Electronic Supplementary Material (ESI) for Chemical Communications.

Photochemical fluoro-amino etherification reactions of aryldiazoacetates with NFSI under stoichiometric conditions

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General Information

Unless otherwise noted, all commercially available compounds were used as provided without further purification. Chemicals used in this manuscript were purchased from Sigma Aldrich, Alfa Aesar, Fluorochem and Carl Roth.

Solvents used in reactions were p.A. grade. All reactions were performed under argon using degassed solvents. Solvents for chromatography were technical grade and distilled prior to use. Analytical thin-layer chromatography (TLC) was performed on Macherey-Nagel silica gel aluminium plates with F-254 indicator, visualised by irradiation with UV light. Column chromatography was performed using silica gel Merck 60 (particle size 0.063 – 0.2 mm). Solvent mixtures are understood as volume/volume.

^{1}H-NMR, ^{19}F-NMR and ^{13}C-NMR were recorded on a Varian AV600/AV400 or an Agilent DD2 400 NMR spectrometer in $CDCl_3$. Data are reported in the following order: chemical shift (δ) in ppm; multiplicities are indicated br (broadened singlet), s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet); coupling constants (*J*) are in Hertz (Hz).

HRMS data were recorded on a ThermoFisher Scientific LTQ Orbitrap XL using ESI ionization or on a Finnigan MAT 95 using EI ionization at 70 eV.

IR spectra were recorded on a Perkin Elmer-100 spectrometer and are reported in terms of frequency of absorption (cm^{-1}).

LEDs used in this manuscript were purchased from Conrad Electronics:

High Power LED-Module, 3 W, 30 lm, 30 °, 470 nm, art.nr. 180745 – 62.

Important safety note

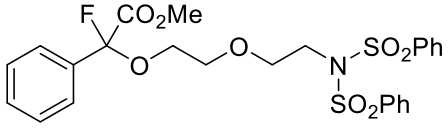
Handling of diazo compounds should only be done in a well-ventilated fume cupboard using an additional blast shield. No incidents occurred handling of diazoalkanes during the preparation of this manuscript, yet the reader should be aware of carcinogenicity and explosiveness of the herein described diazo compounds. General safety precautions when working with diazomethane and its derivatives should be followed. Any reactions described in this manuscript should not be performed without strict risk assessment and proper safety precautions.

General Procedure for rearrangement reaction (GP)

In a test tube and under air, the substrate (0.2 mmol, 1.0 Eq.) and the diazoalkane (1.0 Eq.) was dissolved in 2.0 mL 1,4 - dioxane and irradiated at room temperature with one 3 W LED (distance 1.5 cm, cooling of the setup from the outside with a fan), stirred overnight. The crude reaction mixture was purified by column chromatography using pentane: Et_2O as eluent to afford the final product.

Physical data

methyl 2-fluoro-2-phenyl-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido)ethoxy) ethoxy)acetate (5a)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (94 %, 104 mg).

^{1}H NMR (400 MHz, Chloroform-*d*): δ = 8.19 – 7.76 (m, 4H), 7.66 – 7.57 (m, 4H), 7.57 – 7.48 (m, 4H), 7.43 – 7.38 (m, 3H), 3.91 (t, *J* = 6.1 Hz, 2H), 3.78 – 3.68 (m, 7H), 3.65 – 3.49 (m, 2H) ppm.

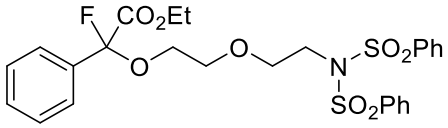
^{13}C NMR (101 MHz, Chloroform-d): δ = 167.0 (d, *J* = 39.4 Hz), 139.6, 135.1 (d, *J* = 27.5 Hz), 133.8, 130.0 (d, *J* = 1.5 Hz), 129.0, 128.5, 128.3, 126.1 (d, *J* = 6.4 Hz), 109.6 (d, *J* = 232.7 Hz), 69.7, 69.4, 64.7 (d, *J* = 2.9 Hz), 53.2, 47.8 ppm.

^{19}F NMR (376 MHz, Chloroform-*d*): δ = -118.7 ppm.

IR (**KBr**): 3501, 3067, 2955, 2884, 2161, 2019, 1902, 1756, 1585, 1478, 1448, 1371, 1267, 1165, 1124, 1084, 1045, 934, 860, 731, 687 cm^{-1}.

HRMS (ESI): mass found: 574.09766, mass calculated for $C_{25}H_{26}NFS_2NaO_8^+$: 574.09761.

ethyl 2-fluoro-2-phenyl-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido)ethoxy) ethoxy)acetate (5b)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (90 %, 102 mg).

^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.11 – 8.03 (m, 4H), 7.67 – 7.63 (m, 4H), 7.54 (t, *J* = 7.9 Hz, 4H), 7.44 – 7.41 (m, 3H), 4.25 (q, *J* = 7.1 Hz, 2H), 3.94 (t, *J* = 6.2 Hz, 2H), 3.82 – 3.72 (m, 4H), 3.68 – 3.57 (m, 2H), 1.26 (t, *J* = 7.1 Hz, 3H) ppm.

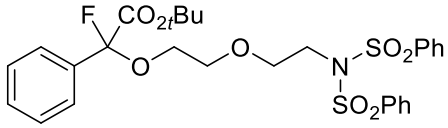
^{13}C NMR (151 MHz, Chloroform-d): δ = 166.5 (d, *J* = 39.6 Hz), 139.7, 135.3 (d, *J* = 27.3 Hz), 133.8, 129.9, 129.0, 128.4, 128.3, 126.1 (d, *J* = 6.2 Hz), 109.6 (d, *J* = 233.1 Hz), 69.8, 69.5, 64.7 (d, *J* = 2.9 Hz), 62.4, 47.9, 13.9 ppm.

^{19}F NMR (565 MHz, Chloroform-*d*): δ = -118.8 ppm

IR (**KBr**): 3493, 3067, 2951, 2326, 2163, 1978, 1903, 1751, 1585, 1449, 1371, 1263, 1165, 1124, 1084, 1041, 929, 859, 755, 729, 687 cm^{-1}.

HRMS (ESI): mass found: 588.11326, mass calculated for $C_{26}H_{28}NFS_2NaO_8^+$: 588.11326.

***tert*-butyl 2-fluoro-2-phenyl-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido)ethoxy) ethoxy)acetate (5c)**

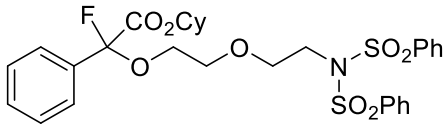


The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (84 %, 100 mg).

^{1}H NMR (400 MHz, Chloroform-*d*): δ = 8.08 – 8.00 (m, 4H), 7.64 – 7.56 (m, 4H), 7.54 – 7.46 (m, 4H), 7.41 – 7.34 (m, 3H), 3.91 (t, *J* = 6.1 Hz, 2H), 3.80 – 3.70 (m, 4H), 3.65 – 3.54

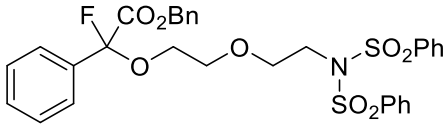
(m, 2H), 1.41 (s, 9H) ppm.
^{13}C NMR (101 MHz, Chloroform-d): δ = 165.4 (d, *J* = 39.1 Hz), 139.6, 135.7 (d, *J* = 27.3 Hz), 133.8, 129.6 (d, *J* = 1.6 Hz), 129.0, 128.3, 128.2, 125.9 (d, *J* = 6.2 Hz), 109.5 (d, *J* = 233.1 Hz), 83.5, 69.8, 69.5, 64.7 (d, *J* = 2.7 Hz), 47.9, 27.7 ppm.
^{19}F NMR (376 MHz, Chloroform-*d*): δ = -118.5 ppm.
IR (**KBr**): 3563, 3362, 3068, 2977, 2933, 2875, 2665, 2327, 2185, 2077, 1987, 1910, 1818, 1727, 1687, 1594, 1477, 1449, 1370, 1253, 1213, 1164, 1081, 984, 927, 852, 755, 686 cm^{-1}.
HRMS (ESI): mass found: 616.14453, mass calculated for $C_{28}H_{32}NFS_2NaO_8^+$: 616.14456.

Cyclohexyl 2-fluoro-2-phenyl-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido)ethoxy) ethoxy)acetate (5d)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (80 %, 99 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.01 – 7.96 (m, 4H), 7.58 – 7.50 (m, 4H), 7.47 – 7.40 (m, 4H), 7.35 – 7.27 (m, 3H), 4.78 – 4.70 (m, 1H), 3.84 (t, *J* = 6.2 Hz, 2H), 3.76 – 3.62 (m, 4H), 3.59 – 3.47 (m, 2H), 1.71 – 1.62 (m, 2H), 1.60 – 1.49 (m, 2H), 1.43 – 1.30 (m, 3H), 1.28 – 1.12 (m, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-d): δ = 165.9 (d, *J* = 39.9 Hz), 139.7, 135.6 (d, *J* = 27.2 Hz), 133.8, 129.8, 129.0, 128.3, 126.0 (d, *J* = 6.1 Hz), 109.6 (d, *J* = 232.7 Hz), 75.0, 69.8, 69.5, 64.8 (d, *J* = 2.8 Hz), 47.9, 31.1, 31.0, 25.1, 23.3 (d, *J* = 6.3 Hz) ppm.
^{19}F NMR (565 MHz, Chloroform-*d*): δ = -118.6 ppm.
IR (**KBr**): 3067, 2938, 2863, 2667, 2523, 2166, 2035, 1971, 1902, 1747, 1585, 1449, 1372, 1264, 1165, 1124, 1085, 1036, 927, 860, 731, 687 cm^{-1}.
HRMS (ESI): mass found: 642.15918, mass calculated for $C_{30}H_{34}NFS_2NaO_8^+$: 642.16021.

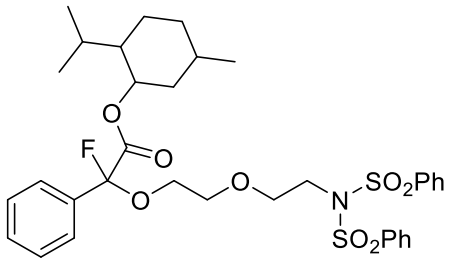
Benzyl 2-fluoro-2-phenyl-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido) ethoxy)ethoxy)acetate (5e)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (99 %, 124 mg).
^{1}H NMR (400 MHz, Chloroform-*d*): δ = 8.10 – 7.99 (m, 4H), 7.65 – 7.58 (m, 4H), 7.51 (t, *J* = 8.0 Hz, 4H), 7.44 – 7.38 (m, 3H), 7.33 – 7.28 (m, 3H), 7.27 – 7.19 (m, 2H), 5.20 (s, 2H), 3.90 (t, *J* = 6.1 Hz, 2H), 3.81 – 3.66 (m, 4H), 3.64 – 3.50 (m, 2H) ppm.
^{13}C NMR (101 MHz, Chloroform-d): δ = 166.4 (d, *J* = 40.0 Hz), 139.6, 135.1 (d, *J* = 27.4 Hz), 134.7, 133.8, 129.9 (d, *J* = 1.7 Hz), 129.0, 128.5, 128.4, 128.3, 128.0, 126.1 (d, *J* = 6.2 Hz), 109.6 (d, *J* = 233.3 Hz), 69.8, 69.4, 67.8, 64.8 (d, *J* = 2.9 Hz), 47.8 ppm.

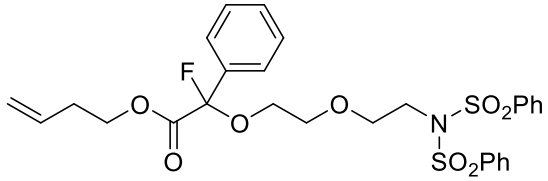
^{19}F NMR (376 MHz, Chloroform-*d*): δ = -118.5 ppm.
IR (**KBr**): 3067, 2952, 2883, 2329, 2164, 2084, 1902, 1754, 1585, 1449, 1371, 1264, 1165, 1125, 1058, 1035, 928, 860, 732, 689 cm^{-1}.
HRMS (ESI): mass found: 650.12909, mass calculated for $C_{31}H_{30}NFS_2NaO_8^+$: 650.12891.

2-isopropyl-5-methylcyclohexyl 2-fluoro-2-phenyl-2-(2-(2-(N-(phenylsulfonyl)phenyl sulfonamido)ethoxy)ethoxy)acetate (5f)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (93 %, 126 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.00 – 7.95 (m, 4H), 7.55 – 7.49 (m, 4H), 7.45 – 7.39 (m, 4H), 7.33 – 7.27 (m, 3H), 4.63 – 4.56 (m, 1H), 3.84 (q, *J* = 6.1 Hz, 2H), 3.78 – 3.62 (m, 4H), 3.60 – 3.47 (m, 2H), 1.85 – 1.80 (m, 1H), 1.59 – 1.50 (m, 2H), 1.48 – 1.22 (m, 3H), 0.94 – 0.85 (m, 2H), 0.81 – 0.71 (m, 4H), 0.65 (dd, *J* = 28.6, 6.9 Hz, 3H), 0.48 – 0.41 (m, 3H) ppm.
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 166.2 (d, *J* = 40.4 Hz, 39.1 Hz*), 139.7, 135.6 (d, J = 26.8 Hz), 135.5 (d, J = 27.5 Hz), 133.8, 129.8, 129.0, 128.37, 128.35, 128.2, 126.0 (d, J = 5.2 Hz, 6.9 Hz*), 125.98, 125.97, 109.7 (d, J = 233.9 Hz), 109.6 (d, J = 232.6 Hz), 69.88, 69.87, 69.5, 64.9 (d, *J* = 2.6 Hz), 64.8 (d, *J* = 2.9 Hz), 47.9, 46.8, 40.2, 34.0, 31.3, 25.8, 25.7, 23.16, 23.11, 21.94, 21.92, 20.59, 20.55, 15.8, 15.7.
^{19}F NMR (565 MHz, Chloroform-*d*): δ = -117.0, -120.2 ppm.
IR (**KBr**): 3856, 3607, 2954, 2871, 2726, 2521, 2327, 2167, 2036, 1993, 1903, 1815, 1746, 1585, 1450, 1373, 1267, 1166, 1127, 1086, 1034, 949, 860, 732, 688 cm^{-1}.
HRMS (ESI): mass found: 698.22278, mass calculated for $C_{34}H_{42}NFS_2NaO_8^+$: 698.22281.

but-3-en-1-yl 2-fluoro-2-phenyl-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido) ethoxy)ethoxy)acetate (5g)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (75 %, 89 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.10 – 8.04 (m, 4H), 7.67 – 7.61 (m, 4H), 7.54 (t, *J* = 7.8 Hz, 4H), 7.45 – 7.38 (m, 3H), 5.72 – 5.62 (m, 1H), 5.04 – 4.96 (m, 2H), 4.29 – 4.17 (m, 2H), 3.94 (t, *J* = 6.2 Hz, 2H), 3.83 – 3.72 (m, 4H), 3.69 – 3.55 (m, 2H), 2.40 – 2.34 (m, 2H)

ppm.

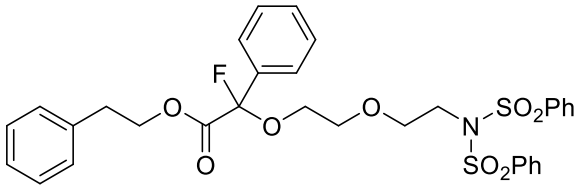
^{13}C NMR (151 MHz, Chloroform-d): δ = 166.5 (d, *J* = 39.8 Hz), 139.7, 135.3 (d, *J* = 27.4 Hz), 133.8, 133.1, 129.9, 129.0, 128.4, 128.3, 126.1 (d, *J* = 6.4 Hz), 117.7, 109.6 (d, *J* = 233.1 Hz), 69.8, 69.5, 65.2, 64.8 (d, *J* = 2.8 Hz), 47.9, 32.7 ppm.

^{19}F NMR (565 MHz, Chloroform-*d*): δ = -118.8 ppm.

IR (**KBr**): 3335, 3071, 2959, 2896, 2519, 2163, 1903, 1753, 1642, 1585, 1449, 1372, 1262, 1165, 1124, 1085, 996, 923, 859, 756, 726, 687 cm^{-1}.

HRMS (ESI): mass found: 614.12811, mass calculated for $C_{28}H_{30}NFS_2NaO_8^+$: 614.12891.

phenethyl 2-fluoro-2-phenyl-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido) ethoxy)ethoxy)acetate (5h)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (74 %, 95 mg).

^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.12 – 8.03 (m, 4H), 7.66 – 7.61 (m, 2H), 7.60 – 7.57 (m, 2H), 7.53 (t, *J* = 7.9 Hz, 4H), 7.45 – 7.38 (m, 3H), 7.28 – 7.20 (m, 3H), 7.13 – 7.09 (m, 2H), 4.45 – 4.36 (m, 2H), 3.93 (t, *J* = 6.2 Hz, 2H), 3.78 – 3.71 (m, 3H), 3.67 – 3.63 (m, 1H), 3.63 – 3.52 (m, 2H), 2.93 (t, *J* = 6.9 Hz, 2H) ppm.

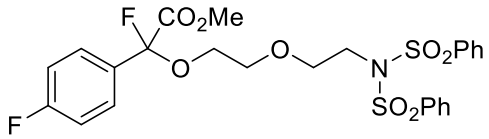
^{13}C NMR (151 MHz, Chloroform-d): δ = 166.4 (d, *J* = 39.9 Hz), 139.7, 137.1, 135.2 (d, *J* = 27.3 Hz), 133.8, 129.9, 129.0, 128.8, 128.5, 128.4, 128.3, 126.6, 126.1 (d, *J* = 6.1 Hz), 109.6 (d, *J* = 233.0 Hz), 69.8, 69.5, 66.6, 64.7 (d, *J* = 2.8 Hz), 47.9, 34.7 ppm.

^{19}F NMR (565 MHz, Chloroform-*d*): δ = -118.6 ppm.

IR (**KBr**): 3066, 3031, 2957, 2327, 2160, 2038, 1901, 1817, 1753, 1585, 1449, 1372, 1261, 1165, 1124, 1085, 929, 860, 752, 689 cm^{-1}.

HRMS (ESI): mass found: 664.14410, mass calculated for $C_{32}H_{32}NFS_2NaO_8^+$: 664.14456.

methyl 2-fluoro-2-(4-fluorophenyl)-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido) ethoxy)ethoxy)acetate (5i)



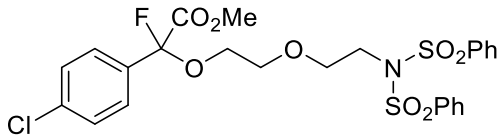
The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (83 %, 94 mg).

^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.14 – 8.10 (m, 2H), 8.09 – 8.04 (m, 4H), 7.70 – 7.66 (m, 2H), 7.60 – 7.55 (m, 4H), 7.24 – 7.18 (m, 2H), 4.00 (s, 3H), 3.95 (t, *J* = 6.0 Hz, 2H), 3.71 (t, *J* = 6.0 Hz, 2H), 3.69 – 3.64 (m, 2H), 3.51 – 3.46 (m, 2H) ppm.

^{13}C NMR (151 MHz, Chloroform-d): δ = 184.1, 166.8 (d, *J* = 258.6 Hz), 163.6, 139.7, 133.9, 133.08, 133.01, 129.0, 128.3, 116.2 (d, *J* = 22.2 Hz), 72.1, 69.2, 61.6, 52.9, 47.9 ppm.

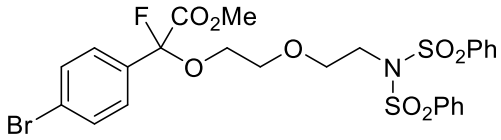
^{19}F NMR (376 MHz, Chloroform-*d*): δ = -111.0, -117.9 ppm.
IR (**KBr**): 3070, 2955, 2884, 2327, 2167, 1985, 1905, 1757, 1605, 1509, 1478, 1448, 1371, 1263, 1236, 1164, 1124, 1086, 936, 844, 736, 685, 658 cm^{-1}.
HRMS (ESI): mass found: 592.08771, mass calculated for $C_{25}H_{25}NF_2S_2NaO_8^+$: 592.08819.

methyl 2-(4-chlorophenyl)-2-fluoro-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido) ethoxy)ethoxy)acetate (5j)



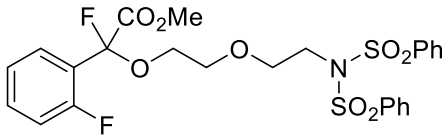
The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (86 %, 101 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.12 – 8.03 (m, 4H), 7.69 – 7.63 (m, 2H), 7.60 – 7.51 (m, 6H), 7.42 – 7.37 (m, 2H), 3.93 (t, *J* = 6.2 Hz, 2H), 3.80 – 3.72 (m, 7H), 3.69 – 3.63 (m, 1H), 3.63 – 3.58 (m, 1H) ppm.
^{13}C NMR (151 MHz, Chloroform-d): δ = 166.7 (d, *J* = 39.7 Hz), 139.7, 136.2, 133.8, 133.6, 129.0, 128.7, 128.3, 127.7 (d, *J* = 6.1 Hz), 109.2 (d, *J* = 233.6 Hz), 69.8, 69.3, 64.9 (d, *J* = 2.7 Hz), 53.3, 47.8 ppm.
^{19}F NMR (565 MHz, Chloroform-*d*): δ = -118.6 ppm.
IR (**KBr**): 3067, 2954, 2883, 2663, 2327, 2109, 1988, 1917, 1757, 1596, 1487, 1447, 1371, 1266, 1166, 1126, 1088, 935, 860, 735, 685, 657 cm^{-1}.
HRMS (ESI): mass found: 608.05823, mass calculated for $C_{25}H_{25}NFClS_2NaO_8^+$: 608.05864.

methyl 2-(4-bromophenyl)-2-fluoro-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido) ethoxy)ethoxy)acetate (5k)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (84 %, 106 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.02 – 7.96 (m, 4H), 7.60 – 7.52 (m, 2H), 7.48 – 7.43 (m, 6H), 7.42 – 7.39 (m, 2H), 3.84 (t, *J* = 6.2 Hz, 2H), 3.69 (s, 3H), 3.68 – 3.63 (m, 4H), 3.58 – 3.48 (m, 2H) ppm.
^{13}C NMR (151 MHz, Chloroform-d): δ = 166.6 (d, *J* = 39.5 Hz), 139.7, 134.2 (d, *J* = 28.2 Hz), 133.8, 131.7, 129.0, 128.3, 127.9 (d, *J* = 6.4 Hz), 124.5, 109.2 (d, *J* = 233.3 Hz), 69.8, 69.3, 64.9 (d, *J* = 2.9 Hz), 53.3, 47.8 ppm.
^{19}F NMR (565 MHz, Chloroform-*d*): δ = -118.8 ppm.
IR (**KBr**): 3322, 3068, 2955, 2884, 2522, 2166, 2030, 1969, 1906, 1757, 1591, 1483, 1447, 1371, 1266, 1165, 1126, 1081, 935, 860, 735, 685, 658 cm^{-1}.
HRMS (ESI): mass found: 652.00793, mass calculated for $C_{25}H_{25}NFBrS_2NaO_8^+$: 652.00812.

methyl 2-fluoro-2-(2-fluorophenyl)-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido) ethoxy)ethoxy)acetate (5l)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (80 %, 91 mg).

^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.09 – 8.01 (m, 4H), 7.73 – 7.69 (m, 1H), 7.66 – 7.62 (m, 2H), 7.53 (t, *J* = 7.9 Hz, 4H), 7.45 – 7.39 (m, 1H), 7.23 – 7.18 (m, 1H), 7.11 – 7.06 (m, 1H), 3.91 (t, *J* = 6.2 Hz, 2H), 3.82 (s, 3H), 3.77 – 3.69 (m, 4H), 3.61 (t, *J* = 5.0 Hz, 2H) ppm.

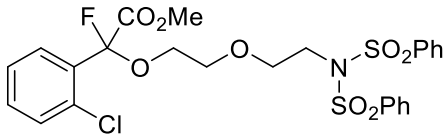
^{13}C NMR (151 MHz, Chloroform-d): δ = 166.1 (d, *J* = 39.2 Hz), 159.7 (d, *J* = 247.8 Hz), 139.6, 133.8, 132.0 (d, *J* = 8.3 Hz), 129.0, 128.3, 128.1 (d, *J* = 2.8 Hz), 128.0 (d, *J* = 2.2 Hz), 124.1 (d, *J* = 3.6 Hz), 116.1 (d, *J* = 20.9 Hz), 106.8 (d, *J* = 231.6 Hz), 69.8, 69.3, 64.83 (d, *J* = 2.8 Hz), 53.3, 47.8 ppm.

^{19}F NMR (565 MHz, Chloroform-*d*): δ = -111.49, -114.41 ppm.

IR (**KBr**): 3484, 2958, 2878, 2792, 2535, 2428, 2165, 2036, 1925, 1762, 1619, 1588, 1546, 1449, 1412, 1371, 1274, 1165, 1086, 1051, 1014, 939, 858, 756, 735, 685, 658 cm^{-1}.

HRMS (ESI): mass found: 592.08716, mass calculated for $C_{25}H_{25}NF_2S_2NaO_8^+$: 592.08819.

methyl 2-(2-chlorophenyl)-2-fluoro-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido) ethoxy)ethoxy)acetate (5m)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (74 %, 87 mg).

^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.09 – 8.06 (m, 4H), 7.87 – 7.82 (m, 1H), 7.68 – 7.63 (m, 2H), 7.57 – 7.52 (m, 4H), 7.44 – 7.34 (m, 3H), 3.92 (t, *J* = 6.2 Hz, 2H), 3.83 (s, 3H), 3.79 – 3.72 (m, 4H), 3.62 (t, *J* = 5.0 Hz, 2H) ppm.

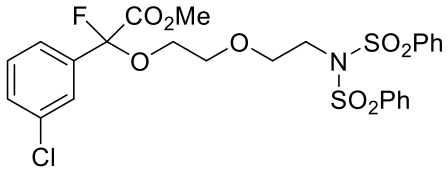
^{13}C NMR (151 MHz, Chloroform-d): δ = 165.8 (d, *J* = 38.1 Hz), 139.7, 133.8, 133.3 (d, *J* = 26.6 Hz), 132.1 (d, *J* = 4.0 Hz), 131.1 (d, *J* = 1.3 Hz), 130.5, 129.0, 128.4 (d, *J* = 7.8 Hz), 128.3, 126.8, 107.5 (d, *J* = 230.4 Hz), 69.8, 69.3, 64.6 (d, *J* = 3.0 Hz), 53.3, 47.8 ppm.

^{19}F NMR (376 MHz, Chloroform-*d*) δ = -111.8 ppm.

IR (**KBr**): 3858, 3426, 3068, 2954, 2883, 2670, 2522, 2327, 2159, 2097, 1993, 1967, 1904, 1819, 1760, 1586, 1473, 1445, 1371, 1269, 1243, 1165, 1067, 970, 860, 751, 685 cm^{-1}.

HRMS (ESI): mass found: 608.05823, mass calculated for $C_{25}H_{25}NFClS_2NaO_8^+$: 608.05864.

methyl 2-(3-chlorophenyl)-2-fluoro-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido) ethoxy)ethoxy)acetate (5n)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (94 %, 111 mg).

^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.10 – 8.06 (m, 4H), 7.68 – 7.62 (m, 3H), 7.59 – 7.50 (m, 5H), 7.44 – 7.40 (m, 1H), 7.37 (t, *J* = 7.8 Hz, 1H), 3.94 (t, *J* = 6.2 Hz, 2H), 3.80 (s, 3H), 3.79 – 3.73 (m, 4H), 3.67 – 3.58 (m, 2H) ppm.

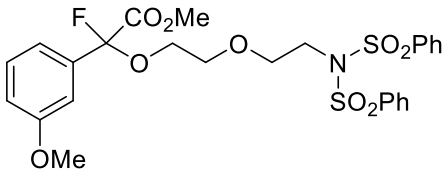
^{13}C NMR (151 MHz, Chloroform-d): δ = 166.5 (d, *J* = 39.4 Hz), 139.7, 137.1 (d, *J* = 28.0 Hz), 134.5, 133.8, 130.2, 129.8, 129.0, 128.3, 126.4 (d, *J* = 6.6 Hz), 124.4 (d, *J* = 6.4 Hz), 108.9 (d, *J* = 234.2 Hz), 69.7, 69.3, 64.9 (d, *J* = 3.0 Hz), 53.3, 47.8 ppm.

^{19}F NMR (565 MHz, Chloroform-*d*): δ = -118.5 ppm.

IR (**KBr**): 3324, 3069, 2928, 2853, 2165, 1979, 1903, 1757, 1622, 1577, 1476, 1447, 1371, 1281, 1246, 1165, 1126, 1084, 937, 860, 754, 683 cm^{-1}.

HRMS (ESI): mass found: 608.05774, mass calculated for $C_{25}H_{25}NFClS_2NaO_8^+$: 608.05864.

methyl 2-fluoro-2-(3-methoxyphenyl)-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido) ethoxy)ethoxy)acetate (5o)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (82 %, 95 mg).

^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.10 – 8.06 (m, 4H), 7.67 – 7.62 (m, 2H), 7.55 (t, *J* = 7.9 Hz, 4H), 7.34 (t, *J* = 8.0 Hz, 1H), 7.24 – 7.19 (m, 1H), 7.18 – 7.15 (m, 1H), 7.01 – 6.94 (m, 1H), 3.93 (t, *J* = 6.2 Hz, 2H), 3.83 (s, 3H), 3.79 (s, 3H), 3.79 – 3.71 (m, 4H), 3.67 – 3.57 (m, 2H) ppm.

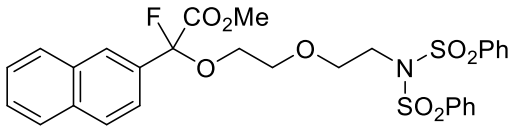
^{13}C NMR (151 MHz, Chloroform-*d*): δ = 166.9 (d, *J* = 39.3 Hz), 159.7, 139.7, 136.5 (d, *J* = 27.8 Hz), 133.8, 129.6, 129.0, 128.3, 118.4 (d, *J* = 6.5 Hz), 115.9, 111.4 (d, *J* = 6.7 Hz), 109.5 (d, *J* = 233.1 Hz), 69.8, 69.4, 64.8 (d, *J* = 2.9 Hz), 55.3, 53.2, 47.8 ppm

^{19}F NMR (565 MHz, Chloroform-d): δ = -118.4 ppm.

IR (**KBr**): 3069, 2954, 2327, 2162, 1927, 1756, 1601, 1486, 1447, 1371, 1274, 1213, 1166, 1123, 1084, 1038, 938, 860, 737, 686 cm^{-1}.

HRMS (ESI): mass found: 604.10815, mass calculated for $C_{26}H_{28}NFS_2NaO_9^+$: 604.10817.

methyl 2-fluoro-2-(naphthalen-2-yl)-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido) ethoxy)ethoxy)acetate (5p)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (63 %, 76 mg).

^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.60 (t, *J* = 1.2 Hz, 1H), 8.08 (dt, *J* = 7.5, 1.3 Hz, 5H), 8.01 (d, *J* = 8.2 Hz, 1H), 7.96 (d, *J* = 8.6 Hz, 1H), 7.92 (d, *J* = 8.2 Hz, 1H), 7.71 – 7.66 (m, 3H), 7.64 – 7.54 (m, 5H), 4.06 (s, 3H), 3.95 (t, *J* = 6.0 Hz, 2H), 3.72 (t, *J* = 6.0 Hz, 2H), 3.69 – 3.64 (m, 2H), 3.51 – 3.47 (m, 2H) ppm.

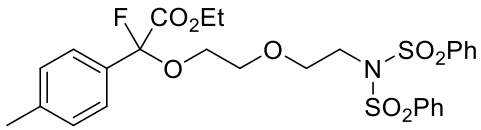
^{13}C NMR (151 MHz, Chloroform-d): δ = 185.9, 164.1, 139.7, 136.4, 133.9, 133.6, 132.3, 130.0, 129.8, 129.6, 129.0, 128.9, 128.3, 127.9, 127.2, 124.0, 72.2, 69.2, 61.6, 52.8, 47.9 ppm.

^{19}F NMR (376 MHz, Chloroform-*d*): δ = -118.5 ppm.

IR (**KBr**): 3295, 3064, 2954, 2884, 2162, 1908, 1755, 1586, 1508, 1447, 1371, 1277, 1225, 1166, 1120, 1084, 940, 860, 823, 753, 685 cm^{-1}.

HRMS (ESI): mass found: 624.11206, mass calculated for $C_{29}H_{28}NFS_2NaO_8^+$: 624.11326.

ethyl 2-fluoro-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido)ethoxy) ethoxy)-2-(p-tolyl)acetate (5q)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (50 %, 58 mg).

^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.10 – 8.06 (m, 4H), 7.67 – 7.63 (m, 2H), 7.57 – 7.50 (m, 6H), 7.23 (d, *J* = 8.0 Hz, 2H), 4.24 (q, *J* = 7.1 Hz, 2H), 3.93 (t, *J* = 6.2 Hz, 2H), 3.81 – 3.71 (m, 4H), 3.66 – 3.57 (m, 2H), 2.39 (s, 3H), 1.26 (t, *J* = 7.1 Hz, 3H) ppm.

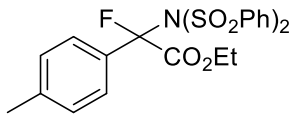
^{13}C NMR (151 MHz, Chloroform-d): δ = 166.7 (d, *J* = 39.7 Hz), 139.9, 139.7, 133.8, 132.4 (d, *J* = 27.8 Hz), 129.1, 129.0, 128.3, 126.0 (d, *J* = 6.1 Hz), 109.7 (d, *J* = 232.7 Hz), 69.8, 69.5, 64.6 (d, *J* = 2.8 Hz), 62.4, 47.9, 21.2, 13.9 ppm.

^{19}F NMR (565 MHz, Chloroform-*d*): δ = -118.5 ppm.

IR (**KBr**): 3068, 2971, 2166, 2017, 1910, 1752, 1612, 1513, 1448, 1371, 1266, 1166, 1118, 1086, 935, 859, 820, 754, 685, 658 cm^{-1}.

HRMS (ESI): mass found: 602.12921, mass calculated for $C_{27}H_{30}NFS_2NaO_8^+$: 602.12891.

ethyl 2-fluoro-2-(N-(phenylsulfonyl)phenylsulfonamido)-2-(p-tolyl)acetate (10a)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless solid (47 %, 46 mg).

^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.92 – 7.84 (m, 4H), 7.70 – 7.61 (m, 2H), 7.51 – 7.45 (m, 4H), 7.16 (d, *J* = 8.1 Hz, 2H), 6.88 (d, *J* = 8.1 Hz, 2H), 4.42 – 4.24 (m, 2H), 2.32 (s, 3H), 1.32 (t, *J* = 7.1 Hz, 3H) ppm.

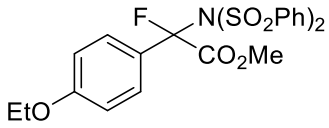
^{13}C NMR (151 MHz, Chloroform-d): δ = 165.9 (d, *J* = 29.7 Hz), 140.6, 140.2, 133.8, 128.6, 128.47, 128.40, 128.3, 128.1 (d, *J* = 1.5 Hz), 100.5 (d, *J* = 233.8 Hz), 63.3, 21.1, 13.7 ppm.

^{19}F NMR (565 MHz, Chloroform-*d*): δ = -118.5 ppm.

IR (**KBr**): 3068, 2926, 2860, 2163, 2011, 1971, 1911, 1748, 1609, 1584, 1512, 1449, 1375, 1266, 1172, 1076, 1046, 999, 954, 929, 900, 843, 792, 755, 722, 682 cm^{-1}.

HRMS (ESI): mass found: 514.07657, mass calculated for $C_{23}H_{22}NFS_2NaO_6^+$: 514.07648.

methyl 2-(4-ethoxyphenyl)-2-fluoro-2-(N-(phenylsulfonyl)phenylsulfonamido)acetate (10b)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless solid (43 %, 44 mg).

^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.90 – 7.84 (m, 4H), 7.67 – 7.60 (m, 2H), 7.53 – 7.44 (m, 4H), 7.16 (d, *J* = 8.6 Hz, 2H), 6.55 (d, *J* = 8.6 Hz, 2H), 4.05 – 3.95 (m, 2H), 3.86 (s, 3H), 1.43 (t, *J* = 7.0 Hz, 3H) ppm.

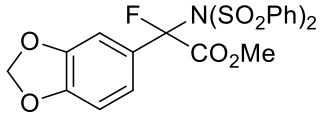
^{13}C NMR (151 MHz, Chloroform-d): δ = 166.6 (d, *J* = 29.6 Hz), 160.2, 140.6, 133.8, 130.1 (d, *J* = 10.0 Hz), 128.7, 128.3, 120.8 (d, *J* = 25.2 Hz), 113.3, 100.5 (d, *J* = 233.4 Hz), 63.5, 53.8, 14.6 ppm.

^{19}F NMR (565 MHz, Chloroform-*d*): δ = -117.7 ppm.

IR (**KBr**): 3509, 3070, 2981, 2952, 2522, 2159, 2035, 1906, 1748, 1675, 1604, 1511, 1477, 1447, 1375, 1253, 1170, 1114, 1076, 1043, 998, 924, 815, 757, 722, 683 cm^{-1}.

HRMS (ESI): mass found: 530.07141, mass calculated for $C_{23}H_{22}NFS_2NaO_7^+$: 530.07139.

methyl 2-(benzo[d][1,3]dioxol-5-yl)-2-fluoro-2-(N-(phenylsulfonyl) phenylsulfonamido)acetate (10c)



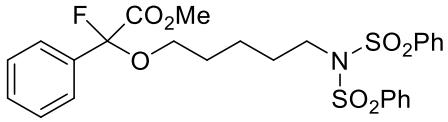
The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et2O 4:1 → 2:1 as yellow solid (74 %, 74 mg).

^{1}H NMR (600 MHz, Chloroform-*d*): δ = 7.84 – 7.77 (m, 4H), 7.59 – 7.50 (m, 2H), 7.46 – 7.39 (m, 4H), 6.73 – 6.66 (m, 1H), 6.62 (d, *J* = 2.0 Hz, 1H), 6.40 (d, *J* = 8.4 Hz, 1H), 5.89 – 5.82 (m, 2H), 3.78 (s, 3H) ppm.

^{13}C NMR (151 MHz, Chloroform-d): δ = 166.4 (d, *J* = 29.6 Hz), 149.2, 147.0 (d, *J* = 2.4 Hz),

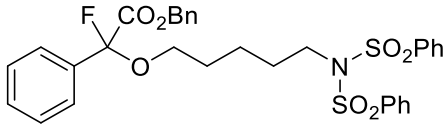
140.5, 134.0, 128.7, 128.3, 123.2 (d, *J* = 10.8 Hz), 122.9 (d, *J* = 25.4 Hz), 109.2 (d, *J* = 10.8 Hz), 107.1, 101.5, 100.3 (d, *J* = 234.7 Hz), 53.9 ppm.
^{19}F NMR (565 MHz, Chloroform-*d*): δ = -116.5 ppm.
IR (**KBr**): 3503, 3073, 2918, 2664, 2329, 2160, 2036, 1910, 1750, 1673, 1602, 1490, 1444, 1369, 1248, 1172, 1075, 1036, 933, 885, 811, 758, 719, 680 cm^{-1}.
HRMS (ESI): mass found: 530.03461, mass calculated for $C_{22}H_{18}NFS_2NaO_8^+$: 530.03501.

methyl 2-fluoro-2-phenyl-2-((5-(N-(phenylsulfonyl)phenylsulfonamido) pentyl)oxy)acetate (16a)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (91 %, 100 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.07 – 8.02 (m, 4H), 7.69 – 7.65 (m, 2H), 7.63 – 7.60 (m, 2H), 7.59 – 7.55 (m, 4H), 7.45 – 7.42 (m, 3H), 3.80 (s, 3H), 3.74 – 3.68 (m, 3H), 3.64 – 3.59 (m, 1H), 1.78 – 1.71 (m, 2H), 1.69 – 1.64 (m, 2H), 1.43 – 1.36 (m, 2H) ppm.
^{13}C NMR (151 MHz, Chloroform-d): δ = 167.3 (d, *J* = 40.5 Hz), 140.0, 135.6 (d, *J* = 27.6 Hz), 133.8, 129.9, 129.1, 128.4, 128.1, 125.9 (d, *J* = 6.3 Hz), 109.6 (d, *J* = 231.9 Hz), 65.2 (d, *J* = 3.0 Hz), 53.1, 49.3, 29.5, 28.9, 22.9 ppm.
^{19}F NMR (565 MHz, Chloroform-*d*): δ = -118.1 ppm.
IR (**KBr**): 3510, 3069, 2952, 2259, 2163, 2035, 1909, 1754, 1585, 1448, 1371, 1269, 1165, 1083, 1044, 907, 880, 830, 727, 687 cm^{-1}.
HRMS (ESI): mass found: 572.11713, mass calculated for $C_{26}H_{28}NFS_2NaO_7^+$: 572.11834.

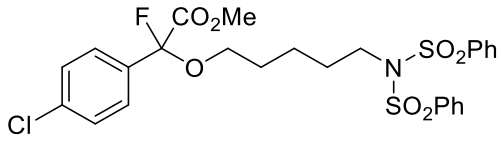
benzyl 2-fluoro-2-phenyl-2-((5-(N-(phenylsulfonyl)phenylsulfonamido) pentyl)oxy)acetate (16b)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (82 %, 103 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.10 – 7.98 (m, 4H), 7.66 (t, *J* = 7.6 Hz, 2H), 7.64 – 7.61 (m, 2H), 7.56 (t, *J* = 7.7 Hz, 4H), 7.46 – 7.39 (m, 3H), 7.36 – 7.31 (m, 3H), 7.28 – 7.23 (m, 2H), 5.29 – 5.15 (m, 2H), 3.74 – 3.66 (m, 3H), 3.60 – 3.54 (m, 1H), 1.77 – 1.68 (m, 2H), 1.66 – 1.58 (m, 2H), 1.39 – 1.25 (m, 2H) ppm.
^{13}C NMR (151 MHz, Chloroform-d): δ = 166.7 (d, *J* = 41.6 Hz), 140.0, 135.6 (d, *J* = 26.9 Hz), 134.9, 133.8, 129.9 (d, *J* = 1.3 Hz), 129.1, 128.58, 128.50, 128.4, 128.1, 128.0, 126.0 (d, *J* = 6.1 Hz), 109.6 (d, *J* = 232.1 Hz), 67.7, 65.3 (d, *J* = 2.9 Hz), 49.3, 29.5, 28.9, 22.9 ppm.
^{19}F NMR (565 MHz, Chloroform-*d*): δ = -117.8 ppm.
IR (**KBr**): 3489, 3067, 3035, 2949, 2867, 2667, 2325, 2173, 2089, 1994, 1907, 1814, 1752,

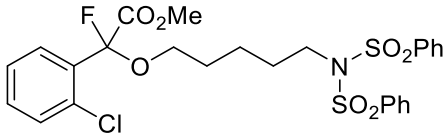
1585, 1449, 1372, 1263, 1165, 1083, 1030, 879, 831, 727, 689 cm^{-1}.
HRMS (ESI): mass found: 648.14917, mass calculated for $C_{32}H_{32}NFS_2NaO_7^+$:648.14964.

methyl 2-(4-chlorophenyl)-2-fluoro-2-((5-(N-(phenylsulfonyl)phenylsulfonamido) pentyl)oxy)acetate (16c)



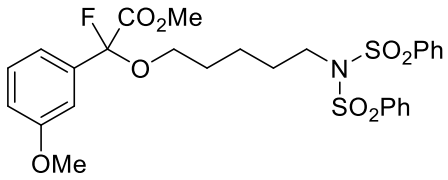
The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (97 %, 113 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.07 – 8.00 (m, 4H), 7.69 – 7.63 (m, 2H), 7.60 – 7.53 (m, 6H), 7.43 – 7.38 (m, 2H), 3.79 (s, 3H), 3.74 – 3.67 (m, 3H), 3.64 – 3.58 (m, 1H), 1.79 – 1.72 (m, 2H), 1.70 – 1.63 (m, 2H), 1.42 – 1.35 (m, 2H) ppm.
^{13}C NMR (151 MHz, Chloroform-d): δ = 167.0 (d, *J* = 40.7 Hz), 140.0, 136.1 (d, *J* = 2.0 Hz), 134.2 (d, *J* = 27.9 Hz), 133.8, 129.1, 128.7, 128.1, 127.5 (d, *J* = 6.0 Hz), 109.2 (d, *J* = 232.5 Hz), 65.4 (d, *J* = 2.8 Hz), 53.2, 49.3, 29.4, 28.8, 22.9 ppm.
^{19}F NMR (565 MHz, Chloroform-*d*): δ = -118.0 ppm.
IR (**KBr**): 3503, 3069, 2952, 2867, 2325, 2165, 2091, 2022, 1912, 1754, 1595, 1488, 1447, 1372, 1266, 1165, 1088, 1052, 1015, 879, 831, 753, 726, 685 cm^{-1}.
HRMS (ESI): mass found: 606.07935, mass calculated for $C_{26}H_{27}NFClS_2NaO_7^+$: 606.07937.

methyl 2-(2-chlorophenyl)-2-fluoro-2-((5-(N-(phenylsulfonyl)phenylsulfonamido) pentyl)oxy)acetate (16d)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (92 %, 108 mg).
^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.07 – 8.01 (m, 4H), 7.85 – 7.81 (m, 1H), 7.69 – 7.64 (m, 2H), 7.56 (t, *J* = 7.8 Hz, 4H), 7.44 – 7.36 (m, 3H), 3.83 (s, 3H), 3.76 – 3.69 (m, 2H), 3.68 – 3.57 (m, 2H), 1.77 – 1.70 (m, 2H), 1.69 – 1.63 (m, 2H), 1.41 – 1.35 (m, 2H) ppm.
^{13}C NMR (151 MHz, Chloroform-d): δ = 166.1 (d, *J* = 38.3 Hz), 140.0, 133.8, 133.6 (d, *J* = 26.6 Hz), 132.0 (d, *J* = 3.7 Hz), 131.0, 130.5, 129.1, 128.3 (d, *J* = 7.8 Hz), 128.1, 126.7, 107.5 (d, *J* = 229.0 Hz), 65.0 (d, *J* = 2.6 Hz), 53.2, 49.3, 29.4, 28.7, 22.9 ppm.
^{19}F NMR (565 MHz, Chloroform-*d*): δ = -111.4 ppm.
IR (**KBr**): 3509, 3069, 2952, 2867, 2327, 2164, 2043, 1979, 1907, 1759, 1586, 1445, 1372, 1268, 1241, 1164, 1114, 1064, 967, 878, 832, 751, 725, 685 cm^{-1}.
HRMS (ESI): mass found: 606.07941, mass calculated for $C_{26}H_{27}NFClS_2NaO_7^+$: 606.07937.

methyl 2-fluoro-2-(3-methoxyphenyl)-2-((5-(N-(phenylsulfonyl)phenylsulfonamido) pentyl)oxy)acetate (16e)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (95 %, 111 mg).

^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.06 – 8.02 (m, 4H), 7.69 – 7.64 (m, 2H), 7.56 (t, *J* = 7.9 Hz, 4H), 7.34 (t, *J* = 8.0 Hz, 1H), 7.21 – 7.18 (m, 1H), 7.17 – 7.14 (m, 1H), 6.99 – 6.95 (m, 1H), 3.84 (s, 3H), 3.79 (s, 3H), 3.73 – 3.67 (m, 3H), 3.65 – 3.56 (m, 1H), 1.78 – 1.71 (m, 2H), 1.70 – 1.64 (m, 2H), 1.43 – 1.34 (m, 2H) ppm.

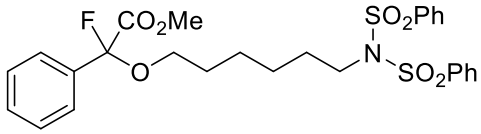
^{13}C NMR (151 MHz, Chloroform-d): δ = 167.2 (d, *J* = 40.2 Hz), 159.6, 140.0, 137.0 (d, *J* = 27.7 Hz), 133.8, 129.6, 129.1, 128.1, 118.2 (d, *J* = 6.1 Hz), 115.6, 111.4 (d, *J* = 6.5 Hz), 109.5 (d, *J* = 232.1 Hz), 65.3 (d, *J* = 2.9 Hz), 55.3, 53.1, 49.3, 29.5, 28.9, 22.9 ppm.

^{19}F NMR (565 MHz, Chloroform-*d*): δ = -117.8 ppm.

IR (**KBr**): 3499, 3068, 2951, 2867, 2327, 2171, 2089, 1996, 1914, 1755, 1595, 1486, 1447, 1372, 1316, 1274, 1211, 1166, 1084, 1037, 939, 877, 829, 790, 727, 686 cm^{-1}.

HRMS (ESI): mass found: 602.12920, mass calculated for $C_{27}H_{30}NFS_2NaO_8^+$: 602.12891.

methyl 2-fluoro-2-phenyl-2-((6-(N-(phenylsulfonyl)phenylsulfonamido)hexyl)oxy)acetate (17)



The titled compound was synthesized according to the general procedure GP. And was obtained after silica gel column chromatography using pentane/Et_2O 4:1 → 2:1 as colorless oil (99 %, 111 mg).

^{1}H NMR (600 MHz, Chloroform-*d*): δ = 8.13 – 7.95 (m, 4H), 7.69 – 7.61 (m, 4H), 7.57 (t, *J* = 7.7 Hz, 4H), 7.46 – 7.40 (m, 3H), 3.80 (s, 3H), 3.75 – 3.68 (m, 3H), 3.66 – 3.60 (m, 1H), 1.75 – 1.69 (m, 2H), 1.68 – 1.62 (m, 2H), 1.43 – 1.36 (m, 2H), 1.32 – 1.25 (m, 2H) ppm.

^{13}C NMR (151 MHz, Chloroform-d): δ = 167.4 (d, *J* = 41.0 Hz), 140.0, 135.7 (d, *J* = 27.4 Hz), 133.8, 129.9, 129.1, 128.4, 128.1, 125.9 (d, *J* = 6.1 Hz), 109.6 (d, *J* = 231.8 Hz), 65.5 (d, *J* = 2.7 Hz), 53.1, 49.4, 29.7, 29.3, 26.1, 25.3 ppm.

^{19}F NMR (565 MHz, Chloroform-*d*): δ = -117.9 ppm.

IR (**KBr**): 3497, 3067, 2946, 2864, 2325, 2166, 2085, 2020, 1909, 1755, 1585, 1448, 1372, 1268, 1165, 1084, 1043, 937, 904, 845, 784, 726, 687 cm^{-1}.

HRMS (ESI): mass found: 586.13422, mass calculated for $C_{27}H_{30}NFS_2NaO_7^+$: 586.13399.

DFT Calculations

Computational Details and Discussion

All of the calculations were performed with the Gaussian 09 program.[1] The hybrid B3LYP functional[2] and the 6-31G(d) basis set[3] were applied for the optimization of all stationary points in the gas phase. Frequency calculations were performed to confirm that each stationary point is either a minimum or a transition structure. Key transition-state structures were confirmed to connect corresponding reactants and products by intrinsic reaction coordinate (IRC) calculations.[4] Solvation energies in 1,4-dioxane (ε = 2.2099) were evaluated by IEFPCM calculations with radii and non-electrostatic terms for SMD solvation model[5] using the gas-phase optimized structures. To improve the calculation accuracy, single-point energies calculations in the chloroform were computed at the B3LYP level of theory with the 6-311+G(2d,2p) basis set[6] for all the atoms. The given Gibbs free energies in 1,4-dioxane were calculated according to the formula: G_{sol} = TCG + ΔG_{sol} + SPE + 1.89 kcal/mol, and an additional term of RTln(11.72/1) = 1.46 kcal/mol at 298 K is added 1,4-dioxane. The CYL View software was employed to show the 3D structures of the studied species.[7]

Figure S1. Potential energy surface and 3D structures of key species for the direct fluorination reaction. The bond lengths in the structures at the bottom are given in Å.

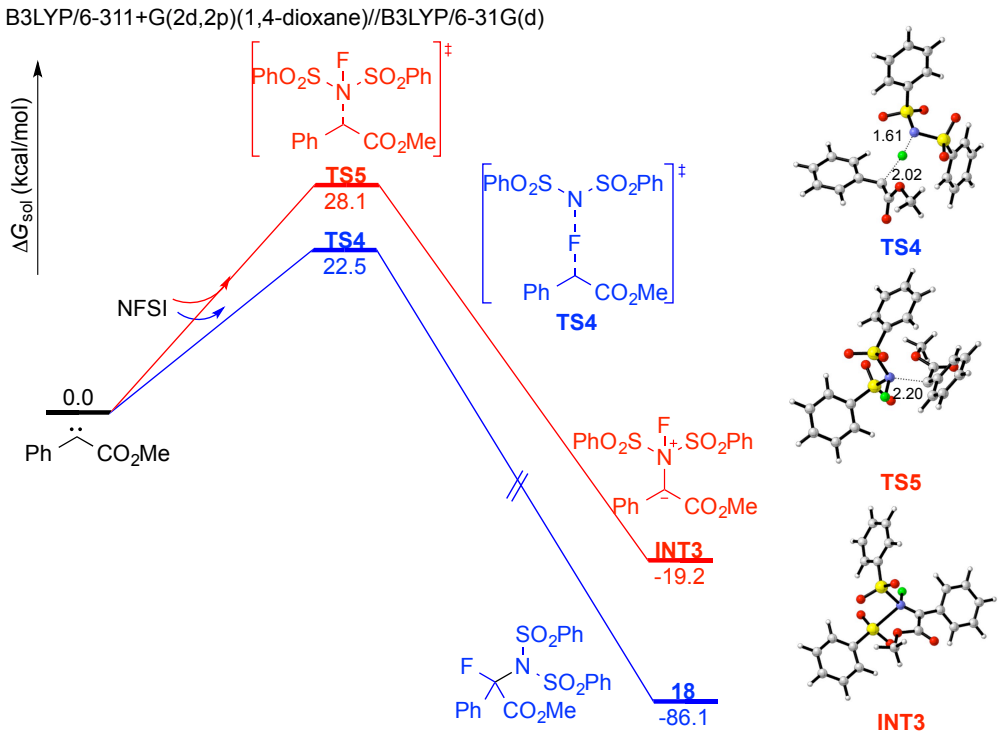


Figure S2. Potential energy surface for electron-rich carbenes.

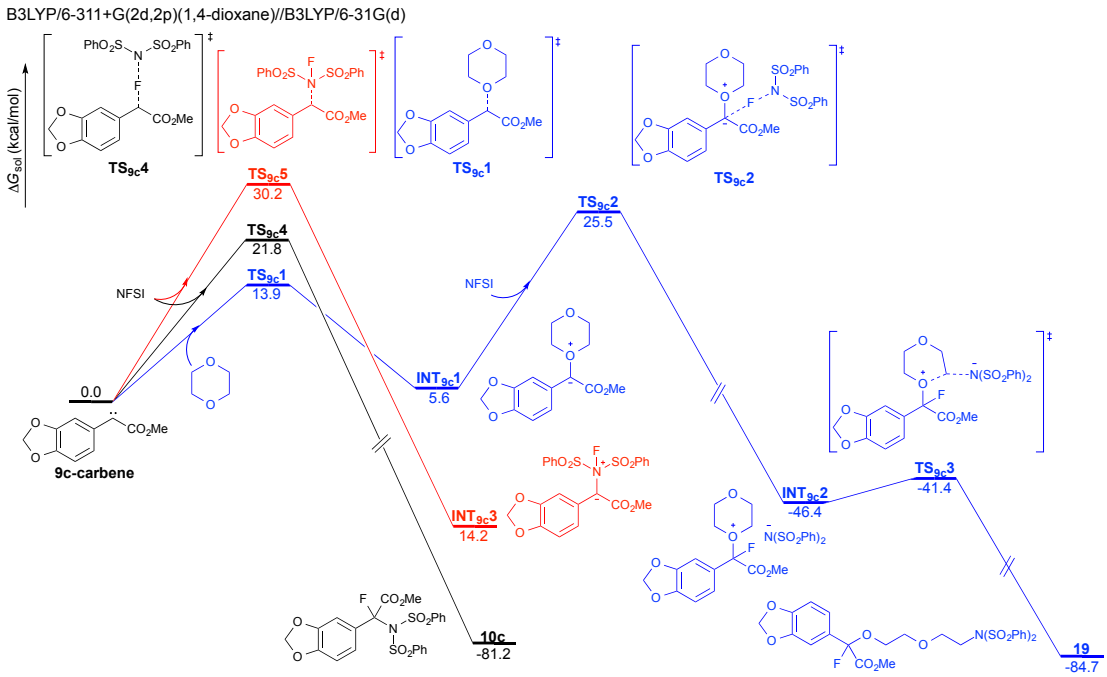
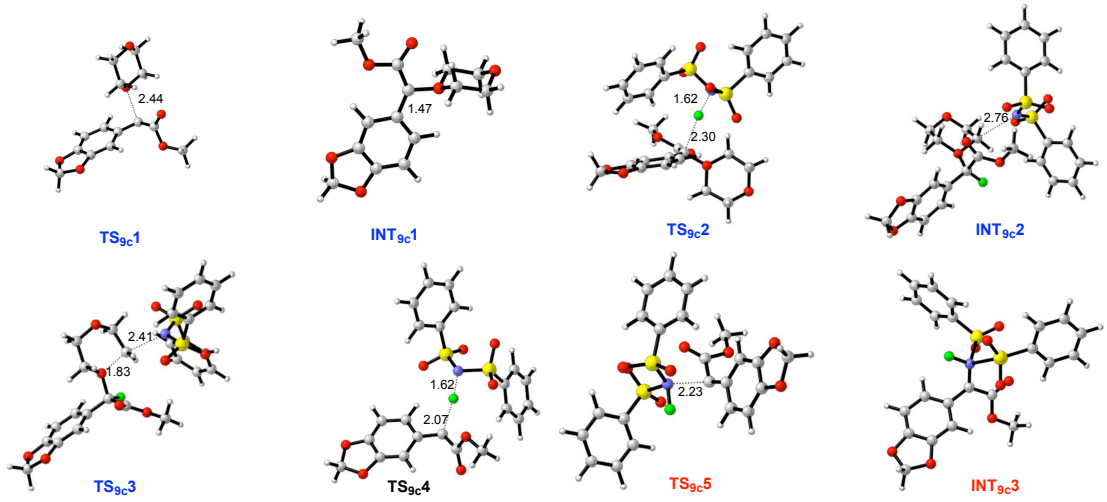


Figure S3. 3D structures of key species for the reaction of electron-rich carbenes. The bond lengths in the structures at the bottom are given in Å.



Computed Energies of All Stationary Points

Table S1. Thermal correction to Gibbs free energies (***TCG***, in Hartree), sum of electronic and thermal enthalpies (***H***, in Hartree), sum of electronic and thermal free energies (***G***, in Hartree), solvation Gibbs free energies in 1,4-dioxane (ΔG_{sol}, in Hartree), and single point energies computed at the B3LYP/6-311+G(2d,2p)//B3LYP/6-31G(d) (***SPE***, in Hartree).

Name	*TCG*/a.u.	*H*/a.u.	*G*/a.u.	ΔG_{sol}/a.u.	*SPE*/a.u.
carbene	0.109730	-497.952560	-498.000926	-0.009770	-498.269390
1,4-dioxane	0.094867	-307.528929	-307.563424	-0.004939	-307.763126
NFSI	0.159487	-1714.703919	-1714.772377	-0.015180	-1715.331037
TS1	0.222245	-805.484796	-805.551031	-0.011701	-806.032200
INT1	0.230133	-805.509801	-805.570855	-0.012777	-806.056101
TS2	0.411942	-2520.211979	-2520.319549	-0.023186	-2521.377684
INT2	0.414278	-2520.313674	-2520.422179	-0.029025	-2521.485652
TS3	0.414123	-2520.312349	-2520.419364	-0.025942	-2521.481856
5a	0.415708	-2520.389464	-2520.497710	-0.020411	-2521.559006
TS4	0.289723	-2212.651829	-2212.748586	-0.020463	-2213.586625
18	0.302320	-2212.839059	-2212.928075	-0.019039	-2213.773652
TS5	0.294355	-2212.651191	-2212.743541	-0.020331	-2213.582404
INT3	0.293240	-2212.727692	-2212.823238	-0.020443	-2213.656522
9c-carbene	0.121963	-686.469304	-686.523442	-0.011948	-686.863690
$TS_{9c}1$	0.237074	-994.000296	-994.069839	-0.012849	-994.623532
$INT_{9c}1$	0.242759	-994.018572	-994.084969	-0.013904	-994.641452
$TS_{9c}2$	0.423887	-2708.721947	-2708.835407	-0.024427	-2709.964136
$INT_{9c}2$	0.425166	-2708.825339	-2708.940753	-0.030404	-2710.073959
$TS_{6c}3$	0.425631	-2708.823593	-2708.936862	-0.027150	-2710.069649
19	0.427393	-2708.899932	-2709.014362	-0.021638	-2710.145984
$TS_{9c}4$	0.301644	-2401.168707	-2401.27159	-0.022971	-2402.181344
10c	0.314348	-2401.349414	-2401.444254	-0.020322	-2402.360760
$TS_{9c}5$	0.305573	-2401.164208	-2401.263194	-0.021490	-2402.173275
$INT_{9c}3$	0.305410	-2401.238008	-2401.339272	-0.021639	-2402.243820

Coordinates of All Stationary Points

carbene

C	2.21633800	1.47969800	-0.00671700
C	0.93965800	0.95532300	0.12385700
C	0.72421900	-0.45186400	0.09665200
C	1.85271200	-1.29807800	-0.06859900
C	3.12737200	-0.76990400	-0.23270200
C	3.30620600	0.61699600	-0.19527100
H	2.37568300	2.55376700	0.02611600
H	0.08779800	1.61162200	0.27582700
H	1.67723900	-2.36911200	-0.07301100
H	3.98193000	-1.42511500	-0.37391400
H	4.30411000	1.03317200	-0.30877600
C	-0.55163200	-1.07794200	0.20497400
C	-1.74776700	-0.29685500	0.31230300
O	-2.10295700	0.10979200	1.41730300
O	-2.48095800	-0.18027900	-0.81820000
C	-3.77624800	0.41961200	-0.64746000
H	-4.23173900	0.41076500	-1.63831900
H	-4.38091400	-0.15883300	0.05621300
H	-3.68794100	1.44572600	-0.27917800

1,4-dioxane

C	1.17174500	0.73743200	-0.19440800
C	1.17158800	-0.73768700	0.19439700
C	-1.17175900	-0.73742900	0.19439500
C	-1.17157300	0.73769200	-0.19440600
H	2.02567300	-1.26326600	-0.24517400
H	1.22556900	0.82863900	-1.29207700
H	2.02595300	1.26283400	0.24513600
H	-2.02597700	-1.26280900	-0.24516300
H	-1.22561400	-0.82862200	1.29206300
H	-1.22537600	0.82890100	-1.29207500
H	-2.02566700	1.26328600	0.24513300
H	1.22542800	-0.82890900	1.29206400
O	-0.00016100	-1.38371500	-0.29294600
O	0.00016300	1.38370200	0.29297400

NFSI

N	0.26387700	0.90064700	-0.46015900
F	0.22963200	0.37132000	-1.77415600
S	-1.38294200	1.59970100	-0.17069700
O	-1.64468200	2.32124300	-1.40900000
O	-1.24088700	2.25957400	1.11907600
S	0.80748100	-0.49315900	0.54801800
O	0.27205000	-1.73490000	-0.00321200
O	0.54033100	-0.06705400	1.91880600
C	2.55619900	-0.40594100	0.20636900
C	3.09774700	-1.24570500	-0.76808800
C	3.33709800	0.49786100	0.93076000
C	4.46737500	-1.17309800	-1.02118900
H	2.45888400	-1.94015700	-1.30212300
C	4.70363200	0.55658000	0.66491700
H	2.88144500	1.13000000	1.68531100
C	5.26495500	-0.27486900	-0.30850100
H	4.91028200	-1.81913700	-1.77328200
H	5.32987900	1.24998600	1.21815800

H	6.33106300	-0.22317800	-0.51096600
C	-2.51879500	0.23084700	-0.04012200
C	-2.86350400	-0.24050300	1.22881900
C	-3.02872600	-0.33481800	-1.21169100
C	-3.75206100	-1.31094500	1.31907100
H	-2.44292400	0.22342200	2.11374400
C	-3.91244300	-1.40635800	-1.10050400
H	-2.74780100	0.06631700	-2.17893400
C	-4.27148500	-1.89164300	0.15979900
H	-4.03723100	-1.69062300	2.29558100
H	-4.32277900	-1.86011500	-1.99769400
H	-4.96171400	-2.72695100	0.23839800

TS1

C	3.20603800	-1.55724700	1.11407600
C	2.46032300	-0.44458900	0.75002300
C	1.66661000	-0.45331400	-0.42991300
C	1.64570300	-1.63696800	-1.21297100
C	2.37690700	-2.75633700	-0.83844900
C	3.15921500	-2.71186500	0.32164300
H	3.81873200	-1.53947900	2.01102400
H	2.48495300	0.45436800	1.35907800
H	1.03025000	-1.63329800	-2.10616700
H	2.34974300	-3.65955300	-1.44102700
H	3.73940000	-3.58426600	0.61210500
C	0.92472300	0.66980500	-0.90270400
C	0.79517900	1.86593100	-0.11661400
O	-0.17563000	2.09906900	0.59974500
O	1.78181100	2.77153100	-0.35945400
C	1.55934300	4.07979700	0.19192200
H	2.41812000	4.67541700	-0.12046700
H	0.63346200	4.51234900	-0.19758700
H	1.49915300	4.04120700	1.28310800
C	-3.85151600	-0.25649600	-0.88552400
C	-2.40439900	0.19397000	-1.04671700
C	-1.87810400	-0.76198800	1.02966400
C	-3.32812900	-1.20705700	1.19178100
H	-2.09317400	0.17948000	-2.09543500
H	-3.99066900	-1.24042900	-1.36533500
H	-4.54065700	0.45927200	-1.34608500
H	-1.19405300	-1.48253600	1.49156600
H	-1.72329500	0.22445800	1.48696300
H	-3.44306200	-2.23827500	0.81576300
H	-3.63233700	-1.18109700	2.24365900
H	-2.27243000	1.20940400	-0.64993000
O	-1.53395400	-0.70513700	-0.35486500
O	-4.20666500	-0.33282200	0.49225700

INT1

C	3.81514000	-0.74034200	0.00002600
C	2.70588600	0.09758900	0.00001900
C	1.38918400	-0.43060100	-0.00003500
C	1.27009700	-1.84257800	-0.00007000
C	2.39198000	-2.66888600	-0.00007200
C	3.67850600	-2.13163400	-0.00001800
H	4.80708700	-0.29355900	0.00007100
H	2.84134100	1.17091600	0.00005400
H	0.28592600	-2.30060300	-0.00012000
H	2.25123700	-3.74778700	-0.00010500
H	4.55194400	-2.77753000	-0.00000800

C	0.22716200	0.42880000	0.00001300	H	4.81316500	3.17790700	-1.19535400
C	-0.02102100	1.81691900	-0.00001600	H	4.07390600	1.69596300	0.63045300
O	-1.15004600	2.34656400	-0.00015900	H	1.77264300	-0.60980200	-2.18439900
O	1.11625900	2.58611500	0.00014300	H	2.55056500	0.84436100	-4.01228700
C	0.88824200	3.99694700	-0.00000200	H	4.06959700	2.76263100	-3.53681400
H	1.88128700	4.45062300	-0.00045300	C	2.44705500	-0.48894700	0.41992000
H	0.32982800	4.30809400	-0.88794100	C	2.59754700	-0.42544300	1.84383100
H	0.33054700	4.30838000	0.88830000	O	2.65170800	-1.40287400	2.59454800
C	-2.95473200	-1.27526600	-1.16472900	O	2.60598000	0.85588000	2.31528300
C	-1.85799100	-0.22815800	-1.23832400	C	2.47266400	0.98124100	3.74092100
C	-1.85777500	-0.22826000	1.23834300	H	2.61356200	2.04237300	3.95128200
C	-2.95470600	-1.27524200	1.16479400	H	1.47353500	0.66592700	4.05244000
H	-1.14784600	-0.41559200	-2.04331700	H	3.22615300	0.38169000	4.25652800
H	-2.51942700	-2.28703200	-1.19505600	C	1.44746000	-4.02712100	-0.55849600
H	-3.61841300	-1.15621600	-2.02662300	C	1.38115000	-2.83514200	0.37167200
H	-1.14762300	-0.41602200	2.04325100	C	3.80521900	-2.55749700	-0.01802900
H	-2.22757800	0.79745100	1.26372800	C	3.73763600	-3.78264000	-0.91350500
H	-2.51949700	-2.28704900	1.19521500	H	0.46813300	-2.26227500	0.25528500
H	-3.61830600	-1.15601700	2.02673100	H	1.21086900	-3.71828500	-1.58763500
H	-2.22795200	0.79749500	-1.26349100	H	0.70240900	-4.76095600	-0.23713600
O	-1.03871300	-0.33187400	-0.00002400	H	4.49838500	-1.80575500	-0.39511900
O	-3.74904800	-1.11471400	0.00006400	H	3.99788600	-2.78946900	1.03051100
				H	3.58605400	-3.46831700	-1.95835700

TS2

H	4.68635900	-4.32464900	-0.84588700				
C	4.14866000	2.34616300	-1.41777600	H	1.58521900	-3.07402900	1.41469500
C	3.73683200	1.50911400	-0.38262100	O	2.46957300	-1.89369000	-0.05475700
C	2.87985700	0.41446600	-0.63551500	O	2.71526700	-4.67202600	-0.50532900
C	2.46350700	0.19929500	-1.96916600	N	-1.43974600	-0.18990500	0.65511300
C	2.89393700	1.03082800	-2.99792800	F	0.18712700	-0.20727500	0.52768200
C	3.73918100	2.11156300	-2.73218900	S	-1.80504300	1.34928600	1.39910600

O	-1.11635900	1.28768200	2.68407900	C	5.32588000	-0.84740100	1.02515100
O	-3.26627500	1.44222500	1.31254200	C	4.58560200	0.07013300	0.26690500
S	-2.00860800	-0.57809400	-0.95514300	C	5.24477300	0.94980300	-0.60724200
O	-1.15478300	-1.70320700	-1.35714000	C	6.63097000	0.90709700	-0.72232700
O	-2.13492600	0.59924100	-1.81650400	C	7.36908800	-0.00678600	0.03508900
C	-3.64103200	-1.20910700	-0.58474400	H	7.28628100	-1.58785200	1.49892100
C	-3.76616700	-2.49068300	-0.04271300	H	4.82261700	-1.53203000	1.69767500
C	-4.75413000	-0.41901800	-0.87295600	H	4.67143700	1.66905900	-1.18216300
C	-5.04142300	-2.98683200	0.21817300	H	7.13586100	1.59144200	-1.39756600
H	-2.88212000	-3.08408900	0.16219200	H	8.45142400	-0.03515400	-0.05254600
C	-6.02415600	-0.93097600	-0.61037800	C	3.08584400	0.17396900	0.35212300
H	-4.61899800	0.57111500	-1.29141400	C	2.41097800	-0.48667500	1.57757600
C	-6.16723900	-2.20833100	-0.06474200	O	2.49985000	-1.68420500	1.75382100
H	-5.15661400	-3.98091400	0.64023000	O	1.80836700	0.40214100	2.33278000
H	-6.90134700	-0.32944900	-0.82962400	C	1.06976500	-0.11821400	3.48076300
H	-7.15957700	-2.59984900	0.14113000	H	1.74166800	-0.71114700	4.10464400
C	-1.08286000	2.66369300	0.42568100	H	0.72103800	0.76955800	4.00482900
C	-1.92627900	3.44515000	-0.36659000	H	0.23682700	-0.71528100	3.10628300
C	0.28828800	2.91297000	0.52017200	C	0.64786500	-0.55821700	-2.51603200
C	-1.37798300	4.50742000	-1.08253300	C	0.92868300	-0.26176500	-1.06241600
H	-2.98563000	3.22292200	-0.40979100	C	2.84708100	-1.86799100	-1.24447100
C	0.82058100	3.97335200	-0.21226300	C	2.41886400	-2.07340200	-2.68981300
H	0.92164900	2.29461100	1.14536000	H	0.76352700	0.77239100	-0.78460200
C	-0.00788100	4.76771300	-1.00781100	H	1.16498300	0.16615400	-3.16367100
H	-2.02056100	5.12823900	-1.70017900	H	-0.42989100	-0.45769900	-2.66399800
H	1.88697300	4.16910300	-0.16587400	H	3.92566200	-1.94068100	-1.11326900
H	0.41625500	5.59349500	-1.57282100	H	2.32213100	-2.51906300	-0.54534400
				H	2.99570400	-1.39795800	-3.34289500

INT2

C	6.71603600	-0.87905900	0.90601500	H	0.46974500	-0.94826200	-0.35124000

O	2.47964300	-0.46456000	-0.89577900	H	-3.15172600	4.60517200	2.29233200
O	1.03372500	-1.88717100	-2.85783300	H	-1.77500900	6.26700200	1.05949300
N	-1.72728500	0.07957300	-0.43769100				
F	2.69643400	1.46219200	0.20746300	**TS3**			
S	-2.72045600	1.14241900	-1.19869500	C	6.66931800	1.10824200	-0.80695700
O	-4.15227400	0.85595100	-1.00173400	C	5.28115000	1.05719600	-0.94759300
O	-2.18462400	1.22530300	-2.57375100	C	4.54279000	0.11711300	-0.21771400
S	-2.10922700	-0.69816900	0.94029000	C	5.20248400	-0.76478600	0.65235600
O	-2.72895200	0.14692500	1.98064400	C	6.58642100	-0.70459800	0.78933800
O	-0.84516700	-1.40155300	1.30707800	C	7.32304200	0.23172000	0.05866100
C	-3.29292300	-2.00845500	0.56601200	H	7.23715900	1.83615300	-1.37898700
C	-4.66118600	-1.74907600	0.65764000	H	4.77874400	1.74619900	-1.61650800
C	-2.81932400	-3.26725600	0.19241500	H	4.63016500	-1.50054300	1.20706800
C	-5.56510300	-2.77040800	0.36554700	H	7.09091000	-1.39276500	1.46130000
H	-5.00378700	-0.76230600	0.94326600	H	8.40350000	0.27454100	0.16323300
C	-3.73225000	-4.28140900	-0.09728700	C	3.03728800	-0.00399200	-0.31614200
H	-1.75047900	-3.44491000	0.14921700	C	2.39156700	0.64639000	-1.56248600
C	-5.10393100	-4.03353200	-0.01193700	O	2.44356700	1.84748900	-1.73377200
H	-6.63225800	-2.57713600	0.43225000	O	1.82771700	-0.24789300	-2.34865000
H	-3.37192200	-5.26571300	-0.38485900	C	1.11923600	0.27591700	-3.50918900
H	-5.81360400	-4.82526800	-0.23790700	H	1.79332800	0.90119500	-4.09821600
C	-2.41088100	2.76689400	-0.46057200	H	0.81271600	-0.60801700	-4.06580800
C	-1.64093600	3.69365000	-1.16499600	H	0.25584600	0.84400800	-3.16015800
C	-2.96396000	3.08683200	0.78225000	C	0.41083900	0.57357500	2.44874500
C	-1.41141800	4.95549000	-0.61247100	C	0.59801600	0.28689700	0.98548400
H	-1.25116400	3.42411800	-2.14062200	C	2.69885400	1.94963900	1.27476900
C	-2.72640400	4.34913200	1.32549100	C	2.17444100	2.11433100	2.69255500
H	-3.55397600	2.35158000	1.31657500	H	0.61606600	-0.73945300	0.65065400
C	-1.95176200	5.28319000	0.63200200	H	0.98283800	-0.14889500	3.04955400
H	-0.81860800	5.68444100	-1.15943600	H	-0.64819000	0.44239300	2.68062500

H	3.78147400	2.07922100	1.22658400	H	-0.90486100	-3.37560200	2.15491800
H	2.20711700	2.61855700	0.56685000	C	-2.11308400	-4.44599800	-1.37309400
H	2.71627900	1.43114600	3.36633200	H	-3.18429700	-2.56639400	-1.39112900
H	2.36350500	3.14332600	3.01470200	C	-1.25542700	-5.28109300	-0.65148300
H	0.31254000	1.03357200	0.25286200	H	-0.15310000	-5.55308900	1.18298600
O	2.40035200	0.56271200	0.88742500	H	-2.46436300	-4.74571100	-2.35680700
O	0.78128900	1.90586300	2.77771900	H	-0.93983000	-6.23117600	-1.07487900
N	-1.72550400	-0.09533700	0.42934900				
F	2.68073600	-1.31837100	-0.22788300	**5a**			
S	-2.60487100	-1.28722400	1.15860800	C	-7.14638300	-1.65915200	-0.42749500
O	-4.04852800	-1.16349800	0.90422800	C	-5.81251000	-1.37082200	-0.72677100
O	-2.11260200	-1.30913400	2.55083100	C	-5.11298400	-0.42709300	0.03326400
S	-2.19598300	0.64352700	-0.96084800	C	-5.76027400	0.21634900	1.09854200
O	-2.77940700	-0.26892100	-1.96041800	C	-7.08916200	-0.07649400	1.39417200
O	-0.99776100	1.42903300	-1.36264800	C	-7.78737200	-1.01515100	0.62985400
C	-3.46299000	1.85808500	-0.54859500	H	-7.68186000	-2.39096800	-1.02611400
C	-4.80812400	1.48572200	-0.56945100	H	-5.31812300	-1.88287100	-1.54410000
C	-3.07380500	3.15750400	-0.21887800	H	-5.21869500	0.95030500	1.68574100
C	-5.77625100	2.43672500	-0.24725300	H	-7.58200100	0.43116500	2.21891400
H	-5.08268900	0.46873800	-0.82066300	H	-8.82533100	-1.24131100	0.85876300
C	-4.05173300	4.09952900	0.10073300	C	-3.64928800	-0.07673900	-0.20392300
H	-2.02220400	3.42167400	-0.23062500	C	-3.11689200	-0.40489600	-1.62015800
C	-5.40097400	3.73960200	0.08808600	O	-3.07794200	-1.53791000	-2.05689300
H	-6.82609200	2.15725600	-0.25789900	O	-2.67229500	0.67541600	-2.26137400
H	-3.75932800	5.11477600	0.35521600	C	-2.05138400	0.43286700	-3.54503200
H	-6.16080300	4.47554800	0.33785100	H	-1.09354800	-0.06780900	-3.39723100
C	-2.06824300	-2.85265100	0.42843900	H	-2.70685500	-0.17489100	-4.17201100
C	-1.21763300	-3.68128800	1.16238200	H	-1.90024500	1.42124500	-3.97754200
C	-2.52840300	-3.22759600	-0.83691300	C	0.27186400	-1.22484900	1.28611000
C	-0.81009300	-4.89952000	0.61495700	C	1.39713500	-1.36194100	0.26368400

C	-2.85528300	-2.05552400	1.00012000	H	-0.70093800	5.24767800	1.84121500
C	-1.69636800	-2.44265200	1.90751100	C	4.90441600	-0.97969200	0.23707600
H	0.98210800	-1.56269300	-0.72399000	C	5.51927600	-0.38937700	-0.87064600
H	-0.37412400	-0.38081600	1.02449200	C	5.25566400	-2.25559500	0.68285400
H	0.68899000	-1.05171400	2.28806800	C	6.50204000	-1.10840000	-1.54864600
H	-3.80782200	-2.28359400	1.49760200	H	5.22154100	0.60093000	-1.19509600
H	-2.79479800	-2.62059800	0.06537500	C	6.24222900	-2.96092900	-0.00797700
H	-1.67177100	-1.78732200	2.79050300	H	4.77391800	-2.67250400	1.56019700
H	-1.87342900	-3.46853700	2.25329400	C	6.86183800	-2.38954100	-1.12048700
H	2.04410200	-2.20208700	0.52865200	H	6.98888100	-0.66531300	-2.41253400
O	-2.76849700	-0.64534800	0.73708000	H	6.52758800	-3.95361800	0.32800500
O	-0.44576100	-2.45242600	1.24130100	H	7.62996400	-2.94193700	-1.65474200
N	2.23722000	-0.14542500	0.17155200				
F	-3.49669700	1.28283600	0.01004000	**TS4**			
S	3.65298400	-0.06752400	1.14597000	C	-4.99744000	2.83624800	-0.54106300
O	3.33530700	-0.83727700	2.34935000	C	-4.46645500	1.70738100	0.06116800
O	4.04223000	1.33751100	1.22087900	C	-3.31216300	1.07363500	-0.48375000
S	1.83838100	1.07663400	-0.99181300	C	-2.70862100	1.63708400	-1.64040000
O	0.82660300	0.44312900	-1.84221900	C	-3.21602900	2.80113200	-2.20146900
O	3.08652600	1.57988100	-1.56114000	C	-4.36442800	3.39157200	-1.66277900
C	1.04352400	2.40070500	-0.08128700	H	-5.89187700	3.30140000	-0.13661800
C	-0.35009600	2.40374100	0.00844800	H	-4.94845800	1.26516800	0.92715400
C	1.82459100	3.40717200	0.49189600	H	-1.82414000	1.16107900	-2.04463100
C	-0.97460900	3.43489800	0.70968400	H	-2.73239900	3.24106400	-3.06838700
H	-0.94003800	1.63361900	-0.47179100	H	-4.77420700	4.28836200	-2.12051000
C	1.18242800	4.43300900	1.18426300	C	-2.78324000	-0.12608500	0.05230300
H	2.90344400	3.37593400	0.40514200	C	-3.20504500	-0.68800600	1.31129600
C	-0.21060700	4.44518300	1.29674900	O	-4.28655900	-1.27008100	1.36695400
H	-2.05714600	3.43686800	0.78742900	O	-2.30759800	-0.61919100	2.30213700
H	1.77396400	5.22324600	1.63731300	C	-2.61575900	-1.35998000	3.49603600

H	-1.68602100	-1.38046000	4.06279200	H	2.43860000	-4.41607800	-2.76624400
H	-3.40681400	-0.85952600	4.06265900	H	-1.61263200	-4.62028900	-1.31971200
H	-2.93856000	-2.37341100	3.24724100	H	0.15707000	-5.38924900	-2.88455100
N	0.74454100	0.10668400	0.44631900				
F	-0.76543200	-0.20331100	-0.01977200	**18**			
S	1.34025200	-1.46140000	0.98386900	C	4.01368400	1.17739300	-0.71382700
O	0.55302800	-1.76340400	2.17353000	C	2.77035200	1.04788500	-0.09358200
O	2.79190100	-1.27147800	1.05329400	C	1.60581300	1.41341700	-0.77909100
S	1.51022600	0.89707700	-0.94627200	C	1.69826800	1.92266900	-2.07926500
O	0.47173200	1.78438600	-1.46975700	C	2.94301700	2.04967400	-2.69195200
O	2.18532200	-0.06105100	-1.82386300	C	4.10465300	1.67735600	-2.01276700
C	2.73071800	1.88291300	-0.08902100	H	4.91125400	0.88998300	-0.17328300
C	2.32772000	3.08690000	0.49465500	H	2.70594700	0.67653200	0.92240100
C	4.05622200	1.44818500	-0.05183200	H	0.79861100	2.21097000	-2.60753700
C	3.28472200	3.87204800	1.13396900	H	3.00321700	2.44231100	-3.70321800
H	1.29060300	3.39859300	0.43801600	H	5.07458500	1.78152900	-2.49183100
C	5.00155100	2.24763400	0.58968900	C	0.23453000	1.36216400	-0.09043400
H	4.33091300	0.50530800	-0.50873200	C	0.39760200	2.12743200	1.25638300
C	4.61728600	3.45288800	1.18131600	O	0.92714500	1.63378600	2.22499700
H	2.99065800	4.81156200	1.59258300	O	0.01558100	3.39799000	1.13750400
H	6.03809800	1.92618200	0.62852700	C	0.16495400	4.18644000	2.33299400
H	5.35908400	4.06926500	1.68158800	H	-0.17160600	5.18703100	2.06233900
C	0.95312100	-2.67558900	-0.27080400	H	-0.45532300	3.77051300	3.13046600
C	1.96135300	-3.09220000	-1.14176100	H	1.20967200	4.20072600	2.65345800
C	-0.33512800	-3.21490500	-0.31637100	N	-0.29568100	0.02173700	0.16172900
C	1.66548800	-4.07758300	-2.08277200	F	-0.67644600	2.04863900	-0.89197400
H	2.94839500	-2.65133500	-1.07840700	S	-1.77562100	-0.08424200	1.14374200
C	-0.61537700	-4.19363900	-1.26755300	O	-1.93104200	1.27012900	1.67715800
H	-1.09349700	-2.87446900	0.37732500	O	-1.62924300	-1.23194300	2.03343600
C	0.38184500	-4.62370300	-2.14690600	S	0.14491100	-1.38176200	-0.78522100

O	0.54203300	-0.94514700	-2.11982300	C	2.26296300	4.00647000	-0.89613000
O	-0.97456000	-2.30259400	-0.60864800	C	3.62102200	3.71230400	-1.04802200
C	1.57279100	-2.05579800	0.06084600	H	5.23087000	2.37511200	-0.51851900
C	2.71179500	-2.33448600	-0.69466100	H	3.78523400	0.88597500	0.83660900
C	1.48457400	-2.37136100	1.41919300	H	0.41503000	3.43337500	0.04913100
C	3.79779800	-2.94475900	-0.06606200	H	1.84084000	4.88614600	-1.37407600
H	2.74236200	-2.06603000	-1.74448500	H	4.25443400	4.36320400	-1.64524300
C	2.58318700	-2.97145000	2.03220200	C	1.12933300	1.23694300	1.36959300
H	0.58397500	-2.14442200	1.98083200	C	1.61999600	0.10608800	2.09917100
C	3.73413200	-3.25950200	1.29247800	O	2.46103000	0.27376000	2.98186100
H	4.69294700	-3.16935200	-0.63876000	O	1.01841500	-1.09264000	1.86974300
H	2.53786300	-3.21604700	3.08930900	C	1.29397500	-2.11166900	2.84078500
H	4.58393300	-3.73095700	1.77850000	H	0.71639400	-2.97764500	2.51673800
C	-3.14730700	-0.36585000	0.02293000	H	2.36179900	-2.34545800	2.86436000
C	-3.81520800	-1.58900800	0.06910800	H	0.97490700	-1.79035300	3.83577300
C	-3.56939900	0.68350200	-0.79595100	N	-0.40938300	0.35114500	0.06607900
C	-4.94092700	-1.76290900	-0.73475300	F	-1.02643600	1.55945200	-0.33445700
H	-3.44948900	-2.37975000	0.71276500	S	-1.77670100	-0.47843400	1.07237800
C	-4.69092600	0.48780500	-1.60028800	O	-1.67615400	0.09684700	2.40429100
H	-3.02890000	1.62241400	-0.80612500	O	-1.62325200	-1.90858800	0.81472500
C	-5.37539300	-0.72974800	-1.56792500	S	-0.08413800	-0.42516300	-1.63876100
H	-5.47445600	-2.70852200	-0.71238000	O	0.52839700	0.68365900	-2.36085100
H	-5.03167700	1.28966600	-2.24866700	O	-1.30317500	-1.07332700	-2.12448500
H	-6.25102700	-0.87341700	-2.19493500	C	1.14795600	-1.66190300	-1.27711600
				C	2.49385100	-1.29920300	-1.36010300

TS5

C	4.17031500	2.59078500	-0.41657500	C	0.73955200	-2.96766200	-0.99682000
C	3.35816100	1.74596700	0.33080600	C	3.45902600	-2.28066300	-1.13959400
C	1.97814200	2.02712300	0.50813800	H	2.77250500	-0.27888600	-1.59742500
C	1.45940600	3.19218800	-0.10658100	C	1.71982900	-3.93419400	-0.78065800
				H	-0.31420000	-3.20974600	-0.94026800

C	3.07290900	-3.59123000	-0.84866300
H	4.51175400	-2.02126900	-1.19969600
H	1.42578800	-4.95629900	-0.56144000
H	3.83063800	-4.35118100	-0.67913200
C	-3.29171800	0.11984800	0.32645900
C	-3.94320900	-0.66650100	-0.62501900
C	-3.82118400	1.33007900	0.78360800
C	-5.16093200	-0.21666600	-1.13505700
H	-3.50384200	-1.59860700	-0.95611200
C	-5.03602900	1.76490400	0.25892800
H	-3.29537400	1.90423500	1.53803000
C	-5.70214200	0.99404000	-0.69801500
H	-5.68508100	-0.81475000	-1.87435400
H	-5.46375000	2.70285000	0.60017800
H	-6.65032100	1.33780200	-1.10195800

INT3

C	-3.34398500	4.14325000	-0.85228700
C	-2.19394500	3.48051800	-0.43198800
C	-2.22894100	2.10130500	-0.15578100
C	-3.44584800	1.40904700	-0.30727600
C	-4.59219000	2.08081700	-0.72001800
C	-4.54624500	3.44907300	-0.99763200
H	-3.29819500	5.20685500	-1.06871400
H	-1.26482700	4.02449100	-0.31809100
H	-3.49621900	0.34836400	-0.08939400
H	-5.52518200	1.53357100	-0.82319600
H	-5.44227500	3.96990200	-1.32407100
C	-1.01151000	1.42005500	0.31117600
C	-0.10005000	2.07281100	1.28687400
O	-0.28652600	3.15966900	1.79421800
O	0.97047200	1.28953400	1.54741600
C	1.87559000	1.77735400	2.55245500
H	2.65708000	1.02219000	2.62254300
H	2.29163600	2.74185800	2.25210200
H	1.35204300	1.88785900	3.50513400
N	-0.60995000	0.21834300	-0.08224400
F	-1.42416800	-0.31956300	-1.08374800
S	-0.28114100	-1.40957100	1.21176800
O	-0.78271800	-1.00855800	2.53267800
O	1.12913500	-1.70962700	0.94037200
S	1.48670400	0.17051200	-1.39863000
O	1.23949300	1.56759100	-1.85268700
O	1.28701800	-0.98597600	-2.32074600
C	3.21445800	0.11720300	-0.85032100
C	3.86871900	1.31375500	-0.55543400
C	3.83575500	-1.12162600	-0.69068400
C	5.19046500	1.26309200	-0.11045600
H	3.35444700	2.25763400	-0.69954400
C	5.15621200	-1.15647200	-0.24325400
H	3.29491000	-2.03165800	-0.92225400
C	5.83162900	0.03178900	0.04793200
H	5.72114300	2.18638800	0.10583900
H	5.65789400	-2.11262500	-0.12292500
H	6.85991500	-0.00183100	0.39756700
C	-1.31090900	-2.70007500	0.52791900
C	-0.94202600	-3.27823900	-0.69081200
C	-2.46838500	-3.06880900	1.21795700
C	-1.75589400	-4.28125600	-1.21261700
H	-0.05864100	-2.93558800	-1.22158200

C	-3.26514900	-4.07817900	0.67822400
H	-2.71904000	-2.58967900	2.15805100
C	-2.90962200	-4.68097000	-0.53084600
H	-1.49106400	-4.74630900	-2.15737900
H	-4.16136400	-4.39357400	1.20429100
H	-3.53785800	-5.46295500	-0.94795400

9c-carbene

C	-1.54794400	-0.59299400	0.06696000
C	-0.19322000	-0.44051400	0.16530900
C	0.33327400	0.89739400	0.09492800
C	-0.56971500	1.98597400	-0.06989900
C	-1.94677500	1.81275800	-0.19489400
C	-2.40612500	0.50500500	-0.11623700
H	0.46999300	-1.28451400	0.31685200
H	-0.13234100	2.97773000	-0.10557000
H	-2.63227900	2.64135300	-0.33168700
C	1.70991800	1.21833100	0.15340400
C	2.69960100	0.18956200	0.30146200
O	2.99262300	-0.24719500	1.41221100
O	3.35541300	-0.14038100	-0.84022800
C	4.47947400	-1.01644600	-0.66438800
H	4.89177000	-1.16358300	-1.66357900
H	5.22640700	-0.56270900	-0.00700700
H	4.16951500	-1.97456800	-0.23695800
O	-2.29583400	-1.74594200	0.11048300
O	-3.68778200	0.08094300	-0.18889500
C	-3.65779200	-1.35443300	-0.04149600
H	-4.23072700	-1.62970800	0.85034000
H	-4.08186800	-1.81121700	-0.94185100

$TS_{9c}1$

C	4.08534200	-1.71095500	0.68210400
C	3.15504700	-0.51883400	0.86867900
C	2.03230100	-1.09592500	-1.11867600
C	2.97304500	-2.28366800	-1.29770000
H	2.95754600	-0.31570300	1.92436500
H	3.68707700	-2.58450300	1.22571200
H	5.08701200	-1.48714200	1.06365500
H	1.03070200	-1.32876200	-1.49611800
H	2.41592300	-0.20754300	-1.63451500
H	2.52016000	-3.18542800	-0.85145800
H	3.16132400	-2.47400200	-2.35963400
H	3.57570200	0.38028300	0.40227800
O	1.88215500	-0.80597400	0.27513800
O	4.23700800	-2.02449100	-0.69900300
C	-2.78879800	-0.09757000	-0.43973500
C	-1.60769400	0.59399400	-0.37594100
C	-0.76904700	0.37480800	0.76745400
C	-1.18945200	-0.54680700	1.76153600
C	-2.38760600	-1.25610900	1.67605000
C	-3.17011600	-1.00426300	0.55847100
H	-1.31872200	1.29915000	-1.14677700
H	-0.52869800	-0.68574200	2.60990000
H	-2.70512500	-1.96028400	2.43689100
C	0.46462700	1.05326900	0.99052200
C	0.94788700	2.07343600	0.08955900
O	1.91885100	2.02648900	-0.65751600
O	0.23873200	3.23190400	0.29755100
C	0.81858600	4.40958700	-0.28018700

H	0.16899900	5.23270700	0.02225100
H	1.83402200	4.56944600	0.09456200
H	0.85576400	4.33543100	-1.37084800
O	-3.76394300	-0.05525300	-1.41024000
O	-4.37434800	-1.55014100	0.25236100
C	-4.77385600	-0.97919800	-1.00881300
H	-4.86329700	-1.78158300	-1.74982200
H	-5.72764000	-0.45718100	-0.87670700

$INT_{9c}1$

C	-3.45753000	-1.79823900	-1.15205400
C	-2.59920100	-0.54855100	-1.23139200
C	-2.58671900	-0.54766700	1.24704700
C	-3.44586200	-1.79741300	1.17717000
H	-1.86900000	-0.58647400	-2.03933200
H	-2.82481600	-2.69978400	-1.18451300
H	-4.13573600	-1.81831700	-2.01060400
H	-1.84860700	-0.58507700	2.04779200
H	-3.15912900	0.38034300	1.27449100
H	-2.81285500	-2.69894300	1.20391800
H	-4.11544700	-1.81683400	2.04248500
H	-3.17192000	0.37940600	-1.25364300
O	-1.77006800	-0.47986100	0.00379600
O	-4.26178200	-1.80170300	0.01663200
C	3.01589600	0.13734700	-0.02386600
C	1.78941100	0.75972400	-0.01716500
C	0.62464900	-0.06522100	-0.01474100
C	0.80177500	-1.46939000	-0.02123200
C	2.07081600	-2.07459900	-0.03038600
C	3.17105900	-1.24612200	-0.02981100
H	1.70628900	1.83694800	-0.01463100
H	-0.06715400	-2.11756800	-0.01598800
H	2.17464400	-3.15493000	-0.04053900
C	-0.69551200	0.53049800	-0.00210500
C	-1.22907300	1.83424800	-0.00039400
O	-2.44464400	2.11558300	0.00750300
O	-0.27841900	2.82671400	-0.00753900
C	-0.79850700	4.15789100	-0.00565200
H	0.07658100	4.81064800	-0.01242400
H	-1.41568100	4.34332100	-0.88982600
H	-1.40375400	4.34555700	0.88628200
O	4.25930900	0.73541100	-0.05826300
O	4.51708500	-1.56607600	-0.07727500
C	5.19174000	-0.32853300	0.15277900
H	5.55607500	-0.29343800	1.19162300
H	6.02100200	-0.22924600	-0.55311800

$TS_{9c}2$

C	-4.20636200	-0.95630000	-0.76316800
C	-3.57436300	-0.16738000	0.17184000
C	-2.44223900	0.58087300	-0.25648700
C	-2.03820700	0.49852100	-1.60742200
C	-2.72138300	-0.28616700	-2.54711800
C	-3.80533400	-1.01287700	-2.09449600
H	-3.91625600	-0.12764200	1.19767600
H	-1.14687500	1.02960800	-1.92232800
H	-2.39483900	-0.34071400	-3.58004900
C	-1.71248800	1.43457300	0.67069900
C	-1.83428100	1.61261000	2.08554700
O	-1.57573400	2.65343300	2.69711000

O	-2.21361500	0.46933600	2.73514700	C	6.07857500	1.41711600	-0.56096500
C	-2.14878200	0.53937800	4.16794500	H	4.06205100	2.18057500	-0.40236300
H	-2.53952200	-0.41591700	4.52135500	C	6.27363100	-0.92147600	-1.17047500
H	-1.11407200	0.66897000	4.49614700	H	4.40265900	-1.97315300	-1.46379600
H	-2.75405900	1.36674200	4.54641000	C	6.86810600	0.29846400	-0.84166000
C	0.29729900	4.32670300	-0.75616000	H	6.54437100	2.36515500	-0.30830000
C	0.00602400	3.32273900	0.33832600	H	6.89047300	-1.78820000	-1.38868400
C	-2.38925800	3.74013500	-0.08224200	H	7.95090900	0.37909600	-0.80388600
C	-1.96447700	4.74681000	-1.13842300	C	0.62752700	-2.62403800	0.92076400
H	0.69608900	2.48691400	0.34289700	C	1.01529800	-3.70246600	0.12280500
H	0.41104100	3.81135600	-1.72102100	C	-0.70626200	-2.40232600	1.27161700
H	1.23587300	4.83757100	-0.52129900	C	0.03731600	-4.58474300	-0.33192100
H	-3.28358700	3.18891000	-0.37198100	H	2.06029600	-3.84283900	-0.12509500
H	-2.48642300	4.16607500	0.91755100	C	-1.67187400	-3.29229200	0.80216000
H	-1.93546800	4.25582500	-2.12405900	H	-0.98365800	-1.55605600	1.88897900
H	-2.69928600	5.55758300	-1.17337500	C	-1.30192000	-4.37902000	0.00669500
H	-0.10473700	3.76569400	1.32725800	H	0.32228400	-5.43118500	-0.95001400
O	-1.32017300	2.70503500	0.01200100	H	-2.71469700	-3.13064400	1.05670400
O	-0.71112900	5.32922900	-0.83277300	H	-2.06069200	-5.07010200	-0.35094800
N	1.91374400	-0.05035000	0.67315900	O	-5.31695700	-1.75404300	-0.58291100
F	0.37805100	0.46971500	0.71611100	O	-4.64740100	-1.84237400	-2.80125400
S	1.89662800	-1.54894000	1.57758100	C	-5.49358000	-2.45061300	-1.82105400
O	1.50669300	-1.13948800	2.92197900	H	-6.53713800	-2.36812200	-2.13916800
O	3.21070000	-2.13843500	1.30042100	H	-5.20712800	-3.50484100	-1.69317800
S	2.32927300	-0.02945500	-1.03108000				
O	1.80159800	1.25947800	-1.49606400				
O	1.96809900	-1.26981700	-1.72032100	C	-6.12033400	-0.54970400	-0.57373200
C	4.11136500	0.09122800	-0.93357600	C	-4.75809700	-0.64785100	-0.75336800
C	4.68971800	1.32056900	-0.60727700	C	-3.96155100	0.31720000	-0.08979500
C	4.88472500	-1.03504300	-1.21649500	C	-4.54668400	1.30977300	0.70990300

$INT_{9c}2$

C	-5.93530700	1.38574400	0.88184800	O	4.81865000	0.81505200	0.86199200
C	-6.69958900	0.43978000	0.22301000	O	2.92588300	1.26367500	2.50373400
H	-4.32361600	-1.42492400	-1.36912000	S	2.66801600	-0.77767300	-0.93648800
H	-3.91410300	2.04431100	1.19459900	O	3.25904200	0.02740200	-2.02449300
H	-6.39153600	2.15426100	1.49527900	O	1.37658800	-1.46435100	-1.23065700
C	-2.46676700	0.32896900	-0.21671200	C	3.84121500	-2.10195800	-0.57788300
C	-1.86726000	-0.43379600	-1.42150700	C	5.21080900	-1.86369000	-0.70391500
O	-2.01777500	-1.63385200	-1.52557300	C	3.35810400	-3.35070800	-0.18350400
O	-1.25253000	0.38092800	-2.24716200	C	6.10609700	-2.89609400	-0.42471800
C	-0.58242900	-0.23653900	-3.38885300	H	5.56140700	-0.88405900	-1.00402100
H	-1.29986700	-0.84308600	-3.94520600	C	4.26272100	-4.37624800	0.09255700
H	-0.22707700	0.60354000	-3.98252800	H	2.28798000	-3.51144400	-0.11406200
H	0.24566400	-0.83818300	-3.01075700	C	5.63545100	-4.14950300	-0.02675900
C	0.03087000	-0.41554100	2.61168400	H	7.17413600	-2.71919400	-0.51782500
C	-0.28941300	-0.17419300	1.15522800	H	3.89473500	-5.35292200	0.39607300
C	-2.29753900	-1.63649200	1.49313200	H	6.33858600	-4.94998200	0.18869400
C	-1.82735300	-1.79429900	2.93156400	C	3.07239400	2.72237600	0.32610800
H	-0.07085800	0.83279500	0.82077400	C	2.33730000	3.68087000	1.02539500
H	-0.41093100	0.37370400	3.23883700	C	3.57871300	2.99230100	-0.94798700
H	1.11763200	-0.38066900	2.71466000	C	2.09502400	4.92357600	0.43610400
H	-3.38300900	-1.63869500	1.40604700	H	1.98458900	3.45059000	2.02494800
H	-1.84841900	-2.36261900	0.81510900	C	3.32870400	4.23577400	-1.52786000
H	-2.32981700	-1.04577800	3.56617900	H	4.14215800	2.23272200	-1.47683500
H	-2.11545800	-2.79298600	3.27623700	C	2.58833200	5.20105000	-0.83975500
H	0.10540900	-0.92029400	0.46571900	H	1.52952800	5.67713100	0.97869500
O	-1.84951600	-0.28631400	1.05116100	H	3.71770900	4.45274100	-2.51925800
O	-0.42733500	-1.69635100	3.03748100	H	2.40186000	6.17006700	-1.29597900
N	2.36323600	0.04325700	0.43580500	O	-7.09834400	-1.35243100	-1.09500000
F	-1.99039100	1.59320700	-0.14593800	O	-8.05356300	0.29705000	0.22733800
S	3.39918100	1.12282100	1.11077100	C	-8.34639200	-0.79716800	-0.65992100

H	-8.91733000	-1.55770900	-0.11913100
H	-8.90456100	-0.42158000	-1.52500200

$TS_{9c}3$

C	-6.10558200	-0.64952900	-0.51300400
C	-4.74482700	-0.73811500	-0.71453500
C	-3.94287900	0.22059100	-0.05238300
C	-4.52060600	1.19706800	0.77007700
C	-5.90766600	1.26460800	0.96428500
C	-6.67777400	0.32495800	0.30448200
H	-4.31661600	-1.50572700	-1.34627400
H	-3.88329600	1.92739600	1.25490600
H	-6.35756800	2.02236400	1.59574500
C	-2.43870100	0.23872300	-0.19082600
C	-1.87299900	-0.48487400	-1.43611300
O	-2.01601200	-1.68237700	-1.58031200
O	-1.26102000	0.34767300	-2.25386200
C	-0.62026700	-0.25253600	-3.41662500
H	-1.35347900	-0.83410400	-3.97920300
H	-0.25717800	0.59367100	-3.99734000
H	0.20379200	-0.87959500	-3.07347600
C	0.23889100	-0.44585100	2.51023500
C	0.02826000	-0.18015600	1.04591300
C	-2.17494200	-1.69133300	1.44257100
C	-1.61600900	-1.85739200	2.84691900
H	0.05875100	0.83745900	0.68701600
H	-0.26523100	0.32723900	3.10875600
H	1.31047400	-0.38209500	2.70962900
H	-3.26480800	-1.74943800	1.43309700
H	-1.75331000	-2.41118400	0.73902900
H	-2.08759400	-1.12274600	3.51933200
H	-1.86246700	-2.86310900	3.20209300
H	0.23816700	-0.96155000	0.32412700
O	-1.79815500	-0.33972400	1.00915800
O	-0.20966800	-1.74217500	2.88277700
N	2.34352600	0.04421200	0.41773000
F	-1.98818500	1.52641000	-0.14780100
S	3.30743000	1.20965700	1.08113500
O	4.73240100	1.00466800	0.77898400
O	2.86803800	1.29487600	2.48833700
S	2.72793800	-0.75574600	-0.96562100
O	3.31343700	0.10009200	-2.01307100
O	1.48186900	-1.49681400	-1.29964000
C	3.95458600	-2.01364100	-0.56333400
C	5.31280600	-1.71135100	-0.67194200
C	3.52134200	-3.27614100	-0.15453800
C	6.25007200	-2.69583700	-0.35904500
H	5.62136200	-0.72146700	-0.98444900
C	4.46850800	-4.25203600	0.15547700
H	2.45915700	-3.48731400	-0.09934200
C	5.83095500	-3.96230900	0.05453800
H	7.31005800	-2.47102800	-0.43821900
H	4.14166100	-5.23927300	0.47092000
H	6.56669800	-4.72484900	0.29650500
C	2.82347000	2.78033000	0.32532400
C	2.04997600	3.67415300	1.06807100
C	3.24880100	3.09435100	-0.96854100
C	1.68496700	4.89701900	0.50127000
H	1.76303400	3.41293300	2.08084200
C	2.87614100	4.31794300	-1.52390100

H	3.84402800	2.38315500	-1.52931100
C	2.09562500	5.21829100	-0.79327800
H	1.08822200	5.60083700	1.07572600
H	3.20065000	4.57046100	-2.52980400
H	1.81311500	6.17192900	-1.23178000
O	-7.08775600	-1.45421300	-1.02820900
O	-8.03367700	0.17190500	0.32928400
C	-8.33133000	-0.89624900	-0.58541800
H	-8.91319700	-1.66438600	-0.06757100
H	-8.88189700	-0.49470000	-1.44472900

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C	6.56788100	-1.00914100	0.32933500
C	5.23852800	-0.86561400	0.66931600
C	4.49468300	0.08798700	-0.05932100
C	5.09793600	0.83483100	-1.07867300
C	6.45217400	0.67291500	-1.40896500
C	7.16458200	-0.26215500	-0.68261300
H	4.78981100	-1.46072400	1.45430600
H	4.50386300	1.56190200	-1.61994000
H	6.92110100	1.25705800	-2.19316200
C	3.00892400	0.31958300	0.18305600
C	2.50919100	-0.08131100	1.59269800
O	2.55779600	-1.22436400	2.00199700
O	1.98795000	0.94639700	2.26155300
C	1.39634700	0.62705300	3.54231700
H	0.48021900	0.05542000	3.38802800
H	2.10198400	0.05944700	4.15226100
H	1.17048500	1.59058300	3.99773300
C	-0.81907600	-1.09547200	-1.32117500
C	-1.92026800	-1.34705200	-0.29433100
C	2.36606600	-1.68076100	-1.07540300
C	1.23443600	-2.13378200	-1.98711500
H	-1.48177100	-1.53679400	0.68543900
H	-0.23809200	-0.21062100	-1.04253600
H	-1.25814200	-0.93034200	-2.31501500
H	3.32894600	-1.81247500	-1.58770000
H	2.36202100	-2.27926100	-0.15950900
H	1.15023500	-1.45672500	-2.84972400
H	1.49033100	-3.13158400	-2.36435400
H	-2.49966200	-2.23050600	-0.57501900
O	2.16511300	-0.29291100	-0.76591200
O	-0.00618400	-2.26314500	-1.31445600
N	-2.85592600	-0.20562000	-0.16565000
F	2.74865500	1.66747400	0.00120200
S	-4.27576300	-0.21428100	-1.13667000
O	-3.90004700	-0.91503400	-2.36526400
O	-4.78229400	1.15460900	-1.16538600
S	-2.54621500	1.01749200	1.02296700
O	-1.48104000	0.44660100	1.85211500
O	-3.82559500	1.40755200	1.61133000
C	-1.86520600	2.41924600	0.13663800
C	-0.47704800	2.52883100	0.03055900
C	-2.72707300	3.37649400	-0.40404600
C	0.05921600	3.61898900	-0.65411100
H	0.17530500	1.79434800	0.48510300
C	-2.17274200	4.46233900	-1.08065500
H	-3.79921400	3.26206600	-0.30479700
C	-0.78615000	4.58140300	-1.20931400
H	1.13744900	3.70387700	-0.74421100

H	-2.82766300	5.21564500	-1.50874700
H	-0.36471000	5.43001000	-1.74140500
C	-5.44007000	-1.25826900	-0.25483600
C	-6.08833300	-0.76257700	0.88015500
C	-5.69084400	-2.54110900	-0.74611400
C	-7.00026700	-1.58533000	1.53881600
H	-5.86998500	0.23630600	1.24008300
C	-6.60792500	-3.35084400	-0.07425300
H	-5.18637700	-2.88399400	-1.64251700
C	-7.25865600	-2.87490700	1.06501900
H	-7.51135100	-1.21675000	2.42344600
H	-6.81486300	-4.35036400	-0.44558500
H	-7.97208900	-3.50862300	1.58462600
O	7.50009500	-1.84429900	0.89775500
O	8.48935300	-0.59786100	-0.79016200
C	8.69102800	-1.68950100	0.11888300
H	8.87970700	-2.60842500	-0.45227400
H	9.53252800	-1.46019500	0.77969000

$TS_{9c}4$

C	-5.16378700	0.57276400	-0.02933400
C	-4.27391000	-0.39742500	0.33004500
C	-2.95812800	-0.33397100	-0.25600900
C	-2.63781200	0.72681900	-1.15559500
C	-3.54781100	1.73195000	-1.46801200
C	-4.81010600	1.62066400	-0.89963000
H	-4.54319300	-1.21189700	0.99206500
H	-1.63505700	0.75688600	-1.56377000
H	-3.29820600	2.55177400	-2.13157900
C	-1.96793200	-1.29149700	0.00756000
C	-2.12102100	-2.34606100	0.98012200
O	-2.86037000	-3.30220800	0.76073600
O	-1.30800100	-2.23232500	2.04644200
C	-1.34155100	-3.31939500	2.98609700
H	-0.54862000	-3.09956200	3.70006400
H	-2.31293800	-3.36650800	3.48765600
H	-1.15450400	-4.27159000	2.48331700
N	1.27447300	0.29936700	0.49491300
F	-0.05652100	-0.50311800	0.04214800
S	2.40875200	-0.96463400	0.94039900
O	1.83251900	-1.56068900	2.14012000
O	3.70605600	-0.28152900	0.97011700
S	1.64640300	1.36180400	-0.86374800
O	0.34479500	1.90210200	-1.26362200
O	2.51991100	0.72628200	-1.85306700
C	2.55233400	2.64680300	-0.01099200
C	1.83895500	3.58876200	0.73463200
C	3.94019100	2.70316100	-0.14035200
C	2.54170500	4.61169600	1.36759400
H	0.75916600	3.51965200	0.80713300
C	4.62823600	3.73584500	0.49577500
H	4.46039700	1.95122400	-0.72119800
C	3.93242700	4.68465500	1.24782700
H	2.00395400	5.35271800	1.95182100
H	5.70879000	3.79612400	0.40544000
H	4.47540000	5.48483200	1.74324200
C	2.42134500	-2.20156300	-0.35208100
C	3.45047500	-2.18830700	-1.29488300
C	1.42589200	-3.18157100	-0.35721200
C	3.47642500	-3.18529200	-2.26937400

H	4.20705200	-1.41438700	-1.26078400
C	1.46263000	-4.16691000	-1.34170300
H	0.64905000	-3.16639000	0.39669900
C	2.48464100	-4.16808100	-2.29460900
H	4.27126800	-3.19171100	-3.00946700
H	0.69287700	-4.93270600	-1.36311100
H	2.50881600	-4.94007900	-3.05898700
O	-5.86475900	2.44399700	-1.07916900
O	-6.47331400	0.73161600	0.35599500
C	-6.94830300	1.91024600	-0.28869500
H	-7.24079300	2.65567200	0.45817400
H	-7.78263100	1.66600500	-0.95430300

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C	3.62929400	0.67959600	-0.27553900
C	2.36696000	0.64119300	0.27550600
C	1.32066300	1.19535400	-0.49485600
C	1.57612500	1.76752400	-1.74362100
C	2.87084900	1.79766100	-2.28425800
C	3.88140800	1.24397800	-1.52349900
H	2.19028100	0.21883600	1.25621200
H	0.75763000	2.19162700	-2.30930600
H	3.06837500	2.23675300	-3.25580500
C	-0.09901200	1.26775600	0.07929300
C	0.03171900	1.93366400	1.48109200
O	0.42457600	1.33026000	2.45306100
O	-0.20224200	3.24348100	1.41726700
C	-0.07726400	3.93990800	2.67116100
H	-0.28566100	4.98493300	2.44256900
H	-0.80340900	3.54683500	3.38664300
H	0.93175800	3.82361000	3.07459900
N	-0.79538400	-0.01559400	0.20511300
F	-0.85968300	2.09514100	-0.74420100
S	-2.35625700	0.00046800	1.05760100
O	-2.40473700	1.33443200	1.65890200
O	-2.41569500	-1.20040300	1.88505300
S	-0.43736900	-1.40730900	-0.79251000
O	0.11411900	-0.95041500	-2.06389100
O	-1.66328300	-2.20048600	-0.75919600
C	0.83280100	-2.28136200	0.12013400
C	1.98585200	-2.66800100	-0.56361500
C	0.60875300	-2.62534200	1.45551000
C	2.94723000	-3.41586700	0.11688900
H	2.12486900	-2.37611000	-1.59848700
C	1.58400500	-3.36633800	2.12100400
H	-0.29862300	-2.31075400	1.96102700
C	2.74771000	-3.76124800	1.45464900
H	3.85282200	-3.72243200	-0.39823500
H	1.43318100	-3.63471400	3.16242700
H	3.50223800	-4.33826300	1.98208800
C	-3.65016600	-0.06216600	-0.18310300
C	-4.44207100	-1.20639800	-0.27300700
C	-3.89134500	1.07370600	-0.95882800
C	-5.50622500	-1.21017700	-1.17360600
H	-4.21646600	-2.06872700	0.34238700
C	-4.95385900	1.04797600	-1.86092000
H	-3.26011000	1.94894300	-0.86153900
C	-5.75932300	-0.08862400	-1.96635700
H	-6.13361500	-2.09255400	-1.25813500
H	-5.15409200	1.91918800	-2.47767700

H	-6.58768700	-0.09974600	-2.66937600
O	5.21598200	1.13017600	-1.82275900
O	4.80108400	0.18488400	0.25111700
C	5.83480000	0.64444300	-0.62415900
H	6.50038100	-0.18695700	-0.87131300
H	6.38911500	1.46304500	-0.14314900

$TS_{9c}5$

C	-2.62059900	-3.30104900	0.09475000
C	-1.64620100	-2.52877900	0.72962700
C	-1.79651100	-1.13670200	0.95413800
C	-3.01012600	-0.49561300	0.53906100
C	-3.97012300	-1.27296500	-0.05438700
C	-3.77873500	-2.64100400	-0.28358600
H	-2.49626300	-4.36362100	-0.08115900
H	-0.72603400	-2.98812300	1.06991400
H	-3.16661900	0.56054300	0.72336300
C	-0.74428800	-0.45635900	1.64388900
C	-0.80838700	0.92196900	2.05437100
O	-0.07115500	1.84750000	1.72855900
O	-1.75635500	1.05575900	3.04150800
C	-1.67143400	2.27300300	3.79378500
H	-2.46983000	2.21291500	4.53567600
H	-0.69917300	2.35794800	4.28839800
H	-1.81377700	3.14443700	3.14836000
N	0.86204800	-0.19077700	0.12092100
F	1.07271500	-1.56406500	-0.15216600
S	2.47558600	0.31246100	0.96021000
O	2.30655200	-0.04921000	2.35816400
O	2.74480400	1.67556700	0.51507700
S	0.61953100	0.46090000	-1.63769900
O	-0.31591100	-0.51375200	-2.19086600
O	1.92512100	0.69548100	-2.25670000
C	-0.21925600	2.01737900	-1.39953700
C	-1.60407500	2.04257600	-1.57806600
C	0.52144800	3.17018000	-1.13338000
C	-2.26517200	3.26579200	-1.47600500
H	-2.13983300	1.12742200	-1.80067700
C	-0.15805000	4.38175000	-1.03169400
H	1.59233500	3.11183100	-0.98752500
C	-1.54388800	4.42970600	-1.20099500
H	-3.34133400	3.30840900	-1.61646700
H	0.39759800	5.28926400	-0.81603900
H	-2.06433200	5.38018000	-1.12105200
C	3.68854800	-0.80241800	0.24918000
C	4.44497200	-0.38266200	-0.84600700
C	3.89477400	-2.03931600	0.86587400
C	5.43219000	-1.23693600	-1.33735200
H	4.25848500	0.58220800	-1.29981600
C	4.88323900	-2.88035900	0.35973900
H	3.29972000	-2.32214900	1.72688500
C	5.64804800	-2.48021300	-0.73957900
H	6.03237300	-0.92776100	-2.18788600
H	5.05846400	-3.84554400	0.82574000
H	6.41844900	-3.13984700	-1.12935400
O	-5.21953100	-0.90723300	-0.50650500
O	-4.88125500	-3.16904600	-0.87973000
C	-5.77567100	-2.06851600	-1.12216500
H	-6.74941100	-2.29468100	-0.67683300
H	-5.86385700	-1.91252400	-2.20468500

$INT_{9c}3$

C	4.36137400	1.11936800	-0.16928500
C	3.01616100	0.99244900	0.20405400
C	2.36191300	-0.25137700	0.20350200
C	3.05565400	-1.42191800	-0.19363800
C	4.37362000	-1.27453900	-0.55820400
C	5.01635000	-0.03672200	-0.54913900
H	4.86692700	2.07858800	-0.15907100
H	2.47223600	1.87943300	0.50901400
H	2.56004000	-2.38323100	-0.22308400
C	0.95611900	-0.35670900	0.61995500
C	0.41694900	-1.34713000	1.56259700
O	-0.77399400	-1.42234900	1.83475700
O	1.36305300	-2.13893100	2.10120300
C	0.88049800	-3.11782000	3.03546400
H	1.77215200	-3.61565000	3.41694400
H	0.32850000	-2.63443700	3.84534100
H	0.22644000	-3.83641300	2.53401800
N	-0.02718600	0.40353700	0.12011300
F	0.42295800	1.27392900	-0.86825500
S	-1.30950100	1.50184000	1.24686100
O	-0.74455800	1.54185200	2.59664000
O	-2.60387100	0.91793000	0.90667400
S	-1.51495700	-1.00323000	-1.24969400
O	-0.47025100	-2.07062600	-1.26360200
O	-1.73682200	-0.14959900	-2.45457600
C	-3.09618500	-1.82976600	-0.90534500
C	-3.15492500	-2.80058700	0.09298800
C	-4.22300900	-1.44568600	-1.63071500
C	-4.37551400	-3.42483900	0.34652400
H	-2.26756600	-3.04576400	0.66548100
C	-5.43718600	-2.08204300	-1.36743500
H	-4.13618600	-0.67980800	-2.39324300
C	-5.51371900	-3.06868400	-0.38251000
H	-4.43896700	-4.18730400	1.11806000
H	-6.32261300	-1.80545100	-1.93353700
H	-6.46281100	-3.55648500	-0.17693300
C	-1.17347100	3.11055800	0.48168900
C	-1.75735000	3.30908300	-0.77320100
C	-0.49257900	4.12201900	1.16224800
C	-1.66262800	4.57340000	-1.34964900
H	-2.25042300	2.49062900	-1.28796700
C	-0.41569000	5.38242000	0.56963000
H	-0.05650100	3.92530500	2.13553600
C	-0.99784200	5.60569500	-0.68022600
H	-2.10558200	4.75111300	-2.32489500
H	0.09643000	6.18851000	1.08666800
H	-0.93089100	6.58864800	-1.13790400
O	5.25865500	-2.24764400	-0.96003600
O	6.31961600	-0.18718600	-0.94213300
C	6.44155100	-1.55390800	-1.36402700
H	7.31299700	-2.00440300	-0.88061700
H	6.53566000	-1.58832000	-2.45806600

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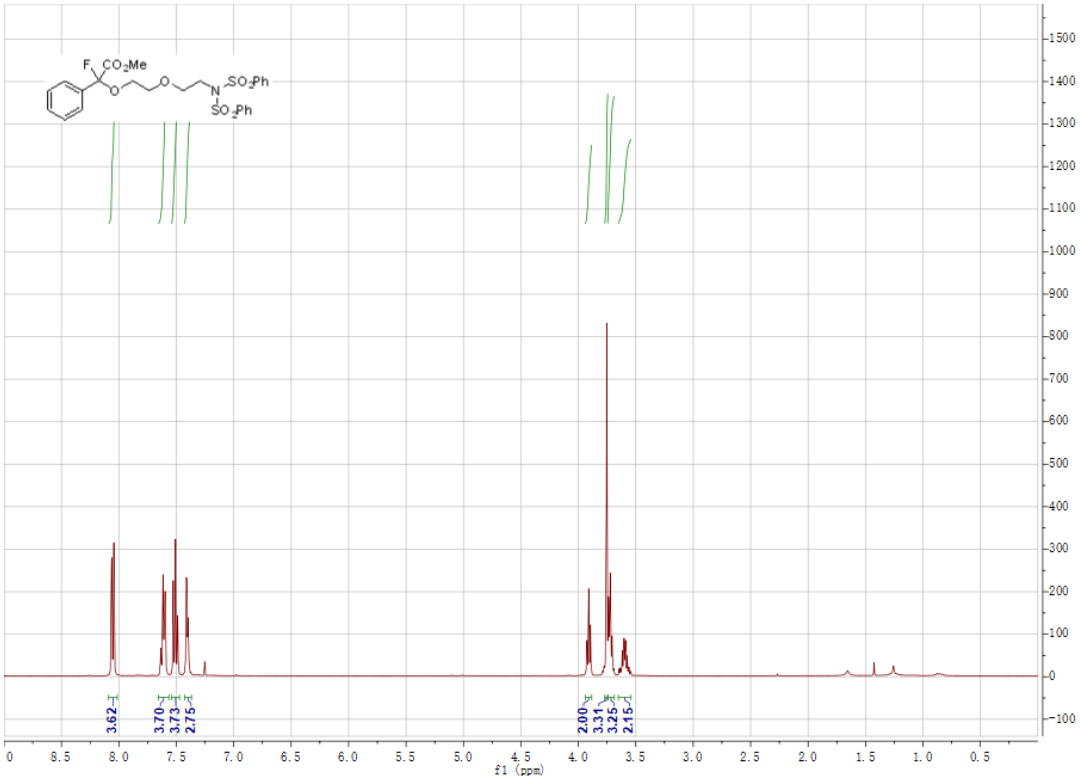
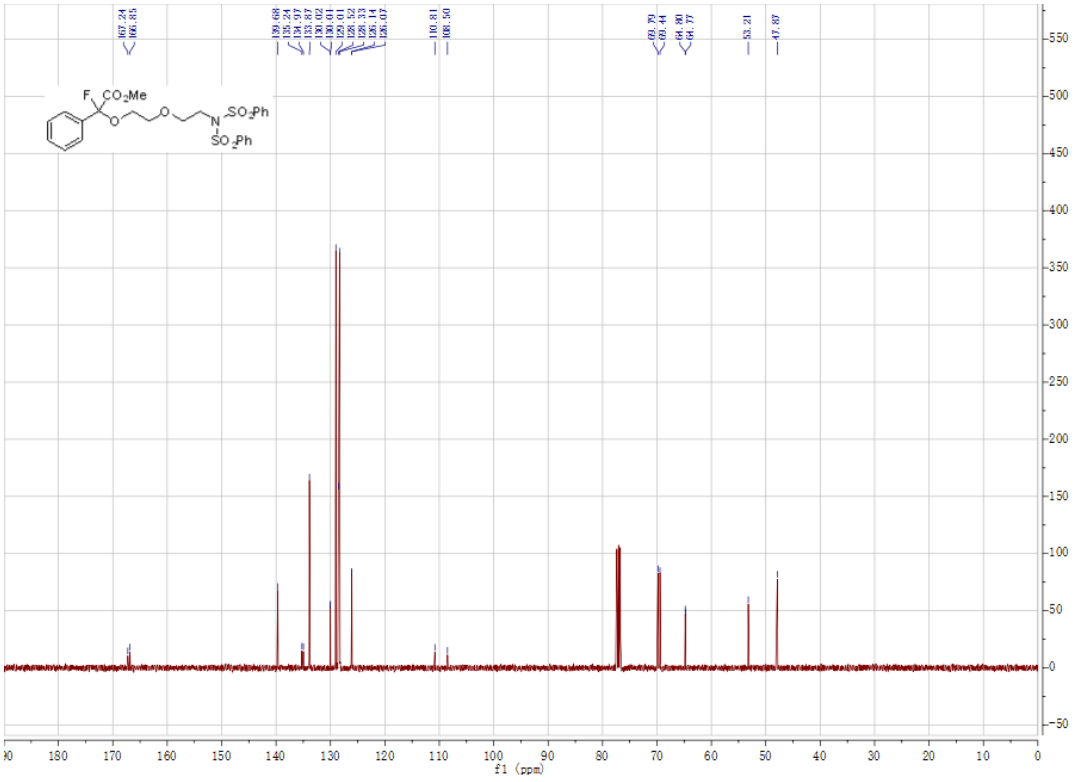
methyl 2-fluoro-2-phenyl-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido)ethoxy) ethoxy)acetate (5a)

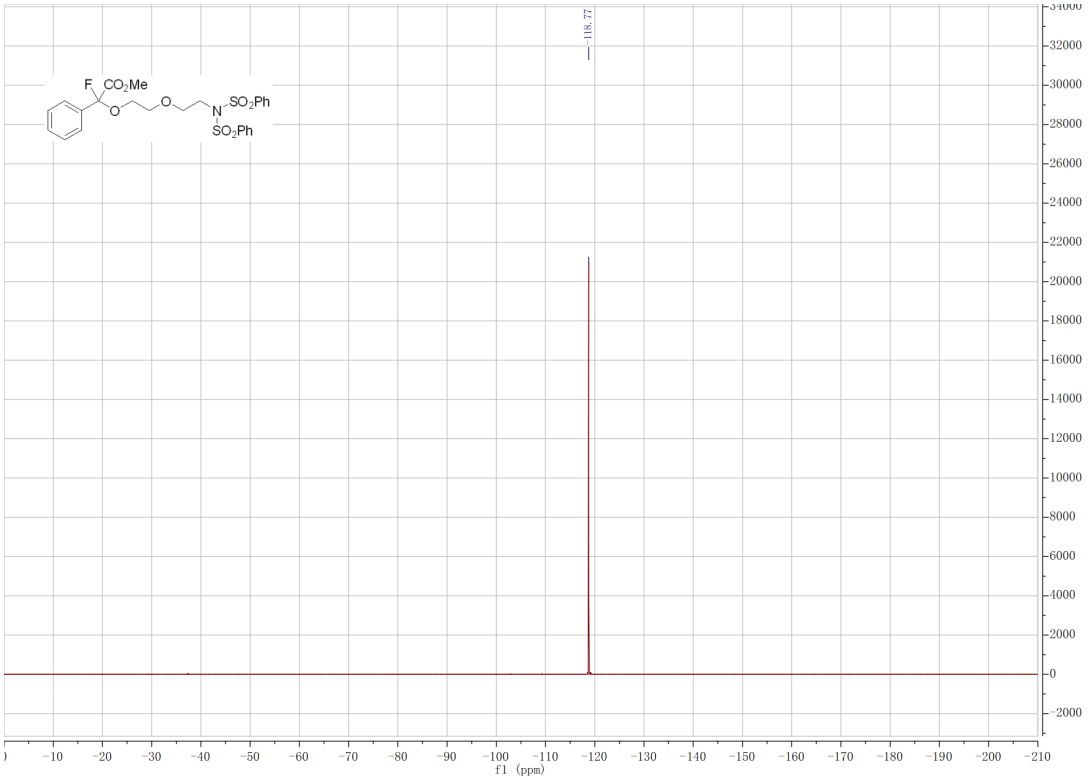
^{1}H NMR (400 MHz, Chloroform-*d*)



^{13}C NMR (101 MHz, Chloroform-*d*)

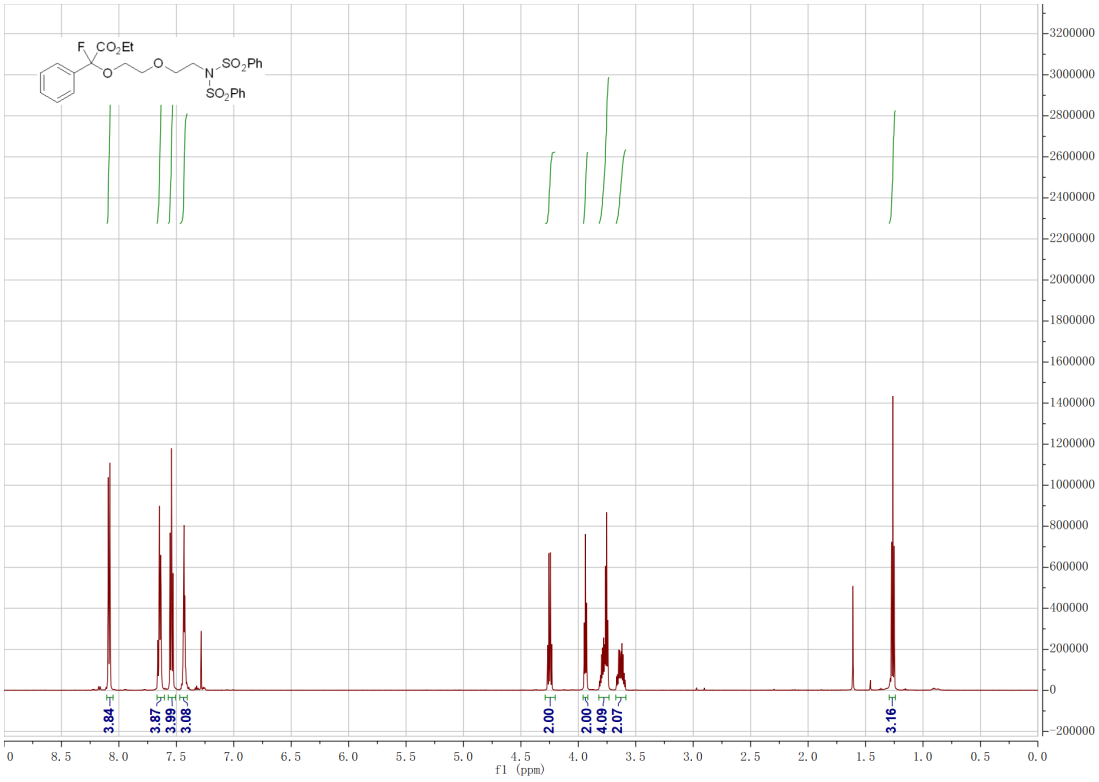


^{19}F NMR (376 MHz, Chloroform-*d*)

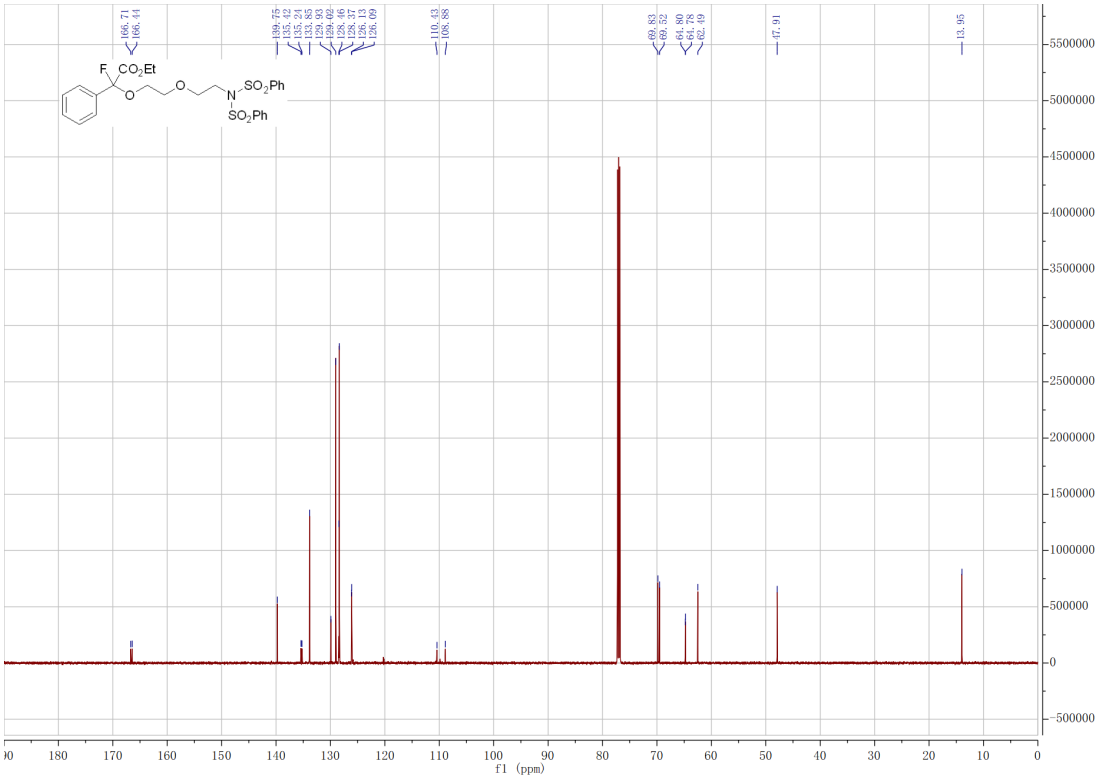


ethyl 2-fluoro-2-phenyl-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido)ethoxy) ethoxy)acetate (5b)

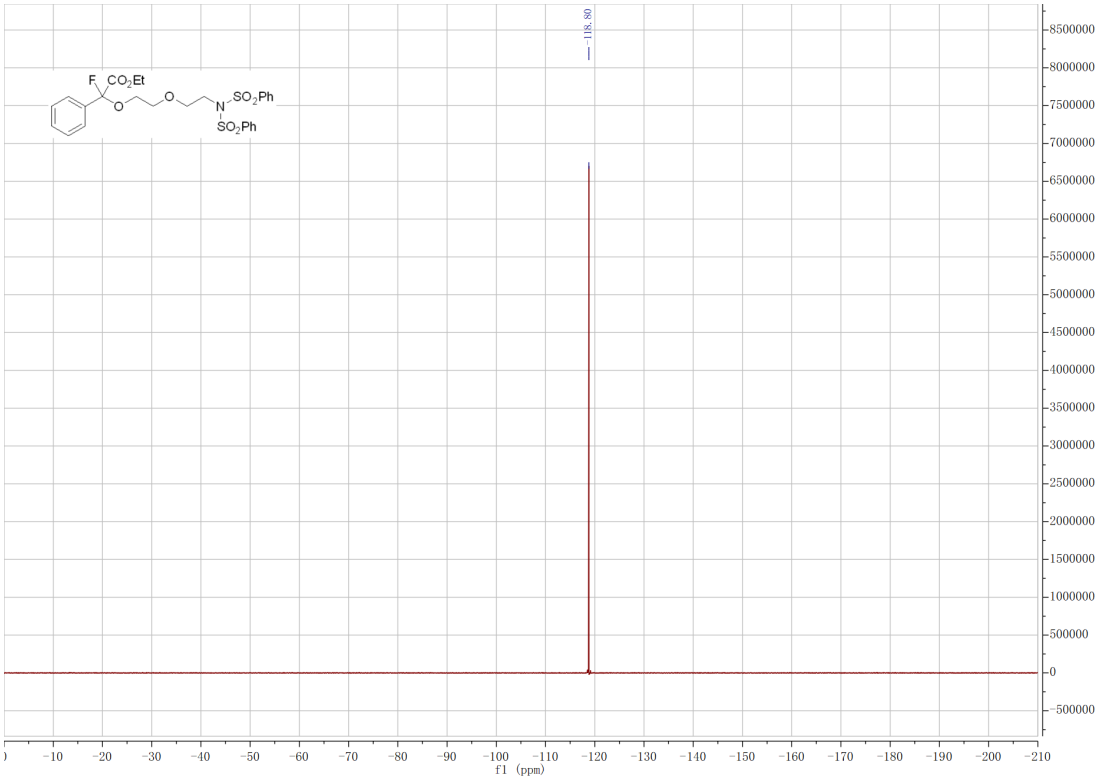
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

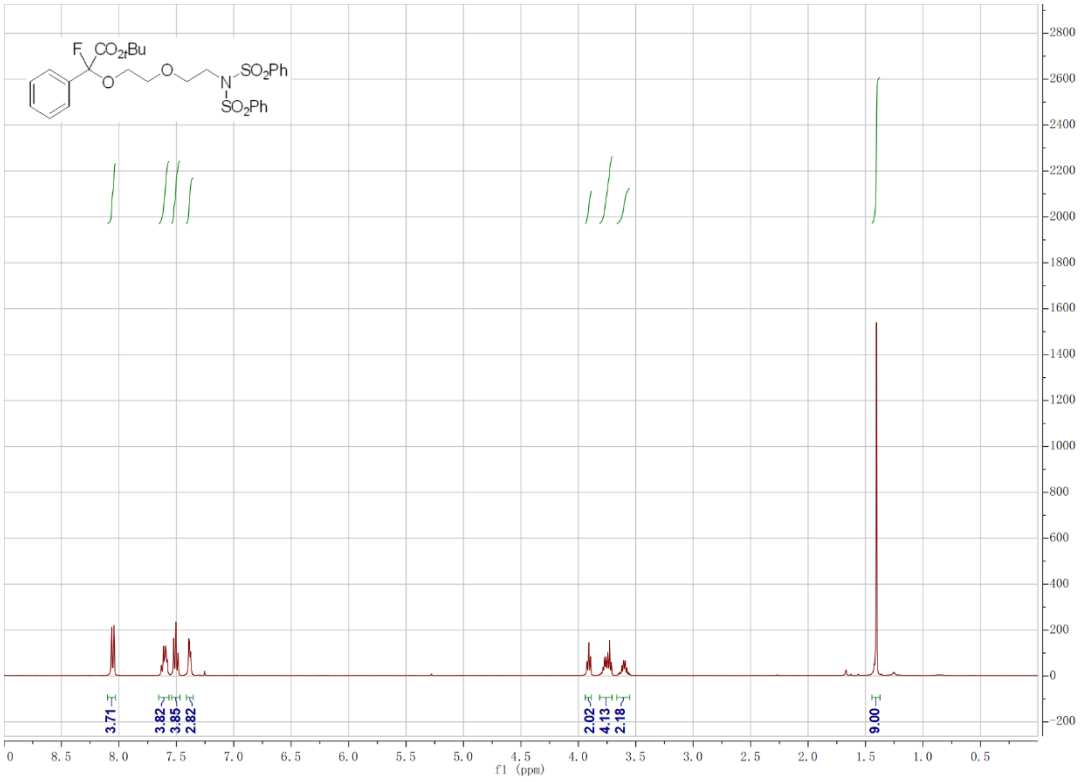


^{19}F NMR (565 MHz, Chloroform-*d*)

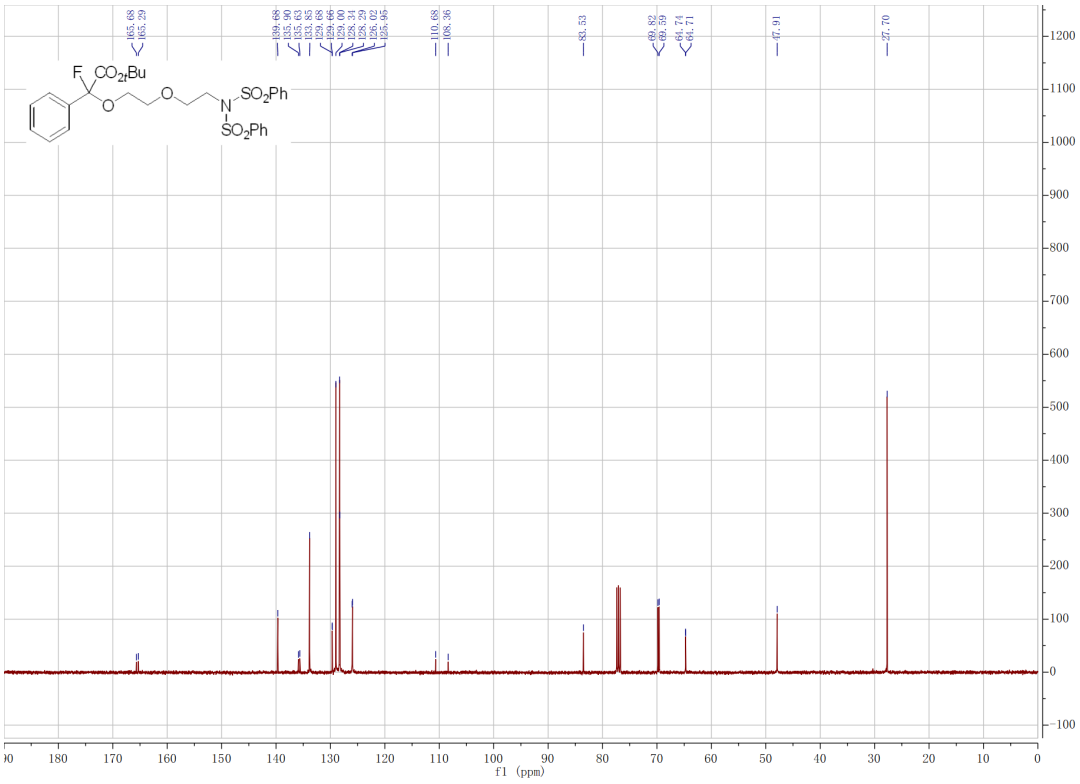


***tert*-butyl 2-fluoro-2-phenyl-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido)ethoxy) ethoxy)acetate (5c)**

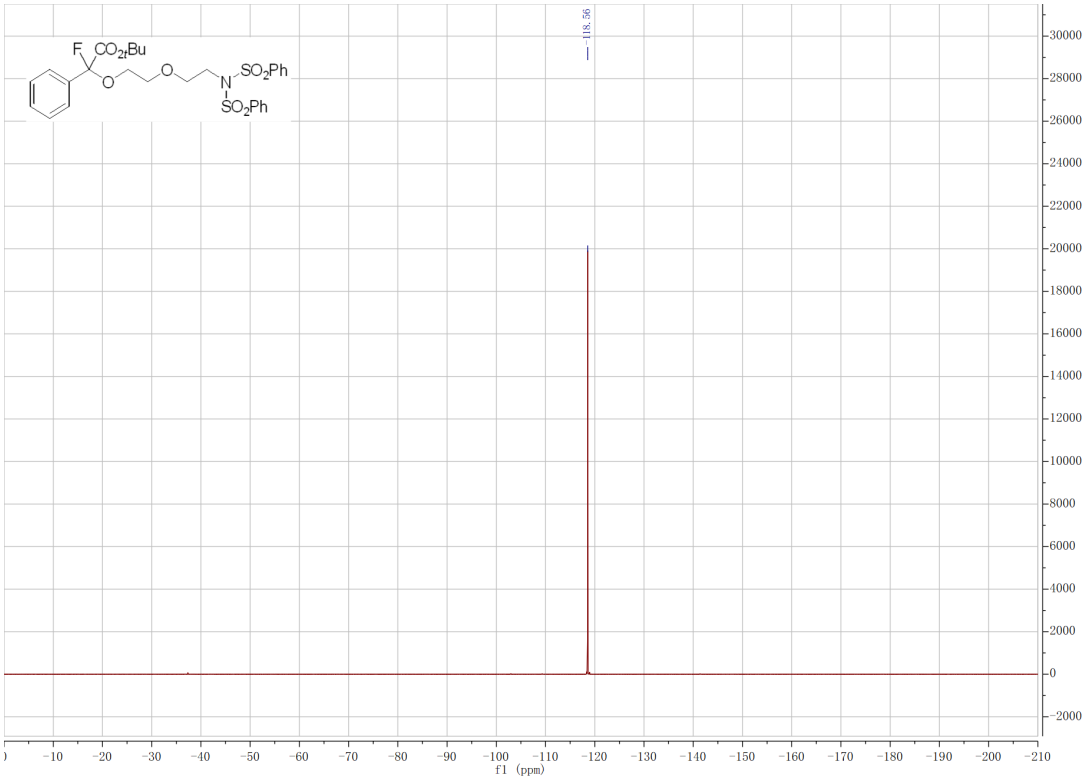
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

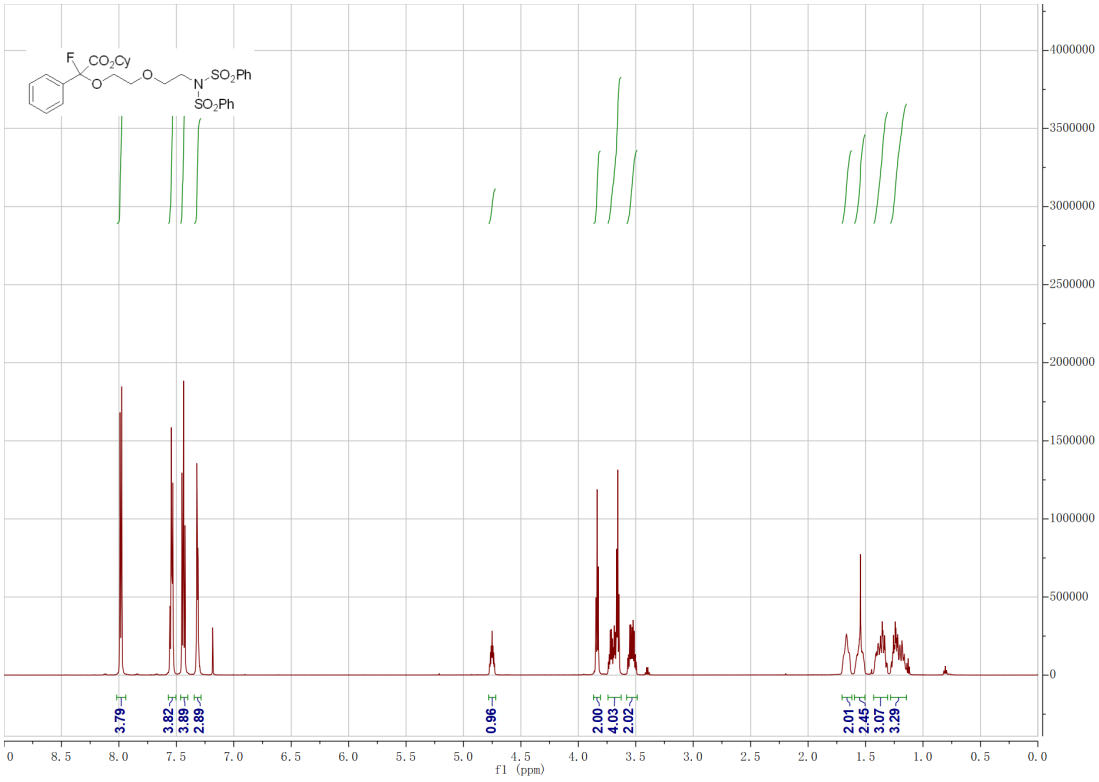


^{19}F NMR (565 MHz, Chloroform-*d*)

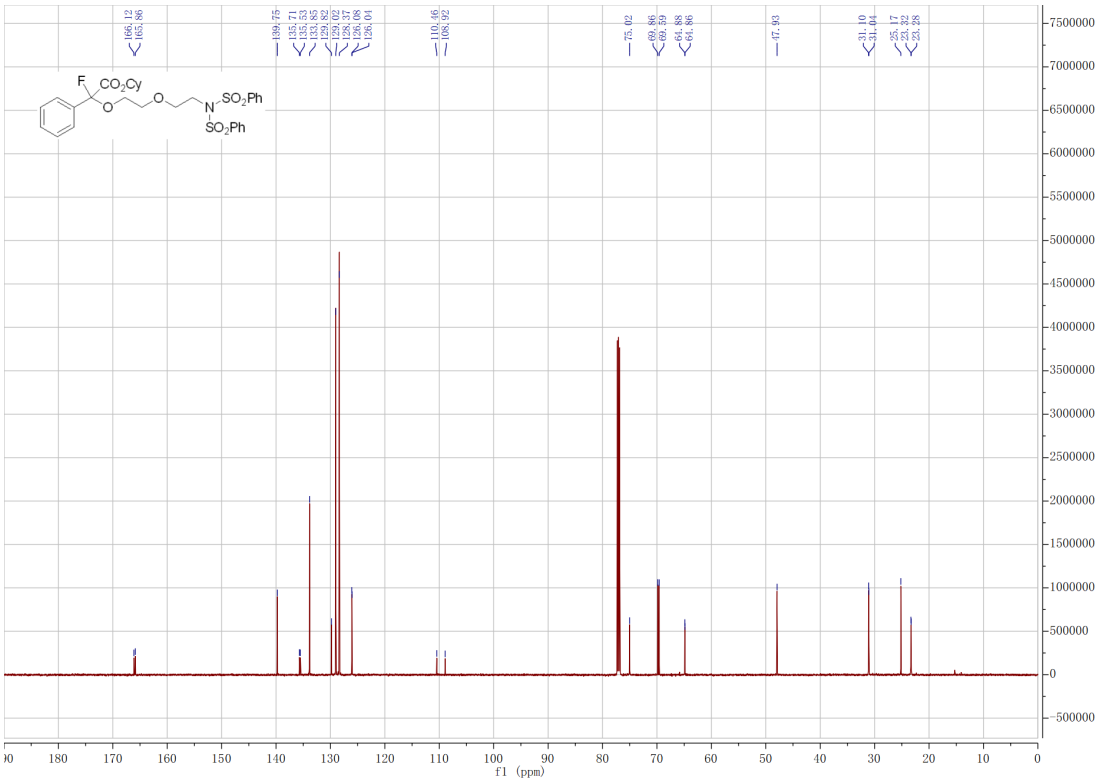


cyclohexyl 2-fluoro-2-phenyl-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido)ethoxy) ethoxy)acetate (5d)

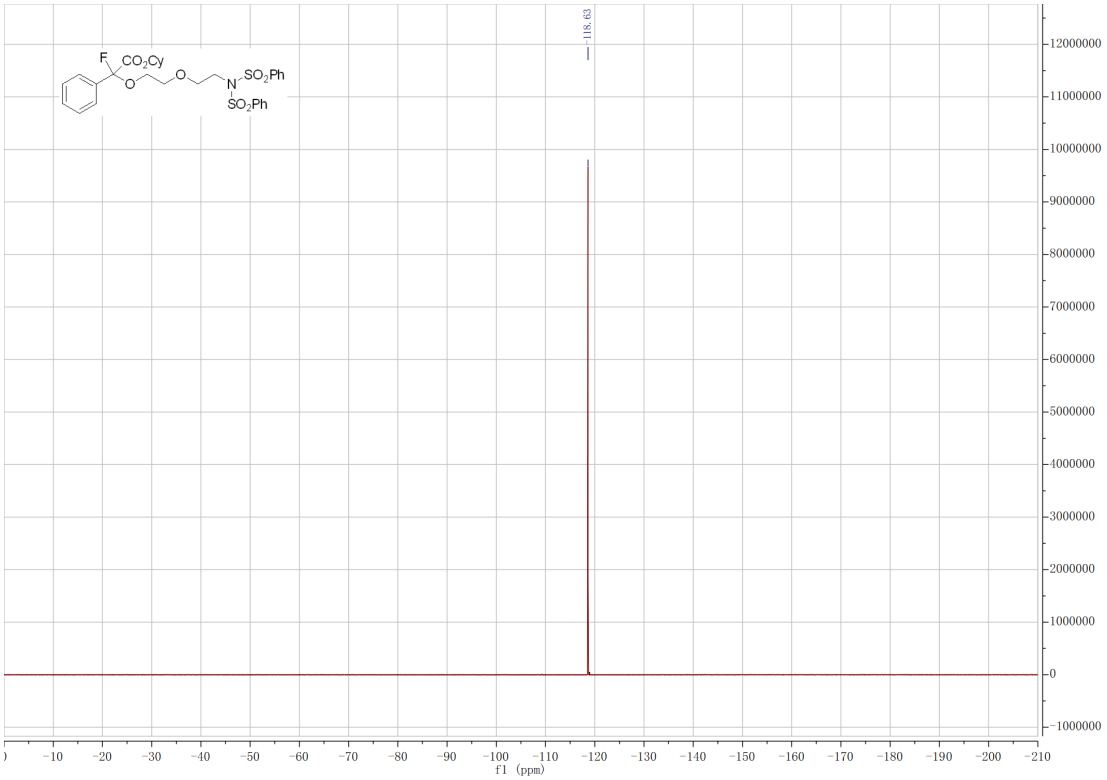
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

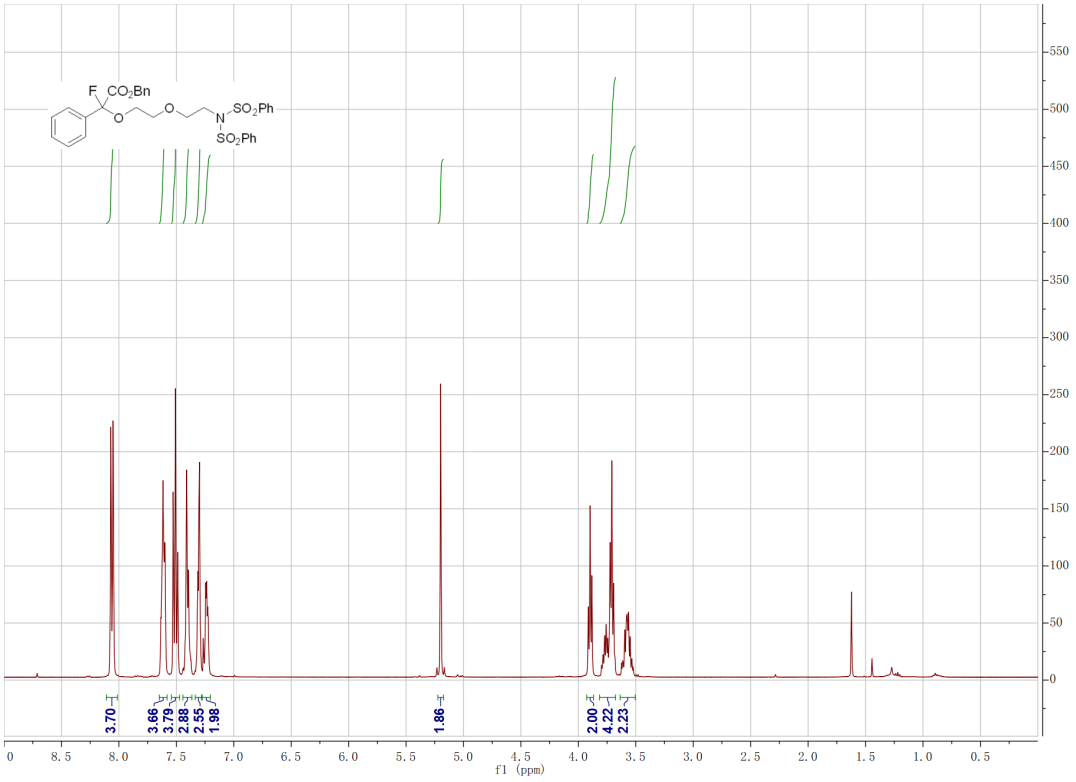


^{19}F NMR (565 MHz, Chloroform-*d*)

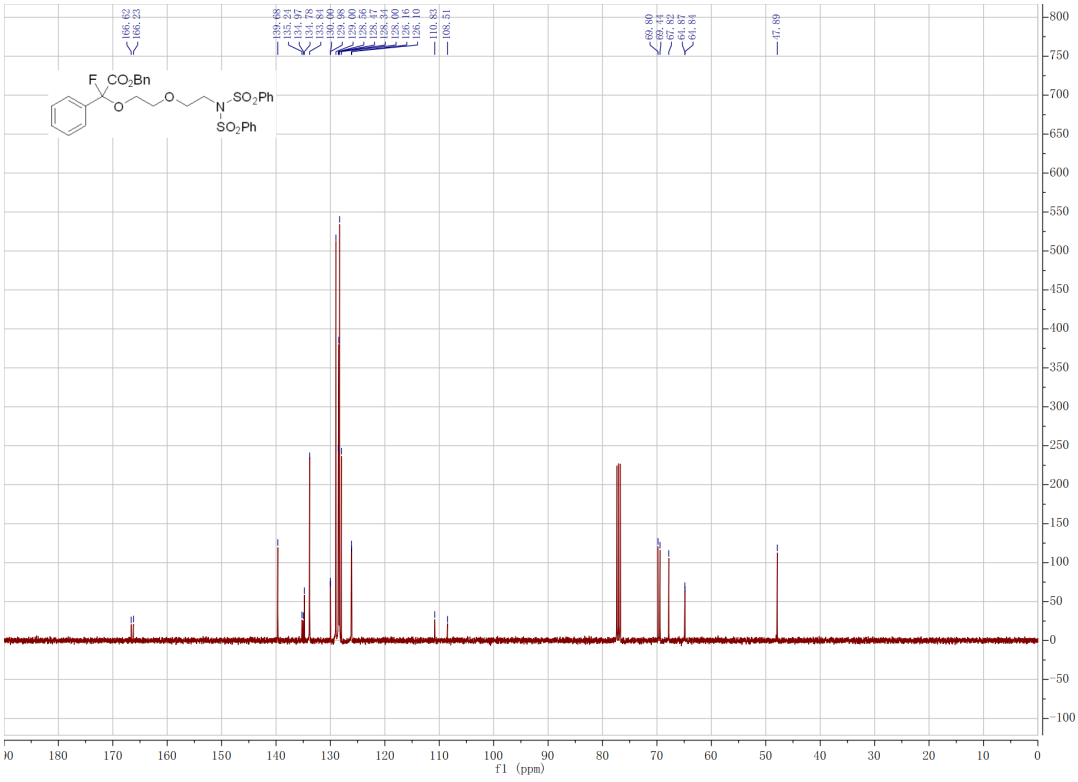


benzyl 2-fluoro-2-phenyl-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido)ethoxy) ethoxy)acetate (5e)

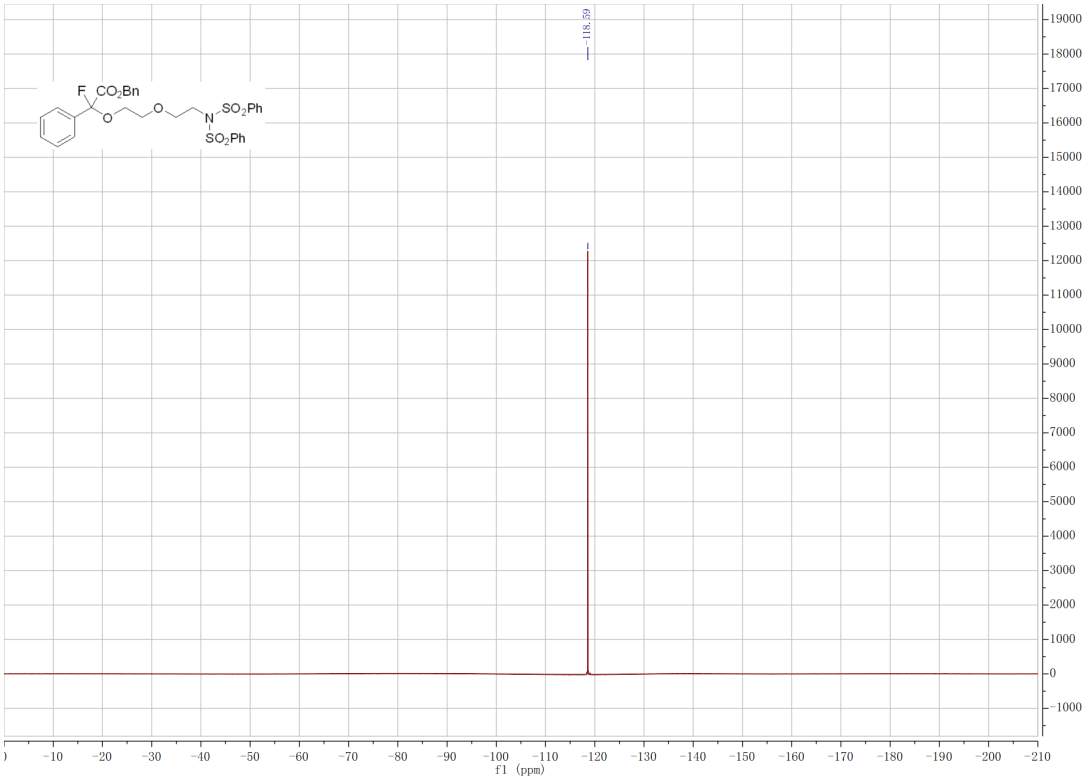
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

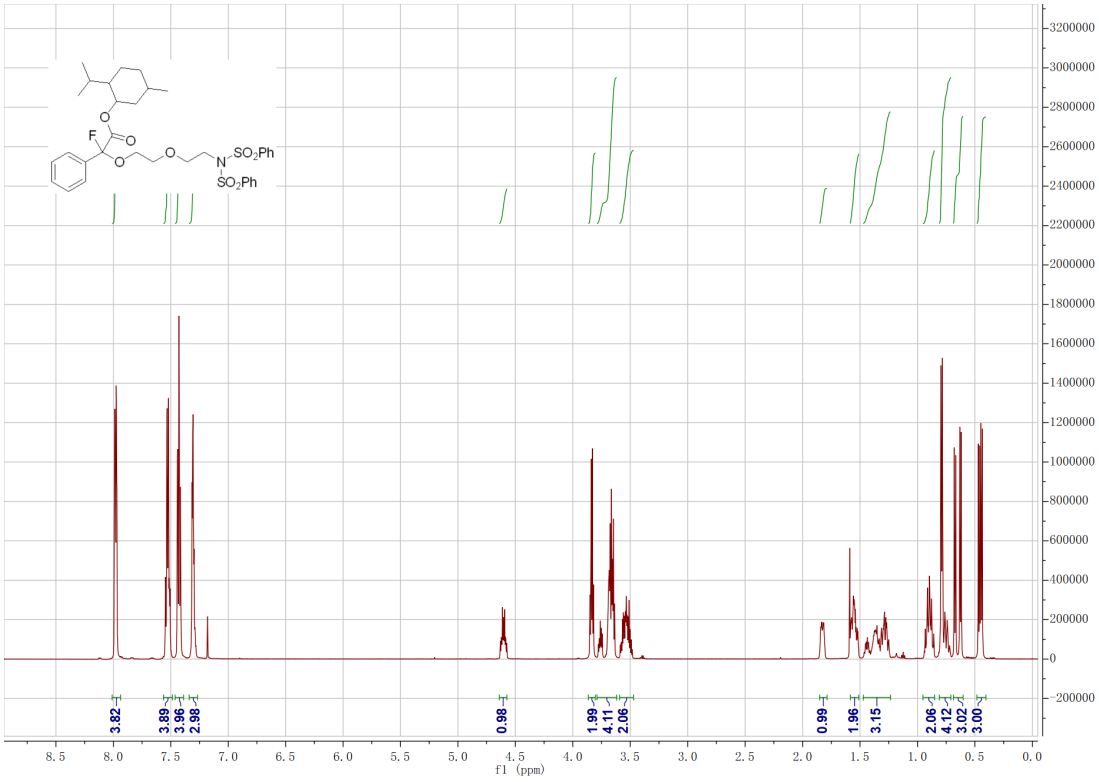


^{19}F NMR (565 MHz, Chloroform-*d*)

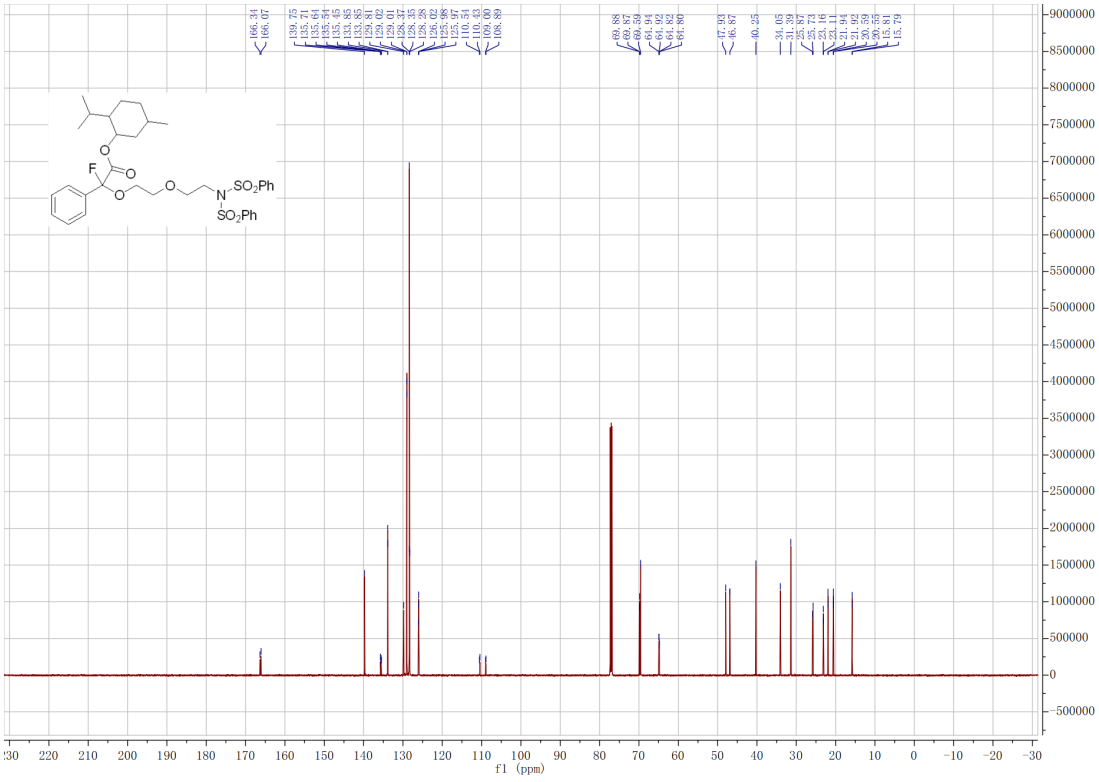


2-isopropyl-5-methylcyclohexyl 2-fluoro-2-phenyl-2-(2-(2-(N-(phenylsulfonyl)phenyl sulfonamido)ethoxy)ethoxy)acetate (5f)

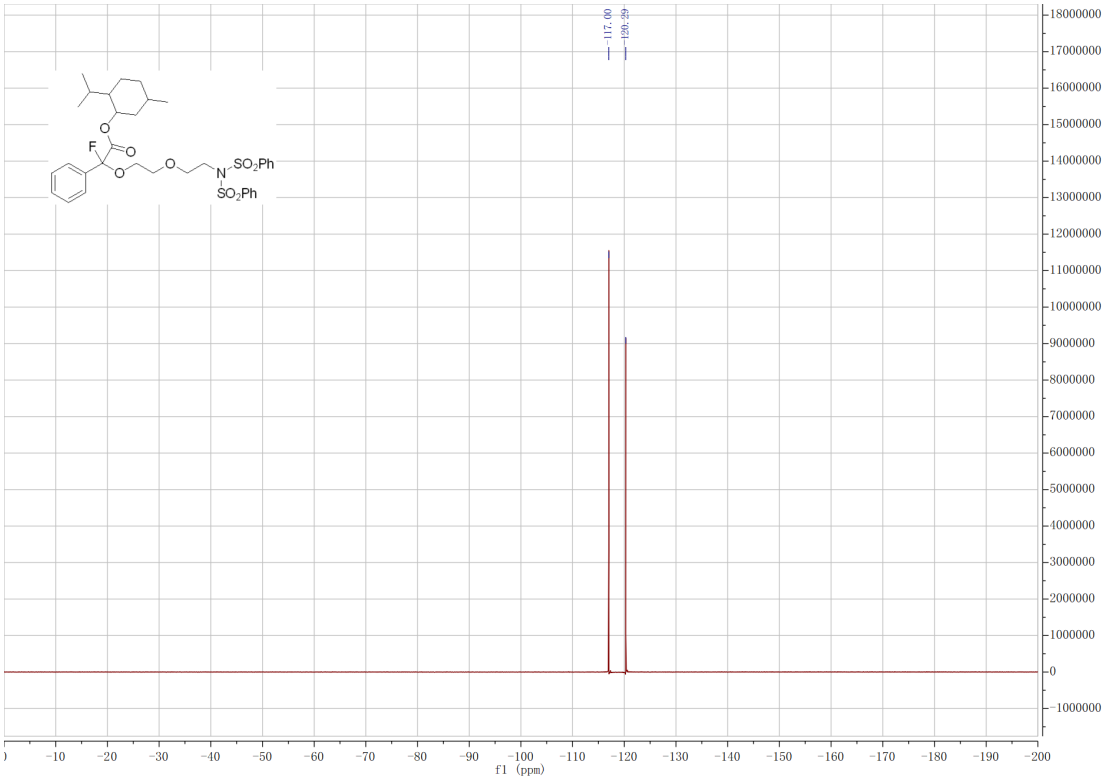
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

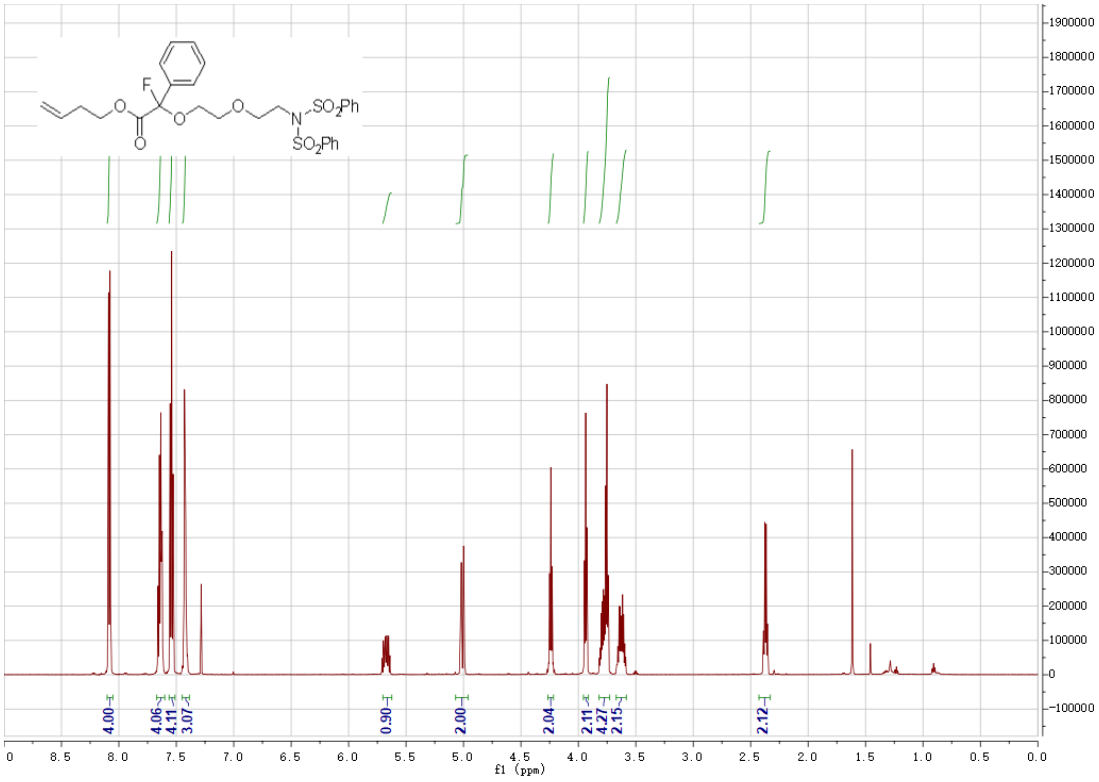


^{19}F NMR (565 MHz, Chloroform-*d*)

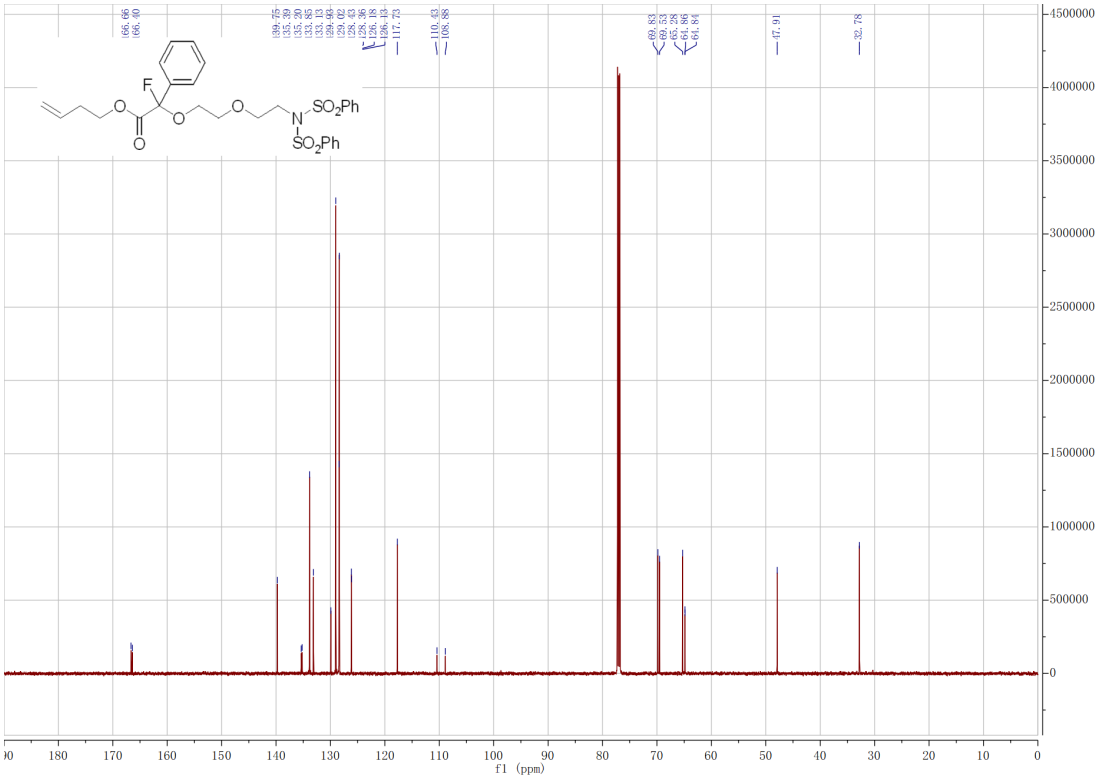


but-3-en-1-yl 2-fluoro-2-phenyl-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido)ethoxy) ethoxy)acetate (5g)

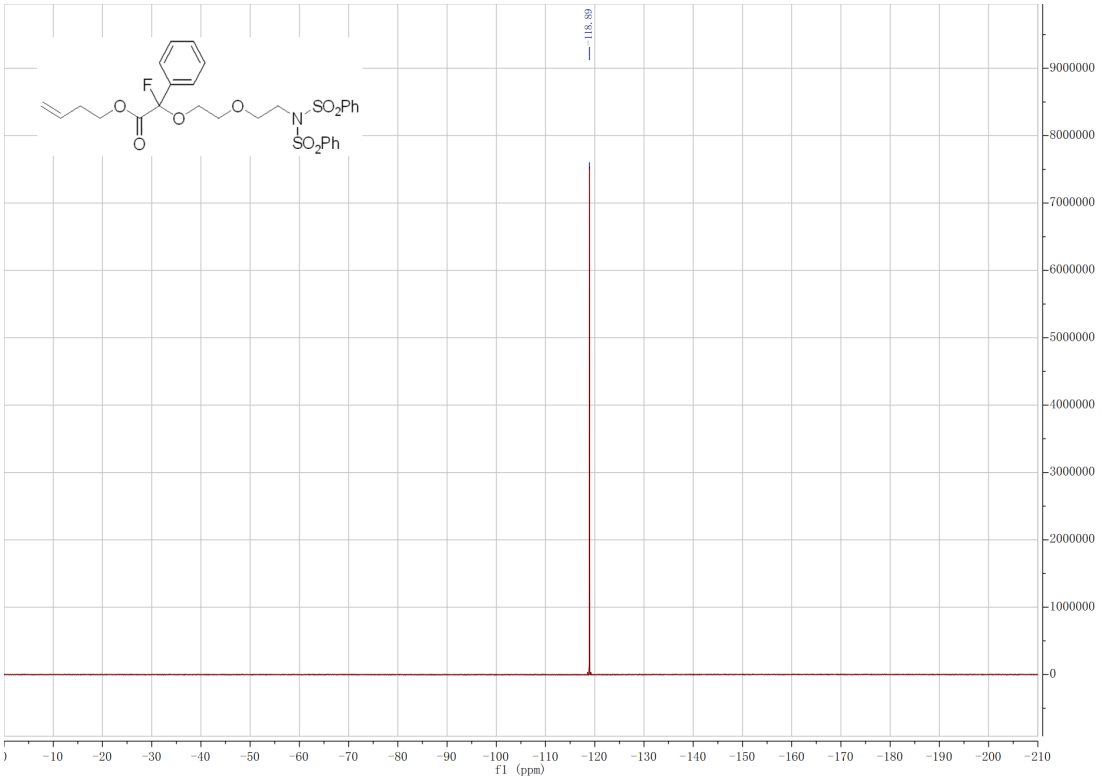
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

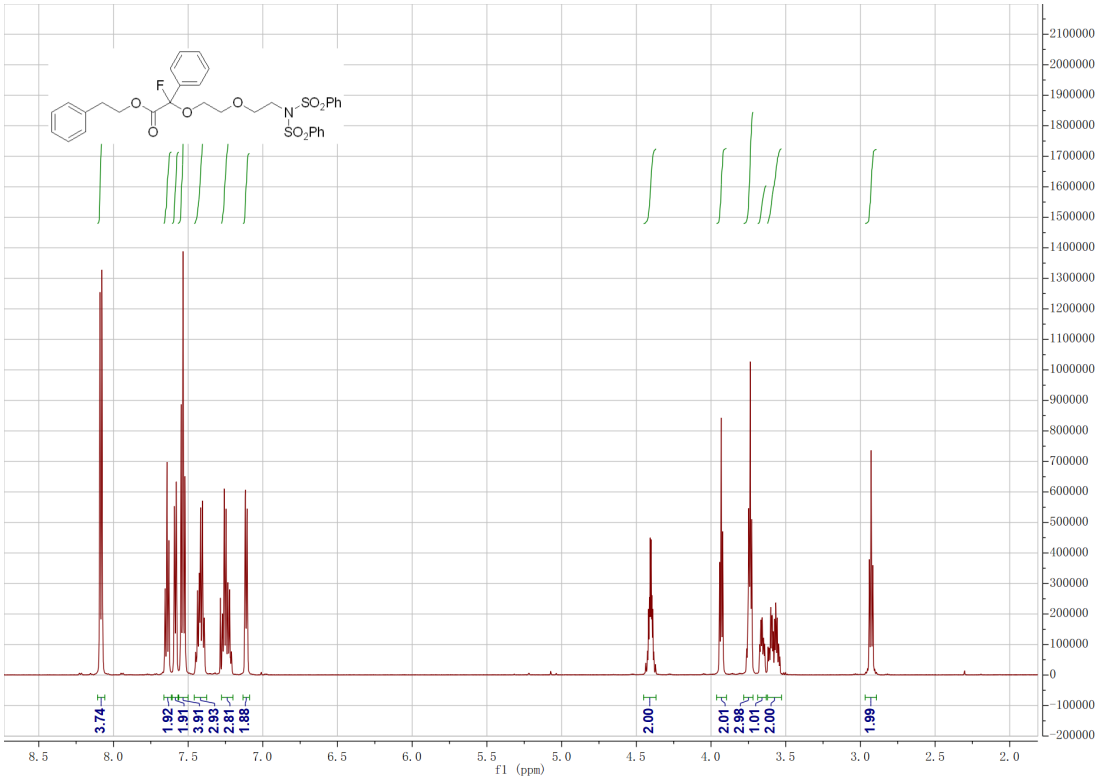


^{19}F NMR (565 MHz, Chloroform-*d*)

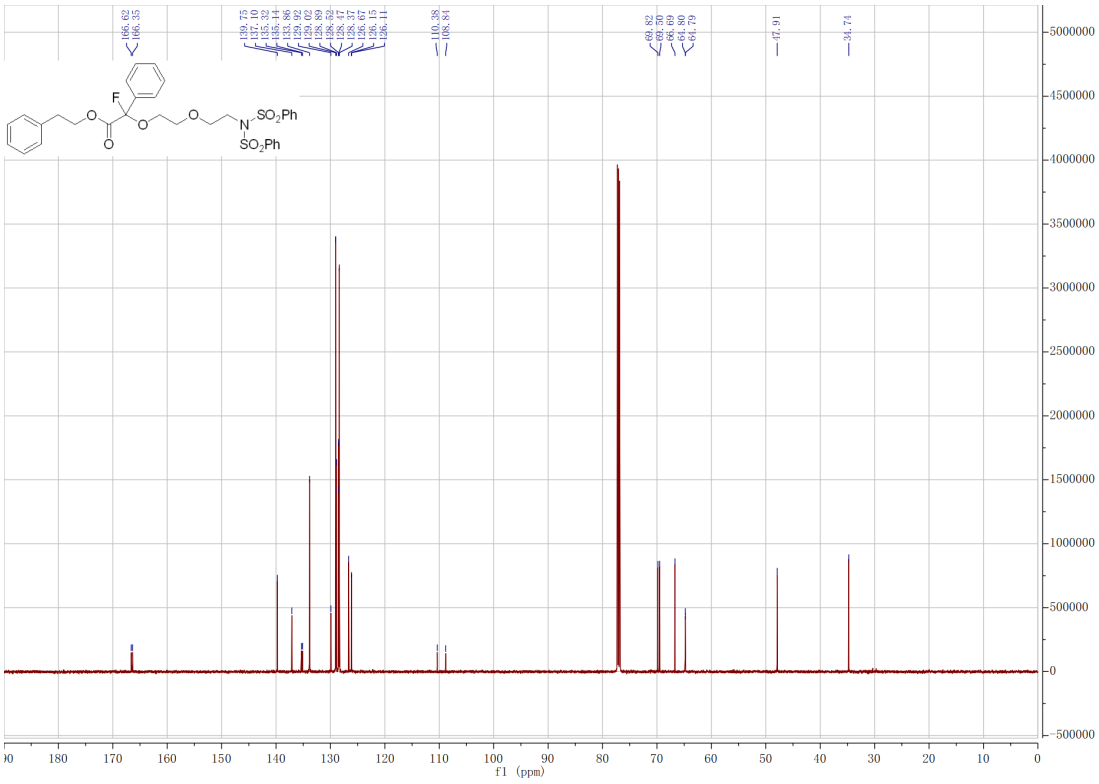


phenethyl 2-fluoro-2-phenyl-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido)ethoxy) ethoxy)acetate (5h)

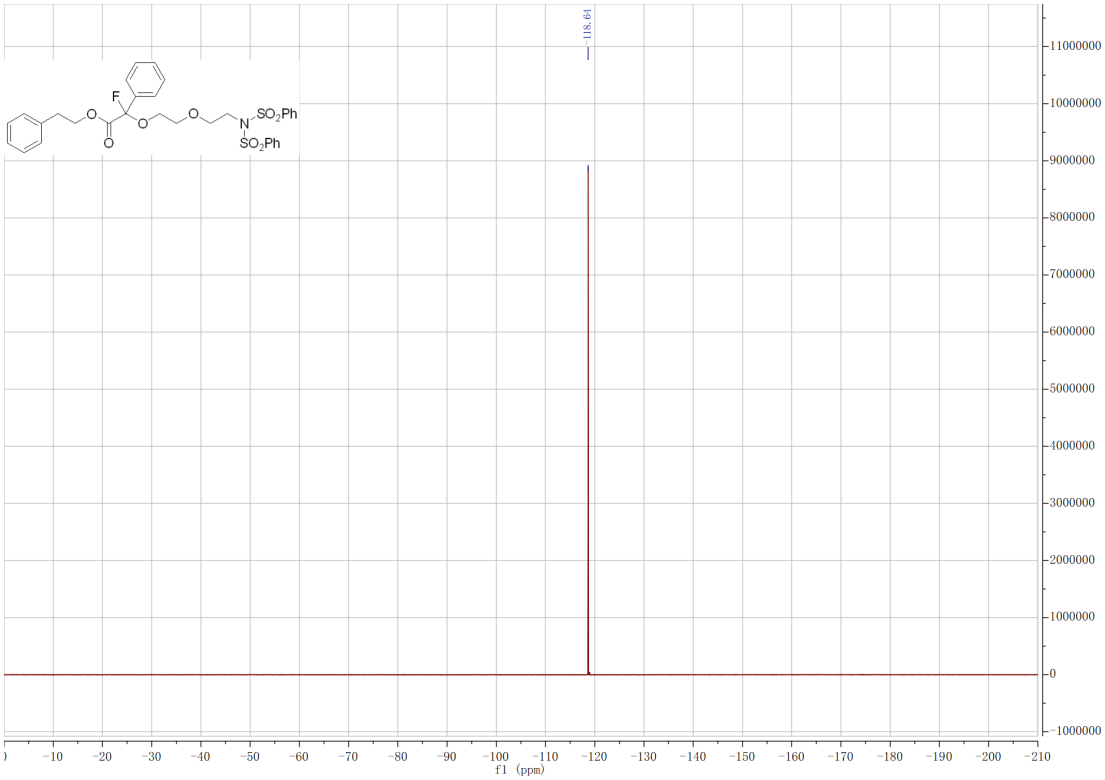
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

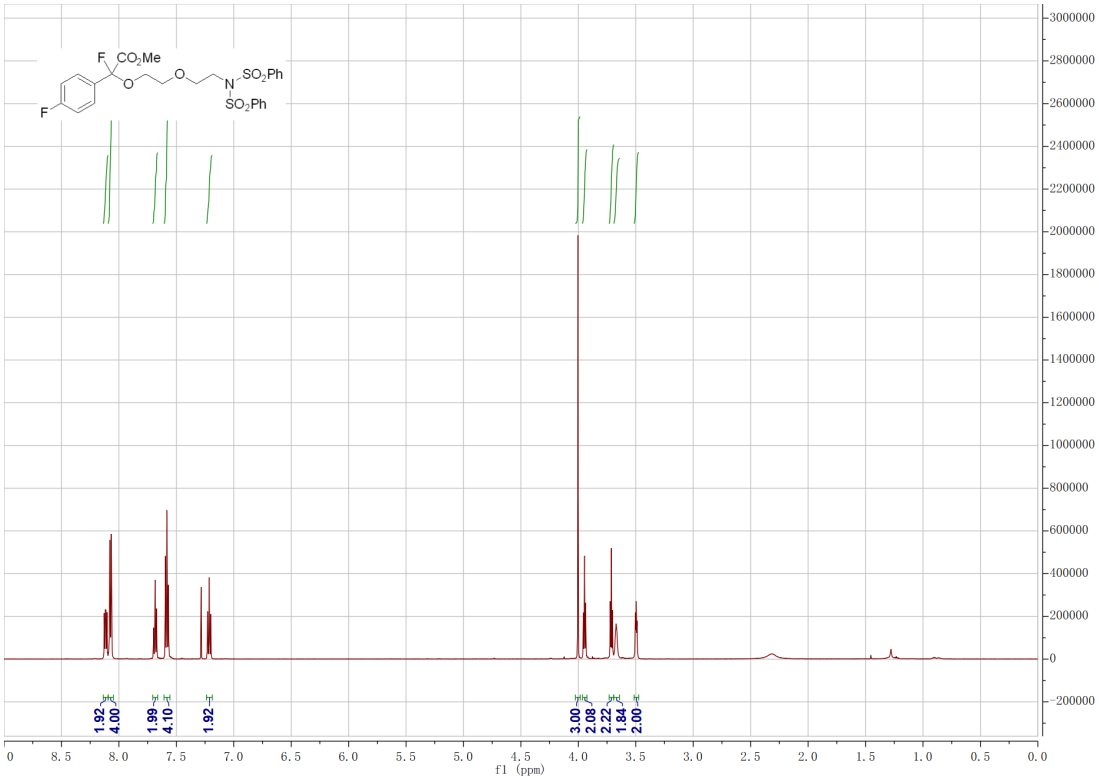


^{19}F NMR (565 MHz, Chloroform-*d*)

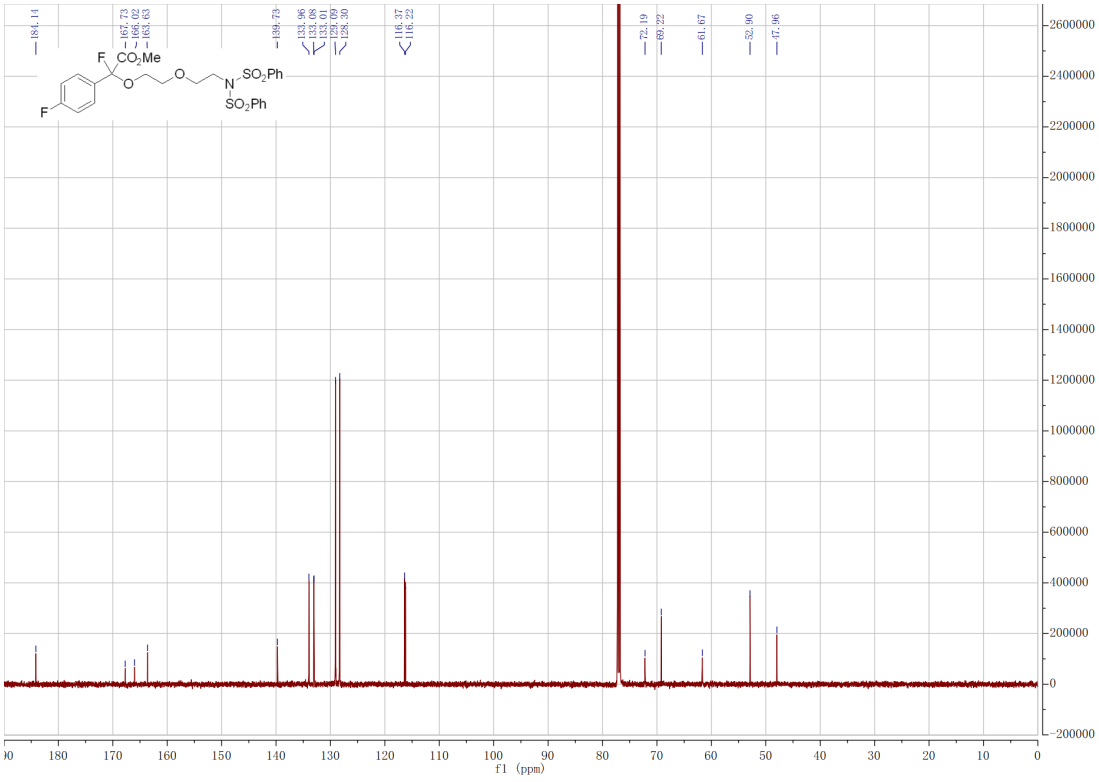


methyl 2-fluoro-2-(4-fluorophenyl)-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido) ethoxy)ethoxy)acetate (5i)

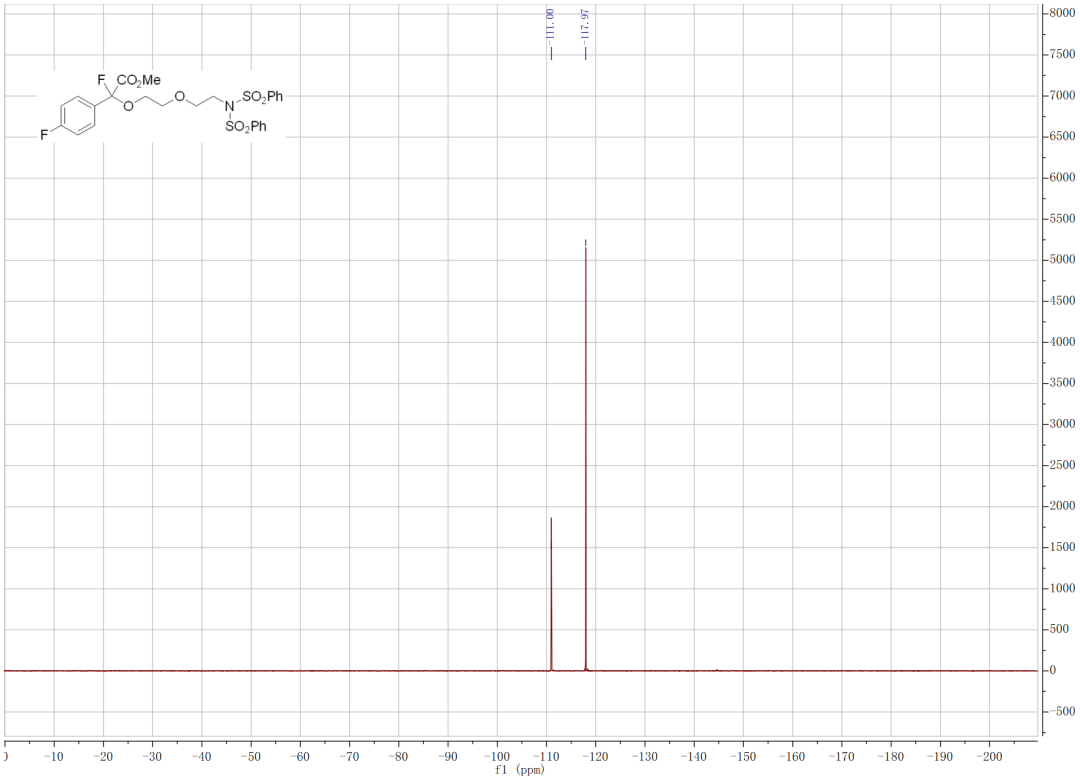
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

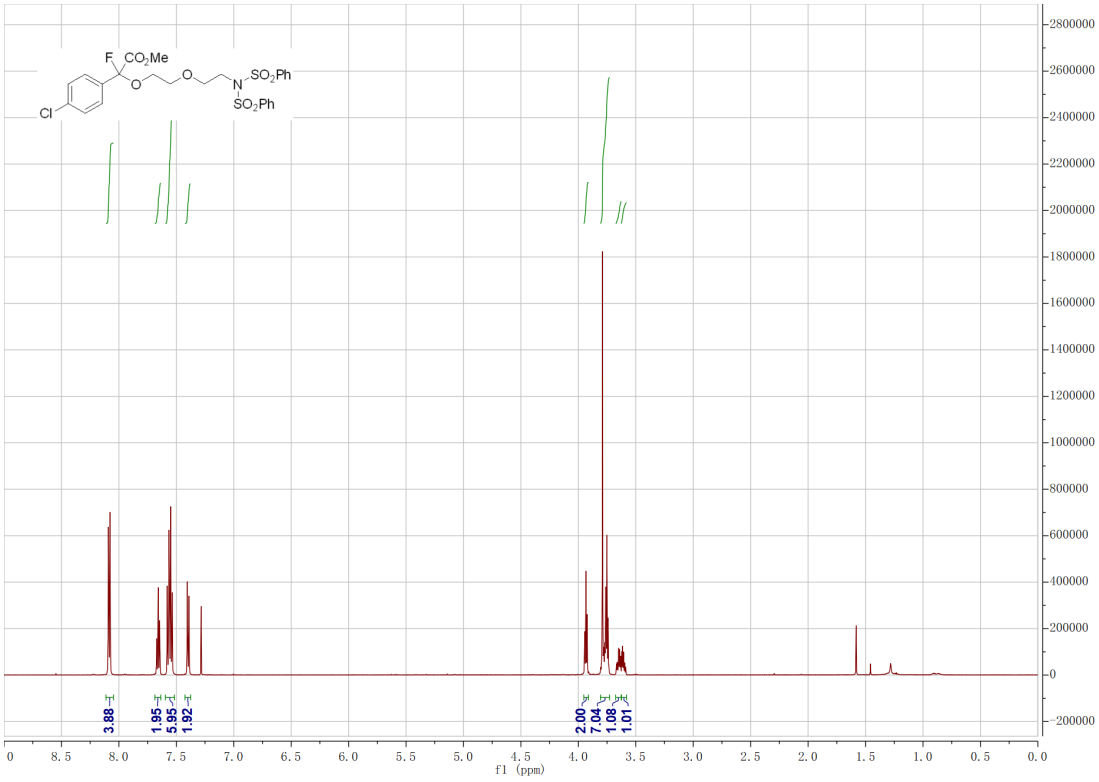


^{19}F NMR (376 MHz, Chloroform-*d*)

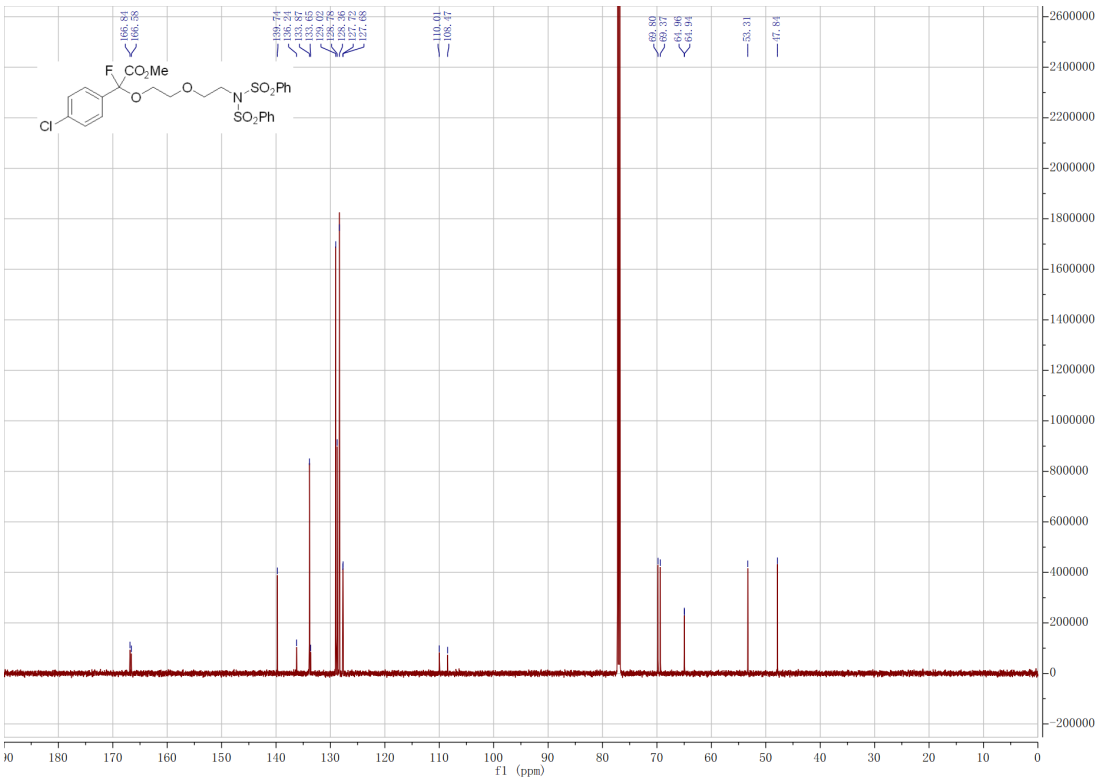


methyl 2-(4-chlorophenyl)-2-fluoro-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido) ethoxy)ethoxy)acetate (5j)

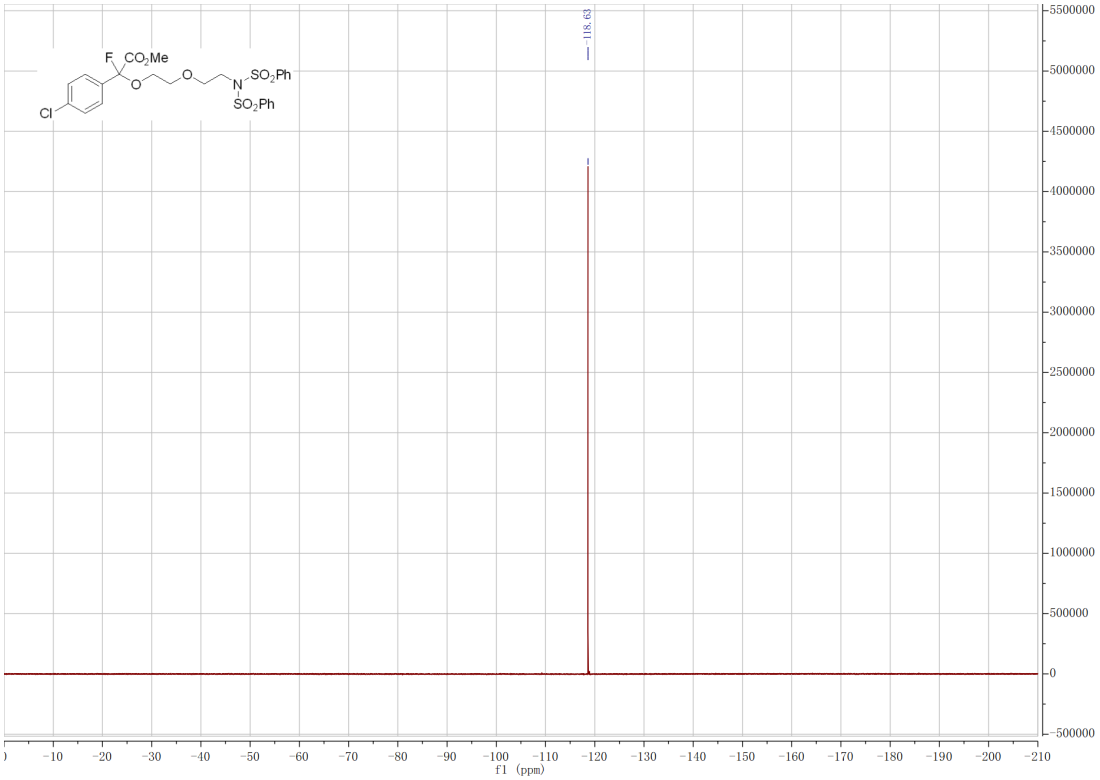
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-*d*)

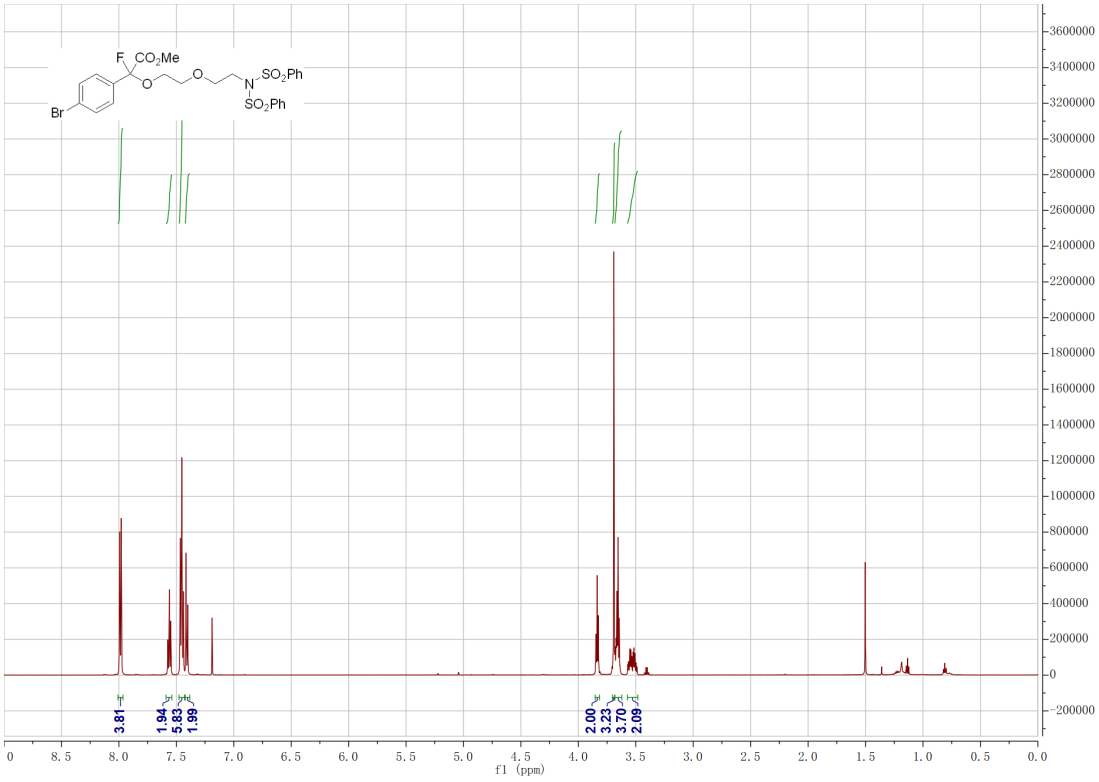


^{19}F NMR (565 MHz, Chloroform-*d*)

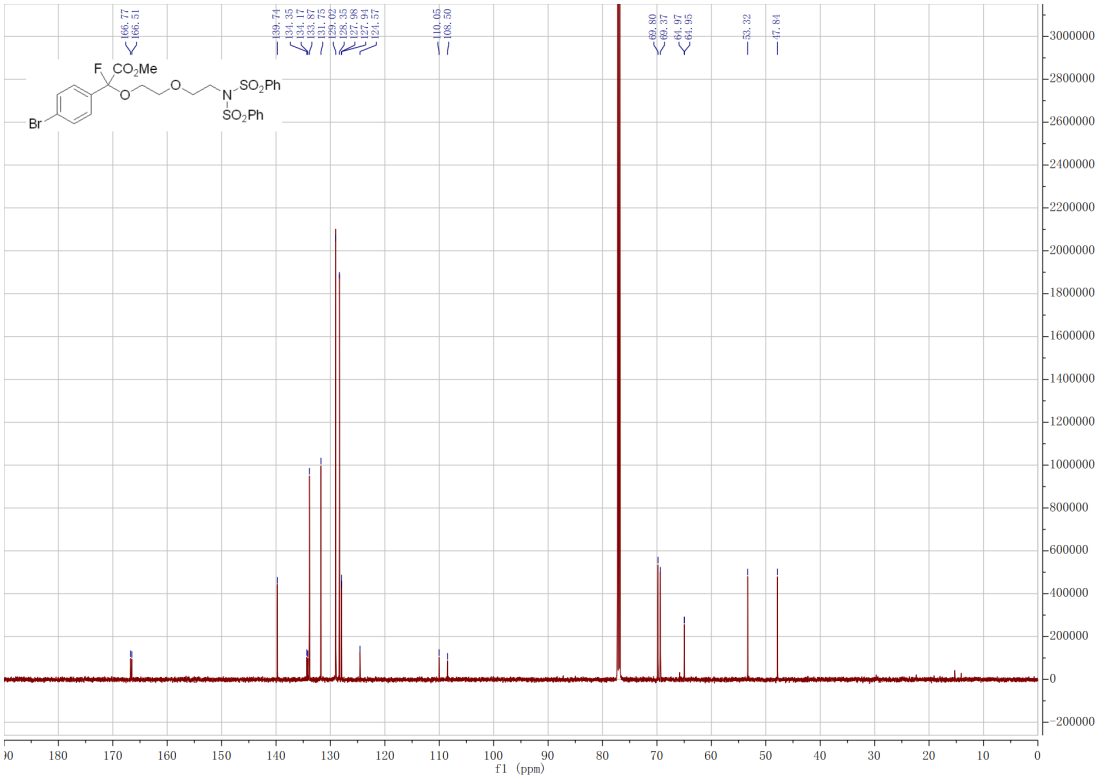


methyl 2-(4-bromophenyl)-2-fluoro-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido) ethoxy)ethoxy)acetate (5k)

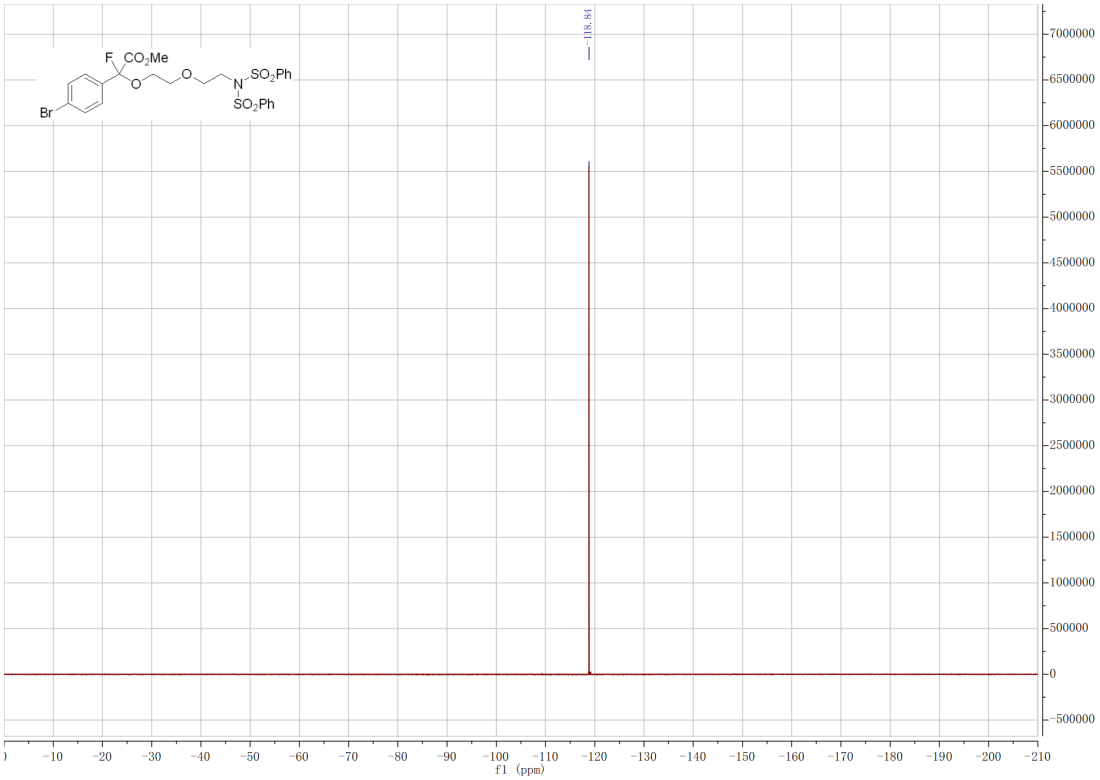
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

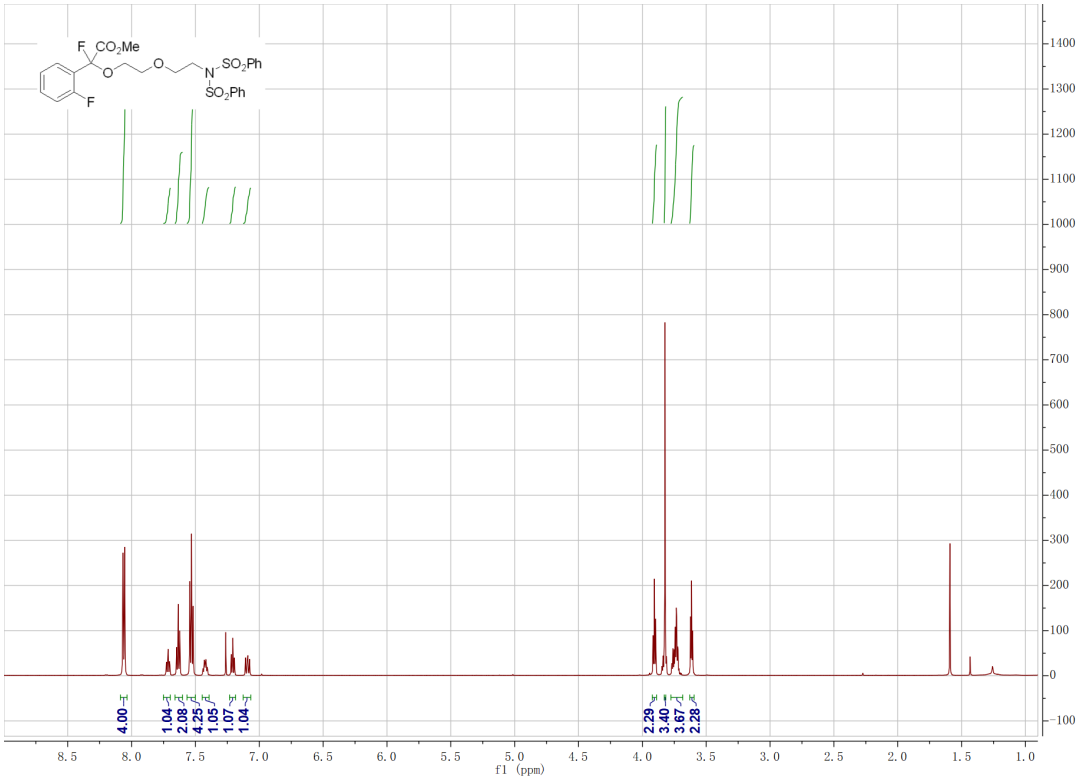


^{19}F NMR (565 MHz, Chloroform-*d*)

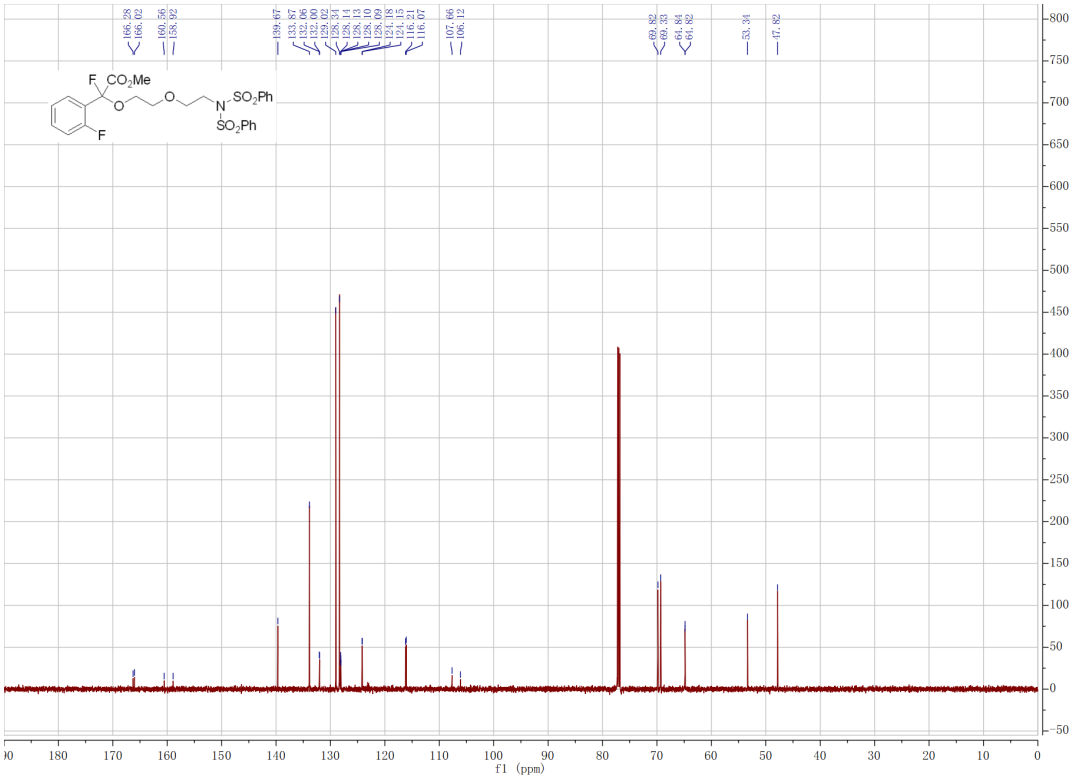


methyl 2-fluoro-2-(2-fluorophenyl)-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido) ethoxy)ethoxy)acetate (5l)

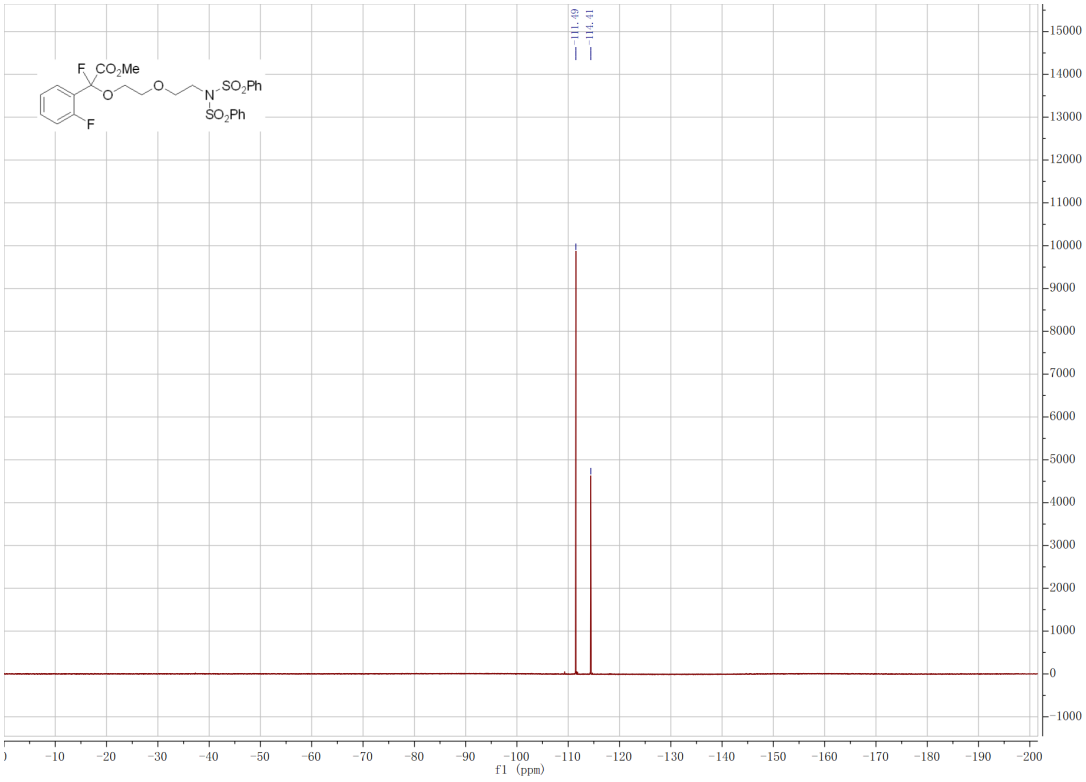
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

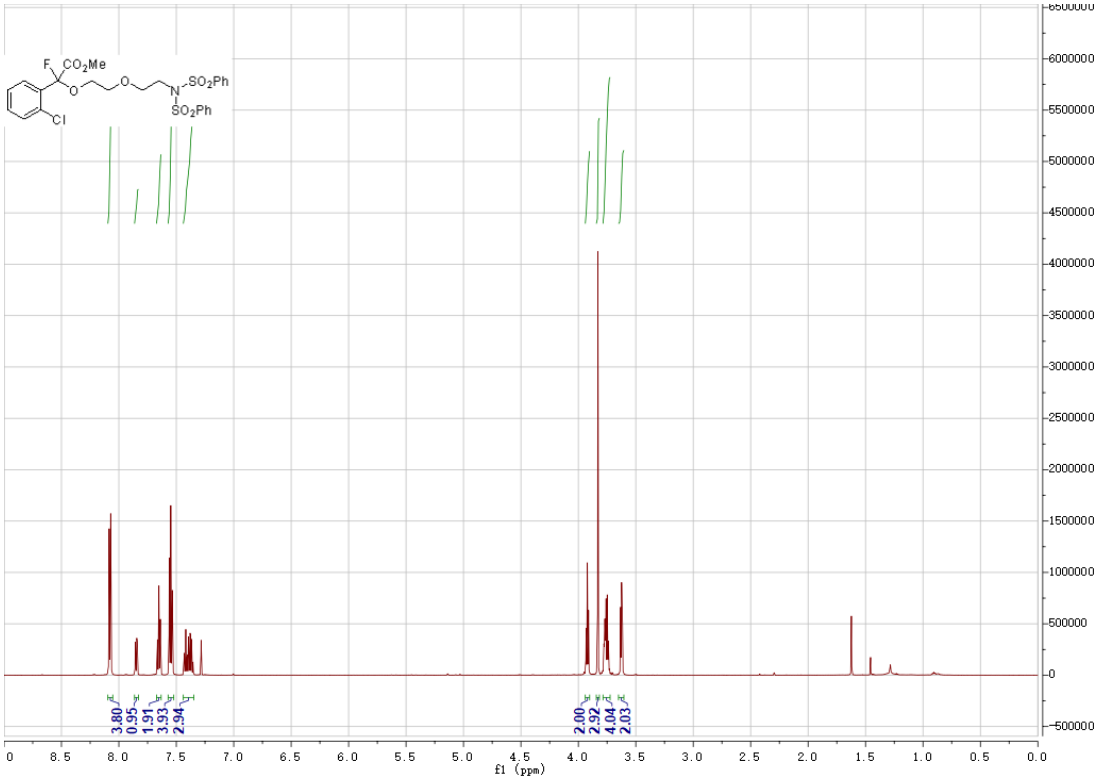


^{19}F NMR (565 MHz, Chloroform-*d*)

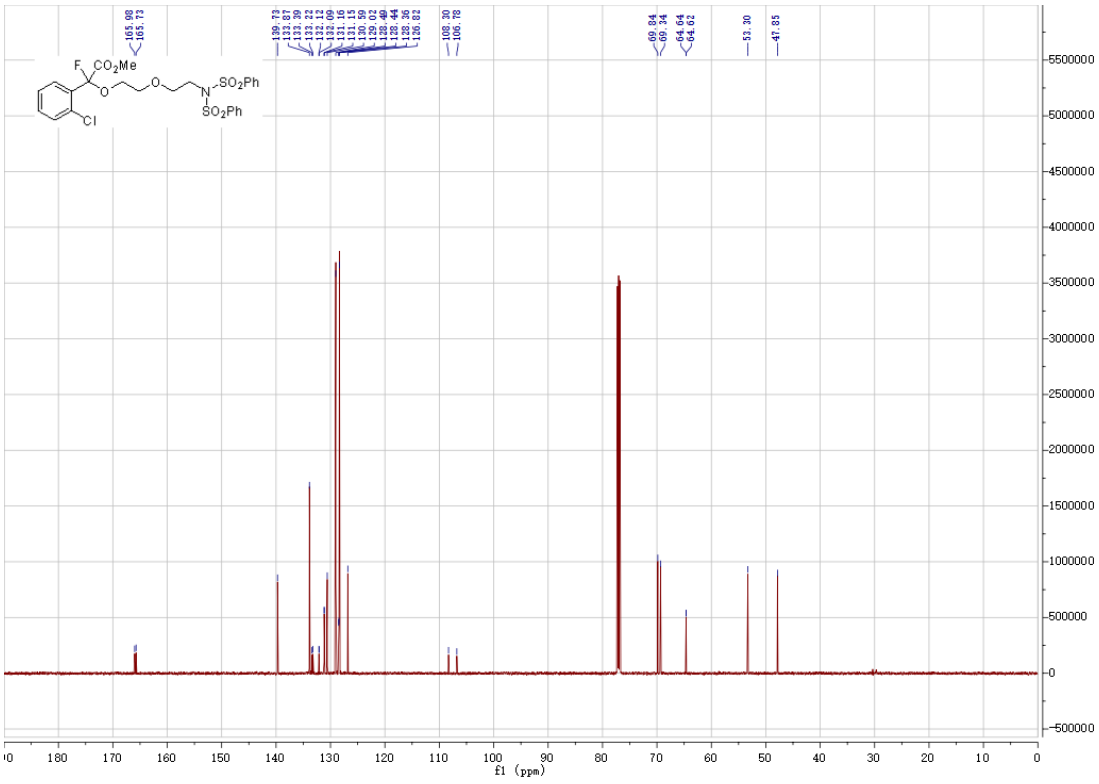


methyl 2-(2-chlorophenyl)-2-fluoro-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido) ethoxy)ethoxy)acetate (5m)

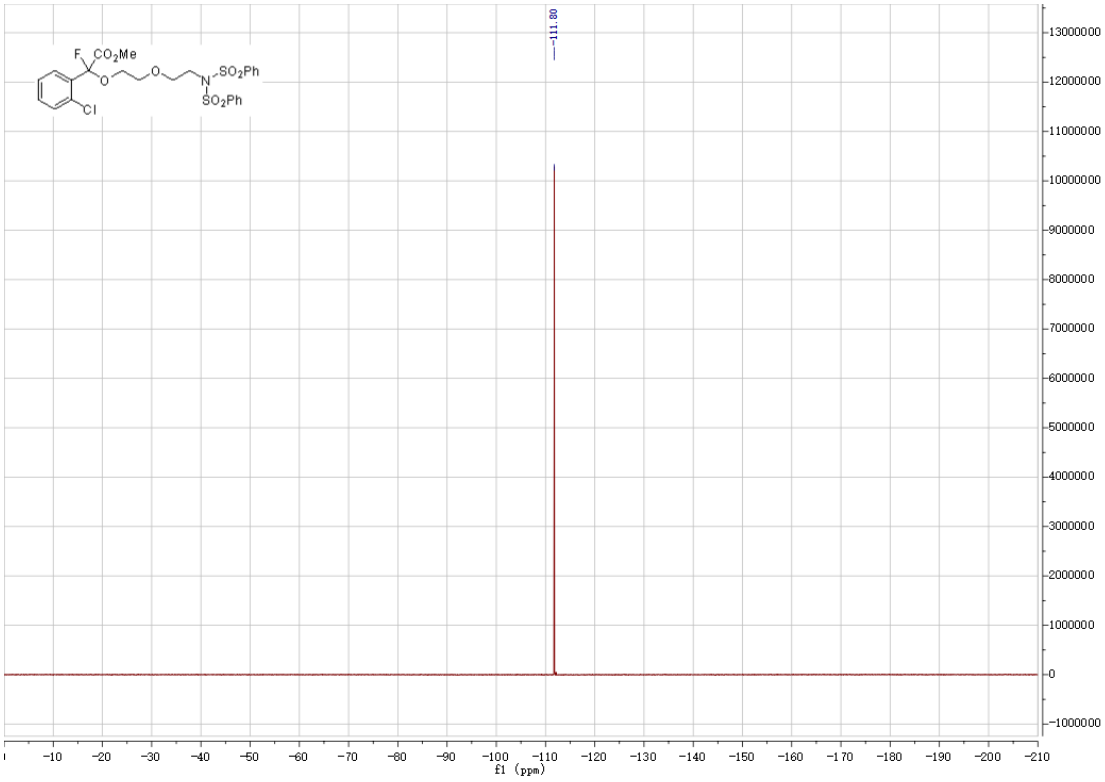
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

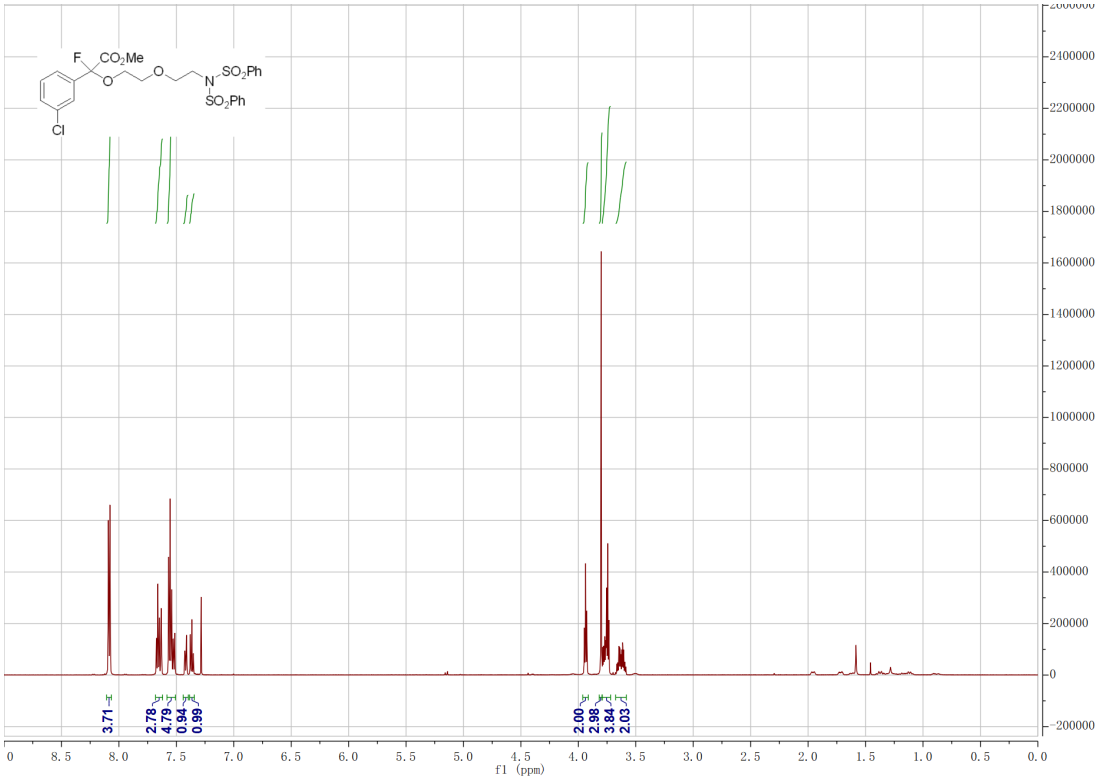


^{19}F NMR (565 MHz, Chloroform-*d*)

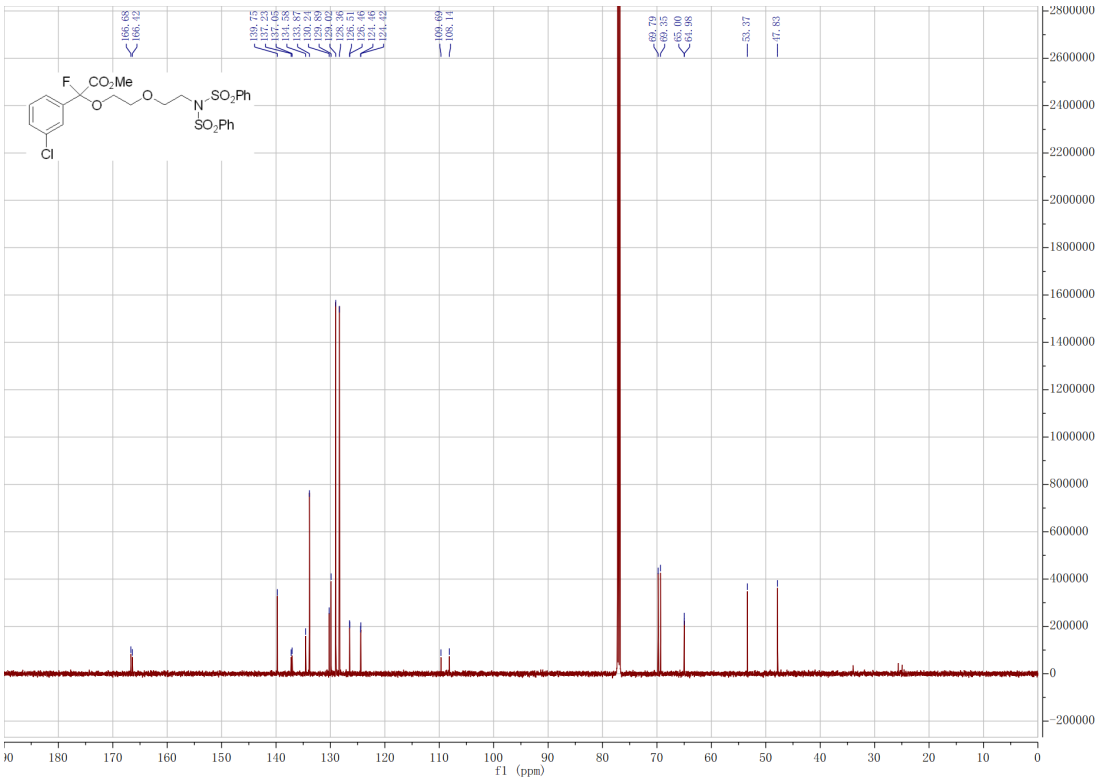


methyl 2-(3-chlorophenyl)-2-fluoro-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido) ethoxy)ethoxy)acetate (5n)

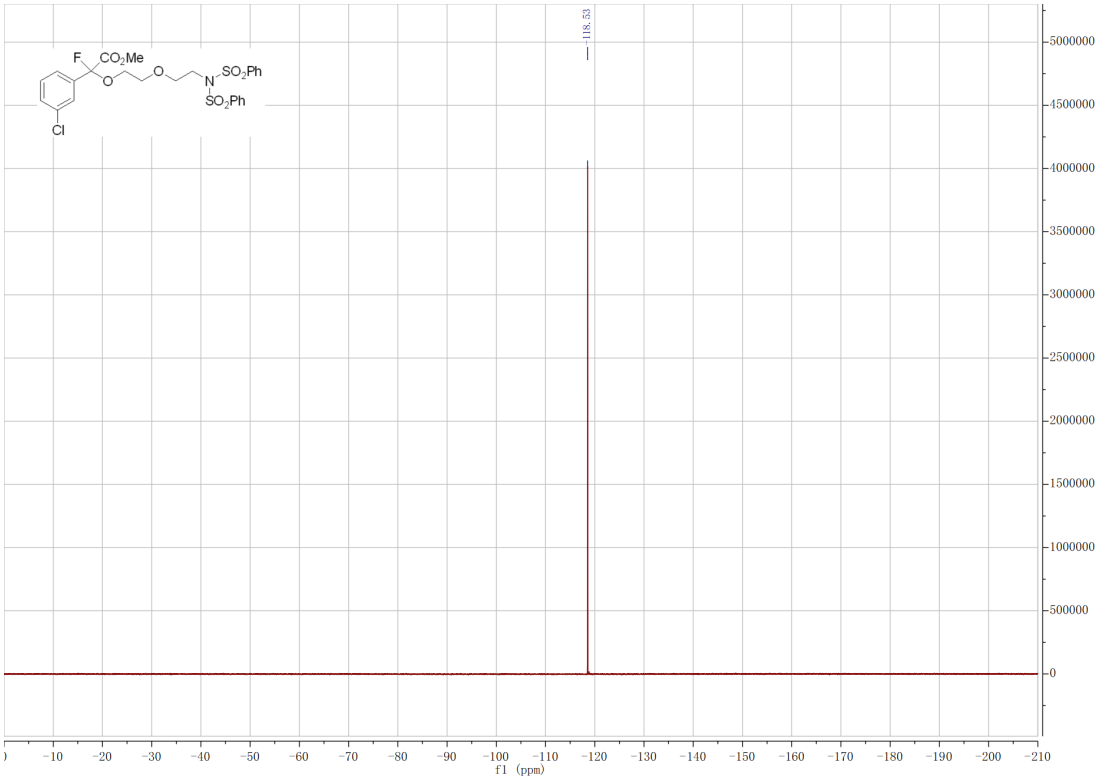
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

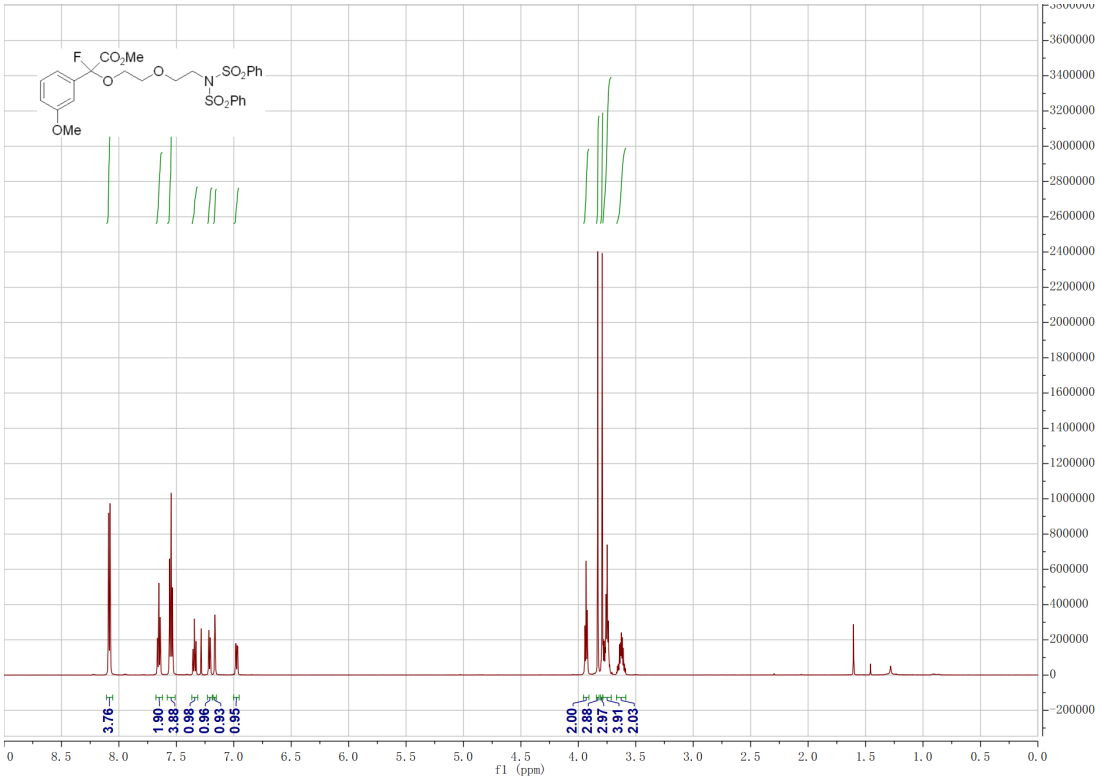


^{19}F NMR (565 MHz, Chloroform-*d*)

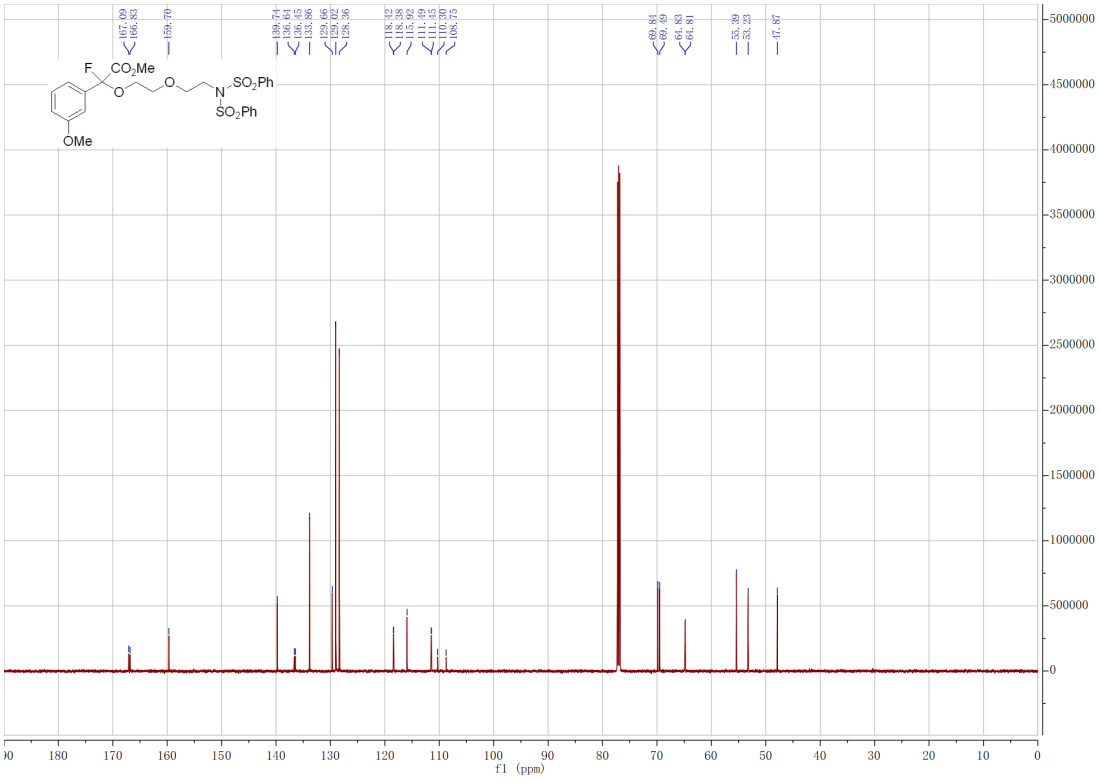


methyl 2-fluoro-2-(3-methoxyphenyl)-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido) ethoxy)ethoxy)acetate (5o)

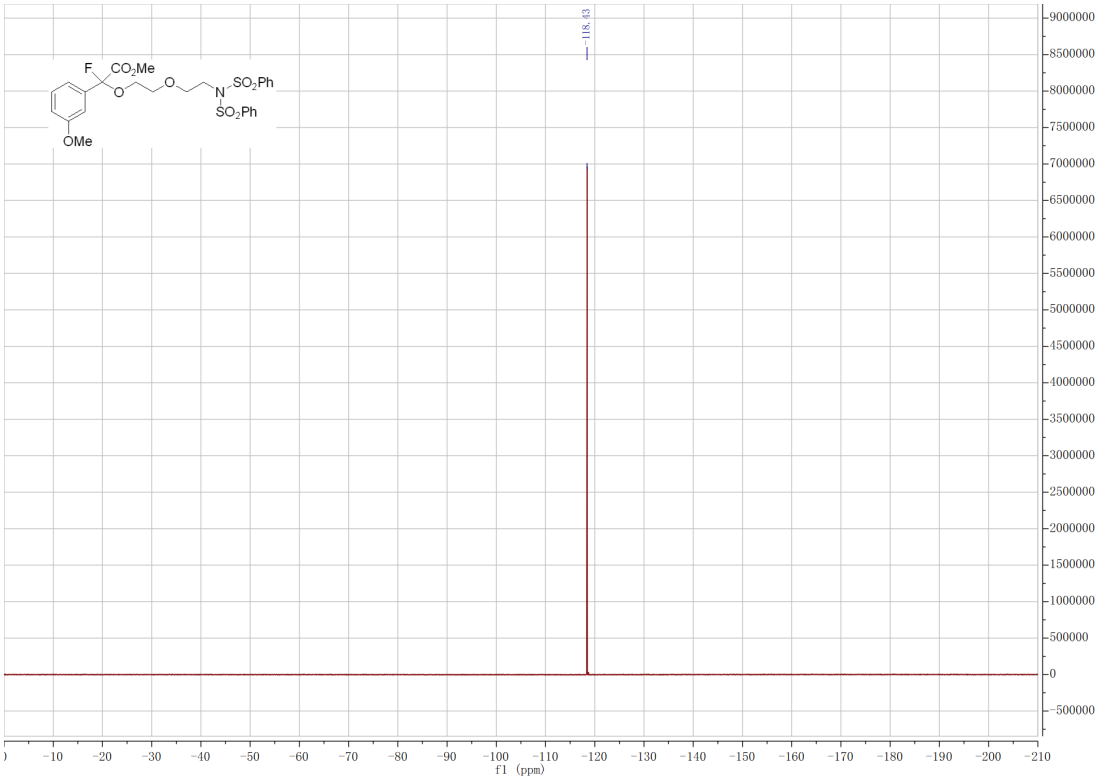
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

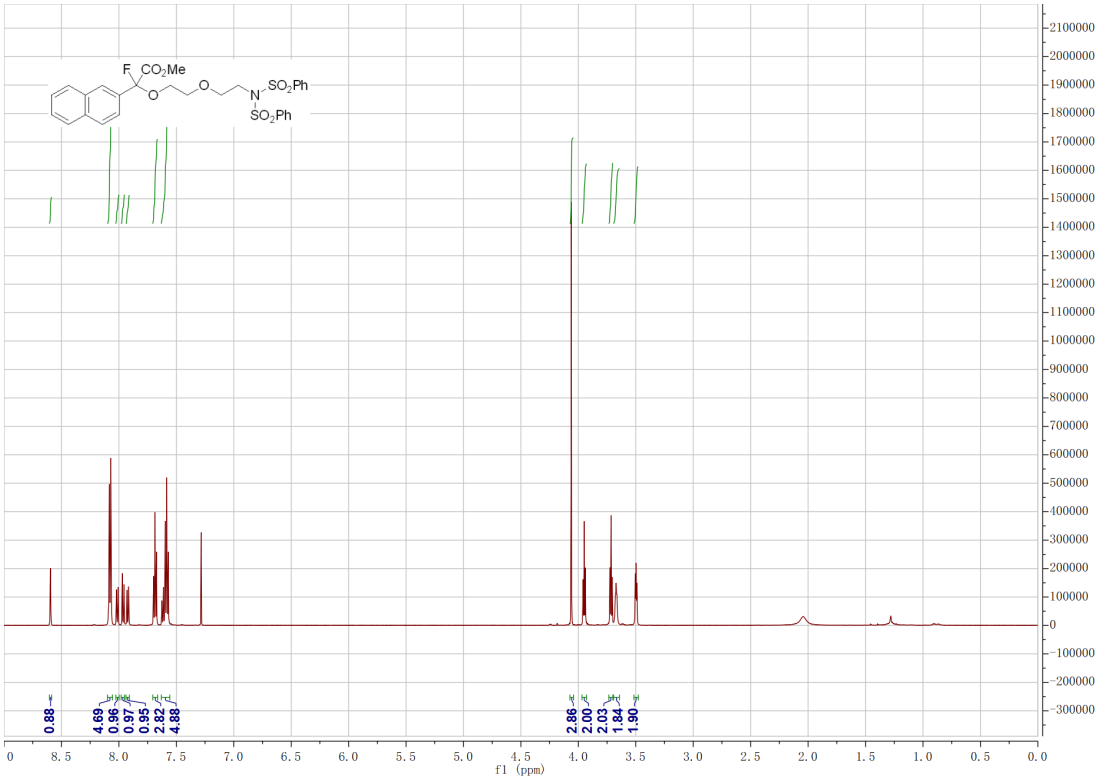


^{19}F NMR (565 MHz, Chloroform-*d*)

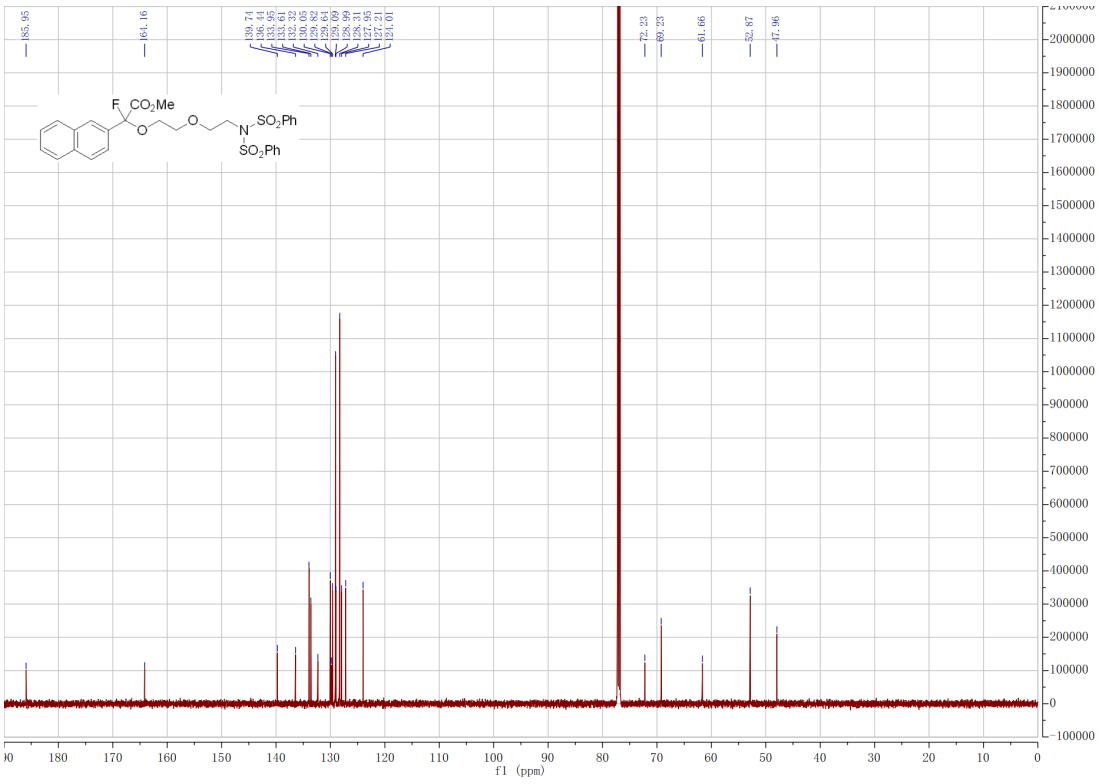


methyl 2-fluoro-2-(naphthalen-2-yl)-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido) ethoxy)ethoxy)acetate (5p)

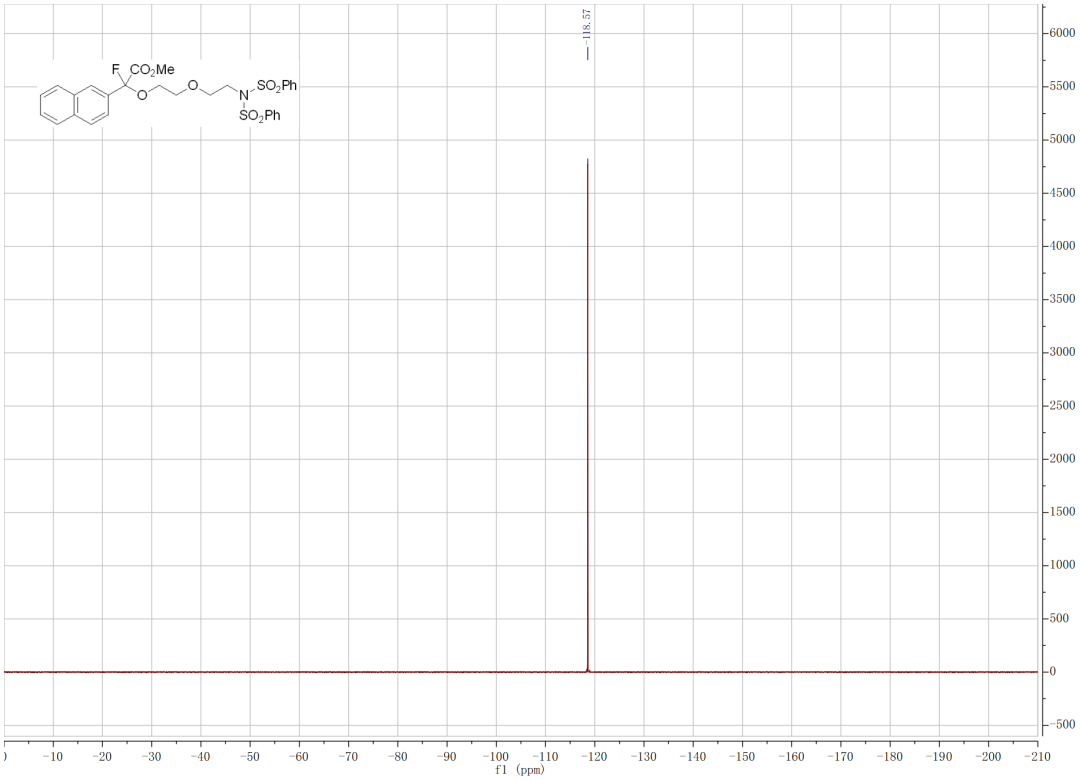
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

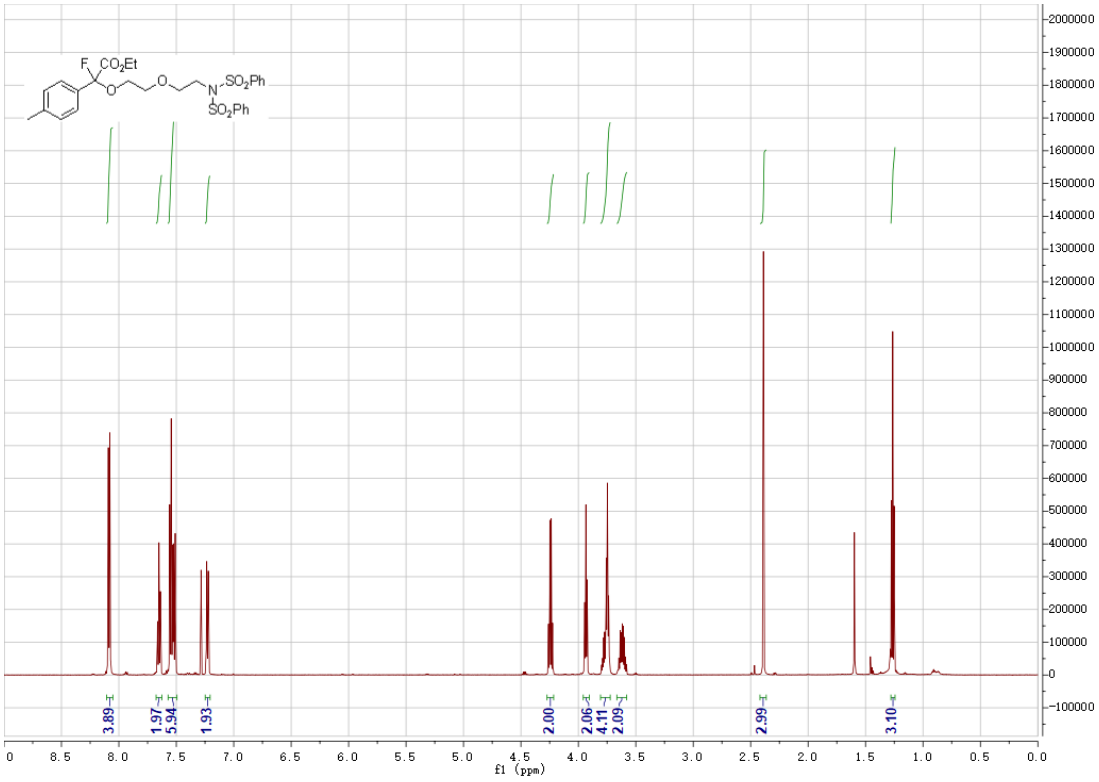


^{19}F NMR (565 MHz, Chloroform-*d*)

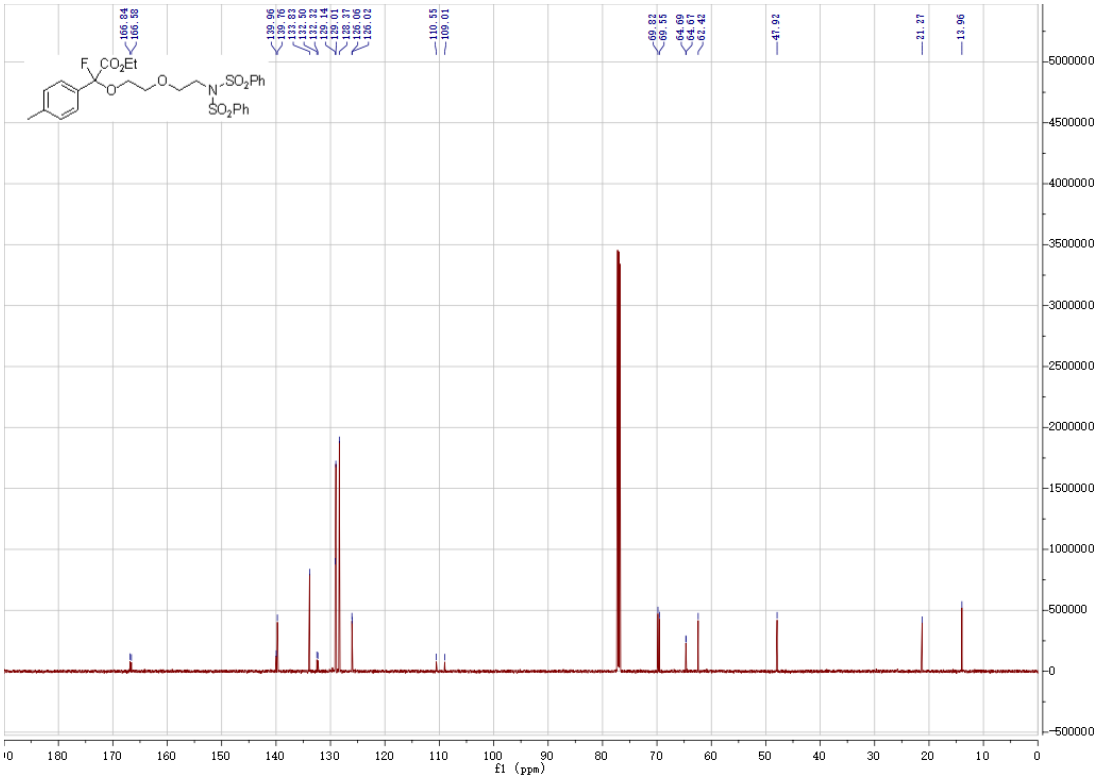


ethyl 2-fluoro-2-(2-(2-(N-(phenylsulfonyl)phenylsulfonamido)ethoxy)ethoxy)-2-(p-tolyl) acetate (5q)

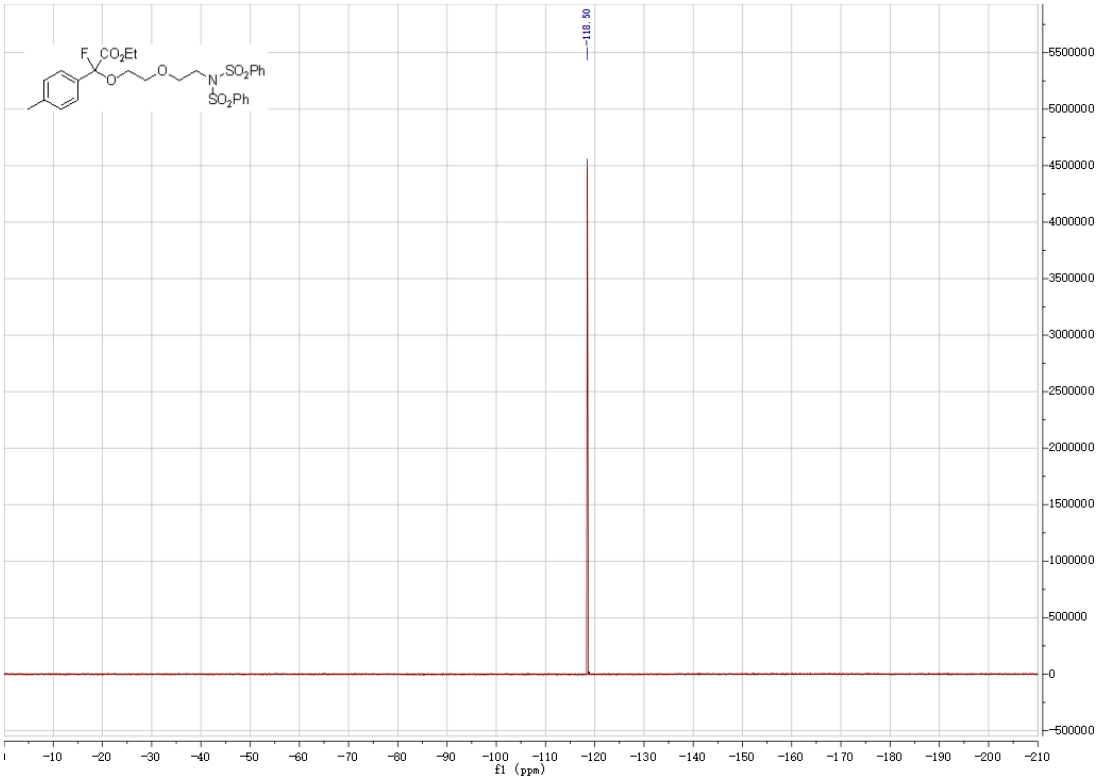
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

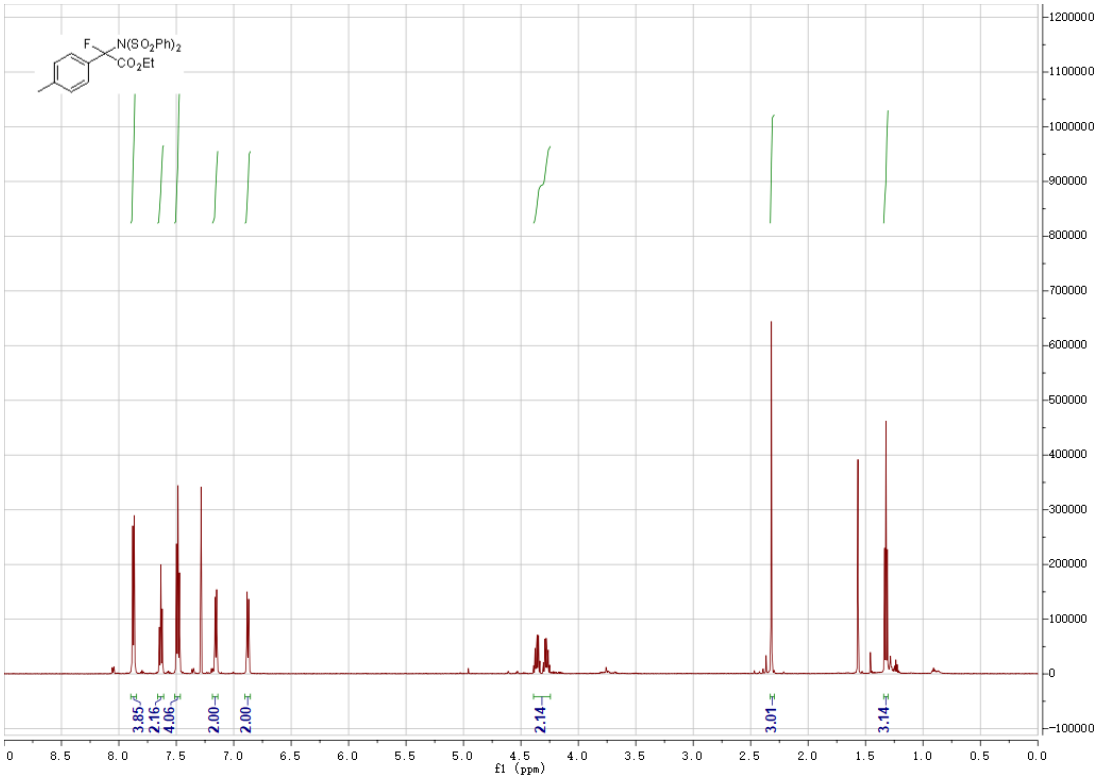


^{19}F NMR (565 MHz, Chloroform-*d*)

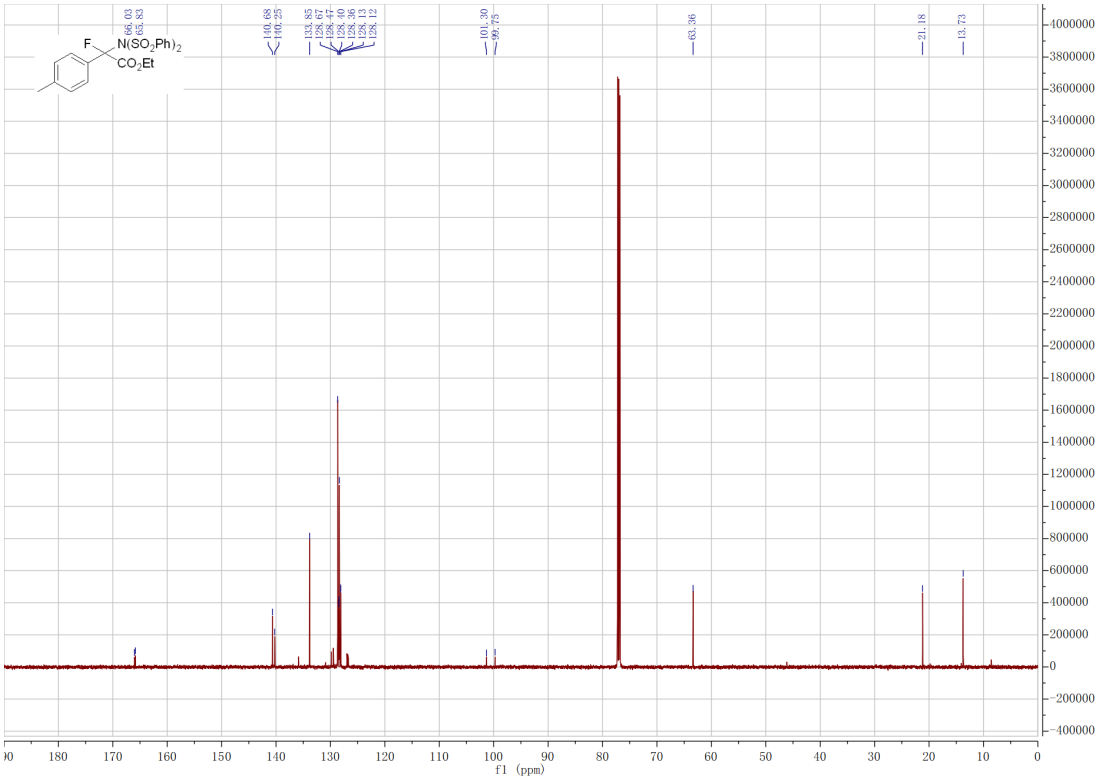


ethyl 2-fluoro-2-(N-(phenylsulfonyl)phenylsulfonamido)-2-(p-tolyl)acetate (10a)

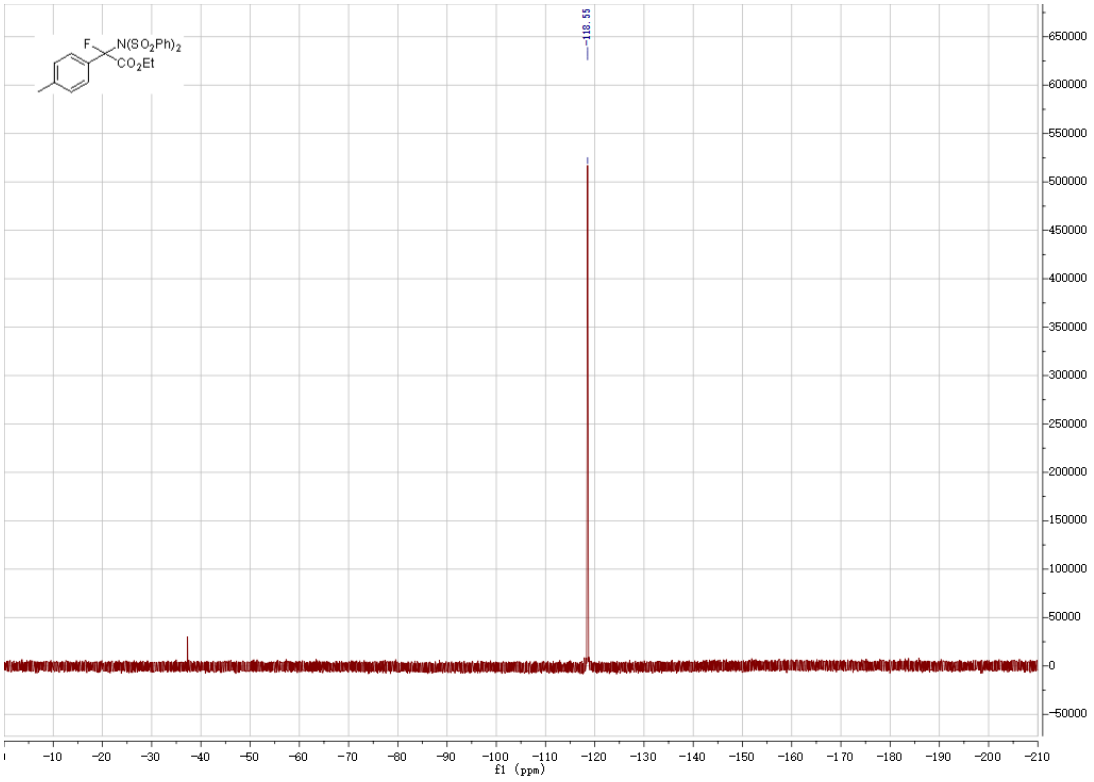
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

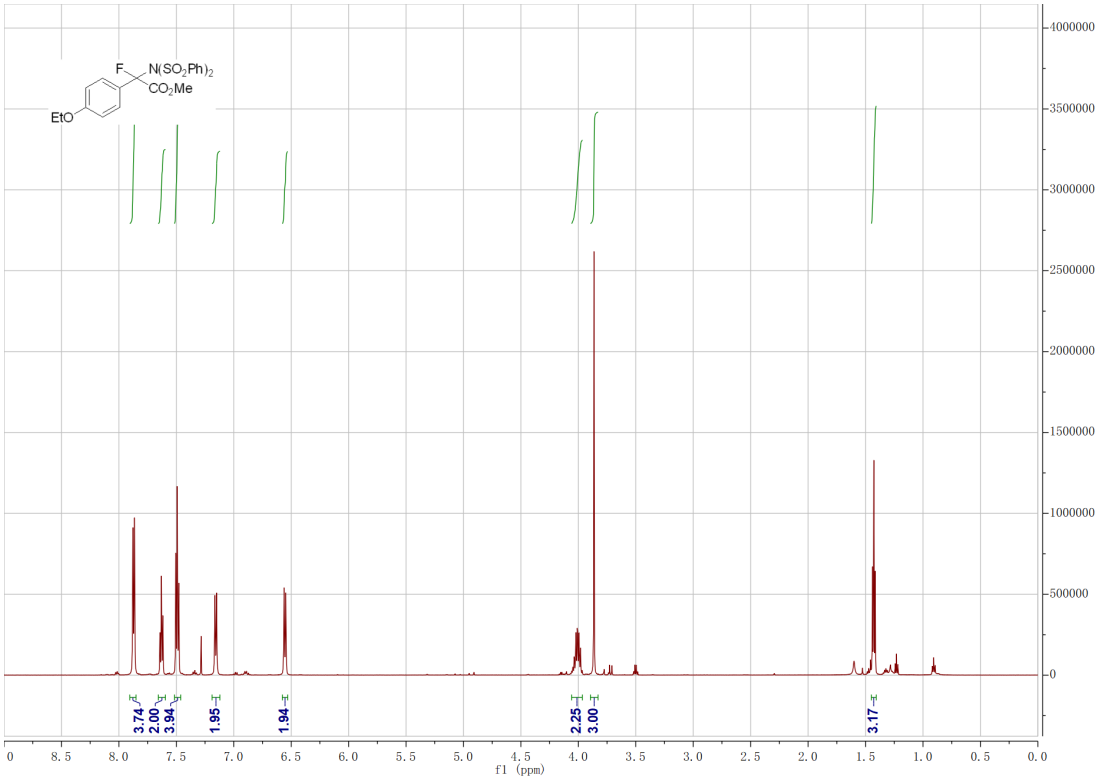


^{19}F NMR (565 MHz, Chloroform-*d*)

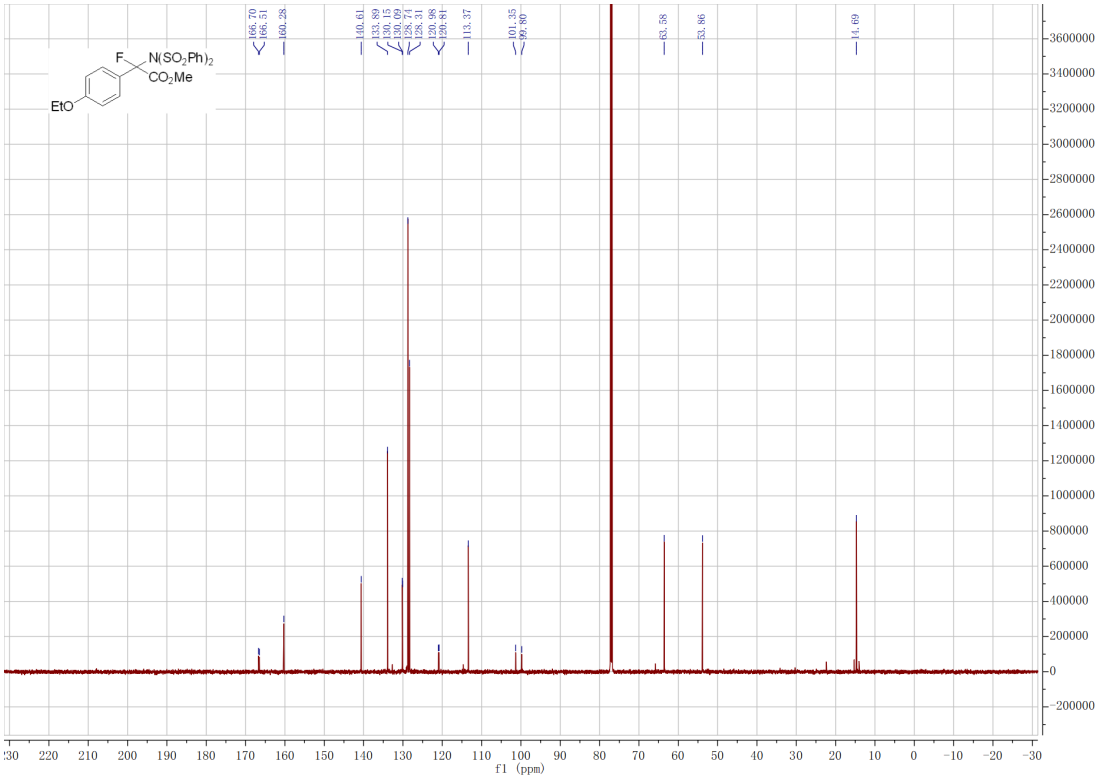


methyl 2-(4-ethoxyphenyl)-2-fluoro-2-(N-(phenylsulfonyl)phenylsulfonamido)acetate (10b)

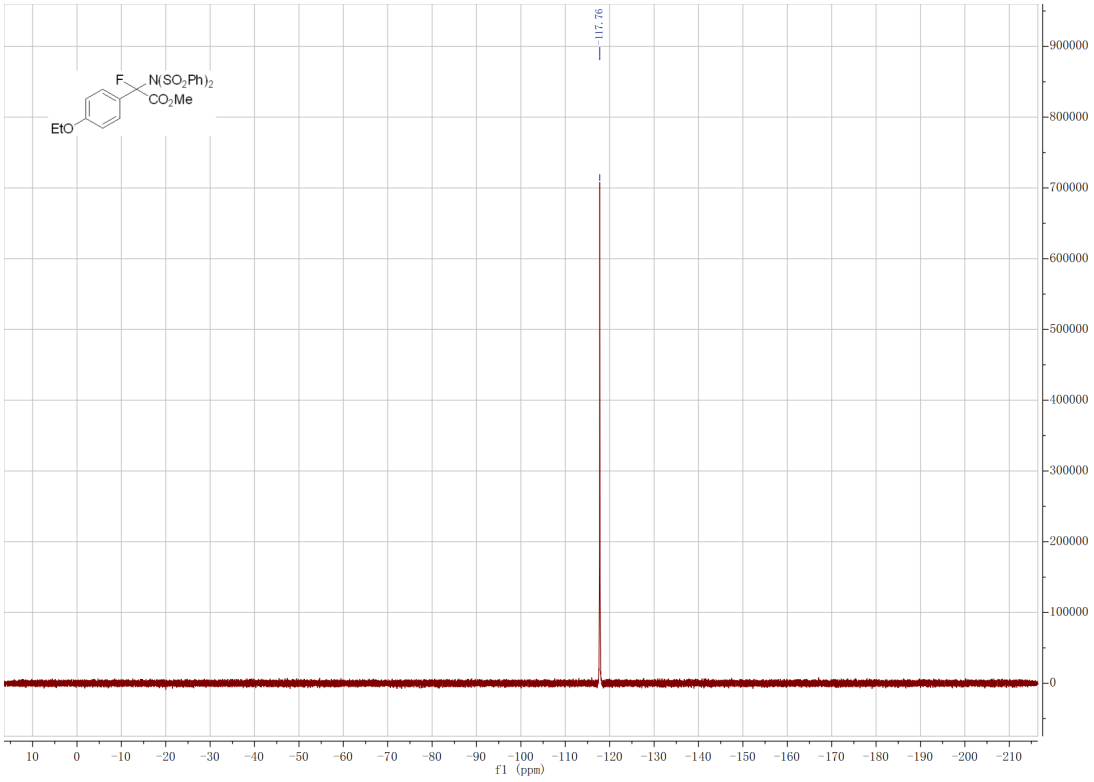
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

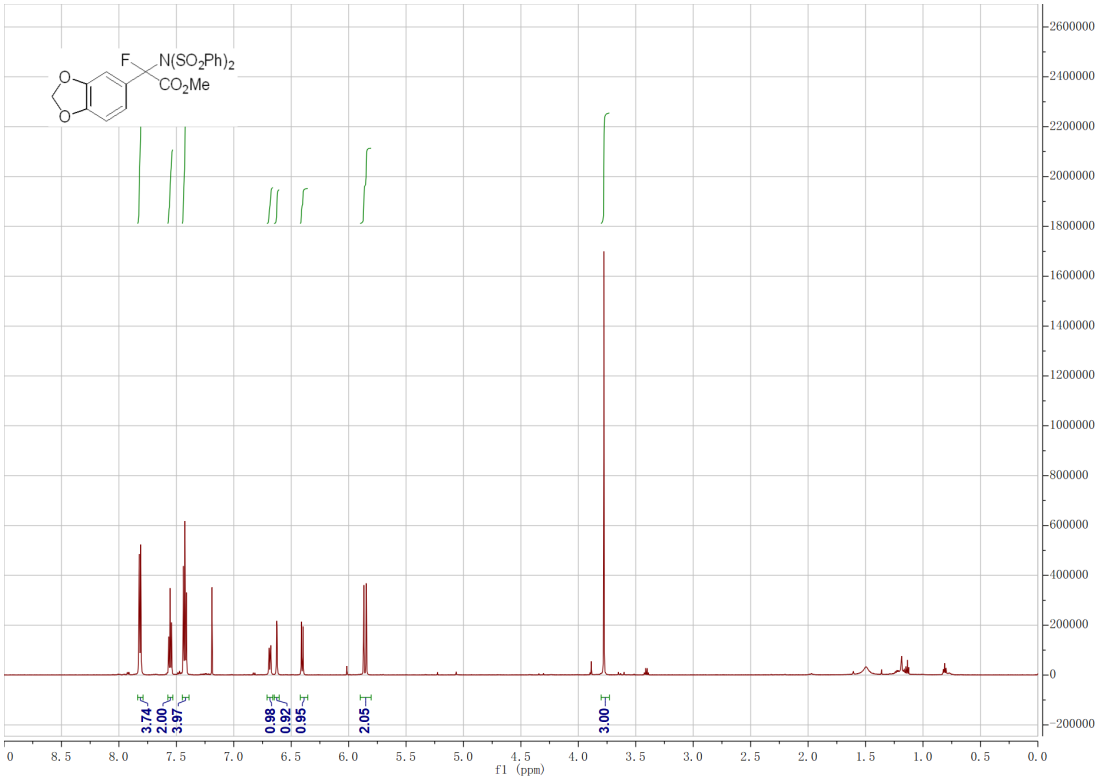


^{19}F NMR (565 MHz, Chloroform-*d*)

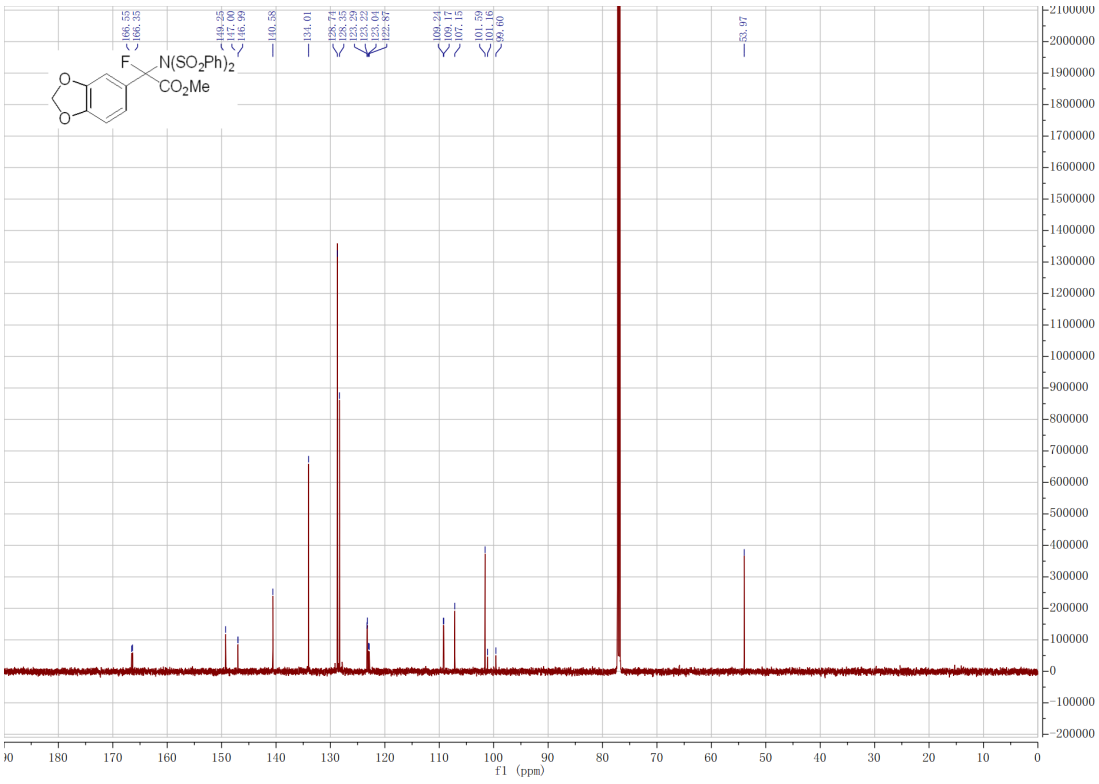


methyl 2-(benzo[d][1,3]dioxol-5-yl)-2-fluoro-2-(N-(phenylsulfonyl)phenylsulfonamido) acetate (10c)

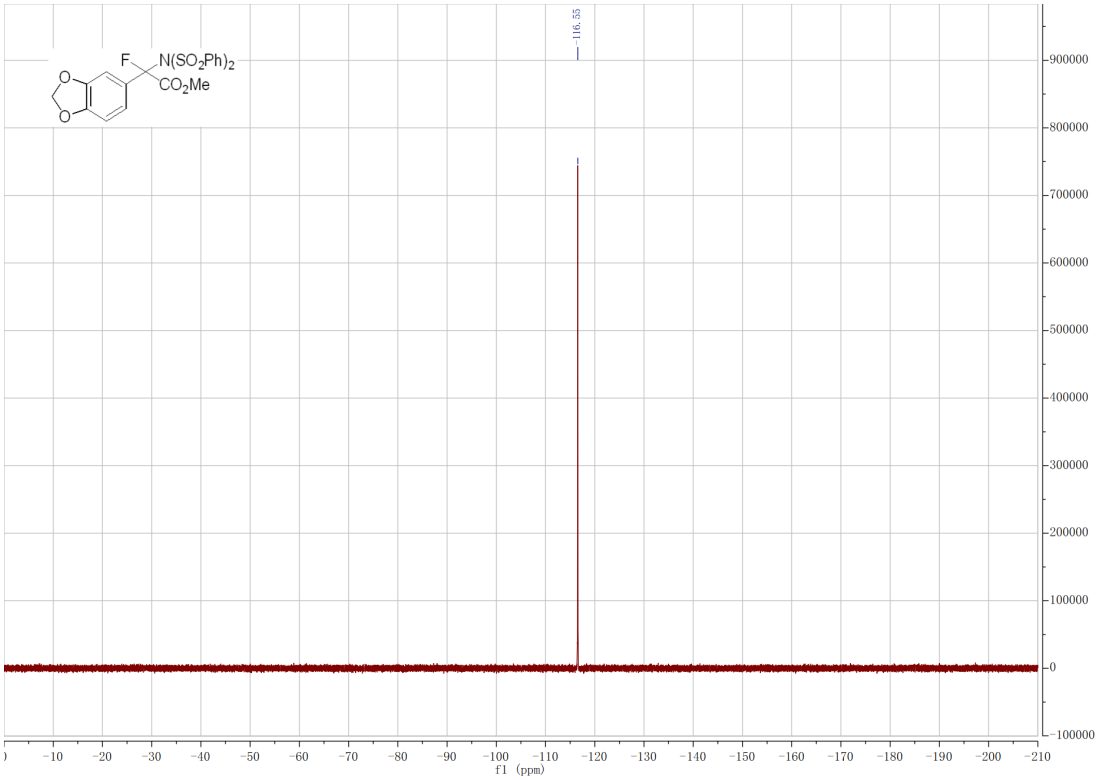
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

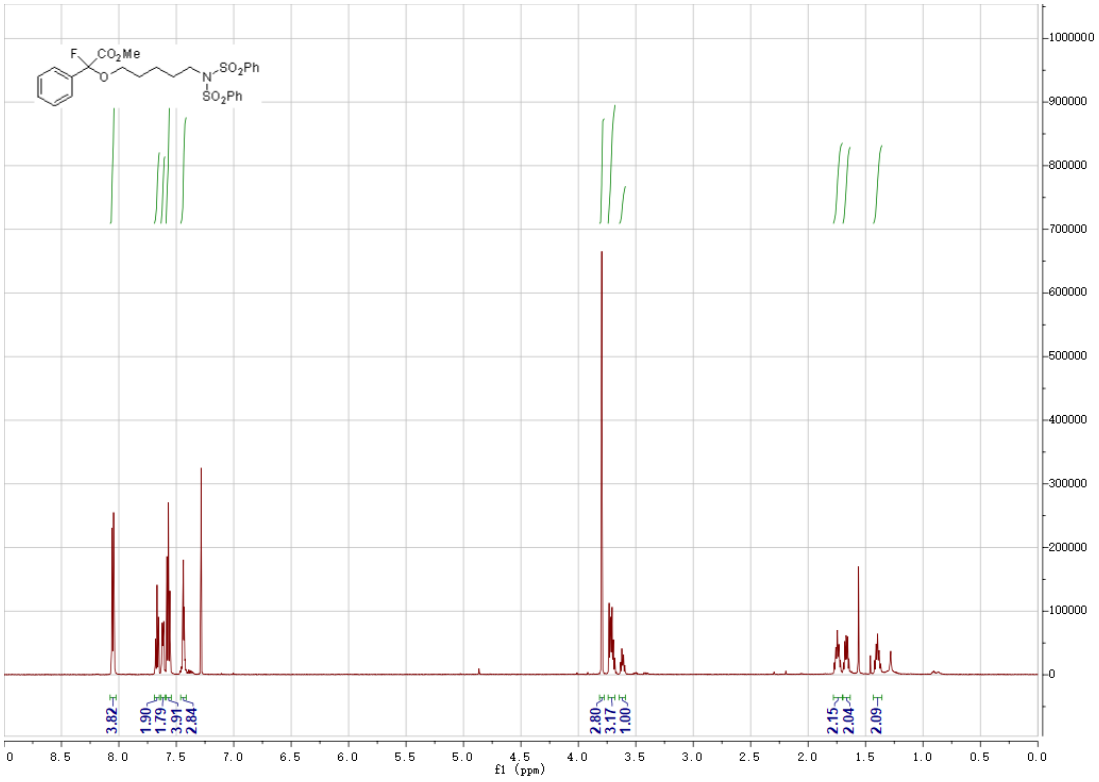


^{19}F NMR (565 MHz, Chloroform-*d*)

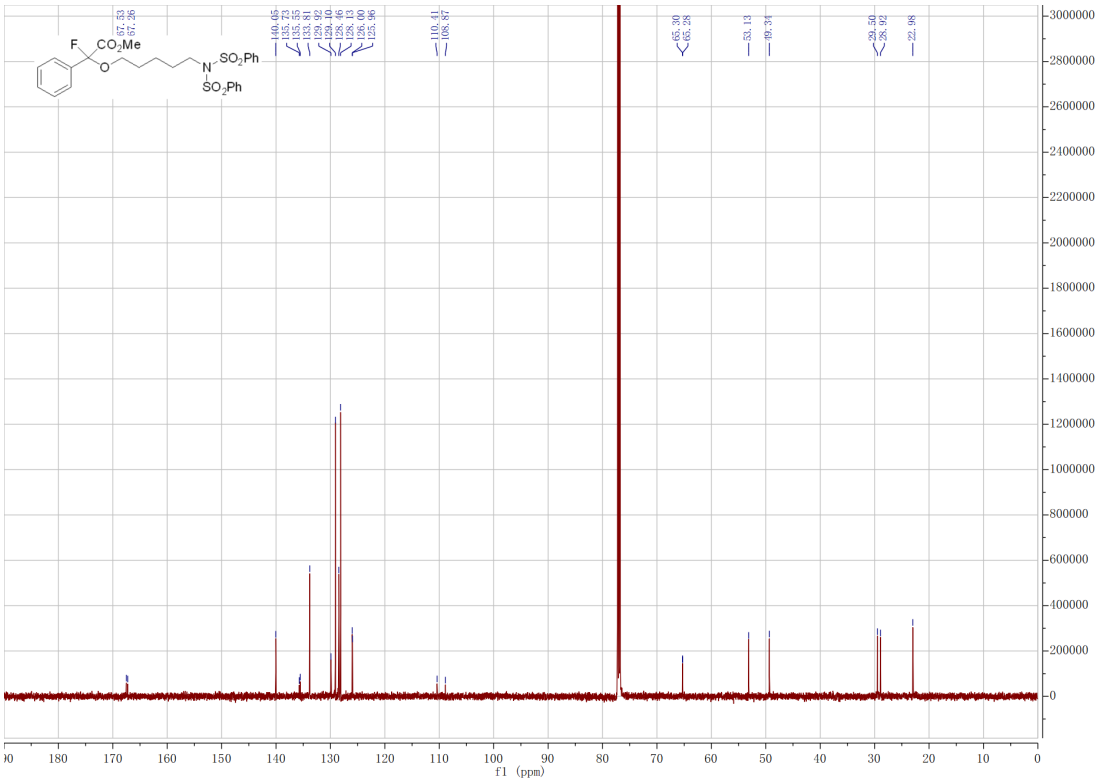


methyl 2-fluoro-2-phenyl-2-((5-(N-(phenylsulfonyl)phenylsulfonamido) pentyl)oxy)acetate (16a)

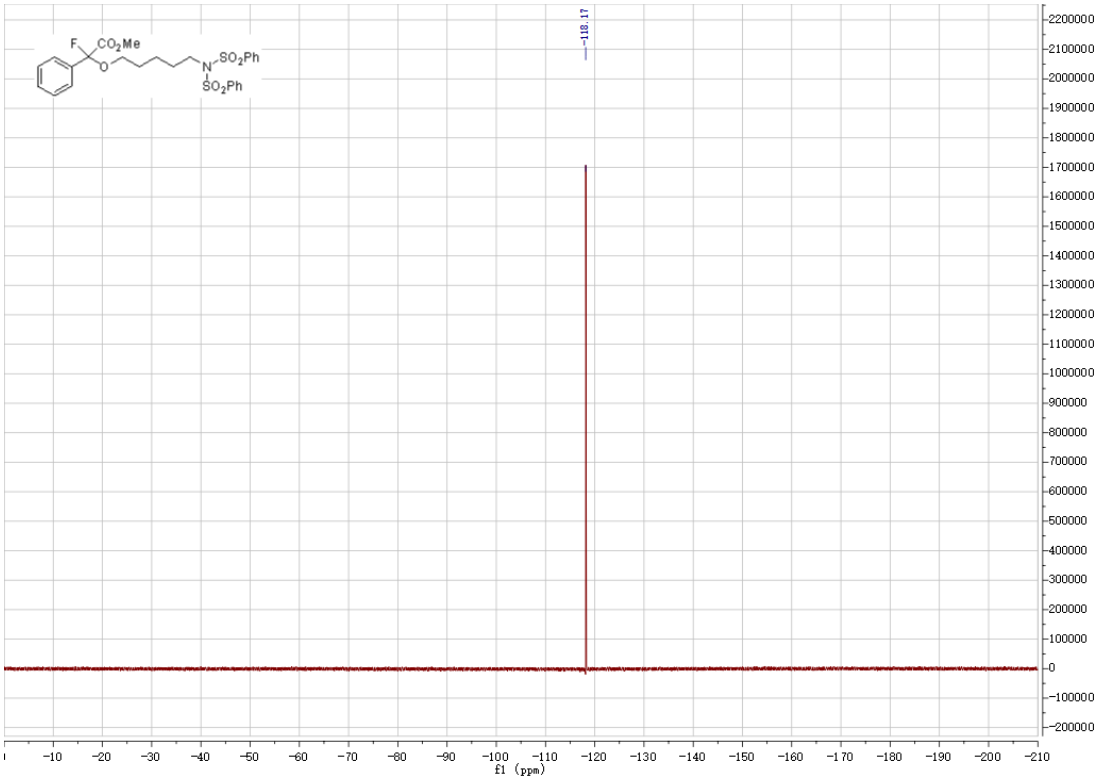
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

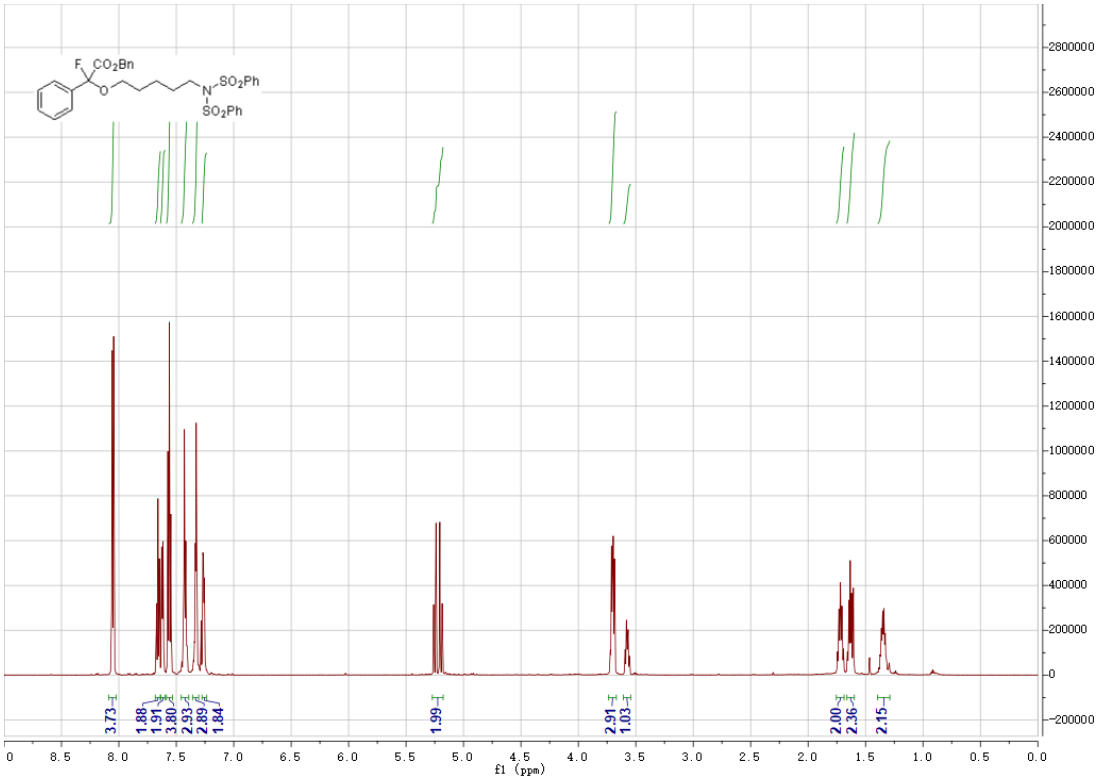


^{19}F NMR (565 MHz, Chloroform-*d*)

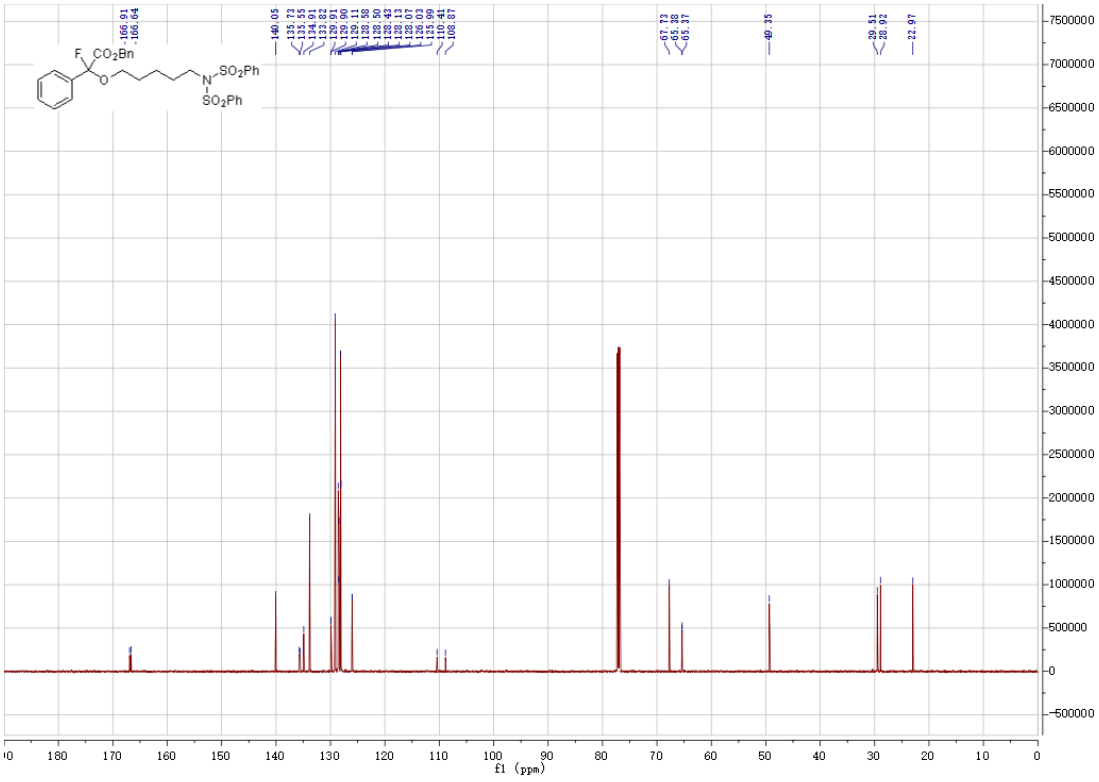


benzyl 2-fluoro-2-phenyl-2-((5-(N-(phenylsulfonyl)phenylsulfonamido) pentyl)oxy)acetate (16b)

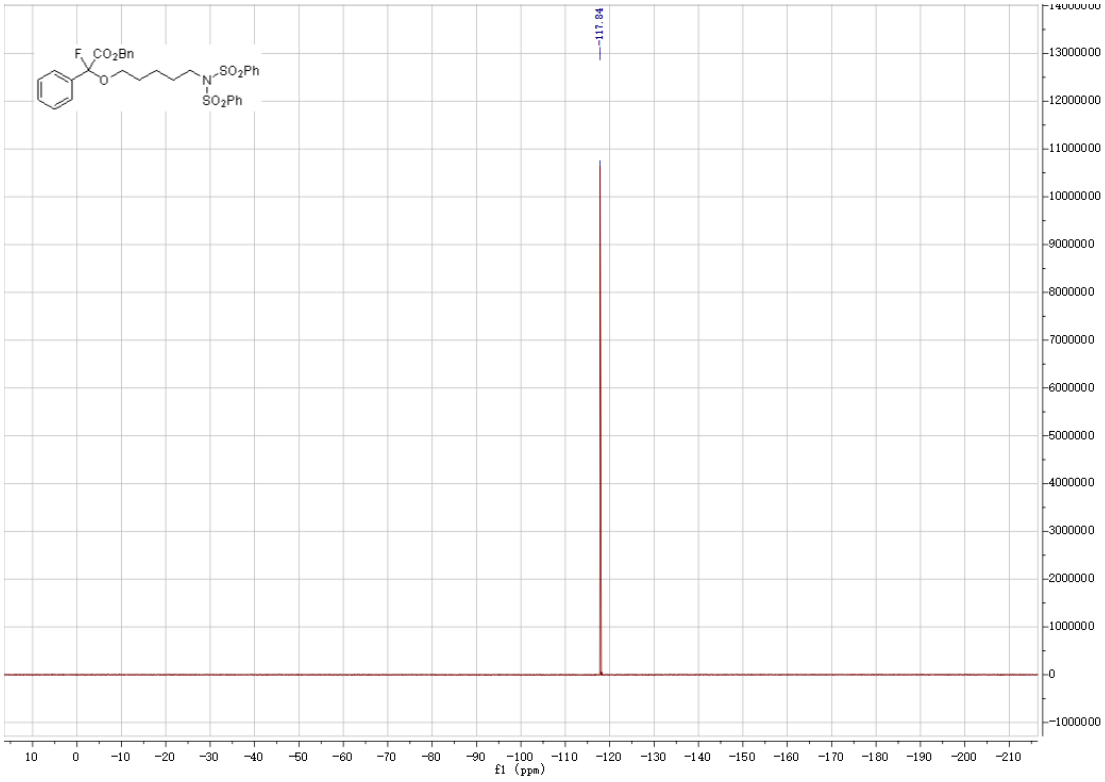
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

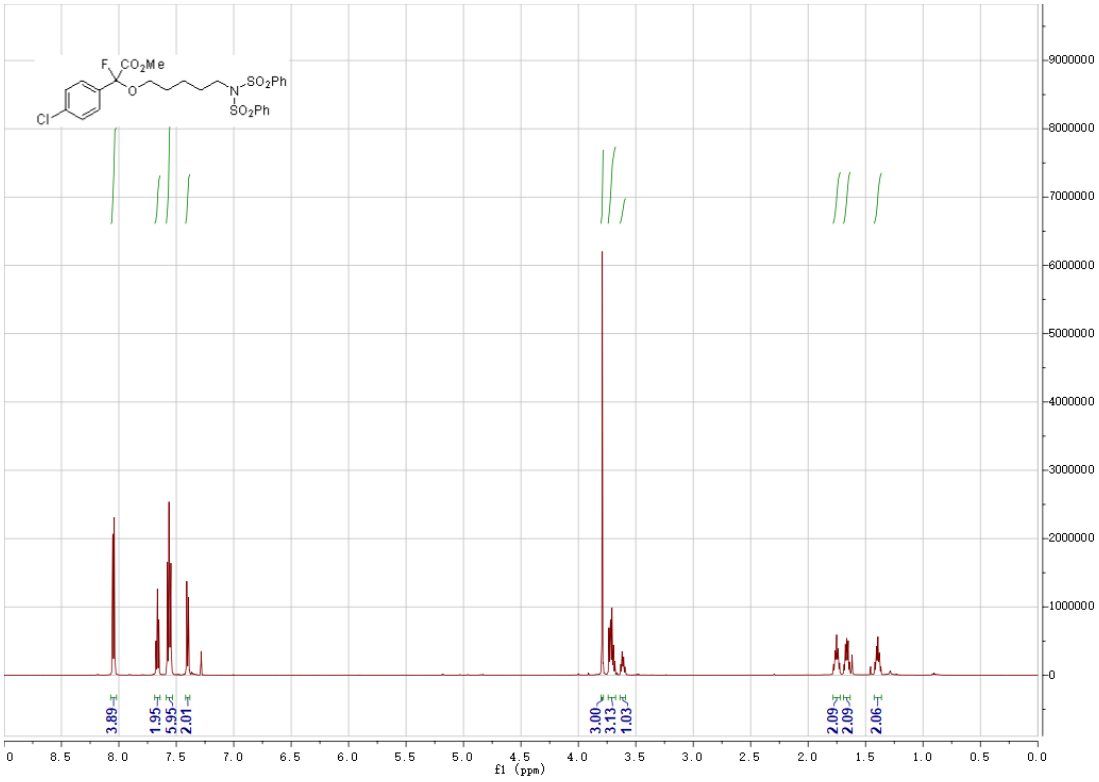


^{19}F NMR (565 MHz, Chloroform-*d*)

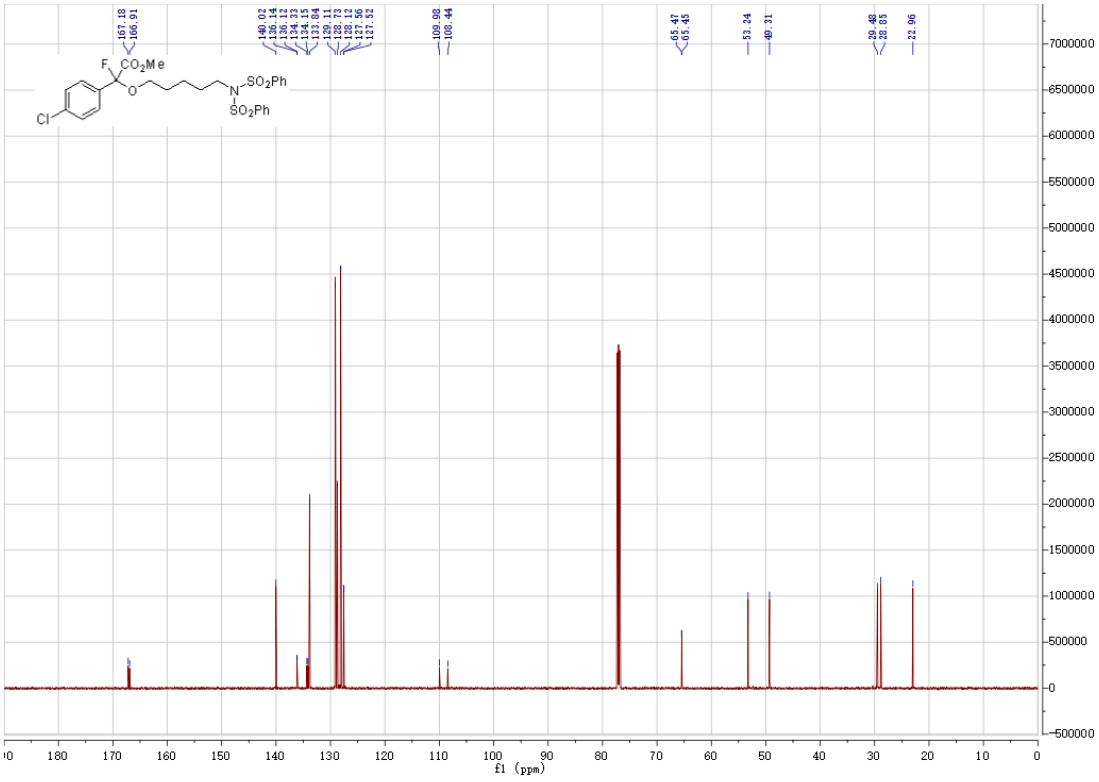


methyl 2-(4-chlorophenyl)-2-fluoro-2-((5-(N-(phenylsulfonyl)phenylsulfonamido) pentyl)oxy)acetate (16c)

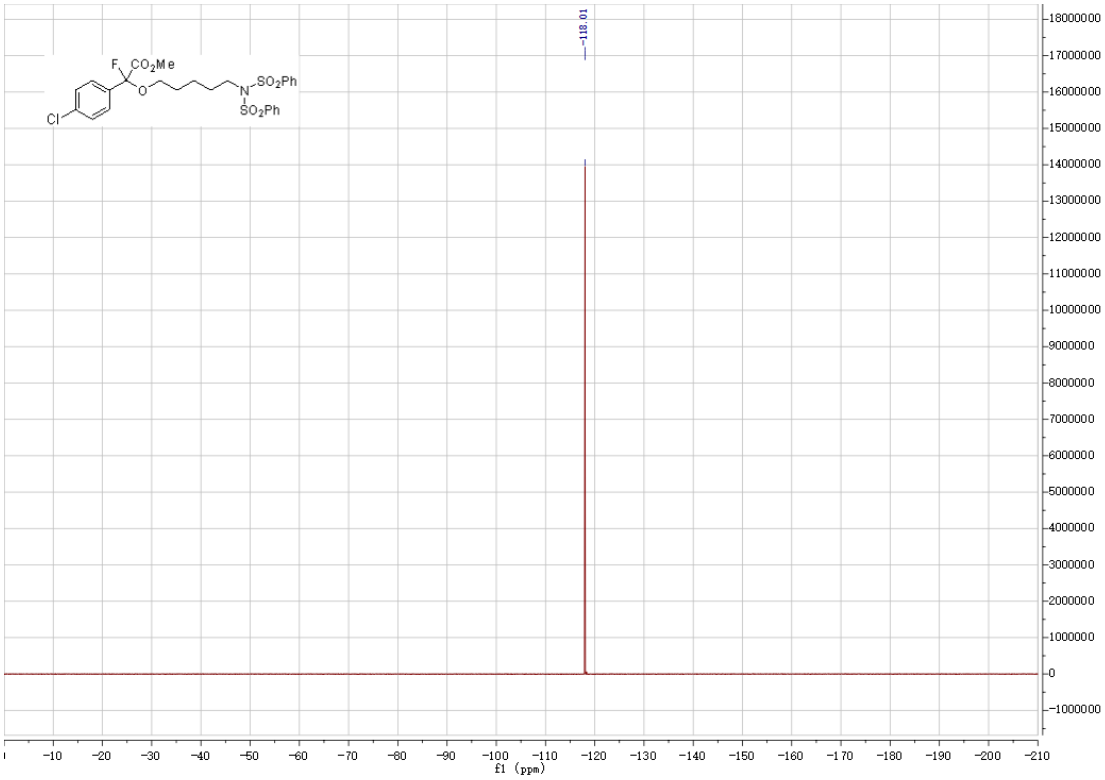
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

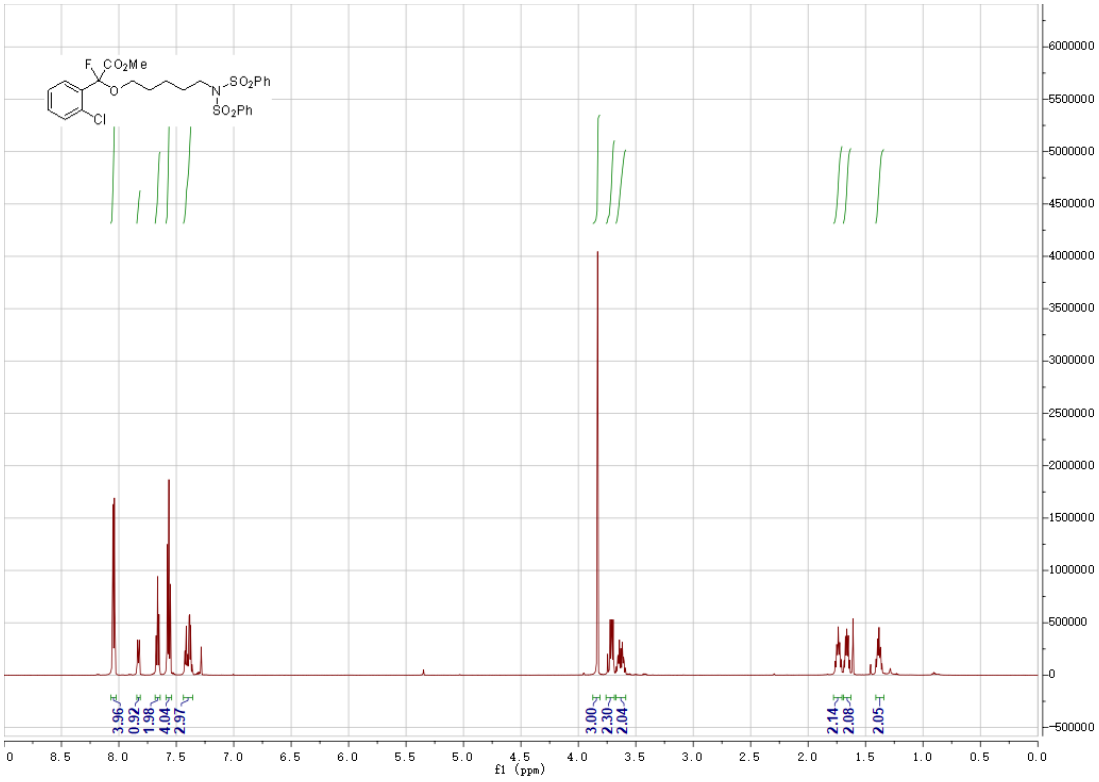


^{19}F NMR (565 MHz, Chloroform-*d*)

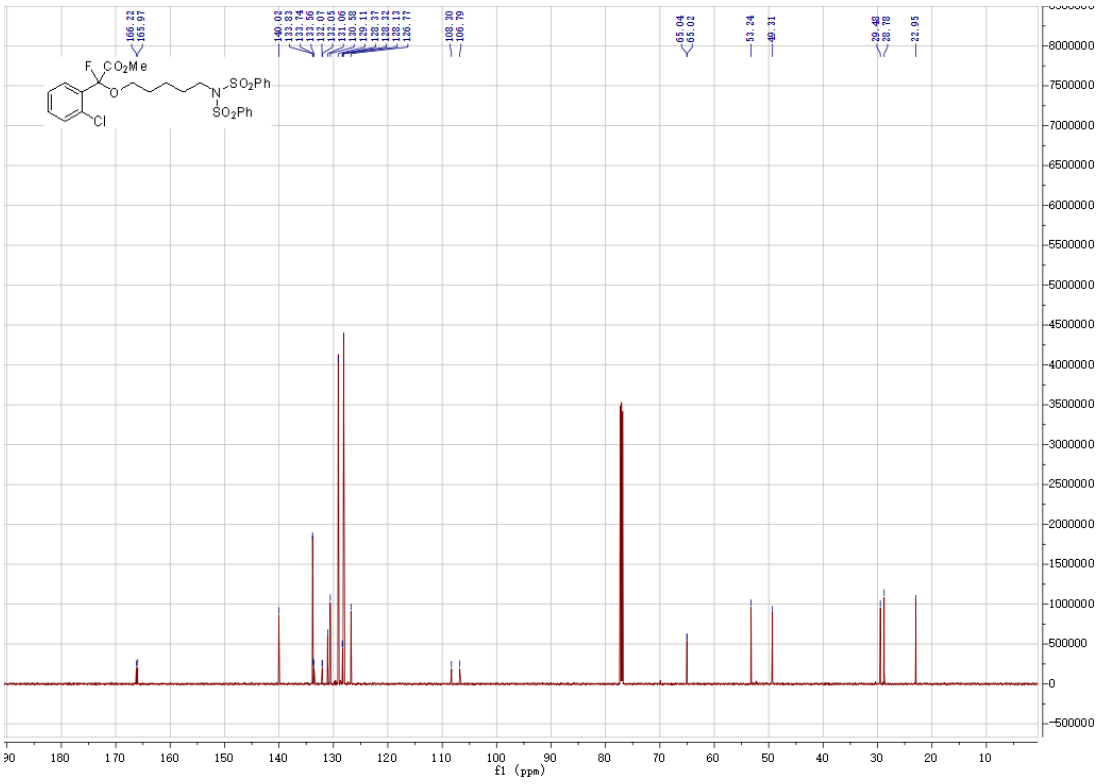


methyl 2-(2-chlorophenyl)-2-fluoro-2-((5-(N-(phenylsulfonyl)phenylsulfonamido) pentyl)oxy)acetate (16d)

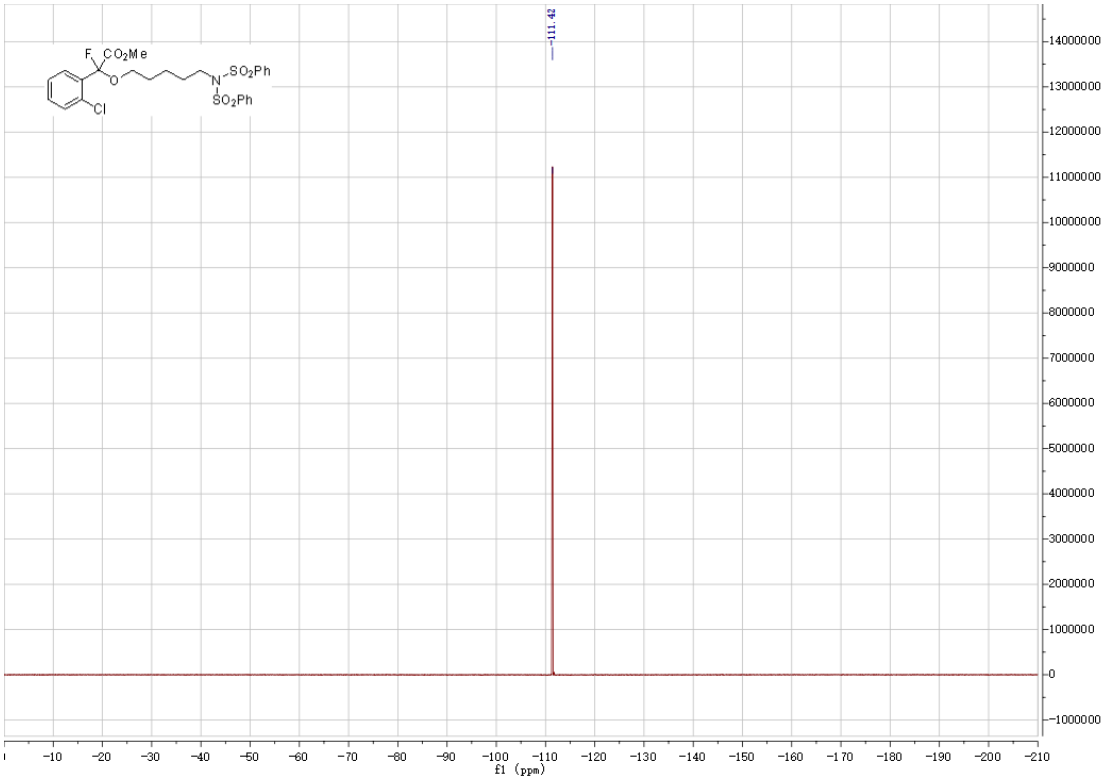
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

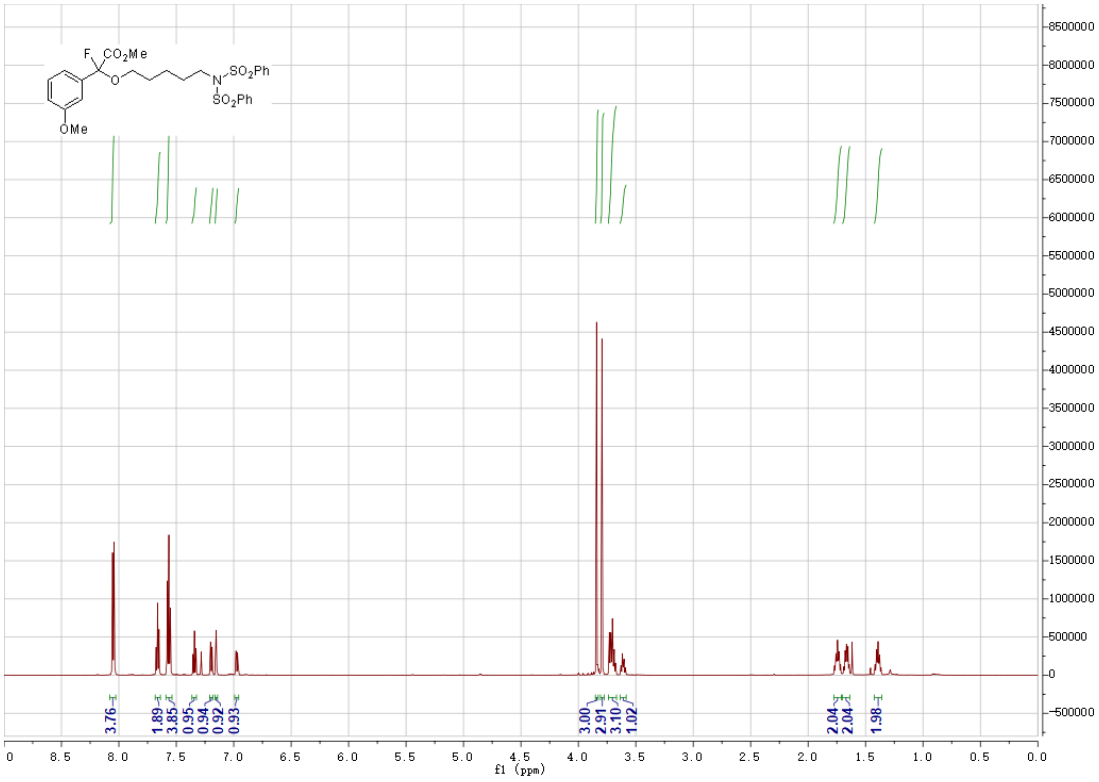


^{19}F NMR (565 MHz, Chloroform-*d*)

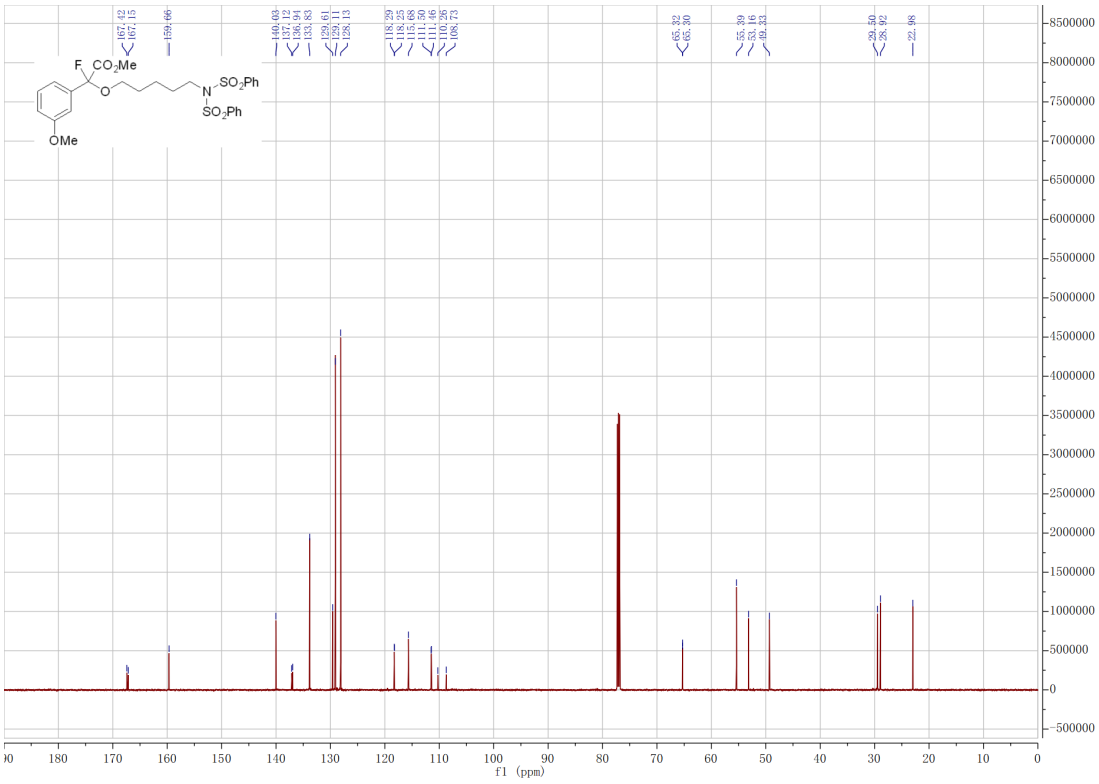


methyl 2-fluoro-2-(3-methoxyphenyl)-2-((5-(N-(phenylsulfonyl)phenylsulfonamido) pentyl)oxy)acetate (16e)

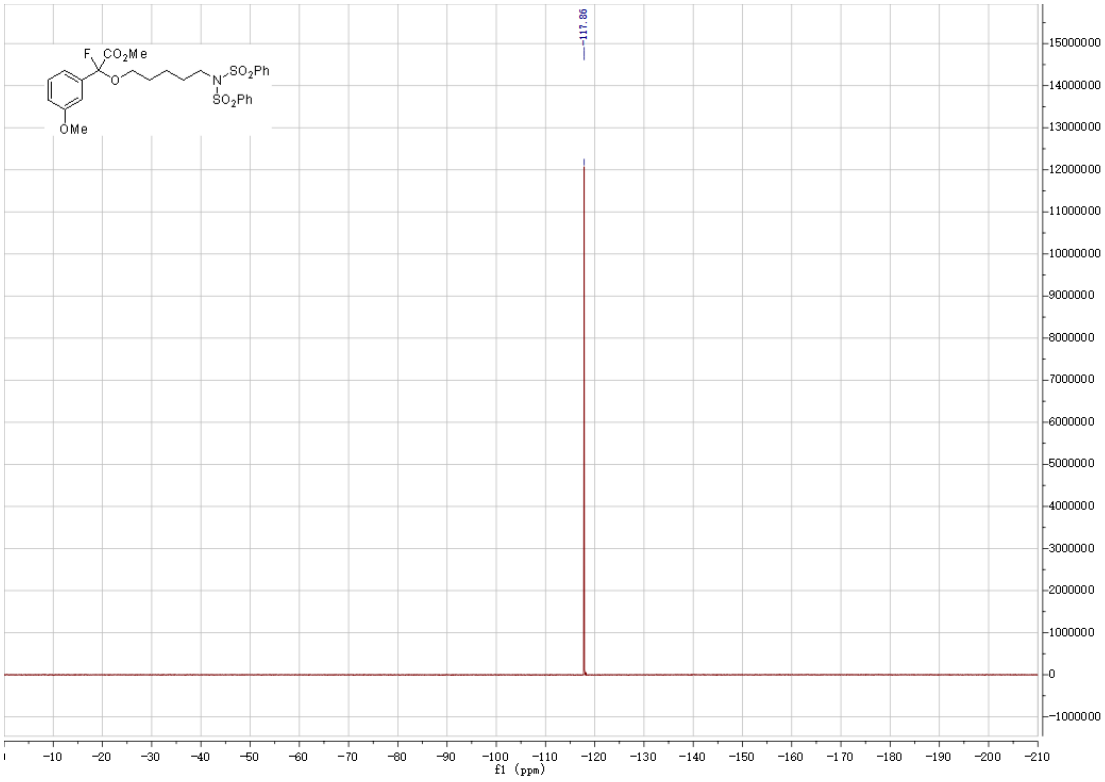
^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)

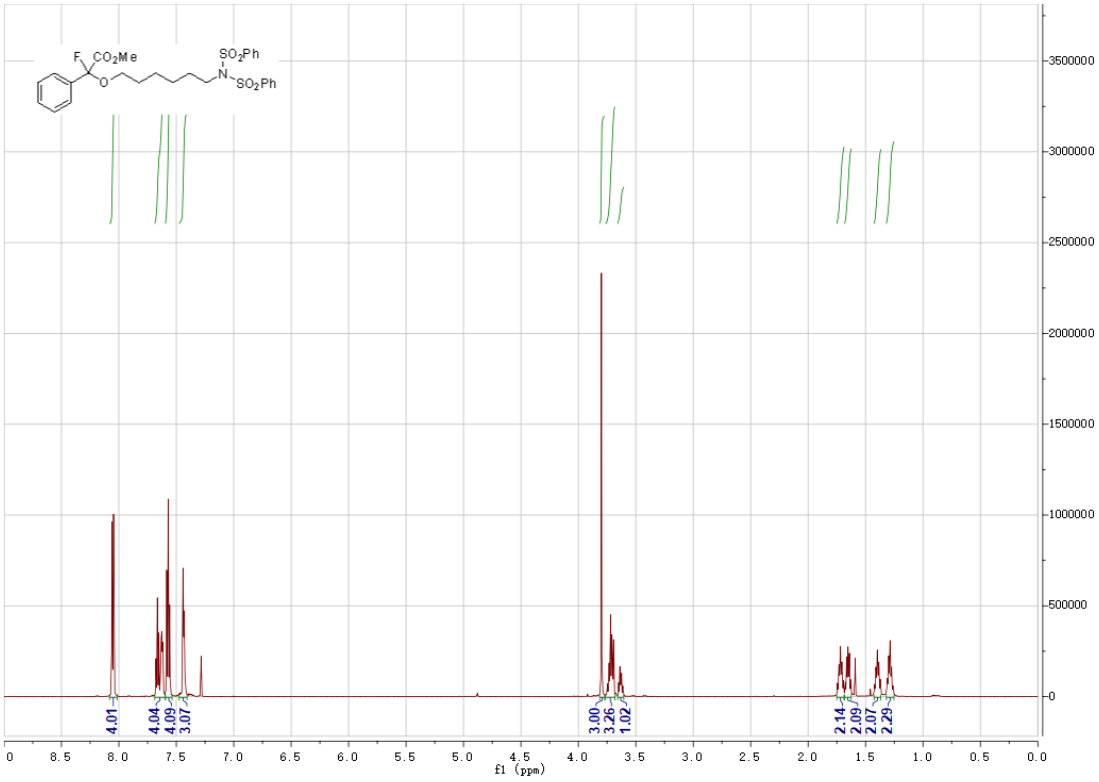


^{19}F NMR (565 MHz, Chloroform-*d*)

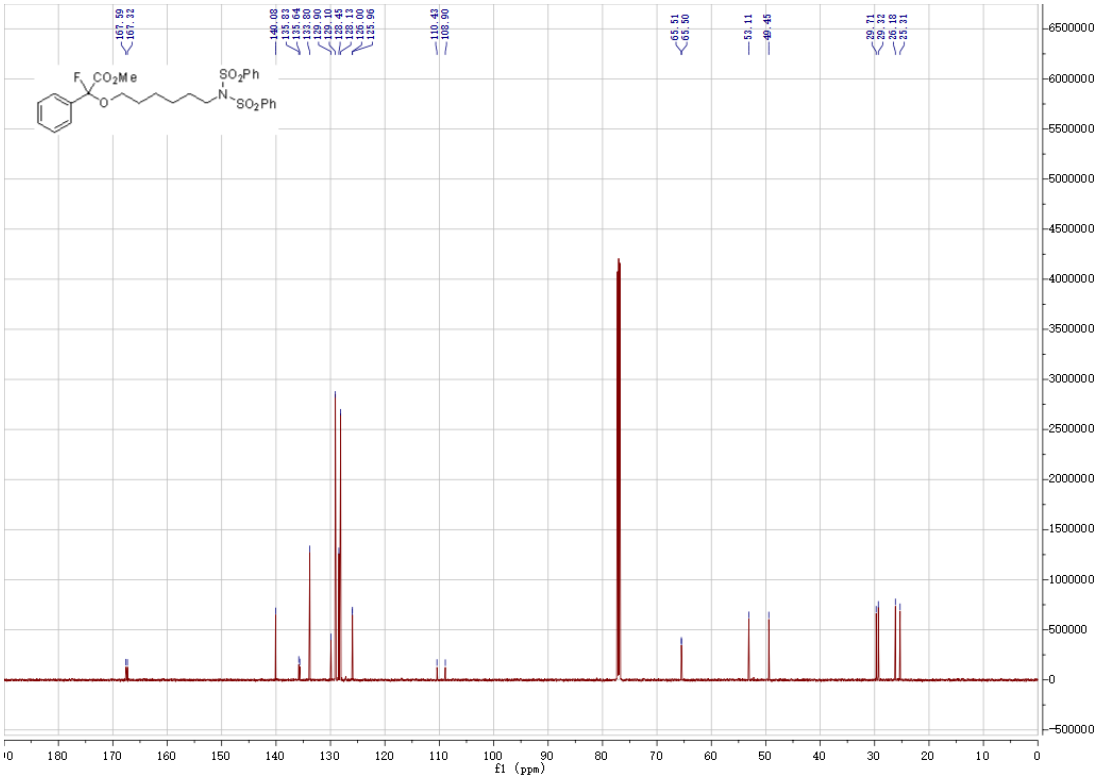


methyl 2-fluoro-2-phenyl-2-((6-(N-(phenylsulfonyl)phenylsulfonamido)hexyl)oxy)acetate (17)

^{1}H NMR (600 MHz, Chloroform-*d*)



^{13}C NMR (151 MHz, Chloroform-d)



^{19}F NMR (565 MHz, Chloroform-*d*)