Supporting Information for:

Iron-catalyzed kinetic resolution of *N*-sulfonyl oxaziridines

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I. General Information

All oxaziridine substrates were stored at 0 ºC and warmed to room temperature immediately prior to use. The syntheses of ligand **6g**,[1] 2-((4-nitrophenyl)sulfonyl)-3-phenyl oxaziridine[2] *N*-(4-methylphenyl)sulfonyl-3-phenyl oxaziridine, [3] *N*-phenylsulfonyl-3-phenyloxaziridine, [4] *N*-phenylsulfonyl-3-(4-nitrophenyl) oxaziridine,[5] *N*-*tert*-butylsulfonyl-3-phenyl oxaziridine,[6] and 2-isopropyl-3-phenyloxaziridine[7]were conducted as previously described, and all spectroscopic data were consistent with those previously reported for these compounds. Toluene, dichloromethane, acetonitrile, and tetrahydrofuran were purified by elution through alumina as described by Grubbs.[8] Dichloroethane was distilled from calcium hydride immediately before use. Aldehydes were distilled prior to use when applicable. All other commercially available reagents were purchased from Aldrich and used without further purification. Flash chromatography was performed with Purasil 60 Å silica gel (230–400 mesh) using the method of Still.[9] All glassware was oven-dried for at least 1 h prior to use.

^{1}H and ^{13}C NMR data were obtained using Varian Inova-500 and Varian Unity-500 spectrometers. ^{1}H NMR spectra were internally referenced to TMS (0.00 ppm); ^{13}C NMR spectra were internally referenced to $CDCl_3$ (77.23 ppm). The NMR facilites at UW-Madison are supported by the NSF (CHE-9629688, CHE-8813550, CHE-9629688) and NIH (1 S10 RR0 4981-10). IR spectral data were obtained using a Bruker ALPHA FT-IR spectrometer (Platinum ATR). Melting points were obtained using a Mel-Temp II (Laboratory Devices, Inc., USA) melting point apparatus. Mass spectrometry was performed with a Micromass LCT (electrospray ionization, time-of-flight analyzer). Mass spectrometry facilities are supported by the NSF (CHE-9304546 and CHE-9974839) and the University of Wisconsin. Enantiomeric ratios were determined by supercritical fluid (SFC) chromatography on a TharSFC investigator instrument equipped with a Waters 2996 photodiode array detector, using chiral columns and methods as noted. Optical rotations were obtained using a Rudolph Autopol III polarimeter. Selectivity factors (*s*) were calculated as described by Kagan.[10] The absolute configurations of

N-(4-methylphenyl)sulfonyl-3-phenyl oxaziridine and *N*-phenylsulfonyl-3-phenyloxaziridine were assigned by correlation to known optical rotations reported by Jørgensen[11] and Torre[12] respectively. All other absolute configurations were assigned by analogy.

II. Racemic Oxaziridine Syntheses

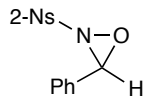
General Procedure 1: Based upon a modification of the procedure originally reported by Davis.[13] Aldehyde (1.2 equiv) and sulfonamide (1 equiv) were dissolved in 1,2-dichloroethane (0.16 M) in a round-bottomed flask containing a stir bar. The flask was fitted with a septum, flushed with N_2, and the solution cooled to 0 °C (ice bath). $TiCl_4$ (1.45 equiv) was then added dropwise over 15 min. The flask was fitted with a reflux condenser, charged with N_2 and heated at reflux for 12 h. The reaction was then cooled to 0 °C, and 10% K_2CO_3 (80% reaction volume) was added with rapid stirring. The solution was transferred to an Erlenmeyer flask. CH_2Cl_2 (60% reaction volume) and water (reaction volume) were then added, and the solution was stirred vigorously to produce a fine white suspension. The mixture was filtered through Celite®, and the layers were separated. The organic layer was washed once with saturated $NaHCO_3$ (40% reaction volume) and the combined aqueous layers were extracted twice with CH_2Cl_2 (40% reaction volume). The organic layer was dried over Na_2SO_4 and concentrated on a rotary evaporator to give the crude imine, which was used without further purification.

In an Erlenmeyer flask equipped with a mechanical stirrer, a solution of the unpurified imine (1.0 equiv, 0.1 M) in toluene was combined with an aqueous solution of K_2CO_3 (7.0 equiv, 1.4 M). An aqueous solution of Oxone® (1.9 equiv, 0.2 M) was then added with vigorous stirring. If after 1 h the reaction had not reached completion, the aqueous layer was removed by siphon and a fresh solution of K_2CO_3 (8.5 equiv, 1.0 M) was added to the Erlenmeyer flask along with a solution of Oxone® (1.6 equiv, 0.2 M). Upon completion of the reaction, the organic and aqueous layers were separated. The aqueous layer was extracted twice with toluene. The combined organic layers were washed with a 5% solution of Na_2SO_3. The organic layer was dried over Na_2SO_4 and concentrated. The resulting solid was recrystallized from EtOAc/hexanes or purified by flash column chromatography to yield the title compound.

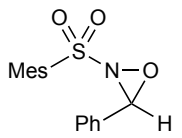
General Procedure 2: Based upon a modification of the procedure originally reported by Davis.[13] Aldehyde (1.3 equiv) and sulfonamide (1 equiv) were dissolved in toluene (0.5 M) in a round-bottomed flask containing flame-dried molecular sieves (4Å, 1 equiv. by weight), Amberlyst® 15 exchange resin (0.016 equiv. by weight), stir bar. The flask was fitted with a Dean–Stark trap and a reflux condenser, flushed with N_2 and heated at reflux for 16 h. The reaction was then cooled to room temperature, and the mixture was filtered through Celite®. The mixture was concentrated on a rotary evaporator to give the crude imine, which was used without further purification.

In an Erlenmeyer flask equipped with a mechanical stirrer; a solution of the unpurified imine (1.0 equiv, 0.1 M) in toluene was combined with an aqueous solution of K_2CO_3 (7.0 equiv, 1.4 M). An aqueous solution of Oxone® (1.9 equiv, 0.2 M) was then added with vigorous stirring. If after 1 h the reaction had not reached completion, the aqueous layer was removed by siphon and a fresh solution of K_2CO_3 (8.5 equiv, 1.0 M) was added to the Erlenmeyer flask along with a solution of Oxone® (1.6 equiv, 0.2 M). Upon completion of the reaction, the organic and aqueous layers were separated. The aqueous layer was extracted twice with toluene. The combined organic layers were washed with a 5% solution of Na_2SO_3.

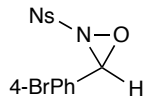
The organic layer was dried over Na_2SO_4 and concentrated. The resulting solid was recrystallized from EtOAc/hexanes or purified by flash column chromatography to yield the title compound.



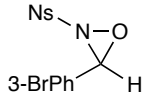
***N*-(2-Nitrophenyl)sulfonyl-3-(phenyl)oxaziridine.** Prepared according to general procedure 1 using 2.5 g 2-nitrobenzenesulfonamide (12.4 mmol) and 1.93 g benzaldehyde (1.85 mL, 16.1 mmol). The title compound was obtained after purification of the crude on silica gel using 30% EtOAc/hexanes as eluent. Yield: 2.62 g (8.6 mmol, 69% yield over two steps). IR (ATR) 3100, 1537, 1361, 1169; ^{1}H NMR: (500 MHz, $CDCl_3$) δ 8.30 (2-Ns**H**, d, J = 7.5 Hz, 1H), 7.83-7.90 (2-Ns**H**, m, 3H), 7.53 (Ph**H**, d, J = 7.7 Hz, 2H), 7.49 (Ph**H**, t, J = 7.5 Hz, 1H), 7.43 (Ph**H**, t, J = 7.5 Hz, 2H), 5.60 (2-Ns-N-C-H, s, 1H); ^{13}C NMR: (126 MHz, $CDCl_3$) δ 149.2, 136.1, 133.1, 132.7, 131.6, 129.9, 128.8, 128.3, 128.3, 125.0, 78.9; HRMS (ESI+) calcd for [$C_{13}H_{11}N_2O_5S$+] requires *m/z* 307.0384, found 307.0383. Isolated as a yellow solid (m.p. 71–75 ºC, decomp). (*Note: This compound was found to have a limited shelf life. Decomposition occurred within days of storage at 0 ºC*)



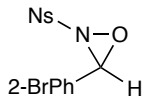
2-(Mesitylsulfonyl)-3-(phenyl)oxaziridine. Prepared according to general procedure 2 using 4.98 g 2,4,6-trimethylbenzenesulfonylamide (25.0 mmol) and 3.18 g benzaldehyde (3.06 mL, 30.0 mmol). The title compound was obtained after recrystallization of the crude with EtOAc/hexanes (1:5). Yield: 2.34 g (7.7 mmol, 31% yield over two steps). IR (ATR) 2981, 1602, 1458, 1336, 1161; ^{1}H NMR: (500 MHz, $CDCl_3$) δ 7.39-7.48 (Ph**H**, m, 5H), 7.04 (Mes**H**, s, 2H), 5.50 (S-N-C-**H**, s, 1H), 2.74 (Mes-C**H**, s, 6H), 2.35 (Mes-C**H**, s, 3H); ^{13}C NMR: (126 MHz, $CDCl_3$) δ 144.8, 142.0, 132.1, 131.3, 130.9, 129.5, 128.7, 128.3, 75.4, 23.2, 21.2; HRMS (ESI+) calcd for [$C_{16}H_{17}N_1O_3S_1N_1H_4$+] requires *m/z* 321.1268, found 321.1259. Isolated as a white solid (m.p. 106–107 ºC).



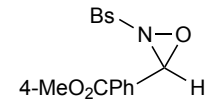
***N*-(4-Nitrophenyl)sulfonyl-3-(4-bromophenyl)oxaziridine.** Prepared according to general procedure 1 using 5.0 g 4-nitrobenzenesulfonamide (24.7 mmol) and 5.95 g 4-bromobenzaldehyde (32.1 mmol). The title compound was obtained after recrystallization of the crude with EtOAc/hexanes (1:4). Yield: 5.6 g (14.5 mmol, 59% yield over two steps). IR (ATR) 3105, 1541, 1347, 1168, 1008; ^{1}H NMR: (500 MHz, $CDCl_3$) δ 8.49 (-Ns**H**, AA'BB', J = 8.8 Hz, 2H), 8.26 (-Ns**H**, AA'BB', J = 8.8 Hz, 2H), 7.58 (4-BrPh**H**, AA'BB', J = 8.5 Hz, 2H), 7.32 (4-BrPh**H**, AA'BB', J = 8.5 Hz, 2H), 5.57 (Ns-N-C-**H**, s, 1H); ^{13}C NMR: (126 MHz, $CDCl_3$) δ 151.6, 140.4, 132.2, 130.8, 129.8, 128.8, 126.5, 124.6, 76.1; HRMS (ESI–) calcd for [$C_{13}H_8BrN_2O_5S$–] requires *m/z* 382.9342, found 382.9362. Isolated as a yellow solid (m.p. 112 ºC, decomp).



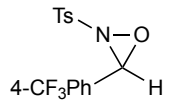
***N*-(4-Nitrophenyl)-sulfonyl-3-(3-bromophenyl)oxaziridine.** Prepared according to general procedure 1 using 2.5 g 4-nitrobenzenesulfonamide (12.4 mmol) and 3.00 g 3-bromobenzaldehyde (1.9 mL, 16.2 mmol). The title compound was obtained after recrystallization of the crude with EtOAc/hexanes (1:4). Yield: 3.10 g (8.1 mmol, 65% yield over two steps). IR (ATR) 3100, 1528, 1347, 1165; ^{1}H NMR: (500 MHz, $CDCl_3$) δ 8.49 (-Ns**H**, AA'BB', J = 8.7 Hz, 2H), 8.26 (-Ns**H**, AA'BB', J = 8.7 Hz, 2H), 7.63 (3-BrPh**H**, d, J = 7.8 Hz, 1H), 7.56 (3-BrPh**H**, s, 1H), 7.42 (3-BrPh**H**, d, J = 7.8 Hz, 1H), 7.31 (3-BrPh**H**, t, J = 7.8 Hz, 1H), 5.56 (Ns-N-C-**H**, s, 1H); ^{13}C NMR: (126 MHz, CDCl3) δ 151.6, 140.4, 134.9, 132.0, 131.1, 130.8, 130.4, 127.1, 124.6, 123.0, 75.6; HRMS (ESI–) calcd for [$C_{13}H_8BrN_2O_5S$–] requires *m/z* 382.9342, found 382.9346. Isolated as a yellow solid (m.p. 114–116 ºC, decomp).



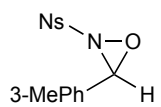
***N*-(4-Nitrophenyl)sulfonyl-3-(2-bromophenyl)oxaziridine.** Prepared according to general 1 procedure using 2.5 g 4-nitrobenzenesulfonamide (12.4 mmol) and 3.00 g 2-bromobenzaldehyde (1.9 mL, 16.2 mmol). The title compound was obtained after recrystallization of the crude with EtOAc/hexanes (1:4). Yield: 2.91 g (7.6 mmol, 61% yield over two steps). IR(ATR) 3108, 1532, 1354, 1178; ^{1}H NMR: (500 MHz, $CDCl_3$) δ 8.48 (-Ns**H**, AA'BB', J = 8.4 Hz, 2H), 8.28 (-Ns**H**, AA'BB', J = 8.4 Hz, 2H), 7.61-7.65 (2-BrPh**H**, m, 1H), 7.32-7.36 (2-BrPh**H**, m, 2H), 7.22-7.27 (2-BrPh**H**, m, 1H), 5.98 (Ns-N-C-**H**, s, 1H); ^{13}C NMR: (126 MHz, CDCl3) δ 151.6, 140.2, 133.0, 132.6, 130.9, 129.5, 128.6, 127.9, 124.5, 124.1, 76.4; HRMS (ESI–) calcd for [$C_{13}H_8BrN_2O_5S$–] requires *m/z* 382.9342, found 382.9345. Isolated as a yellow solid (m.p. 118–119 ºC, decomp).



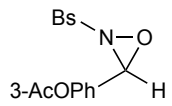
Methyl 4-(2-(phenylsulfonyl)-1,2-oxaziridin-3-yl)benzoate. Prepared according to general procedure 2 using 1.97 g benzenesulfonamide (12.5 mmol) and 2.46 g methyl-4-formylbenzoate (15.0 mmol). The title compound was obtained after recrystallization of the crude with EtOAc/hexanes (1:8). Yield: 1.43 g (4.4 mmol, 35% yield over two steps). IR(ATR) 3071, 2952, 1712, 1354, 1287; ^{1}H NMR: (500 MHz, $CDCl_3$) δ 8.06 (MeO_2CPh**H**, t, J = 7.6 Hz, 4H), 7.78 (-Bs**H**, t, J = 7.6 Hz, 1H), 7.65 (2-Bs**H**, t, J = 7.7 Hz, 2H), 7.53 (2-Bs**H**, d, J = 7.7 Hz, 2H), 5.54 (Bs-N-C-**H**, s, 1H), 3.93 (CO_2C**H**, s, 3H); ^{13}C NMR: (126 MHz, CDCl3) δ 161.2, 135.2, 135.0, 134.5, 132.9, 129.9, 129.5, 129.4, 128.3, 75.5, 52.4; HRMS (ESI+) calcd for [$C_{15}H_{13}N_1O_5S_1N_1H_4$+] requires *m/z* 337.0853, found 337.0863. Isolated as a white solid (m.p. 121–122 ºC).



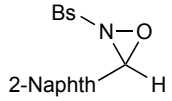
***N*-Tosyl-3-(4-(trifluoromethyl)phenyl)oxaziridine.** Prepared according to general procedure 2 using 5.0 g *p*-toluenesulfonamide (27.1 mmol) and 4.75 g 4-(trifluoromethyl)benzaldehyde (3.8 mL, 27.3 mmol). The title compound was obtained after recrystallization of the crude with EtOAc/hexanes (1:4). Yield: 5.50 g (16.0 mmol, 59% yield over two steps). IR(ATR) 3089, 1593, 1321, 1127, 1064; ^{1}H NMR: (500 MHz, $CDCl_3$) δ 7.93 (-CF_3Ph**H**, AA'BB', J = 8.3 Hz, 2H), 7.66 (Ts**H**, AA'BB', J = 8.2 Hz, 2H), 7.56 (Ts**H**, AA'BB', J = 8.2 Hz, 2H), 7.43 (CF_3Ph**H**, AA'BB', J = 8.1 Hz, 2H), 5.51 (Ts-N-C-**H**, s, 1H), 2.49 (Ts-C**H**, s, 3H); ^{13}C NMR: (126 MHz, CDCl3) δ 146.7, 134.5, 133.3 (F_3C-**C**, q, J = 32.7 Hz), 131.2, 130.2, 129.5, 128.7, 125.7 (F_3C-C-**C**, q, J = 3.7 Hz), 123.6 (F_3**C**, q, J = 272.6 Hz), 75.3, 21.9; ^{19}F NMR (471 MHz, $CDCl_3$) δ -63.1; HRMS (ESI–) calcd for [$C_{15}H_{11}F_3N_1O_3S$–] requires *m/z* 342.0417, found 342.0420. Isolated as a white solid (m.p. 104–107 ºC).



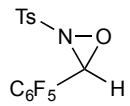
2-((4-Nitrophenyl)sulfonyl)-3-(*m*-tolyl)-1,2-oxaziridine. Prepared according to general procedure 1 using 2.5 g 4-nitrobenzenesulfonamide (12.4 mmol) and 1.95 g *m*-tolualdehyde (1.9 mL, 16.3 mmol). The title compound was obtained after recrystallization of the crude with EtOAc/hexanes (1:10). Yield: 2.81 g (8.8 mmol, 71% yield over two steps). IR(ATR) 3108, 1608, 1521, 1348, 1165; ^{1}H NMR: (500 MHz, $CDCl_3$) δ 8.46-8.48 (-Ns**H**, m, 2H), 8.25-8.27 (-Ns**H**, m, 2H), 7.22-7.33 (3-MePh**H**, m, 4H), 5.56 (Ns-N-C-**H**, s, 1H), 2.36 (Ph-C**H**, s, 1H); ^{13}C NMR: (126 MHz, CDCl3) δ 151.5, 140.6, 138.9, 132.6, 130.7, 129.6, 128.8, 128.6, 125.5, 124.5, 76.6, 21.2; HRMS (ESI+) calcd for [$C_{14}H_{12}N_2O_5S_1N_1H_4$+] requires *m/z* 338.0806, found 338.0801. Isolated as a yellow solid (m.p. 92 ºC, decomp).



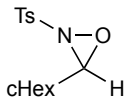
3-(2-(Phenylsulfonyl)-1,2-oxaziridin-3-yl)phenyl acetate. Prepared according to general procedure 2 using 2.6 g benzenesulfonamide (16.7 mmol) and 3.29 g 3-formylphenyl acetate (20.0 mmol). The title compound was obtained after recrystallization of the crude with EtOAc/hexanes (1:8). Yield: 3.30 g (10.3 mmol, 62% yield over two steps). IR(ATR) 3099, 3062, 1736, 1348, 1191; ^{1}H NMR: (500 MHz, $CDCl_3$) δ 8.04 (-Bs**H**, app d, J = 7.3 Hz, 2H), 7.75 (-AcOPh**H**, tt, J = 7.5,1.2 Hz, 1H), 7.63 (-Bs**H**, app t, J = 7.9 Hz, 2H), 7.42 (-Bs**H**, t, J = 7.9 Hz, 1H), 7.34 (-AcOPh**H**, dt, J = 7.8, 1.2 Hz, 1H), 7.20 (-AcOPh**H**, ddd, J = 8.0, 2.4, 1.1 Hz, 1H), 7.17 (-AcOPh**H**, t, J = 1.9 Hz, 1H), 5.48 (Bs-N-C-**H**, s, 1H), 2.28 (-OAc-**H**, s, 3H); ^{13}C NMR: (126 MHz, CDCl3) δ 169.1, 150.9, 135.1, 134.5, 132.2, 129.9, 129.4, 129.4, 125.8, 124.8, 121.3, 75.6, 21.0; HRMS (ESI+) calcd for [$C_{15}H_{13}N_1O_5S_1N_1H_4$+] requires *m/z* 337.0853, found 337.0858. Isolated as a yellow solid (m.p. 77–79 ºC).



3-(Naphthalen-2-yl)-2-(phenylsulfonyl)-1,2-oxaziridine. Prepared according to general procedure 2 using 5.0 g benzenesulfonamide (31.8 mmol) and 6.0 g 2-napthaldehyde (38.4 mmol). The title compound was obtained after recrystallization of the crude with EtOAc/hexanes (1:4). Yield: 7.82 g (25.1 mmol, 79% yield over two steps). IR(ATR) 3066, 1449, 1348, 1173; ^{1}H NMR: (500 MHz, $CDCl_3$) δ 8.09 (-Bs**H**, d, J = 7.8 Hz, 2H), 8.03 (-Naphth**H**, s, 1H), 7.86 (-Naphth**H**, t, J = 9.0 Hz, 2H), 7.76 (-Bs**H**, t, J = 7.5 Hz, 1H), 7.65 (-Bs**H**, t, J = 7.8 Hz, 2H), 7.54 (-Naphth**H**, app p, J = 6.2 Hz, 2H), 7.39 (app d, J = 9.0 Hz, 1H), 5.66 (Bs-N-C-**H**, s, 1H); ^{13}C NMR: (126 MHz, CDCl3) δ 135.0, 134.8, 134.7, 132.6, 129.8, 129.4, 129.4, 128.9, 128.3, 127.8, 127.7, 126.8, 123.4, 76.6; HRMS (ESI–) calcd for [$C_{17}H_{13}N_1O_3S_1N_1H_4$+] requires *m/z* 330.0955, found 330.0960. Isolated as a white solid (m.p. 90–91 ºC, decomp).



3-(Perfluorophenyl)-2-tosyl-1,2-oxaziridine. Prepared according to general procedure 2 using 5 g *p*-toulenesulfonamide (27.1 mmol) and 5.4 g pentafluorobenzaldehyde (3.4 mL, 27.3 mmol). The title compound was obtained after recrystallization of the crude with EtOAc/hexanes (1:4). Yield: 6.12 g (16.8 mmol, 63% yield over two steps). IR(ATR) 3047, 2920, 1656, 1592, 1509, 1352; ^{1}H NMR: (500 MHz, $CDCl_3$) δ 7.91 (-Ts**H**, AA'BB', J = 8.4 Hz, 2H), 7.44 (-Ts**H**, AA'BB', J = 8.0 Hz, 2H), 5.75 (Ts-N-C-**H**, s, 1H), 2.50 (Ts-C**H**, s, 1H); ^{13}C NMR: (126 MHz, CDCl3) δ 147.3-147.5 (m), 147.1, 145.2-145.4 (m), 144.0-144.3 (m), 142.2-141.9 (m), 138.5-138.9 (m), 136.5-136.8 (m), 130.7, 130.3, 129.6, 124.3, 69.6, 21.9; ^{19}F NMR (471 MHz, $CDCl_3$) δ –141.5- –141.5 (m), –148.2 (tt, J = 20.8, 3.9 Hz), –160.2- –160.3 (m); HRMS (ESI–) calcd for [$C_{13}H_8BrN_2O_5S$–] requires *m/z* 364.0072, found 364.0077. Isolated as a white solid (m.p. 91–93 ºC).

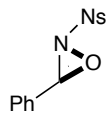


3-Cyclohexyl-2-tosyl-1,2-oxaziridine. Prepared according to general procedure 2 using 5 g *p*-toulenesulfonamide (27.1 mmol) and 3.9 g cyclohexanecarboxaldehyde (4.2 mL, 41.0 mmol). The title compound was obtained after recrystallization of the crude with EtOAc/hexanes (1:4). Yield: 2.25 g (8.1 mmol, 30% yield over two steps). Isolated as a white solid. All spectral data were in accord with previously reported values.[11]

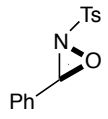
III. Kinetic Resolution of Oxaziridines

General Procedure for oxaziridine resolution. In a nitrogen-atmosphere glovebox, iron(II) chloride (6.1 mg, 0.05 mmol) and ligand **6g** (21.4 mg, 0.06 mmol) were placed in a 1.5 dram vial with a stir bar. The vial was capped with a septum and transferred out of the glove box.

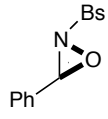
The vessel was then charged with THF (2 mL, 0.5 M) and stirred under nitrogen atmosphere for 1 h. The reaction was then cooled to –78 ºC, the septum was removed, and the oxaziridine (1 mmol) was quickly added. The vessel was sealed, placed under a positive pressure of nitrogen, and stirred for the reported reaction time at 0 ºC. After the allotted time passed, the reaction mixture was immediately passed through a plug of silica using with EtOAc. The solvent was then removed by rotary evaporation, and the crude residue was purified by flash column chromatography to recover the remaining oxaziridine.



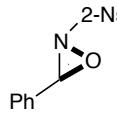
(*S,S*)-*N*-(4-Nitrophenyl)sulfonyl-3-phenyl oxaziridine (**3**). Prepared according to the general procedure using 310.5 mg (1.01 mmol) *N*-(4-nitrophenyl)sulfonyl-3-phenyl oxaziridine. The reaction mixture was stirred 5 min at 0 ºC, filtered through a silica plug, and purified on silica gel using 10% EtOAc/hexanes. Yield: 118 mg (0.39 mmol, 38% yield), 98% ee, s = 17. [Daicel CHIRALCEL®OD-H, 30% MeOH, 3 mL/min, 220 nm; t_1= 3.18 min, t_2=5.02 min], $[\alpha]_D^{22}$ –99.6º (*c*1.00, CH_2Cl_2). Other spectral data were in agreement with reported values.[2]



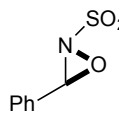
(*S,S*)-*N*-(4-Methylphenyl)sulfonyl-3-phenyl oxaziridine (**7**). Prepared according to the general procedure using 274.1 mg (1.0 mmol) *N*-(4-methylphenyl)sulfonyl-3-phenyl oxaziridine. The reaction mixture was stirred 7 min at 0 ºC, filtered through a silica plug, and purified on silica gel using 10% EtOAc/hexanes. Yield: 112 mg (0.41 mmol, 41% yield), 93% ee, s = 16. [Daicel CHIRALCEL®OD-H, 5% MeOH, 3 mL/min, 220 nm; t_1= 6.18 min, t_2=7.16 min], $[\alpha]_D^{22}$ –106.4º (*c*1.00, CH_2Cl_2); {lit. $[\alpha]_D$ –49.8 (*c*0.58, CH_2Cl_2), 92% ee (*S,S*)}.[11] Other spectral data were in agreement with reported values.[3]



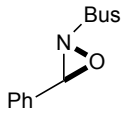
(*S,S*)-*N*-Phenylsulfonyl-3-phenyloxaziridine (**8**). Prepared according to the general procedure using 260.2 mg (1.0 mmol) *N*-phenylsulfonyl-3-phenyl oxaziridine. The reaction mixture was stirred 6 min at 0 ºC, filtered through a silica plug, and purified on silica gel using 10% EtOAc/hexanes. Yield: 110 mg (0.42 mmol, 42% yield), 91% ee, s = 15. [Daicel CHIRALCEL®OD-H, 5% MeOH, 3 mL/min, 220 nm; t_1= 5.58 min, t_2= 6.12 min], $[\alpha]_D^{22}$ –130.2º (*c*1.00, CH_2Cl_2); {lit. $[\alpha]_D$ –130.8 (*c*1–2, $CHCl_3$), (*S,S*)}.[12] Other spectral data were in agreement with reported values.[4]



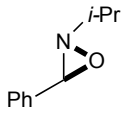
(*S,S*)-*N*-(2-Nitrophenyl)sulphonyl-3-(phenyl)oxaziridine (**9**). Prepared according to the general procedure using 307.2 mg (1.00 mmol) *N*-(2-nitrophenyl)sulfonyl-3-phenyl oxaziridine. The reaction mixture was stirred 2 min at 0 ºC, filtered through a silica plug, and purified on silica gel using 20% EtOAc/hexanes → 30% EtOAc/hexanes. Yield: 123 mg (0.40 mmol, 40% yield), 96% ee, s = 17. [Daicel CHIRALPAK®AD-H, 20% MeOH, 3 mL/min, 220 nm; t_1= 6.85 min, t_2= 7.13 min], $[\alpha]_D^{22}$ +24.5º (*c*2.00, CH_2Cl_2). Other spectral data were in agreement with those reported above.



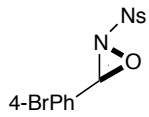
(*S,S*)-2-(Mesitylsulfonyl)-3-phenyl-1,2-oxaziridine (**10**). Prepared according to the general procedure using 302.7 mg (1.00 mmol) 2-(mesitylsulfonyl)-3-phenyl-1,2-oxaziridine. The reaction mixture was stirred 13 min at 0 ºC, filtered through a silica plug, and purified on silica gel using 9% EtOAc/hexanes. Yield: 136 mg (0.45 mmol, 45% yield), 89% ee, s = 18. [Daicel CHIRALCEL®OJ-H, 5% MeOH, 3 mL/min, 220 nm; t_1= 5.66 min, t_2= 6.82 min], $[\alpha]_D^{22}$ –96.0º (*c*1.00, CH_2Cl_2). m.p. 107–109ºC, decomp. Other spectral data were in agreement with those reported above.



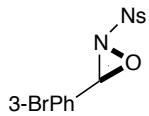
(*S*,*S*)-*N*-*tert*-Butylsulfonyl-3-phenyl oxaziridine (**11**). Prepared according to the general procedure using 255.3 mg (1.00 mmol) *N*-*tert*-butylsulfonyl-3-phenyl oxaziridine. The reaction mixture was stirred 5 min at 0 ºC, filtered through a silica plug, and purified on silica gel using 9% EtOAc/hexanes. Yield: 140. mg (0.55 mmol, 55% yield), 58% ee, s = 10. [Daicel CHIRALCEL®OJ-H, 5% MeOH, 3 mL/min, 220 nm; t_1= 2.42 min, t_2= 2.78 min], $[\alpha]_D^{22}$ –89.6º (*c*0.95, CH_2Cl_2). Other spectral data were in agreement with those previously reported.[6]



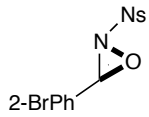
(*S*,*S*)-2-Isopropyl-3-phenyloxaziridine (**12**). Prepared according to the general procedure using 137.3 mg (0.84 mmol) 2-Isopropyl-3-phenyloxaziridine. The reaction mixture was stirred 5 min at 0 ºC, filtered through a silica plug, and purified on silica gel using 97:3:1 hexanes/EtOAc/triethylamine. Yield: 35 mg (0.21 mmol, 25% yield), 53% ee, s = 2. [Daicel CHIRALCEL®OD-H, 5% *i*-PrOH, 3 mL/min, 220 nm; t_1= 2.27 min, t_2= 4.36 min], $[\alpha]_D^{22}$ –53.9º (*c*0.86, CH_2Cl_2). Other spectral data were in agreement with those previously reported.[7]



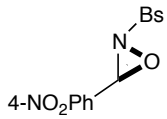
(*S*,*S*)-*N*-(4-Nitrophenyl)sulfonyl-3-(4-bromophenyl)oxaziridine (**13**). Prepared according to a modified general procedure using 387.1 mg (1.01 mmol) *N*-(4-nitrophenyl)sulfonyl-3-(4-bromophenyl) oxaziridine and 4 mL THF (0.25 M). The reaction mixture was stirred 8 min at 0 ºC, and flashed directly on silica gel using 10% EtOAc/hexanes → 30% EtOAc/hexanes. (*Note: This reaction mixture was flashed directly due to the highly crystalline nature of the amide byproduct*). Yield: 185 mg (0.48 mmol, 48% yield), 87% ee, s = 26. [Daicel CHIRALCEL®OD-H, 30% MeOH, 3 mL/min, 220 nm; t_1= 4.38 min, t_2=4.95 min], $[\alpha]_D^{22}$ –49.4º (*c*1.00, CH_2Cl_2). Other spectral data were in agreement with those reported above.



(*S*,*S*)-*N*-(4-Nitrophenyl)sulfonyl-3-(3-bromophenyl)oxaziridine (**14**). Prepared according to the general procedure using 385.3 mg (1.00 mmol) *N*-(4-nitrophenyl)sulfonyl-3-(3-bromophenyl) oxaziridine. The reaction mixture was stirred 10 min at 0 ºC, filtered through a silica plug, and purified on silica gel using 20% EtOAc/hexanes. Yield: 155 mg (0.40 mmol, 40% yield), 98% ee, s = 21. [Daicel CHIRALCEL®OD-H, 30% MeOH, 3 mL/min, 220 nm; t_1= 4.32 min, t_2= 5.23 min], $[\alpha]_D^{22}$ –77.0º (*c*1.00, CH_2Cl_2). Other spectral data were in agreement with those reported above.

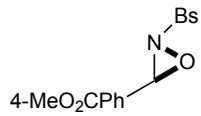


(*S*,*S*)-*N*-(4-Nitrophenyl)sulfonyl-3-(2-bromophenyl)oxaziridine (**15**). Prepared according to a modified general procedure using iron(II) chloride (12.1 mg, 0.1 mmol), ligand **6g** (42.8 mg, 0.12 mmol), and 385.8 mg (1.00 mmol) *N*-(4-nitrophenyl)sulfonyl-3-(2-bromophenyl) oxaziridine. The reaction mixture was stirred 10 min at 0 ºC, filtered through a silica plug, and purified on silica gel using 5% EtOAc/hexanes → 20% EtOAc/hexanes. Yield: 180 mg (0.47 mmol, 47% yield), 76% ee, s = 12. [Daicel CHIRALCEL®OD-H, 40% MeOH, 3 mL/min, 220 nm; t_1= 3.96 min, t_2= 6.52 min], $[\alpha]_D^{22}$ –31.0º (*c*1.00, CH_2Cl_2). Other spectral data were in agreement with those reported above.

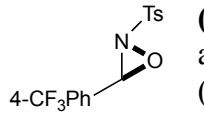


(*S*,*S*)-*N*-Phenylsulfonyl-3-(4-nitrophenyl) oxaziridine (**16**). Prepared according to a modified general procedure using 305.4 mg (1.0 mmol) *N*-phenylsulfonyl- 3-(4-nitrophenyl) oxaziridine. The oxaziridine addition was performed at 0 ºC, the reaction mixture stirred 5 min at room temperature, filtered through a silica plug, and purified on silica gel using 25% EtOAc/hexanes. Yield: 146

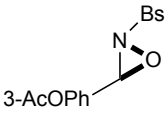
mg (0.48 mmol, 48% yield), 89% ee, s = 30. [Daicel CHIRALCEL®OD-H, 5% MeOH, 3 mL/min, 220 nm; t_1= 3.40 min, t_2=3.90 min], $[\alpha]_D^{22}$ –87.8º (*c*1.00, CH_2Cl_2). Other spectral data were in agreement with reported values.[5]



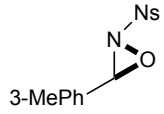
(*S,S*)-Methyl 4-(2-(phenylsulfonyl)-1,2-oxaziridin-3-yl)benzoate (**17**). Prepared according general procedure using 317.9 mg (1.00 mmol) methyl 4-(2-(phenylsulfonyl)-1,2-oxaziridin-3-yl)benzoate. The reaction mixture was stirred 3.5 min at 0ºC, filtered through a silica plug, and purified on silica gel using 13% EtOAc/hexanes. Yield: 123 mg (0.39 mmol, 39% yield), 97% ee, s = 16. [Daicel CHIRALPAK®AS-H, 20% *i*-PrOH, 3 mL/min, 220 nm; t_1= 3.37 min, t_2= 4.53 min], $[\alpha]_D^{22}$ –94.6º (*c*1.00, CH_2Cl_2). m.p. 99–100ºC. Other spectral data were in agreement with those reported above.



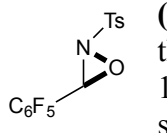
(*S,S*)-*N*-Tosyl-3-(4-(trifluoromethyl)phenyl)oxaziridine (**18**). Prepared according to the general procedure using 343.7 mg (1.00 mmol) *N*-tosyl-3-(4-(trifluoromethyl)phenyl)oxaziridine. The reaction mixture was stirred 2 min at 0 ºC, filtered through a silica plug, and purified on silica gel using 10% EtOAc/hexanes. Yield: 129 mg (0.38 mmol, 38% yield), 96% ee, s = 14. [Daicel CHIRALPAK®AD-H, 40% MeOH, 3 mL/min, 220 nm; t_1= 2.8 min, t_2= 3.51 min], $[\alpha]_D^{22}$ –87.6º (*c*1.00, CH_2Cl_2). m.p. 87–90ºC. Other spectral data were in agreement with those reported above.



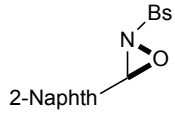
(*S,S*)-3-(2-(Phenylsulfonyl)-1,2-oxaziridin-3-yl)phenyl acetate (**19**). Prepared according general procedure using 317.9 mg (1.00 mmol) 3-(2-(phenylsulfonyl)-1,2-oxaziridin-3-yl)phenyl acetate. The reaction mixture was stirred 7 min at 0 ºC, filtered through a silica plug, and purified on silica gel using 20% EtOAc/hexanes. Yield: 102 mg (0.32 mmol, 32% yield), 93% ee, s = 8. [Daicel CHIRALCEL®OJ-H, 25% MeOH, 3 mL/min, 220 nm; t_1= 2.82 min, t_2= 3.28 min], $[\alpha]_D^{22}$ –109.8º (*c*1.00, CH_2Cl_2). Other spectral data were in agreement with those reported above.



(*S,S*)-2-((4-Nitrophenyl)sulfonyl)-3-(*m*-tolyl)-1,2-oxaziridine (**20**). Prepared according to the general procedure using 322.0 mg (1.01 mmol) 2-((4-nitrophenyl)sulfonyl)-3-(*m*-tolyl)-1,2-oxaziridine. The reaction mixture was stirred 5 min at 0ºC, filtered through a silica plug, and purified on silica gel using 9% EtOAc/hexanes. Yield: 91 mg (0.28 mmol, 28% yield), 97% ee, s = 8. [Daicel CHIRALCEL®OD-H, 30% MeOH, 3 mL/min, 220 nm; t_1= 3.31 min, t_2= 5.96 min], $[\alpha]_D^{22}$ –81.5º (*c*1.00, CH_2Cl_2). Other spectral data were in agreement with those reported above.

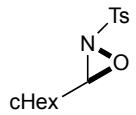


(*S,S*)-3-(Perfluorophenyl)-2-tosyl-1,2-oxaziridine (**21**). Prepared according to the general procedure using 369.1 mg (1.01 mmol) 3-(perfluorophenyl)-2-tosyl-1,2-oxaziridine. The reaction mixture was stirred 4 min at 0 ºC, filtered through a silica plug, and purified on silica gel using 9% EtOAc/hexanes. Yield: 147 mg (0.40 mmol, 40% yield), 85% ee, s = 9. [Daicel CHIRALPAK®AD-H, 10–40% gradient (465 sec) MeOH, 3 mL/min, 220 nm; t_1= 7.8 min, t_2= 8.43 min], $[\alpha]_D^{22}$ –77.4º (*c*1.00, CH_2Cl_2). m.p. 69–70ºC. Other spectral data were in agreement with those reported above.



(*S,S*)-3-(Naphthalen-2-yl)-2-(phenylsulfonyl)-1,2-oxaziridine (**22**). Prepared according to the general procedure using 317.5 mg (1.02 mmol) 3-(naphthalen-2-yl)-2-(phenylsulfonyl)-1,2-oxaziridine. The reaction mixture was stirred 7

min at 0 ºC, filtered through a silica plug, and purified on silica gel using 10% EtOAc/hexanes. Yield: 119 mg (0.38 mmol, 37% yield), 87% ee, s = 9. [Daicel CHIRALCEL®OJ-H, 30% MeOH, 3 mL/min, 220 nm; t_1= 6.57 min, t_2= 7.75 min], $[\alpha]_D^{22}$ –72.0º (*c*1.00, CH_2Cl_2). Other spectral data were in agreement with those reported above.



(*S,S*)-3-(Cyclohexyl)-2-tosyl-1,2-oxaziridine (**23**). Prepared according to the general procedure using 295.4 mg (1.1 mmol) 3-(cyclohexyl)-2-tosyl-1,2-oxaziridine. The reaction mixture was stirred 15 min at 0 ºC, filtered through a silica plug, and purified on silica gel using 9% EtOAc/hexanes. Yield: 209 mg (0.74 mmol, 71% yield), 15% ee, s = 2. [Daicel CHIRALCEL®OJ-H, 5% MeOH, 3 mL/min, 220 nm; t_1= 3.33 min, t_2= 3.64 min], $[\alpha]_D^{22}$ –11.7º (*c*1.04, CH_2Cl_2). m.p. 75–78ºC. Other spectral data were in agreement with those reported above.

IV. Gram-scale resolutions

Gram-scale resolution of *N*-phenylsulfonyl-3-phenyloxaziridine (Scheme 1) In a nitrogen-atmosphere glovebox, iron(II) chloride (36.3 mg, 0.3 mmol) and ligand **6g** (128.2 mg, 0.36 mmol) were placed in a 100 mL flask with a stir bar. The flask was capped with a septum and transferred out of the glove box. The vessel was then charged with THF (24 mL, 0.5 M) and stirred under nitrogen atmosphere for 1 h. The reaction was then cooled to 0 ºC, the septum was removed, and *N*-phenylsulfonyl-3-phenyloxaziridine (3.12 g, 12 mmol) was added in portions with rapid stirring. The vessel was sealed, placed under a positive pressure of nitrogen, and stirred for 25 min at room temperature. The reaction mixture was then immediately passed through a plug of silica washing with EtOAc. The solvent was removed by rotary evaporation, and the crude residue purified on silica gel using 10% EtOAc/hexanes as eluent to recover the remaining *N*-phenylsulfonyl-3-phenyloxaziridine. Yield: 1.18 g (4.5 mmol, 38% yield), 98% ee. s = 17. [Daicel Chiracel OD-H, 5% MeOH, 3 mL/min, 220 nm; t_1= 5.58 min, t_2=6.12 min]. Other spectral data were in agreement with reported values.[4]

Gram-scale resolution of *N-tert*-butylsulfonyl-3-phenyl oxaziridine (Scheme 1) In a nitrogen-atmosphere glovebox, iron(II) chloride (18.2 mg, 0.15 mmol) and ligand **6g** (69.5 mg, 0.18 mmol) were placed in a 50 mL flask with a stir bar. The flask was capped with a septum and transferred out of the glove box. The vessel was then charged with THF (12 mL, 0.5 M) and stirred under nitrogen atmosphere for 1 h. The reaction was then cooled to 0 ºC, the septum was removed, and *N-tert*-butylsulfonyl-3-phenyl oxaziridine (1.44 g, 6.0 mmol) was added in portions with rapid stirring. The vessel was sealed, placed under a positive pressure of nitrogen, and stirred for 25 minutes at room temperature. The reaction mixture was immediately passed through a plug of silica washing with EtOAc. The solvent was removed by rotary evaporation, and the crude residue purified on silica gel using 10% EtOAc/hexanes as eluent to recover the remaining *N*-phenylsulfonyl-3-phenyloxaziridine. Yield: 0.45 g (1.9 mmol, 31% yield), >99% ee. s = 12. [Daicel Chiracel OJ-H, 5% MeOH, 3 mL/min, 220 nm; t_1= 2.71 min]. Other spectral data were in agreement with reported values.[6]

References

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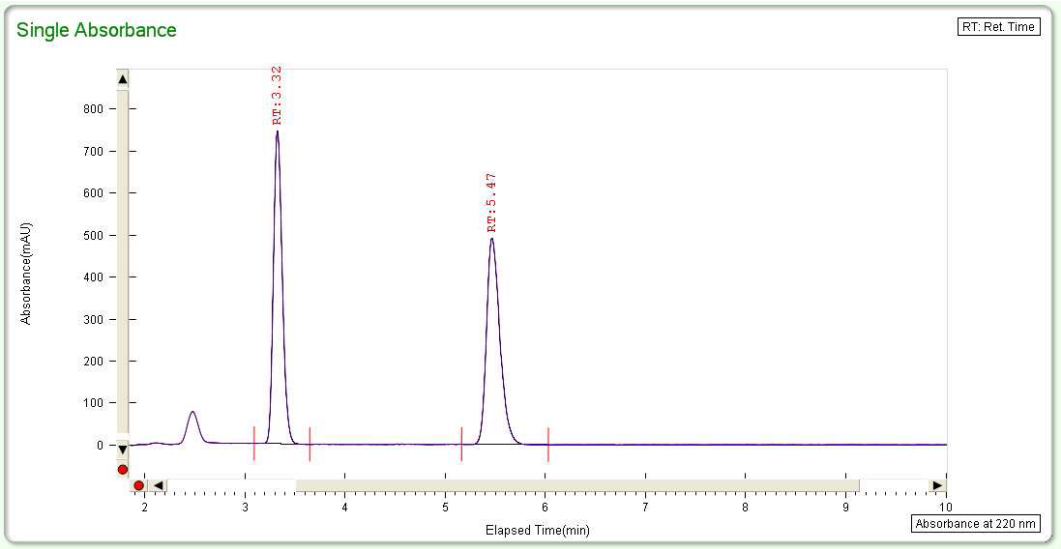
NMR spectra and SFC Chromatograms

(*S,S*)-*N*-(4-nitrophenyl)sulfonyl-3-phenyl oxaziridine (3)

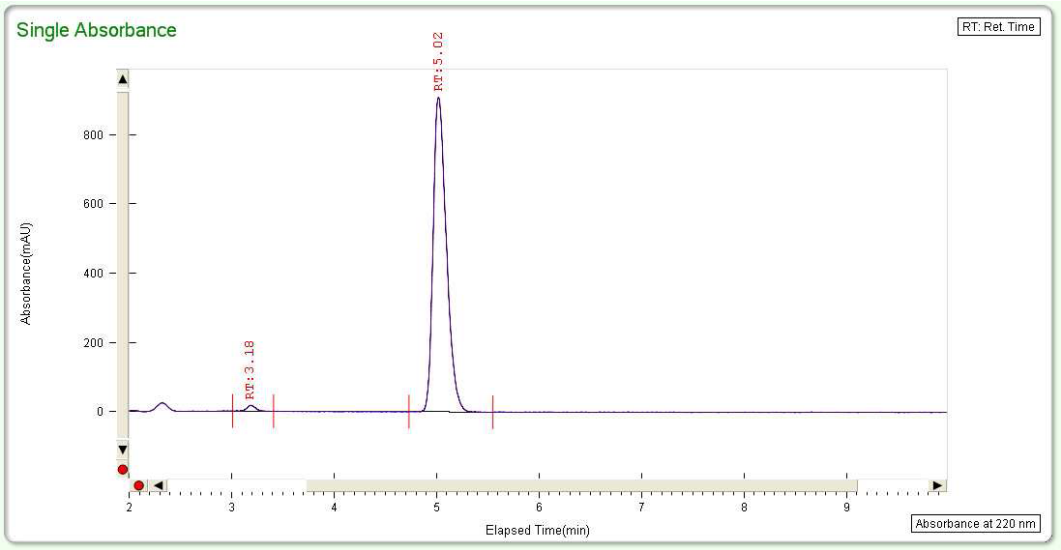
Racemic: (SFC, CHIRALCEL®OD-H, 30% MeOH/CO_2, 3 mL/min, 220nm)



Peak Info

Peak No	% Area	Area	RT (min)	Height (mV)
1	50.0185	4553.8928	3.32	744.9288
2	49.9815	4550.516	5.47	491.4648
Total:	100	9104.4088		

Scalemic: (SFC, CHIRALCEL®OD-H, 30% MeOH/CO_2, 3 mL/min, 220nm)

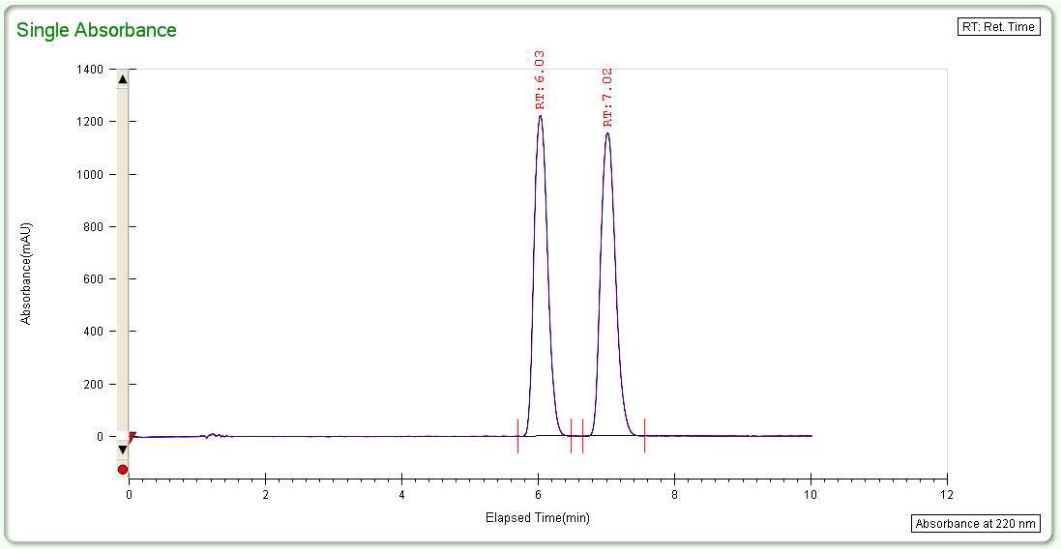


Peak Info

Peak No	% Area	Area	RT (min)	Height (mV)
1	1.0943	90.3084	3.18	16.5937
2	98.9057	8162.0818	5.02	907.8787
Total:	100	8252.3902		

(*S,S*)-*N*-(4-methylphenyl)sulfonyl-3-phenyl oxaziridine (**7**)

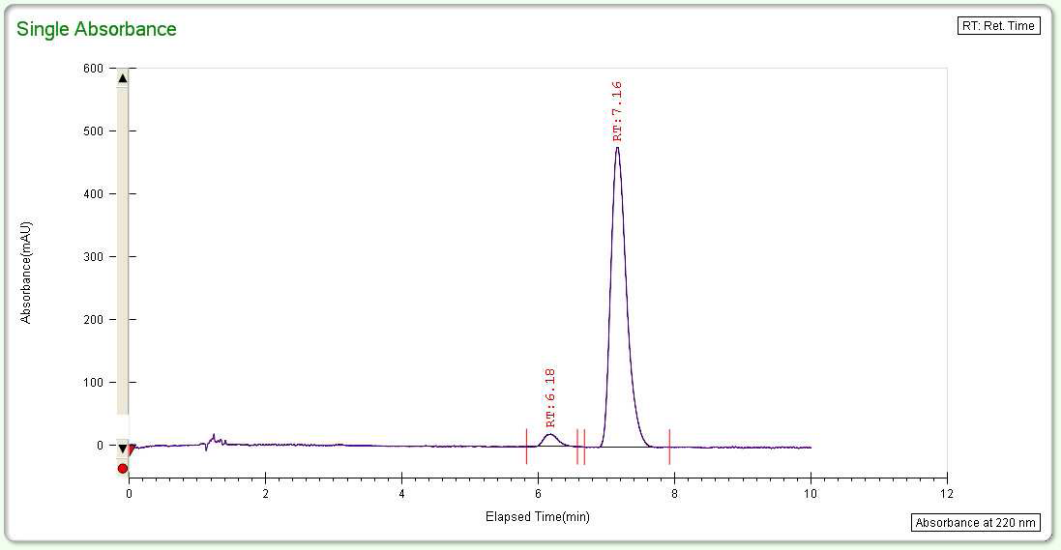
Racemic: (SFC, CHIRALCEL®OD-H, 5% MeOH/CO_2, 3 mL/min, 220nm)



Peak Info

Peak No	**% Area**	**Area**	**RT (min)**	**Height (mV)**
1	49.1007	16807.5378	6.03	1222.21
2	50.8993	17423.2046	7.02	1153.0905
Total:	100	34230.7424		

Scalemic: (SFC, CHIRALCEL®OD-H, 5% MeOH/CO_2, 3 mL/min, 220nm)

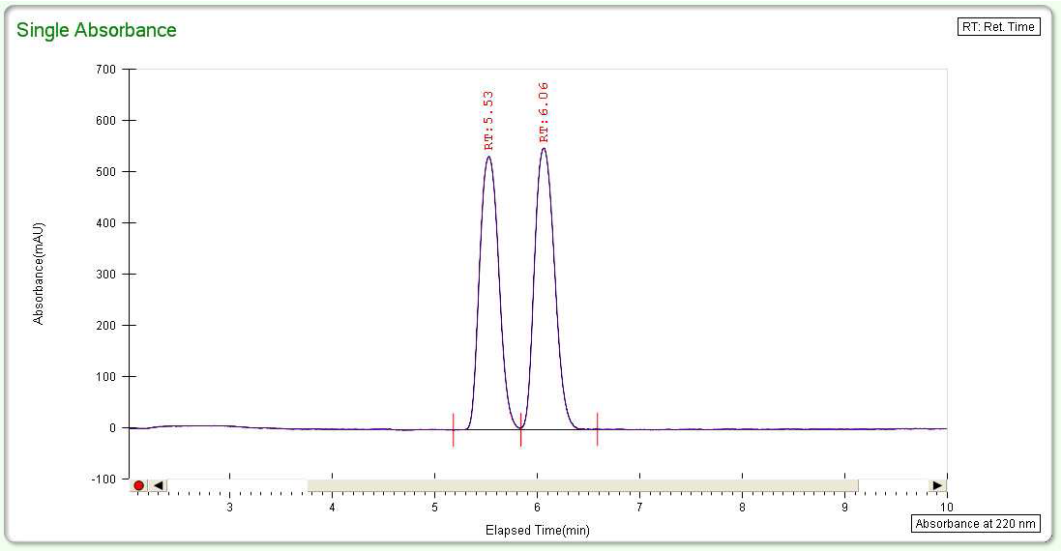


Peak Info

Peak No	**% Area**	**Area**	**RT (min)**	**Height (mV)**
1	3.6733	289.0603	6.18	19.9121
2	96.3267	7580.2176	7.16	476.7903
Total:	100	7869.2779		

(*S,S*)-*N*-phenylsulfonyl-3-phenyl oxaziridine (**8**)

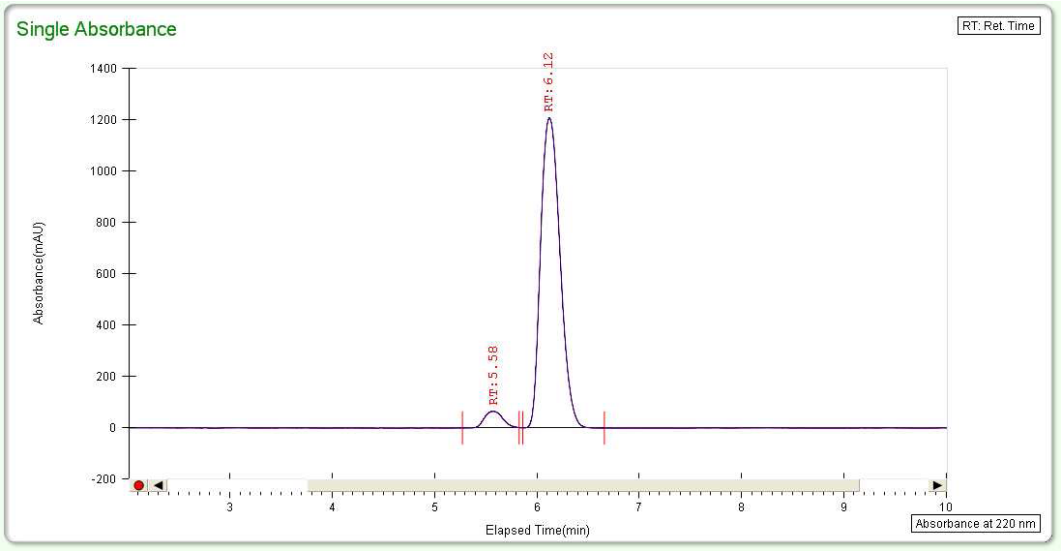
Racemic: (SFC, CHIRALCEL®OD-H, 5% MeOH/CO_2, 3 mL/min, 220nm)



Peak Info

Peak No	**% Area**	**Area**	**RT (min)**	**Height (mV)**
1	48.3023	6938.9887	5.53	533.4303
2	51.6977	7426.75	6.06	549.5026
Total:	100	14365.7387		

Scalemic: (SFC, CHIRALCEL®OD-H, 5% MeOH/CO_2, 3 mL/min, 220nm)

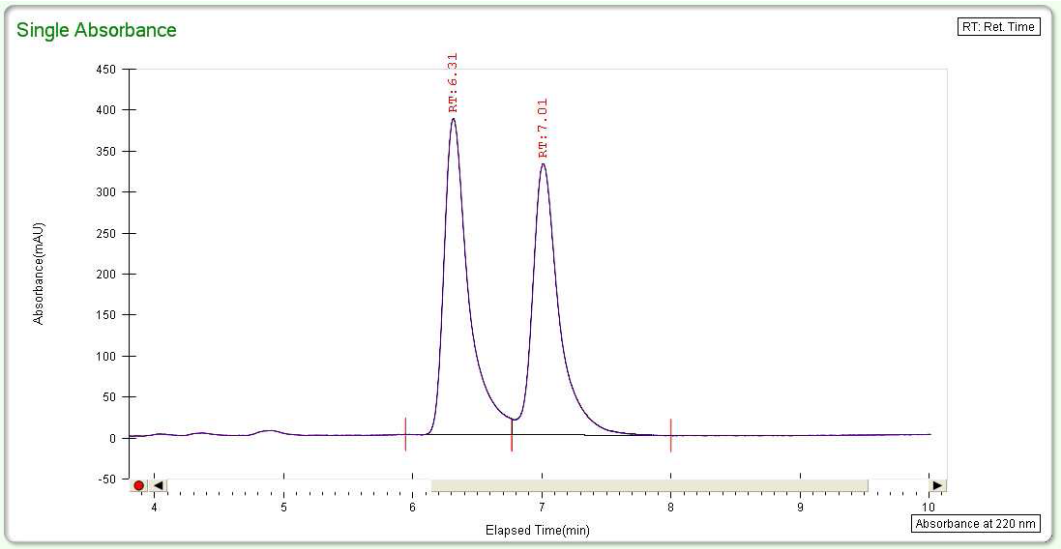


Peak Info

Peak No	**% Area**	**Area**	**RT (min)**	**Height (mV)**
1	4.6954	783.6393	5.58	64.2374
2	95.3046	15905.8962	6.12	1206.9273
Total:	100	16689.5355		

(*S,S*)-*N*-(2-nitrophenyl)sulfonyl-3-phenyl oxaziridine (**9**)

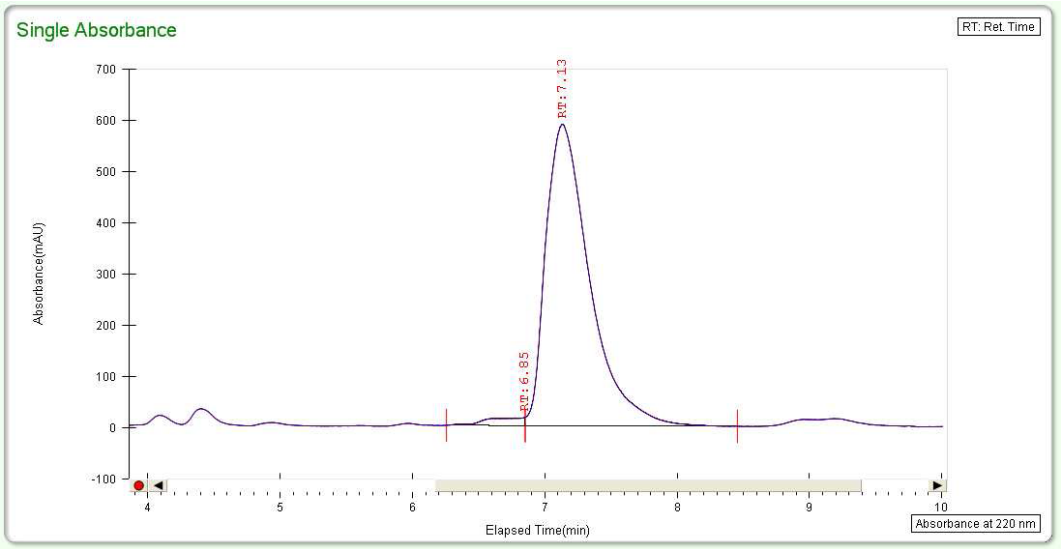
Racemic: (SFC, CHIRALPAK®AD-H, 20% MeOH/CO_2, 3 mL/min, 220nm)



Peak Info

Peak No	% Area	Area	RT (min)	Height (mV)
1	51.9479	5104.3072	6.31	385.3718
2	48.0521	4721.5068	7.01	330.9689
Total:	100	9825.814		

Scalemic: (SFC, CHIRALPAK®AD-H, 20% MeOH/CO_2, 3 mL/min, 220nm)

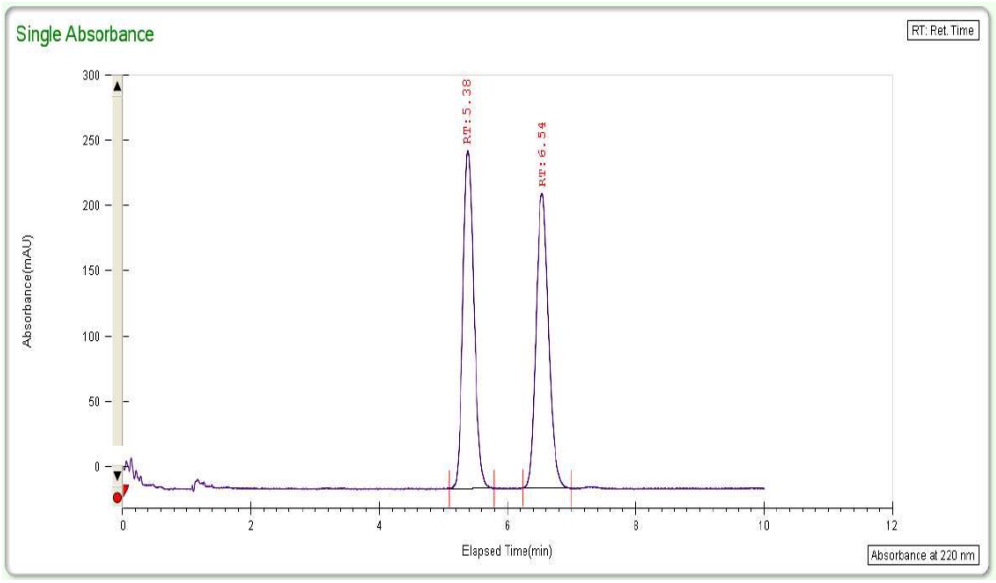


Peak Info

Peak No	% Area	Area	RT (min)	Height (mV)
1	2.2237	307.7125	6.85	16.1509
2	97.7763	13530.3059	7.13	588.2427
Total:	100	13838.0184		

(*S,S*)-*N*-(mesitylsulfonyl)-3-phenyl oxaziridine (10)

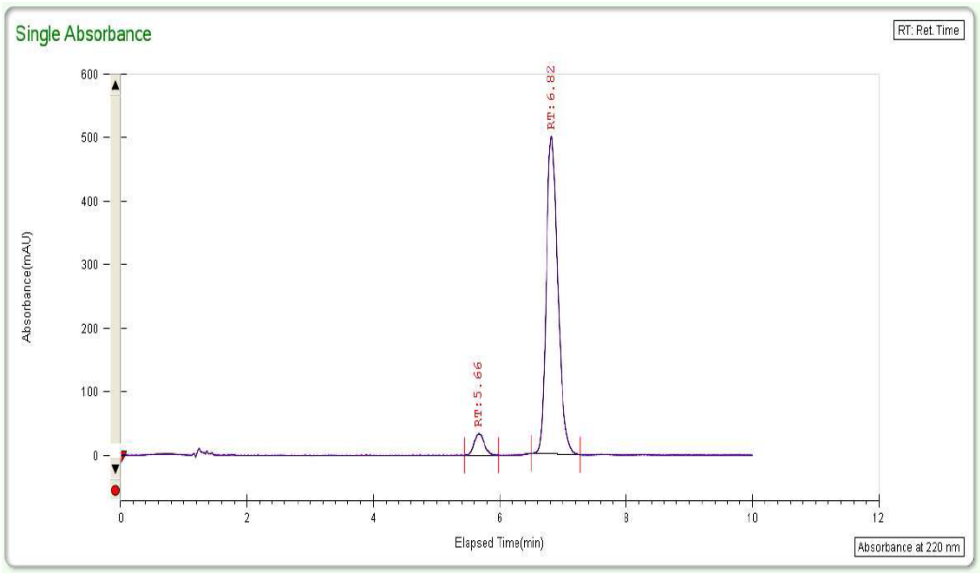
Racemic: (SFC, CHIRALCEL®OJ-H, 5% MeOH/CO_2, 3 mL/min, 220nm)



Peak Info

Peak No	% Area	Area	RT (min)	Height (mV)
1	50.1187	3065.1356	5.38	258.6743
2	48.0521	4721.5068	6.54	225.7642
Total:	100	6115.7566		

Scalemic: (SFC, CHIRALCEL®OJ-H, 5% MeOH/CO_2, 3 mL/min, 220nm)

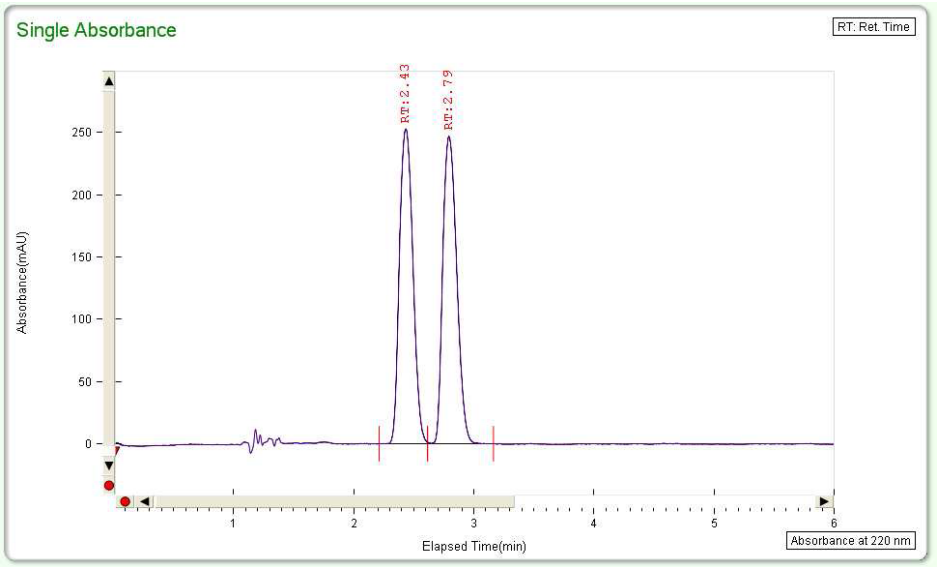


Peak Info

Peak No	% Area	Area	RT (min)	Height (mV)
1	5.5646	371.8924	5.66	33.7333
2	94.4354	6311.234	6.82	500.447
Total:	100	6683.1264		

(*S*,*S*)-*N*-*tert*-butylsulfonyl-3-phenyl oxaziridine (11)

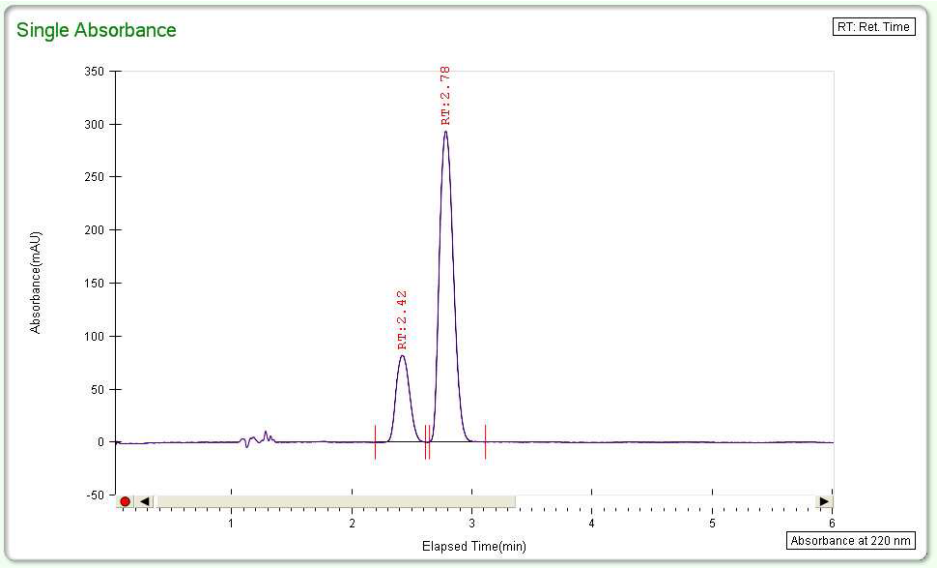
Racemic: (SFC, CHIRALCEL®OJ-H, 5% MeOH/CO_2, 3 mL/min, 220nm)



Peak Info

Peak No	% Area	Area	RT (min)	Height (mV)
1	49.7703	1961.5245	2.43	252.8264
2	50.2297	1979.6311	2.79	246.7777
Total:	100	3941.1556		

Scalemic: (SFC, CHIRALCEL®OJ-H, 5% MeOH/CO_2, 3 mL/min, 220nm)

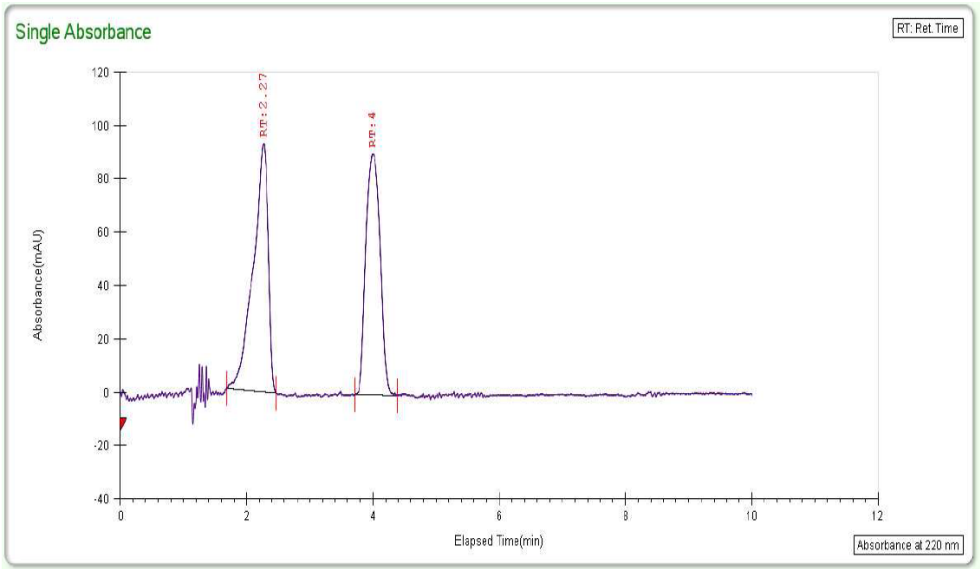


Peak Info

Peak No	% Area	Area	RT (min)	Height (mV)
1	21.2274	633.0596	2.42	81.8917
2	78.7726	2349.2118	2.78	293.4638
Total:	100	2982.2714		

(*S*,*S*)-2-Isopropyl-3-phenyloxaziridine (**12**)

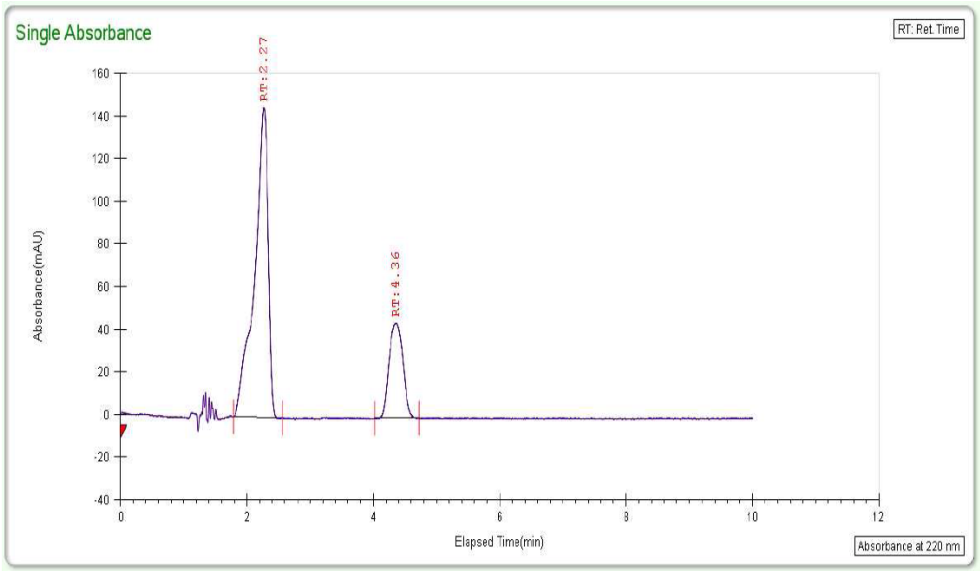
Racemic: (SFC, CHIRALCEL®OD-H, 5% *i*-PrOH/CO_2, 3 mL/min, 220nm)



Peak Info

Peak No	**% Area**	**Area**	**RT (min)**	**Height (mV)**
1	52.0849	1545.5049	2.27	93.1993
2	47.9151	1421.7776	4	90.516
Total:	100	2967.2825		

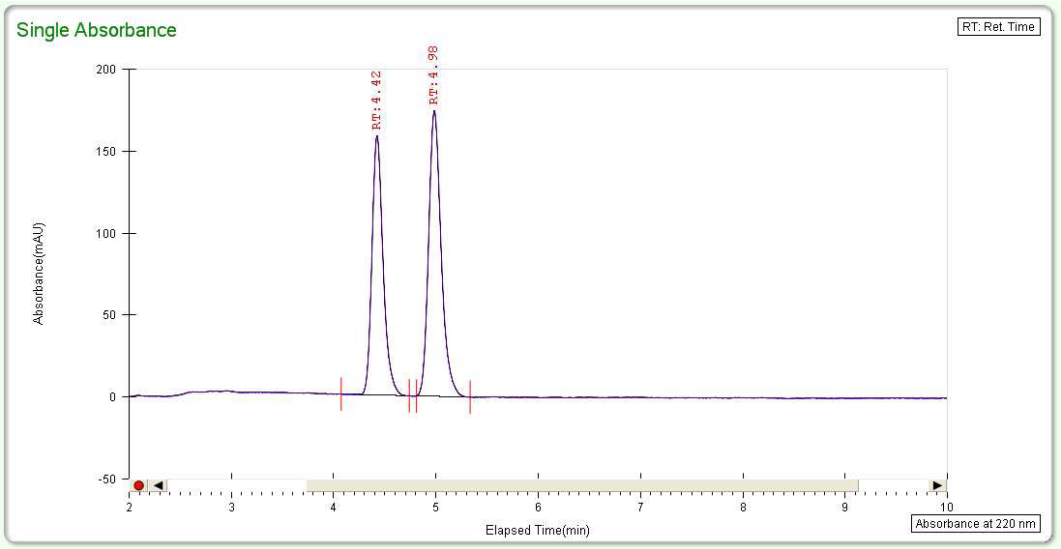
Scalemic: (SFC, CHIRALCEL®OD-H, 5% *i*-PrOH/CO_2, 3 mL/min, 220nm)



Peak Info

Peak No	**% Area**	**Area**	**RT (min)**	**Height (mV)**
1	76.3269	2180.3253	2.27	145.2999
2	23.6731	676.2374	4.36	44.5541
Total:	100	2856.5627		

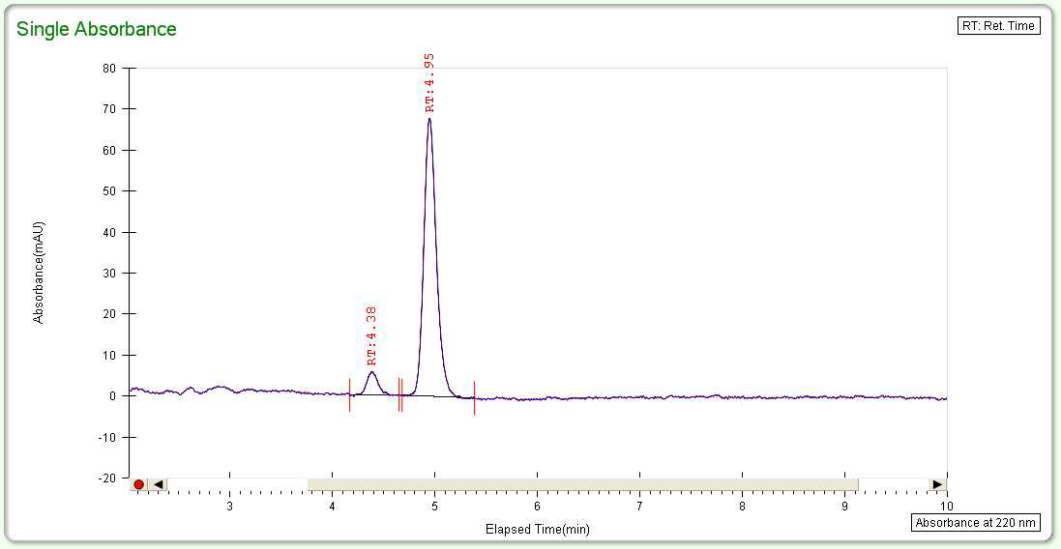
(*S,S*)-*N*-(4-nitrophenyl)sulfonyl-3-(4-bromophenyl)oxaziridine (**13**)
Racemic: (SFC, CHIRALCEL®OD-H, 30% MeOH/CO_2, 3 mL/min, 220nm)



Peak Info

Peak No	**% Area**	**Area**	**RT (min)**	**Height (mV)**
1	44.6666	1196.8482	4.42	158.0366
2	55.3334	1482.6665	4.98	174.1546
Total:	100	2679.5147		

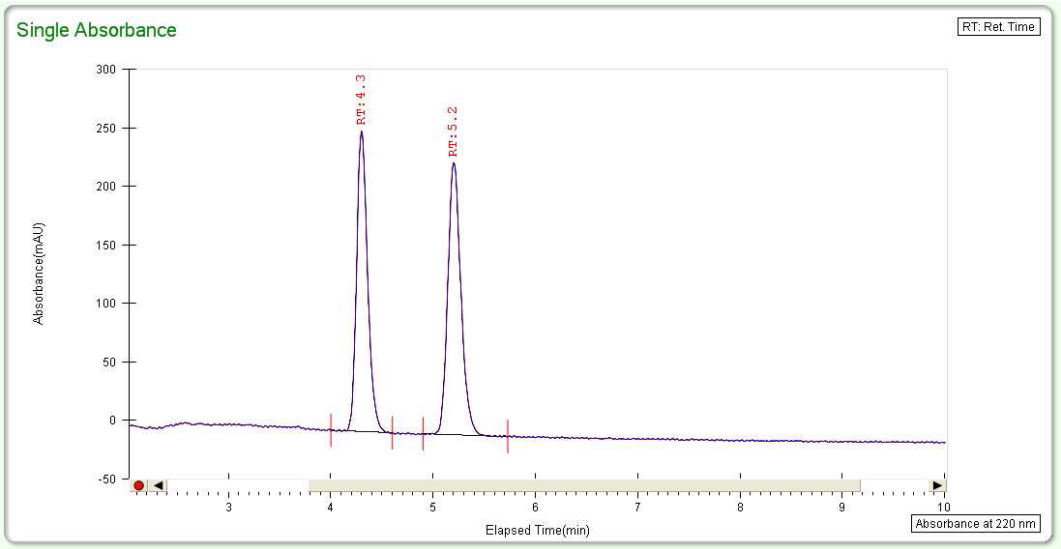
Scalemic: (SFC, CHIRALCEL®OD-H, 30% MeOH/CO_2, 3 mL/min, 220nm)



Peak Info

Peak No	**% Area**	**Area**	**RT (min)**	**Height (mV)**
1	6.726	41.687	4.38	5.5641
2	93.274	578.104	4.95	67.8426
Total:	100	619.791		

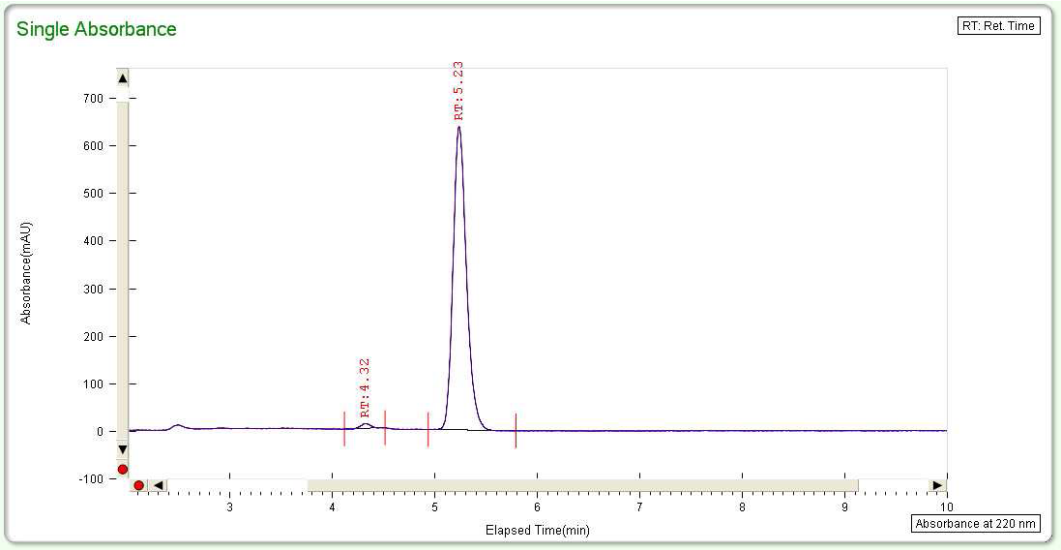
(*S,S*)-*N*-(4-nitrophenyl)sulfonyl-3-(3-bromophenyl)oxaziridine (**14**)
Racemic: (SFC, CHIRALCEL®OD-H, 30% MeOH/CO_2, 3 mL/min, 220nm)



Peak Info

Peak No	**% Area**	**Area**	**RT (min)**	**Height (mV)**
1	47.9602	1917.3299	4.3	256.1938
2	52.0398	2080.425	5.2	232.5002
Total:	100	3997.7549		

Scalemic: (SFC, CHIRALCEL®OD-H, 30% MeOH/CO_2, 3 mL/min, 220nm)

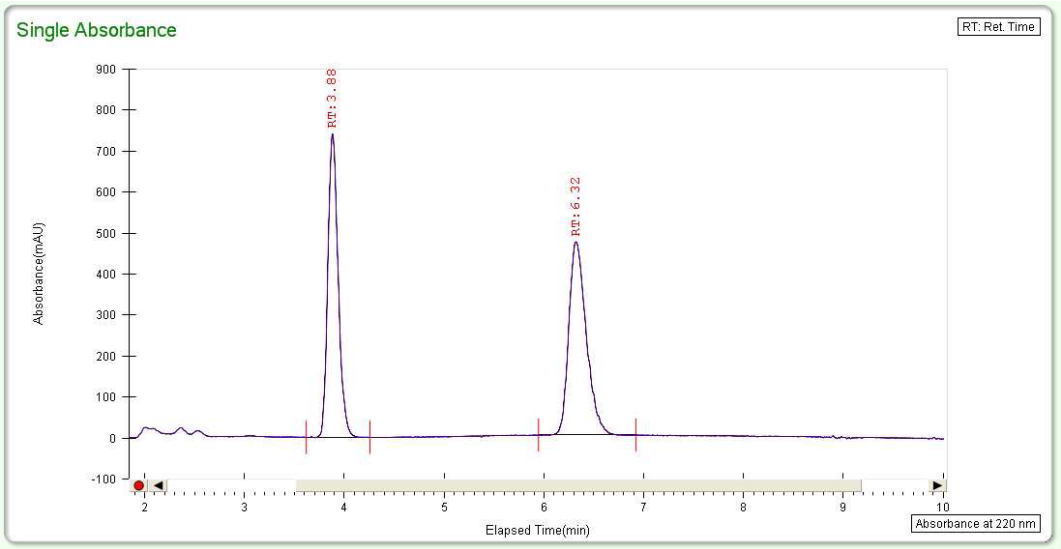


Peak Info

Peak No	**% Area**	**Area**	**RT (min)**	**Height (mV)**
1	1.0807	63.2948	4.32	9.9392
2	98.9193	5793.6904	5.23	638.1039
Total:	100	5856.9852		

(*S,S*)-*N*-(4-nosyl)-3-(2-bromophenyl)oxaziridine (15)

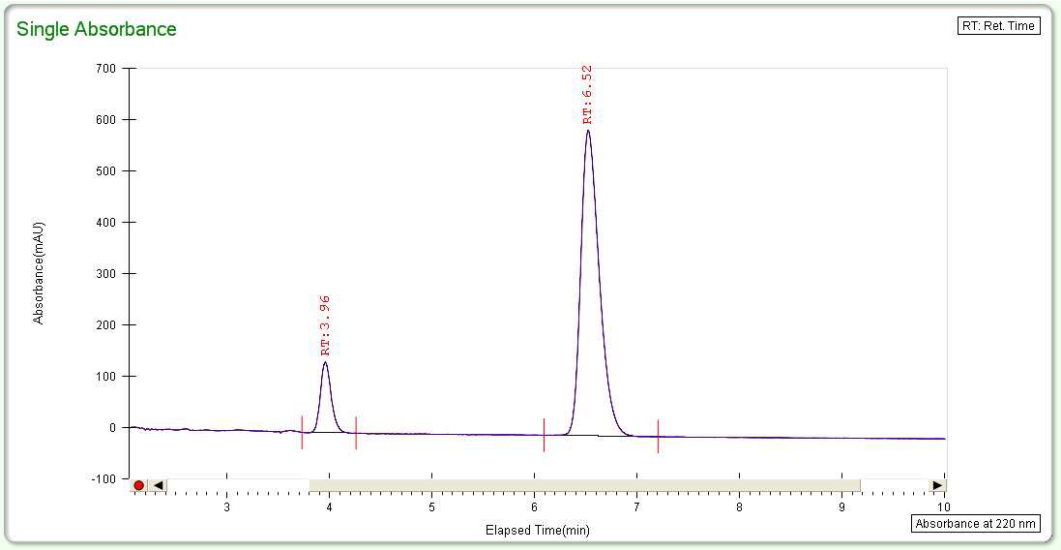
Racemic: (SFC, CHIRALCEL®OD-H, 40% MeOH/CO_2, 3 mL/min, 220nm)



Peak Info

Peak No	% Area	Area	RT (min)	Height (mV)
1	48.2436	5325.3555	3.88	740.5687
2	51.7564	5713.1174	6.32	471.1429
Total:	100	11038.4729		

Scalemic: (SFC, CHIRALCEL®OD-H, 40% MeOH/CO_2, 3 mL/min, 220nm)

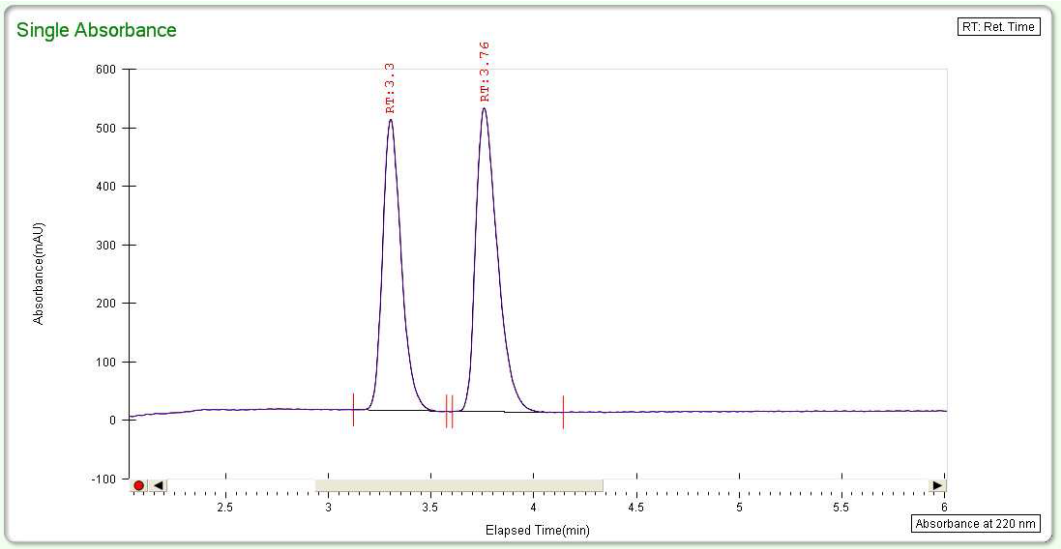


Peak Info

Peak No	% Area	Area	RT (min)	Height (mV)
1	11.8526	1003.4912	3.96	137.235
2	88.1474	7462.9143	6.52	594.3697
Total:	100	8466.4055		

(*S,S*)-*N*-phenylsulfonyl-3-(4-nitrophenyl) oxaziridine (**16**)

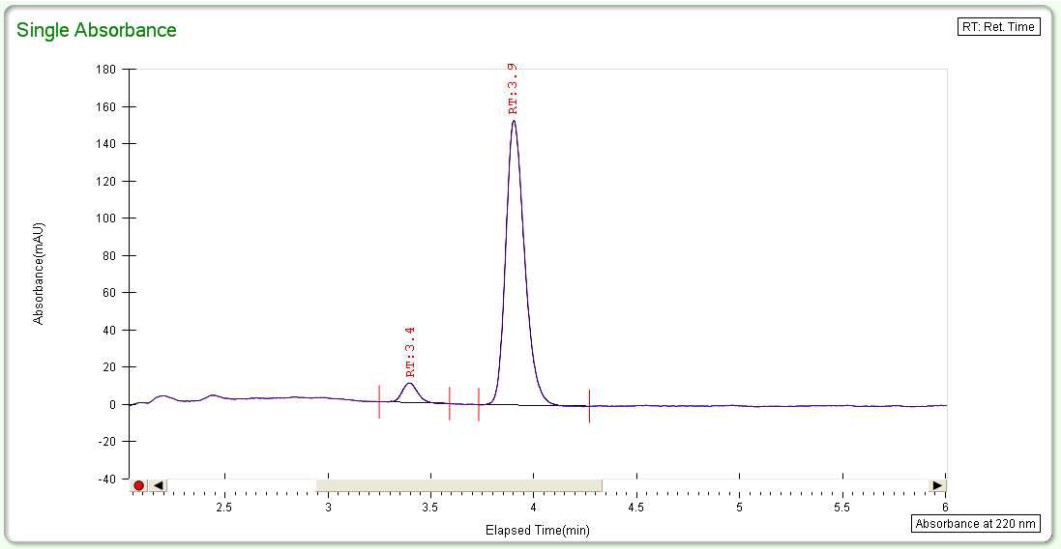
Racemic: (SFC, CHIRALCEL®OD-H, 30% MeOH/CO2, 3 mL/min, 220nm)



Peak Info

Peak No	% Area	Area	RT (min)	Height (mV)
1	45.0969	3122.3577	3.3	497.0033
2	54.9031	3801.3094	3.76	518.6987
Total:	100	6923.6671		

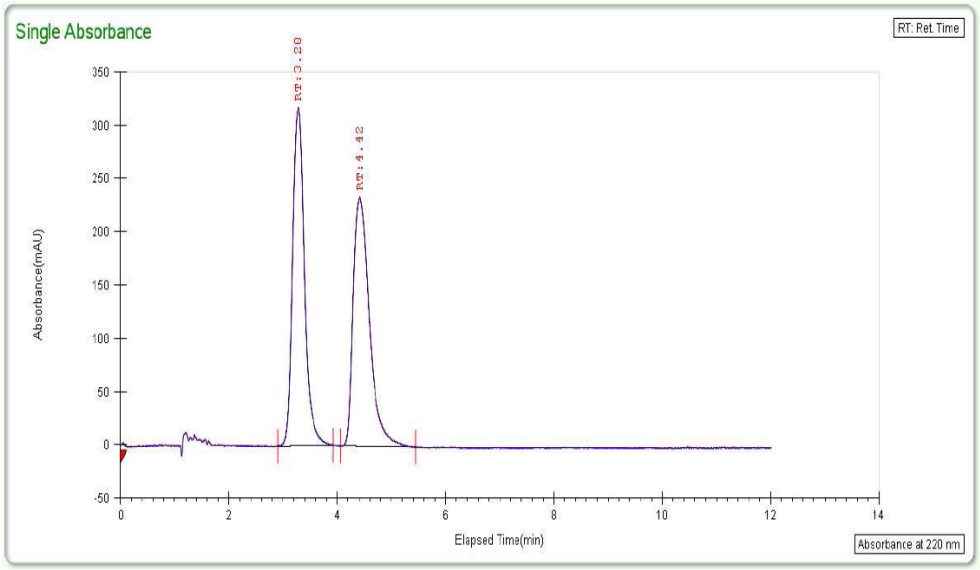
Scalemic: (SFC, CHIRALCEL®OD-H, 30% MeOH/CO2, 3 mL/min, 220nm)



Peak Info

Peak No	% Area	Area	RT (min)	Height (mV)
1	5.3208	54.4884	3.4	10.4546
2	94.6792	969.5753	3.9	152.8081
Total:	100	1024.0637		

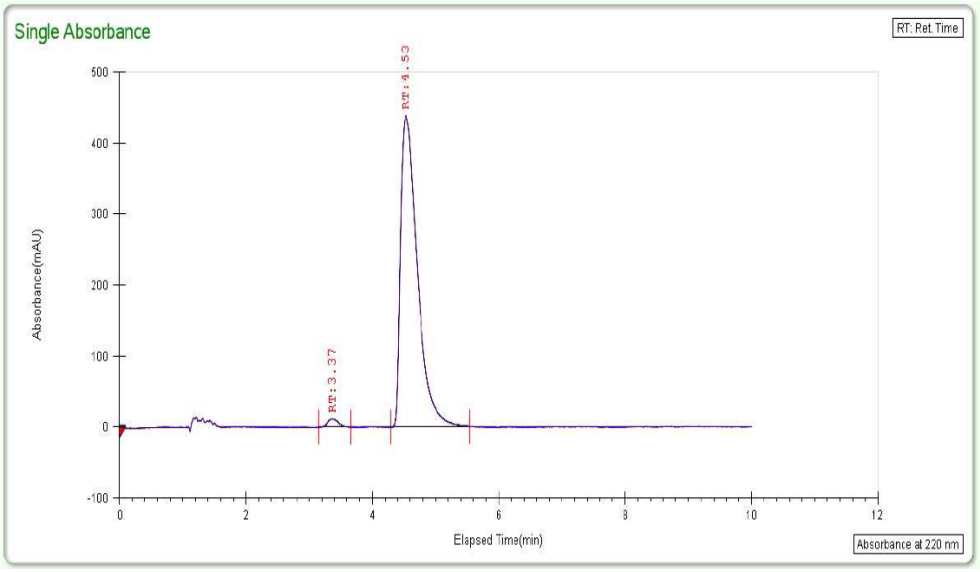
(*S,S*)-methyl 4-(2-(phenylsulfonyl)-1,2-oxaziridin-3-yl)benzoate (**17**)
Racemic: (SFC, CHIRALPAK®AS-H, 20% *i*-PrOH/CO2, 3 mL/min, 220nm)



Peak Info

Peak No	**% Area**	**Area**	**RT (min)**	**Height (mV)**
1	49.9838	4877.6762	3.28	317.6479
2	50.0162	4880.8391	4.42	233.888
Total:	100	9758.5153		

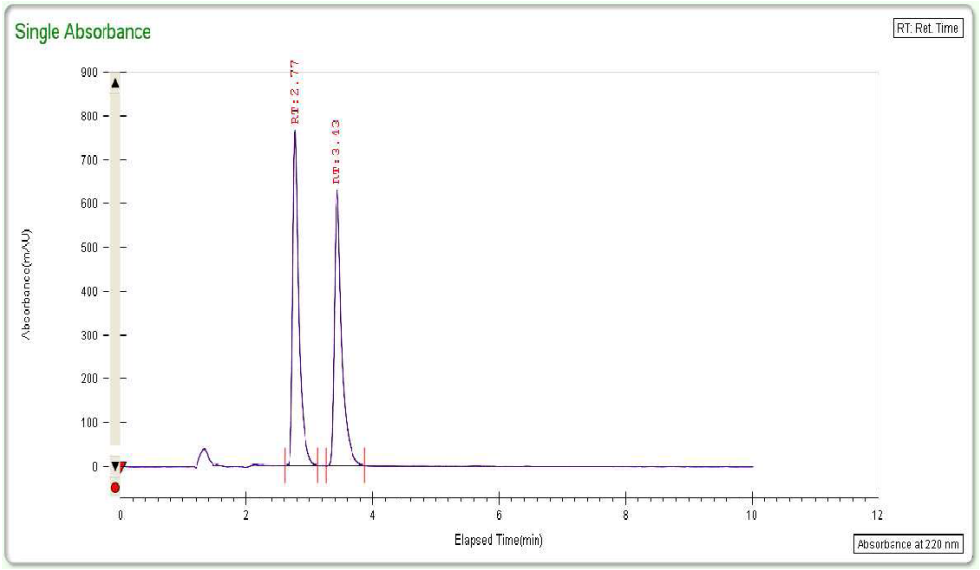
Scalemic: (SFC, CHIRALPAK®AS-H, 20% *i*-PrOH/CO2, 3 mL/min, 220nm)



Peak Info

Peak No	**% Area**	**Area**	**RT (min)**	**Height (mV)**
1	1.6024	131.7158	3.37	11.5568
2	98.3976	8088.1607	4.53	438.3503
Total:	100	8219.8765		

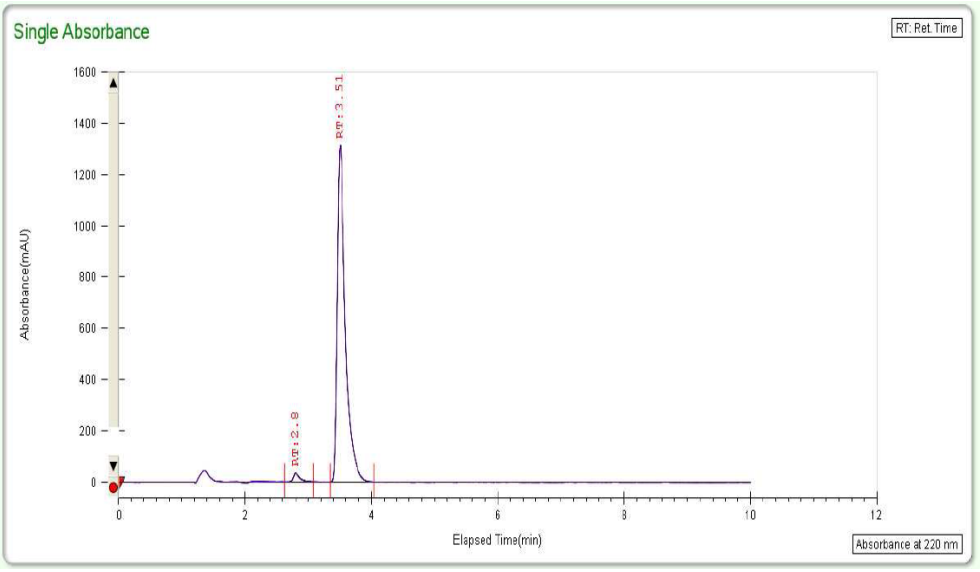
(*S,S*)-*N*-(4-tosyl)-3-(4-(trifluoromethyl)phenyl)oxaziridine (18)
Racemic: (SFC, CHIRALPAK®AD-H, 40% MeOH/CO_2, 3 mL/min, 220nm)



Peak Info

Peak No	% Area	Area	RT (min)	Height (mV)
1	49.8959	5111.9271	2.77	762.918
2	50.1041	5133.2539	3.43	626.5343
Total:	100	10245.181		

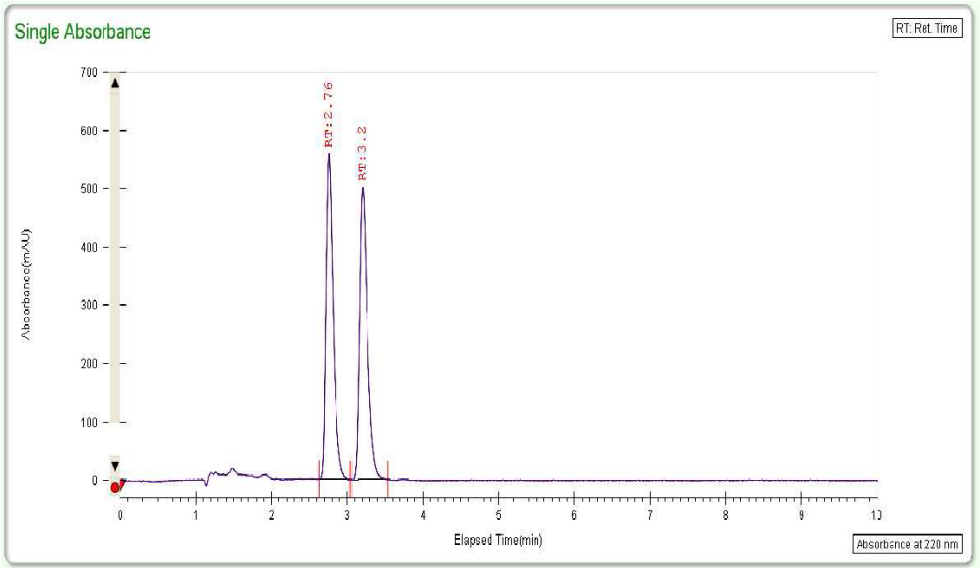
Scalemic: (SFC, CHIRALPAK®AD-H, 40% MeOH/CO_2, 3 mL/min, 220nm)



Peak Info

Peak No	% Area	Area	RT (min)	Height (mV)
1	2.0476	247.2003	2.8	35.9206
2	97.9524	11825.5363	3.51	1314.6334
Total:	100	12072.7366		

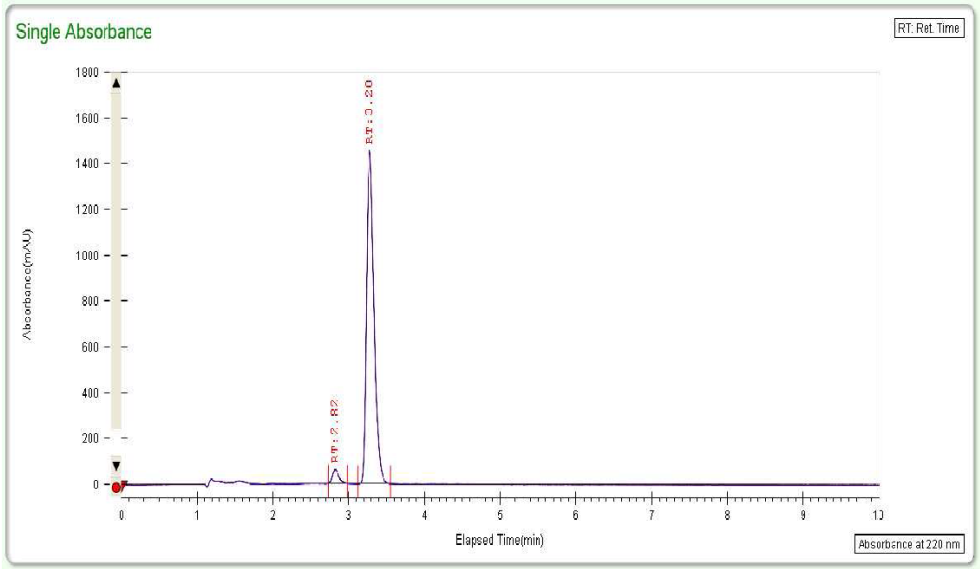
(*S,S*)-3-(2-(phenylsulfonyl)-1,2-oxaziridin-3-yl)phenyl acetate (**19**)
Racemic: (SFC, CHIRALCEL®OJ-H, 25% MeOH/CO_2, 3 mL/min, 220nm)



Peak Info

Peak No	**% Area**	**Area**	**RT (min)**	**Height (mV)**
1	50.176	3577.5127	2.76	557.4579
2	49.824	3552.4103	3.2	500.6532
Total:	100	7129.923		

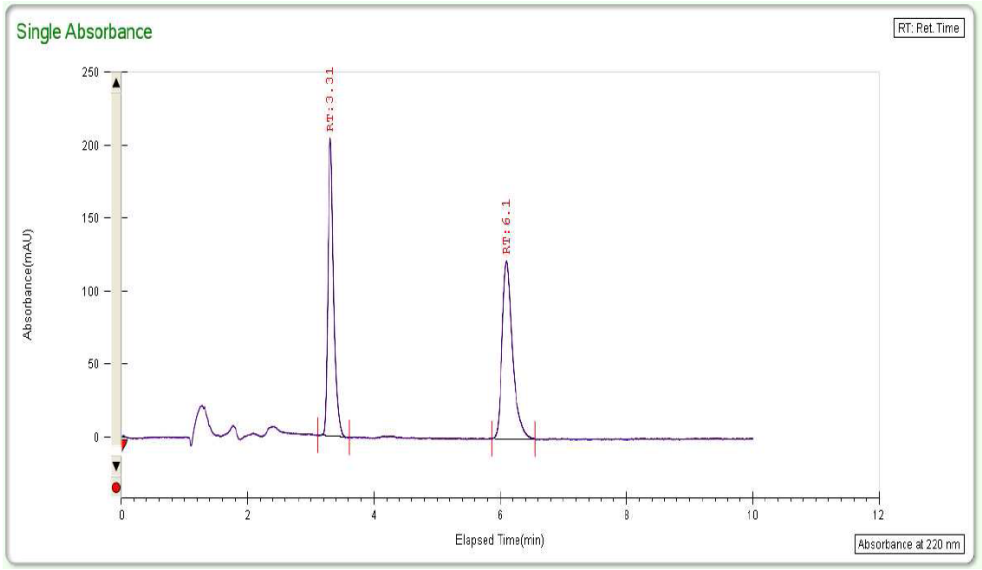
Scalemic: (SFC, CHIRALCEL®OJ-H, 25% MeOH/CO_2, 3 mL/min, 220nm)



Peak Info

Peak No	**% Area**	**Area**	**RT (min)**	**Height (mV)**
1	3.3507	348.0999	2.82	58.621
2	96.6493	10040.6952	3.28	1455.3049
Total:	100	10388.7951		

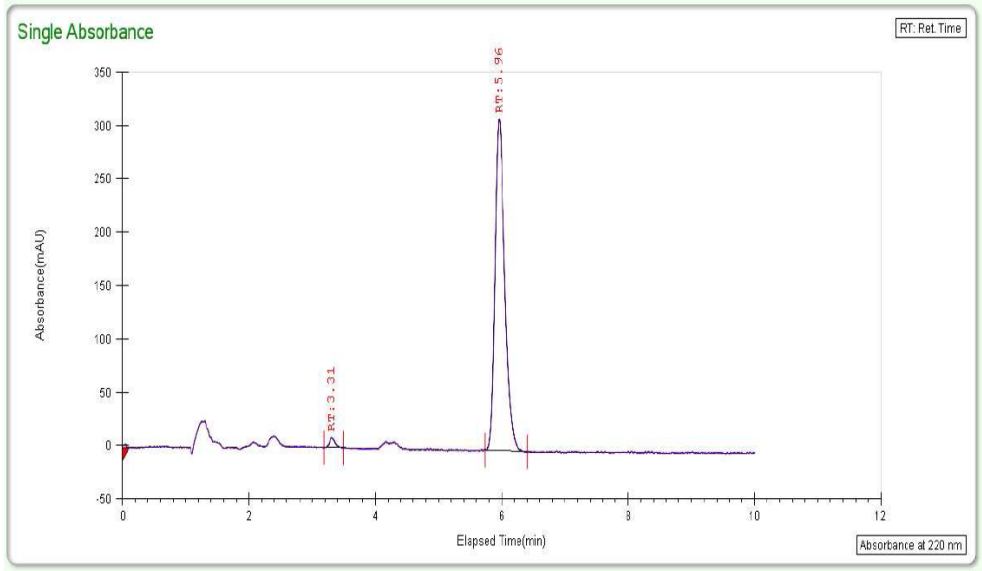
(*S,S*)-*N*-((4-nitrophenyl)sulfonyl)-3-(*m*-tolyl)oxaziridine (20)
Racemic: (SFC, CHIRALCEL®OD-H, 30% MeOH/CO_2, 3 mL/min, 220nm)



Peak Info

Peak No	% Area	Area	RT (min)	Height (mV)
1	48.6624	1309.5671	3.31	203.8318
2	51.3376	1381.5609	6.1	121.724
Total:	100	2691.128		

Scalemic: (SFC, CHIRALCEL®OD-H, 30% MeOH/CO_2, 3 mL/min, 220nm)

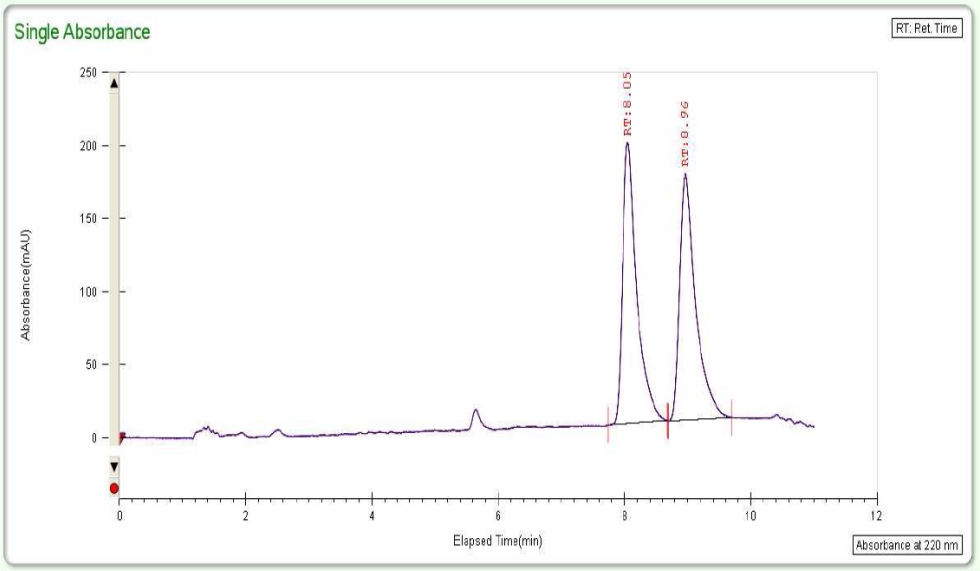


Peak Info

Peak No	% Area	Area	RT (min)	Height (mV)
1	1.7384	58.673	3.31	9.5486
2	98.2616	3316.4382	5.96	310.8549
Total:	100	3375.1112		

(*S,S*)-3-(perfluorophenyl)-2-tosyl-1,2-oxaziridine (**21**)

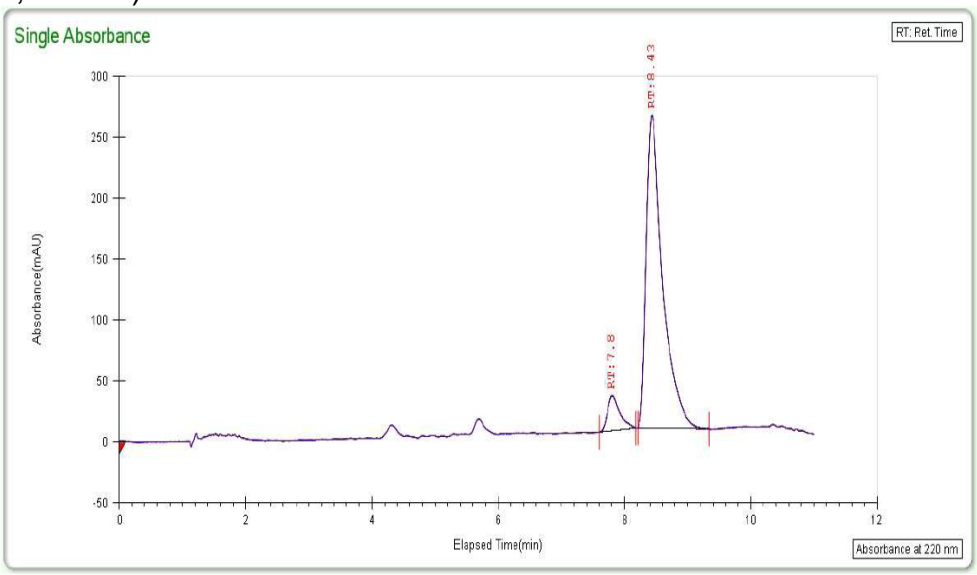
Racemic: (SFC, CHIRALPAK®AD-H, 10–40% gradient (465 sec) MeOH/CO_2, 3 mL/min, 220nm)



Peak Info

Peak No	**% Area**	**Area**	**RT (min)**	**Height (mV)**
1	50.0285	2973.0716	8.05	192.4302
2	49.9715	2969.6842	8.96	168.8506
Total:	100	5942.7558		

Scalemic: (SFC, CHIRALPAK®AD-H, 10–40% gradient (465 sec) MeOH/CO_2, 3 mL/min, 220nm)

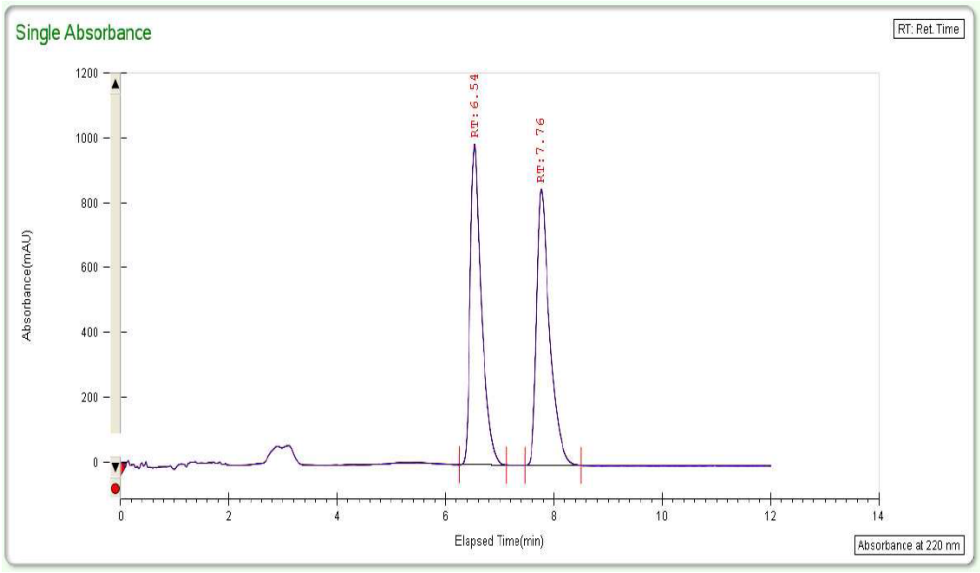


Peak Info

Peak No	**% Area**	**Area**	**RT (min)**	**Height (mV)**
1	7.6707	386.5451	7.8	28.5982
2	92.3293	4652.7152	8.43	256.4473
Total:	100	5039.2603		

(*S,S*)-3-(naphthalen-2-yl)-2-(phenylsulfonyl)oxaziridine (**22**)

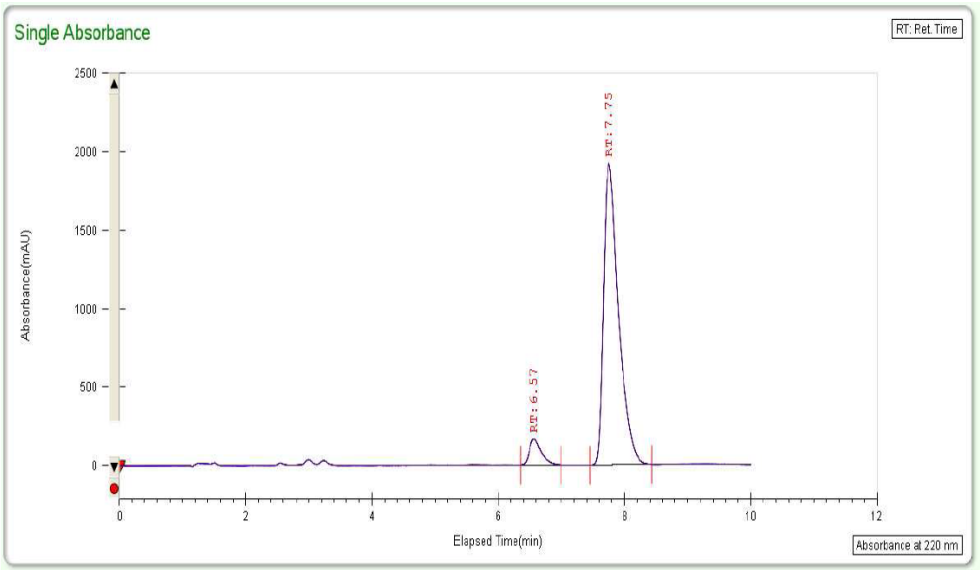
Racemic: (SFC, CHIRALCEL®OJ-H, 30% MeOH/CO_2, 3 mL/min, 220nm)



Peak Info

Peak No	% Area	Area	RT (min)	Height (mV)
1	49.7551	14042.0072	6.54	988.5571
2	50.2449	14180.2294	7.76	852.6082
Total:	100	28222.2366		

Scalemic: (SFC, CHIRALCEL®OJ-H, 30% MeOH/CO_2, 3 mL/min, 220nm)

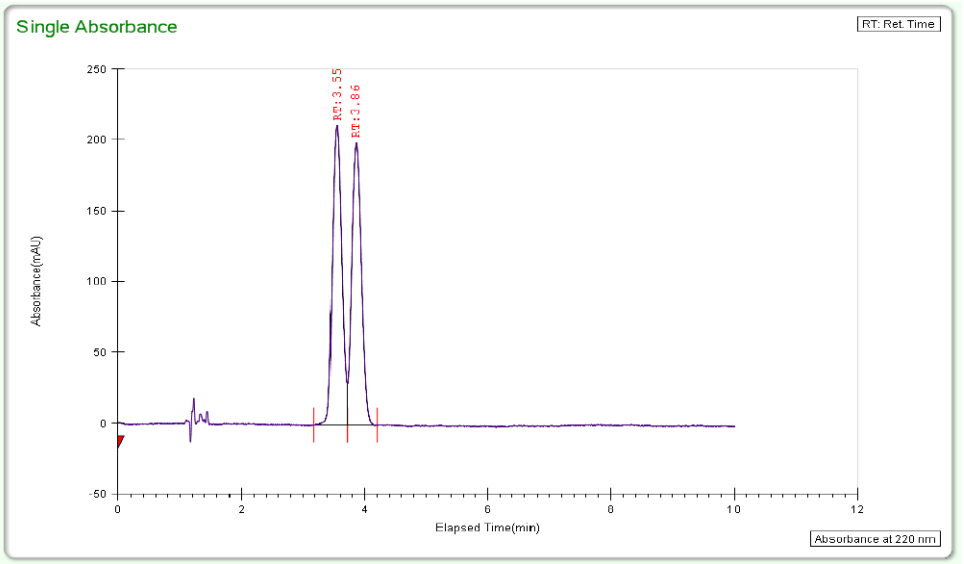


Peak Info

Peak No	% Area	Area	RT (min)	Height (mV)
1	6.4998	2186.3662	6.57	167.7388
2	93.5002	31451.1649	7.75	1920.184
Total:	100	33637.5311		

(*S,S*)-3-(cyclohexyl)-2-tosyl-1,2-oxaziridine (23)

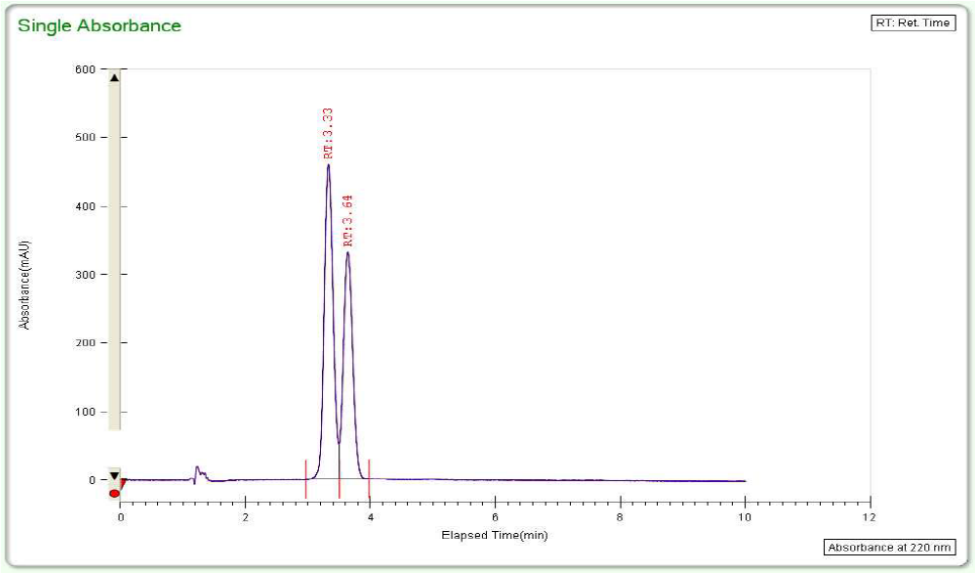
Racemic: (SFC, CHIRALCEL®OJ-H, 5% *i*-PrOH/CO_2, 3 mL/min, 220nm)



Peak Info

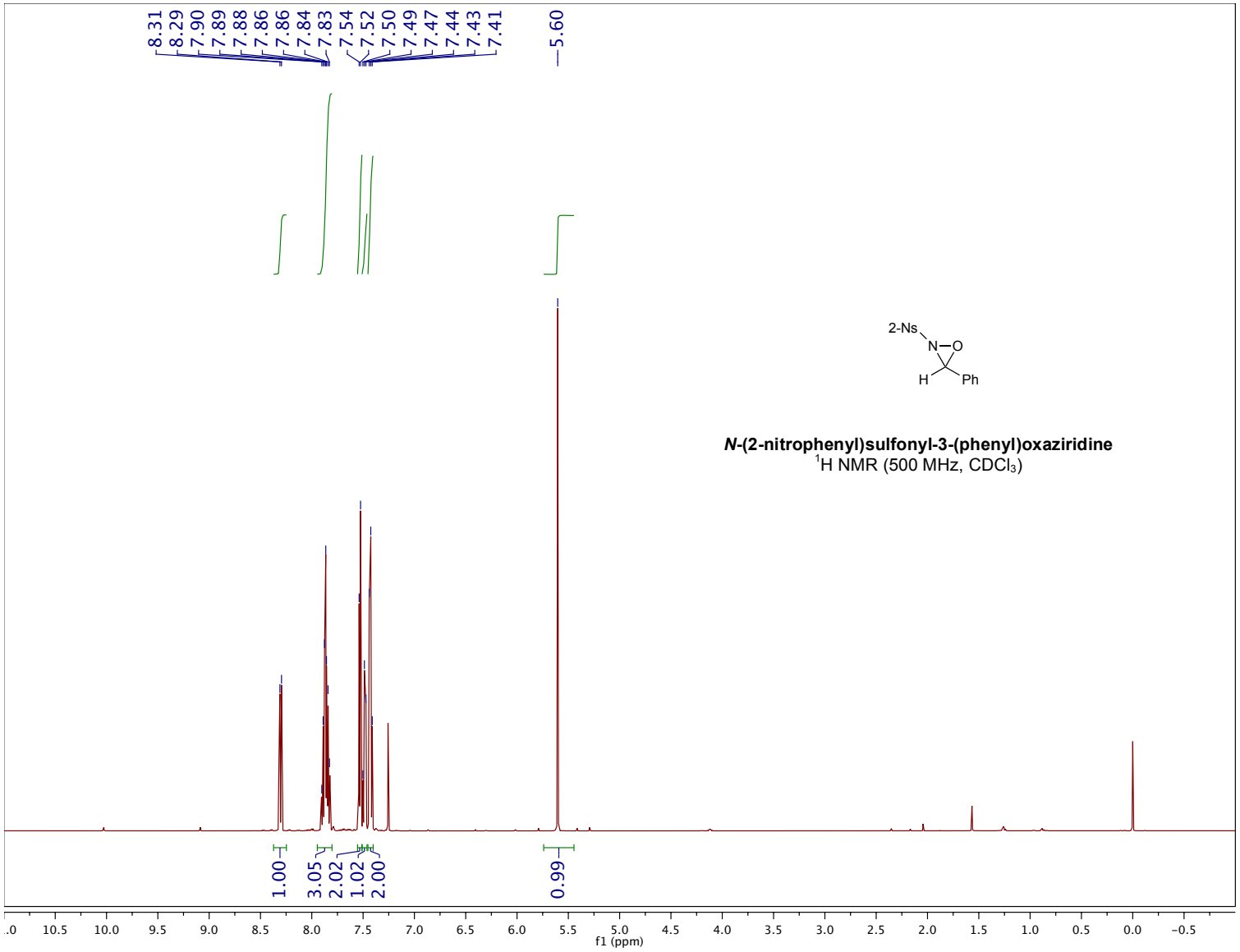
Peak No	% Area	Area	RT (min)	Height (mV)
1	50.2851	2194.6948	3.55	211.2317
2	49.7149	2169.8055	3.86	199.1256
Total:	100	4364.5003		

Scalemic: (SFC, CHIRALCEL®OJ-H, 5% *i*-PrOH /CO_2, 3 mL/min, 220nm)



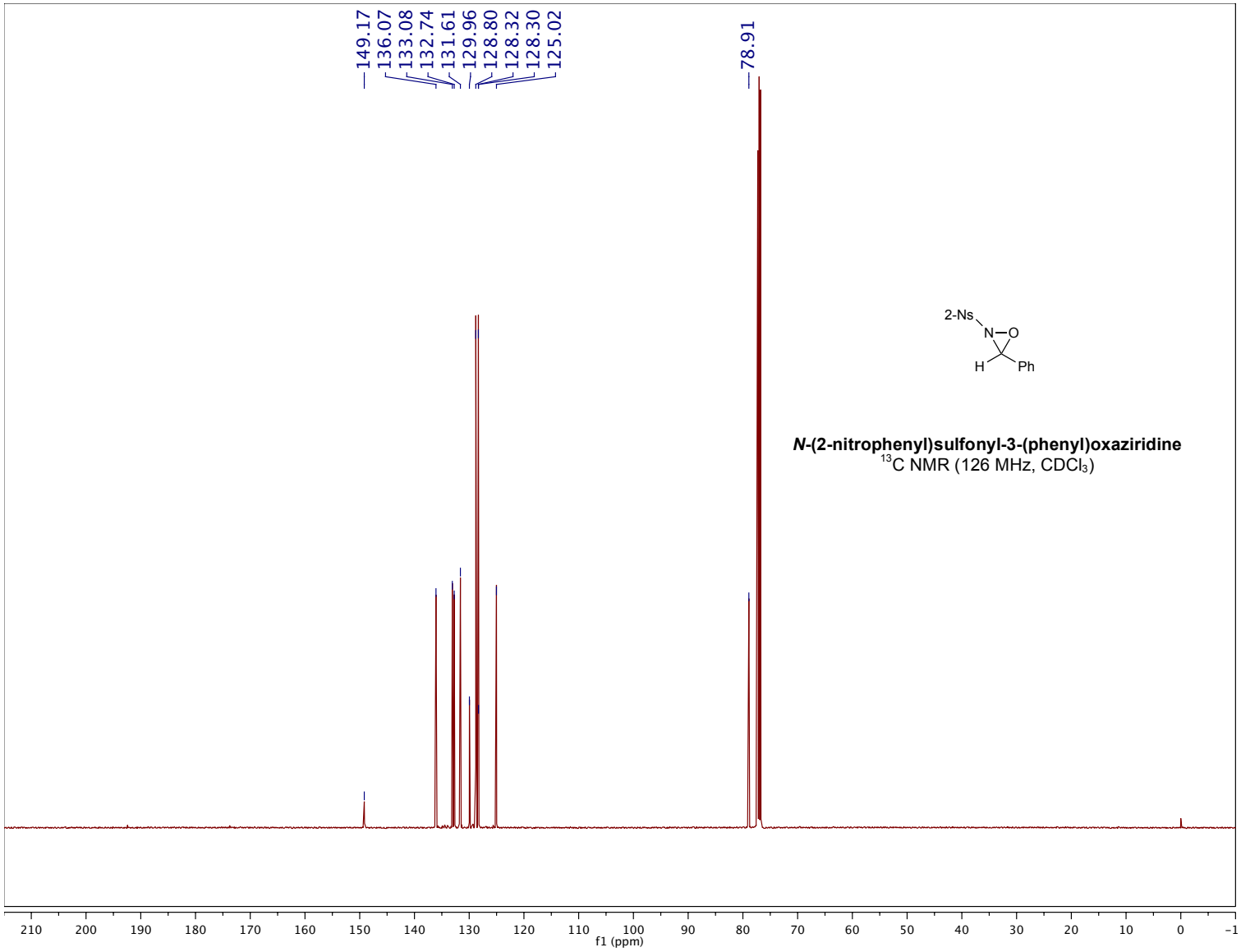
Peak Info

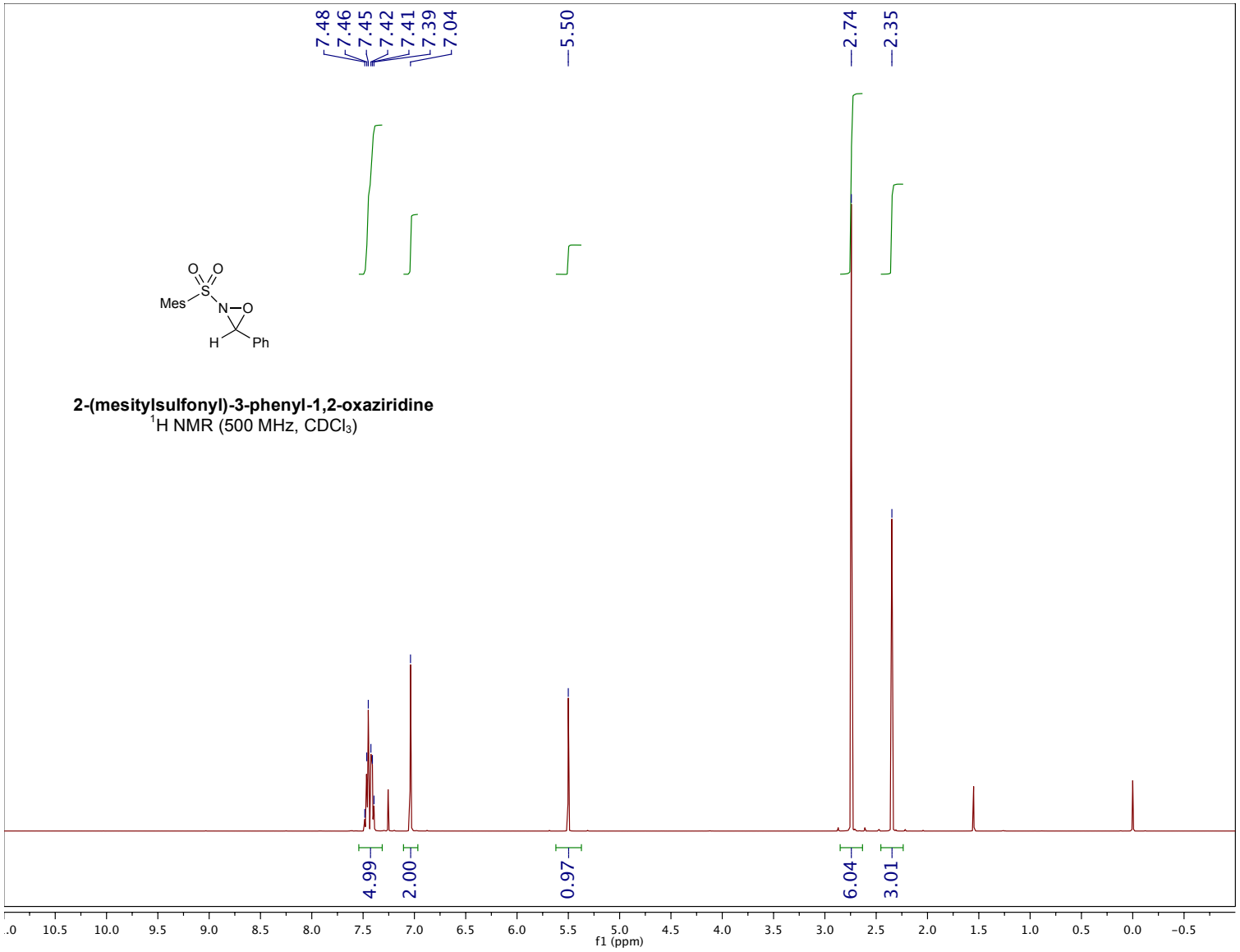
Peak No	% Area	Area	RT (min)	Height (mV)
1	57.3964	4567.535	3.33	459.5881
2	42.6036	3390.3426	3.64	331.4321
Total:	100	7957.8776		



***N*-(2-nitrophenyl)sulfonyl-3-(phenyl)oxaziridine**

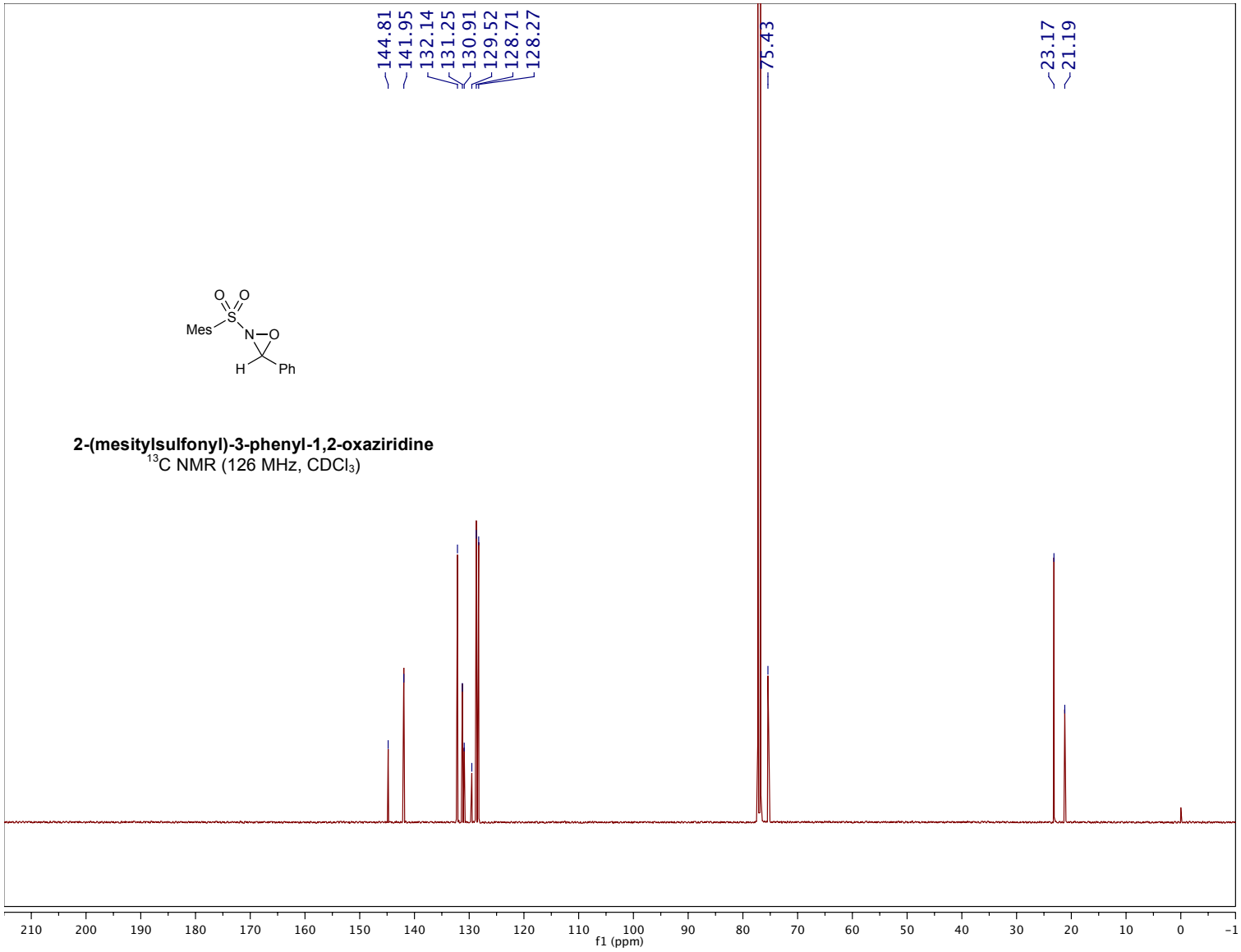
^{1}H NMR (500 MHz, $CDCl_3$)

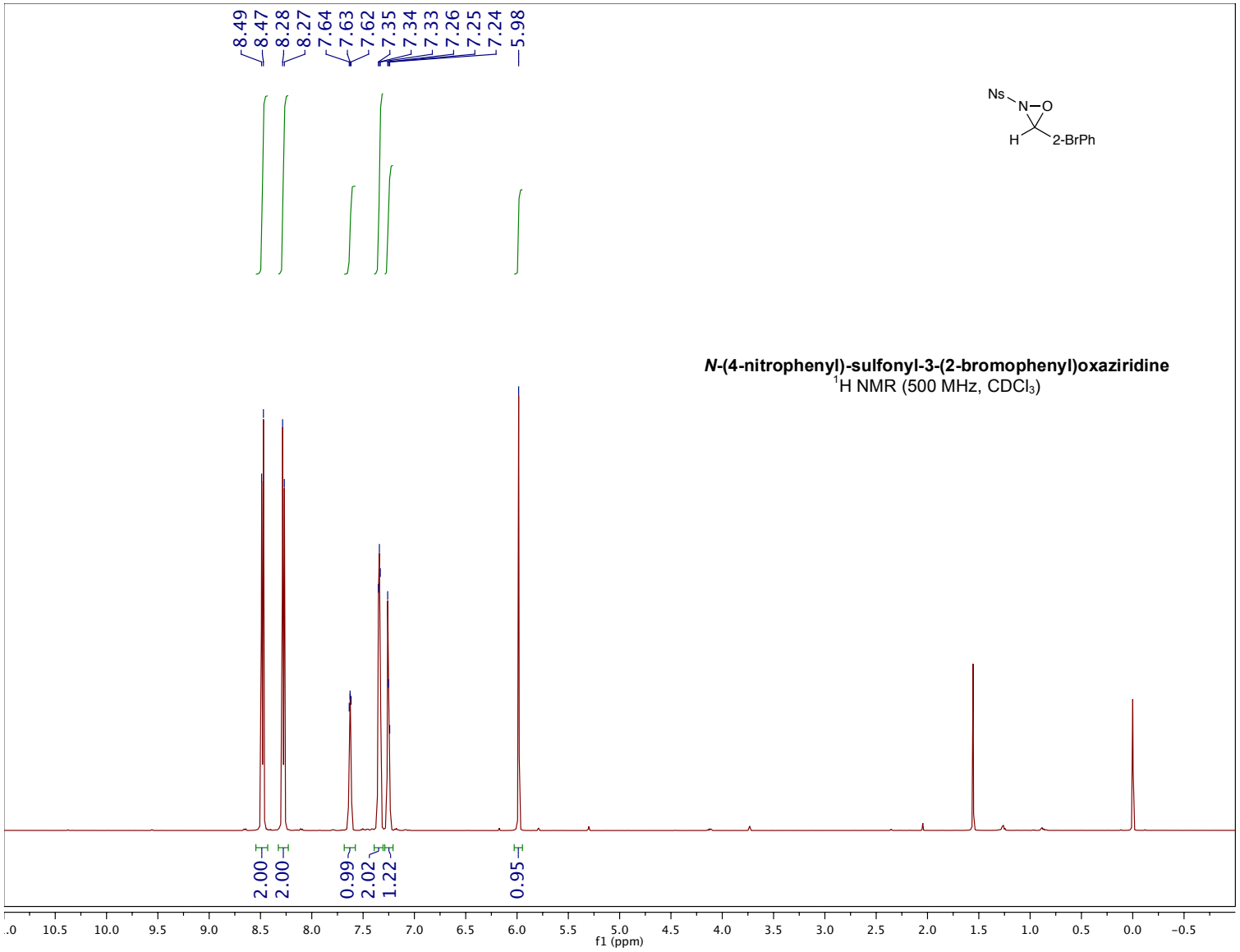

149.17
136.07
133.08
132.74
131.61
129.96
128.80
128.32
128.30
125.02
78.91
2-Ns
N
O
H
Ph
***N*-(2-nitrophenyl)sulfonyl-3-(phenyl)oxaziridine**
^{13}C NMR (126 MHz, $CDCl_3$)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −1
f1 (ppm)



2-(mesitylsulfonyl)-3-phenyl-1,2-oxaziridine

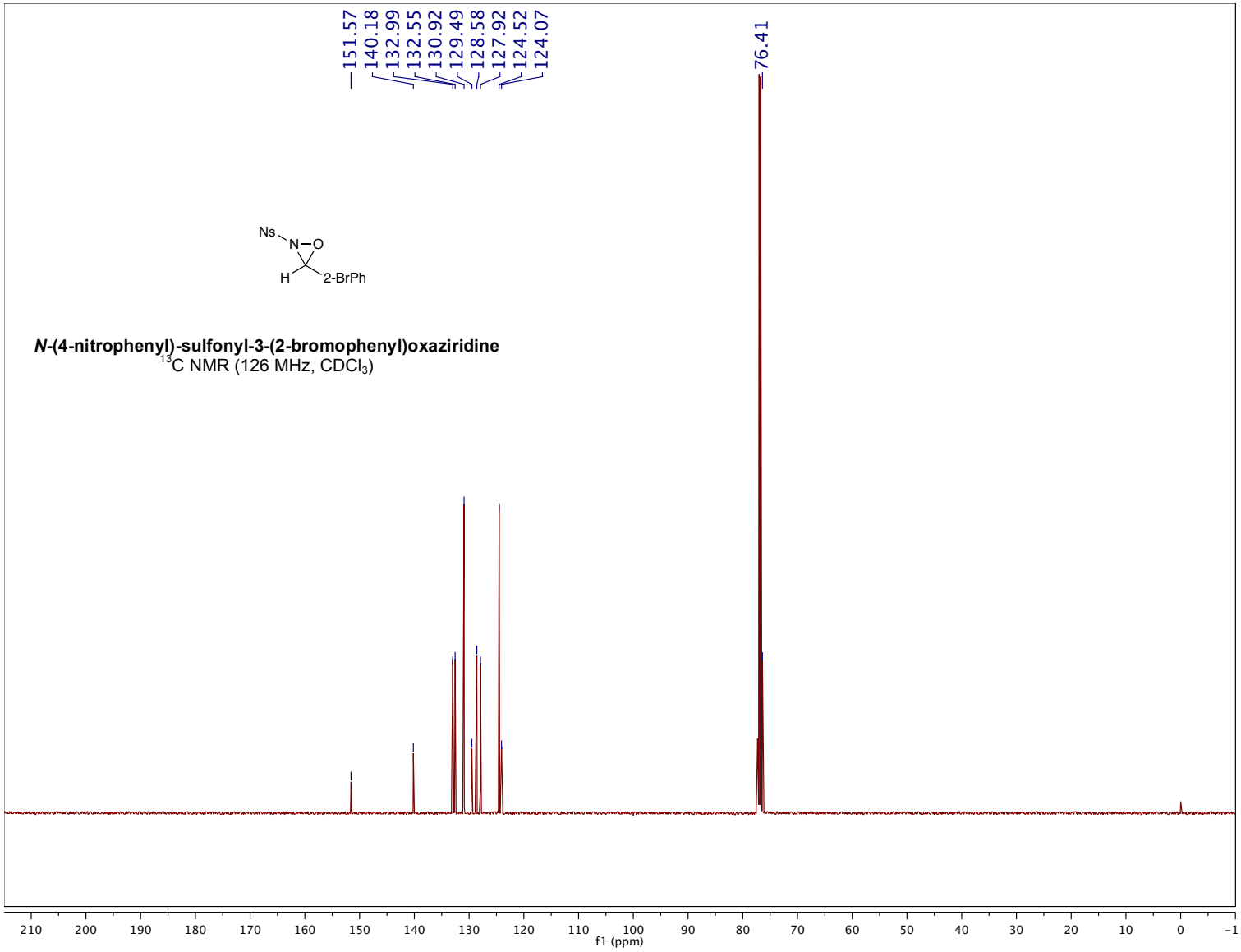
^{1}H NMR (500 MHz, $CDCl_3$)

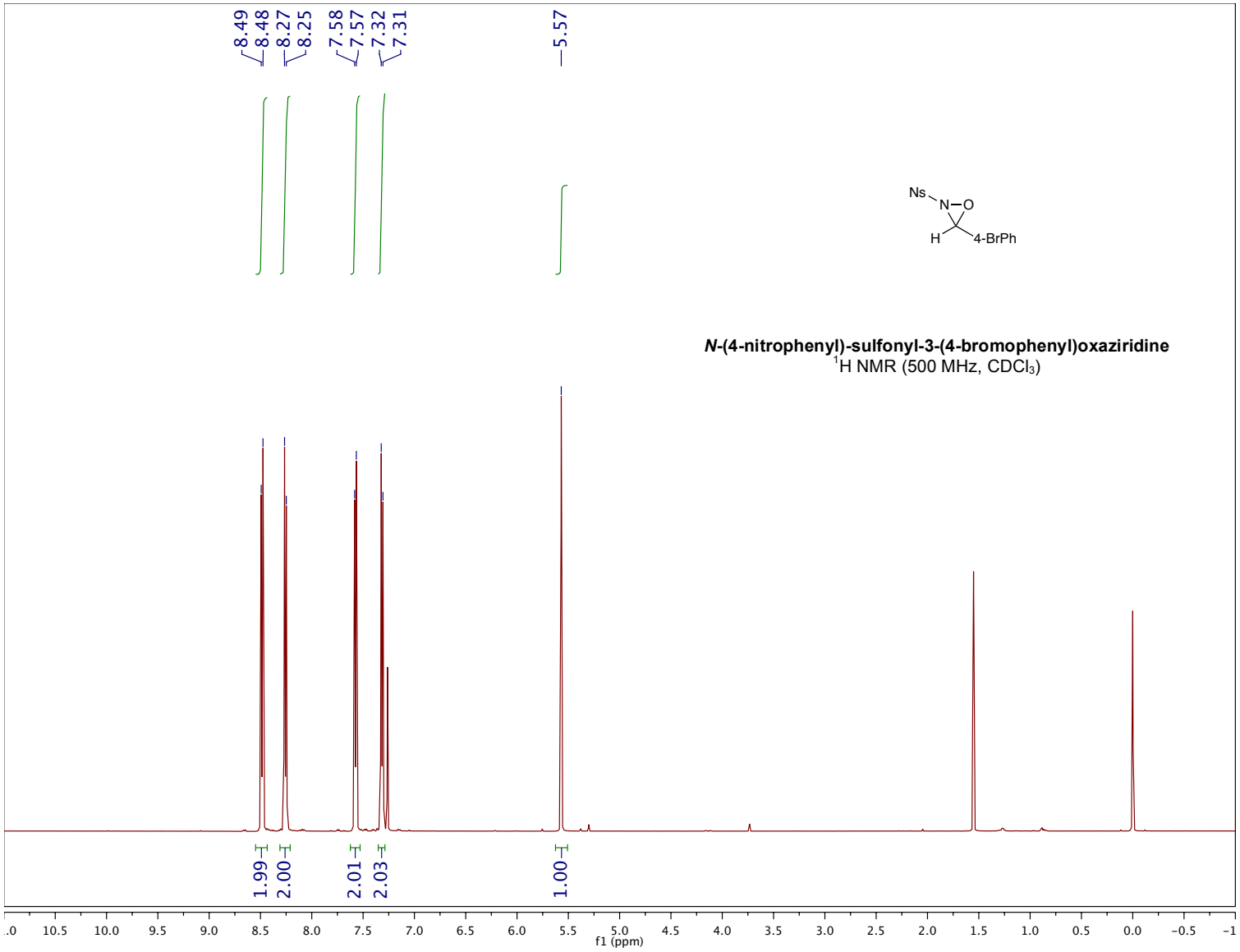

144.81
141.95
132.14
131.25
130.91
129.52
128.71
128.27
75.43
23.17
21.19
O
O
S
Mes
N
O
H
Ph
2-(mesitylsulfonyl)-3-phenyl-1,2-oxaziridine
13C NMR (126 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)



***N*-(4-nitrophenyl)-sulfonyl-3-(2-bromophenyl)oxaziridine**

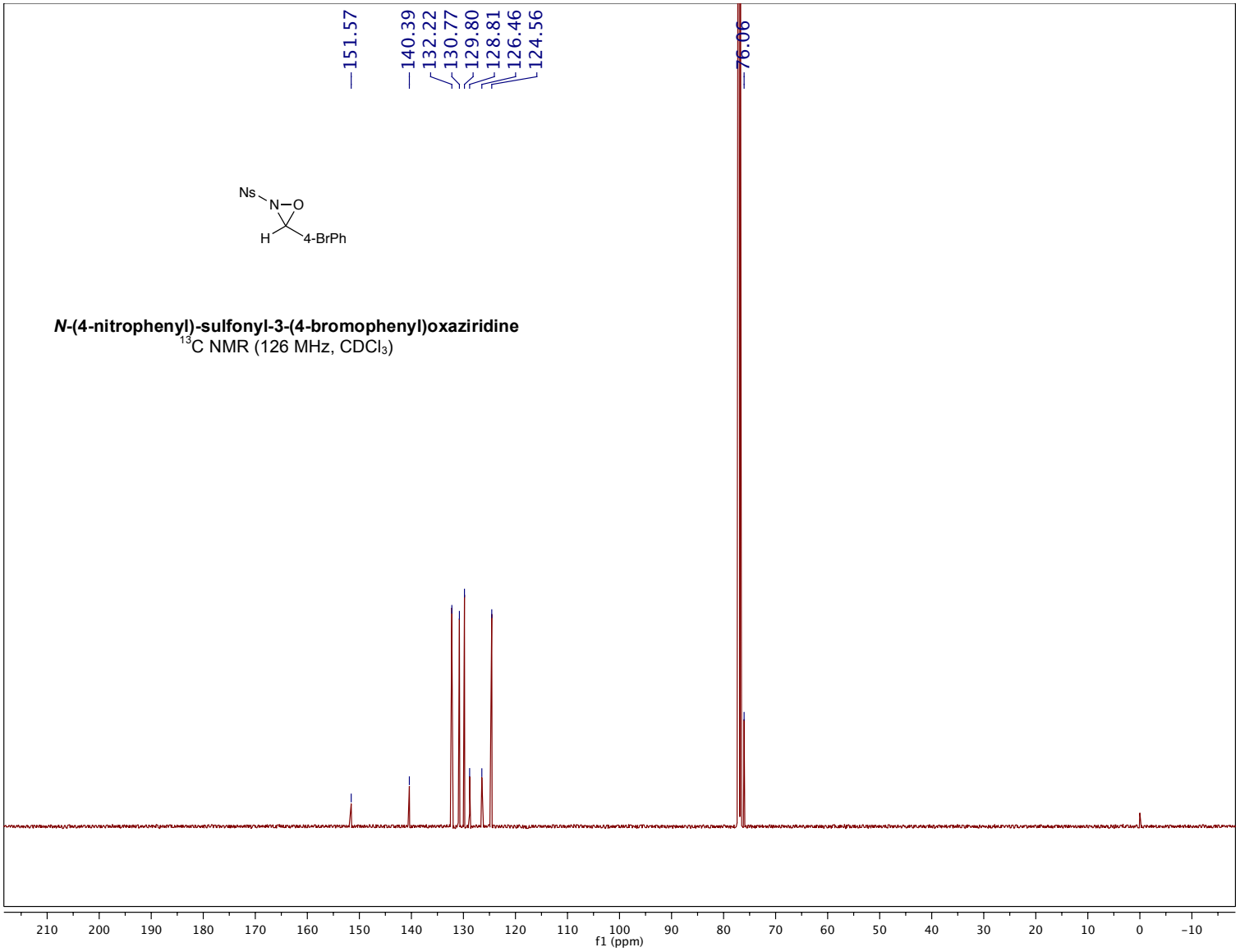
^{1}H NMR (500 MHz, $CDCl_3$)

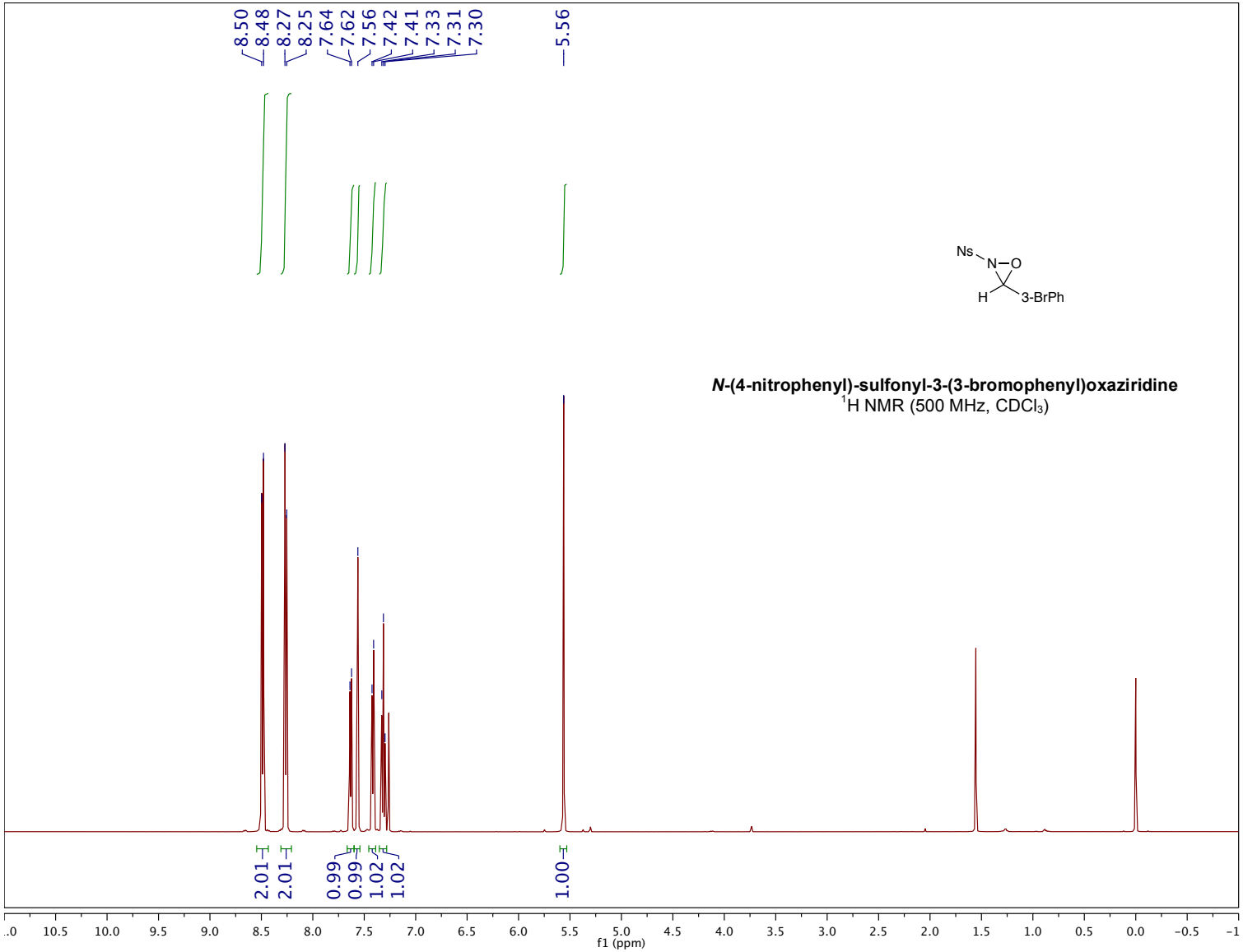

151.57
140.18
132.99
132.55
130.92
129.49
128.58
127.92
124.52
124.07
76.41
Ns
N
O
H
2-BrPh
***N*-(4-nitrophenyl)-sulfonyl-3-(2-bromophenyl)oxaziridine**
^{13}C NMR (126 MHz, $CDCl_3$)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)



***N*-(4-nitrophenyl)-sulfonyl-3-(4-bromophenyl)oxaziridine**

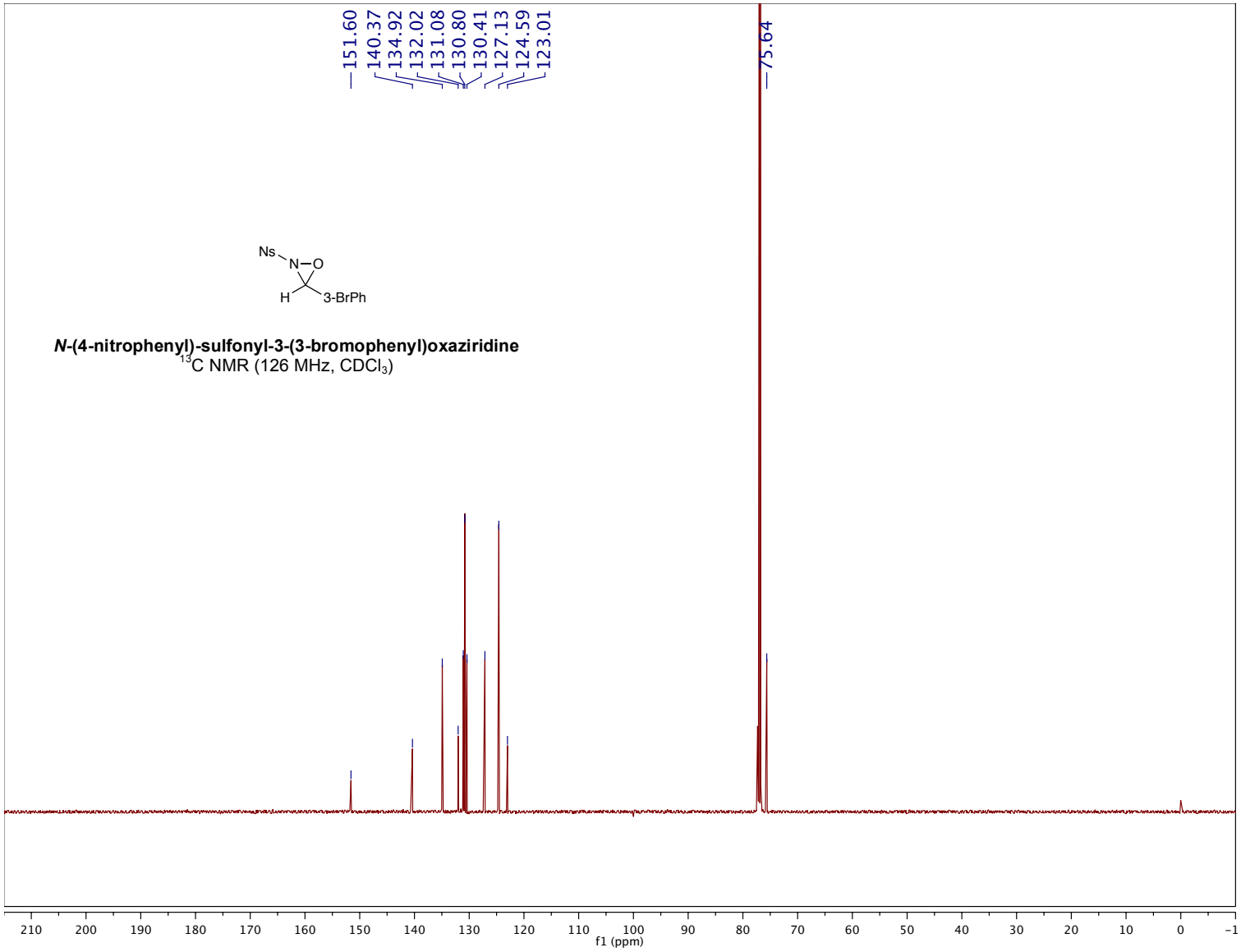
^{1}H NMR (500 MHz, $CDCl_3$)


151.57
140.39
132.22
130.77
129.80
128.81
126.46
124.56
76.06
Ns
N
O
H
4-BrPh
***N*-(4-nitrophenyl)-sulfonyl-3-(4-bromophenyl)oxaziridine**
^{13}C NMR (126 MHz, $CDCl_3$)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)



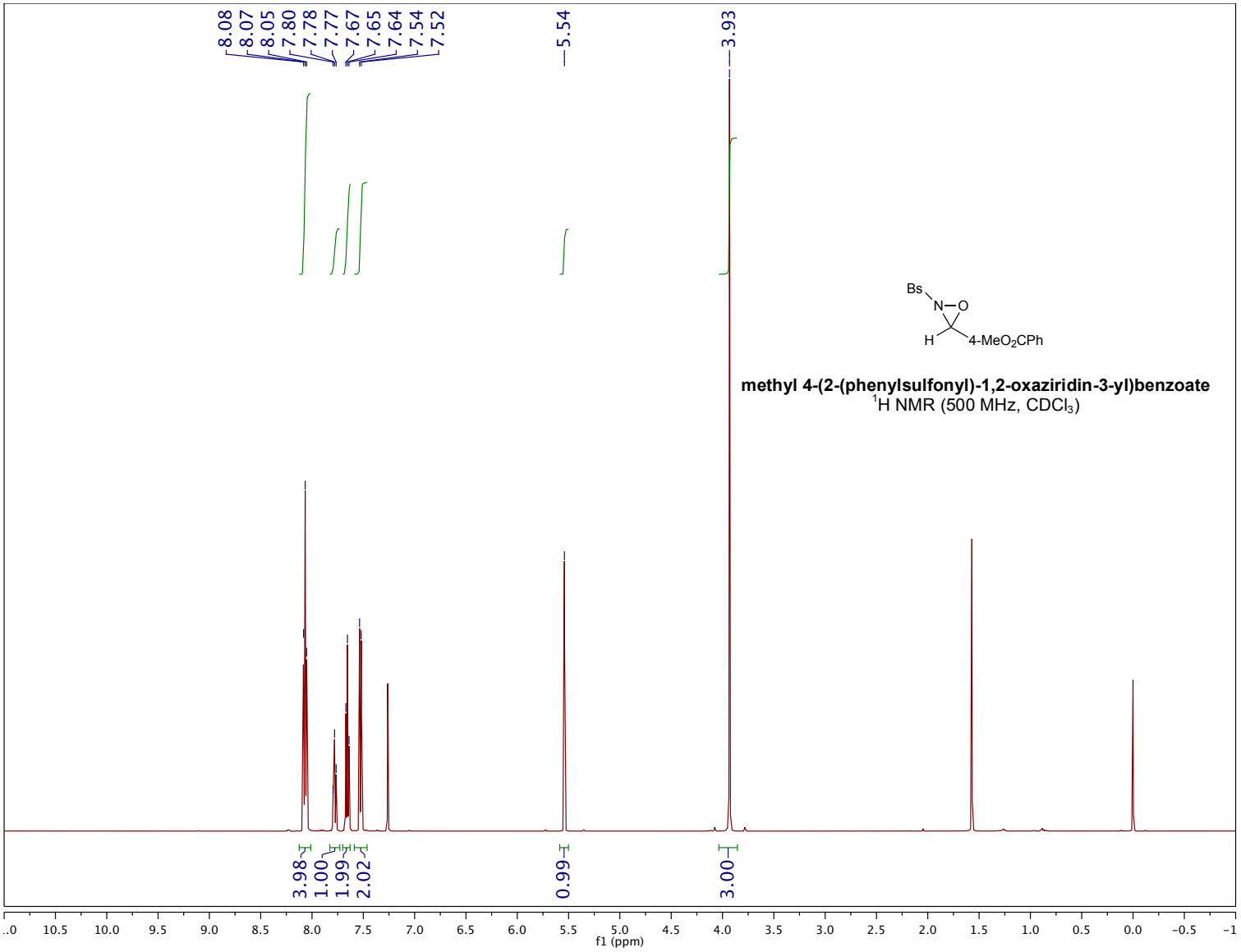
***N*-(4-nitrophenyl)-sulfonyl-3-(3-bromophenyl)oxaziridine**

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



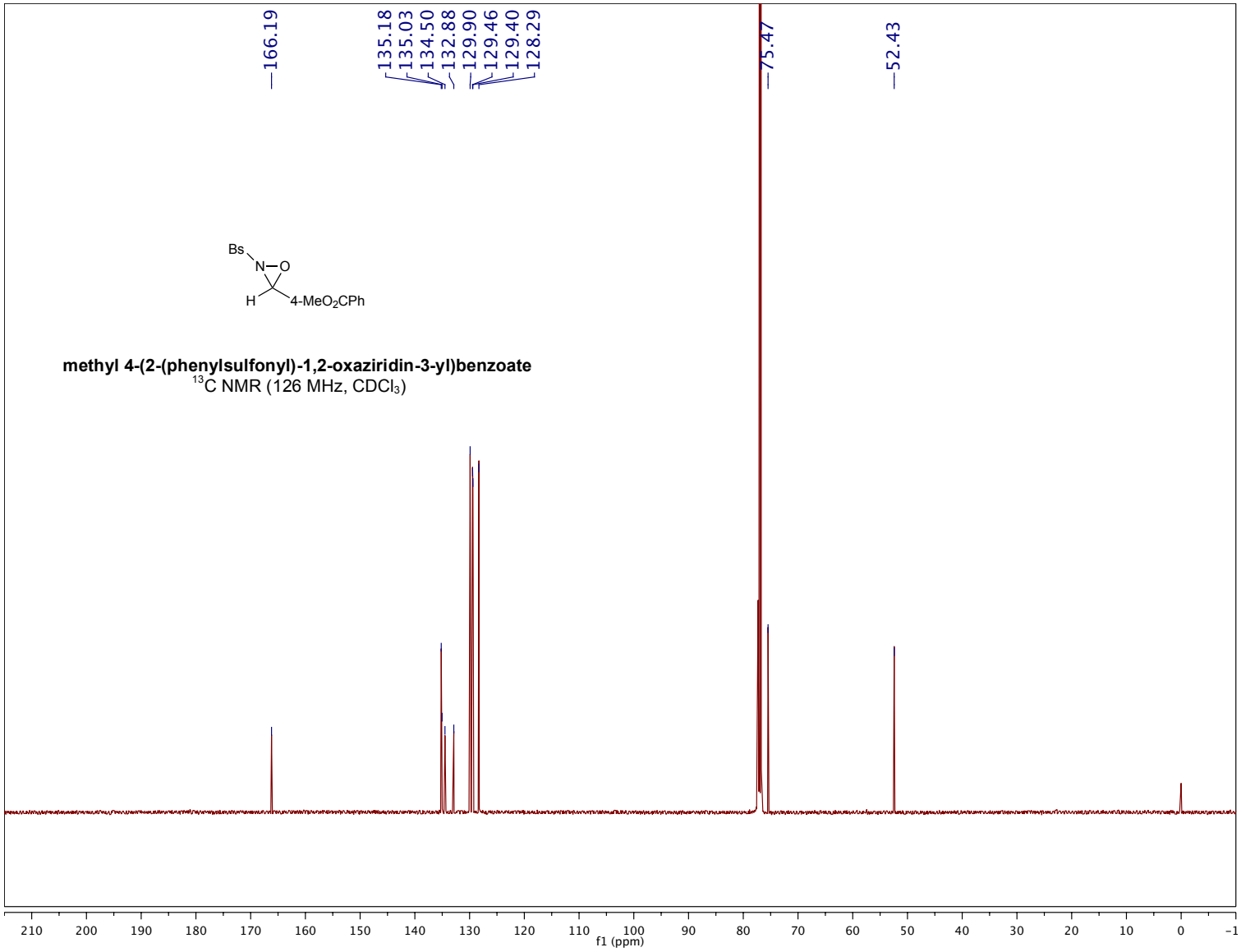
***N*-(4-nitrophenyl)-sulfonyl-3-(3-bromophenyl)oxaziridine**

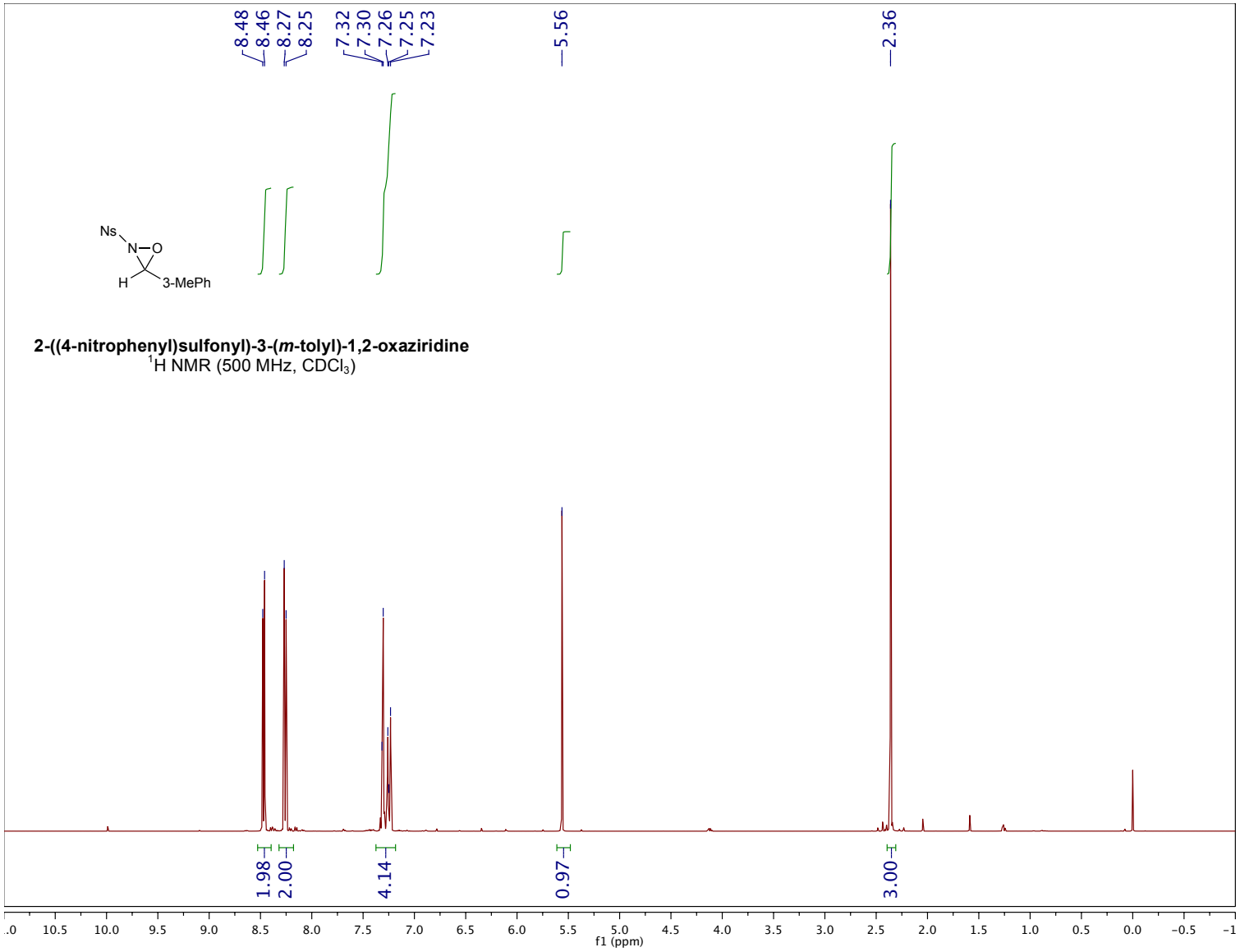
^{13}C NMR (126 MHz, $CDCl_3$)

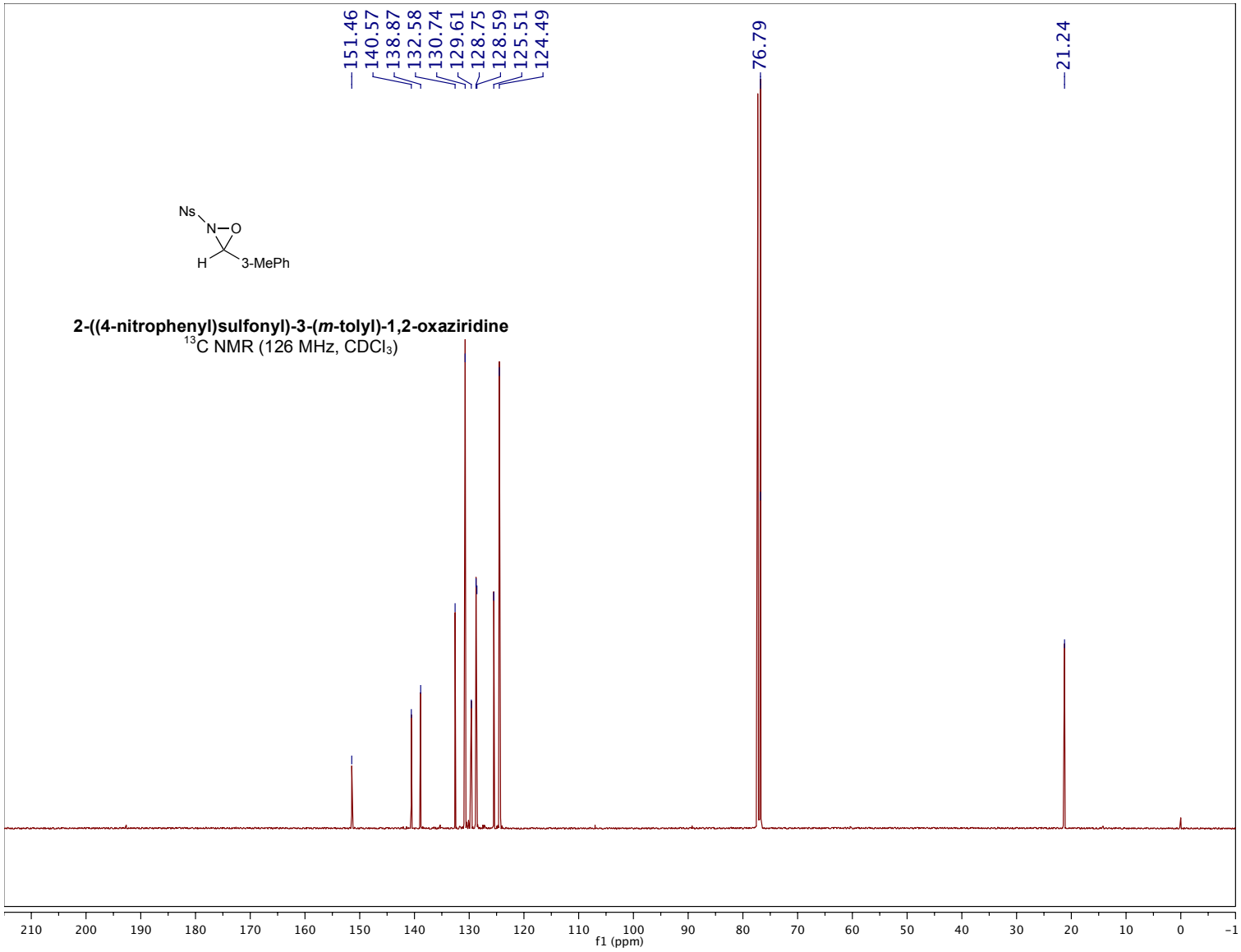


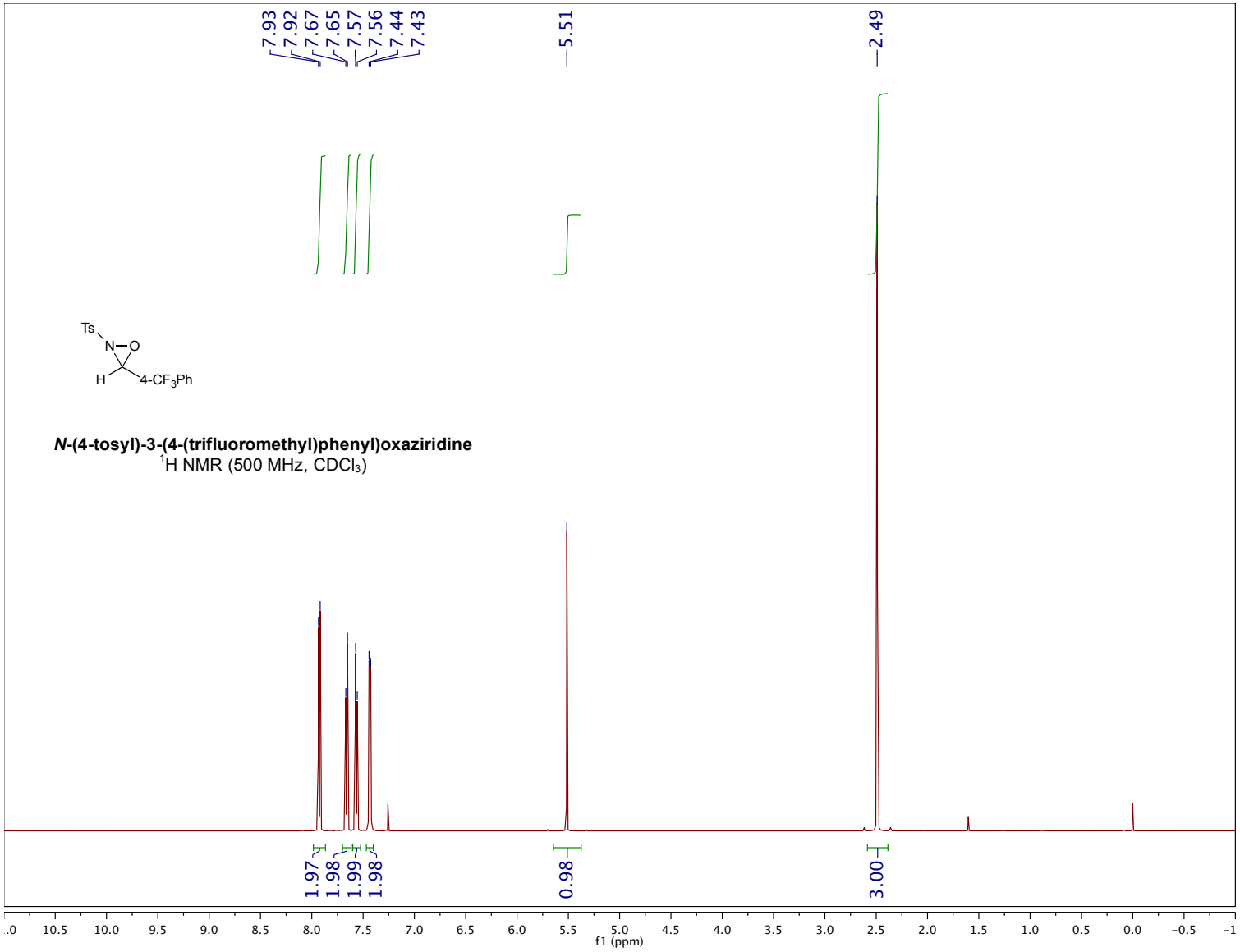
methyl 4-(2-(phenylsulfonyl)-1,2-oxaziridin-3-yl)benzoate

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


166.19
135.18
135.03
134.50
132.88
129.90
129.46
129.40
128.29
75.47
52.43
Bs
N—O
H
4-MeO2CPh
methyl 4-(2-(phenylsulfonyl)-1,2-oxaziridin-3-yl)benzoate
13C NMR (126 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

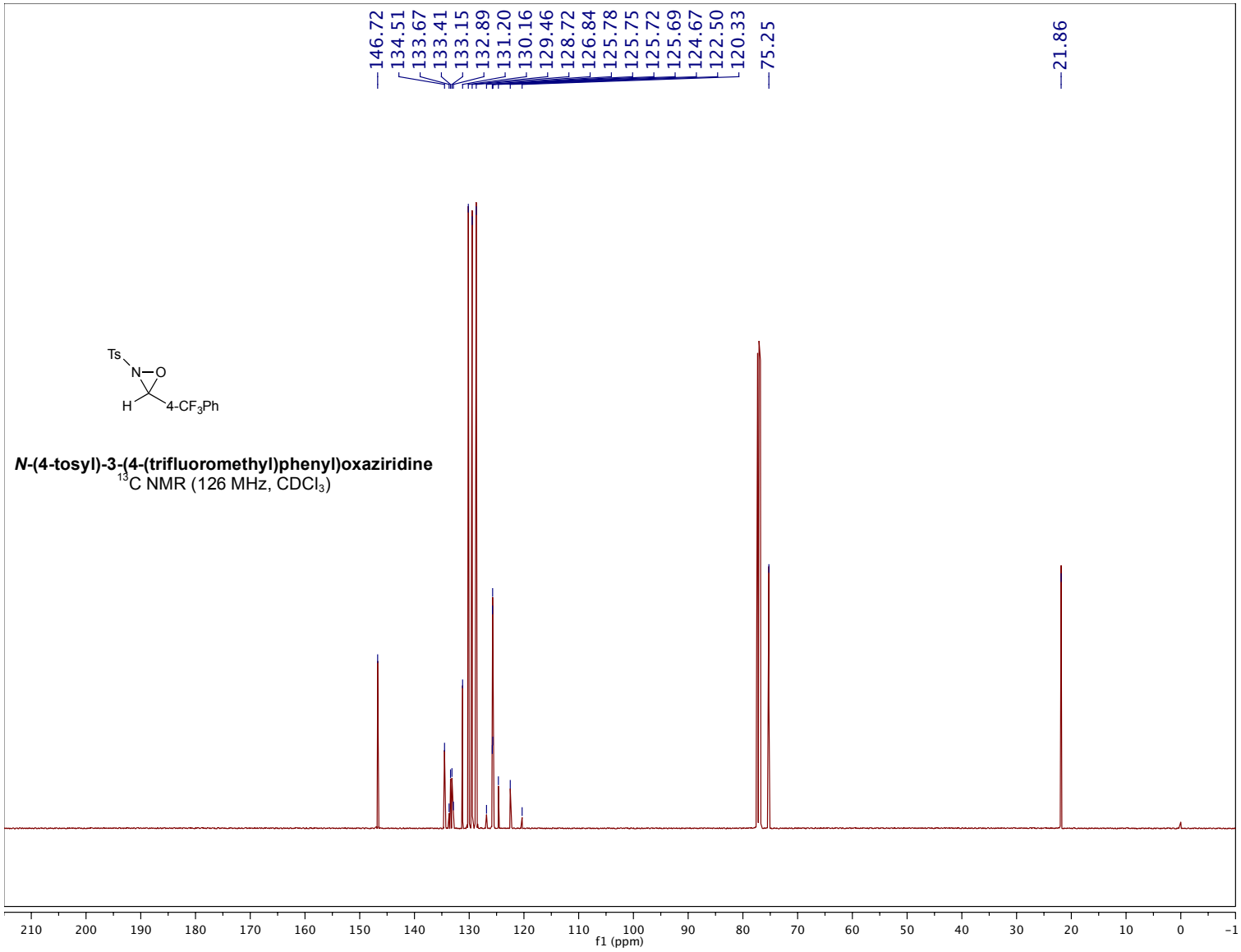

8.48
8.46
8.27
8.25
7.32
7.30
7.26
7.25
7.23
5.56
2.36
Ns
N
O
H
3-MePh
2-((4-nitrophenyl)sulfonyl)-3-(m-tolyl)-1,2-oxaziridine
1H NMR (500 MHz, CDCl3)
1.98
2.00
4.14
0.97
3.00
f1 (ppm)

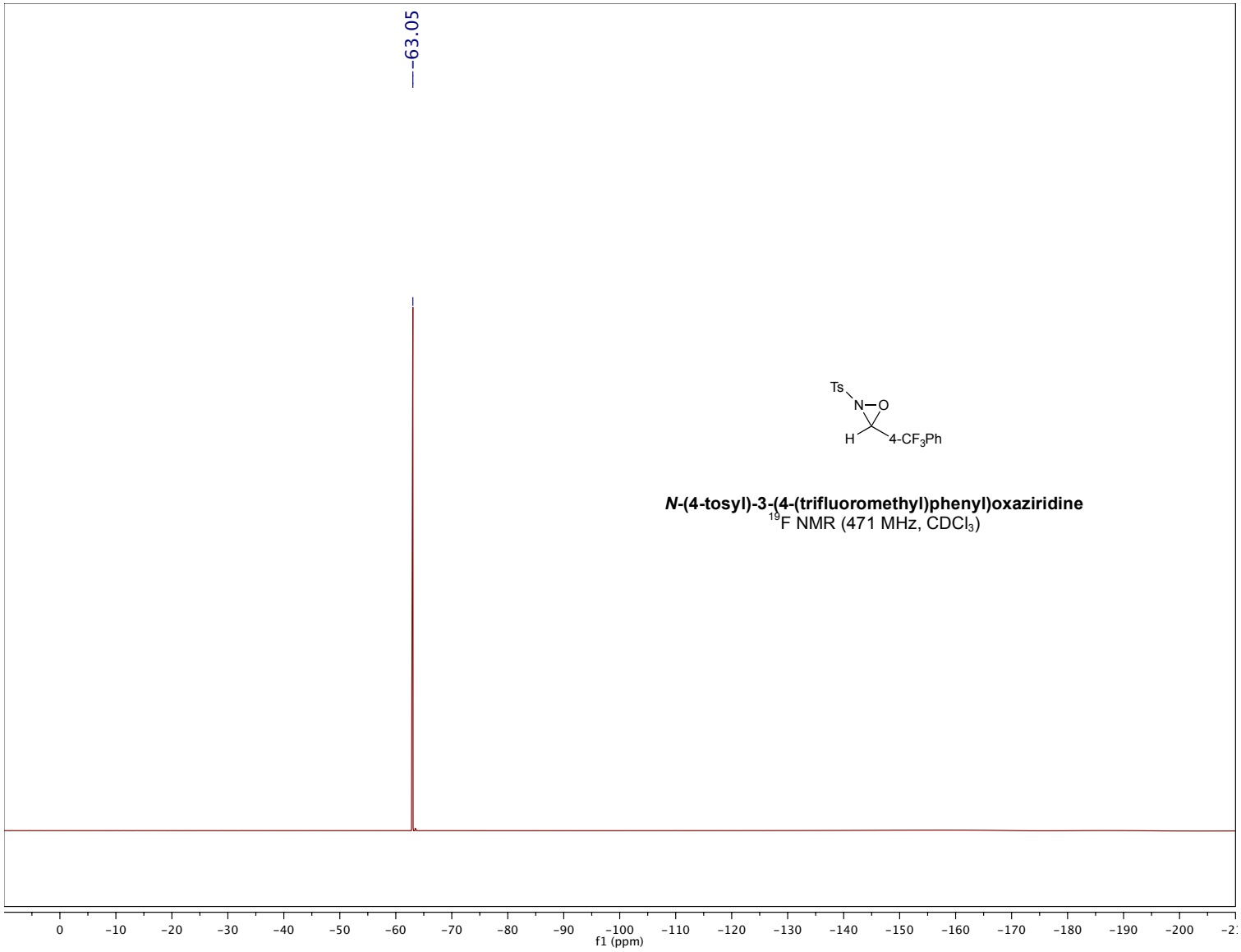

151.46
140.57
138.87
132.58
130.74
129.61
128.75
128.59
125.51
124.49
76.79
21.24
Ns
N
O
H
3-MePh
2-((4-nitrophenyl)sulfonyl)-3-(m-tolyl)-1,2-oxaziridine
13C NMR (126 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)



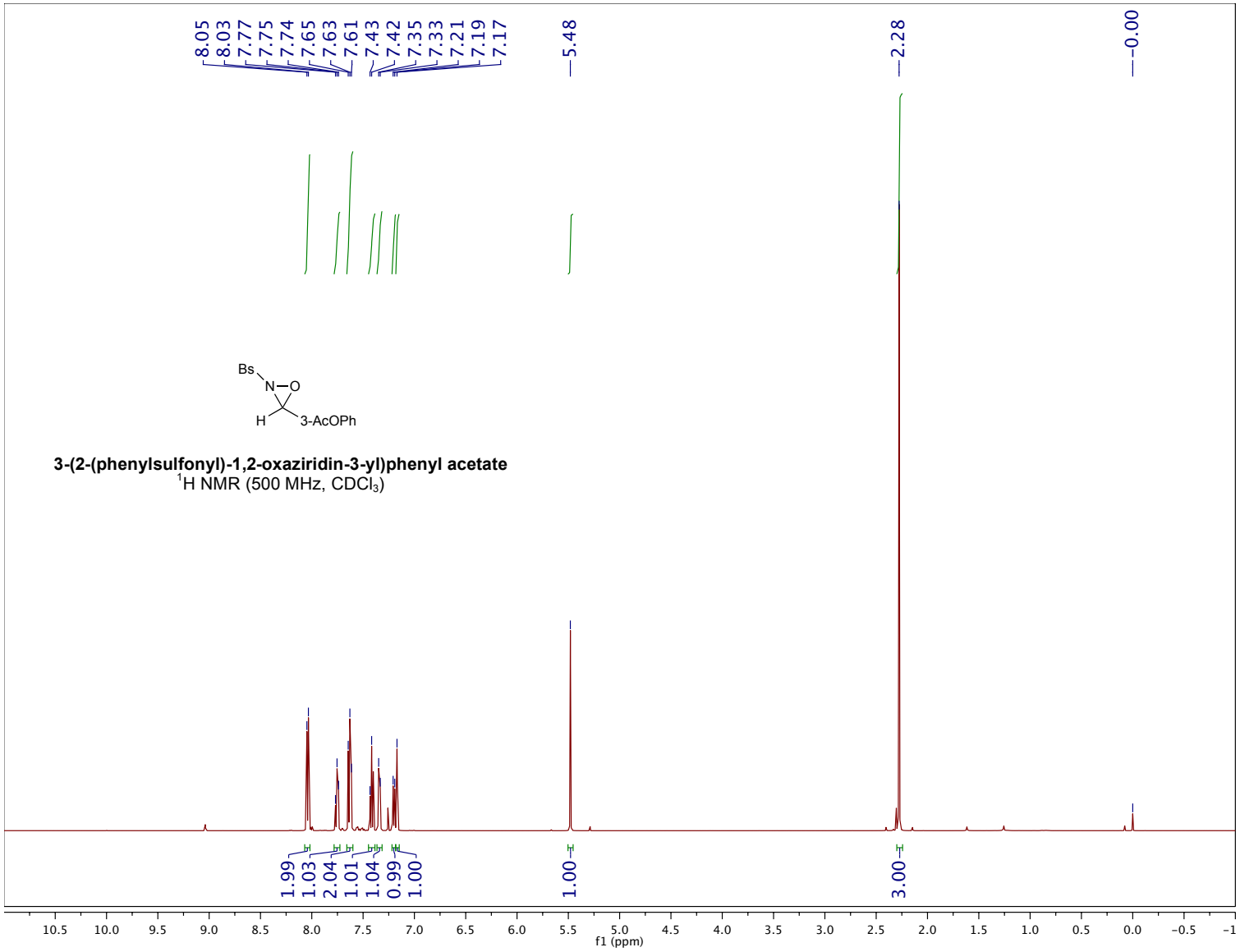
***N*-(4-tosyl)-3-(4-(trifluoromethyl)phenyl)oxaziridine**

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


146.72
134.51
133.67
133.41
133.15
132.89
131.20
130.16
129.46
128.72
126.84
125.78
125.75
125.72
125.69
124.67
122.50
120.33
75.25
21.86
Ts
N
O
H
4-CF3Ph
N-(4-tosyl)-3-(4-(trifluoromethyl)phenyl)oxaziridine
13C NMR (126 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

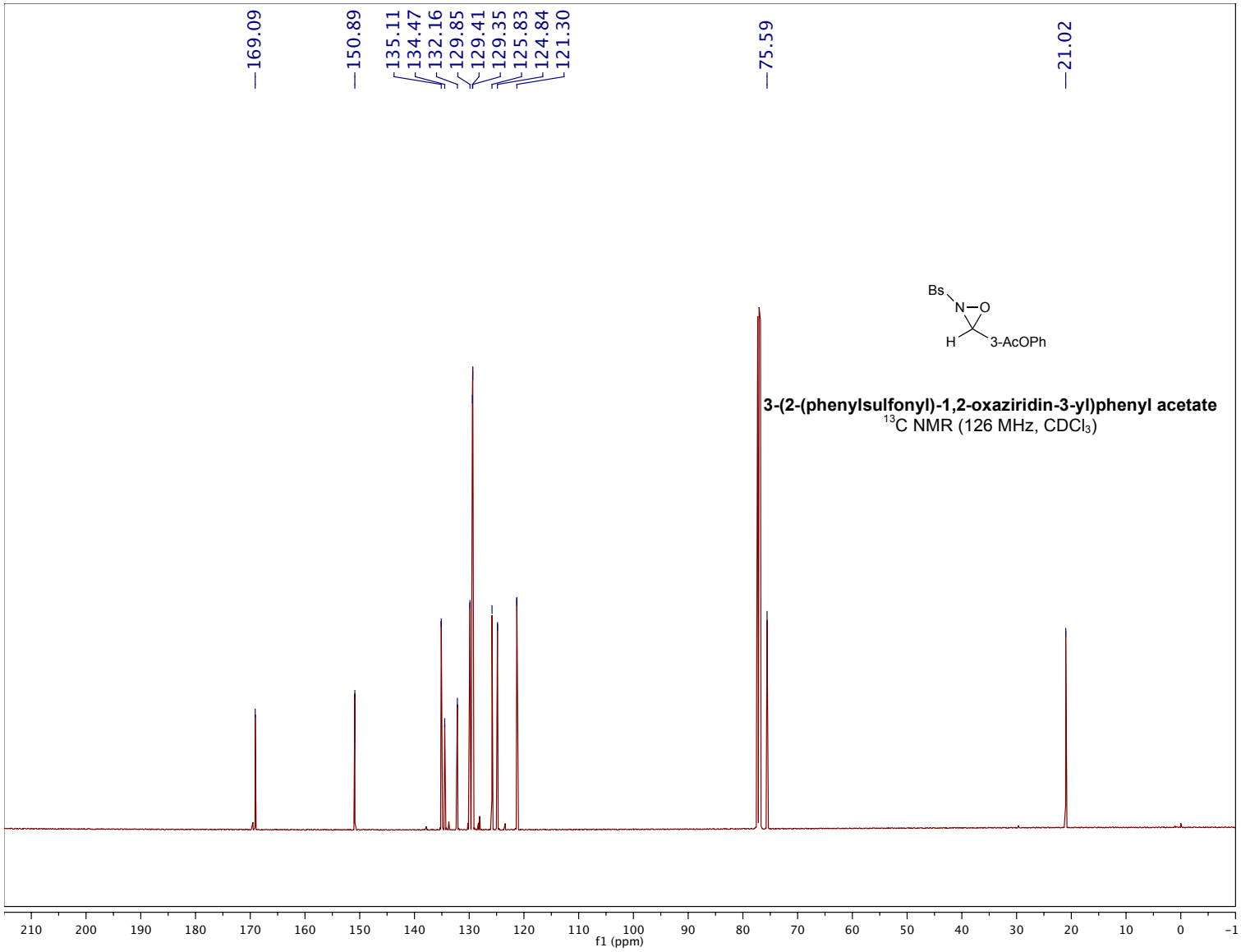


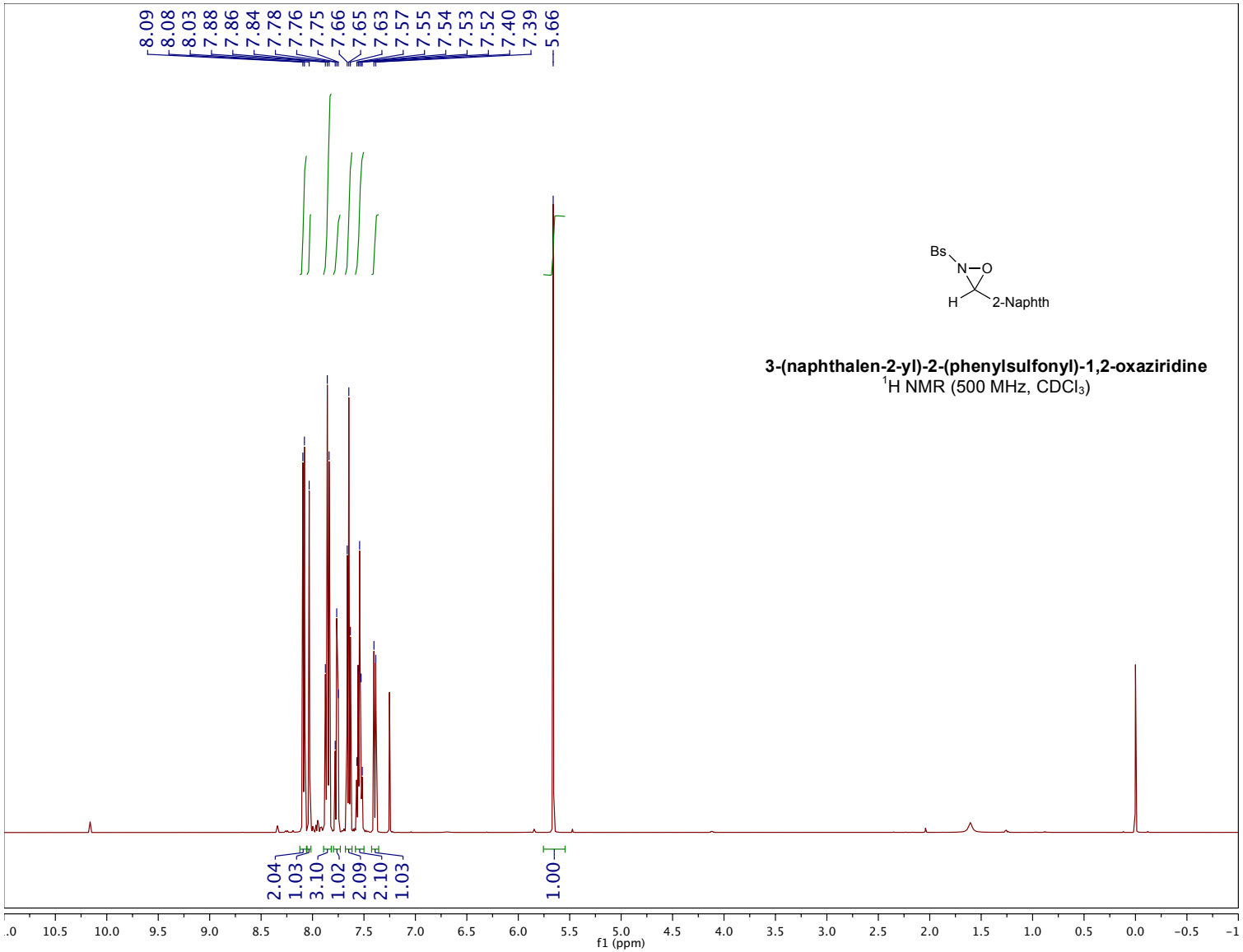
***N*-(4-tosyl)-3-(4-(trifluoromethyl)phenyl)oxaziridine**
^{19}F NMR (471 MHz, $CDCl_3$)

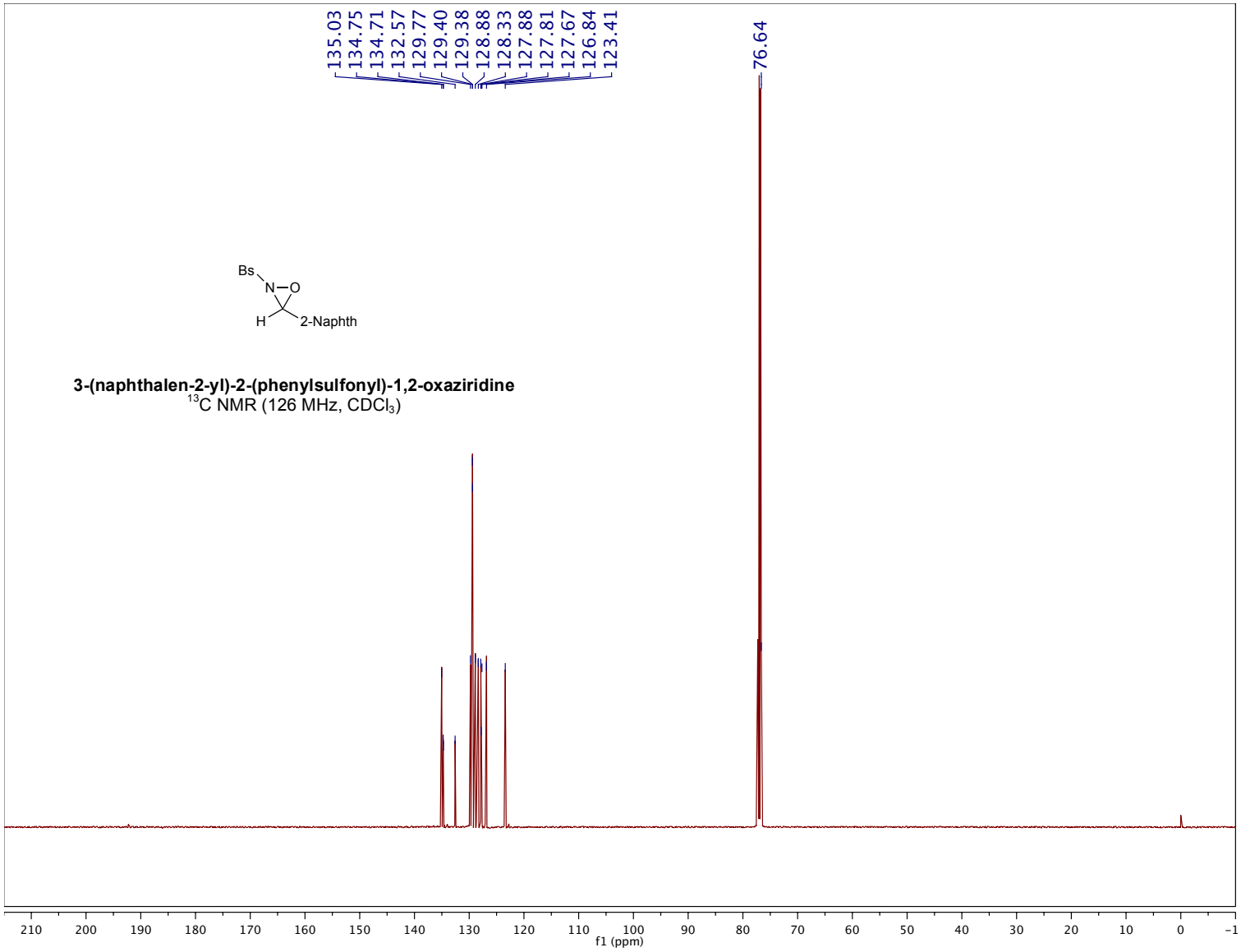


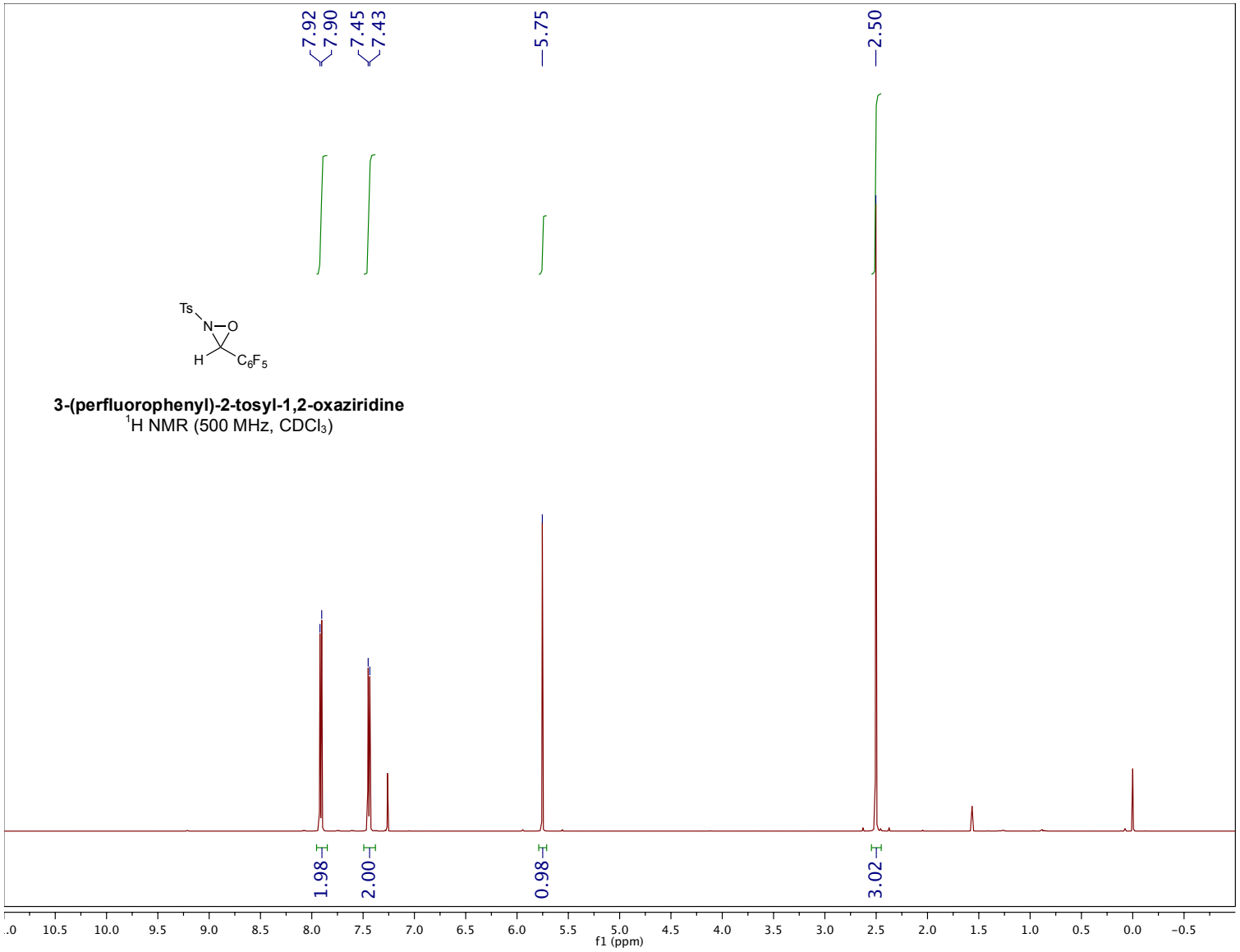
3-(2-(phenylsulfonyl)-1,2-oxaziridin-3-yl)phenyl acetate

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


169.09
150.89
135.11
134.47
132.16
129.85
129.41
129.35
125.83
124.84
121.30
75.59
21.02
Bs
N
O
H
3-AcOPh
3-(2-(phenylsulfonyl)-1,2-oxaziridin-3-yl)phenyl acetate
13C NMR (126 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)

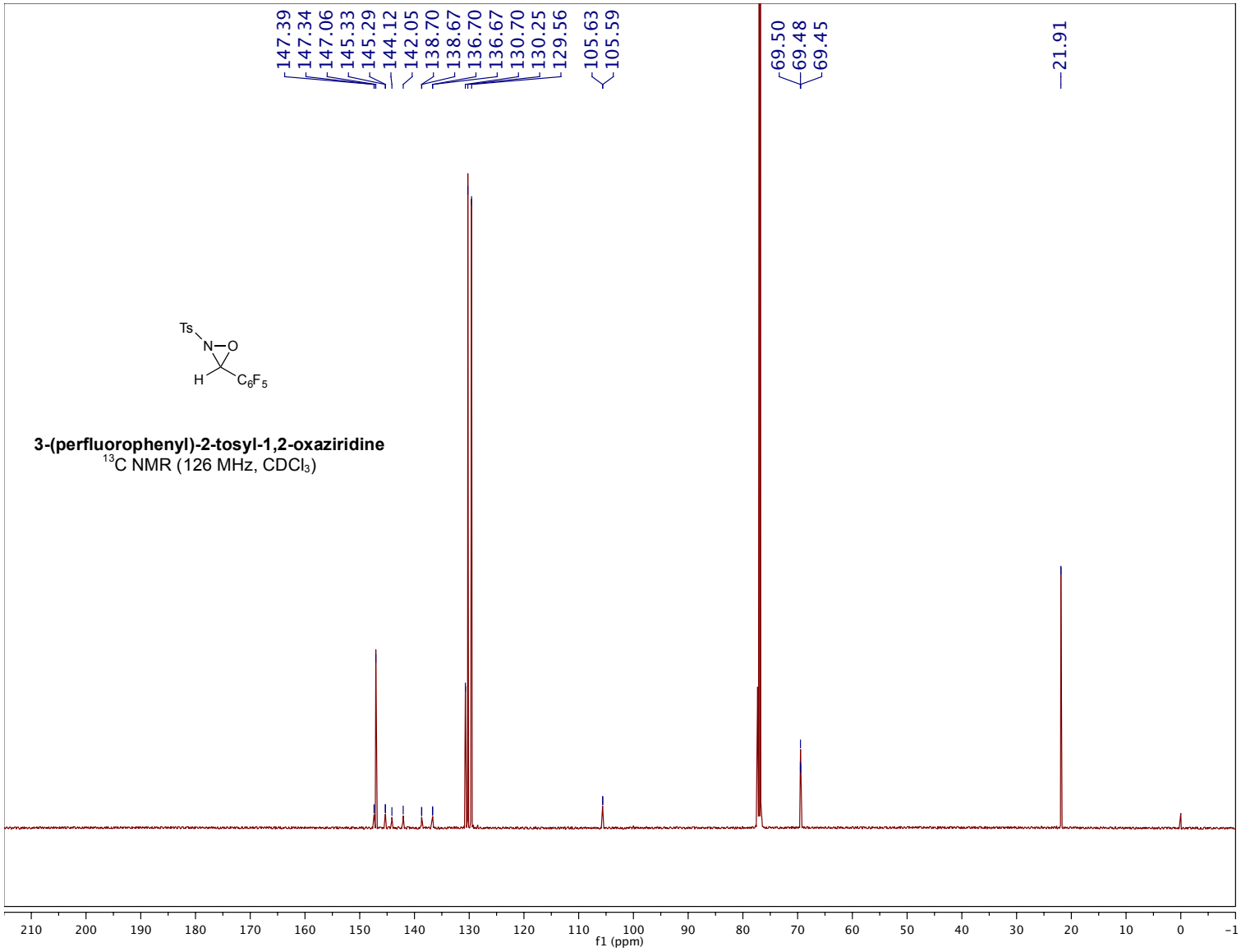

8.09
8.08
8.03
7.88
7.86
7.84
7.78
7.76
7.75
7.66
7.65
7.63
7.57
7.55
7.54
7.53
7.52
7.40
7.39
5.66
Bs
N
O
H
2-Naphth
3-(naphthalen-2-yl)-2-(phenylsulfonyl)-1,2-oxaziridine
1H NMR (500 MHz, CDCl3)
2.04
1.03
3.10
1.02
2.09
2.10
1.03
1.00
f1 (ppm)

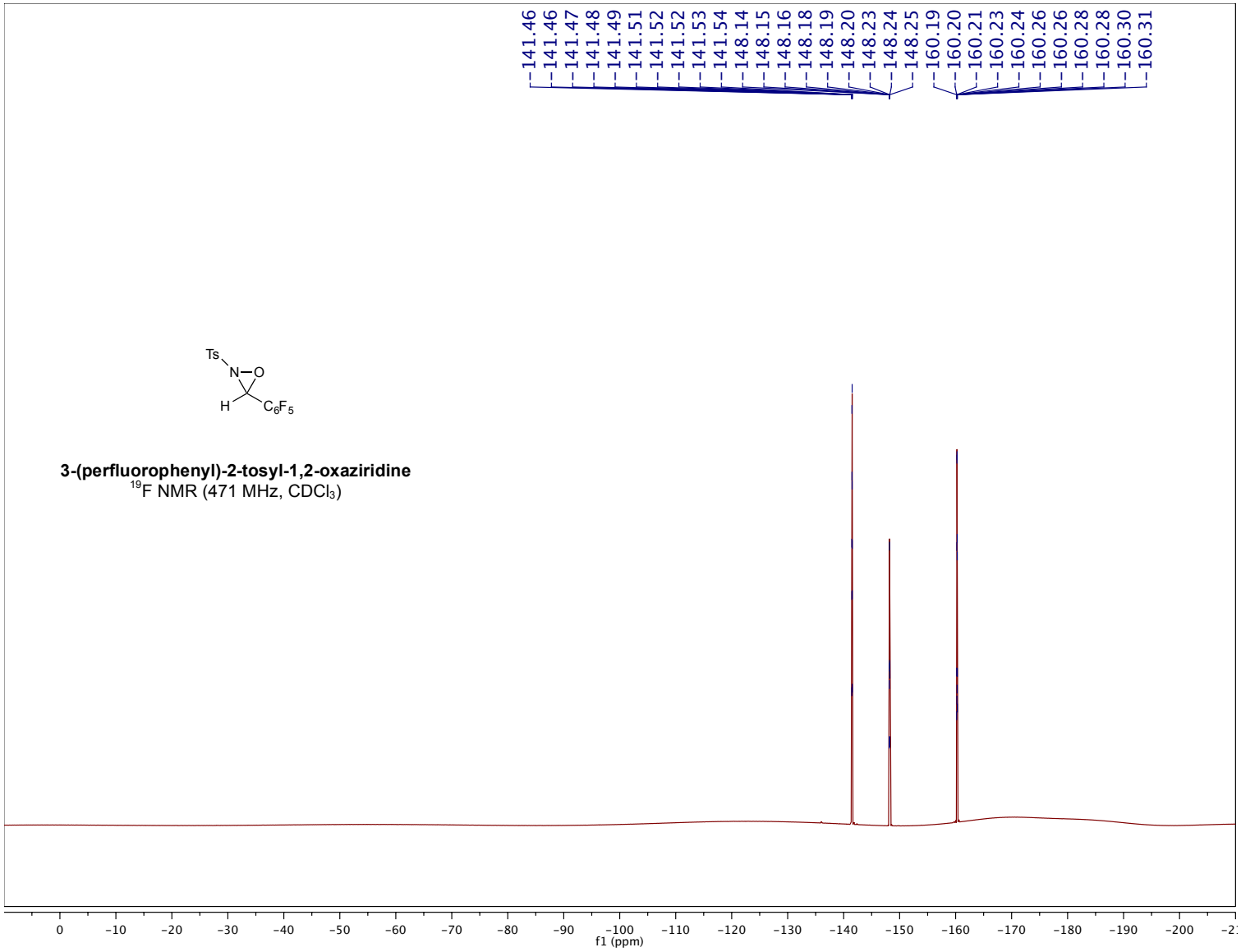

135.03
134.75
134.71
132.57
129.77
129.40
129.38
128.88
128.33
127.88
127.81
127.67
126.84
123.41
76.64
Bs
N
O
H
2-Naphth
3-(naphthalen-2-yl)-2-(phenylsulfonyl)-1,2-oxaziridine
13C NMR (126 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)



3-(perfluorophenyl)-2-tosyl-1,2-oxaziridine

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


147.39
147.34
147.06
145.33
145.29
144.12
142.05
138.70
138.67
136.70
136.67
130.70
130.25
129.56
105.63
105.59
69.50
69.48
69.45
21.91
Ts
N
O
H
C6F5
3-(perfluorophenyl)-2-tosyl-1,2-oxaziridine
13C NMR (126 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


141.46
141.46
141.47
141.48
141.49
141.51
141.52
141.52
141.53
141.54
148.14
148.15
148.16
148.18
148.19
148.20
148.23
148.24
148.25
160.19
160.20
160.21
160.23
160.24
160.26
160.26
160.28
160.28
160.30
160.31
Ts
N
O
H
C6F5
3-(perfluorophenyl)-2-tosyl-1,2-oxaziridine
19F NMR (471 MHz, CDCl3)
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)