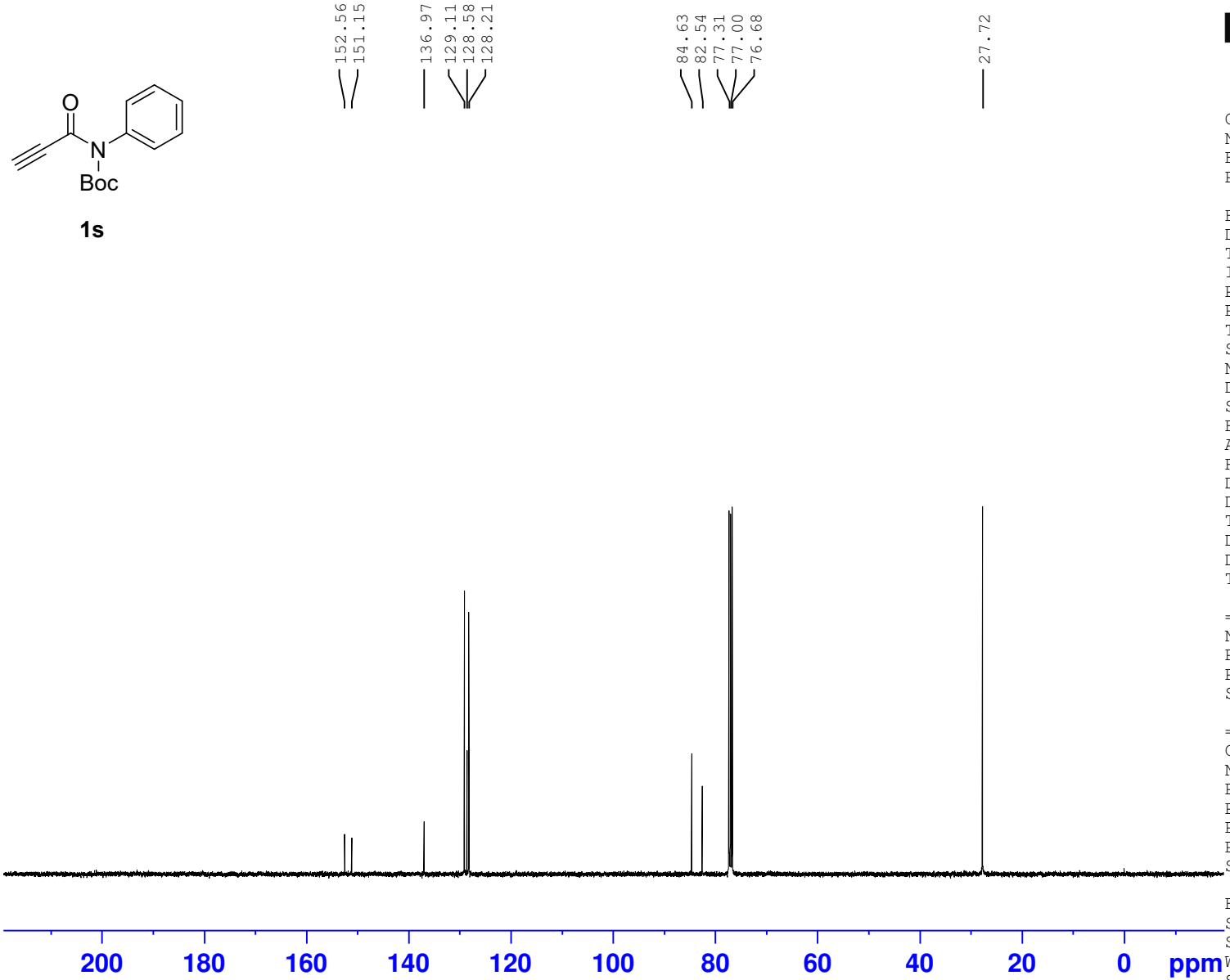





```
Current Data Parameters
NAME       20231003-400m
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231003
Time               19.24
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     6
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9845889 sec
RG                 90.23
DW                60.800 usec
DE                 6.50 usec
TE                291.7 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.90 usec
PLW1        23.00000000 W
SFO1        400.1924713 MHz

F2 - Processing parameters
SI                 65536
SF          400.1900139 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```

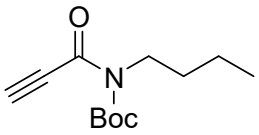
zhl-5-68

1s




```
Current Data Parameters
NAME      20231003-400M?¨1)
EXPNO                    6
PROCNO                   1

F2 - Acquisition Parameters
Date_             20231003
Time                 22.08
INSTRUM              spect
PROBHD    5 mm PADUL 13C
PULPROG            zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     400
DS                       4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    44.2
DW                20.800 usec
DE                 6.50 usec
TE                 292.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.80 usec
PLW1         47.40000153 W
SFO1        100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                   1H
PCPD2              90.00 usec
PLW2         23.00000000 W
PLW12         0.30712000 W
PLW13         0.24877000 W
SFO2        400.1916008 MHz

F2 - Processing parameters
SI                   32768
SF          100.6278642 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

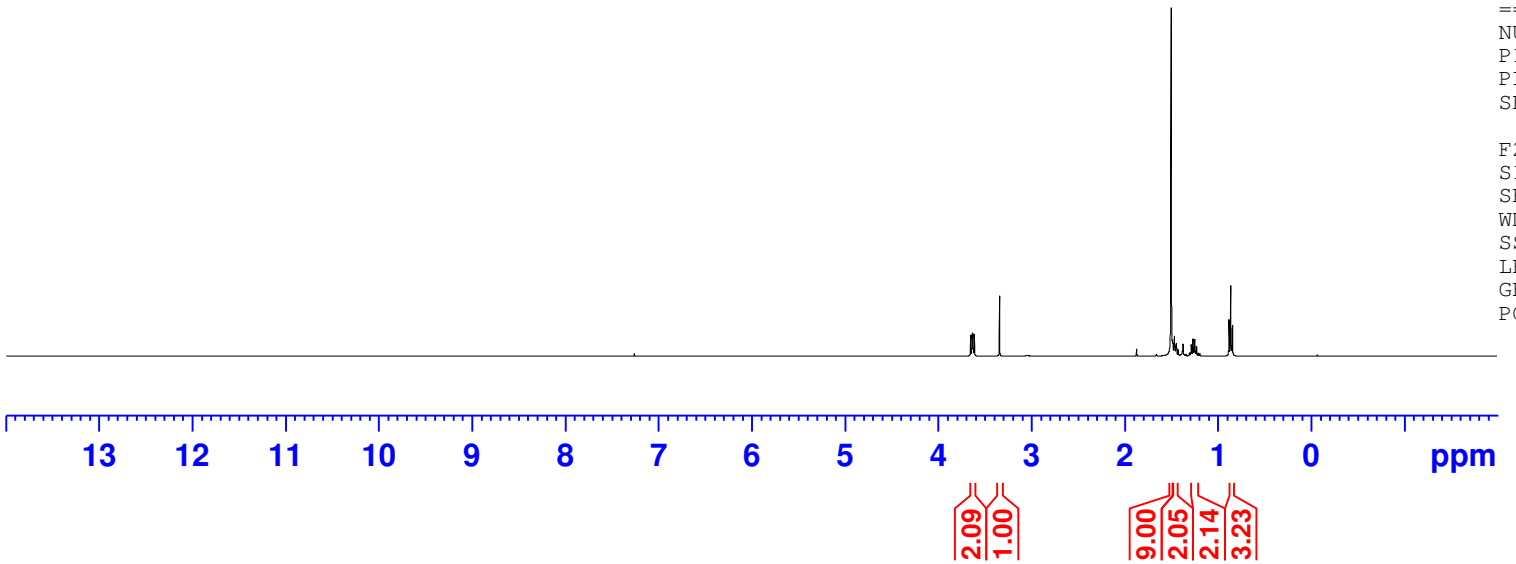
zhl-5-69



1t

7.260

3.649
3.631
3.612
3.341
1.500
1.487
1.484
1.479
1.469
1.464
1.457
1.445
1.441
1.426
1.302
1.284
1.265
1.246
1.228
1.210
1.190
0.879
0.861
0.842



Current Data Parameters
NAME 20231003-400m
EXPNO 2
PROCNO 1

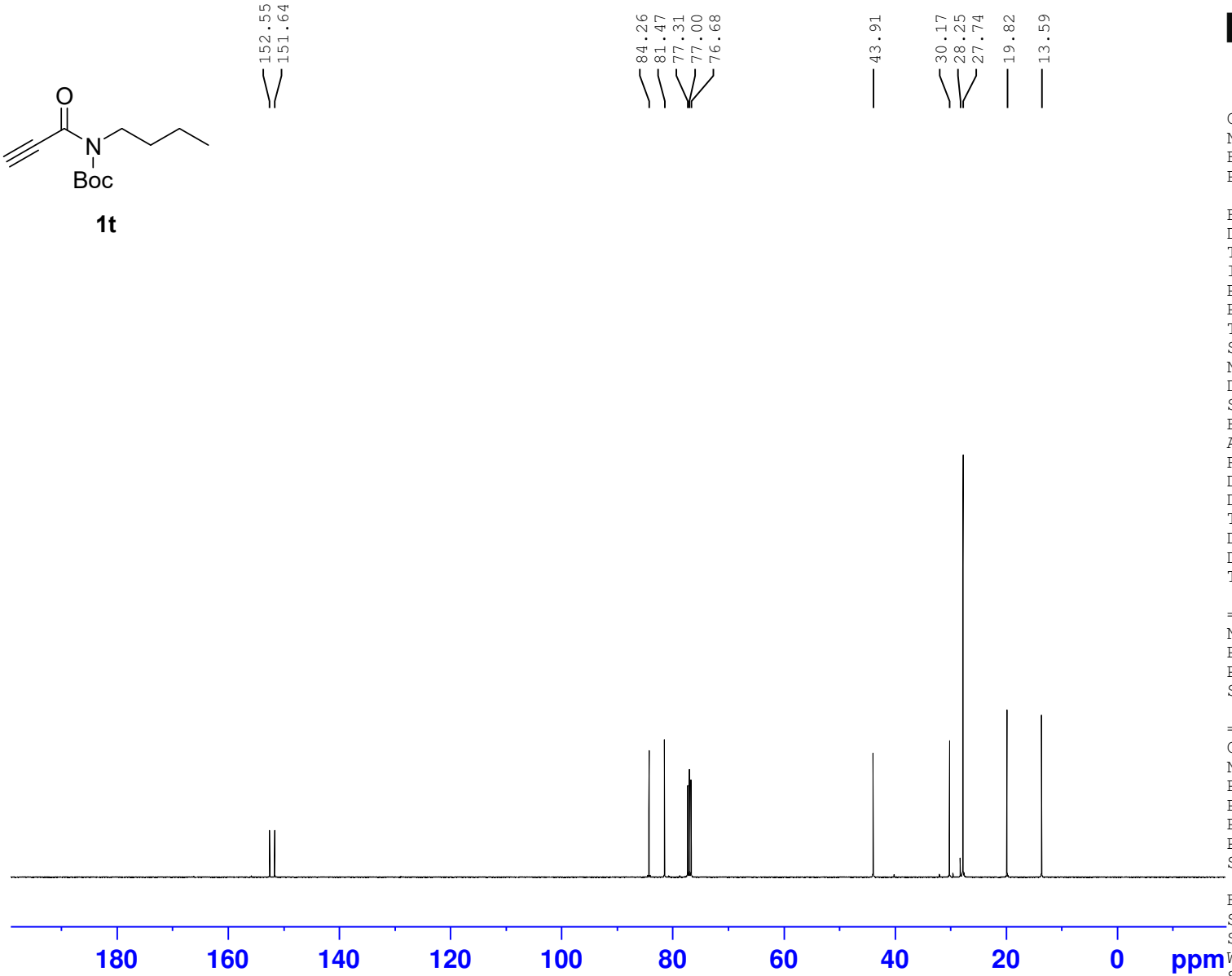
F2 - Acquisition Parameters
Date_ 20231003
Time 19.28
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 15.35
DW 60.800 usec
DE 6.50 usec
TE 291.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900135 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

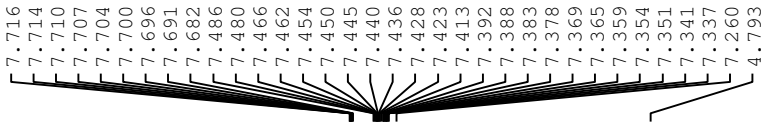
zhl-5-69

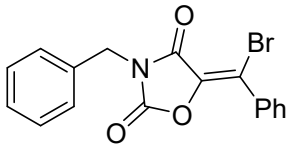
1t



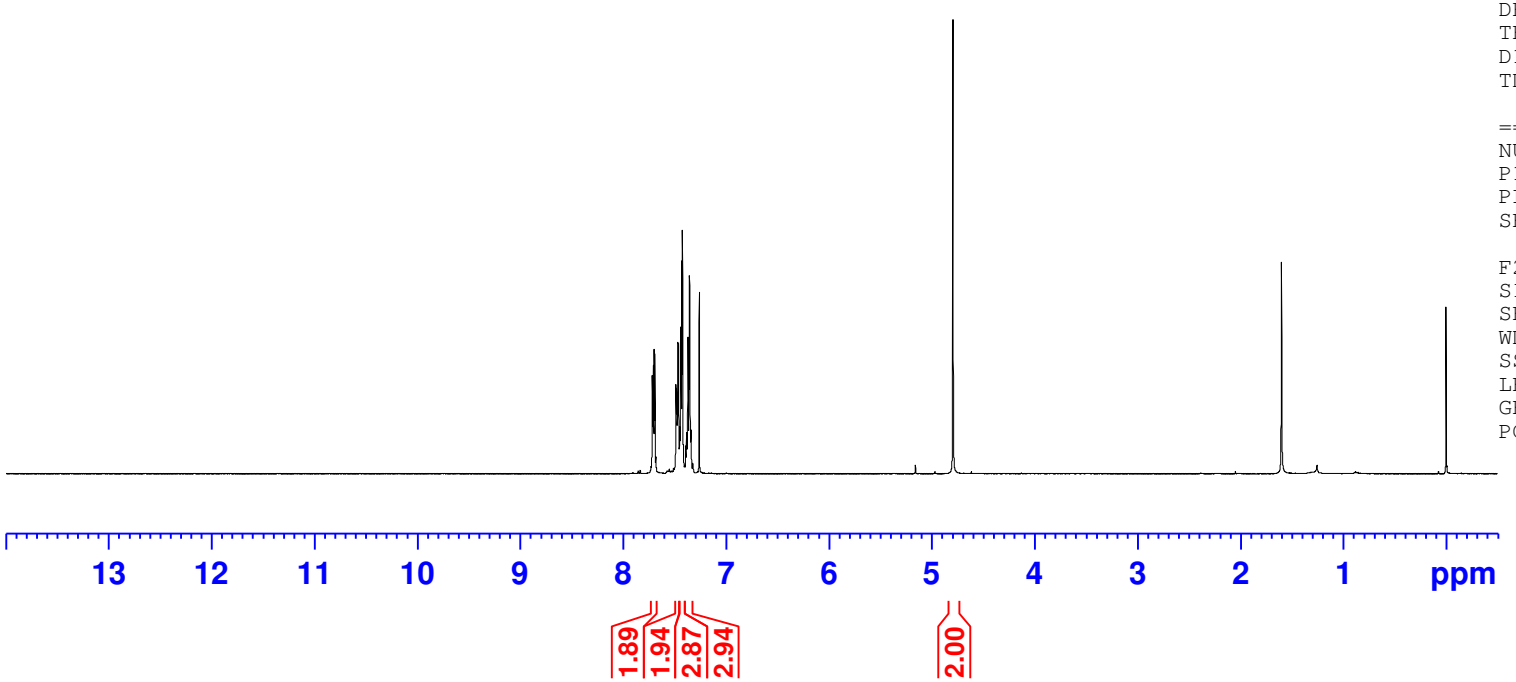

```
Current Data Parameters
NAME      20231003-400M?¨1)
EXPNO                    7
PROCNO                   1

F2 - Acquisition Parameters
Date_             20231003
Time                 22.57
INSTRUM              spect
PROBHD    5 mm PADUL 13C
PULPROG            zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     800
DS                       4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   29.75
DW                 20.800 usec
DE                  6.50 usec
TE                 292.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   9.80 usec
PLW1         47.40000153 W
SFO1        100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                   1H
PCPD2               90.00 usec
PLW2         23.00000000 W
PLW12         0.30712000 W
PLW13         0.24877000 W
SFO2        400.1916008 MHz

F2 - Processing parameters
SI                   32768
SF          100.6278689 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

zhl-35-35a





2a



Current Data Parameters
NAME 20230707-400M
EXPNO 25
PROCNO 1

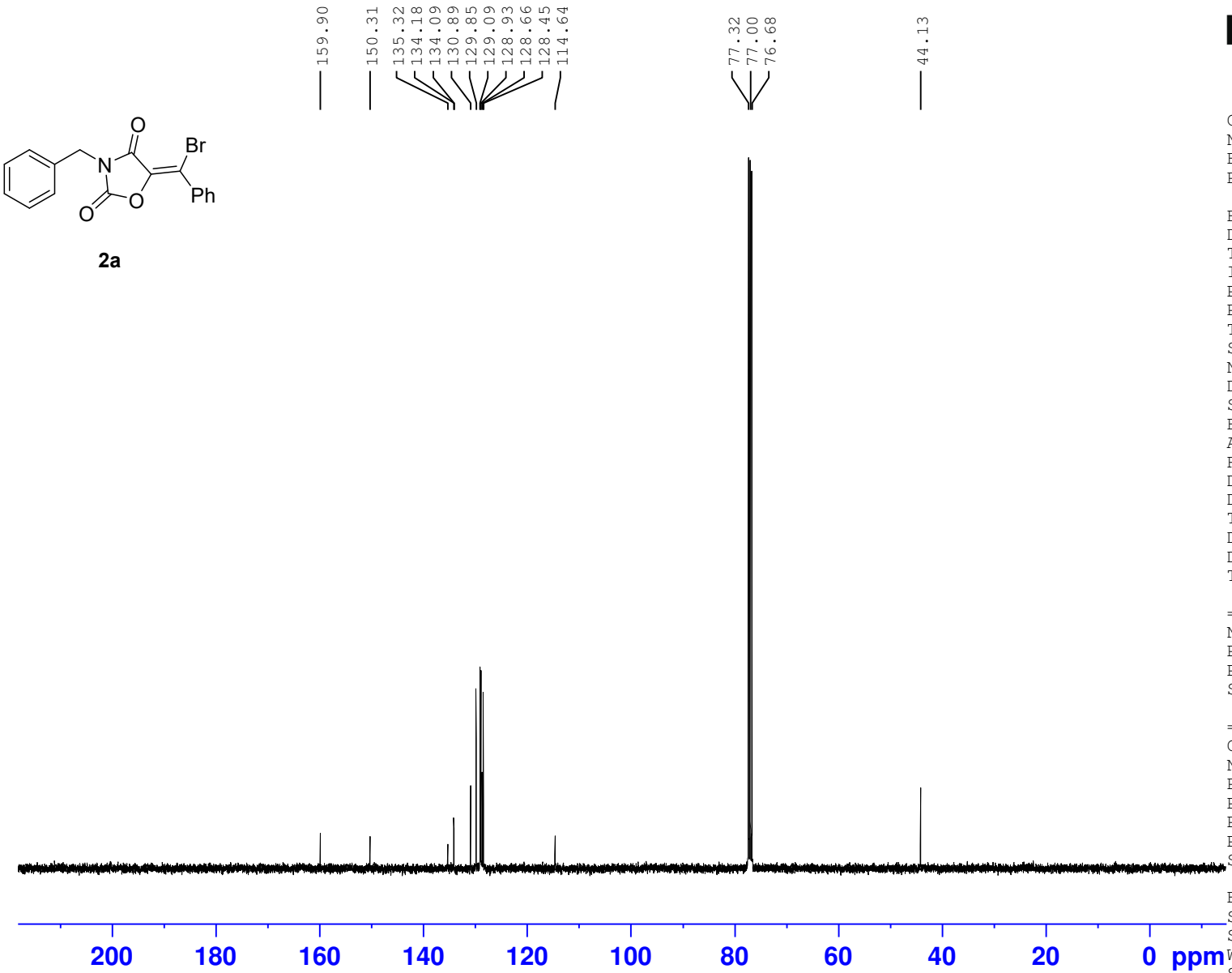
F2 - Acquisition Parameters
Date_ 20230706
Time 23.13
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 154.68
DW 60.800 usec
DE 6.50 usec
TE 290.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900140 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-35a

2a



Current Data Parameters
NAME 20230626-400m
EXPNO 28
PROCNO 1

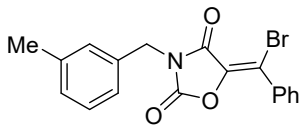
F2 - Acquisition Parameters
Date_ 20230626
Time 2.33
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 300
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 29.75
DW 20.800 usec
DE 6.50 usec
TE 293.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

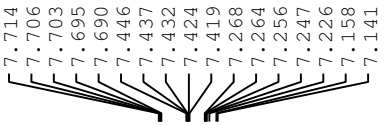
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

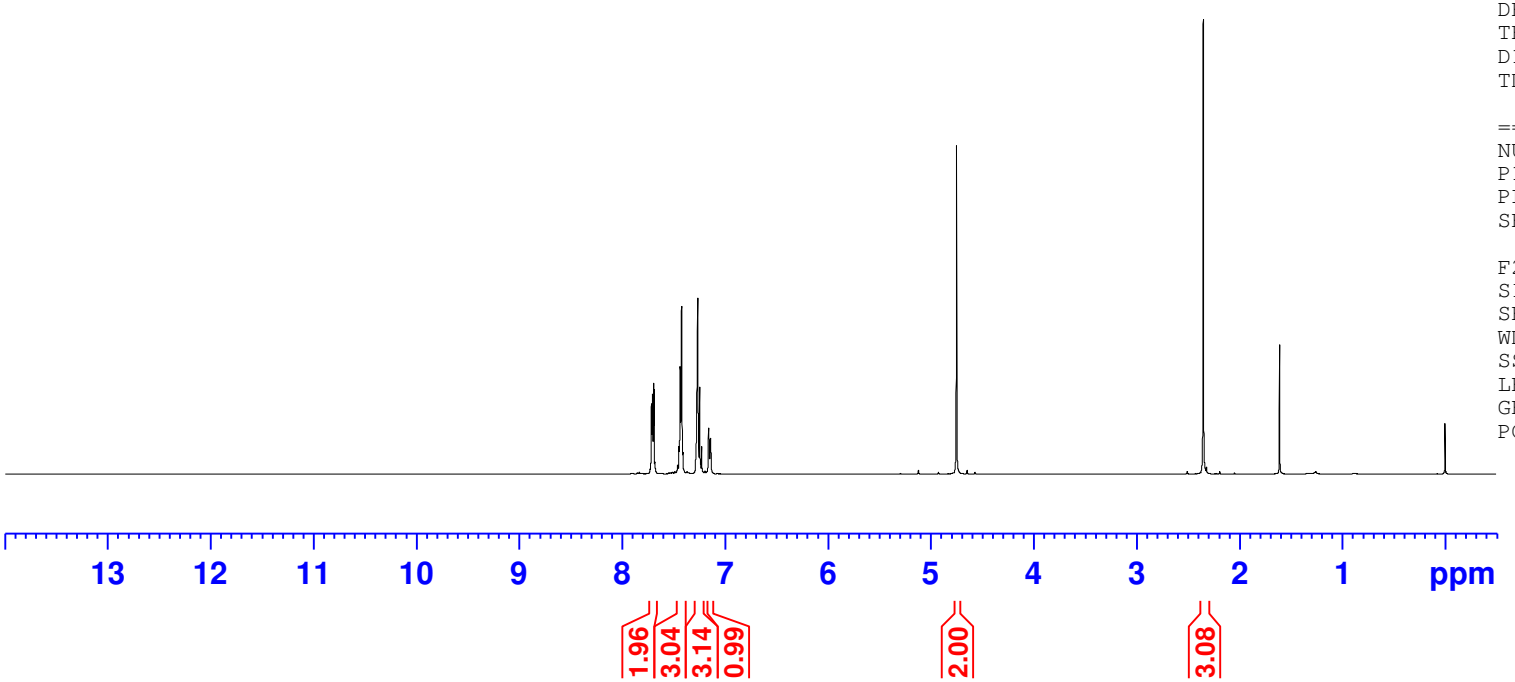
F2 - Processing parameters
SI 32768
SF 100.6273840 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

CB-1-31A



2b

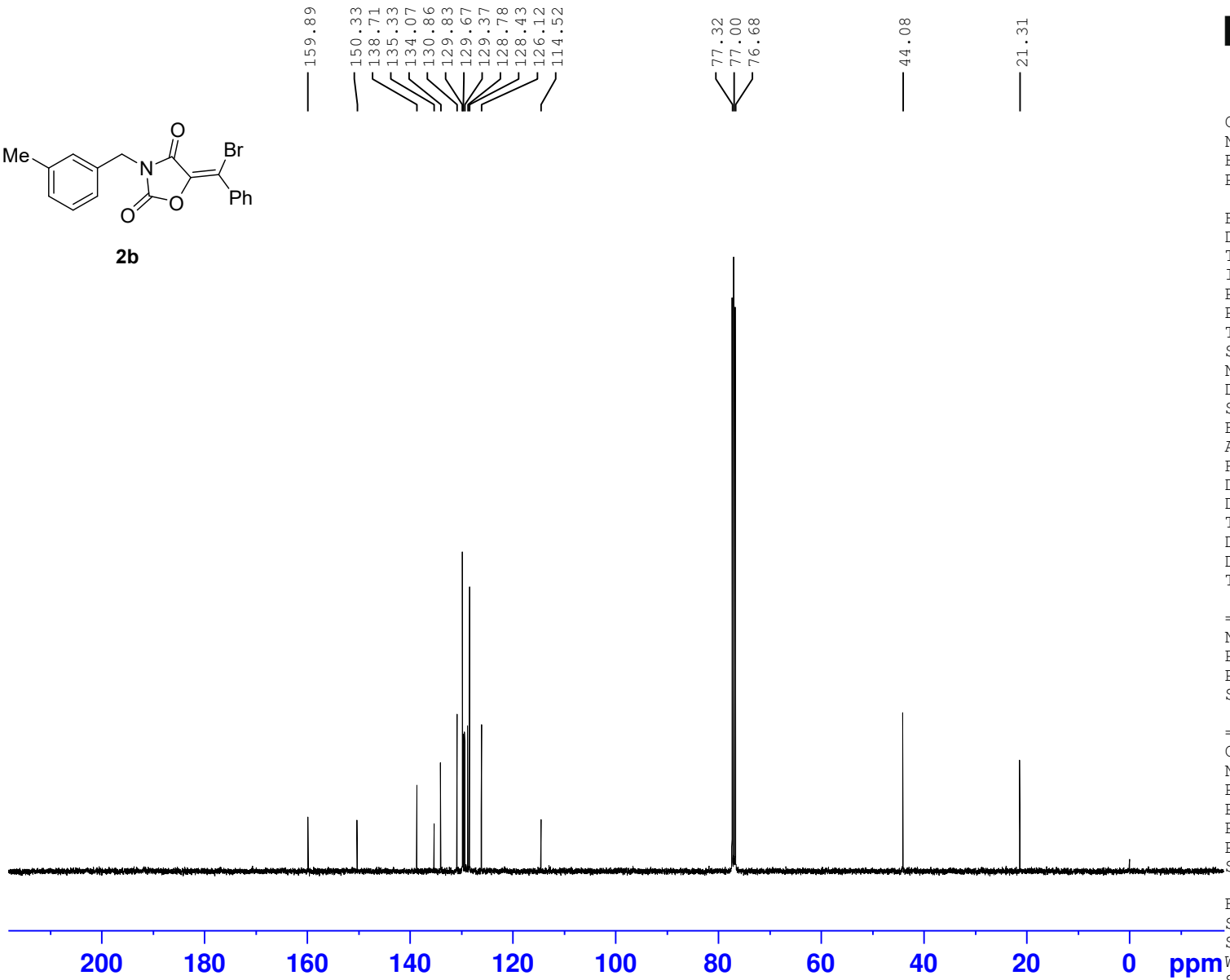





```
Current Data Parameters
NAME          Cb-ketiyi
EXPNO                42
PROCNO                1

F2 - Acquisition Parameters
Date_          20230408
Time              11.29
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   6
DS                   2
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9845889 sec
RG               125.76
DW               60.800 usec
DE                6.50 usec
TE               289.0 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                14.68 usec
PLW1        14.00000000 W
SFO1        400.1924713 MHz

F2 - Processing parameters
SI               65536
SF          400.1900180 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```

CB-1-31A

2b



Current Data Parameters
NAME Cb-ketiyi
EXPNO 43
PROCNO 1

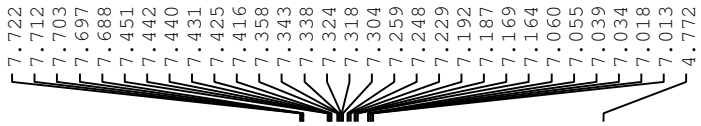
F2 - Acquisition Parameters
Date_ 20230408
Time 11.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 290.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

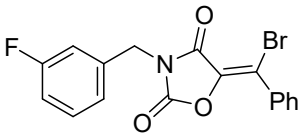
======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278652 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-3-56A





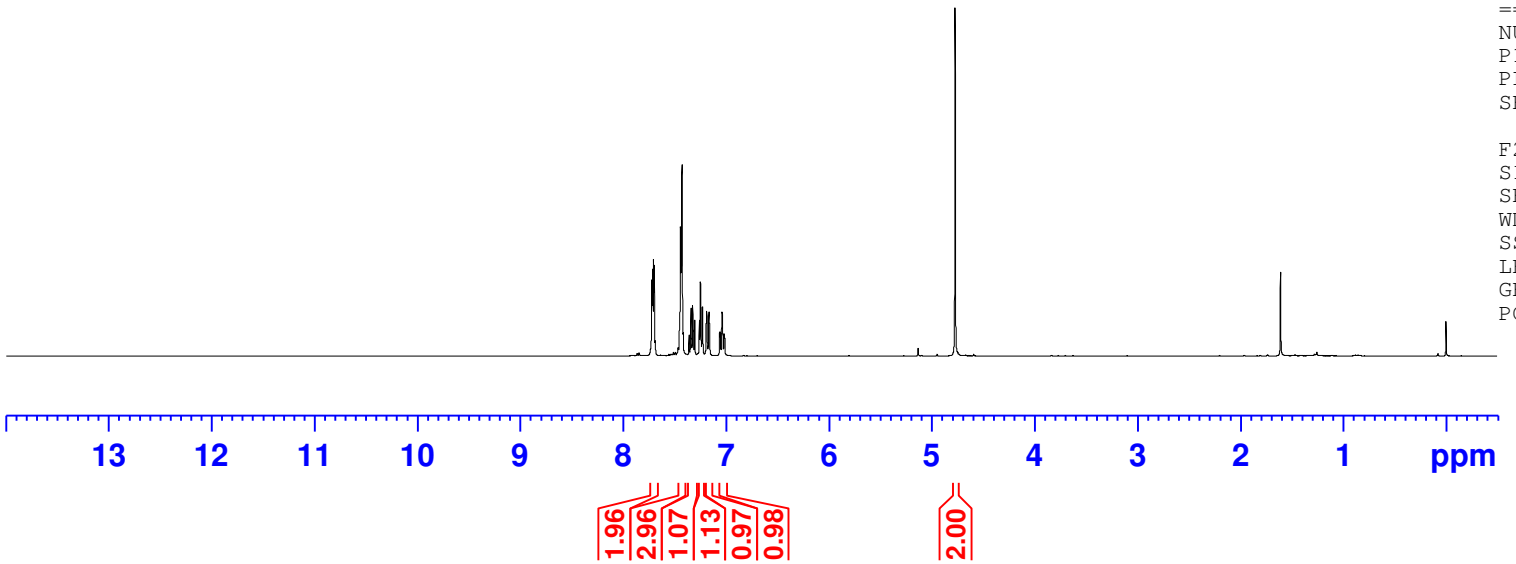
2c

Current Data Parameters
NAME 20230323-400m
EXPNO 138
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230323
Time 1.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 140.02
DW 60.800 usec
DE 6.50 usec
TE 291.9 K
D1 1.00000000 sec
TD0 1

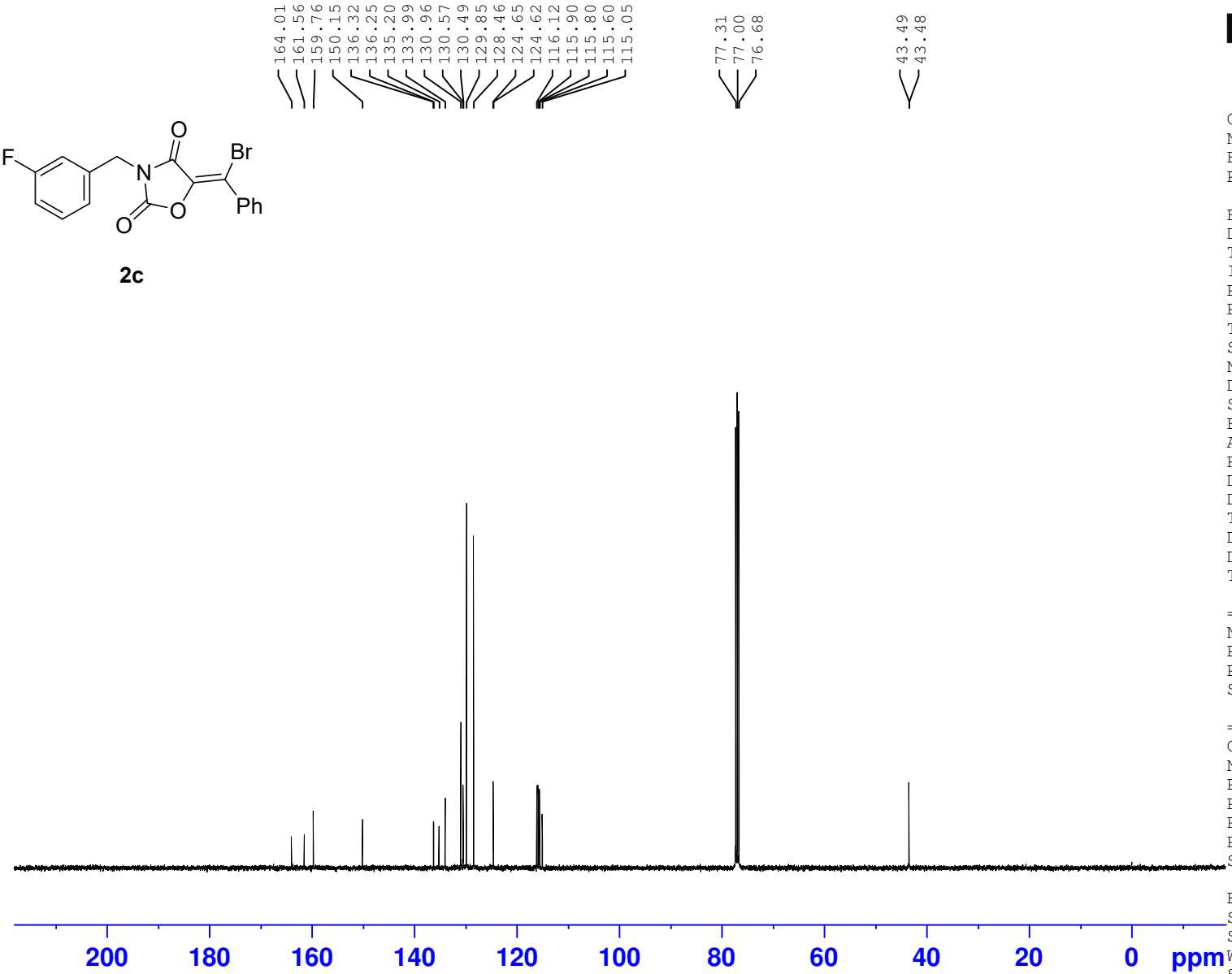
======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900168 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



zhl-3-56A

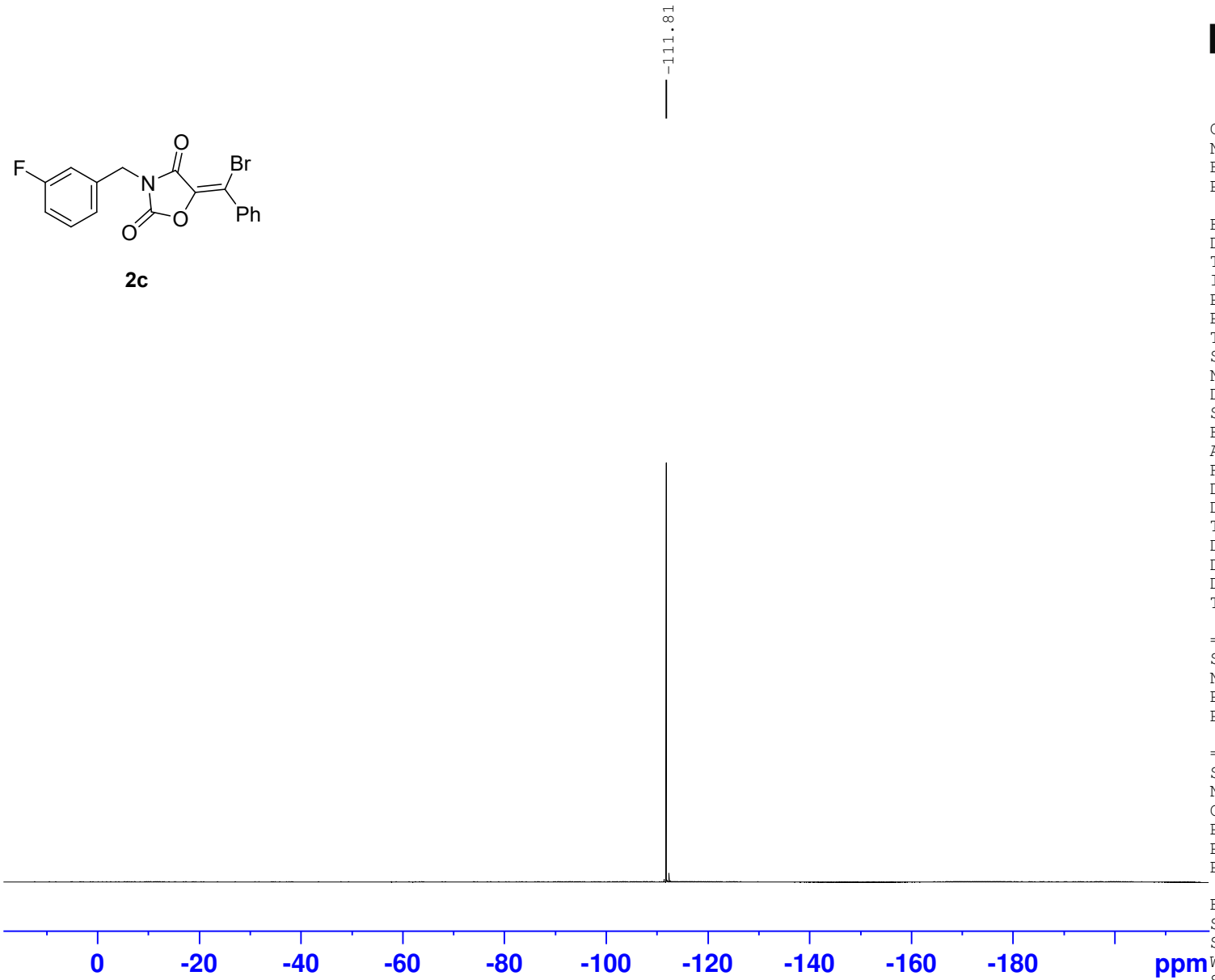
2c




```
Current Data Parameters
NAME      20230323-400m
EXPNO               139
PROCNO                1

F2 - Acquisition Parameters
Date_          20230323
Time               2.15
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE               292.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                12.00 usec
PLW1        53.00000000 W
SFO1       100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.37246999 W
PLW13        0.30170000 W
SFO2       400.1916008 MHz

F2 - Processing parameters
SI                32768
SF         100.6278645 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

zhl-3-56a

2c



Current Data Parameters
NAME 20230323-300M
EXPNO 21
PROCNO 1

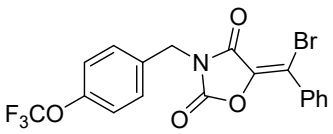
F2 - Acquisition Parameters
Date_ 20230323
Time 13.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn.2
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 0.510897 Hz
AQ 0.9786710 sec
RG 203
DW 7.467 usec
DE 6.50 usec
TE 290.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 282.3761148 MHz
NUC1 19F
P1 14.50 usec
PLW1 10.39999962 W

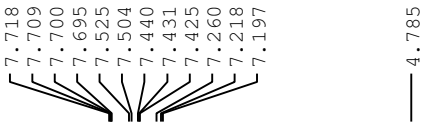
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W

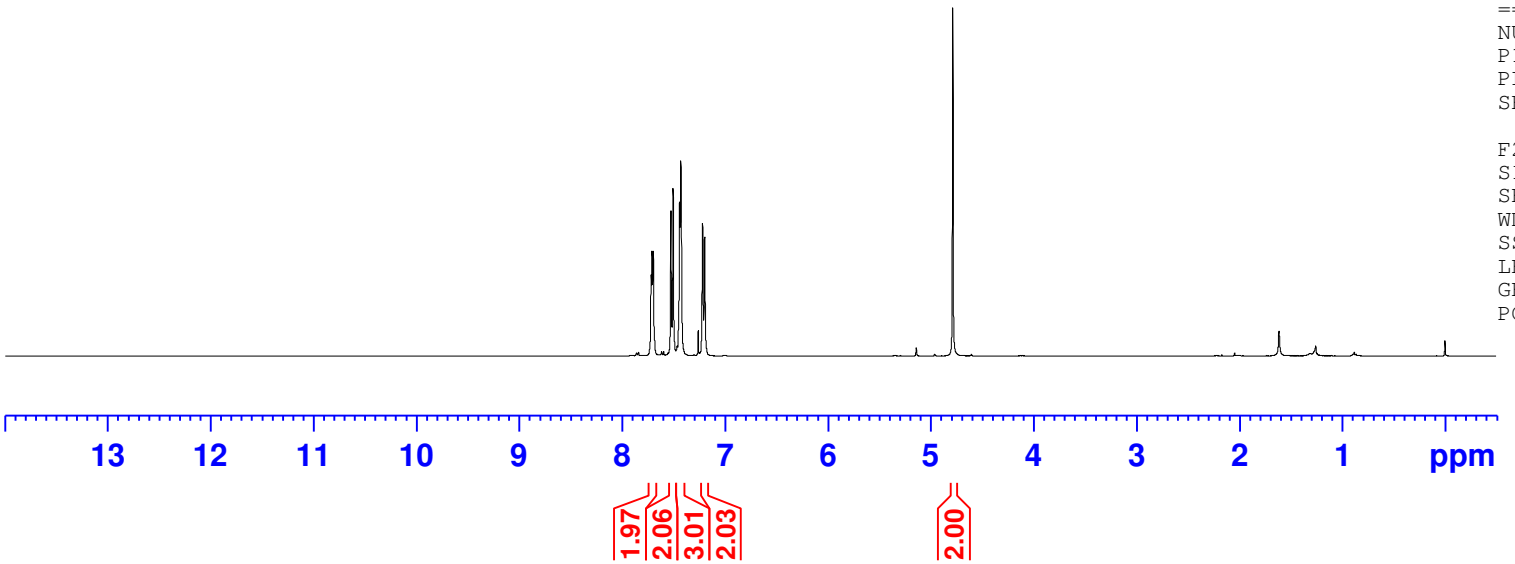
F2 - Processing parameters
SI 65536
SF 282.4043552 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-47a



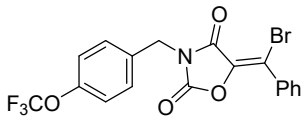
2d






```
Current Data Parameters
NAME       20230427-400M
EXPNO                 26
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230427
Time                0.35
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     6
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9845889 sec
RG                125.76
DW                60.800 usec
DE                 6.50 usec
TE                291.3 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.68 usec
PLW1         14.00000000 W
SFO1         400.1924713 MHz

F2 - Processing parameters
SI                 65536
SF           400.1900169 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

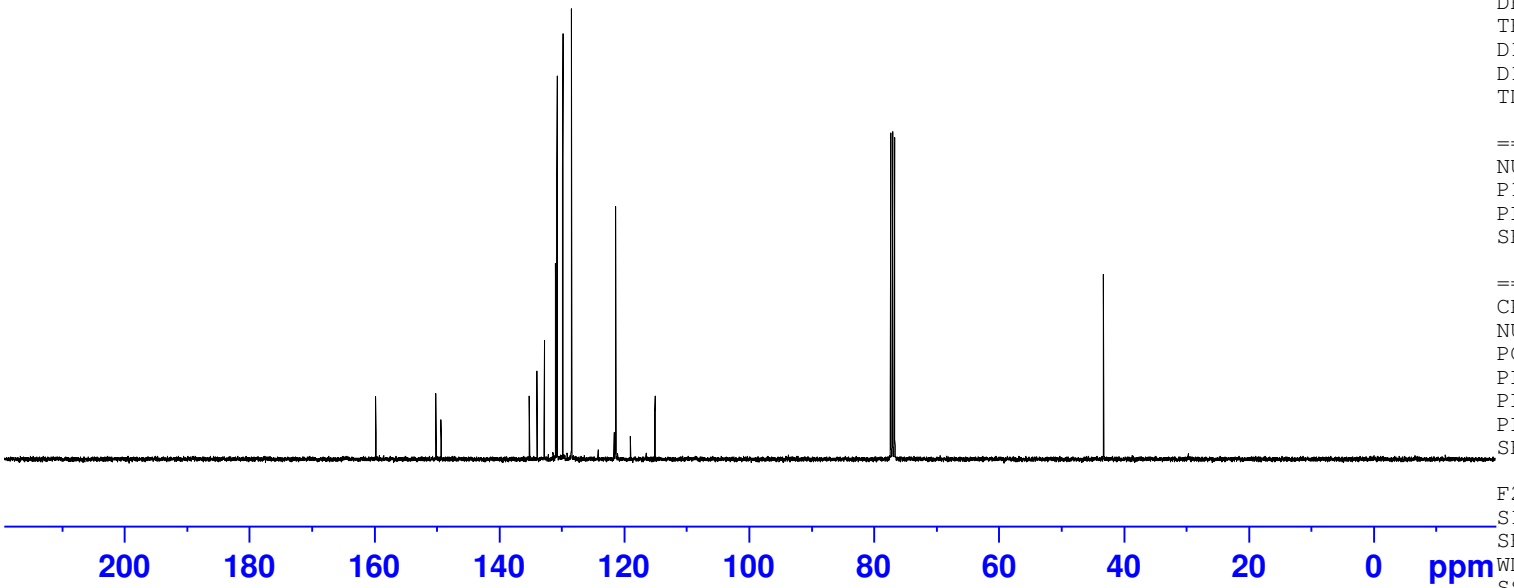
zhl-3-47a



2d

159.78
150.14
149.33
135.18
133.96
132.79
130.96
130.75
129.83
128.45
124.15
121.59
121.35
119.03
116.47
115.07

43.23



Current Data Parameters
NAME 20230506-400m
EXPNO 32
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230506
Time 7.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 292.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

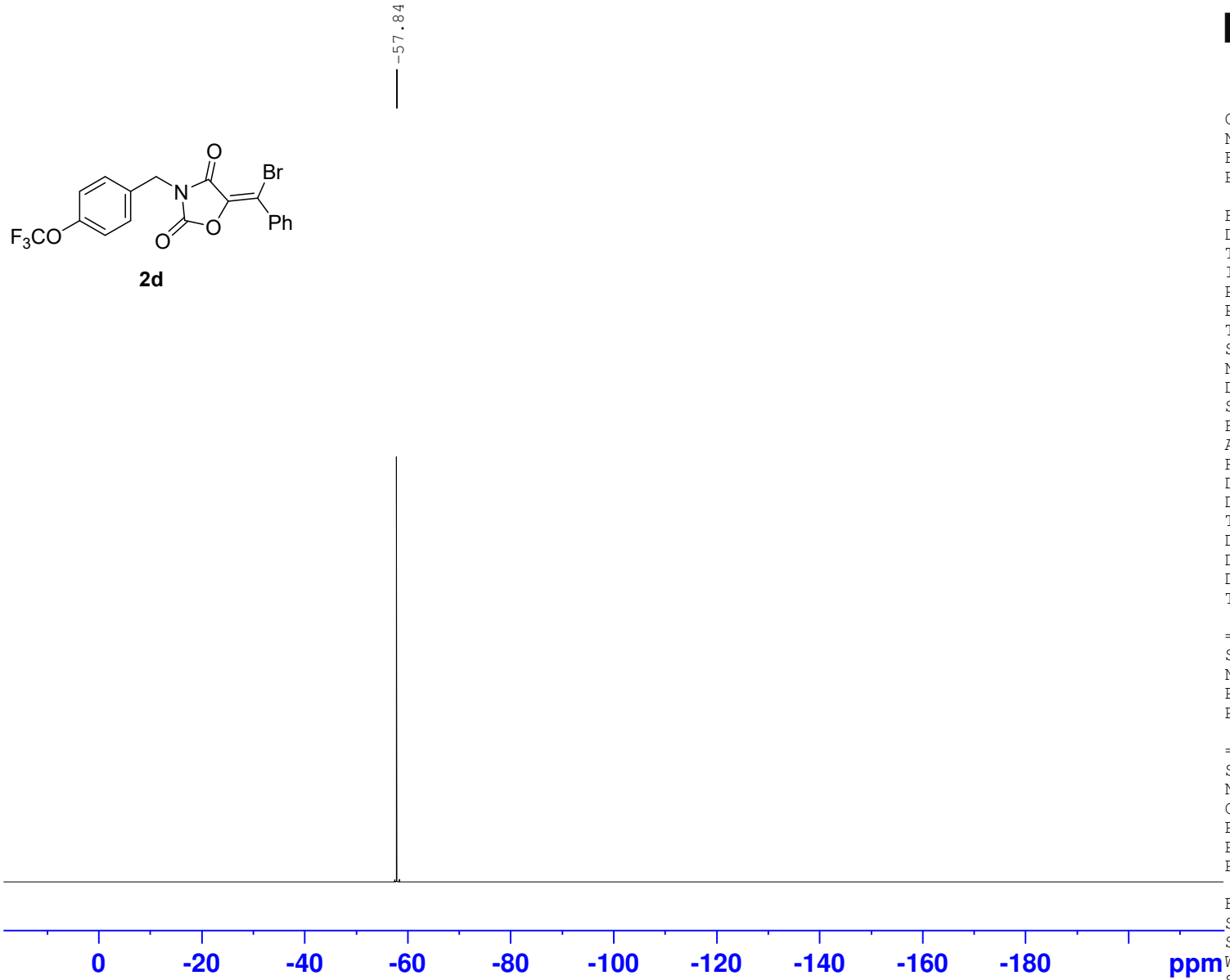
======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278655 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

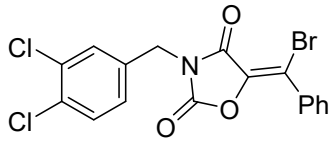
zhl-3-47a

2d

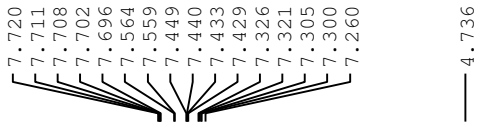


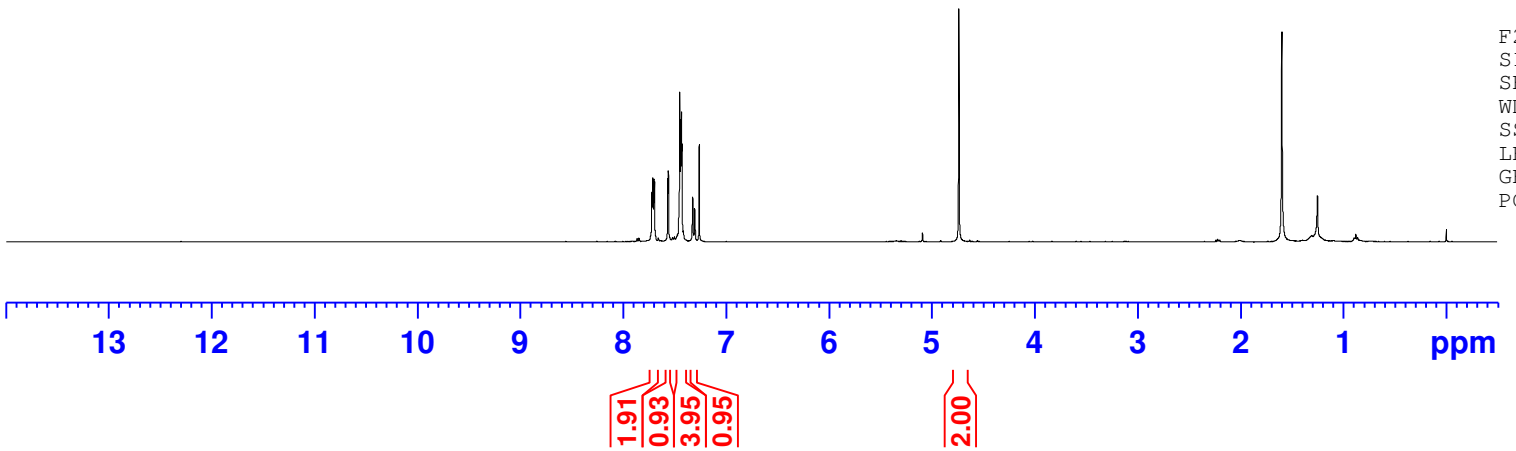

```
Current Data Parameters
NAME      20230627-300M
EXPNO               202
PROCNO                1

F2 - Acquisition Parameters
Date_          20230627
Time              11.56
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG      zgfhigqn.2
TD              131072
SOLVENT           CDCl3
NS                   16
DS                    4
SWH           66964.289 Hz
FIDRES         0.510897 Hz
AQ            0.9786710 sec
RG                  203
DW                7.467 usec
DE                6.50 usec
TE                296.8 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        282.3761148 MHz
NUC1                19F
P1                14.50 usec
PLW1        10.39999962 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.17284000 W

F2 - Processing parameters
SI                65536
SF          282.4043552 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

zhl-3-44a



2e





Current Data Parameters
NAME 20230626-400m
EXPNO 4
PROCNO 1

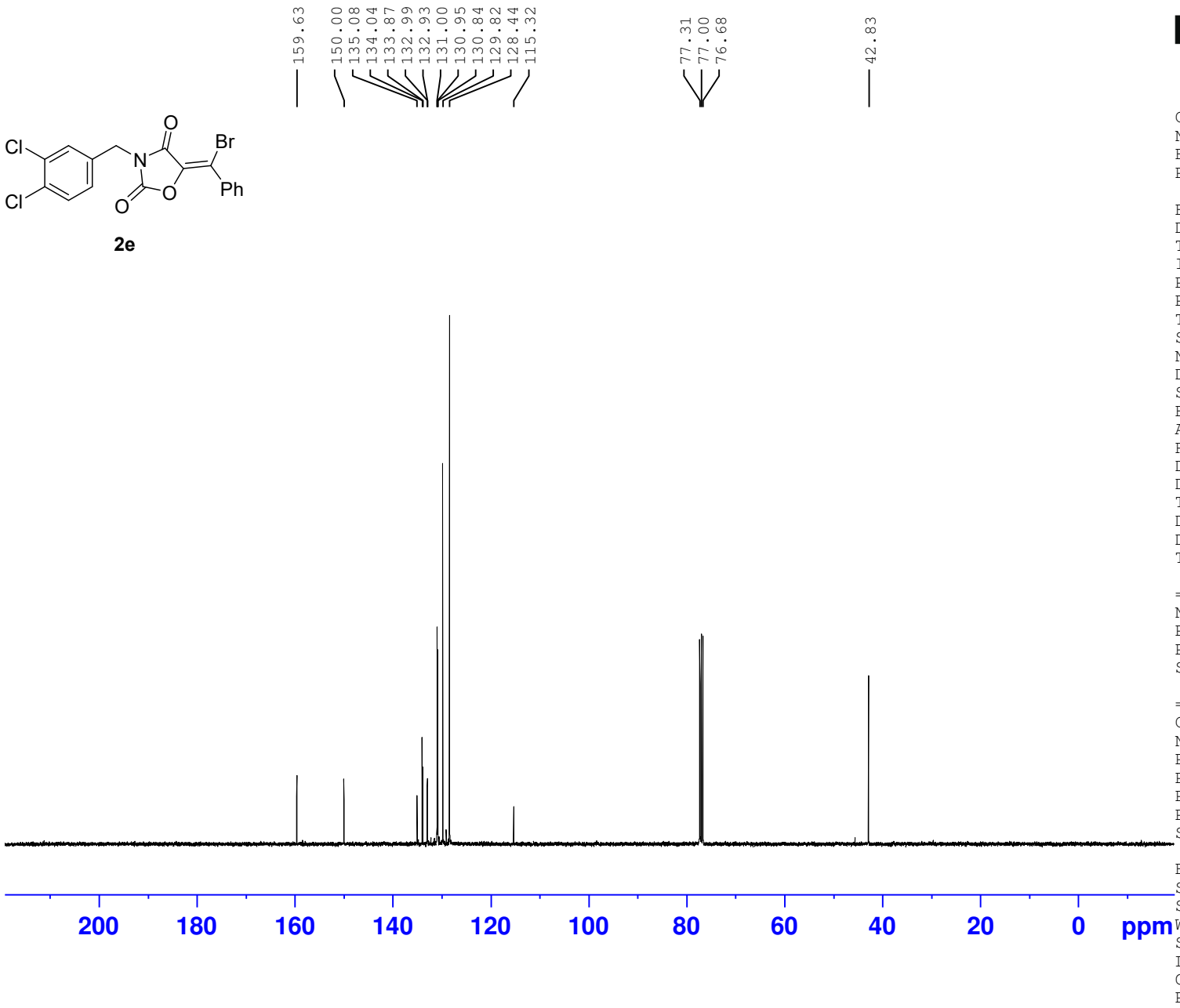
F2 - Acquisition Parameters
Date_ 20230625
Time 21.49
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 193.13
DW 60.800 usec
DE 6.50 usec
TE 292.5 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900140 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

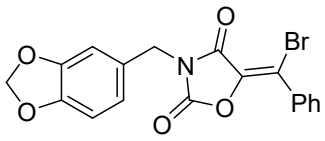
zhl-3-44a

2e

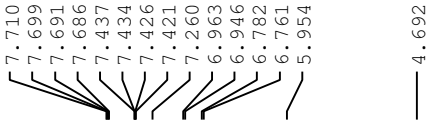


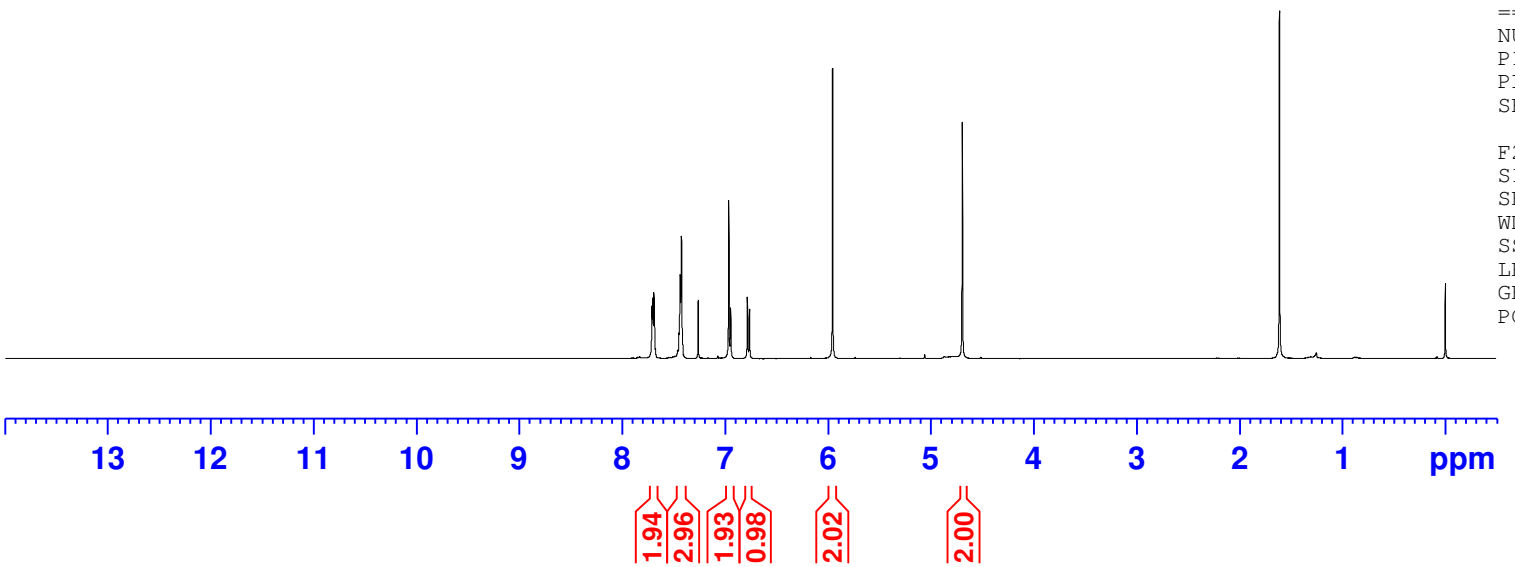

```
Current Data Parameters
NAME      20230506-400m
EXPNO                29
PROCNO                1

F2 - Acquisition Parameters
Date_          20230506
Time               6.45
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  300
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE               292.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                12.00 usec
PLW1        53.00000000 W
SFO1       100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.37246999 W
PLW13        0.30170000 W
SFO2       400.1916008 MHz

F2 - Processing parameters
SI                32768
SF         100.6278688 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

cb-1-30a



2f





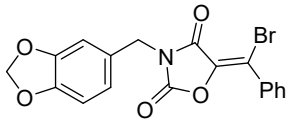
Current Data Parameters
NAME Cb-ketiyi
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230317
Time 22.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 193.13
DW 60.800 usec
DE 6.50 usec
TE 293.4 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

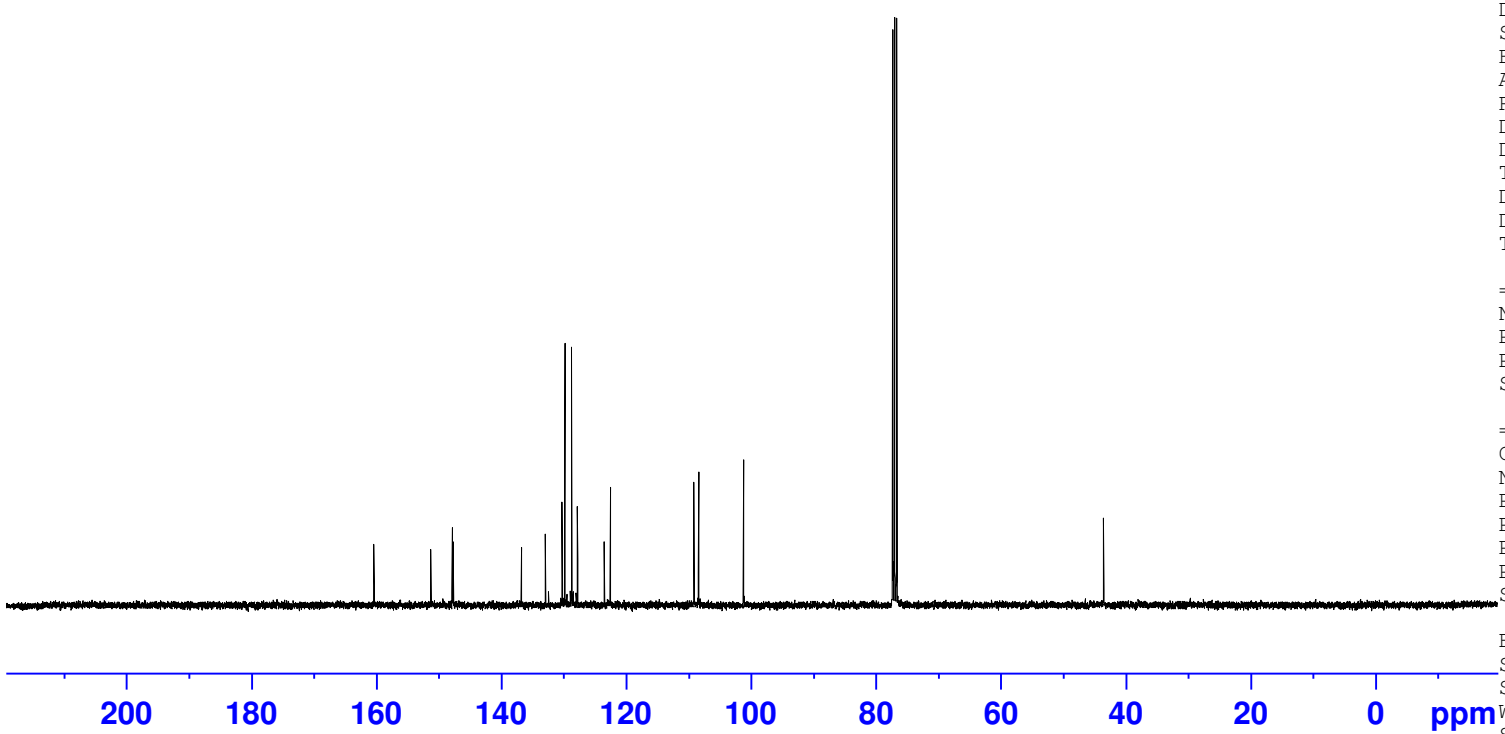
F2 - Processing parameters
SI 65536
SF 400.1900164 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

cb-1-30



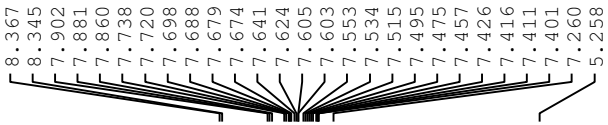
2f

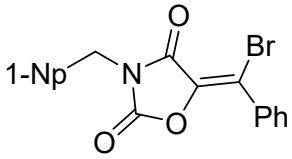
160.40
151.30
147.87
147.72
136.78
132.97
130.27
129.84
128.75
127.79
123.53
122.54
109.19
108.40
101.20
77.31
76.99
76.68
43.55



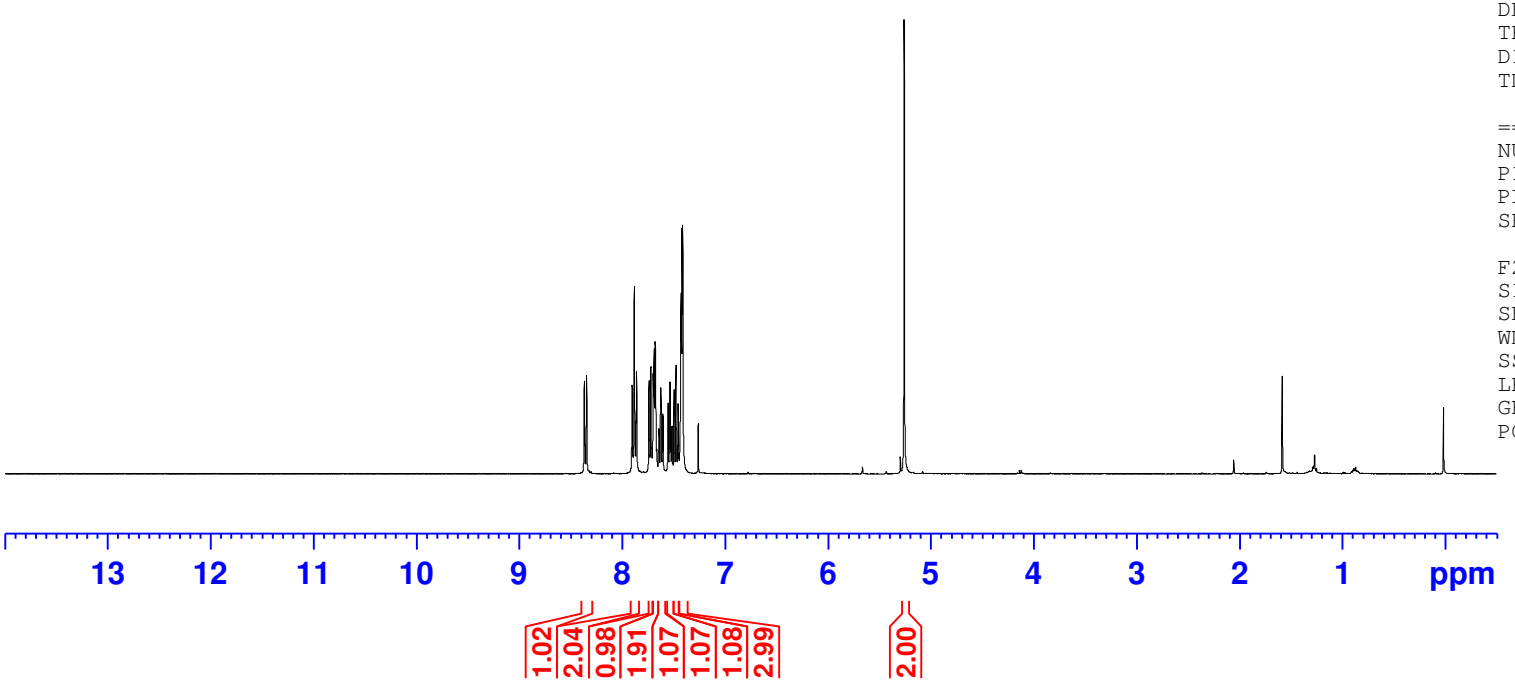

```
Current Data Parameters
NAME          Cb-ketiyi
EXPNO               149
PROCNO                1

F2 - Acquisition Parameters
Date_          20230425
Time               3.10
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  300
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE               290.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                12.00 usec
PLW1        53.00000000 W
SFO1       100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.37246999 W
PLW13        0.30170000 W
SFO2       400.1916008 MHz

F2 - Processing parameters
SI                32768
SF         100.6278645 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

CB-1-28A





2g



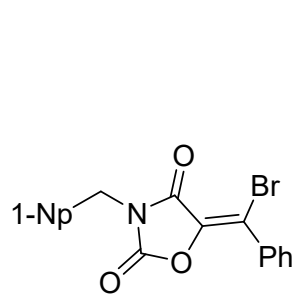
Current Data Parameters
NAME Cb-ketiyi
EXPNO 23
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230309
Time 0.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 140.02
DW 60.800 usec
DE 6.50 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900166 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

cb-1-28

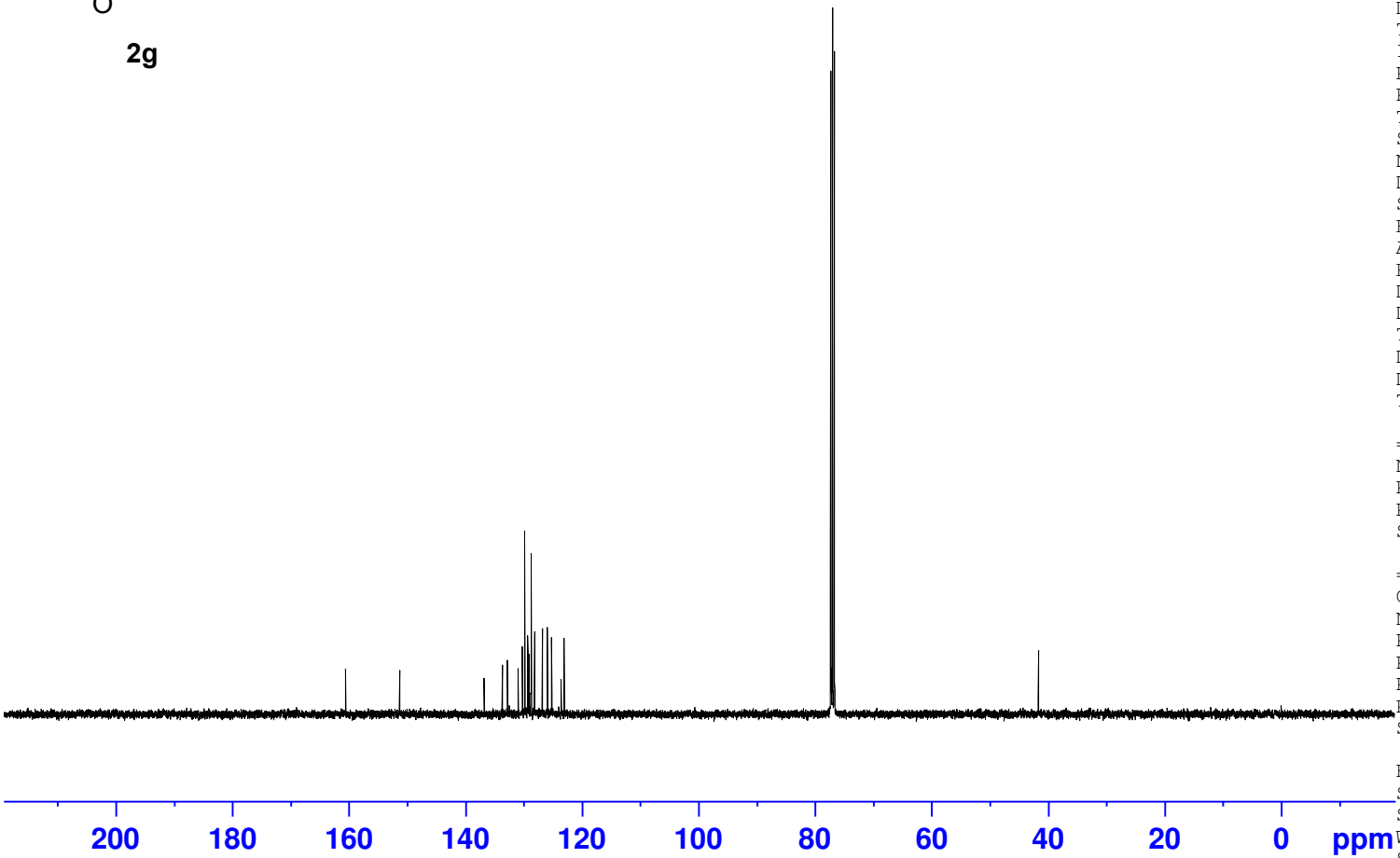


2g

160.60
151.32
136.84
133.70
132.86
130.97
130.25
129.84
129.31
129.09
128.79
128.73
128.16
126.81
125.98
125.22
123.58
123.07

77.32
77.00
76.68

41.65



Current Data Parameters
NAME Cb-ketiyi
EXPNO 151
PROCNO 1

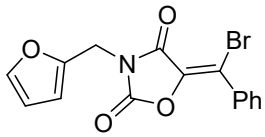
F2 - Acquisition Parameters
Date_ 20230425
Time 3.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 290.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

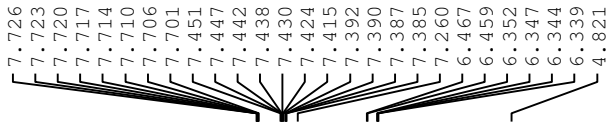
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

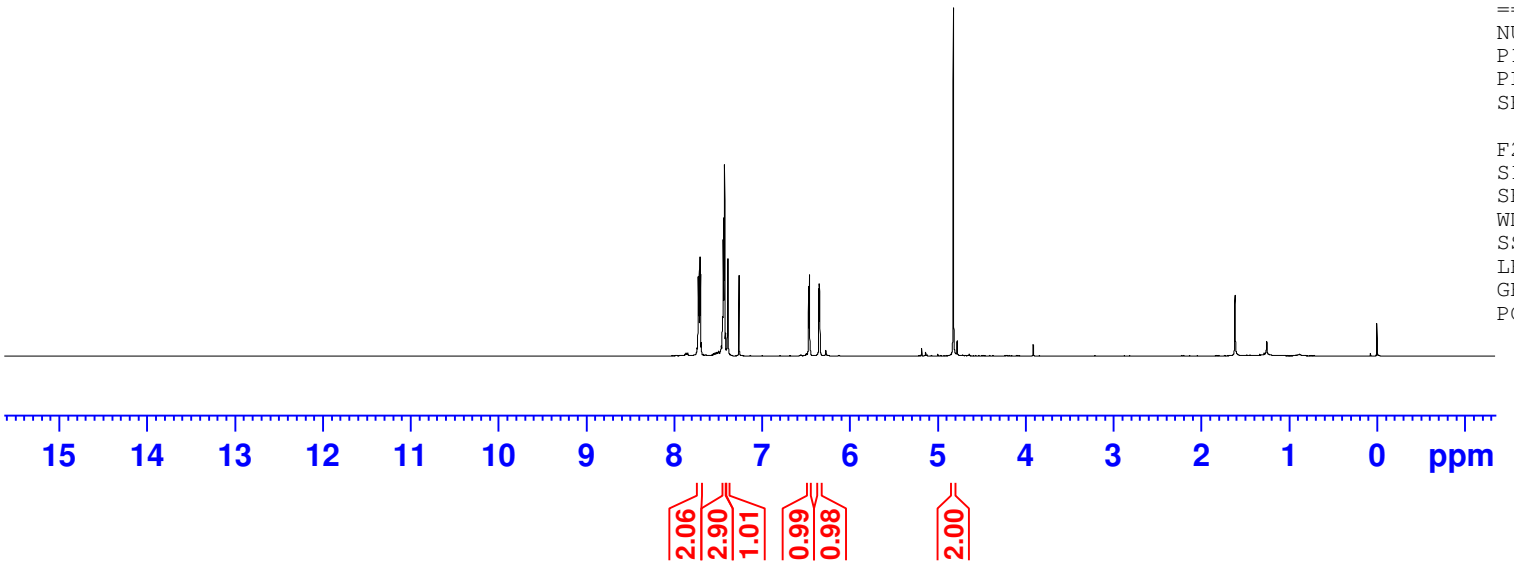
F2 - Processing parameters
SI 32768
SF 100.6278635 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-3-45a



2h





Current Data Parameters
NAME 20231006-400m
EXPNO 5
PROCNO 1

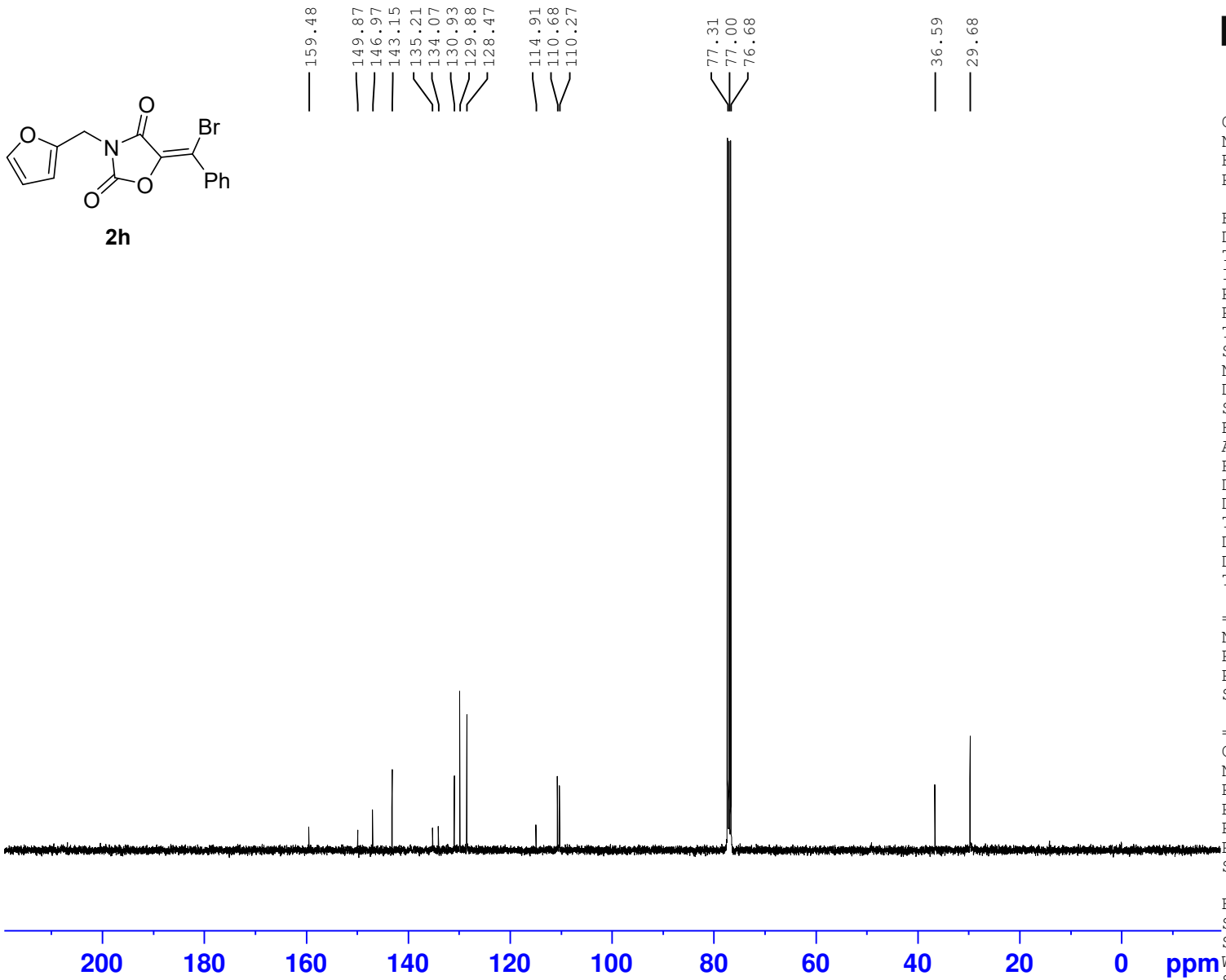
F2 - Acquisition Parameters
Date_ 20231005
Time 23.47
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 140.02
DW 60.800 usec
DE 6.50 usec
TE 291.4 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

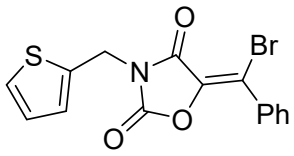
zhl-3-45a

2h

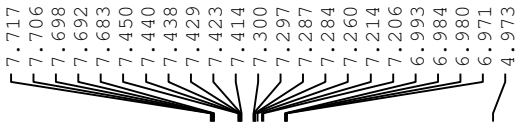


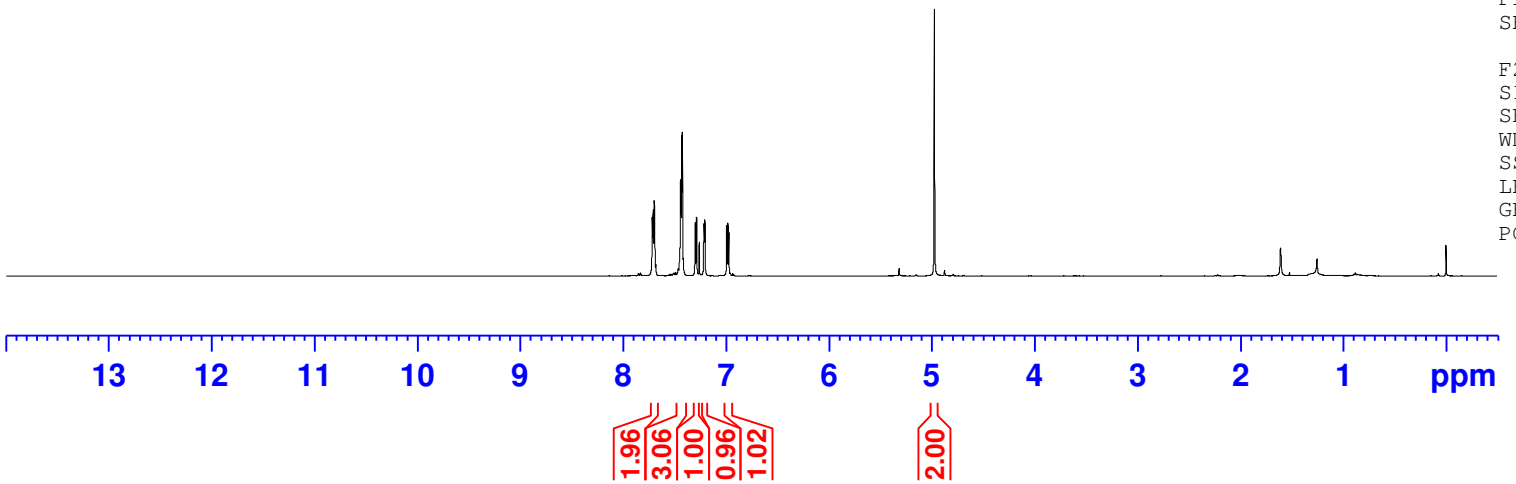

```
Current Data Parameters
NAME       20230722-400M
EXPNO                 33
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230721
Time               23.55
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  500
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                37.77
DW               20.800 usec
DE                6.50 usec
TE                294.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.80 usec
PLW1        47.40000153 W
SFO1       100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2        23.00000000 W
PLW12        0.30712000 W
PLW13        0.24877000 W
SFO2       400.1916008 MHz

F2 - Processing parameters
SI                32768
SF         100.6278612 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

zhl-3-52A



2i





Current Data Parameters
NAME ZHL230423-400m
EXPNO 79
PROCNO 1

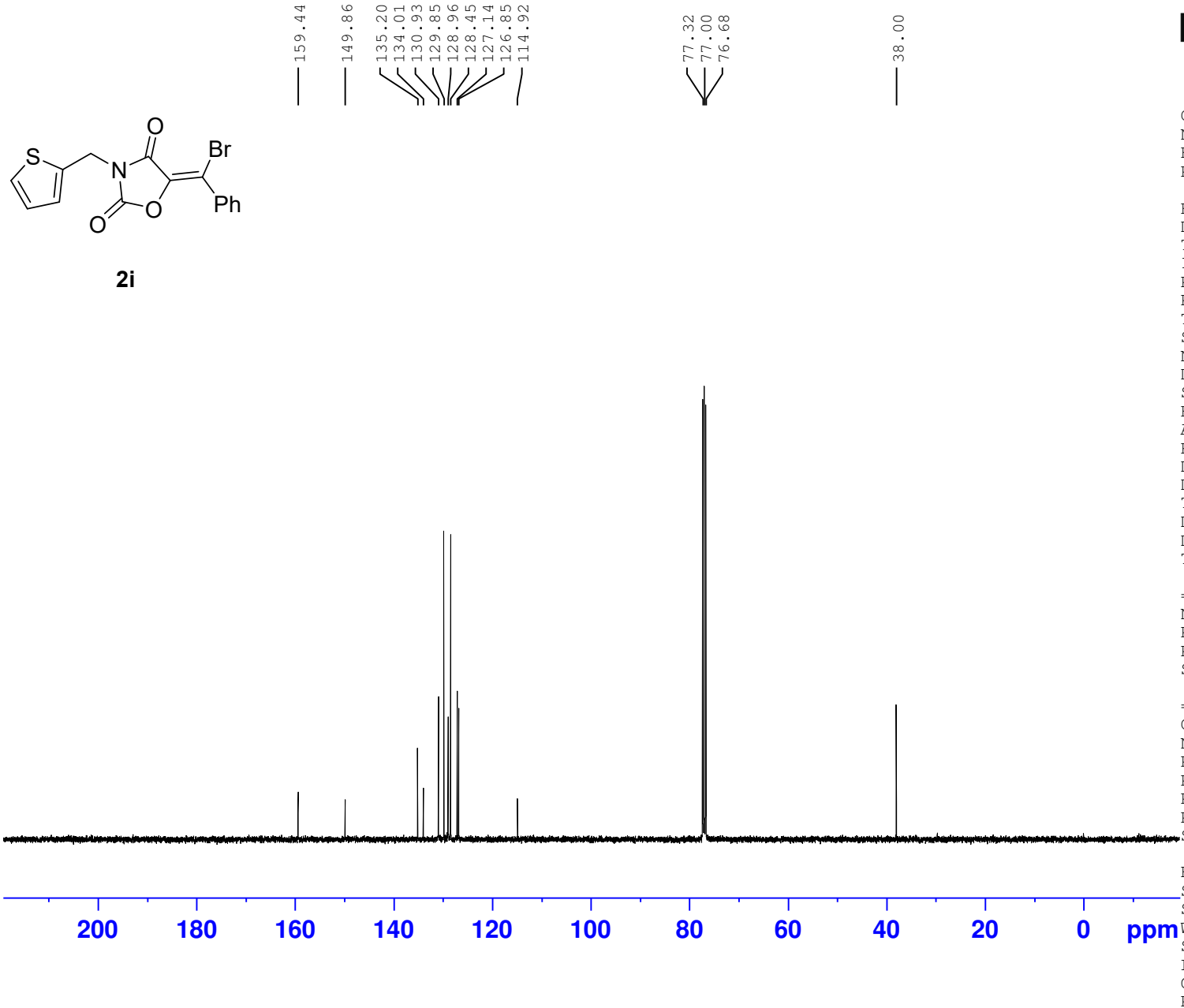
F2 - Acquisition Parameters
Date_ 20230423
Time 2.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 154.68
DW 60.800 usec
DE 6.50 usec
TE 289.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900163 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-52A

2i



Current Data Parameters
NAME ZHL230423-400m
EXPNO 80
PROCNO 1

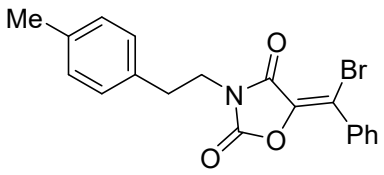
F2 - Acquisition Parameters
Date_ 20230423
Time 2.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 290.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

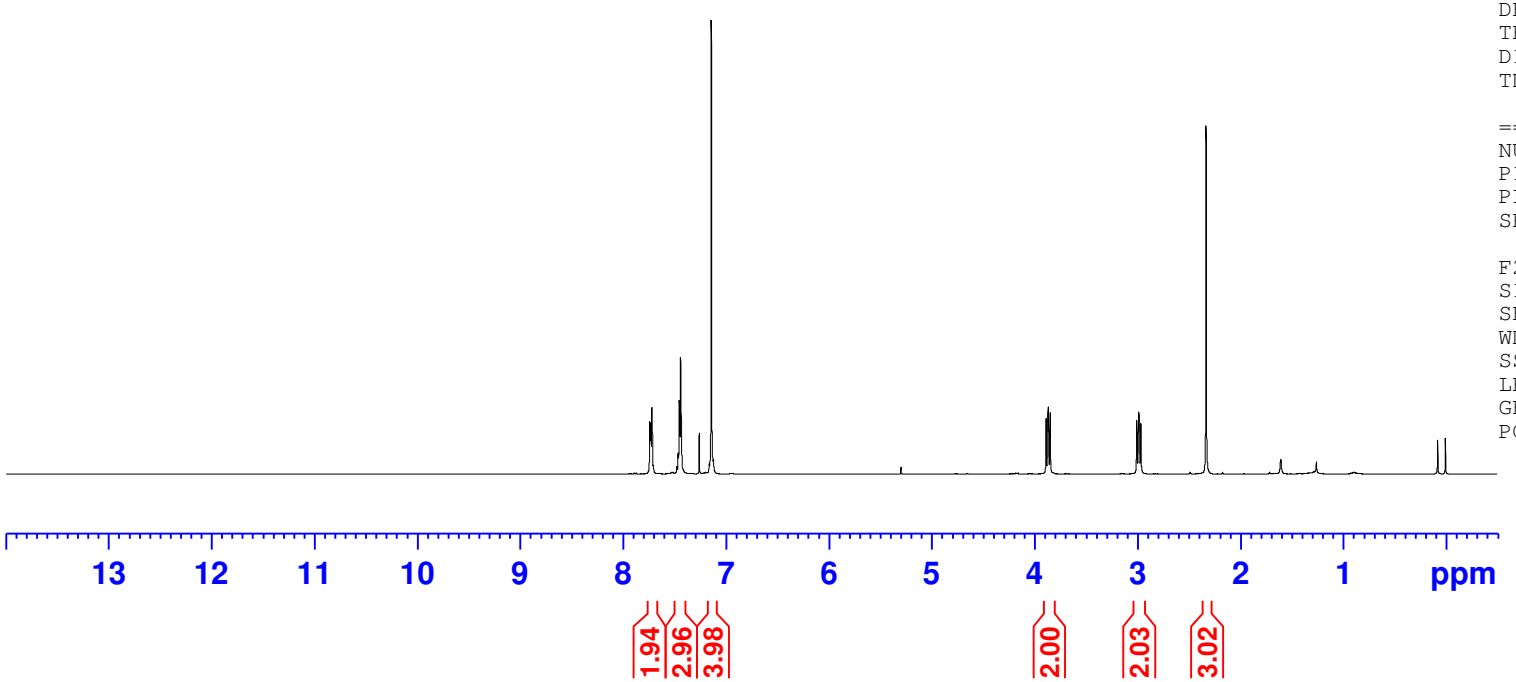
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278645 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

cb-1-34a



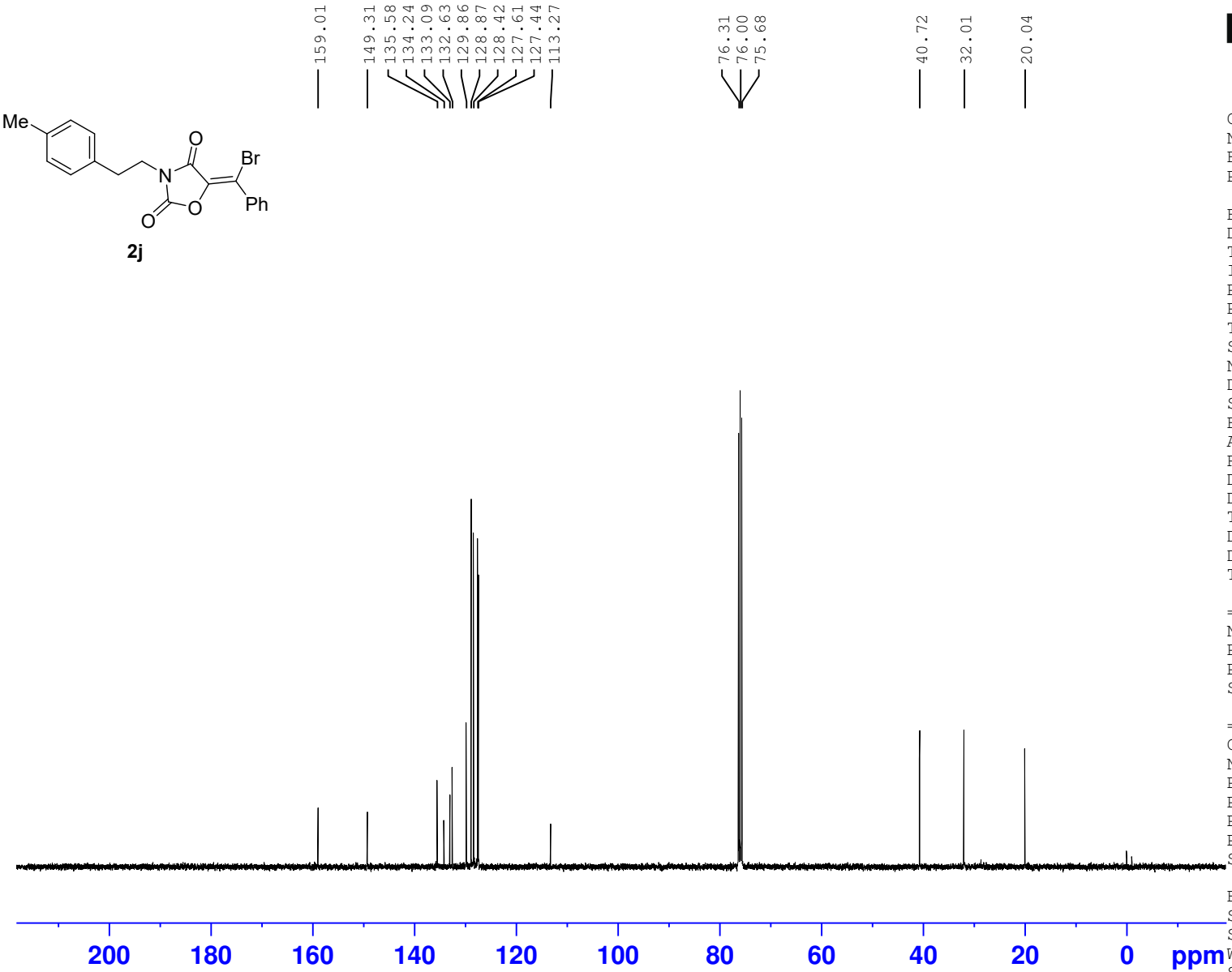
2j




```
Current Data Parameters
NAME          Cb-ketiyi
EXPNO                17
PROCNO                1

F2 - Acquisition Parameters
Date_          20230411
Time               2.31
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    6
DS                    2
SWH            8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9845889 sec
RG               125.76
DW               60.800 usec
DE                6.50 usec
TE                289.8 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.68 usec
PLW1        14.00000000 W
SFO1        400.1924713 MHz

F2 - Processing parameters
SI                65536
SF          400.1900163 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00
```

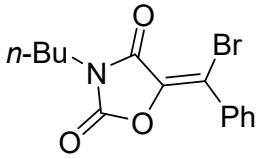
cb-1-34a

2j

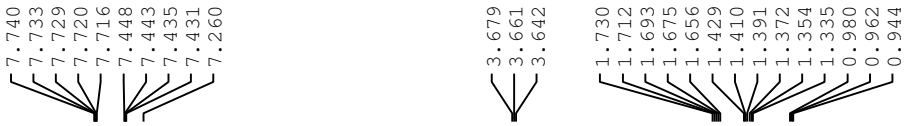


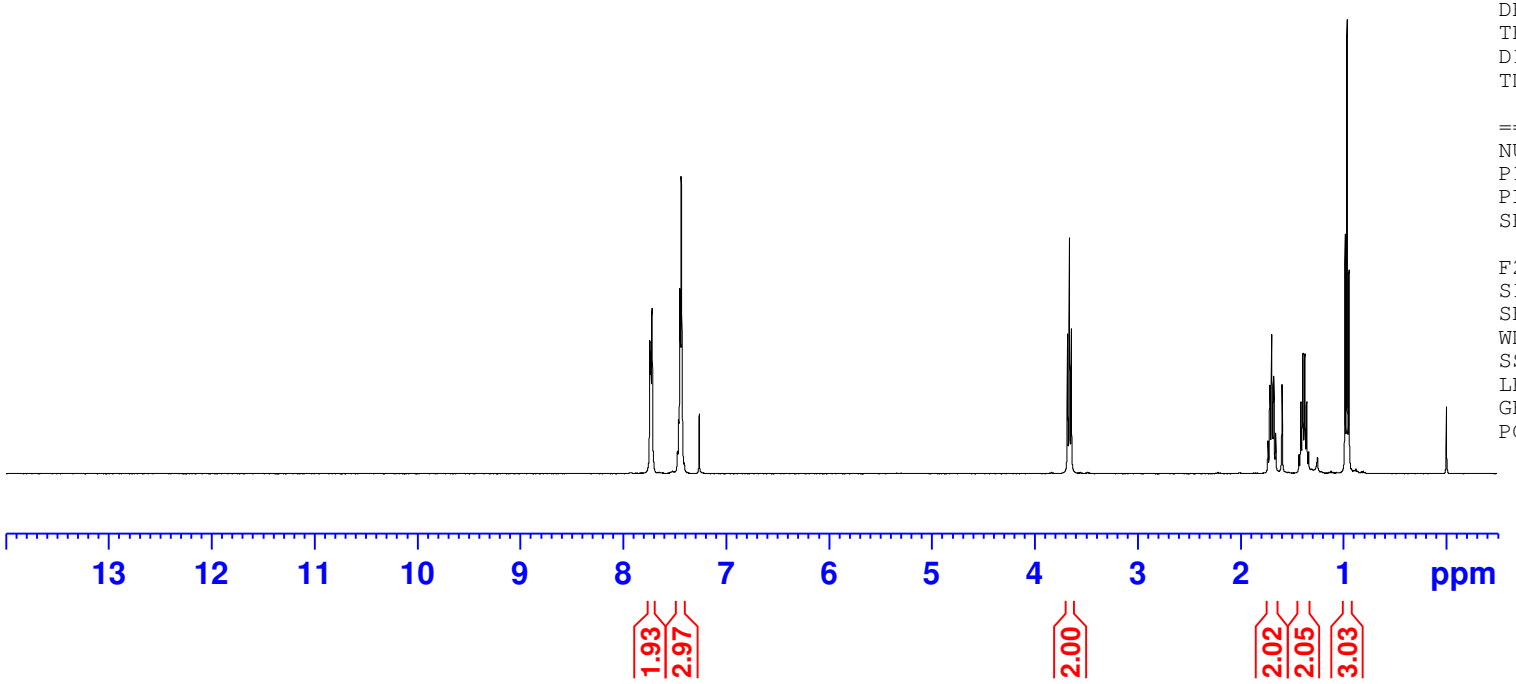

```
Current Data Parameters
NAME          Cb-ketiyi
EXPNO                18
PROCNO                1

F2 - Acquisition Parameters
Date_          20230411
Time               2.55
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE                290.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                12.00 usec
PLW1        53.00000000 W
SFO1       100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.37246999 W
PLW13        0.30170000 W
SFO2       400.1916008 MHz

F2 - Processing parameters
SI                32768
SF         100.6279659 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

zhl-3-83a



2k





Current Data Parameters
NAME 20230509-400M
EXPNO 37
PROCNO 1

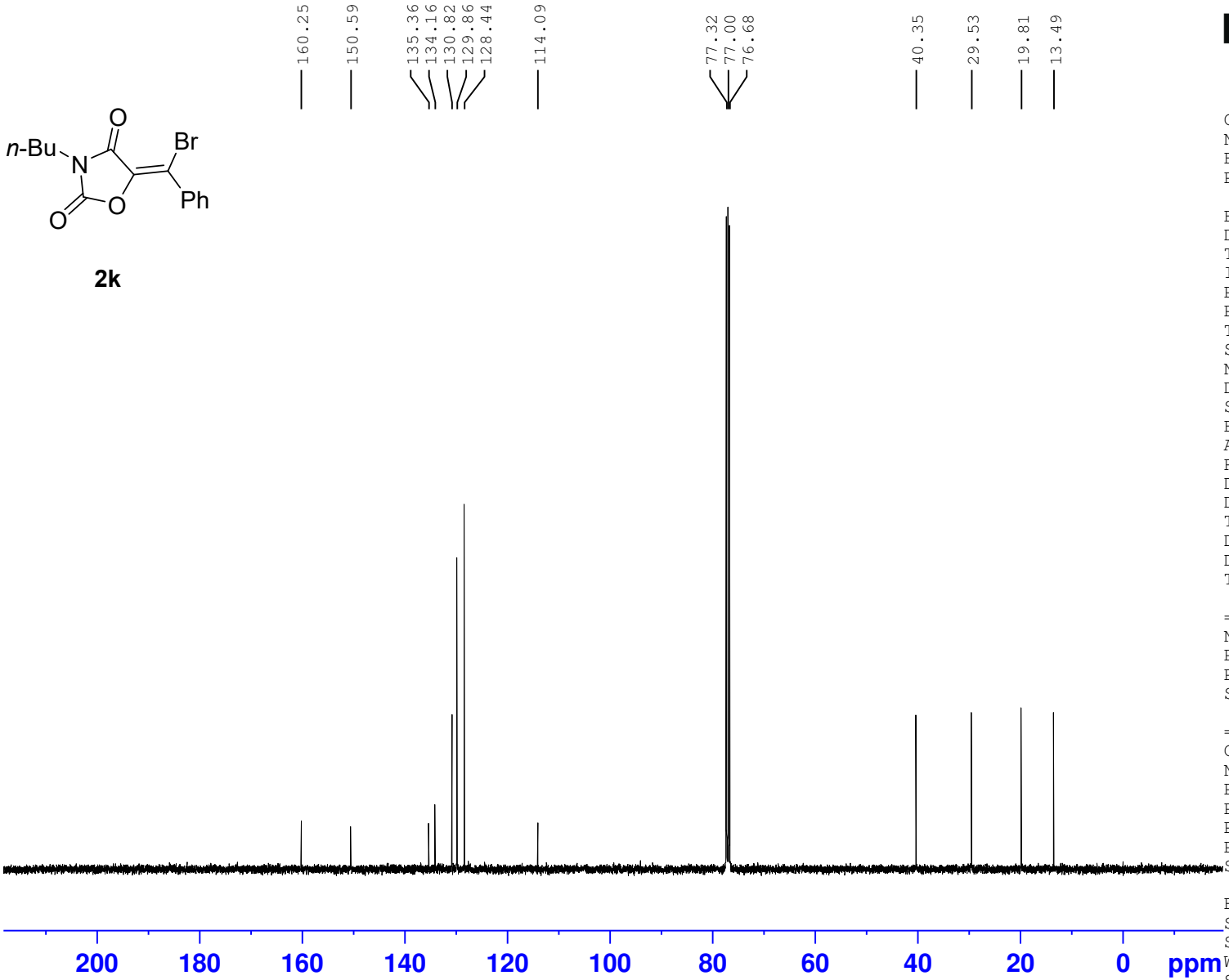
F2 - Acquisition Parameters
Date_ 20230509
Time 8.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 140.02
DW 60.800 usec
DE 6.50 usec
TE 291.4 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900164 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-83a

2k



Current Data Parameters
NAME 20230509-400M
EXPNO 38
PROCNO 1

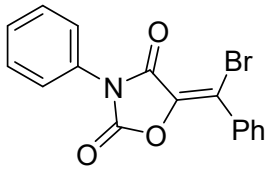
F2 - Acquisition Parameters
Date_ 20230509
Time 8.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 291.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

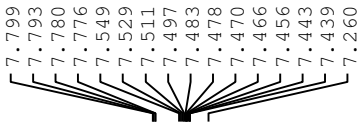
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

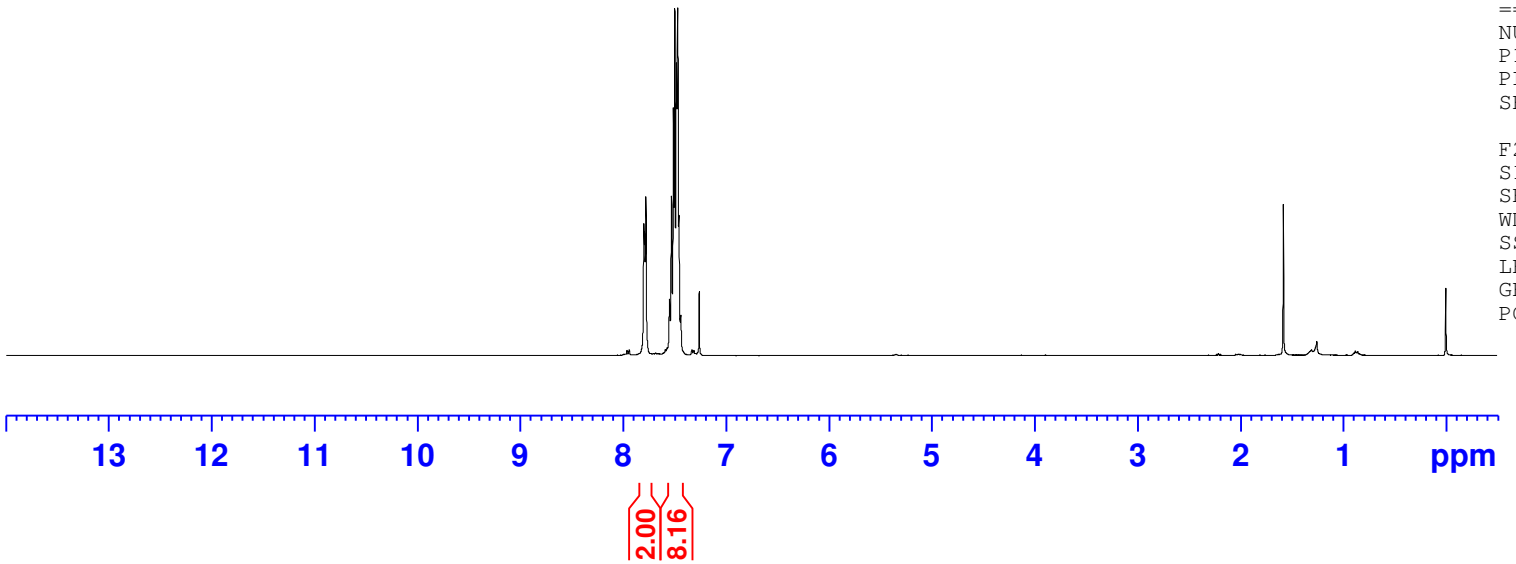
F2 - Processing parameters
SI 32768
SF 100.6278631 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-4-17a



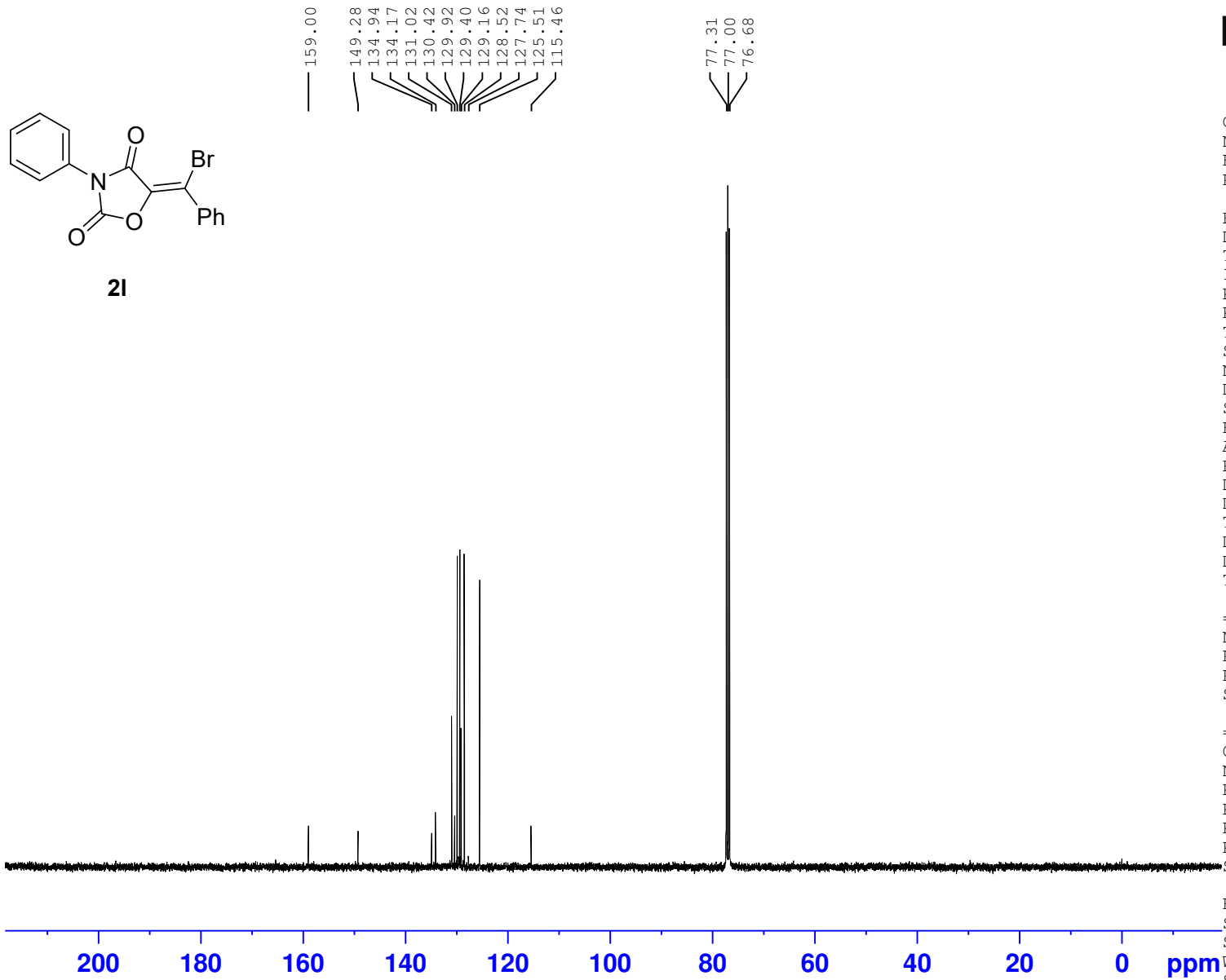
2l






```
Current Data Parameters
NAME            zhl-400m
EXPNO                 32
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230514
Time               20.43
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9845889 sec
RG                181.41
DW                60.800 usec
DE                 6.50 usec
TE                291.1 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.68 usec
PLW1         14.00000000 W
SFO1         400.1924713 MHz

F2 - Processing parameters
SI                 65536
SF           400.1900165 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

zhl-4-17a



2l

Current Data Parameters
NAME zhl-400m
EXPNO 33
PROCNO 1

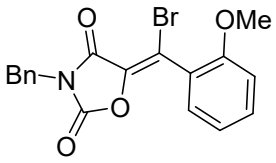
F2 - Acquisition Parameters
Date_ 20230514
Time 21.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 291.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

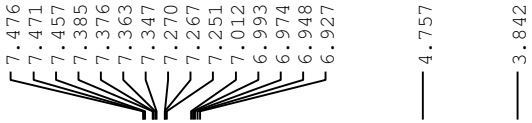
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

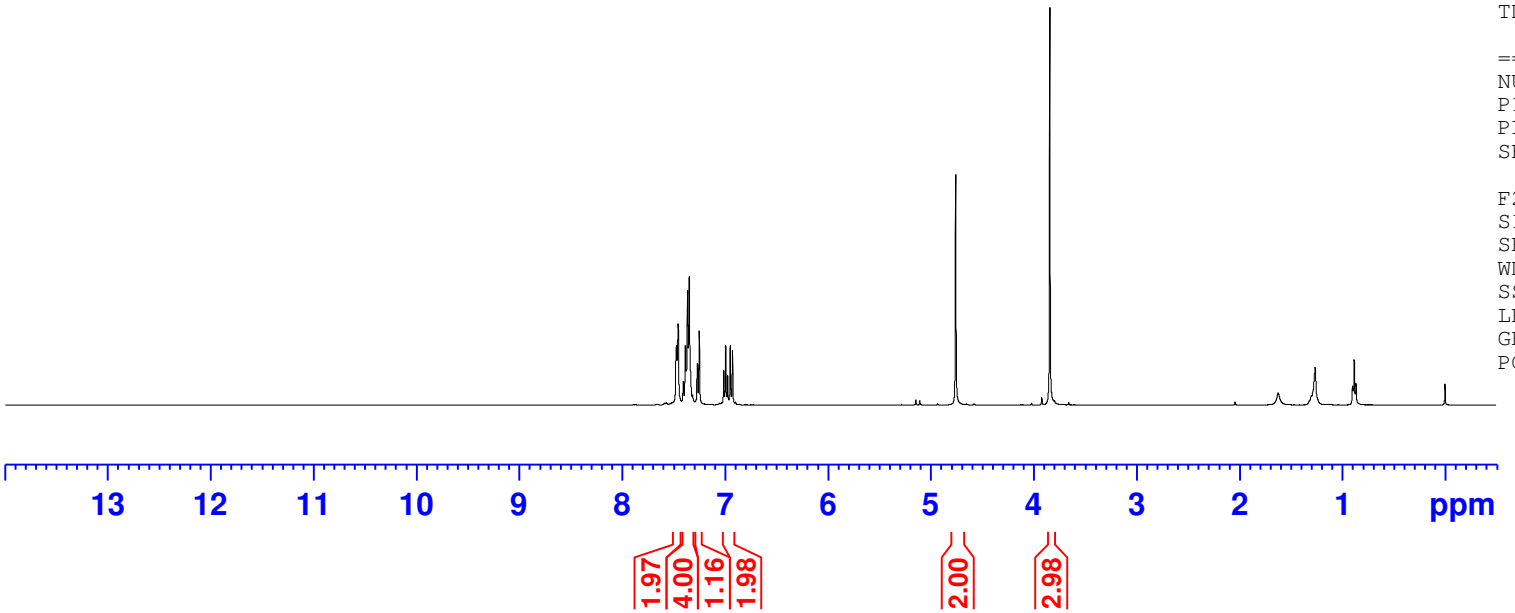
F2 - Processing parameters
SI 32768
SF 100.6278638 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-3-89a



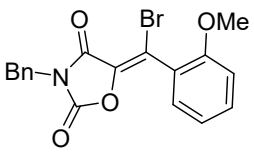
2m





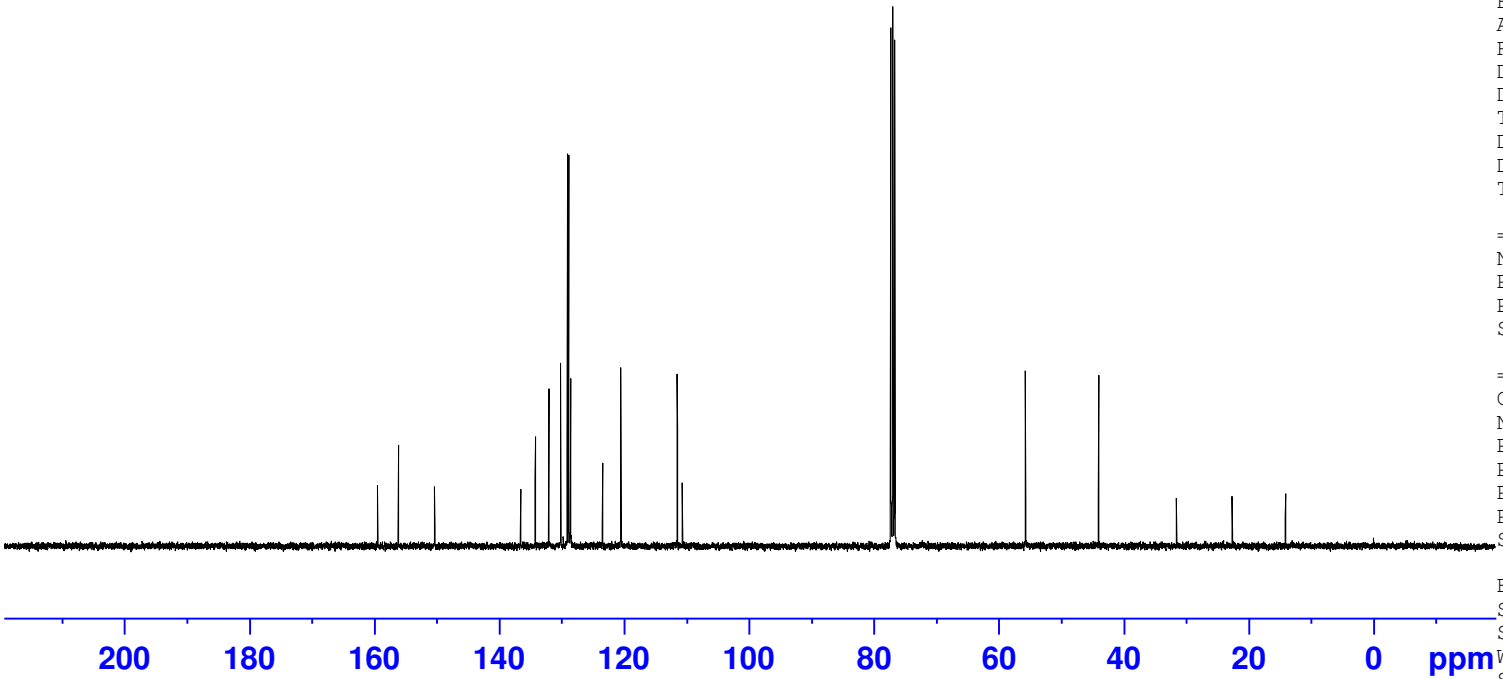

```
Current Data Parameters
NAME       20230721-400M
EXPNO                 29
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230721
Time                0.19
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     6
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9845889 sec
RG                 90.23
DW                60.800 usec
DE                 6.50 usec
TE                294.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.90 usec
PLW1        23.00000000 W
SFO1        400.1924713 MHz

F2 - Processing parameters
SI                 65536
SF          400.1900175 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```

zhl-3-89a



2m

159.52
156.17
150.36
136.60
134.25
132.07
130.19
129.11
128.87
128.58
123.48
120.54
111.49
110.69
77.31
77.00
76.68
55.73
44.01



Current Data Parameters
NAME 20230721-400M
EXPNO 30
PROCNO 1

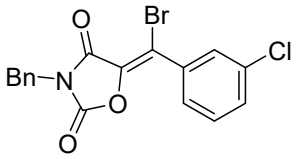
F2 - Acquisition Parameters
Date_ 20230721
Time 0.43
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 35.06
DW 20.800 usec
DE 6.50 usec
TE 294.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

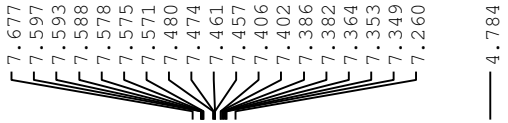
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

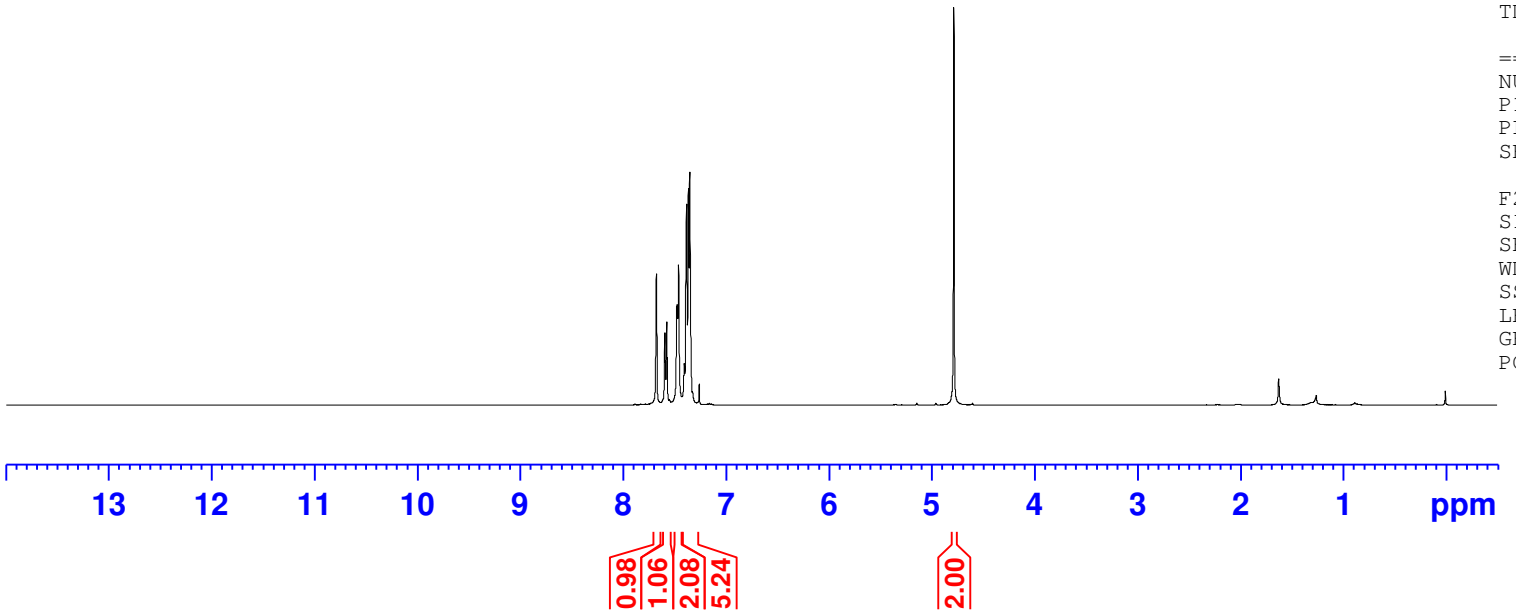
F2 - Processing parameters
SI 32768
SF 100.6278646 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZHL-3-68A



2n

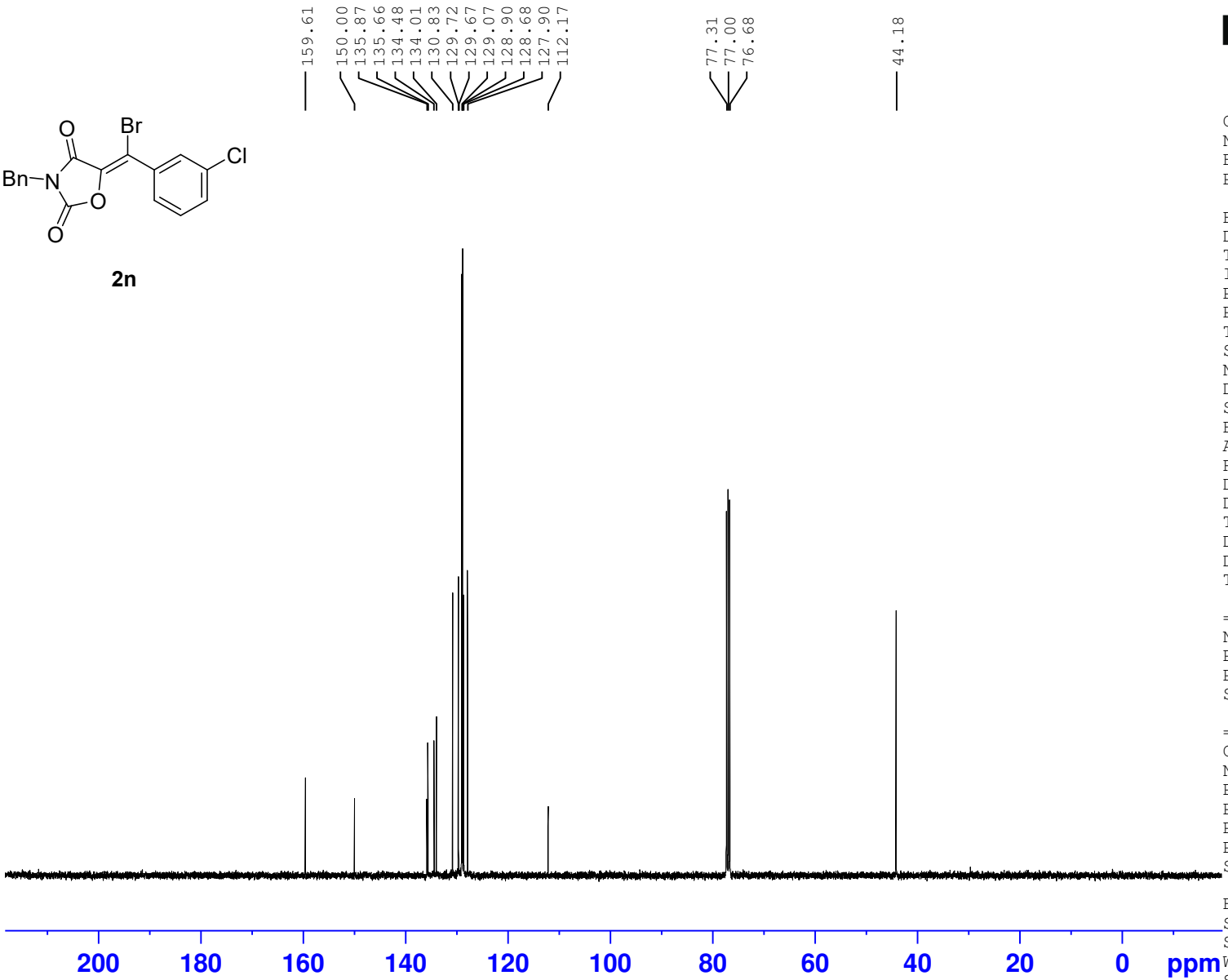





```
Current Data Parameters
NAME      20230429-400m
EXPNO                28
PROCNO                1

F2 - Acquisition Parameters
Date_          20230427
Time              23.56
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    6
DS                    2
SWH            8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9845889 sec
RG               113.67
DW               60.800 usec
DE                6.50 usec
TE               290.9 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.68 usec
PLW1        14.00000000 W
SFO1        400.1924713 MHz

F2 - Processing parameters
SI                65536
SF          400.1900166 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

zhl-3-68a

2n



Current Data Parameters
NAME 20230506-400m
EXPNO 30
PROCNO 1

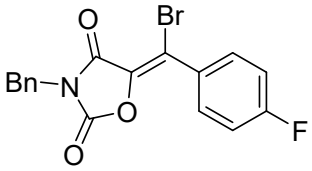
F2 - Acquisition Parameters
Date_ 20230506
Time 7.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 292.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

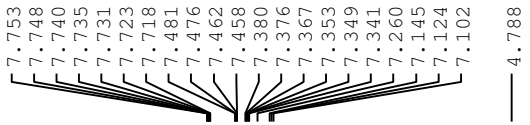
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

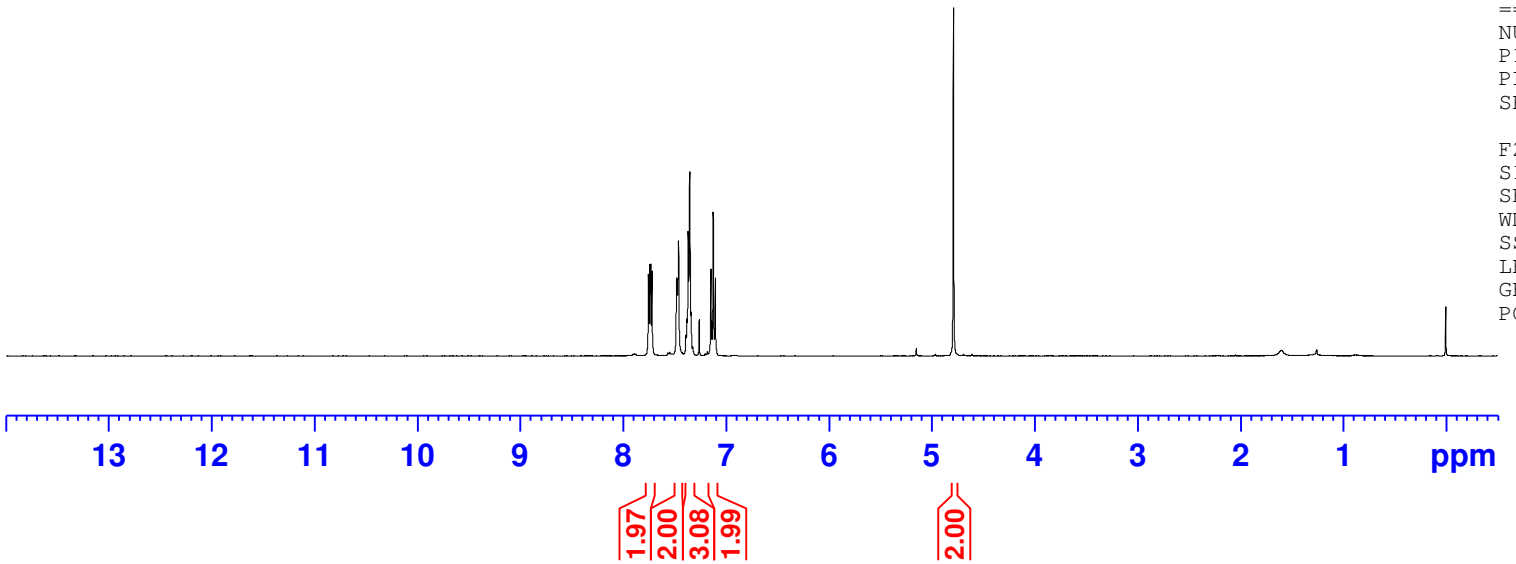
F2 - Processing parameters
SI 32768
SF 100.6278674 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-3-66A



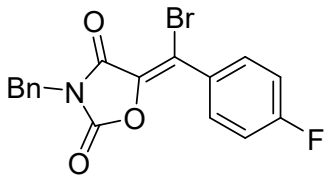
2o



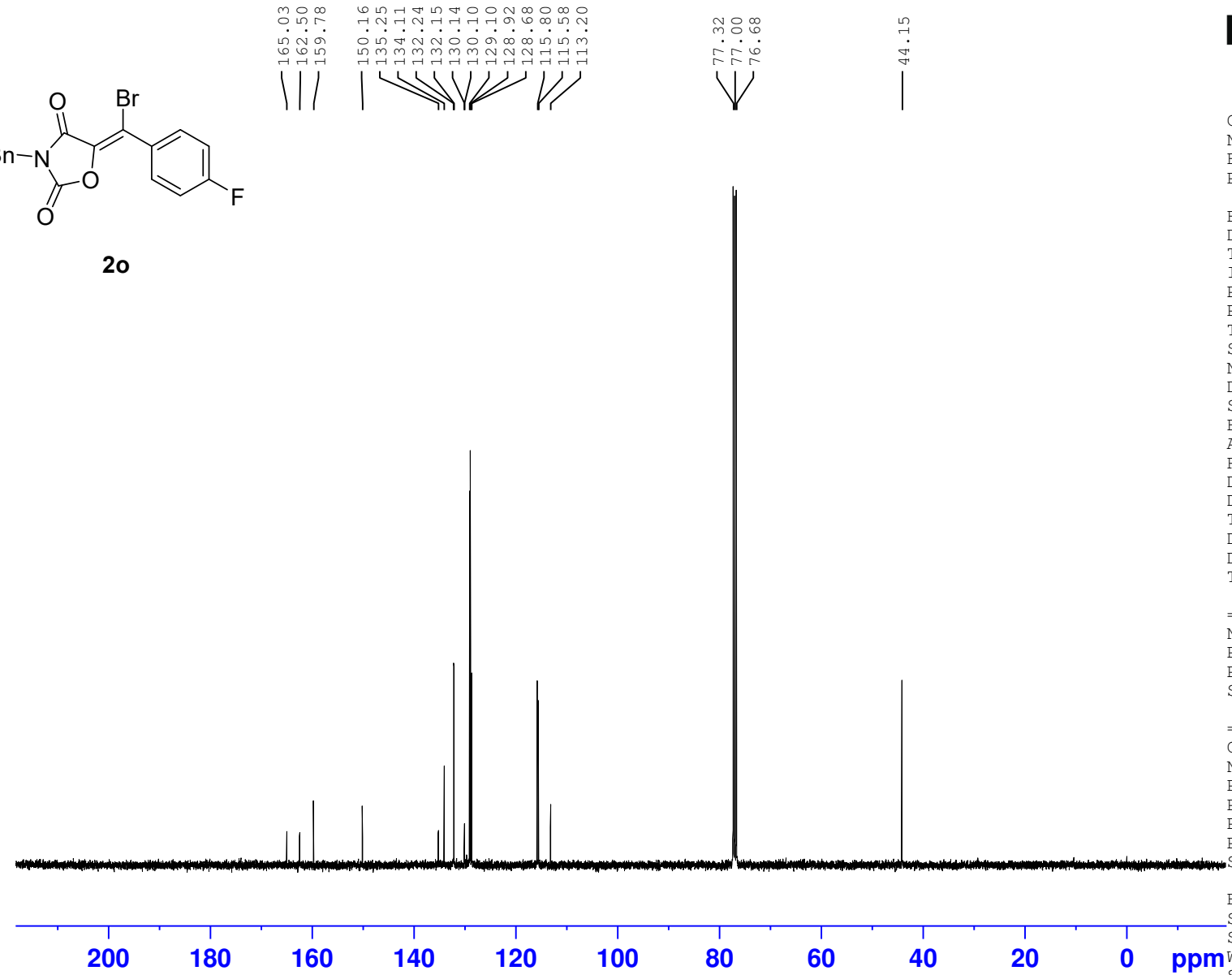



```
Current Data Parameters
NAME      20230509-400M
EXPNO                35
PROCNO                1

F2 - Acquisition Parameters
Date_          20230509
Time               7.53
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    6
DS                    0
SWH            8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9845889 sec
RG               140.02
DW               60.800 usec
DE                6.50 usec
TE               291.3 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.68 usec
PLW1        14.00000000 W
SFO1        400.1924713 MHz

F2 - Processing parameters
SI                65536
SF          400.1900163 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00
```

zhl-3-66A



2o



Current Data Parameters
NAME 20230509-400M
EXPNO 36
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230509
Time 8.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 292.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

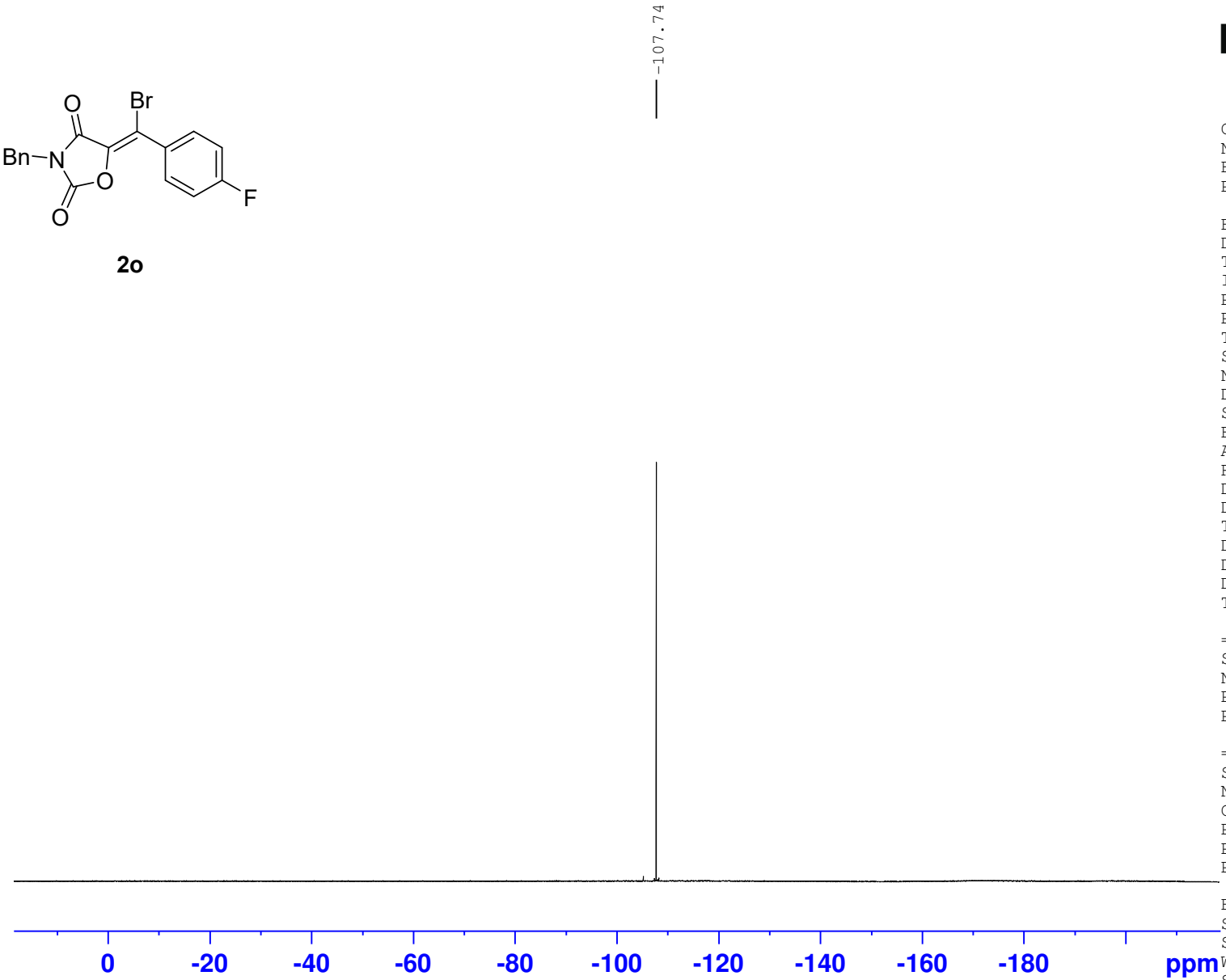
======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278639 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-3-66a

2o



Current Data Parameters
NAME 20230627-300M
EXPNO 203
PROCNO 1

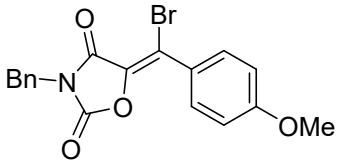
F2 - Acquisition Parameters
Date_ 20230627
Time 12.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn.2
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 0.510897 Hz
AQ 0.9786710 sec
RG 203
DW 7.467 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 282.3761148 MHz
NUC1 19F
P1 14.50 usec
PLW1 10.39999962 W

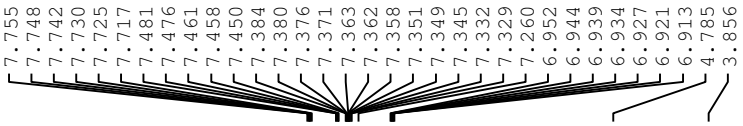
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W

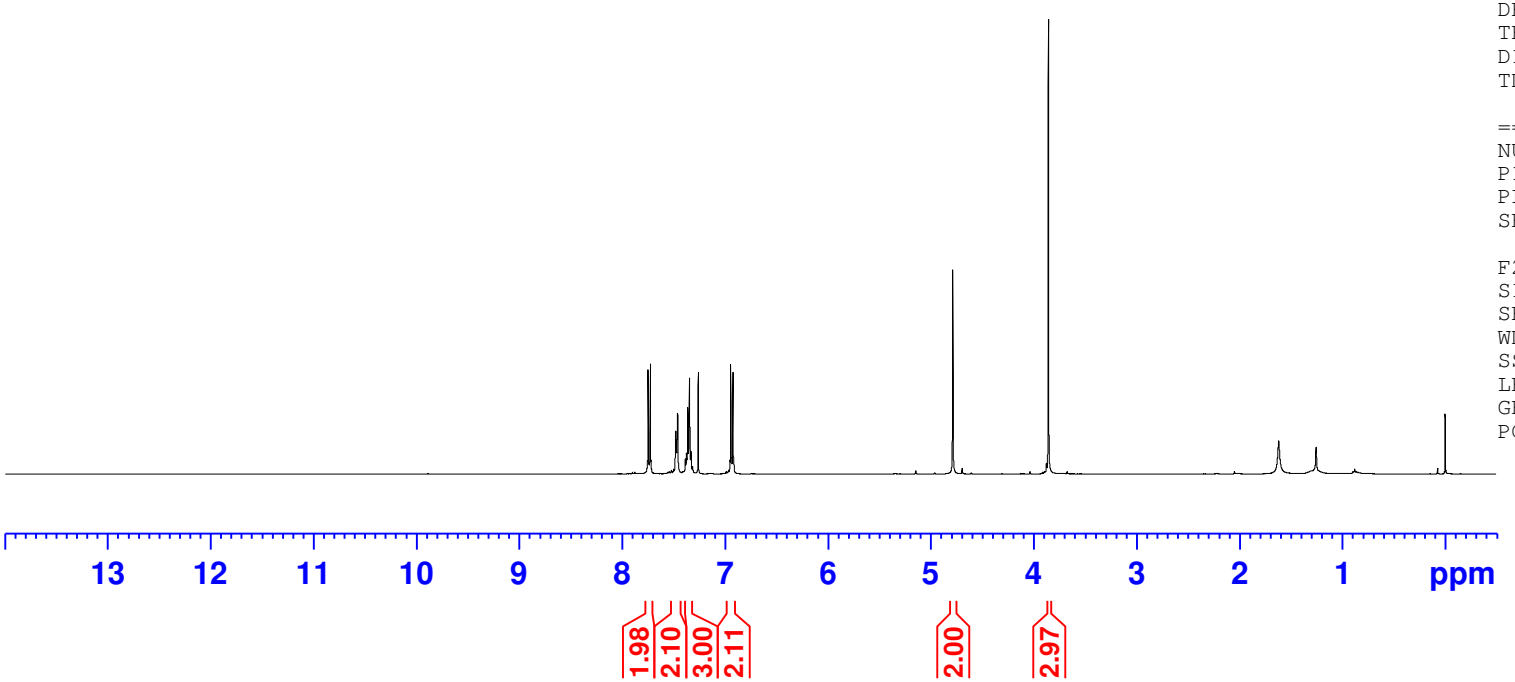
F2 - Processing parameters
SI 65536
SF 282.4043552 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-67a



2p





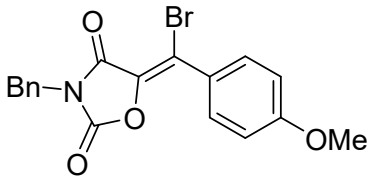
Current Data Parameters
NAME 20230628-400M
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230627
Time 21.54
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 140.02
DW 60.800 usec
DE 6.50 usec
TE 291.7 K
D1 1.00000000 sec
TD0 1

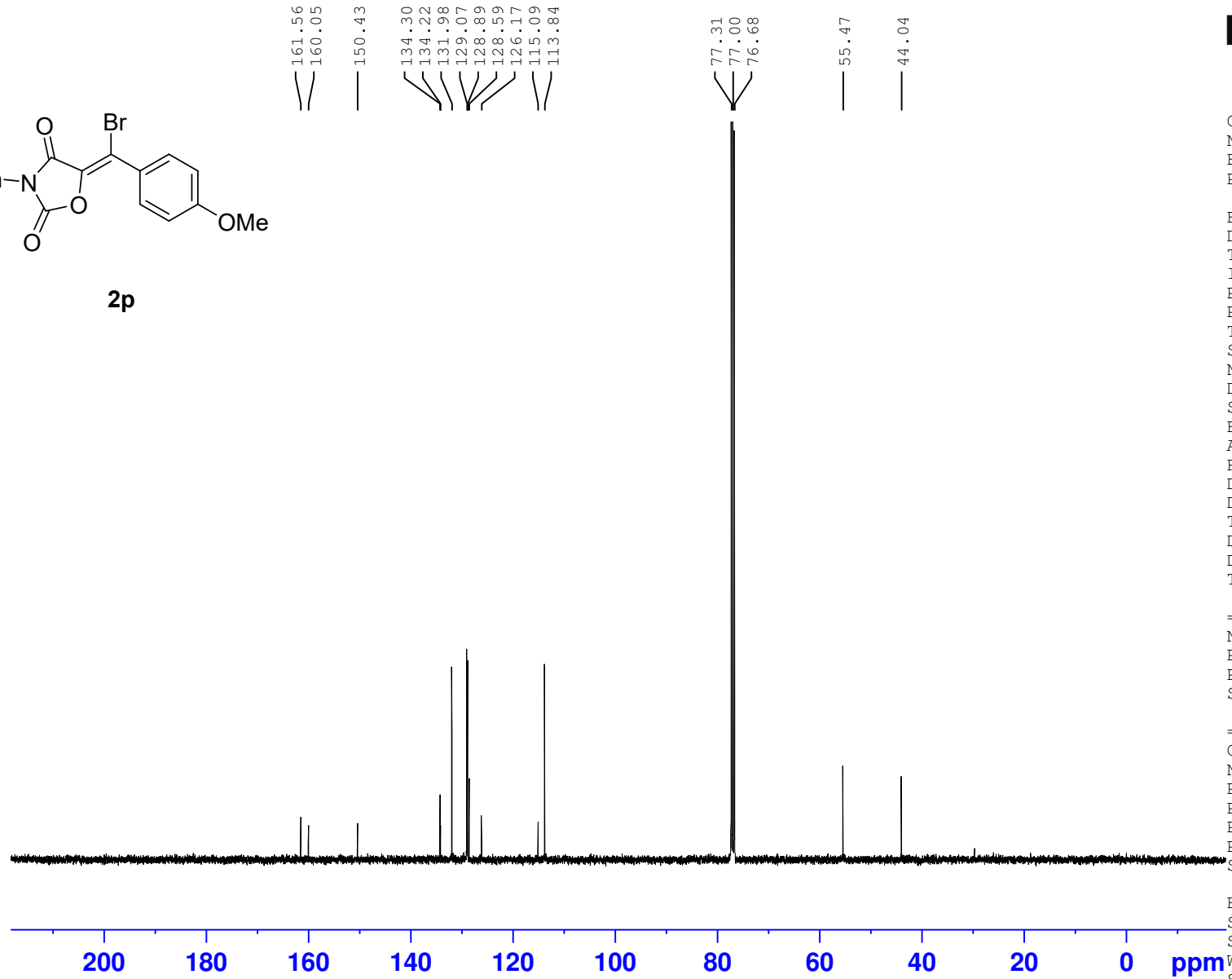
======== CHANNEL f1 ========
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900140 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-67a



2p



Current Data Parameters
NAME 20230629-400m
EXPNO 48
PROCNO 1

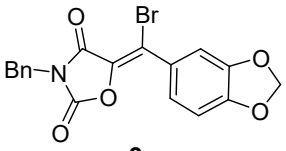
F2 - Acquisition Parameters
Date_ 20230629
Time 5.29
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 29.75
DW 20.800 usec
DE 6.50 usec
TE 291.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

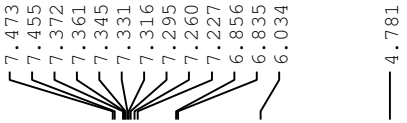
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

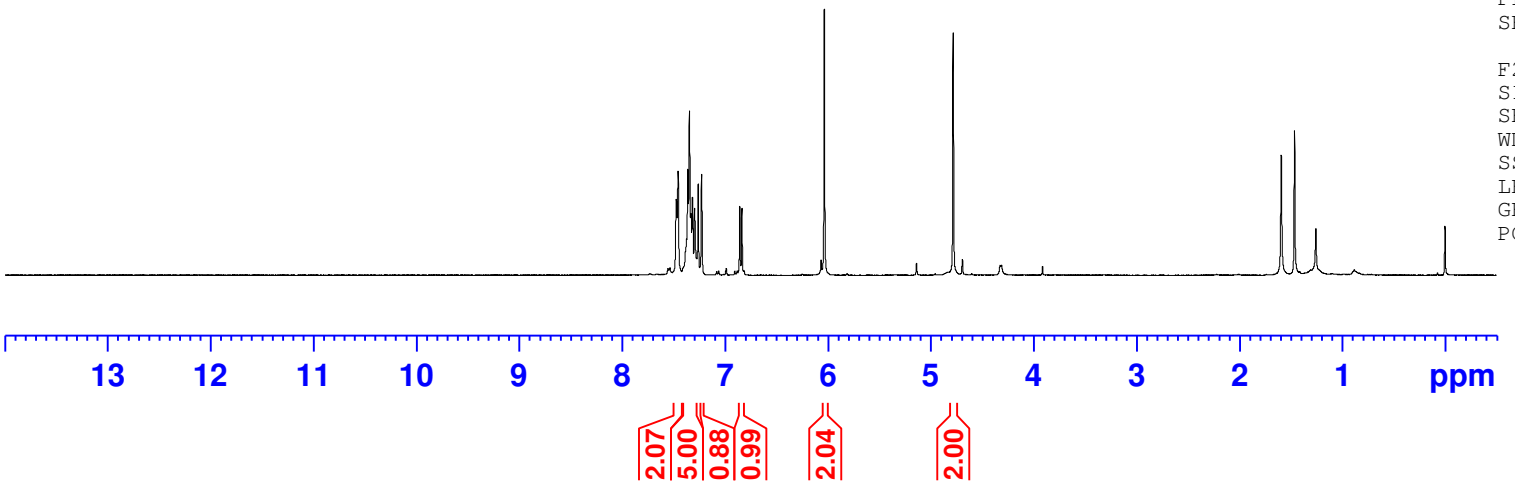
F2 - Processing parameters
SI 32768
SF 100.6278625 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-3-86a



2q





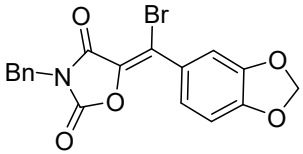
Current Data Parameters
NAME 20230712-400M
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230711
Time 22.50
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 154.68
DW 60.800 usec
DE 6.50 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

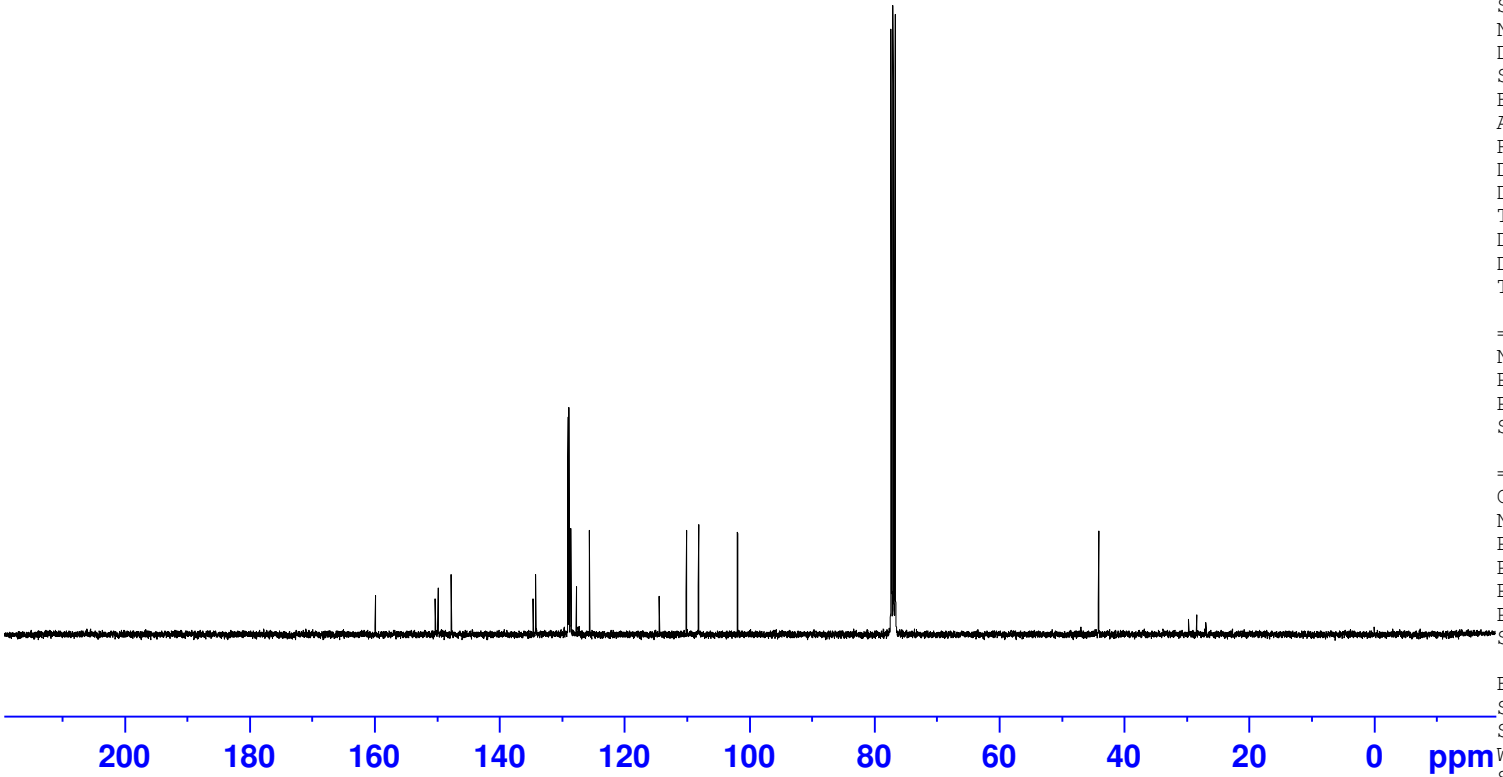
F2 - Processing parameters
SI 65536
SF 400.1900147 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-86a



2q

159.91
150.30
149.84
147.74
134.62
134.24
129.07
128.90
128.61
127.70
125.61
114.43
110.09
108.15
101.91
77.31
77.00
76.68
44.08



Current Data Parameters
NAME 20230818-400M
EXPNO 22
PROCNO 1

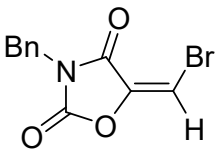
F2 - Acquisition Parameters
Date_ 20230817
Time 23.17
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 44.2
DW 20.800 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

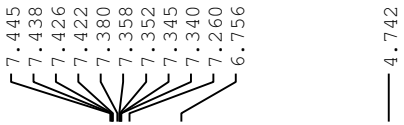
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

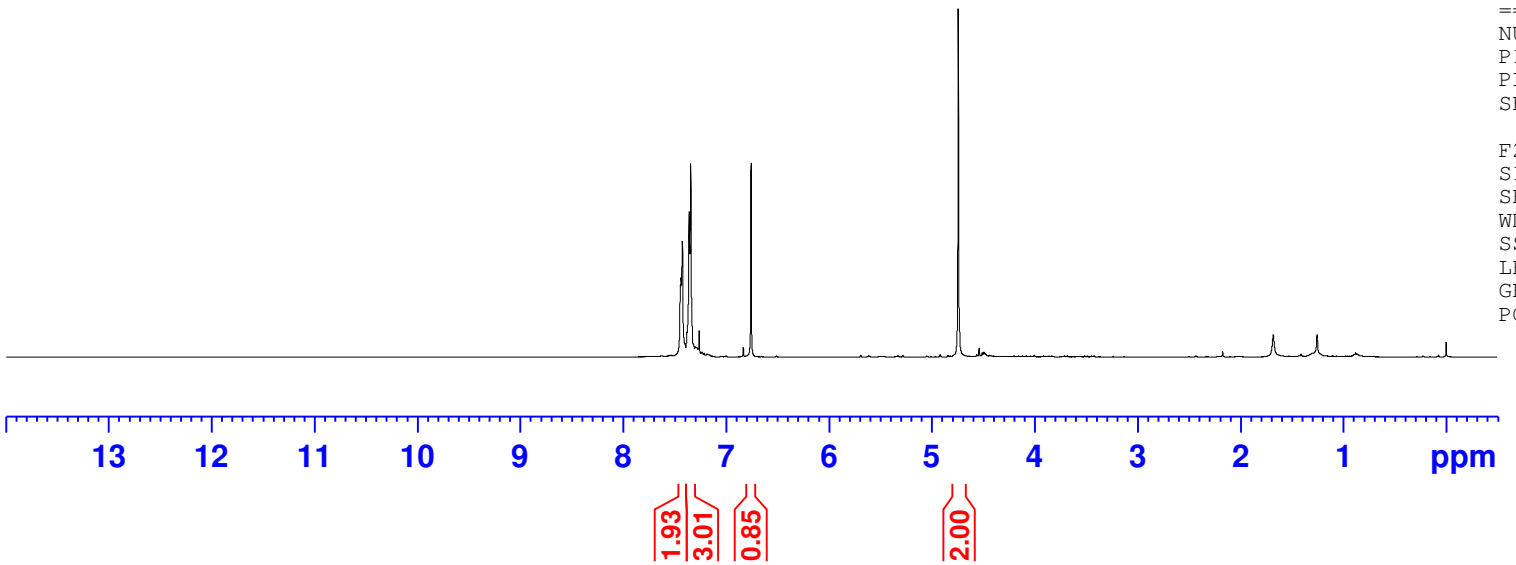
F2 - Processing parameters
SI 32768
SF 100.6278622 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-3-81a



2r

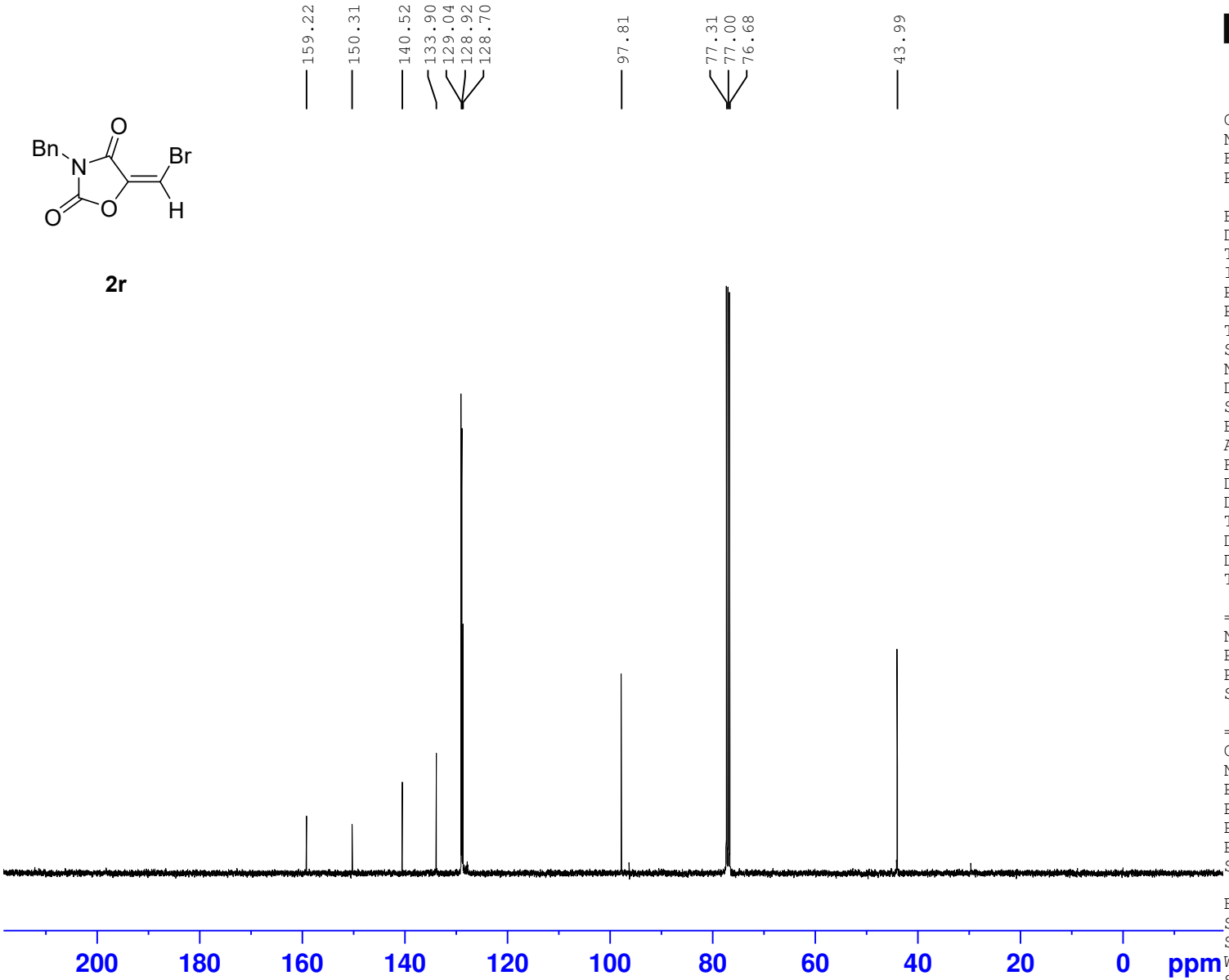





```
Current Data Parameters
NAME          202305-21
EXPNO                23
PROCNO                1

F2 - Acquisition Parameters
Date_          20230521
Time               0.49
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    2
SWH            8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9845889 sec
RG               125.76
DW               60.800 usec
DE                6.50 usec
TE                288.5 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.68 usec
PLW1        14.00000000 W
SFO1        400.1924713 MHz

F2 - Processing parameters
SI                65536
SF          400.1900167 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

zhl-3-81a

2r



Current Data Parameters
NAME 202305-21
EXPNO 24
PROCNO 1

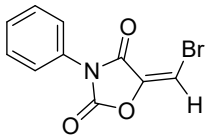
F2 - Acquisition Parameters
Date_ 20230521
Time 1.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 289.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

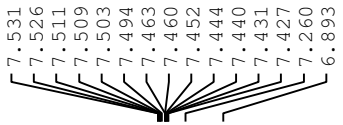
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

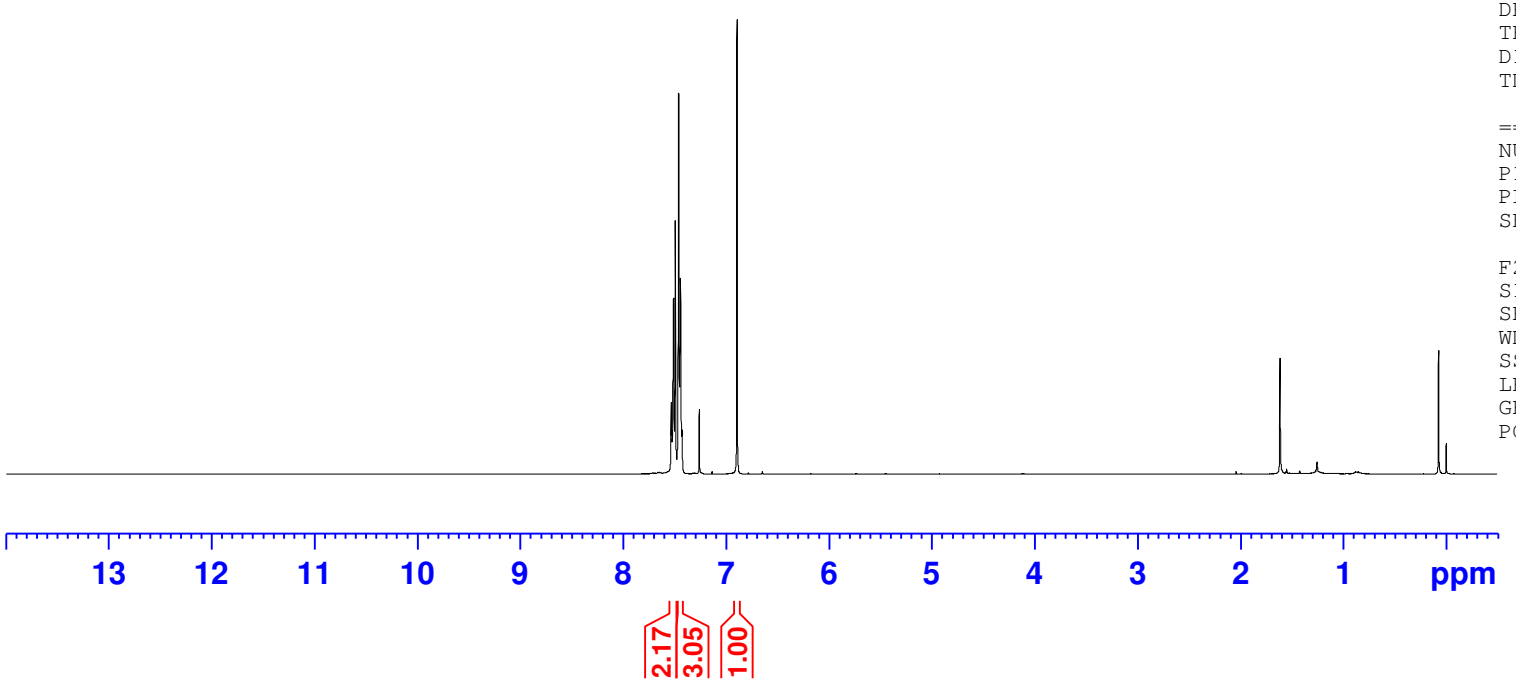
F2 - Processing parameters
SI 32768
SF 100.6278663 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-5-72



2s





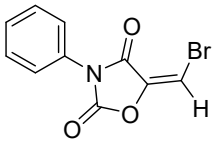
Current Data Parameters
NAME 20231005-400m
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231004
Time 22.45
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 125.76
DW 60.800 usec
DE 6.50 usec
TE 291.4 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

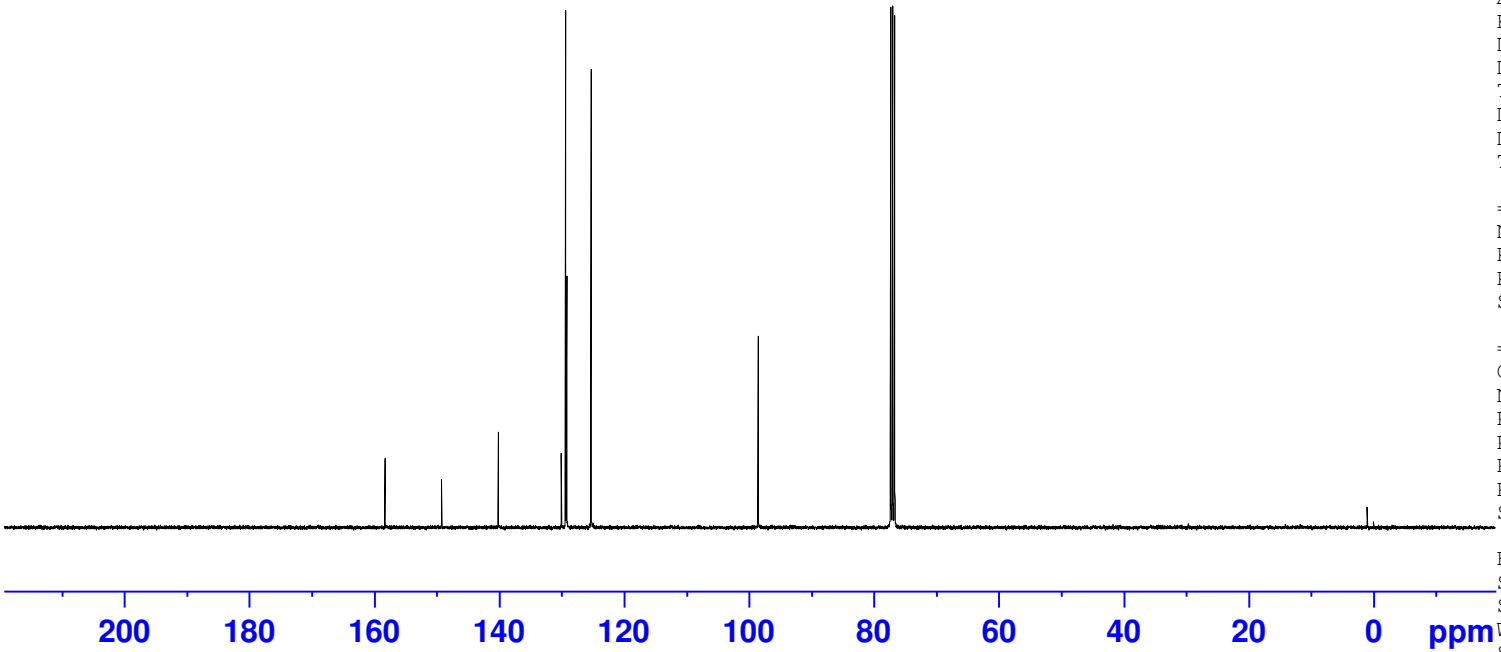
F2 - Processing parameters
SI 65536
SF 400.1900138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-5-72



2s

158.29
149.26
140.16
130.09
129.41
129.22
125.32
98.55
77.32
77.00
76.68



Current Data Parameters
NAME 20231005-400m
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231004
Time 23.45
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 24.67
DW 20.800 usec
DE 6.50 usec
TE 292.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

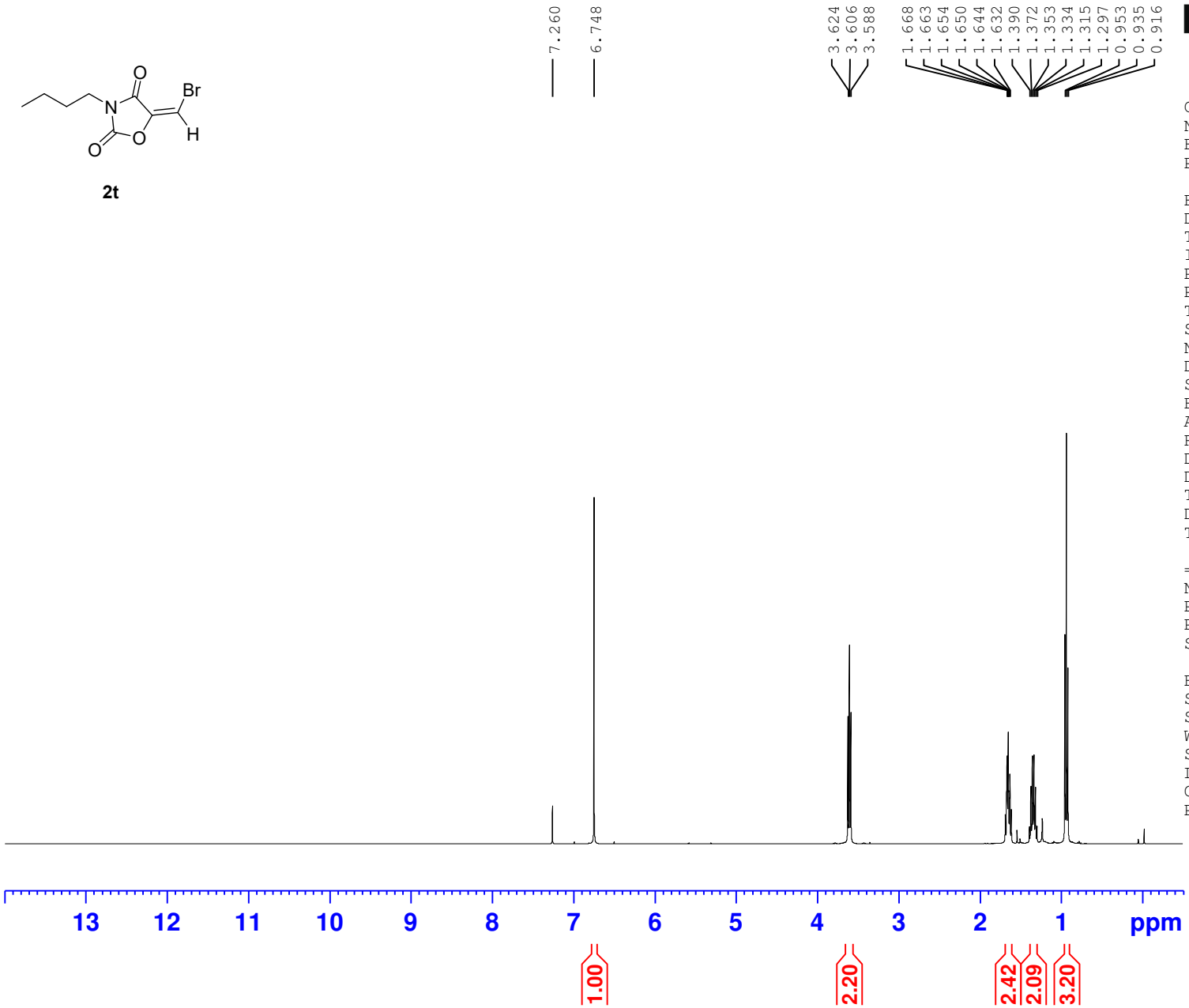
======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278652 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-5-74

2t

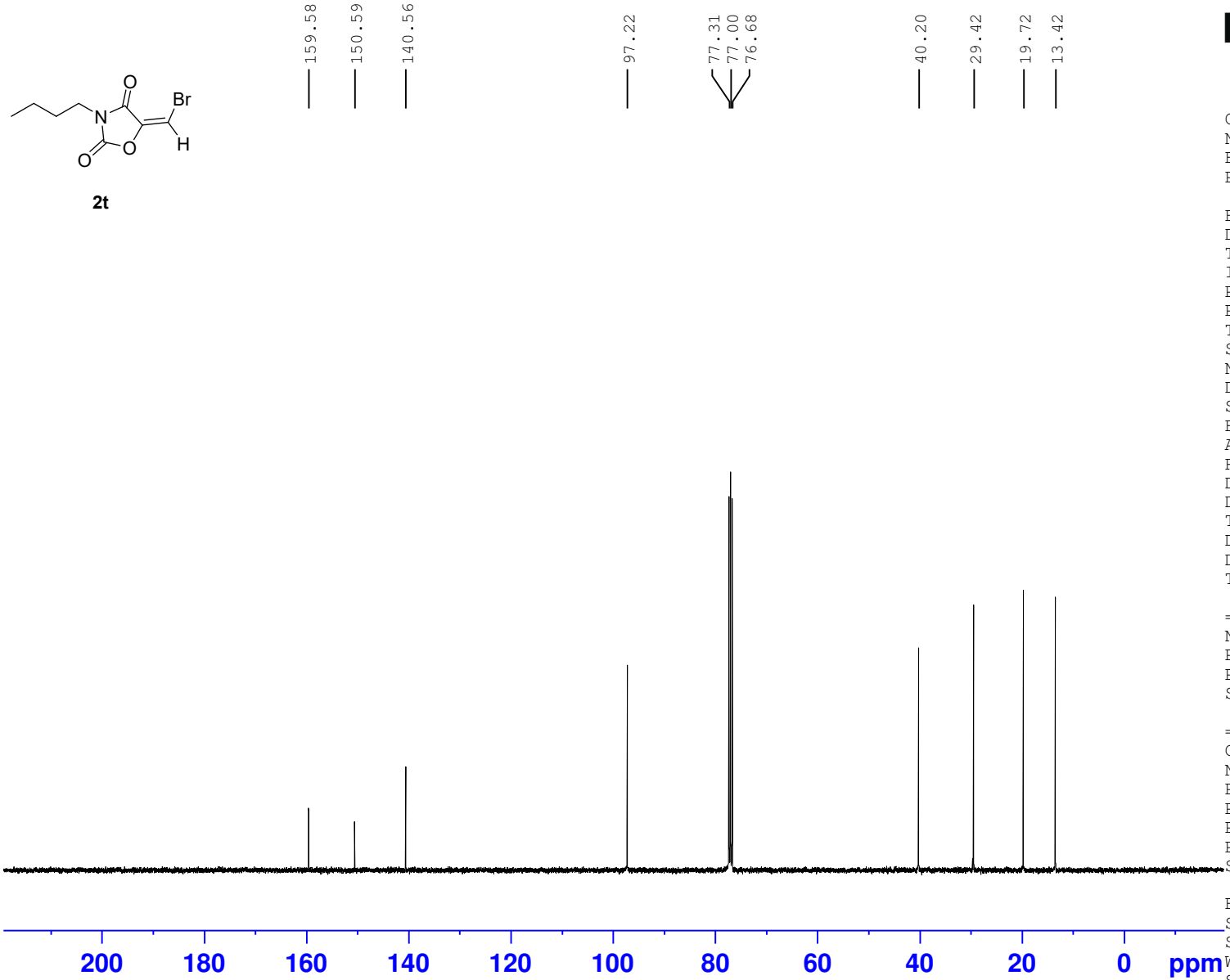


BRUKER

```
Current Data Parameters
NAME       20231005-400m
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231004
Time               23.50
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9845889 sec
RG                 75.43
DW                60.800 usec
DE                 6.50 usec
TE                291.4 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.90 usec
PLW1        23.00000000 W
SFO1        400.1924713 MHz

F2 - Processing parameters
SI                 65536
SF          400.1900139 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```

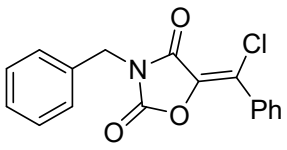
zhl-5-74

2t

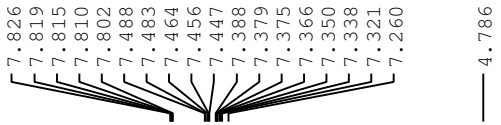


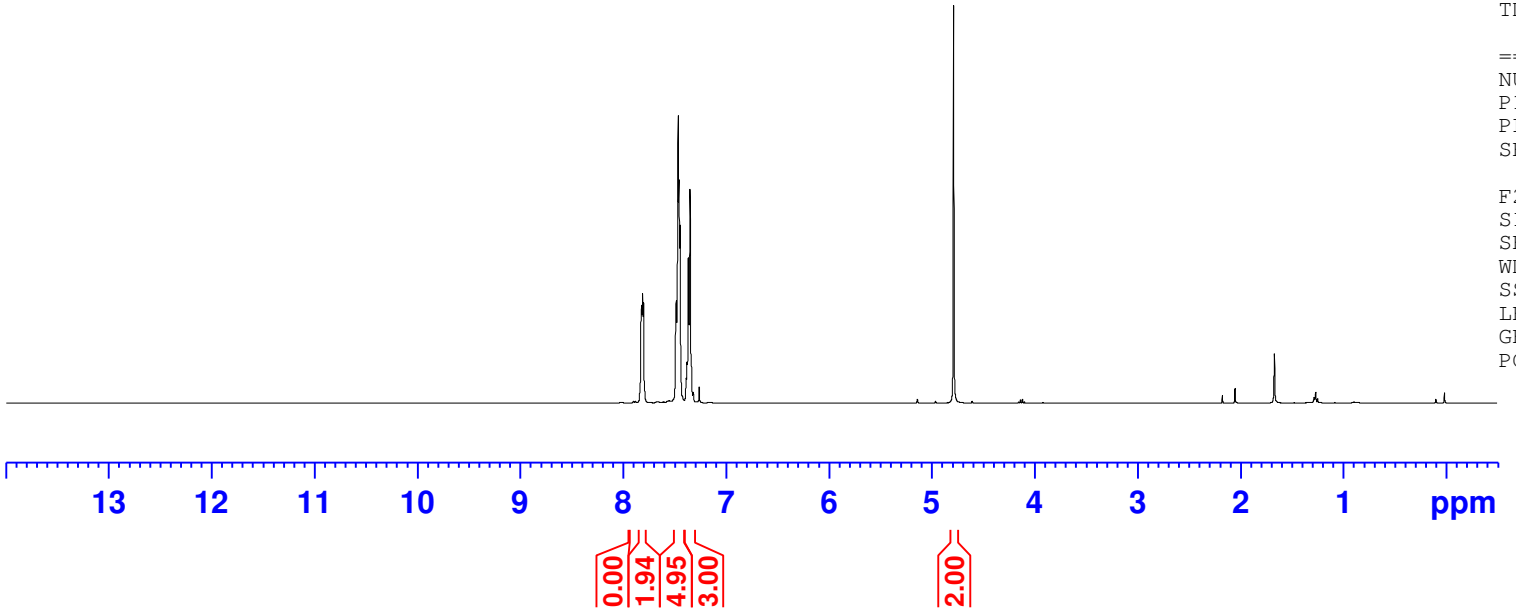

```
Current Data Parameters
NAME      20231005-400m
EXPNO                7
PROCNO               1

F2 - Acquisition Parameters
Date_          20231005
Time               0.09
INSTRUM           spect
PROBHD   5 mm PADUL 13C
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  300
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                 44.2
DW               20.800 usec
DE                6.50 usec
TE               292.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                9.80 usec
PLW1        47.40000153 W
SFO1       100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2                1H
PCPD2            90.00 usec
PLW2        23.00000000 W
PLW12        0.30712000 W
PLW13        0.24877000 W
SFO2       400.1916008 MHz

F2 - Processing parameters
SI                 32768
SF          100.6278645 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                 1.40
```

zhl-3-88



2a'





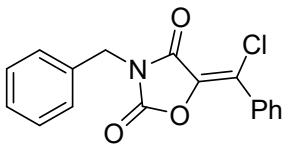
Current Data Parameters
NAME 20230418-400M
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230418
Time 6.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 75.43
DW 60.800 usec
DE 6.50 usec
TE 291.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

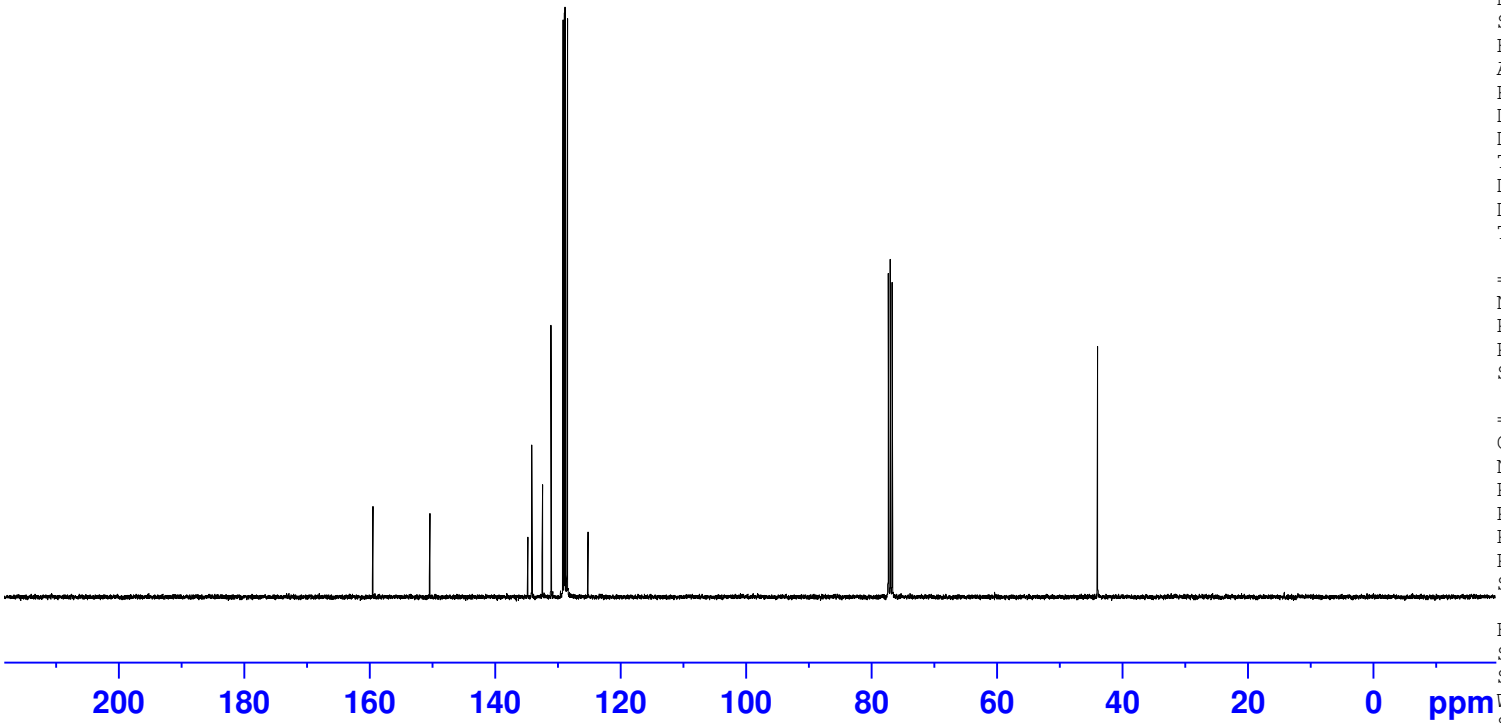
F2 - Processing parameters
SI 65536
SF 400.1900168 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-88



2a'

159.53
150.45
134.82
134.17
132.49
131.10
129.21
129.02
128.86
128.58
128.49
125.19
77.32
77.00
76.68
43.94



Current Data Parameters
NAME 20230418-400M
EXPNO 21
PROCNO 1

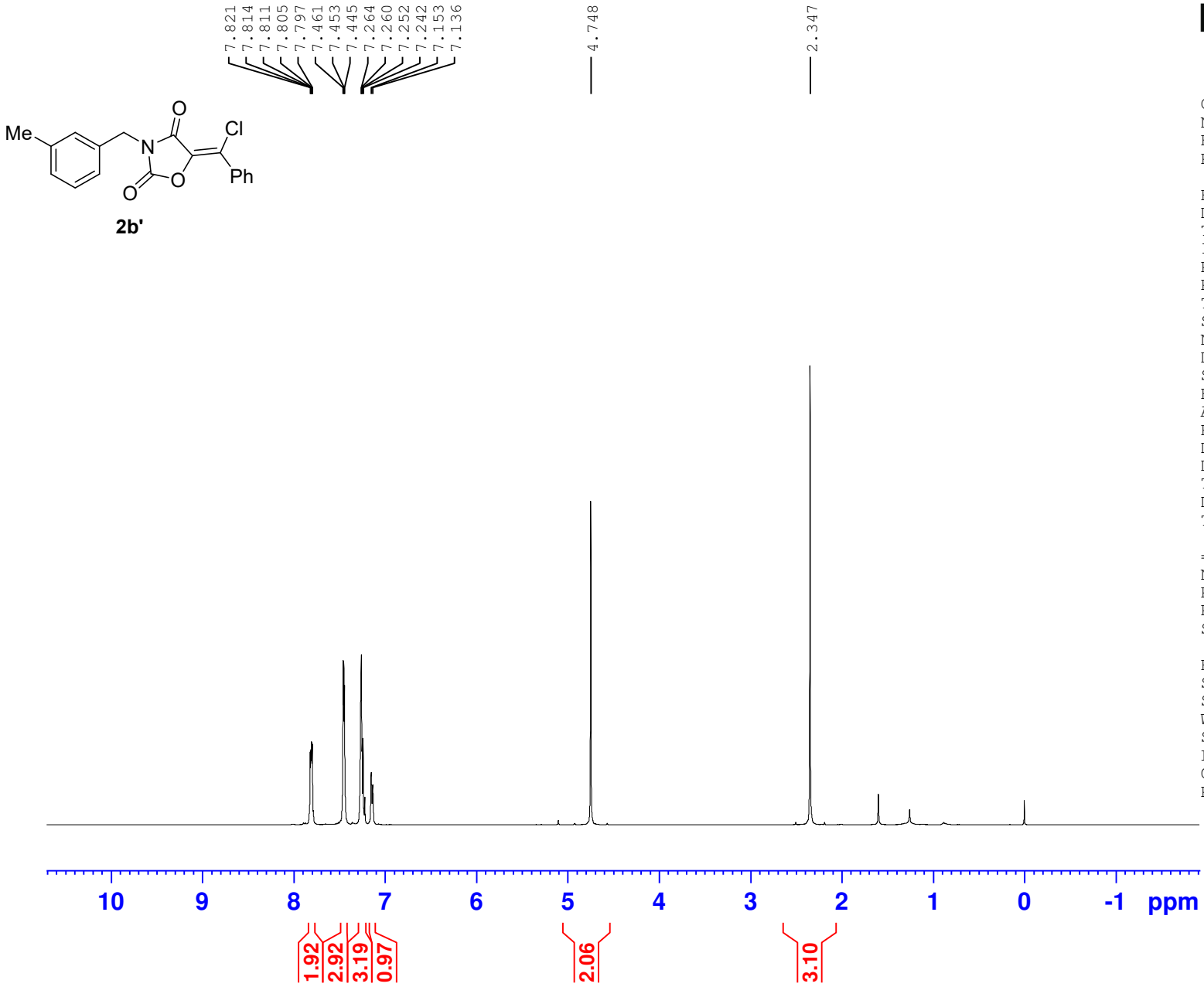
F2 - Acquisition Parameters
Date_ 20230418
Time 6.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 292.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-3-93



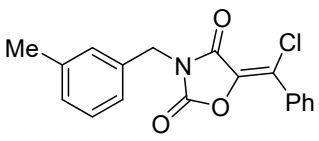
Current Data Parameters
NAME 20230509-400M
EXPNO 32
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230509
Time 7.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 113.67
DW 60.800 usec
DE 6.50 usec
TE 291.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

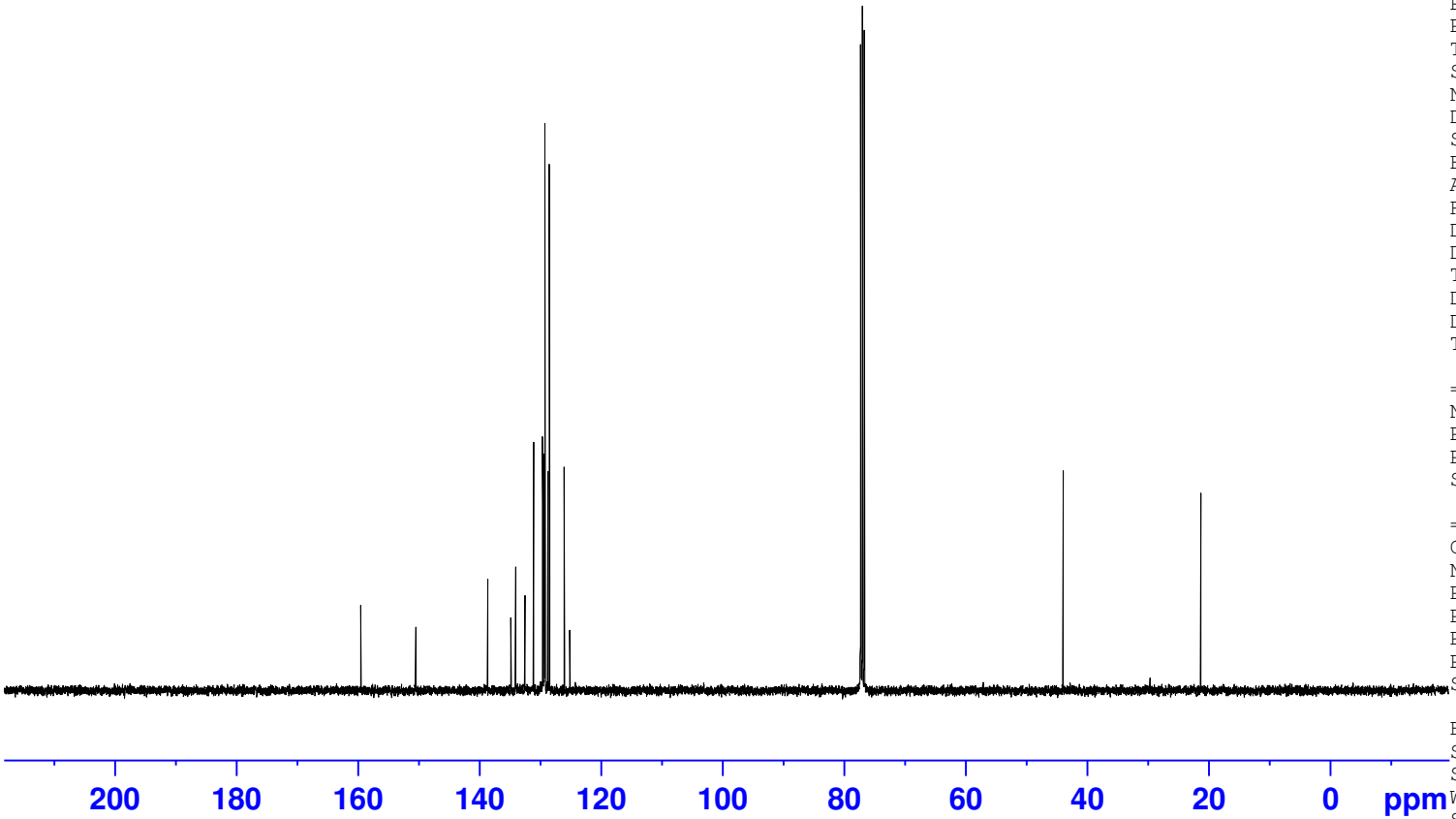
F2 - Processing parameters
SI 65536
SF 400.1900194 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-93



2b'

159.59
150.52
138.70
134.87
134.10
132.54
131.13
129.64
129.36
129.24
128.78
128.52
126.08
125.20
77.31
77.00
76.68
43.97
21.30



Current Data Parameters
NAME 20230509-400M
EXPNO 33
PROCNO 1

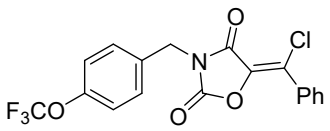
F2 - Acquisition Parameters
Date_ 20230509
Time 7.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 292.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278652 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

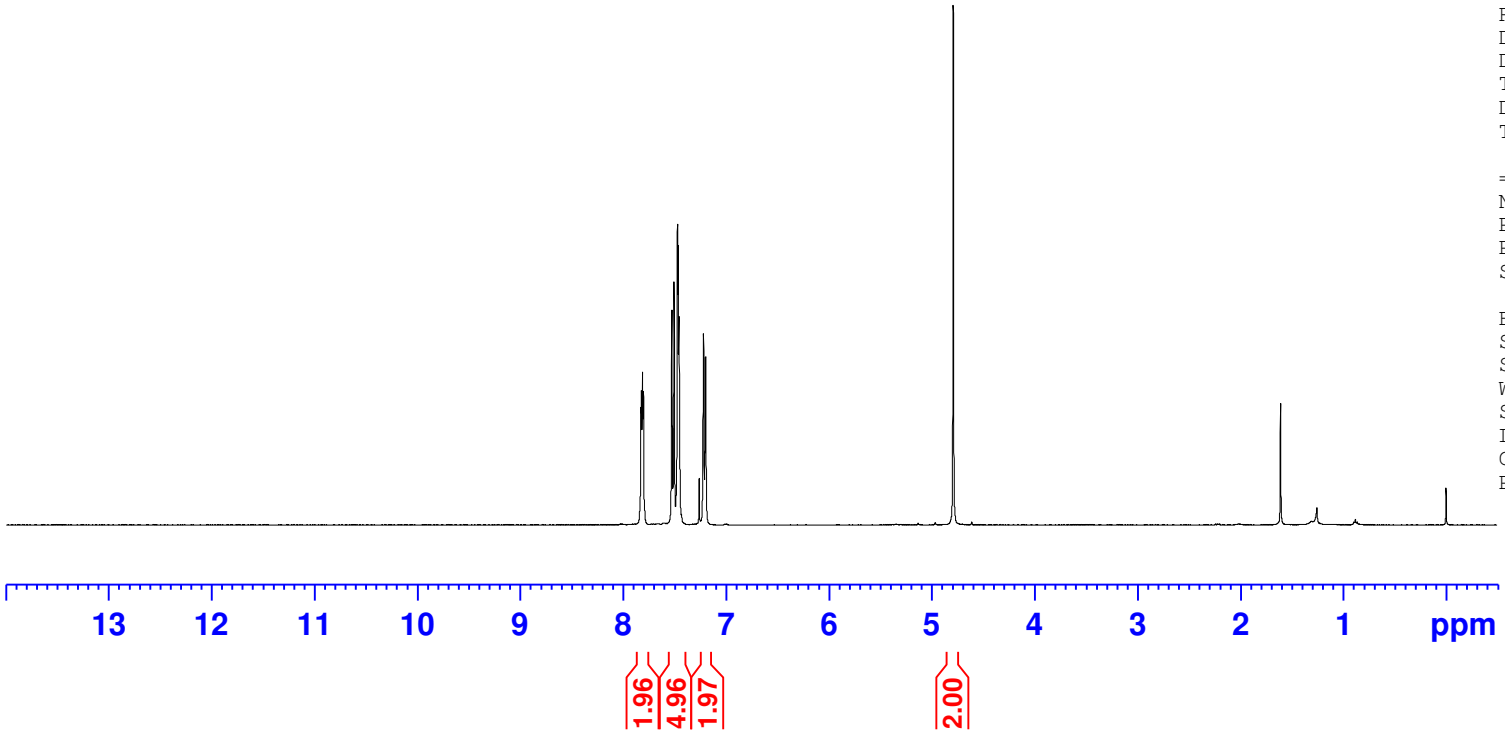
ZHL-3-97



2c'

7.826
7.821
7.811
7.802
7.526
7.505
7.471
7.465
7.456
7.260
7.218
7.198

4.790



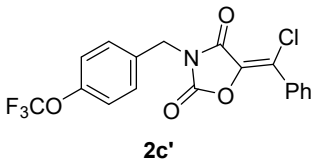
Current Data Parameters
NAME 20230429-400m
EXPNO 23
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230427
Time 23.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 140.02
DW 60.800 usec
DE 6.50 usec
TE 290.9 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900164 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-97

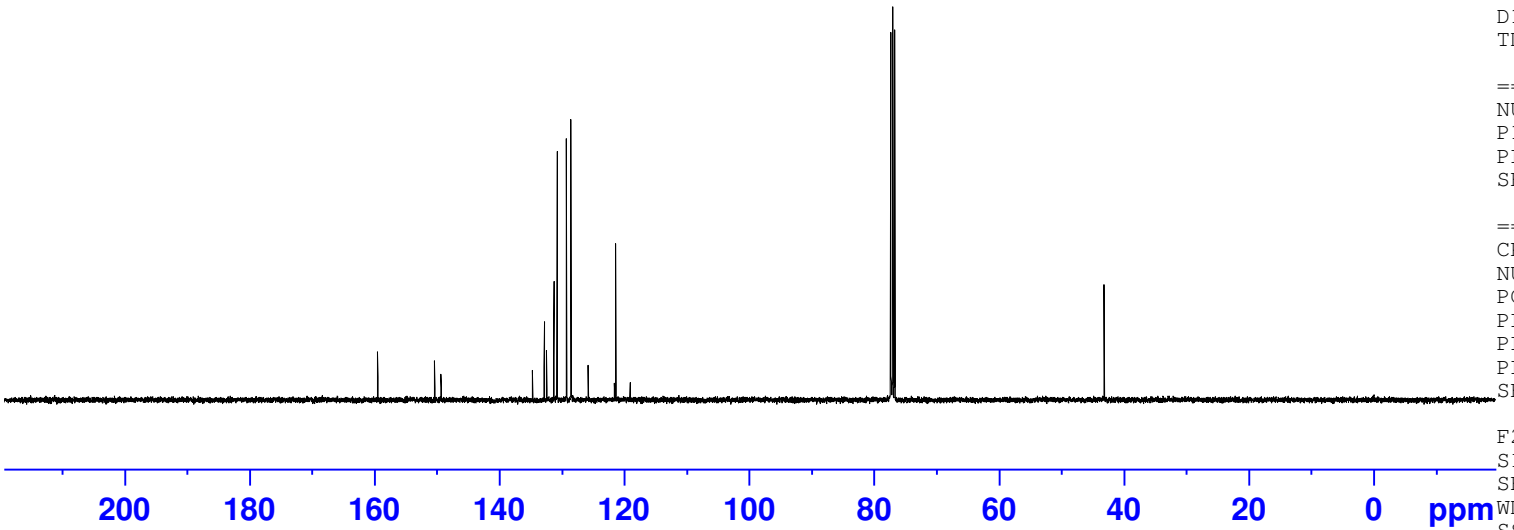


2c'

159.49
150.37
149.36
134.72
132.82
132.43
131.28
130.75
129.27
128.57
125.80
123.78
121.60
121.38
119.05
116.95

77.31
77.00
76.68

43.15



Current Data Parameters
NAME 20230506-400m
EXPNO 33
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230506
Time 8.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 292.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

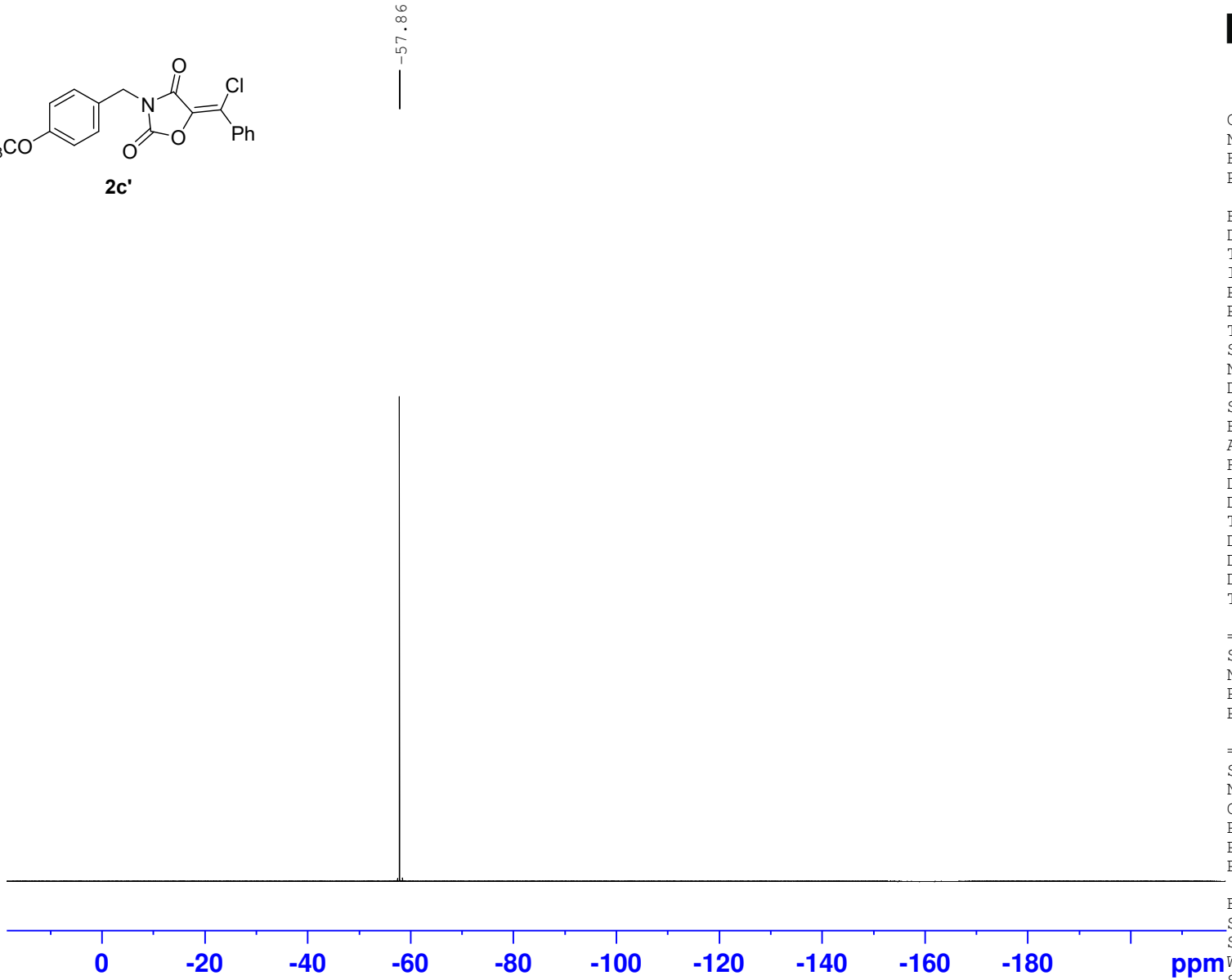
======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278631 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-3-97

2c'



Current Data Parameters
NAME 20230706-300M
EXPNO 241
PROCNO 1

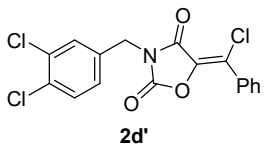
F2 - Acquisition Parameters
Date_ 20230706
Time 11.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn.2
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 0.510897 Hz
AQ 0.9786710 sec
RG 203
DW 7.467 usec
DE 6.50 usec
TE 297.8 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 282.3761148 MHz
NUC1 19F
P1 14.50 usec
PLW1 10.39999962 W

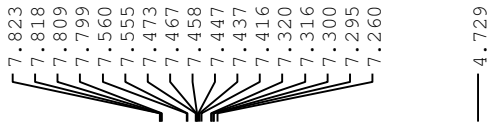
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W

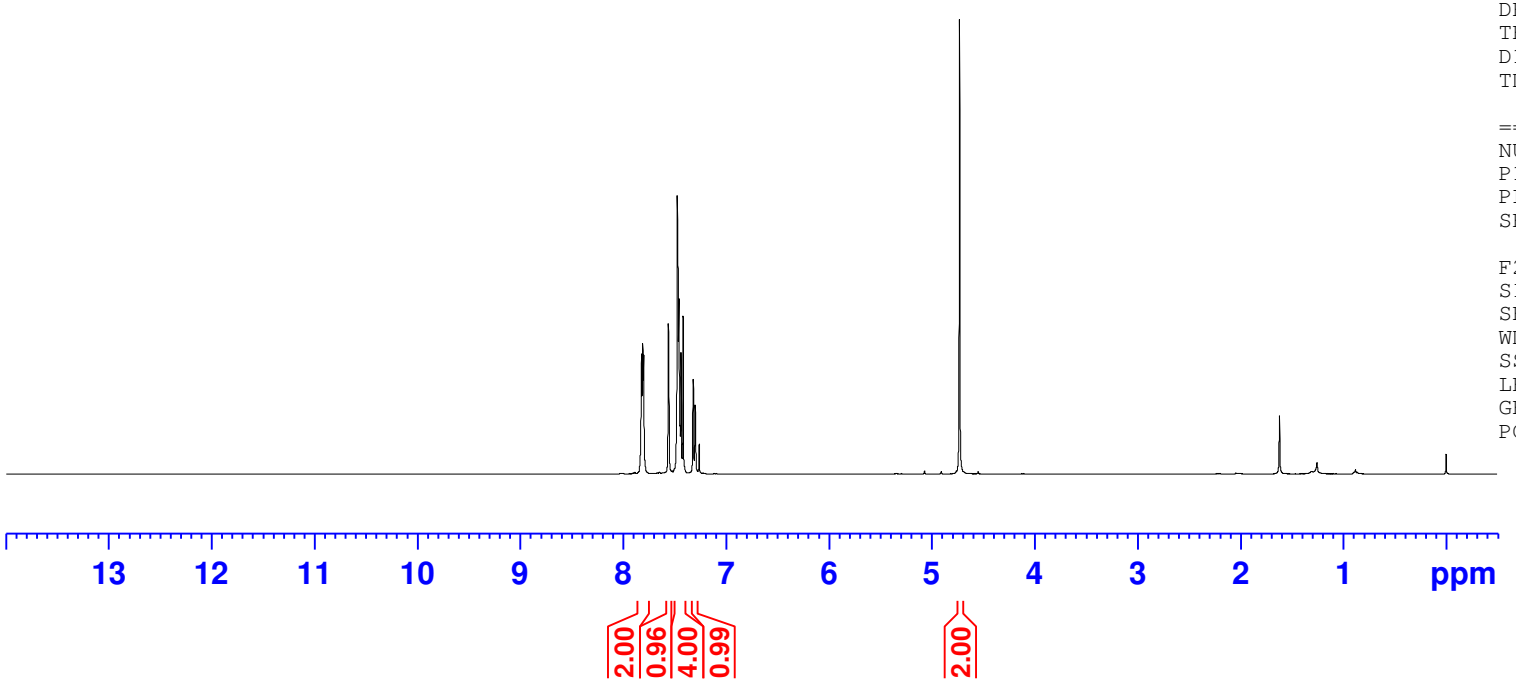
F2 - Processing parameters
SI 65536
SF 282.4043552 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZHL-3-94



2d'





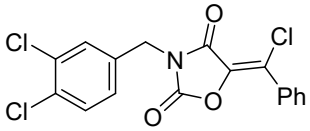
Current Data Parameters
NAME 20230429-400m
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230427
Time 22.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 125.76
DW 60.800 usec
DE 6.50 usec
TE 291.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

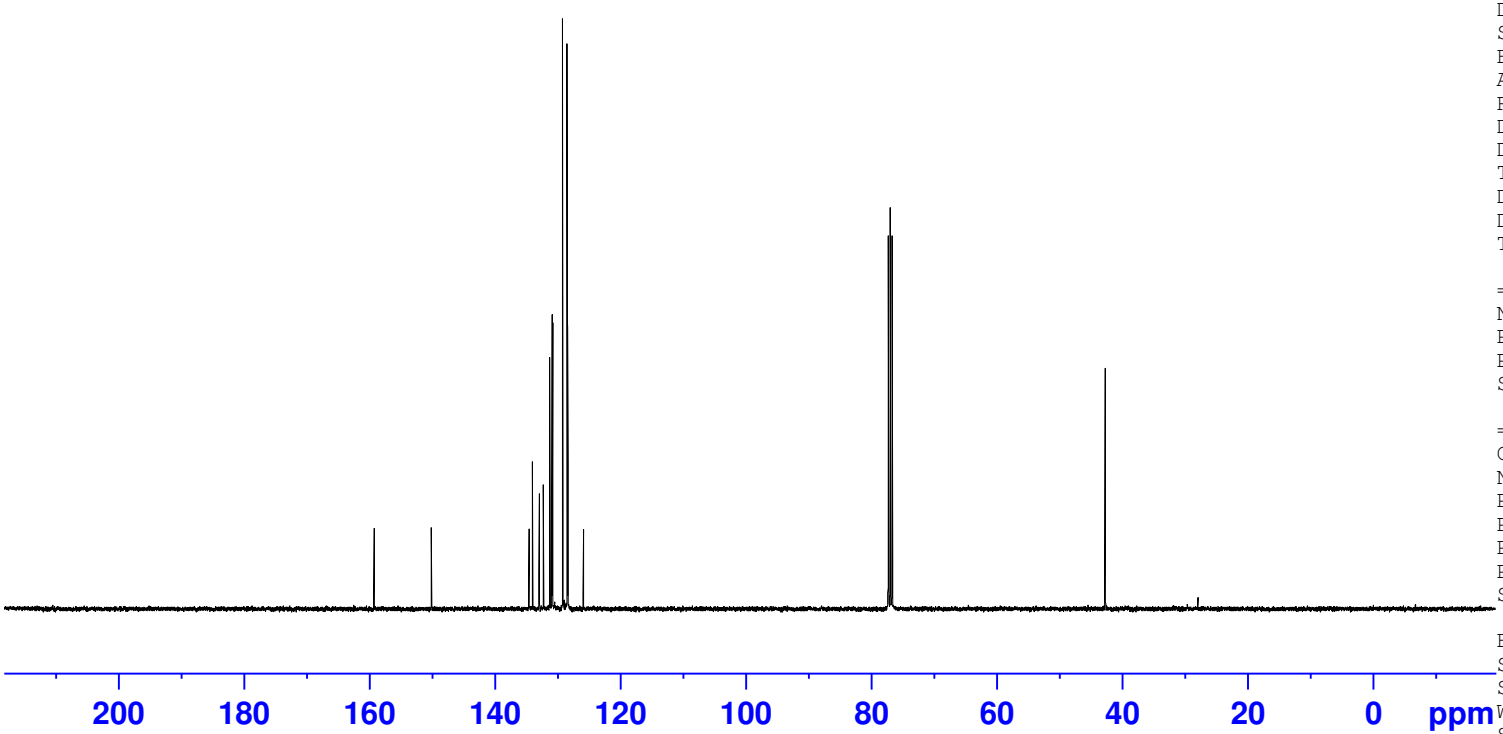
F2 - Processing parameters
SI 65536
SF 400.1900164 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-94



2d'

159.33
150.21
134.61
134.06
133.00
132.94
132.31
131.30
130.94
130.85
129.24
128.54
128.41
125.95
77.31
77.00
76.68
42.72
27.95



Current Data Parameters
NAME ZHL230423-400m
EXPNO 78
PROCNO 1

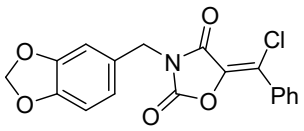
F2 - Acquisition Parameters
Date_ 20230423
Time 2.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 290.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278683 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

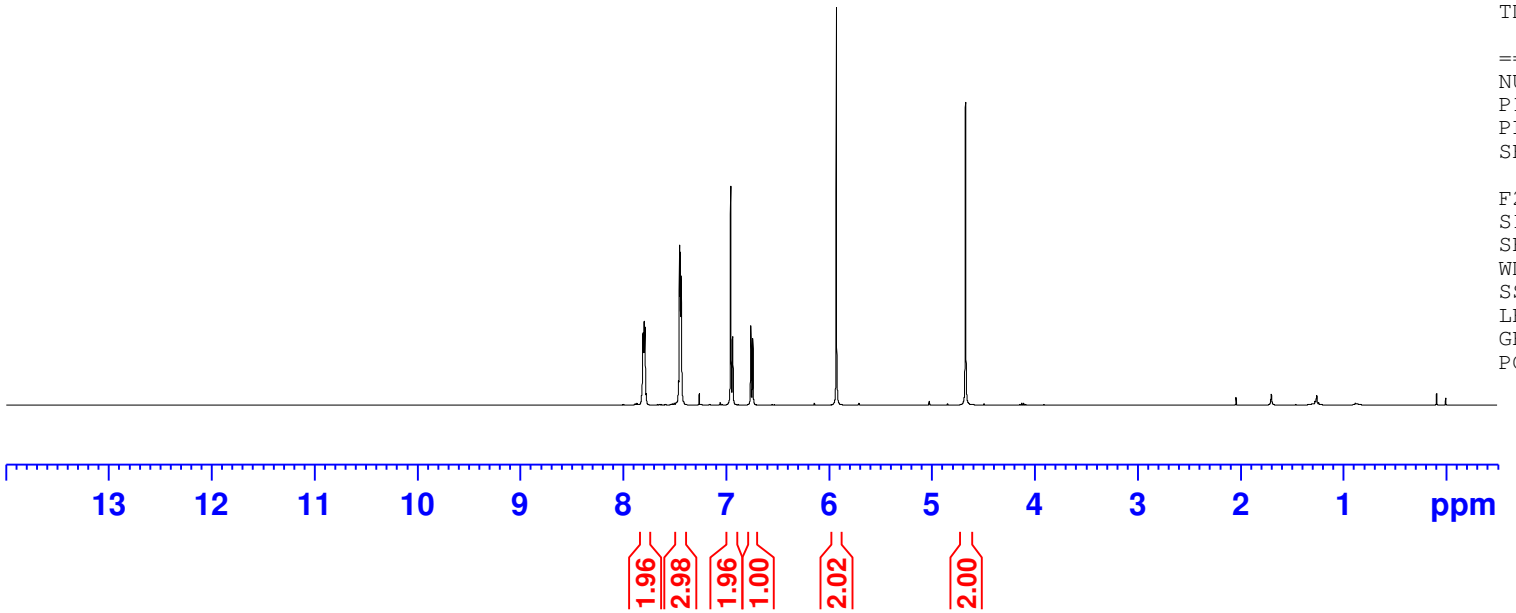
zhl-3-98



2e'

7.811
7.804
7.800
7.795
7.786
7.776
7.462
7.452
7.445
7.436
7.260
6.955
6.936
6.932
6.759
6.738
5.927

4.671



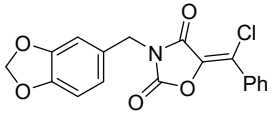
Current Data Parameters
NAME ZHL230423-400m
EXPNO 67
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230422
Time 23.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 68.24
DW 60.800 usec
DE 6.50 usec
TE 290.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

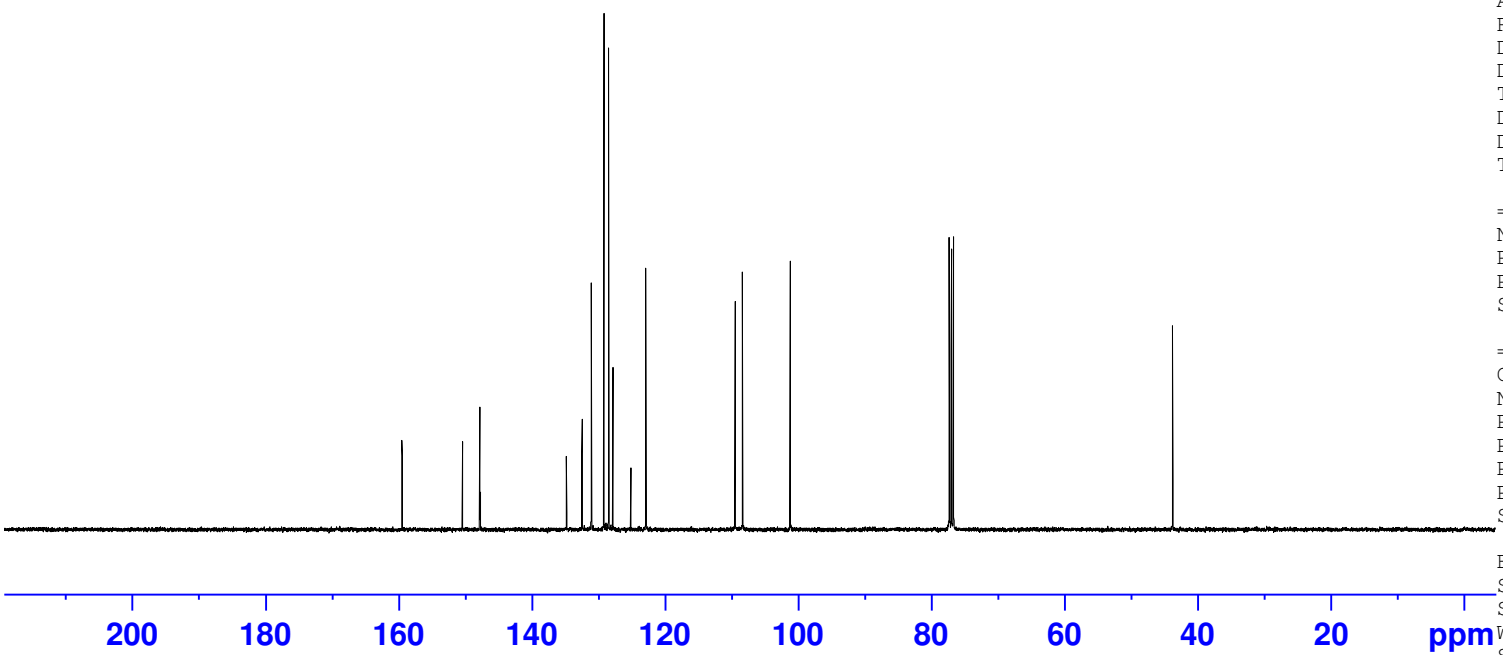
F2 - Processing parameters
SI 65536
SF 400.1900165 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-98



2e'

159.50
150.43
147.84
147.77
134.80
132.47
131.09
129.19
128.47
127.83
125.13
122.89
109.47
108.38
101.20
77.31
77.00
76.68
43.75



Current Data Parameters
NAME 20230505-400m
EXPNO 28
PROCNO 1

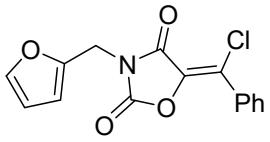
F2 - Acquisition Parameters
Date_ 20230505
Time 4.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 292.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

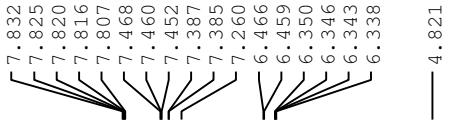
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

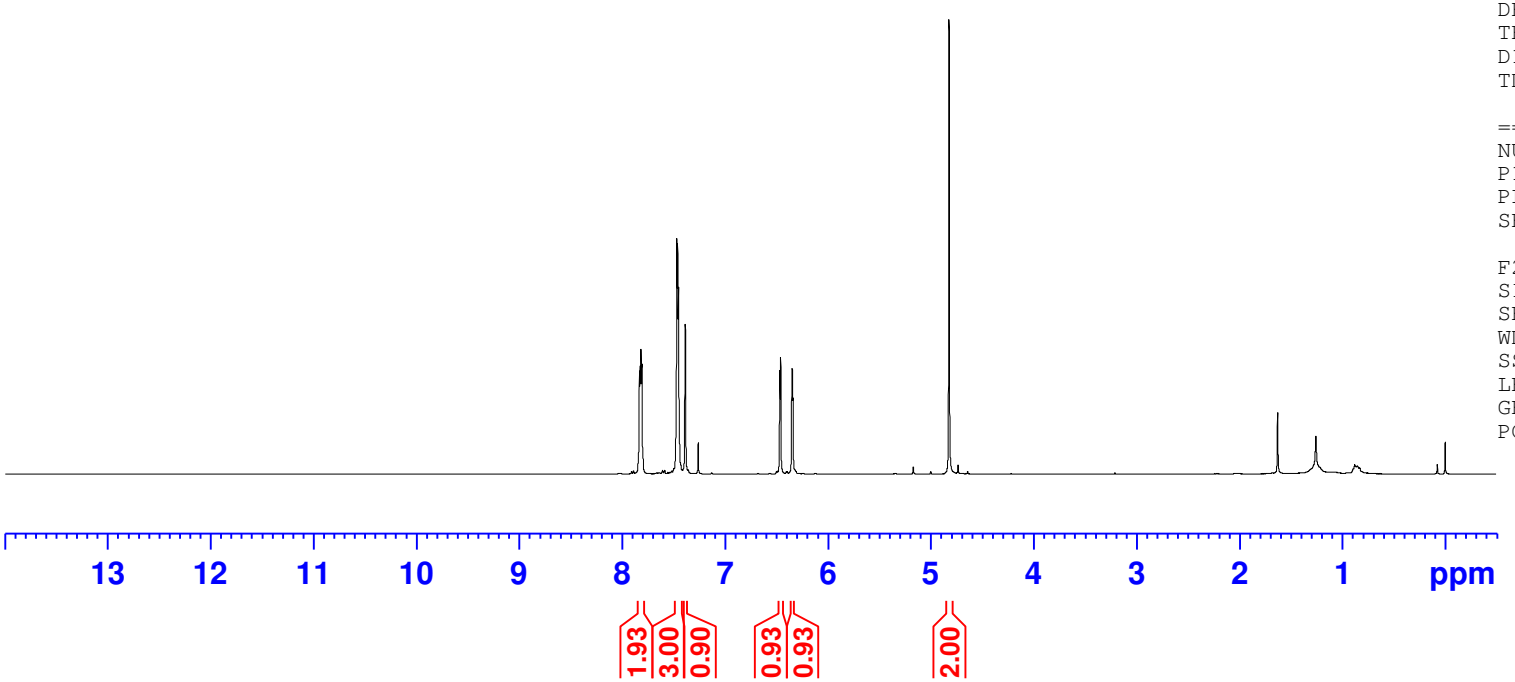
F2 - Processing parameters
SI 32768
SF 100.6278693 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-3-100



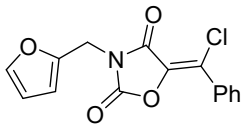
2f'





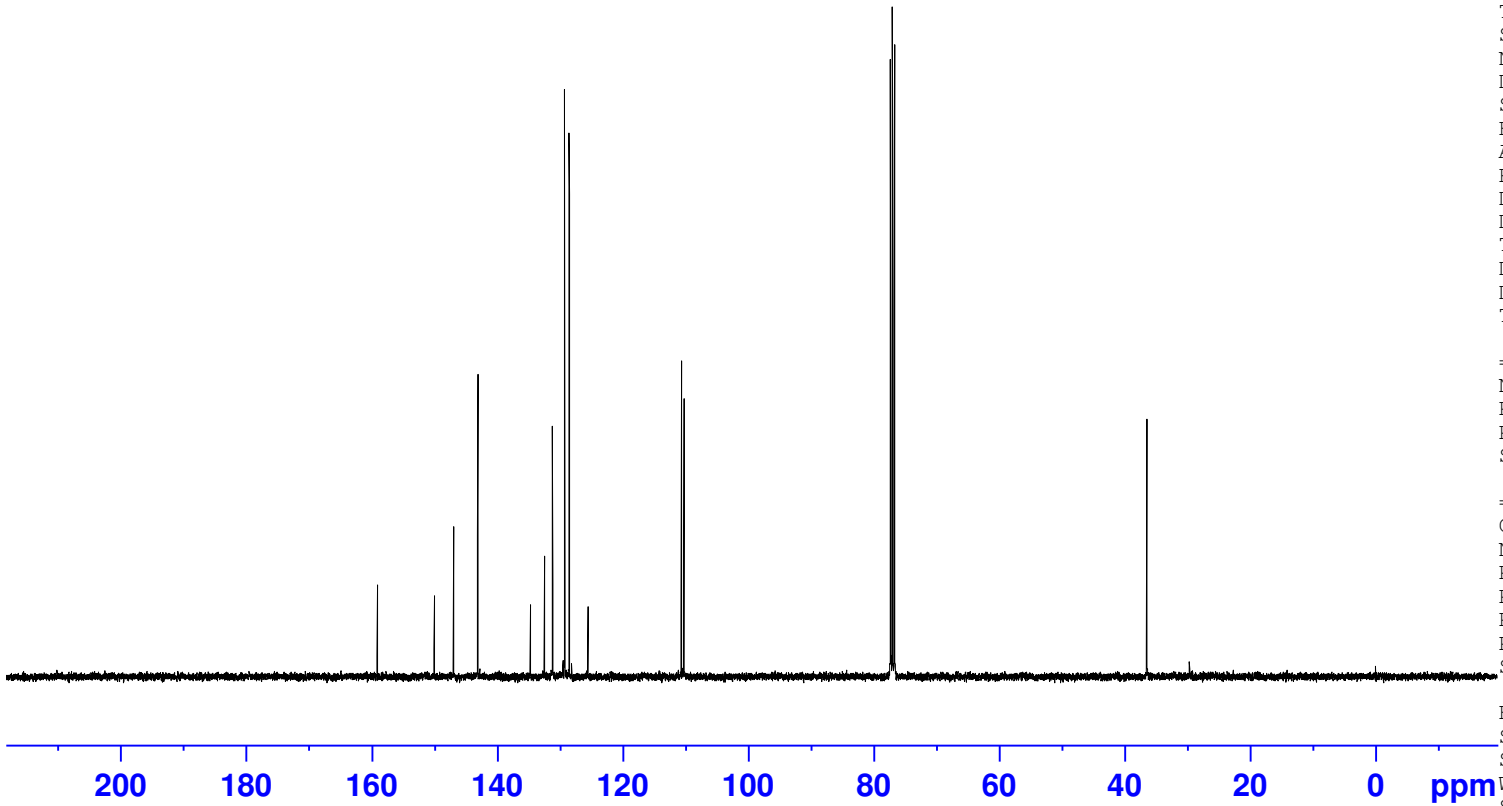

```
Current Data Parameters
NAME            zhl-400m
EXPNO                 30
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230514
Time               20.15
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9845889 sec
RG                125.76
DW                60.800 usec
DE                 6.50 usec
TE                291.2 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.68 usec
PLW1         14.00000000 W
SFO1         400.1924713 MHz

F2 - Processing parameters
SI                 65536
SF           400.1900163 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```

zhl-3-100



2f'

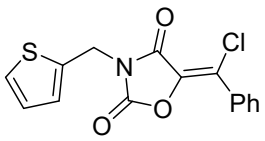
159.13
150.05
146.98
143.12
134.71
132.48
131.19
129.25
128.53
125.52
110.65
110.22
77.31
77.00
76.68
36.45



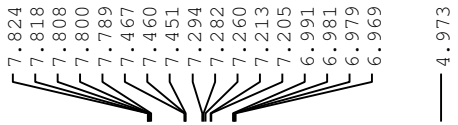
BRUKER

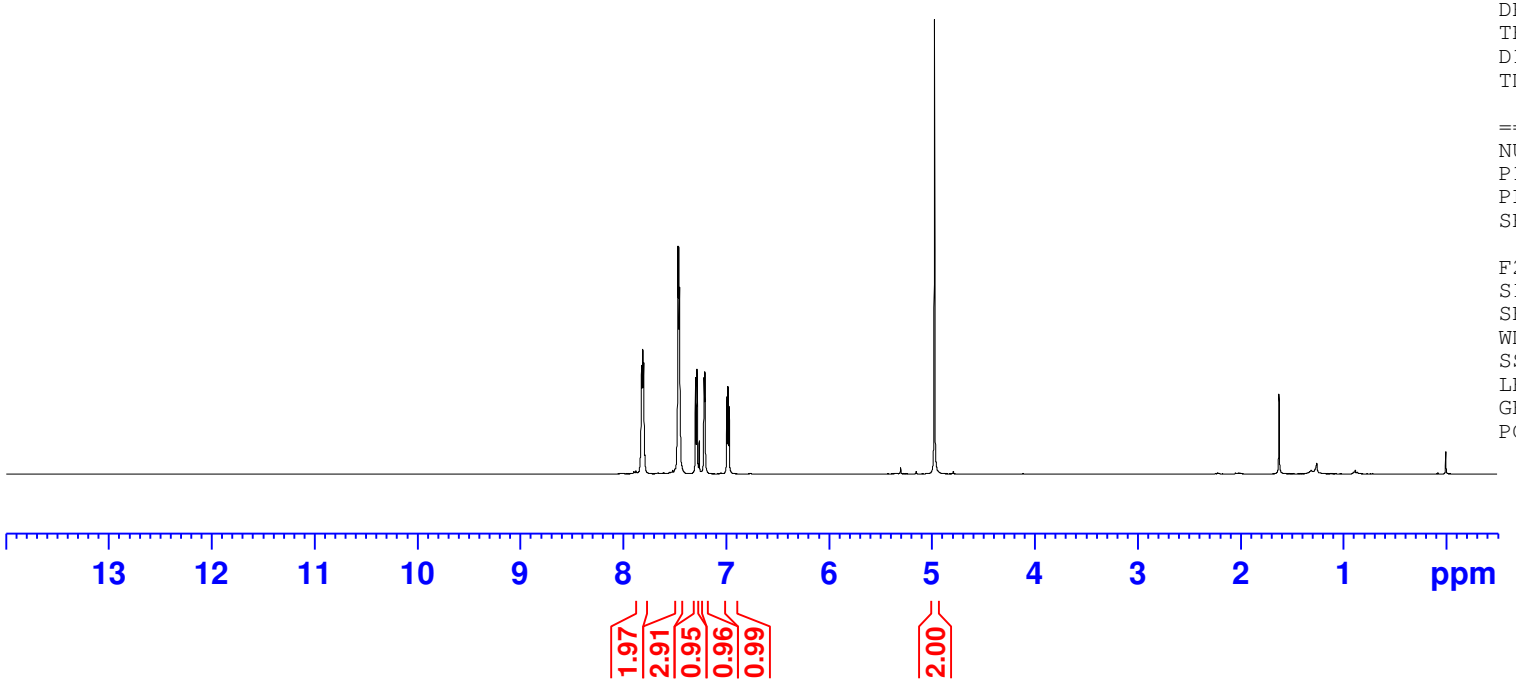
```
Current Data Parameters
NAME            zhl-400m
EXPNO                 31
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230514
Time               20.39
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE               291.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                12.00 usec
PLW1         53.00000000 W
SFO1        100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2         14.00000000 W
PLW12         0.37246999 W
PLW13         0.30170000 W
SFO2        400.1916008 MHz

F2 - Processing parameters
SI                32768
SF          100.6278653 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

ZHL-3-99



2g'





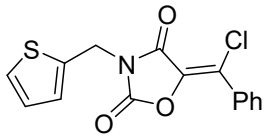
Current Data Parameters
NAME 20230429-400m
EXPNO 24
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230427
Time 23.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 140.02
DW 60.800 usec
DE 6.50 usec
TE 290.9 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

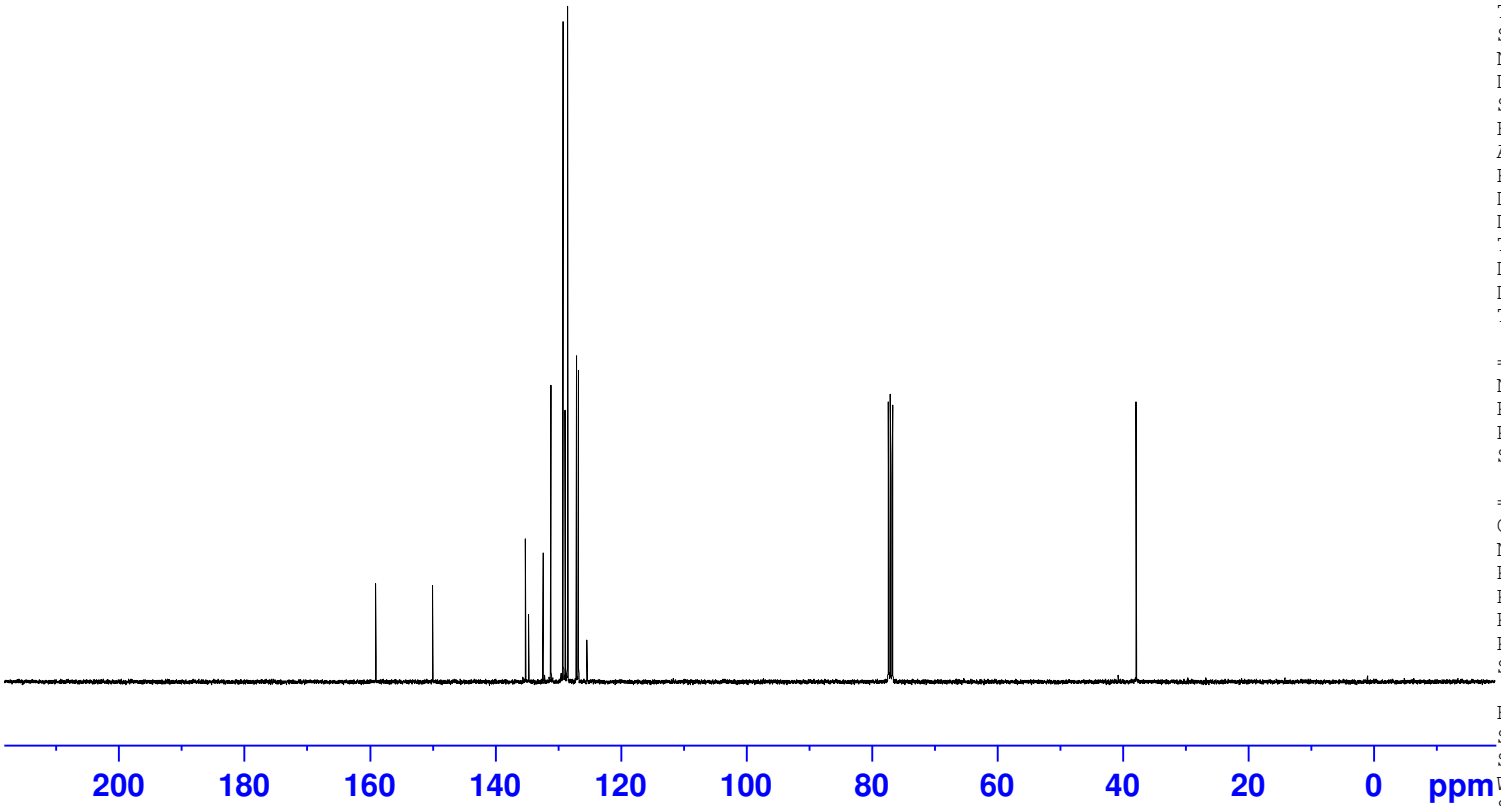
F2 - Processing parameters
SI 65536
SF 400.1900167 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-99



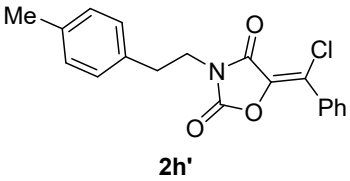
2g'

159.06
150.00
135.22
134.69
132.40
131.14
129.20
128.88
128.48
127.07
126.77
125.41
77.32
77.00
76.68
37.83

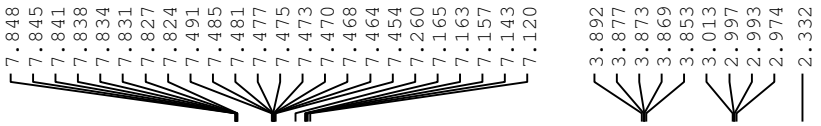


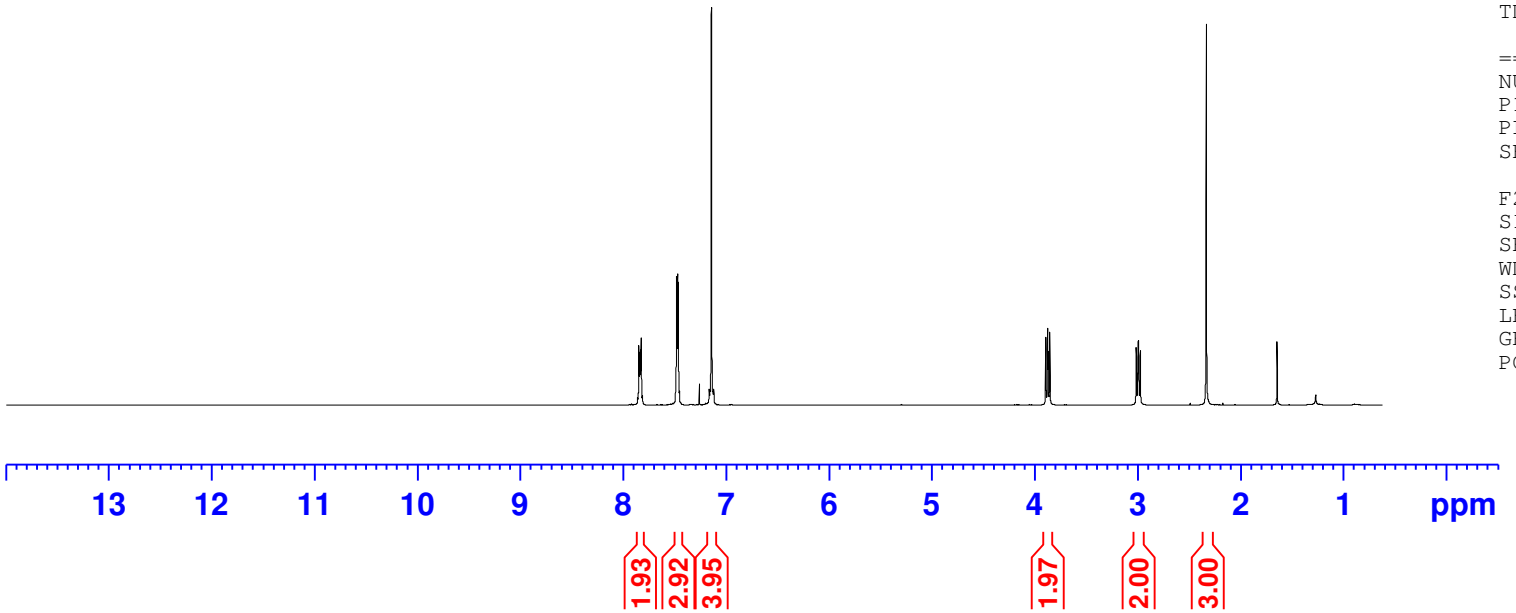

```
Current Data Parameters
NAME      ZHL230423-400m
EXPNO                 64
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230422
Time               22.58
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE               290.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                12.00 usec
PLW1        53.00000000 W
SFO1       100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.37246999 W
PLW13        0.30170000 W
SFO2       400.1916008 MHz

F2 - Processing parameters
SI                32768
SF         100.6278711 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

zhl-4-25A



2h'





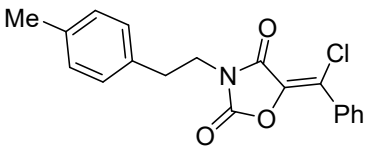
Current Data Parameters
NAME 2023-6-22-400
EXPNO 59
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230622
Time 5.03
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 68.24
DW 60.800 usec
DE 6.50 usec
TE 292.3 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

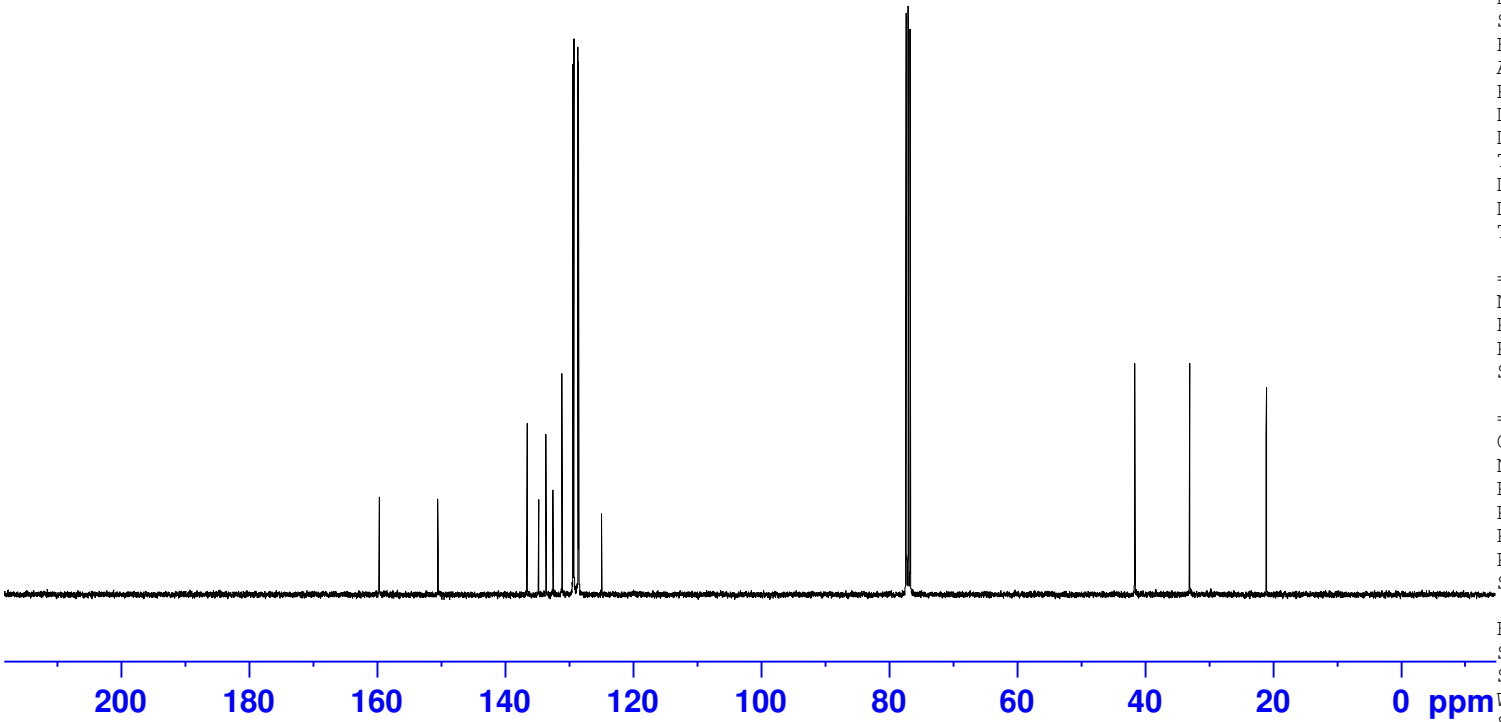
F2 - Processing parameters
SI 65536
SF 400.1881130 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-4-25A



2h'

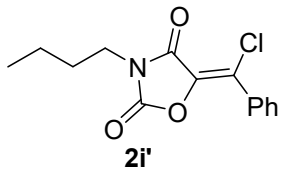
159.67
150.50
136.55
134.76
133.63
132.54
131.10
129.40
129.24
128.59
128.51
124.92
77.31
77.00
76.68
41.58
32.98
21.02



BRUKER

```
Current Data Parameters
NAME       2023-6-22-400
EXPNO                 60
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230622
Time                5.33
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG           zgpg30
TD                 65536
SOLVENT              DMSO
NS                     500
DS                       4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                 50.16
DW                20.800 usec
DE                 6.50 usec
TE                292.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  9.80 usec
PLW1         47.40000153 W
SFO1        100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                  1H
PCPD2              90.00 usec
PLW2         23.00000000 W
PLW12         0.30712000 W
PLW13         0.24877000 W
SFO2        400.1916008 MHz

F2 - Processing parameters
SI                 32768
SF          100.6273886 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

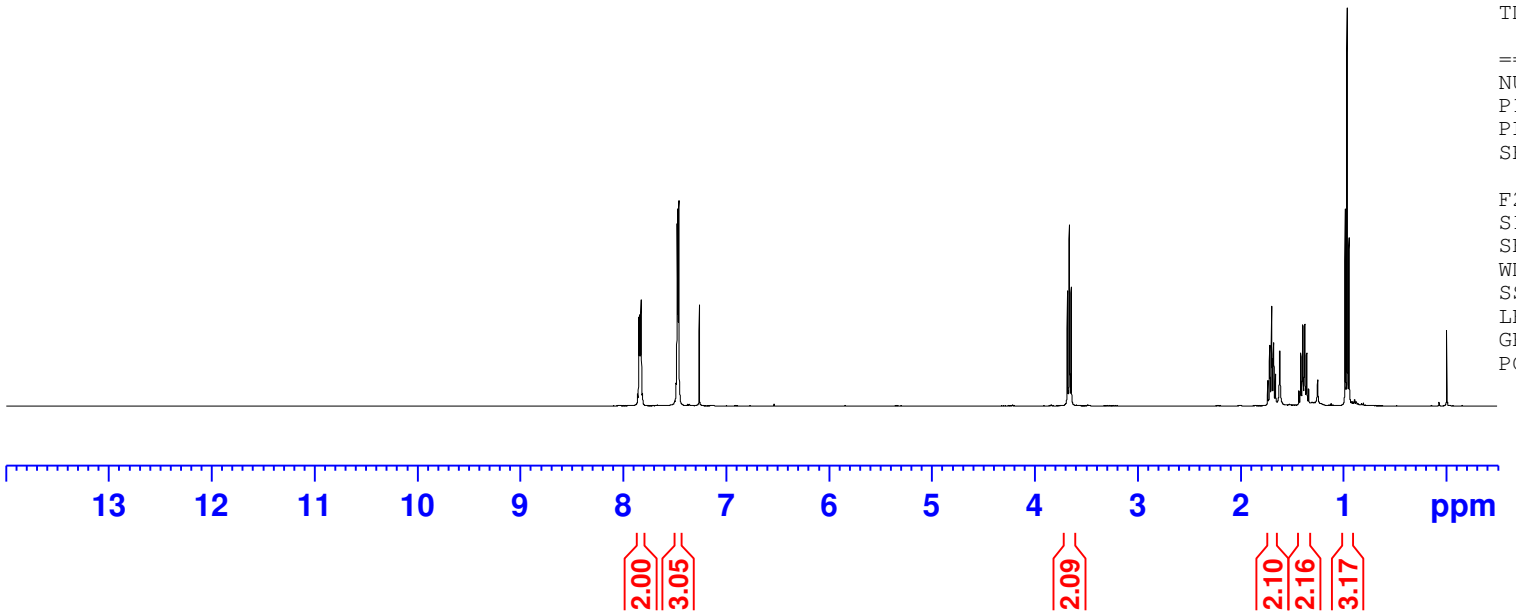
zhl-4-28



2i'

7.847
7.844
7.841
7.838
7.833
7.829
7.826
7.823
7.476
7.467
7.459
7.260

3.681
3.663
3.644
1.732
1.713
1.708
1.699
1.695
1.689
1.676
1.657
1.429
1.411
1.392
1.373
1.354
1.336
0.980
0.962
0.943



Current Data Parameters
NAME 20230707-400M
EXPNO 23
PROCNO 1

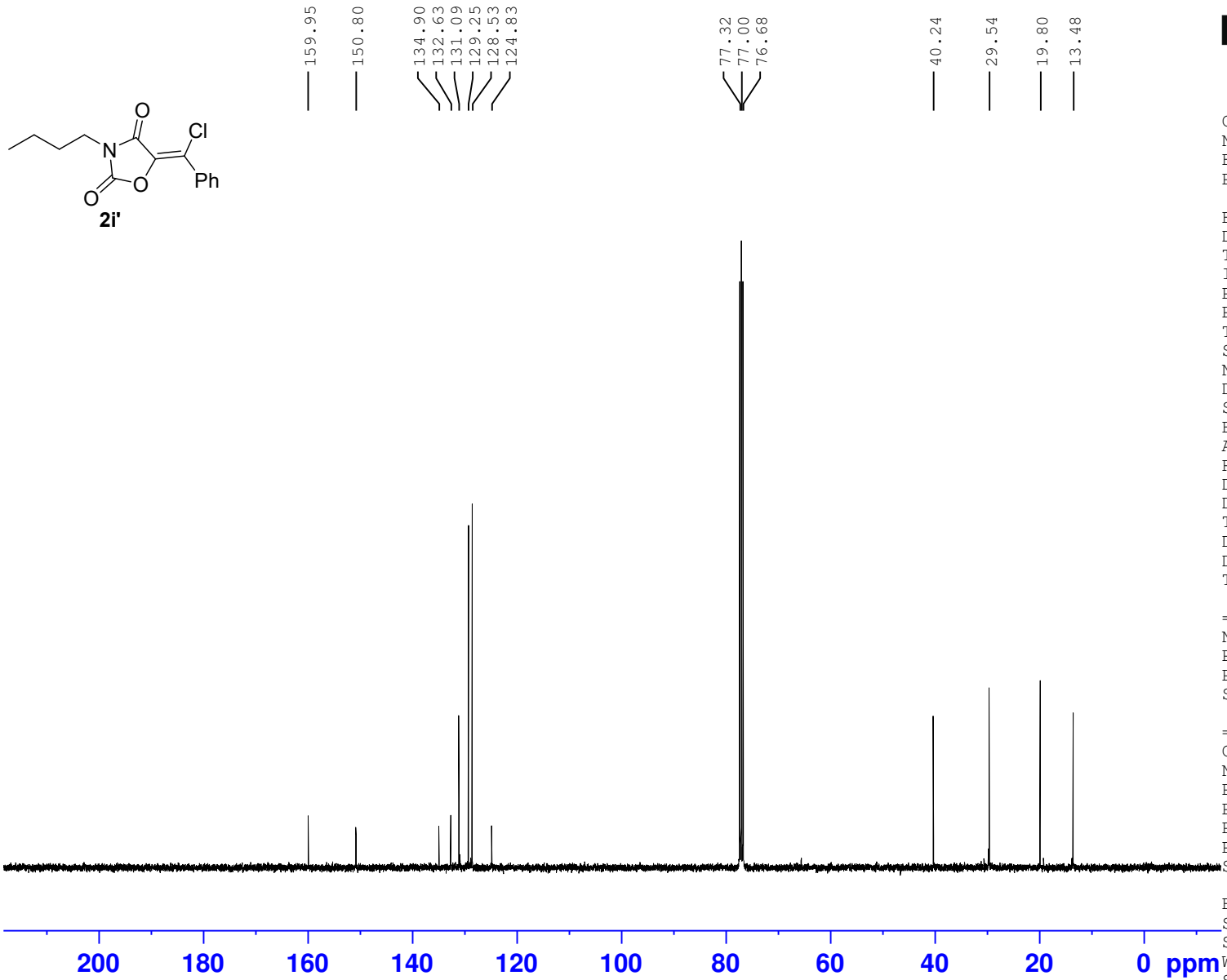
F2 - Acquisition Parameters
Date_ 20230706
Time 23.06
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 113.67
DW 60.800 usec
DE 6.50 usec
TE 290.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900141 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

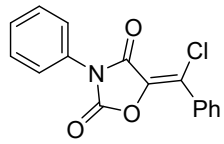
zhl-4-28

2i'

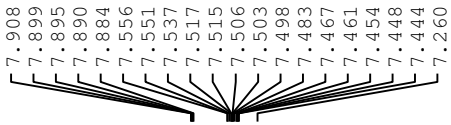


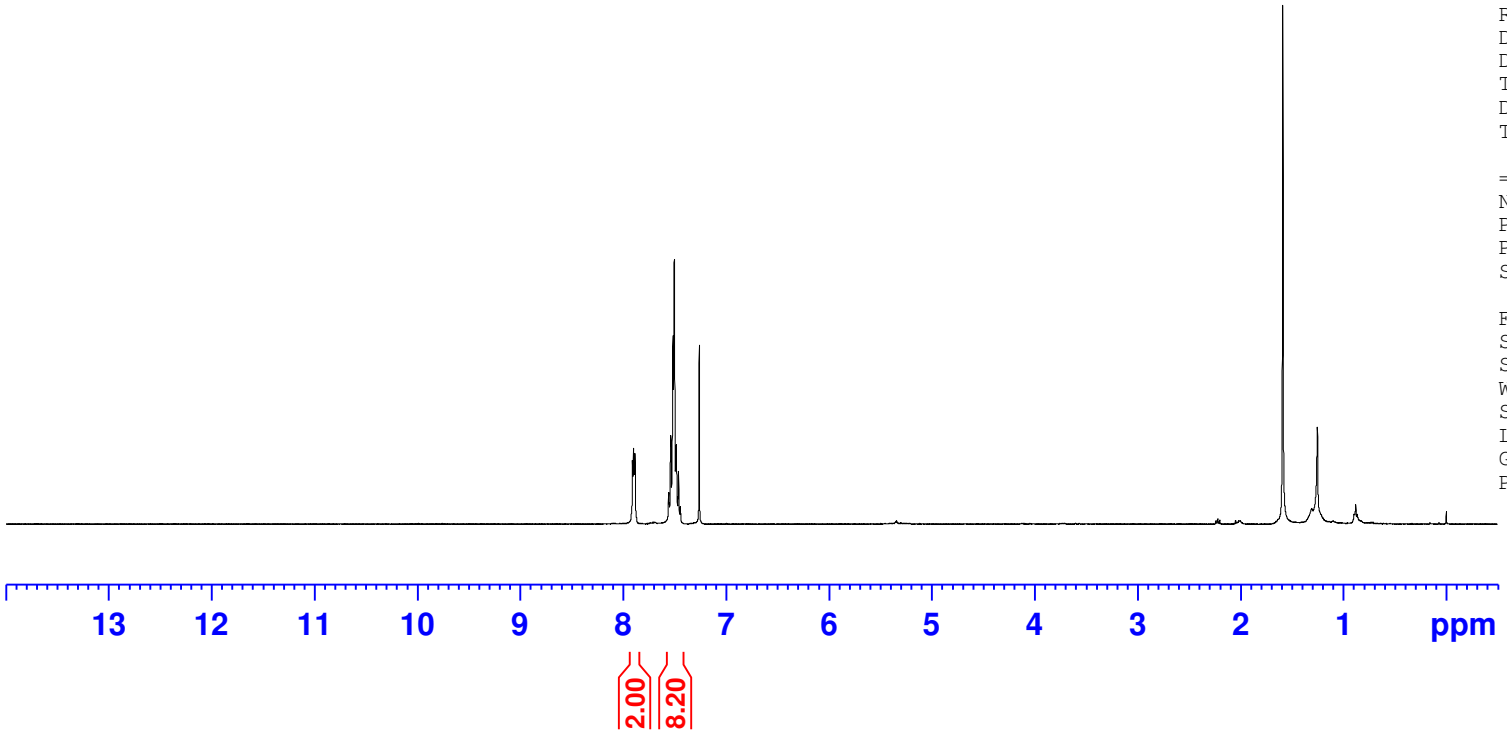

```
Current Data Parameters
NAME      20230524-400m
EXPNO                31
PROCNO                1

F2 - Acquisition Parameters
Date_          20230524
Time               3.20
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE               292.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                12.00 usec
PLW1        53.00000000 W
SFO1       100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.37246999 W
PLW13        0.30170000 W
SFO2       400.1916008 MHz

F2 - Processing parameters
SI                32768
SF         100.6278630 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

ZHL-4-19A



2j'





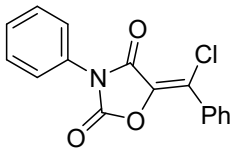
Current Data Parameters
NAME 20230627-400m
EXPNO 28
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230627
Time 5.28
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 193.13
DW 60.800 usec
DE 6.50 usec
TE 292.4 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

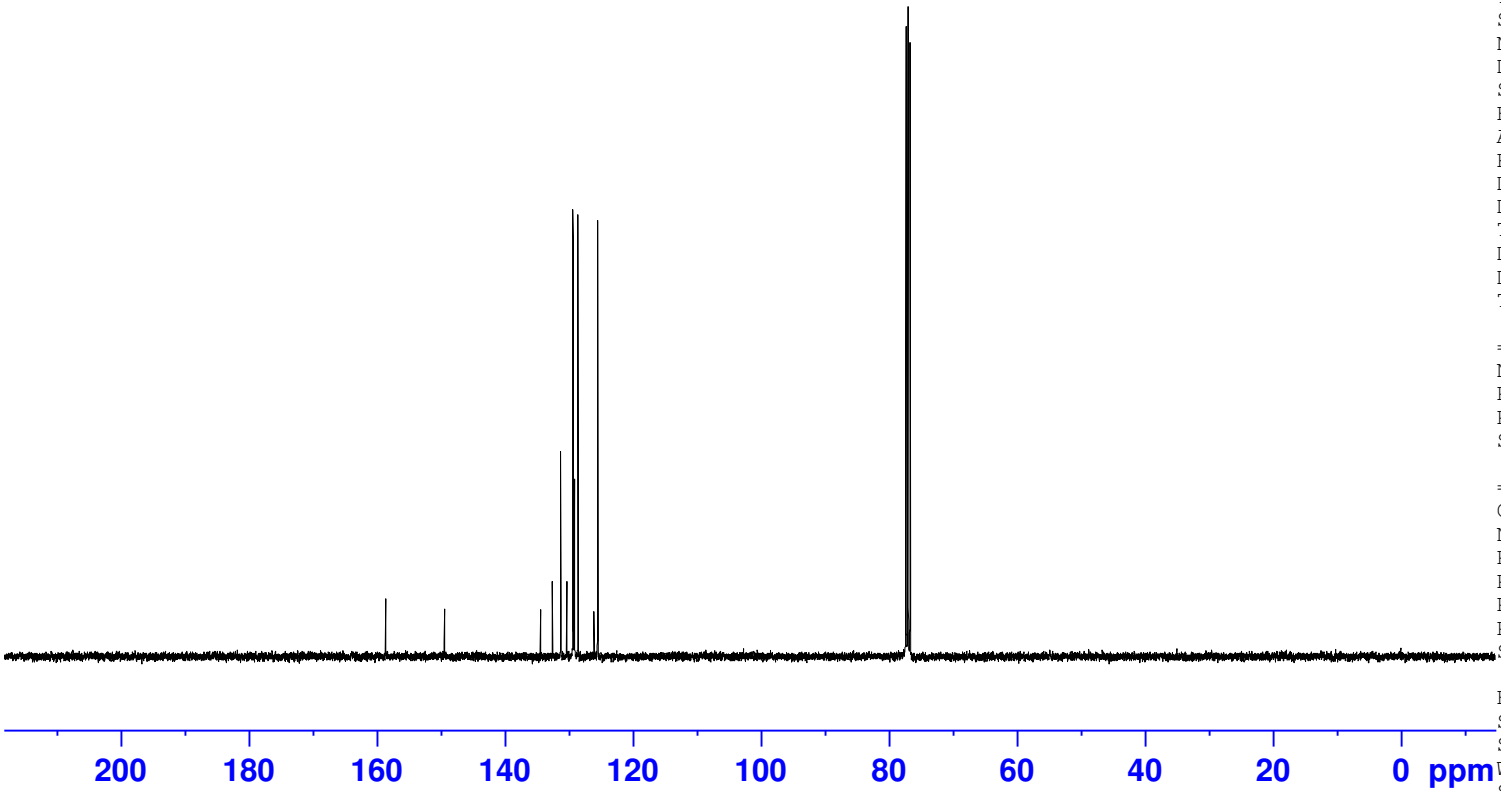
F2 - Processing parameters
SI 65536
SF 400.1900140 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-4-19a



2j'

158.66
149.49
134.47
132.61
131.30
130.36
129.41
129.33
129.15
128.60
126.10
125.53
77.32
77.00
76.68

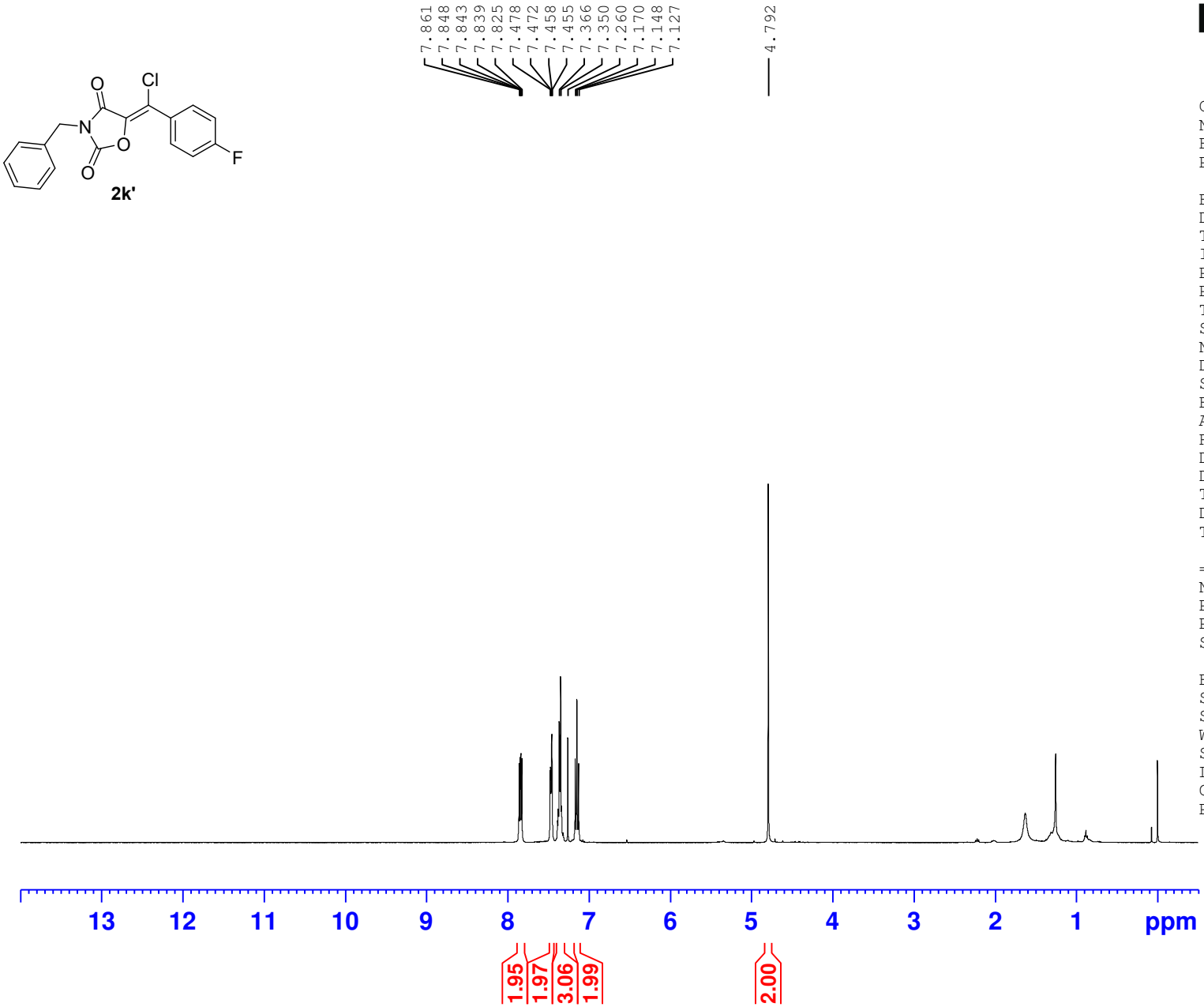


BRUKER

```
Current Data Parameters
NAME                  37(1)
EXPNO                    37
PROCNO                    1

F2 - Acquisition Parameters
Date_              20230514
Time                  22.46
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      400
DS                        4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                   193.13
DW                   20.800 usec
DE                    6.50 usec
TE                   291.9 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                   12.00 usec
PLW1           53.00000000 W
SFO1          100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                    1H
PCPD2                90.00 usec
PLW2           14.00000000 W
PLW12           0.37246999 W
PLW13           0.30170000 W
SFO2          400.1916008 MHz

F2 - Processing parameters
SI                      32768
SF            100.6278645 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40
```

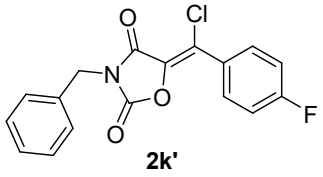
zhl-4-30

2k'

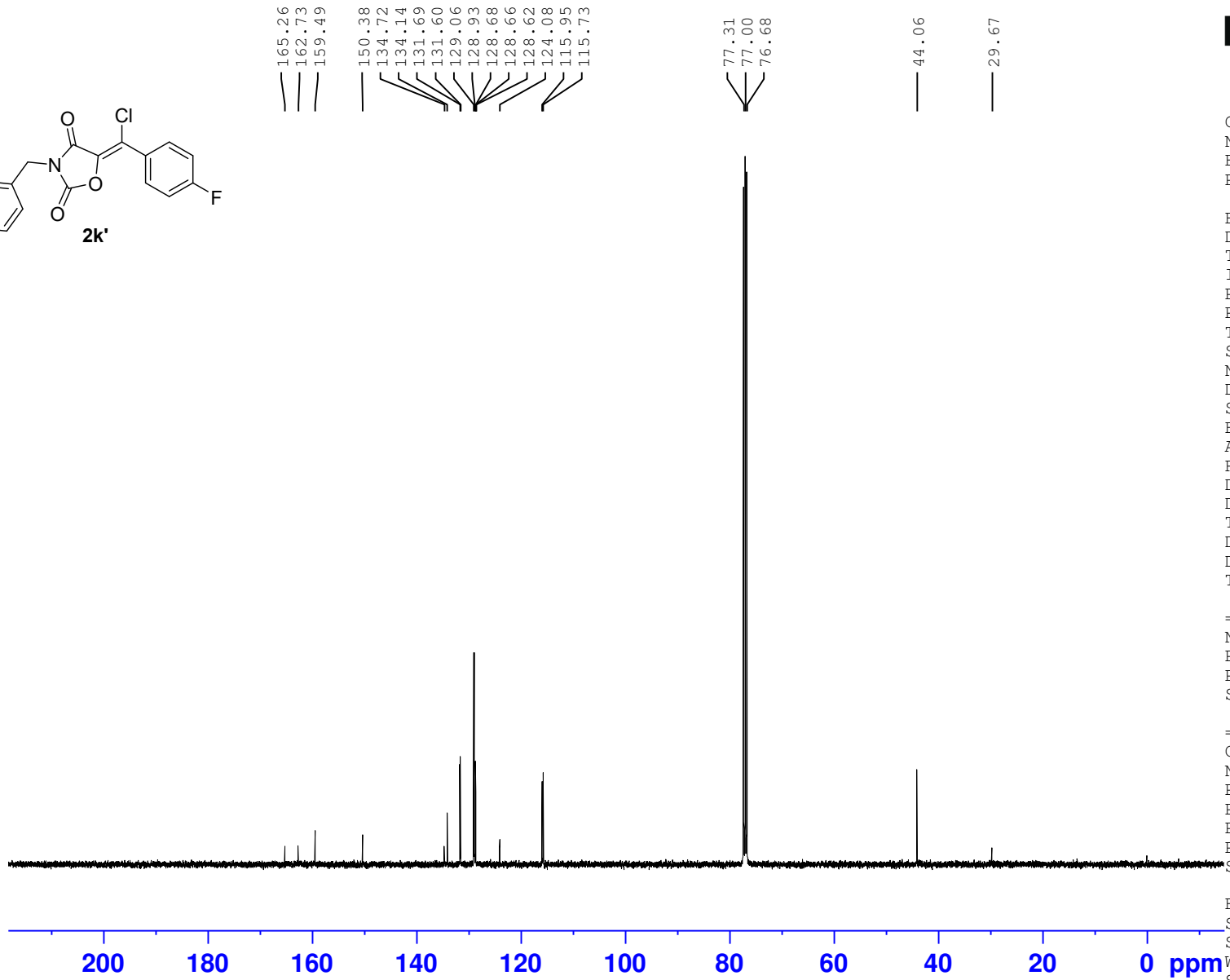



```
Current Data Parameters
NAME       20230720-400M
EXPNO                 34
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230720
Time                3.02
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     6
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9845889 sec
RG                154.68
DW                60.800 usec
DE                 6.50 usec
TE                294.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.90 usec
PLW1        23.00000000 W
SFO1        400.1924713 MHz

F2 - Processing parameters
SI                 65536
SF          400.1900140 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

zhl-4-30



2k'



Current Data Parameters
NAME 20230720-400M
EXPNO 35
PROCNO 1

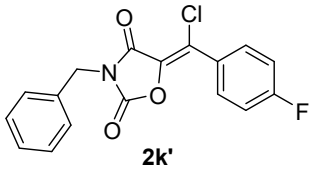
F2 - Acquisition Parameters
Date_ 20230720
Time 3.38
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 600
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 37.77
DW 20.800 usec
DE 6.50 usec
TE 294.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

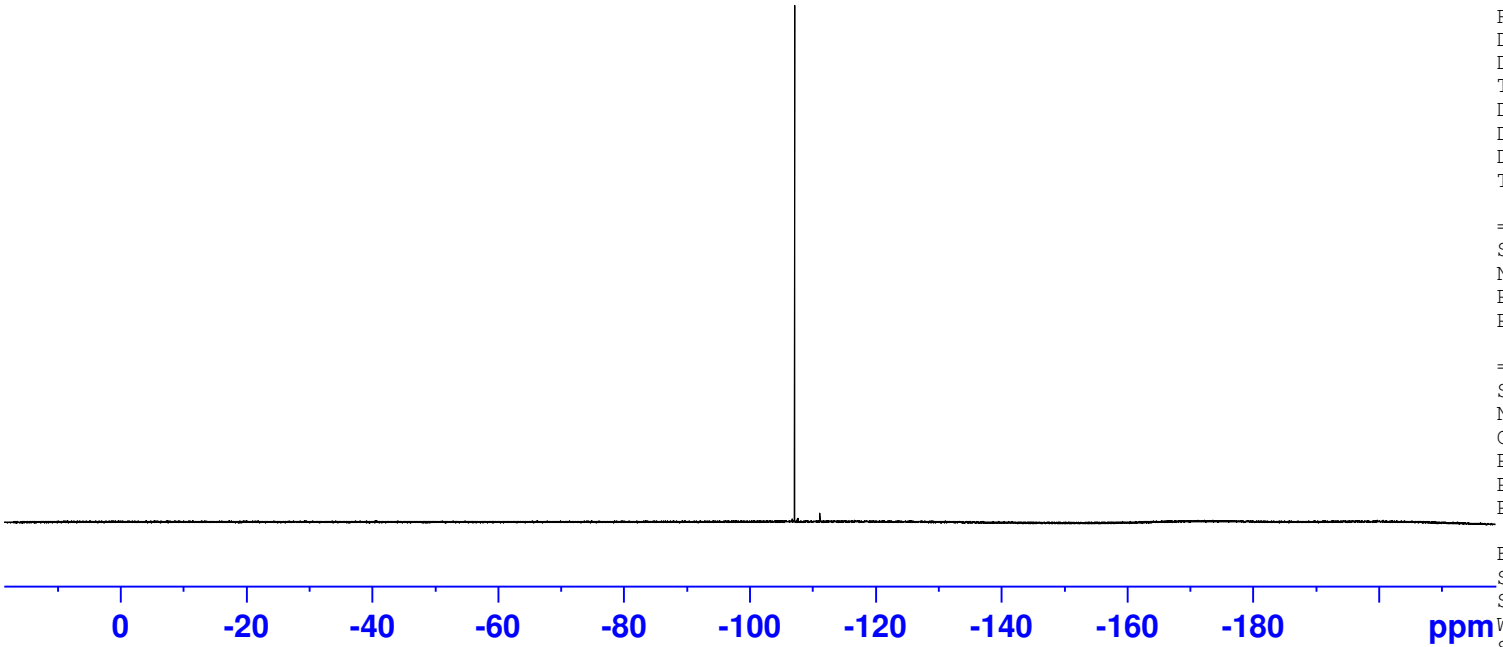
F2 - Processing parameters
SI 32768
SF 100.6278615 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-4-30



2k'

-107.13



Current Data Parameters
NAME 20230707-300m
EXPNO 250
PROCNO 1

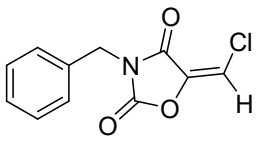
F2 - Acquisition Parameters
Date_ 20230707
Time 11.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn.2
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 0.510897 Hz
AQ 0.9786710 sec
RG 203
DW 7.467 usec
DE 6.50 usec
TE 297.5 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 282.3761148 MHz
NUC1 19F
P1 14.50 usec
PLW1 10.39999962 W

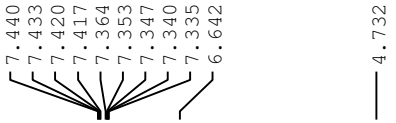
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W

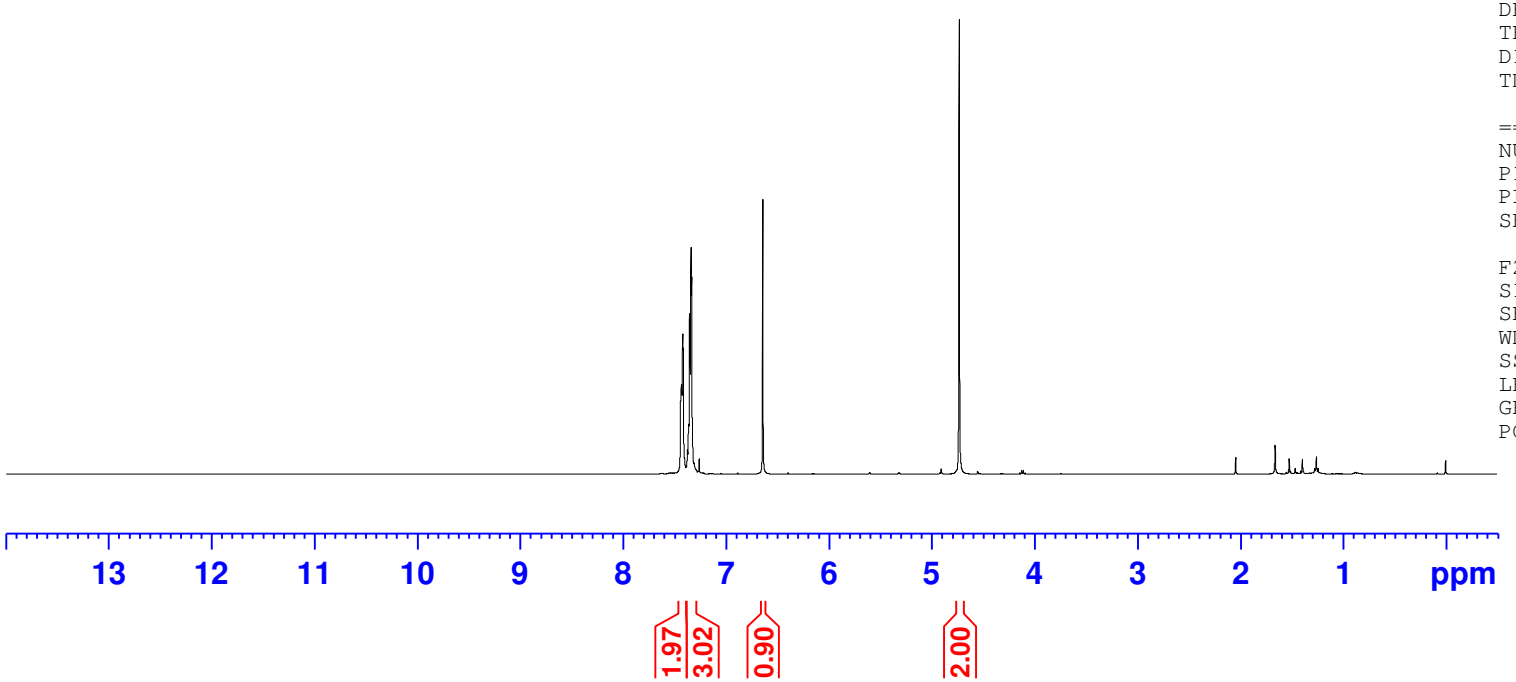
F2 - Processing parameters
SI 65536
SF 282.4043552 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-4-18a



2l'

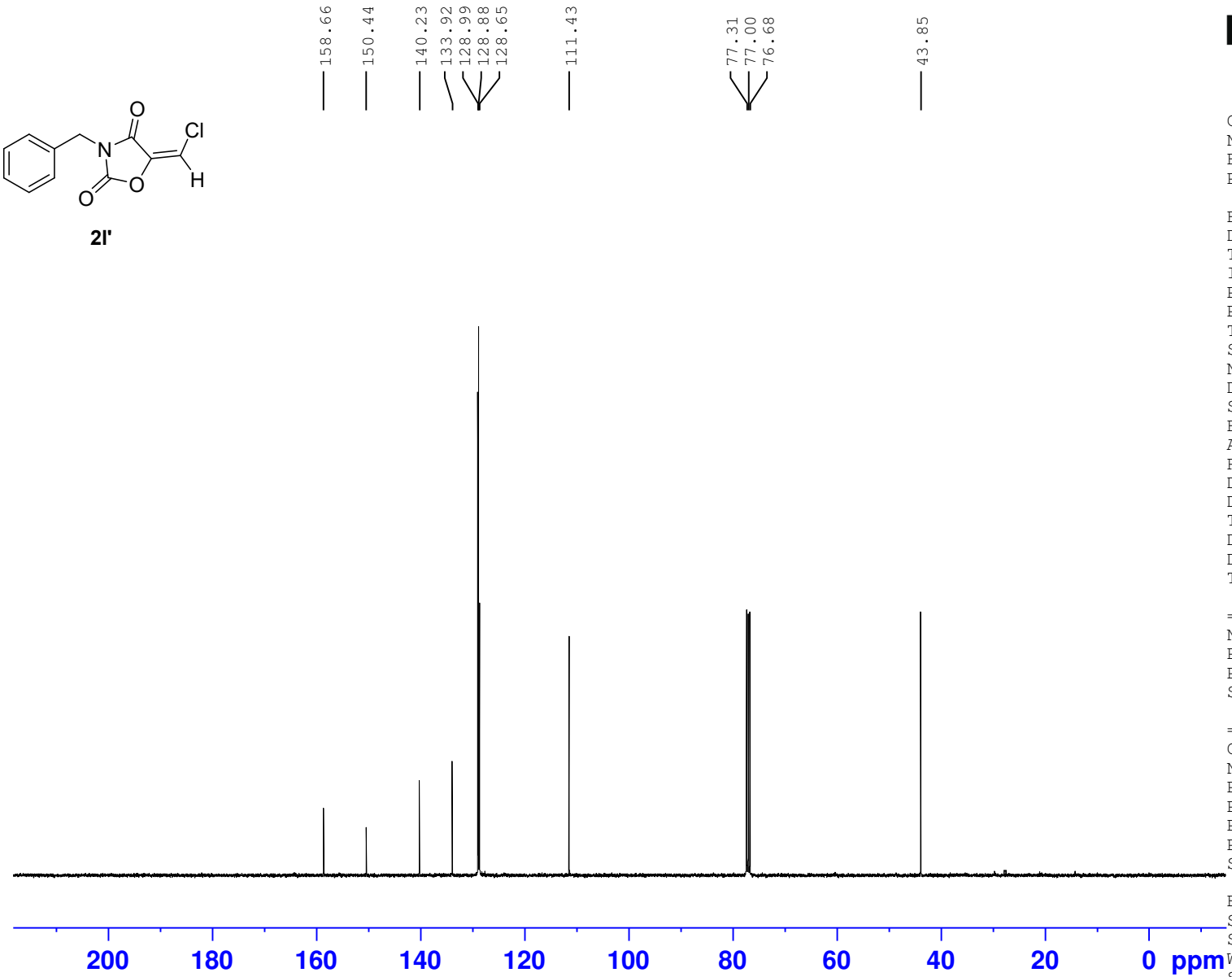





```
Current Data Parameters
NAME            zhl-400m
EXPNO                 34
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230514
Time               21.12
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9845889 sec
RG                 90.23
DW                60.800 usec
DE                 6.50 usec
TE                291.1 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.68 usec
PLW1         14.00000000 W
SFO1         400.1924713 MHz

F2 - Processing parameters
SI                 65536
SF           400.1900165 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```

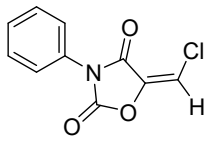
zhl-4-18a

2l'

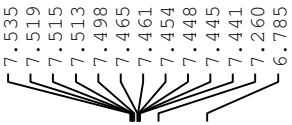


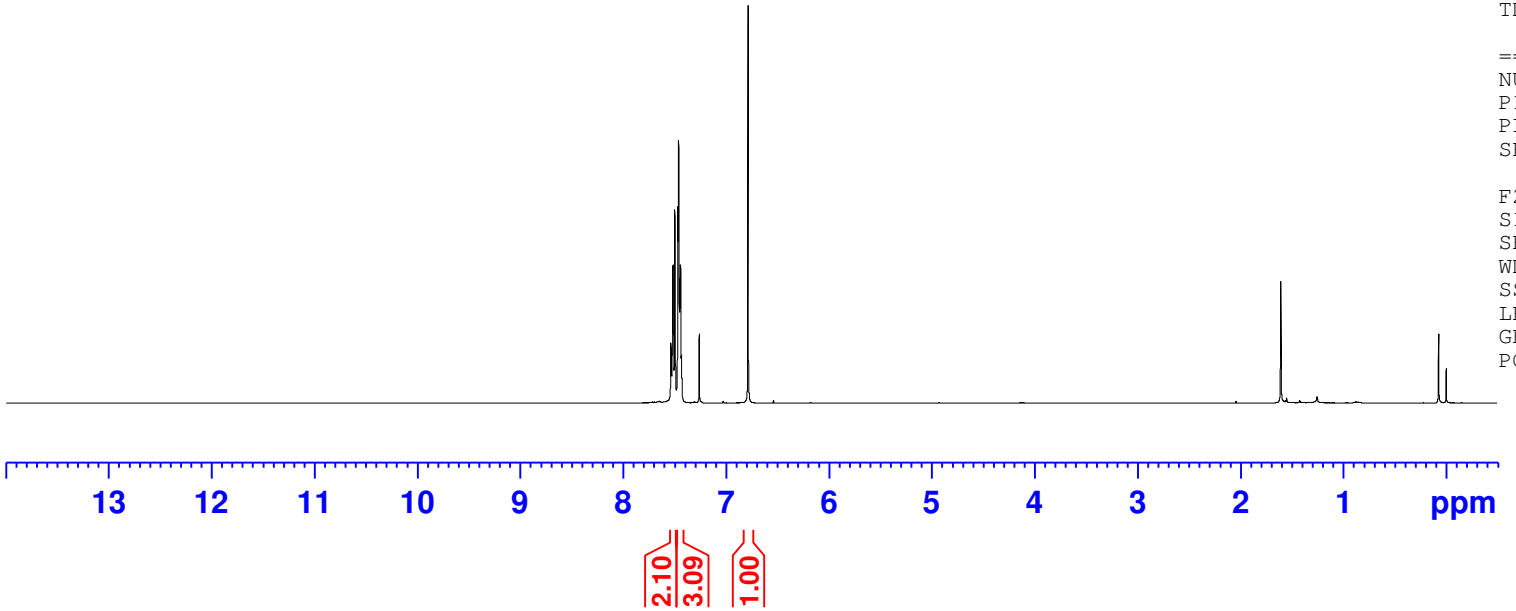

```
Current Data Parameters
NAME            zhl-400m
EXPNO                 35
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230514
Time               21.36
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               193.13
DW               20.800 usec
DE                6.50 usec
TE                291.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                12.00 usec
PLW1        53.00000000 W
SFO1       100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.37246999 W
PLW13        0.30170000 W
SFO2       400.1916008 MHz

F2 - Processing parameters
SI                32768
SF         100.6278685 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

zhl-5-93



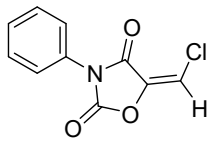
2m'





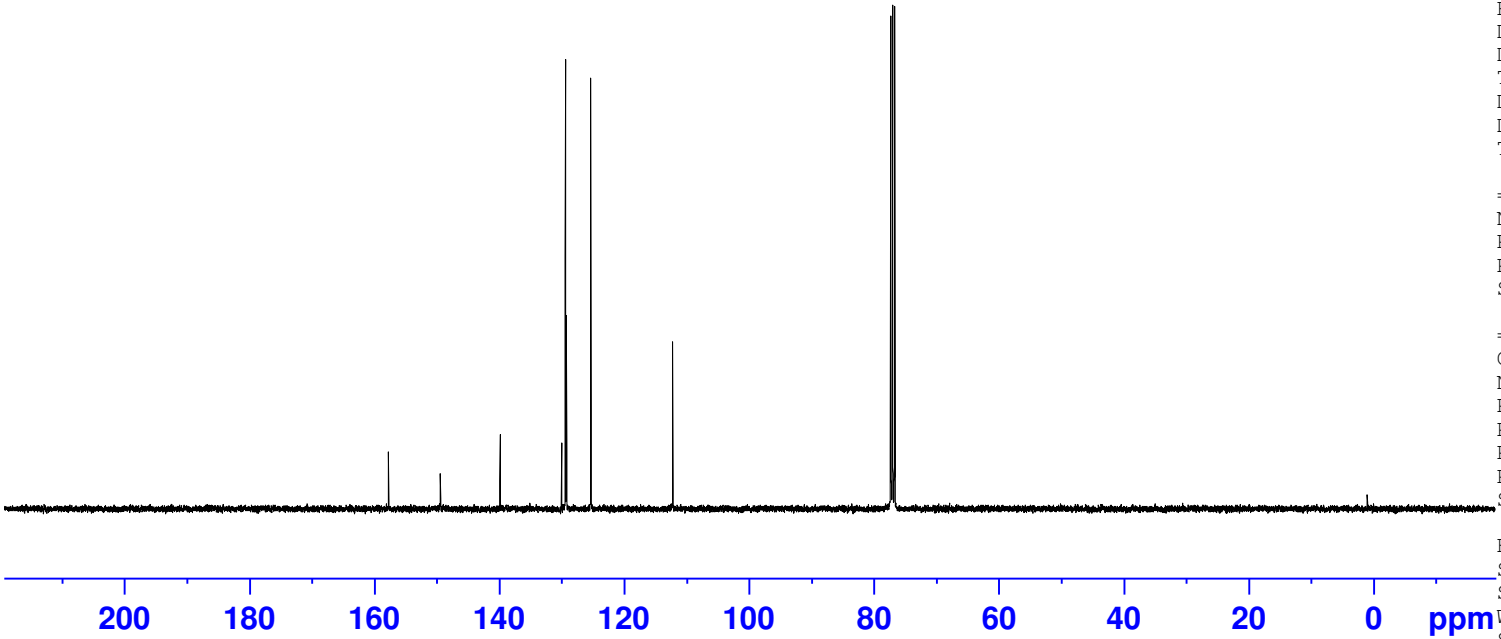

```
Current Data Parameters
NAME       20231005-400m
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231004
Time               22.22
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     6
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9845889 sec
RG                140.02
DW                60.800 usec
DE                 6.50 usec
TE                291.3 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 9.90 usec
PLW1        23.00000000 W
SFO1        400.1924713 MHz

F2 - Processing parameters
SI                 65536
SF          400.1900139 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```

zhl-5-93



2m'

157.75
149.44
139.89
130.02
129.43
129.24
125.34
112.24
77.31
77.00
76.68



Current Data Parameters
NAME 20231005-400m
EXPNO 3
PROCNO 1

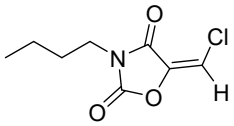
F2 - Acquisition Parameters
Date_ 20231004
Time 22.41
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 44.2
DW 20.800 usec
DE 6.50 usec
TE 292.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

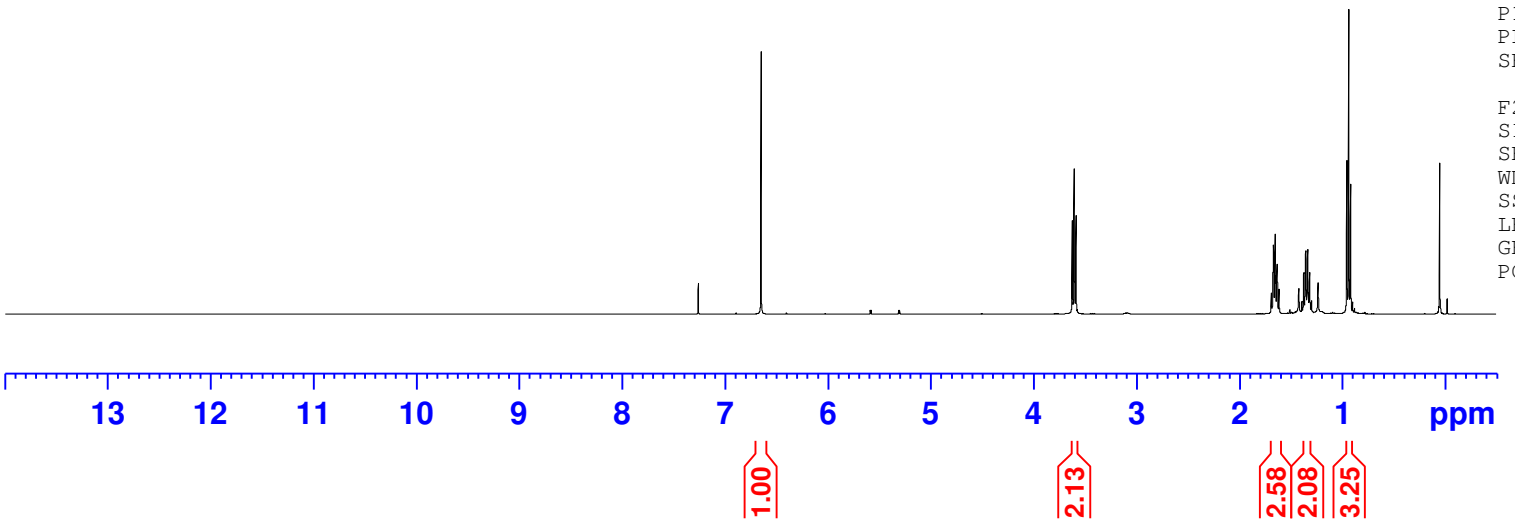
F2 - Processing parameters
SI 32768
SF 100.6278645 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-5-75



2n'

7.260
6.649
3.624
3.606
3.588
1.688
1.667
1.655
1.651
1.645
1.632
1.613
1.421
1.373
1.354
1.334
1.316
1.232
0.954
0.936
0.918



Current Data Parameters
NAME 20231005-400m
EXPNO 8
PROCNO 1

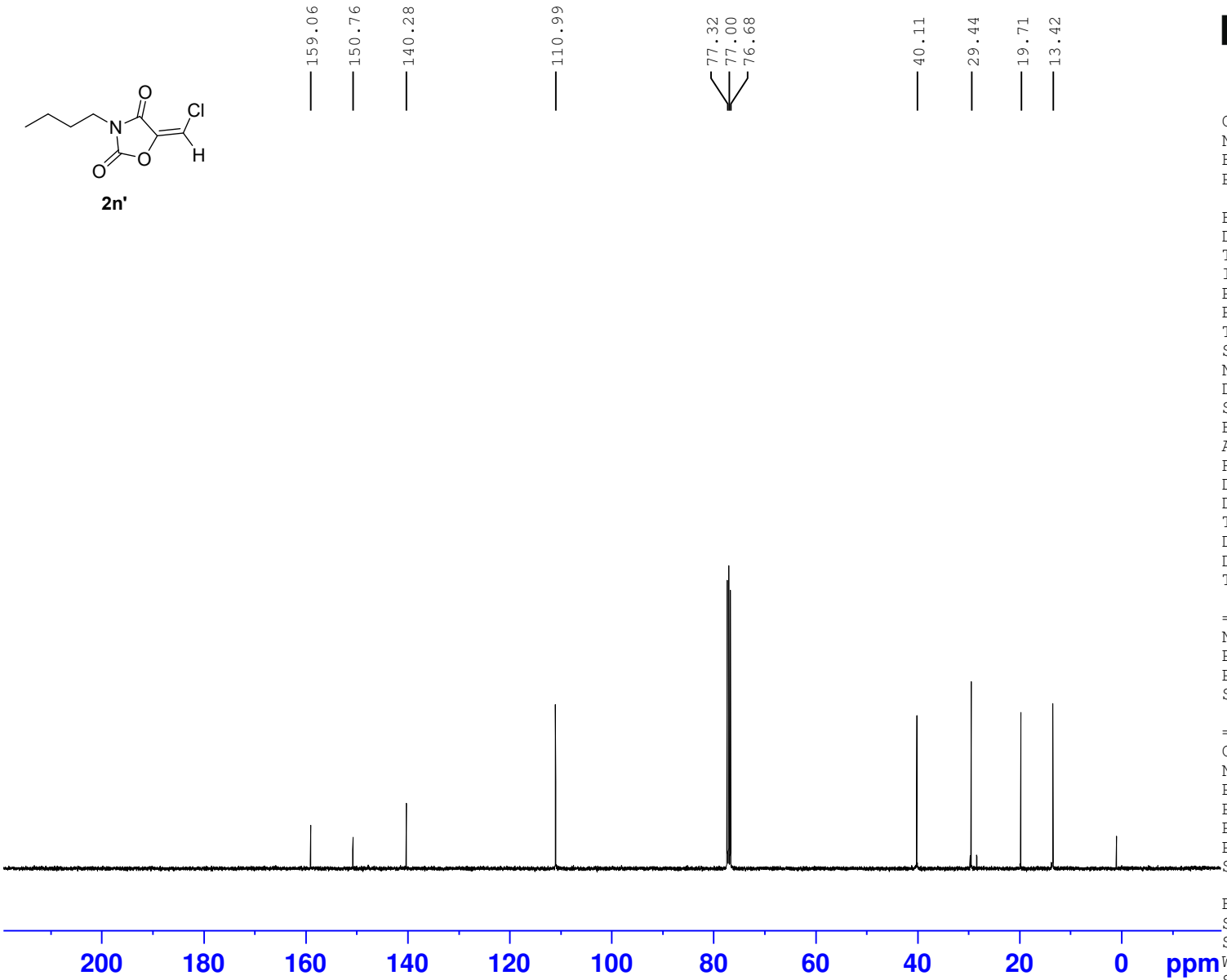
F2 - Acquisition Parameters
Date_ 20231005
Time 0.13
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 75.43
DW 60.800 usec
DE 6.50 usec
TE 291.4 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900138 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-5-75

2n'



Current Data Parameters
NAME 20231005-400m
EXPNO 9
PROCNO 1

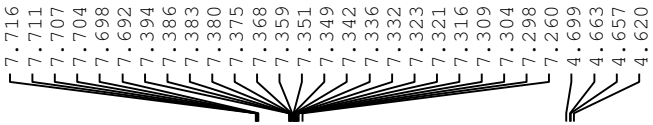
F2 - Acquisition Parameters
Date_ 20231005
Time 0.31
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 44.2
DW 20.800 usec
DE 6.50 usec
TE 291.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

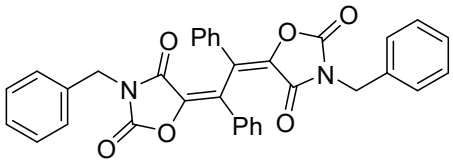
======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

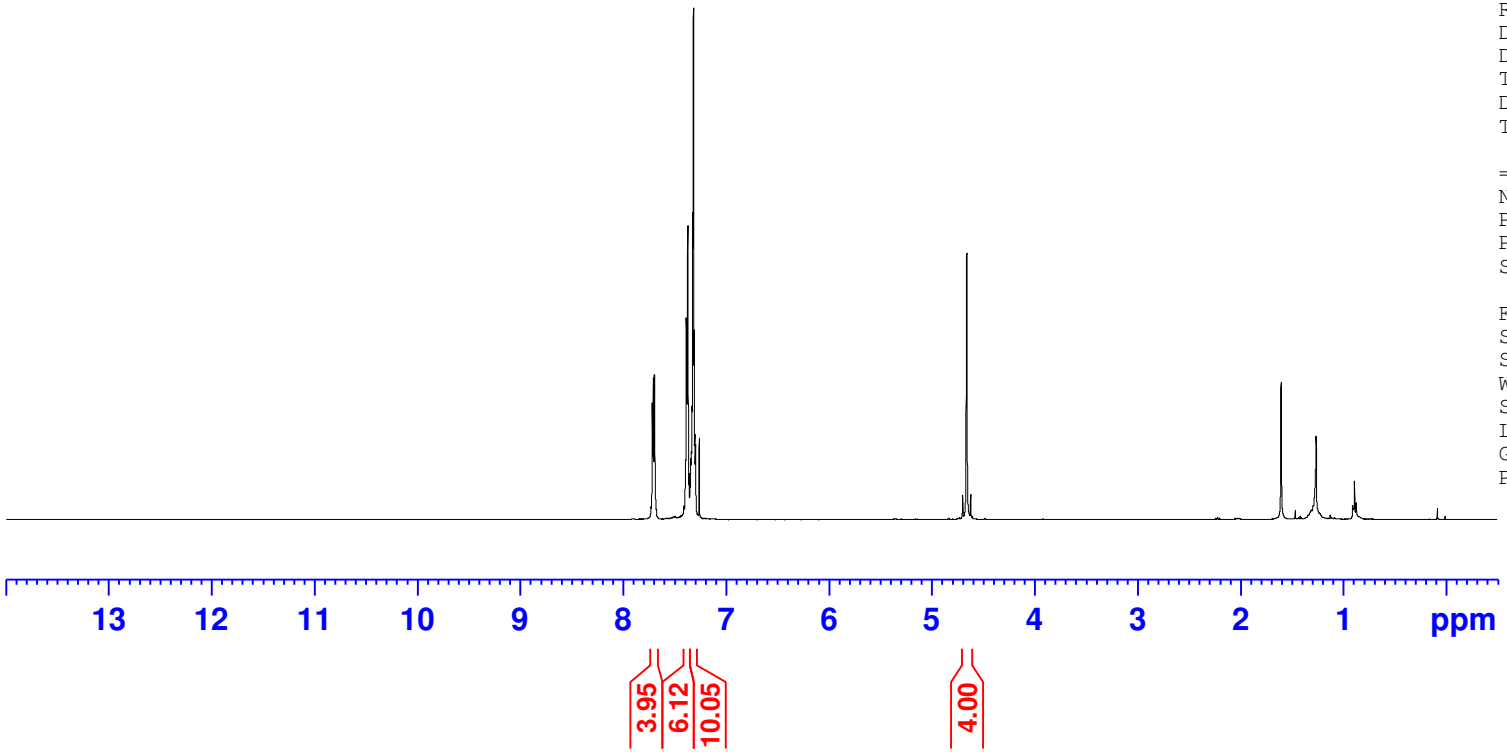
F2 - Processing parameters
SI 32768
SF 100.6278638 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZHL-3d-35B





3a



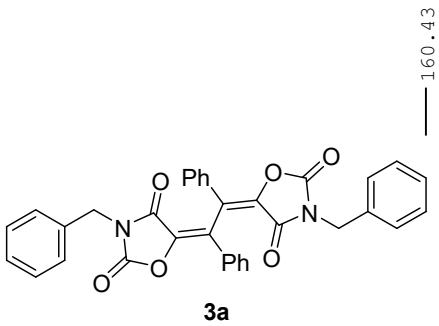
Current Data Parameters
NAME 20230627-400m
EXPNO 32
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230627
Time 6.24
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 125.76
DW 60.800 usec
DE 6.50 usec
TE 292.5 K
D1 1.00000000 sec
TD0 1

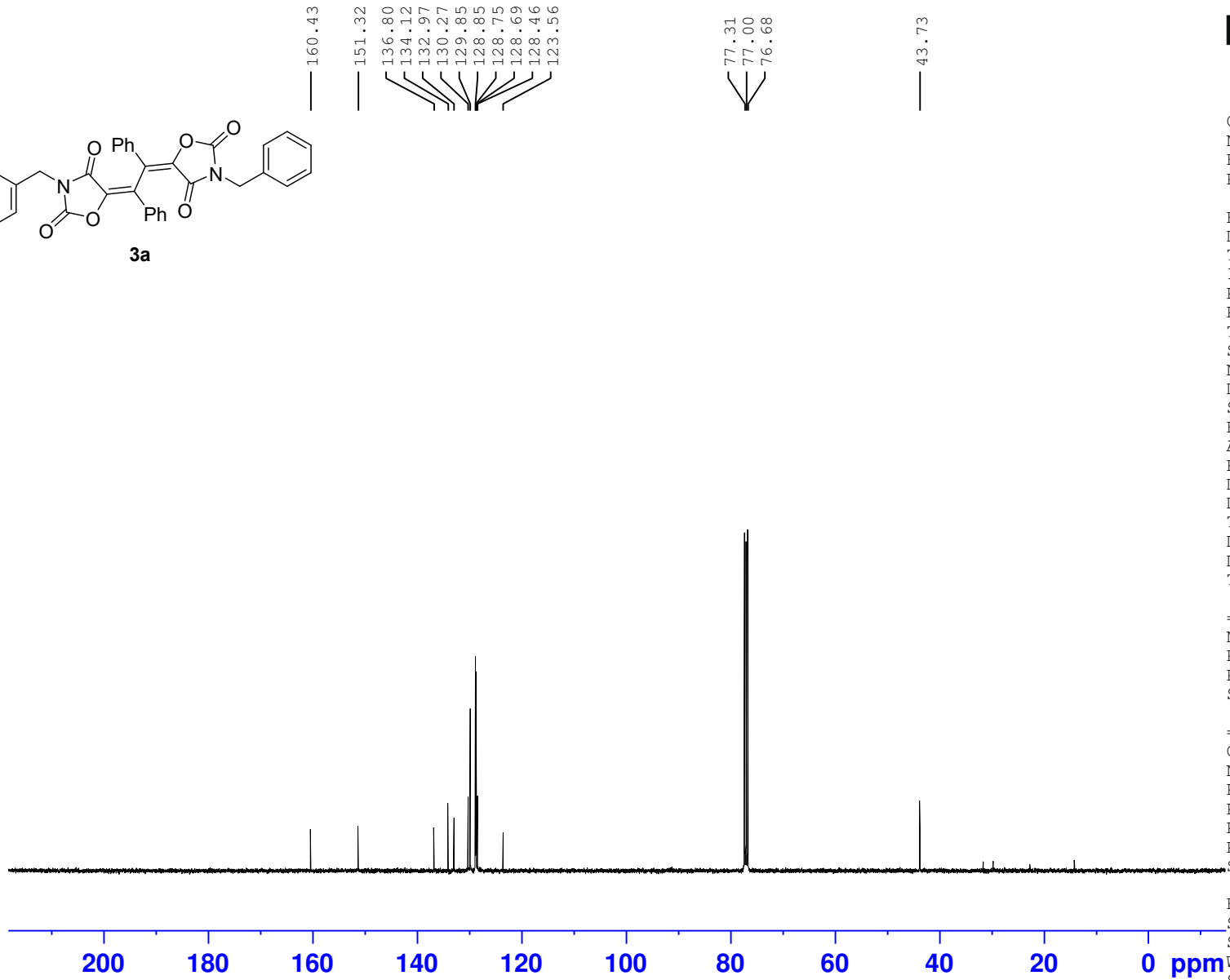
======== CHANNEL f1 ========
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900140 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZHL-3d-35B



3a



BRUKER

Current Data Parameters
NAME 20230627-400m
EXPNO 33
PROCNO 1

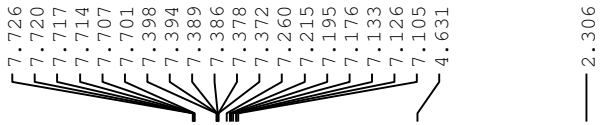
F2 - Acquisition Parameters
Date_ 20230627
Time 6.48
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 29.75
DW 20.800 usec
DE 6.50 usec
TE 292.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

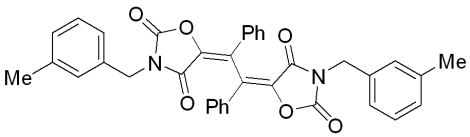
======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

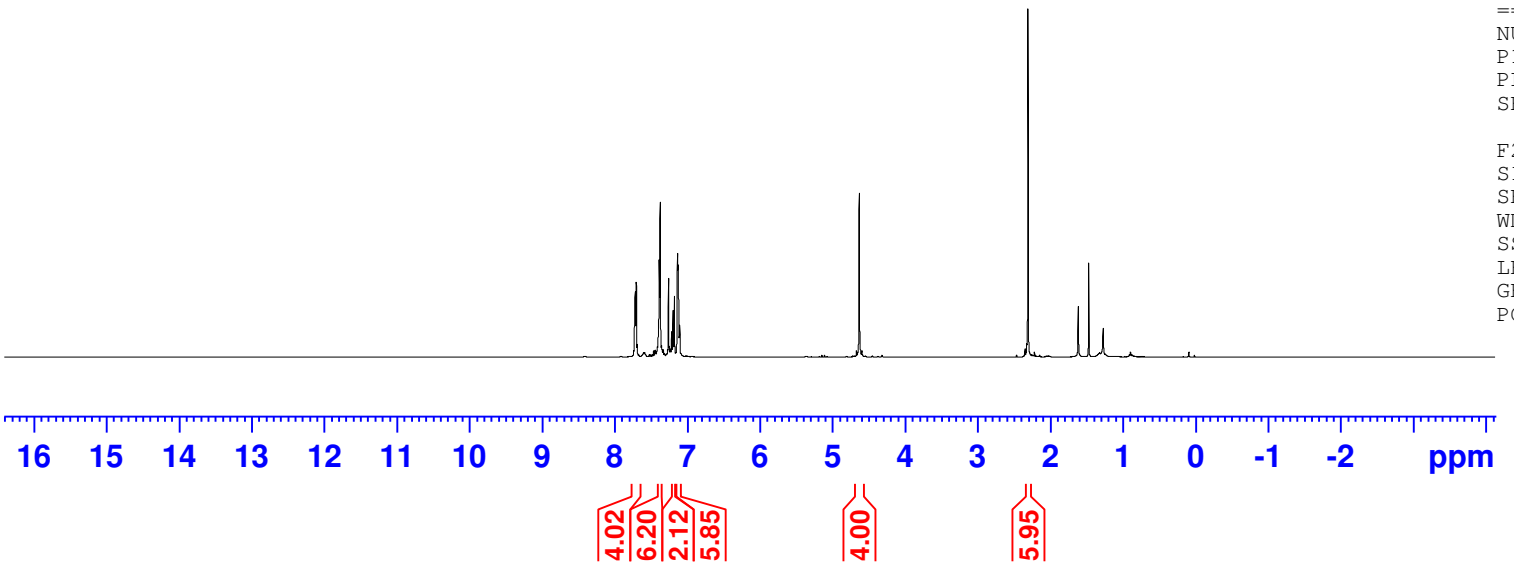
F2 - Processing parameters
SI 32768
SF 100.6278635 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

ZHL-4-56A





3b



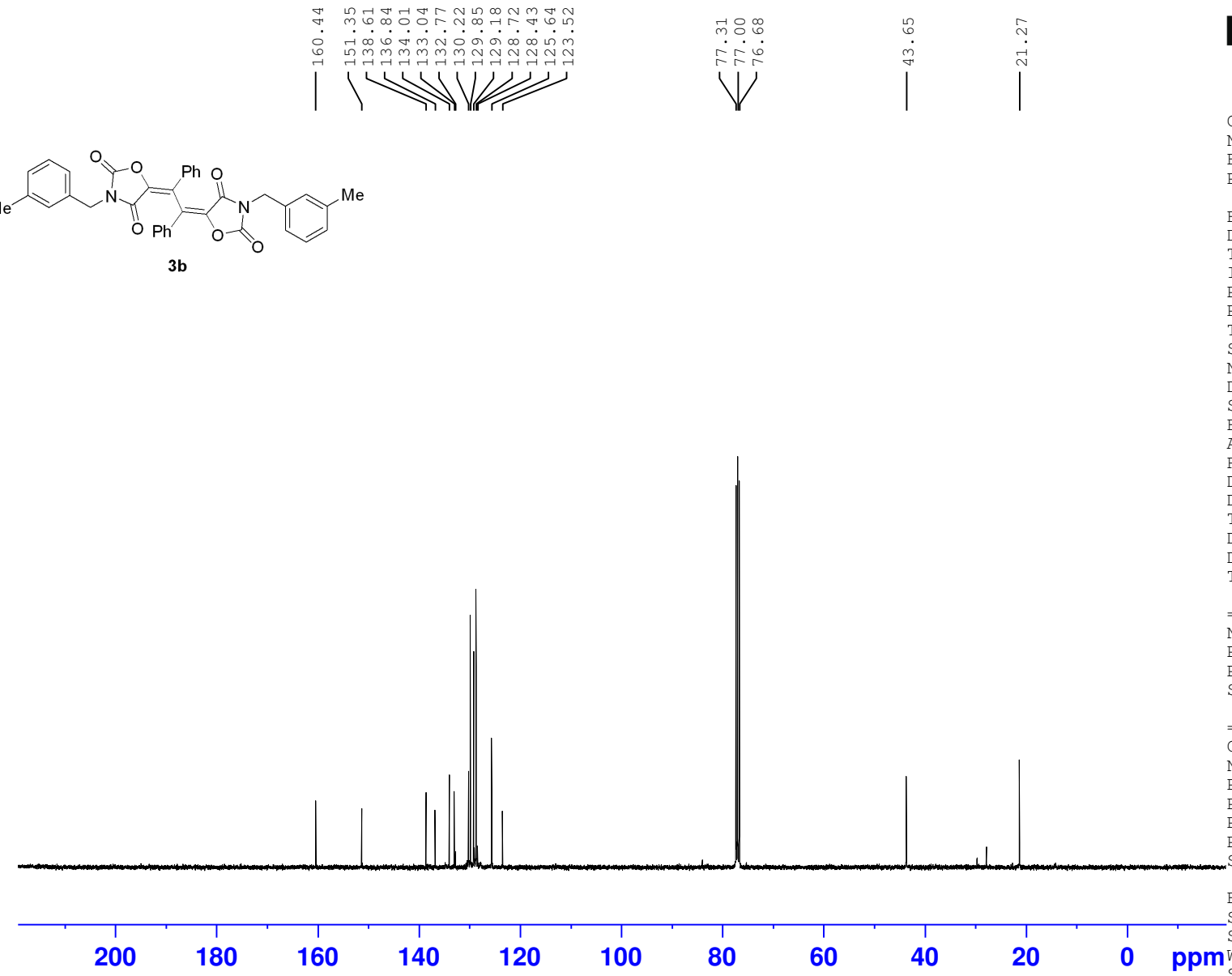
Current Data Parameters
NAME 20230627-400m
EXPNO 35
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230627
Time 7.23
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 90.23
DW 60.800 usec
DE 6.50 usec
TE 292.3 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900140 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZHL-4-56A



Current Data Parameters
NAME 20230627-400m
EXPNO 36
PROCNO 1

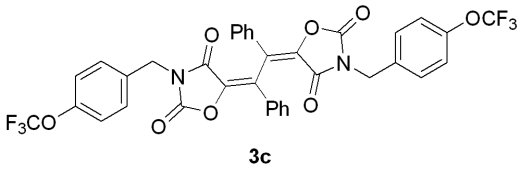
F2 - Acquisition Parameters
Date_ 20230627
Time 7.47
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 29.75
DW 20.800 usec
DE 6.50 usec
TE 292.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

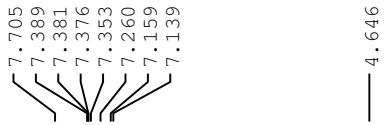
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

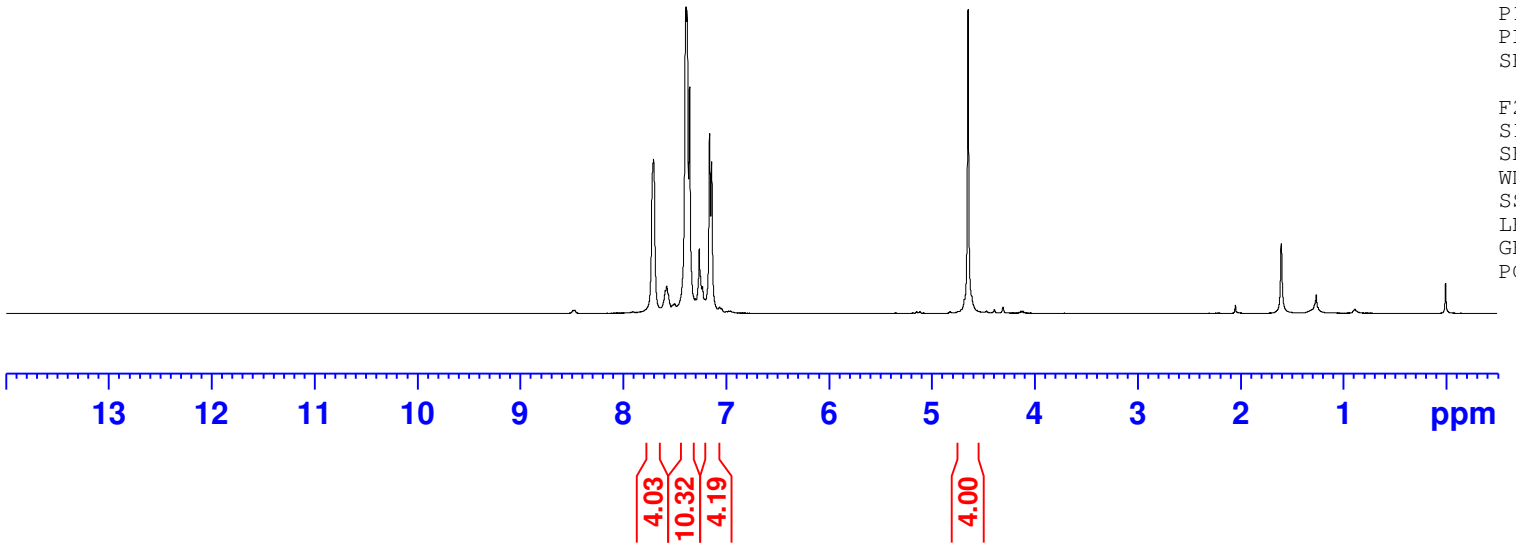
F2 - Processing parameters
SI 32768
SF 100.6278653 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-3-51a



3c





Current Data Parameters
NAME 20230628-400M
EXPNO 13
PROCNO 1

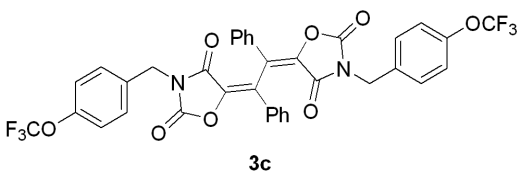
F2 - Acquisition Parameters
Date_ 20230627
Time 22.05
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 100.49
DW 60.800 usec
DE 6.50 usec
TE 291.6 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

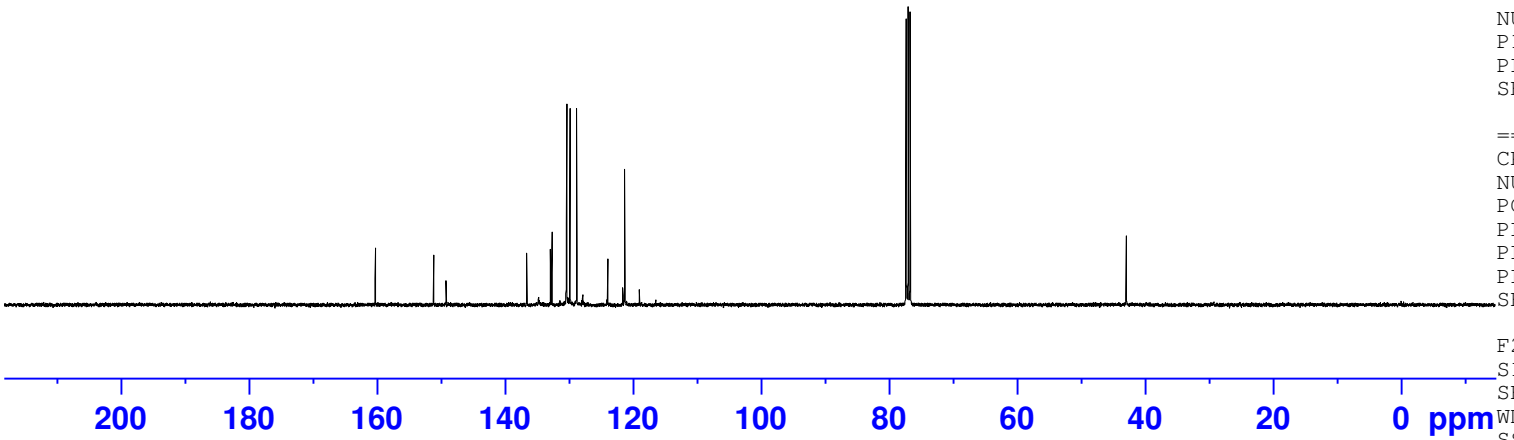
F2 - Processing parameters
SI 65536
SF 400.1900140 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-51a

160.31
151.17
149.25
136.61
132.90
132.69
130.45
130.37
129.86
128.80
123.96
121.58
121.31
119.03
77.31
77.00
76.68
42.90



3c



Current Data Parameters
NAME 20230629-400m
EXPNO 47
PROCNO 1

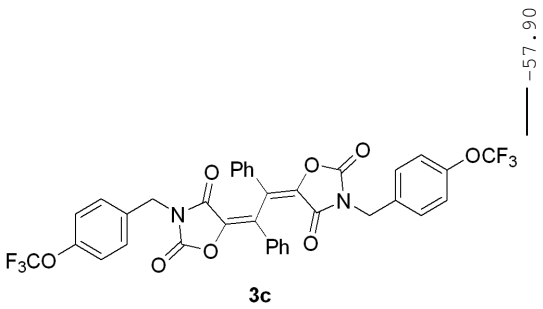
F2 - Acquisition Parameters
Date_ 20230629
Time 5.02
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 35.06
DW 20.800 usec
DE 6.50 usec
TE 291.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

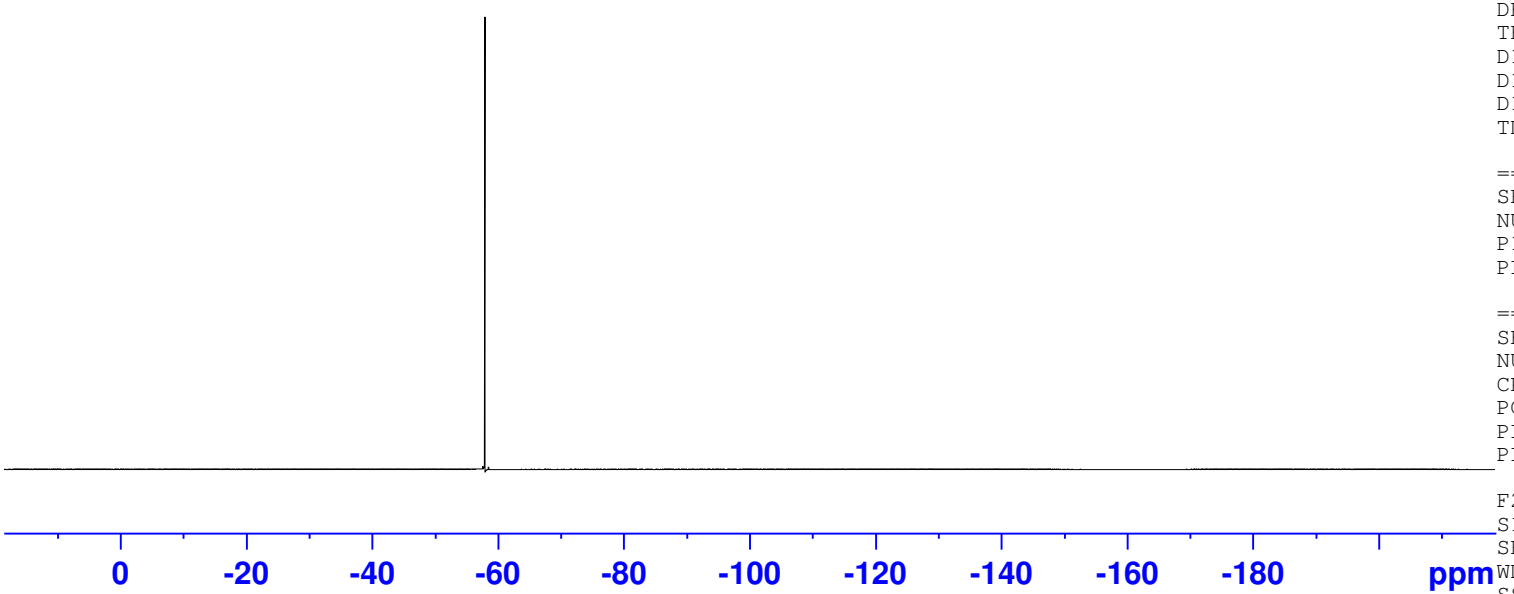
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278637 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-4-51a



3c



Current Data Parameters
NAME 20230706-300M
EXPNO 239
PROCNO 1

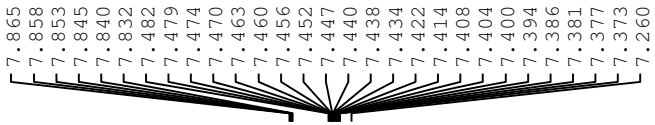
F2 - Acquisition Parameters
Date_ 20230706
Time 11.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn.2
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 0.510897 Hz
AQ 0.9786710 sec
RG 203
DW 7.467 usec
DE 6.50 usec
TE 297.8 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

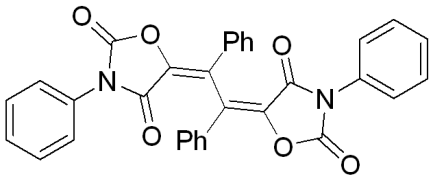
======== CHANNEL f1 ========
SFO1 282.3761148 MHz
NUC1 19F
P1 14.50 usec
PLW1 10.39999962 W

======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W

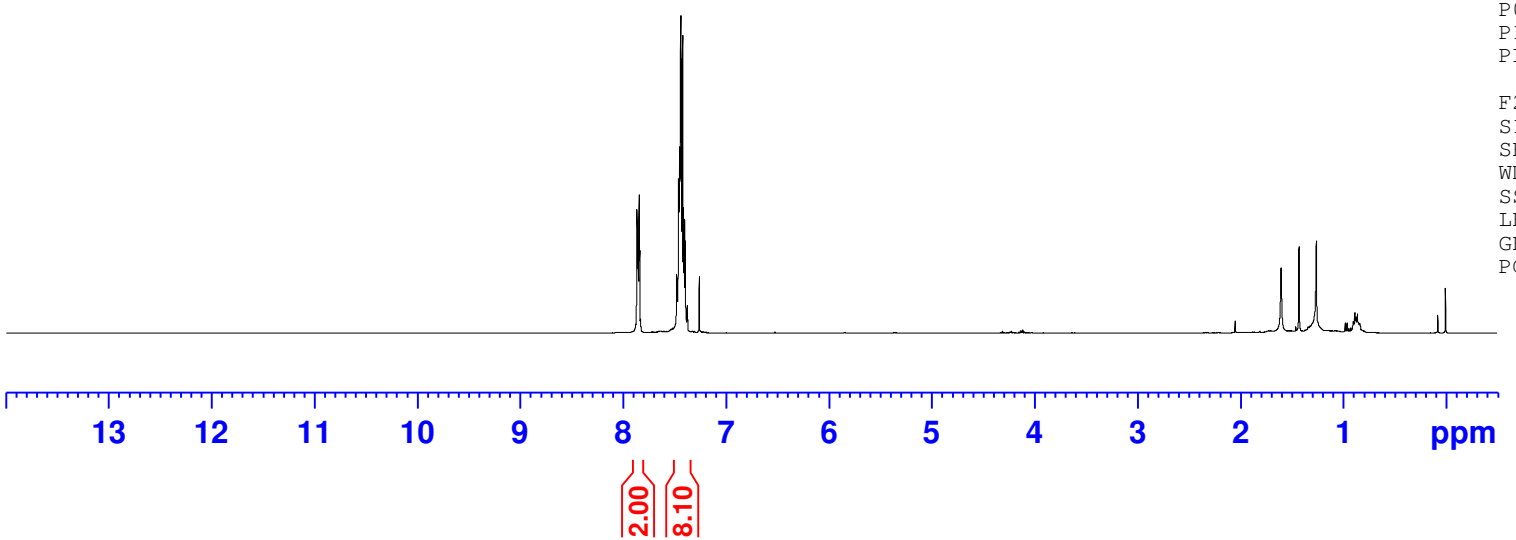
F2 - Processing parameters
SI 65536
SF 282.4043552 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-1-62





3d



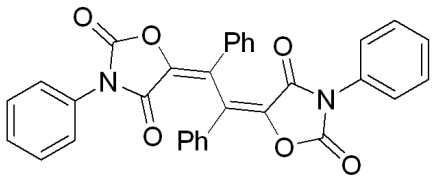
Current Data Parameters
NAME zhl-1-62a
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220830
Time 20.58 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 13.54 usec
TE 291.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 20.73200035 W

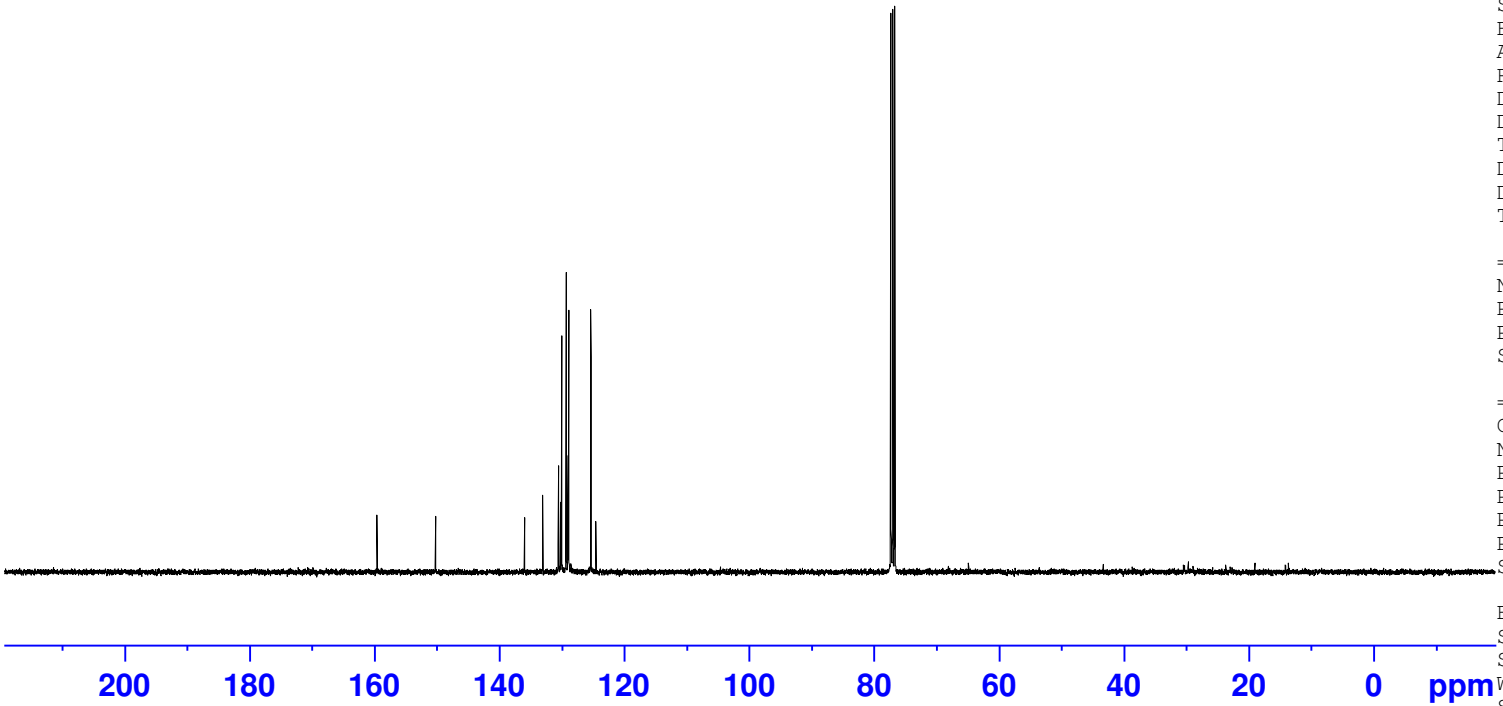
F2 - Processing parameters
SI 65536
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZHL-3-37b

159.61
150.24
135.97
133.07
130.56
130.21
130.03
129.29
129.02
128.89
125.35
124.57
77.32
77.00
76.68



3d



Current Data Parameters
NAME 20230726-400M
EXPNO 2
PROCNO 1

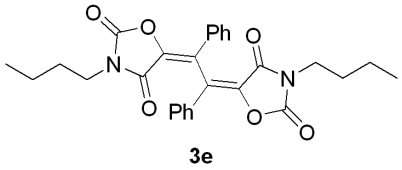
F2 - Acquisition Parameters
Date_ 20230725
Time 21.54
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 600
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 37.77
DW 20.800 usec
DE 6.50 usec
TE 292.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

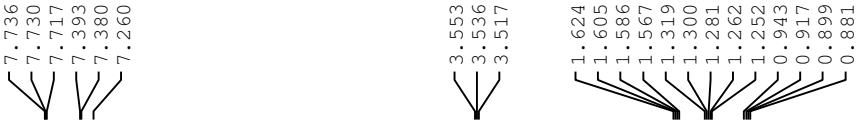
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

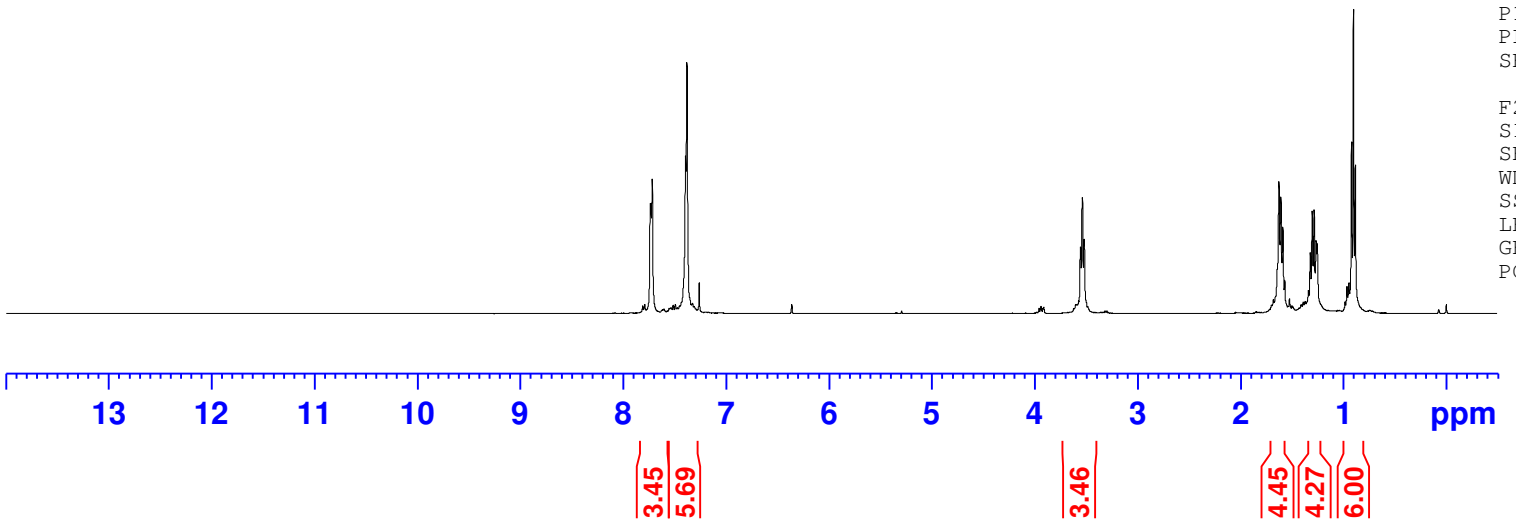
F2 - Processing parameters
SI 32768
SF 100.6278633 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-4-27b



3e

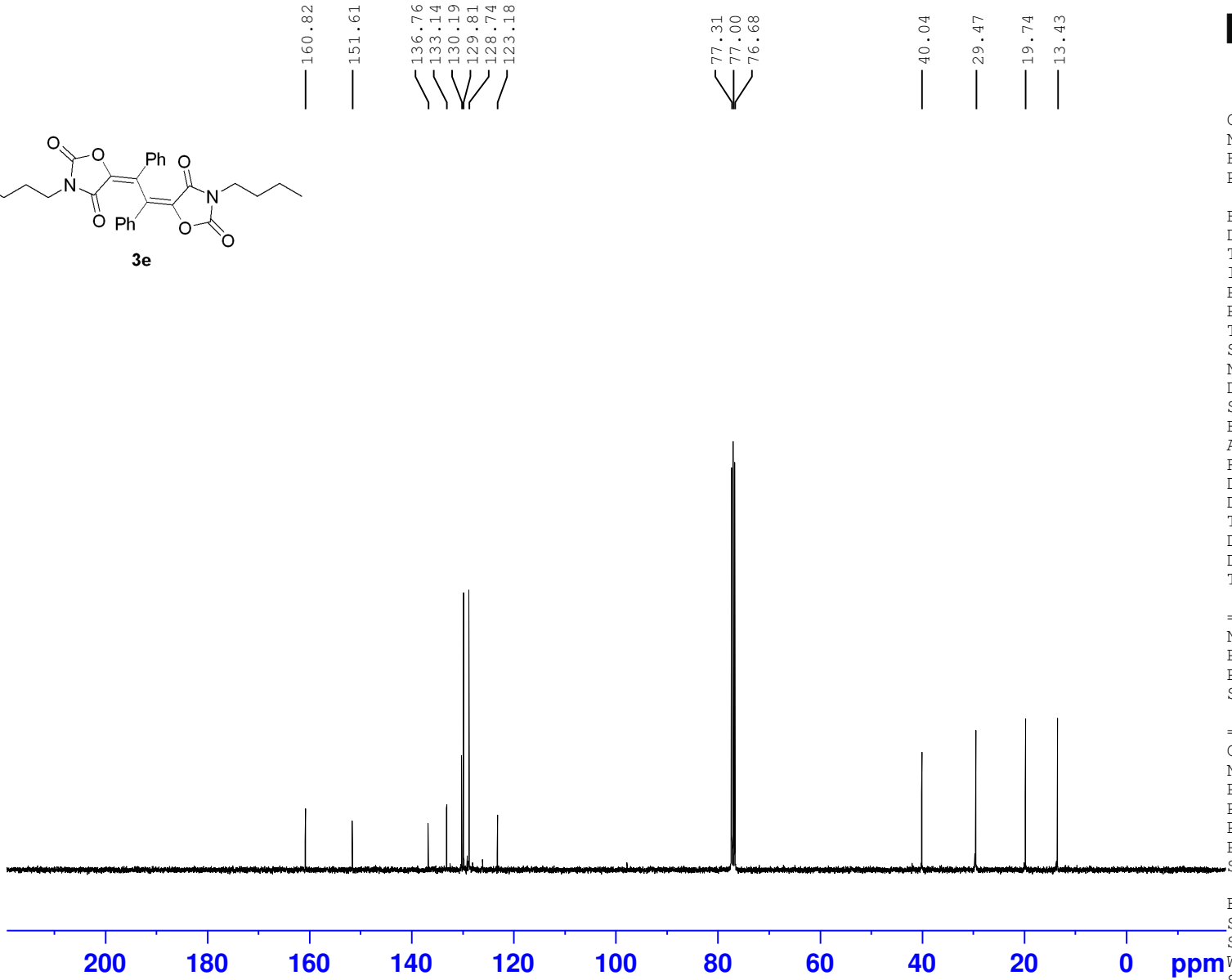





```
Current Data Parameters
NAME       20230602-400m
EXPNO                 19
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230601
Time                5.17
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     6
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9845889 sec
RG                 113.67
DW                 60.800 usec
DE                  6.50 usec
TE                 293.2 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.68 usec
PLW1         14.00000000 W
SFO1         400.1924713 MHz

F2 - Processing parameters
SI                 65536
SF           400.1900171 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

zhl-4-27b

3e



Current Data Parameters
NAME 20230602-400m
EXPNO 20
PROCNO 1

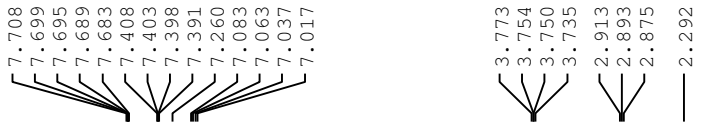
F2 - Acquisition Parameters
Date_ 20230601
Time 5.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 293.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

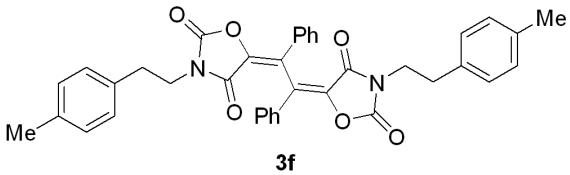
======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

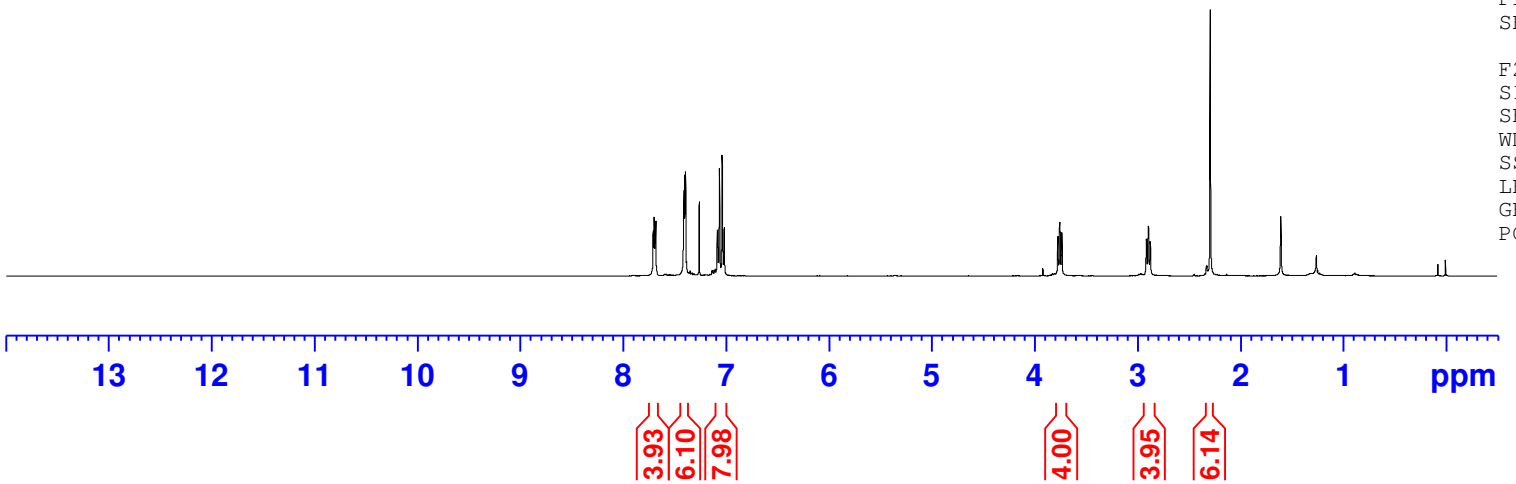
F2 - Processing parameters
SI 32768
SF 100.6278631 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-4-38b



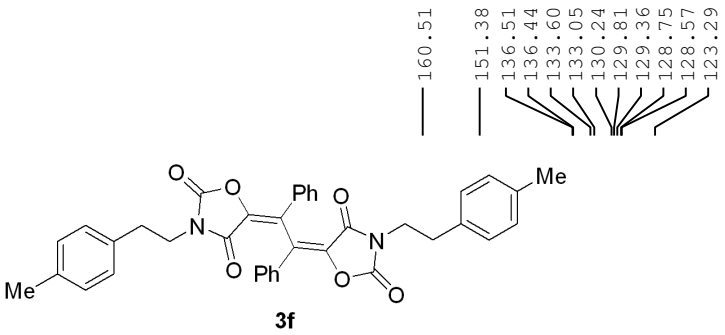


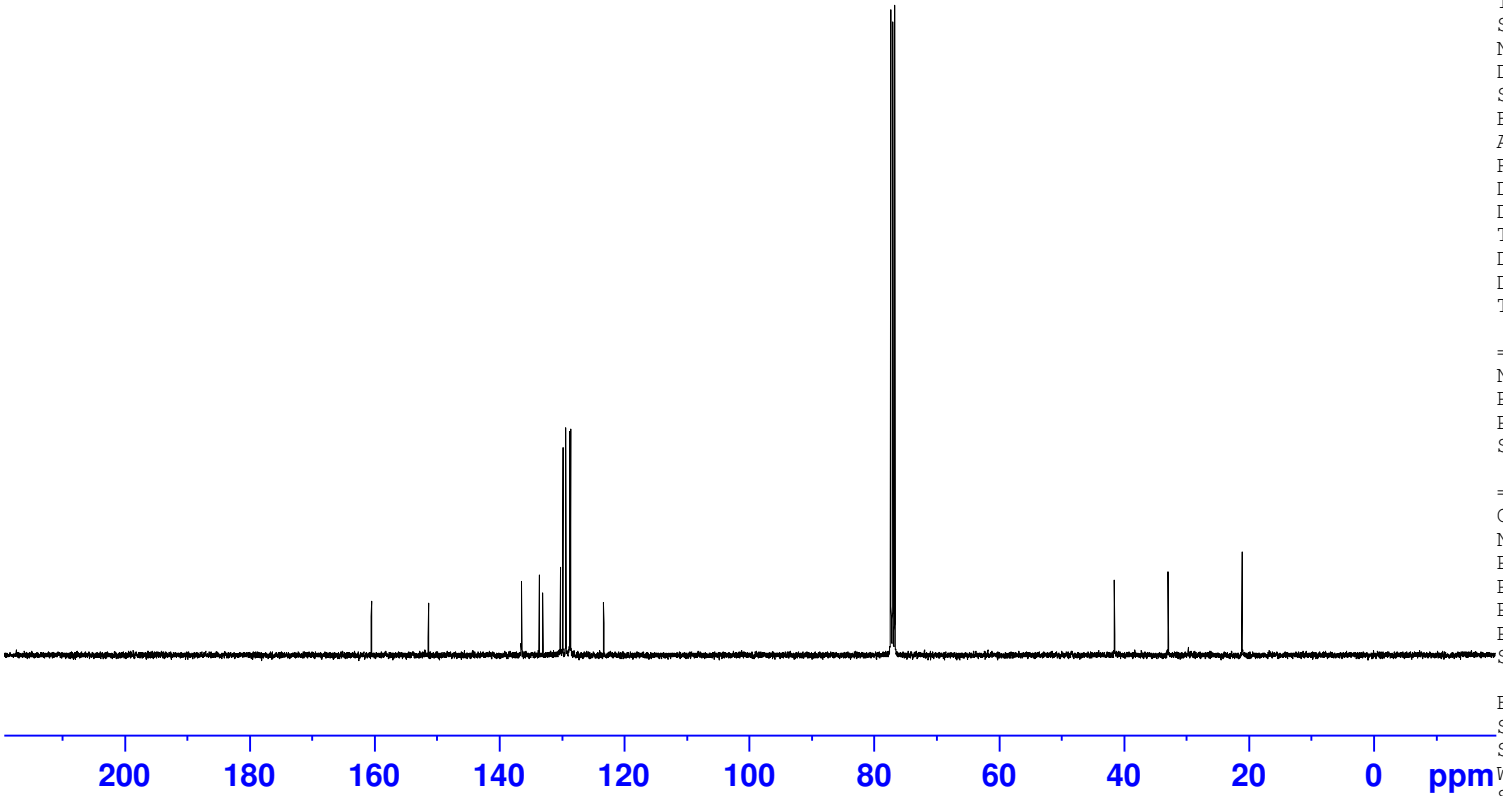
3f




```
Current Data Parameters
NAME       20230630-400M
EXPNO                 41
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230630
Time                2.06
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     6
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9845889 sec
RG                 113.67
DW                 60.800 usec
DE                  6.50 usec
TE                 291.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  9.90 usec
PLW1         23.00000000 W
SFO1         400.1924713 MHz

F2 - Processing parameters
SI                 65536
SF           400.1900139 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

zhl-4-38b





Current Data Parameters
NAME 20230630-400M
EXPNO 42
PROCNO 1

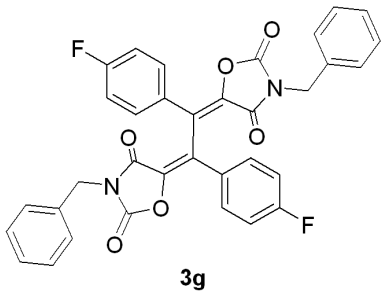
F2 - Acquisition Parameters
Date_ 20230630
Time 2.36
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 29.75
DW 20.800 usec
DE 6.50 usec
TE 291.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

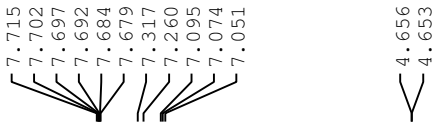
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

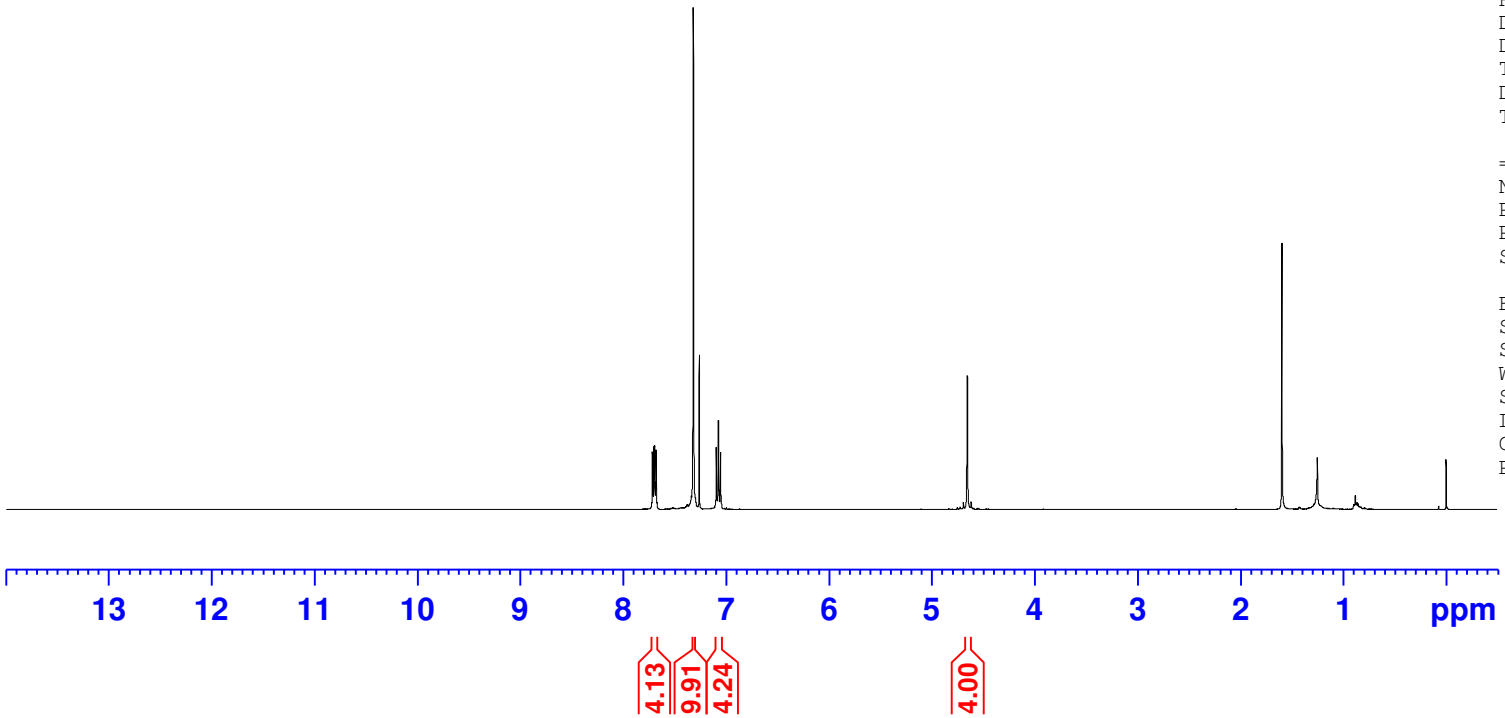
F2 - Processing parameters
SI 32768
SF 100.6278635 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-4-67b



3g





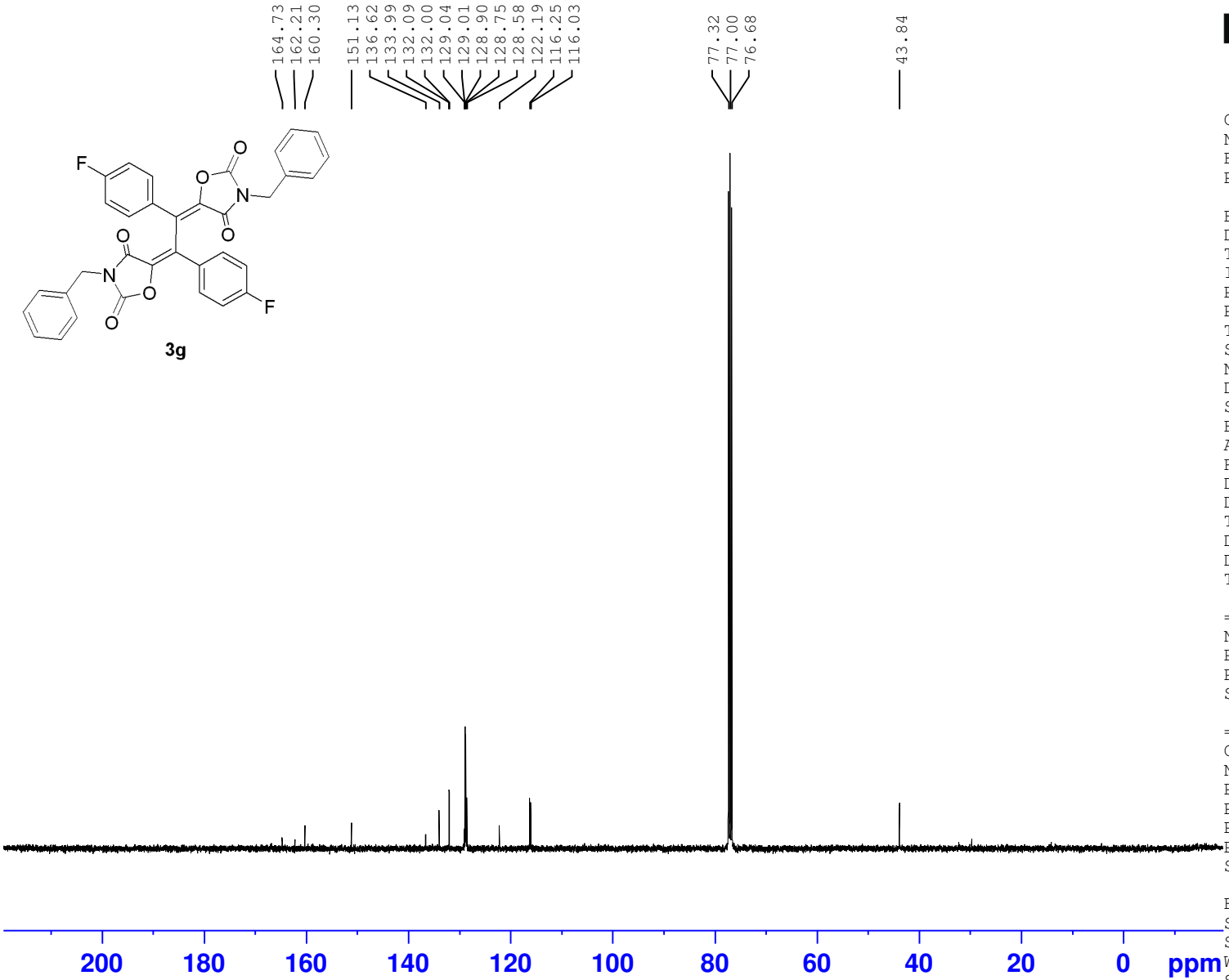
Current Data Parameters
NAME 20230630-400M
EXPNO 43
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230630
Time 2.39
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 181.41
DW 60.800 usec
DE 6.50 usec
TE 291.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 9.90 usec
PLW1 23.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900140 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-4-67b



Current Data Parameters
NAME 20230630-400M
EXPNO 44
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230630
Time 3.09
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 29.75
DW 20.800 usec
DE 6.50 usec
TE 291.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.80 usec
PLW1 47.40000153 W
SFO1 100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 23.00000000 W
PLW12 0.30712000 W
PLW13 0.24877000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278616 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-4-17b

3g

Current Data Parameters
NAME 20230707-300m
EXPNO 252
PROCNO 1

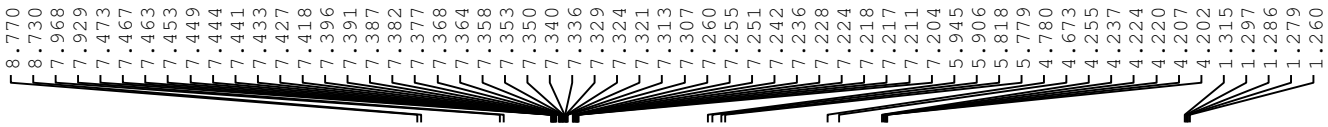
F2 - Acquisition Parameters
Date_ 20230707
Time 11.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn.2
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 66964.289 Hz
FIDRES 0.510897 Hz
AQ 0.9786710 sec
RG 203
DW 7.467 usec
DE 6.50 usec
TE 297.5 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

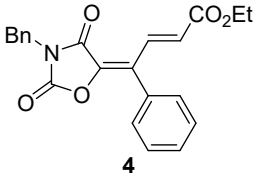
======== CHANNEL f1 ========
SFO1 282.3761148 MHz
NUC1 19F
P1 14.50 usec
PLW1 10.39999962 W

======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W

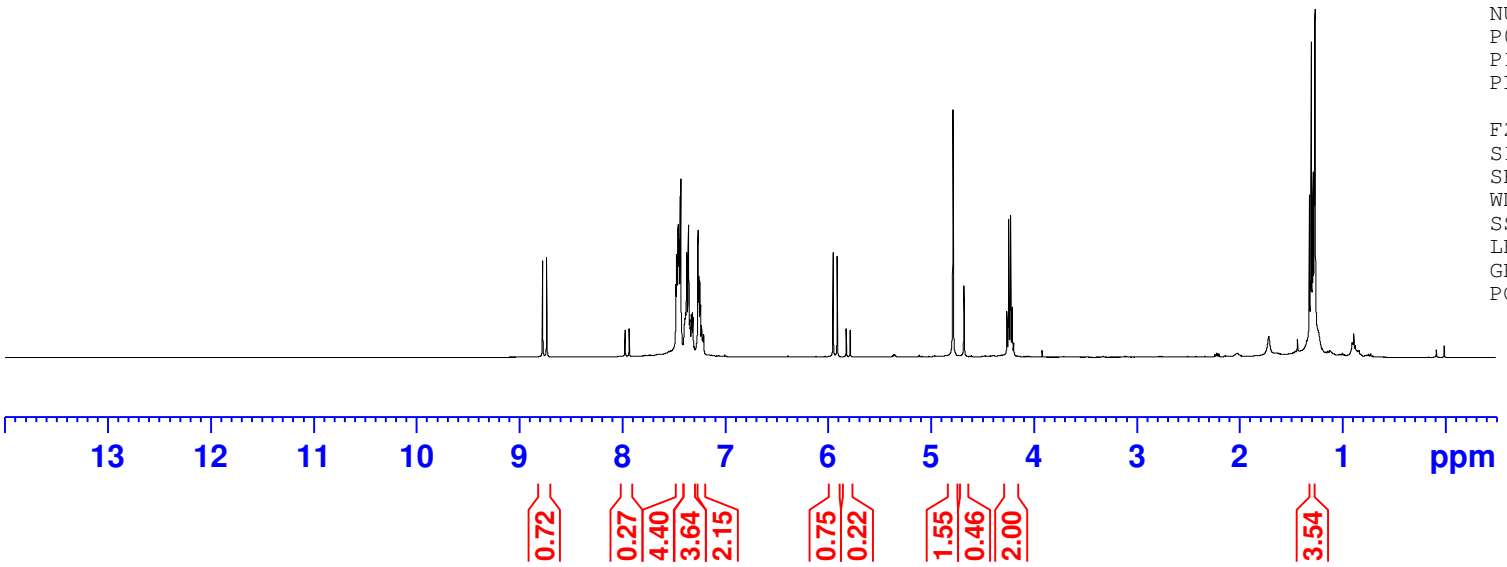
F2 - Processing parameters
SI 65536
SF 282.4043552 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ZHL-4-13 B



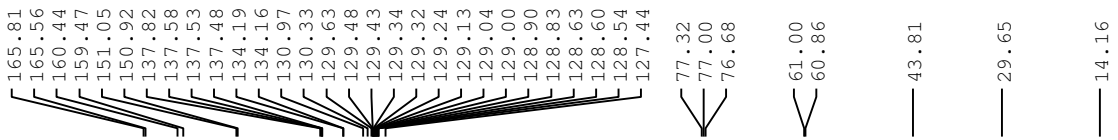


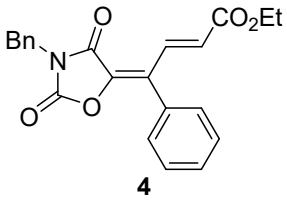
4



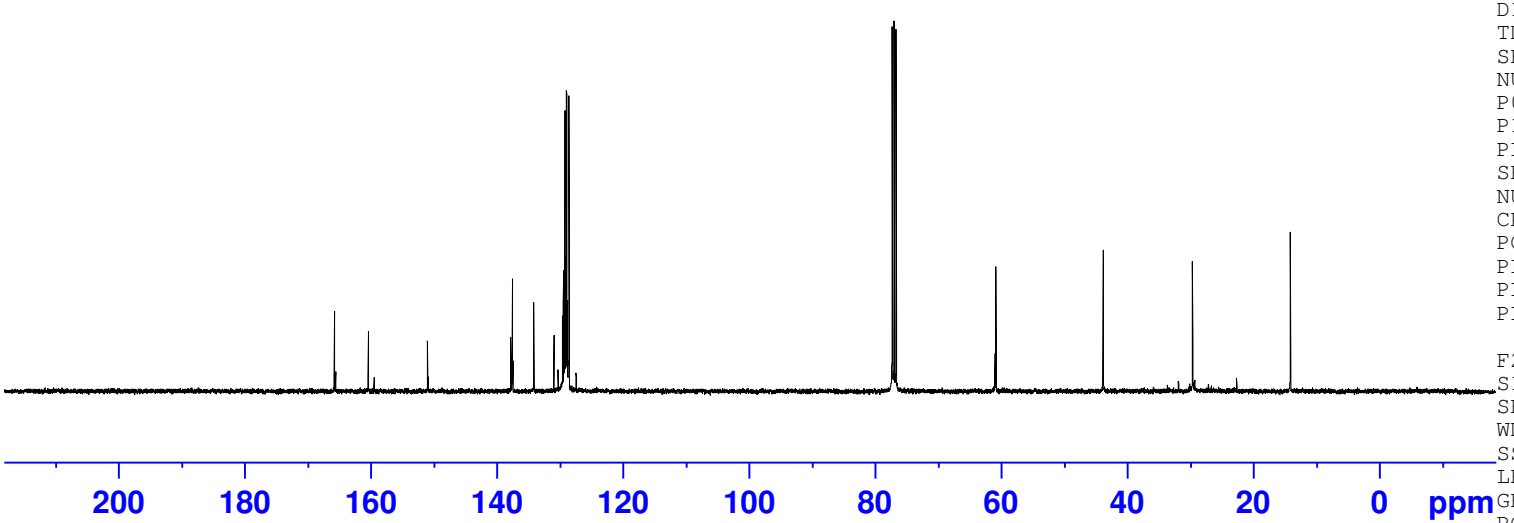

```
Current Data Parameters
NAME                  0729HH
EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_              20230730
Time                   1.19 h
INSTRUM              Avance
PROBHD    Z116098_0833 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8196.722 Hz
FIDRES             0.250144 Hz
AQ                3.9976959 sec
RG                   76.5931
DW                   61.000 usec
DE                    13.54 usec
TE                    294.7 K
D1              1.00000000 sec
TD0                       1
SFO1           400.1324708 MHz
NUC1                    1H
P0                    3.33 usec
P1                   10.00 usec
PLW1           20.73200035 W

F2 - Processing parameters
SI                    65536
SF             400.1300101 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

ZHL-4-13 B



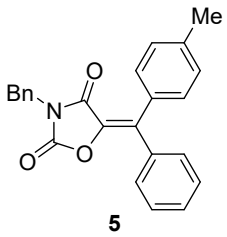


4

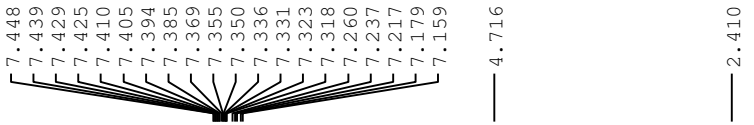


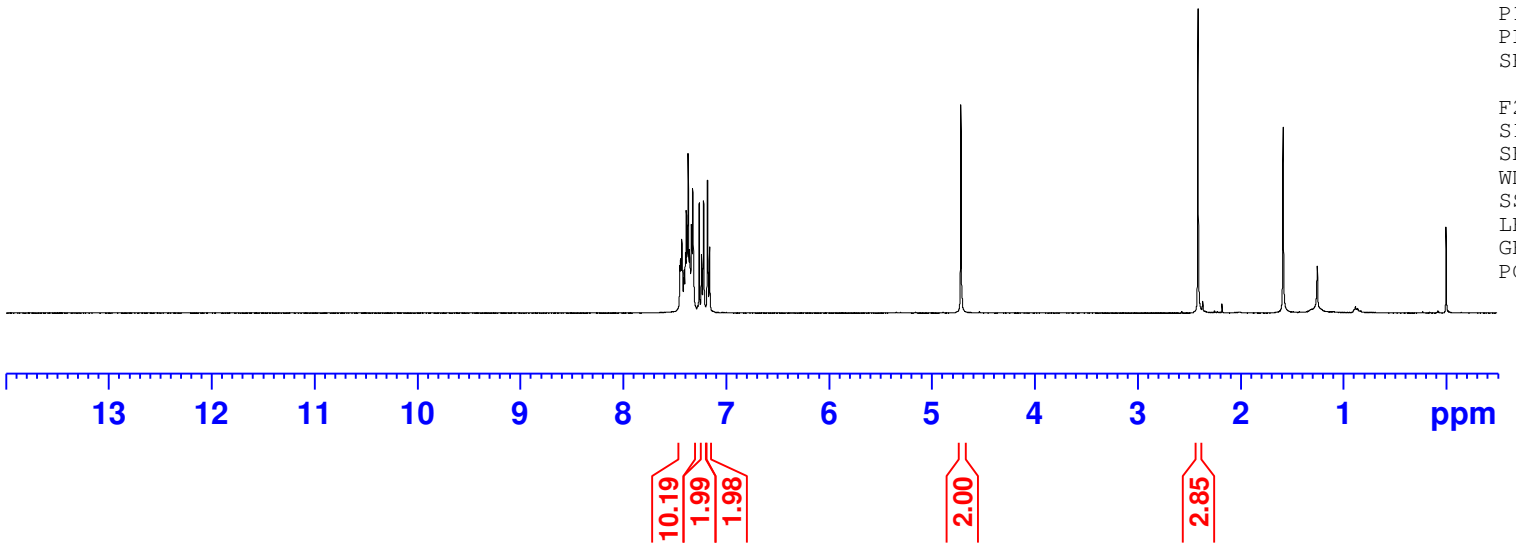

```
Current Data Parameters
NAME                  0729HH
EXPNO                      4
PROCNO                     1

F2 - Acquisition Parameters
Date_              20230730
Time                   2.19 h
INSTRUM              Avance
PROBHD    Z116098_0833 (
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH              23809.523 Hz
FIDRES            0.726609 Hz
AQ                1.3762560 sec
RG                  46.0295
DW                  21.000 usec
DE                   6.50 usec
TE                   295.3 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1
SFO1           100.6228298 MHz
NUC1                    13C
P0                   3.33 usec
P1                  10.00 usec
PLW1           87.89900208 W
SFO2           400.1316005 MHz
NUC2                    1H
CPDPRG[2          waltz65
PCPD2                90.00 usec
PLW2           20.73200035 W
PLW12           0.25595000 W
PLW13           0.12874000 W

F2 - Processing parameters
SI                    32768
SF             100.6127766 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

zhl-3-90



5





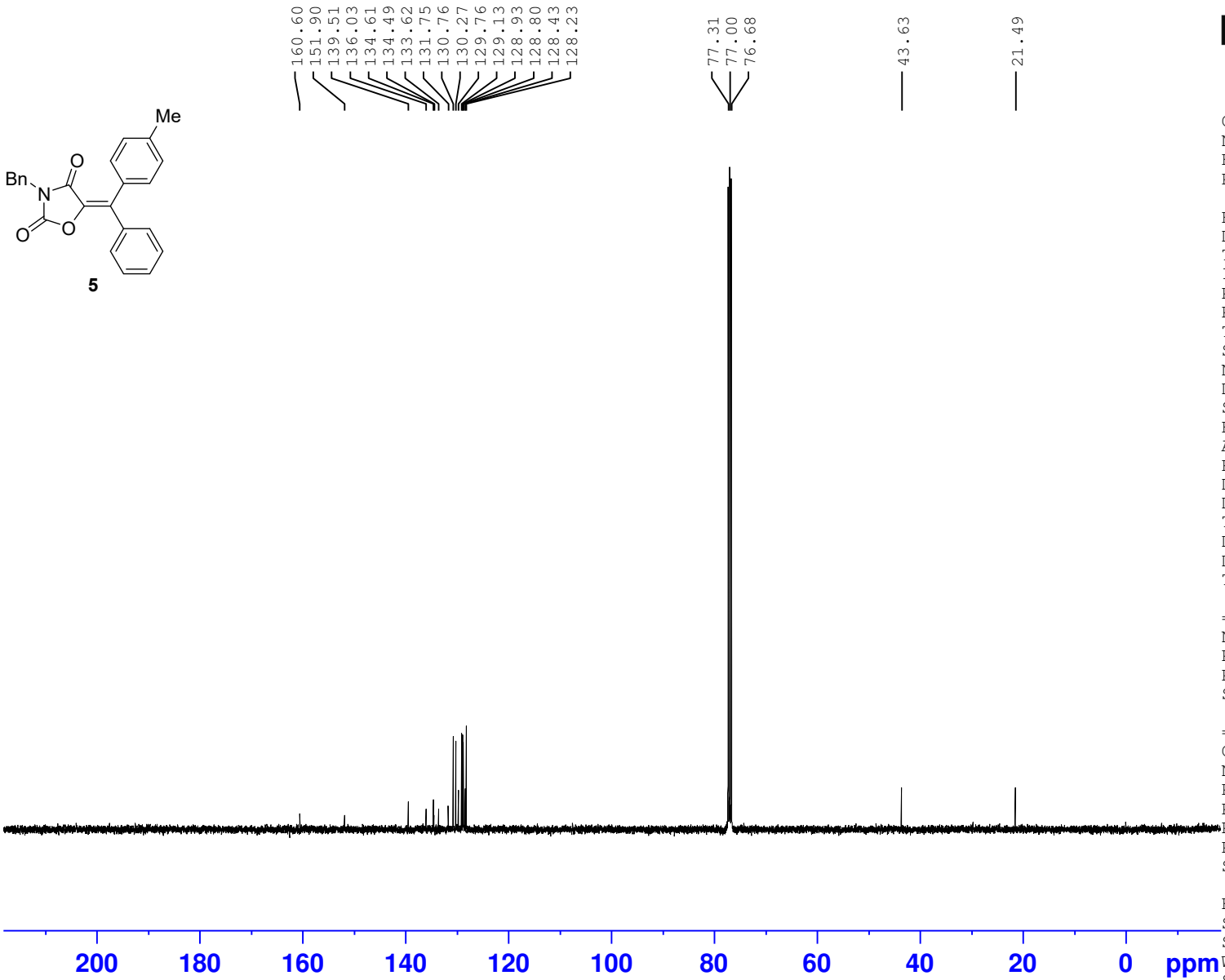
Current Data Parameters
NAME 202305-21
EXPNO 19
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230520
Time 23.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 193.13
DW 60.800 usec
DE 6.50 usec
TE 288.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

F2 - Processing parameters
SI 65536
SF 400.1900164 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-90



Current Data Parameters
NAME 202305-21
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230521
Time 0.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 289.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

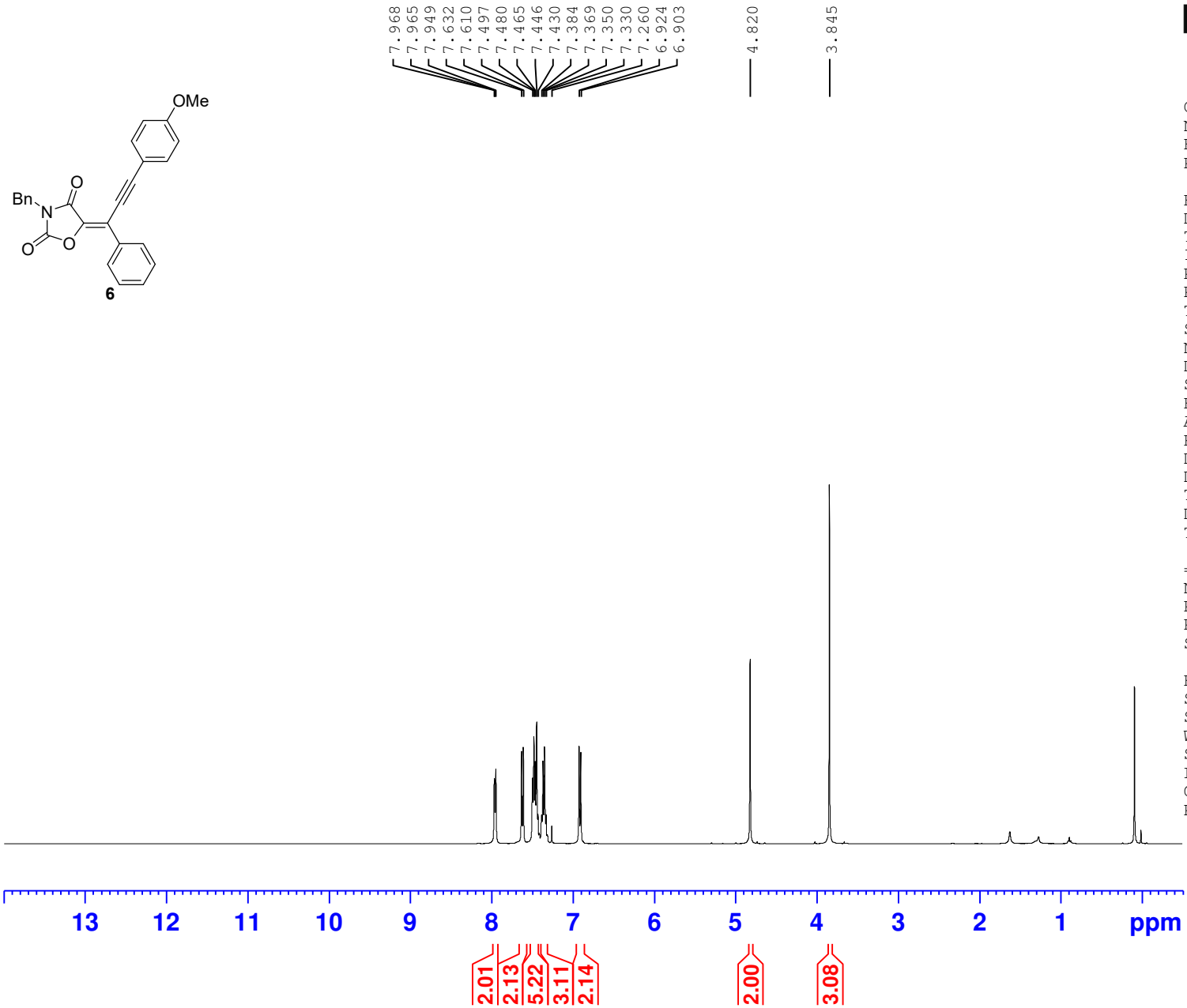
======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278630 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

zhl-3-96

6



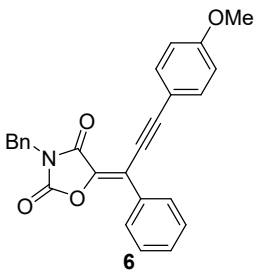
Current Data Parameters
NAME 20230524-400m
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230524
Time 1.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 100.49
DW 60.800 usec
DE 6.50 usec
TE 291.8 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.68 usec
PLW1 14.00000000 W
SFO1 400.1924713 MHz

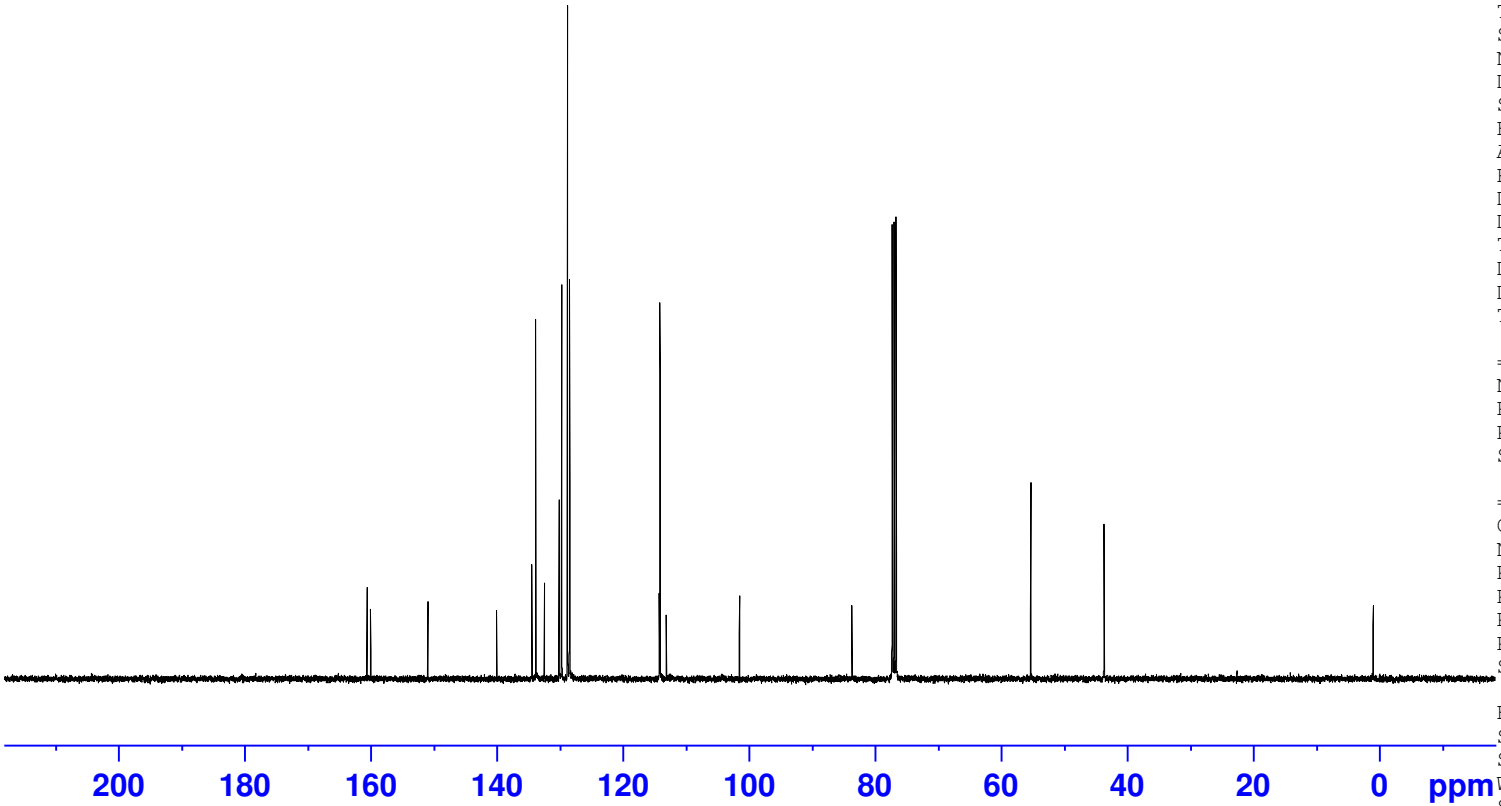
F2 - Processing parameters
SI 65536
SF 400.1900167 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

zhl-3-96



6

160.62
160.05
150.96
140.06
134.48
133.87
132.49
130.16
129.74
128.84
128.52
128.45
114.27
114.14
113.15
101.54
83.71
77.31
77.00
76.68
55.32
43.69



Current Data Parameters
NAME 20230526-400M
EXPNO 34
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230526
Time 5.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 291.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 12.00 usec
PLW1 53.00000000 W
SFO1 100.6379178 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

F2 - Processing parameters
SI 32768
SF 100.6278665 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40