Supplementary Information

Catalytic Asymmetric Synthesis of α-Tertiary Aminoketones from Sulfoxonium Ylides Bearing Two Aryl Groups

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NMR Spectra and HPLC Traces

I. General Information

Flash column chromatography was performed over silica gel (200-300 mesh) purchased from Qindao Puke Co., China. All air or moisture sensitive reactions were conducted in oven-dried glassware under nitrogen atmosphere using anhydrous solvents. Anhydrous acetonitrile was purified by the Innovative® solvent purification system or purchased from J&K Scientific Ltd. Trimethylsulfoxonium iodide, KO*t*Bu, aryl bromides, aryl acyl chloride used in this study were purchased from Energy Chemical, and used as received. XPhos and anilines used in this study were purchased from Shanghai Haohong Scientific Co., Ltd (Leyan). Other solvents (such as DCM, MeOH, THF, EA, and *n*-hexane) used in this study all were purchased from Energy Chemical, and directly used without further purification. ^{1}H, ^{13}C and ^{19}F NMR spectra were collected on a Bruker AV 400 or 300 MHz NMR spectrometer using residue solvent peaks as an internal standard (^{1}H NMR: $CDCl_3$ at 7.26 ppm; ^{13}C NMR: $CDCl_3$ at 77.0 ppm). Mass spectra were collected on an Agilent GC/MS 5975C system, a MALDI Micro MX mass spectrometer, or an API QSTAR XL System. Optical rotations were measured on Shanghai Shenguang polarimeter with $[\alpha]_D$ values reported in degrees. The enantiomeric excess values were determined by chiral HPLC using an Agilent 1260 LC system with a Daicel CHIRALCEL OD-H column, or a Daicel CHIRALPAK AD-H or IC column. Unless otherwise noted, the racemic samples in this study were prepared using the racemic catalyst 1,1′-binaphthyl-2,2′-diyl hydrogenphosphate (20 mol%).

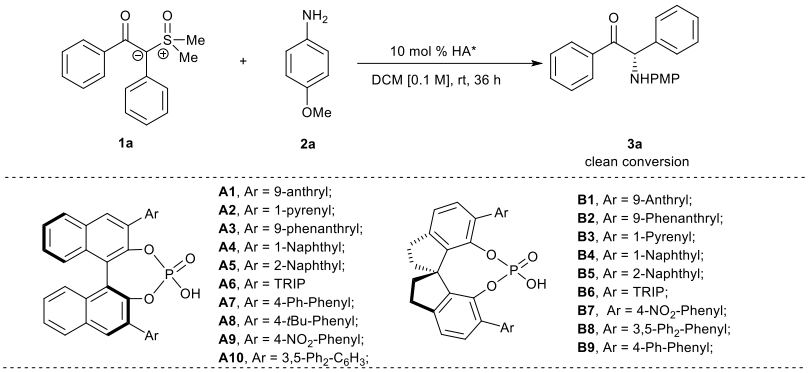
II. Synthesis of Sulfoxonium Ylide

All the sulfoxonium ylides used in this work are known compounds and were synthesized according to the literature procedure.[1]

1 W. Guo, F. Jiang, S. Li and J. Sun, *Chem. Sci.*, 2022, **13**, 11648–11655.

III. Optimization of Reaction Conditions

Table S1 Evaluation of reaction conditions.[a]



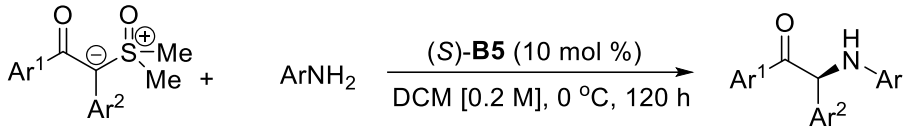
Entry	**HA***	solvent	conv. (%)[b]	ee (%)[c]
1	**A1**	DCM	>95	30
2	**A2**	DCM	>95	26
3	**A3**	DCM	>95	38
4	**A4**	DCM	>95	36
5	**A5**	DCM	>95	43
6	**A6**	DCM	<20	N. D.
7	**A7**	DCM	>95	34
8	**A8**	DCM	>95	49
9	**A9**	DCM	>90	30
10	**A10**	DCM	>90	72
11	**B1**	DCM	>95	57
12	**B2**	DCM	>95	65
13	**B3**	DCM	>95	67
14	**B4**	DCM	>95	64
15	**B5**	DCM	>95	79
16	**B6**	DCM	<20	N.D.
17	**B7**	DCM	>95	76
18	**B8**	DCM	>95	60
19	**B9**	DCM	>95	76
20	**B5**	$CHCl_3$	>95	72
21	**B5**	DCE	>95	78
22	**B5**	toluene	<20	N.D.
23	**B5**	THF	<20	N.D.
24[d]	**B5**	DCM	78(72)	80
25[d,e]	**B5**	DCM	90(85)	80

[a] Rection conditions: unless otherwise noted, all the reaction were conducted by employing **1a** (0.1 mmol, 1.0 equiv), **2a** (0.11 mmol, 1.1 equiv), and chiral phosphoric

acid **A** or **B** (10 mol %) in the corresponding solvent (1.0 mL) at room temperature. Yields in parentheses were isolated yield after purification by column chromatography on silica gel. [b] Determined by ^{1}H NMR analysis using CH_2Br_2 as an internal standard. [c] Determined by chiral HPLC. [d] At 0 °C for 120 h. [e] in 0.5 mL of DCM.

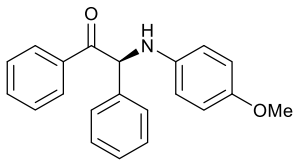
IV. Catalytic Asymmetric Synthesis of α-Tertiary Amino Ketones

General Procedure.



1 **2** **3**

An oven-dried 4-mL vial equipped with a magnetic stirring bar was charged with the sulfoxonium ylide **1** (0.1 mmol, 1.0 equiv) and the CPA catalyst (*S*)-**B5** (5.6 mg, 0.01 mmol, 10 mol%). The vial was carefully sealed with a puncturable screw-cap and electrical tape and then cooled to 0 °C Then, DCM (0.5 mL) was injected into the vial through the cap, and the resulted suspension was stirred at 0 °C for 2 min before addition of aniline **2** (0.11 mmol, 1.1 equiv). Then, the reaction mixture was stirred at the same temperature and monitored by TLC. Upon completion (120 h), the mixture was directly subjected to flash column chromatography on silica gel (eluent: hexanes/ethyl acetate = 10:1 to 5:1) to give the desired product **3**.



3a

(*S*)-2-((4-Methoxyphenyl)amino)-1,2-diphenylethan-1-one (3a) was prepared as a yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 26.9 mg, 85% yield, 80% ee).

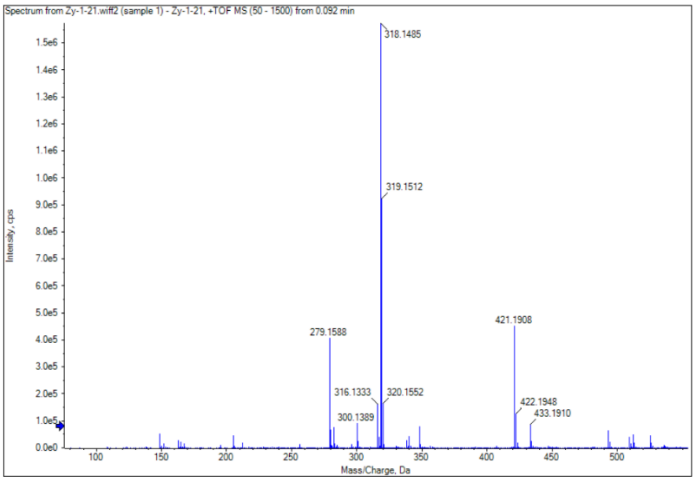
$[\alpha]_D^{25}$: +101.6 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK®

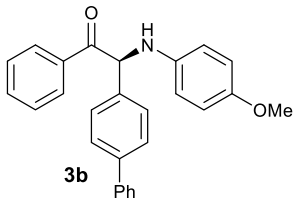
OD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 15.0 min (major), 25.0 min (minor).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.92 – 7.89 (m, 2H), 7.46 – 7.31 (m, 5H), 7.22 – 7.09 (m, 3H), 6.66 – 6.55 (m, 4H), 5.90 (s, 1H), 3.61 (s, 3H) (NH is not displayed) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 197.5, 152.5, 140.2, 137.8, 135.2, 133.5, 129.1, 128.9, 128.7, 128.2, 128.1, 115.2, 114.9, 63.9, 55.7 ppm.

HRMS (ESI+) Calcd for $C_{21}H_{20}NO_2$ $[M+H]^+$: 318.1494, found: 318.1485.





(*S*)-2-([1,1'-Biphenyl]-4-yl)-2-((4-methoxyphenyl)amino)-1-phenylethan-1-one (3b) was prepared as a yellow oil according to the General Procedure (eluent: hexanes /EtOAc = 10:1, 28.7 mg, 73% yield, 83%ee).

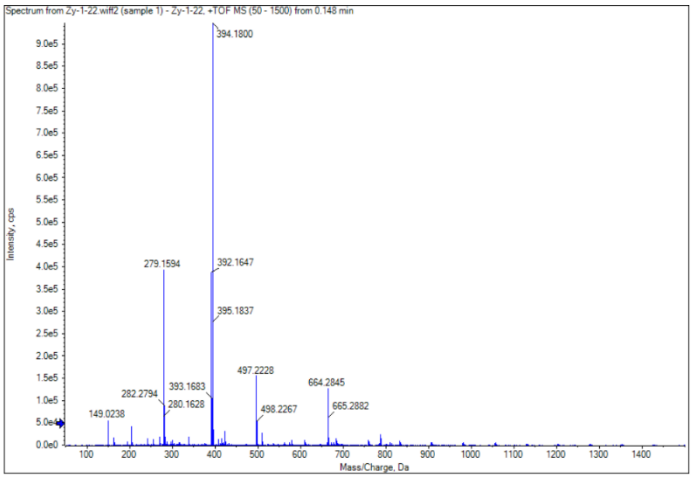
$[\alpha]_D^{25}$: +71.2 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 21.0 min (major), 24.5 min (minor).

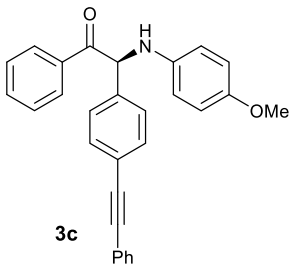
^{1}H NMR (300 MHz, acetone-d_6) δ 8.22 – 8.19 (m, 2H), 7.67 – 7.64 (m, 2H), 7.61 – 7.49 (m, 7H), 7.43 – 7.38 (m, 2H), 7.34 – 7.29 (m, 1H), 6.83 – 6.68 (m, 4H), 6.40 (s, 1H), 5.62 (br, 1H), 3.64 (s, 3H) ppm.

^{13}C NMR (75 MHz, acetone-d_6) δ 198.2, 153.1, 141.9, 141.3, 141.2, 138.8, 136.4, 134.4,

129.9, 129.8, 129.7, 128.3, 128.2, 128.1, 127.7, 115.8, 115.4, 63.1, 55.8 ppm.

HRMS (ESI+) Calcd for $C_{27}H_{24}NO_2$ [M+H]$^+$: 394.1807, found: 394.1800.





3c

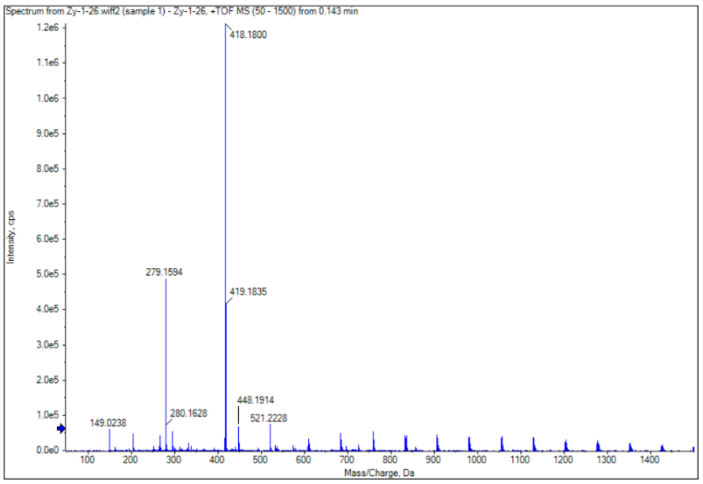
(*S*)-2-((4-Methoxyphenyl)amino)-1-phenyl-2-(4-(phenylethynyl)phenyl)ethan-1-one (3c) was prepared as a yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 30.1 mg, 72% yield, 83%ee).

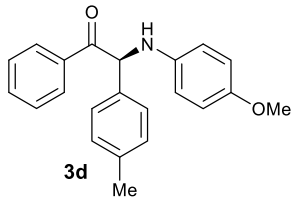
$[\alpha]_D^{25}$: +95.6 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 16.6 min (major), 18.3 min (minor).

^{1}H NMR (300 MHz, acetone-d_6) δ 8.18 – 8.15 (m, 2H), 7.63 – 7.59(m, 3H), 7.53 – 7.45 (m, 6H), 7.40 – 7.37 (m, 3H), 6.81 – 6.78 (m, 2H), 6.71 – 6.68 (m, 2H), 6.38 (s, 1H), 5.64 (br, 1H), 3.64 (s, 3H) ppm.

^{13}C NMR (75 MHz, acetone-d_6) δ 197.9, 153.2, 141.6, 140.3, 136.4, 134.5, 132.7, 132.4, 129.8, 129.7, 129.6, 129.5 (two C), 124.0, 123.5, 115.9, 115.4, 90.4, 89.6, 63.3, 55.8 ppm.

HRMS (ESI+) Calcd for $C_{29}H_{24}NO_2$ [M+H]$^+$: 418.1807, found: 418.1800.





3d

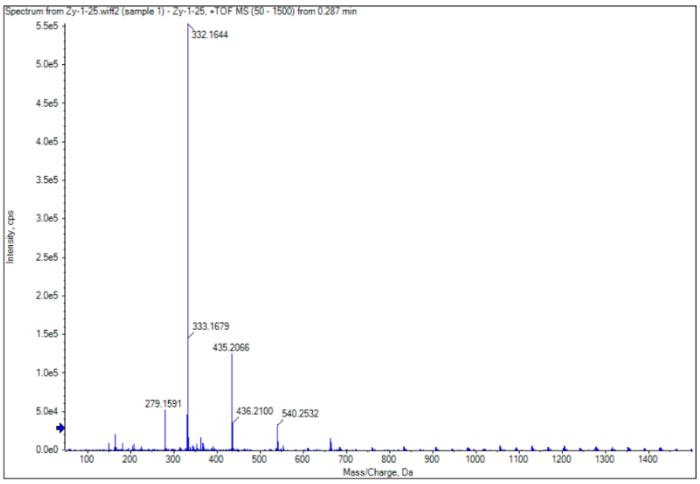
(*S*)-2-((4-Methoxyphenyl)amino)-1-phenyl-2-(*p*-tolyl)ethan-1-one (3d) was prepared as a yellow oil according to the General Procedure (eluent: hexanes /EtOAc = 10:1, 28.8 mg, 87% yield, 82% ee).

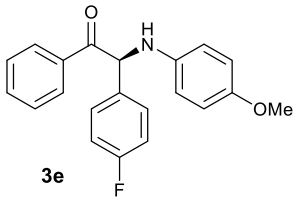
$[\alpha]_D^{25}$: +55.4 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 16.8 min (major), 20.0 min (minor).

^{1}H NMR (300 MHz, acetone-d_6) δ 8.16 – 8.13 (m, 2H), 7.62 – 7.56 (m, 1H), 7.51 – 7.42 (m, 4H), 7.09 – 7.06 (m, 2H), 6.78 – 6.75 (m, 2H), 6.70 – 6.66 (m, 2H), 6.28 (d, *J* = 6 Hz, 1H), 5.50 (br, 1H), 3.64 (s, 3H), 2.20 (s, 3H) ppm.

^{13}C NMR (75 MHz, acetone-d_6) δ 198.3, 153.0, 141.9, 138.3, 136.54, 136.46, 134.2, 130.3, 129.8, 129.6, 129.2, 115.8, 115.4, 63.2, 55.8, 21.1 ppm.

HRMS (ESI+) Calcd for $C_{22}H_{22}NO_2$ $[M+H]^+$: 332.1651, found: 332.1644.





3e

(*S*)-2-(4-Fluorophenyl)-2-((4-methoxyphenyl)amino)-1-phenylethan-1-one (3e) was prepared as a yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 24.6 mg, 73% yield, 87% ee).

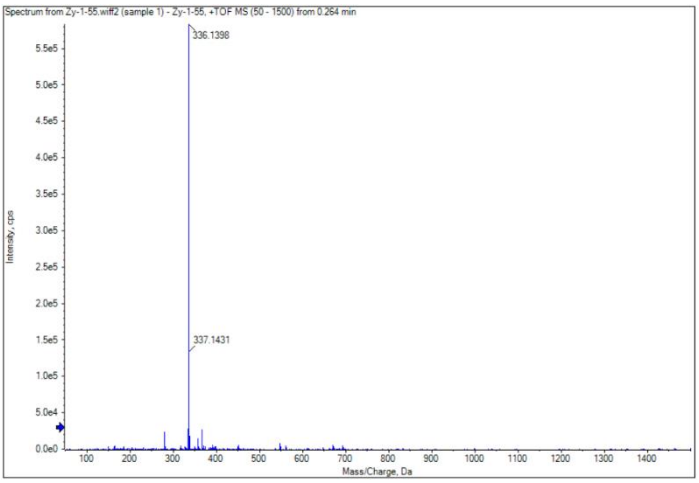
$[\alpha]_D^{25}$: +74.4 (*c* = 1.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 14.2 min (major), 15.8 min (minor).

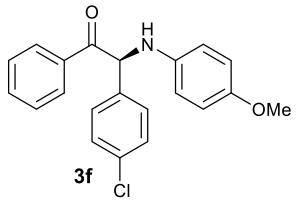
^{1}H NMR (300 MHz, acetone-d_6) δ 8.17 – 8.14 (m, 2H), 7.63 – 7.58 (m, 3H), 7.53 – 7.48 (m, 2H), 7.08 – 7.02 (m, 2H), 6.79 – 6.75 (m, 2H), 6.71 – 6.67 (m, 2H), 6.35 (d, *J* = 6 Hz, 1H), 5.57 (d, *J* = 6 Hz,1H), 3.64 (s, 3H) ppm.

^{13}C NMR (75 MHz, acetone-d_6) δ 198.1, 163.1 (d, $^1J_{C\text{-}F}$ = 243 Hz), 153.2, 141.6, 136.3, 135.7 (d, $^4J_{C\text{-}F}$ = 3 Hz), 134.4, 131.2 (d, $^3J_{C\text{-}F}$ = 8 Hz), 129.7, 129.6, 116.3 (d, $^2J_{C\text{-}F}$ = 22 Hz), 115.8, 115.4, 62.6, 55.7 ppm.

^{19}F NMR (282 MHz, Acetone-d_6) δ –116.1 ppm.

HRMS (ESI+) Calcd for $C_{21}H_{19}FNO_2$ $[M+H]^+$: 336.1400, found: 336.1398.





3f

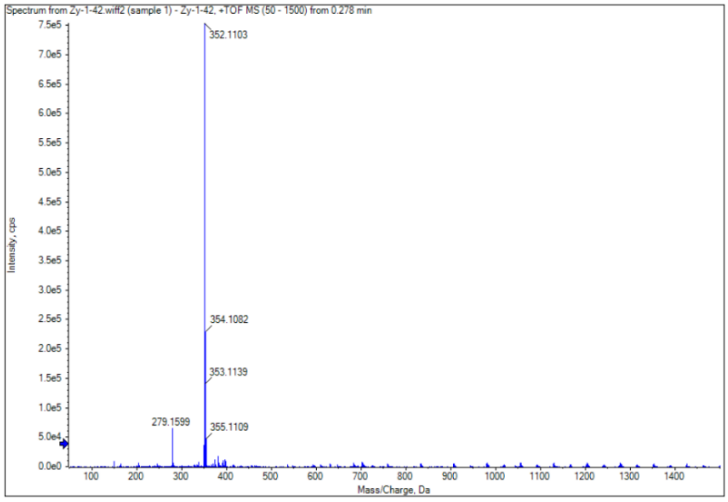
(*S*)-2-(4-Chlorophenyl)-2-((4-methoxyphenyl)amino)-1-phenylethan-1-one (3f) was prepared as a yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 23.1 mg, 66% yield, 87% ee).

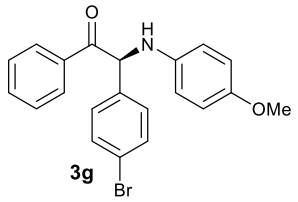
$[\alpha]_D^{25}$: +81.3 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 13.9 min (major), 15.4 min (minor).

^{1}H NMR (300 MHz, acetone-d_6) δ 8.17 – 8.14 (m, 2H), 7.59 – 7.48 (m, 5H), 7.32 – 7.30 (m, 2H), 6.79 – 6.67 (m, 4H), 6.36 (d, *J* = 6 Hz, 1H), 5.61 (d, *J* = 6 Hz, 1H), 3.64 (s, 3H) ppm.

^{13}C NMR (75 MHz, acetone-d_6) δ 197.9, 153.2, 141.5, 138.7, 136.2, 134.5, 133.9, 131.0, 129.8, 129.7, 129.6, 115.9, 115.4, 62.7, 55.7 ppm.

HRMS (ESI+) Calcd for $C_{21}H_{19}ClNO_2$ $[M+H]^+$: 352.1104, found: 352.1103.





3g

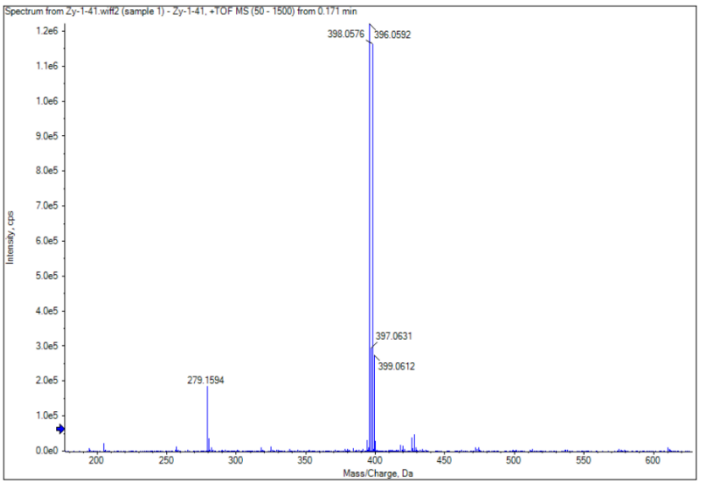
(*S*)-2-(4-Bromophenyl)-2-((4-methoxyphenyl)amino)-1-phenylethan-1-one (3g) was prepared as a yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 21 mg, 53% yield, 86% ee).

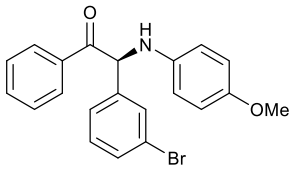
$[\alpha]_D^{25}$: +71.5 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 14.5 min (major), 16.1 min (minor).

^{1}H NMR (300 MHz, acetone-d_6) δ 8.16 – 8.14 (m, 2H), 7.53 – 7.44 (m, 7H), 6.79 – 6.67(m, 4H), 6.35 (d, *J* = 9 Hz, 1H), 5.62 – 5.60 (m, 1H), 3.64 (s, 3H) ppm.

^{13}C NMR (75 MHz, acetone-d_6) δ 197.8, 153.2, 141.5, 139.2, 136.2, 134.4, 132.6, 131.3, 129.74, 129.66, 122.1, 115.8, 115.4, 62.8, 55.7 ppm.

HRMS (ESI+) Calcd for $C_{21}H_{19}BrNO_2$ $[M+H]^+$: 396.0599, found: 396.0592.





3h

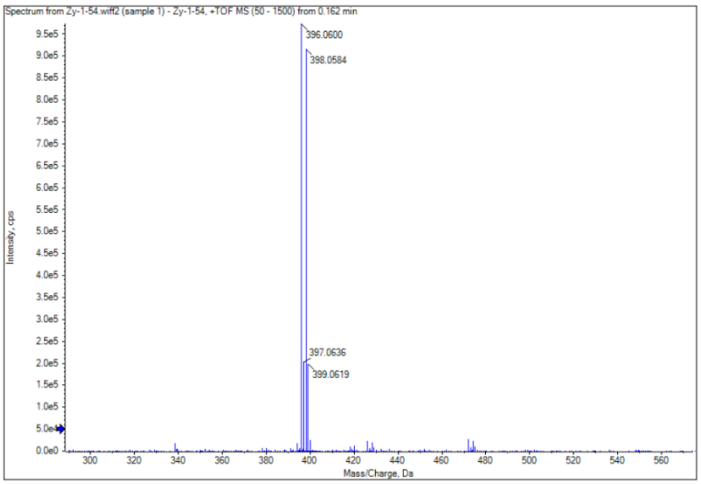
(*S*)-2-(3-Bromophenyl)-2-((4-methoxyphenyl)amino)-1-phenylethan-1-one (3h) was prepared as a yellow solid according to the General Procedure (eluent: hexanes/ EtOAc = 10:1, 29.7 mg, 75% yield, 87% ee).

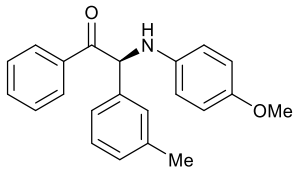
$[\alpha]_D^{25}$: +56.7 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 13.0 min (major), 14.8 min (minor).

^{1}H NMR (300 MHz, acetone-d_6) δ 8.19 – 8.16 (m, 2H), 7.76 – 7.75 (m, 1H), 7.66 – 7.49 (m, 4H), 7.40 – 7.36 (m, 1H), 7.27 – 7.22 (m, 1H), 6.81 – 6.68 (m, 4H), 6.38 – 6.36 (m, 1H), 5.67 – 5.65 (m, 1H), 3.65 (s, 3H) ppm.

^{13}C NMR (75 MHz, acetone-d_6) δ 197.8, 153.3, 142.5, 141.5, 136.2, 134.6, 131.9, 131.7, 131.5, 129.8, 129.7, 128.3, 123.2, 115.9, 115.4, 62.7, 55.7 ppm.

HRMS (ESI+) Calcd for $C_{21}H_{19}BrNO_2$ $[M+H]^+$: 396.0599, found: 396.0600.





3i

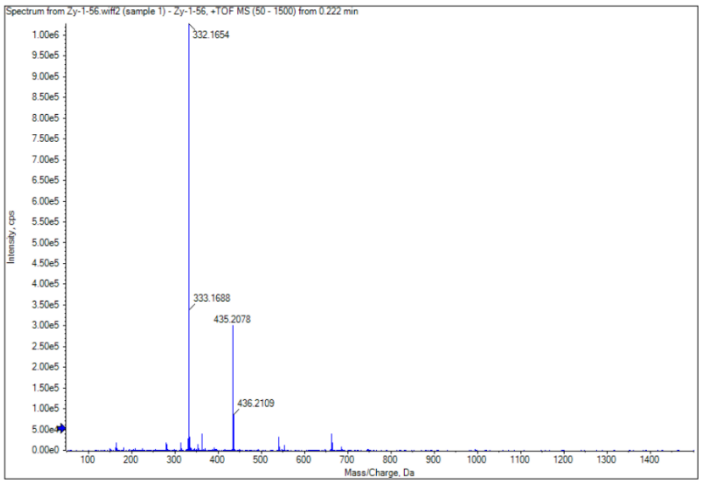
(*S*)-2-((4-Methoxyphenyl)amino)-1-phenyl-2-(*m*-tolyl)ethan-1-one (3i) was prepared as a yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 22.9 mg, 69% yield, 81% ee).

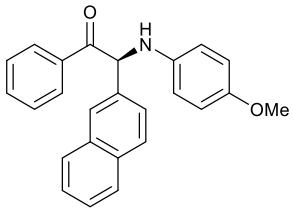
$[\alpha]_D^{25}$: +82.0 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 15.7 min (major), 18.8 min (minor).

^{1}H NMR (300 MHz, acetone-d_6) δ 8.17 – 8.14 (m, 2H), 7.61 – 7.36 (m, 5H), 7.19 – 7.13 (m, 1H), 7.01 – 6.99 (m, 1H), 6.79 – 6.67 (m, 4H), 6.26 (br, 1H), 5.53 (br, 1H), 3.64 (s, 3H), 2.23 (s, 3H) ppm.

^{13}C NMR (75 MHz, acetone-d_6) δ 198.3, 153.0, 141.9, 139.5, 139.1, 136.4, 134.2, 129.7, 129.64, 129.56, 129.4, 129.3, 126.5, 115.7, 115.3, 63.5, 55.7, 21.4 ppm.

HRMS (ESI+) Calcd for $C_{22}H_{22}NO_2$ $[M+H]^+$: 332.1651, found: 332.1654.





3j

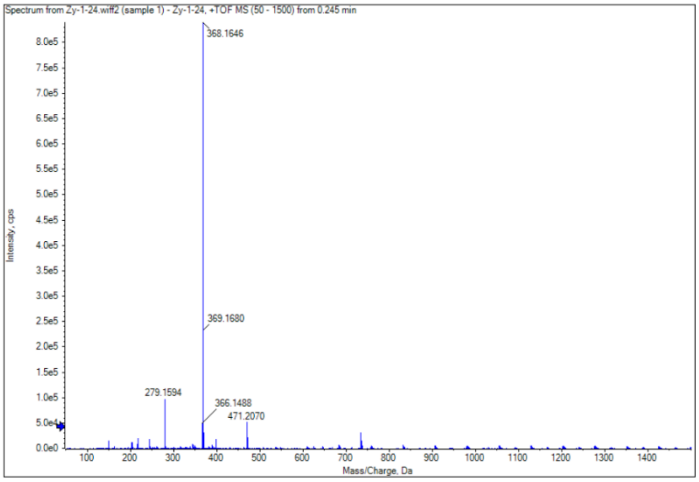
(*S*)-2-((4-Methoxyphenyl)amino)-2-(naphthalen-2-yl)-1-phenylethan-1-one (3j) was prepared as a yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 30.1 mg, 82% yield, 87% ee).

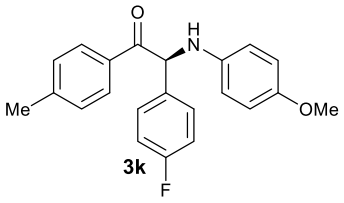
$[\alpha]_D^{25}$: +49.7 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 19.5 min (major), 23.3 min (minor).

^{1}H NMR (300 MHz, acetone-d_6) δ 8.22 – 8.13 (m, 3H), 7.85 – 7.78 (m, 3H), 7.68 – 7.64 (m, 1H), 7.57 – 7.54 (m, 1H), 7.50 – 7.40 (m, 4H), 6.86 – 6.81 (m, 2H), 6.69 – 6.66 (m, 2H), 6.51 (d, *J* = 6 Hz, 1H), 5.66 (d, *J* = 6 Hz, 1H), 3.61 (s, 3H) ppm.

^{13}C NMR (75 MHz, acetone-d_6) δ 198.1, 153.1, 141.8, 137.2, 136.4, 134.4, 134.3, 133.9, 129.8, 129.6, 129.4, 128.8, 128.7, 128.5, 127.2, 127.1, 126.6, 115.8, 115.4, 63.7, 55.7 ppm.

HRMS (ESI+) Calcd for $C_{25}H_{22}NO_2$ $[M+H]^+$: 368.1651, found: 368.1646.





3k

(*S*)-2-(4-Fluorophenyl)-2-((4-methoxyphenyl)amino)-1-(*p*-tolyl)ethan-1-one (3k) was prepared as a yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 21.1 mg, 60% yield, 85% ee).

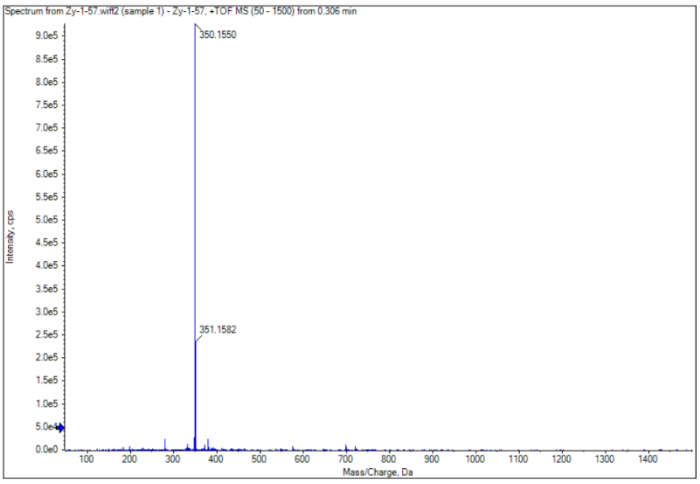
$[\alpha]_D^{25}$: +48.5 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® OD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 21.9 min (major), 28.7 min (minor).

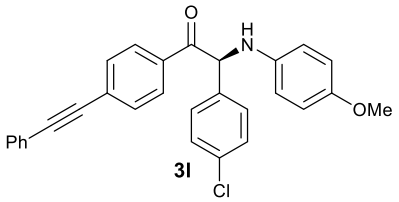
^{1}H NMR (300 MHz, acetone-d_6) δ 8.06 (d, *J* = 9 Hz, 2H), 7.62 – 7.57 (m, 2H), 7.31 (d, *J* = 9 Hz, 2H), 7.07 – 7.01 (m, 2H), 6.78 – 6.67 (m, 4H), 6.32 (s, 1H), 5.56 (br, 1H), 3.64 (s, 3H), 2.36 (s, 3H) ppm.

^{13}C NMR (75 MHz, acetone-d_6) δ 197.6, 163.0 (d, $^1J_{C\text{-}F}$ = 243 Hz), 153.1, 145.3, 141.7, 136.0 (d, $^4J_{C\text{-}F}$ = 3 Hz), 133.7, 131.1 (d, $^3J_{C\text{-}F}$ = 8 Hz), 130.3, 129.9, 116.2 (d, $^2J_{C\text{-}F}$ = 22 Hz), 115.8, 115.4, 62.4, 55.7, 21.6 ppm.

^{19}F NMR (282 MHz, acetone-d_6) δ –116.2 ppm.

HRMS (ESI+) Calcd for $C_{22}H_{21}FNO_2$ $[M+H]^+$: 350.1556, found: 350.1550.





3l

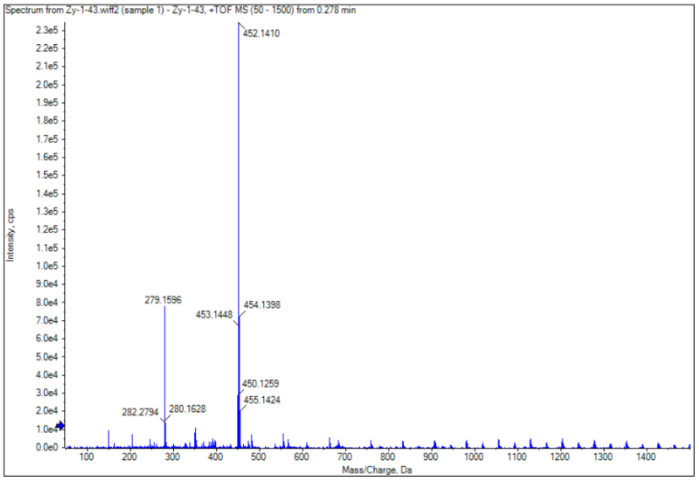
(*S*)-2-(4-Chlorophenyl)-2-((4-methoxyphenyl)amino)-1-(4-(phenylethynyl)phenyl)-ethan-1-one (3l) was prepared as a yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 22.9 mg, 51% yield, 83% ee).

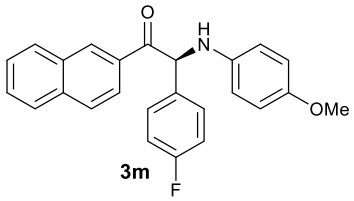
$[\alpha]_D^{25}$: –39.6 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 17.2 min (major), 15.7 min (minor).

^{1}H NMR (300 MHz, acetone-d_6) δ 8.20 – 8.17 (m, 2H), 7.65 – 7.56 (m, 6H), 7.45 – 7.43 (m, 3H), 7.34 – 7.31 (m, 2H), 6.80– 6.68 (m, 4H), 6.38 (d, *J* = 8Hz, 1H), 5.63 – 5.61 (m, 1H), 3.65 (s, 3H) ppm.

^{13}C NMR (75 MHz, acetone-d_6) δ 197.3, 153.3, 141.5, 138.5, 135.6, 134.0, 132.61, 132.5, 131.0, 130.1, 130.0, 129.7, 129.6, 129.2, 123.4, 115.9, 115.4, 93.6, 89.2, 62.9, 55.8 ppm.

HRMS (ESI+) Calcd for $C_{29}H_{23}ClNO_2$ $[M+H]^+$: 452.1417, found: 452.1410.





3m

(*S*)-2-(4-Fluorophenyl)-2-((4-methoxyphenyl)amino)-1-(naphthalen-2-yl)ethan-1-one (3m) was prepared as a yellow solid according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 30.8 mg, 80% yield, 91% ee).

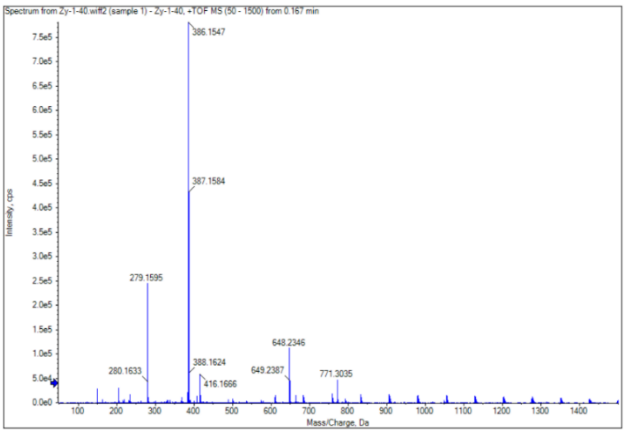
$[\alpha]_D^{25}$: –28.5 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 18.1 min (major), 23.7 min (minor).

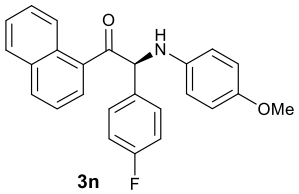
^{1}H NMR (300 MHz, acetone-d_6) δ 8.96 (s, 1H), 8.13 – 8.08 (m, 2H), 7.99 – 7.94 (m, 2H), 7.71 – 7.58 (m, 4H), 7.07 – 7.01 (m, 2H), 6.84 – 6.81 (m, 2H), 6.72 – 6.69 (m, 2H), 6.57 – 6.55 (m, 1H), 5.67 – 5.65 (m, 1H), 3.65 (s, 3H) ppm.

^{13}C NMR (75 MHz, acetone-d_6) δ 198.1, 163.0 (d, $^1J_{C\text{-}F}$ = 243 Hz), 153.2, 141.7, 136.6, 135.9 (d, $^4J_{C\text{-}F}$ = 3 Hz), 133.54, 133.49, 131.7, 131.2 (d, $^3J_{C\text{-}F}$ = 8 Hz), 130.6, 129.7, 129.5, 128.6, 127.9, 125.2, 116.3 (d, $^2J_{C\text{-}F}$ = 21 Hz), 115.8, 115.4, 62.6, 55.7 ppm.

^{19}F NMR (282 MHz, acetone-d_6) δ –116.0 ppm.

HRMS (ESI+) Calcd for $C_{25}H_{21}FNO_2$ $[M+H]^+$: 386.1556, found: 386.1547.





3n

(*S*)-2-(4-Fluorophenyl)-2-((4-methoxyphenyl)amino)-1-(naphthalen-1-yl)ethan-1-one (3n) was prepared as a yellow solid according to the General Procedure (eluent: hexanes/EtOAc = 5:1, 17 mg, 44% yield, 84% ee).

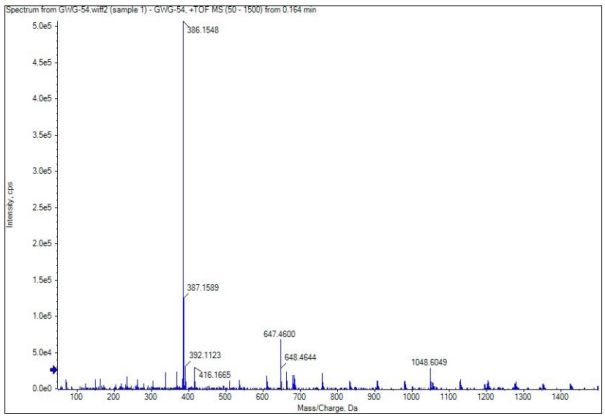
$[\alpha]_D^{25}$: +7.6 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 24.5 min (major), 28.3 min (minor).

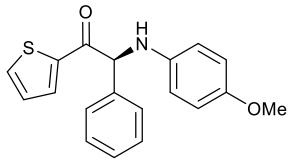
^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.92 – 7.86 (m, 2H), 7.80 – 7.75 (m, 2H), 7.46 – 7.35 (m, 3H), 7.24 – 7.21 (m, 2H), 6.81 – 6.76 (m, 2H), 6.65 – 6.53 (m, 4H), 5.88 (S, 1H), 3.60 (s, 3H) (NH is not displayed) ppm.

^{13}C NMR (100 MHz, CD_2Cl_2) δ 199.8, 167.6, 162.5, (d, $^1J_{C\text{-}F}$ = 263 Hz), 152.4, 139.9, 134.7, 133.7, 133.1 (d, $^4J_{C\text{-}F}$ = 3 Hz), 132.6, 130.4, 129.6 (d, $^3J_{C\text{-}F}$ = 8 Hz), 128.3, 127.8, 126.7, 126.6, 124.8, 124.2, 115.7 (d, $^2J_{C\text{-}F}$ = 22 Hz), 114.7, 65.8, 55.5 ppm.

^{19}F NMR (376 MHz, CD_2Cl_2) δ –114.6 ppm.

HRMS (ESI+) Calcd for $C_{25}H_{21}FNO_2$ $[M+H]^+$: 386.1556, found: 386.1548.





3o

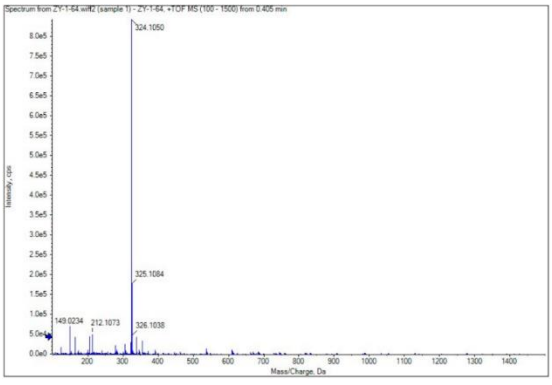
(*S*)-2-((4-Methoxyphenyl)amino)-2-phenyl-1-(thiophen-2-yl)ethan-1-one (3o) was prepared as a light yellow oil according to the General Procedure (eluent: hexanes/ EtOAc = 10:1 to 5:1, 27.5 mg, 85% yield, 82% ee).

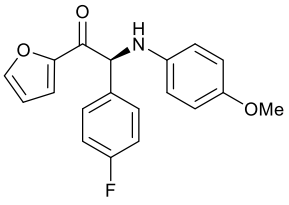
$[\alpha]_D^{25}$: +84.4 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 32.8 min (major), 29.8 min (minor).

^{1}H NMR (300 MHz, acetone-d_6) δ 8.28 – 8.26 (m, 1H), 7.92 – 7.90 (m, 1H), 7.64 – 7.61 (m, 2H), 7.35 – 7.30 (m, 2H) 7.26 – 7.21 (m, 2H), 6.79 – 6.75 (m, 2H), 6.71 – 6.67 (m, 2H), 6.12 (d, *J* = 8 Hz, 1H), 5.52 (d, *J* = 8 Hz, 1H), 3.64 (s, 3H) ppm.

^{13}C NMR (75 MHz, acetone-d_6) δ 191.5, 153.2, 143.0, 141.8, 139.7, 135.9, 134.6, 129.6, 129.4, 129.1, 128.8, 115.8, 115.3, 64.7, 55.7 ppm.

HRMS (ESI+) Calcd for $C_{19}H_{18}NO_2S$ $[M+H]^+$: 324.1058, found: 324.1050.





3p

(*S*)-2-(4-Fluorophenyl)-1-(furan-2-yl)-2-((4-methoxyphenyl)amino)ethan-1-one (3p) was prepared as a light yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 5:1, 28.8 mg, 90% yield, 77% ee).

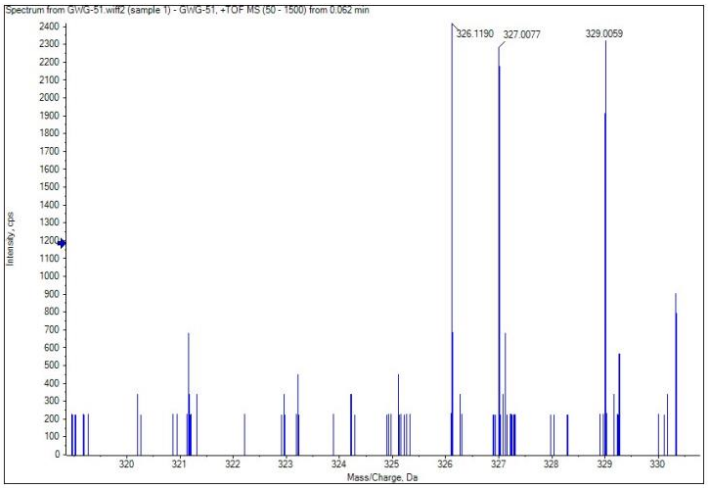
$[\alpha]_D^{25}$: +30.0 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 25.3 min (major), 24.0 min (minor).

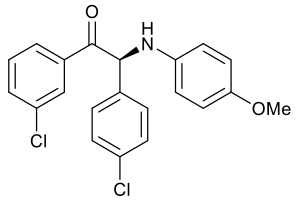
^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.56 – 7.55 (m, 1H), 7.42 – 7.39 (m, 2H), 7.64 – 7.61 (m, 2H), 7.22 – 7.21 (m, 1H) 6.62 – 6.60 (m, 2H), 6.52 – 6.46 (m, 3H), 5.73 (s, 1H), 4.98 (br, 1H), 3.58 (s, 3H) ppm.

^{13}C NMR (100 MHz, CD_2Cl_2) δ 185.6, 162.5 (d, $^1J_{C\text{-}F}$ = 245 Hz), 152.4, 150.9, 147.2, 139.9, 133.8 (d, $^4J_{C\text{-}F}$ = 3 Hz), 129.8 (d, $^3J_{C\text{-}F}$ = 8 Hz), 119.0, 115.7 (d, $^2J_{C\text{-}F}$ = 22 Hz), 114.8, 114.7, 112.7, 62.7, 55.5 ppm.

^{19}F NMR (376 MHz, CD_2Cl_2) δ –114.6 ppm.

HRMS (ESI+) Calcd for $C_{19}H_{17}FNO_3$ $[M+H]^+$: 326.1192, found: 326.1190.





3q

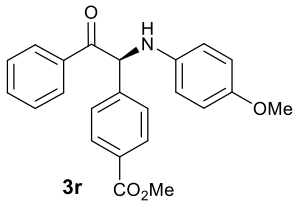
(*S*)-1-(3-Chlorophenyl)-2-(4-chlorophenyl)-2-((4-methoxyphenyl)amino)ethan-1-one (3q) was prepared as a yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1 to 5:1, 22.4 mg, 58% yield, 87% ee).

$[\alpha]_D^{25}$: +84.4 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 14.3 min (major), 15.3 min (minor).

^{1}H NMR (400MHz, CD_2Cl_2) δ 7.83 –7.74(m, 2H), 7.45 – 7.42 (m, 1H), 7.32 – 7.17 (m, 5H), 6.63 – 6.50(m, 4H) 5.84 (s, 1H), 4.99(s, 1H), 3.58 (s, 3H) ppm.

^{13}C NMR (100 MHz, CD_2Cl_2) δ 195.8, 152.6, 139.8, 136.6, 136.2, 135.0, 134.0, 133.5, 130.2, 129.6, 129.2, 128.7, 126.9, 115.0,114.7, 63.0, 55.5 ppm.

Note: It's a known compound[2].



3r

Methyl (*S*)-4-(1-((4-methoxyphenyl)amino)-2-oxo-2-phenylethyl)benzoate (3r) was prepared as a light yellow oil according to the General Procedure (eluent: hexanes/ EtOAc = 5:1, 32 mg, 84% yield, 89% ee).

$[\alpha]_D^{25}$: +32.4 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® OD-H column; 15% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 25.3 min (major), 24.0 min (minor).

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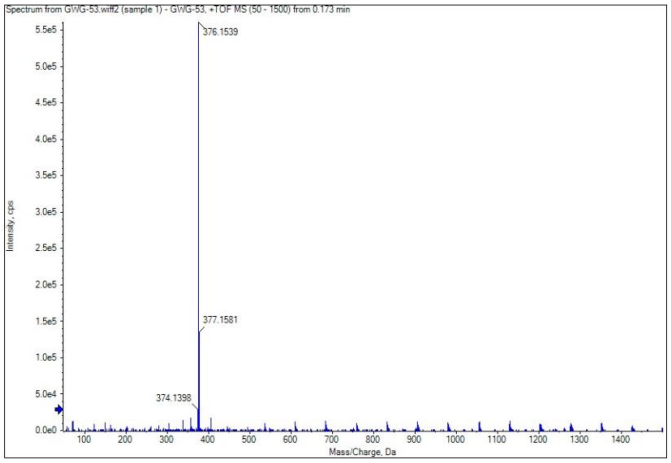
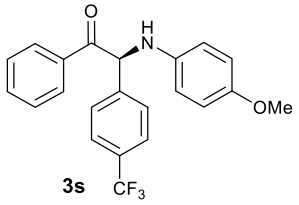
2. A. Z. Gonzalez, J. Eksterowicz, M. D. Bartberger, H. P. Beck, J. Canon, A. Chen, D. Chow, J. Duquette, B. M. Fox, J. S. Fu, X. Huang, J. B. Houze, L. X. Jin, Y. H. Li, Z. H. Li, Y. Ling, M. C. Lo, A. M. Long, L. R. McGee, J. McIntosh, D. L. McMinn, J. D. Oliner, T. Osgood, Y. Rew, A. Y. Saiki, P. Shaffer, S. Wortman, P. Yakowec, X. L. Yan, Q. P. Ye, D. Y. Yu, X. N. Zhao, J. Zhou, S. H. Olson, J. C. Medina and D. Q. Sun, *J. Med. Chem.*, 2014, **57**, 2472–2488

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.90 – 7.83 (m, 4H), 7.50 – 7.35 (m, 5H), 6.63 – 6.53 (m, 4H), 5.98 (s, 1H), 5.14 (br, 1H), 3.74 (s, 1H), 3.59 (s, 3H) ppm.

^{13}C NMR (100 MHz, CD_2Cl_2) δ 196.7, 166.3, 152.5, 143.2, 139.9, 134.9, 133.7, 130.04, 129.99, 128.8, 128.7, 128.2, 114.9, 114.7, 63.3, 55.5, 52.0 ppm.

HRMS (ESI+) Calcd for $C_{23}H_{22}NO_4$ $[M+H]^+$: 376.1549, found: 376.1539.





3s

(*S*)-2-((4-Methoxyphenyl)amino)-1-phenyl-2-(4-(trifluoromethyl)phenyl)ethan-1-one (3s) was prepared as a light yellow oil according to the General Procedure (eluent: hexanes/ EtOAc = 5:1, 15 mg, 39% yield, 93% ee).

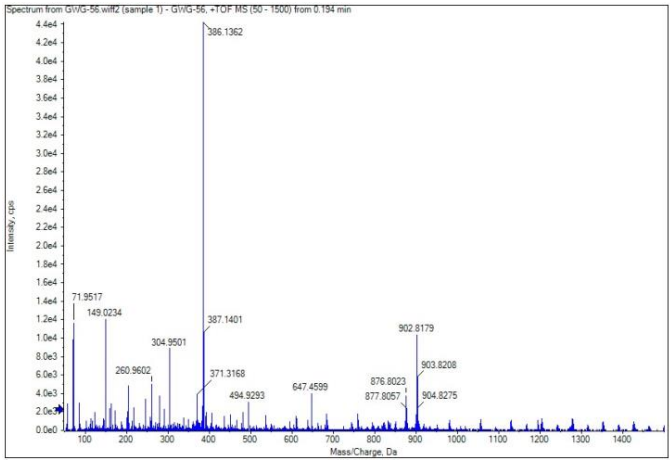
$[\alpha]_D^{25}$: +80.3 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 16.1 min (major), 17.7 min (minor).

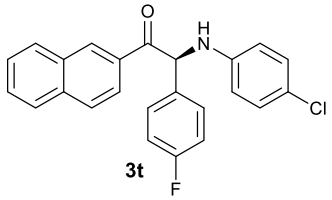
^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.90 – 7.88 (m, 2H), 7.50 – 7.44 (m, 5H), 7.39 – 7.35 (m, 2H), 6.64 – 6.61 (m, 2H) 6.55 – 6.52 (m, 2H), 6.00 (s, 1H), 5.12 (br, 1H), 3.58 (s, 3H) ppm.

^{13}C NMR (100 MHz, CD_2Cl_2) δ 196.6, 152.6, 142.5, 139.8, 134.8, 133.8, 129.9 (q, $^2J_{C\text{-}F}$ = 32 Hz), 128.85, 128.79, 128.6, 125.9 (q, $^3J_{C\text{-}F}$ = 4 Hz), 124.0 (q, $^1J_{C\text{-}F}$ = 271 Hz), 114.9, 114.8, 63.0, 55.5 ppm.

^{19}F NMR (376 MHz, CD_2Cl_2) δ –62.9 ppm.

HRMS (ESI+) Calcd for $C_{22}H_{19}F_3NO_2$ $[M+H]^+$: 386.1368, found: 386.1362.





3t

(*S*)-2-((4-Chlorophenyl)amino)-2-(4-fluorophenyl)-1-(naphthalen-2-yl)ethan-1-one (3t) was prepared as a yellow oil according to the General Procedure (eluent: hexane /EtOAc = 10:1 to 5:1, 29.2 mg, 75% yield, 90% ee).

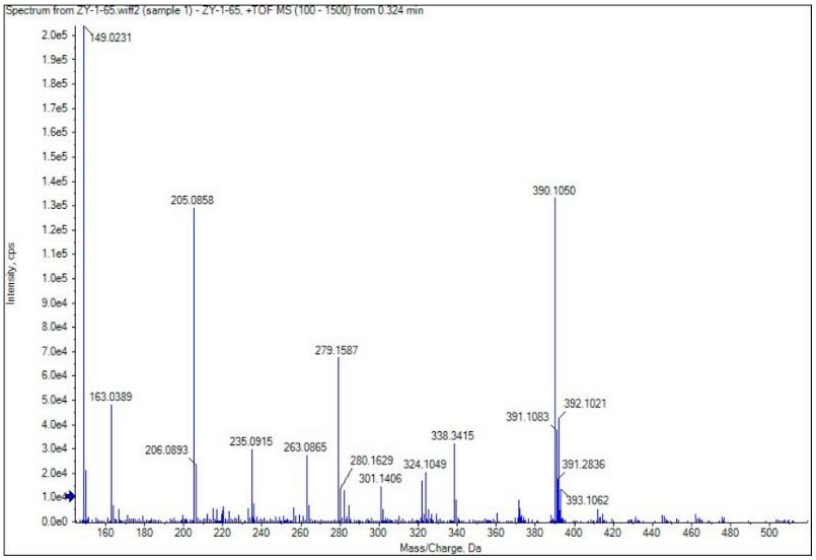
$[\alpha]_D^{25}$: –31.2 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 12.9 min (major), 14.6 min (minor).

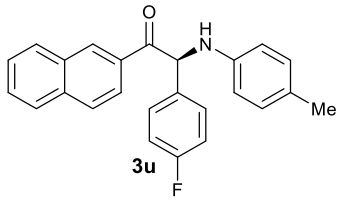
^{1}H NMR (300 MHz, acetone-d_6) δ 8.98 (s, 1H), 8.13 – 8.08 (m, 2H), 7.99 – 7.94 (m, 2H), 7.73 – 7.59 (m, 4H), 7.10 – 7.02 (m, 4H), 6.89 – 6.87 (m, 2H), 6.63 (d, *J* = 8 Hz, 1H), 6.20 (d, *J* = 8 Hz, 1H) ppm.

^{13}C NMR (75 MHz, acetone-d_6) δ 197.4, 163.1 (d, $^1J_{C\text{-}F}$ = 244 Hz), 146.5, 136.6, 135.2 (d, $^4J_{C\text{-}F}$ = 3 Hz), 133.4, 133.2, 131.8, 131.2 (d, $^3J_{C\text{-}F}$ = 8 Hz), 130.5, 129.8, 129.50, 129.46, 128.6, 127.9, 125.1, 122.1, 116.4 (d, $^2J_{C\text{-}F}$ = 22 Hz), 115.8, 61.7 ppm.

^{19}F NMR (282 MHz, acetone-d_6) δ –115.6 ppm.

HRMS (ESI+) Calcd for $C_{24}H_{18}ClFNO$ $[M+H]^+$: 390.1061, found: 390.1050.





(*S*)-2-(4-Fluorophenyl)-1-(naphthalen-2-yl)-2-(*p*-tolylamino)ethan-1-one (3u) was prepared as a yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1 to 5:1, 32.5 mg, 88% yield, 92% ee).

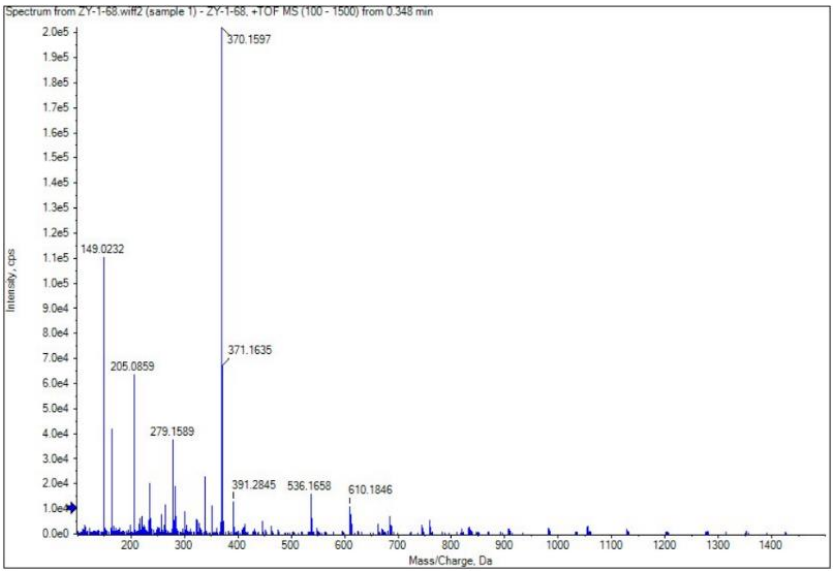
$[\alpha]_D^{25}$: –27.8 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 17.0 min (major), 17.9 min (minor).

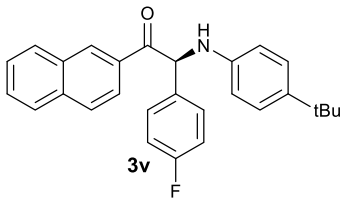
^{1}H NMR (300 MHz, acetone-d_6) δ 8.97 (s, 1H), 8.14 – 8.08 (m, 2H), 8.00 – 7.95 (m, 2H), 7.71 – 7.61 (m, 4H), 7.07 – 7.01 (m, 2H), 6.91 – 6.88 (m, 2H), 6.78 – 6.75 (m, 2H), 6.59 (s, 1H), 5.81 (br, 1H), 2.13 (s, 3H) ppm.

^{13}C NMR (75 MHz, acetone-d_6) δ 197.9, 163.1 (d, $^1J_{C\text{-}F}$ = 243 Hz), 145.3, 136.6, 135.8 (d, $^4J_{C\text{-}F}$ = 3 Hz), 133.51, 133.49, 131.7, 131.2 (d, $^3J_{C\text{-}F}$ = 8 Hz), 130.6, 130.3, 129.8, 129.5, 128.7, 127.9, 126.9, 125.2, 116.3 (d, $^2J_{C\text{-}F}$ = 22 Hz), 114.8, 62.0, 20.5 ppm.

^{19}F NMR (282 MHz, acetone-d_6) δ –116.1 ppm.

HRMS (ESI+) Calcd for $C_{25}H_{21}FNO$ $[M+H]^+$: 370.1607,found: 370.1597.





(*S*)-2-((4-(*Tert*-butyl)phenyl)amino)-2-(4-fluorophenyl)-1-(naphthalen-2-yl)ethan-1-one (3v) was prepared as a yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 34.5 mg, 84% yield,90% ee).

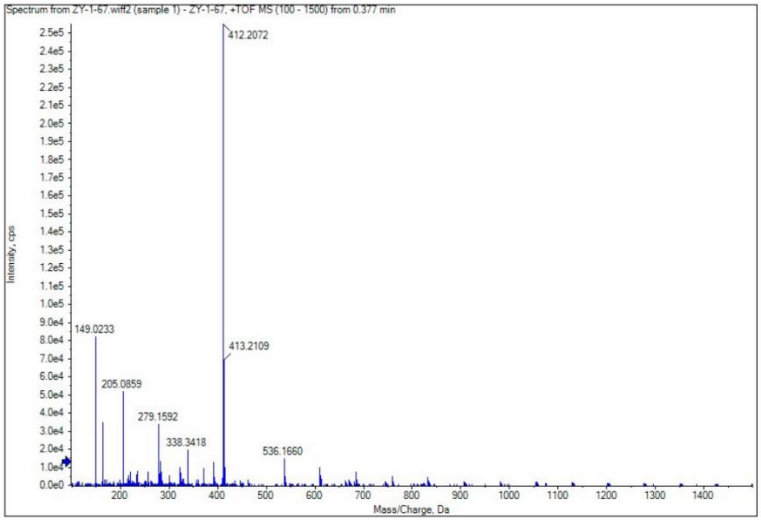
$[\alpha]_D^{25}$: –16.8 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 11.5 min (major), 21.0 min (minor).

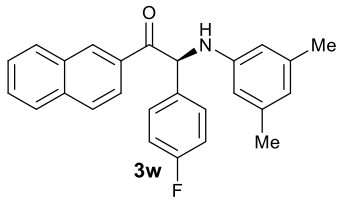
^{1}H NMR (300 MHz, acetone-d_6) δ 8.97 (s, 1H), 8.14 – 8.08 (m, 2H), 7.99 – 7.94 (m, 2H), 7.73 – 7.61 (m, 4H), 7.15 – 7.02 (m, 4H), 6.81 – 6.78 (m, 2H), 6.58 (d, *J* = 8 Hz, 1H), 5.86 (d, *J* = 8 Hz, 1H), 1.21 (s, 9H) ppm.

^{13}C NMR (75 MHz, acetone-d_6) δ 198.0, 163.0 (d, $^1J_{C\text{-}F}$ = 243 Hz), 145.2, 140.6, 136.6, 135.9 (d, $^4J_{C\text{-}F}$ = 3 Hz), 133.48, 133.46, 131.7, 131.2 (d, $^3J_{C\text{-}F}$ = 8 Hz), 130.6, 129.8, 129.5, 128.6, 127.9, 126.5, 125.2, 116.3 (d, $^2J_{C\text{-}F}$ = 22 Hz), 114.2, 62.0, 34.3, 31.9 ppm.

^{19}F NMR (282 MHz, acetone-d_6) δ –115.9 ppm.

HRMS (CI+) Calcd for $C_{28}H_{27}FNO$ $[M+H]^+$: 412.2077, found: 412.2072.





(*S*)-2-((3,5-Dimethylphenyl)amino)-2-(4-fluorophenyl)-1-(naphthalen-2-yl)ethan-1-one (3w) was prepared as a yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 34.5 mg, 90% yield, 92% ee).

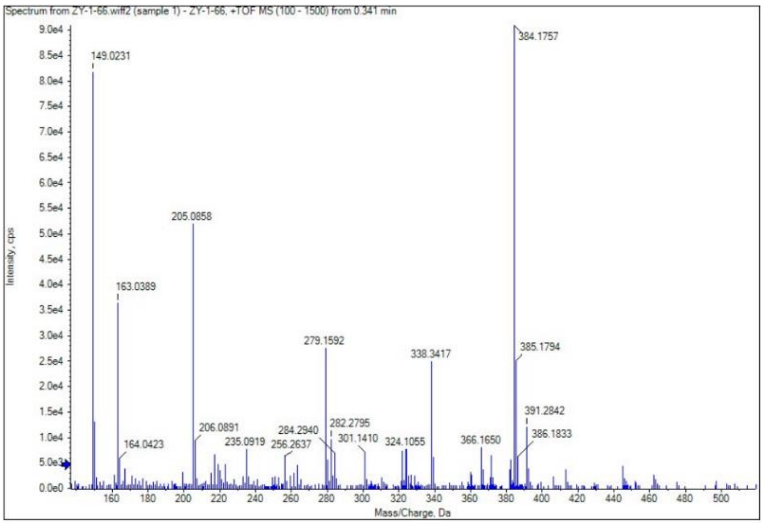
$[\alpha]_D^{25}$: –26.4 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 12.0 min (major), 11.3 min (minor).

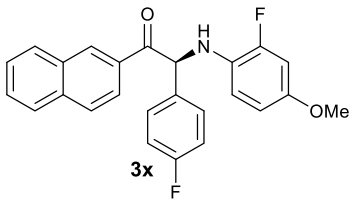
^{1}H NMR (300 MHz, acetone-d_6) δ 8.95 (s, 1H), 8.13 – 8.08 (m, 2H), 7.99 – 7.94 (m, 2H), 7.72 – 7.60 (m, 4H), 7.07 – 7.01 (m, 2H), 6.61 – 6.58 (d, *J* =8 Hz, 1H), 6.49 (s, 2H), 6.27 (s, 1H), 5.81 (d, *J* = 8 Hz, 1H), 2.13 (s, 6H) ppm.

^{13}C NMR (75 MHz, acetone-d_6) δ 197.9, 163.0 (d, $^1J_{C\text{-}F}$ = 243 Hz), 147.5, 139.0, 136.6, 135.9 (d, $^4J_{C\text{-}F}$ = 3 Hz), 133.5, 133.4, 131.7, 131.1 (d, $^3J_{C\text{-}F}$ = 8 Hz), 130.6, 129.7, 129.4, 128.6, 127.9, 125.2, 120.2, 116.3 (d, $^2J_{C\text{-}F}$ = 22 Hz), 112.6, 61.8, 21.6 ppm.

^{19}F NMR (282 MHz, acetone-d_6) δ –116.0 ppm.

HRMS (ESI+) Calcd for $C_{26}H_{23}FNO$ $[M+H]^+$: 384.1764, found: 384.1757.





(*S*)-2-((2-Fluoro-4-methoxyphenyl)amino)-2-(4-fluorophenyl)-1-(naphthalen-2-yl)ethan-1-one (3x) was prepared as a yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 23.6 mg, 58% yield, 86% ee).

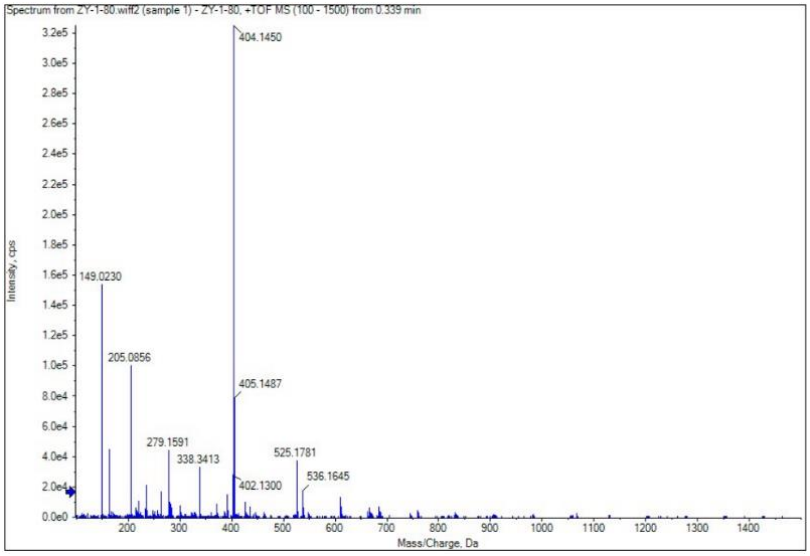
$[\alpha]_D^{25}$: –9.3 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 19.6 min (major), 25.3 min (minor).

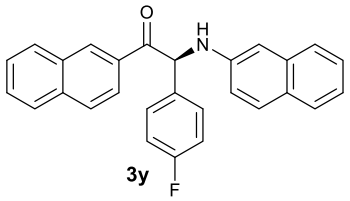
^{1}H NMR (300 MHz, acetone-d_6) δ 8.95 (s, 1H), 8.13 – 8.09 (m, 2H), 8.00 – 7.95 (m, 2H), 7.72 – 7.59 (m, 4H), 7.08 – 7.02 (m, 2H), 6.90 (t, *J* = 9 Hz 1H), 6.73 – 6.61 (m, 2H), 6.56 – 6.52 (m, 1H), 5.53 – 5.49 (m, 1H), 3.68 (s, 3H) ppm.

^{13}C NMR (75 MHz, acetone-d_6) δ 197.6, 163.1 (d, $^1J_{C\text{-}F}$ = 254 Hz), 153.2, 153.070, 153.069 (d, $^1J_{C\text{-}F}$ = 238 Hz), 136.7, 135.4 (d, $^4J_{C\text{-}F}$ = 3 Hz), 133.3 (d, $^2J_{C\text{-}F}$ = 22 Hz), 131.9, 131.1 (d, $^3J_{C\text{-}F}$ = 8 Hz), 130.6, 129.9, 129.5, 129.2 (d, $^3J_{C\text{-}F}$ = 12 Hz), 128.7, 128.0, 125.2, 116.5 (d, $^2J_{C\text{-}F}$ = 22 Hz), 116.0 (d, $^3J_{C\text{-}F}$ = 5 Hz), 110.2 (d, $^4J_{C\text{-}F}$ = 3 Hz), 103.0 (d, $^2J_{C\text{-}F}$ = 22 Hz), 62.2, 56.0 ppm.

^{19}F NMR (282 MHz, acetone-d_6) δ –115.6, –133.7 ppm.

HRMS (ESI+) Calcd for $C_{25}H_{20}FNO_2$ $[M+H]^+$: 404.1462, found: 404.1450.





3y

(*S*)-2-(4-Fluorophenyl)-1-(naphthalen-2-yl)-2-(naphthalen-2-ylamino)ethan-1-one (3y) was prepared as a yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 29.9 mg, 74% yield, 94% ee).

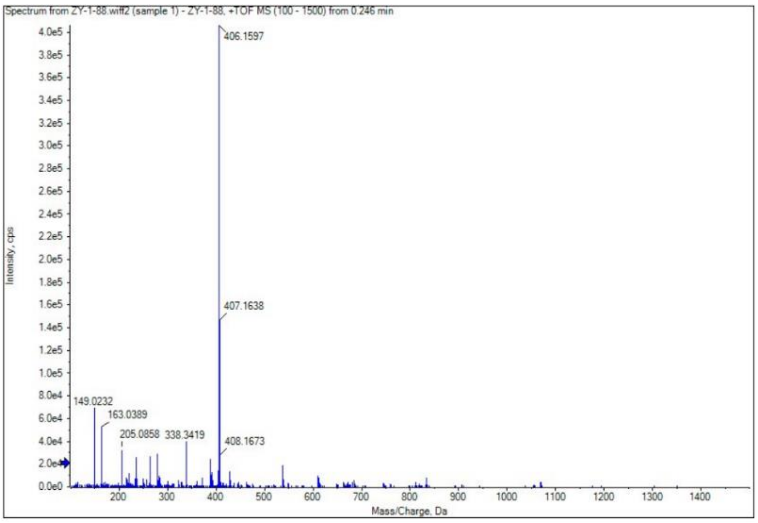
$[\alpha]_D^{25}$: –4.4 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 24.8 min (major), 21.8 min (minor).

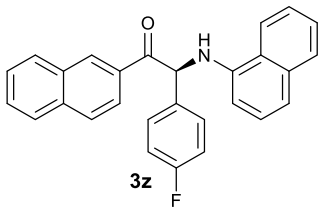
^{1}H NMR (400 MHz, acetone-d_6) δ 9.02 (s, 1H), 8.15 – 8.12 (m, 2H), 8.01 – 7.95 (m, 2H), 7.81– 7.77 (m, 2H), 7.69 – 7.51 (m, 5H), 7.31 – 7.26 (m, 2H), 7.15 – 7.04 (m, 4H), 6.77 (d, *J* = 8 Hz, 1H), 6.31 (d, *J* = 7 Hz, 1H) ppm.

^{13}C NMR (100 MHz, acetone-d_6) δ 197.6, 163.1 (d, $^1J_{C\text{-}F}$ = 243 Hz), 145.4, 136.7, 136.1, 135.5 (d, $^4J_{C\text{-}F}$ = 3 Hz), 133.5, 133.4, 131.8, 131.3 (d, $^3J_{C\text{-}F}$ = 8 Hz), 130.6, 129.8, 129.6, 129.5, 128.7, 128.6,128.4, 128.0, 126.9, 126.6, 125.2, 122.7, 119.6, 116.4 (d, $^2J_{C\text{-}F}$ = 22 Hz), 106.2, 61.9 ppm.

^{19}F NMR (282 MHz, acetone-d_6) δ –115.8 ppm.

HRMS (ESI+) Calcd for $C_{28}H_{21}FNO$ $[M+H]^+$: 406.1607, found: 406.1597.





3z

(*S*)-2-(4-Fluorophenyl)-2-(naphthalen-1-ylamino)-1-(naphthalen-2-yl)ethan-1-one (3z) was prepared as a yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 26.3 mg, 65% yield, 88% ee).

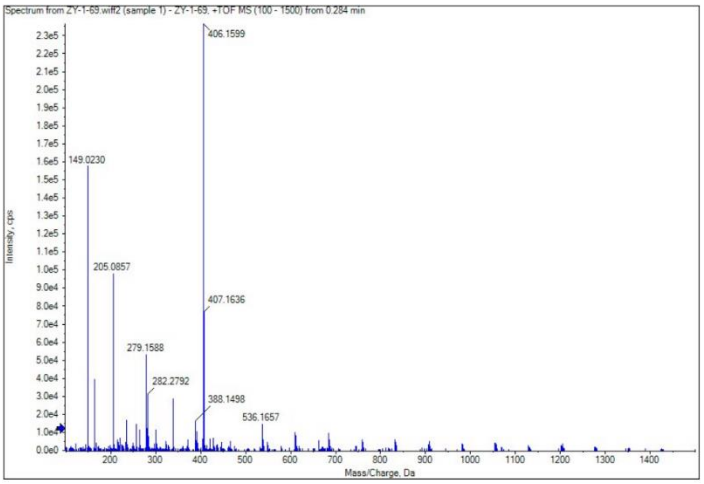
$[\alpha]_D^{25}$: –95.4 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 18.6 min (major), 15.2 min (minor).

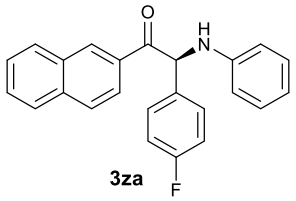
^{1}H NMR (300 MHz, acetone-d_6) δ 9.05 (s, 1H), 8.23 – 8.13 (m, 3H), 8.02 – 7.95 (m, 2H), 7.83 – 7.79 (m, 3H), 7.70 – 7.60 (m, 2H), 7.55 – 7.45 (m, 2H), 7.23 – 7.21 (m, 2H), 7.08 – 7.02 (m, 2H), 6.80 – 6.75 (m, 2H, overlap with the proton of NH), 6.62 (d, *J* = 7 Hz, 1H) ppm.

^{13}C NMR (75 MHz, acetone-d_6) δ 197.8, 163.1 (d, $^1J_{C\text{-}F}$ = 244 Hz), 142.2, 136.7, 135.4, 135.3 (d, $^4J_{C\text{-}F}$ = 3 Hz), 133.5, 133.2, 131.9, 131.3 (d, $^3J_{C\text{-}F}$ = 8 Hz), 130.6, 129.8, 129.5, 129.3, 128.7, 127.9, 127.2, 126.6, 125.6, 125.2, 124.6, 121.3, 118.3, 116.4 (d, $^2J_{C\text{-}F}$ = 22 Hz), 106.5, 61.9 ppm.

^{19}F NMR (282 MHz, acetone-d_6) δ –115.7 ppm

HRMS (ESI+) Calcd for $C_{28}H_{21}FNO$ $[M+H]^+$: 406.1607, found: 406.1599.





3za

(S)-2-(4-Fluorophenyl)-1-(naphthalen-2-yl)-2-(phenylamino)ethan-1-one (3za) was prepared as a yellow oil according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 20.2 mg, 57% yield, 92% ee).

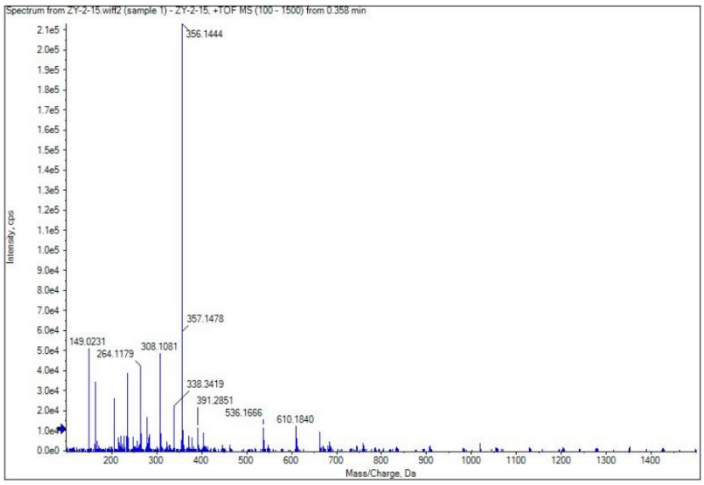
$[\alpha]_D^{25}$: –35.8 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 18.8 min (major), 17.4 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 8.98 (s, 1H), 8.14 – 8.09 (m, 2H), 8.00 – 7.95 (m, 2H), 7.72 – 7.60 (m, 4H), 7.10 – 7.03 (m, 4H), 6.85 (d, *J* = 8 Hz, 2H), 6.62 – 6.58 (m, 2H, overlap with proton of NH), 5.99 (d, *J* = 7 Hz, 1H) ppm.

^{13}C NMR (100 MHz, acetone-d_6) δ 196.9, 162.2 (d, $^1J_{C\text{-}F}$ = 243 Hz), 146.7, 135.7, 134.8 (d, $^4J_{C\text{-}F}$ = 3 Hz), 132.6, 132.5, 130.9, 130.3 (d, $^3J_{C\text{-}F}$ = 8 Hz), 129.7, 128.9 (two carbon), 128.6, 127.7, 127.0, 124.3, 117.2, 115.4 (d, $^2J_{C\text{-}F}$ = 22 Hz), 113.6, 60.8 ppm.

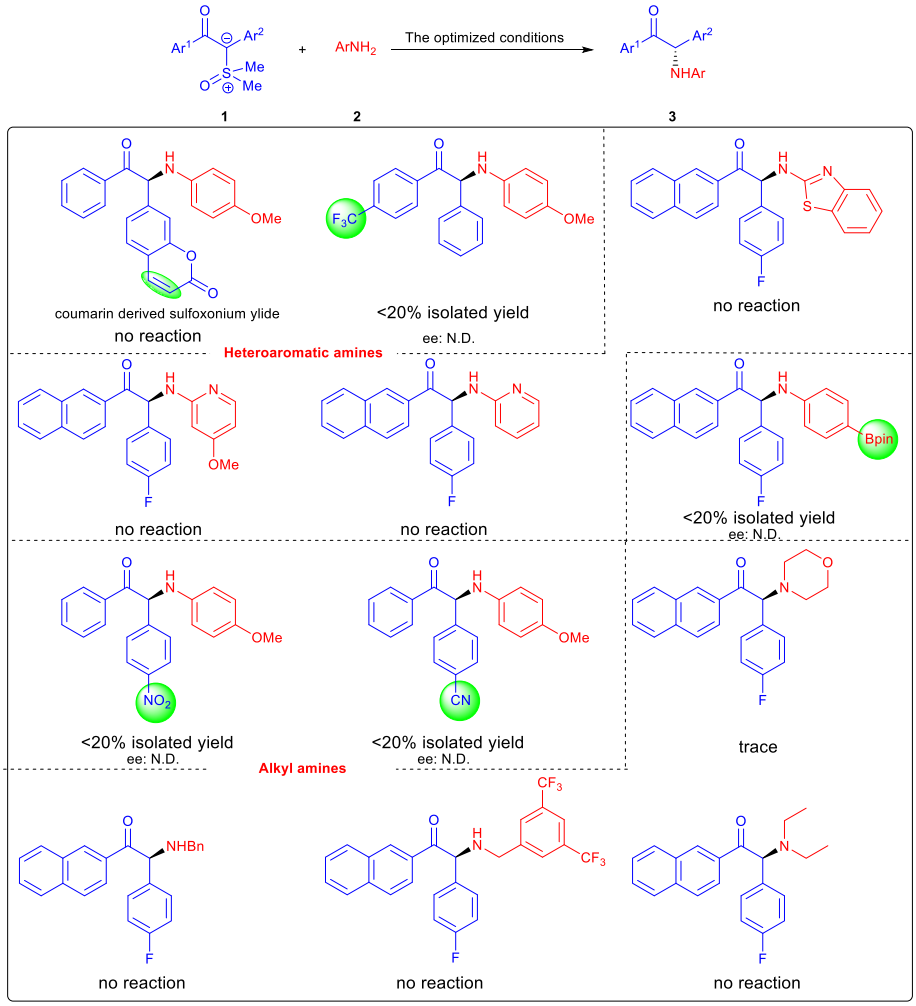
^{19}F NMR (376 MHz, acetone-d_6) δ –115.9 ppm

HRMS (ESI+) Calcd for $C_{24}H_{19}FNO$ $[M+H]^+$: 356.1451, found: 356.1444.

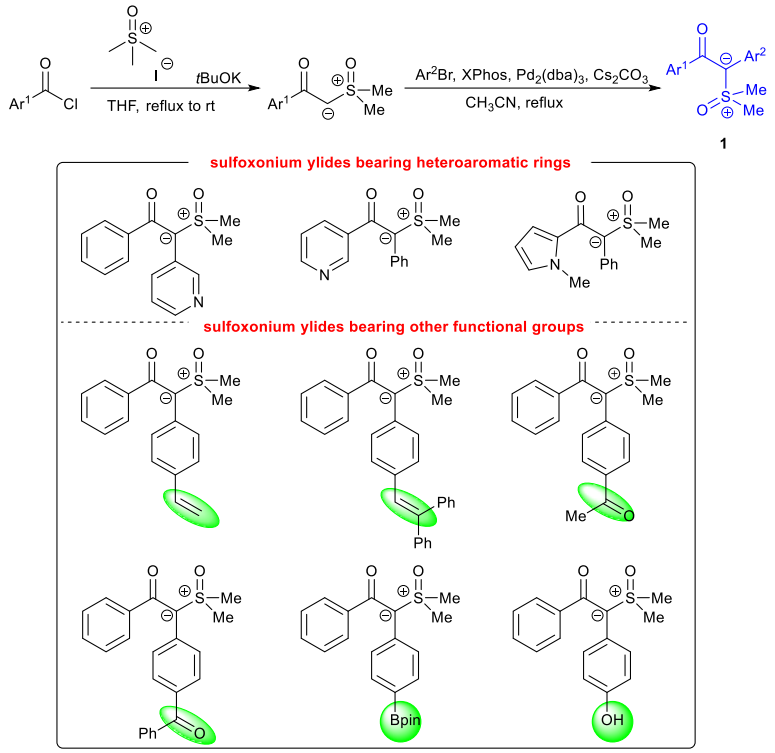


V. Some Unsuccessful Examples

(a) No desired products **3** could be detected or **3** was isolated in very low yields.

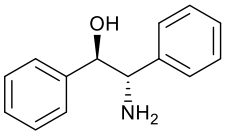


(b) We failed to prepare the following sulfoxonium ylides.



VI. The Procedure for Synthetic Transformation

4a was prepared based on the reported procedure:[3]



4a

(1*R*,2*S*)-2-amino-1,2-diphenylethan-1-ol (4a) was prepared from **3a** (95.2 mg, 0.3 mmol, 1.0 equiv) as a light-yellow solid (eluent: hexanes/EtOAc = 10:1 to 5:1, 41.6 mg, 65% yield, 99% ee after recrystallization).

$[\alpha]_D^{25}$: –17.4 (*c* = 0.4, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 20% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 10.8 min (major), 10.2 min (minor).

3 J. Wang, X. Lin, P.-L. Shao, J. Song, J. Wen, and X. Zhang, *ACS Catal.*, 2021, **11**, 12729–12735

^{1}H NMR (300 MHz, $CDCl_3$) 7.30 – 7.20 (m, 10H), 4.72 (d, *J* = 6 Hz, 2H), 4.14 (d, *J* = 6 Hz 2H), 1.60 (br, 3H) ppm.

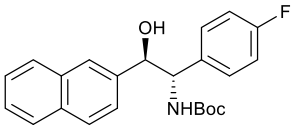
^{13}C NMR (75 MHz, $CDCl_3$) δ 141.5, 140.7, 128.3, 128.2, 127.8, 127.7, 127.6, 127.0, 78.4, 61.9 ppm.

It's a known compound.[3]

General procedure for synthesis of 1,2-aminoalcohol bearing different aryl groups:

(1) To a solution of selected enantioenriched amino ketone **3** (0.3 mmol) and Boc_2O (131 mg, 0.6 mmol, 2.0 equiv) in CH_3CN (5.0 mL) was added the aqueous solution of $Ce(NH_4)_2(NO_3)_6$ (CAN) (657.9 mg, 1.2 mmol, 4.0 equiv in 3 mL H_2O) at 0 °C. Upon addition of CAN, the color of the reaction mixture suddenly becomes dark brown, and then gradually turned to light brown during reaction. After being stirred at the same temperature for 12 h, the reaction mixture was diluted with diethyl ether (10 mL) and washed with $NaHCO_3$. The aqueous layer was extracted with diethyl ether (3*10 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered, and concentrated. The residue was directly used for next step without further purification.

(2) The residue was dissolved in EtOH (5 mL), and cooled to –10 °C. Then, $NaBH_4$ (68.1 mg, 6.0 equiv refers to the amount of aminoketone **3**) was added in one-partition. The reaction mixture was stirred at the same temperature for 4 h, then quenched with slow addition of NH_4Cl (5 mL). The resulted mixture was extracted with DCM (3*10 mL), the combined organic layers were dried over anhydrous Na_2SO_4, filtered, and concentrated in vacuo. The residue was subjected to flash column chromatography on silica gel (eluent: hexanes/EtOAc = 10:1 to 5:1) to afford the desired the product a colorless solid.



4m

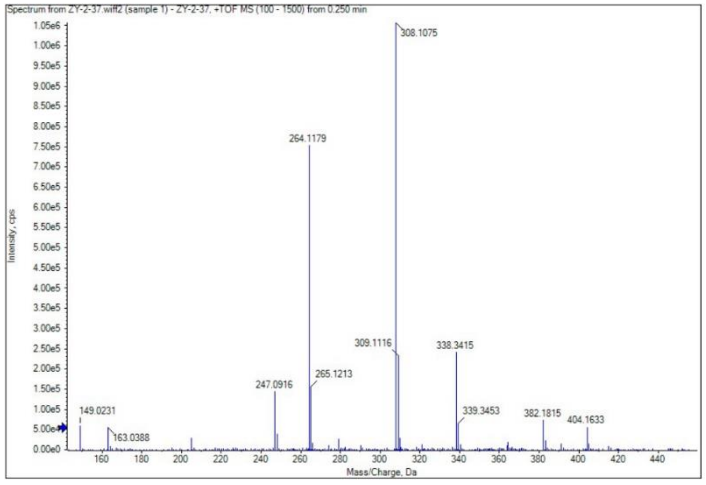
(1*R*,2*S*)-2-amino-2-(4-fluorophenyl)-1-(naphthalen-2-yl)ethan-1-ol (4m) was prepared as a colorless solid from **3m** (115.6 mg, 0.3 mmol, 1.0 equiv) according to the General Procedure (eluent: hexanes/EtOAc = 10:1 to 5:1, 41.2 mg, 36% yield, 89% ee). $[\alpha]_D^{25}$: –71.112 (*c* = 0.18, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 7.8 min (major), 9.2 min (minor).

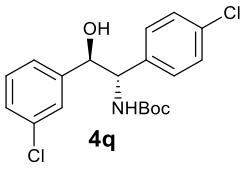
^{1}H NMR (400 MHz, DMSO-d_6) 7.87 – 7.80 (m, 4H), 7.52 – 7.44 (m, 3H), 7.36 – 7.33 (m, 3H), 7.10 – 7.06 (m, 2H), 5.50 (d, *J* = 5 Hz, 1H), 4.83 – 4.80 (m, 1H), 4.72 – 4.67 (m, 1H), 1.11 (s, 9H) ppm.

^{13}C NMR (100 MHz, DMSO-d_6) δ 161.6 (d, $^1J_{C\text{-}F}$ = 240 Hz), 155.0, 141.3, 138.1 (d, $^4J_{C\text{-}F}$ = 3 Hz), 133.0, 132.8, 130.4 (d, $^3J_{C\text{-}F}$ = 8 Hz), 128.1, 128.0, 127.4, 126.3, 126.1, 125.7, 114.7 (d, $^2J_{C\text{-}F}$ = 21 Hz), 78.2, 75.7, 59.8, 28.4 ppm.

^{19}F NMR (376 MHz, DMSO-d_6) δ –116.4 ppm.

HRMS (ESI+) Calcd for $C_{23}H_{25}FNO_3$ $[M+H]^+$: 382.1818, found: 382.1815.





4q

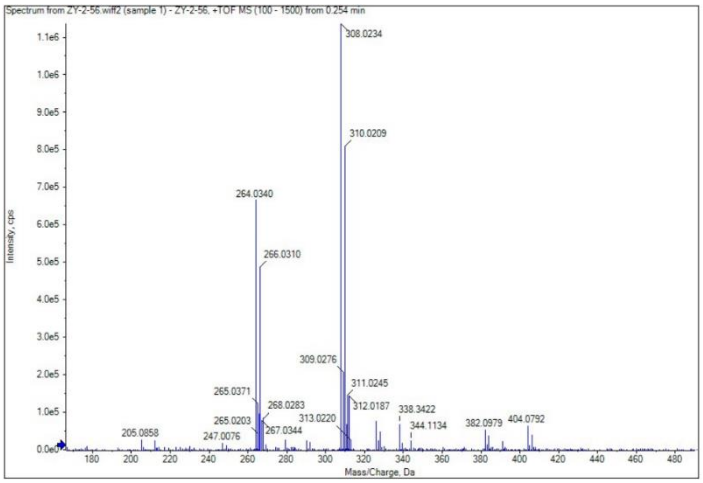
Tert-butyl((1*S*,2*R*)-2-(3-chlorophenyl)-1-(4-chlorophenyl)-2-hydroxyethyl) carbamate (4q) was prepared as a light-yellow oil from **3q** (115.6 mg, 0.3 mmol, 1.0 equiv) according to the General Procedure (eluent: hexanes/EtOAc = 10:1, 26.4 mg, 23% yield, 85% ee).

$[\alpha]_D^{25}$: –33.0 (*c* = 0.2, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 6.9 min (major), 8.4 min (minor).

^{1}H NMR (400 MHz, DMSO) 7.42 – 7.25 (m, 8H), 5.53 (d, *J* = 5 Hz, 1H), 4.63 – 4.51 (m, 2H), 3.36 (s, 1H), 1.21 (s, 9H) ppm.

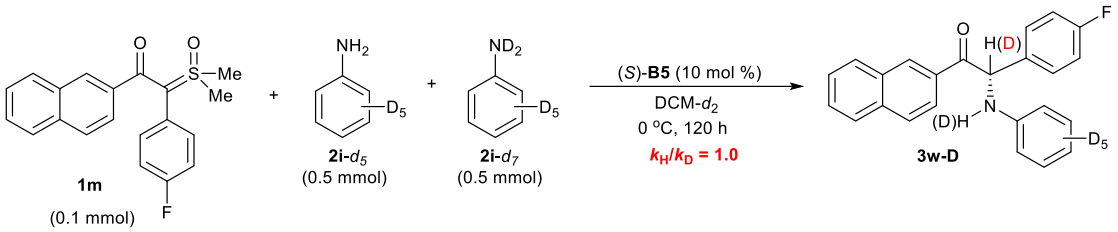
^{13}C NMR (100 MHz, DMSO) δ 154.9, 146.3, 140.8, 132.7, 131.8, 130.4, 129.9, 128.0, 127.4, 127.3, 126.1, 78.3, 74.9, 59.8, 28.5 ppm.

HRMS (ESI+) Calcd for $C_{19}H_{22}Cl_2NO_3$ $[M+H]^+$: 382.0977, found: 382.0979.



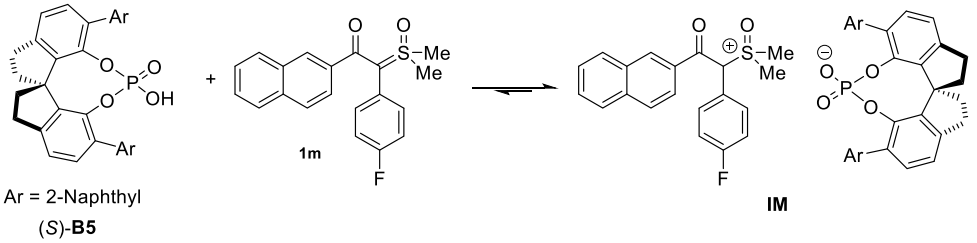
VII. Mechanistic Study

Kinetic isotope effect (KIE)

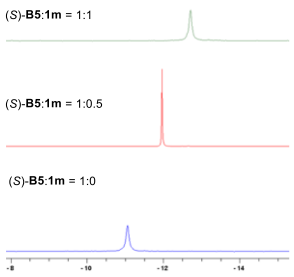


At room temperature, to a solution of (*S*)-**B5** (5.6 mg, 10 mol%), aniline-d5 (49.1 mg, 0.5 mmol, 5.0 equiv), and aniline-d7 (50.1 mg, 5.0 mmol, 5.0 equiv) in CD_2Cl_2 (0.25 mL). The resulted solution was cooled to 0 °C, and then addition of the solution of sulfonium ylide **1a** (0.1 mmol, 34 mg, 1.0 equiv, in 0.25 mL CD_2Cl_2) in one portion. The reaction mixture was stirred at 0 °C until full conversion of 1m (~120 h). The mixture was transferred to an NMR tube for analysis, which indicated 50% D-incorporation at the α-position in the **3w** product.

The reversible protonation:



entry	(*S*)-**B5**:**1m**	δ (^{31}P NMR) ppm	the plot
1	1:0	–11.06	
2	1:0.5	–11.96	

3	1:1	–12.70	

VIII. The Stereochemistry of Product

The absolute stereochemistry of the product derivative **3m** was determined by X-ray crystallography. The X-ray data have been deposited at the Cambridge Crystallographic Data Center (2219238). The stereochemistry of other products was assumed by analogy.

The single crystal of compound **3m** was obtained by slow evaporation of its solution in hexanes/EtOAc (20:1) at 0 °C.

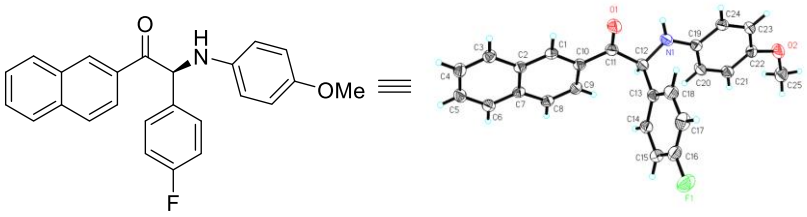


Table 1. Crystal data and structure refinement for **3m**.

Identification code	**3m**	
Empirical formula	$C_{25}H_{20}FNO_2$	
Formula weight	385.42	
Temperature	293(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 10.7905(3) Å	α= 90°.

	b = 6.0625(2) Å	β= 107.9640(10)°.
	c = 15.4957(4) Å	γ = 90°.
Volume	964.27(5) $Å^3$	
Z	2	
Density (calculated)	1.327 Mg/m^3	
Absorption coefficient	0.734 mm^{-1}	
F(000)	404	
Crystal size	0.200 x 0.160 x 0.120 mm^3	
Theta range for data collection	4.307 to 67.953°.	
Index ranges	-12<=h<=12, -6<=k<=7, -18<=l<=16	
Reflections collected	15778	
Independent reflections	3354 [R(int) = 0.0381]	
Completeness to theta = 67.679°	96.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7533 and 0.4911	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3354 / 1 / 264	
Goodness-of-fit on F^2	1.045	
Final R indices [I>2sigma(I)]	R1 = 0.0321, wR2 = 0.0867	
R indices (all data)	R1 = 0.0326, wR2 = 0.0873	
Absolute structure parameter	0.04(6)	
Extinction coefficient	0.031(8)	
Largest diff. peak and hole	0.146 and -0.125 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3m**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1)	10517(2)	2256(4)	9597(1)	88(1)
O(1)	5716(2)	1732(3)	5550(1)	64(1)
O(2)	2851(2)	6732(4)	9456(1)	72(1)
N(1)	4927(2)	3825(4)	6784(1)	56(1)
C(1)	7287(2)	3419(3)	4585(1)	41(1)
C(2)	8083(2)	4301(3)	4093(1)	40(1)
C(3)	8336(2)	3150(4)	3375(1)	48(1)
C(4)	9113(2)	4048(4)	2919(2)	55(1)
C(5)	9690(2)	6129(4)	3168(2)	54(1)
C(6)	9463(2)	7290(4)	3851(1)	48(1)
C(7)	8645(2)	6428(3)	4333(1)	41(1)
C(8)	8359(2)	7603(3)	5033(1)	45(1)
C(9)	7586(2)	6720(3)	5491(1)	45(1)
C(10)	7053(2)	4569(3)	5285(1)	40(1)
C(11)	6242(2)	3495(4)	5788(1)	45(1)
C(12)	6128(2)	4568(4)	6658(1)	45(1)
C(13)	7333(2)	3963(3)	7449(1)	43(1)
C(14)	8353(2)	5430(4)	7794(2)	50(1)
C(15)	9430(2)	4865(5)	8520(2)	57(1)
C(16)	9468(2)	2819(5)	8888(2)	58(1)
C(17)	8488(3)	1318(4)	8575(2)	64(1)
C(18)	7421(2)	1901(4)	7849(2)	56(1)
C(19)	4516(2)	4554(4)	7505(1)	43(1)
C(20)	4932(2)	6517(4)	7961(2)	51(1)
C(21)	4418(2)	7289(4)	8622(2)	51(1)
C(22)	3469(2)	6091(4)	8837(1)	50(1)
C(23)	3073(2)	4097(4)	8410(1)	50(1)
C(24)	3591(2)	3322(4)	7760(1)	46(1)
C(25)	3285(3)	8686(5)	9951(2)	75(1)

Table 3. Bond lengths [Å] and angles [°] for **3m**.

F(1)-C(16)	1.356(3)
O(1)-C(11)	1.213(3)
O(2)-C(22)	1.382(3)
O(2)-C(25)	1.411(3)
N(1)-C(19)	1.395(3)
N(1)-C(12)	1.441(2)
N(1)-H(1)	0.8600
C(1)-C(10)	1.376(3)
C(1)-C(2)	1.417(3)
C(1)-H(1A)	0.9300
C(2)-C(3)	1.410(3)
C(2)-C(7)	1.425(3)
C(3)-C(4)	1.365(3)
C(3)-H(3)	0.9300
C(4)-C(5)	1.407(4)
C(4)-H(4)	0.9300
C(5)-C(6)	1.355(3)
C(5)-H(5)	0.9300
C(6)-C(7)	1.421(3)
C(6)-H(6)	0.9300
C(7)-C(8)	1.409(3)
C(8)-C(9)	1.361(3)
C(8)-H(8)	0.9300
C(9)-C(10)	1.421(3)
C(9)-H(9)	0.9300
C(10)-C(11)	1.489(3)
C(11)-C(12)	1.535(3)
C(12)-C(13)	1.532(3)
C(12)-H(12)	0.9800
C(13)-C(18)	1.385(3)
C(13)-C(14)	1.388(3)
C(14)-C(15)	1.388(3)
C(14)-H(14)	0.9300
C(15)-C(16)	1.360(4)
C(15)-H(15)	0.9300
C(16)-C(17)	1.365(4)

C(17)-C(18)	1.385(3)
C(17)-H(17)	0.9300
C(18)-H(18)	0.9300
C(19)-C(20)	1.387(3)
C(19)-C(24)	1.398(3)
C(20)-C(21)	1.388(3)
C(20)-H(20)	0.9300
C(21)-C(22)	1.377(3)
C(21)-H(21)	0.9300
C(22)-C(23)	1.381(3)
C(23)-C(24)	1.376(3)
C(23)-H(23)	0.9300
C(24)-H(24)	0.9300
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600
C(25)-H(25C)	0.9600

C(22)-O(2)-C(25)	117.60(19)
C(19)-N(1)-C(12)	122.05(17)
C(19)-N(1)-H(1)	119.0
C(12)-N(1)-H(1)	119.0
C(10)-C(1)-C(2)	121.43(17)
C(10)-C(1)-H(1A)	119.3
C(2)-C(1)-H(1A)	119.3
C(3)-C(2)-C(1)	122.34(18)
C(3)-C(2)-C(7)	118.90(18)
C(1)-C(2)-C(7)	118.75(17)
C(4)-C(3)-C(2)	120.7(2)
C(4)-C(3)-H(3)	119.6
C(2)-C(3)-H(3)	119.6
C(3)-C(4)-C(5)	120.4(2)
C(3)-C(4)-H(4)	119.8
C(5)-C(4)-H(4)	119.8
C(6)-C(5)-C(4)	120.6(2)
C(6)-C(5)-H(5)	119.7
C(4)-C(5)-H(5)	119.7
C(5)-C(6)-C(7)	120.7(2)
C(5)-C(6)-H(6)	119.6

C(7)-C(6)-H(6)	119.6
C(8)-C(7)-C(6)	122.55(19)
C(8)-C(7)-C(2)	118.80(17)
C(6)-C(7)-C(2)	118.65(18)
C(9)-C(8)-C(7)	121.17(18)
C(9)-C(8)-H(8)	119.4
C(7)-C(8)-H(8)	119.4
C(8)-C(9)-C(10)	120.94(18)
C(8)-C(9)-H(9)	119.5
C(10)-C(9)-H(9)	119.5
C(1)-C(10)-C(9)	118.83(18)
C(1)-C(10)-C(11)	118.12(17)
C(9)-C(10)-C(11)	123.05(17)
O(1)-C(11)-C(10)	121.44(18)
O(1)-C(11)-C(12)	118.88(19)
C(10)-C(11)-C(12)	119.58(17)
N(1)-C(12)-C(13)	113.20(17)
N(1)-C(12)-C(11)	107.80(16)
C(13)-C(12)-C(11)	108.83(16)
N(1)-C(12)-H(12)	109.0
C(13)-C(12)-H(12)	109.0
C(11)-C(12)-H(12)	109.0
C(18)-C(13)-C(14)	118.0(2)
C(18)-C(13)-C(12)	119.88(18)
C(14)-C(13)-C(12)	122.12(19)
C(15)-C(14)-C(13)	121.3(2)
C(15)-C(14)-H(14)	119.3
C(13)-C(14)-H(14)	119.3
C(16)-C(15)-C(14)	118.3(2)
C(16)-C(15)-H(15)	120.8
C(14)-C(15)-H(15)	120.8
F(1)-C(16)-C(15)	118.6(2)
F(1)-C(16)-C(17)	118.8(2)
C(15)-C(16)-C(17)	122.6(2)
C(16)-C(17)-C(18)	118.5(2)
C(16)-C(17)-H(17)	120.8
C(18)-C(17)-H(17)	120.8
C(17)-C(18)-C(13)	121.3(2)

C(17)-C(18)-H(18)	119.4
C(13)-C(18)-H(18)	119.4
C(20)-C(19)-N(1)	123.22(19)
C(20)-C(19)-C(24)	117.46(19)
N(1)-C(19)-C(24)	119.24(19)
C(19)-C(20)-C(21)	121.73(19)
C(19)-C(20)-H(20)	119.1
C(21)-C(20)-H(20)	119.1
C(22)-C(21)-C(20)	119.8(2)
C(22)-C(21)-H(21)	120.1
C(20)-C(21)-H(21)	120.1
C(21)-C(22)-O(2)	125.0(2)
C(21)-C(22)-C(23)	119.30(19)
O(2)-C(22)-C(23)	115.72(19)
C(24)-C(23)-C(22)	120.90(18)
C(24)-C(23)-H(23)	119.5
C(22)-C(23)-H(23)	119.5
C(23)-C(24)-C(19)	120.76(19)
C(23)-C(24)-H(24)	119.6
C(19)-C(24)-H(24)	119.6
O(2)-C(25)-H(25A)	109.5
O(2)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
O(2)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3m**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F(1)	82(1)	111(2)	59(1)	16(1)	2(1)	15(1)
O(1)	72(1)	59(1)	71(1)	-22(1)	35(1)	-26(1)
O(2)	75(1)	86(1)	69(1)	-22(1)	43(1)	-21(1)
N(1)	43(1)	69(1)	61(1)	-20(1)	24(1)	-16(1)
C(1)	39(1)	36(1)	43(1)	-3(1)	7(1)	-1(1)
C(2)	36(1)	41(1)	38(1)	1(1)	5(1)	3(1)
C(3)	47(1)	49(1)	47(1)	-7(1)	12(1)	2(1)
C(4)	50(1)	70(2)	47(1)	-3(1)	17(1)	8(1)
C(5)	46(1)	66(1)	49(1)	11(1)	16(1)	2(1)
C(6)	44(1)	50(1)	47(1)	11(1)	9(1)	-1(1)
C(7)	39(1)	40(1)	38(1)	4(1)	4(1)	2(1)
C(8)	48(1)	37(1)	44(1)	-2(1)	7(1)	-5(1)
C(9)	51(1)	41(1)	42(1)	-6(1)	13(1)	-1(1)
C(10)	37(1)	41(1)	41(1)	-2(1)	9(1)	2(1)
C(11)	40(1)	46(1)	48(1)	-6(1)	13(1)	-4(1)
C(12)	40(1)	46(1)	52(1)	-5(1)	19(1)	-5(1)
C(13)	45(1)	44(1)	44(1)	-6(1)	20(1)	-2(1)
C(14)	51(1)	49(1)	50(1)	-2(1)	17(1)	-8(1)
C(15)	53(1)	70(2)	46(1)	-6(1)	13(1)	-11(1)
C(16)	58(1)	71(2)	43(1)	2(1)	14(1)	9(1)
C(17)	82(2)	51(1)	62(1)	8(1)	25(1)	7(1)
C(18)	62(1)	49(1)	59(1)	-1(1)	19(1)	-10(1)
C(19)	36(1)	49(1)	46(1)	-1(1)	12(1)	0(1)
C(20)	45(1)	52(1)	63(1)	-6(1)	26(1)	-10(1)
C(21)	53(1)	48(1)	56(1)	-9(1)	20(1)	-7(1)
C(22)	46(1)	61(1)	44(1)	0(1)	16(1)	-1(1)
C(23)	45(1)	59(1)	48(1)	4(1)	18(1)	-11(1)
C(24)	42(1)	45(1)	48(1)	-1(1)	10(1)	-6(1)
C(25)	87(2)	76(2)	71(2)	-16(1)	40(1)	-6(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **3m**.

	x	y	z	U(eq)
H(1)	4448	2903	6402	67
H(1A)	6916	2032	4432	49
H(3)	7971	1764	3210	58
H(4)	9260	3281	2440	66
H(5)	10233	6711	2862	64
H(6)	9847	8668	4005	58
H(8)	8704	9008	5184	54
H(9)	7404	7535	5946	54
H(12)	6094	6174	6581	54
H(14)	8315	6820	7533	59
H(15)	10108	5859	8749	68
H(17)	8536	-64	8844	77
H(18)	6750	890	7626	68
H(20)	5571	7339	7820	62
H(21)	4714	8610	8920	62
H(23)	2448	3266	8564	60
H(24)	3324	1963	7488	55
H(25A)	3217	9894	9538	112
H(25B)	4177	8514	10317	112
H(25C)	2757	8981	10336	112

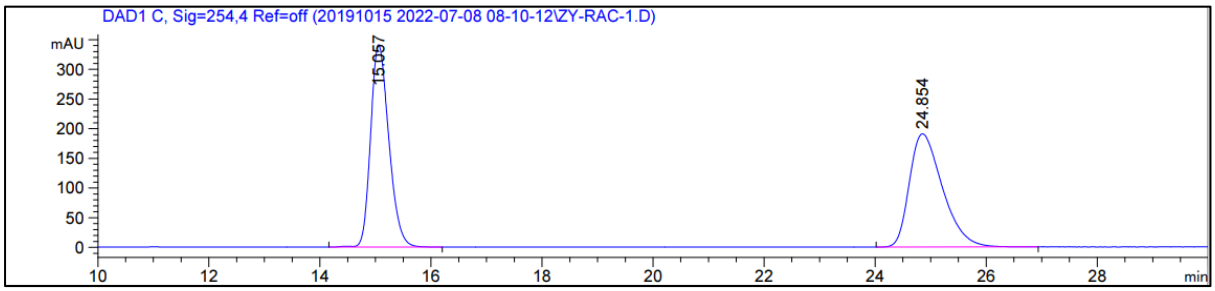
Table 6. Torsion angles [°] for **3m**.

C(10)-C(1)-C(2)-C(3)	179.92(17)
C(10)-C(1)-C(2)-C(7)	-0.1(3)
C(1)-C(2)-C(3)-C(4)	-179.70(18)
C(7)-C(2)-C(3)-C(4)	0.3(3)
C(2)-C(3)-C(4)-C(5)	1.0(3)
C(3)-C(4)-C(5)-C(6)	-1.4(3)
C(4)-C(5)-C(6)-C(7)	0.5(3)
C(5)-C(6)-C(7)-C(8)	-178.47(18)
C(5)-C(6)-C(7)-C(2)	0.9(3)
C(3)-C(2)-C(7)-C(8)	178.11(17)
C(1)-C(2)-C(7)-C(8)	-1.9(2)
C(3)-C(2)-C(7)-C(6)	-1.3(3)
C(1)-C(2)-C(7)-C(6)	178.76(16)
C(6)-C(7)-C(8)-C(9)	-179.06(18)
C(2)-C(7)-C(8)-C(9)	1.6(3)
C(7)-C(8)-C(9)-C(10)	0.7(3)
C(2)-C(1)-C(10)-C(9)	2.3(3)
C(2)-C(1)-C(10)-C(11)	-178.02(16)
C(8)-C(9)-C(10)-C(1)	-2.6(3)
C(8)-C(9)-C(10)-C(11)	177.72(18)
C(1)-C(10)-C(11)-O(1)	-5.6(3)
C(9)-C(10)-C(11)-O(1)	174.0(2)
C(1)-C(10)-C(11)-C(12)	170.92(17)
C(9)-C(10)-C(11)-C(12)	-9.4(3)
C(19)-N(1)-C(12)-C(13)	61.4(3)
C(19)-N(1)-C(12)-C(11)	-178.2(2)
O(1)-C(11)-C(12)-N(1)	-27.7(3)
C(10)-C(11)-C(12)-N(1)	155.73(18)
O(1)-C(11)-C(12)-C(13)	95.5(2)
C(10)-C(11)-C(12)-C(13)	-81.1(2)
N(1)-C(12)-C(13)-C(18)	41.3(3)
C(11)-C(12)-C(13)-C(18)	-78.6(2)
N(1)-C(12)-C(13)-C(14)	-138.0(2)
C(11)-C(12)-C(13)-C(14)	102.1(2)
C(18)-C(13)-C(14)-C(15)	-0.2(3)
C(12)-C(13)-C(14)-C(15)	179.04(19)

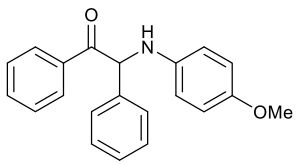
C(13)-C(14)-C(15)-C(16)	0.3(3)
C(14)-C(15)-C(16)-F(1)	180.0(2)
C(14)-C(15)-C(16)-C(17)	-0.5(4)
F(1)-C(16)-C(17)-C(18)	-179.9(2)
C(15)-C(16)-C(17)-C(18)	0.6(4)
C(16)-C(17)-C(18)-C(13)	-0.6(4)
C(14)-C(13)-C(18)-C(17)	0.4(3)
C(12)-C(13)-C(18)-C(17)	-178.9(2)
C(12)-N(1)-C(19)-C(20)	22.9(3)
C(12)-N(1)-C(19)-C(24)	-160.4(2)
N(1)-C(19)-C(20)-C(21)	174.2(2)
C(24)-C(19)-C(20)-C(21)	-2.5(3)
C(19)-C(20)-C(21)-C(22)	-0.1(3)
C(20)-C(21)-C(22)-O(2)	-177.4(2)
C(20)-C(21)-C(22)-C(23)	2.1(3)
C(25)-O(2)-C(22)-C(21)	-4.5(4)
C(25)-O(2)-C(22)-C(23)	175.9(2)
C(21)-C(22)-C(23)-C(24)	-1.5(3)
O(2)-C(22)-C(23)-C(24)	178.0(2)
C(22)-C(23)-C(24)-C(19)	-1.1(3)
C(20)-C(19)-C(24)-C(23)	3.1(3)
N(1)-C(19)-C(24)-C(23)	-173.79(19)

Symmetry transformations used to generate equivalent atoms:

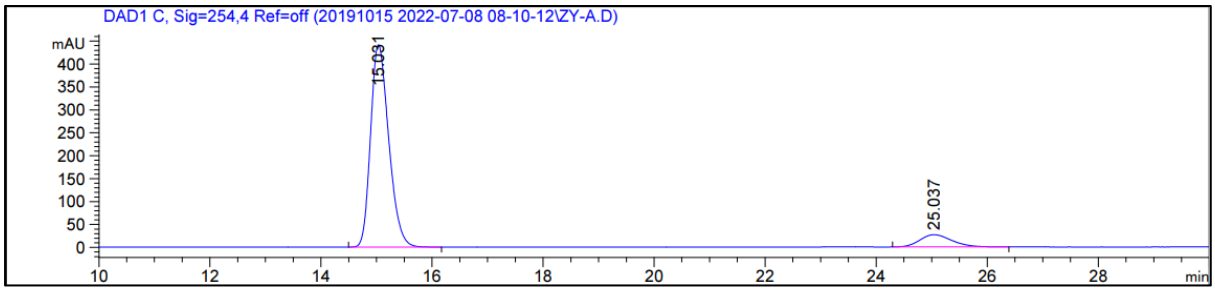
3a, HPLC conditions: Daicel CHIRALPAK® OD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



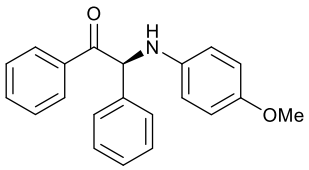
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	15.057	VB	0.3513	7775.93848	341.05212	49.6209
2	24.854	BB	0.6368	7894.74951	190.76564	50.3791



3a
racemic

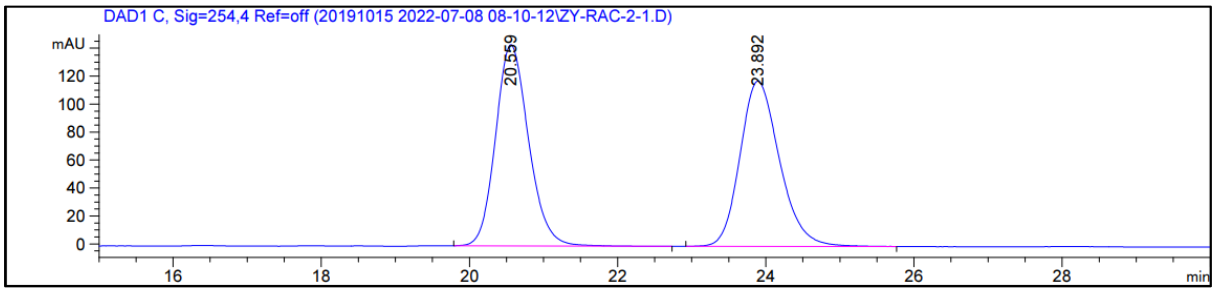


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	15.031	BB	0.3508	1.00167e4	441.26749	90.3332
2	25.037	BB	0.5979	1071.90906	26.72767	9.6668

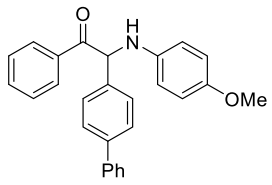


3a
enantioenriched

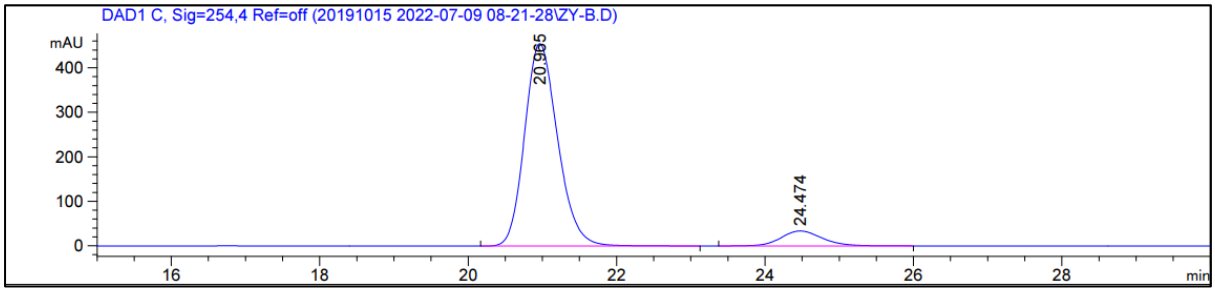
3b, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



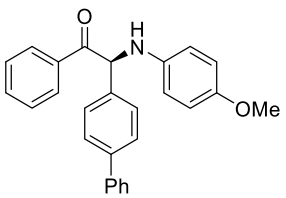
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	20.559	BB	0.4772	4454.99951	143.88319	50.4233
2	23.892	BB	0.5683	4380.19775	118.20825	49.5767



3b
racemic

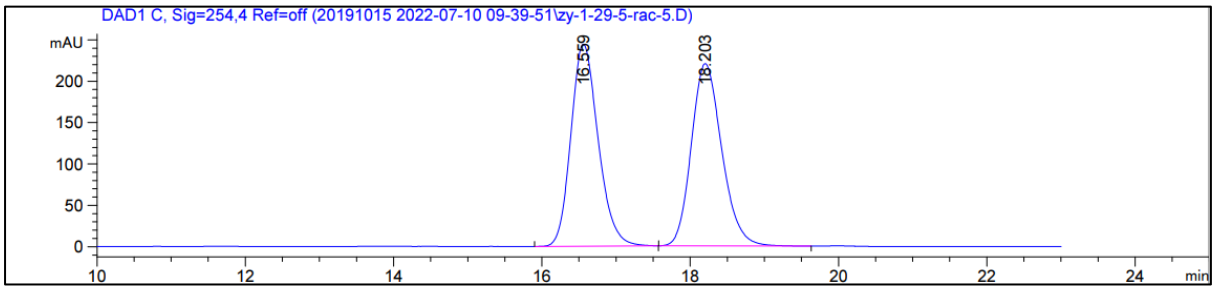


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	20.965	BB	0.4791	1.40769e4	454.83563	91.5252
2	24.474	BB	0.5843	1303.45642	33.62487	8.4748

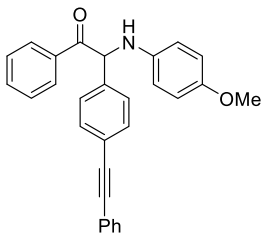


3b
enantioenriched

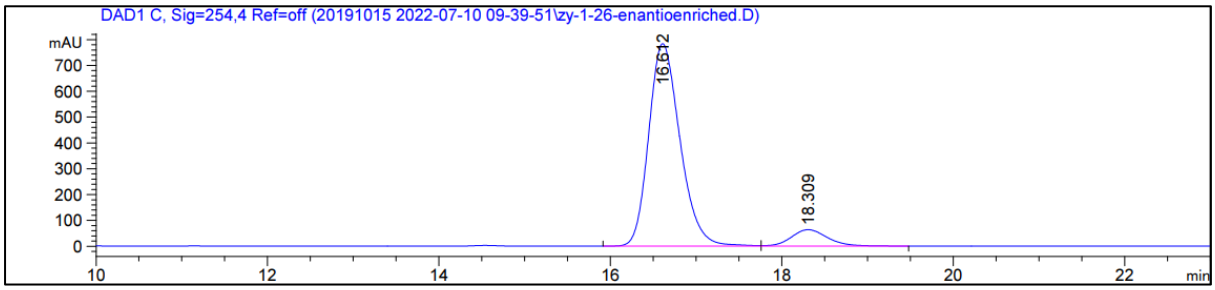
3c, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



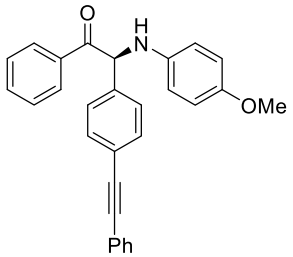
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.559	BB	0.3916	6229.21338	244.22531	49.8152
2	18.203	BB	0.4405	6275.42041	220.21399	50.1848



3c
racemic

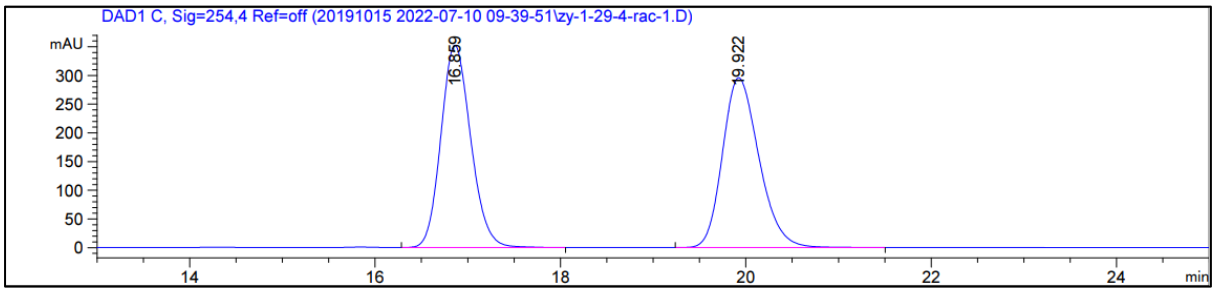


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.612	BV	0.3913	1.98458e4	784.07031	91.4936
2	18.309	VB	0.4517	1845.11768	63.36763	8.5064

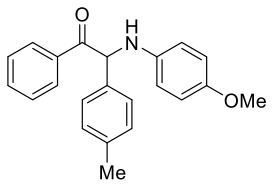


3c
enantioenriched

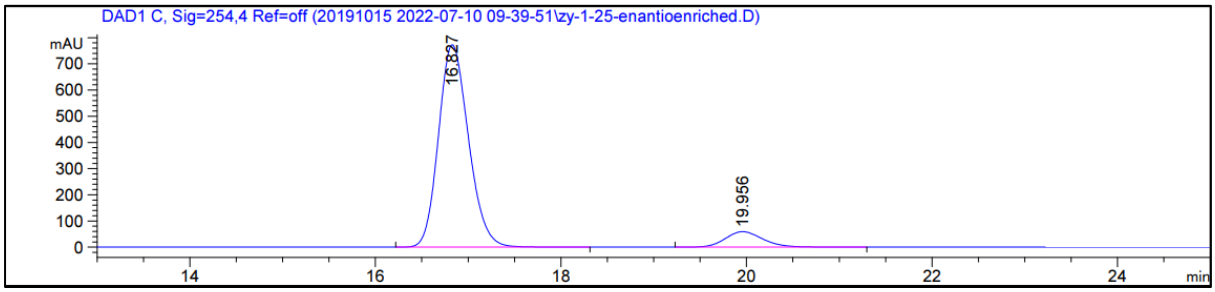
3d, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



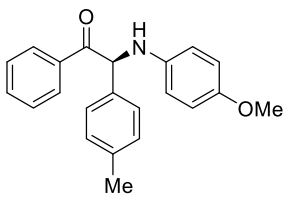
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.859	BB	0.3466	7876.24414	352.59164	49.3935
2	19.922	BB	0.4225	8069.67383	295.59326	50.6065



3d
racemic

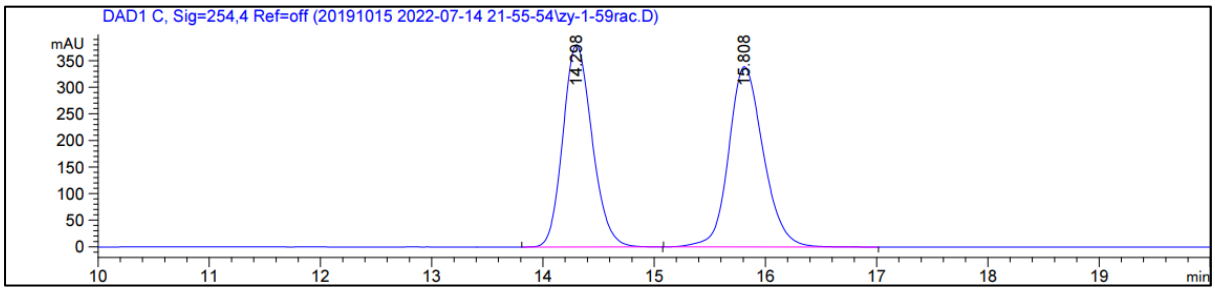


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.827	BB	0.3478	1.73465e4	773.08997	91.2318
2	19.956	BB	0.4269	1667.15039	59.14516	8.7682

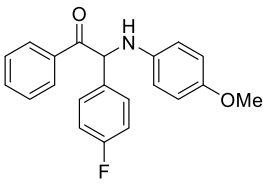


3d
enantioenriched

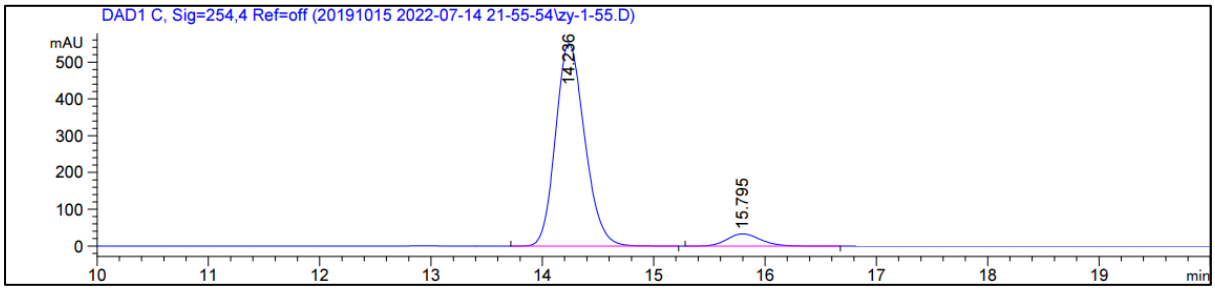
3e, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



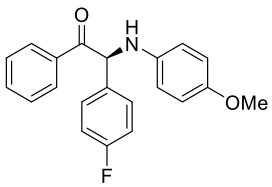
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	14.298	BB	0.2828	6940.29541	380.57504	48.6680
2	15.808	BB	0.3299	7320.18555	339.07407	51.3320



3e
racemic

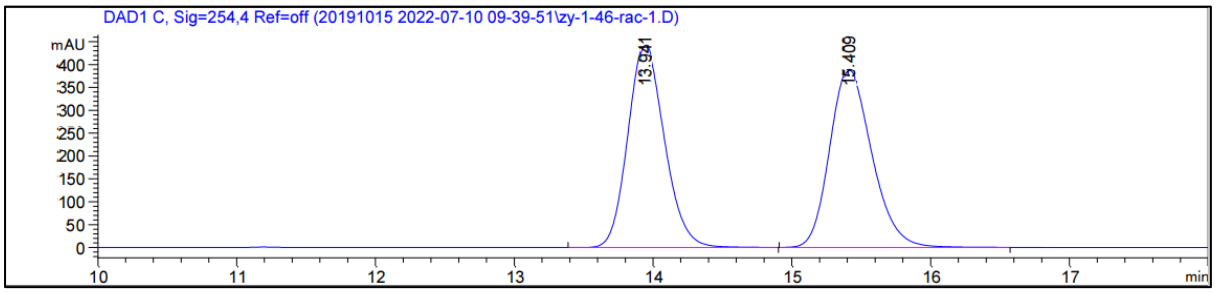


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	14.236	BB	0.2823	1.00147e4	550.36304	93.4765
2	15.795	BB	0.3274	698.89441	33.22435	6.5235

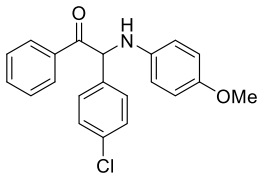


3e
enantioenriched

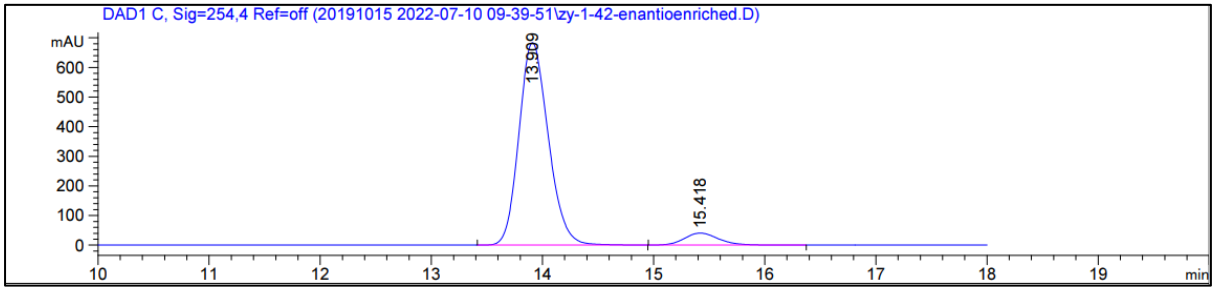
3f, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



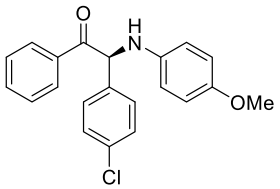
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.941	BB	0.2841	8125.21680	442.67456	49.7651
2	15.409	BB	0.3258	8201.91992	389.25922	50.2349



3f
racemic

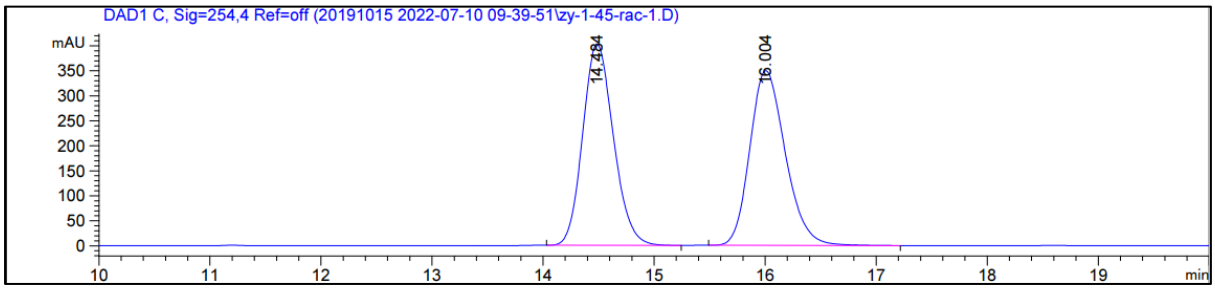


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.909	BB	0.2856	1.25139e4	683.54022	93.5875
2	15.418	BB	0.3280	857.44379	40.33133	6.4125

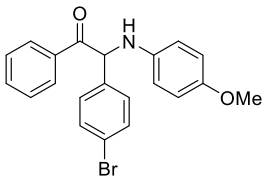


3f
enantioenriched

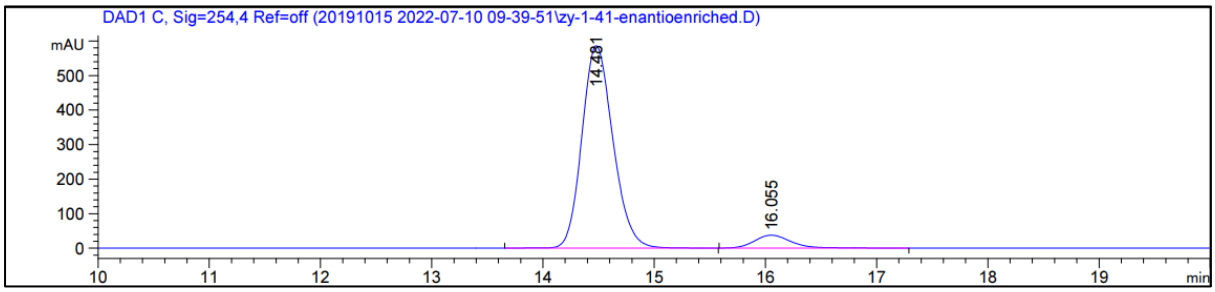
3g, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



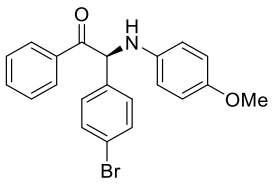
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	14.484	BB	0.2982	7742.84082	402.84247	49.9453
2	16.004	BB	0.3410	7759.79639	349.55884	50.0547



3g
racemic

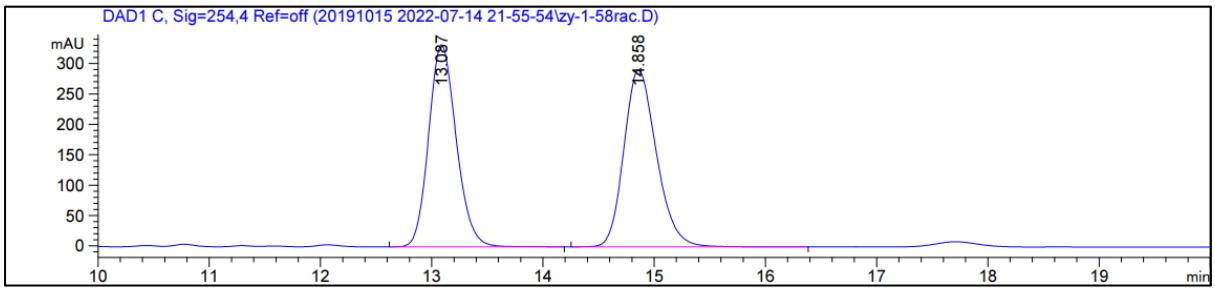


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	14.481	BB	0.3003	1.13652e4	586.02698	93.0116
2	16.055	BB	0.3487	853.91681	37.35254	6.9884

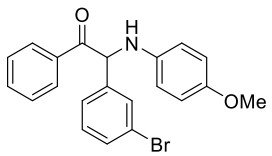


3g
enantioenriched

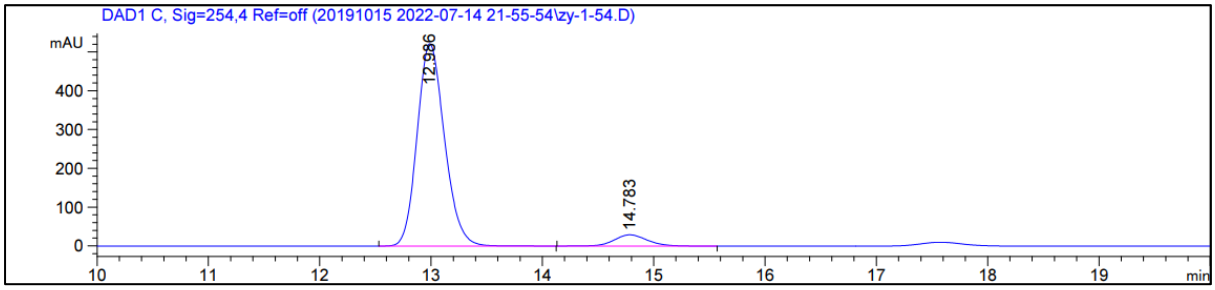
3h, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



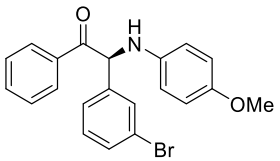
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.087	BB	0.2669	5725.53516	332.44357	49.1639
2	14.858	BB	0.3158	5920.27393	290.50995	50.8361



3h
racemic

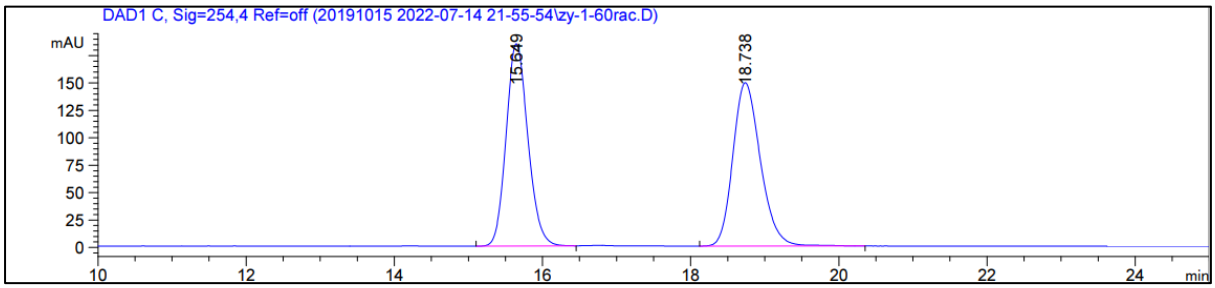


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.986	BB	0.2629	8895.15918	521.78088	93.6458
2	14.783	BB	0.3203	603.57068	29.06090	6.3542

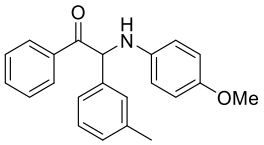


3h
enantioenriched

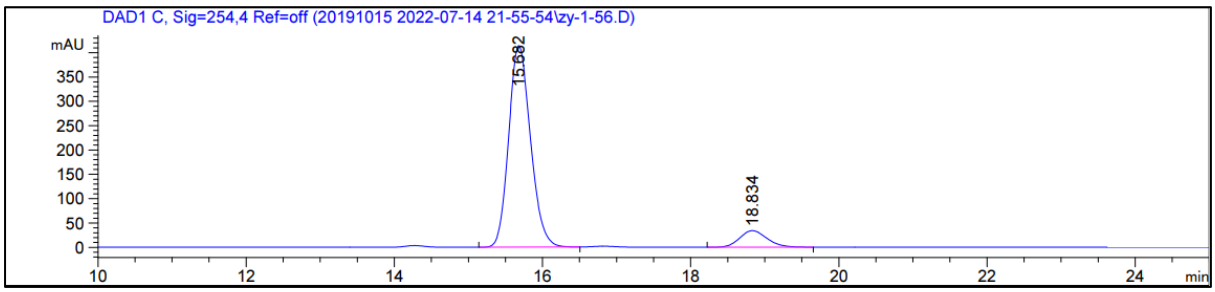
3i, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



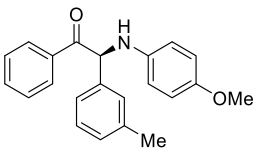
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	15.649	BB	0.3161	3767.24268	184.62012	49.4855
2	18.738	BB	0.3988	3845.58032	149.14952	50.5145



3i
racemic

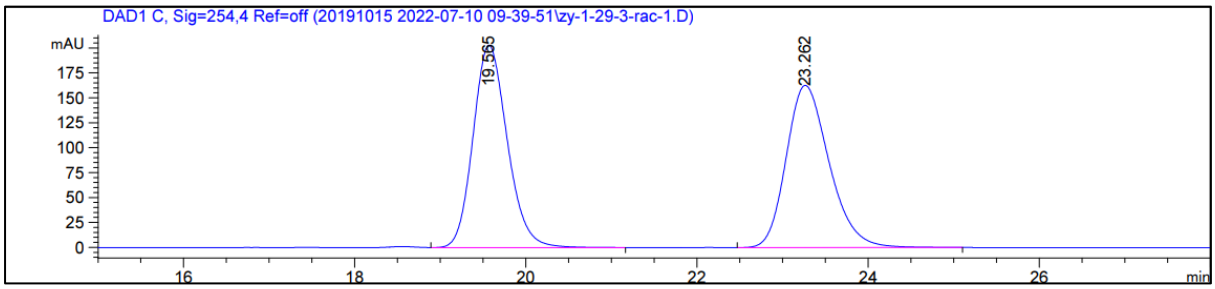


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	15.682	BB	0.3164	8463.91992	414.24954	90.6731
2	18.834	BB	0.3967	870.62244	34.00251	9.3269

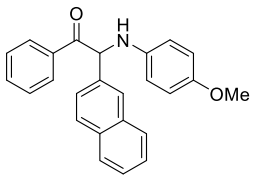


3i
enantioenriched

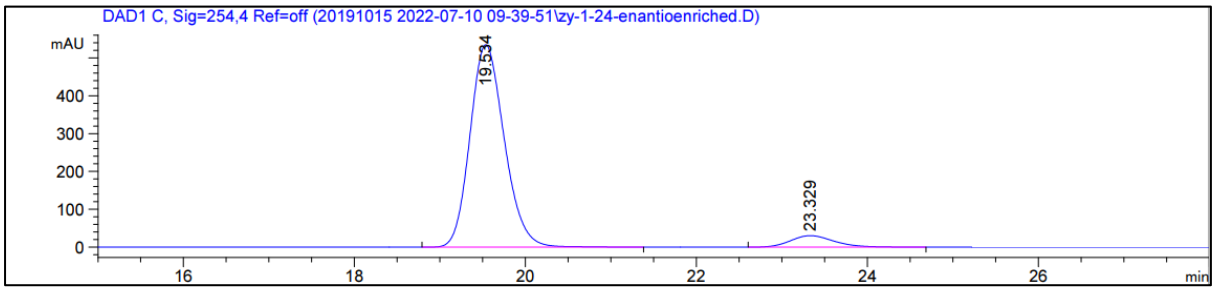
3j, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



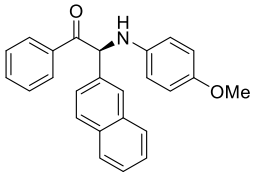
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	19.565	BB	0.4279	5639.56592	203.10912	49.8324
2	23.262	BB	0.5371	5677.50488	162.68896	50.1676



3j
racemic

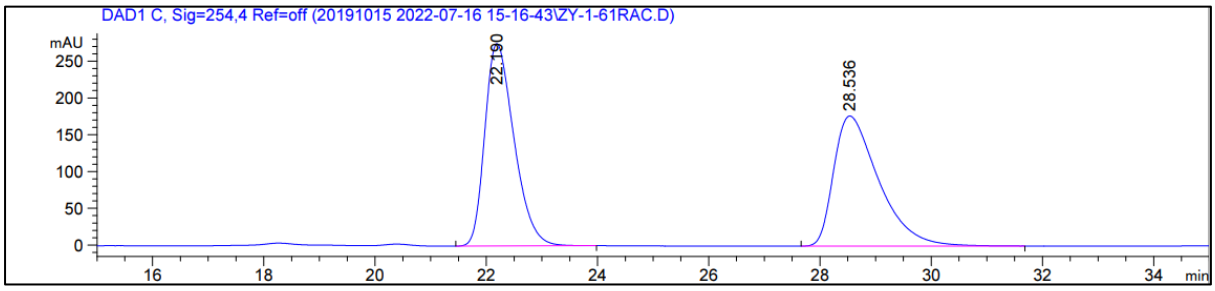


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	19.534	BB	0.4310	1.48935e4	534.62555	93.2568
2	23.329	BB	0.5360	1076.92285	30.34501	6.7432

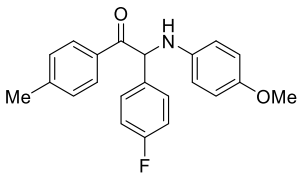


3j
enantioenriched

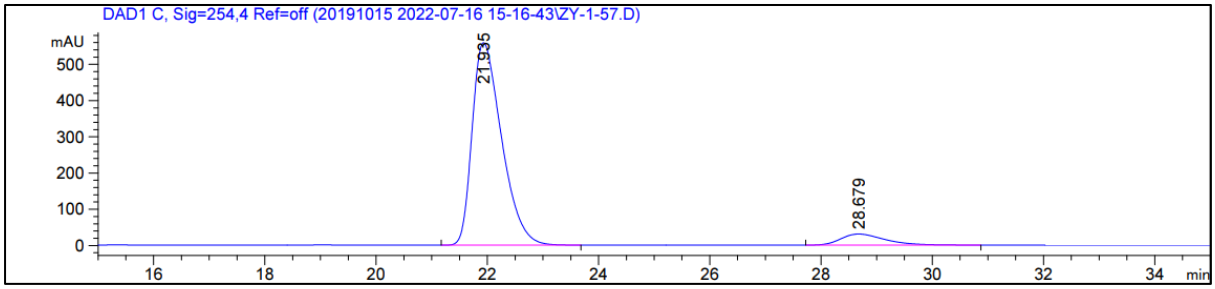
3k, HPLC conditions: Daicel CHIRALPAK® OD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



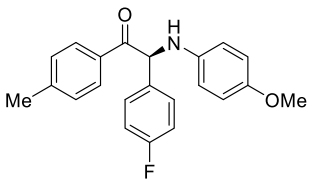
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	22.190	BB	0.5608	1.00143e4	275.05948	50.1714
2	28.536	BB	0.8482	9945.85547	176.82585	49.8286



3k
racemic

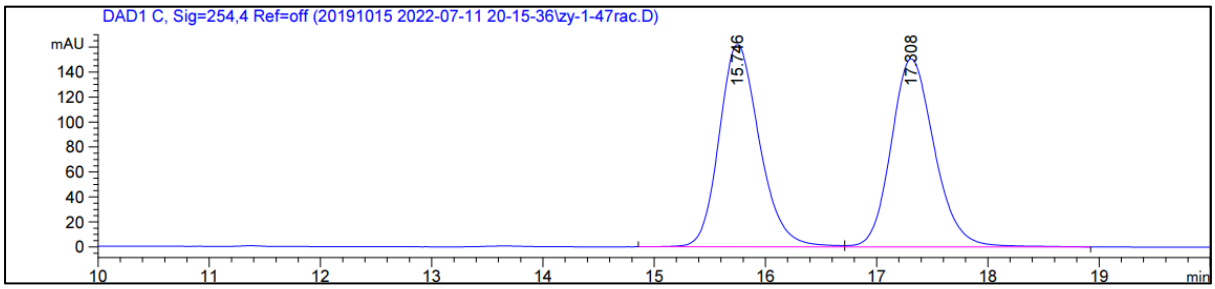


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	21.935	BB	0.5646	2.05343e4	558.91528	92.4363
2	28.679	BB	0.7965	1680.25415	30.60397	7.5637

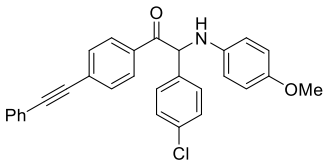


3k
enantioenriched

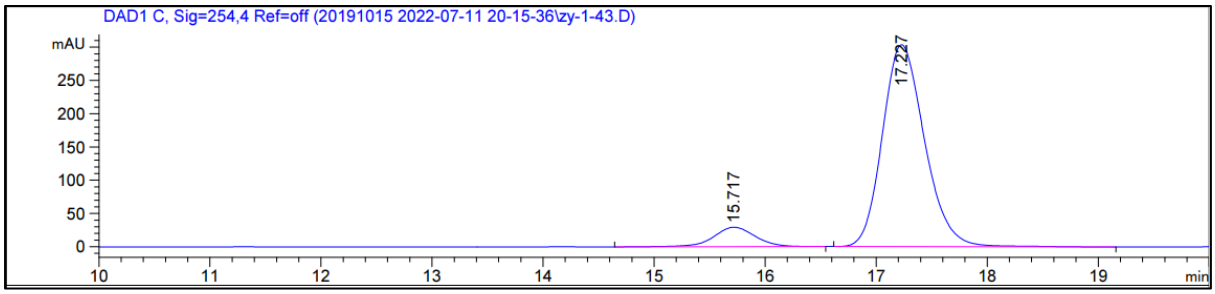
3l, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



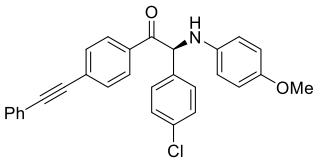
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	15.746	BV	0.3861	4080.66748	161.87164	50.0796
2	17.308	VB	0.4150	4067.70020	150.67944	49.9204



3l
racemic

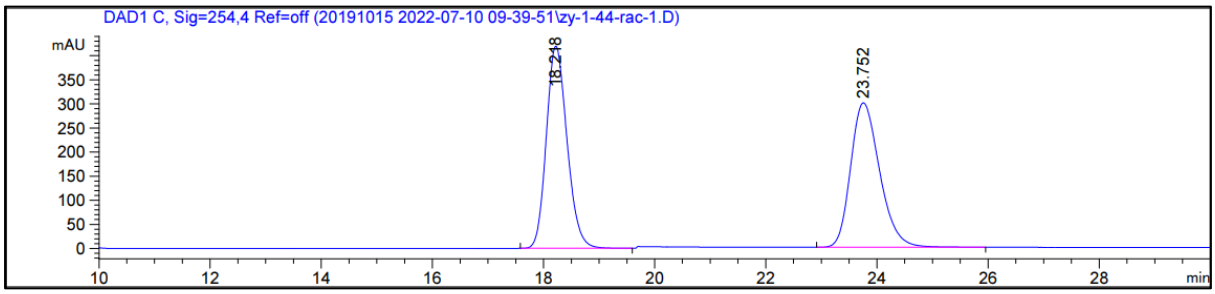


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	15.717	BB	0.4016	772.31616	29.29640	8.7915
2	17.227	BB	0.4079	8012.47949	303.62354	91.2085

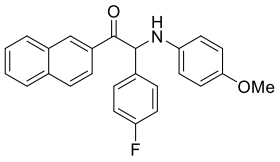


3l
enantioenriched

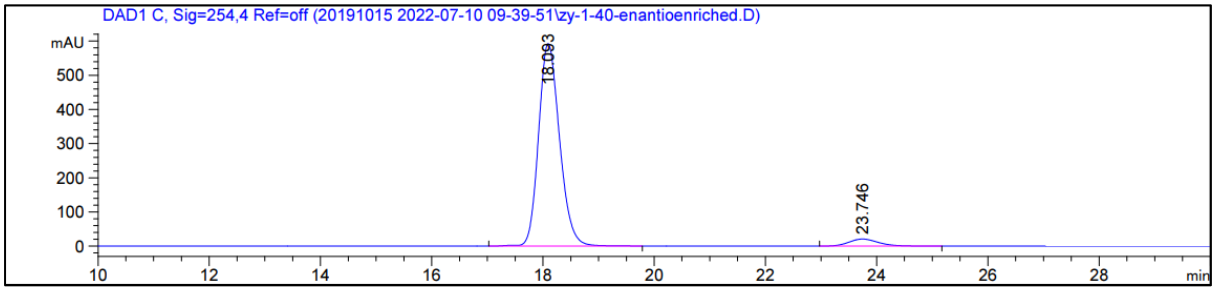
3m, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



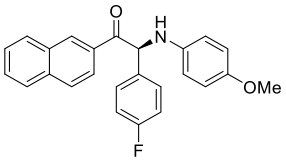
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	18.218	BB	0.3999	1.08564e4	419.53085	49.9874
2	23.752	BB	0.5609	1.08619e4	299.67621	50.0126



3m
racemic

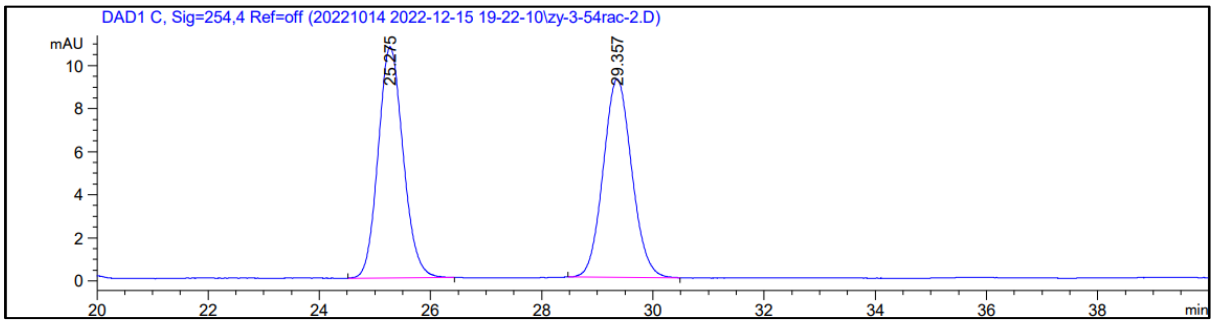


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	18.093	BB	0.4052	1.54895e4	592.13104	95.3662
2	23.746	BB	0.5557	752.63293	20.62856	4.6338

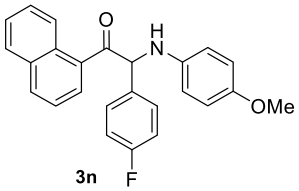


3m
enantioenriched

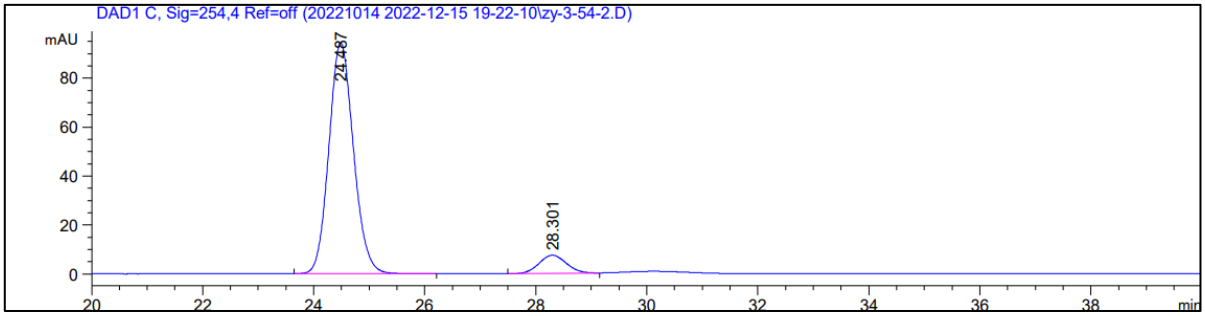
3n, HPLC conditions: Daicel CHIRALPAK® AD-H column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



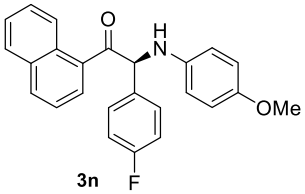
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	25.275	BB	0.4827	335.58197	10.73636	50.4855
2	29.357	BB	0.5428	329.12799	9.21168	49.5145



3n
racemic

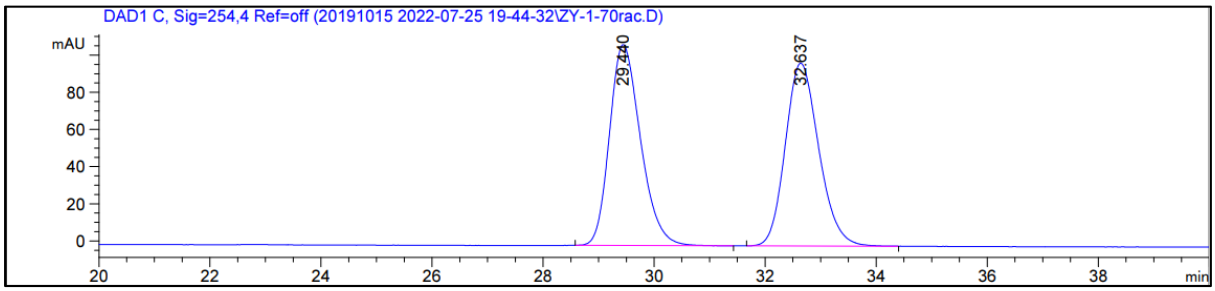


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	24.487	BB	0.4743	2899.63379	94.42235	91.9998
2	28.301	BB	0.5163	252.15015	7.42257	8.0002

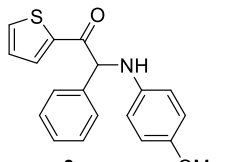


3n
enantioenriched

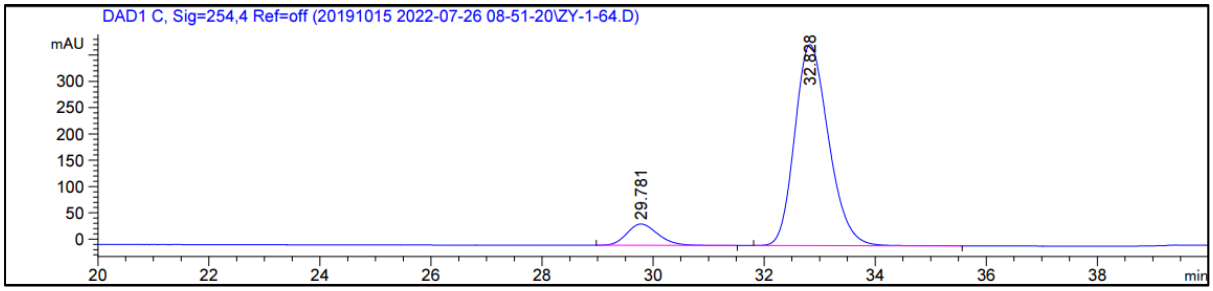
3o, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



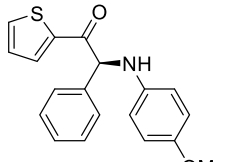
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	29.440	BB	0.5931	4198.45557	108.10249	50.4635
2	32.637	BB	0.6528	4121.32422	98.36447	49.5365



3o
racemic

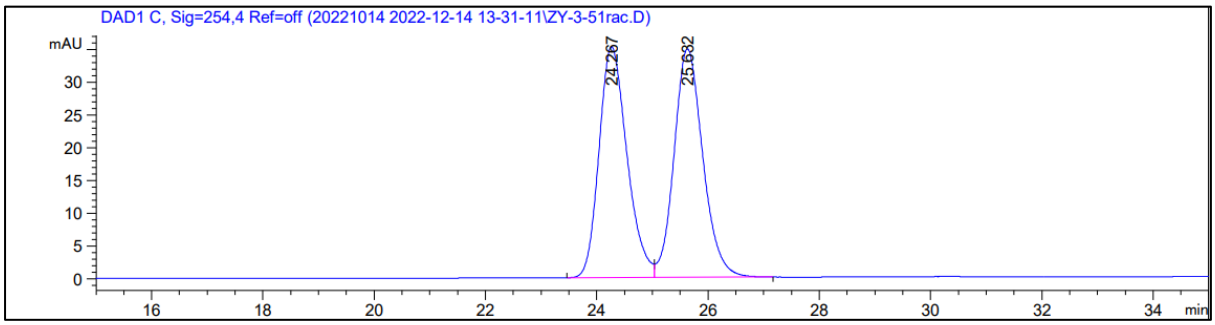


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	29.781	BB	0.5884	1579.38464	40.55428	8.8935
2	32.828	BB	0.6556	1.61795e4	382.42383	91.1065

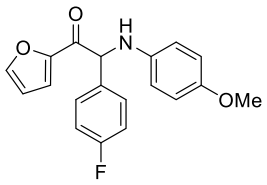


3o
enantioenriched

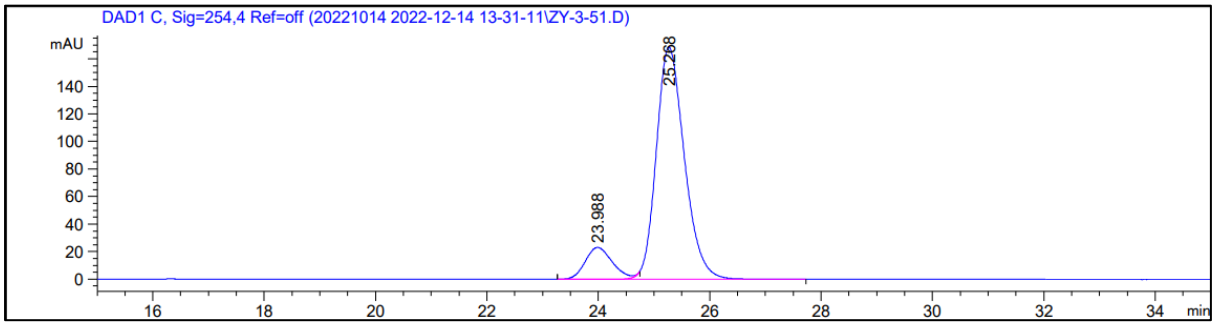
3p, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



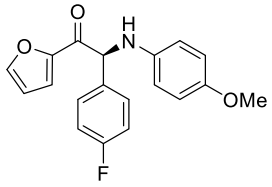
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	24.267	BV	0.5352	1228.03638	35.18452	49.5060
2	25.632	VB	0.5478	1252.54309	34.81116	50.4940



3p
racemic

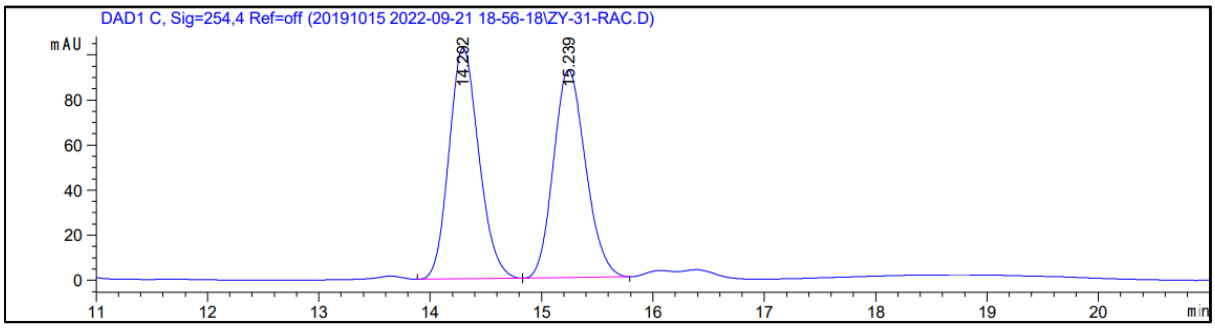


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	23.988	BV E	0.5198	780.37152	23.12164	11.6595
2	25.268	VB R	0.5387	5912.62158	168.77208	88.3405

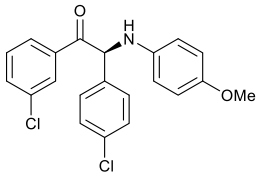


3p
enantioenriched

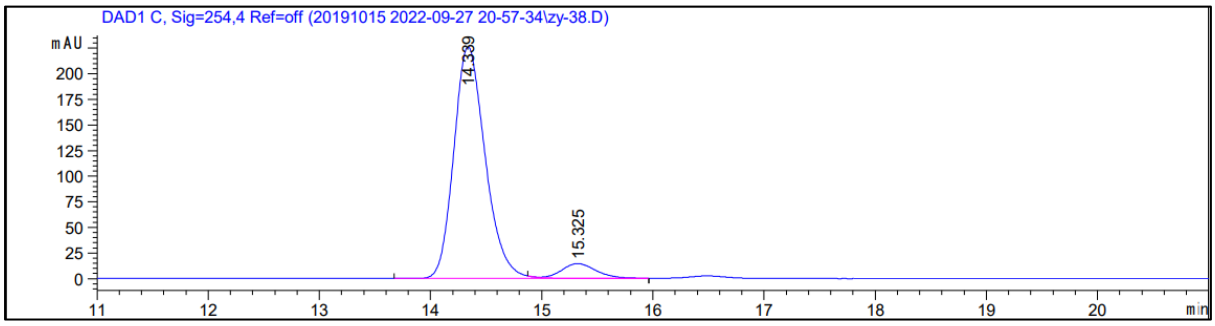
3q, HPLC conditions: Daicel CHIRALPAK® IC column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



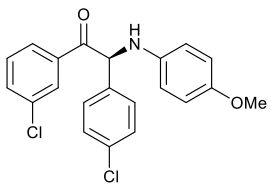
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	14.292	BB	0.2874	1910.42761	102.51716	50.7738
2	15.239	BB	0.3124	1852.19604	92.20248	49.2262



3q
racemic

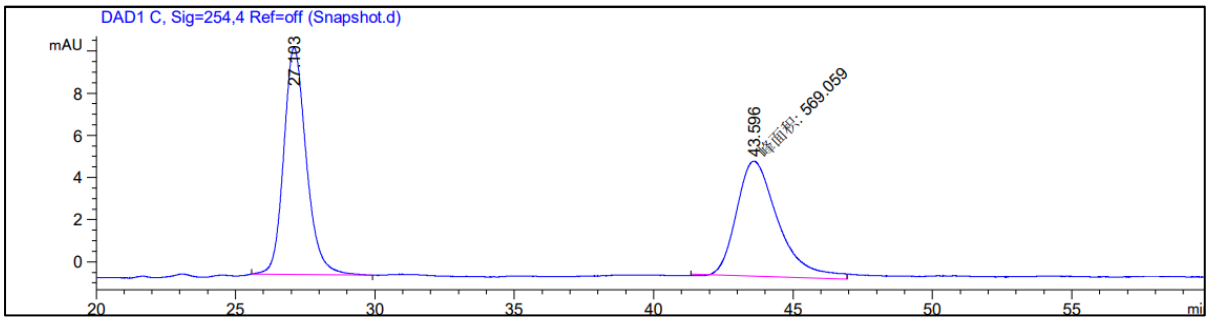


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	14.339	BV R	0.3007	4436.50244	226.27330	93.5513
2	15.325	VB E	0.3285	305.81699	14.35881	6.4487

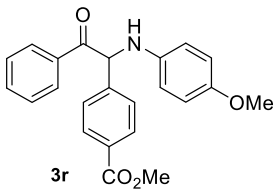


3q
enantioenriched

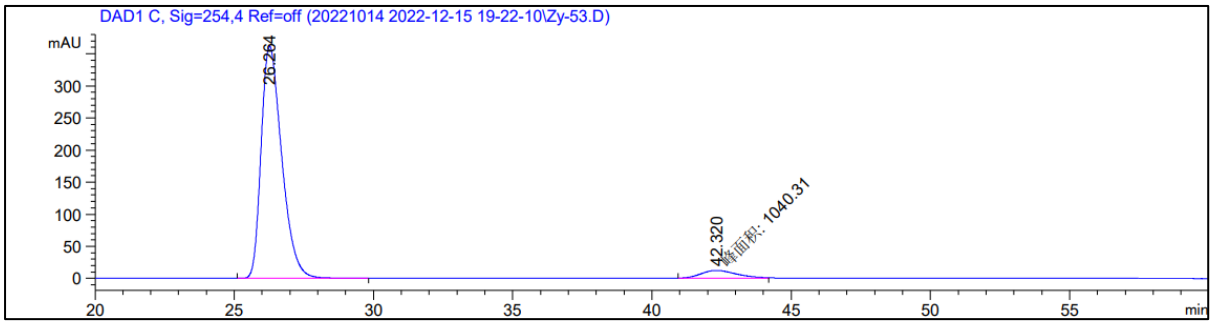
3r, HPLC conditions: Daicel CHIRALPAK® OD-H column; 15% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



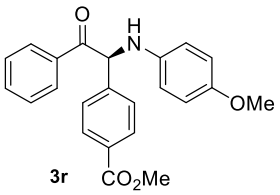
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	27.103	BB	0.8361	609.71545	10.77638	51.7245
2	43.596	MM	1.7350	569.05945	5.46659	48.2755



3r
racemic

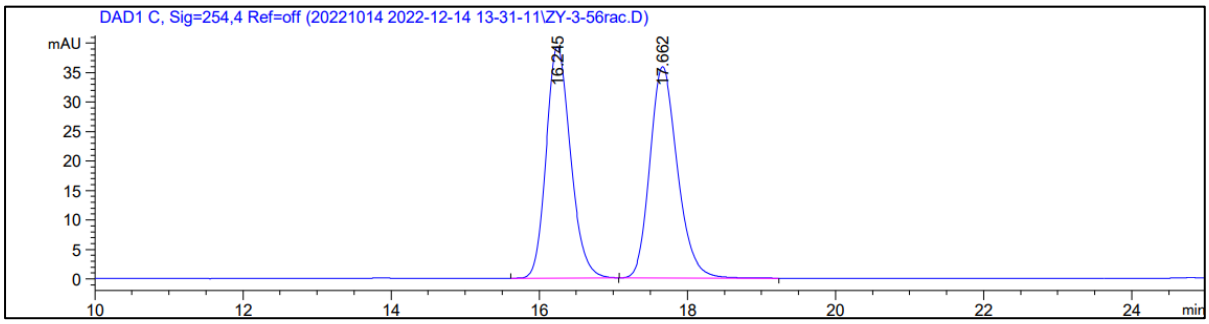


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	26.264	BB	0.7911	1.86002e4	362.19839	94.7032
2	42.320	MM	1.4499	1040.31079	11.95880	5.2968

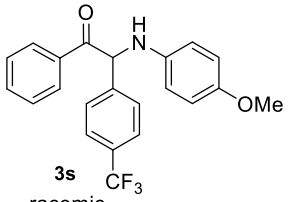


3r
enantioenriched

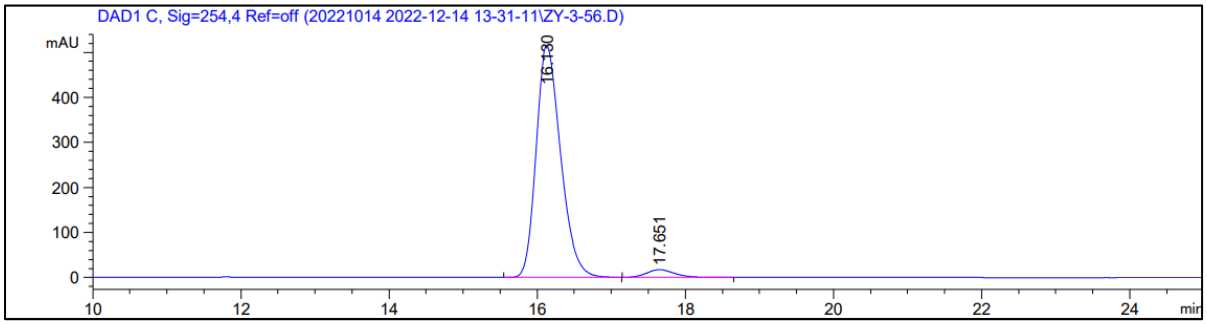
3s, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



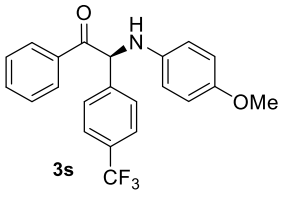
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.245	BB	0.3503	895.84930	39.25415	49.2316
2	17.662	BB	0.3966	923.81293	35.85202	50.7684



3s
racemic

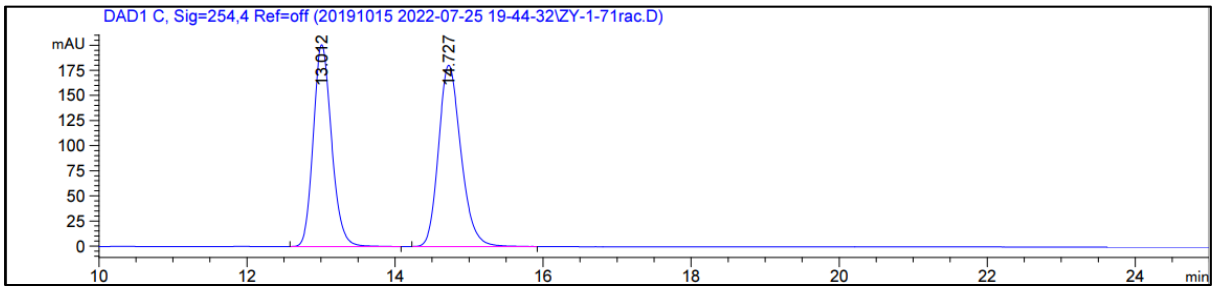


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.130	BB	0.3542	1.18301e4	514.52289	96.4121
2	17.651	BB	0.4024	440.25143	16.98342	3.5879

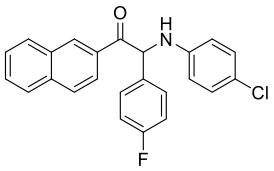


3s
enantioenriched

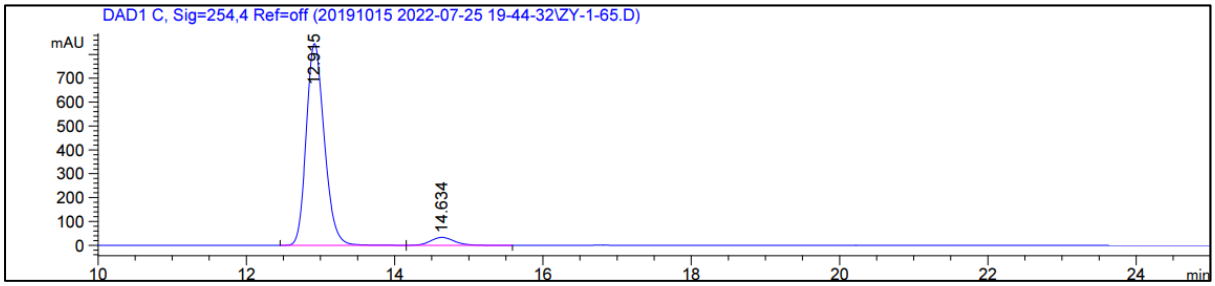
3t, HPLC conditions: Daicel CHIRALPAK® IC column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



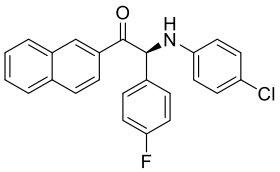
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.012	BB	0.2642	3450.26074	732.69775	47.6561
2	14.727	BB	0.3230	180.45224	646.95306	52.3439



3t
racemic

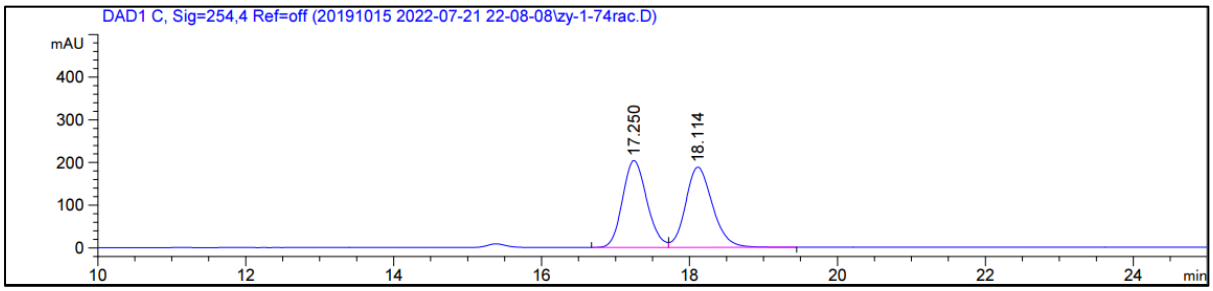


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.915	BB	0.2614	1.43059e4	845.71478	95.1202
2	14.634	BB	0.3417	733.91992	33.22506	4.8798

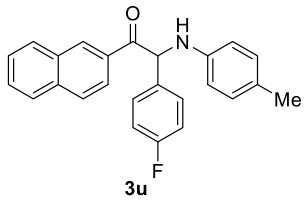


3t
enantioenriched

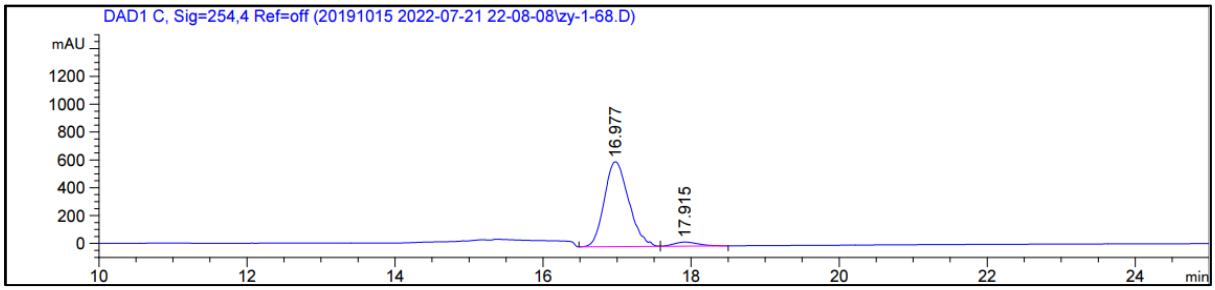
3u, HPLC conditions: Daicel CHIRALPAK® IC column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



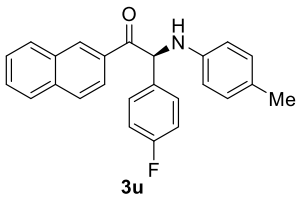
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	17.250	BV	0.3548	4653.64893	203.53154	49.5317
2	18.114	VB	0.3882	4741.65332	188.04225	50.4683



3u
racemic

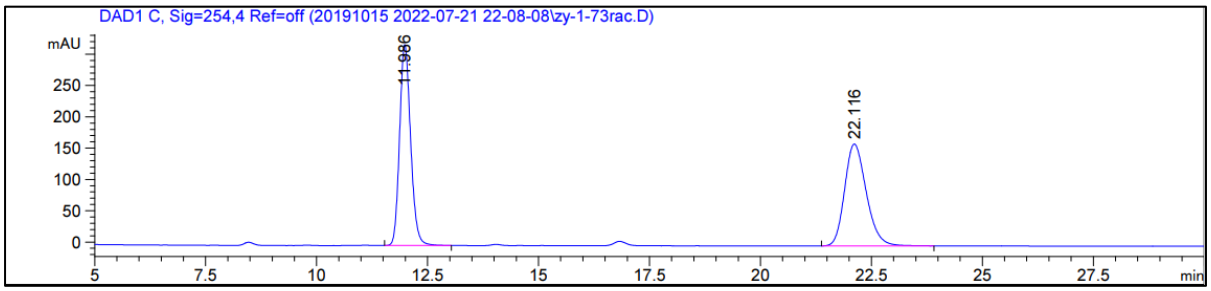


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.977	BV R	0.3505	1.39458e4	609.04877	95.6017
2	17.915	VB	0.3483	641.58942	28.97882	4.3983

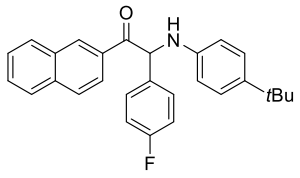


3u
enantioenriched

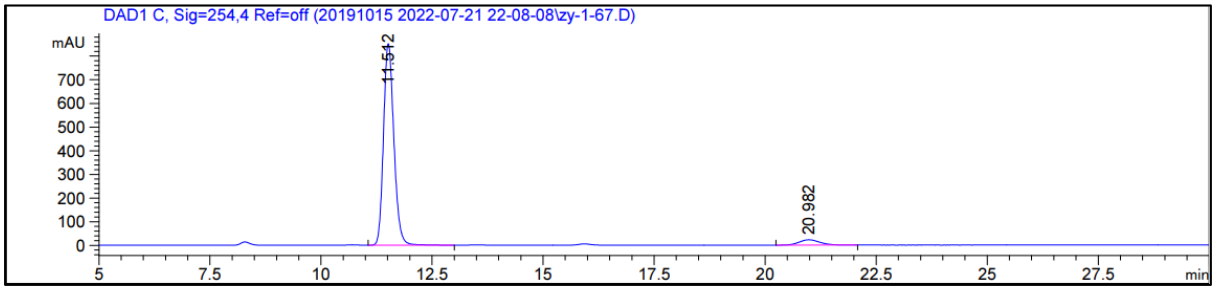
3v, HPLC conditions: Daicel CHIRALPAK® IC column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



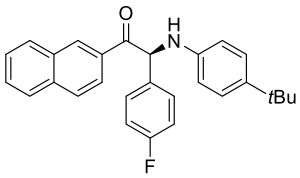
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.986	BB	0.2652	5534.65869	320.89365	50.1105
2	22.116	BB	0.5211	5510.25684	162.68878	49.8895



3v
racemic

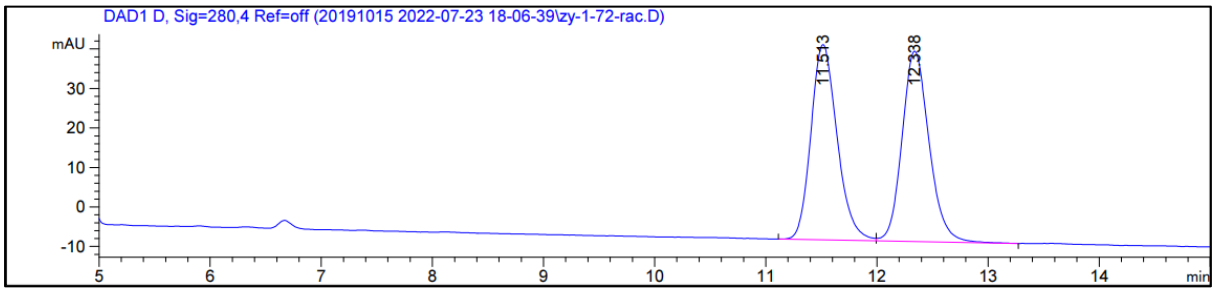


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.512	BB	0.2451	7574.02930	477.48260	95.1550
2	20.982	BB	0.4651	385.64624	11.93104	4.8450

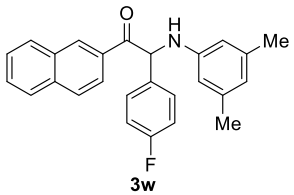


3v
enantioenriched

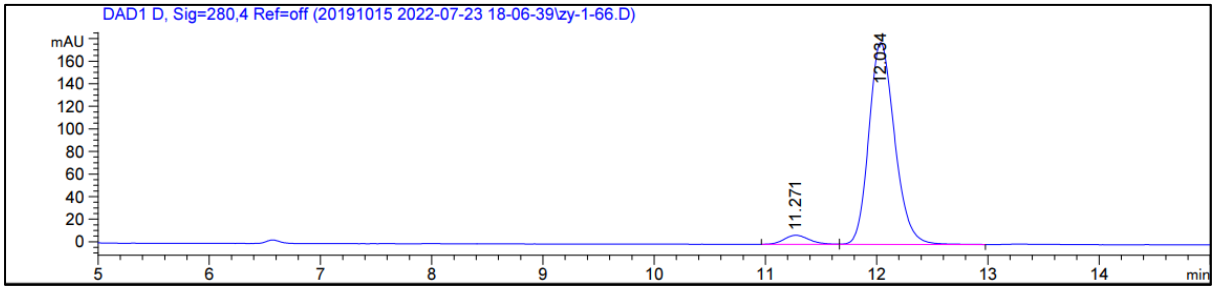
3w, HPLC conditions: Daicel CHIRALPAK® IC column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 280 nm.



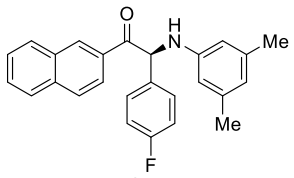
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.513	BV	0.2511	810.81116	49.49159	49.8551
2	12.338	VB	0.2613	815.52350	48.21384	50.1449



3w
racemic

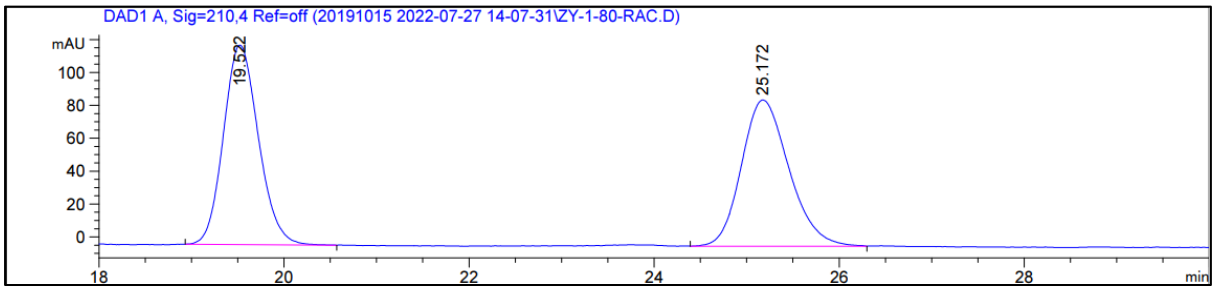


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.271	BV	0.2402	125.75422	8.05407	4.1934
2	12.034	VB	0.2473	2873.11646	178.95538	95.8066

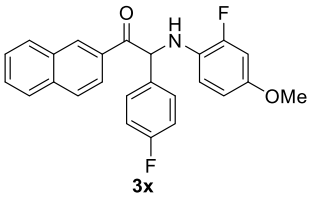


3w
enantioenriched

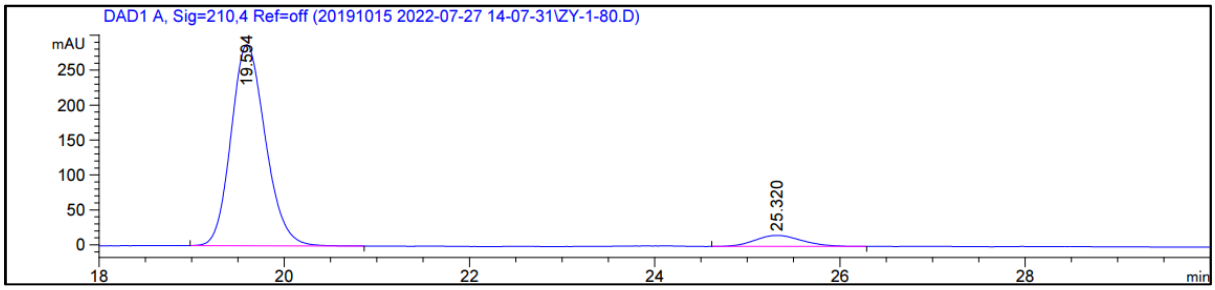
3x, HPLC conditions: Daicel CHIRALPAK® IC column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 210 nm.



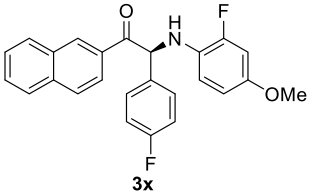
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	19.522	BB	0.4063	3183.41064	121.27193	50.1100
2	25.172	BB	0.5521	3169.43896	88.87357	49.8900



3x
racemic

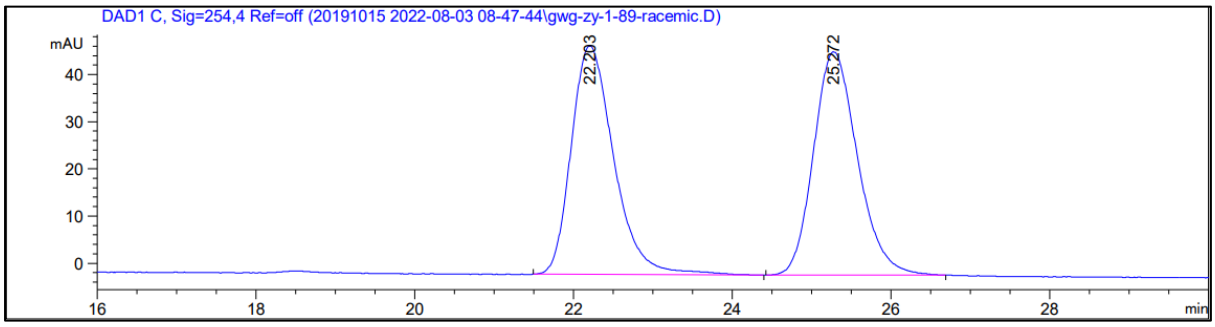


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	19.594	BB	0.3981	7398.1	287.7	92.929
2	25.320	BB	0.4452	56.3	15.8	7.071

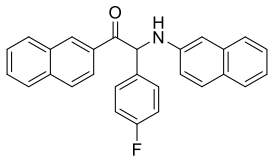


3x
enantioenriched

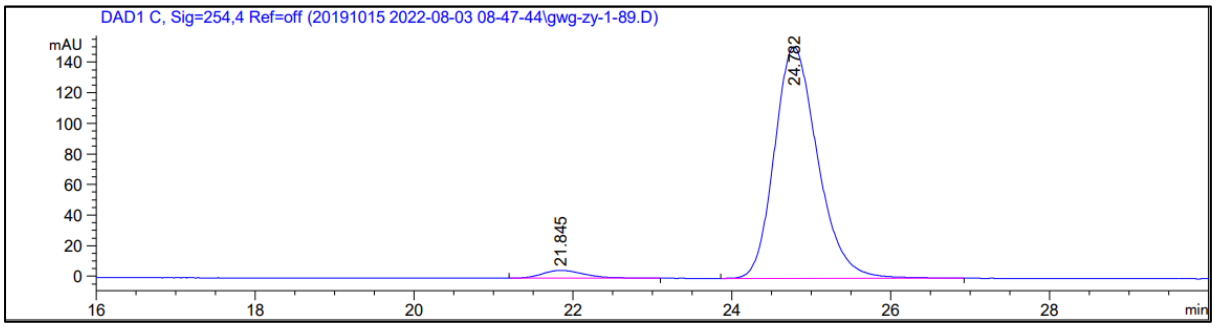
3y, HPLC conditions: Daicel CHIRALPAK® IC column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



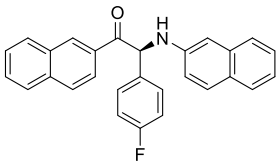
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	22.203	BB	0.5714	1806.78979	48.40806	49.7935
2	25.272	BB	0.5790	1821.77502	47.33804	50.2065



3y
racemic

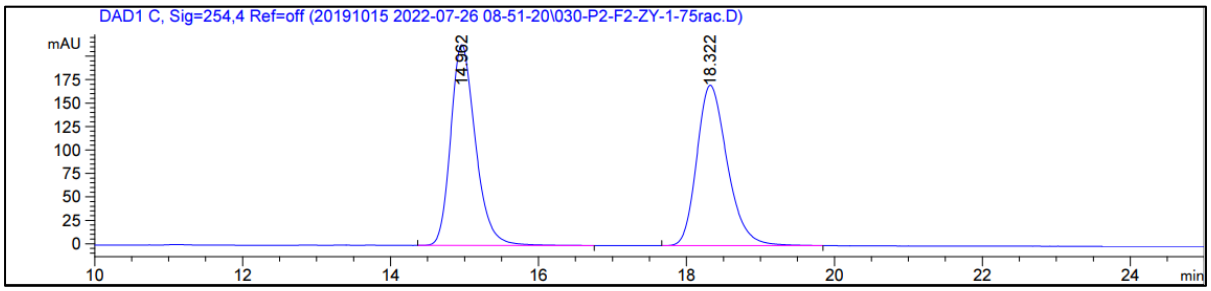


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	21.845	BB	0.4406	187.55370	5.12967	3.1814
2	24.782	BB	0.5783	5707.79736	151.22894	96.8186

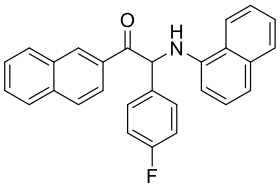


3y
enantioenriched

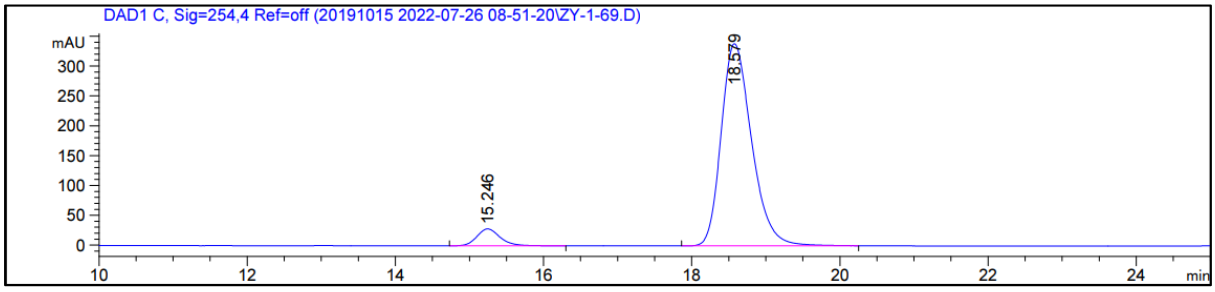
3z, HPLC conditions: Daicel CHIRALPAK® IC column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



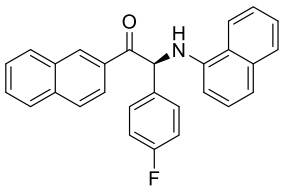
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	14.962	BB	0.3559	4989.40869	214.07133	50.4847
2	18.322	BB	0.4415	4893.61084	171.16895	49.5153



3z
racemic

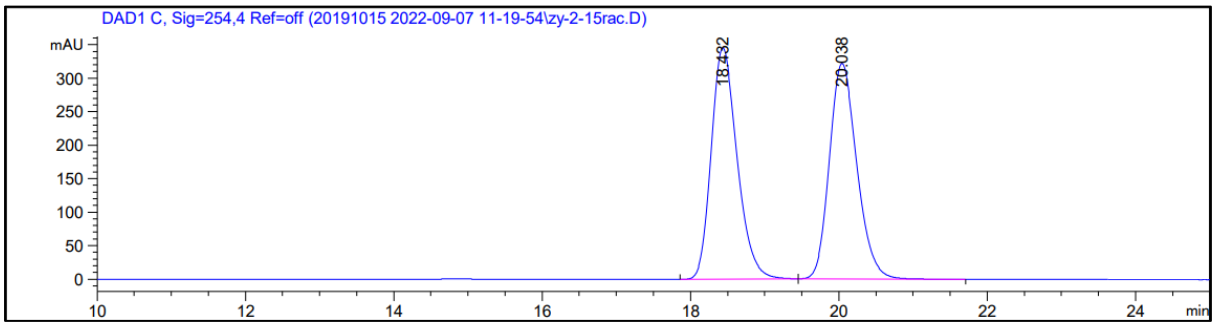


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	15.246	BB	0.3344	618.21783	28.34908	6.0164
2	18.579	BB	0.4427	9657.38770	338.67868	93.9836

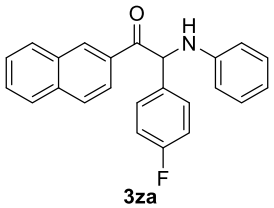


3z
enantioenriched

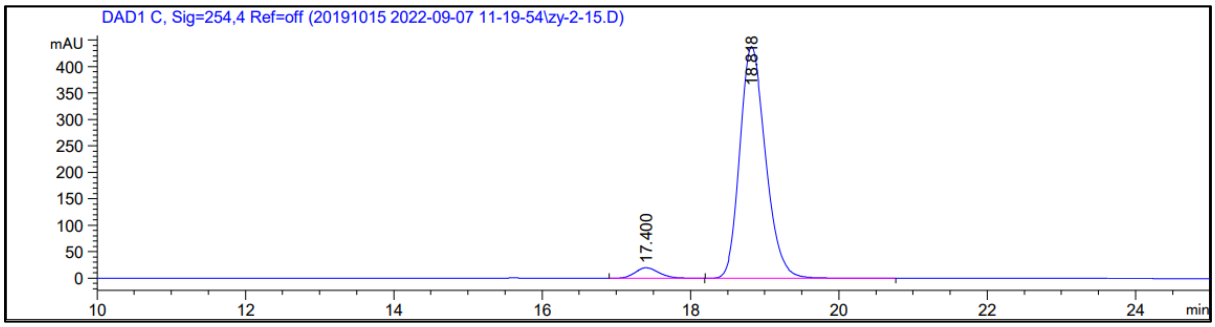
3za, HPLC conditions: Daicel CHIRALPAK® IC column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



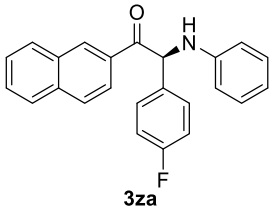
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	18.432	BB	0.3748	8372.31738	345.44525	50.3319
2	20.038	BB	0.3975	8261.91113	321.81729	49.6681



3za
racemic

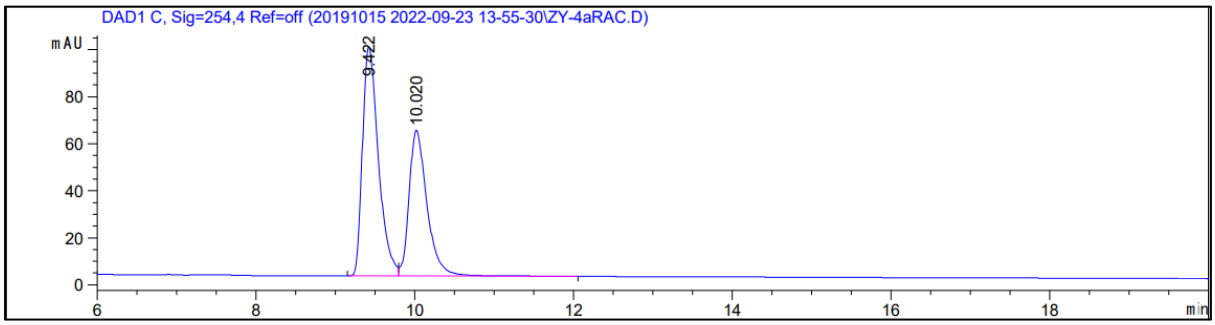


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	17.400	BB	0.3517	453.38593	19.91009	4.1145
2	18.818	BB	0.3736	1.05658e4	437.67453	95.8855

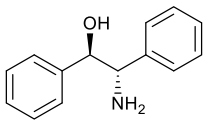


3za
enantioenriched

4a, HPLC conditions: Daicel CHIRALPAK® IC column; 20% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.

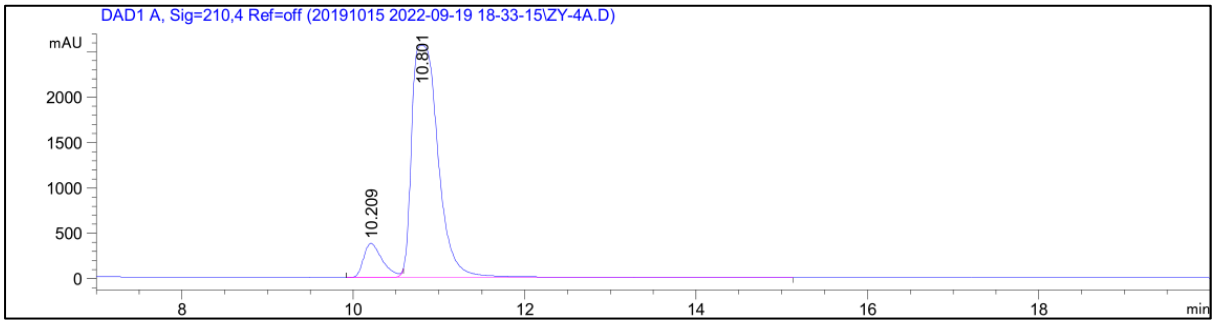


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.422	BV	0.2124	1358.57605	97.58514	58.0477
2	10.020	VB	0.2387	981.87177	62.00480	41.9523

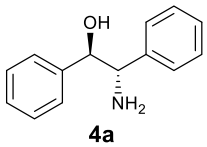


4a

racemic

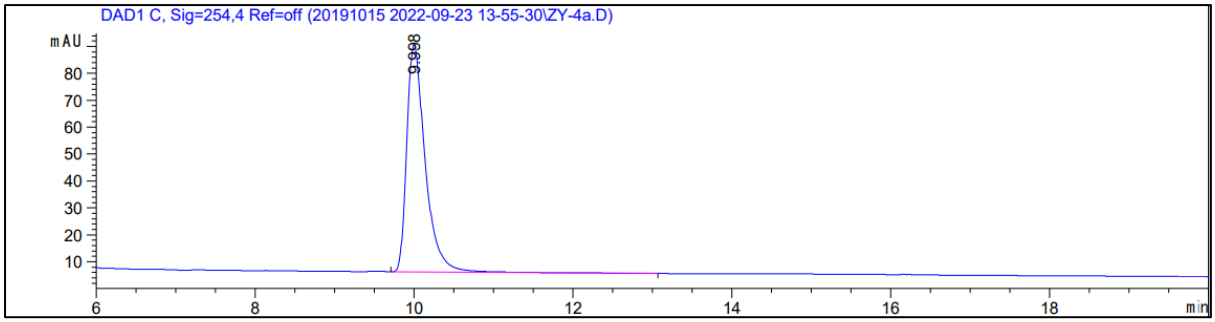


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.209	BV E	0.2307	5685.62061	375.39987	9.3490
2	10.801	VB R	0.3374	5.51299e4	2558.84985	90.6510



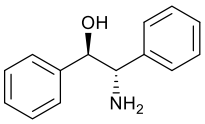
4a

enantioenriched



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.998	BB	0.2425	1363.84961	84.39232	100.0000

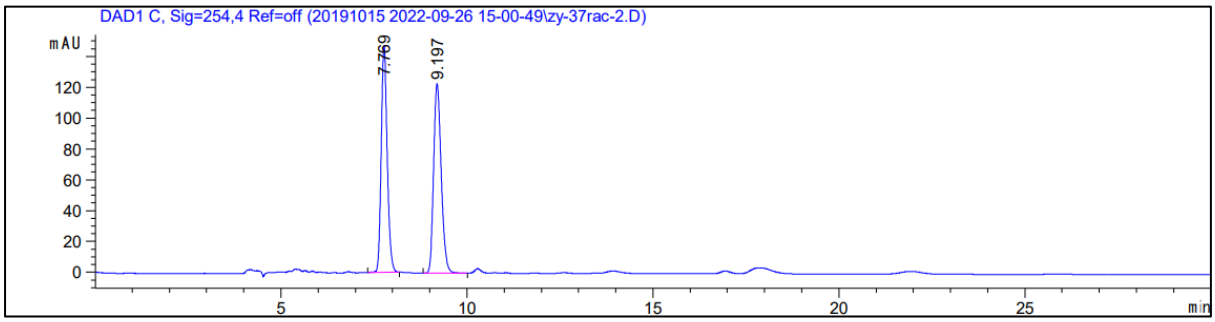
After recrystallization.



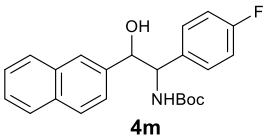
4a

enantioenriched

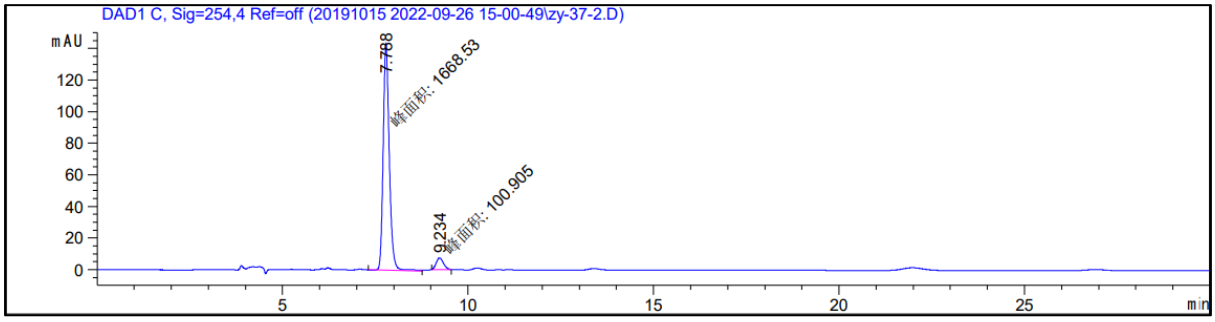
4m, HPLC conditions: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 254 nm.



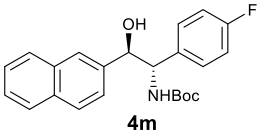
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	7.769	BB	0.1762	1665.39172	146.93123	48.9803
2	9.197	BB	0.2165	1734.73621	123.00260	51.0197



4m
racemic

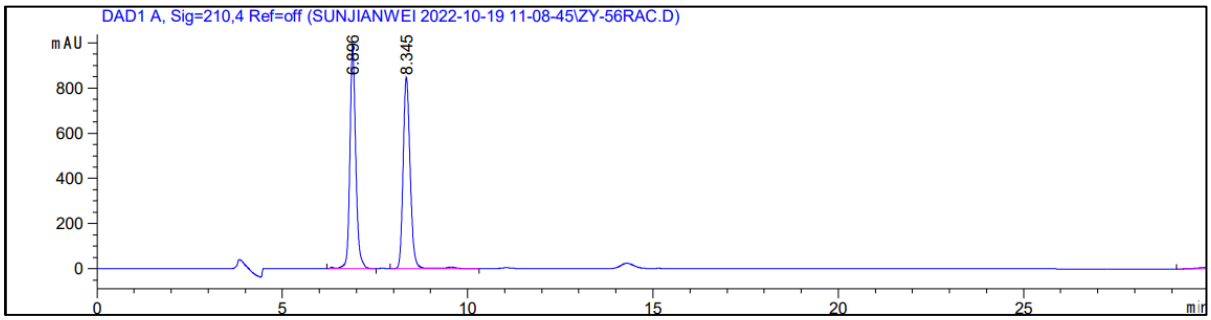


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	7.788	MM	0.1940	1668.53076	143.32246	94.2973
2	9.234	MM	0.2261	100.90502	7.43684	5.7027

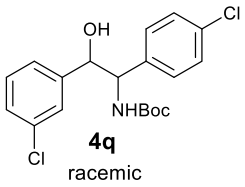


4m
enantioenriched

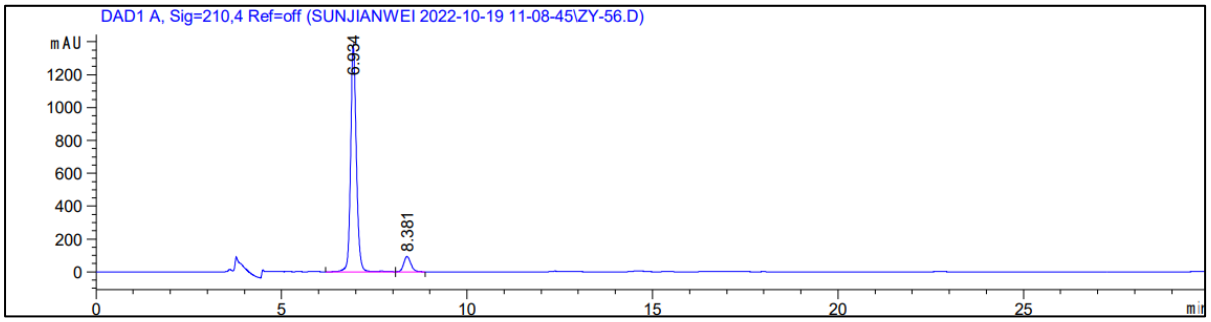
4q, HPLC conditions: Daicel CHIRALPAK® IC column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min, λ = 210 nm.



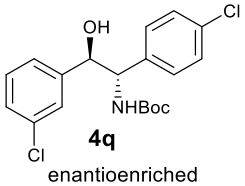
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	6.896	VB R	0.1704	1.10838e4	988.64435	49.9954
2	8.345	BV R	0.1986	1.10859e4	848.49969	50.0046



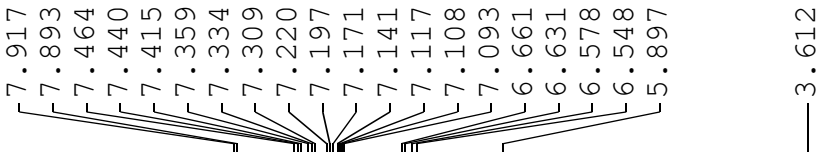
4q
racemic

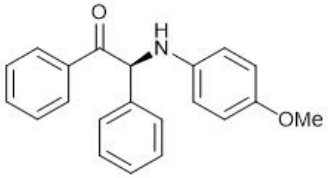


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	6.934	BV R	0.1671	1.50611e4	1375.09656	92.4721
2	8.381	VB	0.2042	1226.08057	92.78487	7.5279



4q
enantioenriched





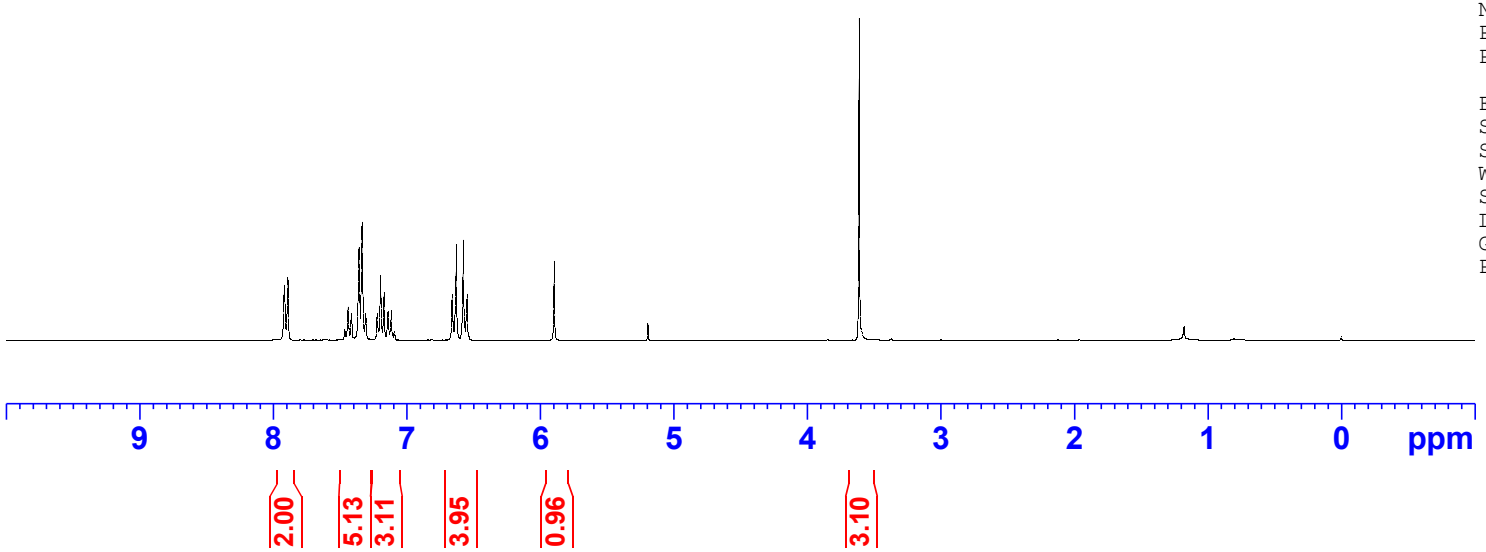
3a

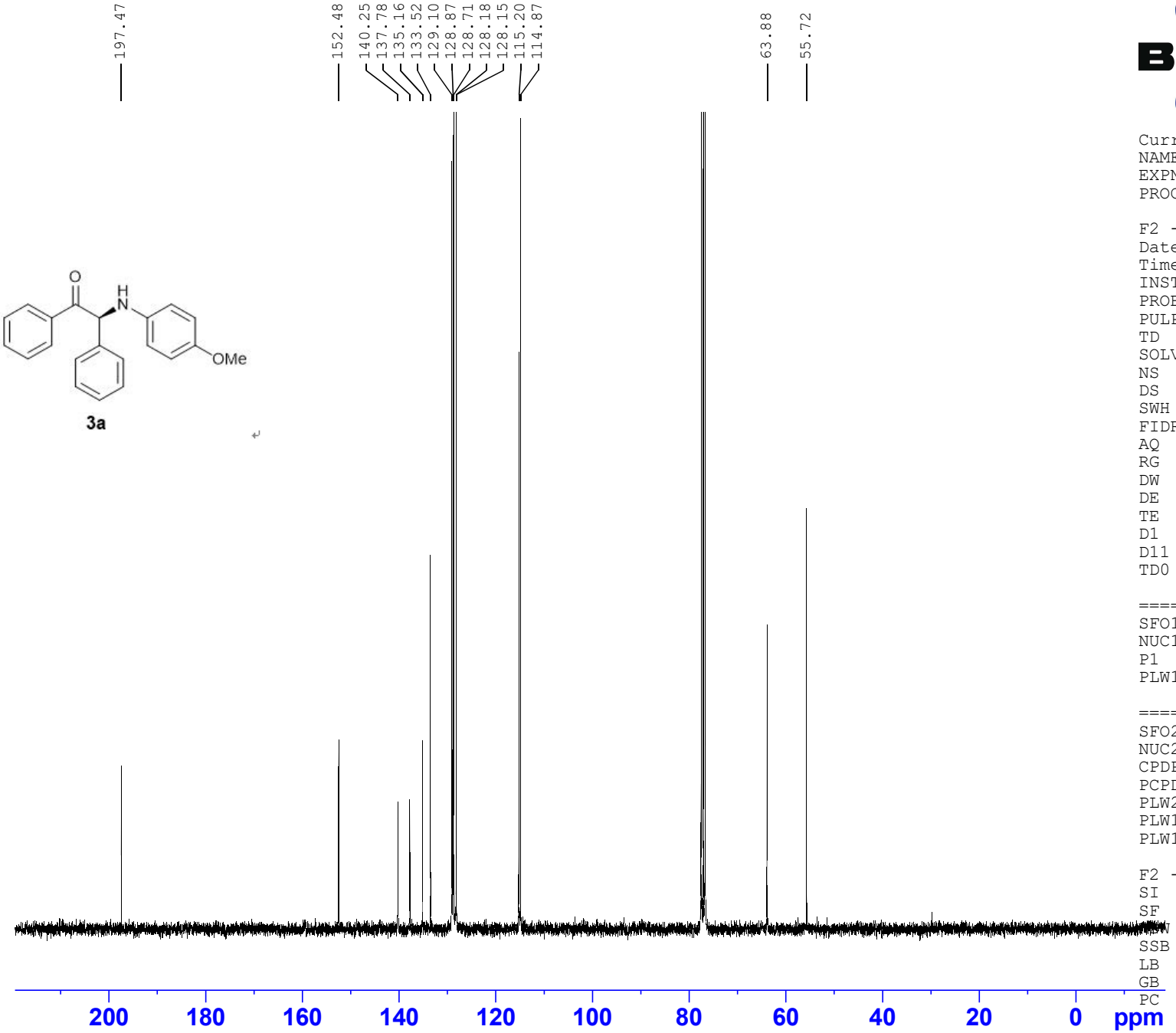
Current Data Parameters
NAME HNMR-ZY-1-8
EXPNO 87
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220602
Time 10.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 114
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300344 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





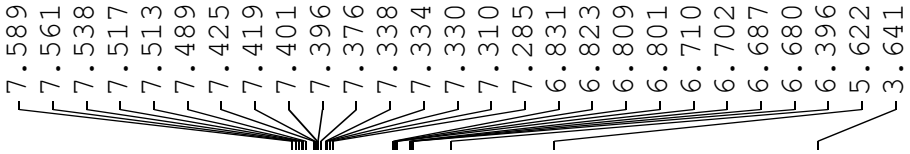
Current Data Parameters
NAME CNMR-ZY-1-8
EXPNO 88
PROCNO 1

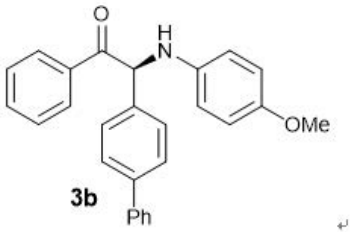
F2 - Acquisition Parameters
Date_ 20220602
Time 11.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4677485 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



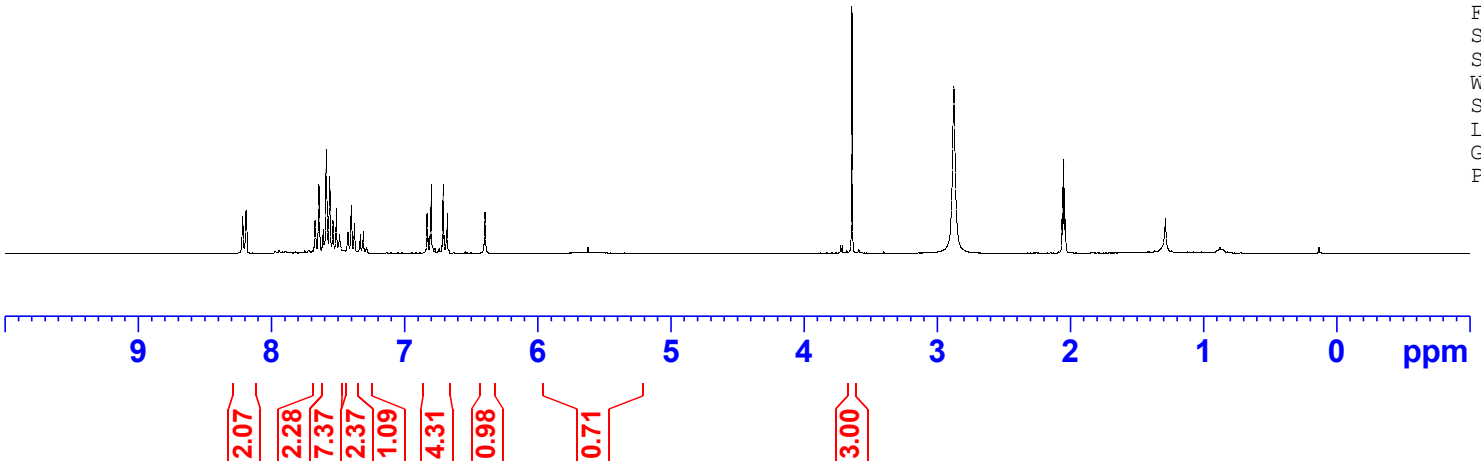


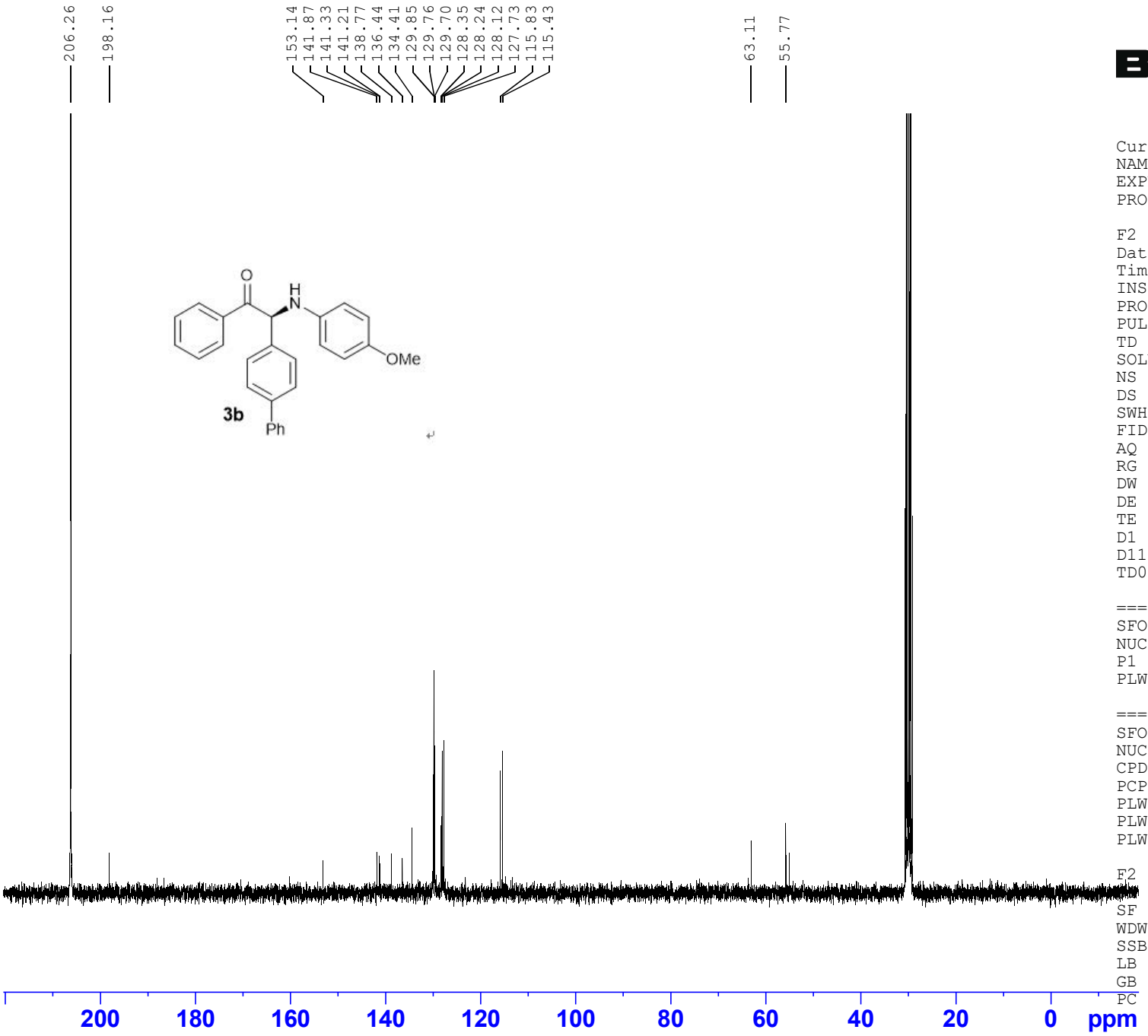
Current Data Parameters
NAME HNMR-1-29-1
EXPNO 184
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220624
Time 14.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 203
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





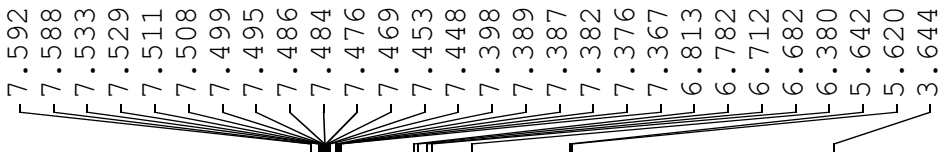
Current Data Parameters
NAME CNMR-ZY-1-29-1
EXPNO 192
PROCNO 1

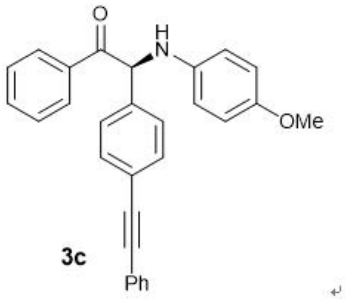
F2 - Acquisition Parameters
Date_ 20220628
Time 10.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 400
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
32768
SF 75.4676755 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



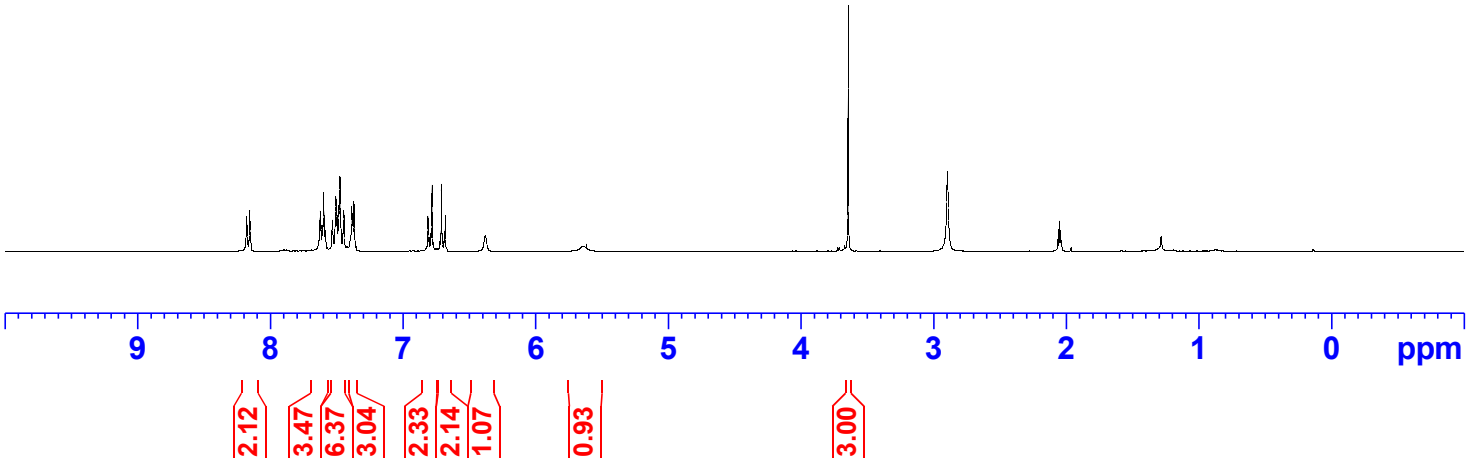


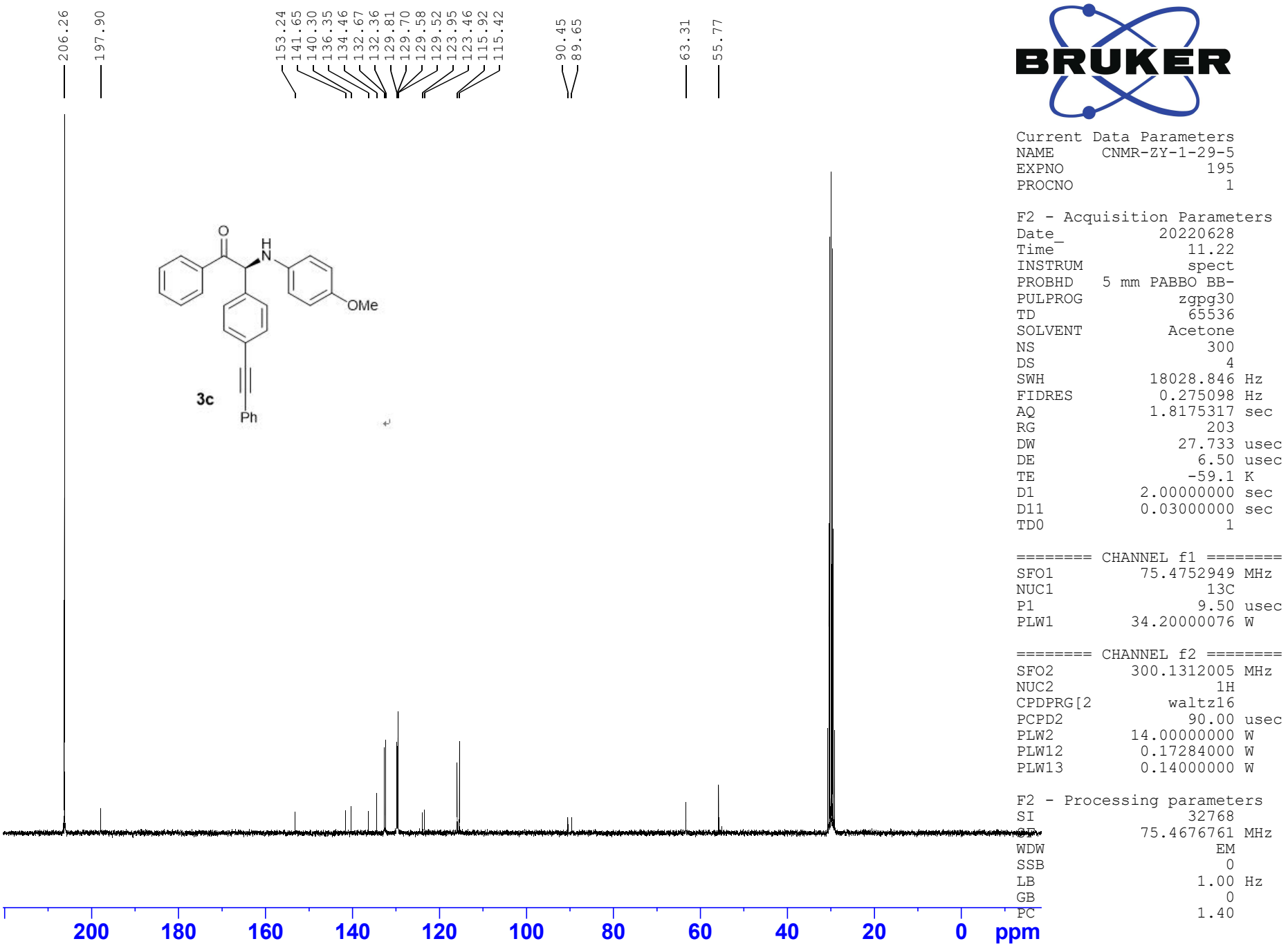
Current Data Parameters
NAME HNMR-1-29-5
EXPNO 188
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220624
Time 15.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 128
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

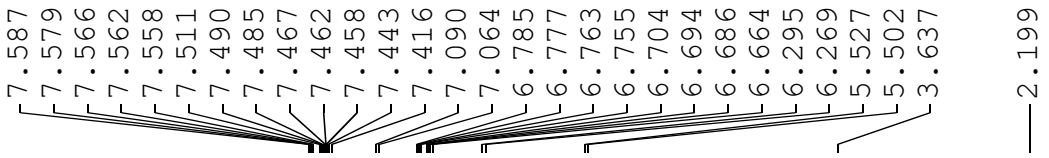
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

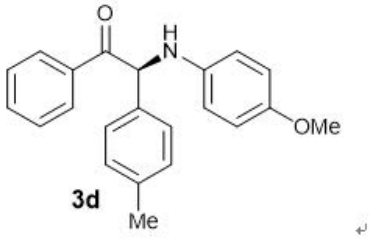
F2 - Processing parameters
SI 65536
SF 300.1300050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00






```
Current Data Parameters
NAME      CNMR-ZY-1-29-5
EXPNO                195
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220628
Time               11.22
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT          Acetone
NS                  300
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                  203
DW               27.733 usec
DE                6.50 usec
TE                -59.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                9.50 usec
PLW1        34.20000076 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.17284000 W
PLW13        0.14000000 W

F2 - Processing parameters
SI                 32768
SF          75.4676761 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC                1.40
```



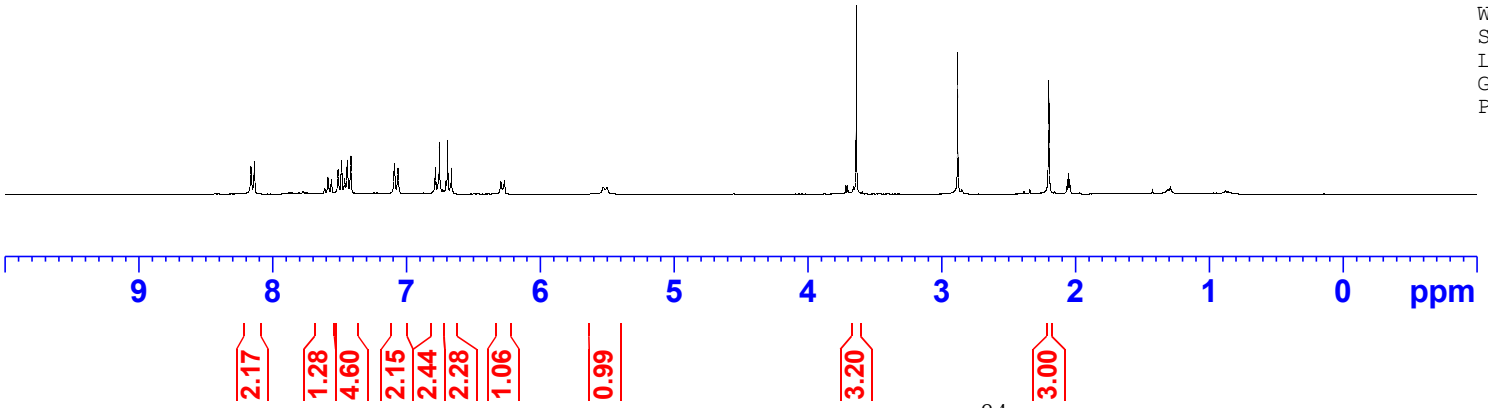


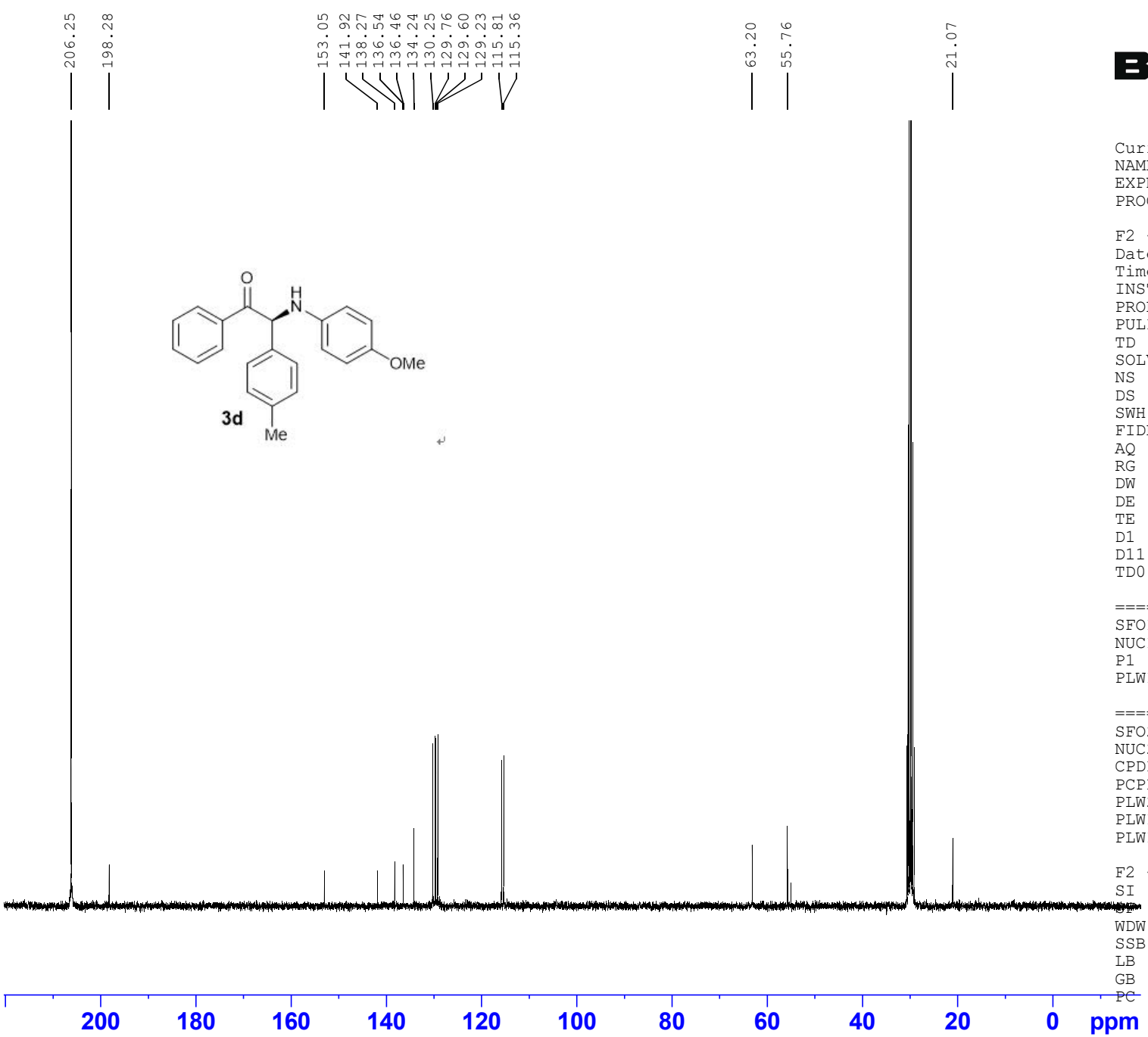
Current Data Parameters
NAME HNMR-1-29-4
EXPNO 185
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220624
Time 14.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 128
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





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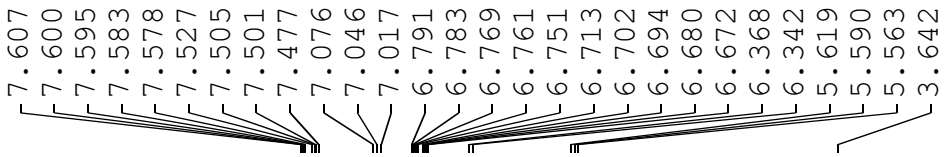
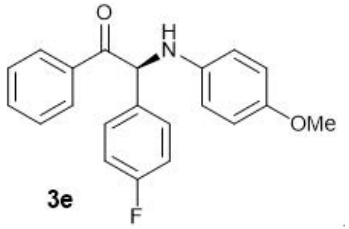
```
Current Data Parameters
NAME      CNMR-ZY-1-29-4
EXPNO                194
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220628
Time               10.58
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT          Acetone
NS                  300
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                  203
DW               27.733 usec
DE                6.50 usec
TE                -59.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                 9.50 usec
PLW1        34.20000076 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        14.00000000 W
PLW12        0.17284000 W
PLW13        0.14000000 W

F2 - Processing parameters
SI                 32768
SF            75.4676771 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```





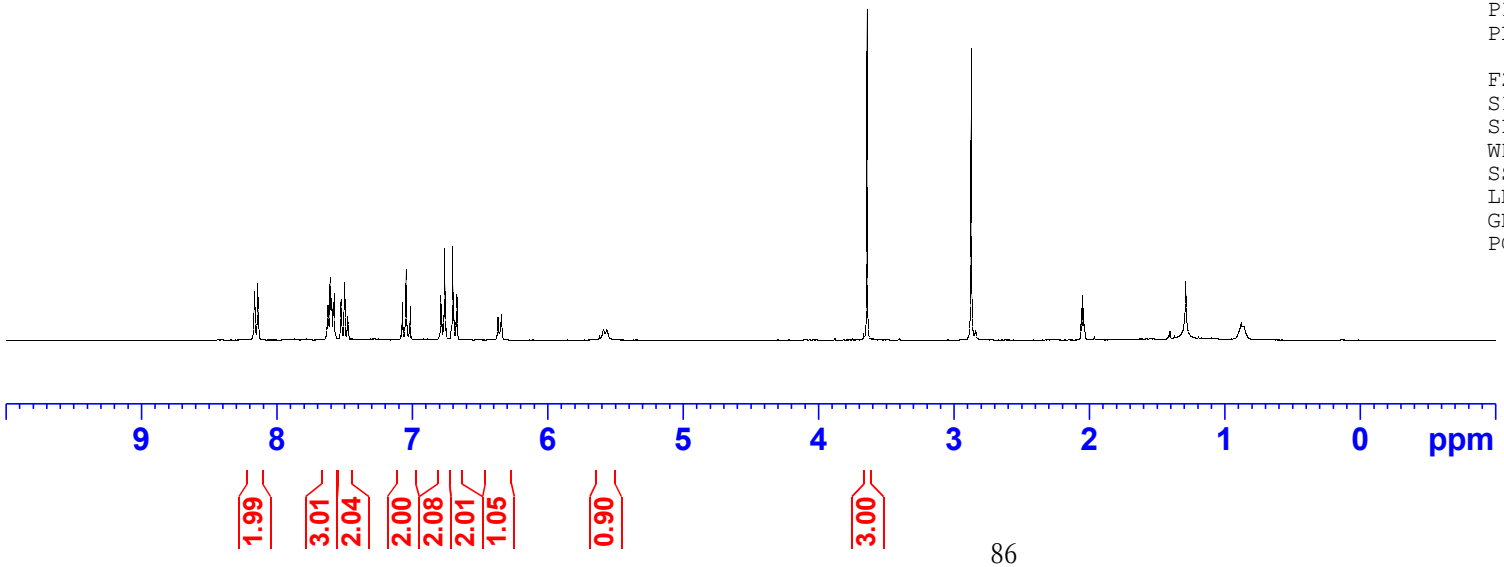
3e

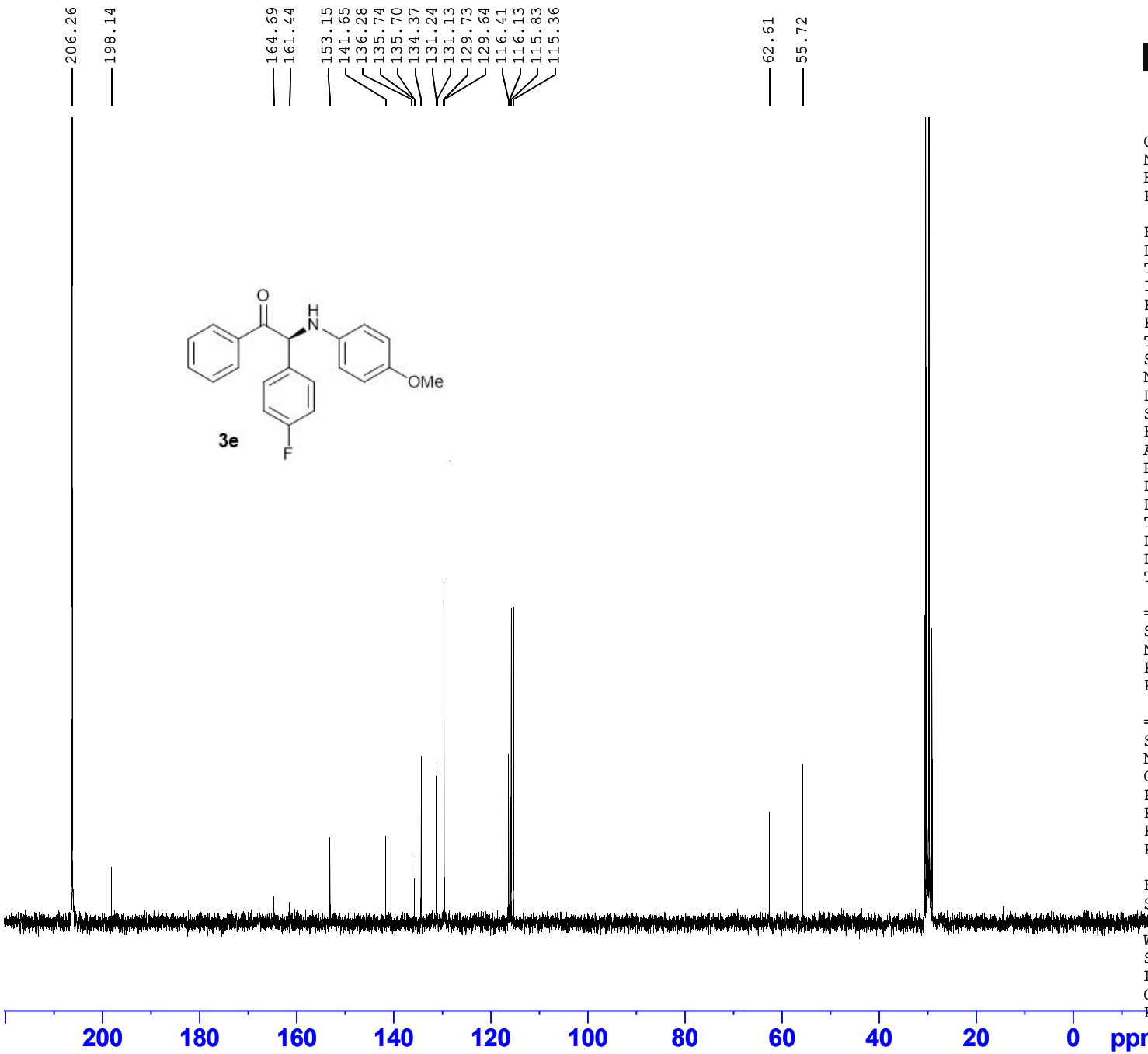
Current Data Parameters
NAME HNMR-ZY-1-59
EXPNO 401
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220712
Time 14.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 144
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





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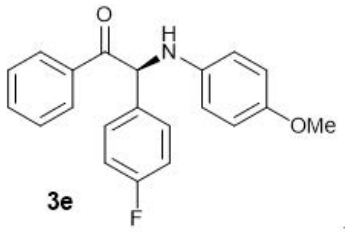
Current Data Parameters
NAME CNMR-ZY-1-59
EXPNO 420
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220713
Time 22.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 300
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

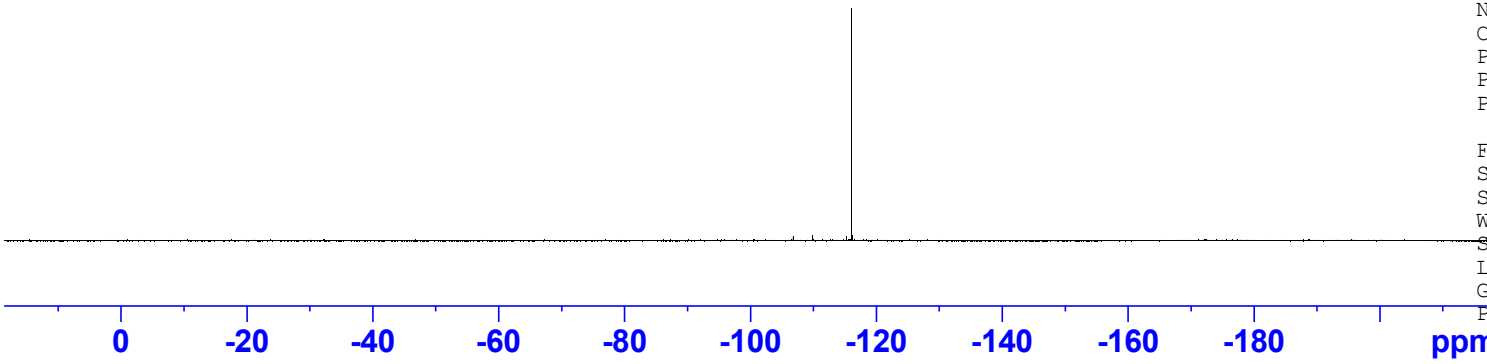
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
75.4676799 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



3e

-116.08



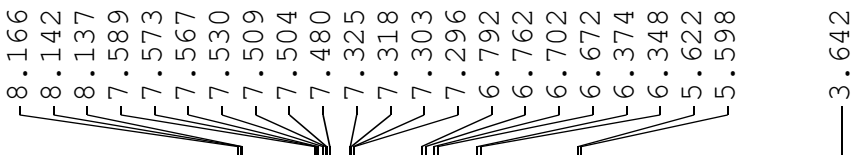
Current Data Parameters
NAME FNMR-ZY-1-59
EXPNO 485
PROCNO 1

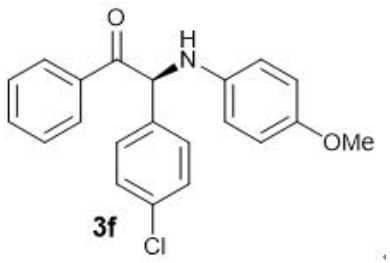
F2 - Acquisition Parameters
Date_ 20220722
Time 15.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn.2
TD 131072
SOLVENT Acetone
NS 4
DS 4
SWH 66964.289 Hz
FIDRES 0.510897 Hz
AQ 0.9786710 sec
RG 203
DW 7.467 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 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



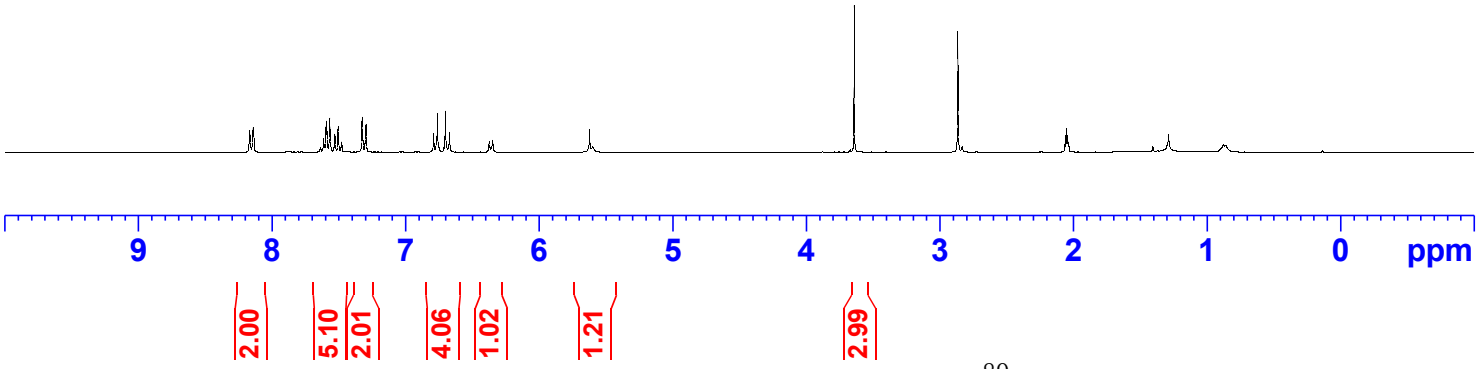


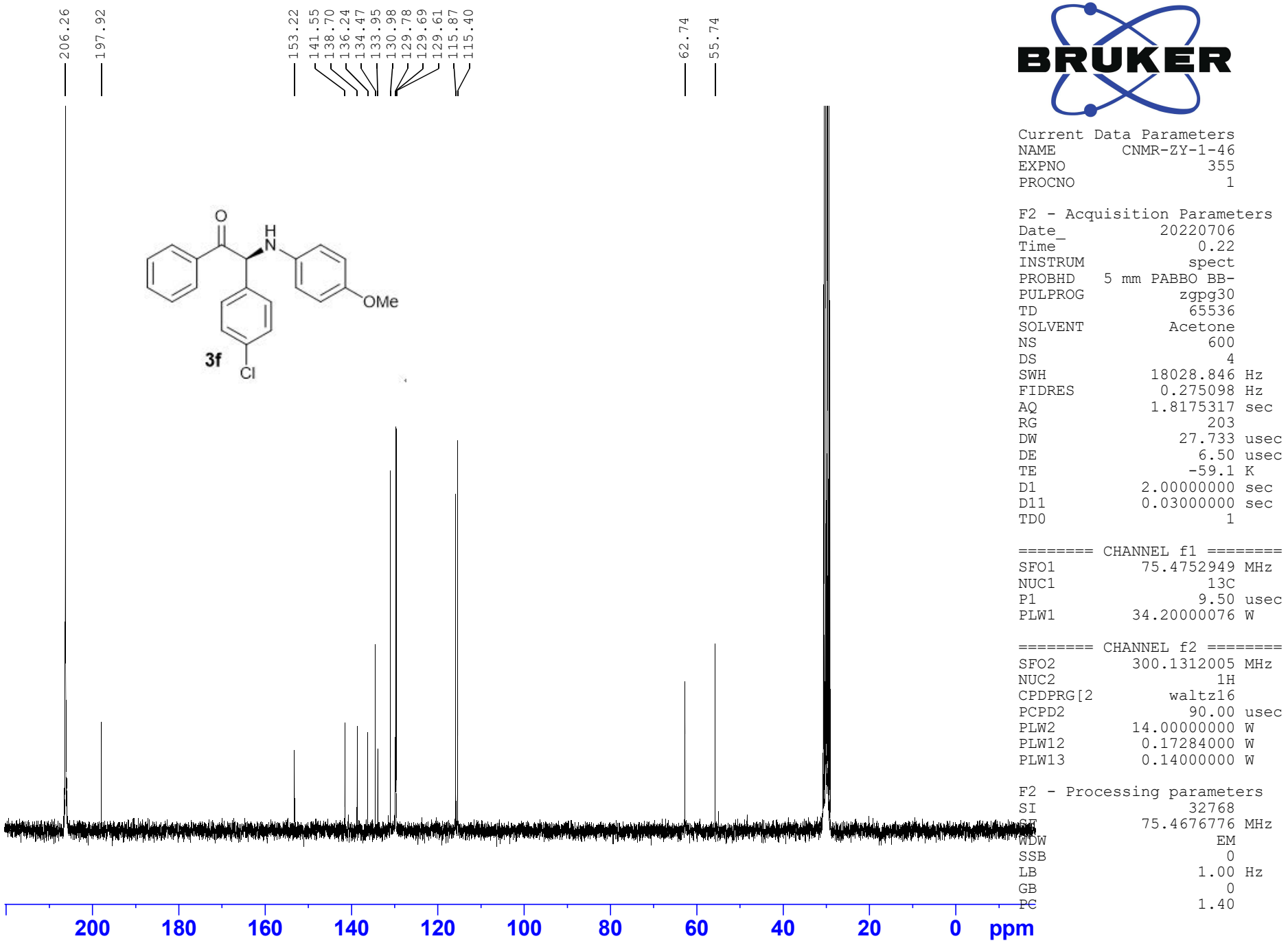

```
Current Data Parameters
NAME        HNMR-ZY-1-46
EXPNO                349
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220704
Time                16.30
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                    16
DS                     2
SWH              6009.615 Hz
FIDRES           0.091699 Hz
AQ               5.4525952 sec
RG                   181
DW                83.200 usec
DE                 6.50 usec
TE                -59.1 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1318534 MHz
NUC1                   1H
P1                 10.00 usec
PLW1         14.00000000 W

F2 - Processing parameters
SI                 65536
SF           300.1300050 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```





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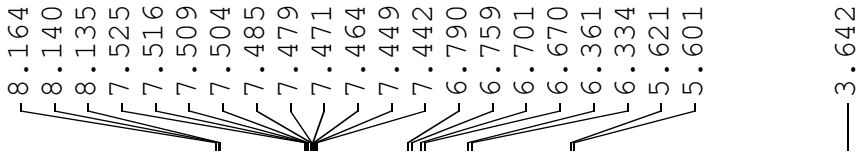
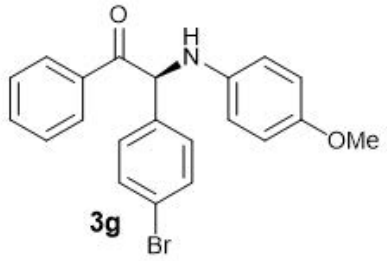
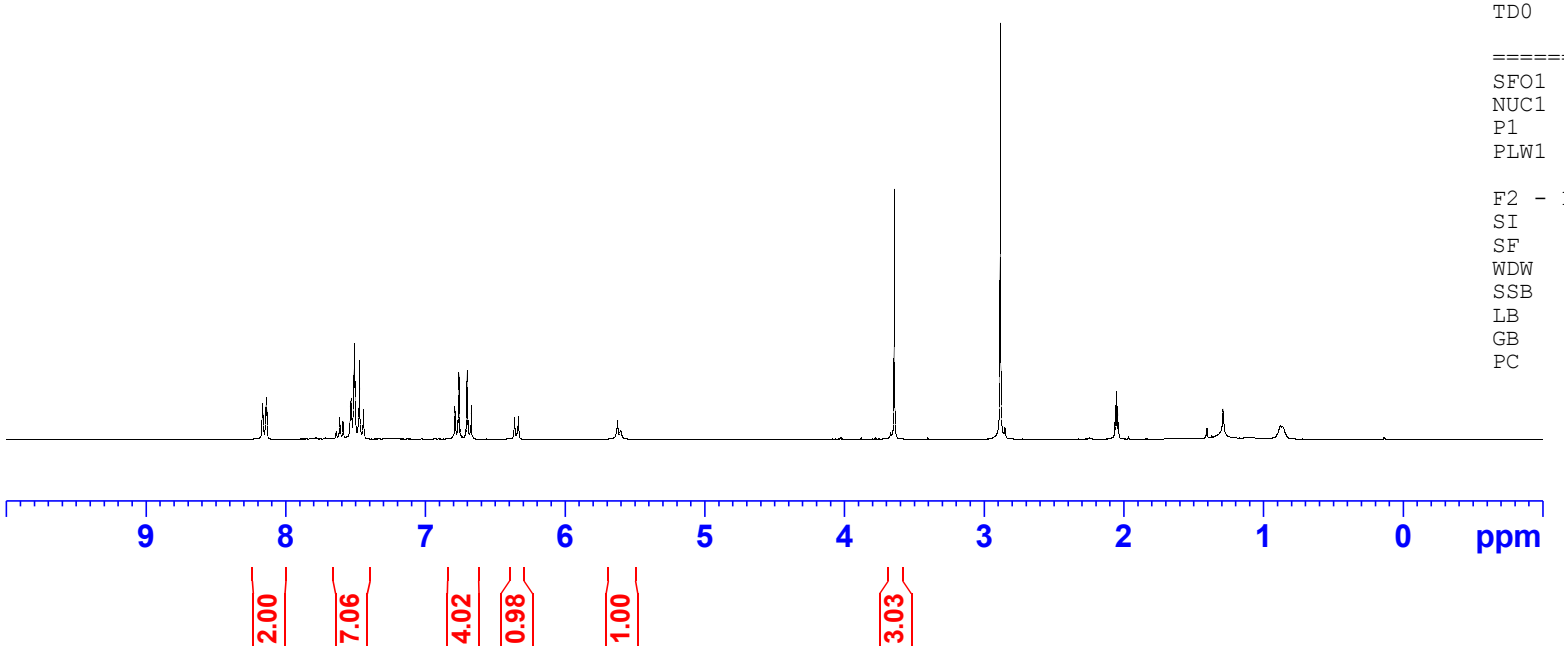
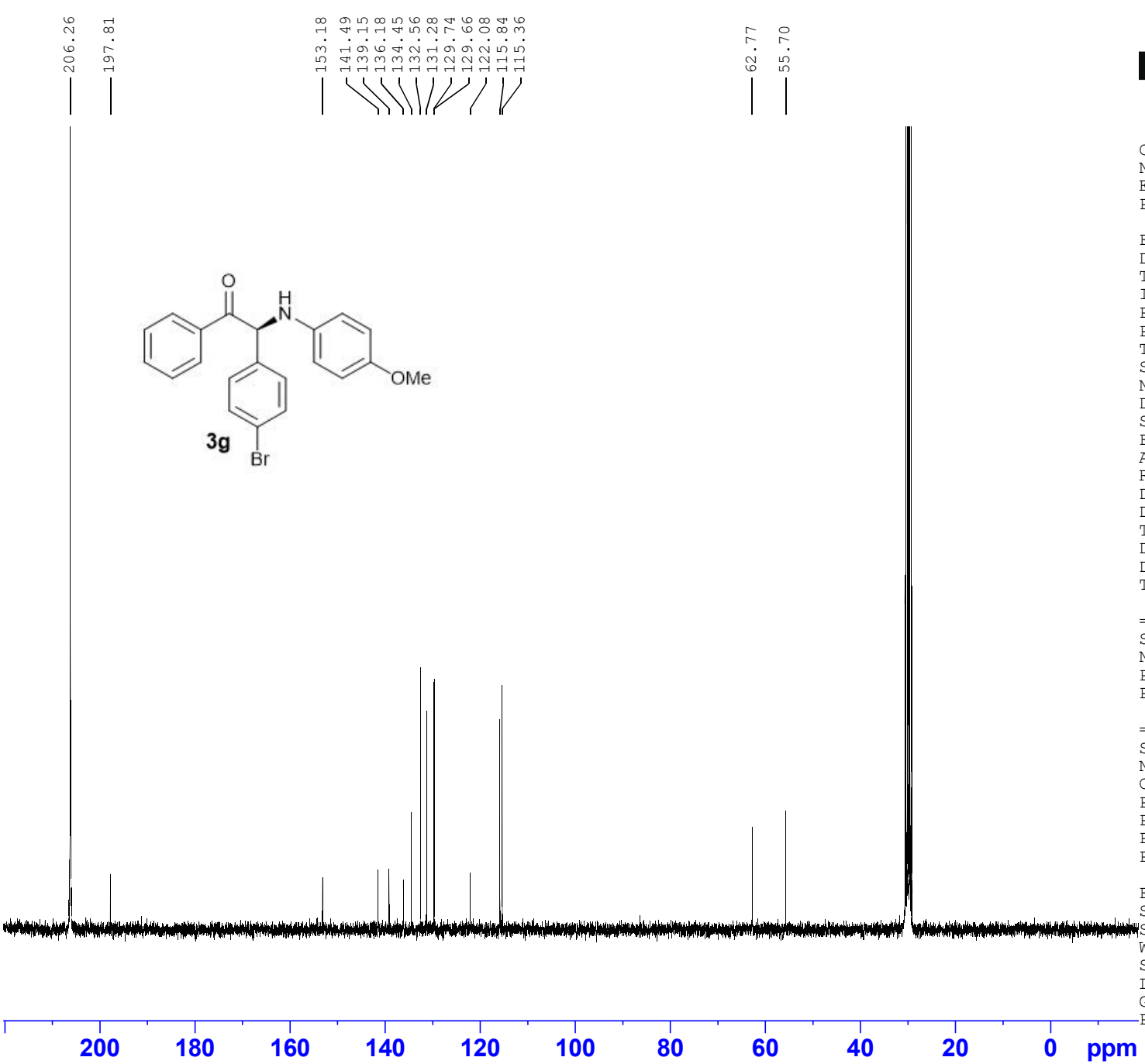
```
Current Data Parameters
NAME       CNMR-ZY-1-46
EXPNO               355
PROCNO                1

F2 - Acquisition Parameters
Date_          20220706
Time               0.22
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                 600
DS                   4
SWH          18028.846 Hz
FIDRES        0.275098 Hz
AQ           1.8175317 sec
RG                 203
DW              27.733 usec
DE               6.50 usec
TE               -59.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                9.50 usec
PLW1        34.20000076 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.17284000 W
PLW13        0.14000000 W

F2 - Processing parameters
SI                 32768
SF           75.4676776 MHz
WDW                   EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



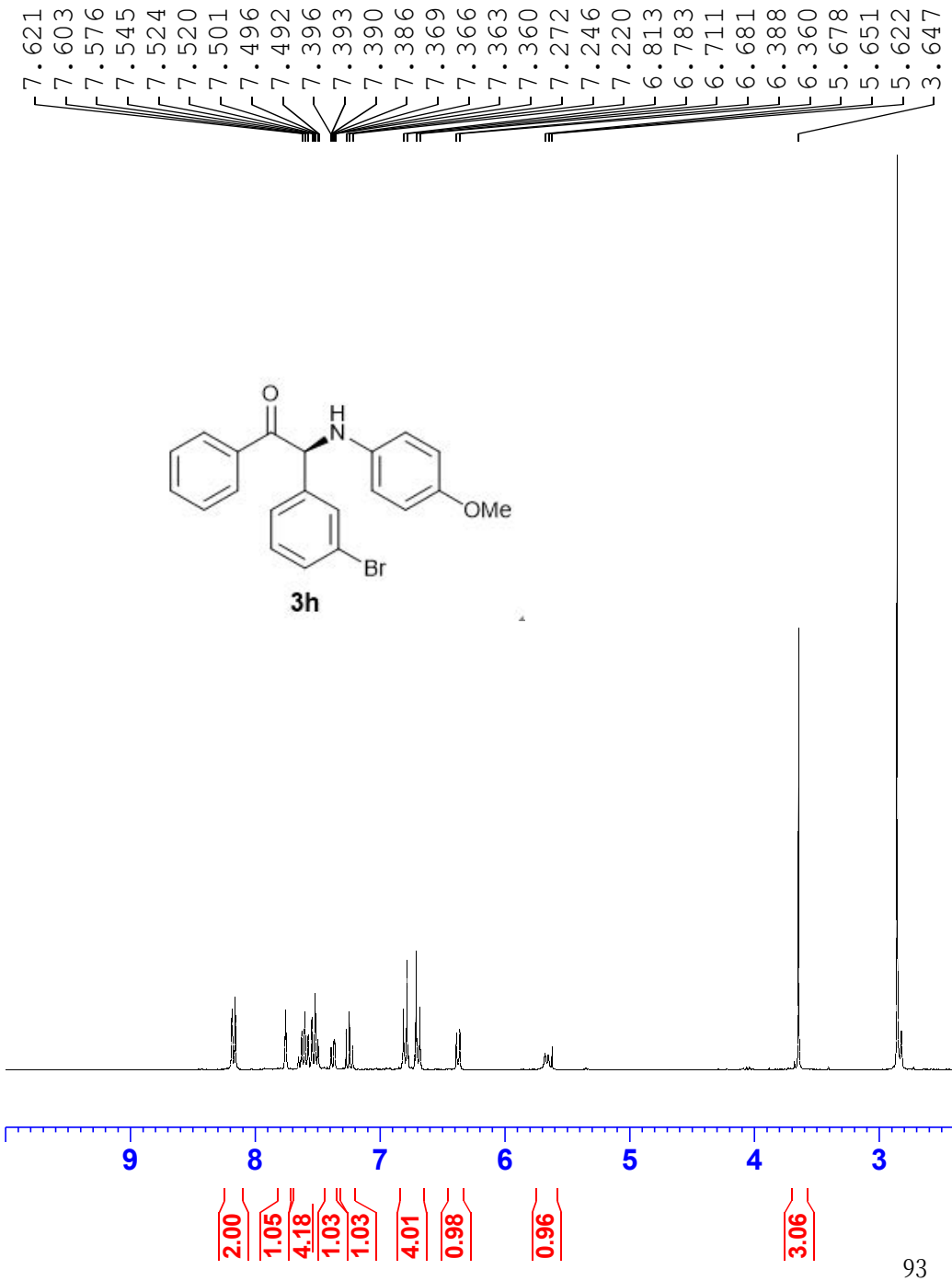





```
Current Data Parameters
NAME       HNMR-ZY-1-45
EXPNO               348
PROCNO                1

F2 - Acquisition Parameters
Date_          20220704
Time              16.25
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    2
SWH            6009.615 Hz
FIDRES        0.091699 Hz
AQ            5.4525952 sec
RG                  161
DW               83.200 usec
DE                6.50 usec
TE                -59.1 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        300.1318534 MHz
NUC1                1H
P1                10.00 usec
PLW1        14.00000000 W

F2 - Processing parameters
SI                65536
SF          300.1300051 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```




```
Current Data Parameters
NAME       CNMR-ZY-1-45
EXPNO               354
PROCNO                1

F2 - Acquisition Parameters
Date_          20220705
Time              23.40
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  600
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                  203
DW               27.733 usec
DE                6.50 usec
TE                -59.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                 9.50 usec
PLW1        34.20000076 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        14.00000000 W
PLW12        0.17284000 W
PLW13        0.14000000 W

F2 - Processing parameters
SI                 32768
SF          75.4676804 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

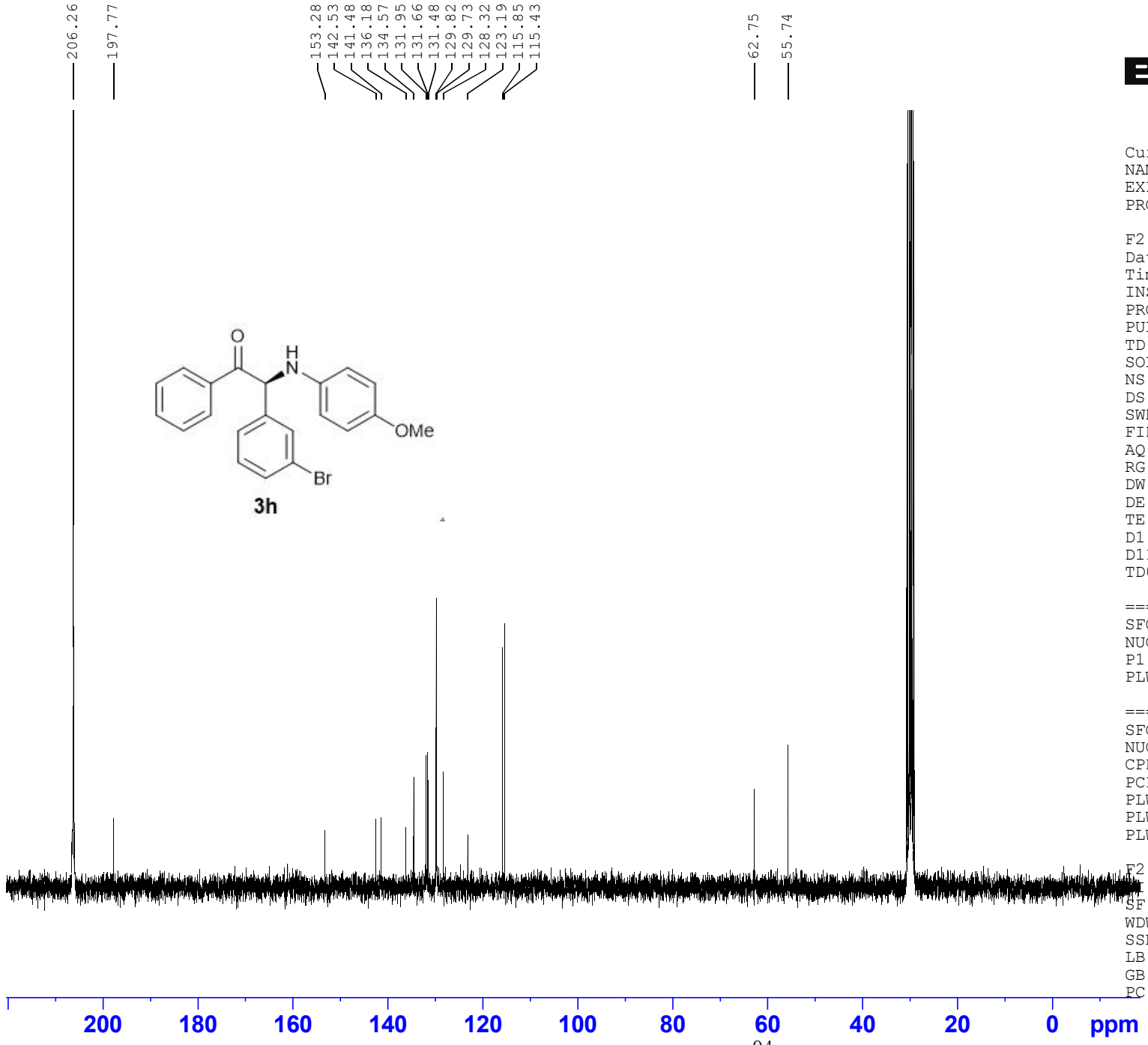


Current Data Parameters
NAME HNMR-ZY-1-58
EXPNO 400
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220712
Time 14.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 203
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



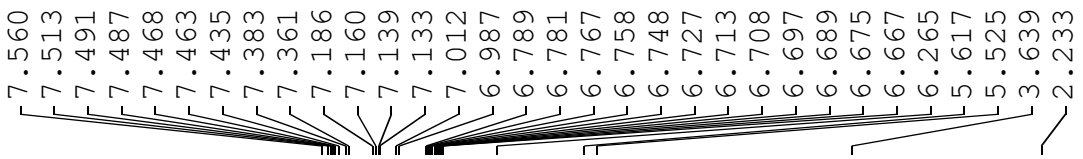
Current Data Parameters
NAME CNMR-ZY-1-58
EXPNO 416
PROCNO 1

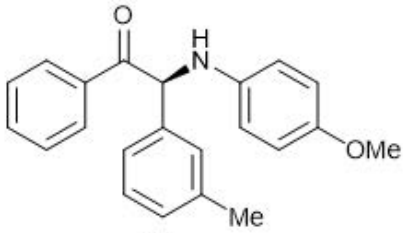
F2 - Acquisition Parameters
Date_ 20220713
Time 21.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 500
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

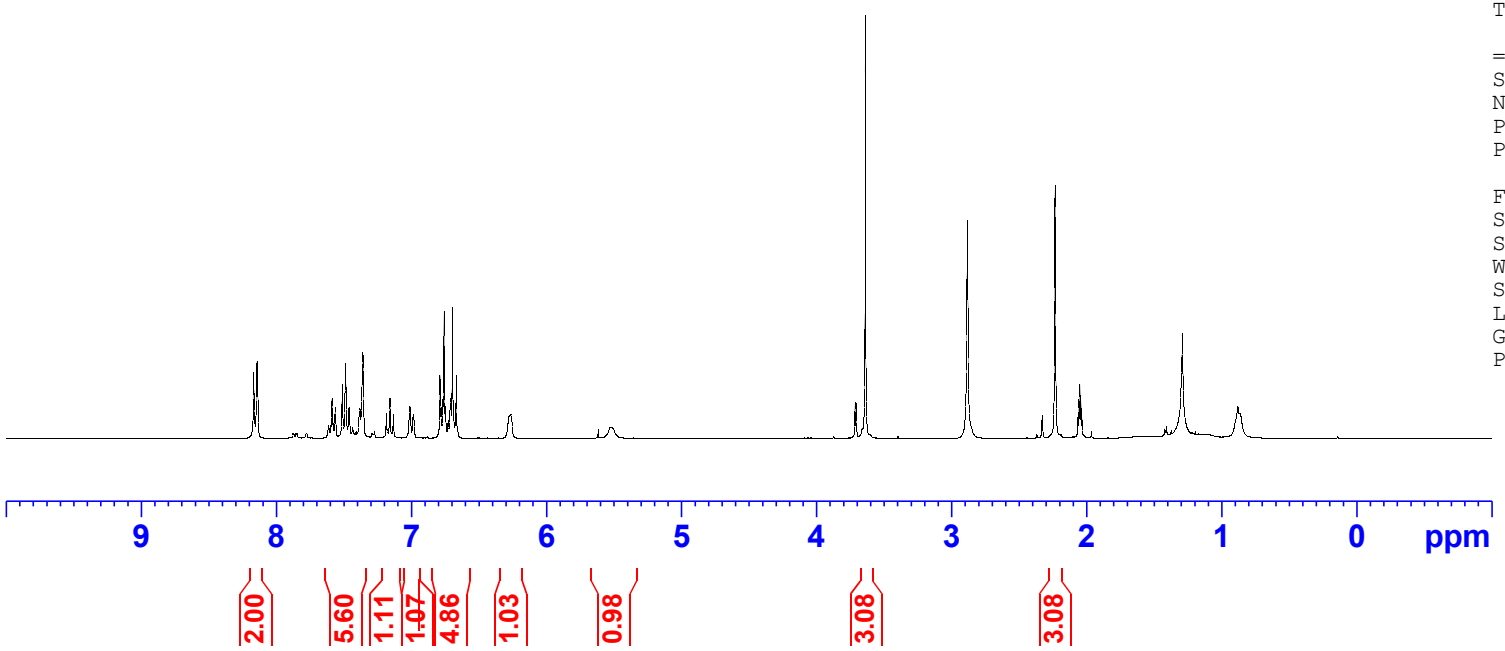
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4676774 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





3i

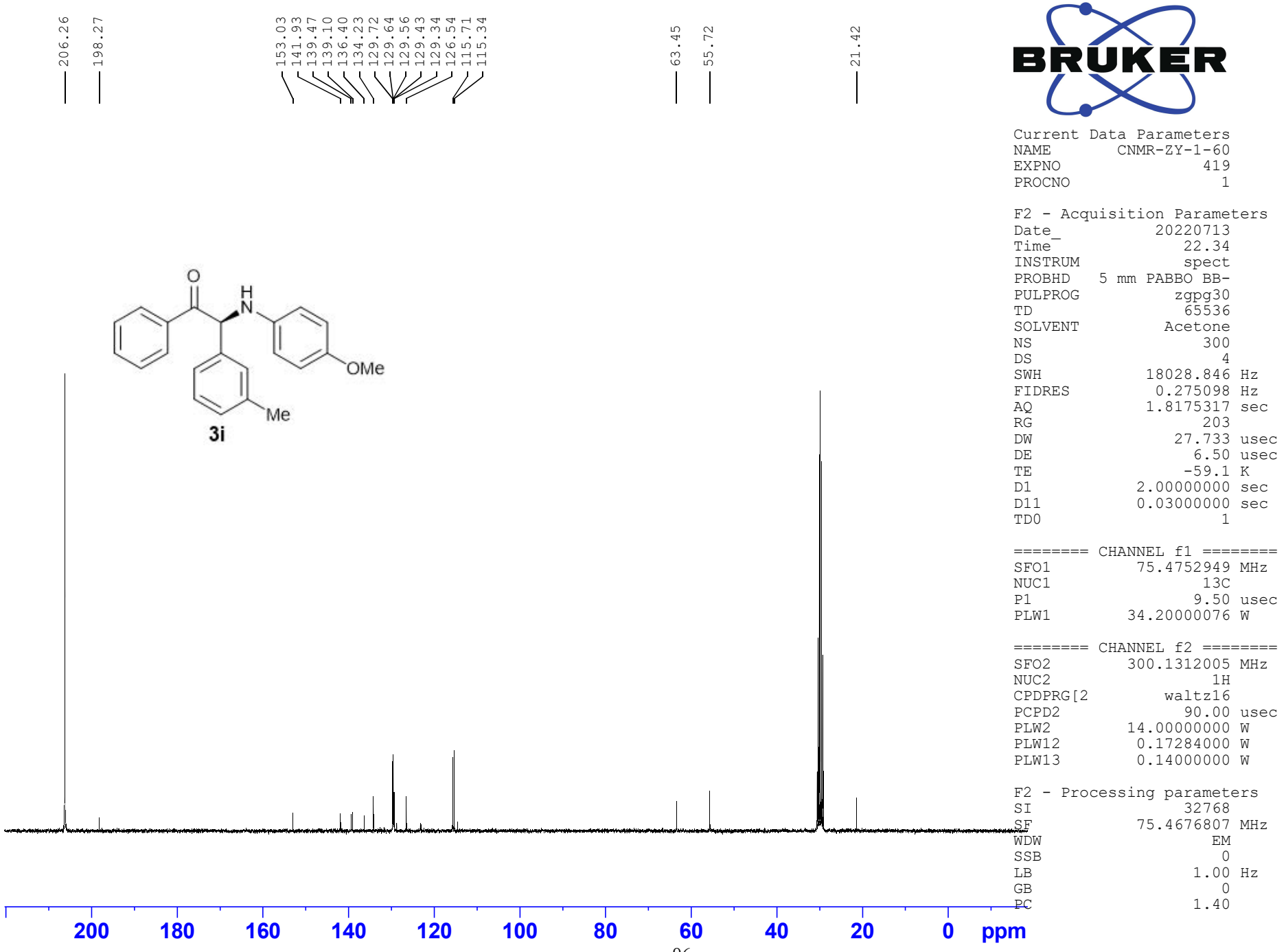


Current Data Parameters
NAME HNMR-ZY-1-60
EXPNO 399
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220712
Time 14.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 114
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



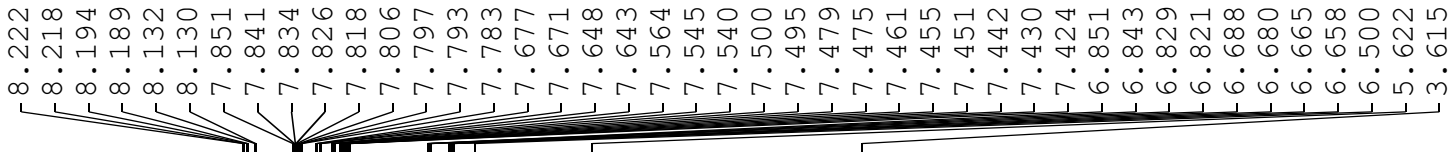
Current Data Parameters
NAME CNMR-ZY-1-60
EXPNO 419
PROCNO 1

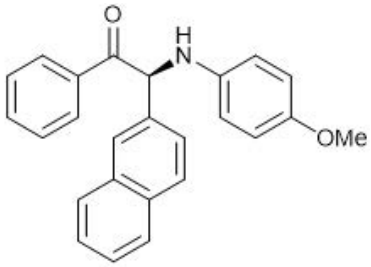
F2 - Acquisition Parameters
Date_ 20220713
Time 22.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 300
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

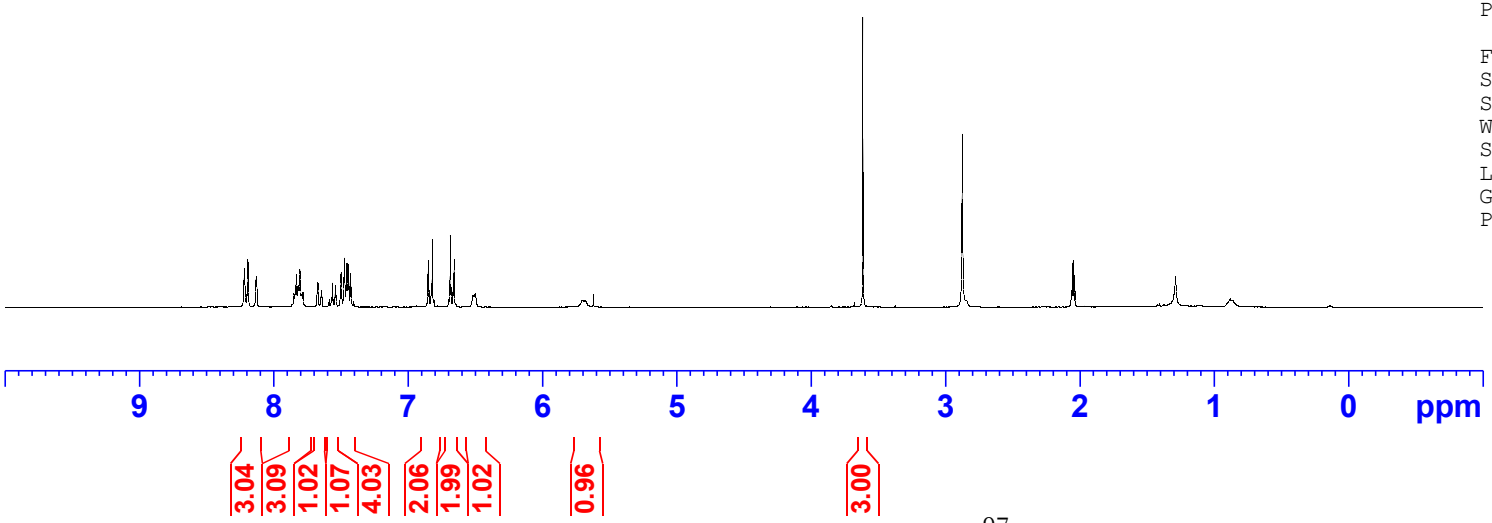
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4676807 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

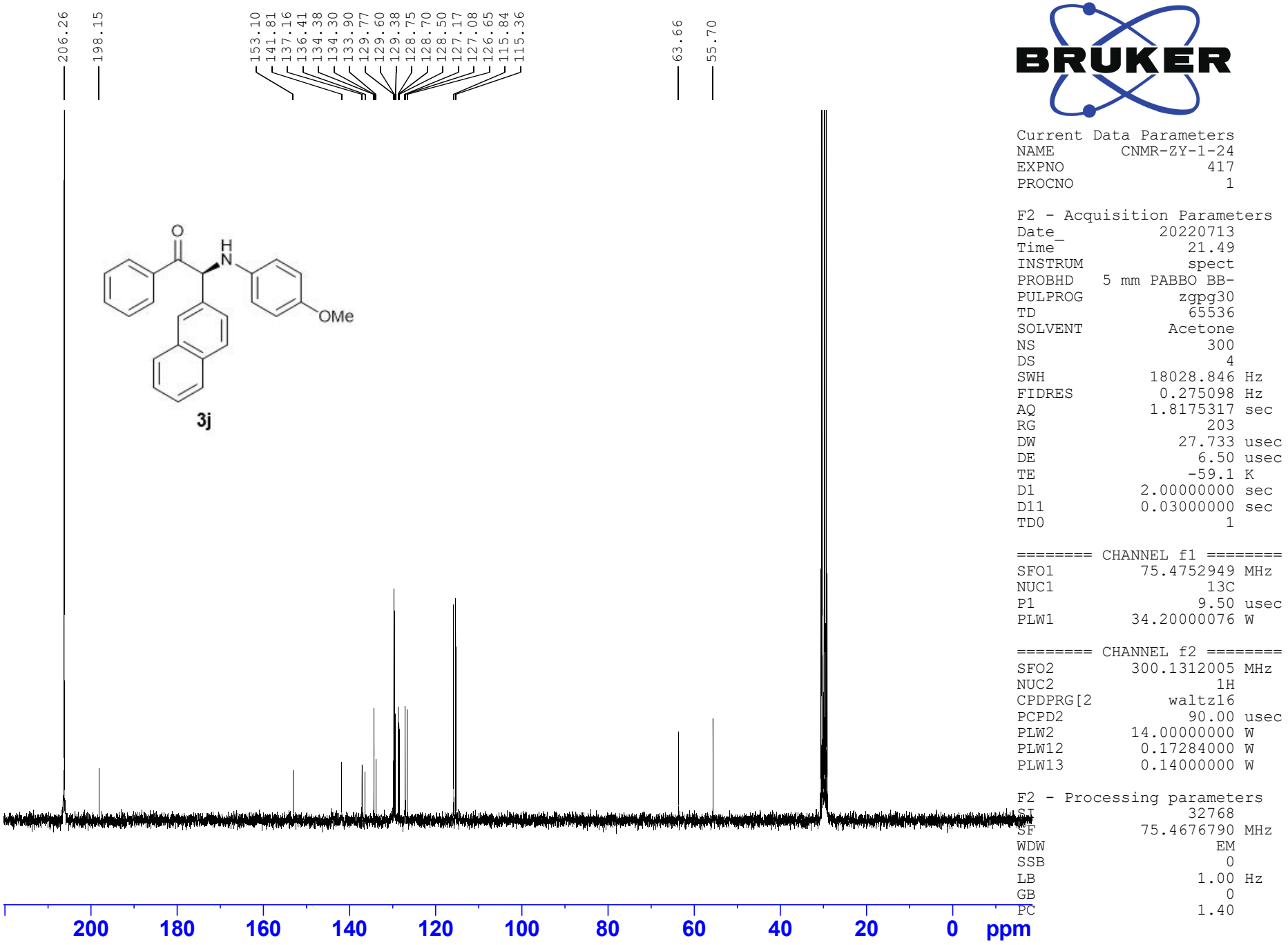




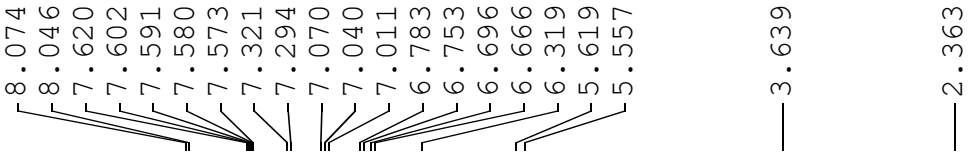
3j

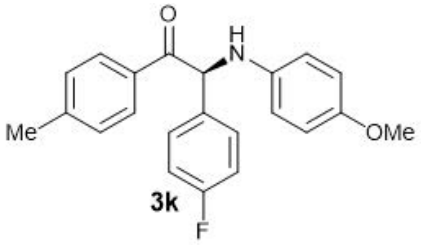


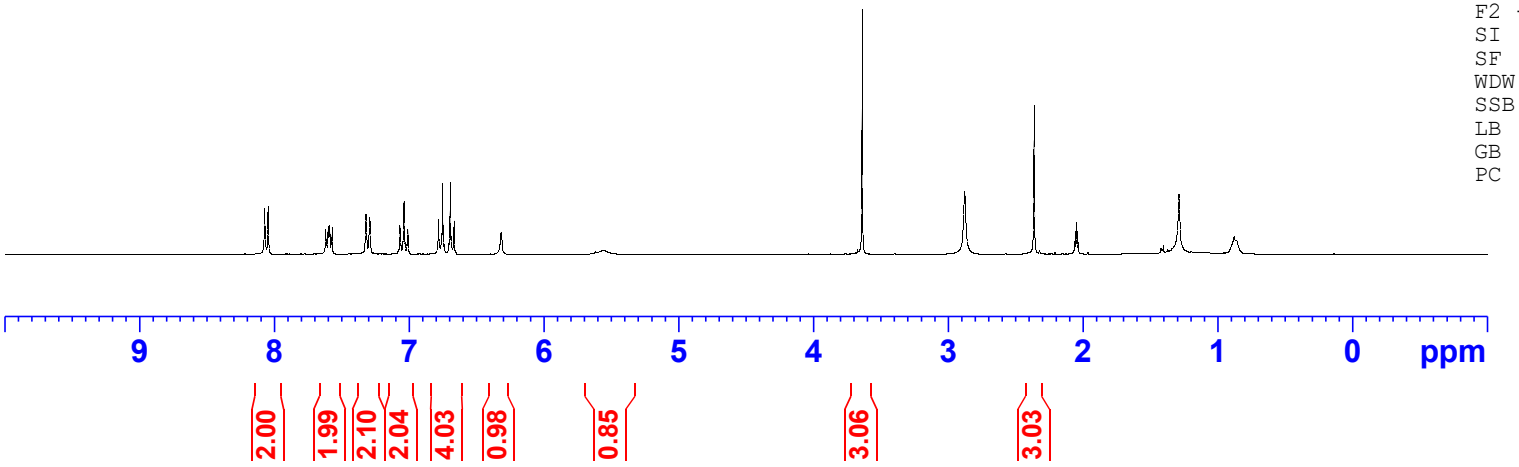

```
Current Data Parameters
NAME       HNMR-ZY-1-24
EXPNO               397
PROCNO                1

F2 - Acquisition Parameters
Date_          20220712
Time              13.56
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    2
SWH            6009.615 Hz
FIDRES        0.091699 Hz
AQ            5.4525952 sec
RG                  161
DW               83.200 usec
DE                6.50 usec
TE                -59.1 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        300.1318534 MHz
NUC1                  1H
P1                10.00 usec
PLW1        14.00000000 W

F2 - Processing parameters
SI                65536
SF          300.1300051 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```




```
Current Data Parameters
NAME       CNMR-ZY-1-24
EXPNO               417
PROCNO                1

F2 - Acquisition Parameters
Date_          20220713
Time              21.49
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD                65536
SOLVENT         Acetone
NS                  300
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                  203
DW               27.733 usec
DE                6.50 usec
TE                -59.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                 9.50 usec
PLW1        34.20000076 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        14.00000000 W
PLW12        0.17284000 W
PLW13        0.14000000 W

F2 - Processing parameters
SI                 32768
SF            75.4676790 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```





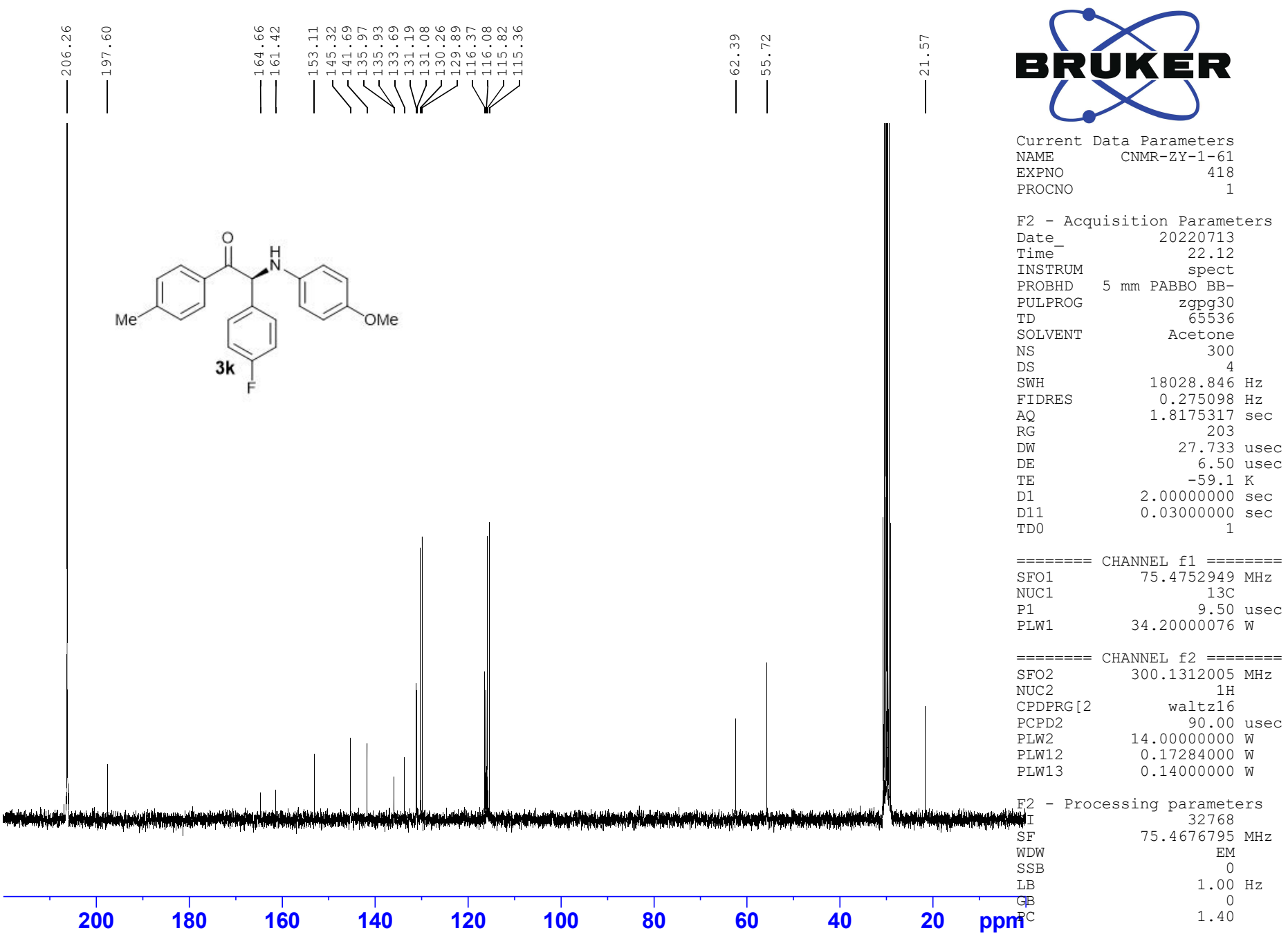


Current Data Parameters
NAME HNMR-ZY-1-61
EXPNO 398
PROCNO 1

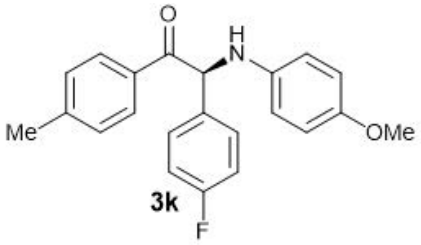
F2 - Acquisition Parameters
Date_ 20220712
Time 14.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 128
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

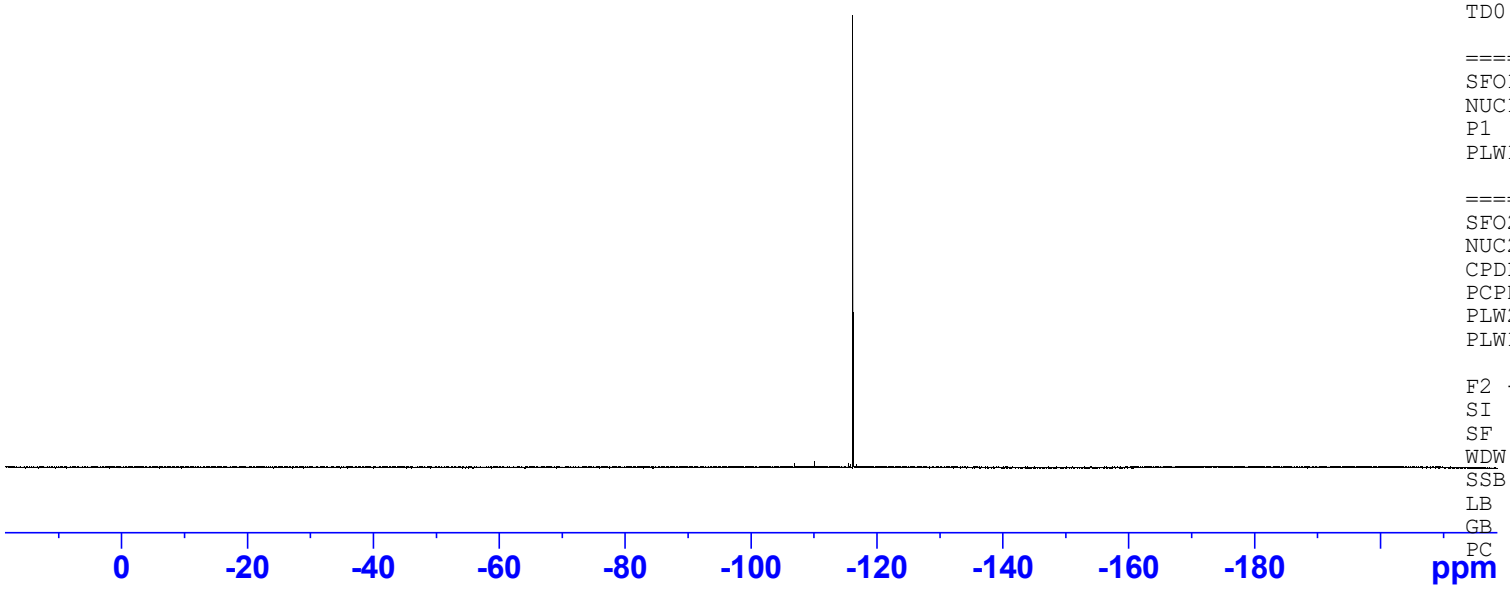
F2 - Processing parameters
SI 65536
SF 300.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00




```
Current Data Parameters
NAME       CNMR-ZY-1-61
EXPNO               418
PROCNO                1

F2 - Acquisition Parameters
Date_          20220713
Time              22.12
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD                65536
SOLVENT         Acetone
NS                  300
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                  203
DW               27.733 usec
DE                6.50 usec
TE                -59.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                 9.50 usec
PLW1        34.20000076 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.17284000 W
PLW13        0.14000000 W

F2 - Processing parameters
SI                32768
SF           75.4676795 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



-116.17



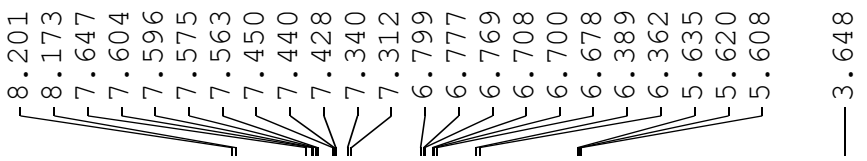
Current Data Parameters
NAME FNMR-ZY-1-61
EXPNO 482
PROCNO 1

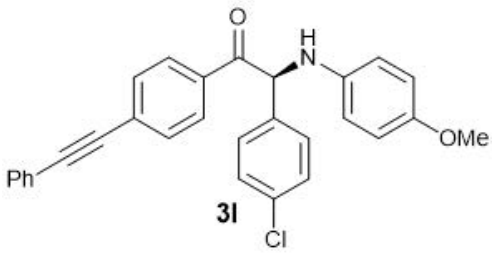
F2 - Acquisition Parameters
Date_ 20220722
Time 14.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn.2
TD 131072
SOLVENT Acetone
NS 4
DS 4
SWH 66964.289 Hz
FIDRES 0.510897 Hz
AQ 0.9786710 sec
RG 203
DW 7.467 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

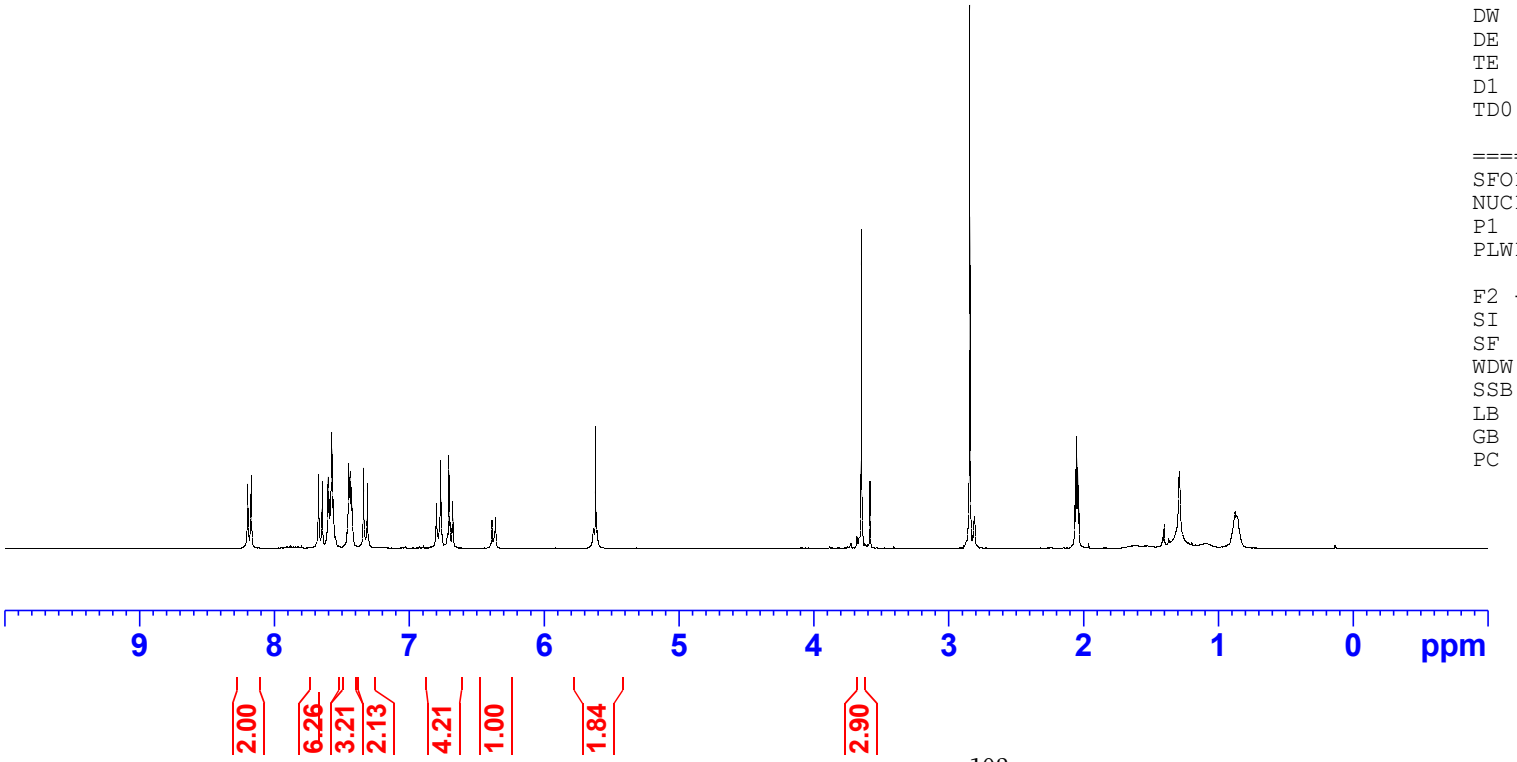
======== CHANNEL f1 ========
SFO1 282.3761148 MHz
NUC1 19F
P1 14.50 usec
PLW1 10.39999962 W

======== 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





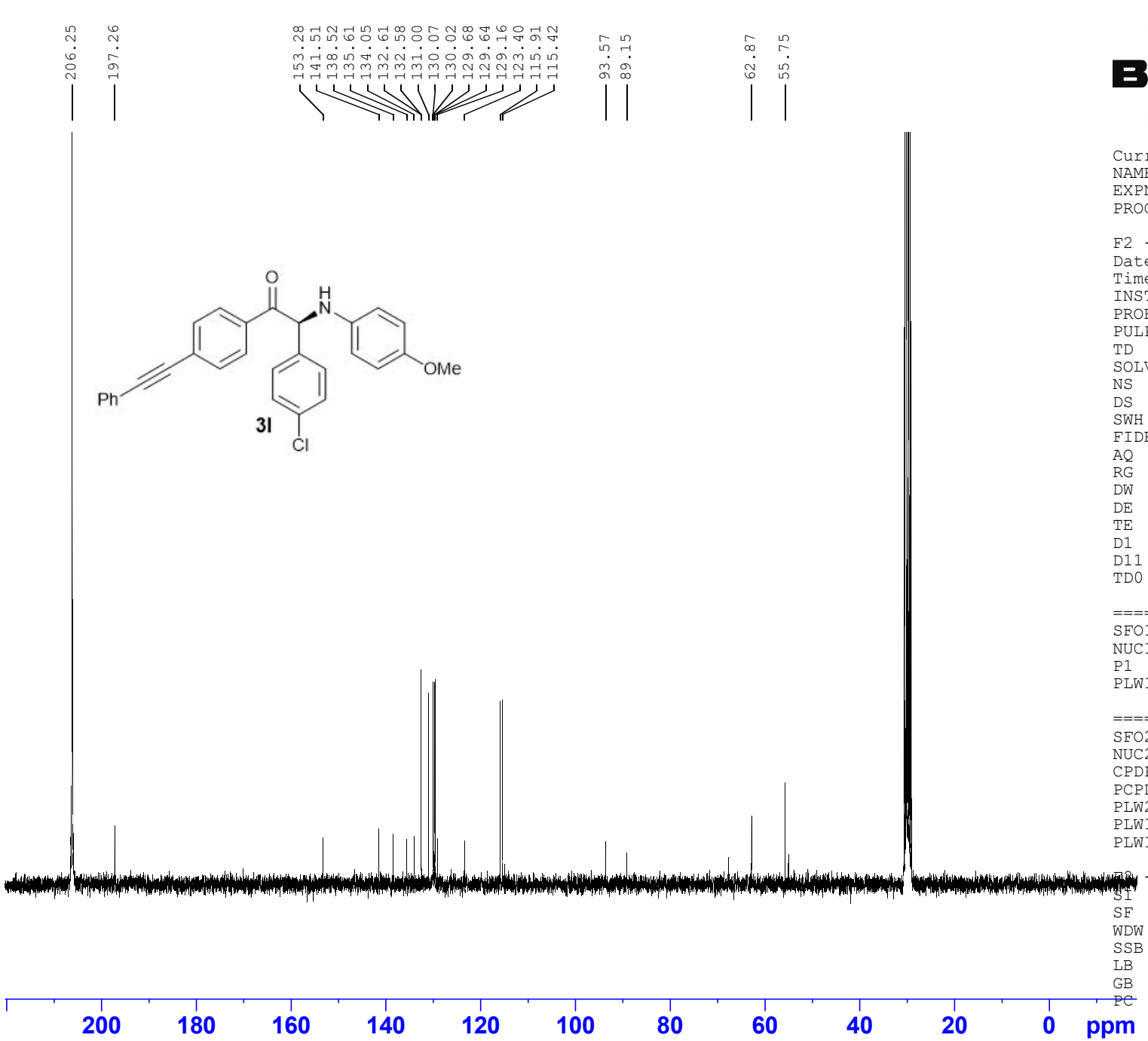


Current Data Parameters
NAME HNMR-ZY-1-47
EXPNO 378
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220708
Time 14.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 203
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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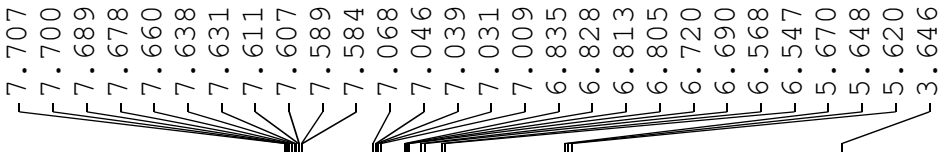
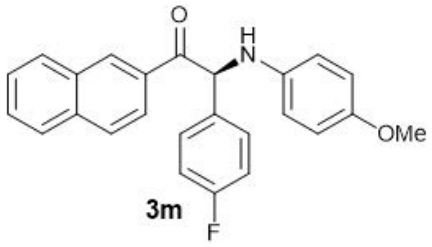
```
Current Data Parameters
NAME          CNMR-1-47
EXPNO               387
PROCNO                1

F2 - Acquisition Parameters
Date_          20220709
Time               2.07
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  600
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                  203
DW               27.733 usec
DE                6.50 usec
TE                -59.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                 9.50 usec
PLW1        34.20000076 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        14.00000000 W
PLW12        0.17284000 W
PLW13        0.14000000 W

F2 - Processing parameters
SI                 32768
SF          75.4676766 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                 1.40
```



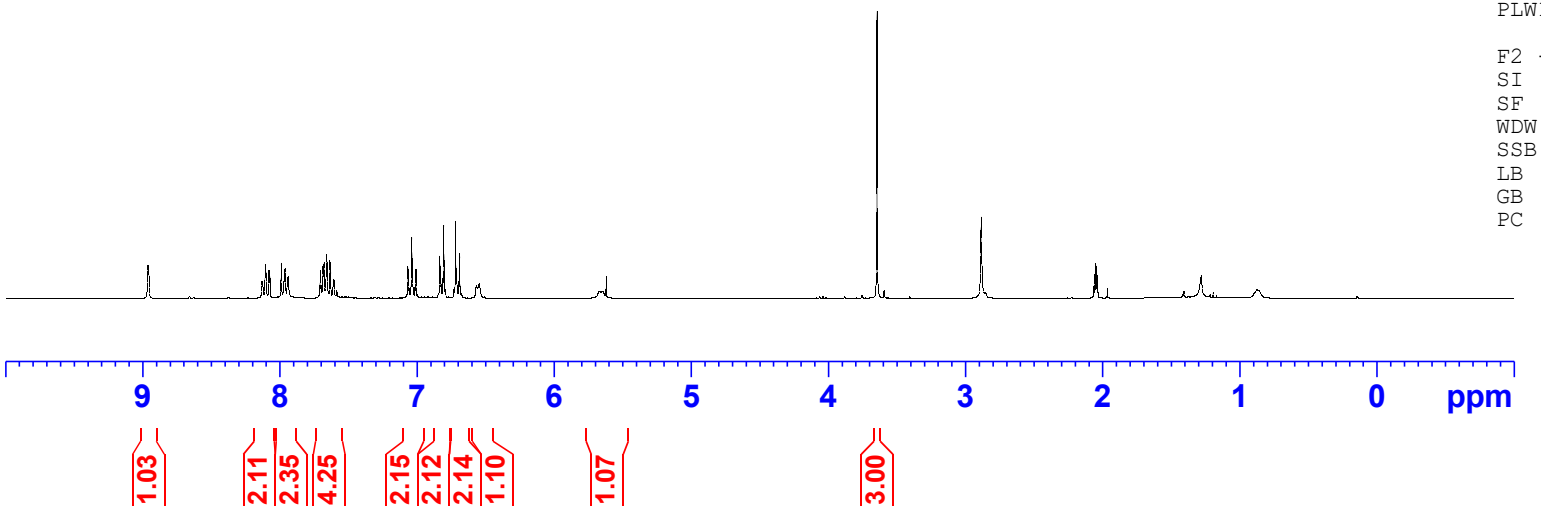


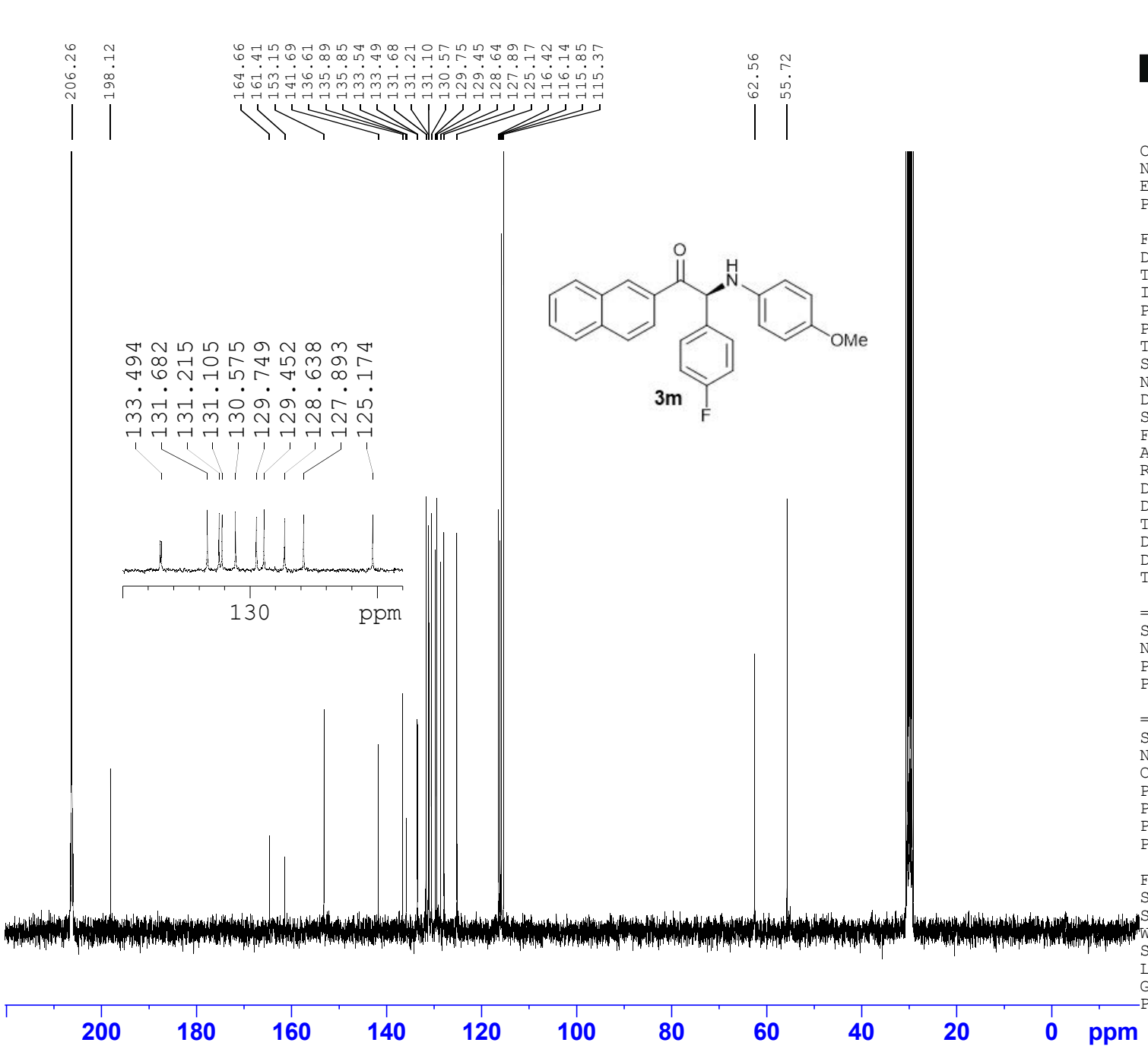
Current Data Parameters
NAME HNMR-ZY-1-44
EXPNO 347
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220704
Time 16.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 128
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





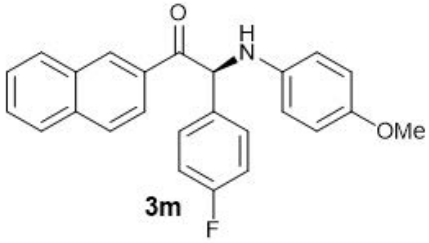
Current Data Parameters
NAME CNMR-ZY-1-44
EXPNO 356
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220706
Time 1.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 600
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4676810 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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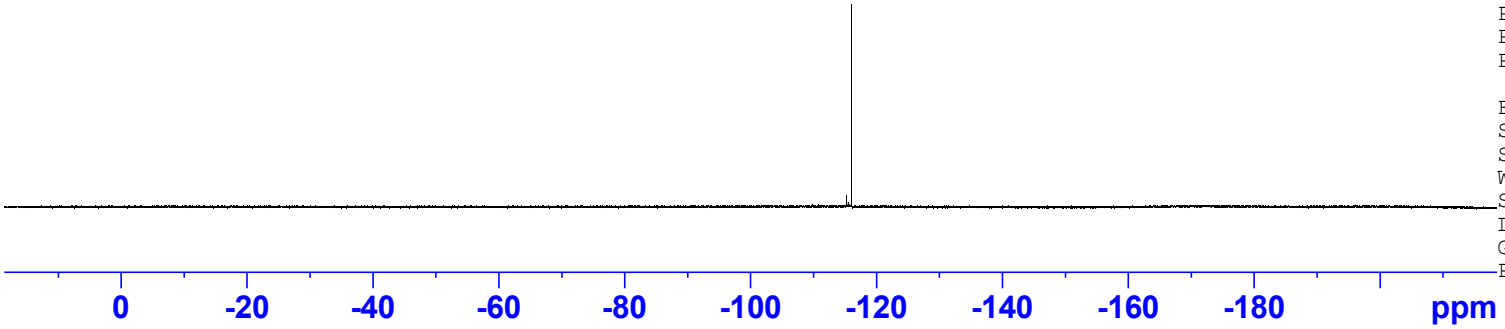
-116.04



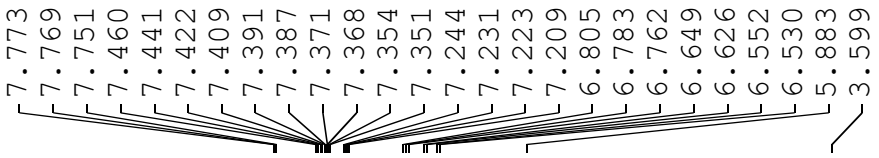
Current Data Parameters
NAME FNMR-ZY-1-44
EXPNO 479
PROCNO 1

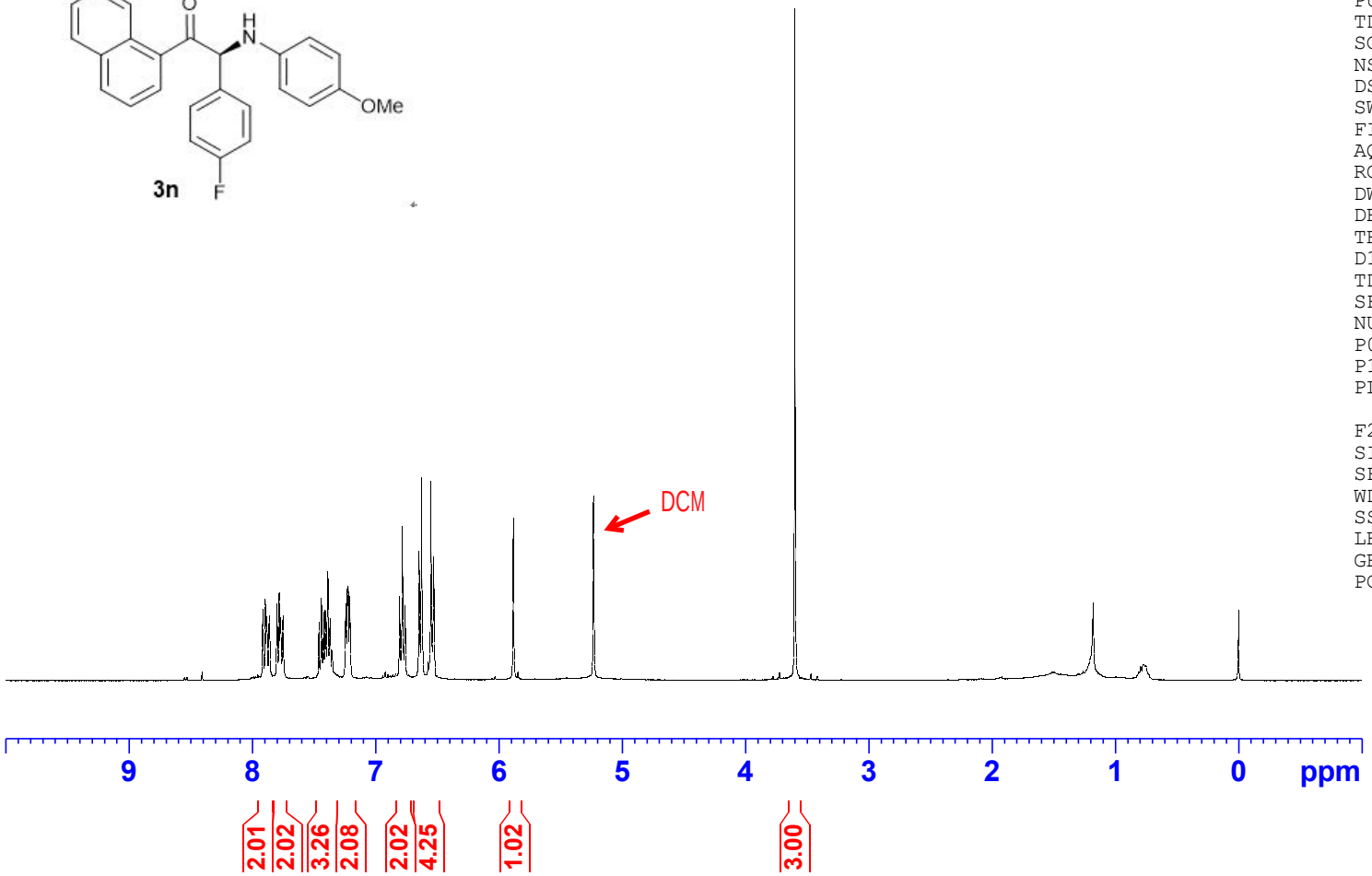
F2 - Acquisition Parameters
Date_ 20220722
Time 14.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn.2
TD 131072
SOLVENT Acetone
NS 4
DS 4
SWH 66964.289 Hz
FIDRES 0.510897 Hz
AQ 0.9786710 sec
RG 203
DW 7.467 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 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

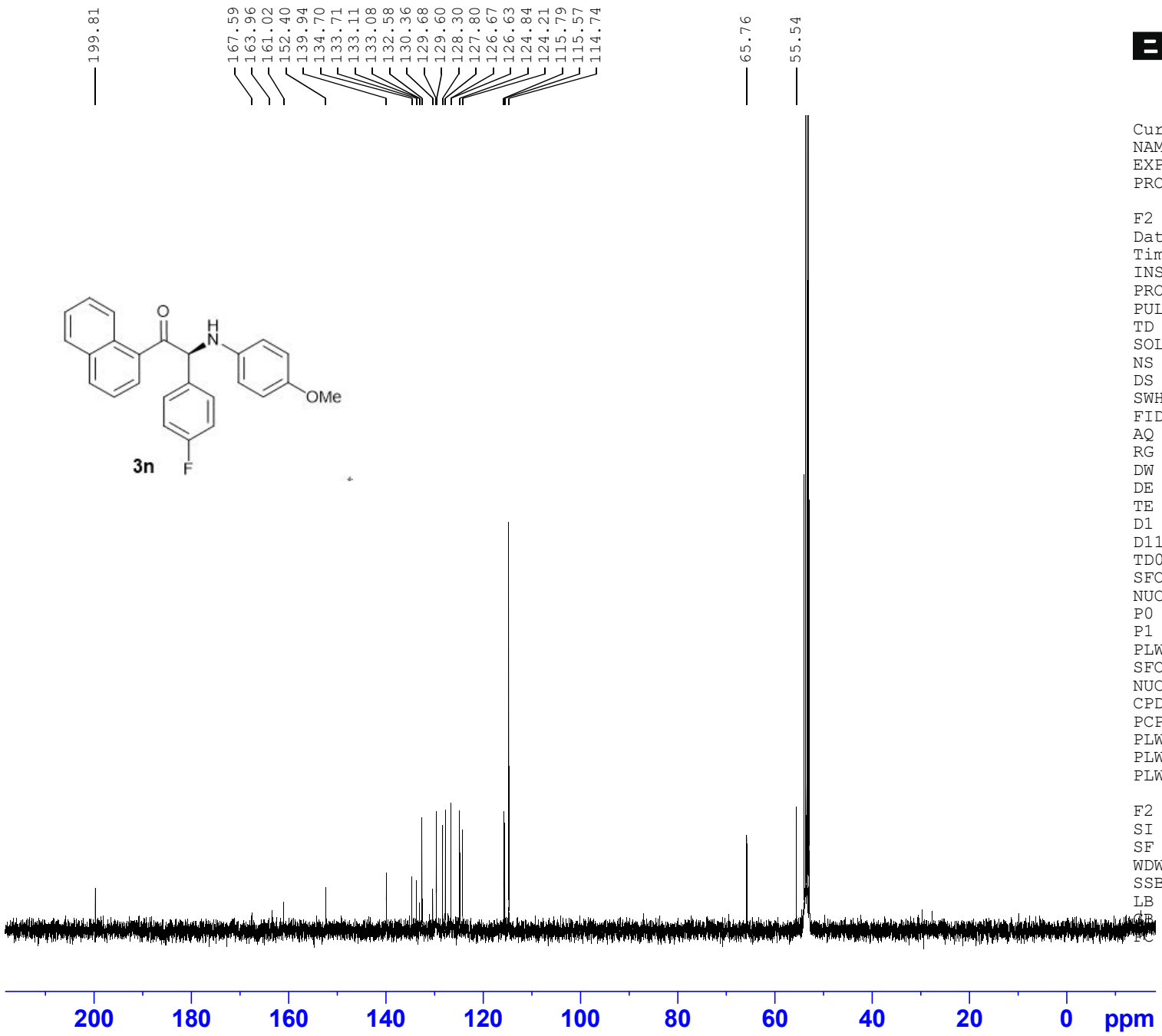




Current Data Parameters
NAME HNMR-zy-3-54
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221217
Time 1.29 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zg30
TD 65536
SOLVENT CD2Cl2
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 295.0 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 400.1300509 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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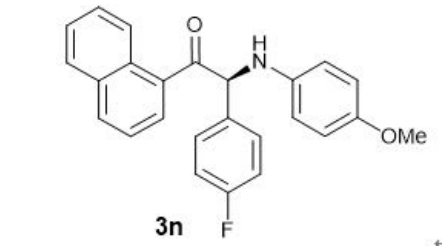
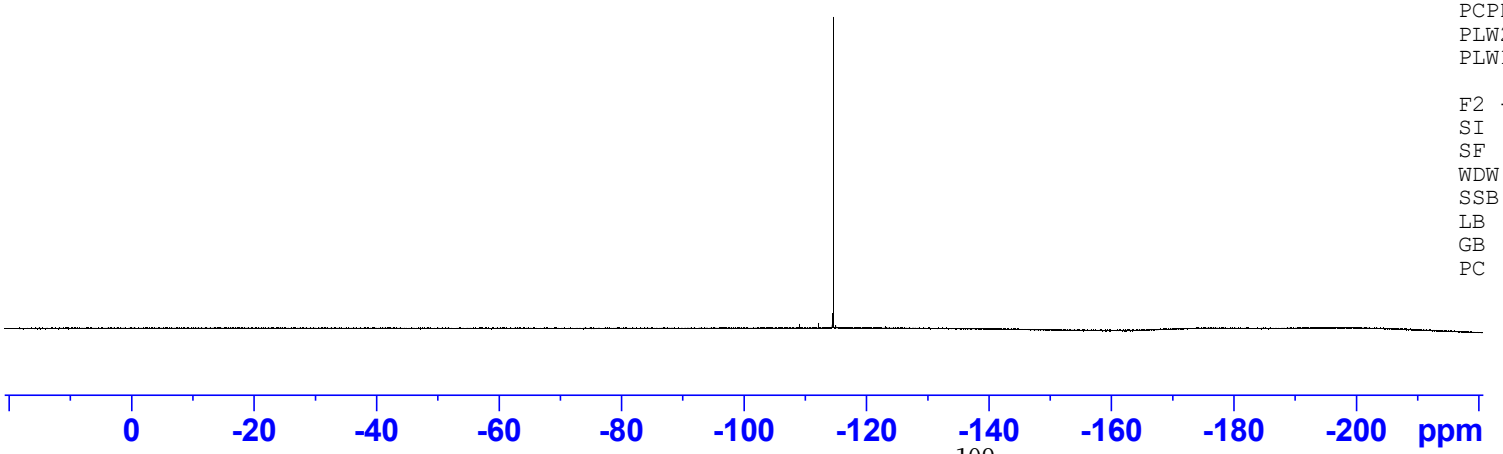
Current Data Parameters
NAME HNMR-zy-3-54
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221217
Time 1.53 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgpg30
TD 65536
SOLVENT CD2Cl2
NS 400
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 295.7 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

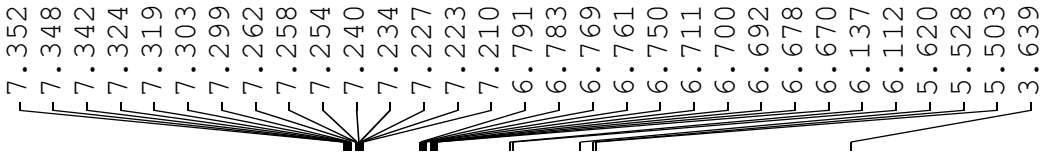
F2 - Processing parameters
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
1.40

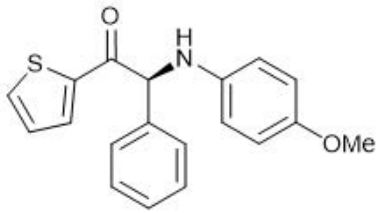


-114.63




```
Current Data Parameters
NAME       HNMR-zy-3-54
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20221217
Time               1.55 h
INSTRUM           Avance
PROBHD   Z116098_0833 (
PULPROG            zgig
TD               131072
SOLVENT          CD2Cl2
NS                   16
DS                    4
SWH           90909.094 Hz
FIDRES         1.387163 Hz
AQ            0.7208960 sec
RG                  101
DW                5.500 usec
DE                6.50 usec
TE                295.4 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        376.4607164 MHz
NUC1                19F
P1                18.00 usec
PLW1        16.73100090 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        20.73200035 W
PLW12        0.25595000 W

F2 - Processing parameters
SI                65536
SF          376.4983662 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```





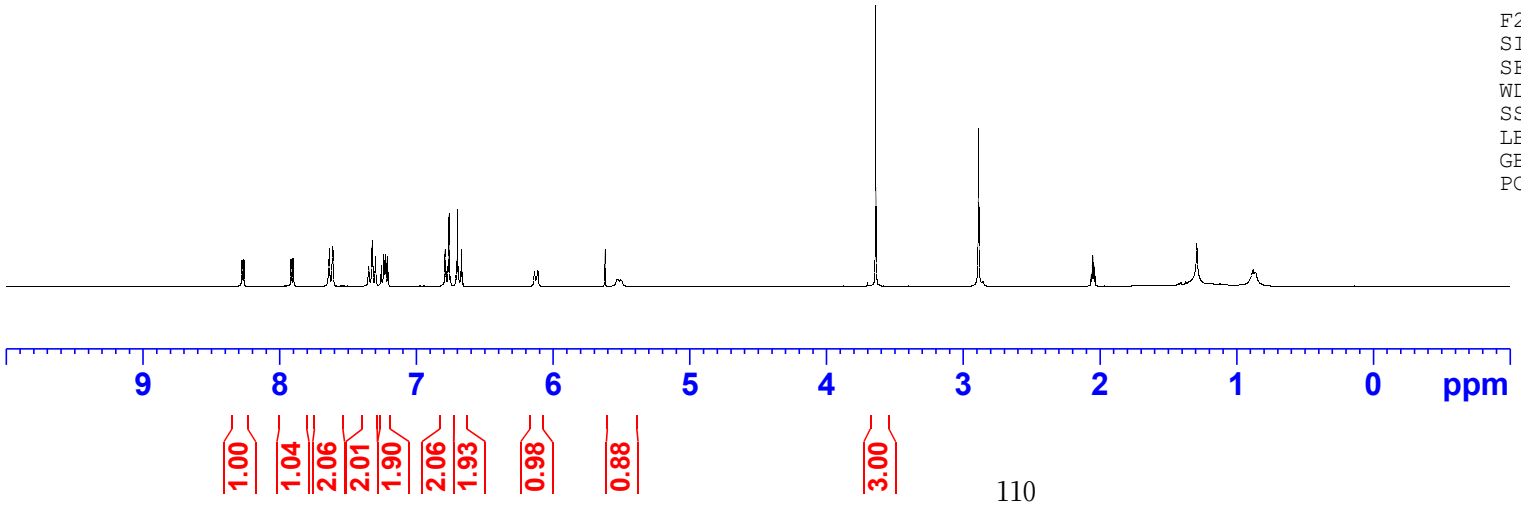
3o

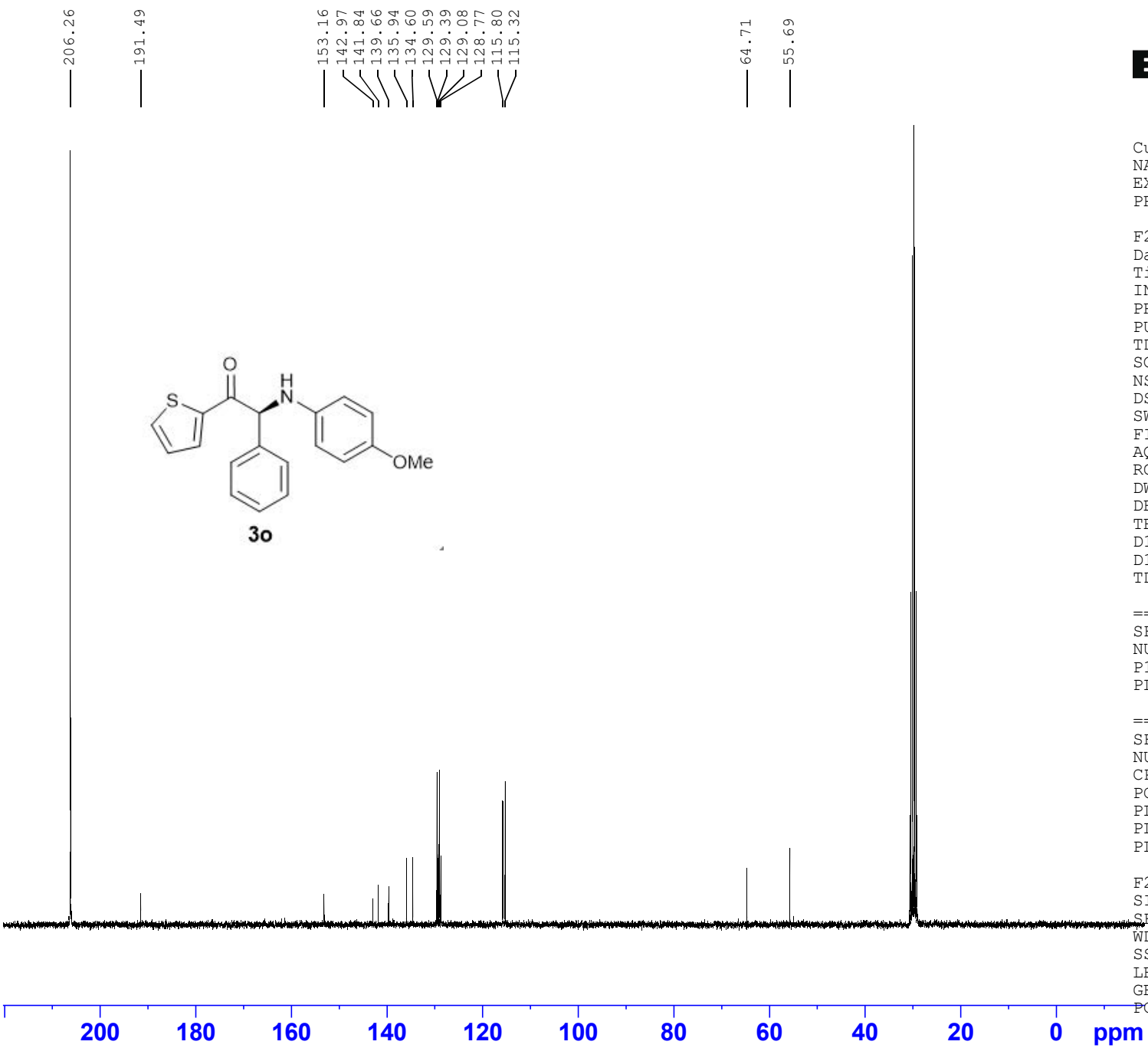
Current Data Parameters
NAME HNMR-ZY-1-70
EXPNO 457
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220721
Time 13.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 128
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

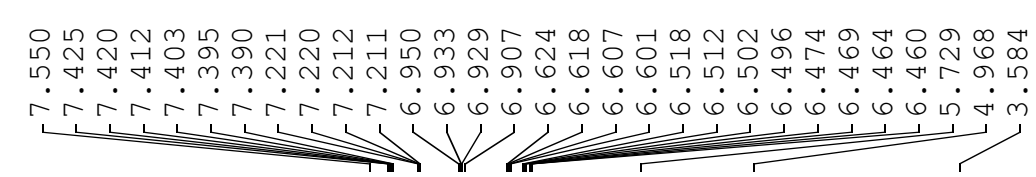
======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

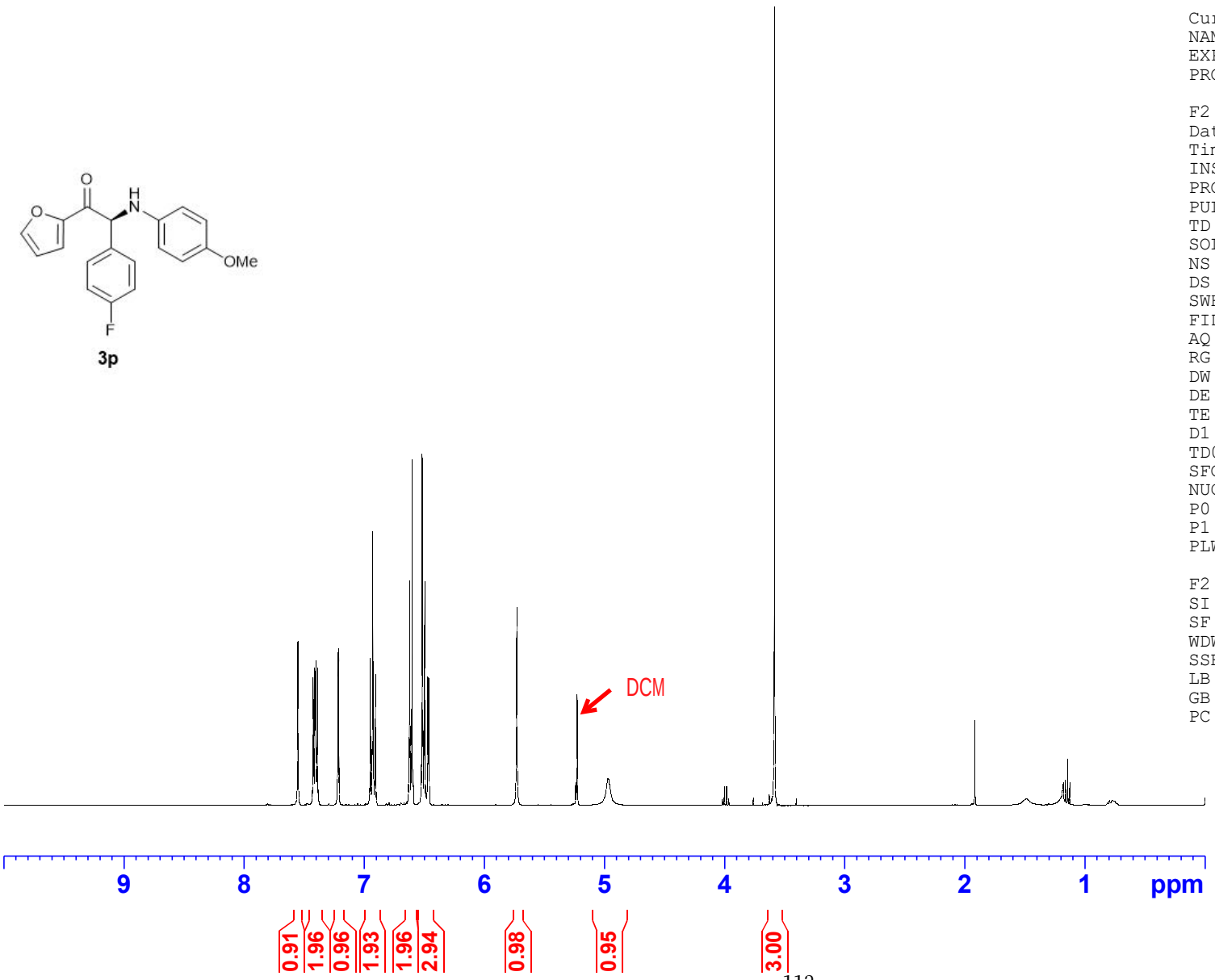




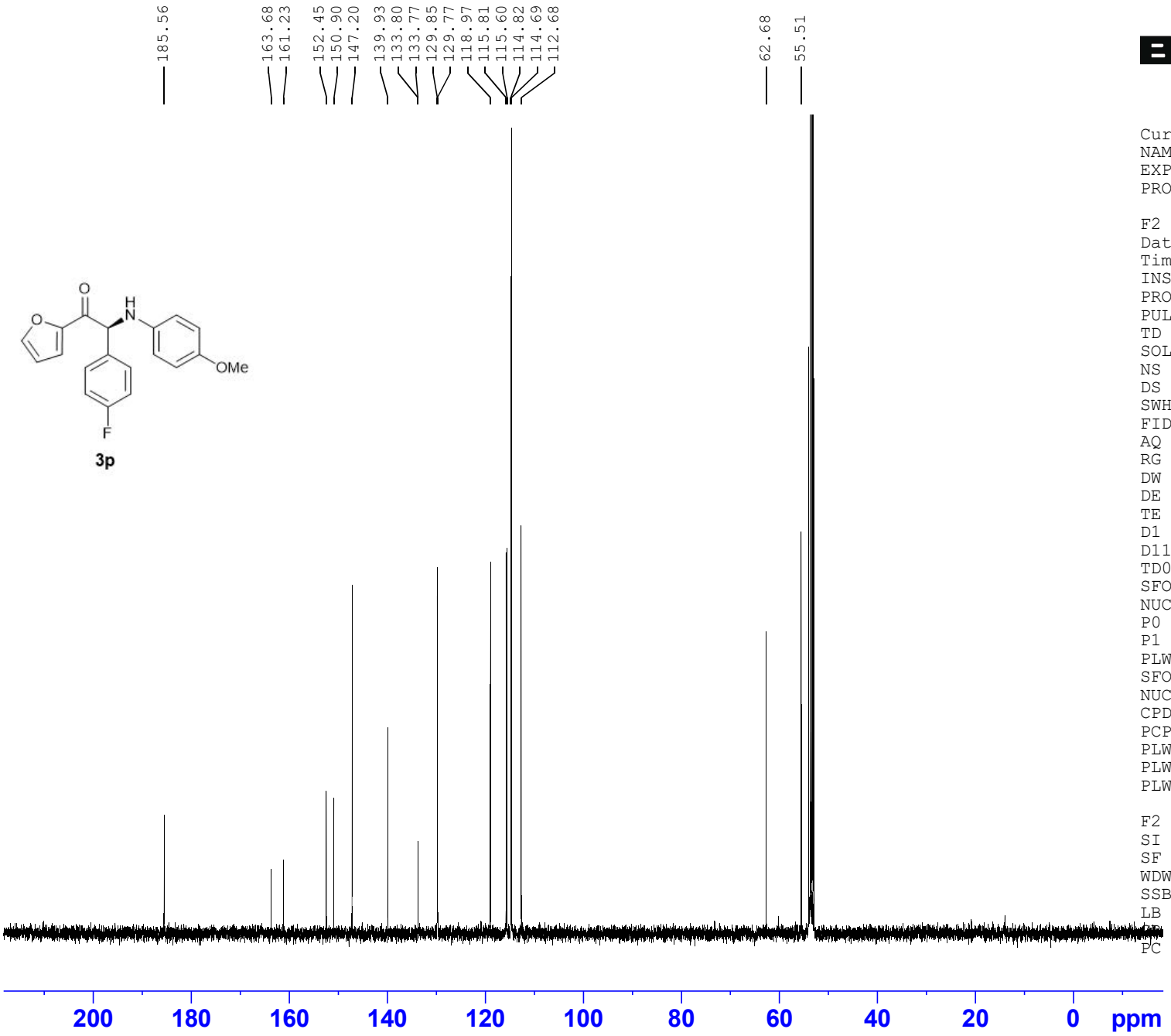

```
Current Data Parameters
NAME       CNMR-ZY-1-70
EXPNO               463
PROCNO                1

F2 - Acquisition Parameters
Date_          20220721
Time              21.21
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  200
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                  203
DW               27.733 usec
DE                6.50 usec
TE                -59.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                 9.50 usec
PLW1        34.20000076 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        14.00000000 W
PLW12        0.17284000 W
PLW13        0.14000000 W

F2 - Processing parameters
SI                 32768
SF          75.4676817 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



3p




```
Current Data Parameters
NAME        HNMR-ZY-3-51
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20221214
Time              23.32 h
INSTRUM           Avance
PROBHD   Z116098_0833 (
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
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                 294.8 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           400.1300525 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



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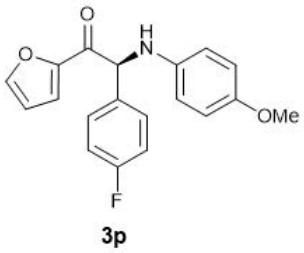
Current Data Parameters
NAME HNMR-ZY-3-51
EXPNO 2
PROCNO 1

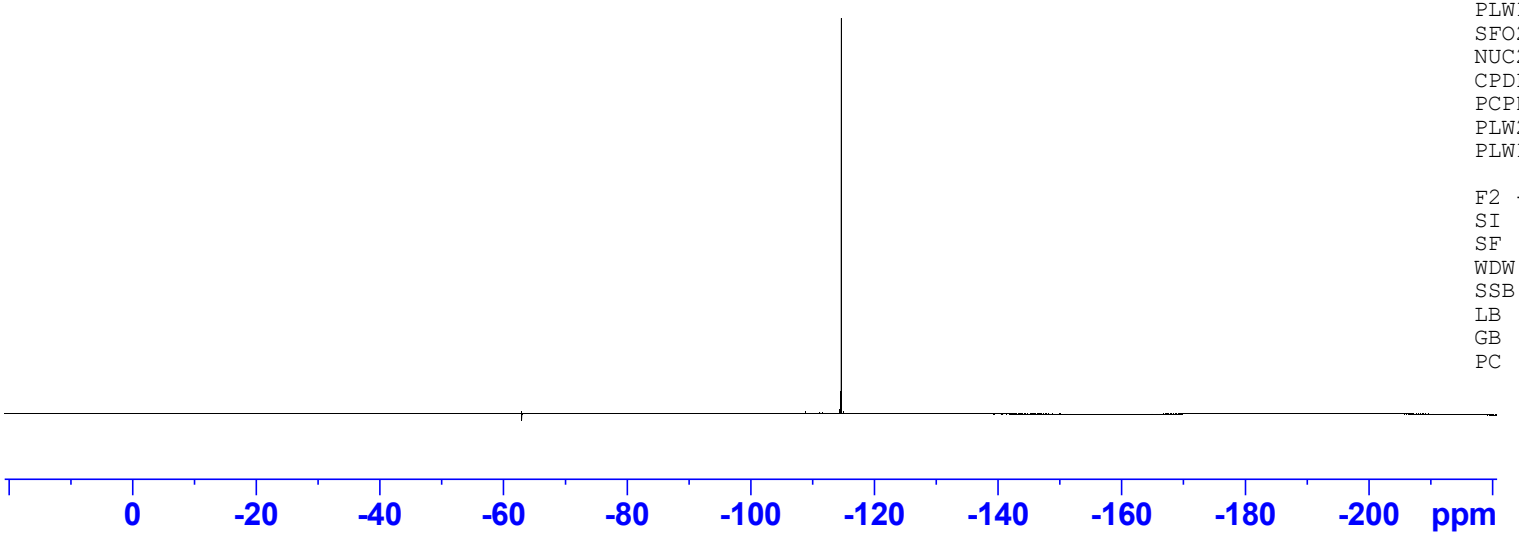
F2 - Acquisition Parameters
Date_ 20221214
Time 23.30 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgpg30
TD 65536
SOLVENT CD2Cl2
NS 450
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 49.9878
DW 21.000 usec
DE 6.50 usec
TE 295.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 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 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



3p

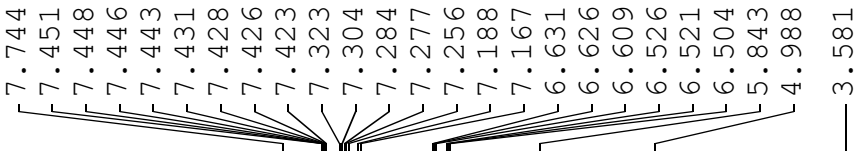
-114.56

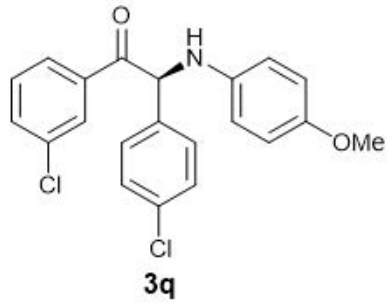


Current Data Parameters
NAME HNMR-ZY-3-51
EXPNO 3
PROCNO 1

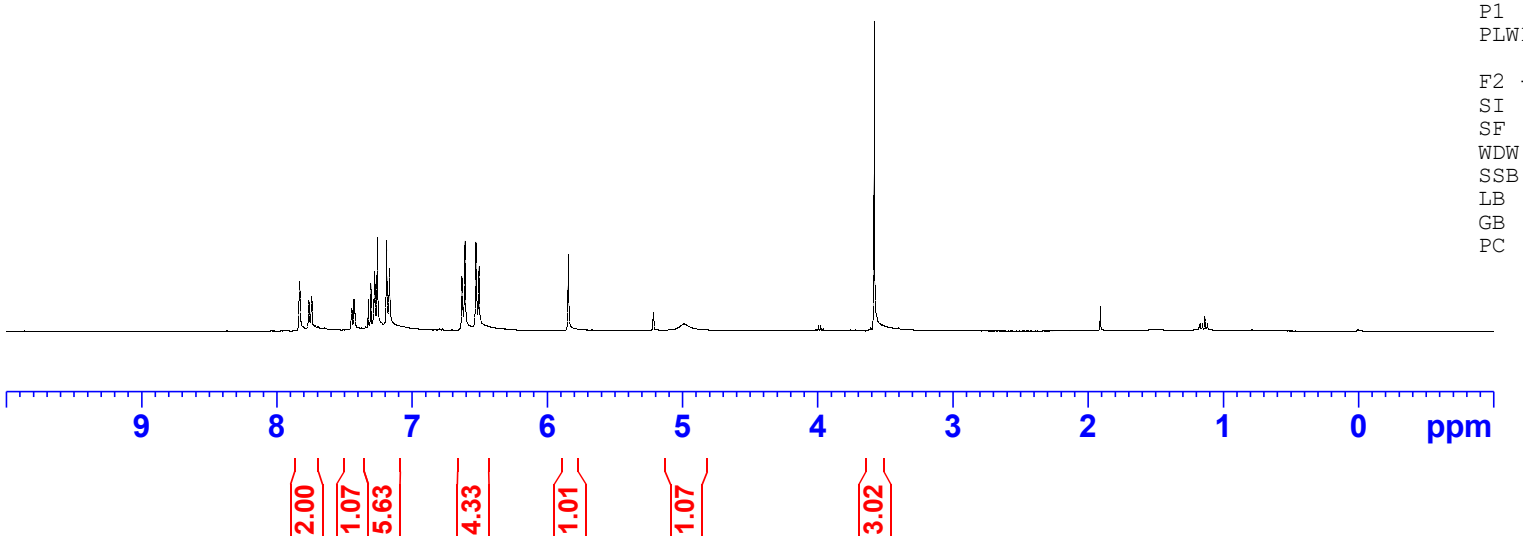
F2 - Acquisition Parameters
Date_ 20221214
Time 23.34 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgig
TD 131072
SOLVENT CD2Cl2
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 294.9 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 376.4607164 MHz
NUC1 19F
P1 18.00 usec
PLW1 16.73100090 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 20.73200035 W
PLW12 0.25595000 W

F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

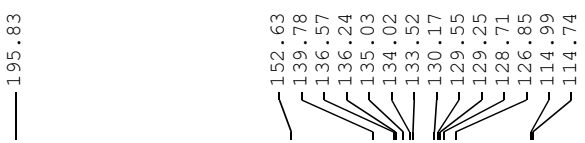


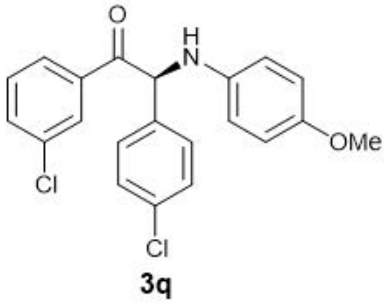


3q

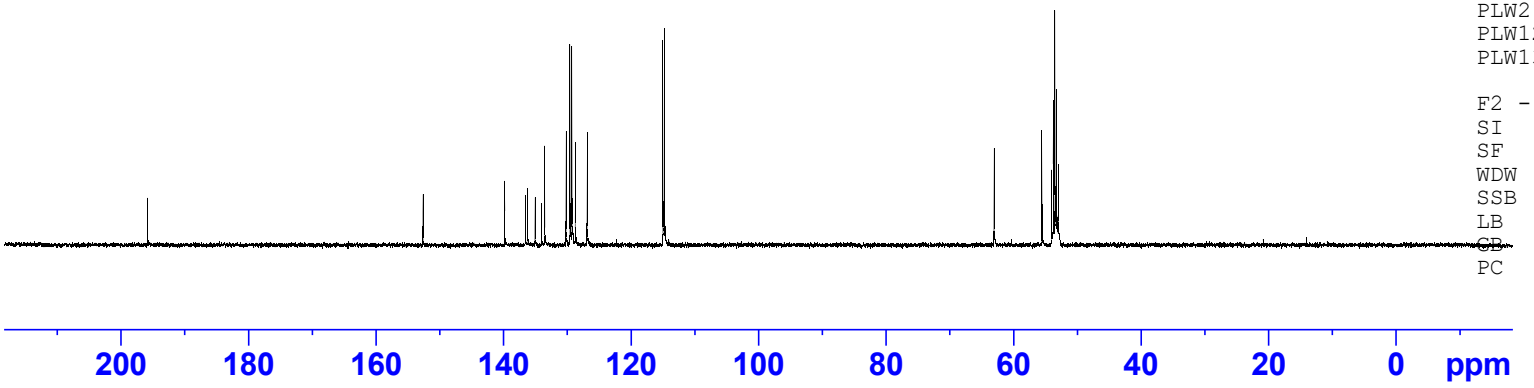



```
Current Data Parameters
NAME        HNMR-ZY-2-38
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220928
Time               7.49 h
INSTRUM           Avance
PROBHD   Z116098_0833 (
PULPROG             zg30
TD                 65536
SOLVENT           CD2Cl2
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ             3.9976959 sec
RG               89.6057
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          400.1300582 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

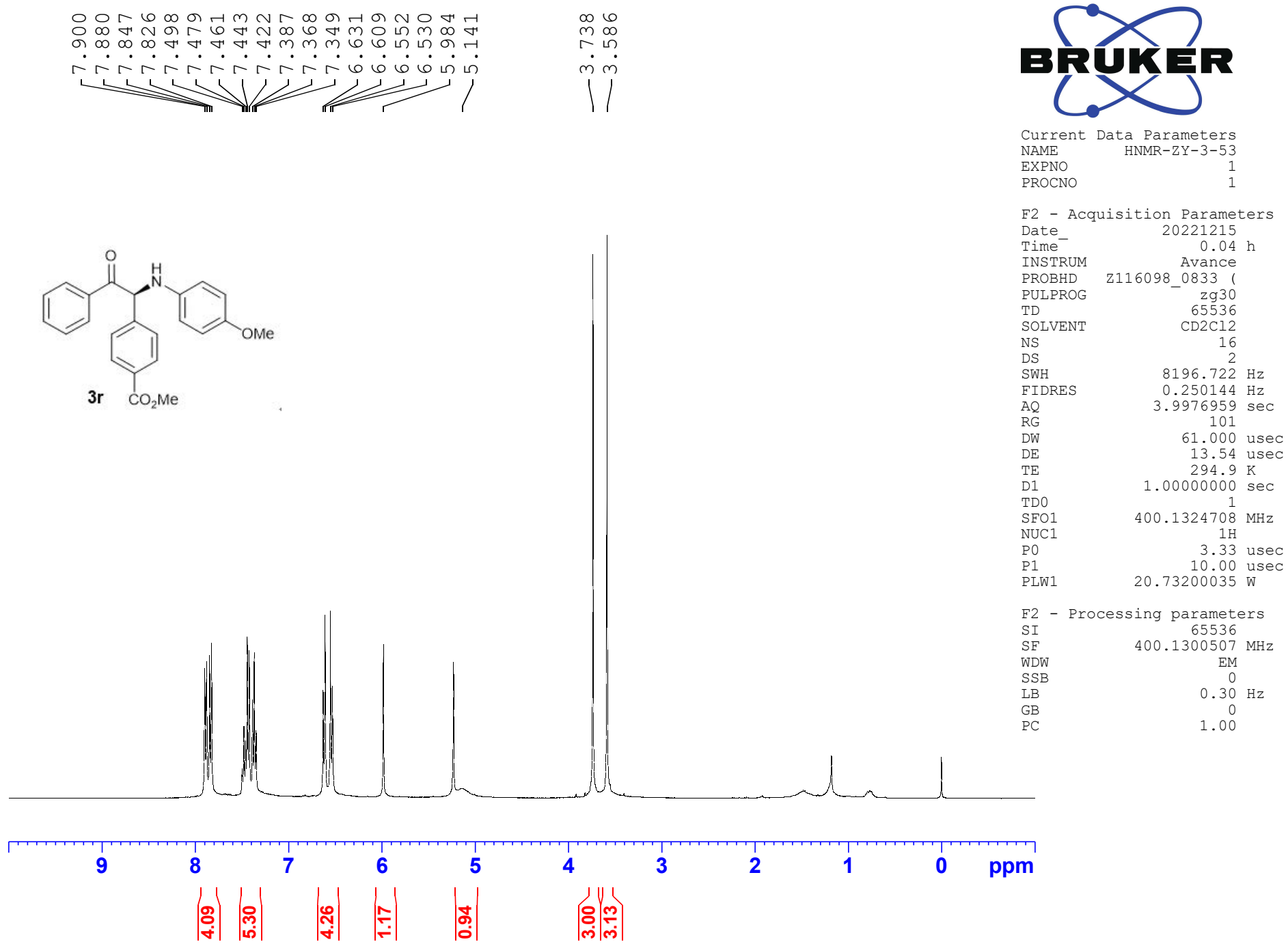




3q



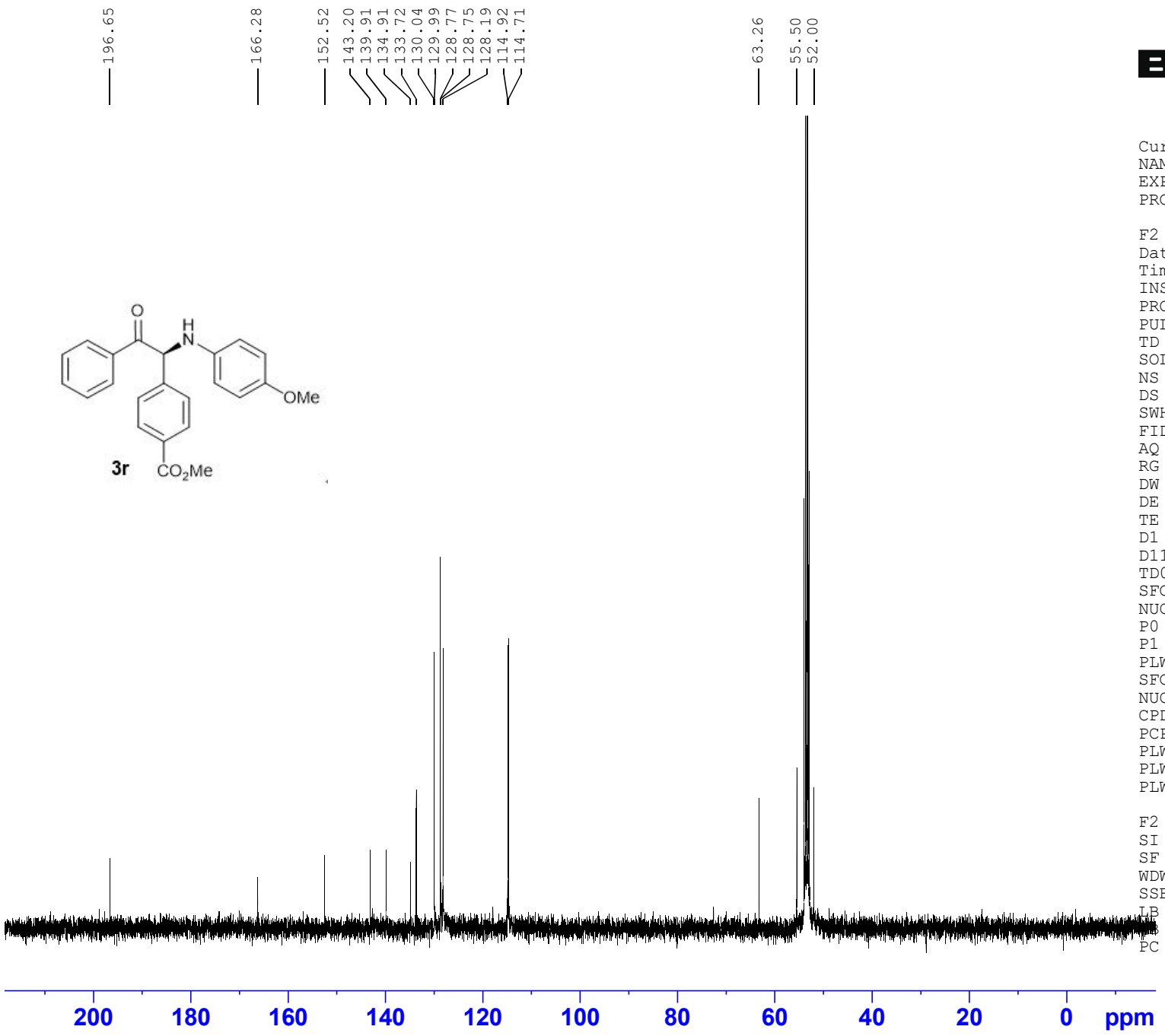

```
Current Data Parameters
NAME       CNMR-ZY-2-38
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20220928
Time              8.13 h
INSTRUM           Avance
PROBHD   Z116098_0833 (
PULPROG          zgpg30
TD                65536
SOLVENT           CD2Cl2
NS                  400
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ             1.3762560 sec
RG               48.6724
DW               21.000 usec
DE                6.50 usec
TE                295.1 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          100.6127685 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



Current Data Parameters
NAME HNMR-ZY-3-53
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221215
Time 0.04 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zg30
TD 65536
SOLVENT CD2Cl2
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 294.9 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 400.1300507 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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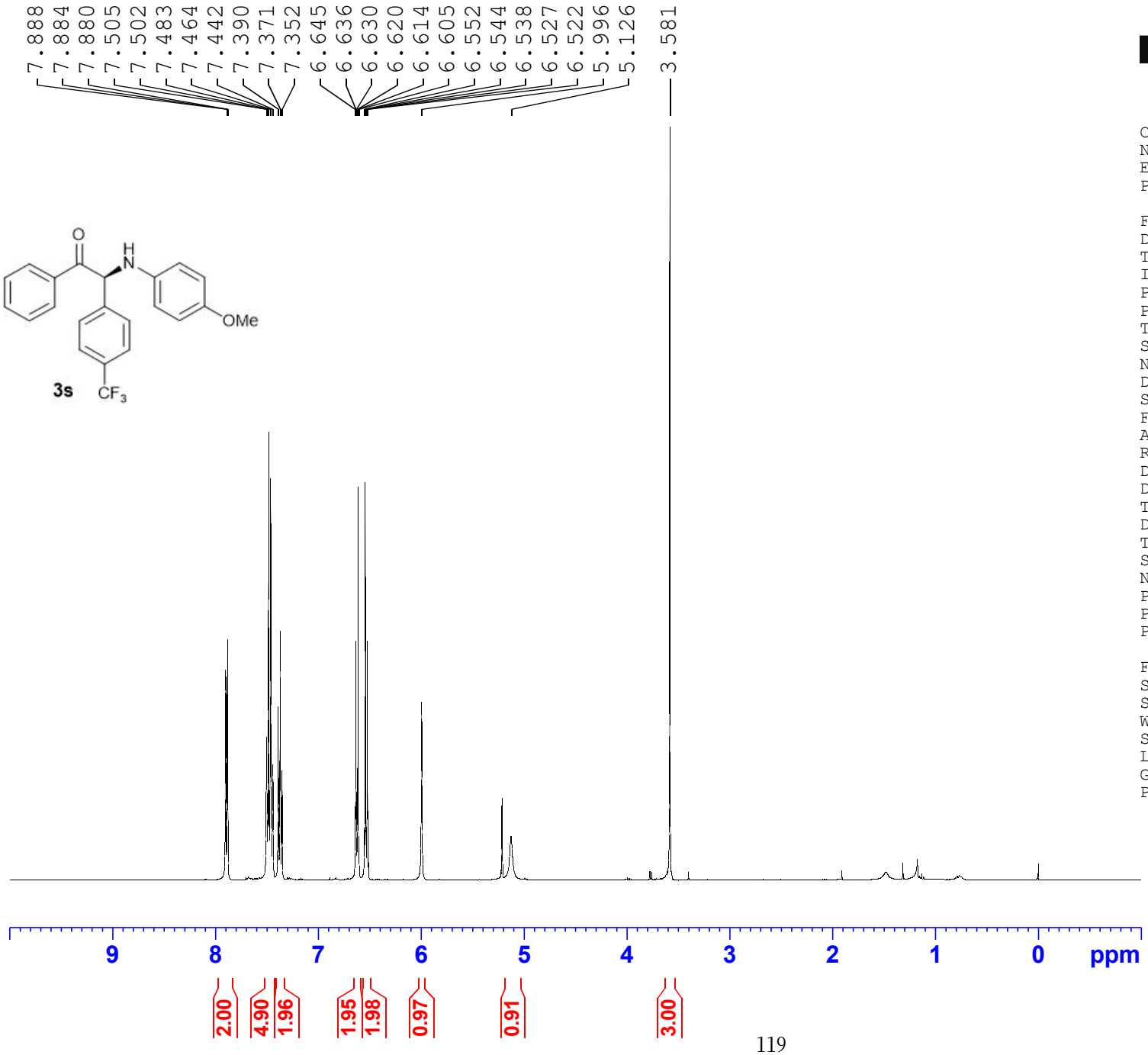
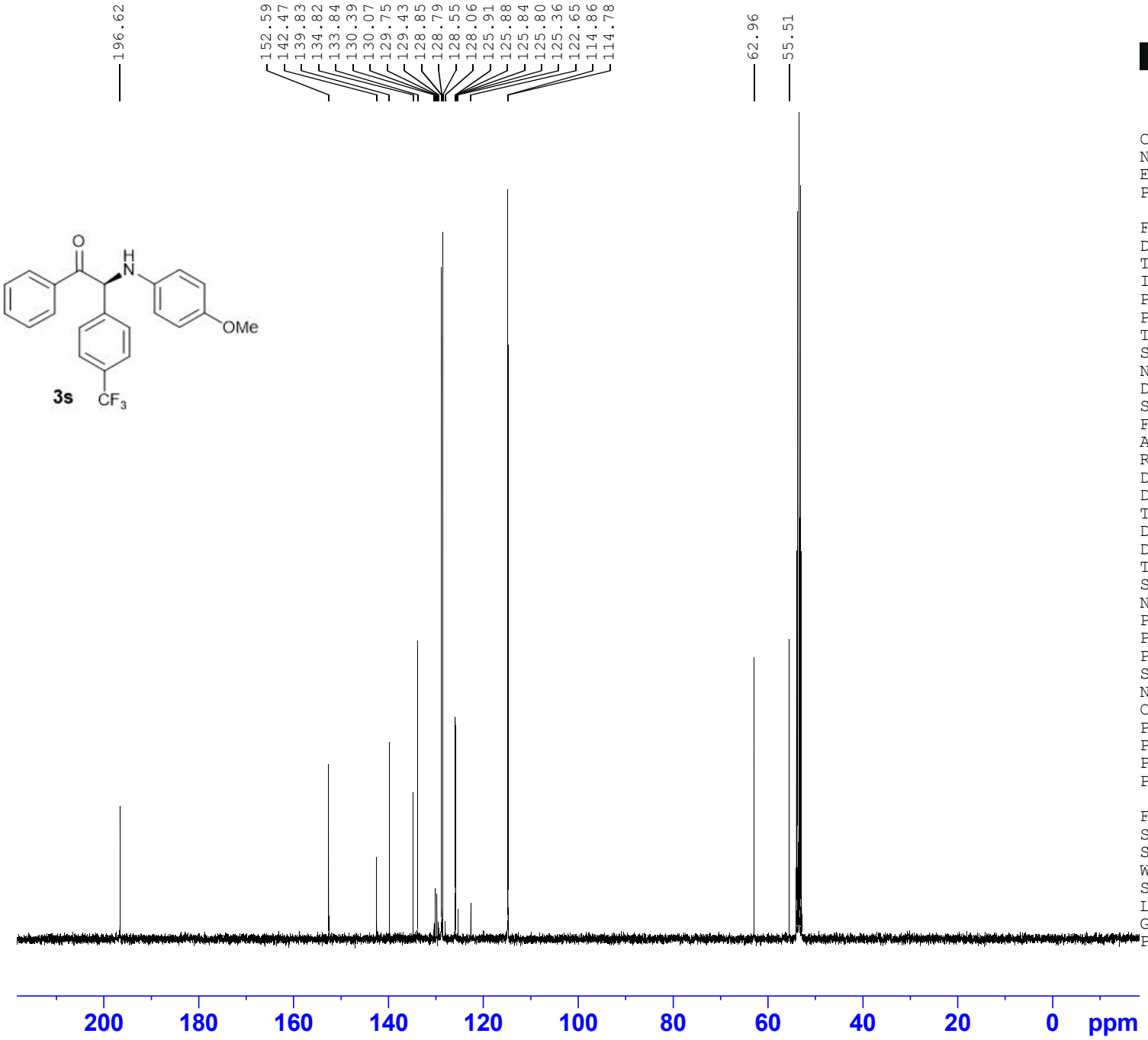
```
Current Data Parameters
NAME        HNMR-ZY-3-53
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20221215
Time                0.02 h
INSTRUM           Avance
PROBHD   Z116098_0833 (
PULPROG          zgpg30
TD                65536
SOLVENT          CD2Cl2
NS                  400
DS                    4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ             1.3762560 sec
RG              50.1934
DW               21.000 usec
DE                6.50 usec
TE                295.4 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          100.6127685 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
                       0
PC                  1.40
```



Current Data Parameters
NAME HNMR-ZY-3-56
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221215
Time 4.28 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zg30
TD 65536
SOLVENT CD2Cl2
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 295.4 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

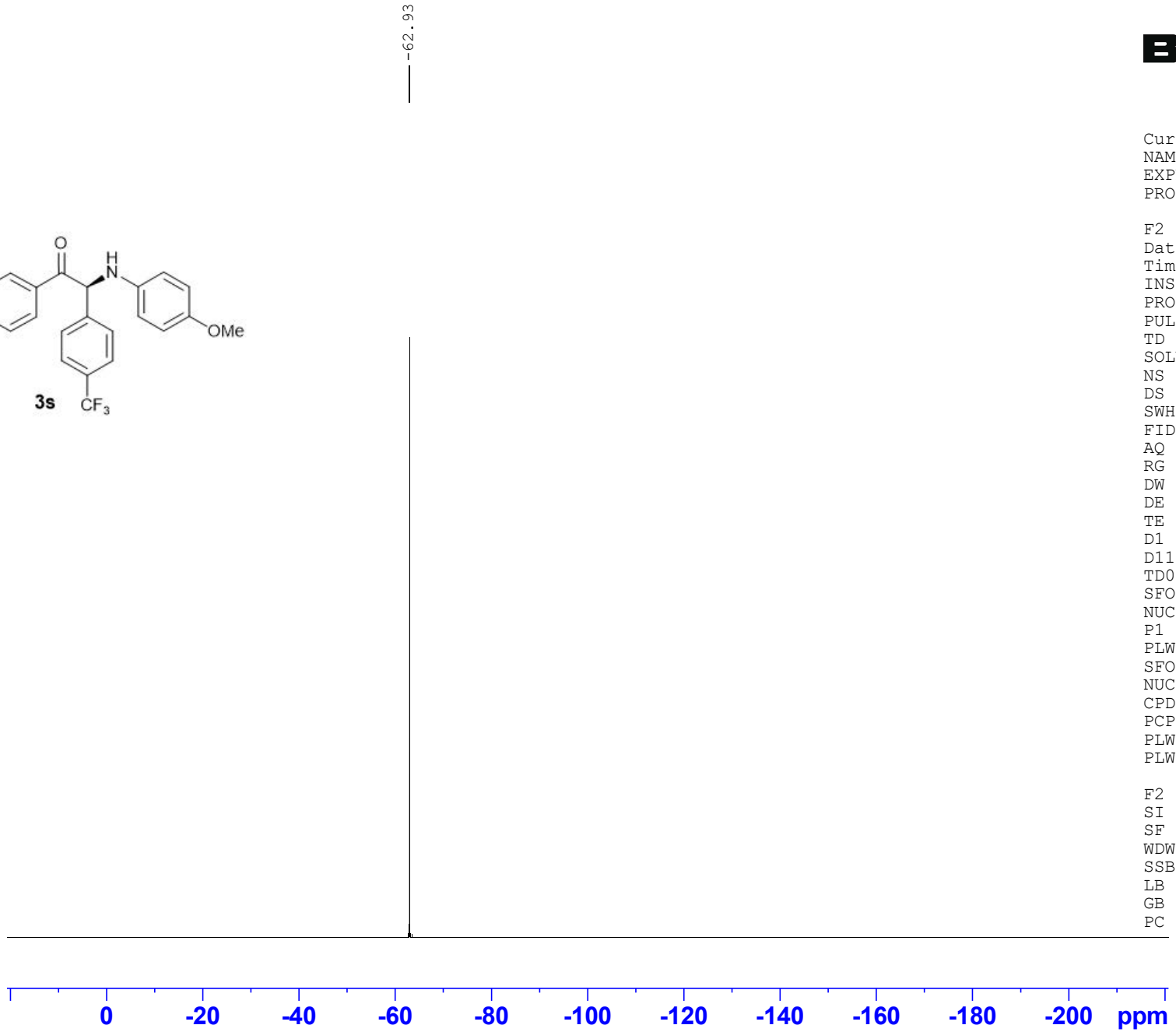
F2 - Processing parameters
SI 65536
SF 400.1300579 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



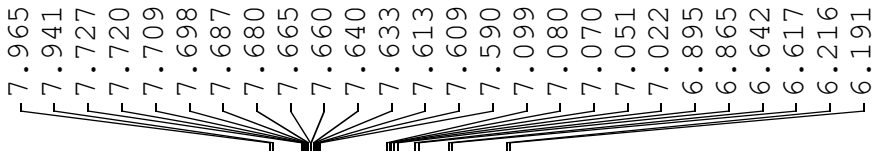
Current Data Parameters
NAME HNMR-ZY-3-56
EXPNO 2
PROCNO 1

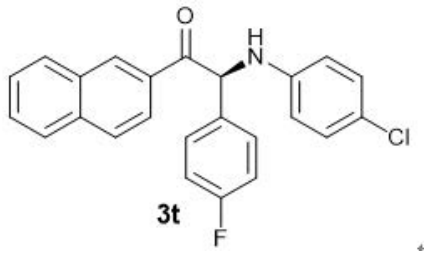
F2 - Acquisition Parameters
Date_ 20221215
Time 4.55 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgpg30
TD 65536
SOLVENT CD2Cl2
NS 450
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 50.1934
DW 21.000 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 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 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40




```
Current Data Parameters
NAME       HNMR-ZY-3-56
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20221215
Time              4.56 h
INSTRUM           Avance
PROBHD   Z116098_0833 (
PULPROG            zgig
TD               131072
SOLVENT          CD2Cl2
NS                   16
DS                    4
SWH           90909.094 Hz
FIDRES         1.387163 Hz
AQ            0.7208960 sec
RG                  101
DW                5.500 usec
DE                6.50 usec
TE                295.8 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        376.4607164 MHz
NUC1                19F
P1                18.00 usec
PLW1        16.73100090 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        20.73200035 W
PLW12        0.25595000 W

F2 - Processing parameters
SI                65536
SF          376.4983662 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```





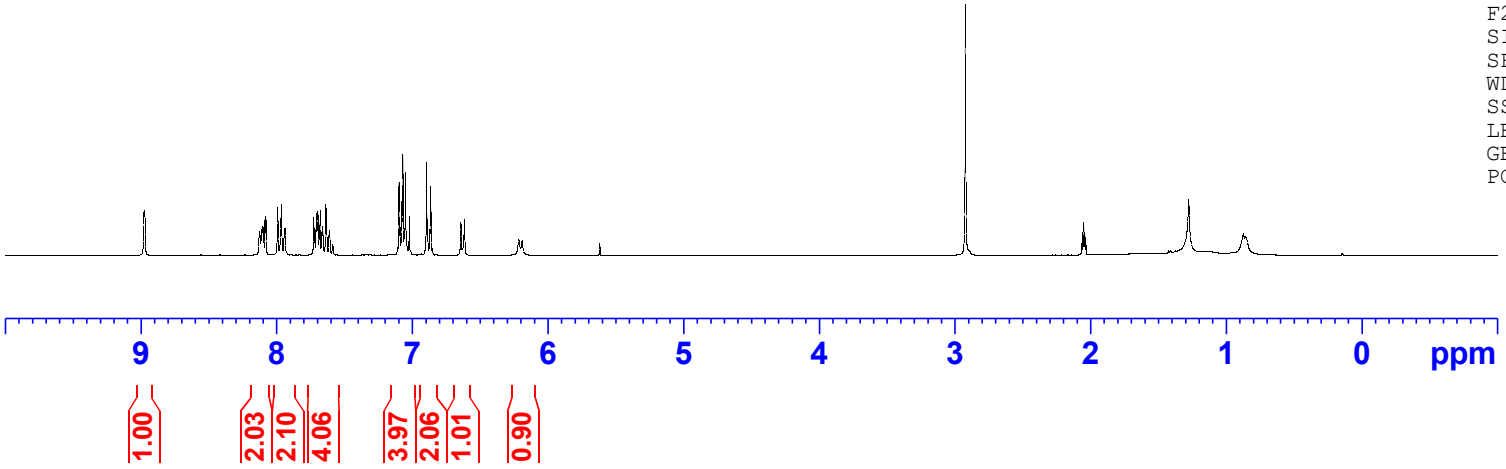
3t

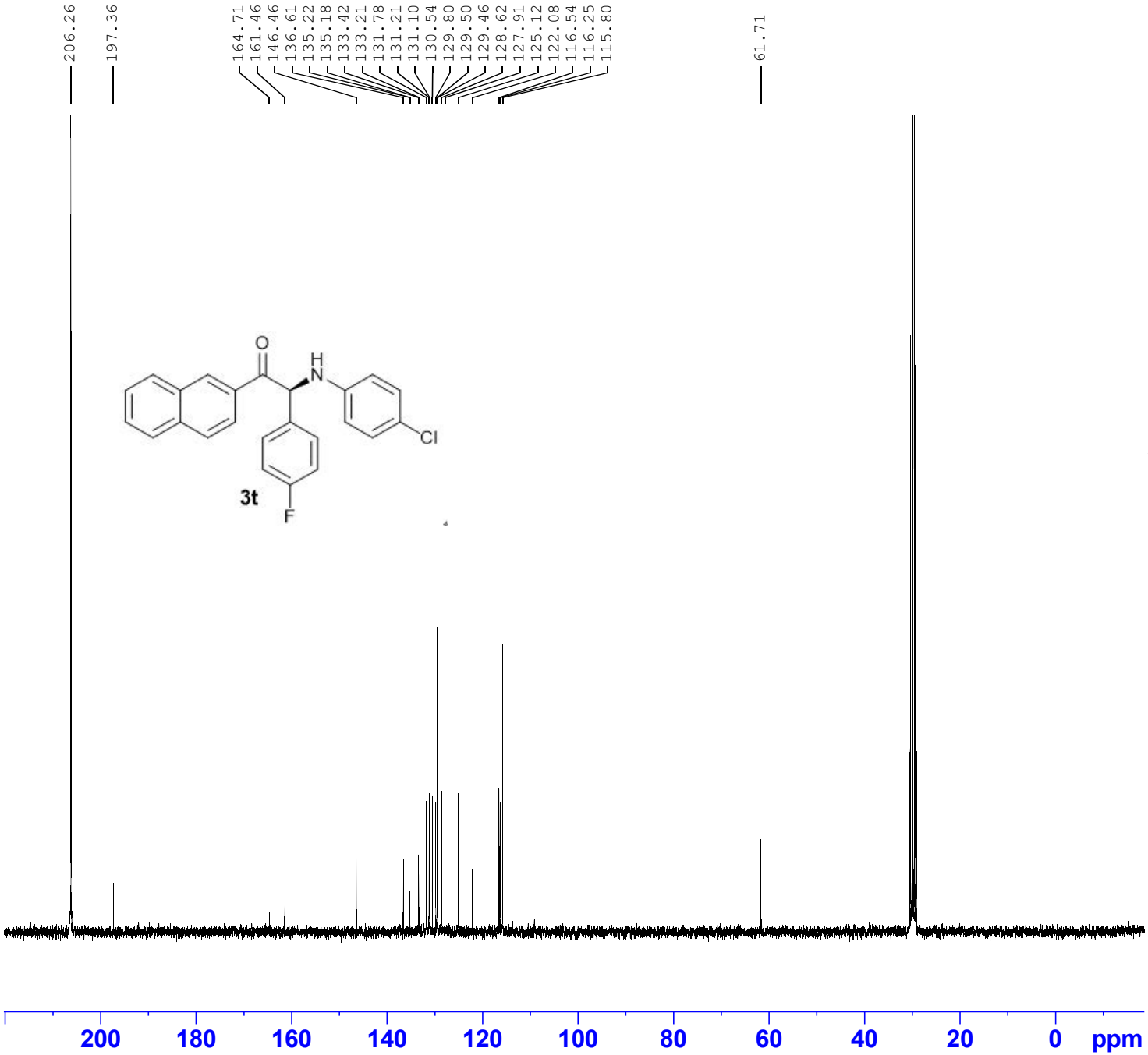
Current Data Parameters
NAME HNMR-ZY-1-71
EXPNO 458
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220721
Time 13.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 114
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





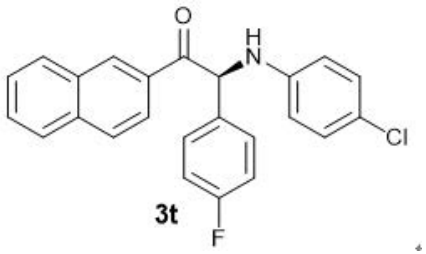
Current Data Parameters
NAME CNMR-ZY-1-71
EXPNO 464
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220721
Time 21.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 200
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

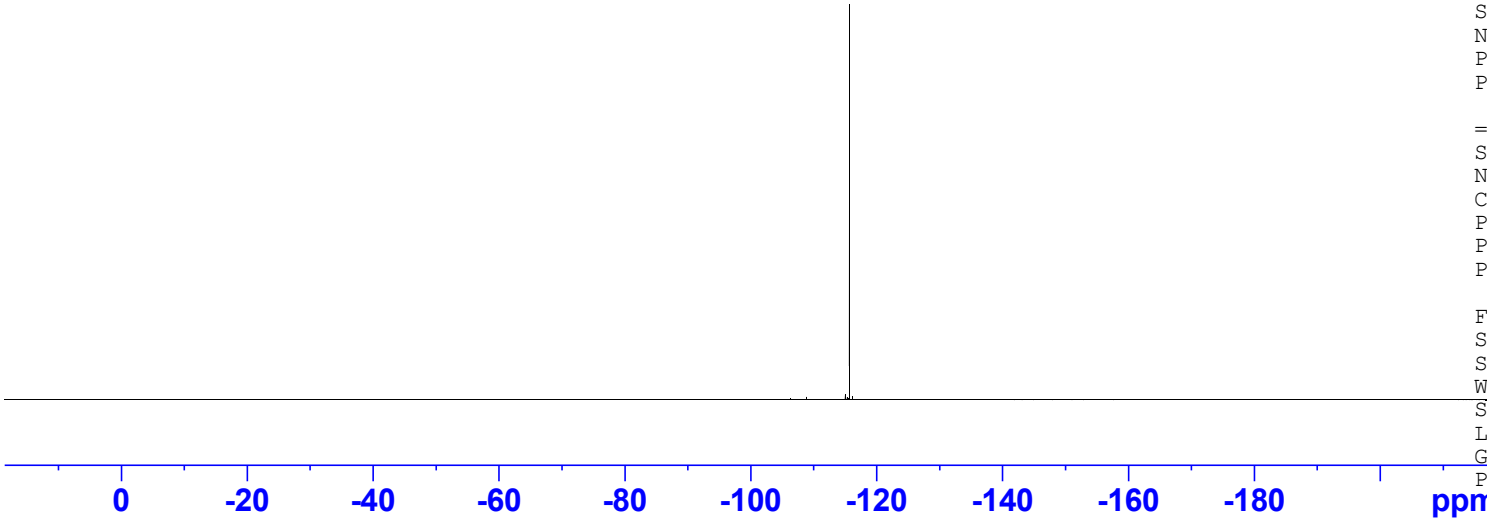
======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

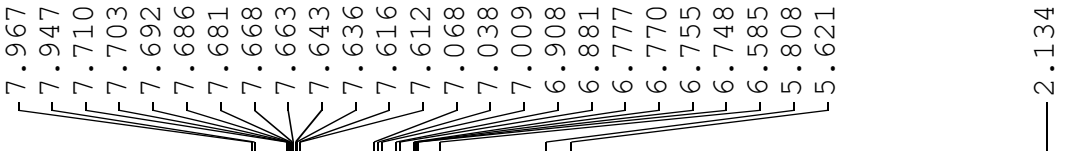
F2 - Processing parameters
SI 32768
SF 75.4676841 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

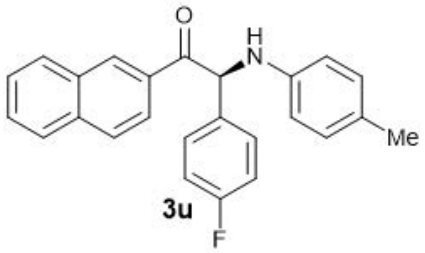


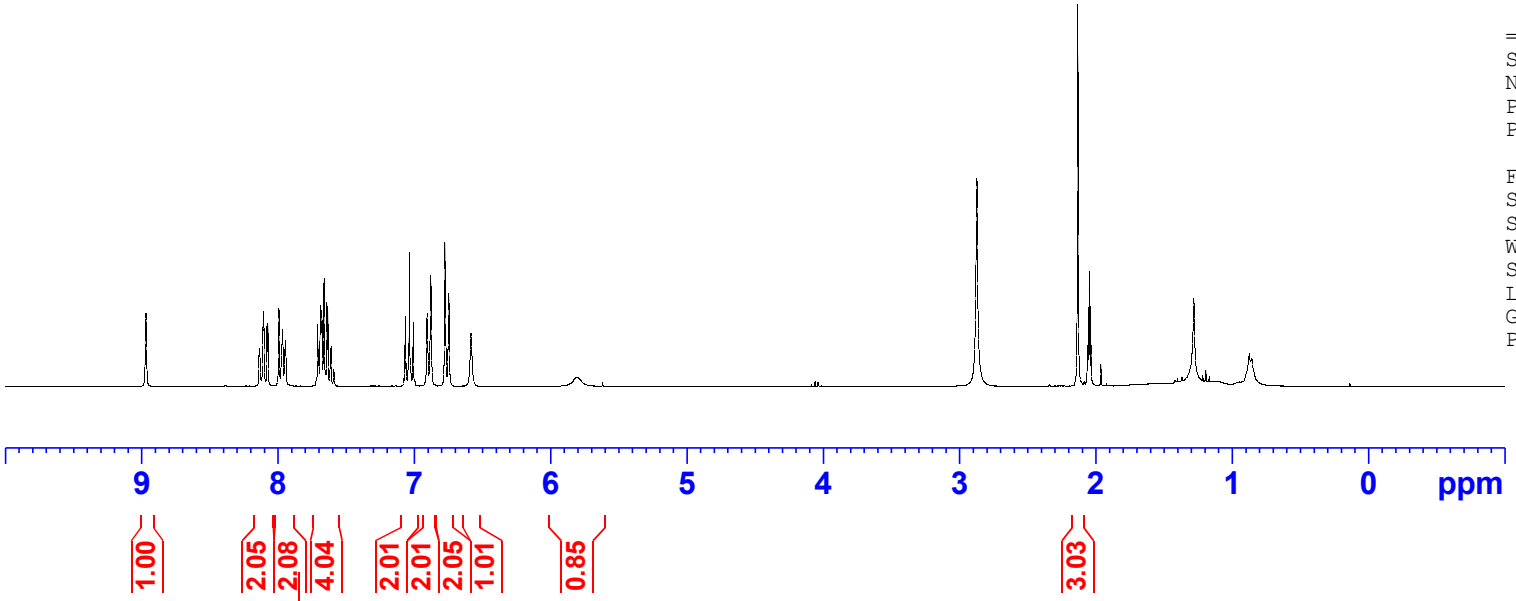
-115.62




```
Current Data Parameters
NAME       FNMR-ZY-1-71
EXPNO               470
PROCNO                1

F2 - Acquisition Parameters
Date_          20220722
Time              14.10
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG      zgfhigqn.2
TD               131072
SOLVENT         Acetone
NS                    4
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                -59.1 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
```





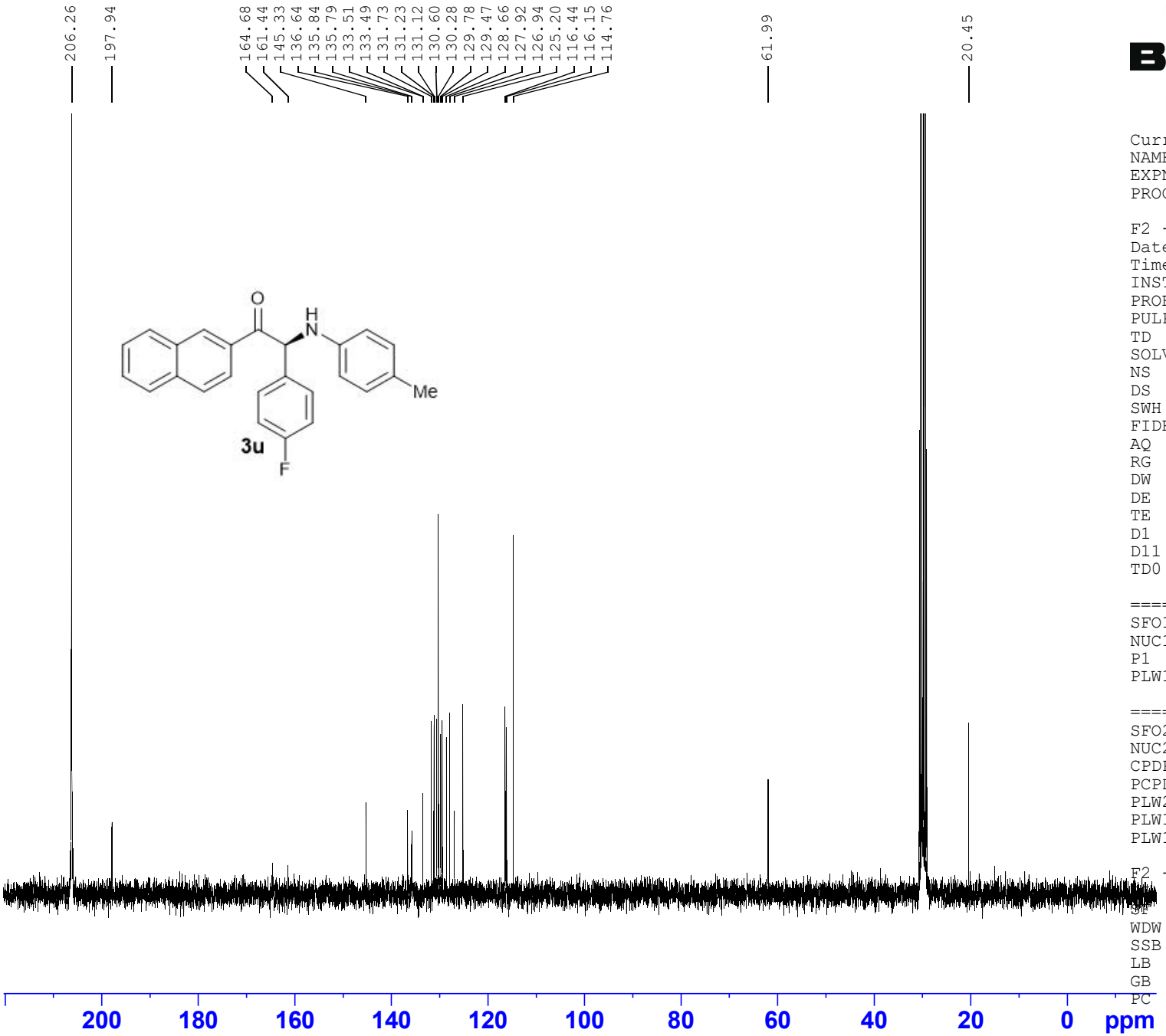


Current Data Parameters
NAME HNMR-ZY-1-74
EXPNO 453
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220720
Time 13.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 161
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



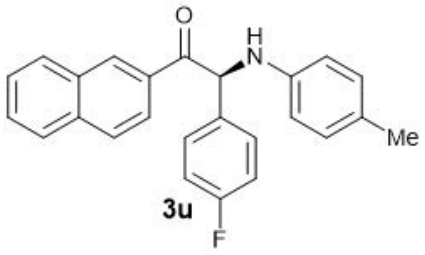
Current Data Parameters
NAME CNMR-ZY-1-74
EXPNO 467
PROCNO 1

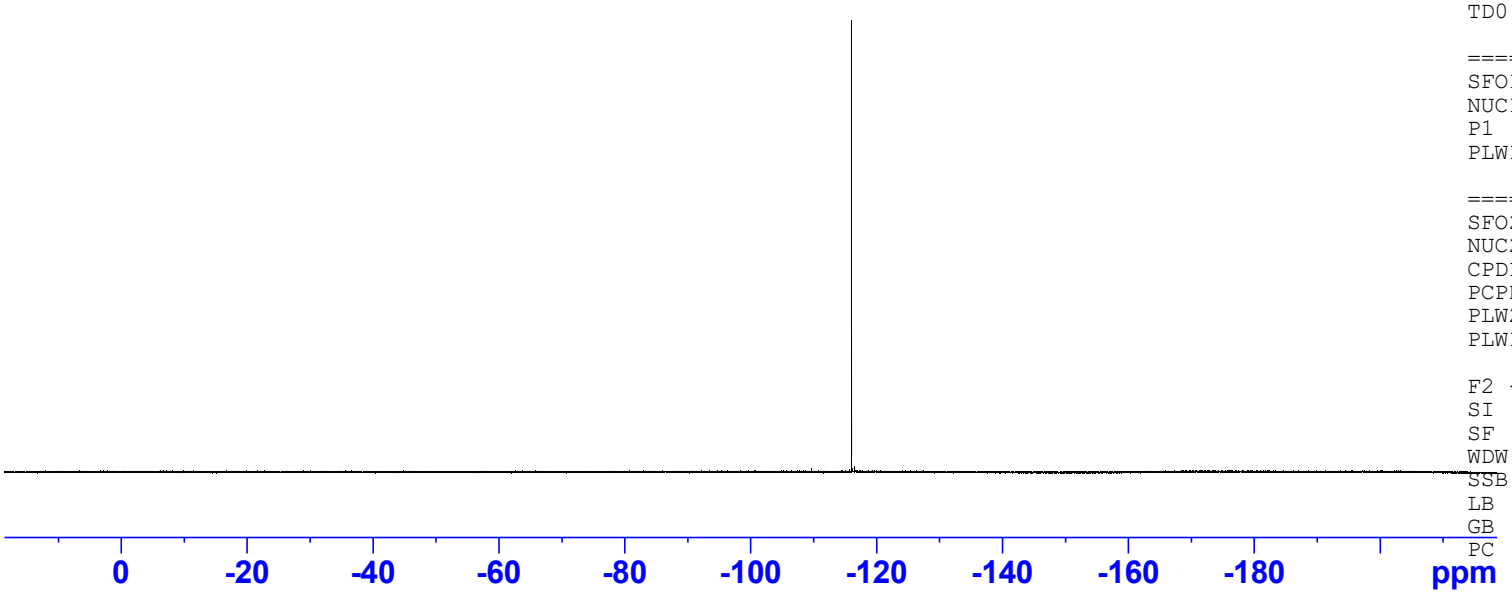
F2 - Acquisition Parameters
Date_ 20220721
Time 22.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 200
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

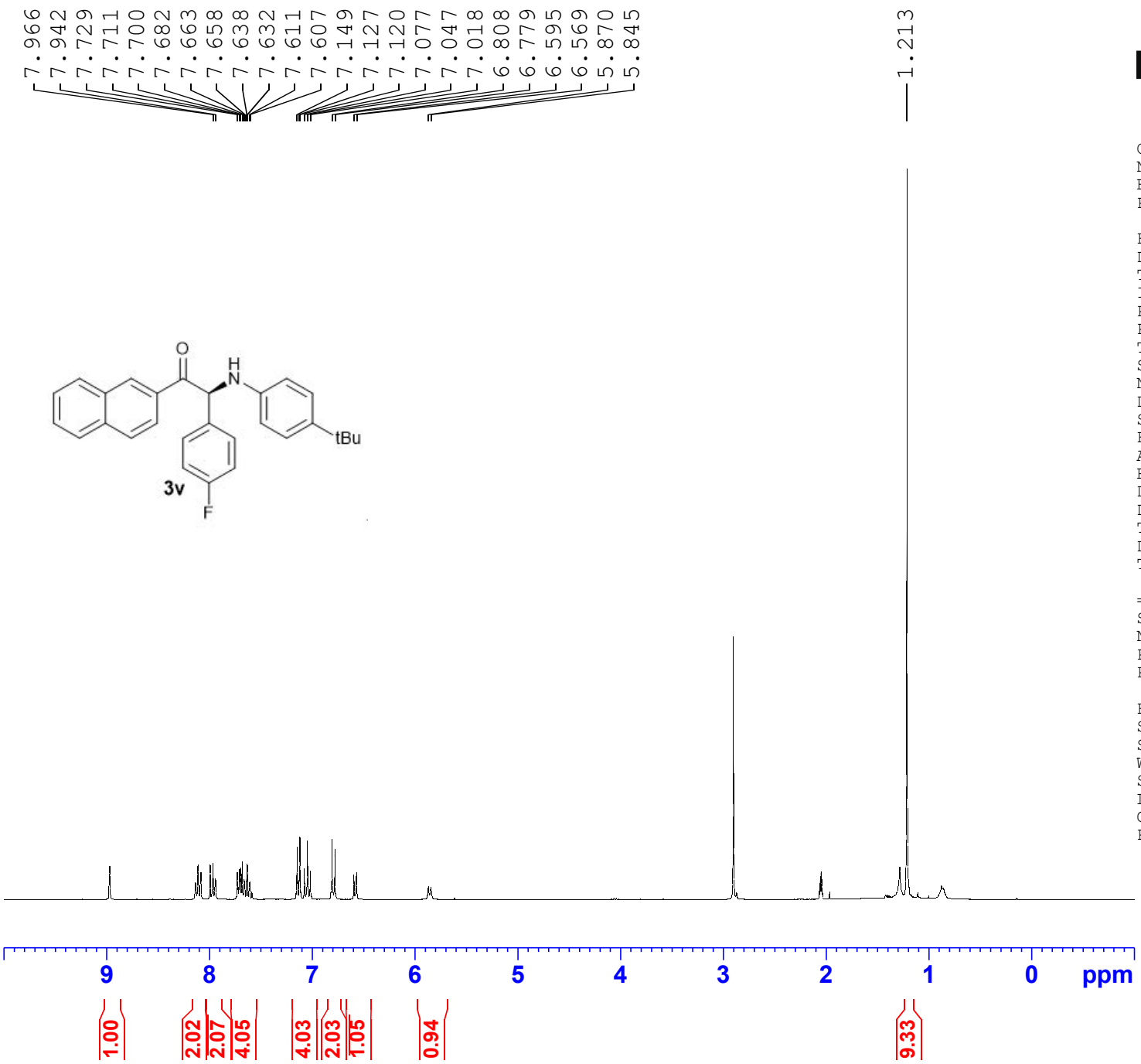
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4676796 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40






```
Current Data Parameters
NAME       FNMR-ZY-1-74
EXPNO               473
PROCNO                1

F2 - Acquisition Parameters
Date_          20220722
Time              14.19
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG      zgfhigqn.2
TD               131072
SOLVENT         Acetone
NS                    4
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                -59.1 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
```

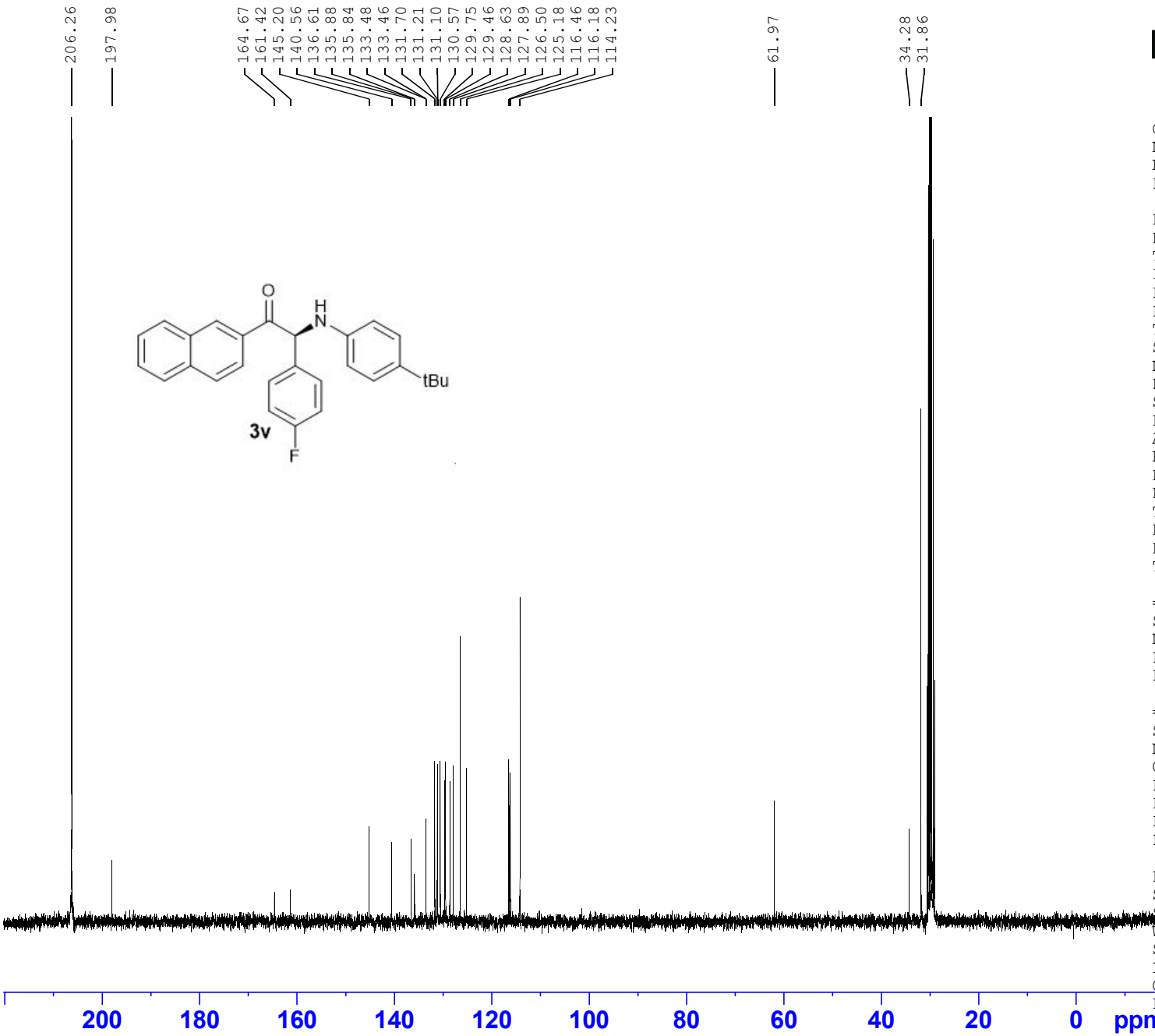


Current Data Parameters
NAME HNMR-ZY-1-73
EXPNO 452
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220720
Time 13.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 101
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

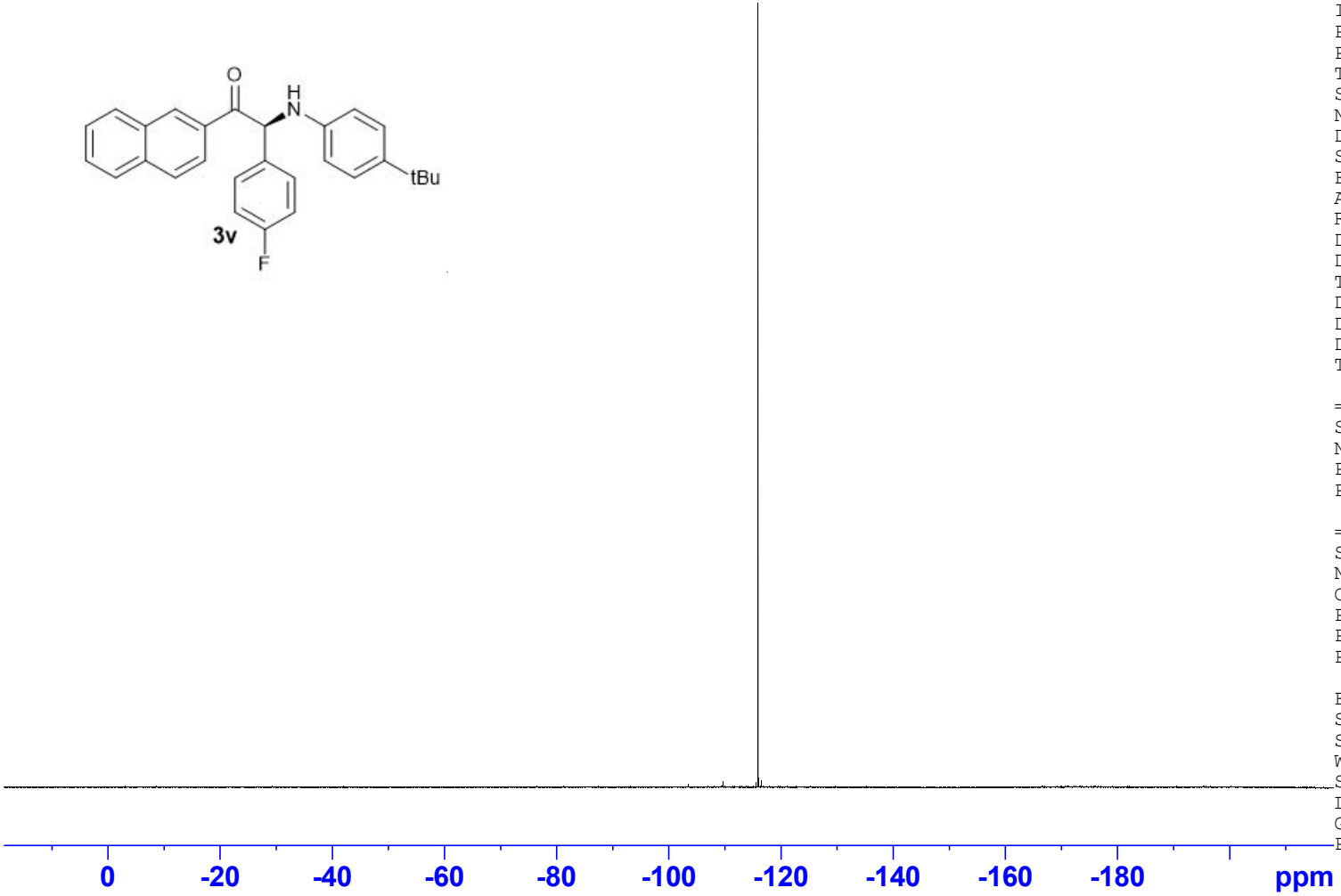
F2 - Processing parameters
SI 65536
SF 300.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



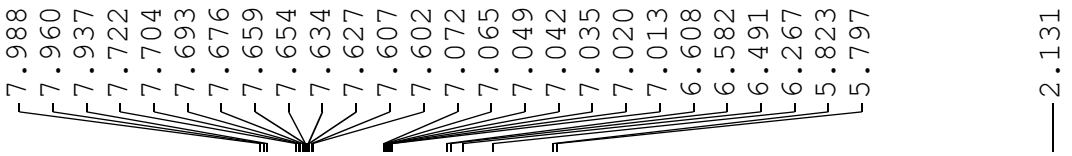
BRUKER

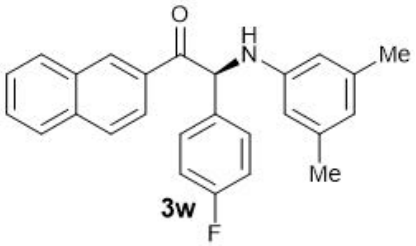
```
Current Data Parameters
NAME       CNMR-ZY-1-73
EXPNO               466
PROCNO                1

F2 - Acquisition Parameters
Date_          20220721
Time              22.10
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  200
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                  203
DW               27.733 usec
DE                6.50 usec
TE                -59.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                 9.50 usec
PLW1        34.20000076 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        14.00000000 W
PLW12        0.17284000 W
PLW13        0.14000000 W

F2 - Processing parameters
SI                 32768
SF            75.4676822 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

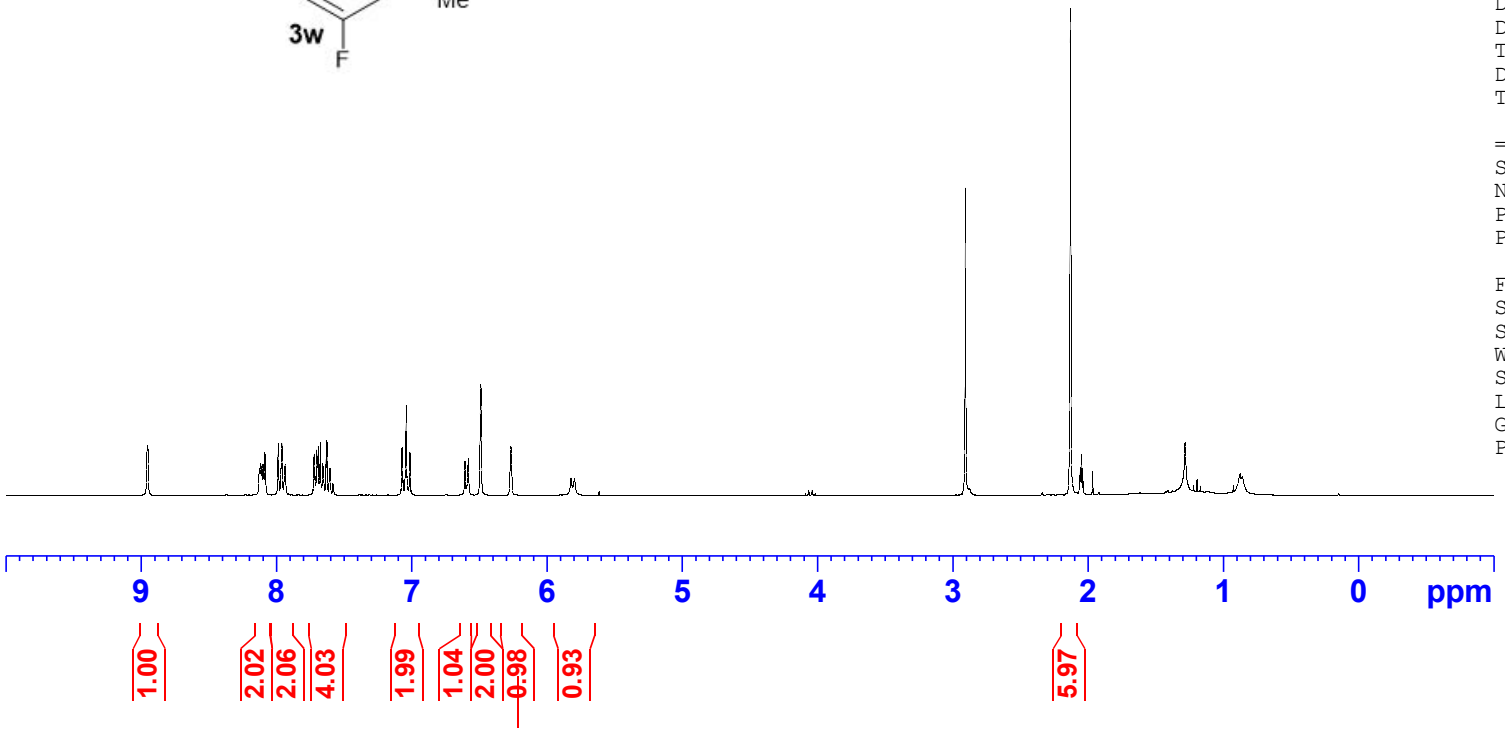
-115.95




```
Current Data Parameters
NAME       FNMR-ZY-1-73
EXPNO               472
PROCNO                1

F2 - Acquisition Parameters
Date_          20220722
Time              14.16
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG      zgfhigqn.2
TD               131072
SOLVENT          Acetone
NS                     4
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                -59.1 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
```





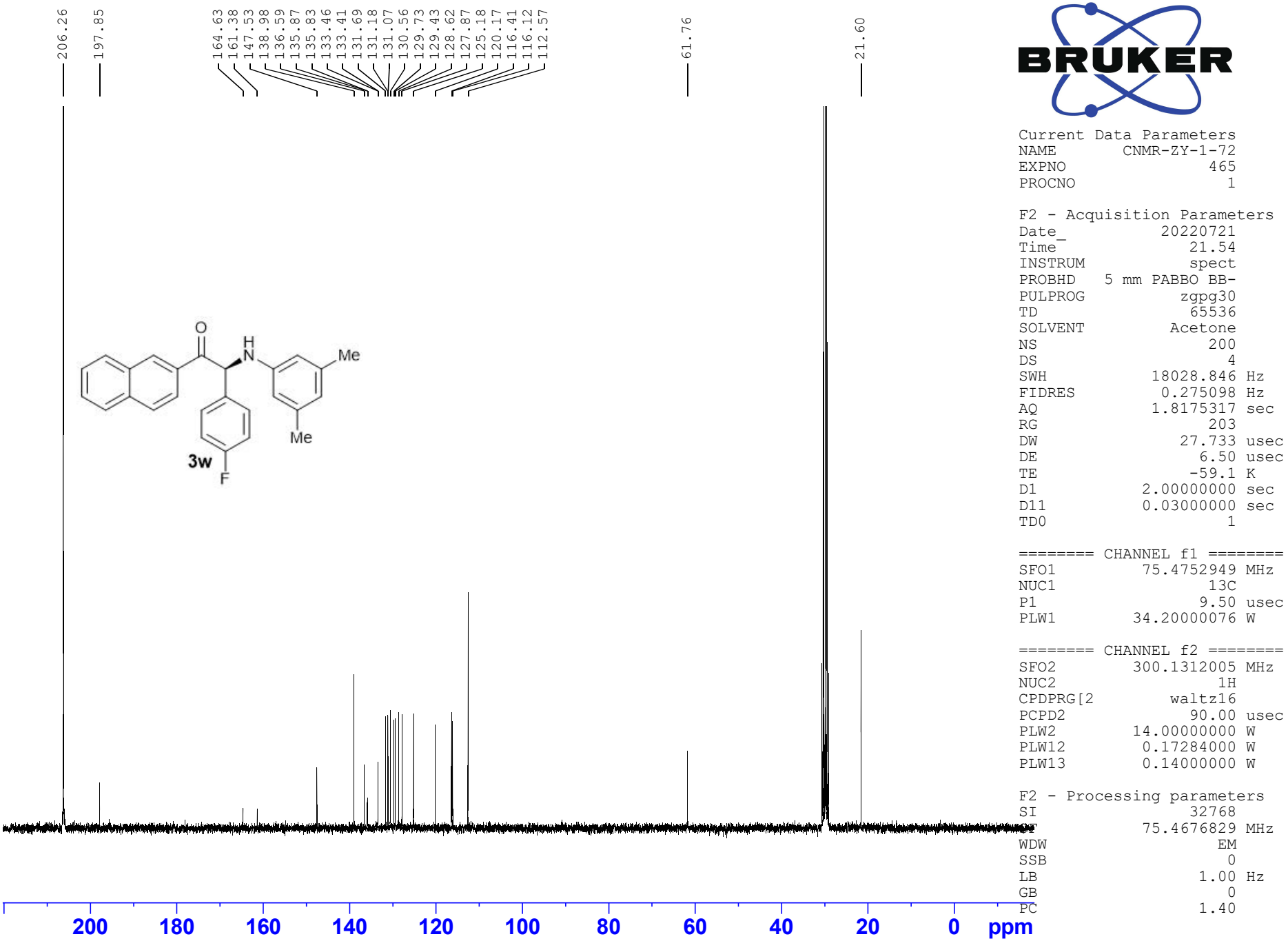


Current Data Parameters
NAME HNMR-ZY-1-72
EXPNO 451
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220720
Time 13.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 101
DW 83.200 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 300.1318534 MHz
NUC1 1H
P1 10.00 usec
PLW1 14.00000000 W

F2 - Processing parameters
SI 65536
SF 300.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME CNMR-ZY-1-72
EXPNO 465
PROCNO 1

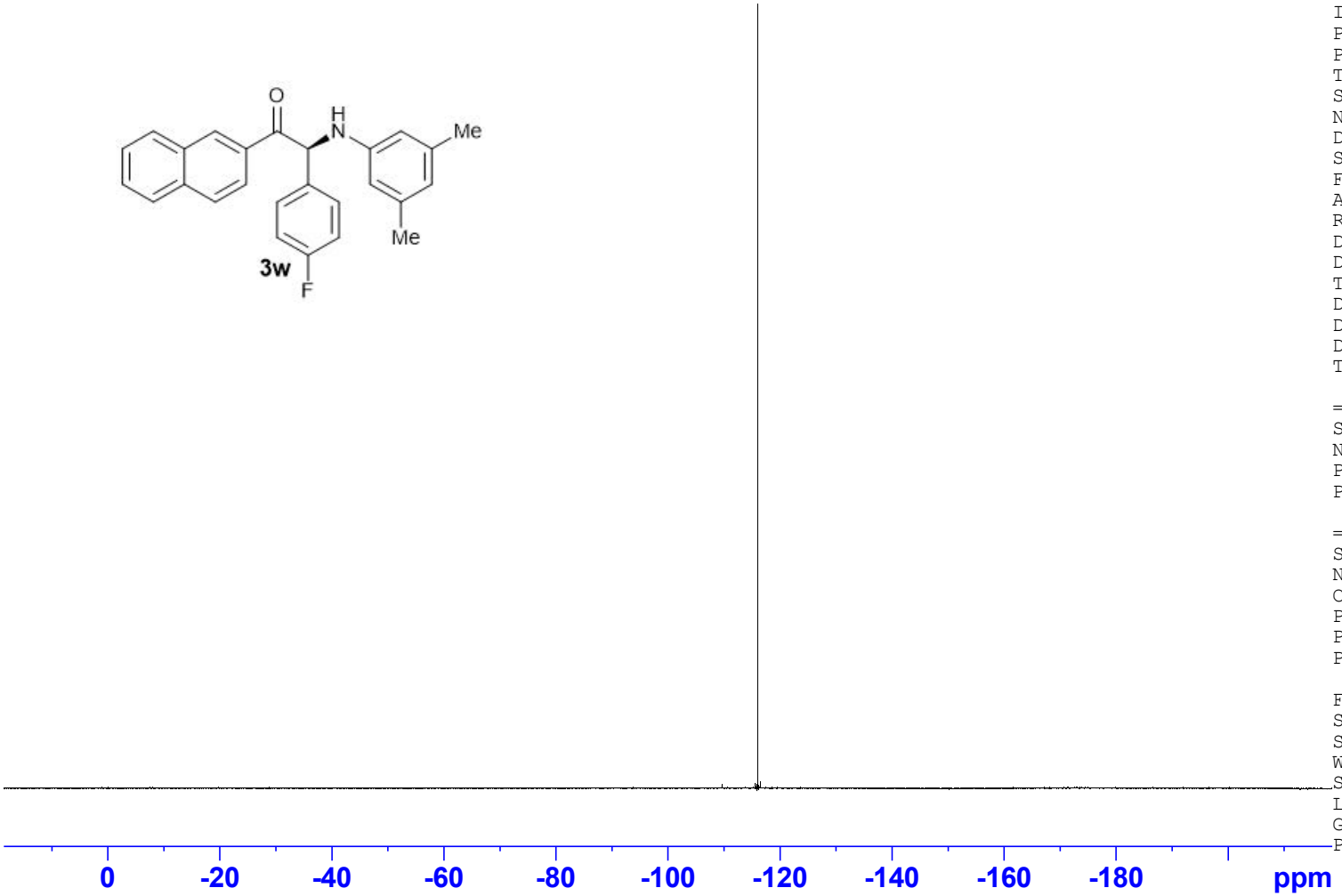
F2 - Acquisition Parameters
Date_ 20220721
Time 21.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 200
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4676829 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

-115.99



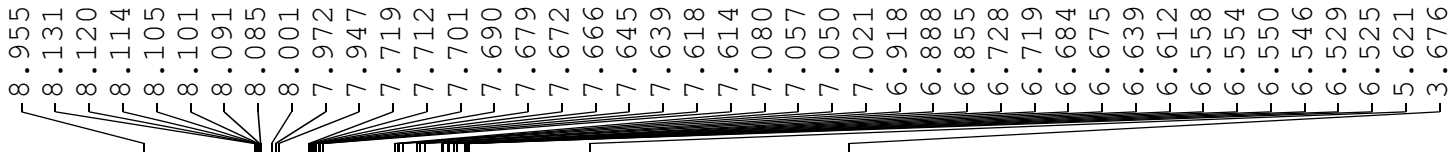
Current Data Parameters
NAME FNMR-ZY-1-72
EXPNO 471
PROCNO 1

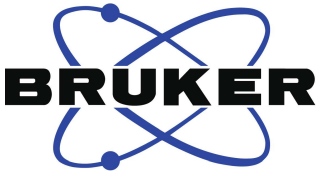
F2 - Acquisition Parameters
Date_ 20220722
Time 14.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn.2
TD 131072
SOLVENT Acetone
NS 4
DS 4
SWH 66964.289 Hz
FIDRES 0.510897 Hz
AQ 0.9786710 sec
RG 203
DW 7.467 usec
DE 6.50 usec
TE -59.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

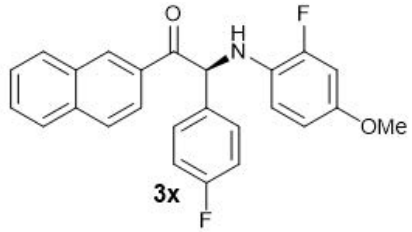
======== CHANNEL f1 ========
SFO1 282.3761148 MHz
NUC1 19F
P1 14.50 usec
PLW1 10.39999962 W

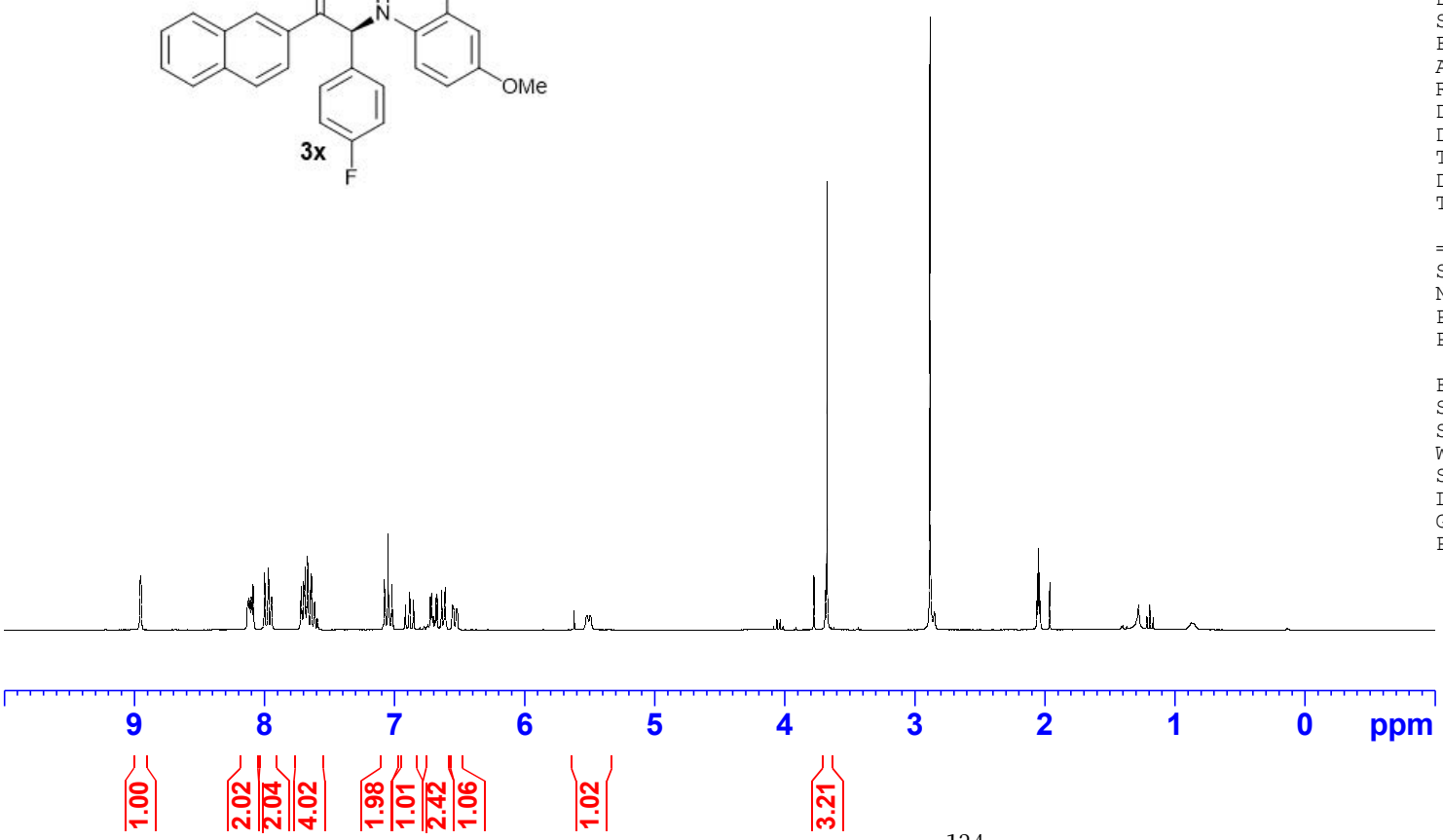
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W

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

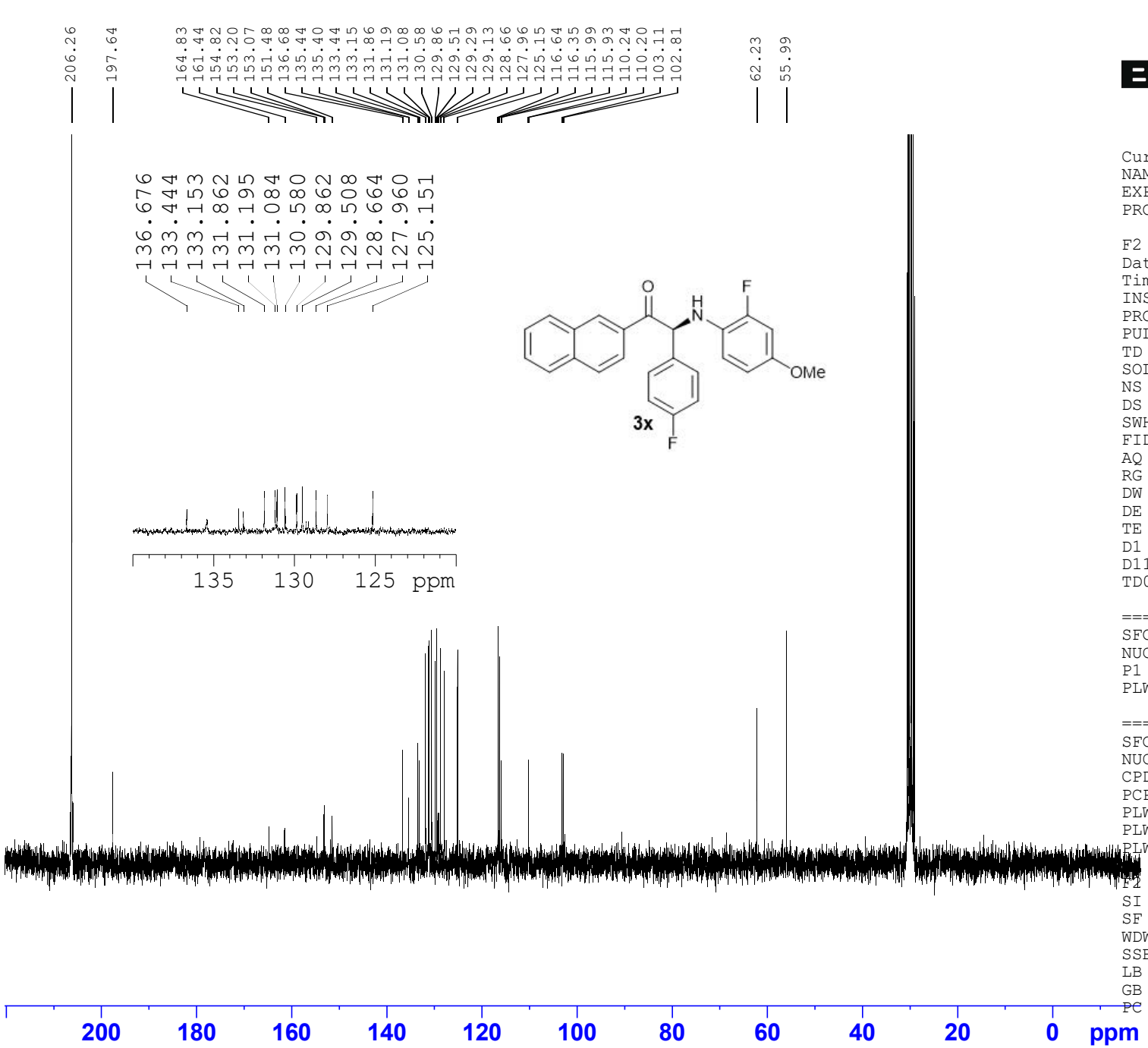









```
Current Data Parameters
NAME       HNMR-ZY-1-92
EXPNO               515
PROCNO                1

F2 - Acquisition Parameters
Date_          20220805
Time              13.57
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    2
SWH            6009.615 Hz
FIDRES        0.091699 Hz
AQ            5.4525952 sec
RG                  161
DW               83.200 usec
DE                6.50 usec
TE                -59.1 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        300.1318534 MHz
NUC1                1H
P1                10.00 usec
PLW1        14.00000000 W

F2 - Processing parameters
SI                65536
SF          300.1300052 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



Current Data Parameters

NAME	CNMR-ZY-1-92
EXPNO	516
PROCNO	1

F2 - Acquisition Parameters

Date_	20220805
Time	14.15
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	250
DS	4
SWH	18028.846 Hz
FIDRES	0.275098 Hz
AQ	1.8175317 sec
RG	203
DW	27.733 usec
DE	6.50 usec
TE	-59.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

======== CHANNEL f1 ========

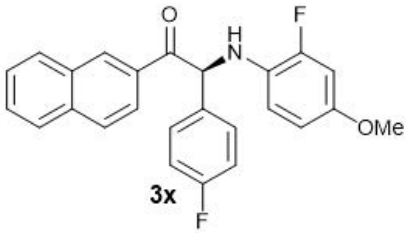
SFO1	75.4752949 MHz
NUC1	13C
P1	9.50 usec
PLW1	34.20000076 W

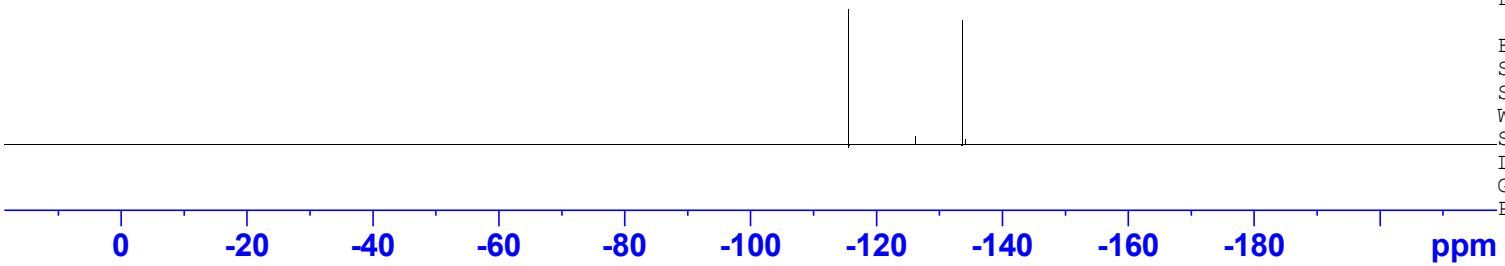
======== CHANNEL f2 ========

SFO2	300.1312005 MHz
NUC2	1H
CPDPRG[2	waltz16
PCPD2	90.00 usec
PLW2	14.00000000 W
PLW12	0.17284000 W
PLW13	0.14000000 W

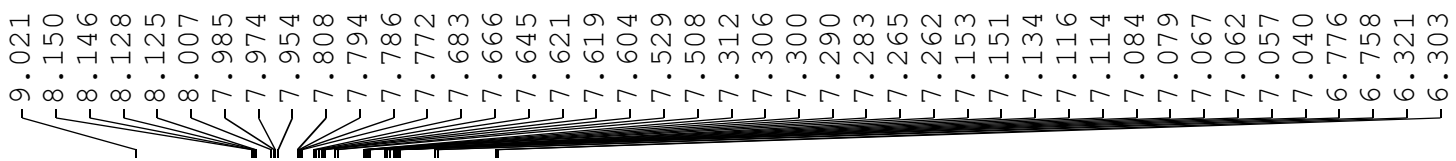
F2 - Processing parameters

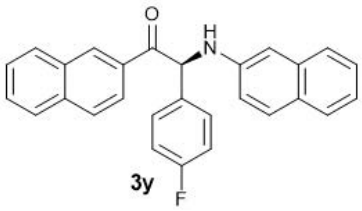
SI	32768
SF	75.4676805 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



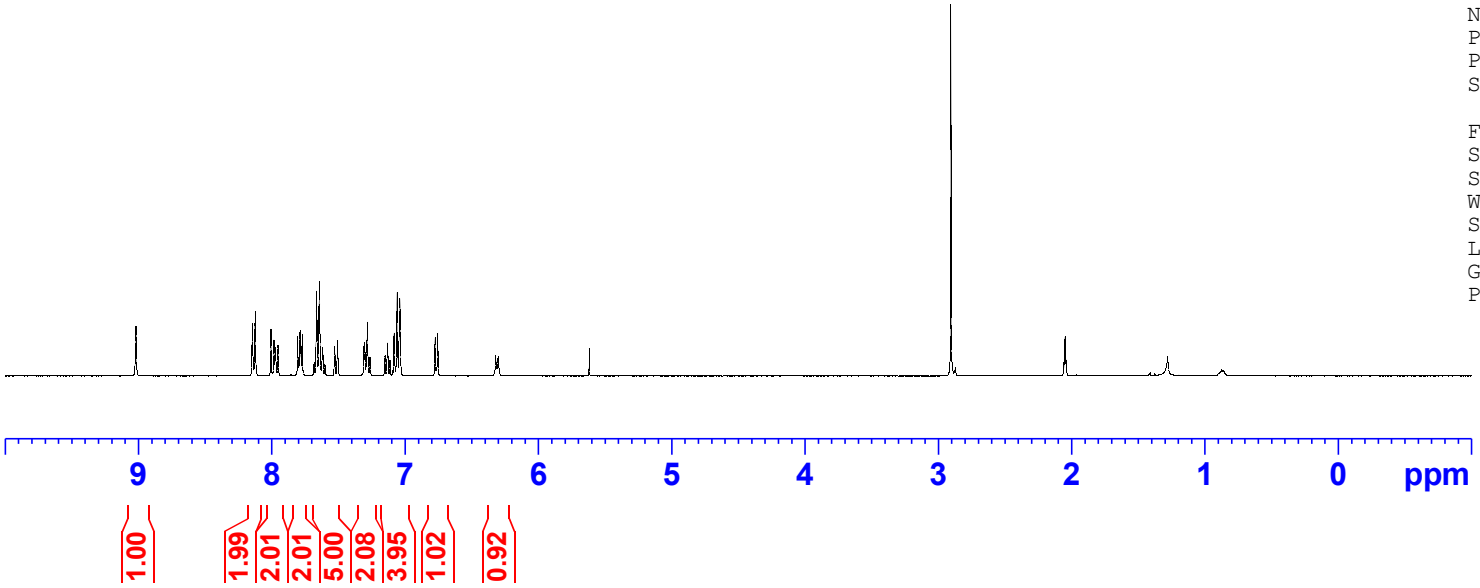


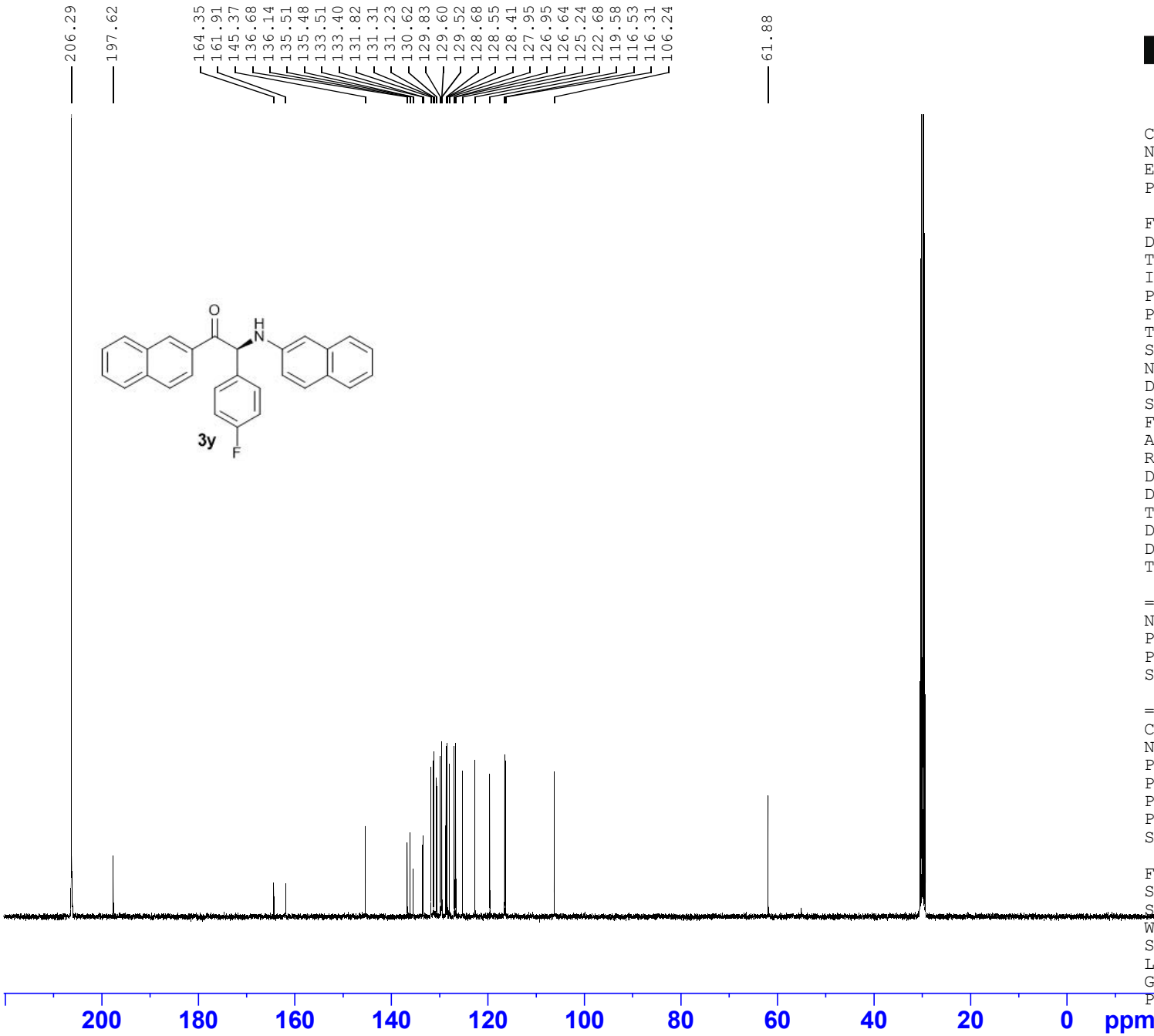

```
Current Data Parameters
NAME       FNMR-ZY-1-92
EXPNO               517
PROCNO                1

F2 - Acquisition Parameters
Date_          20220805
Time              14.17
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG      zgfhigqn.2
TD               131072
SOLVENT         Acetone
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                -59.1 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
```






```
Current Data Parameters
NAME      HNMR-4ZY-1-89
EXPNO               31
PROCNO               1

F2 - Acquisition Parameters
Date_          20220804
Time               22.54
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                     8
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                294.9 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          400.1900120 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```





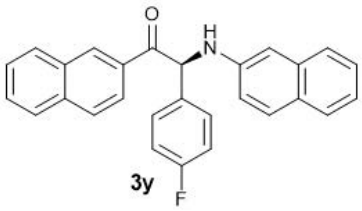
Current Data Parameters
NAME CNMR-4ZY-1-89
EXPNO 32
PROCNO 1

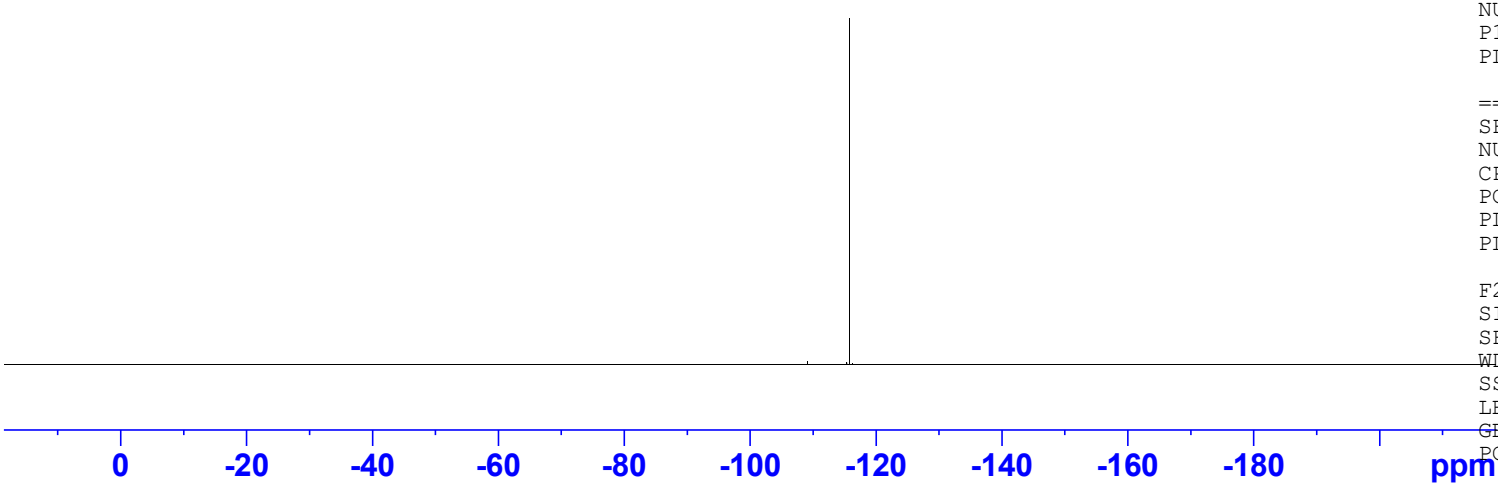
F2 - Acquisition Parameters
Date_ 20220804
Time 23.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 600
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 193.13
DW 20.800 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

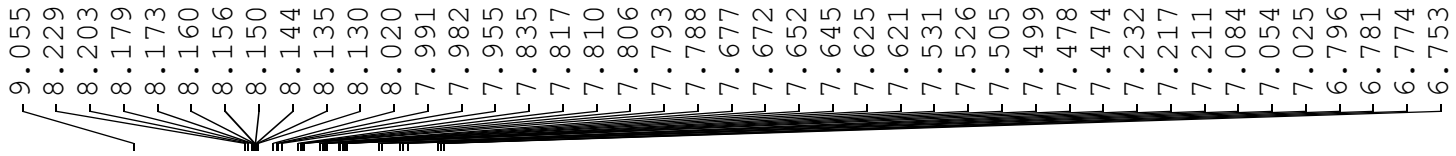
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.37246999 W
PLW13 0.30170000 W
SFO2 400.1916008 MHz

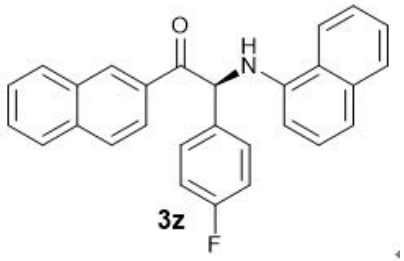
F2 - Processing parameters
SI 32768
SF 100.6277654 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



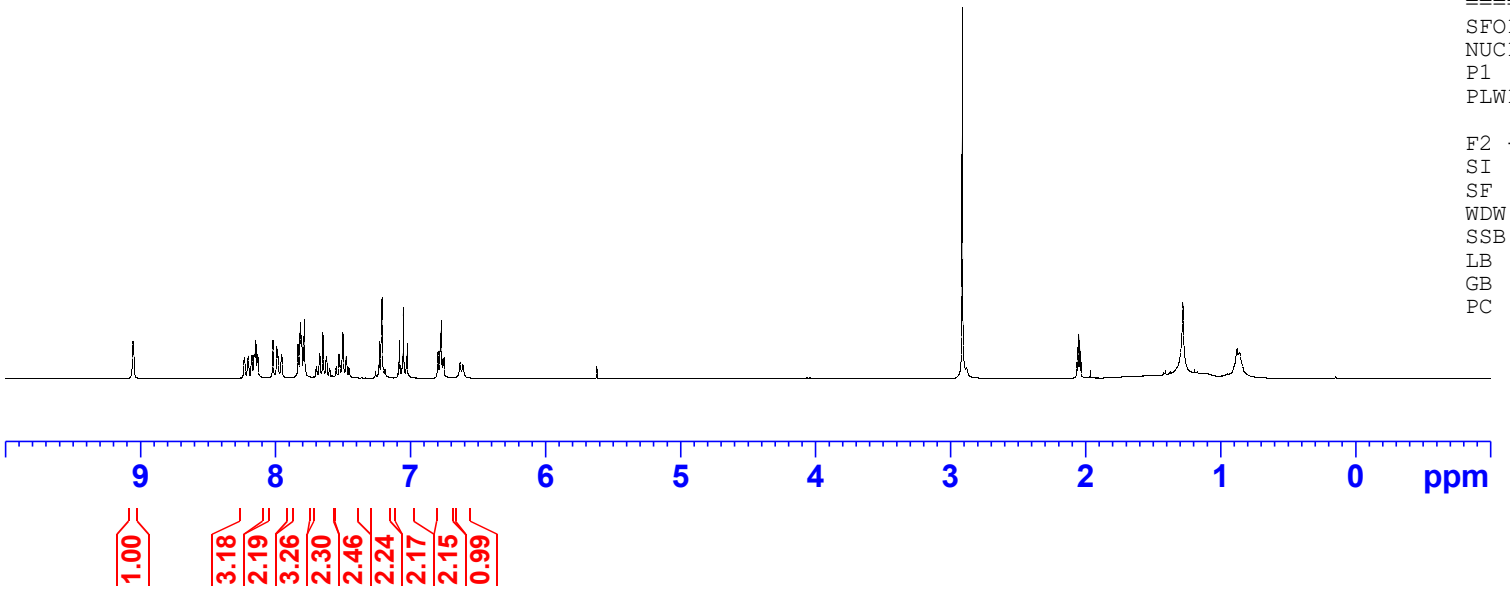


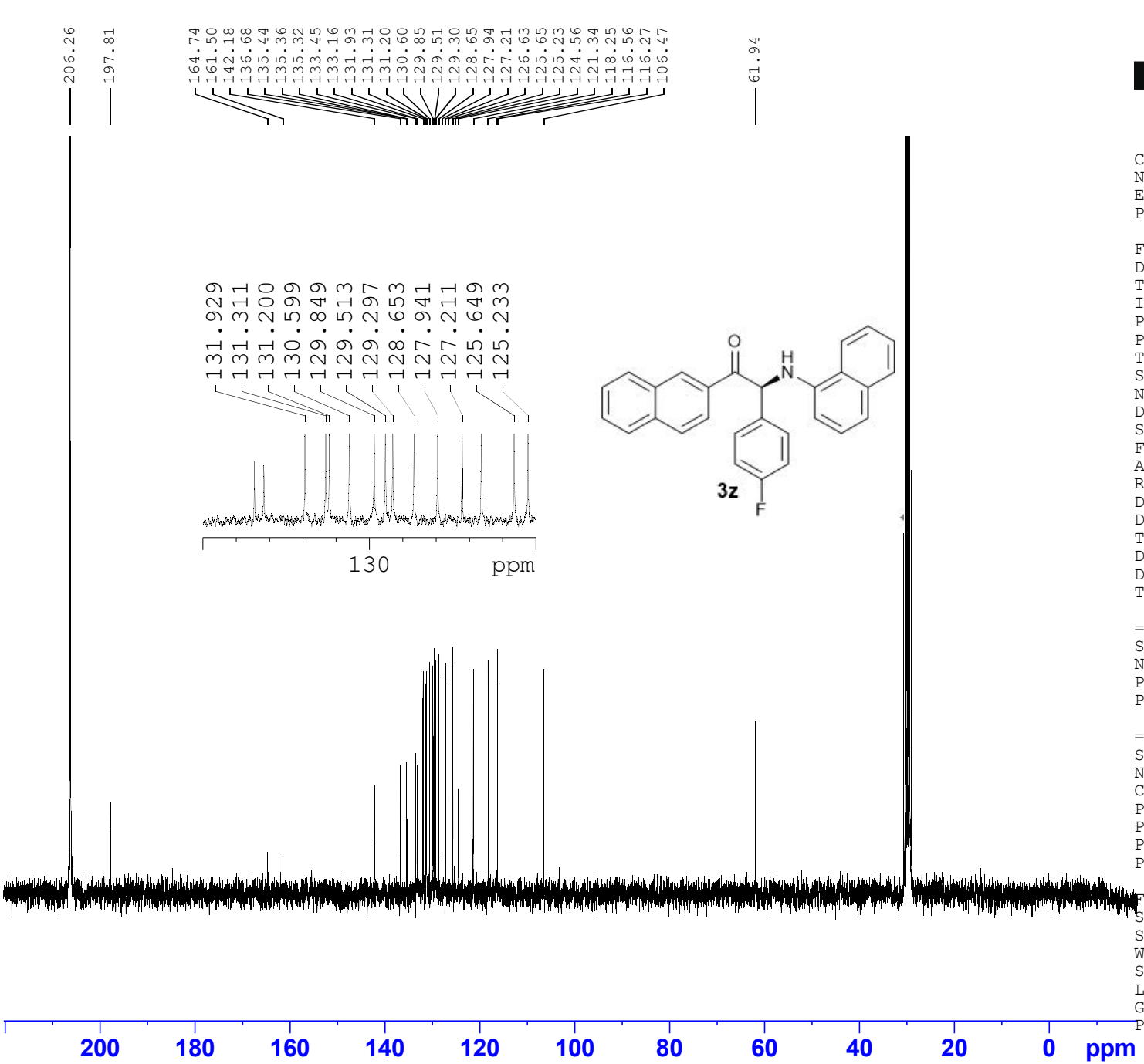

```
Current Data Parameters
NAME       FNMR-ZY-1-89
EXPNO               520
PROCNO                1

F2 - Acquisition Parameters
Date_          20220809
Time              14.07
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG      zgfhigqn.2
TD               131072
SOLVENT          Acetone
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                -59.1 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
```






```
Current Data Parameters
NAME       HNMR-ZY-1-75
EXPNO               459
PROCNO                1

F2 - Acquisition Parameters
Date_          20220721
Time              13.42
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    2
SWH            6009.615 Hz
FIDRES        0.091699 Hz
AQ            5.4525952 sec
RG                  114
DW               83.200 usec
DE                6.50 usec
TE                -59.1 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        300.1318534 MHz
NUC1                  1H
P1                10.00 usec
PLW1        14.00000000 W

F2 - Processing parameters
SI                65536
SF          300.1300051 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```





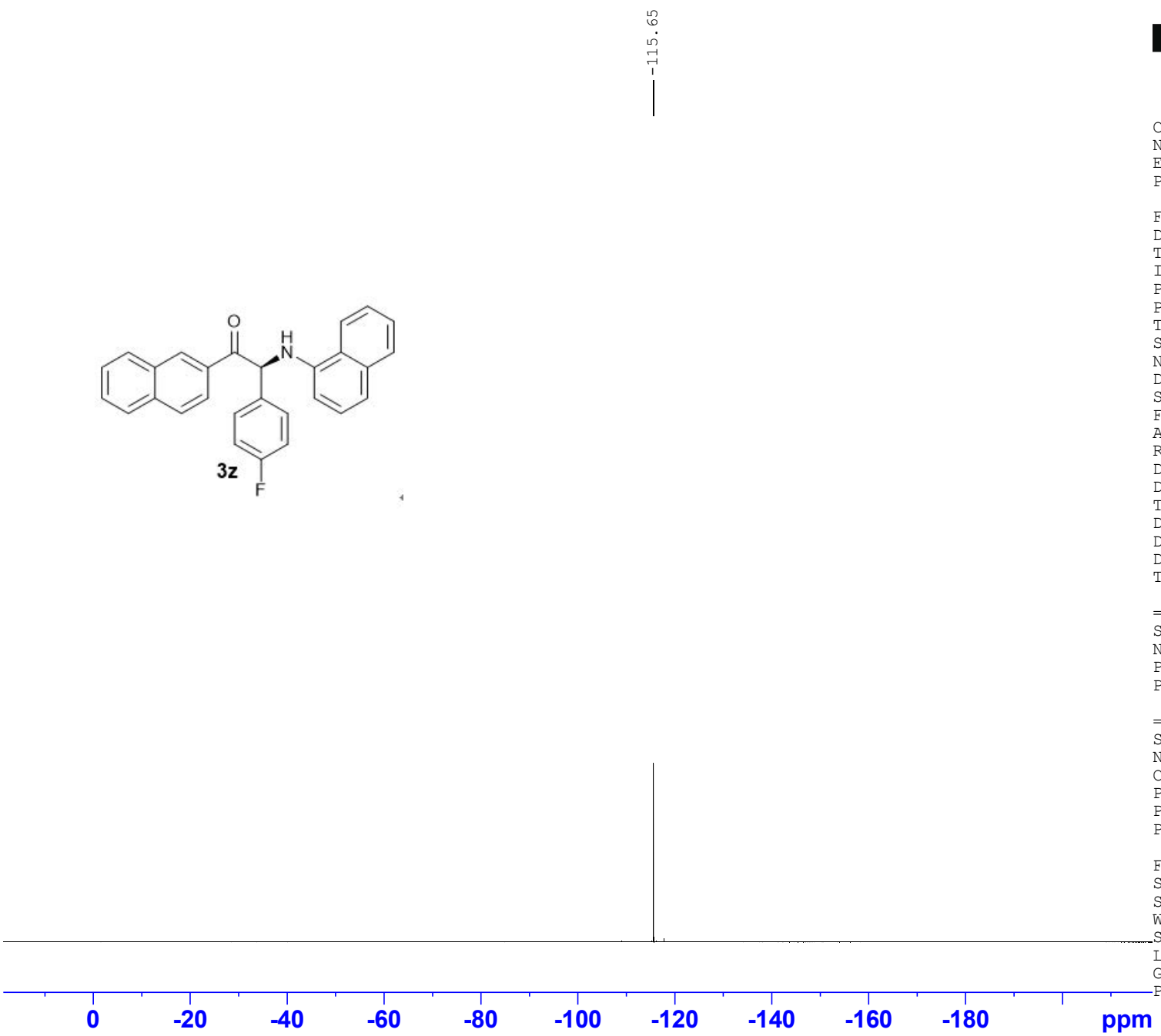
Current Data Parameters
NAME CNMR-ZY-1-75
EXPNO 468
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220721
Time 22.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 200
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175317 sec
RG 203
DW 27.733 usec
DE 6.50 usec
TE -59.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

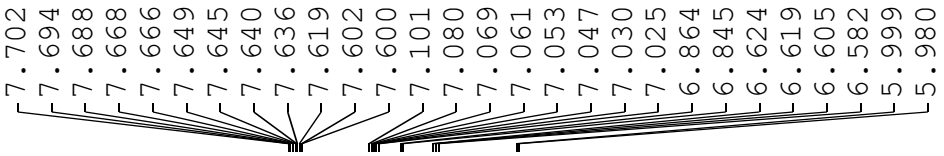
======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.50 usec
PLW1 34.20000076 W

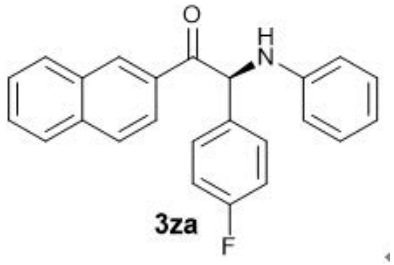
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 14.00000000 W
PLW12 0.17284000 W
PLW13 0.14000000 W

F2 - Processing parameters
SI 32768
SF 75.4676829 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40




```
Current Data Parameters
NAME       FNMR-ZY-1-75
EXPNO               474
PROCNO                1

F2 - Acquisition Parameters
Date_          20220722
Time              14.23
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG      zgfhigqn.2
TD               131072
SOLVENT          Acetone
NS                     4
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                -59.1 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
```

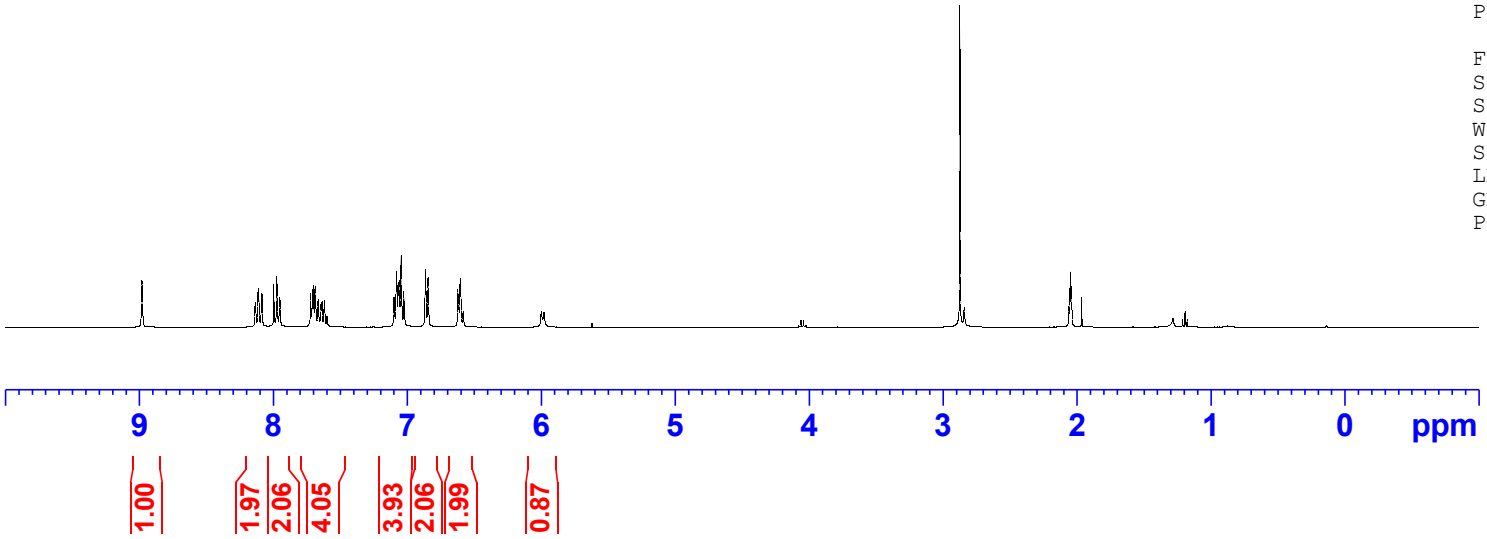


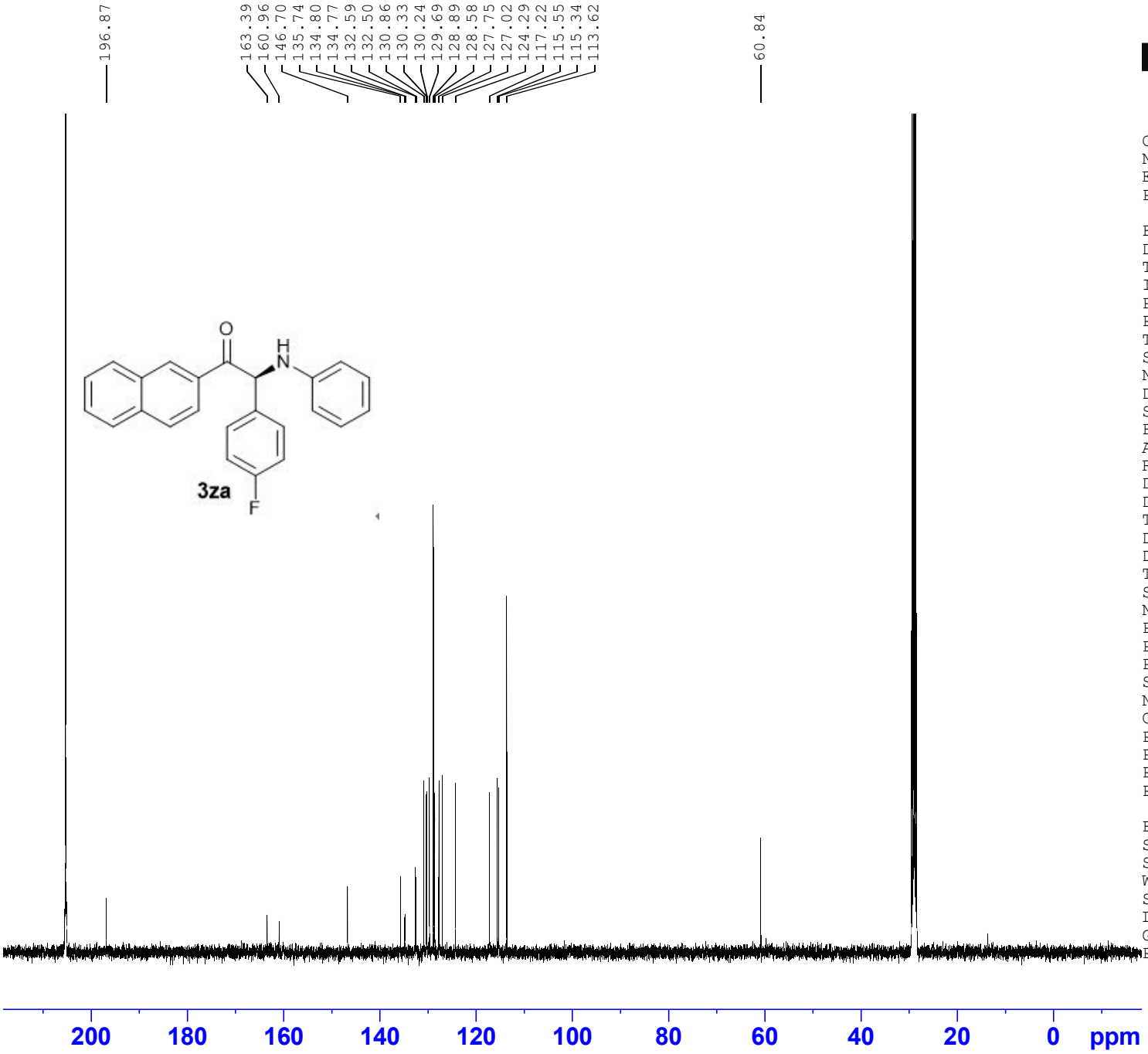


Current Data Parameters
NAME HNMR-ZY-2-15
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220917
Time 9.38 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zg30
TD 65536
SOLVENT Acetone
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 294.9 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 400.1300069 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



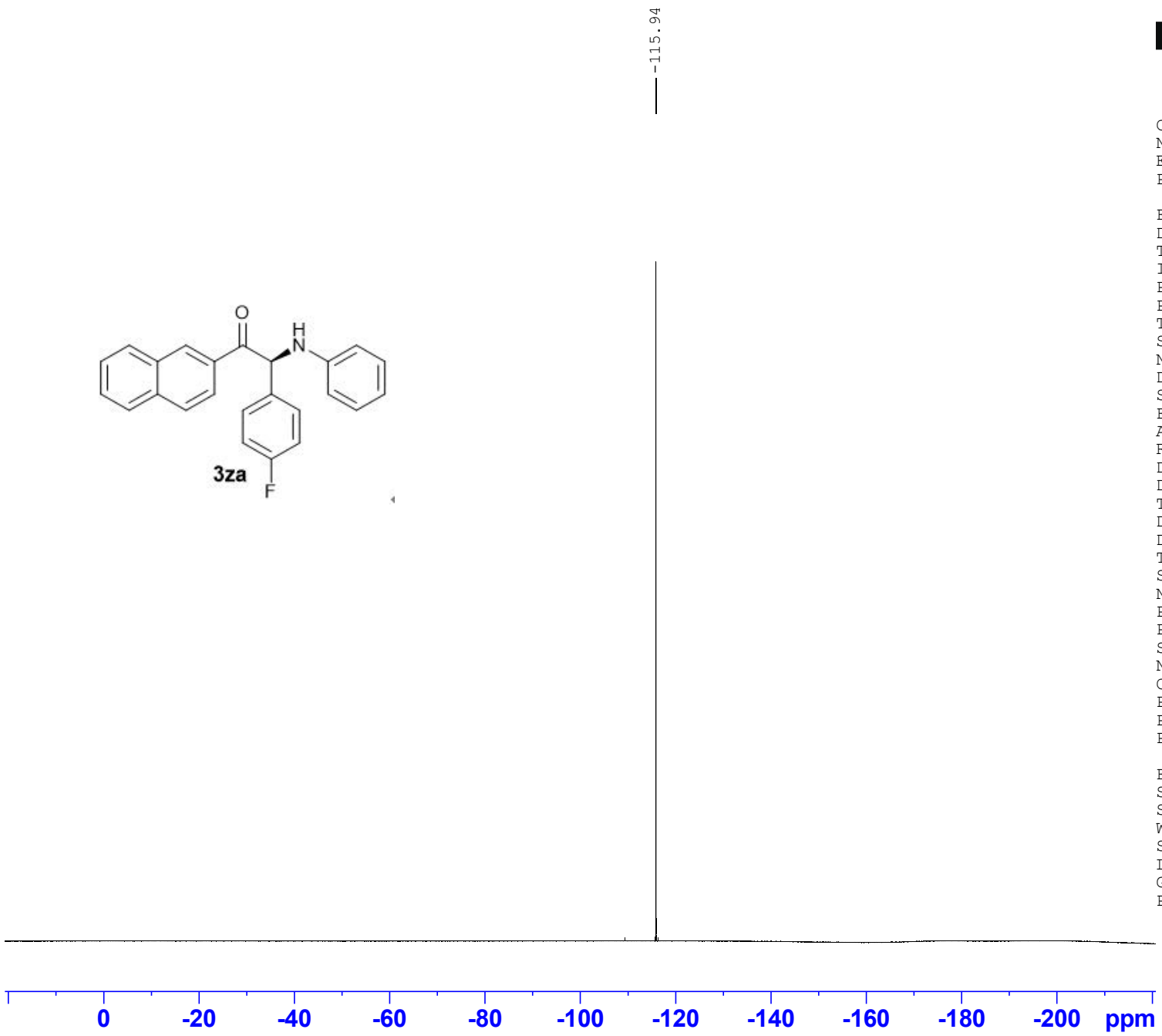


BRUKER

Current Data Parameters
NAME CNMR-ZY-2-15
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220917
Time 9.57 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 300
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 48.6724
DW 21.000 usec
DE 6.50 usec
TE 295.7 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

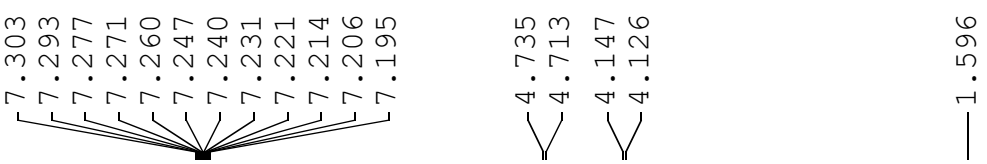
F2 - Processing parameters
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

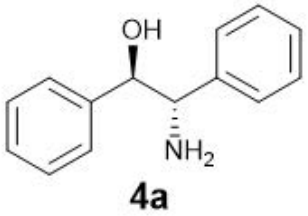


Current Data Parameters
NAME FNMR-ZY-2-15
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220917
Time 9.58 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgig
TD 131072
SOLVENT Acetone
NS 16
DS 4
SWH 90909.094 Hz
FIDRES 1.387163 Hz
AQ 0.7208960 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 376.4607164 MHz
NUC1 19F
P1 18.00 usec
PLW1 16.73100090 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 20.73200035 W
PLW12 0.25595000 W

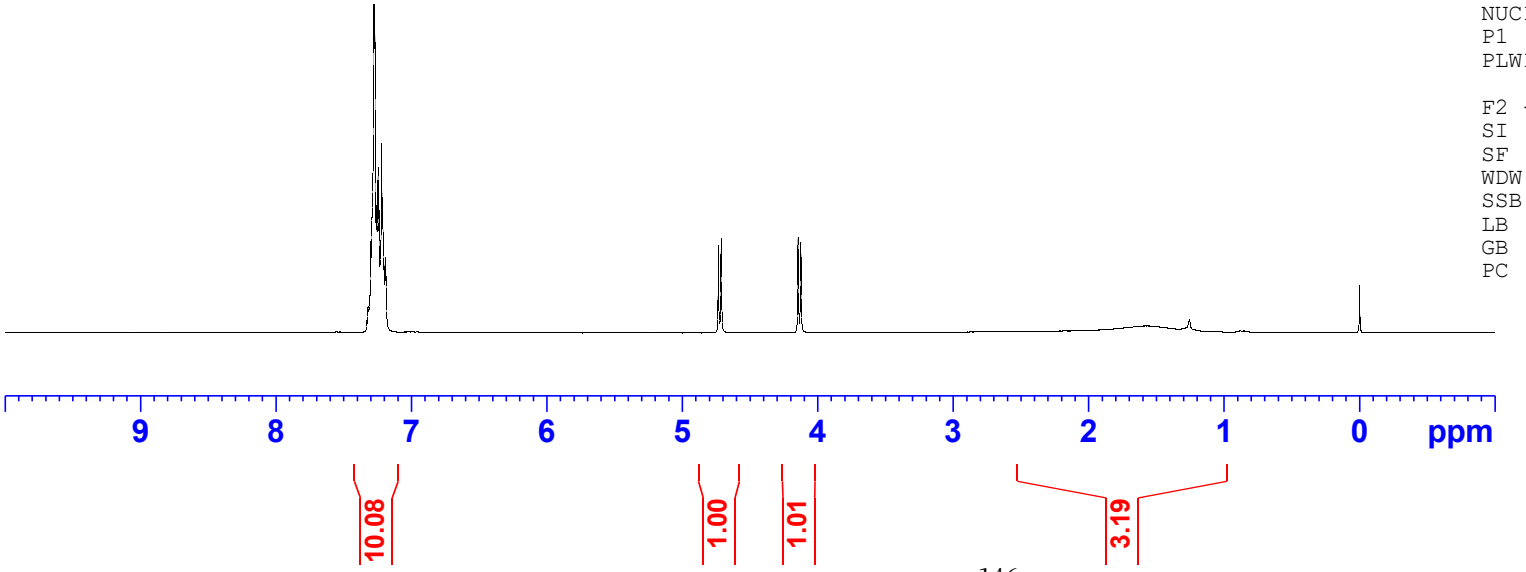
F2 - Processing parameters
SI 65536
SF 376.4983662 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

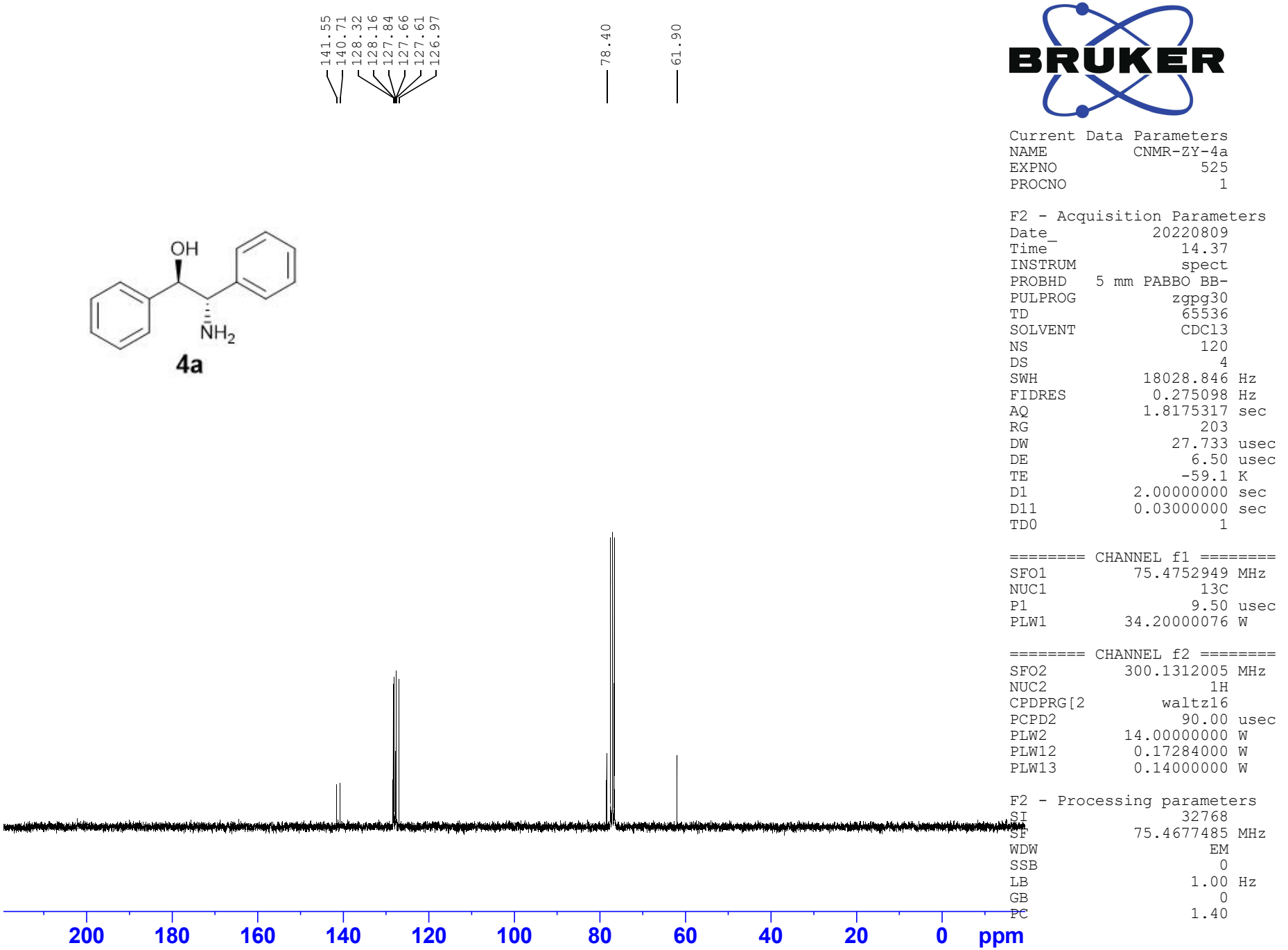




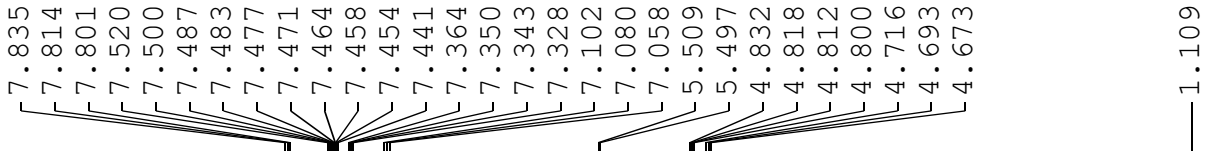
4a

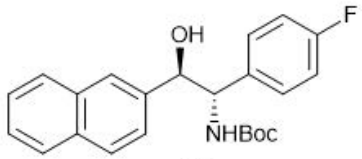
```
Current Data Parameters
NAME          HNMR-ZY-4a
EXPNO                524
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220809
Time              14.28
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            6009.615 Hz
FIDRES        0.091699 Hz
AQ           5.4525952 sec
RG                  181
DW               83.200 usec
DE                6.50 usec
TE               -59.1 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        300.1318534 MHz
NUC1                1H
P1              10.00 usec
PLW1        14.00000000 W

F2 - Processing parameters
SI                65536
SF          300.1300095 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



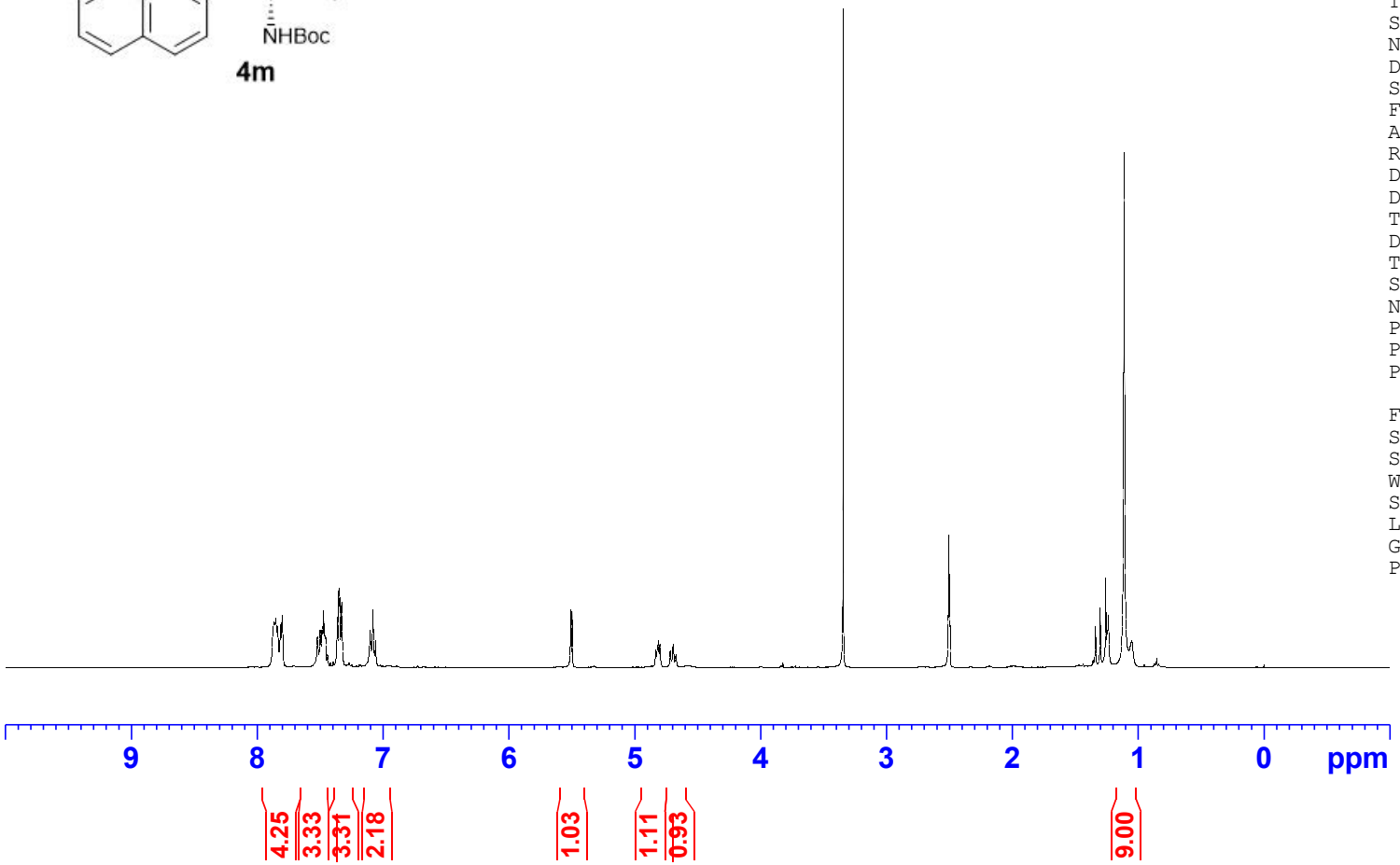



```
Current Data Parameters
NAME          CNMR-ZY-4a
EXPNO                525
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220809
Time               14.37
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  120
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175317 sec
RG                  203
DW               27.733 usec
DE                6.50 usec
TE                -59.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         75.4752949 MHz
NUC1                13C
P1                 9.50 usec
PLW1        34.20000076 W

======== CHANNEL f2 ========
SFO2        300.1312005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        14.00000000 W
PLW12        0.17284000 W
PLW13        0.14000000 W

F2 - Processing parameters
SI                 32768
SF           75.4677485 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

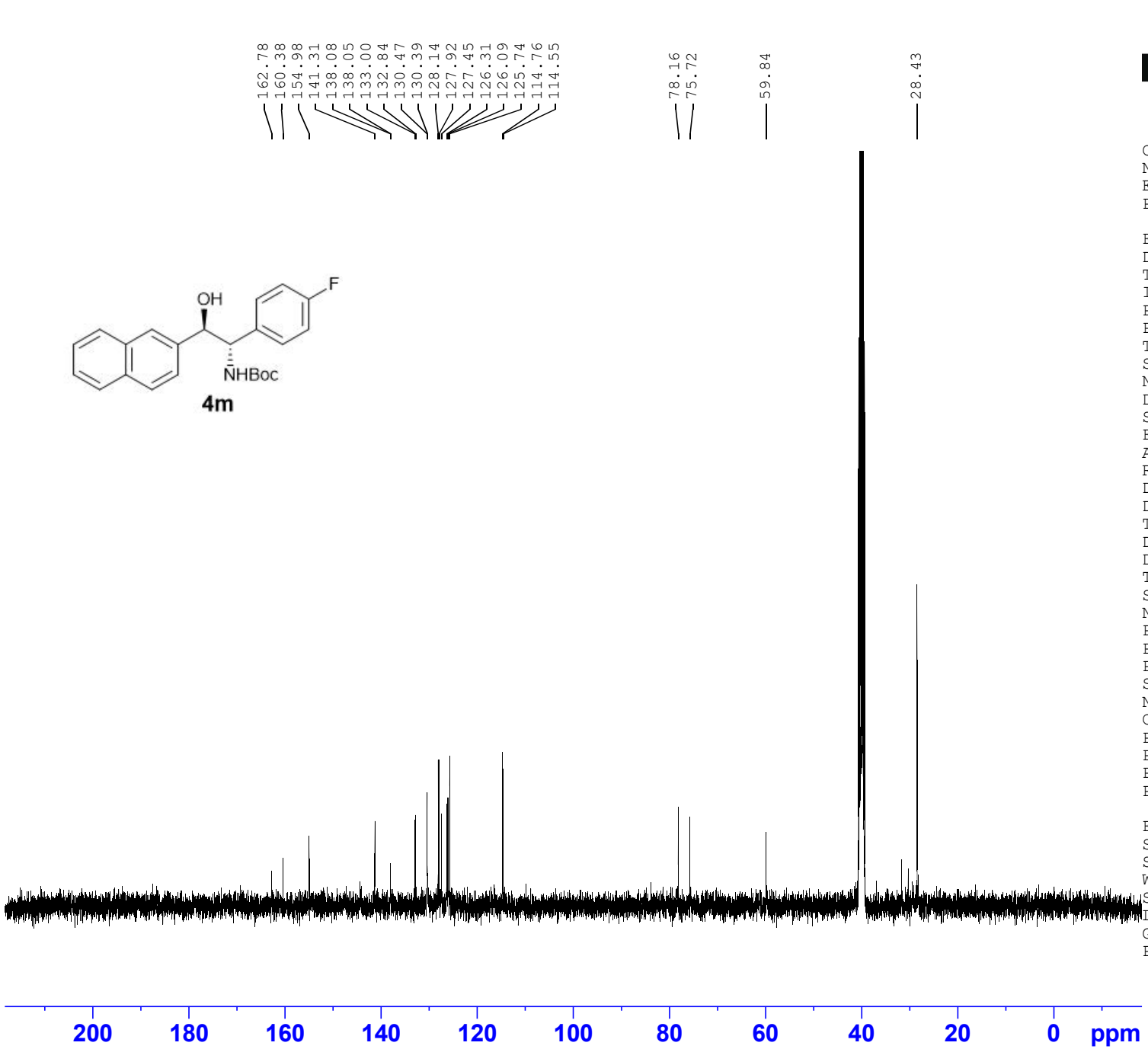




4m



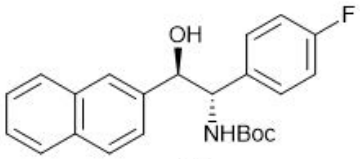

```
Current Data Parameters
NAME        HNMR-ZY-2-37
EXPNO                  7
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220924
Time                5.08 h
INSTRUM            Avance
PROBHD   Z116098_0833 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
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                294.9 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            400.1300025 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



Current Data Parameters
NAME CNMR-ZY-2-37
EXPNO 7
PROCNO 1

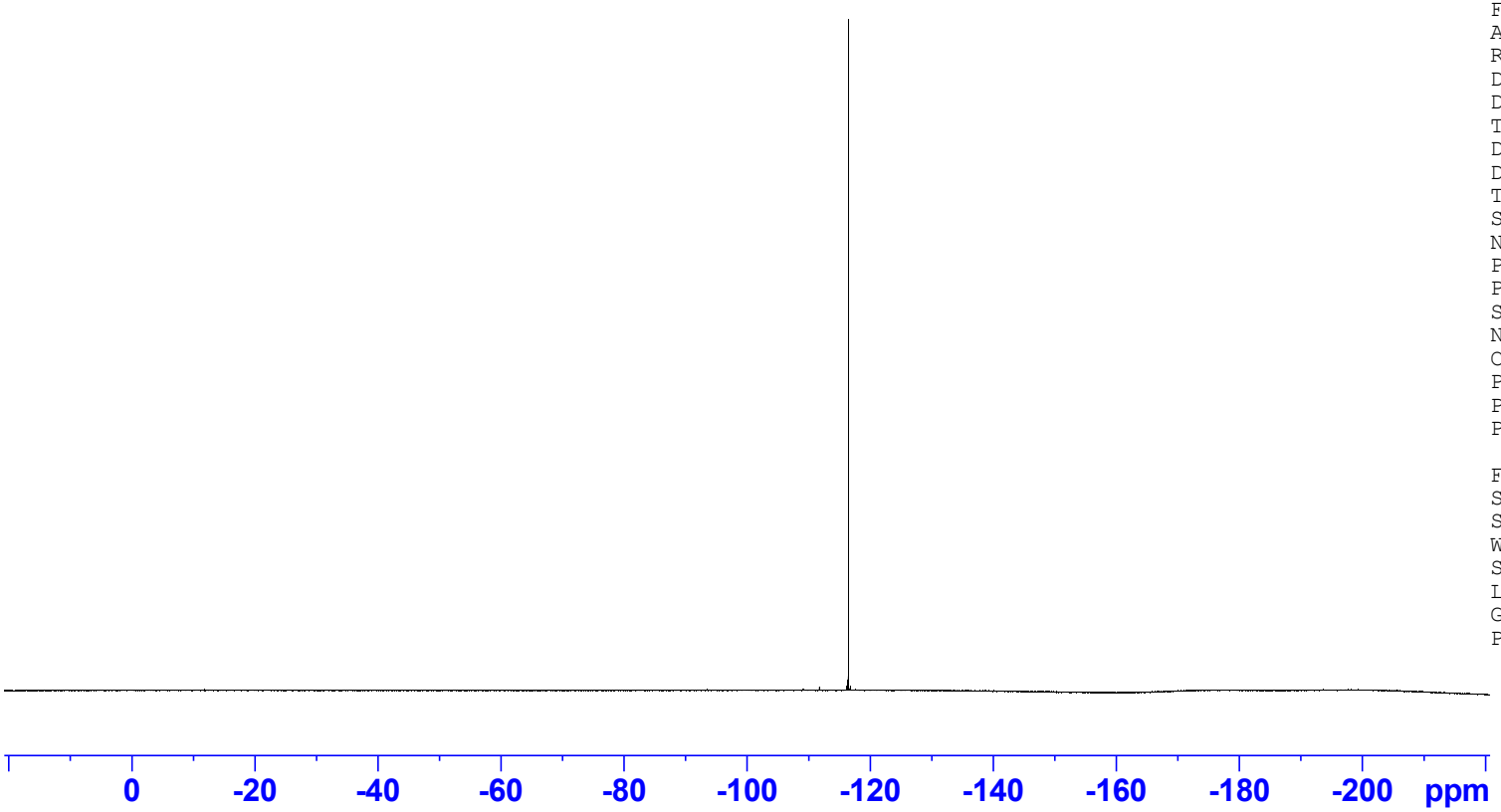
F2 - Acquisition Parameters
Date_ 20220927
Time 10.31 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 500
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 51.55
DW 21.000 usec
DE 6.50 usec
TE 295.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 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 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

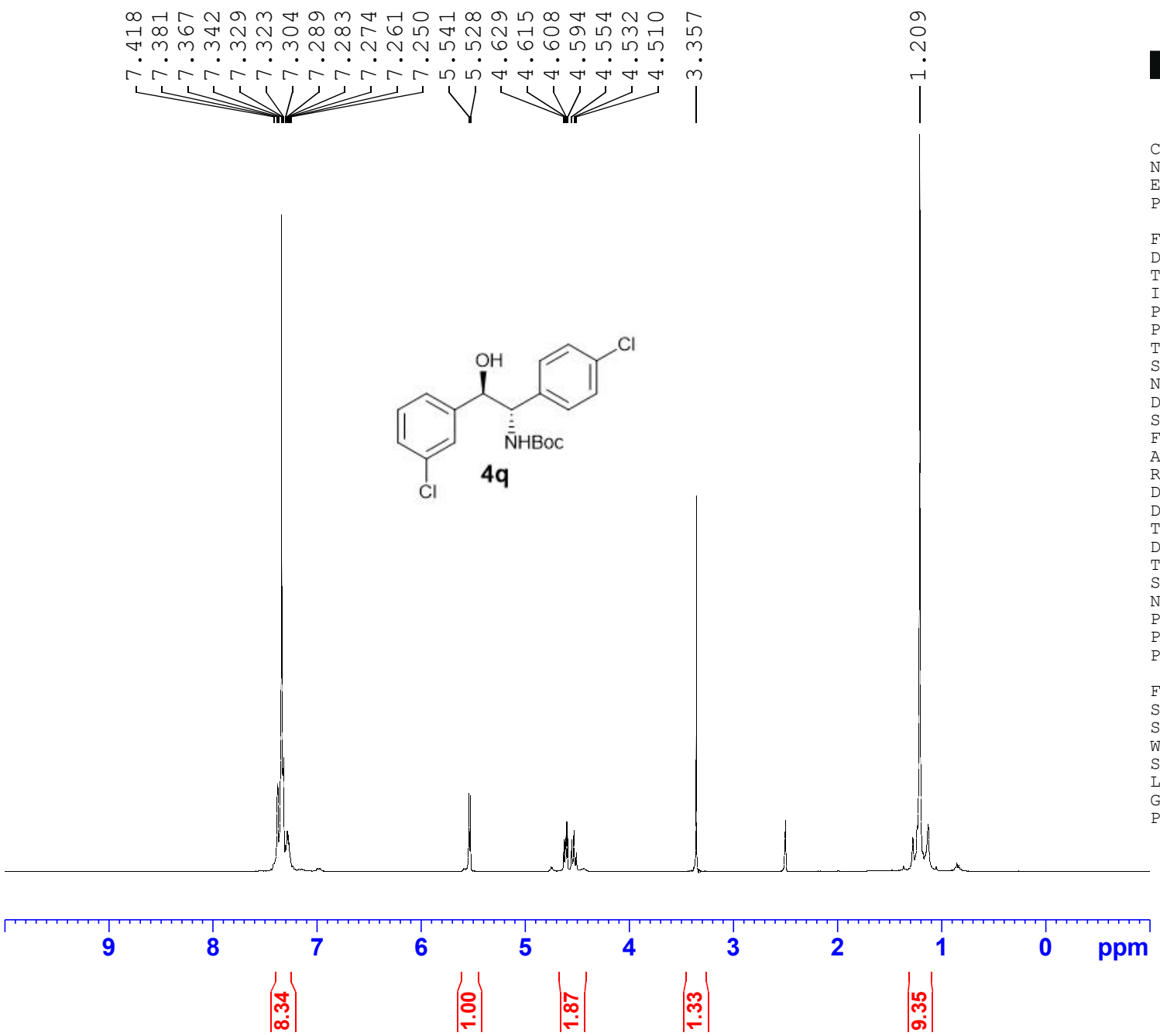


4m

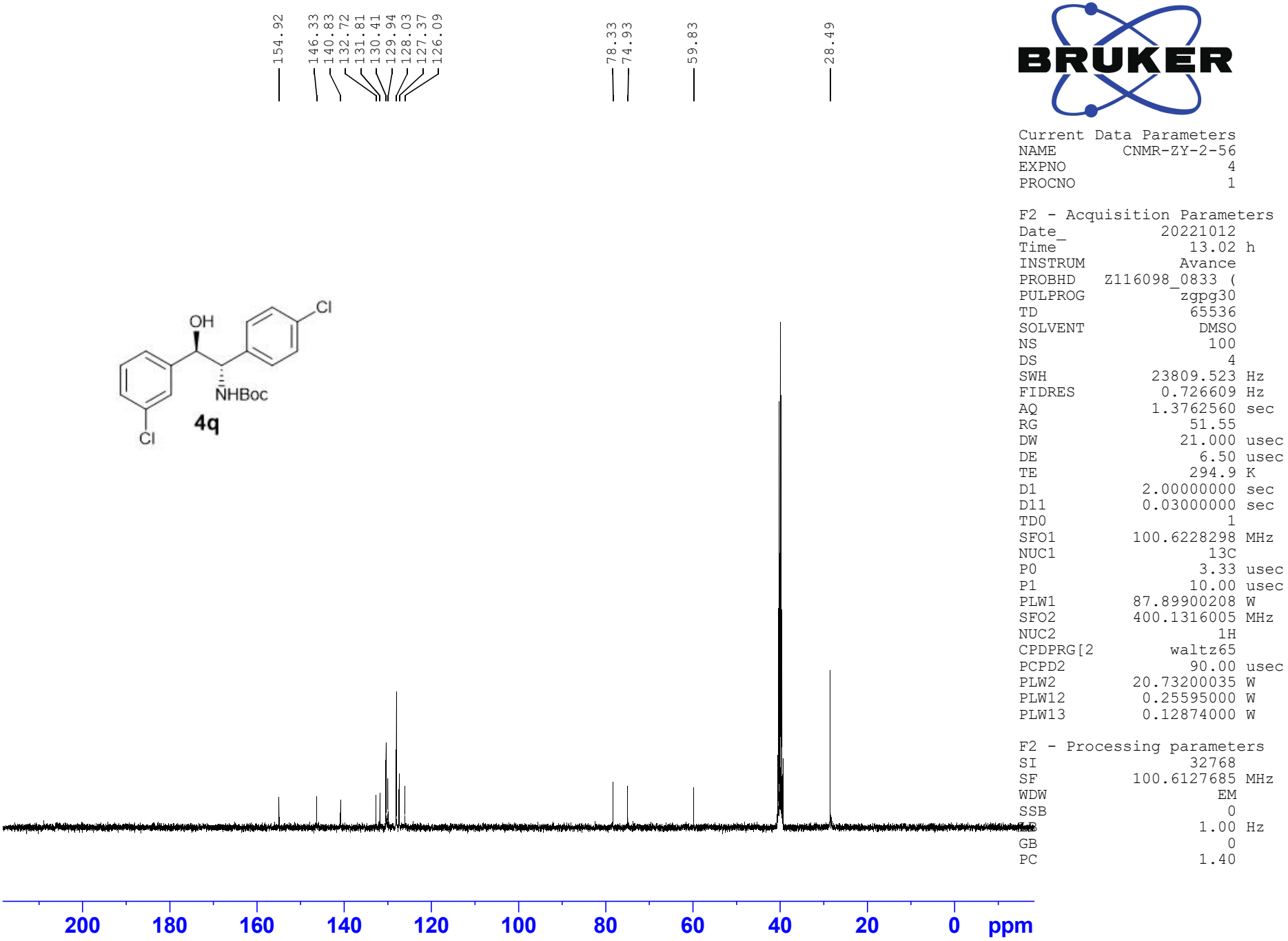
-116.45




```
Current Data Parameters
NAME       FNMR-ZY-2-37
EXPNO                 9
PROCNO                1

F2 - Acquisition Parameters
Date_          20220924
Time               5.25 h
INSTRUM           Avance
PROBHD   Z116098_0833 (
PULPROG            zgig
TD               131072
SOLVENT             DMSO
NS                    16
DS                     4
SWH            90909.094 Hz
FIDRES          1.387163 Hz
AQ             0.7208960 sec
RG                   101
DW                 5.500 usec
DE                 6.50 usec
TE                 295.4 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         376.4607164 MHz
NUC1                 19F
P1                18.00 usec
PLW1         16.73100090 W
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         20.73200035 W
PLW12         0.25595000 W

F2 - Processing parameters
SI                 65536
SF           376.4983662 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME        HNMR-ZY-2-56
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20221012
Time              12.55 h
INSTRUM           Avance
PROBHD   Z116098_0833 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH             8196.722 Hz
FIDRES          0.250144 Hz
AQ             3.9976959 sec
RG               83.1117
DW                61.000 usec
DE                13.54 usec
TE                294.1 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          400.1300028 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



Current Data Parameters
NAME CNMR-ZY-2-56
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221012
Time 13.02 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 100
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 51.55
DW 21.000 usec
DE 6.50 usec
TE 294.9 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 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40