SUPPORTING INFORMATION

Enantioselective Catalytic Synthesis of α-Aryl-α-SCF_3-$\beta^{2,2}$-Amino Acids

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1. General Information:

1.1. General Methods

^{1}H- and ^{13}C-NMR spectra were recorded on a Bruker Avance III 300 MHz spectrometer with a broad band observe probe and a sample changer for 16 samples and on a Bruker Avance III 700 MHz spectrometer with an Ascend magnet and TCI cryoprobe, which are both property of the Austro-Czech NMR-Research Center "RERI-uasb". NMR spectra were referenced on the solvent peak and chemical shifts are given in ppm.

High resolution mass spectra were obtained using a Thermo Fisher Scientific LTQ Orbitrap XL with an Ion Max API Source. Analyses were made in the positive ionization mode if not otherwise stated. Purine (exact mass for $[M+H]^+ = 121.050873$) and 1,2,3,4,5,6-hexakis(2,2,3,3-tetrafluoropropoxy)-1,3,5,2,4,6-triazatriphosphinane (exact mass for $[M+H]^+ = 922.009798$) were used for internal mass calibration.

HPLC was performed using a Thermo Scientific Dionex Ultimate 3000 system with diode array detector with a CHIRALPAK AD-H, CHIRAL ART Cellulose-SB or Amylose-SA (250 x 4.6 mm, 5 µm) chiral stationary phase. Optical rotations were recorded on a Schmidt + Haensch Polarimeter Model UniPol L1000 at 589 nm.

All chemicals were purchased from commercial suppliers and used without further purification unless otherwise stated. K_2CO_3 and Cs_2CO_3 were flame-dried *in vacuo* prior to use. Dry solvents were obtained from an MBraun-SPS-800 solvent purification system. All reactions were carried out under argon atmosphere.

4-Aryl-isoxazolidin-5-ones[1] **1** and trifluoromethylthiolating reagents[2] **3** were prepared following established procedures.

[1] a) M. N. Oliveira, S. Arseniyadis, J. Cossy, *Chem. Eur. J.*, **2008**, 24, 4810 – 4814; b) D. Best, M. Jean, P. Weghe, *J. Org. Chem.*, **2016**, 81, 7760 – 7770.
[2] a) C. Xu, Q. Shen, *Org. Lett.*, **2014**, 16, 7, 2046 – 2049; b) C. Xu, B. Ma, Q. Shen, *Angew. Chem. Int. Ed.*, **2014**, 53, 9316 – 9320.

1.2. Single-Crystal Analysis

Single-crystal structure analyses were carried out on a Bruker D8 Quest Eco diffractometer operating with Mo-K_α radiation (λ= 0.71073 Å). Further crystallographic and refinement data can be found in Table S1. The structures were solved by direct methods (SHELXS-97)[3] and refined by full-matrix least squares on F^2 (SHELXL-97).[4] The H atoms were calculated geometrically, and a riding model was applied in the refinement process. CCDC 1914375 contains the supplementary crystallographic data for compound **2a**. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre at www.ccdc.cam.ac.uk.

Table 1: Crystal Data, Data Collection and Structure Refinement Details for Compound **2a**.

Crystal Data	**2a**
Empirical formula	$C_{15}H_{16}NO_4F_3S$
Formula weight [g/mol]	363.35
Color	colorless
Crystal size [mm]	0.70 × 0.47 × 0.20
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a [Å]	6.2580(3)
b [Å]	10.6081(5)
c [Å]	25.7799(12)
α [°]	90
β [°]	90
γ [°]	90
V [Å^3]	1711.41(14)
Z	4
D_{calc} [g/cm^3]	1.410
μ [mm^{-1}]	0.24
T [K]	296
θ range [°]	3.1-25.0
No. of reflections measured	13540
No. of independent reflections	3037
Obs. Reflections with $I > 2\sigma(I)$	2401
No. of Parameters refined/restraints	221/0
Absorption correction	multi-scan
T_{min}, T_{max}	0.85, 0.95
$\Delta\rho_{min}/\Delta\rho_{max}$ [e Å^{-3}]	−0.19/0.19
F(000)	752
R_{int}	0.046

[3] G. M. Sheldrick, SHELXS-97, Program for the Solution of Crystal Structures, Göttingen, Germany, 1997. See also: G. M. Sheldrick, *Acta Crystallographica*, **1990**, *A46*, 467 – 473.
[4] G. M. Sheldrick, SHELXL-97, Program for crystal structure refinement, Göttingen, Germany, 1997. See also: G. M. Sheldrick, *Acta Crystallographica*, **2008**, *A64*, 112 – 122.

R_1 ($R[F^2 \geq 2\sigma(F^{2)})]$)	0.039
wR_2 ($wR(F^2)$)	0.084
GooF	1.09
Flack x	−0.03(5)
CCDC no.	1914375

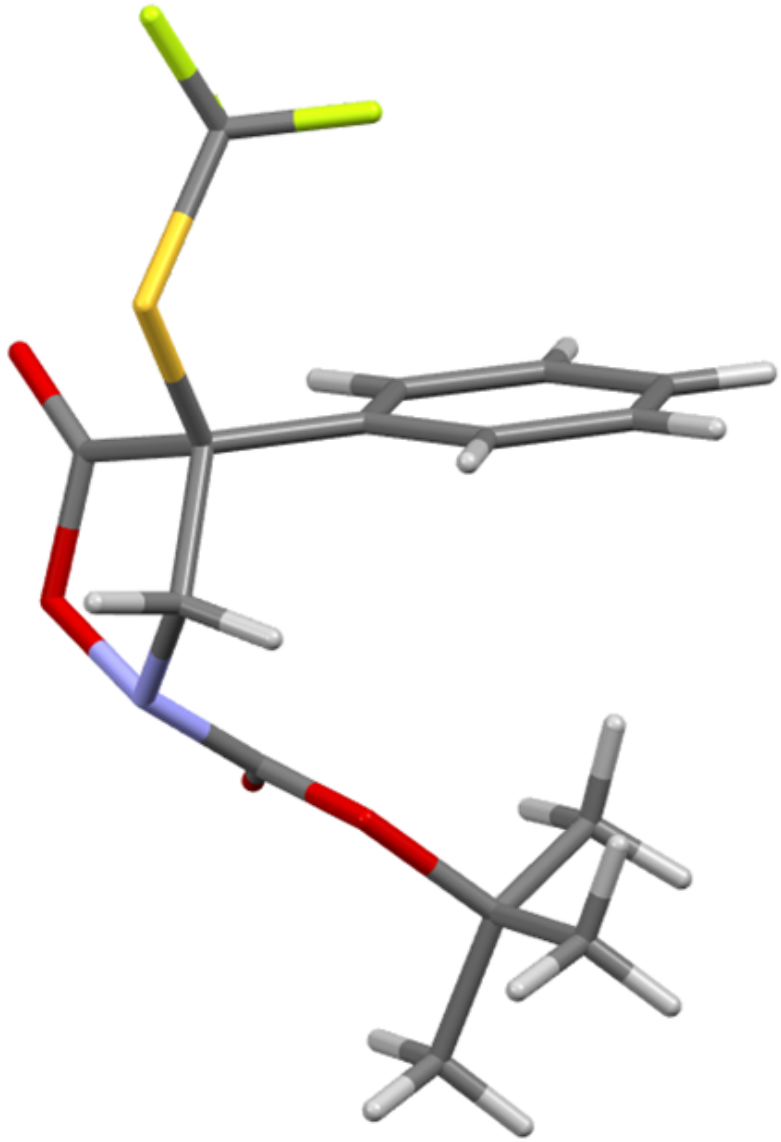
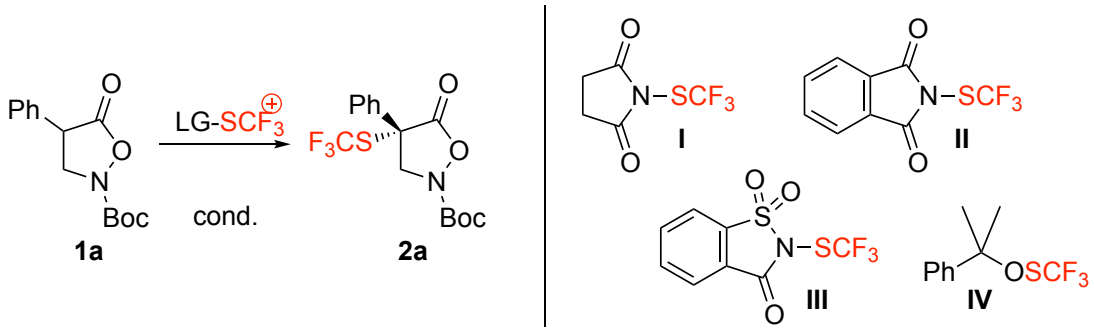


Figure 1: Single Crystal Structure of (S)-**2a**.

2. Detailed Screening Tables

Screening of reaction conditions for the formation of **2a** was conducted using the following general procedure:

Isoxazolidin-5-one **1a** (0.05 mmol), RN-SCF_3-reagent **I-IV**, base and catalyst were dissolved in the respective solvent and stirred for the given time and at the temperature indicated. In case of reactions performed below room temperature, electrophile **I-IV** was added with a delay of 15 min after mixing all other components. After completion of the reaction, the mixture was diluted with Et_2O and washed with water and brine. The organic phase was dried over Na_2SO_4, filtered and concentrated *in vacuo*. Where necessary, the crude mixture was purified by column chromatography (silica gel, heptanes/EtOAc = 5/1) to yield **2a**.

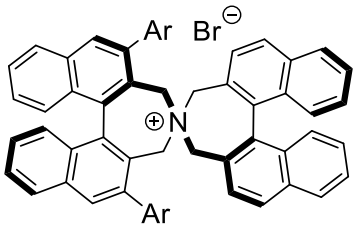


2.1 Trifluoromethylthiolating Agent Screening

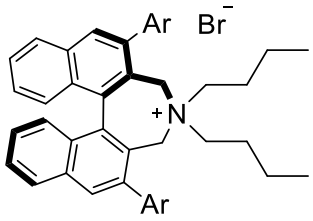
Table 2: LG-SCF_3^+-Reagent Screening: Reactions were run at r.t. for 20 h using 0.1 mmol **1a** and 0.15 or 0.30 mmol **I-IV** in Et_2O (c = 0.1 M with respect to **1a**); [a] Isolated yields; [b] Determined by HPLC using a chiral stationary phase.

entry	catalyst (mol%)	LG (eq.)	base	base-eq.	**2a** yield / %[a]	**2a** e.r.[b]
1	**TEBAC** (10)	Saccharin (1.5) (**III**)	Cs_2CO_3	1.1	-	-
2	**A2** (5)	Saccharin (1.5) (**III**)	Cs_2CO_3	1.1	-	-
3	**A2** (5)	Saccharin (3) (**III**)	Cs_2CO_3	2	-	-
4	**A2** (5)	Phthalimide (3) (**II**)	Cs_2CO_3	2	70	75 : 15
5	**A2** (10)	Succinimide (3) (**I**)	Cs_2CO_3	2	80	82 : 18
6	**A2** (20)	Cumyl-OH (1.5) (**IV**)	Cs_2CO_3	2	-	-

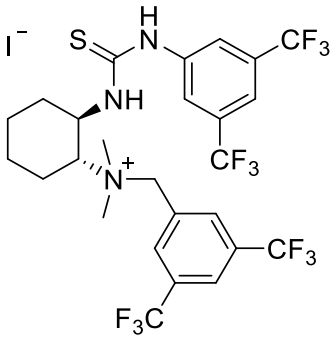
2.2 Catalyst Screening



A1 (Ar = 3,4,5-F_3-C_6H_2)
A2 (Ar = 3,5-CF_3-C_6H_3)



A3 (Ar = 3,4,5-F-C_6H_2)



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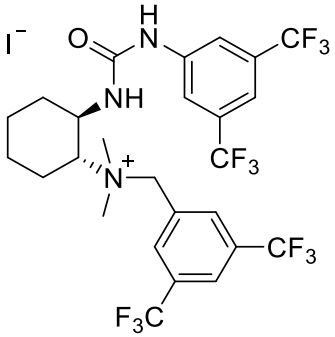
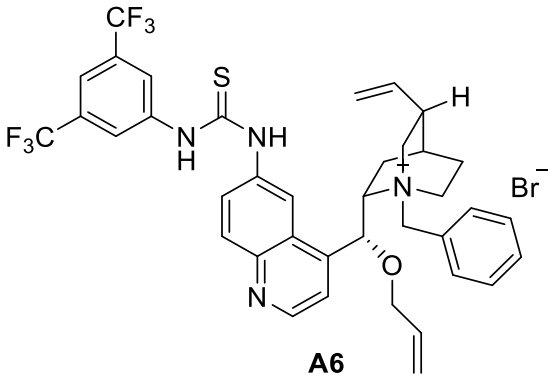


A5



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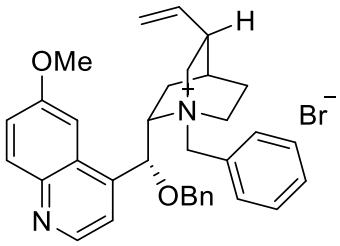

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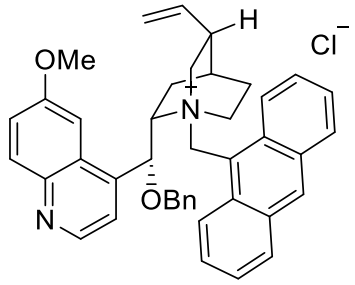

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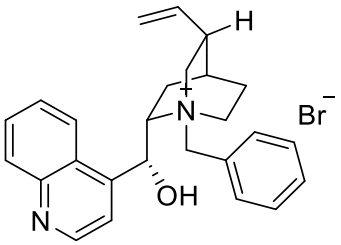


A9

Figure 2: Catalysts tested for the asymmetric trifluoromethylthiolation of **1a**.

Table 3: Catalyst Screening: Reactions were run at r.t. for 20 h using 0.10 mmol **1a**, 0.15 mmol **I** or **II** and 0.11 mmol base in the solvent indicated and at c = 0.1 M (with respect to **1a**); [a] Isolated yields; [b] Determined by HPLC using a chiral stationary phase.[c] Determined by ^{1}H NMR of the crude product.

entry	catalyst (mol%)	LG (eq.)	solvent	base	**2a** yield / %[a]	**2a** e.r.[b]
8	**A1** (5)	SuccN (1.5) (**I**)	Et_2O	Cs_2CO_3	77	90 : 10
9	**A3** (5)	SuccN (1.5) (**I**)	iPr_2O	K_2CO_3	70	59 : 51
10	**A4** (10)	PhthN (1.5) (**II**)	iPr_2O	K_2CO_3	62	67 : 33
11	**A5** (10)	PhthN (1.5) (**II**)	iPr_2O	K_2CO_3	54	58 : 42
12	**A6** (10)	SuccN (1.5) (**I**)	MTBE | toluene	K_2CO_3	70	50 : 50
13	**A7** (20)	PhthN (1.5) (**II**)	iPr_2O	K_2CO_3	60	50 : 50
14	**A8** (20)	PhthN (1.5) (**II**)	iPr_2O	K_2CO_3	55	53 : 47
15	**A9** (20)	PhthN (1.5) (**II**)	iPr_2O	K_2CO_3	57	50 : 50
16	-	SuccN (1.5) (**I**)	iPr_2O	Cs_2CO_3	75 (conv.)[c]	-

2.3 Solvent Screening

Table 4: Solvent Screening: Reactions were run at r.t. for 20 h using 0.10 mmol **1a**, 0.15 mmol $SuccNSCF_3$ (**I**), 0.005 mmol **A1** and 0.02 mmol K_2CO_3 at c = 0.1 M (with respect to **1a**); [a] Isolated yields; [b] Determined by HPLC using a chiral stationary phase.

entry	solvent	**2a** yield / %[a]	**2a** e.r.[b]
17	C_5H_9-O-CH_3	85	87 : 13
18	MTBE	82	87 : 13
19	iPr_2O	87	88 : 12
20	2-Me-THF	73	81 : 19
21	THF	66	76 : 24
22	1,4-dioxane	79	76 : 24
23	DCM	53	75 : 25
24	toluene	56	84 : 16
25	Et_2O	89	89 : 11

2.4 Base Screening

Table 5: Solvent Screening: Reactions were run at r.t. for 20 h using 0.10 mmol **1a**, 0.12 mmol $SuccNSCF_3$ (**I**), indicated amount of catalyst and 0.02 mmol of base in Et_2O at c = 0.1 M (with respect to **1a**); [a] Isolated yields; [b] Determined by HPLC using a chiral stationary phase.

entry	catalyst (mol%)	base (20 mol%)	**2a** yield / %[a]	**2a** e.r.[b]
26	**A1** (5)	$KHCO_3$	79	88 : 12
27	**A1** (5)	Na_2CO_3	80	89 : 11
28	**A1** (5)	Li_2CO_3	34	87 : 13

29	**A1** (5)	K_2HPO_4	88	90 : 10
30	**A1** (5)	Rb_2CO_3	65	83 : 17
31	**A1** (5)	KOAc	25	90 : 10
32	**A1** (5)	Na-phenoxide	71	89 : 11
33	**A1** (5)	DBU	56	55 : 45

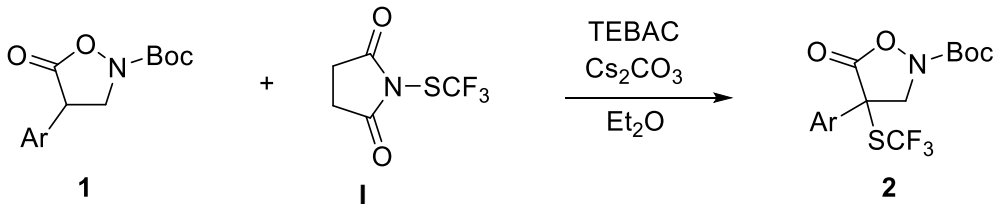
2.5 Further Conditions tested

Table 6: LG-SCF_3^+-Reagent Screening: Reactions were run for 20 h using 0.1 mmol **1a** and 0.12 or 0.105 mmol SuccNSCF$_3$ (**I**), 0.005 mmol **A1** and 0.02 mmol of base in Et_2O; [a] Isolated yields; [b] Determined by HPLC using a chiral stationary phase. [c] 0.1 M SuccNSCF$_3$ (**I**)-solution (in Et_2O) added over 5 h via syringe pump.

entry	solvent (c)	base (20 mol%)	*T* / °C	yield / %[a]	e.r.[b]
35	Et_2O (0.1 M)	K_2HPO_4	-40	72	93 : 7
36	Et_2O (0.05 M)	K_2HPO_4	25	82	91 : 9
37	Et_2O (0.01 M)	K_2HPO_4	25	82	92 : 9
38	Et_2O (0.01 M)[c]	K_2HPO_4	25	86	93 : 7
39	Et_2O (0.01 M)[c]	K_2HPO_4	-20	90	95 : 5
40	Et_2O (0.05 M)	K_2HPO_4	-20	90	93 : 7
41	Et_2O (0.05 M)	K-Phthalimide	-20	84	93 : 7

3. Syntheses

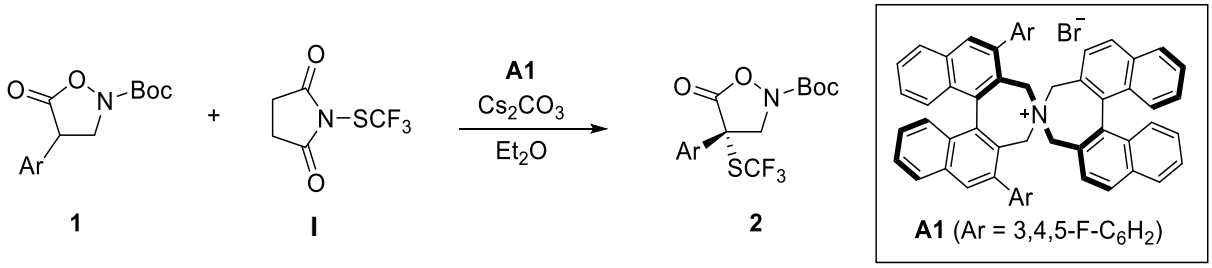
3.1 Synthesis of racemic 4-SCF_3-4-Aryl-Isoxazolidin-5-ones 2



1 I 2

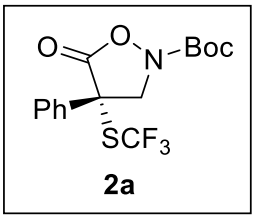
4-Aryl-Isoxazolidin-5-ones **1** (0.10 mmol), N-SCF_3-Succinimide **I** (0.12 mmol), TEBAC (0.01 mmol) and Cs_2CO_3 (0.11 mmol) were dissolved in Et_2O (2 mL) and stirred overnight. After completion of the reaction, the mixture was diluted with Et_2O (20 mL) and washed two times with water (20 mL) and brine (20 mL). The organic phase was dried over Na_2SO_4, filtered and concentrated *in vacuo*. If necessary, the crude mixture was purified by column chromatography (silica gel, heptanes/EtOAc) to give the respective racemic 4-SCF_3-Isoxazolidin-5-ones **2**.

3.2 Asymmetric Synthesis of enantioenriched 4-SCF_3-4Aryl-Isoxazolidin-5-ones 2



1 I 2

4-Aryl-Isoxazolidin-5-ones **1** (0.10 mmol), (*R,R*)-catalyst **A1** (0.005 mmol) and K_2HPO_4 (0.02 mmol) were dissolved in Et_2O (2 mL) at -20 °C. N-SCF_3-Succinimide **I** (0.105 mmol) was added and the mixture was stirred for 20 h at -20 °C. After completion of the reaction, the mixture was diluted with Et_2O (20 mL) and washed two times with water (20 mL) and brine (20 mL). The organic phase was dried over Na_2SO_4, filtered and concentrated *in vacuo*. If necessary, the crude mixture was purified by column chromatography (silica gel, heptanes/EtOAc) to give the respective scalemic 4-SCF_3-Isoxazolidin-5-ones **2**. Analytical data for new compounds are given below.

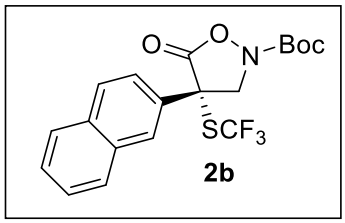


2a

Compound **2a** (***tert*-butyl (*S*)-5-oxo-4-phenyl-4-((trifluoromethyl)thio)isoxazolidine-2-carboxylate**): Prepared following the general procedure using 1 mmol **1a** and 3 mol% **A1**. Obtained as colourless crystals (327.7 mg, 0.90 mmol, 90 %, e.r. = 93:7 (98:2 after single recryst. from DCM/*n*-hexane)). m.p. = 69 – 71 °C. R_f (heptanes/EtOAc = 5/1) = 0.55. $[a]_D^{22}$ (c = 1.00, $CHCl_3$) = -23.4°. ^1H NMR (300 MHz, δ, $CDCl_3$, 298 K): 7.67 – 7.58 (m, 2H), 7.48 – 7.39 (m, 3H), 4.94 (d,

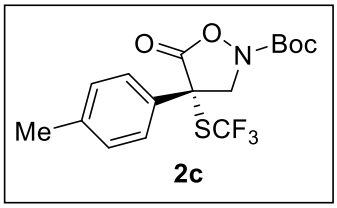
J = 12.8 Hz, 1H), 4.59 (d, *J* = 12.8 Hz, 1H), 1.35 (s, 9H).^{13}C NMR (75 MHz, δ, $CDCl_3$, 298 K): 170.5, 155.5, 131.8, 130.2, 129.5, 128.5 (q, *J* = 311.0 Hz) 127.6, 85.1, 59.7, 59.7, 56.8, 27.9. ^{19}F NMR (282 MHz, δ, $CDCl_3$, 298 K): -36.7. HRMS (ESI): calcd *m/z* for $C_{15}H_{16}F_3NO_4S$: 381.1090 $[M+NH_4]^+$; found: 381.1090. HPLC (YMC CHIRAL ART Cellulose-SB, eluent: hexane:*i*-PrOH = 100:1, 0.5 mL/min, 10 °C) retention times: t_{minor} = 28.0 min, t_{major} = 34.6 min.

Compound **2b** (***tert*-butyl (*S*)-4-(naphthalen-2-yl)-5-oxo-4-((trifluoromethyl)thio)isoxazolidine-2-carboxylate**): Prepared according to the general procedure and obtained as a colourless oil (35.9 mg, 0.087 mmol, 87 %, e.r. = 94:6). R_f (heptanes/EtOAc = 5/1) = 0.55. $[a]_D^{22}$ (c = 1.00, $CHCl_3$) = -40.5°; ^{1}H NMR (300 MHz, δ, $CDCl_3$, 298 K): 8.07 (d, *J* = 2.1 Hz, 1H), 7.93 (d, *J* = 8.8 Hz, 1H), 7.90 – 7.80 (m, 2H), 7.70 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.63 – 7.49 (m, 2H), 5.06 (d, *J* = 12.8 Hz, 1H), 4.67 (d, *J* = 12.8 Hz, 1H), 1.25 (s, 9H). ^{13}C NMR (75 MHz, δ, $CDCl_3$, 298 K): 170.6, 155.5, 133.6, 132.9, 129.7, 128.7, 128.7, 128.6 (q, *J* = 310.8 Hz) 127.9, 127.8, 127.4, 127.3, 124.1, 85.1, 59.7, 59.7, 57.1, 57.1, 27.8. ^{19}F NMR (282 MHz, δ, $CDCl_3$, 298 K): -36.6. HRMS (ESI): calcd *m/z* for $C_{19}H_{18}F_3NO_4S$: 431.1247 $[M+NH_4]^+$; found: 431.1242. HPLC (Chiralpak AD-H, eluent: hexane:*i*-PrOH = 100:1, 0.5 mL/min, 10 °C) retention times: t_{major} = 35.5 min, t_{minor} = 39.5 min.



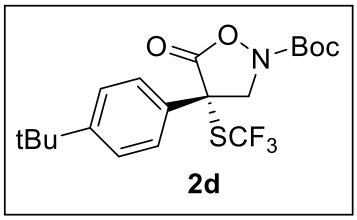
2b

Compound **2c** (***tert*-butyl (*S*)-5-oxo-4-(p-tolyl)-4-((trifluoromethyl)thio)isoxazolidine-2-carboxylate**): Prepared according to the general procedure and obtained as a colourless oil (34.2 mg, 0.091 mmol, 91 %, e.r. = 94:6). R_f (heptanes/EtOAc = 5/1) = 0.55. $[a]_D^{22}$ (c = 1.00, $CHCl_3$) = -24.2°; ^{1}H NMR (300 MHz, δ, $CDCl_3$, 298 K): 7.49 (d, *J* = 8.4 Hz, 2H), 7.23 (d, *J* = 8.2 Hz, 2H), 4.93 (d, *J* = 12.7 Hz, 1H), 4.56 (d, *J* = 12.7 Hz, 1H), 2.36 (s, 3H), 1.35 (s, 9H). ^{13}C NMR (75 MHz, δ, $CDCl_3$, 298 K): 170.7, 155.5, 140.5, 130.2, 128.7 (q, *J* = 310.8 Hz), 128.6, 127.5, 85.0, 59.7, 56.7, 27.8, 21.2. ^{19}F NMR (282 MHz, δ, $CDCl_3$, 298 K): -36.8. HRMS (ESI): calcd *m/z* for $C_{16}H_{18}F_3NO_4S$: 395.1247 $[M+NH_4]^+$; found: 395.1250. HPLC (Chiralpak AD-H, eluent: hexane:*i*-PrOH = 300:1, 0.5 mL/min, 10 °C) retention times: t_{major} = 36.6 min, t_{minor} = 42.0 min.



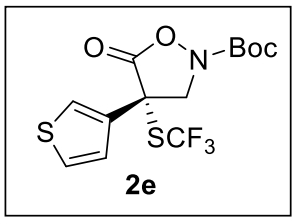
2c

Compound **2d** (***tert*-butyl (*S*)-4-(4-(*tert*-butyl)phenyl)-5-oxo-4-((trifluoromethyl) thio)isoxazolidine-2-carboxylate**): Prepared according to the general procedure and obtained as a colourless solid (33.1 mg, 0.079 mmol, 79 %, e.r. = 95:5). m.p. = 84 – 86 °C. R_f (heptanes/EtOAc = 5/1) = 0.60. $[a]_D^{22}$ (c = 1.00, $CHCl_3$) = -10.0°; ^{1}H NMR (700 MHz, δ, $CDCl_3$, 298 K): 7.51 (d, *J* = 8.7 Hz, 2H), 7.43 (d, *J* = 8.7 Hz, 2H), 4.99 (d, *J* = 12.8 Hz, 1H), 4.55 (d, *J* = 12.7 Hz, 1H), 1.30 (s, 9H), 1.30 (s, 9H). ^{13}C NMR (176 MHz, δ, $CDCl_3$, 298 K): 170.9, 155.6, 153.7, 128.7 (q, *J* = 310.8 Hz), 128.2, 127.4, 126.5, 84.9, 59.6, 56.8, 34.9, 31.2, 27.8. ^{19}F NMR (282 MHz, δ, $CDCl_3$, 298 K): -36.8. HRMS (ESI): calcd *m/z* for $C_{19}H_{24}F_3NO_4S$: 437.1716 $[M+NH_4]^+$; found: 437.1712. HPLC (YMC CHIRAL ART Amylose-SA, eluent: hexane:*i*-PrOH = 300:1, 0.5 mL/min, 10 °C) retention times: t_{minor} = 17.3 min, t_{major} = 21.5 min.



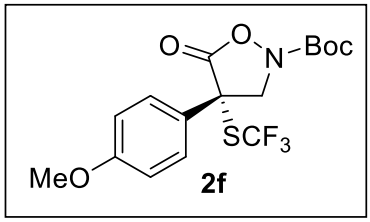
2d

Compound **2e** (***tert*-butyl (*S*)-5-oxo-4-(thiophen-3-yl)-4-((trifluoromethyl)thio)isoxazolidine-2-carboxylate**): Prepared according to the general procedure and obtained as a light-yellow oil (30.2 mg, 0.082 mmol, 82 %, e.r. = 94:6). R_f (heptanes/EtOAc = 5/1) = 0.50. $[a]_D^{23}$ (c = 1.00, $CHCl_3$) = -29.3°; ^{1}H NMR (300 MHz, δ, $CDCl_3$, 298 K): 7.57 (dd, *J* = 3.0, 1.4 Hz, 1H), 7.41 (dd, *J* = 5.2, 3.0 Hz, 1H), 7.27 – 7.24 (m, 1H), 4.90 (d, *J* = 12.7 Hz, 1H), 4.59 (d, *J* = 12.7 Hz, 1H), 1.40 (s, 9H). ^{13}C NMR (75 MHz, δ, $CDCl_3$, 298 K): 170.3, 155.6, 131.9, 128.7 (q, *J* = 311.0 Hz) 128.0, 126.5, 126.0, 85.2, 60.1, 60.1, 60.1, 60.0, 53.8, 53.7, 27.9. ^{19}F NMR (282 MHz, δ, $CDCl_3$, 298 K): -37.0. HRMS (ESI): calcd *m/z* for $C_{13}H_{14}F_3NO_4S_2$: 387.0655 $[M+NH_4]^+$; found: 387.0655. HPLC (YMC CHIRAL ART Amylose-SB, eluent: hexane:*i*-PrOH = 100:1, 0.5 mL/min, 10 °C) retention times: t_{minor} = 23.0 min, t_{major} = 37.5 min.



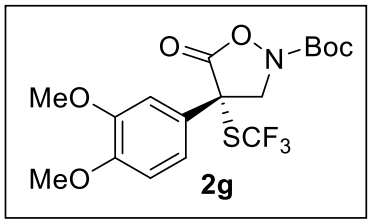
2e

Compound **2f** (***tert*-butyl (*S*)-4-(4-methoxyphenyl)-5-oxo-4-((trifluoromethyl)thio)isoxazolidine-2-carboxylate**): Prepared according to the general procedure and obtained as a colourless oil (30.6 mg, 0.76 mmol, 78 %, e.r. = 94:6). R_f (heptanes/EtOAc = 5/1) = 0.35. $[a]_D^{22}$ (c = 1.00, $CHCl_3$) = -33.0°; ^{1}H NMR (300 MHz, δ, $CDCl_3$, 298 K): 7.59 – 7.47 (m, 2H), 6.99 – 6.87 (m, 2H), 4.94 (d, *J* = 12.7 Hz, 1H), 4.56 (d, *J* = 12.7 Hz, 1H), 3.81 (s, 3H), 1.35 (s, 9H). ^{13}C NMR (75 MHz, δ, $CDCl_3$, 298 K): 170.7, 160.9, 155.6, 129.1, 128.7 (q, *J* = 311.0 Hz), 123.0, 114.8, 85.0, 59.7, 59.6, 56.6, 56.6, 55.6, 27.9. ^{19}F NMR (282 MHz, δ, $CDCl_3$, 298 K): -36.9. HRMS (ESI): calcd *m/z* for $C_{16}H_{18}F_3NO_5S$: 411.1196 $[M+NH_4]^+$; found: 411.1195. HPLC (YMC CHIRAL ART Amylose-SB, eluent: hexane:*i*-PrOH = 100:1, 0.5 mL/min, 10 °C) retention times: t_{minor} = 32.5 min, t_{major} = 37.4 min.



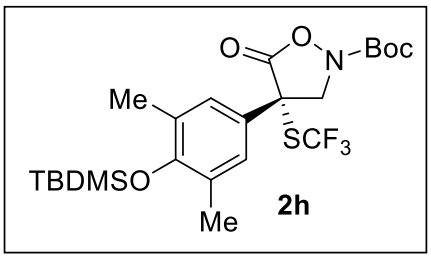
2f

Compound **2g** (***tert*-butyl (*S*)-4-(3,4-dimethoxyphenyl)-5-oxo-4-((trifluoromethyl)thio)isoxazolidine-2-carboxylate**): Prepared according to the general procedure and obtained as a colourless oil (34.0 mg, 0.080 mmol, 80 %, e.r. = 94:6). R_f (heptanes/EtOAc = 5/1) = 0.30. $[a]_D^{22}$ (c = 0.70, $CHCl_3$) = -43.0°; ^{1}H NMR (300 MHz, δ, $CDCl_3$, 298 K): 7.17 – 7.08 (m, 2H), 6.91 – 6.82 (m, 1H), 4.97 (d, *J* = 12.8 Hz, 1H), 4.56 (d, *J* = 12.8 Hz, 1H), 3.91 (s, 3H), 3.89 (s, 3H), 1.36 (s, 9H). ^{13}C NMR (75 MHz, δ, $CDCl_3$, 298 K): 170.7, 155.6, 150.6, 149.6, 128.7 (q, *J* = 311.0 Hz), 123.2, 120.3, 111.3, 110.6, 85.0, 59.6, 56.8, 56.2, 56.2, 27.9. ^{19}F NMR (282 MHz, δ, $CDCl_3$, 298 K): -36.9. HRMS (ESI): calcd *m/z* for $C_{17}H_{20}F_3NO_6S$: 441.1302 $[M+NH_4]^+$; found: 441.1305. HPLC (Chiralpak AD-H, eluent: hexane:*i*-PrOH = 95:5, 0.5 mL/min, 10 °C) retention times: t_{major} = 23.2 min, t_{minor} = 24.7 min.



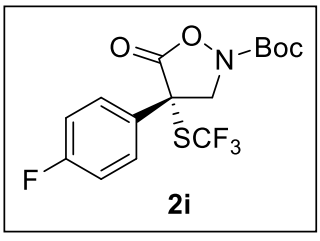
2g

Compound **2h** (***tert*-butyl (*S*)-4-(4-((tert-butyldimethylsilyl)oxy)-3,5-dimethylphenyl)-5-oxo-4-((trifluoromethyl)thio)isoxazolidine-2-carboxylate**): Prepared according to the general procedure and obtained as a colourless oil (46.1 mg, 0.088 mmol, 88 %, e.r. = 95:5). R_f (heptanes/EtOAc = 5/1) = 0.60. $[a]_D^{22}$ (c = 1.00, $CHCl_3$) = -45.8°; ^{1}H NMR (300 MHz, δ, $CDCl_3$, 298 K): 7.18 (s, 2H), 4.98 (d, *J* = 12.7 Hz, 1H), 4.50 (d, *J* = 12.7 Hz, 1H), 2.21 (s, 6H), 1.34 (s, 9H), 1.02 (s, 9H), 0.17 (s, 6H). ^{13}C NMR (75 MHz, δ, $CDCl_3$, 298 K): 171.0, 155.6, 153.9, 130.0, 128.7 (q, *J* = 311.0 Hz), 128.0, 123.1, 84.7, 59.5, 56.7, 27.9, 26.1, 18.9, 18.1, -2.8. ^{19}F NMR (282 MHz, δ, $CDCl_3$, 298 K): -37.0. HRMS (ESI): calcd *m/z* for $C_{23}H_{34}F_3NO_5SSi$: 539.2217$[M+NH_4]^+$; found: 539.2221. HPLC (Chiralpak AD-H, eluent: hexane:*i*-PrOH = 300:1, 0.5 mL/min, 10 °C) retention times: t_{major} = 15.3 min, t_{minor} = 19.0 min.



2h

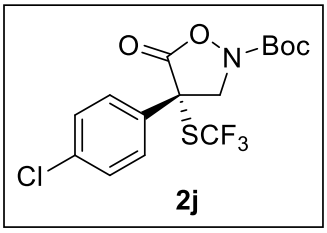
Compound **2i** (***tert*-butyl (*S*)-4-(4-fluorophenyl)-5-oxo-4-((trifluoromethyl)thio)isoxazolidine-2-carboxylate**): Prepared according the general procedure and obtained as a colourless oil (32.0 mg, 0.084 mmol, 84 %, e.r. = 93:7). R_f (heptanes/EtOAc = 5/1) = 0.55. $[a]_D^{22}$ (c = 1.00, $CHCl_3$) = -15.1°; ^{1}H NMR (300 MHz, δ, $CDCl_3$, 298 K): 7.69 – 7.59 (m, 2H), 7.19 – 7.06 (m, 2H), 4.88 (d, *J* = 12.8 Hz, 1H), 4.61 (d, *J* = 12.9 Hz, 1H), 1.39 (s, 9H). ^{13}C NMR (75 MHz, δ, $CDCl_3$, 298 K): 170.2, 163.5 (d, *J* = 250.8 Hz), 155.5, 128.4 (q, *J* = 311.7 Hz), 129.8 (d, *J* = 8.6 Hz), 116.6 (d, *J* = 22.1 Hz) 85.4, 77.6, 76.7, 59.7, 56.1, 27.9. ^{19}F NMR (282 MHz, δ, $CDCl_3$, 298 K): -36.8, -110.2. HRMS (ESI): calcd *m/z* for $C_{15}H_{15}F_4NO_4S$: 399.0996 $[M+NH_4]^+$; found:



2i

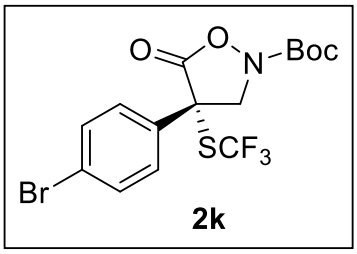
399.0999. HPLC (YMC CHIRAL ART Amylose-SB, eluent: hexane:*i*-PrOH = 100:1, 0.5 mL/min, 10 °C) retention times: t_{minor} = 24.6 min, t_{major} = 34.4 min.

Compound **2j** (***tert*-butyl (*S*)-4-(4-chlorophenyl)-5-oxo-4-((trifluoromethyl)thio)isoxazolidine-2-carboxylate**): Prepared according the general procedure and obtained as a colourless oil (33.9 mg, 0.085 mmol, 85 %, e.r. = 91:9). R_f (heptanes/EtOAc = 5/1) = 0.50. $[a]_D^{22}$ (c = 1.00, $CHCl_3$) = -10.5°; ^{1}H NMR (300 MHz, δ, $CDCl_3$, 298 K): 7.64 – 7.53 (m, 2H), 7.45 – 7.39 (m, 2H), 4.85 (d, *J* = 13.0 Hz, 1H), 4.61 (d, *J* = 12.9 Hz, 1H), 1.41 (s, 9H). ^{13}C NMR (75 MHz, δ, $CDCl_3$, 298 K): 170.0, 155.4, 136.5, 130.6, 129.7, 129.0, 128.6 (q, *J* = 309.7 Hz), 85.4, 77.6, 77.2, 76.7, 59.6, 56.1, 27.9. ^{19}F NMR (282 MHz, δ, $CDCl_3$, 298 K): -36.7. HRMS (ESI): calcd *m/z* for $C_{15}H_{15}ClF_3NO_4S$: 415.0701[M+NH_4]$^+$; found: 415.0705. HPLC (YMC CHIRAL ART Amylose-SB, eluent: hexane:*i*-PrOH = 100:1, 0.5 mL/min, 10 °C) retention times: t_{minor} = 33.9 min, t_{major} = 35.4 min.



2j

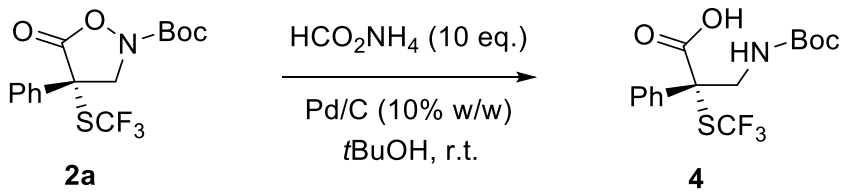
Compound **2k** (***tert*-butyl (*S*)-4-(4-bromophenyl)-5-oxo-4-((trifluoromethyl)thio)isoxazolidine-2-carboxylate**): Prepared according to the general procedure and obtained as a colourless oil (35.8 mg, 0.081 mmol, 81 %, e.r. = 91:9). R_f (heptanes/EtOAc = 5/1) = 0.45. $[a]_D^{22}$ (c = 1.00, $CHCl_3$) = -11.6°; ^{1}H NMR (700 MHz, δ, $CDCl_3$, 298 K): 7.60 – 7.55 (m, 2H), 7.53 – 7.50 (m, 2H), 4.83 (d, *J* = 12.9 Hz, 1H), 4.61 (d, *J* = 12.9 Hz, 1H), 1.41 (s, 9H). ^{13}C NMR (176 MHz, δ, $CDCl_3$, 298 K): 169.9, 155.4, 132.7, 131.2, 129.2, 128.6 (q, *J* = 310.6 Hz) 124.7, 85.5, 77.3, 77.2, 77.0, 59.6, 56.1, 27.9. ^{19}F NMR (282 MHz, δ, $CDCl_3$, 298 K): -36.6. HRMS (ESI): calcd *m/z* for $C_{15}H_{15}BrF_3NO_4S$: 459.0196 [M+NH_4]$^+$; found: 459.0198. HPLC (YMC CHIRAL ART Amylose-SB, eluent: hexane:*i*-PrOH = 100:1, 0.5 mL/min, 10 °C) retention times: t_{minor} = 41.7 min, t_{major} = 43.0 min.



2k

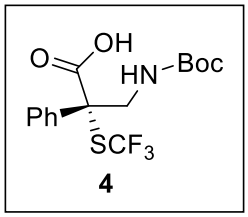
4. Further Transformations

4.1 Reductive Cleavage of the Isoxazolidin-5-one N-O Bond

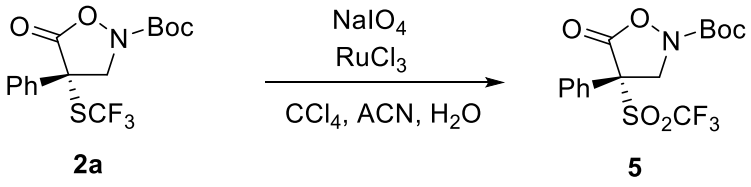


Under an Argon atmosphere, product **2a** (0.5 mmol), HCO_2NH_4 (5 mmol) and Pd/C (10% w/w) were placed in a round bottom flask and *t*BuOH (4 mL) was added. The suspension was stirred vigorously at r.t. overnight. After completion of the reaction, the mixture was filtered through a short pad of Celite® (washed with DCM). The solvent was removed *in vacuo*, giving **4** in high purity.

Compound **4** (**(*S*)-3-((*tert*-butoxycarbonyl)amino)-2-phenyl-2-((trifluoromethyl)thio) propanoic acid**): Prepared following the method described above and obtained as a colourless powder (166.2 mg, 0.45 mmol, 97%). R_f (heptanes/EtOAc = 1/1) = 0.45. m.p. = 146 °C (decomp.). ^{1}H NMR (300 MHz, δ, CD_3OD, 298 K): 7.56 – 7.51 (m, 2H), 7.42 – 7.34 (m, 3H), 4.70 (d, *J* = 15.2 Hz, 1H), 4.43 (d, *J* = 15.1 Hz, 1H), 1.40 (s, 9H). ^{13}C NMR (75 MHz, δ, CD_3OD, 298 K): 175.2, 158.1, 138.3, 131.5 (q, *J* = 307.3 Hz), 129.7, 129.5, 129.3, 82.8, 67.1, 57.7, 28.4. ^{19}F NMR (282 MHz, δ, CD_3OD, 298 K): -38.3. HRMS (ESI): calcd *m/z* for $C_{15}H_{18}F_3NO_4S$: 383.1247 $[M+NH_4]^+$; found: 383.1250.



4.2 Oxidation of SCF_3-Isoxazolidin-5-one 2a

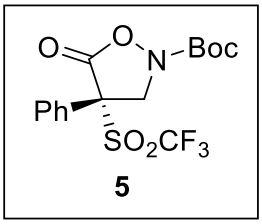


Using an analogous procedure as was reported by Su[5], sulfone **5** was prepared as follows: SCF_3-Isoxazolidin-5-one **2a** (0.10 mmol) was dissolved in CCl_4/ACN/H_2O at room temperature. $NaIO_4$ (0.30 mmol) and $RuCl_3 \cdot H_2O$ (0.005 mmol) were added and the suspension was stirred vigorously overnight. The crude mixture was then filtered and the filtrate treated with DCM (20 mL) and H_2O (20 mL). The aqueous phase was extracted with DCM (20 mL) and the combined organic phases were washed with

[5] W. Su, *Tetrahedron Lett.*, **1994**, 35, 4955 - 4958

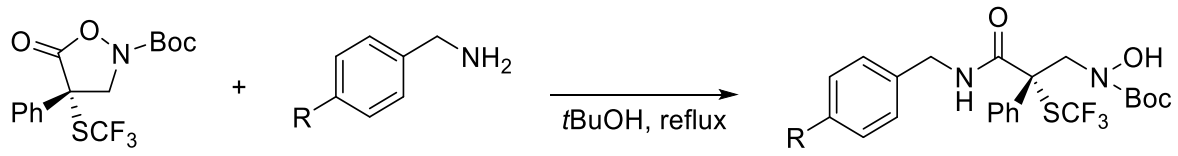
saturated aq. $NaHCO_3$ solution (20 mL), dried over Na_2SO_4, filtered and concentrated *in vacuo* to yield **5**.

Compound **5**: (***tert*-butyl (*S*)-5-oxo-4-phenyl-4-((trifluoromethyl)sulfonyl)isoxazolidine-2-carboxylate**): Prepared following the method described above and obtained as a light-yellow oil. (38.6 mg, 0.098 mmol, 98%). R_f (heptanes/EtOAc = 5/1) = 0.40. ^{1}H NMR (300 MHz, δ, $CDCl_3$, 298 K): 7.81 – 7.70 (m, 2H), 7.57 – 7.48 (m, 3H), 5.29 (d, *J* = 13.3 Hz, 1H), 4.89 (d, *J* = 13.3 Hz, 1H), 1.35 (s, 9H). ^{13}C NMR (75 MHz, δ, $CDCl_3$, 298 K): 165.3, 155.0, 131.7, 129.8, 128.9, 125.7, 120.0 (q, *J* = 331.3 Hz), 85.8, 74.3, 55.8, 27.8. ^{19}F NMR (282 MHz, δ, $CDCl_3$, 298 K): -68.3. HRMS (ESI): calcd *m/z* for $C_{15}H_{16}F_3NO_6S$: 413.0989 $[M+NH_4]^+$; found: 413.0991.



5

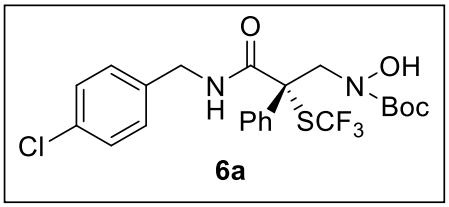
4.3 Nucleophilic Ring-Opening of SCF_3-Isoxazolidin-5-one 2a



2a **9** **6**

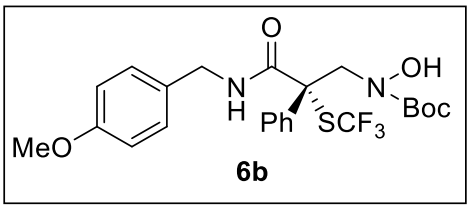
In a pressure Schlenk-tube, SCF_3-Isoxazolidin-5-one **2a** (0.1 mmol) and substituted benzylamine **9** (0.5 mmol) were dissolved in *t*BuOH and stirred at 90 °C overnight. Volatiles were removed in vacuo and the crude mixture was purified by column chromatography (silica gel, heptanes/EtOAc) to yield amides **6**.

Compound **6a**: (***tert*-butyl (*S*)-(3-((4-chlorobenzyl)amino)-3-oxo-2-phenyl-2-((trifluoromethyl) thio)propyl)(hydroxy)carbamate**): Prepared following the method described above and obtained as a white solid. (38.0 mg, 0.075 mmol, 75%). m.p. = 116 – 118 °C. R_f (heptanes/EtOAc = 1/1) = 0.35. ^{1}H NMR (300 MHz, δ, $CDCl_3$, 298 K): 8.06 (s, 1H), 7.42 – 7.35 (m, 2H), 7.36 – 7.26 (m, 5H), 7.15 (d, *J* = 8.4 Hz, 2H), 6.82 – 6.68 (m, 1H), 4.57 (d, *J* = 15.2 Hz, 1H), 4.51 – 4.36 (m, 3H), 1.30 (s, 9H). ^{13}C NMR (75 MHz, δ, $CDCl_3$, 298 K): 171.4, 155.6, 135.6, 135.6, 133.7, 129.5, 129.4 (q, *J* = 310.4 Hz), 129.2, 129.0, 128.8, 128.1, 82.3, 64.9, 58.1, 44.1, 28.1. ^{19}F NMR (282 MHz, δ, $CDCl_3$, 298 K): -36.1. HRMS (ESI): calcd *m/z* for $C_{22}H_{24}ClF_3N_2O_4S$: 522.1436 $[M+NH_4]^+$; found: 522.1434.



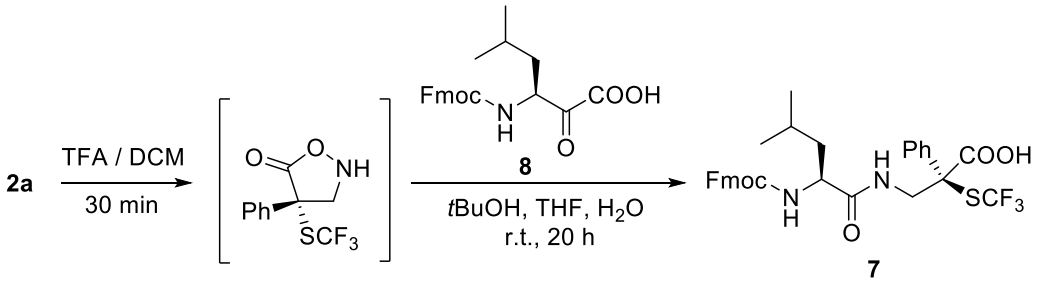
6a

Compound **6b**: (***tert*-butyl (*S*)-(3-((4-methoxybenzyl)amino)-3-oxo-2-phenyl-2-((trifluoromethyl) thio)propyl)(hydroxy)carbamate**): Prepared following the method described above and obtained as a colourless oil. (35.9 mg, 0.071 mmol, 71%). R_f (heptanes/EtOAc = 1/1) = 0.25. ^{1}H NMR (300 MHz, δ, $CDCl_3$, 298 K): 8.13 (s, 1H), 7.42 – 7.35 (m, 2H), 7.34 – 7.28 (m, 3H), 7.20 – 7.11 (m, 2H), 6.88 – 6.79 (m, 2H), 6.69 – 6.58 (m, 1H), 4.60 (d, *J* = 15.2 Hz, 1H), 4.46 – 4.35 (m, 3H), 3.78 (s, 3H), 1.30 (s, 9H). ^{13}C NMR (75 MHz, δ, $CDCl_3$, 298 K): 171.4, 159.4, 155.3, 135.5, 129.5, 129.4 (q, *J* = 310.6 Hz), 129.1, 128.9, 128.8, 128.1, 114.2, 82.0, 64.8, 55.4, 44.4, 32.0, 28.1. ^{19}F NMR (282 MHz, δ, $CDCl_3$, 298 K): -36.0. HRMS (ESI): calcd *m/z* for $C_{22}H_{24}ClF_3N_2O_4S$: 518.1931 $[M+NH_4]^+$; found: 518.1931.



6b

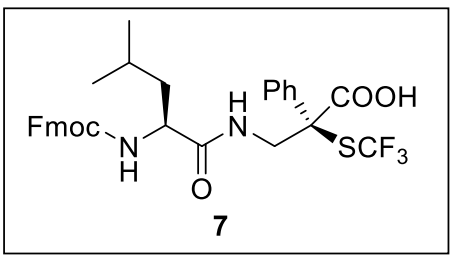
4.4 KAHA Ligation with *N*-Fmoc-Leu α-oxo-acid 7



7

2a (0.1 mmol, e.r. = 93:7) was dissolved in DCM (1 mL) and TFA (0.5 mL) was added. After stirring for 30 min at room temperature, the solvent was removed under reduced pressure, giving a colourless oily residue, which was dried for 1 h under high vacuum and directly used for the next step. *N*-Deprotected **2a** was dissolved in *t*BuOH/THF/H_2O (1/1/1; 1.5 mL), **8** (prepared following a reported procedure[6], 0.11 mmol) was added and the mixture was stirred for 20 h at room temperature. After completion of the reaction, water (20 mL) and EtOAc (30 mL) were added and the phases were separated. The aqueous phase was washed three times with EtOAc (15 mL), the combined organic phases were dried over Na_2SO_4, filtered and concentrated *in vacuo*. **7** was isolated by column chromatography (silica gel, DCM/MeOH) as a colourless oil.

N-protected dipeptide **7**: (**(*S*)-3-((*S*)-2-((((9H-fluoren-9-yl)methoxy)carbonyl)amino)-4-methylpentanamido)-2-phenyl-2-((trifluoromethyl)thio) propanoic acid**): Obtained as a colourless oil (41.8 mg, 0.070 mmol, 70%, d.r. = 13:1). R_f (DCM/MeOH = 20/1) = 0.15. ^{1}H NMR (300 MHz, δ, $CDCl_3$, 298 K): 7.80 – 7.72 (m, 2H), 7.59 – 7.51 (m, 2H), 7.43 – 7.34 (m, 4H), 7.33 – 7.28 (m,

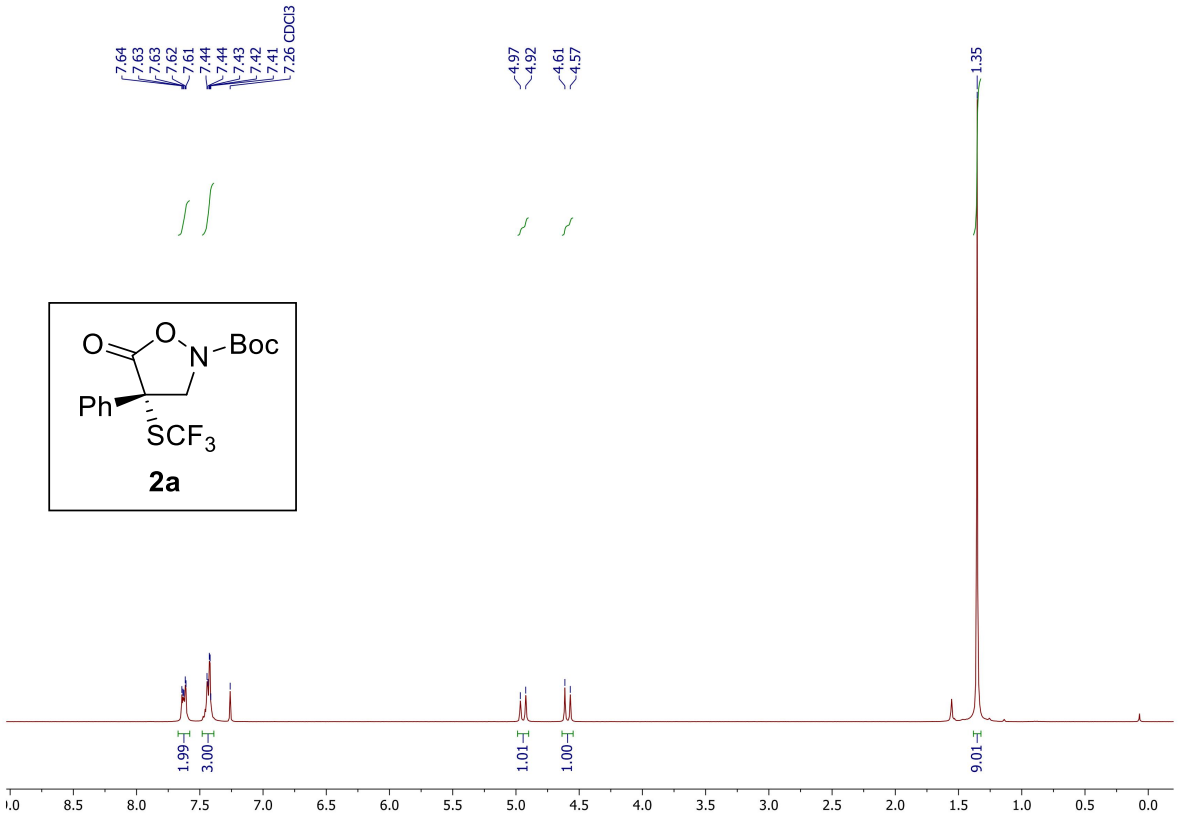


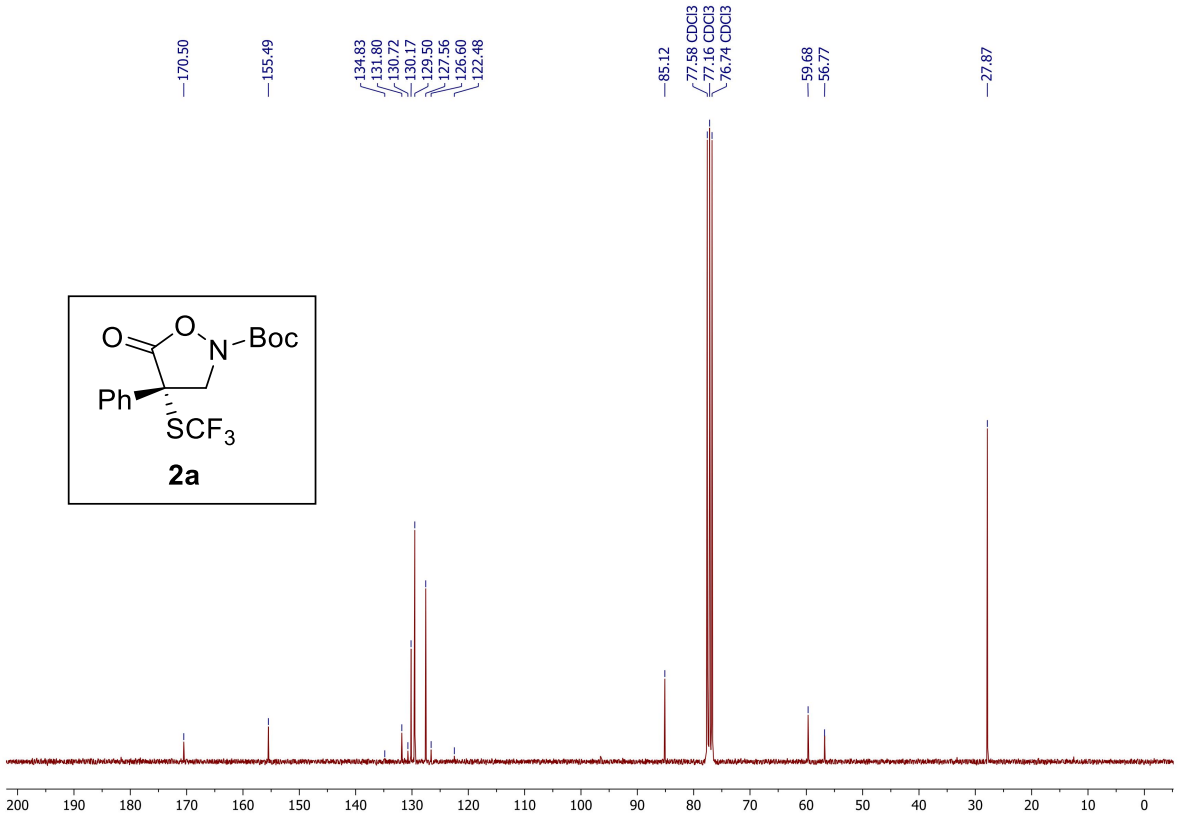
7

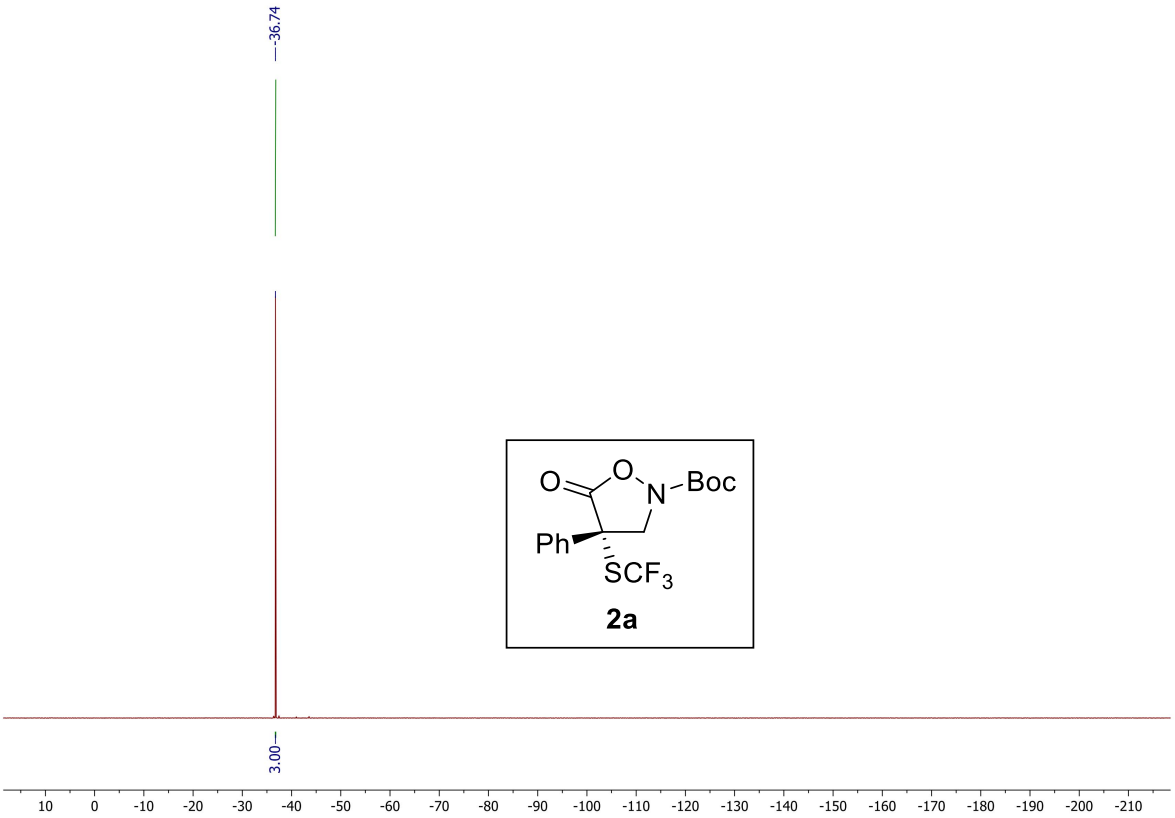
[6] T. Nanjo, N. Kato, Y. Takemoto, *Org. Lett*, **2018**, 20, 5766-5769

2H), 7.23 – 7.09 (m, 2H), 7.04 – 6.87 (m, 1H), 5.49 – 5.32 (m, 1H), 4.76 – 4.62 (m, 1H), 4.47 – 4.36 (m, 1H), 4.19 – 4.15 (m, 1H), 3.91 – 3.77 (m, 1H), 1.46 – 1.36 (m, 2H), 1.26 – 1.25 (m, 1H), 0.90 – 0.74 (m, 6H). ^{13}C NMR (75 MHz, δ, $CDCl_3$, 298 K): 175.6, 170.9, 143.8, 143.6, 141.4, 130.0 (q, J = 310.3 Hz), 128.6, 128.0, 127.6, 127.3, 127.2, 125.4, 125.1, 120.2, 73.0, 69.6, 67.8, 66.9, 47.1, 24.6, 22.8, 22.0. ^{19}F NMR (282 MHz, δ, $CDCl_3$, 298 K): -36.6. HRMS (ESI): calcd *m/z* for $C_{31}H_{31}F_3N_2O_5S$: 601.1979 $[M+H]^+$; found: 601.1980.

5. Copies of NMR Spectra of New Compounds



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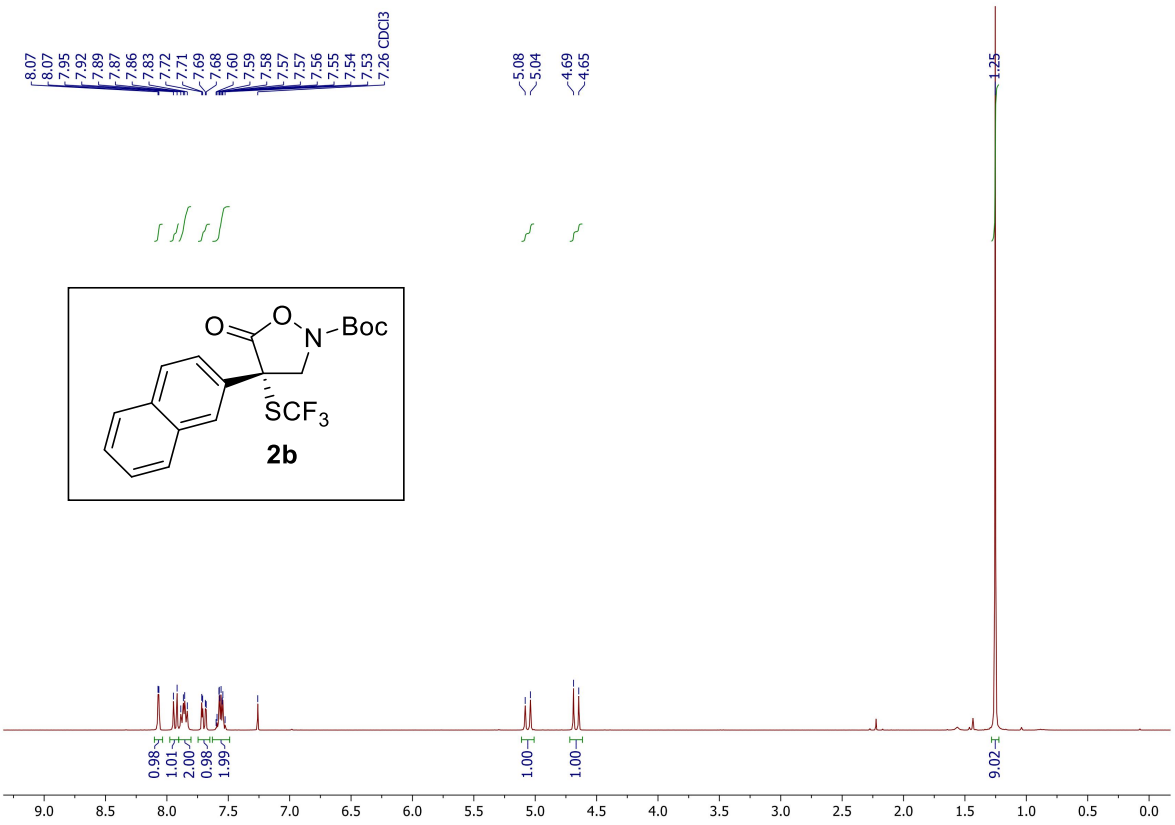
2a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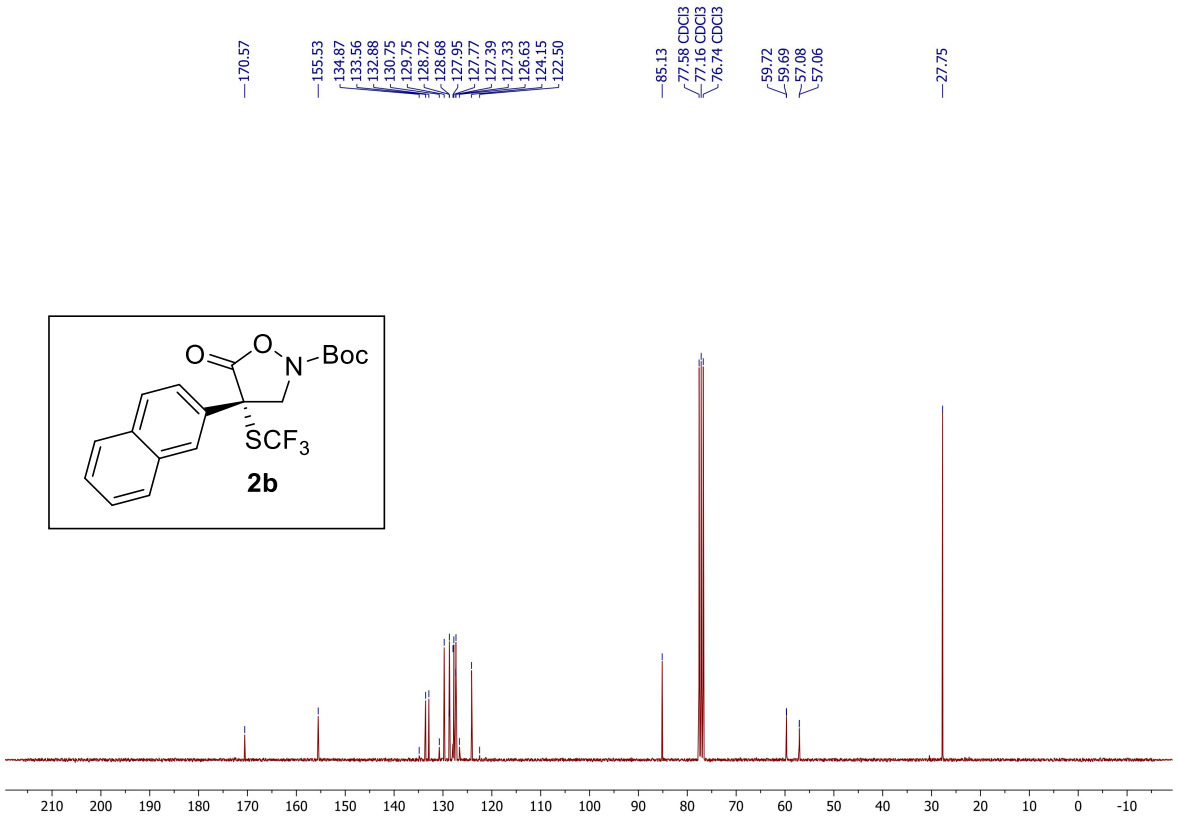
2b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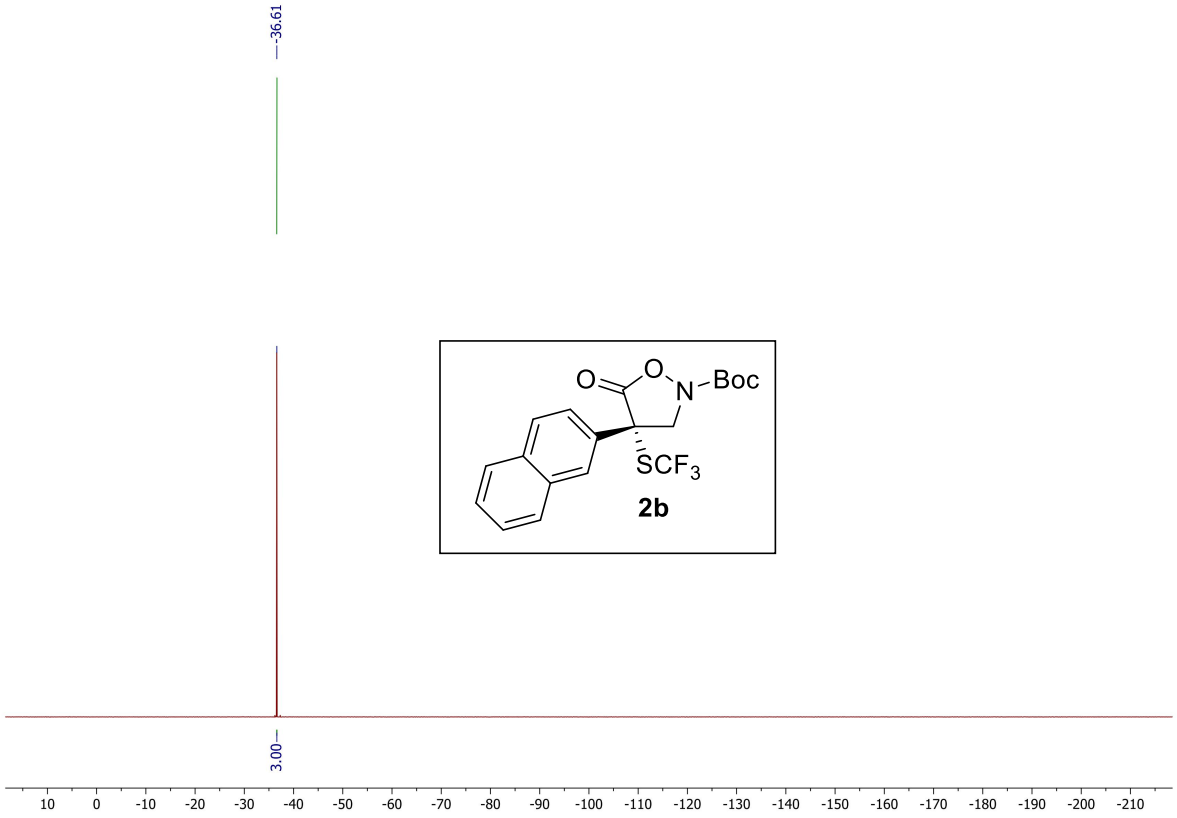
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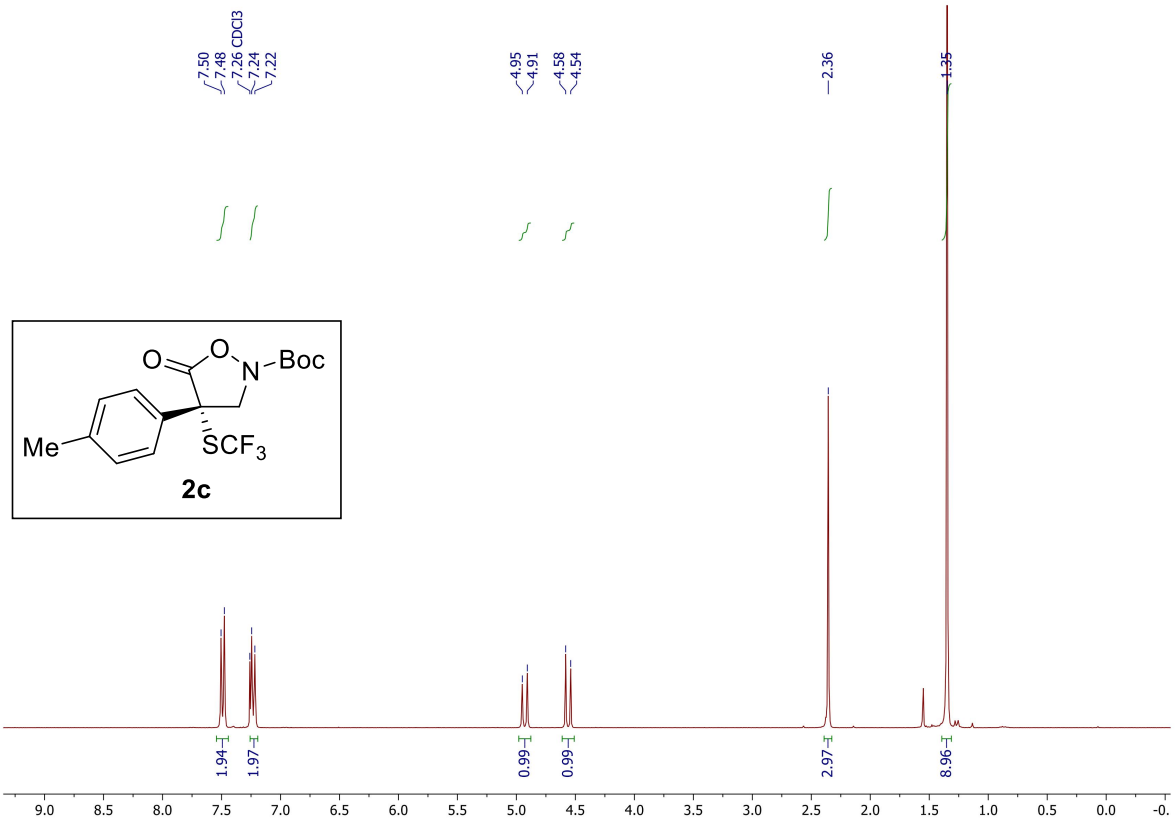
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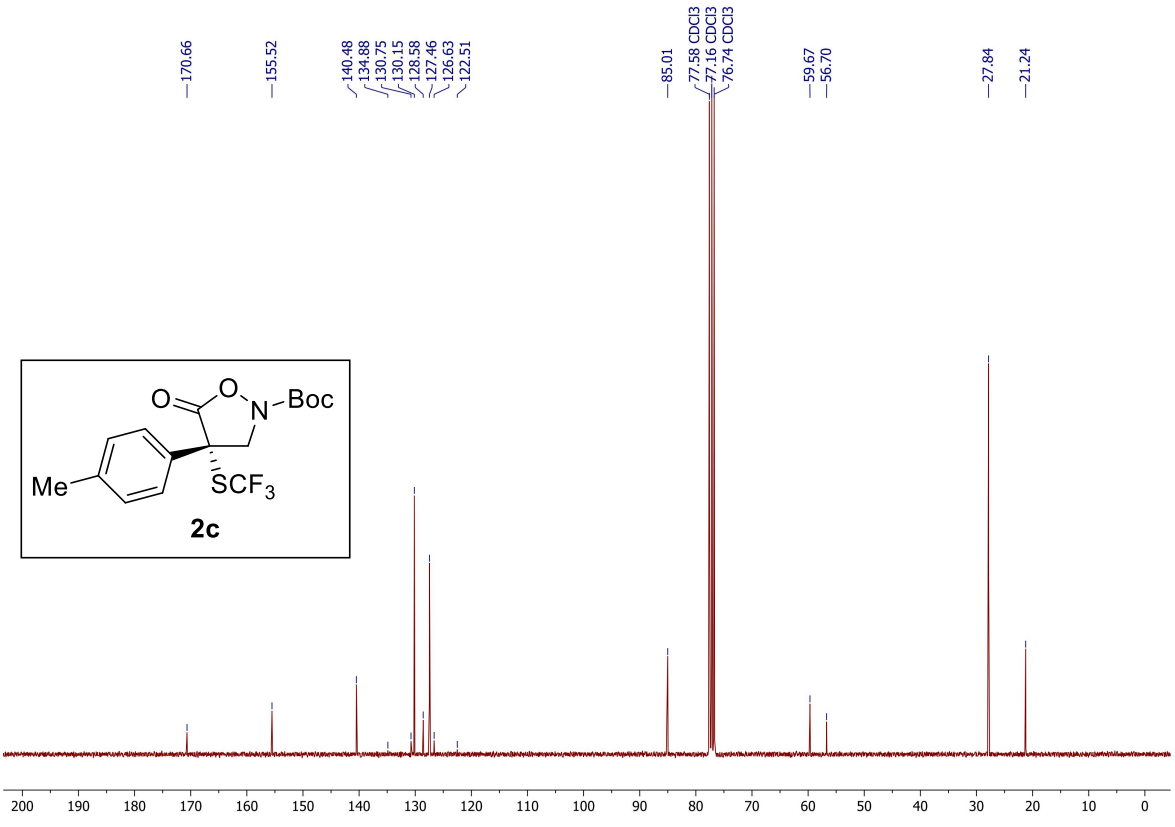
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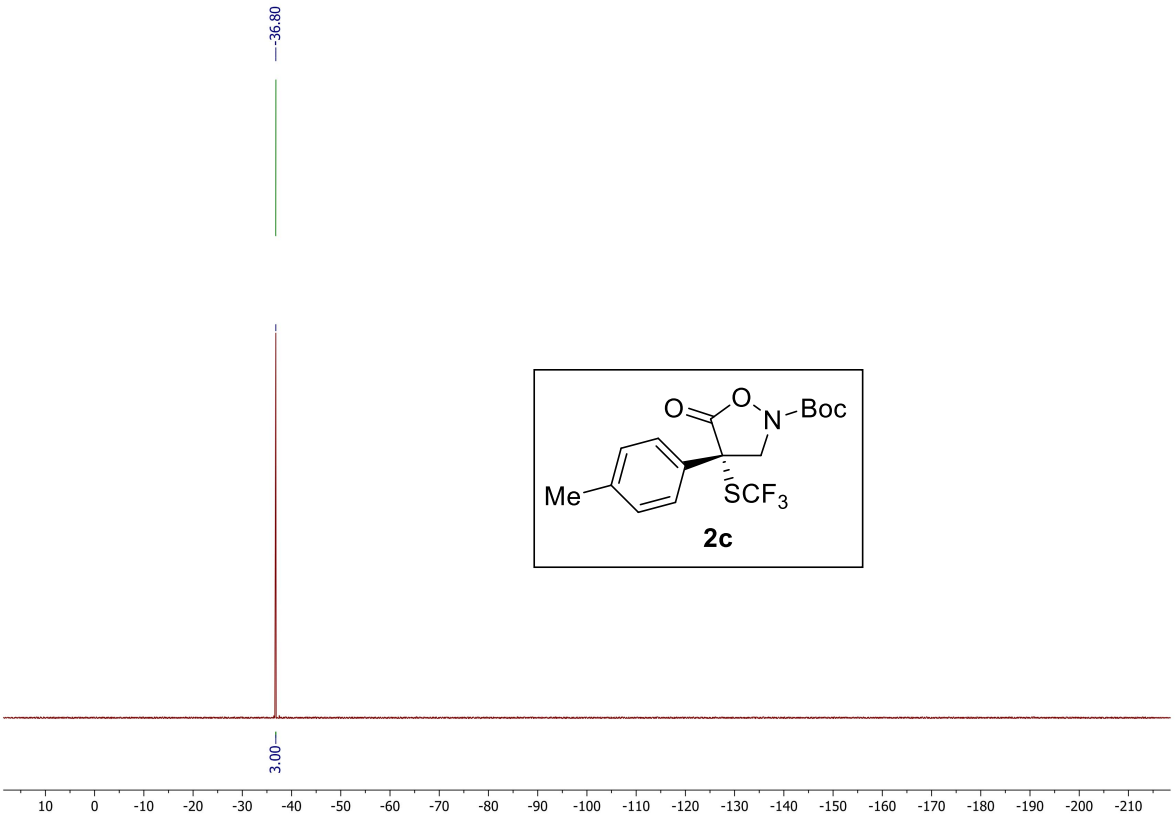
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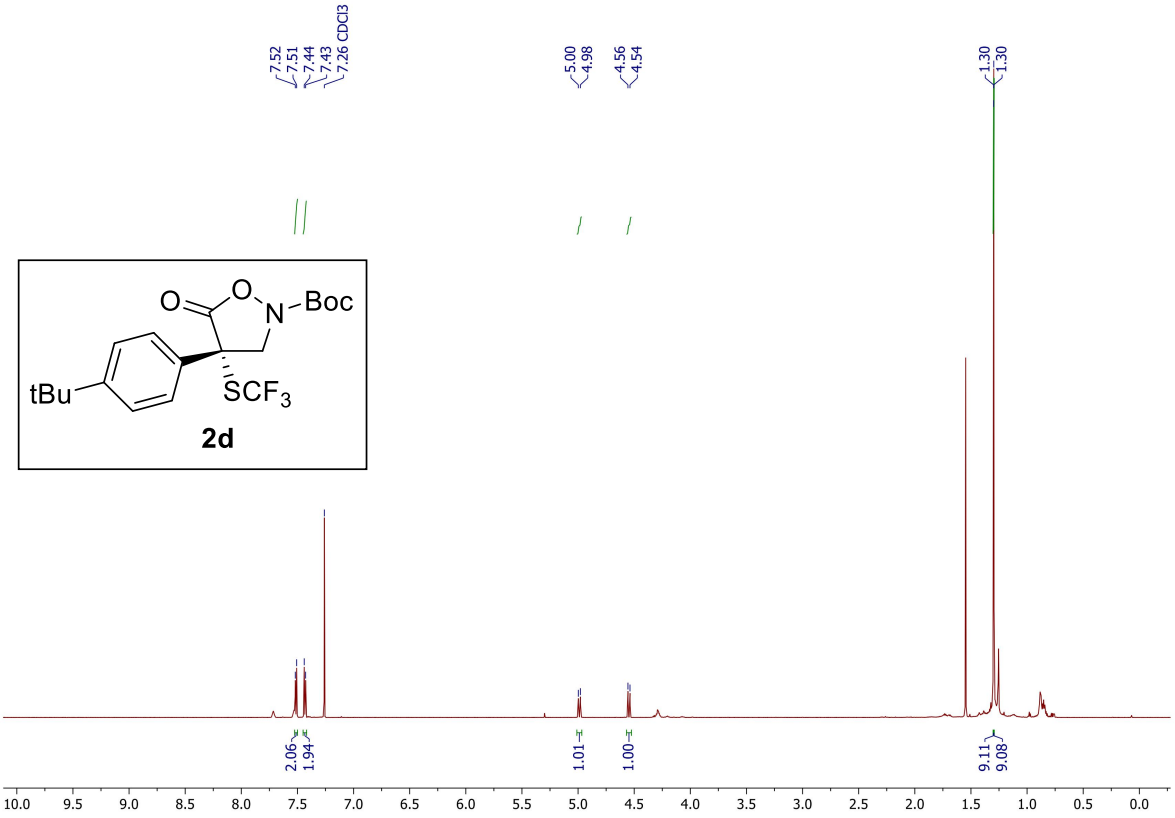
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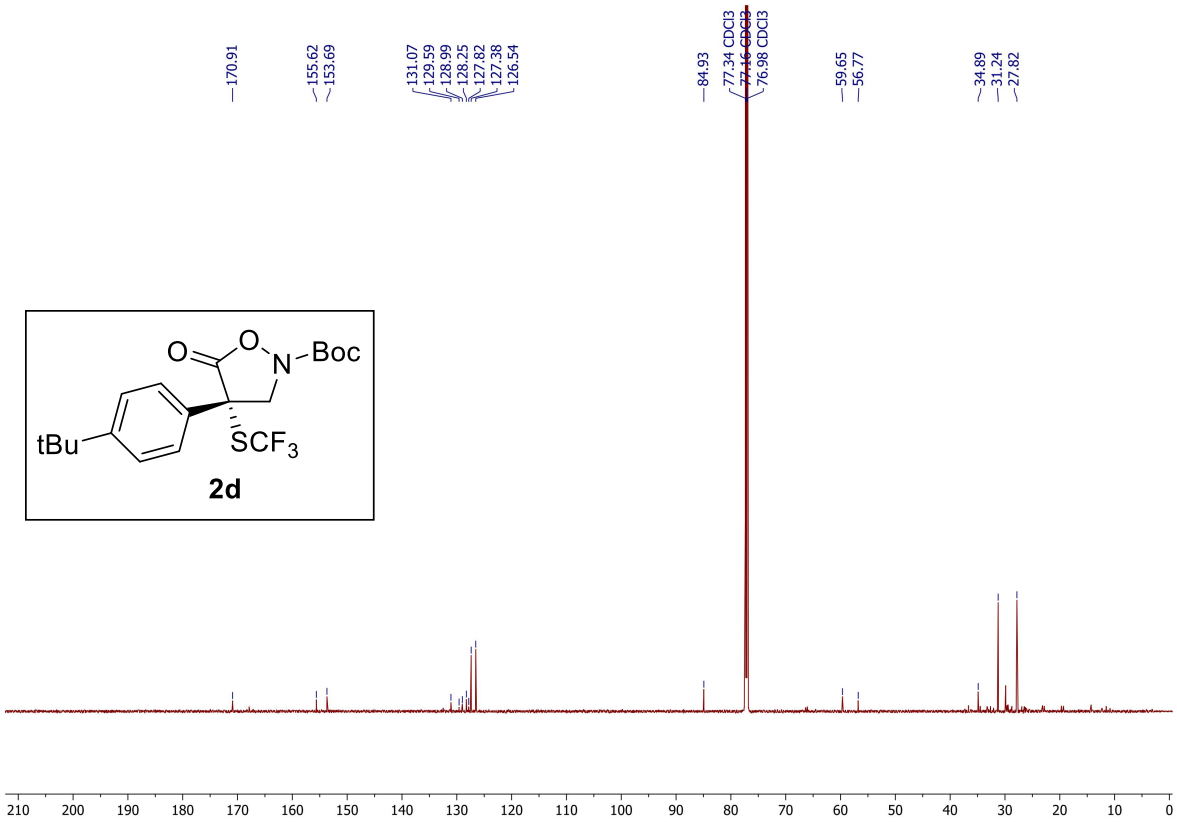
2d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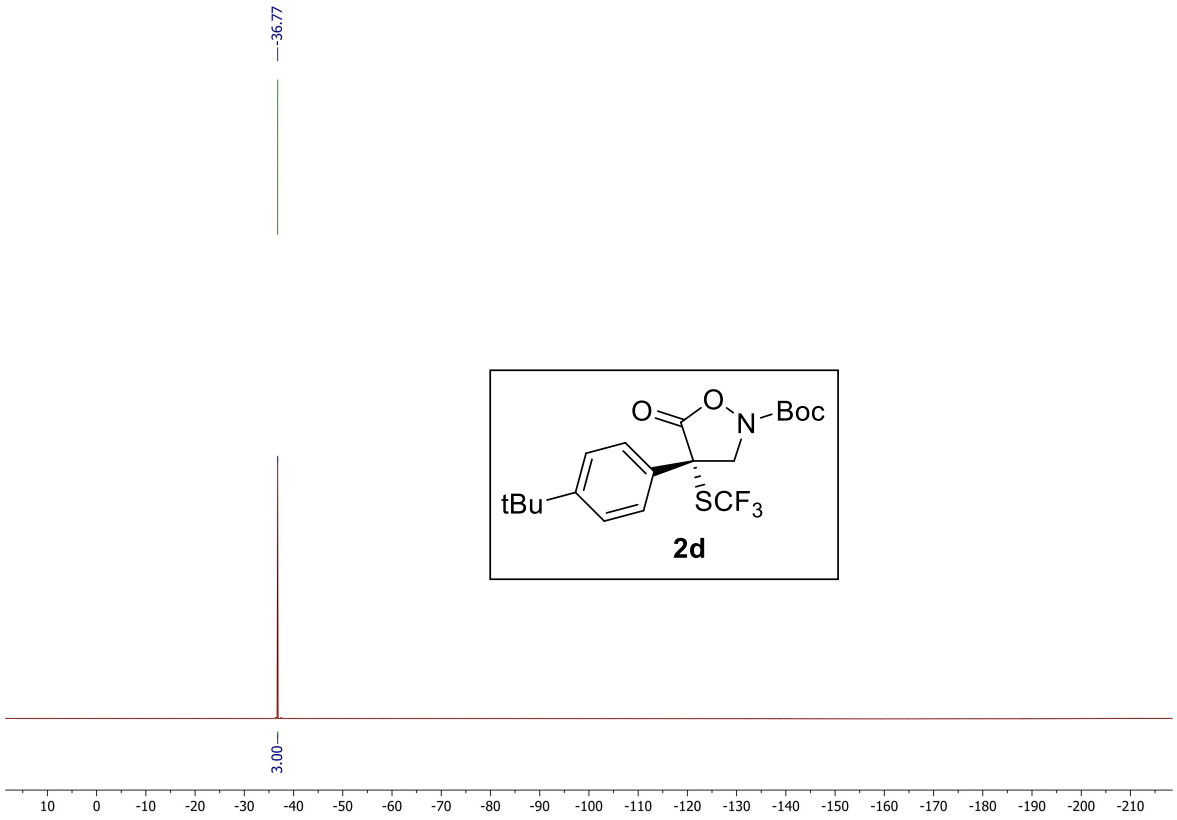
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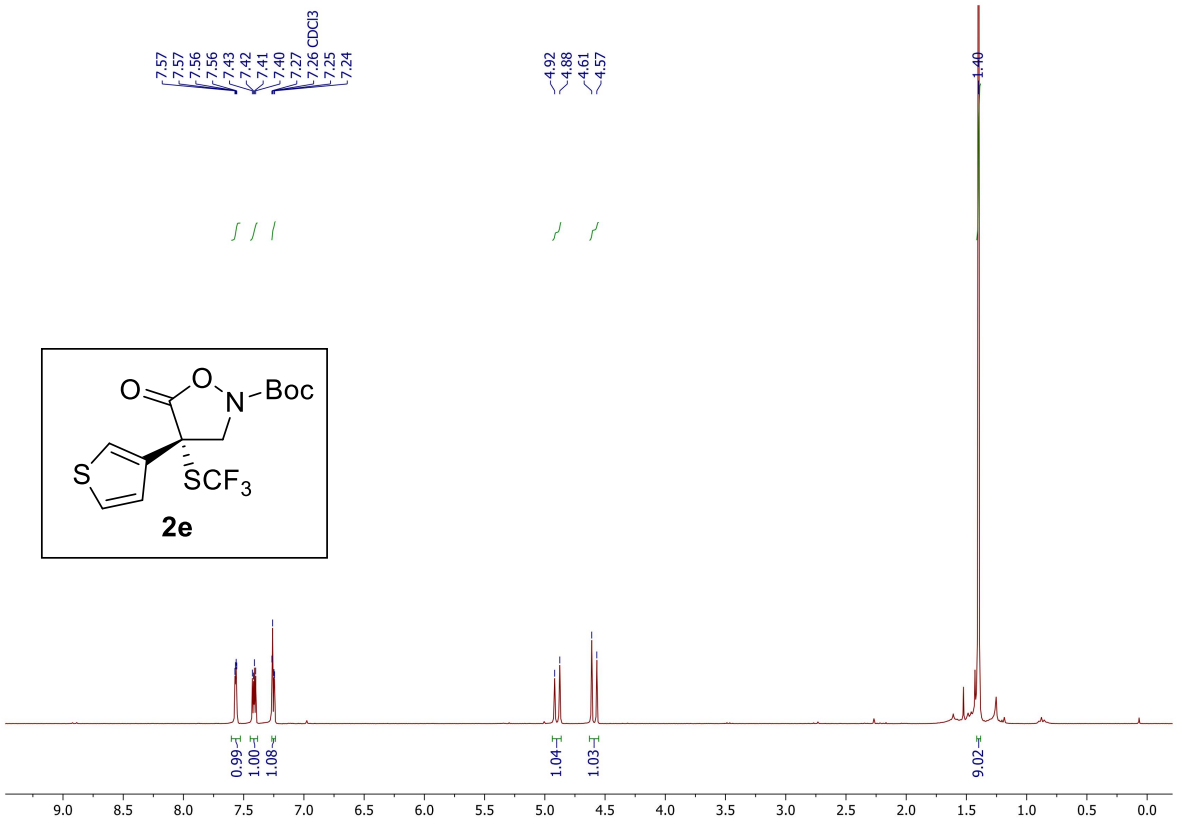
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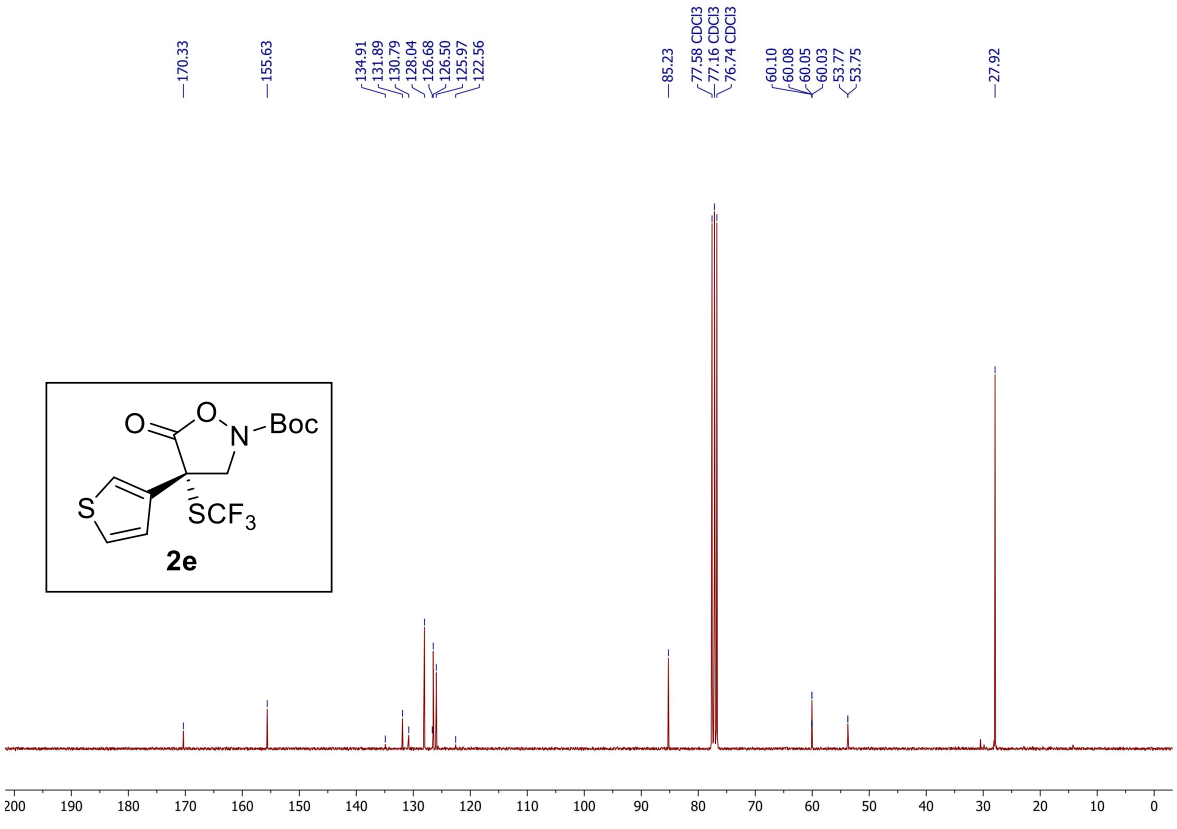
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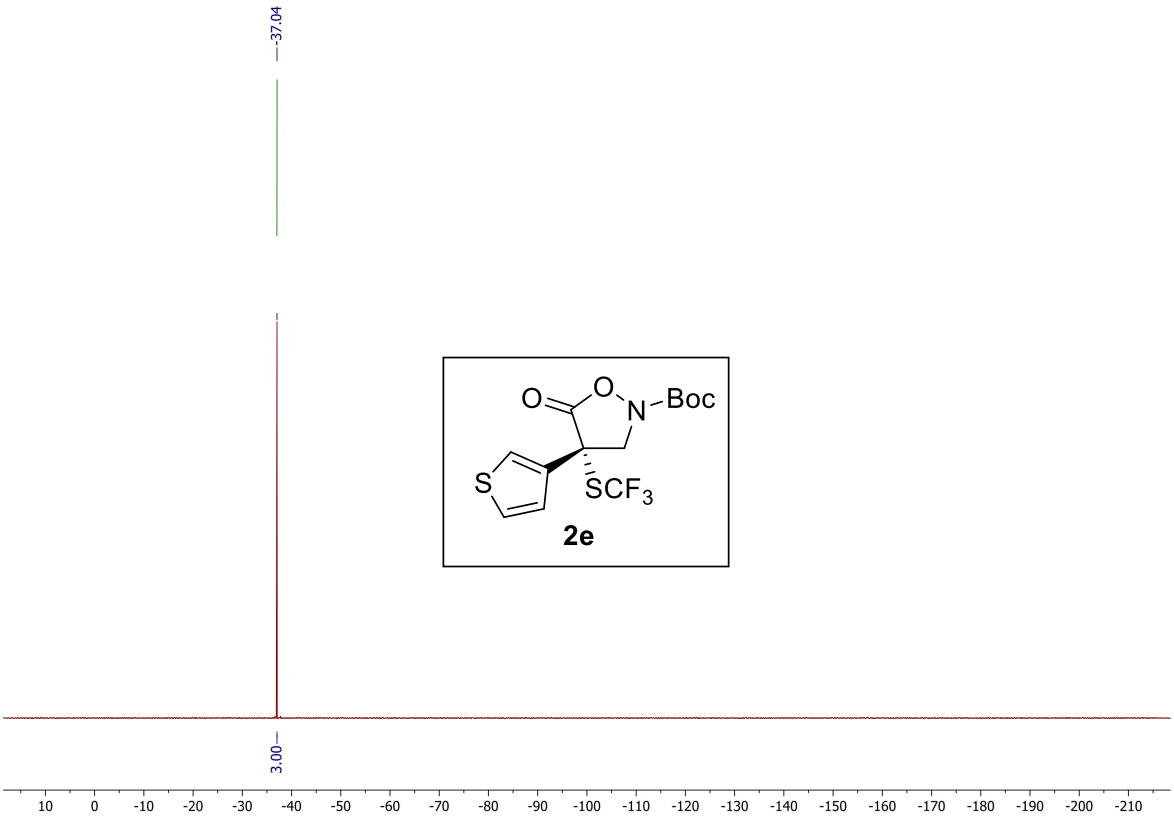
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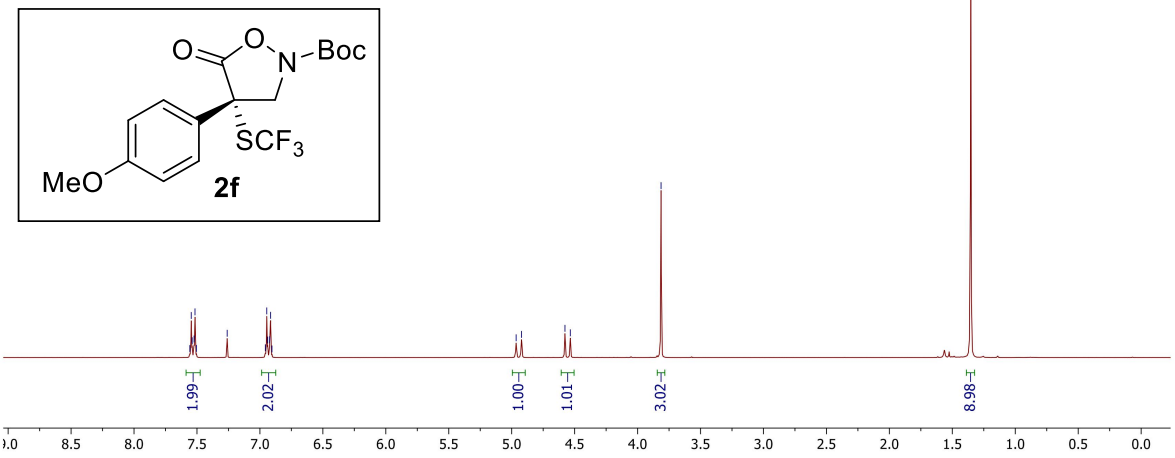
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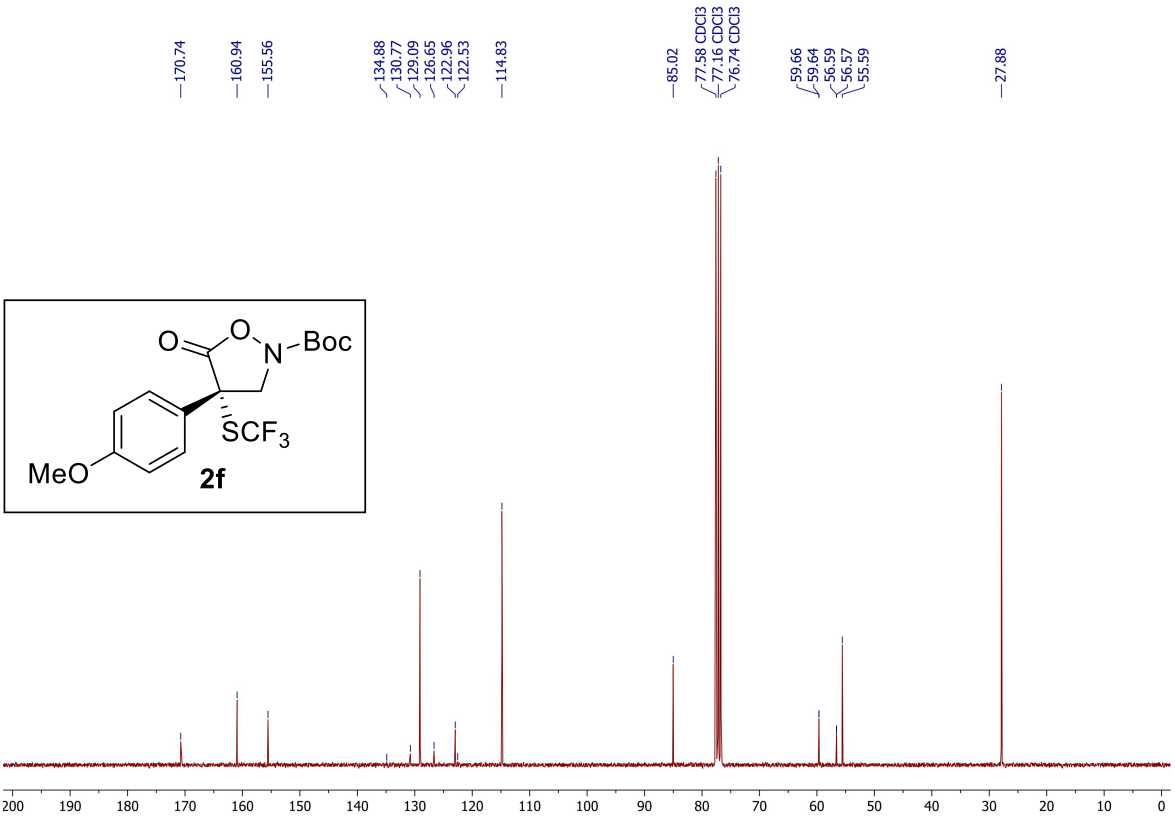
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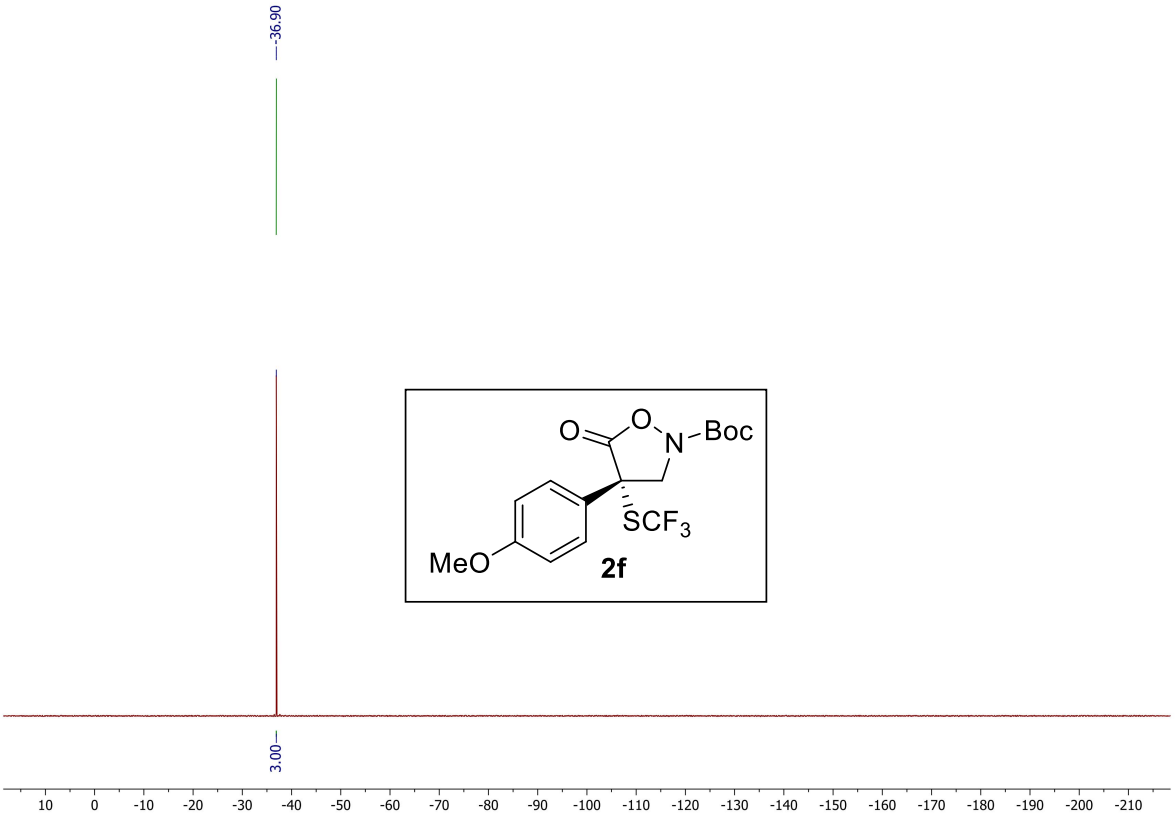
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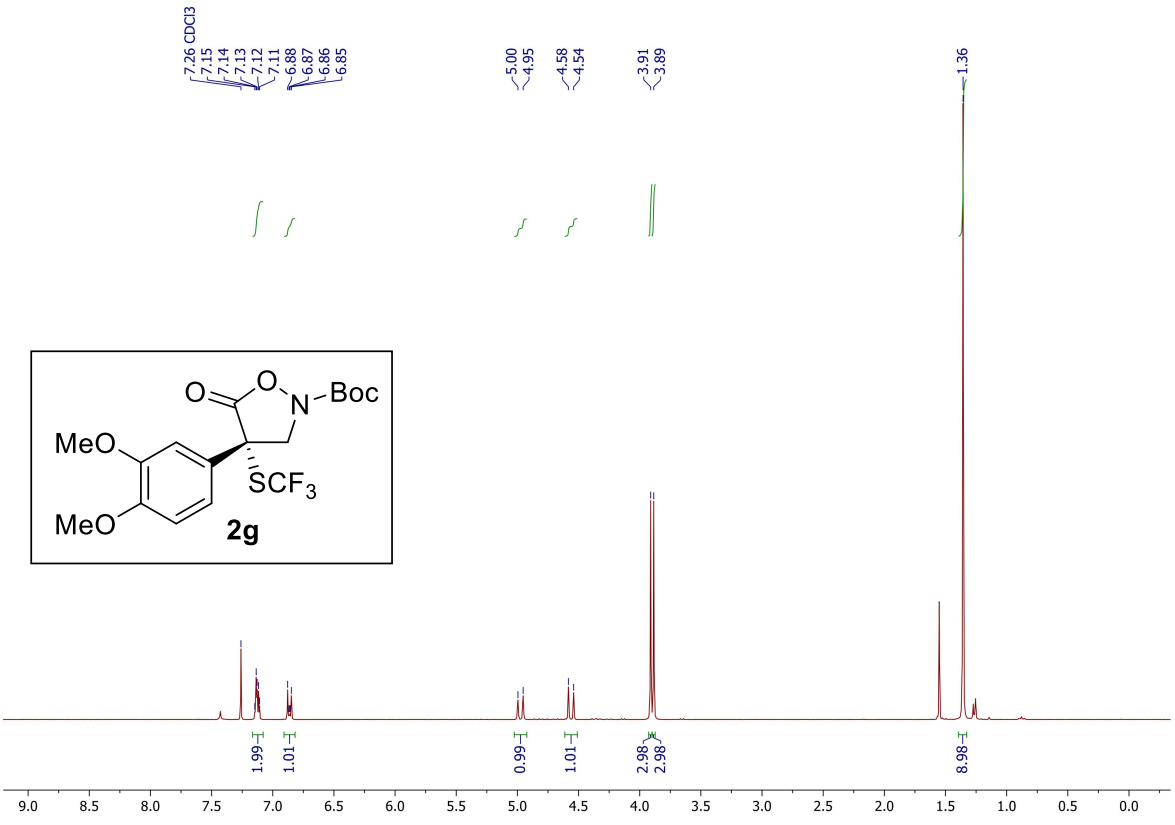
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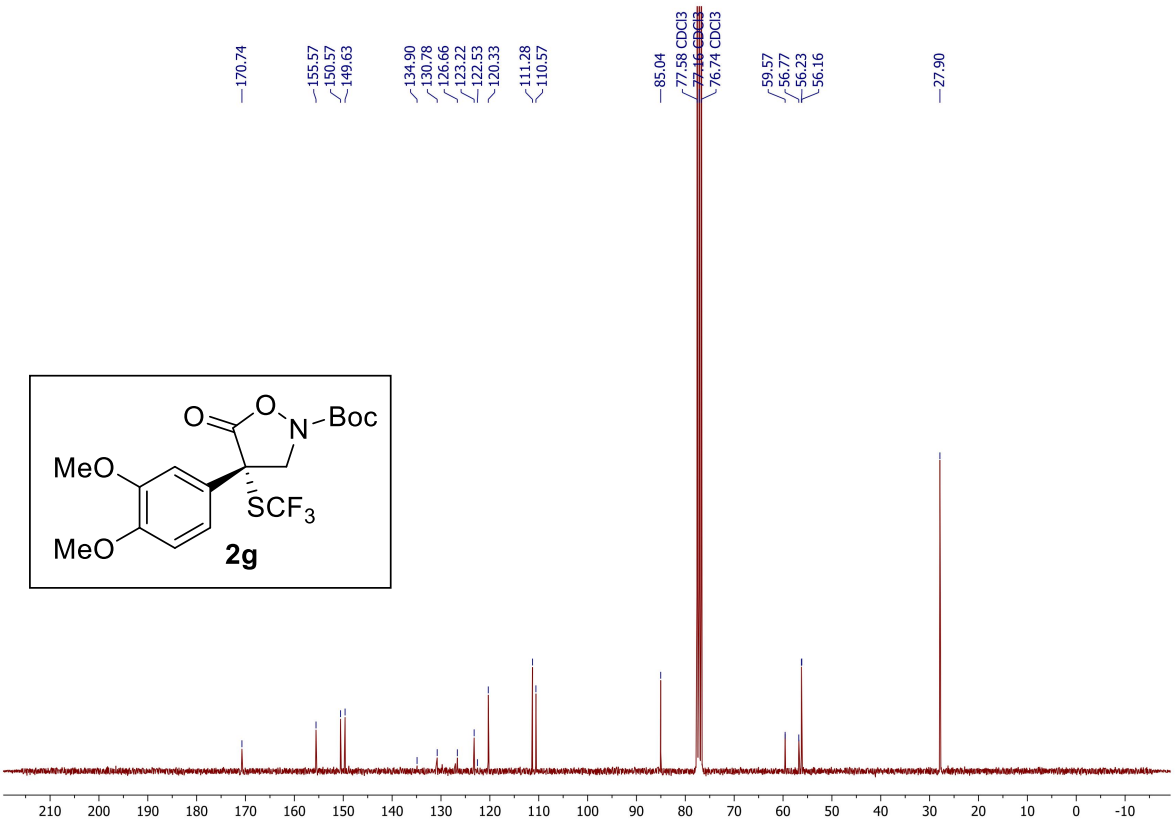
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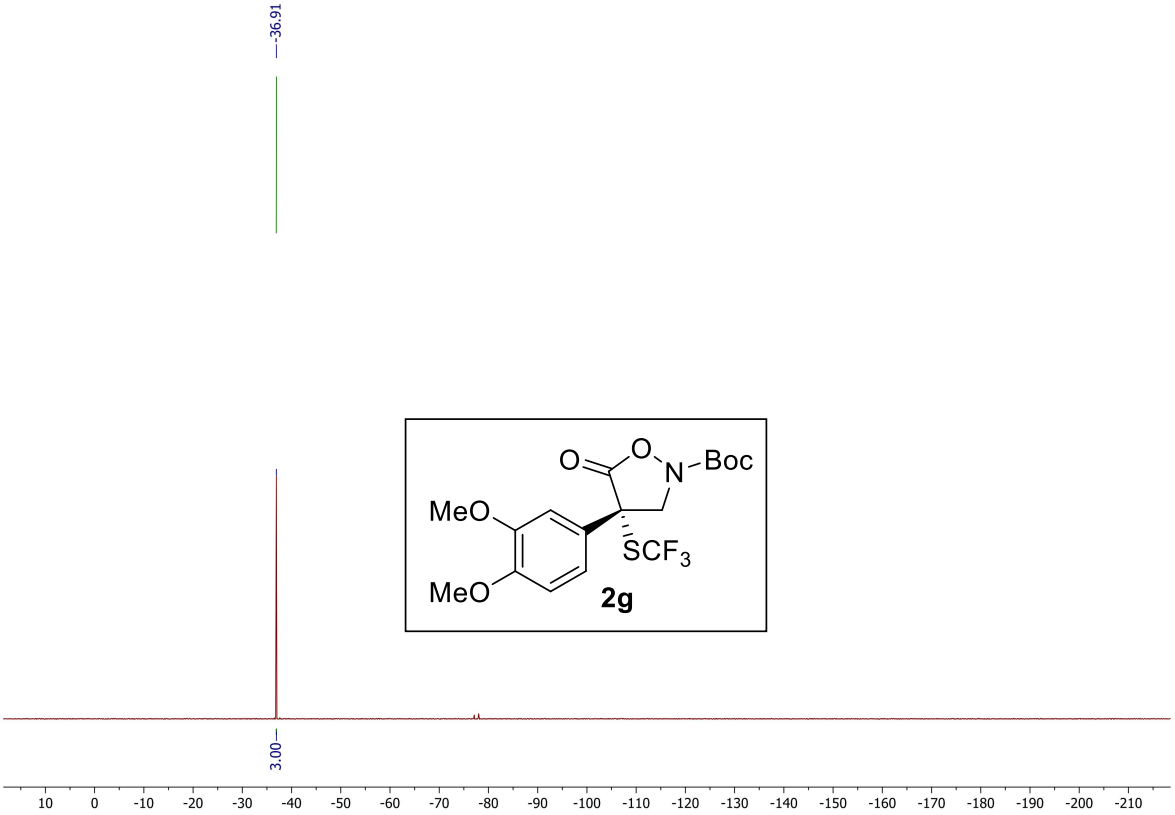
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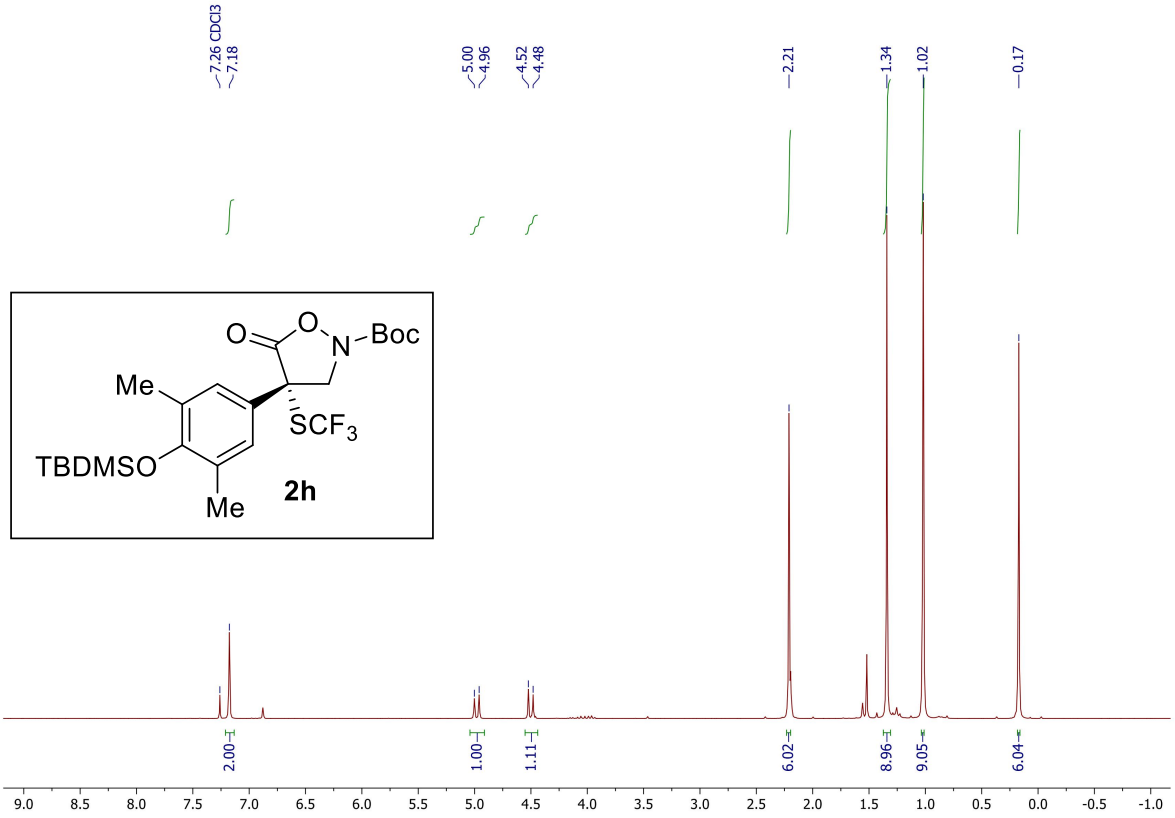
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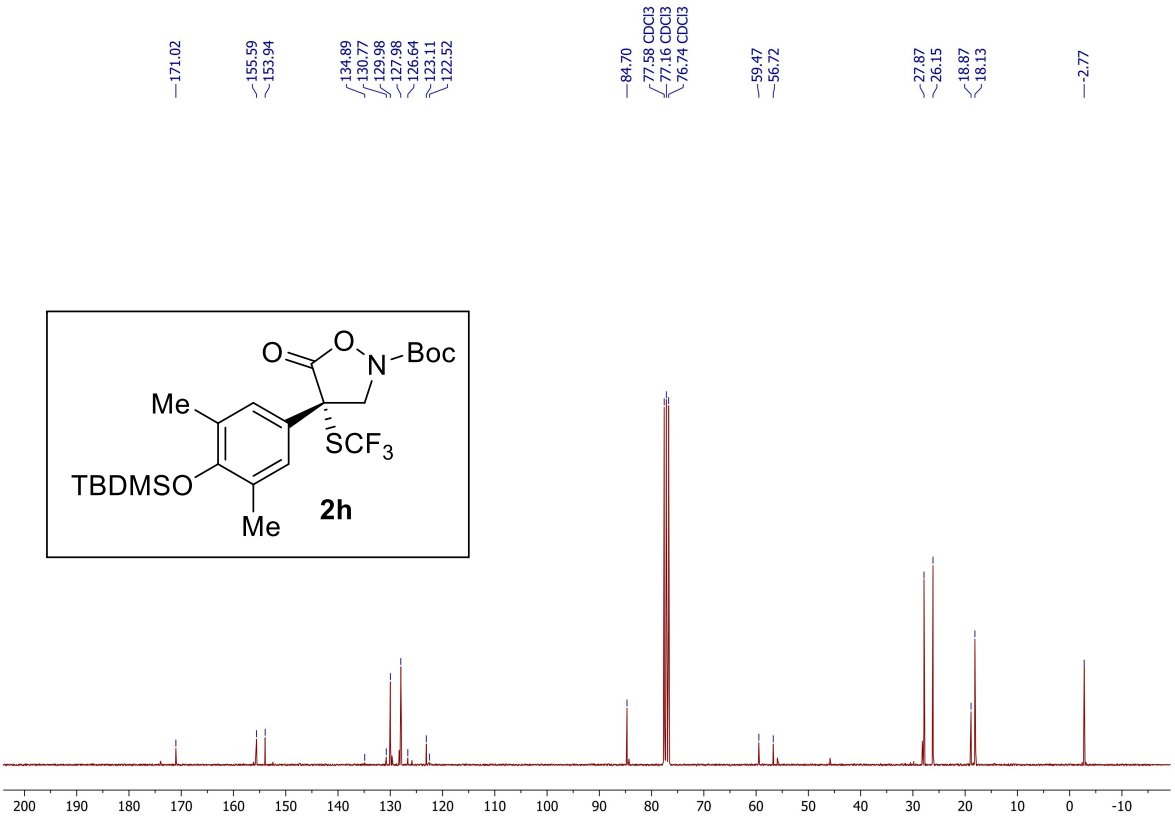
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76.74 CDCl3
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18.87
18.13
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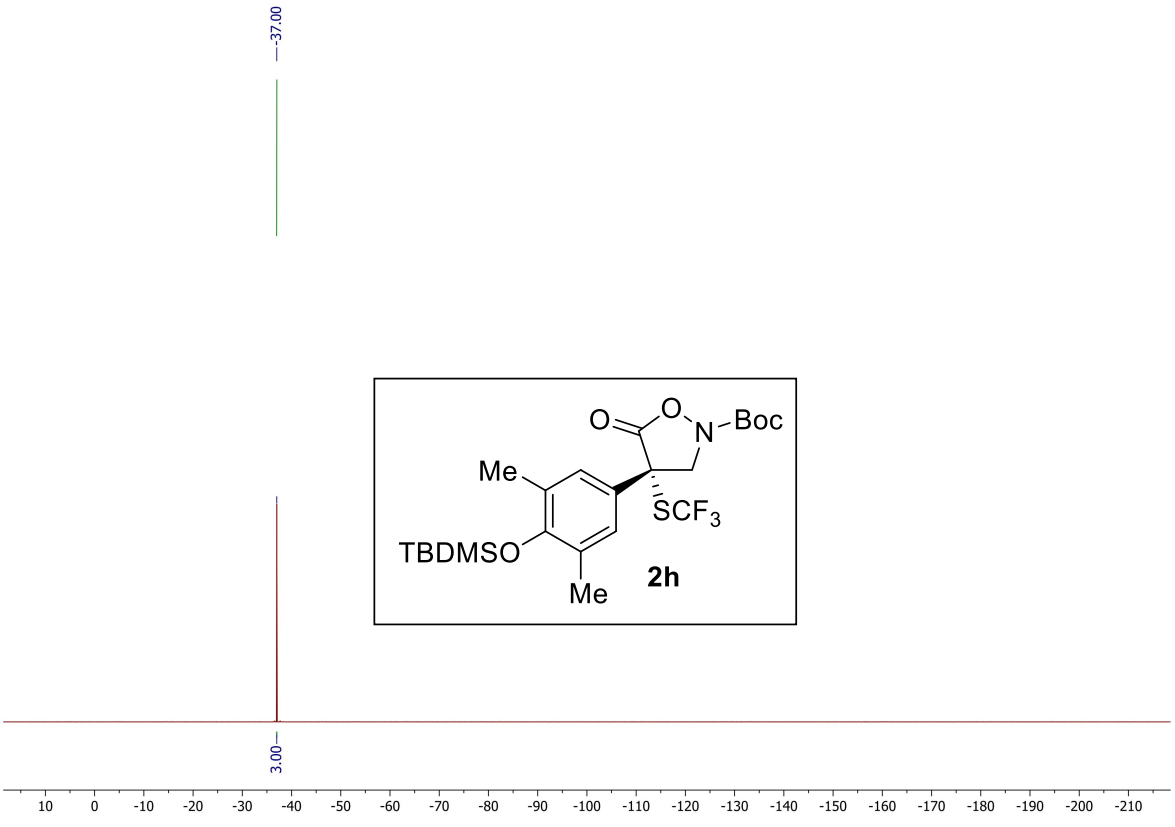
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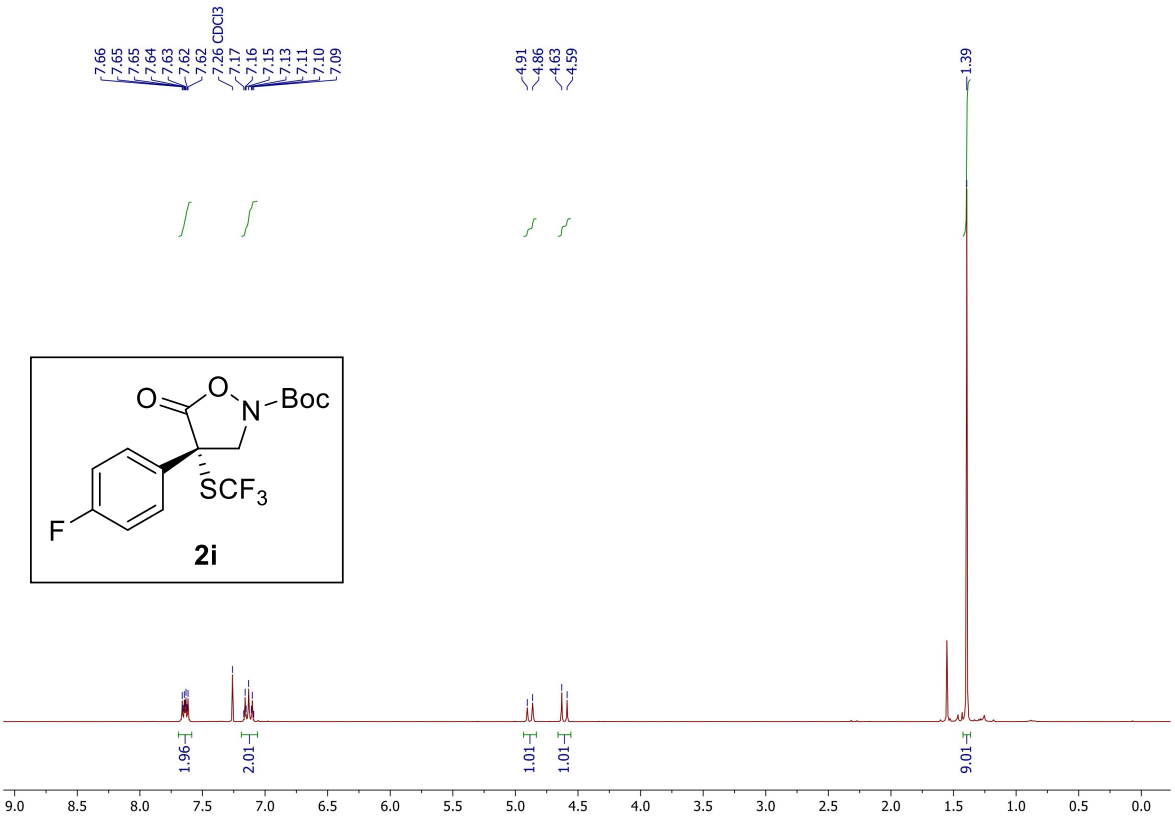
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4.63
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O
O
N
Boc
SCF3
F
2i
1.96
2.01
1.01
1.01
9.01
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8.0
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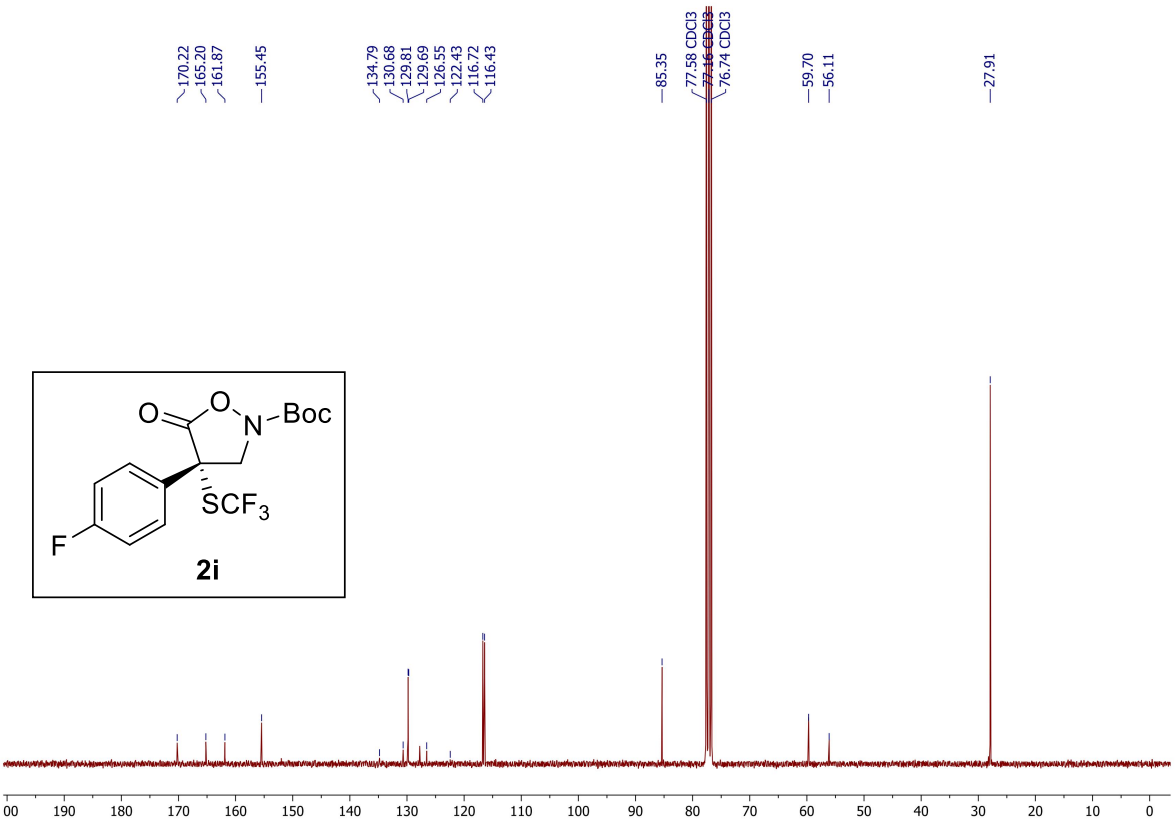
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N
Boc
SCF3
F
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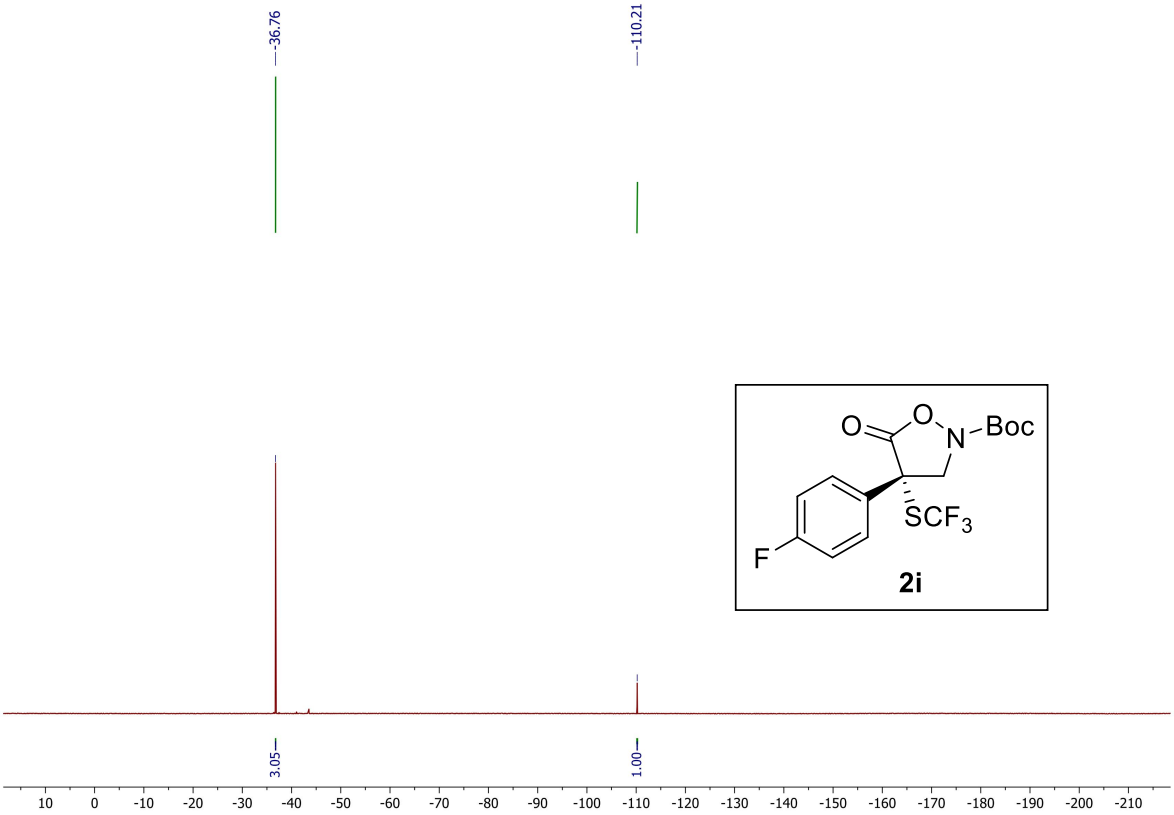
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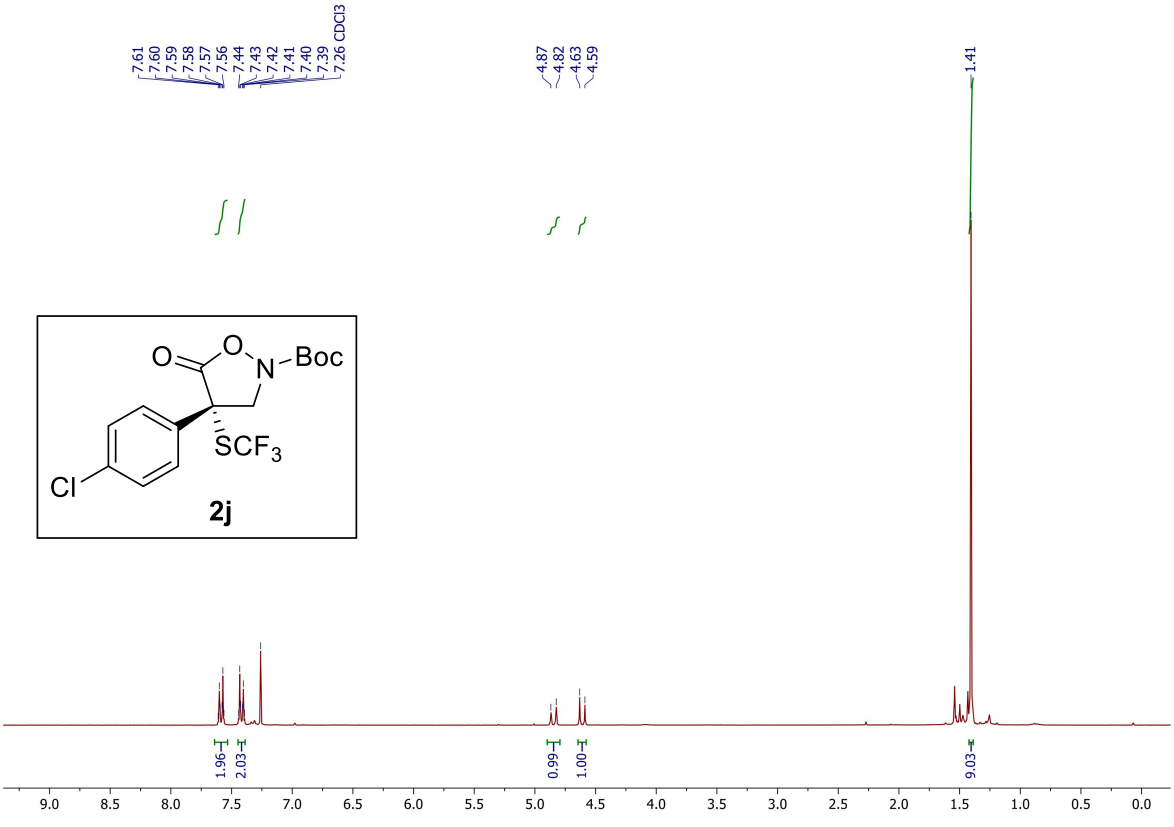
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4.63
4.59
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N
Boc
SCF3
Cl
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2.03
0.99
1.00
9.03
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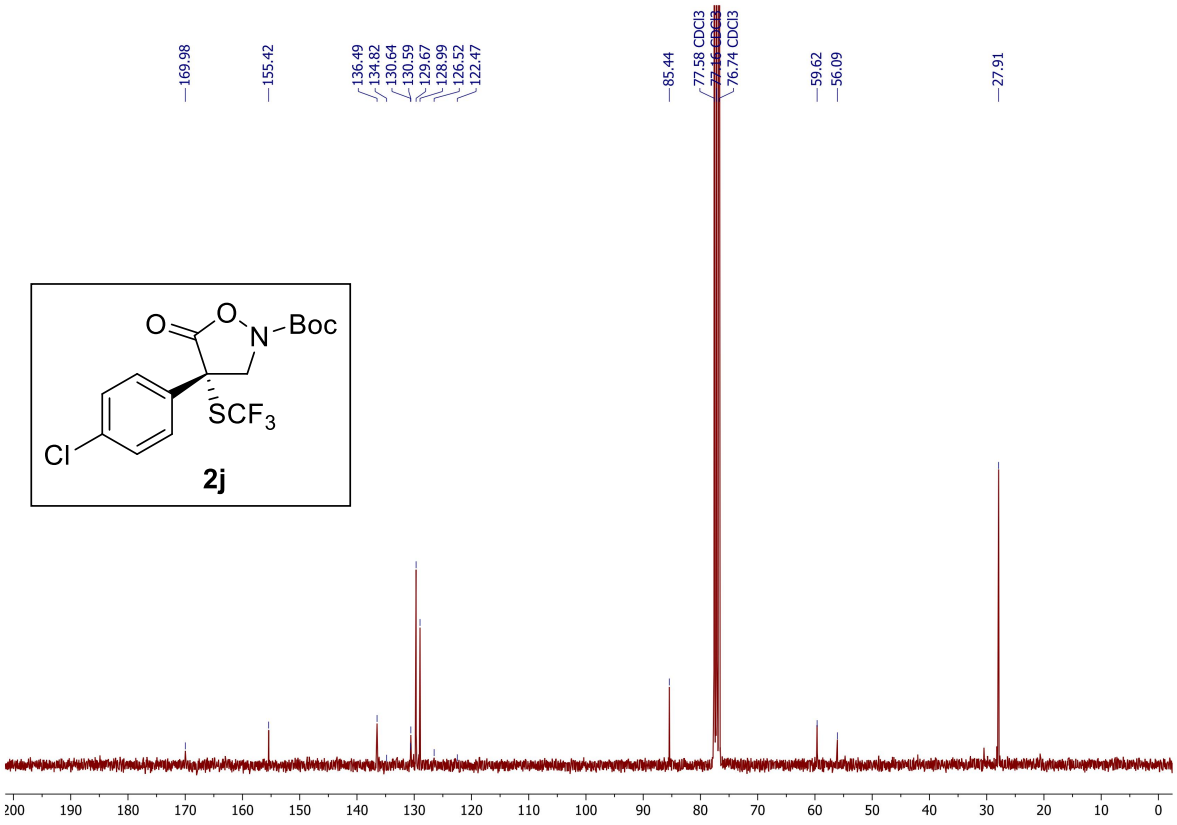
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77.16 CDCl3
76.74 CDCl3
59.62
56.09
27.91
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O
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Boc
SCF3
Cl
2j
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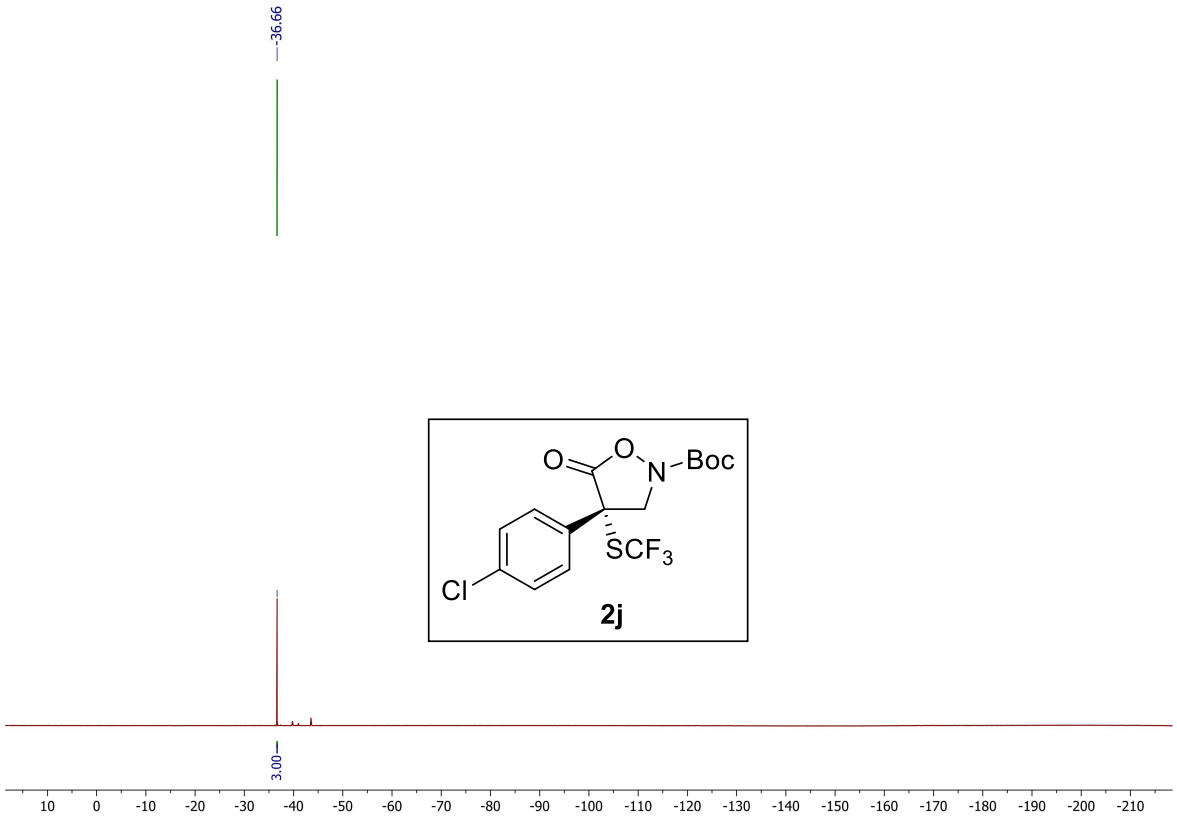
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-200
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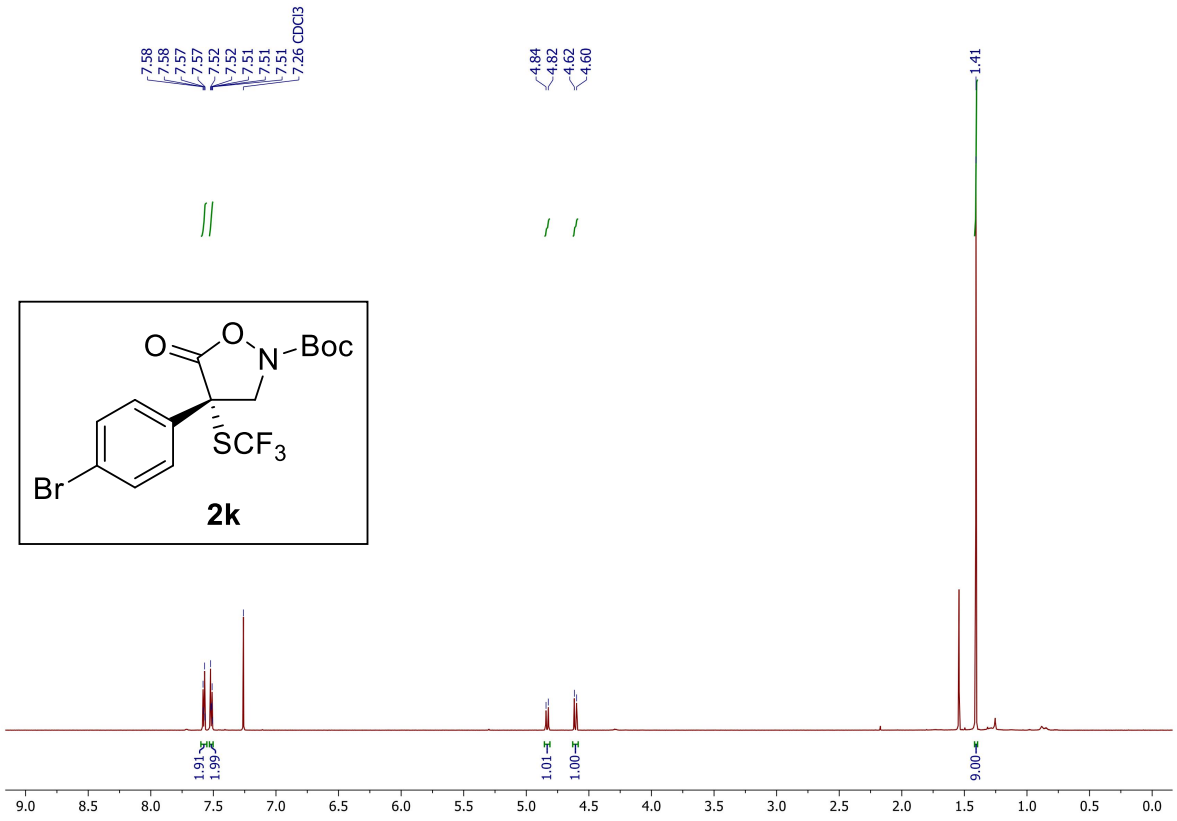
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4.62
4.60
1.41
O
O
N
Boc
SCF3
Br
2k
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1.99
1.01
1.00
9.00
9.0
8.5
8.0
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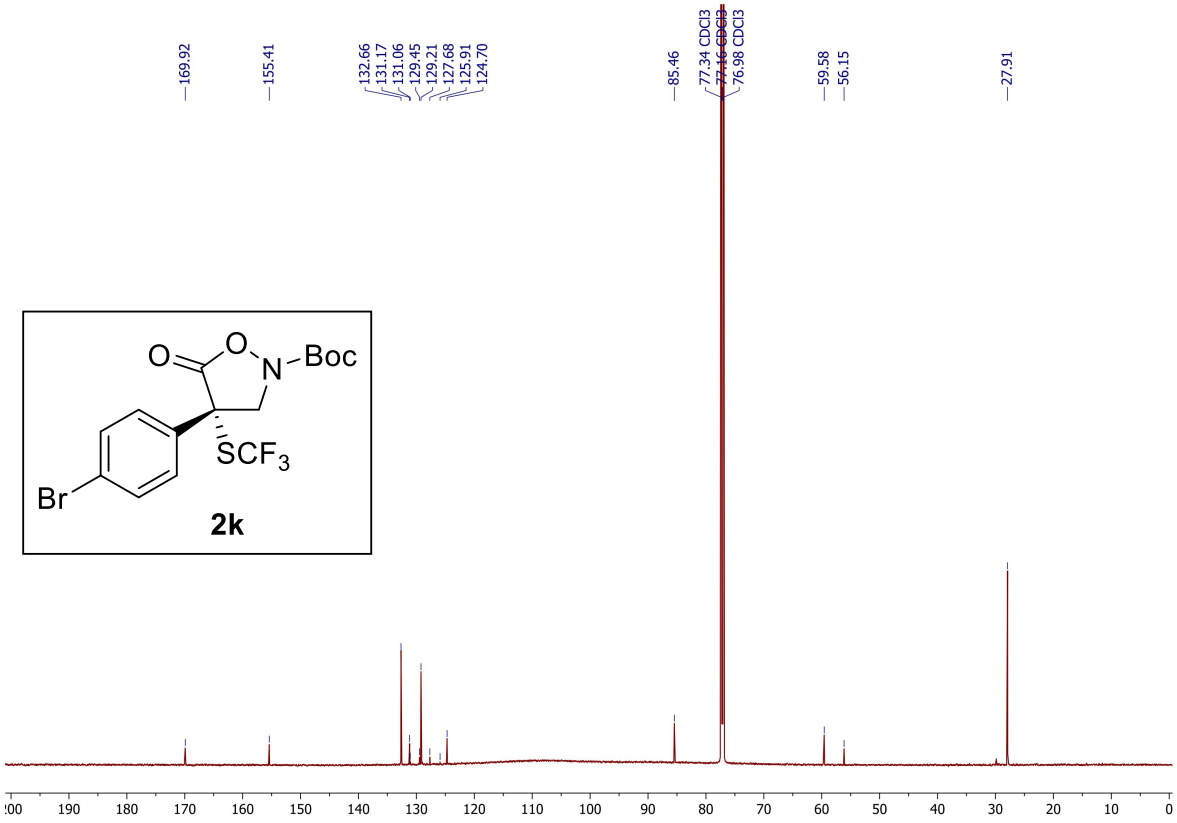
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76.98 CDCl3
59.58
56.15
27.91
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O
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Boc
SCF3
Br
2k
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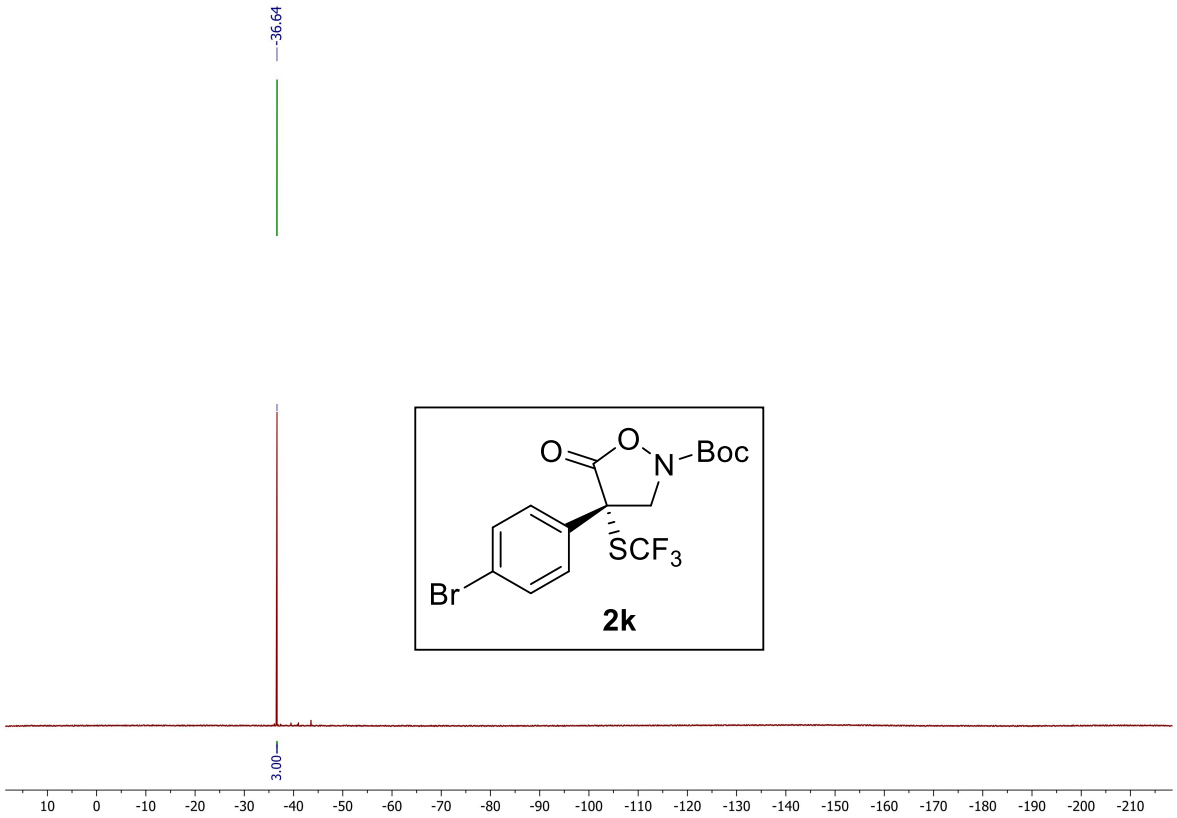
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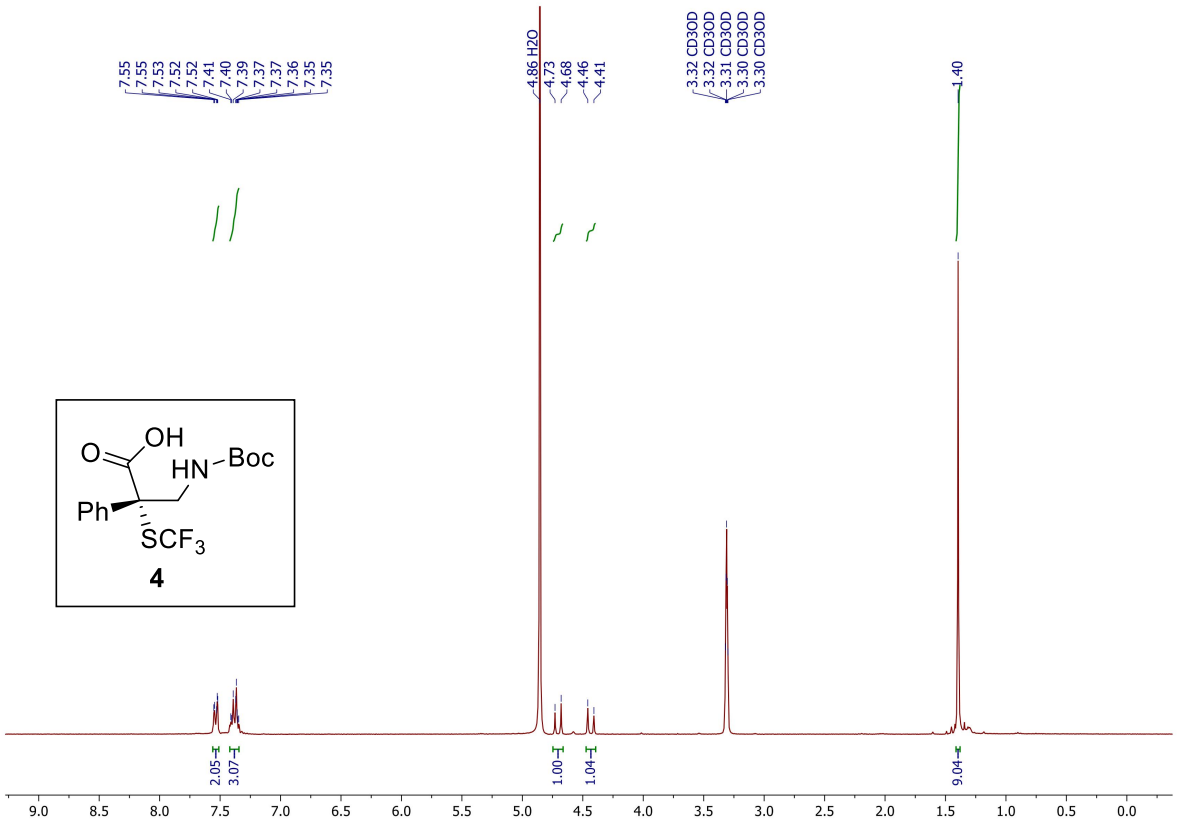
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4.46
4.41
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3.32 CD3OD
3.31 CD3OD
3.30 CD3OD
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1.40
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OH
HN
Boc
Ph
SCF3
4
2.05
3.07
1.00
1.04
9.04
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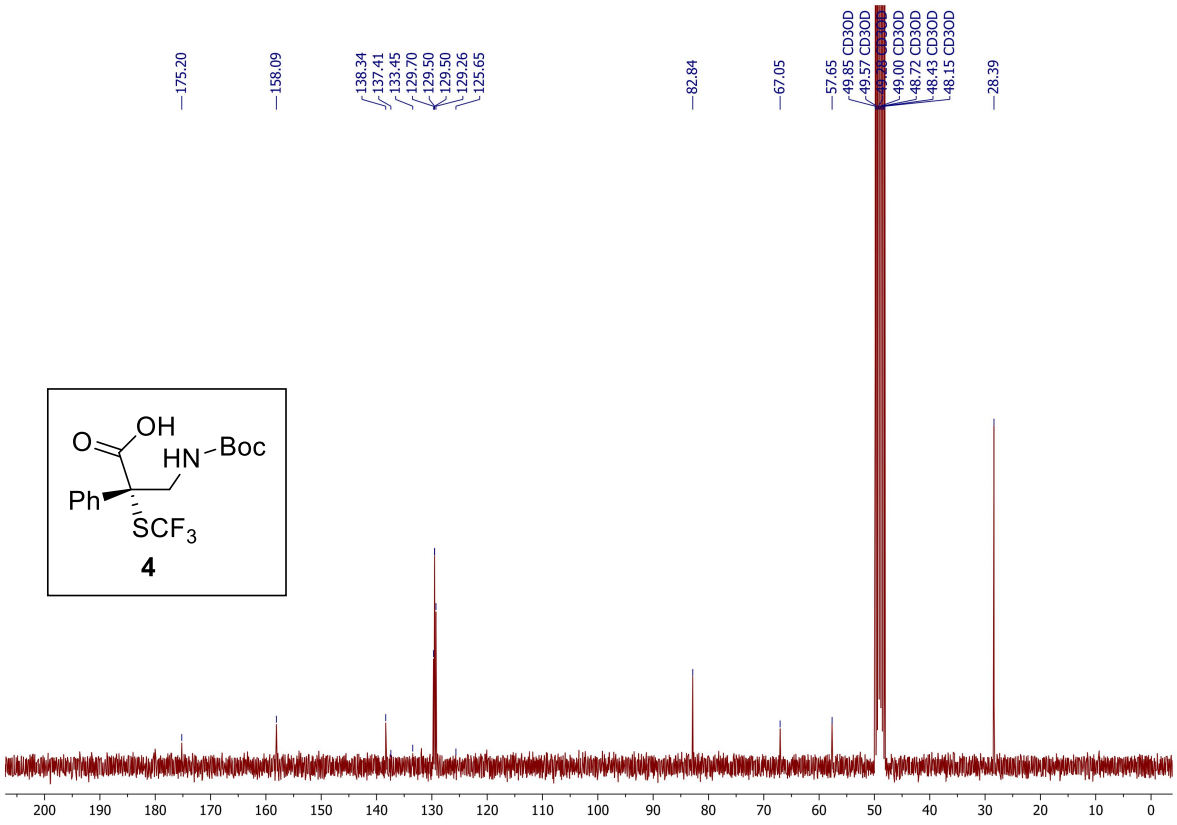
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O
HN
Boc
Ph
SCF3
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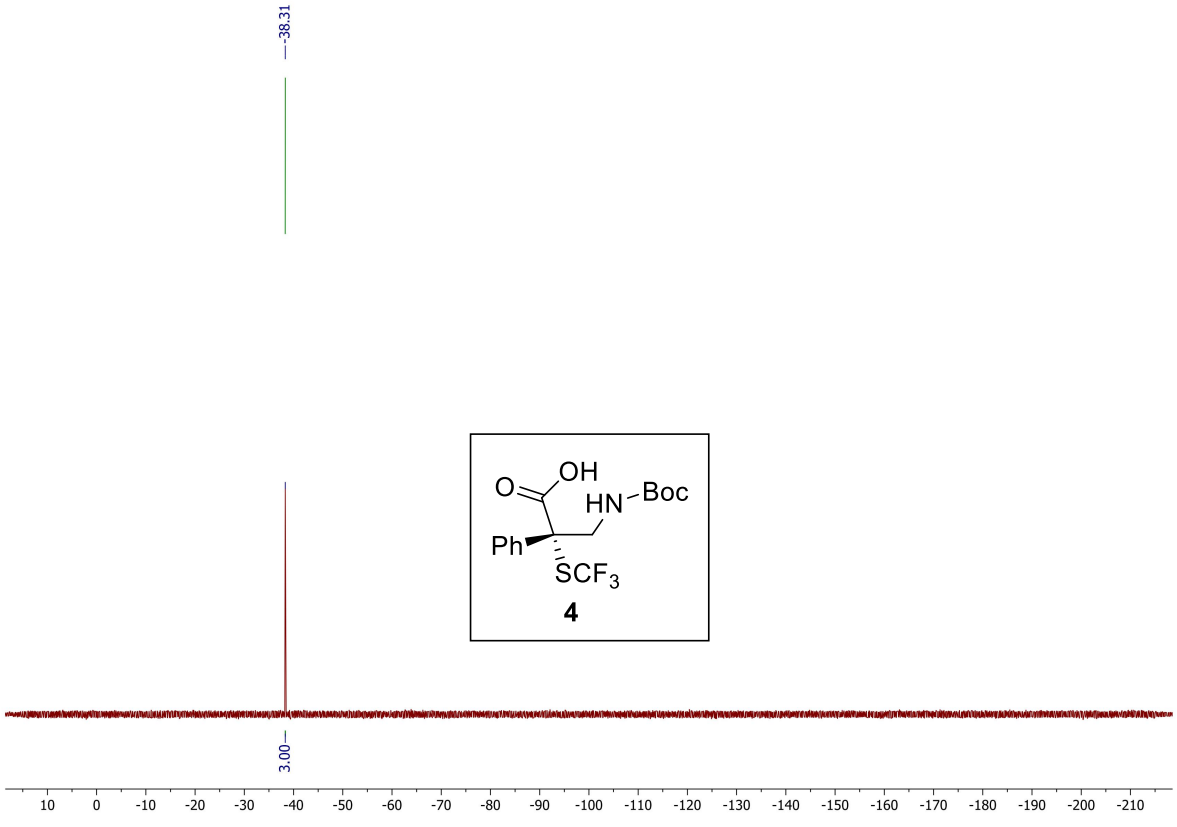
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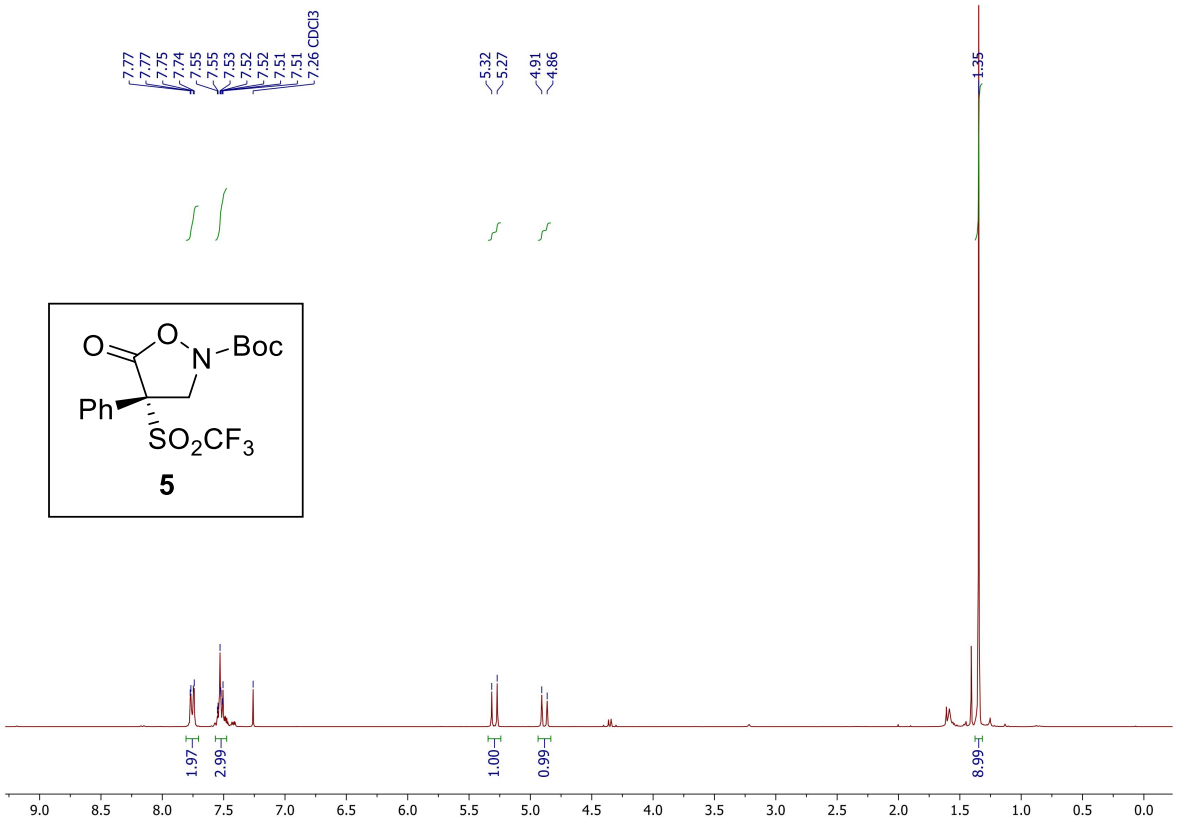
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5.27
4.91
4.86
1.35
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O
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Boc
Ph
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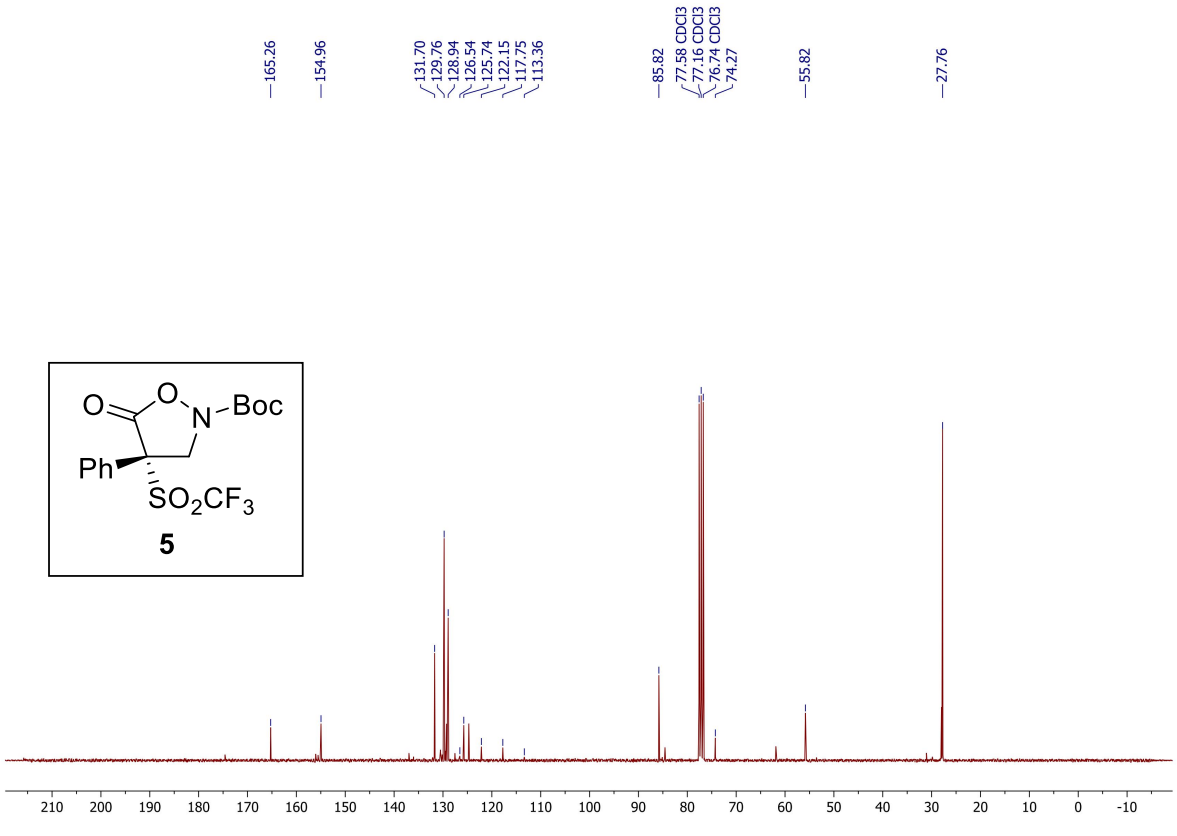
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N
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Ph
SO2CF3
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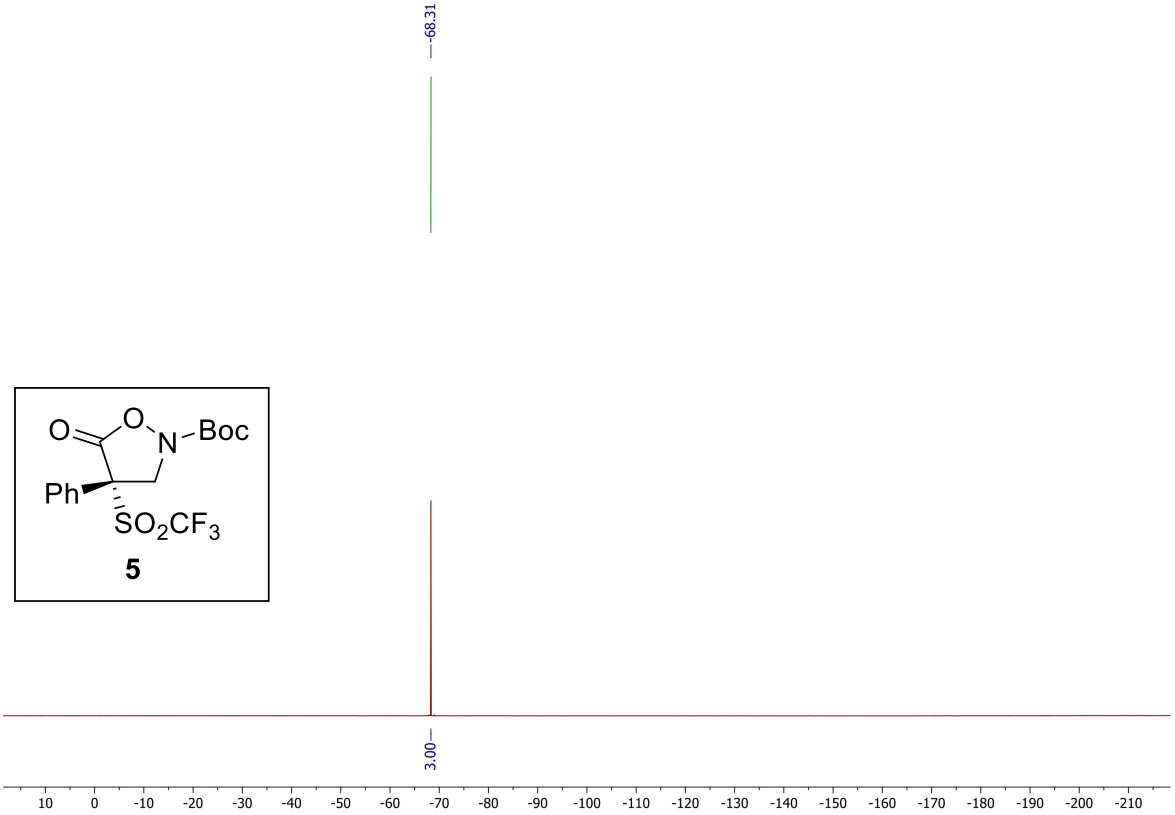
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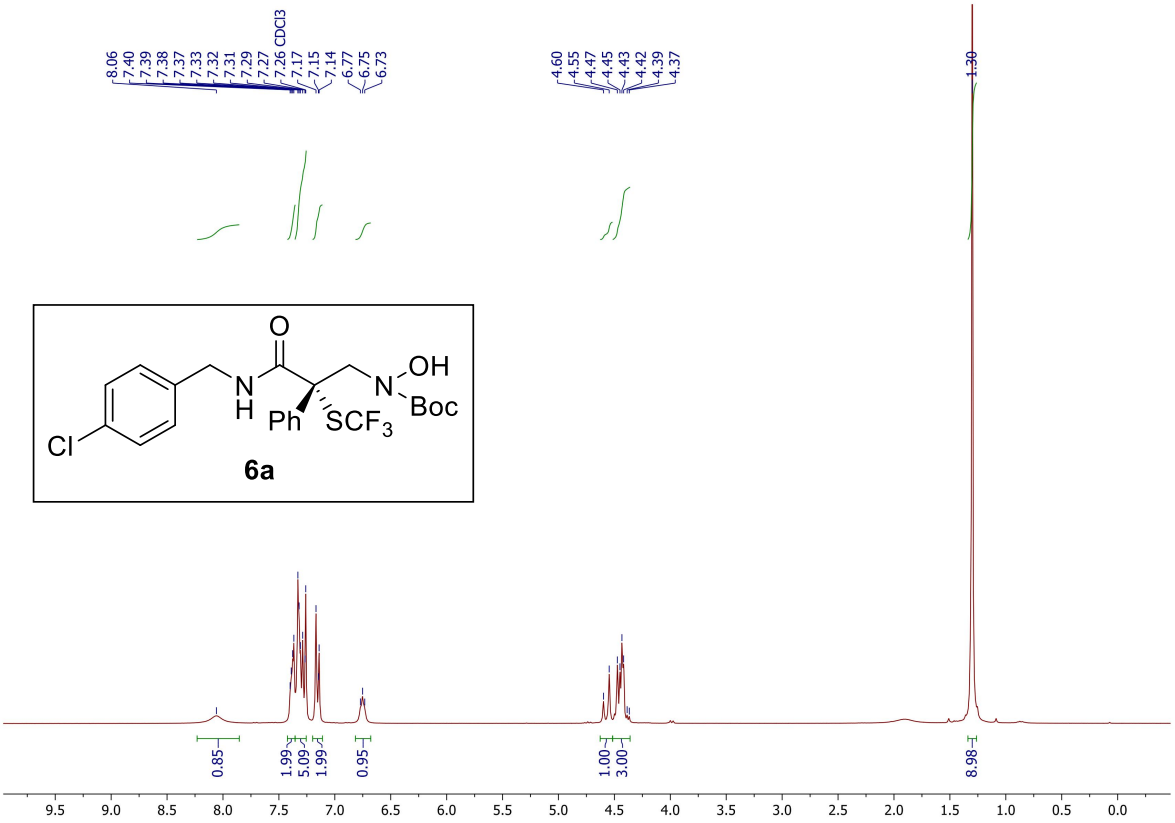
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H
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Boc
Ph
SCF3
Cl
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0.85 1.99 5.09 1.99 0.95 1.00 3.00 8.98
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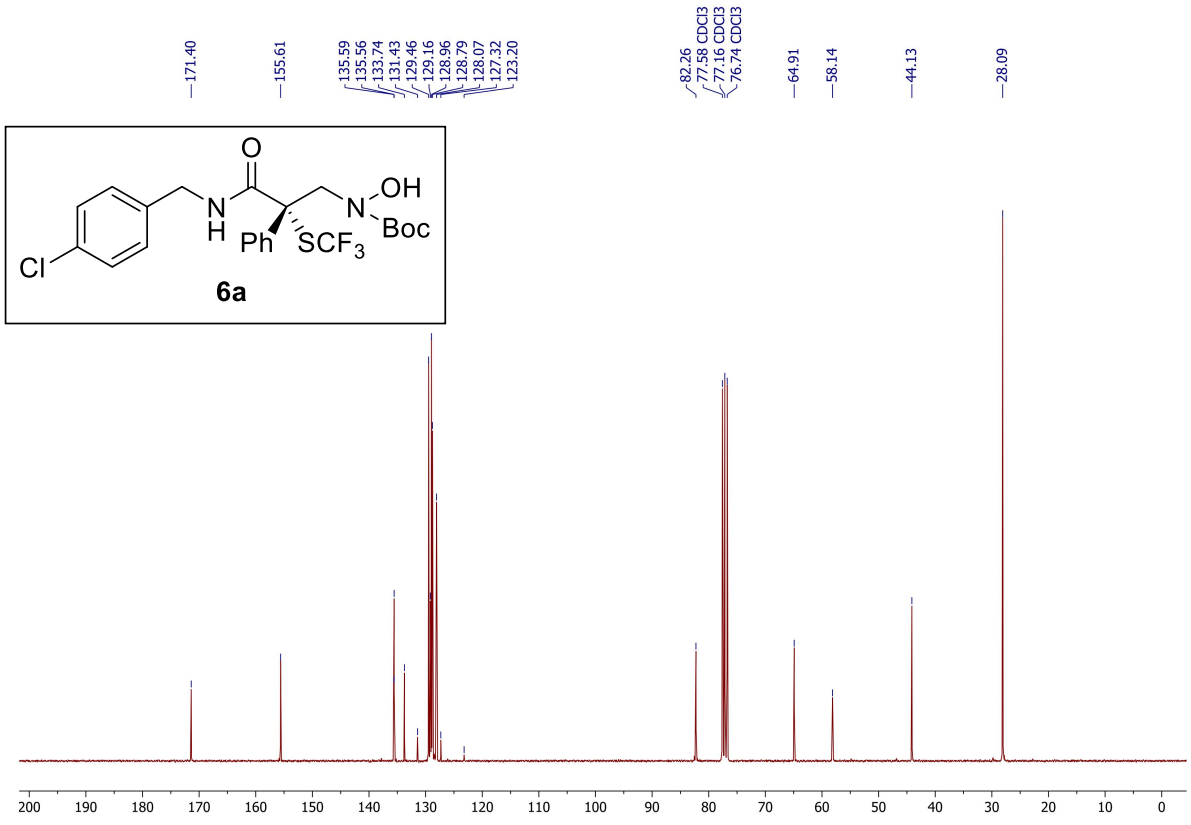
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77.16 CDCl3
76.74 CDCl3
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SCF3
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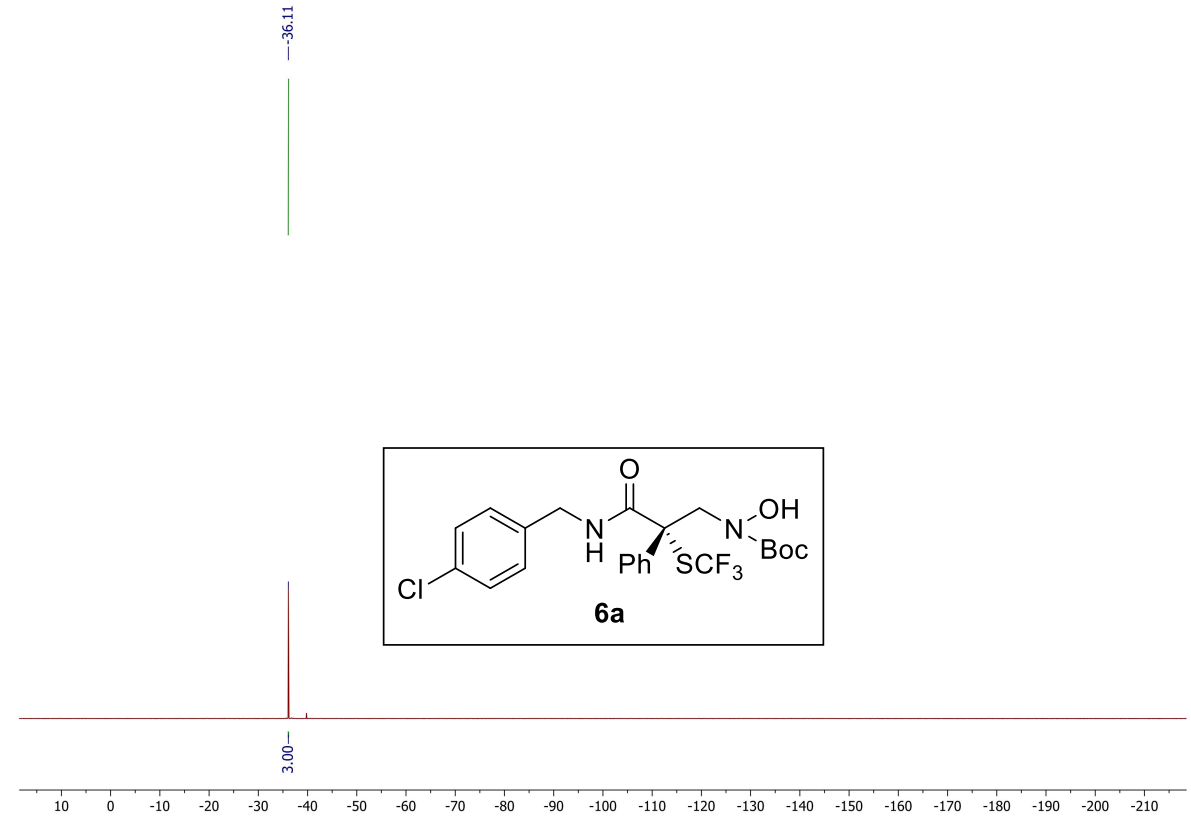
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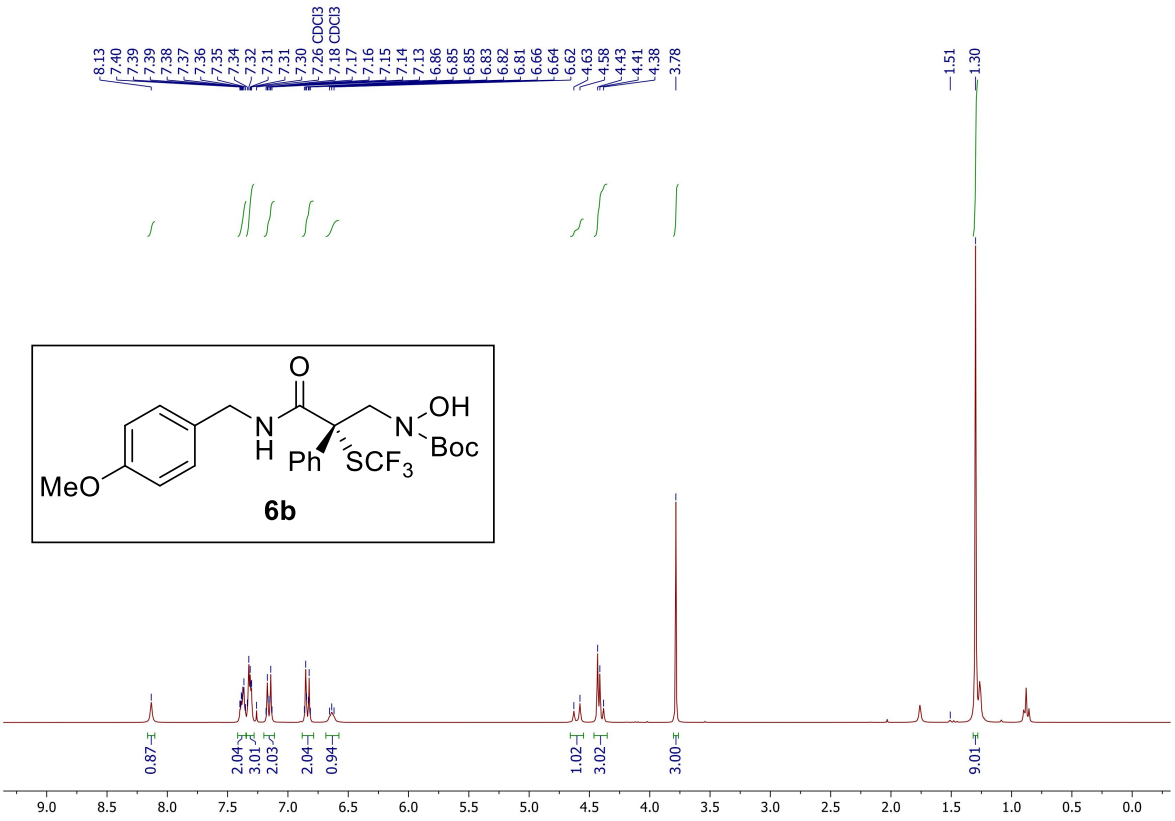
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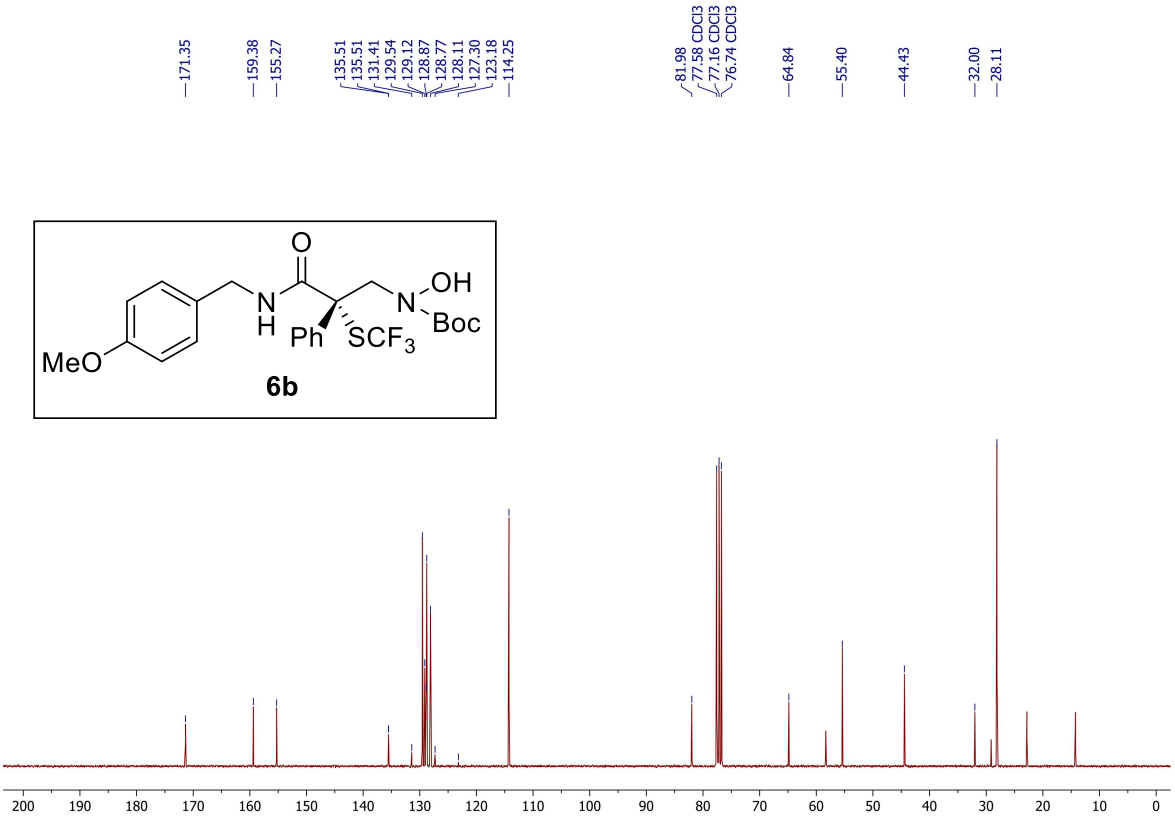
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81.98
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77.16 CDCl3
76.74 CDCl3
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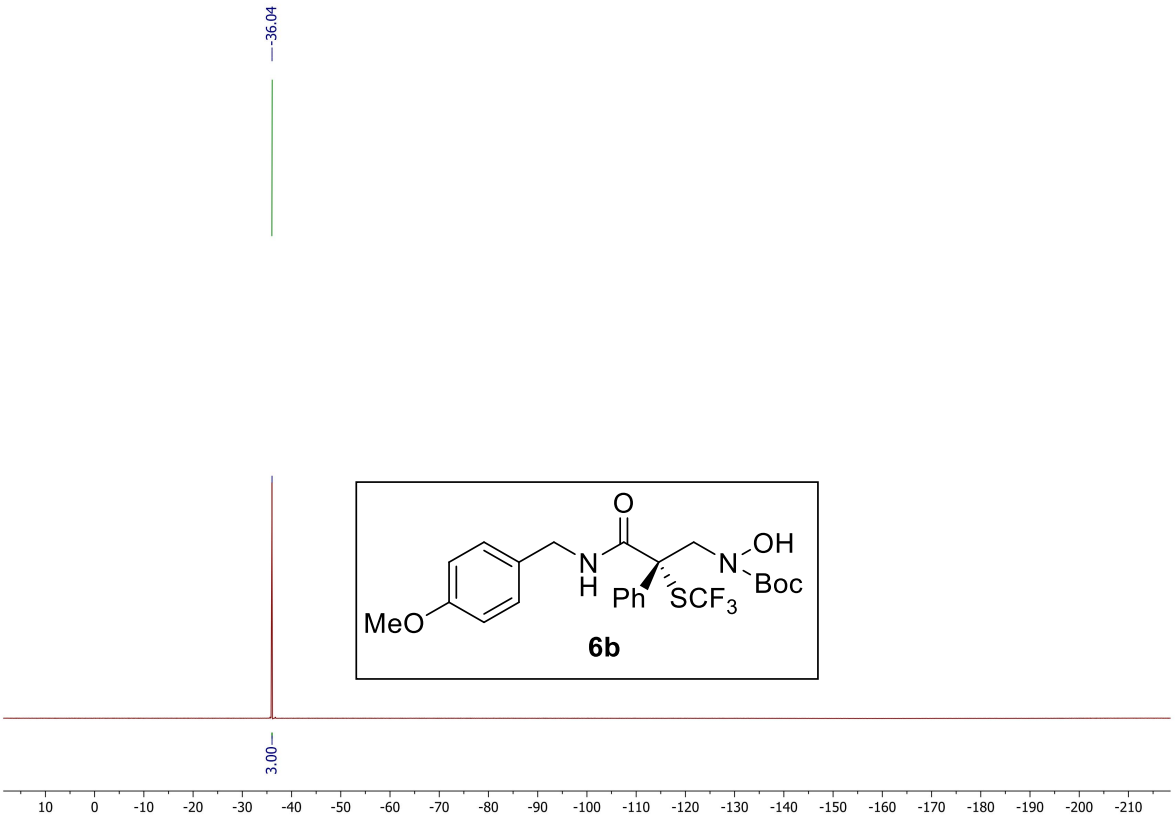
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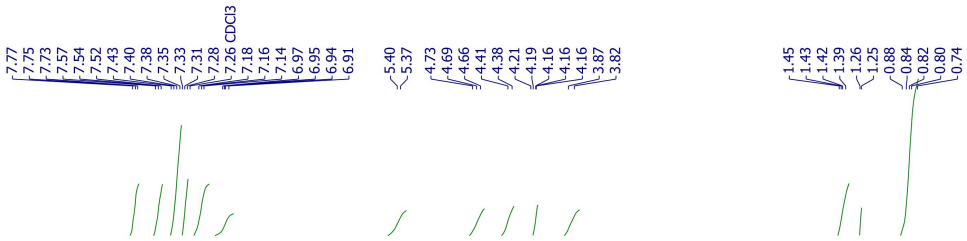
OH
N
Boc
Ph
SCF3
MeO

6b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5.40 5.37 4.73 4.69 4.66 4.41 4.38 4.21 4.19 4.16 4.16 4.16 3.87 3.82
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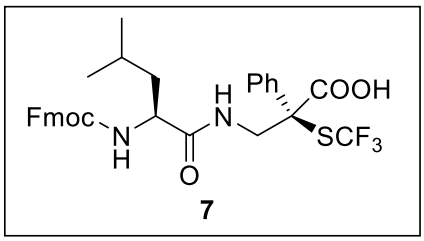
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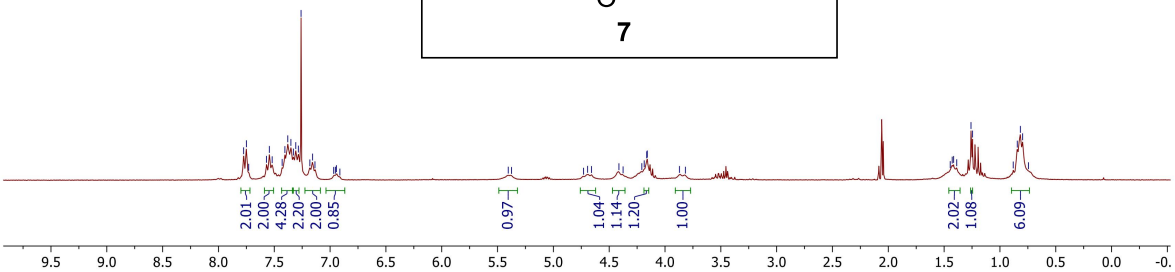
7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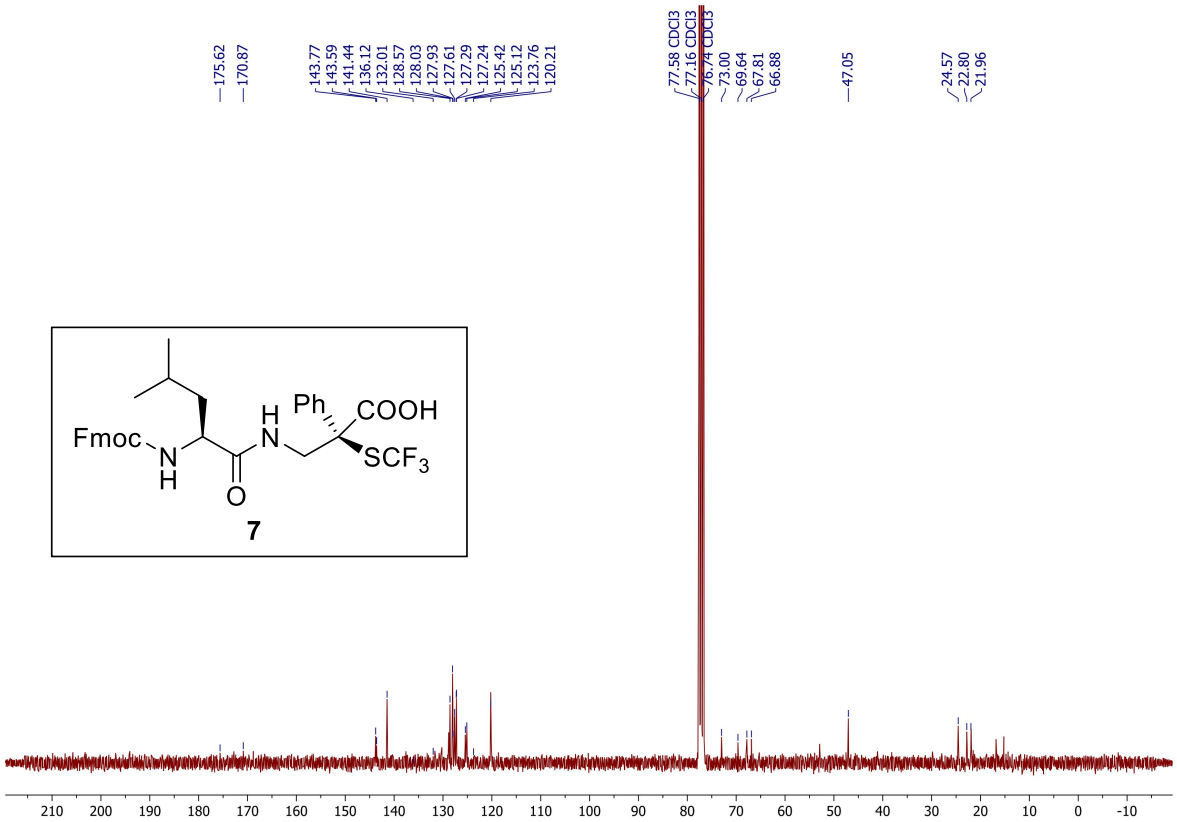
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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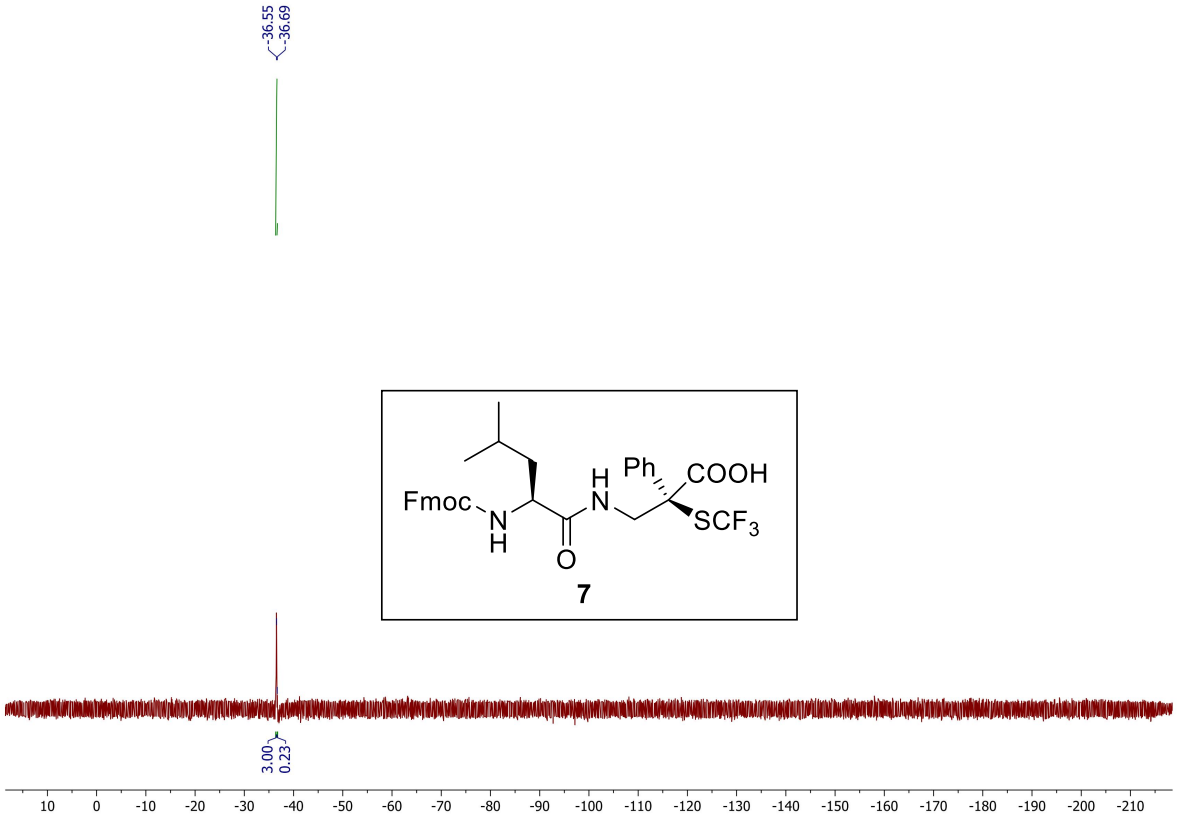
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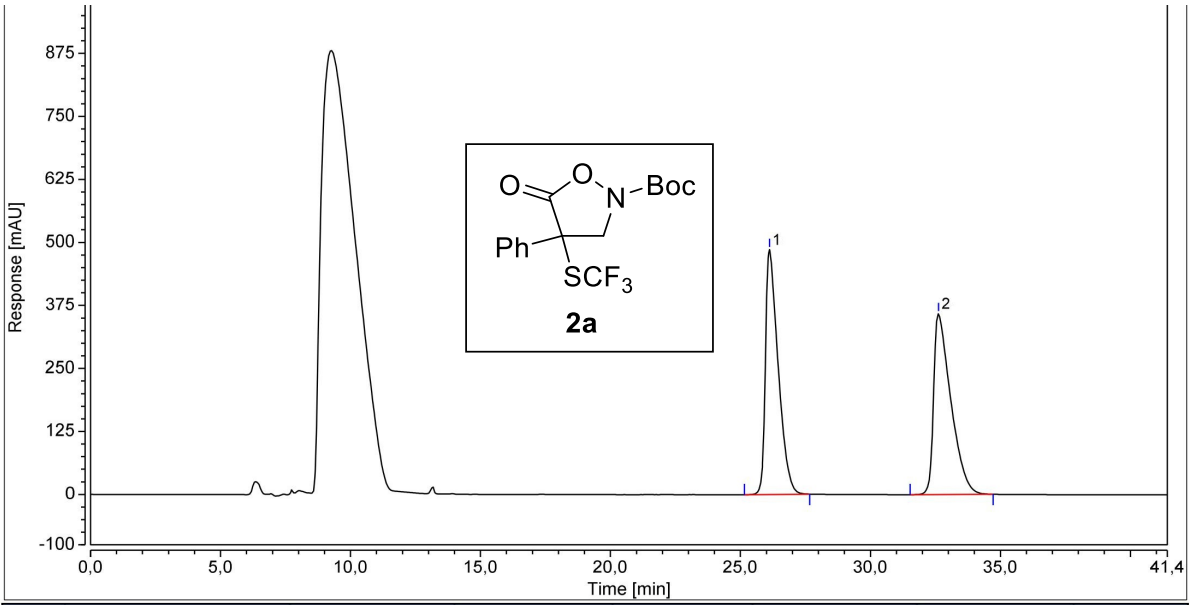
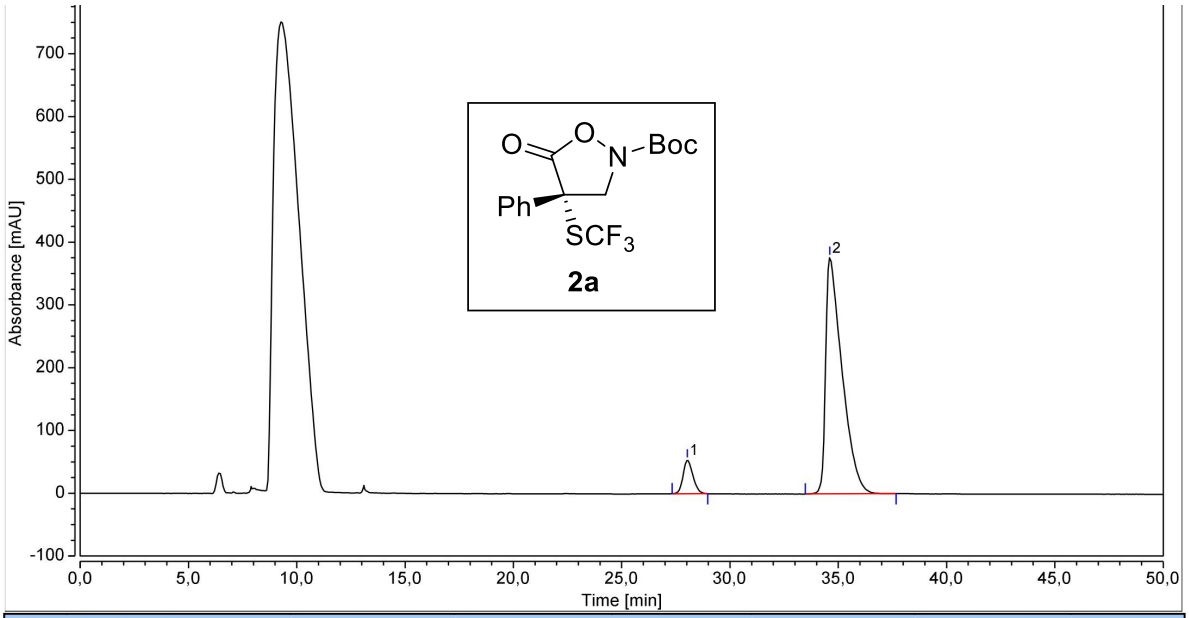
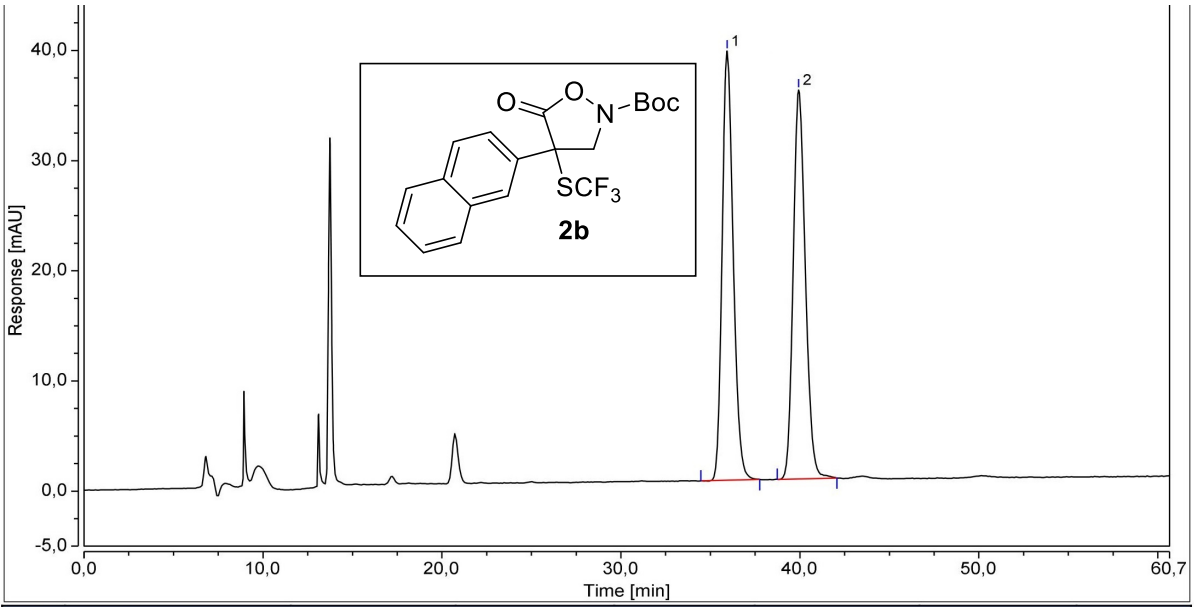
6. Copies of HPLC Chromatograms



Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		26,117	275,069	485,909	49,99	57,52	n.a.
2		32,617	275,158	358,824	50,01	42,48	n.a.
Total:			**550,227**	**844,733**	**100,00**	**100,00**	

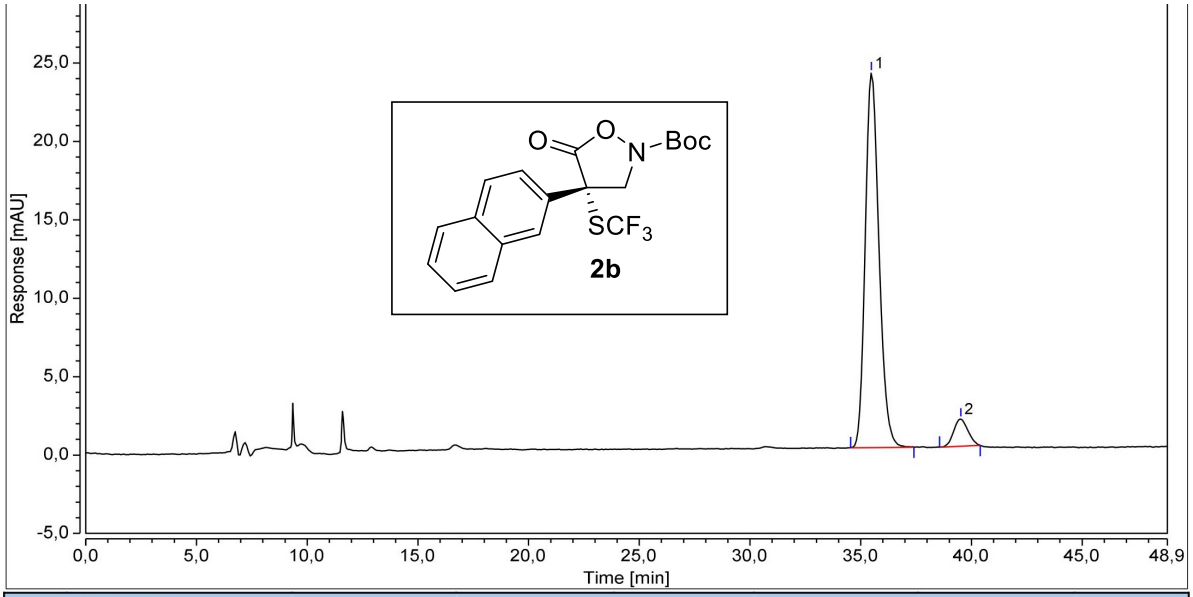


Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		28,033	28,277	53,558	7,90	12,46	n.a.
2		34,610	329,642	376,401	92,10	87,54	n.a.
Total:			**357,919**	**429,959**	**100,00**	**100,00**	



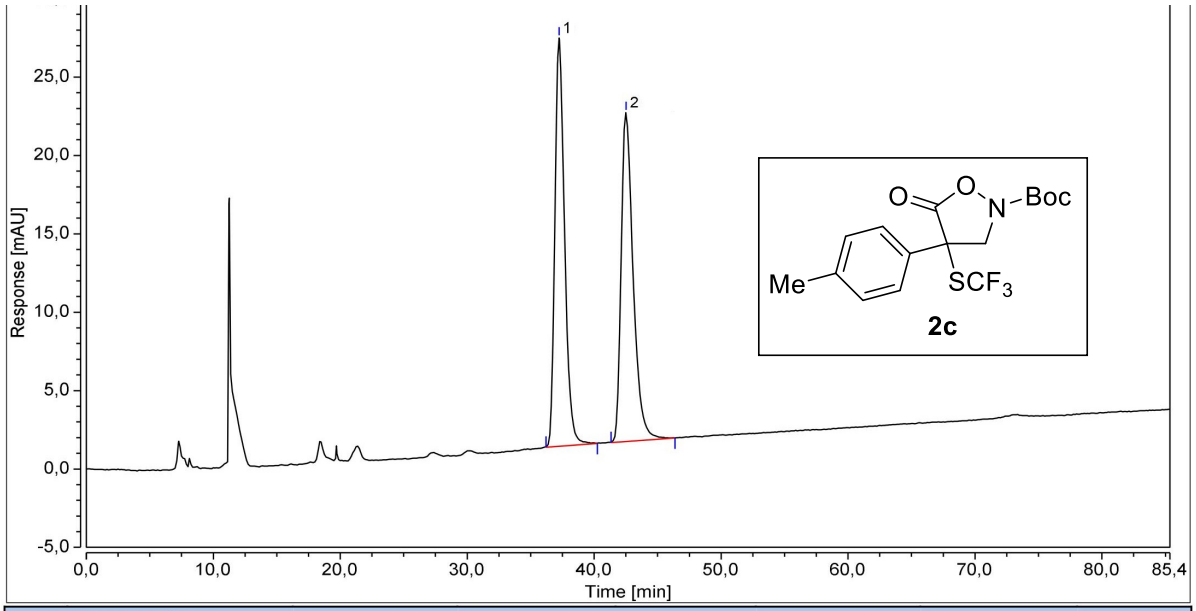
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		35,933	27,774	38,968	49,99	52,47	n.a.
2		39,933	27,783	35,304	50,01	47,53	n.a.
Total:			**55,557**	**74,272**	**100,00**	**100,00**	

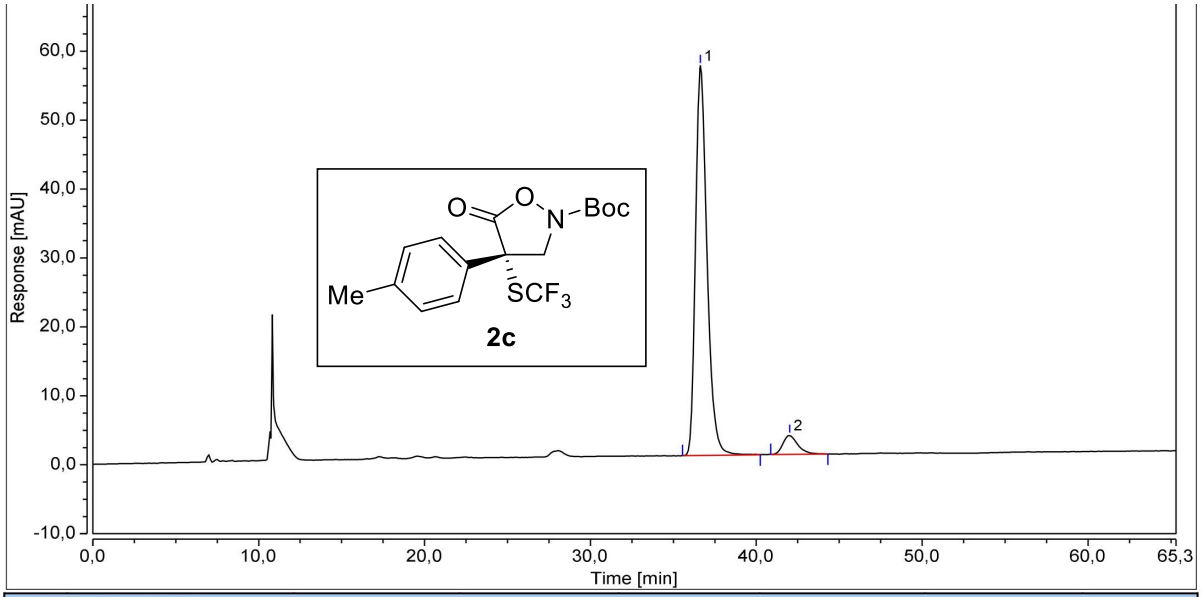


Integration Results

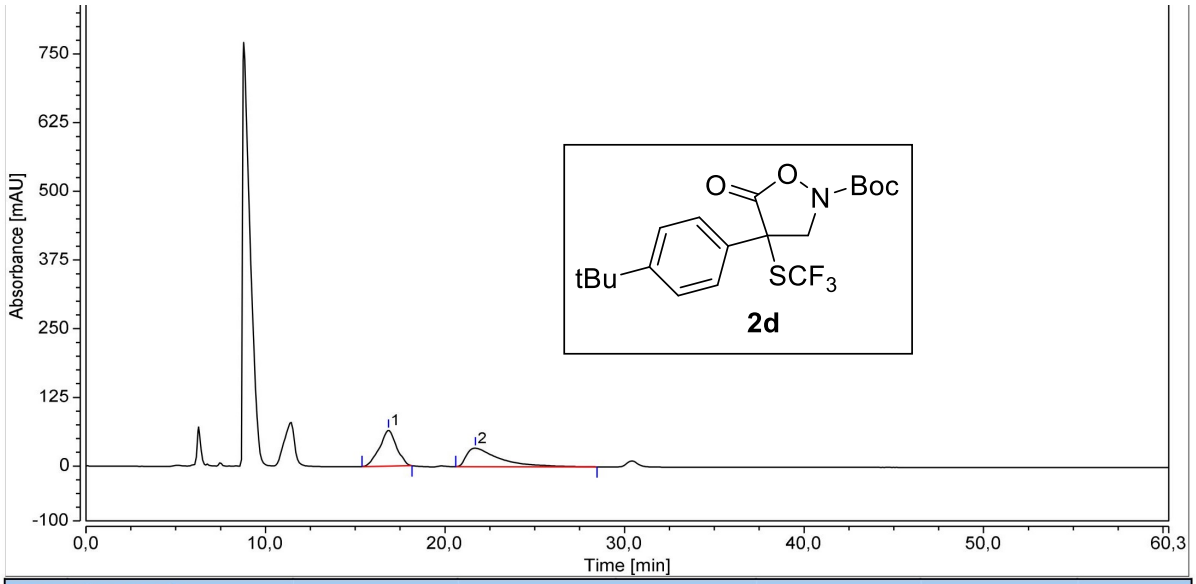
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		35,483	17,172	23,894	92,97	93,23	n.a.
2		39,525	1,298	1,736	7,03	6,77	n.a.
Total:			**18,471**	**25,630**	**100,00**	**100,00**	



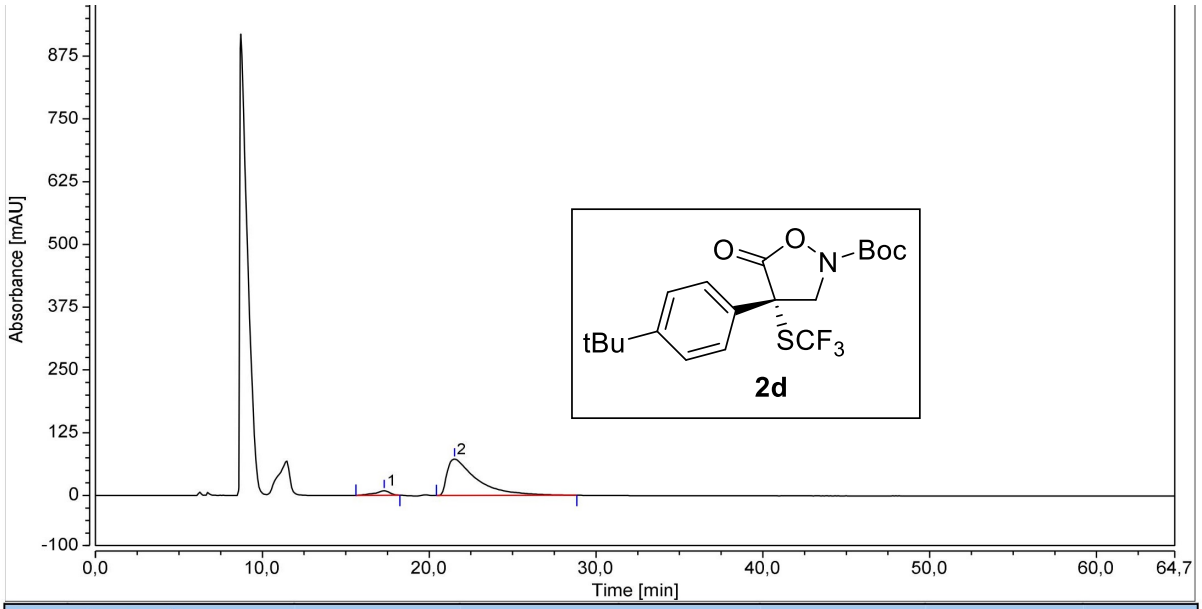
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		37,233	23,045	26,044	50,05	55,38	n.a.
2		42,508	23,003	20,981	49,95	44,62	n.a.
Total:			**46,048**	**47,025**	**100,00**	**100,00**	



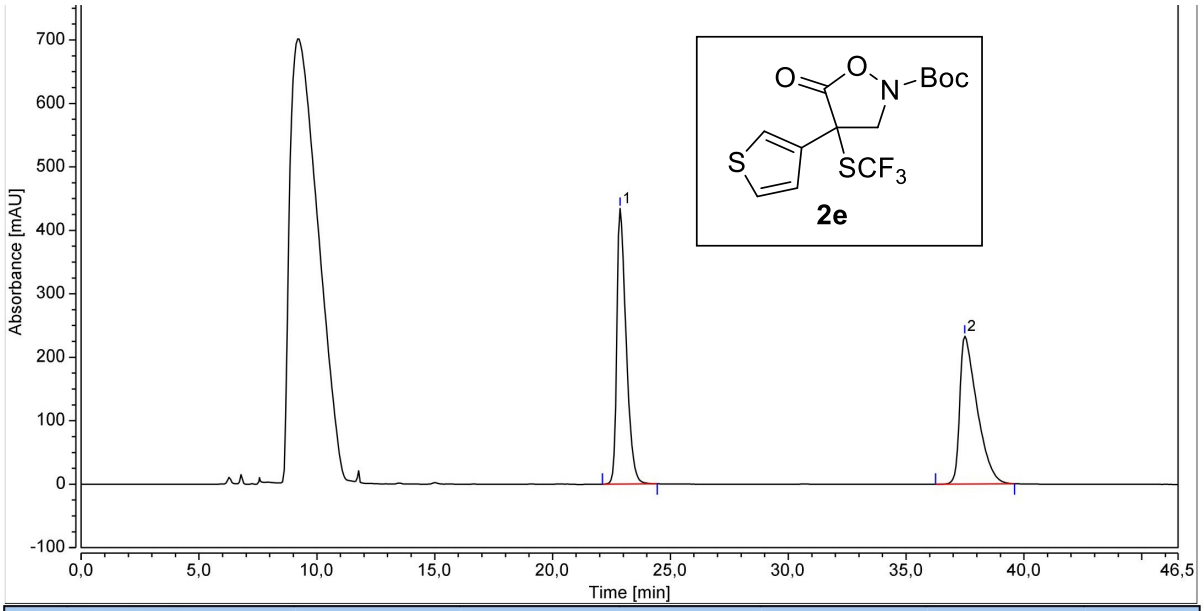
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		36,633	45,519	56,504	93,98	95,37	n.a.
2		42,017	2,914	2,742	6,02	4,63	n.a.
Total:			**48,433**	**59,245**	**100,00**	**100,00**	



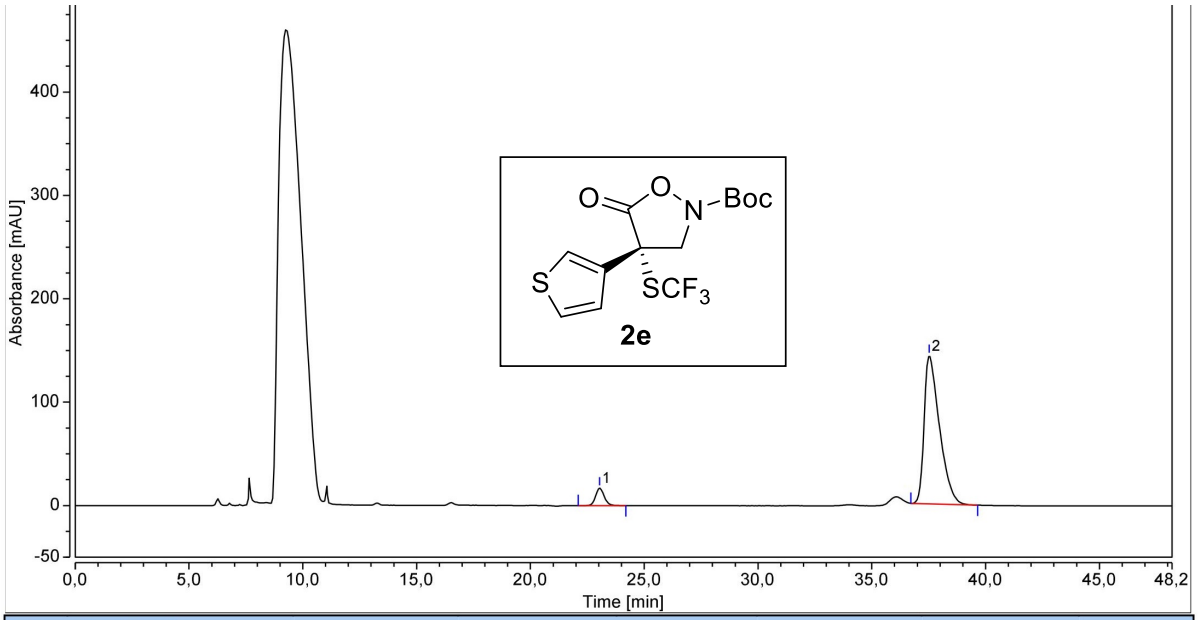
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		16,847	71,813	65,179	50,17	65,91	n.a.
2		21,690	71,341	33,715	49,83	34,09	n.a.
Total:			**143,154**	**98,894**	**100,00**	**100,00**	



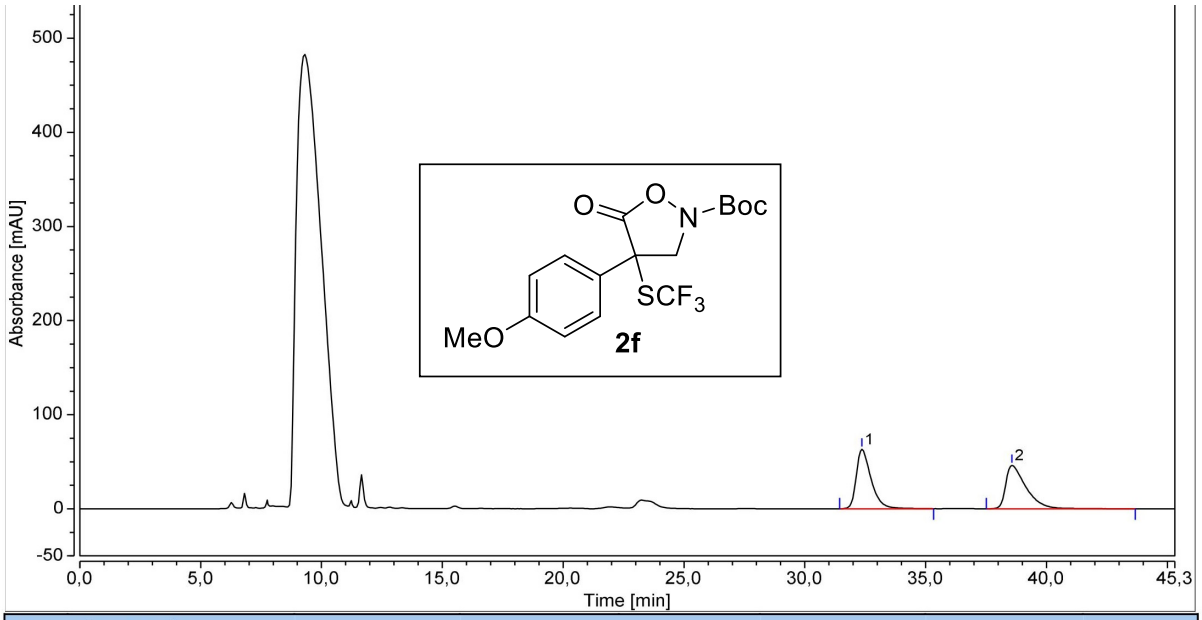
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		17,310	9,378	9,030	5,89	11,04	n.a.
2		21,513	149,853	72,731	94,11	88,96	n.a.
Total:			**159,231**	**81,761**	**100,00**	**100,00**	



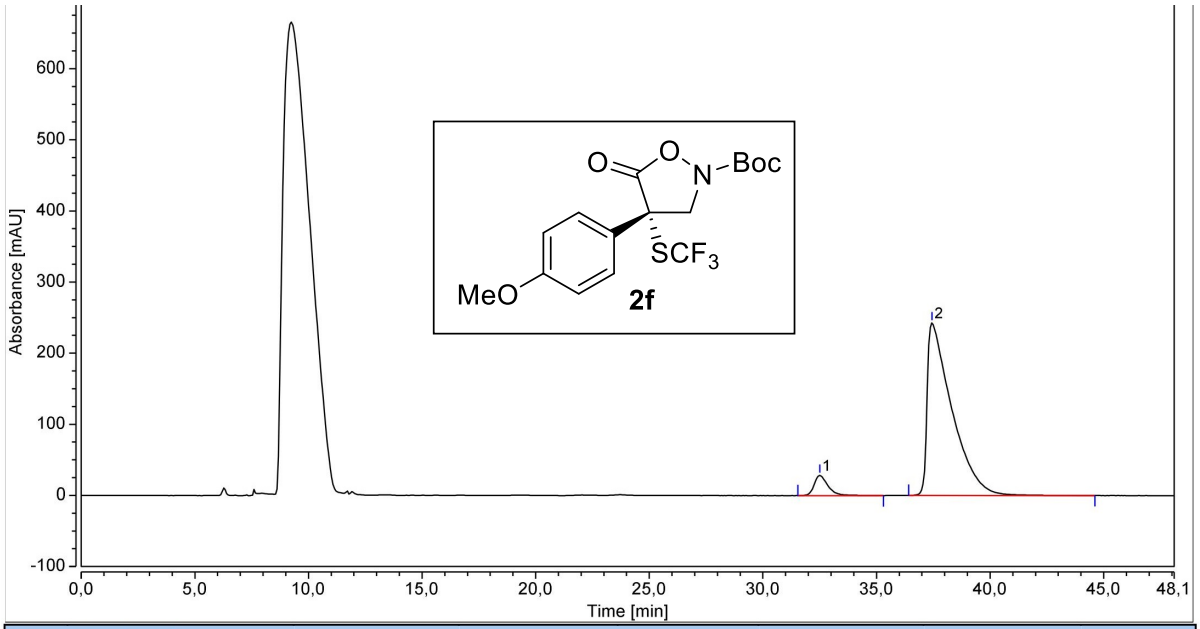
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		22,867	198,843	434,354	50,08	65,08	n.a.
2		37,490	198,228	233,104	49,92	34,92	n.a.
Total:			**397,071**	**667,459**	**100,00**	**100,00**	



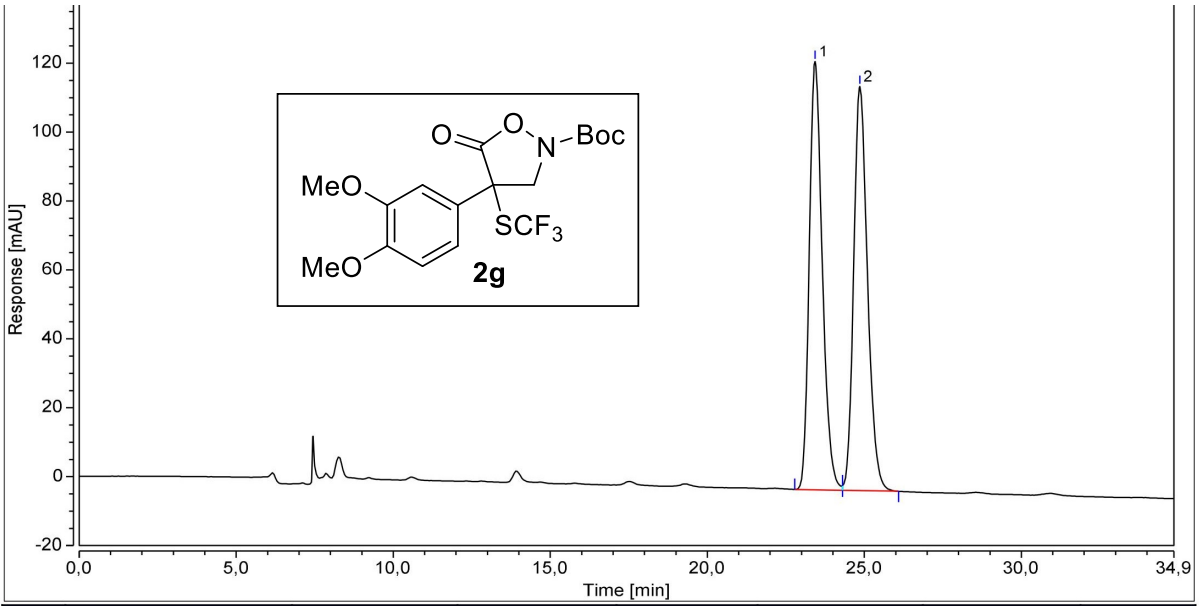
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		23,040	7,481	17,009	6,26	10,60	n.a.
2		37,523	112,073	143,502	93,74	89,40	n.a.
Total:			**119,554**	**160,510**	**100,00**	**100,00**	



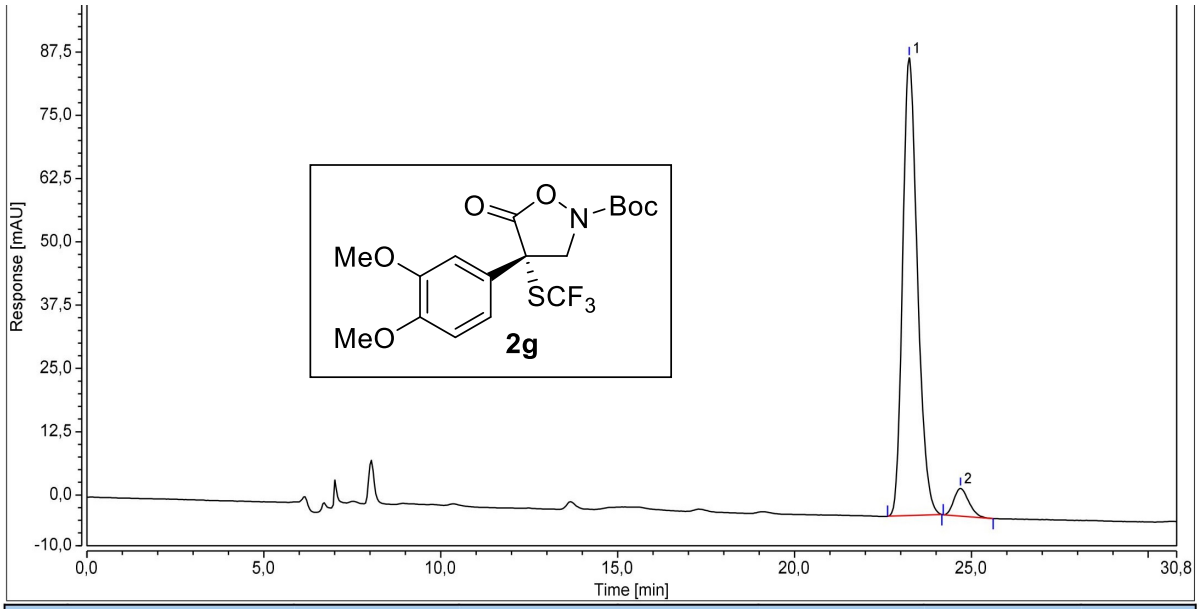
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		32,360	45,002	63,178	49,89	57,78	n.a.
2		38,570	45,194	46,165	50,11	42,22	n.a.
Total:			**90,196**	**109,344**	**100,00**	**100,00**	



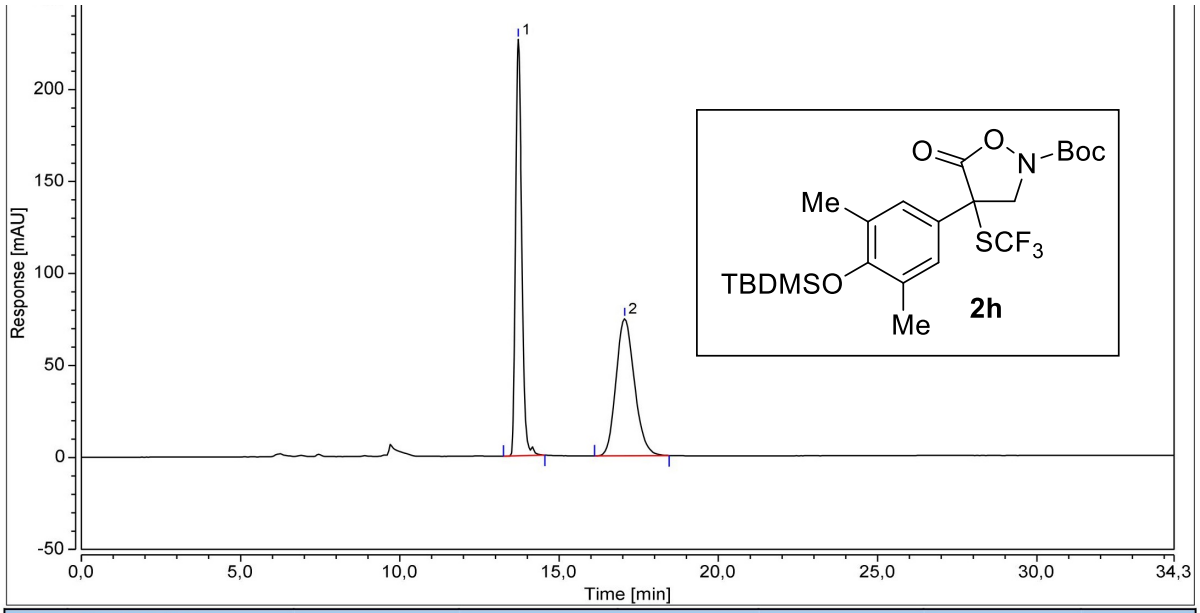
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		32,500	20,103	28,245	6,18	10,43	n.a.
2		37,440	305,080	242,617	93,82	89,57	n.a.
Total:			**325,183**	**270,862**	**100,00**	**100,00**	



Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		23,433	59,555	124,269	49,93	51,45	n.a.
2		24,858	59,724	117,270	50,07	48,55	n.a.
Total:			**119,279**	**241,538**	**100,00**	**100,00**	

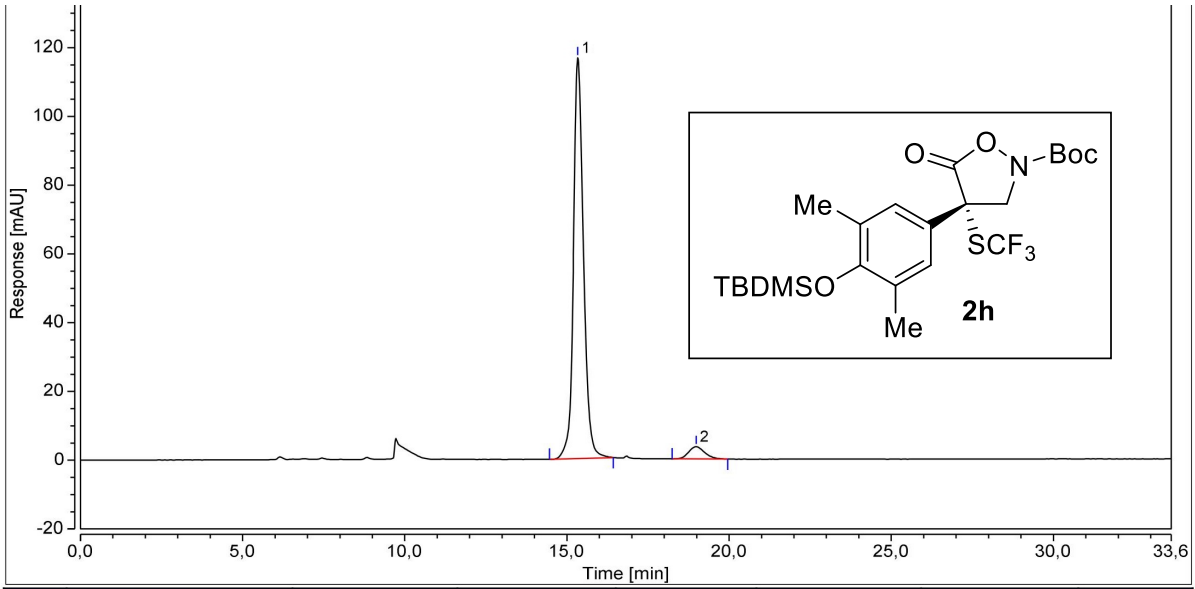


Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		23,242	43,831	90,423	94,23	94,28	n.a.
2		24,692	2,682	5,491	5,77	5,72	n.a.
Total:			**46,513**	**95,914**	**100,00**	**100,00**	



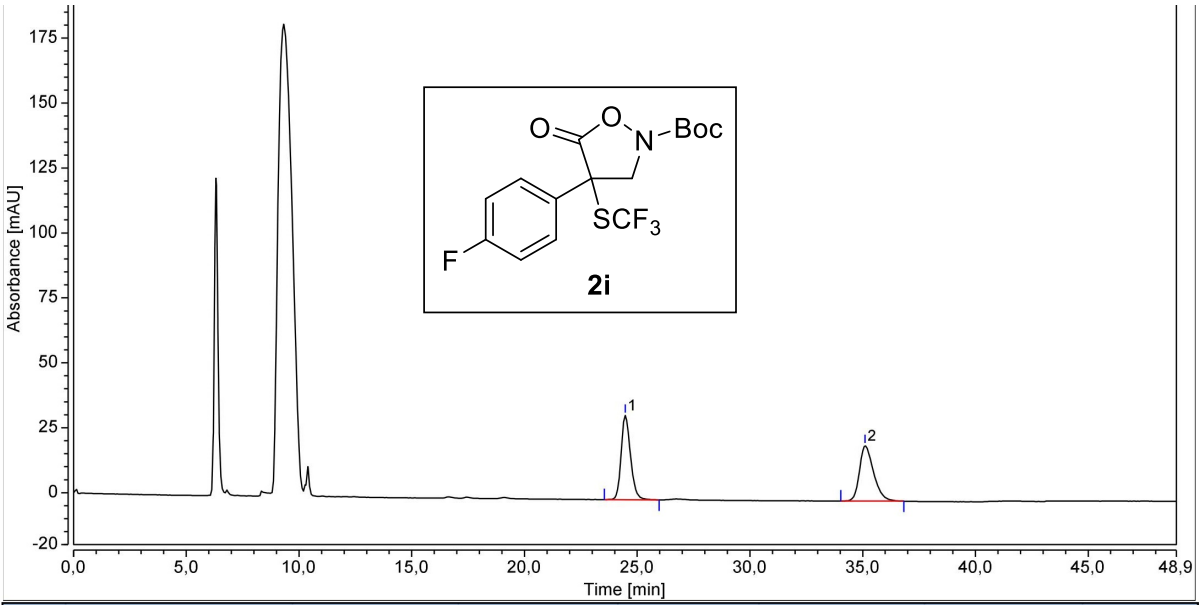
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		13,717	50,382	226,314	50,21	75,23	n.a.
2		17,058	49,970	74,531	49,79	24,77	n.a.
Total:			**100,352**	**300,846**	**100,00**	**100,00**	

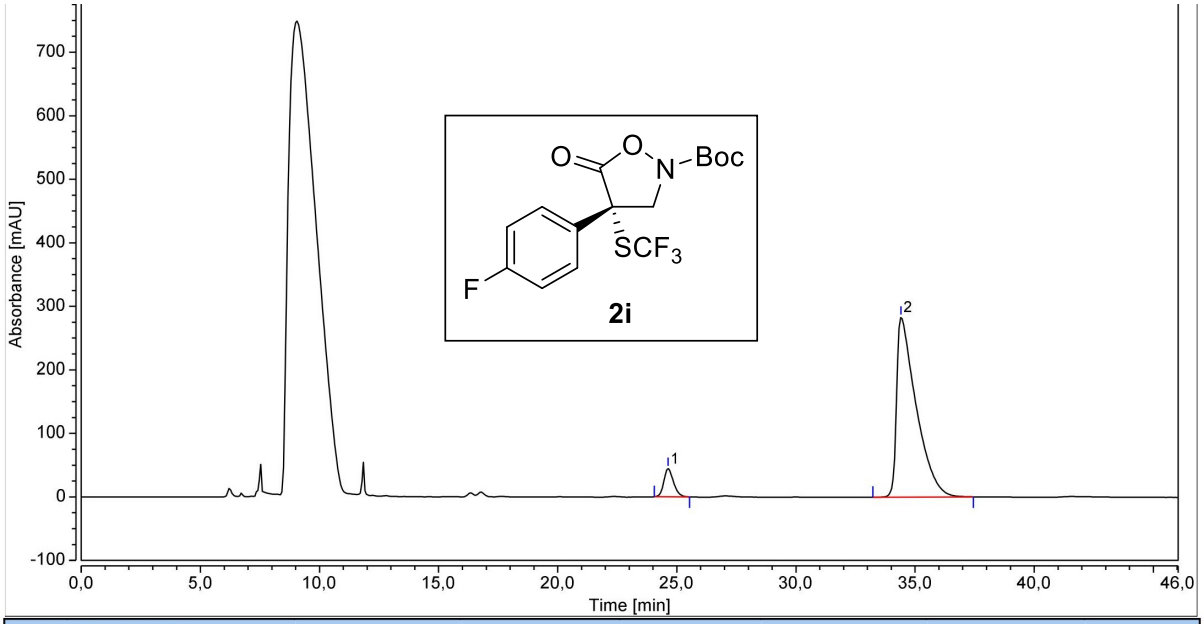


Integration Results

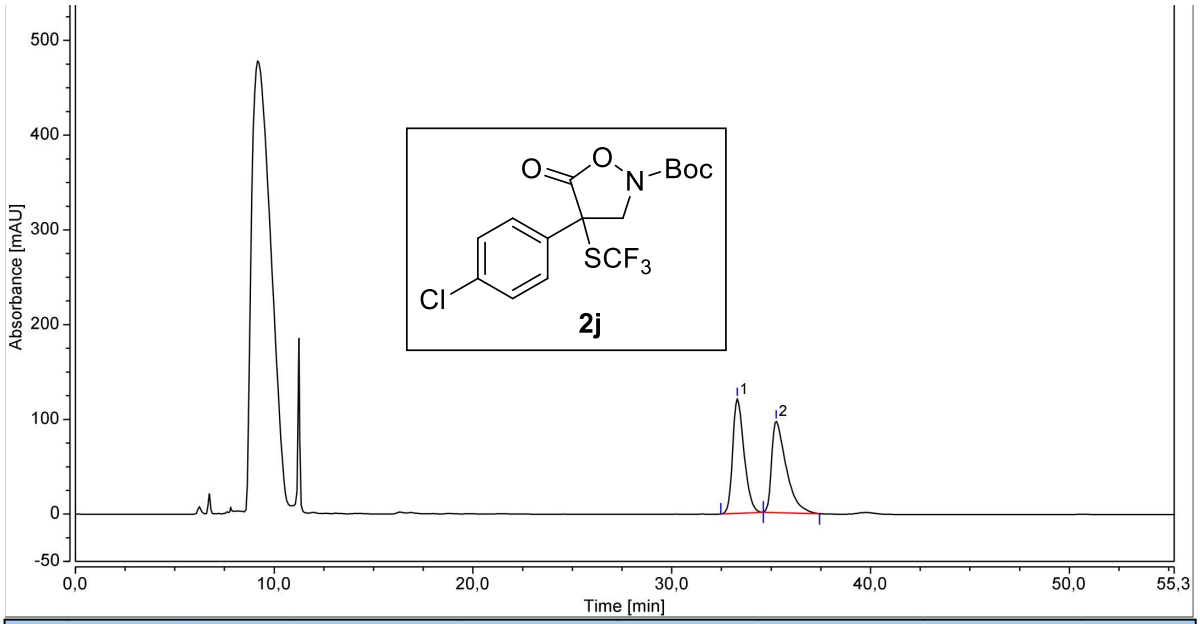
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		15,333	41,595	116,572	95,32	97,04	n.a.
2		18,983	2,041	3,550	4,68	2,96	n.a.
Total:			**43,636**	**120,122**	**100,00**	**100,00**	



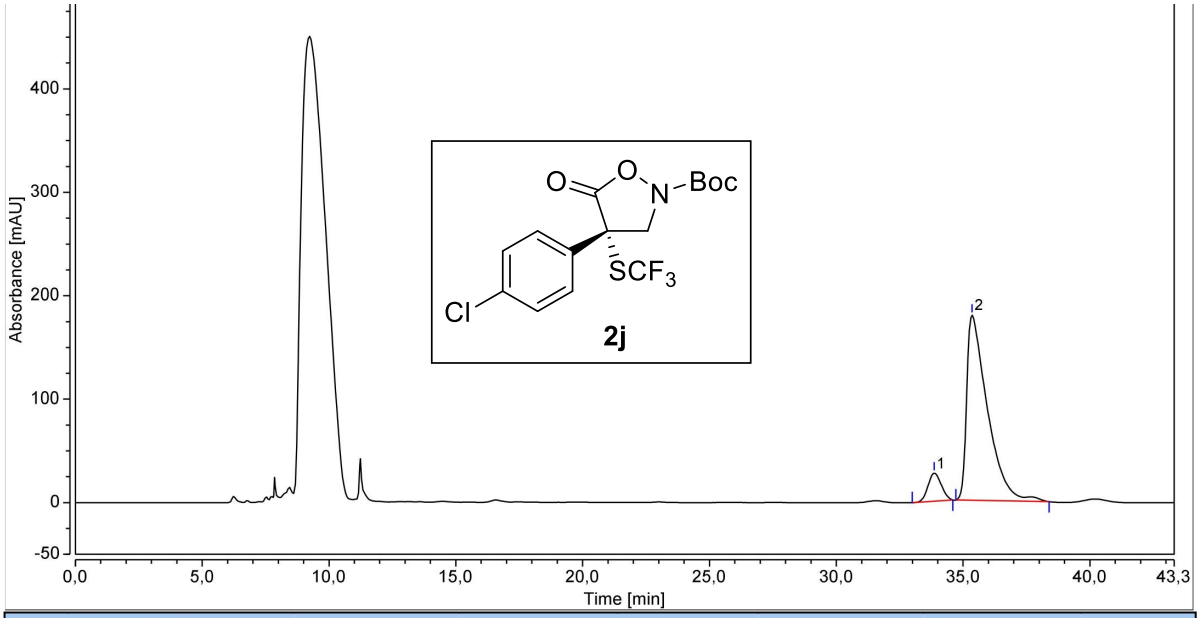
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		24,470	15,651	32,486	50,30	60,38	n.a.
2		35,107	15,466	21,314	49,70	39,62	n.a.
Total:			**31,116**	**53,800**	**100,00**	**100,00**	



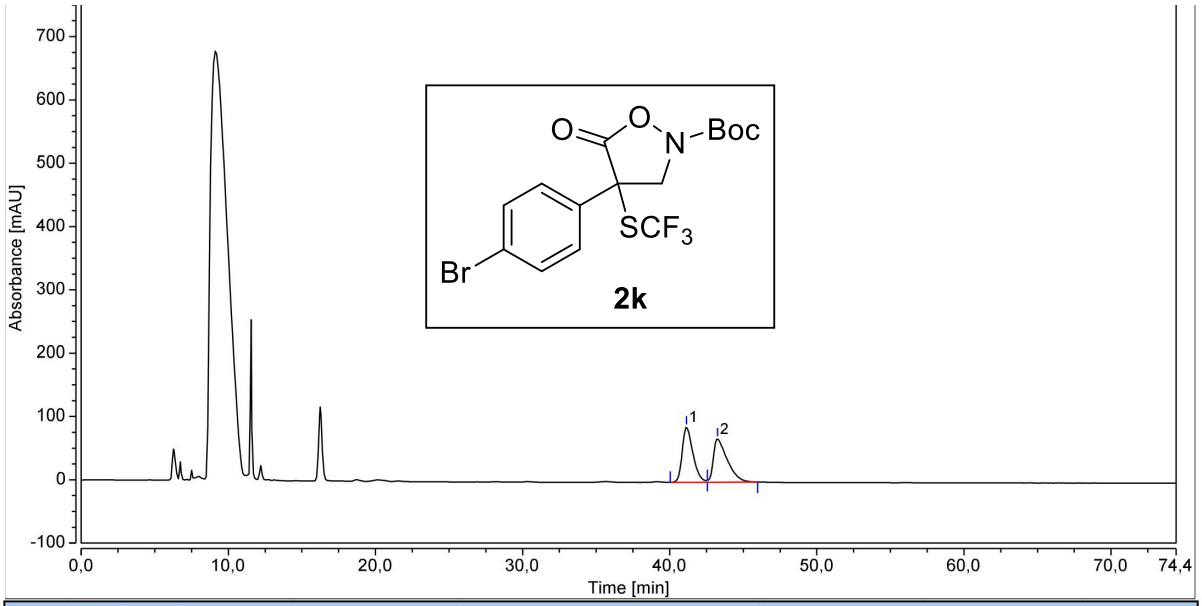
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		24,627	20,978	44,372	7,23	13,54	n.a.
2		34,410	269,288	283,401	92,77	86,46	n.a.
Total:			**290,266**	**327,774**	**100,00**	**100,00**	



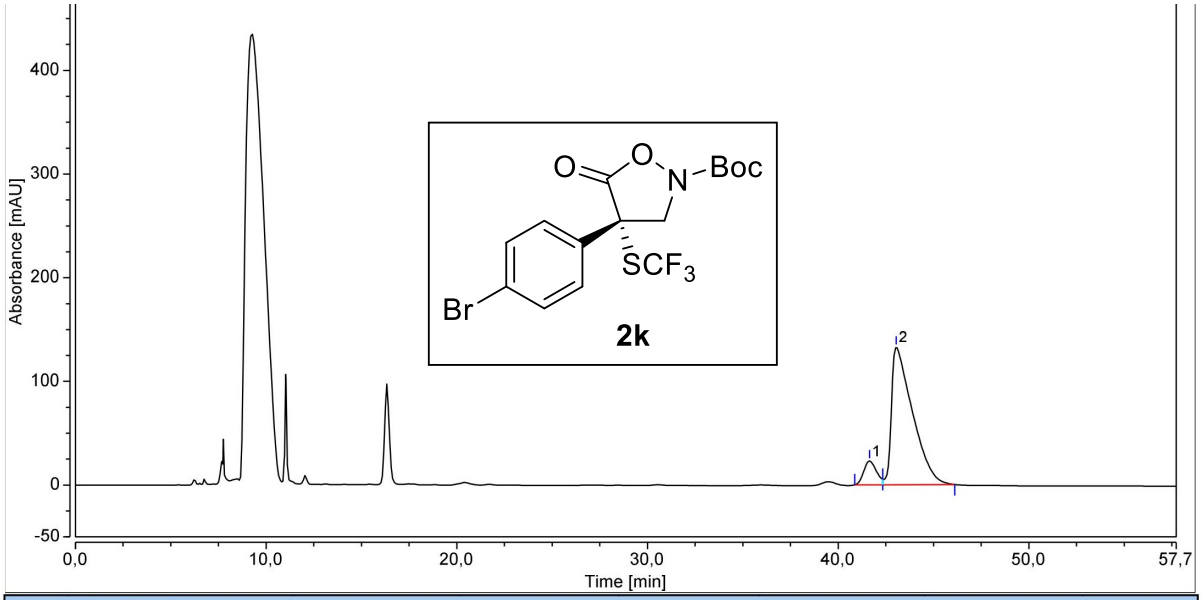
Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		33,293	80,250	120,880	49,53	55,61	n.a.
2		35,250	81,779	96,490	50,47	44,39	n.a.
Total:			**162,029**	**217,370**	**100,00**	**100,00**	



Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		33,860	16,538	27,140	8,88	13,16	n.a.
2		35,350	169,644	179,159	91,12	86,84	n.a.
Total:			**186,183**	**206,299**	**100,00**	**100,00**	



Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		41,133	73,917	87,240	49,66	56,07	n.a.
2		43,243	74,925	68,364	50,34	43,93	n.a.
Total:			**148,843**	**155,603**	**100,00**	**100,00**	



Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		41,650	17,647	22,936	9,41	14,73	n.a.
2		43,047	169,868	132,787	90,59	85,27	n.a.
Total:			**187,515**	**155,724**	**100,00**	**100,00**	