Supplementary Information
Organic base-catalyzed stereodivergent synthesis of (*R*)- and (*S*)-3-amino-4,4,4-trifluorobutanoic acids

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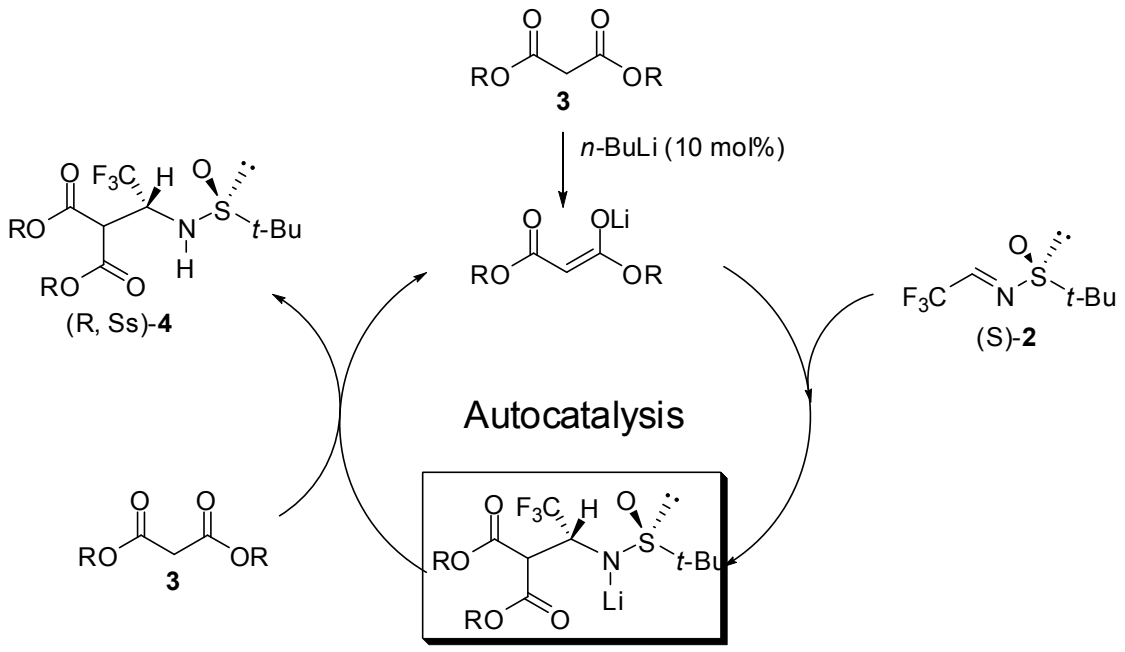
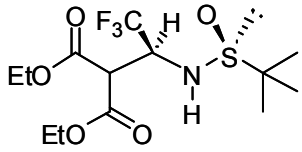


Fig. S1. Auto-catalytic scenario of the reaction of dialkyl malonates **3** with imine (*S*)-**2** catalyzed *n*-BuLi.

General Methods.

All reactions were performed in oven-dried glassware under a positive pressure of nitrogen. Solvents were transferred *via* syringe and were introduced into the reaction vessels through a rubber septum. All reactions were monitored by TLC on 0.25 mm Merck aluminum plates, silica gel 60, F_{254}. The TLC plates were visualized with UV light and 7% phosphomolybdic acid or $KMnO_4$ in water/heat. Column chromatography was carried out on a column packed with silica gel 60N spherical neutral size 63-210 μm. The ^{1}H-NMR (300 MHz), ^{13}C-NMR (75.5 MHz) and ^{19}F-NMR (282 MHz) spectra for solution in $CDCl_3$ or CD_3OD were recorded on a Varian Mercury 300. Chemical shifts (δ) are expressed in ppm and referenced to the internal TMS or residual solvent peak. Mass spectra were recorded on a SHIMAZU LCMS-2010EV (ESI-MS). Optical rotations were measured on a HORIBA SEPA-300. Infrared spectra were recorded on a JASCO FT/IR-4100 spectrometer.

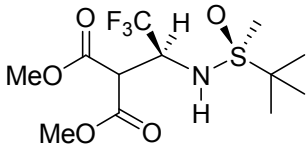
(*S*)-Diethyl 2-[(*S*)-1-(*tert*-butanesulfinamido)- 2,2,2-trifluoroethyl]malonate (4a). General Procedure



To a solution of diethyl malonate (0.30 mmol; 45.5µl) in dry toluene (1.0 ml) P_2-Et (0.03 mmol; 10.0 µl) was added with stiring at -78 ˚C. After 10 min at -78 ˚C (S_S)-*N*-*tert*-butanesulfinyl (3,3,3)-trifluoroacetaldimine **2** (0.36 mmol; 72.4 mg) was added dropwise. Stirring was continued at -78 ˚C for 24 h, then the reaction was quenched with saturated NH_4Cl (3.0 ml), followed by H_2O (10.0 ml) and the mixture was brought to room temperature. The organic layer was taken and the aqueous layer was extracted with diethyl ether (3 × 10 ml). The combined organic layers were washed with brine (15 ml), dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. After purification by chromatography on silica-gel (hexane/EtOAc = 4/1), **3** (91.1 mg, 84%) was obtained as a colorless oil; $[\alpha]_D^{25}$ +20.1 (*c* 1.52, $CHCl_3$).

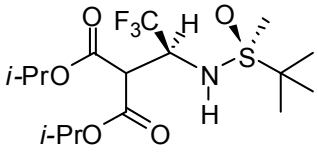
^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.21 (s, 9H), 1.29 (t, *J* = 7.2 Hz, 3H), 1.31 (t, *J* = 7.2 Hz, 3H), 3.81 (d, *J* = 3.6 Hz, 1H), 4.22 (q, *J* = 7.2 Hz, 2H), 4.27 (q, *J* = 7.2 Hz, 2H), 4.47 (dqd, *J* = 3.6, 7.2, 10.8 Hz, 1H), 5.08 (d, *J* = 10.8 Hz, 1H); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 13.7, 13.7, 22.3, 50.2, 57.2, 58.3 (q, *J* = 32.1 Hz), 62.1, 62.6, 123.9 (q, *J* = 284.3 Hz), 165.5, 166.7; ^{19}F NMR (282 MHz, $CDCl_3$): δ = –74.0 (d, *J* = 7.2 Hz); IR (NaCl): 3294, 2984, 1733, 1471, 1263, 1181, 1130, 1092, 882, 493 cm^{-1}; MS (ESI): m/z = 384.5 $[M+Na]^+$; HRMS (ESI) Calcd for $C_{13}H_{22}F_3NNaO_5S$: $(M+Na^+)$: 384.1068, found: 384.1052.

(*S*)-Dimethyl 2-[(*S*)-1-(*tert*-butanesulfinamido)- 2,2,2-trifluoroethyl]malonate (4b)



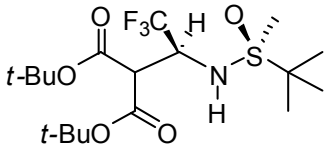
^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.21 (s, 9H), 3.78 (s, 3H), 3.81 (s, 3H), 3.87 (d, *J* = 3.9 Hz, 1H), 4.48 (dqd, *J* = 3.9, 7.2, 10.8 Hz,1H), 5.03 (d, *J* = 10.8 Hz, 1H); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 22.3, 50.0, 53.1, 53.3, 57.3, 58.4 (q, *J* = 31.5 Hz), 123.9 (q, *J* = 283.8 Hz), 166.0, 167.1; ^{19}F NMR (282 MHz, $CDCl_3$): δ = –74.0 (d, *J* = 7.2 Hz); IR (NaCl): 3472, 3331, 2959, 1749, 1438, 1365, 1263, 1173, 1131, 1086, 424 cm^{-1}; MS (ESI): m/z = 356.5 $[M+Na]^+$; HRMS (ESI) Calcd for $C_{11}H_{18}F_3NNaO_5S$: $(M+Na^+)$: 356.0755, found: 356.0757; $[\alpha]_D^{25}$ +18.5 (c 0.90, $CHCl_3$).

(*S*)-Diisopropyl 2-[(*S*)-1-(*tert*-butanesulfinamido)- 2,2,2-trifluoroethyl]malonate (4c)



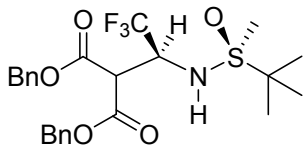
^{1}H NMR (300 MHz, $CDCl_3$): 1.22 (s, 9H), 1.25-1.31 (m, 12H), 3.75 (d, J = 3.3 Hz, 1H), 4.46 (dqd, J = 3.3, 7.2, 10.8 Hz, 1H), 5.04 (sept, J = 6.3, 1H), 5.12 (sept, J = 6.3, 1H), 5.14 (d, J = 10.8 Hz, 1H); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 21.3, 21.3, 21.4, 21.4, 22.4, 50.5, 57.3, 58.2 (q, J = 32.1 Hz), 70.0, 70.7, 124.1 (q, J = 283.0 Hz), 165.1, 166.3; ^{19}F NMR (282 MHz, $CDCl_3$): δ = –74.0 (d, J = 7.2 Hz); IR (NaCl): 3324, 2983, 1742, 1469, 1375, 1264, 1183, 1130, 908, 496 cm^{-1}; MS (ESI): m/z = 412.6 $[M+Na]^+$; HRMS (ESI) Calcd for $C_{15}H_{26}F_3NNaO_5S$: ($M+Na^+$): 412.1381, found: 412.1386; $[\alpha]_D^{25}$ +14.5 (c 0.97, $CHCl_3$).

(*S*)-Di-*tert*-butyl 2-[(*S*)-1-(*tert*-butanesulfinamido)- 2,2,2-trifluoroethyl]malonate (4d)



^{1}H NMR (300 MHz, $CDCl_3$): 1.24 (s, 9H), 1.47 (s, 9H), 1.49 (s, 9H), 3.65 (d, J = 3.3 Hz, 1H), 4.36-4.41 (m, 1H), 5.13 (d, J = 10.5 Hz, 1H); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 22.6, 27.6, 27.7, 51.5, 57.3, 58.0 (q, J = 31.0 Hz), 83.2, 83.7, 124.3 (q, J = 284.4 Hz), 164.7, 166.2; ^{19}F NMR (282 MHz, $CDCl_3$): δ = –74.0 (d, J = 7.9 Hz); IR (KBr): 3324, 2987, 1733, 1458, 1368, 1265, 1151, 1082, 985, 619 cm^{-1}; MS (ESI): m/z = 440.6 $[M+Na]^+$; Mp = 93–94 ºC; HRMS (ESI) Calcd for $C_{17}H_{30}F_3NNaO_5S$: ($M+Na^+$): 440.1694, found: 440.1681; $[\alpha]_D^{25}$ +7.5 (c 1.04, $CHCl_3$).

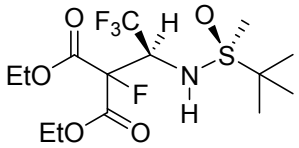
(*S*)-Dibenzyl 2-[(*S*)-1-(*tert*-butanesulfinamido)- 2,2,2-trifluoroethyl]malonate (4e)



^{1}H NMR (300 MHz, $CDCl_3$): 1.09 (s, 9H), 3.93 (d, J = 3.3 Hz, 1H), 4.49 (dqd, J = 3.3, 7.2, 10.8 Hz, 1H), 4.97 (d, J = 10.8 Hz, 1H), 5.10-5.25 (m, 4H), 7.21-7.37 (m, 10H); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 22.3, 50.5, 57.3, 58.4 (q, J = 32.1 Hz), 68.1, 68.3, 123.9 (q, J = 284.3 Hz), 128.3, 128.5, 128.6, 128.7, 128.7, 128.8, 134.2, 134.3, 165.3, 166.4; ^{19}F NMR (282 MHz, $CDCl_3$): δ = –73.9 (d, J = 7.2 Hz); IR (NaCl): 3337, 2960, 1746, 1457, 1344, 1263, 1220, 1170, 1129, 1088, 698, 465 cm^{-1}; MS (ESI): m/z = 508.4 $[M+Na]^+$; HRMS (ESI) Calcd for

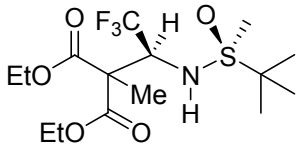
$C_{23}H_{26}F_3NNaO_5S$: ($M+Na^+$): 508.1381, found: 508.1378; $[\alpha]_D^{25}$ +3.3 (c 1.06, $CHCl_3$).

(*S*)-Diethyl 2-[(*S*)-1-(*tert*-butanesulfinamido)-2,2,2-trifluoroethyl]- 2-fluoromalonate (4f)



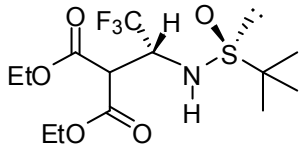
^1H NMR (300 MHz, $CDCl_3$): 1.21 (s, 9H), 1.33 (t, J = 7.2 Hz, 3H), 1.34 (t, J = 7.2 Hz, 3H), 3.99 (d, J = 11.1 Hz, 1H), 4.19-4.40 (m, 4H), 4.79-4.97 (m, 1H); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 13.7, 13.7, 22.3, 57.4, 61.3 (dq, J = 19.9, 31.0 Hz), 63.5, 63.7, 93.7 (d, J = 211.3 Hz), 123.0 (q, J = 284.9 Hz), 162.5 (d, J = 24.9 Hz), 162.8 (d, J = 24.9 Hz); ^{19}F NMR (282 MHz, $CDCl_3$): δ = –69.7 (dd, J = 6.9, 8.7 Hz), –179.8 (dq, J = 23.7, 8.7 Hz); IR (NaCl): 3286, 2985, 1771, 1472, 1254, 1166, 1094, 1046, 881, 492 cm^{-1}; MS (ESI): m/z = 402.5 $[M+Na]^+$; HRMS (ESI) Calcd for $C_{13}H_{21}F_4NNaO_5S$: ($M+Na^+$): 402.0974, found: 402.0988; $[\alpha]_D^{25}$ +0.9 (c 1.12, $CHCl_3$).

(*S*)-Diethyl 2-[(*S*)-1-(*tert*-butanesulfinamido)- 2,2,2-trifluoroethyl]- 2-methylmalonate (4g)



^1H NMR (300 MHz, $CDCl_3$): 1.20 (s, 9H), 1.28 (t, J = 7.2 Hz, 3H), 1.30 (t, J = 7.2 Hz, 3H), 1.56 (d, J = 1.5 Hz, 3H), 4.17-4.30 (m, 4H), 4.57-4.59 (m, 2H); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 13.7, 13.7, 17.2, 22.5, 56.6, 57.1, 62.2, 62.3, 62.6 (q, J = 29.9 Hz), 124.3 (q, J = 285.5 Hz), 168.5, 168.7; ^{19}F NMR (282 MHz, $CDCl_3$): δ = –67.4 (d, J = 7.2 Hz); IR (NaCl): 3470, 3286, 2984, 1740, 1469, 1252, 1184, 1155, 1097, 734, 417 cm^{-1}; MS (ESI): m/z = 398.6 $[M+Na]^+$; HRMS (ESI) Calcd for $C_{14}H_{24}F_3NNaO_5S$: ($M+Na^+$): 398.1225, found: 398.1217; $[\alpha]_D^{25}$ +6.2 (c 0.57, $CHCl_3$).

(*R*)-Diethyl 2-[(*S*)-1-(*tert*-butanesulfinamido)- 2,2,2-trifluoroethyl]malonate (5a). General Procedure

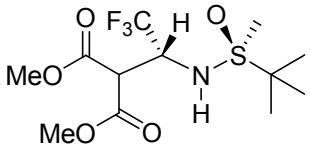


To a solution of diethyl malonate (0.3 mmol; 45.5µl) and DMAP (0.03 mmol; 3.7 mg) in dry toluene (1.0 ml) (S_S)-*N*-*tert*-butanesulfinyl (3,3,3)-trifluoroacetaldimine **2** (0.30 mmol; 60.4 mg) was added with stirring at room temperature. After 48 h the solvent was removed under reduced pressure. Purification by chromatography on silica-gel (hexane/EtOAc = 4/1) gave **4** (94.6 mg,

87%) as colorless oil; $[\alpha]_D^{25}$ +71.9 (c 1.48, $CHCl_3$).

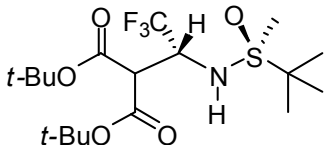
^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.24 (s, 9H), 1.29 (t, *J* = 6.9 Hz, 3H), 1.31 (t, *J* = 7.2 Hz, 3H), 3.81 (d, *J* = 3.0 Hz, 1H), 4.21 (q, *J* = 6.9 Hz, 2H), 4.27 (q, *J* = 7.2 Hz, 2H), 4.47 (dqd, *J* = 3.0, 6.6, 9.3 Hz, 1H), 5.59 (d, *J* = 9.3 Hz, 1H); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 13.6, 22.2, 49.5, 56.8, 58.6 (q, *J* = 31.6 Hz), 62.2, 63.1, 124.1 (q, *J* = 282.1 Hz), 165.1, 167.4; ^{19}F NMR (282 MHz, $CDCl_3$): δ = –75.6 (d, *J* = 6.6 Hz); IR (NaCl): 3328, 2984, 1747, 1469, 1263, 1182, 1130, 1092, 878, 461 cm^{-1}; MS (ESI): m/z = 384.1 $[M+Na]^+$; HRMS (ESI) Calcd for $C_{13}H_{22}F_3NNaO_5S$: $(M+Na^+)$: 384.1068, found: 384.1068.

(*R*)-Dimethyl 2-[(*S*)-1-(*tert*-butanesulfinamido)- 2,2,2-trifluoroethyl]malonate (5b)



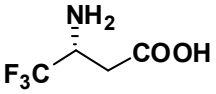
^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.25 (s, 9H), 3.83 (s, 3H), 3.86 (d, *J* = 3.9 Hz, 1H), 3.88 (s, 3H), 4.53–4.41 (m, 1H), 5.55 (d, *J* = 9.3 Hz, 1H); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 22.3, 49.4, 53.1, 53.8, 56.9, 58.8 (q, *J* = 31.6 Hz), 124.1 (q, *J* = 282.1 Hz), 165.6, 167.9; ^{19}F NMR (282 MHz, $CDCl_3$): δ = –75.7 (d, *J* = 7.9 Hz); IR (NaCl): 3479, 3298, 2960, 1738, 1438, 1360, 1264, 1174, 1130, 1090, 929, 472 cm^{-1}; MS (ESI): m/z = 356.6 $[M+Na]^+$; HRMS (ESI) Calcd for $C_{11}H_{18}F_3NNaO_5S$: $(M+Na^+)$: 356.0755, found: 356.0770; $[\alpha]_D^{25}$ +78.9 (c 1.18, $CHCl_3$).

(*R*)-Di-*tert*-butyl 2-[(*S*)-1-(*tert*-butanesulfinamido)- 2,2,2-trifluoroethyl]malonate (5d)



^{1}H NMR (300 MHz, $CDCl_3$): 1.24 (s, 9H), 1.50 (s, 9H), 1.53 (s, 9H), 3.64 (d, *J* = 2.4 Hz, 1H), 4.43 (dqd, *J* = 2.4, 7.9, 8.7 Hz, 1H), 5.56 (d, *J* = 8.7 Hz, 1H); ^{13}C NMR (75.5 MHz, $CDCl_3$): δ = 22.4, 27.7, 27.8, 50.8, 56.9, 58.1(q, *J* = 30.4 Hz), 83.4, 84.5, 124.5 (q, *J* = 282.7 Hz),164.3, 166.7; ^{19}F NMR (282 MHz, $CDCl_3$): δ = –75.5 (d, *J* = 7.9 Hz); IR (NaCl): 3288, 2980, 1724, 1459, 1370, 1263, 1175, 1094, 845, 488 cm^{-1}; MS (ESI): m/z = 440.5 $[M+Na]^+$; HRMS (ESI) Calcd for $C_{17}H_{30}F_3NNaO_5S$: $(M+Na^+)$: 440.1694, found: 440.1693; $[\alpha]_D^{25}$ +61.0 (c 2.13, $CHCl_3$).

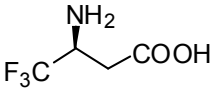
(*S*)-3-Amino-4,4,4-trifluorobutanoic acid (1). General Procedure



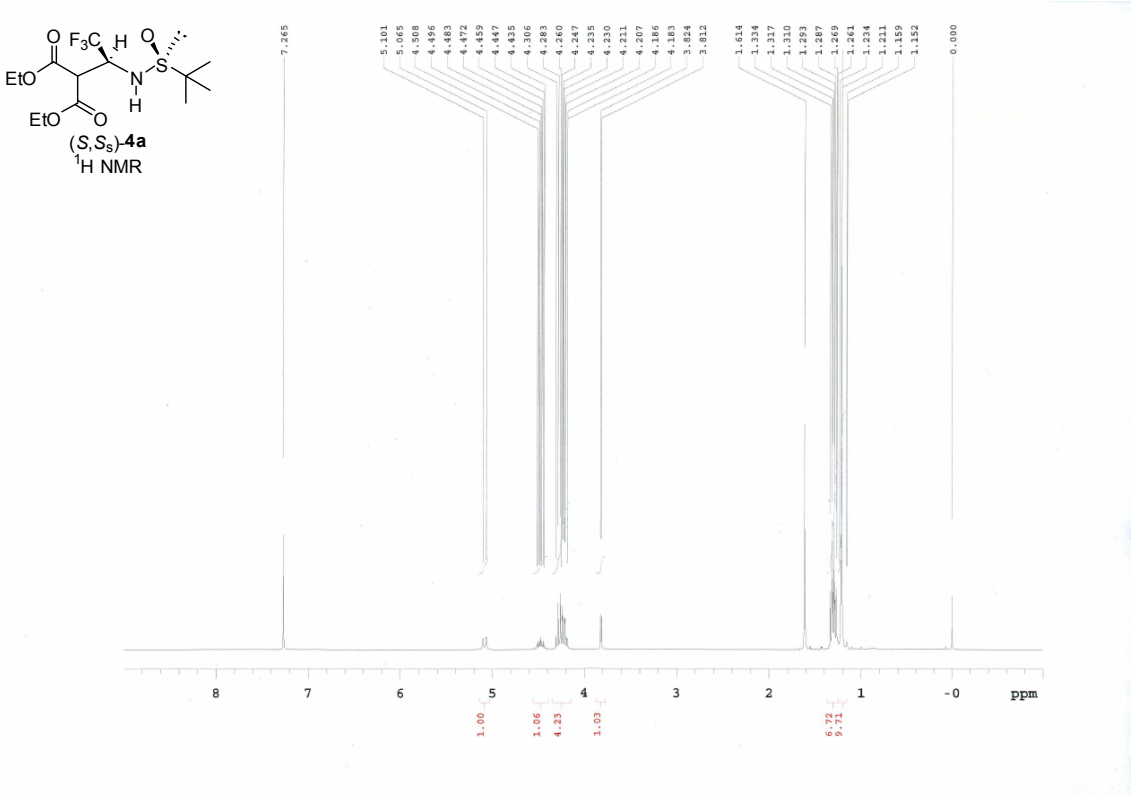
A solution of (*S*)-diethyl 2-[(*S*)-1-(*tert*-butanesulfinamido)-2,2,2-trifluoroethyl]malonate **3** (2.50 mmol; 903.5mg) in 6N HCl (10.0 ml) was refluxed for 12 h. The reaction mixture was brought to room temperature and the aqueous layer was extracted with diethyl ether (3 × 10.0 ml). The aqueous layer was concentrated under reduced pressure to dryness. The resulting solid was treated with propylene oxide (10.0 ml) and stirred for 1 h at room temperature. Precipitate was filtered off and washed with hexane (2 × 5.0 ml) to provide (*S*)-**1** (376.9 mg, 96%) as a white solid; $[\alpha]_D^{25}$ -25.9 (c 1.02, 6N HCl).

^{1}H NMR (300 MHz, CD_3OD): 2.49 (dd, *J* = 9.6, 16.5 Hz, 1H), 2.71 (dd, *J* = 3.6, 16.5 Hz, 1H), 3.81-3.91 (m, 1H); ^{13}C NMR (75.5 MHz, CD_3OD): δ = 35.2, 51.8 (q, *J* = 30.4 Hz), 127.0 (q, *J* = 280.5 Hz), 173.7; ^{19}F NMR (282 MHz, CD_3OD): δ = –77.1 (d, *J* = 7.1 Hz); IR (KBr): 2894, 2724, 2132, 1620, 1526, 1381, 1133, 902, 655; MS (ESI): m/z = 158.0 $[M+H]^+$; Mp = 174–175 ºC; HRMS (ESI) Calcd for $C_4H_7F_3NO_2$: ($M+H^+$): 158.0429, found: 158.0427.

(*R*)-3-Amino-4,4,4-trifluorobutanoic acid (1)



This compound was synthesized according to procedure for (*S*)-**3** starting from (R,S_S)-**4** on 1.0 mmol scale; yield 149.4 mg (95%); white solid; $[\alpha]_D^{25}$ +24.4 (c 1.05, 6N HCl).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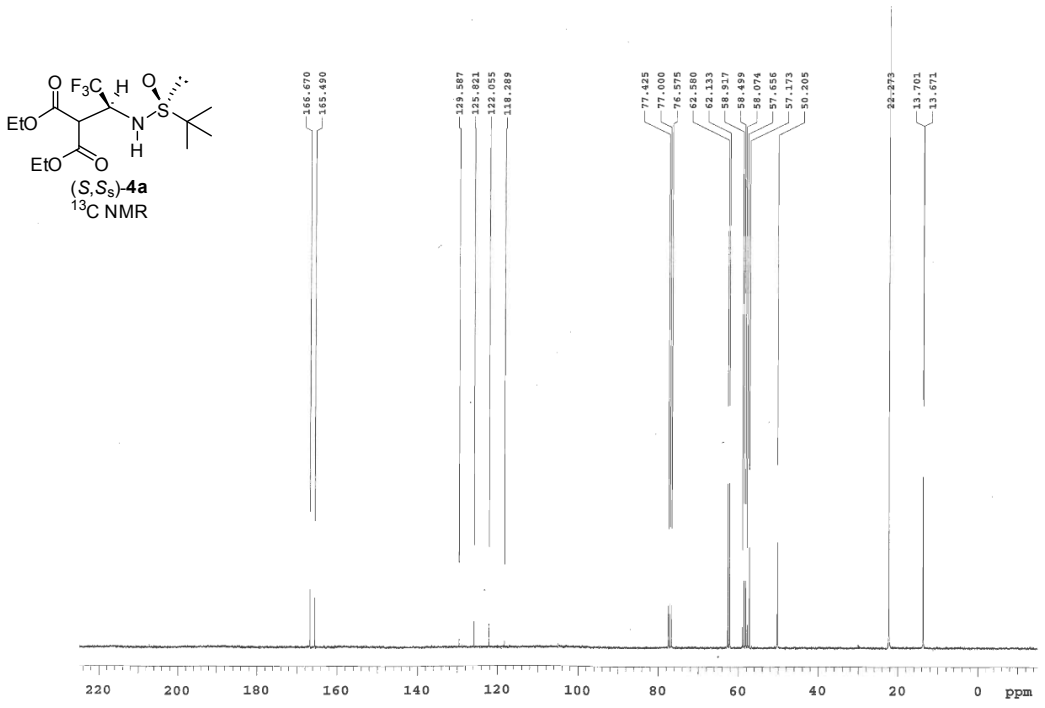
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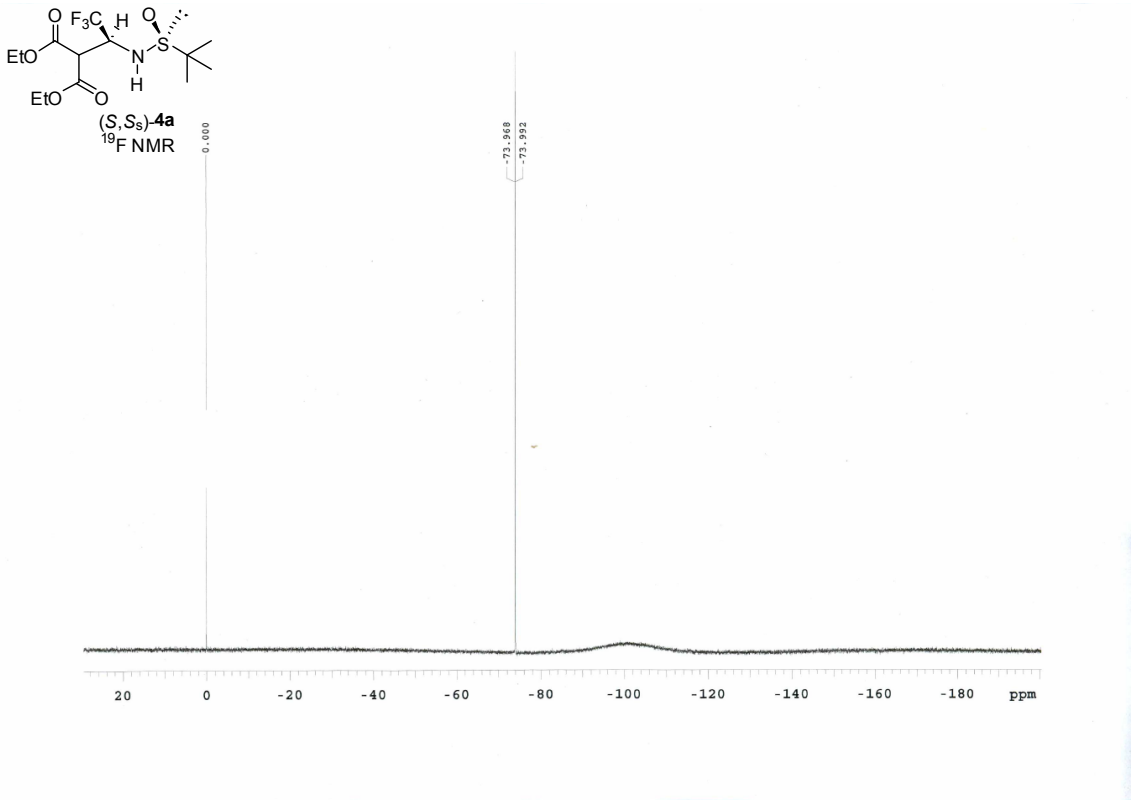
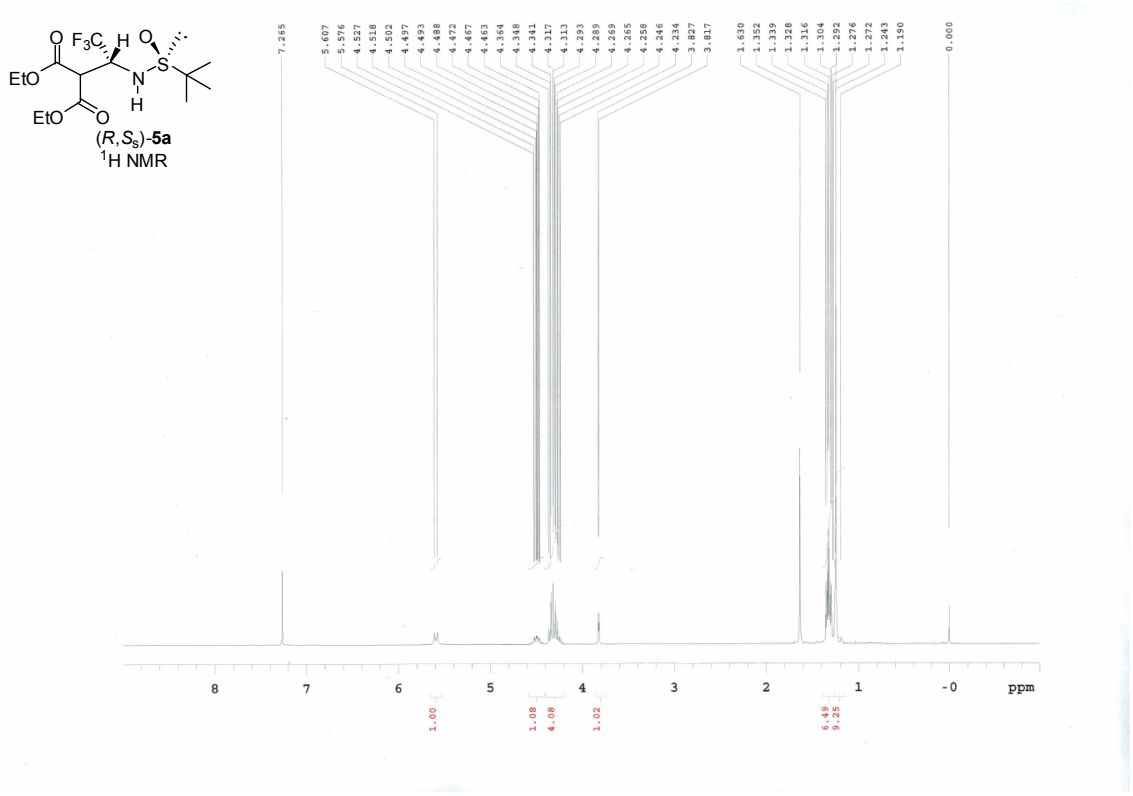
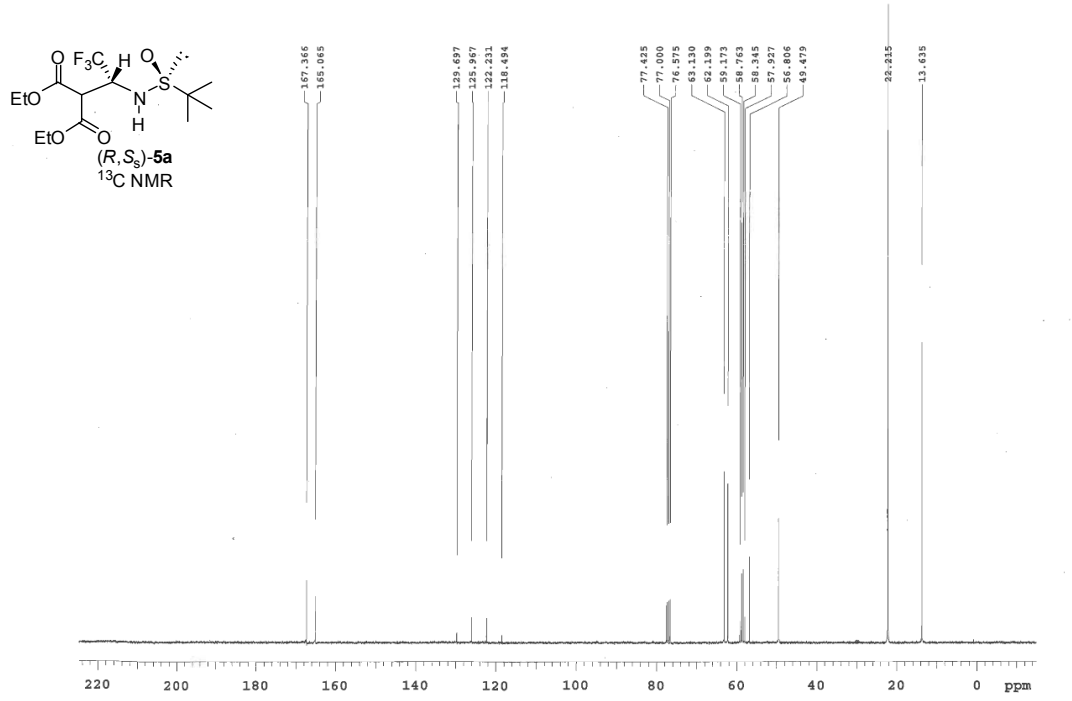
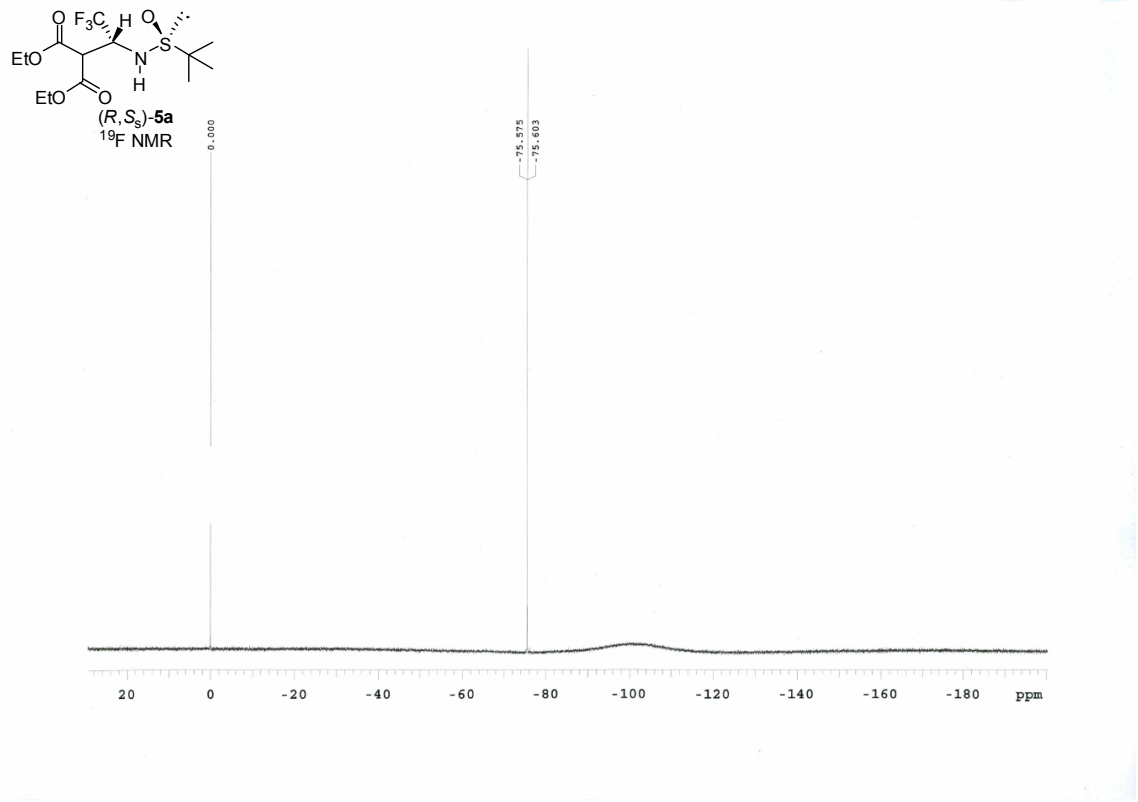
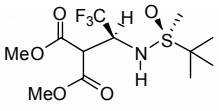
140
120
100
80
60
40
20
0
ppm


(S,Ss)-4a
19F NMR
0.000
-73.968
-73.992
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm

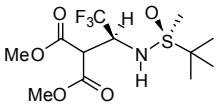

(R,Ss)-5a
1H NMR
7.265
5.607
5.576
4.527
4.518
4.502
4.497
4.493
4.488
4.472
4.467
4.463
4.364
4.348
4.341
4.317
4.313
4.293
4.289
4.269
4.265
4.258
4.246
4.234
3.827
3.817
1.630
1.352
1.339
1.328
1.316
1.304
1.292
1.276
1.272
1.243
1.190
0.000
8
7
6
5
4
3
2
1
-0
ppm
1.00
1.08
4.08
1.02
6.49
9.25


(R,Sₛ)-5a
13C NMR
167.366
165.065
139.697
125.967
122.231
118.494
77.425
77.000
76.575
63.130
62.199
59.173
58.763
58.345
57.927
56.806
49.479
22.915
13.635
220
200
180
160
140
120
100
80
60
40
20
0
ppm

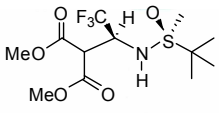

(R,Sₛ)-5a
19F NMR
0.000
-75.575
-75.603
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm



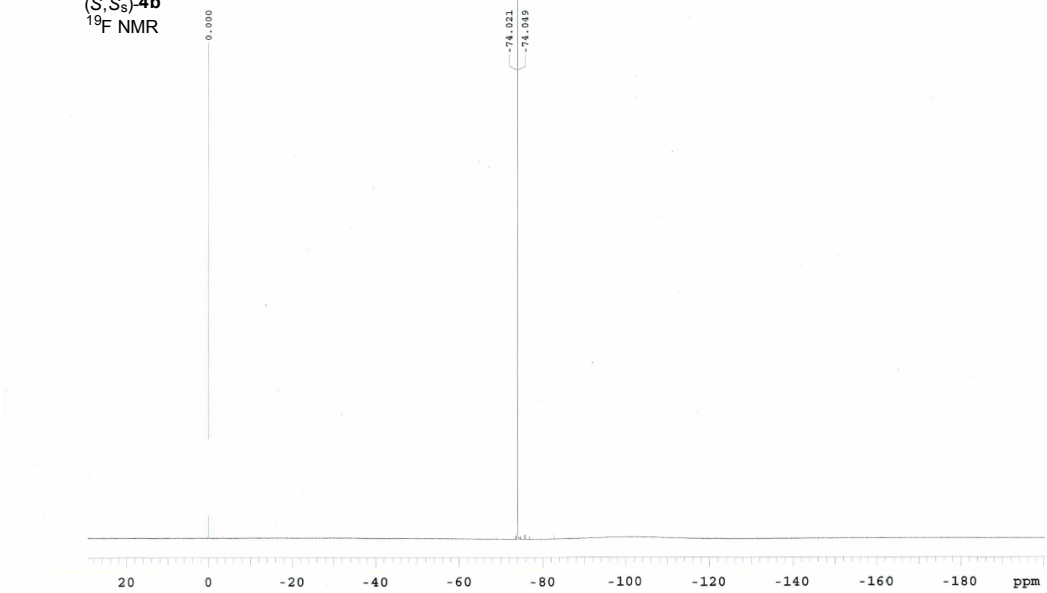
(S,S_S)-**4b**
^{1}H NMR

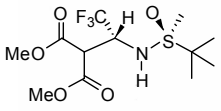


(S,S_S)-**4b**
^{13}C NMR

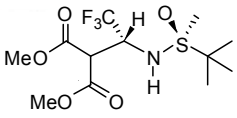


(S,S_S)-**4b**
^{19}F NMR

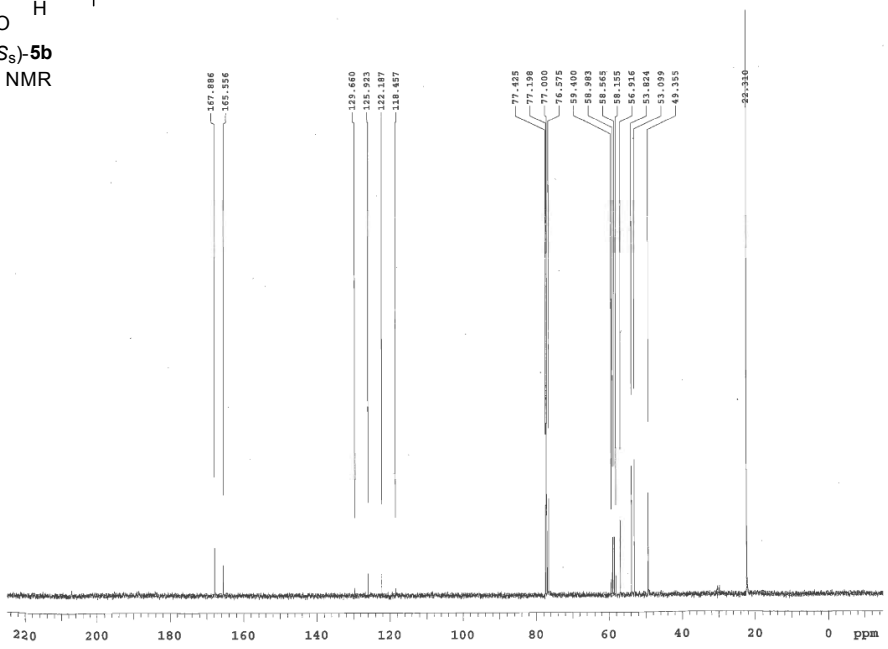


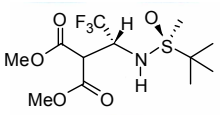


(R,S_S)-**5b**
^{1}H NMR

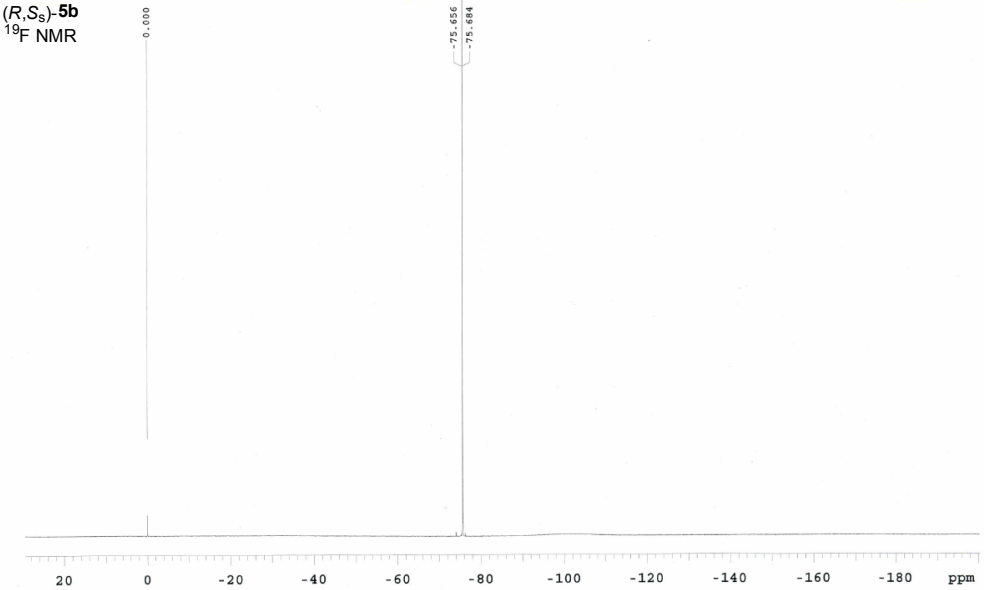


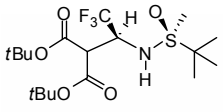
(R,S_S)-**5b**
^{13}C NMR



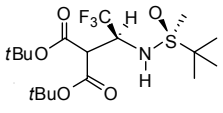


(R,S_S)-**5b**
^{19}F NMR

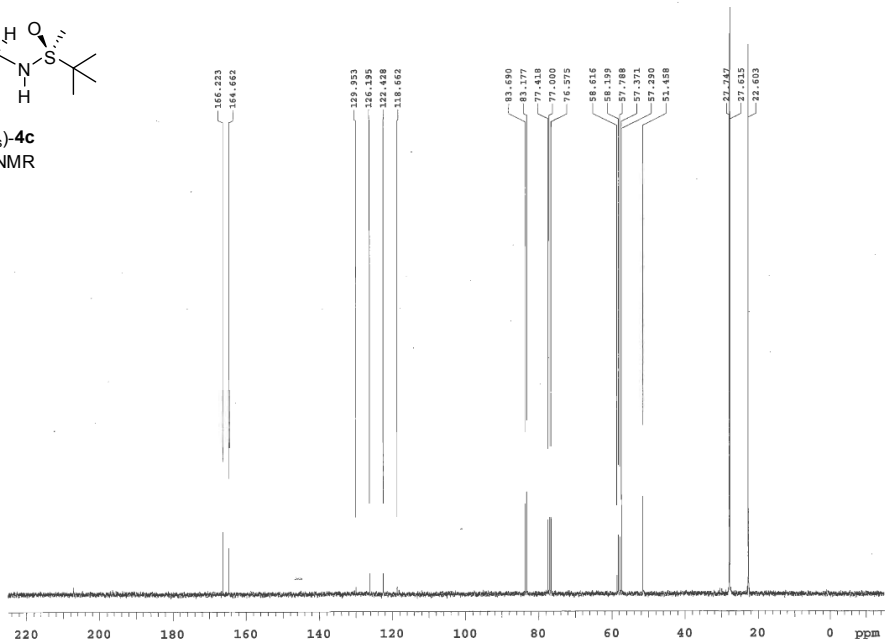


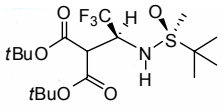


(*S*,*S*$_S$)-**4c**
^{1}H NMR

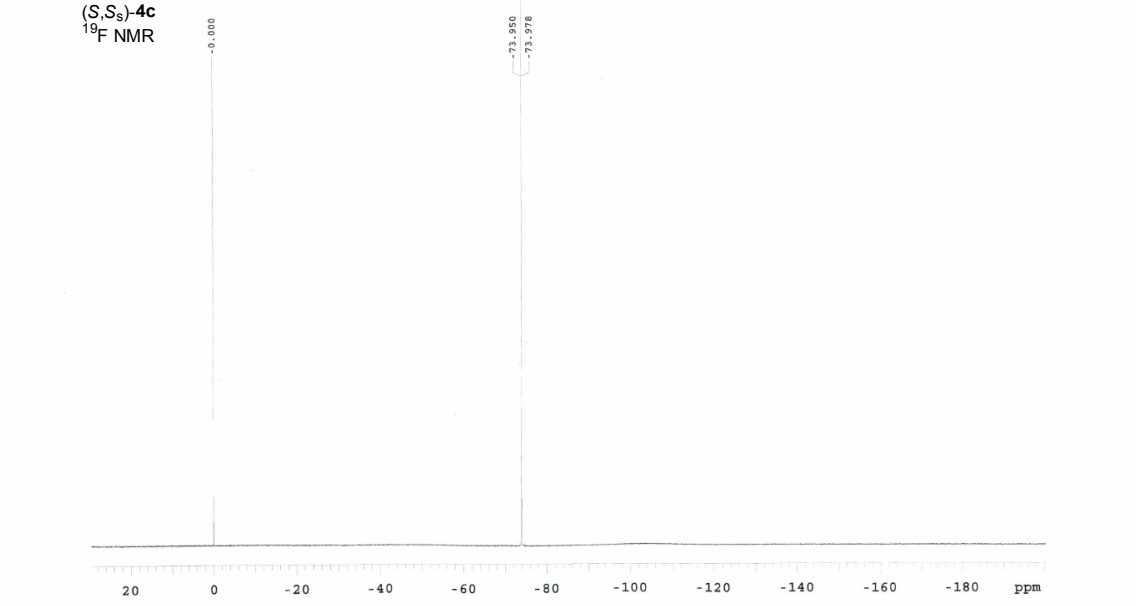


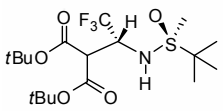
(*S*,*S*$_S$)-**4c**
^{13}C NMR



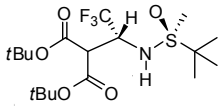


(S,S_S)-**4c**
^{19}F NMR

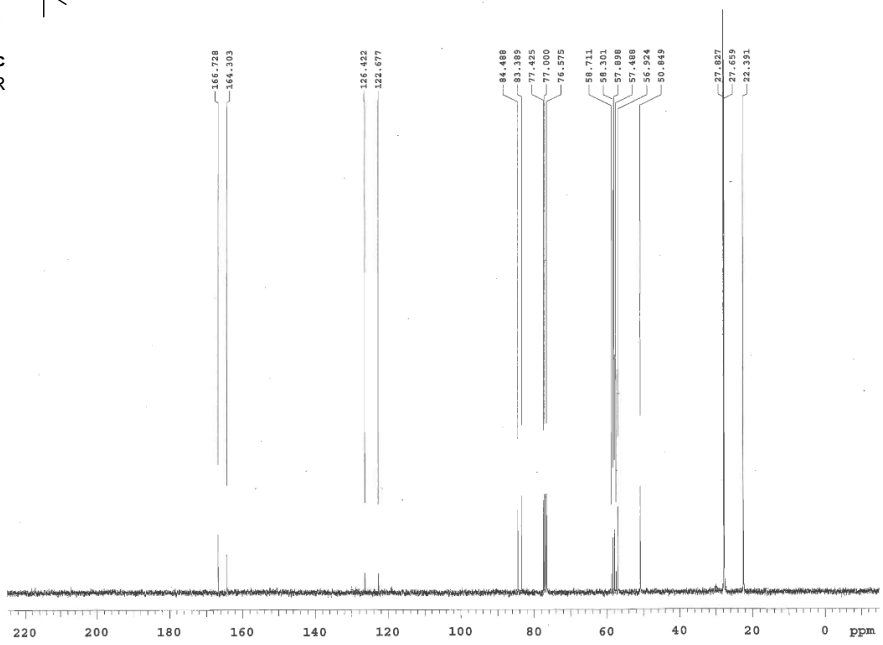


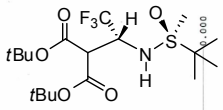


(R,S_S)-**5c**
^{1}H NMR

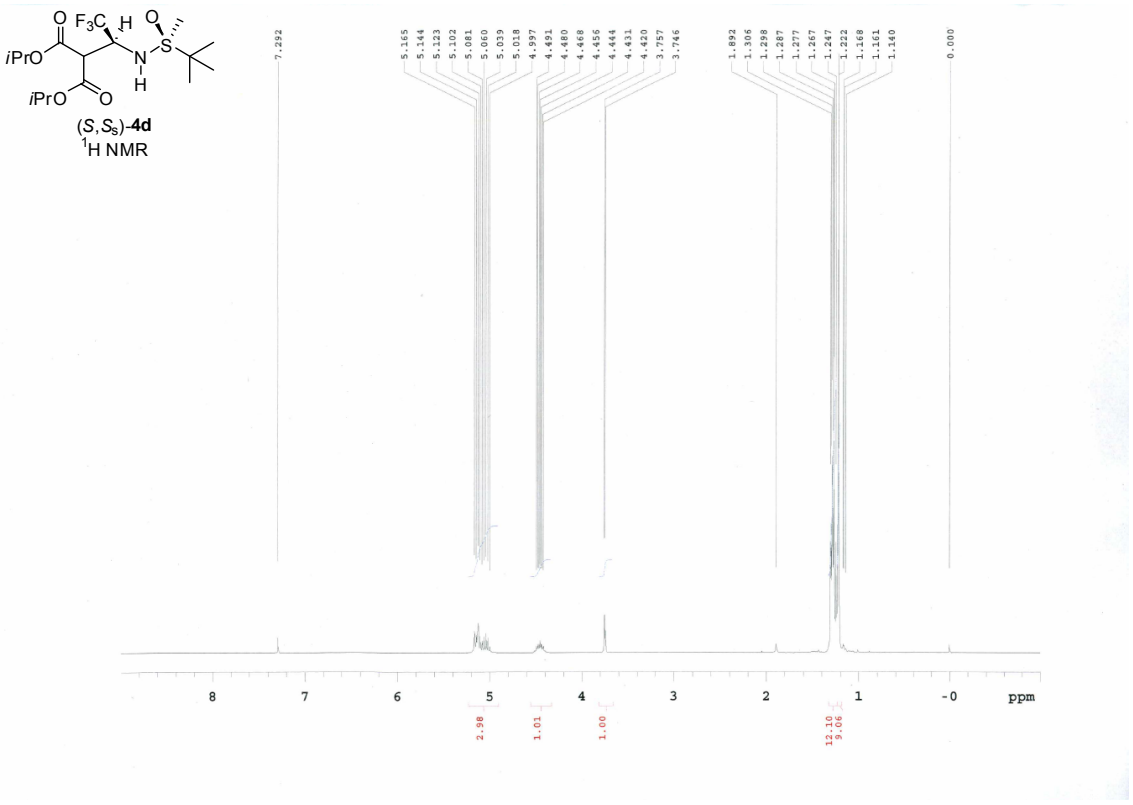


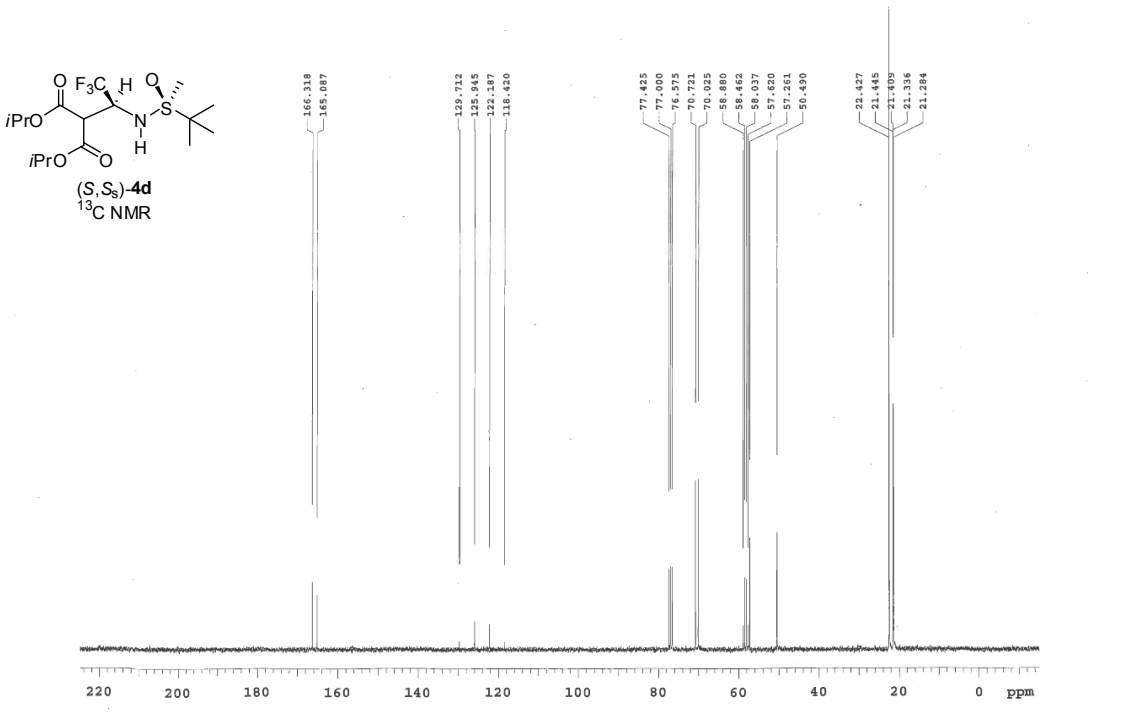
(R,S_S)-**5c**
^{13}C NMR

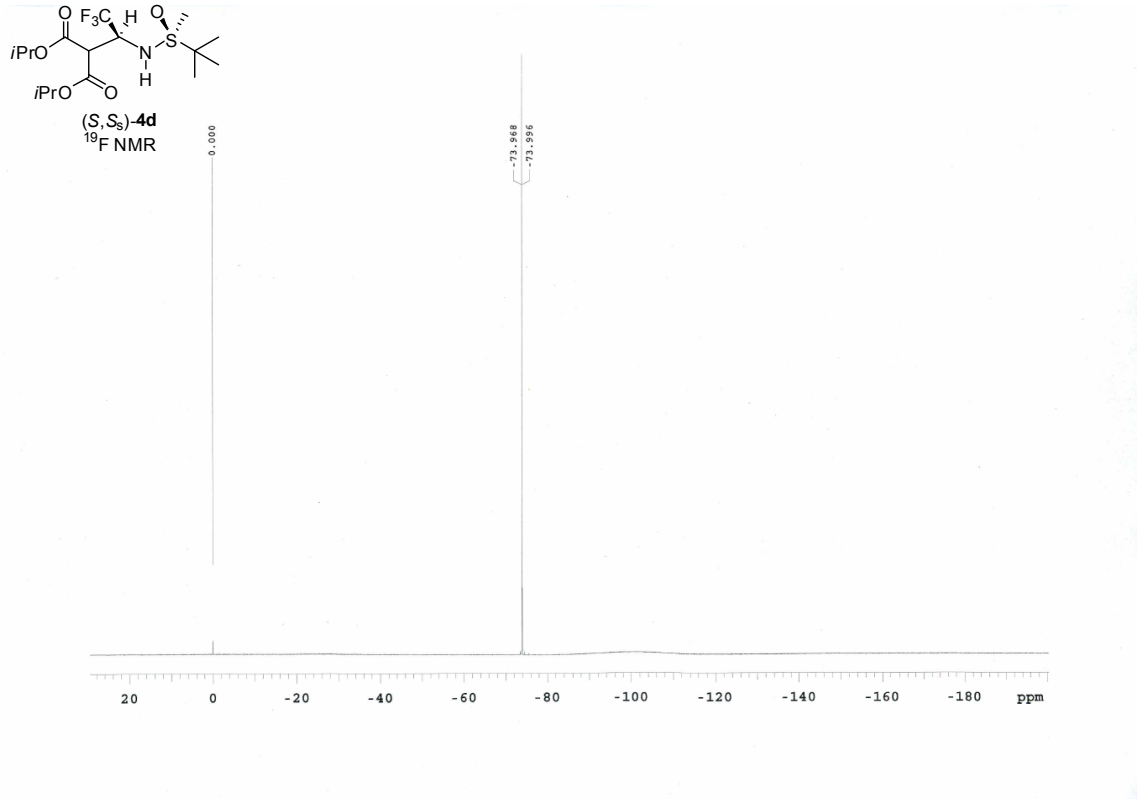


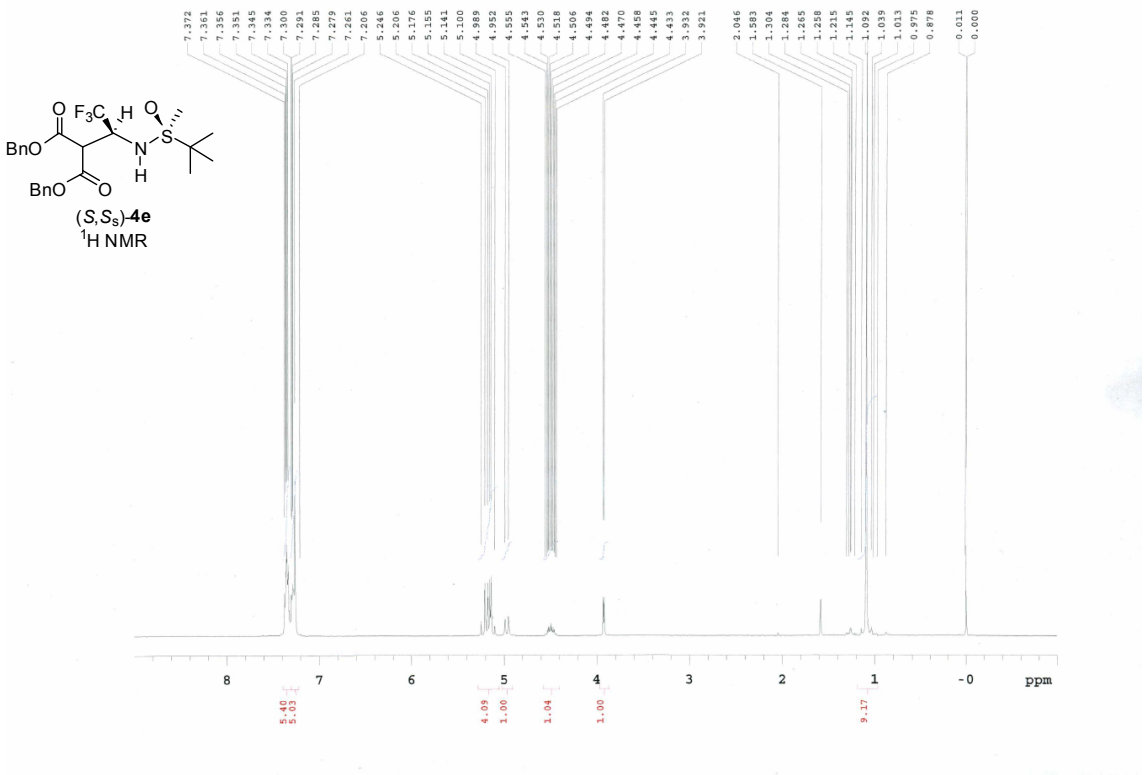


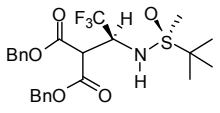
(R,S_S)-**5c**
^{19}F NMR


(S,Ss)-4d
1H NMR
7.292
5.165
5.144
5.123
5.102
5.081
5.060
5.039
5.018
4.597
4.491
4.480
4.468
4.456
4.444
4.431
4.420
3.757
3.746
1.892
1.306
1.298
1.287
1.277
1.267
1.247
1.222
1.168
1.161
1.140
0.000
8
7
6
5
4
3
2
1
-0
ppm
2.98
1.01
1.00
12.10
9.06

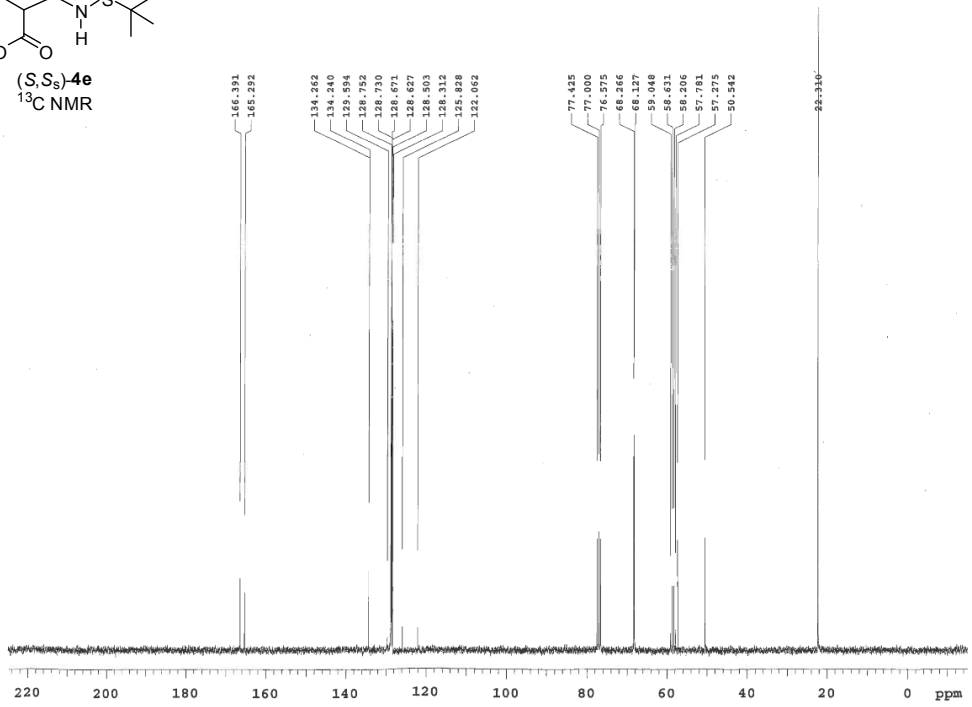

(S,Ss)-4d
13C NMR
166.318
165.087
129.712
125.945
122.187
118.420
77.425
77.000
76.575
70.721
70.025
58.880
58.462
58.037
57.620
57.261
50.490
22.427
21.445
21.409
21.336
21.284
220
200
180
160
140
120
100
80
60
40
20
0
ppm

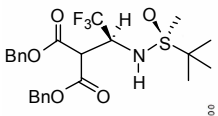

iPrO
iPrO
F3C
H
N
H
S
(S,Ss)-4d
19F NMR
0.000
-73.968
-73.956
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm


BnO
BnO
F3C
H
N
H
S
(S,Ss)-4e
1H NMR
8
7
6
5
4
3
2
1
-0
ppm

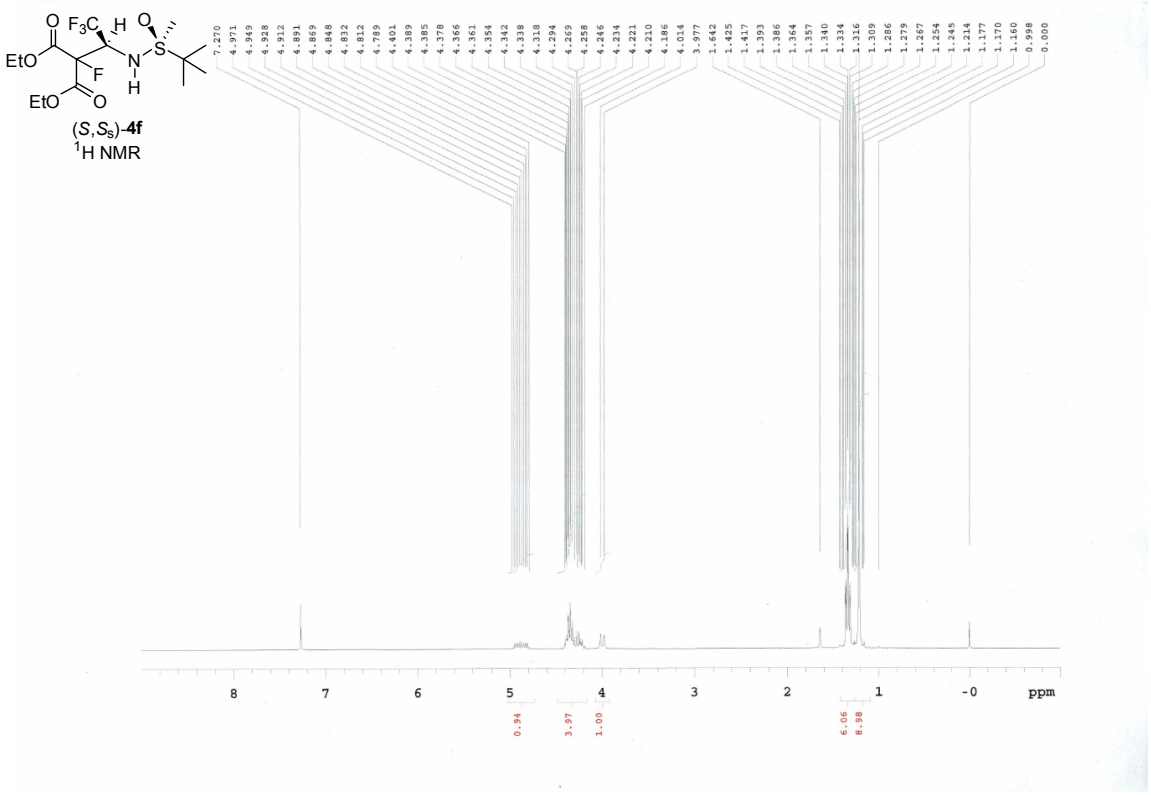


(*S*,*S*$_s$)-**4e**
^{13}C NMR





(*S*,*S*$_s$)-**4e**
^{19}F NMR


(S,Ss)-4f
1H NMR
7.270
4.971
4.949
4.928
4.912
4.891
4.869
4.848
4.832
4.812
4.789
4.401
4.389
4.385
4.378
4.366
4.361
4.354
4.342
4.338
4.318
4.294
4.269
4.258
4.246
4.234
4.221
4.210
4.186
4.014
3.977
1.642
1.425
1.417
1.393
1.386
1.364
1.357
1.340
1.334
1.316
1.309
1.286
1.279
1.267
1.254
1.245
1.214
1.177
1.170
1.160
0.998
0.000
8
7
6
5
4
3
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1
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ppm
0.94
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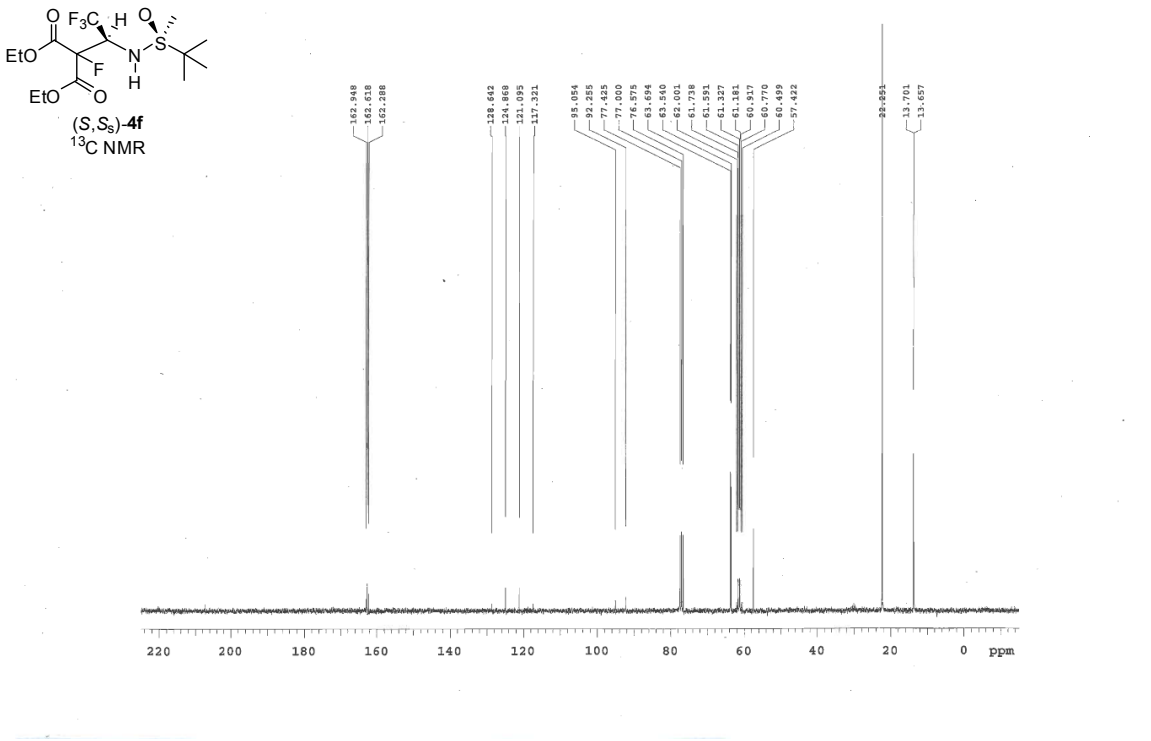
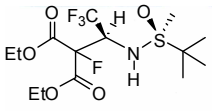
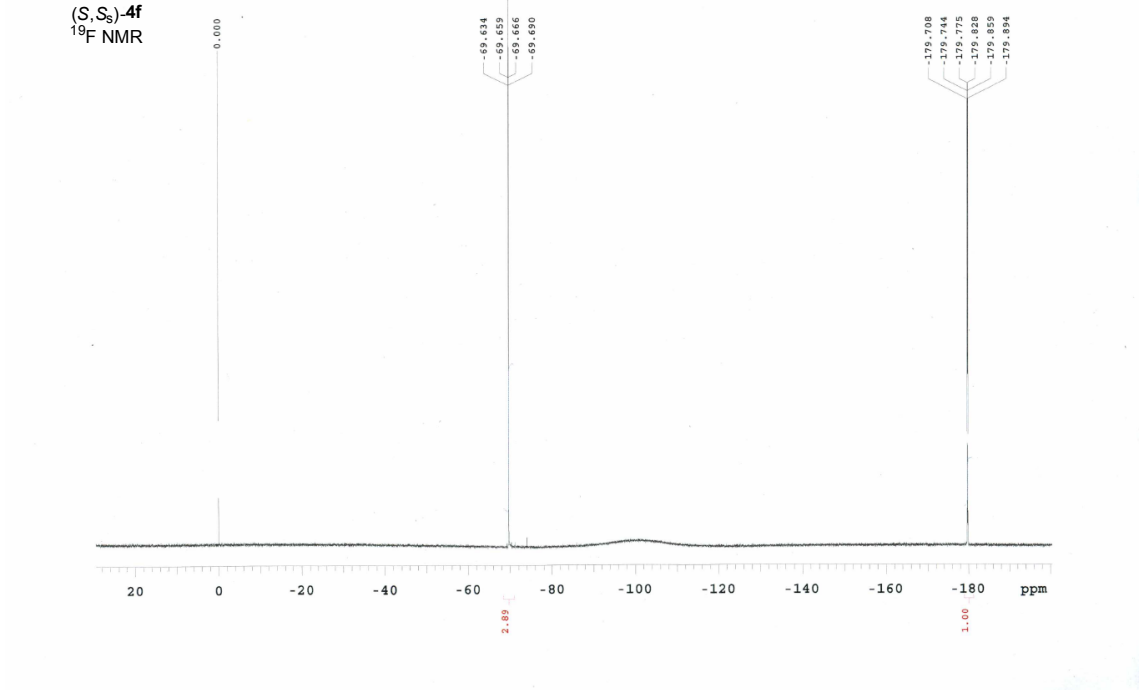
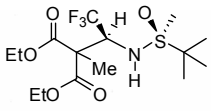
1.00
6.06
8.98


(S,Ss)-4f
13C NMR
162.948
162.618
162.288
128.642
124.868
121.095
117.321
95.054
92.255
77.425
77.000
76.575
63.694
63.540
62.001
61.738
61.591
61.327
61.181
60.917
60.770
60.499
57.422
20.691
13.701
13.657
220
200
180
160
140
120
100
80
60
40
20
0
ppm

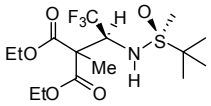


(S,S_s)-**4f**
^{19}F NMR

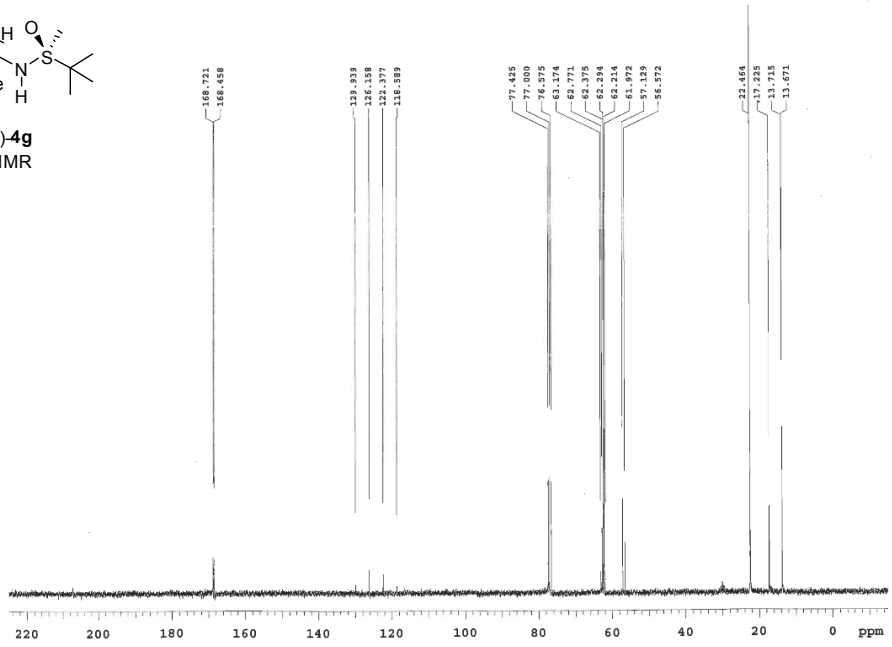


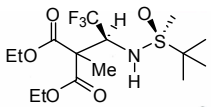


(S,S_s)-**4g**
^{1}H NMR

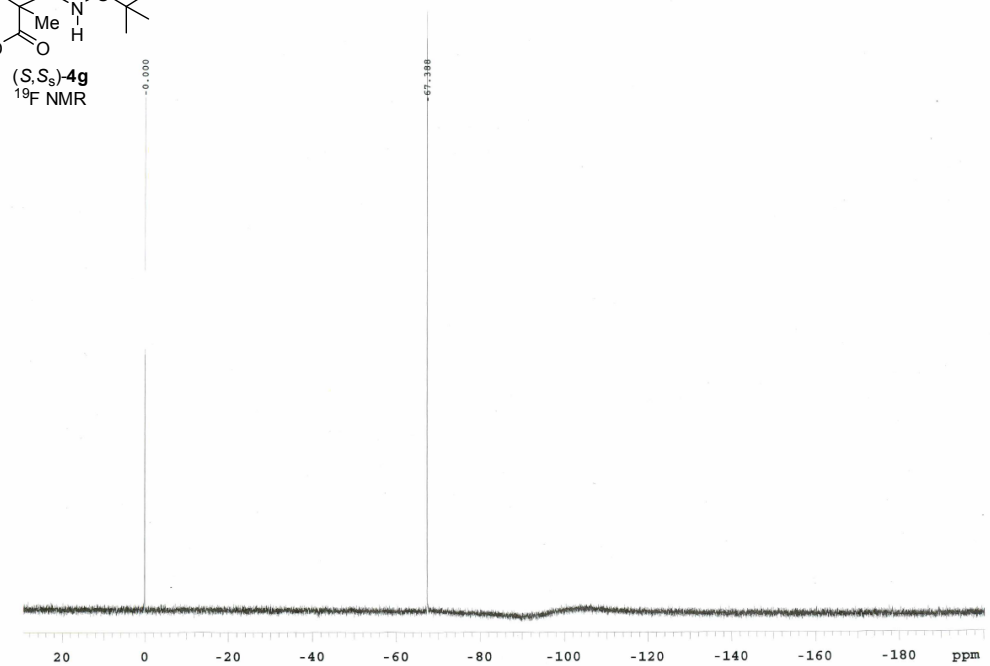


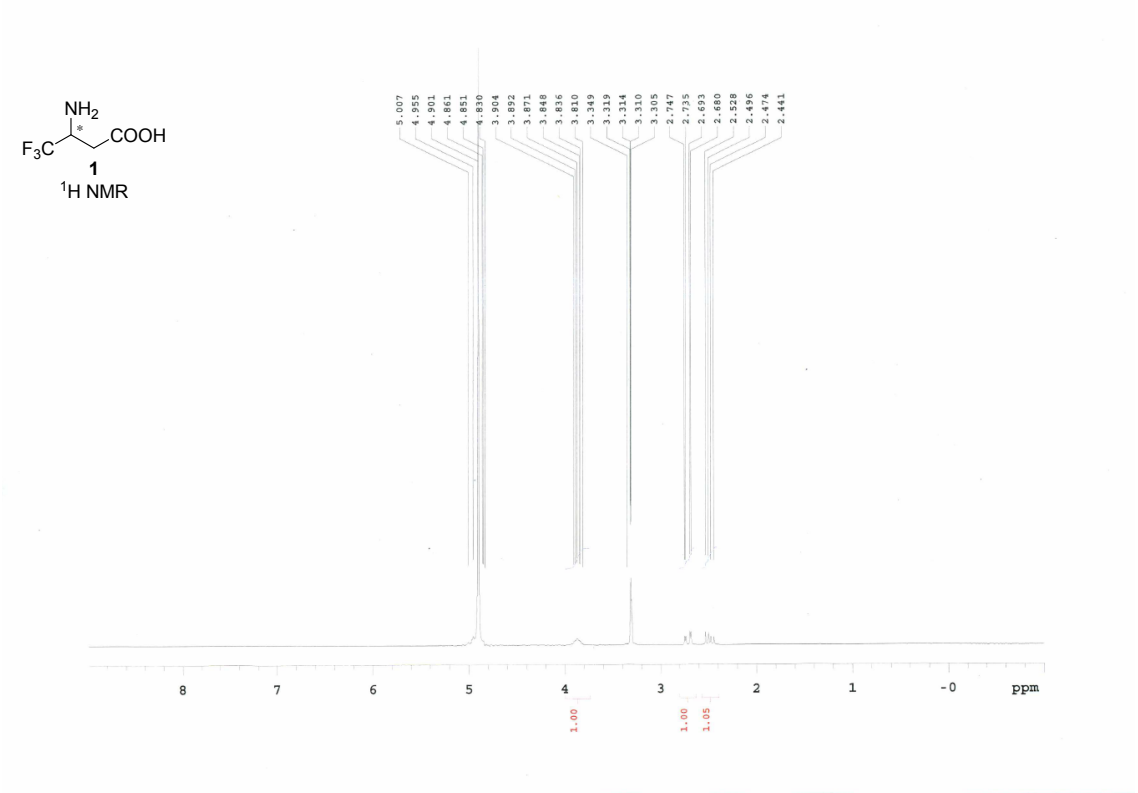
(*S*,*S*$_s$)-**4g**
^{13}C NMR

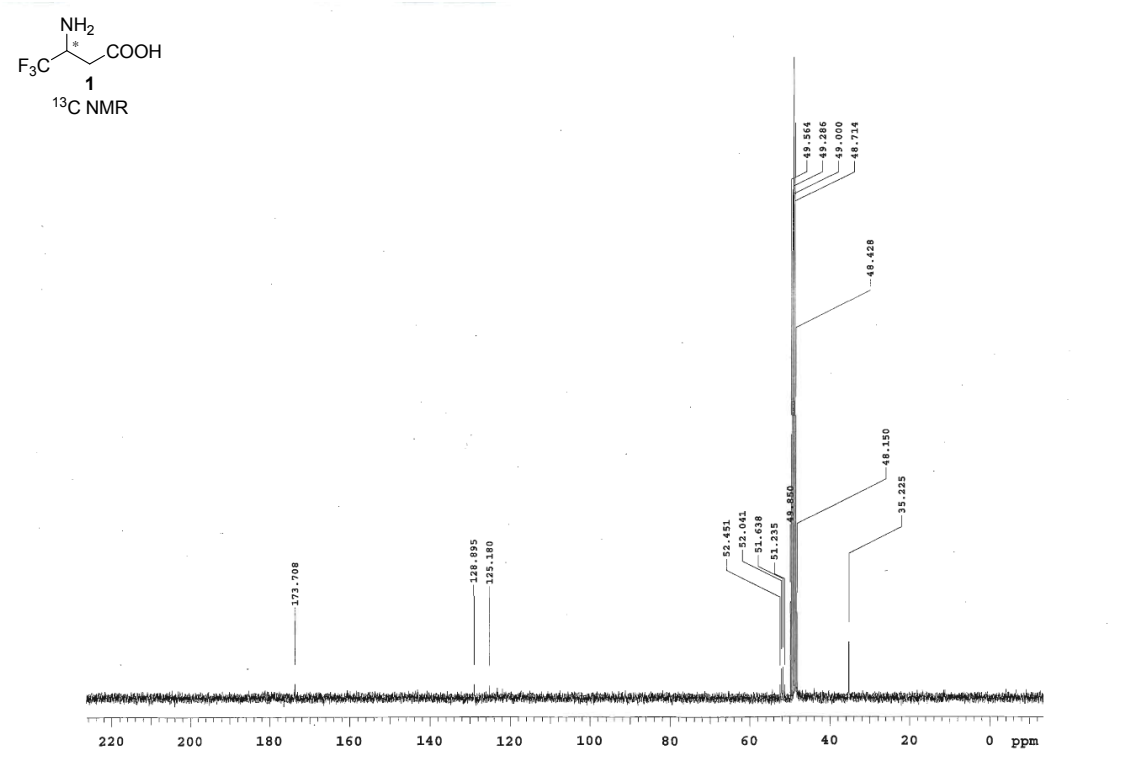


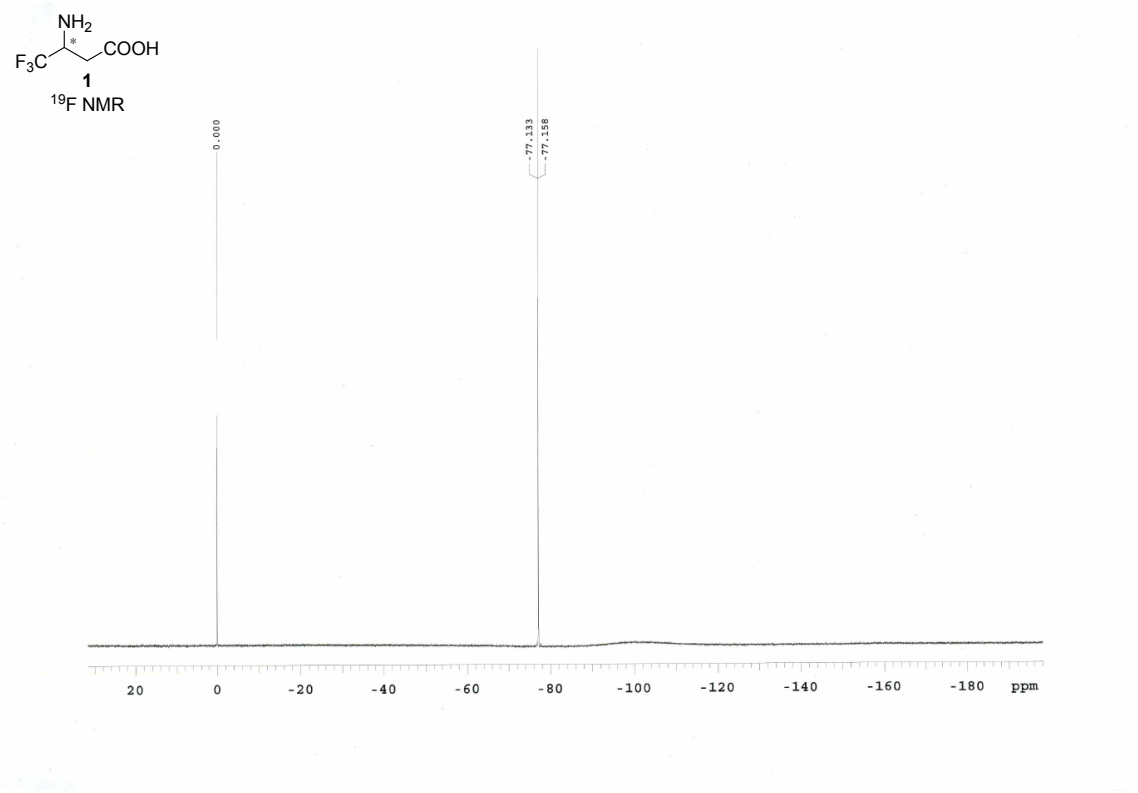


(*S*,*S*$_s$)-**4g**
^{19}F NMR




NH2
F3C
COOH
1
1H NMR
5.007
4.955
4.901
4.861
4.851
4.830
3.904
3.892
3.871
3.848
3.836
3.810
3.349
3.319
3.314
3.310
3.305
2.747
2.735
2.693
2.680
2.528
2.496
2.474
2.441
8
7
6
5
4
3
2
1
-0
ppm
1.00
1.00
1.05


NH2
F3C
COOH
1
13C NMR
49.564
49.286
49.000
48.714
48.428
48.150
35.225
52.451
52.041
51.638
51.235
173.708
128.895
125.180
220
200
180
160
140
120
100
80
60
40
20
0
ppm


NH2
F3C
COOH
1
19F NMR
0.000
-77.133
-77.158
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
ppm