Supplementary Information

Organocatalytic Asymmetric Azidation of Sulfoxonium Ylides: Mild Synthesis of Enantioenriched α-Azido Ketones Bearing a Labile Tertiary Stereocenter

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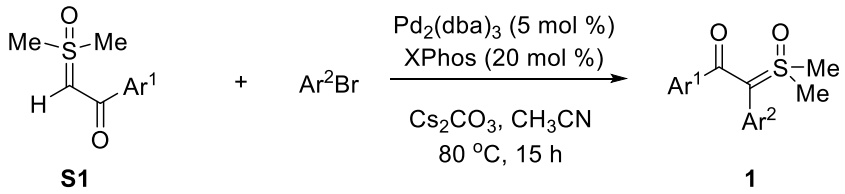
I. General Information

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. Anhydrous methyl *tert*-butyl ether (MTBE), $ZnCl_2$ (0.5 M in THF), *s*-BuLi (1.3 M in *n*-hexane), $Pd(OAc)_2$, trimethylsulfoxonium iodide, KO*t*Bu, aryl bromides, aryl acyl chloride used in this study were purchased from Energy Chemical, and used as received. (+)-Sparteine was purchased from Nanjing Chemlin Chemical Industry Co., Ltd. *N*-Boc-D-*tert*-Leucine, 1-pyrenyl bromide, XPhos, and 3,4-Dimethoxy-3-cyclobutene-1,2-dione 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 commercial sources, 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%).

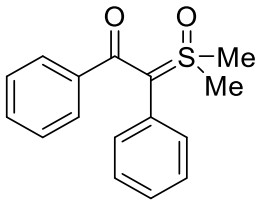
II. Substrate Preparation

The sulfoxonium ylides were prepared according to a modified literature procedure.[1] The detailed procedure is shown below.

General Procedure A.



Under N_2, to a 100-mL round-bottomed flask equipped with a magnetic stir bar were sequentially added Xphos (477.0 mg, 1.0 mmol, 20 mol%), $Pd_2(dba)_3$ (229.0 mg, 0.25 mmol, 5 mol%), Cs_2CO_3 (1.8 g, 5.5 mmol, 1.1 equiv), and anhydrous CH_3CN (10.0 mL). The resulting mixture was stirred at room temperature for 10 min followed by addition of the aryl bromide (10.0 mmol, 2.0 equiv) and sulfoxonium ylide **S1** (5.0 mmol, 1.0 equiv). The mixture was then heated with stirring at 80 °C. Upon completion (~ 15 h), the reaction mixture was cooled to room temperature and filtered through a short plug of silica gel, which was washed with DCM/MeOH (*v*/*v* = 50:1, 50 mL). The filtrate was concentrated, and the residue was purified by flash column chromatography on silica gel to afford the desired product sulfoxonium ylide **1**.



1a

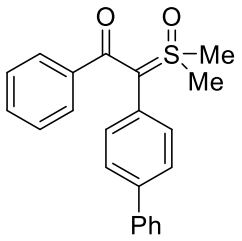
2-(Dimethyl(oxo)-λ⁶-sulfanylidene)-1,2-diphenylethan-1-one (1a) was prepared as a

(1) C. Janot, J. B. Chagnoleau, N. R. Halcovitch, J. Muir, C. Aïssa, *J. Org. Chem.*, **2020**, *85*, 1126–1137.

light brown solid according to the General Procedure A (eluent: DCM/MeOH = 50:1, 0.9 g, 64% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37 – 7.34 (m, 2H), 7.24 – 7.10 (m, 8H), 3.6 (s, 6H) ppm.

It's a known compound, and the spectral data are consistent with the literature report.[2]



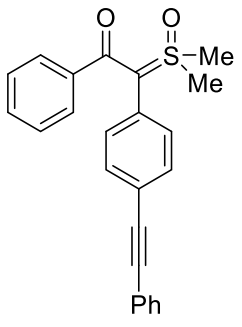
1b

2-([1,1'-Biphenyl]-4-yl)-2-(dimethyl(oxo)-λ^6-sulfanylidene)-1-phenylethan-1-one (1b) was prepared as a light brown solid according to the General Procedure A (eluent: DCM/MeOH = 50:1, 0.8 g, 47% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.56 (m, 2H), 7.48 – 7.45 (m, 2H), 7.43 – 7.39 (m, 4H), 7.33 – 7.29 (m, 1H), 7.26 – 7.21 (m, 3H), 7.18 – 7.14 (m, 2H), 3.66 (s, 6H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 183.1, 140.5, 140.1, 139.7, 135.0, 131.1, 129.5, 128.8 (2C), 127.6, 127.3, 127.0, 126.9, 86.4, 43.1 ppm.

HRMS (ESI-TOF) Calcd for $C_{22}H_{20}NaO_2S$ $[M+Na]^+$: 371.1082, found: 371.1083.



1c

2-(Dimethyl(oxo)-λ^6-sulfanylidene)-1-phenyl-2-(4-(phenylethynyl)phenyl)ethan-1-one (1c) was prepared as a brown solid according to the General Procedure A (eluent:

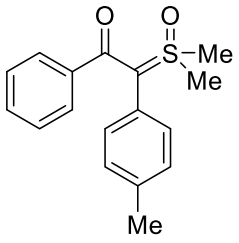
(2) A. G. Talero, B. S. Martins, A. C. B. Burtoloso, *Org. Lett.*, **2018**, *20*, 7206–7211.

DCM/MeOH = 50:1, 521 mg, 28% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.49 (m, 2H), 7.38 – 7.36 (m, 4H), 7.35 – 7.32 (m, 3H), 7.26 – 7.23 (m, 1H), 7.19 – 7.12 (m, 4H), 3.64 (s, 6H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 183.3, 140.0, 134.3, 132.3, 131.6, 131.4, 129.6, 128.7, 128.4, 128.3, 127.7, 123.3, 121.7, 90.1, 89.4, 86.3, 43.2 ppm.

HRMS (ESI-TOF) Calcd for $C_{24}H_{20}NaO_2S$ $[M+Na]^+$: 395.1082, found: 395.1079.



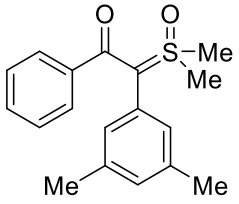
1d

2-(Dimethyl(oxo)-λ^6-sulfanylidene)-1-phenyl-2-(*p*-tolyl)ethan-1-one (1d) was prepared as a light yellow solid according to the General Procedure A (eluent: DCM/MeOH = 50:1, 650 mg, 45% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.41 (m, 2H), 7.28 – 7.24 (m, 1H), 7.21 – 7.17 (m, 2H), 7.11 – 7.06 (m, 4H), 3.66 (s, 6H), 2.34 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 182.9, 140.2, 137.3, 134.7, 129.3, 129.2, 128.8, 128.7, 127.5, 86.7, 43.0, 21.3 ppm.

HRMS (ESI-TOF) Calcd for $C_{17}H_{18}NaO_2S$ $[M+Na]^+$: 309.0925, found: 309.0922.



1e

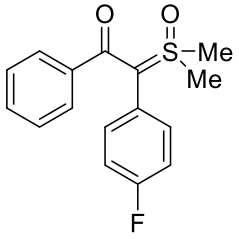
2-(Dimethyl(oxo)-λ^6-sulfanylidene)-2-(3,5-dimethylphenyl)-1-phenylethan-1-one (1e) was prepared as a light brown solid according to the General Procedure A (eluent: DCM/MeOH = 50:1, 700 mg, 47% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.38 (m, 2H), 7.26 – 7.19 (m, 1H), 7.16 – 7.12 (m,

2H), 6.86 (s, 1H), 6.80 (s, 2H), 3.61 (s, 6H), 2.21 (s, 6H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 182.7, 140.2, 137.6, 132.7, 131.5, 129.4, 129.3, 128.6, 127.4, 87.2, 43.1, 21.2 ppm.

HRMS (ESI-TOF) Calcd for $C_{18}H_{20}NaO_2S$ $[M+Na]^+$: 323.1082, found: 323.1083.



1f

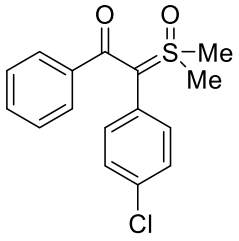
2-(Dimethyl(oxo)-λ^6-sulfanylidene)-2-(4-fluorophenyl)-1-phenylethan-1-one (1f) was prepared as a light yellow solid according to the General Procedure A (eluent: DCM/MeOH = 50:1, 610 mg, 42% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.34 (m, 2H), 7.25 – 7.22 (m, 1H), 7.18 – 7.10 (m, 4H), 6.95 – 6.89 (m, 2H), 3.64 (s, 6H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 183.1, 162.2 (d, $^1J_{C\text{-}F}$ = 246 Hz), 140.0, 136.4 (d, $^3J_{C\text{-}F}$ = 8 Hz), 129.5, 128.6, 127.9 (d, $^4J_{C\text{-}F}$ = 3 Hz), 127.6, 115.3 (d, $^2J_{C\text{-}F}$ = 21 Hz), 85.5, 43.0 ppm.

^{19}F NMR (282 MHz, $CDCl_3$) δ –114.6 ppm.

HRMS (ESI-TOF) Calcd for $C_{16}H_{15}FNaO_2S$ $[M+Na]^+$: 313.0674, found: 313.0670.



1g

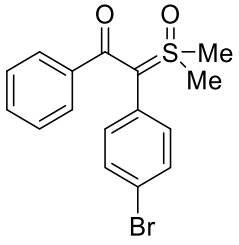
2-(4-Chlorophenyl)-2-(dimethyl(oxo)-λ^6-sulfanylidene)-1-phenylethan-1-one (1g) was prepared as a light yellow solid according to the General Procedure A (eluent: DCM/MeOH = 50:1, 580 mg, 38% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.34 (m, 2H), 7.27 – 7.24 (m, 1H), 7.19 – 7.16 (m,

4H), 7.09 – 7.06 (m, 2H), 3.63 (s, 6H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 183.3, 139.9, 135.8, 133.2, 130.6, 129.6, 128.7, 128.4, 127.7, 85.4, 43.1 ppm.

HRMS (ESI-TOF) Calcd for $C_{16}H_{15}ClNaO_2S$ $[M+Na]^+$: 329.0379, found: 329.0377.



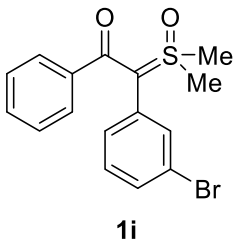
1h

2-(4-Bromophenyl)-2-(dimethyl(oxo)-λ⁶-sulfanylidene)-1-phenylethan-1-one (1h) was prepared as a light brown solid according to the General Procedure A (eluent: DCM/MeOH = 50:1, 640 mg, 36% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37 – 7.31 (m, 4H), 7.28 – 7.15 (m, 3H), 7.02 – 6.99 (mm, 2H), 3.64 (s, 6H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 183.3, 139.9, 136.0, 131.4, 131.1, 129.6, 128.7, 127.7, 121.5, 85.5, 43.1 ppm.

HRMS (ESI-TOF) Calcd for $C_{16}H_{15}BrNaO_2S$ $[M+Na]^+$: 372.9874, found: 372.9875.



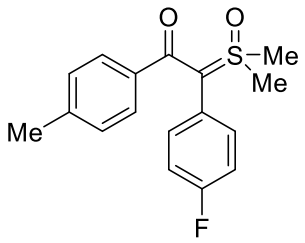
1i

2-(3-Bromophenyl)-2-(dimethyl(oxo)-λ⁶-sulfanylidene)-1-phenylethan-1-one (1i) was prepared as a brown solid according to the General Procedure A (eluent: DCM/MeOH = 50:1, 460 mg, 26% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.34 (m, 4H), 7.30 – 7.27 (m, 1H), 7.23 – 7.19 (m, 2H), 7.10 – 7.07 (m, 2H), 3.67 (s, 6H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 183.4, 139.8, 137.0, 134.3, 133.3, 130.1, 129.7, 129.5, 128.7, 127.7, 121.8, 85.7, 43.2 ppm.

HRMS (ESI-TOF) Calcd for $C_{16}H_{15}BrNaO_2S$ $[M+Na]^+$: 372.9874, found: 372.9876.



1j

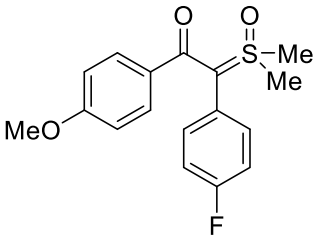
2-(Dimethyl(oxo)-λ^6-sulfanylidene)-2-(4-fluorophenyl)-1-(*p*-tolyl)ethan-1-one (1j) was prepared as a yellow solid according to the General Procedure A (eluent: DCM/MeOH = 50:1, 365 mg, 24% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.27 – 7.24 (m, 2H), 7.15 – 7.11 (m, 2H), 6.99 – 6.88 (m, 4H), 3.60 (s, 6H), 2.26 (s, 3H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 183.0, 162.2 (d, $^1J_{C\text{-}F}$ = 246 Hz), 139.6, 137.1, 136.4 (d, $^3J_{C\text{-}F}$ = 8 Hz), 128.7, 128.3, 128.2 (d, $^4J_{C\text{-}F}$ = 3 Hz), 115.3 (d, $^2J_{C\text{-}F}$ = 21 Hz), 85.2, 43.0, 21.3 ppm.

^{19}F NMR (282 MHz, $CDCl_3$) δ –114.7 ppm.

HRMS (ESI-TOF) Calcd for $C_{17}H_{17}FNaO_2S$ $[M+Na]^+$: 327.0831, found: 327.0830.



1k

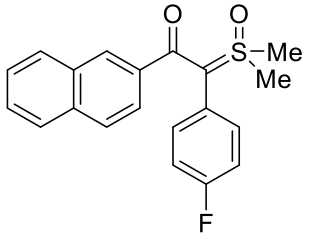
2-(Dimethyl(oxo)-λ^6-sulfanylidene)-2-(4-fluorophenyl)-1-(4-methoxyphenyl)ethan-1-one (1k) was prepared as a brown solid according to the General Procedure A (eluent: DCM/MeOH = 50:1, 200 mg, 12% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35 – 7.31 (m, 2H), 7.17 – 7.12 (m, 2H), 6.97 – 6.91 (m, 2H), 6.70 – 6.66 (m, 2H), 3.76 (s, 3H), 3.62 (s, 6H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 182.4, 162.2 (d, $^1J_{C\text{-}F}$ = 246 Hz), 160.6, 136.4 (d, $^3J_{C\text{-}F}$ = 8 Hz), 132.3, 130.5, 128.2 (d, $^4J_{C\text{-}F}$ = 3 Hz), 115.3 (d, $^2J_{C\text{-}F}$ = 21 Hz), 112.8, 84.7, 55.2, 43.2 ppm.

^{19}F NMR (282 MHz, $CDCl_3$) δ –114.7 ppm.

HRMS (ESI-TOF) Calcd for $C_{17}H_{17}FNaO_3S$ $[M+Na]^+$: 343.0780, found: 343.0771.



1l

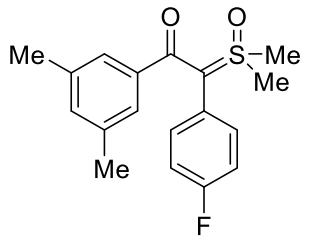
2-(Dimethyl(oxo)-λ^6-sulfanylidene)-2-(4-fluorophenyl)-1-(naphthalen-2-yl)ethan-1-one (1l) was prepared as a light brown solid according to the General Procedure A (eluent: DCM/MeOH = 50:1, 812 mg, 48% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (s, 1H), 7.79 – 7.73 (m, 2H), 7.64 (d, *J* = 8.6 Hz, 1H), 7.51 – 7.43 (m, 3H), 7.22 – 7.19 (m, 2H), 6.97 – 6.92 (m, 2H), 3.70 (s, 6H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 182.8, 162.2 (d, $^1J_{C\text{-}F}$ = 246 Hz), 137.4, 136.5 (d, $^3J_{C\text{-}F}$ = 8 Hz), 133.8, 132.6, 129.0, 128.8, 127.9 (d, $^4J_{C\text{-}F}$ = 3 Hz), 127.5, 127.0, 126.8, 126.0, 125.9, 115.4 (d, $^2J_{C\text{-}F}$ = 21 Hz), 85.9, 43.0 ppm.

^{19}F NMR (376 MHz, $CDCl_3$) δ –114.4 ppm.

HRMS (ESI-TOF) Calcd for $C_{20}H_{17}FNaO_2S$ $[M+Na]^+$: 363.0831, found: 363.0831.



1m

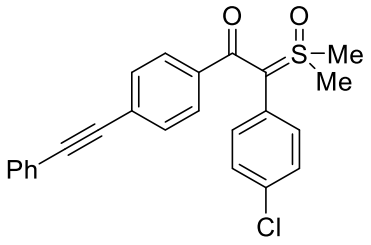
2-(dimethyl(oxo)-λ^6-sulfanylidene)-1-(3,5-dimethylphenyl)-2-(4-fluorophenyl)ethan-1-one (1m) was prepared as a light brown solid according to the General Procedure A (eluent: DCM/MeOH = 50:1, 580 mg, 36% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.15 – 7.10 (m, 2H), 6.96 – 6.86 (m, 5H), 3.58 (s, 6H), 2.14 (s, 6H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 183.4, 162.1 (d, $^1J_{C\text{-}F}$ = 246 Hz), 139.9, 136.9, 136.4 (d, $^3J_{C\text{-}F}$ = 8 Hz), 131.1, 128.2 (d, $^4J_{C\text{-}F}$ = 3 Hz), 126.5, 115.1 (d, $^2J_{C\text{-}F}$ = 21 Hz), 85.5, 42.9, 21.1 ppm.

^{19}F NMR (282 MHz, $CDCl_3$) δ –114.8 ppm.

HRMS (ESI-TOF) Calcd for $C_{18}H_{19}FNaO_2S$ $[M+Na]^+$: 341.0987, found: 341.0989.



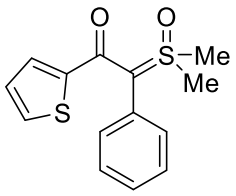
1n

2-(4-Chlorophenyl)-2-(dimethyl(oxo)-λ^6-sulfanylidene)-1-(4-(phenylethynyl)phenyl)ethan-1-one (1n) was prepared as a light brown powder according to the General Procedure A (eluent: DCM/MeOH = 50:1, 300 mg, 15% yield)

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.51 – 7.48 (m, 2H), 7.34 – 7.31 (m, 7H), 7.21 – 7.18 (m, 2H), 7.09 – 7.06 (m, 2H), 3.63 (s, 6H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 182.2, 139.5, 135.7, 133.5, 131.6, 130.9, 130.3, 128.7, 128.6, 128.44, 128.38, 124.4, 123.0, 90.8, 89.1, 86.0, 43.0 ppm.

HRMS (ESI-TOF) Calcd for $C_{24}H_{19}ClNaO_2S$ $[M+Na]^+$: 429.0692, found: 429.0689.



1o

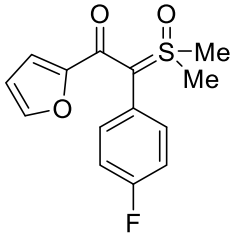
2-(Dimethyl(oxo)-λ^6-sulfanylidene)-2-phenyl-1-(thiophen-2-yl)ethan-1-one (1o) was prepared as a light brown solid according to the General Procedure A (eluent: DCM/MeOH = 50:1, 1.0 g, 76% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42 – 7.35 (m, 5H), 7.28 – 7.26 (m, 1H), 6.79 – 6.76 (m,

1H), 6.59 – 6.58 (m, 1H), 3.62 (s, 6H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 173.8, 145.9, 135.8, 131.1, 129.3, 129.0, 128.9, 128.8, 127.0, 85.5, 43.3 ppm.

HRMS (ESI-TOF) Calcd for $C_{14}H_{14}NaO_2S_2$ $[M+Na]^+$: 301.0333, found: 301.0321.



1p

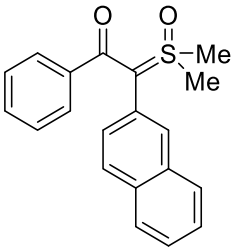
2-(Dimethyl(oxo)-λ^6-sulfanylidene)-2-(4-fluorophenyl)-1-(furan-2-yl)ethan-1-one (1p) was prepared as a light brown solid according to the General Procedure A (eluent: DCM/MeOH = 50:1, 0.9 g, 64% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33 – 7.25 (m, 3H), 7.10 – 7.03 (m, 2H), 6.23 – 6.21 (m, 1H), 5.90 – 5.88 (m, 1H), 3.62 (s, 6H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 170.6, 163.0 (d, $^1J_{C\text{-}F}$ = 247 Hz), 152.2, 143.5, 137.1 (d, $^3J_{C\text{-}F}$ = 8 Hz), 126.8 (d, $^4J_{C\text{-}F}$ = 3 Hz), 115.7 (d, $^2J_{C\text{-}F}$ = 21 Hz), 113.9, 110.9, 83.9, 43.2 ppm.

^{19}F NMR (282 MHz, $CDCl_3$) δ –113.0 ppm.

HRMS (ESI-TOF) Calcd for $C_{14}H_{13}FNaO_3S$ $[M+Na]^+$: 303.0467, found: 303.0453.



1q

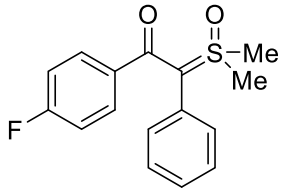
2-(Dimethyl(oxo)-λ^6-sulfanylidene)-2-(naphthalen-2-yl)-1-phenylethan-1-one (1q) was prepared as a light brown solid according to the General Procedure A (eluent: DCM/MeOH = 50:1, 630 mg, 39% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 – 7.79 (m, 1H), 7.77 – 7.71 (m, 3H), 7.49 – 7.44 (m,

4H), 7.29 – 7.27 (m, 1H), 7.24 – 7.20 (m, 1H), 7.16 – 7.12 (m, 2H), 3.71 (s, 6H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 183.3, 140.1, 133.5, 133.4, 132.6, 132.4, 129.53, 129.50, 128.7, 128.0, 127.7, 127.61, 127.56, 126.1, 125.9, 87.0, 43.2 ppm.

HRMS (ESI-TOF) Calcd for $C_{20}H_{18}NaO_2S$ $[M+Na]^+$: 345.0925, found: 345.0924.



1r

2-(Dimethyl(oxo)-λ^6-sulfanylidene)-1-(4-fluorophenyl)-2-phenylethan-1-one (1r) was prepared as a light brown solid according to the General Procedure A (eluent: DCM/MeOH = 50:1, 510 mg, 35% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.38 (m, 2H), 7.30 – 7.26 (m, 3H), 7.21 – 7.18 (m, 2H), 6.87 – 6.83 (m, 2H), 3.66 (s, 6H) ppm.

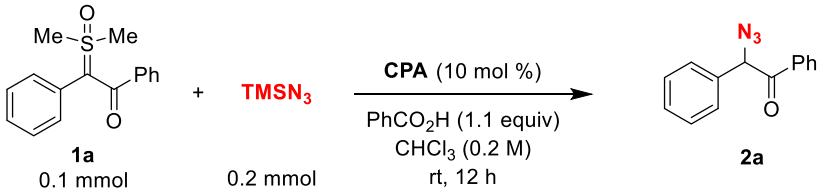
^{13}C NMR (75 MHz, $CDCl_3$) δ 181.7, 163.2 (d, $^1J_{C\text{-}F}$ = 248 Hz), 136.2 (d, $^4J_{C\text{-}F}$ = 3 Hz), 134.8, 131.9, 130.8 (d, $^3J_{C\text{-}F}$ = 9 Hz), 128.4, 127.5, 114.4 (d, $^2J_{C\text{-}F}$ = 21 Hz), 86.8, 43.0 ppm.

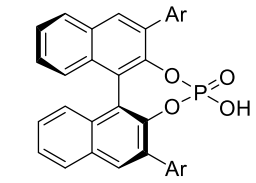
^{19}F NMR (282 MHz, $CDCl_3$) δ –111.2 ppm.

HRMS (ESI-TOF) Calcd for $C_{16}H_{15}FNaO_2S$ $[M+Na]^+$: 313.0674, found: 313.0672.

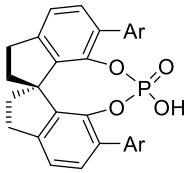
III. Catalytic Asymmetric Synthesis of Chiral α-Amino Esters

Table S1. Screening of CPAs for the H–N_3 Insertion Reaction.





Ar = 9-anthryl, **CPA1**
Ar = 9-((10-Ph)-anthracenyl), **CPA3**
Ar = TRIP, **CPA4**
Ar = 1-pyrenyl, **CPA5**
Ar = 2,6-Me_2-4-*t*Bu-C_6H_2, **CPA6**

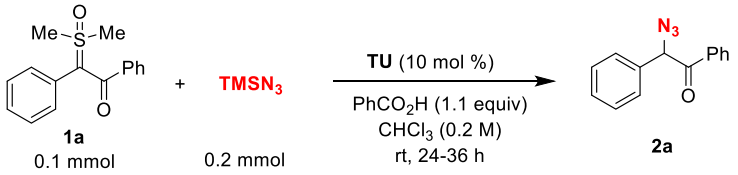


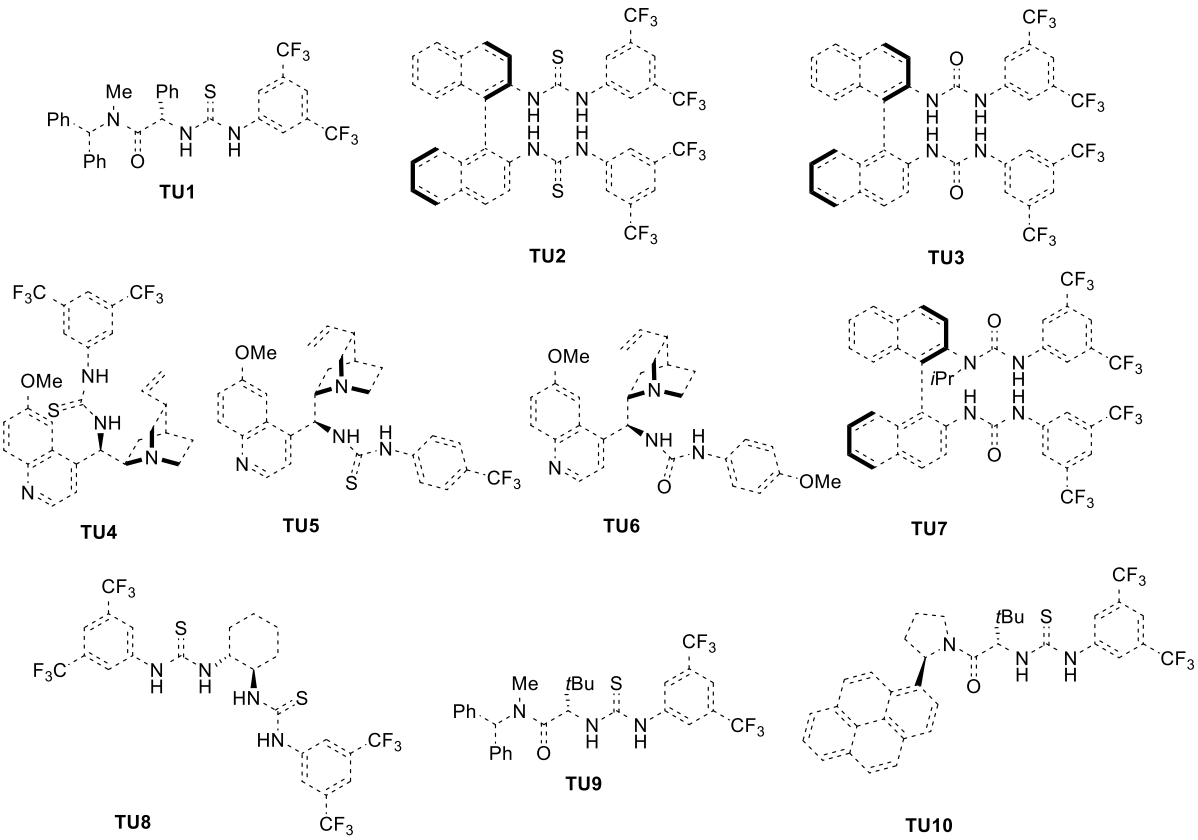
Ar = 9-anthryl, **CPA2**
Ar = 9-phenanthracenyl, **CPA7**
Ar = 9-((10-Ph)-anthracenyl), **CPA8**
Ar = 1-pyrenyl, **CPA9**
Ar = 2,4,6-Me_3-C_6H_2, **CPA10**

entry	CPA	yield (%)[a]	ee (%)[b]
1	**CPA1**	>95	0
2	**CPA2**	>95	0
3	**CPA3**	>95	0
4	**CPA4**	>95	0
5	**CPA5**	>95	0
6	**CPA6**	>95	0
7	**CPA7**	>95	0
8	**CPA8**	52	0
9	**CPA9**	>95	0
10	**CPA10**	>95	0

[a] Determined by crude ^{1}H NMR anaylsis using CH_2Br_2 as an internal standard. All the reactions described above provided clean conversion. [b] Determined by Chiral HPLC analysis.

Table S2. Screening of Chiral Hydrogen Bonding Organocatalysts.

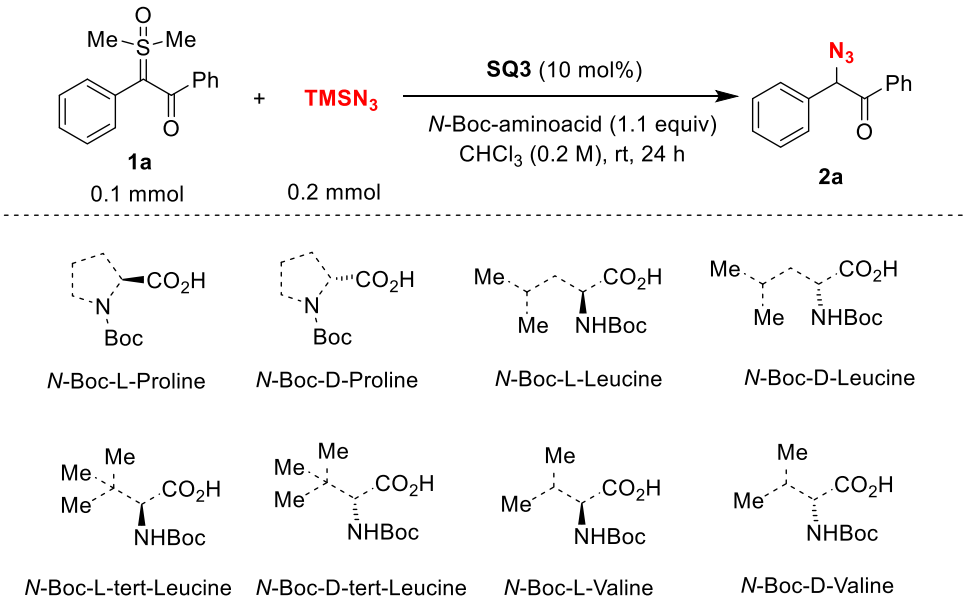




entry	TU	yield (%)[a]	ee (%)[b]
1	**TU1**	>95	0
2	**TU2**	>95	0
3	**TU3**	>95	0
4[c]	**TU4**	<20	0
5[c]	**TU5**	<20	0
6[c]	**TU6**	<20	14
7	**TU7**	>95	0
8	**TU8**	>95	0
9	**TU9**	>95	40
10	**TU10**	>95	52

[a] Determined by crude ^{1}H NMR anaylsis using CH_2Br_2 as an internal standard. [b] Determined by Chiral HPLC analysis. [c] The reaction gave a messy mixture, likely due to the incompatibility of the reaction with the basic cinchona alkaloid functionality.

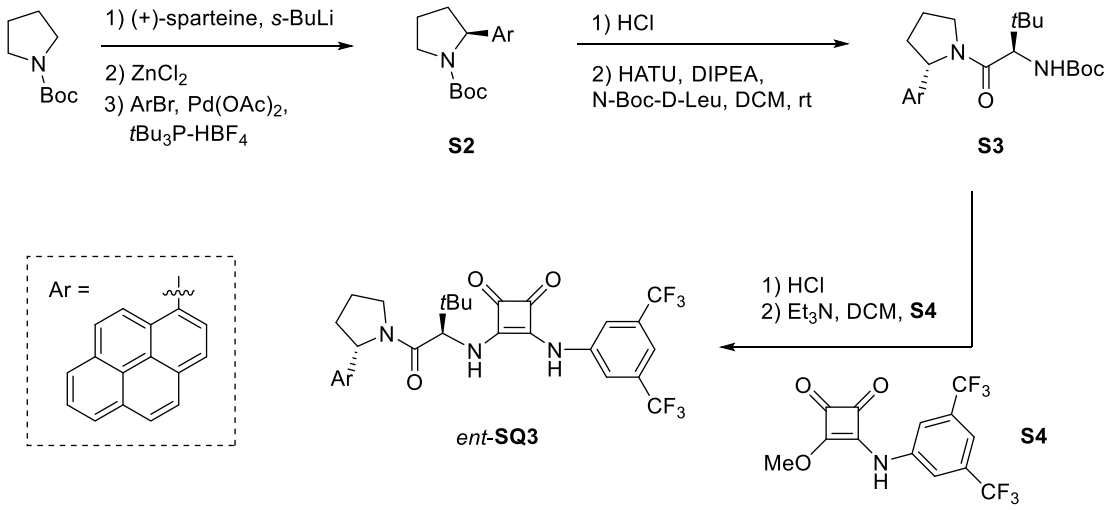
Table S3. Screening of other Chiral Proton Sources.



entry	*N*-Boc-AminoAcids	conv. (%)[a]	ee (%)[b]
1	*N*-Boc-L-Proline	>95	71
2	*N*-Boc-D-Proline	>95	71
3[c]	*N*-Boc-L-Proline	>95	71
4[c]	*N*-Boc-D-Proline	>95	71
5	*N*-Boc-L-Leucine	>95	71
6	*N*-Boc-D-Leucine	>95	71
7	*N*-Boc-L-tert-Leucine	>95	71
8	*N*-Boc-D-tert-Leucine	>95	71
9	*N*-Boc-L-Valine	>95	71
10	*N*-Boc-D-Valine	>95	71

[a] Determined by crude ^{1}H NMR analysis using CH_2Br_2 as an internal standard. [b] Determined by chiral HPLC analysis. [c] *ent*-**SQ3** was used as the catalyst.

Synthesis of *ent*-SQ3



***tert*-Butyl (*S*)-2-(pyren-1-yl)pyrrolidine-1-carboxylate (S2)** was prepared according to a modified literature procedure.[3] To a solution of *N*-Boc-pyrrolidine (2.0 g, 11.4 mmol, 1.7 equiv) and (+)-sparteine (2.7 g, 11.4 mmol, 1.7 equiv) in anhydrous methyl *tert*-butyl ether (MTBE, 24 mL) at –78 °C was added *s*-BuLi (8.8 mL, 1.3 M in *n*-hexane, 11.4 mmol, 1.7 equiv) dropwise, with the temperature kept below –68 °C. During addition, the color of the mixture gradually changed from pale yellow to orange. The resulting solution was stirred at –74 °C for 3 h. A solution of $ZnCl_2$ in THF (13.6 mL, 0.5 M, 6.8 mmol, 1.0 equiv) was slowly added to the reaction mixture with rapid stirring and the temperature kept below –68 °C. The resulting light suspension was stirred at –74 °C for 30 min before it was warmed to room temperature. The resulting homogeneous solution was stirred for 30 min at room temperature, at which point a slightly turbid solution was obtained. Then, 1-bromopyrene (2.7 g, 9.5 mmol, 1.4 equiv) was added in one portion, followed by $Pd(OAc)_2$ (102 mg, 0.46 mmol, 7 mol%) and tBu$_3$P·HBF$_4$ (166 mg, 0.58 mmol, 8 mol%). The mixture was stirred at the same temperature for 24 h, during which time zinc salts were precipitated. Then, an aqueous ammonia (0.7 mL, 25 wt%) was carefully added into the reaction mixture to

(3) (a) K. R. Campos, A. Klapars, J. H. Waldman, P. G. Dormer, C.-Y. Chen, *J. Am. Chem. Soc.*, **2006**, *128*, 3538–3539; (b) S. M. Banik, A. Levina, A. M. Hyde, E. N. Jacobsen, *Science*, **2017**, *358*, 761–764; (c) M. R. Netherton, G. C. Fu, *Org. Lett.*, **2001**, *3*, 4295–4298.

quench and facilitate filtration of the reaction mixture. The resulting suspension was stirred for an addition hour at room temperature before it was filtered through a plug of celite. The filter cake was washed with MTBE (50 mL). The combined organic solutions were washed with an aqueous solution of HCl (1 M, 50 mL) and brine sequentially, and then dried over Na_2SO_4, filtered, and concentrated. After purification by column chromatography on silica gel (eluent: *n*-hexane to EtOAc/*n*-hexane = 2:3), the desired product **S2** was obtained as a light yellow solid (1.0 g, 40% yield, 98% ee). This intermediate was obtained as a mixture of rotamers at 2:1 ratio.

^{1}H NMR (300 MHz, $CDCl_3$) was integrated based on the sum of hydrogen atoms: δ 8.29 – 8.26 (m, 1H), 8.19 – 8.08 (m, 4H), 8.04 – 8.00 (m, 3H), 7.85 – 7.83 (m, 1H), 6.06 – 5.89 (m, 1H), 3.93 – 3.67 (m, 2H), 2.62 – 2.59 (m, 1H), 2.03 – 1.95 (m, 3H), 1.51 – 1.01 (m, 9H) ppm.

$[\boldsymbol{\alpha}]_D^{25}$: –54.2 (*c* = 1.0, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK® OJ-H column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 19.7 min (major), 10.8 min (minor).

Note: The spectra data are consistent with literature report.[3b]

***tert*-Butyl ((*R*)-3,3-dimethyl-1-oxo-1-((*S*)-2-(pyren-1-yl)pyrrolidin-1-yl)butan-2-yl)carbamate (S3)**. At room temperature, pyrrolidine **S2** (1.0 g, 2.7 mmol, 1.0 equiv) was treated with a solution of HCl in 1,4-dioxane (5.4 mL, 4.0 M, 21.6 mmol, 8.0 equiv). The resulting mixture was stirred at the same temperature for 2 h, and concentrated at reduced pressure to yield a beige foam. The obtained amine hydrochloride was then dissolved in anhydrous DCM (10 mL), to which anhydrous diisopropylethylamine (DIPEA, 349 mg, 2.7 mmol, 1.0 equiv) was added in one portion. The reaction mixture was stirred at room temperature for 30 min to liberate the free amine.

To a solution of *N*-Boc-D-*tert*-Leucine (812 mg, 3.5 mmol, 1.3 equiv) and HATU (1.2 g, 3.5 mmol, 1.3 equiv) in anhydrous DCM (10 mL) was added DIPEA (1.0 g, 8.1 mmol, 3.0 equiv). The suspension was stirred at room temperature for 20 min. Then, the solution of the free amine was slowly added into the solution of the activated *N*-

Boc-D-Leucine. The reaction mixture was stirred at room temperature for 48 h before water (20 mL) was added to quench the reaction. The mixture was extracted with EtOAc (3 × 20 mL), and the combined organic layers were washed with an aqueous HCl solution (1.0 M, 20 mL), brine, and dried over Na_2SO_4, filtered, and evaporated in *vacuo*. The crude product was directly used for the next step without further purification.

3-((3,5-Bis(trifluoromethyl)phenyl)amino)-4-(((*R*)-3,3-dimethyl-1-oxo-1-((*S*)-2-(pyren-1-yl)pyrrolidin-1-yl)butan-2-yl)amino)cyclobut-3-ene-1,2-dione (*ent*-SQ3).[4] To a solution of **S3** (2.7 mmol, 1.0 equiv) in anhydrous DCM (5 mL) was added a solution of HCl in 1,4-dioxane (5.4 mL, 4.0 M, 21.6 mmol, 8.0 equiv). The reaction mixture was stirred at room temperature for 2 h. The mixture was concentrated under reduce pressure to afford the amine hydrochloride.

The residue was then dissolved in anhydrous DCM (10 mL), and treated with triethylamine (1.1 mL, 8.1 mmol, 3.0 equiv) in one portion. The mixture was stirred at room temperature for 30 min to liberate the free amine. **S4** (916 mg, 2.7 mmol, 1.0 equiv) was then added, and the reaction mixture was stirred at room temperature for 48 h. Upon completion, the volatiles were removed under reduced pressure, and the residue was purified by flash column chromatography on silica gel (eluent: *n*-hexane/EtOAc = 3:1 to 2:3) to afford the desired product as a light yellow solid (1.1 g, 58% yield over two steps).

Note: *ent*-**SQ3** was obtained as a mixture of rotamers at 7:1 ratio.

^{1}H NMR (300 MHz, DMSO-d_6) was integrated based on the sum of hydrogen atoms: δ 10.36 (br, 1H), 8.52 – 8.02 (m, 11H), 7.83 – 7.57 (m, 2H), 6.47 – 6.14 (m, 1H), 5.20 (s, 1H), 4.31 – 3.93 (m, 2H), 2.59 (m, 1H), 2.02 – 1.90 (m, 3H), 1.07 (s, 9H) ppm.

^{13}C NMR (75 MHz, DMSO-d_6, major and minor rotamer resonances) δ 185.0, 181.0, 169.6, 168.5, 163.1, 141.5, 137.2, 132.0. 131.6, 131.3, 130.6, 129.9, 127.7, 127.1, 126.9, 126.6,

(4) W. Yang, D.-M. Du, *Org. Lett.*, **2010**, *12*, 5450–5453.

125.6, 125.5, 125.1, 124.7, 124.5, 123.4, 122.8, 122.6, 121.8, 118.4, 115.2, 61.9, 58.8, 48.8, 36.2, 35.8, 34.0, 26.5, 26.2, 23.9 ppm.

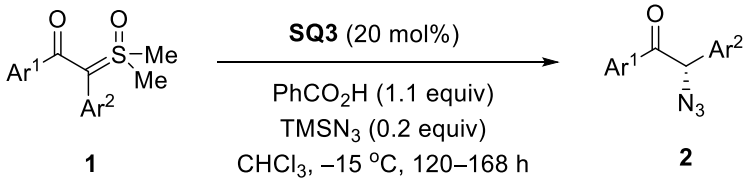
^{19}F NMR (282 MHz, DMSO-d_6, major and minor rotamer resonances) δ –61.8, –61.9 ppm.

HRMS (ESI-TOF) Calcd for $C_{38}H_{31}F_6N_3NaO_3$ [M+Na]$^+$: 714.2167, found: 714.2166.

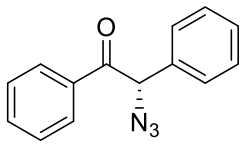
$[\boldsymbol{a}]_D^{25}$: –43.0 (c = 1.0, $CHCl_3$).

The ^{13}C NMR data are consistent with the literature report.[3b]

General Procedure B.



An oven-dried 4-mL vial equipped with a magnetic stirring bar was charged with sulfoxonium ylide **1** (0.2 mmol, 1.0 equiv), benzoic acid (0.22 mmol, 1.1 equiv), catalyst **SQ3** (27.6 mg, 0.04 mmol, 20 mol%), and $CHCl_3$ (1.0 mL). The vial was carefully sealed with a puncturable screw-cap and electric tape before it was cooled to −15 °C. The solution was stirred at the same temperature for 5 min before $TMSN_3$ (52.6 μL, 0.4 mmol, 2.0 equiv) was added by microsyringe. Then, the mixture was stirred at the same temperature and the reaction progress was monitored by TLC. Upon completion, the mixture was directly subjected to flash column chromatography on silica gel (eluent: *n*-hexane/EtOAc = 20:1) to give the desired product **2**.



2a

(*S*)-2-Azido-1,2-diphenylethan-1-one was prepared as a light yellow oil according to the General Procedure B (120 h, 39.4 mg, 83% yield, 90% ee).

$[\boldsymbol{a}]_D^{25}$: +145.1 (c = 2.0, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK® OD-

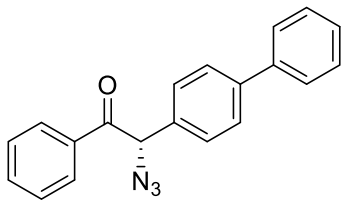
H column; 1% *i*-PrOH in *n*-hexane; 0.5 mL/min; retention times: 29.3 min (major), 45.7 min (minor).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.4 Hz, 2H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.39 – 7.35 (m, 7H), 5.73 (s, 1H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 194.4, 134.3, 133.8 (two C), 129.6, 129.4, 128.9, 128.8, 128.3, 67.9 ppm.

HRMS (ESI-TOF) Calcd for $C_{14}H_{11}N_3NaO$ $[M+Na]^+$: 260.0800, found: 260.0796.

This is a known compound, the spectra data are consistent with those in the previous report.[5]



2b

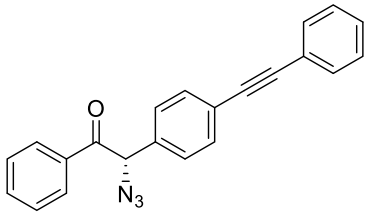
(*S*)-2-([1,1'-Biphenyl]-4-yl)-2-azido-1-phenylethan-1-one (2b) was prepared as a white solid according to the General Procedure B (120 h, 60.2 mg, 96% yield, 85% ee). $[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{25}}$: +133.0 (*c* = 2.0, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 3% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 13.3 min (major), 15.5 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 7.90 (d, *J* = 8.3 Hz, 2H), 7.56 (d, *J* = 8.0 Hz, 2H), 7.48 – 7.41 (m, 5H), 7.33 – 7.26 (m, 4H), 7.21 – 7.17 (m, 1H), 6.11 (s, 1H) ppm.

^{13}C NMR (100 MHz, acetone-d_6) δ 194.5, 141.8, 139.8, 134.6, 133.9, 133.4, 129.1, 128.94, 128.91, 128.88, 127.9, 127.8, 126.9, 66.9 ppm.

HRMS (ESI-TOF) Calcd for $C_{20}H_{15}N_3NaO$ $[M+Na]^+$: 336.1113, found: 336.1106.

(5) (a) W. Wei, H. Cui, H. Yue, D. Yang, *Green Chem.*, **2018**, *20*, 3197–3202; (b) M. I. Hussain, Y. Feng, L. Hu, Q. Deng, X. Zhang, Y. Xiong, *J. Org. Chem.*, **2018**, *83*, 7852–7859.



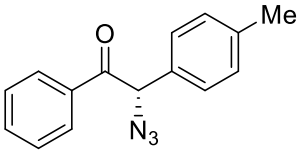
2c

(*S*)-2-Azido-1-phenyl-2-(4-(phenylethynyl)phenyl)ethan-1-one (2c) was prepared as a white solid according to the General Procedure B (120 h, 59.4 mg, 88% yield, 90% ee). $[\boldsymbol{a}]_{\boldsymbol{D}}^{\mathbf{25}}$: +119.8 (*c* = 2.0, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK® OD-H column; 3% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 16.7 min (major), 20.7 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 8.06 (d, *J* = 7.6 Hz, 2H), 7.66 – 7.62 (m, 3H), 7.57 – 7.50 (m, 6H), 7.44 – 7.43 (m, 3H), 6.32 (s, 1H) ppm.

^{13}C NMR (100 MHz, acetone-d_6) δ 194.3, 134.7, 134.5, 133.9, 132.4, 131.5, 128.9 (two C), 128.8 (two C), 128.6, 124.1, 122.8, 90.4, 88.2, 66.8 ppm.

HRMS (ESI-TOF) Calcd for $C_{22}H_{15}N_3NaO$ $[M+Na]^+$: 360.1113, found: 360.1106.



2d

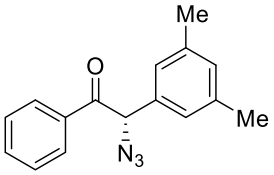
(*S*)-2-Azido-1-phenyl-2-(*p*-tolyl)ethan-1-one (2d) was prepared as a light yellow oil according to the General Procedure B (120 h, 44.7 mg, 89% yield, 88% ee).

$[\boldsymbol{a}]_{\boldsymbol{D}}^{\mathbf{25}}$: +100.5 (*c* = 2.0, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK® OD-H column; 1% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 13.1 min (major), 19.8 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 7.87 – 7.84 (m, 2H), 7.44 – 7.40 (m, 1H), 7.32 – 7.29 (m, 2H), 7.22 – 7.20 (m, 2H), 7.10 – 7.08 (m, 2H), 6.00 (s, 1H), 2.13 (s, 3H) ppm.

^{13}C NMR (100 MHz, acetone-d_6) δ 194.6, 139.2, 134.6, 133.7, 131.4, 130.1, 128.83, 128.80, 128.4, 67.0, 20.3 ppm.

HRMS (ESI-TOF) Calcd for $C_{15}H_{13}N_3NaO$ $[M+Na]^+$: 274.0956, found: 274.0951.



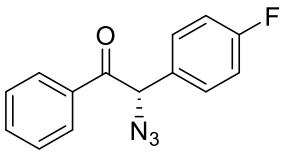
2e

(*S*)-2-Azido-2-(3,5-dimethylphenyl)-1-phenylethan-1-one (2e) was prepared as a colorless oil according to the General Procedure B (120 h, 48.8 mg, 92% yield, 85% ee). $[\boldsymbol{a}]_D^{25}$: +172.5 (*c* = 2.0, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 2% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 9.1 min (major), 11.9 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 7.88 – 7.86 (m, 2H), 7.46 – 7.42 (m, 1H), 7.34 – 7.30 (m, 2H), 6.94 (s, 2H), 6.88 (s, 1H), 5.94 (s, 1H), 2.13 (s, 6H) ppm.

^{13}C NMR (100 MHz, acetone-d_6) δ 194.5, 139.0, 134.6, 134.2, 133.7, 130.8, 128.83, 128.79, 126.1, 67.2, 20.4 ppm.

HRMS (ESI-TOF) Calcd for $C_{16}H_{15}N_3NaO$ $[M+Na]^+$: 288.1113, found: 288.1109.



2f

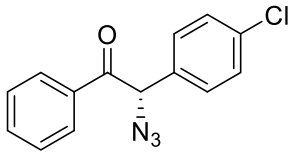
(*S*)-2-Azido-2-(4-fluorophenyl)-1-phenylethan-1-one (2f) was prepared as a colorless oil according to the General Procedure B (168 h, 37.3 mg, 73% yield, 94% ee). $[\boldsymbol{a}]_D^{25}$: +119.9 (*c* = 2.0, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK® OD-H column; 1% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 15.6 min (major), 23.2 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 7.88 – 7.86 (m, 2H), 7.47 – 7.31 (m, 5H), 7.09 – 7.04 (m, 2H), 6.13 (s, 1H) ppm.

^{13}C NMR (100 MHz, acetone-d_6) δ 194.4, 163.0 (d, $^1J_{C\text{-}F}$ = 246 Hz), 134.5, 133.9, 130.723 (d, $^3J_{C\text{-}F}$ = 8 Hz), 130.716, 128.9 (2C), 116.3 (d, $^2J_{C\text{-}F}$ = 22 Hz), 66.3 ppm.

^{19}F NMR (376 MHz, acetone-d_6) δ –113.5 ppm.

HRMS (ESI-TOF) Calcd for $C_{14}H_{10}FN_3NaO$ $[M+Na]^+$: 278.0706, found: 278.0702.



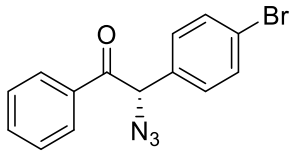
2g

(*S*)-2-Azido-2-(4-chlorophenyl)-1-phenylethan-1-one (2g) was prepared as a colorless oil according to the General Procedure B (168 h, 40.2 mg, 74% yield, 92% ee). $[\boldsymbol{a}]_D^{25}$: +83.2 (*c* = 1.0, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK® OD-H column; 1% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 16.4 min (major), 23.9 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 8.05 (d, *J* = 7.4 Hz, 2H), 7.67 – 7.63 (m, 1H), 7.56 – 7.51 (m, 6H), 6.33 (s, 1H) ppm.

^{13}C NMR (100 MHz, acetone-d_6) δ 194.3, 134.7, 134.4, 133.9, 133.4, 130.2, 129.5, 128.9 (two C), 66.3 ppm.

HRMS (ESI-TOF) Calcd for $C_{14}H_{10}ClNO$ $[M-N_3]^+$: 229.0415, found: 229.0417.



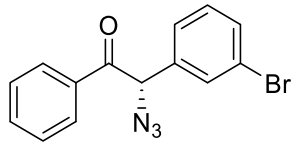
2h

(*S*)-2-Azido-2-(4-bromophenyl)-1-phenylethan-1-one (2h) was prepared as a colorless oil according to the General Procedure B (168 h, 35.4 mg, 56% yield, 91% ee). $[\boldsymbol{a}]_D^{25}$: +90.5 (*c* = 1.0, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK® OD-H column; 1% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 16.5 min (major), 24.4 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 8.05 – 8.03 (m, 2H), 7.67 – 7.62 (m, 3H), 7.53 – 7.46 (m, 4H), 6.30 (s, 1H) ppm.

^{13}C NMR (100 MHz, acetone-d_6) δ 194.2, 134.4, 133.94, 133.90, 132.5, 130.5, 128.9 (2C), 123.0, 66.4 ppm.

HRMS (ESI-TOF) Calcd for $C_{14}H_{10}BrO$ $[M\text{-}N_3]^+$: 272.9910, found: 272.9911.



2i

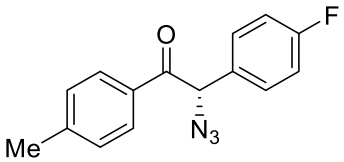
(*S*)-2-Azido-2-(3-bromophenyl)-1-phenylethan-1-one (2i) was prepared as a colorless oil according to the General Procedure B (168 h, 31.6 mg, 50% yield, 84% ee).

$[\boldsymbol{a}]_D^{25}$: +68.9 (*c* = 1.0, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK® OD-H column; 1% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 16.8 min (major), 24.8 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 7.92 – 7.89 (m, 2H), 7.59 – 7.58 (m, 1H), 7.51 – 7.44 (m, 2H), 7.39 – 7.25 (m, 4H), 6.17 (s, 1H) ppm.

^{13}C NMR (100 MHz, acetone-d_6) δ 194.1, 137.0, 134.4, 134.0, 132.3, 131.4, 131.3, 128.94, 128.91, 127.2, 122.7, 66.3 ppm.

HRMS (ESI-TOF) Calcd for $C_{14}H_{10}BrO$ $[M\text{-}N_3]^+$: 272.9910, found: 274.9892.



2j

(*S*)-2-Azido-2-(4-fluorophenyl)-1-(*p*-tolyl)ethan-1-one (2j) was prepared as a colorless oil according to the General Procedure B (168 h, 36.1 mg, 67% yield, 96% ee).

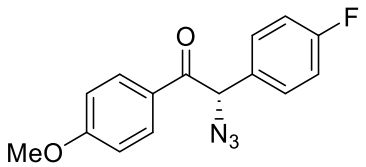
$[\boldsymbol{a}]_D^{25}$: +97.8 (*c* = 1.0, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK® OD-H column; 3% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 8.6 min (major), 10.6 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 7.78 – 7.76 (m, 2H), 7.41 – 7.38 (m, 2H), 7.15 – 7.05 (m, 4H), 6.08 (s, 1H), 2.20 (s, 3H) ppm.

^{13}C NMR (100 MHz, acetone-d_6) δ 194.0, 163.0 (d, $^{1}J_{C\text{-}F}$ = 245 Hz), 144.9, 131.9, 130.9 (d, $^{4}J_{C\text{-}F}$ = 3 Hz), 130.7 (d, $^{3}J_{C\text{-}F}$ = 9 Hz), 129.5, 129.0, 116.2 (d, $^{2}J_{C\text{-}F}$ = 22 Hz), 66.1, 20.7 ppm.

^{19}F NMR (376 MHz, acetone-d_6) δ –113.7 ppm.

HRMS (ESI-TOF) Calcd for $C_{15}H_{12}FN_3NaO$ [M+Na]$^+$: 292.0862, found: 292.0859.



2k

(*S*)-2-Azido-2-(4-fluorophenyl)-1-(4-methoxyphenyl)ethan-1-one (2k) was prepared as a colorless oil according to the General Procedure B (168 h, 47.4 mg, 83% yield, 94% ee).

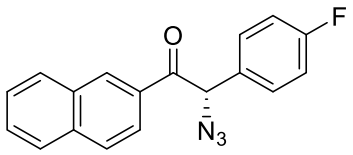
$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{25}}$: +107.9 ($c$ = 2.0, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 10% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 10.4 min (major), 13.6 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 7.87 – 7.83 (m, 2H), 7.41 – 7.38 (m, 2H), 7.08 – 7.04 (m, 2H), 6.85 – 6.81 (m, 2H), 6.02 (s, 1H), 3.69 (s, 3H) ppm.

^{13}C NMR (100 MHz, acetone-d_6) δ 192.8, 164.2, 163.0 (d, $^{1}J_{C\text{-}F}$ = 245 Hz), 131.3, 131.2 (d, $^{4}J_{C\text{-}F}$ = 3 Hz), 130.6 (d, $^{3}J_{C\text{-}F}$ = 8 Hz), 127.1, 116.2 (d, $^{2}J_{C\text{-}F}$ = 22 Hz), 114.1, 65.8, 55.2 ppm.

^{19}F NMR (376 MHz, acetone-d_6) δ –113.7 ppm.

HRMS (ESI-TOF) Calcd for $C_{15}H_{12}FN_3NaO_2$ [M+Na]$^+$: 308.0811, found: 308.0809.



2l

(*S*)-2-Azido-2-(4-fluorophenyl)-1-(naphthalen-2-yl)ethan-1-one (2l) was prepared as a colorless oil according to the General Procedure B (168 h, 53.1 mg, 87% yield, 96% ee).

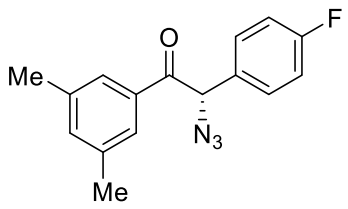
$[\boldsymbol{a}]_{\boldsymbol{D}}^{\mathbf{25}}$: +100.6 (*c* = 1.5, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 3% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 12.3 min (major), 15.9 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 7.79 (s, 1H), 7.14 – 7.11 (m, 2H), 7.07 – 7.01 (m, 2H), 6.76 – 6.66 (m, 4H), 6.33 – 6.28 (m, 2H), 5.59 (s, 1H) ppm.

^{13}C NMR (100 MHz, acetone-d_6) δ 194.6, 163.0 (d, $^1J_{C\text{-}F}$ = 246 Hz), 135.7, 132.4, 131.7, 131.2, 130.84, 130.75 (d, $^3J_{C\text{-}F}$ = 9 Hz), 129.7, 129.2, 128.8, 127.8, 127.2, 123.9, 116.3 (d, $^2J_{C\text{-}F}$ = 22 Hz), 66.3 ppm.

^{19}F NMR (376 MHz, acetone-d_6) δ –113.4 ppm.

HRMS (ESI-TOF) Calcd for $C_{18}H_{12}FN_3NaO$ $[M+Na]^+$: 328.0862, found: 328.0858.



2m

(*S*)-2-azido-1-(3,5-dimethylphenyl)-2-(4-fluorophenyl)ethan-1-one (2m) was prepared as a colorless oil according to the General Procedure B (168 h, 52.7 mg, 79% yield, 91% ee).

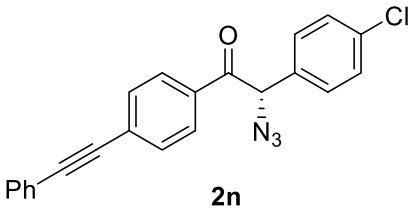
$[\boldsymbol{a}]_{\boldsymbol{D}}^{\mathbf{25}}$: +164.9 (*c* = 1.0, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK® OD-H column; 1% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 13.0 min (major), 23.6 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 7.67 – 7.66 (m, 2H), 7.59 – 7.54 (m, 2H), 7.25 – 7.21 (m, 3H), 6.27 (s, 1H), 2.32 (s, 6H) ppm.

^{13}C NMR (100 MHz, acetone-d_6) δ 194.7, 163.0 (d, $^1J_{C\text{-}F}$ = 246 Hz), 138.6, 135.4, 134.7, 130.9 (d, $^4J_{C\text{-}F}$ = 3 Hz), 130.7 (d, $^3J_{C\text{-}F}$ = 9 Hz), 126.6, 116.2 (d, $^2J_{C\text{-}F}$ = 22 Hz), 66.1, 20.2 ppm.

^{19}F NMR (282 MHz, acetone-d_6) δ –113.6 ppm.

HRMS (ESI-TOF) Calcd for $C_{16}H_{14}FO$ $[M\text{-}N_3]^+$: 241.1023, found: 241.1026.



2n

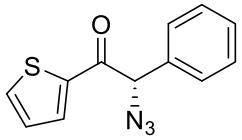
(*S*)-2-Azido-2-(4-chlorophenyl)-1-(4-(phenylethynyl)phenyl)ethan-1-one (2n) was prepared as a colorless oil according to the General Procedure B (168 h, 40.2 mg, 54% yield, 87% ee).

$[\boldsymbol{a}]_{\boldsymbol{D}}^{\mathbf{25}}$: +80.9 (*c* = 1.0, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 1% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 16.7 min (major), 18.2 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 8.07 – 8.05 (m, 2H), 7.66 – 7.64 (m, 2H), 7.59 – 7.49 (m, 6H), 7.46 – 7.43 (m, 3H), 6.33 (s, 1H) ppm.

^{13}C NMR (100 MHz, acetone-d_6) δ 193.5, 134.8, 133.7, 133.3, 131.7, 131.6, 130.3, 130.0, 129.2, 129.1, 128.7, 128.6, 122.3, 92.9, 88.1, 66.4 ppm.

HRMS (ESI-TOF) Calcd for $C_{22}H_{14}ClO$ $[M\text{-}N_3]^+$: 329.0728, found: 329.0727.



2o

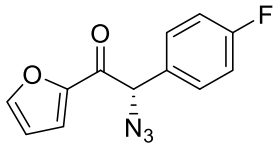
(S)-2-Azido-2-phenyl-1-(thiophen-2-yl)ethan-1-one (2o) was prepared as a colorless oil according to the General Procedure B (168 h, 39.9 mg, 82% yield, 88% ee).

$[\boldsymbol{a}]_{\boldsymbol{D}}^{\mathbf{25}}$: +140.6 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® OD-H column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 11.2 min (major), 13.7 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 7.81 – 7.78 (m, 2H), 7.41 – 7.39 (m, 2H), 7.35 – 7.26 (m, 3H), 7.04 – 7.02 (m, 1H), 5.92 (s, 1H) ppm.

^{13}C NMR (100 MHz, acetone-d_6) δ 187.5, 141.0, 135.7, 134.8, 134.3, 129.4, 129.3, 128.7, 128.3 67.5 ppm.

HRMS (ESI-TOF) Calcd for $C_{12}H_9OS$ $[M\text{-}N_3]^+$: 201.0369, found: 201.0374.



2p

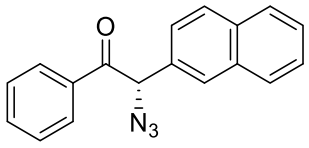
(*S*)-2-Azido-2-(4-fluorophenyl)-1-(furan-2-yl)ethan-1-one (2p) was prepared as a colorless oil according to the General Procedure B (168 h, 25.5 mg, 52% yield, 89% ee). $[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{25}}$: +77.6 (*c* = 0.5, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK® OD-H column; 3% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 9.5 min (major), 11.3 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 7.91 – 7.90 (m, 1H), 7.61 – 7.58 (m, 2H), 7.51 (d, J = 6.4 Hz, 1H), 7.29 – 7.24 (m, 2H), 6.71 – 6.69 (m, 1H), 6.01 (s, 1H) ppm.

^{13}C NMR (100 MHz, acetone-d_6) δ 182.5, 163.1 (d, $^1J_{C\text{-}F}$ = 245 Hz), 150.2, 148.4, 130.7 (d, $^4J_{C\text{-}F}$ = 3 Hz), 130.6 (d, $^3J_{C\text{-}F}$ = 9 Hz), 120.1, 116.1 (d, $^2J_{C\text{-}F}$ = 22 Hz), 112.7, 65.9 ppm.

^{19}F NMR (282 MHz, acetone-d_6) δ –113.7 ppm.

HRMS (ESI-TOF) Calcd for $C_{12}H_8FO_2$ $[M\text{-}N_3]^+$: 203.0503, found: 203.0506.



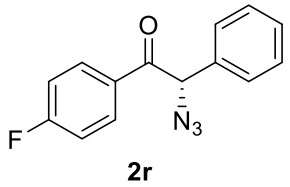
2q

(*S*)-2-Azido-2-(naphthalen-2-yl)-1-phenylethan-1-one (2q) was prepared as a colorless oil according to the General Procedure B (120 h, 43.7 mg, 76% yield, 77% ee). $[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{25}}$: +16.3 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 3% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 12.2 min (major), 15.5 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 8.09 – 8.07 (m, 2H), 8.03 – 8.00 (m, 2H), 7.96 – 7.91 (m, 2H), 7.65 – 7.63 (m, 1H), 7.58 – 7.52 (m, 3H), 7.47 – 7.44 (m, 2H), 6.42 (s, 1H) ppm.

^{13}C NMR (100 MHz, acetone-d_6) δ 194.5, 134.6, 133.8, 133.43, 133.42, 132.0, 129.5, 128.9, 128.8, 128.2, 128.0, 127.8, 127.0, 126.8, 125.7, 67.4 ppm.

HRMS (ESI-TOF) Calcd for $C_{18}H_{13}N_3NaO$ $[M+Na]^+$: 310.0956, found: 310.0954.



2r

(*S*)-2-Azido-1-(4-fluorophenyl)-2-phenylethan-1-one (2r) was prepared as a colorless oil according to the General Procedure B (168 h, 23.5 mg, 46% yield, 67% ee). $[\boldsymbol{a}]_{\boldsymbol{D}}^{\mathbf{25}}$: +58.3 (*c* = 1.0, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK® OD-H column; 3% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 9.8 min (major), 11.4 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 8.13 – 8.08 (m, 2H), 7.50 – 7.39 (m, 5H), 7.26 – 7.21 (m, 2H), 6.21 (s, 1H) ppm.

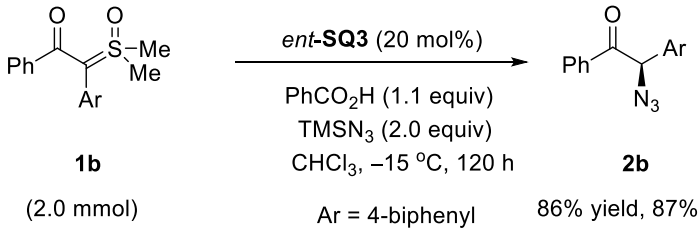
^{13}C NMR (100 MHz, acetone-d_6) δ 193.1, 165.8 (d, $^1J_{C\text{-}F}$ = 253 Hz), 134.3, 131.9 (d, $^3J_{C\text{-}F}$ = 9 Hz), 131.2 (d, $^4J_{C\text{-}F}$ = 3 Hz), 129.5, 129.3, 128.5, 115.8 (d, $^2J_{C\text{-}F}$ = 22 Hz), 67.2 ppm.

^{19}F NMR (376 MHz, acetone-d_6) δ –105.8 ppm.

HRMS (ESI-TOF) Calcd for $C_{14}H_{10}FO$ $[M\text{-}N_3]^+$: 213.0710, found: 213.0713.

IV. Larger-Scale Reaction and Product Transformations

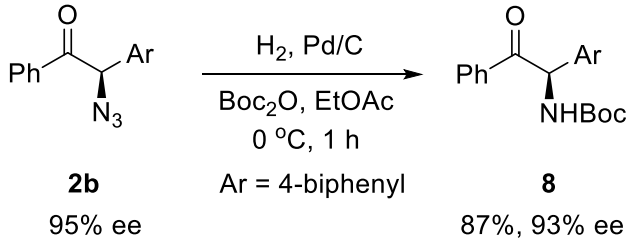
Larger-scale synthesis of (*R*)-2b.



The sulfoxonium ylide **1b** (697 mg, 2.0 mmol, 1.0 equiv), benzoic acid (269 mg, 2.2 mmol, 1.1 equiv), catalyst *ent*-**SQ3** (276 mg, 0.4 mmol, 20 mol %), and $CHCl_3$ (10 mL) were added to a 25-mL flask equipped with a magnetic stir bar. The flask was carefully sealed with a rubber stopper and cooled to –15 °C. The resulted brown solution was stirred at the same temperature for 10 min followed by slow addition of $TMSN_3$ (526 μL, 4.0 mmol, 2.0 equiv) by microsyringe. The mixture was stirred at the same temperature and the reaction progress was monitored by TLC. Upon completion (120 h), it was directly subjected to flash column chromatography on silica gel (eluent: *n*-hexane/EtOAc = 20:1) to afford the desired product (*R*)-**2b** as a colorless solid (539 mg, 86% yield, 87% ee). Moreover, the catalyst *ent*-**SQ3** was recovered in 90% yield (eluent: *n*-hexane/EtOAc = 3:1 to 2:3).

Note: the ACS grade $CHCl_3$ was used for this reaction.

Synthetic transformations of (*R*)-2b.



***tert*-Butyl (*R*)-(1-([1,1'-biphenyl]-4-yl)-2-oxo-2-phenylethyl)carbamate 8**. To a 25 mL round bottomed flask were added (*R*)-**2b** (62 mg, 0.2 mmol, 95% ee after re-crystallization), Pd/C (10% on charcoal wetted with *ca.* 55% water, 12.4 mg, 20 wt %), and EtOAc (2.0 mL). The mixture was degassed three times using vacuum pump

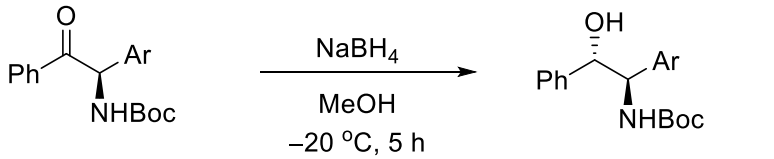
followed by backfilling with N_2. Then, Boc_2O (56 mL, 0.24 mmol, 1.2 equiv) was added into the reaction mixture via syringe. The resulted suspension was stirred at 0 °C for 10 min, and the reaction atmosphere was changed to H_2 (with balloon) and stirred for 1 h. Next, the mixture was filtered through a pad of celite, and the filter cake was washed with EtOAc (10 mL). The combined filtrates was concentrated under reduced pressure to afford a colorless residue, which was directly purified by flash column chromatography on silica gel (eluent: *n*-hexane/EtOAc = 20:1 to 10:1) to get the desired product as a colorless solid (67.4 mg, 87% yield, 93% ee).

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{25}}$: –275.3 (*c* = 1.0, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK® IC column; 5% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 11.2 min (major), 19.3 min (minor).

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.01 – 7.99 (m, 2H), 7.54 – 7.51 (m, 5H), 7.45 – 7.38 (m, 6H), 7.35 – 7.29 (m, 1H), 6.33 (d, *J* = 7.5 Hz, 1H), 6.08 (d, *J* = 7.5 Hz, 1H), 1.45 (s, 9H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 196.1, 155.0, 141.1, 140.3, 136.5, 134.5, 133.7, 129.1, 128.8, 128.7, 128.5, 127.9, 127.5, 127.0, 80.0, 59.4, 28.4 ppm.

HRMS (ESI-TOF) Calcd for $C_{25}H_{25}NNaO_3$ $[M+Na]^+$: 410.1732, found: 410.1729.



8 93% ee

9 78%, 91% ee, dr >20:1

***tert*-Butyl ((1*R*,2*S*)-1-([1,1'-biphenyl]-4-yl)-2-hydroxy-2-phenylethyl)carbamate (9).** Under N_2 at –20 °C, to a solution of the chiral α-aminoketone **8** (0.2 mmol, 77.5 mg, 93% ee) in anhydrous MeOH (2.0 mL) was added $NaBH_4$ (0.6 mmol, 22.7 mg, 3.0 equiv) in one portion. The resulted suspension was stirred at the same temperature until full conversion (~5 h) of the aminoketone **8**. Then, the reaction mixture was carefully quenched by slow addition of water (5.0 mL) and extracted with EtOAc (10 mL×3). The combined organic layers were washed with saturated aqueous NaCl solution (5

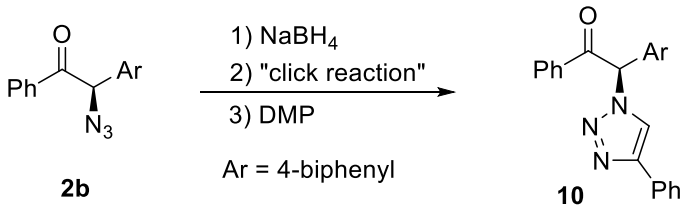
mL), and dried over anhydrous Na_2SO_4. After a filtration, the filtrate was concentrated to afford the crude product, and the d.r. value was determined by crude ^1H NMR analysis. The crude product was further purified by column chromatography on silica gel to afford the desired 1,2-aminoalcohol product **9** as a colorless solid (60.8 mg, 78% yield, 91% ee).

$[\boldsymbol{a}]_{\boldsymbol{D}}^{\mathbf{25}}$: +57.1 (*c* = 1.0, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 15% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 17.2 min (major), 10.0 min (minor).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.58 – 7.55 (m, 2H), 7.48 – 7.40 (m, 4H), 7.36 – 7.31 (m, 1H), 7.26 – 7.23 (m, 3H), 7.10 – 7.08 (m, 4H), 5.38 – 5.35 (m, 1H), 5.07 – 5.02 (m, 2H), 1.41 (s, 9H), 1.26 (s, 1H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 155.7, 140.6, 140.4, 139.9, 136.7, 128.8, 128.2, 128.1, 127.8, 127.3, 127.0, 126.8, 126.6, 80.0, 60.3, 29.7, 28.4 ppm.

HRMS (ESI-TOF) Calcd for $C_{25}H_{27}NNaO_3$ $[M+Na]^+$: 412.1889, found: 412.1888.



(*R*)-2-([1,1'-biphenyl]-4-yl)-1-phenyl-2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethan-1-one (10). To a 25 mL single-neck round bottomed flask were added (*R*)-**2b** (62 mg, 0.2 mmol, 87% ee) and MeOH (1.0 mL). The resulted suspension was cooled to 0 °C. Then, $NaBH_4$ (9.1 mg, 0.24 mmol, 1.2 equiv) was added in one portion. The reaction mixture was stirred at the same temperature until the full conversion of **2b**. Upon completion (1.0 h), a few drops of HCl (1 M) were added to quench the reaction, and the mixture was extracted with Et_2O (3×10 mL). The combined organic layers were washed with brine (10 mL), dried over anhydrous Na_2O_4, filtered, and concentrated *in vacuo* to give the crude β-azido alcohol, which was directly used for the next step without further

purification.

Under N_2, the crude β-azido alcohol (0.2 mmol), $CuSO_4 \cdot 5H_2O$ (10.0 mg, 0.04 mmol, 20 mol %), sodium ascorbate (16.0 mg, 0.08 mmol, 0.4 equiv), *t*BuOH (1.6 mL), and H_2O (0.8 mL) were added into a 10 mL vial. Under vigorous stirring, phenylacetylene (24.4 mg, 0.24 mmol, 1.2 equiv) was added. During which time the color of the reaction mixture was turned to yellow. The reaction mixture was stirred at 40 °C for 24 h, then diluted with DCM (10 mL), filtered through a short pad of celite. The filter cake was washed with DCM (10 mL), and the combined organic layers were concentrated *in vacuo* to give the crude β-hydroxyl triazole, which was directly used for the next step without further purification.

The crude β-hydroxyl triazole (0.2 mmol) was dissolved in anhydrous DCM (2.0 mL), and the resulted mixture was cooled to 0 °C. Then, Dess–Martin periodinane (127 mg, 0.3 mmol, 1.5 equiv) was added. The reaction mixture was stirred at the same temperature until full conversion of β-hydroxyl triazole. Upon completion (~3 h), an aqueous solution of $NaHCO_3$ (10 mL, 1.0 M) was added to quench the reaction. Then, the reaction mixture was extracted with DCM (3×5 mL). The combined organic layers were washed with brine (10 mL), dried over Na_2SO_4, filtered, and concentrated *in vacuo* to give the crude product. The crude product was then purified by flash column chromatography on silica gel (eluent: *n*-hexane/EA = 5:1 to 3:1) to give the desired product **9** as a colorless solid (58.2 mg, 70% yield over three steps, 86% ee).

$[\boldsymbol{\alpha}]_{\boldsymbol{D}}^{\mathbf{25}}$: –59.1 (*c* = 1.0, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK® AD-H column; 20% *i*-PrOH in *n*-hexane; 1.0 mL/min; retention times: 36.1 min (major), 49.9 min (minor).

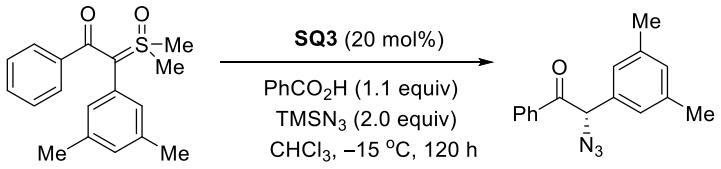
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 – 8.01 (m, 2H), 7.97 (s, 1H), 7.85 – 7.82 (m, 2H), 7.66 – 7.62 (m, 3H), 7.60 – 7.53 (m, 5H), 7.50 – 7.27 (m, 8H) ppm.

^{13}C NMR (75 MHz, $CDCl_3$) δ 191.9, 147.9, 142.9, 139.7, 134.4, 134.1, 132.3, 130.6, 129.21, 129.15, 129.1, 129.0, 128.8, 128.6, 128.1, 128.0, 127.1, 125.8, 120.6, 68.1 ppm.

HRMS (CI+) Calcd for $C_{28}H_{21}N_3NaO$ $[M+Na]^+$: 438.1582, found: 438.1577.

V. Mechanistic Studies

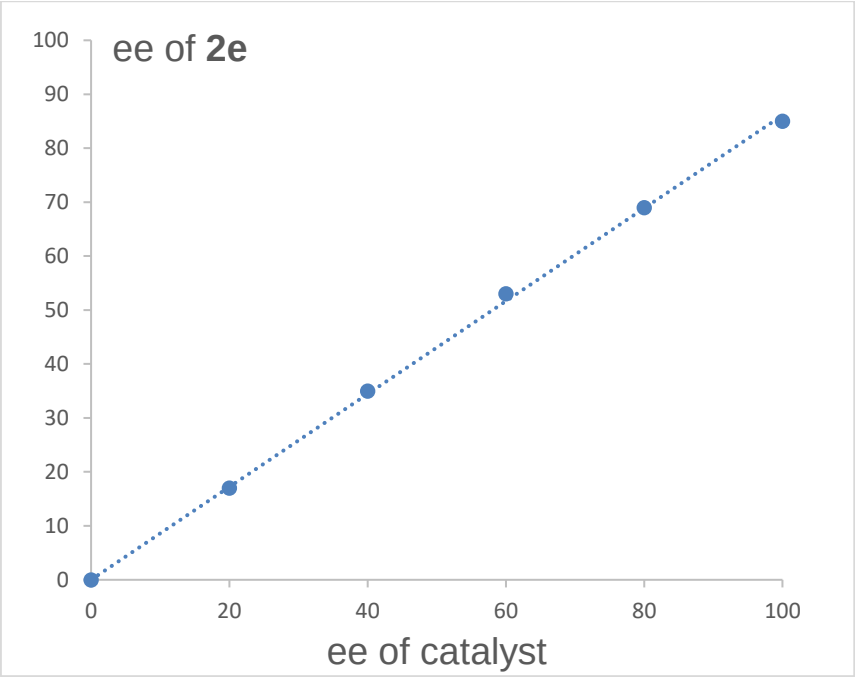
(1) Non-linear effects



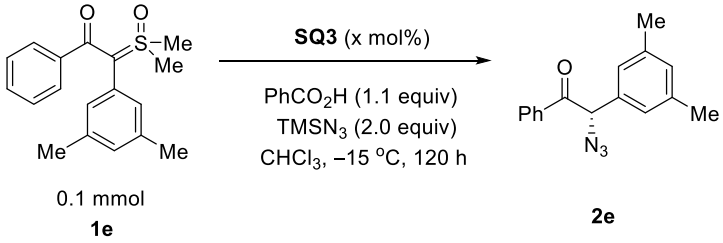
0.1 mmol
1e

2e

entry	ee of **SQ3** (%)	ee of **2e** (%)
1	>99	85
2	80	69
3	60	53
4	40	35
5	20	17
6	0	0



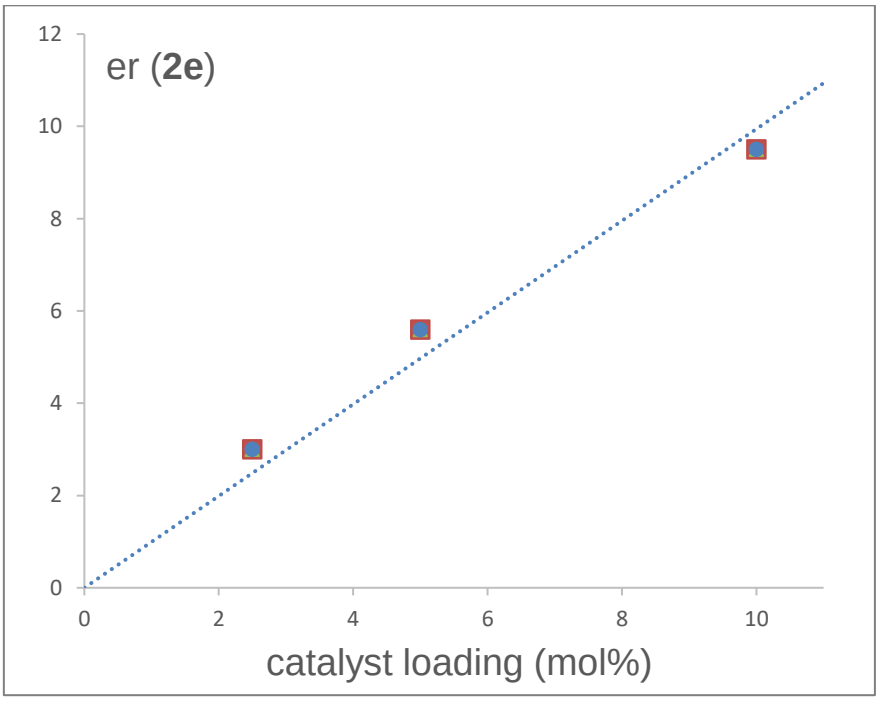
(2) Enantiomeric excess as a function of catalyst loading



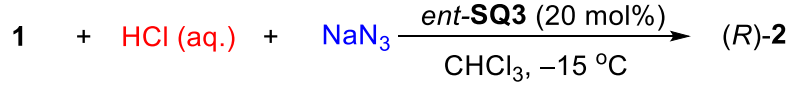
0.1 mmol
1e

2e

entry	x	er of **2e**
1	10	9.5
2	5	5.6
3	2.5	3



(3) The general procedure with HCl and NaN_3 as the HN_3 source

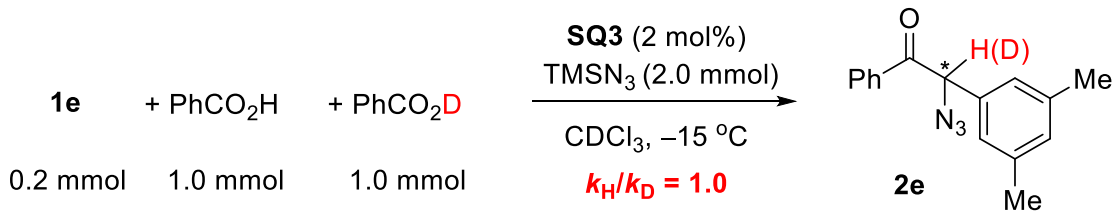


A 4-mL vial equipped with a magnetic stir bar was charged with the sulfoxonium ylide **1** (0.10 mmol, 1.0 equiv), NaN_3 (7.15 mg, 0.11 mmol, 1.1 equiv), *ent*-**SQ3** (13.8 mg, 0.02 mmol, 20 mol%), and $CHCl_3$ (0.5 mL). The vial was carefully sealed with a

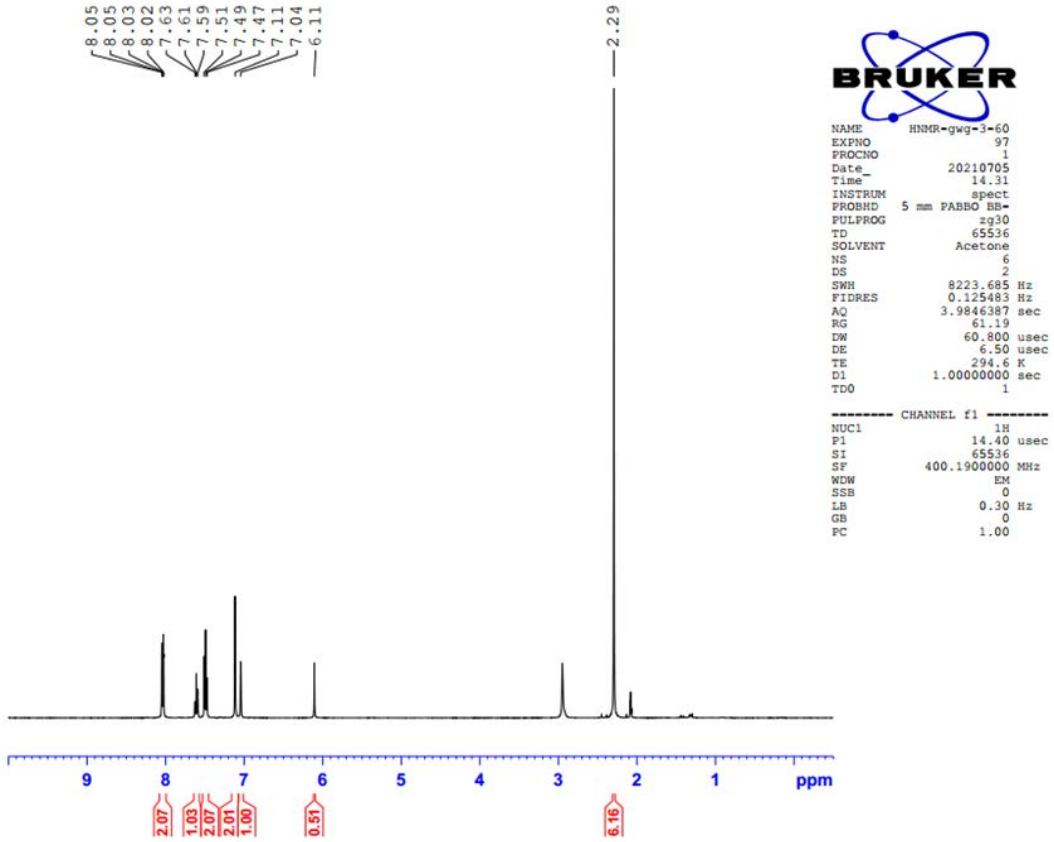
puncturable screw-cap and electrical tape and then cooled to –15 °C. After stirring for 5 min, HCl (27.5 μL, 4.0 M aqueous solution, 0.11 mmol, 1.1 equiv) was injected into the vial by syringe. The mixture was stirred at –15 °C for the indicated time, and then the reaction mixture was directly subjected to flash column chromatography on silica gel (eluent: *n*-hexane/ethyl acetate = 10:1 →5:1) to give the desired product. The results were almost same as those obtained by the standard protocol with $PhCO_2H$ and $TMSN_3$ as the HN_3 source.

entry	(*R*)-**2**	t/h	yield (%)	ee (%)
1	**2a**	120	72	90
2	**2e**	120	79	85
3	**2f**	168	60	94
4	**2p**	168	69	88

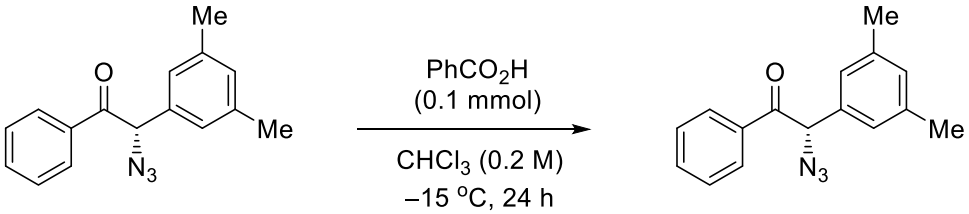
(4) Kinetic isotope effect (KIE)



At room temperature, to an oven-dried 4-mL vial were added sulfoxonium ylide **1e** (0.2 mmol, 60.1 mg, 1.0 equiv), $PhCO_2H$ (611 mg, 1.0 mmol, 5.0 equiv), $PhCO_2D$ (616 mg, 1.0 mmol, 5.0 equiv), and a solution of **SQ3** (27.6 mg, 2 mol%) in $CDCl_3$ (1.0 mL). The vial was sealed with a puncturable screw cap and cooled down to –15 °C. Then, $TMSN_3$ (263 μL, 2.0 mmol, 5.0 equiv) was injected into the vial. The reaction mixture was stirred at the same temperature until full conversion of **1e** (120 h). The mixture was directly subjected to flash column chromatography on silica gel to give the product. ^1H NMR analysis indicated 49% D-incorporation at the α-position in product. The NMR spectrum is shown below.



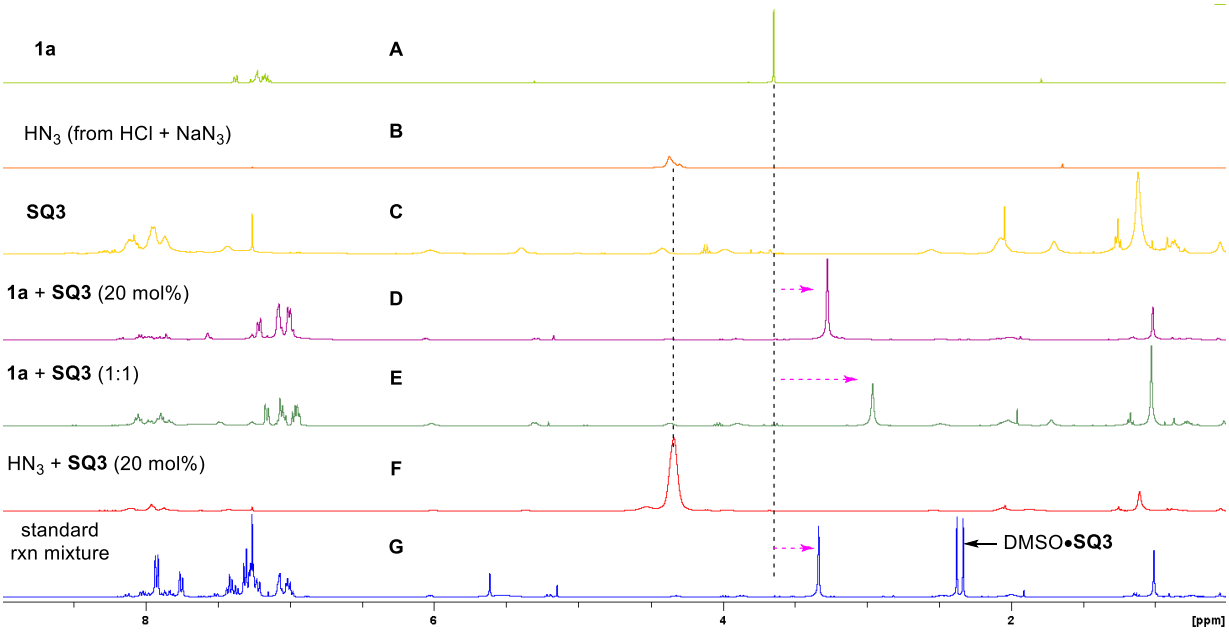
The stability of **2e** has been checked at –15 °C in the presence of benzoic acid. The enantiopurity of **2e** remained intact, indicating no H/D scrambling.



2e
85% ee, 0.1 mmol

2e
85% ee

(5) NMR study to investigate the interactions between substrate and catalyst



A: **1a** (0.1 mmol) in $CDCl_3$ (0.5 mL)

B: HN_3 (0.1 mmol) in $CDCl_3$ (0.5 mL) by mixing HCl (aq.) and NaN_3

C: **SQ3** (0.02 mmol) in $CDCl_3$ (0.5 mL)

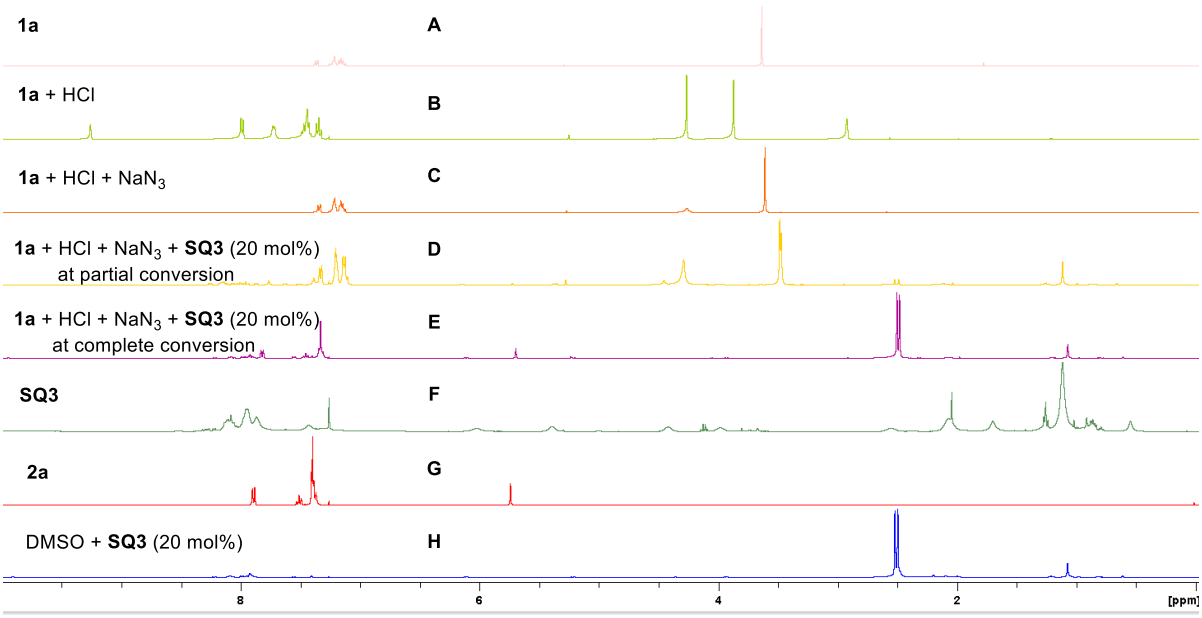
D: **1a** (0.1 mmol) and **SQ3** (0.02 mmol) in $CDCl_3$ (0.5 mL)

E: **1a** (0.02 mmol) and **SQ3** (0.02 mmol) in $CDCl_3$ (0.5 mL)

F: HN_3 (0.1 mmol) and **SQ3** (0.02 mmol) in $CDCl_3$ (0.5 mL) by adding **SQ3** to tube **D**.

G: Standard reaction mixture at particle conversion.

(6) NMR study to investigate the reaction using HCl and NaN_3



A: **1a** (0.1 mmol) in $CDCl_3$ (0.5 mL)

B: **1a** (0.1 mmol), and HCl (0.11 mmol, 4.0 M aqueous solution) in $CDCl_3$ (0.5 mL)

C: **B** + NaN_3 (0.11 mmol)

D: The standard reaction mixture using HCl and NaN_3 at partial conversion

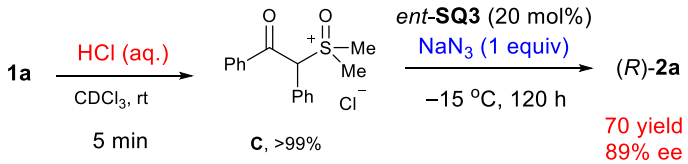
E: The standard reaction mixture using HCl and NaN_3 at complete conversion

F: **SQ3** (0.02 mmol) in $CDCl_3$ (0.5 mL)

G: **2a** (0.1 mmol) in $CDCl_3$ (0.5 mL)

H: DMSO (0.1 mmol) and **SQ3** (0.02 mmol) in $CDCl_3$ (0.5 mL)

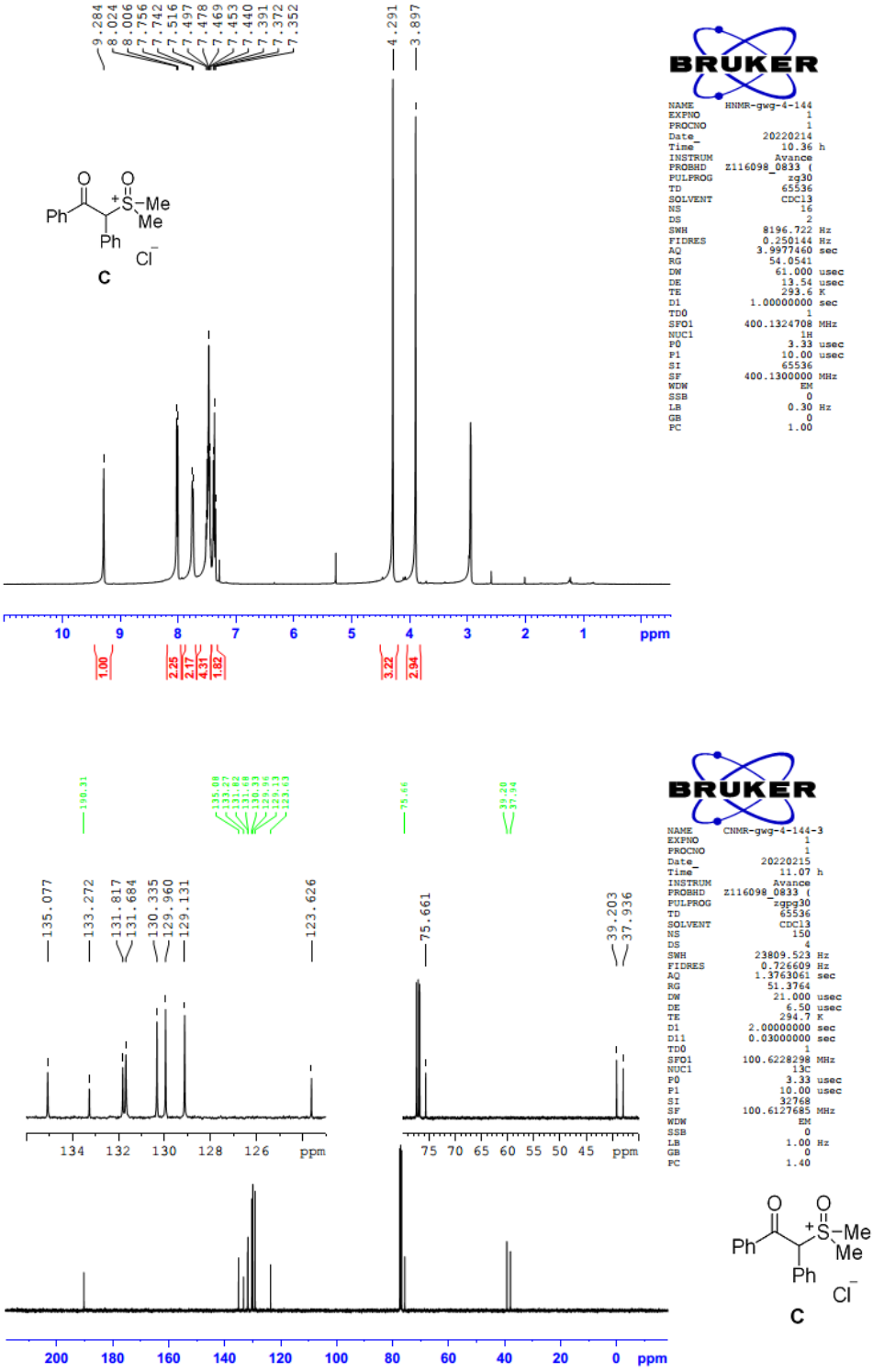
(7) Synthesis and reaction of sulfoxonium chloride salt C



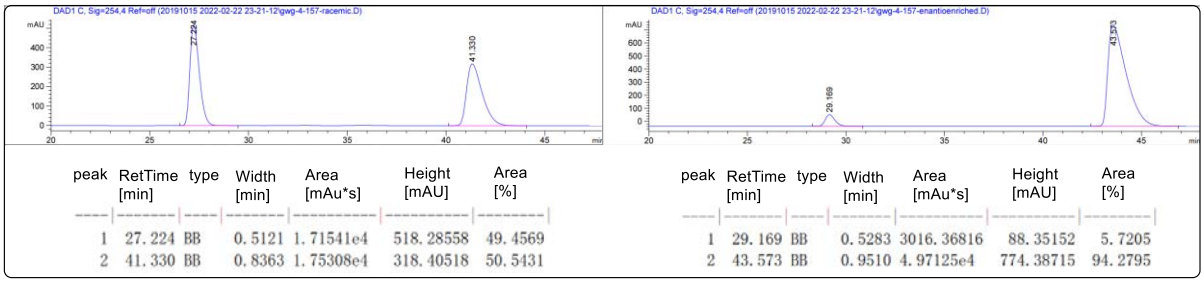
To an NMR tube charged with **1a** (27 mg, 0.1 mmol, 1.0 equiv) and $CDCl_3$ (0.5 mL) was added HCl (27.5 μL, 4.0 M aqueous solution, 0.11 mmol, 1.1 equiv). Upon efficient shaking, **1a** was cleanly converted to the sulfoxonium chloride **C** as indicated by NMR analysis. The diastereotopic relationship between the two methyl groups and the presence of a singlet proton signal at 9.28 ppm are indicative of this structure.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.28 (s, 1H), 8.01 (d, *J* = 4.0 Hz, 2H), 7.75 (d, *J* = 8.0 Hz, 2H), 7.52 – 7.44 (m, 4H), 7.37 (t, *J* = 8.0 Hz, 2H), 4.29 (s, 3H), 3.90 (s, 3H) ppm.

^{13}C NMR (101 MHz, $CDCl_3$) δ 190.3, 135.1, 133.3, 131.8, 131.7, 130.3, 130.0, 129.1, 123.6, 75.7, 39.2, 37.9 ppm.



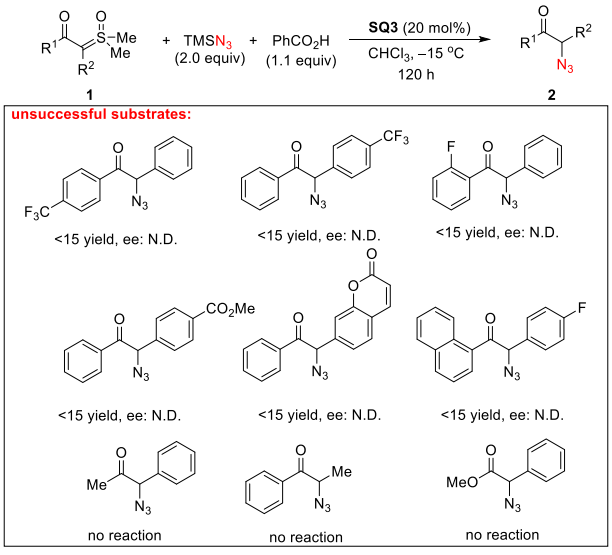
To a 4-mL vial equipped with a magnetic stir bar was were added the above *in situ* generated solution of sulfoxonium chloride **C** (0.10 mmol, 1.0 equiv, 0.2 M) in $CDCl_3$ and ***ent*-SQ3** (13.8 mg, 0.02 mmol, 20 mol%). The vial was carefully sealed with a puncturable screw-cap and cooled to –15 °C. After stirring for 5 min, NaN_3 (7.15 mg, 0.11 mmol, 1.1 equiv) was added, and the reaction mixture was stirred at the same temperature for 120 h. Then, the reaction mixture was directly subjected to flash column chromatography on silica gel (eluent: *n*-hexane/ethyl acetate = 10:1 →5:1) to give the desired product **2a** (70% yield, 89% ee).



peak	RetTime [min]	type	Width [min]	Area [mAu*s]	Height [mAU]	Area [%]
1	27.224	BB	0.5121	1.71541e4	518.28558	49.4569
2	41.330	BB	0.8363	1.75308e4	318.40518	50.5431

peak	RetTime [min]	type	Width [min]	Area [mAu*s]	Height [mAU]	Area [%]
1	29.169	BB	0.5283	3016.36816	88.35152	5.7205
2	43.573	BB	0.9510	4.97125e4	774.38715	94.2795

(8) Unsuccessful substrates for the current research



The reaction conditions: sulfoxonium ylide **1** (0.2 mmol), BzOH (0.22 mmol), $TMSN_3$ (0.4 mmol), **SQ3** (0.04 mmol), $CHCl_3$ (1.0 mL). Yield was determined by ^1H NMR spectra of the crude mixture using CH_2Br_2 as an internal standard.

VI. DFT Calculations

All DFT calculations were carried out with the Gaussian 16 package.[6] All molecular geometries were optimized with the B3LYP-D3(BJ) method and the 6-31G(d) basis set was used for all atoms involved.[7] Single point energies were calculated at B3LYP-D3(BJ)/6-311G(d,p)/SMD($CHCl_3$) level of theory with the optimized structure.[8] The reported free energies and electronic energies were obtained from the above-mentioned single-point calculations combined with the liquid-phase free-energy and ZPE corrections, respectively. Frequency analysis were then performed on the optimized structure. Intrinsic reaction coordinate (IRC) calculation was carried out on the transition state geometries to verify that they are connected to the expected minima.[9] The conformational search was employed with CREST.[10] All energies discussed are Gibbs free relative energies at 298.15 K and 1 atm in kcal mol^{-1}. 3D structures shown in figures were generated by CYLview.[11] In order to reduce the computaional effort, a simplified **SQ3** was employed in which a phenyl group was instead in place of a 1-pyrenyl group.

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(7) (a) S. Grimme, J. Antony, S. Ehrlich, H. A. Krieg, *J. Chem. Phys.*, **2010**, *132*, 154104–154119; (b) S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.*, **2011**, *32*, 1456–1465.
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(11) C. Y. Legault, CYLview, 1.0b, Université de Sherbrooke, **2009**, http://www.cylview.org.

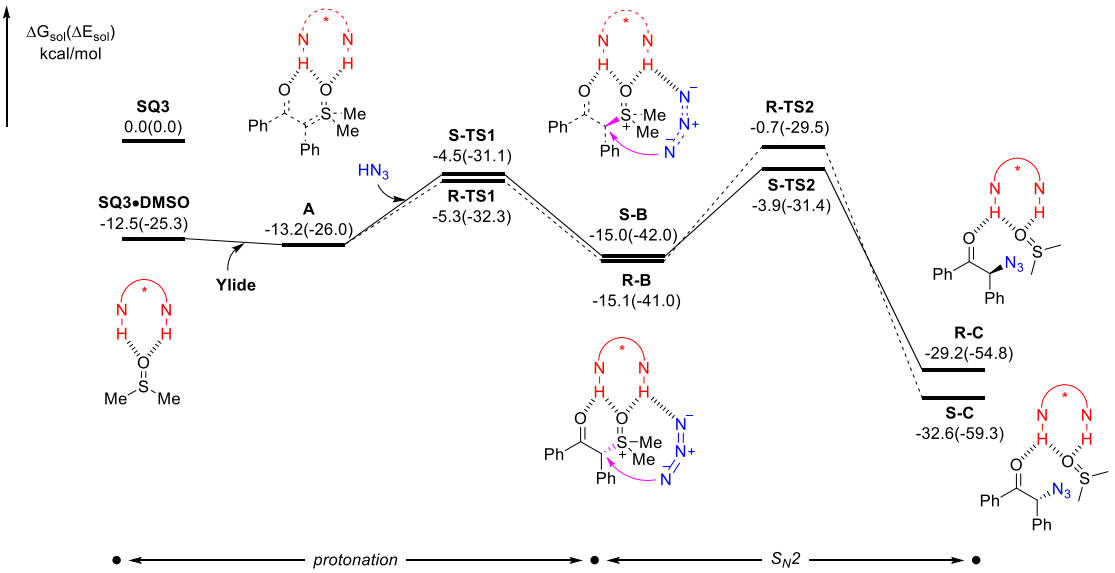
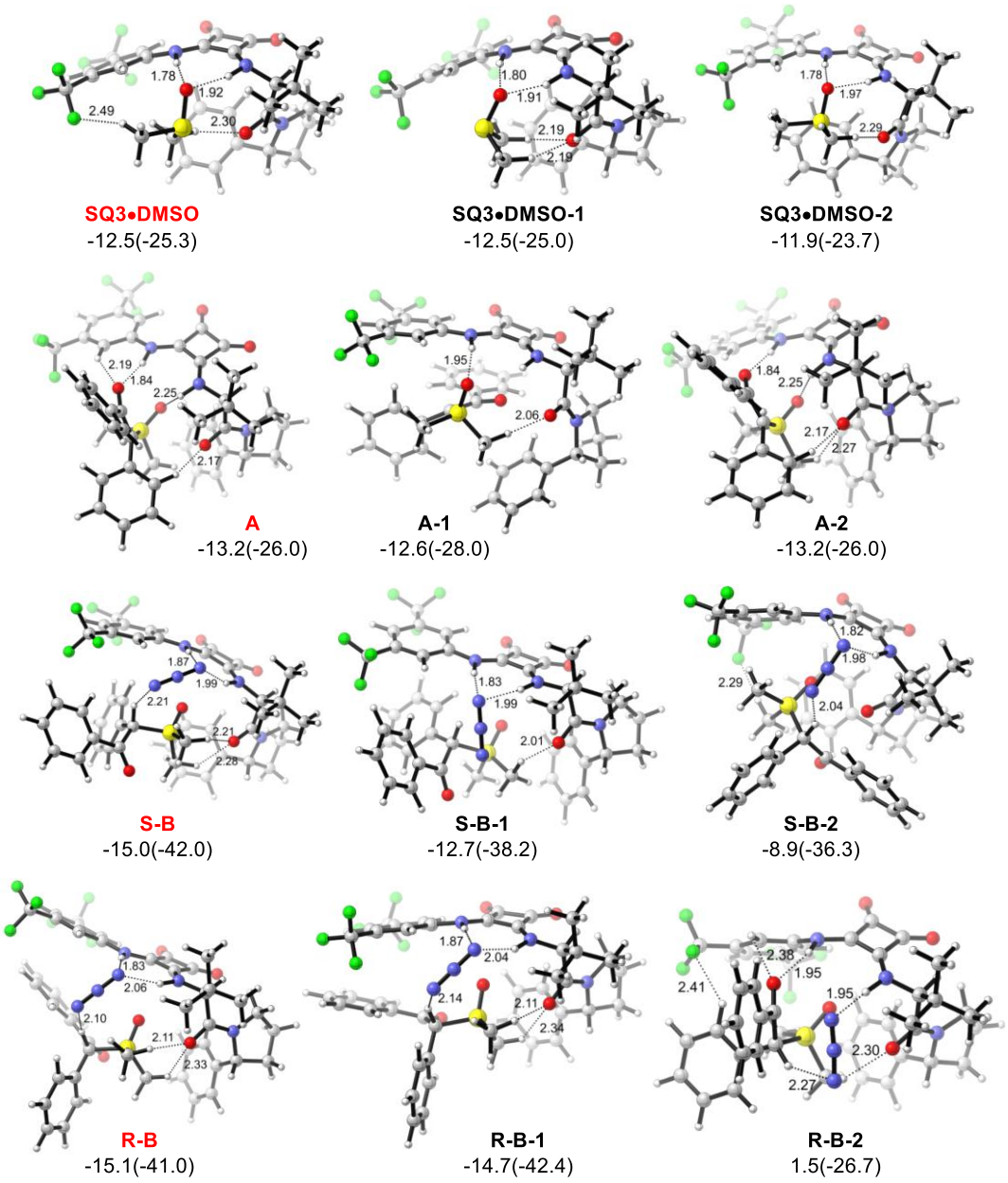


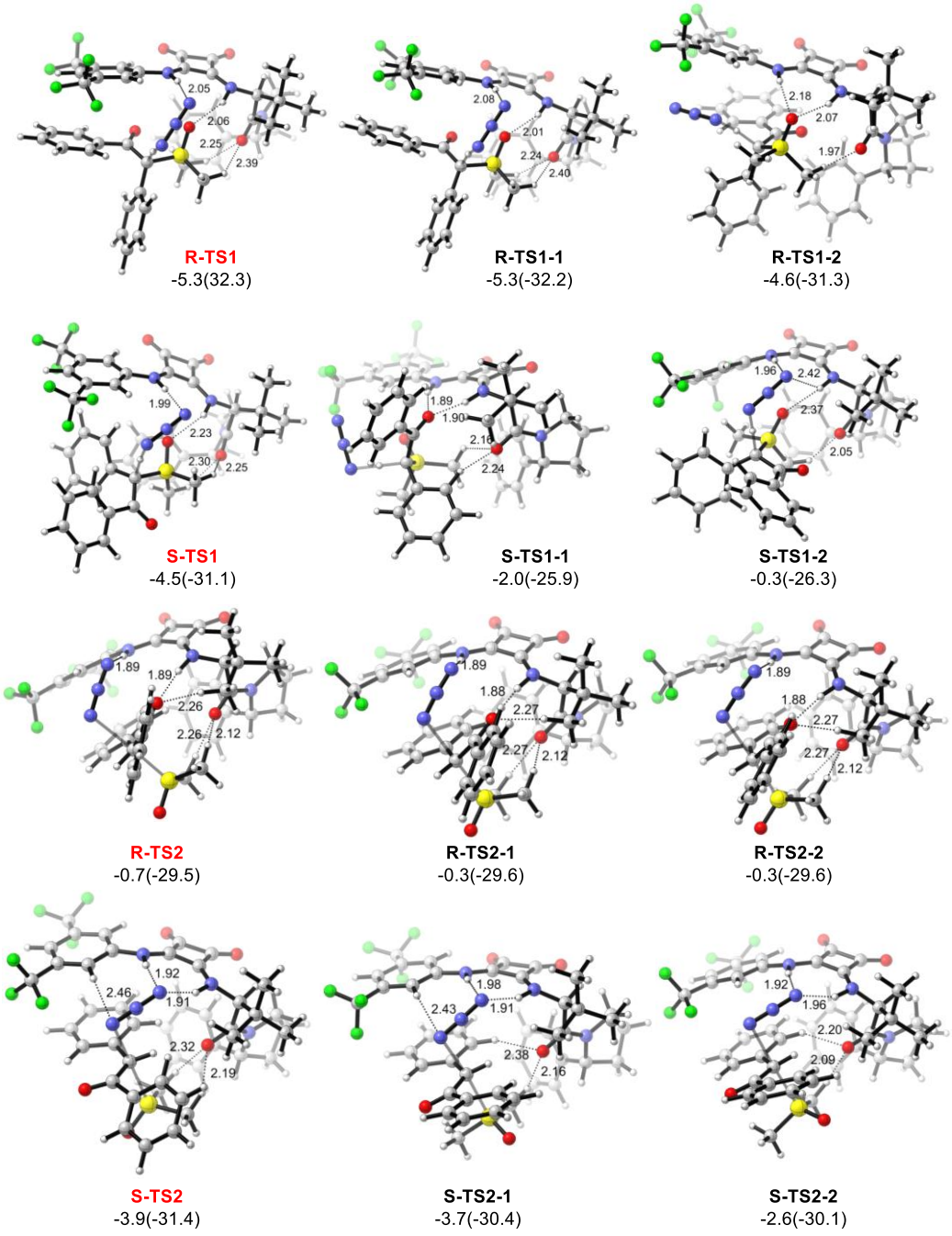
Figure S1. Complete energetic profiles of the asymmetric azidation of sulfur ylides at the B3LYP-D3(BJ)/6-311G(d,p)/SMD($CHCl_3$)//B3LYP-D3(BJ)/6-31G(d) level of theory (kcal/mol).

The reaction starts from the solvent replacement by the sulfoxonium ylide to generate complex **A** through hydrogen-bonding interactions (Figure S1). The subsequent protonation by in situ generated HN_3 leads to intermediate **B** with multiple isomers (Scheme S1). Among them, **S-B** and **R-B** are the preferable isomers. The protonation step is reversible, as indicated by the low energy barrier and the similar energies of **SQ3·DMSO**, **A**, **S-B** and **R-B** . The π-π stacking interaction in **R-TS1** between **SQ3** and ylide results in relatively lower energy barrier (Figure S1). The subsequent S_N2 azide substitution is the rate-determining ($\Delta G^{\neq}$ = 11.2 kcal/mol) and enantio-determining step ($\Delta\Delta G^{\neq}$ = 3.2 kcal/mol). The energy barrier of **S-TS2** to form *R*-configuration product is 3.2 kcal/mol lower than **R-TS2,** which is fundamentally consistent with the *ee* value according to Arrhenius equation. The stability of **S-TS2** might be attributed to the hydrogen bond interactions between N-H motifs of **SQ3** and azide (Scheme S3, N···H1 = 1.91 Å, N···H2 = 1.92 Å) while there is only one N-H···N weak interaction in **R-TS2** (N···H = 1.89 Å). On the other hand, the steric repulsion between azide and carbonyl moiety of the substrate in **R-TS2** leads to higher activation

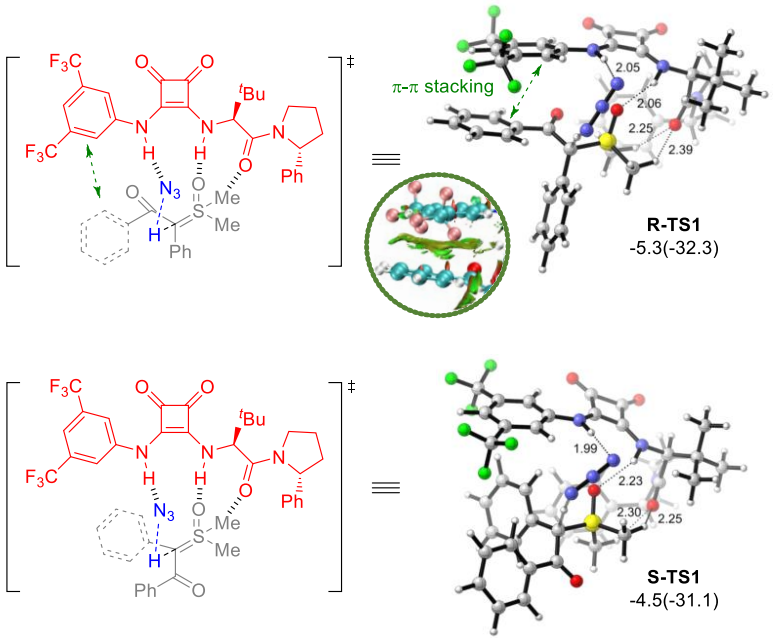
energy according to NCI analysis.



Scheme S1. Multiple isomers of the key intermediates.



Scheme S2. Multiple isomers of the key transition states.



Scheme S3. Computed geometries of the transition states for protonation step.

Energies

Table S1. Absolute electronic energies, thermal corrections to energies and free energies at 298.15 K (in Hartree) of all stationary points. Geometries were optimized in the level of B3LYP-D3(BJ)/6-31G(d). Free energies were obtained from the single point calculation at the level of B3LYP-D3(BJ)/6-311G(d,p)/SMD($CHCl_3$) combined with the free-energy correction mentioned above.

	E	E+ZPE	G
Cat	-2072.420308	-2072.456744	-2072.527697
Ylide	-1167.904295	-1167.922147	-1167.969457
HN3	-164.8082343	-164.8114563	-164.8344543
DMSO	-553.1979785	-553.2036265	-553.2319645
SQ3·DMSO	-2625.658539	-2625.701653	-2625.779596
SQ3·DMSO-1	-2625.658052	-2625.701118	-2625.779509
SQ3·DMSO-2	-2625.656045	-2625.699475	-2625.778585
A	-3240.366012	-3240.421932	-3240.518151
A-1	-3240.369242	-3240.42471	-3240.517154

A-2	-3240.366011	-3240.42193	-3240.518138
S-TS1	-3405.182368	-3405.241546	-3405.338749
S-TS1-1	-3405.174054	-3405.233575	-3405.334801
S-TS1-2	-3405.174719	-3405.233917	-3405.33214
S-B	-3405.199708	-3405.258703	-3405.355438
S-B-1	-3405.193753	-3405.253198	-3405.351864
S-B-2	-3405.190719	-3405.249745	-3405.345855
S-TS2	-3405.182802	-3405.241709	-3405.337868
S-TS2-1	-3405.18125	-3405.240358	-3405.337521
S-TS2-2	-3405.180813	-3405.239669	-3405.335744
R-C	-3405.220216	-3405.280052	-3405.378073
R-TS1	-3405.184379	-3405.243395	-3405.340075
R-TS1-1	-3405.184135	-3405.243161	-3405.340036
R-TS1-2	-3405.182649	-3405.241863	-3405.338927
R-B	-3405.198175	-3405.257269	-3405.355595
R-B-1	-3405.200399	-3405.259283	-3405.354995
R-B-2	-3405.175322	-3405.234281	-3405.329257
R-TS2	-3405.179803	-3405.238078	-3405.332671
R-TS2-1	-3405.180027	-3405.238253	-3405.332055
R-TS2-2	-3405.180032	-3405.238259	-3405.332069
S-C	-3405.227296	-3405.286902	-3405.383548

Table S2. Relative electronic energies, thermal corrections to energies and free energies at 298.15 K (in kcal/mol) of all stationary points. Geometries were optimized in the level of B3LYP-D3(BJ)/6-31G(d). Free energies were obtained from the single point calculation at the level of B3LYP-D3(BJ)/6-311G(d,p)/SMD($CHCl_3$) combined with the free-energy correction mentioned above.

	E	**E+ZPE**	**G**

SQ3·DMSO	-25.3	-25.9	-12.5
SQ3·DMSO-1	-25.0	-25.6	-12.5
SQ3·DMSO-2	-23.7	-24.5	-11.9
A	-26.0	-27.0	-13.2
A-1	-28.0	-28.8	-12.6
A-2	-26.0	-27.0	-13.2
S-TS1	-31.1	-32.1	-4.5
S-TS1-1	-25.9	-27.1	-2.0
S-TS1-2	-26.3	-27.3	-0.3
S-B	-42.0	-42.9	-15.0
S-B-1	-38.2	-39.4	-12.7
S-B-2	-36.3	-37.3	-8.9
S-TS2	-31.4	-32.2	-3.9
S-TS2-1	-30.4	-31.4	-3.7
S-TS2-2	-30.1	-30.9	-2.6
R-C	-54.8	-56.3	-29.2
R-TS1	-32.3	-33.3	-5.3
R-TS1-1	-32.2	-33.1	-5.3
R-TS1-2	-31.3	-32.3	-4.6
R-B	-41.0	-42.0	-15.1
R-B-1	-42.4	-43.3	-14.7
R-B-2	-26.7	-27.6	1.5
R-TS2	-29.5	-30.0	-0.7
R-TS2-1	-29.6	-30.1	-0.3
R-TS2-2	-29.6	-30.1	-0.3
S-C	-59.3	-60.6	-32.6

Cartesian Coordinates (Å)

Cat

C	1.98656000	-2.70607200	-0.63434100
C	0.42933200	-2.68979500	-0.53836600
C	0.50588700	-1.35397000	-1.23897600
C	1.87692100	-1.47904400	-1.44789400
O	2.89081900	-3.32573700	-0.11363500
O	-0.43829100	-3.40034700	-0.08918100
N	-0.25572500	-0.25403300	-1.44810500
H	0.29278600	0.60741500	-1.45756200
N	2.80393900	-0.66201800	-2.04364500
H	2.35146700	0.12249700	-2.50805100
C	-1.61450100	-0.08442700	-1.15920400
C	-2.46356700	-1.15996000	-0.88158400
C	-2.11316800	1.22304300	-1.13554900
C	-3.79338200	-0.90557400	-0.55594400
H	-2.08362300	-2.17459700	-0.85477200
C	-3.44688900	1.45118600	-0.81654600
H	-1.45308200	2.05973000	-1.33792500
C	-4.30286200	0.39103500	-0.52165200
H	-5.34043400	0.57105600	-0.27033300
C	-3.94822000	2.86230800	-0.68933500
C	-4.65821800	-2.05099500	-0.10681100
F	-4.34764600	-3.20116400	-0.73444800
F	-5.96976200	-1.80743500	-0.31617500
F	-4.50603900	-2.27094700	1.22454200
F	-5.24452800	2.96984000	-1.04623800
F	-3.23893400	3.72434100	-1.44829900
F	-3.85884400	3.30306100	0.59236000
C	3.79686200	-0.13197100	-1.08254100
H	4.24486600	-1.00201300	-0.59800700
C	4.91026300	0.67283500	-1.80934400
C	5.86748800	1.27478900	-0.76587800
H	6.37242600	0.49382000	-0.18621800
H	6.64551400	1.85931600	-1.26820700
H	5.34783700	1.94325900	-0.07006700
C	4.32287400	1.81326400	-2.66165800
H	3.70403500	2.48808300	-2.06524700
H	5.13847200	2.39086800	-3.10997000
H	3.71520100	1.42904500	-3.48903900
C	5.68850900	-0.29761500	-2.71345300
H	6.15993100	-1.09344500	-2.12490900
H	5.02591700	-0.76820000	-3.44508400
H	6.47807800	0.23699600	-3.25347600

C	2.96670600	0.68817000	-0.06845100
O	2.08048400	1.45203600	-0.48560500
N	3.15474500	0.47710200	1.24777600
C	2.27915500	1.15084400	2.23756900
C	4.19785900	-0.33550900	1.89179900
C	2.93913400	0.79005700	3.59326400
H	2.33023500	2.22760300	2.04784200
C	4.37116700	0.36636500	3.24091300
H	3.85550000	-1.37193900	2.00790400
H	2.89248700	1.62686300	4.29466800
H	5.01545000	1.24416600	3.11425000
H	4.82394000	-0.28374700	3.99441200
H	5.11248700	-0.34287600	1.30210000
H	2.40025600	-0.04842900	4.04496900
C	0.83113300	0.70863500	2.15667400
C	-0.19558500	1.65482000	2.14743700
C	0.49776500	-0.65204000	2.16650500
C	-1.53356700	1.25583500	2.18258700
H	0.05483600	2.71217400	2.11211800
C	-0.83647700	-1.05444500	2.19239200
H	1.28363000	-1.40360200	2.15480000
C	-1.85587300	-0.09996700	2.21503300
H	-2.32038300	2.00251600	2.15385900
H	-1.08052000	-2.11146600	2.17653100
H	-2.89216700	-0.42013400	2.22502300

Ylide

C	-3.57066000	0.44897700	0.96109400
C	-2.21265300	0.14086300	0.89403300
C	-1.76738800	-0.93089400	0.10923000
C	-2.70879900	-1.69510700	-0.59462500
C	-4.06293500	-1.37702500	-0.54082000
C	-4.49800500	-0.30196000	0.23757400
H	-3.90407800	1.27729700	1.58029400
H	-1.50324900	0.72906200	1.46274300
H	-2.35243300	-2.53959900	-1.17438600
H	-4.78093700	-1.96968600	-1.10113300
H	-5.55507800	-0.05426300	0.28411000
C	-0.32969900	-1.36304500	0.00785100
C	0.71735000	-0.38635600	0.16888000
O	-0.09224900	-2.56862800	-0.20666200
S	2.27372600	-1.03669200	-0.09957700
O	2.75158400	-1.41337200	-1.45746200
C	3.43445000	0.18666900	0.55307000

H	3.23635300	0.38586300	1.60619300
H	4.42985700	-0.23628000	0.40430400
H	3.31854400	1.09686600	-0.03516900
C	2.53870000	-2.43287100	1.02256000
H	3.55522800	-2.79148700	0.84792400
H	2.39681000	-2.09310000	2.04982400
H	1.79198100	-3.17452200	0.74573700
C	0.57411700	1.08524600	-0.01970500
C	0.81237900	1.98664800	1.03096700
C	0.16882600	1.60516900	-1.25941200
C	0.65667500	3.36018700	0.85106900
H	1.09976900	1.59440100	2.00302800
C	-0.00059000	2.97730900	-1.44048700
H	-0.01839300	0.91572400	-2.07667900
C	0.24688500	3.85887700	-0.38707300
H	0.84286400	4.03969000	1.67831900
H	-0.32129500	3.35870000	-2.40584800
H	0.11783700	4.92826700	-0.52828100

HN3

N	0.11256200	1.12756200	0.00000000
H	1.10126400	1.38871200	0.00000000
N	0.00000000	-0.10961400	0.00000000
N	-0.26988500	-1.21633600	0.00000000

DMSO

S	0.25814200	0.43272000	0.00000000
O	-1.09424300	1.10685400	0.00000000
C	0.25814200	-0.80146400	1.35869600
H	1.17707400	-1.39438000	1.32367900
H	0.21036000	-0.24488400	2.29741700
H	-0.62445200	-1.44112900	1.26650700
C	0.25814200	-0.80146400	-1.35869600
H	0.21036000	-0.24488400	-2.29741700
H	1.17707400	-1.39438000	-1.32367900
H	-0.62445200	-1.44112900	-1.26650700

SQ3 • DMSO

C	-1.86389400	-1.35580400	2.34250600
C	-0.34975500	-1.61979700	2.37519500
C	-0.16924300	-0.19536800	1.97175000
C	-1.55478400	0.03648200	1.93521100
O	-2.87909500	-2.01602900	2.48261700
O	0.36368500	-2.59159500	2.54360600

N	0.83731000	0.65061400	1.64338500
H	0.52191200	1.57641900	1.31620500
N	-2.31155200	1.08579800	1.56818100
H	-1.79307000	1.84817100	1.11687900
C	2.13268000	0.32534000	1.24358800
C	2.64179700	-0.98022500	1.23968300
C	2.92935500	1.37456500	0.76223700
C	3.90148000	-1.21719000	0.69546800
H	2.06007900	-1.79738500	1.65518100
C	4.18625900	1.11164700	0.22607700
H	2.54900400	2.39041900	0.79801400
C	4.68537000	-0.18856700	0.17230200
H	5.65599800	-0.39370500	-0.25813100
C	4.95805600	2.26440800	-0.34842200
C	4.36468500	-2.64680600	0.61546500
F	3.60490900	-3.35196200	-0.26479200
F	4.26316800	-3.27471800	1.80217300
F	5.64503500	-2.74918700	0.20271900
F	4.32418400	2.77337000	-1.44413100
F	6.19870400	1.91913100	-0.73633400
F	5.06707400	3.28429300	0.52989700
C	-3.63043800	0.80535300	0.97581600
H	-4.06759600	-0.00233100	1.56262100
C	-4.58165600	2.02693100	1.06308700
C	-5.89981600	1.65310100	0.36318100
H	-5.74785300	1.45755900	-0.70456600
H	-6.35275200	0.76231700	0.81479500
H	-6.62049600	2.47319700	0.45104300
C	-3.98733900	3.28140600	0.39839500
H	-3.05271800	3.59150400	0.87765900
H	-3.78198000	3.11410600	-0.66096200
H	-4.69610500	4.11211400	0.49248000
C	-4.85177600	2.31187800	2.54981000
H	-5.31487200	1.44808800	3.04170100
H	-3.92283600	2.54398600	3.07912200
H	-5.53034600	3.16571100	2.65581200
C	-3.34418300	0.33130900	-0.46113100
O	-2.63744100	1.02536200	-1.20554600
N	-3.77103900	-0.89077800	-0.84976200
C	-3.28625700	-1.43338500	-2.13662000
C	-4.70815700	-1.79745400	-0.15909200
C	-4.18042900	-2.67625300	-2.34111300
H	-3.45548400	-0.68940500	-2.91961100
C	-4.53507500	-3.11985900	-0.91512300

H	-4.45539800	-1.89378600	0.89743500
H	-5.08857500	-2.38517100	-2.88212100
H	-5.43496800	-3.73900600	-0.86991800
H	-3.71240500	-3.69250600	-0.47604600
H	-5.73311800	-1.41717900	-0.25525000
H	-3.67195400	-3.44932800	-2.92183100
C	-1.79671300	-1.74151600	-2.09333700
C	-1.00948000	-1.50367000	-3.22471700
C	-1.18570700	-2.27366100	-0.95139300
C	0.35949600	-1.77516900	-3.21319300
H	-1.47067800	-1.08194800	-4.11495700
C	0.18313000	-2.54521000	-0.93522500
H	-1.77662600	-2.46633700	-0.06285300
C	0.96314200	-2.28874600	-2.06377300
H	0.95608000	-1.57435800	-4.09919600
H	0.63740400	-2.95639700	-0.04005000
H	2.02906100	-2.49030800	-2.03832700
S	-0.36102600	2.98207700	-1.10816000
O	-0.31378300	2.87098500	0.43479400
C	0.31188500	1.43334500	-1.78391300
H	0.35295500	1.52866100	-2.87218900
H	1.30631100	1.24007800	-1.37649000
H	-0.39223700	0.64548600	-1.52277300
C	1.04696100	4.05905700	-1.54303200
H	1.99561800	3.61808100	-1.23044300
H	1.04317200	4.21253300	-2.62642200
H	0.88569400	5.01306000	-1.03653800

SQ3 • DMSO-1

C	1.77437700	-1.39091500	-2.33716800
C	0.25612400	-1.61562100	-2.40699300
C	0.10171200	-0.19012700	-2.00175100
C	1.49129300	0.00137500	-1.90665700
O	2.77736700	-2.06966200	-2.47877200
O	-0.47646800	-2.56978700	-2.59373400
N	-0.89803100	0.68411000	-1.72490300
H	-0.56939500	1.61746100	-1.44207100
N	2.26232600	1.01860400	-1.48889800
H	1.76158300	1.77317200	-1.00237900
C	-2.18971300	0.38353200	-1.28802700
C	-2.71053800	-0.91699300	-1.25853500
C	-2.96167700	1.44515600	-0.79174600
C	-3.95655700	-1.13786300	-0.67723400
H	-2.14966100	-1.74278300	-1.68542200

C	-4.20510100	1.19777800	-0.21809200
H	-2.58068900	2.46006300	-0.84479800
C	-4.71450600	-0.09735200	-0.14062400
H	-5.67523100	-0.28890000	0.31767100
C	-4.94456500	2.35408500	0.39502700
C	-4.43048200	-2.56191300	-0.57018100
F	-3.66668300	-3.25901400	0.31416500
F	-4.34602900	-3.21037700	-1.74701700
F	-5.70675800	-2.64782900	-0.14204700
F	-6.22686600	2.05179400	0.67846500
F	-4.94569500	3.43387200	-0.41706900
F	-4.35797300	2.74378800	1.55498400
C	3.60706300	0.71233400	-0.97369800
H	3.97448500	-0.12855000	-1.56083000
C	4.59916900	1.88694800	-1.16801300
C	5.95091700	1.46657700	-0.56566700
H	6.33020800	0.55201700	-1.03707900
H	6.69674000	2.25390800	-0.71913500
H	5.87234700	1.28928900	0.51340100
C	4.11952500	3.18433400	-0.49533000
H	4.06445100	3.07337800	0.58949800
H	4.82119700	3.99428100	-0.72531800
H	3.13195500	3.48962200	-0.85701700
C	4.75890400	2.12315100	-2.67922700
H	5.12290100	1.22120800	-3.18555000
H	3.80478900	2.40421800	-3.13484300
H	5.47838100	2.92865900	-2.86377200
C	3.38914500	0.28412900	0.48824200
O	2.78003000	1.03634100	1.26434200
N	3.73965100	-0.96448000	0.86371000
C	3.24098200	-1.48267900	2.15566200
C	4.61031800	-1.92403800	0.15585900
C	4.07917900	-2.76386400	2.35520500
H	3.44756700	-0.74661700	2.93662000
C	4.39330400	-3.23159600	0.92719100
H	4.32673000	-2.01610800	-0.89318100
H	5.00685100	-2.51146300	2.88232300
H	5.26629000	-3.88743100	0.87382600
H	3.54191100	-3.77439100	0.50569800
H	5.65426400	-1.59258500	0.22221500
H	3.54385300	-3.50970600	2.94726300
C	1.73853900	-1.72276100	2.11179300
C	0.95798500	-1.43855200	3.23697800
C	1.10905400	-2.23918500	0.97250800

C	-0.42060900	-1.65693600	3.22406300
H	1.43303100	-1.02725200	4.12482300
C	-0.26871200	-2.45868500	0.95509300
H	1.69292900	-2.46217600	0.08658800
C	-1.04061100	-2.16224400	2.07959300
H	-1.01132700	-1.42334800	4.10592400
H	-0.73687300	-2.86231100	0.06348200
H	-2.11270400	-2.32773800	2.05518300
S	-0.23998300	3.09031300	0.95052900
O	0.28820900	2.87948700	-0.48920700
C	1.17868300	3.72942500	1.89180600
H	0.87472400	3.86587400	2.93366900
H	1.99816300	3.01412500	1.80112100
H	1.44457000	4.69275800	1.45167600
C	-0.33671900	1.45512900	1.74420200
H	0.62714800	0.95036400	1.65868000
H	-0.60595700	1.60544100	2.79337300
H	-1.12510100	0.88596100	1.25050700

SQ3 • DMSO-2

C	1.77437700	-1.39091500	-2.33716800
C	0.25612400	-1.61562100	-2.40699300
C	0.10171200	-0.19012700	-2.00175100
C	1.49129300	0.00137500	-1.90665700
O	2.77736700	-2.06966200	-2.47877200
O	-0.47646800	-2.56978700	-2.59373400
N	-0.89803100	0.68411000	-1.72490300
H	-0.56939500	1.61746100	-1.44207100
N	2.26232600	1.01860400	-1.48889800
H	1.76158300	1.77317200	-1.00237900
C	-2.18971300	0.38353200	-1.28802700
C	-2.71053800	-0.91699300	-1.25853500
C	-2.96167700	1.44515600	-0.79174600
C	-3.95655700	-1.13786300	-0.67723400
H	-2.14966100	-1.74278300	-1.68542200
C	-4.20510100	1.19777800	-0.21809200
H	-2.58068900	2.46006300	-0.84479800
C	-4.71450600	-0.09735200	-0.14062400
H	-5.67523100	-0.28890000	0.31767100
C	-4.94456500	2.35408500	0.39502700
C	-4.43048200	-2.56191300	-0.57018100
F	-3.66668300	-3.25901400	0.31416500
F	-4.34602900	-3.21037700	-1.74701700
F	-5.70675800	-2.64782900	-0.14204700

F	-6.22686600	2.05179400	0.67846500
F	-4.94569500	3.43387200	-0.41706900
F	-4.35797300	2.74378800	1.55498400
C	3.60706300	0.71233400	-0.97369800
H	3.97448500	-0.12855000	-1.56083000
C	4.59916900	1.88694800	-1.16801300
C	5.95091700	1.46657700	-0.56566700
H	6.33020800	0.55201700	-1.03707900
H	6.69674000	2.25390800	-0.71913500
H	5.87234700	1.28928900	0.51340100
C	4.11952500	3.18433400	-0.49533000
H	4.06445100	3.07337800	0.58949800
H	4.82119700	3.99428100	-0.72531800
H	3.13195500	3.48962200	-0.85701700
C	4.75890400	2.12315100	-2.67922700
H	5.12290100	1.22120800	-3.18555000
H	3.80478900	2.40421800	-3.13484300
H	5.47838100	2.92865900	-2.86377200
C	3.38914500	0.28412900	0.48824200
O	2.78003000	1.03634100	1.26434200
N	3.73965100	-0.96448000	0.86371000
C	3.24098200	-1.48267900	2.15566200
C	4.61031800	-1.92403800	0.15585900
C	4.07917900	-2.76386400	2.35520500
H	3.44756700	-0.74661700	2.93662000
C	4.39330400	-3.23159600	0.92719100
H	4.32673000	-2.01610800	-0.89318100
H	5.00685100	-2.51146300	2.88232300
H	5.26629000	-3.88743100	0.87382600
H	3.54191100	-3.77439100	0.50569800
H	5.65426400	-1.59258500	0.22221500
H	3.54385300	-3.50970600	2.94726300
C	1.73853900	-1.72276100	2.11179300
C	0.95798500	-1.43855200	3.23697800
C	1.10905400	-2.23918500	0.97250800
C	-0.42060900	-1.65693600	3.22406300
H	1.43303100	-1.02725200	4.12482300
C	-0.26871200	-2.45868500	0.95509300
H	1.69292900	-2.46217600	0.08658800
C	-1.04061100	-2.16224400	2.07959300
H	-1.01132700	-1.42334800	4.10592400
H	-0.73687300	-2.86231100	0.06348200
H	-2.11270400	-2.32773800	2.05518300
S	-0.23998300	3.09031300	0.95052900

O	0.28820900	2.87948700	-0.48920700
C	1.17868300	3.72942500	1.89180600
H	0.87472400	3.86587400	2.93366900
H	1.99816300	3.01412500	1.80112100
H	1.44457000	4.69275800	1.45167600
C	-0.33671900	1.45512900	1.74420200
H	0.62714800	0.95036400	1.65868000
H	-0.60595700	1.60544100	2.79337300
H	-1.12510100	0.88596100	1.25050700

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C	-0.18626100	-2.90034700	-2.57504500
C	-1.67974600	-2.64221900	-2.32558800
C	-1.28607800	-1.27840600	-1.84671300
C	0.07988700	-1.53897700	-2.06202000
O	0.50422100	-3.82241200	-2.98209100
O	-2.70752200	-3.28141800	-2.43094700
N	-1.88779500	-0.16071500	-1.39117400
H	-1.26710100	0.62158000	-1.15402200
N	1.20703300	-0.82504500	-1.88379300
H	1.15182700	-0.07455400	-1.20067600
C	-3.18014400	-0.01301700	-0.88065300
C	-4.14842200	-1.02854900	-0.89900600
C	-3.48874100	1.22392900	-0.29720000
C	-5.38741600	-0.79470400	-0.30580800
H	-3.94114500	-1.98065400	-1.37853800
C	-4.72536600	1.42126200	0.30799000
H	-2.74955100	2.01655700	-0.31492200
C	-5.69110600	0.41825100	0.31566100
H	-6.65400100	0.57627000	0.78296300
C	-4.96146900	2.74104700	0.98279000
C	-6.39314700	-1.91428100	-0.26269500
F	-6.32457300	-2.70047700	-1.35366600
F	-7.65977300	-1.44715600	-0.17314800
F	-6.19398600	-2.71139700	0.81501800
F	-6.18424500	2.83060100	1.54107400
F	-4.82498100	3.77844100	0.12788000
F	-4.05186000	2.94738800	1.97693100
C	2.51858200	-1.48043500	-1.96413000
H	2.35893800	-2.41389400	-2.50108800
C	3.54132500	-0.64570200	-2.78685500
C	4.91936700	-1.31824400	-2.67206100
H	4.88016800	-2.36720100	-2.99111700
H	5.64585800	-0.80505700	-3.31136100

H	5.29776900	-1.28443500	-1.64426100
C	3.62696500	0.81017700	-2.30452900
H	3.95308700	0.87289300	-1.26509500
H	4.33869700	1.36421000	-2.92726600
H	2.66001000	1.31430400	-2.39176800
C	3.07530800	-0.66546900	-4.25235400
H	3.04046800	-1.68805300	-4.64652500
H	2.07532100	-0.23104200	-4.34778100
H	3.76042300	-0.08263900	-4.87810200
C	2.96579900	-1.76780100	-0.52440400
O	3.10516300	-0.84054300	0.28711800
N	3.13618600	-3.05523900	-0.15296400
C	3.46531500	-3.36736300	1.24752400
C	3.09016100	-4.26214200	-1.00776900
C	3.96217400	-4.82656400	1.15846600
H	4.25704800	-2.69098500	1.58263600
C	3.12859300	-5.40677200	0.00977400
H	2.19542200	-4.27919300	-1.63237100
H	5.02706600	-4.83536100	0.89737000
H	3.55065100	-6.32087800	-0.41534000
H	2.11405600	-5.63056900	0.35640500
H	3.97243500	-4.28632000	-1.66038600
H	3.83556800	-5.35953500	2.10362900
C	2.27194300	-3.21256400	2.18032400
C	2.49878300	-3.16545600	3.56218800
C	0.95876700	-3.14491900	1.71167000
C	1.43512500	-3.06416100	4.45712600
H	3.51886600	-3.20761500	3.93825600
C	-0.11005000	-3.03767200	2.60342600
H	0.76497300	-3.14654700	0.64549000
C	0.12234400	-3.00157600	3.97831900
H	1.62871800	-3.03242000	5.52586200
H	-1.12179200	-2.97227100	2.21492600
H	-0.70960900	-2.92588900	4.67302700
C	2.86343600	5.05584400	-2.18533300
C	2.46420500	4.02488300	-1.33747600
C	1.10066300	3.77274500	-1.12458900
C	0.15052300	4.56606600	-1.78452000
C	0.55161500	5.60619600	-2.61781800
C	1.91086400	5.85420200	-2.82050000
H	3.92219800	5.23348000	-2.35102000
H	3.21385900	3.40977300	-0.85759700
H	-0.90017300	4.34452300	-1.63442000
H	-0.19486400	6.21925900	-3.11478500

H	2.22605100	6.66165800	-3.47558900
C	0.58062500	2.65618700	-0.27263600
C	1.35025500	2.11278700	0.78435200
O	-0.57445200	2.20403000	-0.53393400
S	0.51973400	0.81663100	1.56704600
O	0.05352500	-0.32916600	0.74742900
C	1.59145400	0.22272300	2.87967300
H	1.92869500	1.05197700	3.50077000
H	1.00034800	-0.50271000	3.44087500
H	2.42018000	-0.27988400	2.38093800
C	-0.90841500	1.45519700	2.48891800
H	-1.40019800	0.60504800	2.96665200
H	-0.54882000	2.17754800	3.22487400
H	-1.57004800	1.92685800	1.76483700
C	2.54639800	2.70056200	1.43700200
C	2.45039700	3.97662500	2.01800700
C	3.78478700	2.03770300	1.46961200
C	3.56200100	4.58298100	2.59959800
H	1.49727300	4.49666300	1.98778000
C	4.89100600	2.63850900	2.06960600
H	3.86694000	1.05701200	1.01567400
C	4.78620700	3.91246400	2.63093600
H	3.47138300	5.57528200	3.03240300
H	5.84259100	2.11406900	2.08599500
H	5.65291100	4.38111900	3.08846700

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C	-1.58395700	-3.19005600	-0.72208100
C	-0.04883800	-3.26586700	-0.82960100
C	-0.00612900	-2.43403900	0.40844200
C	-1.40170800	-2.41236700	0.52756000
O	-2.54738900	-3.51506300	-1.39625300
O	0.75595000	-3.74102600	-1.60652000
N	0.91379100	-1.81248100	1.18984400
H	0.52852100	-1.16626600	1.88066000
N	-2.25673900	-1.87385200	1.40698000
H	-1.92378100	-1.09328700	1.96893600
C	2.27248300	-1.61459800	0.95100700
C	2.92837800	-2.06529800	-0.20453200
C	2.98365300	-0.87848400	1.91034300
C	4.26888100	-1.73835900	-0.38891500
H	2.39504700	-2.64537700	-0.95101300
C	4.32175800	-0.56282500	1.69728700
H	2.46848800	-0.51373800	2.79121200

C	4.98215100	-0.98636800	0.54537000
H	6.01605300	-0.71812900	0.36628800
C	5.05107500	0.28353100	2.70071700
C	4.94706400	-2.08593300	-1.68555900
F	4.30530400	-3.04680500	-2.36967400
F	6.22147100	-2.49373600	-1.49090600
F	5.01539700	-0.99332500	-2.49619400
F	5.75521200	-0.44339900	3.58999500
F	4.19389500	1.06019100	3.41813200
F	5.92464600	1.12472700	2.09552700
C	-3.68810700	-1.82198000	1.09390800
H	-3.82368800	-2.36827800	0.16172000
C	-4.54359400	-2.54334800	2.18281900
C	-6.03457400	-2.37303900	1.84749600
H	-6.27176500	-2.78267800	0.85855500
H	-6.64794400	-2.90873100	2.58019700
H	-6.33818000	-1.32030100	1.86802200
C	-4.26274000	-1.99136700	3.58893100
H	-4.50654100	-0.92914700	3.66024300
H	-4.85830500	-2.54128900	4.32683600
H	-3.20762900	-2.11705600	3.85381700
C	-4.17747500	-4.03659600	2.13379800
H	-4.35950300	-4.45928200	1.13875100
H	-3.12089100	-4.18744100	2.37560300
H	-4.77486600	-4.59923000	2.86015100
C	-4.06558600	-0.34888300	0.92041400
O	-3.78965500	0.46910200	1.80645500
N	-4.72118300	0.01511300	-0.20553600
C	-5.23641100	1.38929200	-0.33504100
C	-5.11118500	-0.85686800	-1.33025900
C	-6.30316600	1.23251200	-1.44238100
H	-5.68631400	1.67839300	0.61880300
C	-5.73518900	0.12038300	-2.33535600
H	-4.24917600	-1.39786100	-1.73014800
H	-7.24854800	0.90819900	-0.99157100
H	-6.49443500	-0.36179600	-2.95661700
H	-4.96643600	0.52575600	-3.00050800
H	-5.84898300	-1.59710400	-1.00006700
H	-6.48119600	2.16939400	-1.97537500
C	-4.17205200	2.41363800	-0.68752400
C	-3.10969900	2.10572800	-1.54038300
C	-4.28603300	3.72073500	-0.20047800
C	-2.18932800	3.08307900	-1.91485700
H	-2.97787900	1.09110300	-1.88999300

C	-3.36581100	4.70287800	-0.56804500
H	-5.10088800	3.96894300	0.47570400
C	-2.31373400	4.38676800	-1.43197200
H	-1.37346800	2.81467000	-2.57963000
H	-3.46942200	5.71278100	-0.18047500
H	-1.59759400	5.15038000	-1.72352500
C	1.92195500	-0.64639700	-3.51005100
C	1.60874800	0.06010500	-2.34950400
C	0.28780800	0.09451400	-1.87857200
C	-0.70503700	-0.59281100	-2.59554400
C	-0.39390400	-1.28939100	-3.75690000
C	0.92440600	-1.31877400	-4.21593600
H	2.95364100	-0.69553500	-3.84007800
H	2.40208800	0.54779100	-1.79916200
H	-1.70964000	-0.61311300	-2.19110800
H	-1.17022300	-1.83819000	-4.28111600
H	1.17739400	-1.88353000	-5.10843500
C	-0.11561600	0.68432100	-0.56625000
C	0.72835600	1.56570300	0.17518300
O	-1.20464200	0.32032500	-0.05812000
S	0.09582500	1.74971300	1.75734400
O	0.01783400	0.54451700	2.65550900
C	1.17149300	2.95059200	2.56611200
H	1.21742000	3.86985900	1.98125000
H	0.73472900	3.12291200	3.55114600
H	2.16215300	2.50798900	2.66547600
C	-1.51137500	2.58592000	1.82912000
H	-1.63696500	2.96060200	2.84787900
H	-1.50132300	3.39453600	1.09631300
H	-2.27707000	1.84677300	1.59196200
C	1.83096300	2.43420900	-0.30152500
C	1.57216600	3.42910400	-1.25944400
C	3.15006700	2.27836900	0.14950200
C	2.60243700	4.22478000	-1.75862900
H	0.55420500	3.56471700	-1.60771200
C	4.17905500	3.08501300	-0.32943700
H	3.36555100	1.49575400	0.86115700
C	3.90848900	4.05921900	-1.29193700
H	2.38470000	4.98061500	-2.50824600
H	5.18835900	2.93409900	0.04220800
H	4.70910200	4.68304900	-1.67888400

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C	-0.18641300	-2.90005600	-2.57547000

C	-1.67988900	-2.64162600	-2.32622700
C	-1.28599000	-1.27801800	-1.84700300
C	0.07995500	-1.53883100	-2.06209400
O	0.50394300	-3.82203300	-2.98291600
O	-2.70780200	-3.28057700	-2.43181900
N	-1.88765900	-0.16023300	-1.39160200
H	-1.26706500	0.62221400	-1.15484200
N	1.20725000	-0.82530900	-1.88330700
H	1.15204800	-0.07493300	-1.20005100
C	-3.17998000	-0.01244900	-0.88102700
C	-4.14823700	-1.02797700	-0.89906200
C	-3.48854300	1.22461900	-0.29776000
C	-5.38718800	-0.79403500	-0.30574500
H	-3.94101600	-1.98014900	-1.37849400
C	-4.72507700	1.42203900	0.30753700
H	-2.74935300	2.01724500	-0.31568800
C	-5.69081700	0.41899800	0.31553200
H	-6.65363300	0.57708100	0.78296400
C	-4.96108200	2.74189500	0.98223800
C	-6.39270000	-1.91381400	-0.26253200
F	-6.32624000	-2.69796300	-1.35514300
F	-7.65921400	-1.44711600	-0.16949000
F	-6.19109300	-2.71295300	0.81321200
F	-6.18378300	2.83154500	1.54063300
F	-4.82462000	3.77922400	0.12725600
F	-4.05135800	2.94827200	1.97629400
C	2.51868900	-1.48082300	-1.96381100
H	2.35895500	-2.41423000	-2.50083400
C	3.54151800	-0.64614600	-2.78646800
C	4.91947000	-1.31885500	-2.67164100
H	4.88015200	-2.36782100	-2.99067500
H	5.64604800	-0.80578700	-3.31094400
H	5.29783700	-1.28505700	-1.64382500
C	3.62728700	0.80971500	-2.30408200
H	3.95344100	0.87235200	-1.26465000
H	4.33904700	1.36370400	-2.92682900
H	2.66036000	1.31391900	-2.39127000
C	3.07550600	-0.66583500	-4.25196500
H	3.04080100	-1.68838600	-4.64623600
H	2.07545500	-0.23153400	-4.34735900
H	3.76052600	-0.08283700	-4.87766400
C	2.96587600	-1.76842400	-0.52409600
O	3.10595000	-0.84124000	0.28737200
N	3.13514400	-3.05602500	-0.15263400

C	3.46398700	-3.36843500	1.24786800
C	3.08905600	-4.26277200	-1.00764300
C	3.96056000	-4.82771000	1.15869900
H	4.25578800	-2.69224700	1.58317800
C	3.12709300	-5.40756900	0.00974200
H	2.19441000	-4.27956000	-1.63239000
H	5.02550600	-4.83667900	0.89783300
H	3.54902500	-6.32170200	-0.41543700
H	2.11244000	-5.63118700	0.35616000
H	3.97140200	-4.28699100	-1.66015800
H	3.83364200	-5.36081900	2.10374500
C	2.27046700	-3.21341400	2.18045800
C	2.49703100	-3.16654400	3.56237800
C	0.95742000	-3.14512300	1.71153600
C	1.43323100	-3.06479000	4.45709400
H	3.51701400	-3.20923500	3.93866300
C	-0.11154000	-3.03743300	2.60307200
H	0.76385800	-3.14658100	0.64531500
C	0.12058100	-3.00152500	3.97801200
H	1.62661100	-3.03321900	5.52587400
H	-1.12316800	-2.97153300	2.21436100
H	-0.71148100	-2.92543900	4.67255000
C	2.86476900	5.05516100	-2.18531000
C	2.46512500	4.02429300	-1.33752500
C	1.10148700	3.77282100	-1.12449700
C	0.15164700	4.56668600	-1.78421100
C	0.55316000	5.60671500	-2.61743300
C	1.91251300	5.85407000	-2.82025000
H	3.92359700	5.23230000	-2.35110600
H	3.21452300	3.40872900	-0.85781100
H	-0.89913900	4.34564000	-1.63399400
H	-0.19306400	6.22021800	-3.11423900
H	2.22801900	6.66144500	-3.47528800
C	0.58106800	2.65644500	-0.27256100
C	1.35068000	2.11260500	0.78425100
O	-0.57422800	2.20477400	-0.53371000
S	0.51970100	0.81673600	1.56693500
O	0.05318700	-0.32884600	0.74715100
C	1.59134600	0.22213600	2.87926800
H	1.92928700	1.05104500	3.50044900
H	1.00001700	-0.50312900	3.44045200
H	2.41959900	-0.28075500	2.38001000
C	-0.90826800	1.45572100	2.48880400
H	-1.56967600	1.92745300	1.76455800

H	-1.40031300	0.60576100	2.96660000
H	-0.54849400	2.17808000	3.22465900
C	2.54670100	2.70032500	1.43720600
C	2.45065400	3.97630500	2.01835100
C	3.78504500	2.03737300	1.46998700
C	3.56216900	4.58248100	2.60032700
H	1.49760600	4.49647300	1.98793100
C	4.89115800	2.63798900	2.07034900
H	3.86721900	1.05676300	1.01587600
C	4.78630800	3.91186200	2.63188600
H	3.47150000	5.57471100	3.03328800
H	5.84272400	2.11351700	2.08684500
H	5.65293200	4.38034700	3.08974600

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C	-3.05452400	2.74646100	-0.39346700
C	-1.67426600	3.35302200	-0.12567400
C	-1.12849300	2.35407300	-1.08578000
C	-2.39141200	1.75465700	-1.27724500
O	-4.19950900	2.95718100	-0.02414100
O	-1.23177200	4.22539300	0.60156500
N	0.06253500	2.01666200	-1.63118700
H	-0.00092200	1.27432600	-2.34746300
N	-2.80904500	0.68356000	-1.95717600
H	-2.08190700	0.10198200	-2.38749900
C	1.33789900	2.33851500	-1.17727500
C	1.57364200	3.31553000	-0.19944300
C	2.42425000	1.60937800	-1.70194000
C	2.87625700	3.53344800	0.25161700
H	0.74852000	3.89053300	0.21314200
C	3.70862000	1.84734600	-1.22913900
H	2.25934700	0.82482800	-2.43152800
C	3.95495900	2.80865300	-0.24523700
H	4.95841500	2.98346000	0.12166400
C	4.87115500	1.04605700	-1.74283200
C	3.08555500	4.54452400	1.34609200
F	4.38894900	4.85275300	1.51497400
F	2.63636800	4.07506400	2.54358100
F	2.41968400	5.68927700	1.10965000
F	5.49928300	0.39940300	-0.71597900
F	5.80614400	1.82550400	-2.32521900
F	4.50943700	0.10170200	-2.62966100
C	-4.15576600	0.13966200	-1.78684900
H	-4.80607800	0.99451700	-1.60549500

C	-4.66656000	-0.55633800	-3.08018900
C	-6.10212800	-1.04576400	-2.82171100
H	-6.76519100	-0.21519700	-2.55201300
H	-6.50807500	-1.51568900	-3.72383500
H	-6.13751800	-1.78920200	-2.01672900
C	-3.79052700	-1.74932300	-3.50293000
H	-3.80948000	-2.54091800	-2.74998200
H	-4.17538900	-2.16268300	-4.44232100
H	-2.75011100	-1.45525100	-3.68002200
C	-4.67591600	0.48996200	-4.20792200
H	-5.29124000	1.35728200	-3.93975400
H	-3.66462200	0.84432300	-4.42612100
H	-5.08906800	0.05202100	-5.12333300
C	-4.16690400	-0.77653900	-0.54400100
O	-3.38525700	-1.73662800	-0.45251500
N	-5.00266500	-0.46044800	0.47167700
C	-4.91034300	-1.18705900	1.75127900
C	-6.08839200	0.54621800	0.47726600
C	-6.22270300	-0.79516700	2.46196300
H	-4.87124700	-2.26130900	1.54622100
C	-6.47526300	0.62900500	1.95560200
H	-5.73514400	1.50312800	0.09543700
H	-7.02990500	-1.46300900	2.13822700
H	-7.50668000	0.96333000	2.09398100
H	-5.81416100	1.33713700	2.46628800
H	-6.92613400	0.18506100	-0.13204700
H	-6.13416300	-0.86474200	3.54858400
C	-3.67033500	-0.80317700	2.55345900
C	-3.33728700	-1.55641500	3.68705500
C	-2.84970400	0.26831000	2.19642400
C	-2.20287500	-1.24936500	4.43827000
H	-3.96583300	-2.39577900	3.97774700
C	-1.70525200	0.57197600	2.93569800
H	-3.10164300	0.86668900	1.33260500
C	-1.37604900	-0.18675200	4.05917400
H	-1.95762900	-1.84531700	5.31324400
H	-1.07342600	1.39849500	2.62497900
H	-0.47961200	0.04067200	4.62703000
C	5.27983200	-5.21803900	-0.72801900
C	3.96727400	-4.99501900	-0.33412900
C	3.46494600	-3.68350100	-0.27002400
C	4.29717600	-2.60273400	-0.60182100
C	5.61212700	-2.83049500	-0.99424900
C	6.10257700	-4.13543900	-1.05920500

H	5.66599500	-6.23149700	-0.78084400
H	3.30881100	-5.81693500	-0.07508300
H	3.93682900	-1.58454300	-0.55439400
H	6.24137900	-1.98592100	-1.25037600
H	7.12830800	-4.31225600	-1.37006100
C	2.06332000	-3.49804500	0.14514500
C	1.55103100	-2.06384800	0.24352000
O	1.32139000	-4.43311100	0.43900200
S	-0.28434000	-1.96826200	0.00904800
O	-0.62055600	-0.55102300	-0.21158200
C	-1.06995700	-2.65924600	1.45716400
H	-2.13680900	-2.62584900	1.23333600
H	-0.82932900	-2.01288300	2.30050800
H	-0.68059200	-3.66942500	1.58604600
C	-0.76344500	-3.07046900	-1.32939000
H	-1.77927900	-2.75919600	-1.57748400
H	-0.71458500	-4.08875000	-0.94516800
H	-0.04684200	-2.91187800	-2.13845700
C	1.88862200	-1.37307300	1.54143200
C	2.03157100	-2.10299500	2.72990900
C	2.00600800	0.02220100	1.56611300
C	2.30146400	-1.44048700	3.92541000
H	1.93499900	-3.18417300	2.71972400
C	2.27015800	0.68265100	2.76444700
H	1.88324400	0.58670200	0.65132400
C	2.42071200	-0.04889100	3.94384300
H	2.42010800	-2.01148800	4.84143200
H	2.36249200	1.76275300	2.77050200
H	2.63462100	0.46517900	4.87647900
H	1.85548000	-1.48840300	-0.64001600
N	-0.41112600	-0.19839600	-3.42678300
N	0.53950400	-0.84731600	-3.13190800
N	1.48434700	-1.48413700	-2.81852000

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C	-1.99221700	-2.86543600	0.45347800
C	-0.53074600	-3.16258600	0.08446700
C	-0.15624100	-2.02632500	0.96850200
C	-1.49615800	-1.75213800	1.29953600
O	-3.09280300	-3.30122700	0.15165000
O	0.05205000	-3.95778000	-0.63082400
N	0.95647300	-1.35408200	1.35311800
H	0.77366700	-0.45282600	1.82472400
N	-2.06692600	-0.83906200	2.08508500

H	-1.48145100	-0.04787100	2.37651800
C	2.28932000	-1.64160300	1.08047000
C	2.70665400	-2.79888500	0.40507500
C	3.24271400	-0.69667500	1.49146300
C	4.06070200	-2.97141700	0.12891200
H	1.97890300	-3.52989800	0.06522400
C	4.58654900	-0.88970600	1.18976900
H	2.91791900	0.18534500	2.03468400
C	5.01468000	-2.02535100	0.50393100
H	6.06237900	-2.17464700	0.27926300
C	5.56883800	0.19044200	1.54118900
C	4.48620500	-4.17694500	-0.66500800
F	5.78464000	-4.48572600	-0.45862300
F	4.34819100	-3.96101700	-2.00269500
F	3.75228700	-5.26470000	-0.37032600
F	5.53576200	1.19642900	0.62995700
F	6.83773900	-0.25949700	1.58664400
F	5.29183700	0.75473700	2.74230000
C	-3.50480100	-0.79343100	2.32953100
H	-3.85820400	-1.82544000	2.32633400
C	-3.80288400	-0.19557600	3.74135500
C	-5.32673500	-0.10641600	3.93179600
H	-5.80302300	-1.08849800	3.83011000
H	-5.55326800	0.26744900	4.93587700
H	-5.78767700	0.57780500	3.21143000
C	-3.18720800	1.20540800	3.91754400
H	-3.50377100	1.88749400	3.12578600
H	-3.50148300	1.61674700	4.88354600
H	-2.09269200	1.17762300	3.92035300
C	-3.21818700	-1.15102300	4.79569700
H	-3.67087900	-2.14769000	4.72439100
H	-2.13621400	-1.25986000	4.67585600
H	-3.41010200	-0.76407900	5.80263300
C	-4.19111500	-0.00725700	1.20354300
O	-3.76915900	1.10346200	0.86718900
N	-5.26844800	-0.56060000	0.59680800
C	-5.94018000	0.18250000	-0.47890000
C	-5.89097900	-1.87431600	0.85922500
C	-7.27716100	-0.57711200	-0.61969700
H	-6.09041200	1.21590000	-0.15431400
C	-6.88835400	-2.02524400	-0.29636800
H	-5.13456900	-2.66030000	0.85996400
H	-7.99027200	-0.19902200	0.12244800
H	-7.74210000	-2.65154900	-0.02445500

H	-6.39174700	-2.48400000	-1.15741700
H	-6.41049600	-1.85934500	1.82448500
H	-7.71653100	-0.45395500	-1.61252300
C	-5.14905200	0.19561200	-1.77774800
C	-4.19106400	-0.77766700	-2.07517100
C	-5.43075100	1.18459800	-2.72984100
C	-3.54368400	-0.77543000	-3.31252600
H	-3.93321000	-1.53288700	-1.34042600
C	-4.78516300	1.19066100	-3.96581800
H	-6.16318600	1.95488900	-2.49887400
C	-3.84270500	0.20089900	-4.26438000
H	-2.79801200	-1.53612400	-3.52075900
H	-5.01998000	1.96076700	-4.69561700
H	-3.35603800	0.18634600	-5.23668100
C	2.67048500	5.78456300	1.28227400
C	1.81859000	5.21116600	0.34871400
C	1.87234900	3.82970000	0.10366200
C	2.80540900	3.03662200	0.78675400
C	3.66481500	3.61779900	1.71653500
C	3.59216800	4.98733300	1.96983000
H	2.61706600	6.85073200	1.48167300
H	1.08812000	5.80470800	-0.18915900
H	2.89219800	1.97839300	0.57454100
H	4.38900400	3.00129500	2.23539700
H	4.25774000	5.43714800	2.70107000
C	0.94334000	3.27474100	-0.89884700
C	0.86598000	1.74928000	-1.03460500
O	0.33218300	3.97058000	-1.70808300
S	-0.73954500	1.24056600	-1.84776600
O	-0.95008000	-0.20427200	-1.61569700
C	-0.52662600	1.62578600	-3.59035800
H	-1.46615200	1.35600000	-4.07610700
H	0.30107700	1.02050100	-3.96015100
H	-0.30852800	2.69266700	-3.65851100
C	-2.14192900	2.23389800	-1.34626900
H	-2.94528600	1.94857400	-2.03005200
H	-1.85618700	3.28046400	-1.43121800
H	-2.39427600	1.96232100	-0.31976000
C	1.99017100	1.15539200	-1.85724400
C	2.82141000	1.97190000	-2.63758100
C	2.19924100	-0.23067300	-1.84515600
C	3.86682200	1.40838700	-3.36623400
H	2.66413800	3.04447500	-2.66662200
C	3.23965000	-0.79129400	-2.58276900

H	1.53958000	-0.86779200	-1.27254500
C	4.07950600	0.02914700	-3.33699700
H	4.51692900	2.04990200	-3.95339800
H	3.40083600	-1.86220000	-2.55205500
H	4.89904400	-0.40654500	-3.90082900
H	0.78012500	1.24079100	-0.06878700
N	0.10398100	1.16070300	2.36918400
N	-0.33313500	2.10765600	1.78563300
N	-0.74792600	3.03239000	1.19568800

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C	-0.90137500	-3.95409000	1.28841300
C	0.61837000	-3.94001600	1.04134200
C	0.65827900	-2.67747900	1.82555600
C	-0.73444400	-2.66066800	2.00320800
O	-1.84515900	-4.66243800	0.98386700
O	1.40970300	-4.59770600	0.38934900
N	1.59732500	-1.78554500	2.23079400
H	1.23659000	-1.04409800	2.86079400
N	-1.59200300	-1.76733000	2.51729200
H	-1.15628000	-0.88852000	2.82130000
C	2.76008100	-1.45682300	1.54642600
C	3.05717500	-1.96286300	0.26840000
C	3.61395100	-0.50310800	2.12084400
C	4.17453300	-1.49665900	-0.41163400
H	2.41740800	-2.70500400	-0.18588100
C	4.73292300	-0.05672600	1.42171500
H	3.38028100	-0.09722400	3.09946400
C	5.03029500	-0.54220900	0.14834700
H	5.89921000	-0.18752600	-0.39207300
C	5.53985400	1.07746400	1.98606400
C	4.39748100	-1.92009600	-1.83581900
F	3.75674500	-3.05722500	-2.15631300
F	5.70425300	-2.08117000	-2.12254800
F	3.93779400	-0.95814800	-2.69968200
F	6.80935500	1.07815200	1.53031500
F	5.58262700	1.06001600	3.33150700
F	4.99486600	2.27390900	1.62559900
C	-2.93615900	-1.66175400	1.93326400
H	-3.32118500	-2.67846700	1.85170900
C	-3.89409500	-0.85344200	2.85544800
C	-5.19654400	-0.56375800	2.08856100
H	-5.67383100	-1.48697100	1.73958200
H	-5.90922300	-0.05443200	2.74650100

H	-5.02083600	0.08650100	1.22473700
C	-3.27203300	0.47979800	3.30771100
H	-2.94048400	1.06852500	2.45184300
H	-4.02023100	1.05961700	3.86078100
H	-2.41589900	0.32909100	3.97205100
C	-4.20087200	-1.71826000	4.08906100
H	-4.72199500	-2.64167700	3.80823500
H	-3.27824600	-1.99274800	4.60979500
H	-4.83905700	-1.16935400	4.79092400
C	-2.77492800	-1.04776900	0.52440600
O	-2.16401100	0.01823300	0.38971200
N	-3.26193700	-1.74612100	-0.53074300
C	-3.06545900	-1.26696400	-1.91135000
C	-4.12476500	-2.94872800	-0.47752100
C	-4.24223900	-1.93073500	-2.65358700
H	-3.13924900	-0.18000300	-1.92246300
C	-4.35253800	-3.29098500	-1.95524700
H	-3.63557900	-3.75750600	0.06746800
H	-5.15425800	-1.34245600	-2.49334400
H	-5.31241000	-3.78859200	-2.11711100
H	-3.55959300	-3.95767500	-2.30926200
H	-5.07255200	-2.70280300	0.01498100
H	-4.06232700	-2.00578300	-3.72860400
C	-1.71917700	-1.66772900	-2.50321400
C	-0.88081500	-2.60079900	-1.89364400
C	-1.32470800	-1.11331000	-3.72870600
C	0.34579700	-2.94927800	-2.46369600
H	-1.19141700	-3.06561100	-0.96896500
C	-0.10748600	-1.46795700	-4.31107000
H	-1.96731700	-0.38552500	-4.21689700
C	0.74246200	-2.37505900	-3.67017600
H	0.97736700	-3.67501900	-1.96107100
H	0.18298400	-1.02727900	-5.26187300
H	1.70317900	-2.63314100	-4.10556100
C	-5.41052300	2.78877100	-0.87824900
C	-4.17712700	2.43624700	-1.41282900
C	-3.00935700	2.56782200	-0.64563900
C	-3.09013700	3.07833400	0.65794000
C	-4.32734500	3.43686200	1.18726900
C	-5.48724200	3.28835500	0.42559800
H	-6.31197300	2.67736300	-1.47347900
H	-4.09348000	2.05095100	-2.42316200
H	-2.20595700	3.17218100	1.27875800
H	-4.38529300	3.81745900	2.20210300

H	-6.45088600	3.56074300	0.84635300
C	-1.73423700	2.13187100	-1.25956400
C	-0.45274300	2.44744500	-0.49095500
O	-1.66854900	1.66286200	-2.38949700
S	0.86898300	1.18294200	-0.80825000
O	0.57832600	-0.15319200	-0.26986800
C	2.33152300	1.90773000	-0.05615700
H	2.56644900	2.85110200	-0.54836500
H	3.12760400	1.17526700	-0.19082100
H	2.08926500	2.06388700	0.99970500
C	1.27582500	1.12682600	-2.55550700
H	2.15389700	0.48229300	-2.63079400
H	1.47764400	2.14020300	-2.90462500
H	0.41976900	0.68471400	-3.06188800
C	0.03687200	3.84319300	-0.81009100
C	0.01296900	4.33460000	-2.12392000
C	0.51017500	4.65811800	0.22887100
C	0.47711300	5.61989900	-2.39806500
H	-0.38813800	3.71960000	-2.92313800
C	0.96800200	5.94415900	-0.05364200
H	0.52258200	4.27159000	1.24265900
C	0.95820300	6.42531900	-1.36429200
H	0.45420200	5.99435800	-3.41712000
H	1.33342500	6.57098200	0.75424600
H	1.31749600	7.42748600	-1.57897000
H	-0.54464200	2.30576300	0.59462100
N	0.23489000	0.27925700	3.61601000
N	0.27965400	1.30078100	3.01697400
N	0.32818500	2.32688500	2.43499200

S-TS1

C	-3.16697700	2.92779400	-0.64652600
C	-1.80975100	3.60710000	-0.41322900
C	-1.19612800	2.46213300	-1.15161600
C	-2.43620200	1.81305800	-1.30241600
O	-4.33720100	3.18256600	-0.41856400
O	-1.41891900	4.60540400	0.15789500
N	0.02723200	2.10657900	-1.60949800
H	0.03643200	1.31677700	-2.25940000
N	-2.81667500	0.64234000	-1.83576000
H	-2.09387400	-0.06576400	-1.93496100
C	1.28198000	2.54959500	-1.18126300
C	1.44789600	3.54431900	-0.20757900
C	2.41306500	1.90690900	-1.70976200

C	2.73243600	3.84423400	0.24433200
H	0.59034400	4.08318300	0.18423500
C	3.67945400	2.20794600	-1.22311500
H	2.30799400	1.13846900	-2.46370100
C	3.85768000	3.17871300	-0.23866000
H	4.84463900	3.41006500	0.14046800
C	4.85265500	1.38638000	-1.68181900
C	2.88324700	4.82404600	1.37570700
F	4.11663000	5.37178500	1.41192400
F	2.69467500	4.20561100	2.57365500
F	1.98855300	5.82555100	1.30813900
F	5.02519400	0.29949200	-0.87944000
F	6.00703200	2.08441800	-1.63462900
F	4.69844700	0.92690300	-2.93704000
C	-4.19722600	0.15786700	-1.71289700
H	-4.80080300	1.03821500	-1.49987500
C	-4.72842000	-0.44673700	-3.04221200
C	-6.15524700	-0.96272900	-2.78915500
H	-6.80876100	-0.16289000	-2.41992600
H	-6.59098200	-1.34461900	-3.71859300
H	-6.16344600	-1.77922300	-2.05810600
C	-3.84935300	-1.59407800	-3.56717700
H	-3.85780300	-2.44485900	-2.88287700
H	-4.23024300	-1.92994000	-4.53828700
H	-2.81245600	-1.27367700	-3.71895200
C	-4.76417700	0.68287300	-4.08544500
H	-5.39810600	1.51311400	-3.75171900
H	-3.76027200	1.07571700	-4.27238500
H	-5.16619900	0.31013200	-5.03393300
C	-4.24142600	-0.80874800	-0.51547300
O	-3.56567400	-1.84971800	-0.51886900
N	-4.96264700	-0.43897600	0.56647300
C	-4.85598500	-1.20682300	1.81931300
C	-5.95212100	0.65875100	0.66598000
C	-6.09932400	-0.74626100	2.60718500
H	-4.90226900	-2.27434200	1.58417500
C	-6.26349900	0.71153600	2.16419700
H	-5.54821400	1.60004000	0.29320900
H	-6.96953500	-1.33834500	2.29995700
H	-7.25811600	1.11850700	2.36301900
H	-5.52814200	1.34481900	2.67190900
H	-6.84644300	0.39672900	0.08612600
H	-5.96693700	-0.86319500	3.68510000
C	-3.55083400	-0.92792200	2.55928800

C	-3.24006200	-1.69744200	3.68851400
C	-2.64567000	0.05236000	2.14734500
C	-2.04784000	-1.49632400	4.38311400
H	-3.93239900	-2.46911700	4.01875600
C	-1.44578600	0.25003500	2.83280900
H	-2.86091300	0.65113700	1.27159600
C	-1.14050400	-0.52316100	3.95217400
H	-1.82158800	-2.10556500	5.25394100
H	-0.74131000	0.99434000	2.47719900
H	-0.19845500	-0.37861000	4.47078300
C	5.28796700	-5.40719000	0.08123500
C	3.91281600	-5.20486800	0.13613000
C	3.37900700	-3.92538200	-0.07689900
C	4.24099000	-2.85428300	-0.36011000
C	5.61567600	-3.06183100	-0.42276900
C	6.14145800	-4.33544200	-0.19767800
H	5.69729300	-6.39864600	0.25248700
H	3.23076600	-6.02340200	0.34016700
H	3.85235800	-1.86165600	-0.54513300
H	6.26703800	-2.22405800	-0.65122400
H	7.21512800	-4.49547900	-0.24312500
C	1.89901700	-3.76262800	-0.02117000
C	1.39461800	-2.36989800	0.03062500
O	1.14619700	-4.74539200	-0.06148500
S	-0.37596200	-2.24965300	-0.14101600
O	-0.74692300	-0.82562000	-0.32882600
C	-1.20556900	-3.00008200	1.25898800
H	-2.27473400	-2.90861200	1.06689900
H	-0.91295700	-2.43258200	2.14280100
H	-0.85412700	-4.03276900	1.30352100
C	-0.92122800	-3.23836300	-1.54123200
H	-1.98653200	-3.01598000	-1.62377900
H	-0.70491200	-4.28302400	-1.32757200
H	-0.37656400	-2.89413100	-2.41963000
C	1.82778300	-1.51271100	1.18891700
C	2.16263600	-2.10378300	2.41903100
C	1.86358300	-0.11603900	1.08157900
C	2.54683900	-1.31828600	3.50318800
H	2.13127100	-3.18472000	2.52119300
C	2.23012000	0.67296800	2.17119500
H	1.59605500	0.34720000	0.14413200
C	2.57781800	0.07275700	3.38245200
H	2.81592700	-1.79229200	4.44286700
H	2.25382100	1.75256500	2.07554900

H	2.87525100	0.68762300	4.22710400
H	1.74424100	-1.79731600	-1.28596000
N	0.04777700	-0.32933800	-3.37621500
N	0.98089900	-0.85073900	-2.91302900
N	1.95724900	-1.37462100	-2.44155200

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C	0.69166800	-3.34876700	-1.89307800
C	-0.75297900	-3.37822000	-1.40373400
C	-0.71512900	-1.87596700	-1.41488700
C	0.64449600	-1.87716100	-1.80678200
O	1.54964200	-4.17787300	-2.16501700
O	-1.53543500	-4.24694700	-1.06850900
N	-1.54574700	-0.85624700	-1.12051600
H	-1.11664900	0.06734200	-1.09575300
N	1.58663500	-0.93658200	-2.02427100
H	1.37895200	-0.00830600	-1.66071900
C	-2.91485200	-0.88423100	-0.79793000
C	-3.61832900	-2.07591300	-0.58940500
C	-3.57598600	0.34729000	-0.68485300
C	-4.97336400	-2.01807300	-0.27070400
H	-3.11783900	-3.03590000	-0.65888800
C	-4.93019000	0.37671900	-0.36204800
H	-3.03810400	1.27976900	-0.82295300
C	-5.64337400	-0.80211100	-0.15403700
H	-6.69500800	-0.77172500	0.09714300
C	-5.61219400	1.71144300	-0.20402000
C	-5.73116800	-3.30723400	-0.10409600
F	-6.13379500	-3.80496900	-1.29595500
F	-6.84258800	-3.14418100	0.64963400
F	-4.97849400	-4.26012000	0.48608900
F	-6.95900000	1.57915300	-0.13665800
F	-5.34049200	2.53133700	-1.23739600
F	-5.21942800	2.33594500	0.92544300
C	3.00204300	-1.33510700	-1.99837100
H	3.04834400	-2.31453500	-2.47281800
C	3.90239000	-0.36993000	-2.81871700
C	5.32864400	-0.94746200	-2.83293400
H	5.35076700	-1.94491000	-3.28663200
H	5.99177500	-0.30024200	-3.41676900
H	5.74406600	-1.02042200	-1.82105300
C	3.94487400	1.04923700	-2.22735900
H	4.39811700	1.05894000	-1.23375500
H	4.53466700	1.70050600	-2.88211100

H	2.95007500	1.49396100	-2.14473200
C	3.36260500	-0.31451100	-4.25762100
H	3.31959000	-1.31515800	-4.70324800
H	2.35389900	0.10742100	-4.28830400
H	4.01460500	0.30729200	-4.88114200
C	3.40316400	-1.44237700	-0.51779700
O	3.12657400	-0.51411000	0.25823300
N	3.96534400	-2.58171300	-0.06302000
C	4.11411300	-2.77031500	1.39304900
C	4.42626400	-3.75136600	-0.84069200
C	5.02231500	-4.01540000	1.47870900
H	4.59662400	-1.88742800	1.82033900
C	4.63722700	-4.82508800	0.23357700
H	3.67898400	-4.04652800	-1.57819800
H	6.07236100	-3.70494800	1.42059600
H	5.39835300	-5.55325000	-0.05834000
H	3.70165400	-5.36623500	0.40595100
H	5.36723900	-3.50915100	-1.34841800
H	4.87766200	-4.56039800	2.41440200
C	2.76883200	-2.96629400	2.07933800
C	2.62788200	-2.62527300	3.42903500
C	1.67487800	-3.52442100	1.40865200
C	1.42047500	-2.83985100	4.09525100
H	3.47020400	-2.18850900	3.96152800
C	0.45972400	-3.72604400	2.06455100
H	1.76872900	-3.80487700	0.36680400
C	0.32926400	-3.38498300	3.41262100
H	1.32928100	-2.57459800	5.14531500
H	-0.37778500	-4.14884100	1.51677000
H	-0.61304800	-3.54761700	3.92796400
C	1.24033400	4.22027100	-3.66933800
C	0.98071800	3.22594800	-2.73517400
C	0.80619800	3.55299600	-1.37931700
C	0.86272600	4.89833500	-0.98000900
C	1.11482700	5.89165600	-1.92162900
C	1.31353000	5.55565600	-3.26198700
H	1.37744400	3.95958900	-4.71441400
H	0.89653200	2.18811400	-3.03699900
H	0.66766300	5.17379000	0.04900700
H	1.14549500	6.93095500	-1.60971200
H	1.51182300	6.33475300	-3.99244800
C	0.52349800	2.45721700	-0.43019600
C	0.50206600	2.76869800	1.01711700
O	0.28516100	1.30343100	-0.83971000

S	-0.26664900	1.40213200	1.91567200
O	-1.58459500	0.99363000	1.39204500
C	-0.45188600	2.07038800	3.57500400
H	0.52276600	2.32619200	3.99090400
H	-0.95482800	1.29910700	4.16175100
H	-1.08130000	2.95850500	3.45508300
C	0.84776400	0.00791800	2.09823400
H	0.30385700	-0.77612800	2.62846600
H	1.73208700	0.32763100	2.64837000
H	1.14358000	-0.31207300	1.10106800
C	1.79246800	3.22530600	1.64627600
C	2.98684700	2.54033900	1.37568700
C	1.80578100	4.33410700	2.50579200
C	4.17925900	2.96117600	1.96312400
H	2.98150500	1.67237600	0.72310100
C	3.00223200	4.74897900	3.08890500
H	0.88214600	4.87326400	2.69414800
C	4.18926700	4.06336800	2.81990300
H	5.09912500	2.42459200	1.74938700
H	3.00871300	5.61165700	3.74872200
H	5.11985700	4.39052200	3.27486800
H	-0.39119800	3.67372400	1.27586800
N	-2.90745600	4.12536800	-0.17503500
N	-2.19126900	4.34323500	0.70715200
N	-1.40558200	4.54771700	1.61478500

S-TS1-2

C	3.78065000	-1.45716600	-1.94295900
C	2.74530800	-2.59510500	-1.94314400
C	1.71757000	-1.56009400	-2.21804000
C	2.64047300	-0.50680500	-2.09694000
O	4.98908000	-1.35787300	-1.83949400
O	2.75705500	-3.78630200	-1.69065500
N	0.38258000	-1.53881100	-2.48804500
H	0.04061800	-0.64405000	-2.85171300
N	2.52986200	0.82338300	-2.04234200
C	-0.57756900	-2.34445600	-1.88536300
C	-0.23377700	-3.36190800	-0.98200300
C	-1.93548300	-2.08047700	-2.13485700
C	-1.23532100	-4.05415800	-0.30985600
H	0.80442300	-3.62143500	-0.82124000
C	-2.91908800	-2.81234000	-1.47397600
H	-2.22084200	-1.28673000	-2.81500600
C	-2.58629700	-3.79827300	-0.54235800

H	-3.35618700	-4.33983500	-0.00705000
C	-4.37050000	-2.56766700	-1.78393500
C	-0.84389900	-4.97660100	0.80978100
F	0.39177800	-5.48452600	0.66016800
F	-1.70525400	-6.00139300	0.95943100
F	-0.84259800	-4.29556100	1.99795600
F	-4.85147500	-3.45969800	-2.67383800
F	-4.58460300	-1.33622900	-2.29546500
F	-5.13780300	-2.67536700	-0.66798200
C	3.61194600	1.65258400	-1.49303800
H	4.54450000	1.22249600	-1.85786500
C	3.51743900	3.11407700	-2.01415300
C	4.57006600	3.95359400	-1.26987700
H	5.57429000	3.52413300	-1.37554600
H	4.59892200	4.96875700	-1.67983500
H	4.33760100	4.03230500	-0.20237600
C	2.11930900	3.72426500	-1.79390800
H	1.80256300	3.65966500	-0.75104200
H	2.13763800	4.77893800	-2.09192300
H	1.36208500	3.23216000	-2.41459400
C	3.83691300	3.10128900	-3.51841900
H	4.85339900	2.73464100	-3.70778700
H	3.13550600	2.46034100	-4.06146400
H	3.76063100	4.11368500	-3.93044800
C	3.54630800	1.55238000	0.04524000
O	2.51713700	1.87832700	0.64034700
N	4.60678200	1.02757500	0.71129200
C	4.47878200	0.76525200	2.15695300
C	5.97064900	0.77474500	0.20781300
C	5.93969300	0.50708400	2.59152900
H	4.06894500	1.65418500	2.64593500
C	6.59445300	-0.06231600	1.32696600
H	5.94725400	0.23852100	-0.73973100
H	6.41268500	1.45735500	2.86621500
H	7.68555900	0.00500500	1.33667100
H	6.31885500	-1.11372100	1.19261700
H	6.50495500	1.72601200	0.08107700
H	5.99512500	-0.16313300	3.45259900
C	3.55363600	-0.40788900	2.45673900
C	3.27242300	-1.39282500	1.50709200
C	2.98877900	-0.52717700	3.73240900
C	2.42167500	-2.45827600	1.80691100
H	3.72799900	-1.32696700	0.52848900
C	2.14232500	-1.59310200	4.04193100

H	3.20181100	0.22946800	4.48474500
C	1.84343300	-2.55758600	3.07402200
H	2.23237400	-3.22028000	1.05711900
H	1.70965200	-1.66690500	5.03626300
H	1.17564400	-3.38258700	3.30130700
C	-3.06056600	6.52757600	0.76974900
C	-2.21189200	5.44223000	0.95947200
C	-2.56822000	4.17267500	0.48078800
C	-3.77479200	4.00901000	-0.21501000
C	-4.61469500	5.10184300	-0.41649700
C	-4.26507800	6.35805900	0.08183300
H	-2.78334700	7.50616200	1.15094300
H	-1.26299800	5.55302100	1.47329400
H	-4.04593100	3.04378800	-0.62412900
H	-5.54153800	4.97206300	-0.96717800
H	-4.92687400	7.20596100	-0.07133000
C	-1.60292000	3.05981100	0.70859900
C	-2.10030200	1.66353400	0.59028300
O	-0.41410200	3.29354800	0.93640600
S	-0.74306400	0.52755800	0.90349300
O	0.11190800	0.29600900	-0.28140200
C	-1.50379000	-1.02064300	1.41478400
H	-2.06307400	-0.86881100	2.33838400
H	-0.67826900	-1.71951400	1.55760800
H	-2.16133400	-1.36374300	0.61846800
C	0.21916800	0.95380100	2.37101100
H	0.59414500	0.01573000	2.78203500
H	-0.44112200	1.46828900	3.07113300
H	1.03538700	1.58629500	2.02452000
C	-3.38240600	1.25669100	1.25195200
C	-3.70063100	1.69516300	2.54623000
C	-4.27095000	0.40027500	0.58546700
C	-4.87746500	1.27692700	3.16471800
H	-3.02843000	2.37758400	3.06026800
C	-5.44150100	-0.02815800	1.20889400
H	-4.04729000	0.08533100	-0.42761900
C	-5.74562600	0.40769300	2.49959800
H	-5.11635400	1.62696900	4.16484200
H	-6.10776700	-0.70347700	0.68262300
H	-6.65911200	0.07662000	2.98505400
H	-2.26595900	1.49581800	-0.79067700
N	-0.43408900	1.22140500	-3.23753700
N	-1.43473200	1.31336200	-2.64819900
N	-2.47933700	1.37967400	-2.05690700

H	1.58698800	1.18291300	-1.91000200

S-TS2

C	0.41598700	-3.44149100	-1.83720400
C	-1.06827700	-3.24487400	-1.52348600
C	-0.90976800	-1.83647400	-2.00236300
C	0.48221800	-2.00489300	-2.17129100
O	1.22475400	-4.35738700	-1.76990200
O	-1.94474300	-3.91151800	-1.00093100
N	-1.66011200	-0.72711800	-2.15771500
H	-1.13445500	0.08926300	-2.50209800
N	1.49580000	-1.16999200	-2.44299700
H	1.26115000	-0.17272600	-2.47545500
C	-2.92995500	-0.46396900	-1.62331400
C	-3.79780800	-1.48012500	-1.20983900
C	-3.28583800	0.87983700	-1.43462200
C	-4.99623900	-1.13683800	-0.58666300
H	-3.51587800	-2.52241800	-1.30628700
C	-4.48633400	1.19340200	-0.80975900
H	-2.59819200	1.67676200	-1.69455600
C	-5.35756100	0.19198300	-0.38165800
H	-6.27992600	0.44198500	0.12756400
C	-4.84324600	2.63169200	-0.54765700
C	-5.84108600	-2.22750300	0.00869300
F	-5.77216200	-3.37375600	-0.69314500
F	-7.14178100	-1.87381200	0.09499200
F	-5.43142900	-2.51468500	1.27528400
F	-5.42519900	2.77063700	0.67151400
F	-5.72877900	3.10255500	-1.45461600
F	-3.76770900	3.43797400	-0.57447700
C	2.86459700	-1.54587700	-2.09172200
H	3.00357500	-2.57218000	-2.43201900
C	3.90230400	-0.65820800	-2.84318500
C	5.32084000	-1.12043900	-2.46999600
H	5.49074800	-2.16345000	-2.75879100
H	6.06150600	-0.50855400	-2.99548000
H	5.51369400	-1.02362000	-1.39527000
C	3.75394600	0.83484900	-2.50203800
H	3.88589600	1.02223100	-1.43380100
H	4.51717700	1.40410500	-3.04517400
H	2.77765500	1.22694900	-2.80278500
C	3.68741100	-0.85561500	-4.35406900
H	2.69199200	-0.52277600	-4.66001700
H	4.42940100	-0.27862500	-4.91717800

H	3.79489500	-1.91018600	-4.63410900
C	3.00746300	-1.49961800	-0.55445400
O	2.57829400	-0.51805000	0.08356100
N	3.56350500	-2.55690900	0.07051300
C	3.63873600	-2.60350200	1.54449500
C	4.10448900	-3.78958100	-0.55237800
C	4.66698600	-3.72713800	1.78587800
H	4.00519600	-1.63908900	1.90863400
C	4.37181500	-4.70821800	0.64575200
H	3.37813000	-4.21369500	-1.24666200
H	5.68245900	-3.32392900	1.69078600
H	5.19150000	-5.40449900	0.45148500
H	3.47566000	-5.29324600	0.87410400
H	5.03299800	-3.55644400	-1.08272000
H	4.56123600	-4.16772900	2.77978200
C	2.29322500	-2.89891900	2.19357200
C	1.24407700	-3.48951700	1.48509400
C	2.11203900	-2.61276000	3.55205400
C	0.02532000	-3.76220400	2.10930700
H	1.37518400	-3.75289700	0.44439500
C	0.89548800	-2.87949300	4.17966700
H	2.92802100	-2.17112300	4.12122500
C	-0.15597600	-3.44735000	3.45600800
H	-0.77523700	-4.21391300	1.52973300
H	0.76776900	-2.64237600	5.23229900
H	-1.10651800	-3.64760100	3.94154300
C	3.46090900	6.12075400	0.34538400
C	2.24899600	5.56426300	0.74692400
C	1.74456000	4.42824400	0.09875100
C	2.45795300	3.86850500	-0.97110900
C	3.66364000	4.43509300	-1.37832200
C	4.17143200	5.55579900	-0.71646400
H	3.85251400	6.99277600	0.86074000
H	1.68506100	5.97874100	1.57507400
H	2.07384600	3.00930600	-1.50583500
H	4.20227000	4.00289800	-2.21623600
H	5.11600000	5.99053300	-1.03101700
C	0.49177600	3.83225800	0.66141800
C	0.42396600	2.32095300	0.64758600
O	-0.31207200	4.50534900	1.28226600
S	1.88256600	2.15154700	2.37628900
O	1.78935800	3.19615400	3.43590700
C	3.57715100	2.00286100	1.75127500
H	3.83345600	2.94983500	1.27582800

H	3.58953800	1.17467300	1.03820700
H	4.22759500	1.81100600	2.60899700
C	1.61784400	0.50437000	3.05143500
H	2.29759600	0.38802700	3.89816300
H	1.82427400	-0.21932600	2.26210700
H	0.58018800	0.43095800	3.37800400
C	-0.71059300	1.51212600	1.07032200
C	-1.83846900	2.04308300	1.72937600
C	-0.63826900	0.12207100	0.83444400
C	-2.86419300	1.19363500	2.13012800
H	-1.90039400	3.11039400	1.88842100
C	-1.66291500	-0.71713900	1.25353300
H	0.23540100	-0.28845900	0.33759200
C	-2.77927200	-0.18281800	1.90080200
H	-3.74864800	1.61179100	2.59940100
H	-1.60477100	-1.78162200	1.05852000
H	-3.59590400	-0.83695100	2.18887000
H	1.10211600	1.81668500	-0.03579100
N	0.23418100	1.38954300	-2.84756100
N	-0.19925400	2.28304700	-2.19480300
N	-0.64329600	3.15426900	-1.53684200

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C	0.95137900	-3.13233600	-1.95588000
C	-0.52653000	-3.17915400	-1.56664200
C	-0.61075300	-1.74972600	-1.99280100
C	0.78165200	-1.68808400	-2.22147900
O	1.88972400	-3.91618600	-1.97820100
O	-1.26258100	-3.99292300	-1.03373800
N	-1.53135900	-0.76671300	-2.07732100
H	-1.16306300	0.12684200	-2.42252400
N	1.63916400	-0.69940800	-2.49722400
H	1.25848500	0.25149100	-2.49065400
C	-2.83772600	-0.74889800	-1.57178800
C	-3.51610000	-1.91403700	-1.19377500
C	-3.45333200	0.49997000	-1.40835100
C	-4.79109400	-1.80905900	-0.64232300
H	-3.03838900	-2.88405400	-1.27696500
C	-4.73085200	0.57517600	-0.86453900
H	-2.92074100	1.41360800	-1.64748100
C	-5.41583900	-0.57477500	-0.47500700
H	-6.40995700	-0.50992000	-0.05129100
C	-5.33680700	1.92482500	-0.59328000
C	-5.45573100	-3.05046500	-0.11666900

F	-5.14324300	-4.14389500	-0.83632600
F	-6.80145700	-2.93777400	-0.09991900
F	-5.07186800	-3.30133800	1.16601300
F	-6.68633000	1.88948000	-0.66495200
F	-4.90322300	2.86171600	-1.45604300
F	-5.02841600	2.36281800	0.65585700
C	3.06965500	-0.87339800	-2.24770800
H	3.35154300	-1.82836000	-2.69259300
C	3.89886700	0.24093200	-2.95702300
C	5.39628300	-0.06951000	-2.79285900
H	5.66016100	-1.02628800	-3.25715300
H	5.99147400	0.70954500	-3.28063400
H	5.69321200	-0.10084200	-1.73849600
C	3.61537100	1.63839000	-2.37956300
H	3.89087000	1.69471200	-1.32326900
H	4.20725800	2.37963800	-2.92855700
H	2.56500800	1.92723800	-2.47927900
C	3.54361200	0.22294200	-4.45451900
H	3.71012500	-0.76988400	-4.88903800
H	2.49888500	0.49689400	-4.62308300
H	4.17345500	0.93888000	-4.99420900
C	3.29883600	-0.93259000	-0.72029600
O	2.72840400	-0.11873600	0.02732900
N	4.10356500	-1.90263600	-0.23393200
C	4.33136800	-2.03400000	1.21804200
C	4.78506400	-2.97307100	-1.00132400
C	5.56847100	-2.95304100	1.27224700
H	4.54752500	-1.04352900	1.62946000
C	5.33575100	-3.89962800	0.08940700
H	4.07482900	-3.47882400	-1.65672800
H	6.47610500	-2.35814100	1.11508800
H	6.24129600	-4.41897700	-0.23441200
H	4.58650800	-4.65290800	0.35230200
H	5.59678000	-2.54403400	-1.59624300
H	5.65312100	-3.46667900	2.23261700
C	3.13980600	-2.63014600	1.95677500
C	2.11247000	-3.29811700	1.28755100
C	3.08645700	-2.53852500	3.35299900
C	1.03267400	-3.83606700	1.99025900
H	2.15720500	-3.41685900	0.21400500
C	2.00984400	-3.07344500	4.06027900
H	3.88950000	-2.03608500	3.88903200
C	0.97221500	-3.71515200	3.37877500
H	0.24728500	-4.34748700	1.44000500

H	1.98013200	-2.98846100	5.14331000
H	0.13047900	-4.12647200	3.92829800
C	1.49053700	6.77753600	-0.41067400
C	0.62133000	5.90192800	0.22842800
C	0.92756000	4.53556200	0.31275400
C	2.12905700	4.06449700	-0.23492200
C	3.00392600	4.94671300	-0.86411700
C	2.68487900	6.30110900	-0.95957400
H	1.23981900	7.83169100	-0.48419300
H	-0.30976900	6.24914300	0.66198100
H	2.40978500	3.02188800	-0.16057600
H	3.93485400	4.57182200	-1.27792900
H	3.36517000	6.98575100	-1.45814900
C	-0.04911200	3.66298200	1.01787000
C	0.11436800	2.16866500	0.88872200
O	-0.89714900	4.12762000	1.77446400
S	1.49242000	2.07358800	2.74640500
O	2.72814000	2.91129800	2.81681900
C	1.89940500	0.34282800	3.05594200
H	0.99262000	-0.24112700	3.21012600
H	2.54111300	0.32174000	3.93906800
H	2.42345000	-0.00882200	2.16521900
C	0.37547400	2.45740000	4.11964400
H	0.92373800	2.31015600	5.05296600
H	-0.49450000	1.80153200	4.05506400
H	0.06603900	3.49614300	3.99824200
C	-0.88205100	1.16027000	1.23240000
C	-2.14137900	1.46320300	1.78758600
C	-0.53672800	-0.18925300	1.00030000
C	-3.01865200	0.43318700	2.11037100
H	-2.42188800	2.49809600	1.92568300
C	-1.41604200	-1.20986200	1.34063200
H	0.42933500	-0.42350300	0.56239200
C	-2.65935000	-0.90036400	1.89849300
H	-4.00184600	0.67588500	2.49870300
H	-1.15021100	-2.24195000	1.14333700
H	-3.36238900	-1.69582700	2.12148800
H	0.89290000	1.81332600	0.22161900
N	0.01974500	1.68218400	-2.74342700
N	-0.53375300	2.33233100	-1.92299300
N	-1.12263200	2.95074100	-1.10514000

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C	0.43680000	3.50513200	-2.28898100

C	1.81470000	2.83644000	-2.24967600
C	1.10190100	1.52694600	-2.36236900
C	-0.16063900	2.15265900	-2.34911000
O	0.00495900	4.64570400	-2.21863400
O	2.96057400	3.21684600	-2.09052600
N	1.40028500	0.20678700	-2.39267500
H	0.58349300	-0.40069900	-2.55143100
N	-1.42791900	1.71191200	-2.29612900
H	-1.54336700	0.69937300	-2.20354000
C	2.53442800	-0.42113100	-1.86483800
C	3.65492100	0.29683000	-1.43031800
C	2.47945800	-1.81094500	-1.67056800
C	4.67598900	-0.37624100	-0.76356800
H	3.71452500	1.37084900	-1.57434700
C	3.52215600	-2.45927500	-1.02030700
H	1.59744500	-2.37414200	-1.95468100
C	4.63046500	-1.75189800	-0.55354000
H	5.41938100	-2.25622400	-0.01045100
C	3.44844400	-3.94421600	-0.78762700
C	5.75116600	0.43636800	-0.10136300
F	6.07116800	1.54204400	-0.79579200
F	6.88261900	-0.27087600	0.09959800
F	5.33402500	0.85747000	1.13214300
F	4.09366900	-4.63485000	-1.75525200
F	2.18084300	-4.39276600	-0.75077900
F	4.03441000	-4.28497400	0.38878500
C	-2.43248100	2.56000700	-1.64418900
H	-2.28663400	3.56698400	-2.03515100
C	-3.87960000	2.11876300	-1.99874700
C	-4.86373400	3.08541900	-1.31814000
H	-4.70885100	4.11660800	-1.65561600
H	-5.89347100	2.80670100	-1.56553100
H	-4.76817300	3.05999900	-0.22640700
C	-4.18357300	0.68305500	-1.53741800
H	-4.09218100	0.58189300	-0.45290400
H	-5.21070100	0.42510600	-1.82100000
H	-3.52146500	-0.04769000	-2.01310800
C	-4.04471100	2.21196000	-3.52510600
H	-3.84305900	3.22832900	-3.88376900
H	-3.36194300	1.52974100	-4.03903700
H	-5.07004300	1.94975800	-3.80899700
C	-2.12782500	2.54095400	-0.13153100
O	-1.94412800	1.45379200	0.44276800
N	-1.99046900	3.71383000	0.52162400

C	-1.53603000	3.72586200	1.92711800
C	-2.24328700	5.07516800	-0.00251600
C	-1.87642800	5.16352800	2.37522100
H	-2.11622900	2.99233100	2.49307000
C	-1.68823400	5.98852200	1.09662200
H	-1.73446900	5.22126000	-0.95599200
H	-2.92187200	5.20461400	2.70368500
H	-2.20403400	6.95175700	1.12657700
H	-0.62539000	6.18020700	0.92107500
H	-3.32052400	5.22538700	-0.13320300
H	-1.24274400	5.49078600	3.20262700
C	-0.05465100	3.40126100	2.06663800
C	0.86822500	3.72516400	1.06633100
C	0.41756200	2.82965200	3.25401000
C	2.23115700	3.47719900	1.24264200
H	0.52899600	4.17801900	0.14315700
C	1.77850100	2.58130900	3.43597200
H	-0.28674800	2.58242600	4.04598200
C	2.69099400	2.90300000	2.42890900
H	2.92178400	3.71954100	0.44072800
H	2.12504500	2.12790000	4.36063600
H	3.74759200	2.68429600	2.55160900
C	-4.94604000	-5.34284900	-0.74888500
C	-3.74402100	-5.07736300	-0.10533100
C	-3.29065200	-3.75569700	0.03303400
C	-4.07178900	-2.70541800	-0.46853200
C	-5.28242000	-2.97411900	-1.10240300
C	-5.71900300	-4.29032700	-1.24952700
H	-5.28316000	-6.36876000	-0.86436000
H	-3.12837000	-5.87757100	0.28962100
H	-3.76426200	-1.67564500	-0.35606900
H	-5.88052500	-2.15152300	-1.48185600
H	-6.65938700	-4.49800300	-1.75213000
C	-2.00163200	-3.55344000	0.74562500
C	-1.37877600	-2.17466900	0.73721900
O	-1.50147700	-4.44771400	1.42134400
S	-2.49200700	-1.38350100	2.51147200
O	-3.93329200	-1.01772400	2.38445900
C	-1.53944700	0.00756800	3.16516200
H	-0.52183500	-0.31022100	3.39070500
H	-2.06669900	0.34625500	4.06082400
H	-1.54332100	0.76915400	2.38116300
C	-2.24859200	-2.63181500	3.80175200
H	-2.60435400	-2.21606900	4.74714700

H	-1.18648100	-2.88064700	3.84183300
H	-2.82427000	-3.51300800	3.51762000
C	0.00612500	-1.87585100	1.09652200
C	0.86177800	-2.77396500	1.76723000
C	0.46374700	-0.57540700	0.80633500
C	2.12965600	-2.35599600	2.15729000
H	0.52703600	-3.78582500	1.94874200
C	1.72861600	-0.16744400	1.20836700
H	-0.19493800	0.12168800	0.30021300
C	2.56171700	-1.05166700	1.89402800
H	2.79433900	-3.05859600	2.64963400
H	2.06297200	0.83726300	0.98898800
H	3.55318000	-0.72839900	2.19290300
H	-1.82406200	-1.44406800	0.07037000
N	-1.16694900	-1.18624300	-2.58951100
N	-0.97133000	-2.21637000	-2.03540700
N	-0.75553800	-3.22634400	-1.46291600

R-C

C	0.59098000	-3.61082100	2.12440000
C	2.02916900	-3.12792500	1.85373600
C	1.53672000	-1.74731800	2.16260000
C	0.23126100	-2.19711100	2.39318100
O	-0.01269700	-4.66597100	2.07406200
O	3.06420400	-3.63020100	1.46900100
N	2.04698000	-0.49214700	2.20192000
H	1.43839300	0.22439900	2.58625900
N	-0.94830500	-1.58916700	2.65509700
H	-0.92594300	-0.57933300	2.54309100
C	3.16638100	0.00515000	1.52229600
C	3.90546100	-0.77120400	0.62216100
C	3.48962800	1.35449900	1.70829000
C	4.95128400	-0.18106700	-0.07882700
H	3.67018500	-1.81520100	0.46779400
C	4.54539200	1.91840500	1.00158400
H	2.89488000	1.96937600	2.37484900
C	5.29435400	1.15695500	0.10732800
H	6.09656900	1.60689900	-0.46467600
C	4.87764600	3.37208000	1.19337200
C	5.61485900	-0.94426600	-1.18993700
F	5.43535500	-2.27531100	-1.09154100
F	6.94118800	-0.70609700	-1.25148700
F	5.09676500	-0.56580100	-2.39353000
F	5.29830300	3.93884300	0.03811400

F	5.86563000	3.54845400	2.09857000
F	3.81140600	4.08022500	1.62479200
C	-2.14677200	-2.19131300	2.03208900
H	-2.09191100	-3.25906800	2.24201700
C	-3.45569800	-1.64579700	2.66217000
C	-4.65330300	-2.27640400	1.92969400
H	-4.64386700	-3.36773200	2.03095300
H	-5.58838800	-1.91716000	2.37441100
H	-4.66756900	-2.02303300	0.86344300
C	-3.55409700	-0.11456400	2.55248800
H	-3.52070100	0.20581800	1.51049900
H	-4.50181500	0.22106400	2.98921100
H	-2.75191400	0.38899400	3.10484700
C	-3.47966800	-2.05566100	4.14395400
H	-2.62477900	-1.63911400	4.68522200
H	-4.39835800	-1.69607400	4.62106900
H	-3.44872800	-3.14626100	4.25120100
C	-2.00285200	-1.93677400	0.51694600
O	-1.71414900	-0.78980700	0.12749900
N	-2.07529500	-2.98585100	-0.31814900
C	-1.83039200	-2.80122900	-1.76219800
C	-2.53224600	-4.35491900	0.00588000
C	-2.50525100	-4.04399600	-2.37589500
H	-2.35019700	-1.90186900	-2.08109100
C	-2.31252000	-5.12145600	-1.30310900
H	-1.95704100	-4.77135200	0.83454300
H	-3.56967800	-3.82471800	-2.51365200
H	-3.00519300	-5.96138100	-1.40306800
H	-1.29263800	-5.51785300	-1.33939300
H	-3.59417400	-4.33235400	0.27006300
H	-2.07060800	-4.30913300	-3.34264200
C	-0.35290100	-2.68876800	-2.09369200
C	0.63614600	-3.32143700	-1.33254900
C	0.03340500	-1.97216200	-3.23272300
C	1.98134500	-3.23783700	-1.69759100
H	0.35816800	-3.88574700	-0.44976400
C	1.37432300	-1.89601800	-3.60777600
H	-0.72413100	-1.46864400	-3.82918500
C	2.35500400	-2.52713600	-2.83893100
H	2.73218500	-3.72549800	-1.08390700
H	1.65593900	-1.32624600	-4.48890600
H	3.40212200	-2.44585200	-3.11130900
C	-5.56799500	4.80942800	-0.86311300
C	-4.24045200	4.56739800	-1.19912200

C	-3.46512500	3.67228700	-0.44267700
C	-4.04724800	3.02509000	0.65637000
C	-5.38020500	3.26227500	0.98721000
C	-6.14174800	4.15353700	0.23120400
H	-6.15795300	5.50607500	-1.45135800
H	-3.77762700	5.05546800	-2.04992200
H	-3.46765000	2.33919100	1.25643200
H	-5.82103700	2.74816800	1.83596700
H	-7.17975800	4.33891600	0.49231100
C	-2.06931900	3.41540400	-0.90910200
C	-1.16136400	2.45680000	-0.10969000
O	-1.67055400	3.88692600	-1.96019200
S	-4.27428300	0.24637100	-1.32291900
O	-4.56654800	-1.24385500	-1.43685100
C	-3.11320600	0.67327900	-2.67432900
H	-2.12910900	0.30191900	-2.38419500
H	-3.07395600	1.75520800	-2.81669000
H	-3.45433400	0.17471400	-3.58630800
C	-5.72327600	1.11190700	-2.02848900
H	-5.93177300	0.71309800	-3.02503600
H	-5.52882200	2.18650500	-2.06233500
H	-6.56738900	0.91025300	-1.36565500
C	0.22808900	2.32055700	-0.67674200
C	1.05800400	3.44355700	-0.80232800
C	0.69671600	1.06342200	-1.06941800
C	2.33105900	3.31429600	-1.34646700
H	0.69820000	4.41648100	-0.48273000
C	1.97420200	0.93925100	-1.62180900
H	0.06830300	0.18671100	-0.94465800
C	2.78371400	2.06187900	-1.77206400
H	2.97434200	4.18420500	-1.43362500
H	2.33221300	-0.03452700	-1.93011900
H	3.77368700	1.95505600	-2.20291700
H	-1.64691200	1.47275100	-0.09209200
N	-0.12379200	1.54206400	2.91272500
N	-0.59895300	2.20190300	2.10305500
N	-1.12629200	2.96773600	1.31465100

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C	-2.65351700	-2.80497100	0.13450500
C	-1.20671500	-3.11543400	-0.27195300
C	-0.78268700	-2.17590400	0.81284900
C	-2.11657900	-1.80708400	1.07811100
O	-3.76734400	-3.18755500	-0.19589200

O	-0.66588800	-3.75288300	-1.15511300
N	0.35423200	-1.77661900	1.41190800
H	0.23934000	-1.13794500	2.20047500
N	-2.66336000	-0.86986700	1.87911700
H	-2.04635400	-0.08637000	2.07383300
C	1.68191100	-1.94442100	0.99976400
C	2.03591600	-2.52614500	-0.22415000
C	2.68193000	-1.46497500	1.85570600
C	3.38329700	-2.62279400	-0.56136300
H	1.27186200	-2.89166200	-0.90175900
C	4.02137200	-1.57185300	1.49222600
H	2.40890100	-1.00944300	2.80118600
C	4.38925000	-2.15914400	0.28608200
H	5.42797100	-2.21875300	-0.00458800
C	5.05979200	-1.05143500	2.44552700
C	3.73749100	-3.23202400	-1.89016800
F	3.50574800	-4.56137100	-1.91435300
F	5.04221200	-3.04868000	-2.20502400
F	3.00856900	-2.69040800	-2.89536100
F	5.15556300	-1.82639900	3.55076500
F	4.75763700	0.19655000	2.87594900
F	6.28999800	-0.99942600	1.88909500
C	-4.07875200	-0.50895000	1.76571300
H	-4.62390500	-1.44283900	1.63291600
C	-4.58108700	0.14901600	3.08547400
C	-6.04561600	0.57889300	2.89662400
H	-6.68056400	-0.27411000	2.63037900
H	-6.43560900	1.00276200	3.82818400
H	-6.14787100	1.34109000	2.11605800
C	-3.73862900	1.37702500	3.47760100
H	-3.76499100	2.14092500	2.69740600
H	-4.13794200	1.81020500	4.40150200
H	-2.69300200	1.11424500	3.67393700
C	-4.49718800	-0.90401400	4.20324000
H	-5.12286000	-1.77499800	3.97384100
H	-3.46899000	-1.25070700	4.33958100
H	-4.84502300	-0.47882400	5.15130600
C	-4.28135100	0.38804600	0.52554700
O	-3.59935300	1.41313500	0.36711000
N	-5.19084000	0.00276300	-0.39745900
C	-5.30845300	0.75267300	-1.66222600
C	-6.14251600	-1.12785400	-0.32134900
C	-6.65541300	0.25296000	-2.22467000
H	-5.33678600	1.82258200	-1.43812300

C	-6.71793900	-1.20050800	-1.74028000
H	-5.62742800	-2.04719000	-0.04227100
H	-7.47406000	0.83645600	-1.78651700
H	-7.72845100	-1.61721000	-1.75253500
H	-6.08136500	-1.83590400	-2.36402000
H	-6.92645900	-0.90204600	0.41136000
H	-6.70470400	0.35359700	-3.31146300
C	-4.14006800	0.48132500	-2.60028600
C	-3.82944700	1.41064800	-3.60018000
C	-3.37896500	-0.68745100	-2.50696000
C	-2.77345800	1.17872100	-4.48229300
H	-4.41300500	2.32554200	-3.68266200
C	-2.31347600	-0.91882800	-3.37840600
H	-3.61308800	-1.42312400	-1.74908800
C	-2.00712700	0.01522200	-4.36953400
H	-2.54349100	1.91011500	-5.25257800
H	-1.72433200	-1.82509900	-3.26842900
H	-1.17648300	-0.16002800	-5.04704500
C	5.38209600	0.17642500	-2.03037400
C	4.00187400	0.32959700	-1.95367500
C	3.43225800	1.06682700	-0.90614900
C	4.25558700	1.62971600	0.07886000
C	5.63541900	1.45818400	0.00865100
C	6.19973300	0.74152400	-1.04860100
H	5.81641300	-0.40711700	-2.83583100
H	3.34489600	-0.13911600	-2.67702700
H	3.82103600	2.15692400	0.92041400
H	6.26779500	1.86375700	0.79167100
H	7.27683800	0.60866400	-1.09710300
C	1.95157800	1.16839700	-0.85662300
C	1.36251700	2.27842100	-0.05108100
O	1.23766100	0.35468100	-1.44993900
S	-0.39940900	2.01146100	0.02057800
O	-0.70288900	0.78197900	0.77786500
C	-1.08255400	3.43475600	0.87738900
H	-0.92123100	4.34241600	0.29554700
H	-2.14163200	3.19633400	0.99629600
H	-0.57168900	3.49108300	1.84044800
C	-1.22231900	2.06604800	-1.57532400
H	-2.29094100	2.02128600	-1.36203000
H	-0.92724000	2.99302500	-2.07177400
H	-0.88883600	1.19108600	-2.12861300
C	1.75653400	3.68320400	-0.41050400
C	1.90191900	4.05390500	-1.75735800

C	1.98585100	4.64499100	0.58555800
C	2.26308300	5.35471000	-2.10267000
H	1.74504100	3.30952700	-2.53383400
C	2.34140400	5.94775000	0.23810200
H	1.89989800	4.36124700	1.62961800
C	2.47871300	6.30625100	-1.10411200
H	2.37855100	5.62424200	-3.14851200
H	2.52090000	6.68175400	1.01838400
H	2.76074700	7.32064000	-1.37093300
H	1.57178700	2.09905200	1.36540300
N	0.36888700	0.34826300	3.61191400
N	0.97733000	1.20946300	3.12460900
N	1.61278400	2.11259400	2.63789800

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C	-2.63205100	-2.93993500	0.27939100
C	-1.20203000	-3.21187200	-0.19901800
C	-0.74991000	-2.22957800	0.83743900
C	-2.08141900	-1.90318900	1.17029600
O	-3.74850600	-3.36741700	0.01855300
O	-0.69069300	-3.86107000	-1.09136100
N	0.40521100	-1.77454800	1.35653300
H	0.31658400	-1.10545700	2.12267800
N	-2.62590600	-0.98117500	1.98971900
H	-2.03484900	-0.17047600	2.14844500
C	1.72123000	-1.98213200	0.92447700
C	2.04250200	-2.68585100	-0.24513200
C	2.74365000	-1.43796300	1.71157800
C	3.38081500	-2.83776000	-0.59399200
H	1.26128100	-3.11856600	-0.86103500
C	4.07497300	-1.60120400	1.33661600
H	2.49585300	-0.89783500	2.61857600
C	4.40987300	-2.30518700	0.18556800
H	5.44420400	-2.42624000	-0.10617200
C	5.14648800	-1.05486900	2.23754700
C	3.73270000	-3.52483100	-1.88450600
F	2.79673500	-4.41087800	-2.26776300
F	4.91174800	-4.18190800	-1.79563000
F	3.87118300	-2.63393600	-2.90615100
F	5.34087500	-1.84862100	3.31672800
F	4.82474200	0.17048100	2.71218300
F	6.33861600	-0.94738800	1.60938400
C	-4.05897100	-0.67953200	1.94383600
H	-4.57238600	-1.63608800	1.85291000

C	-4.51854200	-0.01939000	3.27791300
C	-6.00614300	0.35208600	3.15833200
H	-6.62052900	-0.52857800	2.93792400
H	-6.36418300	0.77658300	4.10235000
H	-6.17730500	1.09666600	2.37283000
C	-3.70481900	1.24569000	3.60834100
H	-3.79776700	1.99434000	2.81854400
H	-4.07398600	1.67965500	4.54428500
H	-2.64163400	1.02519500	3.75627500
C	-4.33795300	-1.04982200	4.40529500
H	-4.94121900	-1.94697900	4.22133700
H	-3.29182200	-1.35609900	4.49363500
H	-4.65270700	-0.62202300	5.36369000
C	-4.35938500	0.18785900	0.70266600
O	-3.72380200	1.23328300	0.49197100
N	-5.30051700	-0.24500400	-0.16580800
C	-5.50466400	0.47708500	-1.43585800
C	-6.20720600	-1.40536100	-0.02345100
C	-6.85424500	-0.08497500	-1.92935600
H	-5.56621200	1.54889900	-1.22824400
C	-6.84274500	-1.52883600	-1.41295200
H	-5.64789300	-2.30005400	0.25052800
H	-7.67513100	0.47794600	-1.46908700
H	-7.83736500	-1.98037500	-1.37064000
H	-6.21302100	-2.15560600	-2.05210600
H	-6.96504300	-1.19050200	0.73940700
H	-6.95289600	-0.01048600	-3.01489400
C	-4.36761600	0.23589600	-2.41918200
C	-4.11726200	1.17403000	-3.42747400
C	-3.57614600	-0.91507200	-2.35804800
C	-3.09016200	0.96921800	-4.34962100
H	-4.72472300	2.07515700	-3.48469800
C	-2.53981000	-1.11930600	-3.27037000
H	-3.76143900	-1.65669500	-1.59220300
C	-2.29318800	-0.17606800	-4.26957300
H	-2.90692800	1.70747600	-5.12587700
H	-1.92596900	-2.01188300	-3.18587200
H	-1.48544600	-0.33042400	-4.97916900
C	5.24364300	0.18213900	-1.94852600
C	3.86092600	0.30496100	-1.86781500
C	3.28190600	1.11848400	-0.88495500
C	4.10043800	1.79504600	0.03139400
C	5.48349000	1.66086100	-0.04623100
C	6.05613800	0.86171900	-1.03830300

H	5.68167700	-0.46423500	-2.70267000
H	3.21172600	-0.24423900	-2.53821700
H	3.66074600	2.38579400	0.82697200
H	6.11405200	2.15931000	0.68300900
H	7.13587800	0.75399000	-1.08819600
C	1.80015000	1.17571600	-0.82447900
C	1.18139600	2.31032300	-0.07791000
O	1.10648100	0.30141700	-1.35305400
S	-0.56463500	1.97098300	0.05491700
O	-0.78882300	0.77643900	0.89177700
C	-1.29318000	3.40744200	0.84852000
H	-1.17701200	4.29021900	0.21953300
H	-2.33997700	3.13400800	0.99721300
H	-0.77028700	3.52942600	1.79919300
C	-1.42605600	1.89208200	-1.51977900
H	-2.48721000	1.81707300	-1.27933600
H	-1.18102400	2.79774800	-2.07883300
H	-1.06721900	0.99957100	-2.02714900
C	1.50681000	3.70635000	-0.52507300
C	1.61229900	4.00536300	-1.89312100
C	1.71060500	4.73197800	0.41113100
C	1.90968100	5.29894800	-2.31757800
H	1.47474800	3.21183800	-2.62318800
C	2.00188300	6.02708100	-0.01547100
H	1.65581100	4.50413700	1.47095600
C	2.09998600	6.31408800	-1.37825200
H	1.99513500	5.51352400	-3.37889600
H	2.16217200	6.81139800	0.71866100
H	2.33214600	7.32290800	-1.70701600
H	1.43141000	2.21596500	1.33147500
N	0.52808500	0.34916800	3.60094200
N	1.00103200	1.28759800	3.10686400
N	1.49111000	2.27068300	2.60555800

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C	-1.40944900	-3.23695400	-0.95472800
C	0.07448900	-3.06887900	-1.29412400
C	0.19985000	-2.29346100	-0.01746100
C	-1.16932800	-2.44270200	0.27119200
O	-2.38593500	-3.76082800	-1.46926900
O	0.79359300	-3.38202300	-2.22258600
N	1.16964700	-1.65851000	0.67990500
H	0.87525200	-1.19623600	1.53655200
N	-1.96818300	-2.05189100	1.27337900

H	-1.67957100	-1.24809900	1.82727500
C	2.54013900	-1.55688600	0.37586800
C	3.04478000	-1.81307900	-0.90385700
C	3.40535800	-1.16156100	1.40201700
C	4.40693200	-1.64979000	-1.13835000
H	2.39269100	-2.14844600	-1.69962900
C	4.76568400	-1.01035200	1.14330100
H	3.01803800	-0.94781600	2.39099200
C	5.27952300	-1.24853000	-0.12809000
H	6.33477700	-1.11091300	-0.32813900
C	5.69496800	-0.65942500	2.27253600
C	4.96320300	-1.84802800	-2.52064500
F	4.07402300	-2.40318700	-3.36668200
F	6.06264800	-2.63547400	-2.50675600
F	5.34976800	-0.66609400	-3.07179100
F	5.11403400	0.16713000	3.16873300
F	6.82400600	-0.06829700	1.83679200
F	6.06975700	-1.77016900	2.95731100
C	-3.40339300	-2.34348300	1.24177800
H	-3.54546300	-3.08830700	0.46036700
C	-3.89424900	-2.97082600	2.58160900
C	-5.42046400	-3.14661500	2.51023700
H	-5.71121300	-3.76545000	1.65284400
H	-5.78619800	-3.64388300	3.41515600
H	-5.93475300	-2.18242200	2.43023200
C	-3.53047300	-2.10046300	3.79628000
H	-3.99112900	-1.11274500	3.73069200
H	-3.87287500	-2.59079700	4.71477600
H	-2.44627400	-1.96722700	3.87914700
C	-3.22538000	-4.34851400	2.72078000
H	-3.48954200	-5.00580100	1.88383400
H	-2.13540600	-4.25407700	2.74571800
H	-3.54572700	-4.83548900	3.64863700
C	-4.13582700	-1.04749300	0.88200400
O	-3.99035700	-0.03883600	1.58667500
N	-4.91543900	-1.03132200	-0.22016900
C	-5.63211100	0.20333500	-0.58061200
C	-5.26588800	-2.17185300	-1.09456100
C	-6.75035500	-0.32483700	-1.50652500
H	-6.03657200	0.65085600	0.33111200
C	-6.08710900	-1.51545800	-2.21056200
H	-4.37144200	-2.68213000	-1.45776900
H	-7.59603500	-0.66682900	-0.89797400
H	-6.80435900	-2.21049500	-2.65457900

H	-5.42412100	-1.16032900	-3.00625900
H	-5.87500200	-2.89395000	-0.53673200
H	-7.10981800	0.44436600	-2.19393300
C	-4.75033500	1.22860800	-1.27577700
C	-3.60596000	0.86455200	-1.99074100
C	-5.14230100	2.57292100	-1.26877400
C	-2.88645500	1.81872300	-2.71171200
H	-3.26050000	-0.16287900	-1.96335300
C	-4.42469700	3.53010400	-1.98461800
H	-6.02327600	2.86855200	-0.70304100
C	-3.29832800	3.15171200	-2.71961300
H	-1.99521300	1.52106600	-3.25540600
H	-4.74675300	4.56797100	-1.97284700
H	-2.73794200	3.89169300	-3.28421800
C	1.11151600	-0.27561000	-3.59029400
C	0.30000300	0.02627100	-2.50354100
C	0.74527400	0.91358900	-1.50990700
C	2.00993800	1.50815200	-1.63369400
C	2.82321500	1.20109300	-2.71999200
C	2.37748200	0.30783100	-3.69610800
H	0.77582700	-0.99394400	-4.33087500
H	-0.66830100	-0.44433200	-2.38230700
H	2.37595500	2.19083300	-0.87848200
H	3.81791300	1.62843600	-2.78176200
H	3.03038100	0.04099100	-4.52041800
C	-0.10694800	1.09887400	-0.31556000
C	0.36727000	2.03547200	0.75272000
O	-1.15987300	0.46990500	-0.16594100
S	-0.52829700	1.61079500	2.24931000
O	-0.41899300	0.17424400	2.64078200
C	0.24171800	2.61728900	3.52537800
H	0.06210600	3.67133700	3.31031900
H	-0.21696200	2.31574300	4.46920500
H	1.31199800	2.39027800	3.49675900
C	-2.23356200	2.18705400	2.23969000
H	-2.61308200	2.10230500	3.26028500
H	-2.22083700	3.22330400	1.89680100
H	-2.79860400	1.53174300	1.57371400
C	0.24304900	3.50255600	0.42448400
C	-0.83081900	3.95063000	-0.36256100
C	1.18773400	4.43292300	0.88437800
C	-0.95752800	5.30008800	-0.68326200
H	-1.56584200	3.24117300	-0.72825200
C	1.05500600	5.78363300	0.56385600

H	2.02582900	4.08687000	1.48030400
C	-0.01597500	6.22049000	-0.21850400
H	-1.79318600	5.62696600	-1.29516200
H	1.79565500	6.49416600	0.91897000
H	-0.11280500	7.27304300	-0.46865200
H	1.65154000	1.81799600	1.21628100
N	4.74286100	2.15436600	0.64253400
N	3.77249600	1.98494000	1.24505300
N	2.76673500	1.79080600	1.89950900

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C	-1.47487000	-3.02875800	-0.91856800
C	-0.01880100	-2.85908700	-1.36248100
C	0.24381300	-2.27543600	-0.01651600
C	-1.11210200	-2.37879600	0.35822000
O	-2.50362800	-3.47827000	-1.40823800
O	0.61665900	-3.06156600	-2.38133900
N	1.28139400	-1.80447600	0.70180800
H	1.03526100	-1.47220000	1.65100500
N	-1.78330000	-2.00961400	1.45513700
H	-1.29264500	-1.39319200	2.10749700
C	2.63099700	-1.73811600	0.36566900
C	3.11133800	-1.93722700	-0.93694600
C	3.53279500	-1.45171000	1.40394100
C	4.48234800	-1.86882000	-1.17017200
H	2.42366200	-2.15577300	-1.74803100
C	4.89784600	-1.40593500	1.14466600
H	3.15910000	-1.29020700	2.40952500
C	5.39063800	-1.62080700	-0.14170200
H	6.45387800	-1.57612100	-0.34035100
C	5.85073500	-1.04140400	2.24725300
C	4.99828500	-2.08726600	-2.56631100
F	6.14979700	-1.39758000	-2.78330200
F	4.11425800	-1.68288900	-3.50187000
F	5.27371000	-3.38608300	-2.80981600
F	7.05625000	-1.62778400	2.08529200
F	5.38427400	-1.38833300	3.46290200
F	6.07899100	0.30105200	2.28671600
C	-3.21882900	-2.21643600	1.60672500
H	-3.44143700	-3.18070000	1.14936000
C	-3.60971800	-2.32622200	3.11312500
C	-5.11569900	-2.62543200	3.20802600
H	-5.36878600	-3.56484400	2.70317600
H	-5.41175800	-2.72351900	4.25783100

H	-5.71926100	-1.82411700	2.76693100
C	-3.30097200	-1.03913300	3.89968100
H	-3.88392200	-0.19501600	3.52327300
H	-3.56186100	-1.19170900	4.95319500
H	-2.23790500	-0.77640100	3.86674200
C	-2.82111500	-3.49698700	3.72621700
H	-3.00719600	-4.42921200	3.17943000
H	-1.74511800	-3.30383600	3.71341500
H	-3.12677700	-3.64892800	4.76737300
C	-4.00748600	-1.11905900	0.86295800
O	-3.77819100	0.08527100	1.06320300
N	-4.95262000	-1.50343000	-0.02181800
C	-5.68496500	-0.48297900	-0.79322800
C	-5.37706800	-2.87969100	-0.36299100
C	-6.86152400	-1.28914100	-1.38284400
H	-6.03290000	0.29459400	-0.10691800
C	-6.25095600	-2.67750400	-1.60489700
H	-4.50833600	-3.50349000	-0.57159600
H	-7.67394500	-1.34301900	-0.64817900
H	-6.99864900	-3.46727400	-1.71501500
H	-5.62141000	-2.67608800	-2.50049300
H	-5.95866500	-3.30401400	0.46369600
H	-7.25190300	-0.83127300	-2.29472700
C	-4.82810700	0.16851700	-1.86998300
C	-5.24844800	1.38320700	-2.42659500
C	-3.65262200	-0.42157200	-2.34276800
C	-4.50911600	1.99710300	-3.43763400
H	-6.16090700	1.85200200	-2.06317000
C	-2.90583000	0.19534600	-3.34823800
H	-3.31596600	-1.36458400	-1.93004700
C	-3.33070800	1.40470700	-3.90056900
H	-4.84917800	2.93872500	-3.86029800
H	-1.98932800	-0.27401000	-3.69344800
H	-2.74702400	1.88450100	-4.68076800
C	4.01545100	1.46396100	-2.72718600
C	2.70245100	1.87224900	-2.54598100
C	2.21974500	2.15744700	-1.25436800
C	3.07576700	2.01958000	-0.14629900
C	4.39851600	1.63369500	-0.33885100
C	4.86745100	1.35630300	-1.62321900
H	4.37726600	1.21369000	-3.71895600
H	2.02170600	1.96804800	-3.38439600
H	2.72717100	2.18807000	0.86698800
H	5.05085200	1.51266300	0.51722400

H	5.89014500	1.02420500	-1.76583300
C	0.81747800	2.58648200	-1.13906900
C	0.25283900	2.88234300	0.26163000
O	0.07603300	2.72934800	-2.10684600
S	-1.26834700	1.85896500	0.41035800
O	-0.91935300	0.46226400	0.10643800
C	-1.85086000	2.15264900	2.08380300
H	-2.25958200	3.16363300	2.12451100
H	-2.61410500	1.38866400	2.24153800
H	-0.98824500	2.05222500	2.74674300
C	-2.58030200	2.50235100	-0.62188600
H	-3.45870100	1.91462800	-0.35008500
H	-2.69817900	3.56582300	-0.40902900
H	-2.28787700	2.33014300	-1.65584500
C	0.02634200	4.33673200	0.57849900
C	-0.47258000	5.23565000	-0.37472900
C	0.31869800	4.78503600	1.87511800
C	-0.68648600	6.56841100	-0.02691800
H	-0.67218000	4.89082400	-1.38359900
C	0.10233800	6.11961500	2.21435900
H	0.71482500	4.08322400	2.60383900
C	-0.40327700	7.01146200	1.26669700
H	-1.06836000	7.26274700	-0.76949900
H	0.33394100	6.46290700	3.21817800
H	-0.56950400	8.05121600	1.53292500
H	0.83278100	2.41055800	1.06443800
N	0.33659200	-0.63737000	3.11729200
N	0.75958000	0.47032800	3.03681200
N	1.16782400	1.57587800	2.95889400

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C	-2.66742600	-2.97717100	0.03290400
C	-1.21567400	-3.28393200	-0.34790600
C	-0.81203700	-2.45733400	0.82330600
C	-2.14517300	-2.08438300	1.08989900
O	-3.77666900	-3.28534800	-0.38194700
O	-0.65624400	-3.85678500	-1.26713900
N	0.31059500	-2.08228100	1.46829700
H	0.14267000	-1.48436900	2.29368200
N	-2.69309800	-1.20021900	1.93282300
H	-2.04233100	-0.57957900	2.42280900
C	1.62962500	-2.12045400	1.02115900
C	2.00798100	-2.65206200	-0.22034800
C	2.60796200	-1.56738700	1.86289200

C	3.35240700	-2.62877400	-0.58782300
H	1.26293300	-3.08571100	-0.88180200
C	3.94266300	-1.56458700	1.47300900
H	2.32106100	-1.13502100	2.81499200
C	4.33439600	-2.10032100	0.24770000
H	5.37020300	-2.08433700	-0.05695000
C	4.95069400	-0.96389000	2.41191100
C	3.72123800	-3.18782900	-1.93461600
F	3.43726800	-4.50263200	-2.02957100
F	5.03941300	-3.04085400	-2.20988400
F	3.03973100	-2.56981800	-2.93108300
F	4.97497000	-1.60746100	3.59912600
F	4.66898800	0.33479400	2.68532500
F	6.20709100	-0.99859900	1.91072500
C	-4.09621500	-0.80775900	1.82515400
H	-4.65409100	-1.71983900	1.61288600
C	-4.63035600	-0.24550200	3.17598500
C	-6.12674500	0.07185700	3.01214700
H	-6.69754700	-0.82370600	2.74050700
H	-6.53463000	0.45196200	3.95479800
H	-6.29908400	0.83534000	2.24476800
C	-3.88942100	1.02828900	3.62219600
H	-4.03471600	1.84231000	2.90774400
H	-4.28373400	1.35106000	4.59263900
H	-2.81450900	0.85988400	3.74964200
C	-4.45562500	-1.33579000	4.24756100
H	-4.96505300	-2.26235100	3.95665000
H	-3.39939100	-1.56544800	4.41166400
H	-4.88346400	-0.99843600	5.19825600
C	-4.27345700	0.17526300	0.64650200
O	-3.57454300	1.19805400	0.55676000
N	-5.18583600	-0.12304400	-0.30442400
C	-5.30215200	0.73380200	-1.49976400
C	-6.13640100	-1.25727000	-0.33115100
C	-6.63486600	0.26501700	-2.12086000
H	-5.35251300	1.77909500	-1.18084200
C	-6.67621800	-1.22513100	-1.76401000
H	-5.62315200	-2.19253400	-0.10945900
H	-7.46893300	0.79414300	-1.64431900
H	-7.67593200	-1.66117800	-1.83727900
H	-6.00728800	-1.79150700	-2.42002800
H	-6.93767000	-1.08489000	0.39719000
H	-6.67291100	0.45929700	-3.19526200
C	-4.12473900	0.57270800	-2.45344000

C	-3.91777600	1.53392900	-3.45084200
C	-3.25714100	-0.51950000	-2.38100600
C	-2.86086700	1.40536800	-4.35276500
H	-4.58698400	2.38948700	-3.52002000
C	-2.18827200	-0.64495500	-3.26960200
H	-3.42031900	-1.28244000	-1.63303500
C	-1.98681600	0.31782900	-4.25992100
H	-2.71427700	2.15803100	-5.12296200
H	-1.51945900	-1.49599100	-3.17788000
H	-1.15397700	0.22454400	-4.95055900
C	5.26876300	0.11794000	-2.39549600
C	3.90689500	0.38510200	-2.35054800
C	3.35692400	1.05778500	-1.24634500
C	4.18486200	1.44127800	-0.18015700
C	5.55122800	1.18223500	-0.23626100
C	6.09321500	0.52729000	-1.34299700
H	5.68592700	-0.42278100	-3.23848700
H	3.24533300	0.06652200	-3.14673500
H	3.77619600	1.92535000	0.69853900
H	6.18438100	1.46429000	0.59721500
H	7.15845000	0.31735800	-1.37693500
C	1.91010600	1.34524900	-1.27443700
C	1.31841000	2.11132400	-0.08335500
O	1.19156700	1.05395000	-2.22240400
S	-0.48733700	1.73050100	-0.00624000
O	-0.68053100	0.28560000	0.17593300
C	-1.10073400	2.73837500	1.34926000
H	-1.12638900	3.77700300	1.01661200
H	-2.09937400	2.34037500	1.54017700
H	-0.41381600	2.60925500	2.18859600
C	-1.36079900	2.38808400	-1.42583900
H	-2.41526200	2.26994500	-1.16964500
H	-1.07393100	3.43233200	-1.55934900
H	-1.08632800	1.77602900	-2.28151800
C	1.59266500	3.59200500	-0.11614000
C	1.56352900	4.30125500	-1.32483400
C	1.87831400	4.26218100	1.08160600
C	1.80734500	5.67344700	-1.33348100
H	1.36710400	3.77621800	-2.25522300
C	2.12285700	5.63445300	1.06466100
H	1.90358800	3.70015200	2.01124700
C	2.08438300	6.34149000	-0.13897500
H	1.78872800	6.21839200	-2.27250800
H	2.34678100	6.15086400	1.99323600

H	2.27723600	7.41021100	-0.14776600
H	1.62143300	1.68423300	0.88643900
N	-0.35836400	-0.11559800	3.46708500
N	0.47668800	0.69619000	3.23525600
N	1.30734700	1.50189900	2.99341400

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C	2.97875400	-1.14560400	-2.73261900
C	1.69618000	-1.90565200	-3.09525300
C	0.94340300	-0.73379900	-2.59349000
C	2.10995500	-0.02234800	-2.24327100
O	4.17900100	-1.35266700	-2.76835700
O	1.41017300	-3.00874600	-3.52111600
N	-0.39663700	-0.48340000	-2.50642100
H	-0.67134400	0.45544400	-2.21704300
N	2.41241400	1.14067500	-1.66246200
H	1.67526600	1.66753100	-1.16815500
C	-1.31823200	-1.44529500	-2.07221900
C	-2.68343200	-1.11579100	-2.08541200
C	-0.92491500	-2.67612300	-1.52571700
C	-3.61783600	-1.97162200	-1.50927200
H	-2.99598300	-0.16624800	-2.49695500
C	-1.87763900	-3.52381600	-0.96708100
H	0.11465100	-2.96416800	-1.52188800
C	-3.23005200	-3.18562800	-0.93854100
H	-3.95769400	-3.84199100	-0.47723600
C	-1.42574800	-4.74650200	-0.22220400
C	-5.07415000	-1.59978000	-1.51597500
F	-5.69327400	-2.00521400	-0.37693900
F	-5.74343500	-2.15656900	-2.54411700
F	-5.25626800	-0.25908300	-1.60238300
F	-2.29576100	-5.76796600	-0.33024700
F	-1.31957500	-4.47281500	1.11714900
F	-0.21554700	-5.18385400	-0.61741700
C	3.78449200	1.35231500	-1.16863200
H	4.41481500	0.67027900	-1.73585300
C	4.32886800	2.78457700	-1.43613800
C	5.77877700	2.84216400	-0.92223200
H	6.41260800	2.09940800	-1.42075200
H	6.20650100	3.83052900	-1.12163000
H	5.83123800	2.67217200	0.15951400
C	3.50491200	3.88411600	-0.75157700
H	3.44463000	3.73474200	0.32915300
H	3.97181300	4.85771600	-0.94211300

H	2.48424100	3.91785400	-1.13947100
C	4.32254200	3.00849400	-2.95764200
H	4.92292400	2.25043100	-3.47557800
H	3.30415600	2.96420500	-3.35494600
H	4.73922400	3.99346600	-3.19660000
C	3.78047300	0.93768700	0.31379600
O	2.93777200	1.38309800	1.09678800
N	4.68034600	-0.00028500	0.71526600
C	4.58852200	-0.52905000	2.08247000
C	5.80884700	-0.58078300	-0.04195400
C	5.95325500	-1.22639000	2.26800100
H	4.45639700	0.30215500	2.78048200
C	6.27577600	-1.73185500	0.85647400
H	5.49229600	-0.92055500	-1.02920500
H	6.69835300	-0.48832100	2.58755400
H	7.33373200	-1.96499900	0.71042200
H	5.69662500	-2.63540200	0.63797600
H	6.60195900	0.16665300	-0.16128200
H	5.91173700	-2.01978700	3.01828800
C	3.42276800	-1.49423800	2.25352600
C	2.99441500	-1.82104500	3.54753000
C	2.79377900	-2.10375300	1.16485100
C	1.96169600	-2.73703500	3.75019800
H	3.47421700	-1.34911000	4.40240500
C	1.76587700	-3.02724500	1.36296200
H	3.10350700	-1.85198100	0.15689000
C	1.34331500	-3.34679700	2.65431700
H	1.64382200	-2.97867400	4.76094500
H	1.30400400	-3.51040900	0.50933200
H	0.54747200	-4.07073800	2.79853300
C	-3.06988600	5.38200800	-1.91923600
C	-2.64000800	4.08400000	-1.67578900
C	-2.25650700	3.69395800	-0.38344000
C	-2.32352900	4.62420100	0.66487300
C	-2.75315400	5.92603400	0.41493400
C	-3.12699200	6.30812000	-0.87306300
H	-3.36064100	5.67603000	-2.92361600
H	-2.58510400	3.35093300	-2.47250500
H	-2.02906200	4.35484700	1.67135200
H	-2.79332700	6.64207800	1.23022400
H	-3.46333800	7.32343200	-1.06286300
C	-1.82353500	2.28548000	-0.20000600
C	-1.64531200	1.80552700	1.24165300
O	-1.92786100	1.44054200	-1.09660600

S	-0.51153400	0.27264800	1.28100300
O	0.33603300	-0.07032700	0.13316200
C	0.45425300	0.58557400	2.76052200
H	-0.23160500	0.83357500	3.57290800
H	1.02396400	-0.32124700	2.96857100
H	1.12566600	1.41553700	2.52037500
C	-1.55054600	-1.14363200	1.68844300
H	-0.86078900	-1.98553300	1.76609200
H	-2.08869100	-0.96751000	2.61878400
H	-2.24189200	-1.28815200	0.85796300
C	-2.94487100	1.47074700	1.91833500
C	-3.99125600	0.86885200	1.20508400
C	-3.09800600	1.72519400	3.28768900
C	-5.16258200	0.49982000	1.86037500
H	-3.88489900	0.69279000	0.14209200
C	-4.27498600	1.36091400	3.94069500
H	-2.30019500	2.22072900	3.83602300
C	-5.30389200	0.73930700	3.22940200
H	-5.95500400	0.01788800	1.29767000
H	-4.38981000	1.56508800	5.00098600
H	-6.21753800	0.45022800	3.74024100
H	-1.06597100	2.50859000	1.84885900
N	0.43661800	2.88488700	-0.28539600
N	0.64538500	3.39855900	0.77215000
N	0.75511100	3.86964900	1.84120900

R-TS2

C	0.27098700	3.06146100	-1.99467500
C	1.64915100	2.43655600	-2.16883300
C	0.96341700	1.10645800	-2.23841900
C	-0.29924700	1.69405900	-1.99352100
O	-0.17303000	4.19368300	-1.86521500
O	2.79351000	2.85289000	-2.15095500
N	1.32737800	-0.18072300	-2.42629200
H	0.57915000	-0.86046800	-2.63389000
N	-1.54658900	1.25377700	-1.75268300
H	-1.67648500	0.25681000	-1.57364300
C	2.57296200	-0.75631300	-2.14676400
C	3.66047600	-0.01722200	-1.66418900
C	2.68669700	-2.14976200	-2.26849000
C	4.81545500	-0.68302600	-1.26141600
H	3.61226900	1.06355600	-1.60420800
C	3.85298400	-2.78879500	-1.86614000
H	1.85794400	-2.72594500	-2.65741500

C	4.92933800	-2.06857400	-1.34705700
H	5.83069200	-2.57389000	-1.02399000
C	3.92132100	-4.29066200	-1.90038200
C	5.89686400	0.11380700	-0.58935800
F	7.10082400	-0.49016800	-0.65977800
F	5.62338000	0.27284000	0.74299400
F	6.02268400	1.35145900	-1.10029500
F	3.10453200	-4.81872800	-2.83151800
F	3.56244000	-4.82993700	-0.70681600
F	5.17530300	-4.72722100	-2.15659400
C	-2.46538400	2.17123300	-1.05458900
H	-2.21004800	3.16656500	-1.41518100
C	-3.95893500	1.93619800	-1.41267900
C	-4.77472400	3.10462300	-0.83161100
H	-4.44972200	4.06685700	-1.24322500
H	-5.83564700	2.97863100	-1.07292200
H	-4.68929600	3.14973200	0.26095200
C	-4.52045200	0.61877700	-0.85721100
H	-4.58751000	0.65144100	0.23415700
H	-5.53247100	0.46030200	-1.24711200
H	-3.90920900	-0.24142900	-1.13609300
C	-4.08308500	1.94322600	-2.94584100
H	-3.66247000	2.86067600	-3.37379100
H	-3.55672500	1.09442400	-3.39094700
H	-5.13813200	1.88531100	-3.23607100
C	-2.11337300	2.07428600	0.44578800
O	-2.02196400	0.96031000	0.99347200
N	-1.78545000	3.20198300	1.11010600
C	-1.15613700	3.10491900	2.44311500
C	-2.00164500	4.60464200	0.68717500
C	-1.36538900	4.52274400	3.01413700
H	-1.68723300	2.35422000	3.03306100
C	-1.29238200	5.42339100	1.77412500
H	-1.58378500	4.78012200	-0.30491800
H	-2.35970900	4.58630900	3.47241100
H	-1.76684600	6.39670200	1.92373400
H	-0.25006800	5.59908300	1.49317400
H	-3.07517200	4.81948200	0.67202300
H	-0.62051200	4.76877000	3.77434800
C	0.31367400	2.71491300	2.35306400
C	0.89672800	1.97131200	3.38523600
C	1.12608900	3.14470000	1.29599600
C	2.26025900	1.67311300	3.36987800
H	0.27757600	1.62687800	4.21151500

C	2.49066500	2.84898900	1.27691100
H	0.69986000	3.70999500	0.47598500
C	3.06369200	2.11412400	2.31658200
H	2.69236000	1.08531400	4.17492800
H	3.09244700	3.17786800	0.43517000
H	4.11859700	1.85989900	2.28299400
C	-4.99657000	-5.17164500	-0.22237700
C	-3.81733700	-4.48803500	0.07176400
C	-3.38733400	-3.43604400	-0.75130800
C	-4.15009200	-3.09340800	-1.87853000
C	-5.31544500	-3.78985100	-2.17814400
C	-5.74630500	-4.82785500	-1.34750000
H	-5.32370700	-5.97814300	0.42708300
H	-3.25513400	-4.77975100	0.95298000
H	-3.79539100	-2.29230700	-2.51669200
H	-5.88942800	-3.52523500	-3.06142000
H	-6.65984200	-5.36803200	-1.57842300
C	-2.17313600	-2.61537400	-0.47941300
C	-1.22518000	-3.05071300	0.61018100
O	-2.03902800	-1.50634300	-1.01170000
S	-2.16803900	-2.46548000	2.39470600
O	-2.45111900	-3.62874400	3.28177400
C	-1.14995700	-1.22940400	3.23490800
H	-1.14622300	-0.31473900	2.63675900
H	-1.61889500	-1.07880100	4.21113500
H	-0.14414600	-1.63616400	3.34207400
C	-3.65006900	-1.50362300	2.03247700
H	-4.08581800	-1.21214200	2.99148700
H	-3.33425400	-0.63471300	1.44871200
H	-4.33194100	-2.14386300	1.47262700
C	0.13899500	-2.50032500	0.73668700
C	1.16336100	-3.36298500	1.15979800
C	0.41177600	-1.13421200	0.57037700
C	2.43731700	-2.86594100	1.42140200
H	0.95994500	-4.42482100	1.26138200
C	1.68103500	-0.64426600	0.85076600
H	-0.37780000	-0.45912600	0.27496500
C	2.69402200	-1.50092000	1.28245600
H	3.22893200	-3.54520000	1.71913500
H	1.87720600	0.41294500	0.73481000
H	3.68364600	-1.10516000	1.48094900
H	-1.27842400	-4.11363800	0.82999500
N	-0.54727400	-2.27249200	-3.18727300
N	-0.61284700	-3.19210500	-2.45528900

N	-0.73946000	-4.06748100	-1.66285400

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C	-0.02041100	3.09234600	-2.43845700
C	1.41521000	2.58190900	-2.42060900
C	0.85149300	1.20159900	-2.27960400
C	-0.47069000	1.69810700	-2.21743500
O	-0.56707800	4.18159900	-2.53872200
O	2.51559700	3.10399500	-2.41972500
N	1.33269900	-0.05878200	-2.19714800
H	0.65813000	-0.82937100	-2.32451900
N	-1.68818100	1.18744200	-1.96439100
H	-1.74129000	0.23006700	-1.61298000
C	2.58437900	-0.45278300	-1.70740100
C	3.59087400	0.46113900	-1.37128000
C	2.77413300	-1.81727500	-1.43928100
C	4.73973300	0.00537300	-0.72845900
H	3.47770400	1.51622300	-1.59327300
C	3.92791100	-2.24432500	-0.79572000
H	1.99708000	-2.52937800	-1.67711800
C	4.92571500	-1.34138500	-0.42773300
H	5.80753500	-1.67531100	0.10459600
C	4.09260900	-3.69894300	-0.45153000
C	5.71224200	1.01926300	-0.19786500
F	6.95933700	0.51961900	-0.07332800
F	5.33843200	1.43433600	1.05232300
F	5.78192500	2.12374600	-0.96128300
F	2.91425800	-4.35028100	-0.41269200
F	4.67592400	-3.84796300	0.76631500
F	4.88239100	-4.34384100	-1.33895100
C	-2.72794900	2.11821500	-1.48977200
H	-2.53744900	3.05556500	-2.01043700
C	-4.16776300	1.67851900	-1.87412300
C	-5.12058900	2.84384100	-1.55396700
H	-4.85557000	3.74672000	-2.11567500
H	-6.14782300	2.57324700	-1.82089100
H	-5.11212800	3.08733800	-0.48453000
C	-4.64633200	0.42903700	-1.11960200
H	-4.78815100	0.64480300	-0.05658600
H	-5.61219500	0.10576500	-1.52446100
H	-3.94416500	-0.40192400	-1.20828500
C	-4.18945100	1.40611900	-3.38784900
H	-3.82400500	2.27209900	-3.95202500
H	-3.56150600	0.54910800	-3.64645100

H	-5.21353400	1.19462900	-3.71530400
C	-2.47042200	2.31939100	0.01969000
O	-2.31804800	1.33300400	0.76318500
N	-2.29037500	3.57285000	0.48576800
C	-1.75182800	3.77320800	1.84649500
C	-2.59629600	4.85174600	-0.19543200
C	-2.12571600	5.24110400	2.13928600
H	-2.25508500	3.08783200	2.53256900
C	-2.04016500	5.91341200	0.76289500
H	-2.12525900	4.89106300	-1.17842300
H	-3.15293400	5.28488000	2.52095800
H	-2.60542800	6.84729300	0.70665500
H	-0.99886400	6.13685400	0.51370700
H	-3.68051200	4.95456700	-0.30840000
H	-1.46324800	5.68871300	2.88364300
C	-0.25032300	3.52394800	1.90870700
C	0.32426400	3.05345500	3.09478000
C	0.59126700	3.82735600	0.83100900
C	1.70722400	2.90228000	3.20824600
H	-0.31722600	2.80903600	3.93947600
C	1.97522800	3.67647500	0.93978000
H	0.17289300	4.18099500	-0.10364700
C	2.53881800	3.21689800	2.13162600
H	2.13395700	2.52661100	4.13406000
H	2.60203600	3.89949700	0.08172900
H	3.61244300	3.07343200	2.20284800
C	-4.92288100	-4.19705500	-1.69184400
C	-3.85258200	-3.34396100	-1.44763900
C	-3.15072100	-3.41403900	-0.23412100
C	-3.54539400	-4.35274400	0.73133900
C	-4.63142800	-5.19326800	0.48954700
C	-5.32028800	-5.12081300	-0.72141200
H	-5.44860900	-4.14390200	-2.64075800
H	-3.52375400	-2.62880400	-2.19278100
H	-3.02874200	-4.43424500	1.68224900
H	-4.93303400	-5.90940800	1.24812400
H	-6.16036700	-5.78292200	-0.90994000
C	-2.04007400	-2.43953100	-0.03710200
C	-1.14223100	-2.58830300	1.16539300
O	-1.97211300	-1.42302400	-0.73981800
S	-2.26632700	-1.80454500	2.75396700
O	-2.51486700	-2.81863600	3.81662600
C	-1.42955700	-0.34549400	3.41878100
H	-1.45996100	0.44777500	2.66760000

H	-1.98560100	-0.07655700	4.32104500
H	-0.40339500	-0.62396800	3.65961200
C	-3.79288900	-1.07199500	2.13303900
H	-4.32569800	-0.66313000	2.99528200
H	-3.50829900	-0.29078000	1.42285900
H	-4.37091500	-1.86380300	1.65643700
C	0.15539900	-1.89234700	1.27972200
C	1.20740400	-2.55994400	1.92955500
C	0.32435600	-0.55647400	0.88735400
C	2.40253400	-1.89749400	2.19563800
H	1.08747600	-3.60295900	2.20698800
C	1.51587100	0.10145100	1.16914600
H	-0.48932000	-0.02729100	0.41350600
C	2.55204200	-0.55759900	1.83000500
H	3.22065900	-2.43160400	2.66745800
H	1.63145300	1.13550500	0.87450000
H	3.48104000	-0.03417300	2.02719200
H	-1.11813700	-3.59979600	1.56248700
N	-0.33380400	-2.39504900	-2.70384600
N	-0.33767300	-3.17757600	-1.82425800
N	-0.40604400	-3.90833300	-0.89029300

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C	-0.02238300	3.09195000	-2.43868900
C	1.41358600	2.58249500	-2.42068500
C	0.85080200	1.20179900	-2.27962100
C	-0.47172800	1.69741700	-2.21767600
O	-0.56979200	4.18083200	-2.53895400
O	2.51361700	3.10532500	-2.41977300
N	1.33292600	-0.05821500	-2.19694300
H	0.65895200	-0.82935000	-2.32403200
N	-1.68893400	1.18593900	-1.96486600
H	-1.74140500	0.22862800	-1.61320500
C	2.58495800	-0.45125000	-1.70726000
C	3.59065600	0.46339400	-1.37074900
C	2.77587100	-1.81568100	-1.43964400
C	4.73984800	0.00835400	-0.72798000
H	3.47666800	1.51844900	-1.59245100
C	3.92988600	-2.24199400	-0.79604100
H	1.99951900	-2.52831100	-1.67816100
C	4.92688100	-1.33833500	-0.42760800
H	5.80890000	-1.67170000	0.10473900
C	4.09575500	-3.69660700	-0.45236900
C	5.71153400	1.02289900	-0.19711800

F	6.95889100	0.52406400	-0.07202000
F	5.33697900	1.43791100	1.05287700
F	5.78083700	2.12733100	-0.96064800
F	2.91794700	-4.34897300	-0.41423200
F	4.67868200	-3.84550000	0.76567800
F	4.88645100	-4.34056700	-1.33964800
C	-2.72938300	2.11602600	-1.49042500
H	-2.53959400	3.05342400	-2.01126000
C	-4.16885900	1.67508200	-1.87467400
C	-5.12266900	2.83965200	-1.55473100
H	-4.85819500	3.74275100	-2.11633800
H	-6.14962300	2.56827900	-1.82193900
H	-5.11467200	3.08313200	-0.48528500
C	-4.64623200	0.42535900	-1.11980900
H	-4.78705800	0.64104600	-0.05665600
H	-5.61234200	0.10165600	-1.52372000
H	-3.94370400	-0.40523100	-1.20918200
C	-4.19038700	1.40233200	-3.38833300
H	-3.82636600	2.26876100	-3.95274400
H	-3.56118100	0.54623100	-3.64686800
H	-5.21420300	1.18921600	-3.71556900
C	-2.47199700	2.31764700	0.01900000
O	-2.31860700	1.33150500	0.76262400
N	-2.29321400	3.57132500	0.48494900
C	-1.75507600	3.77228900	1.84576100
C	-2.60030800	4.84987200	-0.19635700
C	-2.12984700	5.24005300	2.13814600
H	-2.25809800	3.08677500	2.53187600
C	-2.04449300	5.91202400	0.76158200
H	-2.12974400	4.88934200	-1.17956400
H	-3.15714600	5.28334000	2.51965800
H	-2.60997900	6.84574900	0.70502700
H	-1.00323800	6.13561400	0.51233100
H	-3.68465600	4.95194600	-0.30880400
H	-1.46773800	5.68822900	2.88248100
C	-0.25344700	3.52389200	1.90834900
C	0.32116100	3.05404600	3.09466800
C	0.58819700	3.82758100	0.83077500
C	1.70419200	2.90380000	3.20850000
H	-0.32037100	2.80942400	3.93927400
C	1.97223100	3.67765800	0.93992200
H	0.16980400	4.18072400	-0.10405800
C	2.53583500	3.21874300	2.13201500
H	2.13095400	2.52863000	4.13450400

H	2.59910600	3.90092800	0.08198400
H	3.60954100	3.07605600	2.20354700
C	-4.92035600	-4.19912800	-1.69171100
C	-3.85022900	-3.34580000	-1.44757100
C	-3.14882600	-3.41512300	-0.23375100
C	-3.54375200	-4.35335400	0.73206900
C	-4.62959300	-5.19413900	0.49032200
C	-5.31801900	-5.12240800	-0.72093000
H	-5.44573000	-4.14654800	-2.64085300
H	-3.52115500	-2.63103000	-2.19297300
H	-3.02742600	-4.43430400	1.68320800
H	-4.93138800	-5.90992000	1.24916300
H	-6.15794900	-5.78471800	-0.90941600
C	-2.03828500	-2.44047600	-0.03686500
C	-1.14063700	-2.58874300	1.16589800
O	-1.96998400	-1.42444100	-0.74020500
S	-2.26484600	-1.80509300	2.75434800
O	-2.51259900	-2.81915100	3.81722200
C	-1.42869100	-0.34549400	3.41873400
H	-1.45935600	0.44755000	2.66732800
H	-1.98484500	-0.07650800	4.32091500
H	-0.40242300	-0.62349900	3.65965800
C	-3.79202600	-1.07352800	2.13379000
H	-4.32514000	-0.66558100	2.99628200
H	-3.50818800	-0.29170300	1.42398700
H	-4.36941300	-1.86558800	1.65683400
C	0.15676500	-1.89225600	1.27993500
C	1.20908300	-2.55915200	1.92997100
C	0.32505000	-0.55637100	0.88729400
C	2.40382400	-1.89598000	2.19604400
H	1.08970200	-3.60218000	2.20758900
C	1.51613900	0.10229500	1.16914300
H	-0.48881900	-0.02778000	0.41311700
C	2.55259800	-0.55604900	1.83025100
H	3.22220900	-2.42953500	2.66803800
H	1.63115400	1.13637400	0.87435800
H	3.48124200	-0.03203400	2.02753000
H	-1.11620200	-3.60016800	1.56314000
N	-0.33015500	-2.39746700	-2.70283200
N	-0.33488000	-3.17952000	-1.82283700
N	-0.40400500	-3.90988600	-0.88859400

S-C

C	0.67003600	-2.54502000	-2.82395800

C	-0.84425600	-2.31840200	-2.73395300
C	-0.53086600	-0.93920700	-2.23444800
C	0.85282300	-1.17006800	-2.30630800
O	1.41221100	-3.46490900	-3.12956200
O	-1.84297100	-2.98582800	-2.90772500
N	-1.24443700	0.13652000	-1.84091800
H	-0.70966000	0.96964400	-1.58684700
N	1.96170600	-0.47156300	-1.98068800
H	1.80356600	0.39849000	-1.47960800
C	-2.57637700	0.12048800	-1.39249000
C	-3.20769500	-1.06087000	-0.98425800
C	-3.24879500	1.33852300	-1.27494800
C	-4.49445600	-1.00708000	-0.46498100
H	-2.69938100	-2.00851000	-1.05997500
C	-4.53411500	1.37397500	-0.73666200
H	-2.76711100	2.25630700	-1.59060300
C	-5.17149700	0.20585100	-0.32804400
H	-6.17007100	0.23882000	0.08918400
C	-5.19312900	2.70850400	-0.52423000
C	-5.11457600	-2.25901500	0.08716700
F	-6.44214700	-2.31256900	-0.14249900
F	-4.95552600	-2.32862200	1.44087800
F	-4.56034000	-3.37974400	-0.41937000
F	-4.70744400	3.32481300	0.58474800
F	-6.52753800	2.59431400	-0.35423400
F	-4.98154200	3.54646100	-1.55880600
C	3.15031400	-1.23519300	-1.56425800
H	3.24455400	-2.05610100	-2.27439400
C	4.44268800	-0.37649700	-1.64648800
C	5.60139000	-1.16368000	-1.01217300
H	5.74323900	-2.13375900	-1.50198800
H	6.53590900	-0.60192800	-1.11506900
H	5.43519600	-1.33947800	0.05672300
C	4.27652000	0.96904500	-0.92321800
H	3.91004800	0.83835000	0.09597300
H	5.23510800	1.49839900	-0.88827800
H	3.57807000	1.62043600	-1.45295700
C	4.74927100	-0.11923000	-3.13116200
H	4.95139000	-1.05604600	-3.66369900
H	3.90516900	0.37473100	-3.62220700
H	5.62989700	0.52512500	-3.23230500
C	2.86060200	-1.79593500	-0.15728400
O	2.47282700	-1.03484600	0.74255200
N	2.95744500	-3.12786600	0.04438700

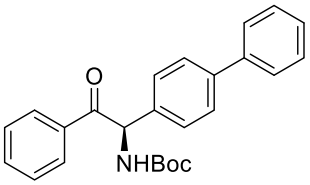
C	2.49114600	-3.70186900	1.32302300
C	3.53453600	-4.14633300	-0.85930200
C	3.12758500	-5.10818800	1.31165000
H	2.88002900	-3.09696900	2.14630700
C	3.17232700	-5.47149200	-0.17797100
H	3.10888900	-4.06549500	-1.86009000
H	4.14432300	-5.05132000	1.71872800
H	3.89469100	-6.25934900	-0.40693100
H	2.18835900	-5.80891600	-0.51725100
H	4.62226200	-4.01819800	-0.91302200
H	2.55605900	-5.81663100	1.91552300
C	0.97274700	-3.73527900	1.42046200
C	0.36176300	-3.61974100	2.67394300
C	0.16421400	-3.93600200	0.29496500
C	-1.02543200	-3.70292100	2.80248100
H	0.97687200	-3.45309400	3.55565200
C	-1.22408300	-4.01652000	0.41943100
H	0.61441100	-4.02519700	-0.68685400
C	-1.82465000	-3.89909500	1.67435200
H	-1.48256100	-3.59659700	3.78218900
H	-1.83175000	-4.16710300	-0.46764900
H	-2.90496600	-3.93977600	1.76546700
C	3.84415800	4.84929800	-1.95498400
C	2.70319200	4.08816600	-1.73783800
C	2.25959600	3.83044600	-0.42825600
C	2.97855300	4.34275100	0.66390600
C	4.13575300	5.08657200	0.43713200
C	4.56606000	5.34584600	-0.86460300
H	4.17465600	5.05573400	-2.96855600
H	2.13476900	3.68425000	-2.56878600
H	2.68139600	4.12434900	1.68494300
H	4.70001600	5.46517900	1.28402800
H	5.46273500	5.93583800	-1.03253700
C	1.05586400	2.98573300	-0.26644200
C	0.18523700	3.16411400	0.98818900
O	0.68789100	2.24544700	-1.18336300
S	2.62668300	1.40350600	2.65939400
O	2.49443500	2.72663900	3.41024400
C	1.82277900	0.11585200	3.67312300
H	1.89974100	-0.83026200	3.13413800
H	2.29497900	0.07600000	4.65840500
H	0.77363700	0.39955700	3.76357100
C	4.34041300	0.81078100	2.89092200
H	4.58764700	0.81660700	3.95603000

H	4.41564700	-0.19272700	2.46569400
H	4.99620200	1.49717600	2.35085600
C	-0.71949000	1.98828500	1.30505300
C	-1.99773100	2.19303900	1.83262800
C	-0.24767900	0.67772000	1.15698600
C	-2.79112400	1.10623600	2.20280900
H	-2.37999000	3.20026400	1.95196800
C	-1.03787700	-0.40440800	1.53259900
H	0.73914200	0.48102100	0.75902500
C	-2.31354600	-0.19518500	2.05770600
H	-3.79003700	1.28459800	2.58852900
H	-0.65393400	-1.40730300	1.39848100
H	-2.93958600	-1.04132000	2.31826700
H	0.81616700	3.37380200	1.85498500
N	-2.07810800	4.59482400	-1.03808000
N	-1.32601000	4.45415700	-0.19237300
N	-0.54061100	4.45070500	0.76615800

VII. Determination of the Product Stereochemistry

The absolute stereochemistry of the product derivative **8** was determined by X-ray crystallography. The X-ray data have been deposited at the Cambridge Crystallographic Data Center (CCDC 2149693). The stereochemistry of other products was assumed by analogy.

The single crystal of compound **8** was obtained by slow evaporation of its solution in *n*-hexane/Et_2O (5:1) at 0 °C.



8

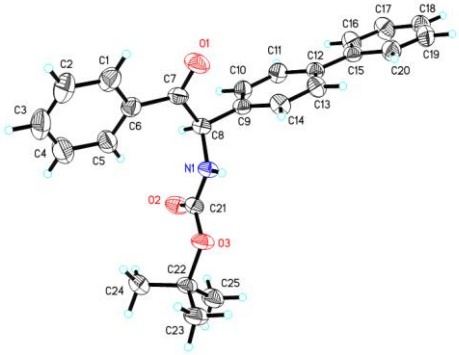


Table S4. Crystal data and structure refinement for **8**.

Identification code	**8**	
Empirical formula	C_{25} H_{25} N O_3	
Formula weight	387.46	
Temperature	293(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 10.5777(2) Å	α= 90°.
	b = 41.8595(7) Å	β= 115.1980(10)°.
	c = 10.6059(2) Å	γ = 90°.
Volume	4249.18(14) $Å^3$	
Z	8	
Density (calculated)	1.211 Mg/m^3	
Absorption coefficient	0.630 mm^{-1}	
F(000)	1648	
Crystal size	0.200 x 0.160 x 0.130 mm^3	
Theta range for data collection	4.607 to 67.496°.	

Index ranges	-12<=h<=12, -50<=k<=50, -11<=l<=12
Reflections collected	39522
Independent reflections	14813 [R(int) = 0.0304]
Completeness to theta = 67.679°	97.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.5692
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14813 / 1 / 1073
Goodness-of-fit on F^2	1.020
Final R indices [I>2sigma(I)]	R1 = 0.0386, wR2 = 0.1030
R indices (all data)	R1 = 0.0425, wR2 = 0.1071
Absolute structure parameter	0.05(5)
Extinction coefficient	n/a
Largest diff. peak and hole	0.132 and -0.106 e.$Å^{-3}$

Table S5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **8**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	2573(2)	3680(1)	6422(2)	54(1)
N(1A)	2477(2)	3699(1)	1371(2)	54(1)
N(1B)	3264(2)	6767(1)	2562(2)	60(1)
N(1C)	3458(2)	6794(1)	7582(2)	57(1)
O(1)	5517(3)	3490(1)	6226(3)	94(1)
O(2)	2027(2)	3691(1)	8270(2)	69(1)
O(3)	378(2)	3629(1)	6049(2)	66(1)
O(1A)	5419(3)	3526(1)	1157(3)	93(1)
O(2A)	1931(2)	3703(1)	3218(2)	68(1)
O(3A)	284(2)	3648(1)	996(2)	63(1)
O(1B)	5409(2)	6760(1)	5046(2)	85(1)
O(2B)	2587(2)	6790(1)	237(2)	72(1)
O(3B)	1603(2)	7103(1)	1322(2)	69(1)
O(1C)	5472(2)	6760(1)	10119(2)	88(1)
O(2C)	2641(2)	6781(1)	5236(2)	72(1)
O(3C)	1722(2)	7112(1)	6323(2)	68(1)
C(1)	5083(4)	2853(1)	6586(4)	80(1)

C(2)	4878(5)	2538(1)	6803(5)	103(1)
C(3)	4135(5)	2456(1)	7542(5)	101(1)
C(4)	3582(4)	2692(1)	8064(4)	96(1)
C(5)	3781(3)	3012(1)	7847(3)	74(1)
C(6)	4530(3)	3095(1)	7103(3)	62(1)
C(7)	4788(2)	3432(1)	6811(3)	58(1)
C(8)	4079(2)	3709(1)	7236(3)	52(1)
C(9)	4647(2)	4029(1)	7078(2)	51(1)
C(10)	5548(3)	4198(1)	8239(3)	61(1)
C(11)	6076(3)	4491(1)	8097(3)	66(1)
C(12)	5718(2)	4632(1)	6798(3)	55(1)
C(13)	4806(3)	4462(1)	5645(3)	64(1)
C(14)	4286(3)	4166(1)	5779(3)	64(1)
C(15)	6235(2)	4955(1)	6643(3)	58(1)
C(16)	7057(3)	5136(1)	7789(3)	76(1)
C(17)	7514(4)	5438(1)	7636(4)	86(1)
C(18)	7173(3)	5567(1)	6356(4)	76(1)
C(19)	6351(4)	5392(1)	5199(4)	82(1)
C(20)	5890(3)	5089(1)	5340(3)	74(1)
C(21)	1682(2)	3670(1)	7027(3)	53(1)
C(22)	-813(2)	3577(1)	6409(3)	59(1)
C(23)	-1967(3)	3476(1)	5014(3)	75(1)
C(24)	-508(3)	3307(1)	7439(3)	69(1)
C(25)	-1152(4)	3884(1)	6931(4)	81(1)
C(1A)	5055(4)	2886(1)	1554(4)	84(1)
C(2A)	4879(5)	2570(1)	1785(5)	109(1)
C(3A)	4149(5)	2486(1)	2535(5)	108(1)
C(4A)	3591(4)	2718(1)	3058(4)	98(1)
C(5A)	3754(3)	3038(1)	2829(3)	76(1)
C(6A)	4489(3)	3126(1)	2067(3)	64(1)
C(7A)	4708(2)	3464(1)	1758(3)	59(1)
C(8A)	3980(2)	3735(1)	2183(3)	55(1)
C(9A)	4534(2)	4059(1)	2028(3)	54(1)
C(10A)	5722(3)	4178(1)	3107(3)	64(1)
C(11A)	6308(3)	4463(1)	2958(3)	67(1)
C(12A)	5719(3)	4644(1)	1757(3)	59(1)
C(13A)	4502(3)	4526(1)	702(3)	76(1)
C(14A)	3923(3)	4240(1)	829(3)	75(1)

C(15A)	6351(3)	4948(1)	1578(3)	62(1)
C(16A)	7779(3)	4995(1)	2192(4)	88(1)
C(17A)	8348(4)	5279(1)	1985(5)	102(1)
C(18A)	7526(4)	5515(1)	1175(4)	86(1)
C(19A)	6123(4)	5471(1)	541(4)	86(1)
C(20A)	5540(3)	5190(1)	731(4)	79(1)
C(21A)	1587(2)	3685(1)	1975(2)	52(1)
C(22A)	-902(2)	3592(1)	1361(3)	58(1)
C(23A)	-2072(3)	3502(1)	-44(3)	78(1)
C(24A)	-1220(3)	3894(1)	1935(4)	80(1)
C(25A)	-605(3)	3315(1)	2352(3)	72(1)
C(1B)	8103(3)	6556(1)	5652(3)	76(1)
C(2B)	9420(3)	6439(1)	5974(4)	90(1)
C(3B)	9619(3)	6203(1)	5192(3)	84(1)
C(4B)	8494(4)	6082(1)	4084(3)	88(1)
C(5B)	7161(3)	6201(1)	3733(3)	76(1)
C(6B)	6945(3)	6440(1)	4513(3)	58(1)
C(7B)	5558(3)	6587(1)	4204(3)	59(1)
C(8B)	4324(3)	6526(1)	2782(3)	55(1)
C(9B)	3735(2)	6188(1)	2652(2)	53(1)
C(10B)	3116(3)	6079(1)	3484(3)	58(1)
C(11B)	2534(3)	5777(1)	3301(3)	64(1)
C(12B)	2561(3)	5572(1)	2275(3)	64(1)
C(13B)	3167(3)	5687(1)	1435(3)	72(1)
C(14B)	3749(3)	5988(1)	1624(3)	65(1)
C(15B)	1958(3)	5245(1)	2044(4)	75(1)
C(16B)	2035(3)	5056(1)	3139(4)	92(1)
C(17B)	1518(4)	4746(1)	2918(6)	115(2)
C(18B)	931(5)	4623(1)	1600(7)	126(2)
C(19B)	800(5)	4808(1)	480(6)	125(2)
C(20B)	1324(4)	5117(1)	709(4)	100(1)
C(21B)	2489(3)	6879(1)	1275(3)	55(1)
C(22B)	813(4)	7301(1)	82(3)	73(1)
C(23B)	30(7)	7526(1)	597(4)	140(2)
C(24B)	1833(5)	7477(1)	-332(4)	107(1)
C(25B)	-187(4)	7096(1)	-1099(4)	91(1)
C(1C)	8109(3)	6493(1)	11002(3)	69(1)
C(2C)	9442(3)	6380(1)	11391(3)	80(1)

C(3C)	9833(3)	6250(1)	10430(3)	75(1)
C(4C)	8884(3)	6235(1)	9056(3)	71(1)
C(5C)	7535(3)	6348(1)	8647(3)	63(1)
C(6C)	7123(2)	6476(1)	9619(3)	54(1)
C(7C)	5704(3)	6610(1)	9268(3)	56(1)
C(8C)	4512(2)	6552(1)	7811(2)	50(1)
C(9C)	3930(2)	6213(1)	7699(2)	47(1)
C(10C)	4332(2)	5971(1)	7059(3)	56(1)
C(11C)	3747(2)	5669(1)	6884(3)	57(1)
C(12C)	2704(2)	5602(1)	7317(2)	51(1)
C(13C)	2323(3)	5846(1)	7977(3)	59(1)
C(14C)	2933(2)	6144(1)	8175(3)	56(1)
C(15C)	2009(3)	5286(1)	7052(3)	56(1)
C(16C)	2743(3)	5007(1)	7137(3)	70(1)
C(17C)	2090(4)	4714(1)	6874(4)	86(1)
C(18C)	689(4)	4694(1)	6506(5)	98(1)
C(19C)	-65(4)	4966(1)	6404(5)	106(1)
C(20C)	585(3)	5260(1)	6676(4)	84(1)
C(21C)	2605(3)	6886(1)	6281(3)	55(1)
C(22C)	934(4)	7309(1)	5076(3)	78(1)
C(23C)	1953(5)	7484(1)	4662(4)	99(1)
C(24C)	142(7)	7534(1)	5603(4)	137(2)
C(25C)	-86(4)	7102(1)	3889(4)	91(1)

Table S6. Bond lengths [Å] and angles [°] for **8**.

N(1)-C(21)	1.348(3)
N(1)-C(8)	1.458(3)
N(1)-H(1)	0.88(3)
N(1A)-C(21A)	1.347(3)
N(1A)-C(8A)	1.458(3)
N(1A)-H(1A)	0.89(3)
N(1B)-C(21B)	1.344(3)
N(1B)-C(8B)	1.452(3)
N(1B)-H(1B)	0.83(4)
N(1C)-C(21C)	1.345(3)

N(1C)-C(8C)	1.448(3)
N(1C)-H(1C)	0.87(4)
O(1)-C(7)	1.201(3)
O(2)-C(21)	1.212(3)
O(3)-C(21)	1.337(3)
O(3)-C(22)	1.480(2)
O(1A)-C(7A)	1.203(3)
O(2A)-C(21A)	1.212(3)
O(3A)-C(21A)	1.336(3)
O(3A)-C(22A)	1.480(2)
O(1B)-C(7B)	1.211(3)
O(2B)-C(21B)	1.208(3)
O(3B)-C(21B)	1.342(3)
O(3B)-C(22B)	1.475(3)
O(1C)-C(7C)	1.207(3)
O(2C)-C(21C)	1.207(3)
O(3C)-C(21C)	1.344(3)
O(3C)-C(22C)	1.478(3)
C(1)-C(2)	1.372(5)
C(1)-C(6)	1.393(4)
C(1)-H(1D)	0.9300
C(2)-C(3)	1.369(7)
C(2)-H(2)	0.9300
C(3)-C(4)	1.377(6)
C(3)-H(3)	0.9300
C(4)-C(5)	1.390(5)
C(4)-H(4)	0.9300
C(5)-C(6)	1.379(4)
C(5)-H(5)	0.9300
C(6)-C(7)	1.497(4)
C(7)-C(8)	1.547(3)
C(8)-C(9)	1.507(3)
C(8)-H(8)	0.9800
C(9)-C(10)	1.387(3)
C(9)-C(14)	1.388(4)
C(10)-C(11)	1.384(4)
C(10)-H(10)	0.9300
C(11)-C(12)	1.395(4)

C(11)-H(11)	0.9300
C(12)-C(13)	1.390(4)
C(12)-C(15)	1.493(3)
C(13)-C(14)	1.386(4)
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
C(15)-C(16)	1.381(4)
C(15)-C(20)	1.390(4)
C(16)-C(17)	1.387(4)
C(16)-H(16)	0.9300
C(17)-C(18)	1.360(5)
C(17)-H(17)	0.9300
C(18)-C(19)	1.375(5)
C(18)-H(18)	0.9300
C(19)-C(20)	1.388(4)
C(19)-H(19)	0.9300
C(20)-H(20)	0.9300
C(22)-C(25)	1.504(4)
C(22)-C(24)	1.508(4)
C(22)-C(23)	1.523(4)
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600
C(25)-H(25C)	0.9600
C(1A)-C(2A)	1.371(6)
C(1A)-C(6A)	1.394(4)
C(1A)-H(1E)	0.9300
C(2A)-C(3A)	1.371(7)
C(2A)-H(2A)	0.9300
C(3A)-C(4A)	1.370(7)
C(3A)-H(3A)	0.9300
C(4A)-C(5A)	1.385(5)
C(4A)-H(4A)	0.9300

C(5A)-C(6A)	1.389(4)
C(5A)-H(5A)	0.9300
C(6A)-C(7A)	1.490(4)
C(7A)-C(8A)	1.542(3)
C(8A)-C(9A)	1.514(3)
C(8A)-H(8A)	0.9800
C(9A)-C(14A)	1.383(4)
C(9A)-C(10A)	1.384(3)
C(10A)-C(11A)	1.385(4)
C(10A)-H(10A)	0.9300
C(11A)-C(12A)	1.380(4)
C(11A)-H(11A)	0.9300
C(12A)-C(13A)	1.388(4)
C(12A)-C(15A)	1.486(4)
C(13A)-C(14A)	1.376(4)
C(13A)-H(13A)	0.9300
C(14A)-H(14A)	0.9300
C(15A)-C(16A)	1.382(4)
C(15A)-C(20A)	1.384(4)
C(16A)-C(17A)	1.392(5)
C(16A)-H(16A)	0.9300
C(17A)-C(18A)	1.354(5)
C(17A)-H(17A)	0.9300
C(18A)-C(19A)	1.357(5)
C(18A)-H(18A)	0.9300
C(19A)-C(20A)	1.384(4)
C(19A)-H(19A)	0.9300
C(20A)-H(20A)	0.9300
C(22A)-C(24A)	1.502(4)
C(22A)-C(25A)	1.506(4)
C(22A)-C(23A)	1.525(4)
C(23A)-H(23D)	0.9600
C(23A)-H(23E)	0.9600
C(23A)-H(23F)	0.9600
C(24A)-H(24D)	0.9600
C(24A)-H(24E)	0.9600
C(24A)-H(24F)	0.9600
C(25A)-H(25D)	0.9600

C(25A)-H(25E)	0.9600
C(25A)-H(25F)	0.9600
C(1B)-C(2B)	1.376(5)
C(1B)-C(6B)	1.391(4)
C(1B)-H(1F)	0.9300
C(2B)-C(3B)	1.362(5)
C(2B)-H(2B)	0.9300
C(3B)-C(4B)	1.365(5)
C(3B)-H(3B)	0.9300
C(4B)-C(5B)	1.389(4)
C(4B)-H(4B)	0.9300
C(5B)-C(6B)	1.378(4)
C(5B)-H(5B)	0.9300
C(6B)-C(7B)	1.492(4)
C(7B)-C(8B)	1.539(3)
C(8B)-C(9B)	1.526(3)
C(8B)-H(8B)	0.9800
C(9B)-C(14B)	1.379(3)
C(9B)-C(10B)	1.380(3)
C(10B)-C(11B)	1.385(4)
C(10B)-H(10B)	0.9300
C(11B)-C(12B)	1.394(4)
C(11B)-H(11B)	0.9300
C(12B)-C(13B)	1.386(4)
C(12B)-C(15B)	1.488(4)
C(13B)-C(14B)	1.381(4)
C(13B)-H(13B)	0.9300
C(14B)-H(14B)	0.9300
C(15B)-C(16B)	1.379(5)
C(15B)-C(20B)	1.390(5)
C(16B)-C(17B)	1.388(5)
C(16B)-H(16B)	0.9300
C(17B)-C(18B)	1.366(7)
C(17B)-H(17B)	0.9300
C(18B)-C(19B)	1.376(7)
C(18B)-H(18B)	0.9300
C(19B)-C(20B)	1.387(5)
C(19B)-H(19B)	0.9300

C(20B)-H(20B)	0.9300
C(22B)-C(23B)	1.502(5)
C(22B)-C(25B)	1.515(5)
C(22B)-C(24B)	1.519(6)
C(23B)-H(23G)	0.9600
C(23B)-H(23H)	0.9600
C(23B)-H(23I)	0.9600
C(24B)-H(24G)	0.9600
C(24B)-H(24H)	0.9600
C(24B)-H(24I)	0.9600
C(25B)-H(25G)	0.9600
C(25B)-H(25H)	0.9600
C(25B)-H(25I)	0.9600
C(1C)-C(2C)	1.374(4)
C(1C)-C(6C)	1.394(4)
C(1C)-H(1G)	0.9300
C(2C)-C(3C)	1.366(5)
C(2C)-H(2C)	0.9300
C(3C)-C(4C)	1.375(4)
C(3C)-H(3C)	0.9300
C(4C)-C(5C)	1.386(4)
C(4C)-H(4C)	0.9300
C(5C)-C(6C)	1.387(4)
C(5C)-H(5C)	0.9300
C(6C)-C(7C)	1.493(3)
C(7C)-C(8C)	1.542(3)
C(8C)-C(9C)	1.529(3)
C(8C)-H(8C)	0.9800
C(9C)-C(14C)	1.379(3)
C(9C)-C(10C)	1.384(3)
C(10C)-C(11C)	1.384(3)
C(10C)-H(10C)	0.9300
C(11C)-C(12C)	1.392(3)
C(11C)-H(11C)	0.9300
C(12C)-C(13C)	1.392(3)
C(12C)-C(15C)	1.480(3)
C(13C)-C(14C)	1.379(4)
C(13C)-H(13C)	0.9300

C(14C)-H(14C)	0.9300
C(15C)-C(16C)	1.385(4)
C(15C)-C(20C)	1.389(4)
C(16C)-C(17C)	1.376(4)
C(16C)-H(16C)	0.9300
C(17C)-C(18C)	1.365(5)
C(17C)-H(17C)	0.9300
C(18C)-C(19C)	1.370(5)
C(18C)-H(18C)	0.9300
C(19C)-C(20C)	1.379(4)
C(19C)-H(19C)	0.9300
C(20C)-H(20C)	0.9300
C(22C)-C(23C)	1.514(6)
C(22C)-C(24C)	1.517(5)
C(22C)-C(25C)	1.531(5)
C(23C)-H(23J)	0.9600
C(23C)-H(23K)	0.9600
C(23C)-H(23L)	0.9600
C(24C)-H(24J)	0.9600
C(24C)-H(24K)	0.9600
C(24C)-H(24L)	0.9600
C(25C)-H(25J)	0.9600
C(25C)-H(25K)	0.9600
C(25C)-H(25L)	0.9600

C(21)-N(1)-C(8)	122.0(2)
C(21)-N(1)-H(1)	117(2)
C(8)-N(1)-H(1)	121(2)
C(21A)-N(1A)-C(8A)	122.1(2)
C(21A)-N(1A)-H(1A)	117.6(17)
C(8A)-N(1A)-H(1A)	120.3(17)
C(21B)-N(1B)-C(8B)	120.2(2)
C(21B)-N(1B)-H(1B)	121(2)
C(8B)-N(1B)-H(1B)	119(2)
C(21C)-N(1C)-C(8C)	120.4(2)
C(21C)-N(1C)-H(1C)	121(2)
C(8C)-N(1C)-H(1C)	118(2)
C(21)-O(3)-C(22)	121.88(19)

C(21A)-O(3A)-C(22A)	121.64(18)
C(21B)-O(3B)-C(22B)	119.8(2)
C(21C)-O(3C)-C(22C)	119.8(2)
C(2)-C(1)-C(6)	120.7(4)
C(2)-C(1)-H(1D)	119.7
C(6)-C(1)-H(1D)	119.7
C(3)-C(2)-C(1)	120.3(4)
C(3)-C(2)-H(2)	119.8
C(1)-C(2)-H(2)	119.8
C(2)-C(3)-C(4)	119.9(3)
C(2)-C(3)-H(3)	120.0
C(4)-C(3)-H(3)	120.0
C(3)-C(4)-C(5)	120.2(4)
C(3)-C(4)-H(4)	119.9
C(5)-C(4)-H(4)	119.9
C(6)-C(5)-C(4)	120.0(3)
C(6)-C(5)-H(5)	120.0
C(4)-C(5)-H(5)	120.0
C(5)-C(6)-C(1)	118.9(3)
C(5)-C(6)-C(7)	123.7(3)
C(1)-C(6)-C(7)	117.4(3)
O(1)-C(7)-C(6)	120.6(2)
O(1)-C(7)-C(8)	120.0(2)
C(6)-C(7)-C(8)	119.4(2)
N(1)-C(8)-C(9)	113.3(2)
N(1)-C(8)-C(7)	107.97(19)
C(9)-C(8)-C(7)	111.49(18)
N(1)-C(8)-H(8)	108.0
C(9)-C(8)-H(8)	108.0
C(7)-C(8)-H(8)	108.0
C(10)-C(9)-C(14)	117.8(2)
C(10)-C(9)-C(8)	120.6(2)
C(14)-C(9)-C(8)	121.6(2)
C(11)-C(10)-C(9)	120.8(2)
C(11)-C(10)-H(10)	119.6
C(9)-C(10)-H(10)	119.6
C(10)-C(11)-C(12)	122.0(2)
C(10)-C(11)-H(11)	119.0

C(12)-C(11)-H(11)	119.0
C(13)-C(12)-C(11)	116.6(2)
C(13)-C(12)-C(15)	121.2(2)
C(11)-C(12)-C(15)	122.2(2)
C(14)-C(13)-C(12)	121.7(2)
C(14)-C(13)-H(13)	119.2
C(12)-C(13)-H(13)	119.2
C(13)-C(14)-C(9)	121.1(2)
C(13)-C(14)-H(14)	119.4
C(9)-C(14)-H(14)	119.4
C(16)-C(15)-C(20)	117.0(3)
C(16)-C(15)-C(12)	121.5(2)
C(20)-C(15)-C(12)	121.5(2)
C(15)-C(16)-C(17)	121.1(3)
C(15)-C(16)-H(16)	119.4
C(17)-C(16)-H(16)	119.4
C(18)-C(17)-C(16)	121.4(3)
C(18)-C(17)-H(17)	119.3
C(16)-C(17)-H(17)	119.3
C(17)-C(18)-C(19)	118.5(3)
C(17)-C(18)-H(18)	120.8
C(19)-C(18)-H(18)	120.8
C(18)-C(19)-C(20)	120.6(3)
C(18)-C(19)-H(19)	119.7
C(20)-C(19)-H(19)	119.7
C(19)-C(20)-C(15)	121.4(3)
C(19)-C(20)-H(20)	119.3
C(15)-C(20)-H(20)	119.3
O(2)-C(21)-O(3)	126.0(2)
O(2)-C(21)-N(1)	124.5(2)
O(3)-C(21)-N(1)	109.5(2)
O(3)-C(22)-C(25)	109.3(2)
O(3)-C(22)-C(24)	110.8(2)
C(25)-C(22)-C(24)	112.6(2)
O(3)-C(22)-C(23)	102.04(19)
C(25)-C(22)-C(23)	112.1(3)
C(24)-C(22)-C(23)	109.4(2)
C(22)-C(23)-H(23A)	109.5

C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(22)-C(25)-H(25A)	109.5
C(22)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(22)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(2A)-C(1A)-C(6A)	120.8(4)
C(2A)-C(1A)-H(1E)	119.6
C(6A)-C(1A)-H(1E)	119.6
C(3A)-C(2A)-C(1A)	120.3(4)
C(3A)-C(2A)-H(2A)	119.8
C(1A)-C(2A)-H(2A)	119.8
C(4A)-C(3A)-C(2A)	119.9(4)
C(4A)-C(3A)-H(3A)	120.0
C(2A)-C(3A)-H(3A)	120.0
C(3A)-C(4A)-C(5A)	120.5(4)
C(3A)-C(4A)-H(4A)	119.8
C(5A)-C(4A)-H(4A)	119.8
C(4A)-C(5A)-C(6A)	120.2(4)
C(4A)-C(5A)-H(5A)	119.9
C(6A)-C(5A)-H(5A)	119.9
C(5A)-C(6A)-C(1A)	118.3(3)
C(5A)-C(6A)-C(7A)	124.0(3)
C(1A)-C(6A)-C(7A)	117.7(3)
O(1A)-C(7A)-C(6A)	120.8(2)
O(1A)-C(7A)-C(8A)	120.0(3)
C(6A)-C(7A)-C(8A)	119.2(2)

N(1A)-C(8A)-C(9A)	113.7(2)
N(1A)-C(8A)-C(7A)	107.87(19)
C(9A)-C(8A)-C(7A)	111.27(19)
N(1A)-C(8A)-H(8A)	107.9
C(9A)-C(8A)-H(8A)	107.9
C(7A)-C(8A)-H(8A)	107.9
C(14A)-C(9A)-C(10A)	117.8(2)
C(14A)-C(9A)-C(8A)	122.8(2)
C(10A)-C(9A)-C(8A)	119.4(2)
C(9A)-C(10A)-C(11A)	120.7(3)
C(9A)-C(10A)-H(10A)	119.7
C(11A)-C(10A)-H(10A)	119.7
C(12A)-C(11A)-C(10A)	121.9(2)
C(12A)-C(11A)-H(11A)	119.0
C(10A)-C(11A)-H(11A)	119.0
C(11A)-C(12A)-C(13A)	116.7(2)
C(11A)-C(12A)-C(15A)	122.4(2)
C(13A)-C(12A)-C(15A)	121.0(3)
C(14A)-C(13A)-C(12A)	121.9(3)
C(14A)-C(13A)-H(13A)	119.0
C(12A)-C(13A)-H(13A)	119.0
C(13A)-C(14A)-C(9A)	120.9(3)
C(13A)-C(14A)-H(14A)	119.5
C(9A)-C(14A)-H(14A)	119.5
C(16A)-C(15A)-C(20A)	116.8(3)
C(16A)-C(15A)-C(12A)	121.6(3)
C(20A)-C(15A)-C(12A)	121.5(2)
C(15A)-C(16A)-C(17A)	120.6(3)
C(15A)-C(16A)-H(16A)	119.7
C(17A)-C(16A)-H(16A)	119.7
C(18A)-C(17A)-C(16A)	121.3(3)
C(18A)-C(17A)-H(17A)	119.4
C(16A)-C(17A)-H(17A)	119.4
C(17A)-C(18A)-C(19A)	119.1(3)
C(17A)-C(18A)-H(18A)	120.4
C(19A)-C(18A)-H(18A)	120.4
C(18A)-C(19A)-C(20A)	120.4(3)
C(18A)-C(19A)-H(19A)	119.8

C(20A)-C(19A)-H(19A)	119.8
C(19A)-C(20A)-C(15A)	121.8(3)
C(19A)-C(20A)-H(20A)	119.1
C(15A)-C(20A)-H(20A)	119.1
O(2A)-C(21A)-O(3A)	125.8(2)
O(2A)-C(21A)-N(1A)	124.6(2)
O(3A)-C(21A)-N(1A)	109.58(19)
O(3A)-C(22A)-C(24A)	109.6(2)
O(3A)-C(22A)-C(25A)	110.8(2)
C(24A)-C(22A)-C(25A)	112.4(2)
O(3A)-C(22A)-C(23A)	102.03(19)
C(24A)-C(22A)-C(23A)	112.1(3)
C(25A)-C(22A)-C(23A)	109.4(2)
C(22A)-C(23A)-H(23D)	109.5
C(22A)-C(23A)-H(23E)	109.5
H(23D)-C(23A)-H(23E)	109.5
C(22A)-C(23A)-H(23F)	109.5
H(23D)-C(23A)-H(23F)	109.5
H(23E)-C(23A)-H(23F)	109.5
C(22A)-C(24A)-H(24D)	109.5
C(22A)-C(24A)-H(24E)	109.5
H(24D)-C(24A)-H(24E)	109.5
C(22A)-C(24A)-H(24F)	109.5
H(24D)-C(24A)-H(24F)	109.5
H(24E)-C(24A)-H(24F)	109.5
C(22A)-C(25A)-H(25D)	109.5
C(22A)-C(25A)-H(25E)	109.5
H(25D)-C(25A)-H(25E)	109.5
C(22A)-C(25A)-H(25F)	109.5
H(25D)-C(25A)-H(25F)	109.5
H(25E)-C(25A)-H(25F)	109.5
C(2B)-C(1B)-C(6B)	120.9(3)
C(2B)-C(1B)-H(1F)	119.5
C(6B)-C(1B)-H(1F)	119.5
C(3B)-C(2B)-C(1B)	120.7(3)
C(3B)-C(2B)-H(2B)	119.6
C(1B)-C(2B)-H(2B)	119.6
C(2B)-C(3B)-C(4B)	119.3(3)

C(2B)-C(3B)-H(3B)	120.4
C(4B)-C(3B)-H(3B)	120.4
C(3B)-C(4B)-C(5B)	120.7(3)
C(3B)-C(4B)-H(4B)	119.7
C(5B)-C(4B)-H(4B)	119.7
C(6B)-C(5B)-C(4B)	120.6(3)
C(6B)-C(5B)-H(5B)	119.7
C(4B)-C(5B)-H(5B)	119.7
C(5B)-C(6B)-C(1B)	117.8(3)
C(5B)-C(6B)-C(7B)	124.4(2)
C(1B)-C(6B)-C(7B)	117.8(3)
O(1B)-C(7B)-C(6B)	120.5(2)
O(1B)-C(7B)-C(8B)	120.0(2)
C(6B)-C(7B)-C(8B)	119.4(2)
N(1B)-C(8B)-C(9B)	111.7(2)
N(1B)-C(8B)-C(7B)	108.4(2)
C(9B)-C(8B)-C(7B)	112.74(19)
N(1B)-C(8B)-H(8B)	107.9
C(9B)-C(8B)-H(8B)	107.9
C(7B)-C(8B)-H(8B)	107.9
C(14B)-C(9B)-C(10B)	118.2(2)
C(14B)-C(9B)-C(8B)	119.4(2)
C(10B)-C(9B)-C(8B)	122.3(2)
C(9B)-C(10B)-C(11B)	121.1(2)
C(9B)-C(10B)-H(10B)	119.5
C(11B)-C(10B)-H(10B)	119.5
C(10B)-C(11B)-C(12B)	121.0(2)
C(10B)-C(11B)-H(11B)	119.5
C(12B)-C(11B)-H(11B)	119.5
C(13B)-C(12B)-C(11B)	117.3(3)
C(13B)-C(12B)-C(15B)	119.7(3)
C(11B)-C(12B)-C(15B)	123.0(3)
C(14B)-C(13B)-C(12B)	121.5(3)
C(14B)-C(13B)-H(13B)	119.2
C(12B)-C(13B)-H(13B)	119.2
C(9B)-C(14B)-C(13B)	121.0(2)
C(9B)-C(14B)-H(14B)	119.5
C(13B)-C(14B)-H(14B)	119.5

C(16B)-C(15B)-C(20B)	117.8(3)
C(16B)-C(15B)-C(12B)	121.5(3)
C(20B)-C(15B)-C(12B)	120.6(3)
C(15B)-C(16B)-C(17B)	121.1(4)
C(15B)-C(16B)-H(16B)	119.4
C(17B)-C(16B)-H(16B)	119.4
C(18B)-C(17B)-C(16B)	119.9(4)
C(18B)-C(17B)-H(17B)	120.0
C(16B)-C(17B)-H(17B)	120.0
C(17B)-C(18B)-C(19B)	120.4(4)
C(17B)-C(18B)-H(18B)	119.8
C(19B)-C(18B)-H(18B)	119.8
C(18B)-C(19B)-C(20B)	119.3(5)
C(18B)-C(19B)-H(19B)	120.3
C(20B)-C(19B)-H(19B)	120.3
C(19B)-C(20B)-C(15B)	121.3(4)
C(19B)-C(20B)-H(20B)	119.3
C(15B)-C(20B)-H(20B)	119.3
O(2B)-C(21B)-O(3B)	125.6(2)
O(2B)-C(21B)-N(1B)	124.4(2)
O(3B)-C(21B)-N(1B)	109.9(2)
O(3B)-C(22B)-C(23B)	102.6(2)
O(3B)-C(22B)-C(25B)	110.5(2)
C(23B)-C(22B)-C(25B)	110.9(4)
O(3B)-C(22B)-C(24B)	109.1(3)
C(23B)-C(22B)-C(24B)	111.7(4)
C(25B)-C(22B)-C(24B)	111.6(3)
C(22B)-C(23B)-H(23G)	109.5
C(22B)-C(23B)-H(23H)	109.5
H(23G)-C(23B)-H(23H)	109.5
C(22B)-C(23B)-H(23I)	109.5
H(23G)-C(23B)-H(23I)	109.5
H(23H)-C(23B)-H(23I)	109.5
C(22B)-C(24B)-H(24G)	109.5
C(22B)-C(24B)-H(24H)	109.5
H(24G)-C(24B)-H(24H)	109.5
C(22B)-C(24B)-H(24I)	109.5
H(24G)-C(24B)-H(24I)	109.5

H(24H)-C(24B)-H(24I)	109.5
C(22B)-C(25B)-H(25G)	109.5
C(22B)-C(25B)-H(25H)	109.5
H(25G)-C(25B)-H(25H)	109.5
C(22B)-C(25B)-H(25I)	109.5
H(25G)-C(25B)-H(25I)	109.5
H(25H)-C(25B)-H(25I)	109.5
C(2C)-C(1C)-C(6C)	120.7(3)
C(2C)-C(1C)-H(1G)	119.6
C(6C)-C(1C)-H(1G)	119.6
C(3C)-C(2C)-C(1C)	120.8(3)
C(3C)-C(2C)-H(2C)	119.6
C(1C)-C(2C)-H(2C)	119.6
C(2C)-C(3C)-C(4C)	119.5(3)
C(2C)-C(3C)-H(3C)	120.2
C(4C)-C(3C)-H(3C)	120.3
C(3C)-C(4C)-C(5C)	120.4(3)
C(3C)-C(4C)-H(4C)	119.8
C(5C)-C(4C)-H(4C)	119.8
C(4C)-C(5C)-C(6C)	120.5(3)
C(4C)-C(5C)-H(5C)	119.8
C(6C)-C(5C)-H(5C)	119.8
C(5C)-C(6C)-C(1C)	118.1(2)
C(5C)-C(6C)-C(7C)	124.1(2)
C(1C)-C(6C)-C(7C)	117.7(2)
O(1C)-C(7C)-C(6C)	120.8(2)
O(1C)-C(7C)-C(8C)	119.4(2)
C(6C)-C(7C)-C(8C)	119.8(2)
N(1C)-C(8C)-C(9C)	112.25(18)
N(1C)-C(8C)-C(7C)	107.50(19)
C(9C)-C(8C)-C(7C)	110.75(18)
N(1C)-C(8C)-H(8C)	108.8
C(9C)-C(8C)-H(8C)	108.8
C(7C)-C(8C)-H(8C)	108.8
C(14C)-C(9C)-C(10C)	117.9(2)
C(14C)-C(9C)-C(8C)	120.7(2)
C(10C)-C(9C)-C(8C)	121.3(2)
C(11C)-C(10C)-C(9C)	121.4(2)

C(11C)-C(10C)-H(10C)	119.3
C(9C)-C(10C)-H(10C)	119.3
C(10C)-C(11C)-C(12C)	120.8(2)
C(10C)-C(11C)-H(11C)	119.6
C(12C)-C(11C)-H(11C)	119.6
C(13C)-C(12C)-C(11C)	117.2(2)
C(13C)-C(12C)-C(15C)	121.7(2)
C(11C)-C(12C)-C(15C)	121.1(2)
C(14C)-C(13C)-C(12C)	121.6(2)
C(14C)-C(13C)-H(13C)	119.2
C(12C)-C(13C)-H(13C)	119.2
C(13C)-C(14C)-C(9C)	121.0(2)
C(13C)-C(14C)-H(14C)	119.5
C(9C)-C(14C)-H(14C)	119.5
C(16C)-C(15C)-C(20C)	117.5(3)
C(16C)-C(15C)-C(12C)	121.5(2)
C(20C)-C(15C)-C(12C)	121.0(2)
C(17C)-C(16C)-C(15C)	121.4(3)
C(17C)-C(16C)-H(16C)	119.3
C(15C)-C(16C)-H(16C)	119.3
C(18C)-C(17C)-C(16C)	120.2(3)
C(18C)-C(17C)-H(17C)	119.9
C(16C)-C(17C)-H(17C)	119.9
C(17C)-C(18C)-C(19C)	119.7(3)
C(17C)-C(18C)-H(18C)	120.2
C(19C)-C(18C)-H(18C)	120.2
C(18C)-C(19C)-C(20C)	120.4(3)
C(18C)-C(19C)-H(19C)	119.8
C(20C)-C(19C)-H(19C)	119.8
C(19C)-C(20C)-C(15C)	120.9(3)
C(19C)-C(20C)-H(20C)	119.6
C(15C)-C(20C)-H(20C)	119.6
O(2C)-C(21C)-O(3C)	125.5(2)
O(2C)-C(21C)-N(1C)	124.6(2)
O(3C)-C(21C)-N(1C)	109.9(2)
O(3C)-C(22C)-C(23C)	109.2(3)
O(3C)-C(22C)-C(24C)	101.9(2)
C(23C)-C(22C)-C(24C)	112.3(4)

O(3C)-C(22C)-C(25C)	110.6(3)
C(23C)-C(22C)-C(25C)	112.0(3)
C(24C)-C(22C)-C(25C)	110.4(4)
C(22C)-C(23C)-H(23J)	109.5
C(22C)-C(23C)-H(23K)	109.5
H(23J)-C(23C)-H(23K)	109.5
C(22C)-C(23C)-H(23L)	109.5
H(23J)-C(23C)-H(23L)	109.5
H(23K)-C(23C)-H(23L)	109.5
C(22C)-C(24C)-H(24J)	109.5
C(22C)-C(24C)-H(24K)	109.5
H(24J)-C(24C)-H(24K)	109.5
C(22C)-C(24C)-H(24L)	109.5
H(24J)-C(24C)-H(24L)	109.5
H(24K)-C(24C)-H(24L)	109.5
C(22C)-C(25C)-H(25J)	109.5
C(22C)-C(25C)-H(25K)	109.5
H(25J)-C(25C)-H(25K)	109.5
C(22C)-C(25C)-H(25L)	109.5
H(25J)-C(25C)-H(25L)	109.5
H(25K)-C(25C)-H(25L)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S7. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **8**. 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}
N(1)	44(1)	72(1)	51(1)	-5(1)	25(1)	-5(1)
N(1A)	44(1)	74(1)	50(1)	-8(1)	24(1)	-7(1)
N(1B)	76(1)	56(1)	52(1)	5(1)	30(1)	11(1)
N(1C)	66(1)	51(1)	53(1)	5(1)	25(1)	12(1)
O(1)	100(2)	67(1)	160(2)	-11(1)	99(2)	-4(1)
O(2)	61(1)	97(1)	58(1)	-17(1)	34(1)	-15(1)
O(3)	44(1)	103(1)	57(1)	3(1)	27(1)	-6(1)
O(1A)	92(2)	80(1)	146(2)	-12(1)	89(2)	-5(1)

O(2A)	60(1)	96(1)	55(1)	-17(1)	32(1)	-16(1)
O(3A)	46(1)	96(1)	54(1)	-1(1)	28(1)	-5(1)
O(1B)	71(1)	112(2)	71(1)	-26(1)	30(1)	-2(1)
O(2B)	81(1)	84(1)	55(1)	3(1)	32(1)	18(1)
O(3B)	95(1)	61(1)	51(1)	7(1)	30(1)	24(1)
O(1C)	65(1)	122(2)	68(1)	-29(1)	22(1)	7(1)
O(2C)	79(1)	83(1)	55(1)	6(1)	31(1)	25(1)
O(3C)	85(1)	67(1)	51(1)	10(1)	27(1)	29(1)
C(1)	80(2)	65(2)	89(2)	-2(1)	31(2)	10(1)
C(2)	125(3)	60(2)	121(3)	8(2)	48(3)	19(2)
C(3)	121(3)	57(2)	107(3)	11(2)	30(2)	0(2)
C(4)	98(2)	86(2)	95(2)	17(2)	35(2)	-17(2)
C(5)	77(2)	63(2)	77(2)	4(1)	30(2)	-10(1)
C(6)	51(1)	59(1)	65(2)	-1(1)	16(1)	-2(1)
C(7)	47(1)	60(1)	71(2)	-7(1)	28(1)	-6(1)
C(8)	47(1)	58(1)	55(1)	-6(1)	25(1)	-5(1)
C(9)	46(1)	52(1)	59(1)	-5(1)	27(1)	0(1)
C(10)	61(1)	60(1)	56(1)	0(1)	17(1)	-4(1)
C(11)	64(1)	60(1)	60(2)	-6(1)	13(1)	-8(1)
C(12)	52(1)	52(1)	65(1)	-4(1)	30(1)	0(1)
C(13)	75(2)	64(1)	57(1)	-4(1)	31(1)	-9(1)
C(14)	72(2)	66(2)	55(1)	-12(1)	28(1)	-14(1)
C(15)	53(1)	52(1)	74(2)	-5(1)	34(1)	1(1)
C(16)	95(2)	62(2)	77(2)	-9(1)	42(2)	-12(1)
C(17)	105(2)	60(2)	101(2)	-16(2)	52(2)	-22(2)
C(18)	82(2)	54(1)	106(2)	2(1)	53(2)	-4(1)
C(19)	82(2)	71(2)	91(2)	17(2)	36(2)	-2(2)
C(20)	72(2)	67(2)	76(2)	3(1)	26(1)	-7(1)
C(21)	52(1)	58(1)	57(1)	-4(1)	30(1)	-4(1)
C(22)	51(1)	78(2)	61(1)	3(1)	35(1)	-4(1)
C(23)	52(1)	110(2)	67(2)	2(2)	30(1)	-7(1)
C(24)	72(2)	73(2)	68(2)	-1(1)	36(1)	-14(1)
C(25)	77(2)	72(2)	115(3)	-5(2)	60(2)	-3(1)
C(1A)	80(2)	79(2)	87(2)	0(2)	29(2)	15(2)
C(2A)	131(3)	67(2)	120(3)	7(2)	45(3)	20(2)
C(3A)	123(3)	67(2)	110(3)	12(2)	27(3)	3(2)
C(4A)	96(2)	91(2)	95(3)	17(2)	29(2)	-18(2)
C(5A)	76(2)	72(2)	76(2)	3(1)	30(2)	-6(1)

C(6A)	52(1)	67(2)	64(2)	-2(1)	15(1)	-1(1)
C(7A)	46(1)	67(2)	67(2)	-8(1)	26(1)	-5(1)
C(8A)	48(1)	66(1)	52(1)	-7(1)	24(1)	-7(1)
C(9A)	49(1)	61(1)	55(1)	-8(1)	26(1)	-3(1)
C(10A)	55(1)	67(2)	62(2)	-2(1)	16(1)	-2(1)
C(11A)	53(1)	67(2)	69(2)	-12(1)	15(1)	-8(1)
C(12A)	55(1)	59(1)	67(2)	-11(1)	30(1)	-2(1)
C(13A)	76(2)	74(2)	65(2)	4(1)	17(1)	-14(1)
C(14A)	66(2)	81(2)	62(2)	0(1)	12(1)	-20(1)
C(15A)	58(1)	61(1)	70(2)	-13(1)	32(1)	-3(1)
C(16A)	62(2)	74(2)	120(3)	9(2)	31(2)	-3(1)
C(17A)	72(2)	94(2)	137(3)	3(2)	42(2)	-19(2)
C(18A)	96(2)	68(2)	101(2)	-8(2)	50(2)	-18(2)
C(19A)	99(2)	64(2)	90(2)	-1(2)	35(2)	-1(2)
C(20A)	68(2)	66(2)	96(2)	-4(2)	28(2)	-2(1)
C(21A)	50(1)	59(1)	52(1)	-6(1)	27(1)	-4(1)
C(22A)	51(1)	76(2)	60(1)	0(1)	34(1)	-6(1)
C(23A)	50(1)	122(3)	68(2)	-4(2)	30(1)	-11(2)
C(24A)	75(2)	78(2)	107(2)	-8(2)	58(2)	-4(1)
C(25A)	76(2)	75(2)	74(2)	-2(1)	40(2)	-17(1)
C(1B)	69(2)	85(2)	71(2)	-12(2)	26(1)	-10(2)
C(2B)	61(2)	109(3)	88(2)	-7(2)	19(2)	-4(2)
C(3B)	68(2)	109(2)	71(2)	15(2)	25(1)	16(2)
C(4B)	81(2)	103(2)	73(2)	0(2)	25(2)	24(2)
C(5B)	70(2)	89(2)	58(2)	-5(1)	18(1)	8(2)
C(6B)	61(1)	63(1)	51(1)	9(1)	24(1)	-3(1)
C(7B)	63(1)	64(1)	51(1)	0(1)	27(1)	-6(1)
C(8B)	60(1)	55(1)	50(1)	4(1)	25(1)	4(1)
C(9B)	52(1)	57(1)	48(1)	6(1)	20(1)	6(1)
C(10B)	61(1)	59(1)	52(1)	2(1)	25(1)	4(1)
C(11B)	62(1)	69(2)	62(2)	11(1)	28(1)	2(1)
C(12B)	57(1)	58(1)	72(2)	6(1)	22(1)	4(1)
C(13B)	83(2)	63(2)	80(2)	-13(1)	43(2)	-7(1)
C(14B)	75(2)	66(2)	64(2)	-6(1)	39(1)	-6(1)
C(15B)	62(2)	62(2)	94(2)	8(1)	27(1)	3(1)
C(16B)	70(2)	76(2)	110(3)	26(2)	21(2)	-1(2)
C(17B)	87(2)	83(2)	157(4)	39(3)	33(3)	-6(2)
C(18B)	107(3)	68(2)	199(6)	-5(3)	61(4)	-22(2)

C(19B)	135(4)	83(3)	157(4)	-27(3)	62(3)	-34(3)
C(20B)	109(3)	76(2)	115(3)	-14(2)	48(2)	-21(2)
C(21B)	66(1)	48(1)	56(1)	2(1)	29(1)	1(1)
C(22B)	101(2)	60(1)	49(1)	6(1)	22(1)	22(1)
C(23B)	212(6)	122(3)	74(2)	19(2)	51(3)	108(4)
C(24B)	133(3)	76(2)	89(2)	27(2)	26(2)	-5(2)
C(25B)	87(2)	80(2)	80(2)	3(2)	10(2)	11(2)
C(1C)	64(2)	78(2)	56(2)	3(1)	18(1)	3(1)
C(2C)	60(2)	95(2)	69(2)	8(2)	11(1)	8(2)
C(3C)	54(1)	71(2)	88(2)	10(1)	19(1)	7(1)
C(4C)	55(1)	74(2)	83(2)	-8(1)	29(1)	-1(1)
C(5C)	51(1)	68(2)	64(2)	-7(1)	20(1)	-4(1)
C(6C)	51(1)	51(1)	54(1)	3(1)	18(1)	-5(1)
C(7C)	54(1)	59(1)	53(1)	-2(1)	22(1)	-4(1)
C(8C)	50(1)	53(1)	47(1)	4(1)	20(1)	6(1)
C(9C)	44(1)	51(1)	40(1)	5(1)	12(1)	7(1)
C(10C)	52(1)	58(1)	64(1)	-2(1)	30(1)	0(1)
C(11C)	57(1)	53(1)	66(1)	-6(1)	30(1)	3(1)
C(12C)	43(1)	56(1)	50(1)	6(1)	15(1)	7(1)
C(13C)	57(1)	60(1)	67(2)	0(1)	33(1)	3(1)
C(14C)	59(1)	55(1)	59(1)	-3(1)	31(1)	5(1)
C(15C)	54(1)	56(1)	59(1)	4(1)	24(1)	3(1)
C(16C)	65(2)	58(1)	88(2)	3(1)	32(1)	6(1)
C(17C)	90(2)	57(2)	113(3)	1(2)	45(2)	5(2)
C(18C)	97(2)	64(2)	136(3)	-7(2)	53(2)	-19(2)
C(19C)	69(2)	82(2)	169(4)	-10(2)	52(2)	-16(2)
C(20C)	60(2)	66(2)	126(3)	-4(2)	40(2)	-2(1)
C(21C)	61(1)	50(1)	56(1)	5(1)	27(1)	6(1)
C(22C)	99(2)	76(2)	51(2)	15(1)	25(1)	38(2)
C(23C)	135(3)	71(2)	78(2)	23(2)	32(2)	11(2)
C(24C)	192(5)	141(4)	77(2)	29(2)	55(3)	118(4)
C(25C)	82(2)	109(3)	67(2)	16(2)	16(2)	23(2)

Table S8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **8**.

	x	y	z	U(eq)
H(1D)	5596	2905	6089	96
H(2)	5246	2378	6445	124
H(3)	4003	2243	7691	122
H(4)	3073	2637	8563	115
H(5)	3409	3170	8205	88
H(8)	4281	3681	8221	63
H(10)	5800	4113	9123	73
H(11)	6688	4598	8893	79
H(13)	4538	4548	4760	77
H(14)	3683	4058	4984	77
H(16)	7308	5054	8679	91
H(17)	8065	5554	8427	103
H(18)	7489	5769	6264	92
H(19)	6103	5477	4315	98
H(20)	5339	4974	4545	88
H(23A)	-2099	3639	4333	112
H(23B)	-2820	3446	5112	112
H(23C)	-1709	3280	4717	112
H(24A)	-94	3132	7163	103
H(24B)	-1362	3238	7463	103
H(24C)	127	3380	8348	103
H(25A)	-385	3943	7792	122
H(25B)	-1978	3856	7081	122
H(25C)	-1308	4050	6253	122
H(1E)	5559	2941	1050	101
H(2A)	5257	2413	1430	131
H(3A)	4032	2271	2689	130
H(4A)	3099	2660	3570	118
H(5A)	3371	3194	3187	91
H(8A)	4185	3705	3168	66
H(10A)	6131	4066	3941	77
H(11A)	7122	4535	3689	80
H(13A)	4064	4644	-114	91
H(14A)	3109	4168	97	90

H(16A)	8365	4836	2749	105
H(17A)	9312	5308	2411	123
H(18A)	7919	5705	1054	103
H(19A)	5549	5631	-23	103
H(20A)	4576	5163	277	95
H(23D)	-2222	3674	-693	118
H(23E)	-2915	3463	64	118
H(23F)	-1815	3313	-389	118
H(24D)	-453	3945	2809	120
H(24E)	-2052	3865	2074	120
H(24F)	-1357	4066	1290	120
H(25D)	-220	3142	2036	108
H(25E)	-1457	3247	2386	108
H(25F)	52	3380	3266	108
H(1F)	7985	6716	6204	92
H(2B)	10182	6521	6733	108
H(3B)	10511	6125	5412	101
H(4B)	8621	5918	3558	106
H(5B)	6407	6119	2965	91
H(8B)	4662	6553	2059	66
H(10B)	3090	6211	4178	69
H(11B)	2119	5709	3872	76
H(13B)	3181	5558	728	87
H(14B)	4158	6058	1051	78
H(16B)	2439	5137	4040	110
H(17B)	1572	4622	3667	139
H(18B)	617	4413	1458	151
H(19B)	365	4728	-421	150
H(20B)	1249	5242	-47	120
H(23G)	-645	7408	794	209
H(23H)	-439	7684	-104	209
H(23I)	675	7629	1432	209
H(24G)	2495	7591	458	160
H(24H)	1331	7625	-1067	160
H(24I)	2318	7326	-650	160
H(25G)	336	6951	-1398	136
H(25H)	-756	7230	-1865	136
H(25I)	-772	6976	-784	136

H(1G)	7861	6582	11669	83
H(2C)	10086	6392	12319	97
H(3C)	10734	6171	10704	90
H(4C)	9149	6149	8396	85
H(5C)	6901	6337	7715	75
H(8C)	4882	6578	7113	60
H(10C)	5009	6012	6739	67
H(11C)	4055	5510	6473	69
H(13C)	1640	5808	8291	71
H(14C)	2669	6301	8636	67
H(16C)	3696	5018	7377	84
H(17C)	2605	4529	6947	103
H(18C)	248	4496	6326	117
H(19C)	-1020	4953	6151	128
H(20C)	63	5444	6606	101
H(23J)	2610	7599	5449	149
H(23K)	1451	7630	3919	149
H(23L)	2443	7332	4355	149
H(24J)	-533	7416	5795	206
H(24K)	-328	7693	4907	206
H(24L)	786	7637	6441	206
H(25J)	430	6958	3579	137
H(25K)	-666	7236	3129	137
H(25L)	-661	6982	4215	137
H(1A)	2120(30)	3684(6)	450(30)	52(7)
H(1)	2210(30)	3667(7)	5510(30)	65(8)
H(1C)	3330(30)	6857(8)	8290(40)	72(9)
H(1B)	3150(30)	6835(8)	3240(40)	73(9)

Table S9. Torsion angles [°] for **8**.

C(6)-C(1)-C(2)-C(3)	-0.5(6)
C(1)-C(2)-C(3)-C(4)	0.4(7)
C(2)-C(3)-C(4)-C(5)	-0.3(6)
C(3)-C(4)-C(5)-C(6)	0.3(6)
C(4)-C(5)-C(6)-C(1)	-0.4(5)

C(4)-C(5)-C(6)-C(7)	179.5(3)
C(2)-C(1)-C(6)-C(5)	0.5(5)
C(2)-C(1)-C(6)-C(7)	-179.4(3)
C(5)-C(6)-C(7)-O(1)	175.7(3)
C(1)-C(6)-C(7)-O(1)	-4.4(4)
C(5)-C(6)-C(7)-C(8)	-5.8(4)
C(1)-C(6)-C(7)-C(8)	174.1(2)
C(21)-N(1)-C(8)-C(9)	-109.9(3)
C(21)-N(1)-C(8)-C(7)	126.2(2)
O(1)-C(7)-C(8)-N(1)	114.0(3)
C(6)-C(7)-C(8)-N(1)	-64.5(3)
O(1)-C(7)-C(8)-C(9)	-11.0(4)
C(6)-C(7)-C(8)-C(9)	170.5(2)
N(1)-C(8)-C(9)-C(10)	132.2(2)
C(7)-C(8)-C(9)-C(10)	-105.8(3)
N(1)-C(8)-C(9)-C(14)	-47.3(3)
C(7)-C(8)-C(9)-C(14)	74.7(3)
C(14)-C(9)-C(10)-C(11)	-0.7(4)
C(8)-C(9)-C(10)-C(11)	179.7(2)
C(9)-C(10)-C(11)-C(12)	0.9(4)
C(10)-C(11)-C(12)-C(13)	-0.4(4)
C(10)-C(11)-C(12)-C(15)	177.3(2)
C(11)-C(12)-C(13)-C(14)	-0.3(4)
C(15)-C(12)-C(13)-C(14)	-178.0(2)
C(12)-C(13)-C(14)-C(9)	0.6(4)
C(10)-C(9)-C(14)-C(13)	0.0(4)
C(8)-C(9)-C(14)-C(13)	179.5(2)
C(13)-C(12)-C(15)-C(16)	175.1(3)
C(11)-C(12)-C(15)-C(16)	-2.4(4)
C(13)-C(12)-C(15)-C(20)	-3.7(4)
C(11)-C(12)-C(15)-C(20)	178.7(3)
C(20)-C(15)-C(16)-C(17)	0.0(4)
C(12)-C(15)-C(16)-C(17)	-178.9(3)
C(15)-C(16)-C(17)-C(18)	-0.1(5)
C(16)-C(17)-C(18)-C(19)	0.3(5)
C(17)-C(18)-C(19)-C(20)	-0.4(5)
C(18)-C(19)-C(20)-C(15)	0.3(5)
C(16)-C(15)-C(20)-C(19)	-0.1(4)

C(12)-C(15)-C(20)-C(19)	178.8(3)
C(22)-O(3)-C(21)-O(2)	-5.3(4)
C(22)-O(3)-C(21)-N(1)	173.8(2)
C(8)-N(1)-C(21)-O(2)	1.8(4)
C(8)-N(1)-C(21)-O(3)	-177.3(2)
C(21)-O(3)-C(22)-C(25)	72.5(3)
C(21)-O(3)-C(22)-C(24)	-52.2(3)
C(21)-O(3)-C(22)-C(23)	-168.6(2)
C(6A)-C(1A)-C(2A)-C(3A)	-0.5(7)
C(1A)-C(2A)-C(3A)-C(4A)	0.0(7)
C(2A)-C(3A)-C(4A)-C(5A)	0.3(7)
C(3A)-C(4A)-C(5A)-C(6A)	-0.1(6)
C(4A)-C(5A)-C(6A)-C(1A)	-0.4(5)
C(4A)-C(5A)-C(6A)-C(7A)	179.5(3)
C(2A)-C(1A)-C(6A)-C(5A)	0.7(5)
C(2A)-C(1A)-C(6A)-C(7A)	-179.2(3)
C(5A)-C(6A)-C(7A)-O(1A)	175.9(3)
C(1A)-C(6A)-C(7A)-O(1A)	-4.3(4)
C(5A)-C(6A)-C(7A)-C(8A)	-5.7(4)
C(1A)-C(6A)-C(7A)-C(8A)	174.2(3)
C(21A)-N(1A)-C(8A)-C(9A)	-109.4(3)
C(21A)-N(1A)-C(8A)-C(7A)	126.7(2)
O(1A)-C(7A)-C(8A)-N(1A)	113.3(3)
C(6A)-C(7A)-C(8A)-N(1A)	-65.1(3)
O(1A)-C(7A)-C(8A)-C(9A)	-12.1(4)
C(6A)-C(7A)-C(8A)-C(9A)	169.5(2)
N(1A)-C(8A)-C(9A)-C(14A)	-29.5(3)
C(7A)-C(8A)-C(9A)-C(14A)	92.5(3)
N(1A)-C(8A)-C(9A)-C(10A)	152.3(2)
C(7A)-C(8A)-C(9A)-C(10A)	-85.7(3)
C(14A)-C(9A)-C(10A)-C(11A)	-2.8(4)
C(8A)-C(9A)-C(10A)-C(11A)	175.5(2)
C(9A)-C(10A)-C(11A)-C(12A)	1.9(4)
C(10A)-C(11A)-C(12A)-C(13A)	0.3(4)
C(10A)-C(11A)-C(12A)-C(15A)	-179.1(2)
C(11A)-C(12A)-C(13A)-C(14A)	-1.5(5)
C(15A)-C(12A)-C(13A)-C(14A)	178.0(3)
C(12A)-C(13A)-C(14A)-C(9A)	0.4(5)

C(10A)-C(9A)-C(14A)-C(13A)	1.7(4)
C(8A)-C(9A)-C(14A)-C(13A)	-176.5(3)
C(11A)-C(12A)-C(15A)-C(16A)	32.1(4)
C(13A)-C(12A)-C(15A)-C(16A)	-147.3(3)
C(11A)-C(12A)-C(15A)-C(20A)	-151.3(3)
C(13A)-C(12A)-C(15A)-C(20A)	29.3(4)
C(20A)-C(15A)-C(16A)-C(17A)	1.8(5)
C(12A)-C(15A)-C(16A)-C(17A)	178.6(3)
C(15A)-C(16A)-C(17A)-C(18A)	-0.4(6)
C(16A)-C(17A)-C(18A)-C(19A)	-0.8(6)
C(17A)-C(18A)-C(19A)-C(20A)	0.5(6)
C(18A)-C(19A)-C(20A)-C(15A)	0.9(5)
C(16A)-C(15A)-C(20A)-C(19A)	-2.1(5)
C(12A)-C(15A)-C(20A)-C(19A)	-178.9(3)
C(22A)-O(3A)-C(21A)-O(2A)	-6.0(4)
C(22A)-O(3A)-C(21A)-N(1A)	173.8(2)
C(8A)-N(1A)-C(21A)-O(2A)	0.8(4)
C(8A)-N(1A)-C(21A)-O(3A)	-179.1(2)
C(21A)-O(3A)-C(22A)-C(24A)	71.5(3)
C(21A)-O(3A)-C(22A)-C(25A)	-53.2(3)
C(21A)-O(3A)-C(22A)-C(23A)	-169.6(2)
C(6B)-C(1B)-C(2B)-C(3B)	-0.8(5)
C(1B)-C(2B)-C(3B)-C(4B)	-0.3(6)
C(2B)-C(3B)-C(4B)-C(5B)	1.3(6)
C(3B)-C(4B)-C(5B)-C(6B)	-1.1(5)
C(4B)-C(5B)-C(6B)-C(1B)	0.1(4)
C(4B)-C(5B)-C(6B)-C(7B)	178.9(3)
C(2B)-C(1B)-C(6B)-C(5B)	0.9(5)
C(2B)-C(1B)-C(6B)-C(7B)	-178.1(3)
C(5B)-C(6B)-C(7B)-O(1B)	168.6(3)
C(1B)-C(6B)-C(7B)-O(1B)	-12.5(4)
C(5B)-C(6B)-C(7B)-C(8B)	-13.4(4)
C(1B)-C(6B)-C(7B)-C(8B)	165.5(2)
C(21B)-N(1B)-C(8B)-C(9B)	-89.9(3)
C(21B)-N(1B)-C(8B)-C(7B)	145.3(2)
O(1B)-C(7B)-C(8B)-N(1B)	16.0(3)
C(6B)-C(7B)-C(8B)-N(1B)	-162.0(2)
O(1B)-C(7B)-C(8B)-C(9B)	-108.2(3)

C(6B)-C(7B)-C(8B)-C(9B)	73.8(3)
N(1B)-C(8B)-C(9B)-C(14B)	118.1(3)
C(7B)-C(8B)-C(9B)-C(14B)	-119.5(3)
N(1B)-C(8B)-C(9B)-C(10B)	-58.5(3)
C(7B)-C(8B)-C(9B)-C(10B)	63.9(3)
C(14B)-C(9B)-C(10B)-C(11B)	0.5(4)
C(8B)-C(9B)-C(10B)-C(11B)	177.1(2)
C(9B)-C(10B)-C(11B)-C(12B)	0.3(4)
C(10B)-C(11B)-C(12B)-C(13B)	-1.2(4)
C(10B)-C(11B)-C(12B)-C(15B)	179.6(2)
C(11B)-C(12B)-C(13B)-C(14B)	1.5(4)
C(15B)-C(12B)-C(13B)-C(14B)	-179.4(3)
C(10B)-C(9B)-C(14B)-C(13B)	-0.3(4)
C(8B)-C(9B)-C(14B)-C(13B)	-177.0(2)
C(12B)-C(13B)-C(14B)-C(9B)	-0.7(5)
C(13B)-C(12B)-C(15B)-C(16B)	144.6(3)
C(11B)-C(12B)-C(15B)-C(16B)	-36.3(4)
C(13B)-C(12B)-C(15B)-C(20B)	-34.0(4)
C(11B)-C(12B)-C(15B)-C(20B)	145.1(3)
C(20B)-C(15B)-C(16B)-C(17B)	1.2(5)
C(12B)-C(15B)-C(16B)-C(17B)	-177.5(3)
C(15B)-C(16B)-C(17B)-C(18B)	0.4(6)
C(16B)-C(17B)-C(18B)-C(19B)	-2.4(7)
C(17B)-C(18B)-C(19B)-C(20B)	2.7(8)
C(18B)-C(19B)-C(20B)-C(15B)	-1.0(7)
C(16B)-C(15B)-C(20B)-C(19B)	-0.9(6)
C(12B)-C(15B)-C(20B)-C(19B)	177.8(4)
C(22B)-O(3B)-C(21B)-O(2B)	-10.4(4)
C(22B)-O(3B)-C(21B)-N(1B)	169.6(2)
C(8B)-N(1B)-C(21B)-O(2B)	1.3(4)
C(8B)-N(1B)-C(21B)-O(3B)	-178.7(2)
C(21B)-O(3B)-C(22B)-C(23B)	-177.0(4)
C(21B)-O(3B)-C(22B)-C(25B)	64.6(4)
C(21B)-O(3B)-C(22B)-C(24B)	-58.5(4)
C(6C)-C(1C)-C(2C)-C(3C)	0.3(5)
C(1C)-C(2C)-C(3C)-C(4C)	0.7(5)
C(2C)-C(3C)-C(4C)-C(5C)	-0.8(5)
C(3C)-C(4C)-C(5C)-C(6C)	-0.1(4)

C(4C)-C(5C)-C(6C)-C(1C)	1.0(4)
C(4C)-C(5C)-C(6C)-C(7C)	178.7(2)
C(2C)-C(1C)-C(6C)-C(5C)	-1.1(4)
C(2C)-C(1C)-C(6C)-C(7C)	-178.9(3)
C(5C)-C(6C)-C(7C)-O(1C)	-169.0(3)
C(1C)-C(6C)-C(7C)-O(1C)	8.6(4)
C(5C)-C(6C)-C(7C)-C(8C)	11.7(4)
C(1C)-C(6C)-C(7C)-C(8C)	-170.6(2)
C(21C)-N(1C)-C(8C)-C(9C)	-84.5(3)
C(21C)-N(1C)-C(8C)-C(7C)	153.5(2)
O(1C)-C(7C)-C(8C)-N(1C)	21.4(3)
C(6C)-C(7C)-C(8C)-N(1C)	-159.4(2)
O(1C)-C(7C)-C(8C)-C(9C)	-101.6(3)
C(6C)-C(7C)-C(8C)-C(9C)	77.7(3)
N(1C)-C(8C)-C(9C)-C(14C)	-36.5(3)
C(7C)-C(8C)-C(9C)-C(14C)	83.7(2)
N(1C)-C(8C)-C(9C)-C(10C)	140.3(2)
C(7C)-C(8C)-C(9C)-C(10C)	-99.5(3)
C(14C)-C(9C)-C(10C)-C(11C)	0.7(3)
C(8C)-C(9C)-C(10C)-C(11C)	-176.2(2)
C(9C)-C(10C)-C(11C)-C(12C)	1.7(4)
C(10C)-C(11C)-C(12C)-C(13C)	-2.5(4)
C(10C)-C(11C)-C(12C)-C(15C)	176.0(2)
C(11C)-C(12C)-C(13C)-C(14C)	1.1(4)
C(15C)-C(12C)-C(13C)-C(14C)	-177.4(2)
C(12C)-C(13C)-C(14C)-C(9C)	1.3(4)
C(10C)-C(9C)-C(14C)-C(13C)	-2.1(3)
C(8C)-C(9C)-C(14C)-C(13C)	174.8(2)
C(13C)-C(12C)-C(15C)-C(16C)	-144.0(3)
C(11C)-C(12C)-C(15C)-C(16C)	37.5(4)
C(13C)-C(12C)-C(15C)-C(20C)	37.5(4)
C(11C)-C(12C)-C(15C)-C(20C)	-141.0(3)
C(20C)-C(15C)-C(16C)-C(17C)	-0.7(5)
C(12C)-C(15C)-C(16C)-C(17C)	-179.2(3)
C(15C)-C(16C)-C(17C)-C(18C)	0.7(5)
C(16C)-C(17C)-C(18C)-C(19C)	-0.2(6)
C(17C)-C(18C)-C(19C)-C(20C)	-0.2(7)
C(18C)-C(19C)-C(20C)-C(15C)	0.2(7)

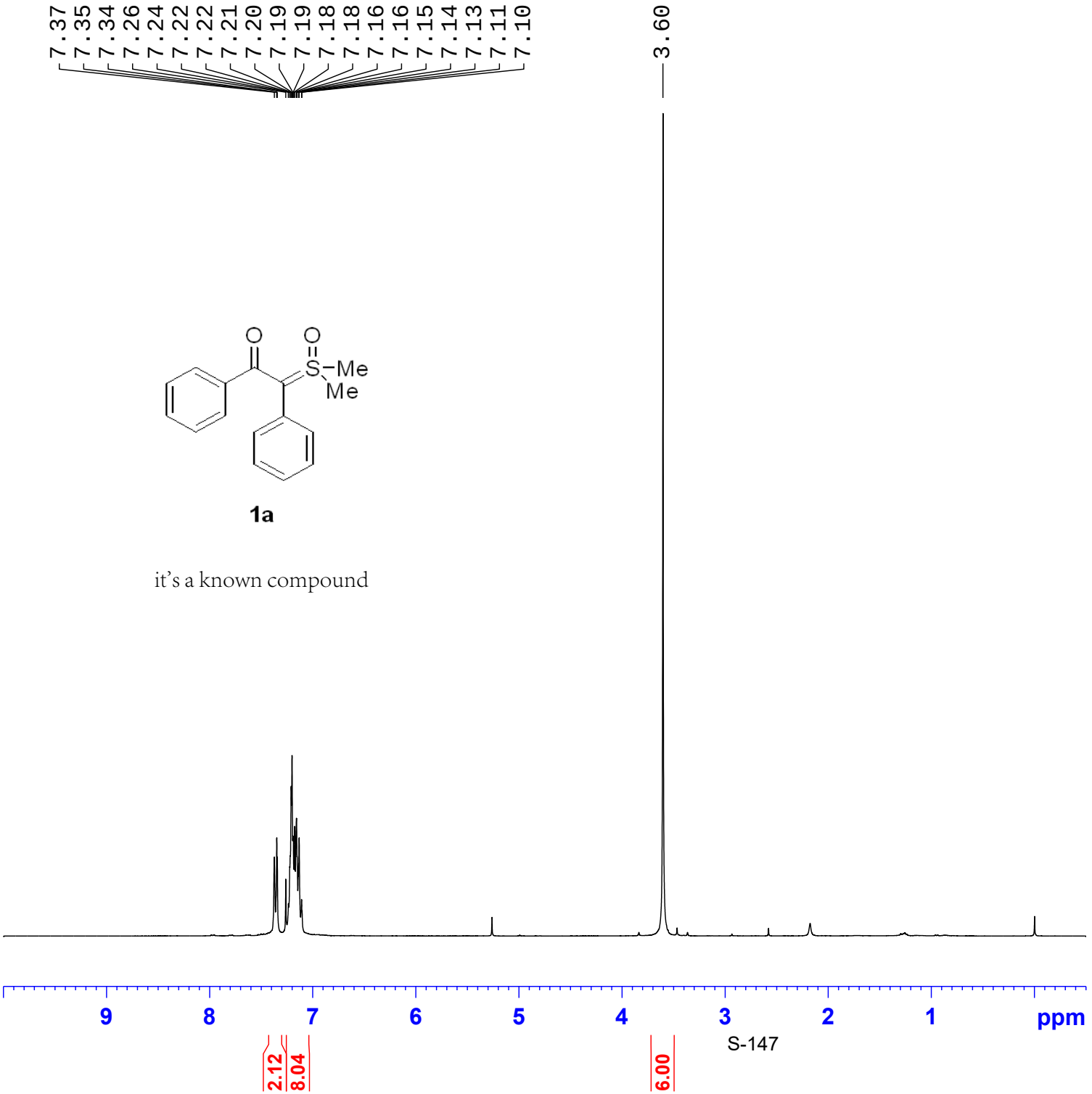
C(16C)-C(15C)-C(20C)-C(19C)	0.2(5)
C(12C)-C(15C)-C(20C)-C(19C)	178.8(3)
C(22C)-O(3C)-C(21C)-O(2C)	-15.2(4)
C(22C)-O(3C)-C(21C)-N(1C)	164.5(3)
C(8C)-N(1C)-C(21C)-O(2C)	-0.1(4)
C(8C)-N(1C)-C(21C)-O(3C)	-179.8(2)
C(21C)-O(3C)-C(22C)-C(23C)	-58.8(4)
C(21C)-O(3C)-C(22C)-C(24C)	-177.7(4)
C(21C)-O(3C)-C(22C)-C(25C)	64.9(4)

Table S10. Hydrogen bonds for **8** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1B)-H(1B)...O(2C)	0.83(4)	2.41(4)	3.174(3)	154(3)
N(1C)-H(1C)...O(2B)#1	0.87(4)	2.51(4)	3.314(3)	155(3)
N(1)-H(1)...O(2A)	0.88(3)	2.32(3)	3.171(3)	162(3)
N(1A)-H(1A)...O(2)#2	0.89(3)	2.27(3)	3.116(3)	159(2)
C(25C)-H(25J)...O(2C)	0.96	2.37	2.941(4)	117.9
C(23C)-H(23L)...O(2C)	0.96	2.46	3.027(4)	117.5
C(8C)-H(8C)...O(1B)	0.98	2.60	3.554(3)	165.8
C(25B)-H(25G)...O(2B)	0.96	2.37	2.952(4)	118.6
C(24B)-H(24I)...O(2B)	0.96	2.40	2.977(4)	118.0
C(25A)-H(25F)...O(2A)	0.96	2.42	2.929(3)	112.6
C(24A)-H(24D)...O(2A)	0.96	2.58	3.120(4)	116.2
C(23A)-H(23E)...O(1A)#3	0.96	2.50	3.399(3)	155.7
C(25)-H(25A)...O(2)	0.96	2.60	3.148(4)	116.2
C(24)-H(24C)...O(2)	0.96	2.43	2.921(3)	111.8
C(23)-H(23B)...O(1)#3	0.96	2.51	3.415(3)	157.1

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z+1 #2 x,y,z-1 #3 x-1,y,z



1a

it's a known compound

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PROCNO                   1
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TD                   65536
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FIDRES            0.091699 Hz
AQ                5.4526453 sec
RG                     80.6
DW                   83.200 usec
DE                    6.50 usec
TE                   291.1 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           300.1318534 MHz
NUC1                   1H
P1                  10.00 usec
SI                   65536
SF             300.1300065 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
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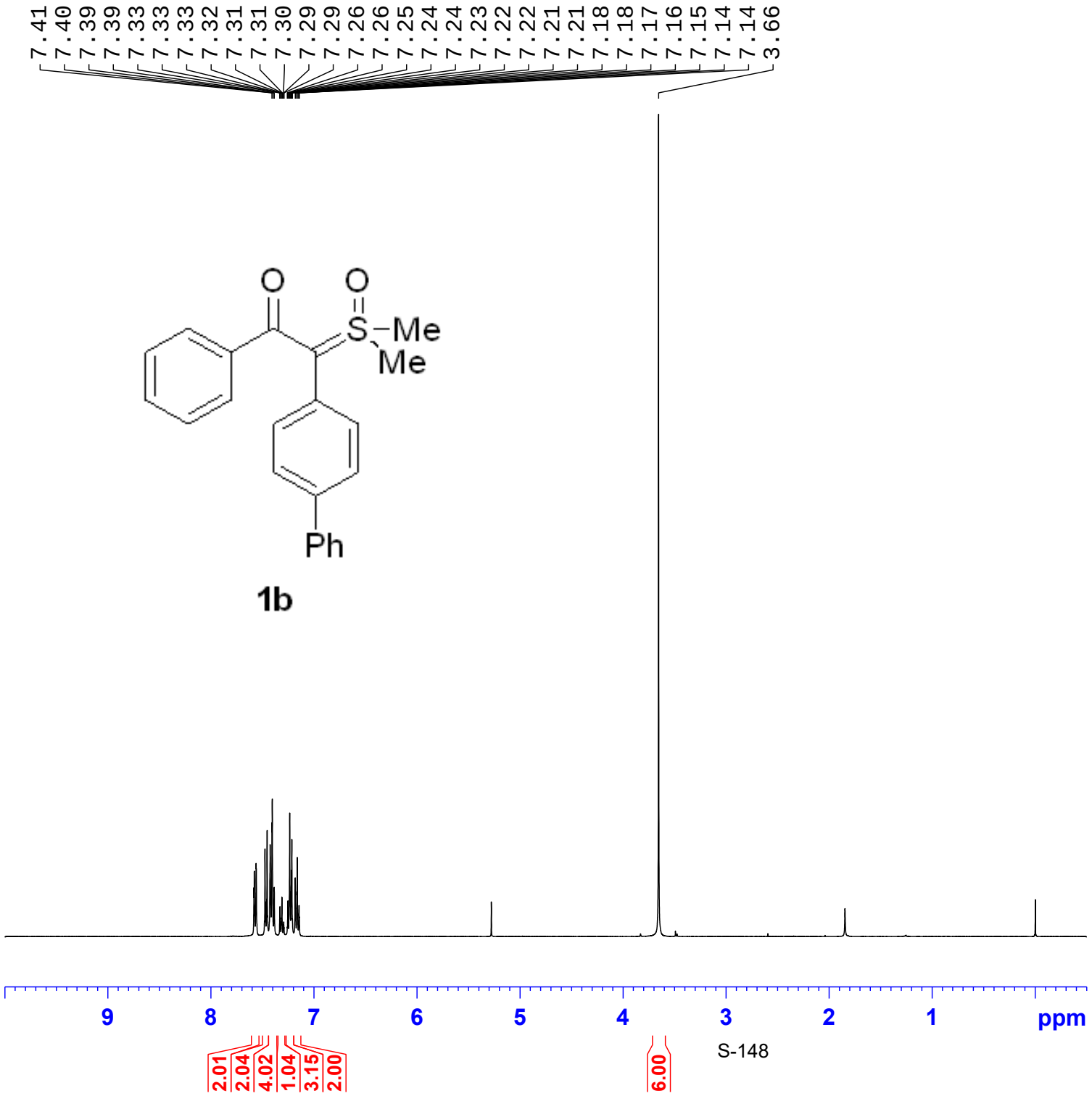

BRUKER

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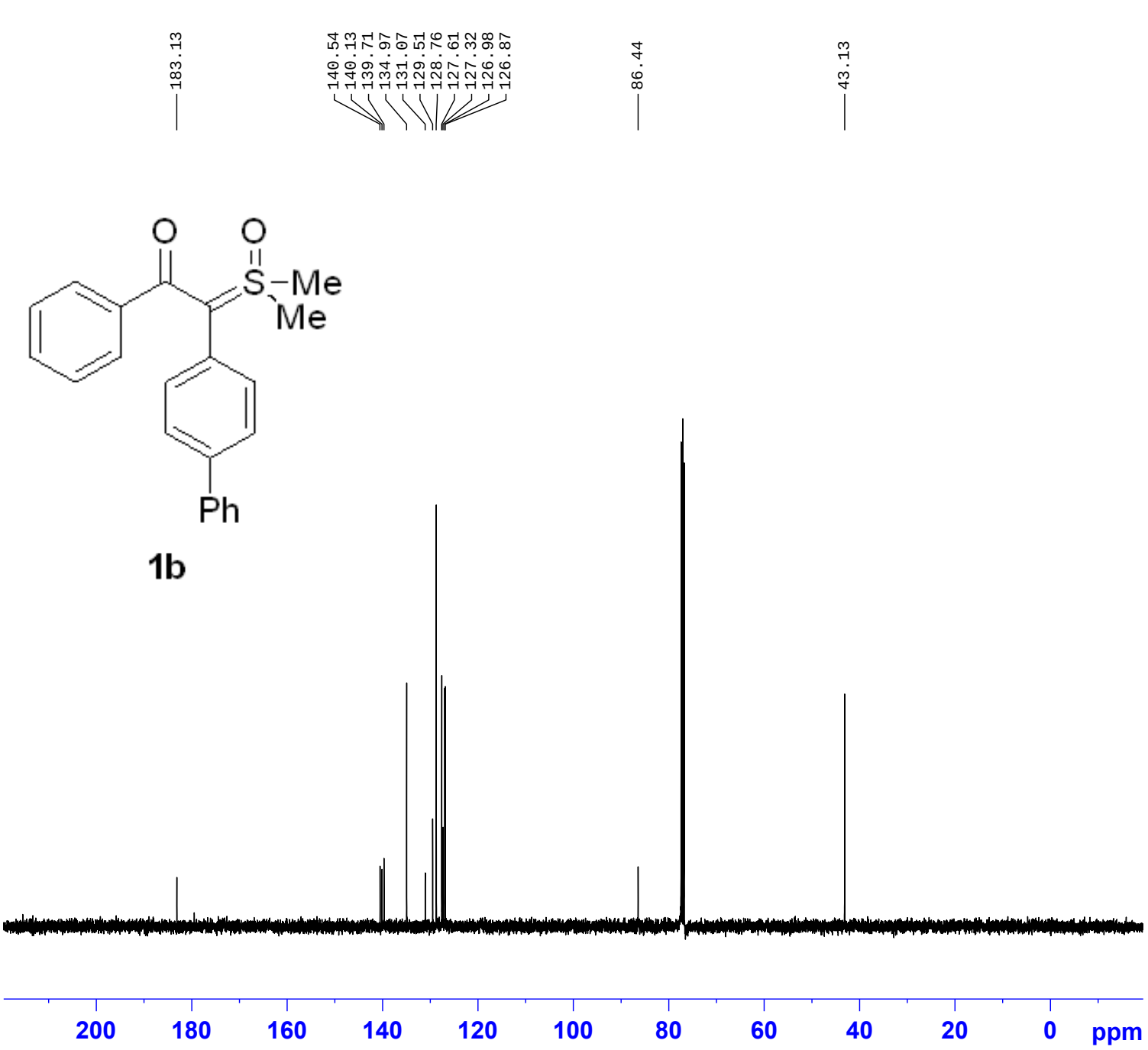
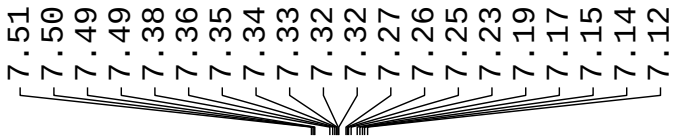
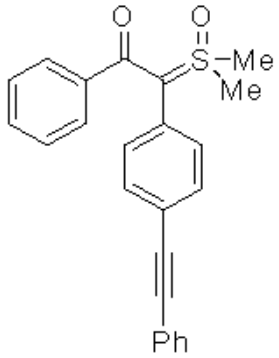
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	100.49
DW	60.800 usec
DE	6.50 usec
TE	293.8 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.40 usec
SI	65536
SF	400.1900182 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



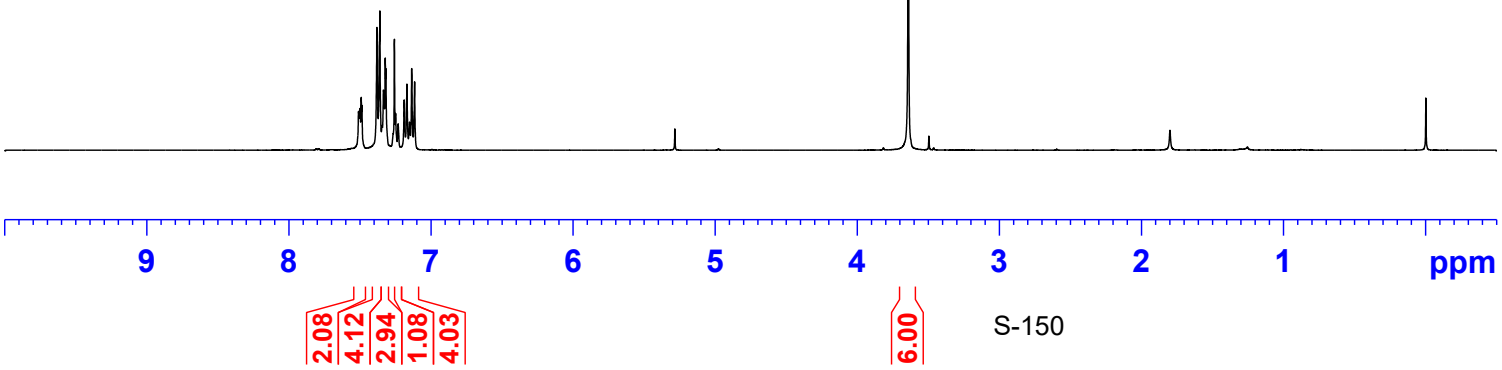

```
NAME          CNMR-gwg-1-37
EXPNO                    86
PROCNO                    1
Date_              20210401
Time                  14.47
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       62
DS                        4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                   193.13
DW                   20.800 usec
DE                    6.50 usec
TE                   294.4 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    9.90 usec
SI                   32768
SF            100.6278560 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

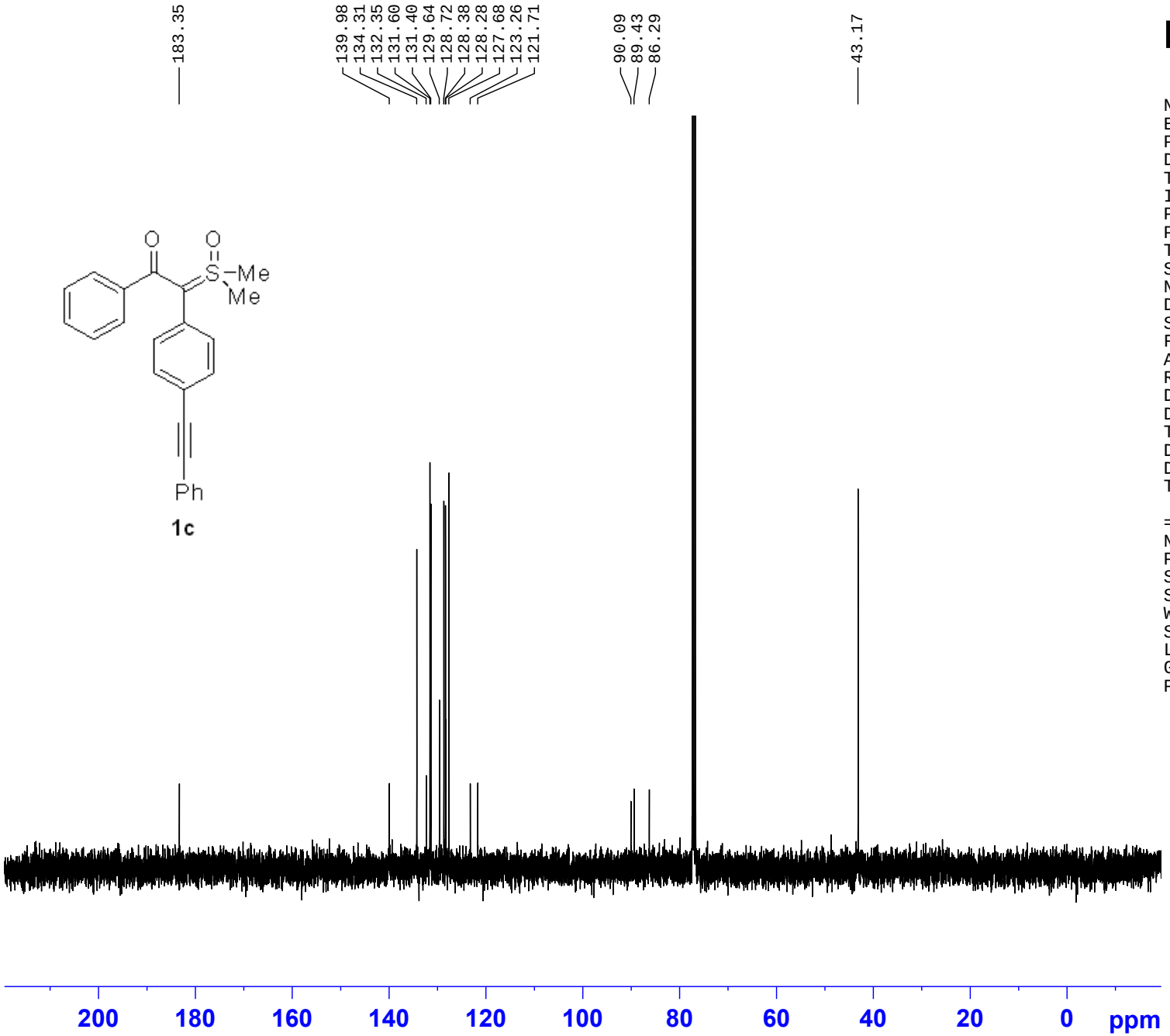




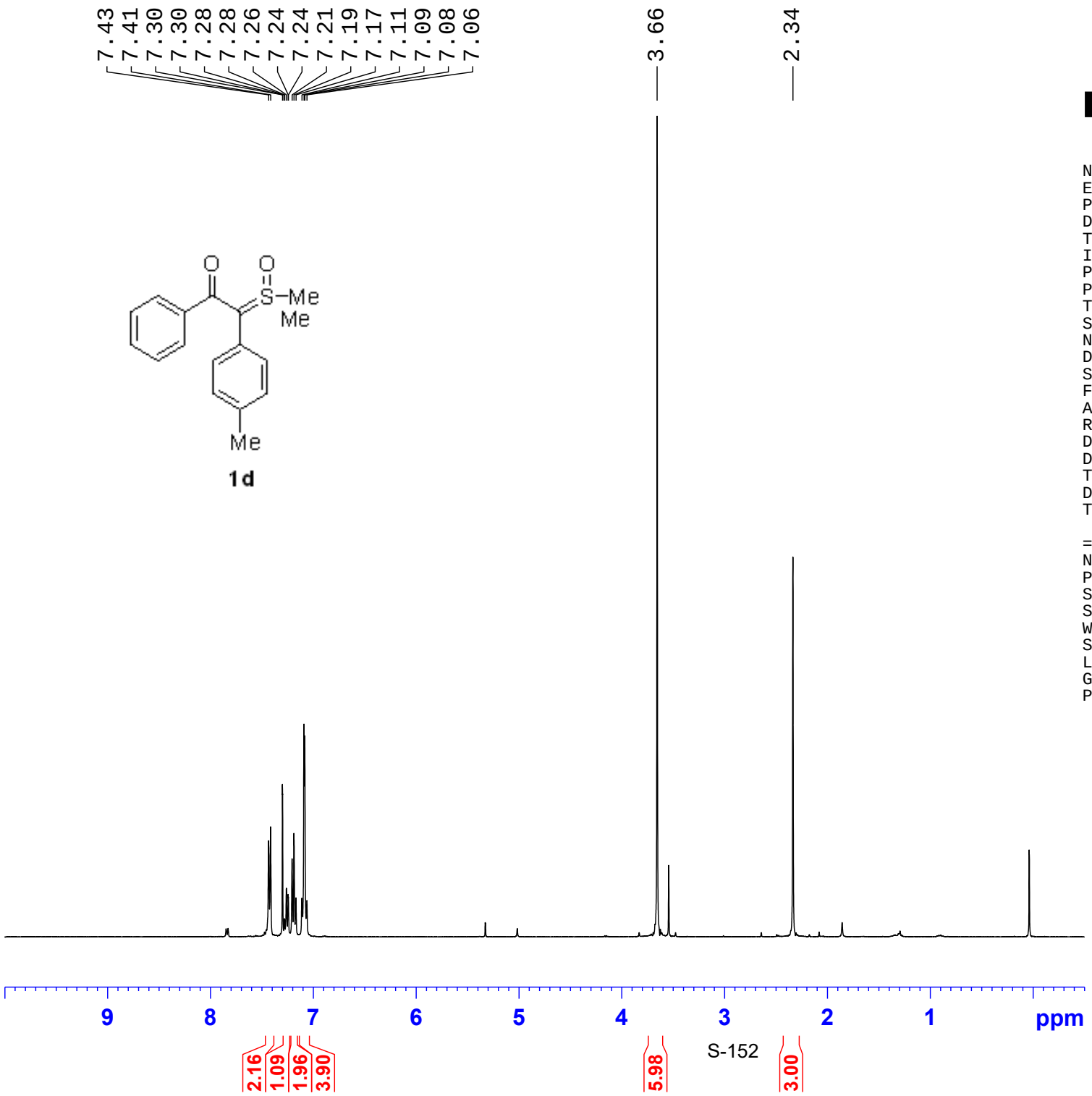
1c

```
NAME        HNMR-gwg-wm-1-29
EXPNO                    117
PROCNO                     1
Date_             20210412
Time                  14.34
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        6
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                    140.02
DW                    60.800 usec
DE                     6.50 usec
TE                    293.7 K
D1              1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                    14.40 usec
SI                    65536
SF             400.1900163 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                     1.00
```

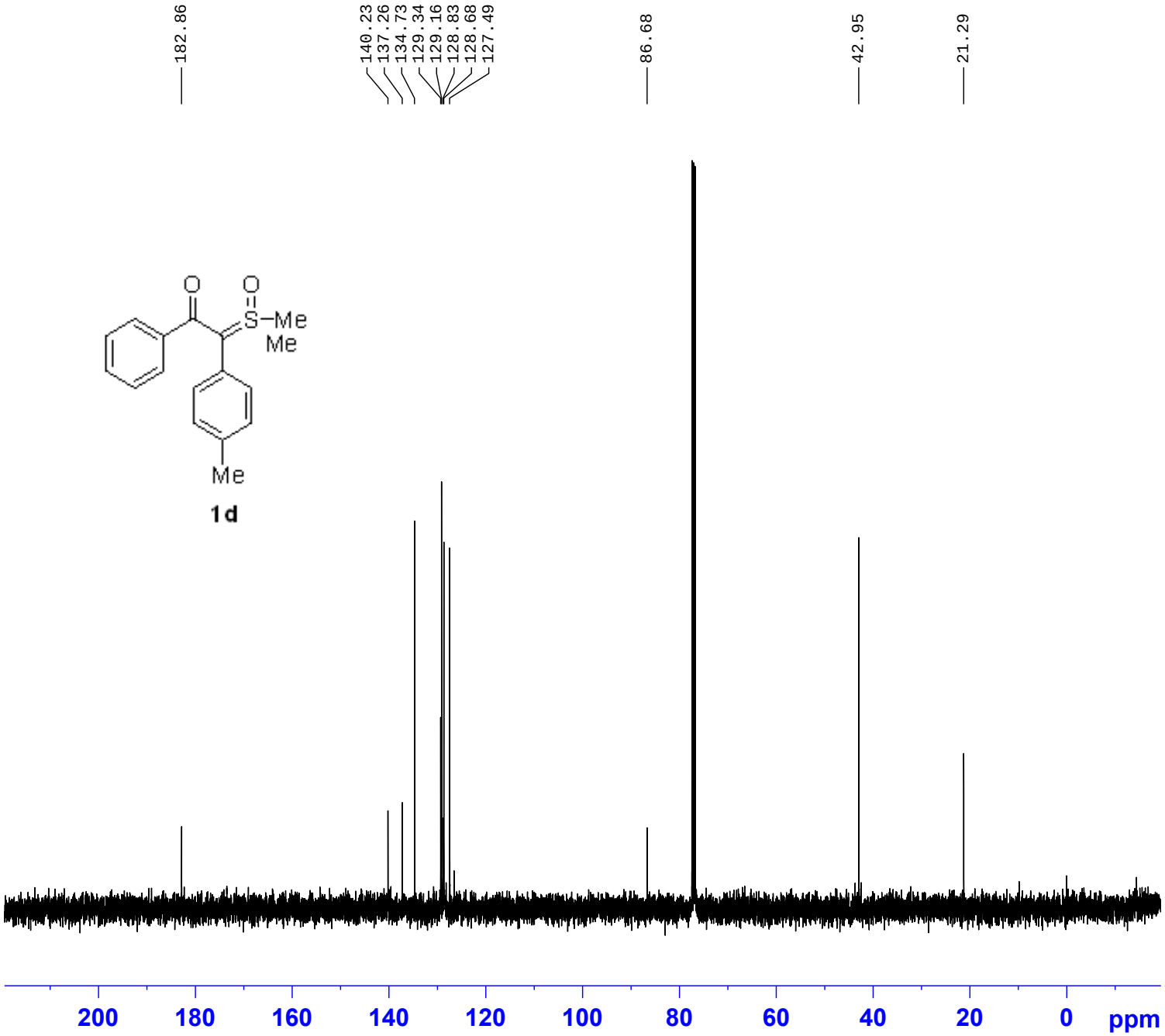





```
NAME        CNMR-gwg-wm-1-29
EXPNO                    118
PROCNO                     1
Date_             20210412
Time                  14.37
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       53
DS                        4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                   193.13
DW                   20.800 usec
DE                    6.50 usec
TE                   294.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    9.90 usec
SI                   32768
SF            100.6278560 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```




```
NAME          HNMR-gwg-1-16
EXPNO                    21
PROCNO                    1
Date_              20210322
Time                  15.26
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        6
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                    140.02
DW                    60.800 usec
DE                     6.50 usec
TE                    293.8 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                    14.40 usec
SI                    65536
SF             400.1900000 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    1.00
```

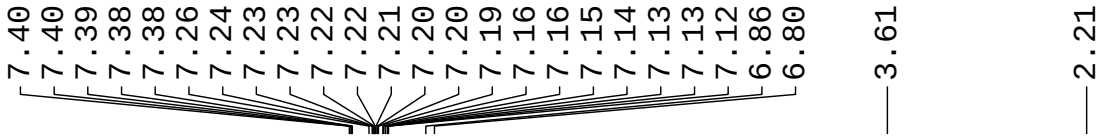


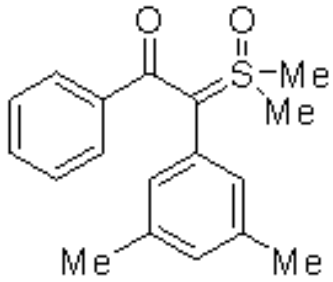
BRUKER

NAME	CNMR-gwg-1-16
EXPNO	23
PROCNO	1
Date_	20210323
Time	15.03
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	35
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	193.13
DW	20.800 usec
DE	6.50 usec
TE	294.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

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

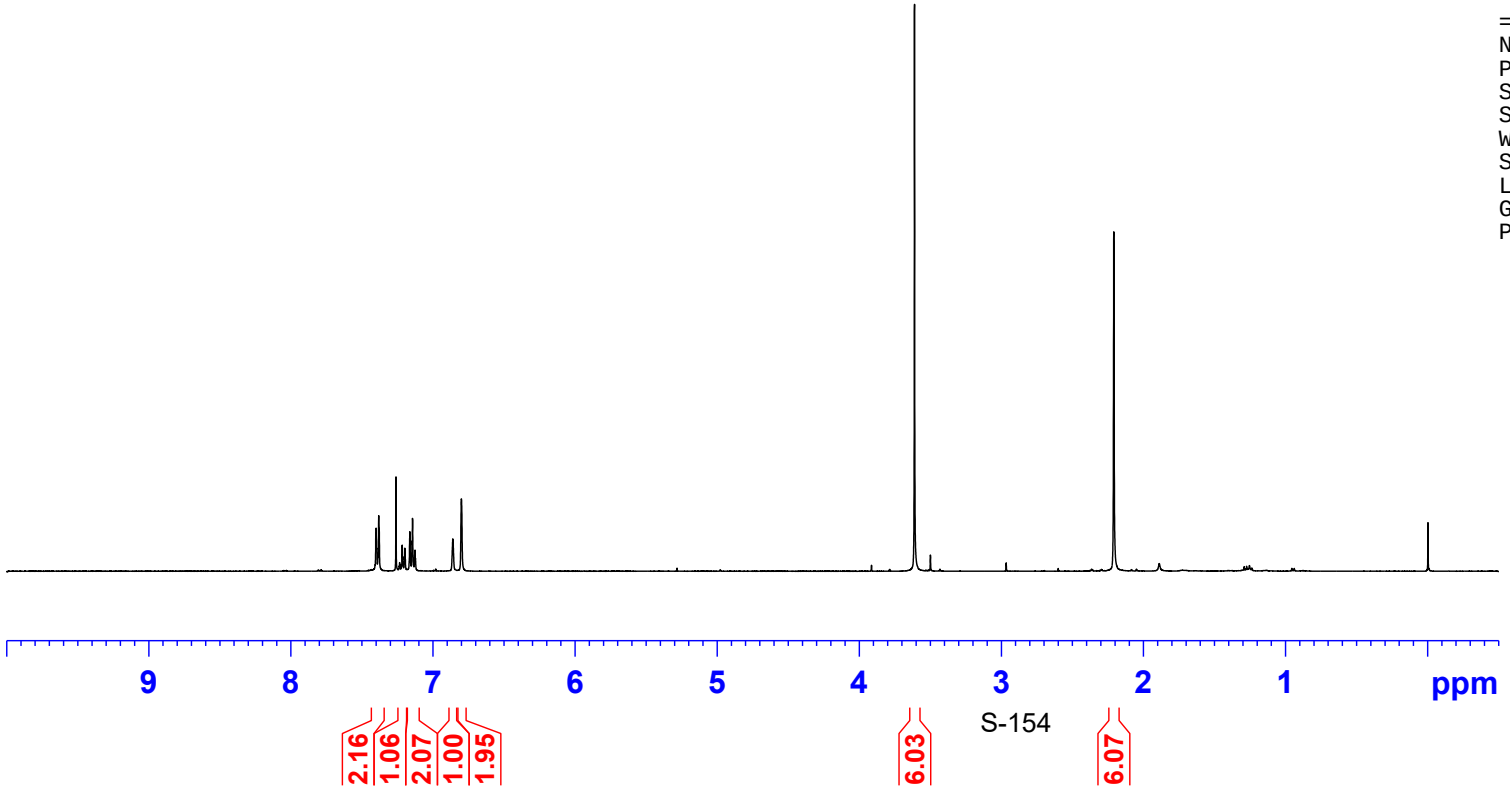
NUC1	13C
P1	9.90 usec
SI	32768
SF	100.6278560 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

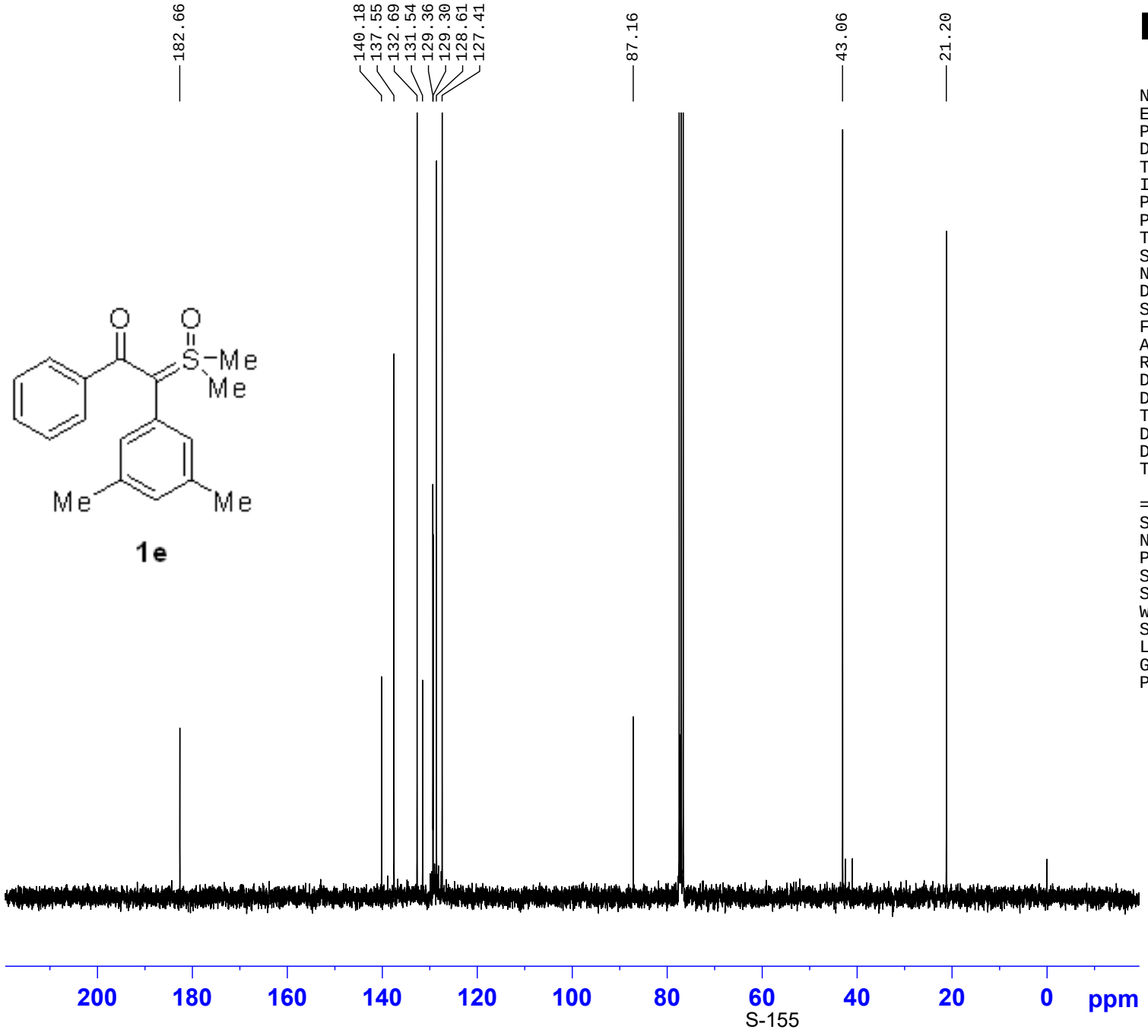




1e

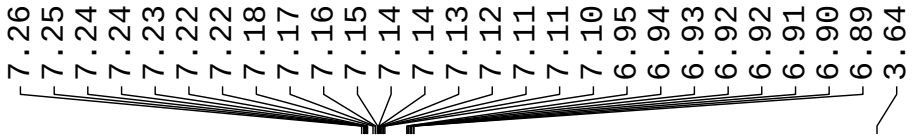
```
NAME        HNMR-gwg-3-22
EXPNO                 58
PROCNO                 1
Date_           20210624
Time               14.39
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     6
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                 100.49
DW                 60.800 usec
DE                  6.50 usec
TE                 295.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.40 usec
SI                 65536
SF          400.1900156 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```

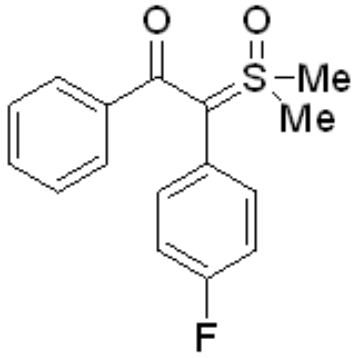




BRUKER

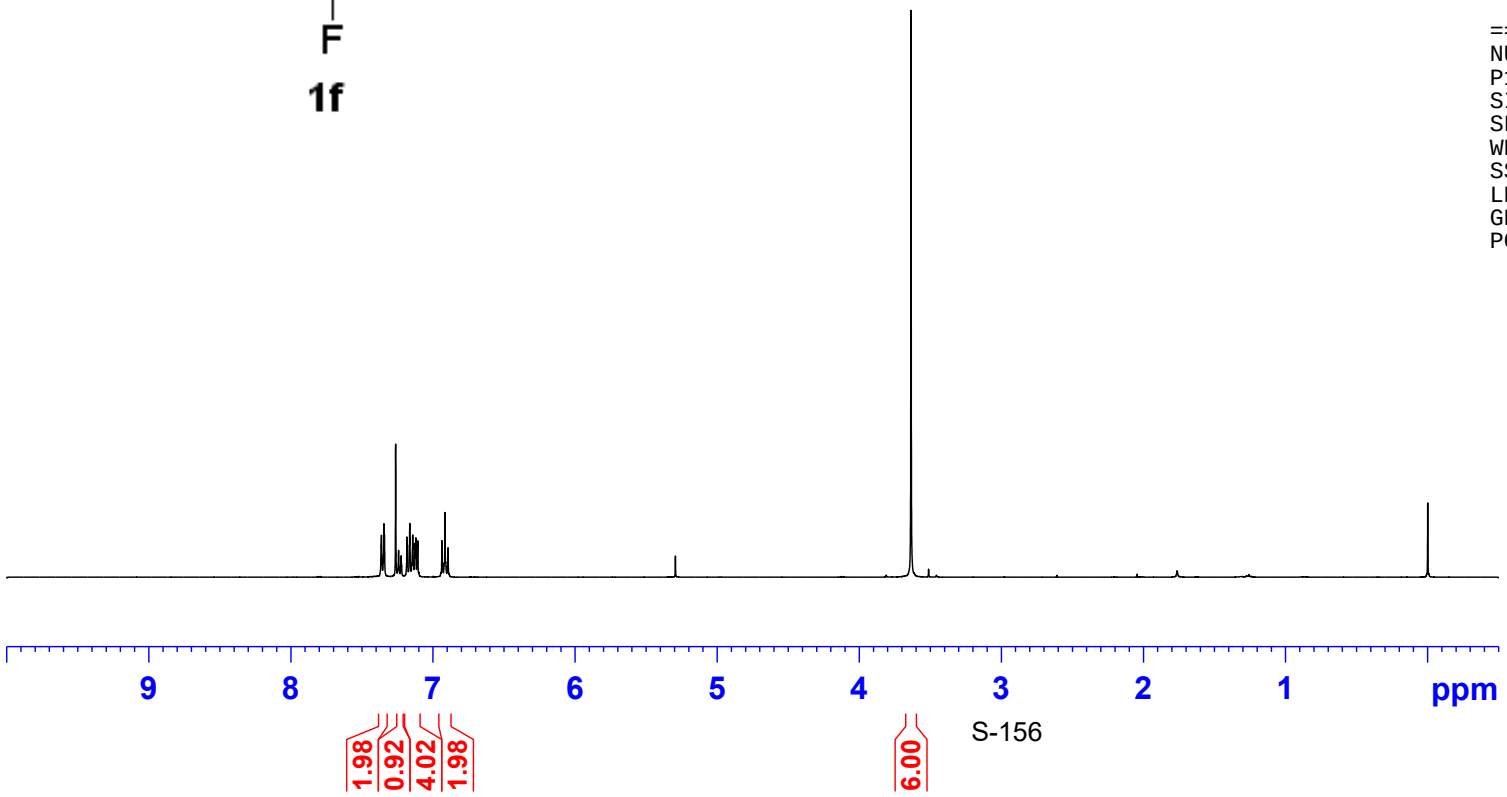
NAME	CNMR-gwg-3-22
EXPNO	4286
PROCNO	1
Date_	20210625
Time	11.26
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	600
DS	4
SWH	18028.846 Hz
FIDRES	0.275098 Hz
AQ	1.8175818 sec
RG	203
DW	27.733 usec
DE	6.50 usec
TE	296.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	75.4752949 MHz
NUC1	13C
P1	9.50 usec
SI	32768
SF	75.4677485 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

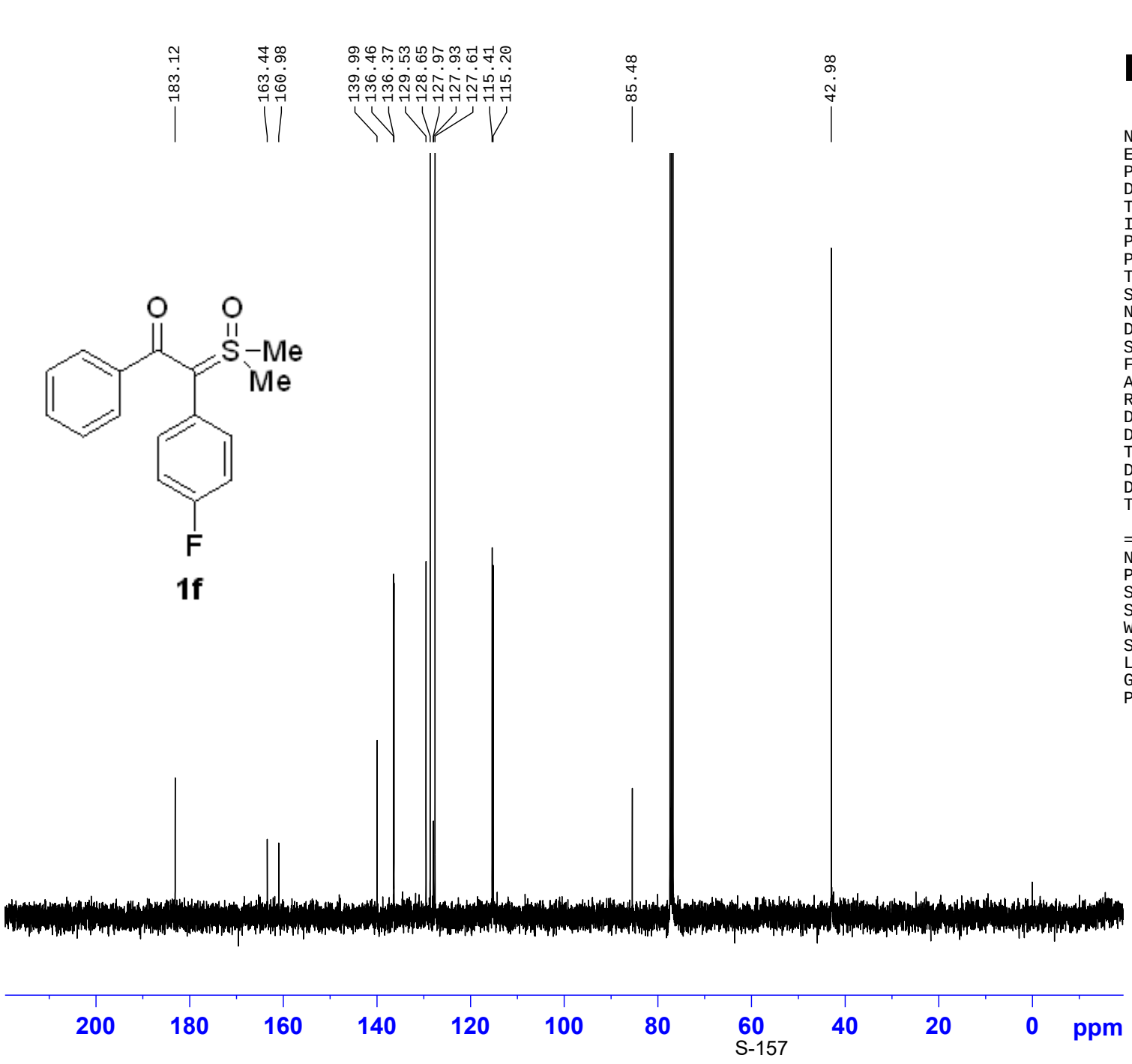




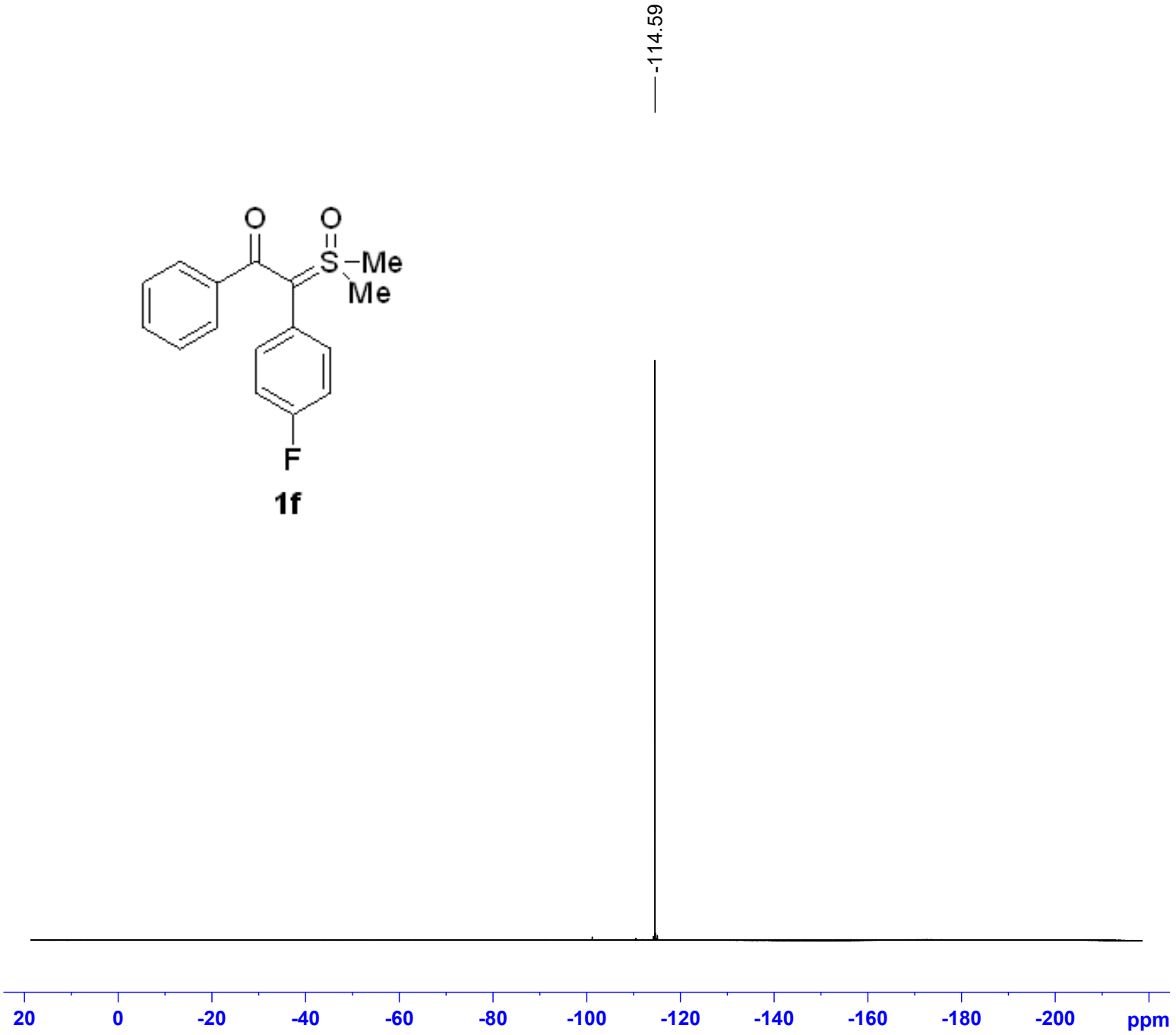
1f

```
NAME        HNMR-gwg-1-13
EXPNO                 20
PROCNO                 1
Date_           20210322
Time               15.24
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     6
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                140.02
DW                60.800 usec
DE                 6.50 usec
TE                293.7 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.40 usec
SI                 65536
SF          400.1900138 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```

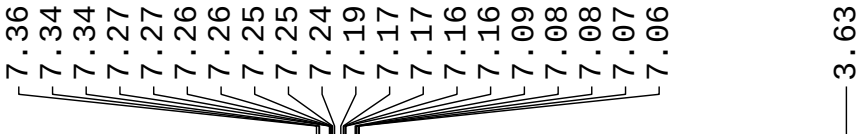


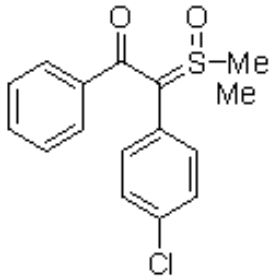



```
NAME          CNMR-gwg-1-13
EXPNO                    22
PROCNO                    1
Date_              20210323
Time                  14.59
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       56
DS                        4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631988 sec
RG                   193.13
DW                   20.800 usec
DE                    6.50 usec
TE                   294.1 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    9.90 usec
SI                   32768
SF            100.6278560 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```



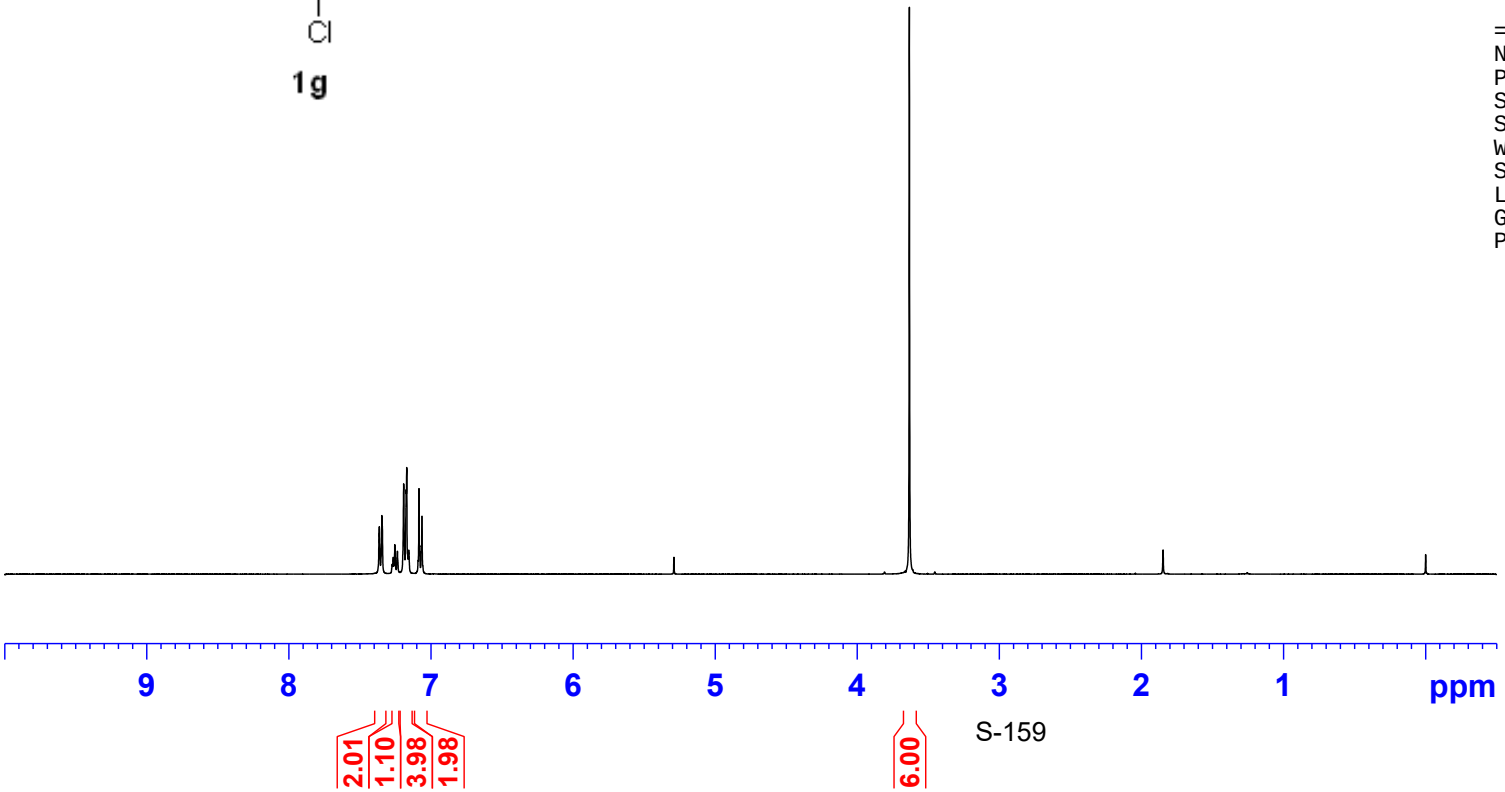

```
NAME          FNMR-gwg-1-13
EXPNO                  2808
PROCNO                    1
Date_              20210330
Time                  10.48
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG         zgfhigqn.2
TD                    131072
SOLVENT               CDCl3
NS                       16
DS                        4
SWH               66964.289 Hz
FIDRES             0.510897 Hz
AQ                 0.9787210 sec
RG                      203
DW                    7.467 usec
DE                    6.50 usec
TE                    296.2 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
SI                    65536
SF              282.4043552 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

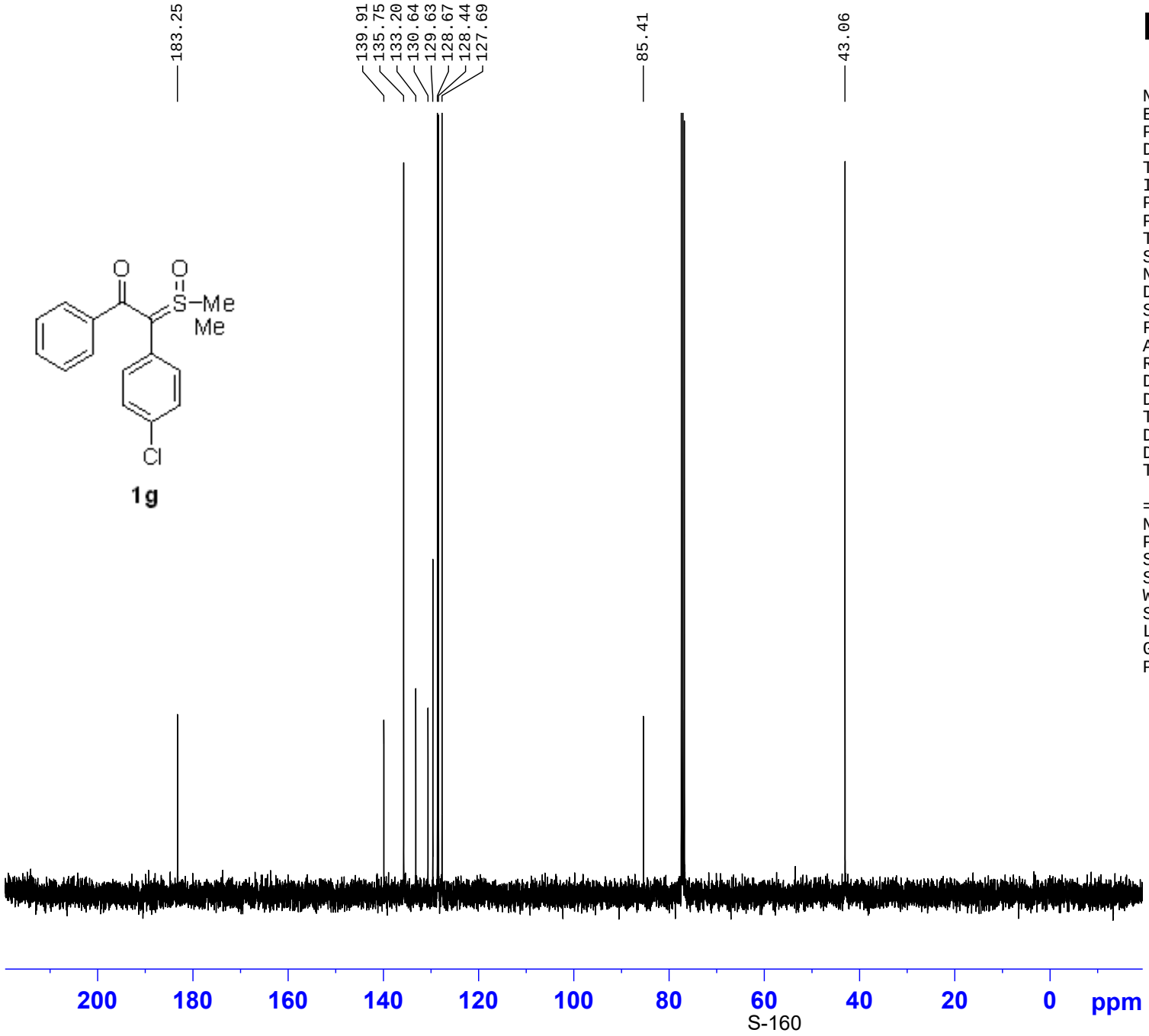




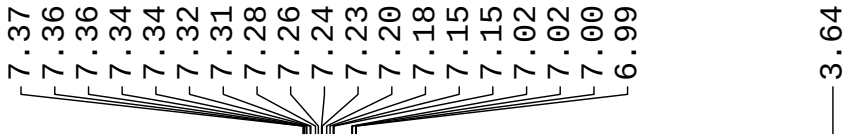
1g

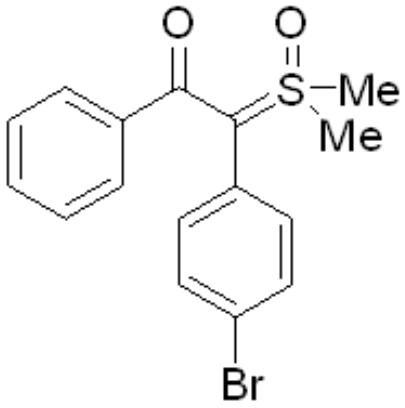
```
NAME        HNMR-gwg-1-30
EXPNO                 59
PROCNO                 1
Date_           20210329
Time               14.41
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     6
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                 125.76
DW                 60.800 usec
DE                  6.50 usec
TE                 293.9 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.40 usec
SI                 65536
SF          400.1900136 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```





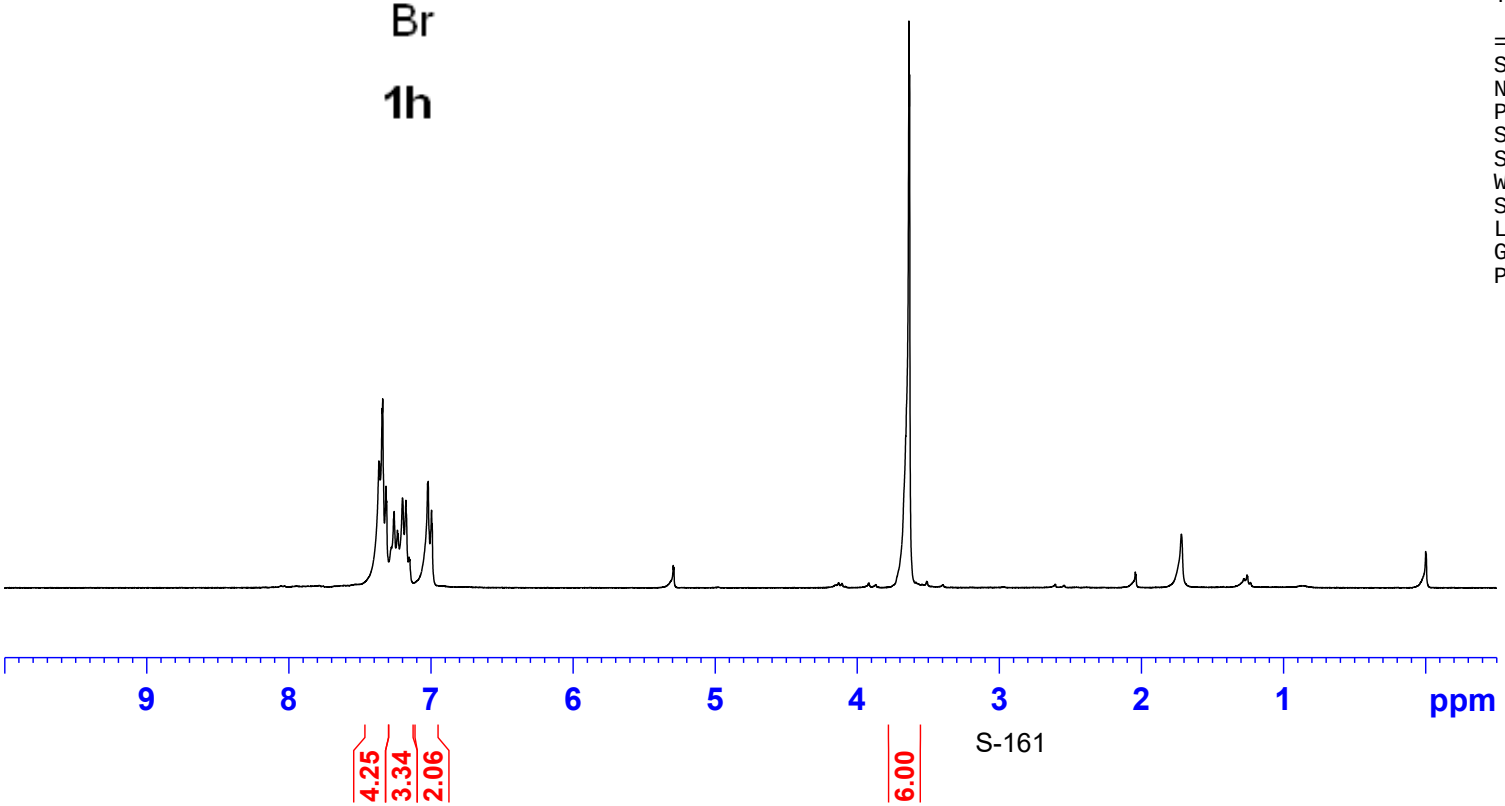

```
NAME          CNMR-gwg-1-30
EXPNO                    69
PROCNO                    1
Date_             20210330
Time                 14.39
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      67
DS                       4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                  193.13
DW                  20.800 usec
DE                   6.50 usec
TE                  294.5 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   9.90 usec
SI                  32768
SF           100.6278560 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

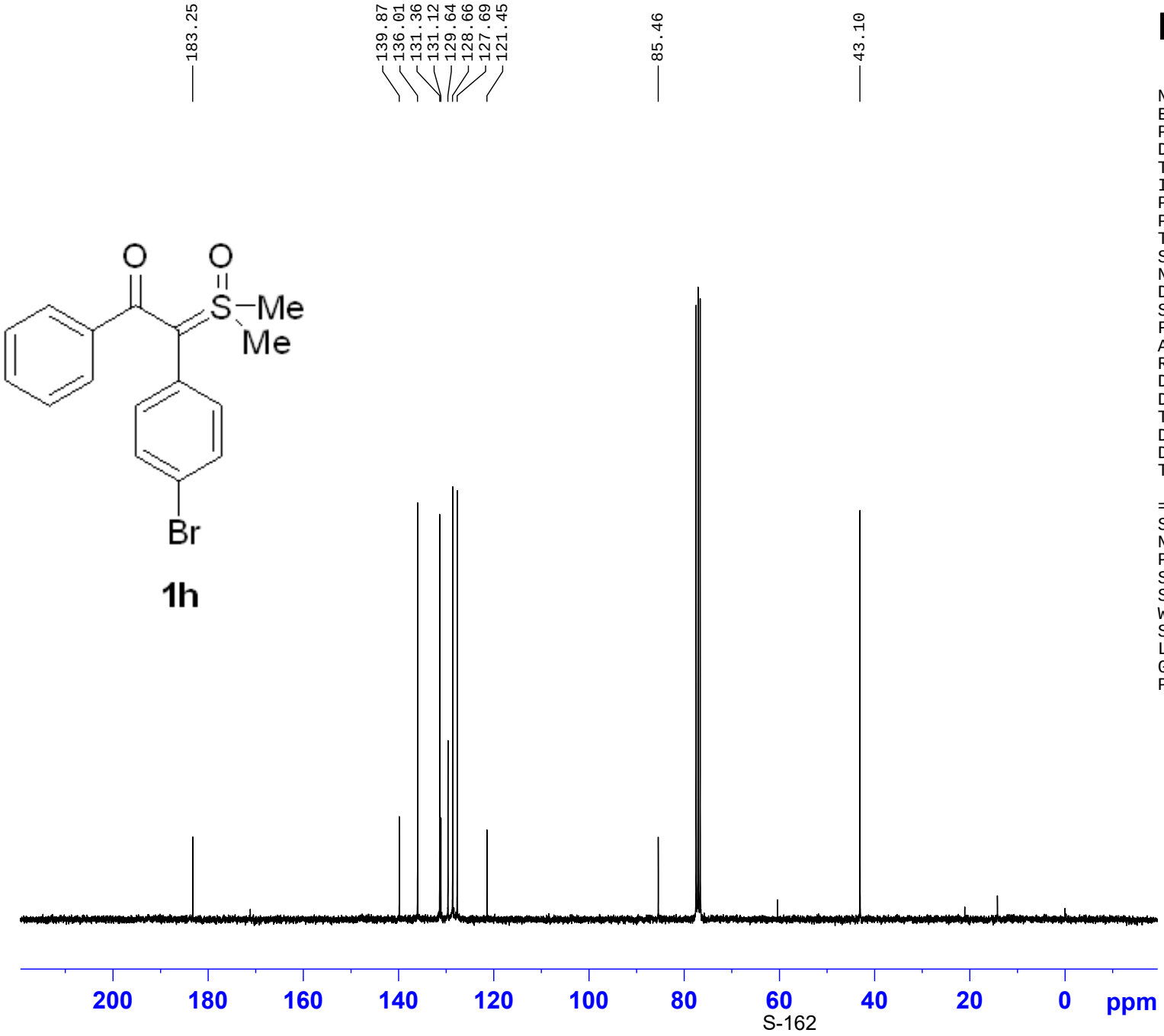




1h

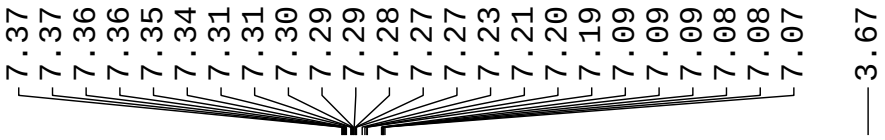
```
NAME          HNMR-gwg-1-75
EXPNO                 3095
PROCNO                   1
Date_             20210417
Time                  9.58
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               6009.615 Hz
FIDRES            0.091699 Hz
AQ                5.4526453 sec
RG                     203
DW                  83.200 usec
DE                   6.50 usec
TE                  296.2 K
D1               1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           300.1318534 MHz
NUC1                   1H
P1                  10.00 usec
SI                   65536
SF             300.1300060 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

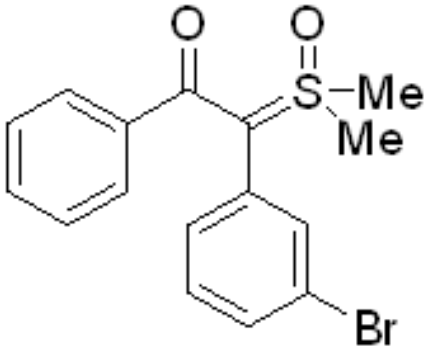




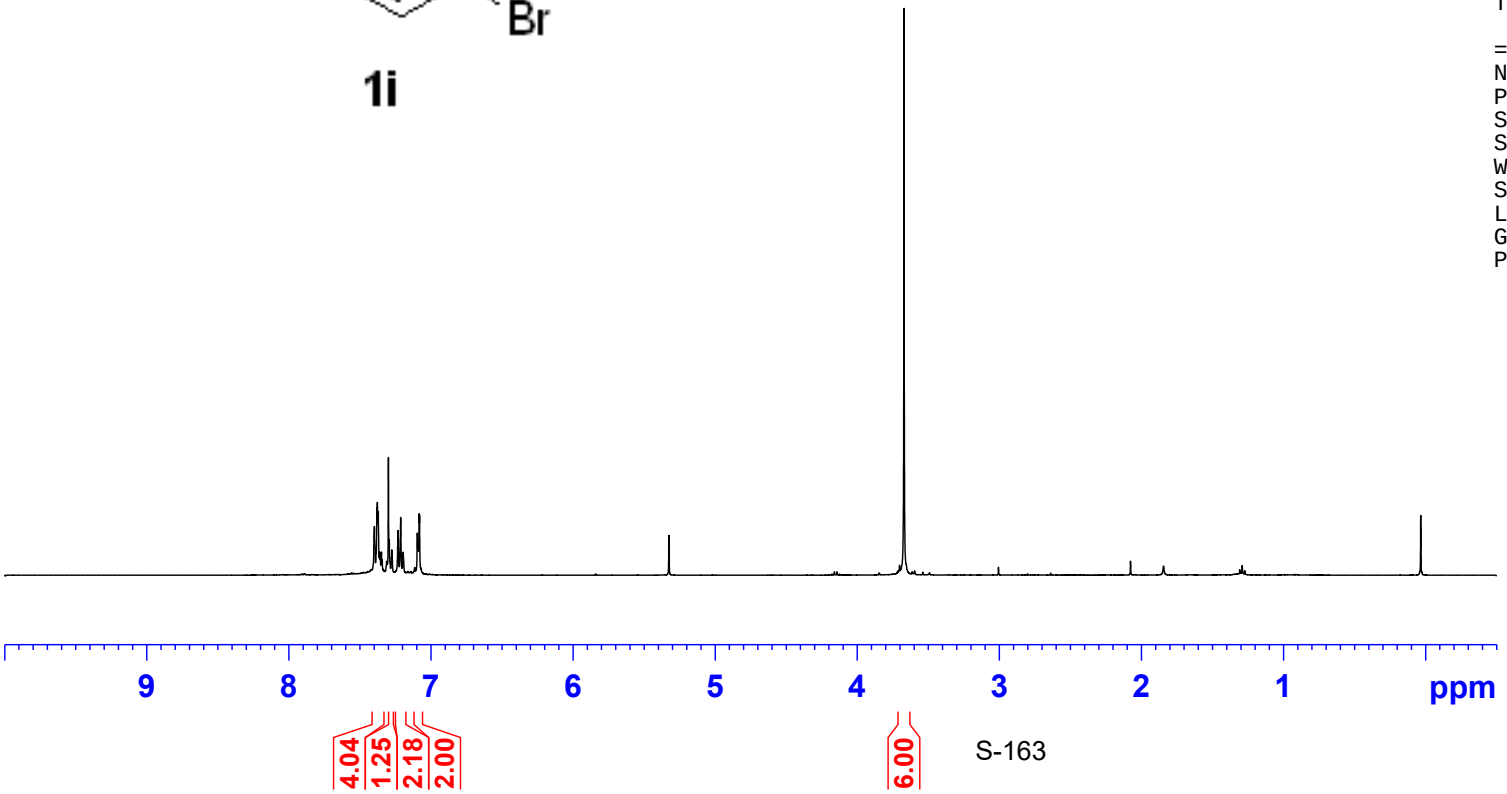
BRUKER

```
NAME          CNMR-gwg-1-75
EXPNO                  3121
PROCNO                    1
Date_           20210419
Time                 11.31
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             1.8175818 sec
RG                    203
DW                27.733 usec
DE                 6.50 usec
TE                296.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          75.4752949 MHz
NUC1                  13C
P1                 9.50 usec
SI                 32768
SF            75.4677485 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

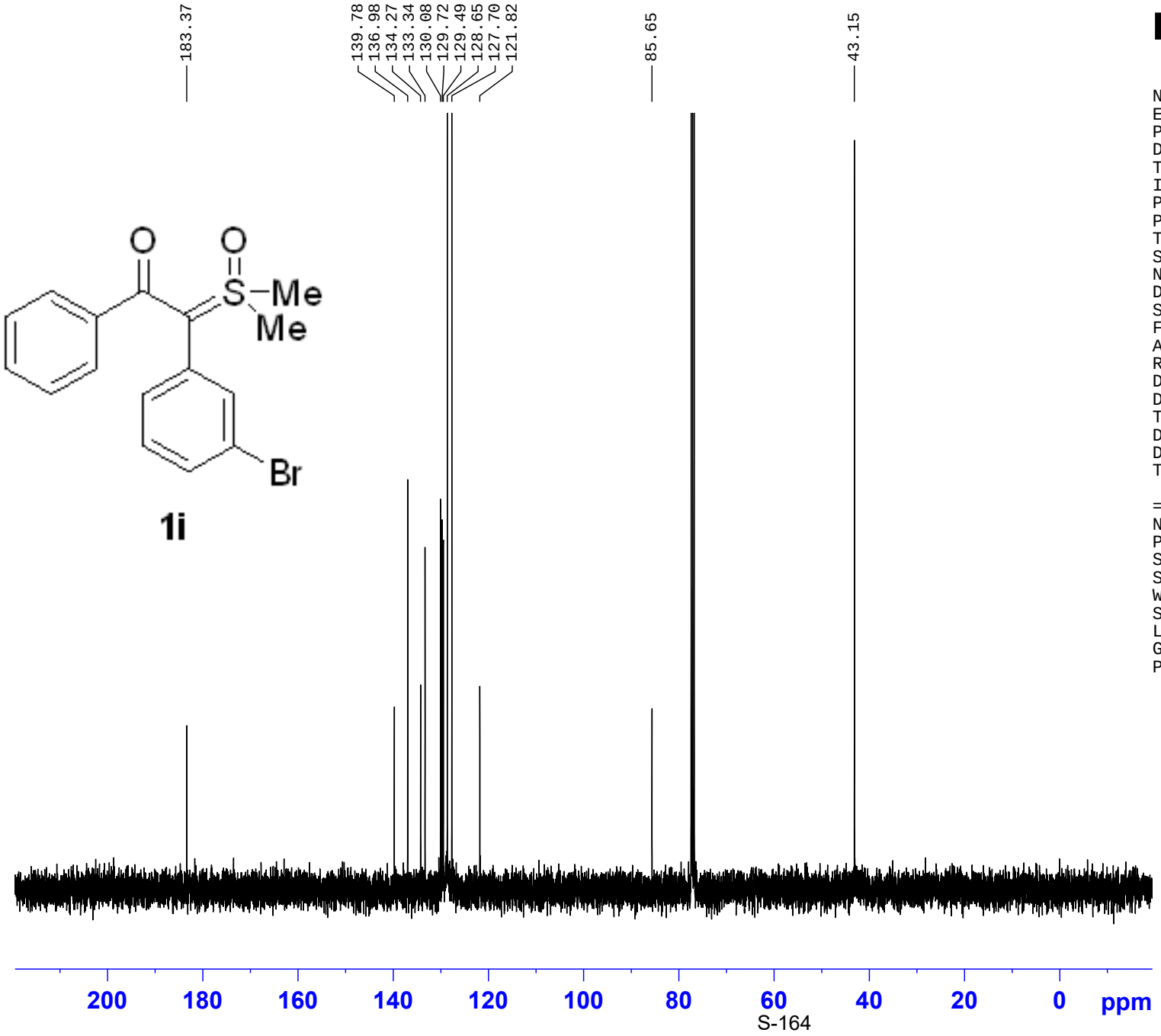




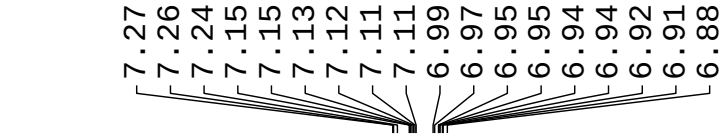
1i

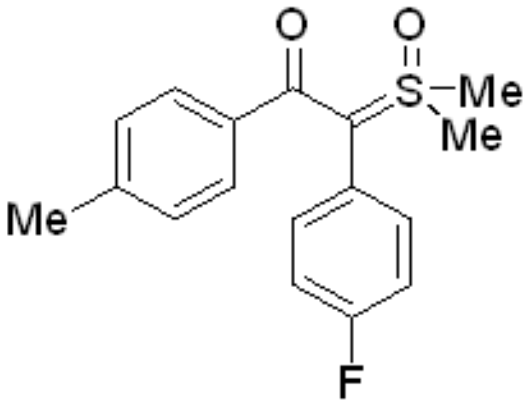



```
NAME        HNMR-gwg-1-34
EXPNO                  63
PROCNO                  1
Date_           20210330
Time               14.14
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     6
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                 90.23
DW                60.800 usec
DE                 6.50 usec
TE                294.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.40 usec
SI                 65536
SF          400.1900000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```



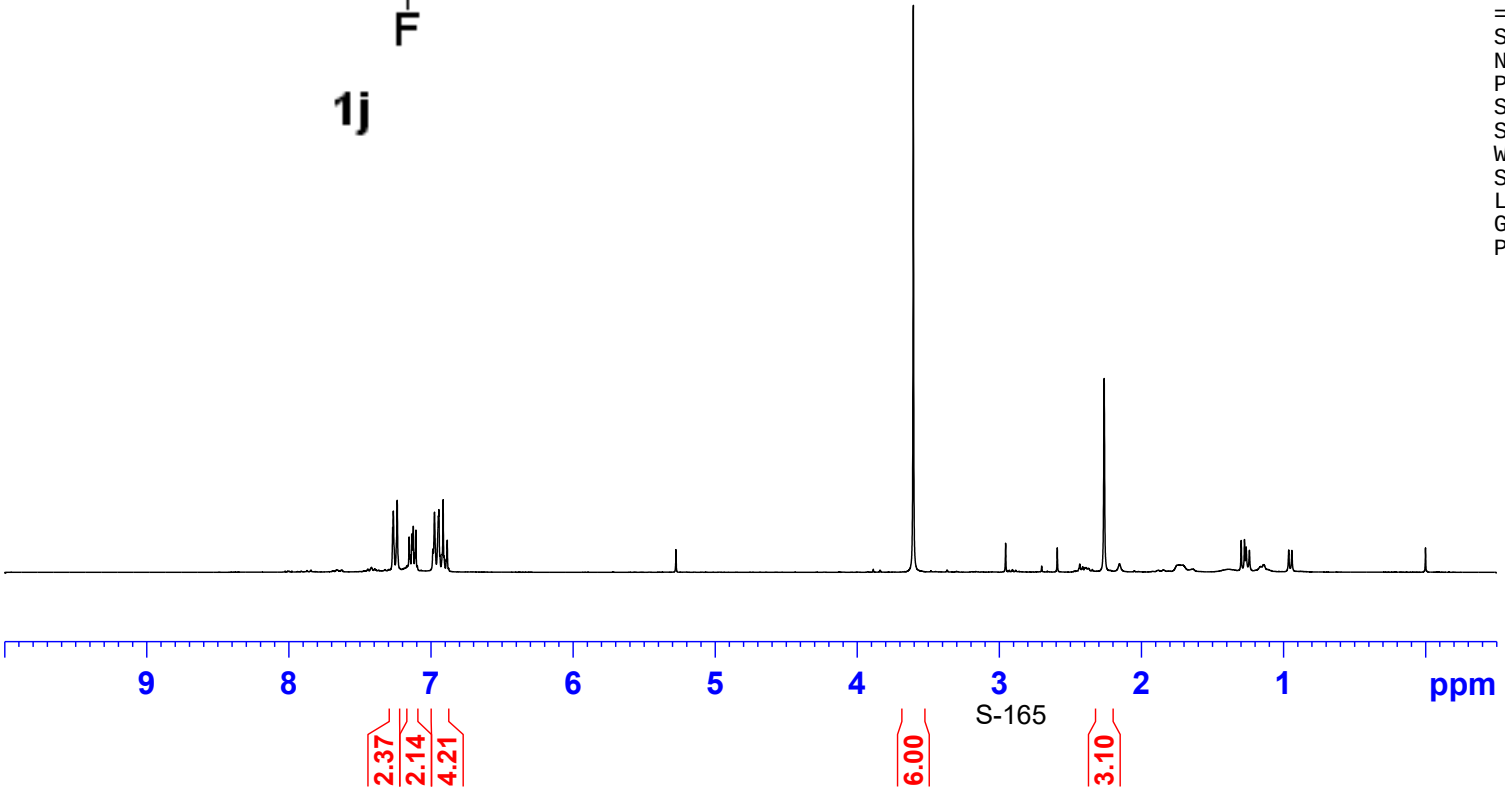

```
NAME          CNMR-gwg-1-34
EXPNO                    78
PROCNO                    1
Date_             20210331
Time                 14.41
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      68
DS                       4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                  193.13
DW                  20.800 usec
DE                   6.50 usec
TE                  294.4 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.90 usec
SI                   32768
SF           100.6278560 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

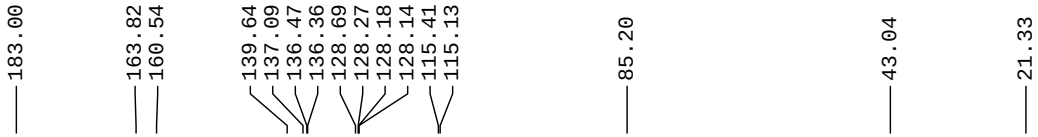


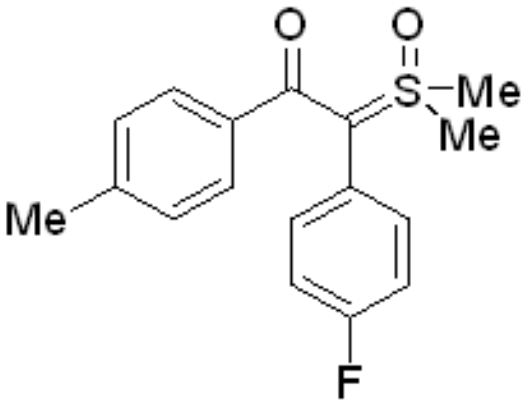


1j

```
NAME          HNMR-gwg-1-86
EXPNO                 3242
PROCNO                   1
Date_             20210426
Time                 10.03
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                5.4526453 sec
RG                     71.8
DW                  83.200 usec
DE                   6.50 usec
TE                  296.2 K
D1               1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           300.1318534 MHz
NUC1                   1H
P1                  10.00 usec
SI                   65536
SF             300.1300043 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

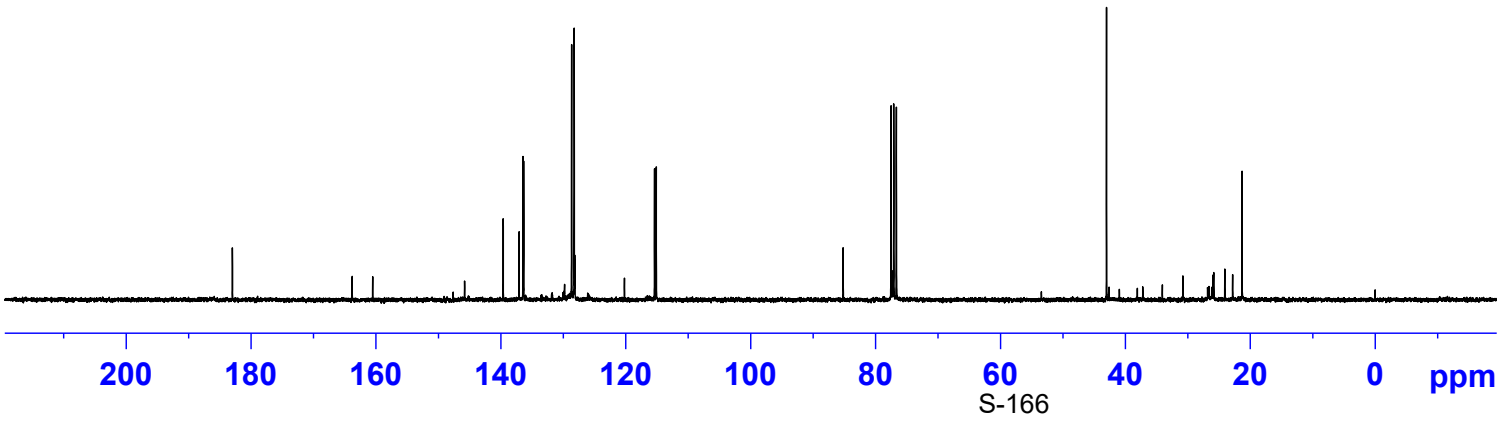


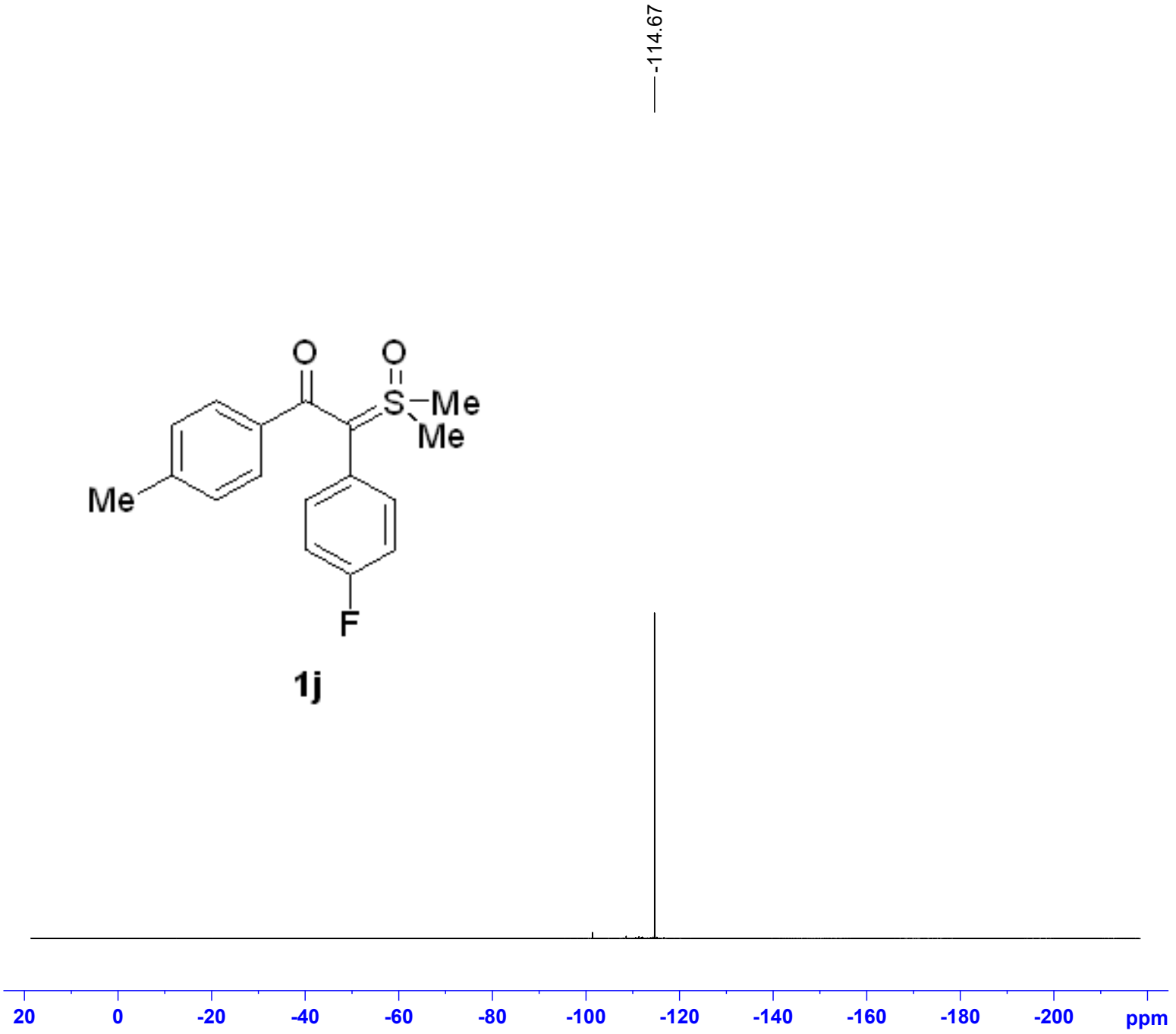




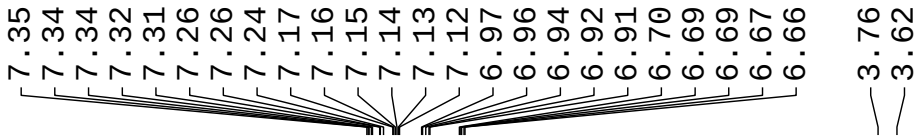
1j

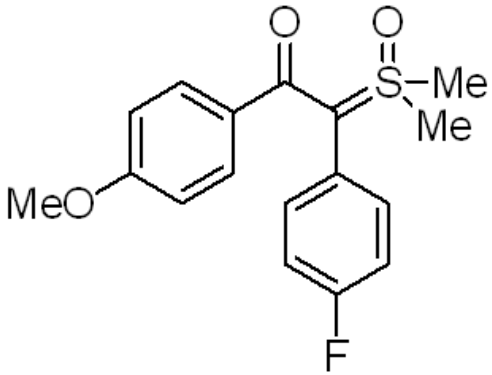
```
NAME          CNMR-gwg-1-86
EXPNO                 3244
PROCNO                   1
Date_           20210426
Time                10.46
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   600
DS                     4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ             1.8175818 sec
RG                   203
DW                27.733 usec
DE                 6.50 usec
TE                296.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          75.4752949 MHz
NUC1                 13C
P1                 9.50 usec
SI                32768
SF            75.4677485 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```





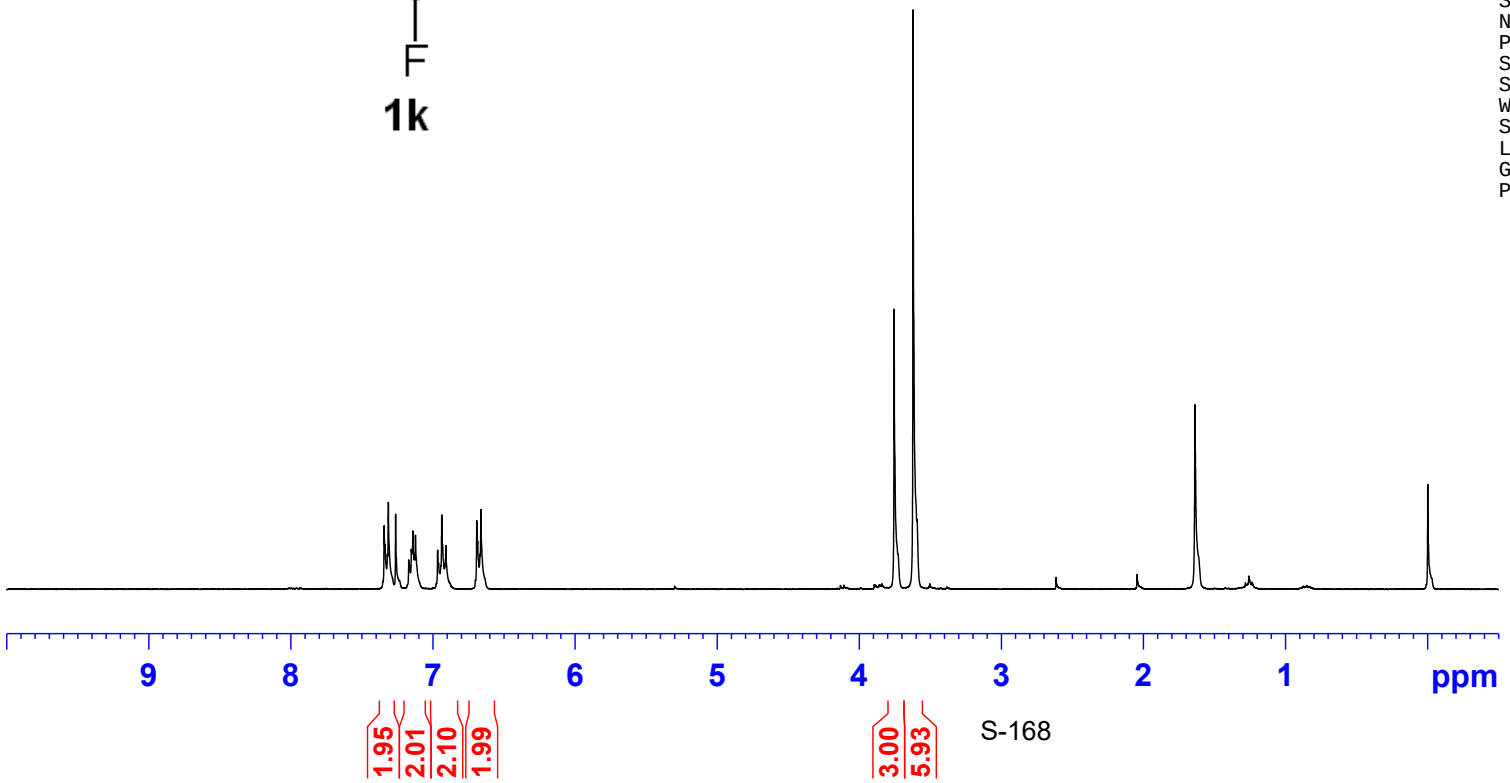

```
NAME        FNMR-gwg-1-86
EXPNO               3243
PROCNO                 1
Date_           20210426
Time               10.05
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG       zgfhigqn.2
TD                131072
SOLVENT             CDCl3
NS                     16
DS                      4
SWH             66964.289 Hz
FIDRES          0.510897 Hz
AQ              0.9787210 sec
RG                    203
DW                7.467 usec
DE                 6.50 usec
TE                296.1 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
SI                 65536
SF           282.4043552 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

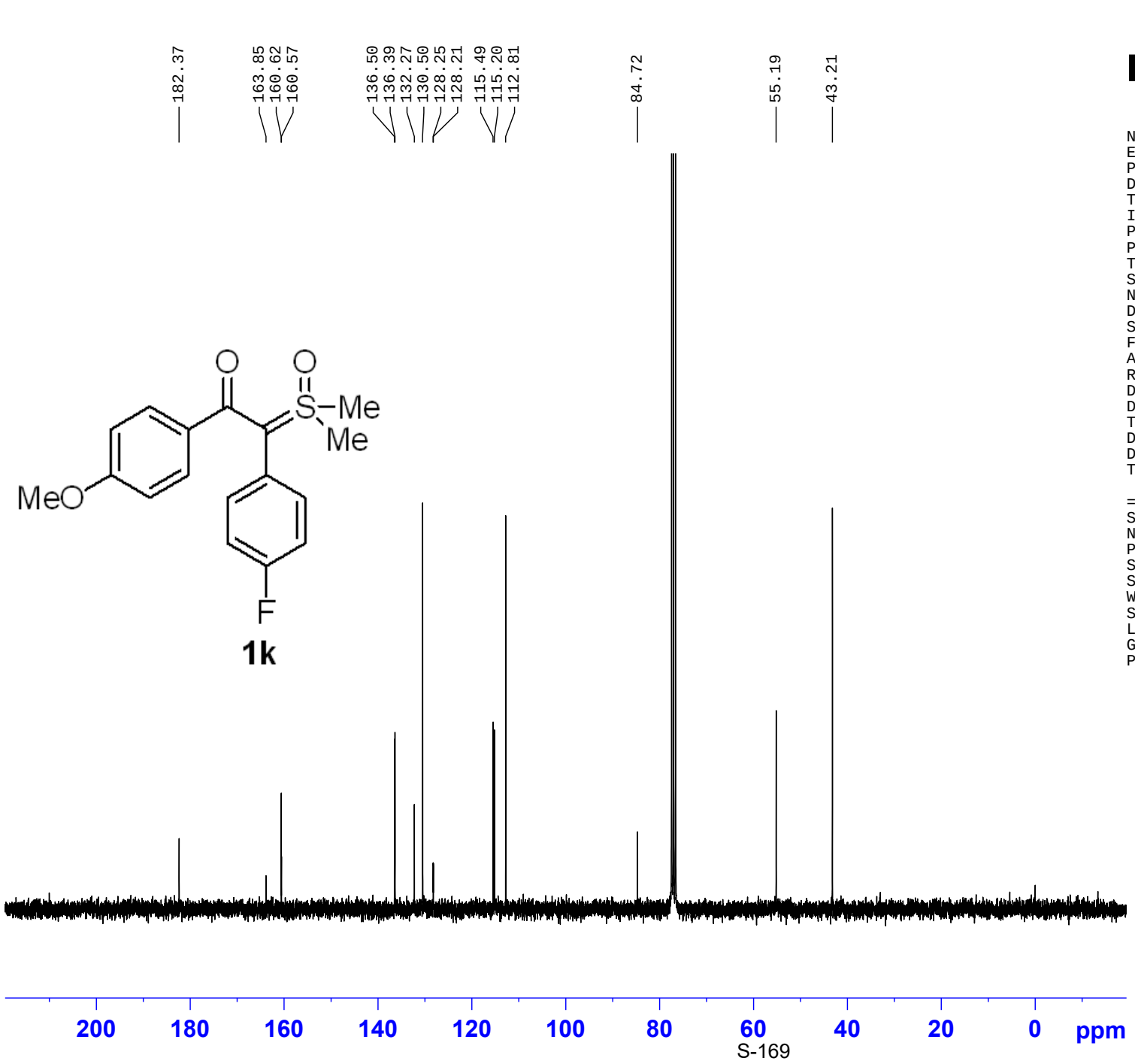




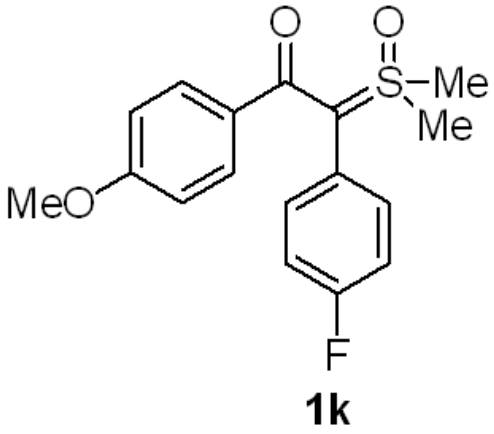
1k

```
NAME      HNMR-gwg-wm-1-38-p-OMe
EXPNO               3157
PROCNO                 1
Date_           20210422
Time                9.51
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             5.4526453 sec
RG                   203
DW                83.200 usec
DE                 6.50 usec
TE                296.1 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        300.1318534 MHz
NUC1                  1H
P1                10.00 usec
SI                 65536
SF          300.1300067 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



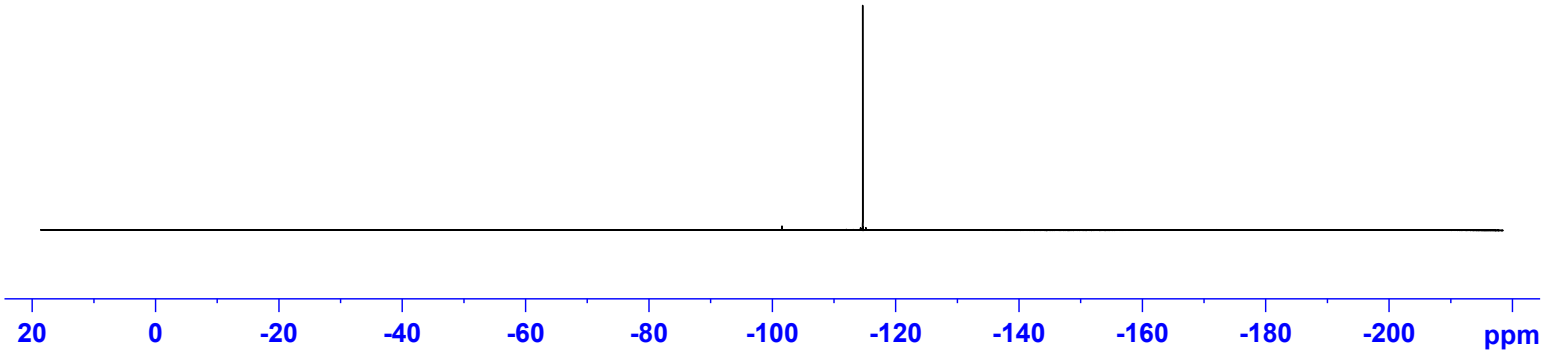



```
NAME       CNMR-gwg-wm-1-38-p-OMe
EXPNO                        3203
PROCNO                          1
Date_                    20210423
Time                        11.25
INSTRUM                     spect
PROBHD   5 mm PABBO BB-
PULPROG                   zgpg30
TD                         65536
SOLVENT                    CDCl3
NS                           600
DS                             4
SWH                    18028.846 Hz
FIDRES                  0.275098 Hz
AQ                     1.8175818 sec
RG                           203
DW                        27.733 usec
DE                         6.50 usec
TE                        296.1 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                            1

======== CHANNEL f1 ========
SFO1                  75.4752949 MHz
NUC1                         13C
P1                         9.50 usec
SI                        32768
SF                    75.4677485 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.40
```

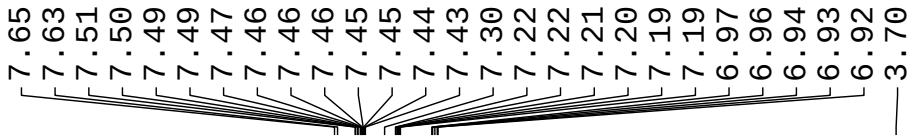


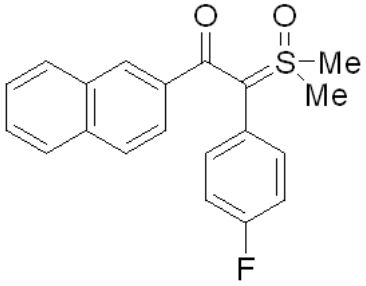
1k

-114.67



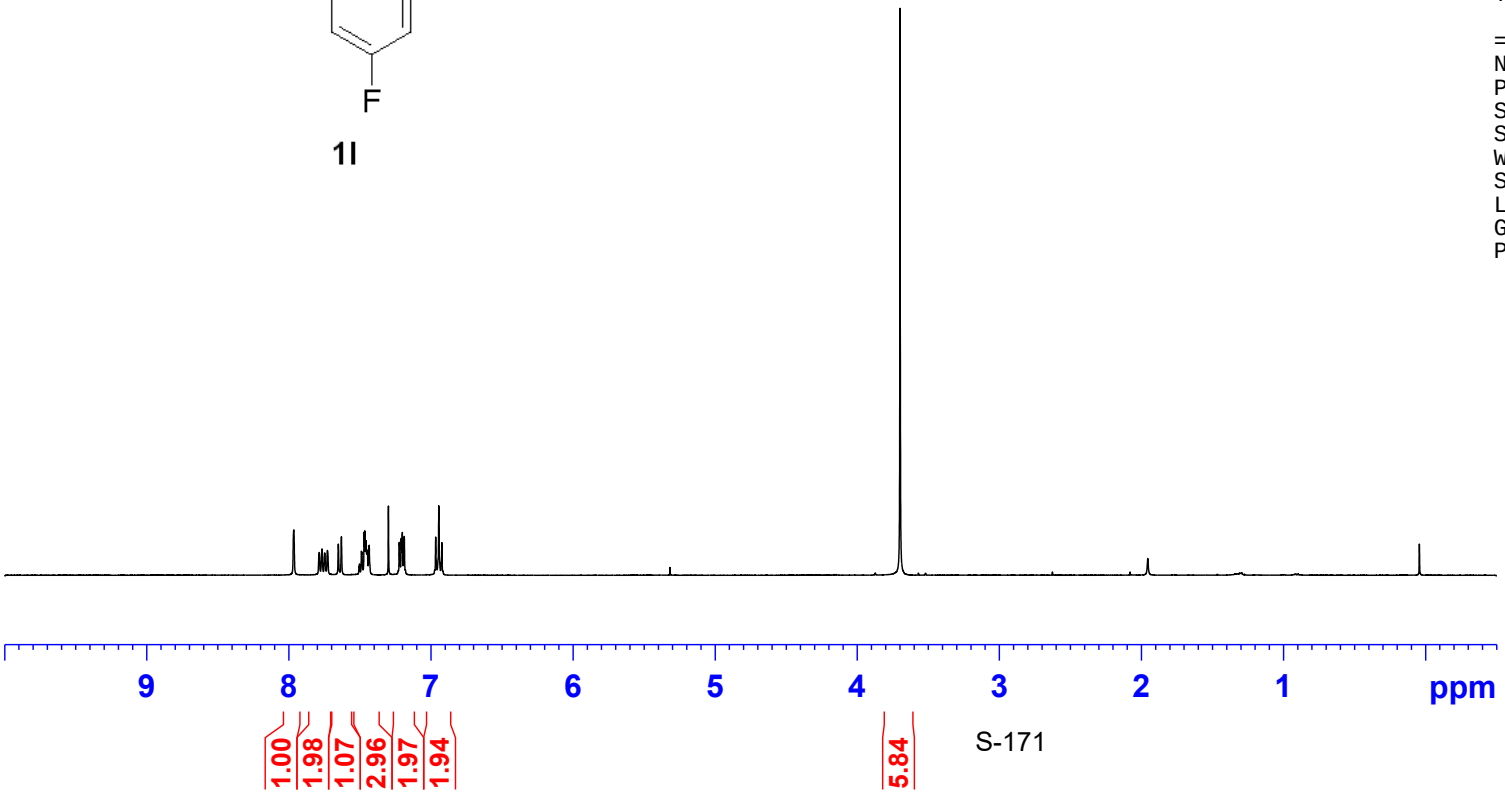

```
NAME      FNMR-gwg-wm-1-38-p-OMe
EXPNO                       3202
PROCNO                         1
Date_                   20210423
Time                       10.44
INSTRUM                    spect
PROBHD   5 mm PABBO BB-
PULPROG              zgfhigqn.2
TD                        131072
SOLVENT                    CDCl3
NS                            16
DS                             4
SWH                    66964.289 Hz
FIDRES                 0.510897 Hz
AQ                     0.9787210 sec
RG                           203
DW                         7.467 usec
DE                         6.50 usec
TE                         296.2 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
SI                         65536
SF                  282.4043552 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```

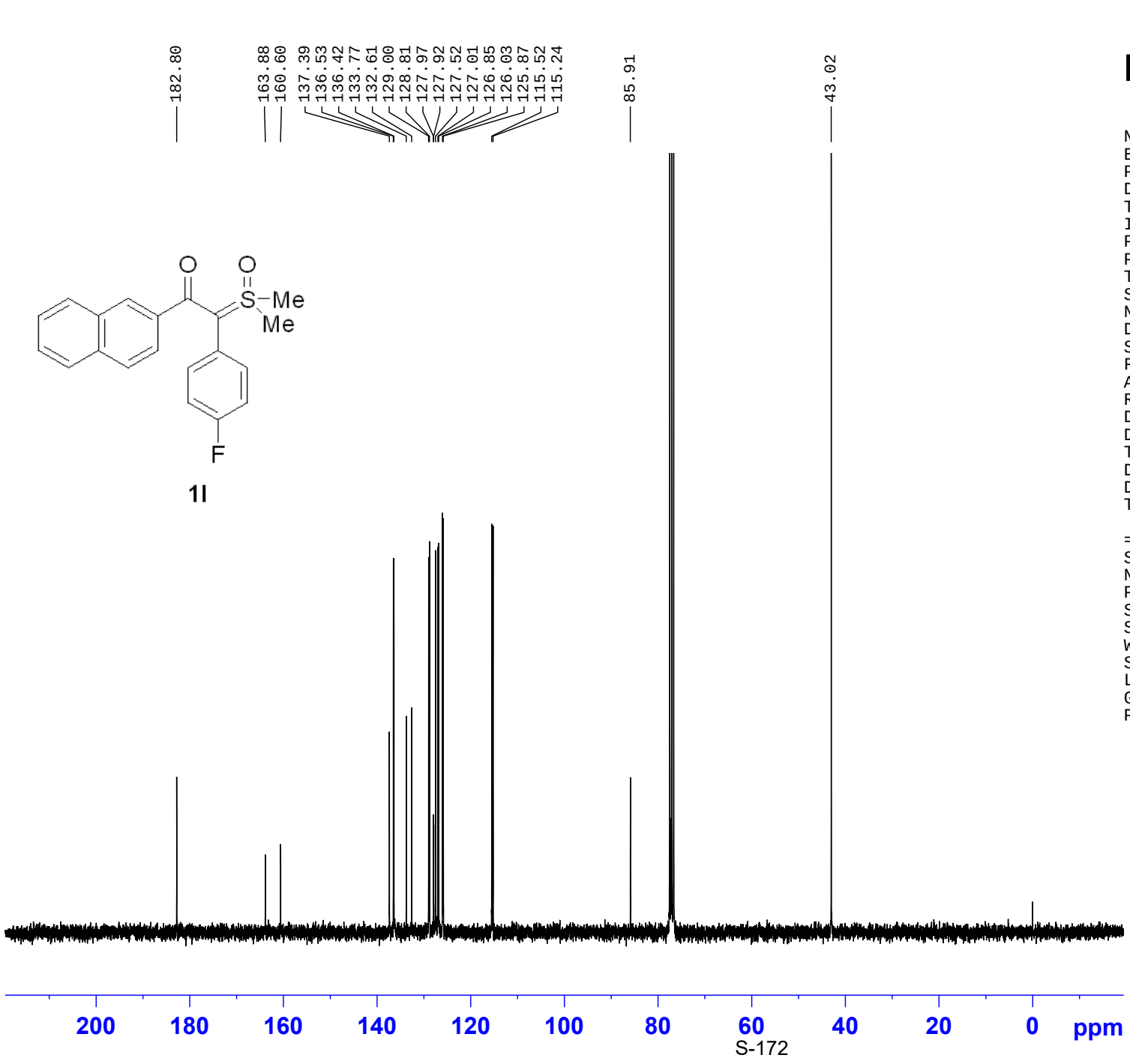




1l

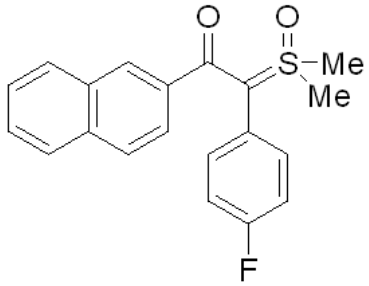
```
NAME        HNMR-gwg-1-80
EXPNO                 24
PROCNO                 1
Date_           20210422
Time               14.30
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     6
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                113.67
DW                60.800 usec
DE                 6.50 usec
TE                294.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.40 usec
SI                 65536
SF          400.1900000 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```





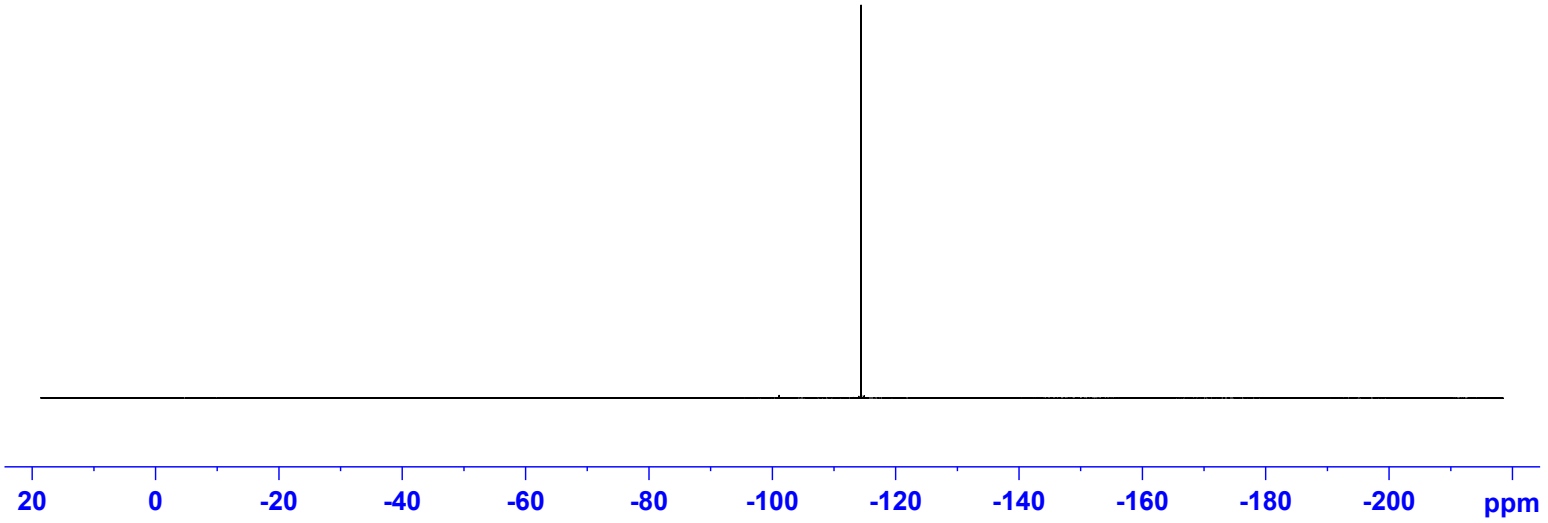
BRUKER

NAME	CNMR-gwg-1-80
EXPNO	3184
PROCNO	1
Date_	20210422
Time	23.19
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	500
DS	4
SWH	18028.846 Hz
FIDRES	0.275098 Hz
AQ	1.8175818 sec
RG	203
DW	27.733 usec
DE	6.50 usec
TE	296.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	75.4752949 MHz
NUC1	13C
P1	9.50 usec
SI	32768
SF	75.4677485 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

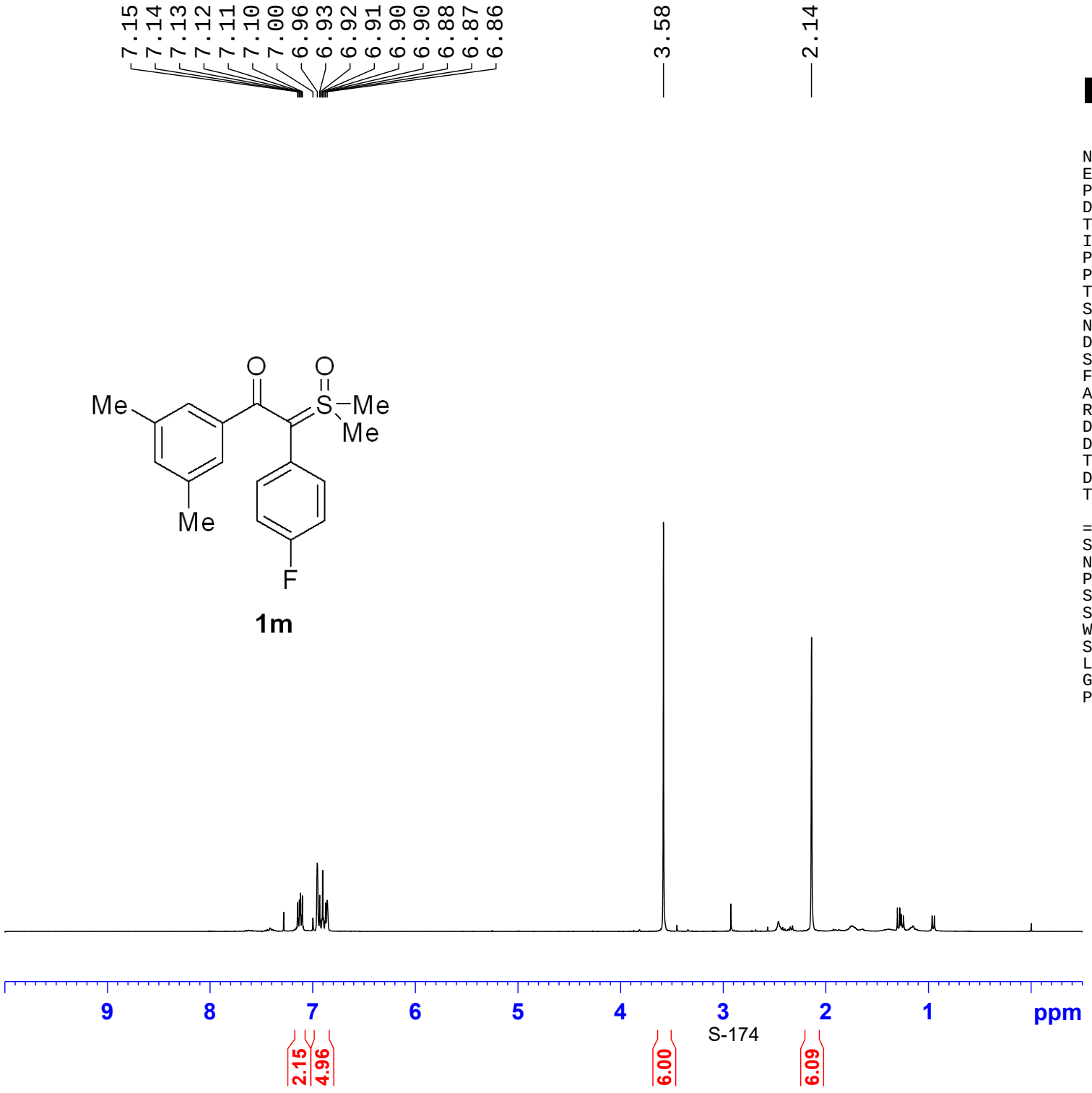


1l

-114.40

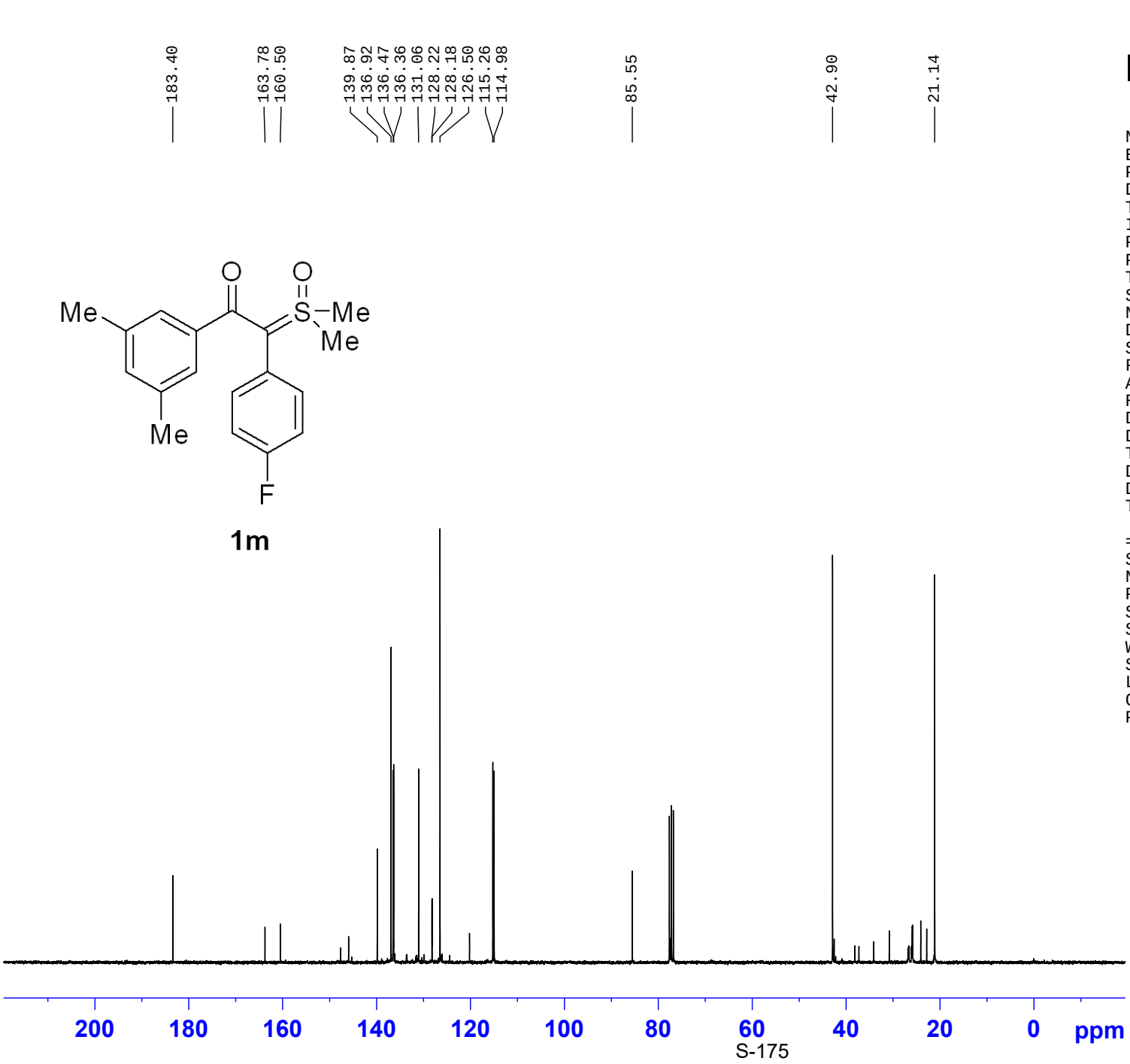



```
NAME        FNMR-gwg-1-80
EXPNO               3185
PROCNO                 1
Date_           20210422
Time               23.21
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG       zgfhigqn.2
TD                131072
SOLVENT             CDCl3
NS                     16
DS                      4
SWH             66964.289 Hz
FIDRES          0.510897 Hz
AQ              0.9787210 sec
RG                    203
DW                7.467 usec
DE                 6.50 usec
TE                296.1 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
SI                65536
SF           282.4043552 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



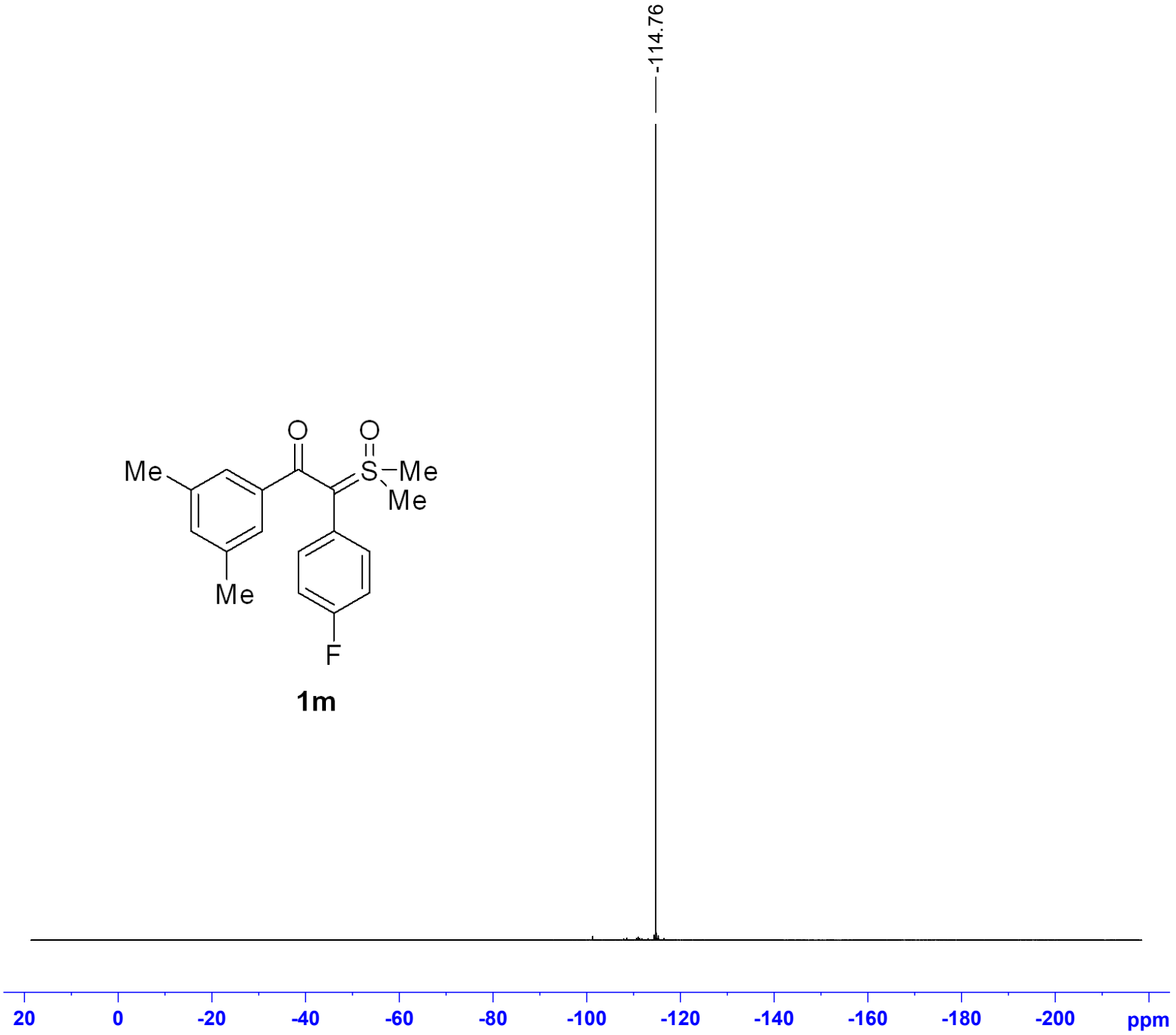
BRUKER

NAME	HNMR-gwg-2-24
EXPNO	3563
PROCNO	1
Date_	20210518
Time	11.16
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	5.4526453 sec
RG	32
DW	83.200 usec
DE	6.50 usec
TE	296.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	300.1318534 MHz
NUC1	1H
P1	10.00 usec
SI	65536
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

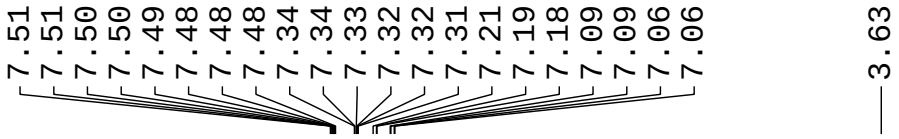


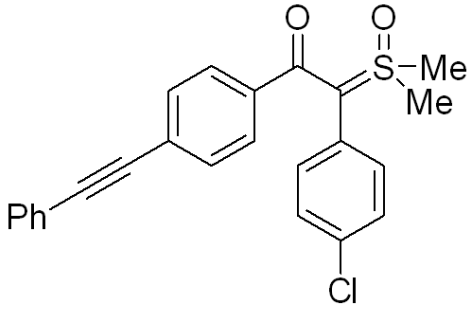

```
NAME          CNMR-gwg-2-24
EXPNO                  3565
PROCNO                    1
Date_              20210518
Time                  11.58
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      600
DS                        4
SWH               18028.846 Hz
FIDRES             0.275098 Hz
AQ                1.8175818 sec
RG                      203
DW                   27.733 usec
DE                    6.50 usec
TE                   296.1 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             75.4752949 MHz
NUC1                    13C
P1                    9.50 usec
SI                   32768
SF               75.4677485 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

1m

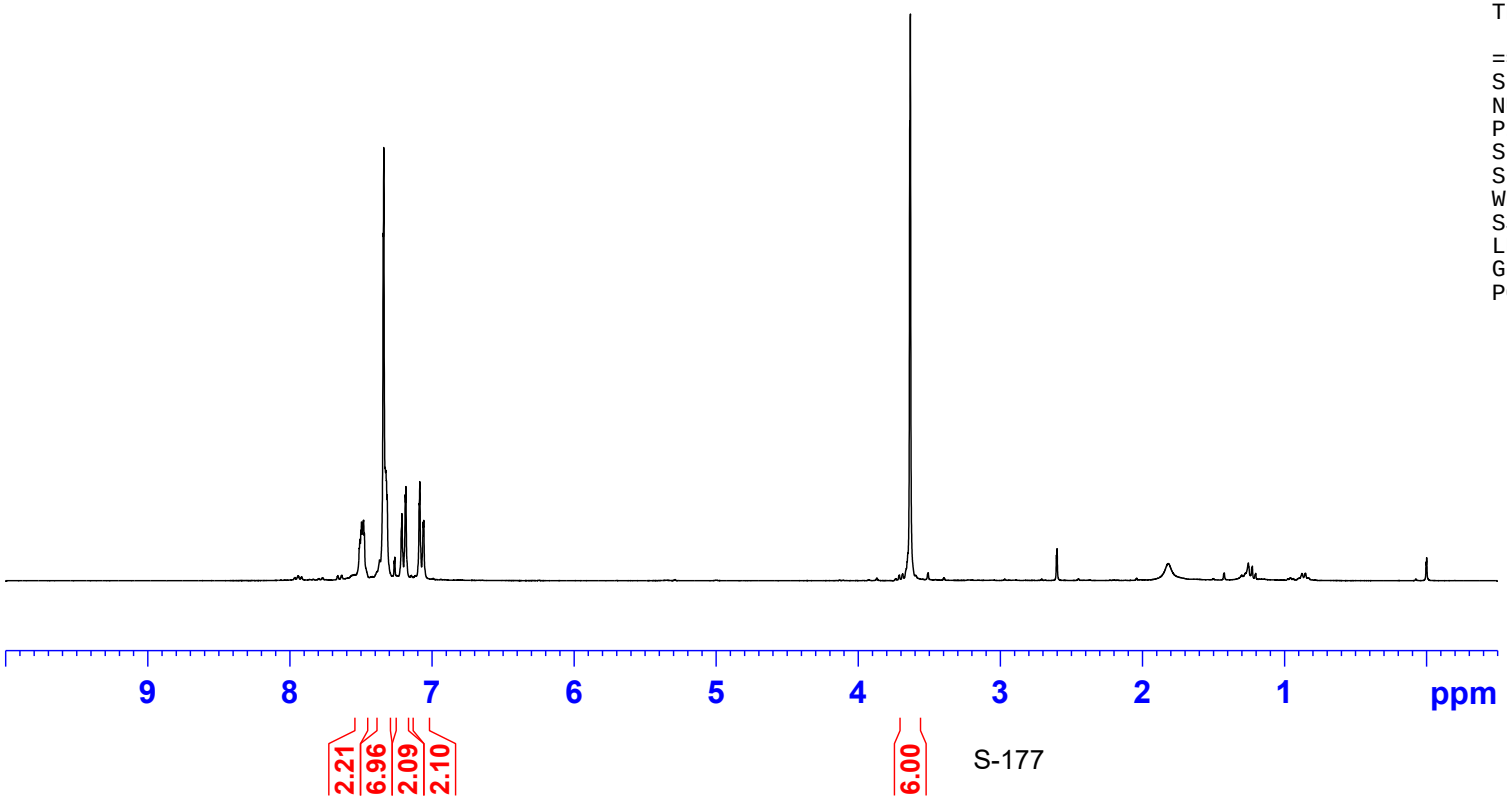



```
NAME        FNMR-gwg-2-24
EXPNO                3564
PROCNO                  1
Date_            20210518
Time                11.18
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG       zgfhigqn.2
TD                 131072
SOLVENT             CDCl3
NS                     16
DS                      4
SWH             66964.289 Hz
FIDRES          0.510897 Hz
AQ              0.9787210 sec
RG                    203
DW                7.467 usec
DE                6.50 usec
TE                296.2 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
SI                  65536
SF            282.4043552 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

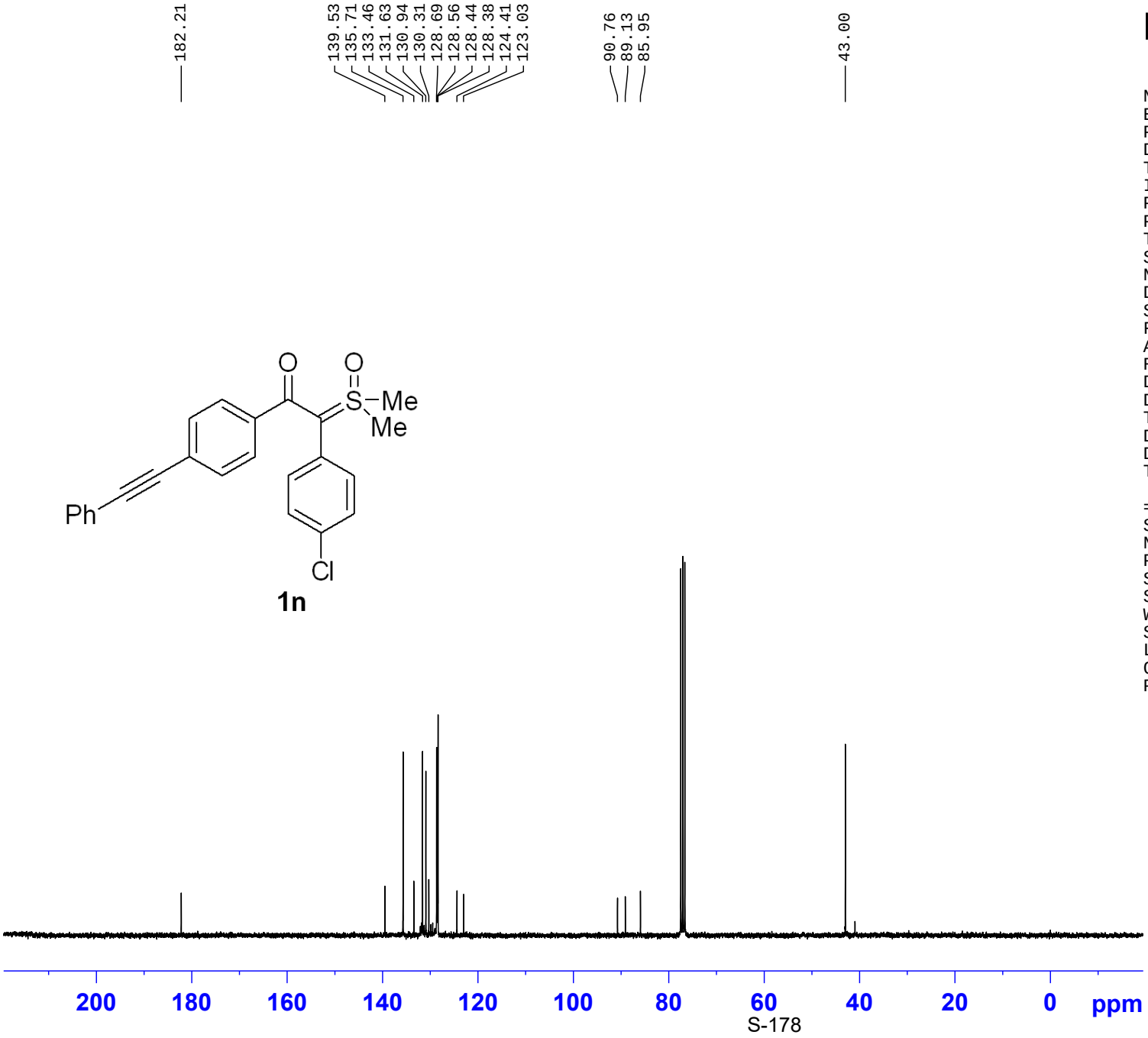




1n

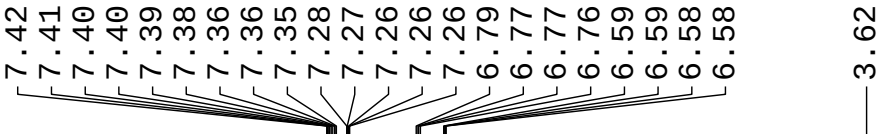


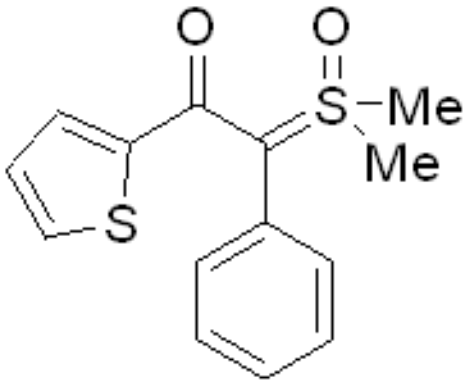

```
NAME        HNMR-gwg-2-83
EXPNO               3952
PROCNO                 1
Date_           20210603
Time                9.58
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ              5.4526453 sec
RG                   144
DW                83.200 usec
DE                 6.50 usec
TE                296.1 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1318534 MHz
NUC1                   1H
P1                 10.00 usec
SI                 65536
SF           300.1300067 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



BRUKER

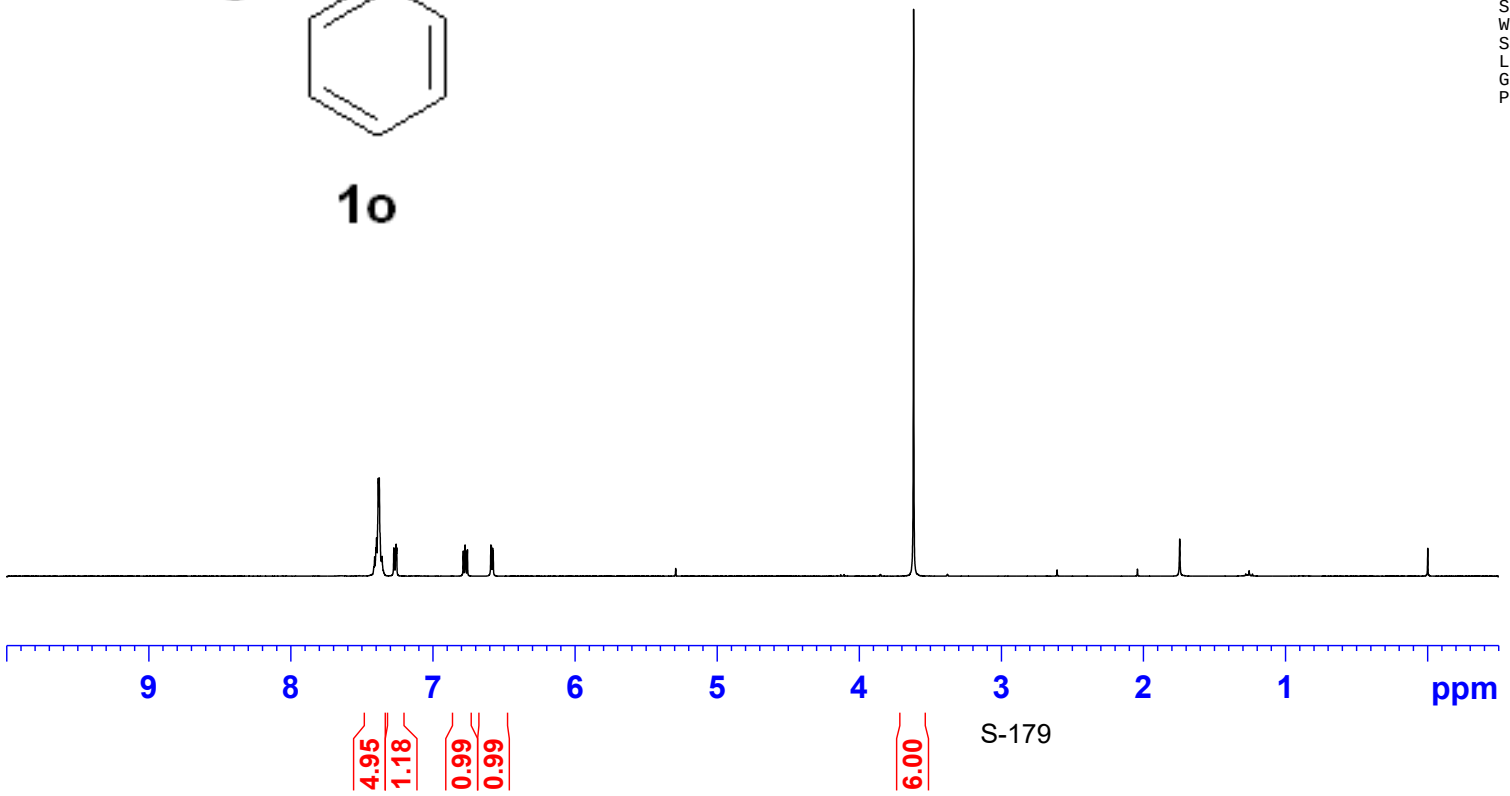
NAME	CNMR-gwg-2-83
EXPNO	4006
PROCNO	1
Date_	20210605
Time	11.44
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	18028.846 Hz
FIDRES	0.275098 Hz
AQ	1.8175818 sec
RG	203
DW	27.733 usec
DE	6.50 usec
TE	296.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	75.4752949 MHz
NUC1	13C
P1	9.50 usec
SI	32768
SF	75.4677485 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

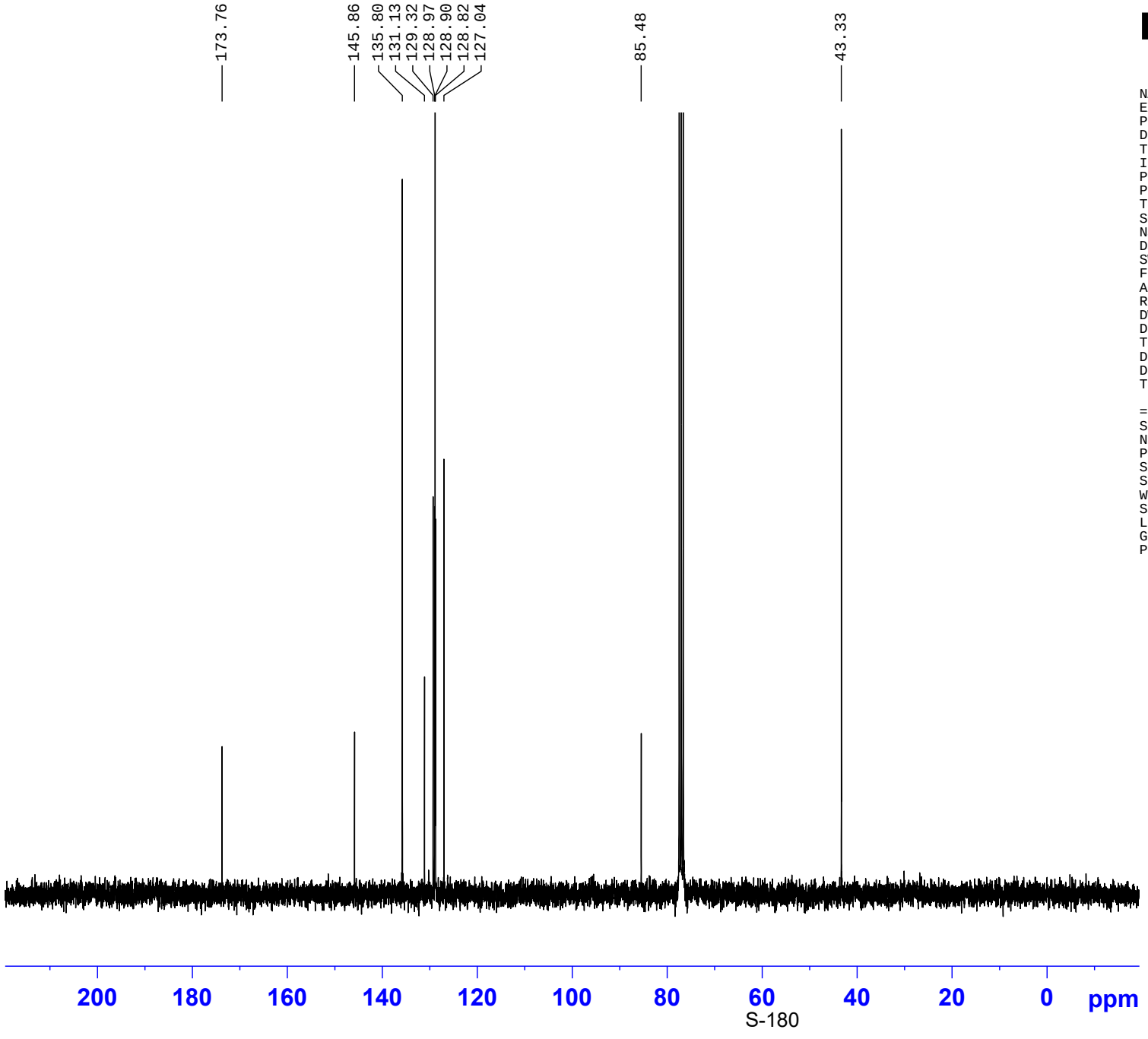




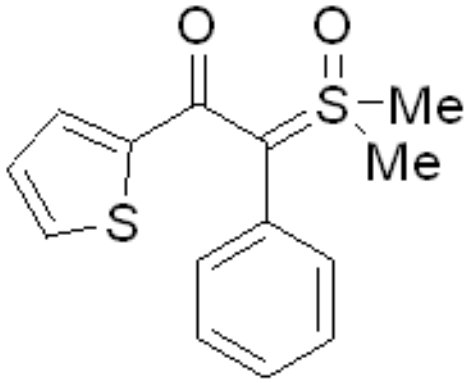
1o

```
NAME      HNMR-gwg-wm-1-41-thiophenyl
EXPNO               3227
PROCNO                 1
Date_           20210425
Time                9.56
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              5.4526453 sec
RG                   181
DW                83.200 usec
DE                 6.50 usec
TE                296.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1318534 MHz
NUC1                   1H
P1                 10.00 usec
SI                 65536
SF           300.1300060 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

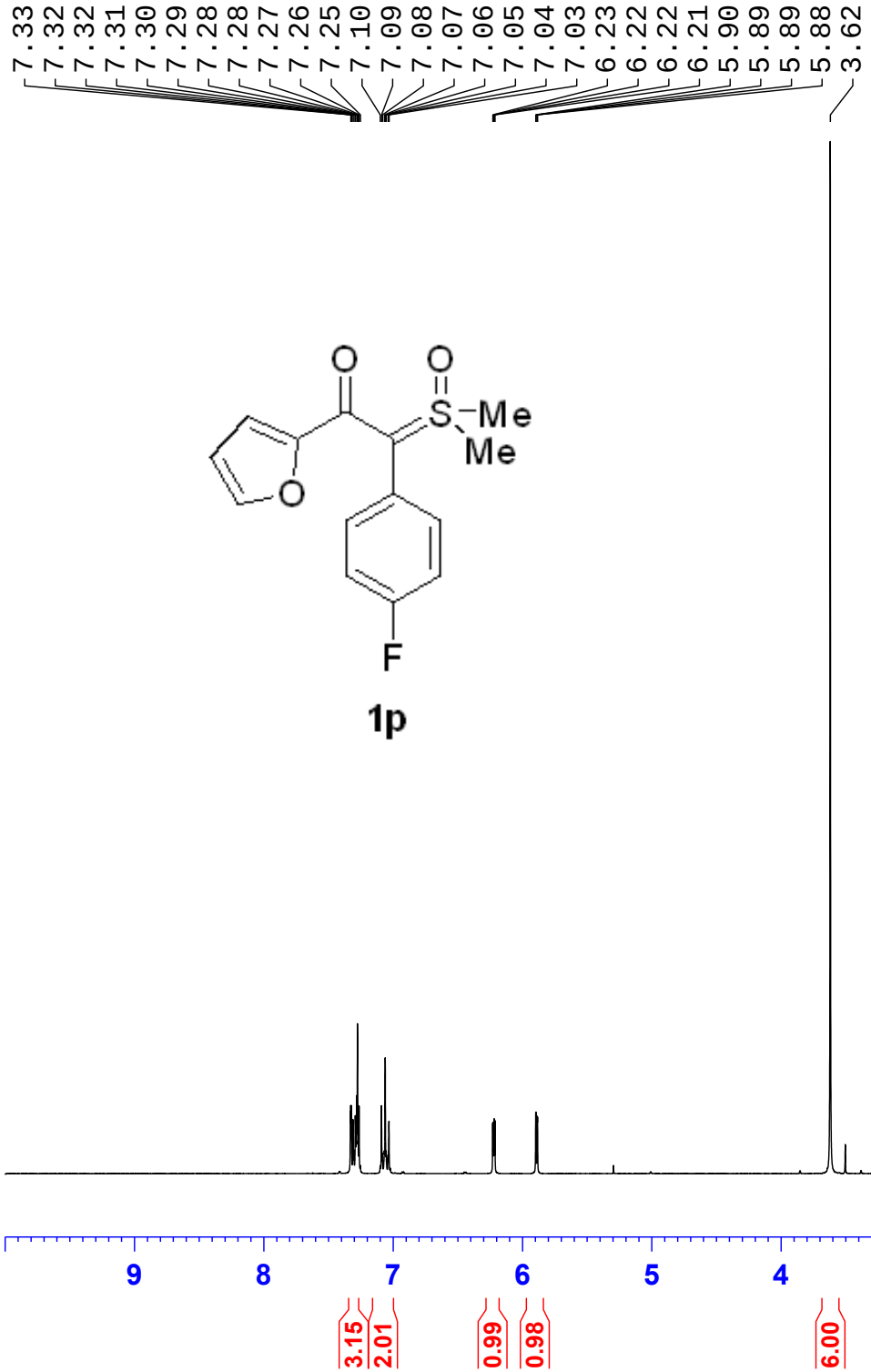





```
NAME      CNMR-gwg-wm-1-41-thiophenyl
EXPNO               3248
PROCNO                 1
Date_           20210426
Time               12.16
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  600
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ             1.8175818 sec
RG                  203
DW                27.733 usec
DE                 6.50 usec
TE                296.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1          75.4752949 MHz
NUC1              13C
P1                 9.50 usec
SI                32768
SF            75.4677485 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```

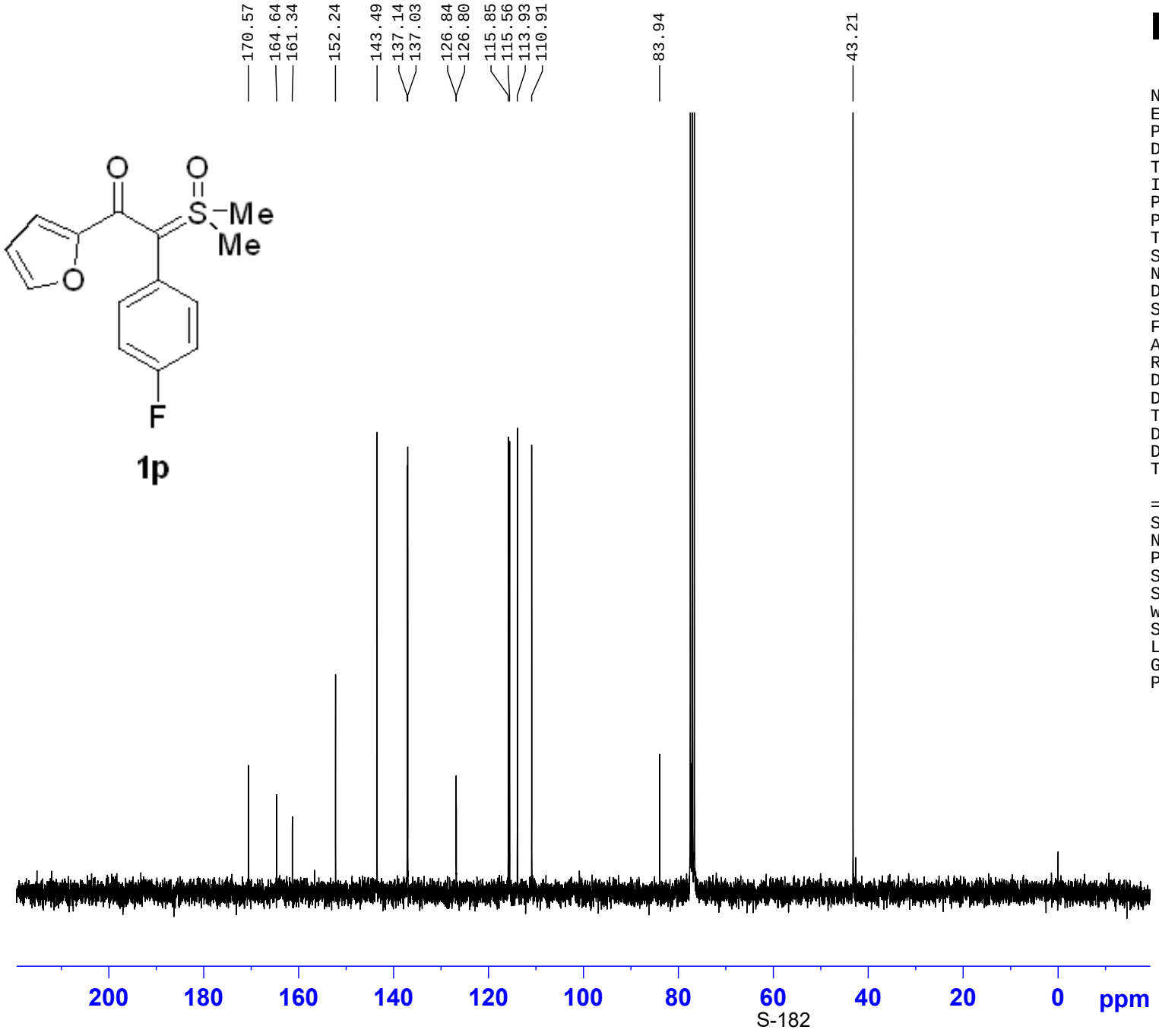


1o

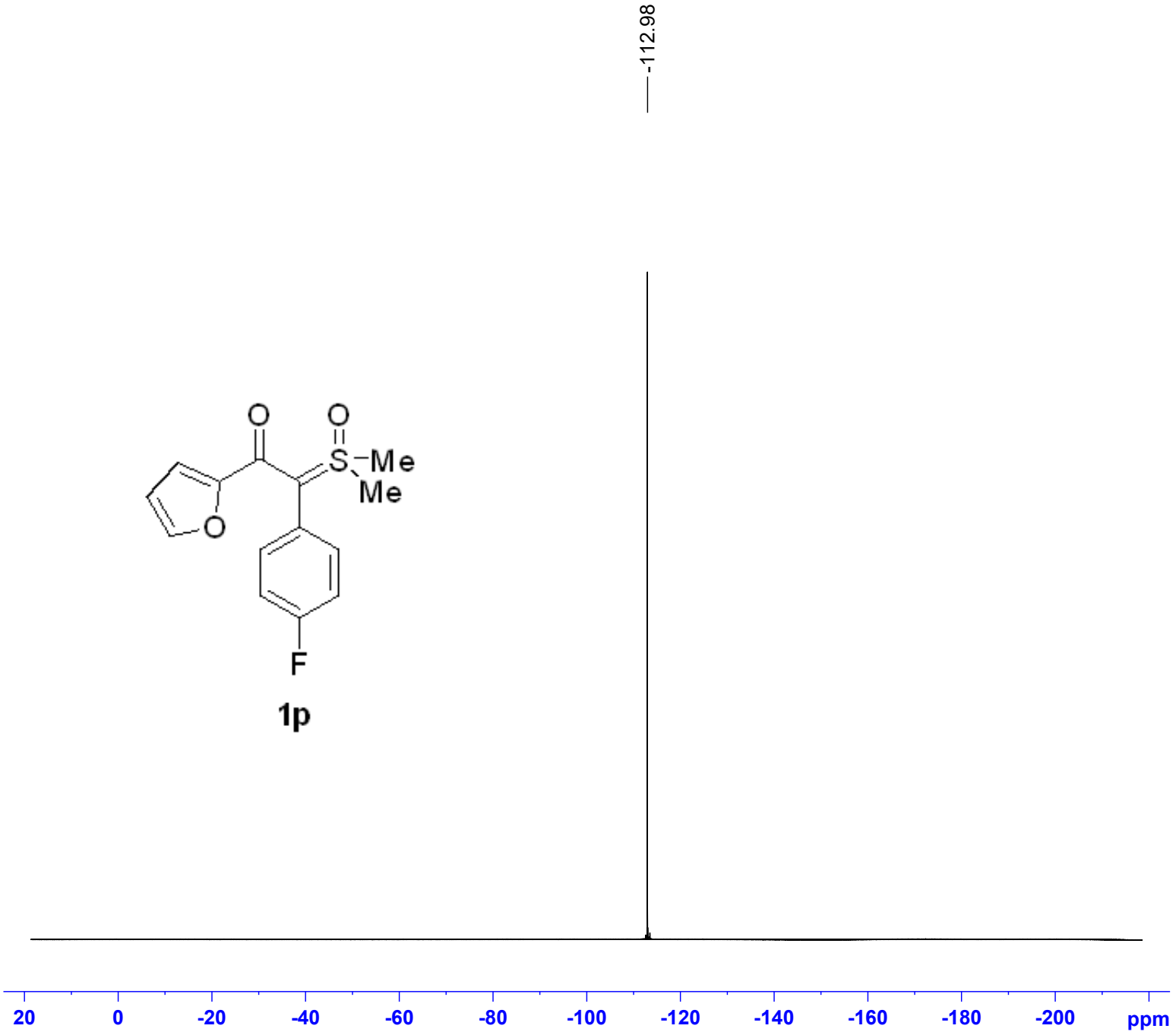


BRUKER

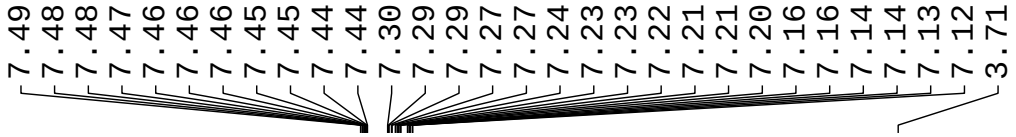
```
NAME        HNMR-gwg-1-85
EXPNO               3228
PROCNO                 1
Date_           20210425
Time               10.01
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             6009.615 Hz
FIDRES          0.091699 Hz
AQ              5.4526453 sec
RG                   144
DW                83.200 usec
DE                 6.50 usec
TE                296.1 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         300.1318534 MHz
NUC1                   1H
P1                 10.00 usec
SI                 65536
SF           300.1300024 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

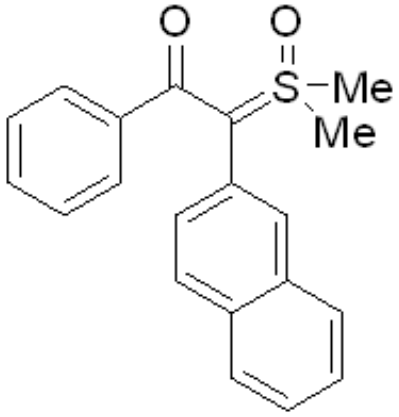



```
NAME          CNMR-gwg-1-85
EXPNO                 3230
PROCNO                   1
Date_             20210425
Time                 10.25
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   300
DS                     4
SWH            18028.846 Hz
FIDRES          0.275098 Hz
AQ              1.8175818 sec
RG                   203
DW                27.733 usec
DE                 6.50 usec
TE                296.1 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1           75.4752949 MHz
NUC1                  13C
P1                  9.50 usec
SI                 32768
SF             75.4677485 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



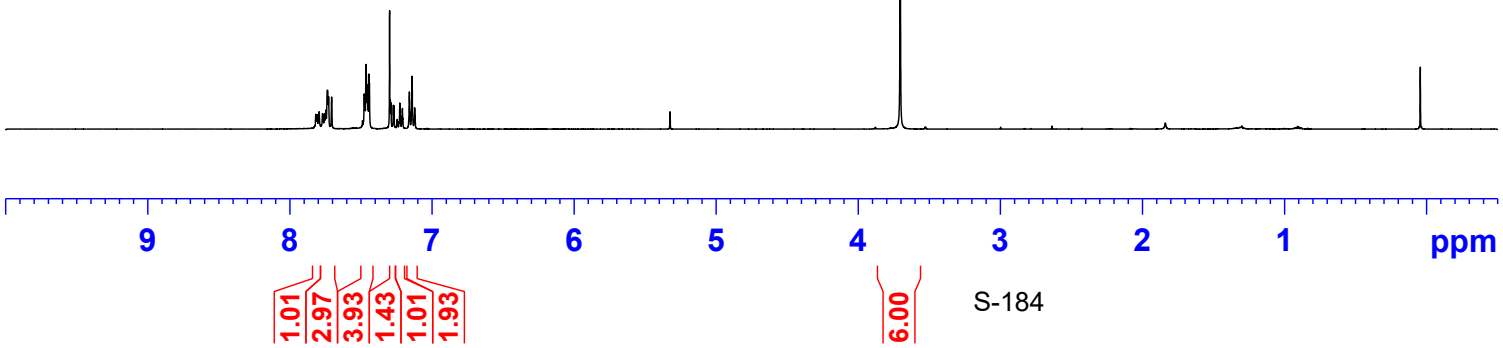

```
NAME       FNMR-gwg-1-85
EXPNO              3229
PROCNO                1
Date_          20210425
Time              10.04
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG      zgfhigqn.2
TD               131072
SOLVENT            CDCl3
NS                    16
DS                     4
SWH            66964.289 Hz
FIDRES         0.510897 Hz
AQ             0.9787210 sec
RG                   203
DW                 7.467 usec
DE                 6.50 usec
TE                296.1 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
SI                65536
SF           282.4043552 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

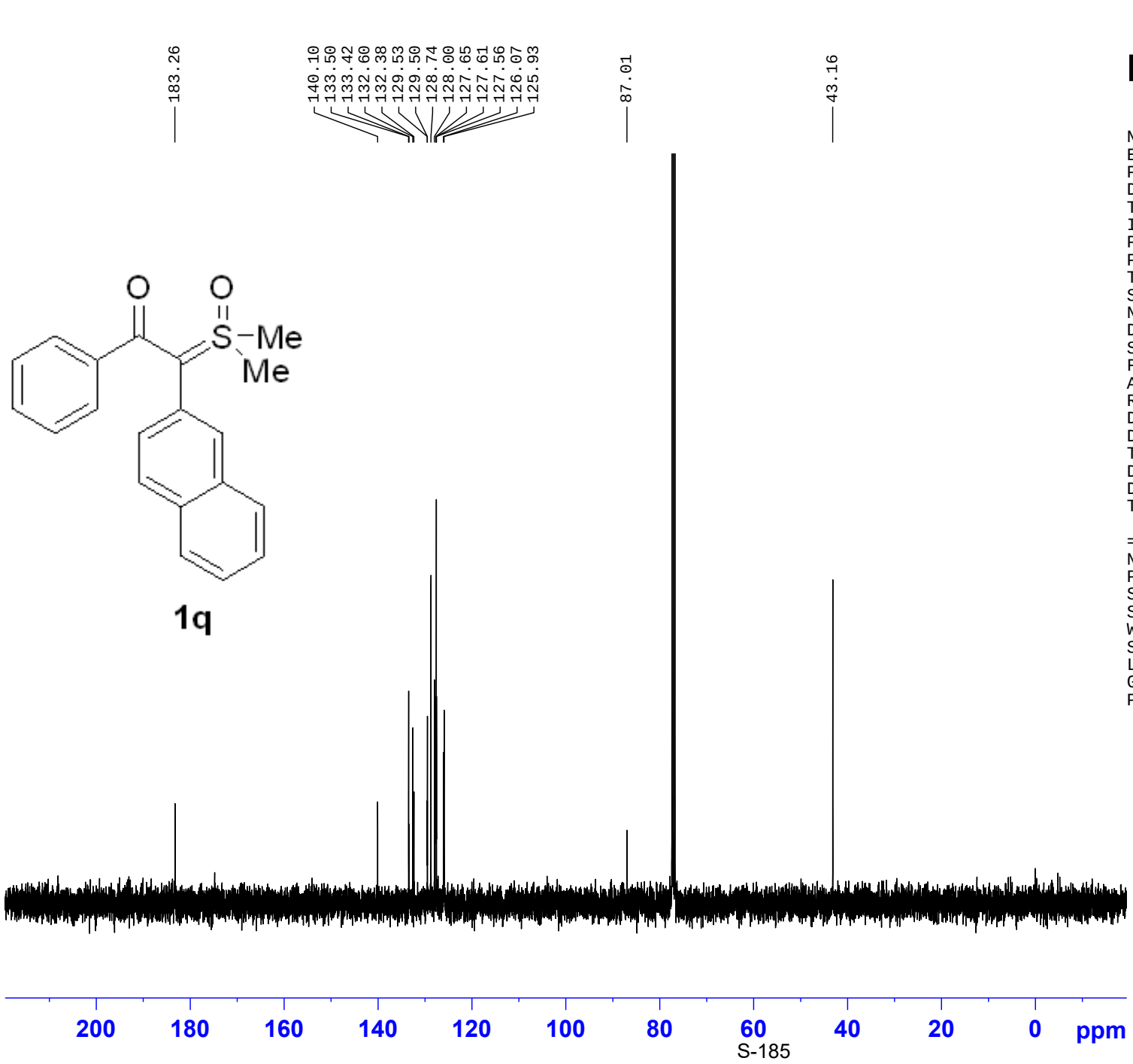




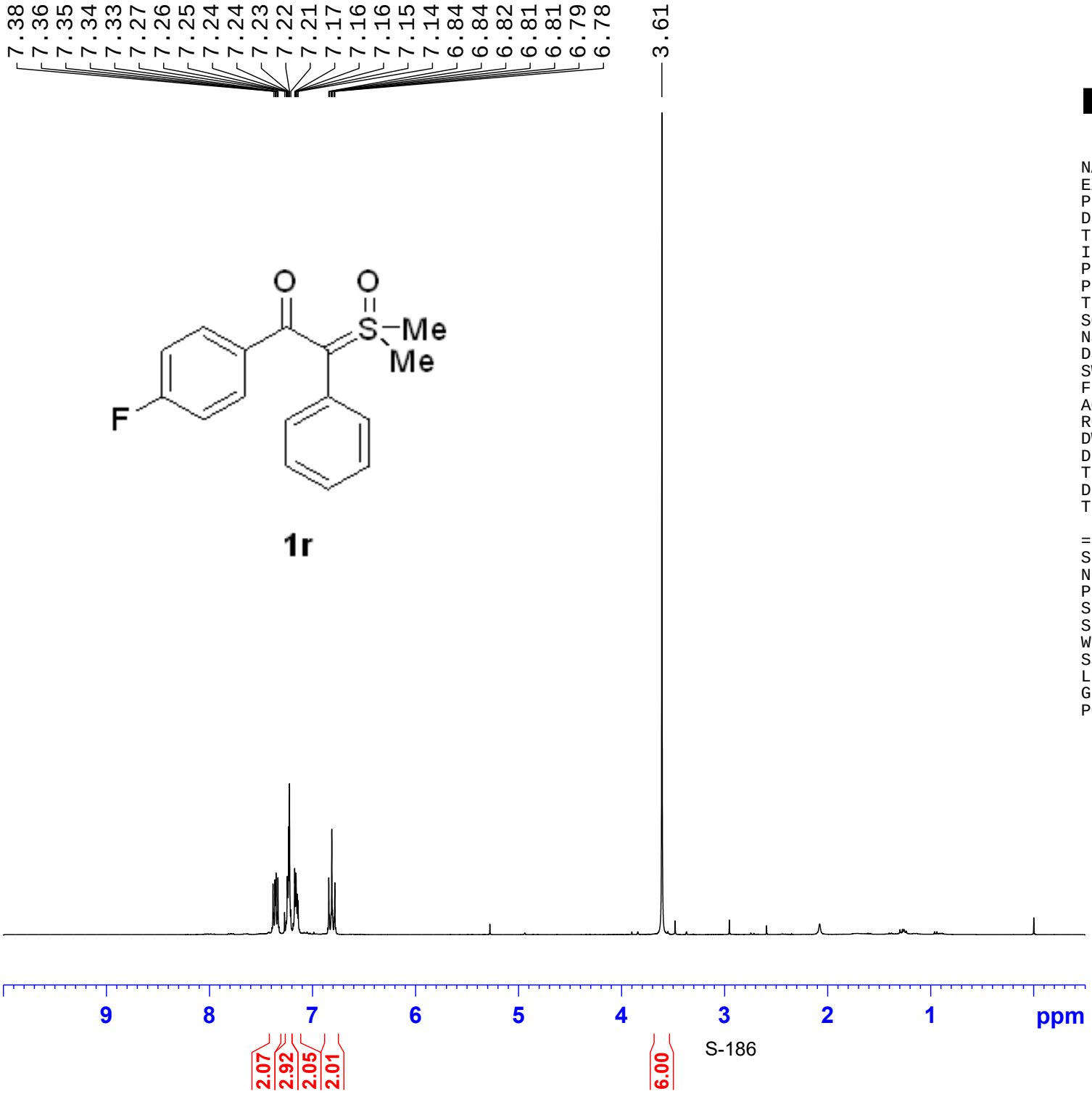
1q

```
NAME          HNMR-gwg-1-27
EXPNO                    43
PROCNO                    1
Date_             20210325
Time                 15.11
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       6
DS                       2
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                   100.49
DW                   60.800 usec
DE                    6.50 usec
TE                   293.7 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.40 usec
SI                   65536
SF            400.1900000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



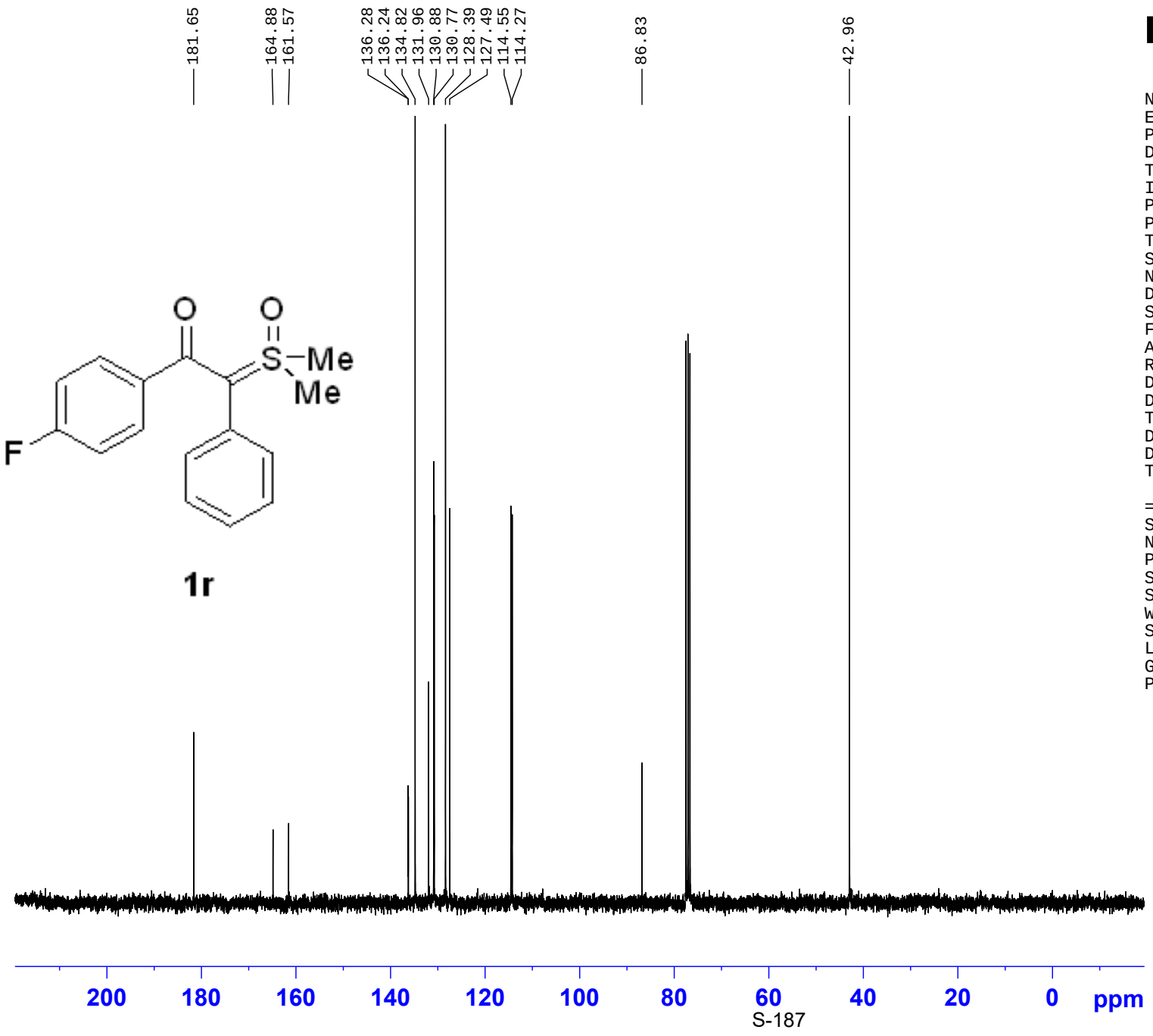



```
NAME          CNMR-gwg-1-27
EXPNO                    53
PROCNO                    1
Date_              20210326
Time                  15.19
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       33
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                1.3631988 sec
RG                   193.13
DW                   20.800 usec
DE                    6.50 usec
TE                   294.5 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                     9.90 usec
SI                    32768
SF             100.6278560 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```



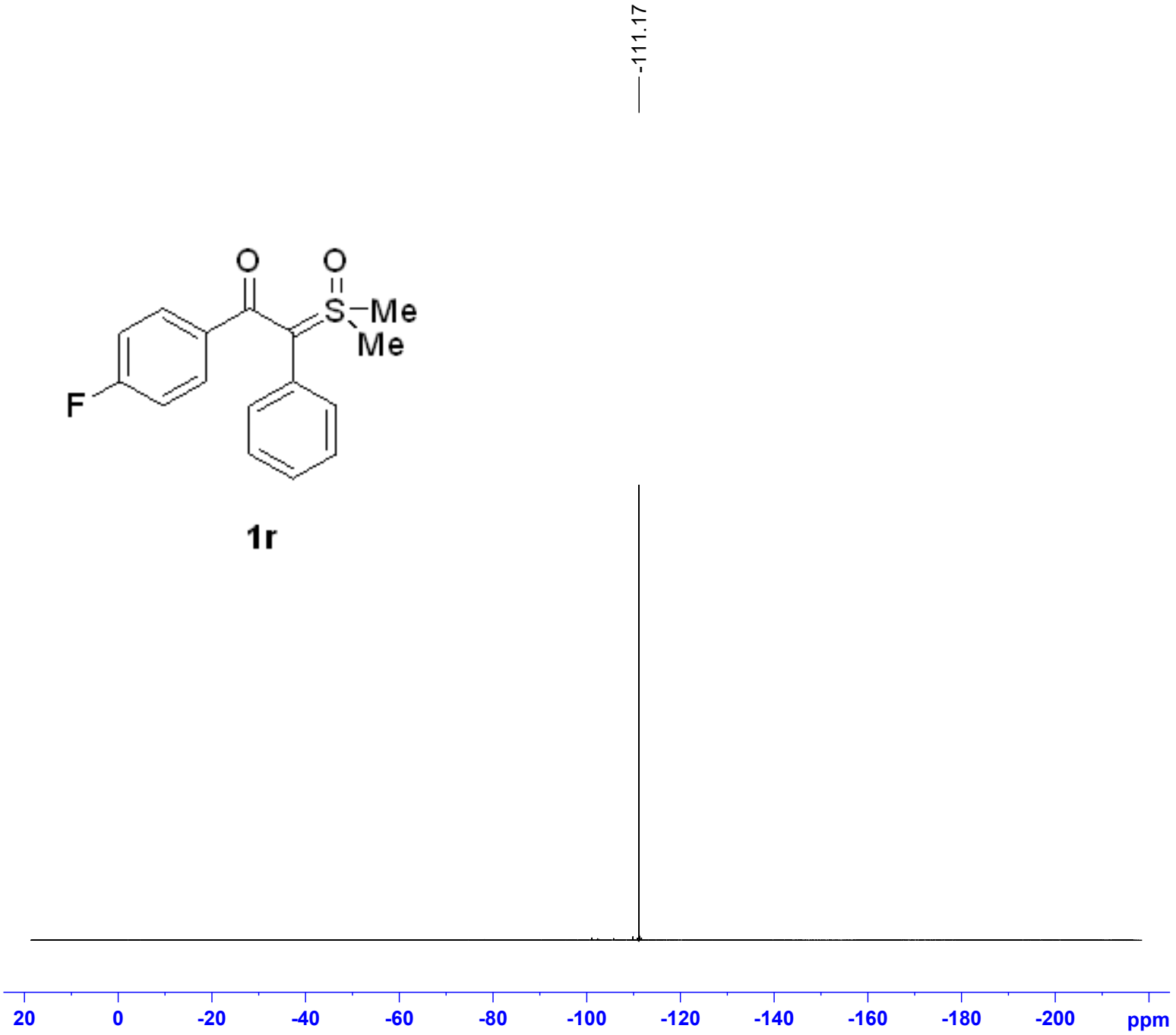
BRUKER

```
NAME      HNMR-gwg-1-49-wm
EXPNO                 5329
PROCNO                   1
Date_          20210914
Time                11.04
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               5.4526453 sec
RG                    90.5
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
SI                  65536
SF           300.1300041 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

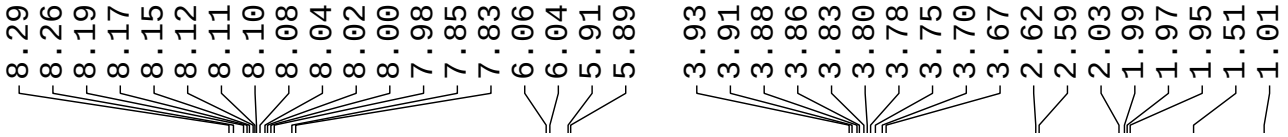


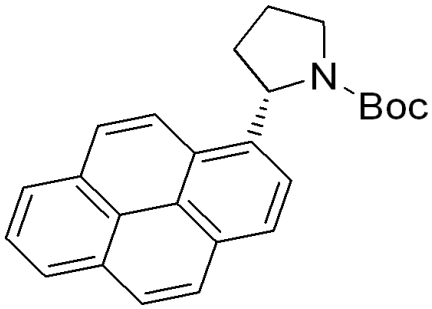

```
NAME        CNMR-gwg-1-49-wm
EXPNO                   5331
PROCNO                     1
Date_               20210914
Time                   11.27
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       300
DS                         4
SWH                18028.846 Hz
FIDRES              0.275098 Hz
AQ                  1.8175818 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
SI                     32768
SF                 75.4677485 MHz
WDW                       EM
SSB                        0
LB                     1.00 Hz
GB                         0
PC                     1.40
```

1r



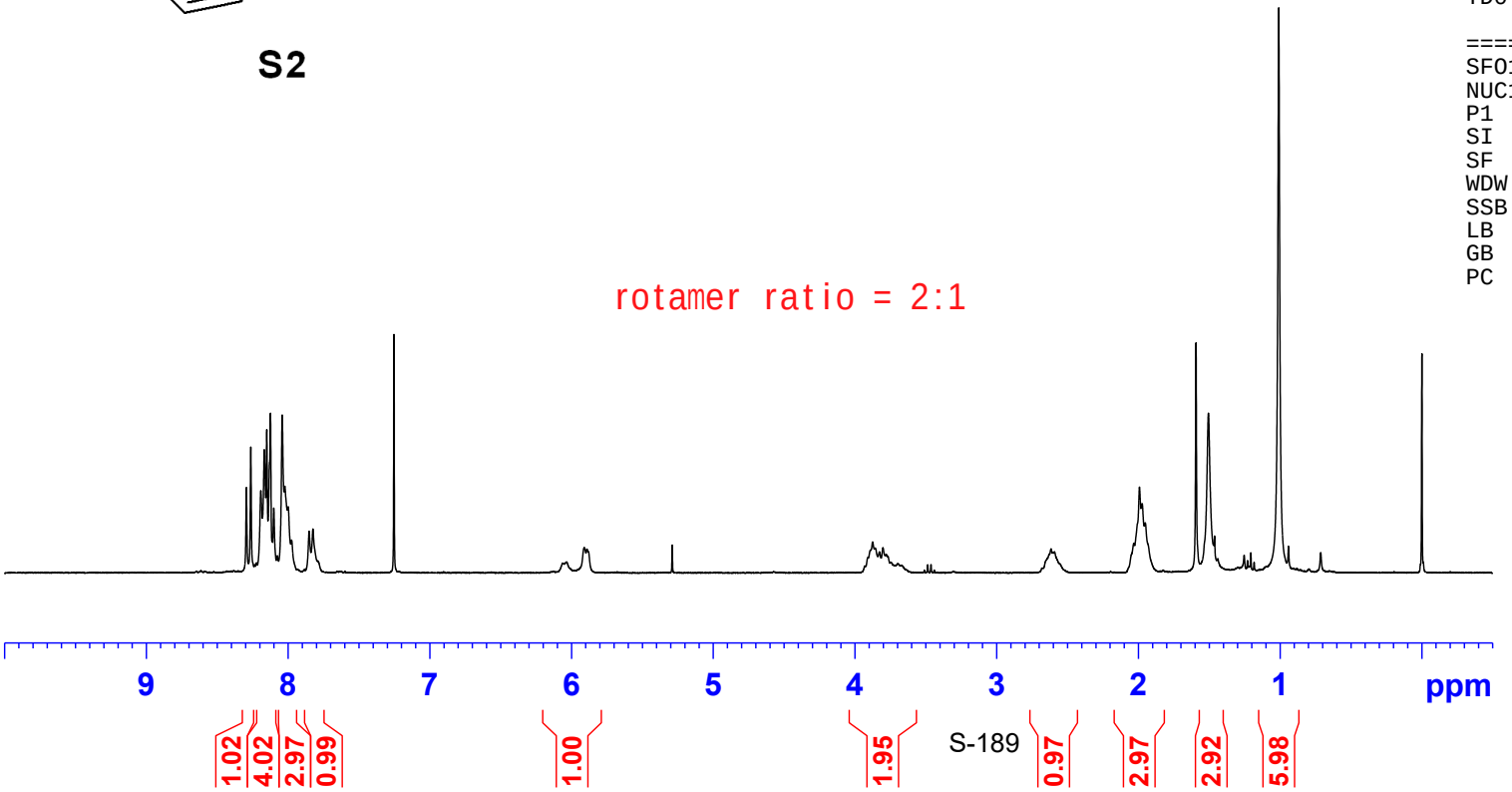

```
NAME      FNMR-gwg-1-49-wm
EXPNO                5330
PROCNO                  1
Date_            20210914
Time                11.06
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG       zgfhigqn.2
TD                 131072
SOLVENT             CDCl3
NS                     16
DS                      4
SWH             66964.289 Hz
FIDRES           0.510897 Hz
AQ               0.9787210 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
SI                  65536
SF            282.4043552 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

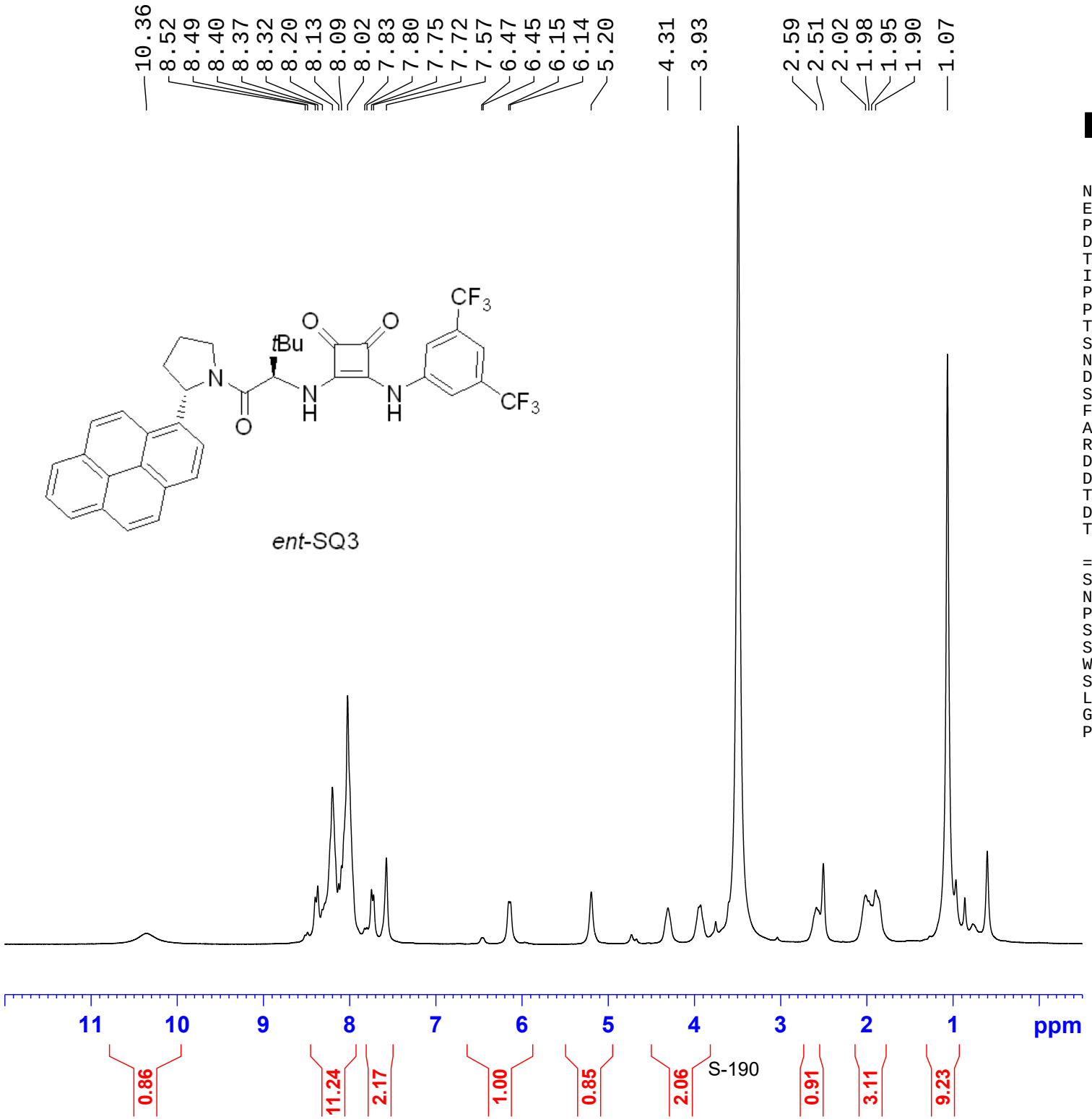




S2

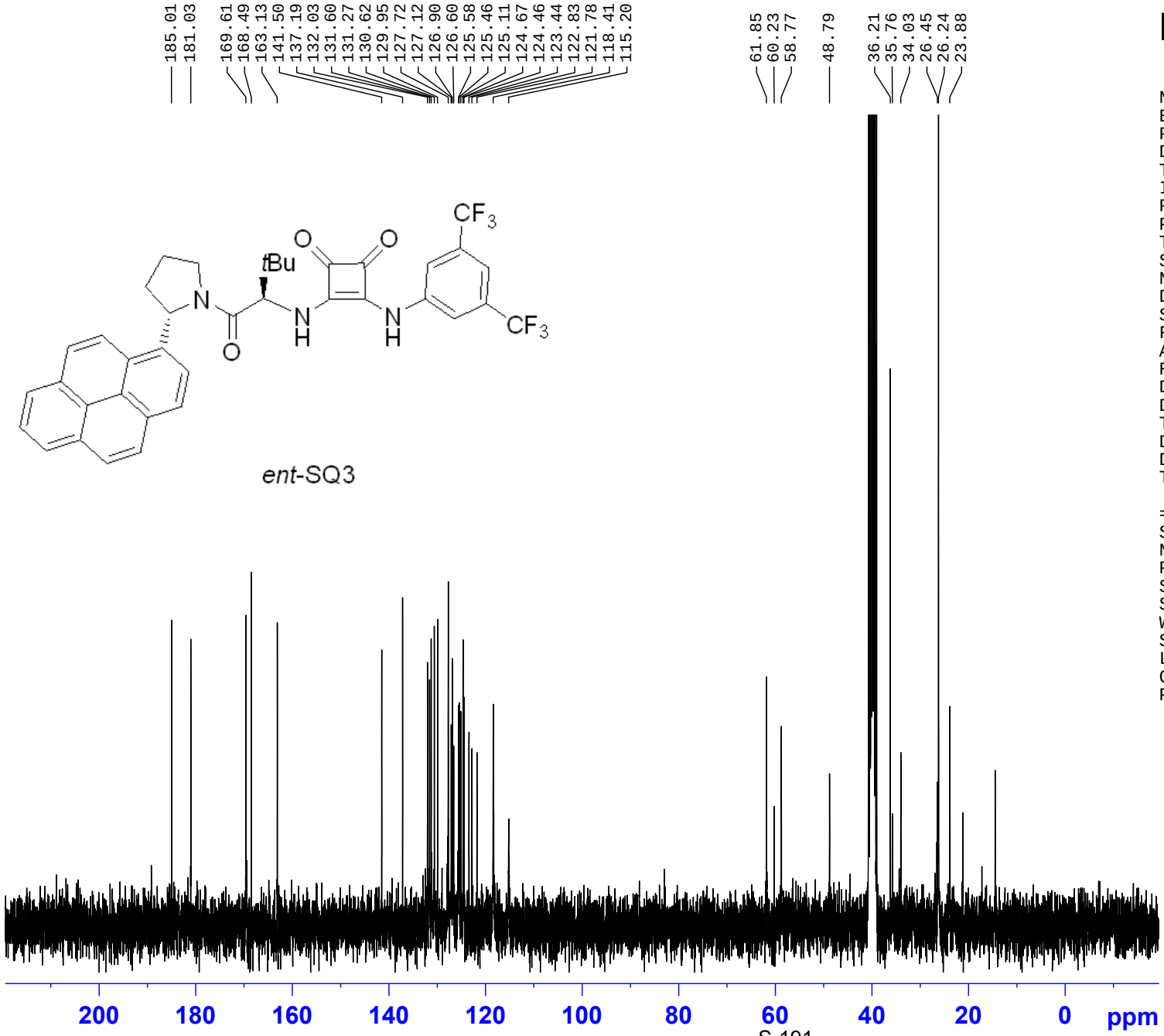
```
NAME          HNMR-gwg-3-90
EXPNO                  4859
PROCNO                    1
Date_              20210727
Time                  10.50
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                6009.615 Hz
FIDRES             0.091699 Hz
AQ                 5.4526453 sec
RG                       203
DW                    83.200 usec
DE                     6.50 usec
TE                    296.1 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            300.1318534 MHz
NUC1                      1H
P1                    10.00 usec
SI                    65536
SF              300.1300093 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```





BRUKER

NAME	HNMR-gwg-3-99
EXPNO	4979
PROCNO	1
Date_	20210804
Time	9.28
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	6009.615 Hz
FIDRES	0.091699 Hz
AQ	5.4526453 sec
RG	32
DW	83.200 usec
DE	6.50 usec
TE	296.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	300.1318534 MHz
NUC1	1H
P1	10.00 usec
SI	65536
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

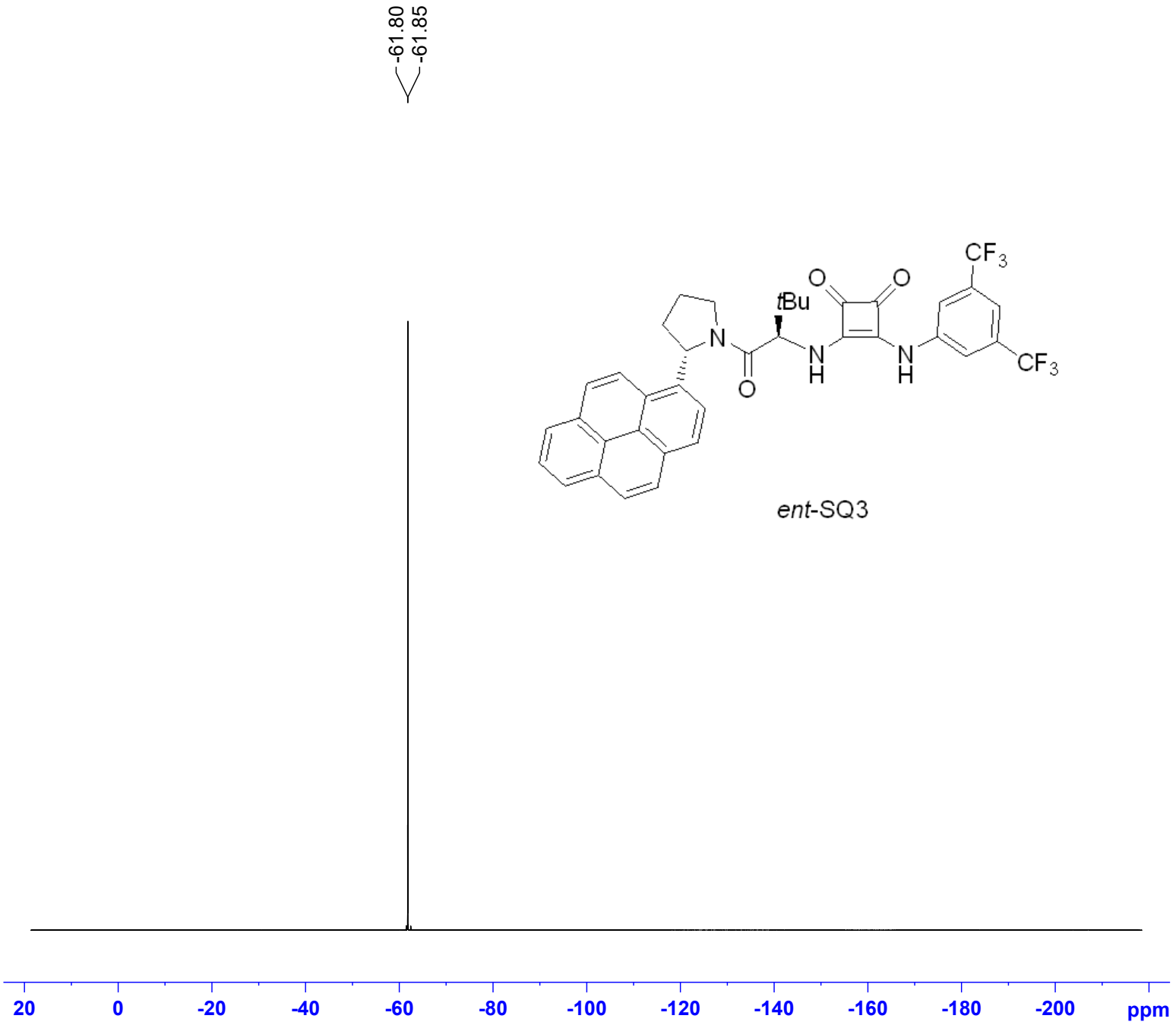


BRUKER

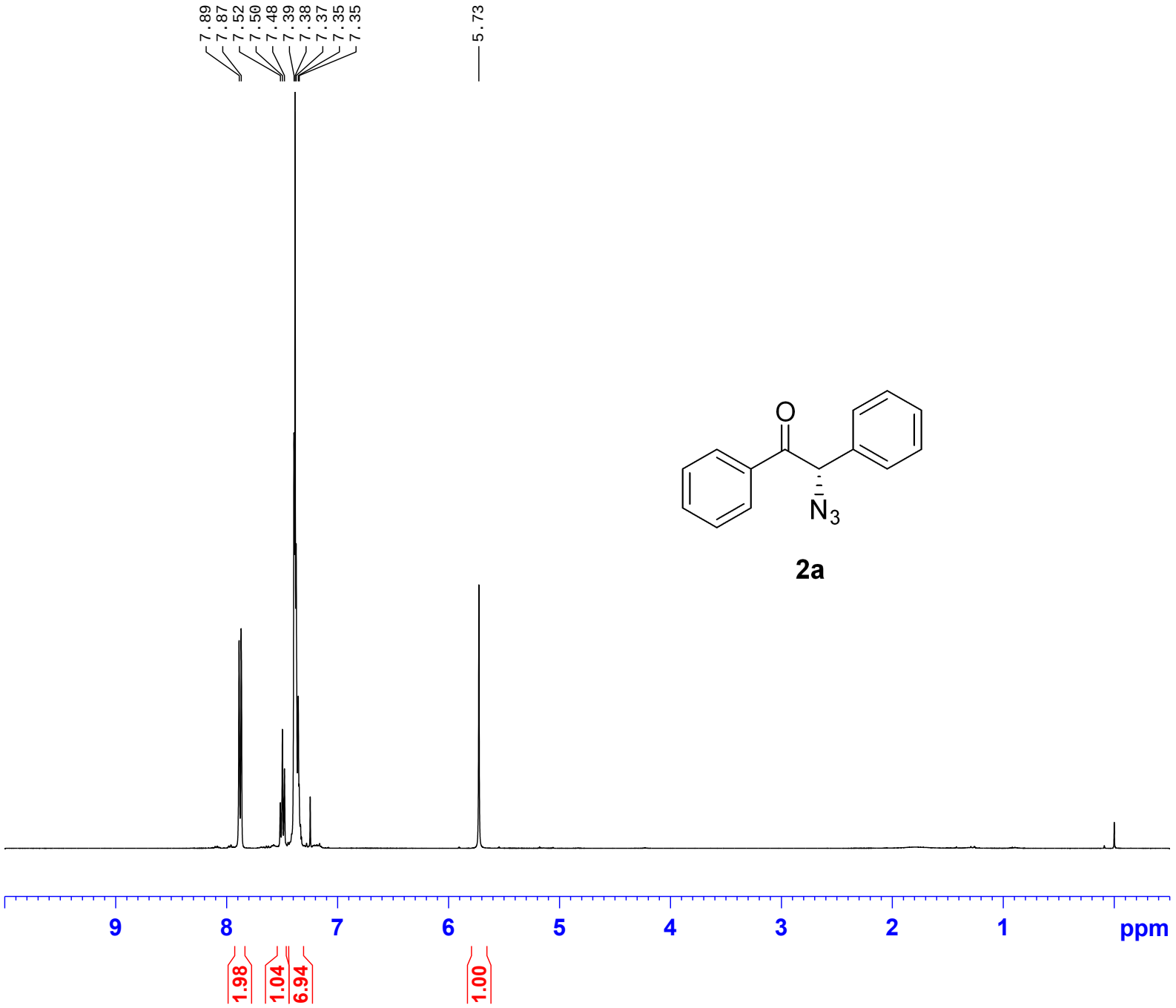
NAME	HNMR-gwg-3-99
EXPNO	5343
PROCNO	1
Date_	20210915
Time	13.36
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	500
DS	4
SWH	18028.846 Hz
FIDRES	0.275098 Hz
AQ	1.8175818 sec
RG	203
DW	27.733 usec
DE	6.50 usec
TE	-59.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1

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

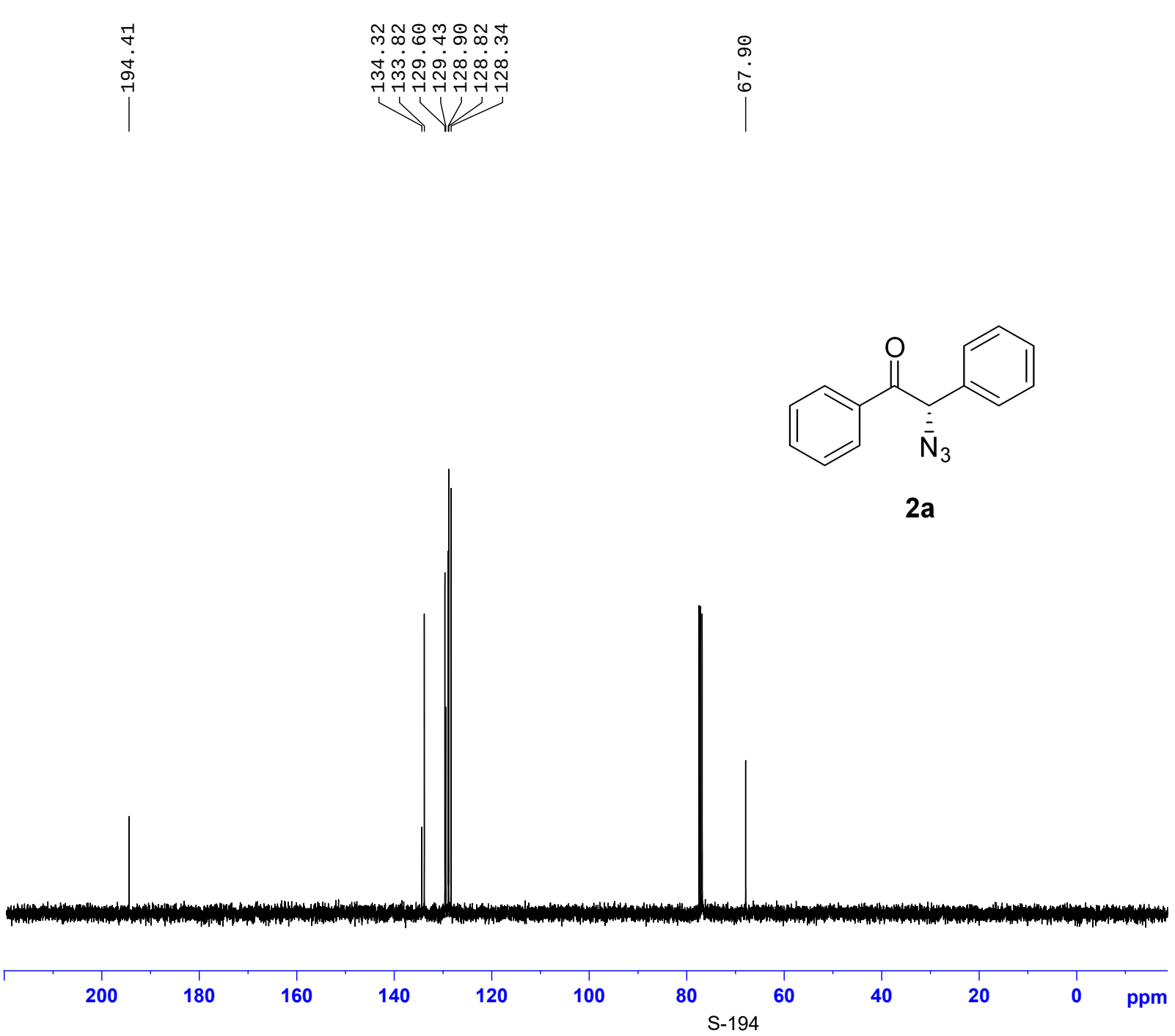
SFO1	75.4752949 MHz
NUC1	13C
P1	9.50 usec
SI	32768
SF	75.4677485 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



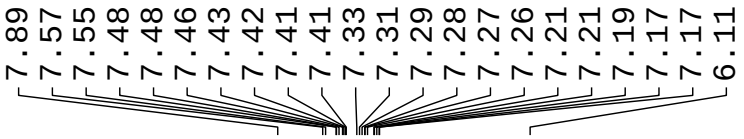

```
NAME          HNMR-gwg-3-99
EXPNO                  5342
PROCNO                    1
Date_              20210915
Time                  13.04
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG         zgfhigqn.2
TD                    131072
SOLVENT                DMSO
NS                        16
DS                         4
SWH               66964.289 Hz
FIDRES             0.510897 Hz
AQ                 0.9787210 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
SI                    65536
SF              282.4043552 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

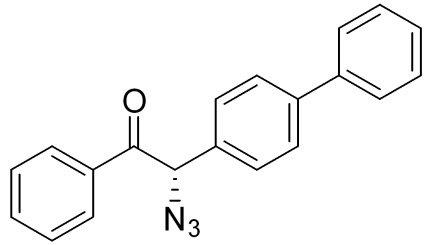



```
NAME      HNMR-gwg-9-93-1
EXPNO                   1
PROCNO                  1
Date_            20201120
Time                14.36
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      4
DS                      0
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                  34.77
DW                  62.400 usec
DE                   6.50 usec
TE                  296.9 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                    1H
P1                  14.50 usec
SI                  65536
SF            400.1300154 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



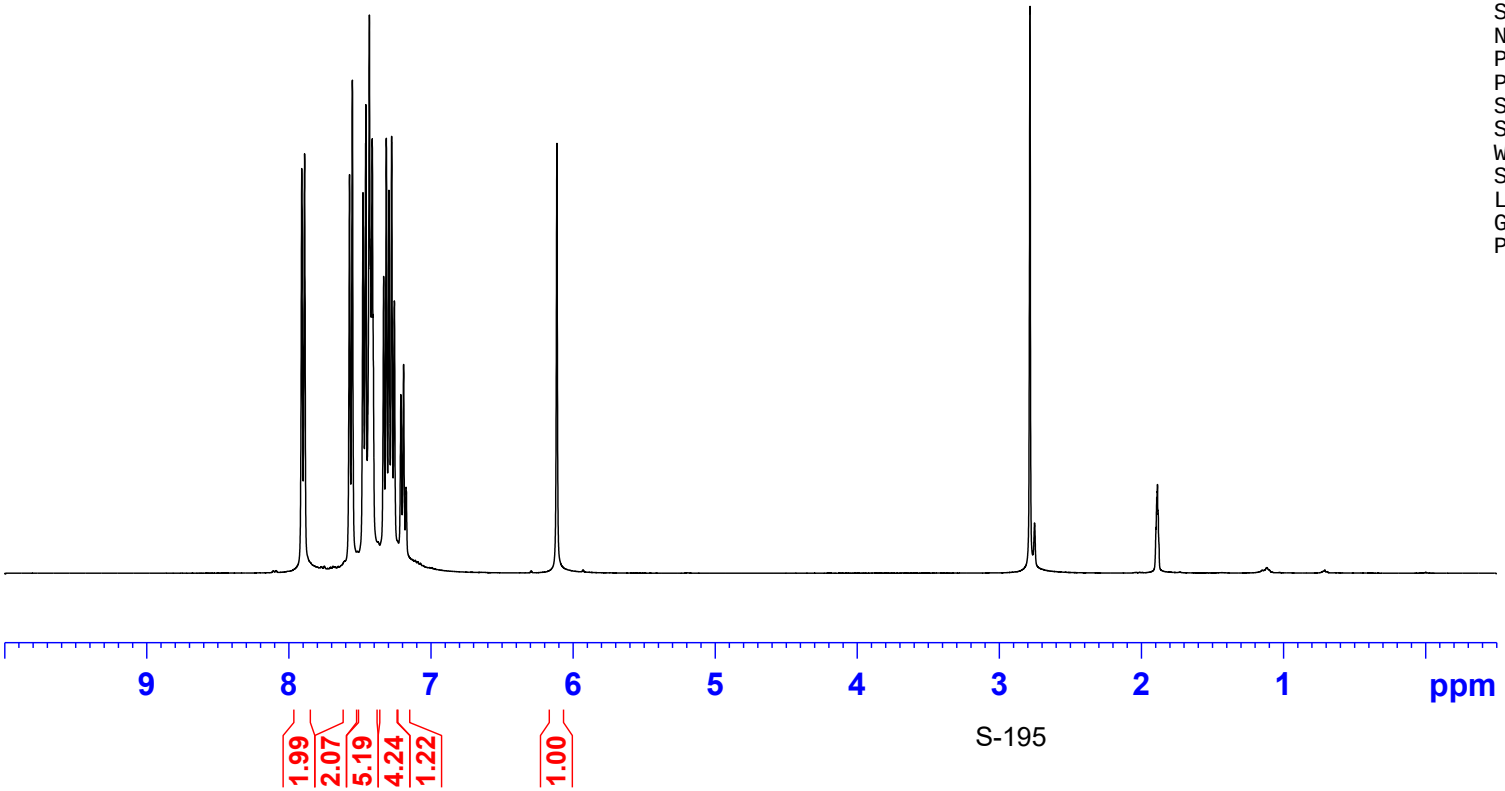
NAME	CNMR-gwg-9-93-1
EXPNO	1
PROCNO	1
Date_	20201120
Time	14.38
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	5
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	297.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

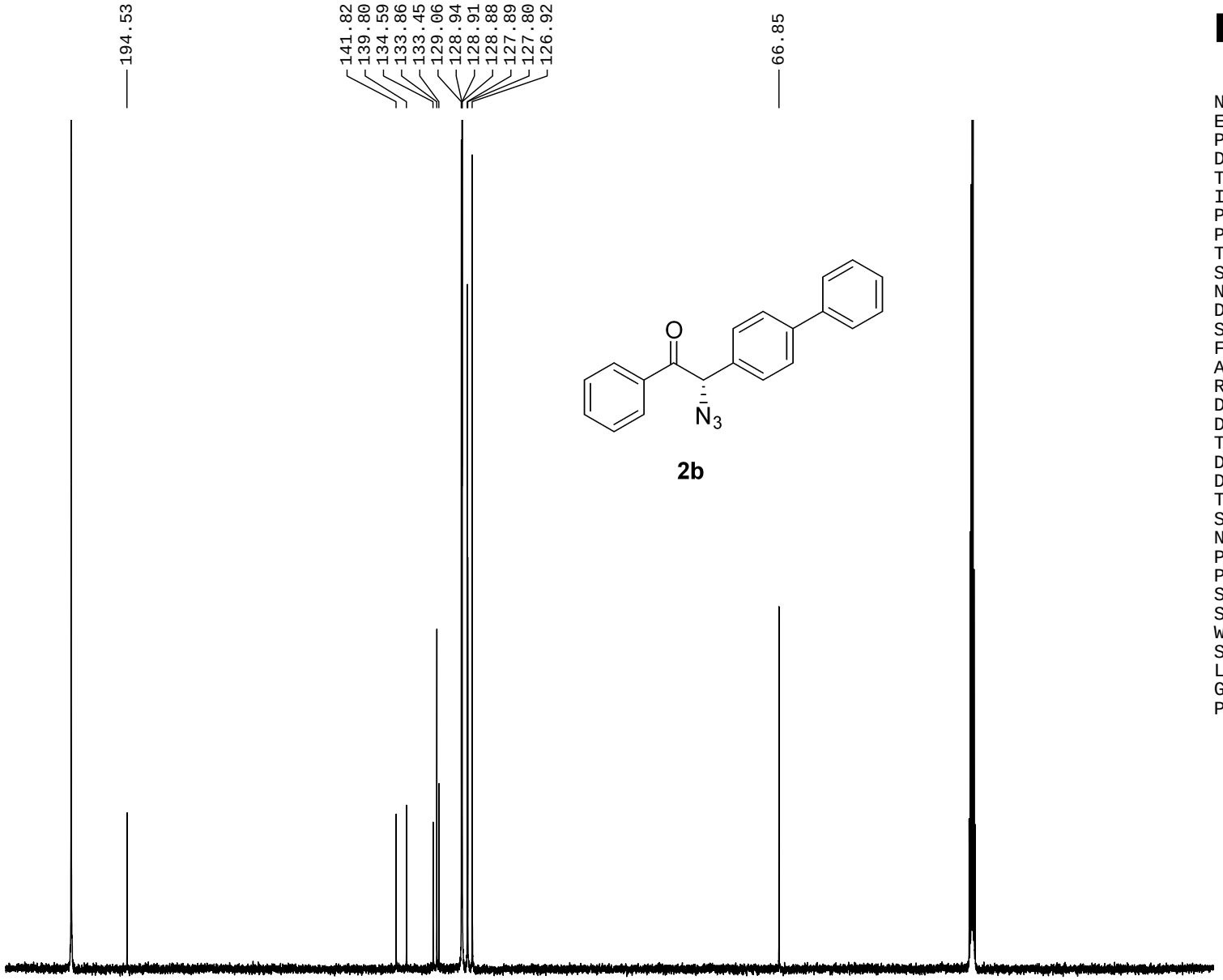




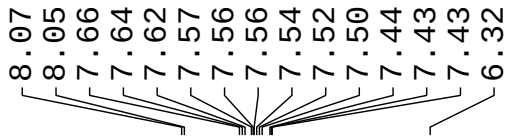
2b

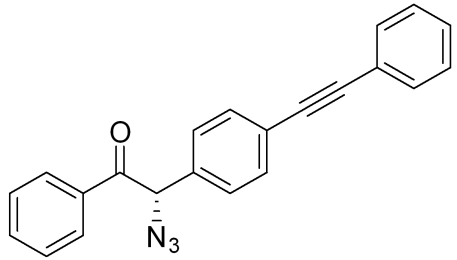
```
NAME          HNMR-gwg-2-66
EXPNO                    1
PROCNO                   1
Date_             20210609
Time                23.35 h
INSTRUM           Avance
PROBHD    Z116098_0833 (
PULPROG              zg30
TD                  65536
SOLVENT           Acetone
NS                      16
DS                       2
SWH              8196.722 Hz
FIDRES           0.250144 Hz
AQ               3.9977460 sec
RG                 52.6316
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
SI                  65536
SF            400.1300716 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                  1.00
```





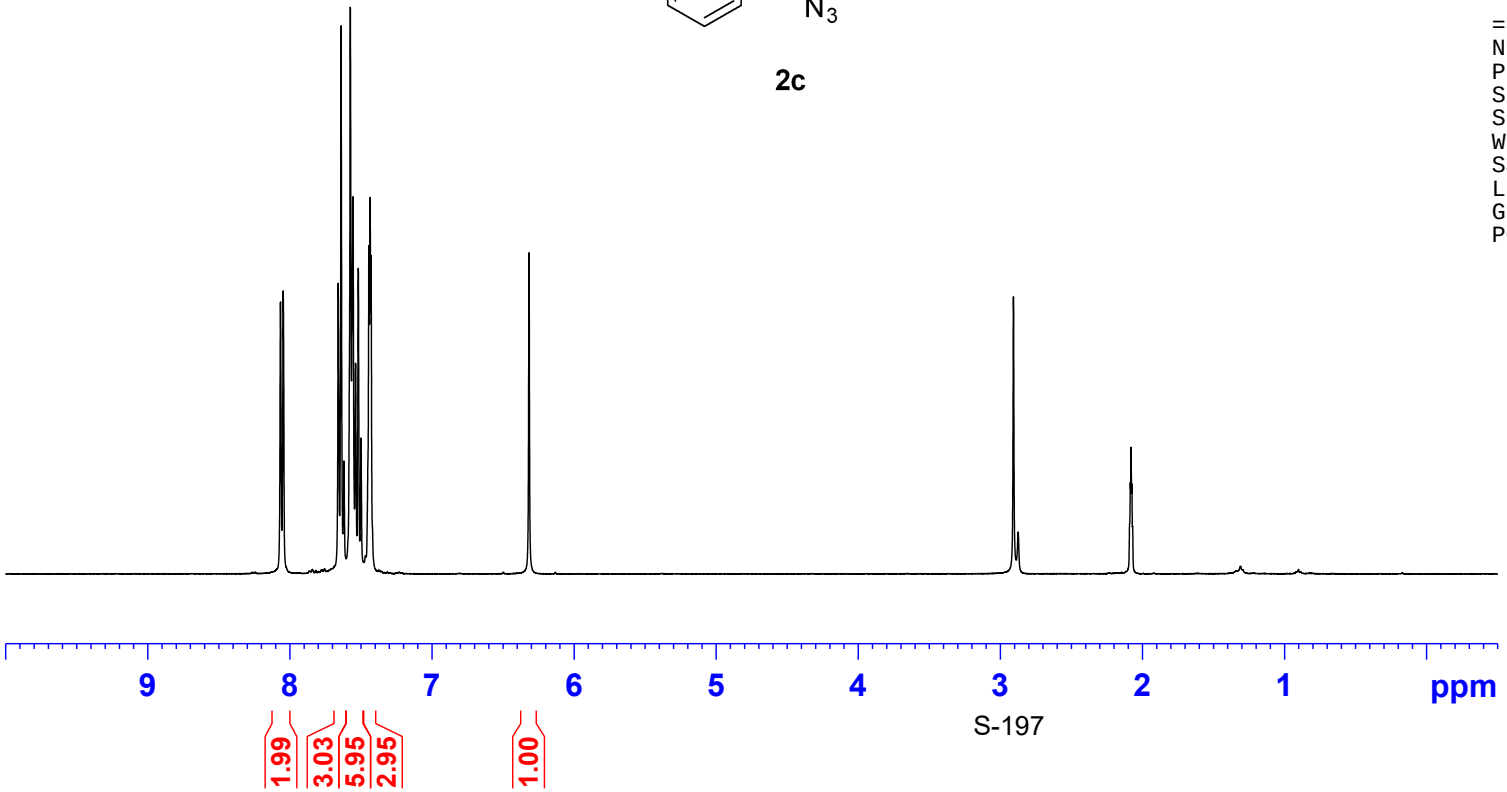
NAME	CNMR-gwg-2-66
EXPNO	2
PROCNO	1
Date_	20210609
Time	23.47 h
INSTRUM	Avance
PROBHD	Z116098_0833 (
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	200
DS	4
SWH	23809.523 Hz
FIDRES	0.726609 Hz
AQ	1.3763061 sec
RG	51.55
DW	21.000 usec
DE	6.50 usec
TE	295.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	100.6228298 MHz
NUC1	13C
P0	3.33 usec
P1	10.00 usec
SI	32768
SF	100.6127685 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

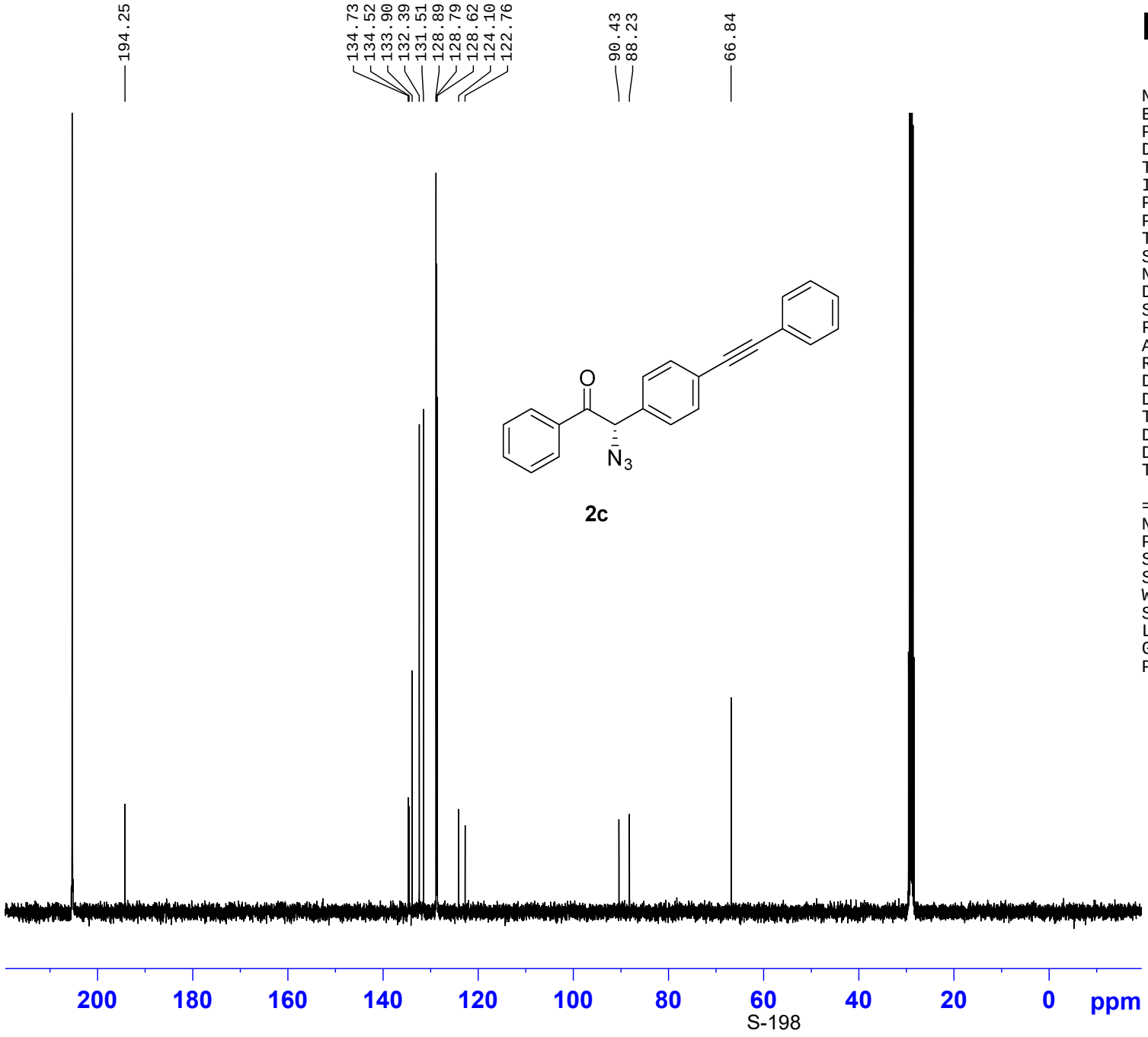




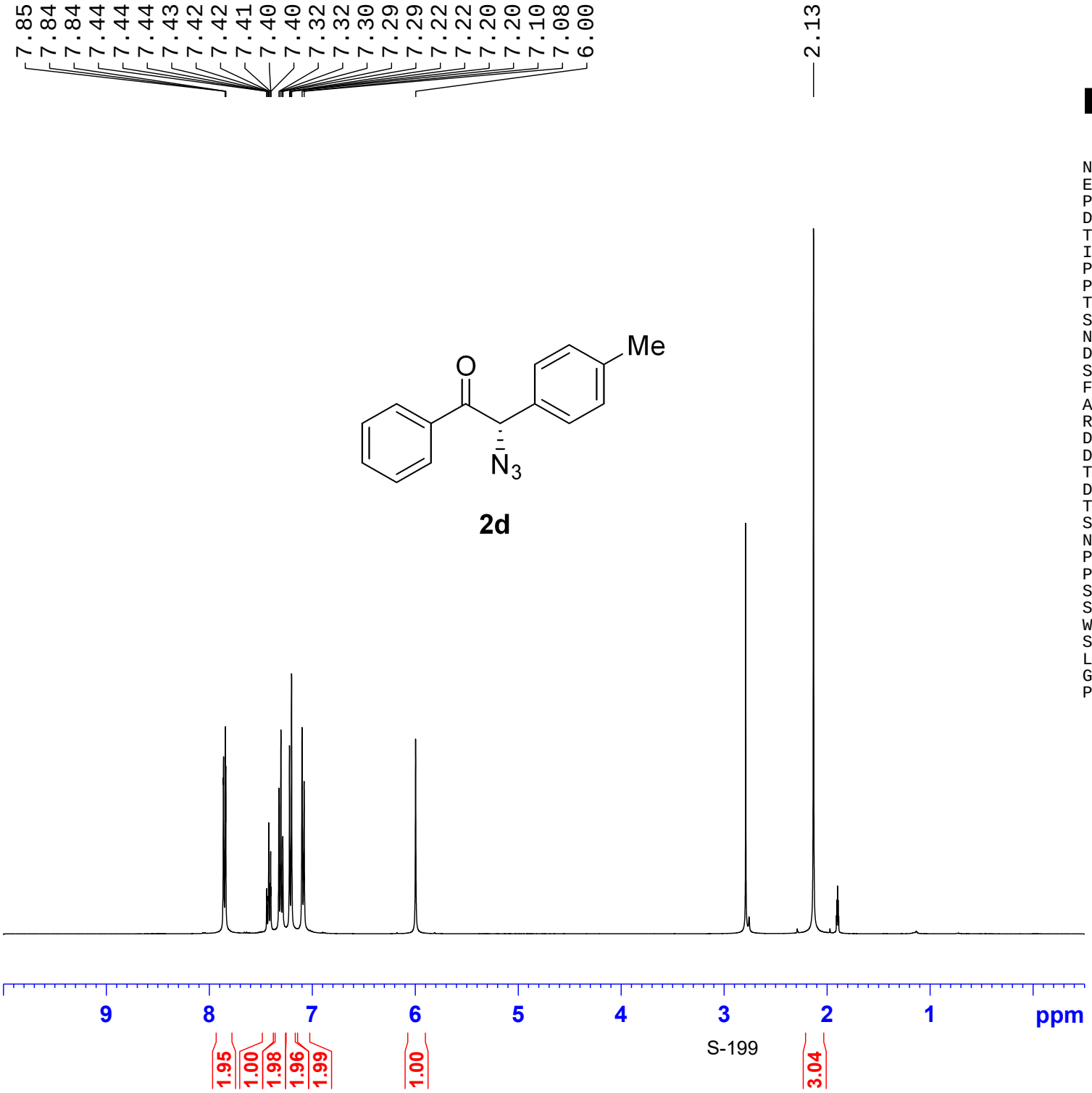
2c

```
NAME          HNMR-gwg-2-45
EXPNO                   173
PROCNO                    1
Date_              20210601
Time                 14.31
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT             Acetone
NS                        6
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 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                    14.40 usec
SI                    65536
SF             400.1900000 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    1.00
```

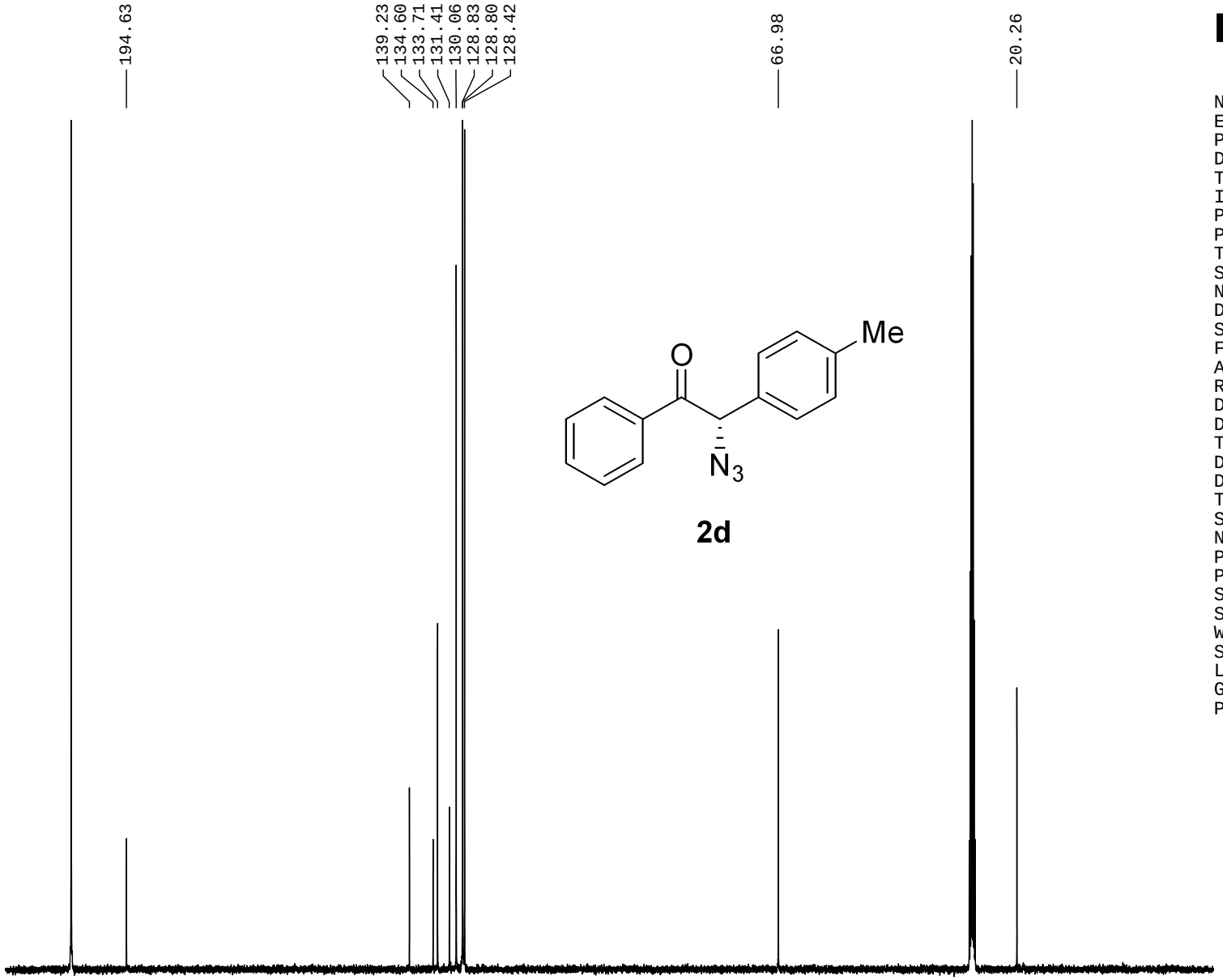




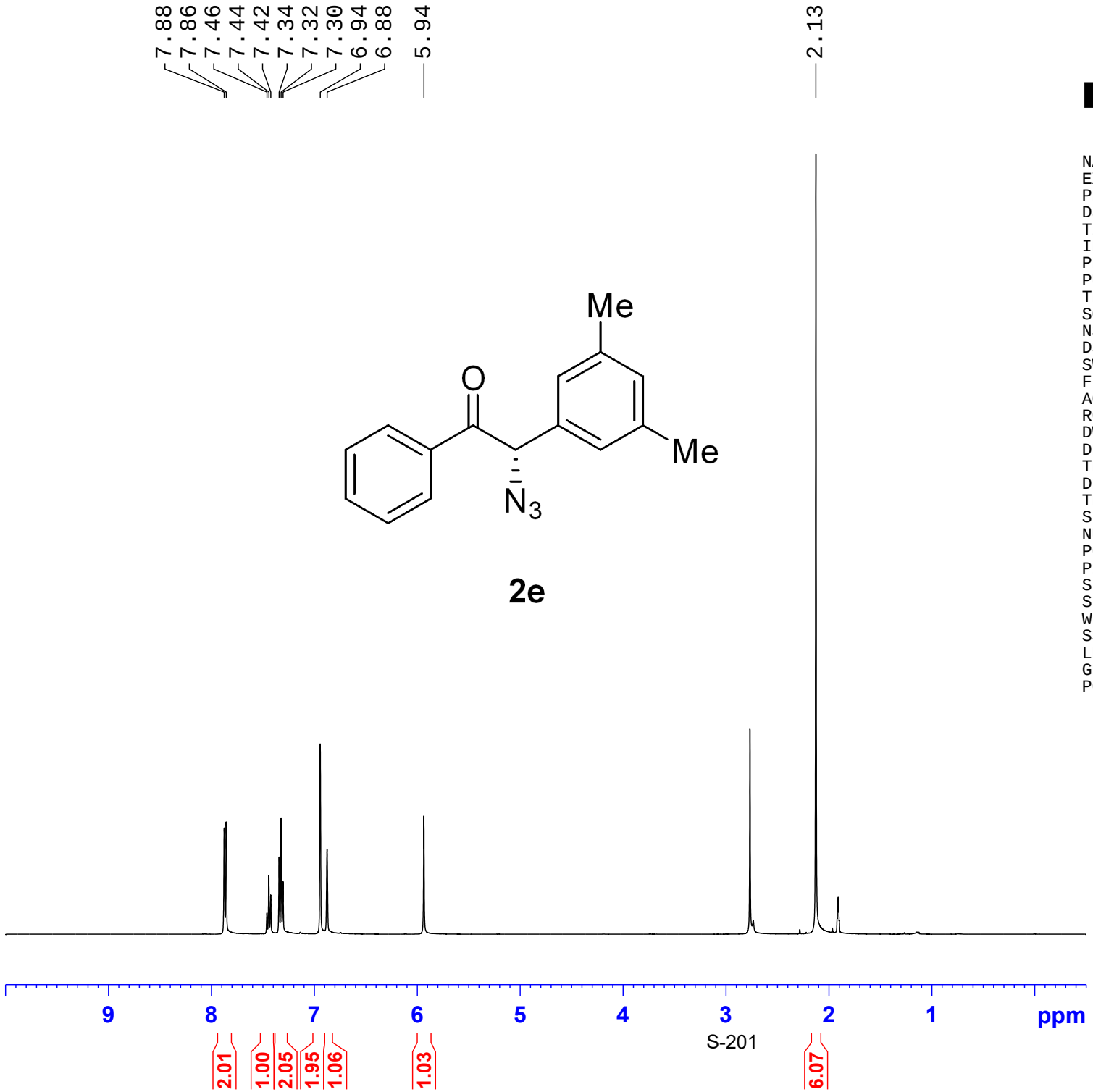

```
NAME          CNMR-gwg-2-45
EXPNO                   174
PROCNO                    1
Date_              20210601
Time                  14.39
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                       101
DS                         4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                   193.13
DW                   20.800 usec
DE                    6.50 usec
TE                   295.3 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                    13C
P1                     9.90 usec
SI                    32768
SF           100.6278560 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```



NAME	HNMR-gwg-2-67
EXPNO	5
PROCNO	1
Date_	20210610
Time	0.09 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	3.9977460 sec
RG	50
DW	61.000 usec
DE	13.54 usec
TE	294.6 K
D1	1.00000000 sec
TD0	1
SFO1	400.1324708 MHz
NUC1	1H
P0	3.33 usec
P1	10.00 usec
SI	65536
SF	400.1300675 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

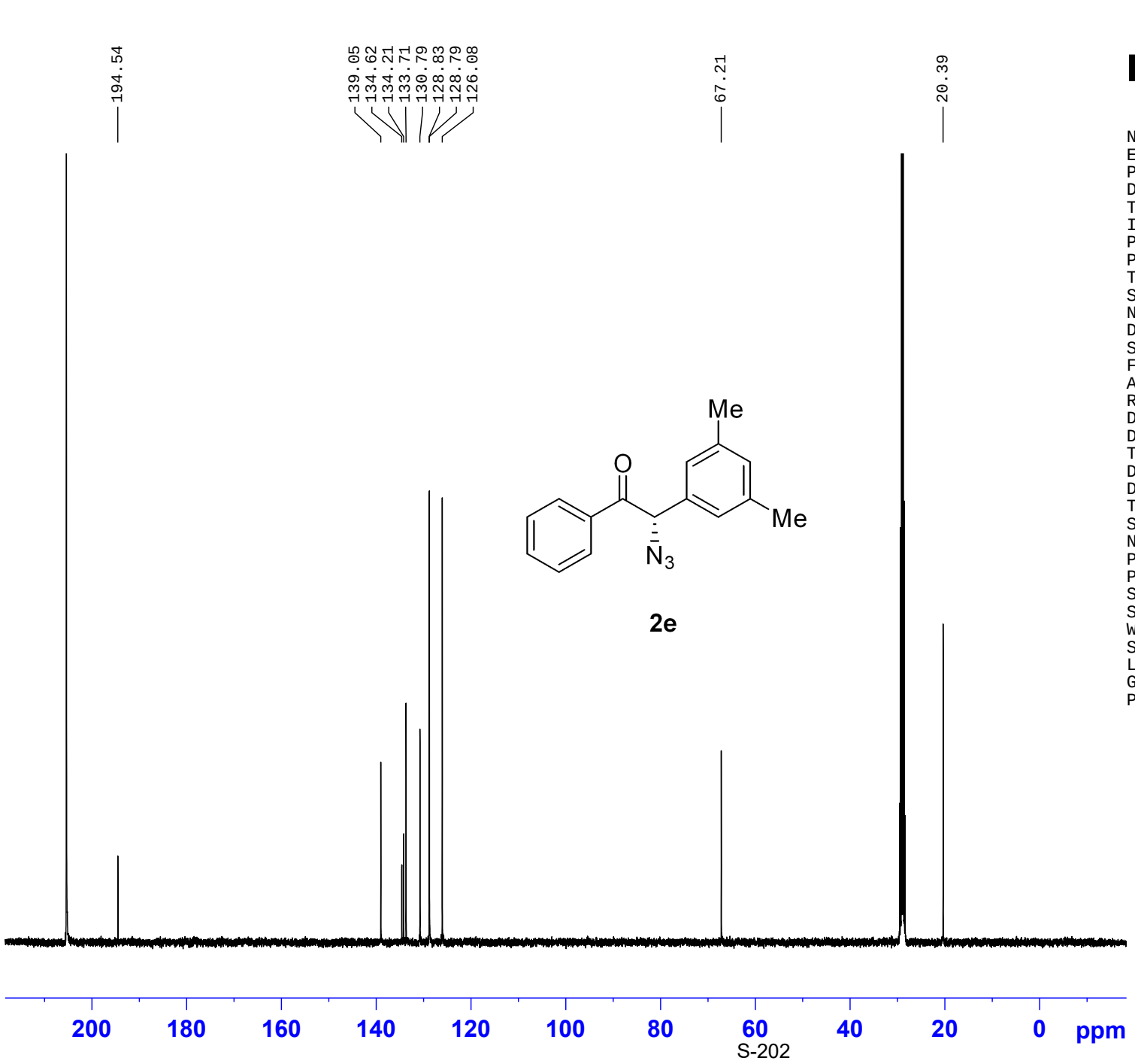


NAME	CNMR-gwg-2-67
EXPNO	6
PROCNO	1
Date_	20210610
Time	0.21 h
INSTRUM	Avance
PROBHD	Z116098_0833 (
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	200
DS	4
SWH	23809.523 Hz
FIDRES	0.726609 Hz
AQ	1.3763061 sec
RG	50.1934
DW	21.000 usec
DE	6.50 usec
TE	295.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	100.6228298 MHz
NUC1	13C
P0	3.33 usec
P1	10.00 usec
SI	32768
SF	100.6127685 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

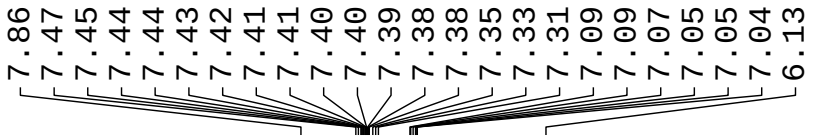


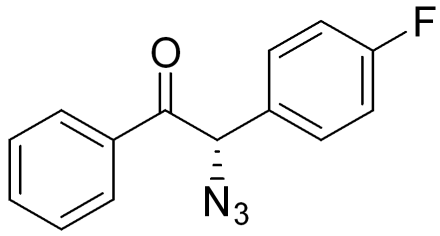
BRUKER

NAME	HNMR-gwg-3-28
EXPNO	3
PROCNO	1
Date_	20210630
Time	6.37 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	3.9977460 sec
RG	72.8863
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
SI	65536
SF	400.1300627 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



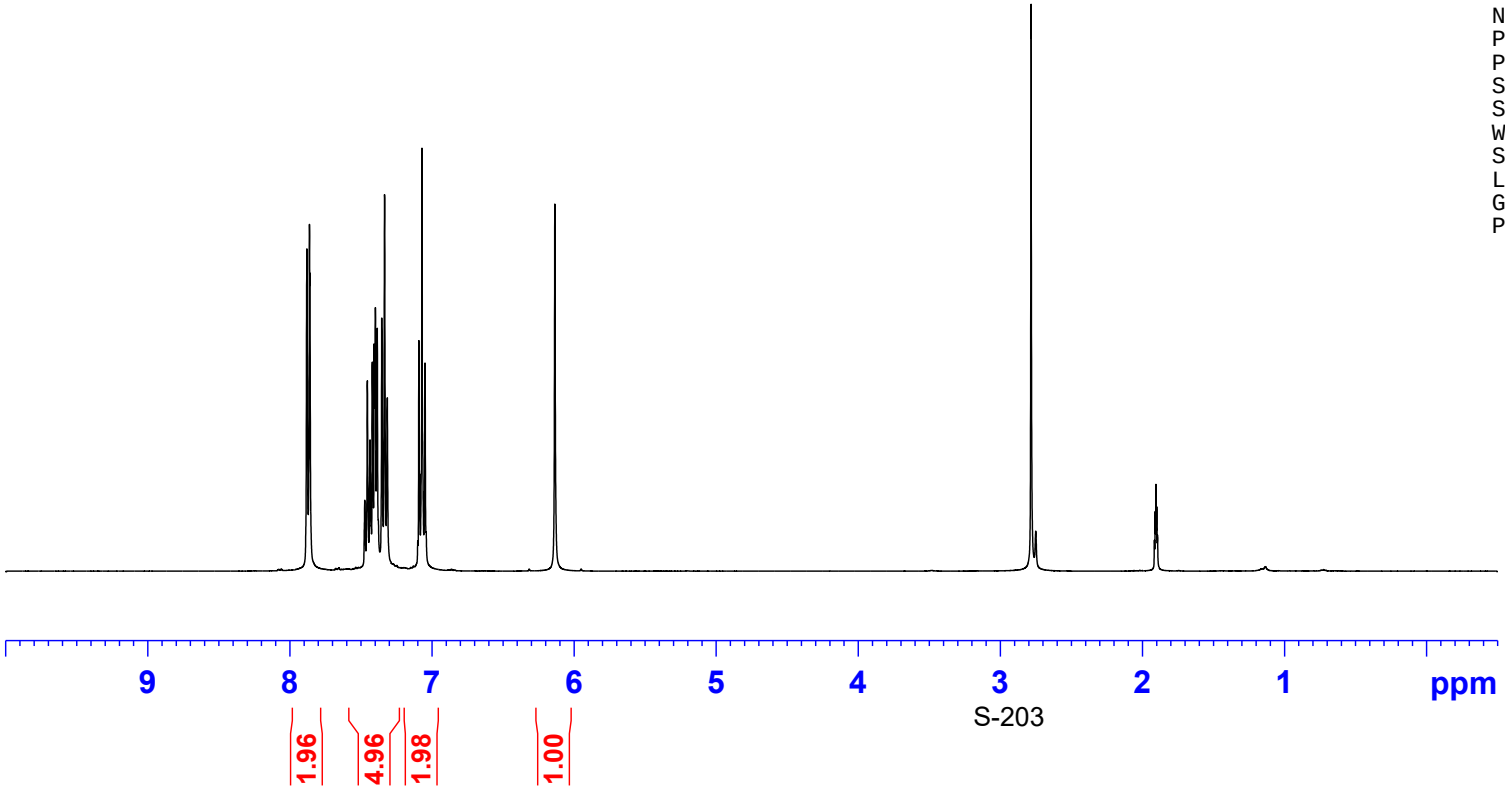
NAME	CNMR-gwg-3-28
EXPNO	4
PROCNO	1
Date_	20210630
Time	6.48 h
INSTRUM	Avance
PROBHD	Z116098_0833 (
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	160
DS	4
SWH	23809.523 Hz
FIDRES	0.726609 Hz
AQ	1.3763061 sec
RG	48.6724
DW	21.000 usec
DE	6.50 usec
TE	295.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	100.6228298 MHz
NUC1	13C
P0	3.33 usec
P1	10.00 usec
SI	32768
SF	100.6127685 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

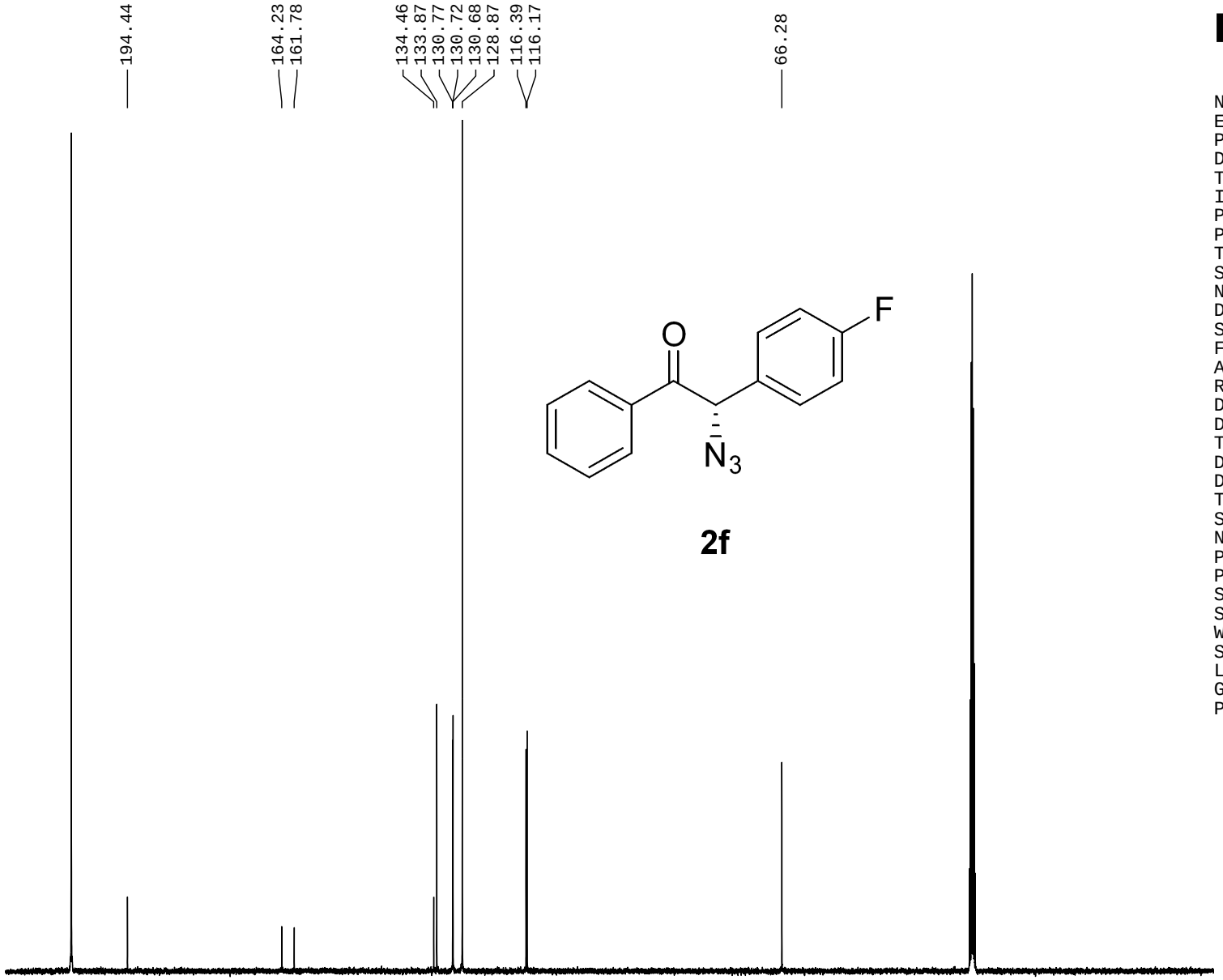




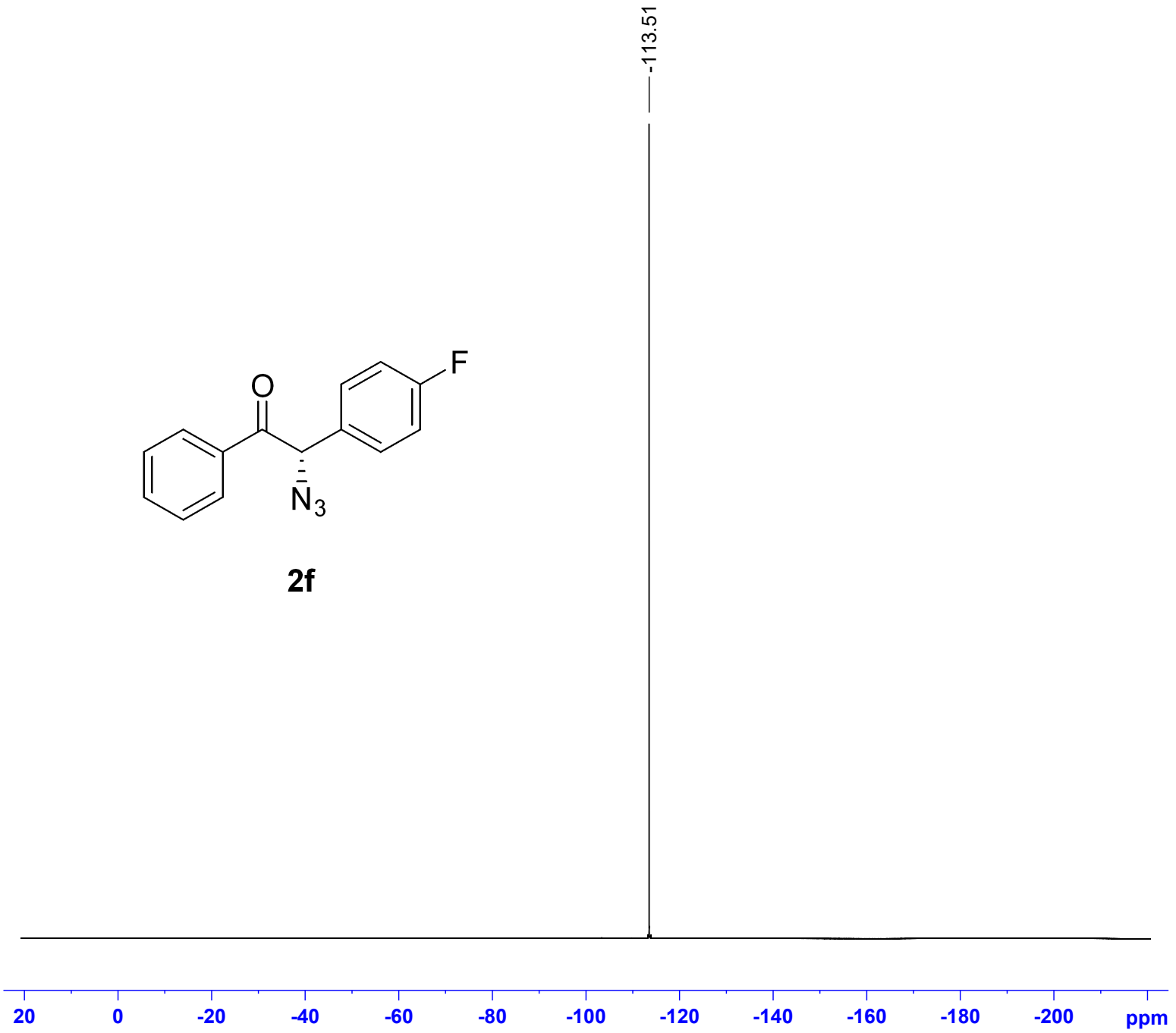
2f

NAME	HNMR-gwg-2-68
EXPNO	1
PROCNO	1
Date_	20210610
Time	20.52 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	3.9977460 sec
RG	81.1688
DW	61.000 usec
DE	13.54 usec
TE	294.5 K
D1	1.00000000 sec
TD0	1
SFO1	400.1324708 MHz
NUC1	1H
P0	3.33 usec
P1	10.00 usec
SI	65536
SF	400.1300649 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

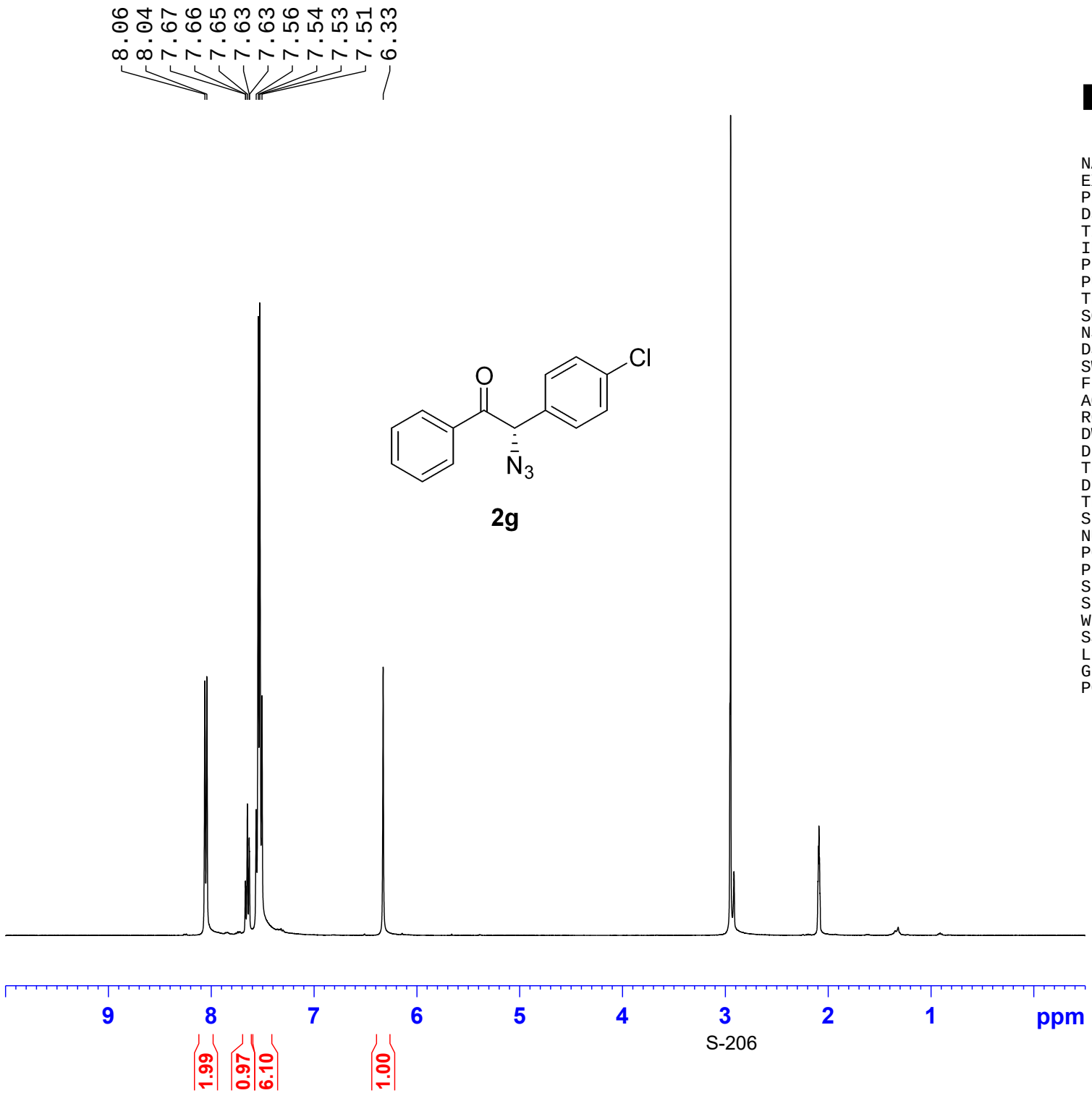




NAME	CNMR-gwg-2-68
EXPNO	2
PROCNO	1
Date_	20210610
Time	21.05 h
INSTRUM	Avance
PROBHD	Z116098_0833 (
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	200
DS	4
SWH	23809.523 Hz
FIDRES	0.726609 Hz
AQ	1.3763061 sec
RG	48.6724
DW	21.000 usec
DE	6.50 usec
TE	294.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	100.6228298 MHz
NUC1	13C
P0	3.33 usec
P1	10.00 usec
SI	32768
SF	100.6127685 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

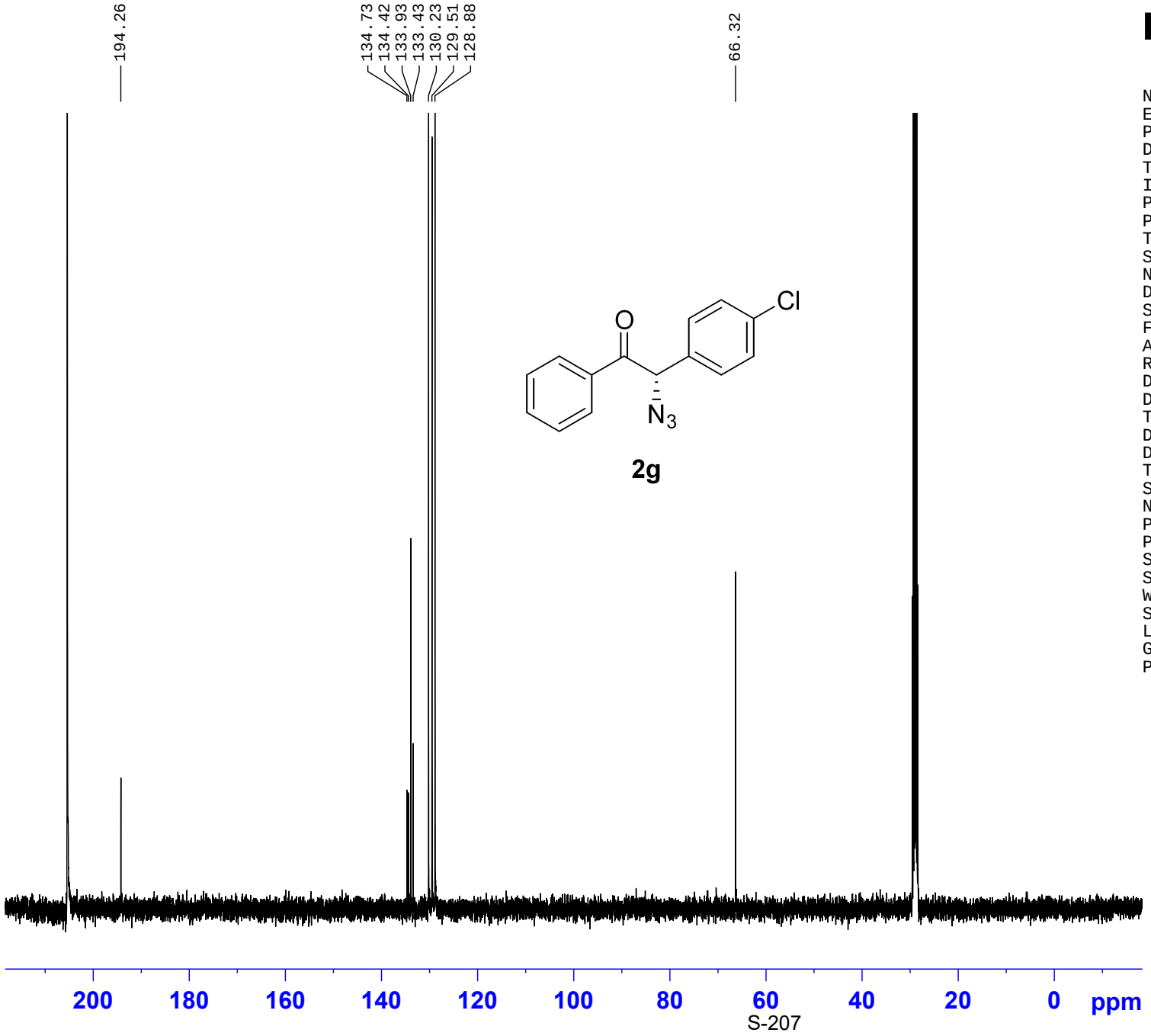


NAME	FNMR-gwg-2-68
EXPNO	3
PROCNO	1
Date_	20210610
Time	21.07 h
INSTRUM	Avance
PROBHD	Z116098_0833 (
PULPROG	zgig
TD	131072
SOLVENT	Acetone
NS	16
DS	4
SWH	90909.094 Hz
FIDRES	1.387163 Hz
AQ	0.7209460 sec
RG	101
DW	5.500 usec
DE	6.50 usec
TE	294.7 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	376.4607164 MHz
NUC1	19F
P1	18.00 usec
SI	65536
SF	376.4983662 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



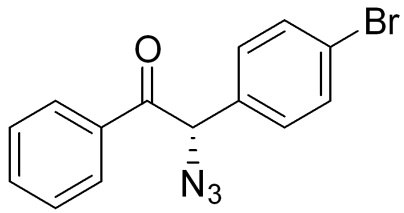
BRUKER

NAME	HNMR-gwg-2-47
EXPNO	1
PROCNO	1
Date_	20210602
Time	20.29 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	3.9977460 sec
RG	101
DW	61.000 usec
DE	13.54 usec
TE	294.3 K
D1	1.00000000 sec
TD0	1
SFO1	400.1324708 MHz
NUC1	1H
P0	3.33 usec
P1	10.00 usec
SI	65536
SF	400.1299908 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



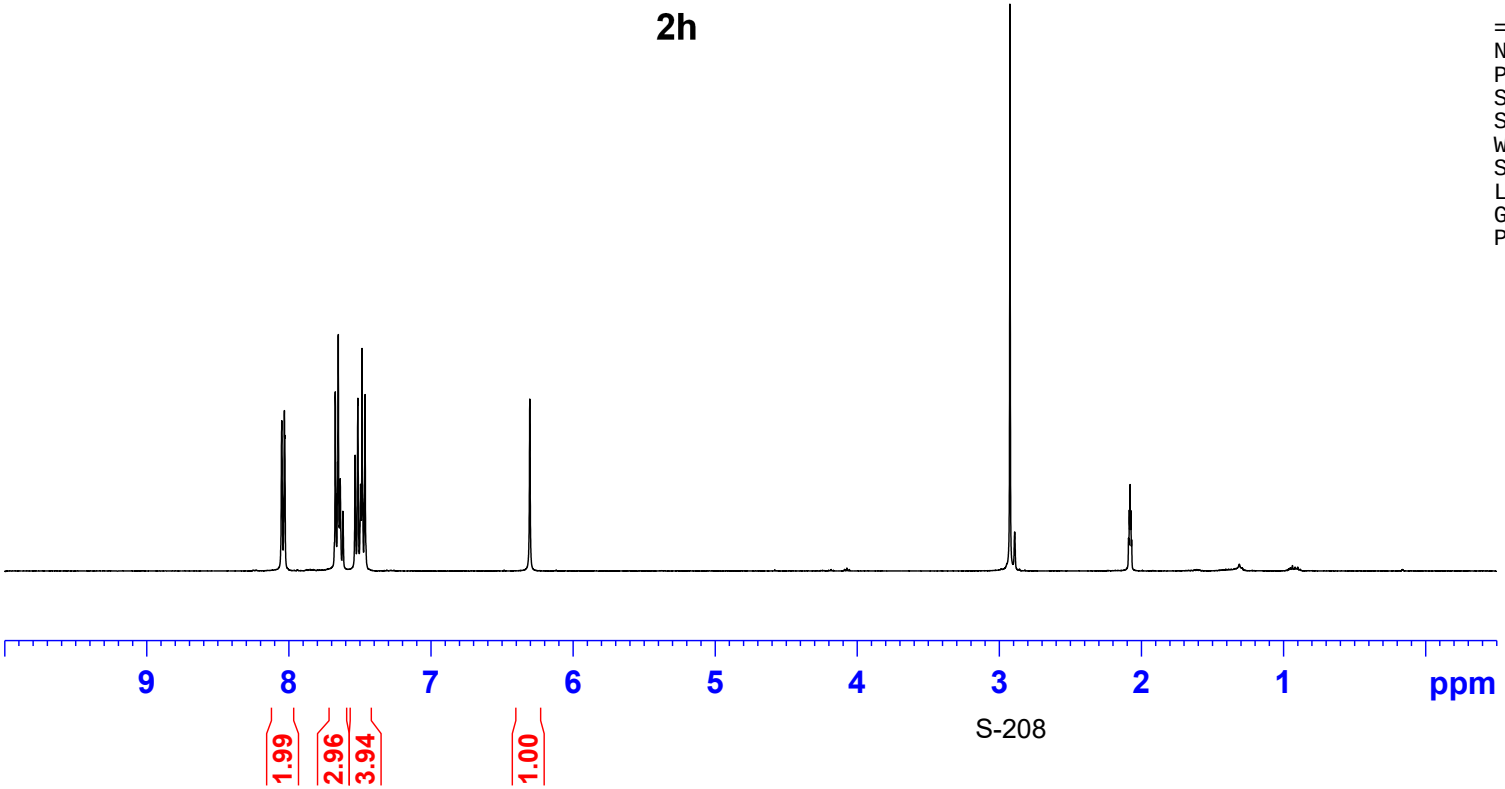
NAME	CNMR-gwg-2-47
EXPNO	2
PROCNO	1
Date_	20210602
Time	20.37 h
INSTRUM	Avance
PROBHD	Z116098_0833 (
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	100
DS	4
SWH	23809.523 Hz
FIDRES	0.726609 Hz
AQ	1.3763061 sec
RG	47.4244
DW	21.000 usec
DE	6.50 usec
TE	294.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	100.6228298 MHz
NUC1	13C
P0	3.33 usec
P1	10.00 usec
SI	32768
SF	100.6127685 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

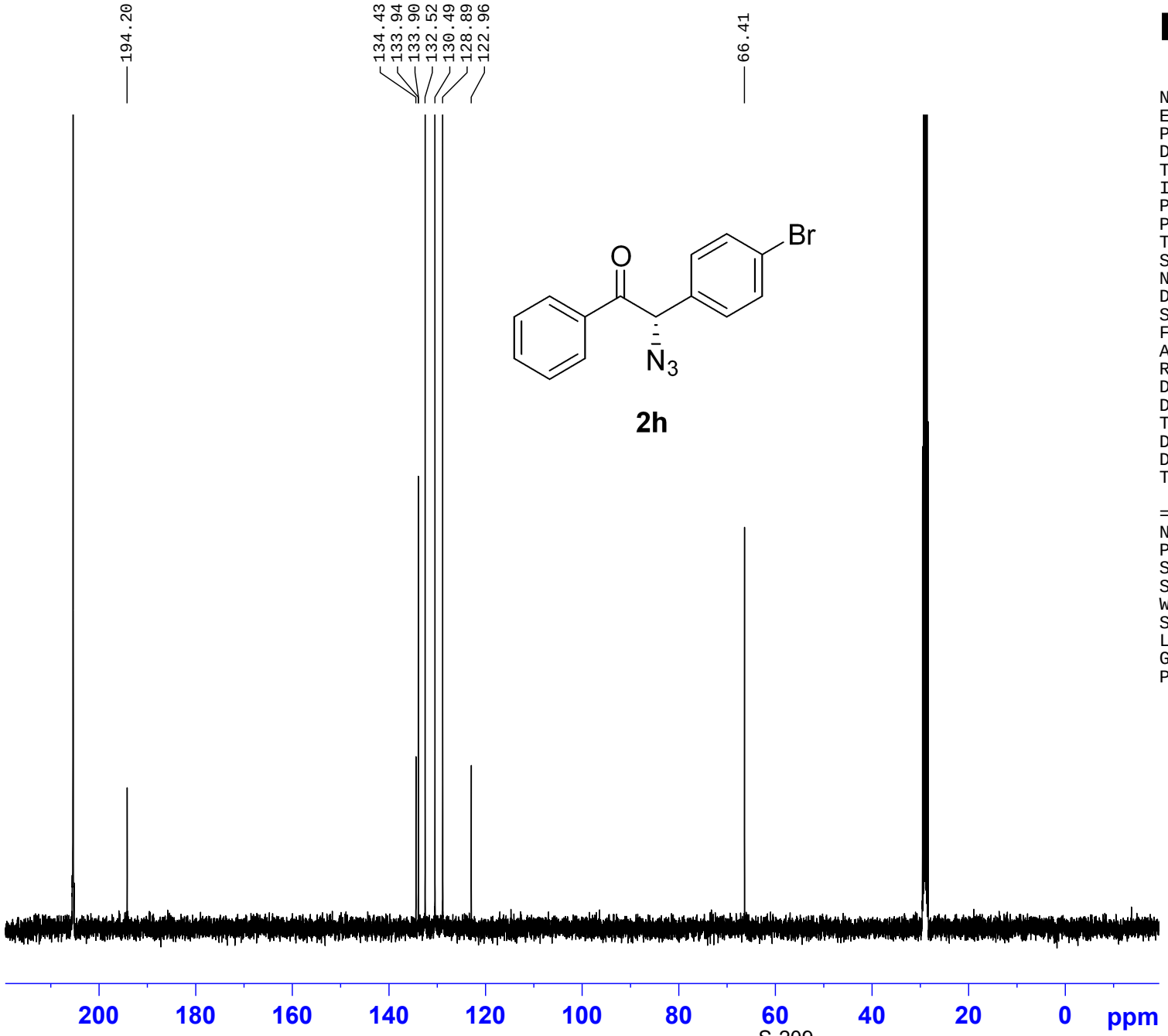
8.05
8.03
8.03
7.67
7.66
7.65
7.65
7.64
7.64
7.62
7.53
7.51
7.49
7.48
7.46
6.30



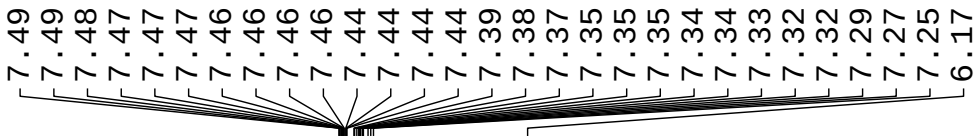
2h

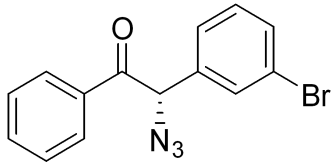
```
NAME          HNMR-gwg-2-46
EXPNO                   180
PROCNO                    1
Date_              20210602
Time                 14.31
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT            Acetone
NS                         6
DS                         2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                   100.49
DW                   60.800 usec
DE                    6.50 usec
TE                   294.7 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     14.40 usec
SI                     65536
SF              400.1900000 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                     1.00
```





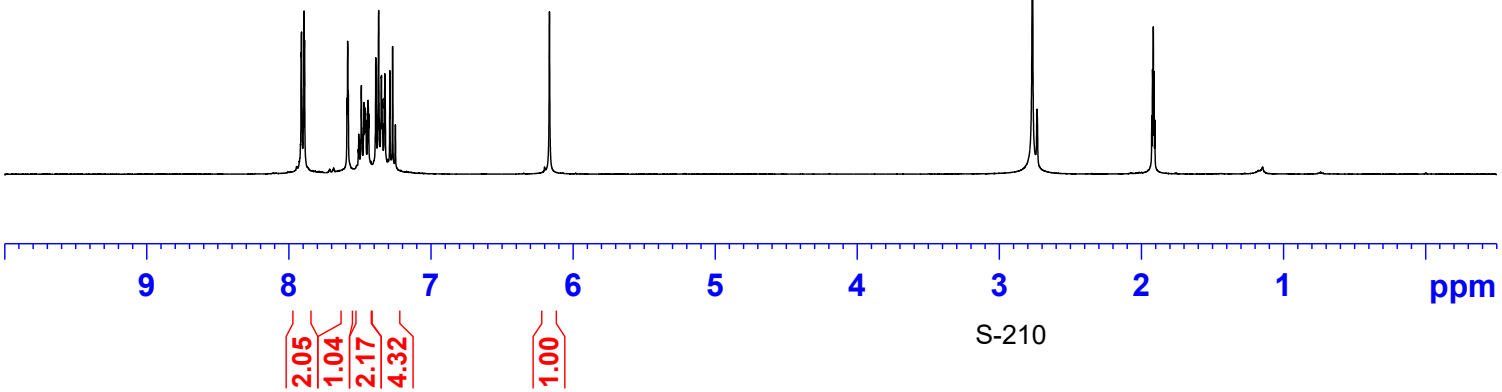

```
NAME          CNMR-gwg-2-46
EXPNO                   181
PROCNO                    1
Date_              20210602
Time                  14.41
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT             Acetone
NS                      167
DS                        4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                   193.13
DW                   20.800 usec
DE                    6.50 usec
TE                   295.2 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                     9.90 usec
SI                    32768
SF           100.6278560 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

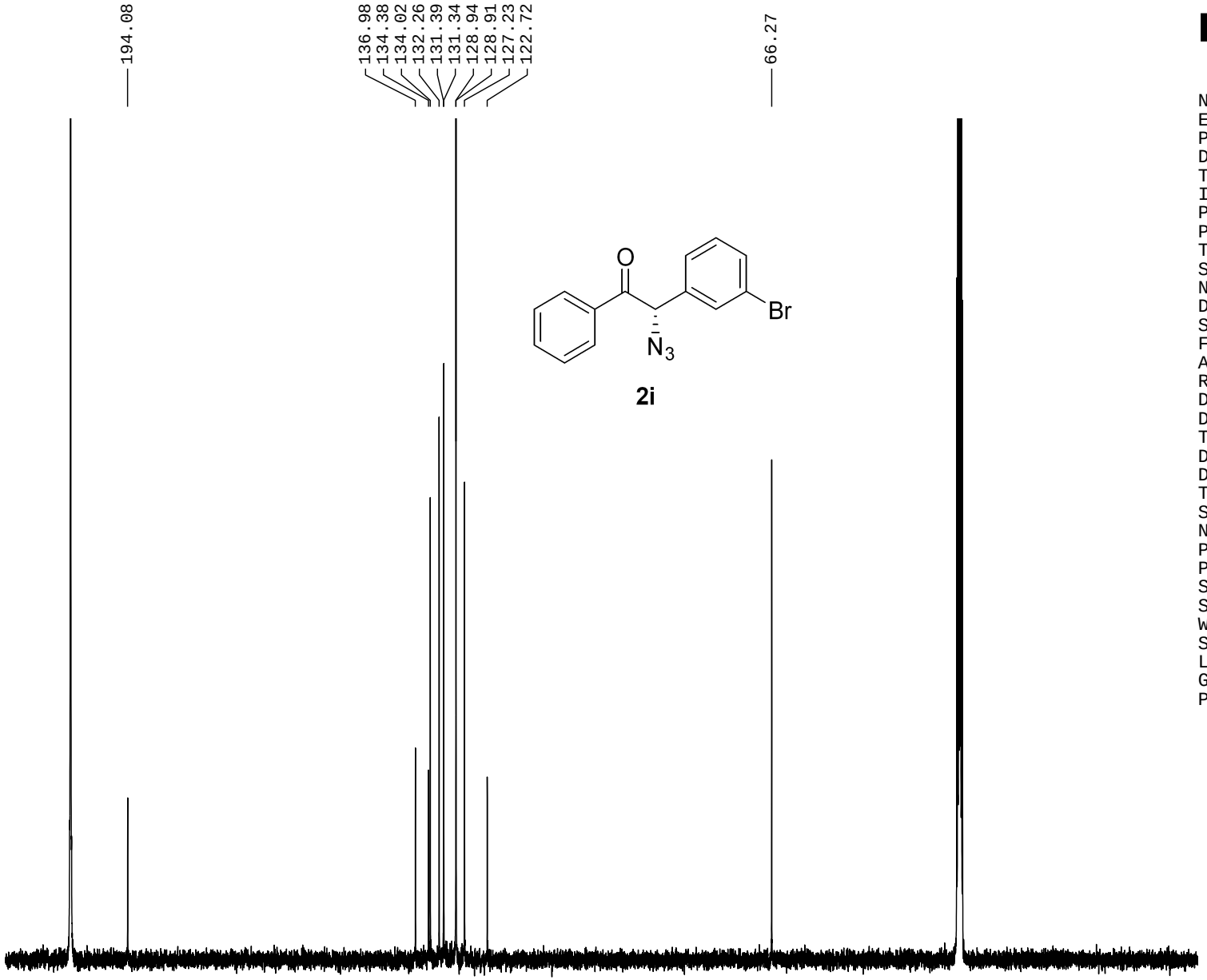




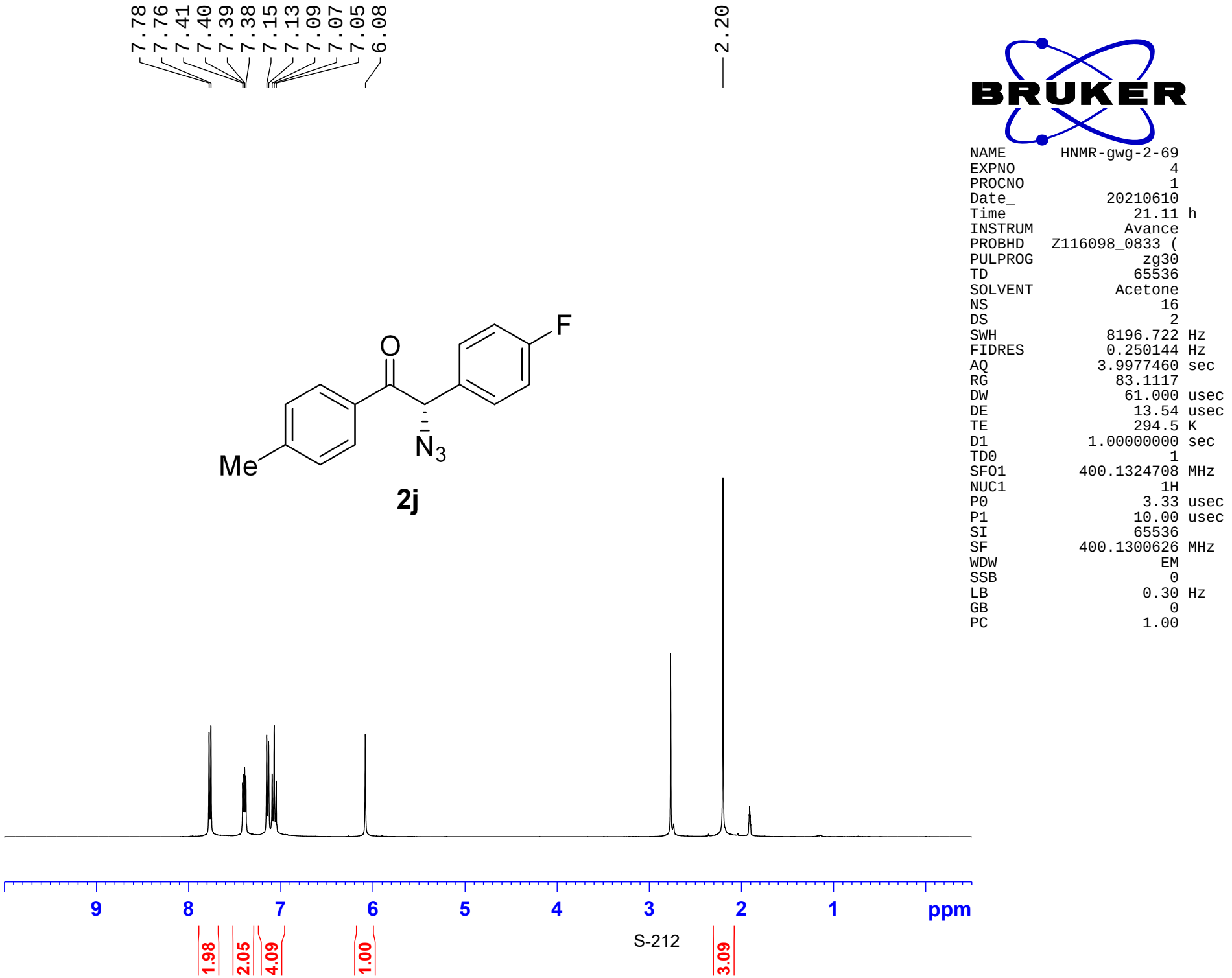
2i

NAME	HNMR-gwg-3-6
EXPNO	3
PROCNO	1
Date_	20210622
Time	23.00 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	3.9977460 sec
RG	101
DW	61.000 usec
DE	13.54 usec
TE	294.3 K
D1	1.00000000 sec
TD0	1
SFO1	400.1324708 MHz
NUC1	1H
P0	3.33 usec
P1	10.00 usec
SI	65536
SF	400.1300603 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

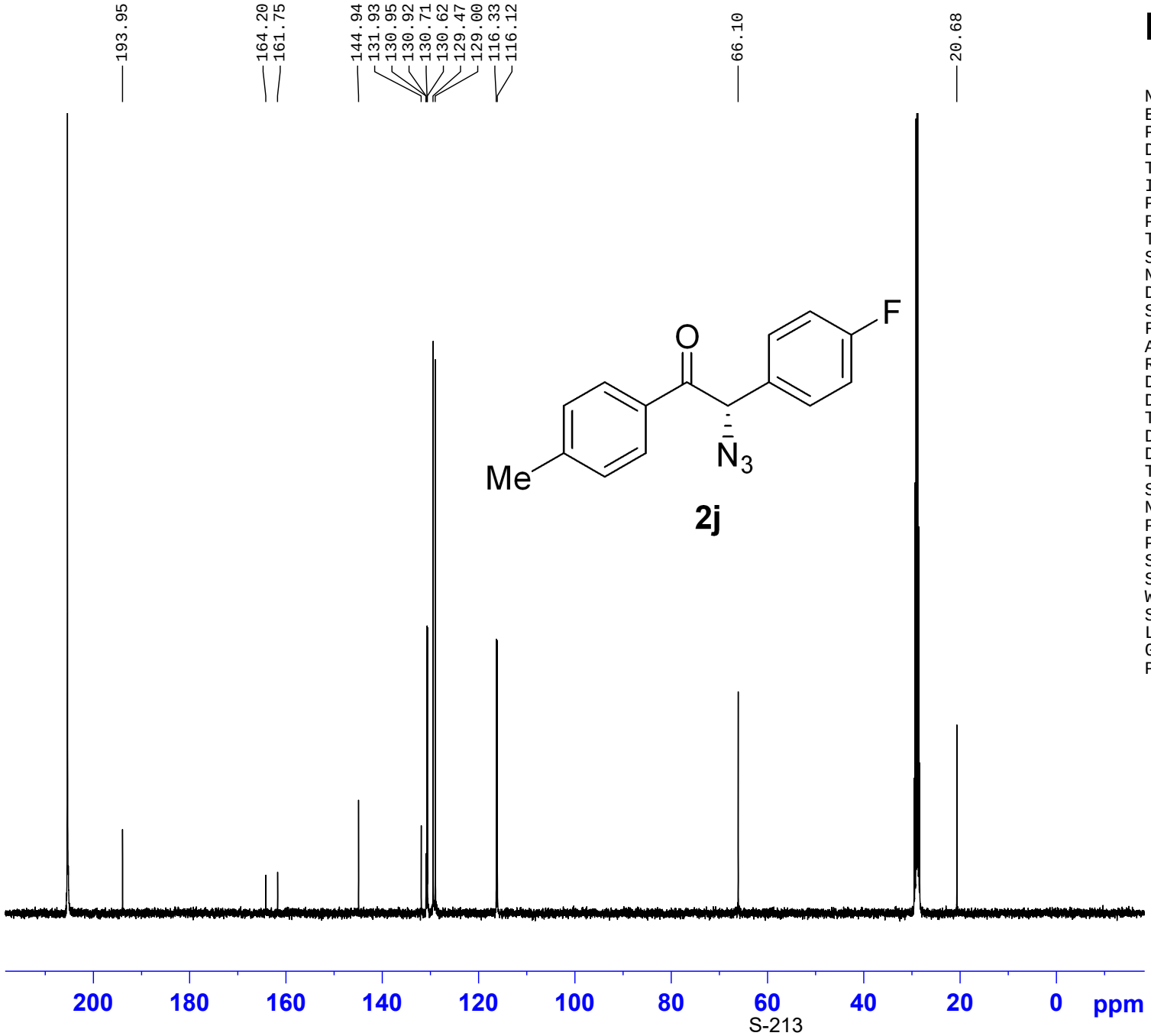




NAME	CNMR-gwg-3-6
EXPNO	4
PROCNO	1
Date_	20210623
Time	0.00 h
INSTRUM	Avance
PROBHD	Z116098_0833 (
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	1024
DS	4
SWH	23809.523 Hz
FIDRES	0.726609 Hz
AQ	1.3763061 sec
RG	48.6724
DW	21.000 usec
DE	6.50 usec
TE	295.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	100.6228298 MHz
NUC1	13C
P0	3.33 usec
P1	10.00 usec
SI	32768
SF	100.6127685 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



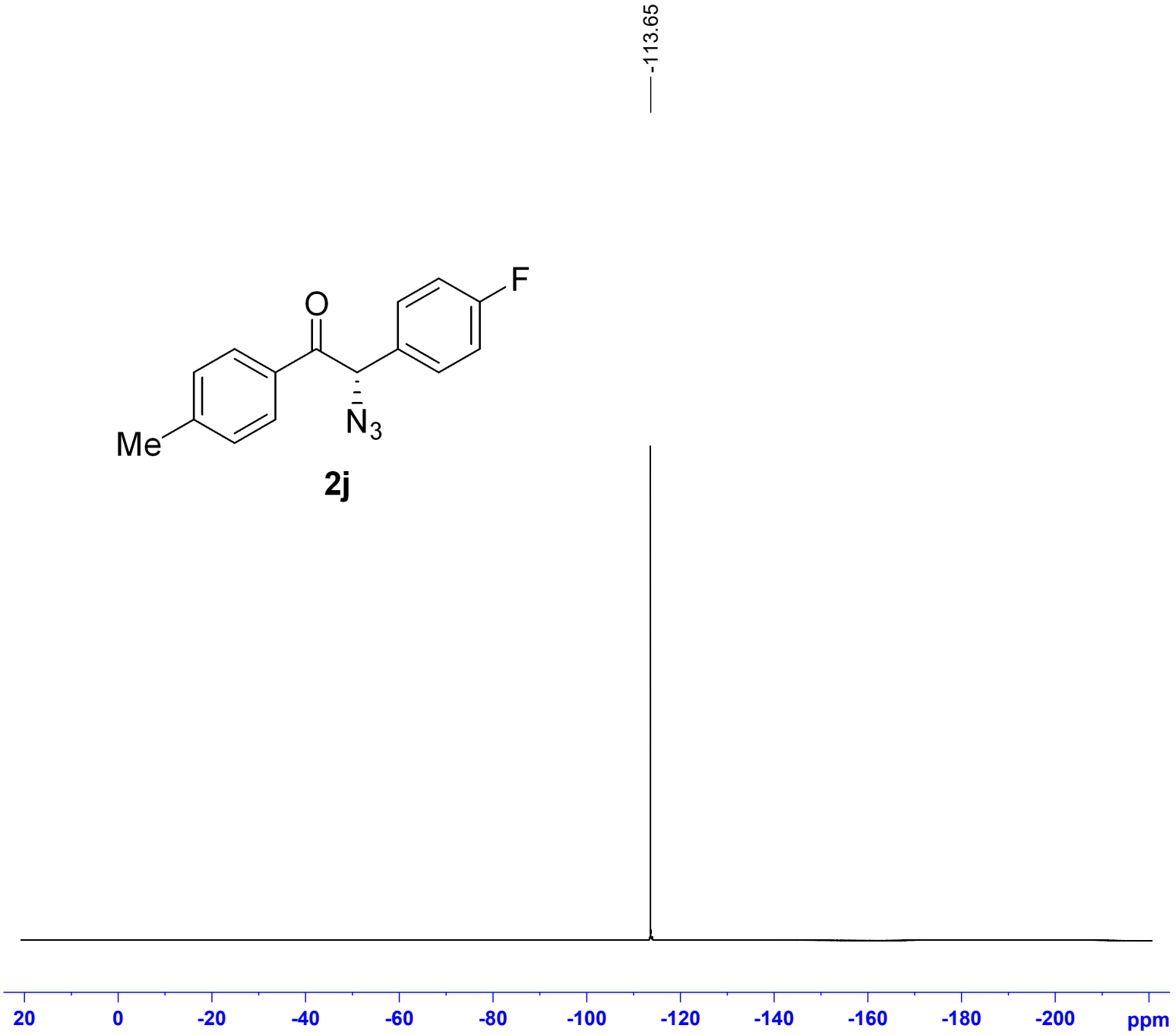
NAME	HNMR-gwg-2-69
EXPNO	4
PROCNO	1
Date_	20210610
Time	21.11 h
INSTRUM	Avance
PROBHD	Z116098_0833 (
PULPROG	zg30
TD	65536
SOLVENT	Acetone
NS	16
DS	2
SWH	8196.722 Hz
FIDRES	0.250144 Hz
AQ	3.9977460 sec
RG	83.1117
DW	61.000 usec
DE	13.54 usec
TE	294.5 K
D1	1.00000000 sec
TD0	1
SFO1	400.1324708 MHz
NUC1	1H
P0	3.33 usec
P1	10.00 usec
SI	65536
SF	400.1300626 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



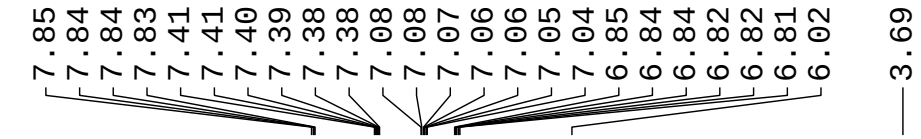
BRUKER

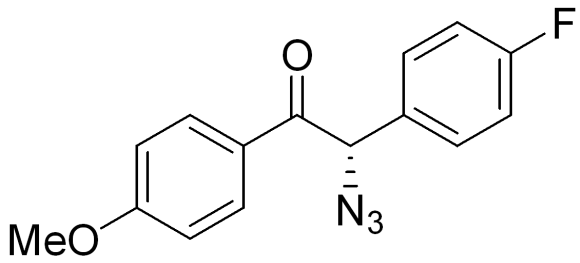
NAME	CNMR-gwg-2-69
EXPNO	5
PROCNO	1
Date_	20210610
Time	21.24 h
INSTRUM	Avance
PROBHD	Z116098_0833 (
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	200
DS	4
SWH	23809.523 Hz
FIDRES	0.726609 Hz
AQ	1.3763061 sec
RG	51.55
DW	21.000 usec
DE	6.50 usec
TE	295.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	100.6228298 MHz
NUC1	13C
P0	3.33 usec
P1	10.00 usec
SI	32768
SF	100.6127685 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

2j



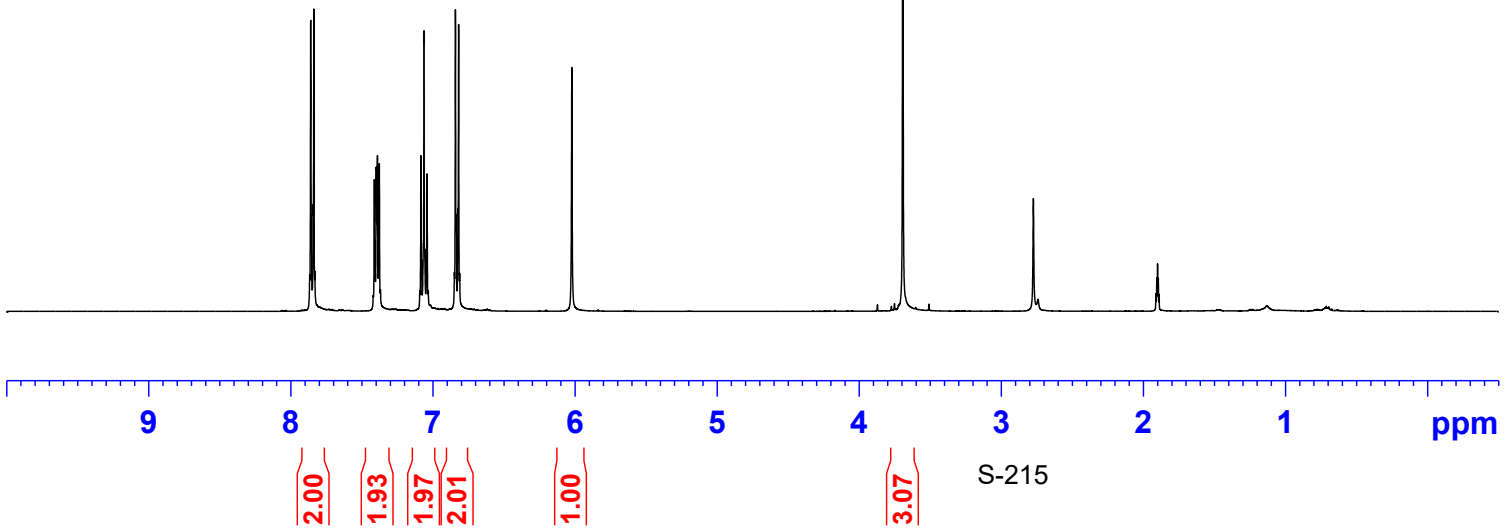
NAME	FNMR-gwg-2-69
EXPNO	6
PROCNO	1
Date_	20210610
Time	21.26 h
INSTRUM	Avance
PROBHD	Z116098_0833 (
PULPROG	zgig
TD	131072
SOLVENT	Acetone
NS	16
DS	4
SWH	90909.094 Hz
FIDRES	1.387163 Hz
AQ	0.7209460 sec
RG	101
DW	5.500 usec
DE	6.50 usec
TE	294.7 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	376.4607164 MHz
NUC1	19F
P1	18.00 usec
SI	65536
SF	376.4983662 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

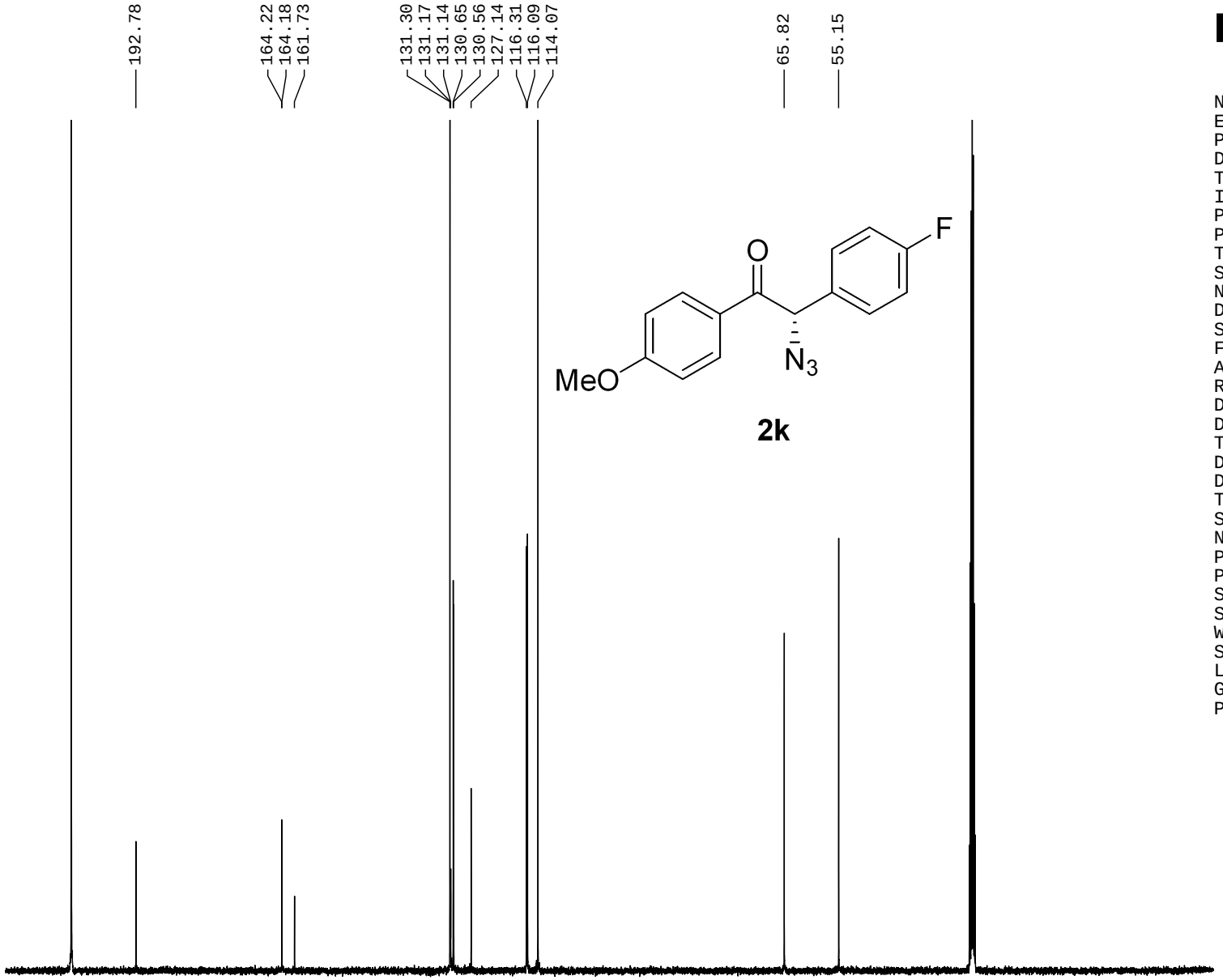




2k

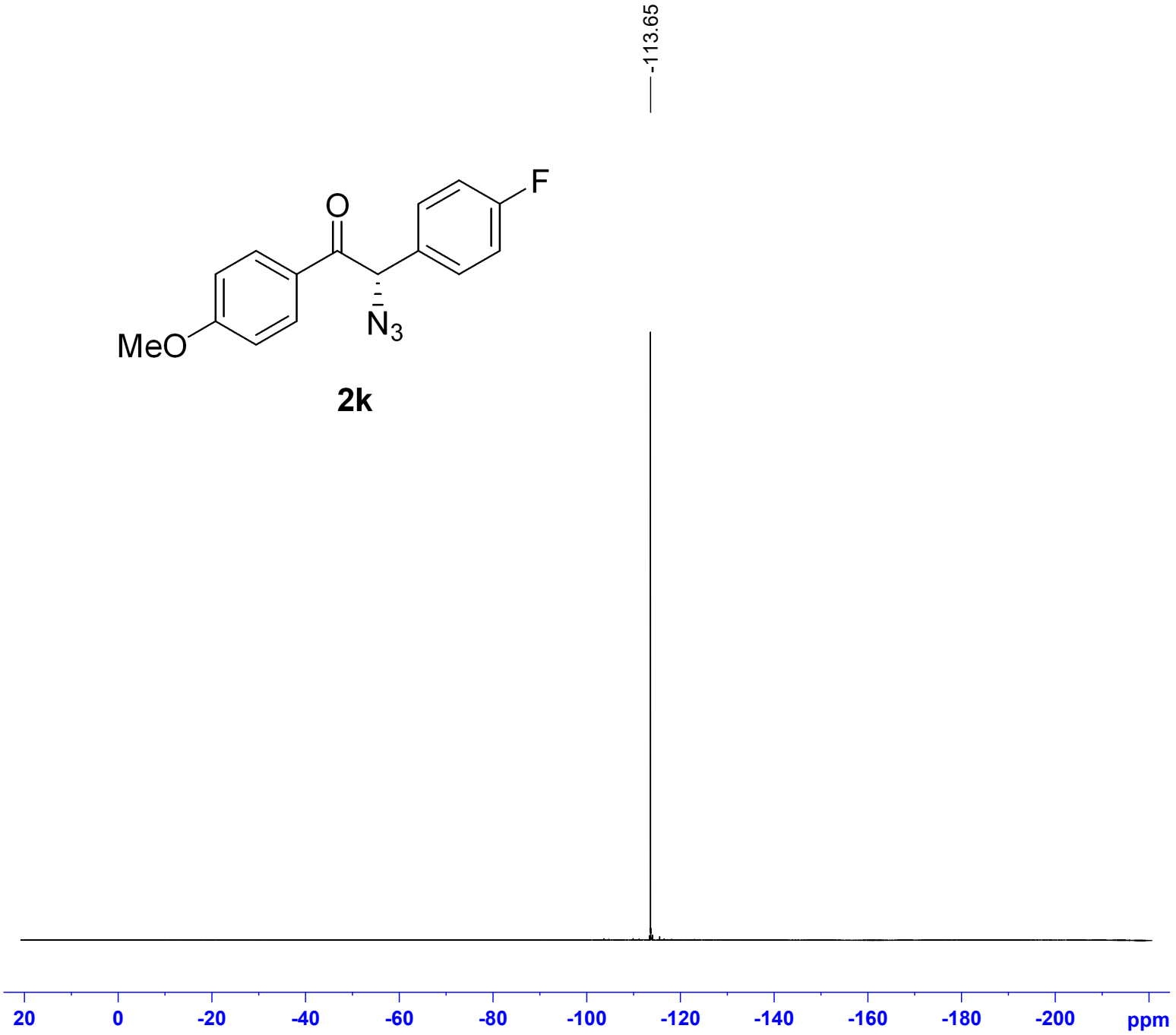
NAME HNMR-gwg-3-53
EXPNO 1
PROCNO 1
Date_ 20210710
Time 6.12 h
INSTRUM Avance
PROBHD Z116098_0833 (
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9977460 sec
RG 47.619
DW 61.000 usec
DE 13.54 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
SI 65536
SF 400.1300665 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



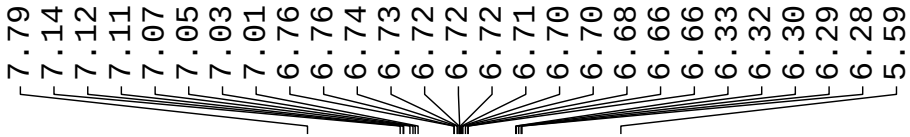


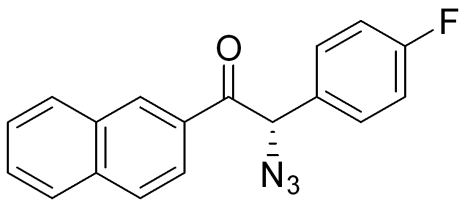
NAME	CNMR-gwg-3-53
EXPNO	2
PROCNO	1
Date_	20210710
Time	6.25 h
INSTRUM	Avance
PROBHD	Z116098_0833 (
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	200
DS	4
SWH	23809.523 Hz
FIDRES	0.726609 Hz
AQ	1.3763061 sec
RG	47.4244
DW	21.000 usec
DE	6.50 usec
TE	295.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	100.6228298 MHz
NUC1	13C
P0	3.33 usec
P1	10.00 usec
SI	32768
SF	100.6127685 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

2k



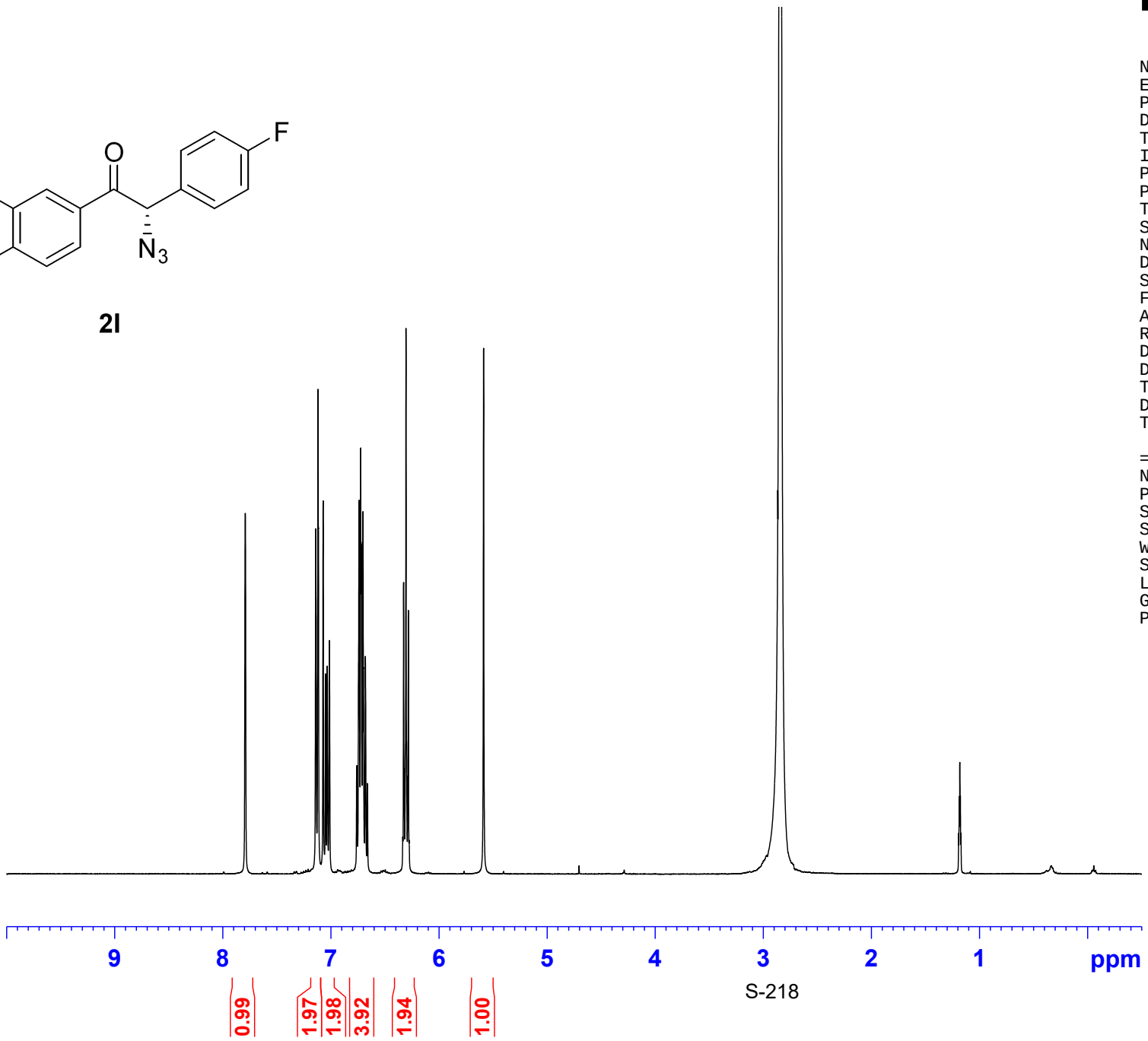
NAME	FNMR-gwg-3-53	
EXPNO	3	
PROCNO	1	
Date_	20210710	
Time	6.27	h
INSTRUM	Avance	
PROBHD	Z116098_0833 (	
PULPROG	zgig	
TD	131072	
SOLVENT	Acetone	
NS	16	
DS	4	
SWH	90909.094	Hz
FIDRES	1.387163	Hz
AQ	0.7209460	sec
RG	101	
DW	5.500	usec
DE	6.50	usec
TE	294.7	K
D1	1.00000000	sec
D11	0.03000000	sec
TD0	1	
SFO1	376.4607164	MHz
NUC1	19F	
P1	18.00	usec
SI	65536	
SF	376.4983662	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

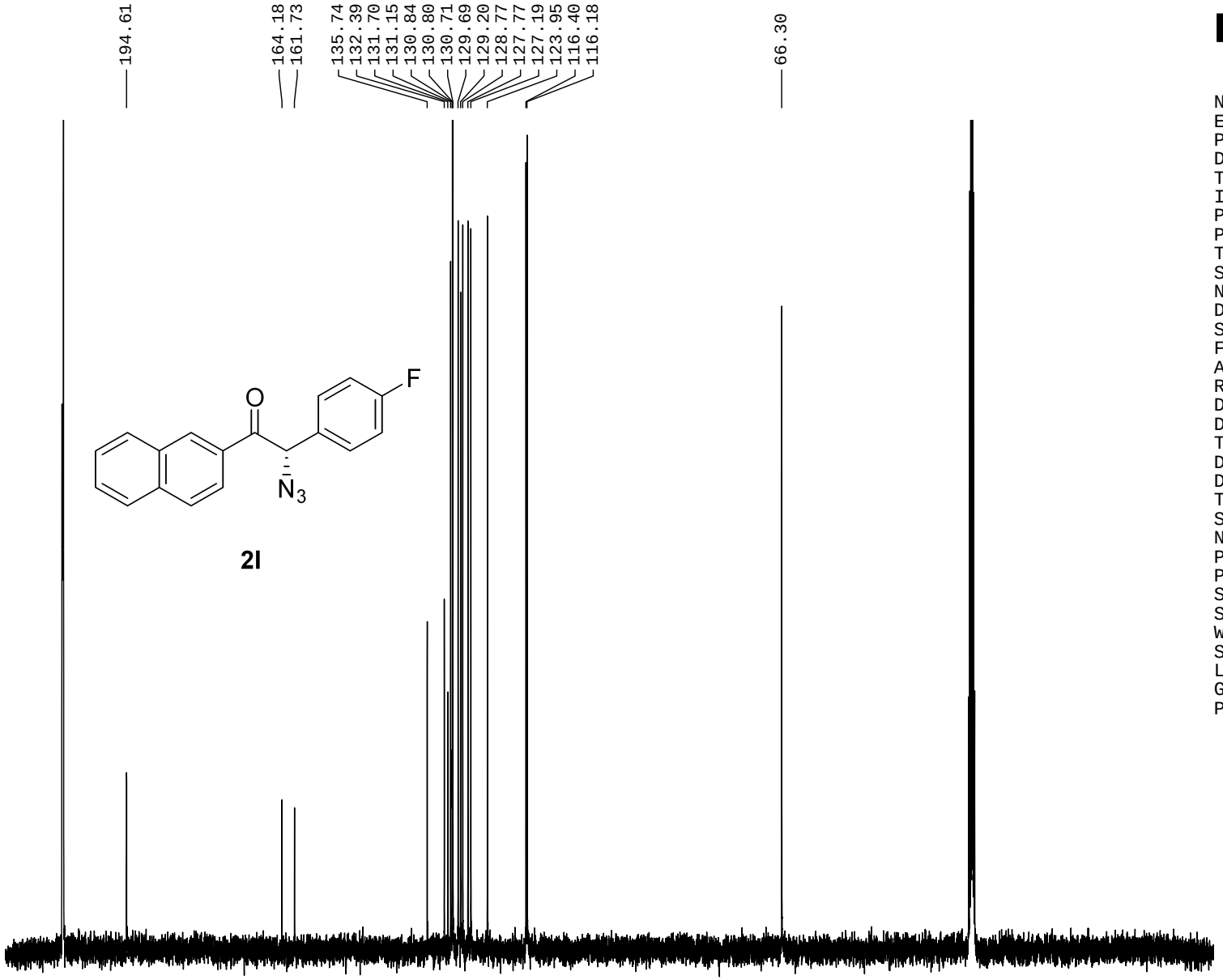




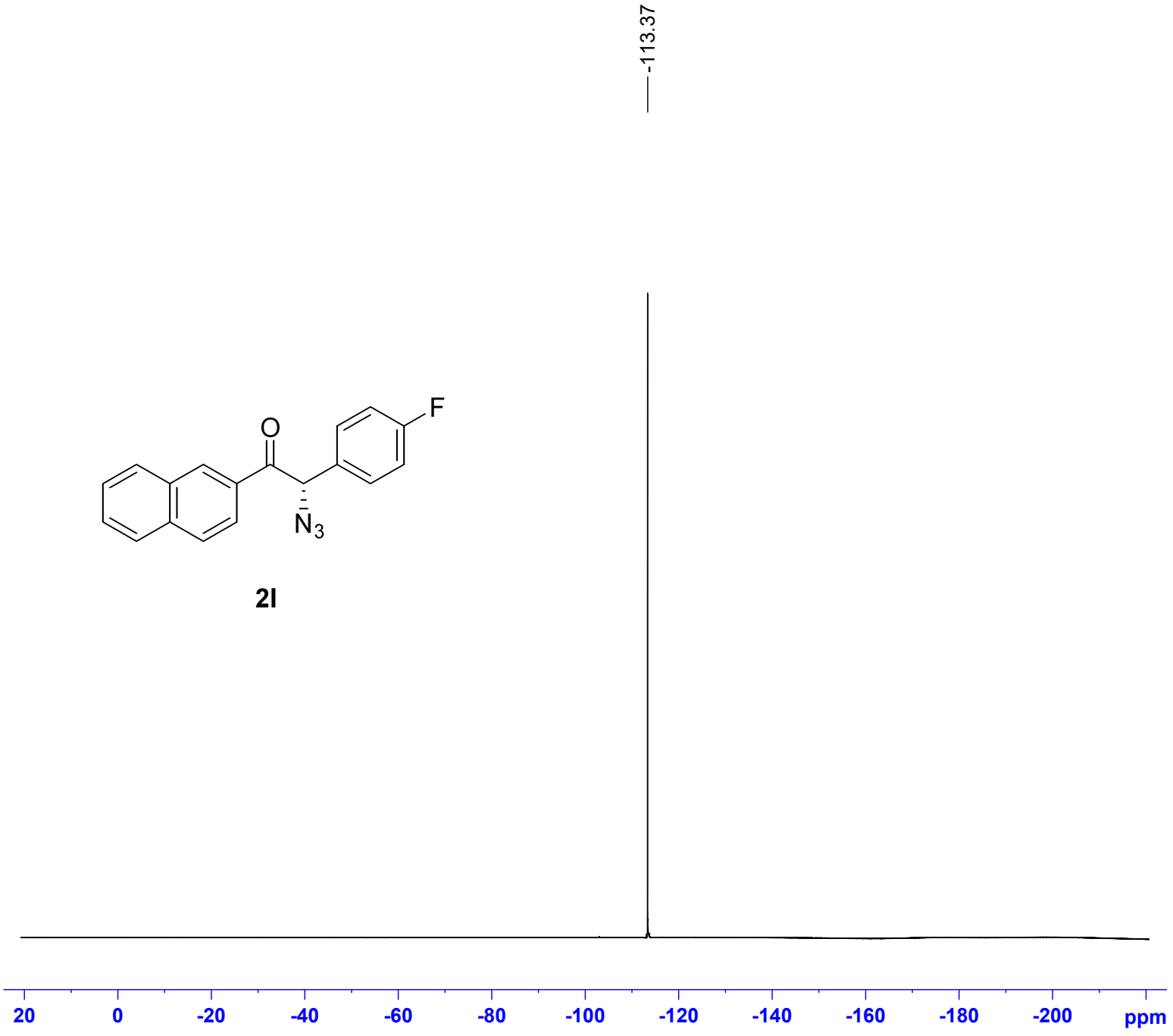
2l

```
NAME      HNMR-gwg-2-48-2
EXPNO                188
PROCNO                 1
Date_           20210603
Time               14.48
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                     6
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                 21.42
DW                60.800 usec
DE                 6.50 usec
TE                294.5 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.40 usec
SI                 65536
SF          400.1903591 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```

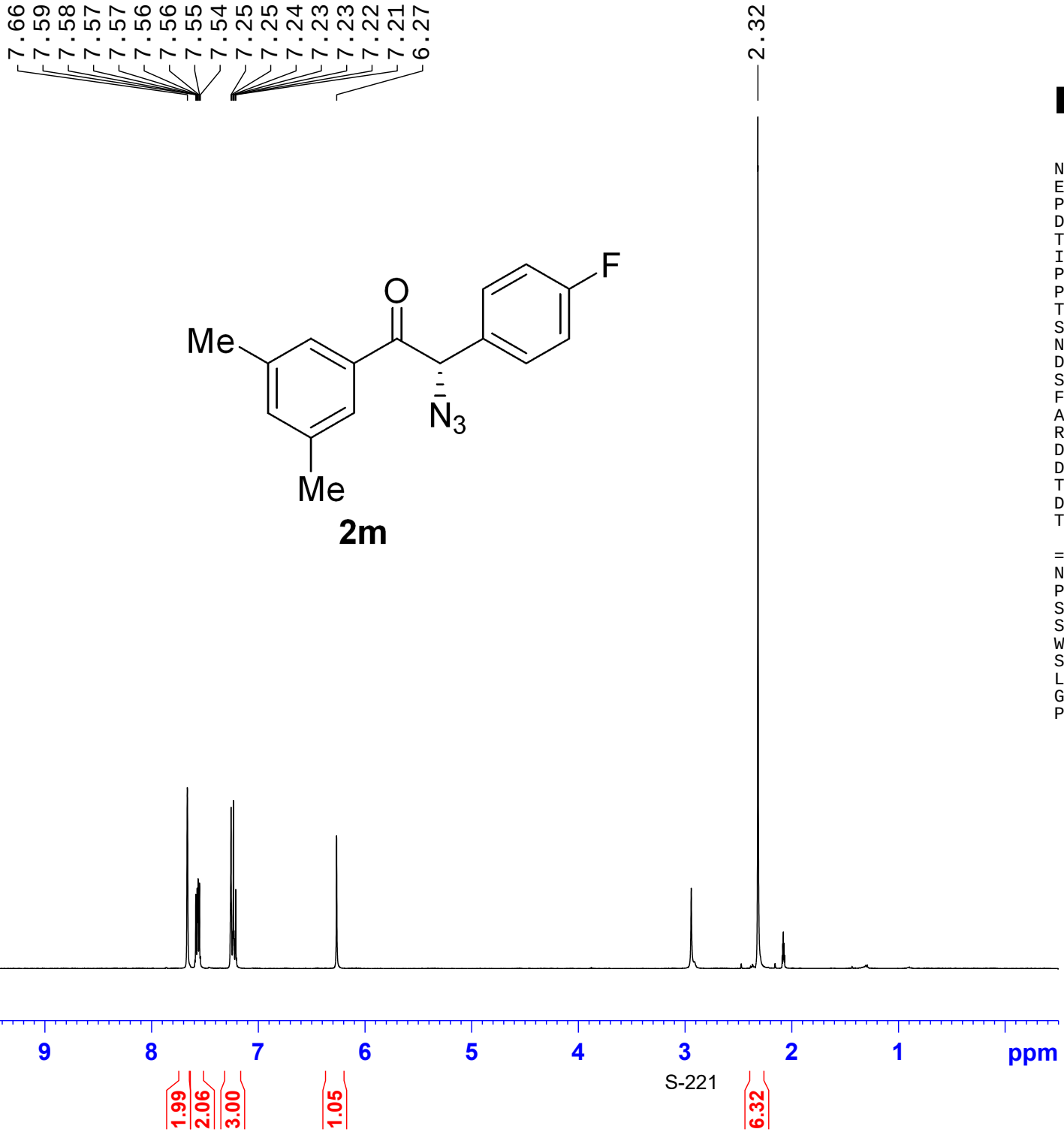




NAME	CNMR-gwg-2-48
EXPNO	4
PROCNO	1
Date_	20210602
Time	20.48 h
INSTRUM	Avance
PROBHD	Z116098_0833 (
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	100
DS	4
SWH	23809.523 Hz
FIDRES	0.726609 Hz
AQ	1.3763061 sec
RG	51.55
DW	21.000 usec
DE	6.50 usec
TE	294.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	100.6228298 MHz
NUC1	13C
P0	3.33 usec
P1	10.00 usec
SI	32768
SF	100.6127685 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

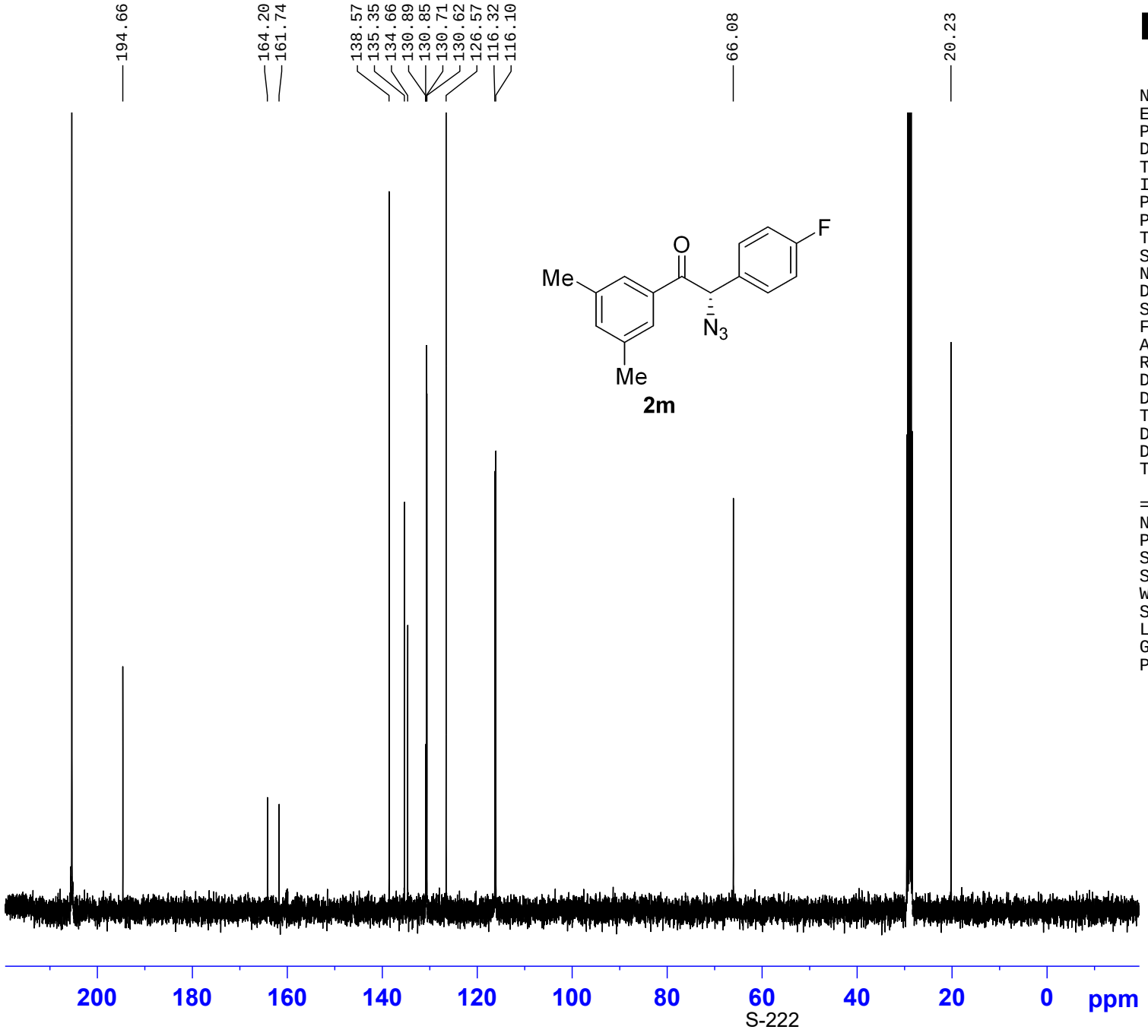


NAME	FNMR-gwg-2-48
EXPNO	5
PROCNO	1
Date_	20210602
Time	20.49 h
INSTRUM	Avance
PROBHD	Z116098_0833 (
PULPROG	zgig
TD	131072
SOLVENT	Acetone
NS	16
DS	4
SWH	90909.094 Hz
FIDRES	1.387163 Hz
AQ	0.7209460 sec
RG	101
DW	5.500 usec
DE	6.50 usec
TE	294.4 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	376.4607164 MHz
NUC1	19F
P1	18.00 usec
SI	65536
SF	376.4983662 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

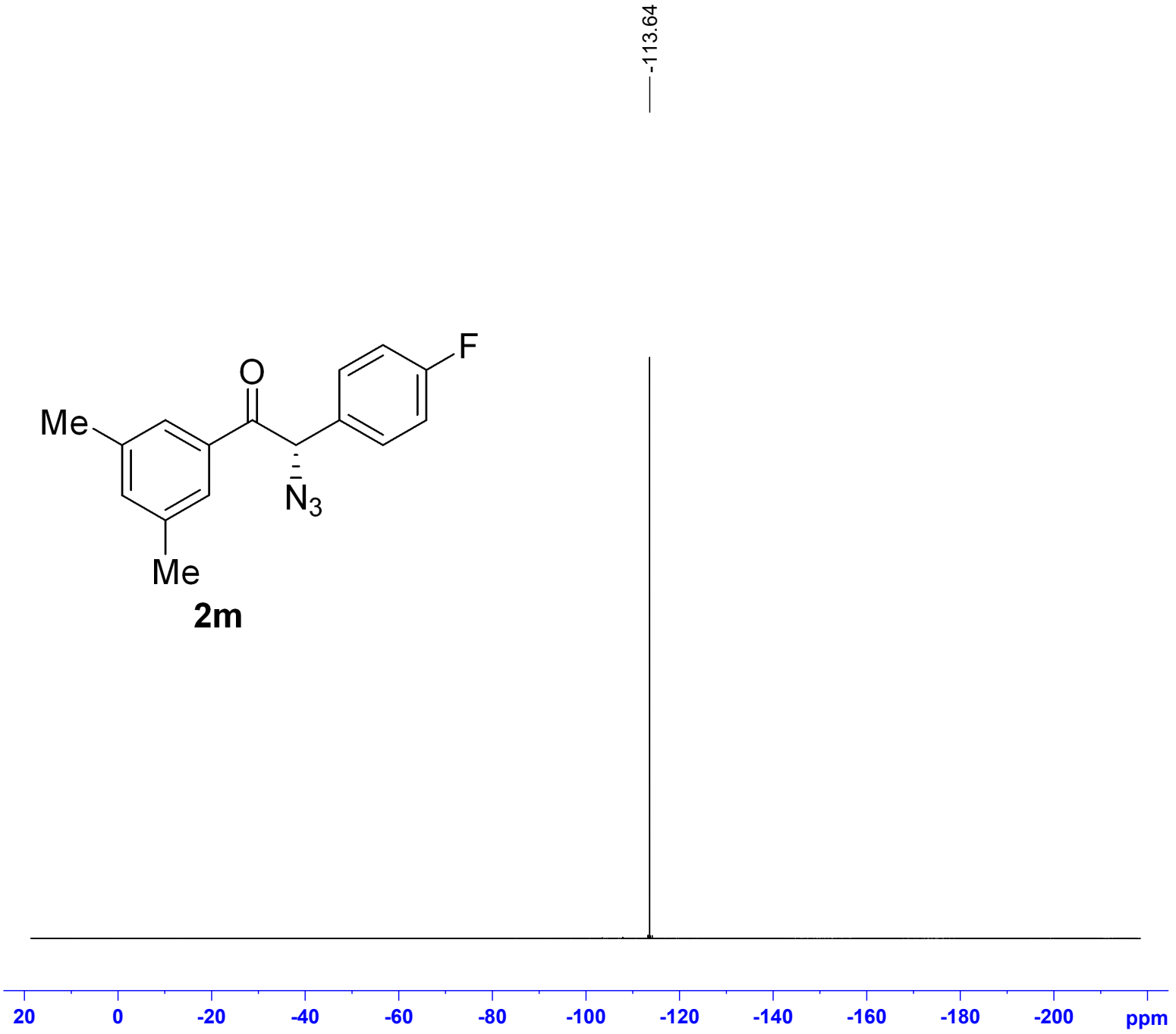


NAME HNMR-gwg-3-5
EXPNO 59
PROCNO 1
Date_ 20210624
Time 14.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 6
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 68.24
DW 60.800 usec
DE 6.50 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1

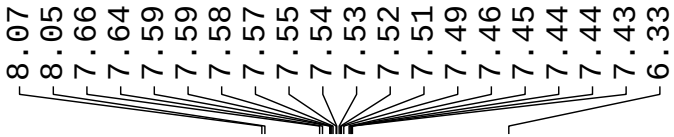
======== CHANNEL f1 ========
NUC1 1H
P1 14.40 usec
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

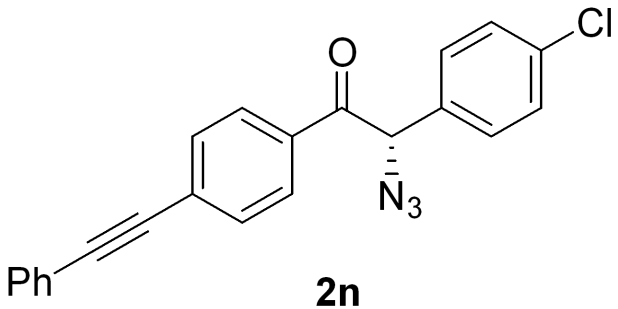



```
NAME          CNMR-gwg-3-5
EXPNO                   60
PROCNO                   1
Date_             20210624
Time                 14.58
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT            Acetone
NS                       258
DS                         4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                   193.13
DW                   20.800 usec
DE                    6.50 usec
TE                   295.2 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                    13C
P1                     9.90 usec
SI                    32768
SF            100.6278560 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```



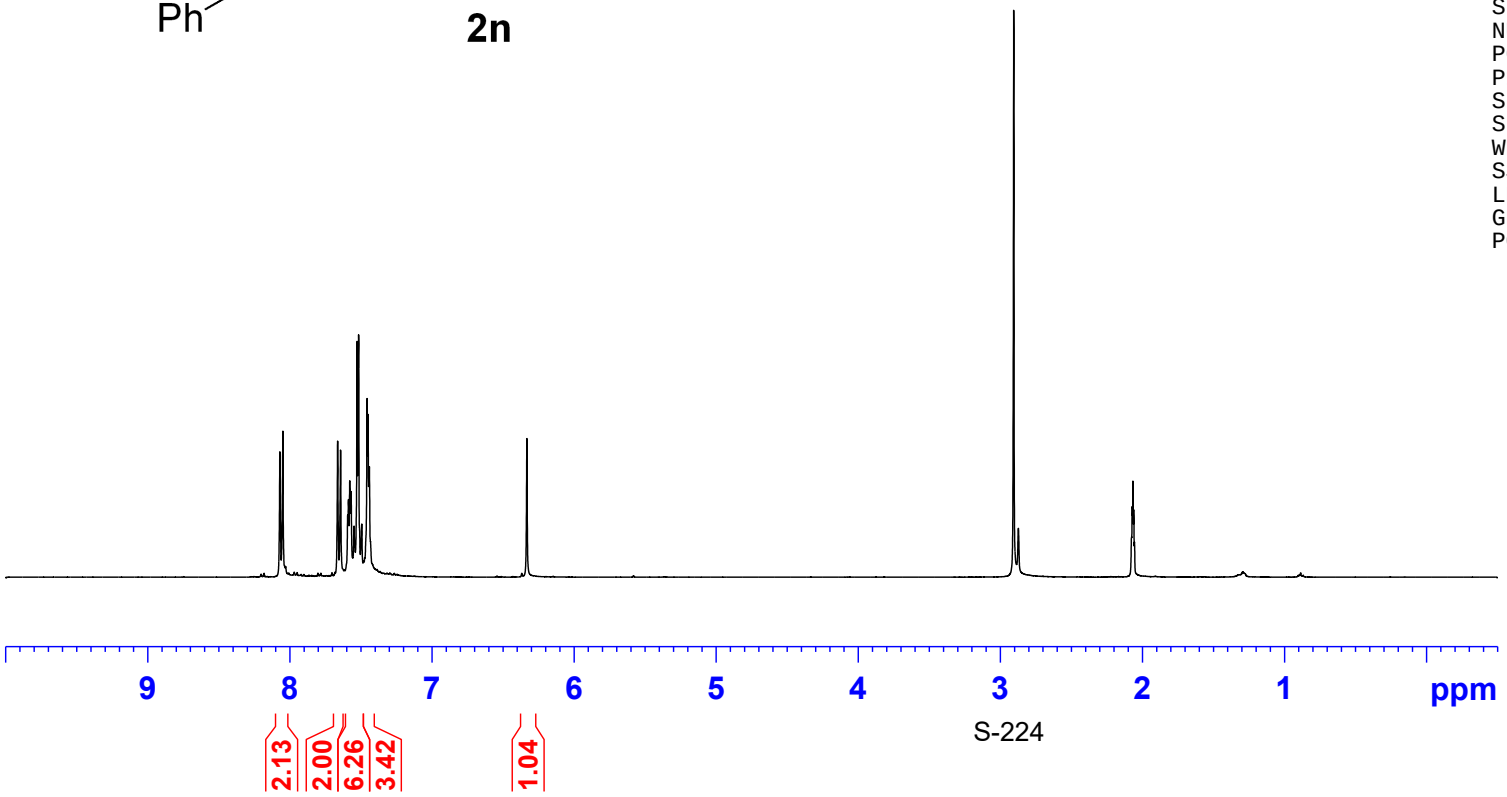

```
NAME          FNMR-gwg-3-5
EXPNO                 4288
PROCNO                   1
Date_             20210625
Time                 12.13
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG        zgfhigqn.2
TD                   131072
SOLVENT           Acetone
NS                       16
DS                        4
SWH               66964.289 Hz
FIDRES             0.510897 Hz
AQ                 0.9787210 sec
RG                      203
DW                    7.467 usec
DE                    6.50 usec
TE                   296.1 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
SI                   65536
SF              282.4043552 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

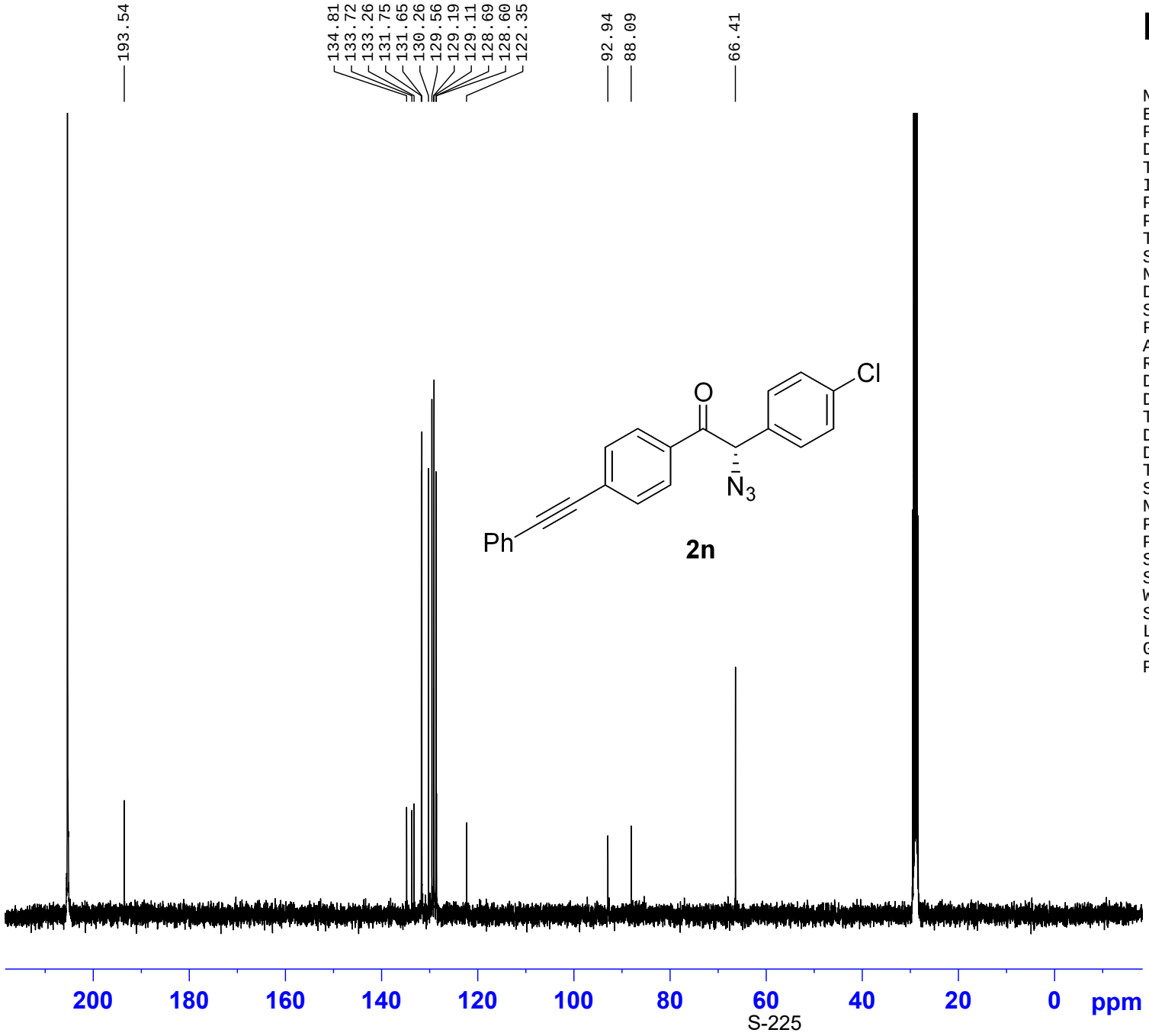




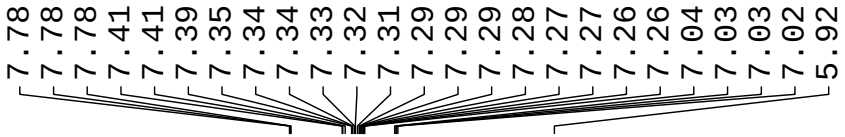
2n

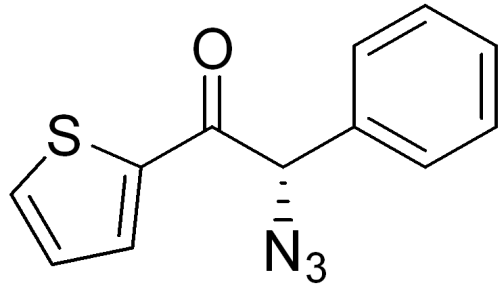
```
NAME          HNMR-gwg-3-23
EXPNO                    5
PROCNO                   1
Date_             20210630
Time                 6.51 h
INSTRUM            Avance
PROBHD    Z116098_0833 (
PULPROG              zg30
TD                  65536
SOLVENT           Acetone
NS                      16
DS                       2
SWH              8196.722 Hz
FIDRES           0.250144 Hz
AQ               3.9977460 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
SI                   65536
SF            400.1300000 MHz
WDW                     EM
SSB                      0
LB                   0.30 Hz
GB                       0
PC                    1.00
```





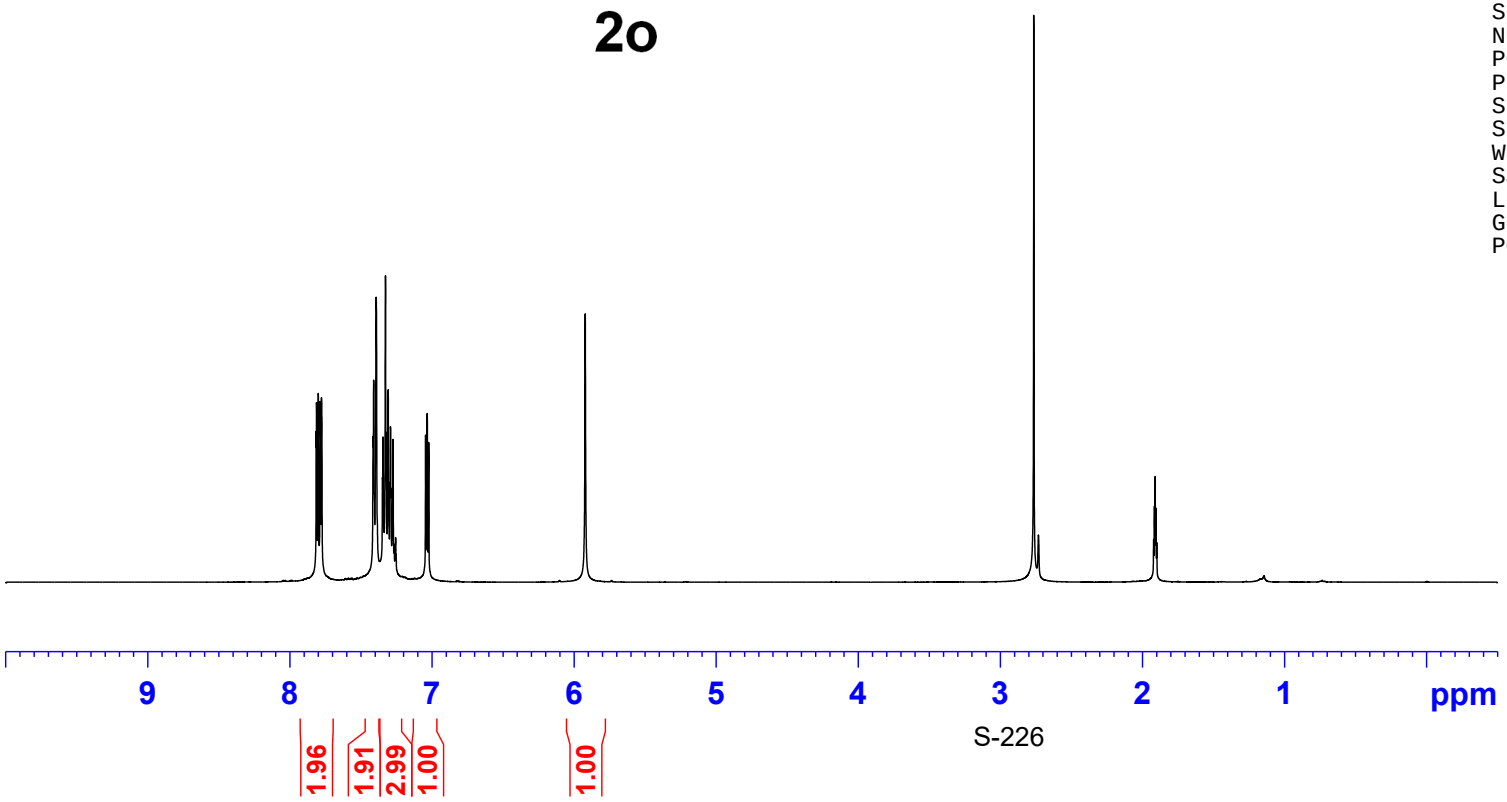
NAME	CNMR-gwg-3-23
EXPNO	6
PROCNO	1
Date_	20210630
Time	7.02 h
INSTRUM	Avance
PROBHD	Z116098_0833 (
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	160
DS	4
SWH	23809.523 Hz
FIDRES	0.726609 Hz
AQ	1.3763061 sec
RG	51.55
DW	21.000 usec
DE	6.50 usec
TE	295.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	100.6228298 MHz
NUC1	13C
P0	3.33 usec
P1	10.00 usec
SI	32768
SF	100.6127685 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

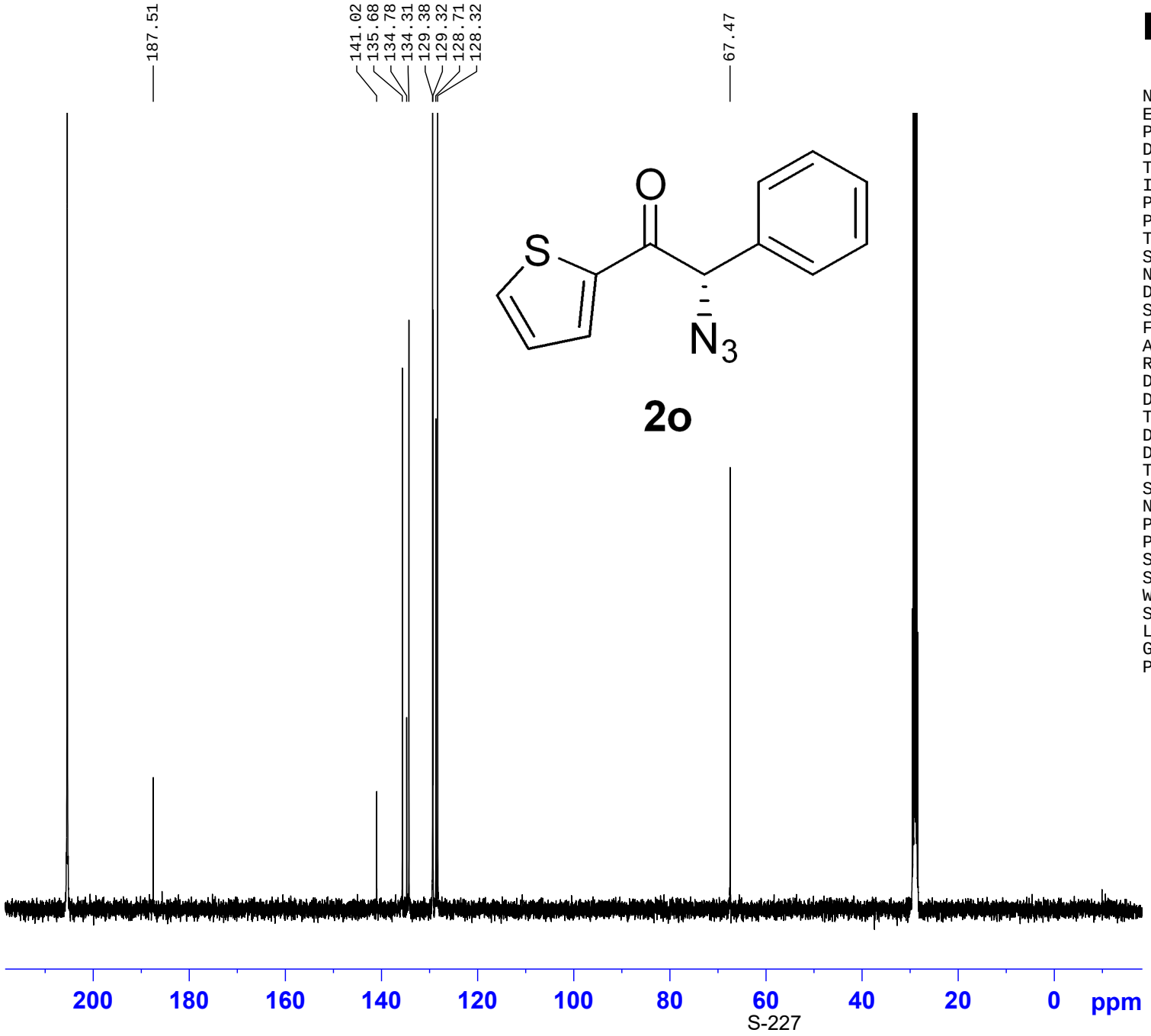




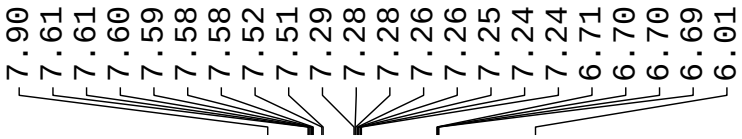
2o

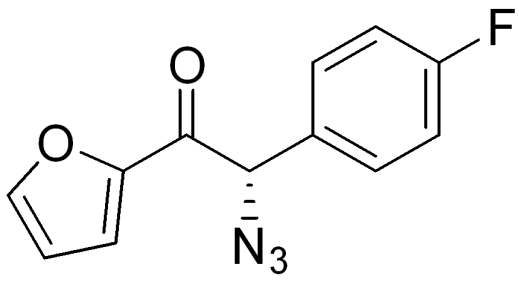
```
NAME          HNMR-gwg-3-4
EXPNO                    1
PROCNO                   1
Date_             20210622
Time                22.43 h
INSTRUM            Avance
PROBHD    Z116098_0833 (
PULPROG              zg30
TD                  65536
SOLVENT           Acetone
NS                       16
DS                        2
SWH              8196.722 Hz
FIDRES           0.250144 Hz
AQ               3.9977460 sec
RG                     101
DW                61.000 usec
DE                13.54 usec
TE                294.5 K
D1             1.00000000 sec
TD0                      1
SFO1          400.1324708 MHz
NUC1                    1H
P0                 3.33 usec
P1                10.00 usec
SI                   65536
SF            400.1300627 MHz
WDW                     EM
SSB                      0
LB                0.30 Hz
GB                       0
PC                1.00
```





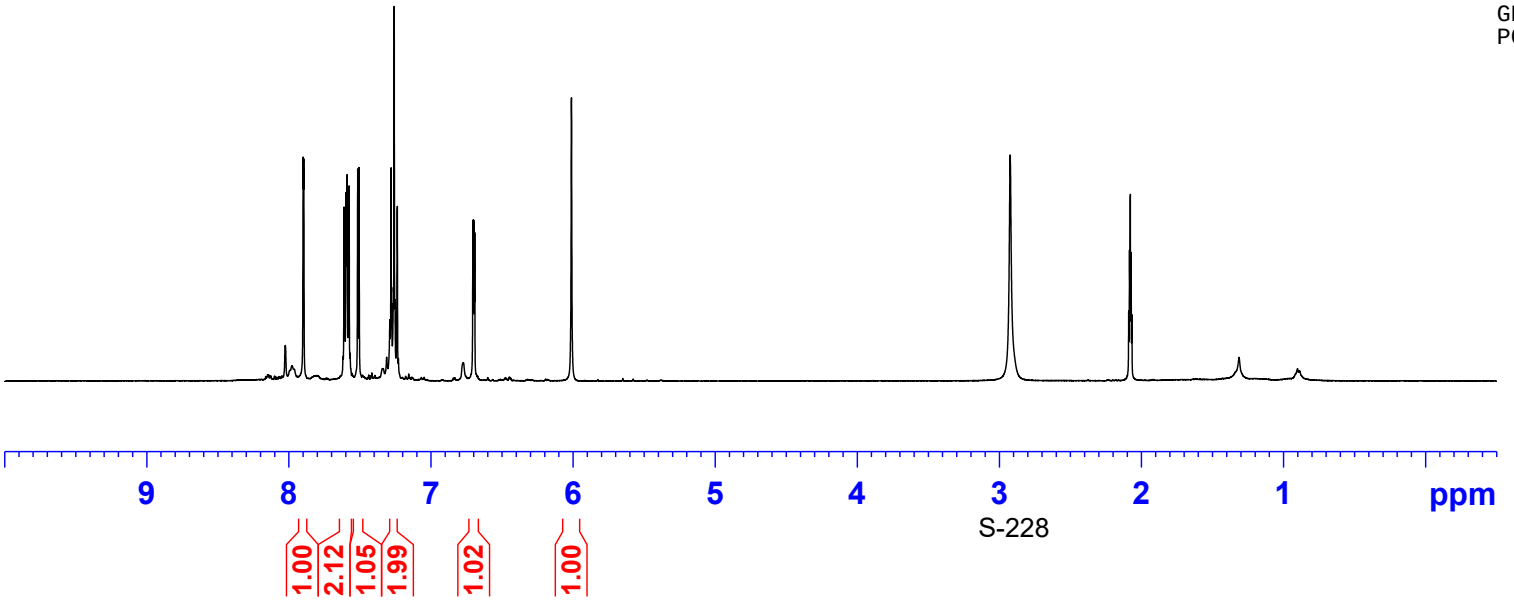
NAME	CNMR-gwg-3-4
EXPNO	2
PROCNO	1
Date_	20210622
Time	22.56 h
INSTRUM	Avance
PROBHD	Z116098_0833 (
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	200
DS	4
SWH	23809.523 Hz
FIDRES	0.726609 Hz
AQ	1.3763061 sec
RG	47.4244
DW	21.000 usec
DE	6.50 usec
TE	295.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	100.6228298 MHz
NUC1	13C
P0	3.33 usec
P1	10.00 usec
SI	32768
SF	100.6127685 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

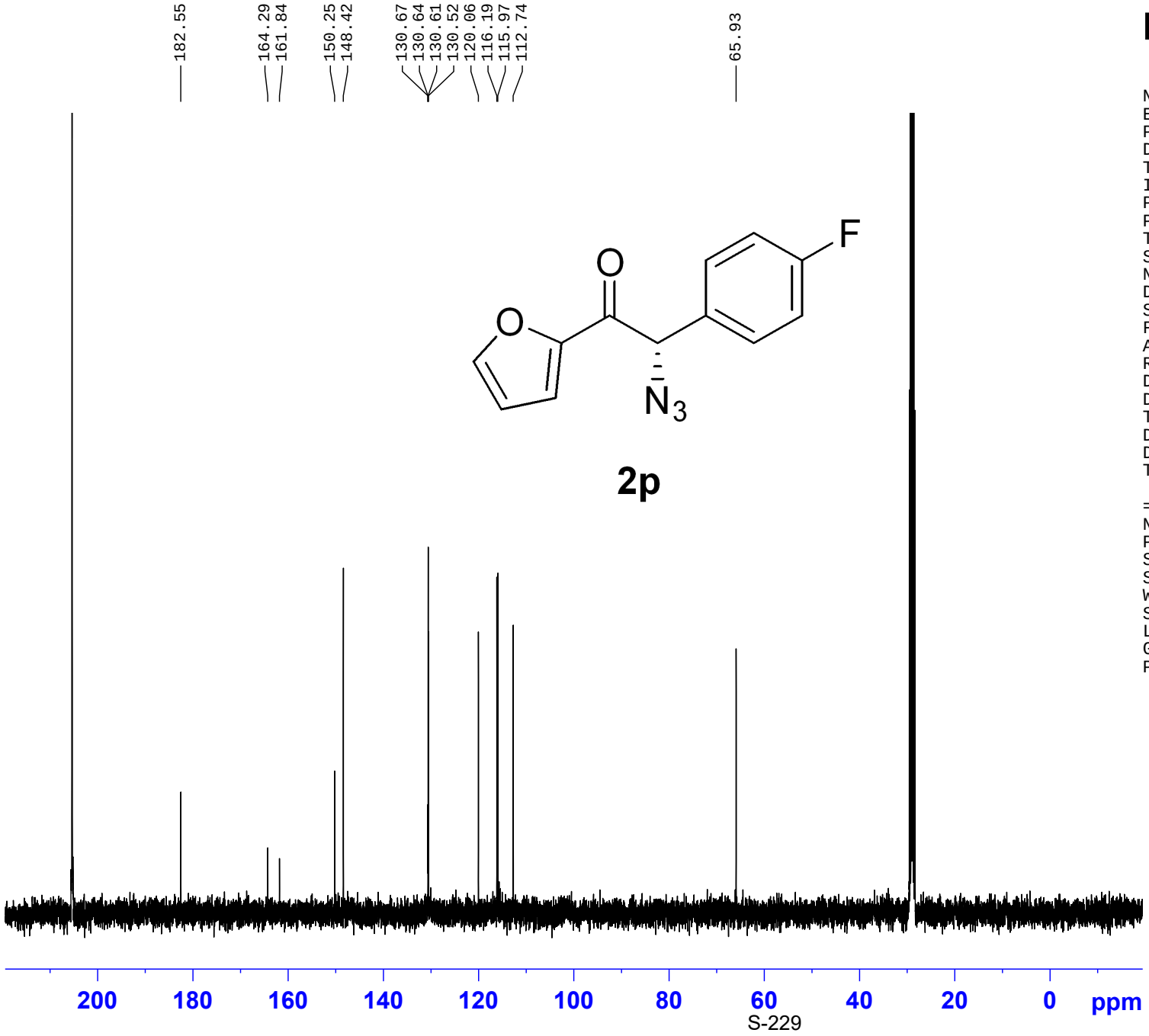




2p

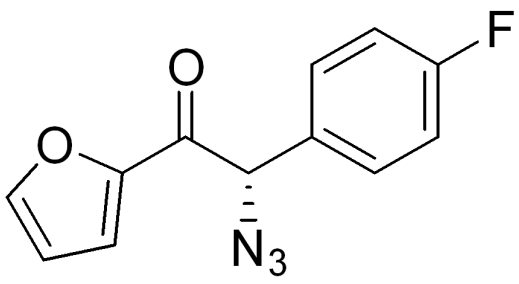
```
NAME          HNMR-gwg-3-3
EXPNO                  102
PROCNO                   1
Date_             20210706
Time                 14.45
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT           Acetone
NS                       6
DS                       2
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                   100.49
DW                   60.800 usec
DE                    6.50 usec
TE                   294.6 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.40 usec
SI                   65536
SF            400.1900000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



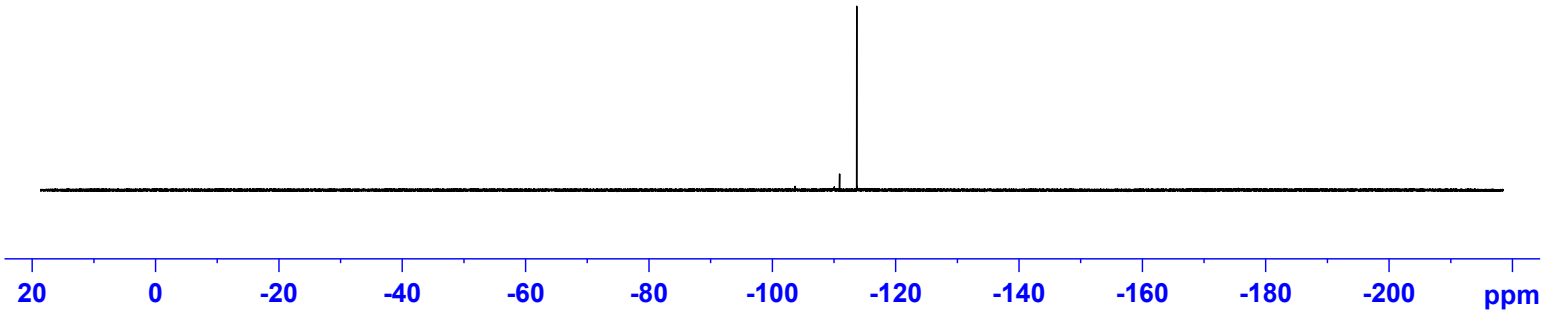



```
NAME          CNMR-gwg-3-3
EXPNO                  105
PROCNO                   1
Date_             20210706
Time                 15.03
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT           Acetone
NS                    106
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                 193.13
DW                 20.800 usec
DE                  6.50 usec
TE                 295.1 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.90 usec
SI                  32768
SF           100.6278560 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

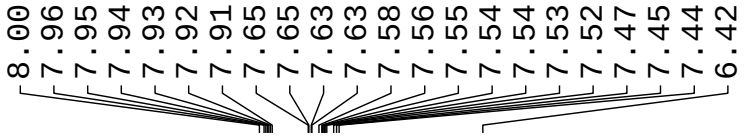
-113.70

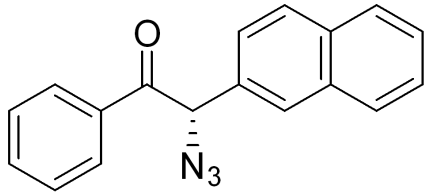


2p



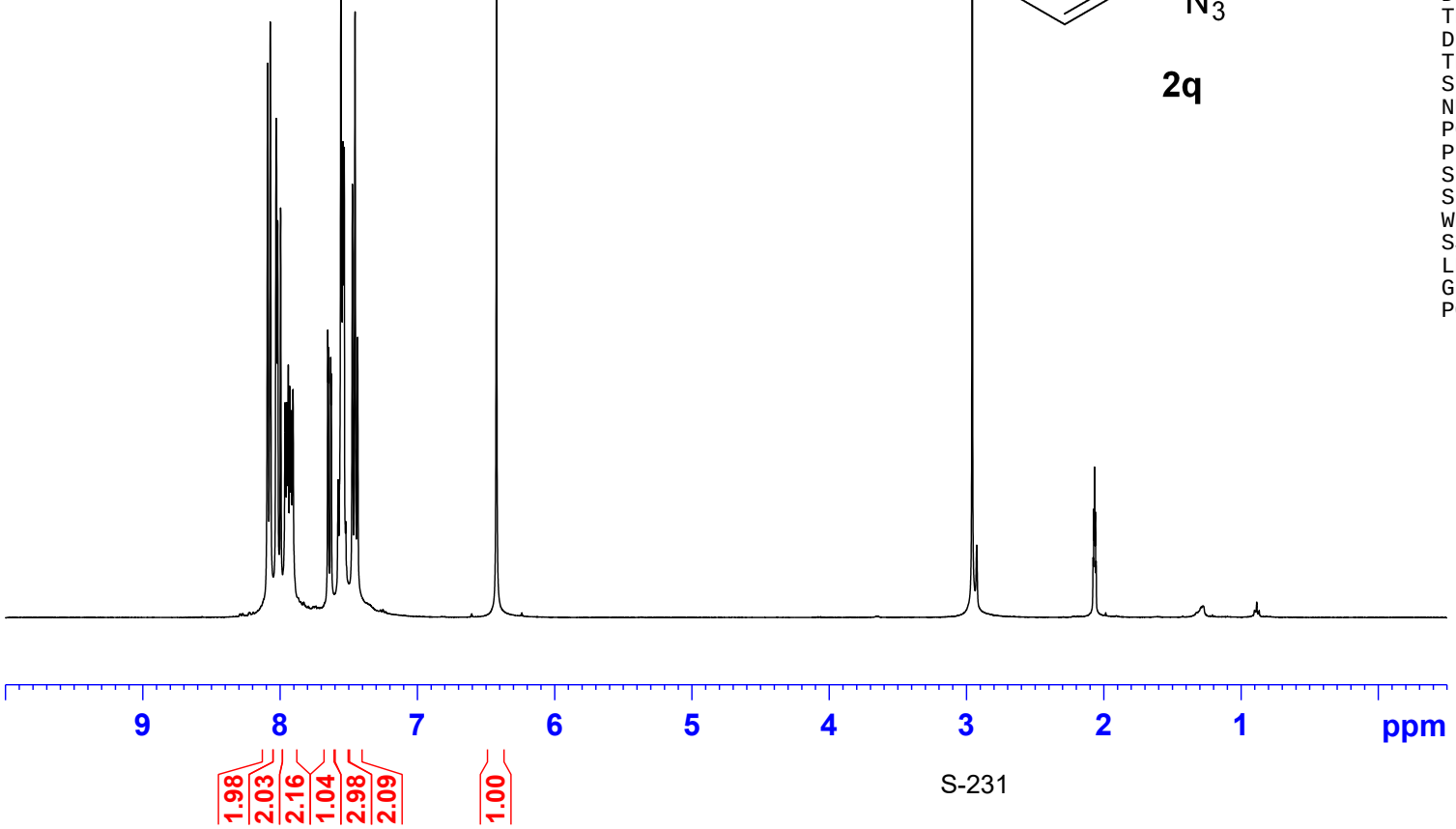

```
NAME          FNMR-gwg-3-3
EXPNO                 4461
PROCNO                   1
Date_             20210707
Time                 9.12
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG        zgfhigqn.2
TD                  131072
SOLVENT           Acetone
NS                       16
DS                        4
SWH              66964.289 Hz
FIDRES            0.510897 Hz
AQ                0.9787210 sec
RG                      203
DW                  7.467 usec
DE                  6.50 usec
TE                  296.2 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
SI                   65536
SF            282.4043552 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

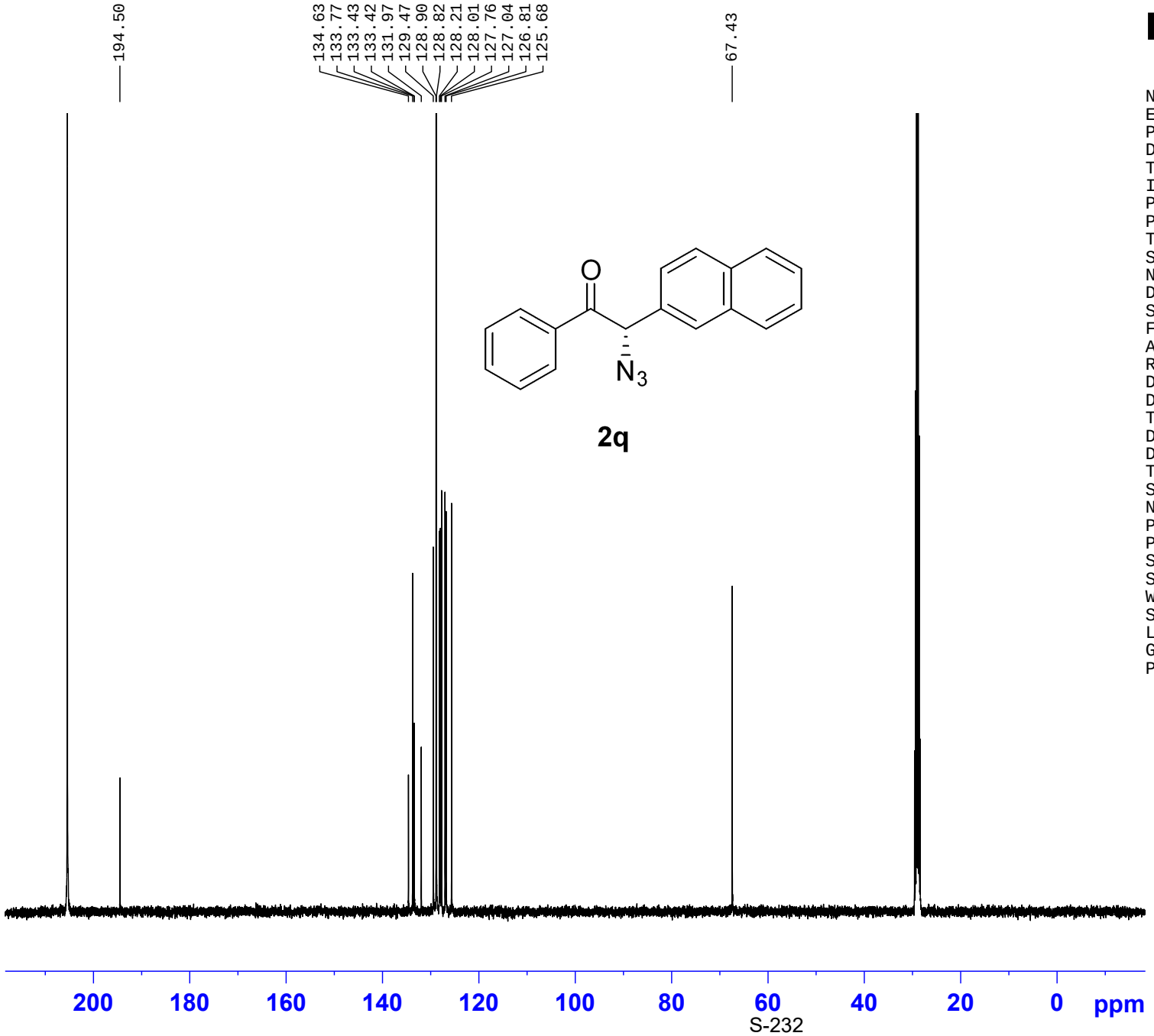




2q

NAME	HNMR-gwg-2-70
EXPNO	3
PROCNO	1
Date_	20210609
Time	23.52 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	3.9977460 sec
RG	79.9233
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
SI	65536
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

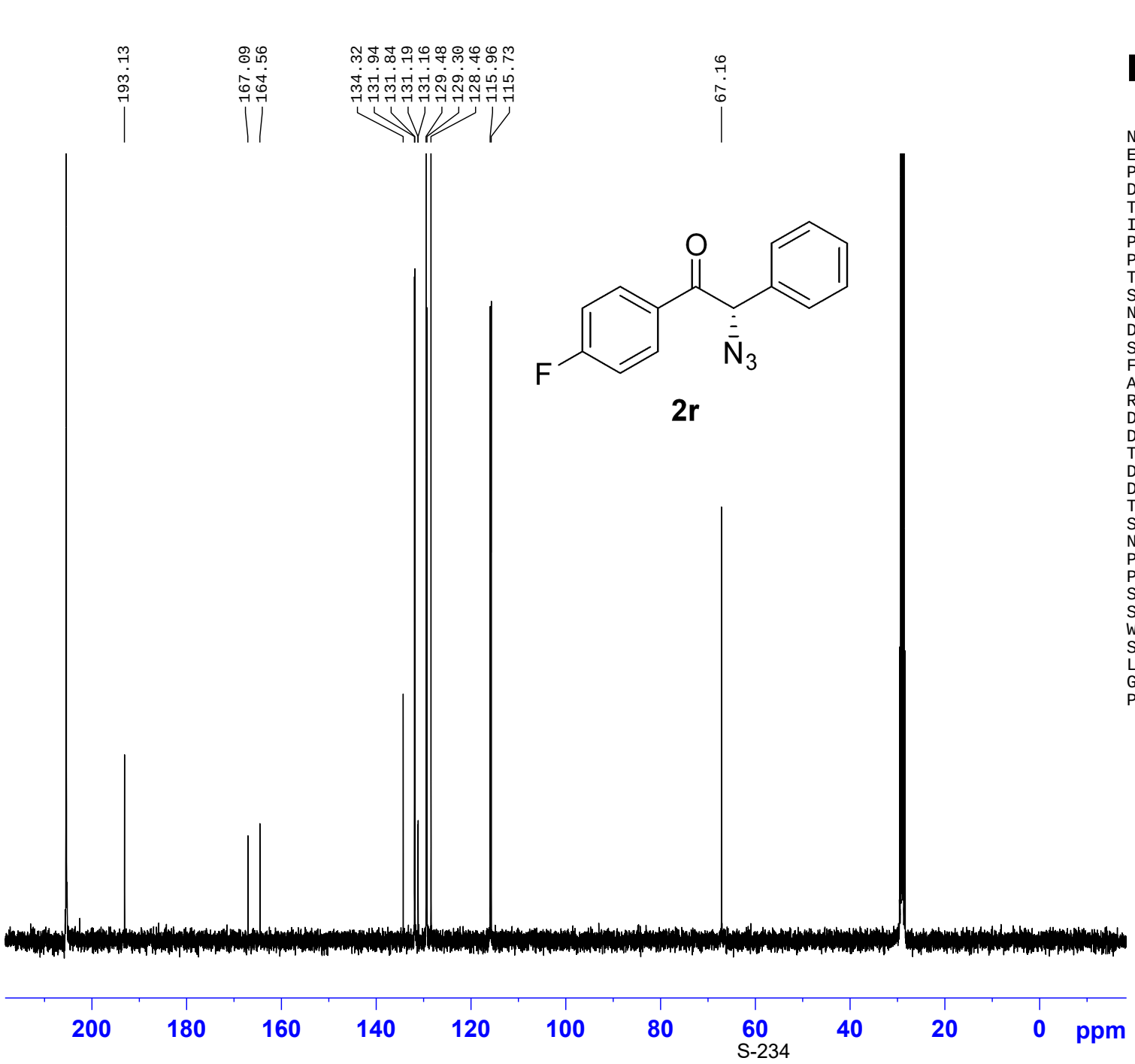




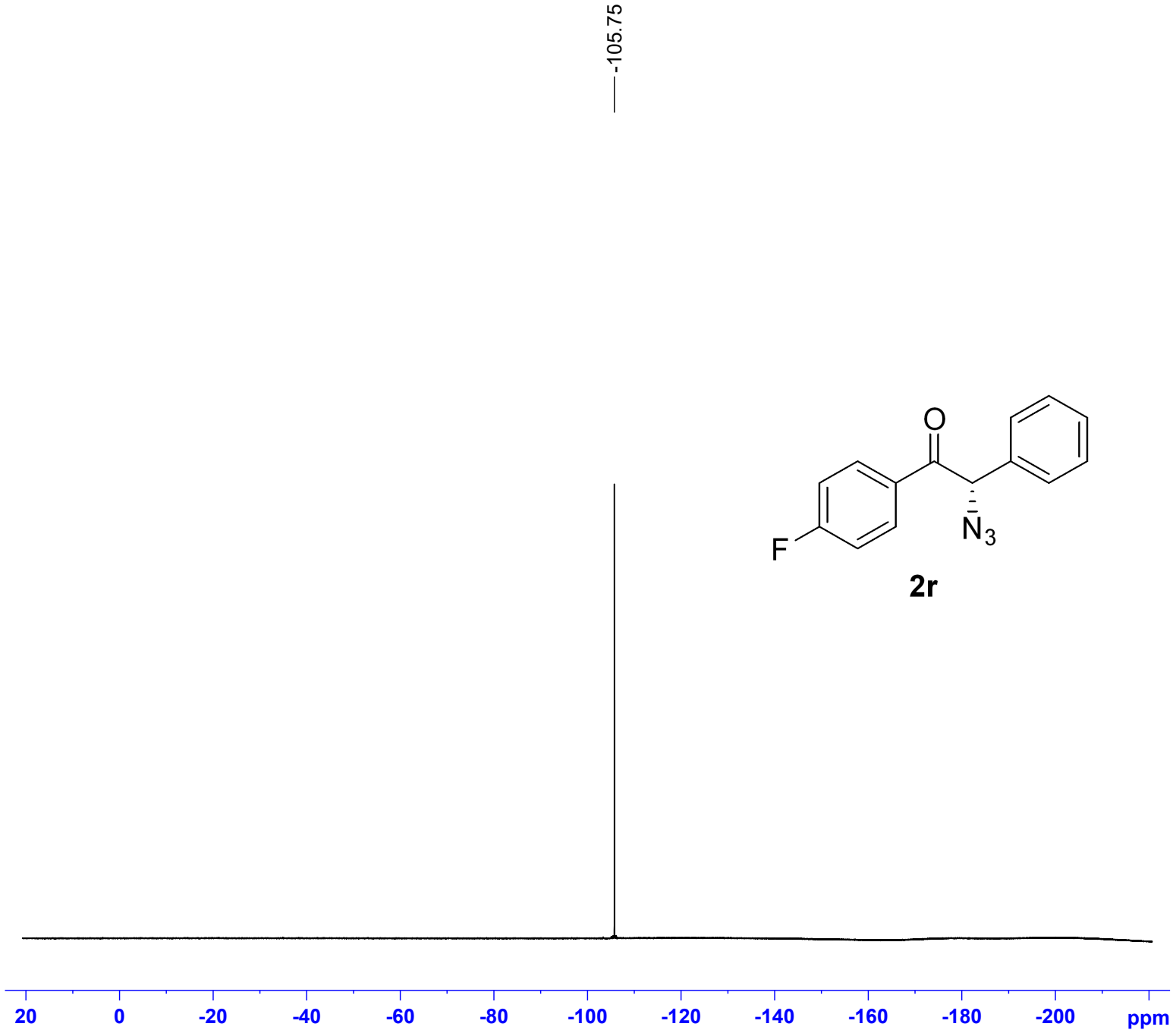
BRUKER

NAME	CNMR-gwg-2-70	
EXPNO	4	
PROCNO	1	
Date_	20210610	
Time	0.04	h
INSTRUM	Avance	
PROBHD	Z116098_0833 (	
PULPROG	zgpg30	
TD	65536	
SOLVENT	Acetone	
NS	200	
DS	4	
SWH	23809.523	Hz
FIDRES	0.726609	Hz
AQ	1.3763061	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
SI	32768	
SF	100.6127685	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	

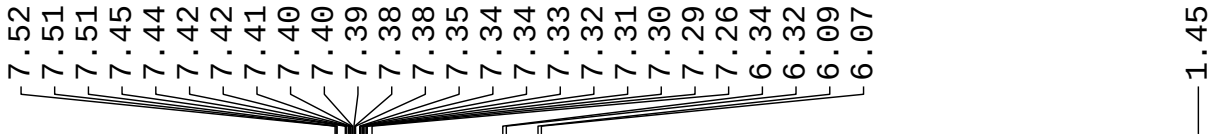
NAME	HNMR-gwg-3-75
EXPNO	1
PROCNO	1
Date_	20210719
Time	23.32 h
INSTRUM	Avance
PROBHD	Z116098_0833 (
PULPROG	zg30
TD	65536
SOLVENT	Acetone
NS	16
DS	2
SWH	8196.722 Hz
FIDRES	0.250144 Hz
AQ	3.9977460 sec
RG	101
DW	61.000 usec
DE	13.54 usec
TE	294.9 K
D1	1.00000000 sec
TD0	1
SFO1	400.1324708 MHz
NUC1	1H
P0	3.33 usec
P1	10.00 usec
SI	65536
SF	400.1300044 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

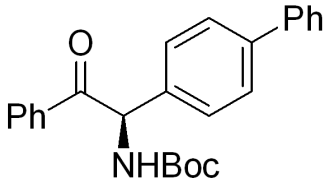



```
NAME          CNMR-gwg-3-75
EXPNO                    2
PROCNO                   1
Date_             20210719
Time                23.45 h
INSTRUM             Avance
PROBHD    Z116098_0833 (
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                     200
DS                       4
SWH             23809.523 Hz
FIDRES           0.726609 Hz
AQ              1.3763061 sec
RG                 48.6724
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
SI                   32768
SF            100.6127685 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                 1.40
```



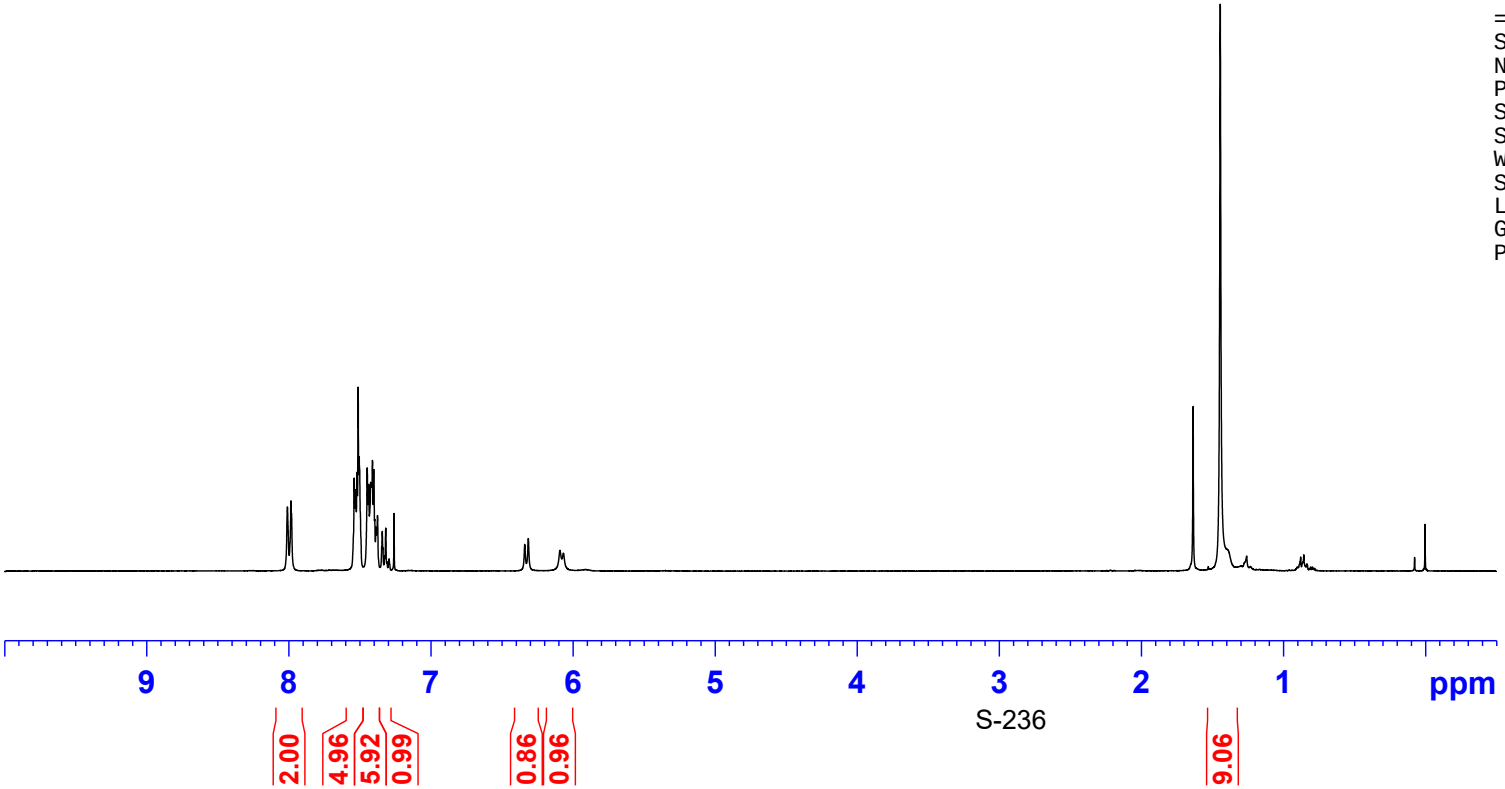
NAME	FNMR-gwg-3-75
EXPNO	3
PROCNO	1
Date_	20210719
Time	23.47 h
INSTRUM	Avance
PROBHD	Z116098_0833 (
PULPROG	zgig
TD	131072
SOLVENT	Acetone
NS	16
DS	4
SWH	90909.094 Hz
FIDRES	1.387163 Hz
AQ	0.7209460 sec
RG	101
DW	5.500 usec
DE	6.50 usec
TE	295.3 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	376.4607164 MHz
NUC1	19F
P1	18.00 usec
SI	65536
SF	376.4983662 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

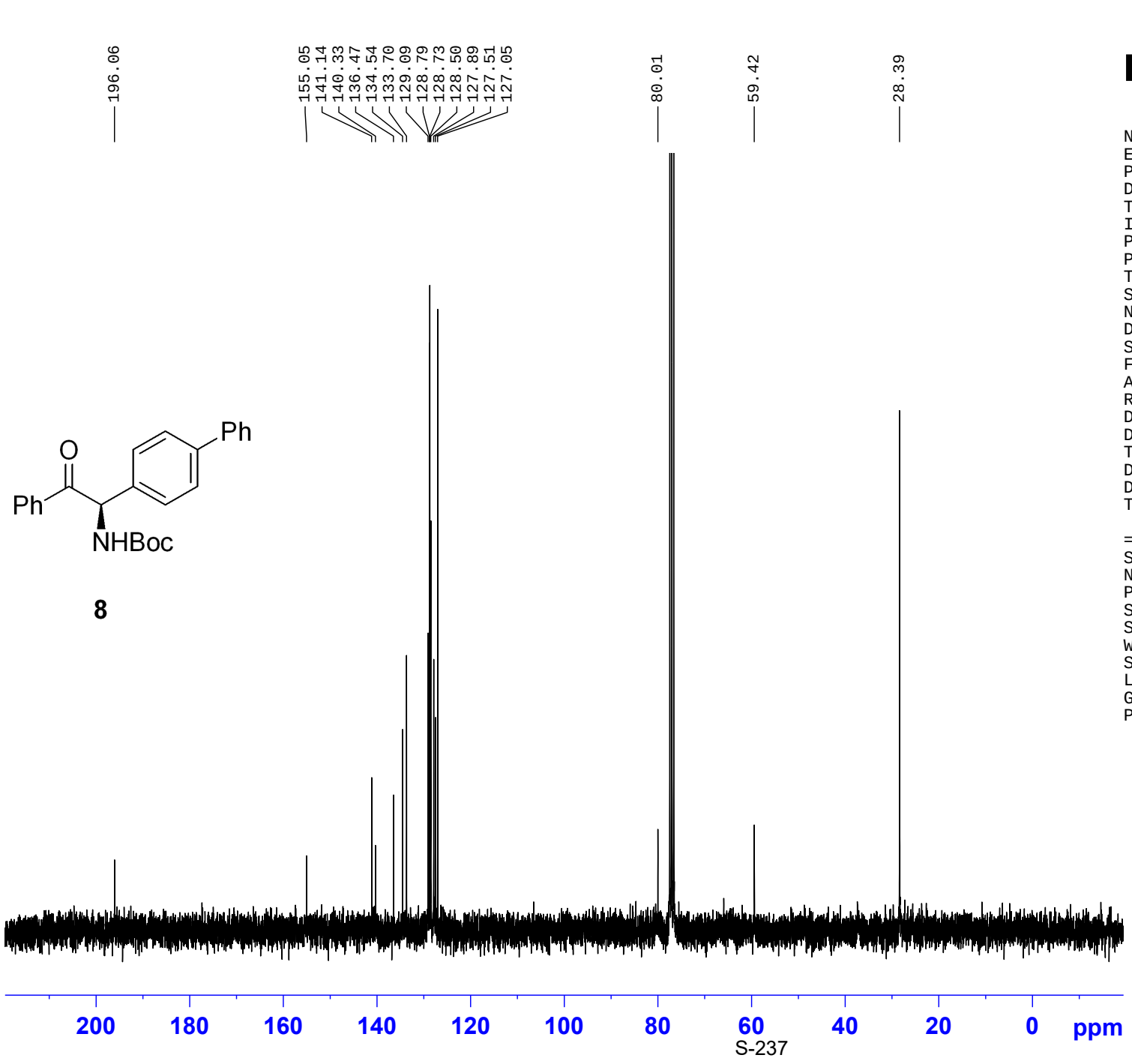




8

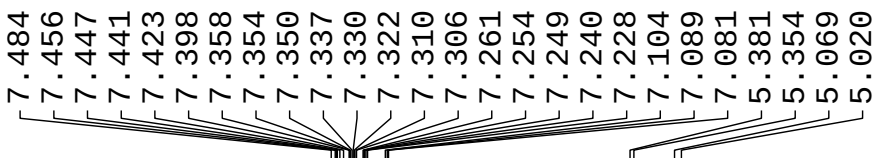
```
NAME          HNMR-gwg-3-89
EXPNO                 4780
PROCNO                   1
Date_             20210722
Time                  9.37
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               6009.615 Hz
FIDRES           0.091699 Hz
AQ               5.4526453 sec
RG                     161
DW                  83.200 usec
DE                   6.50 usec
TE                  296.2 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           300.1318534 MHz
NUC1                   1H
P1                  10.00 usec
SI                   65536
SF             300.1300072 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

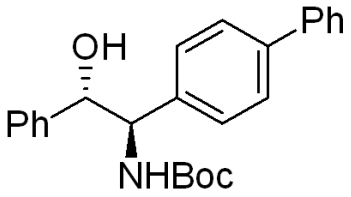




BRUKER

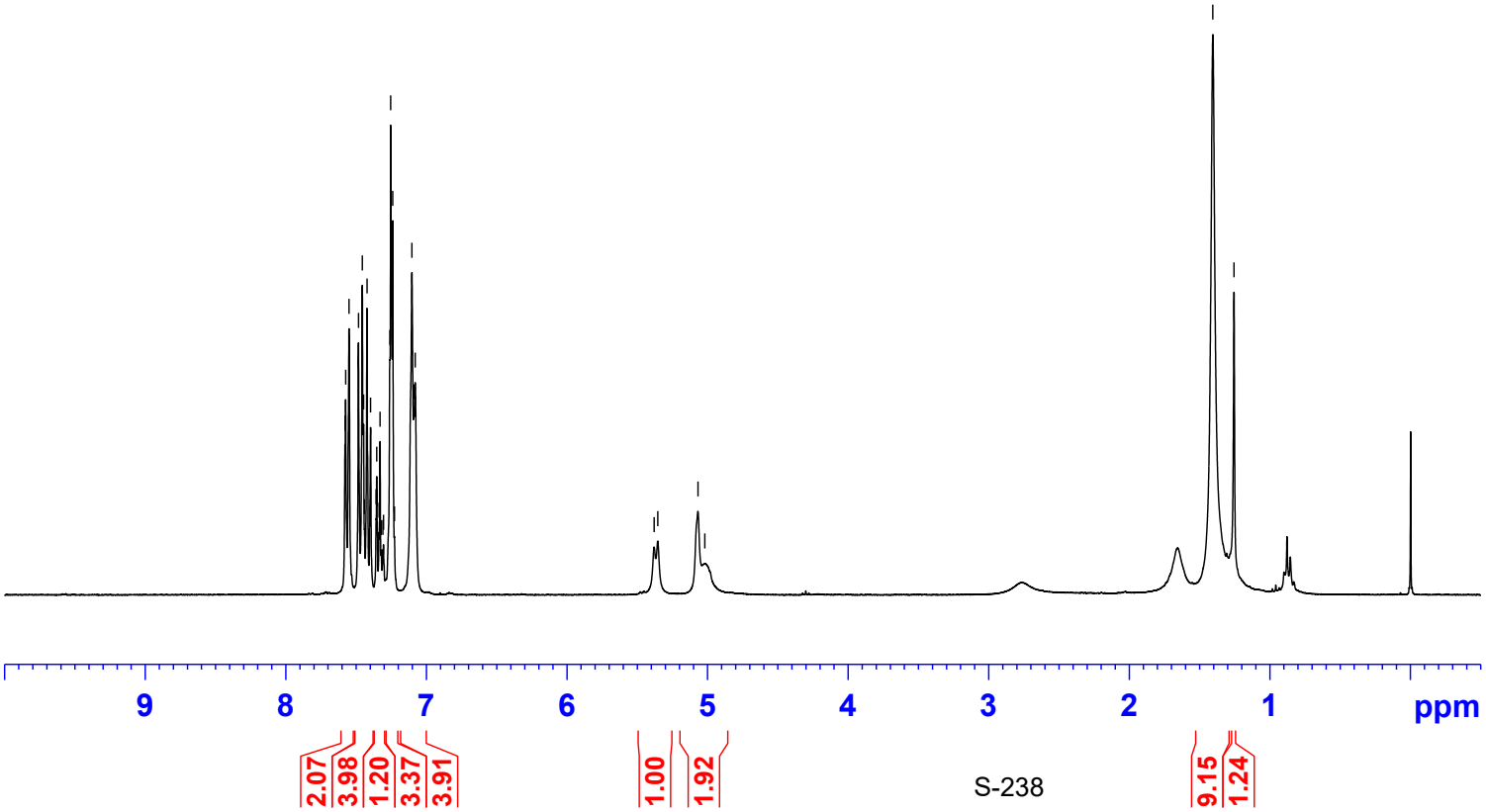
NAME	CNMR-gwg-3-89
EXPNO	4841
PROCNO	1
Date_	20210724
Time	18.28
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	300
DS	4
SWH	18028.846 Hz
FIDRES	0.275098 Hz
AQ	1.8175818 sec
RG	203
DW	27.733 usec
DE	6.50 usec
TE	296.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	75.4752949 MHz
NUC1	13C
P1	9.50 usec
SI	32768
SF	75.4677485 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

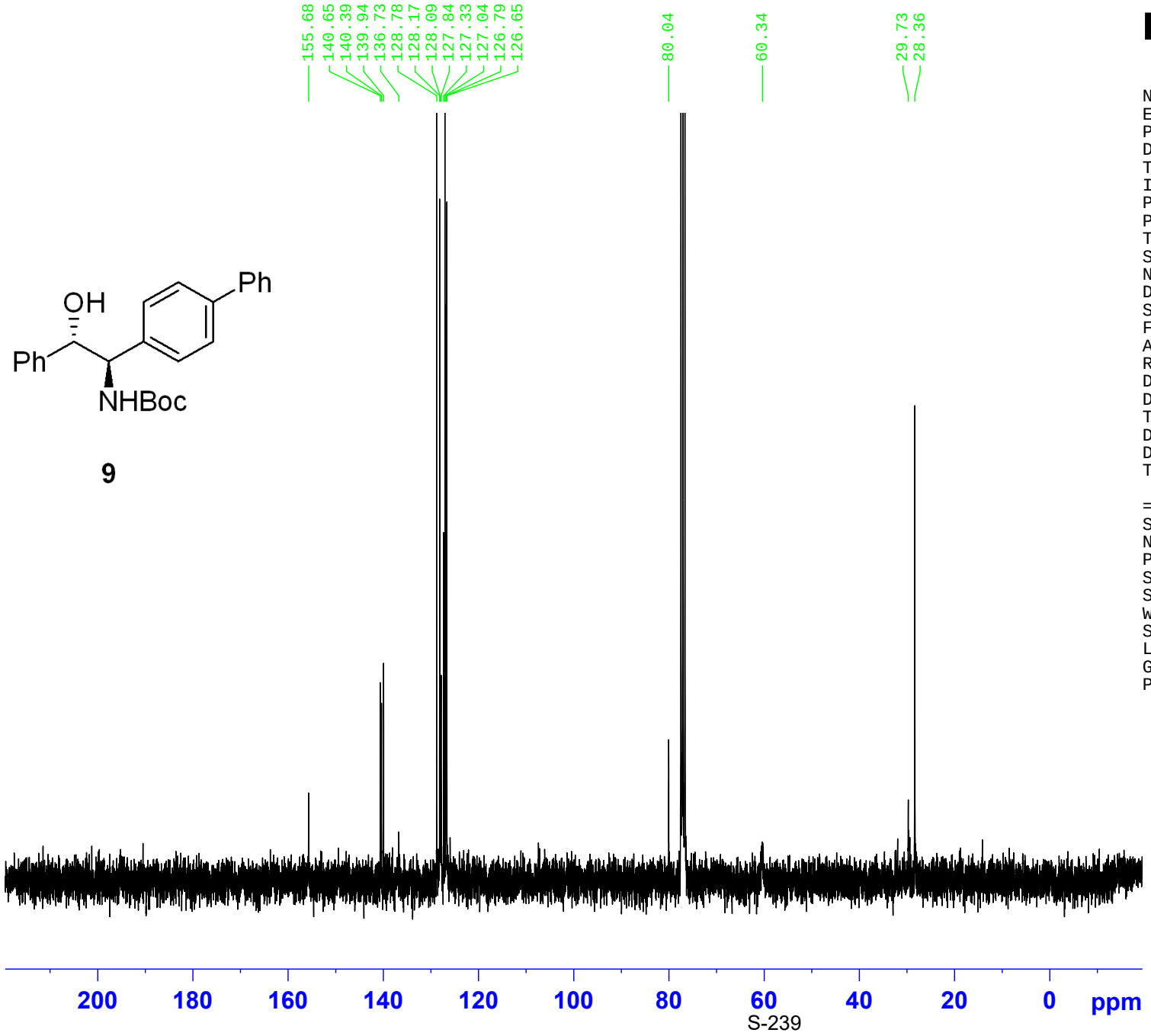




9

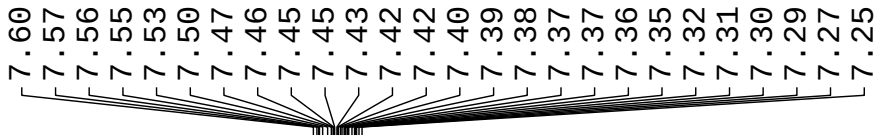
```
NAME        HNMR-gwg-3-155
EXPNO                 5524
PROCNO                   1
Date_             20211014
Time                 9.53
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               6009.615 Hz
FIDRES            0.091699 Hz
AQ                5.4526453 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
SI                   65536
SF             300.1300092 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                    1.00
```

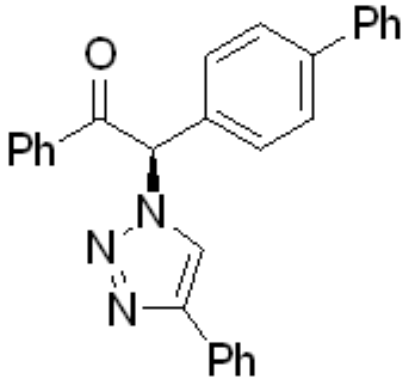




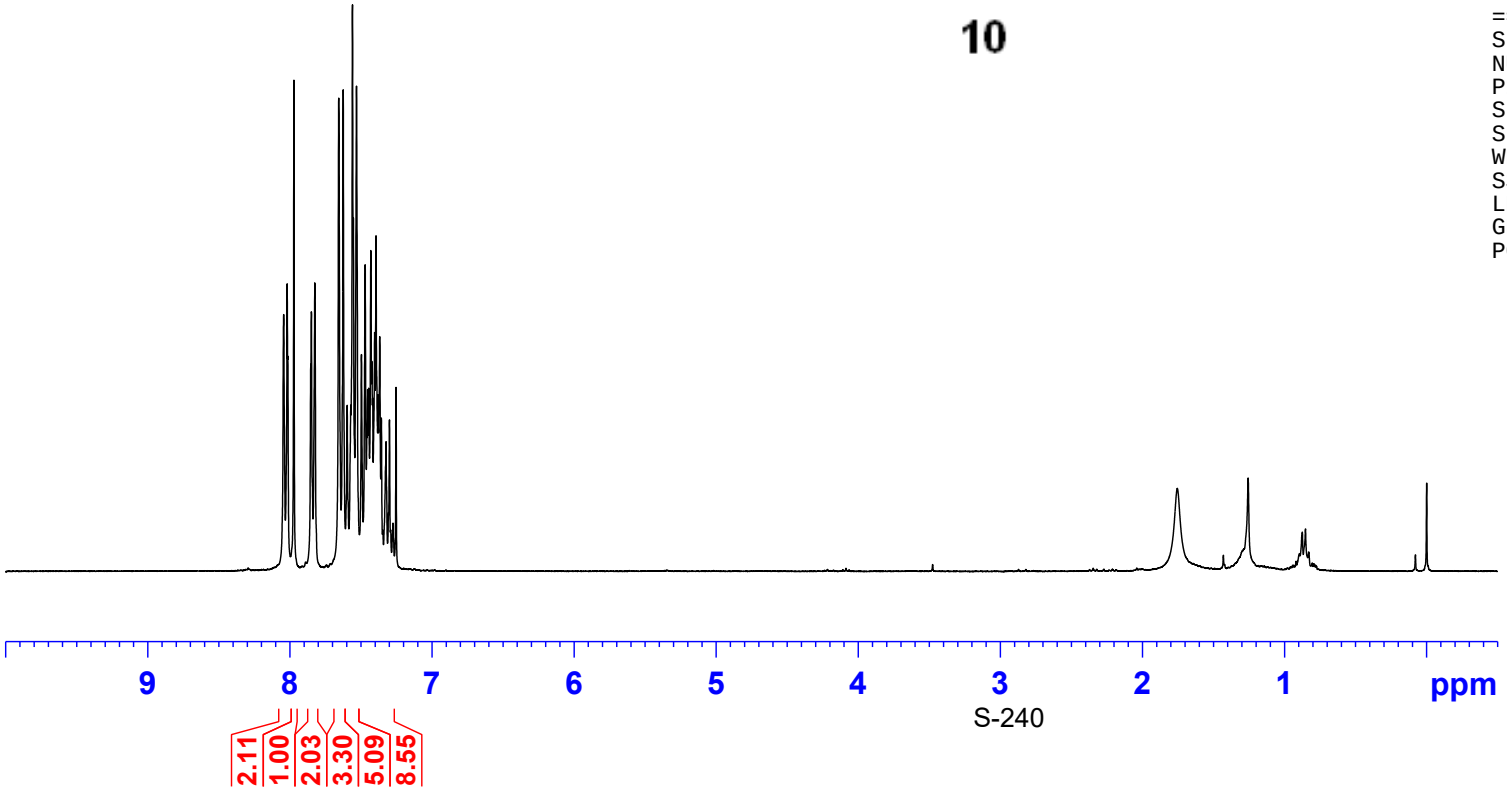
BRUKER

```
NAME        CNMR-gwg-3-155
EXPNO                 5525
PROCNO                   1
Date_          20211014
Time                10.27
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   500
DS                     4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ             1.8175818 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
SI                32768
SF            75.4677485 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

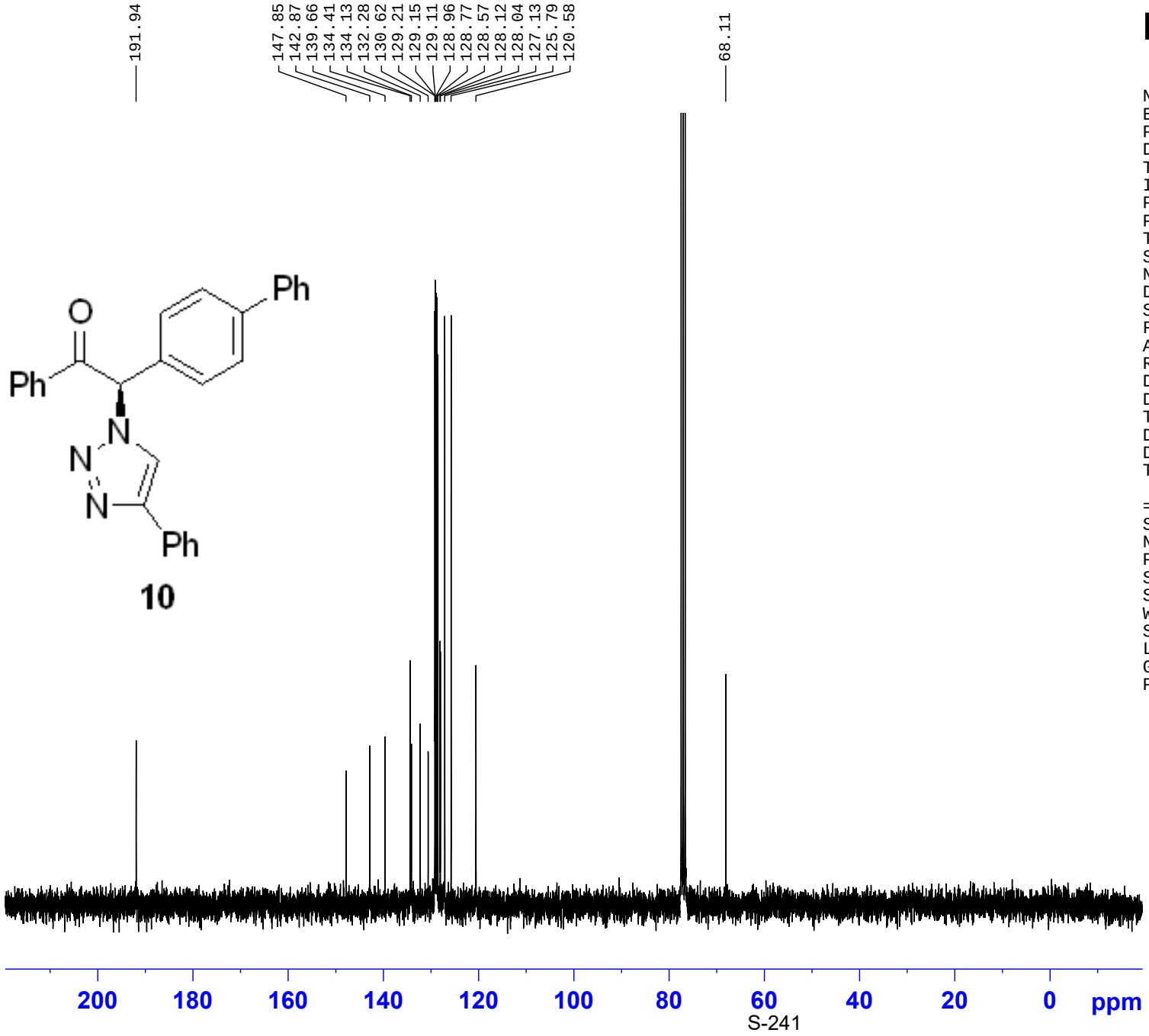




10

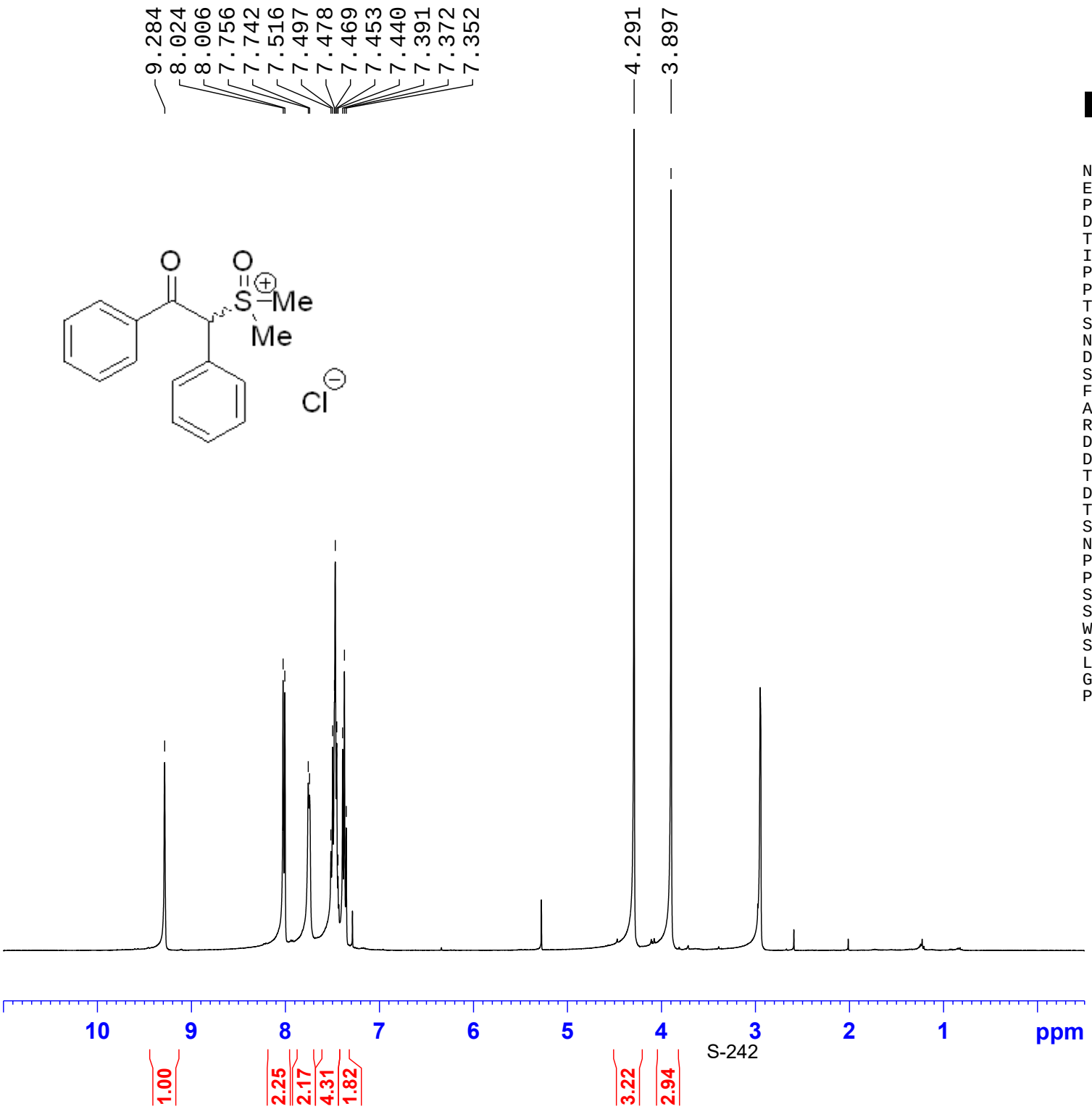



```
NAME          HNMR-gwg-3-92
EXPNO                 4862
PROCNO                   1
Date_             20210727
Time                 11.06
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               6009.615 Hz
FIDRES            0.091699 Hz
AQ                5.4526453 sec
RG                     161
DW                  83.200 usec
DE                   6.50 usec
TE                  296.1 K
D1               1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           300.1318534 MHz
NUC1                   1H
P1                  10.00 usec
SI                   65536
SF             300.1300092 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

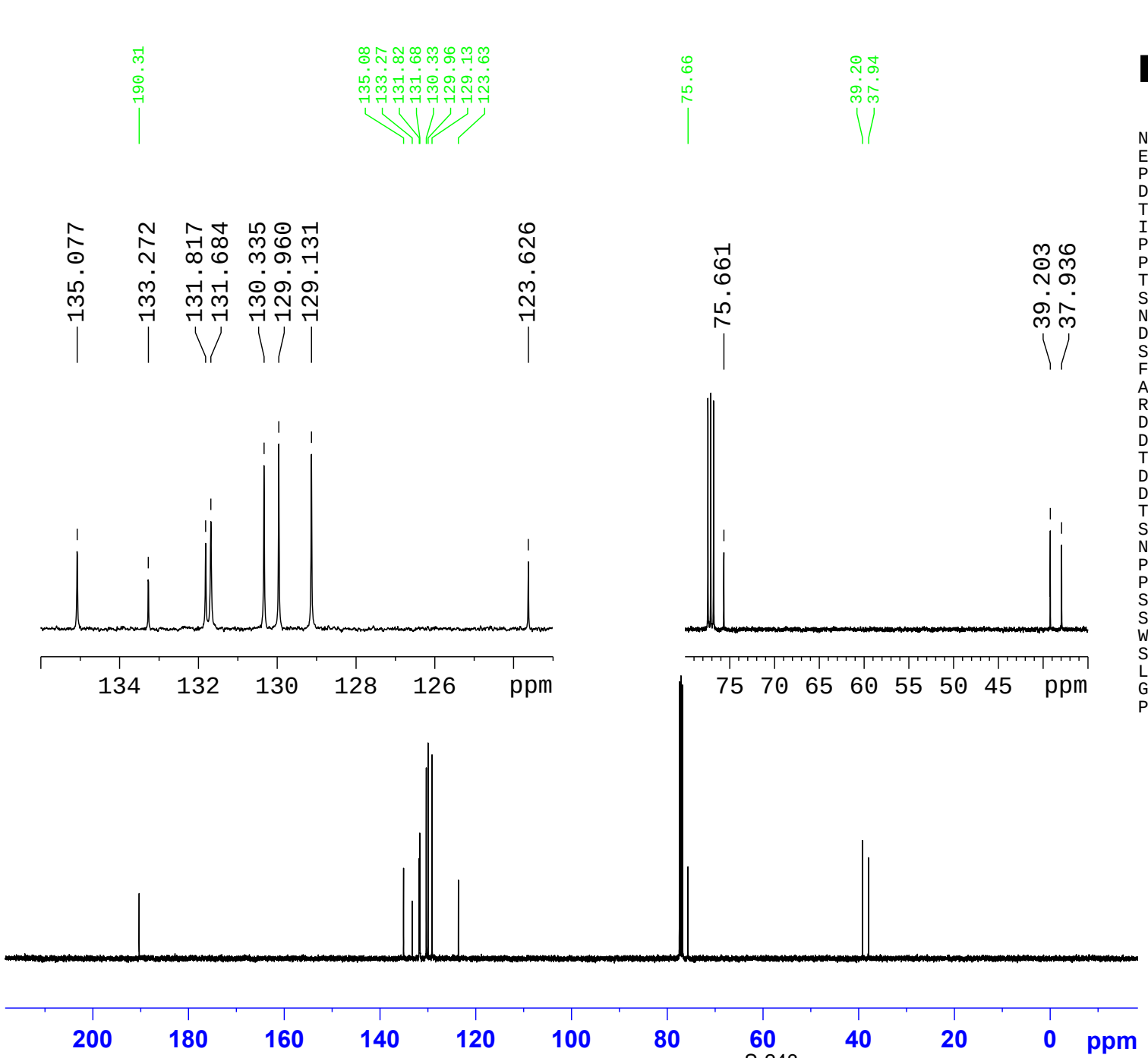


BRUKER

NAME	CNMR-gwg-3-92
EXPNO	4863
PROCNO	1
Date_	20210727
Time	11.27
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	300
DS	4
SWH	18028.846 Hz
FIDRES	0.275098 Hz
AQ	1.8175818 sec
RG	203
DW	27.733 usec
DE	6.50 usec
TE	296.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	75.4752949 MHz
NUC1	13C
P1	9.50 usec
SI	32768
SF	75.4677485 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

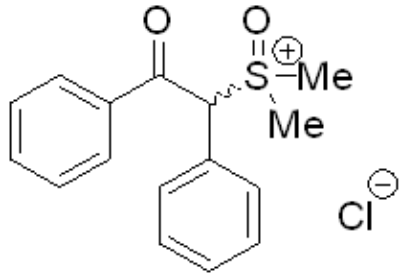


NAME	HNMR-gwg-4-144
EXPNO	1
PROCNO	1
Date_	20220214
Time	10.36 h
INSTRUM	Avance
PROBHD	Z116098_0833 (
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8196.722 Hz
FIDRES	0.250144 Hz
AQ	3.9977460 sec
RG	54.0541
DW	61.000 usec
DE	13.54 usec
TE	293.6 K
D1	1.00000000 sec
TD0	1
SFO1	400.1324708 MHz
NUC1	1H
P0	3.33 usec
P1	10.00 usec
SI	65536
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



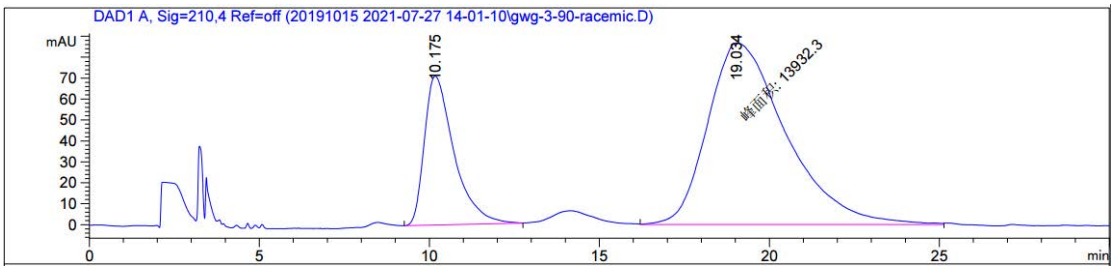
BRUKER

NAME	CNMR-gwg-4-144-3
EXPNO	1
PROCNO	1
Date_	20220215
Time	11.07 h
INSTRUM	Avance
PROBHD	Z116098_0833 (
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	150
DS	4
SWH	23809.523 Hz
FIDRES	0.726609 Hz
AQ	1.3763061 sec
RG	51.3764
DW	21.000 usec
DE	6.50 usec
TE	294.7 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
SI	32768
SF	100.6127685 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

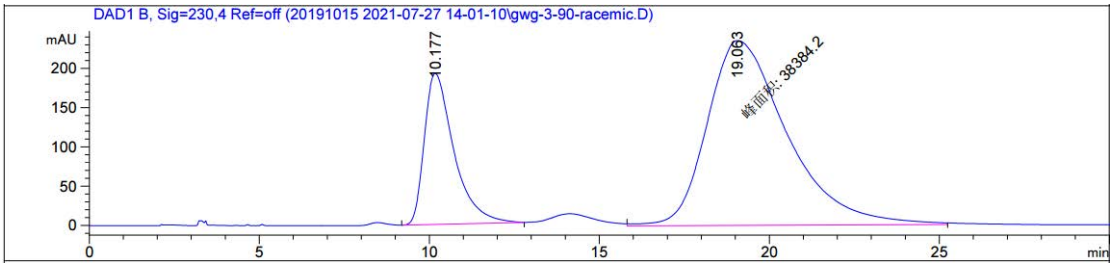


Sample Name: gwg-3-90-racemic

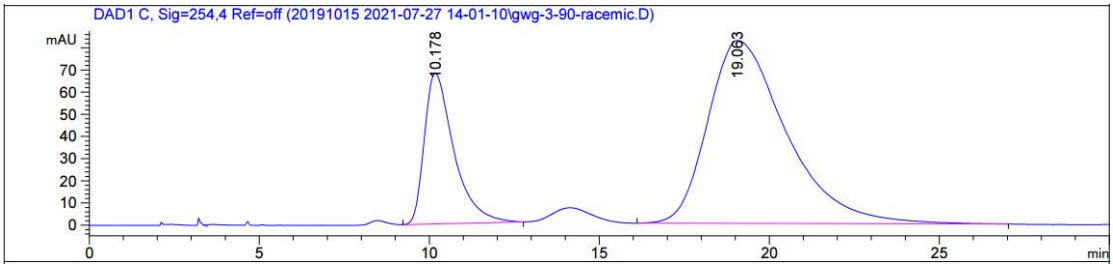
HPLC Condition: OJH, *n*-Hexane/*i*PrOH = 95:5, 1.0 mL/min



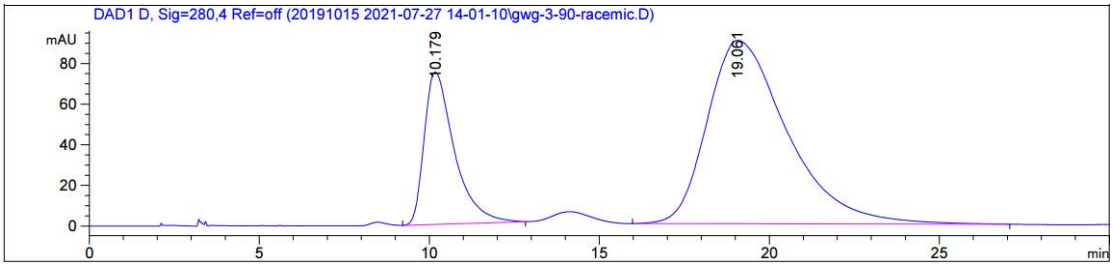
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.175	BB	0.9032	4301.76611	71.16495	23.5919
2	19.034	MM	2.6744	1.39323e4	86.82592	76.4081



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.177	BB	0.9099	1.15992e4	192.25169	23.2062
2	19.063	MM	2.7207	3.83842e4	235.13536	76.7938

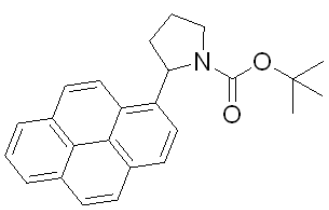


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.178	BB	0.9048	4092.76416	67.93699	23.5749
2	19.063	BB	1.9885	1.32679e4	82.48836	76.4251



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.179	BB	0.9084	4606.88037	75.02094	23.7194
2	19.061	BB	2.0542	1.48156e4	90.30022	76.2806

End of Report

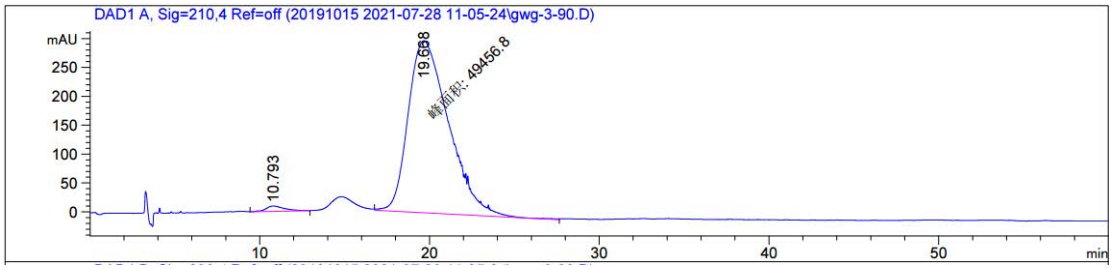


S2

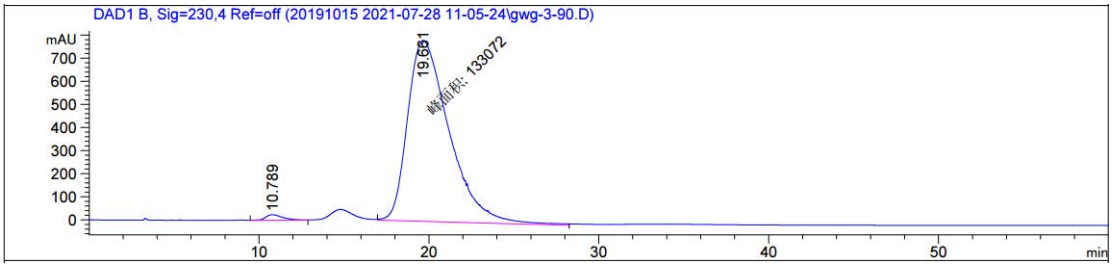
mixture of S2 and ent-S2

Sample Name: gwg-3-90 (using (+)-Sparteine as the chiral ligand)

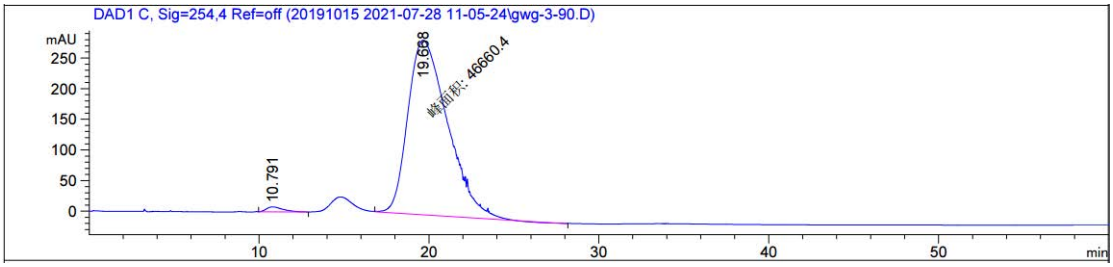
HPLC Condition: OJH, *n*-Hexane/*i*PrOH = 95:5, 1.0 mL/min



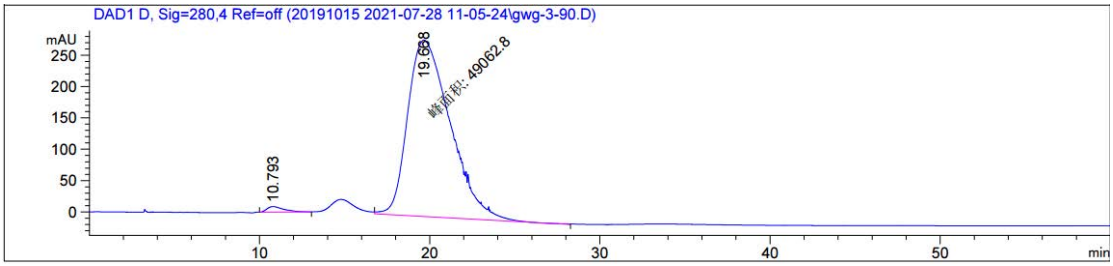
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.793	BB	0.8999	684.00684	9.15239	1.3642
2	19.668	MM	2.7659	4.94568e4	298.02026	98.6358



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.789	BB	0.9610	1642.58740	23.92318	1.2193
2	19.661	MM	2.8333	1.33072e5	782.79388	98.7807

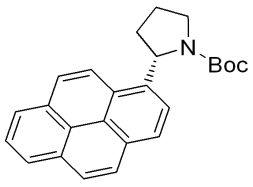


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.791	BB	0.8247	539.35315	8.05997	1.1427
2	19.668	MM	2.7263	4.66604e4	285.24786	98.8573



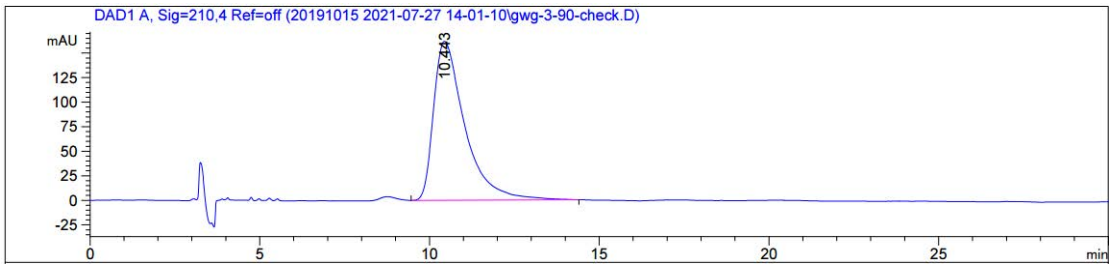
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.793	BB	0.8886	615.61188	8.97056	1.2392
2	19.668	MM	2.9064	4.90628e4	281.34576	98.7608

End of Report

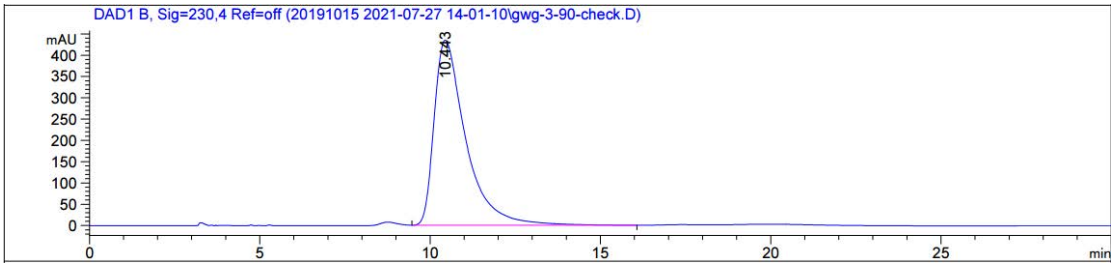


Sample Name: gwg-3-90-check ee (using (–)-Sparteine as the chiral ligand)

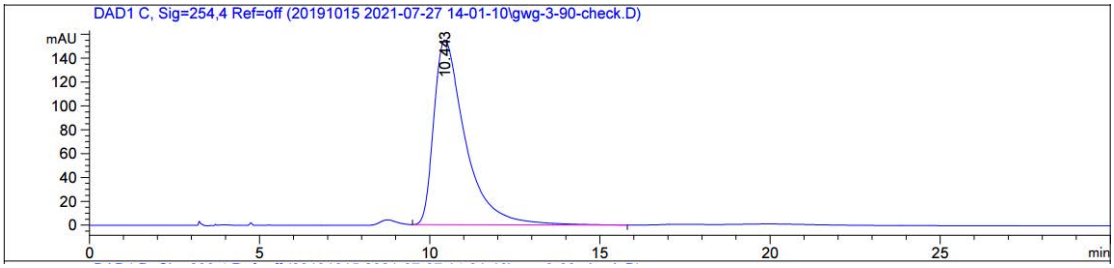
HPLC Condition: OJH, *n*-Hexane/*i*PrOH = 95:5, 1.0 mL/min



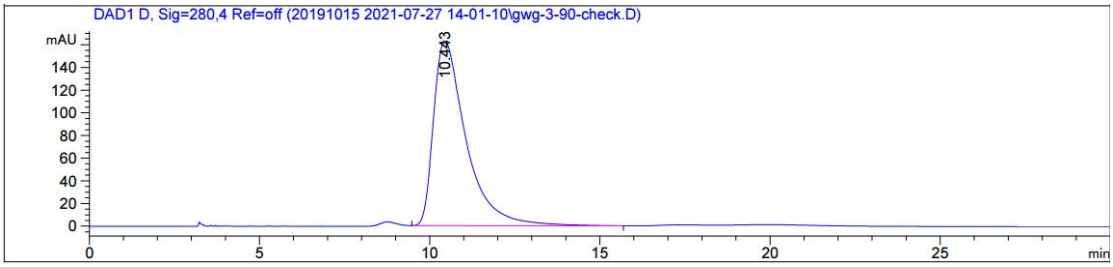
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.443	BB	0.9334	1.03471e4	161.95375	100.0000
2	--	--	--	--	--	--



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.443	BB	0.9541	2.80896e4	434.58441	100.0000
2	--	--	--	--	--	--

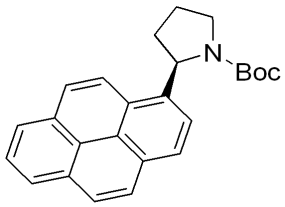


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.443	BB	0.9508	9937.71680	154.82727	100.0000
2	--	--	--	--	--	--



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.443	BB	0.9867	1.08583e4	163.09874	100.0000
2	--	--	--	--	--	--

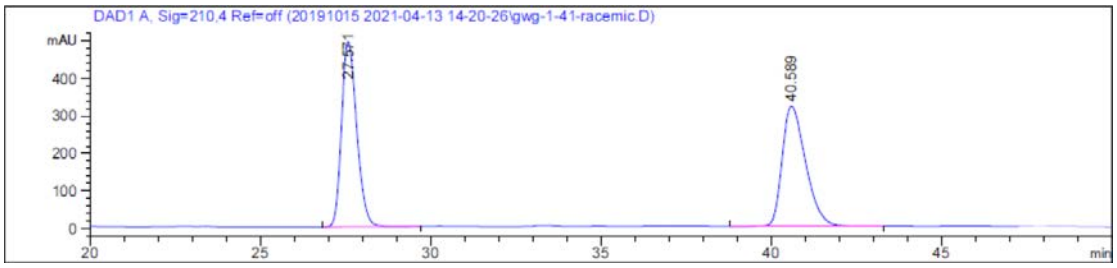
End of Report



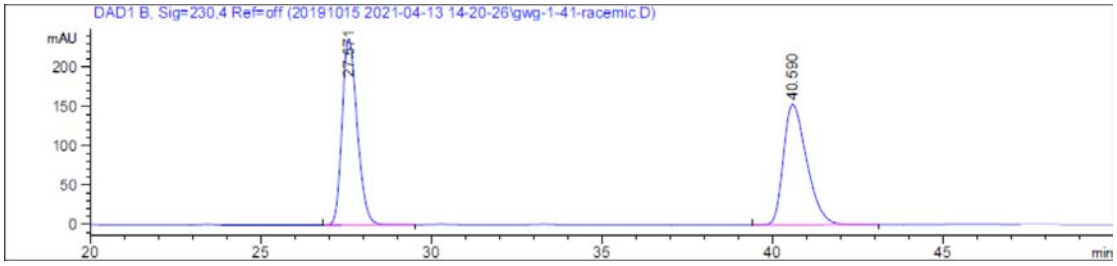
cm-S2 for checking ee

Sample Name: gwg-1-41-racemic

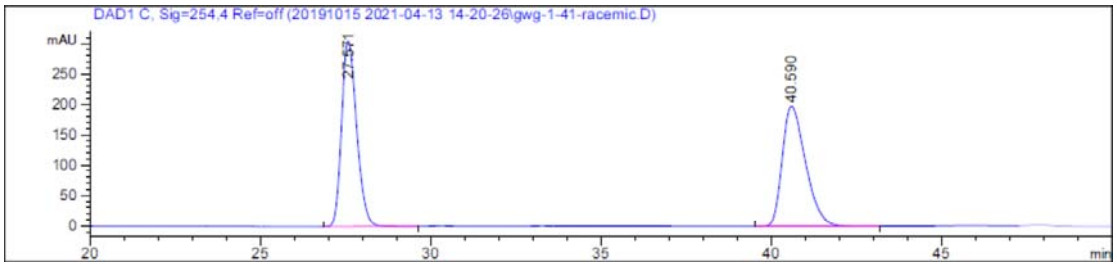
HPLC Condition: OD-H, *n*-Hexane:*i*PrOH = 99:1, 0.5 mL/min



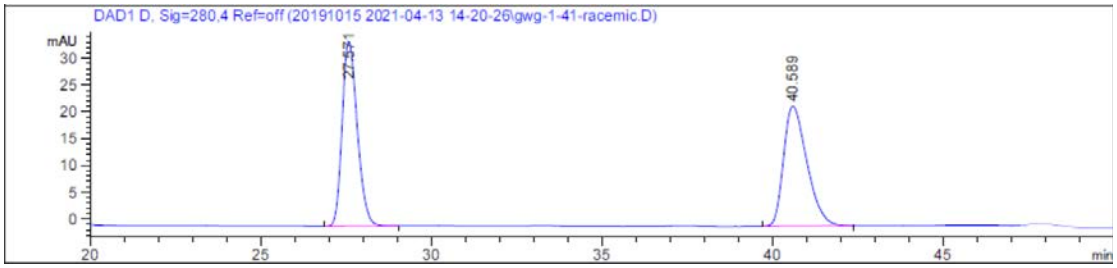
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	27.571	BB	0.4784	1.52143e4	492.54242	49.9347
2	40.589	BB	0.7369	1.52540e4	319.57141	50.0653



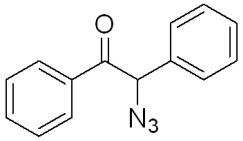
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	27.571	BB	0.4742	7267.94043	236.74677	50.0272
2	40.590	BB	0.7302	7260.03076	152.83063	49.9728



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	27.571	BB	0.4763	9382.03418	305.44919	50.0006
2	40.590	BB	0.7327	9381.79102	197.32199	49.9994



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	27.571	BB	0.4752	1062.21313	34.50259	49.9082
2	40.589	BB	0.7219	1066.12280	22.37579	50.0918

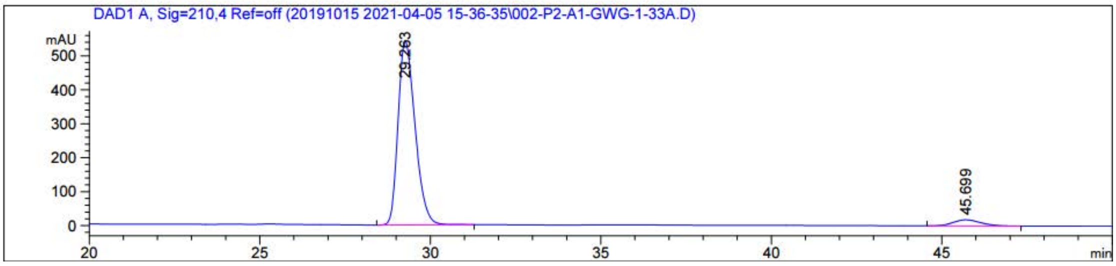


2a

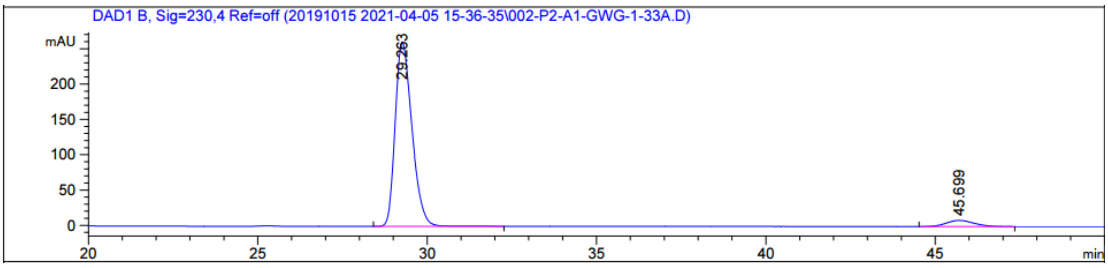
racemic

Sample Name: gwg-1-41-enantioenriched

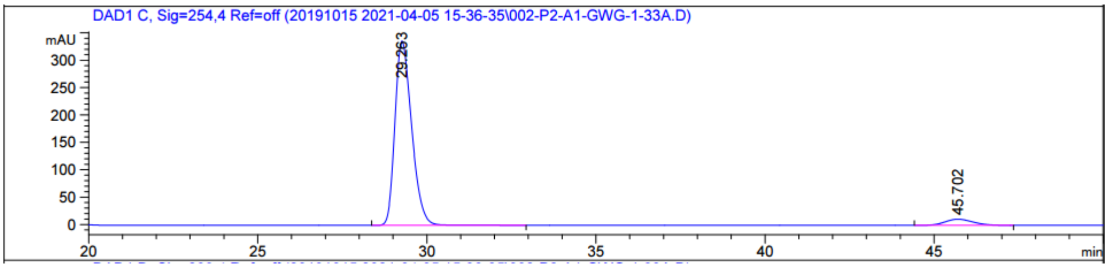
HPLC Condition: OD-H, *n*-Hexane/*i*PrOH = 99:1, 0.5 mL/min



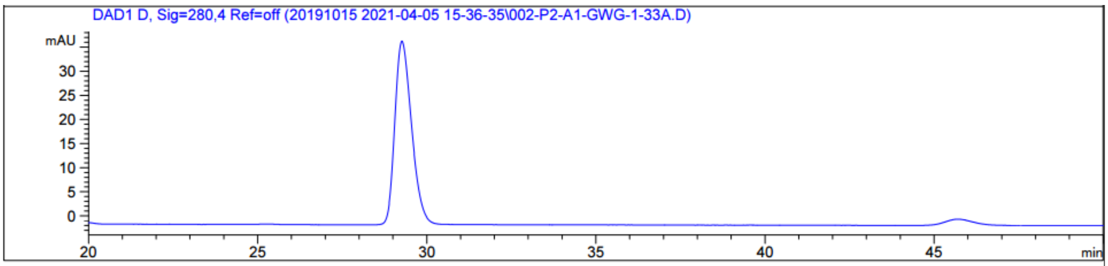
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	29.263	BB	0.5348	1.87597e4	543.32391	94.8477
2	45.699	BB	0.8245	1019.06128	17.94446	5.1523



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	29.263	BB	0.5306	8972.75391	261.28308	94.7803
2	45.699	BB	0.8246	494.14722	8.64814	5.2197



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	29.263	BB	0.5309	1.15658e4	336.59842	94.7581
2	45.702	BB	0.8248	639.80573	11.16127	5.2419



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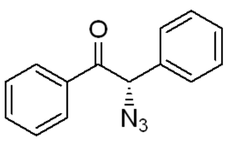
End of report

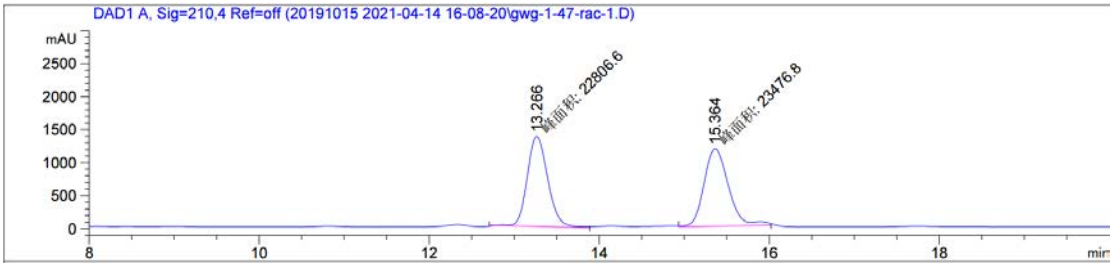


2a

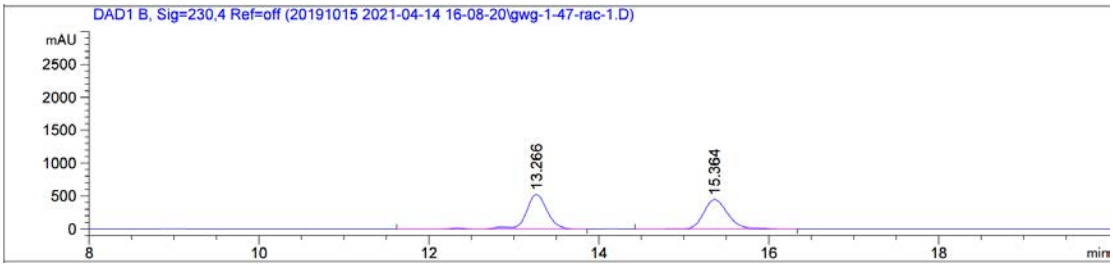
enantioenriched

Sample Name: gwg-1-47-racemic

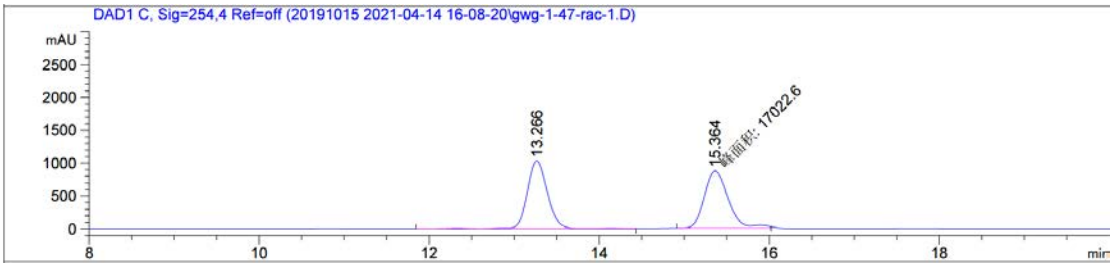
HPLC Condition: IC, *n*-Hexane/*i*PrOH = 97/3, 1.0 mL/min



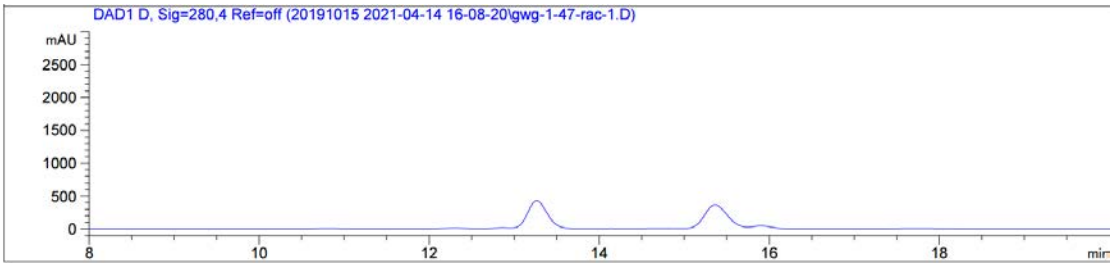
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.266	MM	0.2784	2.28066e4	1365.44788	49.2761
2	15.364	MM	0.3332	2.34768e4	1174.31628	50.7239



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.266	VB R	0.2526	9109.55859	523.79852	50.6746
2	15.364	BB	0.3052	8867.00977	447.42209	49.3254



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.266	VV R	0.2515	1.71665e4	1031.35742	50.2105
2	15.364	MM	0.3265	1.70226e4	868.92230	49.7895



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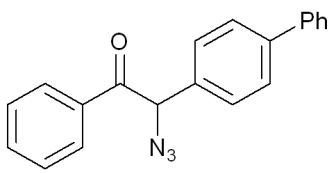
End of Report

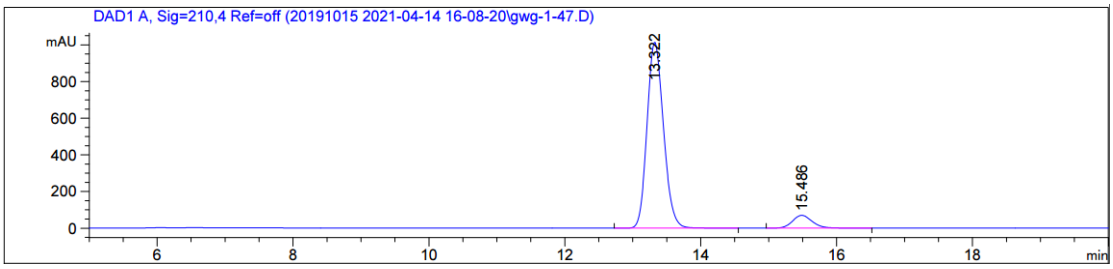


2b

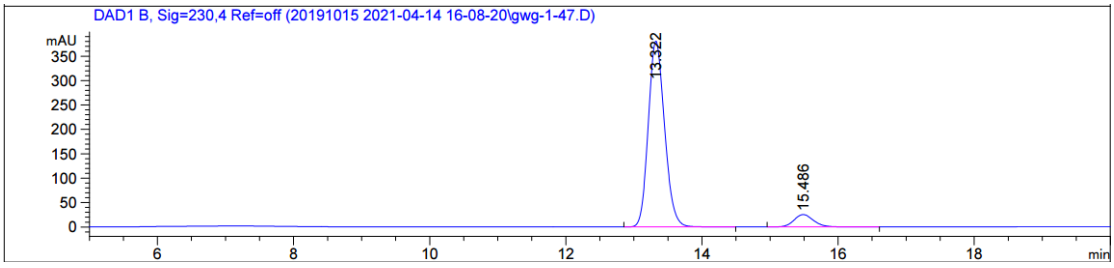
racemic

Sample Name: gwg-1-47-enantioenriched

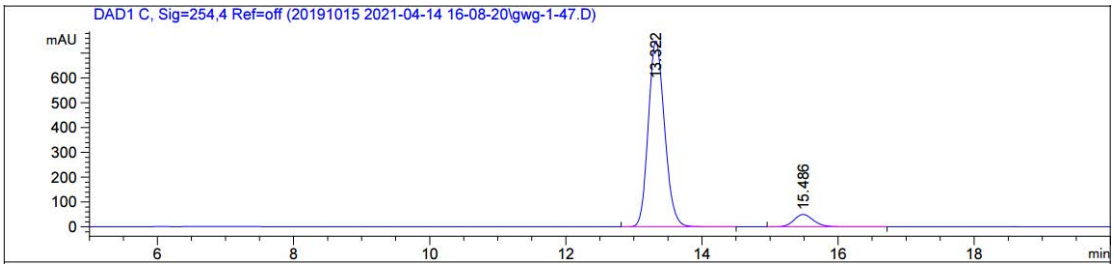
HPLC Condition: IC, *n*-Hexane/*i*PrOH = 97:3, 1.0 mL/min



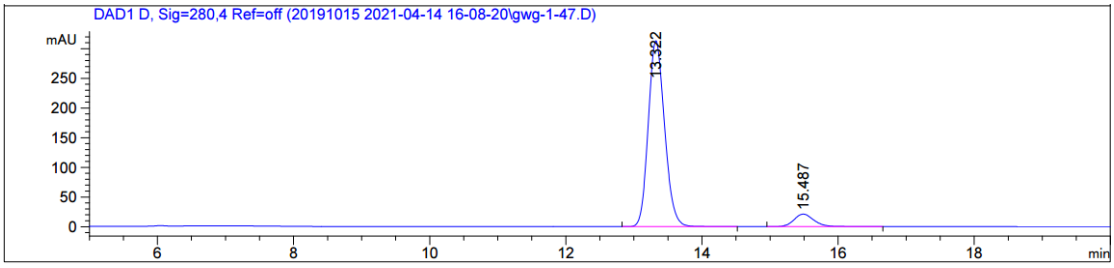
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.322	BB	0.2599	1.70318e4	1014.15057	92.4095
2	15.486	BB	0.3102	1398.98914	69.70102	7.5905



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.322	BB	0.2578	6324.69775	380.80521	92.6128
2	15.486	BB	0.3088	504.48703	25.28175	7.3872

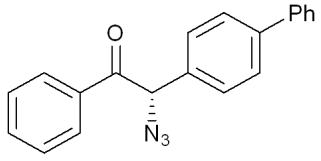


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.322	BB	0.2575	1.24294e4	749.45618	92.6018
2	15.486	BB	0.3078	993.01617	49.55843	7.3982



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.322	BB	0.2581	5214.35596	313.35446	92.4075
2	15.487	BB	0.3134	428.42780	21.05302	7.5925

End of Report

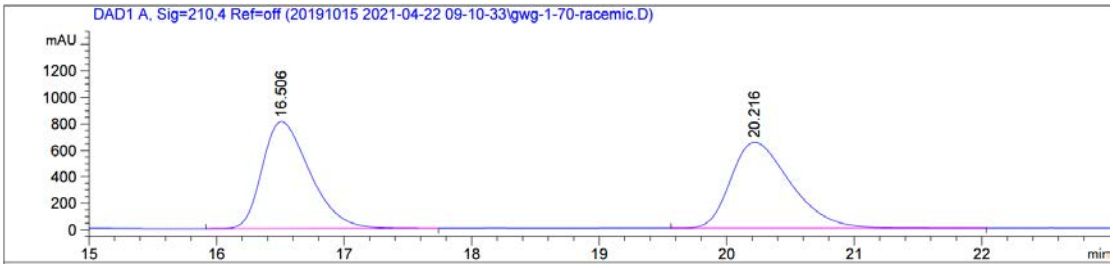


2b

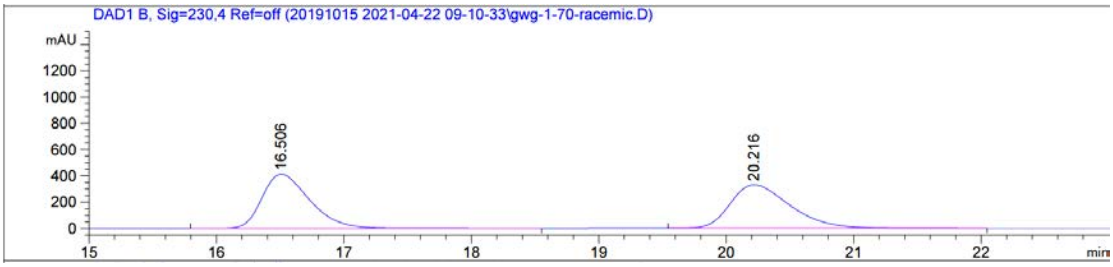
enantioenriched

Sample Name: gwg-1-70-racemic

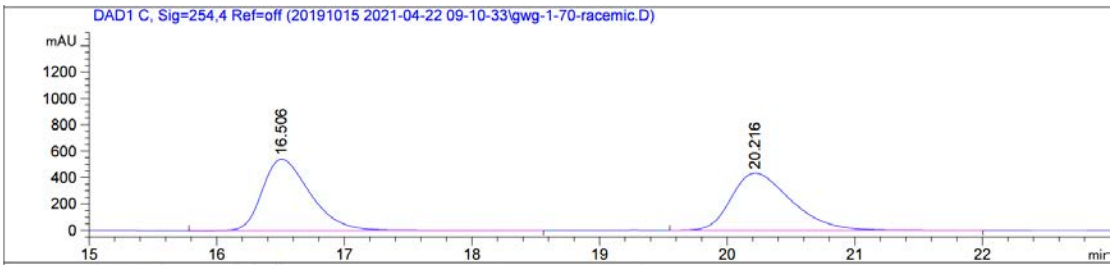
HPLC Condition: ODH, *n*-Hexane/*i*PrOH = 97:3, 1.0 mL/min



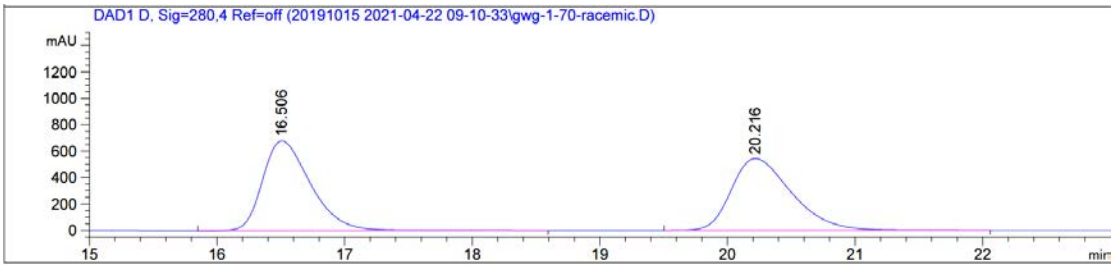
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.506	BB	0.3981	2.09364e4	808.45325	49.7208
2	20.216	BB	0.5028	2.11715e4	648.70923	50.2792



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.506	BB	0.3980	1.06764e4	412.46991	49.8799
2	20.216	BB	0.4991	1.07278e4	330.13751	50.1201

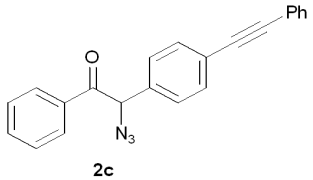


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.506	BB	0.3974	1.39574e4	540.32098	49.9010
2	20.216	BB	0.4981	1.40128e4	432.35681	50.0990



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.506	BB	0.3977	1.75513e4	678.67181	49.8416
2	20.216	BB	0.4990	1.76628e4	543.69885	50.1584

End of Report

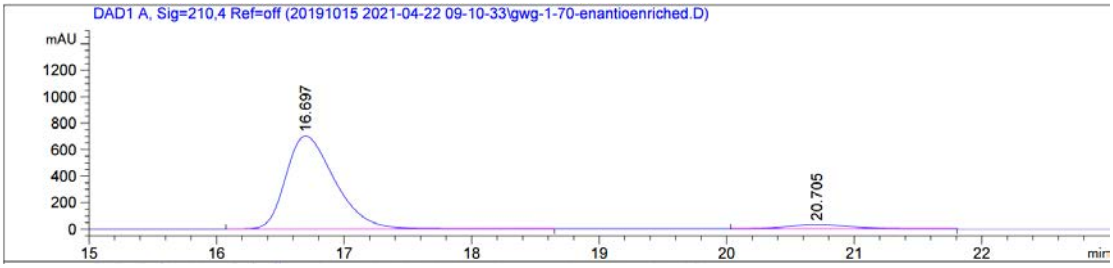


2c

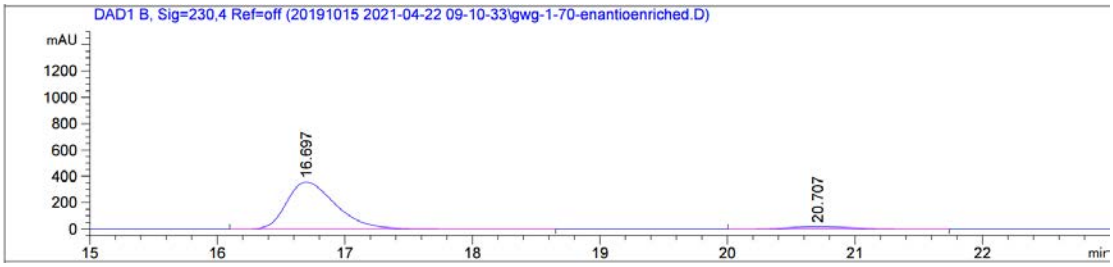
racemic

Sample Name: gwg-1-70-enantioenriched

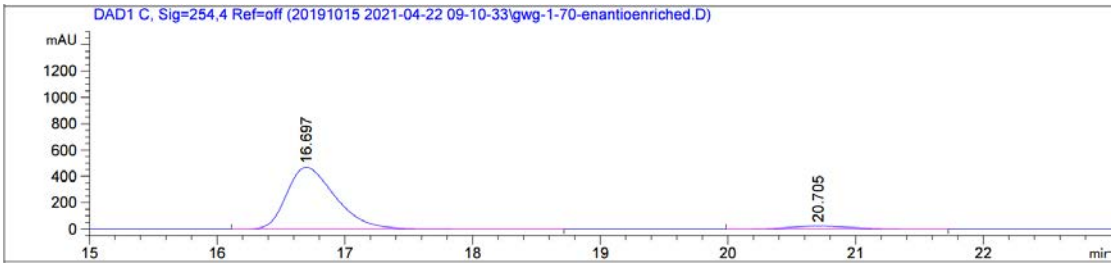
HPLC Condition: ODH, *n*-Hexane/*i*PrOH = 97:3, 1.0 mL/min



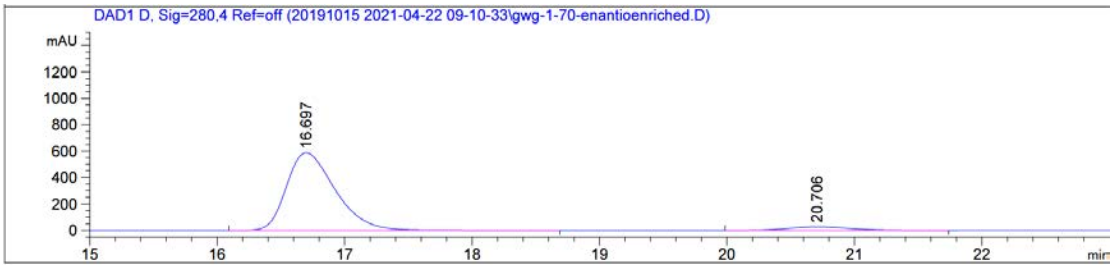
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.697	BB	0.4101	1.86602e4	701.98755	94.7017
2	20.705	BB	0.4988	1043.98413	32.32163	5.2983



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.697	BB	0.4072	9466.77734	357.16183	94.7803
2	20.707	BB	0.4906	521.34979	16.23601	5.2197

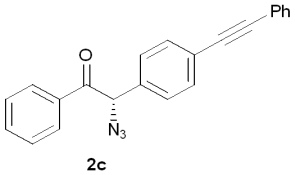


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.697	BB	0.4067	1.23817e4	467.91214	94.7920
2	20.705	BB	0.4991	680.26526	21.16079	5.2080



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.697	BB	0.4070	1.55784e4	588.23163	94.7855
2	20.706	BB	0.5009	857.02344	26.66719	5.2145

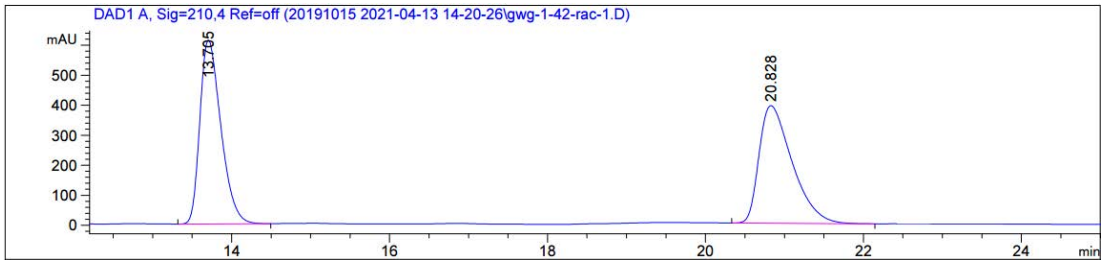
End of Report



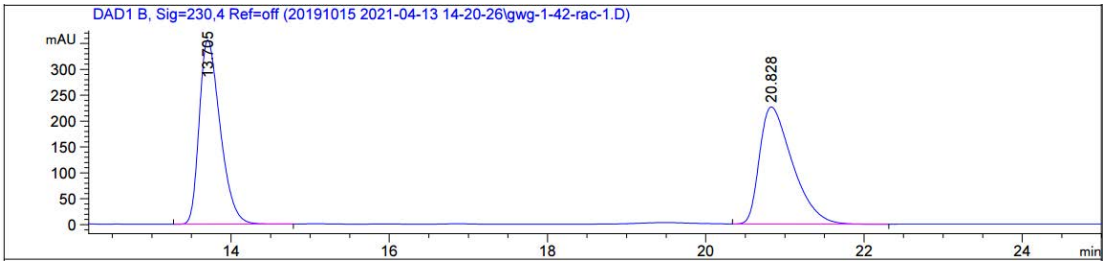
2c
enantioenriched

Sample Name: gwg-1-42-racemic

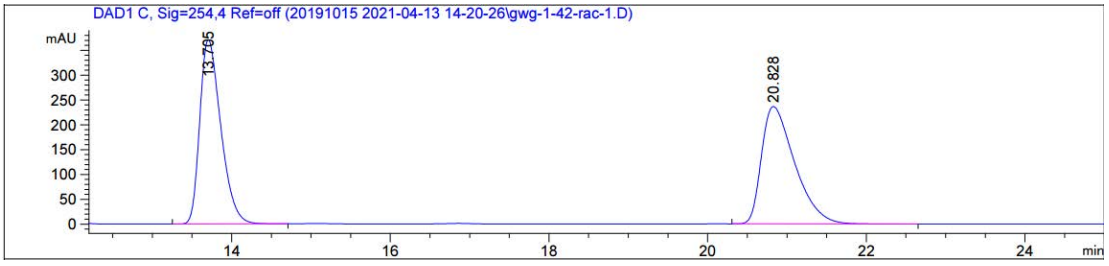
HPLC condition: OD-H, *n*-Hexane/*i*PrOH = 99:1, 1.0 mL/min



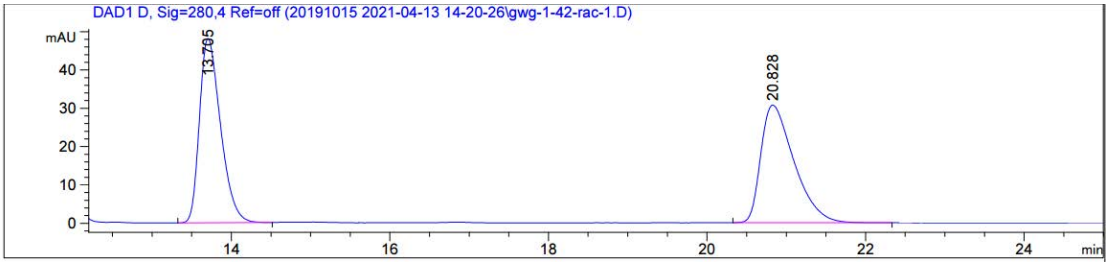
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.705	BB	0.2855	1.13173e4	612.70325	49.8690
2	20.828	BB	0.4409	1.13767e4	391.62283	50.1310



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.705	BB	0.2826	6552.40527	356.17844	50.0262
2	20.828	BB	0.4397	6545.55371	226.14812	49.9738

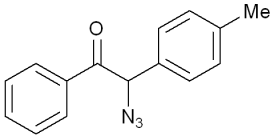


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.705	BB	0.2827	6828.00000	371.04672	49.8981
2	20.828	BB	0.4424	6855.89795	236.37073	50.1019



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.705	BB	0.2827	6828.00000	371.04672	49.8981
2	20.828	BB	0.4424	6855.89795	236.37073	50.1019

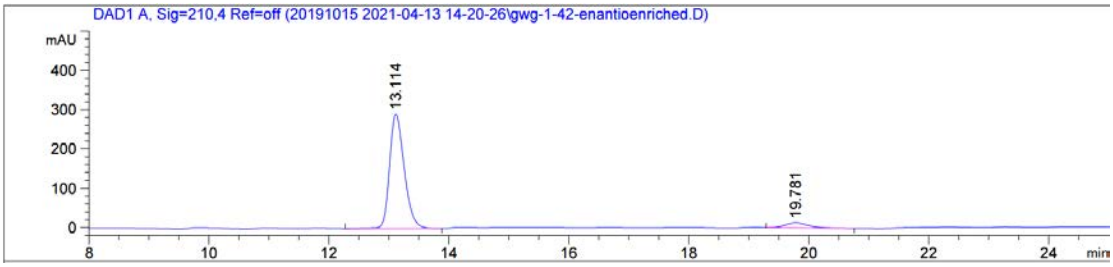
End of Report



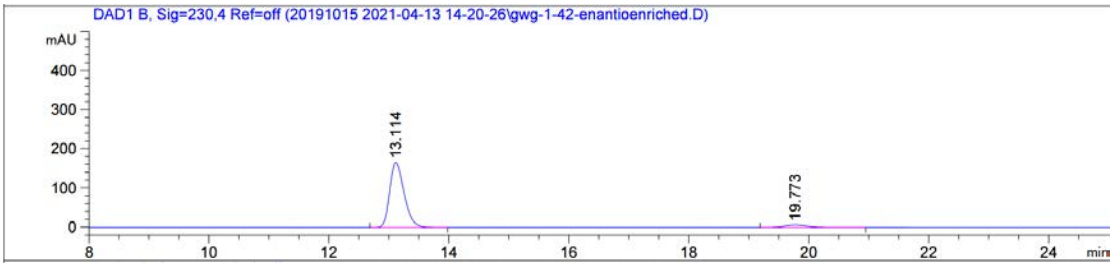
2d
racemic

Sample Name: gwg-1-42-enantioenriched

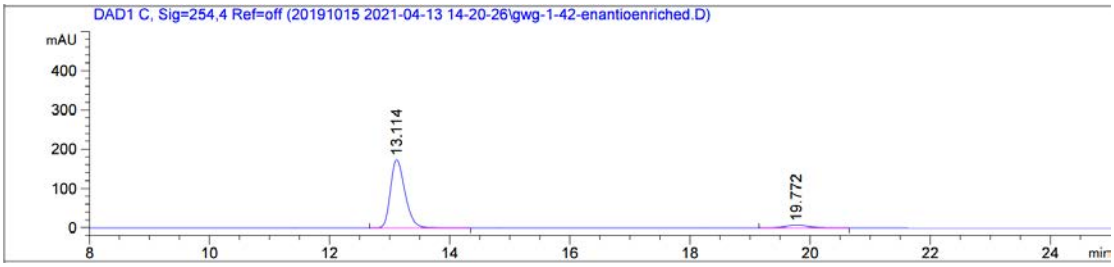
HPLC Condition: OD-H, *n*-Hexane/*i*PrOH = 99:1, 1.0 mL/min



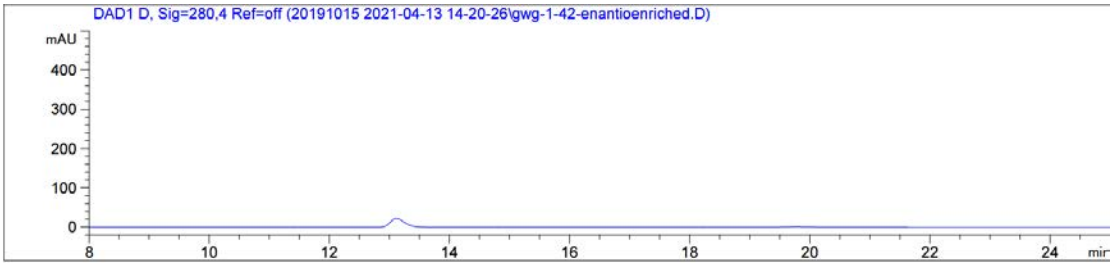
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.114	BB	0.2595	4925.44873	290.97800	93.7527
2	19.781	BB	0.3901	328.21225	12.75865	6.2473



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.114	BB	0.2568	2779.88892	166.45003	93.9195
2	19.773	BB	0.3936	179.97446	7.00917	6.0805



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.114	BB	0.2572	2913.18262	174.11984	93.9621
2	19.772	BB	0.3965	187.19635	7.31652	6.0379



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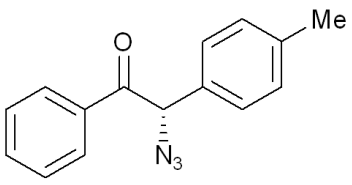
End of Report

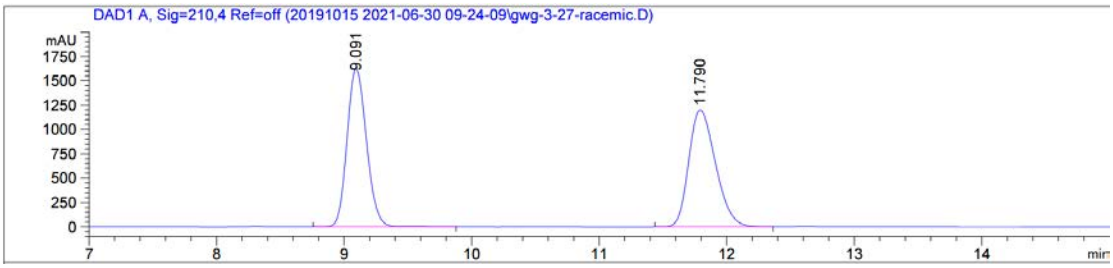


2d

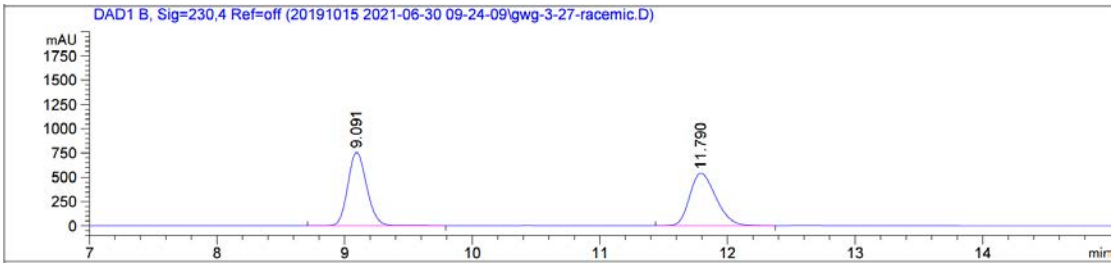
enantioenriched

Sample Name: gwg-3-27-racemic

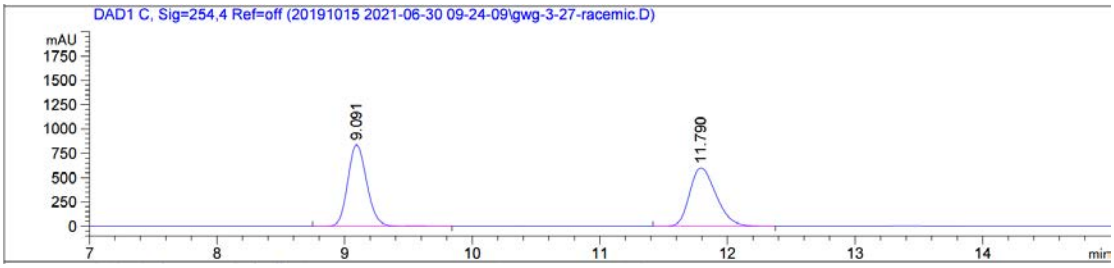
HPLC Condition: IC, *n*-Hexane/*i*PrOH = 98:2, 1.0 mL/min



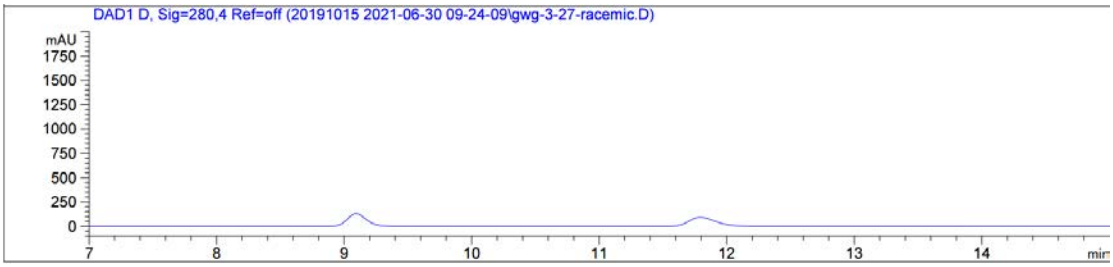
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.091	BV R	0.1653	1.72059e4	1623.42700	49.5919
2	11.790	BB	0.2259	1.74891e4	1200.97192	50.4081



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.091	BV R	0.1596	7779.95410	757.57751	50.0978
2	11.790	BB	0.2228	7749.58936	541.94916	49.9022



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.091	BV R	0.1600	8640.17285	837.97394	50.0711
2	11.790	BB	0.2231	8615.62891	601.35620	49.9289



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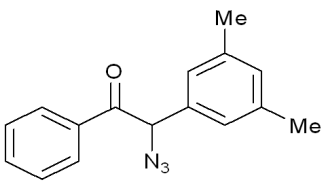
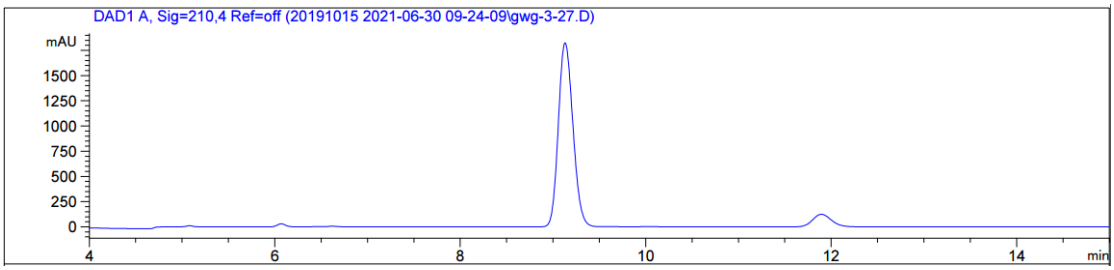
End of Report

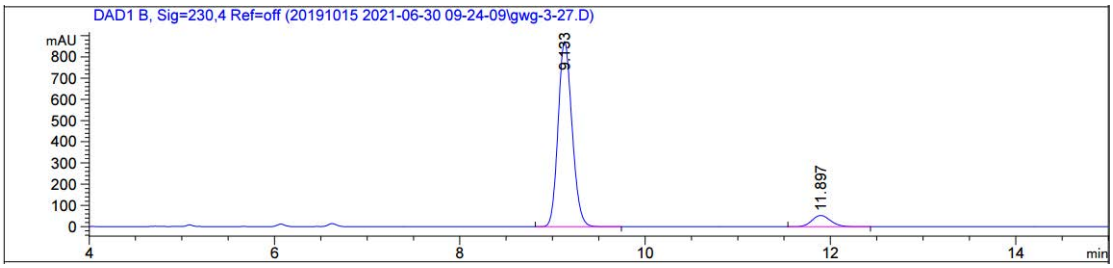


2e
racemic

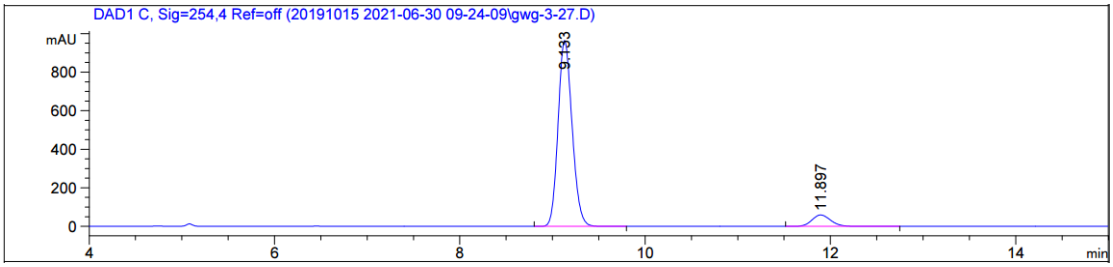
Sample Name: gwg-3-27-enantioenriched

HPLC Condition: IC, *n*-Hexane/*i*PrOH = 98:2, 1.0 mL/min

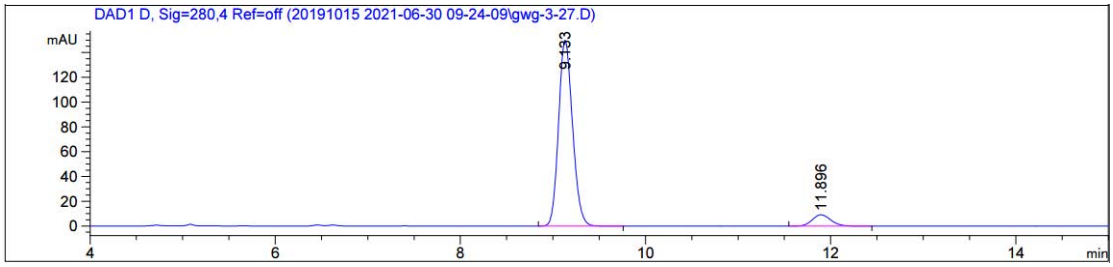




Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.133	BB	0.1623	9151.08398	873.17218	92.4898
2	11.897	BB	0.2174	743.06964	53.04055	7.5102



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.133	BB	0.1628	1.01523e4	964.74243	92.4236
2	11.897	BB	0.2178	832.22565	59.27462	7.5764



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.133	BB	0.1625	1575.54138	150.00868	92.4455
2	11.896	BB	0.2178	128.75119	9.17229	7.5545

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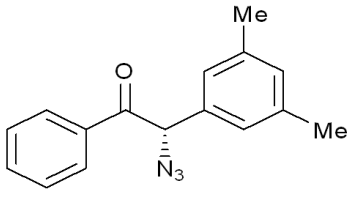
End of Report

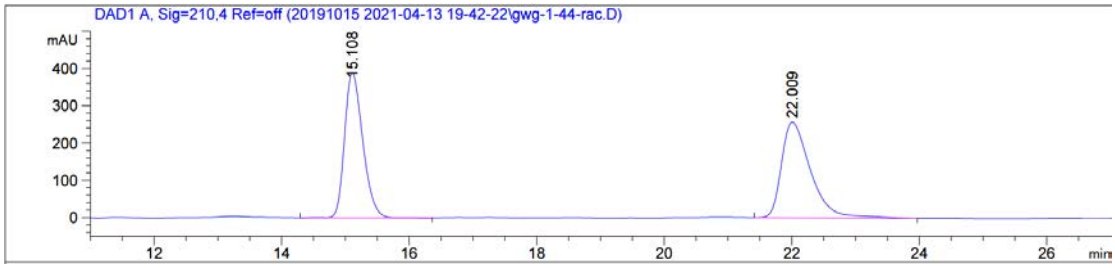


2e

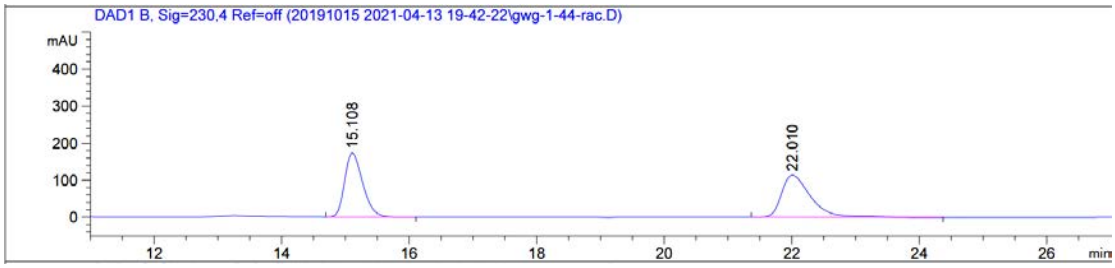
enantioenriched

Sample Name: gwg-1-44-racemic

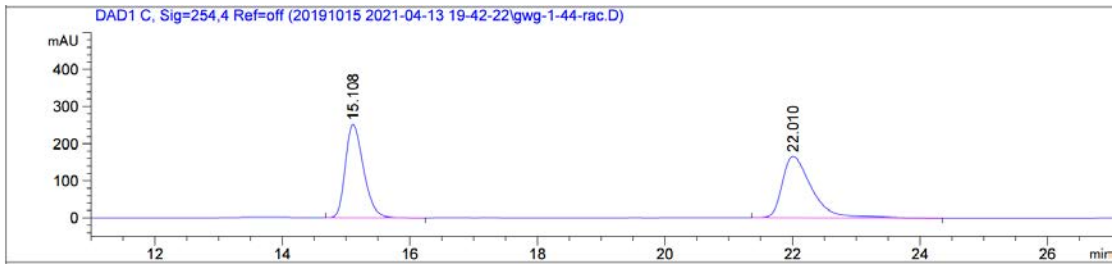
HPLC Condition: ODH, *n*-Hexane/*i*PrOH = 99:1, 1.0 mL/min



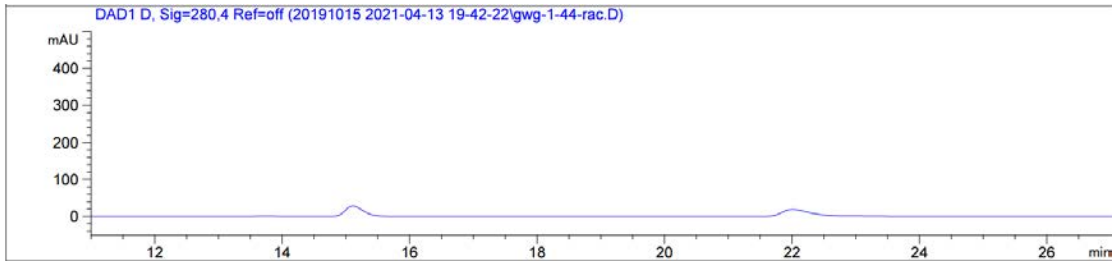
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	15.108	BB	0.3047	7692.92529	389.07913	48.8497
2	22.009	BB	0.4771	8055.23828	256.00125	51.1503



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	15.108	BB	0.3034	3395.94946	172.68091	48.5985
2	22.010	BB	0.4790	3591.82056	113.54807	51.4015



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	15.108	BB	0.3039	4955.11670	251.47105	48.5262
2	22.010	BB	0.4809	5256.09717	165.32623	51.4738



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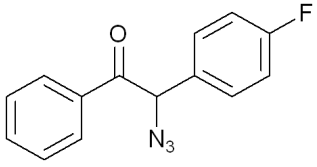
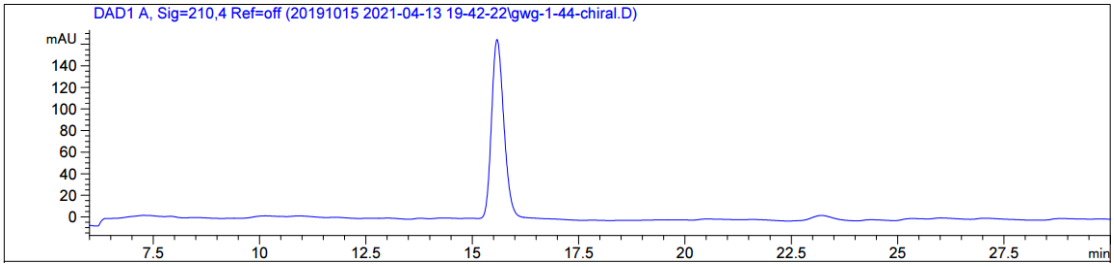
End of Report

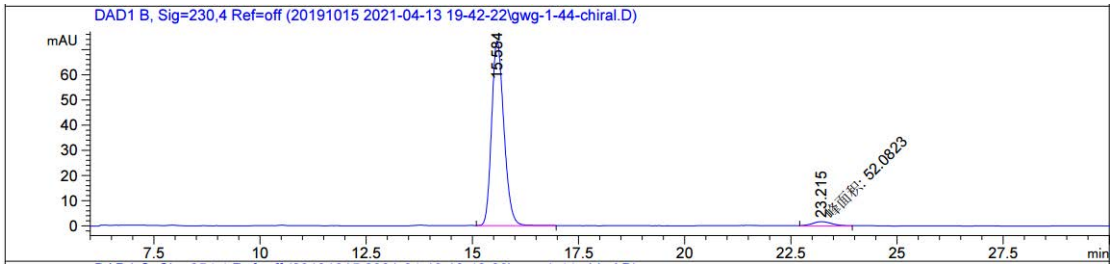


2f
racemic

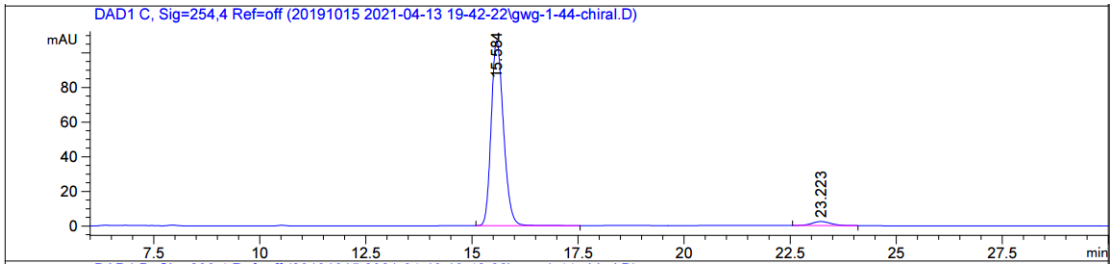
Sample Name: gwg-1-44-enantioenriched

HPLC Condition: ODH, *n*-Hexane/*i*PrOH = 99:1, 1.0 mL/min

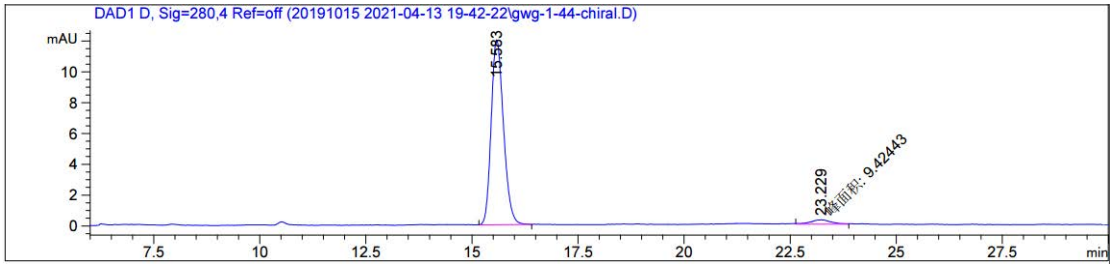




Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	15.584	BB	0.3108	1475.24658	73.30584	96.5900
2	23.215	MM	0.5249	52.08226	1.65381	3.4100



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	15.584	BB	0.3132	2151.47949	106.71661	96.8492
2	23.223	BB	0.4387	69.99355	2.28908	3.1508



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	15.583	BB	0.3125	241.19707	11.99922	96.2396
2	23.229	MM	0.5680	9.42443	2.76542e-1	3.7604

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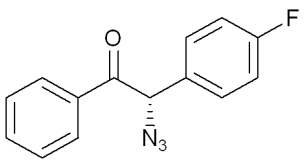
End of Report

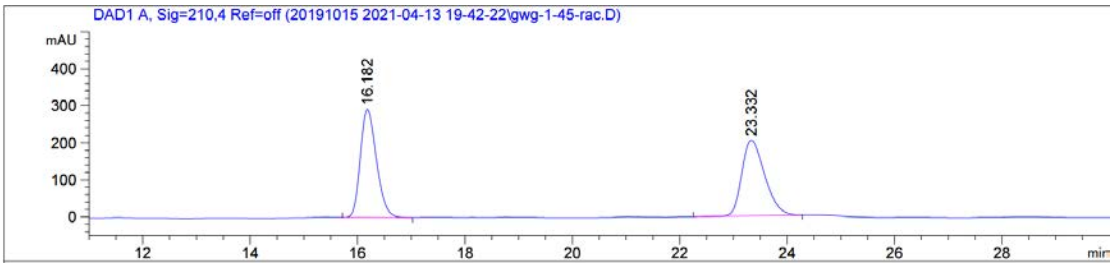


2f

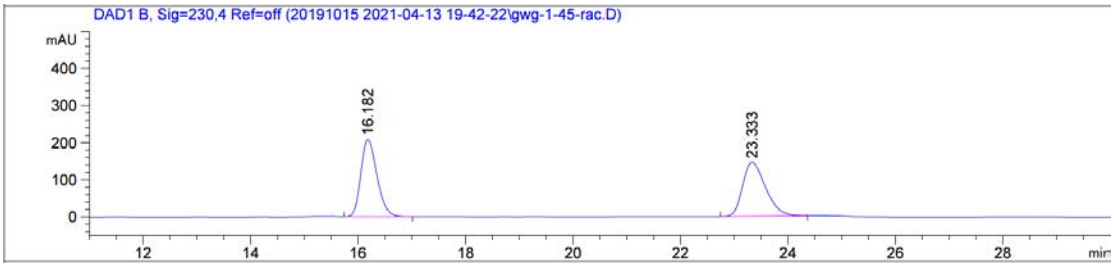
enantioenriched

Sample Name: gwg-1-45-racemic

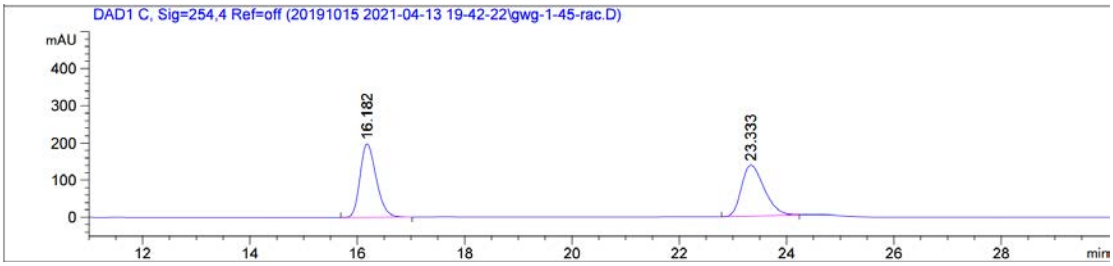
HPLC Condition: ODH, *n*-Hexane/*i*PrOH = 99:1, 1.0 mL/min



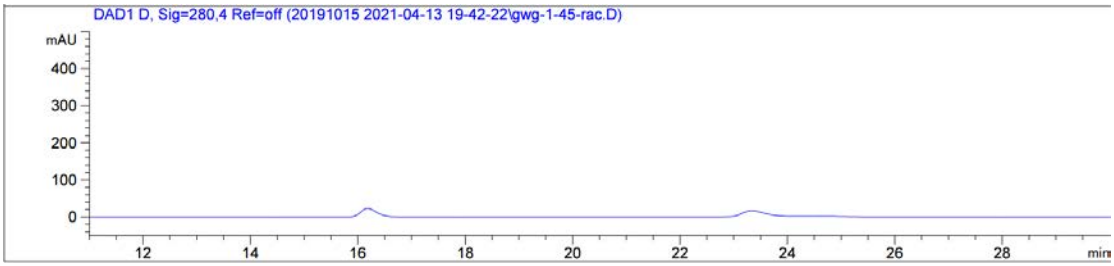
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.182	BB	0.3238	6108.70459	292.34091	50.1951
2	23.332	BB	0.4562	6061.22217	204.27145	49.8049



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.182	BB	0.3208	4325.56348	207.86732	50.2204
2	23.333	BB	0.4570	4287.60254	144.97192	49.7796



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.182	BB	0.3216	4122.50684	197.40228	50.6515
2	23.333	BB	0.4526	4016.45874	136.77499	49.3485



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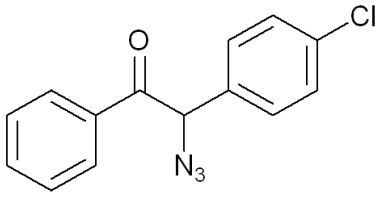
End of Report

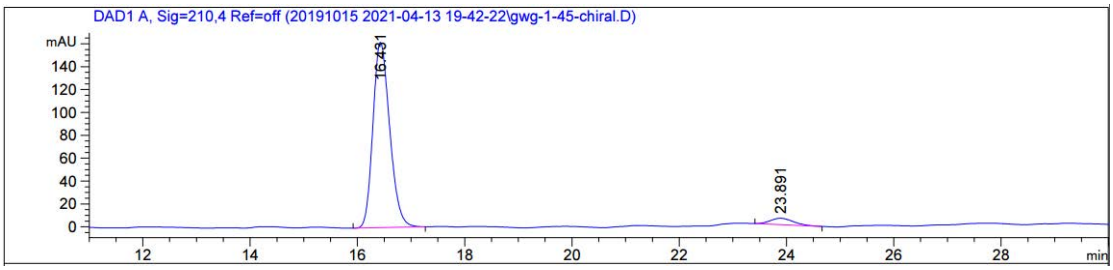


2g

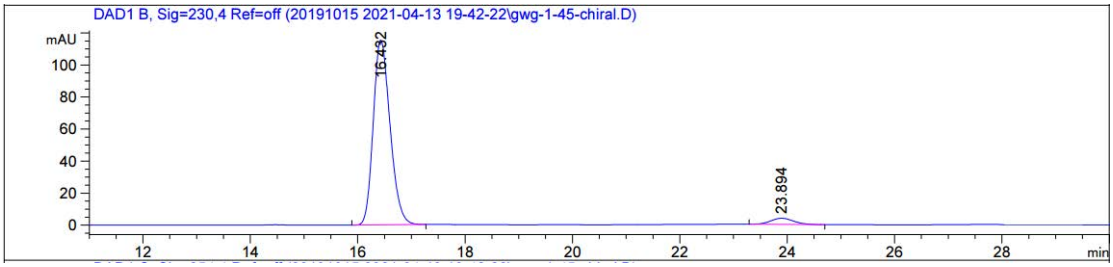
racemic

Sample Name: gwg-1-45-enantioenriched

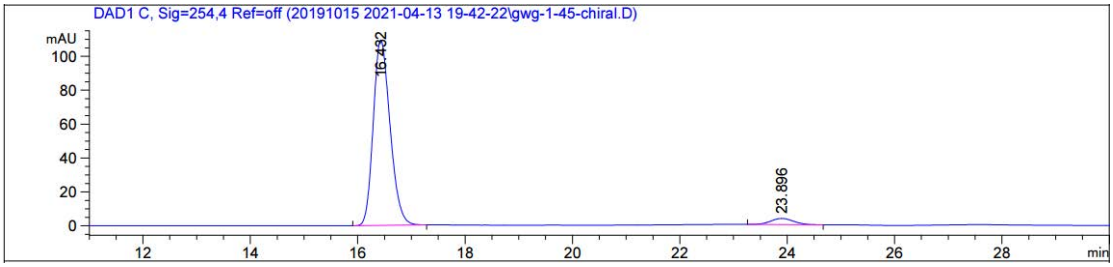
HPLC Condition: ODH, *n*-Hexane/*i*PrOH = 99:1, 1.0 mL/min



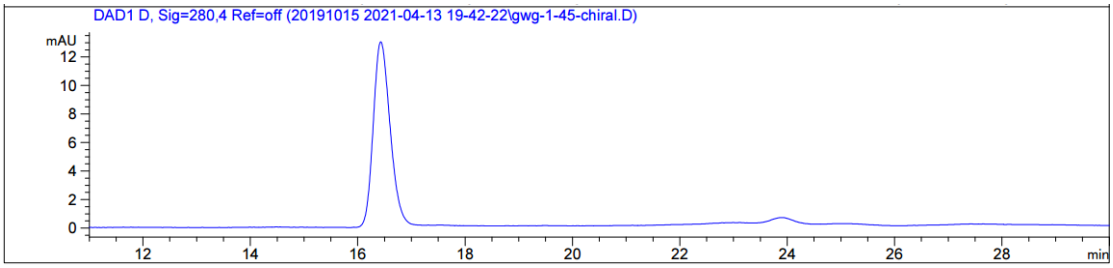
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.431	BB	0.3375	3521.53052	162.07024	95.4833
2	23.891	BB	0.4517	166.58087	5.58906	4.5167



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.432	BB	0.3377	2510.08228	115.43481	95.7134
2	23.894	BB	0.4391	112.41541	3.82309	4.2866



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.432	BB	0.3378	2381.09204	109.43916	95.7777
2	23.896	BB	0.4439	104.96941	3.60300	4.2223



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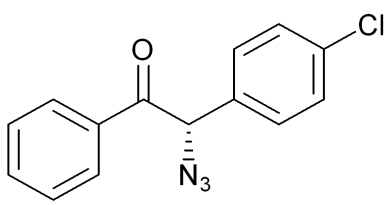
End of Report

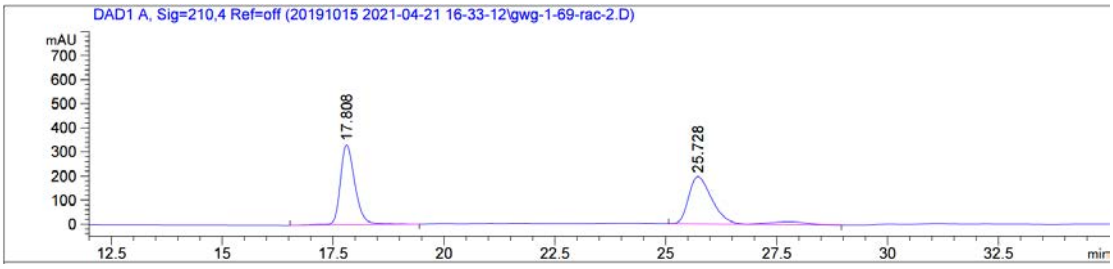


2g

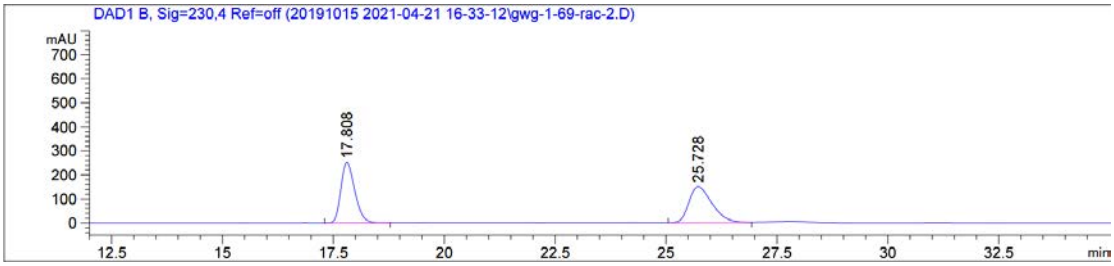
enantioenriched

Sample Name: gwg-1-69-racemic

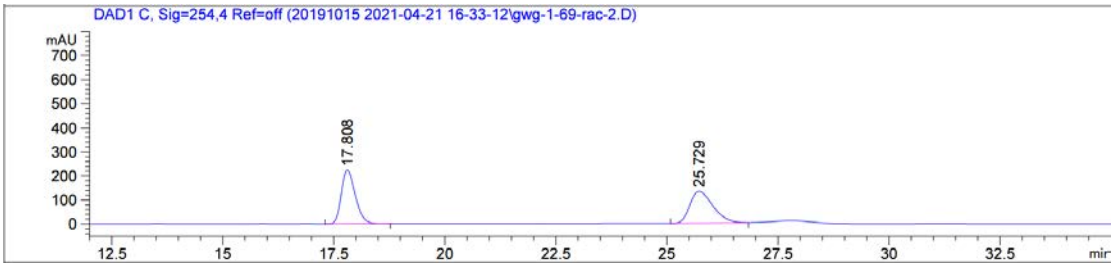
HPLC Condition: ODH, *n*-Hexane/*i*PrOH = 99:1, 1.0 mL/min



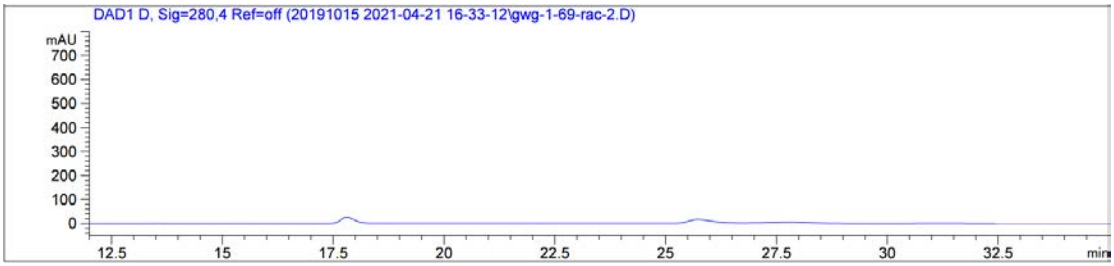
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	17.808	BB	0.3544	7696.07617	332.11020	49.6066
2	25.728	BV R	0.5586	7818.13721	195.73138	50.3934



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	17.808	BB	0.3389	5478.79736	250.78078	50.4163
2	25.728	BB	0.5571	5388.31396	149.29057	49.5837



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	17.808	BB	0.3391	4899.62891	224.07776	50.5858
2	25.729	BB	0.5553	4786.15576	133.16766	49.4142



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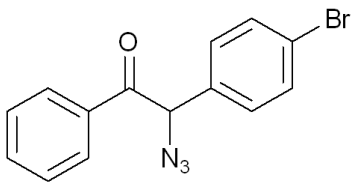
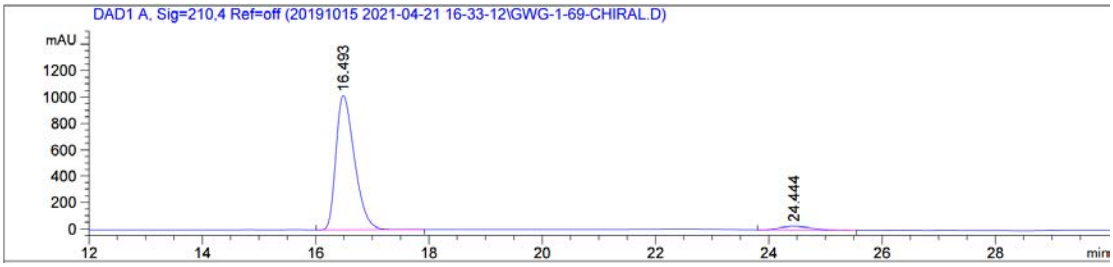
End of Report



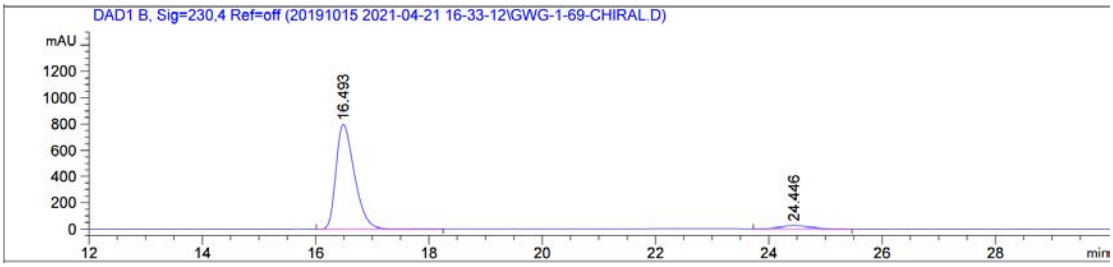
2h
racemic

Sample Name: gwg-1-69-enantioenriched

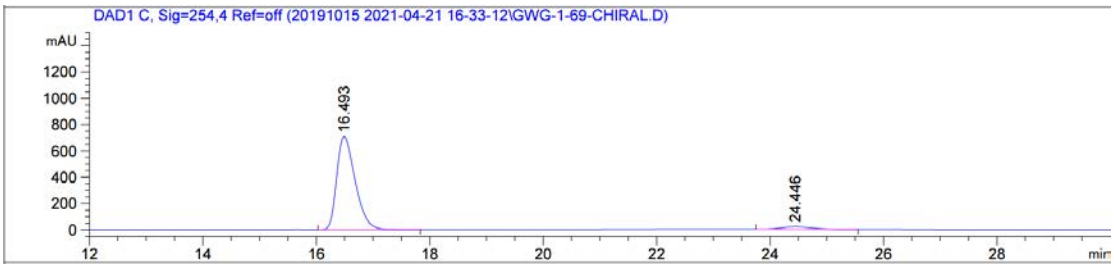
HPLC Condition: ODH, *n*-Hexane/*i*PrOH = 99:1, 1.0 mL/min



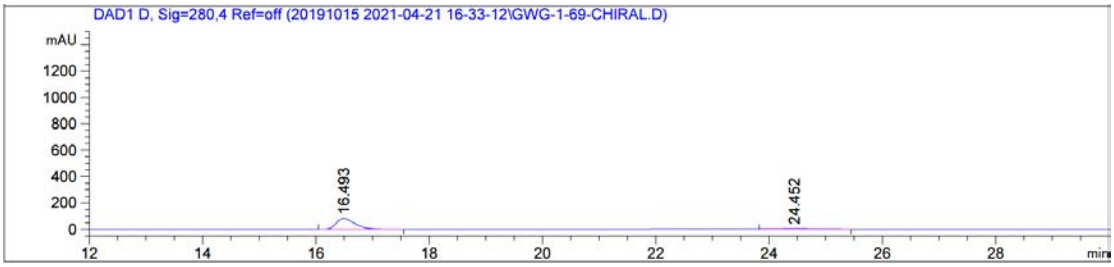
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.493	BB	0.3512	2.31659e4	1019.07037	95.5994
2	24.444	BB	0.5730	1066.35999	28.86527	4.4006



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.493	BB	0.3472	1.79595e4	796.10510	95.5967
2	24.446	BB	0.5739	827.24628	22.44786	4.4033

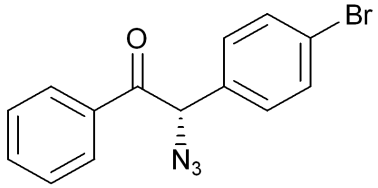


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.493	BB	0.3474	1.60041e4	708.77216	95.5521
2	24.446	BB	0.5756	744.98035	20.13910	4.4479



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.493	BB	0.3508	1852.25269	81.60120	95.4108
2	24.452	BB	0.5267	89.09206	2.36912	4.5892

End of Report

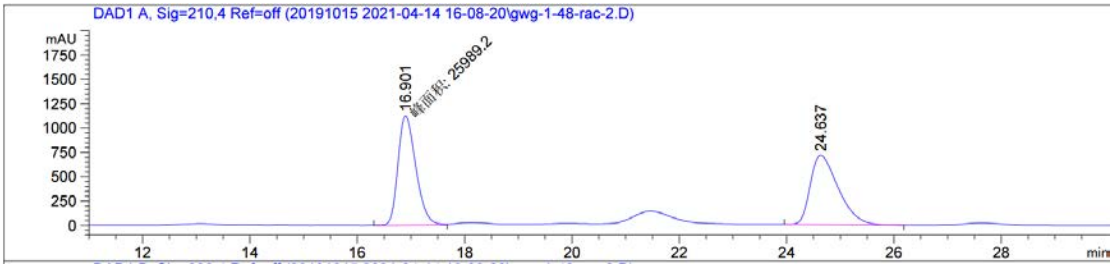


2h

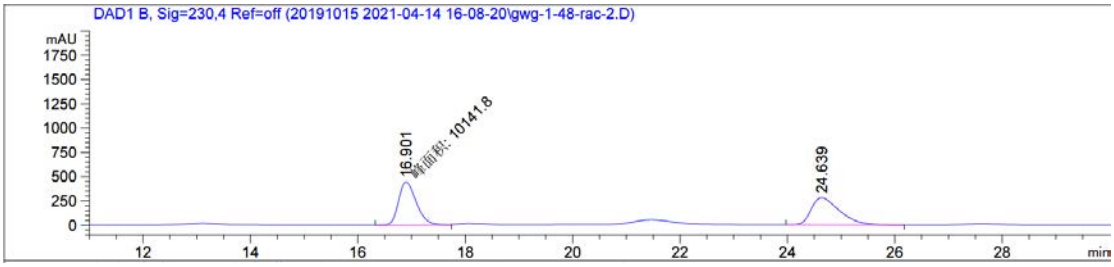
S-262 enantioenriched

Sample Name: gwg-1-48-racemic

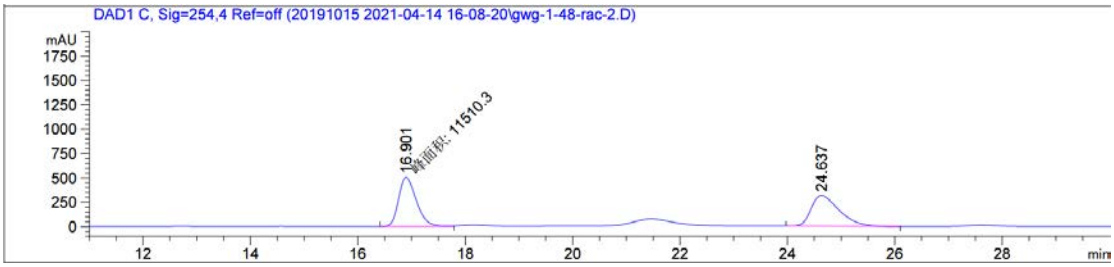
HPLC Condition: ODH, *n*-Hexane/*i*PrOH = 99:1, 1.0 mL/min



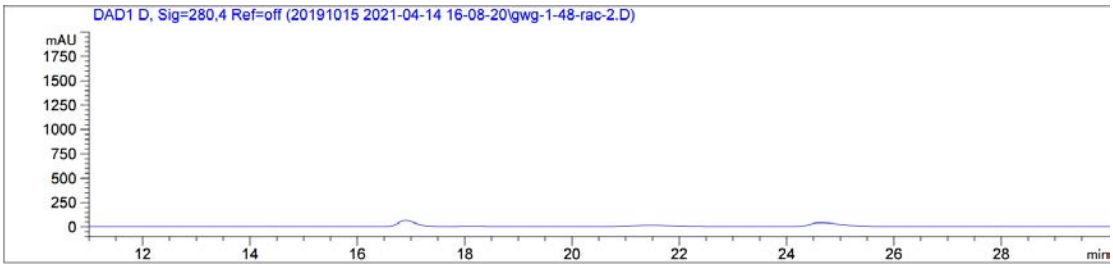
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.901	MM	0.3848	2.59892e4	1125.60767	50.2913
2	24.637	BB	0.5557	2.56882e4	710.64301	49.7087



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.901	MM	0.3802	1.01418e4	444.53177	50.0810
2	24.639	BB	0.5570	1.01090e4	277.48788	49.9190



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.901	MM	0.3810	1.15103e4	503.56229	50.5229
2	24.637	BB	0.5507	1.12720e4	314.09879	49.4771



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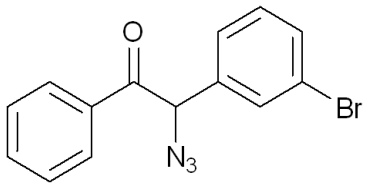
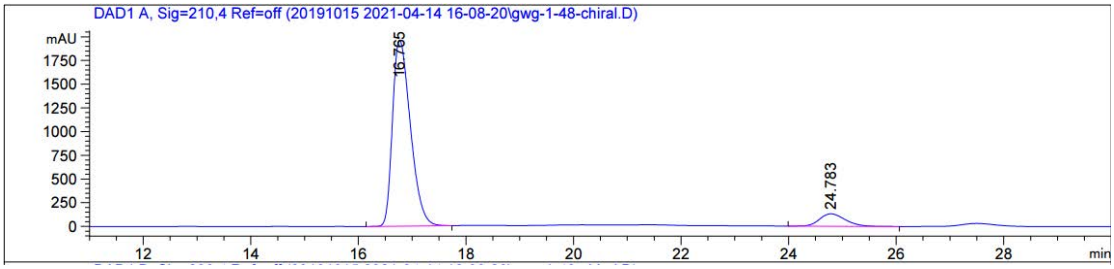
End of Report



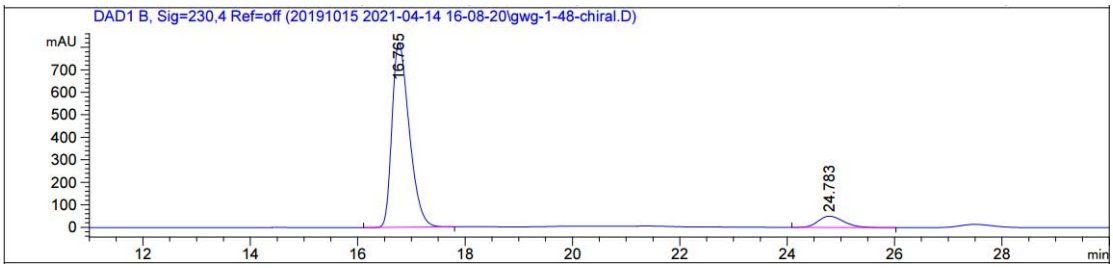
2i
racemic

Sample Name: gwg-1-48-enantioenriched

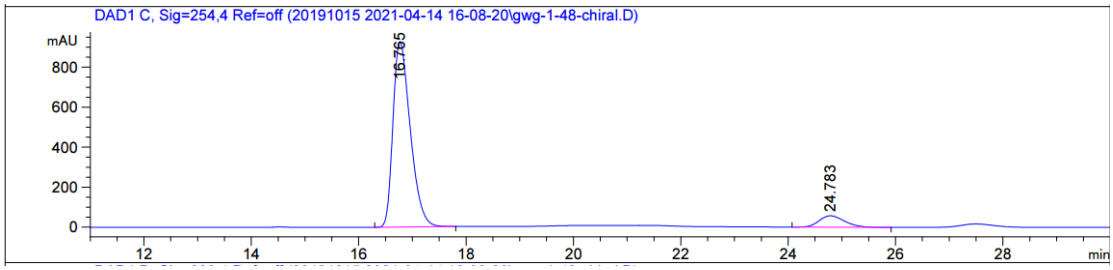
HPLC Condition: ODH, *n*-Hexane/*i*PrOH = 99:1, 1.0 mL/min



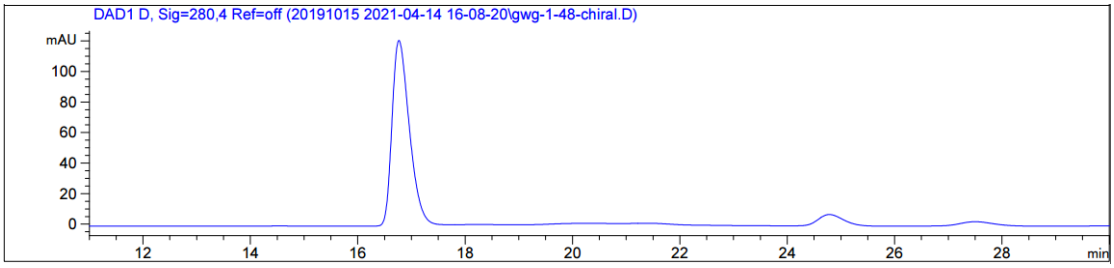
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.765	BB	0.3596	4.53575e4	1962.81848	91.2625
2	24.783	BB	0.5149	4342.53906	130.93690	8.7375



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.765	BB	0.3440	1.83041e4	821.47205	91.7526
2	24.783	BB	0.5095	1645.30847	50.05591	8.2474



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.765	BB	0.3446	2.07164e4	927.45416	91.7391
2	24.783	BB	0.5105	1865.46594	56.89314	8.2609



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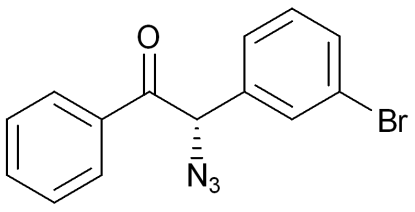
End of Report

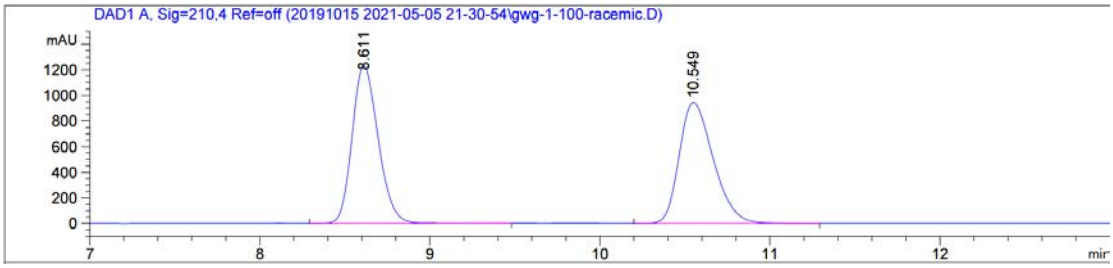


2i

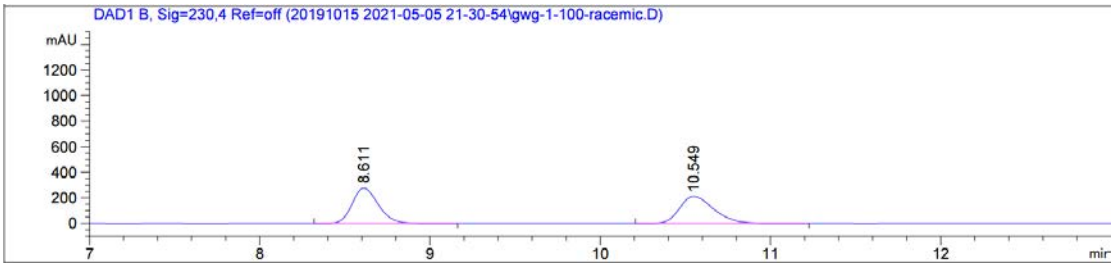
enantioenriched

Sample Name: gwg-1-100-racemic

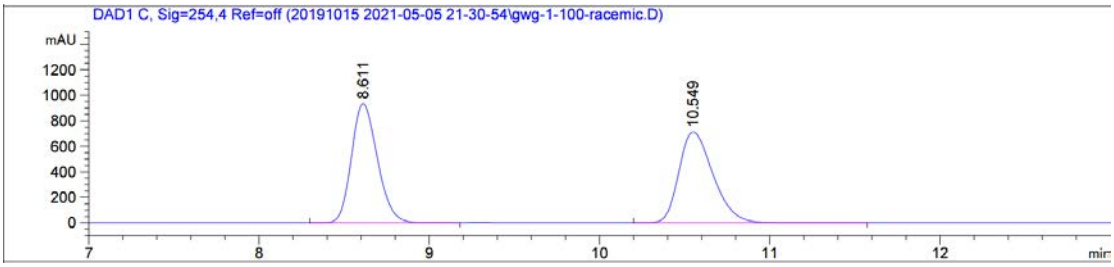
HPLC Condition: ODH, *n*-Hexane/*i*PrOH = 97:3, 1.0 mL/min



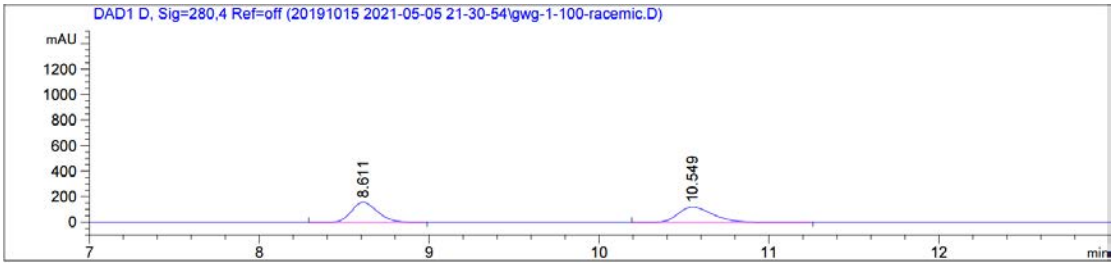
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	8.611	BV R	0.1662	1.31242e4	1231.74316	49.9860
2	10.549	BB	0.2162	1.31315e4	944.38702	50.0140



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	8.611	BB	0.1654	2928.03125	276.73859	49.9673
2	10.549	BB	0.2159	2931.86011	211.23080	50.0327

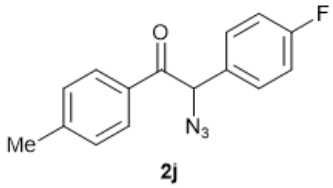


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	8.611	BB	0.1653	9886.88770	935.62610	49.9634
2	10.549	BB	0.2158	9901.36621	714.15643	50.0366



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	8.611	BB	0.1653	1637.08777	154.89624	49.8418
2	10.549	BB	0.2162	1647.47949	118.48223	50.1582

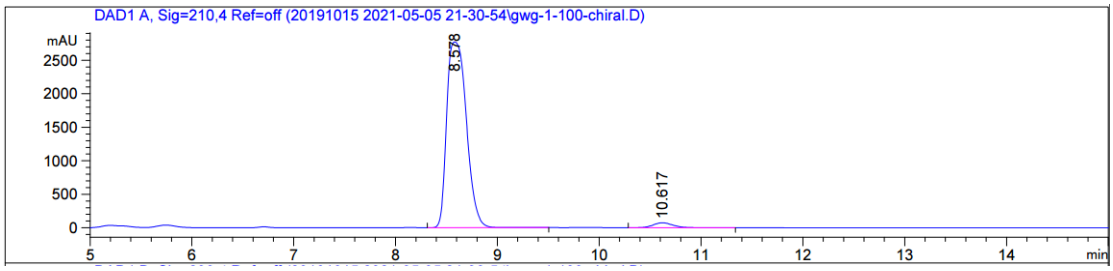
End of Report



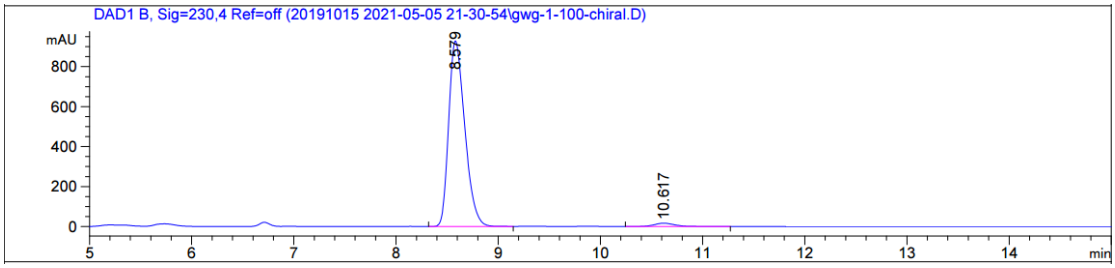
2j
racemic

Sample Name: gwg-1-100-enantioenriched

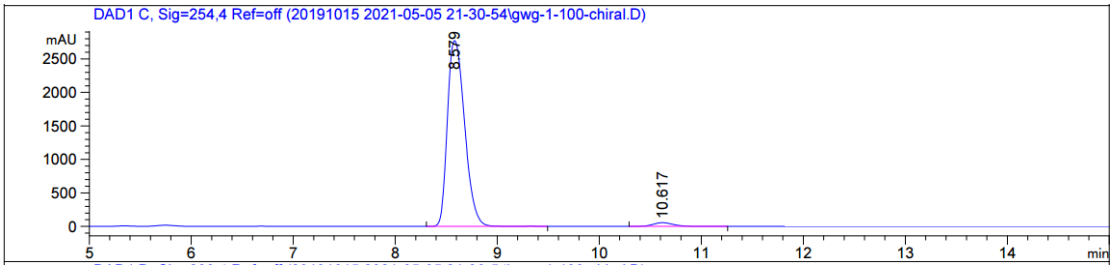
HPLC Condition: ODH, *n*-Hexane/*i*PrOH = 97:3, 1.0 mL/min



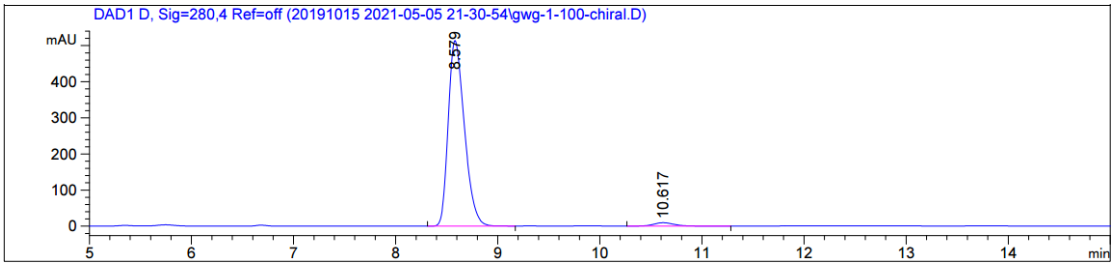
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	8.578	BV R	0.2141	3.71387e4	2773.76392	97.4015
2	10.617	BB	0.2106	990.78931	72.87672	2.5985



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	8.579	BB	0.1675	1.01611e4	929.60577	97.8416
2	10.617	BB	0.2107	224.15475	16.27779	2.1584

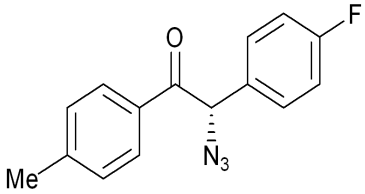


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	8.579	BV R	0.1846	3.24921e4	2774.04077	97.7591
2	10.617	BB	0.2086	744.81122	54.79323	2.2409



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	8.579	BB	0.1681	5650.28760	514.55536	97.8252
2	10.617	BB	0.2115	125.61207	9.18944	2.1748

End of Report

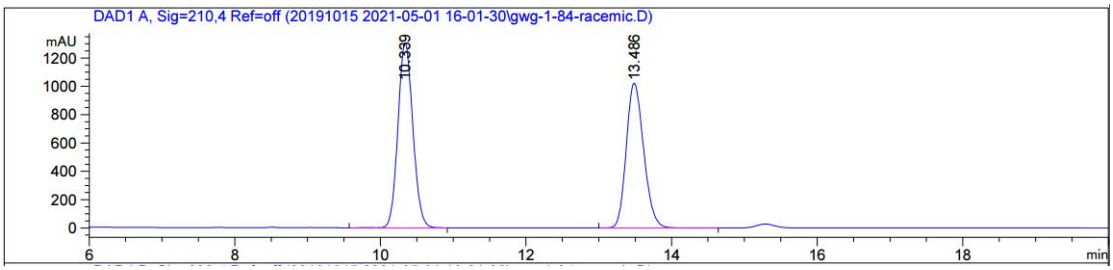


2j

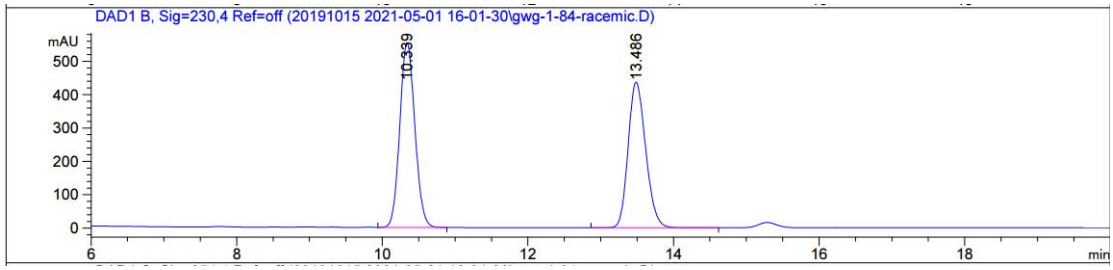
enantioenriched

Sample Name: gwg-1-84-racemic

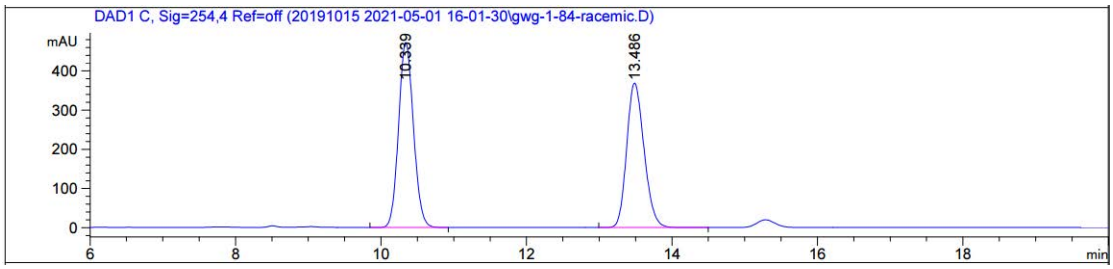
HPLC Condition: IC, *n*-Hexane/*i*PrOH = 90:10, 1.0 mL/min



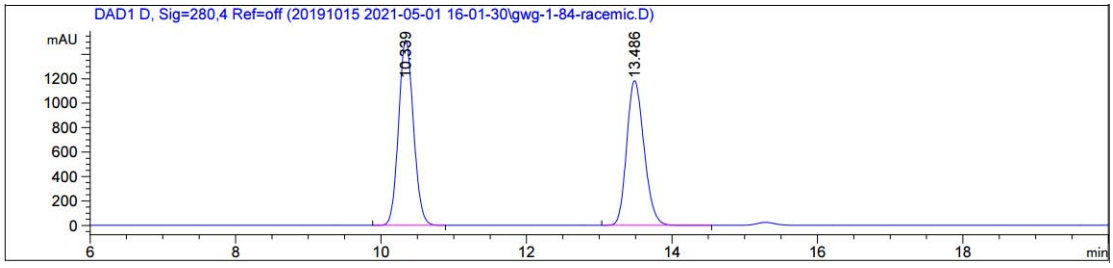
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.339	VB R	0.2201	1.86183e4	1306.32776	52.3446
2	13.486	BB	0.2576	1.69504e4	1021.42572	47.6554



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.339	BB	0.2256	7961.01270	554.09009	52.1544
2	13.486	BB	0.2615	7303.30811	435.87149	47.8456

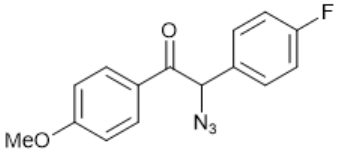


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.339	BB	0.2198	6713.04395	472.35962	52.3369
2	13.486	BB	0.2575	6113.54346	368.55103	47.6631



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.339	BB	0.2199	2.15408e4	1515.25928	52.3540
2	13.486	BB	0.2572	1.96038e4	1183.94238	47.6460

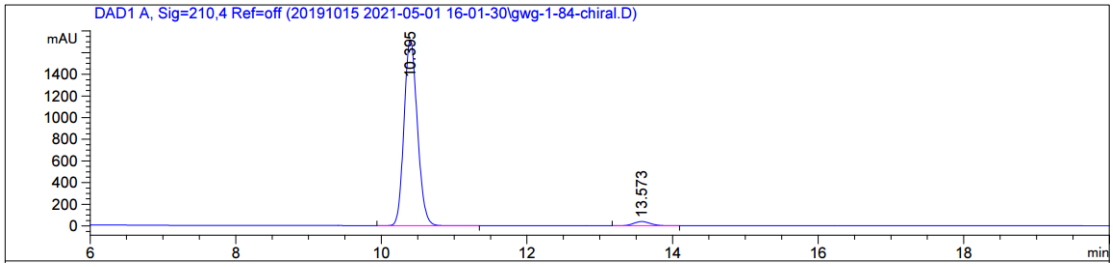
End of Report



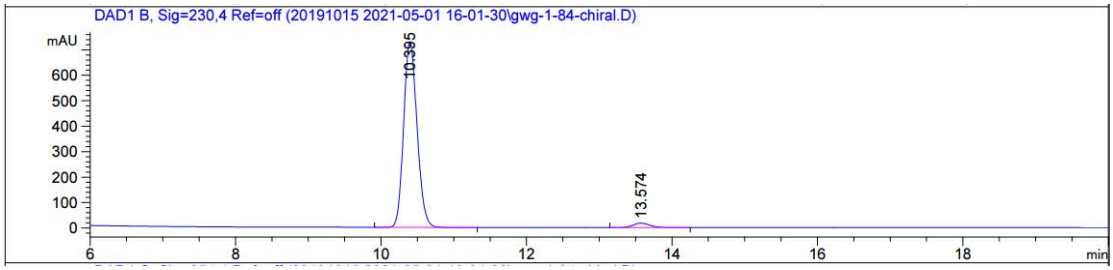
2k
racemic

Sample Name: gwg-1-84-enantioenriched

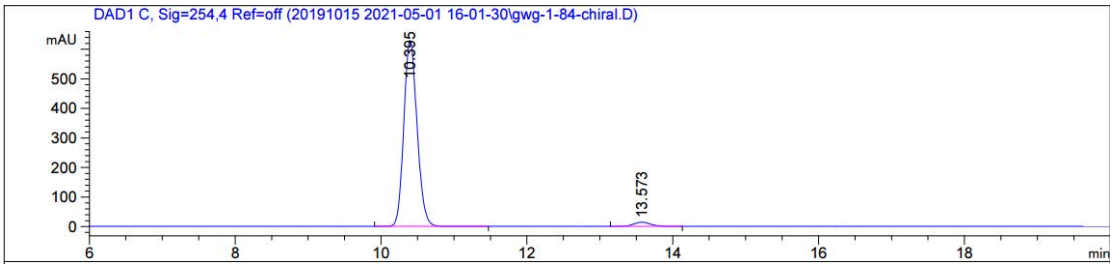
HPLC Condition: IC, *n*-Hexane/*i*PrOH = 90:10, 1.0 mL/min



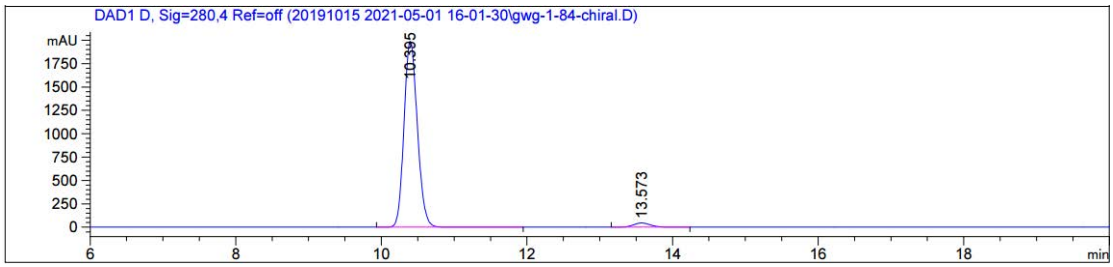
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.395	BB	0.1985	2.18530e4	1716.43066	97.1783
2	13.573	BB	0.2517	634.52686	39.03366	2.8217



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.395	BB	0.1995	9352.90918	729.99243	97.0893
2	13.574	BB	0.2520	280.39456	17.22071	2.9107

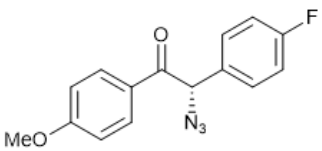


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.395	BB	0.1951	7938.87744	629.60620	97.1804
2	13.573	BB	0.2521	230.34195	14.13673	2.8196



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.395	BB	0.1985	2.53288e4	1989.65771	97.1872
2	13.573	BB	0.2520	733.06873	45.00504	2.8128

End of Report

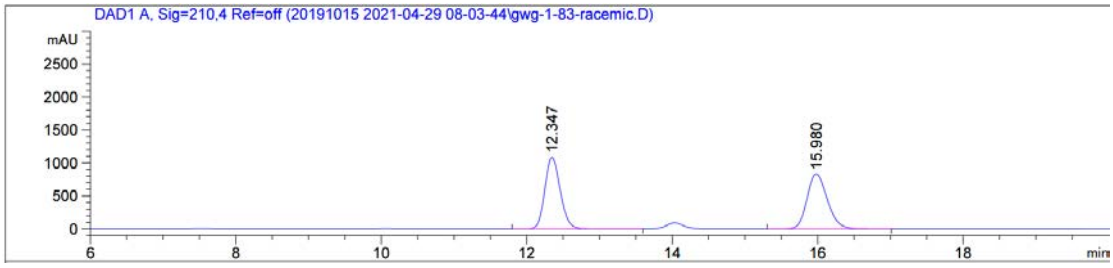


2k

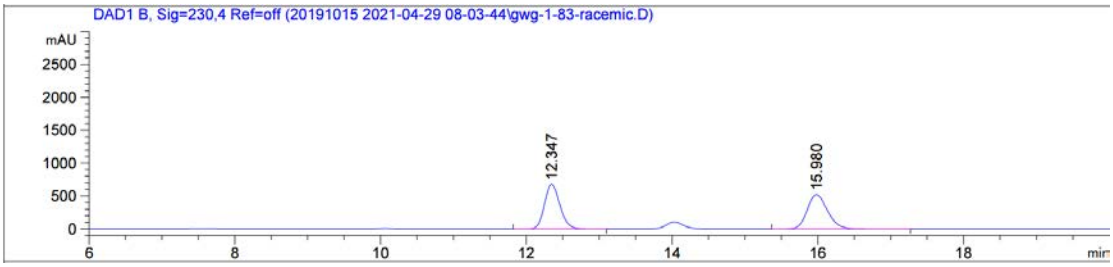
enantioenriched

Sample Name: gwg-1-83-racemic

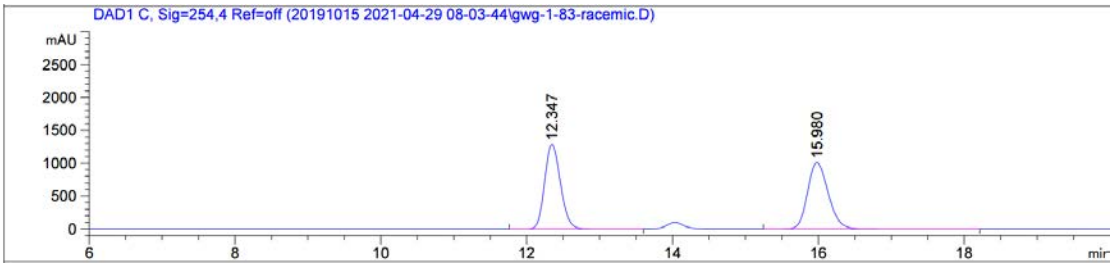
HPLC Condition: IC, *n*-Hexane/*i*PrOH = 97:3, 1.0 mL/min



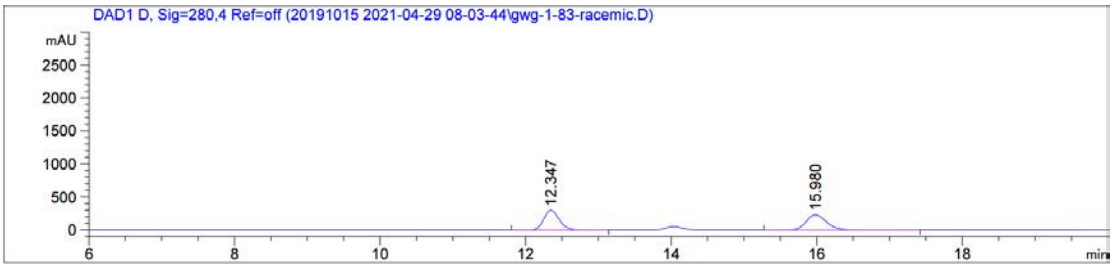
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.347	BB	0.2272	1.59776e4	1088.83655	49.8670
2	15.980	BB	0.2984	1.60628e4	834.99329	50.1330



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.347	BB	0.2269	9910.62598	676.71509	49.7790
2	15.980	BB	0.2989	9998.62891	518.77405	50.2210

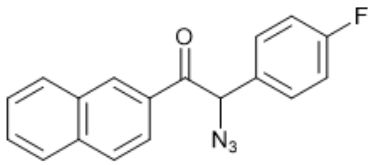


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.347	BB	0.2359	1.93601e4	1284.25586	49.4009
2	15.980	BB	0.3055	1.98296e4	1007.84265	50.5991



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.347	BB	0.2268	4367.92432	298.31885	49.7459
2	15.980	BB	0.2991	4412.54297	228.68457	50.2541

End of Report

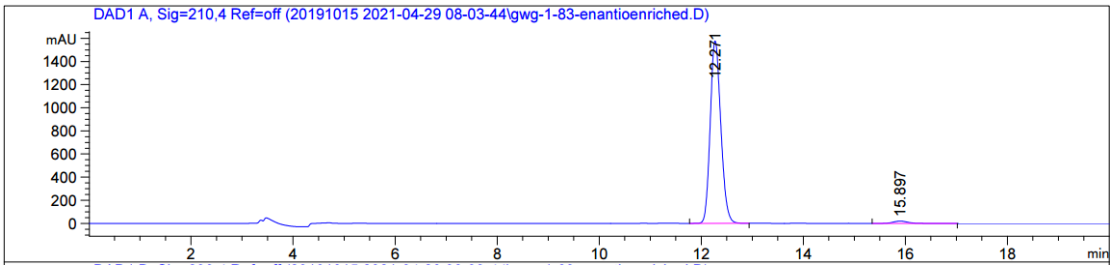


2l

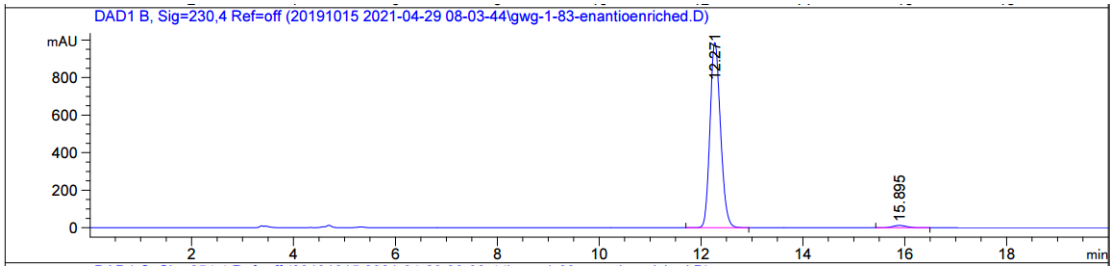
racemic

Sample Name: gwg-1-83-enantioenriched

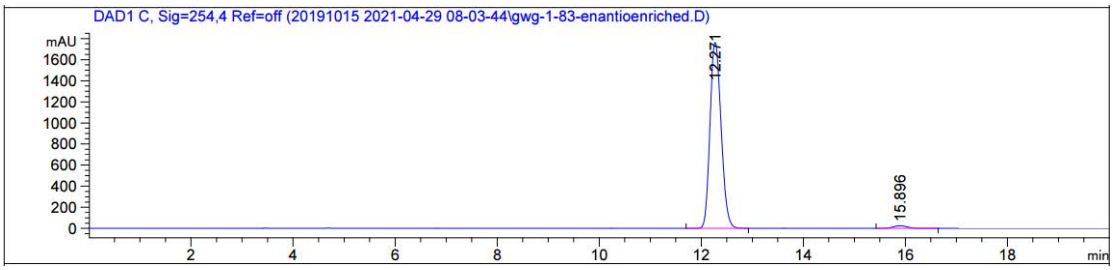
HPLC Condition: IC, *n*-Hexane/*i*PrOH = 97:3, 1.0 mL/min



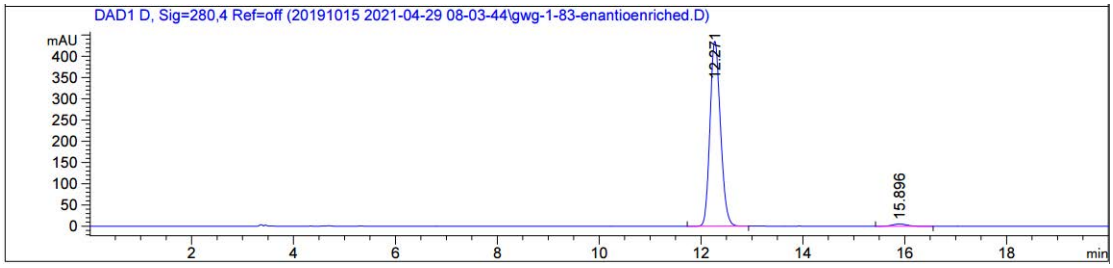
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.271	BB	0.2242	2.27529e4	1577.95251	98.2427
2	15.897	BB	0.3055	406.99643	20.33627	1.7573



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.271	BB	0.2216	1.41702e4	986.48230	98.3779
2	15.895	BB	0.2940	233.63748	12.39243	1.6221

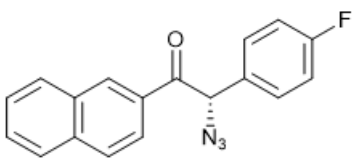


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.271	BB	0.2384	2.66524e4	1762.35132	98.2216
2	15.896	BB	0.2922	482.57474	25.56369	1.7784



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.271	BB	0.2214	6245.13623	435.26337	98.3793
2	15.896	BB	0.2898	102.87933	5.46074	1.6207

End of Report

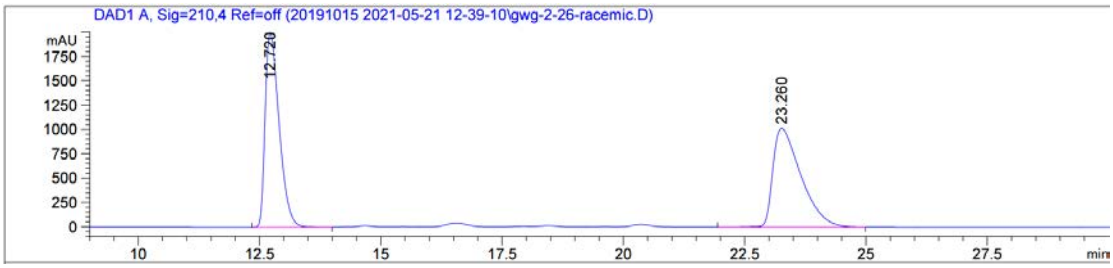


2l

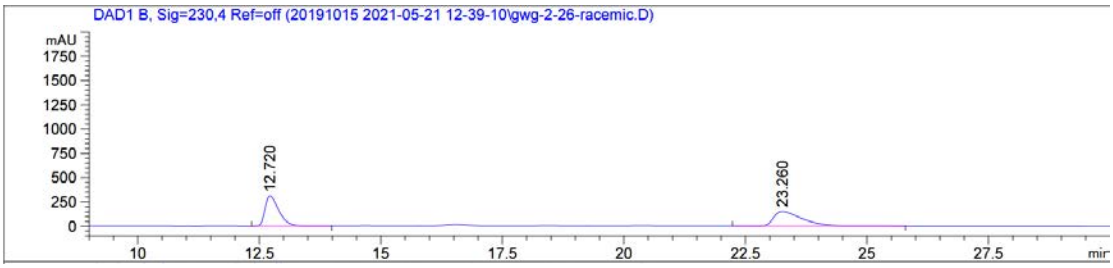
enantioenriched

Sample Name: gwg-2-26-racemic

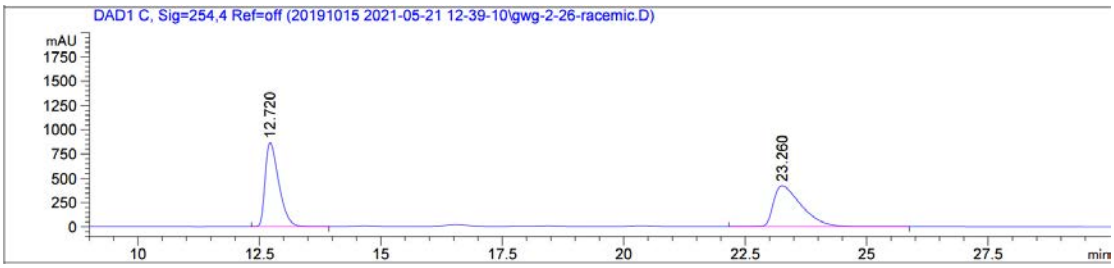
HPLC Condition: ODH, *n*-Hexane/*i*PrOH = 99:1, 1.0 mL/min



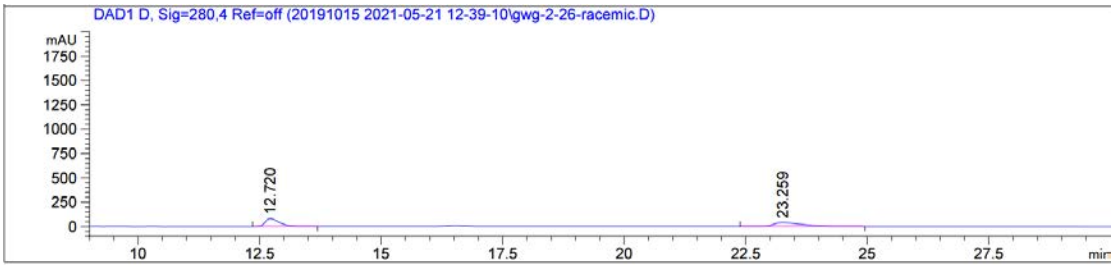
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.720	BB	0.3072	3.98587e4	1994.03394	49.4495
2	23.260	BB	0.6089	4.07461e4	1013.77081	50.5505



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.720	BB	0.3000	6075.55078	310.85889	49.9846
2	23.260	BB	0.6087	6079.30469	151.32632	50.0154

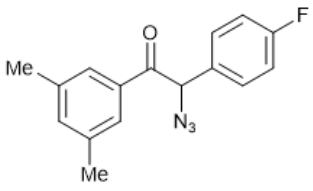


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.720	BB	0.2991	1.68637e4	866.25348	49.9803
2	23.260	BB	0.6056	1.68771e4	421.09863	50.0197



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.720	BB	0.3007	1573.90833	80.30427	49.9183
2	23.259	BB	0.6023	1579.05750	39.33966	50.0817

End of Report

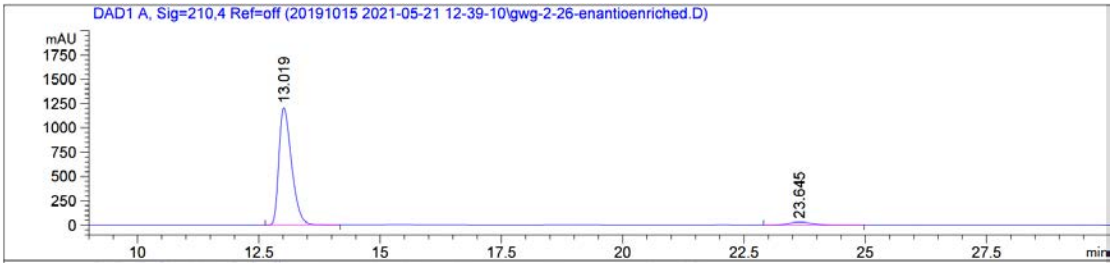


2m

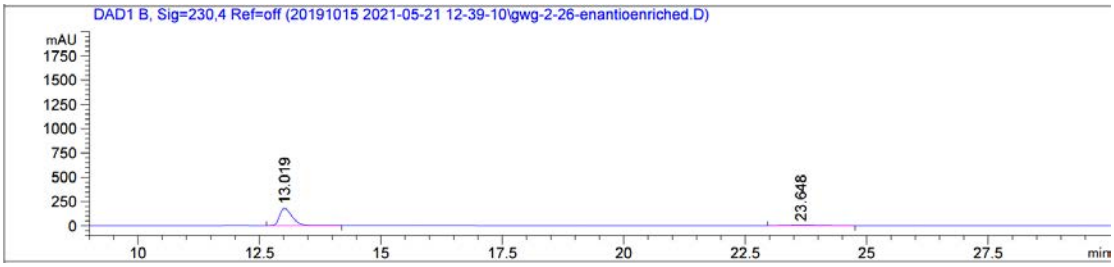
racemic

Sample Name: gwg-2-26-enantioenriched

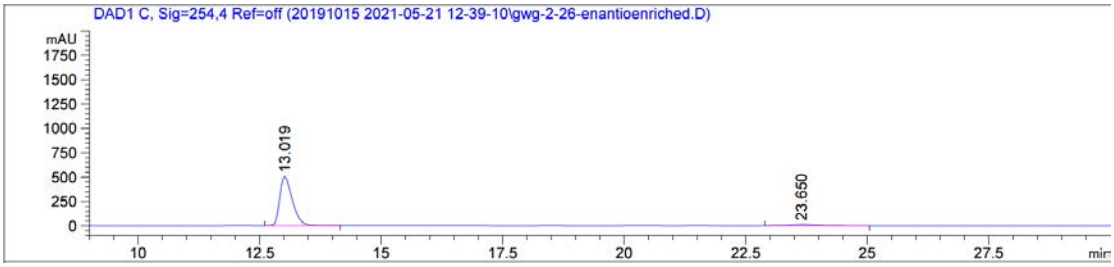
HPLC Condition: ODH, *n*-Hexane/*i*PrOH = 99:1, 1.0 mL/min



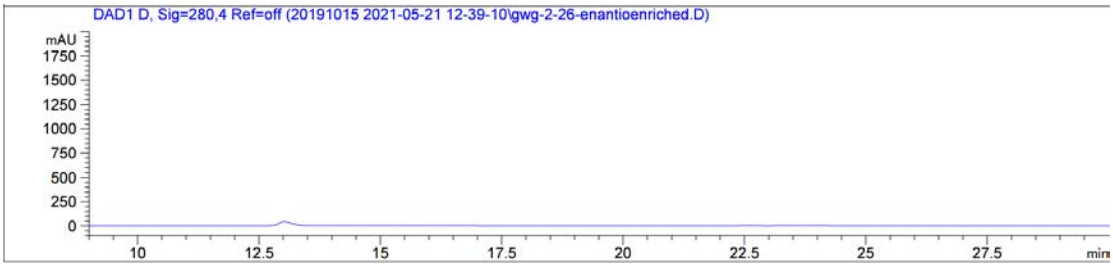
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.019	BB	0.2799	2.19037e4	1206.11572	95.5716
2	23.645	BB	0.5330	1014.93628	29.24023	4.4284



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.019	BB	0.2797	3275.80103	180.51335	95.5904
2	23.648	BB	0.5104	151.11218	4.35972	4.4096



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	13.019	BB	0.2788	9077.93652	502.49368	95.5686
2	23.650	BB	0.5342	420.93219	12.08856	4.4314



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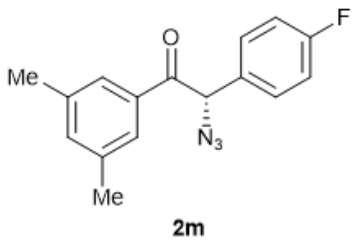
End of Report

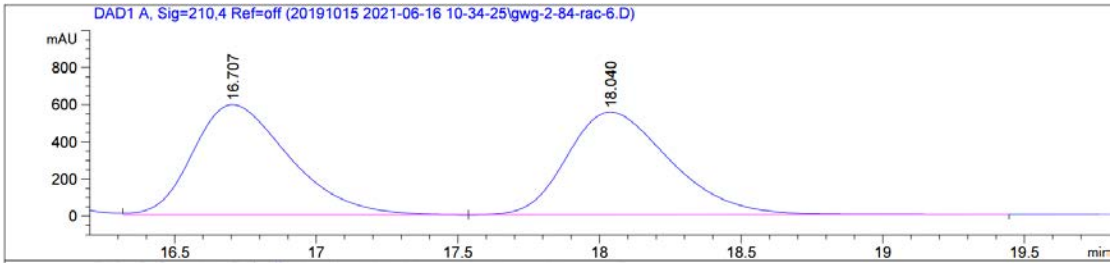


2m

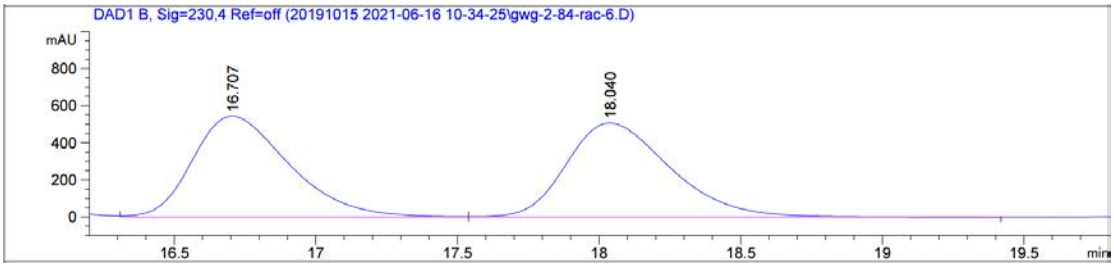
enantioenriched

Sample Name: gwg-2-84-racemic

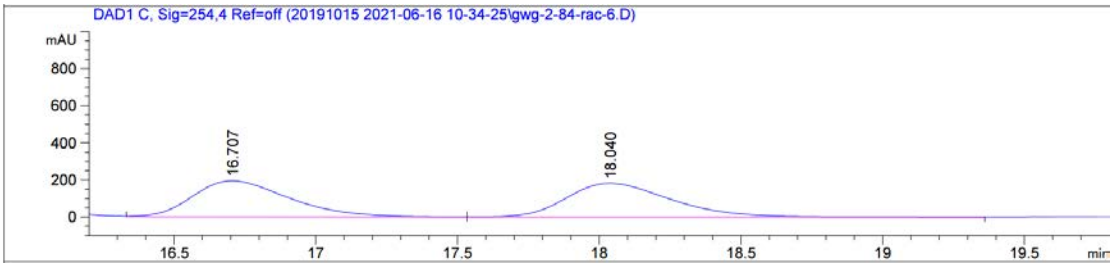
HPLC Condition: IC, *n*-Hexane/*i*PrOH = 99:1, 1.0 mL/min



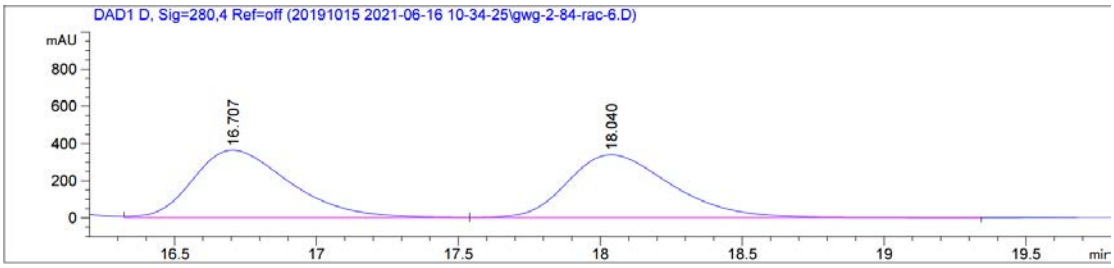
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.707	VB	0.3635	1.39926e4	592.47137	50.0315
2	18.040	BB	0.3915	1.39750e4	551.69586	49.9685



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.707	VV	0.3644	1.28769e4	543.43390	49.9632
2	18.040	VB	0.3929	1.28959e4	506.68484	50.0368

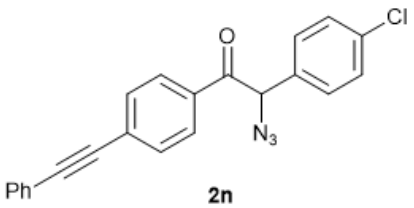


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.707	VV	0.3638	4592.26074	194.25298	50.0039
2	18.040	VB	0.3919	4591.54150	181.02127	49.9961



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.707	VV	0.3640	8568.51758	362.23358	50.0423
2	18.040	VB	0.3917	8554.02832	337.47238	49.9577

End of Report

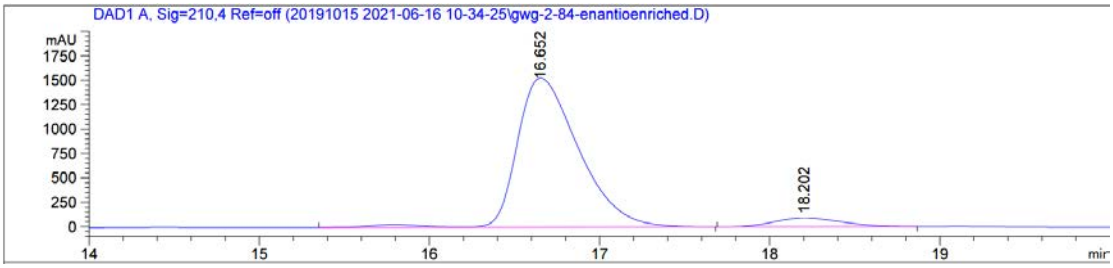


2n

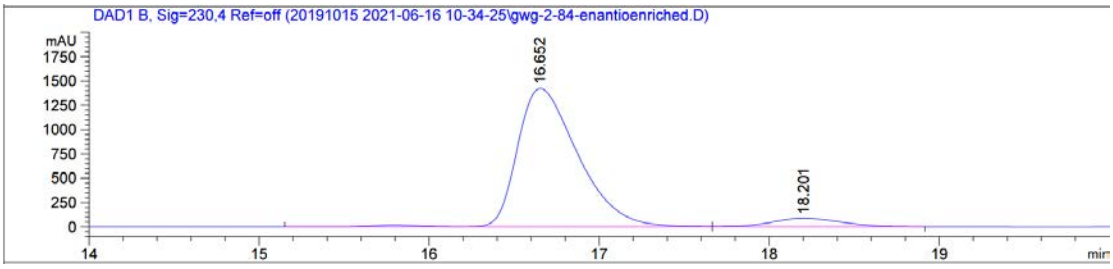
racemic

Sample Name: gwg-2-84-enantioenriched

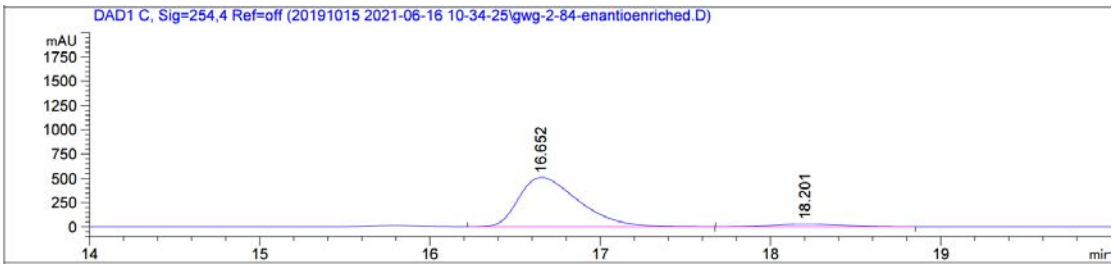
HPLC Condition: IC, *n*-Hexane/*i*PrOH = 99:1, 1.0 mL/min



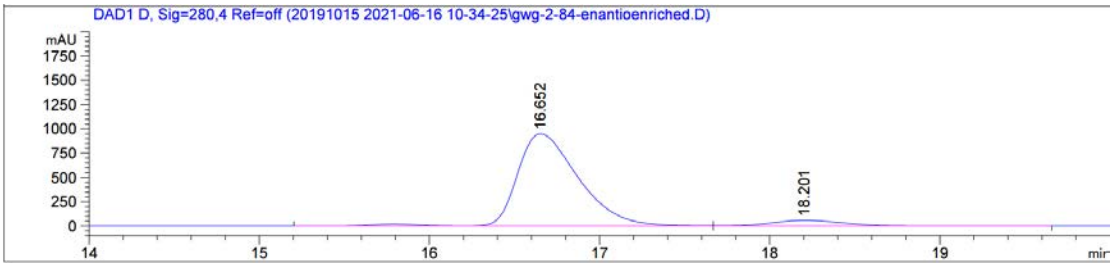
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.652	VB R	0.3830	3.83610e4	1527.83594	93.9066
2	18.202	BB	0.4167	2489.15186	92.27799	6.0934



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.652	VV R	0.3789	3.53668e4	1423.77454	93.4617
2	18.201	VB	0.4475	2474.15039	88.68900	6.5383

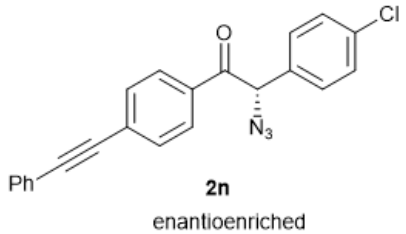


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.652	VB	0.3753	1.24761e4	510.12561	93.6930
2	18.201	BB	0.4409	839.83295	31.11443	6.3070



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	16.652	VV R	0.3792	2.38199e4	951.67157	93.1087
2	18.201	VB	0.4612	1762.98303	60.28823	6.8913

End of Report

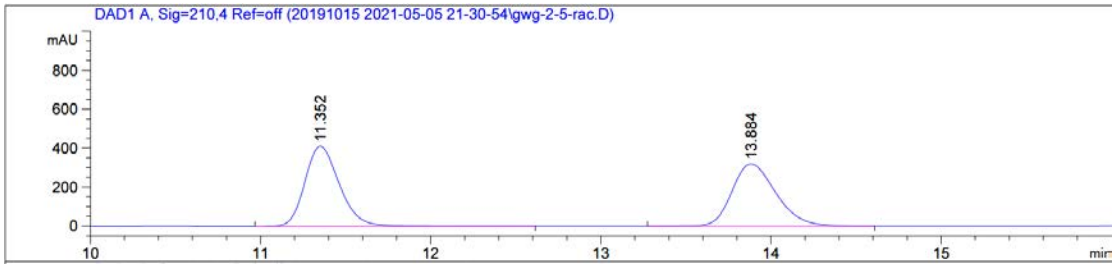


2n

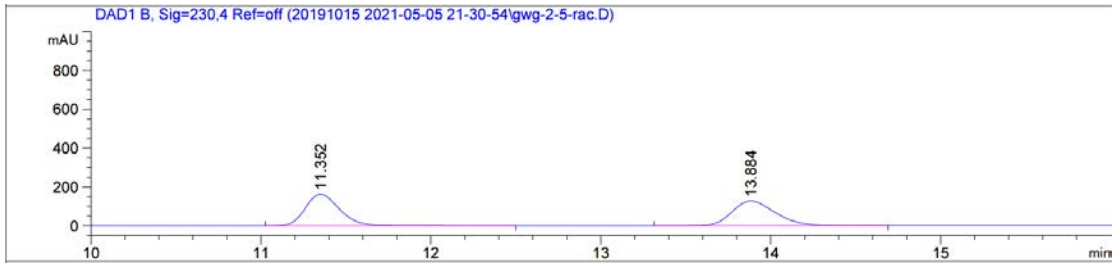
enantioenriched

Sample Name: gwg-1-95-racemic

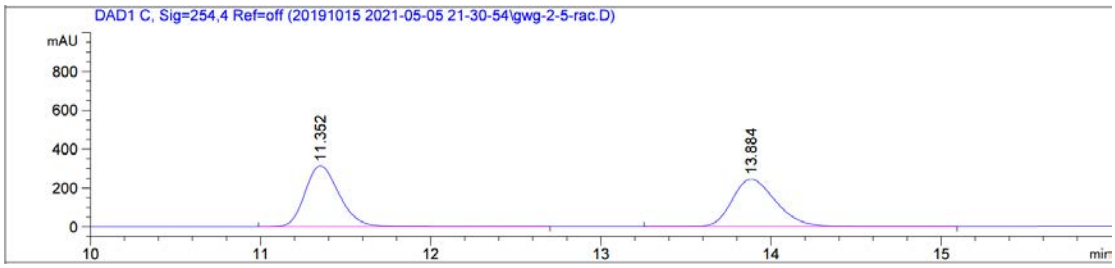
HPLC Condition: ODH, *n*-Hexane/*i*PrOH = 95:5, 1.0 mL/min



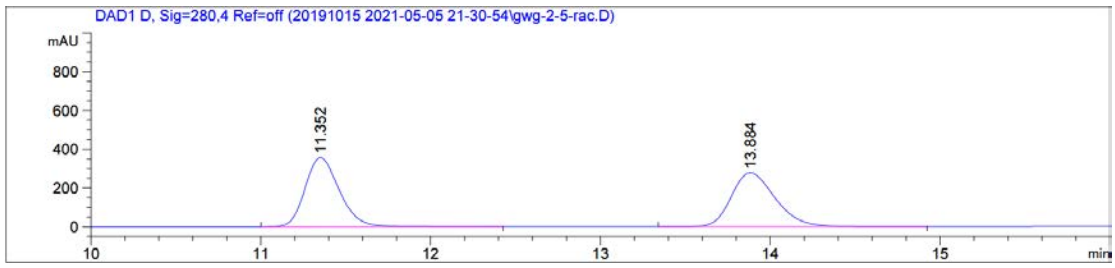
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.352	BB	0.2177	5750.46387	409.82306	50.1876
2	13.884	BB	0.2762	5707.47656	319.77087	49.8124



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.352	BB	0.2178	2286.07813	162.79077	50.2914
2	13.884	BB	0.2758	2259.58838	126.86114	49.7086

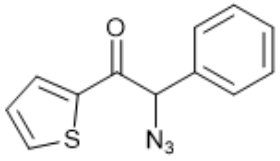


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.352	BB	0.2177	4411.17139	314.37024	50.2565
2	13.884	BB	0.2760	4366.14648	244.86259	49.7435



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.352	BB	0.2150	4971.68701	355.79819	50.1780
2	13.884	BB	0.2755	4936.41260	277.55780	49.8220

End of Report

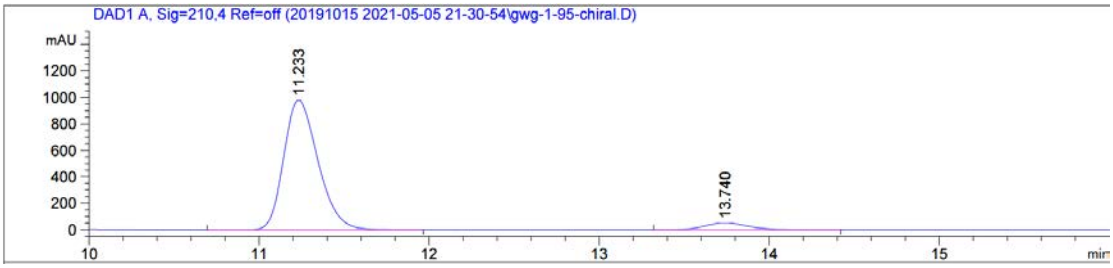


2o

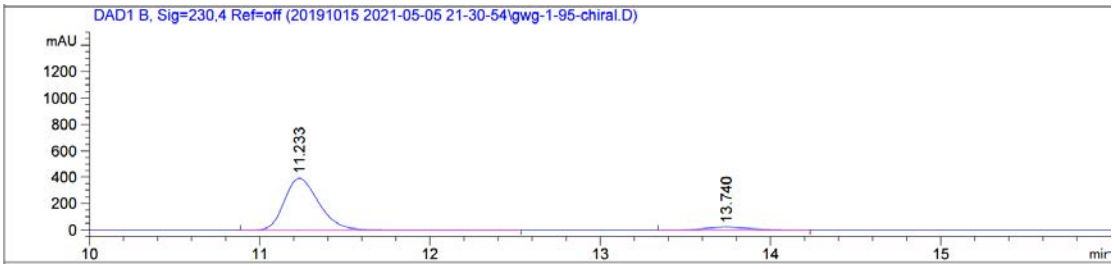
racemic

Sample Name: gwg-1-95-enantioenriched

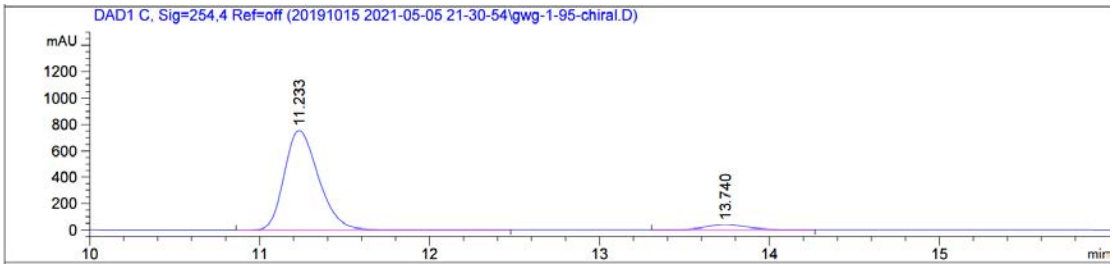
HPLC Condition: ODH, *n*-Hexane/*i*PrOH = 95:5, 1.0 mL/min



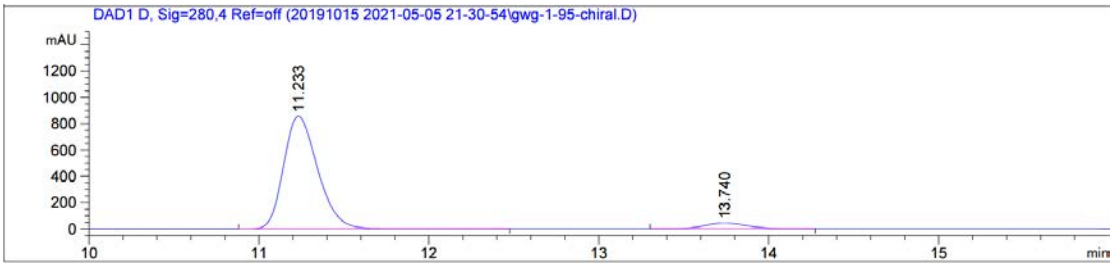
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.233	BB	0.2167	1.36727e4	980.37939	93.9481
2	13.740	BB	0.2640	880.76270	51.90536	6.0519



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.233	BB	0.2170	5468.70752	391.44571	94.0680
2	13.740	BB	0.2623	344.86127	20.49823	5.9320

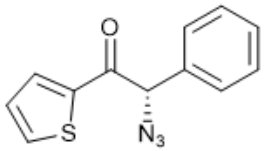


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.233	BB	0.2169	1.05350e4	754.38928	94.0079
2	13.740	BB	0.2631	671.50848	39.74366	5.9921



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.233	BB	0.2166	1.19407e4	856.66187	94.0045
2	13.740	BB	0.2634	761.56921	45.01426	5.9955

End of Report

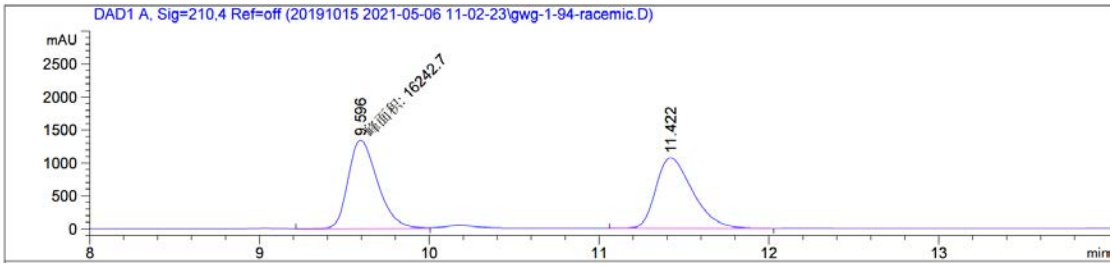


2o

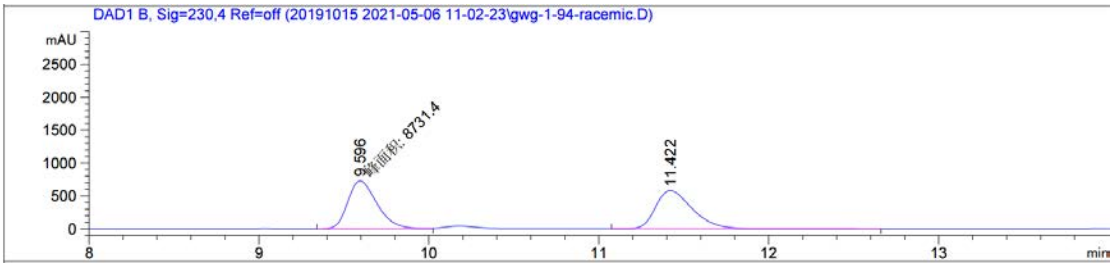
enantioenriched

Sample Name: gwg-1-94-racemic

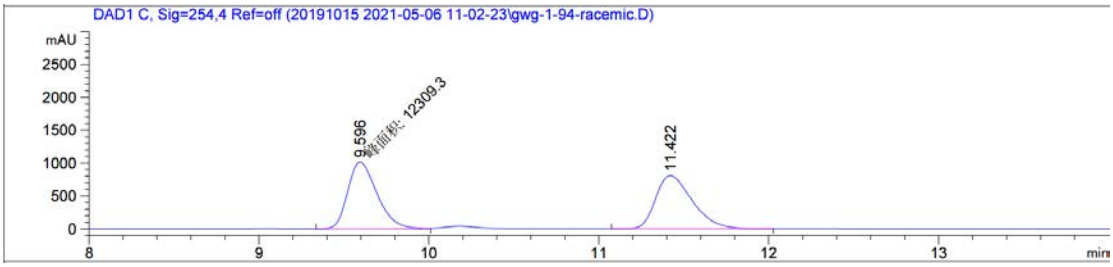
HPLC Condition: ODH, *n*-Hexane/*i*PrOH = 95:5, 1.0 mL/min



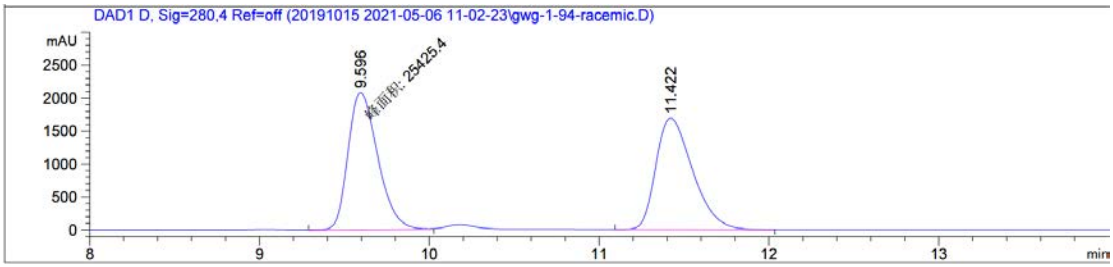
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.596	MM	0.2015	1.62427e4	1343.46545	50.4782
2	11.422	BB	0.2301	1.59349e4	1067.92371	49.5218



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.596	MM	0.1990	8731.40234	731.17902	50.1956
2	11.422	BV R	0.2297	8663.35449	579.43475	49.8044

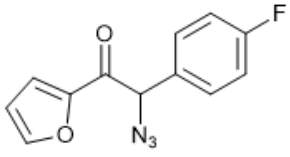


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.596	MM	0.2013	1.23093e4	1019.26355	50.5376
2	11.422	BB	0.2301	1.20474e4	807.33246	49.4624



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.596	MM	0.2034	2.54254e4	2083.47119	50.0346
2	11.422	BB	0.2333	2.53902e4	1690.00122	49.9654

End of Report

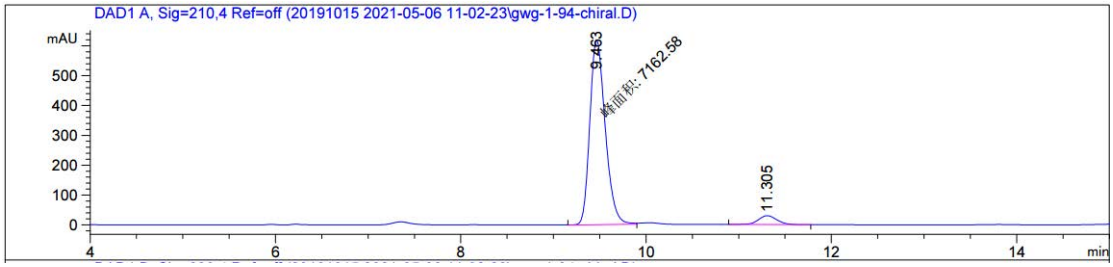


2p

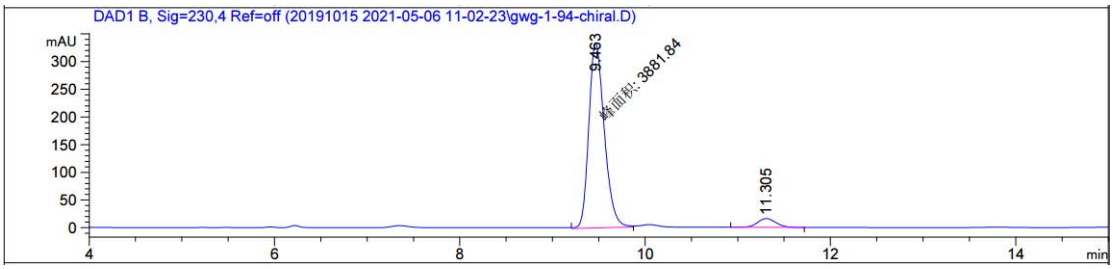
racemic

Sample Name: gwg-1-94-enantioenriched

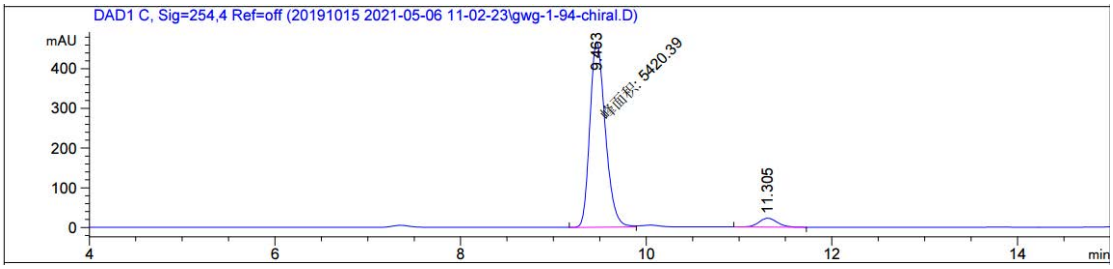
HPLC Condition: ODH, *n*-Hexane/*i*PrOH = 95:5, 1.0 mL/min



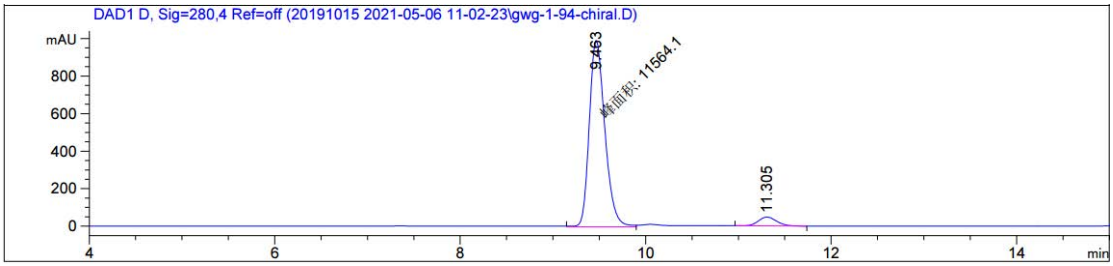
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.463	MM	0.1926	7162.58203	619.95569	94.6258
2	11.305	BB	0.2132	406.79056	29.44935	5.3742



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.463	MM	0.1933	3881.84277	334.69803	94.6896
2	11.305	BB	0.2144	217.70306	15.83468	5.3104

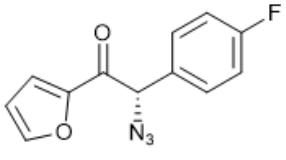


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.463	MM	0.1927	5420.38721	468.70099	94.6717
2	11.305	BB	0.2119	305.07013	22.26280	5.3283



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.463	MM	0.1941	1.15641e4	993.20239	94.7434
2	11.305	BB	0.2115	641.60291	46.93247	5.2566

End of Report

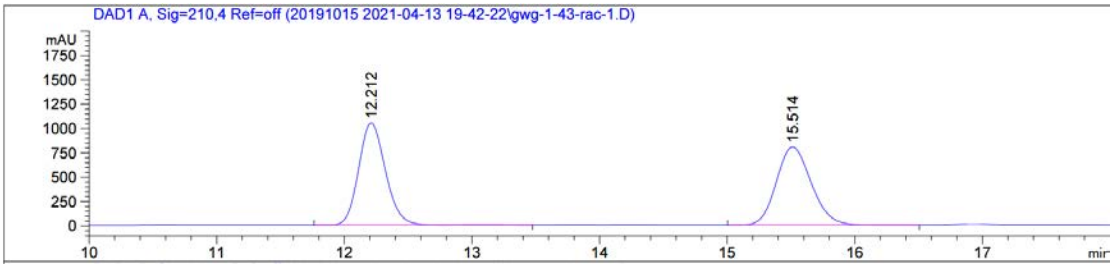


2p

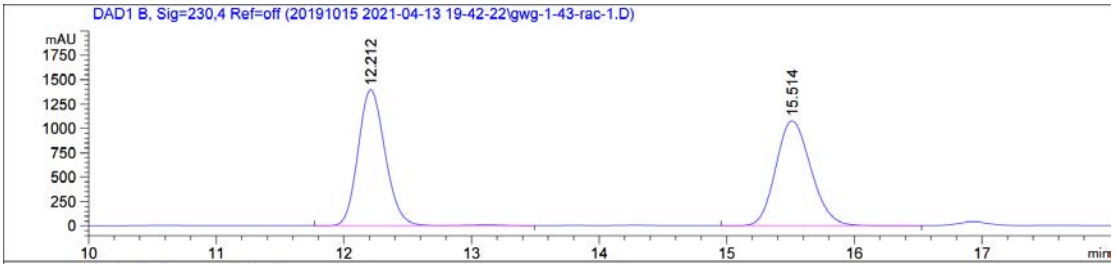
enantioenriched

Sample Name: gwg-1-43

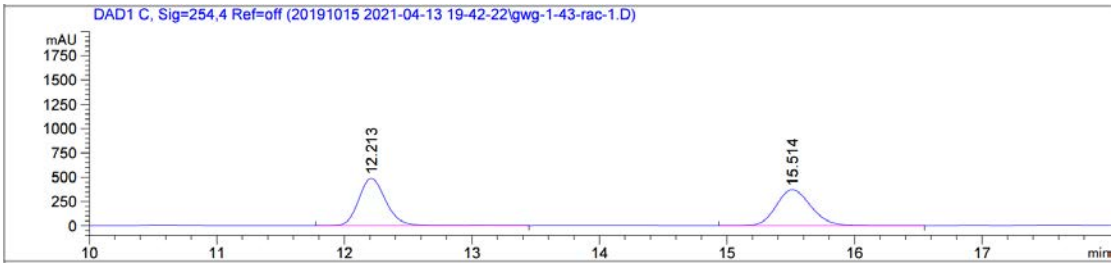
HPLC Condition: IC, *n*-Hexane/*i*PrOH = 97/3, 1.0 mL/min



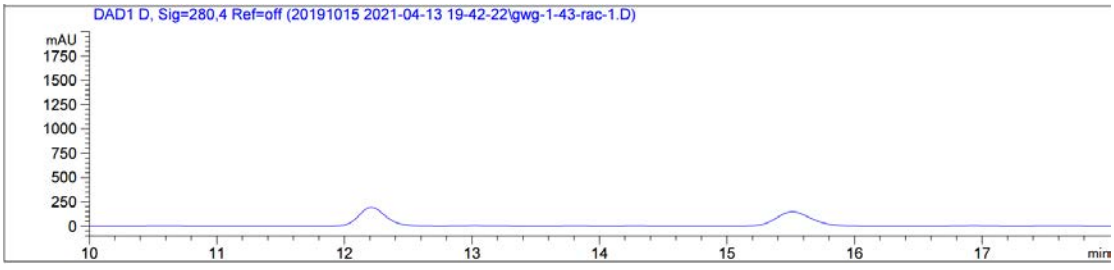
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.212	BV R	0.2257	1.53946e4	1048.64185	50.3487
2	15.514	BB	0.2950	1.51814e4	801.47662	49.6513



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.212	BV R	0.2276	2.06605e4	1393.35242	50.0805
2	15.514	BB	0.2971	2.05941e4	1076.97510	49.9195



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.213	BV R	0.2275	7246.02197	488.16440	50.6952
2	15.514	BB	0.2952	7047.29541	371.72296	49.3048



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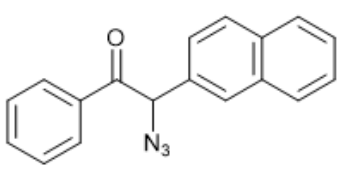
End of Report

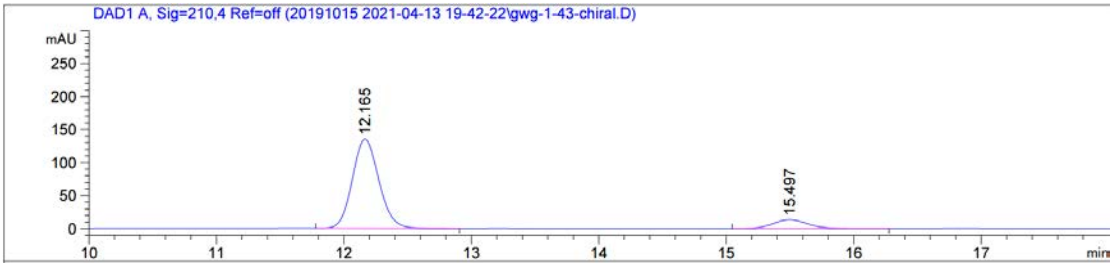


2q

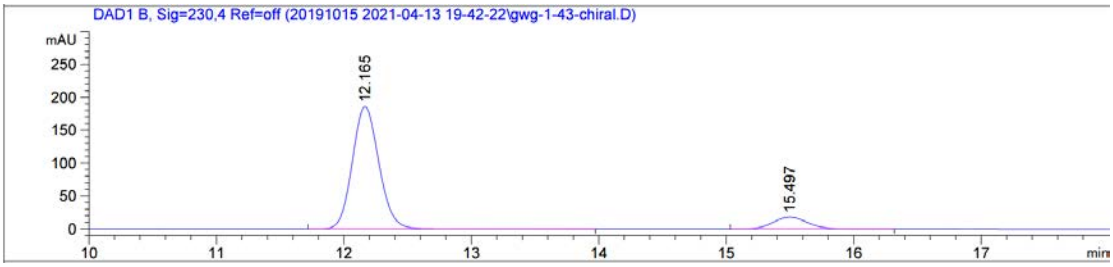
racemic

Sample Name: gwg-1-43-enantioenriched

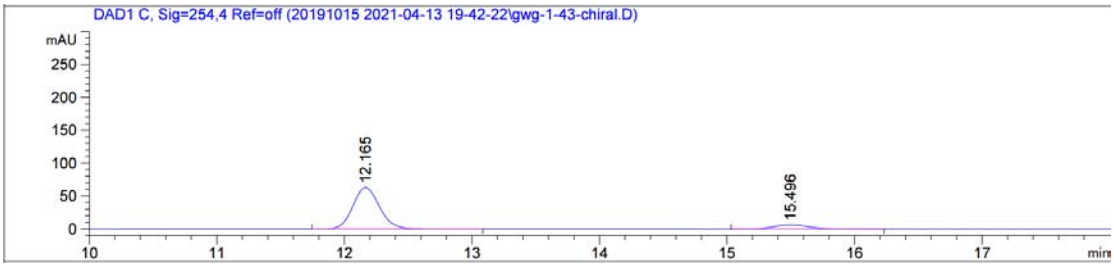
HPLC Condition: IC, *n*-Hexane/*i*PrOH = 97:3, 1.0 mL/min



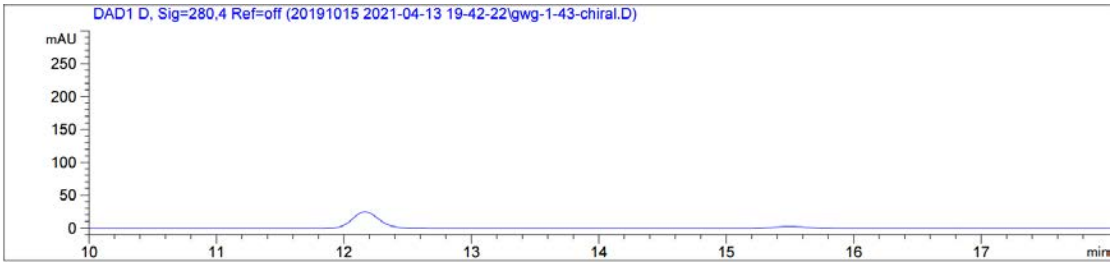
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.165	BB	0.2248	1955.87842	135.14792	88.0918
2	15.497	BB	0.2931	264.39392	13.82425	11.9082



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.165	BB	0.2252	2698.12500	185.98920	88.4731
2	15.497	BB	0.2910	351.52969	18.72474	11.5269



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	12.165	BB	0.2248	909.48560	62.86038	88.4258
2	15.496	BB	0.2938	119.04402	6.31809	11.5742



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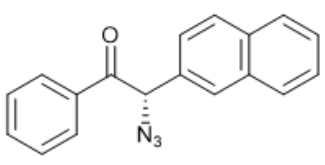
End of Report

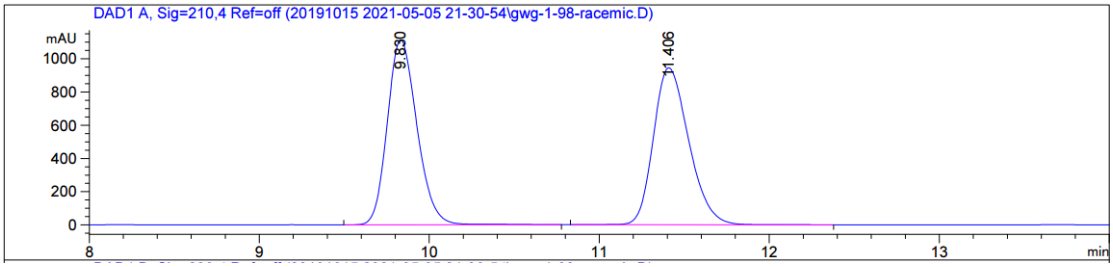


2q

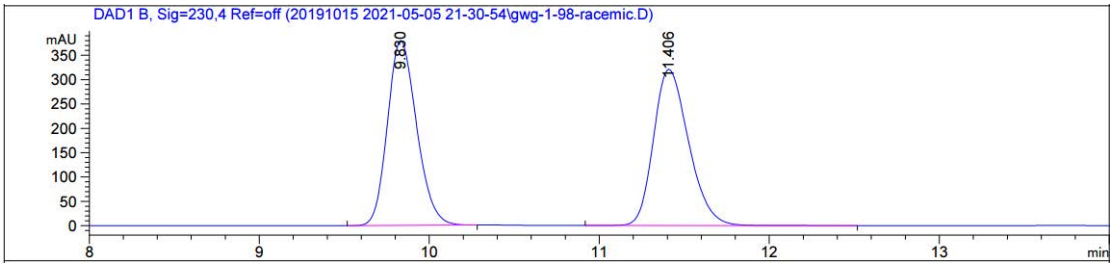
enantioenriched

Sample Name: gwg-1-98-racemic

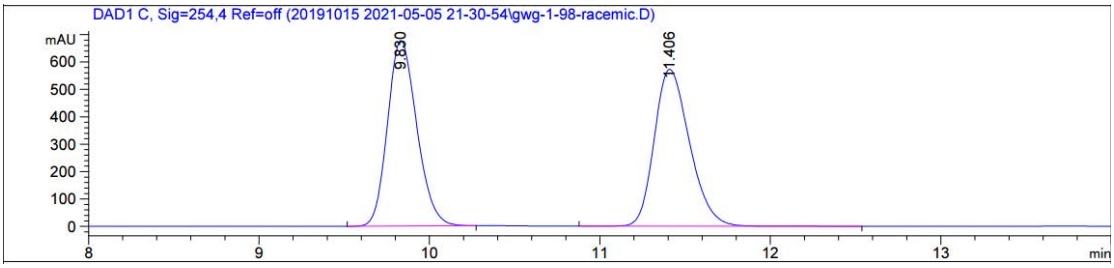
HPLC Condition: ODH, *n*-Hexane/*i*PrOH = 97:3, 1.0 mL/min



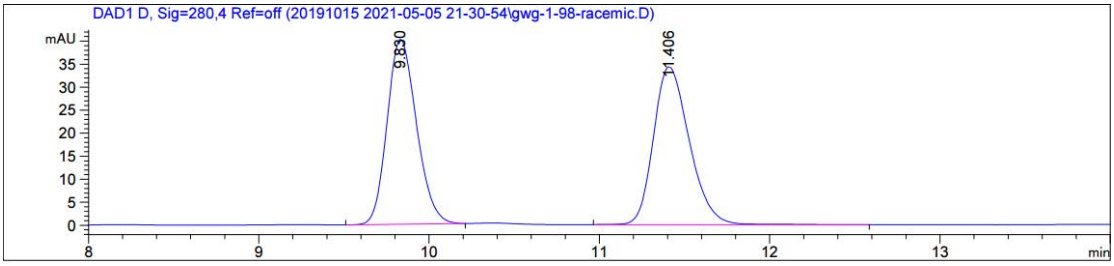
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.830	BB	0.1871	1.34759e4	1114.00635	49.7018
2	11.406	BB	0.2244	1.36376e4	944.70026	50.2982



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.830	BB	0.1851	4525.84668	379.67108	49.5618
2	11.406	BB	0.2235	4605.88330	320.75357	50.4382

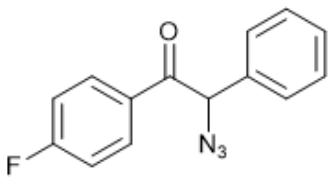


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.830	BB	0.1851	8071.86914	677.09534	49.5510
2	11.406	BB	0.2235	8218.15234	572.52954	50.4490



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.830	BB	0.1859	481.83469	40.18430	49.0166
2	11.406	BB	0.2264	501.16901	34.31062	50.9834

End of Report

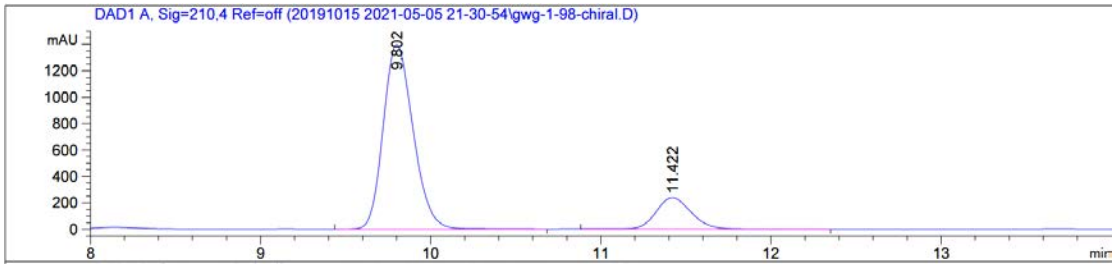


2r

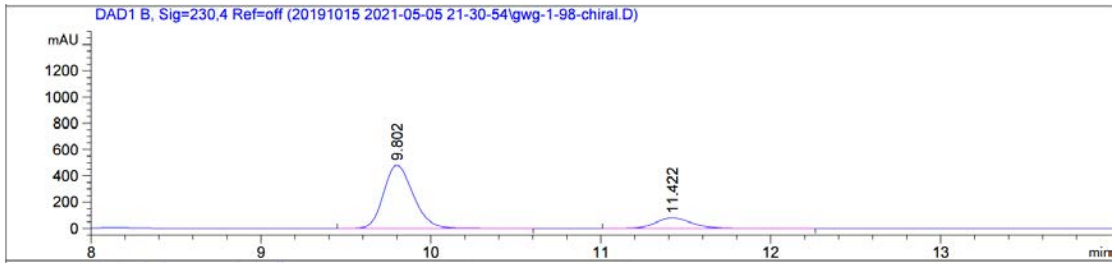
racemic

Sample Name: gwg-1-98-enantioenriched

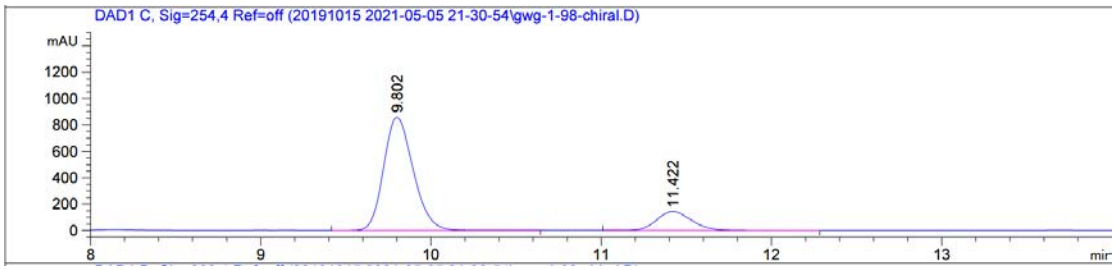
HPLC Condition: ODH, *n*-Hexane/*i*PrOH = 97:3, 1.0 mL/min



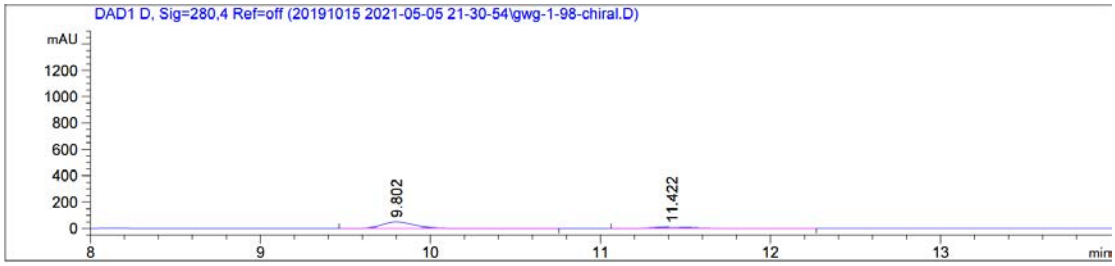
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.802	BB	0.1902	1.70337e4	1397.91956	83.3647
2	11.422	BB	0.2201	3399.04932	238.75194	16.6353



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.802	BB	0.1864	5798.85889	481.94672	83.6837
2	11.422	BB	0.2191	1130.63684	79.91781	16.3163

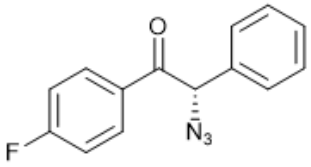


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.802	BB	0.1866	1.03469e4	858.86169	83.6700
2	11.422	BB	0.2190	2019.41943	142.82462	16.3300



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	9.802	BB	0.1885	620.61389	50.80875	83.0422
2	11.422	BB	0.2234	126.73378	8.72981	16.9578

End of Report

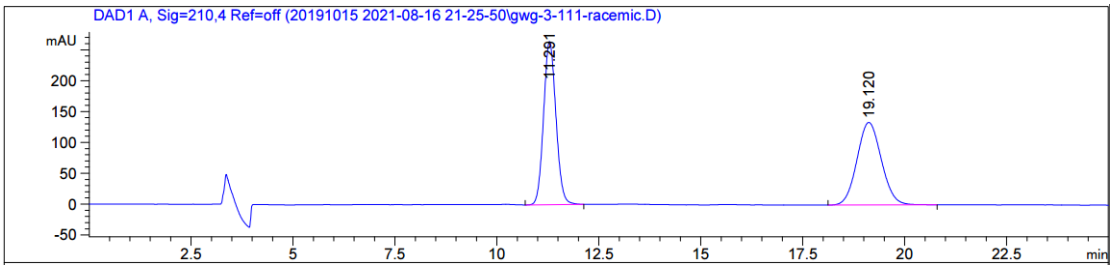


2r

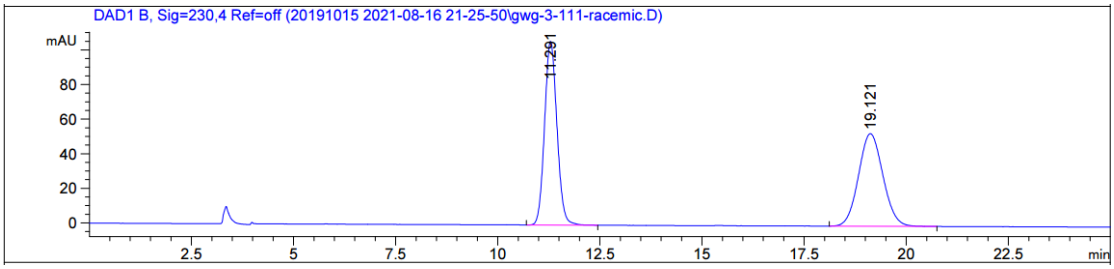
enantioenriched

Sample Name: gwg-3-111-racemic

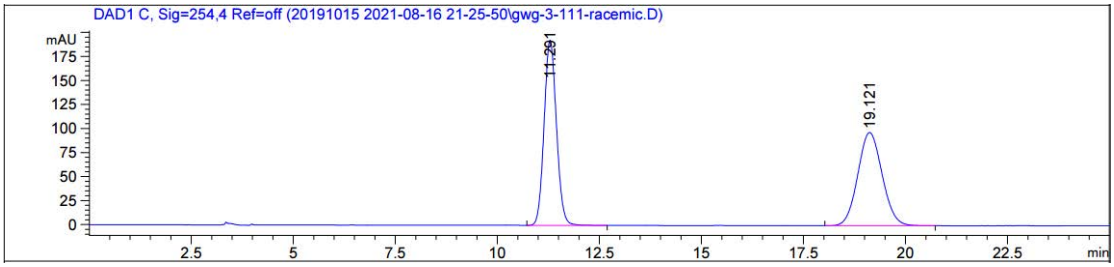
HPLC Condition: IC, *n*-Hexane/*i*PrOH = 95:5, 1.0 mL/min



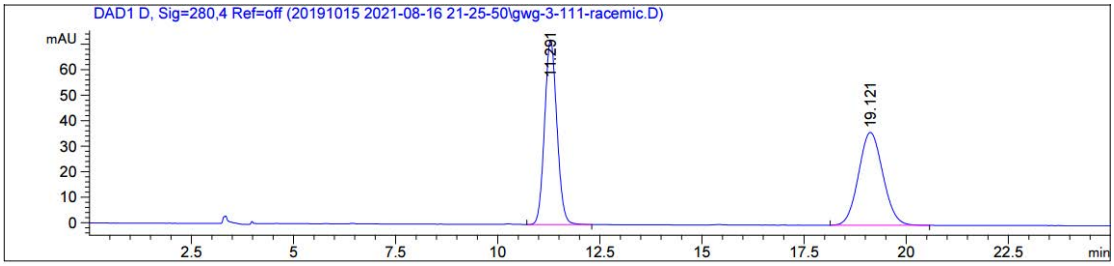
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.291	BB	0.3298	5570.95068	264.46167	50.0996
2	19.120	BB	0.6521	5548.79639	133.72734	49.9004



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.291	BB	0.3275	2235.96362	106.24183	50.1587
2	19.121	BB	0.6444	2221.81738	53.51153	49.8413

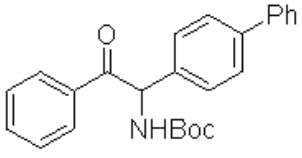


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.291	BB	0.3249	4047.90723	192.83478	50.1326
2	19.121	BB	0.6482	4026.49194	97.02424	49.8674



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.291	BB	0.3248	1518.07654	72.35809	50.1605
2	19.121	BB	0.6375	1508.36279	36.39727	49.8395

End of Report

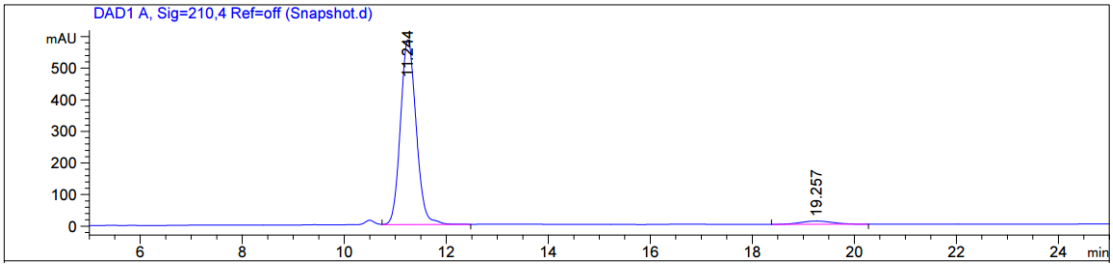


8

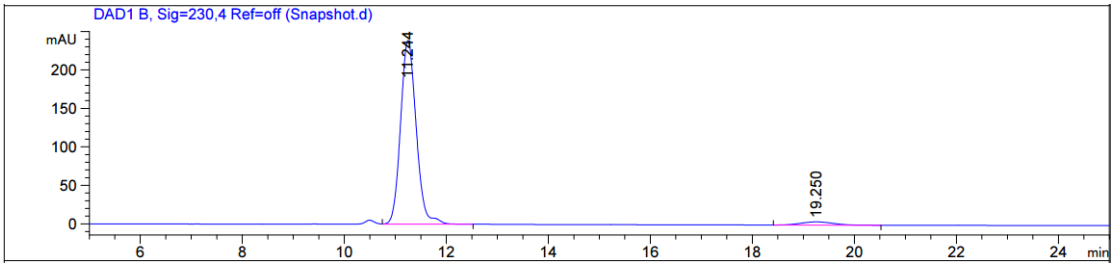
racemic

Sample Name: gwg-3-111-enantioenriched

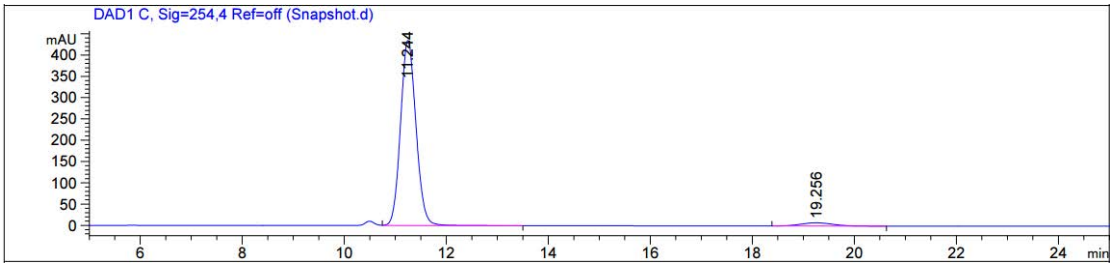
HPLC Condition: IC, *n*-Hexane/*i*PrOH = 95:5, 1.0 mL/min



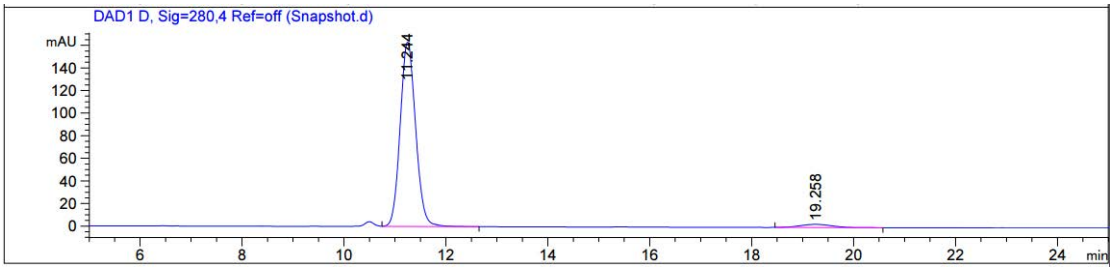
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.244	VB	0.3310	1.24881e4	585.01758	96.5272
2	19.257	BB	0.6160	449.29156	10.31904	3.4728



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.244	VB	0.3306	5087.86963	238.73804	96.5466
2	19.250	BB	0.5579	181.98700	4.16407	3.4534

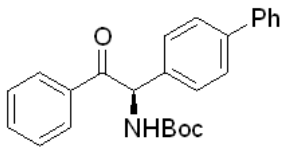


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.244	VB	0.3273	9138.28125	434.59372	96.5592
2	19.256	BB	0.6125	325.63535	7.56076	3.4408



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	11.244	VB	0.3276	3433.52026	163.12679	96.6052
2	19.258	BB	0.5286	120.65544	2.82308	3.3948

End of Report

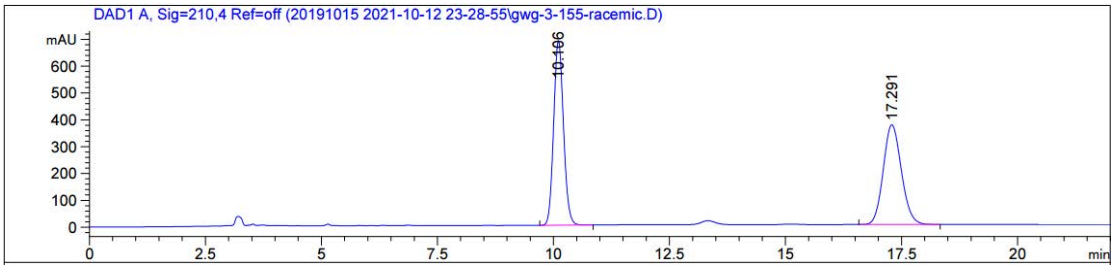


8

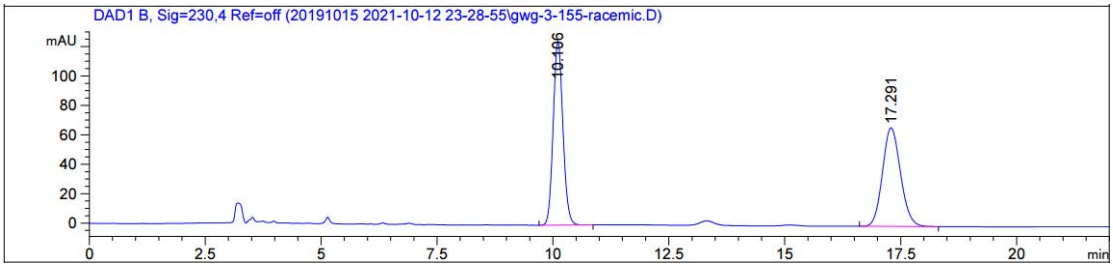
enantioenriched

Sample Name: gwg-3-155-racemic

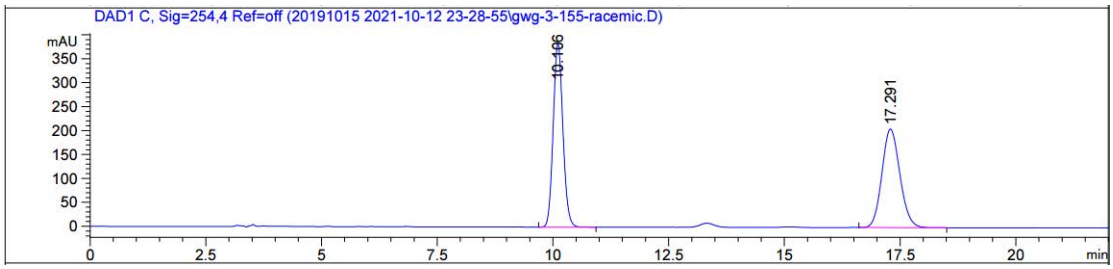
HPLC Condition: ADH, *n*-Hexane/*i*PrOH = 85:15, 1.0 mL/min



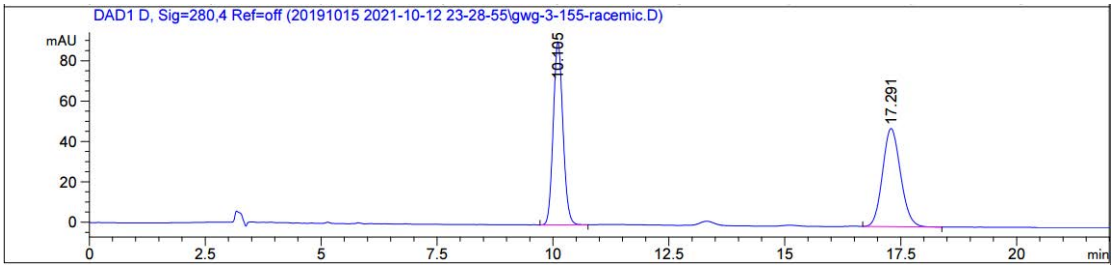
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.106	BB	0.2266	1.00618e4	688.26166	49.9883
2	17.291	BB	0.4202	1.00665e4	371.43140	50.0117



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.106	BB	0.2253	1814.52002	125.02724	50.0452
2	17.291	BB	0.4191	1811.24402	67.07168	49.9548

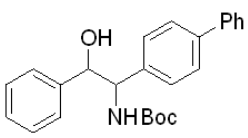


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.106	BB	0.2253	5587.44824	385.12701	50.1401
2	17.291	BB	0.4169	5556.22217	205.87775	49.8599



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.105	BB	0.2253	1316.55640	90.71405	50.1318
2	17.291	BB	0.4185	1309.63330	48.58440	49.8682

End of Report

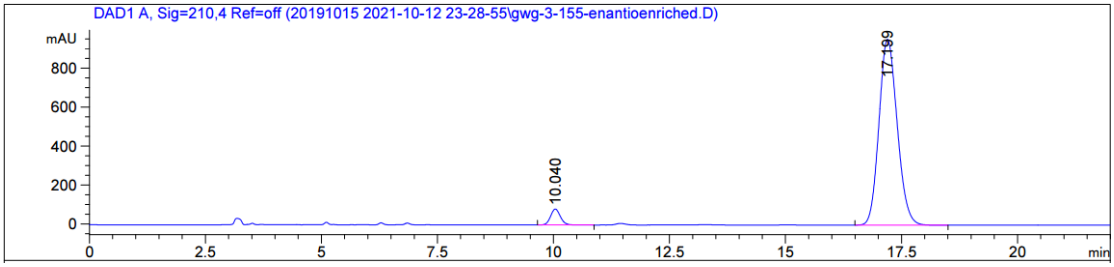


9

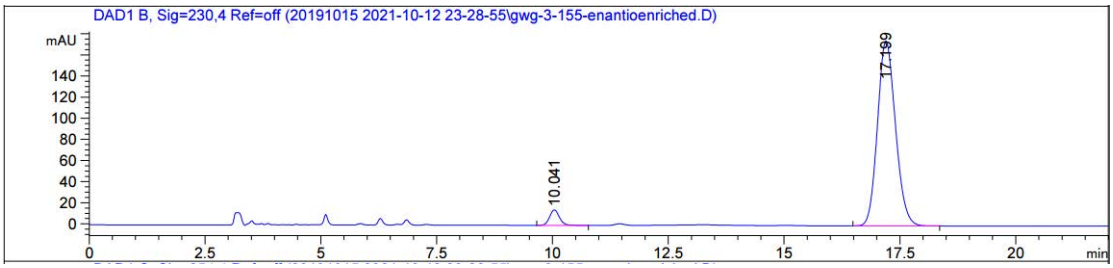
racemic

Sample Name: gwg-3-155-enantioenriched

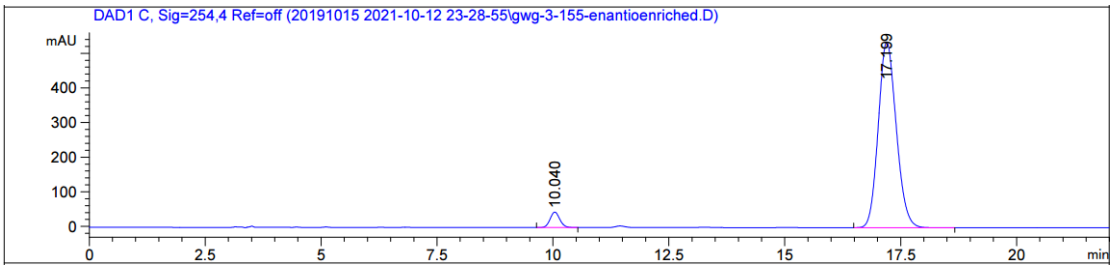
HPLC Condition: ADH, *n*-Hexane/*i*PrOH = 85:15, 1.0 mL/min



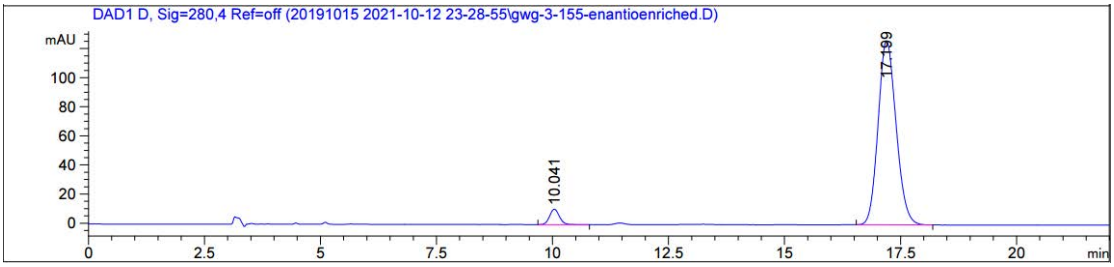
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.040	BB	0.2254	1199.77747	81.64992	4.4138
2	17.199	BB	0.4240	2.59824e4	953.29797	95.5862



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.041	BB	0.2276	217.04330	14.58637	4.3973
2	17.199	BB	0.4166	4718.78760	175.01804	95.6027

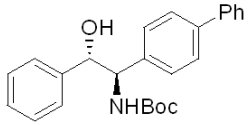


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.040	BB	0.2239	648.34186	44.51392	4.2908
2	17.199	BB	0.4165	1.44616e4	536.49506	95.7092



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	10.041	BB	0.2271	155.12466	10.58029	4.3516
2	17.199	BB	0.4164	3409.64160	126.50976	95.6484

End of Report



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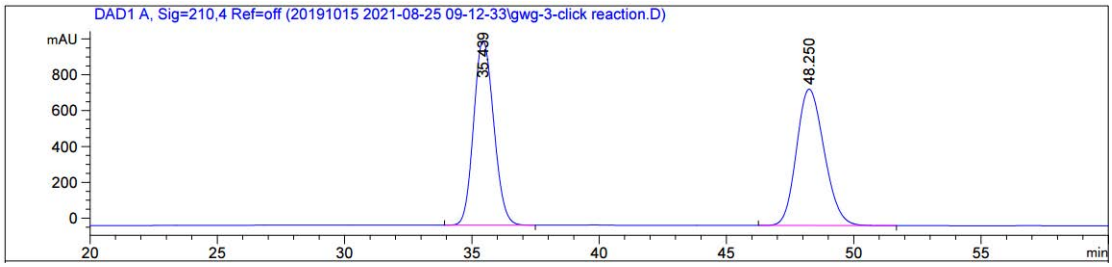
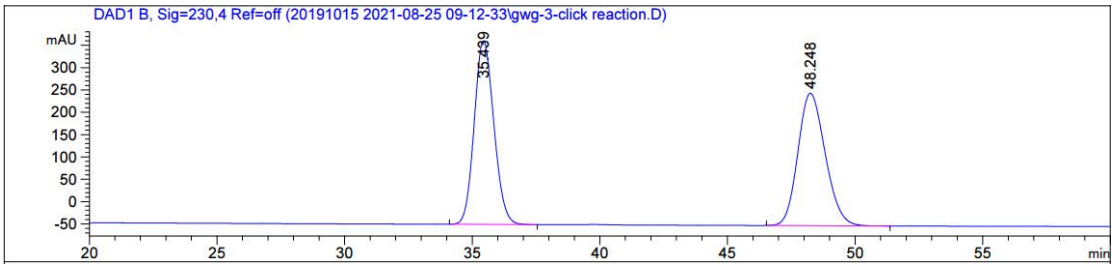
enantioenriched

Sample Name: gwg-3-114-racemic

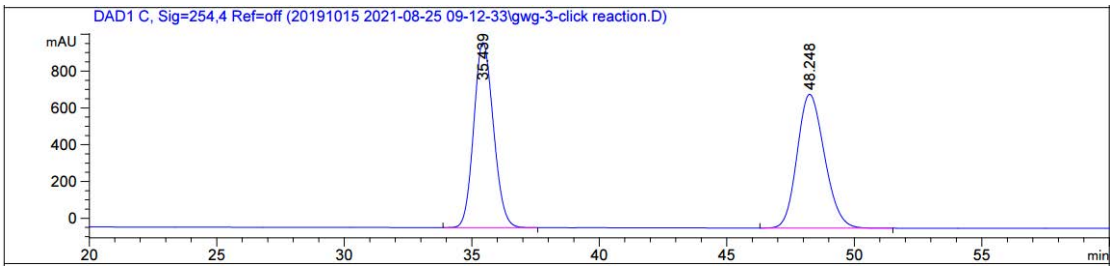
HPLC Condition: ADH, *n*-Hexane/*i*PrOH = 80:20, 1.0 mL/min



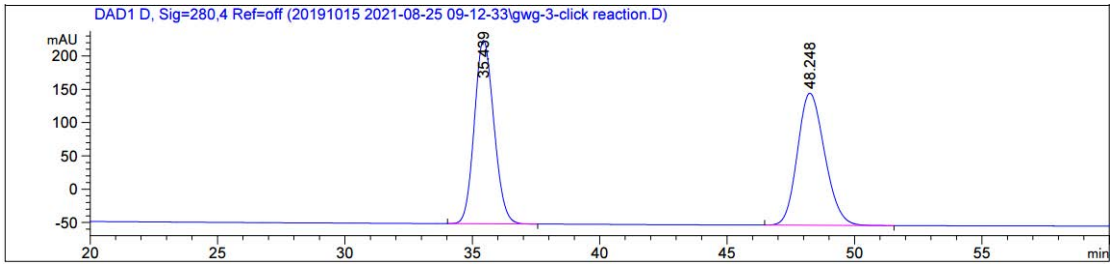
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	35.439	BB	0.8651	5.65630e4	1029.29639	49.5387
2	48.250	BB	1.1755	5.76164e4	760.85791	50.4613



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	35.439	BB	0.8316	2.19696e4	411.04282	49.9256
2	48.248	BB	1.1438	2.20350e4	296.22345	50.0744

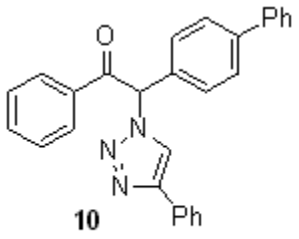


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	35.439	BB	0.8378	5.39580e4	1006.00275	49.8936
2	48.248	BB	1.1576	5.41883e4	727.03790	50.1064



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	35.439	BB	0.8315	1.47183e4	275.39395	49.9441
2	48.248	BB	1.1441	1.47513e4	198.24451	50.0559

End of Report



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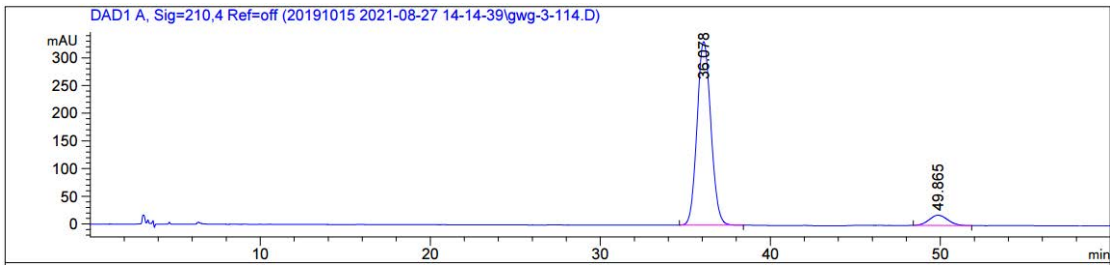
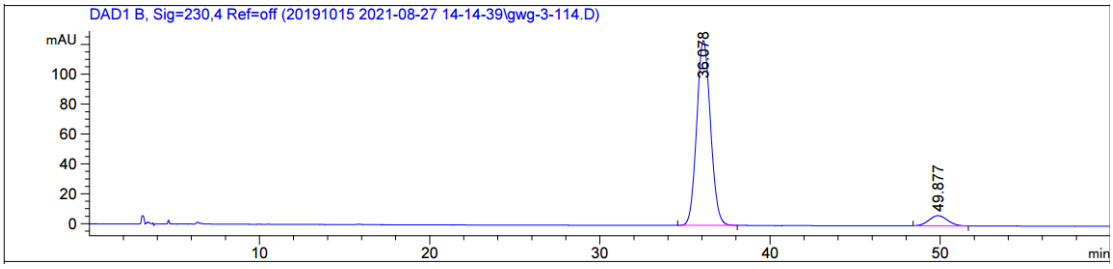
racemic

Sample Name: gwg-3-114-enantioenriched

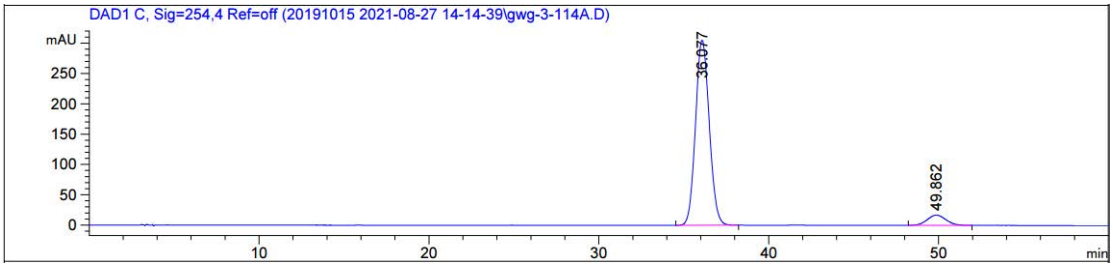
HPLC Condition: ADH, *n*-Hexane/*i*PrOH = 80:20, 1.0 mL/min



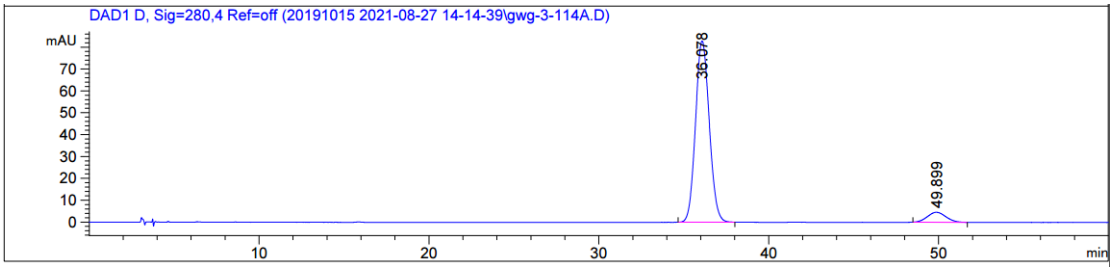
Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	36.078	BB	0.8748	1.87056e4	331.27939	93.0017
2	49.865	BB	0.9043	1407.58472	18.52926	6.9983



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	36.078	BB	0.8724	6963.04785	123.75789	93.1159
2	49.877	BB	0.8884	514.78400	6.80636	6.8841

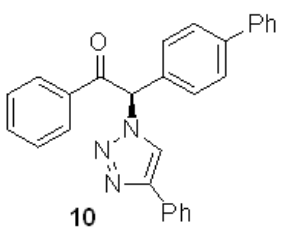


Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	36.077	BB	0.8743	1.71613e4	305.07858	92.9823
2	49.862	BB	0.9841	1295.23450	16.89993	7.0177



Peak	RetTime[min]	Type	Width[min]	Area[mAu*s]	Height[mAU]	Area[%]
1	36.078	BB	0.8641	4662.72803	82.90699	93.1309
2	49.899	BB	0.8998	343.90897	4.55016	6.8691

End of Report



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enantioenriched