Supporting Information

A Ruthenium-(Ph-BPE) Catalyst for Asymmetric Alkynylation of Fluoral: Enantioselection from 1 of 12 Fluxional Stereogenic-at-Ruthenium Complexes

Weijia Shen,[†§] Sebastian Höthker,[†§] Colin E. Hayter,[†] Nicholas K. Bowers,[†]
Andrea Pellegrini,[‡⊥] Stefan Grimme[‡] and Michael J. Krische*[†]

[⊥]Department of Industrial Chemistry Toso Montanari, University of Bologna, 40129 Bologna, Italy

[‡]Mulliken Center for Theoretical Chemistry, University of Bonn, 53115 Bonn, Germany

[†]Department of Chemistry, University of Texas at Austin, Austin, Texas 78712, United States

EMAIL: grimme@thch.uni-bonn.de, mkrische@cm.utexas.edu

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I. General Information

All reactions were run under an atmosphere of argon unless otherwise indicated. Resealable pressure tubes (13x100 mm) were purchased from Fisher Scientific (catalog number 14–959–35C) and were oven-dried prior to use. All commercial reagents, which include $RuHCl(CO)(PPh_3)_3$, KI, (*S*,*S*)-PhBPE, alkynes, fluoral, difluoroaldehydes, and solvents were used as received from vendors without further purification. 4Å Molecular Sieves were flame-dried prior to use. Purification of reaction products was carried out by flash column chromatography using 40-63 μm silica gel. Analytical thin-layer chromatography (TLC) was carried out using 0.25 mm commercial silica gel plates (Dynamic Adsorbents F254).

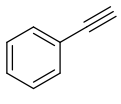
II. Spectroscopy, Spectrometry and Data Collection

Infrared spectra were recorded on a Perkin-Elmer 1600 spectrometer. High-resolution mass spectra (HRMS) were recorded on a Karatos MS9 and are reported as m/z. Electron spray ionization (ESI) was used unless otherwise indicated. Accurate masses are reported for the molecular ion (M^+, $M+H^+$, $M+Na^+$), or a suitable fragment ion. Proton nuclear magnetic resonance (^1H NMR) spectra were recorded on a Varian INOVA (400, 500, MHz) spectrometer equipped with a Bruker AVANCE III cryoprobe. Data are reported alongside their respective multiplicities (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet). Integration and coupling constants are reported in Hertz (Hz). Carbon-13 nuclear magnetic resonance (^{13}C NMR) spectra were recorded with a Varian INOVA (101, 126, 151 MHz) spectrometer and were routinely run with broadband decoupling. Fluorine-19 nuclear magnetic resonance (^{19}F NMR) spectra were recorded with a Varian INOVA (376, 471 MHz) spectrometer. Specific optical rotations were recorded on the polarimeter Azzota Corp AP45 (589 nm) in $CHCl_3$ or CH_2Cl_2. The concentrations of the employed solutions are given in the units of 10^{-2} g mL^{-1}. The absolute stereochemical assignments of products **3a**-**3y** and **5a**-**5f** were made in analogy to those observed for compound **3d** and **5b** which were determined *via* single crystal X-ray diffraction.

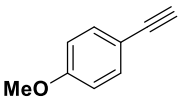
III. Known Reagents

The following reagents were either obtained from commercial sources or prepared following the given procedures.

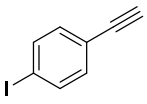
Alkynes



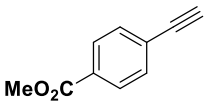
1a
commercial



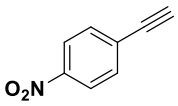
1b
commercial



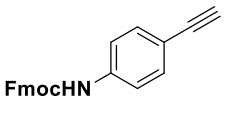
1c
Ref.1



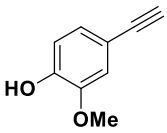
1d
commercial



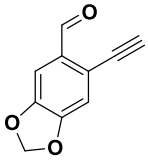
1e
commercial



1f
Ref.2



1g
Ref.3



1h
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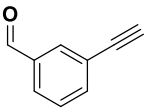
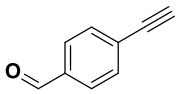
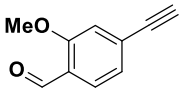


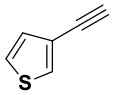
1i
Ref.5



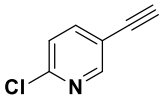
1k
Commercial



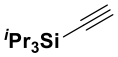
1l
Ref.5



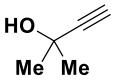
1m
commercial



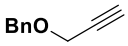
1n
Ref.6



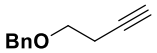
1r
commercial



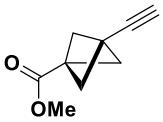
1s
Commercial



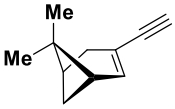
1t
Commercial



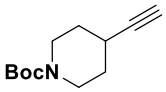
1u
Ref.7



1v
Ref.8

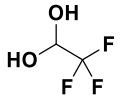


1w
Ref.9

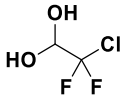


1y
commercial

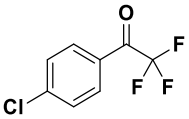
Fluorinated electrophiles



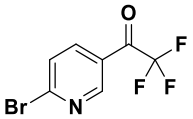
2a
commercial



4a
commercial



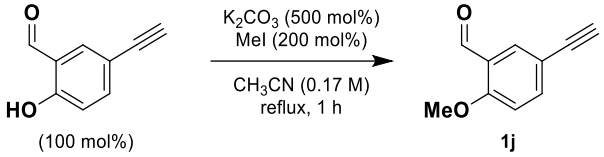
6a
commercial



6b
commercial

IV. Preparation of Alkynes

5-ethynyl-2-methoxybenzaldehydedifluoroacetate (1j)



An oven-dried 50 mL round-bottom flask equipped with a magnetic stir bar under an atmosphere of argon was charged with 5-ethynyl-2-hydroxybenzaldehyde[10] (250.0 mg, 1.70 mmol, 100 mol%) and K_2CO_3 (1.20 g, 8.65 mmol, 500 mol%). To the reaction vessel was added acetonitrile (10 mL, 0.17 M) and methyl iodide (485.4 mg, 3.42 mmol, 200 mol%). The reaction vessel was placed in an oil bath and heated at 82 °C. After stirring for one hour, the reaction mixture was allowed to reach ambient temperature and was filtered through silica gel with the aid of ethyl acetate. The mixture was transferred to a separatory funnel, and the organic layer was washed with water and brine, dried (Na_2SO_4), filtered, and concentrated *in vacuo*. The residue was subjected to flash column chromatography (SiO_2: 10:90 EtOAc:hexanes) to furnish the title compound **1j** as a yellow solid in 70% yield (190.8 mg, 1.19 mmol).

TLC (SiO_2): R_f = 0.5 (1:19 EtOAc:hexanes).

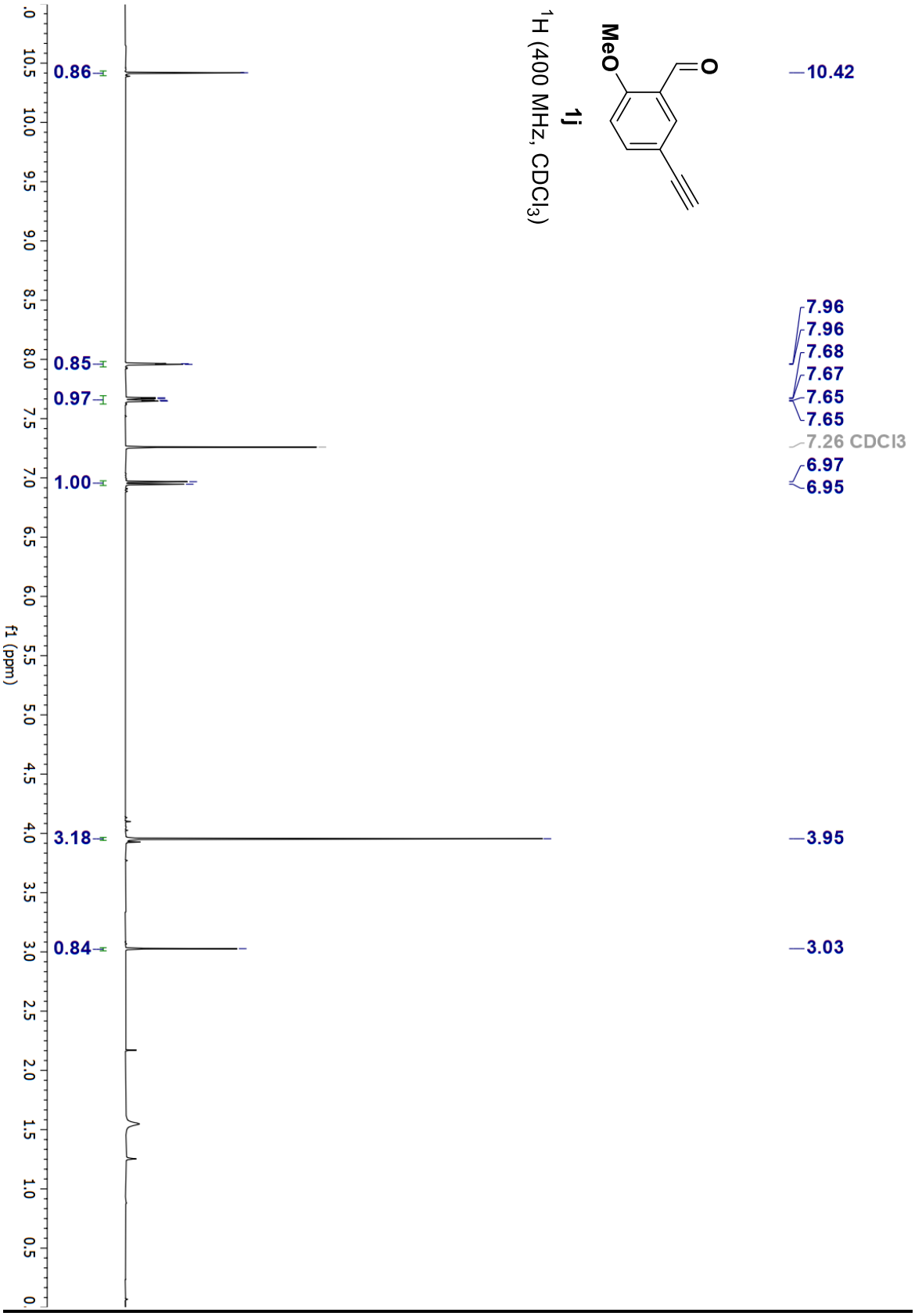
^{1}H NMR (400 MHz, $CDCl_3$): δ 10.42 (s, 1H), 7.96 (d, *J* = 2.2 Hz, 1H), 7.66 (dd, *J* = 8.7, 2.2 Hz, 1H), 6.96 (d, *J* = 8.6 Hz, 1H), 3.95 (s, 3H), 3.03 (s, 1H) ppm.

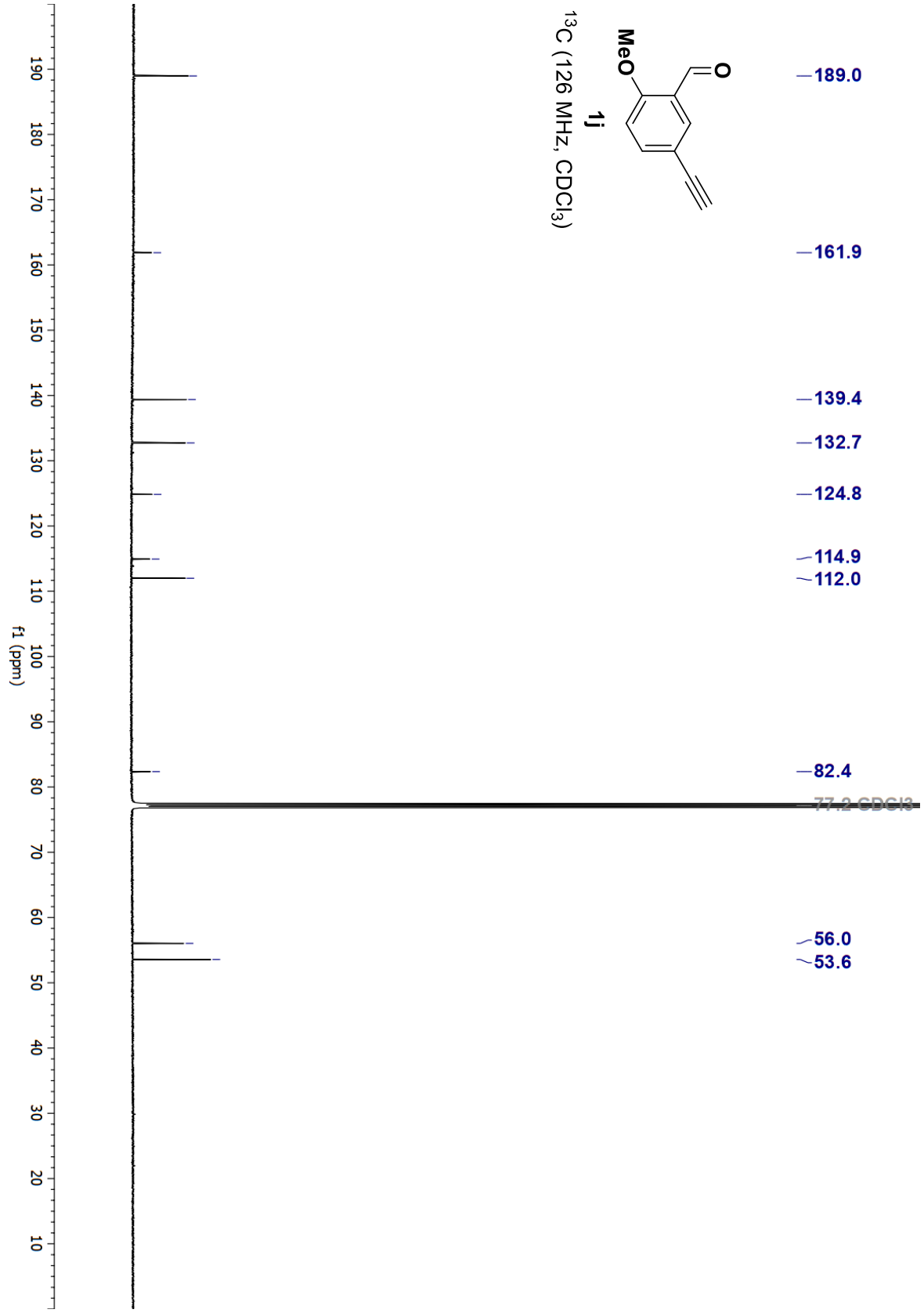
^{13}C NMR (126 MHz, $CDCl_3$): δ 189.0, 161.9, 139.4, 132.7, 124.8, 114.9, 112.0, 82.4, 56.0, 53.6 ppm.

HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_{10}H_9O_2^+$: 161.0597; found = 161.0597.

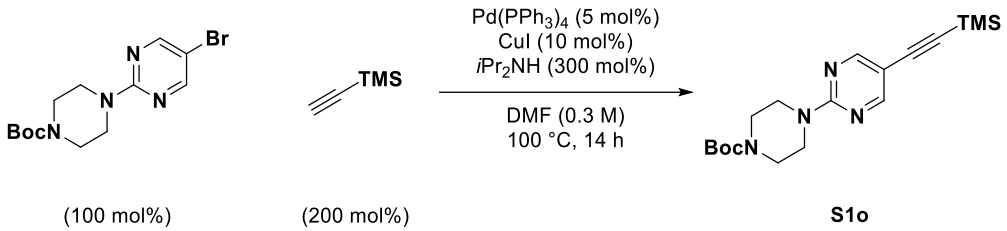
FTIR (neat): 3217, 2942, 2874, 2845, 1668, 1607, 1492, 1255, 1177, 1108, 1022, 829, 646, 572 cm^{-1}.

m.p.: 75 °C.


1j
^{1}H (400 MHz, CDCl$_3$)
MeO
O
10.42
7.96
7.96
7.68
7.67
7.65
7.65
7.26 CDCl3
6.97
6.95
3.95
3.03
0.86
0.85
0.97
1.00
3.18
0.84
f1 (ppm)


MeO
O
1j
^{13}C (126 MHz, CDCl$_3$)
189.0
161.9
139.4
132.7
124.8
114.9
112.0
82.4
77.2 CDCl3
56.0
53.6
f1 (ppm)

tert-butyl 4-(5-((trimethylsilyl)ethynyl)pyrimidin-2-yl)piperazine-1-carboxylate (S1o)



(100 mol%) (200 mol%) **S1o**

An oven-dried 125 mL round-bottom flask equipped with a magnetic stir bar under an atmosphere of argon was charged with dimethylformamide (20 mL, 0.3 M), which was sparged with argon for five minutes. To the reaction vessel, $Pd(PPh_3)_4$ (341.6 mg, 0.3 mmol, 5 mol%), copper(I) iodide (113.0 mg, 0.6 mmol, 10 mol%), diisopropylamine (2.5 mL, 18.3 mmol, 313 mol%), *tert*-butyl 4-(5-bromopyrimidin-2-yl)piperazine-1-carboxylate (2.0 g, 5.9 mmol, 100 mol%) and ethynyltrimethylsilane (1.2 mL, 8.4 mmol, 144 mol%) were added. The reaction vessel was placed in an oil bath and was allowed to stir for 14 hours at 100 °C. The reaction mixture was allowed to reach ambient temperature and was filtered through silica gel with the aid of ethyl acetate (100 mL). The filtrate was concentrated *in vacuo* and the residue was subjected to flash column chromatography (SiO_2: CH_2Cl_2:EtOAc 100:0–95:5) to furnish the title compound **S1o** as a pale yellow solid in 71% yield (1.50 g, 5.9 mmol).

TLC (SiO_2): R_f = 0.7 (9:1 CH_2Cl_2:EtOAc).

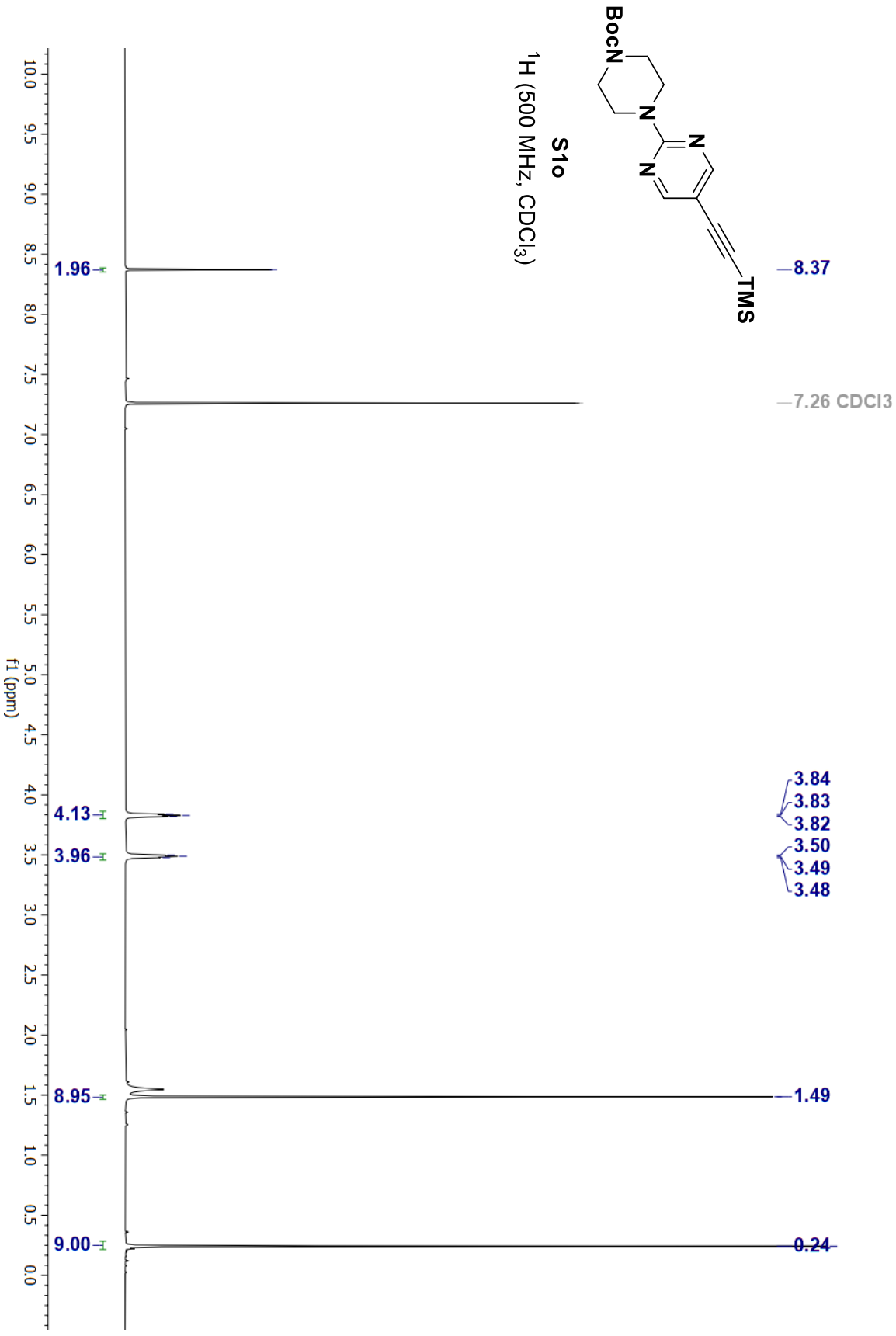
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.37 (s, 2H), 3.83 (t, *J* = 5.3 Hz, 4H), 3.49 (t, *J* = 5.3 Hz, 4H), 1.49 (s, 9H), 0.24 (s, 9H) ppm.

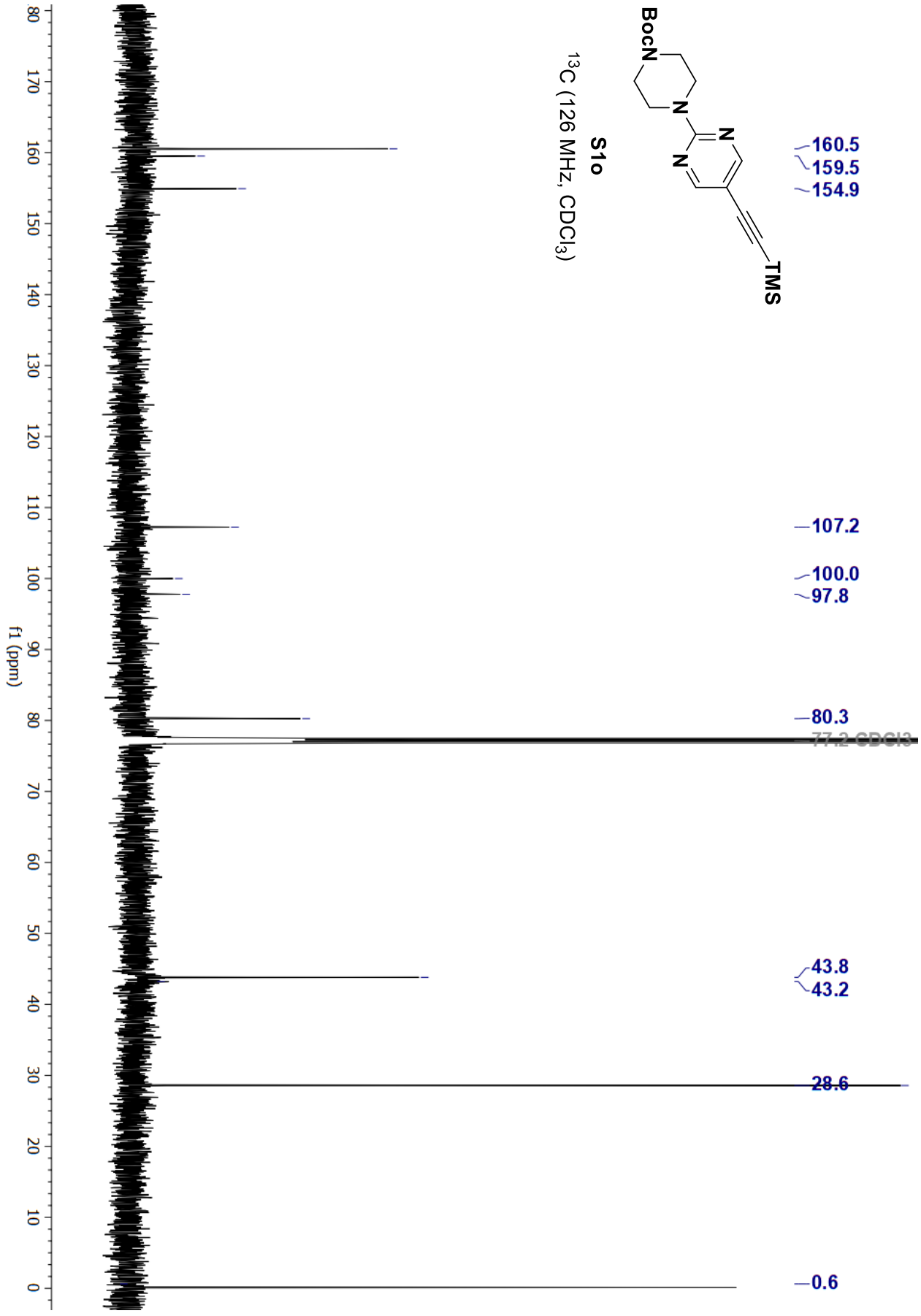
^{13}C NMR (126 MHz, $CDCl_3$): δ 160.5, 159.5, 154.9, 107.2, 100.0, 97.8, 80.3, 43.8, 43.2 (bs), 28.6, 0.6 ppm.

HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_{18}H_{29}N_4O_2Si^+$: 361.2054; found = 361.2060.

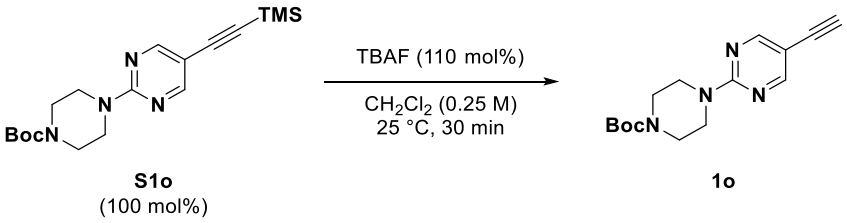
FTIR (neat): 2979, 2899, 2853, 2155, 1678, 1594, 1518, 1425, 1405, 1361, 1312, 1241, 1160, 1134, 1077, 993, 940, 836, 790, 758, 725, 699, 659, 633, 599, 552, 536, 484, 430, 420, 409 cm^{-1}.

m.p.: 175 °C.


S1o
^{1}H (500 MHz, CDCl$_3$)
BocN
N
N
N
TMS
f1 (ppm)
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1.96
4.13
3.96
8.95
9.00
8.37
7.26 CDCl3
3.84
3.83
3.82
3.50
3.49
3.48
1.49
0.24


S1o
^{13}C (126 MHz, $CDCl_3$)
BocN
N
N
TMS
160.5
159.5
154.9
107.2
100.0
97.8
80.3
77.2 CDCl3
43.8
43.2
28.6
0.6
f1 (ppm)

tert-butyl 4-(5-ethynylpyrimidin-2-yl)piperazine-1-carboxylate (1o)



S1o
(100 mol%)

1o

A 125 mL round-bottom flask equipped with a magnetic stir bar under an atmosphere of argon was charged with alkyne **S1o** (1.7 g, 4.7 mmol, 100 mol%) and dichloromethane (20 mL, 0.25 M). To the reaction vessel, a solution of tetra-*n*-butylammonium fluoride (1.0 M in THF, 5.0 mL, 5.0 mmol, 110 mol%) was added and the reaction mixture was allowed to stir at ambient temperature for 30 min. The volatiles were removed *in vacuo* and the residue was subjected to flash column chromatography (SiO_2: CH_2Cl_2:EtOAc 100:0–96:4) to furnish the title compound **1o** as an orange solid in 65% yield (884.0 mg, 3.1 mmol).

TLC (SiO_2): R_f = 0.7 (9:1 CH_2Cl_2:EtOAc).

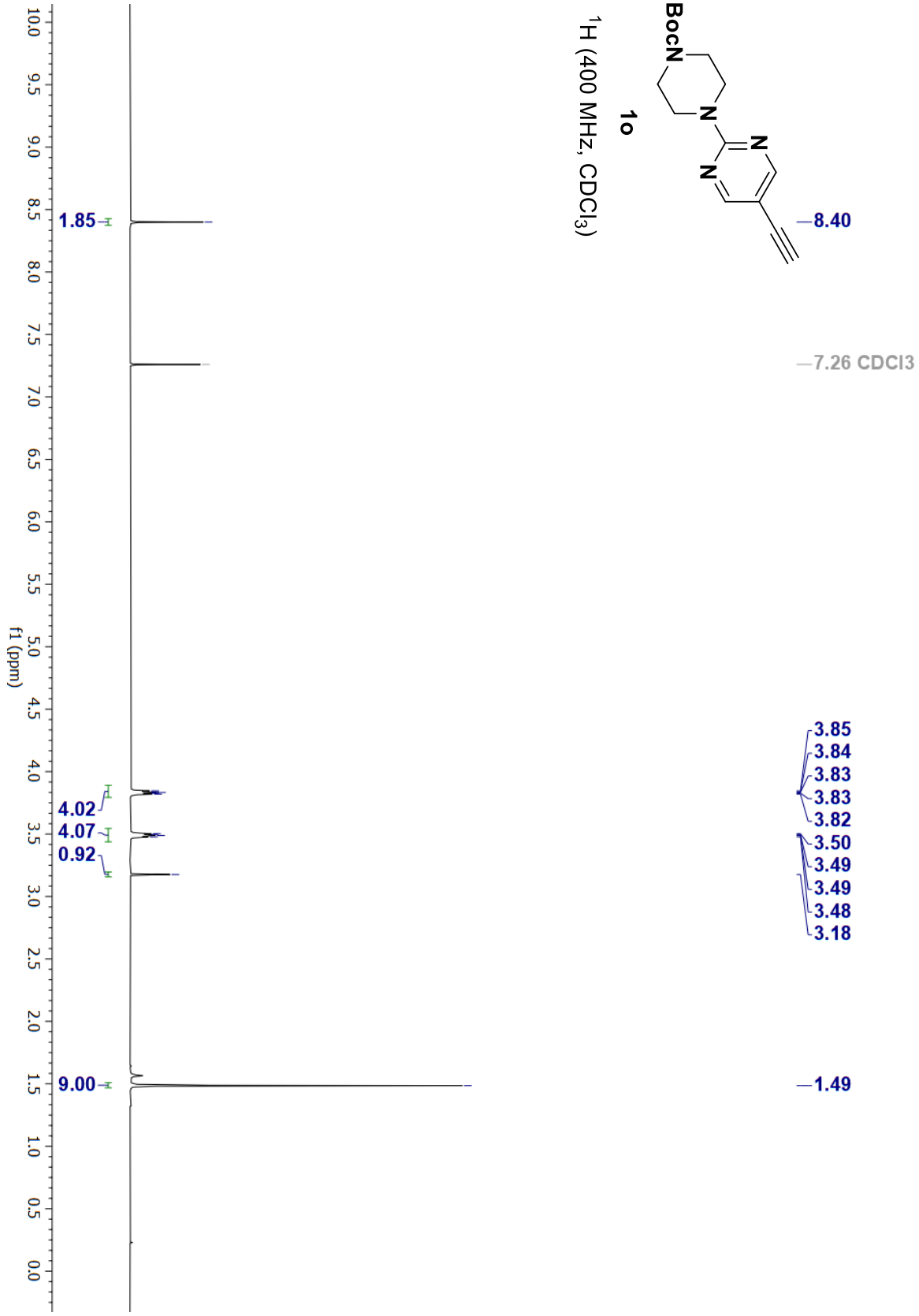
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.40 (s, 2H), 3.83 (dd, *J* = 6.3, 4.3 Hz, 4H), 3.49 (dd, *J* = 6.5, 4.0 Hz, 4H), 3.18 (s, 1H), 1.49 (s, 9H) ppm.

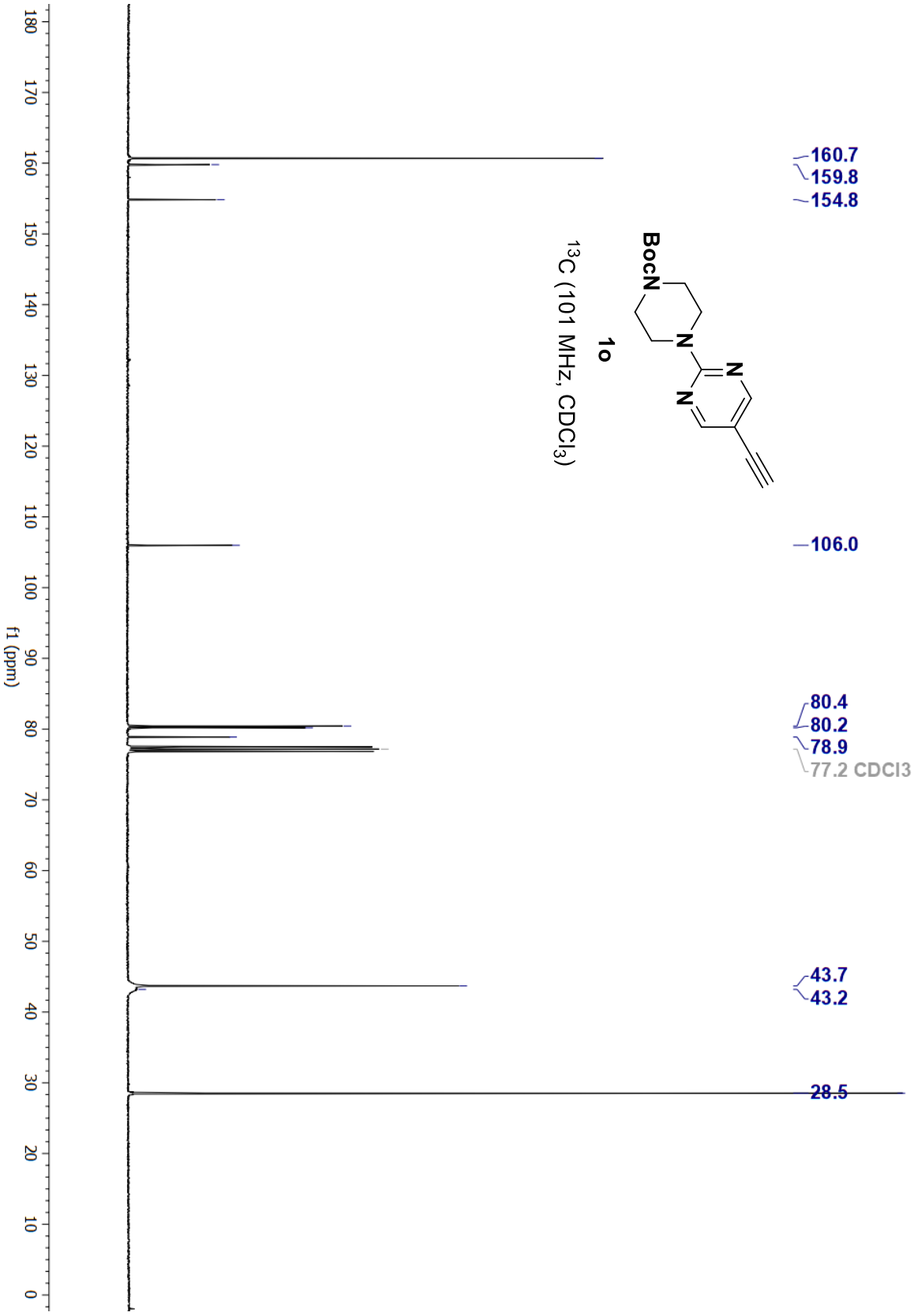
^{13}C NMR (101 MHz, $CDCl_3$): δ 160.7, 159.8, 154.8, 106.0, 80.4, 80.2, 78.9, 43.7, 43.2, 28.5 ppm.

HRMS (ESI(+)): m/z [M+Na^+] calcd. for $C_{15}H_{20}N_4NaO_2^+$: 311.1478; found = 311.1488.

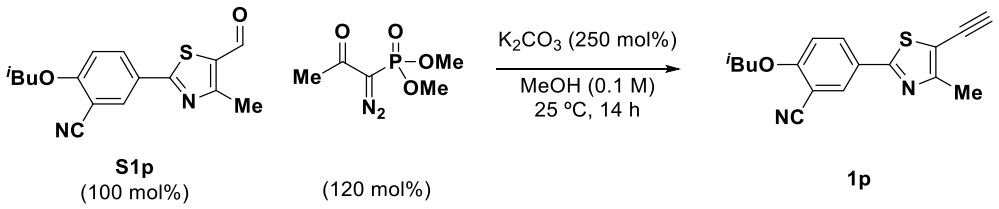
FTIR (neat): 3274, 3226, 3010, 2978, 2896, 2855, 2099, 1674, 1597, 1511, 1476, 1422, 1403, 1390, 1362, 1309, 1281, 1246, 1217, 1161, 1128, 1088, 1075, 994, 946, 862, 838, 791, 769, 723, 679, 658, 612, 572, 537, 519, 467, 420 cm^{-1}.

m.p.: 110 °C.


1o
^{1}H (400 MHz, CDCl$_3$)
BocN
N
N
N
8.40
7.26 CDCl3
3.85
3.84
3.83
3.83
3.82
3.50
3.49
3.49
3.48
3.18
1.49
1.85
4.02
4.07
0.92
9.00
f1 (ppm)


160.7
159.8
154.8
106.0
80.4
80.2
78.9
77.2 CDCl3
43.7
43.2
28.5
BocN
N
N
N
1o
^{13}C (101 MHz, CDCl$_3$)
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

5-(5-ethynyl-4-methylthiazol-2-yl)-2-isobutoxybenzonitrile (1p)



A 250 mL round-bottom flask equipped with a magnetic stir bar under an atmosphere of nitrogen was charged with **S1p**[11] (1.5 g, 5.0 mmol, 100 mol%), K_2CO_3 (1.7 g, 12.5 mmol, 250 mol%) and methanol (50 mL, 0.1 M). To the reaction vessel, dimethyl (1-diazo-2-oxopropyl)phosphonate (0.9 mL, 6.0 mmol, 120 mol%) was added dropwise and the reaction mixture was allowed to stir at ambient temperature for 14 hours. The reaction mixture was concentrated *in vacuo*. Water and diethyl ether were added to the resulting residue, and the mixture was transferred to a separatory funnel. The organic layer was washed with brine, dried (Na_2SO_4), filtered, and concentrated *in vacuo*. The residue was subjected to flash column chromatography (SiO_2: 40:60 EtOAc:hexanes) to furnish the title compound **1p** as a yellow solid in 81% yield (1.2 g, 4.1 mmol).

TLC (SiO_2): R_f = 0.3 (1:1 EtOAc:hexanes).

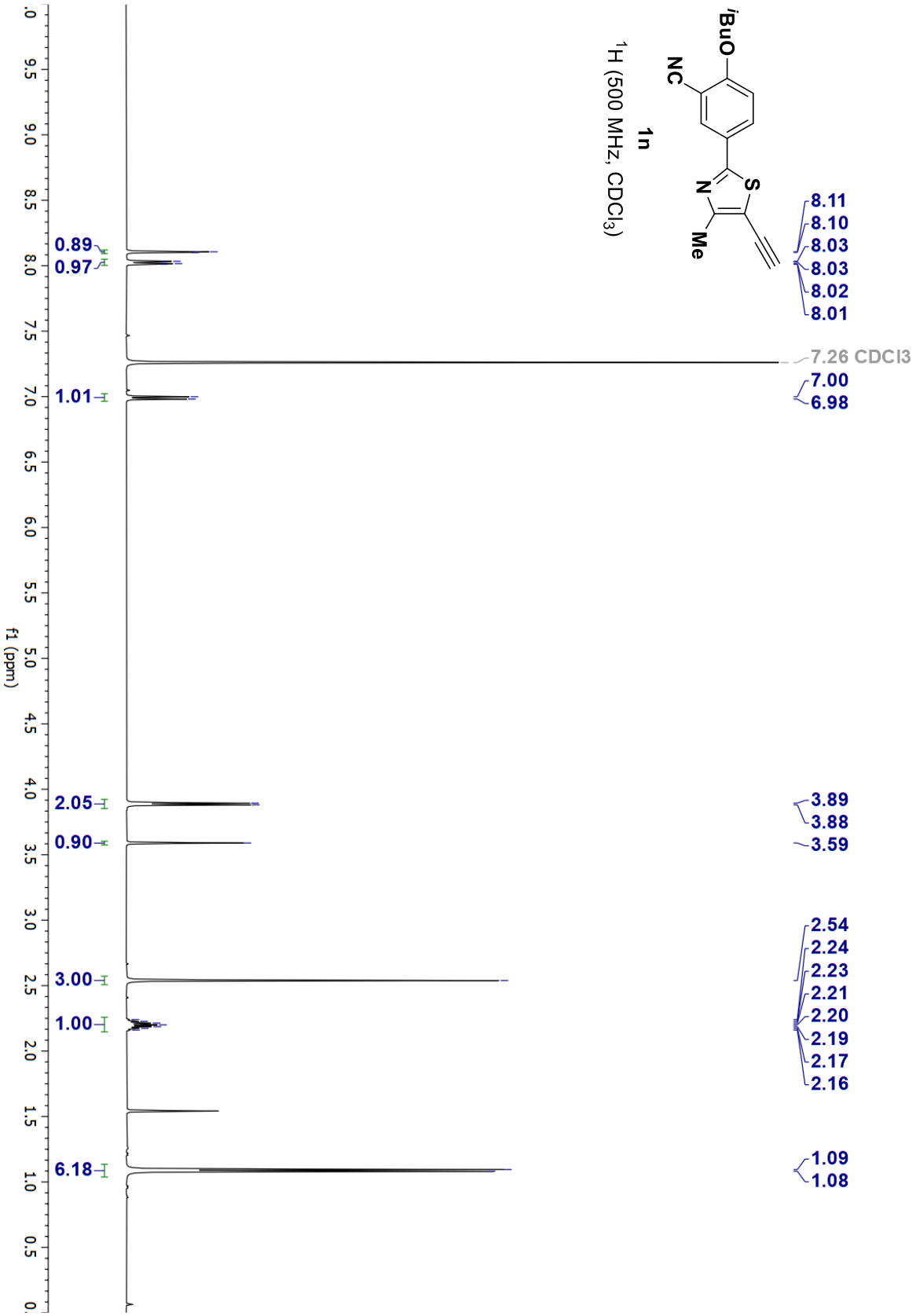
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.10 (d, *J* = 2.4 Hz, 1H), 8.02 (dd, *J* = 8.9, 2.3 Hz, 1H), 6.99 (d, *J* = 8.8 Hz, 1H), 3.89 (d, *J* = 6.4 Hz, 2H), 3.59 (s, 1H), 2.54 (s, 3H), 2.27 – 2.13 (m, 1H), 1.09 (d, *J* = 6.5 Hz, 6H) ppm.

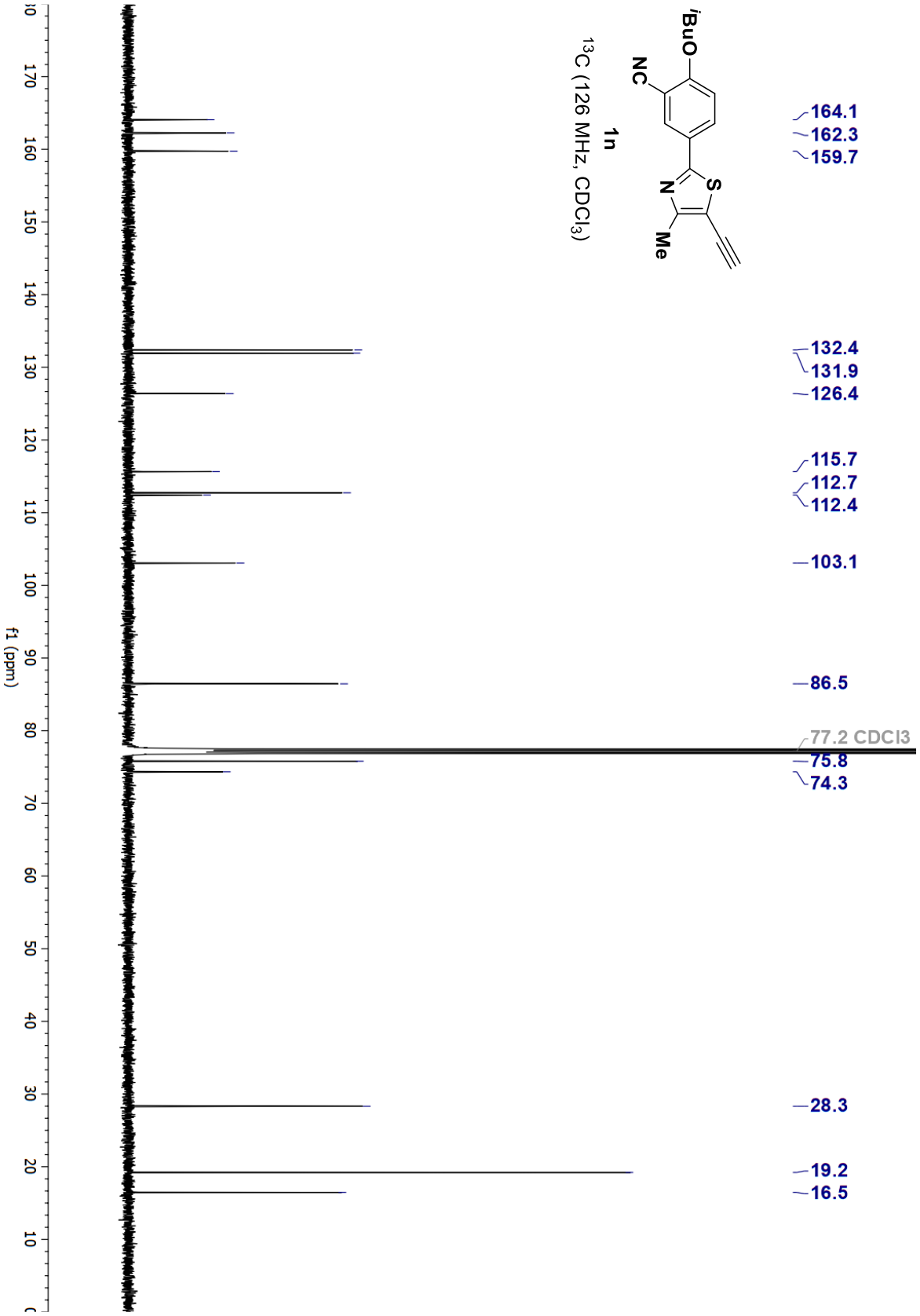
^{13}C NMR (126 MHz, $CDCl_3$): δ 164.1, 162.3, 159.7, 132.4, 131.9, 126.4, 115.7, 112.7, 112.4, 103.1, 86.5, 75.8, 74.3, 28.3, 19.2, 16.5 ppm.

HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_{17}H_{17}N_2OS^+$: 297.1056; found = 297.1061.

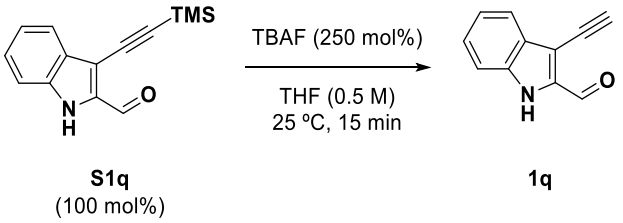
FTIR (neat): 3270, 2958, 2220, 1607, 1282, 1006, 832, 592, 494 cm^{-1}.

m.p.: 138 °C.


1n
^{1}H (500 MHz, CDCl$_3$)
^{i}BuO
NC
N
S
Me
8.11
8.10
8.03
8.03
8.02
8.01
7.26 CDCl3
7.00
6.98
3.89
3.88
3.59
2.54
2.24
2.23
2.21
2.20
2.19
2.17
2.16
1.09
1.08
0.89
0.97
1.01
2.05
0.90
3.00
1.00
6.18
f1 (ppm)


1n
^{13}C (126 MHz, CDCl$_3$)
^{i}BuO
NC
N
S
Me
164.1
162.3
159.7
132.4
131.9
126.4
115.7
112.7
112.4
103.1
86.5
77.2 CDCl3
75.8
74.3
28.3
19.2
16.5
f1 (ppm)

3-ethynyl-1*H*-indole-2-carbaldehyde (1q)



S1q
(100 mol%)

1q

A 50 mL round-bottom flask equipped with a magnetic stir bar under an atmosphere of nitrogen was charged with **S1q**[12] (482 mg, 2.0 mmol, 100 mol%) and THF (4 mL, 0.5 M). To the reaction vessel, tetra-*n*-butylammonium fluoride (1.0 M in THF, 5.0 mL, 5.0 mmol, 250 mol%) was added. It was allowed to stir at ambient temperature for 15 minutes. The reaction mixture was concentrated *in vacuo* and the resulting residue was diluted with water and diethyl ether and transferred to a separatory funnel. The organic layer was washed with brine, dried (Na_2SO_4), filtered, and concentrated *in vacuo*. The residue was subjected to flash column chromatography (SiO_2: 35:65 EtOAc:hexanes) to furnish the title compound **1q** as a brown solid in 99% yield (334.8 mg, 2.0 mmol).

TLC (SiO_2): R_f = 0.3 (1:2 EtOAc:hexanes).

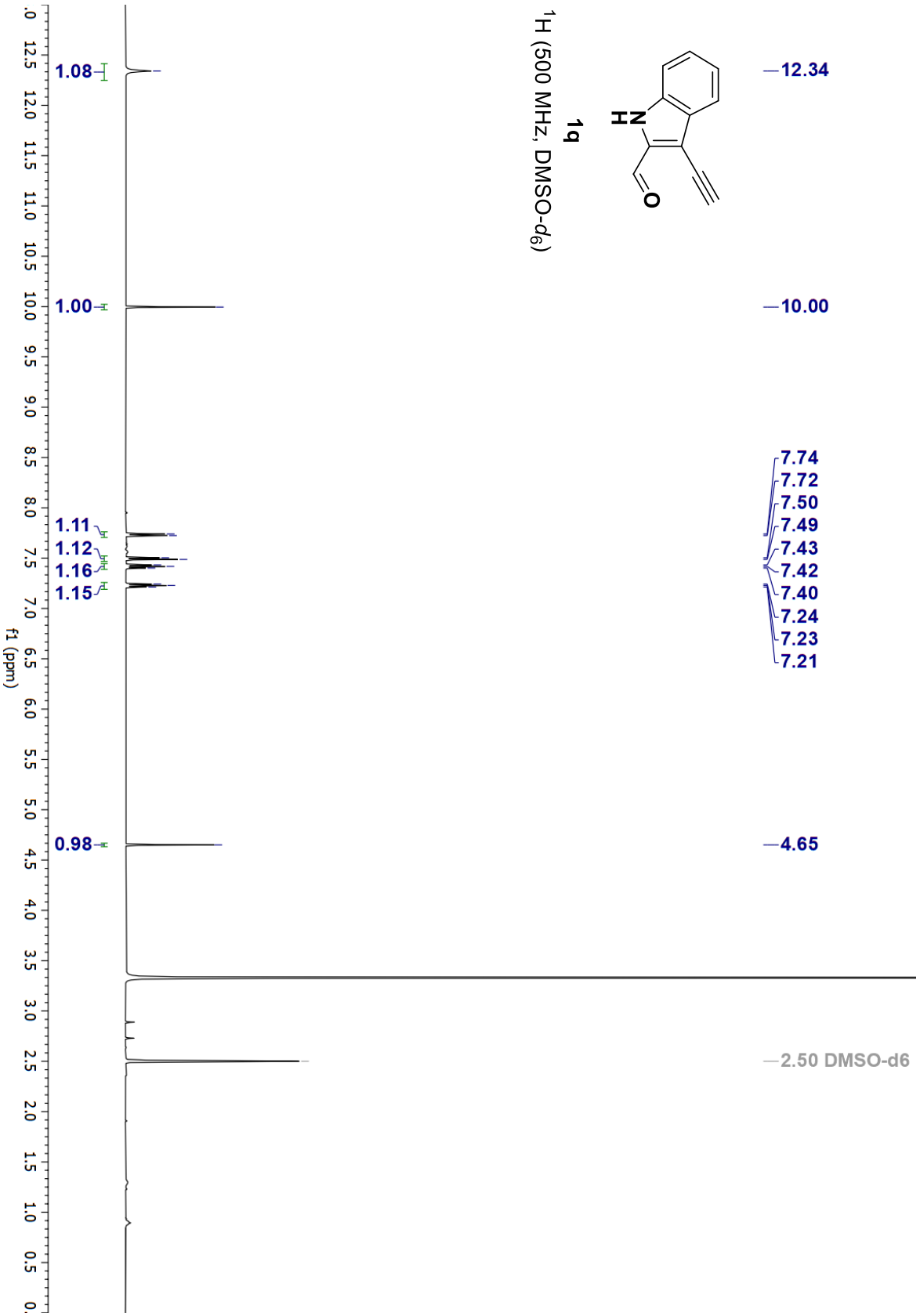
^{1}H NMR (500 MHz, DMSO-d_6): δ 12.34 (s, 1H), 10.00 (s, 1H), 7.73 (d, J = 8.1 Hz, 1H), 7.50 (d, J = 8.4 Hz, 1H), 7.42 (t, J = 7.7 Hz, 1H), 7.26 – 7.20 (m, 1H), 4.65 (s, 1H) ppm.

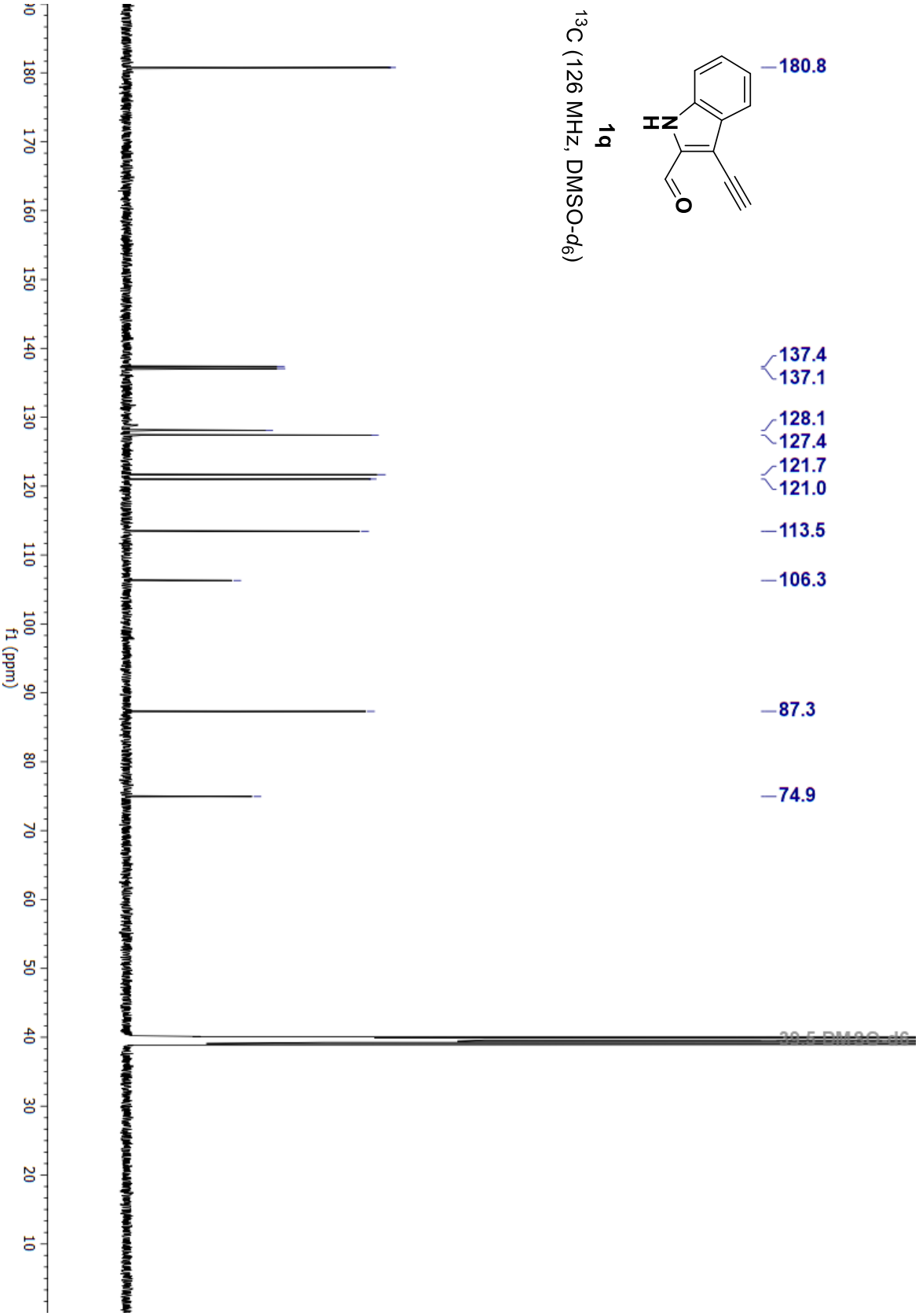
^{13}C NMR (126 MHz, DMSO-d_6): δ 180.8, 137.4, 137.1, 128.1, 127.4, 121.7, 121.0, 113.5, 106.3, 87.3, 74.9 ppm.

HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_{11}H_8NO^+$: 170.0600; found = 170.0594.

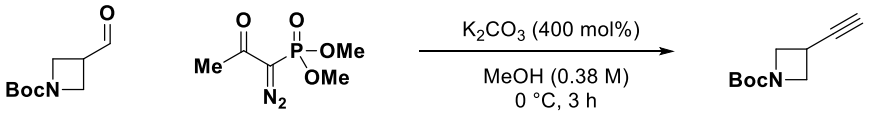
FTIR (neat): 3268, 2853, 1656, 1463, 1334, 1234, 740, 676, 612 cm^{-1}.

m.p.: 160 °C.


1q
^{1}H (500 MHz, DMSO-d_6)
12.34
10.00
7.74
7.72
7.50
7.49
7.43
7.42
7.40
7.24
7.23
7.21
4.65
2.50 DMSO-d6
1.08
1.00
1.11
1.12
1.16
1.15
0.98
f1 (ppm)


1q
^{13}C (126 MHz, DMSO-d_6)
180.8
137.4
137.1
128.1
127.4
121.7
121.0
113.5
106.3
87.3
74.9
39.5 DMSO-d6
f1 (ppm)

tert-butyl 3-ethynylazetidine-1-carboxylate (1x)



S1x (100 mol%) (115 mol%) **1x**

A 125 mL round-bottom flask equipped with a magnetic stir bar under an atmosphere of nitrogen was charged with aldehyde **S1x** (1.10 g, 5.7 mmol, 100 mol%), K_2CO_3 (3.10 g, 22.7 mmol, 400 mol%), and methanol (14.9 mL, 0.38 M). To the reaction vessel, dimethyl (1-diazo-2-oxopropyl)phosphonate (1.20 g, 6.5 mmol, 115 mol%) was added dropwise at 0 ºC and the reaction mixture was allowed to stir for three hours. The reaction mixture was concentrated *in vacuo*. Water and diethyl ether were added to the resulting residue, and the mixture was transferred to a separatory funnel. The organic layer was washed with saturated $NaHCO_3$ and brine, dried (Na_2SO_4), filtered, and concentrated *in vacuo*. The residue was subjected to flash column chromatography (SiO_2: 0:100–5:95 EtOAc:hexanes) to furnish the title compound **1x** as a colorless oil in 80% yield (817.4 mg, 4.5 mmol).

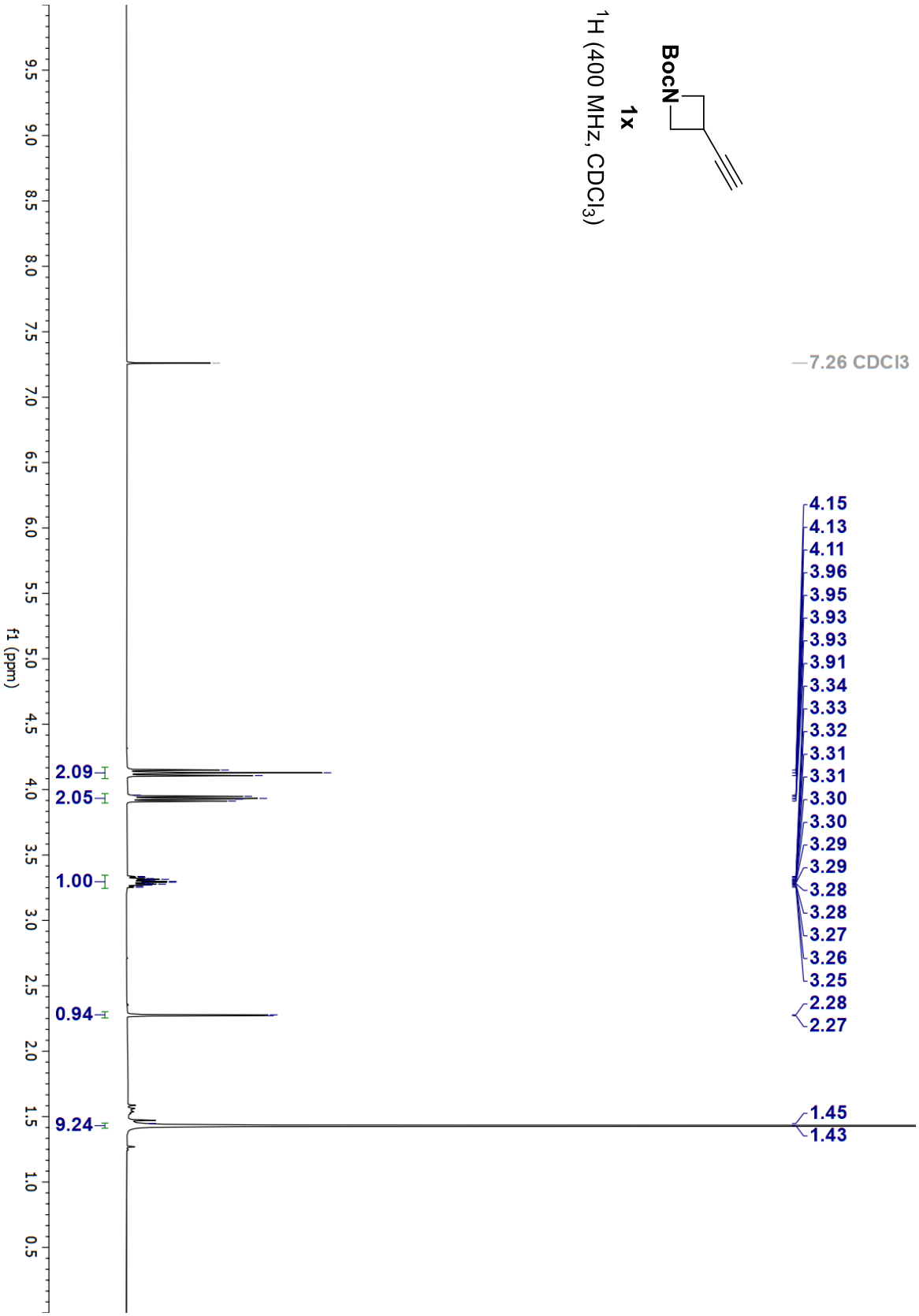
TLC (SiO_2): R_f = 0.7 (1:3 EtOAc:hexanes).

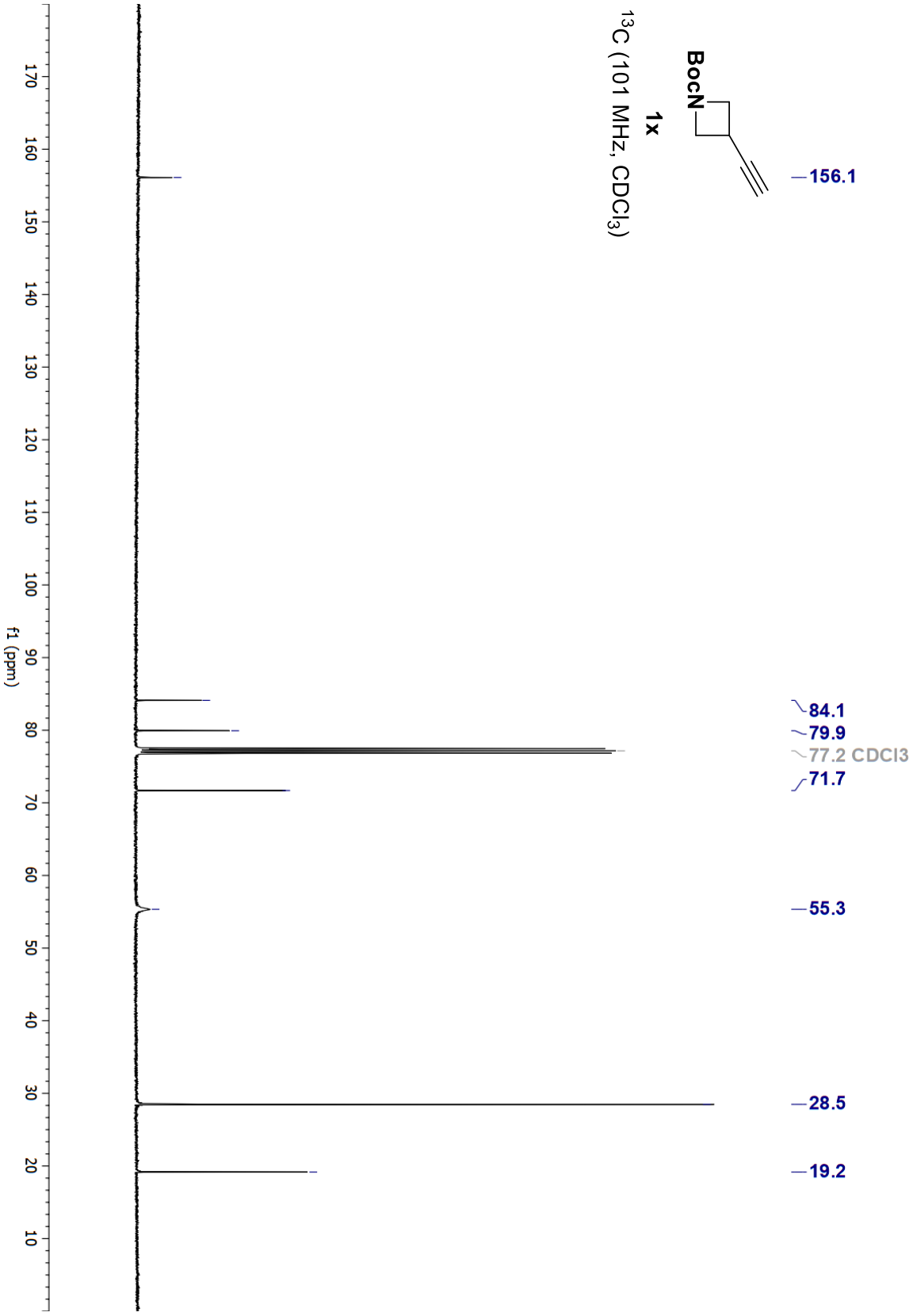
^{1}H NMR (400 MHz, $CDCl_3$): δ 4.13 (t, *J* = 8.5 Hz, 2H), 3.93 (dd, *J* = 8.2, 6.3 Hz, 2H), 3.29 (ttd, *J* = 8.8, 6.3, 2.5 Hz, 1H), 2.27 (d, *J* = 2.5 Hz, 1H), 1.43 (s, 9H) ppm.

^{13}C NMR (101 MHz, $CDCl_3$): δ 156.1, 84.1, 79.9, 71.7, 55.3, 28.5, 19.2 ppm.

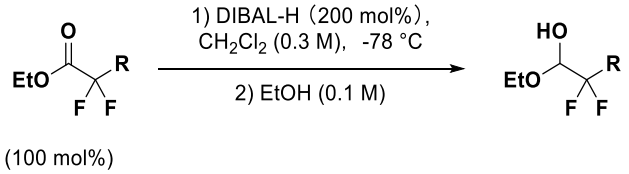
HRMS (ESI(+)): m/z [M+Na^+] calcd. for $C_{10}H_{25}NNaO_2^+$: 204.0995; found = 204.0998.

FTIR (neat): 3295, 2974, 2891, 1693, 1478, 1390, 1366, 1324, 1295, 1254, 1130, 927, 858, 773 cm^{-1}.


1H (400 MHz, CDCl3)
1x
BocN
7.26 CDCl3
4.15
4.13
4.11
3.96
3.95
3.93
3.93
3.91
3.34
3.33
3.32
3.31
3.31
3.30
3.30
3.29
3.29
3.28
3.28
3.27
3.26
3.25
2.28
2.27
1.45
1.43
2.09
2.05
1.00
0.94
9.24
f1 (ppm)


BocN
1x
^{13}C (101 MHz, $CDCl_3$)
156.1
84.1
79.9
77.2 CDCl3
71.7
55.3
28.5
19.2
f1 (ppm)

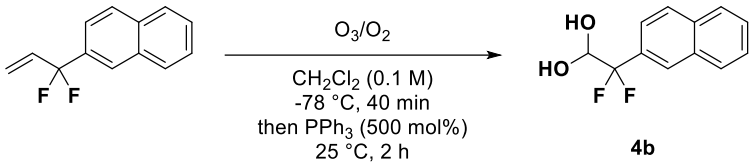
V. Preparation of Difluoroaldehydes



(100 mol%)

General Procedure A: A round-bottom flask equipped with a magnetic stir bar under an atmosphere of argon was charged with the respective difluoroester (100 mol%) and dichloromethane (0.3 M). The reaction mixture was cooled to -78 °C and DIBAL-H (1.0 M in hexanes, 200 mol%) was added dropwise. Upon full consumption of the starting material, ethanol was added dropwise. After Fieser work-up, the organic layer was filtered and concentrated *in vacuo*. Ethanol (0.1 M) was added to the resulting residue, and the mixture was allowed to stir for 14 hours. The mixture was concentrated *in vacuo* to furnish the corresponding hemiacetals which were used directly unless specified otherwise.

2,2-difluoro-2-(naphthalen-2-yl)ethane-1,1-diol (4b)



4b

A 50 mL round-bottom flask equipped with a magnetic stir bar was charged with 2-(1,1-difluoroallyl)naphthalene[13](404.0 mg, 1.9 mmol, 100 mol%) and dichloromethane (20 mL, 0.1 M). The reaction mixture was allowed to stir at -78 °C, while a stream of O_3/O_2 was passed through the solution. After 40 min, the solution was purged with nitrogen for 10 min before adding PPh_3 (2.6 g, 9.8 mmol, 500 mol%) and allowing it to stir for two hours at ambient temperature. The reaction mixture was concentrated *in vacuo* and the resulting residue was subjected to flash column chromatography (SiO_2: EtOAc:hexanes 20:80–25:75) to furnish the title compound **4b** as a colorless solid in 19% yield (85.0 mg, 0.4 mmol).

TLC (SiO_2): R_f = 0.3 (40:60 EtOAc:hexanes).

^{1}H NMR (400 MHz, DMSO-d_6): δ 8.08 (s, 1H), 8.04 (dd, J = 7.8, 1.9 Hz, 1H), 8.00–7.92 (m, 2H), 7.66 – 7.53 (m, 4H), 6.70 (d, J = 6.2 Hz, 2H), 5.16 (q, J = 5.8 Hz, 1H) ppm.

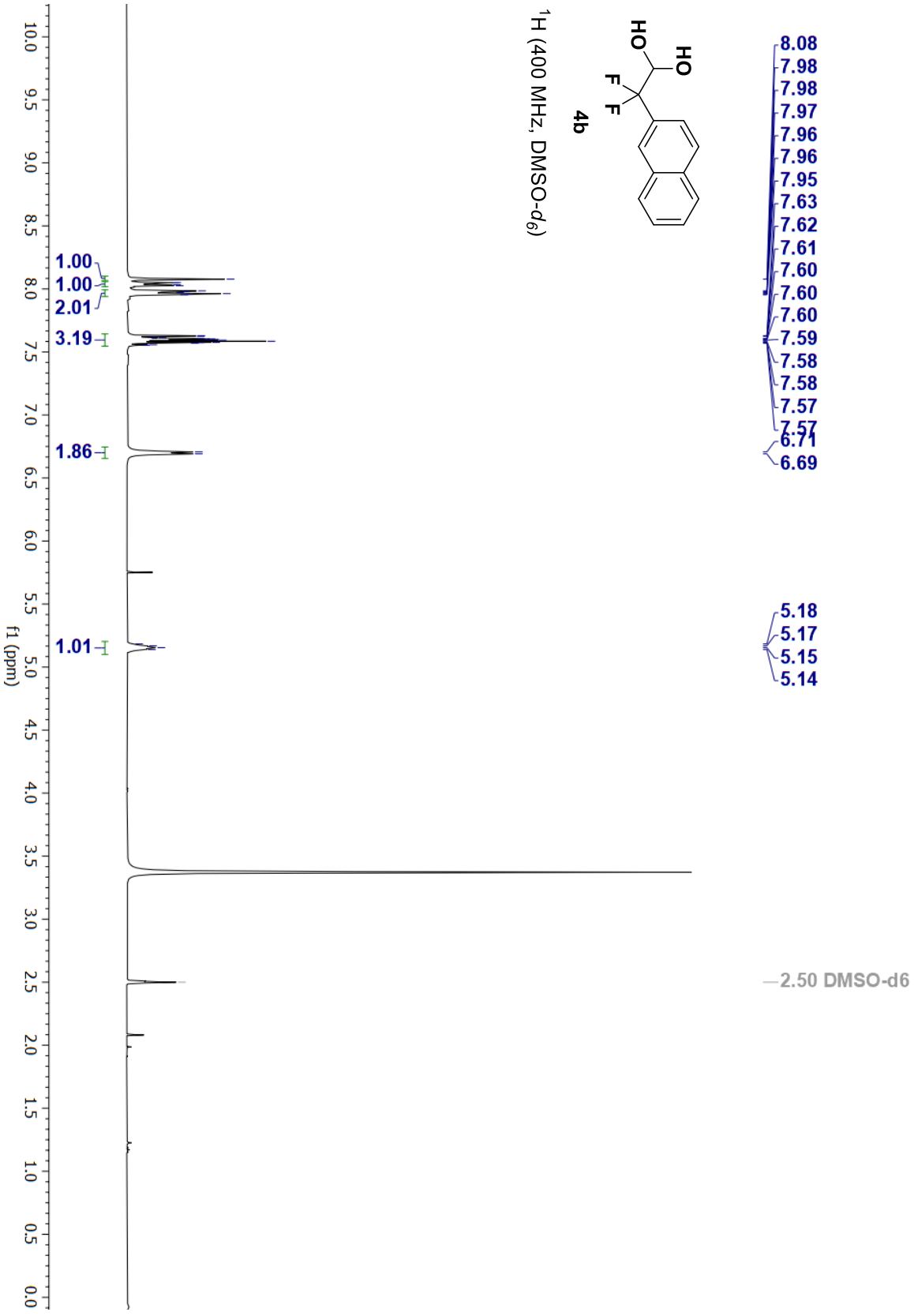
^{13}C NMR (101 MHz, DMSO-d_6): δ 133.3, 131.9, 131.4 (t, J = 25.3 Hz), 128.5, 127.5, 127.4, 127.1, 126.6, 126.2 (t, J = 7.0 Hz), 123.9 (t, J = 5.7 Hz), 120.0 (t, J = 246.2 Hz), 89.3 (t, J = 34.3 Hz) ppm.

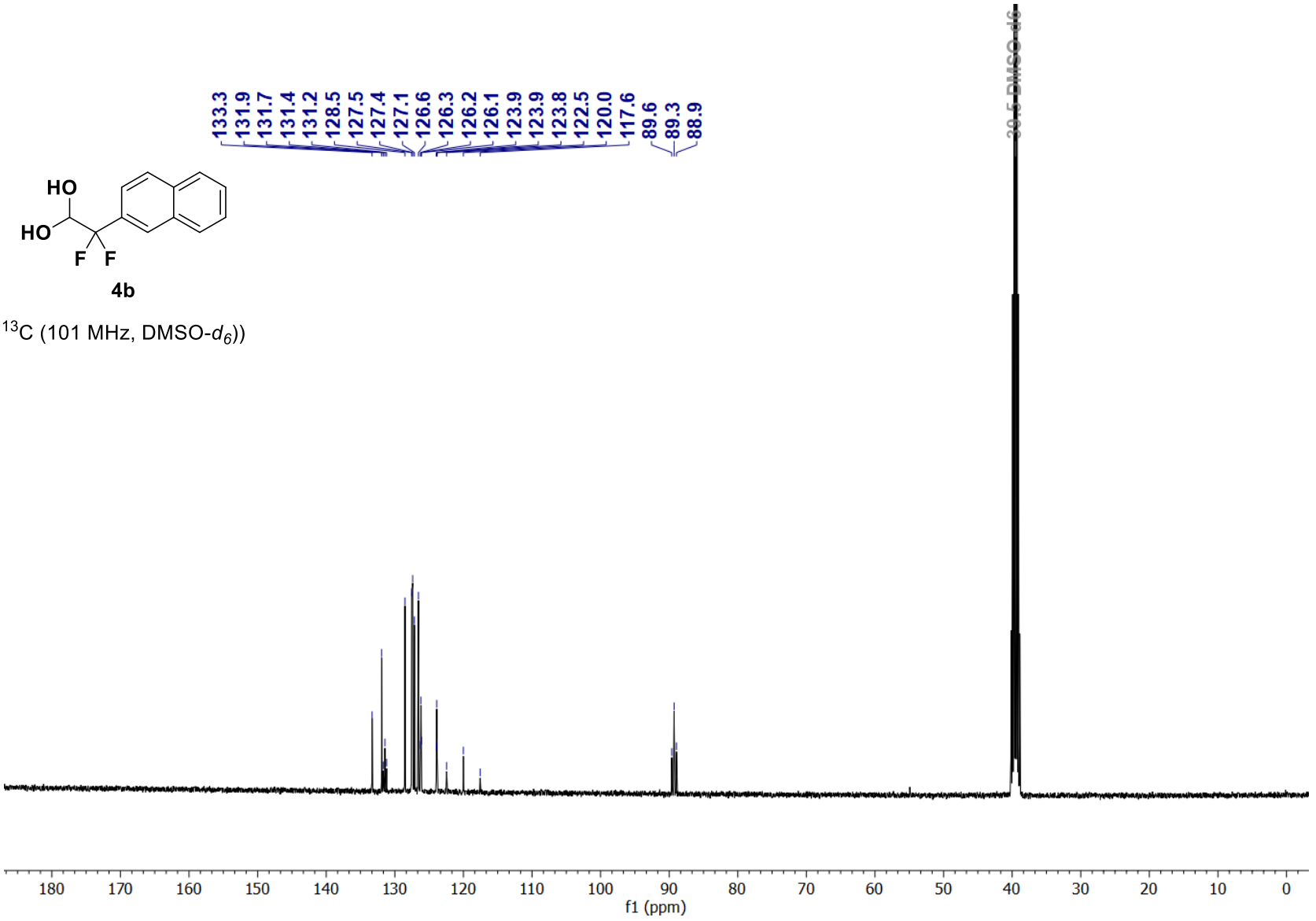
^{19}F NMR (376 MHz, DMSO-d_6): δ -108.3 (d, J = 6.3 Hz) ppm.

HRMS (ESI(+)): m/z [M+Na^+] calcd. for $C_{12}H_{10}F_2O_2Na^+$: 247.0541; found = 247.0541.

FTIR (neat): 3232, 3055, 1275, 1262, 1222, 1184, 1080, 1055, 1017, 1001, 969 cm^{-1}.

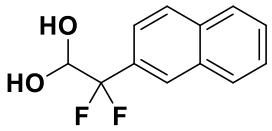
m.p.: 128 °C.


^{1}H (400 MHz, DMSO-d_6)
4b
HO
HO
F
F
8.08
7.98
7.98
7.97
7.96
7.96
7.95
7.63
7.62
7.61
7.60
7.60
7.60
7.59
7.58
7.58
7.57
7.57
6.71
6.69
5.18
5.17
5.15
5.14
2.50 DMSO-d6
1.00
1.00
2.01
3.19
1.86
1.01
f1 (ppm)



4b

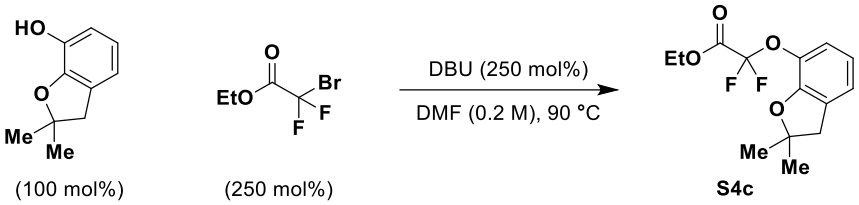
^{13}C (101 MHz, DMSO-d_6))



4b

^{19}F (376 MHz, DMSO-d_6)

Ethyl 2-((2,2-dimethyl-2,3-dihydrobenzofuran-7-yl)oxy)-2,2-difluoroacetate (S4c)



A 100 mL round-bottom flask equipped with a magnetic stir bar under an atmosphere of argon was charged with 2,2-dimethyl-2,3-dihydrobenzofuran-7-ol (1.64 g, 10.0 mmol, 100 mol%) and dimethylformamide (50 mL, 0.2 M).To the reaction vessel, ethyl 2-bromo-2,2-difluoroacetate (5.07 g, 25.0 mmol, 250 mol%) and 1,8-diazabicyclo[5.4.0]undec-7-ene (3.81 g, 25.0 mmol, 250 mol%) were added. The reaction vessel was placed in an oil bath and was allowed to stir at 90 °C. After 16 hours, the reaction mixture was allowed to reach ambient temperature and was diluted with ethyl acetate. The reaction mixture was transferred to a separatory funnel with the aid of ethyl acetate, and the organic layer was washed with water and brine, dried (Na_2SO_4), filtered, and concentrated *in vacuo*. The resulting residue was subjected to flash column chromatography (SiO_2: 6:94 EtOAc:hexanes) to furnish the title compound **S4c** as a pale yellow oil in 65% yield (1.85 g, 6.46 mmol).

TLC (SiO_2): R_f = 0.3 (1:5 EtOAc:hexanes).

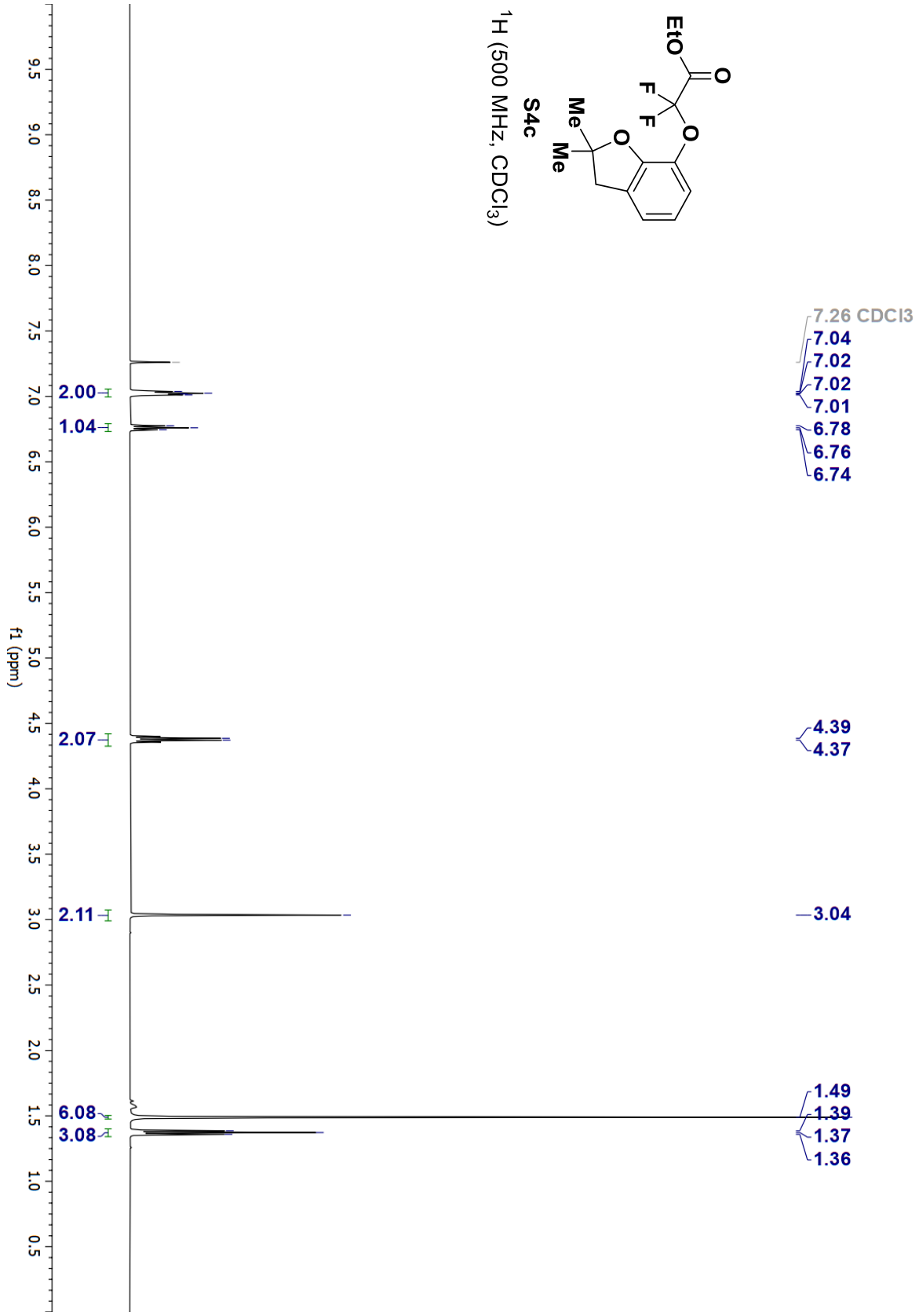
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.05 – 7.00 (m, 2H), 6.76 (t, *J* = 7.8 Hz, 1H), 4.38 (q, *J* = 7.1 Hz, 2H), 3.04 (s, 2H), 1.49 (s, 6H), 1.37 (t, *J* = 7.1 Hz, 3H) ppm.

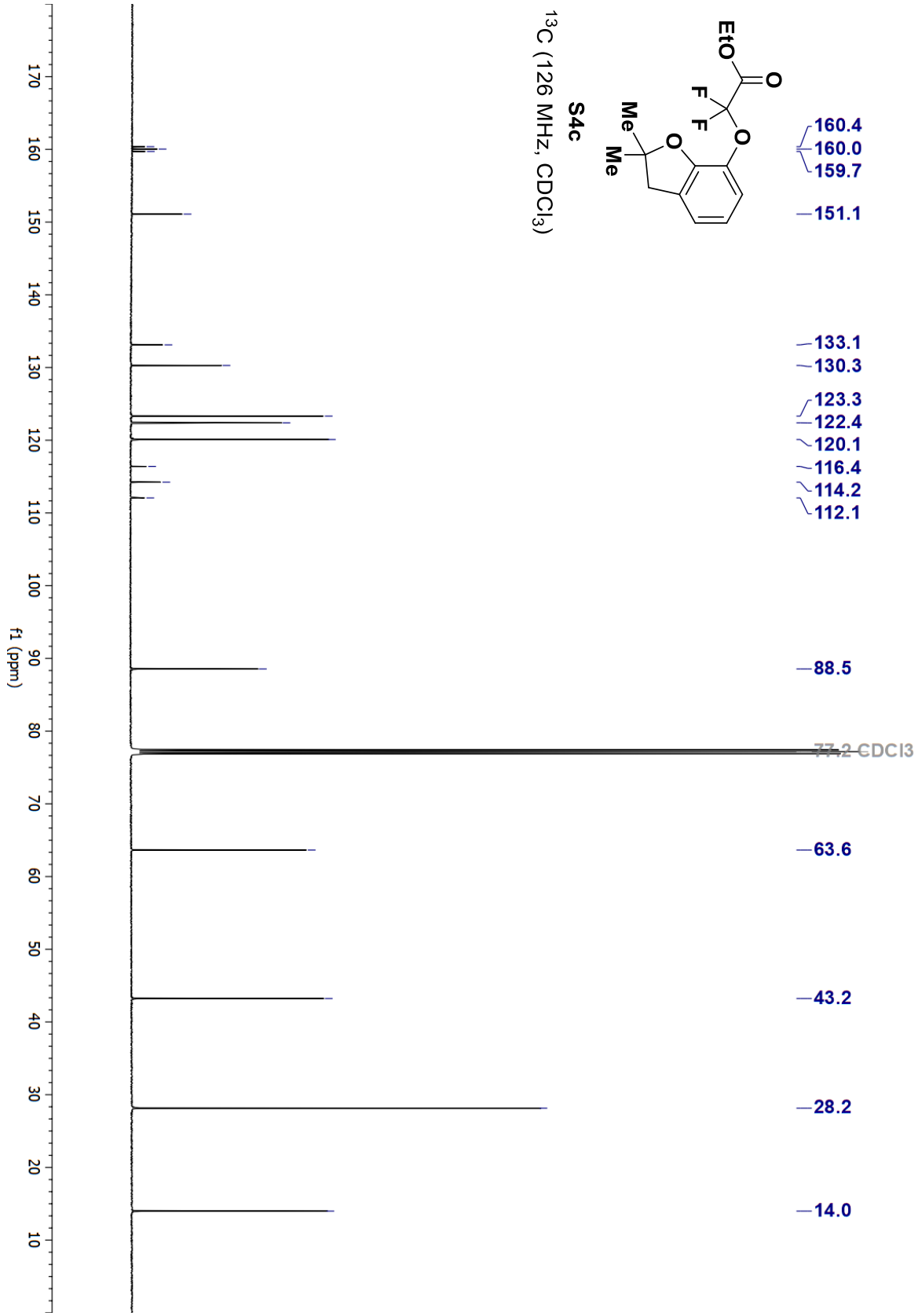
^{13}C NMR (126 MHz, $CDCl_3$): δ 160.0 (t, *J* = 41.6 Hz), 151.1, 133.1 (t, *J* = 2.3 Hz), 130.3, 123.3, 122.4, 120.1, 114.2 (t, *J* = 272.5 Hz), 88.5, 63.6, 43.2, 28.2, 14.0 ppm.

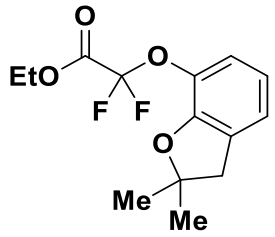
^{19}F NMR (471 MHz, $CDCl_3$): δ -76.4 ppm.

HRMS (ESI(+)): m/z [M+Na^+] calcd. for $C_{14}H_{16}F_2NaO_4^+$: 309.0909; found = 309.0907.

FTIR (neat): 2978, 2932, 1772, 1618, 1597, 1480, 1467, 1372, 1332, 1296, 1259, 1234, 1128, 1053, 998, 874, 855, 810, 774, 753, 717, 560 cm^{-1}.


S4c
^{1}H (500 MHz, CDCl$_3$)
EtO
O
F
F
O
O
Me
Me
f1 (ppm)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
2.00
1.04
2.07
2.11
6.08
3.08
7.26 CDCl3
7.04
7.02
7.02
7.01
6.78
6.76
6.74
4.39
4.37
3.04
1.49
1.39
1.37
1.36

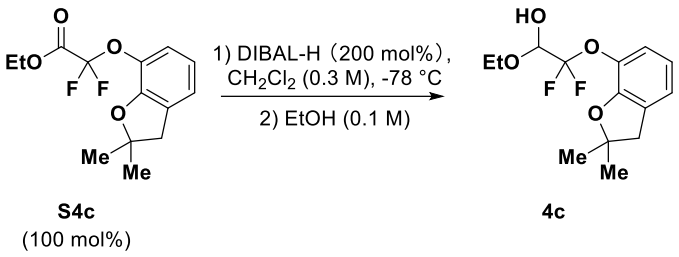

S4c
^{13}C (126 MHz, CDCl$_3$)
EtO
O
F
F
O
O
Me
Me
160.4
160.0
159.7
151.1
133.1
130.3
123.3
122.4
120.1
116.4
114.2
112.1
88.5
77.2 CDCl3
63.6
43.2
28.2
14.0
f1 (ppm)



S4c

^{19}F (471 MHz, $CDCl_3$)

2-((2,2-dimethyl-2,3-dihydrobenzofuran-7-yl)oxy)-1-ethoxy-2,2-difluoroethan-1-ol (4c)



S4c
(100 mol%)

4c

The reaction was performed according to **General Procedure A** using **S4c** (1.00 g, 3.5 mmol, 100 mol%). The concentrated reaction mixture was subjected to flash column chromatography (SiO_2: 24:76 EtOAc:hexanes) to furnish the title compound **4c** as an unstable oil in 36% yield (364.5 mg, 1.3 mmol). It was redissolved in ethanol and allowed to stir at ambient temperature overnight. The mixture was concentrated *in vacuo*, and the resulting residue (containing residual ethanol) was used directly in the next step.

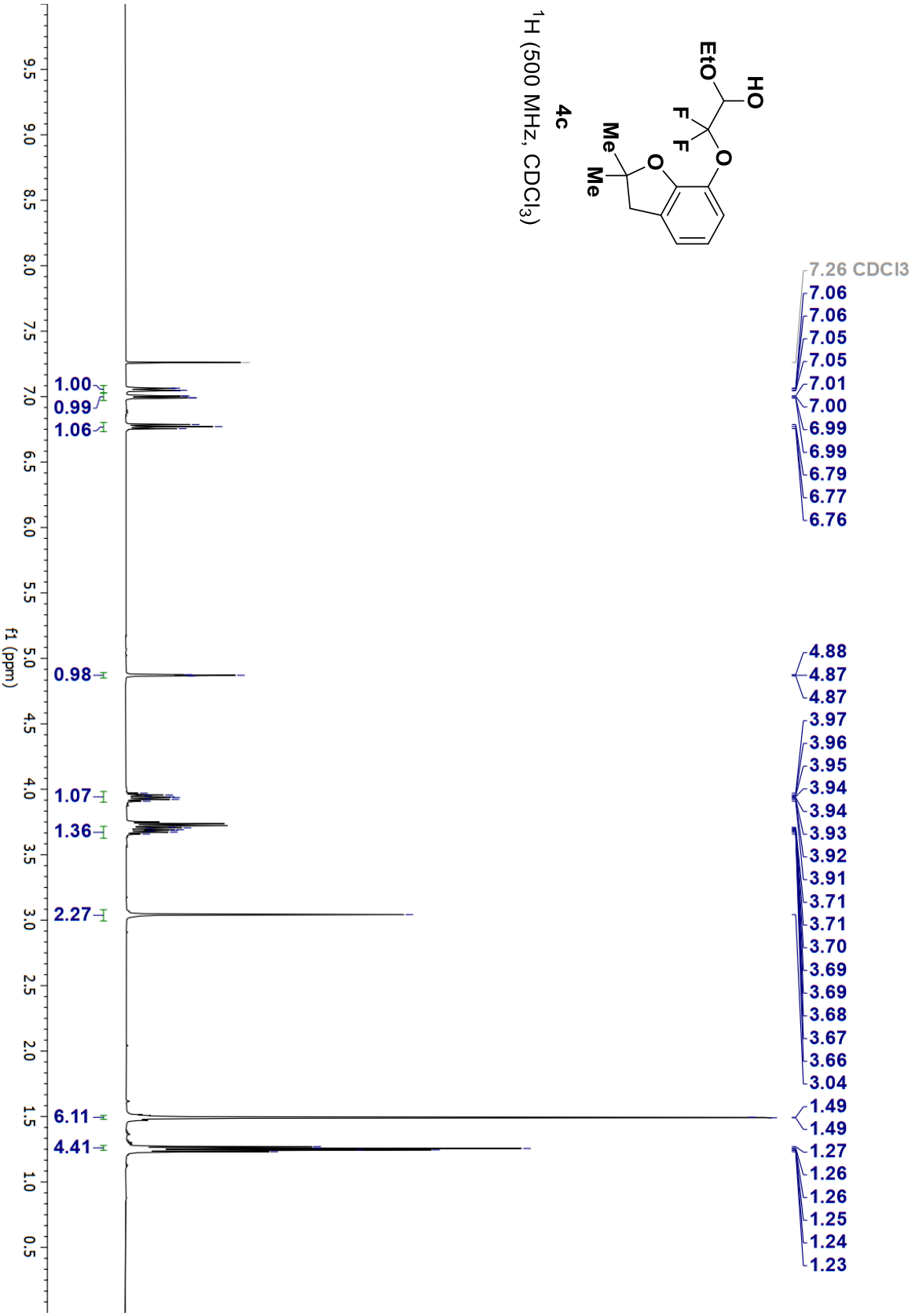
TLC (SiO_2): R_f = 0.3 (30:70 EtOAc:hexanes).

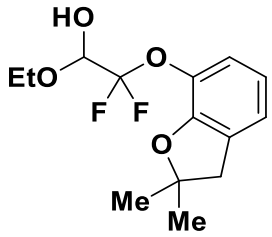
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.05 (dd, *J* = 8.2, 1.6 Hz, 1H), 7.00 (dd, *J* = 7.4, 1.2 Hz, 1H), 6.77 (t, *J* = 7.8 Hz, 1H), 4.87 (t, *J* = 2.3 Hz, 1H), 3.94 (dq, *J* = 9.7, 7.1 Hz, 1H), 3.71 – 3.65 (m, 1H), 3.04 (s, 2H), 1.49 (d, *J* = 1.8 Hz, 6H), 1.31 – 1.20 (m, 3H) ppm.

^{19}F NMR (471 MHz, $CDCl_3$): δ -84.6 – -85.0 (m), -85.0 – -85.3 (m) ppm.

HRMS (ESI(+)): m/z [M+Na^+] calcd. for $C_{14}H_{18}F_2NaO_4^+$: 311.1065; found = 311.1068.

Due to the instability of **4c**, it was used without further characterization.

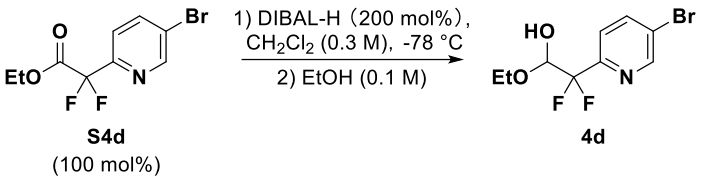

4c
^{1}H (500 MHz, CDCl$_3$)
HO
EtO
F
F
O
O
Me
Me
7.26 CDCl3
7.06
7.06
7.05
7.05
7.01
7.00
6.99
6.99
6.79
6.77
6.76
4.88
4.87
4.87
3.97
3.96
3.95
3.94
3.94
3.93
3.92
3.91
3.71
3.71
3.70
3.69
3.69
3.68
3.67
3.66
3.04
1.49
1.49
1.27
1.26
1.26
1.25
1.24
1.23
1.00
0.99
1.06
0.98
1.07
1.36
2.27
6.11
4.41
f1 (ppm)



4c

^{19}F (471 MHz, $CDCl_3$)

2-(5-bromopyridin-2-yl)-1-ethoxy-2,2-difluoroethan-1-ol (4d)



The reaction was performed according to **General Procedure A** using **S4d**[14](1.00 g, 3.6 mmol, 100 mol%). The concentrated reaction mixture was subjected to flash column chromatography (SiO_2: 50:50 EtOAc:hexanes) to furnish the title compound **4d** as an unstable oil in 30% yield (303.4 mg, 1.1 mmol). **4d** was dissolved in ethanol and allowed to stir at ambient temperature overnight. The mixture was concentrated *in vacuo*, and the resulting residue (94 wt% solution in ethanol) was used directly in the next step.

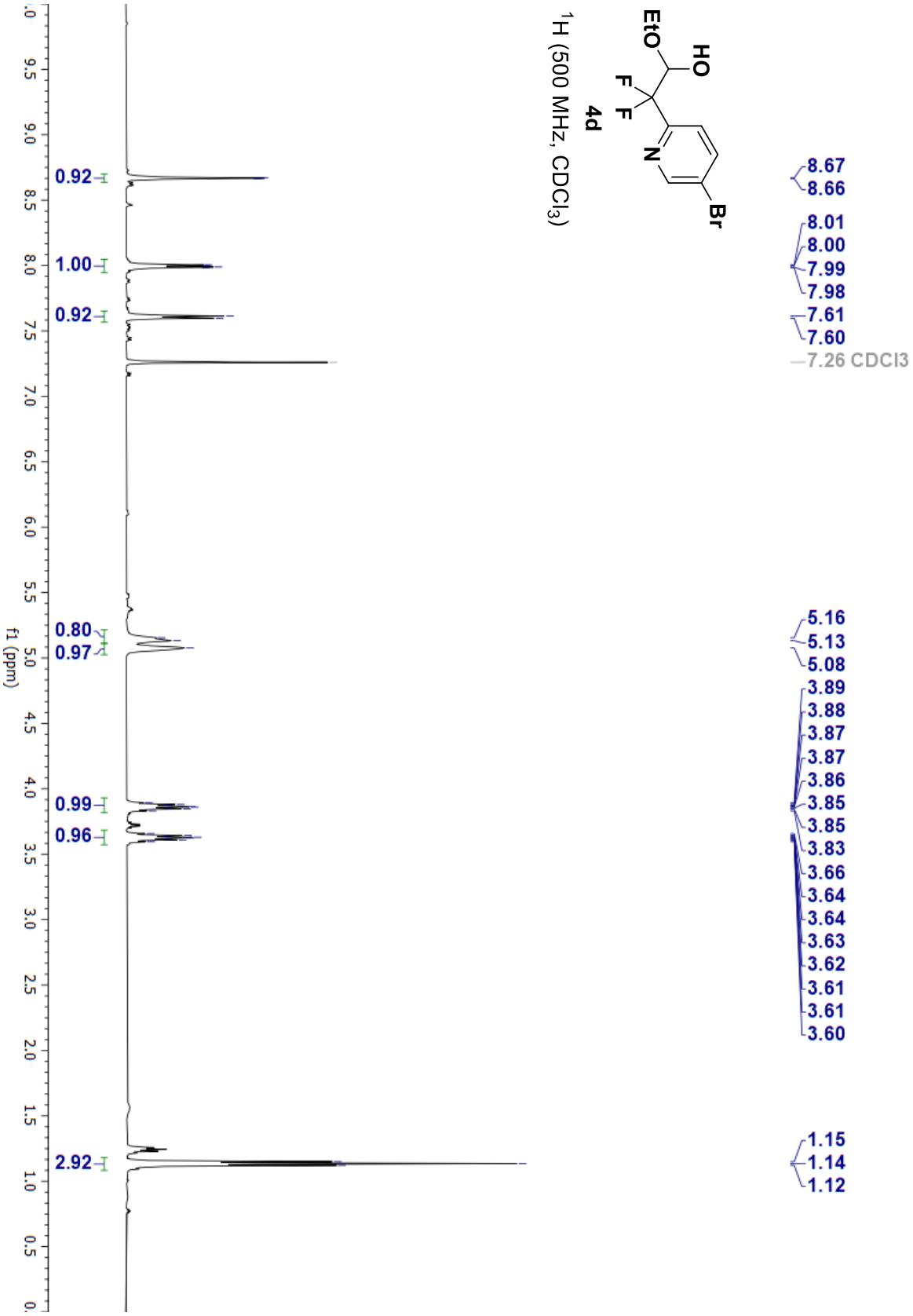
TLC (SiO_2): R_f = 0.3 (40:60 EtOAc:hexanes).

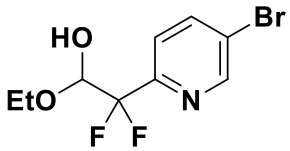
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.67 (d, *J* = 2.4 Hz, 1H), 7.99 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.61 (d, *J* = 8.4 Hz, 1H), 5.16 – 5.13 (m, 1H), 5.08 (s, 1H), 3.86 (dq, *J* = 9.8, 7.1 Hz, 1H), 3.63 (dq, *J* = 9.8, 7.0 Hz, 1H), 1.14 (t, *J* = 7.0 Hz, 3H) ppm.

^{19}F NMR (471 MHz, $CDCl_3$): δ -103.8 (d, *J* = 267.2 Hz), -116.7 (dd, *J* = 267.3, 4.6 Hz) ppm.

HRMS (ESI(+)): m/z [M+H^+] calcd. for $C_9H_{11}BrF_2NO_2^+$: 281.9936; found = 281.9933.

Due to the instability of **4d**, it was used without further characterization.

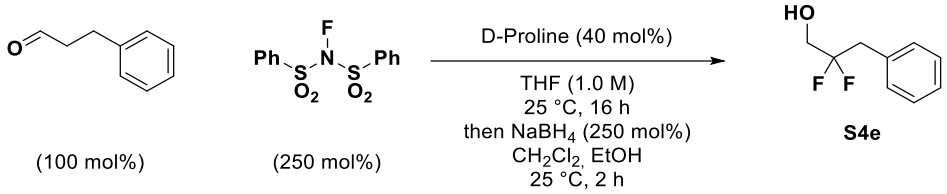

4d
^{1}H (500 MHz, CDCl$_3$)
EtO
HO
F
F
N
Br
8.67
8.66
8.01
8.00
7.99
7.98
7.61
7.60
7.26 CDCl3
5.16
5.13
5.08
3.89
3.88
3.87
3.87
3.86
3.85
3.85
3.83
3.66
3.64
3.64
3.63
3.62
3.61
3.61
3.60
1.15
1.14
1.12
0.92
1.00
0.92
0.80
0.97
0.99
0.96
2.92
f1 (ppm)



4d

^{19}F (471 MHz, $CDCl_3$)

2,2-difluoro-3-phenylpropan-1-ol (S4e)



A round-bottom flask equipped with a magnetic stir bar under an atmosphere of nitrogen was charged with hydrocinnamaldehyde (1.3 mL, 10.1 mmol, 100 mol%) and THF (25 mL, 0.40 M). To the reaction vessel, *N*-fluorosulfinimide (7.8 g, 24.9 mmol, 250 mol%) and D-proline (0.46 g, 4.02 mmol, 40 mol%) were added, and the reaction mixture was allowed to stir for 16 hours at ambient temperature. The reaction mixture was filtered through silica gel with the aid of diethyl ether and concentrated *in vacuo*. The residue was dissolved in dichloromethane (20 mL) and ethanol (10 mL), and sodium borohydride (95.7 mg, 2.53 mmol, 250 mol%) was added at ambient temperature and the solution was allowed to stir for 2 hours. The reaction mixture was quenched with saturated NH_4Cl (20 mL) and transferred to a separatory funnel. The aqueous phase was extracted with diethyl ether (3 × 20 mL), and the combined organic layers were washed with brine, dried (Na_2SO_4), filtered, and concentrated *in vacuo*. The resulting residue was subjected to flash column chromatography (SiO_2: 20:80 EtOAc:hexanes) to furnish the title compound **S4e** as a colorless oil in 45% yield (774.6 mg, 4.5 mmol).

TLC (SiO_2): R_f = 0.4 (EtOAc:hexanes 20:80).

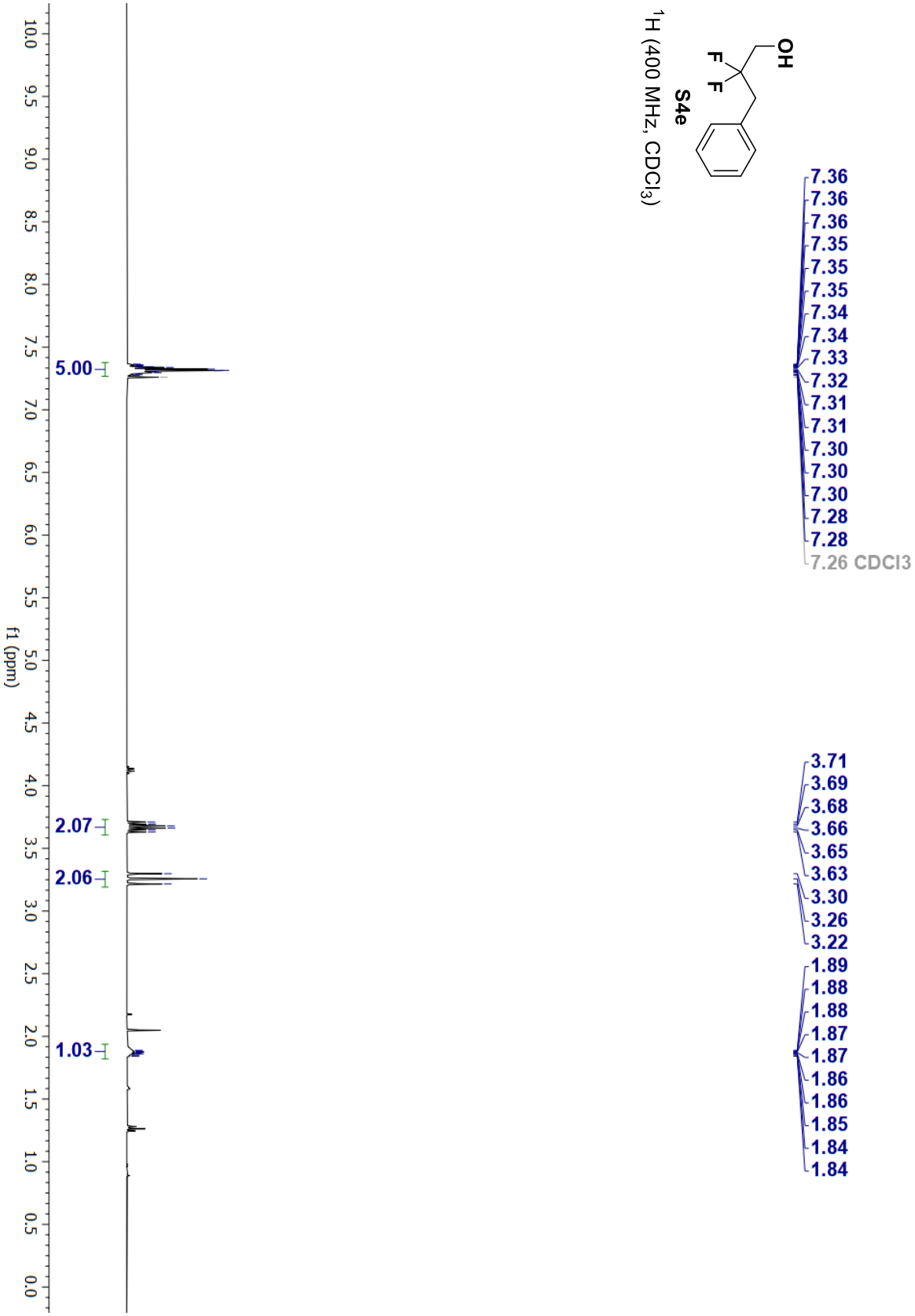
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40 – 7.30 (m, 5H), 3.69 (td, *J* = 12.4, 7.0 Hz, 2H), 3.28 (t, *J* = 16.4 Hz, 2H), 1.98 – 1.81 (m, 1H) ppm.

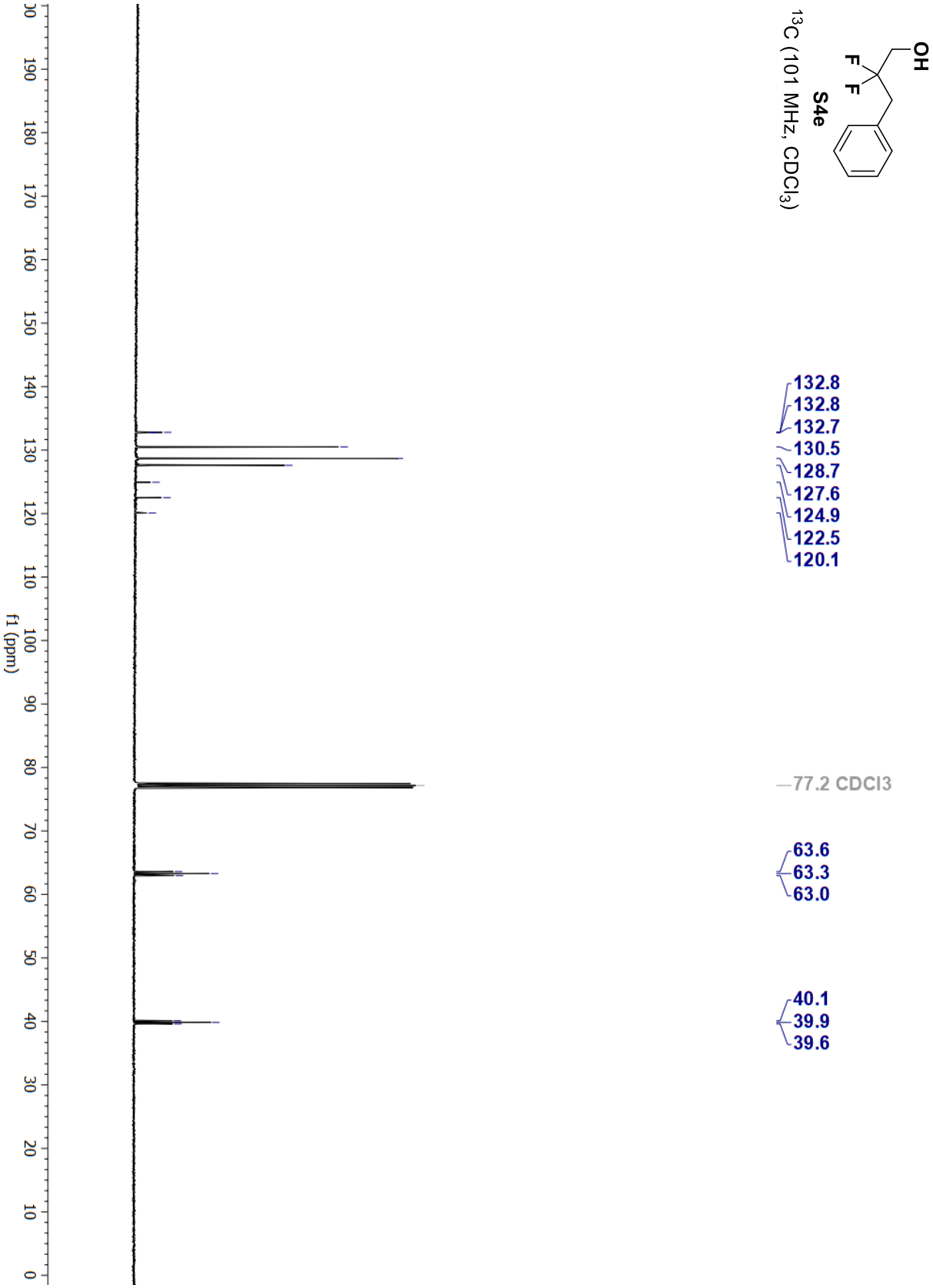
^{13}C NMR (101 MHz, $CDCl_3$): δ 132.8 (t, *J* = 4.9 Hz), 130.5, 128.7, 127.6, 122.5 (t, *J* = 243.5 Hz), 63.3 (t, *J* = 31.8 Hz), 39.9 (t, *J* = 24.7 Hz) ppm.

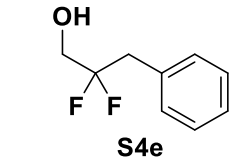
^{19}F NMR (376 MHz, $CDCl_3$): δ -106.9 (tt, *J* = 16.6, 12.6 Hz) ppm.

HRMS: Known compound, see reference 15.

The spectral data are in agreement with the literature.[15]


S4e
^{1}H (400 MHz, CDCl$_3$)
OH
F
F
7.36
7.36
7.36
7.35
7.35
7.35
7.34
7.34
7.33
7.32
7.31
7.31
7.30
7.30
7.30
7.28
7.28
7.26 CDCl3
3.71
3.69
3.68
3.66
3.65
3.63
3.30
3.26
3.22
1.89
1.88
1.88
1.87
1.87
1.86
1.86
1.85
1.84
1.84
5.00
2.07
2.06
1.03
f1 (ppm)

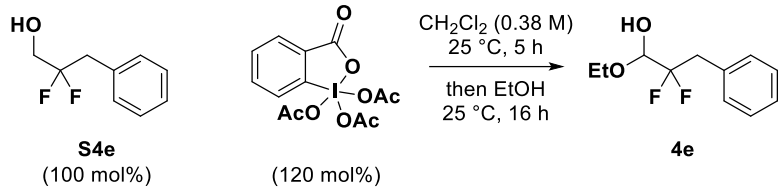

S4e
^{13}C (101 MHz, CDCl$_3$)
OH
F
F
132.8
132.8
132.7
130.5
128.7
127.6
124.9
122.5
120.1
77.2 CDCl3
63.6
63.3
63.0
40.1
39.9
39.6
f1 (ppm)



S4e

^{19}F (376 MHz, $CDCl_3$)

1-ethoxy-2,2-difluoro-3-phenylpropan-1-ol (4e)



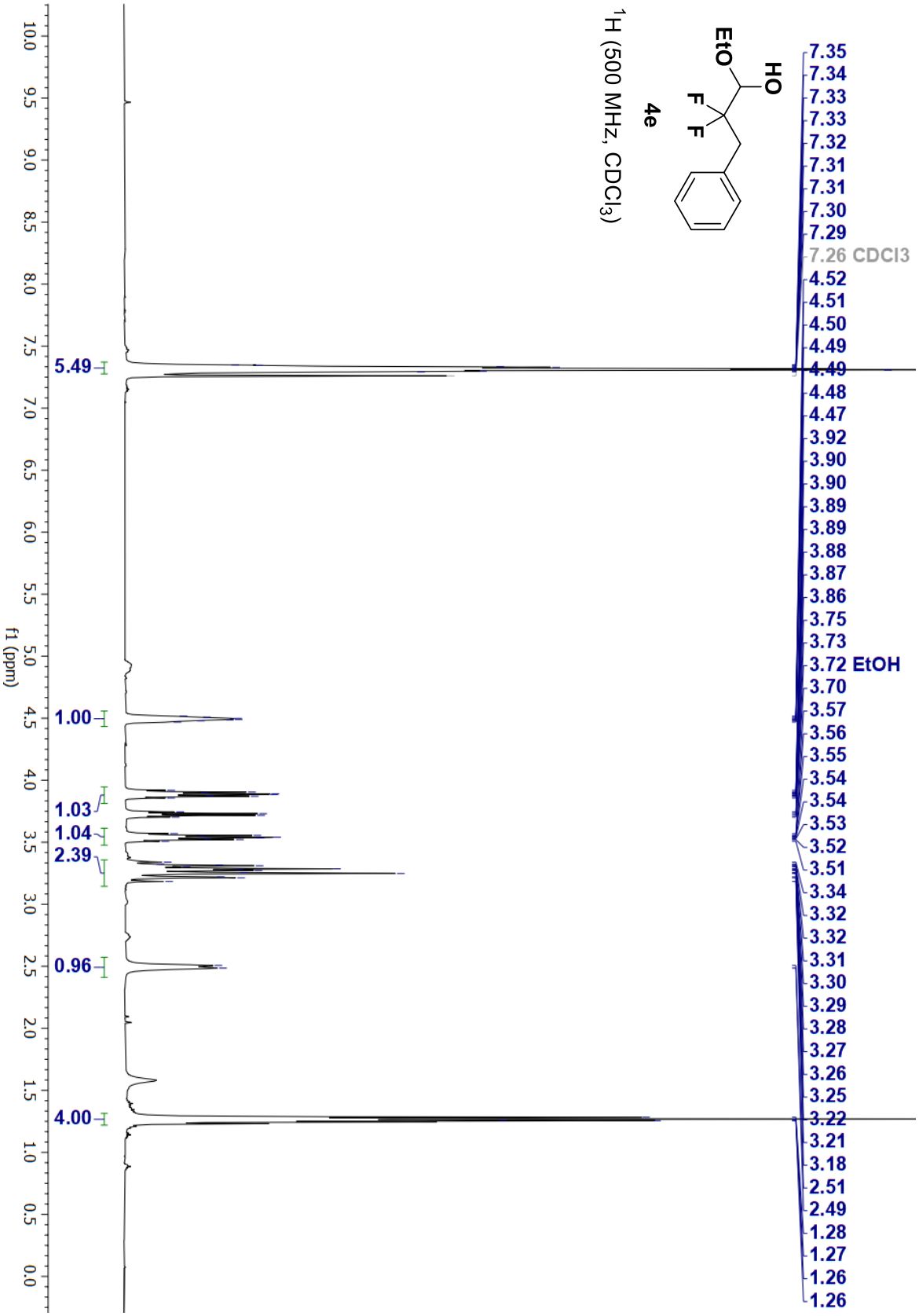
A 50 mL round-bottom flask equipped with a magnetic stir bar under an atmosphere of argon was charged with **S4e** (655.9 mg, 3.80 mmol, 100 mol%) and dichloromethane (10 mL, 0.38 M). To the reaction vessel, Dess-Martin periodinane (1.92 g, 4.53 mmol, 120 mol%) was added in one portion at ambient temperature, and the reaction mixture was allowed to stir for five hours. The reaction mixture was diluted with EtOAc (30 mL) and quenched with saturated $NaHCO_3$ (30 mL) and saturated $Na_2S_2O_3$ (30 mL) and transferred to a separatory funnel. The aqueous phase was extracted with EtOAc (3 × 20 mL), and the combined organic layers were washed with brine, dried (Na_2SO_4), filtered, and concentrated *in vacuo*. The residue was subjected to flash column chromatography (SiO_2: 20:80–50:50 EtOAc:hexanes), and the collected material was dissolved in ethanol (5 mL) and allowed to stir at ambient temperature for 16 hours. Concentration *in vacuo* furnished the title compound **4e** as a colorless oil in 34% yield (94 wt% solution in ethanol, 300.5 mg, 1.3 mmol).

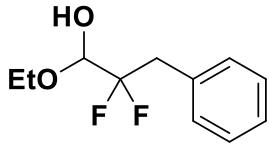
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.36 – 7.27 (m, 5H), 4.59 – 4.42 (m, 1H), 3.89 (dq, J = 9.5, 7.1 Hz, 1H), 3.54 (dq, J = 9.6, 7.0 Hz, 1H), 3.38 – 3.16 (m, 2H), 2.50 (d, J = 10.9 Hz, 1H), 1.27 (t, J = 7.1 Hz, 3H) ppm.

^{19}F{^{1}H} NMR (471 MHz, $CDCl_3$): δ -110.9 (d, J = 251.7 Hz), -116.6 (d, J = 251.9 Hz) ppm.

HRMS (ESI(+)): m/z [M+Na^+] calcd. for $C_{11}H_{14}F_2O_2^+$: 239.0854; found = 239.0856.

Due to the instability of **4e**, it was used without further characterization.

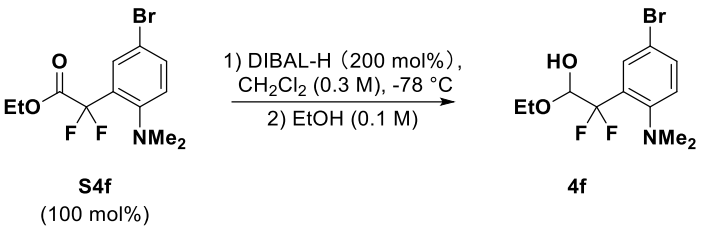

4e
^{1}H (500 MHz, CDCl$_3$)
EtO
HO
F
F
f1 (ppm)
5.49
1.00
1.03
1.04
2.39
0.96
4.00
7.35
7.34
7.33
7.33
7.32
7.31
7.31
7.30
7.29
7.26 CDCl3
4.52
4.51
4.50
4.49
4.49
4.48
4.47
3.92
3.90
3.90
3.89
3.89
3.88
3.87
3.86
3.75
3.73
3.72 EtOH
3.70
3.57
3.56
3.55
3.54
3.54
3.53
3.52
3.51
3.34
3.32
3.32
3.31
3.30
3.29
3.28
3.27
3.26
3.25
3.22
3.21
3.18
2.51
2.49
1.28
1.27
1.26
1.26



4e

^{19}F (471 MHz, $CDCl_3$)

2-(5-bromo-2-(dimethylamino)phenyl)-1-ethoxy-2,2-difluoroethan-1-ol (4f)



S4f
(100 mol%)

4f

The reaction was performed according to **General Procedure A** using **S4f**[16] (610.0 mg, 1.89 mmol, 100 mol%). The concentrated reaction mixture was subjected to flash column chromatography (SiO_2: 24:76 EtOAc:hexanes) to furnish the title compound **4f** as an unstable oil in 74% yield (451.4 mg, 1.39 mmol). **4f** was dissolved in ethanol and allowed to stir at ambient temperature overnight. The mixture was concentrated *in vacuo*, and the resulting residue (95 wt% solution in ethanol) was used directly in the next step.

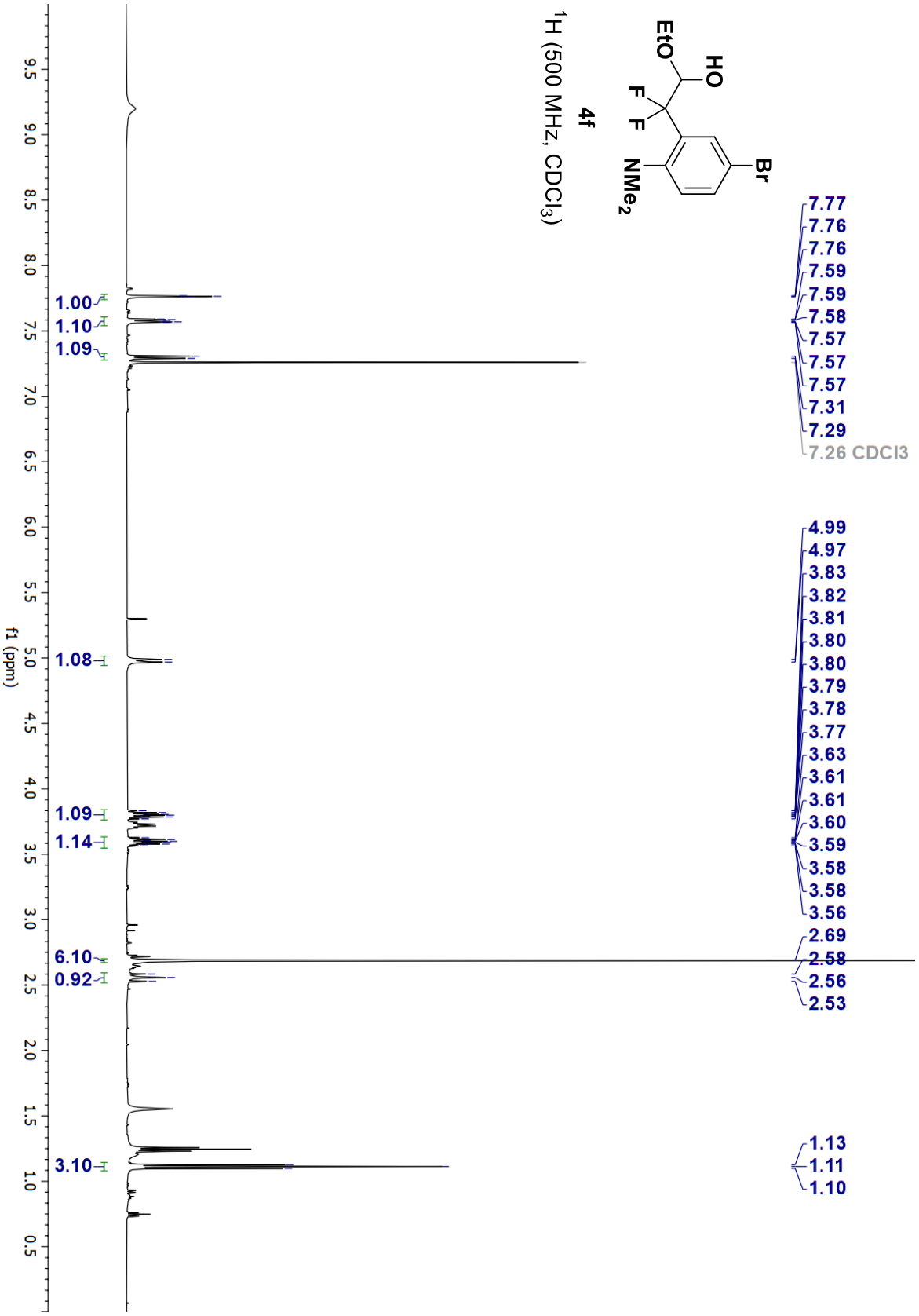
TLC (SiO_2): R_f = 0.3 (30:70 EtOAc:hexanes).

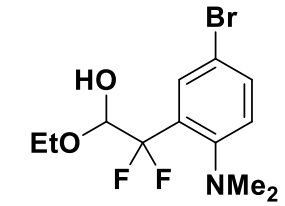
^{1}H NMR (500 MHz, $CDCl_3$): δ 7.76 (t, *J* = 2.0 Hz, 1H), 7.58 (dt, *J* = 8.6, 1.9 Hz, 1H), 7.30 (d, *J* = 8.5 Hz, 1H), 4.98 (d, *J* = 10.3 Hz, 1H), 3.80 (dq, *J* = 10.0, 7.1 Hz, 1H), 3.60 (dq, *J* = 10.0, 7.0 Hz, 1H), 2.69 (s, 6H), 2.58 – 2.53 (m, 1H), 1.11 (t, *J* = 7.0 Hz, 3H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ -92.8 (d, *J* = 265.5 Hz), -107.0 (dd, *J* = 265.4, 10.3 Hz) ppm.

HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_{12}H_{17}BrF_2NO_2^+$: 324.0405; found = 324.0412.

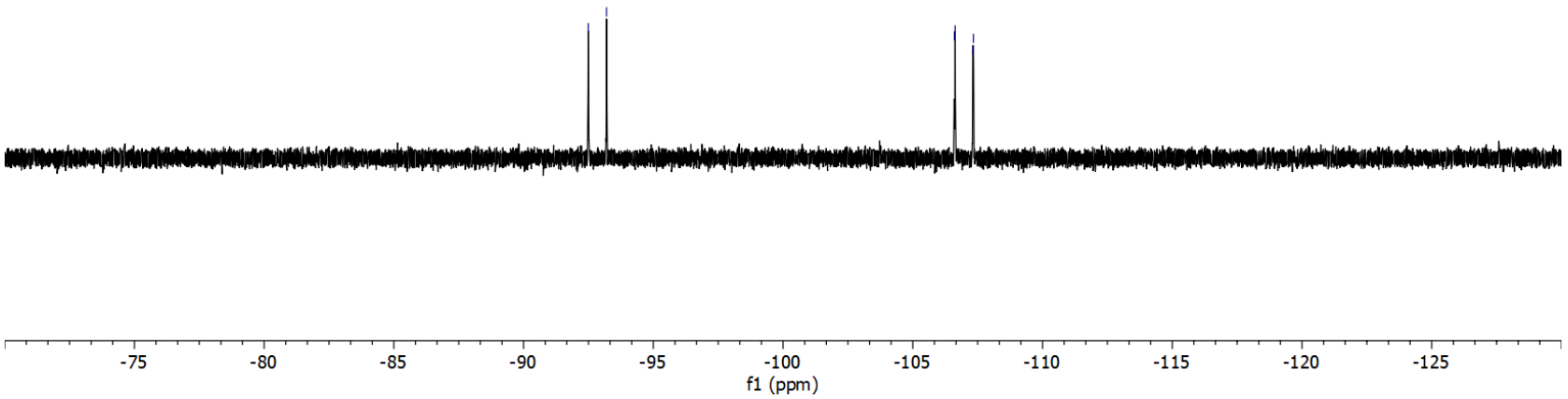
Due to the instability of **4f**, it was used without further characterization.


4f
^{1}H (500 MHz, CDCl$_3$)
EtO
HO
F
F
NMe$_2$
Br
7.77
7.76
7.76
7.59
7.59
7.58
7.57
7.57
7.57
7.31
7.29
7.26 CDCl3
4.99
4.97
3.83
3.82
3.81
3.80
3.80
3.79
3.78
3.77
3.63
3.61
3.61
3.60
3.59
3.58
3.58
3.56
2.69
2.58
2.56
2.53
1.13
1.11
1.10
1.00
1.10
1.09
1.08
1.09
1.14
6.10
0.92
3.10
f1 (ppm)

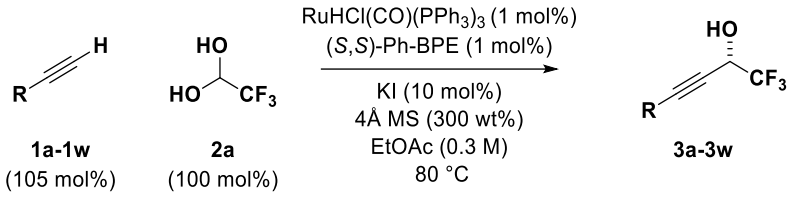


4f

^{19}F (376 MHz, $CDCl_3$)



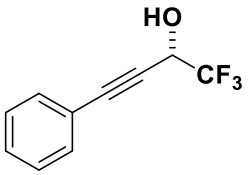
VI. Products 3a-3y



1a-1w (105 mol%) **2a** (100 mol%) **3a-3w**

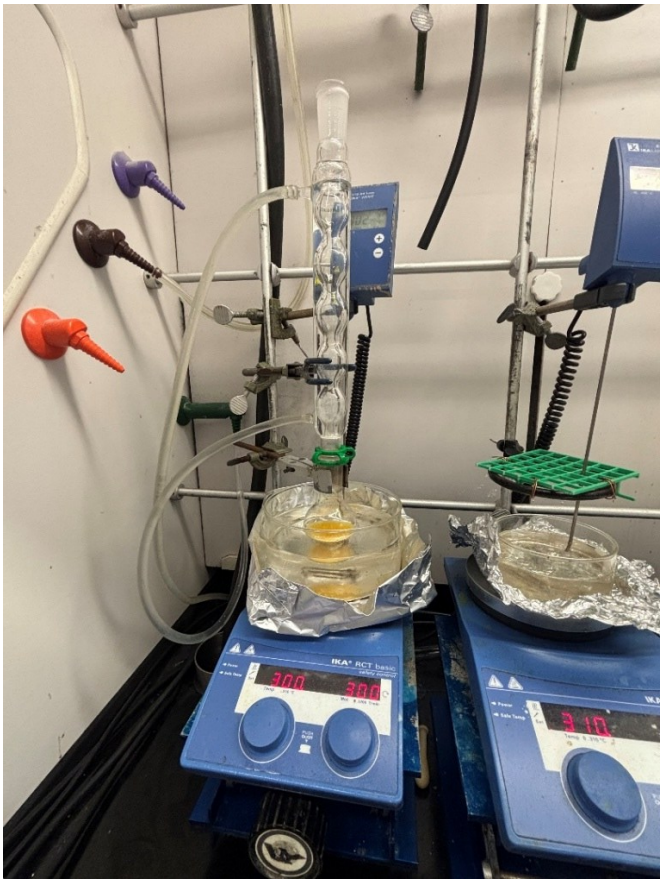
General Procedure B: A pressure tube equipped with a magnetic stir bar was charged with $RuHCl(CO)(PPh_3)_3$ (1.9 mg, 0.002 mmol, 1 mol%), (*S*,*S*)-Ph-BPE (1.0 mg, 0.002 mmol, 1 mol%), KI (3.2 mg, 0.02 mmol, 10 mol%), 4Å molecular sieves (90 mg, 300 wt%) and ethyl acetate (0.67 mL) under air. The tube was sealed with a PTFE-lined cap, placed in an oil bath and was allowed to stir at 80 ºC. After 15 minutes, the reaction mixture was allowed to reach ambient temperature. The cap was removed from the tube and the respective terminal alkyne **1** (0.21 mmol, 105 mol%) and fluoral (**2a**, 76 wt% in H_2O, 21 μL, 0.2 mmol, 100 mol%) were added. The tube was resealed with the cap, placed in an oil bath and was allowed to stir for 24 hours at 80 ºC. The reaction mixture was allowed to reach ambient temperature, and the residue was subjected to flash column chromatography (SiO_2) under the noted conditions to furnish products **3a**-**3y**.

(*S*)-1,1,1-trifluoro-4-phenylbut-3-yn-2-ol (3a)



Alkyne **1a** (23 μL, 0.21 mmol, 105 mol%) was subjected to standard reaction conditions (80 °C, 24 h) at 1 mol% catalyst loading. Upon flash column chromatography (SiO_2: 5:95–10:90 EtOAc:hexanes), the title compound **3a** was isolated as a colorless oil in 89% yield (35.6 mg, 0.18 mmol, 99% ee).

2mmol scale reaction: A 25 mL round bottom flask connected to a water condenser was charged with $RuHCl(CO)(PPh_3)_3$ (19 mg, 0.02 mmol, 1 mol%), (*S*,*S*)-Ph-BPE (10 mg, 0.02 mmol, 1 mol%), KI (32 mg, 0.2 mmol, 10 mol%), 4Å molecular sieves (150 mg, 50 wt%) and ethyl acetate (6.7 mL) under air. The flask was placed in an oil bath and was allowed to stir at 80 ºC. After 15 minutes, the reaction mixture was allowed to reach ambient temperature, before adding alkyne **1a** (230 μL 2.1 mmol, 105 mol%) and fluoral (**2a**, 76 wt% in H_2O, 210 μL, 2 mmol, 100 mol%) were added to the reaction mixture and was allowed to stir for 24 hours at 80 ºC. The reaction mixture was allowed to reach ambient temperature, and the residue was subjected to flash column chromatography (SiO_2) to furnish the title compound **3a** as a color less oil in 88% yield (352 mg, 1.8 mmol, 99% ee).



TLC (SiO_2): R_f = 0.2 (10:90 hexanes:EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57 – 7.46 (m, 2H), 7.43 – 7.30 (m, 3H), 4.91 (dq, *J* = 8.5, 5.7 Hz, 1H), 2.46 (d, *J* = 8.3 Hz, 1H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ 132.2, 129.7, 128.6, 122.9 (q, *J* = 281.9 Hz), 121.0, 88.2, 80.5 (q, *J* = 2.5 Hz), 63.1 (q, *J* = 36.6 Hz) ppm.

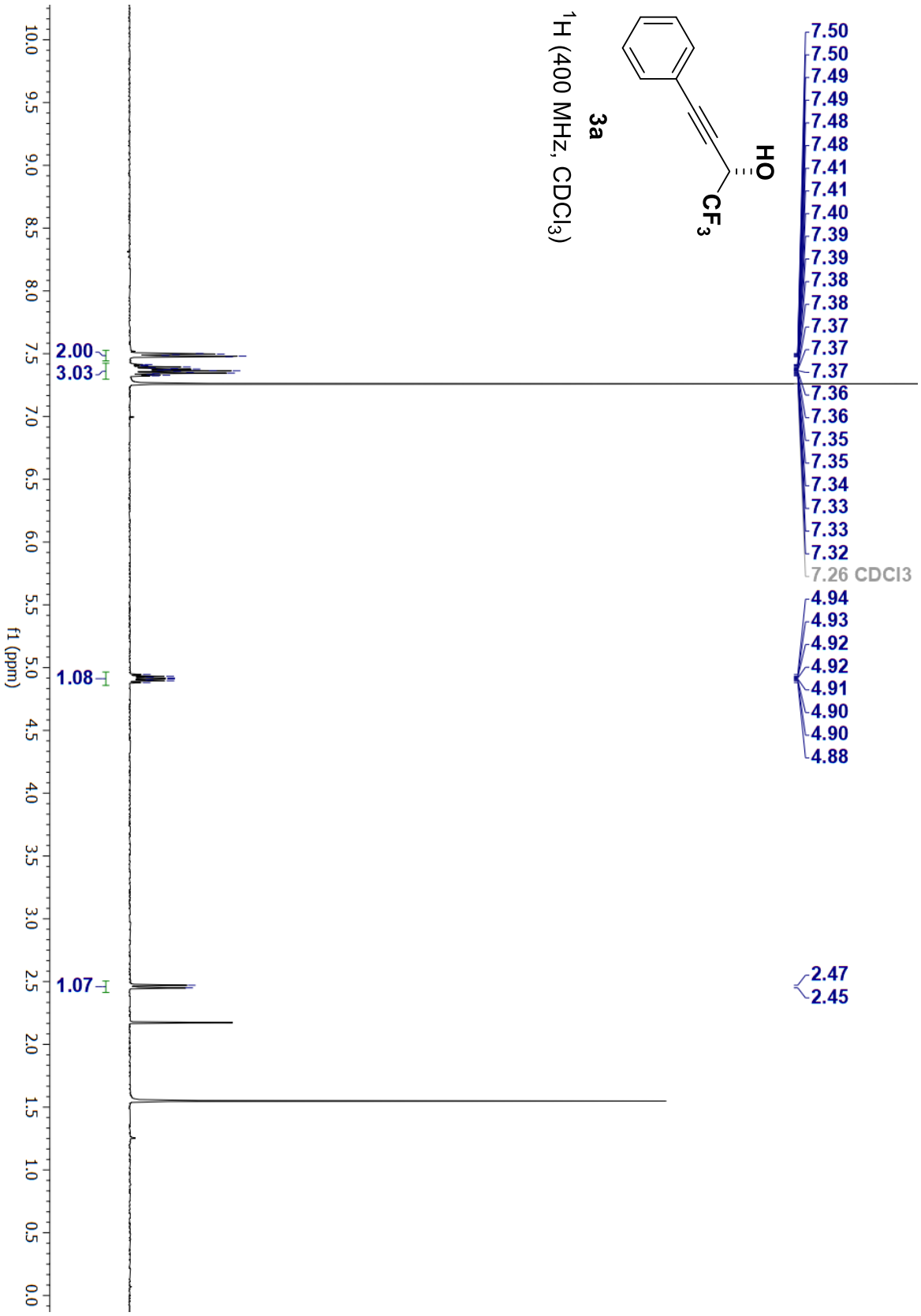
^{19}F NMR (471 MHz, $CDCl_3$): -79.4 (d, *J* = 6.0 Hz) ppm.

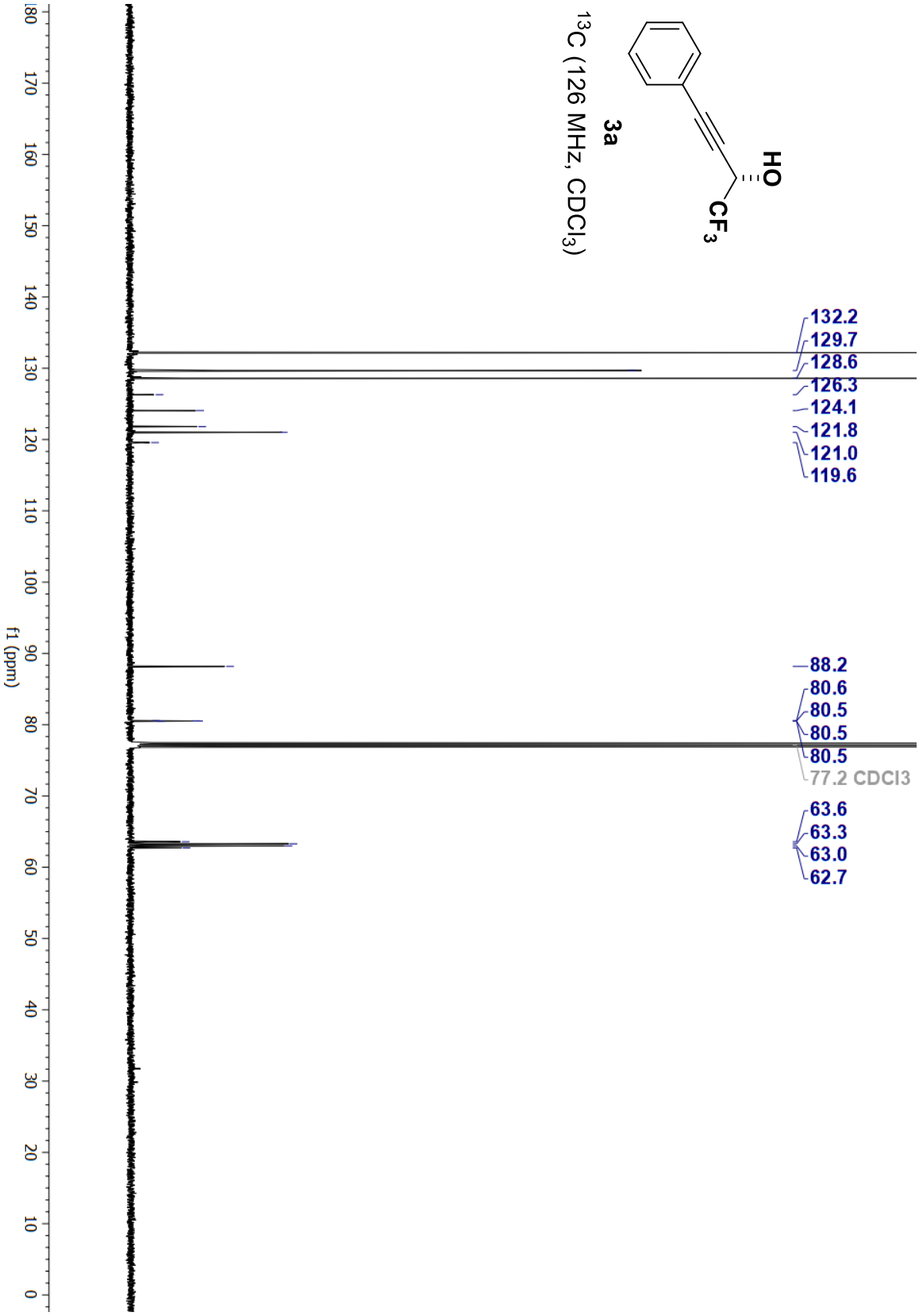
HRMS: Known compound, see reference 17.

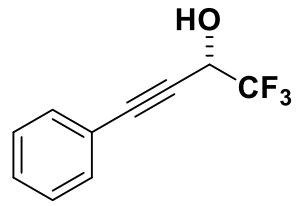
HPLC (CHIRALPAK AD-H, hexanes:2-PrOH = 98:2, 1.0 mL/min, 254 nm): ee = 99%.

$[\alpha]_D^{20}$= -22° ($CHCl_3$, c = 0.5).

The analytical data are in agreement with the literature.[17]

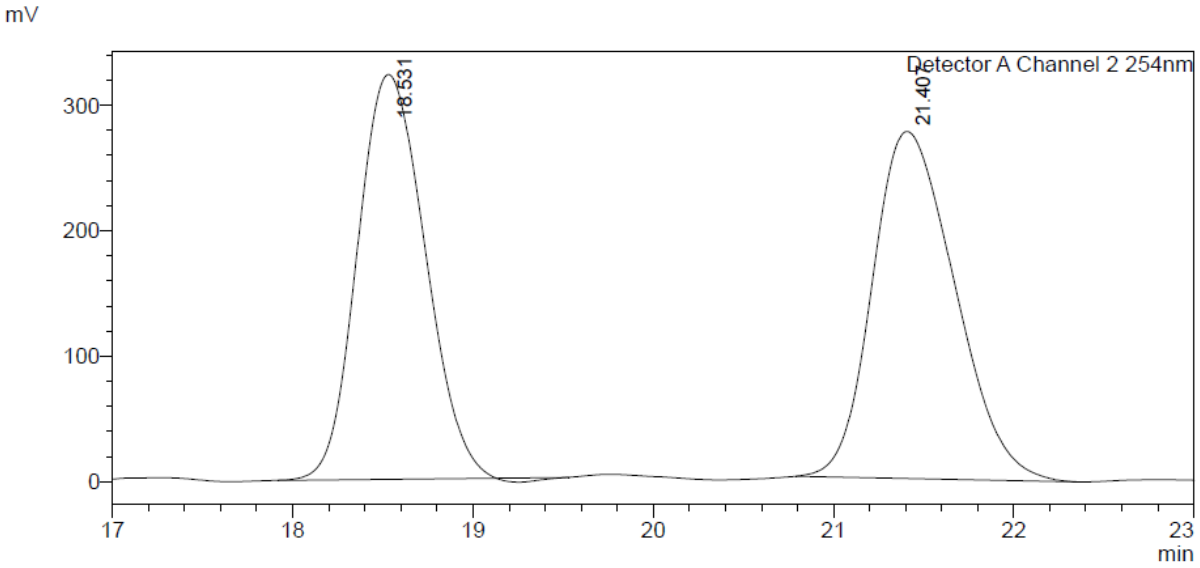

3a
^{1}H (400 MHz, CDCl$_3$)
HO
CF$_3$
7.50
7.50
7.49
7.49
7.48
7.48
7.41
7.41
7.40
7.39
7.39
7.38
7.38
7.37
7.37
7.37
7.36
7.36
7.35
7.35
7.34
7.33
7.33
7.32
7.26 CDCl3
4.94
4.93
4.92
4.92
4.91
4.90
4.90
4.88
2.47
2.45
2.00
3.03
1.08
1.07
f1 (ppm)


3a
^{13}C (126 MHz, CDCl$_3$)
HO
CF$_3$
132.2
129.7
128.6
126.3
124.1
121.8
121.0
119.6
88.2
80.6
80.5
80.5
80.5
77.2 CDCl3
63.6
63.3
63.0
62.7
f1 (ppm)



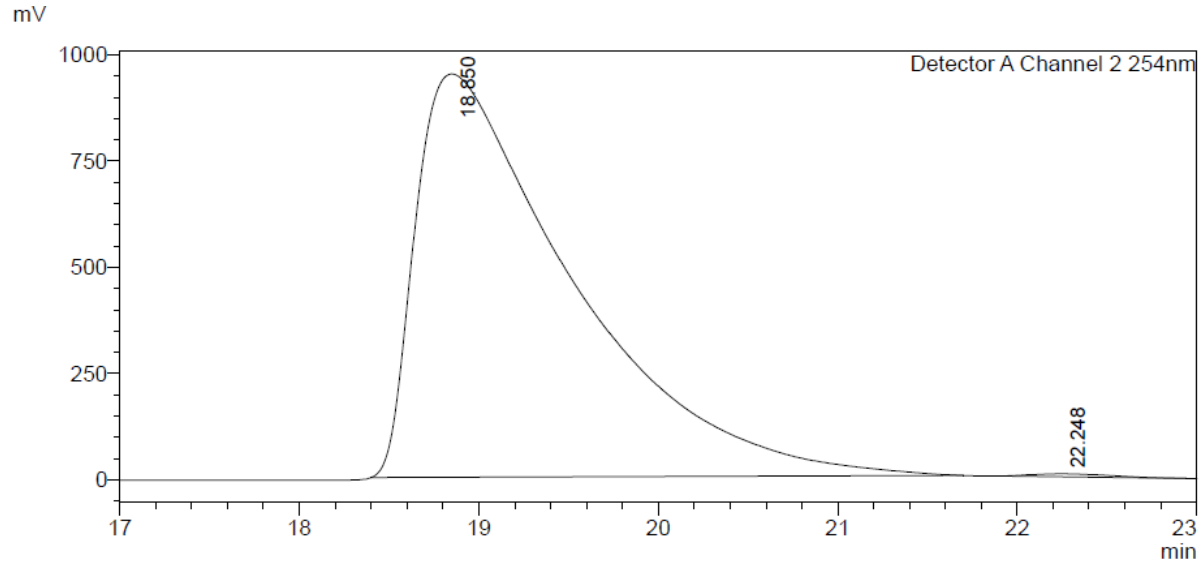
3a

^{19}F (471 MHz, $CDCl_3$)



Detector A Channel 2 254nm

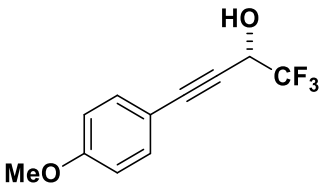
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	18.531	8389346	322625	48.798		M	
2	21.407	8802753	276660	51.202		M	
Total		17192099	599285				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	18.850	57714739	948885	99.615		M	
2	22.248	222881	7222	0.385		M	
Total		57937620	956107				

(*S*)-1,1,1-trifluoro-4-(4-methoxyphenyl)but-3-yn-2-ol (3b)



Alkyne **1b** (27 μL, 0.21 mmol, 105 mol%) was subjected to standard reaction conditions (80 °C, 24 h) at 1 mol% catalyst loading. Upon flash column chromatography (SiO_2: 8:92–12:88 EtOAc:hexanes), the title compound **3b** was isolated as viscous brown oil in 83% yield (38.1 mg, 0.17 mmol, 96% ee).

TLC (SiO_2): R_f = 0.2 (10:90 EOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.41 (d, *J* = 8.8 Hz, 2H), 6.86 (d, *J* = 8.8 Hz, 2H), 4.99 – 4.76 (m, 1H), 3.82 (s, 3H), 2.79 – 2.61 (m, 1H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ 160.6, 133.8, 123.0 (q, *J* = 281.9 Hz), 114.2, 113.0, 88.2, 79.4 (q, *J* = 2.4 Hz), 63.2 (q, *J* = 36.5 Hz), 55.5 ppm.

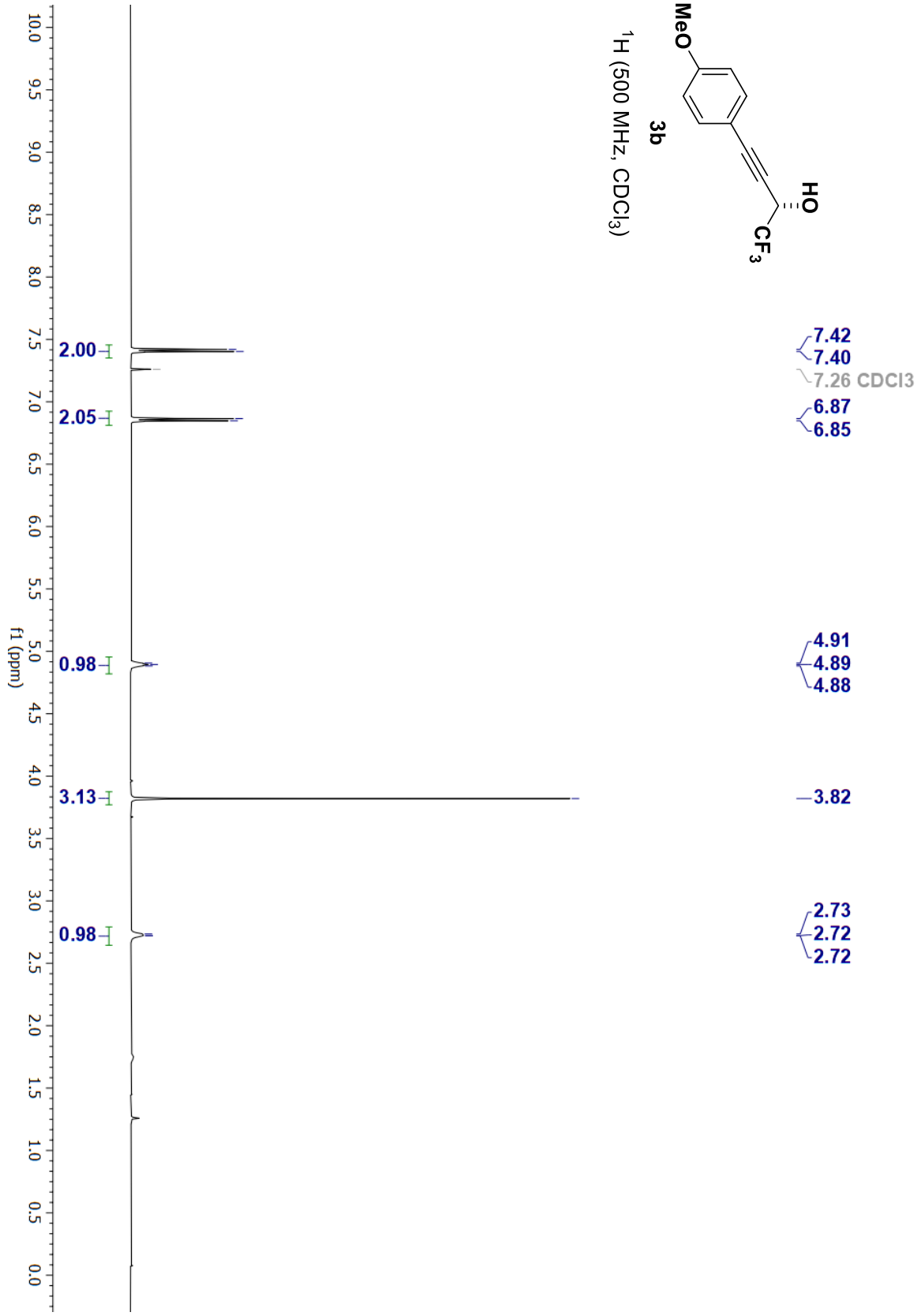
^{19}F NMR (471 MHz, $CDCl_3$): δ -79.4 (d, *J* = 5.9 Hz) ppm.

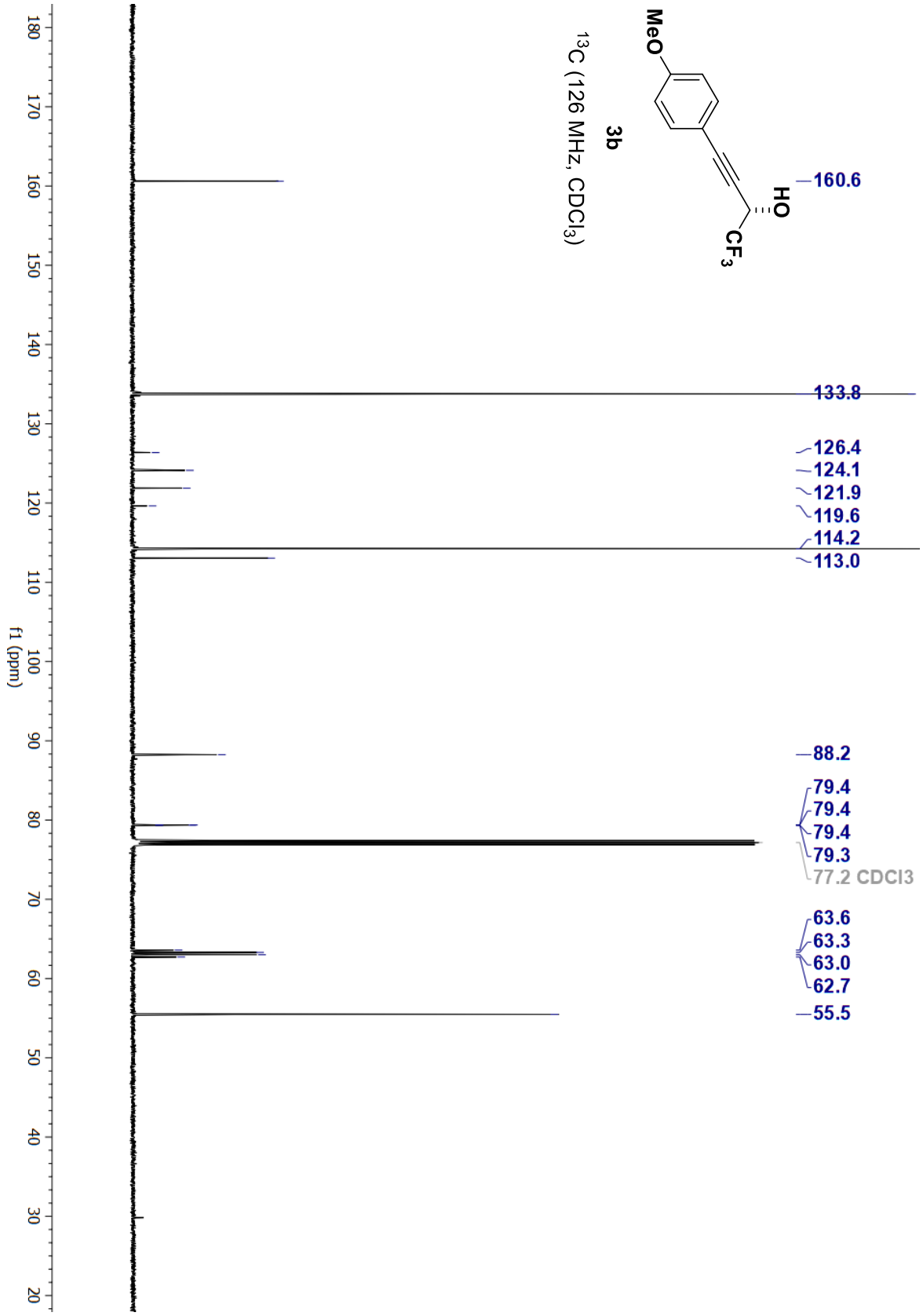
HRMS: Known compound, see reference 17.

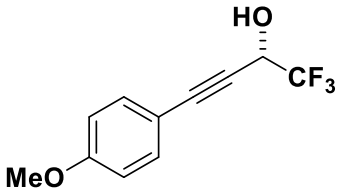
HPLC (PHENOMENEX Cellulose 5, hexanes:2-PrOH = 98:2, 1.0 mL/min, 254 nm): ee = 96%.

$[\alpha]_D^{20}$ = -17° ($CHCl_3$, c = 1.0).

The analytical data are in agreement with the literature.[17]

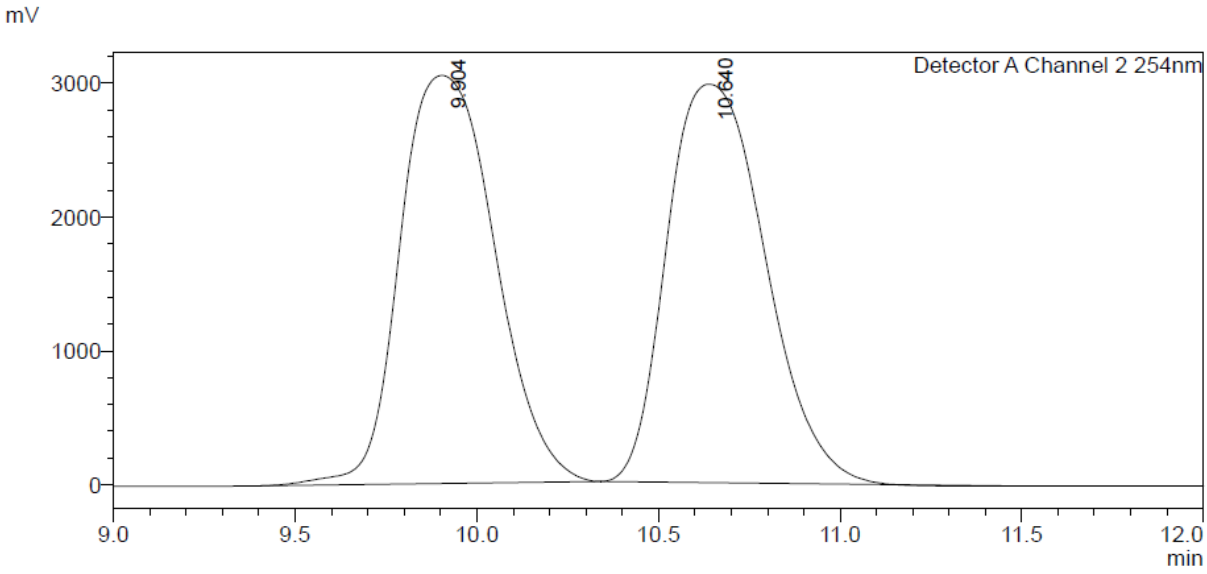

MeO
HO
CF3
3b
1H (500 MHz, CDCl3)
7.42
7.40
7.26 CDCl3
6.87
6.85
4.91
4.89
4.88
3.82
2.73
2.72
2.72
2.00
2.05
0.98
3.13
0.98
f1 (ppm)


MeO
HO
CF3
3b
13C (126 MHz, CDCl3)
160.6
133.8
126.4
124.1
121.9
119.6
114.2
113.0
88.2
79.4
79.4
79.4
79.3
77.2 CDCl3
63.6
63.3
63.0
62.7
55.5
f1 (ppm)



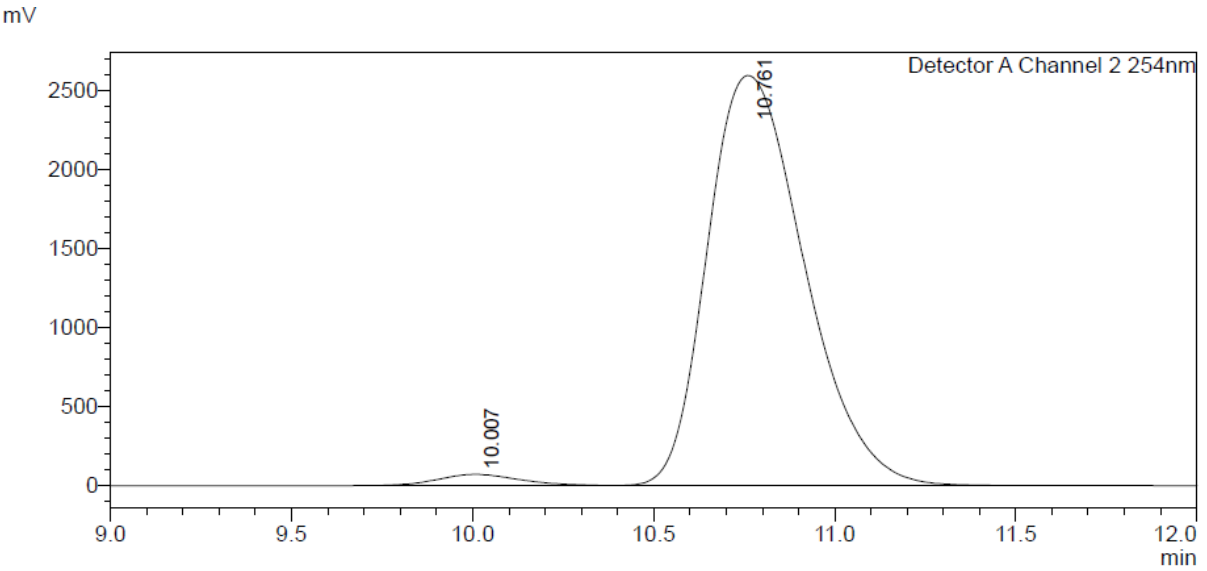
3b

^{19}F (471 MHz, $CDCl_3$)



Detector A Channel 2 254nm

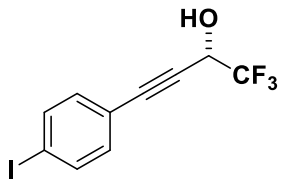
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	9.904	55471705	3049459	49.729		M	
2	10.640	56076099	2979633	50.271		M	
Total		111547804	6029092				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	10.007	1061567	69501	2.153		M	
2	10.761	48243694	2591172	97.847		M	
Total		49305261	2660673				

(*S*)-1,1,1-trifluoro-4-(4-iodophenyl)but-3-yn-2-ol (3c)



Alkyne **1c** (47.7 mg, 0.21 mmol, 105 mol%) was subjected to standard reaction conditions (80 °C, 24 h) at 1 mol% catalyst loading. Upon flash column chromatography (SiO_2: 7:93 EtOAc:hexanes), the title compound **3c** was isolated as a white solid in 83% yield (54.1 mg, 0.17 mmol, 99% ee).

TLC (SiO_2): R_f = 0.4 (1:10 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.70 (d, *J* = 8.4 Hz, 1H), 7.20 (d, *J* = 8.4 Hz, 1H), 4.89 (dq, *J* = 7.9, 5.5 Hz, 1H), 2.43 (d, *J* = 8.1 Hz, 1H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ 137.8, 133.6, 122.8 (q, *J* = 281.9 Hz), 120.5, 96.0, 87.2, 82.9 – 79.9 (m), 63.1 (q, *J* = 36.6 Hz) ppm.

^{19}F NMR (471 MHz, $CDCl_3$): δ -79.3 (d, *J* = 5.3 Hz) ppm.

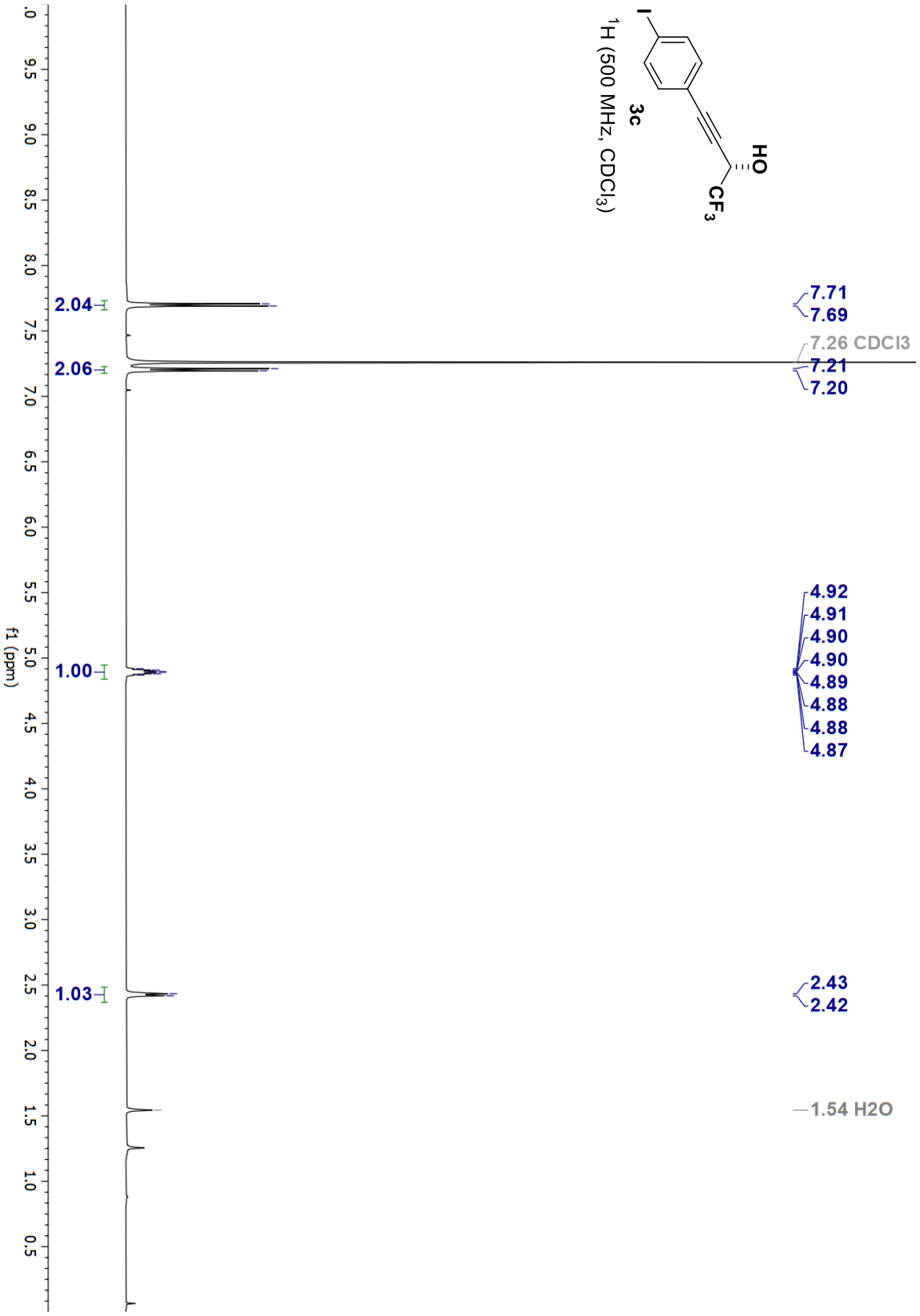
HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_{10}H_7F_3IO^+$: 326.9488; found = 326.9481.

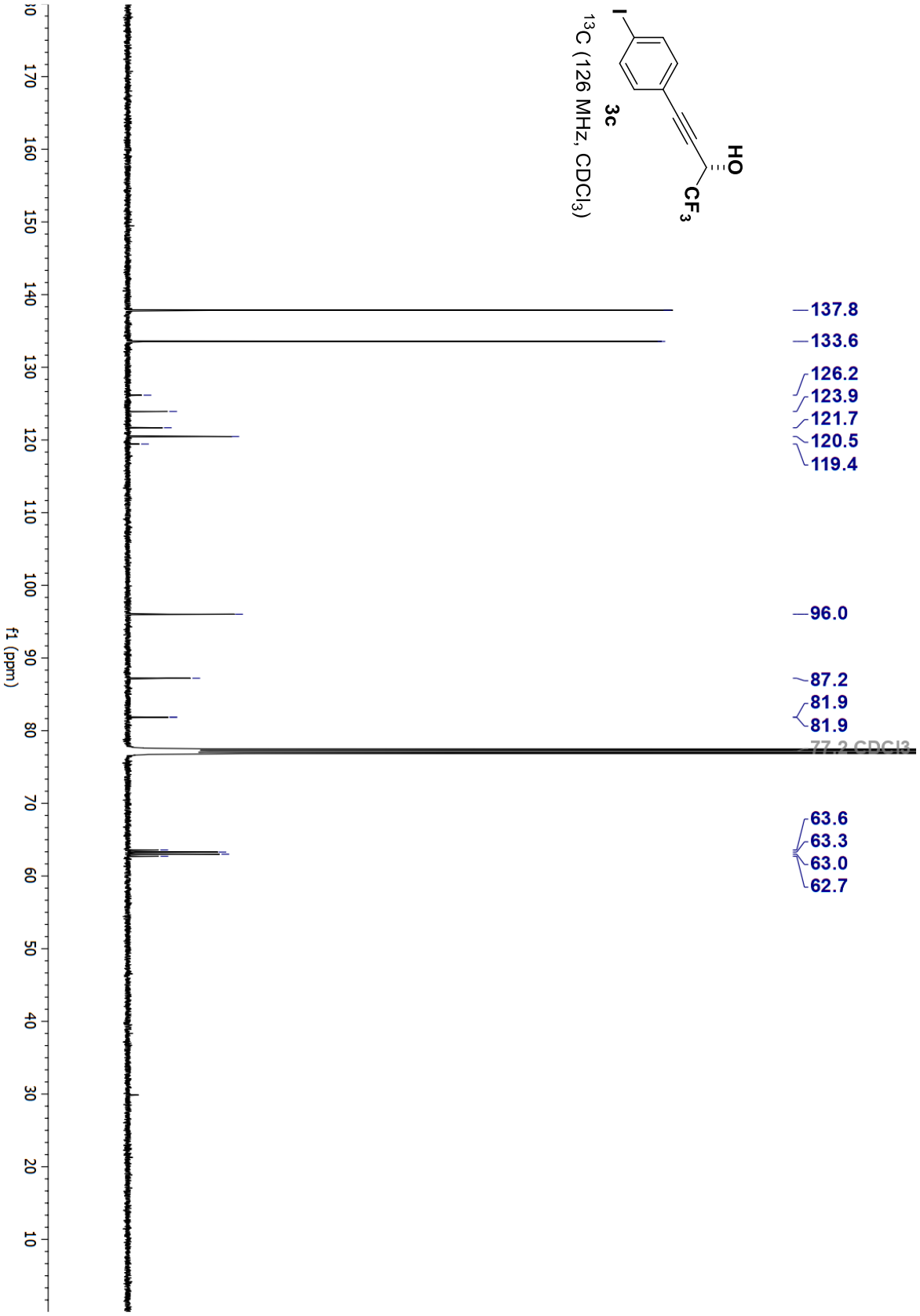
FTIR (neat): 3304, 2919, 2226, 1907, 1253, 1122, 813, 697, 520 cm^{-1}.

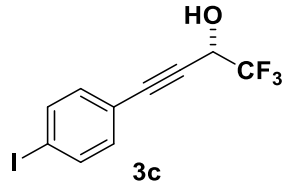
HPLC (CHIRALPAK AD-H, hexanes:2-PrOH = 98:2, 1.0 mL/min, 254 nm): ee = 99%.

$[\alpha]_D^{20}$ = -11° ($CHCl_3$, c = 1.0).

m.p.: 103 °C.

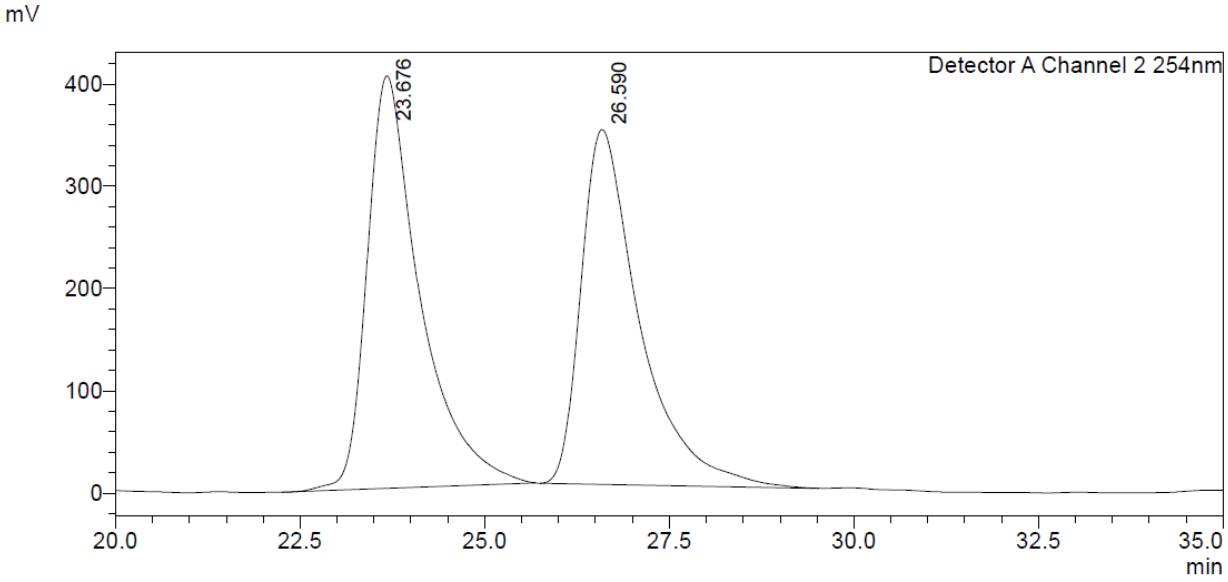

3c
^{1}H (500 MHz, CDCl$_3$)
I
HO
CF$_3$
f1 (ppm)
2.04
2.06
1.00
1.03
7.71
7.69
7.26 CDCl3
7.21
7.20
4.92
4.91
4.90
4.90
4.89
4.88
4.88
4.87
2.43
2.42
1.54 H2O


3c
^{13}C (126 MHz, CDCl$_3$)
I
HO
CF$_3$
137.8
133.6
126.2
123.9
121.7
120.5
119.4
96.0
87.2
81.9
81.9
77.2 CDCl3
63.6
63.3
63.0
62.7
f1 (ppm)



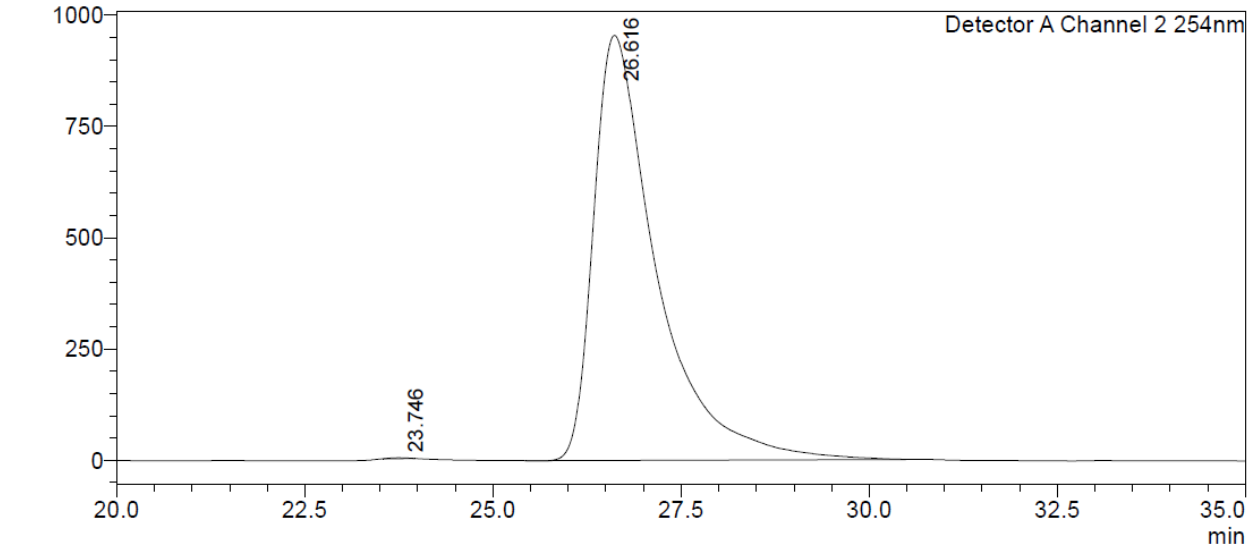
3c

^{19}F (471 MHz, $CDCl_3$)



Detector A Channel 2 254nm

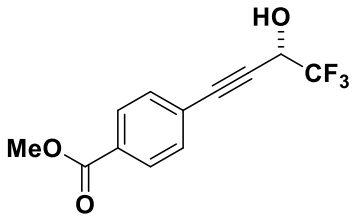
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	23.676	20047694	402962	51.249		M	
2	26.590	19070814	346592	48.751		M	
Total		39118507	749554				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	23.746	32095	1978	0.058		M	
2	26.616	55551817	954010	99.942		M	
Total		55583912	955988				

methyl (*S*)-4-(4,4,4-trifluoro-3-hydroxybut-1-yn-1-yl)benzoate (3d)



Alkyne **1d** (33.6 mg, 0.21 mmol, 105 mol%) was subjected to standard reaction conditions (80 °C, 24 h) at 1 mol% catalyst loading. Upon flash column chromatography (SiO_2: 8:92 EtOAc:hexanes), the title compound **3d** was isolated as a white solid in 84% yield (43.3 mg, 0.17 mmol, 98% ee).

TLC (SiO_2): R_f = 0.1 (1:9 EtOAc:hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.05 – 7.97 (m, 2H), 7.57 – 7.50 (m, 2H), 4.94 (dq, *J* = 8.3, 5.7 Hz, 1H), 3.93 (s, 3H), 2.79 (dt, *J* = 8.5, 2.0 Hz, 1H) ppm.

^{13}C NMR (101 MHz, $CDCl_3$): δ 166.5, 132.1, 130.9, 129.7, 125.6, 122.8 (q, *J* = 282.3 Hz), 87.1, 83.2 (q, *J* = 2.4 Hz), 63.1 (q, *J* = 36.6 Hz), 52.6 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ -79.2 (d, *J* = 5.6 Hz) ppm.

HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_{12}H_{10}F_3O_3^+$: 259.0577; found = 259.0584.

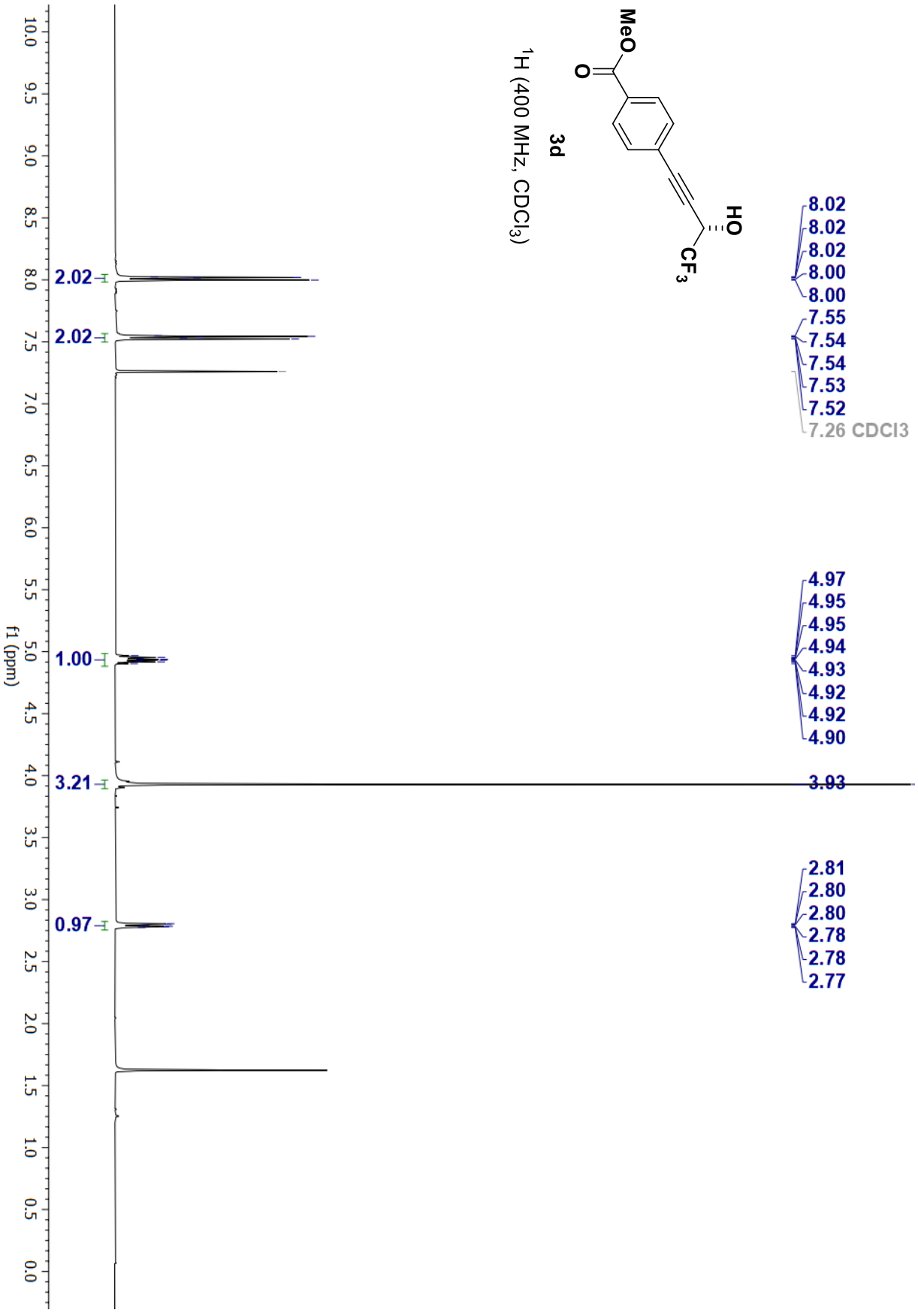
FTIR (neat): 3374, 2965, 1702, 1605, 1442, 1406, 1350, 1311, 1267, 1175, 1140, 1115, 1076, 1016, 976, 953, 858, 828, 771, 699, 615, 536, 459 cm^{-1}.

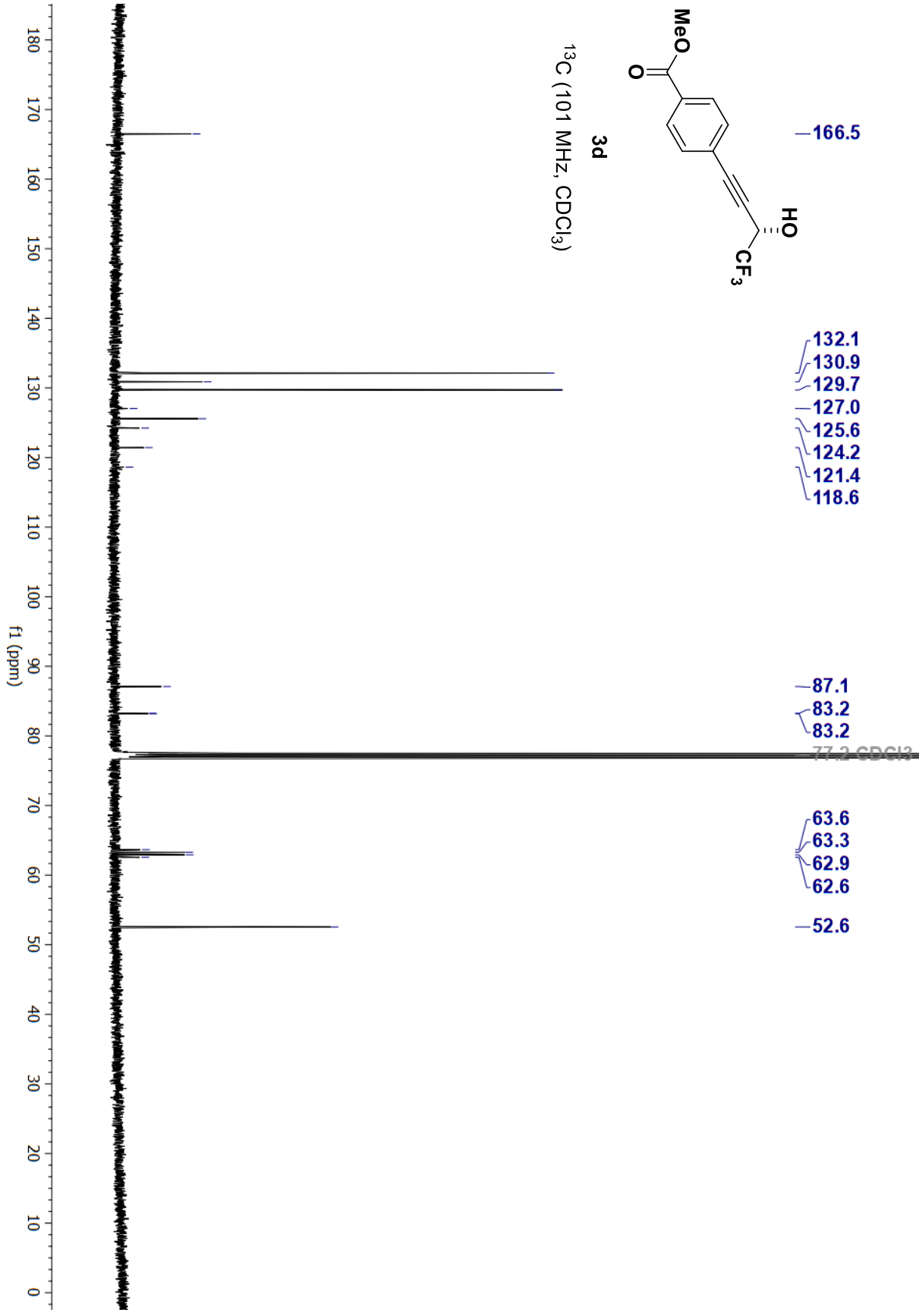
HPLC (PHENOMENEX Cellulose 5, hexanes:2-PrOH = 97:3, 1.0 mL/min, 254 nm): ee = 98%.

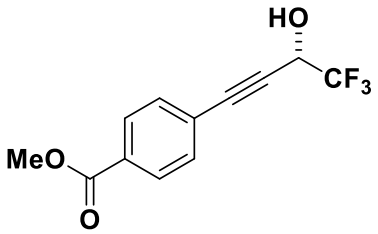
$[\alpha]_D^{20}$ = -182° ($CHCl_3$, c = 1.0).

m.p.: 96 °C.

A single crystal suitable for X-Ray analysis was obtained by vapor diffusion using Et_2O and Pentane.

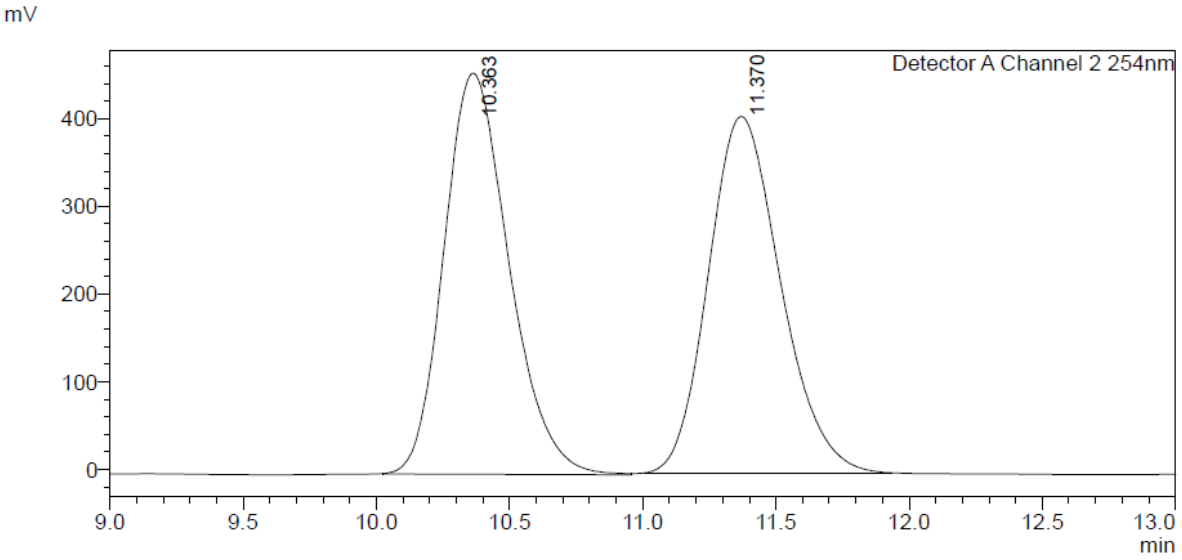

MeO
O
HO
CF3
3d
1H (400 MHz, CDCl3)
8.02
8.02
8.02
8.00
8.00
7.55
7.54
7.54
7.53
7.52
7.26 CDCl3
4.97
4.95
4.95
4.94
4.93
4.92
4.92
4.90
3.93
2.81
2.80
2.80
2.78
2.78
2.77
2.02
2.02
1.00
3.21
0.97
f1 (ppm)


3d
^{13}C (101 MHz, CDCl$_3$)
MeO
O
HO
CF$_3$
166.5
132.1
130.9
129.7
127.0
125.6
124.2
121.4
118.6
87.1
83.2
83.2
77.2 CDCl3
63.6
63.3
62.9
62.6
52.6
f1 (ppm)



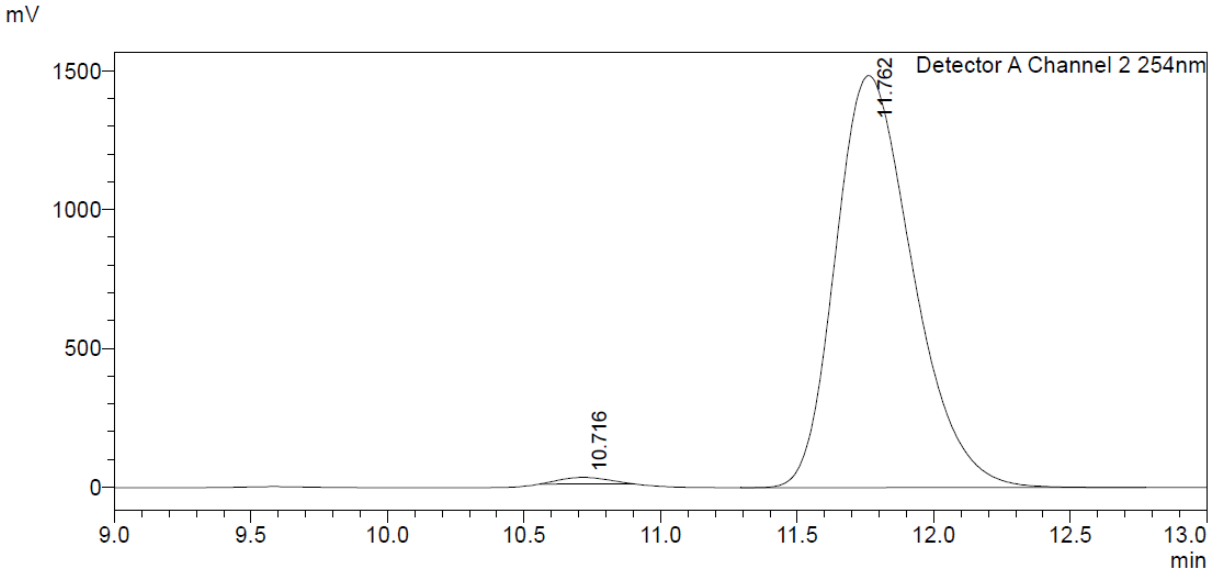
3d

^{19}F (376 MHz, $CDCl_3$)



Detector A Channel 2 254nm

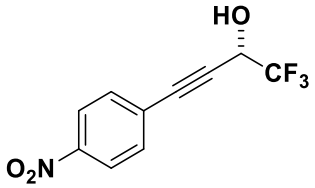
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	10.363	7757581	457008	50.298		M	
2	11.370	7665597	406400	49.702		M	
Total		15423178	863408				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	10.716	285735	23582	0.970		M	
2	11.762	29179270	1484183	99.030		M	
Total		29465004	1507765				

(*S*)-1,1,1-trifluoro-4-(4-nitrophenyl)but-3-yn-2-ol (3e)



Alkyne **1e** (30.8 mg, 0.21 mmol, 105 mol%) was subjected to standard reaction conditions (80 °C, 24 h) at 1 mol% catalyst loading. Upon flash column chromatography (SiO_2: 4:96 EtOAc:hexanes), the title compound **3e** was isolated as a waxy orange solid in 90% yield (44.1 mg, 0.18 mmol, 99% ee).

TLC (SiO_2): R_f = 0.4 (1:10 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.23 (d, *J* = 8.5 Hz, 2H), 7.66 (d, *J* = 8.6 Hz, 2H), 4.96 (dq, *J* = 10.8, 6.0 Hz, 1H), 2.53 (d, *J* = 8.2 Hz, 1H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ 148.1, 133.1, 127.7, 123.8, 122.7 (q, *J* = 282.0 Hz), 85.9, 85.4 – 85.1 (m), 63.1 (q, *J* = 36.7 Hz) ppm.

^{19}F NMR (471 MHz, $CDCl_3$): δ -79.1 (d, *J* = 5.3 Hz) ppm .

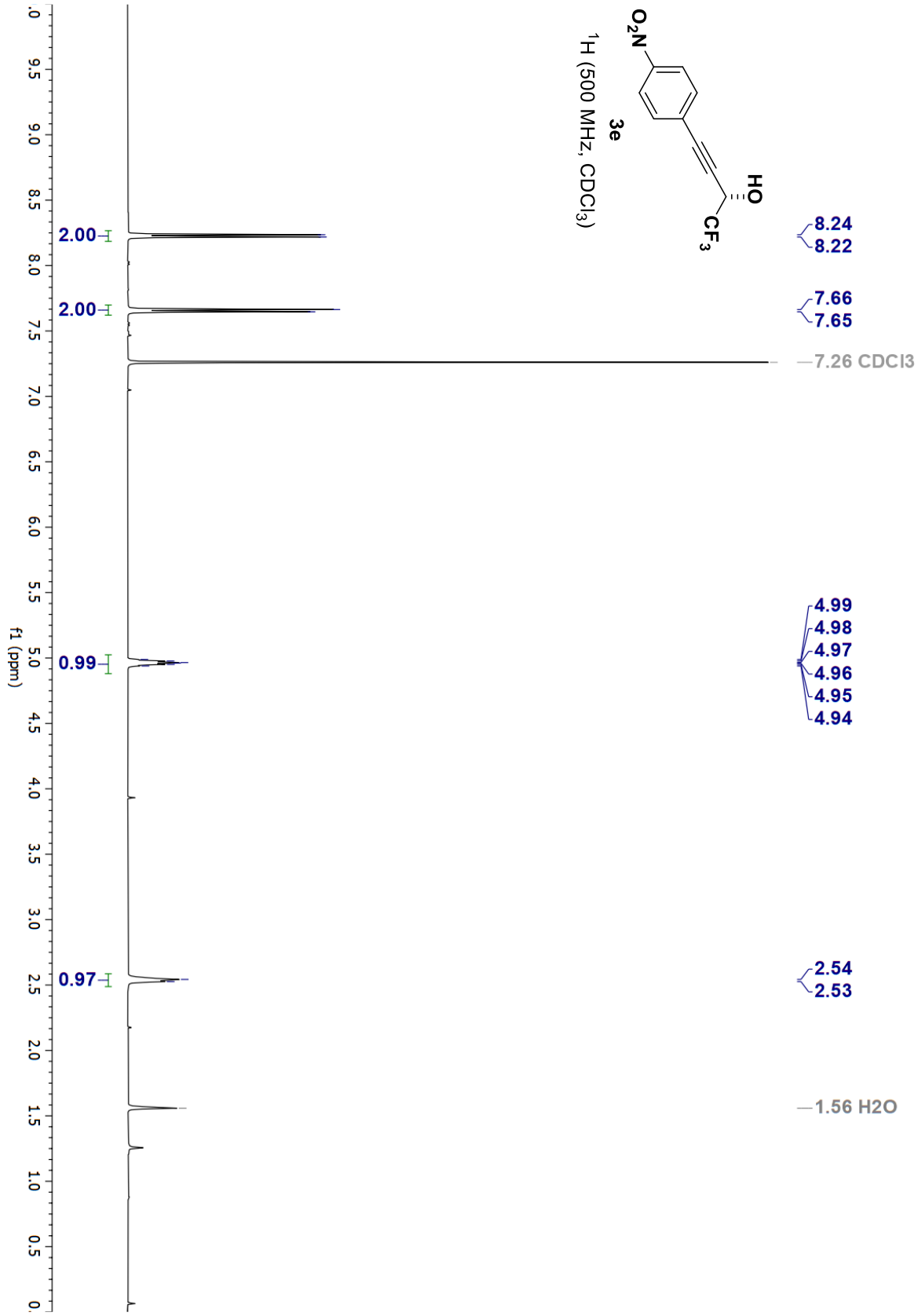
HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_{10}H_7F_3NO_3^+$: 246.0373; found = 246.0368.

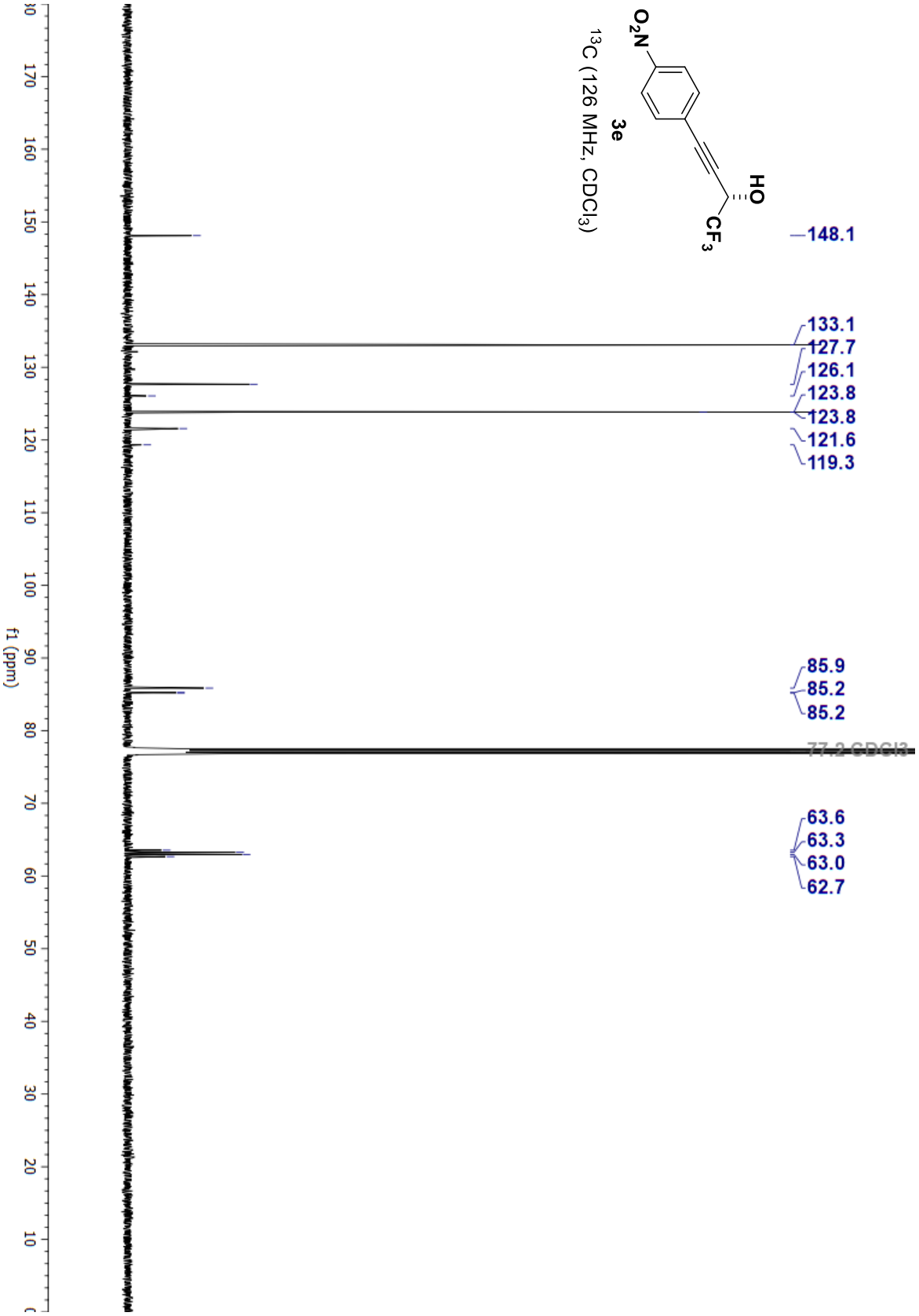
FTIR (neat): 3454, 3108, 2848, 1508, 1341, 1131, 855, 686, 476 cm^{-1}.

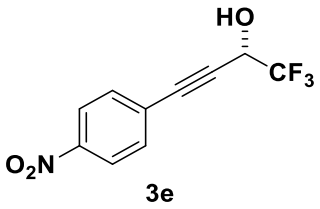
HPLC (CHIRALPAK AD-H, hexanes:2-PrOH = 93:7, 0.5 mL/min, 254 nm): ee = 99%.

$[\alpha]_D^{20}$ = -22° ($CHCl_3$, c = 1.0).

m.p.: 66 °C.

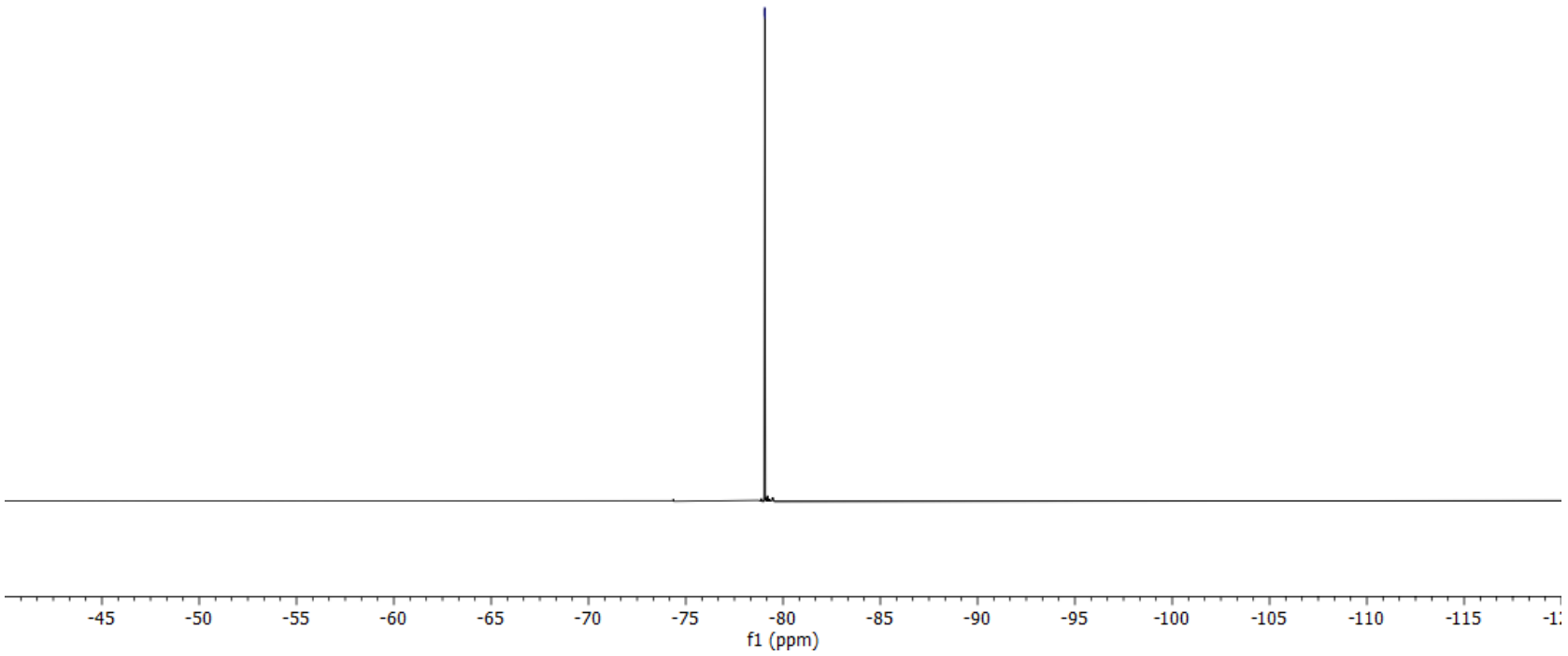

3e
^{1}H (500 MHz, $CDCl_3$)
O_2N
HO
CF_3
8.24
8.22
7.66
7.65
7.26 CDCl3
4.99
4.98
4.97
4.96
4.95
4.94
2.54
2.53
1.56 H2O
2.00
2.00
0.99
0.97
f1 (ppm)

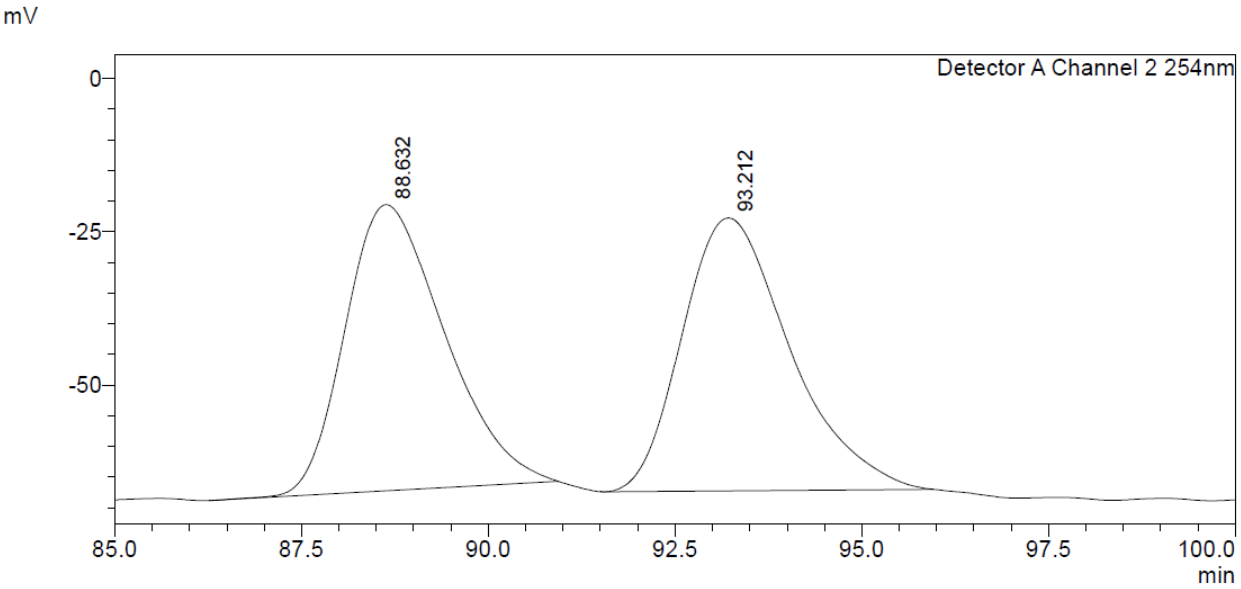

3e
^{13}C (126 MHz, CDCl$_3$)
O_2N
HO
CF_3
148.1
133.1
127.7
126.1
123.8
123.8
121.6
119.3
85.9
85.2
85.2
77.2 CDCl3
63.6
63.3
63.0
62.7
f1 (ppm)



3e

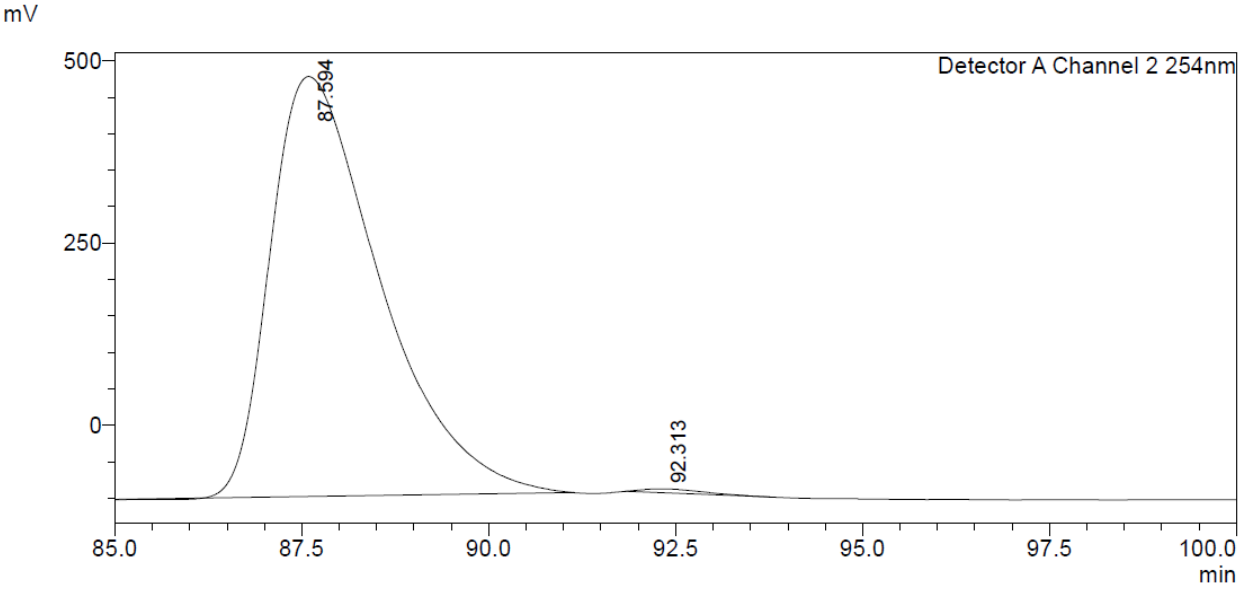
^{19}F (471 MHz, $CDCl_3$)





Detector A Channel 2 254nm

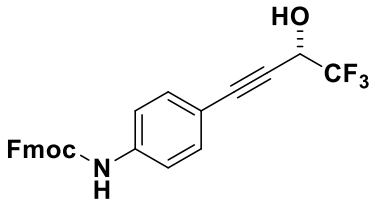
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	88.632	4320082	46655	49.177		M	
2	93.212	4464736	44507	50.823		M	
Total		8784818	91162				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	87.594	58607632	575299	99.466		M	
2	92.313	314671	5263	0.534		M	
Total		58922303	580562				

(9*H*-fluoren-9-yl)methyl (*S*)-(4-(4,4,4-trifluoro-3-hydroxybut-1-yn-1-yl)phenyl)carbamate (3f)



Alkyne **1f** (105.8 mg, 0.31 mmol) was subjected to standard reaction conditions (80 °C, 24 h) at 1 mol% catalyst loading. Upon flash column chromatography (SiO_2: 1:9–2:8 EtOAc:Hexanes), the title compound **3f** was isolated as a yellow solid in 75% yield (65.3 mg, 0.15 mmol, 98% ee).

TLC (SiO_2): R_f = 0.2 (2:8 EtOAc:Hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 (d, *J* = 7.5 Hz, 2H), 7.61 (d, *J* = 7.5 Hz, 2H), 7.42 (t, *J* = 7.8 Hz, 4H), 7.34 (td, *J* = 7.4, 1.2 Hz, 4H), 6.69 (s, 1H), 5.01 – 4.78 (m, 1H), 4.58 (d, *J* = 6.4 Hz, 2H), 4.27 (t, *J* = 6.4 Hz, 1H), 2.47 (d, *J* = 8.3 Hz, 1H) ppm.

^{13}C NMR (101 MHz, $CDCl_3$): δ 153.2, 143.7, 141.5, 138.9, 133.2, 128.0, 127.3, 125.0, 123.7 (q, *J* = 280.8 Hz), 120.2, 118.4, 115.8, 87.8, 80.1 (q, *J* = 2.5 Hz), 67.2, 63.1 (q, *J* = 36.5 Hz), 47.2 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ -79.3 (d, *J* = 5.6 Hz) ppm.

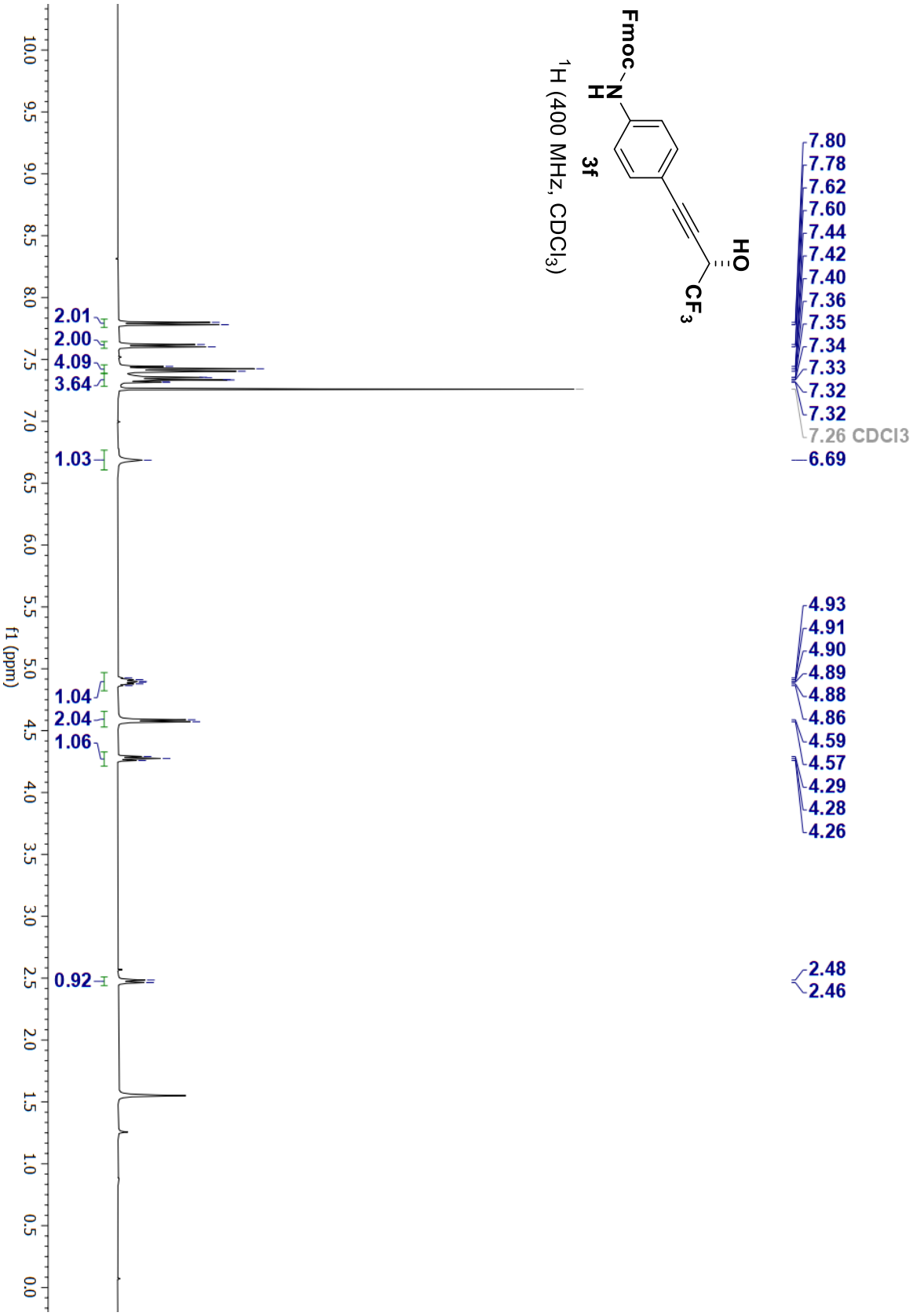
HRMS (ESI) m/z: [M+Na^+] calcd. for $C_{25}H_{18}F_3NO_3^+$: 460.1131; found =460.1137.

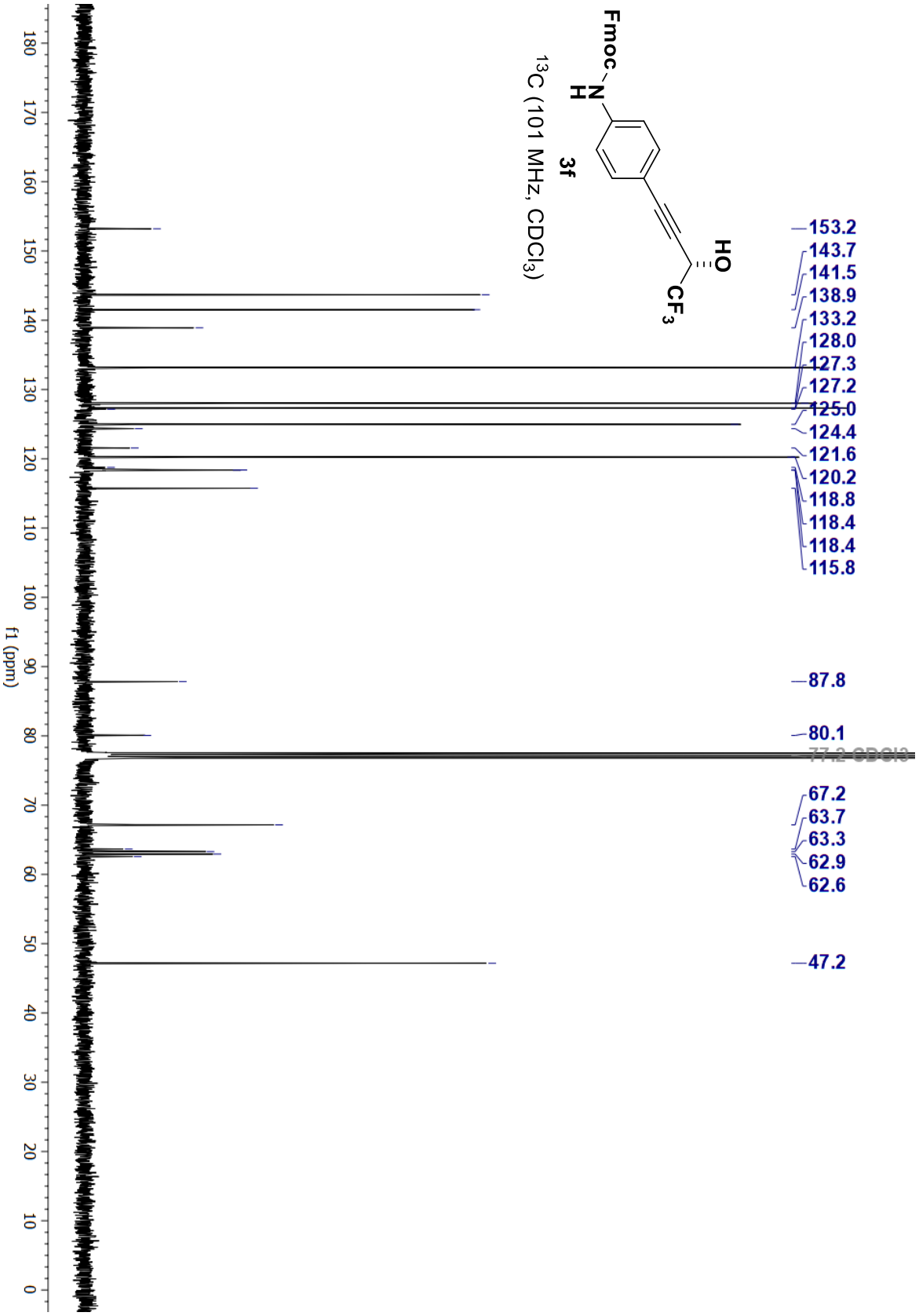
FTIR (neat): 3450, 3331, 3068, 3044, 2227, 1528, 1257, 1227, 1190, 1177, 1123, 1104, 1080, 1059, 830, 732, 536 cm^{-1}.

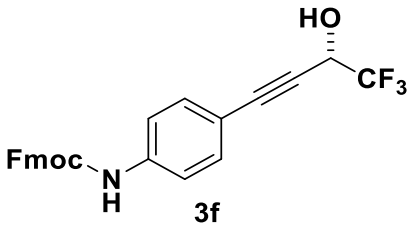
HPLC (Phenomenex Cellulose 5 column, Hexanes:2-PrOH = 95:5, 1.0 mL/min, 254 nm): ee = 98%

$[\alpha]_D^{25}$ = +39 (c=0.39, $CHCl_3$).

m.p.: 152 °C.

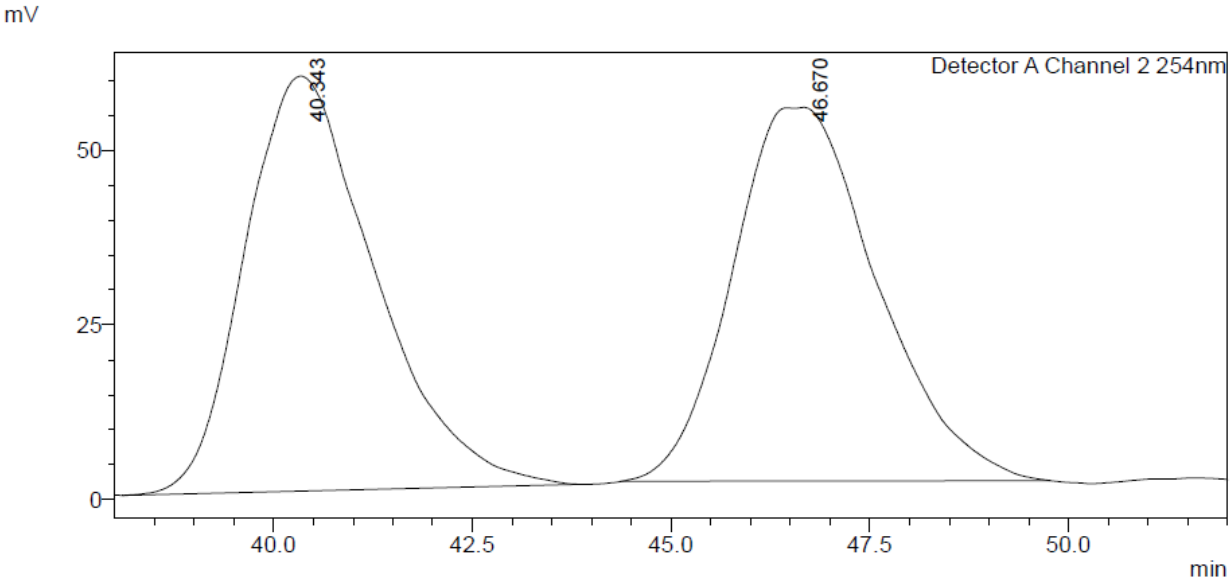

Fmoc
N
H
HO
CF3
3f
1H (400 MHz, CDCl3)
7.80
7.78
7.62
7.60
7.44
7.42
7.40
7.36
7.35
7.34
7.33
7.32
7.32
7.26 CDCl3
6.69
4.93
4.91
4.90
4.89
4.88
4.86
4.59
4.57
4.29
4.28
4.26
2.48
2.46
2.01
2.00
4.09
3.64
1.03
1.04
2.04
1.06
0.92
f1 (ppm)


Fmoc
N
H
HO
CF3
3f
13C (101 MHz, CDCl3)
153.2
143.7
141.5
138.9
133.2
128.0
127.3
127.2
125.0
124.4
121.6
120.2
118.8
118.4
118.4
115.8
87.8
80.1
77.2 CDCl3
67.2
63.7
63.3
62.9
62.6
47.2
f1 (ppm)



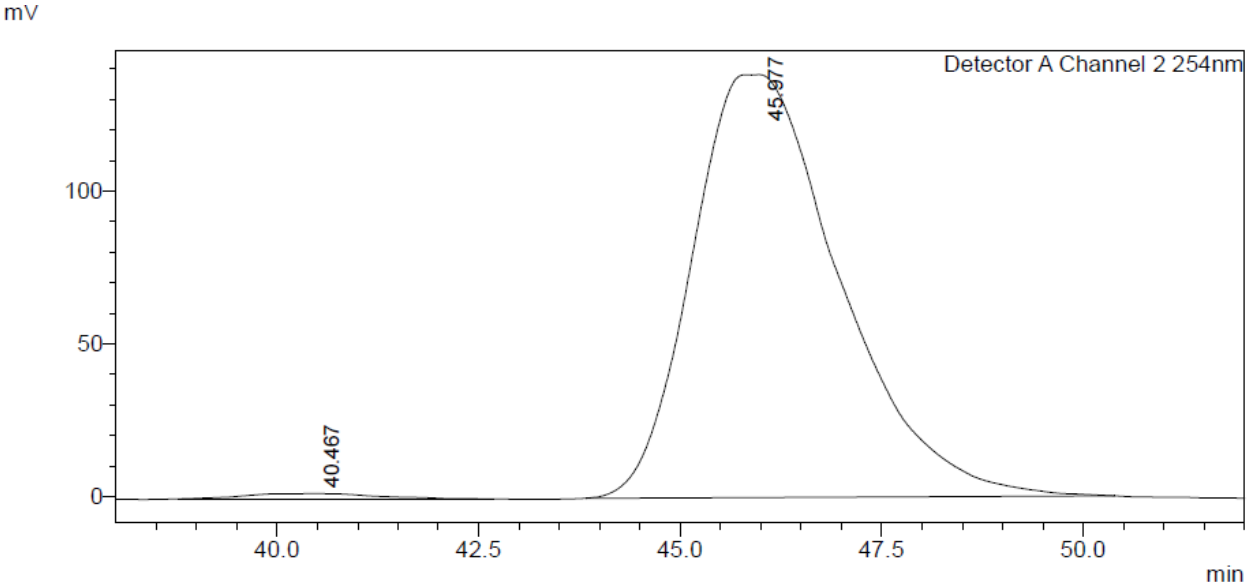
3f

^{19}F (376 MHz, $CDCl_3$)



Detector A Channel 2 254nm

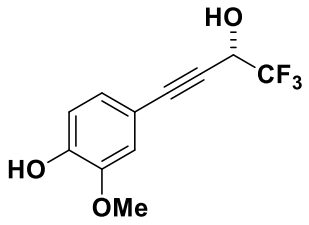
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	40.343	6762105	59343	49.975			
2	46.670	6768923	53440	50.025		M	
Total		13531028	112783				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	40.467	196267	1801	1.102		M	
2	45.977	17608716	138509	98.898		M	
Total		17804983	140310				

(S)-2-methoxy-4-(4,4,4-trifluoro-3-hydroxybut-1-yn-1-yl)phenol (3g)



Alkyne **1g** (31.1 mg, 0.21 mmol, 105 mol%) was subjected to standard reaction conditions (80 °C, 24 h) at 5 mol% catalyst loading. Upon flash chromatography (SiO2: 20:80 EtOAc:hexanes) the title compound **3g** was isolated as a pale yellow solid in 81% yield (39.8 mg, 0.16 mmol, 91% ee).

TLC (SiO_2): R_f = 0.3 (1:3 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.04 (d, 1H), 6.96 (s, 1H), 6.87 (d, *J* = 8.2 Hz, 1H), 5.80 (s, 1H), 4.89 (dq, *J* = 10.9, 5.7 Hz, 1H), 3.90 (s, 3H), 2.42 (d, *J* = 8.0 Hz, 1H) ppm.

^{13}C NMR (101 MHz, $CDCl_3$): δ 147.3, 146.2, 126.3, 122.8 (q, *J* = 281.9 Hz), 114.6, 114.1, 112.3, 88.4, 78.7 – 78.5 (m), 63.0 (q, *J* = 36.5 Hz), 56.1 ppm.

^{19}F NMR (471 MHz, $CDCl_3$): δ -79.4 (d, *J* = 5.8 Hz) ppm.

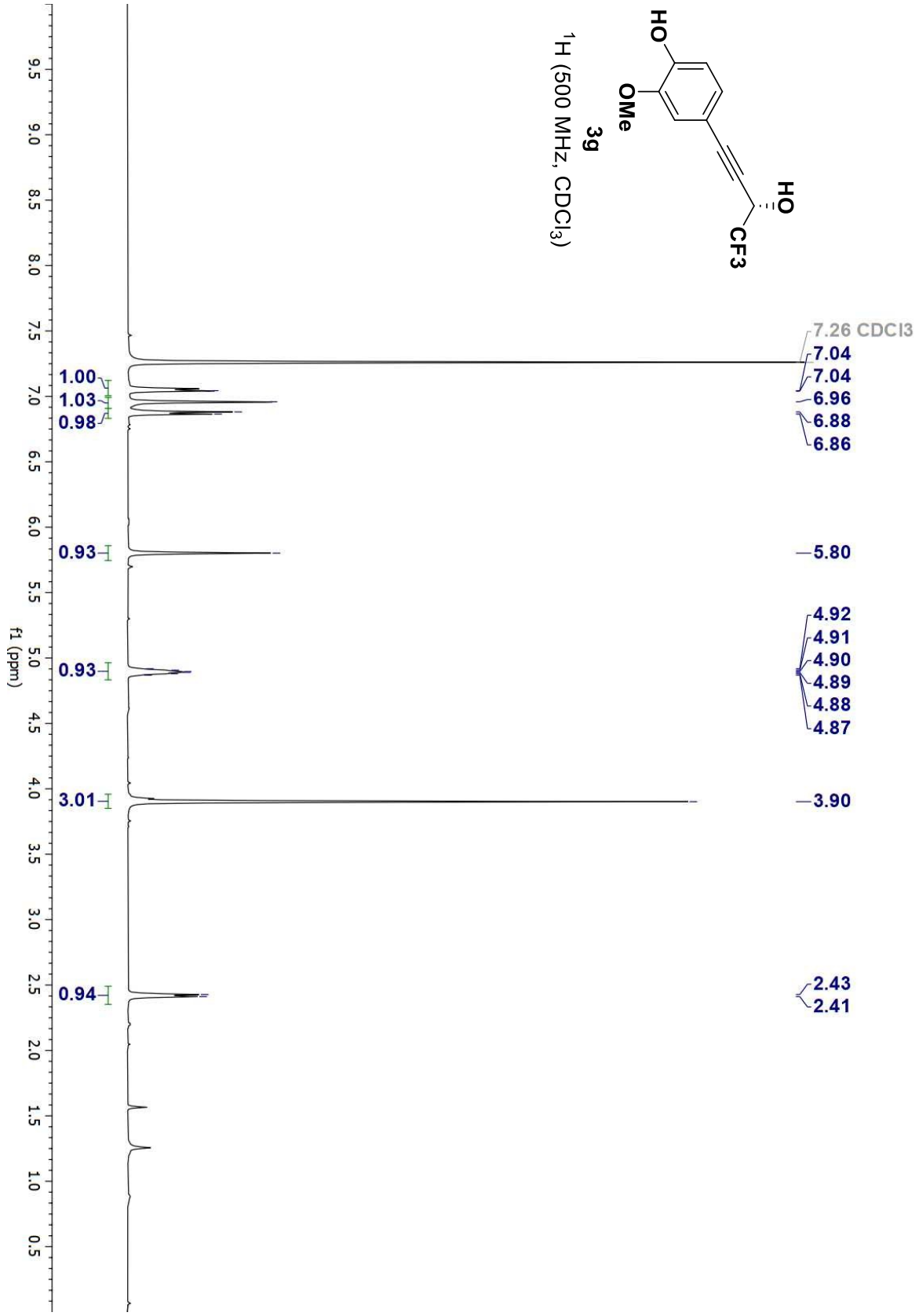
HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_{11}H_{10}F_3O_3^+$: 247.0577; found = 247.0577.

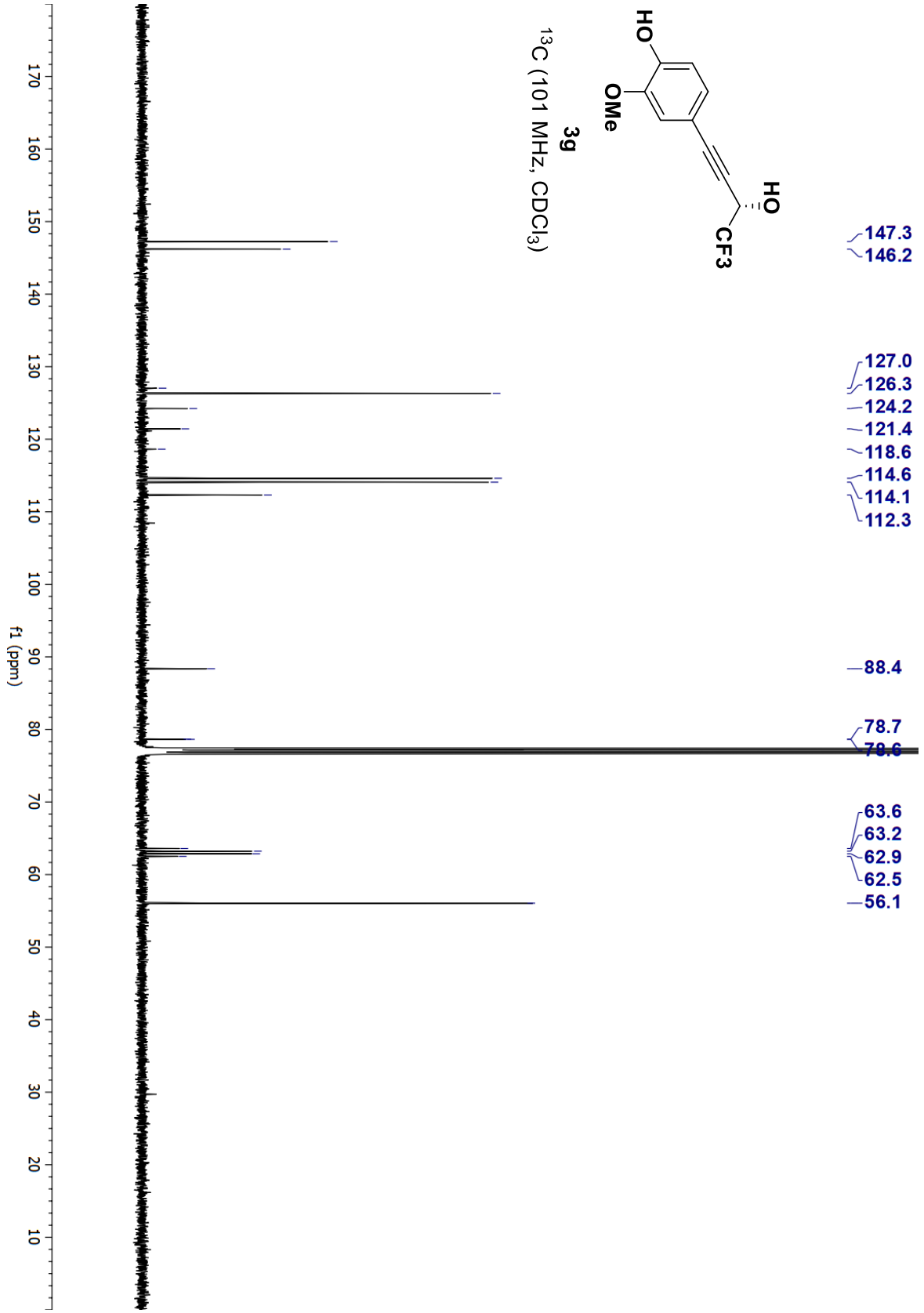
FTIR (neat): 3464, 3323, 2236, 1510, 1182, 1166, 1130, 1118, 1068, 1023, 997, 861, 681, 618 cm^{-1}.

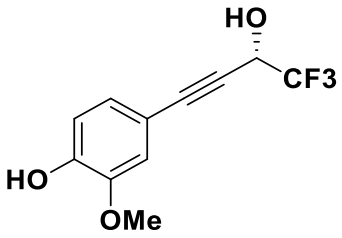
HPLC (PHENOMENEX Cellulose 5, hexanes:2-PrOH = 96:4, 0.5 mL/min, 254 nm): ee = 91%.

$[\alpha]_D^{20}$ = -77.1° ($CHCl_3$, c = 1.0).

m.p.: 112 °C.

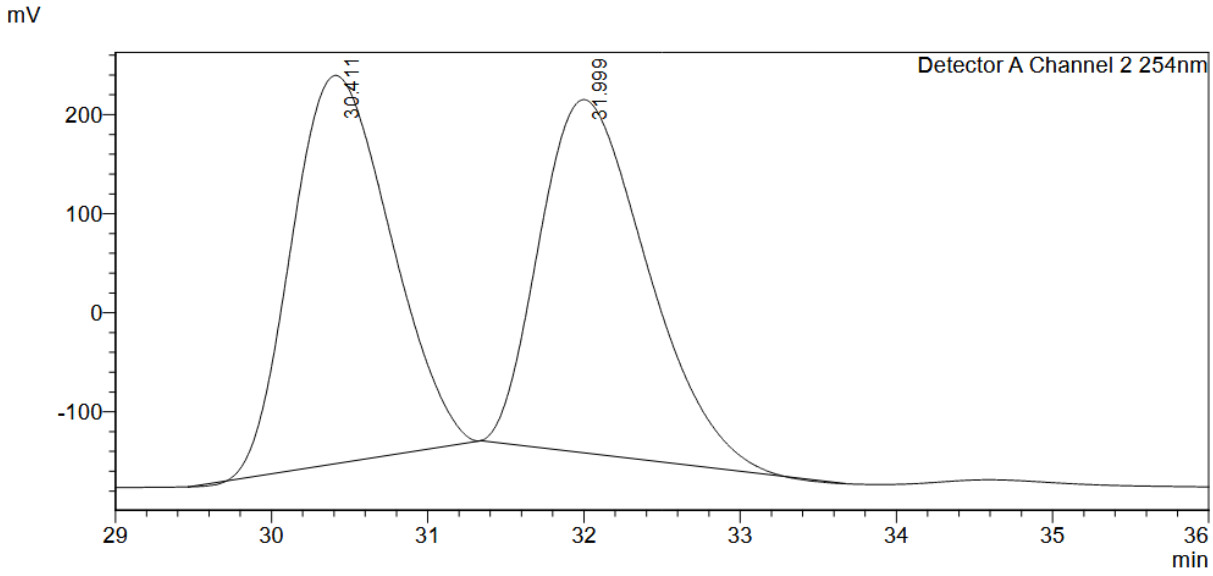

3g
^{1}H (500 MHz, CDCl$_3$)
HO
OMe
HO
CF3
f1 (ppm)
7.26 CDCl3
7.04
7.04
6.96
6.88
6.86
5.80
4.92
4.91
4.90
4.89
4.88
4.87
3.90
2.43
2.41
1.00
1.03
0.98
0.93
0.93
3.01
0.94


3g
^{13}C (101 MHz, CDCl$_3$)
HO
OMe
HO
CF3
147.3
146.2
127.0
126.3
124.2
121.4
118.6
114.6
114.1
112.3
88.4
78.7
78.6
63.6
63.2
62.9
62.5
56.1
f1 (ppm)



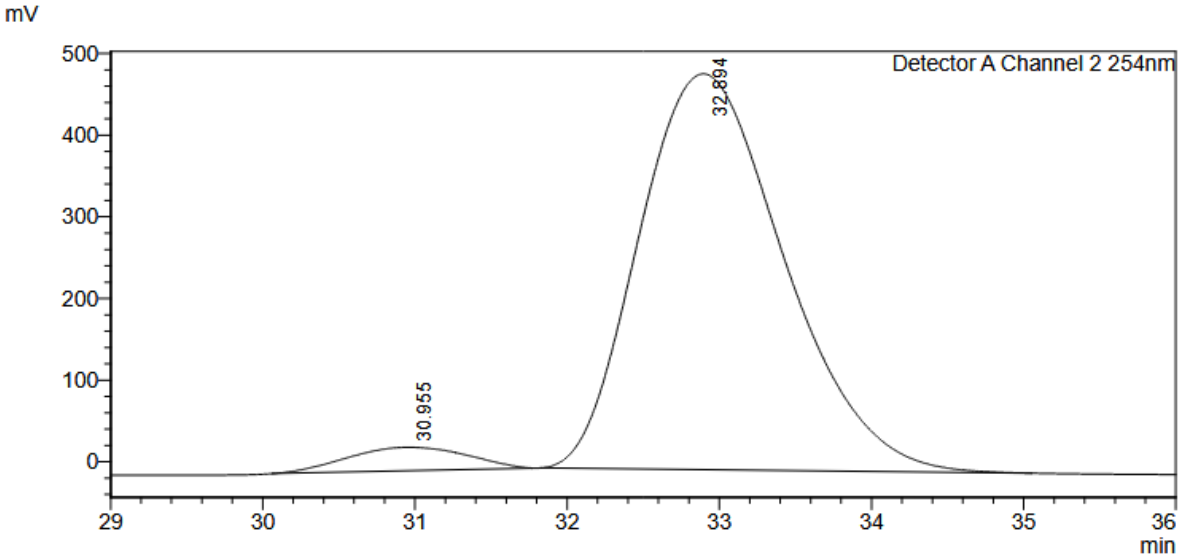
3g

^{19}F (471 MHz, $CDCl_3$)



Detector A Channel 2 254nm

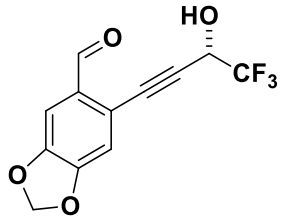
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	30.411	17185073	391860	50.121		M	
2	31.999	17101816	356566	49.879		M	
Total		34286889	748426				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	30.955	1566659	28652	4.661		M	
2	32.894	32043291	484935	95.339		M	
Total		33609950	513587				

(*S*)-6-(4,4,4-trifluoro-3-hydroxybut-1-yn-1-yl)benzo[d][1,3]dioxole-5-carbaldehyde (3h)



Alkyne **1h** (36.5 mg, 0.21 mmol, 105 mol%) was subjected to standard reaction conditions (80 °C, 24 h) at 1 mol% catalyst loading. Upon flash column chromatography (SiO_2: 10:90 EtOAc:hexanes), the title compound **3h** was isolated as a waxy brown solid in 62% yield (33.7 mg, 0.12 mmol, 99% ee).

TLC (SiO_2): R_f = 0.4 (1:10 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 10.28 (s, 1H), 7.36 (s, 1H), 6.98 (s, 1H), 6.11 (s, 2H), 5.05 – 4.90 (m, 1H), 2.89 – 2.65 (m, 1H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ 189.3, 152.5, 149.8, 133.3, 122.8 (q, J = 282.0 Hz), 120.6, 112.6, 106.7, 102.8, 87.1 – 85.1 (m), 83.7, 63.2 (q, J = 36.7 Hz) ppm.

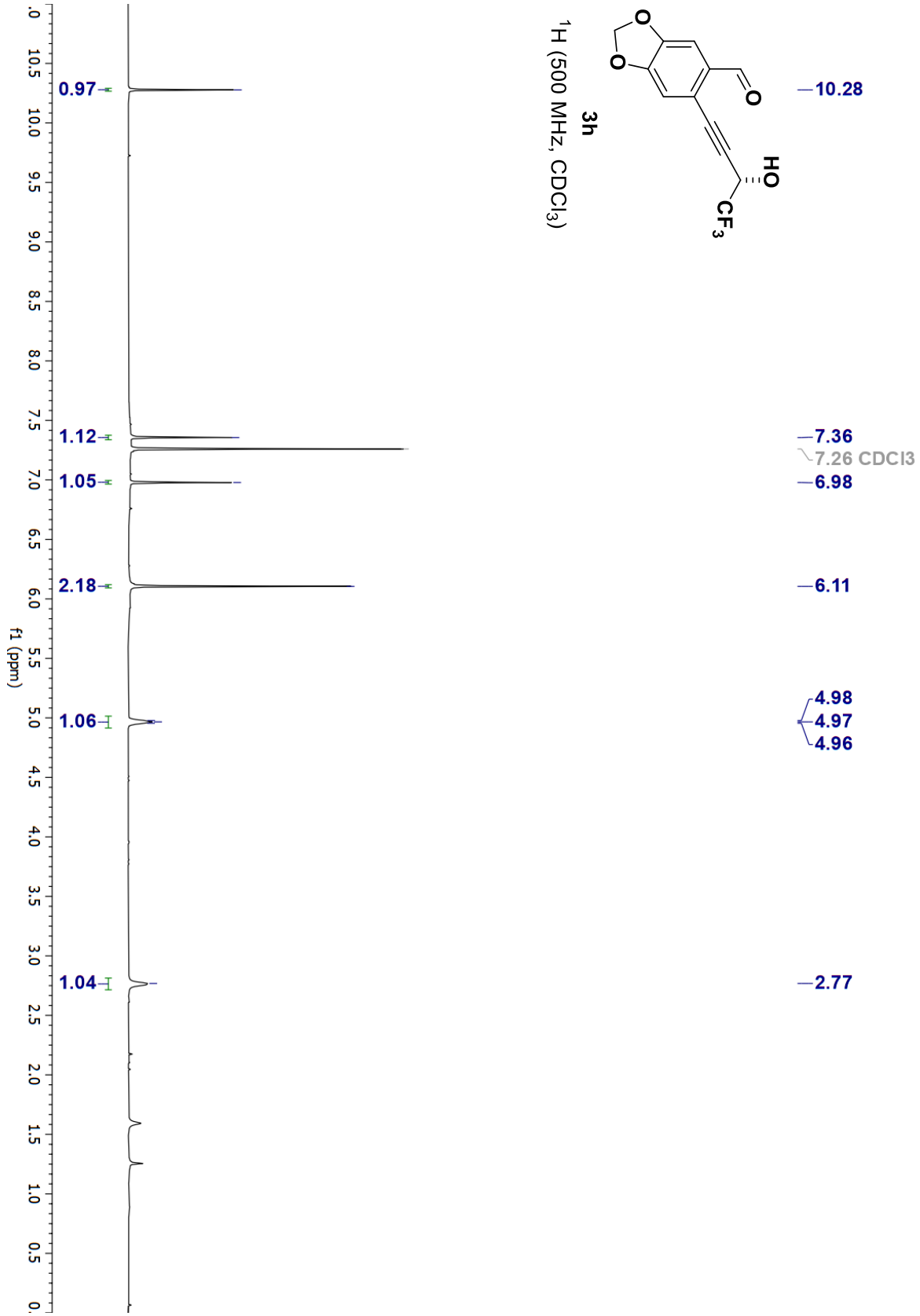
^{19}F NMR (471 MHz, $CDCl_3$): δ -79.1 (d, J = 5.4 Hz) ppm.

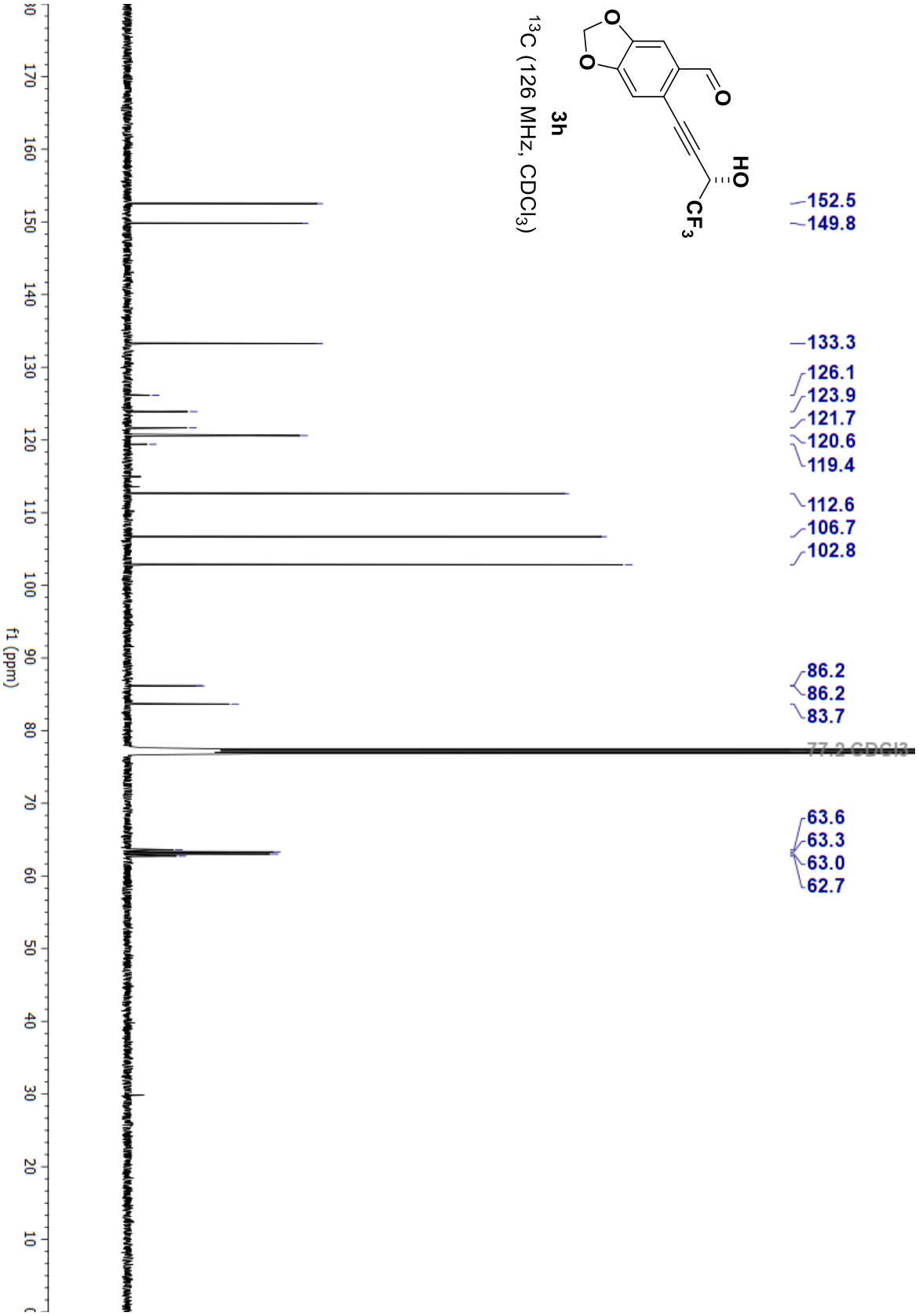
HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_{12}H_8F_3O_4^+$: 273.0369; found = 273.0364.

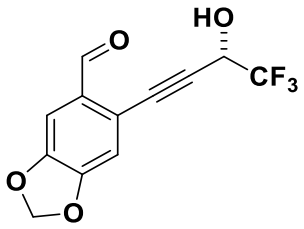
FTIR (neat): 3226, 2917, 2233, 1664, 1479, 1261, 1029, 695, 590 cm^{-1}.

HPLC (PHENOMENEX Cellulose 5, hexanes:2-PrOH = 95:5, 1.0 mL/min, 254 nm): ee = 99%.

$[\alpha]_D^{20}$ = -18° ($CHCl_3$, c = 0.5).

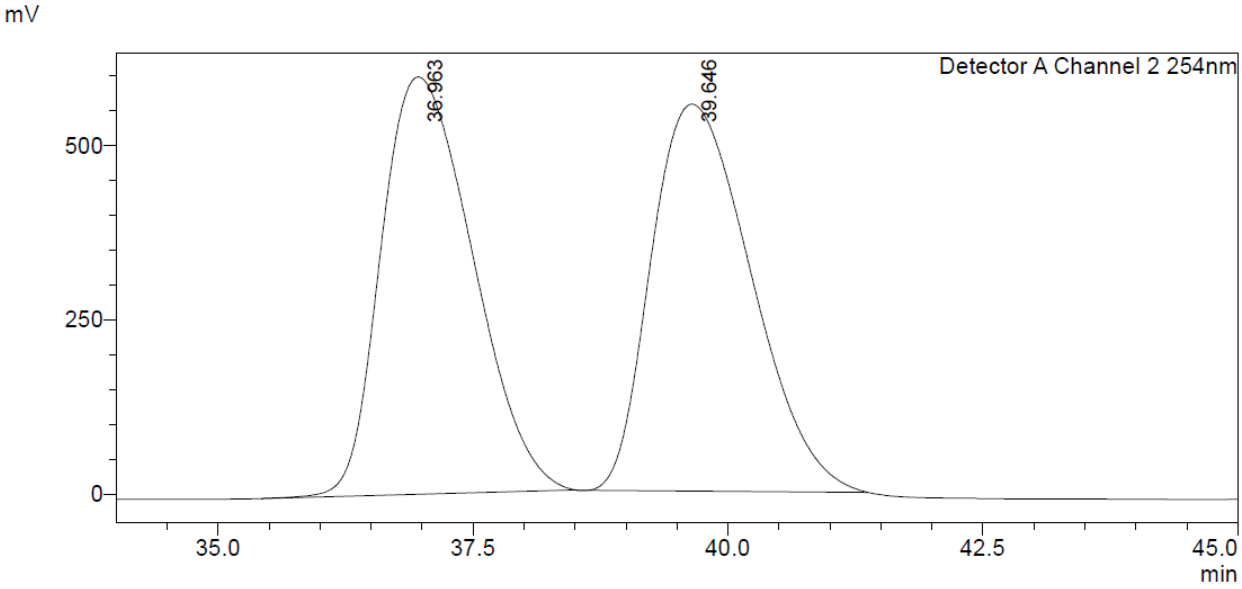

3h
^{1}H (500 MHz, CDCl$_3$)
HO
CF$_3$
O
O
O
10.28
7.36
7.26 CDCl3
6.98
6.11
4.98
4.97
4.96
2.77
0.97
1.12
1.05
2.18
1.06
1.04
f1 (ppm)


3h
^{13}C (126 MHz, CDCl$_3$)
O
O
O
HO
CF$_3$
152.5
149.8
133.3
126.1
123.9
121.7
120.6
119.4
112.6
106.7
102.8
86.2
86.2
83.7
77.2 CDCl3
63.6
63.3
63.0
62.7
f1 (ppm)



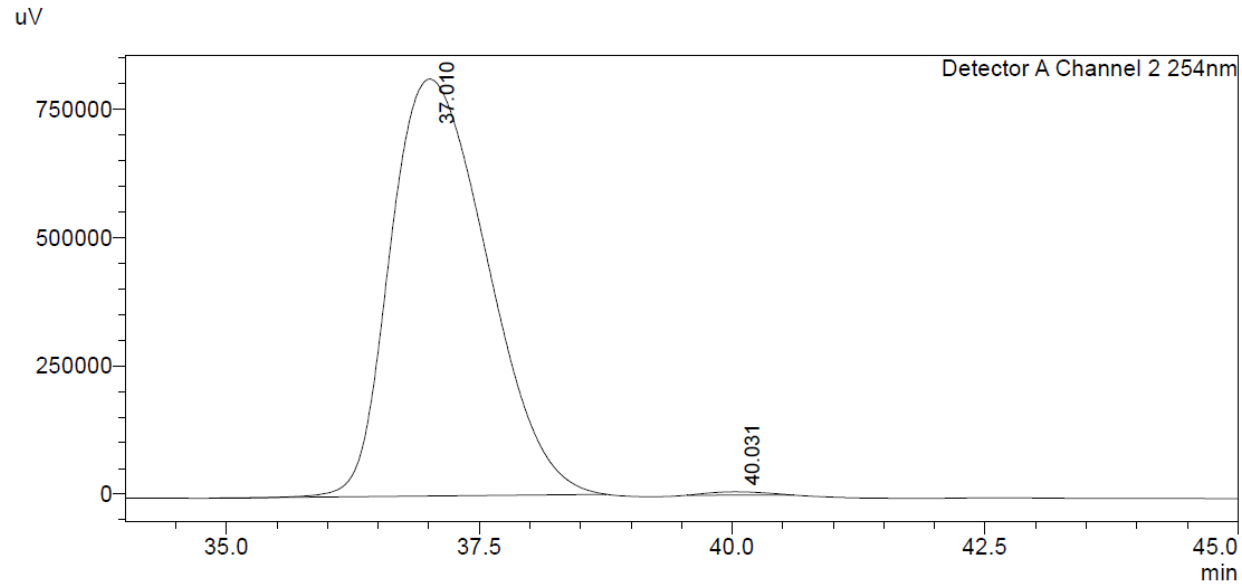
3h

^{19}F (471 MHz, $CDCl_3$)



Detector A Channel 2 254nm

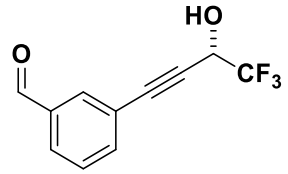
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	36.963	37378865	597857	49.715		M	
2	39.646	37806930	554347	50.285		M	
Total		75185795	1152204				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	37.010	54023249	812757	99.531		M	
2	40.031	254424	6650	0.469		M	
Total		54277673	819408				

(*S*)-3-(4,4,4-trifluoro-3-hydroxybut-1-yn-1-yl)benzaldehyde (3i)



Alkyne **1i** (27.3 mg, 0.21 mmol, 105 mol%) was subjected to standard reaction conditions (80 °C, 24 h) at 1 mol% catalyst loading. Upon flash column chromatography (SiO_2: 8:92 EtOAc:hexanes), the title compound **3i** was isolated as a yellow oil in 93% yield (42.4 mg, 0.19 mmol, 99% ee).

TLC (SiO_2): R_f = 0.4 (1:10 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 10.00 (s, 1H), 7.99 (s, 1H), 7.90 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.73 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.54 (t, *J* = 7.7 Hz, 1H), 5.03 – 4.83 (m, 1H), 2.92 – 2.69 (m, 1H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ 191.4, 137.6, 136.6, 133.4, 130.4, 129.4, 122.8 (q, *J* = 282.0 Hz), 122.3, 86.5, 82.2 (q, *J* = 2.2 Hz), 63.1 (q, *J* = 36.7 Hz) ppm.

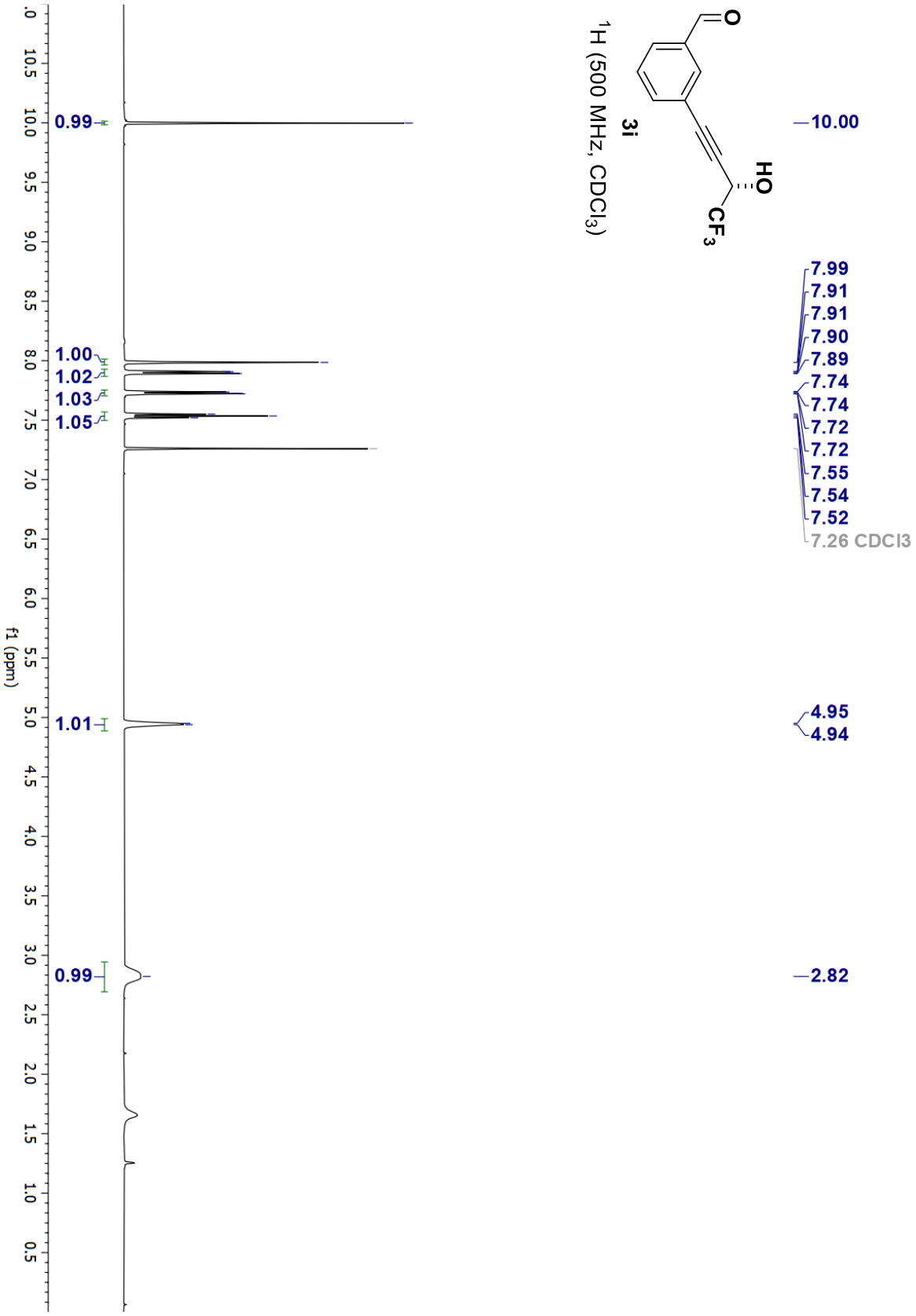
^{19}F NMR (471 MHz, $CDCl_3$): δ -79.2 (d, *J* = 5.6 Hz) ppm.

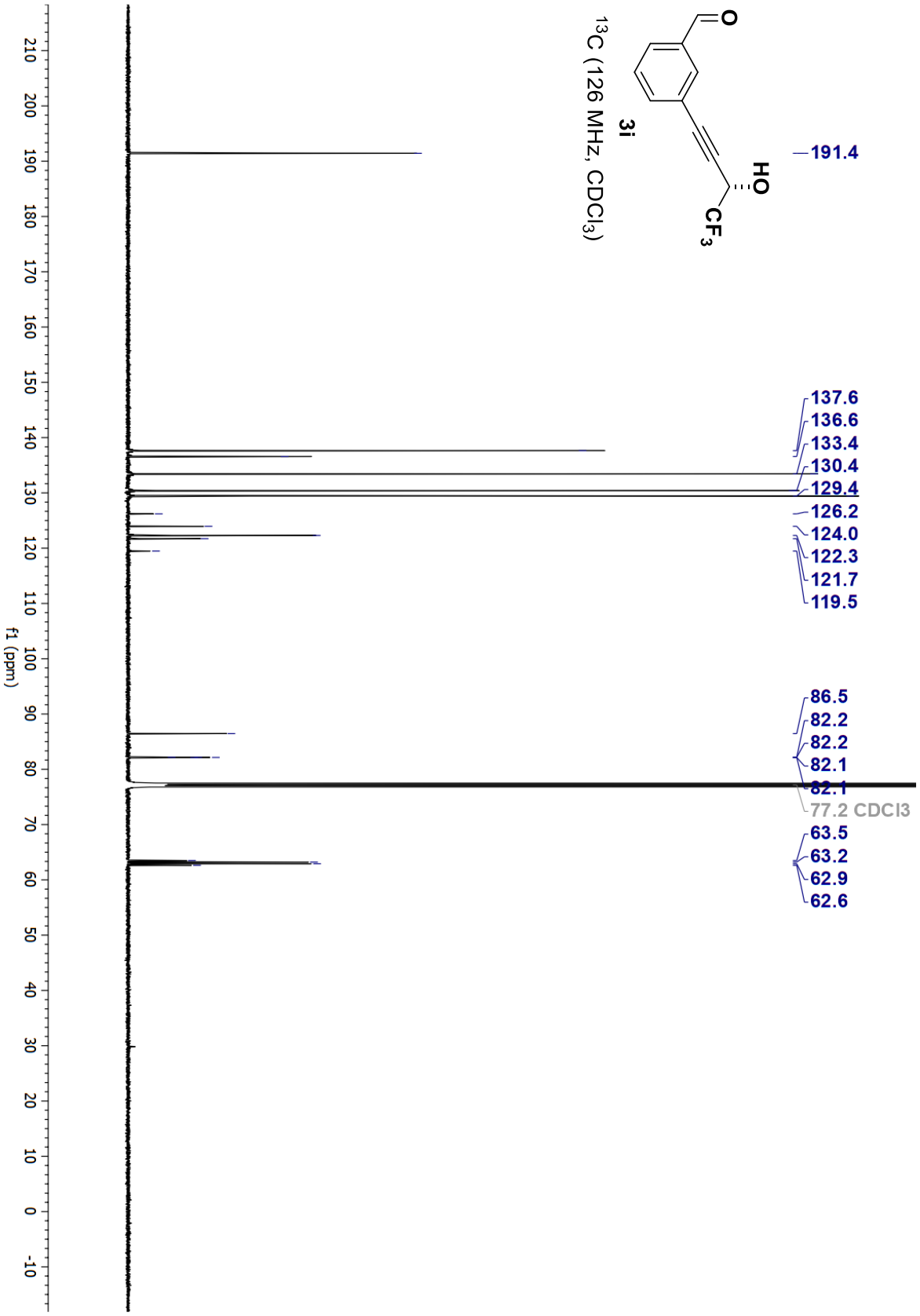
HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_{11}H_8F_3O_2^+$: 229.0471; found = 229.0463.

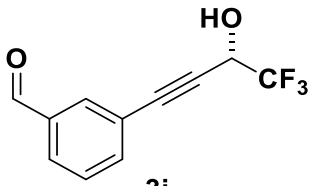
FTIR (neat): 3362, 2848, 2238, 1686, 1258, 1131, 1074, 640, 414 cm^{-1}.

HPLC (CHIRALPAK AD-H, hexanes:2-PrOH = 95:5, 1.0 mL/min, 254 nm): ee = 99%.

$[\alpha]_D^{20}$ = -16° ($CHCl_3$, c = 0.5).

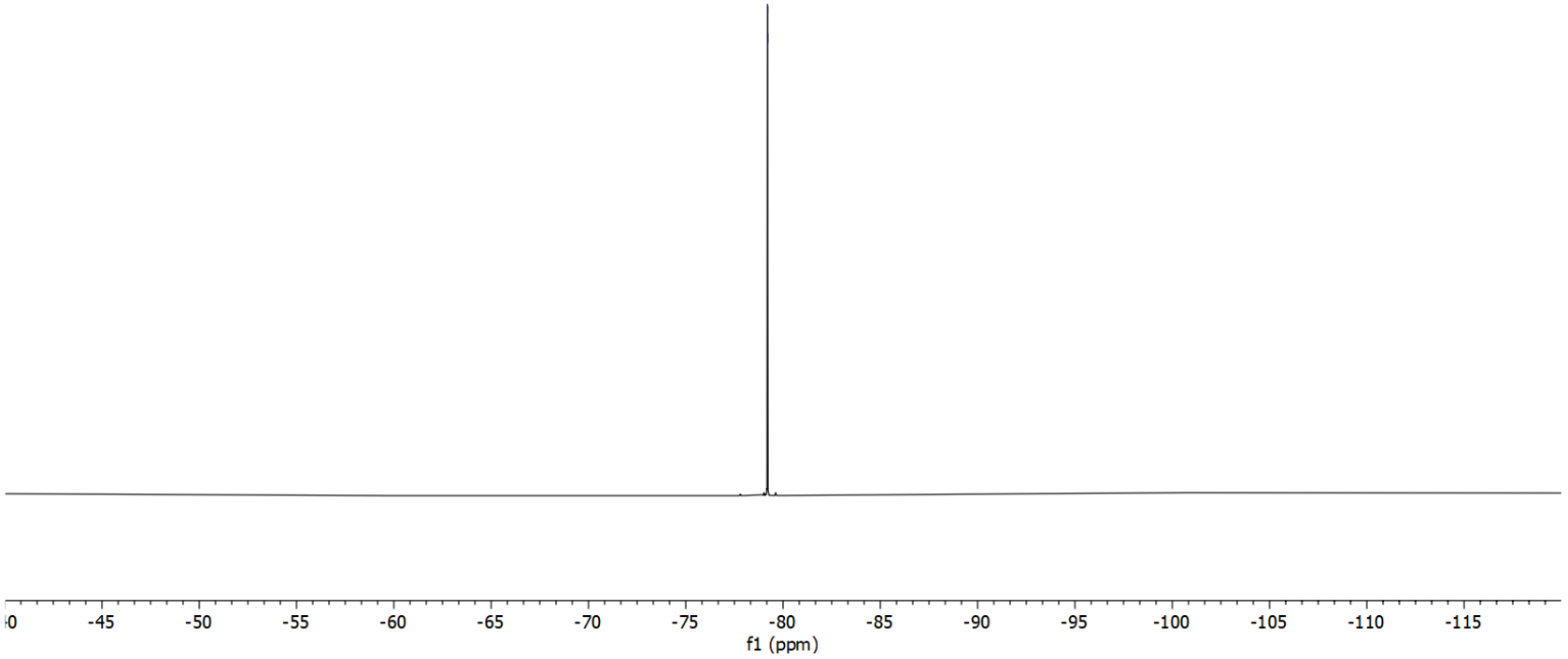

3i
^{1}H (500 MHz, CDCl$_3$)
O
HO
CF$_3$
10.00
7.99
7.91
7.91
7.90
7.89
7.74
7.74
7.72
7.72
7.55
7.54
7.52
7.26 CDCl3
4.95
4.94
2.82
0.99
1.00
1.02
1.03
1.05
1.01
0.99
f1 (ppm)

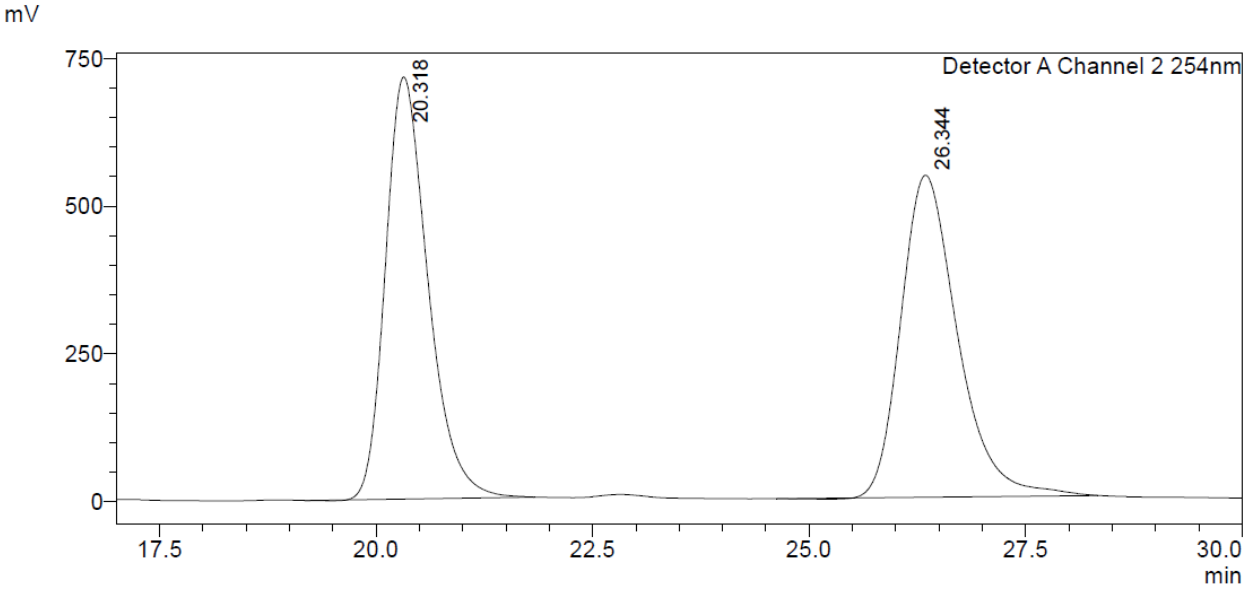

3i
^{13}C (126 MHz, CDCl$_3$)
O
HO
CF$_3$
191.4
137.6
136.6
133.4
130.4
129.4
126.2
124.0
122.3
121.7
119.5
86.5
82.2
82.2
82.1
82.1
77.2 CDCl3
63.5
63.2
62.9
62.6
f1 (ppm)



3i

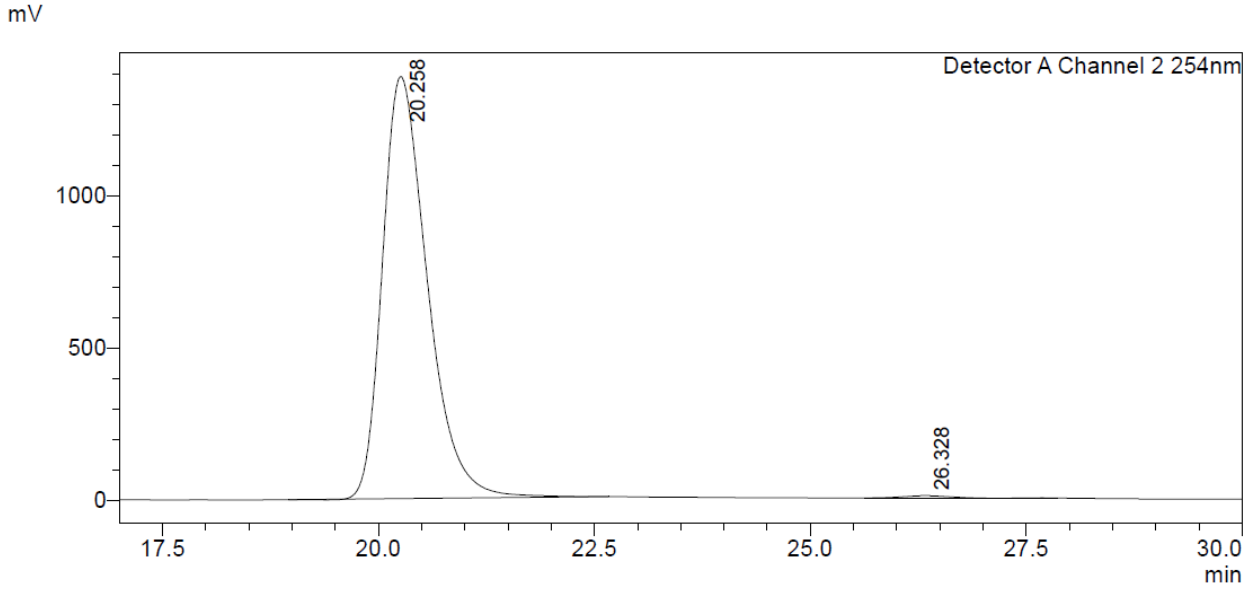
^{19}F (471 MHz, $CDCl_3$)





Detector A Channel 2 254nm

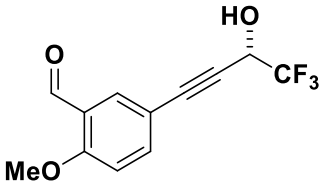
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	20.318	24425023	714696	49.610		M	
2	26.344	24808683	545424	50.390		M	
Total		49233706	1260120				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	20.258	50111200	1385693	99.463		M	
2	26.328	270450	7669	0.537		M	
Total		50381650	1393362				

(*S*)-2-methoxy-5-(4,4,4-trifluoro-3-hydroxybut-1-yn-1-yl)benzaldehyde (3j)



Alkyne **1j** (33.6 mg, 0.21 mmol, 105 mol%) was subjected to standard reaction conditions (80 °C, 24 h) at 1 mol% catalyst loading. Upon flash column chromatography (SiO_2: 8:92 EtOAc:hexanes), the title compound **3j** was isolated as a brown oil in 82% yield (42.3 mg, 0.16 mmol, 97% ee).

TLC (SiO_2): R_f = 0.4 (1:10 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 10.45 (s, 1H), 7.80 (d, *J* = 7.9 Hz, 1H), 7.15 (d, *J* = 7.9 Hz, 1H), 7.09 (s, 1H), 5.01 – 4.88 (m, 1H), 3.95 (s, 3H), 2.67 – 2.46 (m, 1H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ 189.2, 161.4, 128.8, 128.2, 125.4, 124.6, 122.8 (q, *J* = 281.9 Hz), 115.2, 87.1, 83.9 – 83.5 (m), 63.1 (q, *J* = 36.6 Hz), 56.0 ppm.

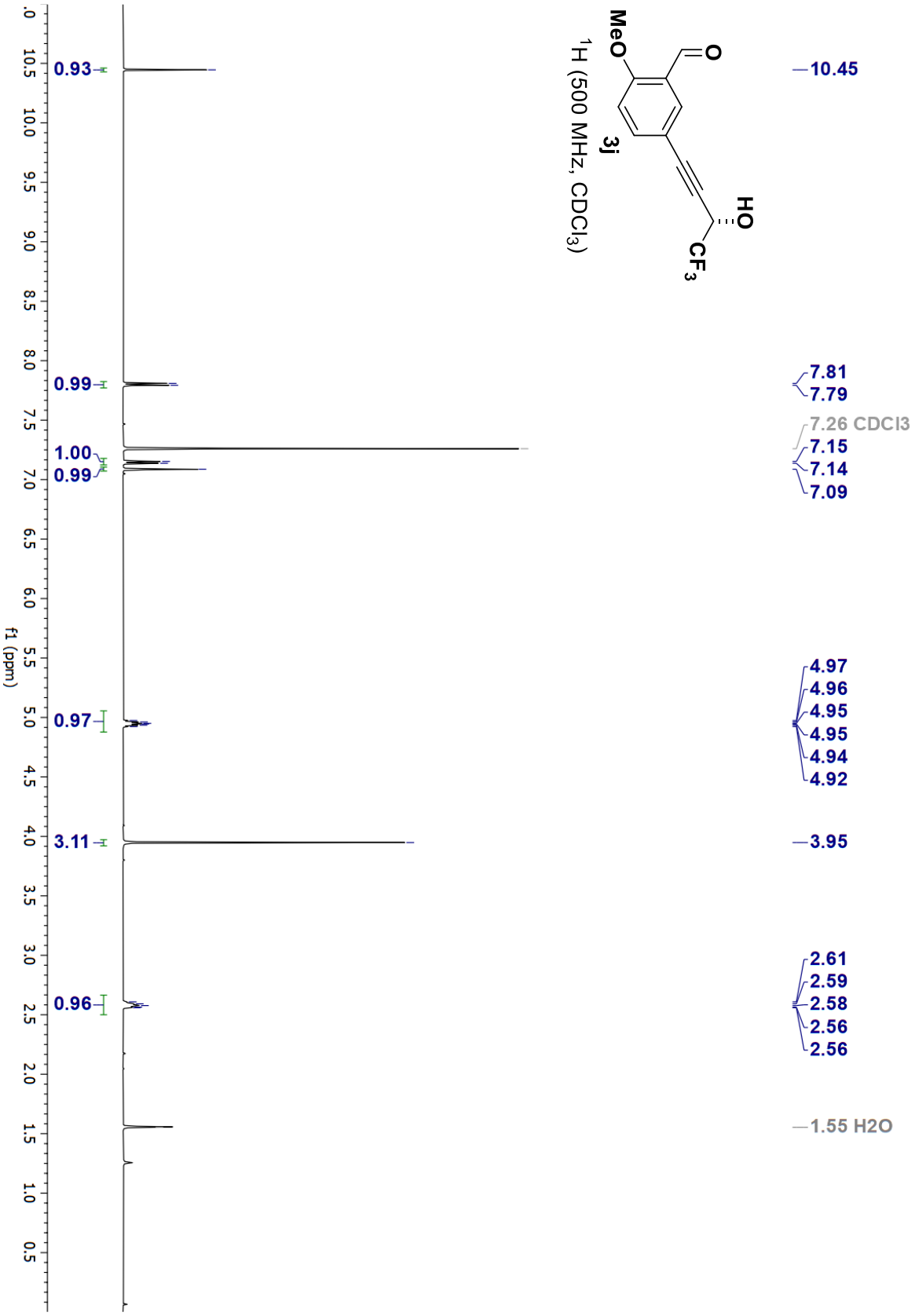
^{19}F NMR (471 MHz, $CDCl_3$): δ -79.1 (d, *J* = 5.8 Hz) ppm.

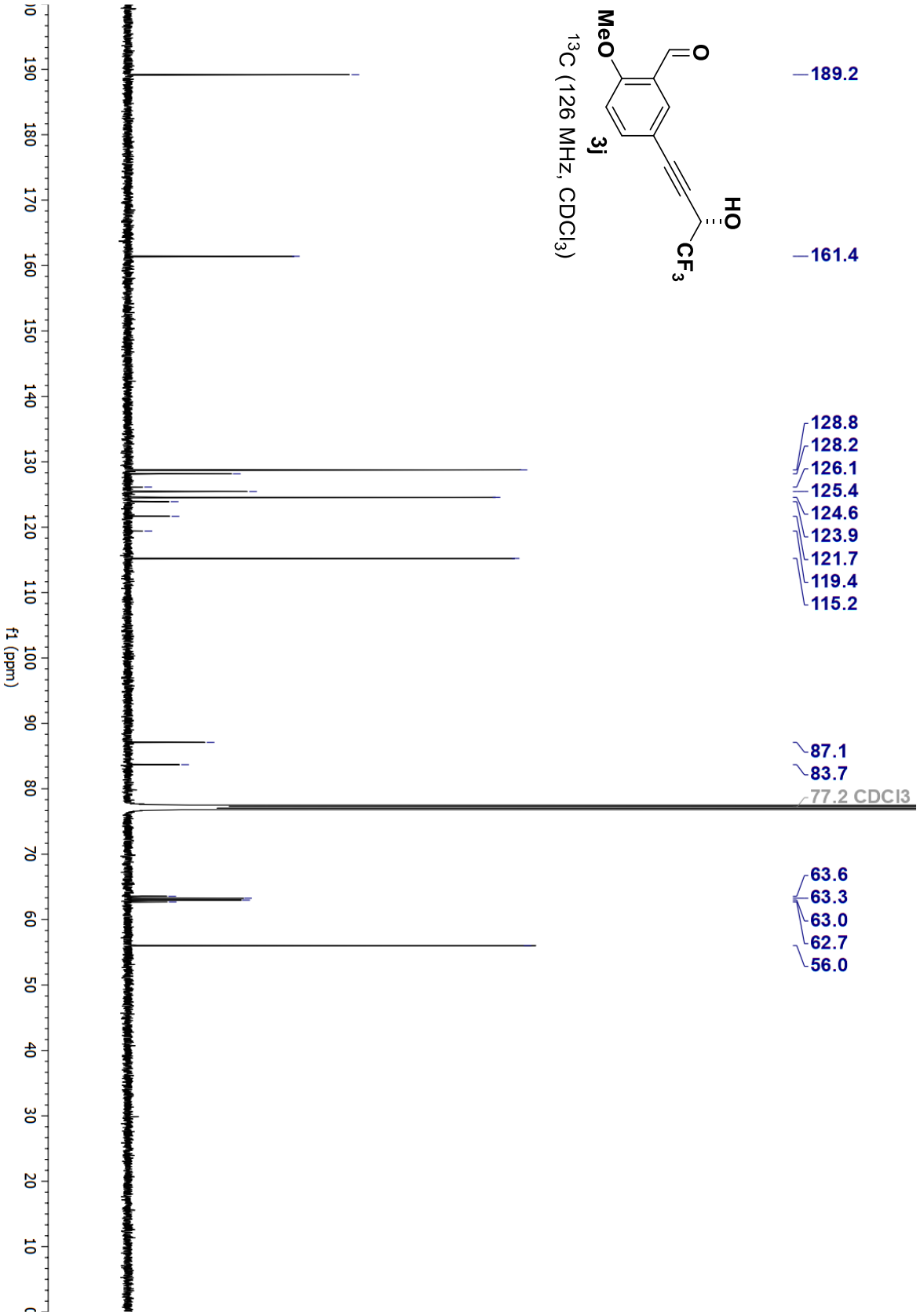
HRMS (ESI(+)): m/z [M+Na^+] calcd. for $C_{12}H_9F_3NaO_3^+$: 281.0396; found = 281.0382.

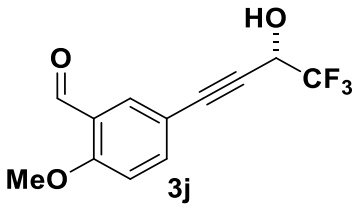
FTIR (neat): 3343, 2850, 2232, 1669, 1604, 1495, 1165, 820, 522 cm^{-1}.

HPLC (CHIRALPAK AD-H, hexanes:2-PrOH = 90:10, 1.0 mL/min, 254 nm): ee = 97%.

$[\alpha]_D^{20}$ = -4° ($CHCl_3$, c = 0.5).

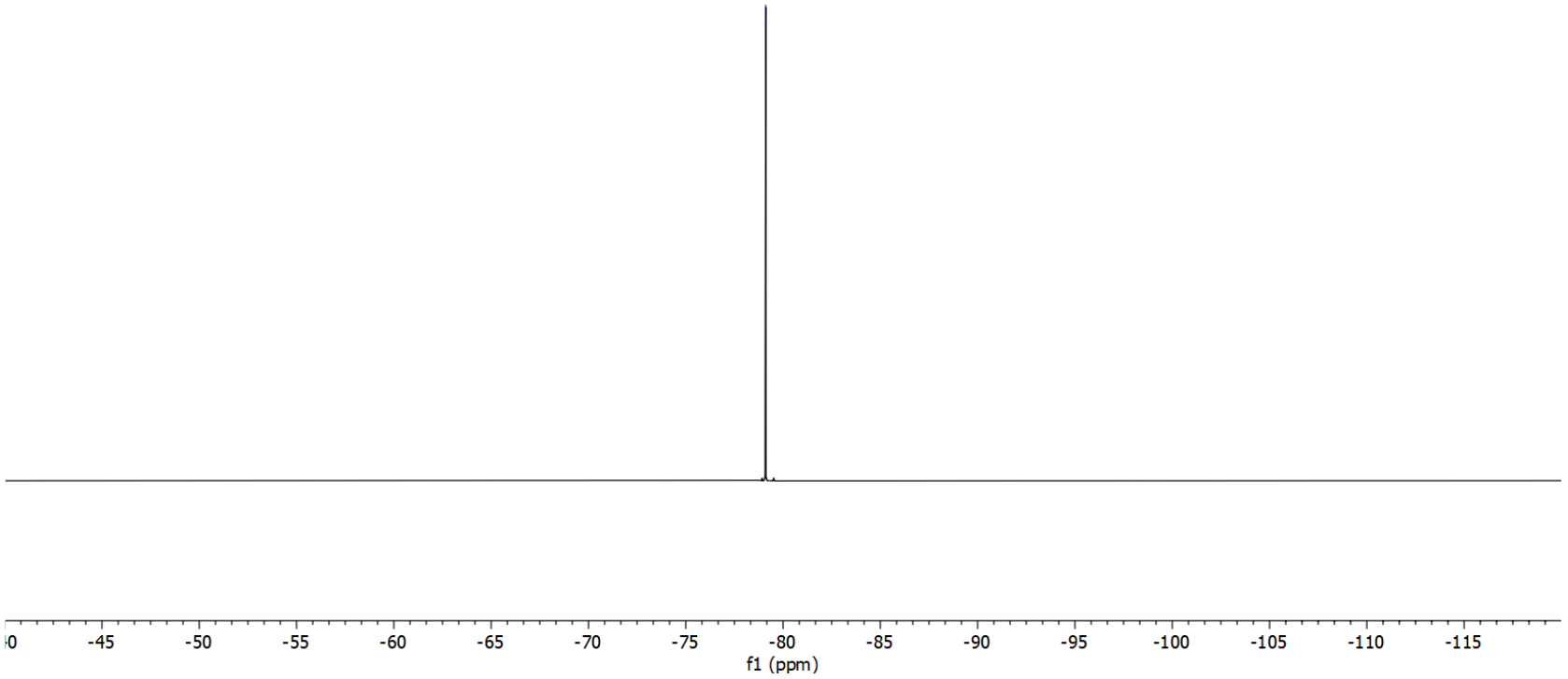

3j
^{1}H (500 MHz, CDCl$_3$)
MeO
O
HO
CF$_3$
10.45
7.81
7.79
7.26 CDCl3
7.15
7.14
7.09
4.97
4.96
4.95
4.95
4.94
4.92
3.95
2.61
2.59
2.58
2.56
2.56
1.55 H2O
0.93
0.99
1.00
0.99
0.97
3.11
0.96
f1 (ppm)

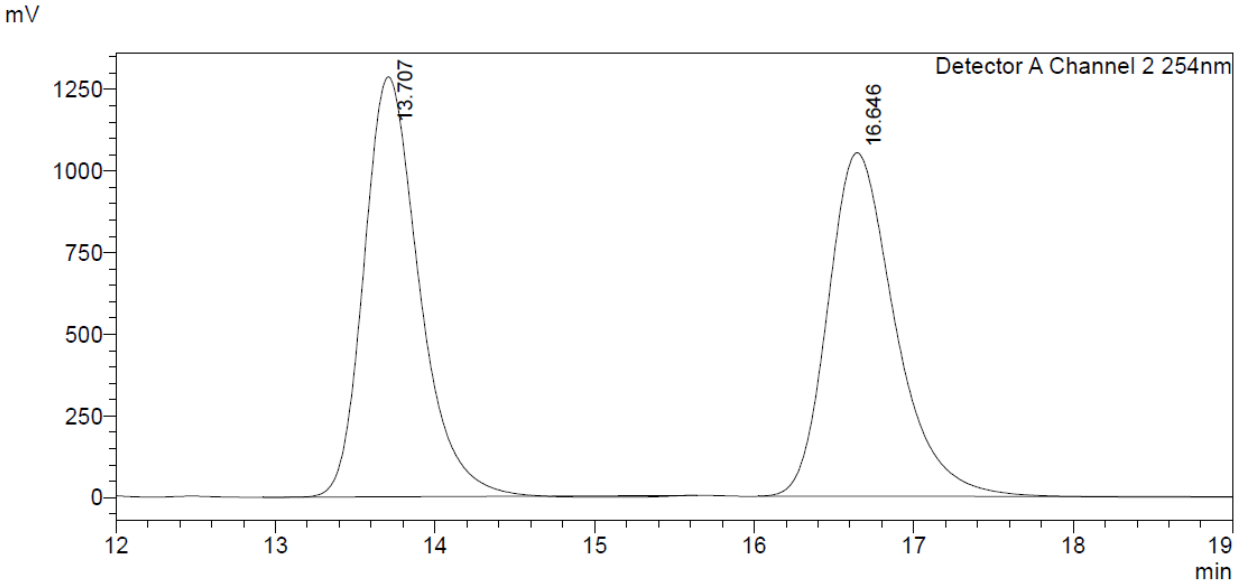

3j
^{13}C (126 MHz, CDCl$_3$)
MeO
O
HO
CF$_3$
189.2
161.4
128.8
128.2
126.1
125.4
124.6
123.9
121.7
119.4
115.2
87.1
83.7
77.2 CDCl3
63.6
63.3
63.0
62.7
56.0
f1 (ppm)



3j

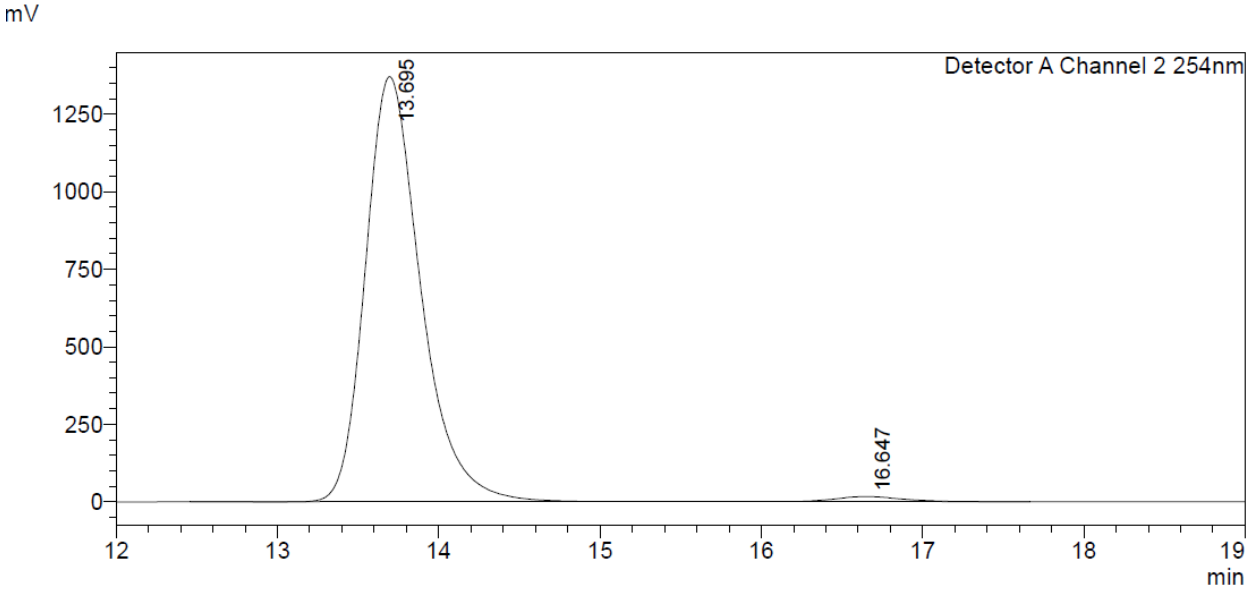
^{19}F (471 MHz, $CDCl_3$)





Detector A Channel 2 254nm

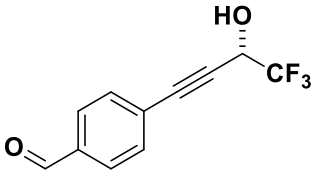
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	13.707	30749149	1285163	49.985		M	
2	16.646	30768019	1051450	50.015		M	
Total		61517169	2336612				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	13.695	32613468	1369473	98.690		M	
2	16.647	432907	15664	1.310		M	
Total		33046375	1385136				

(*S*)-4-(4,4,4-trifluoro-3-hydroxybut-1-yn-1-yl)benzaldehyde (3k)



Alkyne **1k** (27.3 mg, 0.21 mmol, 105 mol%) was subjected to standard reaction conditions (80 °C, 24 h) at 1 mol% catalyst loading. Upon flash column chromatography (SiO_2: 8:92 EtOAc:hexanes), the title compound **3k** was isolated as a yellow solid in 79% yield (36.0 mg, 0.16 mmol, 99% ee).

TLC (SiO_2): R_f = 0.4 (1:10 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 10.03 (s, 1H), 7.87 (d, *J* = 8.0 Hz, 2H), 7.64 (d, *J* = 8.0 Hz, 2H), 5.01 – 4.90 (m, 1H), 2.71 – 2.48 (m, 1H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ 191.5, 136.6, 132.8, 129.7, 127.1, 122.8 (q, *J* = 281.8 Hz), 86.9, 85.0 – 83.5 (m), 63.1 (q, *J* = 36.7 Hz) ppm.

^{19}F NMR (471 MHz, $CDCl_3$): δ -79.1 (d, *J* = 5.2 Hz) ppm.

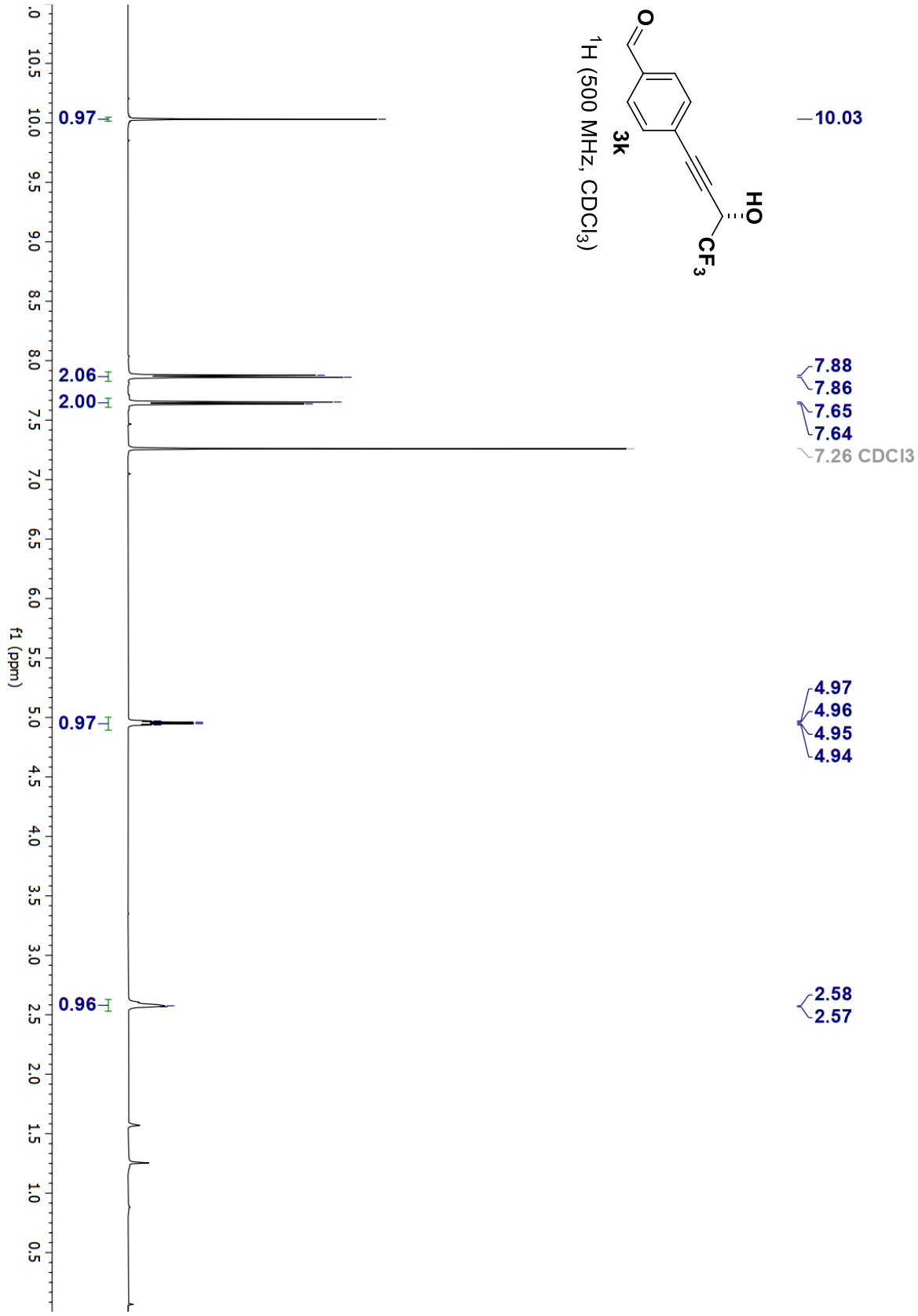
HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_{11}H_8F_3O_2^+$: 229.0471; found = 229.0470.

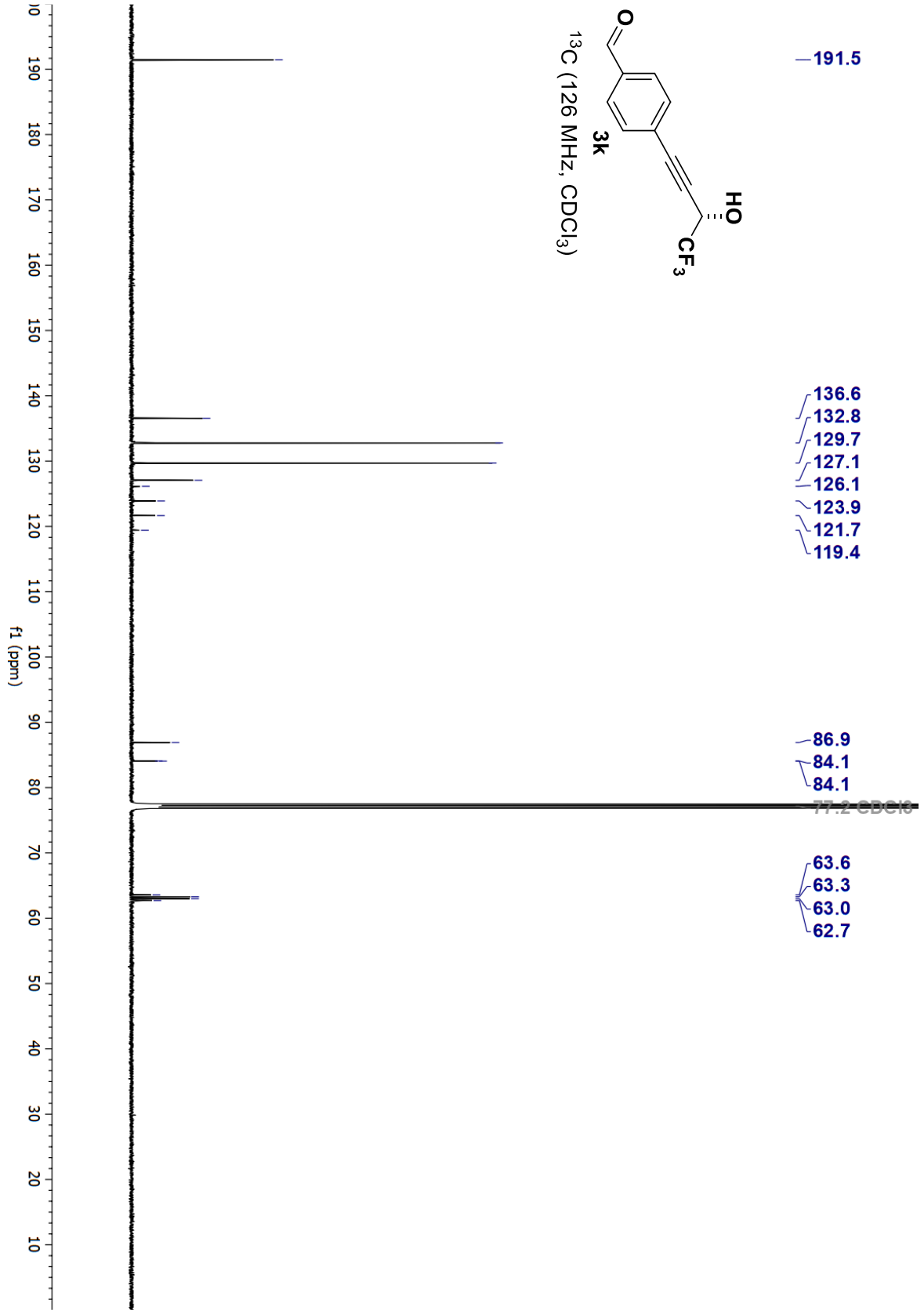
FTIR (neat): 3293, 2887, 1669, 1165, 1132, 1082, 829, 533, 499 cm^{-1}.

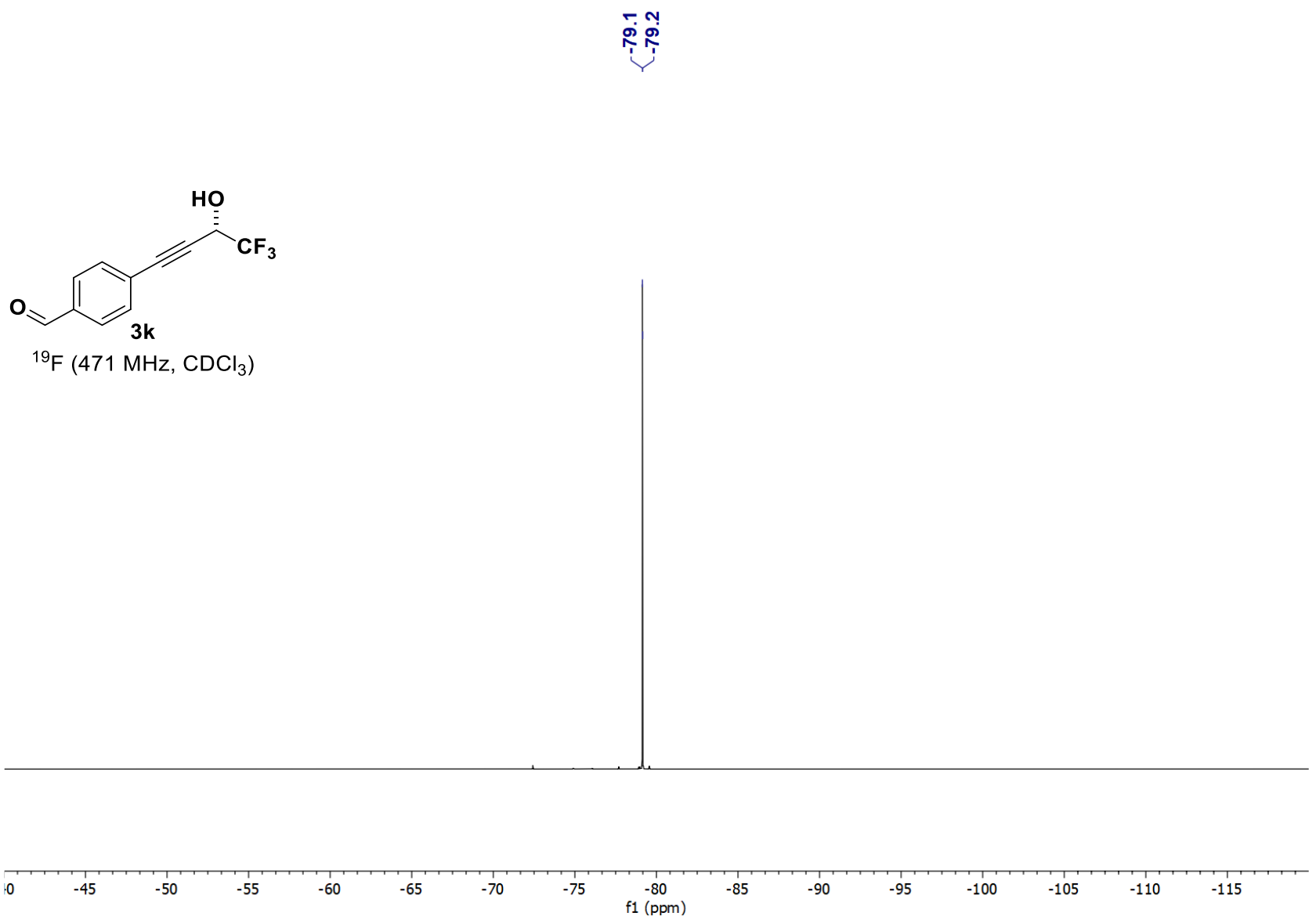
HPLC (CHIRALCEL OJ-H, hexanes:2-PrOH = 95:5, 1.0 mL/min, 254 nm): ee = 99%.

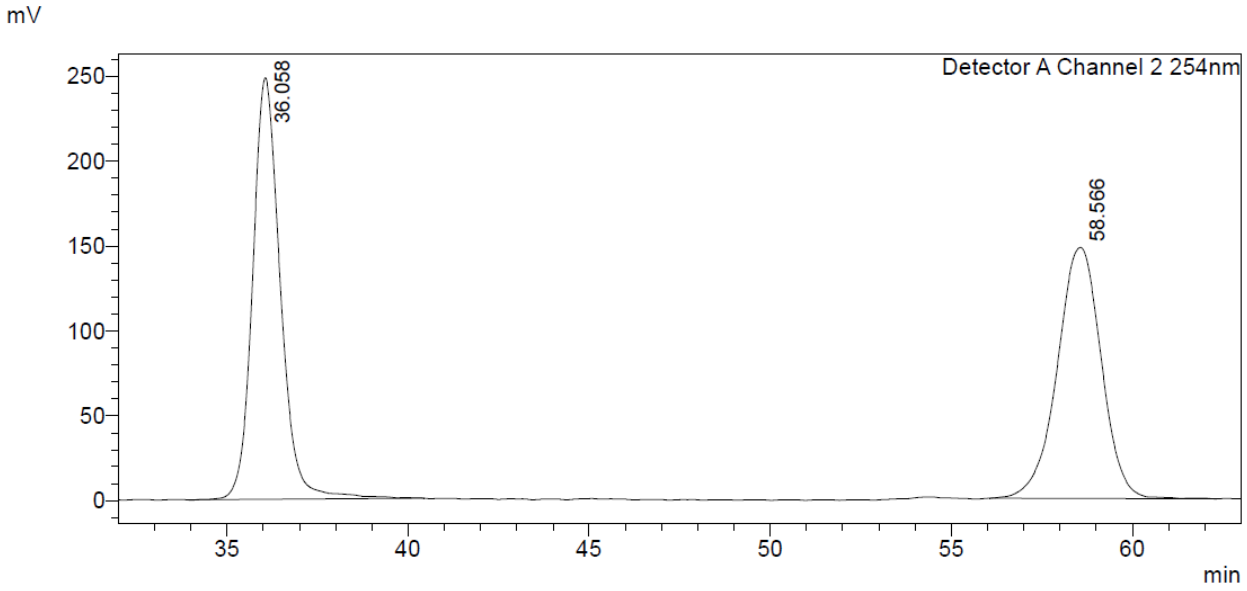
$[\alpha]_D^{20}$ = -42° ($CHCl_3$, c = 1.0).

m.p.: 78 °C.


^{1}H (500 MHz, CDCl$_3$)
3k
O
HO
CF$_3$
10.03
7.88
7.86
7.65
7.64
7.26 CDCl3
4.97
4.96
4.95
4.94
2.58
2.57
0.97
2.06
2.00
0.97
0.96
f1 (ppm)

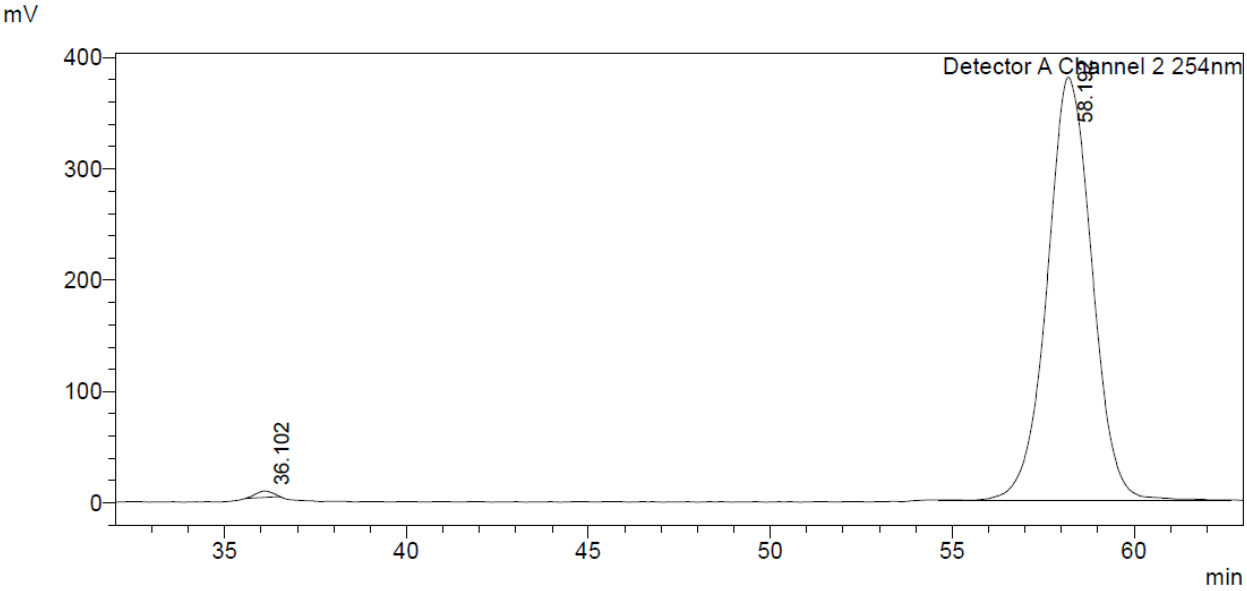

3k
^{13}C (126 MHz, CDCl$_3$)
O
HO
CF$_3$
191.5
136.6
132.8
129.7
127.1
126.1
123.9
121.7
119.4
86.9
84.1
84.1
77.2 CDCl3
63.6
63.3
63.0
62.7
f1 (ppm)


-79.1
-79.2
HO
CF3
O
3k
19F (471 MHz, CDCl3)
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
f1 (ppm)



Detector A Channel 2 254nm

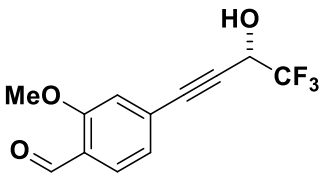
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	36.058	13241053	248300	51.423		M	
2	58.566	12508182	147854	48.577		M	
Total		25749235	396154				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	36.102	180853	5579	0.554		M	
2	58.192	32479681	379638	99.446		M	
Total		32660534	385216				

(*S*)-2-methoxy-4-(4,4,4-trifluoro-3-hydroxybut-1-yn-1-yl)benzaldehyde (3l)



Alkyne **1l** (33.6 mg, 0.21 mmol, 105 mol%) was subjected to standard reaction conditions (80 °C, 24 h) at 1 mol% catalyst loading. Upon flash column chromatography (SiO_2: 8:92 EtOAc:hexanes), the title compound **3l** was isolated as a white solid in 88% yield (45.4 mg, 0.18 mmol, 99% ee).

TLC (SiO_2): R_f = 0.4 (1:10 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 10.41 (s, 1H), 7.96 (s, 1H), 7.66 (d, *J* = 8.7 Hz, 1H), 6.98 (d, *J* = 8.6 Hz, 1H), 4.94 – 4.86 (m, 1H), 3.97 (s, 3H), 2.71 – 2.55 (m, 1H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ 188.8, 162.3, 139.3, 132.8, 124.9, 122.9 (q, *J* = 281.9 Hz), 113.7, 112.1, 86.8, 82.2 – 79.4 (m), 63.1 (q, *J* = 36.5 Hz), 56.1 ppm.

^{19}F NMR (471 MHz, $CDCl_3$): δ -79.3 (d, *J* = 5.8 Hz) ppm.

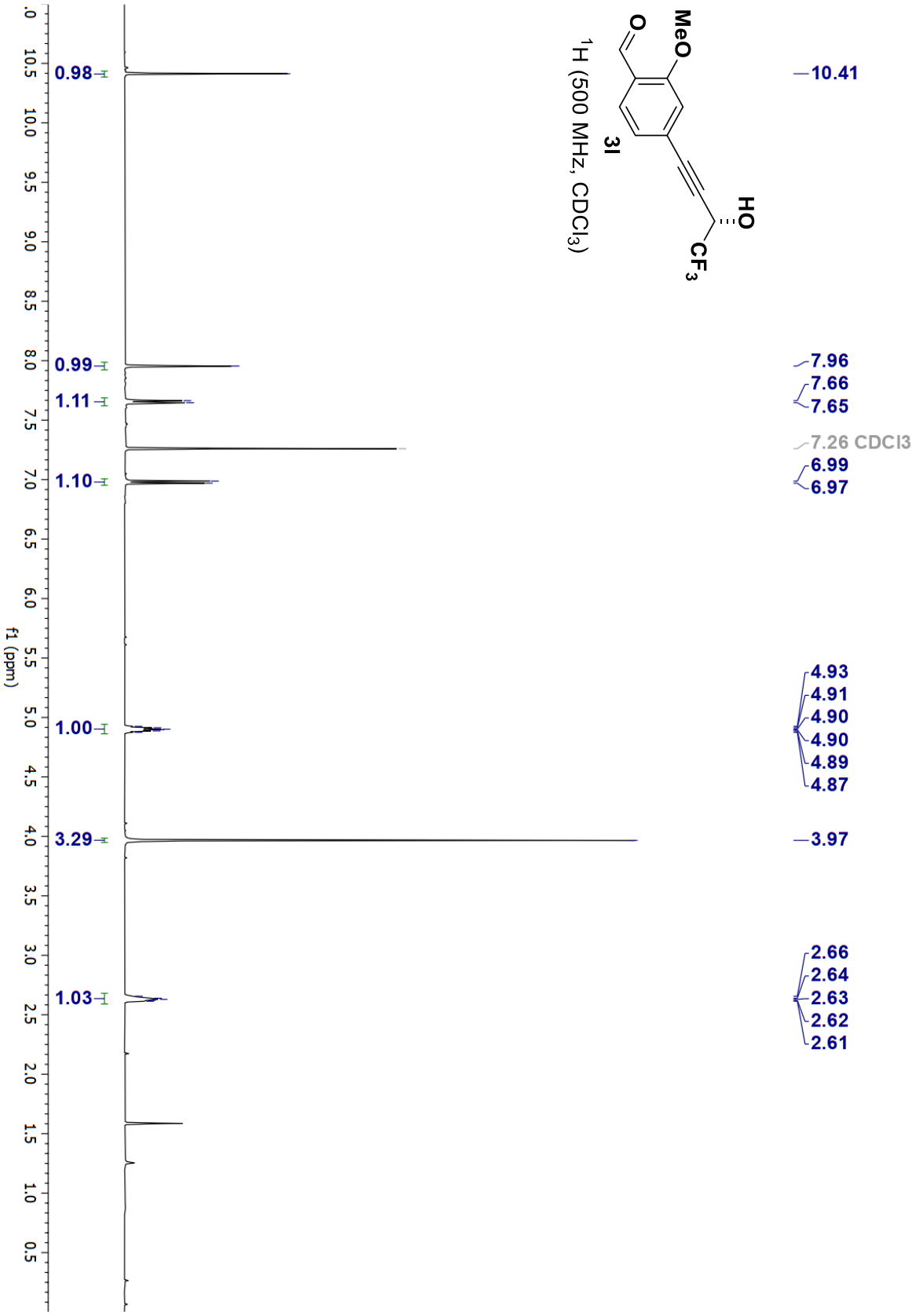
HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_{12}H_{10}F_3O_3^+$: 259.0477; found = 259.0571.

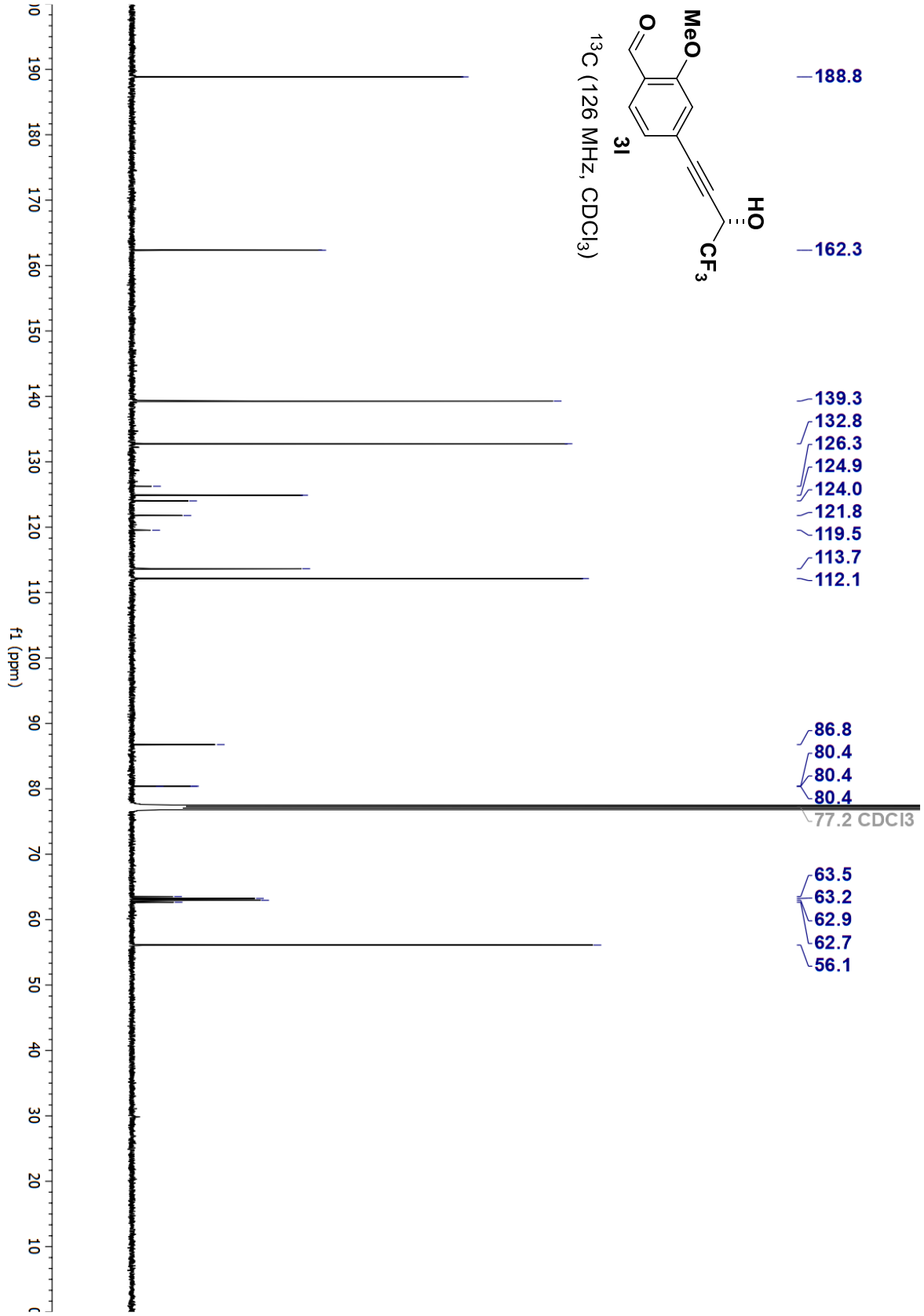
FTIR (neat): 3335, 2981, 2776, 2240, 1683,1401, 1172, 688 cm^{-1}.

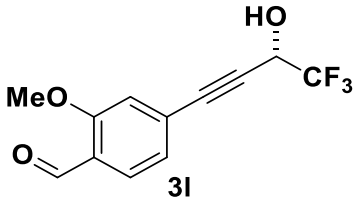
HPLC (CHIRALPAK AD-H, hexanes:2-PrOH = 95:5, 1.0 mL/min, 254 nm): ee = 99%.

$[\alpha]_D^{20}$ = -28° ($CHCl_3$, c = 1.0).

m.p.: 95 °C.

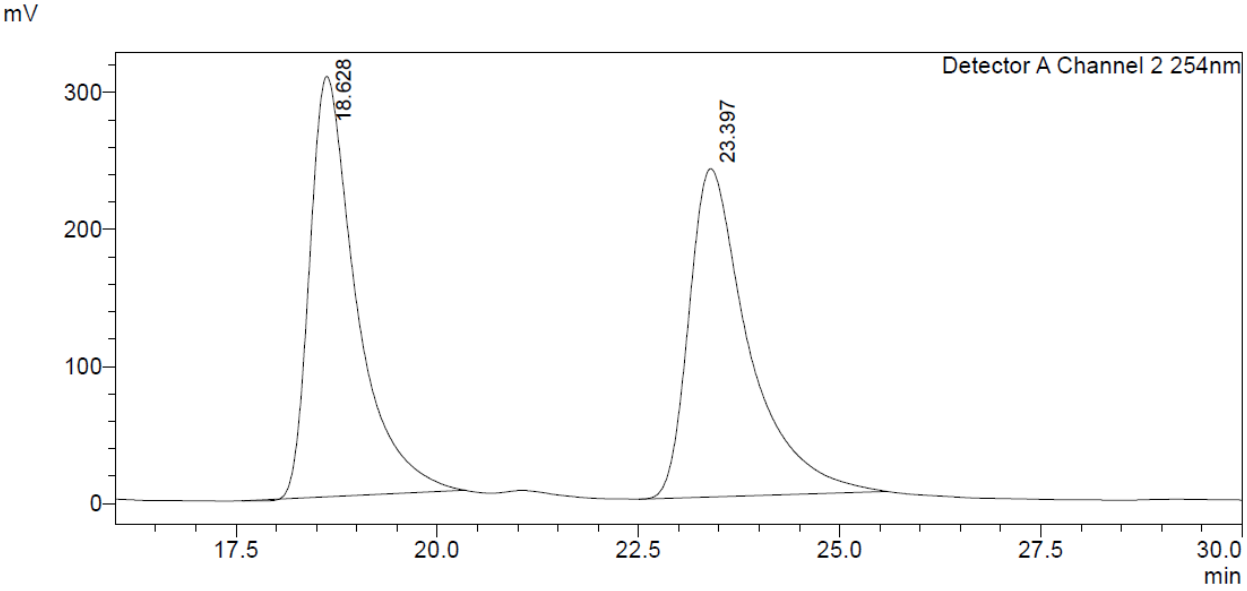

3l
^{1}H (500 MHz, CDCl$_3$)
MeO
O
HO
CF$_3$
10.41
7.96
7.66
7.65
7.26 CDCl3
6.99
6.97
4.93
4.91
4.90
4.90
4.89
4.87
3.97
2.66
2.64
2.63
2.62
2.61
0.98
0.99
1.11
1.10
1.00
3.29
1.03
f1 (ppm)


3l
^{13}C (126 MHz, CDCl$_3$)
MeO
O
HO
CF$_3$
188.8
162.3
139.3
132.8
126.3
124.9
124.0
121.8
119.5
113.7
112.1
86.8
80.4
80.4
80.4
77.2 CDCl3
63.5
63.2
62.9
62.7
56.1
f1 (ppm)



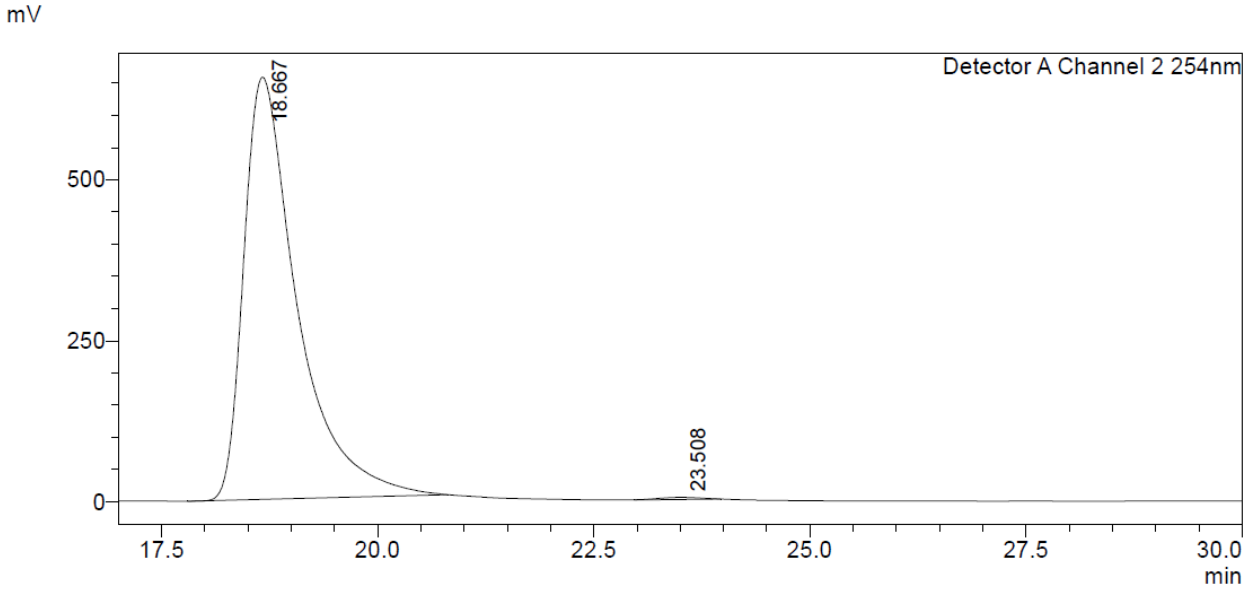
3l

^{19}F (471 MHz, $CDCl_3$)



Detector A Channel 2 254nm

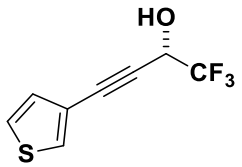
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	18.628	12370599	306970	50.015		M	
2	23.397	12363249	239629	49.985		M	
Total		24733847	546599				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	18.667	28156432	655299	99.607		M	
2	23.508	111200	3392	0.393		M	
Total		28267632	658691				

(*S*)-1,1,1-trifluoro-4-(thiophen-3-yl)but-3-yn-2-ol (3m)



Alkyne **1m** (21 μL, 0.21 mmol, 105 mol%) was subjected to standard reaction conditions (80 °C, 48 h) at 2.5 mol% catalyst loading. Upon flash column chromatography (SiO_2: 5:95–10:90 Et_2O:hexanes), the title compound **3m** was isolated as a pale, yellow oil in 80% yield (33.1 mg, 0.16 mmol, 97% ee).

TLC (SiO_2): R_f = 0.2 (1:9 Et_2O:hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57 (dd, *J* = 3.0, 1.2 Hz, 1H), 7.30 (dd, *J* = 5.0, 3.0 Hz, 1H), 7.15 (dd, *J* = 5.0, 1.2 Hz, 1H), 4.89 (dq, *J* = 8.1, 5.7 Hz, 1H), 2.51 (dd, *J* = 8.3, 2.1 Hz, 1H) ppm.

^{13}C NMR (101 MHz, $CDCl_3$): δ 130.9, 129.8, 125.8, 122.8 (q, *J* = 281.7 Hz), 119.9, 83.3, 80.2–80.1 (m), 63.1 (q, *J* = 36.0 Hz) ppm.

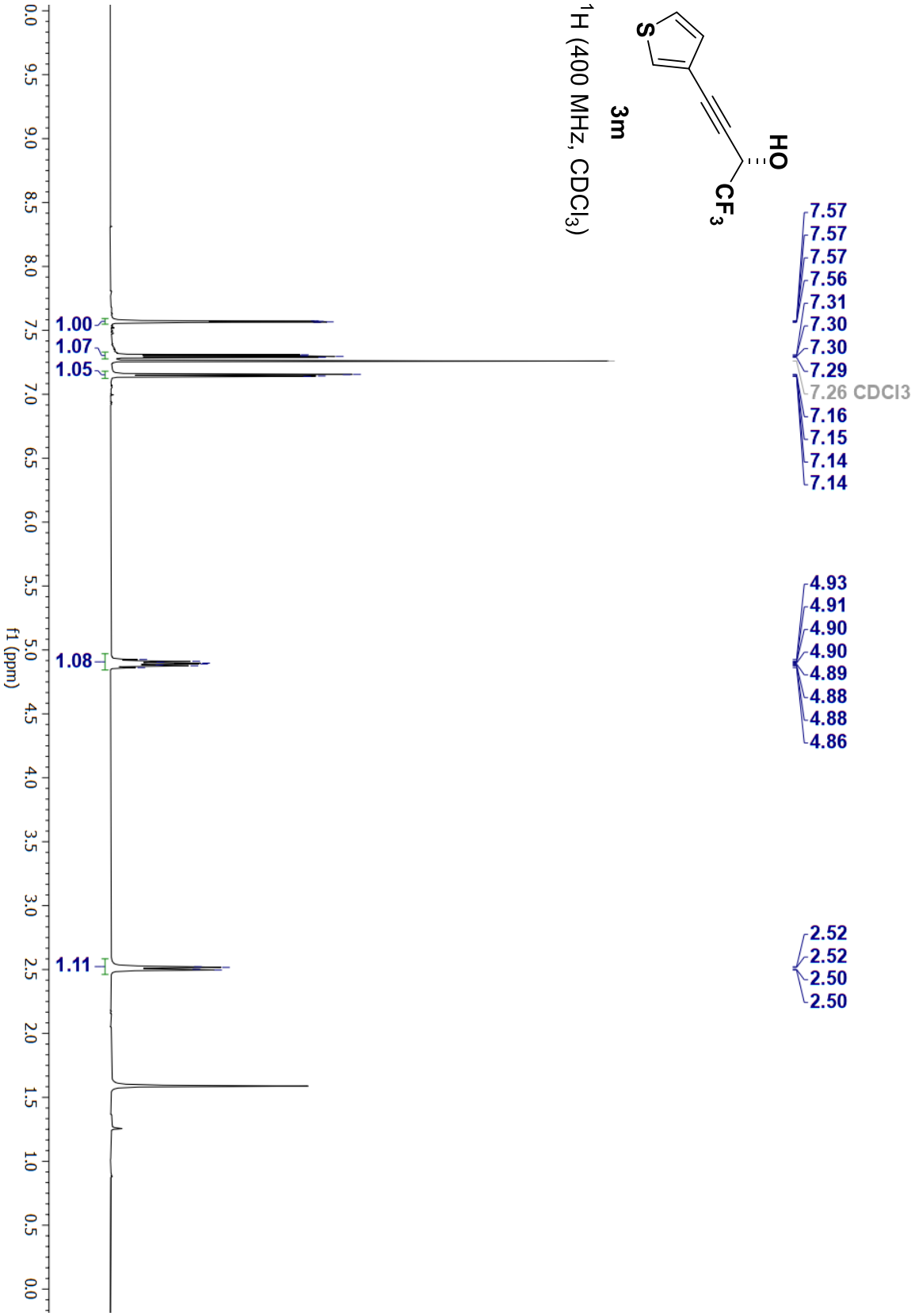
^{19}F NMR (376 MHz, $CDCl_3$): δ -79.3 (d, *J* = 5.8 Hz) ppm.

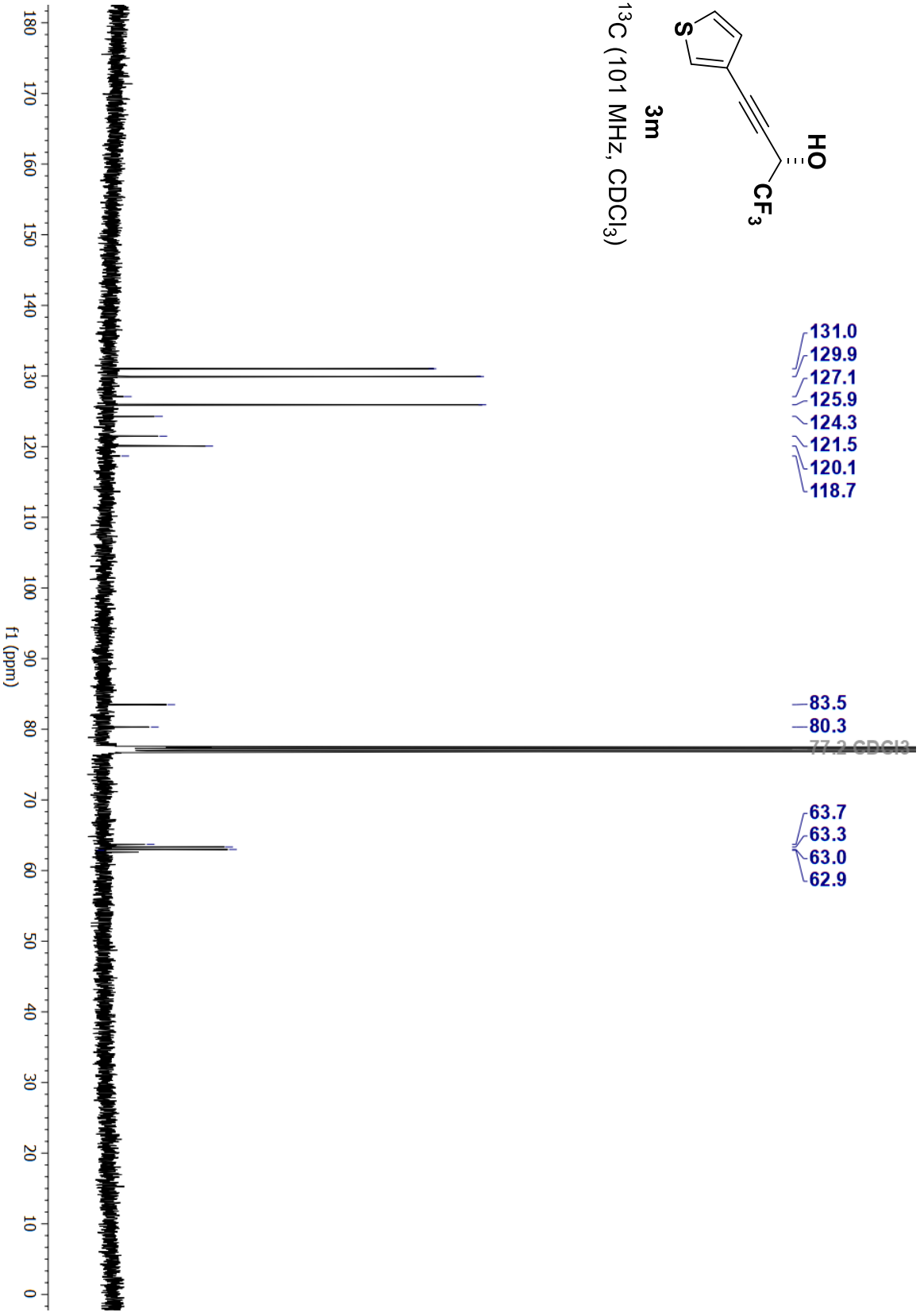
HRMS (EI(+)): Known compound, see reference 17.

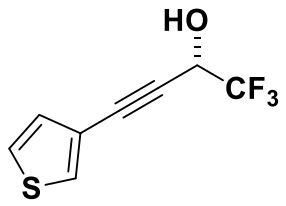
HPLC (CHIRALCEL OB-H, hexanes:2-PrOH = 98:2, 1.0 mL/min, 254 nm): ee = 97%.

$[\alpha]_D^{20}$ = +34° ($CHCl_3$, c = 1.0).

The analytical data are in agreement with the literature.[17]

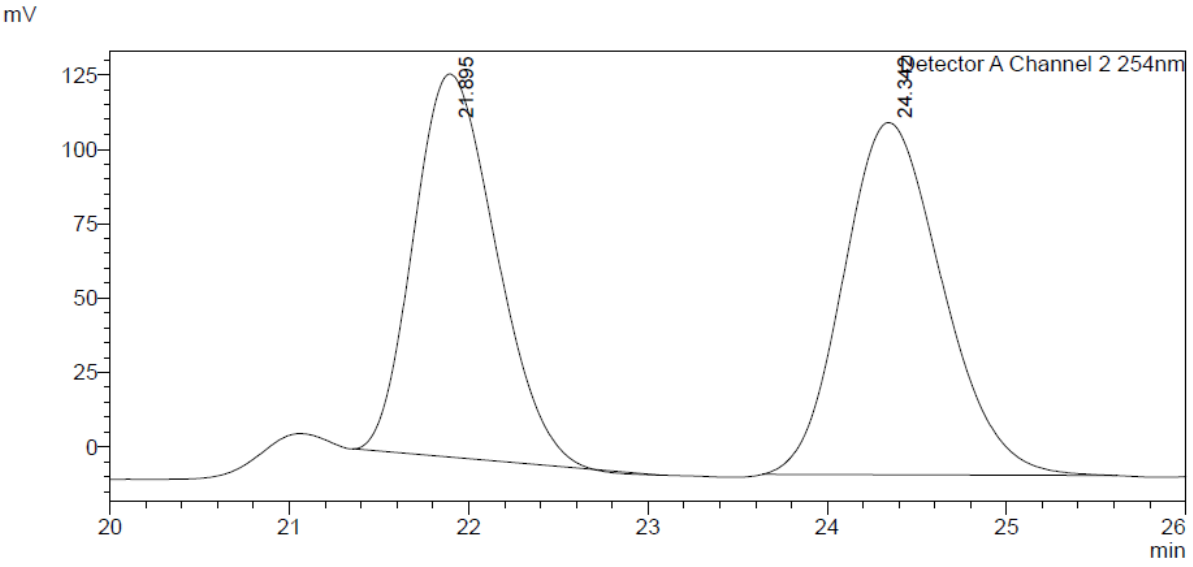

3m
^{1}H (400 MHz, CDCl$_3$)
S
HO
CF$_3$
7.57
7.57
7.57
7.56
7.31
7.30
7.30
7.29
7.26 CDCl3
7.16
7.15
7.14
7.14
4.93
4.91
4.90
4.90
4.89
4.88
4.88
4.86
2.52
2.52
2.50
2.50
1.00
1.07
1.05
1.08
1.11
f1 (ppm)


3m
^{13}C (101 MHz, $CDCl_3$)
S
HO
CF_3
131.0
129.9
127.1
125.9
124.3
121.5
120.1
118.7
83.5
80.3
77.2 CDCl3
63.7
63.3
63.0
62.9
f1 (ppm)



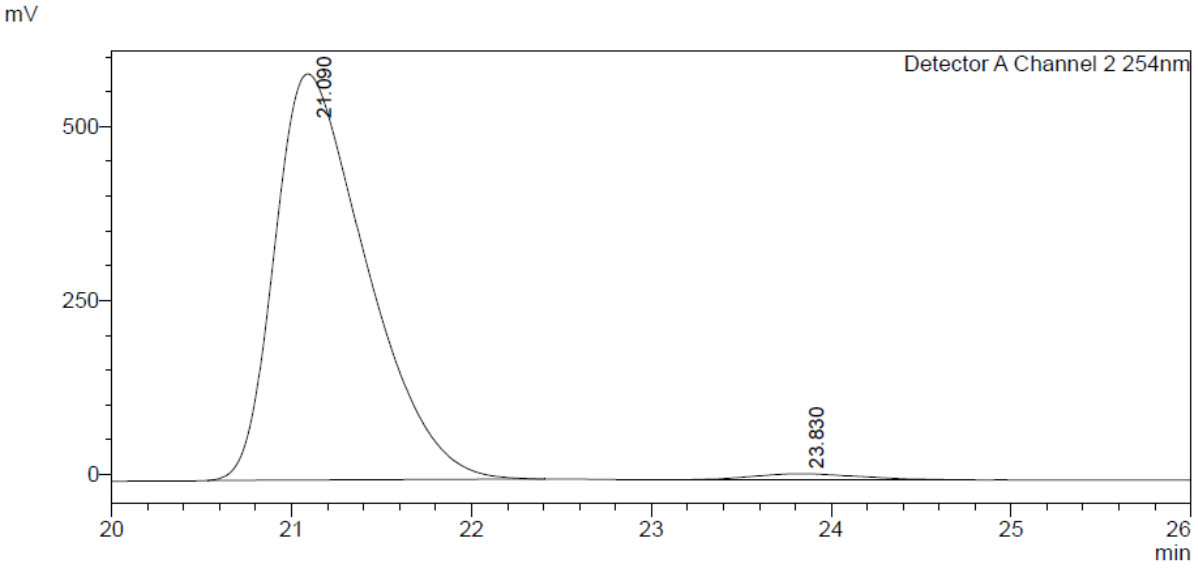
3m

^{19}F (376 MHz, $CDCl_3$)



Detector A Channel 2 254nm

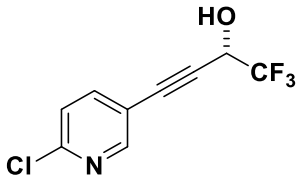
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	21.895	4084892	128600	47.410		M	
2	24.342	4531222	118387	52.590		M	
Total		8616114	246987				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	21.090	20668407	583167	98.363		M	
2	23.830	344023	8584	1.637		M	
Total		21012430	591752				

(*S*)-4-(6-chloropyridin-3-yl)-1,1,1-trifluorobut-3-yn-2-ol (3n)



Alkyne **1n** (29.9 mg, 0.21 mmol, 105 mol%) was subjected to standard reaction conditions (80 °C, 48 h) at 1 mol% catalyst loading. Upon flash column chromatography (SiO_2: 10:90–15:85 EtOAc:hexanes), the title compound **3n** was isolated as a brown oil in 78% yield (36.7 mg, 0.16 mmol, 98% ee).

TLC (SiO_2): R_f = 0.1 (1:9 EtOAc:hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.50 (d, *J* = 2.3 Hz, 1H), 7.73 (dd, *J* = 8.3, 2.3 Hz, 1H), 7.34 (dd, *J* = 8.3, 0.7 Hz, 1H), 4.96 (q, *J* = 5.9 Hz, 1H) ppm.

^{13}C NMR (101 MHz, $CDCl_3$): δ 152.1, 151.6, 141.8, 124.4, 122.8 (q, *J* = 282.2 Hz), 117.4, 86.1 (q, *J* = 2.3 Hz), 82.6, 62.7 (q, *J* = 36.4 Hz) ppm.

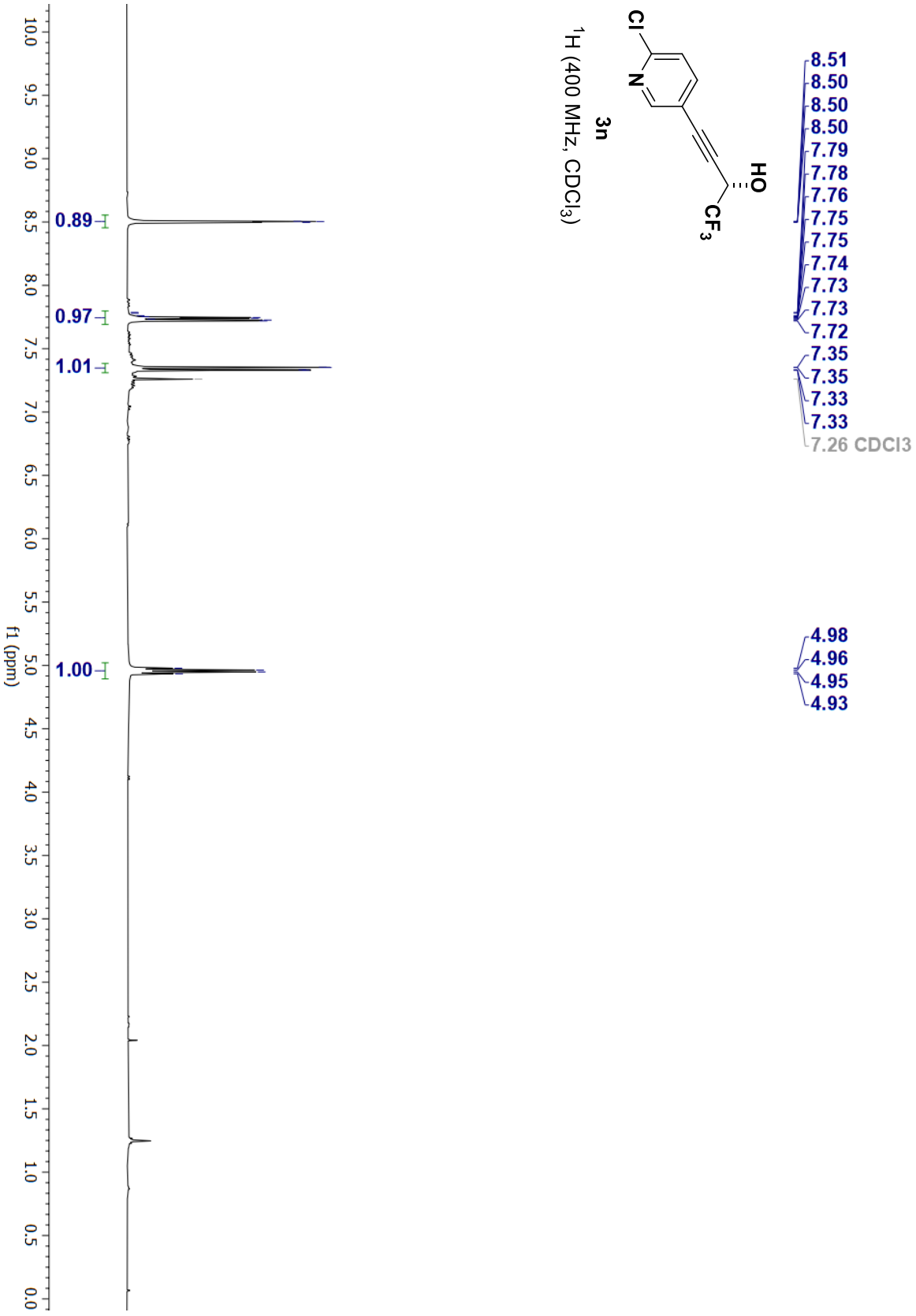
^{19}F NMR (376 MHz, $CDCl_3$): δ -79.1 (d, *J* = 5.6 Hz) ppm.

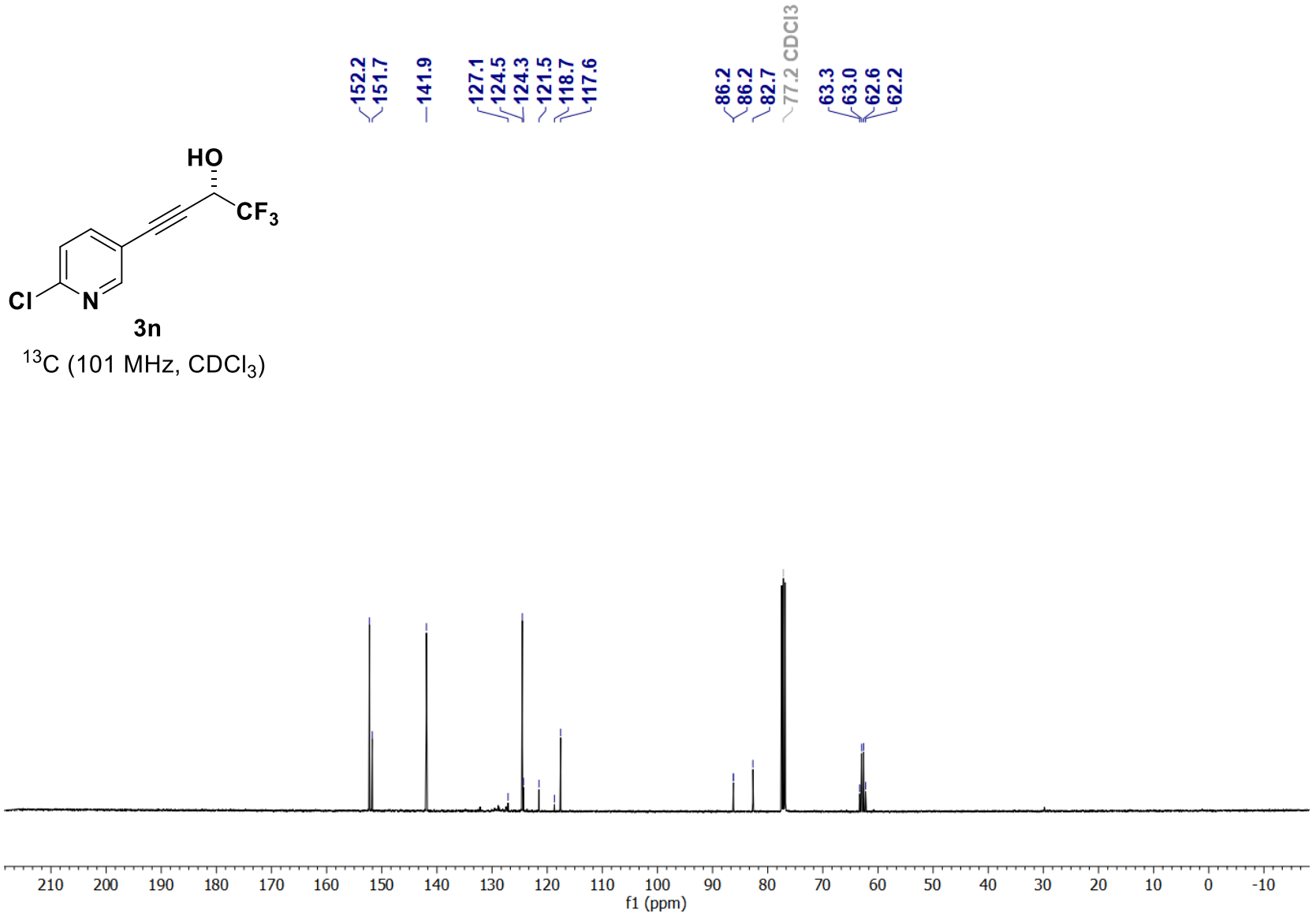
HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_9H_6ClF_3NO^+$: 236.0085; found = 236.0085.

FTIR (neat): 3166, 2851, 2723, 1981, 1585, 1549, 1457, 1359, 1258, 1177, 1131, 1110, 1071, 1026, 982, 928, 836, 789, 753, 734, 710, 693, 648, 629, 597, 537, 481 cm^{-1}.

HPLC (CHIRALPAK AD-H, hexanes:2-PrOH = 98:2, 1.0 mL/min, 254 nm): ee = 98% ee.

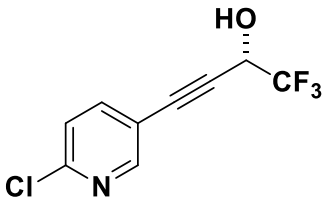
$[\alpha]_D^{20}$ = –4° ($CHCl_3$, c = 1.0).


3n
^{1}H (400 MHz, CDCl$_3$)
Cl
N
HO
CF$_3$
8.51
8.50
8.50
8.50
7.79
7.78
7.76
7.75
7.75
7.74
7.73
7.73
7.72
7.35
7.35
7.33
7.33
7.26 CDCl3
4.98
4.96
4.95
4.93
0.89
0.97
1.01
1.00
f1 (ppm)



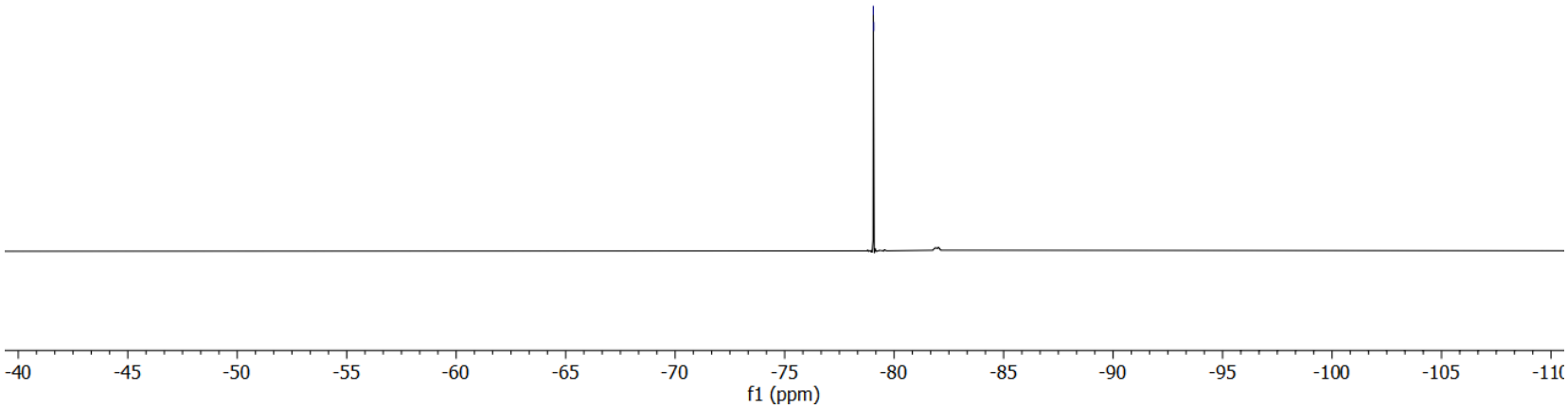
3n

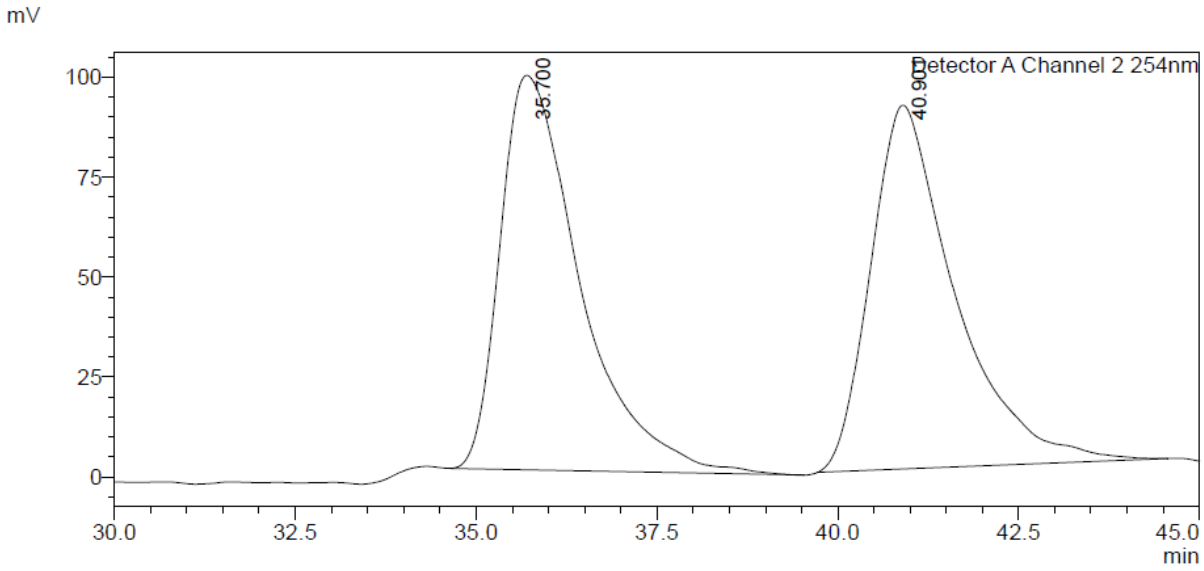
^{13}C (101 MHz, $CDCl_3$)



3n

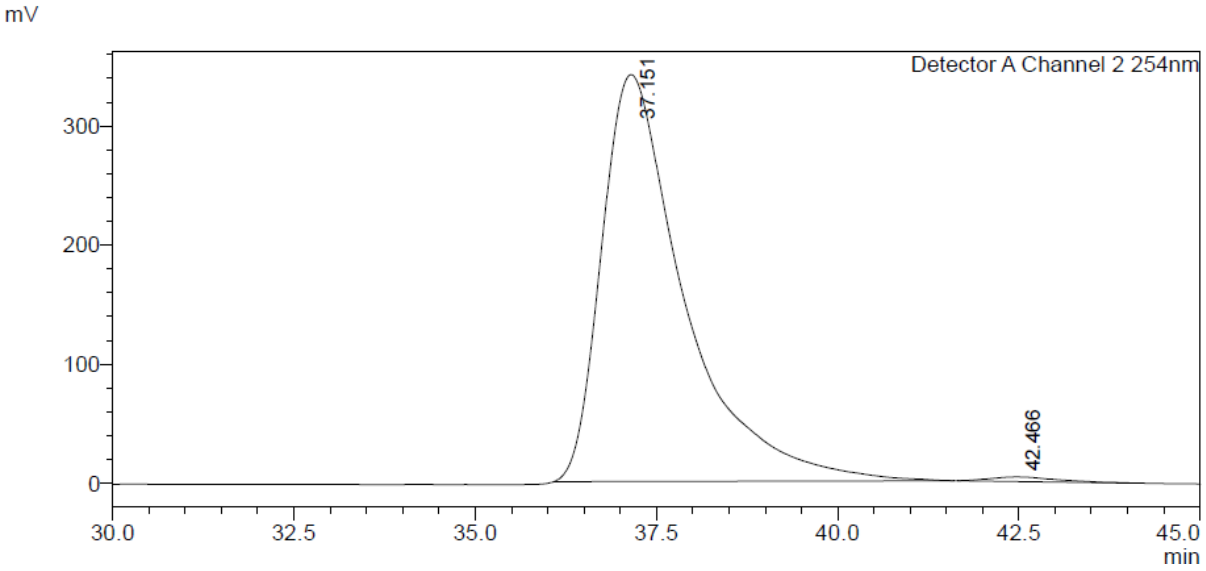
^{19}F (376 MHz, $CDCl_3$)





Detector A Channel 2 254nm

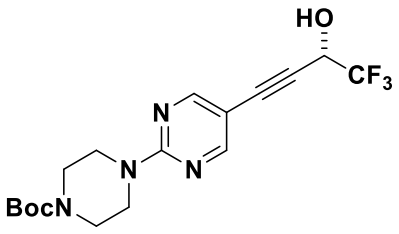
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	35.700	7580517	98687	50.605		M	
2	40.901	7399216	90999	49.395		M	
Total		14979732	189686				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	37.151	27183901	341545	99.113		M	
2	42.466	243296	3782	0.887		M	
Total		27427196	345327				

tert-butyl (_S_)-4-(5-(4,4,4-trifluoro-3-hydroxybut-1-yn-1-yl)pyrimidin-2-yl)piperazine-1-carboxylate (3o)



Alkyne **1o** (61.2 mg, 0.21 mmol, 105 mol%) was subjected to standard reaction conditions (80 °C, 24 h) at 2.5 mol% catalyst loading. Upon flash column chromatography (SiO_2: 5:95–15:85 EtOAc:CH_2Cl_2), the title compound **3o** was isolated as a pale, yellow solid in 87% yield (66.9 mg, 0.17 mmol, 98% ee).

TLC (SiO_2): R_f = 0.3 (9:1 CH_2Cl_2:EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.40 (s, 2H), 5.44 – 5.06 (m, 1H), 4.89 (q, *J* = 5.9 Hz, 1H), 3.96 – 3.63 (m, 4H), 3.56 – 3.33 (m, 4H), 1.46 (s, 9H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ 160.7, 160.0, 154.9, 122.9 (q, *J* = 282.0 Hz), 104.8, 84.3–84.0 (m), 83.5, 80.4, 63.2 (q, *J* = 36.3 Hz), 43.8, 42.2 (bs), 28.6 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ -79.2 (d, *J* = 5.8 Hz) ppm.

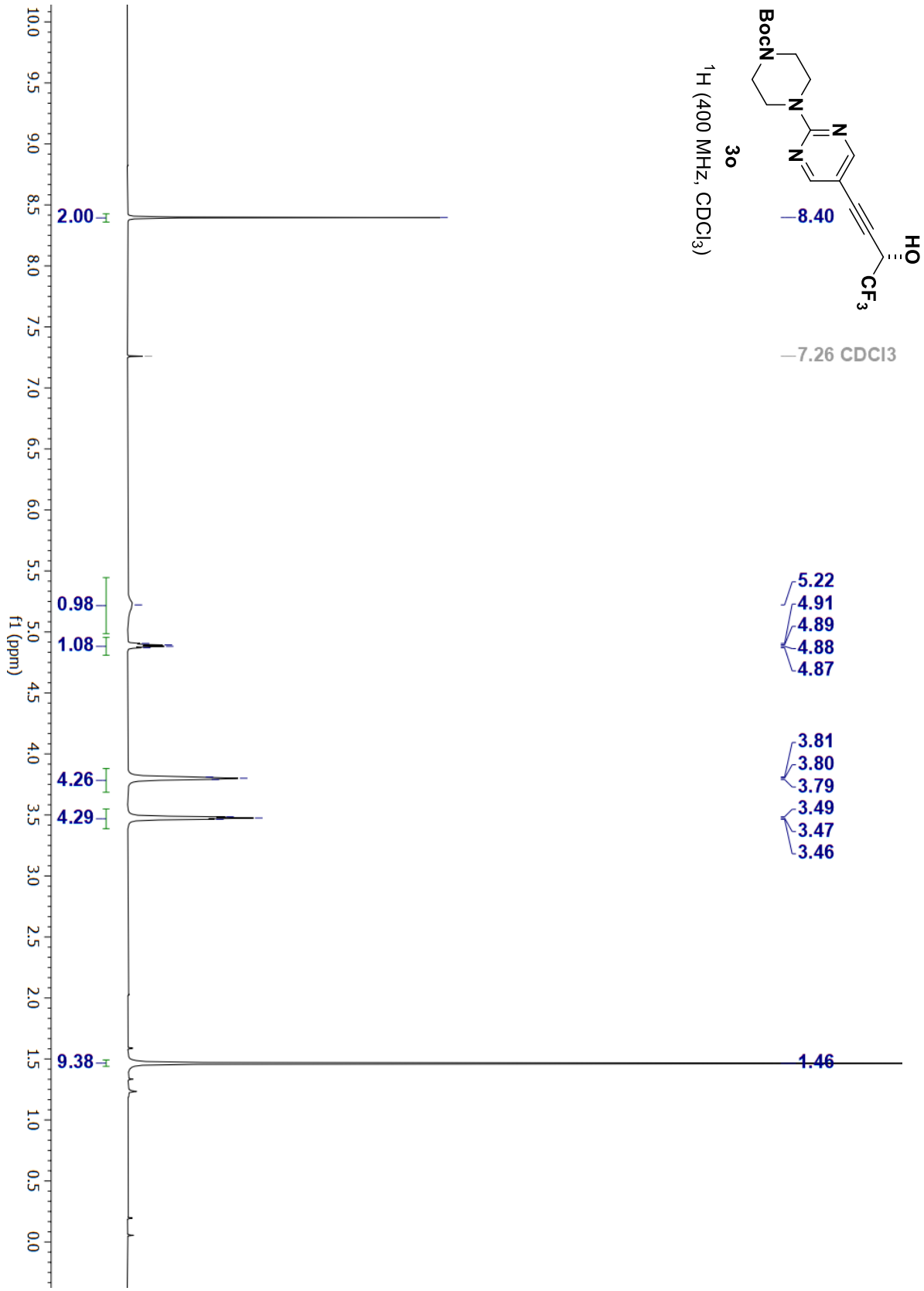
HRMS (ESI(+)): m/z [M+Na^+] calcd. for $C_{17}H_{21}F_3N_4NaO_3^+$: 409.1458; found = 409.1464.

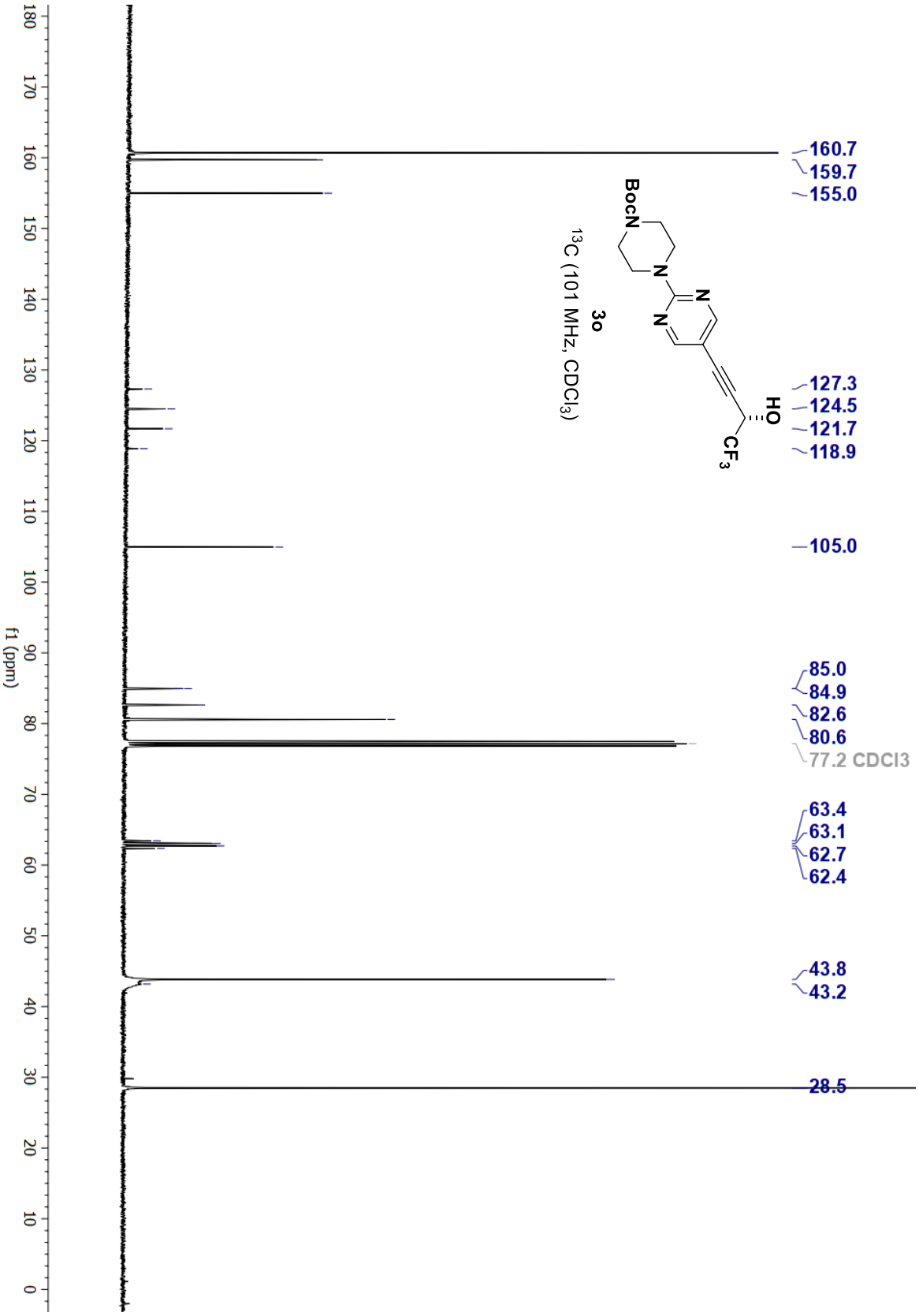
FTIR (neat): 3307, 2972, 2916, 2862, 2359, 2343, 2230, 1655, 1604, 1517, 1477, 1428, 1362, 1307, 1283, 1246, 1174, 1159, 1132, 1087, 997, 972, 946, 858, 836, 790, 770, 715, 668, 656, 593, 523, 451, 443, 424, 417 cm^{-1}.

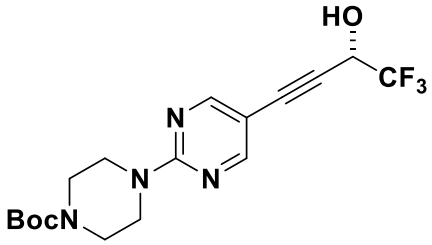
HPLC (CHIRALPAK AD-H, hexanes:2-PrOH = 95:5, 1.0 mL/min, 254 nm): ee = 98%.

$[\alpha]_D^{20}$ = +77° ($CHCl_3$, c = 0.9).

m.p.: 187 °C.

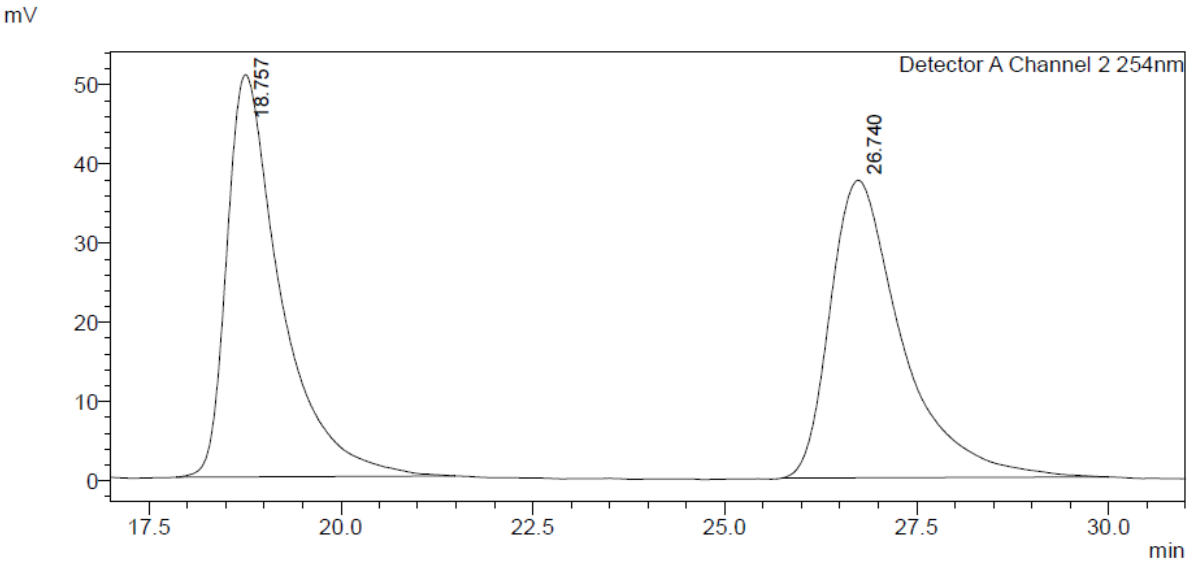

3o
^{1}H (400 MHz, CDCl$_3$)
BocN
N
N
N
HO
CF$_3$
8.40
7.26 CDCl3
5.22
4.91
4.89
4.88
4.87
3.81
3.80
3.79
3.49
3.47
3.46
1.46
2.00
0.98
1.08
4.26
4.29
9.38
f1 (ppm)


160.7
159.7
155.0
127.3
124.5
121.7
118.9
105.0
85.0
84.9
82.6
80.6
77.2 CDCl3
63.4
63.1
62.7
62.4
43.8
43.2
28.5
BocN
N
N
N
HO
CF3
3o
13C (101 MHz, CDCl3)
f1 (ppm)



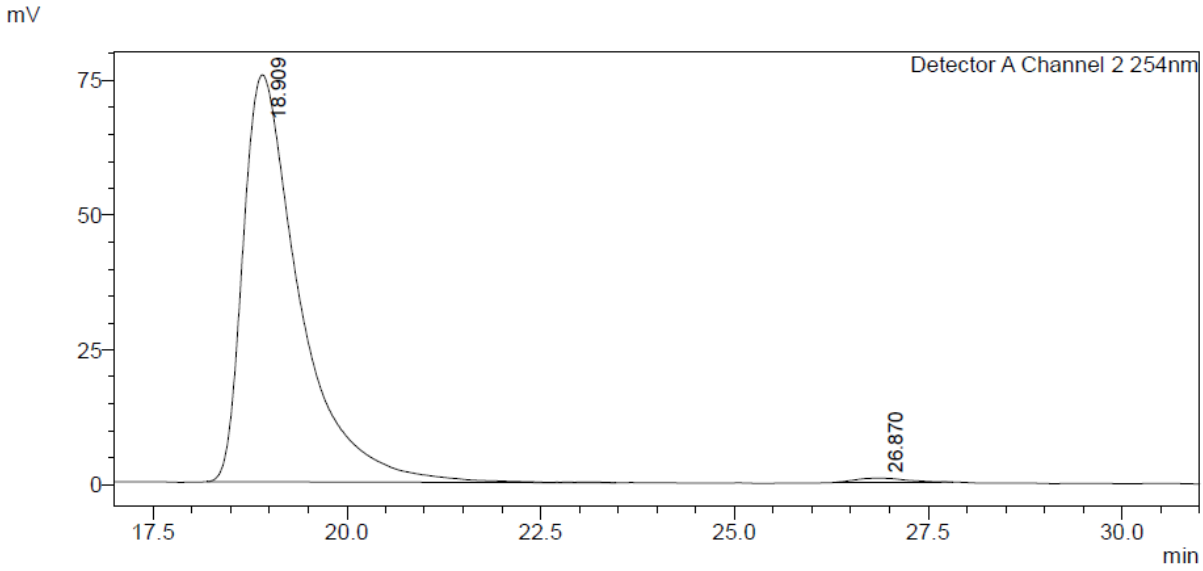
3o

^{19}F (376 MHz, $CDCl_3$)



Detector A Channel 2 254nm

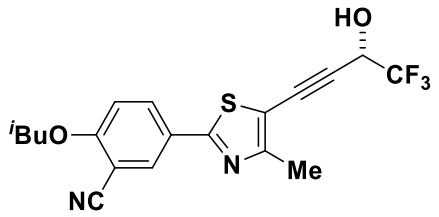
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	18.757	2484454	50779	50.365		M	
2	26.740	2448422	37574	49.635		M	
Total		4932876	88353				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	18.909	3839360	75538	99.052		M	
2	26.870	36730	816	0.948		M	
Total		3876090	76354				

(*S*)-2-isobutoxy-5-(4-methyl-5-(4,4,4-trifluoro-3-hydroxybut-1-yn-1-yl)thiazol-2-yl)benzonitrile (3p)



Alkyne **1p** (62.1 mg, 0.21 mmol, 105 mol%) was subjected to standard reaction conditions (80 °C, 24 h) at 1 mol% catalyst loading. Upon flash column chromatography (SiO_2: 50:50 EtOAc:hexanes), the title compound **3p** was isolated as a yellow solid in 90% yield (70.9 mg, 0.18 mmol, 99% ee).

2 mmol scale reaction: A 25 mL round bottom flask equipped with a water condenser was charged with $RuHCl(CO)(PPh_3)_3$ (19 mg, 0.02 mmol, 1 mol%), (*S*,*S*)-Ph-BPE (10 mg, 0.02 mmol, 1 mol%), KI (32 mg, 0.2 mmol, 10 mol%), 4Å molecular sieves (150 mg, 50 wt%) and ethyl acetate (6.7 mL) under air. The flask was placed in an oil bath and was allowed to stir at 80 ºC. After 15 minutes, the mixture was allowed to reach ambient temperature, before adding alkyne **1p** (621 mg, 2.1 mmol, 105 mol%) and fluoral (**2a**, 76 wt% in H_2O, 210 μL, 2 mmol, 100 mol%) were added to the reaction mixture and was allowed to stir for 24 hours at 80 ºC. The reaction mixture was allowed to reach ambient temperature, and the residue was subjected to flash column chromatography (SiO_2: 50:50 EtOAc:hexanes) to furnish the title compound **3p** as a yellow solid in 86% yield (677 mg, 1.7 mmol, 99% ee).

TLC (SiO_2): R_f = 0.3 (1:1 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.10 (d, *J* = 2.3 Hz, 1H), 8.02 (dd, *J* = 8.9, 2.3 Hz, 1H), 7.00 (d, *J* = 8.9 Hz, 1H), 5.03 – 4.94 (m, 1H), 3.89 (d, *J* = 6.5 Hz, 2H), 2.82 – 2.61 (m, 1H), 2.53 (s, 3H), 2.19 (dq, *J* = 13.4, 6.7 Hz, 1H), 1.09 (d, *J* = 6.7 Hz, 6H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ 165.3, 162.4, 160.7, 132.5, 132.0, 126.1, 122.7 (q, *J* = 281.6 Hz), 115.6, 112.8, 111.0, 103.1, 89.4, 79.0, 75.8, 63.3 (q, *J* = 36.7 Hz), 28.3, 19.2, 16.6 ppm.

^{19}F NMR (471 MHz, $CDCl_3$): δ -79.0 (d, *J* = 5.9 Hz) ppm.

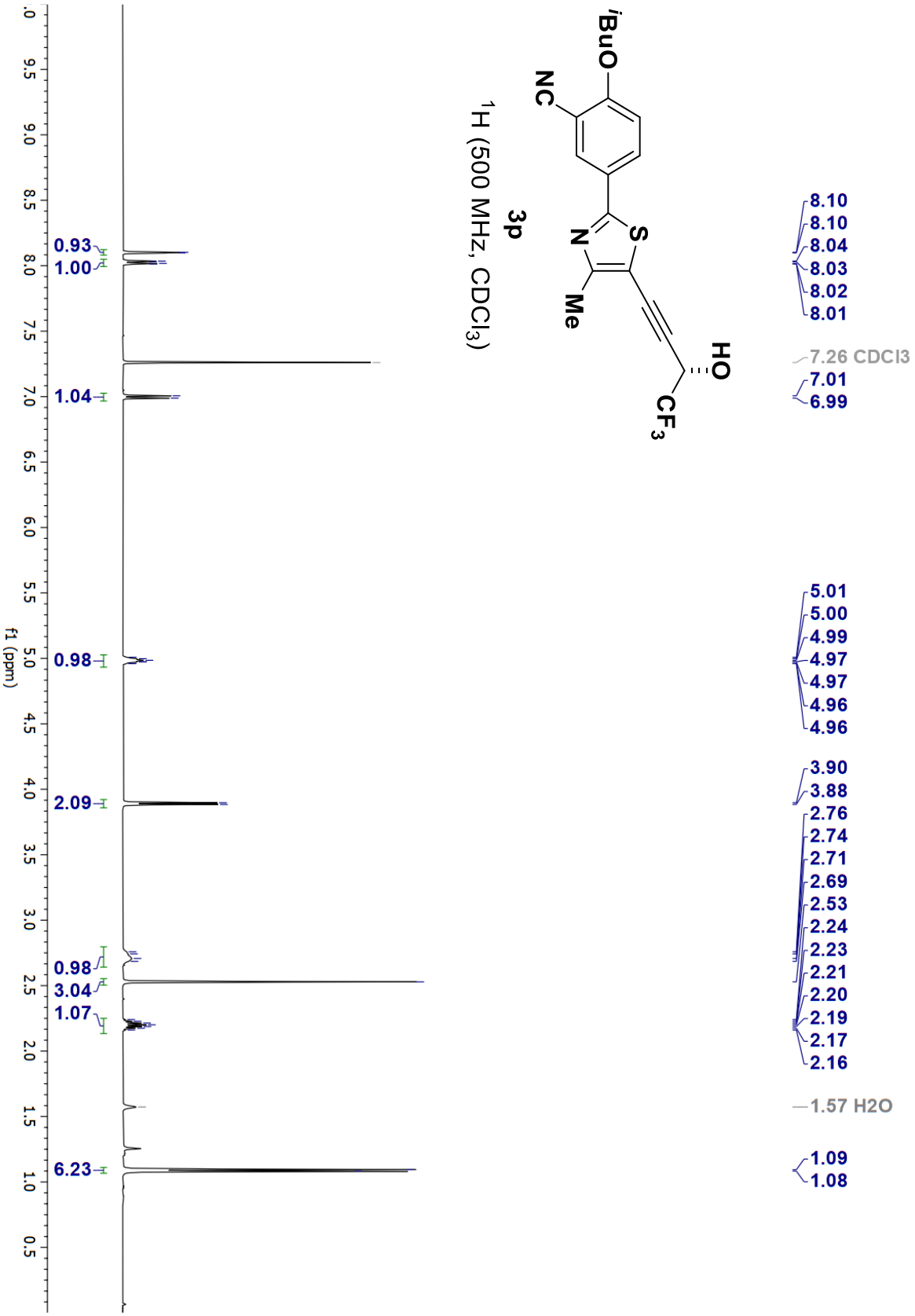
HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_{19}H_{18}F_3N_2O_2S^+$: 395.1036; found = 395.1029.

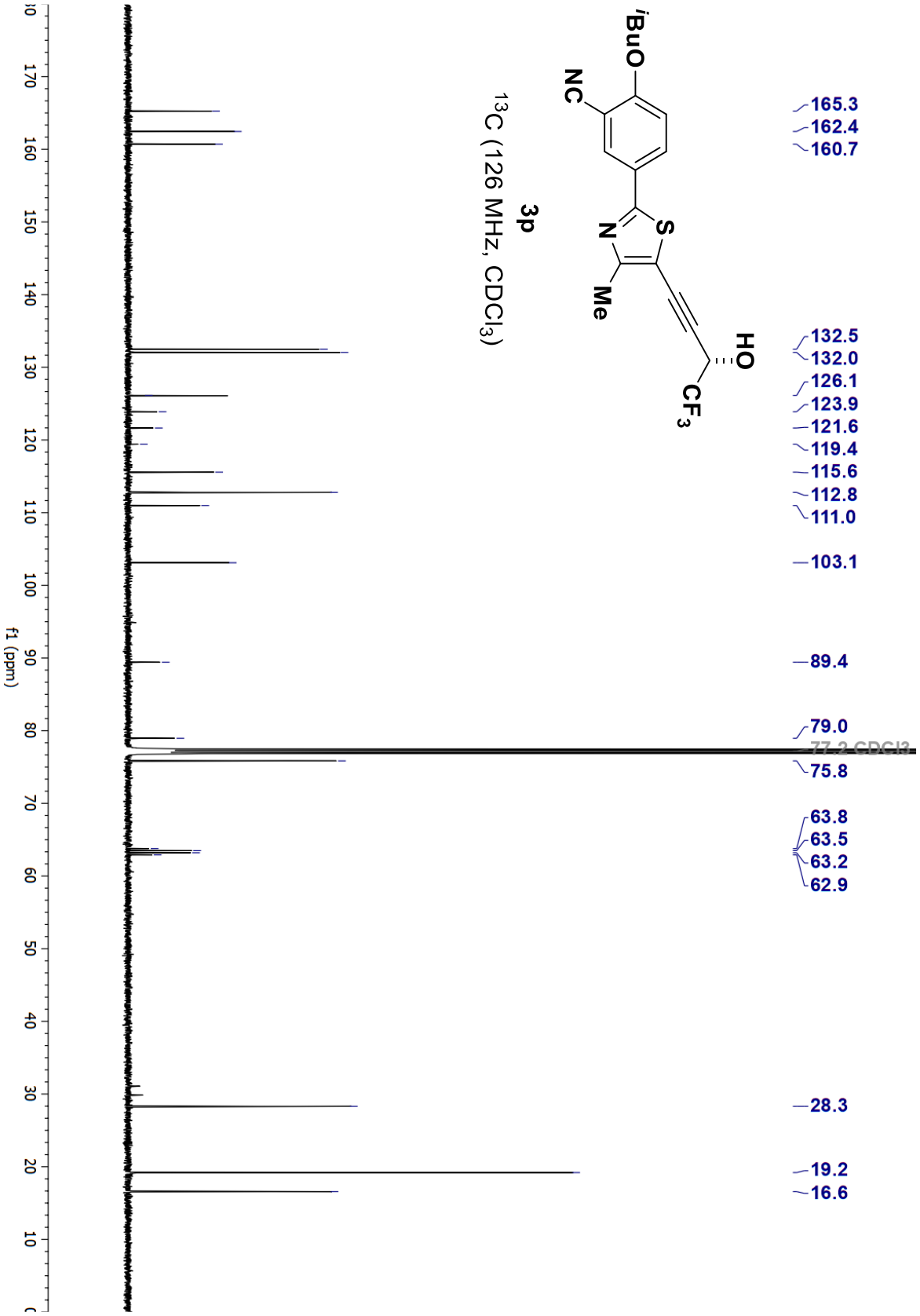
FTIR (neat): 3153, 2873, 2226, 1607, 1305, 1135, 831, 662, 491 cm^{-1}.

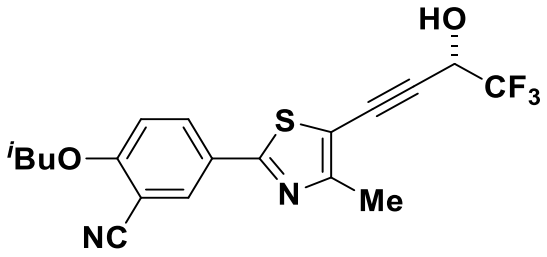
HPLC (PHENOMENEX Amylose 3, hexanes:2-PrOH = 93:7, 1.0 mL/min, 254 nm): ee = 99%.

$[\alpha]_D^{20}$ = -19° ($CHCl_3$, c = 1.0).

m.p.: 157 °C.

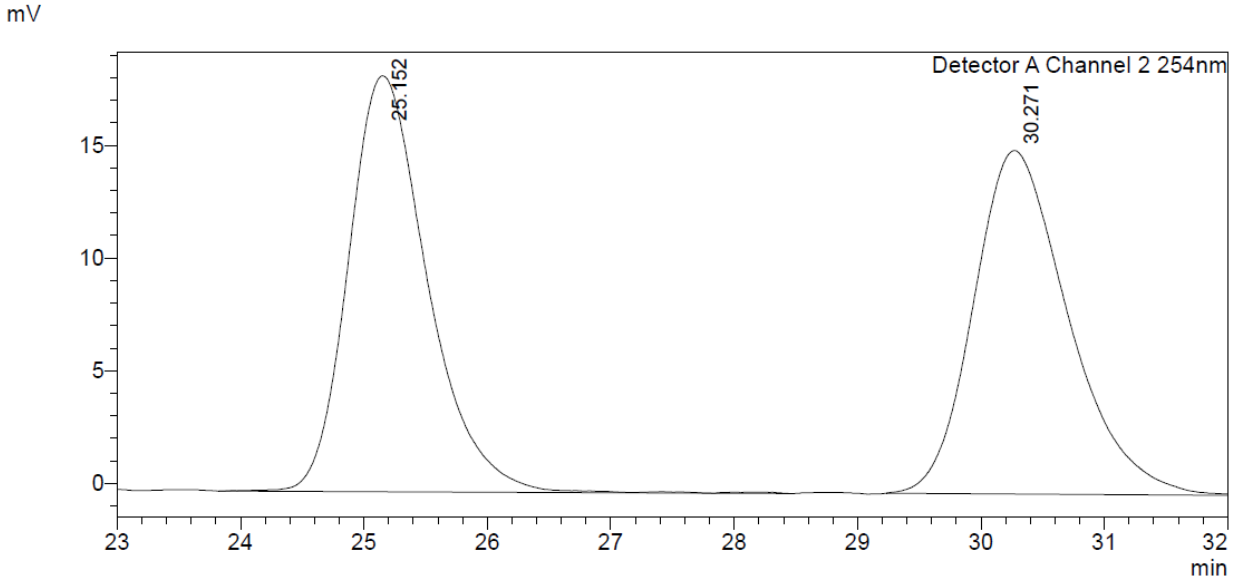

3p
^{1}H (500 MHz, CDCl$_3$)
^{i}BuO
NC
N
S
Me
HO
CF$_3$
8.10
8.10
8.04
8.03
8.02
8.01
7.26 CDCl3
7.01
6.99
5.01
5.00
4.99
4.97
4.97
4.96
4.96
3.90
3.88
2.76
2.74
2.71
2.69
2.53
2.24
2.23
2.21
2.20
2.19
2.17
2.16
1.57 H2O
1.09
1.08
0.93
1.00
1.04
0.98
2.09
0.98
3.04
1.07
6.23
f1 (ppm)


3p
^{13}C (126 MHz, CDCl$_3$)
^{i}BuO
NC
N
S
Me
HO
CF$_3$
165.3
162.4
160.7
132.5
132.0
126.1
123.9
121.6
119.4
115.6
112.8
111.0
103.1
89.4
79.0
77.2 CDCl3
75.8
63.8
63.5
63.2
62.9
28.3
19.2
16.6
f1 (ppm)



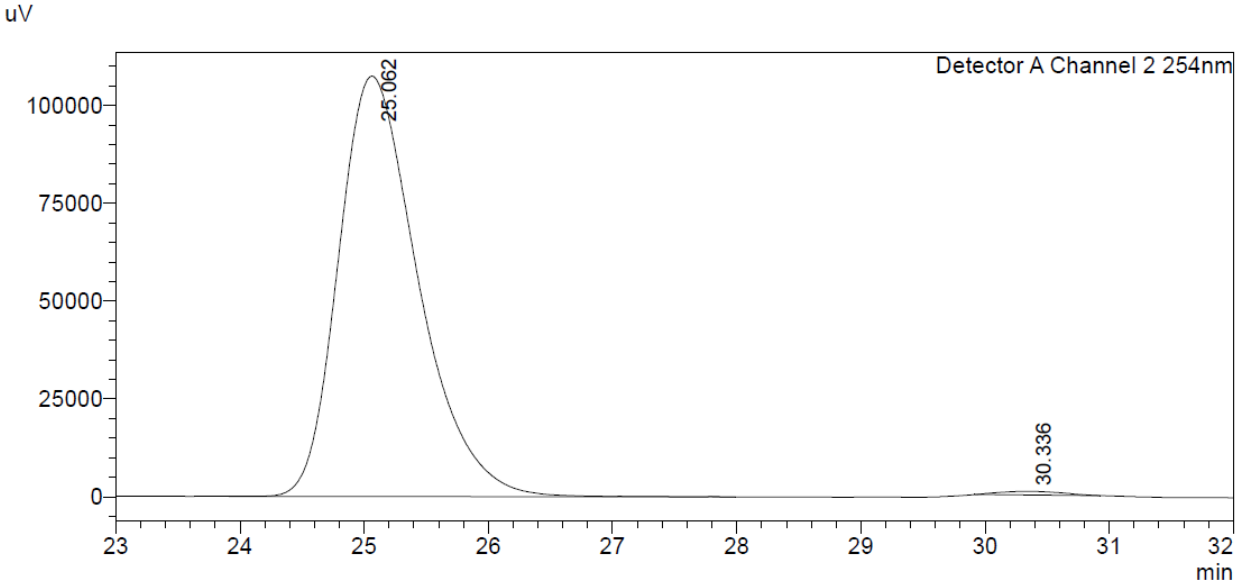
3p

^{19}F (471 MHz, $CDCl_3$)



Detector A Channel 2 254nm

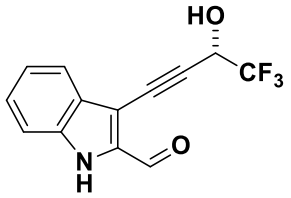
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	25.152	821591	18449	50.313		M	
2	30.271	811366	15232	49.687		M	
Total		1632957	33681				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	25.062	4793441	107299	99.319		M	
2	30.336	32866	950	0.681		M	
Total		4826307	108250				

(*S*)-3-(4,4,4-trifluoro-3-hydroxybut-1-yn-1-yl)-1H-indole-2-carbaldehyde (3q)



Alkyne **1q** (35.5 mg, 0.21 mmol, 105 mol%) was subjected to modified reaction conditions (80 °C, 24 h) at 5 mol% catalyst loading. Upon flash column chromatography (SiO_2: 20:80 EtOAc:hexanes), the title compound **3q** was isolated as a rust solid in 62% yield (33.1 mg, 0.12 mmol, 99% ee).

TLC (SiO_2): R_f = 0.3 (1:5 EtOAc:hexanes).

^{1}H NMR (500 MHz, DMSO-d_6): δ 12.46 (s, 1H), 9.97 (s, 1H), 7.70 (d, *J* = 8.1 Hz, 1H), 7.52 (d, *J* = 8.3 Hz, 1H), 7.43 (t, *J* = 7.7 Hz, 1H), 7.31 (d, *J* = 7.1 Hz, 1H), 7.26 (t, *J* = 7.5 Hz, 1H), 5.47 – 5.27 (m, 1H) ppm.

^{13}C NMR (126 MHz, DMSO-d_6): δ 180.9, 137.5, 137.3, 128.0, 127.8, 123.9 (q, *J* = 282.6 Hz), 122.3, 121.1, 113.9, 105.3, 90.8 – 86.6 (m), 77.7, 61.6 (q, *J* = 34.7 Hz) ppm.

^{19}F NMR (471 MHz, DMSO-d_6): δ -77.7 (d, *J* = 6.7 Hz) ppm.

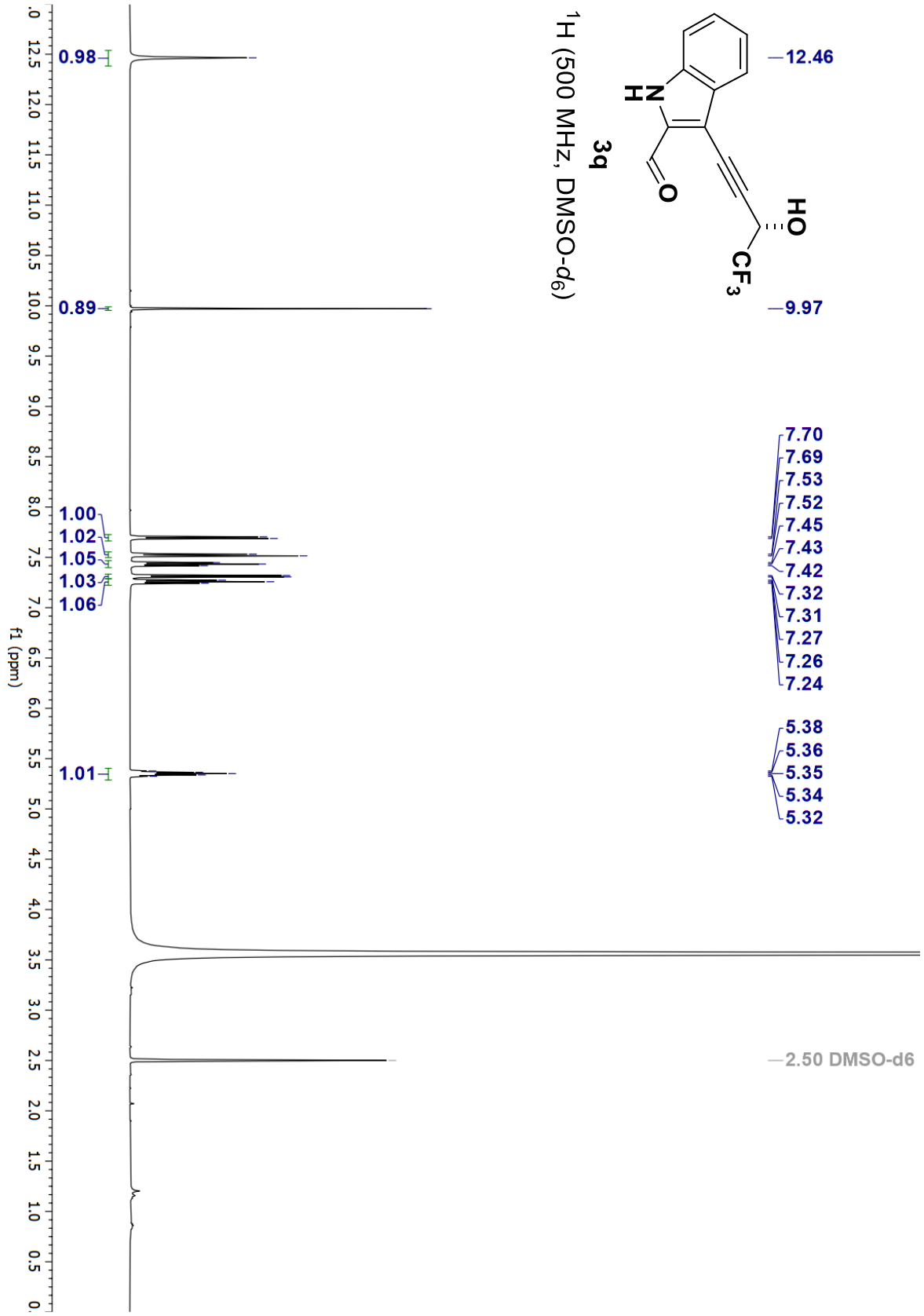
HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_{13}H_9F_3NO_2^+$: 268.0580; found = 268.0584.

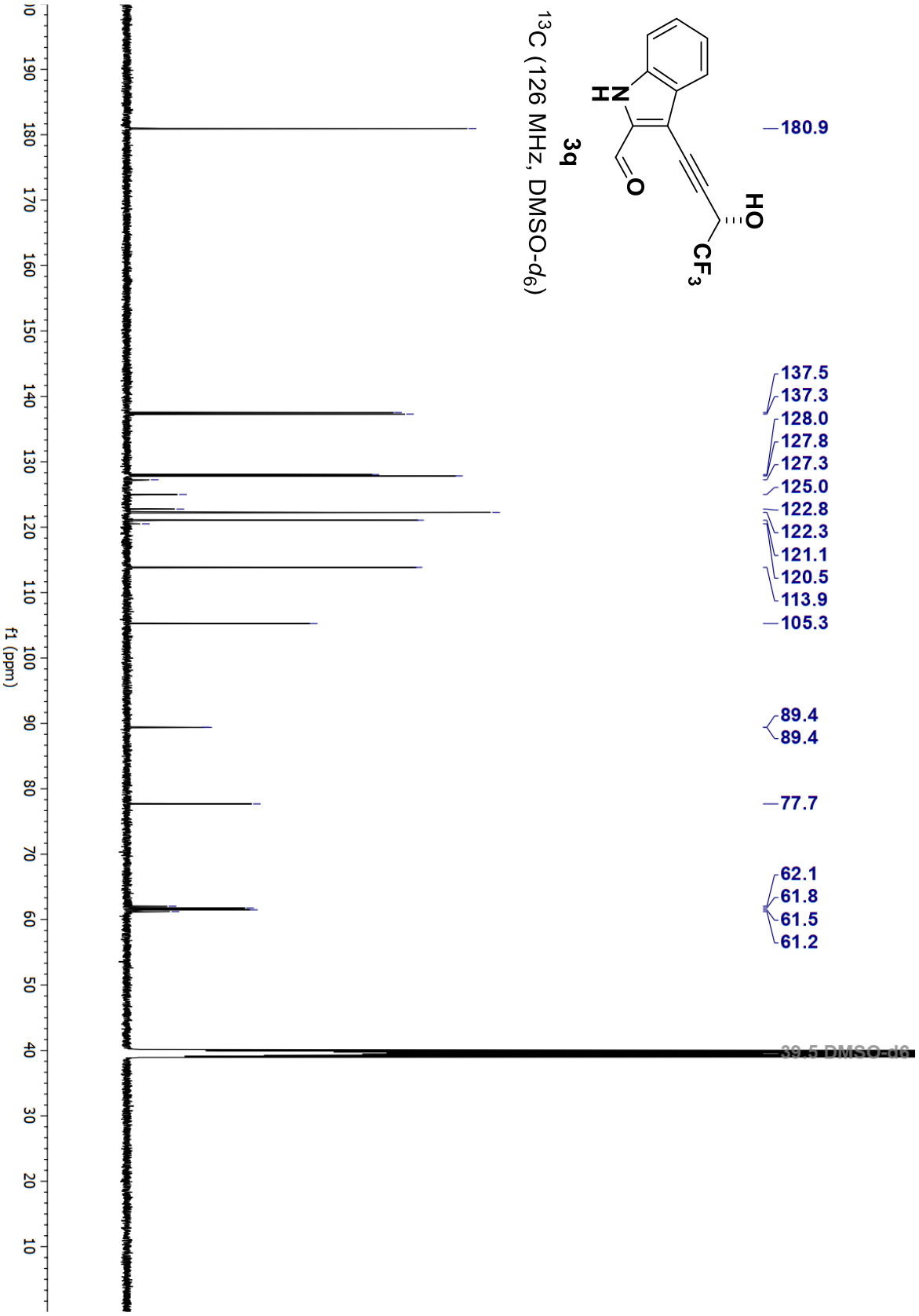
FTIR (neat): 3434, 3224, 2836, 2222, 1643, 1181, 744, 660, 377 cm^{-1}.

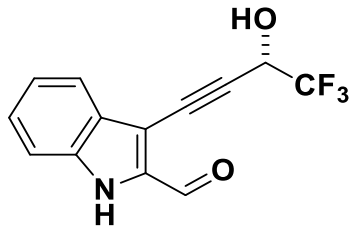
HPLC (CHIRALPAK AD-H, hexanes:2-PrOH = 90:10, 1.0 mL/min, 254 nm): ee = 99%.

$[\alpha]_D^{20}$ = -90° ($CHCl_3$, c = 0.3).

m.p.: 155 °C.

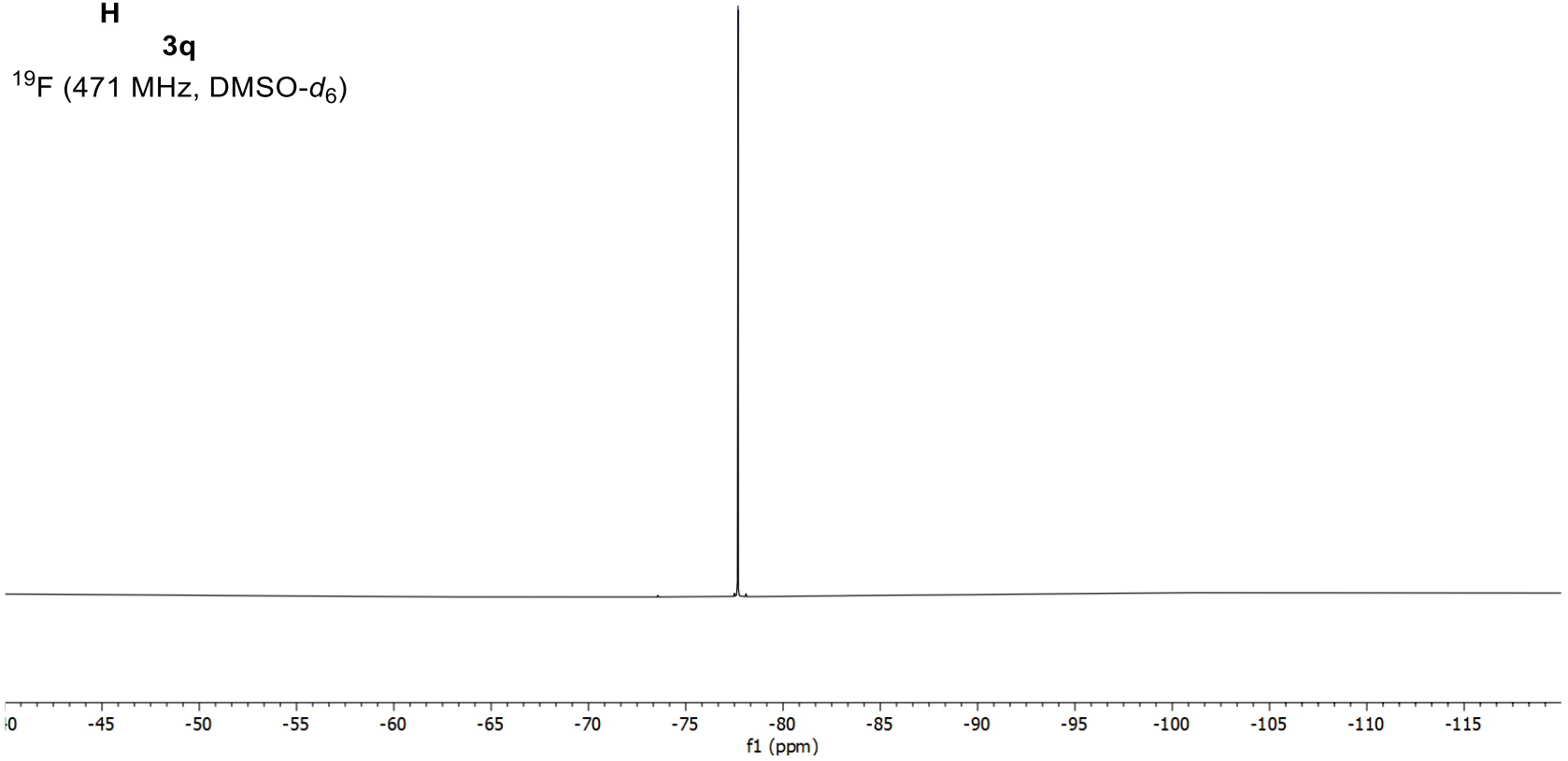

3q
^{1}H (500 MHz, DMSO-d_6)
12.46
9.97
7.70
7.69
7.53
7.52
7.45
7.43
7.42
7.32
7.31
7.27
7.26
7.24
5.38
5.36
5.35
5.34
5.32
2.50 DMSO-d6
0.98
0.89
1.00
1.02
1.05
1.03
1.06
1.01
f1 (ppm)

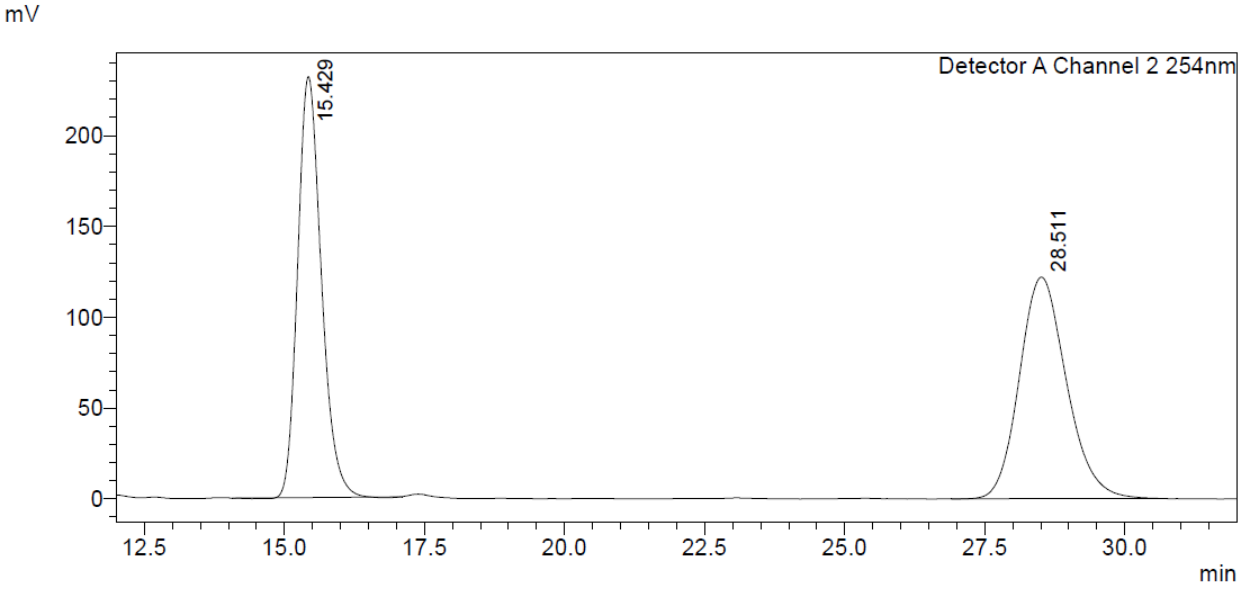

3q
^{13}C (126 MHz, DMSO-d_6)
180.9
137.5
137.3
128.0
127.8
127.3
125.0
122.8
122.3
121.1
120.5
113.9
105.3
89.4
89.4
77.7
62.1
61.8
61.5
61.2
39.5 DMSO-d6
f1 (ppm)



3q

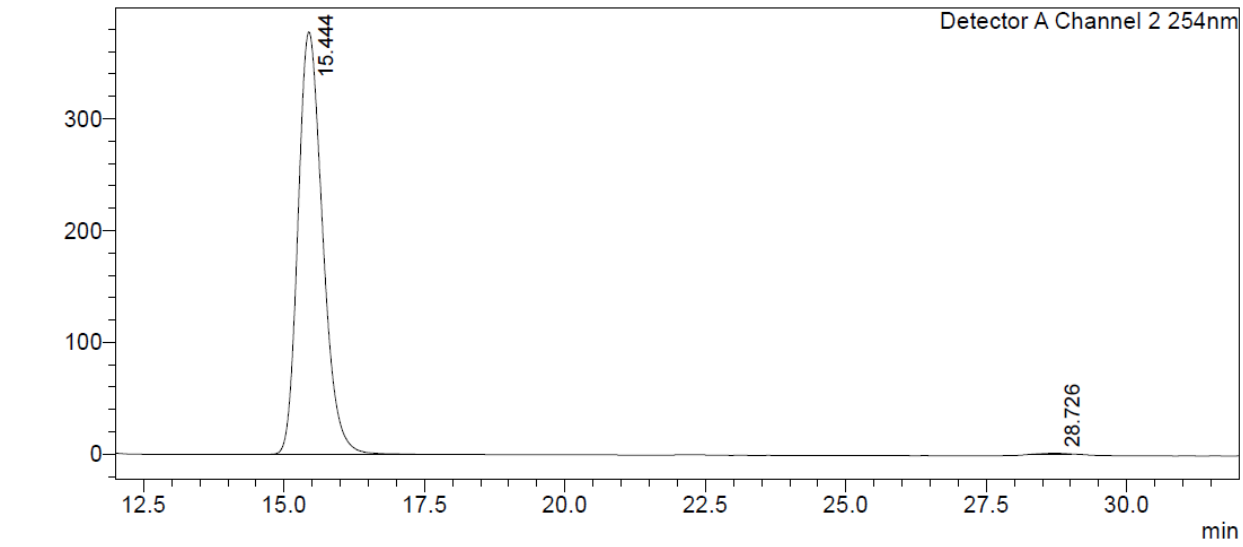
^{19}F (471 MHz, DMSO-d_6)





Detector A Channel 2 254nm

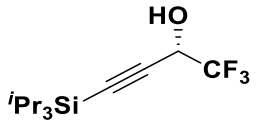
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	15.429	6794717	231670	48.783		M	
2	28.511	7133876	121993	51.217		M	
Total		13928593	353663				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	15.444	11500543	378004	99.822		M	
2	28.726	20531	790	0.178		M	
Total		11521074	378794				

(*S*)-1,1,1-trifluoro-4-(triisopropylsilyl)but-3-yn-2-ol (3r)



Alkyne **1r** (67 μL, 0.30 mmol, 150 mol%) was subjected to modified reaction conditions (80 °C, 48 h) at 5 mol% catalyst loading. Upon flash column chromatography (SiO_2: 0:100–2:98 EtOAc:hexanes), the title compound **3r** was isolated as a pale, yellow oil in 70% yield (39.3 mg, 0.14 mmol, 99% ee).

TLC (SiO_2): R_f = 0.1 (2:98 EtOAc:hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ 4.69 (dq, *J* = 8.3, 5.7 Hz, 1H), 2.33 (d, *J* = 8.4 Hz, 1H), 1.12 – 1.03 (m, 21H) ppm.

^{13}C NMR (101 MHz, $CDCl_3$): δ 122.8 (q, *J* = 281.9 Hz), 98.5 – 98.3 (m), 91.3, 62.9 (q, *J* = 36.3 Hz), 18.6, 11.1 ppm.

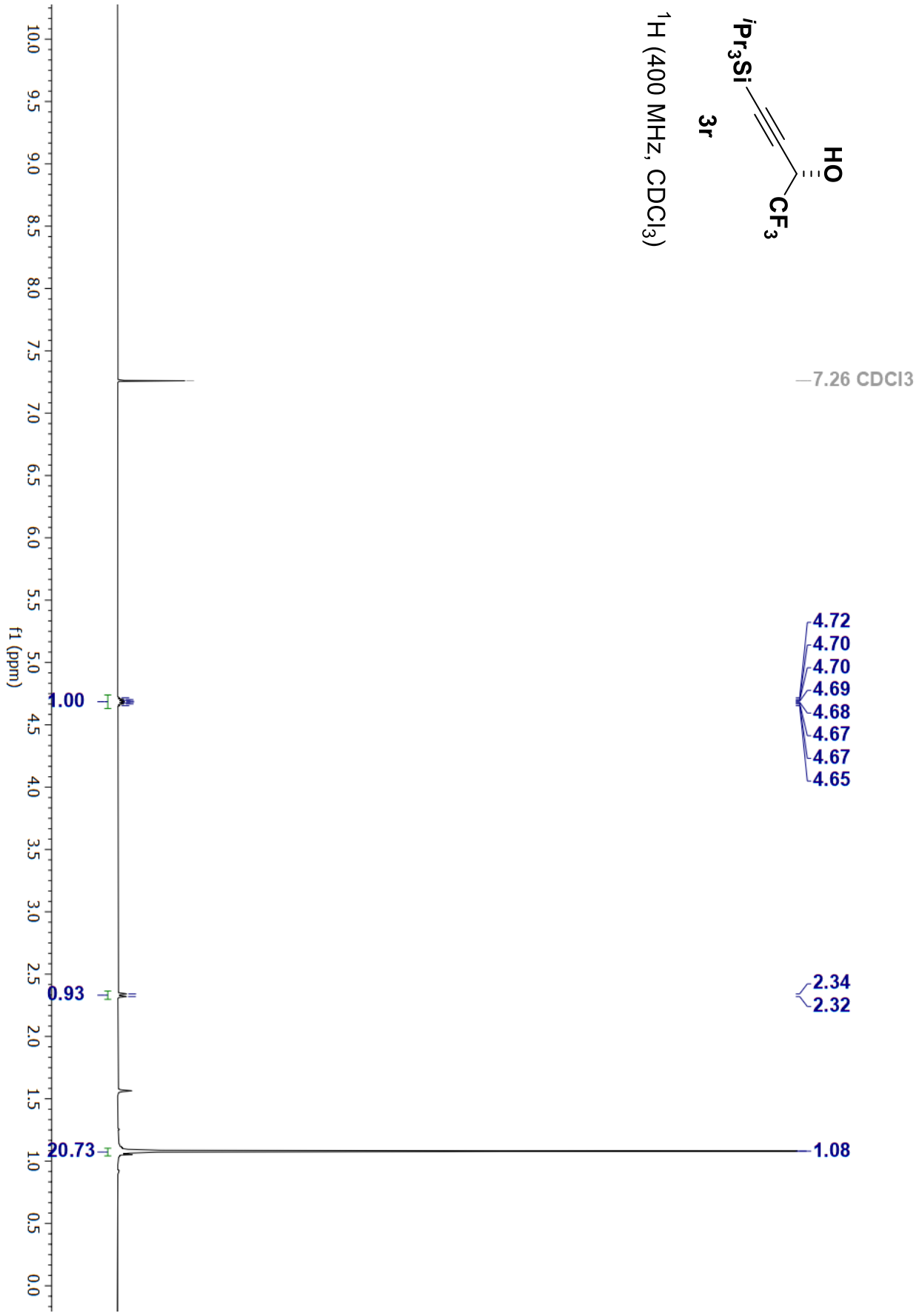
^{19}F NMR (376 MHz, $CDCl_3$): δ -79.6 (d, *J* = 5.6 Hz) ppm.

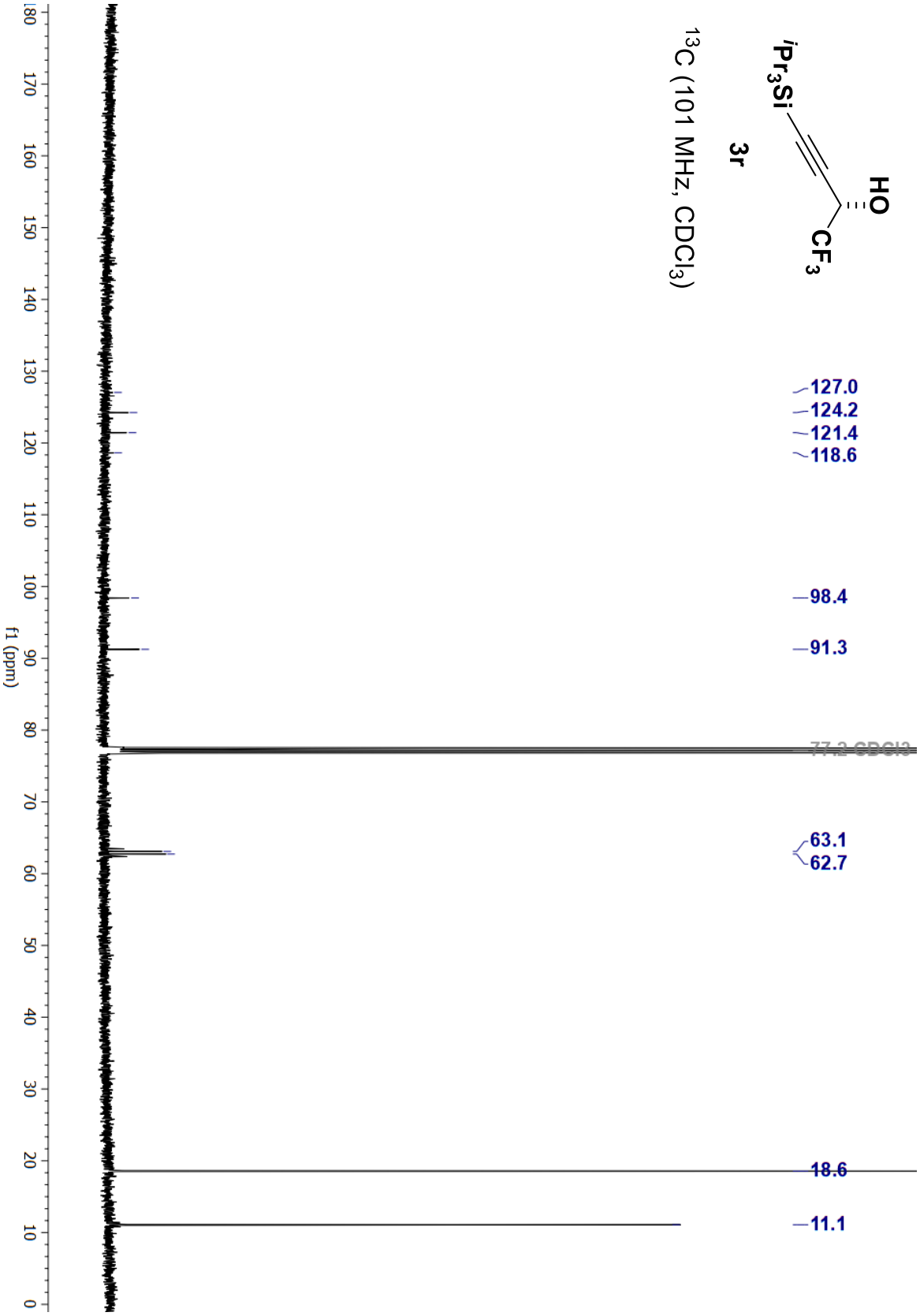
HRMS (ESI(–)): m/z [M–H$^+$] calcd. for $C_{13}H_{22}F_3OSi^-$: 279.1397; found = 279.1404.

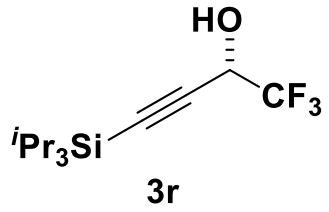
FTIR (neat): 3336, 2945, 2894, 2868, 1464, 1385, 1349, 1270, 1182, 1141, 1087, 1007, 920, 882, 838, 721, 669, 600, 570, 519, 459, 421, 410 cm^{-1}.

HPLC (The product **3r** was derivatized to give its respective benzoyl ester prior to HPLC analysis. CHIRALPAK AD-H, hexanes, 1.0 mL/min, 254 nm): ee = 99%.

$[\alpha]_D^{20}$ = -15° (CH_2Cl_2, c = 1.0).

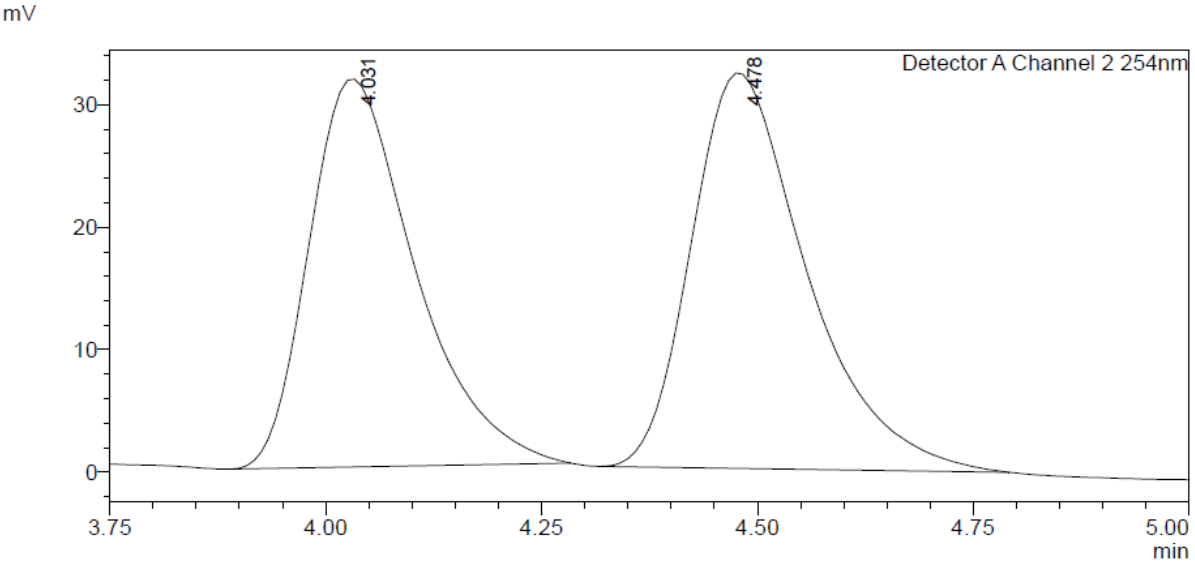

^{1}H (400 MHz, CDCl$_3$)
3r
^{i}Pr$_3$Si
HO
CF$_3$
7.26 CDCl3
4.72
4.70
4.70
4.69
4.68
4.67
4.67
4.65
2.34
2.32
1.08
1.00
0.93
20.73
f1 (ppm)


^{13}C (101 MHz, $CDCl_3$)
3r
$^{i}Pr_3Si$
HO
CF_3
127.0
124.2
121.4
118.6
98.4
91.3
77.2 $CDCl_3$
63.1
62.7
18.6
11.1
f1 (ppm)



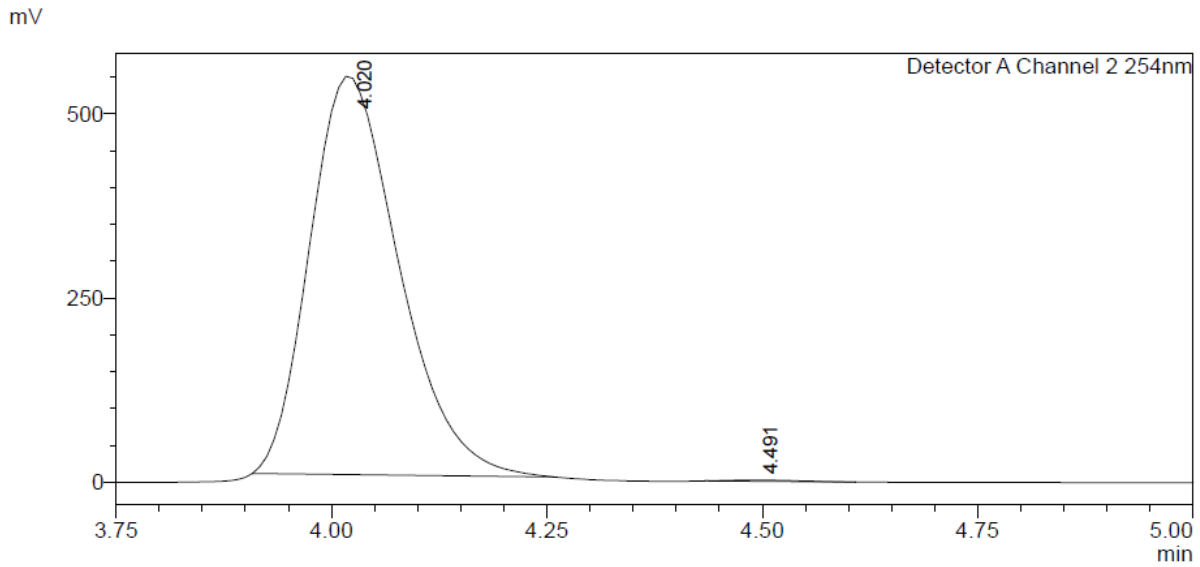
3r

^{19}F (376 MHz, $CDCl_3$)



Detector A Channel 2 254nm

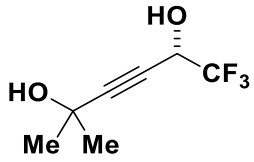
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	4.031	270517	31673	47.392		M	
2	4.478	300296	32280	52.608		M	
Total		570813	63953				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	4.020	3902152	540516	99.751		M	
2	4.491	9729	1834	0.249		M	
Total		3911882	542350				

(*S*)-1,1,1-trifluoro-5-methylhex-3-yne-2,5-diol (3s)



Alkyne **1s** (17.7 mg, 0.21 mmol, 105 mol%) was subjected to modified reaction conditions (100 °C, 48 h) at 5 mol% catalyst loading. Upon flash column chromatography (SiO_2: 25:75 EtOAc:hexanes), the title compound **3s** was isolated as a colorless waxy solid in 69% yield (25.4 mg, 0.14 mmol, 99% ee).

TLC (SiO_2): R_f = 0.2 (1:3 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 4.70 (q, *J* = 5.7 Hz, 1H), 2.44 (s, 1H), 1.96 (s, 1H), 1.55 (s, 6H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ 122.8 (q, *J* = 281.6 Hz), 92.8, 74.2 (d, *J* = 2.7 Hz), 65.3, 62.5 (q, *J* = 36.5 Hz), 31.1, 31.0 ppm.

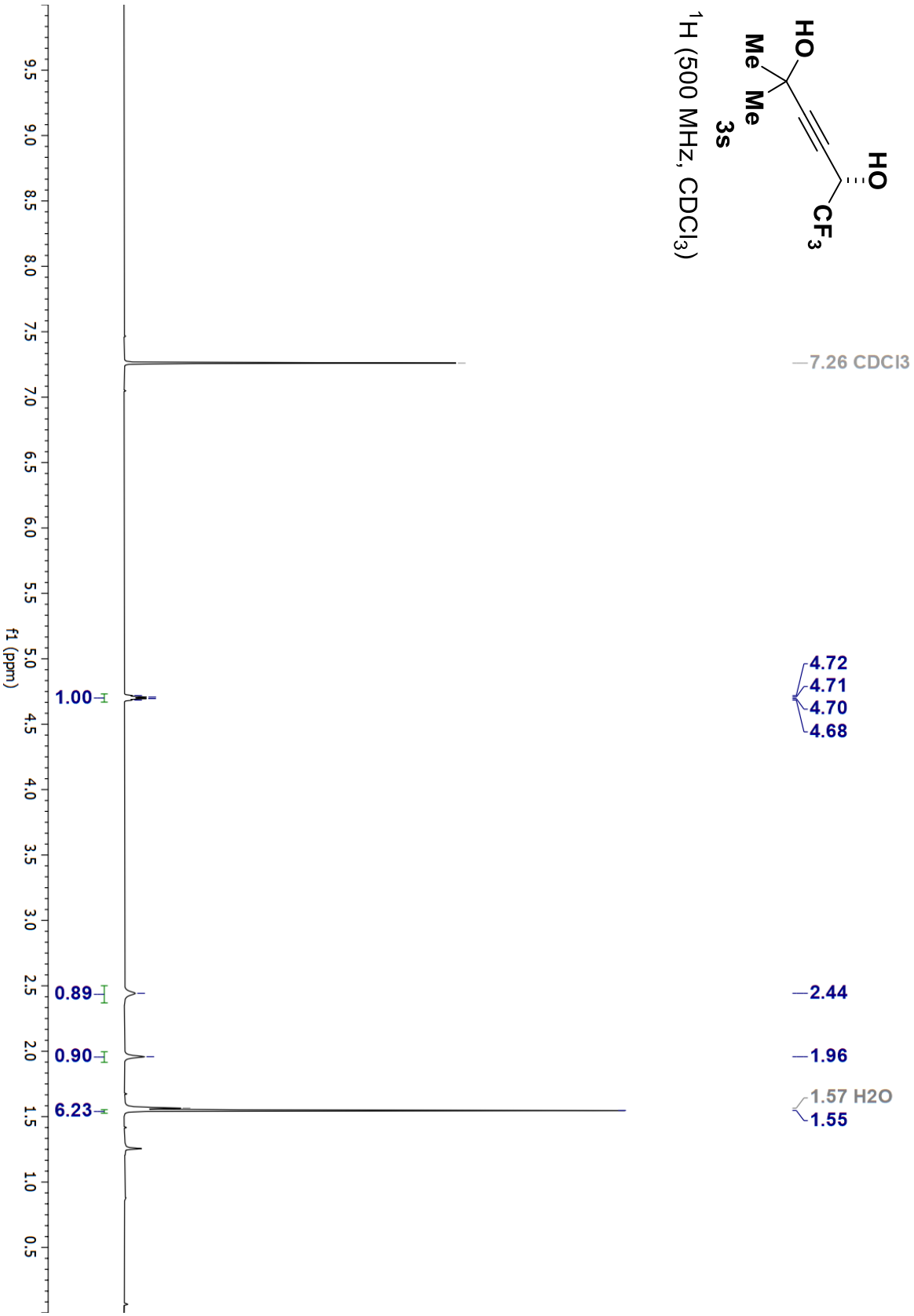
^{19}F NMR (471 MHz, $CDCl_3$): δ -79.6 (d, *J* = 5.9 Hz) ppm.

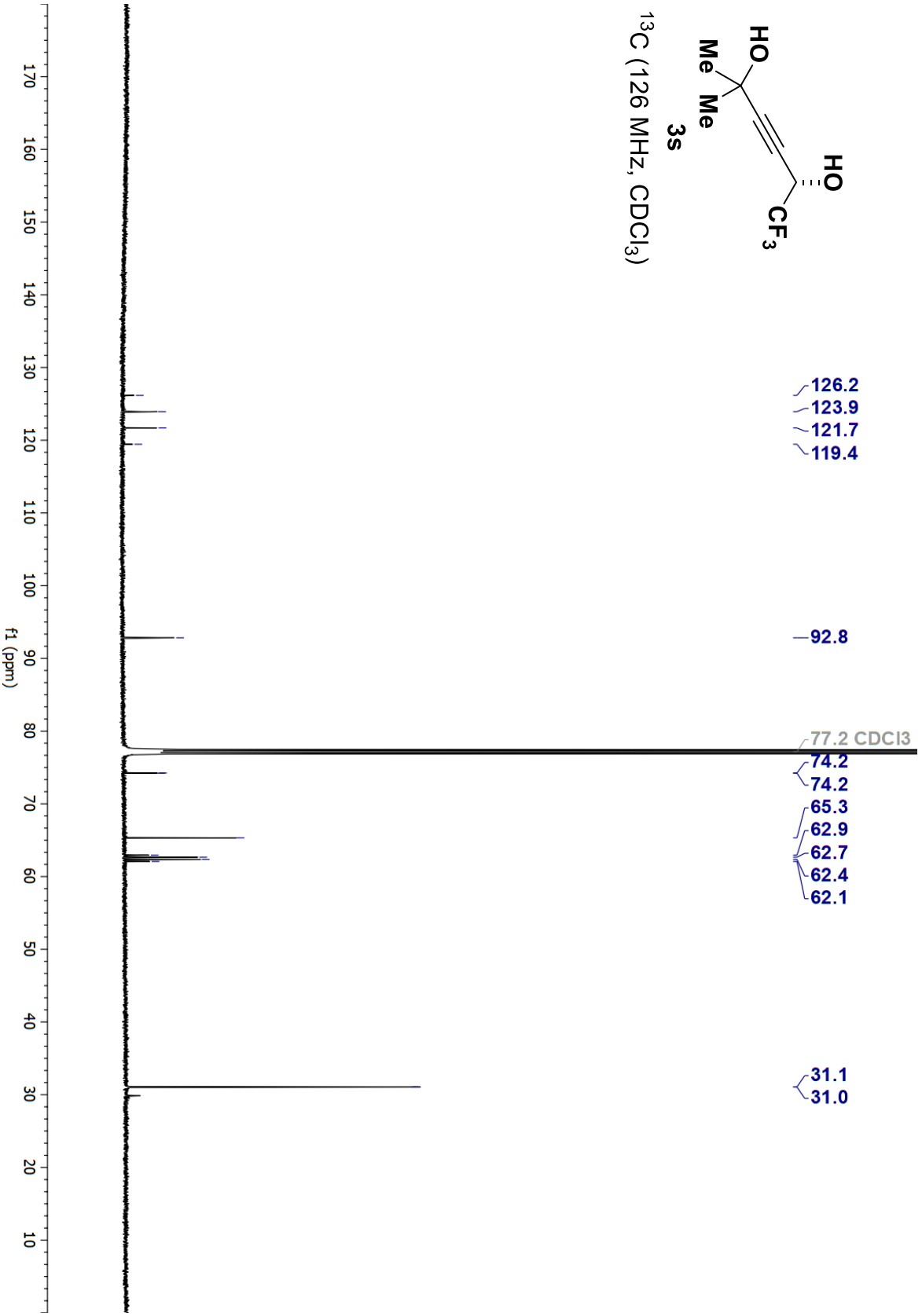
HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_7H_{10}F_3O_2^+$: 183.0627; found = 183.0623.

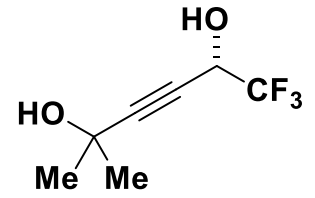
FTIR (neat): 3362, 3147, 2992, 2920, 2850, 2727, 2362, 2344, 2245, 2167, 2027, 2009, 1977, 1379, 1364, 1355, 1272, 1237, 1183, 1141, 1097, 1035, 947, 870, 835, 735, 668, 598 cm^{-1}.

HPLC (The product **3s** was derivatized to give its respective monobenzoyl ester prior to HPLC analysis. PHENOMENEX Cellulose 5, hexanes:2-PrOH = 97:3, 0.5 mL/min, 254 nm): ee = 99%.

$[\alpha]_D^{20}$ = -126° ($CHCl_3$, c = 1.0).

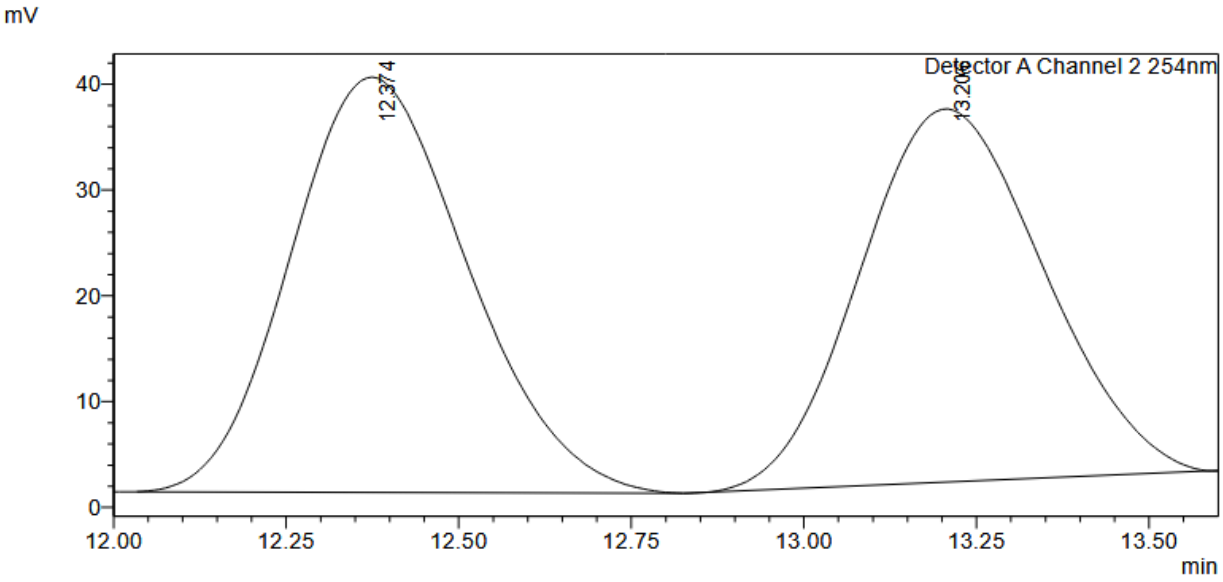

3s
^{1}H (500 MHz, CDCl$_3$)
HO
Me
Me
HO
CF$_3$
7.26 CDCl3
4.72
4.71
4.70
4.68
2.44
1.96
1.57 H2O
1.55
1.00
0.89
0.90
6.23
f1 (ppm)


3s
^{13}C (126 MHz, CDCl$_3$)
HO
Me Me
HO
CF$_3$
126.2
123.9
121.7
119.4
92.8
77.2 CDCl3
74.2
74.2
65.3
62.9
62.7
62.4
62.1
31.1
31.0
f1 (ppm)



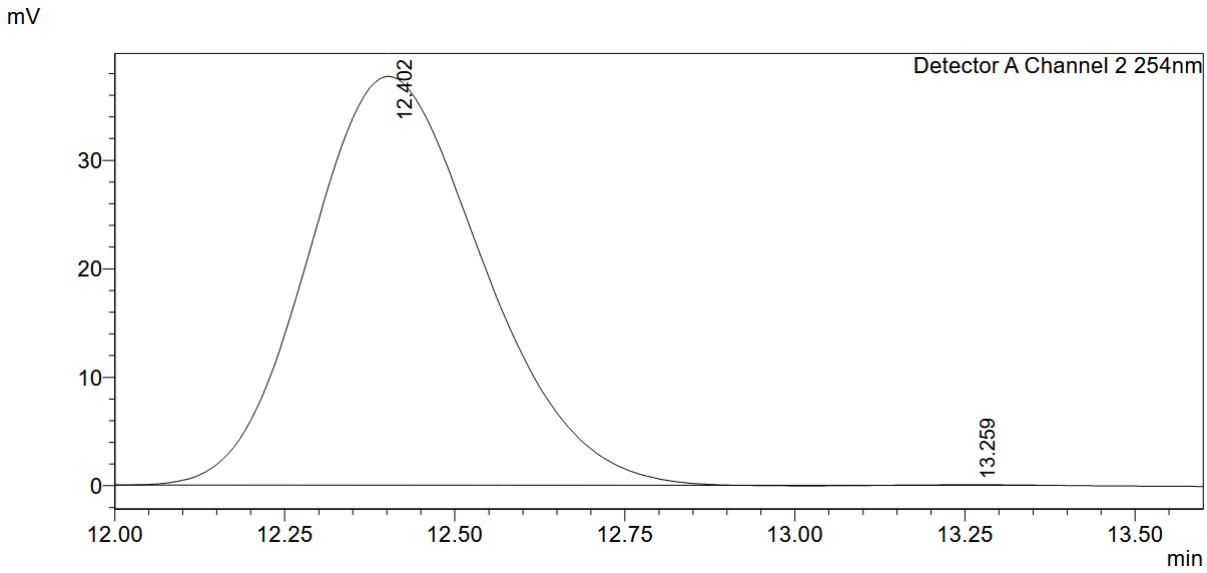
3s

^{19}F (471 MHz, $CDCl_3$)



Detector A Channel 2 254nm

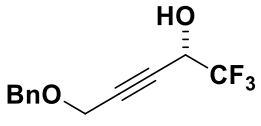
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	12.374	698988	39238	51.796		M	
2	13.206	650510	35260	48.204		M	
Total		1349498	74498				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	12.402	671265	37675	99.937		M	
2	13.259	422	57	0.063		M	
Total		671687	37732				

(*S*)-5-(benzyloxy)-1,1,1-trifluoropent-3-yn-2-ol (3t)



Alkyne **1t** (58.4 mg, 0.4 mmol, 200 mol%) was subjected to modified reaction conditions (100 °C, 48 h) at 5 mol% catalyst loading. Upon flash column chromatography (SiO_2: 10:90 EtOAc:hexanes), the title compound **3t** was isolated as a clear orange oil in 65% yield (31.7 mg, 0.13 mmol, 97% ee).

TLC (SiO_2): R_f = 0.4 (1:5 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.43 – 7.28 (m, 5H), 4.82 – 4.67 (m, 1H), 4.60 (s, 2H), 4.24 (s, 2H), 2.54 (d, *J* = 7.9 Hz, 1H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ 137.0, 128.7, 128.3, 128.3, 122.8 (q, *J* = 281.8 Hz), 84.6, 78.6 – 78.4 (m), 72.1, 62.6 (q, *J* = 36.6 Hz), 57.1 ppm.

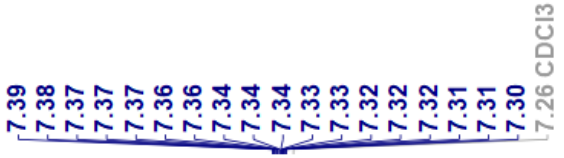
^{19}F NMR (471 MHz, $CDCl_3$): δ -79.4 (d, *J* = 5.9 Hz) ppm.

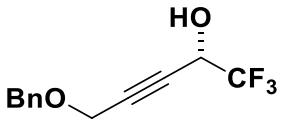
HRMS (ESI(+)): m/z [M+Na^+] calcd. for $C_{11}H_{11}F_3NaO_2^+$: 267.0603; found = 267.0597.

FTIR (neat): 3320, 3032, 2859, 2161, 2020, 1268, 1121, 696, 541 cm^{-1}.

HPLC (PHENOMENEX Cellulose 5, hexanes:2-PrOH = 98:2, 1.0 mL/min, 210 nm): ee = 97%.

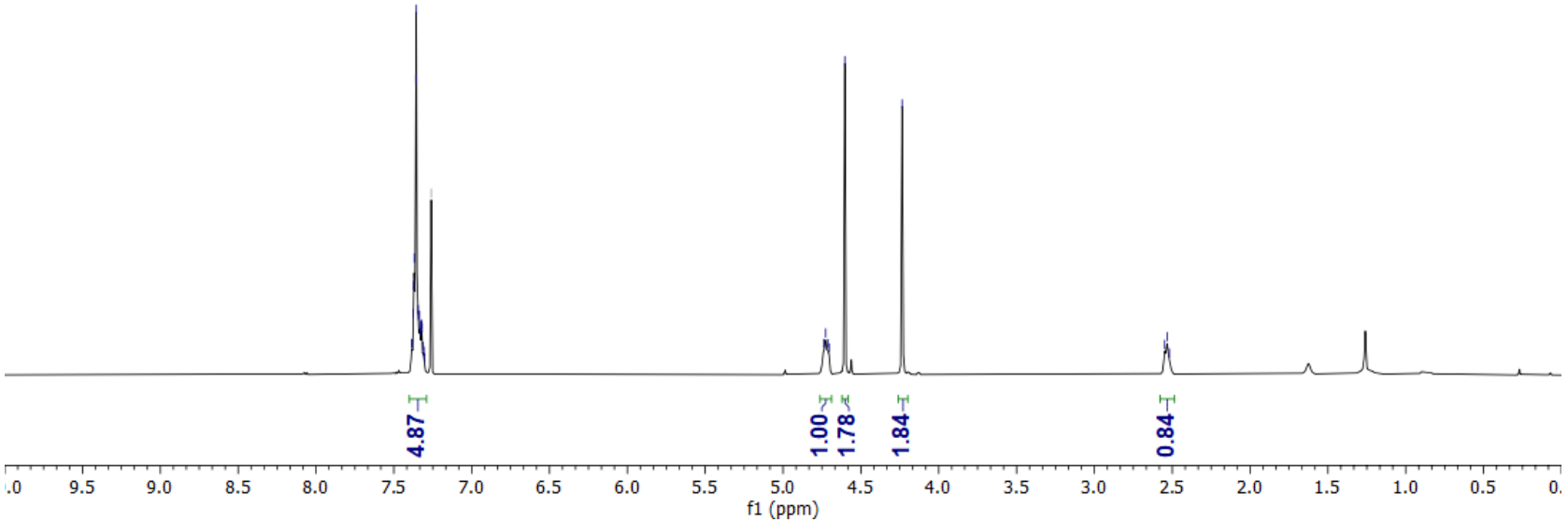
$[\alpha]_D^{20}$ = -30° ($CHCl_3$, c = 0.3).

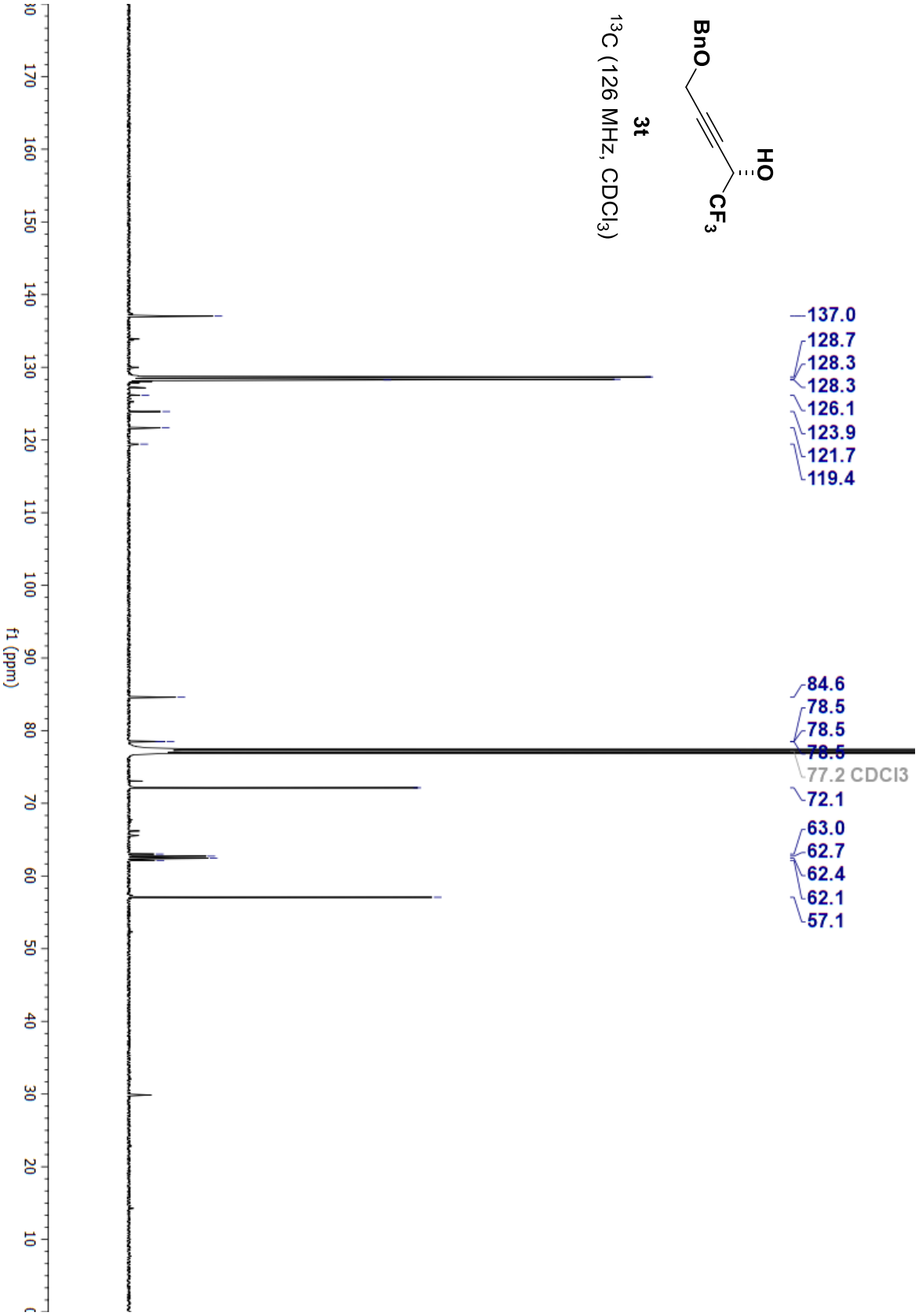


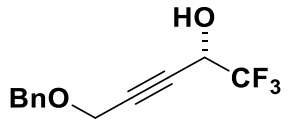


3t

^{1}H (500 MHz, $CDCl_3$)

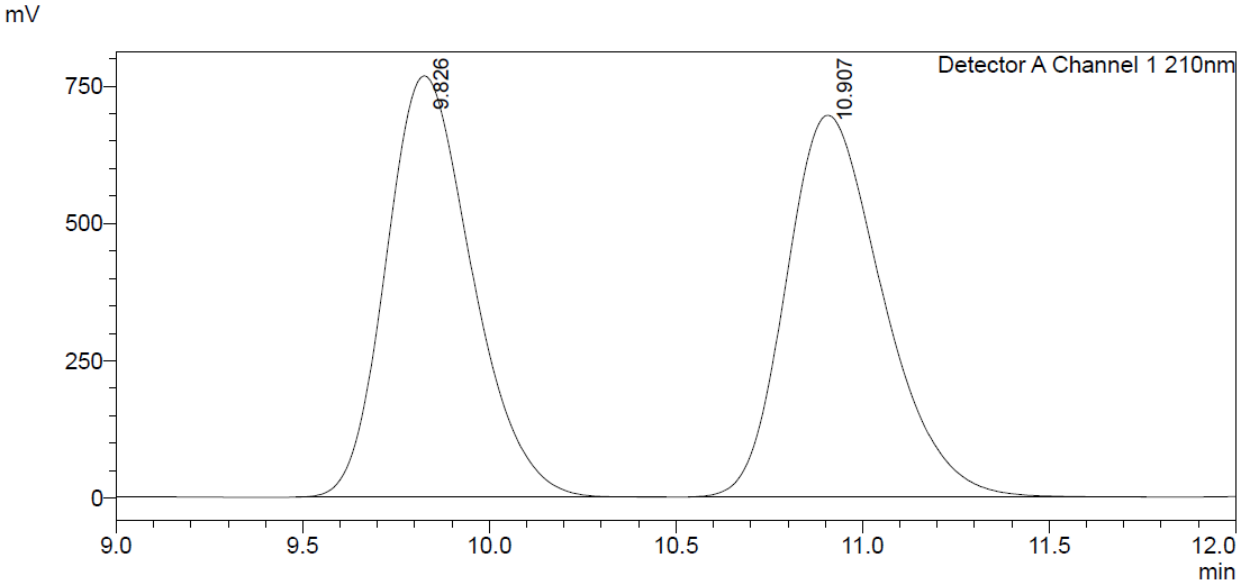



3t
^{13}C (126 MHz, CDCl$_3$)
BnO
HO
CF$_3$
137.0
128.7
128.3
128.3
126.1
123.9
121.7
119.4
84.6
78.5
78.5
78.5
77.2 CDCl3
72.1
63.0
62.7
62.4
62.1
57.1
f1 (ppm)



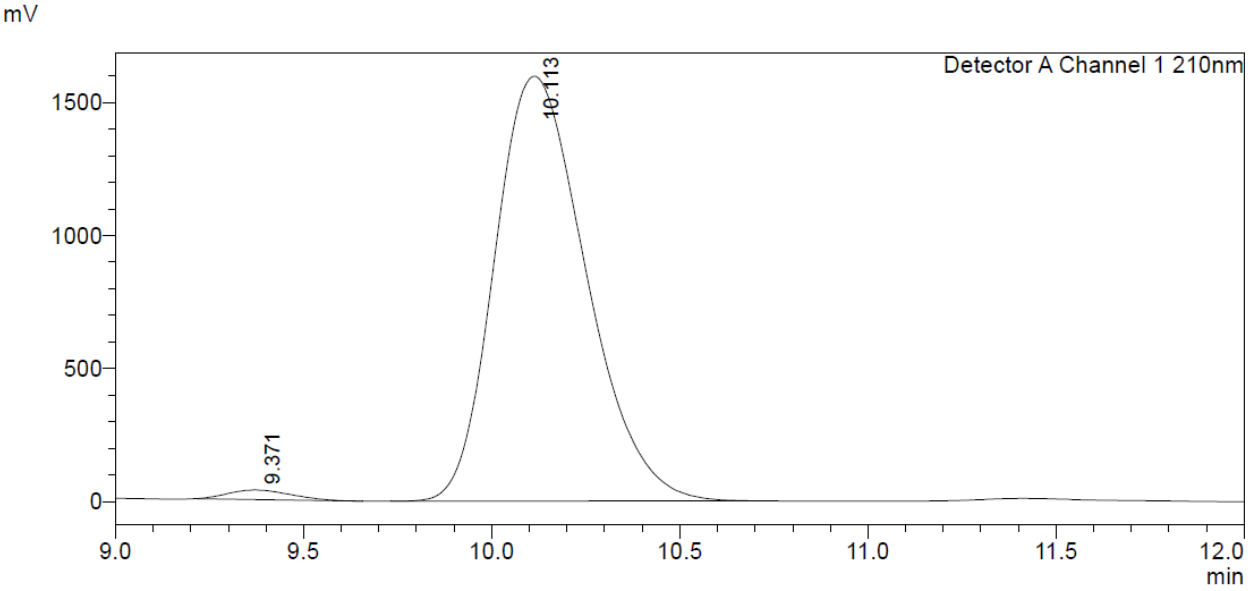
3t

^{19}F (471 MHz, $CDCl_3$)



Detector A Channel 1 210nm

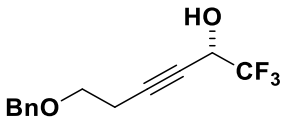
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	9.826	12288194	766874	49.530		M	
2	10.907	12521506	694766	50.470		M	
Total		24809700	1461640				



Detector A Channel 1 210nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	9.371	424242	36274	1.548		M	
2	10.113	26989438	1597231	98.452		M	
Total		27413680	1633504				

(*S*)-6-(benzyloxy)-1,1,1-trifluorohex-3-yn-2-ol (3u)



Alkyne **1u** (48.8 mg, 0.30 mmol, 150 mol%) was subjected to modified reaction conditions (100 °C, 48 h) at 5 mol% catalyst loading. Upon flash column chromatography (SiO_2: 5:95–10:90 EtOAc:hexanes), the title compound **3u** was isolated as a pale yellow oil in 68% yield (34.9 mg, 0.14 mmol, 90% ee).

TLC (SiO_2): R_f = 0.1 (1:9 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.39 – 7.33 (m, 4H), 7.30 (td, *J* = 5.9, 2.4 Hz, 1H), 4.68 – 4.60 (m, 1H), 4.56 (s, 2H), 3.61 (t, *J* = 6.7 Hz, 2H), 2.64 – 2.49 (m, 3H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ 137.9, 128.6, 128.0, 127.9, 122.9 (q, *J* = 281.6 Hz), 86.5, 73.4 – 73.3 (m), 73.2, 67.7, 62.6 (q, *J* = 36.3 Hz), 20.2 ppm.

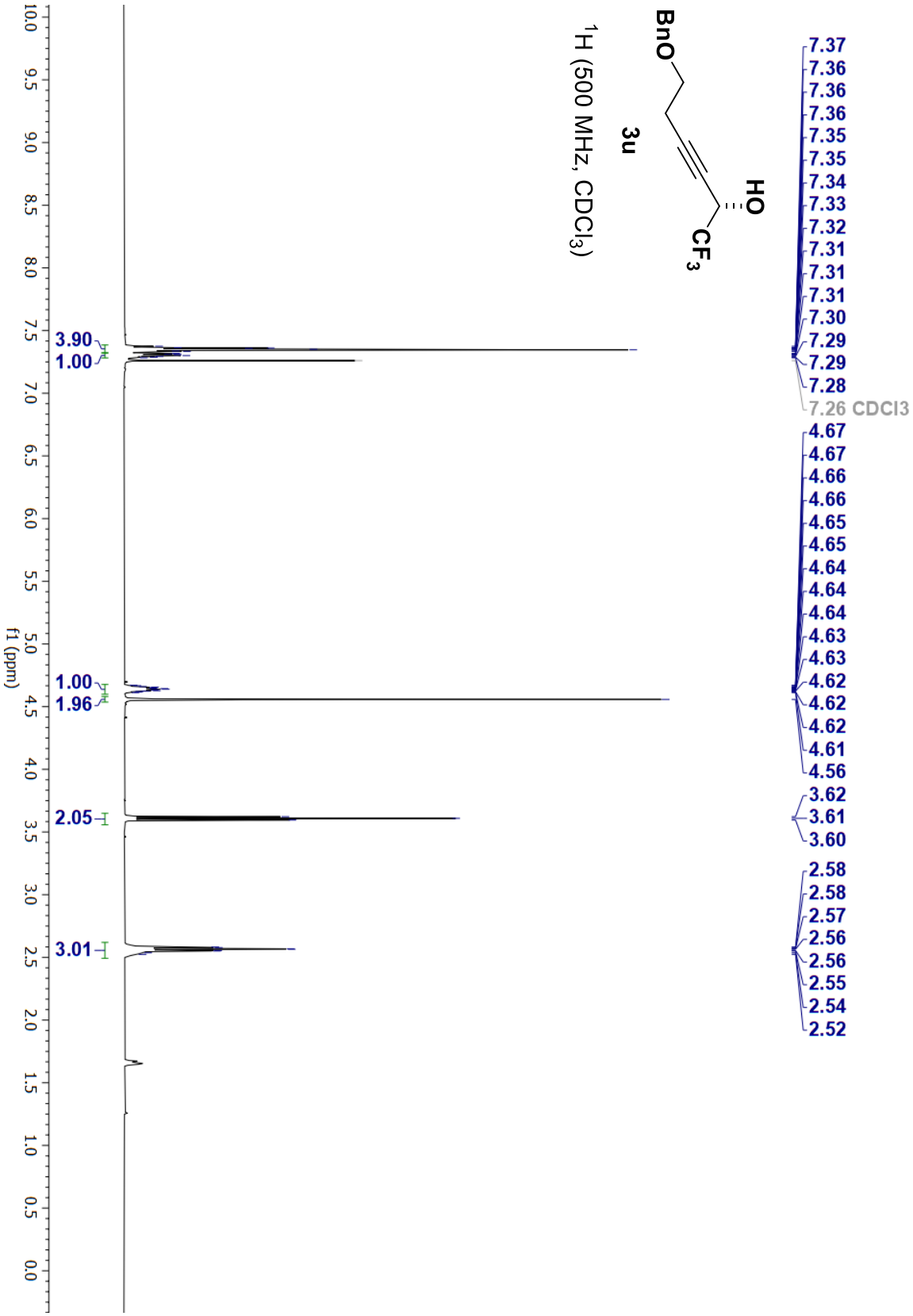
^{19}F NMR (471 MHz, $CDCl_3$): δ -79.7 (d, *J* = 5.6 Hz) ppm.

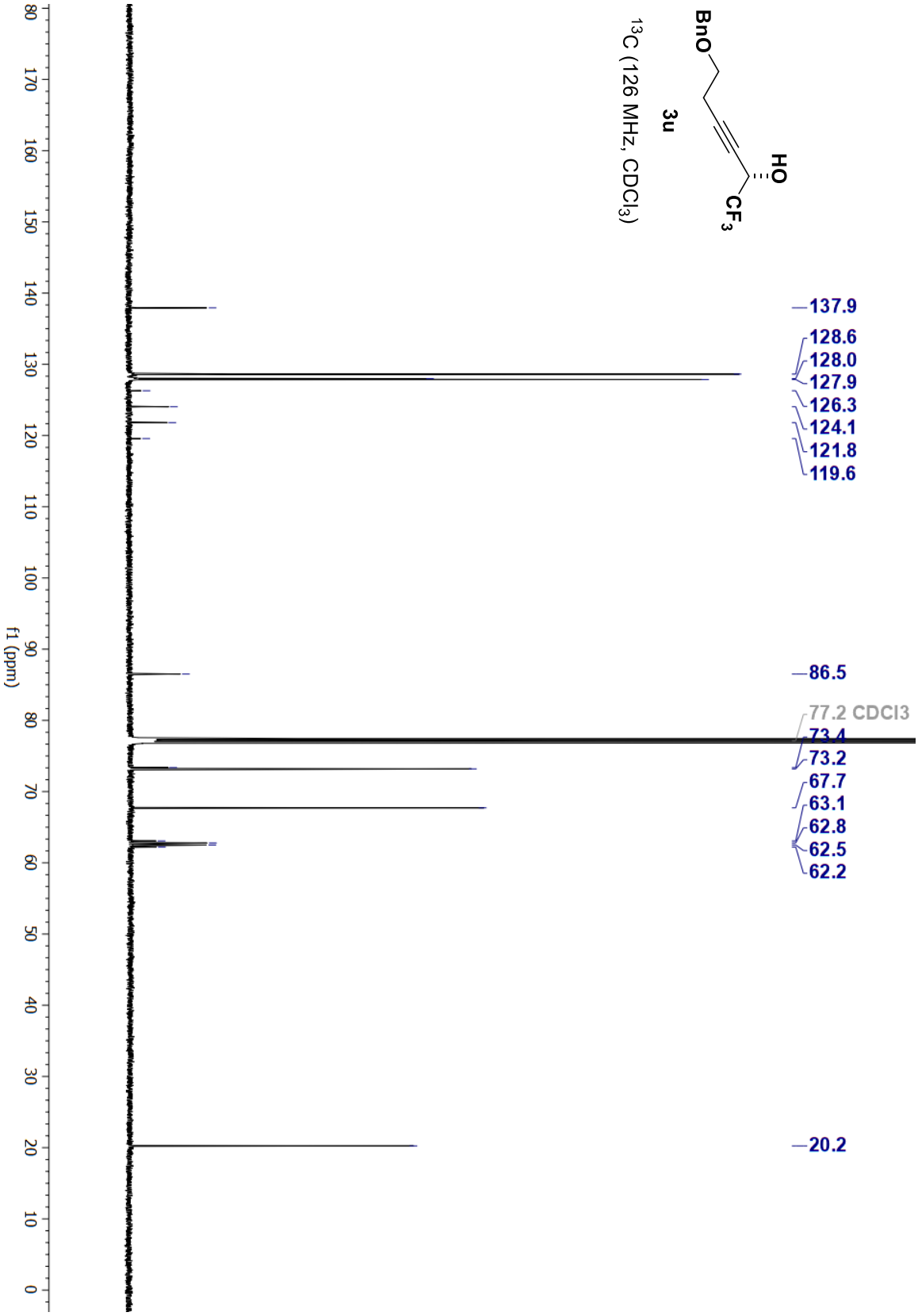
HRMS (ESI(+)): m/z [M+NH_4^+] calcd. for $C_{13}H_{17}F_3NO_2^+$: 276.1206; found = 276.1213.

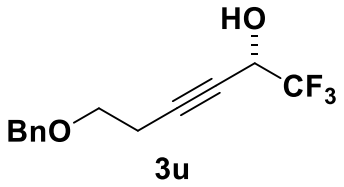
FTIR (neat): 3351, 3066, 3033, 2919, 2871, 2250, 1455, 1360, 1269, 1174, 1156, 1129, 1055, 843, 823, 790, 738, 696, 599, 527, 456, 418 cm^{-1}.

HPLC (PHENOMENEX Amylose-3, hexanes:2-PrOH = 99:1, 1.0 mL/min, 210 nm): ee = 90%.

$[\alpha]_D^{20}$ = -22° (CH_2Cl_2, c = 1.0).

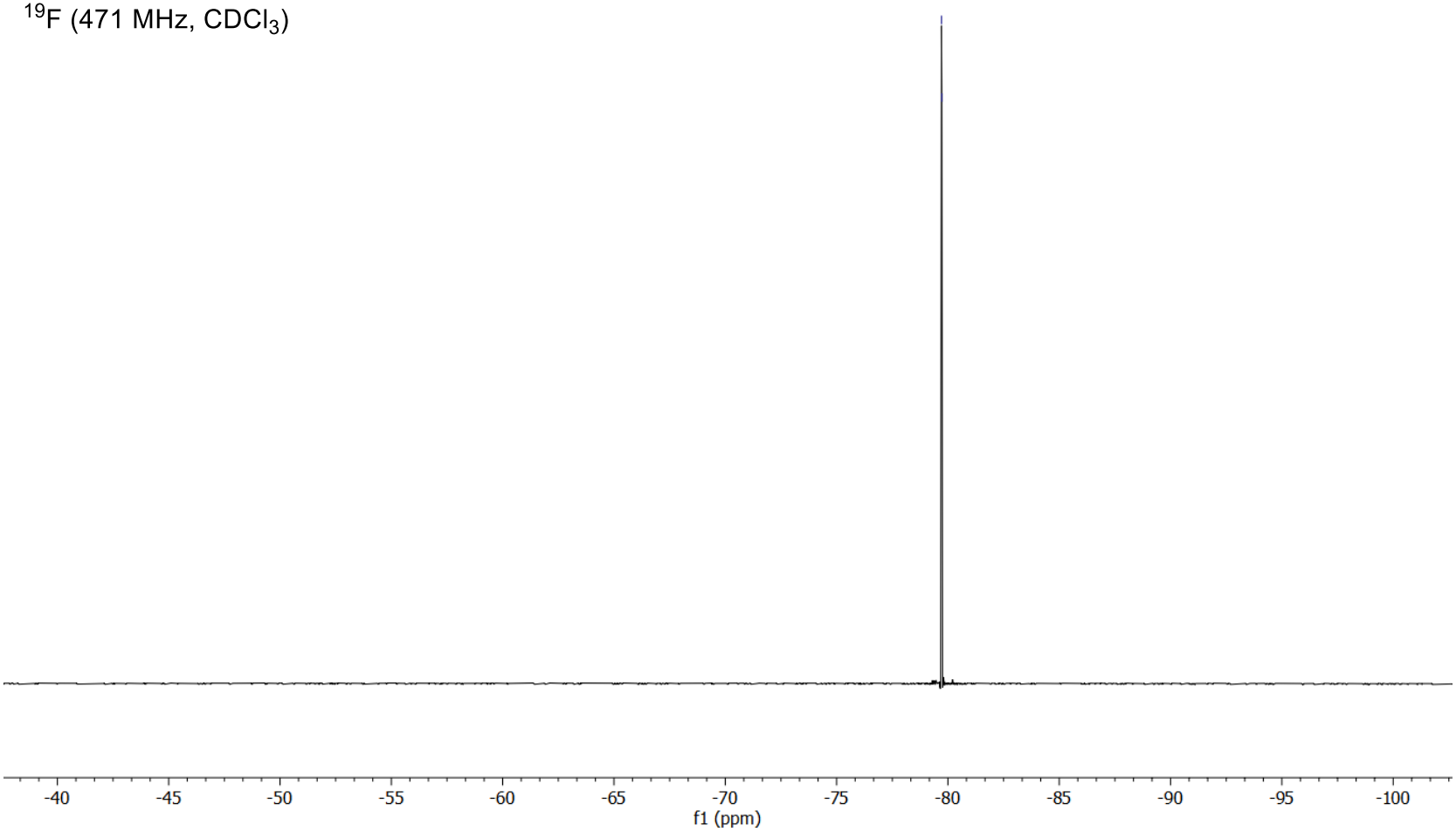

3u
^{1}H (500 MHz, CDCl$_3$)
BnO
HO
CF$_3$
7.37
7.36
7.36
7.36
7.35
7.35
7.34
7.33
7.32
7.31
7.31
7.31
7.30
7.29
7.29
7.28
7.26 CDCl3
4.67
4.67
4.66
4.66
4.65
4.65
4.64
4.64
4.64
4.63
4.63
4.62
4.62
4.62
4.61
4.56
3.62
3.61
3.60
2.58
2.58
2.57
2.56
2.56
2.55
2.54
2.52
3.90
1.00
1.00
1.96
2.05
3.01
f1 (ppm)

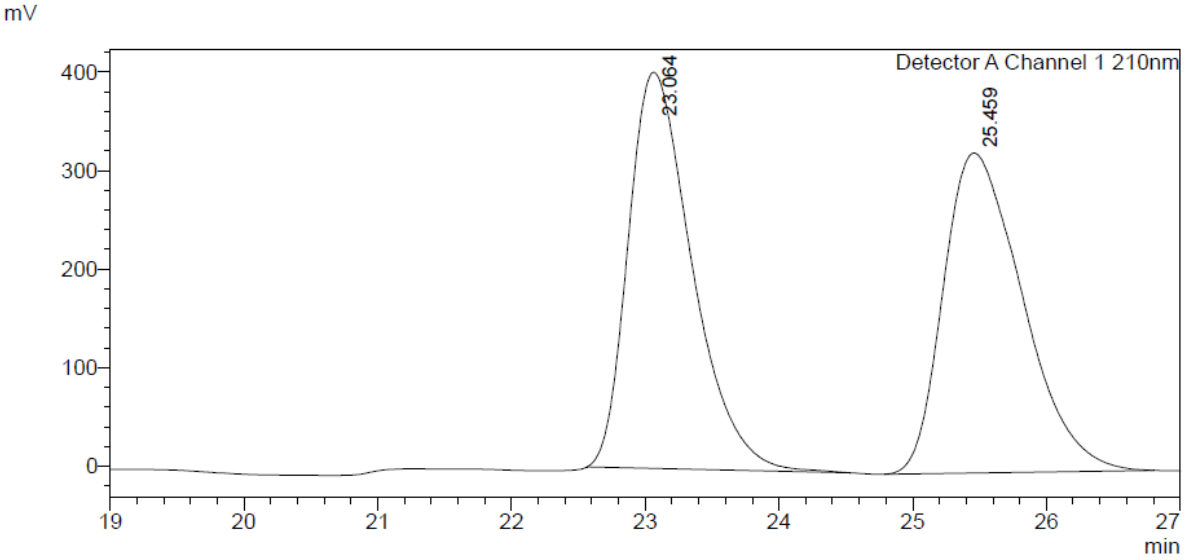

BnO
HO
CF3
3u
13C (126 MHz, CDCl3)
137.9
128.6
128.0
127.9
126.3
124.1
121.8
119.6
86.5
77.2 CDCl3
73.4
73.2
67.7
63.1
62.8
62.5
62.2
20.2
f1 (ppm)



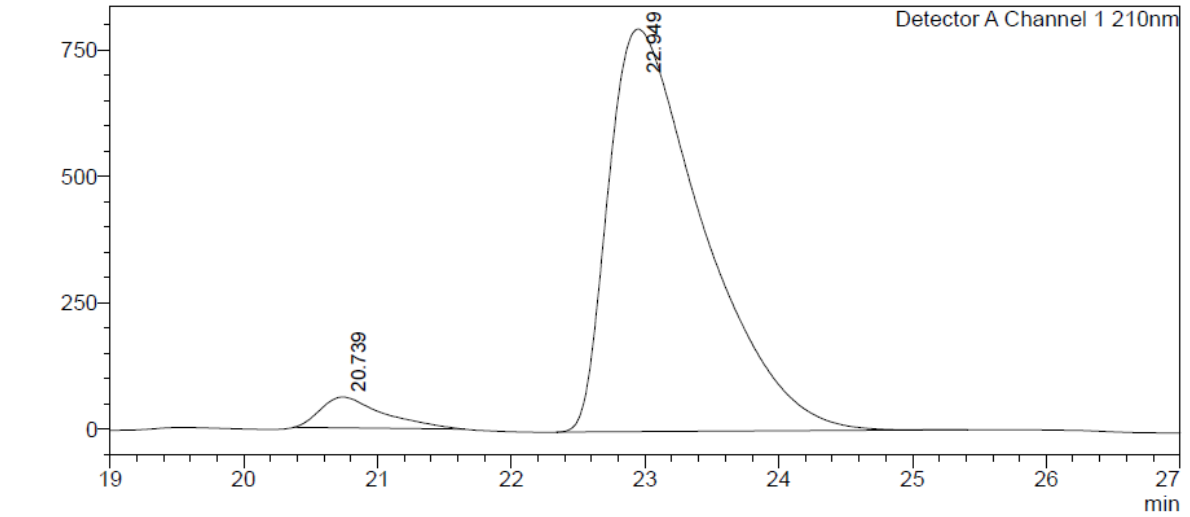
3u

^{19}F (471 MHz, $CDCl_3$)



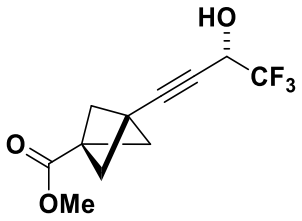


Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	23.064	13318025	401896	49.914		M	
2	25.459	13363852	324704	50.086		M	
Total		26681878	726600				



Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	20.739	1989661	60827	4.818		M	
2	22.949	39302874	795749	95.182		M	
Total		41292535	856576				

Methyl (*S*)-3-(4,4,4-trifluoro-3-hydroxybut-1-yn-1-yl)bicyclo[1.1.1]pentane-1-carboxylate (3v)



Alkyne **1v** (31.5 mg, 0.21 mmol, 105 mol%) was subjected to standard reaction conditions (80 °C, 24 h) at 5 mol% catalyst loading. Upon flash chromatography (SiO_2: 16:84 EtOAc:hexanes), the title compound **3v** was isolated as a waxy, pale-yellow solid in 81% yield (40.2 mg, 0.16 mmol, 92% ee).

TLC (SiO_2): R_f = 0.3 (1:4 EtOAc:hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ 4.67 (dq, *J* = 8.3, 5.7 Hz, 1H), 3.67 (s, 3H), 2.38 (s, 1H), 2.35 (s, 6H) ppm.

^{13}C NMR (101 MHz, $CDCl_3$): δ 169.5, 122.7 (q, *J* = 281.3 Hz), 86.6, 72.4 (q, *J* = 2.4 Hz), 62.7 (q, *J* = 36.5 Hz), 55.8, 52.0, 40.0, 27.9 ppm.

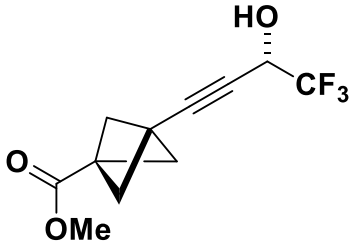
^{19}F NMR (376 MHz, $CDCl_3$): δ -79.4 (d, *J* = 6.1 Hz) ppm.

HRMS (ESI(+)): m/z [M+H^+] calcd. for $C_{11}H_{12}F_3O_3^+$: 249.0733; found = 249.0729.

FTIR (neat): 3299, 2998, 2977, 2956, 2923, 2883, 2852, 1713, 1439, 1352, 1278, 1216, 1182, 1130, 1111, 1074, 976, 929, 827, 803, 714, 654, 626, 526, 497, 462, 432, 420 cm^{-1}.

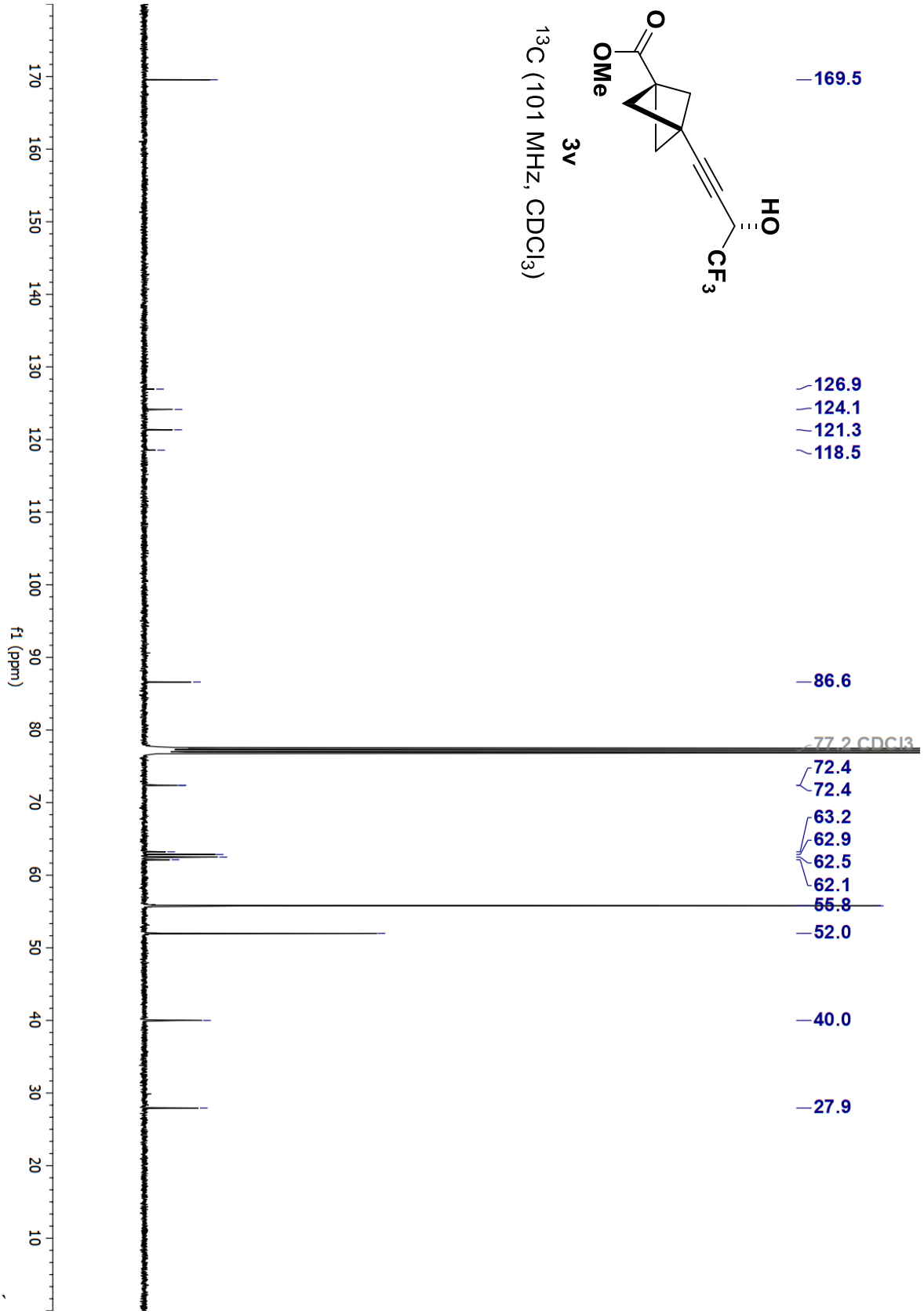
HPLC (The product **3v** was derivatized to give its respective tosylate prior to chiral HPLC analysis. PHENOMENEX Cellulose 5, hexanes:2-PrOH = 98:2, 1.0 mL/min, 210 nm): ee = 92%.

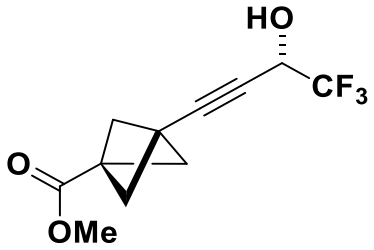
$[\alpha]_D^{20}$ = +43° ($CHCl_3$, c = 1.0).



3v

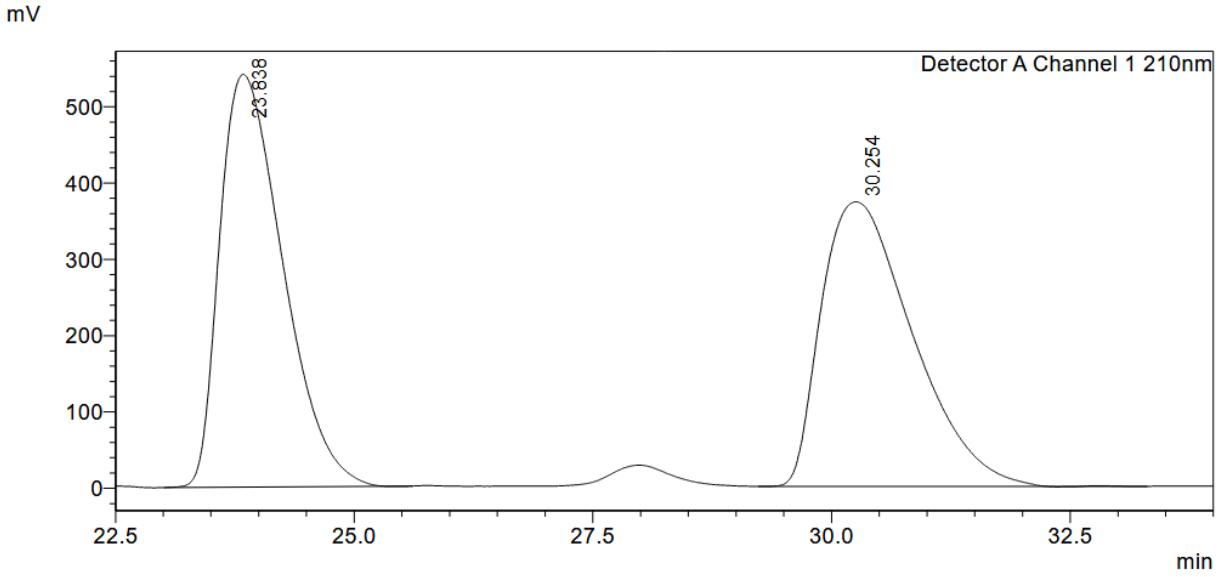
^{1}H (400 MHz, $CDCl_3$)


3v
^{13}C (101 MHz, CDCl$_3$)
O
OMe
HO
CF$_3$
169.5
126.9
124.1
121.3
118.5
86.6
77.2 CDCl3
72.4
72.4
63.2
62.9
62.5
62.1
55.8
52.0
40.0
27.9
f1 (ppm)

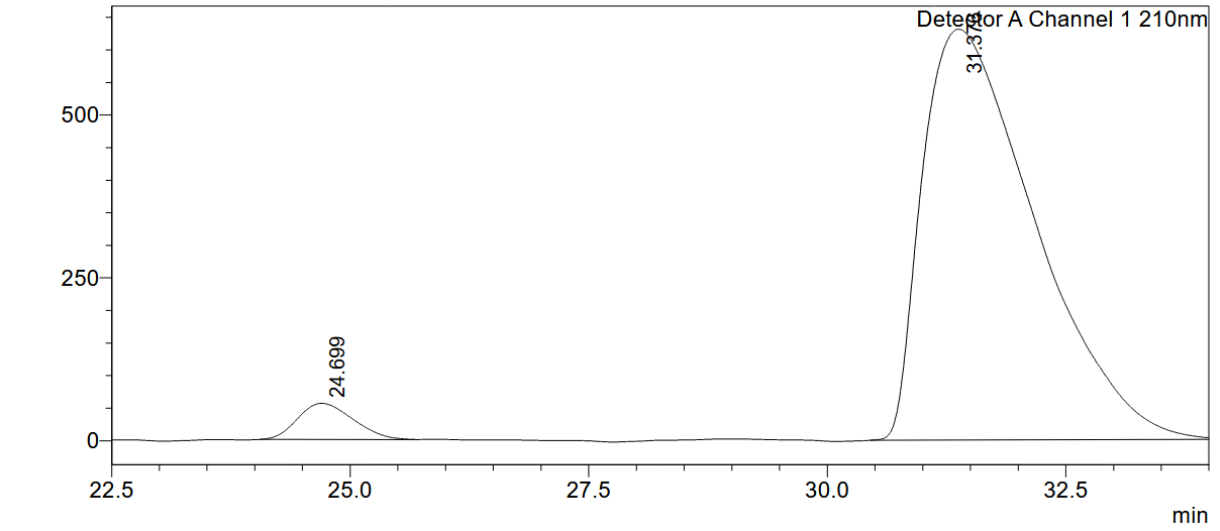


3v

^{19}F (376 MHz, $CDCl_3$)

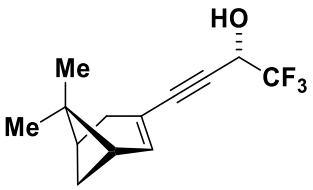


Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	23.838	24907725	540843	50.109		M	
2	30.254	24798984	372944	49.891		M	
Total		49706709	913787				



Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	24.699	2238774	55631	4.150		M	
2	31.376	51702853	630770	95.850		M	
Total		53941627	686401				

(2*S*)-4-((1*S*)-6,6-dimethylbicyclo[3.1.1]hept-2-en-3-yl)-1,1,1-trifluorobut-3-yn-2-ol (3w)



Alkyne **1w** (43.9 mg, 0.30 mmol, 150 mol%) was subjected to modified reaction conditions (48 h, 100 °C) at 2.5 mol% catalyst loading. Upon flash column chromatography (SiO_2: 1:24 EtOAc:hexanes), the title compound **3w** was isolated as a viscous, red-orange oil in 69% yield (33.7 mg, 0.14 mmol, >20:1 dr).

TLC (SiO_2): R_f = 0.5 (1:5 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 6.32 – 5.86 (m, 1H), 4.80 (dq, *J* = 8.3, 5.8 Hz, 1H), 2.51 – 2.30 (m, 4H), 2.27 (td, *J* = 5.6, 1.4 Hz, 1H), 2.12 (ttd, *J* = 5.9, 2.8, 1.3 Hz, 1H), 1.30 (s, 3H), 1.23 (d, *J* = 9.1 Hz, 1H), 0.88 (s, 3H) ppm.

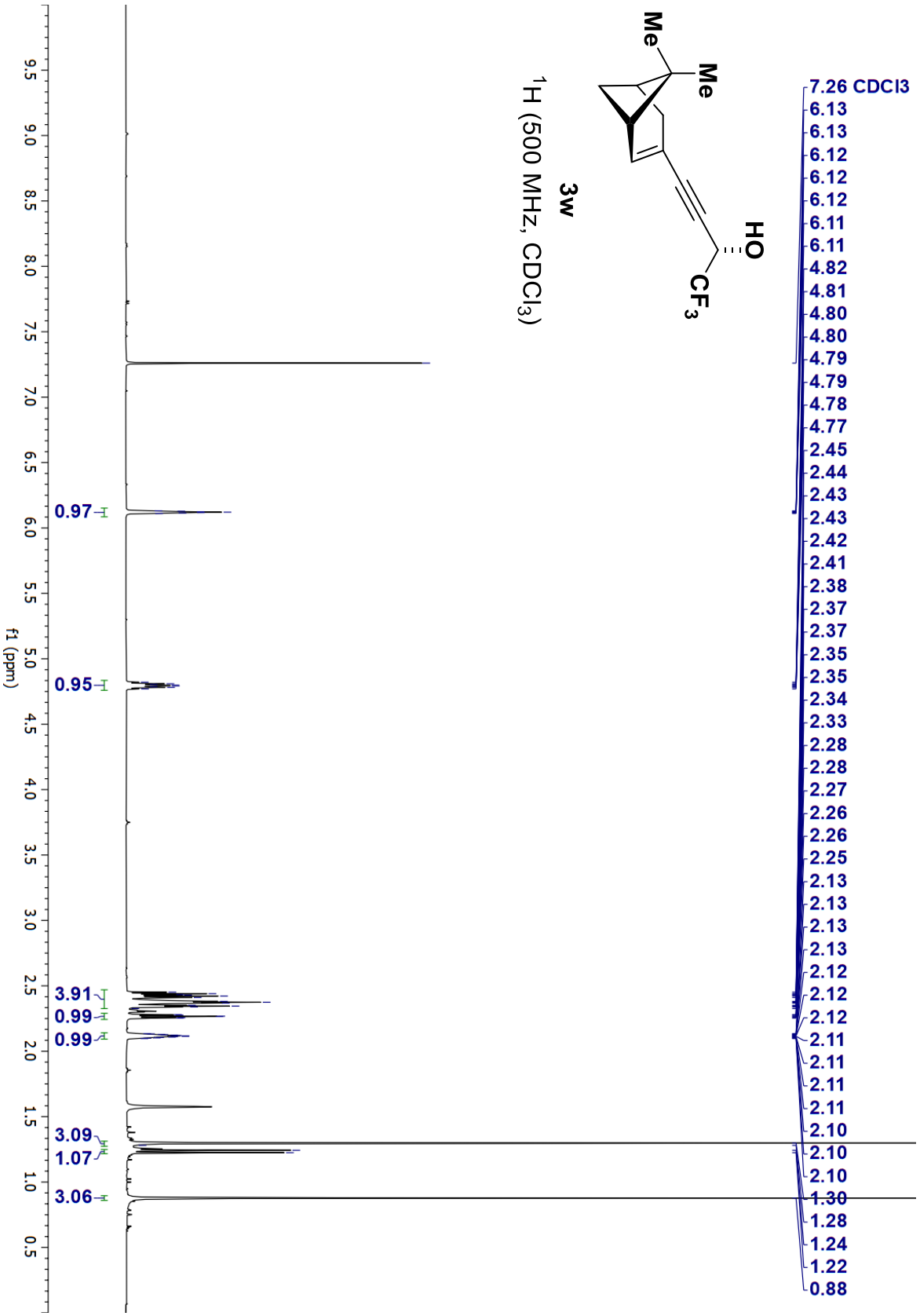
^{13}C NMR (126 MHz, $CDCl_3$): δ 134.4, 128.4, 122.9 (q, *J* = 281.7 Hz), 88.7, 80.2 (q, *J* = 2.5 Hz), 63.2 (q, *J* = 36.3 Hz), 46.6, 40.2, 38.1, 32.3, 31.5, 26.1, 21.1 ppm.

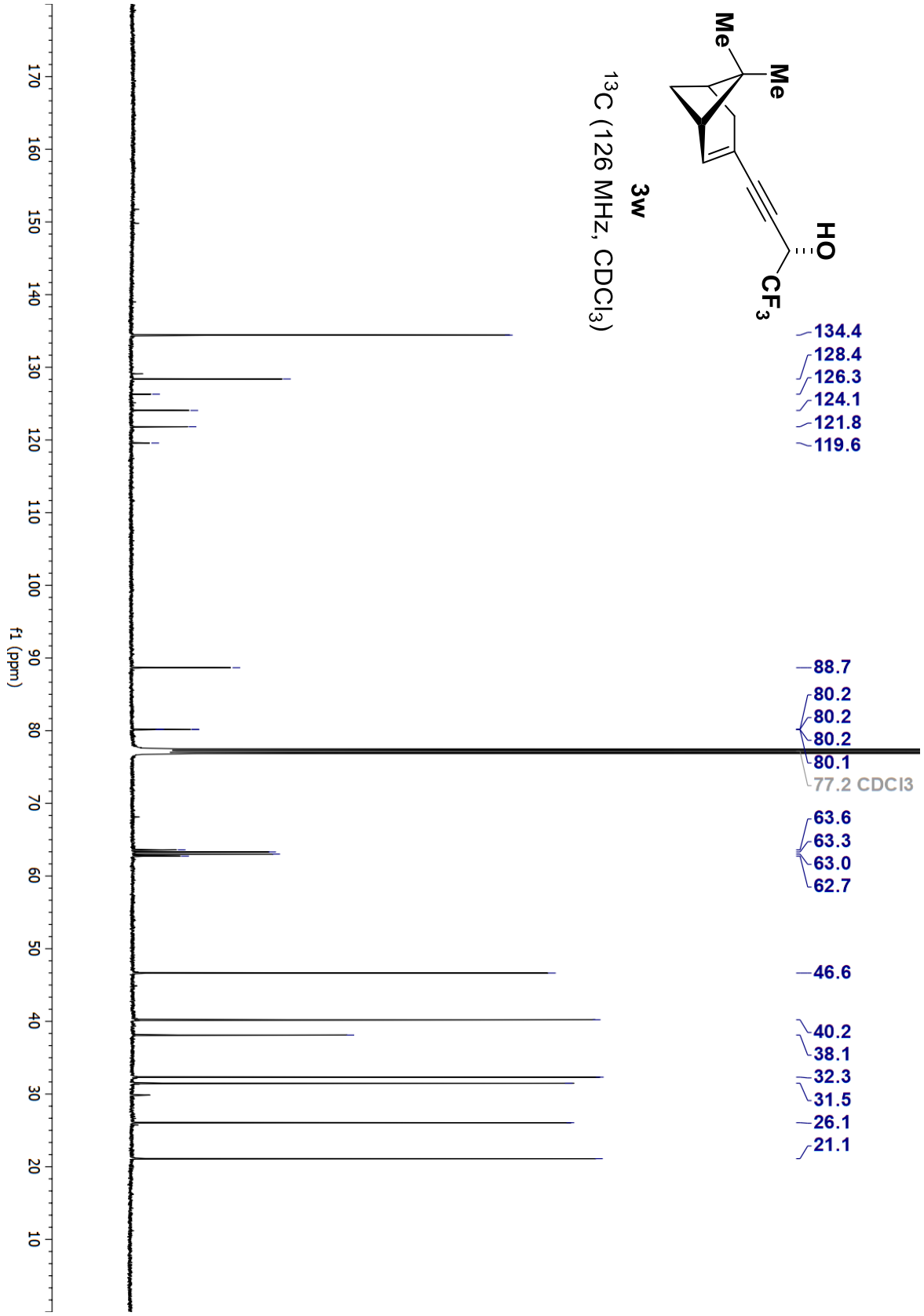
^{19}F NMR (376 MHz, $CDCl_3$): δ -79.5 (d, *J* = 5.6 Hz) ppm.

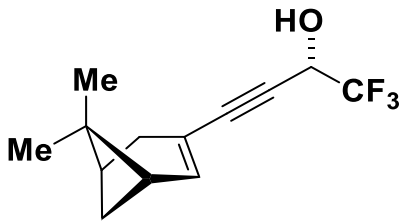
HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_{13}H_{16}F_3O^+$: 245.1148; found = 245.1156.

FTIR (neat): 3359, 2926, 1705, 1369, 1268, 1174, 1133, 1074, 955, 835 cm^{-1}.

$[\alpha]_D^{20}$ = +40° ($CHCl_3$, c = 1.0).


3w
^{1}H (500 MHz, $CDCl_3$)
Me
Me
HO
CF_3
7.26 CDCl3
6.13
6.13
6.12
6.12
6.12
6.11
6.11
4.82
4.81
4.80
4.80
4.79
4.79
4.78
4.77
2.45
2.44
2.43
2.43
2.42
2.41
2.38
2.37
2.37
2.35
2.35
2.34
2.33
2.28
2.28
2.27
2.26
2.26
2.25
2.13
2.13
2.13
2.13
2.12
2.12
2.12
2.11
2.11
2.11
2.11
2.10
2.10
2.10
1.30
1.28
1.24
1.22
0.88
0.97
0.95
3.91
0.99
0.99
3.09
1.07
3.06
f1 (ppm)

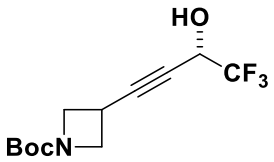

Me
Me
HO
CF3
3w
13C (126 MHz, CDCl3)
134.4
128.4
126.3
124.1
121.8
119.6
88.7
80.2
80.2
80.2
80.1
77.2 CDCl3
63.6
63.3
63.0
62.7
46.6
40.2
38.1
32.3
31.5
26.1
21.1
f1 (ppm)



3w

^{19}F (376 MHz, $CDCl_3$)

tert-butyl (*S*)-3-(4,4,4-trifluoro-3-hydroxybut-1-yn-1-yl)azetidine-1-carboxylate (3x)



Alkyne **1x** (38.1 mg, 0.21 mmol, 105 mol%) was subjected to modified reaction conditions (100 °C, 48 h) at 2.5 mol% catalyst loading. Upon flash column chromatography (SiO_2: 2:9 EtOAc:hexanes), the title compound **3x** was isolated as a pale-yellow oil in 65% yield (36.4 mg, 0.13 mmol, 97% ee).

TLC (SiO_2): R_f = 0.3 (1:2 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 4.80 – 4.58 (m, 1H), 4.16 (t, *J* = 8.5 Hz, 2H), 3.95 (dd, *J* = 8.4, 6.2 Hz, 2H), 3.62 – 3.04 (m, 2H), 1.44 (s, 9H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ 156.2, 122.9 (q, *J* = 282.0 Hz), 88.4 – 88.0 (m), 80.5 – 80.3 (m), 76.0 – 75.7 (m), 62.6 (q, *J* = 36.6 Hz), 55.1 (bs), 28.5, 19.2 ppm.

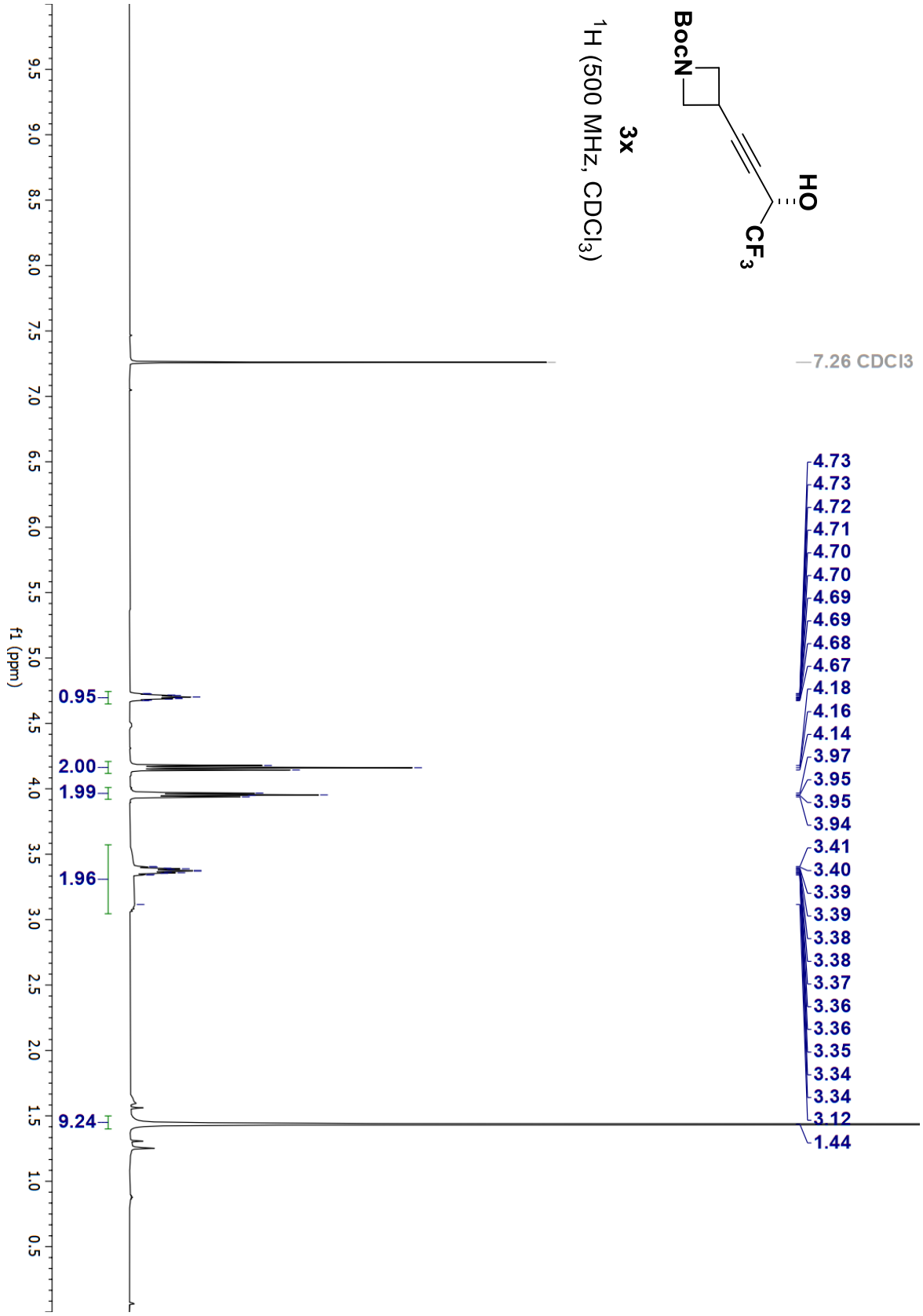
^{19}F NMR (376 MHz, $CDCl_3$): δ -79.5 (d, *J* = 6.0 Hz) ppm.

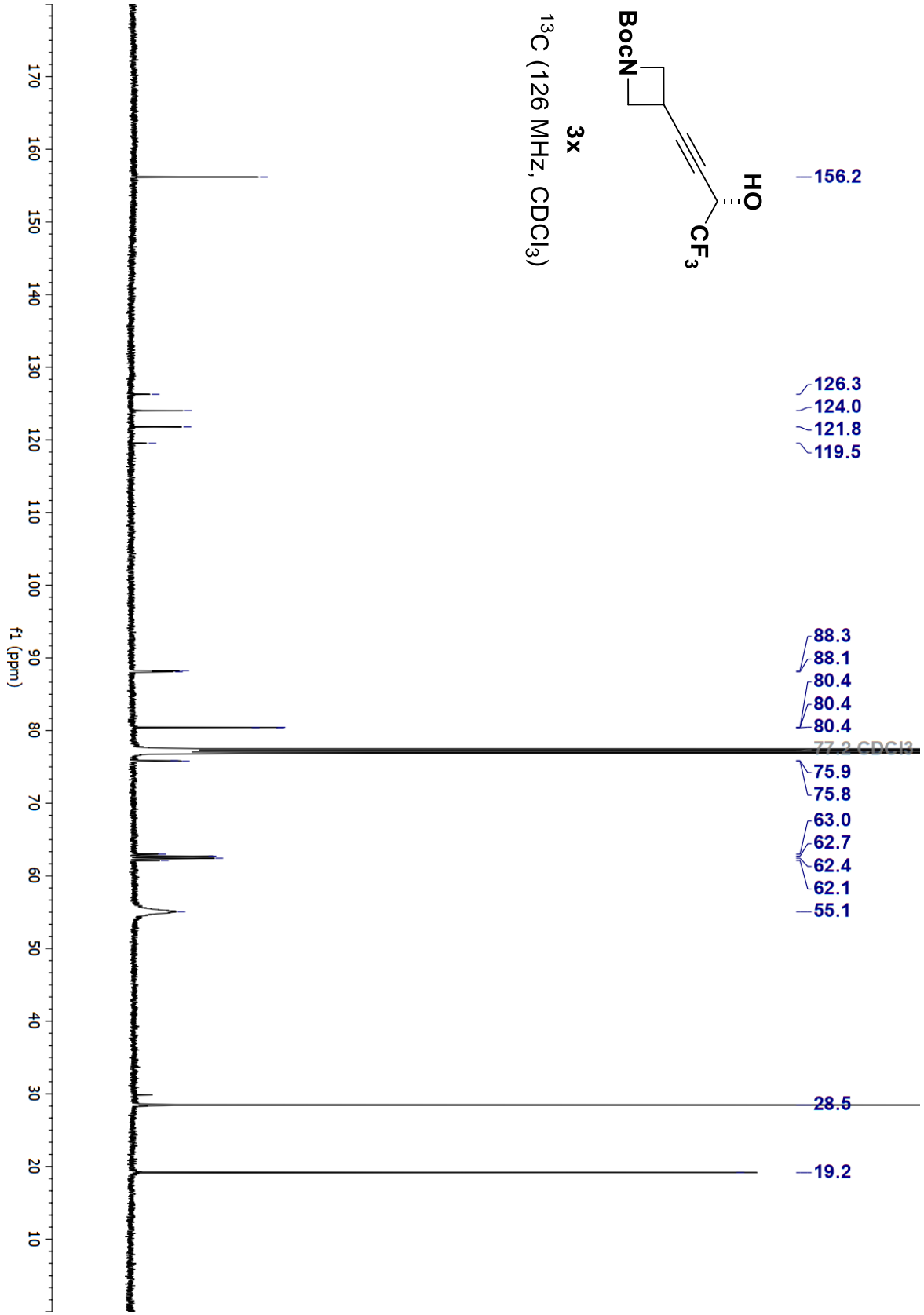
HRMS (ESI(+)): m/z [M+Na^+] calcd. for $C_{12}H_{16}F_3NNaO_3^+$: 302.0974; found = 302.0983.

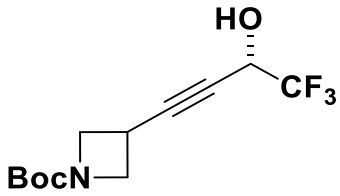
FTIR (neat): 3314, 2978, 1674, 1479, 1418, 1368, 1269, 1171, 1130, 1081 cm^{-1}.

HPLC (The product **3x** was derivatized to give its respective *o*-methoxybenzoyl ester prior to HPLC analysis. CHIRALPAK AD-H hexanes:2-PrOH = 98:2, 1.0 mL/min, 210 nm): ee = 97%.

$[\alpha]_D^{20}$ = +5° ($CHCl_3$, c = 1.0).

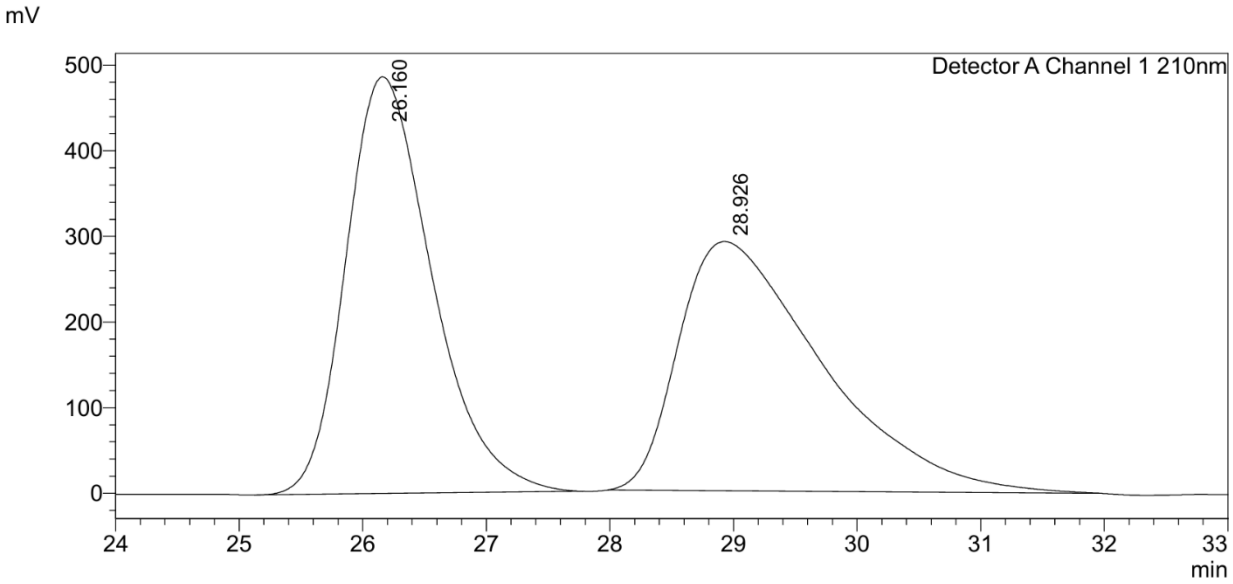

3x
^{1}H (500 MHz, CDCl$_3$)
BocN
HO
CF$_3$
7.26 CDCl3
4.73
4.73
4.72
4.71
4.70
4.70
4.69
4.69
4.68
4.67
4.18
4.16
4.14
3.97
3.95
3.95
3.94
3.41
3.40
3.39
3.39
3.38
3.38
3.37
3.36
3.36
3.35
3.34
3.34
3.12
1.44
0.95
2.00
1.99
1.96
9.24
f1 (ppm)


3x
^{13}C (126 MHz, CDCl$_3$)
BocN
HO
CF$_3$
156.2
126.3
124.0
121.8
119.5
88.3
88.1
80.4
80.4
80.4
77.2 CDCl3
75.9
75.8
63.0
62.7
62.4
62.1
55.1
28.5
19.2
f1 (ppm)

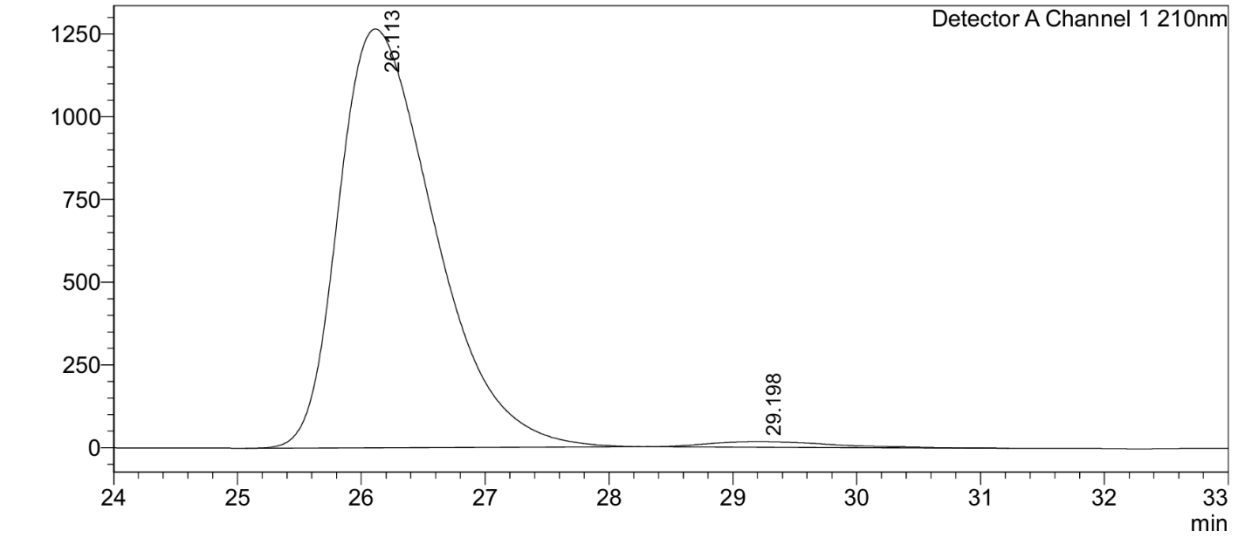


3x

^{19}F (376 MHz, $CDCl_3$)

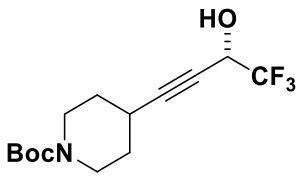


Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	26.160	23609851	486580	50.137		M	
2	28.926	23480922	290936	49.863		M	
Total		47090773	777516				



Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	26.113	68244388	1265292	98.298		M	
2	29.198	1181954	16977	1.702		M	
Total		69426342	1282269				

tert-butyl (*S*)-4-(4,4,4-trifluoro-3-hydroxybut-1-yn-1-yl)piperidine-1-carboxylate (3y)



Alkyne **1y** (43.9 mg, 0.21 mmol, 105 mol%) was subjected to modified reaction conditions (100 °C, 48 h) at 5 mol% catalyst loading. Upon flash column chromatography (SiO_2: 15:85 EtOAc:hexanes), the title compound **3y** was isolated as a clear oil in 67% yield (41.2 mg, 0.13 mmol, 99% ee).

TLC (SiO_2): R_f = 0.4 (1:5 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 4.67 (dq, *J* = 7.8, 3.7 Hz, 1H), 3.72 – 3.50 (m, 2H), 3.31 – 3.06 (m, 2H), 3.07 – 2.90 (m, 1H), 2.69 – 2.60 (m, 1H), 1.88 – 1.68 (m, 2H), 1.65 – 1.51 (m, 2H), 1.45 (s, 9H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ 154.9, 123.0 (q, *J* = 281.6 Hz), 90.7, 80.0, 74.4 – 73.8 (m), 62.6 (q, *J* = 36.2 Hz), 44.8 – 40.5 (m), 30.9, 28.6, 26.9 ppm.

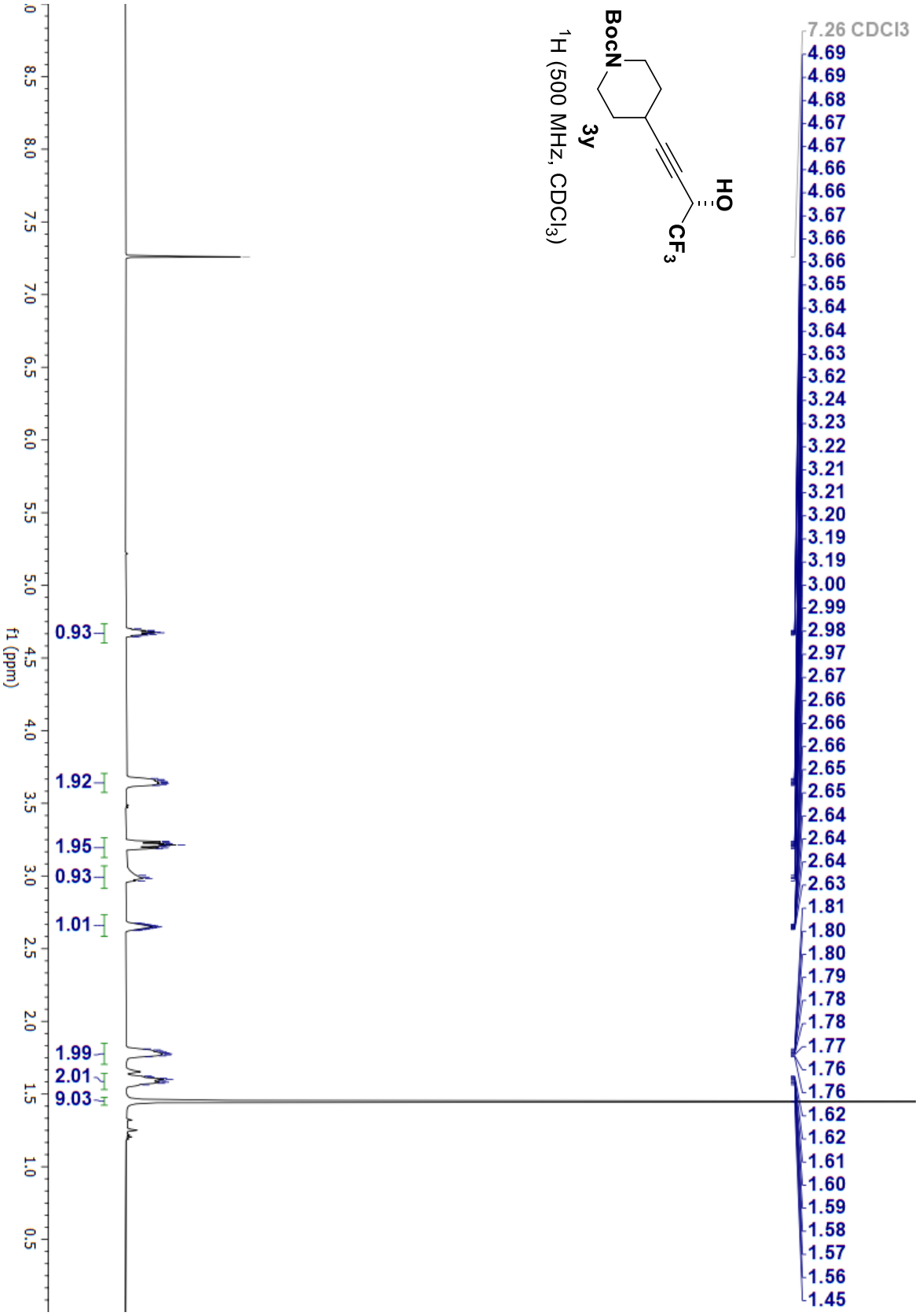
^{19}F NMR (471 MHz, $CDCl_3$): δ -79.8 (d, *J* = 5.9 Hz) ppm.

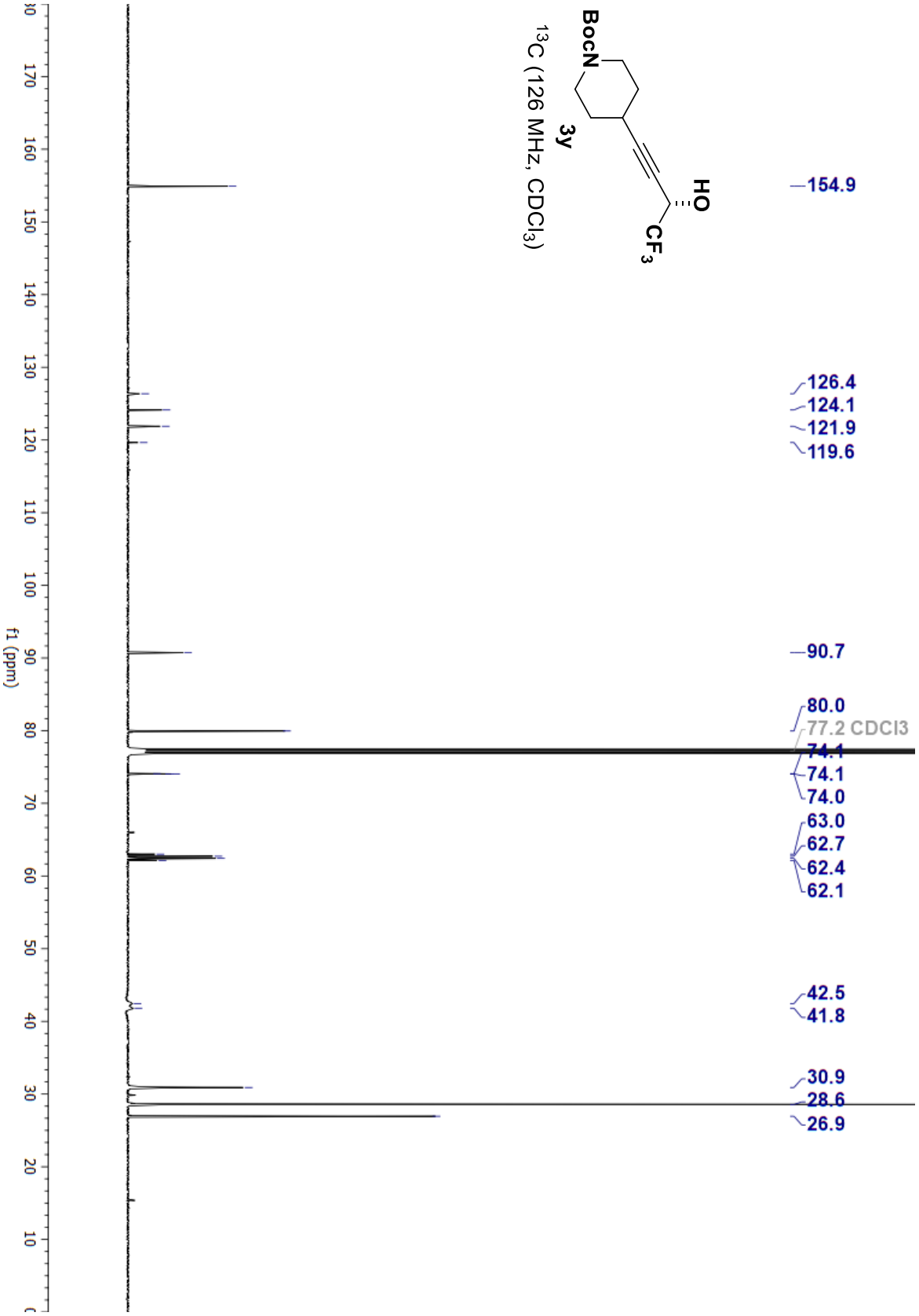
HRMS (ESI(+)): m/z [M+Na^+] calcd. for $C_{14}H_{20}F_3NNaO_3^+$: 330,1287; found = 330.1293.

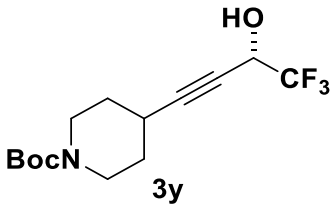
FTIR (neat): 3337, 2930, 2247, 1683, 1430, 1130, 1071, 708, 529 cm^{-1}.

HPLC (The product **3y** was derivatized to give its respective benzoyl ester prior to HPLC analysis. CHIRALPAK AD-H, hexanes:2-PrOH = 98:2, 1.0 mL/min, 254 nm): ee = 99%.

$[\alpha]_D^{20}$ = -4° ($CHCl_3$, c = 1.0).

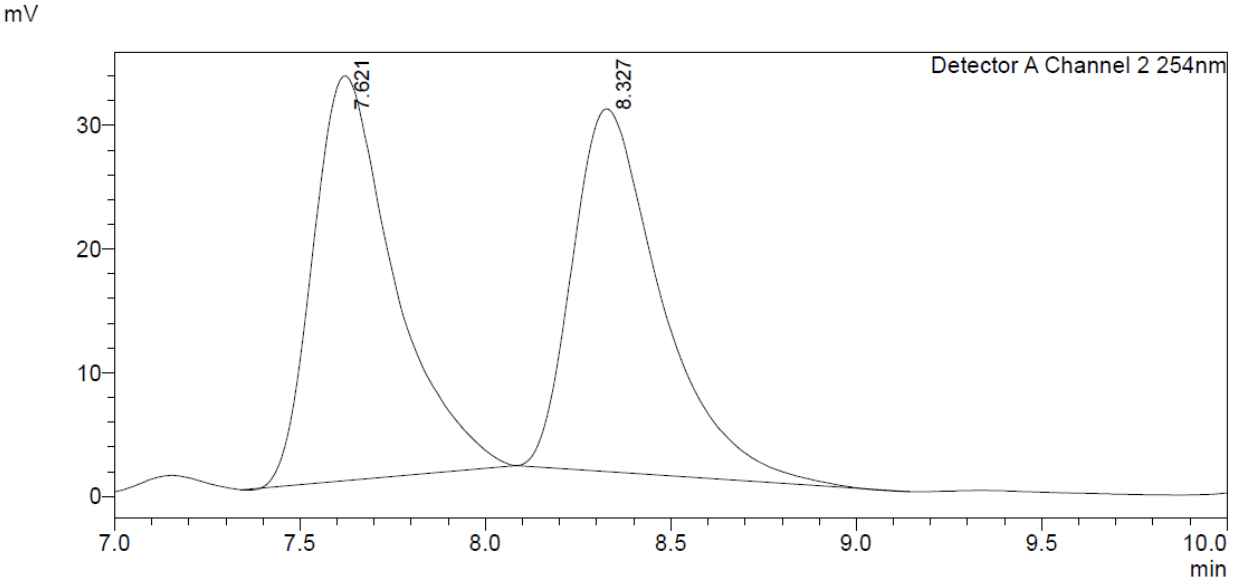

BocN
HO
CF3
3y
1H (500 MHz, CDCl3)
7.26 CDCl3
4.69
4.69
4.68
4.67
4.67
4.66
4.66
3.67
3.66
3.66
3.65
3.64
3.64
3.63
3.62
3.24
3.23
3.22
3.21
3.21
3.20
3.19
3.19
3.00
2.99
2.98
2.97
2.67
2.66
2.66
2.66
2.65
2.65
2.64
2.64
2.64
2.63
1.81
1.80
1.80
1.79
1.78
1.78
1.77
1.76
1.76
1.62
1.62
1.61
1.60
1.59
1.58
1.57
1.56
1.45
0.93
1.92
1.95
0.93
1.01
1.99
2.01
9.03
f1 (ppm)


BocN
HO
CF3
3y
13C (126 MHz, CDCl3)
154.9
126.4
124.1
121.9
119.6
90.7
80.0
77.2 CDCl3
74.1
74.1
74.0
63.0
62.7
62.4
62.1
42.5
41.8
30.9
28.6
26.9
f1 (ppm)



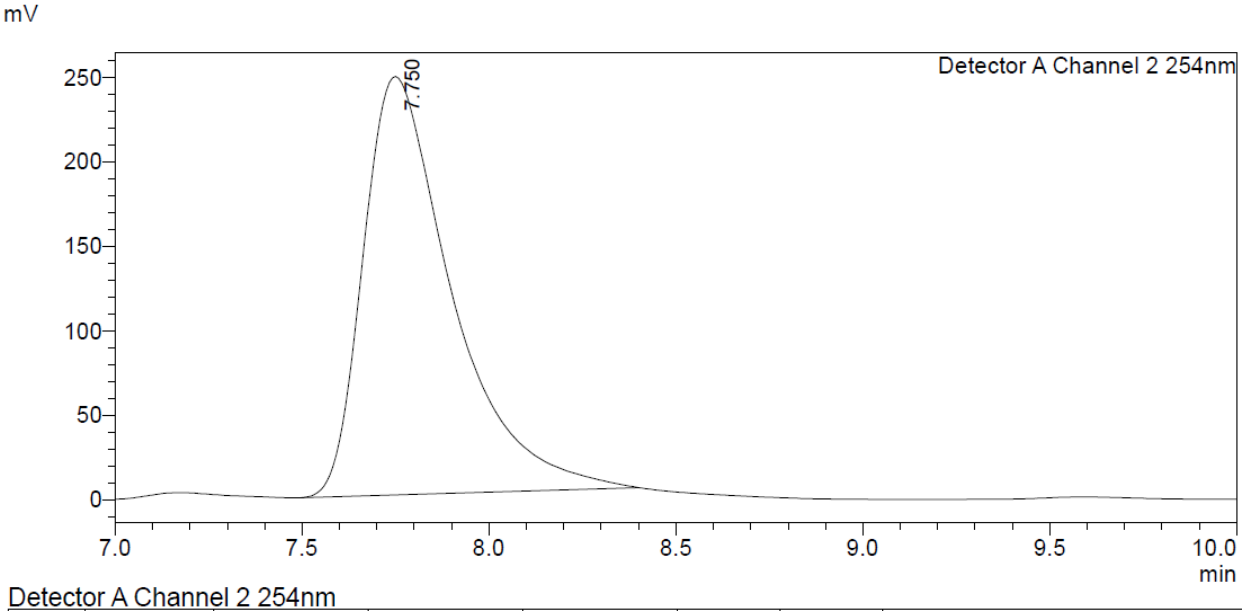
3y

^{19}F (471 MHz, $CDCl_3$)



Detector A Channel 2 254nm

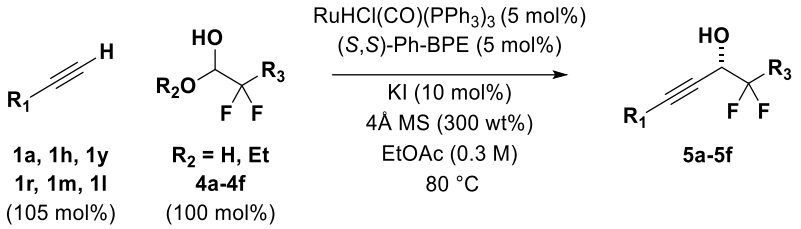
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	7.621	499458	32717	50.493		M	
2	8.327	489712	29335	49.507		M	
Total		989170	62052				



Detector A Channel 2 254nm

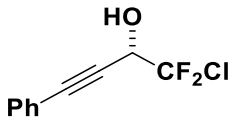
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	7.750	4082493	247705	100.000		M	
Total		4082493	247705				

VII. Products 5a-5f



General Procedure C: A pressure tube equipped with a magnetic stir bar was charged with $RuHCl(CO)(PPh_3)_3$ (9.5 mg, 0.01 mmol, 5 mol%), (*S*,*S*)-Ph-BPE (5.1 mg, 0.01 mmol, 5 mol%), KI (3.2 mg, 0.02 mmol, 10 mol%), 4Å molecular sieves (300 wt%), and ethyl acetate (0.67 mL, 0.3 M) under air. The tube was sealed with a PTFE-lined cap, placed in an oil bath and was allowed to stir at 80 ºC. After 15 minutes, the reaction mixture was allowed to reach ambient temperature. The cap was removed from the tube and the respective terminal alkyne **1** (0.21 mmol, 105 mol%) and difluoroaldehyde **4** (0.2 mmol, 100 mol%) were added. The tube was resealed with the cap, placed in an oil bath and was allowed to stir for 24 hours at 80 ºC. The reaction mixture was allowed to reach ambient temperature and the residue was subjected to flash column chromatography (SiO_2) under the noted conditions to furnish products **5a-5f**.

(*S*)-1-chloro-1,1-difluoro-4-phenylbut-3-yn-2-ol (5a)



Alkyne **1a** (23 μL, 0.21 mmol, 105 mol%) and 2-chloro-2,2-difluoroacetaldehyde hydrate **4a** (75 wt% in H_2O, 34.5 mg, 0.20 mmol) were subjected to standard reaction conditions (80 °C, 24 h) at 5 mol% catalyst loading. Upon flash column chromatography (SiO_2: 5:95–10:90 EtOAc:hexanes), the title compound **5a** was isolated as a light brown oil in 81% yield (34.2 mg, 0.16 mmol, 99% ee).

TLC (SiO_2): R_f = 0.2 (1:9 EtOAc:hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.45–7.39 (m, 1H), 7.36–7.22 (m, 2H), 4.87 (t, *J* = 6.2 Hz, 1H), 2.86 (s, 1H) ppm.

^{13}C NMR (101 MHz, $CDCl_3$): δ 132.2, 129.6, 128.6, 127.6 (t, *J* = 296.3 Hz), 121.1, 88.2, 81.4 (t, *J* = 3.1 Hz), 67.9 (t, *J* = 32.0 Hz) ppm.

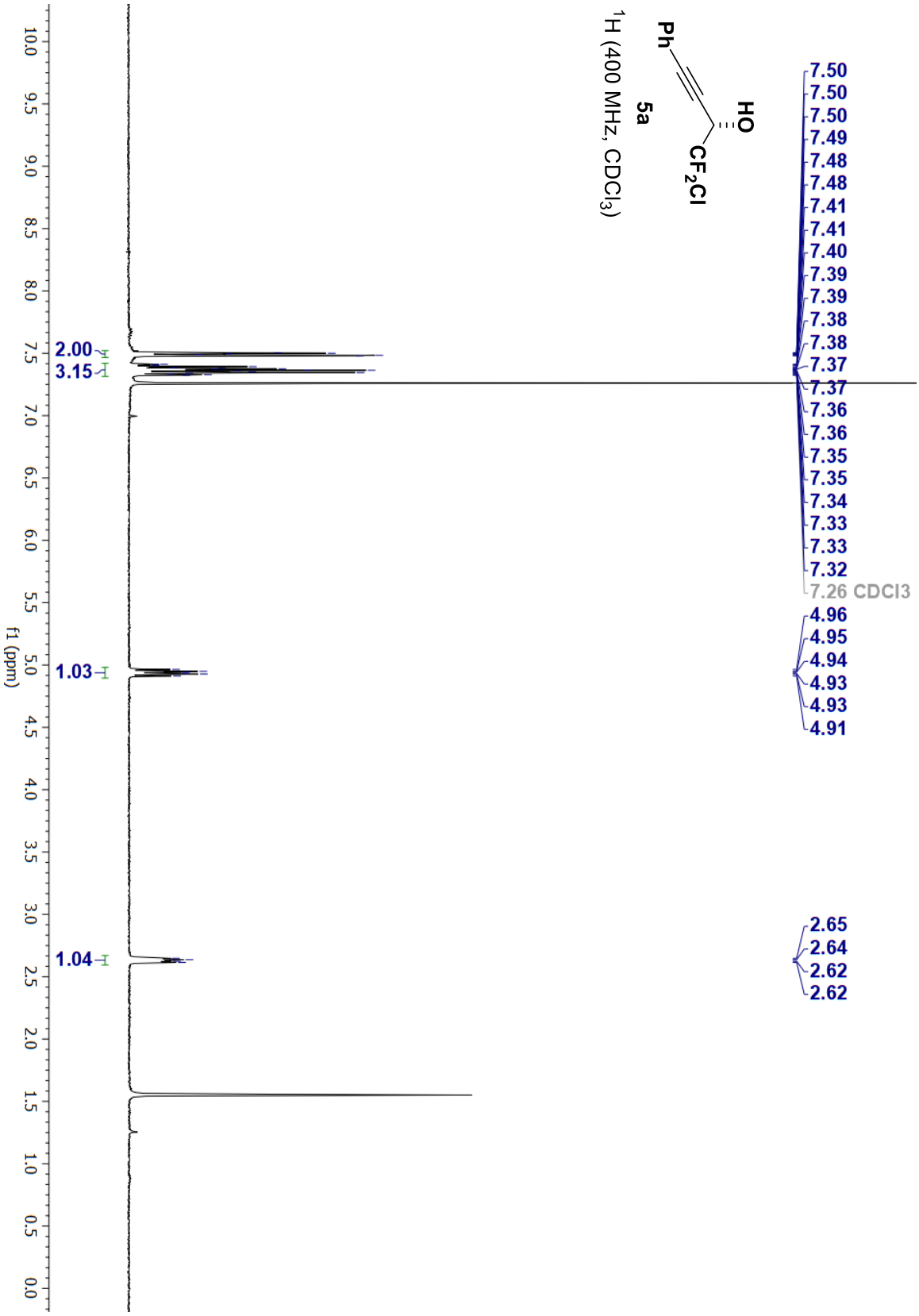
^{19}F NMR (376 MHz, $CDCl_3$): δ -64.7 (dd, *J* = 160.2, 5.7 Hz), -65.2 (dd, *J* = 162.8, 8.2 Hz) ppm. (*Signals display extreme roofing toward each other*.)

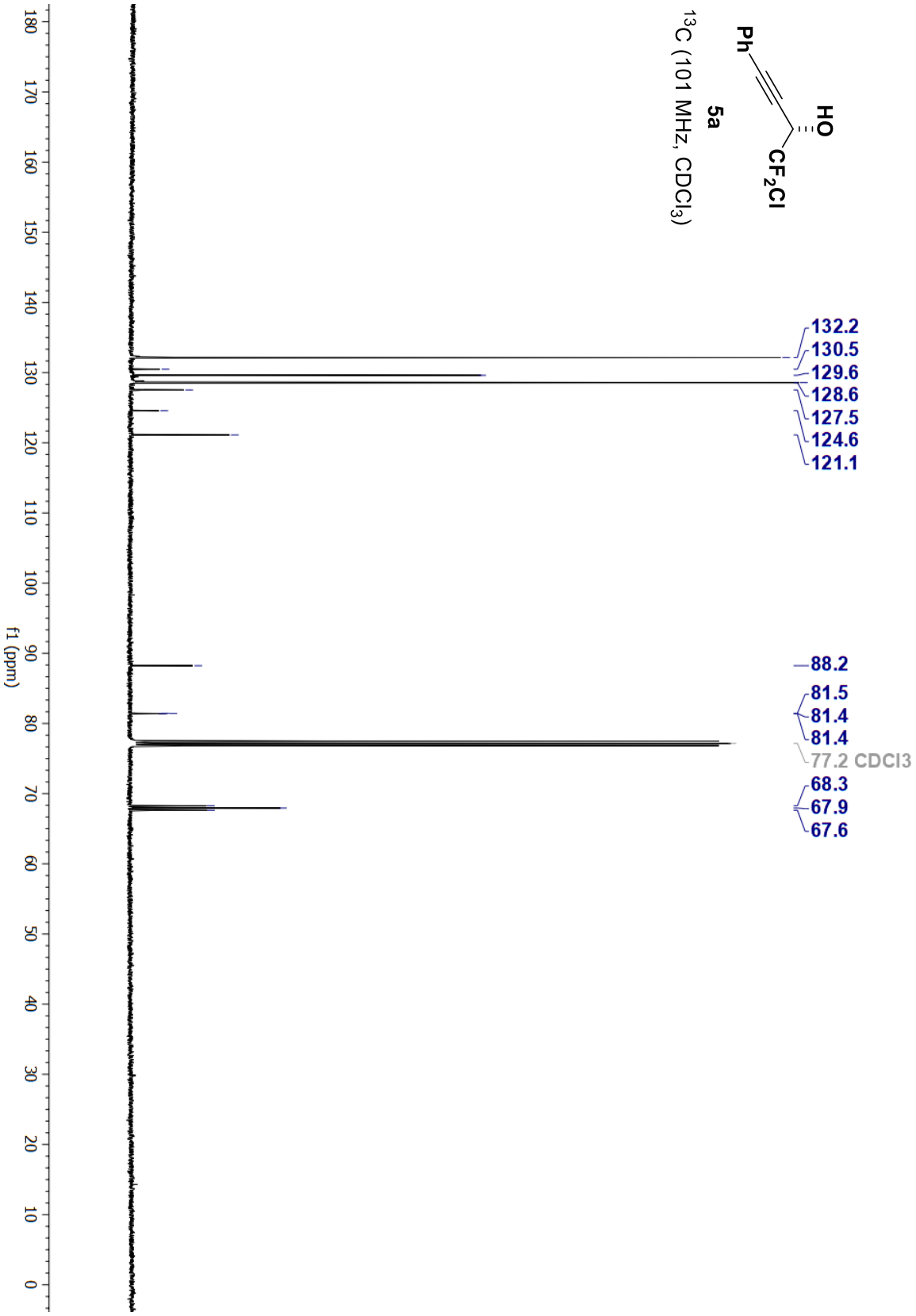
HRMS (FI(+)): m/z [M^+] calcd. for $C_{10}H_7ClF_2O^+$: 216.01480; found = 216.01440.

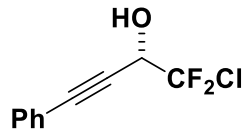
HPLC (CHIRALPAK AD-H, hexanes:2-PrOH = 98:2, 1.0 mL/min, 210 nm): 99% ee.

$[\alpha]_D^{20}$ = -9° (CH_2Cl_2, c = 1.0)

The analytical data are in agreement with the literature.[18]

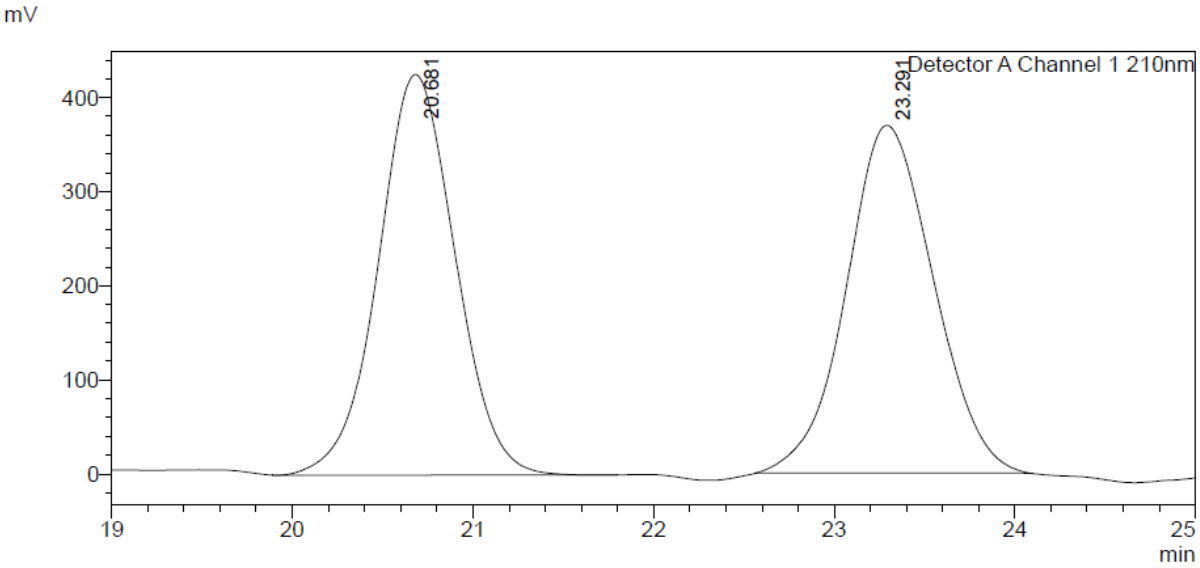

Ph
HO
CF2Cl
5a
1H (400 MHz, CDCl3)
7.50
7.50
7.50
7.49
7.48
7.48
7.41
7.41
7.40
7.39
7.39
7.38
7.38
7.37
7.37
7.36
7.36
7.35
7.35
7.34
7.33
7.33
7.32
7.26 CDCl3
4.96
4.95
4.94
4.93
4.93
4.91
2.65
2.64
2.62
2.62
2.00
3.15
1.03
1.04
f1 (ppm)


Ph
HO
CF2Cl
5a
13C (101 MHz, CDCl3)
132.2
130.5
129.6
128.6
127.5
124.6
121.1
88.2
81.5
81.4
81.4
77.2 CDCl3
68.3
67.9
67.6
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

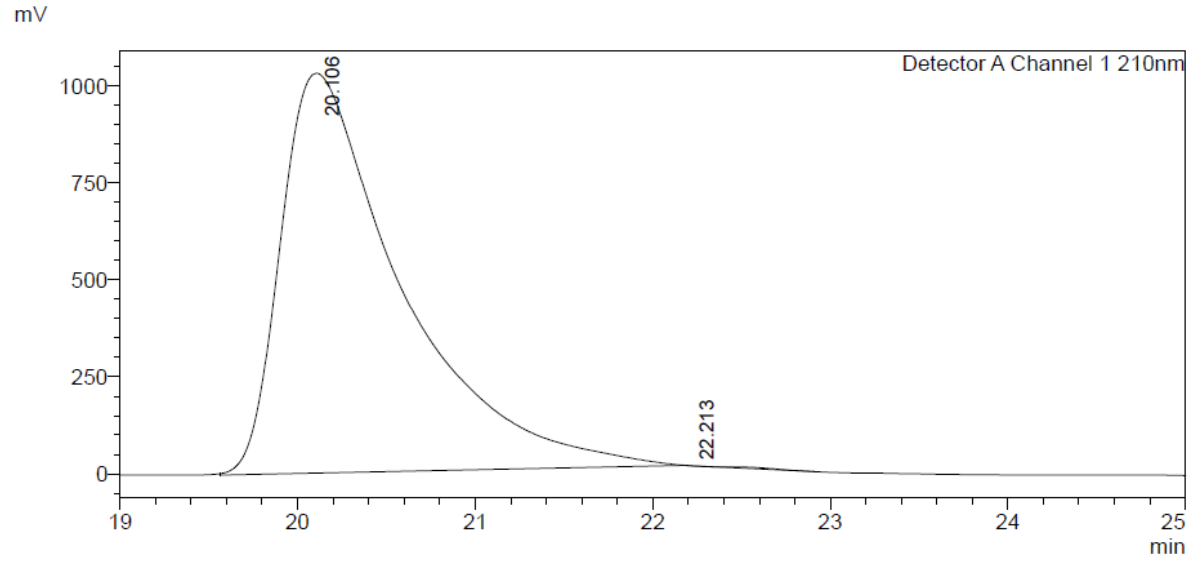


5a

^{19}F (376 MHz, $CDCl_3$)

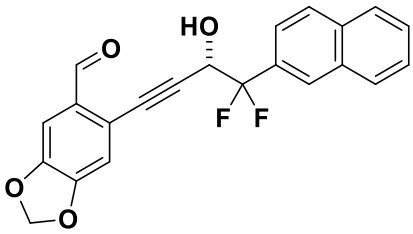


Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	20.681	12600509	425636	50.328		M	
2	23.291	12436110	369622	49.672		M	
Total		25036619	795258				



Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	20.106	48793000	1030340	99.885		M	
2	22.213	56261	6	0.115		M	
Total		48849261	1030347				

(*S*)-6-(4,4-difluoro-3-hydroxy-4-(naphthalen-2-yl)but-1-yn-1-yl)benzo[d][1,3]dioxole-5-carbaldehyde (5b)



Alkyne **1h** (36.6 mg, 0.21 mmol, 105 mol%) and hydrate **4b** (44.8 mg, 0.20 mmol) were subjected to standard reaction conditions (80 °C, 24 h) at 5 mol% catalyst loading. Upon flash column chromatography (SiO_2: 1:5 EtOAc:hexanes), the title compound **5b** was isolated as a yellow solid in 88% yield (67.2 mg, 0.18 mmol, 99% ee).

TLC (SiO_2): R_f = 0.5 (2:3 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 10.13 (d, *J* = 1.2 Hz, 1H), 8.12 (s, 1H), 7.97 – 7.87 (m, 3H), 7.66 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.61 – 7.54 (m, 2H), 7.30 (s, 1H), 6.86 (s, 1H), 6.07 (s, 2H), 5.10 (q, *J* = 8.3 Hz, 1H), 2.49 (t, *J* = 7.4 Hz, 1H) ppm.

^{13}C NMR (151 MHz, $CDCl_3$): δ 189.5, 152.4, 149.4, 134.3, 133.0, 132.5, 130.4 (t, *J* = 25.4 Hz), 128.8, 128.5, 128.0, 127.7, 127.1, 126.7 (t, *J* = 6.9 Hz), 122.9 (t, *J* = 5.7 Hz), 121.5, 119.8 (t, *J* = 249.5 Hz), 112.5, 106.4, 102.7, 89.2 (t, *J* = 4.4 Hz), 83.6, 67.4 (t, *J* = 35.5 Hz) ppm.

^{19}F NMR (471 MHz, $CDCl_3$): δ -105.8 (dd, *J* = 245.7, 7.7 Hz), -106.8 (dd, *J* = 246.1, 9.4 Hz) ppm.

HRMS (ESI(+)): m/z [M+Na^+] calcd. for $C_{22}H_{14}F_2NaO_4^+$: 403.0752; found = 403.0752.

FTIR (neat): 3347, 2918, 1679, 1605, 1502, 1477, 1435, 1408, 1359, 1267, 1224, 1191, 1157, 1127, 1059, 1031 cm^{-1}.

HPLC (CHIRALPAK AD-H, hexanes:2-PrOH = 85:15, 1.0 mL/min, 254 nm): ee = 99%.

$[\alpha]_D^{20}$ = +17° ($CHCl_3$, c = 1.0).

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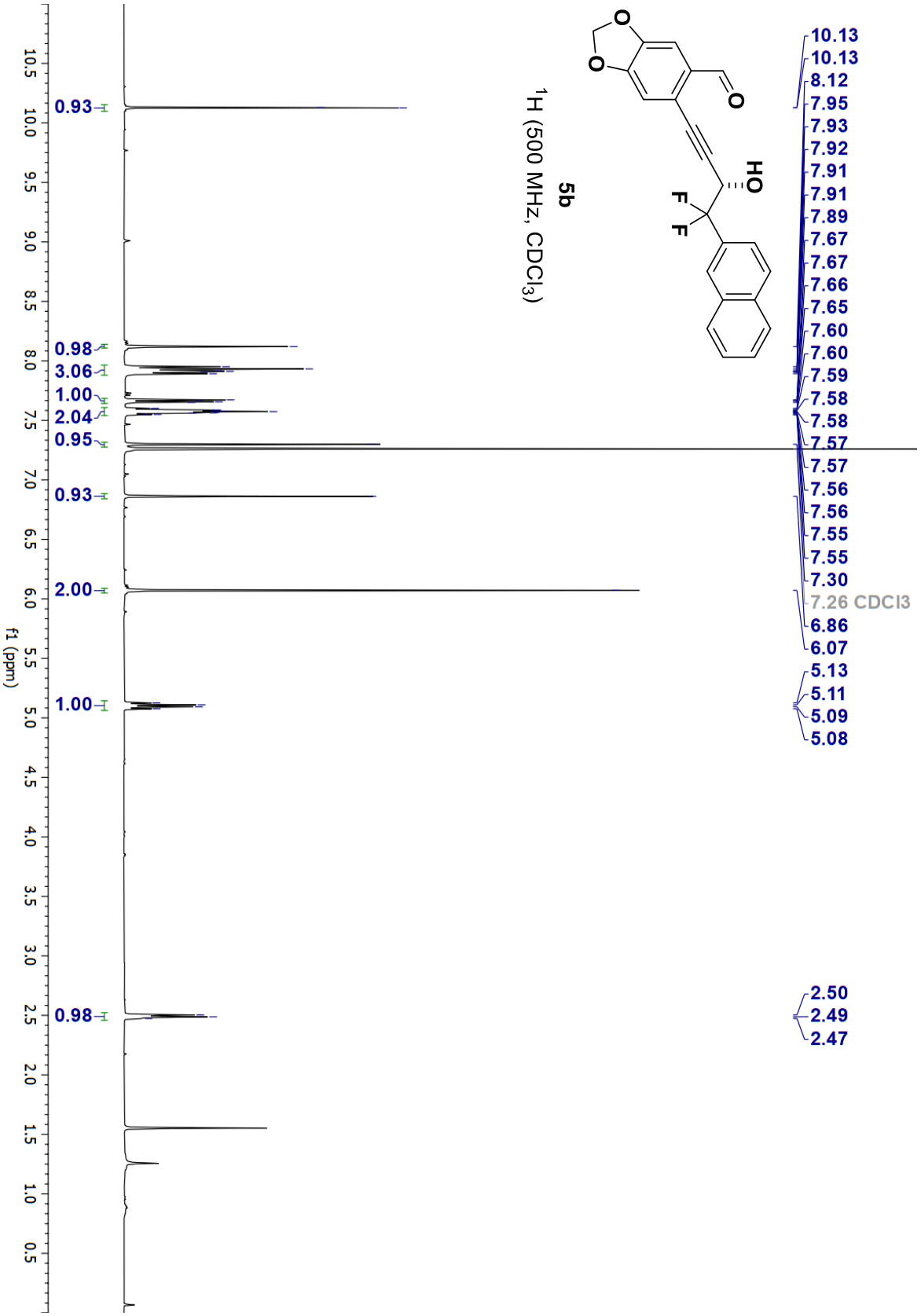
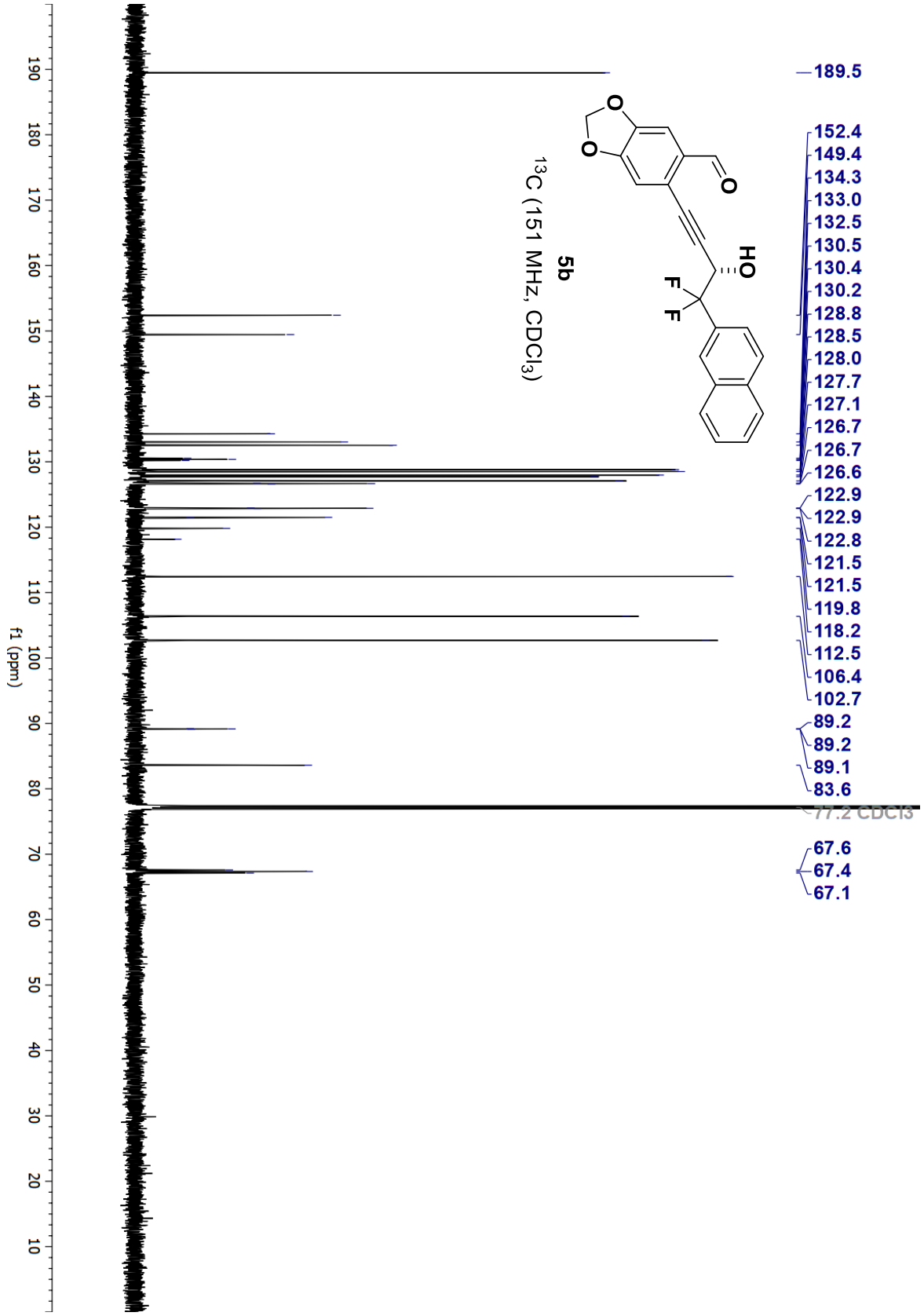
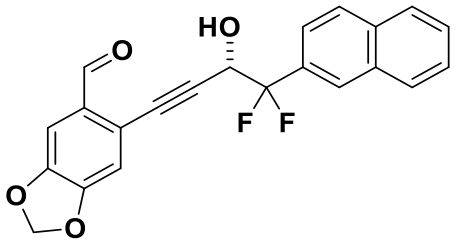
m.p.: 103 °C.

A single crystal suitable for X-Ray analysis was obtained by vapor diffusion using DCM and Pentane.

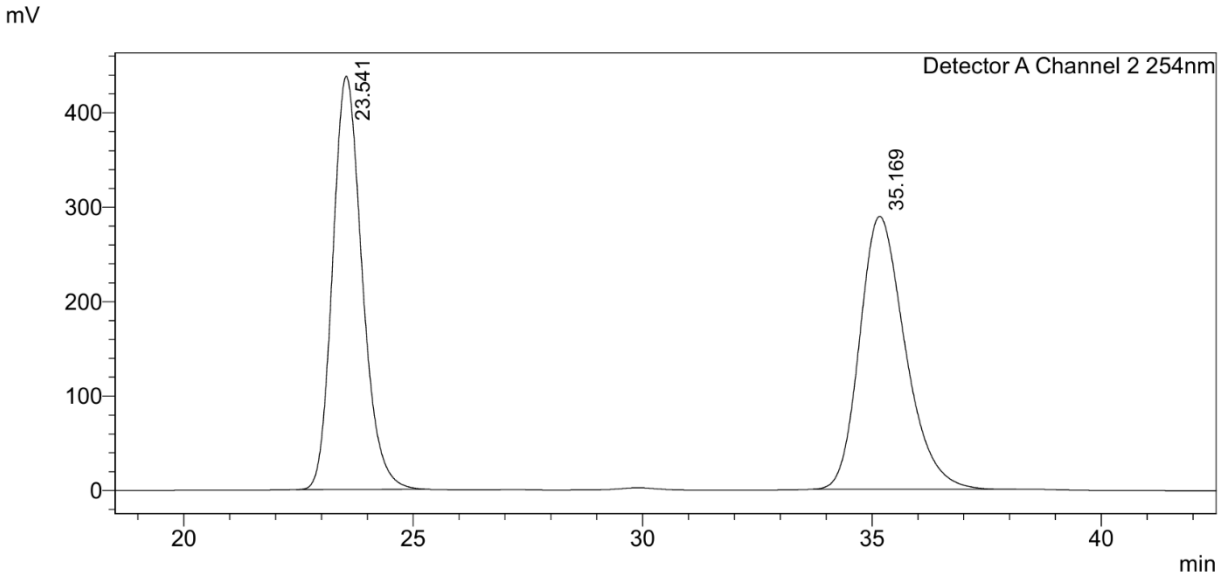

5b
^{1}H (500 MHz, CDCl$_3$)
HO
F
F
O
O
O
10.13
10.13
8.12
7.95
7.93
7.92
7.91
7.91
7.89
7.67
7.67
7.66
7.65
7.60
7.60
7.59
7.58
7.58
7.57
7.57
7.56
7.56
7.55
7.55
7.30
7.26 CDCl3
6.86
6.07
5.13
5.11
5.09
5.08
2.50
2.49
2.47
0.93
0.98
3.06
1.00
2.04
0.95
0.93
2.00
1.00
0.98
f1 (ppm)


5b
^{13}C (151 MHz, CDCl$_3$)
HO
F
F
O
O
O
189.5
152.4
149.4
134.3
133.0
132.5
130.5
130.4
130.2
128.8
128.5
128.0
127.7
127.1
126.7
126.7
126.6
122.9
122.9
122.8
121.5
121.5
119.8
118.2
112.5
106.4
102.7
89.2
89.2
89.1
83.6
77.2 CDCl3
67.6
67.4
67.1
f1 (ppm)



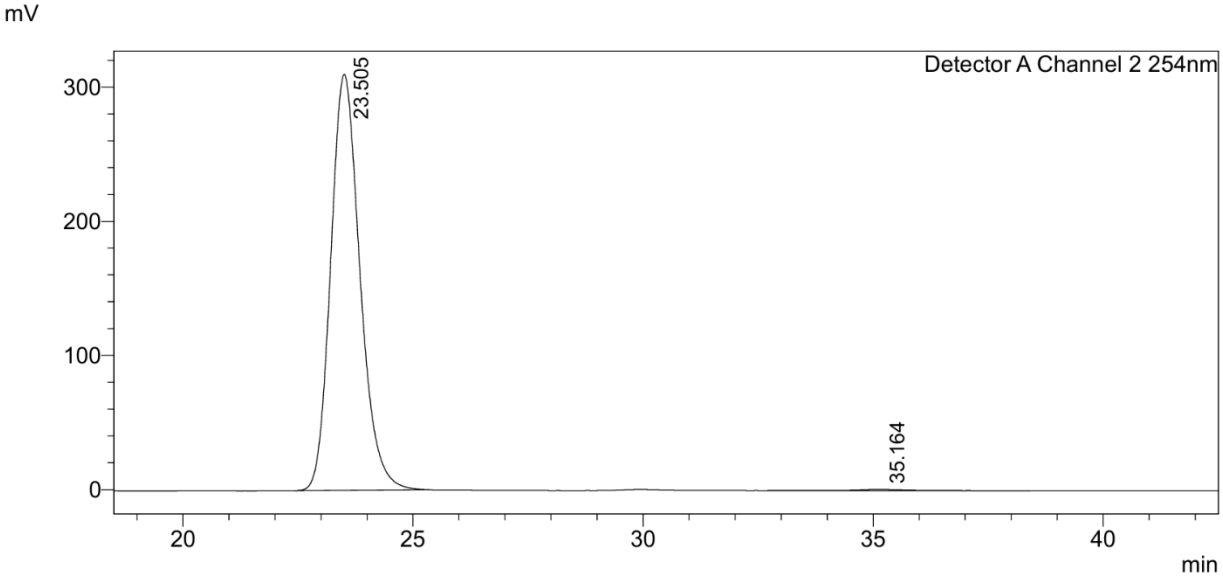
5b

^{19}F (471 MHz, $CDCl_3$)



Detector A Channel 2 254nm

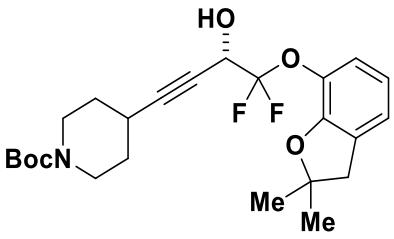
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	23.541	19575455	437802	49.548		M	
2	35.169	19932269	288994	50.452		M	
Total		39507724	726796				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	23.505	13699018	310007	99.539		M	
2	35.164	63415	793	0.461		M	
Total		13762433	310800				

tert-butyl (_S_)-4-(4-((2,2-dimethyl-2,3-dihydrobenzofuran-7-yl)oxy)-4,4-difluoro-3-hydroxybut-1-yn-1-yl)piperidine-1-carboxylate (5c)



Alkyne **1y** (43.9 mg, 0.21 mmol, 105 mol%) and ethyl hemiacetal **4c** (57.7 mg, 0.20 mmol) were subjected to standard reaction conditions (80 °C, 24 h) at 5 mol% catalyst loading. Upon flash column chromatography (SiO_2: 20:80 EtOAc:hexanes), the title compound **5c** was isolated as an orange oil in 67% yield (60.6 mg, 0.13 mmol, 93% ee).

TLC (SiO_2): R_f = 0.4 (1:3) EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.03 (dd, *J* = 14.9, 7.9 Hz, 2H), 6.86 – 6.75 (m, 1H), 4.71 (ddt, *J* = 7.4, 5.4, 2.8 Hz, 1H), 3.61 (ddd, *J* = 12.9, 7.3, 3.3 Hz, 2H), 3.52 (d, *J* = 7.4 Hz, 1H), 3.24 (ddd, *J* = 12.6, 8.0, 3.3 Hz, 2H), 3.05 (s, 2H), 2.63 (ddq, *J* = 7.7, 3.8, 1.9 Hz, 1H), 1.73 (tt, *J* = 7.2, 3.5 Hz, 2H), 1.63 – 1.53 (m, 2H), 1.50 (s, 6H), 1.44 (s, 9H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ 154.8, 150.8, 133.7, 129.7, 123.1, 123.0, 121.7 (t, *J* = 271.0 Hz), 120.6, 89.5, 89.0, 79.6, 75.5 (d, *J* = 2.6 Hz), 63.7 (dd, *J* = 39.0, 35.4 Hz), 43.2, 42.0 (d, *J* = 89.4 Hz), 31.0, 28.6, 28.2 (d, *J* = 4.2 Hz), 26.9 ppm.

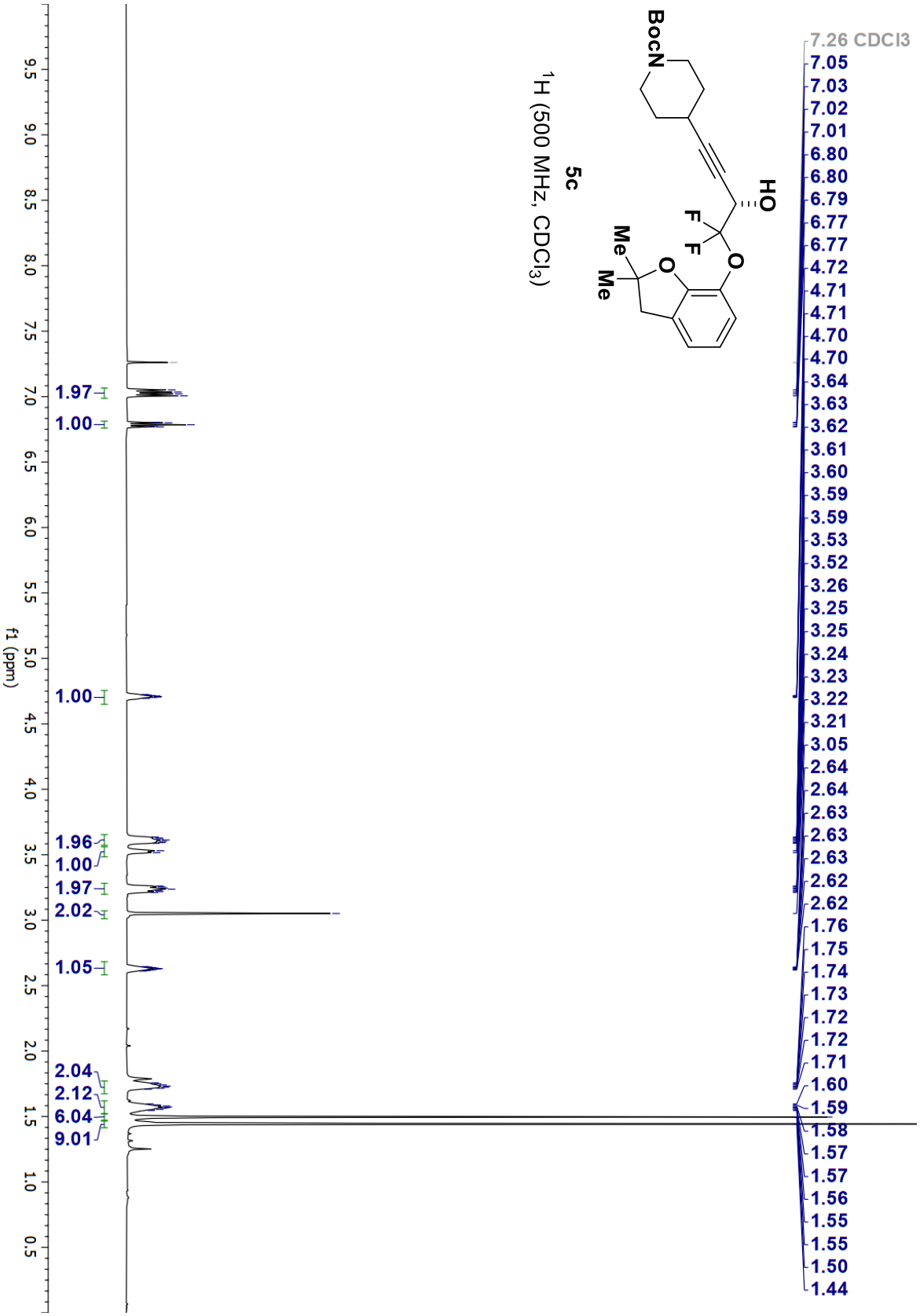
^{19}F NMR (471 MHz, $CDCl_3$): δ -81.0 (d, *J* = 139.9 Hz), -83.8 (d, *J* = 140.3 Hz) ppm.

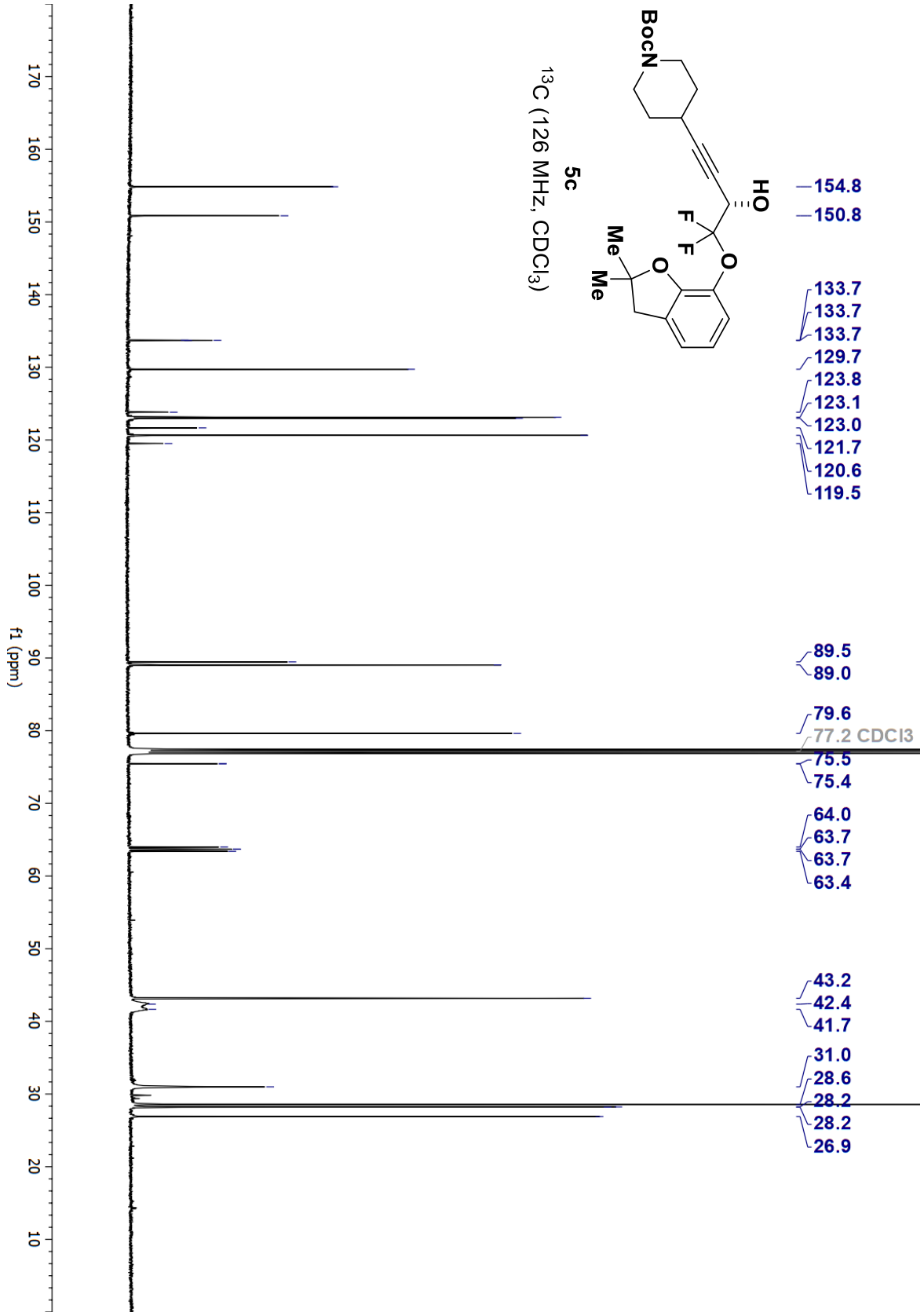
HRMS (ESI(+)): m/z [M+Na^+] calcd. for $C_{24}H_{31}F_2NNaO_5^+$: 474.2063; found = 474.2059.

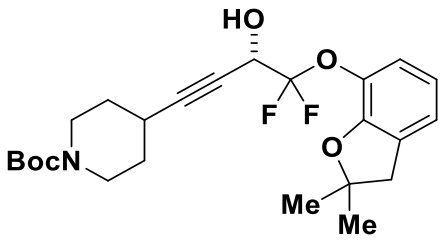
FTIR (neat): 3362, 2971, 2922, 2851, 2248, 2157, 2023, 1979, 1665, 1481, 1465, 1426, 1366, 1297, 1262, 1233, 1154, 1131, 1106, 1071, 1053, 1015, 908, 873, 787, 774, 727, 645, 524 cm^{-1}.

HPLC (PHENOMENEX Cellulose 5, hexanes:2-PrOH = 95:5, 1.0 mL/min, 210 nm): ee = 93%.

$[\alpha]_D^{20}$ = -126° ($CHCl_3$, c = 1.0).

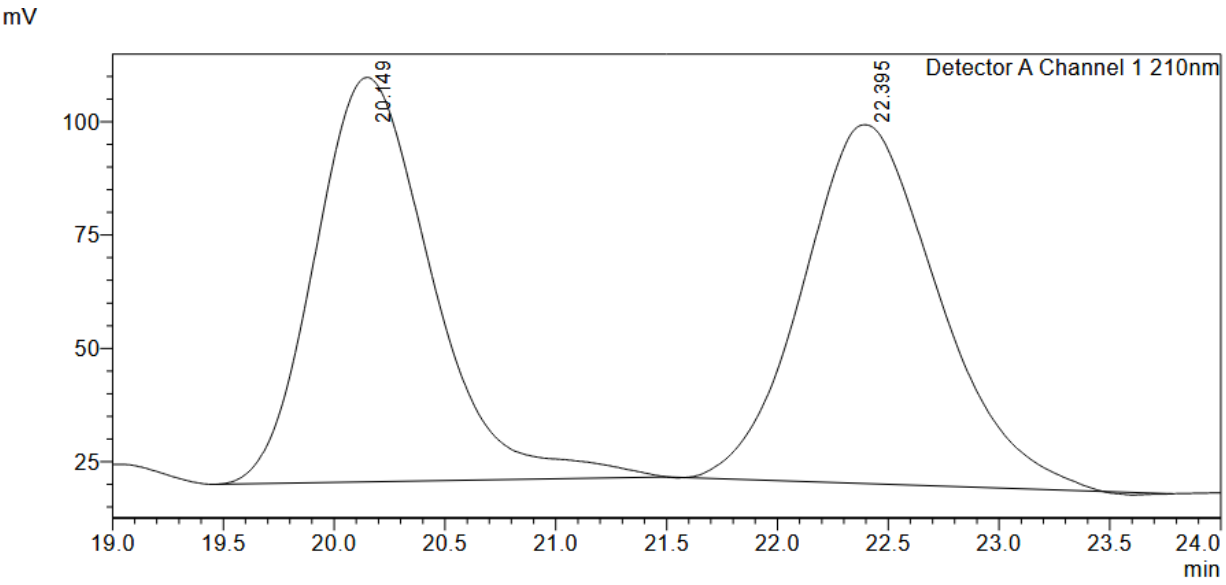

5c
^{1}H (500 MHz, CDCl$_3$)
BocN
HO
F
F
O
O
Me
Me
7.26 CDCl3
7.05
7.03
7.02
7.01
6.80
6.80
6.79
6.77
6.77
4.72
4.71
4.71
4.70
4.70
3.64
3.63
3.62
3.61
3.60
3.59
3.59
3.53
3.52
3.26
3.25
3.25
3.24
3.23
3.22
3.21
3.05
2.64
2.64
2.63
2.63
2.63
2.62
2.62
1.76
1.75
1.74
1.73
1.72
1.72
1.71
1.60
1.59
1.58
1.57
1.57
1.56
1.55
1.55
1.50
1.44
1.97
1.00
1.00
1.96
1.00
1.97
2.02
1.05
2.04
2.12
6.04
9.01
f1 (ppm)


5c
^{13}C (126 MHz, CDCl$_3$)
BocN
HO
F
F
O
O
Me
Me
154.8
150.8
133.7
133.7
133.7
129.7
123.8
123.1
123.0
121.7
120.6
119.5
89.5
89.0
79.6
77.2 CDCl3
75.5
75.4
64.0
63.7
63.7
63.4
43.2
42.4
41.7
31.0
28.6
28.2
28.2
26.9
f1 (ppm)

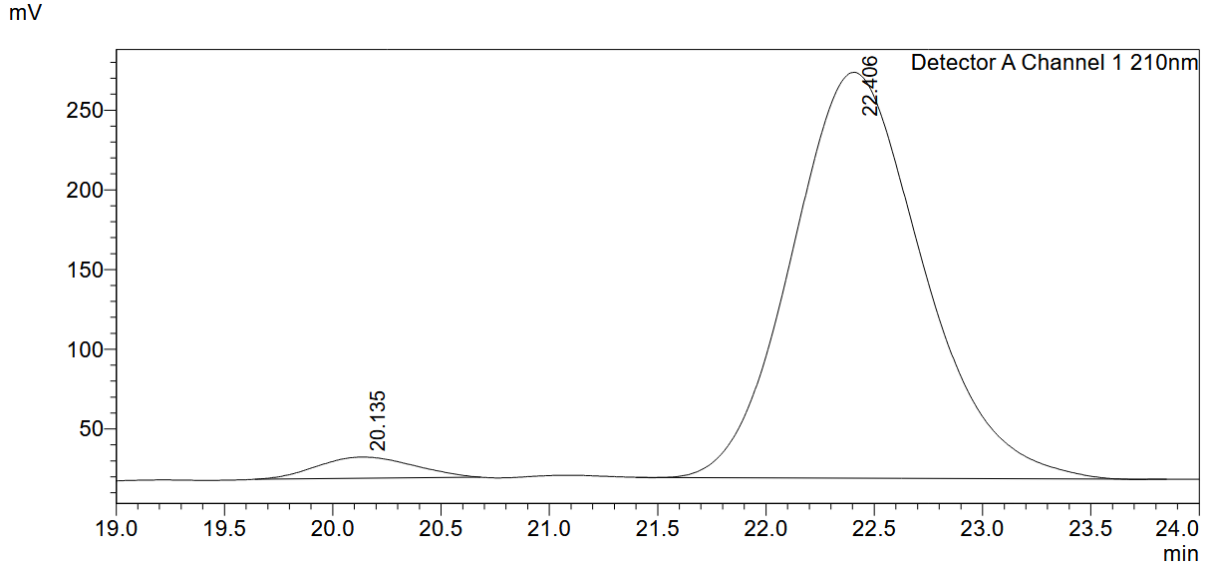


5f

^{19}F (471 MHz, $CDCl_3$)

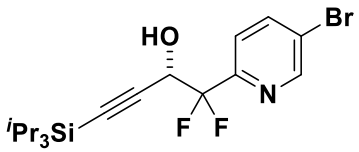


Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	20.149	3272966	89216	49.271		M	
2	22.395	3369777	79162	50.729		M	
Total		6642743	168379				



Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	20.135	412331	13309	3.722		M	
2	22.406	10667112	254558	96.278		M	
Total		11079443	267867				

(*S*)-1-(5-bromopyridin-2-yl)-1,1-difluoro-4-(triisopropylsilyl)but-3-yn-2-ol (5d)



Alkyne **1r** (38.2 mg, 0.21 mmol, 105 mol%) and aldehyde **4d** (94 wt% in ethanol, 52.6 mg, 0.19 mmol) were subjected to standard reaction conditions (80 °C, 24 h) at 5 mol% catalyst loading. Upon flash column chromatography (SiO_2: 10:90 EtOAc:hexanes), the title compound **5d** was isolated as a brown oil in 98% yield (82.6 mg, 0.19 mmol, 99% ee).

TLC (SiO_2): R_f = 0.3 (1:4 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.68 (d, *J* = 2.3 Hz, 1H), 7.98 (dd, *J* = 8.4, 2.3 Hz, 1H), 7.62 (d, *J* = 8.4 Hz, 1H), 5.01 (ddd, *J* = 9.5, 8.6, 7.6 Hz, 1H), 3.99 (d, *J* = 9.5 Hz, 1H), 0.94 (s, 21H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ 151.9 (dd, *J* = 31.3, 27.6 Hz), 150.6 – 149.6 (m), 140.2, 123.0 – 122.7 (m), 122.7 – 122.5 (m), 116.2 (t, *J* = 248.4 Hz), 101.9 (dd, *J* = 5.5, 2.0 Hz), 90.0, 66.0 (t, *J* = 31.8 Hz), 18.5, 11.0 ppm.

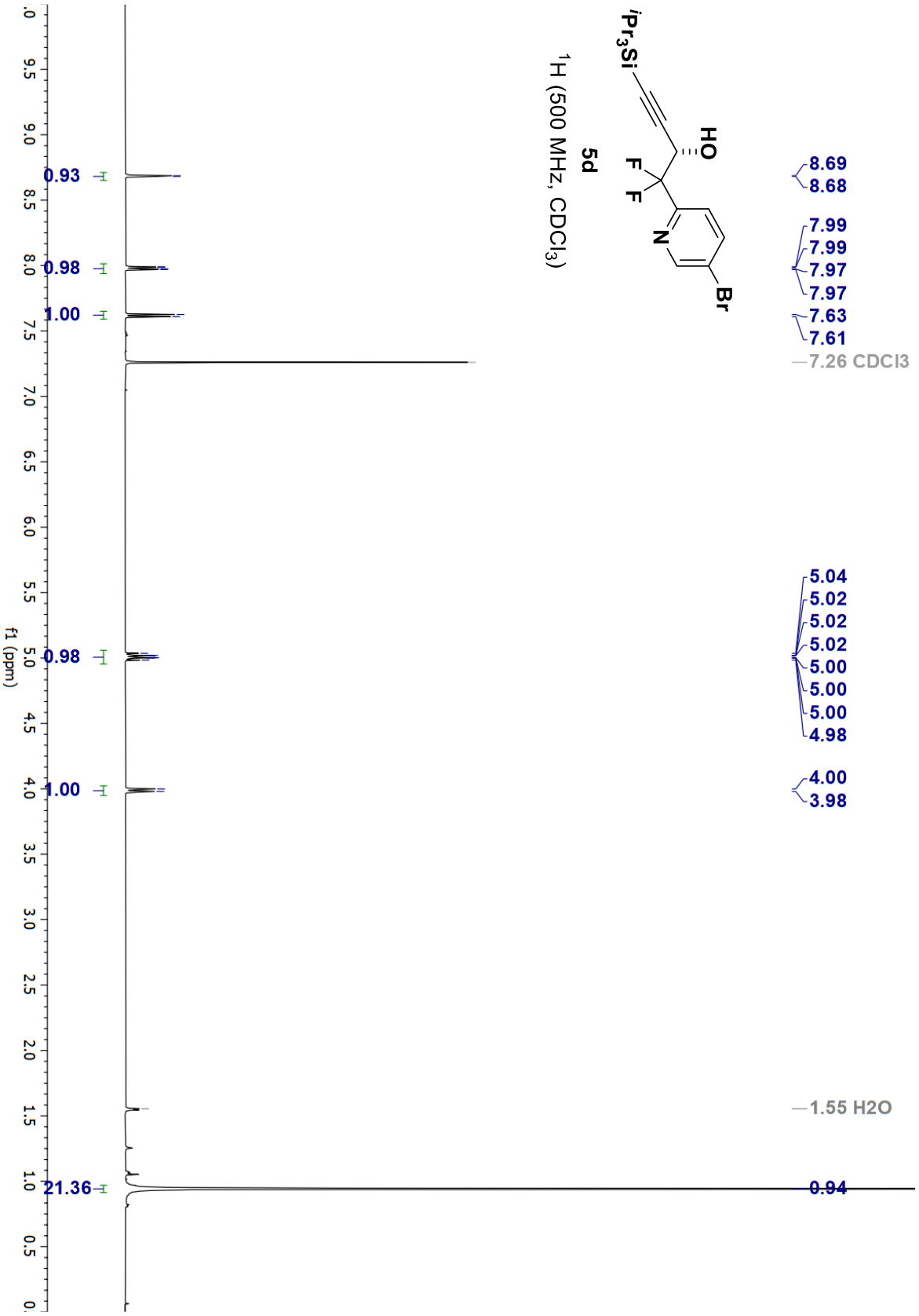
^{19}F NMR (471 MHz, $CDCl_3$): δ -104.7 (d, *J* = 260.5 Hz), -111.1 (dd, *J* = 260.7, 8.6 Hz) ppm.

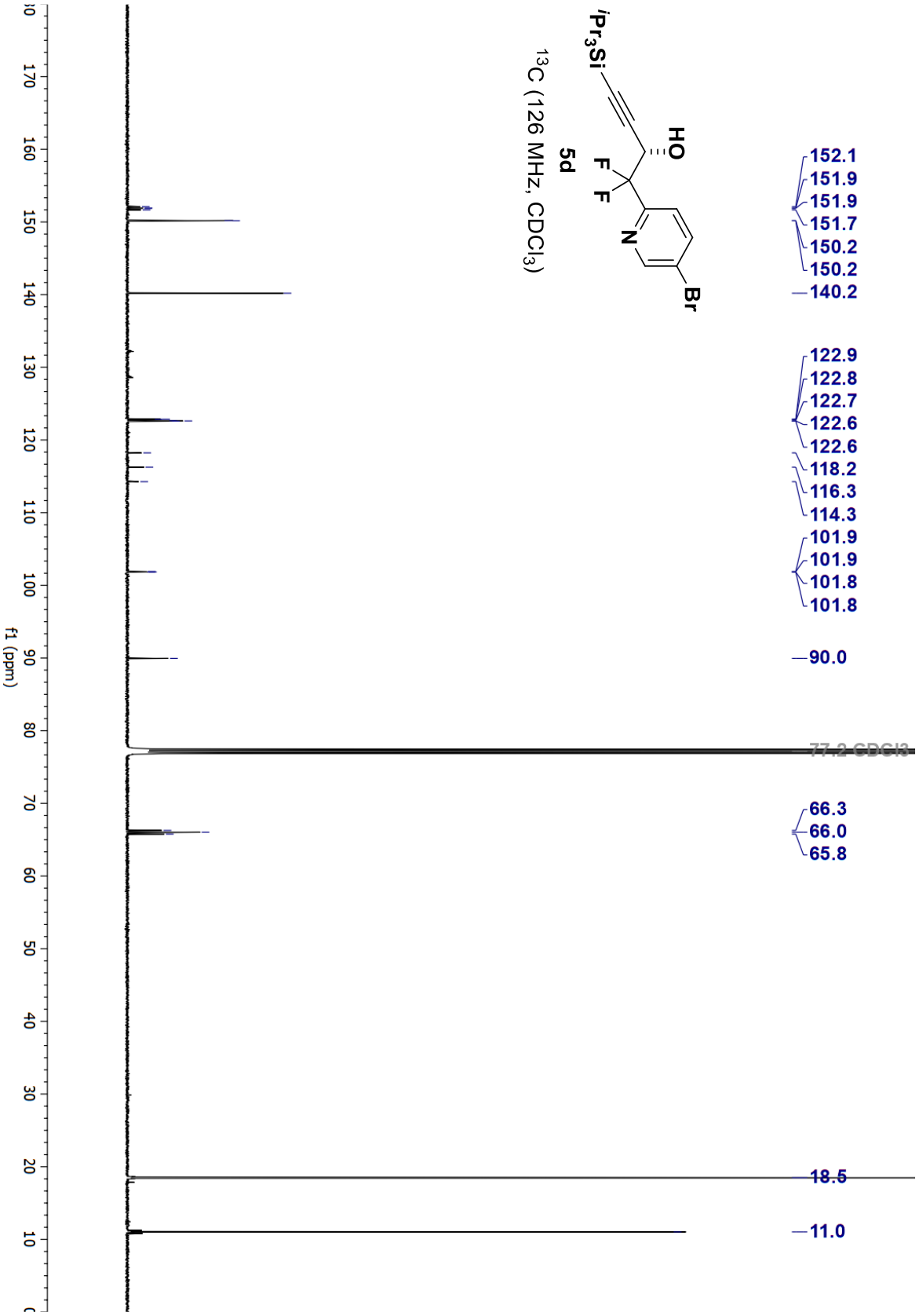
HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_{18}H_{27}BrF_2NOSi^+$: 418.1008; found = 418.1011.

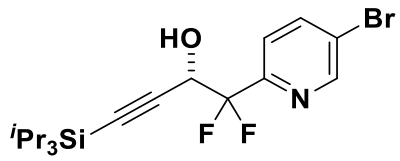
FTIR (neat): 3351, 2941, 2863, 2177, 1462, 1073, 958, 672, 410 cm^{-1}.

HPLC (CHIRALPAK AD-H, hexanes:2-PrOH = 97:3, 1.0 mL/min, 254 nm), ee = 99%.

$[\alpha]_D^{20}$ = -158° ($CHCl_3$, c = 1.0).

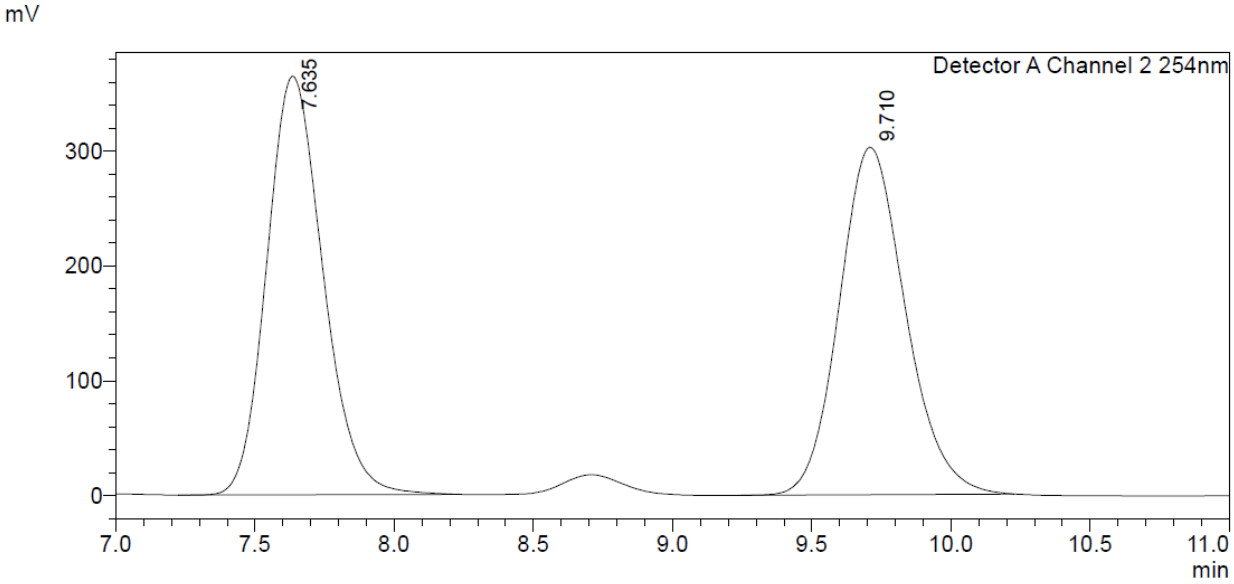

5d
^{1}H (500 MHz, CDCl$_3$)
^{i}Pr$_3$Si
HO
F
F
N
Br
8.69
8.68
7.99
7.99
7.97
7.97
7.63
7.61
7.26 CDCl3
5.04
5.02
5.02
5.02
5.00
5.00
5.00
4.98
4.00
3.98
1.55 H2O
0.94
0.93
0.98
1.00
0.98
1.00
21.36
f1 (ppm)


^{13}C (126 MHz, CDCl$_3$)
5d
^{i}Pr$_3$Si
HO
F
F
N
Br
152.1
151.9
151.9
151.7
150.2
150.2
140.2
122.9
122.8
122.7
122.6
122.6
118.2
116.3
114.3
101.9
101.9
101.8
101.8
90.0
77.2 CDCl3
66.3
66.0
65.8
18.5
11.0
f1 (ppm)



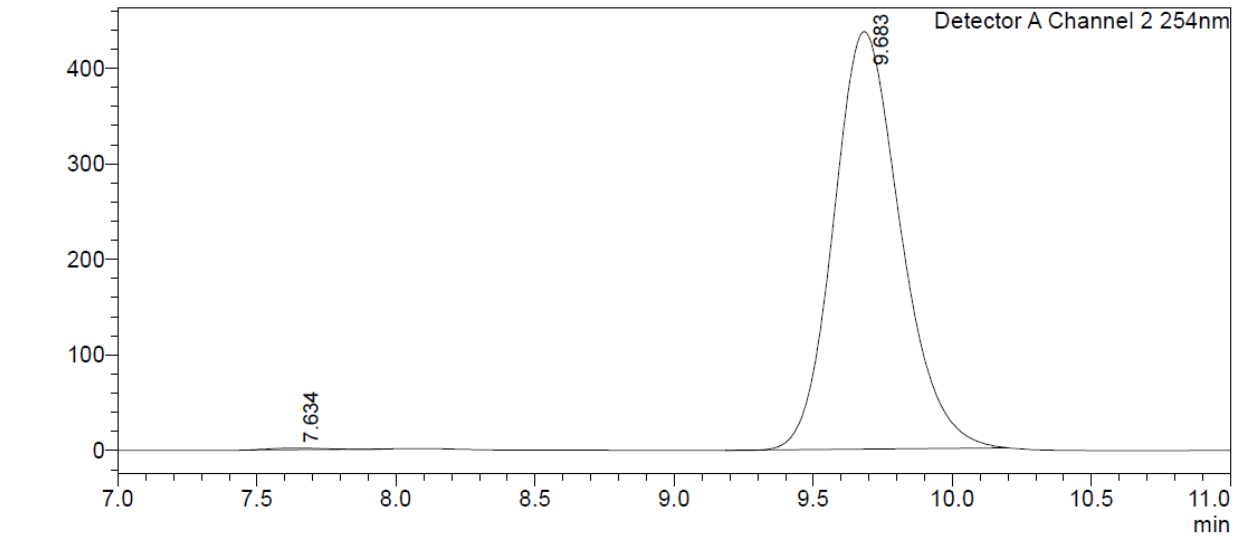
5d

^{19}F (471 MHz, $CDCl_3$)



Detector A Channel 2 254nm

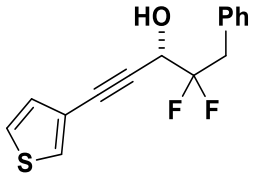
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	7.635	5122074	364280	50.515		M	
2	9.710	5017729	302436	49.485		M	
Total		10139803	666717				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	7.634	19334	1702	0.264		M	
2	9.683	7316316	437096	99.736		M	
Total		7335650	438797				

(*S*)-4,4-difluoro-5-phenyl-1-(thiophen-3-yl)pent-1-yn-3-ol (5e)



Alkyne **1m** (21 μL, 0.21 mmol, 105 mol%) and ethyl hemiacetal **4e** (94 wt% in EtOH, 44.8 mg, 0.19 mmol) were subjected to standard reaction conditions (80 °C, 24 h) at 5 mol% catalyst loading. Upon flash column chromatography (SiO_2: 5:95–10:90 EtOAc:hexanes), the title compound **5e** was isolated as a brown oil in 89% yield (48.3 mg, 0.17 mmol, 94% ee).

TLC (SiO_2): R_f = 0.2 (1:9 EtOAc:hexanes).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.43 (dd, *J* = 3.0, 1.2 Hz, 1H), 7.28 – 7.14 (m, 6H), 7.04 (dd, *J* = 5.0, 1.2 Hz, 1H), 4.53 (td, *J* = 9.5, 5.9 Hz, 1H), 3.44 – 3.19 (m, 2H), 2.33 (d, *J* = 7.2 Hz, 1H) ppm.

^{13}C NMR (101 MHz, $CDCl_3$): δ 132.3 (t, *J* = 4.1 Hz), 130.7, 130.3, 130.0, 128.7, 127.7, 125.7, 121.2 (t, *J* = 249.8 Hz), 120.8, 83.1 (t, *J* = 4.0 Hz), 83.0, 64.8 (t, *J* = 31.3 Hz), 39.2 (t, *J* = 24.1 Hz) ppm.

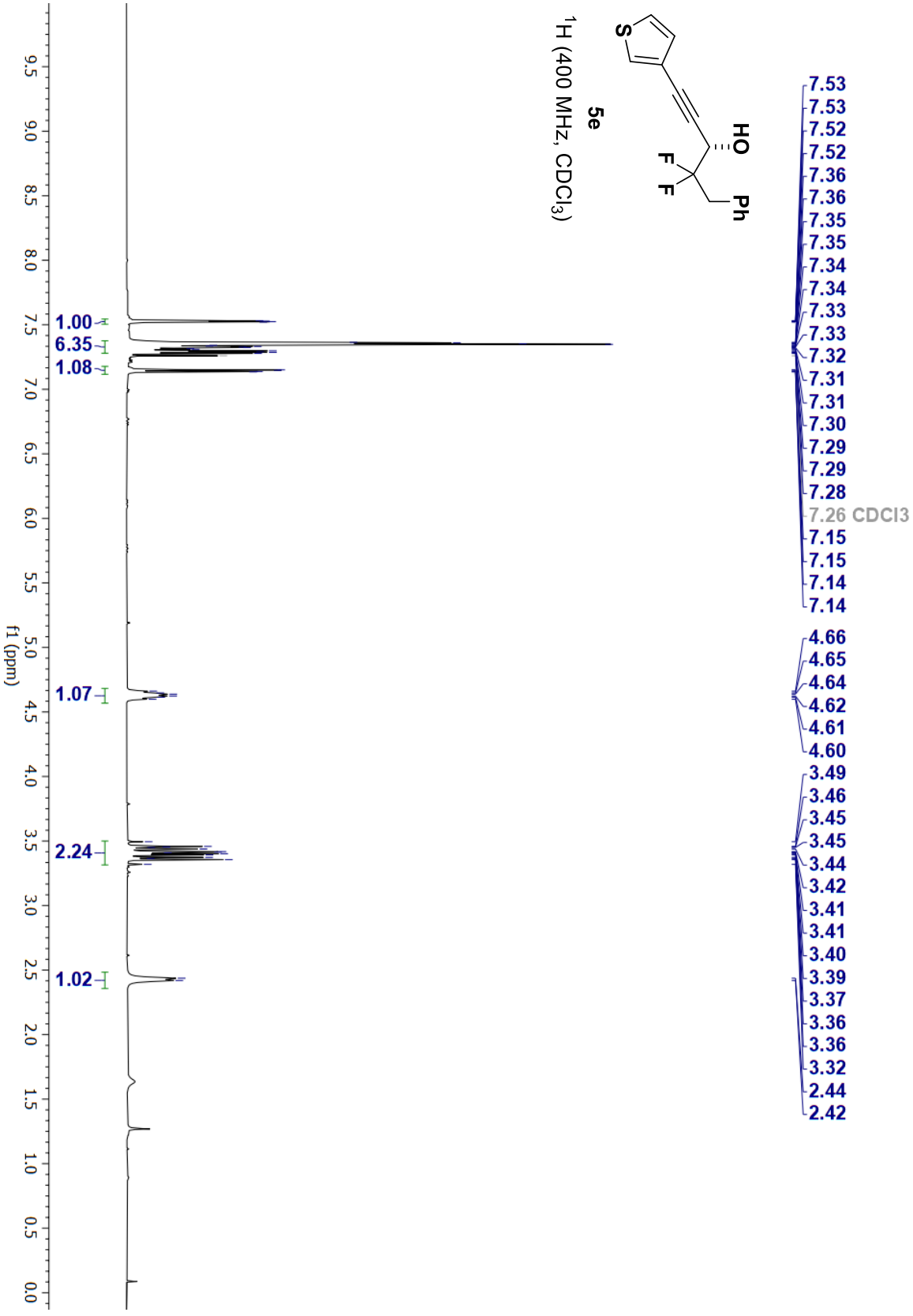
^{19}F NMR (376 MHz, $CDCl_3$): δ -108.0 – -108.9 (m), -109.1 – -110.1 (m) ppm.

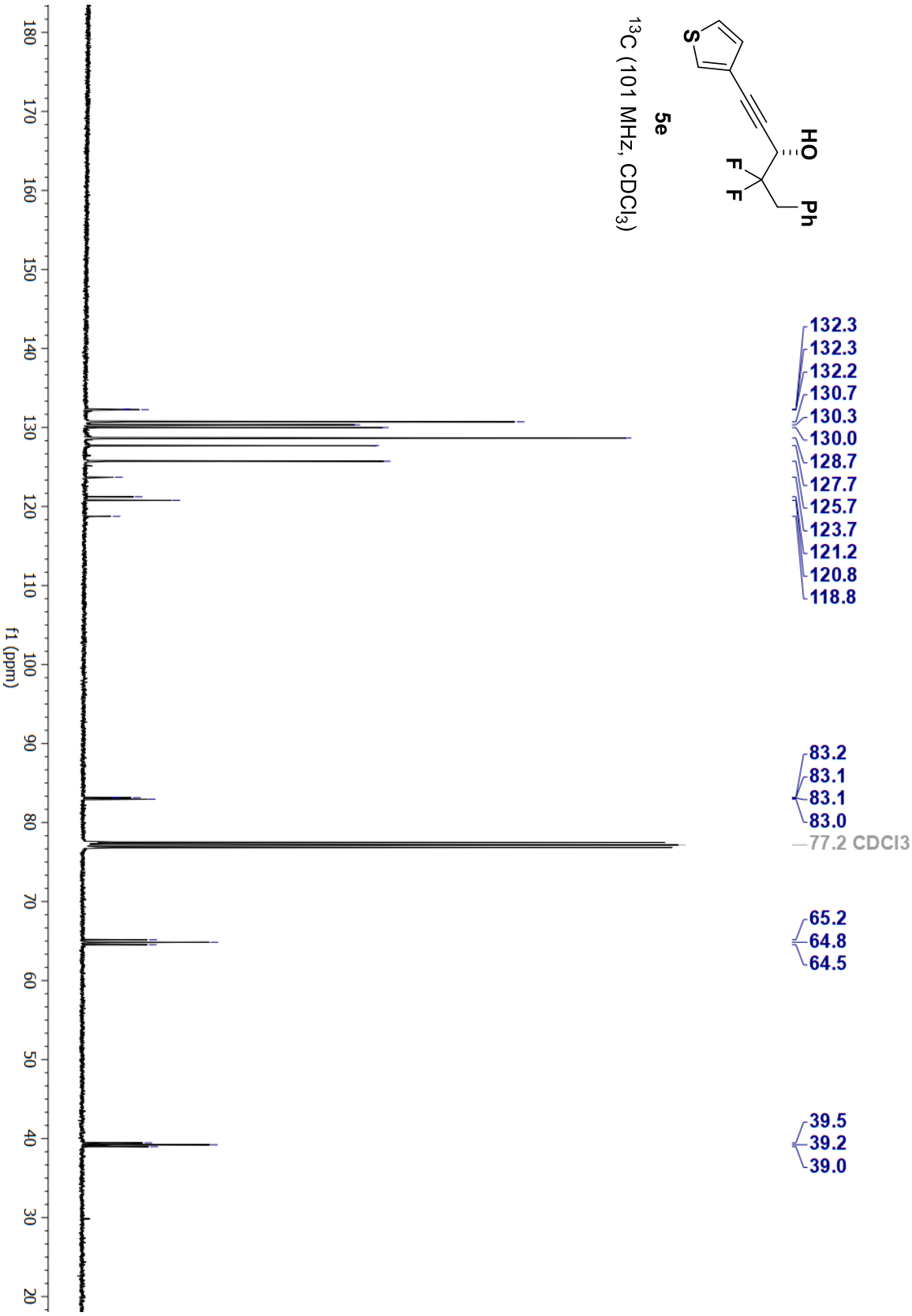
HRMS (ESI(+)): m/z [M+Na^+] calcd. for $C_{15}H_{12}F_2NaOS^+$: 301.0469; found = 301.0457.

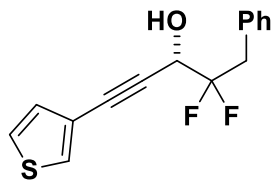
FTIR (neat): 3324, 3106, 3063, 3030, 2927, 2241, 2223, 1604, 1496, 1454, 1429, 1356, 1230, 1178, 1124, 1056, 1033, 993, 889, 863, 835, 821, 781, 734, 698, 650, 624, 576, 540, 518, 477, 421, 405 cm^{-1}.

HPLC (CHIRALPAK AD-H, hexanes:2-PrOH = 98:2, 1.0 mL/min, 254 nm): ee =94%.

$[\alpha]_D^{20}$ = –78° ($CHCl_3$, c = 1.0).

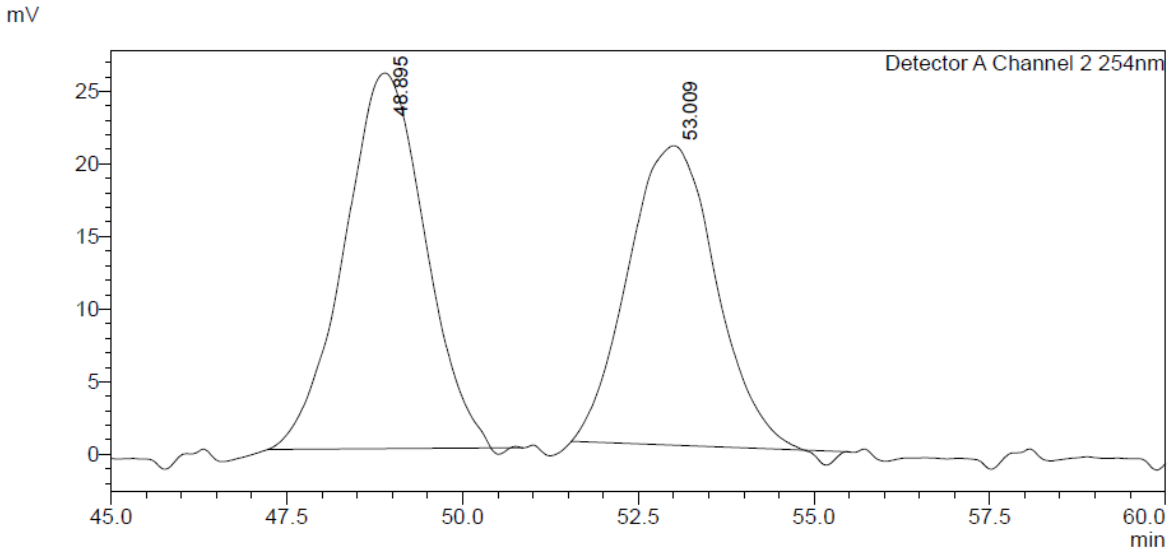

5e
^{1}H (400 MHz, $CDCl_3$)
HO
Ph
F
F
S
7.53
7.53
7.52
7.52
7.36
7.36
7.35
7.35
7.34
7.34
7.33
7.33
7.32
7.31
7.31
7.30
7.29
7.29
7.28
7.26 CDCl3
7.15
7.15
7.14
7.14
4.66
4.65
4.64
4.62
4.61
4.60
3.49
3.46
3.45
3.45
3.44
3.42
3.41
3.41
3.40
3.39
3.37
3.36
3.36
3.32
2.44
2.42
1.00
6.35
1.08
1.07
2.24
1.02
f1 (ppm)


5e
^{13}C (101 MHz, CDCl$_3$)
S
HO
F
F
Ph
132.3
132.3
132.2
130.7
130.3
130.0
128.7
127.7
125.7
123.7
121.2
120.8
118.8
83.2
83.1
83.1
83.0
77.2 CDCl3
65.2
64.8
64.5
39.5
39.2
39.0
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20



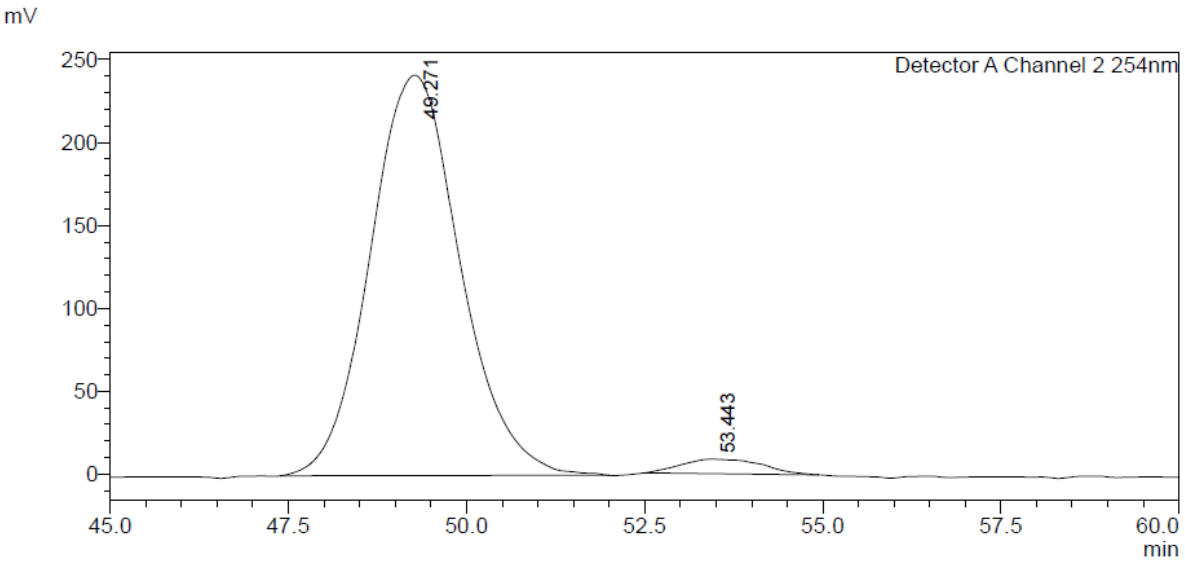
5e

^{19}F (376 MHz, $CDCl_3$)



Detector A Channel 2 254nm

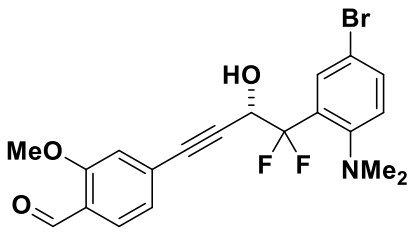
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	48.895	2071980	25844	53.700		M	
2	53.009	1786484	20613	46.300		M	
Total		3858464	46457				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	49.271	21254644	241353	96.830		M	
2	53.443	695737	8920	3.170		M	
Total		21950381	250272				

(*S*)-4-(4-(5-bromo-2-(dimethylamino)phenyl)-4,4-difluoro-3-hydroxybut-1-yn-1-yl)-2-methoxybenzaldehyde (5f)



Alkyne **1l** (33.6 mg, 0.21 mmol, 105 mol%) and ethyl hemiacetal **4f** (55.6 mg, 0.20 mmol) were subjected to modified reaction conditions (80 °C, 48 h) at 5 mol% catalyst loading. Upon flash column chromatography (SiO_2: 16:84 EtOAc:hexanes), the title compound **5f** was isolated as a dark yellow oil in 52% yield (45.3 mg, 0.10 mmol, 98% ee).

TLC (SiO_2): R_f = 0.4 (1:19 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 10.39 (s, 1H), 7.85 (m, 2H), 7.70 (d, *J* = 7.9 Hz, 1H), 7.63 (dd, *J* = 8.6, 2.4 Hz, 1H), 7.34 (d, *J* = 8.5 Hz, 1H), 6.87 (d, *J* = 7.9 Hz, 1H), 6.80 (m, 1H), 5.17 (dt, *J* = 11.5, 2.5 Hz, 1H), 3.88 (s, 3H), 2.73 (s, 6H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$): δ 189.1, 161.3, 150.7 (d, *J* = 5.4 Hz), 134.9, 133.9 – 132.7 (m), 131.2 (dd, *J* = 14.7, 6.4 Hz), 129.3, 128.6, 125.1, 124.9, 124.2, 119.7 (dd, *J* = 262.0, 241.7 Hz), 119.6 (m, *J* = 3.7 Hz), 114.9, 89.1 (d, *J* = 7.3 Hz), 85.9 (d, *J* = 2.0 Hz), 67.6 (dd, *J* = 37.1, 33.7 Hz), 55.9, 46.7 ppm.

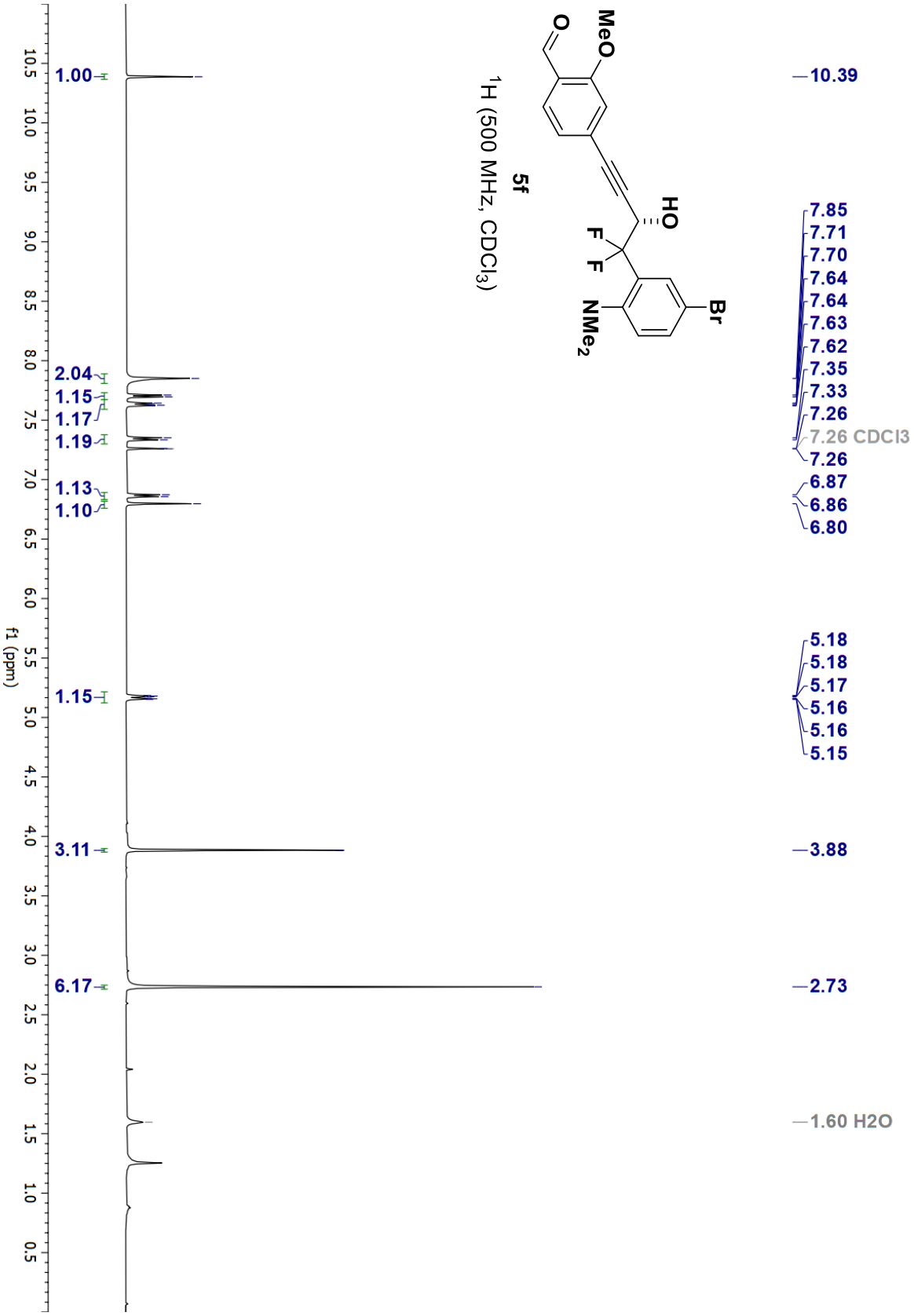
^{19}F NMR (471 MHz, $CDCl_3$): δ -96.0 (d, *J* = 259.0 Hz), -101.7 (dd, *J* = 258.9, 11.5 Hz) ppm.

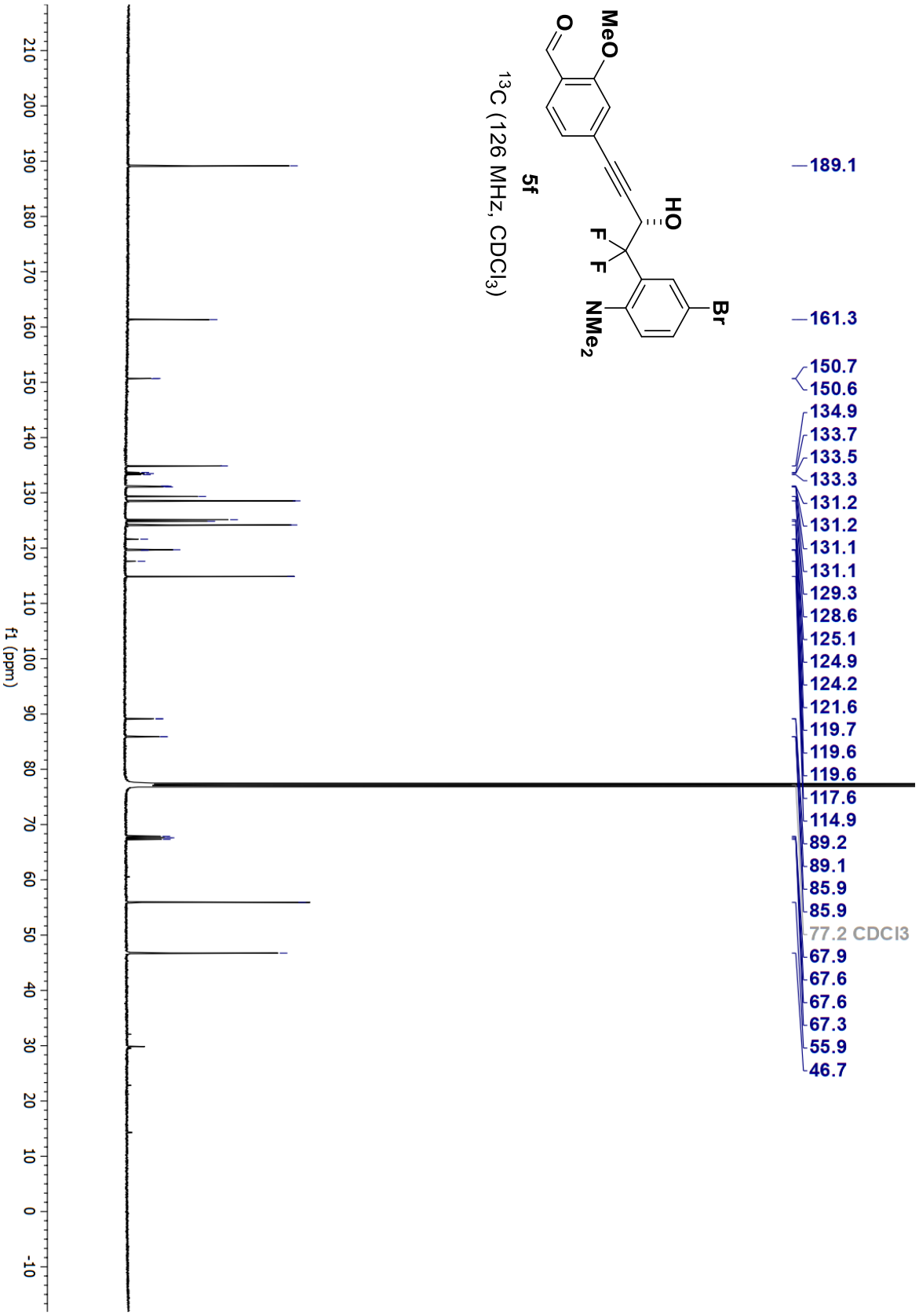
HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_{20}H_{19}BrF_2NO_3^+$: 438.0511; found = 438.0513.

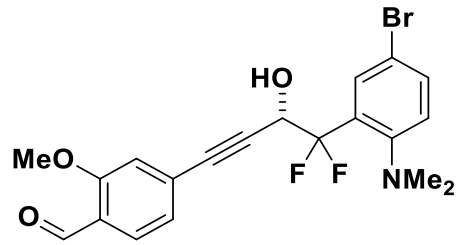
FTIR (neat): 3340, 3073, 2936, 2860, 2831, 2787, 1676, 1599, 1482, 1454, 1403, 1394, 1264, 1204, 1169, 1134, 1107, 1061, 1028, 979, 855, 825, 802, 768, 728, 705, 669, 605, 569, 556, 528 cm^{-1}.

HPLC (CHIRALPAK AD-H, hexanes:2-PrOH = 95:5, 1.0 mL/min, 254 nm): ee = 98%.

$[\alpha]_D^{20}$ = -120° ($CHCl_3$, c = 1.0).

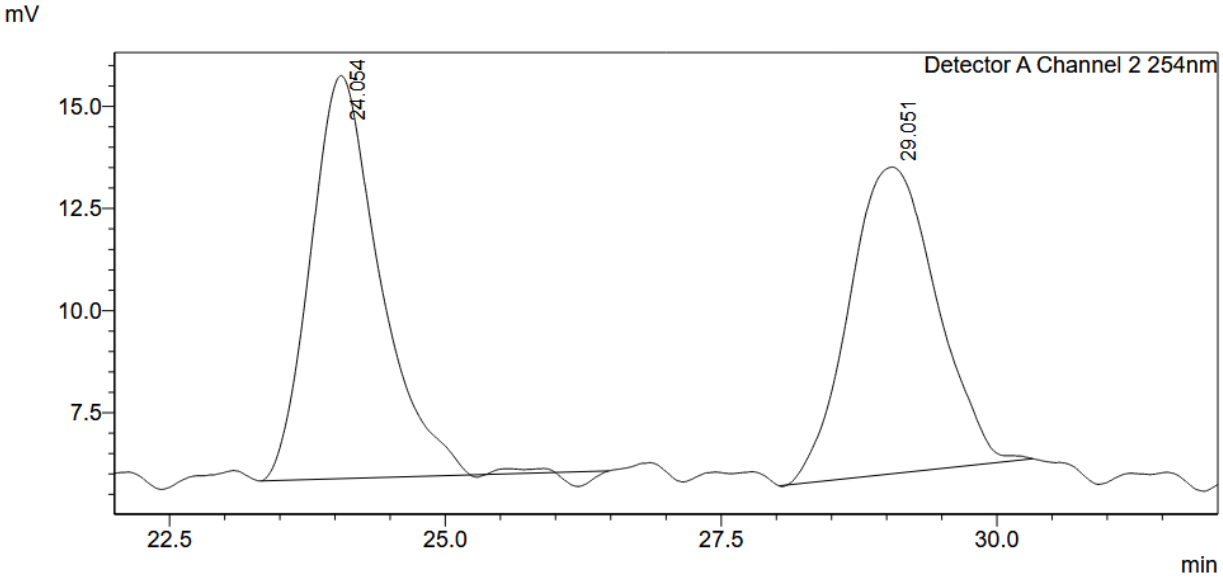

5f
^{1}H (500 MHz, $CDCl_3$)
MeO
O
HO
F
F
NMe$_2$
Br
10.39
7.85
7.71
7.70
7.64
7.64
7.63
7.62
7.35
7.33
7.26
7.26 CDCl3
7.26
6.87
6.86
6.80
5.18
5.18
5.17
5.16
5.16
5.15
3.88
2.73
1.60 H2O
1.00
2.04
1.15
1.17
1.19
1.13
1.10
1.15
3.11
6.17
f1 (ppm)


5f
^{13}C (126 MHz, CDCl$_3$)
MeO
O
HO
F
F
NMe$_2$
Br
189.1
161.3
150.7
150.6
134.9
133.7
133.5
133.3
131.2
131.2
131.1
131.1
129.3
128.6
125.1
124.9
124.2
121.6
119.7
119.6
119.6
117.6
114.9
89.2
89.1
85.9
85.9
77.2 CDCl3
67.9
67.6
67.6
67.3
55.9
46.7
f1 (ppm)



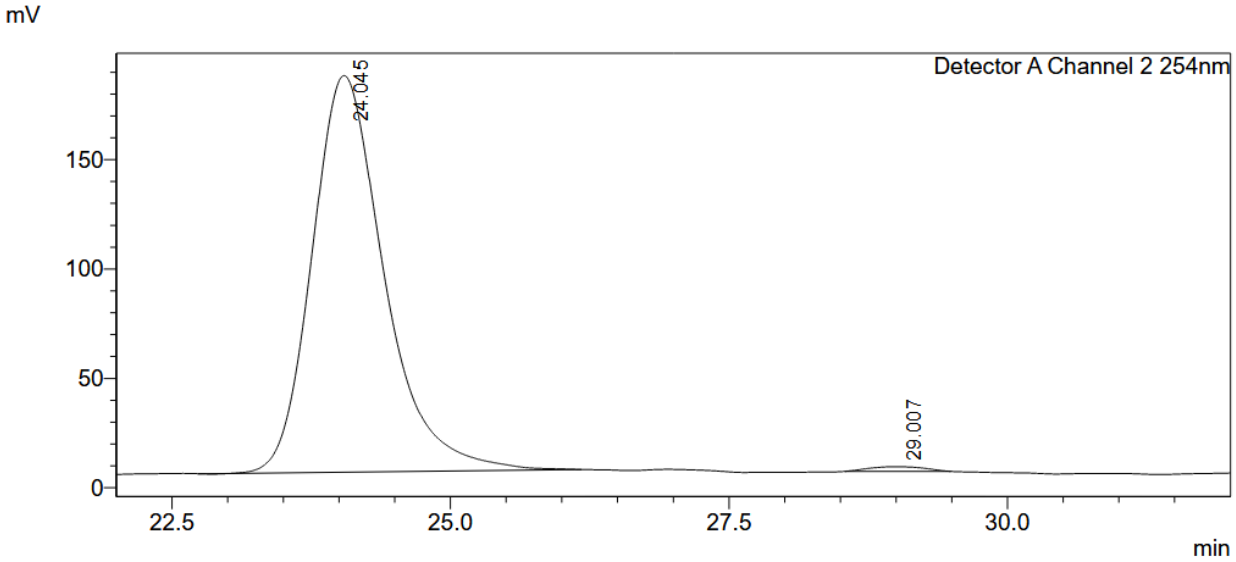
5f

^{19}F (471 MHz, $CDCl_3$)



Detector A Channel 2 254nm

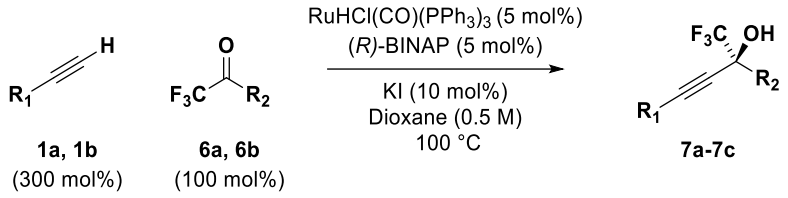
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	24.054	428414	9863	50.766		M	
2	29.051	415490	7507	49.234		M	
Total		843904	17369				



Detector A Channel 2 254nm

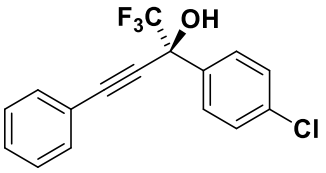
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	24.045	8168283	181295	99.099		M	
2	29.007	74277	2142	0.901		M	
Total		8242560	183436				

VIII Products 7a-7c



General Procedure D: An oven dried pressure tube equipped with a magnetic stir bar was charged with the respective terminal alkyne **1a, 1b** (0.60 mmol, 300 mol%), the respective CF_3-ketone **6a, 6b** (0.20 mmol, 100 mol%), $RuHCl(CO)(PPh_3)_3$ (9.5 mg, 0.01 mmol, 5 mol%), (*R*)-BINAP (6.2 mg, 0.01 mmol, 5 mol%), KI (3.2 mg, 0.02 mmol, 10 mol%), and dioxane (0.40 mL, 0.5 M) under air. The tube was sealed with a PTFE-lined cap, placed in an oil bath and was allowed to stir for 48 hours at 100 ºC. The reaction mixture was allowed to reach ambient temperature, and the residue was subjected to flash column chromatography (SiO_2) under the noted conditions to furnish products **7a-7c**.

(*S*)-2-(4-chlorophenyl)-1,1,1-trifluoro-4-phenylbut-3-yn-2-ol (7a)



Alkyne **1a** (61.3 mg, 66 µL, 0.60 mmol, 300 mol%) and CF_3-ketone **6a** (41.4 mg, 0.20 mmol, 100 mol%) were subjected to standard reaction conditions (100 °C, 48 h) at 5 mol% catalyst loading. Upon flash column chromatography (SiO_2: 8:92 EtOAc:hexanes), the title compound **7a** was isolated as a colorless oil in 60% yield (24.5 mg, 0.12 mmol, 99% ee).

TLC (SiO_2): R_f = 0.3 (1:9 hexanes:EtOAc).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.58 – 7.48 (m, 2H), 7.48 – 7.29 (m, 5H), 3.09 (s, 1H) ppm.

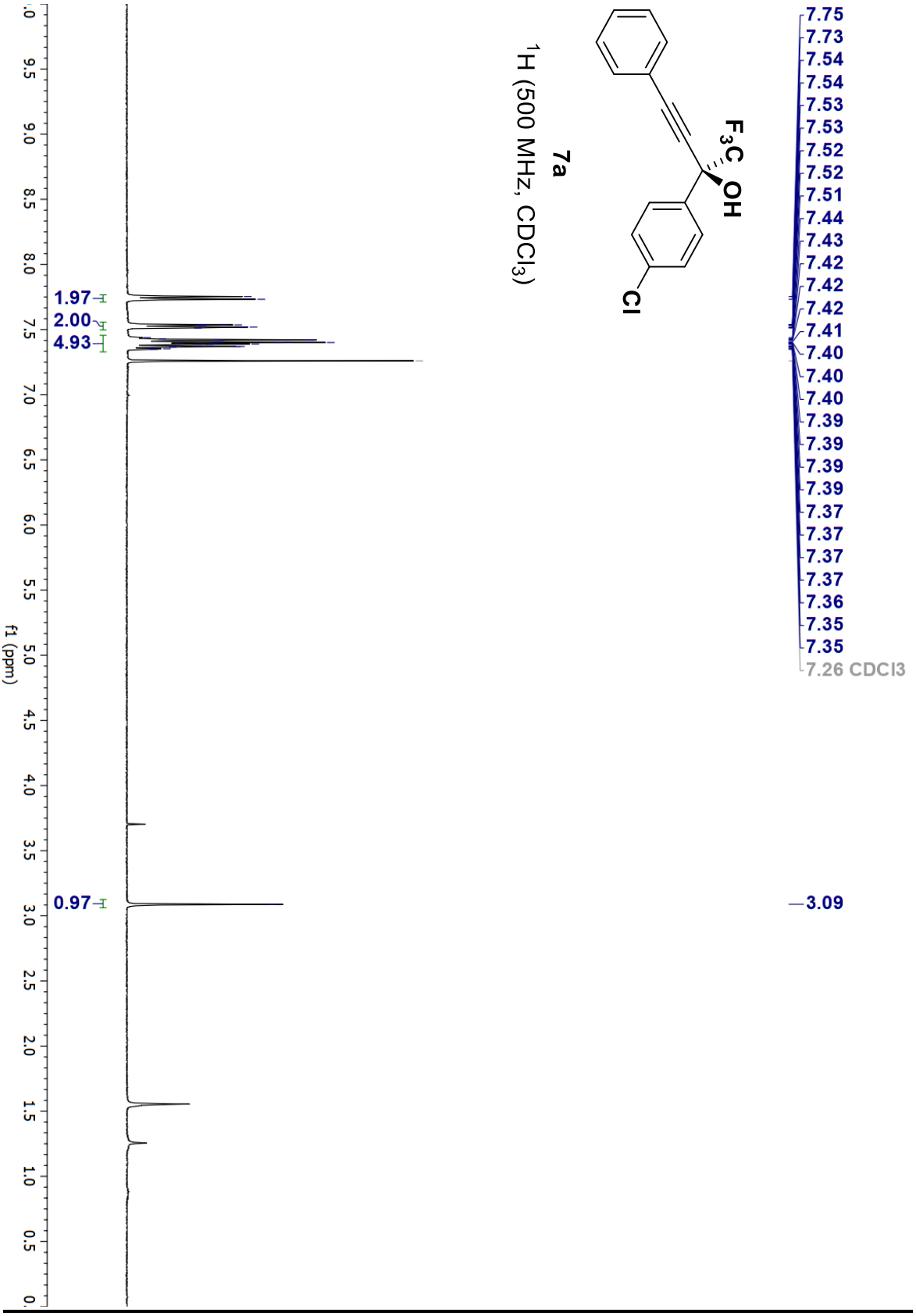
^{19}F NMR (376 MHz, $CDCl_3$): δ -80.4 ppm.

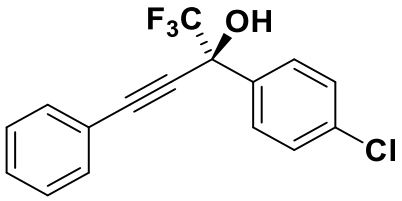
HRMS: Known compound, see reference 19.

HPLC (CHIRALPAK AD-H, hexanes:2-PrOH = 98:2, 1.0 mL/min, 254 nm): ee = 99%.

$[\alpha]_D^{20}$= -21° ($CHCl_3$, c = 1.0).

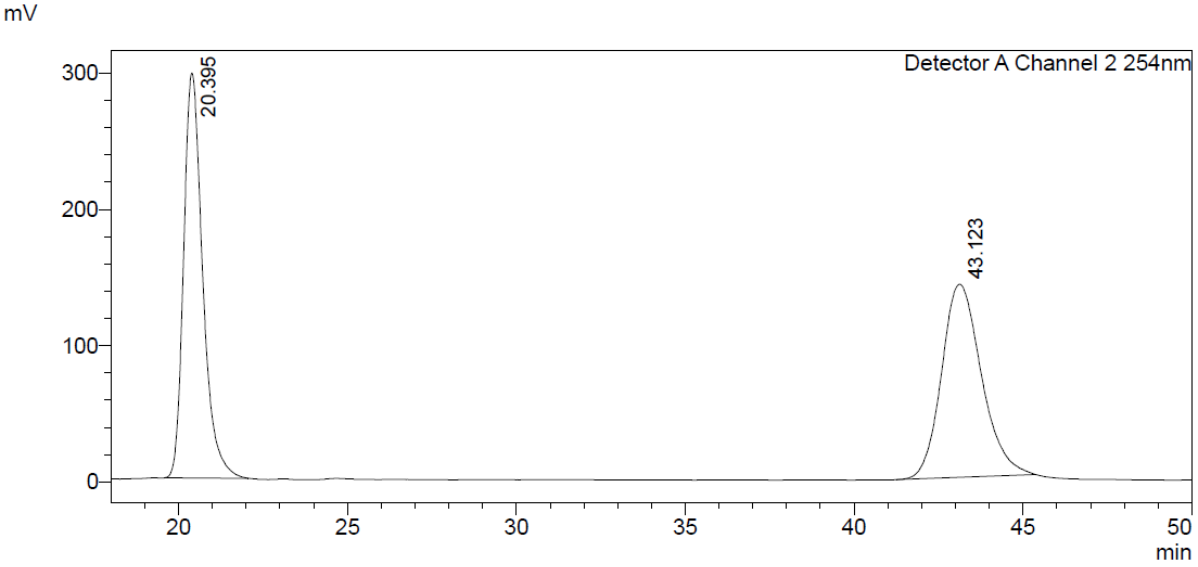
The analytical data including absolute stereochemistry are in agreement with the literature.[19]


7a
^{1}H (500 MHz, CDCl$_3$)
F$_3$C
OH
Cl
7.75
7.73
7.54
7.54
7.53
7.53
7.52
7.52
7.51
7.44
7.43
7.42
7.42
7.42
7.41
7.40
7.40
7.40
7.39
7.39
7.39
7.39
7.37
7.37
7.37
7.37
7.36
7.35
7.35
7.26 CDCl3
3.09
1.97
2.00
4.93
0.97
f1 (ppm)



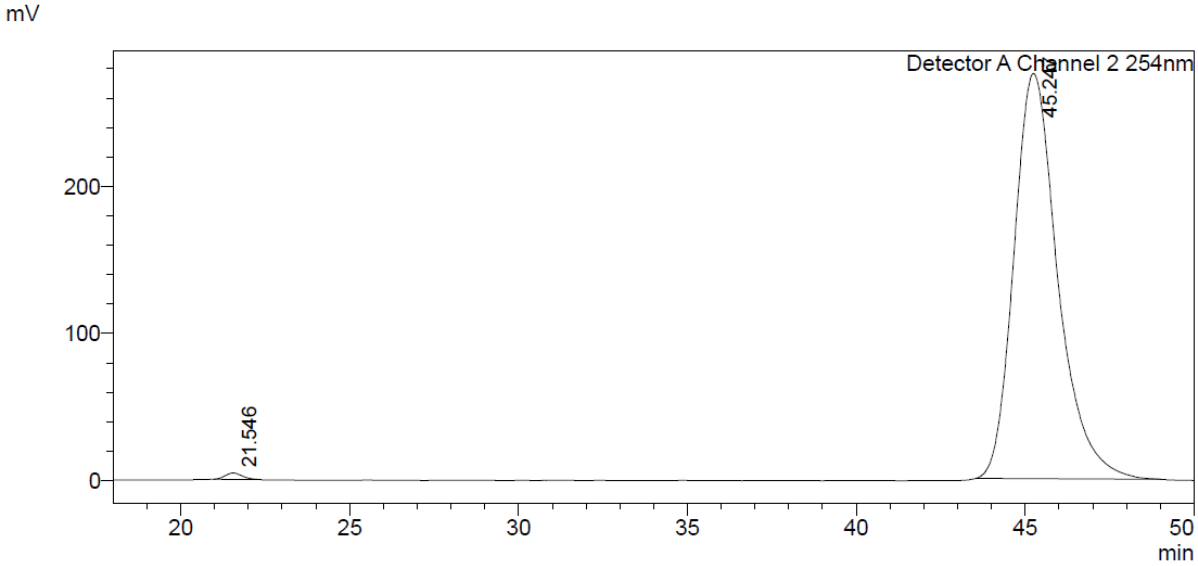
7a

^{19}F (437 MHz, $CDCl_3$)



Detector A Channel 2 254nm

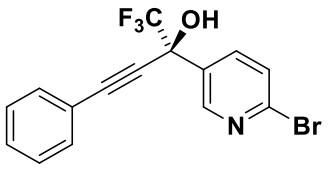
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	20.395	11648148	297254	49.998		M	
2	43.123	11649168	141812	50.002		M	
Total		23297316	439065				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	21.546	150486	4306	0.600		M	
2	45.247	24930636	275452	99.400		M	
Total		25081122	279758				

(*R*)-2-(6-bromopyridin-3-yl)-1,1,1-trifluoro-4-phenylbut-3-yn-2-ol (7b)



Alkyne **1a** (61.3 mg, 66 µL, 0.60 mmol, 300 mol%) and CF_3-ketone **6b** (51.1 mg, 0.20 mmol, 100 mol%) were subjected to standard reaction conditions (100°C, 48h) at 5 mol% catalyst loading. Upon flash chromatography (SiO_2: 7.5:92.5 EtOAc:hexanes) the title compound **7b** was isolated as a viscous brown oil in 90% yield (64.5 mg, 0.18 mmol, 91% ee).

TLC (SiO_2): Rf = 0.3 (1:4 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 8.80 (d, *J* = 2.6 Hz, 1H), 7.96 (dd, *J* = 8.4, 2.6 Hz, 1H), 7.55 (d, *J* = 8.4 Hz, 1H), 7.51 – 7.45 (m, 2H), 7.43 – 7.39 (m, 1H), 7.35 (dd, *J* = 8.2, 6.7 Hz, 2H), 4.11 (s, 1H) ppm.

^{13}C NMR (126 MHz, CDCl3) δ 149.4, 143.5, 137.8, 132.2, 131.4, 130.1, 128.7, 127.9, 123.1 (q, *J* = 285.3 Hz), 120.4, 89.4, 82.9, 71.8 (q, *J* = 33.3 Hz) ppm.

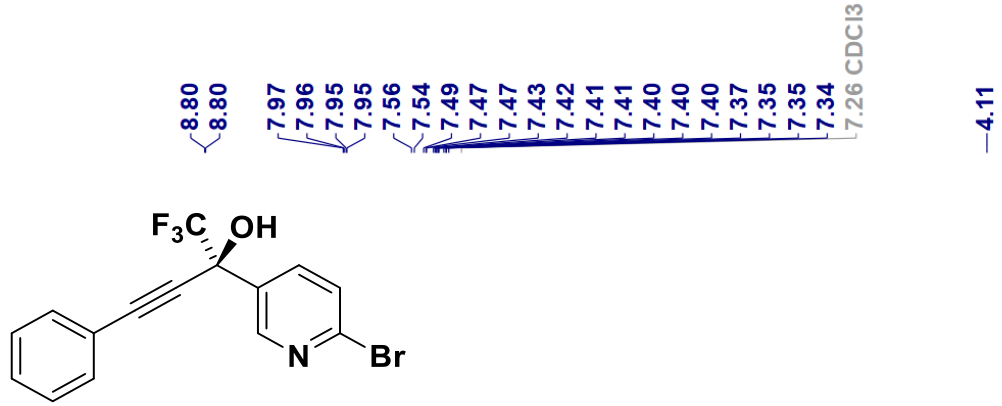
^{19}F NMR (471 MHz, CDCl3) δ -80.5 ppm.

HRMS (ESI(+)): m/z [M+H$^+$] calcd. for $C_{15}H_{10}BrF_3NO^+$: 355.9892; found = 355.9889.

FTIR (neat): 3058, 2922, 2851, 2231, 1172, 1107, 1085, 1012, 997, 915, 755, 744, 688.

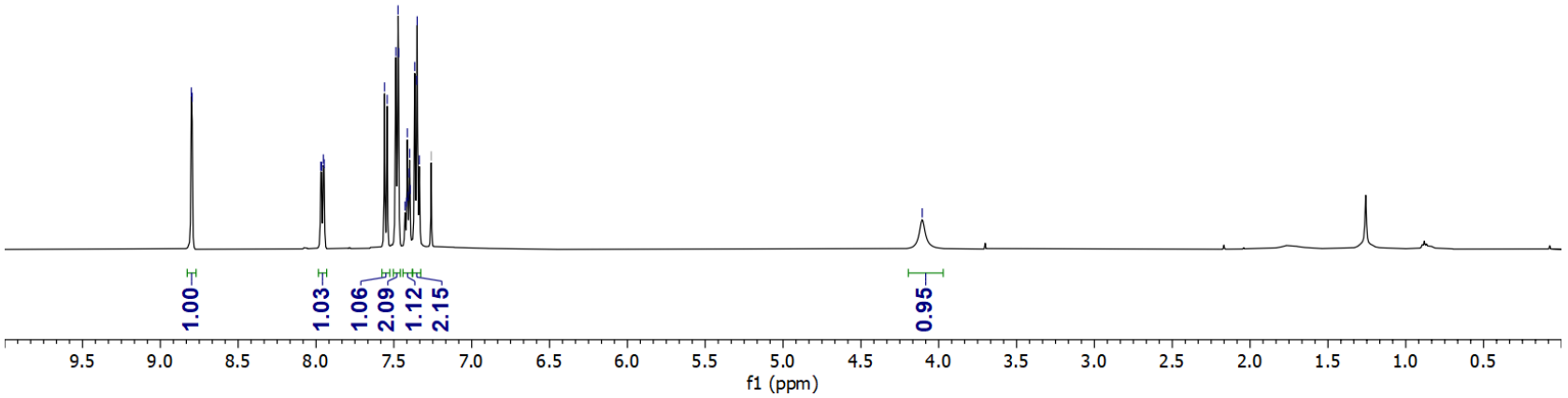
HPLC (CHIRALPAK AD-H, hexanes:2-PrOH = 97:3, 1.0 mL/min, 254 nm): ee = 91%.

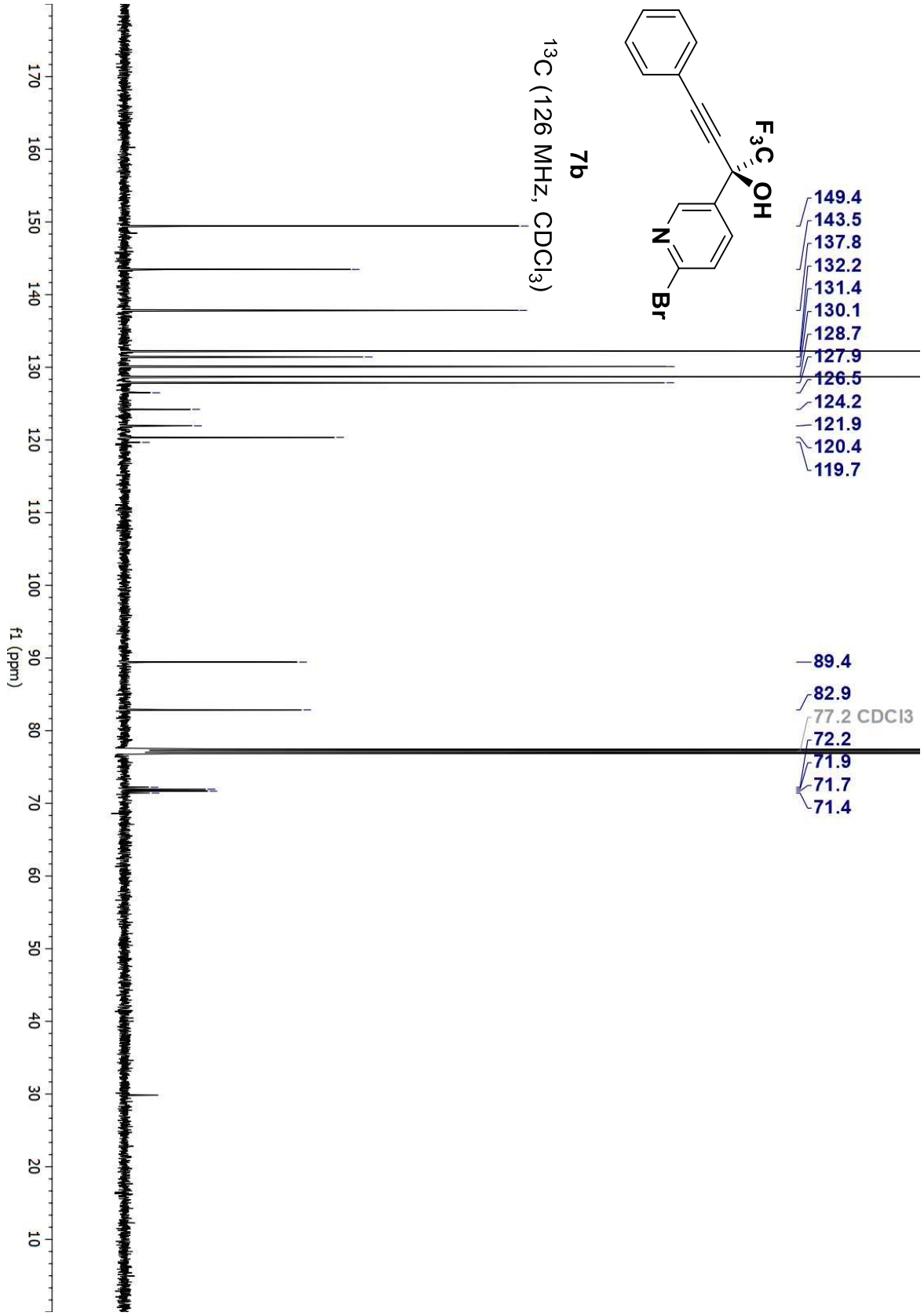
$[\alpha]_D^{20}$ = +3° ($CHCl_3$, c = 1.0).

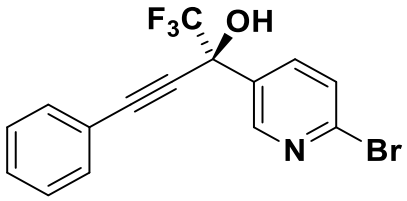


7b

^{1}H (500 MHz, $CDCl_3$)

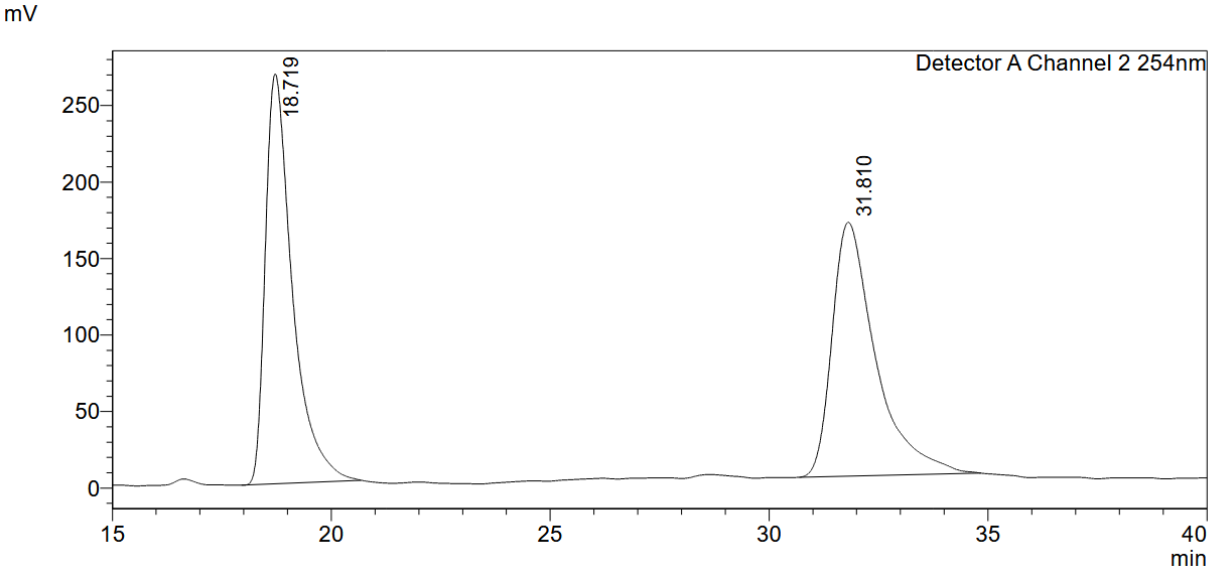



7b
^{13}C (126 MHz, $CDCl_3$)
F_3C
OH
N
Br
149.4
143.5
137.8
132.2
131.4
130.1
128.7
127.9
126.5
124.2
121.9
120.4
119.7
89.4
82.9
77.2 CDCl3
72.2
71.9
71.7
71.4
f1 (ppm)



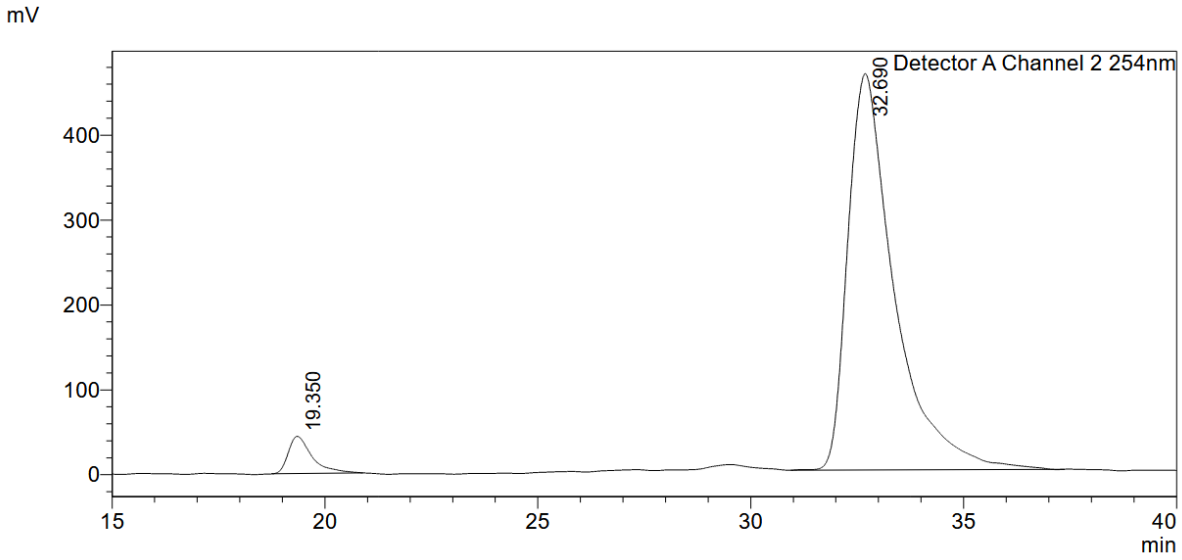
7b

^{19}F (471 MHz, $CDCl_3$)



Detector A Channel 2 254nm

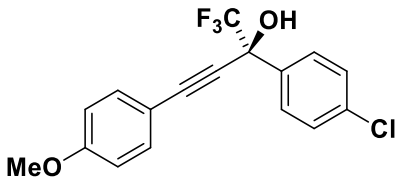
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	18.719	11504560	267916	50.016		M	
2	31.810	11497126	165871	49.984		M	
Total		23001686	433788				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	19.350	1706291	43907	4.590		M	
2	32.690	35470685	466784	95.410		M	
Total		37176976	510691				

(*S*)-2-(4-chlorophenyl)-1,1,1-trifluoro-4-(4-methoxyphenyl)but-3-yn-2-ol (7c)



Alkyne **1b** (79.3 mg, 0.60 mmol, 300 mol%) and CF_3-ketone **6a** (41.7 mg, 0.20 mmol, 100 mol%) were subjected to standard reaction conditions (100 °C, 48 h) at 5 mol% catalyst loading. Upon flash chromatography (SiO_2: 5:95 EtOAc:hexanes) the title compound **7c** was isolated as a brown oil in 95% yield (64.6 mg, 0.19 mmol, 88% ee).

TLC (SiO_2): R_f = 0.4 (1:9 EtOAc:hexanes).

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.47 – 7.43 (m, 2H), 7.42 – 7.38 (m, 2H), 6.92 – 6.84 (m, 2H), 3.83 (s, 3H), 3.21-3.20 (m, 1H) ppm.

^{13}C NMR (126 MHz, $CDCl_3$) δ 160.8, 135.8, 134.2, 133.8, 128.9, 128.6, 123.4 (q, *J* = 286.3 Hz), 114.3, 112.8, 88.7, 82.9, 73.1 (q, *J* = 32.7 Hz), 55.5 ppm.

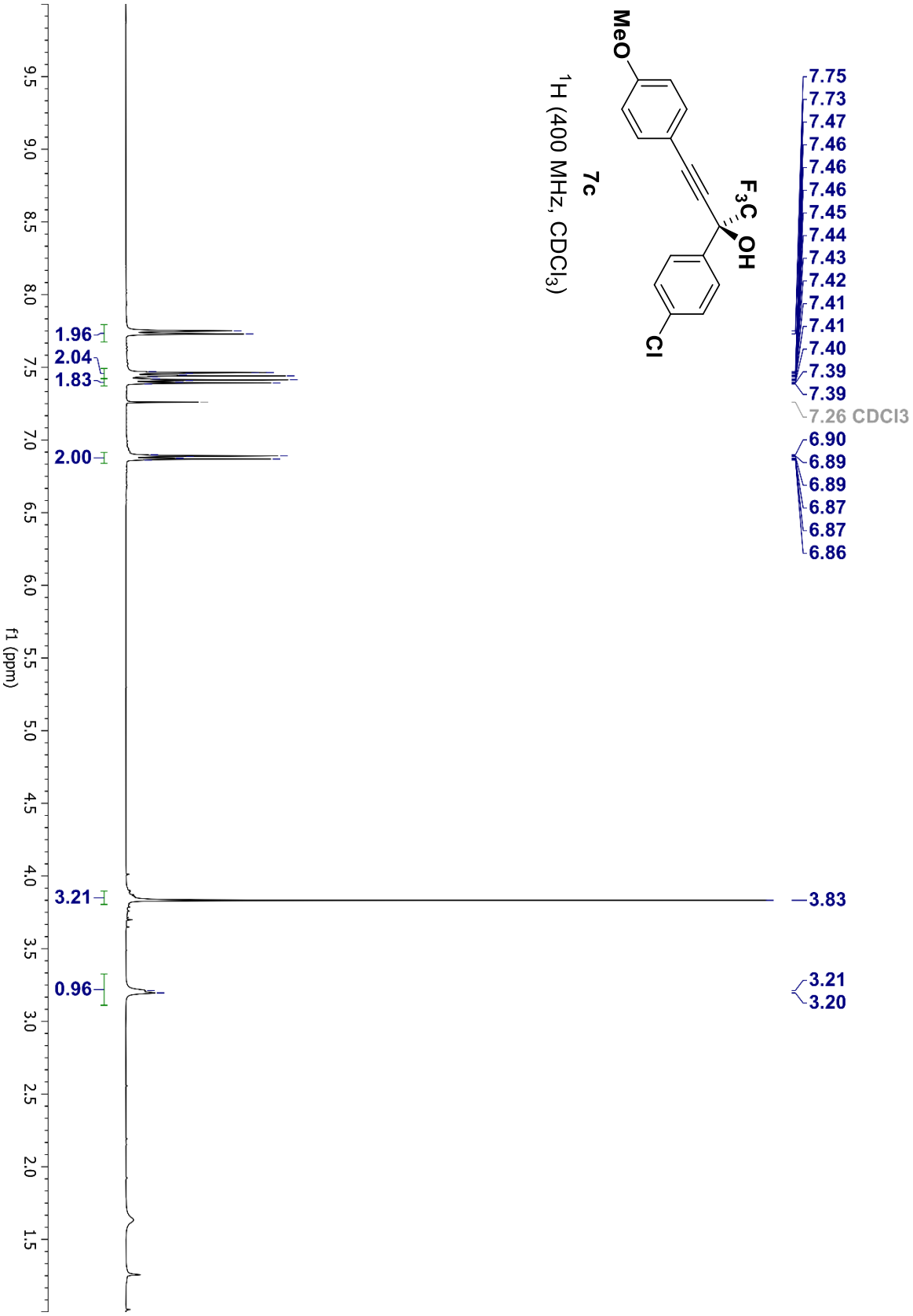
^{19}F NMR (471 MHz, CDCl3) δ -80.4 ppm.

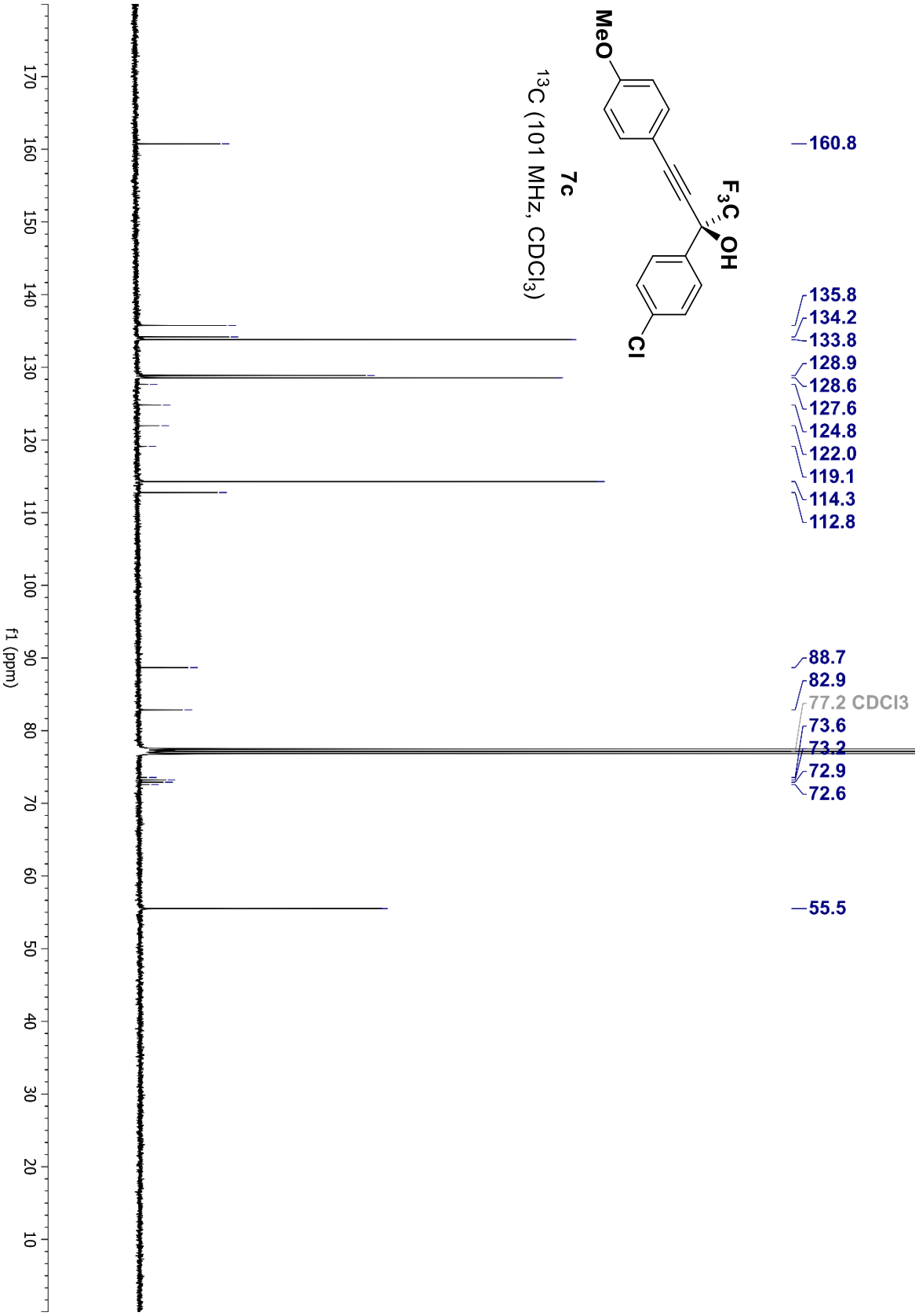
HRMS (FI(+)): m/z [M^+] calcd. for $C_{17}H_{12}ClF_3O_2^+$: 340.04724; found = 340.04787.

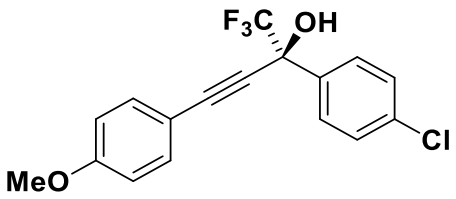
HPLC (CHIRALPAK AD-H, hexanes:2-PrOH = 98:2, 1.0 mL/min, 254 nm): ee = 99%.

$[\alpha]_D^{20}$= -20° ($CHCl_3$, c = 0.84).

The analytical data are in agreement with the literature.[20]

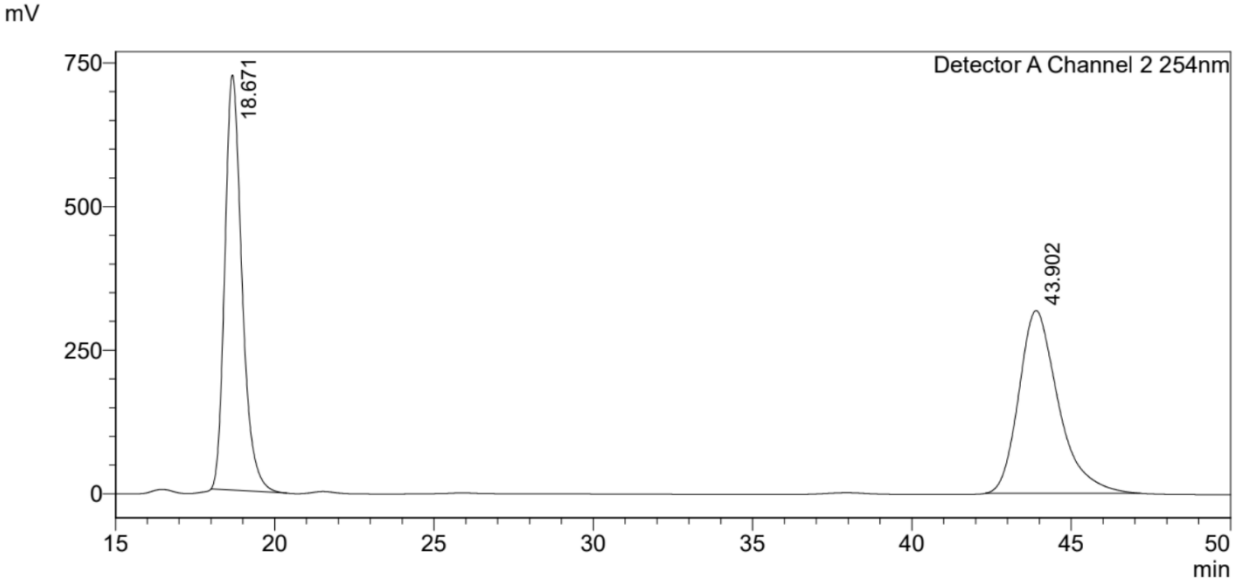

7c
^{1}H (400 MHz, CDCl$_3$)
MeO
F$_3$C
OH
Cl
7.75
7.73
7.47
7.46
7.46
7.46
7.45
7.44
7.43
7.42
7.41
7.41
7.40
7.39
7.39
7.26 CDCl3
6.90
6.89
6.89
6.87
6.87
6.86
3.83
3.21
3.20
1.96
2.04
1.83
2.00
3.21
0.96
f1 (ppm)


7c
^{13}C (101 MHz, CDCl$_3$)
MeO
F$_3$C
OH
Cl
160.8
135.8
134.2
133.8
128.9
128.6
127.6
124.8
122.0
119.1
114.3
112.8
88.7
82.9
77.2 CDCl3
73.6
73.2
72.9
72.6
55.5
f1 (ppm)



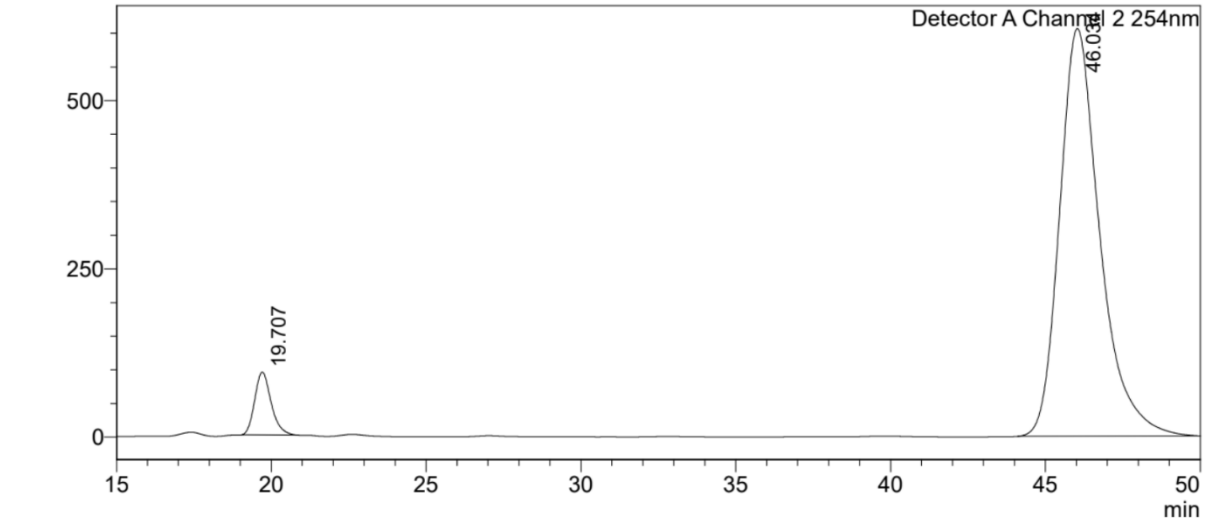
7c

^{19}F (471 MHz, $CDCl_3$)



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	18.671	26991628	722469	49.568		M	
2	43.902	27462492	318219	50.432		M	
Total		54454120	1040688				

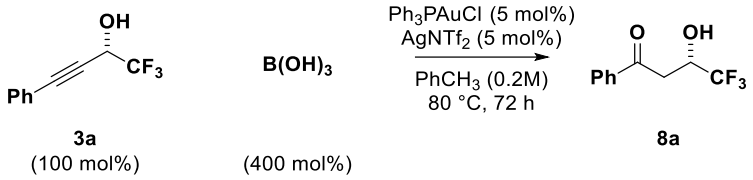


Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	19.707	3431807	93162	5.901		M	
2	46.034	54727809	605649	94.099		M	
Total		58159616	698811				

IX Gold catalyzed hydration 8a

(*S*)-4,4,4-trifluoro-3-hydroxy-1-phenylbutan-1-one (8a)



3a (100 mol%) | $B(OH)_3$ (400 mol%) | **8a**

A pressure tube was charged successively with **3a** (40.8 mg, 203 μmol, 100 mol%), Ph_3PAuCl (5.5 mg, 11 μmol, 5 mol%), $AgNTf_2$ (4.1 mg, 11 μmol, 5 mol%), freshly distilled toluene (1.0 mL, 0.2M) and boric acid (50.2 mg, 812 μmol, 398 mol%). The mixture was placed in an oil bath at 80 °C and allowed to stir for 72 h. After, allowing the mixture to cool to ambient temperature, it was purified by flash chromatography (SiO_2, Hexanes:Et_2O 90:10–85:15). The product **8a** was obtained as a colorless solid in 69% yield (30.8 mg, 141 μmol, 99% ee).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 – 7.94 (m, 2H), 7.63 (td, *J* = 7.2, 1.3 Hz, 1H), 7.54 – 7.48 (m, 2H), 4.77 – 4.63 (m, 1H), 3.70 – 3.26 (m, 3H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ -79.2 (d, *J* = 6.9 Hz) ppm.

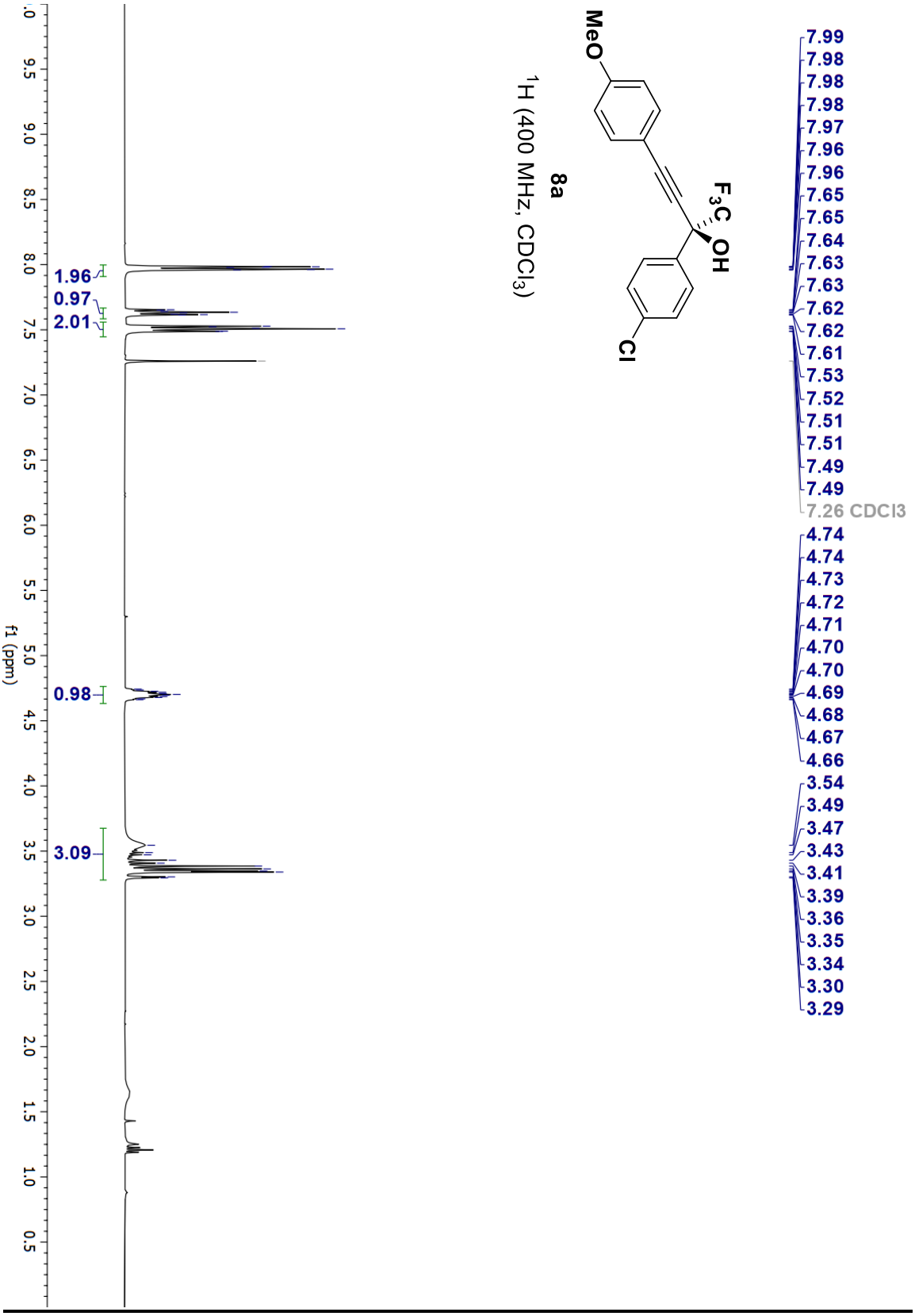
HRMS: Known compound, see reference 21.

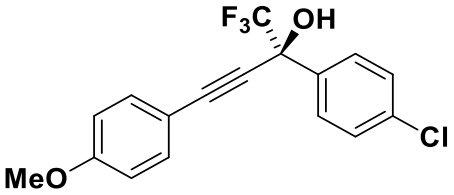
HPLC (CHIRALPAK AD-H, hexanes:2-PrOH = 95:5, 1.0 mL/min, 254 nm): ee = 99%.

$[\alpha]_D^{20}$ = -31° ($CHCl_3$, c = 1.0).

m.p. 50 °C.

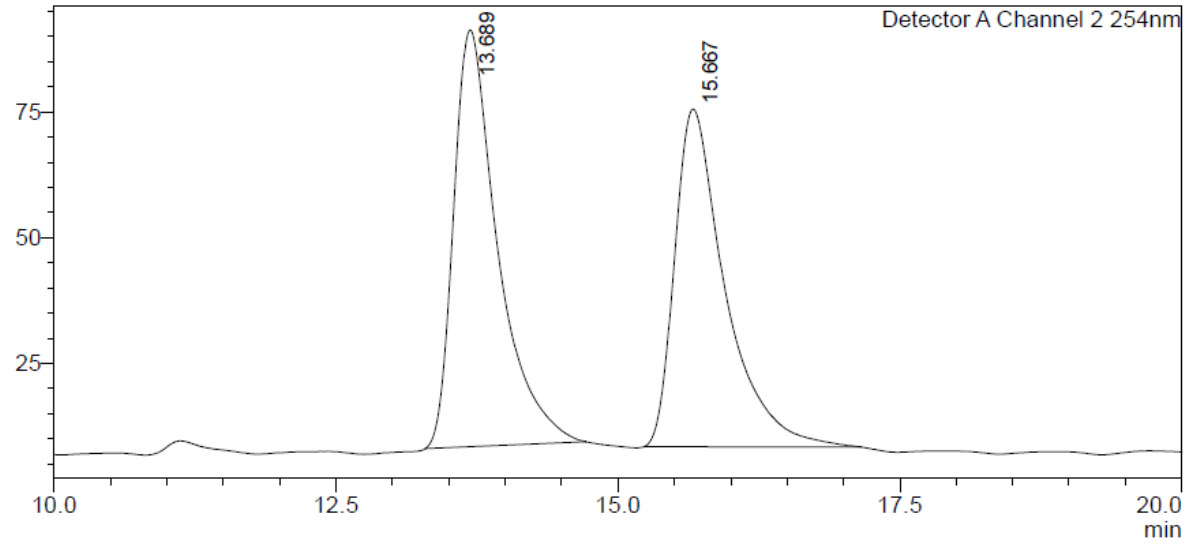
The analytical data are in good agreement with the literature.[21]


8a
^{1}H (400 MHz, CDCl$_3$)
MeO
F$_3$C
OH
Cl
7.99
7.98
7.98
7.98
7.97
7.96
7.96
7.65
7.65
7.64
7.63
7.63
7.62
7.62
7.61
7.53
7.52
7.51
7.51
7.49
7.49
7.26 CDCl3
4.74
4.74
4.73
4.72
4.71
4.70
4.70
4.69
4.68
4.67
4.66
3.54
3.49
3.47
3.43
3.41
3.39
3.36
3.35
3.34
3.30
3.29
1.96
0.97
2.01
0.98
3.09
f1 (ppm)



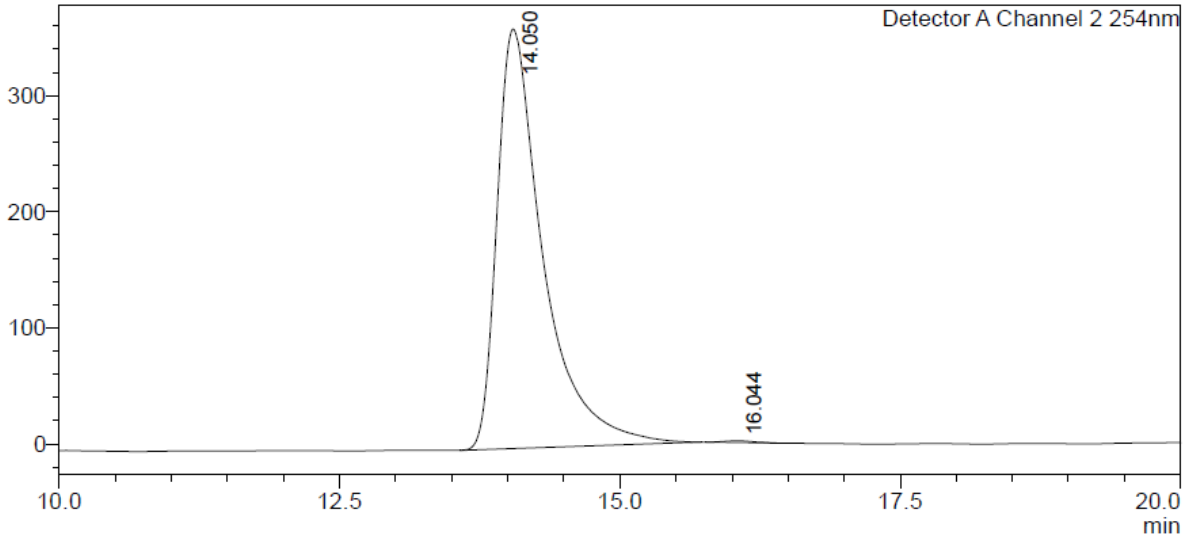
8a

^{19}F (376 MHz, $CDCl_3$)



Detector A Channel 2 254nm

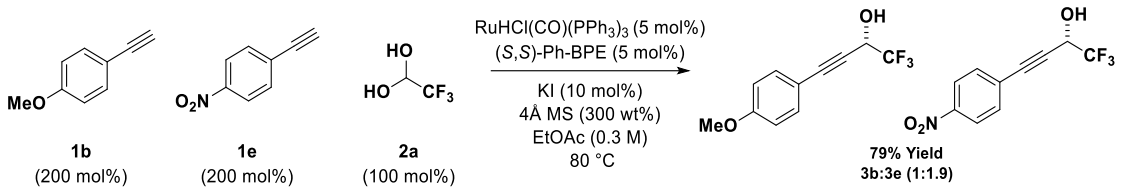
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	13.689	2248519	82891	51.842		M	
2	15.667	2088722	67148	48.158		M	
Total		4337240	150039				



Detector A Channel 2 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	14.050	10339479	361242	99.710		M	
2	16.044	30085	1556	0.290		M	
Total		10369564	362798				

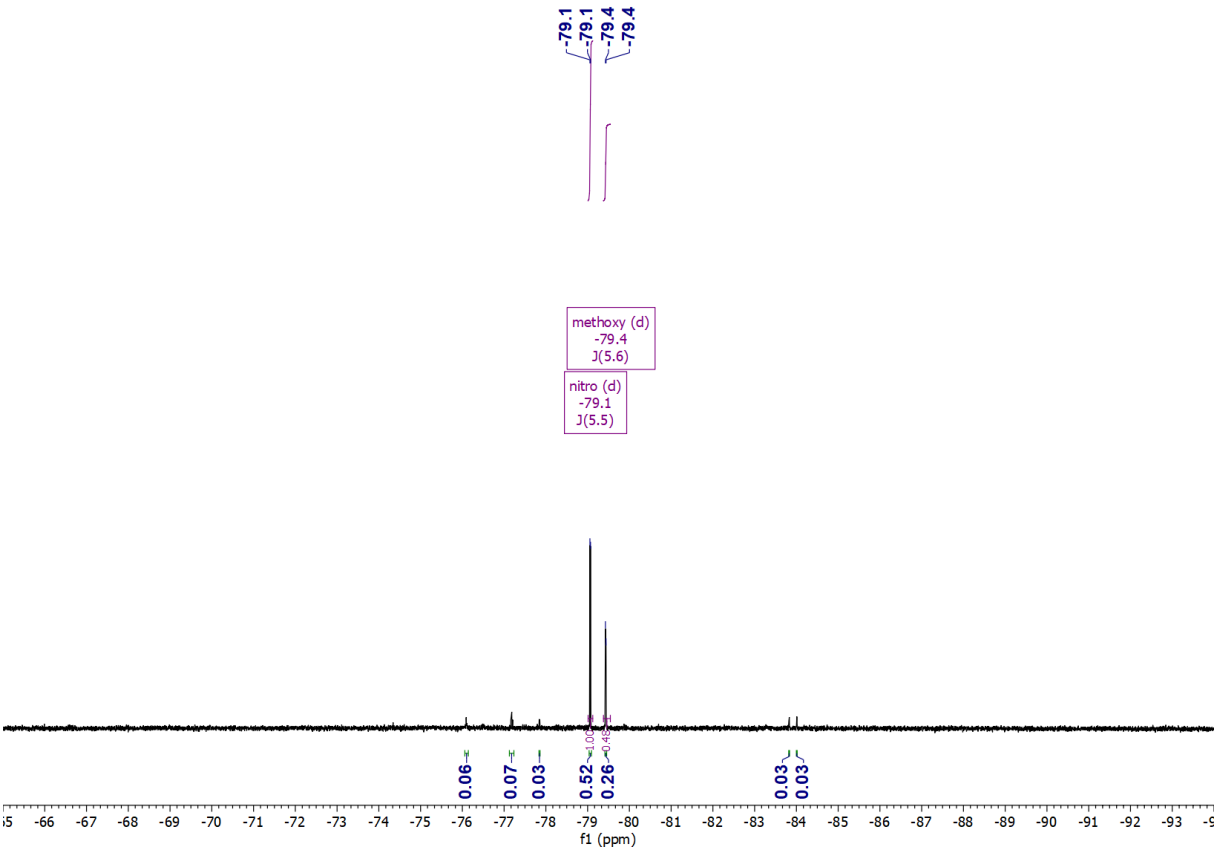
X Competitive Experiment



1b (200 mol%) **1e** (200 mol%) **2a** (100 mol%)

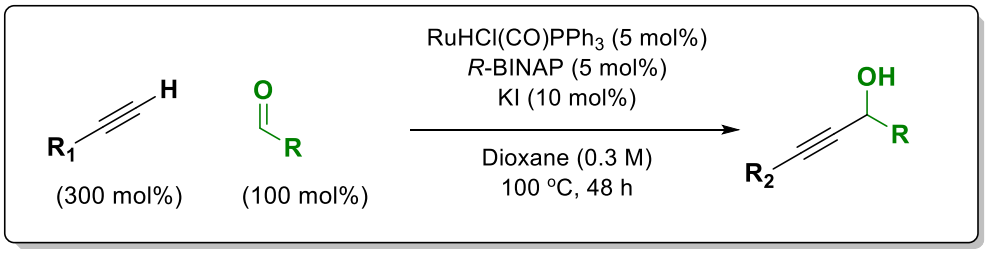
79% Yield
3b:3e (1:1.9)

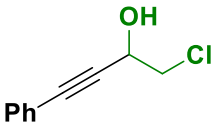
A pressure tube equipped with a magnetic stir bar was charged with $RuHCl(CO)(PPh_3)_3$ (9.5 mg, 0.01 mmol, 5 mol%), (*S*,*S*)-Ph-BPE (5.1 mg, 0.01 mmol, 5 mol%), KI (3.2 mg, 0.02 mmol, 10 mol%), 4Å molecular sieves (90 mg, 300 wt%) and ethyl acetate (0.67 mL) under air. The tube was sealed with a PTFE-lined cap, placed in an oil bath and was allowed to stir at 80 ºC. After 15 minutes, the reaction mixture was allowed to reach ambient temperature. The cap was removed from the tube and the terminal alkyne **1b**,**1e** (0.21 mmol, 105 mol%) and fluoral (**2a**, 76 wt% in H_2O, 21 μL, 0.2 mmol, 100 mol%) were added. The tube was resealed with the cap, placed in an oil bath and was allowed to stir for 24 hours at 80 ºC. The reaction mixture was allowed to reach ambient temperature, and the overall yield and ratio was determined by crude ^{19}F NMR.



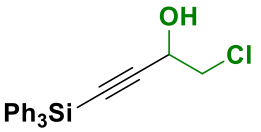
XI. Other Substrates That Were Investigated

The following table displays some selected results of alkynylations of non-fluorinated aldehydes. While some less activated aldehydes seem to be competent electrophiles for alkynylation under the developed conditions, they yield products of unsatisfactory enantiomeric excess.

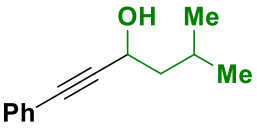




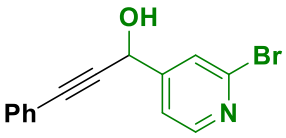
99% Yield, 23% ee
(*S*,*S*)-Ph-BPE



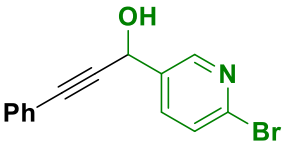
99% Yield, 52% ee
(*S*,*S*)-Ph-BPE



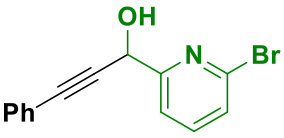
21% Yield, 26% ee



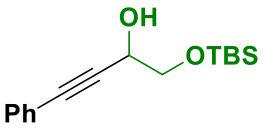
80% Yield, 14% ee



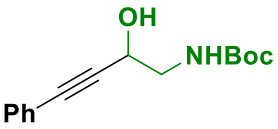
87% Yield, 10% ee
using 3 eq. of TFE



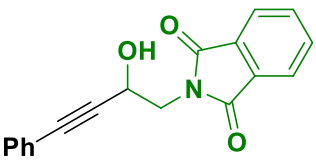
99% Yield, 36% ee
using 3 eq. of TFE



94% Yield, 7% ee
(*S*,*S*)-Ph-BPE



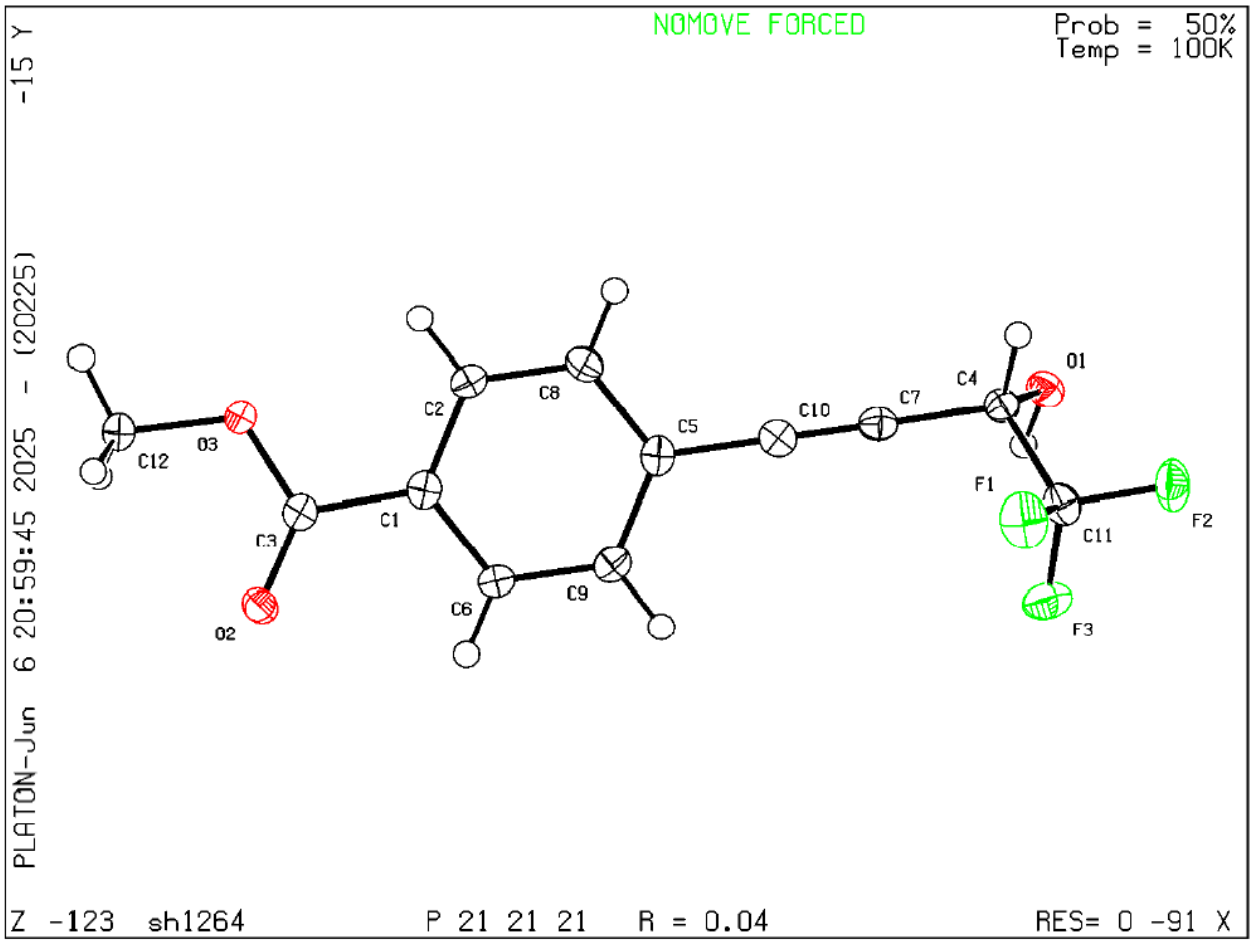
53% Yield, 11% ee
(*S*,*S*)-Ph-BPE



86% Yield, 4% ee

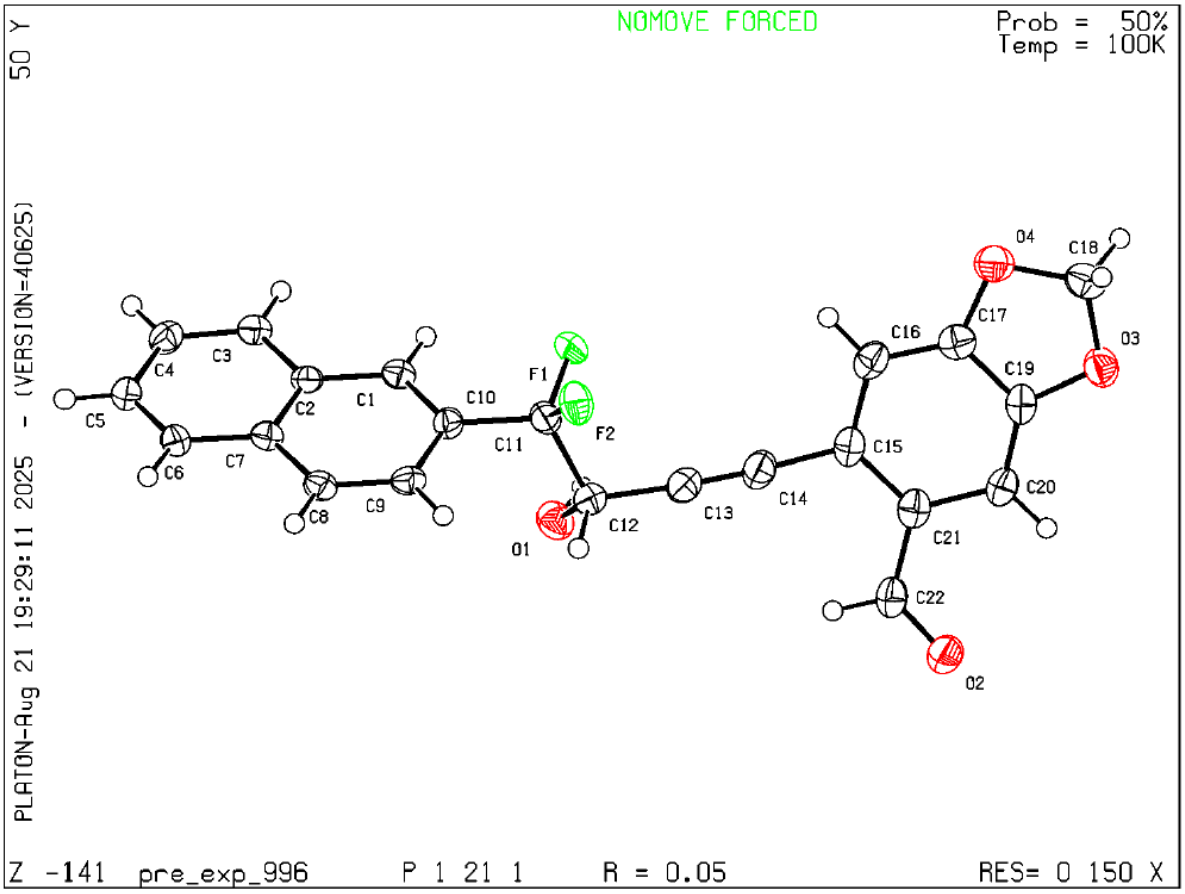
XII. Single Crystal Diffraction Data

Crystal data and structure refinement for **3d**



Crystal data	
Chemical formula	$C_{12}H_9F_3O_3$
M_r	258.19
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	100
***a*, *b*, *c* (Å)**	6.11735 (14), 7.1588 (2), 25.3548 (6)
***V* (Å3)**	1110.36 (5)
Z	4
Radiation type	Cu $K\alpha$
μ **(mm^{-1})**	1.26
Crystal size (mm)	0.4 × 0.02 × 0.02
Data collection	
Diffractometer	XtaLAB Synergy, Single source at home/near, HyPix
Absorption correction	Multi-scan *CrysAlis PRO* 1.171.43.144a (Rigaku Oxford Diffraction, 2024) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.492, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9573, 2203, 2107
R_{int}	0.041
(sin $\theta/\lambda)_{max}$ (Å−1)	0.629
Refinement	
$R[F^2 > 2\sigma(F2)]$, $wR(F^2)$, S	0.040, 0.102, 1.11
No. of reflections	2203
No. of parameters	168
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ **(e Å−3)**	0.36, −0.26
Absolute structure	Flack x determined using 819 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	-0.10 (9)

Crystal data and structure refinement for **5b**



Crystal data	
Chemical formula	$C_{22}H_{14}F_2O_4$
M_r	380.33
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	100
a, b, c (Å)	11.3663 (3), 5.7598 (1), 13.2621 (3)
β (°)	95.504 (2)
V (Å3)	864.24 (3)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.97
Crystal size (mm)	0.23 × 0.07 × 0.05
Data collection	
Diffractometer	SuperNova, Dual, Cu at home/near, HyPix
Absorption correction	Multi-scan
CrysAlis PRO 1.171.43.144a (Rigaku Oxford Diffraction, 2024) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	
T_{min}, T_{max}	0.492, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15521, 3473, 3233
R_{int}	0.095
(sin $\theta/\lambda)_{max}$ (Å−1)	0.632
Refinement	
$R[F^2 > 2\sigma(F2)]$, $wR(F^2)$, S	0.045, 0.124, 1.09
No. of reflections	3473
No. of parameters	257
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å−3)	0.21, −0.20
Absolute structure	Flack x determined using 1275 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	0.15 (15)

XIII. Computational Data

The computational study mainly focused on identifying the factors responsible for the enantioselectivity toward one specific product enantiomer: i) the formation of diastereotopic complexes between the catalyst, ligands, and reactants, and ii) the nucleophilic addition step.

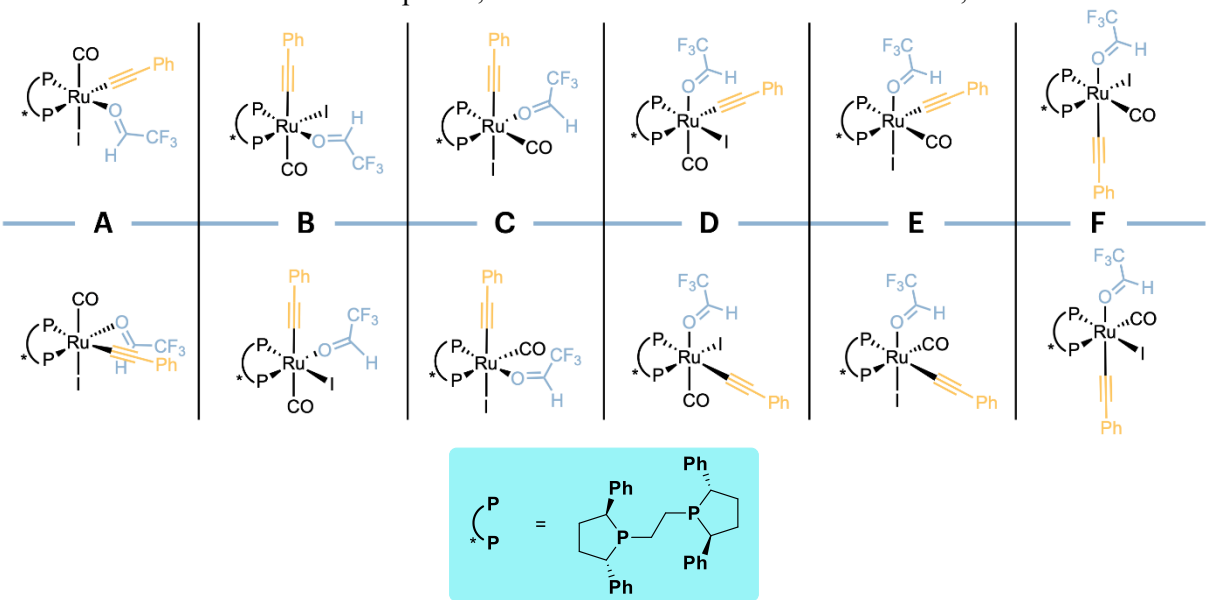
First, a conformational analysis was carried out for the geometries of each complex using the metadynamic at GFN2-xTB[22] implemented in CREST[23] (version 3.0.2) implementing APLB[24] to implicitly include the solvent ethyl acetate. The resulting ensemble was clustered on the dihedral angle using the *k*-mean algorithm and PCA statistical analysis. The reduced ensemble was refined using ORCA (version 6.1.0)[25] at different levels of theory: i) a single point energy evaluation to remove high-lying conformers at PBE[26]-D4[27]/def2-SV(P)[28] [CPCM(ethyl acetate)][29], ii) optimization of the remaining conformers at r^{2}SCAN-3c[30] [CPCM(ethyl acetate)] level of theory, and iii) evaluation of the final energies at ωB97X-D4rev[31,32]/def2-QZVPP [CPCM(ethyl acetate)] to refine the electronic energy and re-rank the final ensemble. This analysis was necessary to identify the most suitable conformer as the starting point for the subsequent reaction study. The selected conformer was employed to construct the product structure, providing the two critical points required for a Nudged Elastic Band (NEB) calculation to generate a reliable transition state (TS) guess. From this geometry, an initial constrained optimization was performed, followed by a full optimization toward the saddle point. To account for the potential flexibility of the complex, an additional CREST run was carried out on the TS geometry—with the reacting atoms constrained—followed by a subsequent TS optimization. The *pre-* and *post-*reaction complexes were then obtained by optimizing the geometries generated through displacement of the TS structure along its unique imaginary frequency. Every geometry optimization was conducted at the r^{2}SCAN-3c [CPCM(ethyl acetate)] level of theory, and the final electronic energy was evaluated using ωB97X-D4rev/def2-QZVPP [CPCM(ethyl acetate)]. Therefore, the final free Gibbs energy is calculated as:

$$G = E_{\omega B97X-D4rev} + G_{thr,r2SCAN-3c}$$

where $E_{\omega B97X\text{-}D4rev}$ is the electronic energy at ωB97X-D4rev/def2-QZVPP [CPCM(ethyl acetate)] and $G_{thr,r2SCAN\text{-}3c}$ is the thermal correction obtained at the r^{2}SCAN-3c level under standard conditions and at the reaction temperature of 353K.

Evaluation of the diastereomeric complexes

It is possible to generate six-different pseudo-enantiomeric complexes, that are in fact diastereomeric by virtue of the enantiomerically pure ligand (*S*,*S*)-Ph-BPE. For the following discussion, to differentiate between these diastereomeric complexes, the bottom row will be addressed as **A'** ,**B'** *etc*.



The computed respective populations of these complexes are reported in the following table.

Complex	Conformers	ΔG_{av} / kcal mol^{-1}	Population (%)
A	4	9.58	0.00
A'	3	6.82	0.01
B	1	7.14	0.00
B'	1	5.36	0.04
C	1	14.17	0.00
C'	2	13.15	0.00
D	3	1.45	11.23
D'	4	0.00	88.72
E	7	21.74	0.00
E'	1	18.63	0.00
F	1	9.86	0.00
F'	7	9.35	0.00

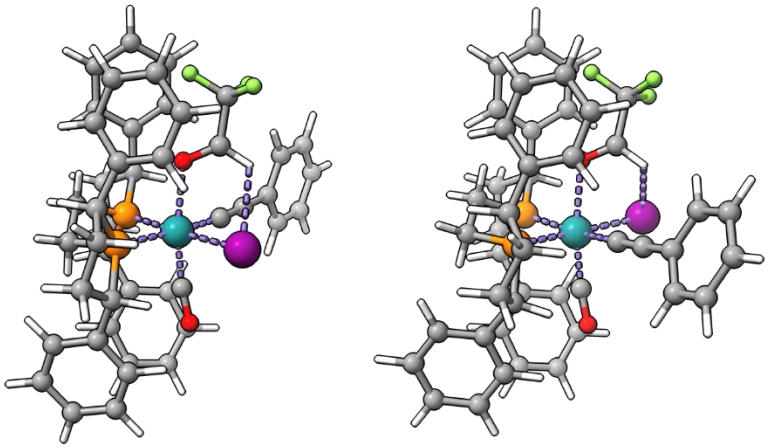
The average free energy has been calculated as:

$$G_{av} = \sum_i p_i G_i$$

$$\frac{p_i}{p_{tot}} = \frac{g_i exp\{-\Delta G_i/RT\}}{\sum_j g_j \, exp\{-\Delta G_j/RT\}}$$

where g_i is the degeneracy of the conformer, R is the gas constant, and T is the absolute temperature.

The following figure shows the best conformers for **D** and **D'**.



D *D′*

As reported previously[33], the important interactions between the hydrogen atom of the aldehyde and Ruthenium-bound iodide are highlighted.

TS optimization

Each complex was used to find its transition state, always considering the stabilizing interaction of the hydrogen atom of the aldehyde pointing toward the iodide, thus reducing the possible approachable diastereotopic faces to one. The following table features the energies obtained from the optimization of the ten reactions. Like their respective ground states, the transition states originating from **D** and **D'** account for >99% of all populated states.

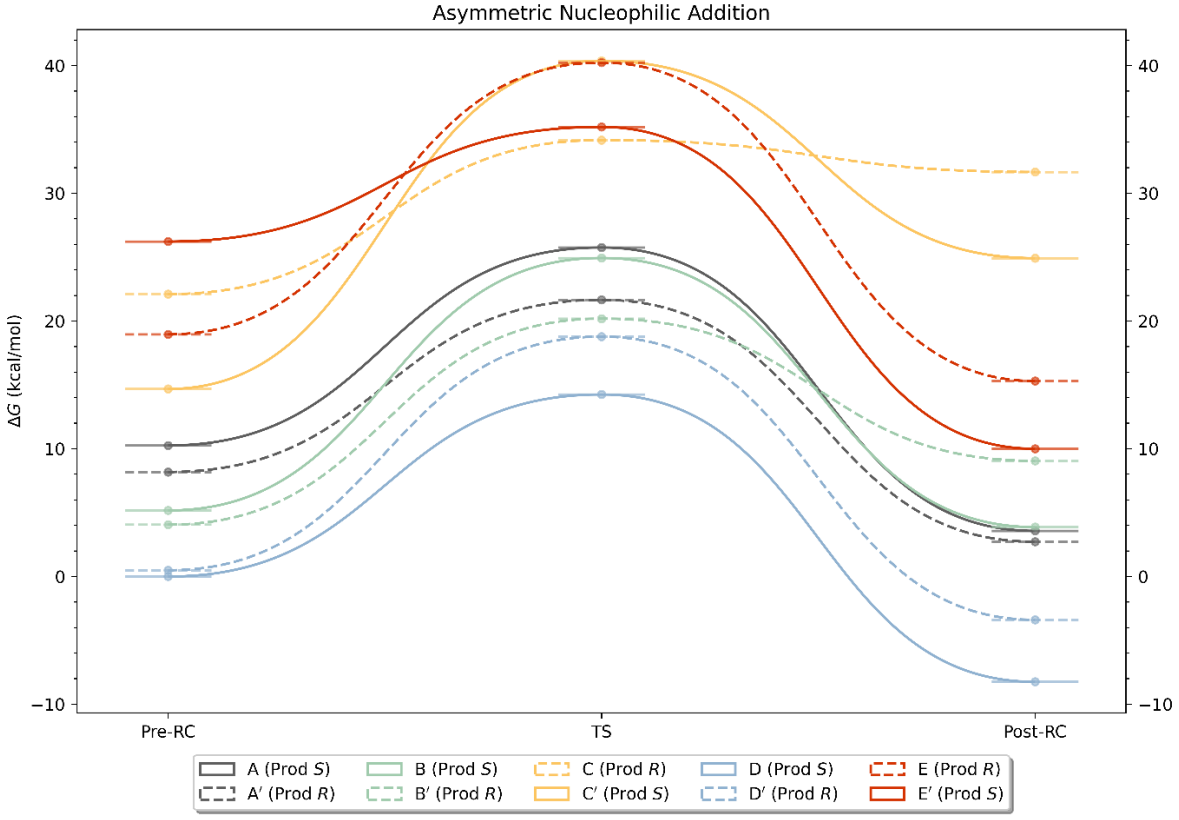
	A	A'	B	B'	C	C'	D	D'	E	E'
Pre-RC	10.26	8.18	5.18	4.06	22.11	14.68	0	0.49	18.96	26.22
TS	25.76	21.66	24.94	20.19	34.16	40.37	**14.25**	**18.78**	40.23	35.19
Post-RC	3.57	2.73	3.87	9.06	31.67	24.92	-8.24	-3.39	15.3	10
TS Population	0	0	0	0.02	0	0	99.82	0.16	0	0
Enantiomer	S	R	S	R	R	S	S	R	R	S

The enantiomeric excess was evaluated from the Boltzmann populations evaluated on the TS's energies, then summing the populations that led to the (*S*)-enantiomer minus the sum of the populations toward the (*R*)-enantiomer.

$$ee_{\%} = \sum_{i}^{S} p_i - \sum_{j}^{R} p_j$$

Pre- and post-reaction complexes (Pre-RC/Post-RC) describe the optimized geometries coming from the displacement along the imaginary frequency of the TS.

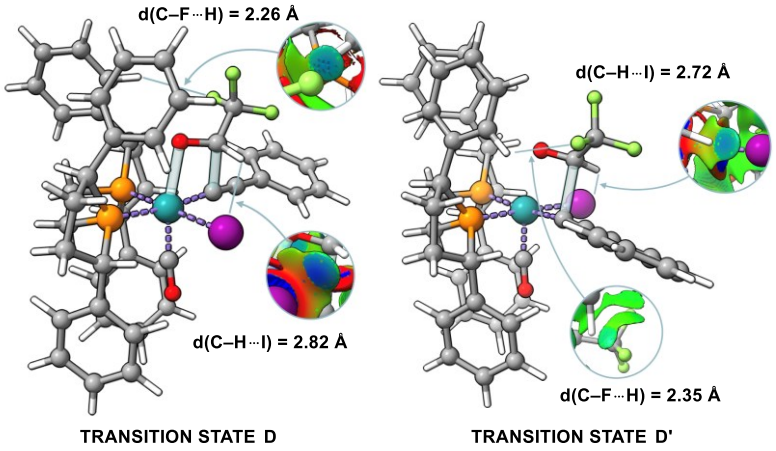
The computed enantiomeric excess is 99.6% in favor of the (*S*)-enantiomer, which is in perfect agreement with the experimentally obtained value of ee > 99%.



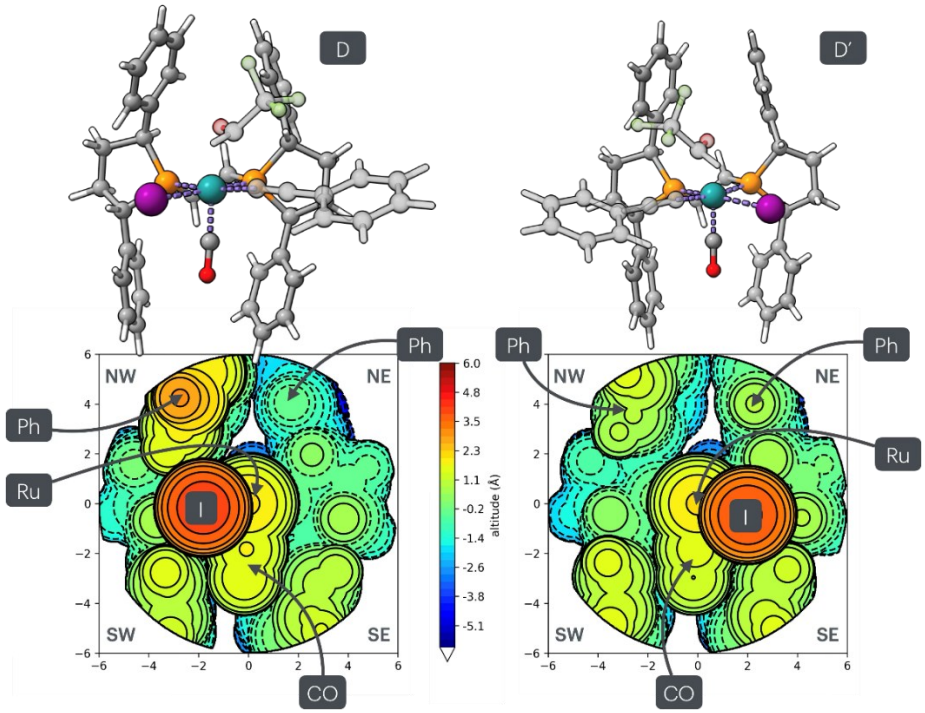
Rationalization from calculation

To study the interactions involved during the TS, a Non-Covalent Interaction analysis *via* NCIplot (version 4.2) [34] software was performed. This qualitative analysis was only carried out on the **D** and **D'** transition states (based on their population). The most important interactions are shown in the following

figure. The colors were chosen following the default coloring scheme: a blue surface represents an attractive interaction, a green one represents a van-der-Waals interaction, and a red one represents a repulsive interaction. The darker the color, the stronger the respective interaction. This figure shows that in the **D** transition state geometry non-covalent interactions appear more intense compared to those in the **D'** geometry.



Furthermore, steric hindrance was analyzed by evaluating the free volume around the metal center at the TS using the buried volume ($\%V_{bur}$) approach, as commonly employed in ligand steric analysis. A spherical region with a radius of 6 Å was defined around the ruthenium atom, and the volume occupied by the surrounding atoms was subtracted from this sphere to obtain $\%V_{bur}$. The sphere was subsequently dissected into octants to numerically assess the distribution of occupied and free space. These calculations were performed using the SEQCrow[35] toolkit within the ChimeraX[36] environment. The following figure displays maps in which the color represents the distance of the atoms from the ruthenium center.



D				D'			
FNE	FNW	FSW	FSE	FNE	FNW	FSW	FSE
0.8%	6.6%	5.0%	3.3%	2.7%	**2.2%**	2.8%	6.2%

The buried volume was calculated from these maps. The values are reported as the percentage of buried volume for the frontal four octants of the sphere. The reaction takes place in the frontal north-eastern quadrant (FNE) for the **D** complex and in the frontal north-western (FNW) quadrant for **D′**. As shown from the table above, the quadrant in which the reaction occurs exhibits more free volume in the TS of the **D** complex than in the **D′** one, providing a plausible explanation for the observed $\Delta\Delta G^{\ddagger}$ of 4.53 kcal/mol and the resulting high enantioselectivity.

To gain further insight into the reaction's chemoselectivity for fluorinated aldehydes in the presence of non-fluorinated ones, C–C bond formations through complexes following configurations **D** and **D′** were computed using acetaldehyde instead of fluoral (ωB97X-D4rev/def2-QZVPP [CPCM]//r^{2}SCAN-3c level at 353K). Both pathways show increased reaction barriers and are in fact endergonic for acetaldehyde.

	D (acetaldehyde)	**D′ (acetaldehyde)**
Pre-RC	2.0 kcal mol^{-1}	0.0 kcal mol^{-1}
TS	25.2 kcal mol^{-1}	29.8 kcal mol^{-1}
Post-RC	9.3 kcal mol^{-1}	14.0 kcal mol^{-1}

Further conformational relaxation at the ωB97X-D4rev/def2-QZVPP [CPCM]//r^{2}SCAN-3c level of theory (353K) may slightly lower the energy of the Post-RCs (ΔG(**D**)=7.9 kcal mol^{-1}; ΔG(**D′**)=11.8 kcal mol^{-1}), yet the reactions remain endergonic.

Natural Bond Orbital Analysis and "Fuzzy" Bond Order

Natural Bond Order (NBO) was carried out on 6 optimized TSs of the general configurations **D** and **D′**: **i)** using the experimentally employed Ru–I complex and trifluoroacetaldehyde, **ii)** using the experimentally employed Ru–I complex and acetaldehyde, and **iii)** using the analogous Ru-Cl complex and trifluoroacetaldehyde. These computations should give insight into the strength of formyl-hydrogen bonds upon exchange of the hydrogen bond donor or acceptor. Thus, the stabilization energy originating from this interaction was computed as the sum of the individual stabilization energies involving the halogens' orbitals with the formyl C-H σ*-orbital.

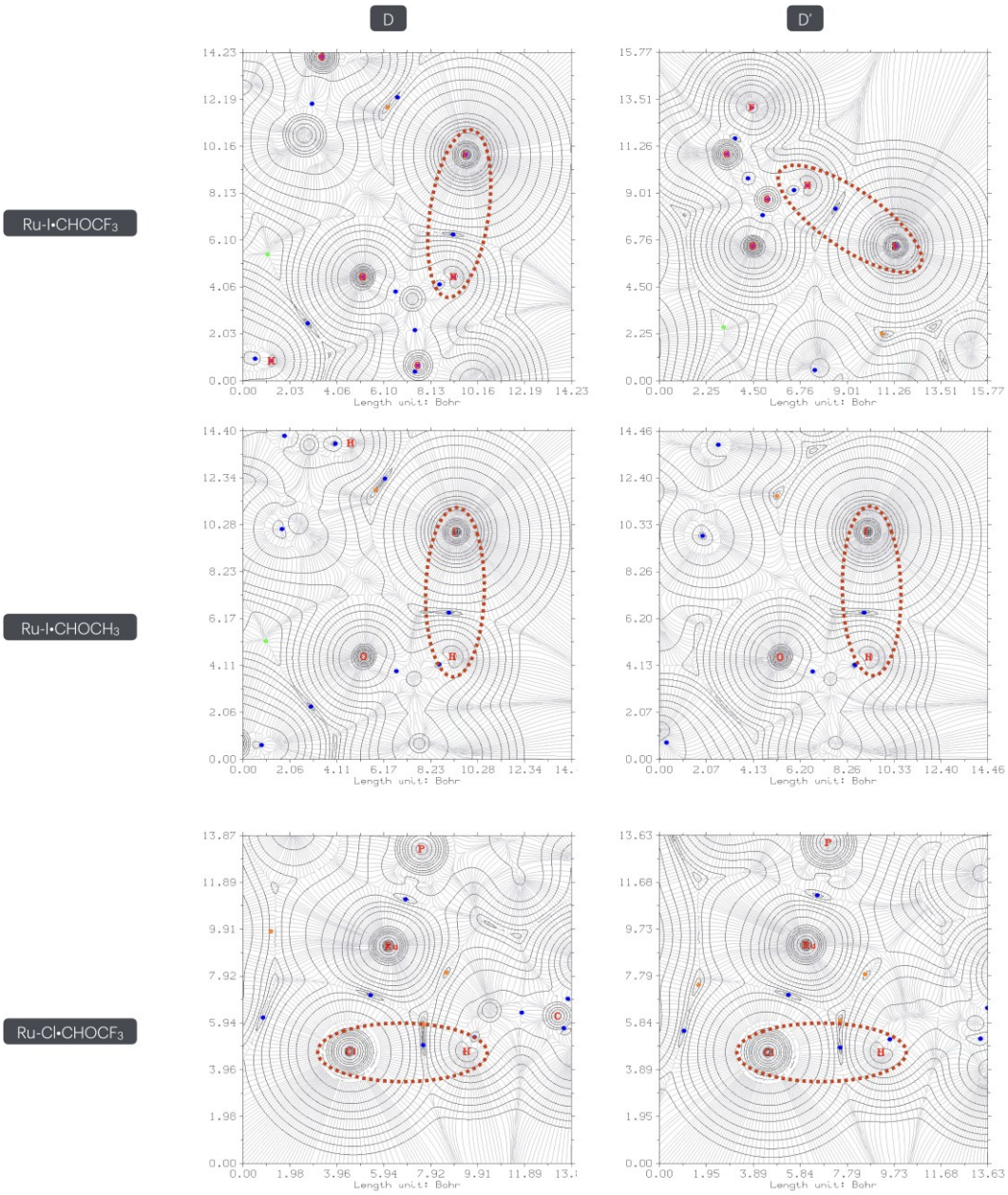
E (C–H···X)	**i)** [Ru]–I / CF_3CHO	**ii)** [Ru]–I / CH_3CHO	**iii)** [Ru]–Cl / CF_3CHO
D	3.21 kcal mol^{-1}	1.62 kcal mol^{-1}	1.81 kcal mol^{-1}
D′	4.61 kcal mol^{-1}	1.37 kcal mol^{-1}	3.26 kcal mol^{-1}

Furthermore, using MultiWFN[37], *fuzzy* bond order (FBO) analyses have been carried out on these transition states.

FBO	**i)** [Ru]–I / CF_3CHO	**ii)** [Ru]–I / CH_3CHO	**iii)** [Ru]–Cl / CF_3CHO
D	0.0753	0.0682	<0.05
D′	0.0910	0.0662	0.0633

Stabilizing orbital overlap as well as FBO are the most pronounced for the Ru–I complex with trifluoroacetaldehyde. Exchanging either trifluoroacetaldehyde for acetaldehyde or iodide for chloride leads to a significant decrease in both categories. The decrease upon exchanging the aldehyde may contribute to the observed chemoselectivity for fluorinated aldehydes over non-fluorinated ones. Decreases in stabilizing overlap and FBO upon exchanging the iodide-bound complex for the chloride-bound one, hint at the role of iodide as a more competent hydrogen bond acceptor in this specific case.

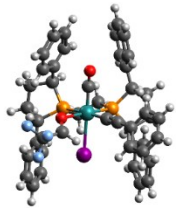
Additionally, Atom In Molecule (AIM) analyses were performed, and the gradient of the density was plotted along the plane spanned by the formyl C-H and the Ru-bound halide. Each of the 6 TSs shows bond critical points between the formyl hydrogen and the halide.



These points were characterized by the value of the density ($\rho(\mathbf{r})$), the value of the potential energy density ($V(\mathbf{r})$), the energy of the density ($H(\mathbf{r})$) and the Laplacian of the density ($\nabla^2\rho(\mathbf{r})$). From the positive values of $H(\mathbf{r})$ and $\nabla^2\rho(\mathbf{r})$, the presence of the non-covalent interaction can be confirmed.

	i) [Ru]–I / CF_3CHO		**ii)** [Ru]–I / CH_3CHO		**iii)** [Ru]–Cl / CF_3CHO	
	D	**D′**	**D**	**D′**	**D**	**D′**
$\rho(\mathbf{r})$ / a.u.	0.0137	0.0161	0.0123	0.0116	0.0133	0.0168
$V(\mathbf{r})$ / E_h	-0.0078	-0.0095	-0.0069	-0.0064	-0.0084	-0.0112
$H(\mathbf{r})$ / E_h	0.000705	0.000394	0.000874	0.000900	0.001378	0.001174
$\nabla^2\rho(\mathbf{r})$	0.0367	0.0411	0.0345	0.0326	0.0448	0.0544

A Pre-Reaction Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.5189794400
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6406168867
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9632962512
Imaginary Frequency (cm^{-1}): None

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C	-0.26021	-2.29712	1.84295
P	0.17057	0.46569	1.59900
P	0.23639	-2.32584	0.05571
C	-0.57797	-3.84365	-0.71396
C	0.20922	-5.01253	-0.09726
C	1.68758	-4.67125	-0.23593
C	1.92891	-3.18710	0.15590
C	1.47447	1.62858	2.29588
C	1.02132	1.80148	3.75382
C	-0.47115	2.11191	3.71915
C	-1.21295	1.21537	2.68161
C	-2.34886	1.98440	2.06251
C	3.02799	-2.56346	-0.65943
C	2.93431	1.30223	2.13061
C	-2.07046	-3.99902	-0.65135
C	-2.82399	-3.89001	-1.82340
C	-4.20367	-4.06316	-1.80633
C	-4.85652	-4.34861	-0.60973
C	-4.11392	-4.47690	0.56230
C	-2.73219	-4.31233	0.54050
C	3.70048	2.03688	1.21972
C	5.06928	1.82603	1.09631
C	5.70465	0.87619	1.89162
C	4.95775	0.14412	2.81041
C	3.58719	0.35661	2.93199
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C	-4.73304	2.40002	1.90385
C	-4.49616	3.50211	1.08590
C	-3.18489	3.85405	0.76988
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C	4.18887	-2.09745	-0.04056
C	5.24412	-1.58945	-0.79487
C	5.14924	-1.53584	-2.18163
C	3.98890	-1.98664	-2.80967
C	2.93923	-2.49599	-2.05558
Ru	0.02345	-0.03209	-0.64164
C	1.79699	0.32999	-0.97987
I	-2.76621	-0.37931	-0.54874
O	2.83767	0.68975	-1.33049
C	-0.30157	1.87284	-1.21967
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H	0.21278	-1.04372	3.55829
H	1.57019	-1.31590	2.45522
H	-0.01999	-3.24184	2.34440
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H	-0.28934	-3.76602	-1.77354
H	-0.06897	-5.14812	0.95417
H	-0.03827	-5.94393	-0.62017
H	2.32218	-5.32719	0.36941
H	1.98449	-4.80793	-1.28142
H	2.21182	-3.13149	1.21421
H	1.27626	2.57106	1.76301
H	1.22578	0.89456	4.33261
H	1.58320	2.61700	4.22343
H	-0.93910	2.00170	4.70308
H	-0.60187	3.15525	3.41318
H	-1.63361	0.33560	3.18282
H	-2.32124	-3.65355	-2.75899
H	-4.77055	-3.96907	-2.72865
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H	-4.61243	-4.71066	1.49921
H	-2.17095	-4.42797	1.46330
H	3.21260	2.78467	0.59915
H	5.64084	2.40890	0.37925
H	6.77492	0.71276	1.80131
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H	4.26818	-2.13262	1.04360
H	6.13970	-1.23317	-0.29356
H	5.97114	-1.14017	-2.77183
H	3.90056	-1.93718	-3.89171
H	2.03848	-2.84159	-2.55933
H	-2.68775	3.82152	-2.90530
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H	-1.52074	7.93515	-3.36015
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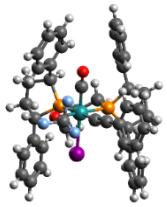
H	1.14309	5.13885	-1.47076
H	-1.66522	0.69402	-3.16600

A TS



Gibbs Energy @ r^2SCAN-3c[CPCM]: -3264.5063134800
Thermal Correction @ r^2SCAN-3c[CPCM]: 0.6436110065
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^2SCAN-3c[CPCM]: -3266.9386020638
Imaginary Frequency (cm^{-1}): -173.16

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P	0.14215	-2.45547	0.11504
C	-0.67417	-4.02309	-0.55157
C	0.19874	-5.14557	0.03877
C	1.64943	-4.75835	-0.20769
C	1.86353	-3.26674	0.16327
C	1.32472	1.62487	2.13827
C	0.91400	1.82752	3.60552
C	-0.59177	2.07188	3.61976
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C	-2.48624	1.86920	1.99156
C	2.92535	-2.62955	-0.68897
C	2.79317	1.35719	1.94026
C	-2.14830	-4.24602	-0.36214
C	-2.99113	-4.26358	-1.47695
C	-4.35190	-4.51698	-1.34236
C	-4.89676	-4.75555	-0.08318
C	-4.06386	-4.75879	1.03363
C	-2.70048	-4.51702	0.89439
C	3.50441	2.10650	0.99727
C	4.87732	1.95166	0.84095
C	5.57333	1.04382	1.63465
C	4.88223	0.29918	2.58620
C	3.50775	0.45677	2.74141
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C	-4.87765	2.26446	1.88640
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C	-3.37232	3.70047	0.67669
C	-2.28928	2.97140	1.15561
C	4.09478	-2.13608	-0.10840
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C	3.81462	-2.06451	-2.87241
C	2.79615	-2.58265	-2.08262
Ru	-0.15489	-0.23467	-0.67769
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C	-0.55047	2.80723	-1.88155
C	-0.62065	4.14745	-2.31264
C	-1.86658	4.74915	-2.58118
C	-1.92582	6.06548	-3.01340
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C	0.48543	6.21787	-2.91588
C	0.55813	4.89858	-2.49303
C	-0.92870	0.43433	-3.17538
C	-0.41130	1.15522	-4.42966
F	0.89177	1.47909	-4.35221
F	-0.55418	0.32199	-5.49440
F	-1.11460	2.27142	-4.70301
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H	1.54074	-1.29735	2.41381
H	0.02398	-3.28158	2.44570
H	-1.36099	-2.24984	2.00884
H	-0.47066	-3.96869	-1.63159
H	-0.00249	-5.26041	1.11030
H	-0.05157	-6.09860	-0.44195
H	2.34835	-5.38793	0.35338
H	1.87545	-4.89001	-1.27140
H	2.17397	-3.19639	1.21316
H	1.07341	2.54142	1.58296
H	1.18084	0.95030	4.20388
H	1.45537	2.68177	4.02801
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H	-0.77759	3.10527	3.30928
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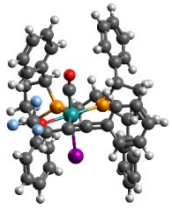
H	1.39759	6.79231	-3.04885
H	1.51773	4.43031	-2.29563
H	-2.00487	0.56992	-2.99447

A Post-Reaction Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.5643600904
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6490364662
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9739540516
Imaginary Frequency (cm^{-1}): None

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P	0.08761	-2.08053	-0.12770
C	-0.82915	-3.61834	-0.69736
C	-0.02335	-4.75157	-0.03413
C	1.44983	-4.47035	-0.29812
C	1.75978	-2.97501	-0.02426
C	1.64954	2.07749	1.14492
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C	-4.24891	-3.99459	0.94537
C	-2.87374	-3.85389	0.78629
C	4.07115	1.37569	1.04412
C	5.24033	0.90890	1.64137
C	5.25278	0.57274	2.99087
C	4.08744	0.71743	3.74320
C	2.92528	1.19354	3.14783
C	-2.95700	0.81078	2.85713
C	-4.33211	0.63877	2.95587
C	-5.19447	1.51139	2.29386
C	-4.66547	2.55791	1.54402
C	-3.28713	2.72183	1.43923
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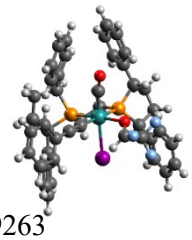
C	5.10791	-1.58063	-1.14969
C	4.99557	-1.65154	-2.53469
C	3.81281	-2.11727	-3.10728
C	2.75674	-2.51815	-2.29921
Ru	-0.15326	-0.06337	-1.17440
C	1.61139	0.26566	-1.54572
I	-2.93885	-0.15840	-0.90320
O	2.65428	0.66333	-1.86156
C	-0.64915	1.25179	-3.12740
O	-0.46359	-1.07088	-3.04546
C	-0.53797	2.32883	-2.56119
C	-0.49369	3.63399	-2.00911
C	-1.69540	4.31107	-1.73672
C	-1.66002	5.59347	-1.20596
C	-0.43810	6.21002	-0.94008
C	0.75605	5.54481	-1.21664
C	0.73549	4.26412	-1.75137
C	-0.79728	-0.01832	-3.87194
C	0.09885	0.00854	-5.12169
F	1.40859	0.14546	-4.81886
F	-0.03143	-1.14003	-5.82208
F	-0.23260	1.02920	-5.95140
H	0.24657	-0.31276	3.14393
H	1.56138	-0.79392	2.07052
H	-0.08103	-2.66879	2.26156
H	-1.39757	-1.59654	1.71482
H	-0.62631	-3.64001	-1.77853
H	-0.23258	-4.79022	1.04135
H	-0.33015	-5.71406	-0.45907
H	2.10654	-5.10279	0.30844
H	1.66854	-4.68702	-1.34907
H	2.06517	-2.85421	1.02257
H	1.88372	2.33927	0.10784
H	1.34040	3.28770	2.92487
H	1.61699	4.22966	1.45631
H	-0.84886	4.16997	2.33409
H	-0.65642	3.68179	0.64609
H	-0.54114	1.78601	3.03635
H	-2.73537	-3.68927	-2.59583
H	-5.17386	-3.97236	-2.31979
H	-6.15818	-4.14571	-0.04302
H	-4.66827	-4.08024	1.94420
H	-2.23964	-3.84402	1.66795
H	4.07203	1.63123	-0.01133
H	6.14339	0.80862	1.04562
H	6.16310	0.20642	3.45720
H	4.08579	0.46361	4.79979
H	2.02871	1.31026	3.75209
H	-2.29250	0.13519	3.39228
H	-4.73311	-0.17298	3.55694
H	-6.27036	1.38257	2.37247
H	-5.32874	3.25036	1.03255
H	-2.89383	3.54017	0.84352
H	4.14098	-1.92294	0.74190
H	6.02398	-1.21445	-0.69445
H	5.82265	-1.34075	-3.16707
H	3.71018	-2.16118	-4.18815
H	1.83259	-2.86381	-2.75764
H	-2.64077	3.81698	-1.93907
H	-2.59014	6.11277	-0.99425
H	-0.41608	7.21194	-0.52141
H	1.70777	6.02813	-1.01611
H	1.66009	3.74038	-1.97538
H	-1.83676	-0.06878	-4.25790

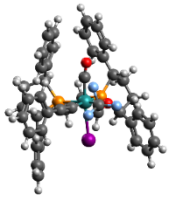
A' Pre-Reaction Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.5217080700
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6421720210
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9666032868
Imaginary Frequency (cm^{-1}): None

C	0.46929	-1.64101	2.31100
C	-0.23457	-2.35232	1.15663
P	0.40251	0.22136	2.14796
P	0.34967	-1.63271	-0.44994
C	-0.49989	-2.62100	-1.80497
C	0.17008	-3.99889	-1.66873
C	1.67790	-3.76640	-1.58846
C	2.00188	-2.51609	-0.71654
C	1.84801	0.73392	3.25684
C	1.35233	0.33757	4.65545
C	-0.06162	0.89420	4.79687
C	-0.87011	0.70315	3.47546
C	-1.71695	1.91921	3.20471
C	3.10691	-1.69281	-1.32236
C	3.23787	0.26900	2.91410
C	-1.99904	-2.66076	-1.87968
C	-2.64874	-1.99683	-2.92412
C	-4.03249	-2.04689	-3.05218
C	-4.79323	-2.76587	-2.13353
C	-4.15495	-3.44510	-1.09789
C	-2.76945	-3.39938	-0.97570
C	4.10610	1.13896	2.24495
C	5.42487	0.78267	1.98704
C	5.90896	-0.45564	2.40063
C	5.05904	-1.33166	3.06970
C	3.73768	-0.97340	3.32631
C	-3.09741	1.86461	3.40963
C	-3.89009	2.99668	3.24525
C	-3.31056	4.20671	2.87204
C	-1.93206	4.27608	2.67969
C	-1.14272	3.14318	2.85098
C	4.31105	-1.52311	-0.63893
C	5.36982	-0.83163	-1.22299
C	5.23488	-0.29317	-2.49826
C	4.03139	-0.44719	-3.18551
C	2.97960	-1.14377	-2.60491
Ru	0.19859	0.63738	-0.23200
C	1.97522	1.05361	-0.48687
I	-2.59006	0.42980	0.02734
O	3.01541	1.51115	-0.70112
C	-0.10119	0.79421	-2.21815
O	-0.08785	2.84020	-0.11865
C	-0.28592	0.89083	-3.42856
C	-0.55548	0.95253	-4.82030
C	0.48935	0.90833	-5.76458
C	0.21513	0.94986	-7.12579
C	-1.10094	1.03727	-7.57933
C	-2.14497	1.08392	-6.65563
C	-1.88066	1.04269	-5.29263
C	-0.91856	3.40464	-0.80882
C	-0.98171	4.93491	-0.82278
F	-2.22410	5.34432	-0.49735
F	-0.10807	5.49553	0.02002
F	-0.71449	5.37203	-2.07217
H	0.04551	-1.95976	3.26913
H	1.53353	-1.90808	2.31483
H	-0.03562	-3.42980	1.19574
H	-1.31803	-2.19510	1.20331
H	-0.12864	-2.14413	-2.72339
H	-0.20094	-4.52015	-0.77997
H	-0.08776	-4.61904	-2.53473
H	2.20606	-4.64273	-1.19942
H	2.05667	-3.58153	-2.59857
H	2.31592	-2.82877	0.28662
H	1.84395	1.83200	3.19474
H	1.35748	-0.75105	4.77351
H	2.01900	0.74874	5.42280
H	-0.59965	0.44090	5.63594
H	0.00494	1.96895	4.99714
H	-1.53067	-0.16729	3.55661
H	-2.05925	-1.42141	-3.63402
H	-4.51699	-1.51973	-3.86981
H	-5.87483	-2.80505	-2.22833
H	-4.73852	-4.01789	-0.38219
H	-2.29309	-3.94717	-0.16751
H	3.74193	2.11437	1.93282
H	6.07741	1.47779	1.46588
H	6.94113	-0.73419	2.20681
H	5.42670	-2.29733	3.40632
H	3.10954	-1.66178	3.88335
H	-3.55687	0.91881	3.68696
H	-4.96323	2.93138	3.40328
H	-3.92615	5.09189	2.73832
H	-1.46910	5.21858	2.40144
H	-0.06787	3.21741	2.69973
H	4.42175	-1.93176	0.36294
H	6.29970	-0.71200	-0.67417
H	6.05941	0.24745	-2.95470
H	3.91084	-0.01975	-4.17743
H	2.04523	-1.24651	-3.15217
H	1.51475	0.84127	-5.41159
H	1.03432	0.91438	-7.83910
H	-1.31133	1.07007	-8.64443
H	-3.17331	1.15292	-7.00057
H	-2.69369	1.07879	-4.57263
H	-1.63467	2.88334	-1.45973

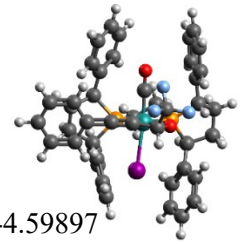
A' TS



Gibbs Energy @ r^2SCAN-3c[CPCM]: -3264.5096365000
Thermal Correction @ r^2SCAN-3c[CPCM]: 0.6453239240
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^2SCAN-3c[CPCM]: -3266.9451342802
Imaginary Frequency (cm^{-1}): -180.94

C	0.42986	-1.70901	2.36358
C	-0.26886	-2.38975	1.18666
P	0.35312	0.15639	2.25291
P	0.25607	-1.56358	-0.39001
C	-0.59069	-2.51865	-1.77412
C	0.13245	-3.87547	-1.72052
C	1.63241	-3.59495	-1.65843
C	1.93174	-2.37363	-0.73779
C	1.84353	0.66442	3.30192
C	1.39743	0.27026	4.71883
C	-0.00175	0.84435	4.91281
C	-0.86488	0.63220	3.63128
C	-1.73609	1.83756	3.39188
C	2.99086	-1.48618	-1.33447
C	3.22560	0.19974	2.92686
C	-2.08859	-2.61457	-1.81127
C	-2.79322	-1.91779	-2.79635
C	-4.17729	-2.01140	-2.89039
C	-4.88395	-2.81184	-1.99635
C	-4.19085	-3.52617	-1.02133
C	-2.80523	-3.43383	-0.93260
C	4.09849	1.08897	2.28996
C	5.41563	0.73583	2.01945
C	5.89317	-0.51975	2.38545
C	5.03895	-1.41499	3.02320
C	3.72035	-1.05859	3.29548
C	-3.08243	1.80242	3.76131
C	-3.88939	2.92780	3.62169
C	-3.35897	4.10790	3.10511
C	-2.01378	4.15566	2.74502
C	-1.20776	3.03247	2.89965
C	4.21123	-1.31663	-0.68089
C	5.23309	-0.56930	-1.26170
C	5.04465	0.02571	-2.50435
C	3.82477	-0.12848	-3.16180
C	2.80920	-0.87940	-2.58423
Ru	0.04382	0.67738	-0.05015
C	1.79600	1.16466	-0.33123
I	-2.72756	0.33005	0.31174
O	2.81553	1.66865	-0.53932
C	-0.33621	1.14163	-2.03918
O	-0.28378	2.95833	-0.14188
C	-0.42458	1.12794	-3.27411
C	-0.53779	1.15984	-4.67806
C	0.60466	1.37241	-5.47617
C	0.49439	1.39938	-6.85846
C	-0.74899	1.22300	-7.46603
C	-1.88823	1.02119	-6.68597
C	-1.78991	0.98742	-5.30311
C	-0.86679	2.94751	-1.26893
C	-0.39907	4.01176	-2.27498
F	-0.61671	5.24106	-1.73688
F	0.91389	3.93098	-2.55814
F	-1.08883	3.95969	-3.43240
H	0.01162	-2.05792	3.31362
H	1.49505	-1.96983	2.35541
H	-0.02966	-3.45934	1.16882
H	-1.35577	-2.27431	1.25871
H	-0.26174	-1.99049	-2.68143
H	-0.19897	-4.45167	-0.85040
H	-0.12298	-4.46285	-2.60984
H	2.19580	-4.46951	-1.31786
H	1.98629	-3.35424	-2.66590
H	2.28541	-2.71839	0.24140
H	1.83672	1.76259	3.23943
H	1.39372	-0.81924	4.83350
H	2.09954	0.67161	5.45910
H	-0.50848	0.41425	5.78303
H	0.08341	1.92292	5.08544
H	-1.50886	-0.24643	3.75029
H	-2.24410	-1.28765	-3.49158
H	-4.70431	-1.45685	-3.66227
H	-5.96562	-2.88691	-2.06409
H	-4.73186	-4.16206	-0.32575
H	-2.28771	-4.00828	-0.16962
H	3.74029	2.07755	2.01555
H	6.07217	1.44757	1.52652
H	6.92384	-0.79632	2.18101
H	5.40195	-2.39372	3.32540
H	3.09189	-1.76096	3.83432
H	-3.50565	0.87723	4.14621
H	-4.93666	2.87980	3.90788
H	-3.98890	4.98490	2.98464
H	-1.58973	5.06982	2.33830
H	-0.16237	3.08405	2.60515
H	4.36446	-1.77082	0.29536
H	6.17644	-0.45158	-0.73604
H	5.84048	0.60896	-2.95918
H	3.66560	0.33886	-4.12978
H	1.86305	-0.98536	-3.11097
H	1.56536	1.51689	-4.99167
H	1.37901	1.56236	-7.46718
H	-0.83144	1.24717	-8.54885
H	-2.85627	0.89138	-7.16103
H	-2.67269	0.83984	-4.68812
H	-1.93353	2.69302	-1.36504

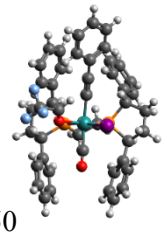
A' Post-Reaction Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.5337907000
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6484030532
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9753027900
Imaginary Frequency (cm^{-1}): None

C	0.86138	-1.33000	1.70406
C	-0.12933	-1.98544	0.73936
P	0.43733	0.46739	1.76638
P	-0.06222	-1.12571	-0.91495
C	-1.61278	-1.63692	-1.89821
C	-1.10613	-2.51616	-3.06978
C	0.37116	-2.23097	-3.32303
C	1.04625	-2.26223	-1.94995
C	1.64753	1.31215	2.91436
C	1.20617	0.82366	4.30284
C	-0.30804	0.99373	4.36229
C	-0.96568	0.44398	3.06958
C	-2.29459	1.08444	2.78510
C	2.53035	-2.04493	-1.90930
C	3.11220	1.17218	2.60979
C	-2.70978	-2.28025	-1.08803
C	-3.91363	-1.60550	-0.86531
C	-4.94048	-2.19557	-0.13180
C	-4.78068	-3.47274	0.39744
C	-3.58766	-4.15962	0.17699
C	-2.56664	-3.57088	-0.56104
C	3.82739	2.28054	2.14694
C	5.18795	2.18875	1.87383
C	5.85843	0.98293	2.06050
C	5.15916	-0.12486	2.53453
C	3.79882	-0.03055	2.81222
C	-3.42233	0.28036	2.60336
C	-4.68054	0.84657	2.42018
C	-4.82934	2.23059	2.42497
C	-3.70964	3.04115	2.60128
C	-2.45354	2.47343	2.77510
C	3.28032	-2.59066	-0.86000
C	4.65847	-2.41855	-0.80145
C	5.31688	-1.70899	-1.80396
C	4.58459	-1.18272	-2.86381
C	3.20357	-1.34870	-2.91583
Ru	0.42384	1.13665	-0.42510
C	2.23247	0.83745	-0.47849
I	-2.26916	1.88059	-0.79504
O	3.38157	0.75457	-0.57516
C	0.78647	2.81132	-2.10776
O	0.75737	3.15672	0.19929
C	0.63956	2.07513	-3.07194
C	0.41648	1.33335	-4.25973
C	1.48600	1.01259	-5.11253
C	1.24947	0.28965	-6.27445
C	-0.04430	-0.11715	-6.59763
C	-1.11066	0.21261	-5.76118
C	-0.88950	0.93715	-4.59897
C	0.84618	3.80701	-1.01382
C	2.14610	4.62162	-1.11718
F	2.22622	5.51646	-0.10794
F	3.25298	3.84943	-1.05608
F	2.20347	5.31659	-2.28086
H	0.80488	-1.79128	2.69697
H	1.88955	-1.42615	1.33681
H	0.08335	-3.05337	0.62387
H	-1.15588	-1.89677	1.11974
H	-1.98787	-0.68703	-2.29335
H	-1.22412	-3.57431	-2.81245
H	-1.71782	-2.32621	-3.95877
H	0.81977	-2.97819	-3.98836
H	0.49253	-1.25147	-3.79697
H	0.84370	-3.25088	-1.50916
H	1.37560	2.37428	2.81919
H	1.49164	-0.22424	4.45108
H	1.70470	1.41184	5.08147
H	-0.74624	0.49120	5.23133
H	-0.53766	2.05988	4.45403
H	-1.14016	-0.63181	3.19347
H	-4.04110	-0.60359	-1.26478
H	-5.86860	-1.65217	0.02386
H	-5.57986	-3.93351	0.97138
H	-3.45239	-5.15988	0.57946
H	-1.64450	-4.12385	-0.72317
H	3.30509	3.22070	1.98624
H	5.72411	3.06140	1.51086
H	6.92053	0.90721	1.84471
H	5.67569	-1.06755	2.69387
H	3.27576	-0.90103	3.19783
H	-3.31376	-0.80268	2.60529
H	-5.54547	0.20376	2.28051
H	-5.81086	2.67624	2.28927
H	-3.81394	4.12272	2.58974
H	-1.58709	3.12105	2.88643
H	2.77743	-3.17126	-0.08880
H	5.22150	-2.84855	0.02254
H	6.39438	-1.57628	-1.76254
H	5.08937	-0.63659	-3.65638
H	2.64894	-0.93208	-3.75043
H	2.49024	1.33271	-4.85163
H	2.07881	0.04047	-6.92986
H	-0.22257	-0.68563	-7.50585
H	-2.11999	-0.09599	-6.01755
H	-1.70823	1.19931	-3.93499
H	0.02919	4.53980	-1.18273

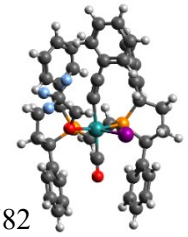
B Pre-Reaction Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.5271643900
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6433149603
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9713985650
Imaginary Frequency (cm^{-1}): None

C	-0.21246	-1.10061	2.31469
C	-1.05171	-2.01355	1.42086
P	-0.39915	0.66937	1.76462
P	-0.62388	-1.61445	-0.33887
C	-1.70190	-2.71186	-1.41053
C	-1.11361	-4.10905	-1.16322
C	0.40177	-3.97665	-1.31191
C	0.91729	-2.68679	-0.60773
C	1.11175	1.63285	2.38425
C	0.56458	2.69271	3.37261
C	-0.93640	2.88664	3.14452
C	-1.53672	1.48335	3.02364
C	-3.01511	1.36542	2.79326
C	2.07157	-2.06670	-1.34537
C	2.20089	0.73615	2.91725
C	-3.18960	-2.57765	-1.25689
C	-3.93218	-1.95444	-2.26475
C	-5.31276	-1.82366	-2.15874
C	-5.97718	-2.31385	-1.03778
C	-5.25021	-2.94734	-0.03231
C	-3.86973	-3.08402	-0.14280
C	3.24824	0.34676	2.07548
C	4.25553	-0.50068	2.52833
C	4.22809	-0.98870	3.83185
C	3.17798	-0.62667	4.67349
C	2.17463	0.22487	4.22101
C	-3.66137	0.15864	3.09176
C	-5.02888	0.01163	2.89271
C	-5.78130	1.07913	2.40570
C	-5.15311	2.28875	2.12651
C	-3.78084	2.43165	2.31591
C	3.31545	-1.95549	-0.72437
C	4.41371	-1.44365	-1.41202
C	4.28094	-1.04303	-2.73685
C	3.04284	-1.15264	-3.36779
C	1.94844	-1.65823	-2.67780
Ru	-0.81010	0.67183	-0.48747
C	-2.70865	0.54352	-0.31938
I	-1.27760	3.44569	-0.77544
O	-3.86092	0.56167	-0.31813
C	1.14319	1.13567	-0.87170
O	-1.00417	0.51004	-2.68636
C	2.20596	1.62406	-1.25083
C	3.40238	2.21404	-1.73127
C	3.61874	2.36024	-3.11681
C	4.78803	2.93309	-3.59696
C	5.77443	3.37479	-2.71438
C	5.56949	3.24740	-1.34136
C	4.39889	2.68061	-0.85150
C	-0.39600	1.23239	-3.45738
C	-0.50279	0.97843	-4.96355
F	0.73430	0.79994	-5.47537
F	-1.24145	-0.09830	-5.25354
F	-1.05092	2.05282	-5.56553
H	-0.48834	-1.20318	3.37012
H	0.85256	-1.35363	2.23018
H	-0.86445	-3.06800	1.65419
H	-2.12111	-1.81247	1.55280
H	-1.43551	-2.40704	-2.43424
H	-1.38412	-4.47005	-0.16465
H	-1.52119	-4.82283	-1.88823
H	0.93063	-4.85119	-0.91893
H	0.64364	-3.90345	-2.37749
H	1.25353	-2.93034	0.40747
H	1.48234	2.12616	1.48012
H	0.72378	2.36389	4.40401
H	1.11566	3.63007	3.24390
H	-1.40117	3.43337	3.97332
H	-1.11126	3.45656	2.22485
H	-1.29380	0.93506	3.94870
H	-3.41734	-1.56001	-3.13824
H	-5.86985	-1.33313	-2.95223
H	-7.05491	-2.20933	-0.95020
H	-5.76061	-3.34356	0.84135
H	-3.32511	-3.59969	0.64263
H	3.25551	0.69888	1.04752
H	5.06312	-0.77975	1.85646
H	5.01438	-1.64794	4.18880
H	3.13829	-1.00946	5.68977
H	1.35998	0.47914	4.89360
H	-3.08526	-0.67019	3.49892
H	-5.51039	-0.93390	3.12730
H	-6.85125	0.96913	2.25258
H	-5.73209	3.12900	1.75285
H	-3.30744	3.37983	2.08181
H	3.42524	-2.27283	0.30997
H	5.37466	-1.36236	-0.91047
H	5.13358	-0.63845	-3.27496
H	2.92944	-0.83509	-4.40076
H	0.98664	-1.73396	-3.18262
H	2.85893	2.00565	-3.80714
H	4.93361	3.03424	-4.66938
H	6.68989	3.81978	-3.09334
H	6.32590	3.59750	-0.64387
H	4.24342	2.59789	0.22008
H	0.24871	2.06444	-3.14174

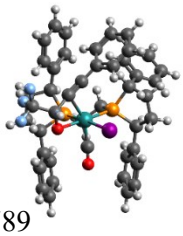
B TS



Gibbs Energy @ r^2SCAN-3c[CPCM]: -3264.5105224900
Thermal Correction @ r^2SCAN-3c[CPCM]: 0.6453963533
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^2SCAN-3c[CPCM]: -3266.9399082485
Imaginary Frequency (cm^{-1}): -277.78

C	-0.28430	-1.18349	2.14056
C	-1.25541	-2.02336	1.30474
P	-0.42834	0.60040	1.61860
P	-0.85115	-1.67509	-0.47153
C	-1.98595	-2.73878	-1.51310
C	-1.46354	-4.16106	-1.26667
C	0.05339	-4.09777	-1.42532
C	0.62721	-2.87868	-0.65650
C	1.12712	1.57204	2.09705
C	0.71913	2.44730	3.30800
C	-0.77936	2.73267	3.23924
C	-1.45042	1.37596	3.01048
C	-2.94583	1.33363	2.88829
C	1.94438	-2.40523	-1.20640
C	2.39249	0.79133	2.33207
C	-3.46006	-2.52304	-1.32310
C	-4.18840	-1.83546	-2.29891
C	-5.55526	-1.62374	-2.15220
C	-6.21817	-2.09430	-1.02205
C	-5.50485	-2.78821	-0.04720
C	-4.13870	-3.00561	-0.19791
C	3.51827	1.03200	1.54020
C	4.71878	0.36924	1.77919
C	4.81218	-0.55806	2.81220
C	3.69910	-0.80253	3.61548
C	2.50513	-0.12759	3.38386
C	-3.62423	0.15380	3.22025
C	-5.00835	0.07205	3.12359
C	-5.74417	1.18049	2.70917
C	-5.08260	2.36584	2.40251
C	-3.69511	2.44299	2.48995
C	3.03039	-2.22081	-0.34534
C	4.29338	-1.91522	-0.84508
C	4.48893	-1.78180	-2.21644
C	3.40625	-1.93050	-3.08137
C	2.14800	-2.24095	-2.57911
Ru	-1.02004	0.62534	-0.60230
C	-2.85952	0.50587	-0.24598
I	-1.48099	3.42382	-0.56102
O	-4.00810	0.52125	-0.14063
C	0.88577	1.09490	-1.41334
O	-1.22502	0.54731	-2.81066
C	2.00190	1.59670	-1.61925
C	3.17962	2.34135	-1.83562
C	4.30114	1.78638	-2.47993
C	5.44838	2.54545	-2.65727
C	5.50133	3.85873	-2.18953
C	4.39520	4.41987	-1.55009
C	3.23836	3.67511	-1.37782
C	-0.25165	1.33221	-3.06276
C	0.53777	1.02888	-4.34422
F	1.64312	1.78974	-4.46181
F	0.89577	-0.25877	-4.46770
F	-0.26385	1.32627	-5.40380
H	-0.48336	-1.29166	3.21224
H	0.75051	-1.50484	1.96483
H	-1.15139	-3.08808	1.54309
H	-2.29376	-1.72687	1.48914
H	-1.72485	-2.45216	-2.54324
H	-1.74070	-4.50822	-0.26478
H	-1.90956	-4.85621	-1.98719
H	0.54283	-5.01231	-1.07278
H	0.28615	-3.99831	-2.48974
H	0.80746	-3.17875	0.38246
H	1.27661	2.22097	1.22482
H	0.94346	1.90878	4.23657
H	1.31568	3.36624	3.30915
H	-1.14633	3.18536	4.16805
H	-0.99886	3.42010	2.41555
H	-1.17511	0.73805	3.86495
H	-3.67272	-1.45571	-3.17814
H	-6.10231	-1.08486	-2.92096
H	-7.28488	-1.92641	-0.90304
H	-6.01485	-3.16686	0.83450
H	-3.60362	-3.56194	0.56630
H	3.45641	1.75741	0.73479
H	5.58112	0.57918	1.15210
H	5.74604	-1.08144	2.99780
H	3.76345	-1.51594	4.43268
H	1.65492	-0.31481	4.03515
H	-3.05872	-0.70702	3.57219
H	-5.51433	-0.85424	3.38224
H	-6.82655	1.12233	2.63555
H	-5.64827	3.23884	2.08818
H	-3.19629	3.37231	2.23595
H	2.89254	-2.33728	0.72827
H	5.12595	-1.79184	-0.15912
H	5.47717	-1.55766	-2.60923
H	3.54291	-1.80978	-4.15280
H	1.31801	-2.36192	-3.26711
H	4.25052	0.76278	-2.83412
H	6.30870	2.11226	-3.15937
H	6.40429	4.44698	-2.32584
H	4.43570	5.44385	-1.19023
H	2.36845	4.10165	-0.88646
H	-0.33083	2.41433	-2.88363

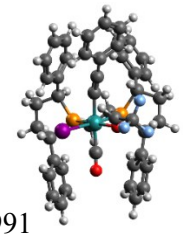
B Post-Reaction Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.5307282800
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6484750521
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9734762425
Imaginary Frequency (cm^{-1}): None

C	0.16388	-1.03395	1.62802
C	-0.88509	-1.86970	0.88941
P	-0.01396	0.76665	1.17156
P	-0.71752	-1.45973	-0.91143
C	-1.98016	-2.43770	-1.89151
C	-1.33723	-3.81793	-2.09202
C	0.12088	-3.56511	-2.45478
C	0.72643	-2.63074	-1.38710
C	1.60872	1.62031	1.60613
C	1.13539	3.03136	2.01197
C	-0.26237	2.99780	2.68596
C	-0.81474	1.56385	2.67888
C	-2.29710	1.38072	2.86402
C	2.11418	-2.16227	-1.73749
C	2.40416	0.86657	2.63932
C	-3.38730	-2.43056	-1.36441
C	-4.37279	-1.71065	-2.04653
C	-5.68771	-1.69552	-1.59276
C	-6.03906	-2.39933	-0.44408
C	-5.06708	-3.12731	0.23946
C	-3.75339	-3.14717	-0.21926
C	3.31877	-0.10697	2.21594
C	4.06465	-0.83837	3.13332
C	3.91280	-0.60826	4.49961
C	3.01888	0.36701	4.93338
C	2.27314	1.09996	4.01268
C	-2.76857	0.15848	3.36380
C	-4.12811	-0.07161	3.53727
C	-5.04917	0.92909	3.23348
C	-4.59260	2.15456	2.75961
C	-3.23086	2.37902	2.57348
C	3.16135	-2.40558	-0.84063
C	4.48742	-2.17651	-1.20219
C	4.79100	-1.70279	-2.47544
C	3.75554	-1.43065	-3.36833
C	2.43188	-1.65175	-3.00114
Ru	-0.96149	0.83842	-0.96671
C	-2.62263	0.62362	-0.25817
I	-1.50080	3.60584	-0.96716
O	-3.72490	0.52664	0.07425
C	0.40504	1.34912	-2.92454
O	-1.83728	0.70986	-2.92054
C	1.38986	1.65133	-2.27046
C	2.54885	2.17392	-1.63839
C	3.61604	1.34293	-1.26716
C	4.73283	1.88371	-0.64575
C	4.79297	3.25081	-0.37954
C	3.73483	4.08153	-0.74748
C	2.61600	3.55442	-1.37789
C	-0.84463	1.24421	-3.70790
C	-0.65487	0.41906	-4.98875
F	0.37000	0.88558	-5.74173
F	-0.40611	-0.88861	-4.73845
F	-1.77142	0.46641	-5.74691
H	0.09744	-1.16305	2.71397
H	1.17425	-1.34559	1.33193
H	-0.73404	-2.94027	1.06986
H	-1.89929	-1.60894	1.21418
H	-1.97802	-1.91071	-2.85598
H	-1.40314	-4.41330	-1.17263
H	-1.86458	-4.36572	-2.88128
H	0.70651	-4.49061	-2.49798
H	0.17467	-3.09431	-3.44215
H	0.81955	-3.21587	-0.46277
H	2.20668	1.67436	0.69552
H	1.88775	3.49598	2.65756
H	1.07080	3.63652	1.10215
H	-0.22431	3.35859	3.72040
H	-0.92805	3.66238	2.13179
H	-0.32377	1.00680	3.49108
H	-4.09715	-1.14529	-2.93358
H	-6.43816	-1.12725	-2.13548
H	-7.06439	-2.38576	-0.08530
H	-5.33337	-3.68665	1.13229
H	-3.01235	-3.73102	0.31975
H	3.44913	-0.28465	1.15070
H	4.77121	-1.58508	2.78046
H	4.49503	-1.17661	5.21939
H	2.90334	0.56558	5.99545
H	1.59897	1.87065	4.37590
H	-2.05666	-0.62026	3.62884
H	-4.46850	-1.02956	3.92125
H	-6.11259	0.75595	3.37287
H	-5.30033	2.94473	2.52379
H	-2.90691	3.33737	2.18232
H	2.93755	-2.81207	0.14365
H	5.28290	-2.38535	-0.49183
H	5.82415	-1.53673	-2.76722
H	3.97854	-1.04344	-4.35882
H	1.64272	-1.43841	-3.71326
H	3.54731	0.27929	-1.45408
H	5.55358	1.23292	-0.35736
H	5.66443	3.67025	0.11484
H	3.78105	5.14668	-0.54020
H	1.78182	4.18901	-1.66020
H	-1.06381	2.27375	-4.06704

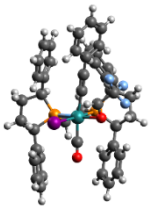
B' Pre-Reaction Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.5286906900
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6422840088
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9731789135
Imaginary Frequency (cm^{-1}): None

C	-0.41969	-1.00600	2.47299
C	-1.17936	-2.04925	1.65533
P	-0.59745	0.66374	1.67607
P	-0.68170	-1.87084	-0.12545
C	-1.67010	-3.16963	-1.05454
C	-0.95827	-4.48082	-0.68624
C	0.53541	-4.22285	-0.85824
C	0.92541	-2.89087	-0.16570
C	0.85418	1.74515	2.24073
C	0.22008	2.96096	2.96087
C	-1.25411	3.07270	2.56958
C	-1.83292	1.65769	2.68644
C	-3.28617	1.46876	2.36402
C	2.16160	-2.27738	-0.75826
C	1.89156	0.99155	3.03066
C	-3.16320	-3.15772	-0.88227
C	-3.97311	-2.73788	-1.94235
C	-5.35895	-2.72738	-1.82423
C	-5.96288	-3.13773	-0.63892
C	-5.16846	-3.57540	0.41870
C	-3.78204	-3.59267	0.29642
C	3.06568	0.56297	2.40406
C	4.03120	-0.15314	3.10718
C	3.83458	-0.46381	4.44960
C	2.65995	-0.05713	5.08092
C	1.69851	0.66176	4.37855
C	-3.94637	0.32105	2.82136
C	-5.29399	0.11665	2.55084
C	-6.01288	1.06800	1.82910
C	-5.37055	2.21853	1.38286
C	-4.01689	2.41686	1.64363
C	3.28451	-2.06445	0.04293
C	4.46258	-1.55703	-0.50092
C	4.53250	-1.26287	-1.85876
C	3.41694	-1.47570	-2.66689
C	2.24264	-1.97691	-2.12135
Ru	-0.90846	0.35250	-0.59098
C	-2.80574	0.15663	-0.52902
I	-1.13033	0.01954	-3.37812
O	-3.95434	0.10455	-0.61411
C	1.05045	0.84817	-0.89323
O	-1.21477	2.53297	-0.91098
C	2.08510	1.46175	-1.15031
C	3.25823	2.16725	-1.52697
C	3.98310	2.93490	-0.59467
C	5.12622	3.62467	-0.98046
C	5.57063	3.57214	-2.30081
C	4.85555	2.82520	-3.23751
C	3.71439	2.13064	-2.85991
C	-0.57841	3.16233	-1.73933
C	-0.75690	4.67988	-1.83257
F	-1.15239	5.01896	-3.07535
F	-1.64931	5.15148	-0.95507
F	0.43334	5.27365	-1.59683
H	-0.76605	-0.97337	3.51196
H	0.65401	-1.23613	2.49294
H	-0.97524	-3.06134	2.02338
H	-2.25972	-1.87274	1.71071
H	-1.44609	-2.94671	-2.10764
H	-1.18942	-4.77693	0.34396
H	-1.30342	-5.28805	-1.34245
H	1.14631	-5.03831	-0.45603
H	0.76058	-4.14334	-1.92750
H	1.12258	-3.08934	0.89543
H	1.30885	2.06835	1.29885
H	0.28713	2.83202	4.04582
H	0.77648	3.86950	2.70764
H	-1.79413	3.76743	3.22322
H	-1.34938	3.44319	1.54155
H	-1.66140	1.30756	3.71735
H	-3.50540	-2.39957	-2.86399
H	-5.96755	-2.39193	-2.65953
H	-7.04488	-3.12615	-0.54180
H	-5.62977	-3.91288	1.34297
H	-3.18551	-3.96002	1.12625
H	3.21380	0.78069	1.34932
H	4.93919	-0.46977	2.60073
H	4.58744	-1.02072	5.00033
H	2.49095	-0.30196	6.12613
H	0.78349	0.95712	4.88597
H	-3.39772	-0.41315	3.40845
H	-5.78723	-0.78176	2.91215
H	-7.06786	0.91381	1.62061
H	-5.92348	2.96763	0.82249
H	-3.53278	3.31892	1.28155
H	3.23432	-2.29467	1.10489
H	5.32694	-1.39582	0.13813
H	5.44789	-0.86247	-2.28583
H	3.45913	-1.23699	-3.72621
H	1.37130	-2.11299	-2.75782
H	3.63596	2.98718	0.43345
H	5.67243	4.21023	-0.24570
H	6.46392	4.11315	-2.59929
H	5.19130	2.78409	-4.27037
H	3.15948	1.54499	-3.58686
H	0.14559	2.71290	-2.43188

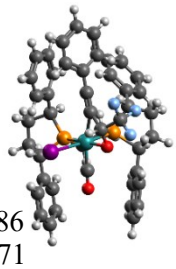
B' TS



Gibbs Energy @ r^2SCAN-3c[CPCM]: -3264.5172755500
Thermal Correction @ r^2SCAN-3c[CPCM]: 0.6461990674
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^2SCAN-3c[CPCM]: -3266.9474773609
Imaginary Frequency (cm^{-1}): -290.84

C	-0.49615	-0.91620	2.41915
C	-1.20311	-1.99219	1.59979
P	-0.72422	0.74692	1.61953
P	-0.71825	-1.79286	-0.18359
C	-1.63864	-3.16842	-1.08012
C	-0.84450	-4.42786	-0.70038
C	0.62859	-4.08287	-0.89068
C	0.94226	-2.72025	-0.21787
C	0.72340	1.84666	2.16908
C	0.08078	3.07172	2.86844
C	-1.40432	3.14802	2.50973
C	-1.94904	1.72205	2.65795
C	-3.40717	1.49676	2.38512
C	2.13976	-2.05686	-0.83750
C	1.75503	1.10347	2.97622
C	-3.12768	-3.24757	-0.88364
C	-3.97984	-2.87872	-1.92983
C	-5.36154	-2.95290	-1.78893
C	-5.92005	-3.40042	-0.59485
C	-5.08281	-3.79007	0.44822
C	-3.70010	-3.72134	0.30346
C	2.90988	0.62430	2.35018
C	3.87044	-0.08823	3.06331
C	3.68736	-0.34645	4.41863
C	2.53025	0.10695	5.05009
C	1.57418	0.82229	4.33664
C	-4.03570	0.36250	2.91470
C	-5.38781	0.12784	2.69547
C	-6.14135	1.03384	1.95127
C	-5.52898	2.16927	1.42977
C	-4.17165	2.39853	1.64072
C	3.28878	-1.84514	-0.07375
C	4.45110	-1.34160	-0.65544
C	4.47797	-1.04901	-2.01458
C	3.33175	-1.24700	-2.78367
C	2.17280	-1.74205	-2.20004
Ru	-1.10821	0.42351	-0.64033
C	-2.94054	0.06861	-0.45166
I	-1.48009	-0.03747	-3.40330
O	-4.08513	-0.07704	-0.44897
C	0.78652	1.27348	-1.10560
O	-1.39930	2.59071	-0.89010
C	1.94543	1.67263	-1.30787
C	3.21583	2.20666	-1.60253
C	3.98830	2.82455	-0.59989
C	5.23572	3.34891	-0.90575
C	5.72454	3.27845	-2.21014
C	4.95836	2.68696	-3.21559
C	3.71518	2.15146	-2.91923
C	-0.37361	2.80921	-1.62200
C	0.31277	4.16356	-1.38265
F	-0.60384	5.15074	-1.55179
F	0.81392	4.30249	-0.13864
F	1.30656	4.38782	-2.26518
H	-0.85560	-0.89229	3.45394
H	0.58435	-1.10693	2.45568
H	-0.95089	-2.99270	1.96964
H	-2.29098	-1.86933	1.65648
H	-1.44645	-2.95202	-2.14039
H	-1.04649	-4.72234	0.33616
H	-1.14535	-5.26461	-1.34136
H	1.29289	-4.85471	-0.48678
H	0.83770	-4.00036	-1.96321
H	1.16116	-2.89154	0.84362
H	1.18486	2.16330	1.23029
H	0.17658	2.97427	3.95429
H	0.61349	3.98239	2.57721
H	-1.94325	3.83770	3.16970
H	-1.52937	3.49713	1.47832
H	-1.73772	1.38328	3.68527
H	-3.54952	-2.51277	-2.85863
H	-6.00285	-2.65542	-2.61413
H	-6.99899	-3.45536	-0.48002
H	-5.50702	-4.15689	1.37907
H	-3.06959	-4.05280	1.12305
H	3.05049	0.79780	1.28653
H	4.76318	-0.44290	2.55475
H	4.43623	-0.89958	4.97844
H	2.37011	-0.09861	6.10506
H	0.67300	1.15214	4.84687
H	-3.45690	-0.33780	3.51430
H	-5.85692	-0.75900	3.11307
H	-7.19980	0.85635	1.78272
H	-6.10885	2.88230	0.84997
H	-3.71072	3.28732	1.22054
H	3.27612	-2.08805	0.98608
H	5.33746	-1.18795	-0.04529
H	5.38197	-0.65755	-2.47277
H	3.33990	-1.00759	-3.84358
H	1.28131	-1.88034	-2.80814
H	3.59536	2.89228	0.40971
H	5.82808	3.82071	-0.12723
H	6.70075	3.69261	-2.44577
H	5.33646	2.64329	-4.23287
H	3.11137	1.68541	-3.69116
H	-0.35862	2.51482	-2.68187

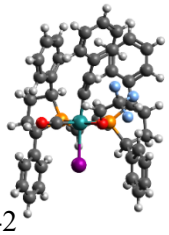
B' Post-Reaction Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.5271604500
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6458230951
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9652086668
Imaginary Frequency (cm^{-1}): None

C	-0.52875	-0.86911	2.43592
C	-1.16909	-1.96192	1.58528
P	-0.76056	0.79714	1.64126
P	-0.64972	-1.73125	-0.18854
C	-1.49823	-3.15355	-1.08929
C	-0.68451	-4.38065	-0.65189
C	0.78515	-4.00214	-0.79288
C	1.04215	-2.59457	-0.18145
C	0.70795	1.88728	2.16278
C	0.07728	3.12494	2.85483
C	-1.41729	3.19828	2.53347
C	-1.96208	1.77478	2.69765
C	-3.42372	1.55286	2.43771
C	2.20523	-1.93599	-0.86835
C	1.72959	1.13236	2.97306
C	-2.99039	-3.27447	-0.93907
C	-3.82213	-2.90963	-2.00288
C	-5.20485	-3.02121	-1.90269
C	-5.78539	-3.50454	-0.73323
C	-4.96803	-3.88963	0.32692
C	-3.58411	-3.78196	0.22333
C	2.84043	0.57067	2.33470
C	3.79010	-0.15502	3.04840
C	3.63771	-0.34940	4.41834
C	2.52011	0.17864	5.06170
C	1.57586	0.90925	4.34729
C	-4.07497	0.48010	3.05866
C	-5.42937	0.24833	2.84660
C	-6.16038	1.09627	2.01706
C	-5.52359	2.17025	1.40207
C	-4.16504	2.39572	1.60550
C	3.42860	-1.82969	-0.20426
C	4.57369	-1.40833	-0.87854
C	4.50699	-1.09389	-2.23129
C	3.28385	-1.17175	-2.89712
C	2.14185	-1.58166	-2.22101
Ru	-1.16148	0.50193	-0.61134
C	-2.89760	0.03359	-0.34377
I	-1.53042	0.06574	-3.37243
O	-4.02391	-0.21782	-0.26618
C	0.56828	2.04402	-1.36441
O	-1.71354	2.54486	-0.86513
C	1.79747	2.05822	-1.47158
C	3.18575	2.17525	-1.64502
C	4.02217	2.54356	-0.57174
C	5.37669	2.74012	-0.78732
C	5.90803	2.60361	-2.07062
C	5.08364	2.26841	-3.14440
C	3.73283	2.04191	-2.93786
C	-0.63003	2.94894	-1.58871
C	-0.23220	4.39758	-1.24967
F	-1.28732	5.22851	-1.40422
F	0.20803	4.54763	0.02175
F	0.75469	4.84607	-2.06537
H	-0.93509	-0.85917	3.45358
H	0.55242	-1.03592	2.52055
H	-0.88589	-2.95316	1.95724
H	-2.26237	-1.88615	1.61838
H	-1.27761	-2.95344	-2.14766
H	-0.91988	-4.65987	0.38126
H	-0.93500	-5.23977	-1.28518
H	1.45185	-4.73527	-0.32582
H	1.03890	-3.96217	-1.85830
H	1.28554	-2.69897	0.88334
H	1.16958	2.19119	1.21870
H	0.20017	3.04492	3.93885
H	0.60219	4.03074	2.53744
H	-1.93894	3.88958	3.20565
H	-1.57103	3.53847	1.50431
H	-1.74018	1.43602	3.72248
H	-3.37572	-2.51770	-2.91301
H	-5.82986	-2.72676	-2.74141
H	-6.86530	-3.59006	-0.65087
H	-5.40838	-4.28289	1.23930
H	-2.96942	-4.10881	1.05661
H	2.95498	0.68900	1.26046
H	4.65156	-0.56798	2.53020
H	4.37870	-0.91173	4.97934
H	2.38077	0.02064	6.12770
H	0.70537	1.29514	4.87048
H	-3.51302	-0.17455	3.72240
H	-5.91712	-0.59033	3.33618
H	-7.22015	0.92150	1.85362
H	-6.08530	2.83597	0.75228
H	-3.68001	3.22553	1.10147
H	3.48894	-2.10745	0.84521
H	5.51981	-1.34349	-0.34738
H	5.39868	-0.77676	-2.76395
H	3.22037	-0.91199	-3.95029
H	1.19365	-1.64459	-2.75206
H	3.59340	2.68978	0.41394
H	6.01997	3.01857	0.04193
H	6.96866	2.77073	-2.23558
H	5.49998	2.17507	-4.14293
H	3.07953	1.77401	-3.76147
H	-0.79457	2.93979	-2.68725

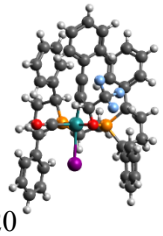
C Pre-Reaction Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.5030225100
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6429153210
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9444162900
Imaginary Frequency (cm^{-1}): None

C	-0.62184	-0.71433	2.40592
C	-1.26222	-1.79868	1.53985
P	-0.74762	0.94110	1.54890
P	-0.54007	-1.76453	-0.16740
C	-1.35018	-3.19684	-1.08854
C	-0.70439	-4.42871	-0.43201
C	0.79653	-4.17405	-0.39081
C	1.09106	-2.71466	0.06235
C	0.41480	2.05942	2.50480
C	-0.19744	2.01480	3.92195
C	-1.71196	2.21266	3.80007
C	-2.25840	1.63696	2.44964
C	-3.10298	2.66899	1.74290
C	2.32571	-2.19745	-0.62316
C	1.91500	1.88388	2.55513
C	-2.84598	-3.27757	-1.20083
C	-3.45147	-3.09653	-2.44731
C	-4.82811	-3.22135	-2.59912
C	-5.62655	-3.52709	-1.50033
C	-5.03284	-3.72540	-0.25567
C	-3.65396	-3.61091	-0.10860
C	2.64243	2.94013	3.12470
C	4.01566	2.84969	3.31945
C	4.69560	1.69375	2.94345
C	3.99010	0.65199	2.35187
C	2.61299	0.74548	2.15339
C	-4.49486	2.57803	1.82804
C	-5.31194	3.55234	1.26345
C	-4.74699	4.63717	0.59686
C	-3.36043	4.74450	0.51732
C	-2.54742	3.77566	1.09778
C	3.50796	-2.04041	0.10038
C	4.69058	-1.66604	-0.53596
C	4.70408	-1.44877	-1.90939
C	3.53030	-1.61457	-2.64320
C	2.35508	-1.98985	-2.00613
Ru	-0.68955	0.41990	-0.87015
C	-0.64143	-0.13771	-2.64719
I	-3.49165	0.34086	-0.98273
O	-0.59542	-0.51089	-3.74032
C	1.23457	0.88218	-0.94006
O	-0.73472	2.60736	-1.21053
C	2.25653	1.53780	-1.16754
C	3.51304	2.15852	-1.39973
C	4.13658	2.92262	-0.39659
C	5.35824	3.53906	-0.63613
C	5.97950	3.41623	-1.87832
C	5.36551	2.67001	-2.88473
C	4.14678	2.04660	-2.65242
C	0.16259	3.04196	-1.93583
C	0.69819	4.44470	-1.63706
F	-0.25251	5.37247	-1.90367
F	1.03875	4.57776	-0.34107
F	1.77364	4.72313	-2.39297
H	-1.12315	-0.67047	3.37865
H	0.43288	-0.93883	2.59597
H	-1.13189	-2.78514	2.00056
H	-2.33686	-1.60980	1.42386
H	-0.93654	-3.10475	-2.10431
H	-1.11096	-4.58843	0.57252
H	-0.93938	-5.32281	-1.02057
H	1.31970	-4.87932	0.26337
H	1.20193	-4.30399	-1.40018
H	1.26263	-2.69578	1.14585
H	0.21585	3.05695	2.08367
H	0.05559	1.05505	4.38733
H	0.24602	2.79671	4.54739
H	-2.24282	1.76432	4.64569
H	-1.92969	3.28506	3.81320
H	-2.89055	0.76119	2.63563
H	-2.83439	-2.84503	-3.30691
H	-5.27816	-3.07222	-3.57675
H	-6.70292	-3.62047	-1.61407
H	-5.64569	-3.97678	0.60573
H	-3.21233	-3.78761	0.86773
H	2.11948	3.84728	3.42046
H	4.55356	3.68420	3.76108
H	5.76868	1.61354	3.09264
H	4.51724	-0.23912	2.02721
H	2.10130	-0.06432	1.64423
H	-4.94241	1.72222	2.32839
H	-6.39214	3.45780	1.33499
H	-5.38175	5.39438	0.14515
H	-2.90703	5.58753	0.00266
H	-1.46952	3.87983	1.02011
H	3.50390	-2.22646	1.17229
H	5.60268	-1.55001	0.04346
H	5.62230	-1.15032	-2.40737
H	3.53105	-1.44706	-3.71687
H	1.45035	-2.12581	-2.59396
H	3.65170	3.01985	0.56907
H	5.82785	4.12110	0.15274
H	6.93355	3.90166	-2.06324
H	5.84166	2.57367	-3.85692
H	3.66931	1.46191	-3.43308
H	0.50069	2.57871	-2.87000

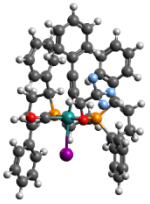
C TS



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.4932411200
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6447582801
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9252051792
Imaginary Frequency (cm^{-1}): -269.90

C	-0.70245	-0.64801	2.40574
C	-1.24334	-1.77085	1.52319
P	-0.83950	1.00388	1.53634
P	-0.52669	-1.66566	-0.18626
C	-1.24958	-3.16186	-1.08732
C	-0.55482	-4.34641	-0.39703
C	0.93231	-4.01838	-0.33193
C	1.15376	-2.52091	0.04358
C	0.33663	2.11262	2.49112
C	-0.25909	2.05385	3.91555
C	-1.77596	2.25155	3.81388
C	-2.33487	1.71099	2.45392
C	-3.16550	2.76807	1.76722
C	2.34252	-1.98780	-0.71057
C	1.83681	1.93720	2.53659
C	-2.73854	-3.31791	-1.21913
C	-3.33947	-3.15016	-2.46997
C	-4.70671	-3.34014	-2.63960
C	-5.50111	-3.70238	-1.55515
C	-4.91133	-3.88932	-0.30684
C	-3.54192	-3.70694	-0.14165
C	2.56759	3.00976	3.07116
C	3.93400	2.90939	3.30544
C	4.60565	1.72590	3.00687
C	3.90132	0.67078	2.43822
C	2.53172	0.77629	2.19579
C	-4.55873	2.69225	1.85117
C	-5.36483	3.68974	1.31144
C	-4.78728	4.78363	0.67083
C	-3.39976	4.87385	0.58915
C	-2.59777	3.88109	1.14407
C	3.56490	-1.84318	-0.05359
C	4.72199	-1.50759	-0.75459
C	4.67025	-1.32143	-2.13124
C	3.45404	-1.46296	-2.79861
C	2.30262	-1.79224	-2.09523
Ru	-0.84020	0.50487	-0.88100
C	-0.87937	-0.09075	-2.64429
I	-3.61701	0.24182	-0.82610
O	-0.89553	-0.50978	-3.72356
C	1.03458	1.25696	-1.09708
O	-1.04905	2.64331	-1.23687
C	2.23328	1.56355	-1.22154
C	3.54478	2.02483	-1.42930
C	4.26011	2.63386	-0.38031
C	5.54858	3.09859	-0.59574
C	6.13495	2.97687	-1.85565
C	5.42745	2.39229	-2.90775
C	4.14358	1.91455	-2.70120
C	0.10353	2.81171	-1.78283
C	0.79615	4.12811	-1.39038
F	-0.05767	5.15895	-1.61705
F	1.13742	4.18154	-0.08638
F	1.90323	4.36164	-2.12465
H	-1.25850	-0.61466	3.34883
H	0.34662	-0.82696	2.66176
H	-1.03327	-2.74625	1.97725
H	-2.32906	-1.67148	1.40427
H	-0.82974	-3.07421	-2.10064
H	-0.97242	-4.51131	0.60148
H	-0.73068	-5.26226	-0.97292
H	1.46858	-4.66507	0.37049
H	1.36909	-4.18236	-1.32300
H	1.35980	-2.43874	1.11818
H	0.13487	3.11461	2.08658
H	-0.00045	1.08996	4.36902
H	0.19290	2.83015	4.54230
H	-2.29559	1.77759	4.65251
H	-1.99720	3.32227	3.86025
H	-2.98054	0.84264	2.62533
H	-2.72653	-2.85920	-3.31986
H	-5.15250	-3.19958	-3.62050
H	-6.57013	-3.84789	-1.68285
H	-5.52007	-4.18357	0.54389
H	-3.10381	-3.87266	0.83817
H	2.04912	3.93429	3.31673
H	4.47260	3.75576	3.72296
H	5.67195	1.63566	3.19391
H	4.42482	-0.23999	2.16620
H	2.02104	-0.04880	1.71124
H	-5.01618	1.83123	2.33313
H	-6.44601	3.60673	1.38277
H	-5.41313	5.55958	0.23882
H	-2.93616	5.72103	0.09063
H	-1.51959	3.96980	1.05846
H	3.61386	-2.02606	1.01730
H	5.66427	-1.40304	-0.22312
H	5.56895	-1.06050	-2.68275
H	3.40313	-1.31488	-3.87405
H	1.36591	-1.91333	-2.63409
H	3.78869	2.73389	0.59047
H	6.09738	3.56279	0.21884
H	7.14361	3.34493	-2.02133
H	5.88442	2.30829	-3.88951
H	3.58456	1.45342	-3.50874
H	0.25971	2.57025	-2.84670

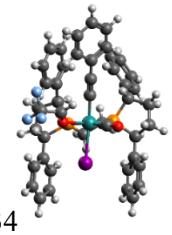
C Post-Reaction Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.4965274600
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6452316842
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9291771354
Imaginary Frequency (cm^{-1}): None

C	-0.72340	-0.60765	2.40551
C	-1.21045	-1.73675	1.50053
P	-0.86180	1.05455	1.54819
P	-0.48150	-1.58261	-0.20238
C	-1.15711	-3.10155	-1.10869
C	-0.45726	-4.27052	-0.39928
C	1.02222	-3.91717	-0.29895
C	1.21377	-2.40663	0.05001
C	0.32976	2.14848	2.50273
C	-0.24815	2.08118	3.93360
C	-1.75611	2.32750	3.83592
C	-2.34486	1.75282	2.50381
C	-3.22545	2.77716	1.83161
C	2.39989	-1.88157	-0.71251
C	1.83082	1.98160	2.52565
C	-2.64098	-3.28175	-1.26816
C	-3.22582	-3.09831	-2.52452
C	-4.58706	-3.30658	-2.71947
C	-5.39215	-3.70551	-1.65590
C	-4.81849	-3.90807	-0.40260
C	-3.45535	-3.70503	-0.21185
C	2.56792	3.09560	2.95754
C	3.93346	3.01019	3.20338
C	4.59905	1.79943	3.02265
C	3.89064	0.70020	2.55047
C	2.52278	0.79158	2.29174
C	-4.61358	2.64910	1.93033
C	-5.46201	3.61733	1.40129
C	-4.93161	4.73293	0.75766
C	-3.54895	4.87462	0.66152
C	-2.70528	3.91109	1.20504
C	3.63046	-1.75942	-0.06526
C	4.79705	-1.49849	-0.78192
C	4.74766	-1.36814	-2.16511
C	3.52111	-1.46889	-2.82175
C	2.35876	-1.71367	-2.10234
Ru	-0.88892	0.59276	-0.87894
C	-0.93398	0.00489	-2.63838
I	-3.62595	0.22332	-0.75875
O	-0.94561	-0.42089	-3.71749
C	0.89087	1.71584	-1.29482
O	-1.26332	2.66453	-1.23583
C	2.14017	1.69716	-1.35032
C	3.51591	1.86120	-1.49684
C	4.29718	2.31117	-0.41019
C	5.64304	2.57517	-0.59089
C	6.22048	2.42075	-1.85332
C	5.45365	1.99989	-2.94116
C	4.11237	1.70594	-2.76927
C	-0.03777	2.90057	-1.74709
C	0.53865	4.25201	-1.29679
F	-0.30785	5.25963	-1.61092
F	0.75518	4.31874	0.03755
F	1.72203	4.51759	-1.90578
H	-1.31024	-0.59177	3.33030
H	0.31717	-0.77248	2.69998
H	-0.96908	-2.70848	1.94629
H	-2.29729	-1.67743	1.36883
H	-0.72216	-3.01203	-2.11532
H	-0.89499	-4.44144	0.58915
H	-0.60135	-5.19170	-0.97583
H	1.54785	-4.54125	0.43150
H	1.48926	-4.09574	-1.27339
H	1.41580	-2.30257	1.12314
H	0.11870	3.15391	2.11332
H	-0.01524	1.10380	4.37203
H	0.23020	2.83703	4.56672
H	-2.28892	1.91173	4.69714
H	-1.93280	3.40773	3.83613
H	-2.96308	0.87253	2.71062
H	-2.60493	-2.78090	-3.35894
H	-5.01975	-3.15302	-3.70432
H	-6.45635	-3.86664	-1.80371
H	-5.43505	-4.22982	0.43245
H	-3.03102	-3.88114	0.77217
H	2.05199	4.03955	3.12078
H	4.47569	3.88872	3.54229
H	5.66323	1.72013	3.22591
H	4.40896	-0.23670	2.37142
H	2.01063	-0.07483	1.88907
H	-5.03339	1.77110	2.41610
H	-6.53860	3.49476	1.48430
H	-5.59011	5.48634	0.33428
H	-3.12275	5.73922	0.15948
H	-1.63196	4.03626	1.10928
H	3.67947	-1.91481	1.00955
H	5.74566	-1.41748	-0.25765
H	5.65575	-1.17954	-2.73012
H	3.47120	-1.35683	-3.90153
H	1.41421	-1.80959	-2.63286
H	3.82312	2.45663	0.55268
H	6.24430	2.91665	0.24652
H	7.27539	2.64025	-1.99270
H	5.91040	1.89437	-3.92051
H	3.50050	1.37515	-3.60148
H	0.01435	2.89656	-2.85734

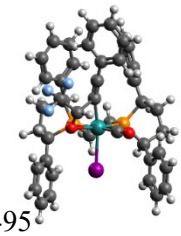
C' Pre-Reaction Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.5117576000
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6410381752
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9562476923
Imaginary Frequency (cm^{-1}): None

C	-0.59925	-0.89156	2.05755
C	-1.35903	-1.83259	1.12421
P	-0.63372	0.86494	1.43905
P	-0.72957	-1.59061	-0.60304
C	-1.60366	-2.89064	-1.65942
C	-0.95443	-4.20566	-1.19264
C	0.55092	-3.98050	-1.18023
C	0.88563	-2.59012	-0.56423
C	0.93313	1.73685	2.08269
C	0.44909	2.88532	3.00036
C	-1.01725	3.18929	2.70133
C	-1.72543	1.83175	2.63983
C	-3.21567	1.84044	2.46583
C	2.08930	-1.99667	-1.24613
C	1.94889	0.81539	2.70373
C	-3.10433	-2.94658	-1.71653
C	-3.75824	-2.63537	-2.91174
C	-5.14169	-2.73072	-3.01669
C	-5.89842	-3.13957	-1.92164
C	-5.25609	-3.47030	-0.73023
C	-3.87095	-3.38394	-0.63141
C	3.07462	0.42384	1.97351
C	4.03515	-0.41438	2.53498
C	3.87694	-0.89416	3.83149
C	2.74491	-0.53239	4.56069
C	1.79322	0.31434	4.00349
C	-3.96517	0.74392	2.90748
C	-5.35060	0.73701	2.80168
C	-6.01501	1.83771	2.26292
C	-5.28014	2.93864	1.83398
C	-3.89145	2.93994	1.93272
C	3.31047	-1.94219	-0.57524
C	4.46388	-1.50440	-1.22485
C	4.40829	-1.12452	-2.56123
C	3.19303	-1.18204	-3.24288
C	2.04543	-1.61297	-2.59094
Ru	-0.88201	0.86106	-0.84201
C	-1.17888	2.70096	-0.87510
I	-3.68098	0.59093	-1.01681
O	-1.34963	3.84295	-0.91039
C	1.04069	1.27994	-1.11530
O	-0.89081	0.50897	-3.01651
C	2.12040	1.76076	-1.45498
C	3.37807	2.27619	-1.85876
C	3.74516	2.28913	-3.21998
C	4.97786	2.78644	-3.61982
C	5.88013	3.28309	-2.67860
C	5.52662	3.28827	-1.32987
C	4.29205	2.79841	-0.92134
C	-0.31046	1.20071	-3.83328
C	-0.20796	0.72543	-5.28607
F	1.09022	0.70013	-5.65555
F	-0.72751	-0.49301	-5.46169
F	-0.85298	1.59219	-6.09286
H	-1.00673	-0.92750	3.07409
H	0.45624	-1.18393	2.12542
H	-1.23294	-2.87193	1.44871
H	-2.42891	-1.59304	1.11504
H	-1.23384	-2.67446	-2.67319
H	-1.32448	-4.48304	-0.19943
H	-1.23142	-5.01521	-1.87816
H	1.08435	-4.76824	-0.63768
H	0.91660	-3.99248	-2.21284
H	1.11582	-2.70606	0.50196
H	1.36671	2.15957	1.17116
H	0.53909	2.59084	4.05084
H	1.08632	3.76387	2.85455
H	-1.46710	3.81711	3.47892
H	-1.11566	3.72742	1.75171
H	-1.50753	1.31207	3.58782
H	-3.17399	-2.30106	-3.76626
H	-5.63009	-2.47846	-3.95401
H	-6.97986	-3.20978	-1.99802
H	-5.83608	-3.80171	0.12692
H	-3.39145	-3.65958	0.30319
H	3.19077	0.77217	0.95050
H	4.90936	-0.69375	1.95268
H	4.62565	-1.54713	4.27096
H	2.60399	-0.90904	5.57027
H	0.91465	0.57777	4.58738
H	-3.45344	-0.11254	3.34252
H	-5.91449	-0.12520	3.14742
H	-7.09858	1.83814	2.18460
H	-5.78854	3.80275	1.41489
H	-3.33610	3.80659	1.58663
H	3.35903	-2.24853	0.46654
H	5.40617	-1.46608	-0.68433
H	5.30353	-0.77880	-3.07059
H	3.14186	-0.88338	-4.28626
H	1.10290	-1.65451	-3.13439
H	3.04998	1.89098	-3.95300
H	5.24004	2.78279	-4.67481
H	6.84577	3.66751	-2.99398
H	6.21715	3.68185	-0.58859
H	4.02105	2.81732	0.13044
H	0.16281	2.16622	-3.60343

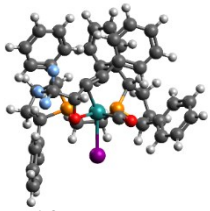
C' TS



Gibbs Energy @ r^2SCAN-3c[CPCM]: -3264.4866097800
Thermal Correction @ r^2SCAN-3c[CPCM]: 0.6456495089
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^2SCAN-3c[CPCM]: -3266.9153126894
Imaginary Frequency (cm^{-1}): -283.81

C	-0.67592	-1.21745	2.11133
C	-1.43288	-2.18011	1.19621
P	-0.86405	0.55246	1.55153
P	-0.82340	-1.89498	-0.53261
C	-1.64014	-3.20953	-1.60861
C	-1.06924	-4.52042	-1.04644
C	0.43876	-4.34057	-0.90962
C	0.79289	-2.90592	-0.41135
C	0.53171	1.41583	2.48408
C	0.09322	1.28199	3.95018
C	-1.36696	1.71317	4.02074
C	-2.17711	1.15675	2.81290
C	-3.23516	2.14695	2.40621
C	2.05253	-2.40881	-1.07114
C	1.96122	1.02513	2.22293
C	-3.13210	-3.21502	-1.78801
C	-3.68198	-2.78978	-2.99999
C	-5.05548	-2.83168	-3.21567
C	-5.90500	-3.30475	-2.21900
C	-5.36655	-3.74135	-1.01031
C	-3.99262	-3.70065	-0.79800
C	2.74018	1.81291	1.36962
C	4.09577	1.56000	1.19032
C	4.70555	0.50969	1.87111
C	3.94318	-0.28703	2.72053
C	2.58443	-0.03452	2.89411
C	-4.58504	1.83730	2.59308
C	-5.57772	2.77232	2.31890
C	-5.23513	4.03478	1.83996
C	-3.89220	4.35842	1.65977
C	-2.90281	3.42688	1.95775
C	3.15474	-2.06241	-0.28629
C	4.38953	-1.78651	-0.86790
C	4.53930	-1.85048	-2.24998
C	3.43550	-2.15219	-3.04610
C	2.20509	-2.42803	-2.46120
Ru	-1.14901	0.56705	-0.73884
C	-1.51523	2.38884	-0.75766
I	-3.89345	0.13930	-0.56691
O	-1.68251	3.52924	-0.84719
C	0.69062	1.07317	-1.49356
O	-1.21446	0.30487	-2.91502
C	1.80945	1.57690	-1.70657
C	2.99058	2.28228	-1.99740
C	4.12047	1.63131	-2.52800
C	5.28151	2.34585	-2.77767
C	5.33832	3.71127	-2.49616
C	4.22227	4.36931	-1.97680
C	3.05160	3.66772	-1.73495
C	-0.27250	1.15568	-3.14684
C	0.59360	0.84707	-4.37610
F	1.53956	1.78858	-4.57817
F	1.19712	-0.35062	-4.32276
F	-0.20645	0.84554	-5.47501
H	-1.01806	-1.32112	3.14661
H	0.39853	-1.44194	2.09927
H	-1.26359	-3.21559	1.51243
H	-2.50978	-1.97700	1.21683
H	-1.18066	-3.02926	-2.59276
H	-1.53118	-4.75467	-0.08242
H	-1.30761	-5.34790	-1.72509
H	0.87865	-5.08421	-0.23663
H	0.89675	-4.48852	-1.89169
H	0.98701	-2.93691	0.66620
H	0.41557	2.46953	2.18730
H	0.21565	0.25107	4.29730
H	0.72364	1.91255	4.58809
H	-1.84071	1.40588	4.95916
H	-1.40879	2.80646	3.98144
H	-2.68435	0.22883	3.10045
H	-3.02369	-2.41180	-3.77905
H	-5.46285	-2.49175	-4.16399
H	-6.97830	-3.33865	-2.38416
H	-6.02043	-4.11590	-0.22727
H	-3.59515	-4.04495	0.15264
H	2.27629	2.65208	0.85833
H	4.67718	2.19245	0.52441
H	5.76725	0.31731	1.74470
H	4.40773	-1.10819	3.26016
H	2.02264	-0.65601	3.58480
H	-4.85952	0.84738	2.94947
H	-6.62150	2.51101	2.47062
H	-6.00846	4.76392	1.61486
H	-3.61249	5.34176	1.29150
H	-1.85828	3.70170	1.83326
H	3.05132	-2.02985	0.79538
H	5.23625	-1.53342	-0.23620
H	5.50570	-1.65331	-2.70660
H	3.53523	-2.17896	-4.12785
H	1.35743	-2.67679	-3.09454
H	4.06462	0.56835	-2.73393
H	6.14939	1.83864	-3.18919
H	6.25291	4.26586	-2.68578
H	4.26770	5.43361	-1.76539
H	2.17521	4.16933	-1.33524
H	-0.48273	2.23686	-3.10245

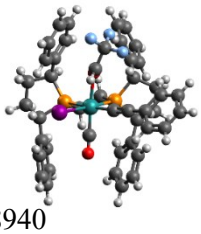
C' Post-Reaction Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.5017560200
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6486286774
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9399278912
Imaginary Frequency (cm^{-1}): None

C	-1.29972	-1.06523	2.15169
C	-1.25483	-2.27282	1.20264
P	-0.91321	0.60029	1.37935
P	-0.62375	-1.88281	-0.50173
C	-1.14820	-3.37129	-1.52237
C	-0.36289	-4.55478	-0.91300
C	0.94607	-4.07122	-0.23662
C	1.14225	-2.54431	-0.40421
C	0.65124	1.17474	2.26679
C	0.23287	1.26647	3.75621
C	-1.29418	1.49083	3.89769
C	-1.95927	1.68756	2.51693
C	-2.09306	3.12962	2.09854
C	2.07147	-2.18954	-1.54051
C	1.97874	0.48113	2.09012
C	-2.62276	-3.61196	-1.72212
C	-3.22799	-3.19175	-2.91139
C	-4.58327	-3.40204	-3.14013
C	-5.36482	-4.04113	-2.18065
C	-4.77308	-4.47444	-0.99718
C	-3.41493	-4.26707	-0.77224
C	3.07267	1.21619	1.61957
C	4.34250	0.65105	1.53973
C	4.54695	-0.66812	1.93262
C	3.47083	-1.40969	2.41466
C	2.20378	-0.83930	2.49941
C	-3.23434	3.53620	1.39982
C	-3.41495	4.86525	1.03196
C	-2.45548	5.81897	1.35981
C	-1.32225	5.43223	2.07144
C	-1.14461	4.10227	2.44181
C	2.97458	-1.13323	-1.38576
C	3.92889	-0.85840	-2.35939
C	3.98482	-1.62258	-3.52299
C	3.08566	-2.67118	-3.69307
C	2.14702	-2.95834	-2.70627
Ru	-1.34813	0.43191	-0.93206
C	-2.06842	2.13076	-1.25370
I	-3.91845	-0.28779	-0.21364
O	-2.51285	3.13574	-1.60180
C	0.16714	0.73073	-2.50999
O	-1.89156	-0.12147	-2.95910
C	0.66095	1.43364	-1.60858
C	1.50783	2.47462	-1.11604
C	2.83520	2.55157	-1.57168
C	3.65032	3.59971	-1.16769
C	3.15711	4.58884	-0.31714
C	1.83372	4.53053	0.11618
C	1.01216	3.48128	-0.27519
C	-0.79536	0.41197	-3.59737
C	-0.25516	-0.49657	-4.70440
F	0.89814	-0.00413	-5.22046
F	-0.01161	-1.75565	-4.29499
F	-1.15097	-0.57748	-5.71675
H	-2.31254	-0.96402	2.55481
H	-0.63519	-1.21486	3.00562
H	-0.66419	-3.08426	1.63726
H	-2.27217	-2.64685	1.05302
H	-0.72397	-3.13467	-2.50486
H	-0.98209	-5.06972	-0.17493
H	-0.15585	-5.28029	-1.70787
H	0.92012	-4.31295	0.82983
H	1.81794	-4.58862	-0.64740
H	1.56835	-2.11712	0.50892
H	0.77347	2.19416	1.88205
H	0.52530	0.34742	4.27284
H	0.80477	2.07699	4.22219
H	-1.74718	0.62267	4.38529
H	-1.51034	2.35690	4.53055
H	-2.95878	1.23955	2.50072
H	-2.62912	-2.67123	-3.65359
H	-5.03043	-3.06322	-4.07083
H	-6.42419	-4.20625	-2.35630
H	-5.36970	-4.98088	-0.24318
H	-2.98085	-4.62610	0.15622
H	2.92955	2.25110	1.32304
H	5.17231	1.24758	1.16996
H	5.53550	-1.11400	1.87000
H	3.61615	-2.43922	2.73073
H	1.39181	-1.43814	2.90093
H	-3.98711	2.79564	1.13884
H	-4.30898	5.15502	0.48674
H	-2.59519	6.85815	1.07574
H	-0.57573	6.17096	2.35059
H	-0.26373	3.83458	3.01871
H	2.94096	-0.53334	-0.48003
H	4.64355	-0.05487	-2.20087
H	4.73044	-1.41012	-4.28407
H	3.11964	-3.27794	-4.59389
H	1.47616	-3.80033	-2.85304
H	3.20848	1.78559	-2.24219
H	4.67668	3.64586	-1.52084
H	3.79904	5.40563	-0.00046
H	1.43581	5.30528	0.76545
H	-0.02051	3.44797	0.05619
H	-0.99597	1.37592	-4.11748

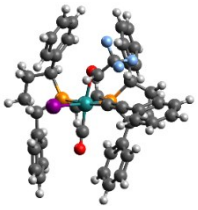
D Pre-Reaction Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.5355955400
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6420995659
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9796456361
Imaginary Frequency (cm^{-1}): None

C	-0.24988	-0.98772	2.58585
C	-1.13221	-2.02734	1.89637
P	-0.13520	0.56382	1.56186
P	-0.57354	-2.22542	0.13499
C	-1.74155	-3.49681	-0.60474
C	-1.22446	-4.83084	-0.04378
C	0.29195	-4.81232	-0.21674
C	0.85617	-3.46446	0.30045
C	1.47091	1.46166	2.03669
C	1.02601	2.84575	2.58016
C	-0.40343	3.14667	2.13034
C	-1.21085	1.86779	2.37780
C	-2.66507	1.87627	2.00293
C	2.14413	-3.05999	-0.36228
C	2.35650	0.67345	2.96662
C	-3.21069	-3.21817	-0.44590
C	-3.94027	-2.73344	-1.53611
C	-5.29919	-2.45872	-1.42317
C	-5.95642	-2.66579	-0.21342
C	-5.24480	-3.16305	0.87638
C	-3.88597	-3.44161	0.76063
C	3.50258	0.04403	2.47472
C	4.32519	-0.70384	3.31383
C	4.01084	-0.84070	4.66245
C	2.86367	-0.22644	5.16346
C	2.04546	0.52161	4.32437
C	-3.51865	0.90895	2.54835
C	-4.86998	0.88528	2.22548
C	-5.39738	1.84411	1.36220
C	-4.56155	2.82043	0.82946
C	-3.20465	2.83561	1.14288
C	3.28048	-2.80440	0.40878
C	4.48666	-2.45406	-0.19220
C	4.57196	-2.35135	-1.57729
C	3.44196	-2.59973	-2.35618
C	2.24084	-2.95514	-1.75350
Ru	-0.39098	0.01237	-0.66558
C	-2.20866	0.16459	-0.66511
I	-0.60970	-0.76532	-3.36250
O	-3.35117	0.28653	-0.78572
C	-0.19844	1.95450	-1.20900
O	1.83797	0.09137	-0.87002
C	0.02589	3.12305	-1.51717
C	0.27917	4.48645	-1.81777
C	1.37538	5.15710	-1.23876
C	1.61873	6.49405	-1.52583
C	0.77788	7.19560	-2.38953
C	-0.31217	6.54458	-2.96650
C	-0.56151	5.20647	-2.68940
C	2.29635	0.65353	-1.85080
C	3.74969	1.13922	-1.87918
F	4.38072	0.64709	-2.96235
F	3.73293	2.48704	-1.98629
F	4.44709	0.81436	-0.78683
H	-0.61992	-0.75018	3.58981
H	0.77404	-1.36770	2.69920
H	-1.09323	-2.98237	2.43310
H	-2.17644	-1.69413	1.86804
H	-1.50255	-3.46265	-1.67804
H	-1.49054	-4.93989	1.01424
H	-1.67993	-5.66914	-0.58382
H	0.77839	-5.64303	0.30603
H	0.52968	-4.91332	-1.28157
H	1.03155	-3.53742	1.38128
H	2.00005	1.59998	1.08878
H	1.06171	2.83531	3.67417
H	1.72710	3.61484	2.23975
H	-0.83193	3.98502	2.69187
H	-0.41688	3.40532	1.06570
H	-1.13550	1.61998	3.44936
H	-3.42814	-2.55445	-2.47875
H	-5.84406	-2.07698	-2.28226
H	-7.01696	-2.44878	-0.12114
H	-5.75024	-3.33979	1.82204
H	-3.35373	-3.84105	1.61891
H	3.74732	0.13477	1.42127
H	5.21475	-1.17987	2.90946
H	4.65213	-1.42130	5.31952
H	2.60404	-0.33164	6.21337
H	1.14741	0.98018	4.73135
H	-3.11821	0.17246	3.24256
H	-5.51477	0.12315	2.65491
H	-6.45433	1.83152	1.11119
H	-4.96420	3.57439	0.15850
H	-2.56762	3.59971	0.70781
H	3.21825	-2.87774	1.49215
H	5.35984	-2.25727	0.42440
H	5.51038	-2.07357	-2.04894
H	3.49622	-2.51296	-3.43827
H	1.36477	-3.12757	-2.37346
H	2.02947	4.61182	-0.56398
H	2.47003	6.99372	-1.07129
H	0.97065	8.24130	-2.61105
H	-0.97232	7.08368	-3.64072
H	-1.40845	4.69947	-3.14236
H	1.71554	0.87132	-2.75818

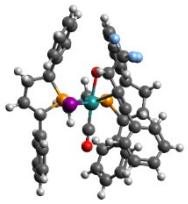
D TS



Gibbs Energy @ r^2SCAN-3c[CPCM]: -3264.5269139300
Thermal Correction @ r^2SCAN-3c[CPCM]: 0.6442641726
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^2SCAN-3c[CPCM]: -3266.9569388291
Imaginary Frequency (cm^{-1}): -133.82

C	-0.24097	-1.02828	2.58223
C	-1.15417	-2.05170	1.91184
P	-0.11932	0.50964	1.54311
P	-0.61804	-2.26422	0.14758
C	-1.82271	-3.51429	-0.56974
C	-1.30492	-4.85778	-0.03157
C	0.20776	-4.85286	-0.23493
C	0.79470	-3.52561	0.30589
C	1.46727	1.42162	2.02534
C	1.00521	2.75567	2.66133
C	-0.40072	3.08567	2.16615
C	-1.22593	1.80604	2.34018
C	-2.66392	1.84546	1.90950
C	2.10938	-3.14810	-0.32193
C	2.44601	0.63515	2.85511
C	-3.28180	-3.21537	-0.35832
C	-4.03382	-2.68335	-1.41051
C	-5.38358	-2.38803	-1.24880
C	-6.00993	-2.62363	-0.02798
C	-5.27658	-3.16853	1.02391
C	-3.92664	-3.46519	0.86000
C	3.62976	0.16451	2.28017
C	4.55839	-0.54470	3.03835
C	4.31343	-0.80584	4.38297
C	3.13072	-0.35143	4.96500
C	2.20859	0.36358	4.20894
C	-3.55718	0.89280	2.41552
C	-4.89638	0.90119	2.04507
C	-5.37225	1.87850	1.17275
C	-4.49751	2.84125	0.67944
C	-3.15266	2.82395	1.04058
C	3.22785	-2.91173	0.47950
C	4.45973	-2.59702	-0.09030
C	4.58824	-2.50921	-1.47299
C	3.47528	-2.73787	-2.28123
C	2.24966	-3.05790	-1.71033
Ru	-0.33696	-0.07207	-0.68272
C	-2.14344	0.17927	-0.75363
I	-0.61206	-0.93643	-3.36392
O	-3.27465	0.34720	-0.92919
C	0.14761	1.85689	-1.27321
O	1.88823	0.01726	-0.85546
C	0.29240	3.06440	-1.51220
C	0.48530	4.43462	-1.78564
C	1.15169	5.26097	-0.85781
C	1.34075	6.60712	-1.13342
C	0.86488	7.15295	-2.32579
C	0.20074	6.34532	-3.24941
C	0.01379	4.99576	-2.98959
C	1.93101	0.91833	-1.74454
C	3.12034	1.89195	-1.71551
F	4.25921	1.18352	-1.93171
F	3.02529	2.80912	-2.69663
F	3.27681	2.54349	-0.54674
H	-0.58866	-0.77669	3.59069
H	0.77841	-1.42550	2.67727
H	-1.12803	-3.00744	2.44803
H	-2.19198	-1.69860	1.89380
H	-1.61801	-3.47592	-1.64932
H	-1.54809	-4.97332	1.03119
H	-1.78100	-5.68632	-0.56877
H	0.69442	-5.70047	0.25999
H	0.42463	-4.93231	-1.30605
H	0.94704	-3.61917	1.38890
H	1.93107	1.63167	1.06018
H	0.98765	2.66109	3.75244
H	1.72272	3.54544	2.41232
H	-0.84749	3.91083	2.73300
H	-0.36919	3.37859	1.11051
H	-1.19875	1.53179	3.40706
H	-3.54697	-2.48562	-2.36272
H	-5.94558	-1.96942	-2.07917
H	-7.06343	-2.39184	0.10180
H	-5.75772	-3.36744	1.97781
H	-3.37727	-3.89830	1.69064
H	3.82022	0.35258	1.22660
H	5.47706	-0.89277	2.57437
H	5.03767	-1.35817	4.97514
H	2.92702	-0.55254	6.01329
H	1.29046	0.70783	4.67892
H	-3.19833	0.14363	3.11877
H	-5.57207	0.14954	2.44433
H	-6.41965	1.89103	0.88451
H	-4.86001	3.60964	0.00198
H	-2.48516	3.57853	0.63487
H	3.13488	-2.97142	1.56200
H	5.32045	-2.42129	0.54904
H	5.54758	-2.26240	-1.91951
H	3.56135	-2.66098	-3.36196
H	1.38681	-3.21140	-2.35288
H	1.51895	4.82867	0.06806
H	1.85920	7.23665	-0.41600
H	1.01286	8.20830	-2.53598
H	-0.16789	6.77142	-4.17801
H	-0.49612	4.35765	-3.70485
H	1.56983	0.74524	-2.76893

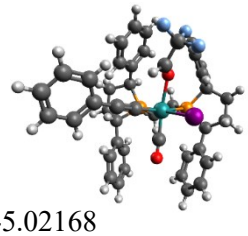
D Post-Reaction Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.5496827600
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6469367297
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9927802806
Imaginary Frequency (cm^{-1}): None

C	-0.04059	-0.88465	2.47815
C	-1.05909	-1.74736	1.73929
P	0.28736	0.66143	1.50158
P	-0.49634	-1.94351	-0.01357
C	-1.84389	-2.95533	-0.84831
C	-1.52416	-4.39255	-0.40321
C	-0.02155	-4.57757	-0.58059
C	0.71785	-3.40860	0.10882
C	1.93401	1.38280	2.07945
C	1.60369	2.79710	2.62331
C	0.23162	3.23576	2.11039
C	-0.70427	2.03974	2.30929
C	-2.14046	2.19858	1.89966
C	2.14155	-3.24213	-0.35001
C	2.69894	0.49531	3.02565
C	-3.26506	-2.50495	-0.64895
C	-3.94180	-1.88534	-1.70416
C	-5.26207	-1.47075	-1.56351
C	-5.93386	-1.67243	-0.36101
C	-5.27769	-2.30539	0.69220
C	-3.95758	-2.72233	0.54893
C	3.80568	-0.22344	2.56493
C	4.52318	-1.05443	3.42200
C	4.13999	-1.18889	4.75333
C	3.03110	-0.48557	5.22132
C	2.31908	0.34809	4.36597
C	-3.09653	1.30142	2.39326
C	-4.43452	1.41328	2.03512
C	-4.84668	2.44206	1.18936
C	-3.90993	3.35426	0.71532
C	-2.56687	3.23297	1.06383
C	3.16583	-3.17780	0.59684
C	4.49847	-3.08621	0.20296
C	4.82658	-3.06373	-1.14904
C	3.81126	-3.12992	-2.10205
C	2.48208	-3.21954	-1.70594
Ru	0.10314	0.13659	-0.74039
C	-1.68309	0.58474	-0.88161
I	-0.11069	-0.70485	-3.45996
O	-2.78481	0.88540	-1.07321
C	1.54923	1.86829	-1.68805
O	2.21695	-0.15668	-0.76966
C	0.66229	2.70688	-1.69185
C	-0.28616	3.76060	-1.77498
C	-0.01130	4.99741	-1.16618
C	-0.93603	6.02960	-1.24972
C	-2.13718	5.84183	-1.93216
C	-2.40605	4.62146	-2.55002
C	-1.48716	3.58407	-2.48094
C	2.57024	0.79929	-1.69745
C	3.97380	1.38242	-1.45940
F	4.89258	0.39711	-1.39901
F	4.32479	2.21013	-2.47386
F	4.08315	2.09830	-0.31424
H	-0.37965	-0.63297	3.48917
H	0.91761	-1.41290	2.57359
H	-1.17540	-2.72385	2.22322
H	-2.04101	-1.26081	1.70973
H	-1.60278	-2.86947	-1.91636
H	-1.81167	-4.55170	0.64292
H	-2.09460	-5.10260	-1.01275
H	0.33265	-5.52748	-0.16515
H	0.21306	-4.57805	-1.65051
H	0.73996	-3.60292	1.18927
H	2.50945	1.46600	1.15665
H	1.58132	2.77581	3.71766
H	2.39109	3.49803	2.32663
H	-0.14060	4.11564	2.64804
H	0.28885	3.49892	1.04784
H	-0.68074	1.76707	3.37725
H	-3.41824	-1.71554	-2.64207
H	-5.76535	-0.98677	-2.39592
H	-6.96439	-1.34762	-0.24741
H	-5.79683	-2.48085	1.63055
H	-3.47400	-3.23049	1.37784
H	4.10087	-0.13484	1.52234
H	5.38633	-1.59709	3.04667
H	4.70014	-1.83573	5.42273
H	2.71966	-0.58610	6.25758
H	1.45200	0.88266	4.74656
H	-2.78864	0.51599	3.08060
H	-5.15873	0.70230	2.42338
H	-5.89261	2.53444	0.91027
H	-4.21917	4.16460	0.06063
H	-1.85350	3.95168	0.67291
H	2.91866	-3.19597	1.65644
H	5.28159	-3.03865	0.95477
H	5.86544	-2.99395	-1.45987
H	4.05563	-3.10530	-3.16084
H	1.70410	-3.24469	-2.46342
H	0.92615	5.13587	-0.63637
H	-0.71997	6.98368	-0.77783
H	-2.86156	6.64932	-1.98756
H	-3.33748	4.47671	-3.08911
H	-1.68737	2.63342	-2.96439
H	2.61485	0.40326	-2.73555

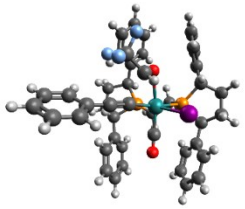
D' Pre-Reaction Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.5353839000
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6446359061
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9788612995
Imaginary Frequency (cm^{-1}): -13.36 (Conformational, thus ignored)

C	-0.34777	-1.59933	2.44973
C	-0.91692	-2.33422	1.23368
P	-0.37283	0.24161	2.15674
P	-0.04435	-1.73292	-0.28734
C	-0.78380	-2.66065	-1.73398
C	-0.17617	-4.06504	-1.59055
C	1.32040	-3.86682	-1.35489
C	1.54771	-2.76287	-0.28806
C	0.88438	1.03885	3.33891
C	0.04616	1.91281	4.30707
C	-1.30199	2.23329	3.66370
C	-1.84492	0.90407	3.12754
C	-3.16309	0.92700	2.40713
C	2.81935	-1.98587	-0.48473
C	1.81287	0.06406	4.01291
C	-2.27560	-2.58662	-1.90025
C	-2.81325	-1.81563	-2.93540
C	-4.18880	-1.72693	-3.12114
C	-5.05429	-2.40958	-2.27065
C	-4.53081	-3.19260	-1.24393
C	-3.15396	-3.28573	-1.06344
C	3.14003	-0.04588	3.59060
C	4.01279	-0.94778	4.19486
C	3.56979	-1.76316	5.23191
C	2.24504	-1.66966	5.65696
C	1.37673	-0.76634	5.05407
C	-3.91058	-0.25367	2.30926
C	-5.13330	-0.27359	1.64832
C	-5.64111	0.89613	1.08607
C	-4.91591	2.07869	1.19430
C	-3.68562	2.09507	1.84638
C	3.73330	-1.86845	0.56583
C	4.92715	-1.17269	0.40010
C	5.21837	-0.57296	-0.82072
C	4.30542	-0.67232	-1.87289
C	3.12062	-1.38151	-1.70863
Ru	-0.07603	0.55488	-0.20019
C	-1.85194	0.54751	-0.59800
I	-0.21752	3.37483	-0.09236
O	-2.95338	0.60620	-0.94382
C	0.37745	0.63899	-2.16905
O	2.10194	0.95568	0.25387
C	0.70923	0.64900	-3.35224
C	1.16700	0.63828	-4.69450
C	0.37160	0.11296	-5.73240
C	0.83610	0.09732	-7.04153
C	2.10006	0.59916	-7.35065
C	2.89785	1.12201	-6.33302
C	2.44098	1.14574	-5.02168
C	2.71688	1.68814	-0.50360
C	3.95928	2.45553	-0.02351
F	4.53202	1.92379	1.06260
F	4.87432	2.53397	-1.00744
F	3.57959	3.71663	0.28022
H	-0.90034	-1.85626	3.36059
H	0.69927	-1.88660	2.61395
H	-0.80680	-3.41922	1.34757
H	-1.98277	-2.11071	1.10622
H	-0.31803	-2.17159	-2.60279
H	-0.63584	-4.60510	-0.75461
H	-0.36303	-4.64910	-2.49883
H	1.81388	-4.79213	-1.03926
H	1.78627	-3.55355	-2.29510
H	1.57488	-3.21922	0.70920
H	1.47708	1.69371	2.69002
H	-0.12670	1.36705	5.24052
H	0.60414	2.82101	4.55872
H	-2.00102	2.67102	4.38617
H	-1.16817	2.95053	2.84537
H	-1.93172	0.20674	3.97525
H	-2.14169	-1.26786	-3.59266
H	-4.58486	-1.11774	-3.92894
H	-6.12931	-2.33827	-2.41005
H	-5.19729	-3.73867	-0.58177
H	-2.76622	-3.91457	-0.26734
H	3.48898	0.57831	2.77431
H	5.04233	-1.01049	3.85211
H	4.24863	-2.46598	5.70671
H	1.88576	-2.30412	6.46271
H	0.34469	-0.71795	5.39273
H	-3.53314	-1.16446	2.77057
H	-5.69566	-1.20107	1.58051
H	-6.59825	0.88516	0.57216
H	-5.30512	2.99705	0.76301
H	-3.13038	3.02561	1.90891
H	3.50530	-2.32667	1.52558
H	5.62586	-1.09311	1.22840
H	6.14677	-0.02547	-0.95441
H	4.52247	-0.20167	-2.82828
H	2.41284	-1.43165	-2.53127
H	-0.61375	-0.27810	-5.49535
H	0.20595	-0.30969	-7.82797
H	2.45931	0.58486	-8.37550
H	3.88312	1.51840	-6.56396
H	3.06126	1.55991	-4.23155
H	2.39931	1.89310	-1.53732

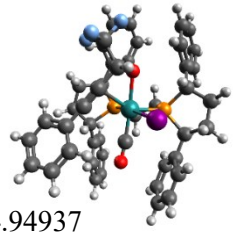
D' TS



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.5160089200
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6456355215
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9497239105
Imaginary Frequency (cm^{-1}): -103.38

C	-0.38491	-1.62310	2.46000
C	-0.95029	-2.29373	1.19891
P	-0.46320	0.22041	2.21455
P	0.06948	-1.68856	-0.23028
C	-0.51784	-2.53509	-1.79296
C	0.06917	-3.95091	-1.69828
C	1.52209	-3.77849	-1.26971
C	1.57512	-2.85760	-0.02953
C	0.69794	1.13297	3.39434
C	-0.20927	1.70028	4.51104
C	-1.57872	2.00353	3.90915
C	-2.01139	0.72624	3.18036
C	-3.31358	0.74701	2.43125
C	2.94941	-2.31840	0.24704
C	1.90651	0.39822	3.90218
C	-1.98321	-2.43926	-2.10817
C	-2.40558	-1.64736	-3.18032
C	-3.75431	-1.54614	-3.50530
C	-4.70631	-2.23600	-2.75960
C	-4.29641	-3.03762	-1.69612
C	-2.94629	-3.14350	-1.37615
C	3.18664	0.83278	3.54463
C	4.31972	0.23251	4.08555
C	4.19178	-0.82156	4.98535
C	2.92186	-1.27726	5.33347
C	1.78946	-0.67076	4.79897
C	-4.02506	-0.44867	2.26787
C	-5.23308	-0.47528	1.58058
C	-5.76357	0.70289	1.05904
C	-5.07744	1.90053	1.23725
C	-3.86179	1.92377	1.91576
C	3.55166	-2.54401	1.48795
C	4.86694	-2.15164	1.72256
C	5.59555	-1.51709	0.72133
C	4.99908	-1.27799	-0.51557
C	3.69010	-1.68151	-0.74989
Ru	-0.11508	0.61703	-0.09841
C	-1.87431	0.47200	-0.53492
I	-0.62244	3.37938	0.27044
O	-2.97668	0.46297	-0.88557
C	0.47422	0.87879	-2.06204
O	2.14603	1.06809	-0.07470
C	0.69563	0.88870	-3.28011
C	0.97777	0.89509	-4.66310
C	0.54762	1.96104	-5.47820
C	0.82160	1.95374	-6.83824
C	1.52773	0.89351	-7.40667
C	1.96029	-0.16630	-6.60897
C	1.68911	-0.17155	-5.24866
C	2.13577	1.77747	-1.11725
C	3.36445	1.78325	-2.04842
F	4.46058	2.11731	-1.32129
F	3.63302	0.62178	-2.66587
F	3.20874	2.72643	-3.00250
H	-0.94276	-1.92519	3.35341
H	0.66449	-1.90858	2.61230
H	-0.90734	-3.38596	1.28342
H	-1.99392	-2.00214	1.03374
H	0.03281	-1.99132	-2.57566
H	-0.48229	-4.55172	-0.96439
H	-0.01140	-4.45695	-2.66707
H	2.00275	-4.73375	-1.03009
H	2.08717	-3.32547	-2.09208
H	1.27822	-3.45399	0.84221
H	1.04102	1.97219	2.77544
H	-0.31817	0.95949	5.31231
H	0.25916	2.59067	4.94512
H	-2.31397	2.26626	4.67885
H	-1.50095	2.84430	3.21113
H	-2.08292	-0.06865	3.93816
H	-1.66603	-1.09600	-3.75760
H	-4.06180	-0.92236	-4.34010
H	-5.76077	-2.15520	-3.00815
H	-5.03115	-3.58777	-1.11443
H	-2.64589	-3.78735	-0.55434
H	3.29260	1.65906	2.84556
H	5.30549	0.58902	3.79960
H	5.07567	-1.28958	5.40983
H	2.81155	-2.10264	6.03172
H	0.80462	-1.02424	5.09498
H	-3.63025	-1.36739	2.69782
H	-5.76647	-1.41462	1.46182
H	-6.70955	0.68746	0.52491
H	-5.48686	2.82599	0.84122
H	-3.33536	2.86517	2.03247
H	2.99079	-3.04466	2.27491
H	5.31979	-2.34250	2.69047
H	6.62234	-1.21088	0.90160
H	5.55783	-0.77816	-1.30158
H	3.23485	-1.49536	-1.71659
H	0.00151	2.78361	-5.02648
H	0.48624	2.77896	-7.45980
H	1.74183	0.89333	-8.47159
H	2.51054	-0.99113	-7.05253
H	2.02263	-0.99146	-4.61948
H	1.59967	2.73586	-1.16846

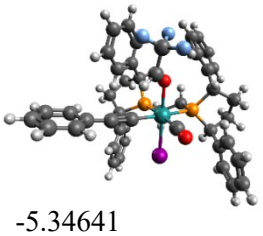
D' Post-Reaction Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.5427755700
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6478604620
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9850466248
Imaginary Frequency (cm^{-1}): None

C	-0.24024	-1.38136	2.10626
C	-0.65849	-2.10534	0.82400
P	-0.27942	0.44940	1.82383
P	0.35634	-1.44598	-0.58017
C	-0.36556	-2.02592	-2.23613
C	0.71758	-2.93085	-2.87672
C	2.07114	-2.63888	-2.22675
C	1.80188	-2.65548	-0.71826
C	0.78048	1.32874	3.11266
C	-0.22990	1.96063	4.10041
C	-1.51867	2.29233	3.35104
C	-1.90943	1.02469	2.58320
C	-3.11075	1.08522	1.68354
C	2.97140	-2.56800	0.21815
C	1.86837	0.52507	3.77524
C	-1.73836	-2.64070	-2.15948
C	-2.83401	-1.97578	-2.71778
C	-4.11284	-2.52276	-2.65036
C	-4.31710	-3.74846	-2.02287
C	-3.23041	-4.42788	-1.47413
C	-1.95395	-3.88068	-1.54491
C	3.20953	0.81464	3.50529
C	4.23143	0.14914	4.17574
C	3.93010	-0.82653	5.12155
C	2.59847	-1.13961	5.38357
C	1.57690	-0.46927	4.71745
C	-3.81252	-0.09373	1.40137
C	-4.92716	-0.08210	0.57116
C	-5.37350	1.11837	0.02173
C	-4.69854	2.29917	0.31590
C	-3.57461	2.28425	1.13755
C	2.86151	-3.09259	1.51298
C	3.94227	-3.06989	2.38604
C	5.15944	-2.52772	1.97833
C	5.28737	-2.02948	0.68571
C	4.20380	-2.05800	-0.18884
Ru	0.37413	0.85291	-0.32403
C	-1.33536	0.89211	-1.01757
I	0.01696	3.68836	0.02287
O	-2.35604	0.98210	-1.55888
C	2.01256	1.58683	-1.98140
O	2.41658	1.08519	0.24761
C	1.26629	1.30780	-2.90646
C	0.45730	1.03986	-4.04255
C	-0.72286	1.76998	-4.26144
C	-1.51846	1.48057	-5.36127
C	-1.14837	0.47375	-6.25185
C	0.03016	-0.24245	-6.04748
C	0.83288	0.03388	-4.94937
C	2.85581	1.87219	-0.80152
C	4.34379	1.67832	-1.14197
F	5.09703	1.69571	-0.02355
F	4.61418	0.52599	-1.79437
F	4.77579	2.68562	-1.94314
H	-0.88662	-1.65592	2.94740
H	0.79055	-1.63698	2.37936
H	-0.52406	-3.18749	0.92421
H	-1.71319	-1.91888	0.58878
H	-0.44159	-1.10510	-2.82457
H	0.46358	-3.98235	-2.70225
H	0.73277	-2.77117	-3.96004
H	2.81841	-3.39390	-2.49650
H	2.45559	-1.65980	-2.54373
H	1.28897	-3.60681	-0.49826
H	1.24864	2.12616	2.52421
H	-0.44916	1.25053	4.90574
H	0.21887	2.84908	4.55814
H	-2.32348	2.57742	4.03880
H	-1.34854	3.12543	2.66146
H	-2.09408	0.23659	3.32998
H	-2.68146	-1.01933	-3.21055
H	-4.95003	-1.98870	-3.09163
H	-5.31421	-4.17620	-1.96711
H	-3.37723	-5.38935	-0.98960
H	-1.11730	-4.42583	-1.11392
H	3.44706	1.56996	2.76120
H	5.26694	0.39353	3.95504
H	4.72762	-1.34723	5.64450
H	2.35217	-1.90606	6.11367
H	0.54293	-0.71964	4.94245
H	-3.48961	-1.02966	1.85307
H	-5.45375	-1.00932	0.36134
H	-6.24737	1.13309	-0.62381
H	-5.04375	3.24154	-0.10094
H	-3.05292	3.21334	1.34221
H	1.92684	-3.55108	1.82957
H	3.83452	-3.47653	3.38733
H	6.00351	-2.50407	2.66176
H	6.23679	-1.62179	0.34886
H	4.32357	-1.68766	-1.19863
H	-1.00399	2.55032	-3.56135
H	-2.43302	2.04321	-5.52369
H	-1.77730	0.25026	-7.10867
H	0.32312	-1.02135	-6.74530
H	1.75130	-0.51987	-4.78038
H	2.76603	2.95787	-0.59062

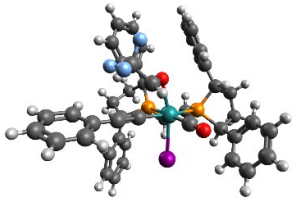
E Pre-Reaction Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.5032315300
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6401582363
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9494365874
Imaginary Frequency (cm^{-1}): None

C	-0.63674	-1.09926	2.51566
C	-1.00242	-1.98612	1.32527
P	-0.76563	0.72501	2.11920
P	-0.07915	-1.39162	-0.16617
C	-0.48608	-2.54244	-1.61439
C	0.70044	-3.54657	-1.69132
C	1.44386	-3.58776	-0.35424
C	1.62341	-2.12986	0.13023
C	0.40404	1.55756	3.38776
C	-0.51716	2.05980	4.52816
C	-1.82393	1.26353	4.52522
C	-2.32676	1.18106	3.06444
C	-3.03545	2.44528	2.64870
C	2.77819	-1.45976	-0.57406
C	1.54256	0.66933	3.82212
C	-1.84579	-3.19450	-1.56877
C	-2.85599	-2.74397	-2.42320
C	-4.10991	-3.34748	-2.43026
C	-4.37656	-4.41684	-1.57927
C	-3.37364	-4.88498	-0.73265
C	-2.11909	-4.28239	-0.73178
C	2.73392	0.66988	3.09087
C	3.80059	-0.14691	3.45399
C	3.69278	-0.99005	4.55704
C	2.50978	-1.00172	5.29310
C	1.44598	-0.18039	4.93044
C	-4.43473	2.46986	2.68956
C	-5.14059	3.62989	2.39249
C	-4.45749	4.79480	2.04633
C	-3.06729	4.78334	2.00016
C	-2.36343	3.61920	2.30096
C	4.03960	-1.48985	0.03046
C	5.15495	-0.96118	-0.61304
C	5.02691	-0.38782	-1.87524
C	3.77481	-0.34887	-2.48581
C	2.66287	-0.88778	-1.84320
Ru	-0.48431	1.00380	-0.25476
C	-0.91614	2.81934	-0.42834
I	-3.15292	0.47625	-0.59301
O	-1.14651	3.92683	-0.65957
C	-0.21733	0.91622	-2.25609
O	1.63705	1.53289	-0.04226
C	0.01269	0.84098	-3.46116
C	0.36086	0.69692	-4.82988
C	0.35863	1.80232	-5.70379
C	0.71769	1.65145	-7.03718
C	1.08528	0.40108	-7.53388
C	1.08988	-0.70249	-6.68116
C	0.73253	-0.56129	-5.34641
C	2.22666	2.18894	-0.88940
C	3.61078	2.75987	-0.57317
F	4.27178	2.05189	0.34913
F	4.35602	2.83412	-1.68754
F	3.44616	4.01897	-0.09947
H	-1.26810	-1.33831	3.37916
H	0.39824	-1.28992	2.81882
H	-0.76254	-3.03118	1.54931
H	-2.07095	-1.92476	1.09095
H	-0.46925	-1.87816	-2.48661
H	0.33584	-4.53969	-1.97148
H	1.38901	-3.22065	-2.47828
H	0.86859	-4.15210	0.38927
H	2.41977	-4.07786	-0.45059
H	1.81455	-2.10855	1.21039
H	0.83565	2.40984	2.84930
H	-0.00880	1.99084	5.49523
H	-0.74150	3.11828	4.36535
H	-1.65510	0.25049	4.90983
H	-2.58383	1.73200	5.16135
H	-3.02103	0.34102	2.94609
H	-2.65509	-1.90579	-3.08531
H	-4.87970	-2.98036	-3.10359
H	-5.35505	-4.88890	-1.58187
H	-3.56588	-5.72690	-0.07306
H	-1.34591	-4.67523	-0.07714
H	2.82422	1.32295	2.22891
H	4.71951	-0.11785	2.87455
H	4.52415	-1.62704	4.84544
H	2.41307	-1.65257	6.15792
H	0.53296	-0.21065	5.51858
H	-4.97409	1.56209	2.95083
H	-6.22673	3.62313	2.42436
H	-5.00601	5.70176	1.80824
H	-2.52299	5.68092	1.71995
H	-1.27895	3.63361	2.23778
H	4.14518	-1.93411	1.01760
H	6.12422	-0.98991	-0.12245
H	5.89331	0.03527	-2.37573
H	3.65704	0.10361	-3.46751
H	1.69404	-0.81344	-2.32871
H	0.07128	2.77664	-5.31915
H	0.70958	2.51622	-7.69535
H	1.36449	0.28739	-8.57737
H	1.37342	-1.68098	-7.05970
H	0.73706	-1.42291	-4.68402
H	1.78887	2.45702	-1.86227

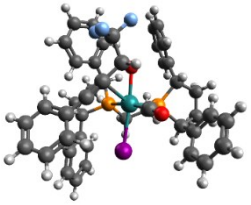
E TS



Gibbs Energy @ r^2SCAN-3c[CPCM]: -3264.4801397100
Thermal Correction @ r^2SCAN-3c[CPCM]: 0.6424949241
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^2SCAN-3c[CPCM]: -3266.9155387979
Imaginary Frequency (cm^{-1}): -140.05

C	-1.01849	-1.25895	2.64675
C	-1.20392	-2.13307	1.40097
P	-0.97365	0.56872	2.24377
P	-0.06846	-1.51103	0.06445
C	-0.20195	-2.61315	-1.46407
C	0.83946	-3.75323	-1.26690
C	1.29607	-3.80354	0.19282
C	1.50939	-2.34585	0.67855
C	0.16317	1.27645	3.55554
C	-0.56143	0.98707	4.88144
C	-2.10063	1.00354	4.67712
C	-2.48790	1.19321	3.18449
C	-2.90886	2.60306	2.84788
C	2.86188	-1.85701	0.22657
C	1.62094	0.90243	3.48459
C	-1.58620	-3.08267	-1.82569
C	-2.21830	-2.56202	-2.95796
C	-3.48441	-2.99960	-3.33435
C	-4.14327	-3.96498	-2.57795
C	-3.51771	-4.50031	-1.45297
C	-2.24771	-4.06785	-1.08443
C	2.48371	1.69724	2.71979
C	3.84771	1.43487	2.66698
C	4.38293	0.37143	3.38958
C	3.53736	-0.43392	4.14531
C	2.16889	-0.17586	4.18953
C	-4.03571	2.81574	2.04688
C	-4.47229	4.10217	1.74807
C	-3.78888	5.20764	2.24656
C	-2.67714	5.01183	3.06195
C	-2.24713	3.72363	3.36611
C	3.95130	-2.10738	1.06912
C	5.25141	-1.83251	0.66274
C	5.48671	-1.31030	-0.60648
C	4.41127	-1.05293	-1.45159
C	3.10709	-1.31735	-1.03639
Ru	-0.64663	0.87479	-0.06176
C	-1.28247	2.63282	-0.04512
I	-3.26226	0.15072	-0.54842
O	-1.66030	3.72313	-0.09803
C	-0.26345	0.93026	-2.08336
O	1.45749	1.47270	-0.26609
C	-0.07357	0.89807	-3.30671
C	0.15724	0.82063	-4.69745
C	-0.31647	1.82733	-5.56157
C	-0.08738	1.73863	-6.92721
C	0.61073	0.65149	-7.45270
C	1.08330	-0.35213	-6.60626
C	0.86302	-0.27240	-5.23927
C	1.34976	2.10959	-1.35238
C	2.55167	2.16462	-2.31383
F	3.65907	2.52933	-1.62262
F	2.83208	1.01523	-2.94394
F	2.32819	3.10396	-3.25819
H	-1.82243	-1.45617	3.36436
H	-0.07427	-1.50553	3.14729
H	-1.00009	-3.17992	1.64597
H	-2.22967	-2.06435	1.02793
H	0.12906	-1.94708	-2.27076
H	0.41378	-4.71249	-1.57652
H	1.70189	-3.55661	-1.91279
H	0.53961	-4.29891	0.81123
H	2.22673	-4.37181	0.30291
H	1.48203	-2.30696	1.77415
H	0.10748	2.35259	3.34395
H	-0.26378	0.00551	5.25899
H	-0.24907	1.72091	5.63310
H	-2.52650	0.06349	5.03957
H	-2.56332	1.80266	5.26329
H	-3.30815	0.52049	2.91136
H	-1.71313	-1.79792	-3.54519
H	-3.95887	-2.58069	-4.21760
H	-5.13395	-4.30527	-2.86605
H	-4.01909	-5.26208	-0.86200
H	-1.76815	-4.50826	-0.21393
H	2.07553	2.53799	2.16464
H	4.49513	2.06908	2.06736
H	5.44956	0.16881	3.35784
H	3.94213	-1.26910	4.71085
H	1.53897	-0.81119	4.80434
H	-4.57273	1.95888	1.65141
H	-5.35229	4.23952	1.12532
H	-4.12696	6.21351	2.01352
H	-2.14627	5.86554	3.47455
H	-1.40298	3.60211	4.03894
H	3.77213	-2.52593	2.05633
H	6.08072	-2.02754	1.33738
H	6.50103	-1.10124	-0.93489
H	4.58999	-0.64412	-2.44053
H	2.27777	-1.09266	-1.70209
H	-0.86050	2.66905	-5.14393
H	-0.45478	2.51920	-7.58707
H	0.78686	0.58579	-8.52253
H	1.62653	-1.19845	-7.01672
H	1.22930	-1.04666	-4.57134
H	0.72774	3.00774	-1.45346

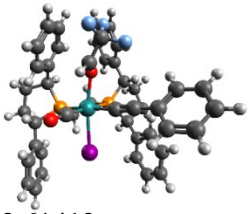
E Post-Reaction Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.5098551800
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6475622712
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9552576574
Imaginary Frequency (cm^{-1}): None

C	-0.97559	-1.21738	2.29424
C	-1.11553	-2.03133	1.01036
P	-0.89769	0.61537	1.96253
P	0.10062	-1.41276	-0.24922
C	-0.06727	-2.58006	-1.73860
C	0.89728	-3.77456	-1.45530
C	1.45058	-3.71557	-0.02544
C	1.67715	-2.23470	0.35843
C	0.16976	1.32767	3.34228
C	-0.72805	1.29960	4.60937
C	-2.21342	1.03010	4.26122
C	-2.48642	1.23785	2.75450
C	-2.89195	2.64757	2.40438
C	2.99252	-1.73573	-0.18972
C	1.55582	0.76417	3.55763
C	-1.46576	-3.00079	-2.11501
C	-2.06352	-2.46658	-3.25918
C	-3.33430	-2.86714	-3.65852
C	-4.03719	-3.80816	-2.91098
C	-3.44812	-4.35701	-1.77313
C	-2.17078	-3.96417	-1.38496
C	2.67162	1.50001	3.14375
C	3.96379	1.04908	3.38952
C	4.17153	-0.15328	4.06085
C	3.07280	-0.89551	4.48407
C	1.77940	-0.43845	4.24125
C	-3.99890	2.85505	1.57548
C	-4.43767	4.13999	1.27329
C	-3.77718	5.24683	1.79909
C	-2.68144	5.05461	2.63625
C	-2.24542	3.76857	2.93905
C	4.06218	-1.57427	0.69654
C	5.34149	-1.28142	0.23322
C	5.57885	-1.15527	-1.13273
C	4.51777	-1.28725	-2.02363
C	3.23618	-1.56227	-1.55625
Ru	-0.33766	1.01580	-0.19330
C	-0.95854	2.77853	-0.14756
I	-2.86575	0.42209	-1.15804
O	-1.38024	3.85055	-0.24563
C	1.19265	1.85111	-1.94091
O	1.64079	1.56055	0.30096
C	0.61746	1.30682	-2.87000
C	0.05348	0.72284	-4.03355
C	-1.20888	1.12849	-4.49809
C	-1.73821	0.55736	-5.64825
C	-1.02139	-0.41228	-6.34705
C	0.23589	-0.81280	-5.89518
C	0.77393	-0.25444	-4.74388
C	1.87512	2.41522	-0.75921
C	3.37393	2.64307	-1.00188
F	3.95039	3.15728	0.10951
F	4.04573	1.52542	-1.32232
F	3.56331	3.53483	-2.00649
H	-1.80606	-1.43126	2.97574
H	-0.05021	-1.49162	2.81035
H	-0.97352	-3.09438	1.22547
H	-2.11104	-1.90356	0.57254
H	0.32162	-1.99318	-2.57900
H	0.37698	-4.72141	-1.62383
H	1.72129	-3.73530	-2.17375
H	0.74263	-4.17286	0.67418
H	2.39073	-4.27266	0.05819
H	1.70098	-2.12250	1.44947
H	0.29699	2.36726	3.01288
H	-0.37431	0.52840	5.29696
H	-0.61364	2.25372	5.13413
H	-2.46671	-0.00040	4.52793
H	-2.87796	1.67839	4.84102
H	-3.27557	0.55960	2.40916
H	-1.52917	-1.72015	-3.84011
H	-3.77687	-2.43676	-4.55312
H	-5.03185	-4.12041	-3.21655
H	-3.98172	-5.10204	-1.18911
H	-1.71917	-4.42370	-0.50958
H	2.52024	2.43464	2.61372
H	4.81142	1.64313	3.05843
H	5.18036	-0.50693	4.25584
H	3.21841	-1.83111	5.01728
H	0.94517	-1.02020	4.62312
H	-4.51849	1.99604	1.16121
H	-5.30118	4.27505	0.62748
H	-4.11770	6.25157	1.56478
H	-2.16289	5.90994	3.06083
H	-1.39905	3.65144	3.60805
H	3.88904	-1.68598	1.76408
H	6.15495	-1.15835	0.94374
H	6.57810	-0.93647	-1.49876
H	4.68255	-1.16135	-3.09047
H	2.42593	-1.63630	-2.27343
H	-1.76083	1.88328	-3.94901
H	-2.71621	0.87131	-6.00090
H	-1.44161	-0.85560	-7.24526
H	0.79775	-1.56540	-6.44059
H	1.75443	-0.55656	-4.38894
H	1.47796	3.44148	-0.59203

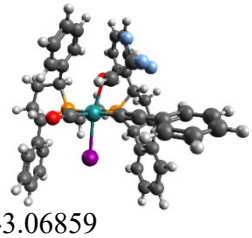
E' Pre-Reaction Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.4962530800
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6454111267
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9378547701
Imaginary Frequency (cm^{-1}): -9.84 (Conformational, thus ignored)

C	-0.14292	-1.34795	2.50864
C	-0.79285	-2.46043	1.69185
P	-0.34799	0.33295	1.72107
P	-0.16704	-2.35573	-0.04975
C	-0.88215	-3.86368	-0.93013
C	-0.07544	-5.02801	-0.33113
C	1.39516	-4.62352	-0.37829
C	1.55664	-3.14075	0.06234
C	0.99378	1.33681	2.60900
C	0.39679	1.56539	4.00848
C	-1.03539	2.02553	3.80193
C	-1.74850	1.10844	2.77252
C	-2.86383	1.86524	2.10235
C	2.59386	-2.41282	-0.74752
C	2.41175	0.83052	2.63235
C	-2.37145	-4.06532	-0.93856
C	-3.08396	-3.87582	-2.12622
C	-4.45826	-4.08184	-2.17747
C	-5.14743	-4.48095	-1.03516
C	-4.44587	-4.68892	0.15050
C	-3.06899	-4.49127	0.19680
C	3.37872	1.46173	1.84517
C	4.71645	1.08564	1.90754
C	5.11782	0.06257	2.76167
C	4.16874	-0.56942	3.56092
C	2.83223	-0.18404	3.50423
C	-4.19233	1.52596	2.36809
C	-5.23916	2.26872	1.82957
C	-4.96911	3.36345	1.01153
C	-3.64610	3.71714	0.75161
C	-2.60367	2.98095	1.30391
C	3.72330	-1.86958	-0.13167
C	4.71083	-1.23744	-0.88237
C	4.56659	-1.10956	-2.25946
C	3.42920	-1.62855	-2.88426
C	2.46205	-2.28860	-2.13497
Ru	-0.40782	-0.08376	-0.73455
C	-0.57457	-0.59114	-2.51283
I	-3.12201	-0.41598	-0.61403
O	-0.72437	-0.93850	-3.60718
C	-0.67864	1.87965	-1.16455
O	1.68869	0.56086	-0.88806
C	-0.73528	3.06373	-1.48647
C	-0.88268	4.45231	-1.73592
C	-0.05402	5.39290	-1.09128
C	-0.21851	6.75413	-1.31483
C	-1.20806	7.21316	-2.18385
C	-2.03391	6.29345	-2.83017
C	-1.87590	4.93052	-2.61413
C	2.08862	1.00909	-1.95429
C	3.28124	1.96905	-2.03045
F	4.19781	1.79086	-1.07673
F	3.87783	1.86212	-3.23375
F	2.80675	3.23376	-1.92238
H	-0.52709	-1.34312	3.53484
H	0.93774	-1.52405	2.56467
H	-0.56780	-3.43764	2.13502
H	-1.88203	-2.33877	1.65312
H	-0.55711	-3.73094	-1.97284
H	-0.39681	-5.22793	0.69695
H	-0.25640	-5.94165	-0.90939
H	2.01940	-5.27194	0.24516
H	1.75421	-4.72181	-1.40860
H	1.84089	-3.09366	1.12053
H	0.98629	2.29847	2.07483
H	0.42912	0.64201	4.59765
H	0.98808	2.31595	4.54670
H	-1.60861	2.04385	4.73547
H	-1.02556	3.04698	3.40543
H	-2.18194	0.24538	3.29195
H	-2.55374	-3.55065	-3.01850
H	-4.99263	-3.92384	-3.11025
H	-6.22182	-4.63818	-1.06997
H	-4.97234	-5.01217	1.04450
H	-2.54063	-4.67189	1.12820
H	3.07477	2.26786	1.18346
H	5.44883	1.59818	1.29046
H	6.16230	-0.23231	2.81297
H	4.46968	-1.35800	4.24539
H	2.12413	-0.66485	4.17195
H	-4.40810	0.66241	2.99357
H	-6.26682	1.98744	2.04365
H	-5.78372	3.93999	0.58182
H	-3.42122	4.56679	0.11186
H	-1.57779	3.25980	1.08041
H	3.83263	-1.94276	0.94833
H	5.58406	-0.82750	-0.38340
H	5.32995	-0.60714	-2.84639
H	3.30626	-1.53074	-3.95970
H	1.59289	-2.70282	-2.64066
H	0.71604	5.03693	-0.41263
H	0.42953	7.46320	-0.80630
H	-1.33469	8.27814	-2.35583
H	-2.80829	6.64191	-3.50849
H	-2.52274	4.21597	-3.11510
H	1.57997	0.85085	-2.91457

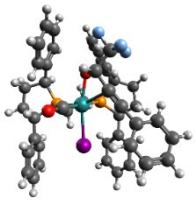
E' TS



Gibbs Energy @ r^2SCAN-3c[CPCM]: -3264.4906559900
Thermal Correction @ r^2SCAN-3c[CPCM]: 0.6440522779
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^2SCAN-3c[CPCM]: -3266.9235653179
Imaginary Frequency (cm^{-1}): -125.50

C	-0.15230	-1.36151	2.51136
C	-0.80641	-2.47172	1.69599
P	-0.30101	0.31305	1.69766
P	-0.17465	-2.37028	-0.04304
C	-0.88370	-3.88263	-0.91723
C	-0.07419	-5.04054	-0.30932
C	1.39528	-4.63039	-0.35803
C	1.55446	-3.14260	0.06848
C	1.13376	1.26592	2.50626
C	0.57712	1.63874	3.89201
C	-0.82958	2.16624	3.68109
C	-1.62004	1.19118	2.77370
C	-2.76833	1.90722	2.11582
C	2.60305	-2.42875	-0.74475
C	2.51419	0.65841	2.57658
C	-2.37283	-4.08480	-0.92753
C	-3.08440	-3.89347	-2.11562
C	-4.45850	-4.10076	-2.16890
C	-5.14874	-4.50277	-1.02835
C	-4.44846	-4.71158	0.15794
C	-3.07188	-4.51253	0.20644
C	3.54283	1.18738	1.79030
C	4.85363	0.74126	1.91613
C	5.16898	-0.25983	2.83010
C	4.15928	-0.79512	3.62554
C	2.85027	-0.33407	3.50917
C	-4.08272	1.58443	2.45874
C	-5.15359	2.29504	1.92332
C	-4.92308	3.34013	1.03204
C	-3.61341	3.67769	0.69362
C	-2.54769	2.97348	1.24162
C	3.74770	-1.91734	-0.13464
C	4.74296	-1.29994	-0.89014
C	4.59901	-1.17053	-2.26727
C	3.45355	-1.67085	-2.88692
C	2.47190	-2.30133	-2.13287
Ru	-0.43595	-0.13781	-0.74494
C	-0.60607	-0.72266	-2.49971
I	-3.16647	-0.40331	-0.59539
O	-0.75007	-1.12559	-3.57619
C	-0.55362	1.85820	-1.24858
O	1.61089	0.56495	-0.84361
C	-0.65793	3.05698	-1.54235
C	-0.80270	4.43137	-1.83036
C	-0.43567	5.40476	-0.87937
C	-0.59511	6.75324	-1.16358
C	-1.12170	7.15473	-2.39136
C	-1.48848	6.20009	-3.34009
C	-1.32997	4.84890	-3.06859
C	1.47816	1.45268	-1.73289
C	2.35523	2.70637	-1.62248
F	3.66255	2.34084	-1.68159
F	2.12482	3.55005	-2.64529
F	2.18635	3.38290	-0.47069
H	-0.55436	-1.33072	3.53033
H	0.92200	-1.56163	2.59080
H	-0.58811	-3.44904	2.14239
H	-1.89461	-2.34422	1.64990
H	-0.55549	-3.75653	-1.95969
H	-0.39634	-5.23525	0.71950
H	-0.25090	-5.95841	-0.88213
H	2.02132	-5.27222	0.27059
H	1.75524	-4.73539	-1.38737
H	1.83760	-3.08681	1.12687
H	1.19936	2.18343	1.90374
H	0.56310	0.75961	4.54673
H	1.22609	2.38634	4.36373
H	-1.36971	2.30732	4.62407
H	-0.77853	3.14321	3.18657
H	-2.02936	0.37962	3.38721
H	-2.55328	-3.56730	-3.00690
H	-4.99175	-3.94175	-3.10217
H	-6.22289	-4.66130	-1.06486
H	-4.97578	-5.03669	1.05078
H	-2.54464	-4.69402	1.13829
H	3.31220	1.97295	1.08022
H	5.63047	1.18110	1.29673
H	6.19177	-0.61268	2.92972
H	4.39104	-1.56546	4.35620
H	2.09901	-0.73800	4.18048
H	-4.26971	0.76017	3.14369
H	-6.17027	2.02707	2.19812
H	-5.75740	3.89067	0.60625
H	-3.42002	4.49082	-0.00177
H	-1.53136	3.23634	0.96406
H	3.86149	-1.99454	0.94452
H	5.62853	-0.91287	-0.39443
H	5.37160	-0.68374	-2.85607
H	3.32789	-1.57347	-3.96212
H	1.59208	-2.69701	-2.63539
H	-0.02664	5.08551	0.07427
H	-0.30948	7.49688	-0.42514
H	-1.24609	8.21167	-2.60877
H	-1.89843	6.51317	-4.29600
H	-1.61279	4.09917	-3.80116
H	1.20268	1.21872	-2.76976

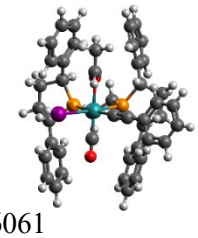
E' Post-Reaction Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3264.5206623700
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6455711967
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3266.9637084474
Imaginary Frequency (cm^{-1}): None

C	-0.01496	-0.95261	2.26956
C	-0.78491	-1.96056	1.41852
P	0.05830	0.69800	1.41688
P	-0.09415	-1.96596	-0.30220
C	-1.03026	-3.32160	-1.21755
C	-0.45368	-4.60542	-0.59620
C	1.06313	-4.45641	-0.59851
C	1.46928	-3.03477	-0.11877
C	1.64191	1.57925	1.98281
C	1.18296	2.87058	2.70228
C	-0.25557	3.18294	2.30045
C	-1.02903	1.86792	2.43032
C	-2.50841	1.91703	2.17823
C	2.71834	-2.56334	-0.81385
C	2.60760	0.73398	2.76769
C	-2.53075	-3.28236	-1.28061
C	-3.15914	-3.04036	-2.50548
C	-4.54571	-3.03944	-2.61095
C	-5.33193	-3.27637	-1.48626
C	-4.71726	-3.53530	-0.26310
C	-3.32916	-3.54883	-0.16290
C	3.78923	0.28689	2.17059
C	4.70586	-0.47997	2.88659
C	4.45026	-0.82365	4.21079
C	3.26733	-0.39635	4.81310
C	2.35686	0.37461	4.09880
C	-3.32691	0.90655	2.69578
C	-4.70240	0.93070	2.49899
C	-5.28901	1.98085	1.79407
C	-4.48649	3.00318	1.29693
C	-3.10753	2.97107	1.48541
C	3.89549	-2.38076	-0.08943
C	5.07594	-2.00696	-0.72893
C	5.09274	-1.81388	-2.10652
C	3.92321	-2.00796	-2.84185
C	2.75047	-2.38632	-2.20086
Ru	0.01209	0.19144	-1.00549
C	-0.04843	-0.39963	-2.76797
I	-2.72538	0.39658	-1.15801
O	-0.16298	-0.81103	-3.84655
C	1.02999	2.26969	-1.81065
O	2.10933	0.43137	-0.90870
C	0.09452	3.04901	-1.72027
C	-0.95746	3.99438	-1.64877
C	-0.81827	5.13165	-0.83154
C	-1.84739	6.05869	-0.75190
C	-3.02391	5.86375	-1.47581
C	-3.16100	4.74691	-2.29777
C	-2.13518	3.81592	-2.39422
C	2.24023	1.42328	-1.85797
C	3.50074	2.28013	-1.63599
F	4.60694	1.50833	-1.61970
F	3.64669	3.18393	-2.63474
F	3.48027	2.97388	-0.47465
H	-0.46711	-0.85049	3.26261
H	1.01969	-1.28558	2.42046
H	-0.72765	-2.96192	1.86202
H	-1.84067	-1.67599	1.33386
H	-0.64434	-3.24831	-2.24527
H	-0.83817	-4.75029	0.41957
H	-0.76990	-5.47277	-1.18685
H	1.55448	-5.21333	0.02195
H	1.42720	-4.58895	-1.62314
H	1.65909	-3.05175	0.96161
H	2.11832	1.83565	1.03482
H	1.22396	2.72938	3.78771
H	1.86483	3.69203	2.45527
H	-0.69836	3.95871	2.93628
H	-0.29307	3.54331	1.26552
H	-0.87925	1.49377	3.45599
H	-2.55112	-2.83920	-3.38449
H	-5.01282	-2.84496	-3.57251
H	-6.41560	-3.27001	-1.56345
H	-5.32096	-3.73547	0.61808
H	-2.87370	-3.77284	0.79708
H	3.98170	0.53565	1.13000
H	5.62190	-0.81121	2.40440
H	5.16464	-1.42085	4.77064
H	3.05393	-0.66469	5.84438
H	1.43601	0.69337	4.58191
H	-2.87855	0.08986	3.25879
H	-5.31971	0.13246	2.90243
H	-6.36467	2.00521	1.64311
H	-4.93261	3.83060	0.75117
H	-2.50010	3.77245	1.07492
H	3.88734	-2.52528	0.98803
H	5.98314	-1.86629	-0.14702
H	6.01013	-1.51722	-2.60741
H	3.92691	-1.86419	-3.91922
H	1.84944	-2.54430	-2.78919
H	0.10207	5.27940	-0.27480
H	-1.73339	6.93544	-0.12125
H	-3.83002	6.58843	-1.40559
H	-4.07298	4.60009	-2.86921
H	-2.23537	2.94479	-3.03115
H	2.35369	1.02729	-2.89287

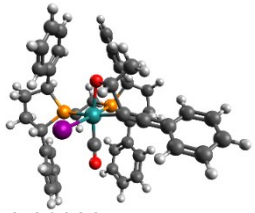
D Pre-Reaction complex with Acetaldehyde



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -2966.7780182900
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6709543095
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -2969.0851310113
Imaginary Frequency (cm^{-1}): -5.63 (Conformational, thus ignored)

C	-0.29212	-0.91575	2.57995
C	-1.20203	-1.94660	1.90926
P	-0.18182	0.61040	1.51965
P	-0.58440	-2.23113	0.17711
C	-1.74627	-3.51283	-0.55635
C	-1.30155	-4.82864	0.09942
C	0.22073	-4.85755	0.00837
C	0.79292	-3.50354	0.50141
C	1.38850	1.58012	1.95914
C	0.90068	2.78118	2.79994
C	-0.48850	3.16906	2.30577
C	-1.32214	1.88112	2.32471
C	-2.73038	1.96704	1.80928
C	2.15599	-3.21377	-0.06337
C	2.52466	0.81743	2.58158
C	-3.21436	-3.19324	-0.49565
C	-3.87571	-2.77600	-1.65515
C	-5.23255	-2.47105	-1.63548
C	-5.95636	-2.57778	-0.45103
C	-5.31322	-3.00682	0.70816
C	-3.95665	-3.31793	0.68547
C	3.73933	0.69745	1.90148
C	4.81963	0.03090	2.47246
C	4.70271	-0.53159	3.74005
C	3.50134	-0.40756	4.43611
C	2.42608	0.26558	3.86540
C	-3.69648	1.08615	2.31007
C	-5.01403	1.14459	1.87080
C	-5.39267	2.10077	0.93075
C	-4.44286	2.99007	0.43657
C	-3.12112	2.92282	0.86788
C	3.24935	-3.05364	0.79025
C	4.53413	-2.87843	0.27905
C	4.74076	-2.85628	-1.09645
C	3.65158	-2.99300	-1.95737
C	2.37273	-3.17138	-1.44521
Ru	-0.37991	-0.01076	-0.68554
C	-2.20001	0.12804	-0.75681
I	-0.45624	-0.85200	-3.38526
O	-3.33727	0.25369	-0.92572
C	-0.21865	1.94419	-1.18038
O	1.82443	-0.05038	-0.83043
C	-0.09433	3.15106	-1.37734
C	0.03913	4.55513	-1.51937
C	1.24897	5.20275	-1.19449
C	1.36778	6.58196	-1.30818
C	0.28946	7.35157	-1.74470
C	-0.91355	6.72435	-2.06837
C	-1.04189	5.34534	-1.96061
C	2.41084	0.52896	-1.74693
C	3.88207	0.52453	-1.88660
H	4.13267	0.12618	-2.87858
H	4.23449	1.56499	-1.87959
H	4.37083	-0.06464	-1.10990
H	-0.65121	-0.65872	3.58320
H	0.72551	-1.31428	2.68616
H	-1.22032	-2.87800	2.48754
H	-2.22932	-1.56961	1.83939
H	-1.44964	-3.54176	-1.61540
H	-1.62713	-4.87183	1.14563
H	-1.75215	-5.68229	-0.42044
H	0.65767	-5.67800	0.58848
H	0.51199	-5.00565	-1.03779
H	0.87884	-3.53145	1.59483
H	1.71229	1.96018	0.98237
H	0.84949	2.49894	3.85845
H	1.61807	3.60467	2.71037
H	-0.95395	3.92978	2.94322
H	-0.42098	3.57020	1.28817
H	-1.37006	1.53615	3.36890
H	-3.31031	-2.67288	-2.57856
H	-5.72346	-2.14294	-2.54766
H	-7.01530	-2.33569	-0.43154
H	-5.87100	-3.10511	1.63567
H	-3.48042	-3.66533	1.59775
H	3.83803	1.14138	0.91543
H	5.75401	-0.04798	1.92349
H	5.54273	-1.05534	4.18760
H	3.40239	-0.83271	5.43120
H	1.50151	0.36388	4.42848
H	-3.40946	0.35069	3.05968
H	-5.74778	0.44860	2.26854
H	-6.42239	2.15344	0.58835
H	-4.72907	3.74007	-0.29606
H	-2.39118	3.61337	0.45663
H	3.09549	-3.07304	1.86764
H	5.37258	-2.76256	0.96033
H	5.74170	-2.72358	-1.49814
H	3.80011	-2.95874	-3.03359
H	1.53072	-3.26269	-2.12800
H	2.08893	4.60521	-0.85040
H	2.30910	7.06169	-1.05285
H	0.38597	8.42985	-1.83193
H	-1.75942	7.31527	-2.40975
H	-1.97929	4.85906	-2.21562
H	1.82896	1.08318	-2.49873

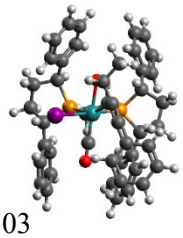
D TS with Acetaldehyde



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -2966.7555603500
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6690730232
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -2969.0481924156
Imaginary Frequency (cm^{-1}): -290.18

C	-0.19002	-1.02526	2.57268
C	-1.12143	-2.02667	1.89477
P	-0.01439	0.49856	1.52038
P	-0.56705	-2.26028	0.13792
C	-1.81040	-3.46960	-0.58768
C	-1.35553	-4.82814	-0.03144
C	0.15859	-4.88709	-0.21142
C	0.79145	-3.57999	0.32575
C	1.59436	1.36497	2.02005
C	1.16743	2.71492	2.64565
C	-0.22309	3.08541	2.13618
C	-1.09016	1.83295	2.30111
C	-2.51817	1.92110	1.84430
C	2.13311	-3.27106	-0.28137
C	2.54135	0.55521	2.86376
C	-3.26086	-3.11709	-0.40251
C	-3.97626	-2.56843	-1.47156
C	-5.31794	-2.22697	-1.33622
C	-5.97328	-2.43217	-0.12519
C	-5.27726	-2.99366	0.94323
C	-3.93536	-3.33677	0.80546
C	3.71595	0.04707	2.30198
C	4.61813	-0.68288	3.07219
C	4.35464	-0.92852	4.41635
C	3.18005	-0.43767	4.98514
C	2.28478	0.29843	4.21704
C	-3.45437	1.00427	2.33839
C	-4.78581	1.05911	1.94416
C	-5.21042	2.04779	1.05828
C	-4.29254	2.97513	0.57572
C	-2.95606	2.91148	0.96160
C	3.24290	-3.06611	0.54085
C	4.50014	-2.81820	-0.00570
C	4.66456	-2.77100	-1.38685
C	3.56174	-2.97289	-2.21603
C	2.30966	-3.22255	-1.66765
Ru	-0.21687	-0.09540	-0.69542
C	-2.02297	0.20519	-0.80700
I	-0.44747	-0.97903	-3.38267
O	-3.13965	0.43070	-1.01832
C	0.34933	1.83512	-1.30164
O	1.94343	-0.03976	-0.85957
C	0.25745	3.05050	-1.52977
C	0.23084	4.43335	-1.78884
C	0.89655	5.33359	-0.92934
C	0.87594	6.69465	-1.19420
C	0.17992	7.18416	-2.29992
C	-0.48965	6.30468	-3.15164
C	-0.46084	4.93971	-2.90939
C	1.98076	0.99660	-1.65804
C	3.11491	1.97813	-1.48452
H	4.04945	1.43081	-1.66585
H	3.03243	2.79041	-2.21230
H	3.15551	2.39865	-0.47653
H	-0.54411	-0.75806	3.57491
H	0.81691	-1.44928	2.68292
H	-1.13097	-2.97990	2.43614
H	-2.14822	-1.64383	1.85994
H	-1.58860	-3.44780	-1.66423
H	-1.61845	-4.92599	1.02852
H	-1.85708	-5.64119	-0.56930
H	0.60219	-5.74955	0.29833
H	0.38744	-4.98591	-1.27838
H	0.92326	-3.66893	1.41184
H	2.07660	1.54644	1.05672
H	1.13607	2.62406	3.73681
H	1.90998	3.48327	2.40281
H	-0.65007	3.92599	2.69579
H	-0.17198	3.37336	1.08038
H	-1.09112	1.56209	3.36902
H	-3.46578	-2.39363	-2.41584
H	-5.85060	-1.79568	-2.17936
H	-7.02053	-2.16423	-0.01584
H	-5.78174	-3.16973	1.88955
H	-3.41633	-3.78353	1.64821
H	3.91738	0.22244	1.24803
H	5.53029	-1.06010	2.61823
H	5.05783	-1.49738	5.01818
H	2.96159	-0.62688	6.03270
H	1.37254	0.67040	4.67728
H	-3.13473	0.24583	3.05065
H	-5.49515	0.33422	2.33443
H	-6.25128	2.09618	0.75074
H	-4.61451	3.75195	-0.11262
H	-2.25439	3.63910	0.56411
H	3.12247	-3.09667	1.62191
H	5.35268	-2.66554	0.65033
H	5.64441	-2.57958	-1.81571
H	3.67632	-2.92839	-3.29589
H	1.45582	-3.35086	-2.32727
H	1.43182	4.94530	-0.06772
H	1.39857	7.38048	-0.53366
H	0.16025	8.25181	-2.49882
H	-1.02936	6.68755	-4.01294
H	-0.97005	4.24655	-3.57198
H	1.72593	0.81303	-2.71514

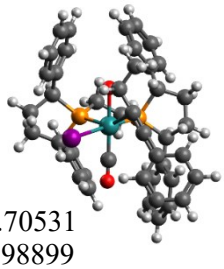
D Post-Reaction Complex with Acetaldehyde



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -2966.7680771100
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6750892533
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -2969.0735672668
Imaginary Frequency (cm^{-1}): None

C	-0.04757	-0.89445	2.46179
C	-1.06040	-1.76138	1.71878
P	0.26912	0.65801	1.48969
P	-0.49954	-1.93912	-0.03797
C	-1.84542	-2.94963	-0.87798
C	-1.52005	-4.39133	-0.45290
C	-0.01717	-4.56764	-0.63580
C	0.71624	-3.40752	0.07328
C	1.91201	1.39116	2.07411
C	1.57040	2.79917	2.62611
C	0.19675	3.23058	2.11286
C	-0.73275	2.02805	2.30118
C	-2.16553	2.18472	1.87837
C	2.14470	-3.23619	-0.36991
C	2.68117	0.50696	3.02000
C	-3.26755	-2.50678	-0.66872
C	-3.94738	-1.86904	-1.71109
C	-5.26940	-1.46289	-1.56214
C	-5.94057	-1.69197	-0.36412
C	-5.28099	-2.34171	0.67675
C	-3.95877	-2.74912	0.52534
C	3.79814	-0.19983	2.56542
C	4.51751	-1.02700	3.42468
C	4.12587	-1.17055	4.75252
C	3.00649	-0.47980	5.21457
C	2.29322	0.35057	4.35719
C	-3.12469	1.28383	2.35861
C	-4.45946	1.39490	1.98836
C	-4.86542	2.42601	1.14272
C	-3.92561	3.34107	0.68068
C	-2.58589	3.22108	1.04190
C	3.15772	-3.16636	0.58867
C	4.49386	-3.06018	0.21122
C	4.83789	-3.02898	-1.13706
C	3.83435	-3.10621	-2.10195
C	2.50164	-3.21116	-1.72142
Ru	0.09591	0.14461	-0.74654
C	-1.69003	0.60797	-0.91961
I	-0.08339	-0.67607	-3.48906
O	-2.78745	0.91164	-1.13609
C	1.60101	1.86449	-1.60664
O	2.17723	-0.19723	-0.72801
C	0.70418	2.69525	-1.63793
C	-0.23449	3.75813	-1.75056
C	0.03287	4.99697	-1.14245
C	-0.88245	6.03542	-1.24903
C	-2.07060	5.85423	-1.95564
C	-2.33249	4.63334	-2.57493
C	-1.42218	3.59023	-2.48103
C	2.63494	0.80109	-1.59414
C	4.02299	1.32495	-1.22838
H	4.71346	0.47478	-1.19542
H	4.37576	2.03640	-1.98387
H	4.02506	1.81731	-0.25117
H	-0.38731	-0.65068	3.47454
H	0.91449	-1.41658	2.55271
H	-1.16833	-2.74163	2.19709
H	-2.04605	-1.28232	1.69356
H	-1.60818	-2.84886	-1.94582
H	-1.80337	-4.56439	0.59221
H	-2.08950	-5.09636	-1.06932
H	0.34137	-5.52349	-0.23789
H	0.21517	-4.54857	-1.70605
H	0.72944	-3.61673	1.15113
H	2.48654	1.48040	1.14927
H	1.54603	2.77032	3.72016
H	2.35273	3.50868	2.33652
H	-0.18249	4.10523	2.65416
H	0.25535	3.49939	1.05217
H	-0.71774	1.75191	3.36831
H	-3.42514	-1.67884	-2.64583
H	-5.77466	-0.96447	-2.38482
H	-6.97279	-1.37477	-0.24436
H	-5.79905	-2.53784	1.61168
H	-3.47210	-3.26963	1.34480
H	4.09748	-0.10697	1.52476
H	5.38821	-1.56062	3.05341
H	4.68688	-1.81507	5.42343
H	2.68749	-0.58778	6.24773
H	1.41777	0.87445	4.73351
H	-2.82171	0.49594	3.04511
H	-5.18605	0.68112	2.36676
H	-5.90870	2.51717	0.85362
H	-4.22945	4.15199	0.02441
H	-1.86992	3.94118	0.65824
H	2.89794	-3.18772	1.64522
H	5.26758	-3.00769	0.97237
H	5.87988	-2.94994	-1.43533
H	4.09079	-3.07882	-3.15780
H	1.73301	-3.24114	-2.48804
H	0.95904	5.13204	-0.59243
H	-0.67031	6.98948	-0.77509
H	-2.78840	6.66582	-2.02901
H	-3.25235	4.49265	-3.13479
H	-1.61898	2.63902	-2.96452
H	2.68029	0.42854	-2.63929

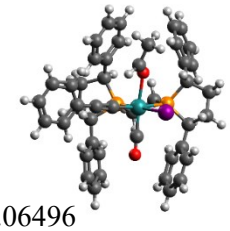
D Post-Reaction Complex with Acetaldehyde after Conformational Search



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -2966.7699545800
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6755447647
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -2969.0757657611
Imaginary Frequency (cm^{-1}): None

C	0.58794	2.66714	-0.29600
C	1.86380	2.08036	0.29263
P	-0.31674	1.33858	-1.21294
P	1.48214	0.49645	1.17520
C	1.07235	0.86771	2.98788
C	2.33500	0.46903	3.78538
C	3.05485	-0.65055	3.03548
C	3.20352	-0.16614	1.58823
C	0.30687	1.27889	-2.99963
C	-0.87376	1.77191	-3.86729
C	-2.17863	1.54907	-3.09952
C	-1.94524	2.13422	-1.70149
C	-3.07425	2.08858	-0.71147
C	3.89812	-1.07292	0.61232
C	1.63348	1.95754	-3.22116
C	0.55332	2.25970	3.24456
C	-0.81597	2.47340	3.43761
C	-1.31614	3.75291	3.66297
C	-0.45717	4.84748	3.69488
C	0.90977	4.64774	3.51422
C	1.40972	3.36765	3.29763
C	1.74210	3.34272	-3.39533
C	2.98567	3.94389	-3.57063
C	4.14520	3.17222	-3.57822
C	4.04904	1.79350	-3.40405
C	2.80681	1.19325	-3.22400
C	-4.12447	1.17451	-0.82218
C	-5.17510	1.18489	0.09199
C	-5.19425	2.10708	1.13353
C	-4.15580	3.02882	1.24925
C	-3.10990	3.02102	0.33373
C	3.86566	-2.46354	0.73865
C	4.51559	-3.27522	-0.18679
C	5.22180	-2.71055	-1.24615
C	5.28819	-1.32355	-1.36149
C	4.63832	-0.51487	-0.43560
Ru	-0.08762	-0.62741	-0.05806
C	-1.48544	-0.26012	1.09682
I	0.16019	-3.00811	1.54388
O	-2.35781	-0.11959	1.85068
C	-0.58804	-2.22231	-1.83529
O	1.44646	-1.22757	-1.37104
C	-1.79246	-2.09591	-1.66661
C	-3.20930	-2.15119	-1.56019
C	-3.82203	-2.41630	-0.32507
C	-5.20503	-2.49063	-0.24039
C	-5.99137	-2.30677	-1.37703
C	-5.38795	-2.05511	-2.60796
C	-4.00457	-1.97518	-2.70531
C	0.88100	-2.34757	-1.98899
C	1.31429	-2.50625	-3.44584
H	2.40763	-2.56569	-3.47562
H	0.90051	-3.42699	-3.87180
H	0.99173	-1.65718	-4.05581
H	-0.08005	3.01202	0.50478
H	0.79664	3.51445	-0.95805
H	2.56819	1.81066	-0.50650
H	2.36709	2.78696	0.96030
H	0.27757	0.14824	3.21850
H	3.00908	1.32748	3.87619
H	2.04577	0.16892	4.79839
H	4.04107	-0.85826	3.46659
H	2.46582	-1.57402	3.07417
H	3.77423	0.77684	1.62054
H	0.45003	0.20661	-3.15810
H	-0.77080	2.84104	-4.08005
H	-0.86859	1.24487	-4.82768
H	-3.02894	2.03730	-3.58922
H	-2.40151	0.47646	-3.03575
H	-1.65901	3.19111	-1.83067
H	-1.49763	1.62821	3.41752
H	-2.38172	3.89146	3.82115
H	-0.84664	5.84633	3.87040
H	1.59355	5.49151	3.54912
H	2.48122	3.23732	3.17447
H	0.85254	3.96712	-3.39062
H	3.04693	5.02071	-3.70349
H	5.11466	3.64194	-3.71905
H	4.94635	1.18062	-3.40644
H	2.73317	0.12265	-3.05050
H	-4.13591	0.45036	-1.62948
H	-5.98172	0.46532	-0.01558
H	-6.01630	2.11603	1.84376
H	-4.16753	3.76627	2.04664
H	-2.31714	3.76061	0.42159
H	3.30781	-2.92138	1.54831
H	4.46981	-4.35554	-0.07684
H	5.72908	-3.34532	-1.96753
H	5.85390	-0.87065	-2.17144
H	4.69992	0.56707	-0.53261
H	-3.20296	-2.56135	0.55484
H	-5.67325	-2.69003	0.71926
H	-7.07372	-2.36269	-1.30405
H	-5.99757	-1.91816	-3.49646
H	-3.52793	-1.77833	-3.66099
H	1.15471	-3.27992	-1.45146

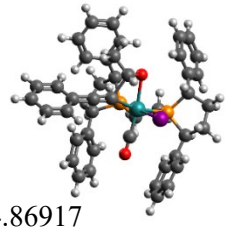
D' Pre-Reaction Complex with Acetaldehyde



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -2966.7793024100
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6689559479
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -2969.0883228161
Imaginary Frequency (cm^{-1}): None

C	-0.35985	-1.59328	2.43685
C	-0.89525	-2.32473	1.20322
P	-0.41126	0.24947	2.15655
P	0.00466	-1.69779	-0.29308
C	-0.68729	-2.62946	-1.76021
C	-0.07749	-4.03088	-1.60223
C	1.41078	-3.82298	-1.32763
C	1.60326	-2.72135	-0.25112
C	0.81460	1.06267	3.35985
C	-0.05356	1.89510	4.33748
C	-1.40044	2.20009	3.68393
C	-1.90899	0.86982	3.11750
C	-3.21684	0.87846	2.37834
C	2.89338	-1.96291	-0.40238
C	1.77371	0.11274	4.02596
C	-2.17331	-2.56238	-1.97156
C	-2.68155	-1.79255	-3.02231
C	-4.05072	-1.71114	-3.25269
C	-4.93958	-2.40001	-2.43172
C	-4.44527	-3.18128	-1.38926
C	-3.07436	-3.26727	-1.16433
C	3.11276	0.07236	3.62924
C	4.01525	-0.79946	4.23370
C	3.59066	-1.65614	5.24474
C	2.25514	-1.63257	5.64474
C	1.35775	-0.75756	5.04274
C	-3.94401	-0.31304	2.26022
C	-5.15647	-0.34723	1.58110
C	-5.67477	0.81870	1.02063
C	-4.96985	2.01152	1.14824
C	-3.74957	2.04219	1.81830
C	3.78532	-1.88500	0.66859
C	5.00347	-1.22165	0.53793
C	5.34619	-0.62736	-0.67181
C	4.45629	-0.68839	-1.74434
C	3.24199	-1.35185	-1.61153
Ru	-0.08223	0.58489	-0.19105
C	-1.85375	0.54897	-0.62211
I	-0.27276	3.41489	-0.03732
O	-2.95133	0.59793	-0.98517
C	0.38865	0.67887	-2.15723
O	2.04587	0.96423	0.31681
C	0.68749	0.67053	-3.34956
C	1.09049	0.64678	-4.70881
C	0.16166	0.40023	-5.74032
C	0.56879	0.36554	-7.06792
C	1.90597	0.57444	-7.40508
C	2.83569	0.82206	-6.39528
C	2.43830	0.85942	-5.06496
C	2.73177	1.71304	-0.38188
C	3.96690	2.36311	0.11009
H	3.71210	3.41968	0.28286
H	4.33225	1.91926	1.03707
H	4.73779	2.34895	-0.66581
H	-0.92487	-1.86786	3.33494
H	0.68842	-1.86585	2.61753
H	-0.77673	-3.40945	1.31143
H	-1.96024	-2.11015	1.05501
H	-0.19852	-2.13556	-2.61350
H	-0.55564	-4.57371	-0.77846
H	-0.23729	-4.61558	-2.51527
H	1.90445	-4.74565	-1.00434
H	1.89661	-3.50049	-2.25462
H	1.59548	-3.18345	0.74386
H	1.38812	1.74395	2.72115
H	-0.22583	1.32371	5.25585
H	0.48091	2.80930	4.61749
H	-2.11644	2.61046	4.40596
H	-1.27131	2.93492	2.88055
H	-1.99562	0.15786	3.95294
H	-1.99107	-1.23970	-3.65521
H	-4.42366	-1.10270	-4.07205
H	-6.00990	-2.33474	-2.60609
H	-5.12986	-3.73187	-0.74964
H	-2.70924	-3.89535	-0.35696
H	3.44752	0.72994	2.83254
H	5.05318	-0.80715	3.91182
H	4.29244	-2.33645	5.71898
H	1.91047	-2.29920	6.43065
H	0.31880	-0.76160	5.36324
H	-3.55842	-1.22152	2.71940
H	-5.70259	-1.28311	1.49757
H	-6.62401	0.79660	0.49256
H	-5.36692	2.92682	0.71758
H	-3.20905	2.98034	1.89435
H	3.52343	-2.34660	1.61817
H	5.68545	-1.17440	1.38268
H	6.29605	-0.11069	-0.77873
H	4.71135	-0.21742	-2.69010
H	2.54894	-1.36710	-2.44881
H	-0.88141	0.24056	-5.48262
H	-0.16438	0.17501	-7.84733
H	2.22000	0.54730	-8.44446
H	3.87965	0.98986	-6.64716
H	3.16342	1.05753	-4.28067
H	2.39923	1.94949	-1.40538

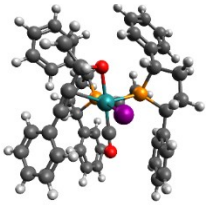
D' TS with Acetaldehyde



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -2966.7451228000
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6731188560
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -2969.0408299223
Imaginary Frequency (cm^{-1}): -297.84

C	-0.54688	-1.60099	2.64023
C	-0.86811	-2.29810	1.31517
P	-0.65344	0.24366	2.40200
P	0.19993	-1.54428	-0.00598
C	-0.15915	-2.47446	-1.58002
C	0.30570	-3.91873	-1.29342
C	1.39826	-3.94736	-0.18762
C	1.79255	-2.51764	0.28137
C	0.47557	1.11513	3.64576
C	-0.47181	1.71404	4.70973
C	-1.81530	2.02374	4.04675
C	-2.22846	0.74477	3.31046
C	-3.48602	0.75537	2.48918
C	3.06613	-2.03266	-0.36813
C	1.61234	0.27733	4.16397
C	-1.54957	-2.32730	-2.13725
C	-1.75462	-1.53942	-3.27406
C	-3.02873	-1.36584	-3.80484
C	-4.12492	-1.97848	-3.20459
C	-3.93266	-2.77512	-2.07796
C	-2.65698	-2.95262	-1.55196
C	2.89443	0.43914	3.62890
C	3.96228	-0.32676	4.09007
C	3.76552	-1.27697	5.08852
C	2.49001	-1.45551	5.62060
C	1.42456	-0.68604	5.16322
C	-4.13600	-0.45801	2.22854
C	-5.29654	-0.49877	1.46496
C	-5.83878	0.68085	0.95825
C	-5.21107	1.89350	1.22657
C	-4.04274	1.93207	1.98395
C	4.06907	-1.47260	0.42872
C	5.31395	-1.15234	-0.10214
C	5.57906	-1.37780	-1.45058
C	4.58545	-1.92377	-2.25942
C	3.34359	-2.25488	-1.72229
Ru	-0.14947	0.71307	0.16542
C	-1.85670	0.50735	-0.45249
I	-0.75648	3.50820	0.48494
O	-2.92555	0.47457	-0.89966
C	0.78822	1.08703	-1.70805
O	2.02693	1.28228	0.47360
C	0.88127	1.01404	-2.94239
C	1.06004	0.91358	-4.33422
C	0.40648	1.80276	-5.21259
C	0.57188	1.67314	-6.58332
C	1.39550	0.67231	-7.10041
C	2.05332	-0.20862	-6.24095
C	1.88478	-0.09905	-4.86917
C	2.16960	1.83213	-0.71235
C	3.46246	1.58561	-1.44386
H	4.27782	1.98731	-0.82783
H	3.63651	0.51882	-1.58879
H	3.46087	2.09798	-2.41091
H	-1.22952	-1.92487	3.43365
H	0.47157	-1.84061	2.96910
H	-0.71943	-3.38012	1.39338
H	-1.91132	-2.11644	1.03079
H	0.53075	-2.00144	-2.29265
H	-0.55035	-4.52030	-0.97609
H	0.67330	-4.36347	-2.22438
H	1.03440	-4.51482	0.67302
H	2.29791	-4.45845	-0.54161
H	1.95624	-2.50922	1.36523
H	0.89492	1.93521	3.04938
H	-0.62932	0.99510	5.52140
H	-0.01497	2.60878	5.14682
H	-2.57692	2.30095	4.78516
H	-1.70305	2.85695	3.34392
H	-2.33302	-0.04817	4.06710
H	-0.90370	-1.05281	-3.74475
H	-3.16365	-0.74791	-4.68848
H	-5.12187	-1.84198	-3.61404
H	-4.78050	-3.26382	-1.60559
H	-2.53013	-3.58763	-0.67968
H	3.04790	1.16433	2.83369
H	4.95224	-0.17894	3.66600
H	4.59816	-1.87418	5.44943
H	2.32257	-2.19715	6.39703
H	0.43587	-0.84703	5.58545
H	-3.72945	-1.38043	2.63942
H	-5.78308	-1.45111	1.27172
H	-6.74762	0.65420	0.36354
H	-5.62899	2.81946	0.84065
H	-3.56066	2.88576	2.17168
H	3.87081	-1.29949	1.48323
H	6.07987	-0.72823	0.54177
H	6.55156	-1.13263	-1.86806
H	4.77990	-2.10791	-3.31271
H	2.60348	-2.72164	-2.36681
H	-0.22828	2.58087	-4.79978
H	0.06152	2.35736	-7.25495
H	1.52476	0.57859	-8.17483
H	2.69444	-0.98633	-6.64587
H	2.38604	-0.78177	-4.18936
H	1.78351	2.86037	-0.82125

D' Post-Reaction Complex with Acetaldehyde



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -2966.7635041800
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6752241363
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -2969.0659994116
Imaginary Frequency (cm^{-1}): None

C	-0.57258	-1.41890	2.29419
C	-0.77080	-2.12583	0.95698
P	-0.51669	0.41922	2.02436
P	0.46656	-1.45083	-0.25346
C	0.14065	-2.39510	-1.86295
C	1.02457	-3.67328	-1.78759
C	1.61034	-3.85614	-0.37895
C	1.98410	-2.46482	0.19136
C	0.53496	1.19982	3.38624
C	-0.45878	1.98304	4.27674
C	-1.69433	2.35413	3.45257
C	-2.13135	1.07133	2.73761
C	-3.30733	1.12941	1.80510
C	3.32656	-2.02279	-0.33611
C	1.43682	0.21833	4.09122
C	-1.32049	-2.63496	-2.15150
C	-1.99280	-1.80237	-3.04973
C	-3.34090	-1.99737	-3.33526
C	-4.04092	-3.03546	-2.72759
C	-3.37853	-3.88141	-1.83920
C	-2.03072	-3.68517	-1.55680
C	2.76103	0.06893	3.66347
C	3.60823	-0.85283	4.27212
C	3.14656	-1.64895	5.31789
C	1.82722	-1.51632	5.74491
C	0.98046	-0.59357	5.13670
C	-3.99560	-0.05212	1.50059
C	-5.08544	-0.04312	0.63824
C	-5.51814	1.15584	0.07452
C	-4.85262	2.33781	0.38489
C	-3.75478	2.32611	1.24201
C	4.44194	-2.13826	0.50131
C	5.72774	-1.91085	0.01918
C	5.92386	-1.56675	-1.31638
C	4.82065	-1.42527	-2.15370
C	3.53519	-1.64320	-1.66600
Ru	0.26489	0.83327	-0.09371
C	-1.40550	0.75860	-0.89489
I	-0.24501	3.66636	0.05907
O	-2.43189	0.80495	-1.43097
C	2.03728	1.48428	-1.55138
O	2.15961	1.22256	0.73752
C	1.31288	1.23516	-2.50716
C	0.59361	1.00507	-3.71414
C	-0.58813	1.71739	-3.97967
C	-1.28997	1.48458	-5.15449
C	-0.82486	0.55022	-6.07914
C	0.35518	-0.14823	-5.82948
C	1.06404	0.07318	-4.65552
C	2.78547	1.88037	-0.33141
C	4.28468	1.62149	-0.38566
H	4.73592	2.02764	0.52581
H	4.49030	0.55220	-0.43761
H	4.73597	2.12047	-1.25089
H	-1.36650	-1.67383	3.00500
H	0.37937	-1.71572	2.75073
H	-0.67903	-3.20959	1.07414
H	-1.76503	-1.91917	0.54373
H	0.51582	-1.73316	-2.65181
H	0.44538	-4.55386	-2.07953
H	1.83860	-3.57701	-2.51220
H	0.87926	-4.33993	0.27746
H	2.49707	-4.49950	-0.40178
H	2.03735	-2.50061	1.28654
H	1.16269	1.90313	2.82728
H	-0.77458	1.36812	5.12587
H	0.03800	2.87039	4.68354
H	-2.50411	2.73046	4.08875
H	-1.44300	3.13200	2.72386
H	-2.35630	0.32292	3.51437
H	-1.45508	-0.98559	-3.52448
H	-3.84259	-1.33452	-4.03519
H	-5.09316	-3.19068	-2.94887
H	-3.91292	-4.70092	-1.36634
H	-1.52897	-4.36018	-0.86812
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H	4.63451	-0.94760	3.92670
H	3.80713	-2.36774	5.79480
H	1.45185	-2.13572	6.55511
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H	-5.60257	-0.97181	0.41183
H	-6.37214	1.16794	-0.59702
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H	-3.24049	3.25545	1.46284
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H	6.57825	-2.00780	0.68858
H	6.92671	-1.39552	-1.69723
H	4.95717	-1.13194	-3.19119
H	2.69308	-1.50141	-2.33379
H	-0.94395	2.44307	-3.25495
H	-2.20545	2.03551	-5.34962
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H	0.72431	-0.87089	-6.55136
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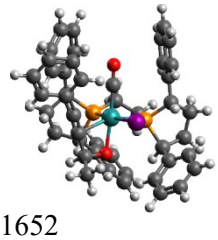
D' Post-Reaction Complex with Acetaldehyde after Conformational Search



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Imaginary Frequency (cm^{-1}): None

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C	-2.38804	-3.71659	-1.06790
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C	-1.45781	3.46558	-2.92372
C	-0.03785	3.79525	-2.45478
C	0.77124	2.51010	-2.67379
C	2.22478	2.49071	-2.30689
C	-2.91812	-2.52554	1.14558
C	-2.97527	1.34814	-2.89996
C	1.46638	-3.29855	-0.75046
C	2.42099	-3.47058	0.25666
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C	3.26203	-3.29744	-2.38244
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C	-4.94595	-0.05605	-2.69204
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C	4.08732	3.19313	-0.92746
C	4.95515	2.39182	-1.66398
C	4.45985	1.64332	-2.72982
C	3.10756	1.69588	-3.04855
C	-3.72361	-1.55157	1.74448
C	-4.13594	-1.67779	3.06616
C	-3.75589	-2.78880	3.81620
C	-2.96807	-3.77326	3.22677
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C	1.68914	-0.03322	-0.05689
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C	-0.36082	2.42207	1.36742
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C	0.83044	2.55589	1.61987
C	2.15266	2.88036	2.02600
C	3.08407	1.89212	2.37988
C	4.35431	2.25781	2.80466
C	4.70969	3.60229	2.89601
C	3.78452	4.58900	2.55679
C	2.51627	4.23700	2.11652
C	-1.83331	2.22855	1.29726
C	-2.46409	2.34355	2.68788
H	-3.54321	2.18383	2.59097
H	-2.04684	1.57653	3.34668
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H	-0.47041	0.06588	-4.04176
H	-2.08377	-1.18997	-2.70948
H	-0.77087	-2.32032	-3.03606
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H	-0.85383	-5.18598	-0.47373
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H	-0.04548	4.07617	-1.39337
H	0.69301	2.25781	-3.74323
H	2.09403	-3.52737	1.29219
H	4.50014	-3.68572	0.75265
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H	3.58336	-3.23222	-3.41852
H	1.19337	-3.11880	-2.88963
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H	-5.71140	-0.50664	-2.06548
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H	-2.22015	1.55744	-4.91405
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H	-4.07690	-2.88936	4.84928
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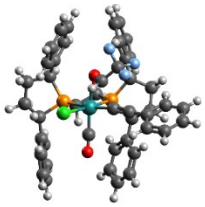
H	-1.95551	-4.43639	1.46504
H	2.79566	0.84779	2.33121
H	5.07000	1.48594	3.07281
H	5.70425	3.88147	3.23169
H	4.05477	5.63870	2.62838
H	1.79497	5.00146	1.84318
H	-2.23531	3.05929	0.67703

D TS using [Ru]-Cl Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3426.9612973100
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Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3429.3898166326
Imaginary Frequency (cm^{-1}): -137.39

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P	-0.60922	-2.27454	0.19447
C	-1.80085	-3.50738	-0.56297
C	-1.31174	-4.85716	-0.01326
C	0.20588	-4.86786	-0.17971
C	0.79701	-3.53921	0.35751
C	1.48758	1.40404	2.03681
C	1.03924	2.73850	2.68077
C	-0.36056	3.08650	2.18100
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C	2.10714	-3.16632	-0.28295
C	2.47327	0.61262	2.85291
C	-3.26260	-3.19519	-0.39928
C	-3.97964	-2.67373	-1.48056
C	-5.33069	-2.36466	-1.36135
C	-5.99215	-2.57398	-0.15433
C	-5.29325	-3.10772	0.92641
C	-3.94231	-3.41963	0.80458
C	3.65409	0.14997	2.26558
C	4.59091	-0.56118	3.01173
C	4.35718	-0.83249	4.35636
C	3.17753	-0.38600	4.95068
C	2.24727	0.33123	4.20673
C	-3.54808	0.93887	2.41129
C	-4.88223	0.96018	2.02332
C	-5.33368	1.93254	1.13275
C	-4.43984	2.87733	0.63888
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C	4.57593	-2.54065	-1.46109
C	3.44765	-2.74077	-2.25587
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Ru	-0.32436	-0.09692	-0.64736
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Cl	-0.47702	-0.93777	-3.01045
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C	0.26384	3.04316	-1.51354
C	0.41685	4.41932	-1.77991
C	1.10101	5.24995	-0.86864
C	1.25089	6.60262	-1.13592
C	0.71737	7.15088	-2.30257
C	0.03510	6.33910	-3.20921
C	-0.11267	4.98303	-2.95834
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C	3.09344	1.89750	-1.76367
F	4.23978	1.20867	-2.00523
F	2.96090	2.81075	-2.74423
F	3.26541	2.55361	-0.59952
H	-0.60666	-0.76369	3.62295
H	0.76685	-1.42564	2.72954
H	-1.13917	-3.00580	2.49548
H	-2.19780	-1.69920	1.92431
H	-1.55878	-3.46471	-1.63487
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H	-1.78233	-5.68077	-0.56268
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H	1.76655	3.52182	2.43988
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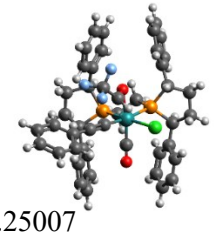
H	3.51843	-2.64580	-3.33622
H	1.35123	-3.18288	-2.30289
H	1.51345	4.81568	0.03707
H	1.78366	7.23540	-0.43196
H	0.83467	8.21139	-2.50605
H	-0.37843	6.76720	-4.11775
H	-0.63619	4.34185	-3.66087
H	1.54905	0.69424	-2.76769

D' TS using [Ru]-Cl Complex



Gibbs Energy @ r^{2}SCAN-3c[CPCM]: -3426.9521216400
Thermal Correction @ r^{2}SCAN-3c[CPCM]: 0.6463107292
Gibbs Energy @ ωB97X-D4rev/def2-QZVPP[CPCM]//r^{2}SCAN-3c[CPCM]: -3429.382583378
Imaginary Frequency (cm^{-1}): -102.36

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P	0.04592	-1.72175	-0.22821
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C	0.06432	-3.99403	-1.68481
C	1.51611	-3.80253	-1.26044
C	1.55881	-2.87760	-0.02269
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C	-0.15649	1.74768	4.44308
C	-1.52127	2.05878	3.83522
C	-1.98789	0.76261	3.16172
C	-3.28937	0.79057	2.41155
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C	-2.44090	-1.72608	-3.16911
C	-3.79211	-1.63863	-3.48773
C	-4.73448	-2.33014	-2.73134
C	-4.31237	-3.11966	-1.66355
C	-2.95968	-3.21224	-1.35041
C	3.21371	0.78815	3.51402
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C	4.18540	-0.85015	4.99560
C	2.90669	-1.28078	5.34386
C	1.78686	-0.66921	4.78919
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C	-5.25241	-0.40347	1.62363
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C	1.73057	-0.09247	-5.25007
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C	3.31765	1.84316	-1.98654
F	4.39894	2.18598	-1.24104
F	3.61527	0.69768	-2.61978
F	3.15175	2.79994	-2.92395
H	-0.97263	-1.93260	3.36166
H	0.64004	-1.93904	2.63126
H	-0.92472	-3.41345	1.30038
H	-2.01410	-2.03262	1.04608
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H	-0.01311	-4.50525	-2.65112
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H	2.07444	-3.34342	-2.08428
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H	0.33430	2.64194	4.84291
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H	3.33634	1.59776	2.79841
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H	5.05965	-1.32194	5.43558
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H	-0.03329	2.81555	-5.01180
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H	2.06990	-0.91640	-4.62930
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