

## **A Mild and Metal-free Oxy- and Amino-Fluorination for the Synthesis of Fluorinated Heterocycles**

Dixit Parmar and Magnus Rueping\*

Institute of Organic Chemistry

RWTH Aachen University, Landoltweg 1, 52074, Aachen, Germany

Email: [magnus.rueping@rwth-aachen.de](mailto:magnus.rueping@rwth-aachen.de)

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## **General Information**

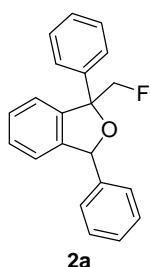
All reagents were obtained from commercial suppliers unless otherwise stated. Organic solvents were routinely dried and/or distilled prior to use and stored over molecular sieves under argon. Solvents for chromatography were technical grade and distilled prior to use. Thin layer chromatography (TLC) was carried out on Merck aluminum support plates Silicagel 60 F<sub>254</sub>. Visualization was achieved under a UV mineral light. Column chromatography was performed using silicagel Merck 60 (particle size 0.2-0.063 mm). Proton NMR (<sup>1</sup>H NMR) spectra were recorded on Varian 400 MHz and 600 MHz spectrometers at 400 and 600 MHz. Carbon NMR (<sup>13</sup>C) spectra were similarly recorded at 100 or 150 MHz, using a broadband decoupled mode. <sup>19</sup>F measurements were performed at 376 and 282 MHz respectively on Varian 400 MHz and Mercury 300 MHz spectrometers. Proton and carbon NMR chemical shifts ( $\delta$ ) are reported in parts per million (ppm) relative to residual proton signals in CDCl<sub>3</sub> ( $\delta$  = 7.26, 77.16). Fluorine NMR chemical shifts ( $\delta$ ) are reported in parts per million (ppm) relative to CCl<sub>4</sub> ( $\delta$  = 0.00). Coupling constants (*J*) are reported in Hertz (Hz) and refer to apparent multiplicities. The following abbreviations are used for the multiplicities: s: singlet, d: doublet, t: triplet, q: quartet, qu: quintet, m: multiplet, br: broad. Mass spectra (EI-MS, 70 eV) were conducted on a Finnigan SSQ 7000 spectrometer. HRMS were recorded on a Thermo Scientific LTQ Orbitrap XL spectrometer. IR spectra were recorded on a Jasco FT/IR-420 spectrometer and are reported in terms of frequency of absorption (cm<sup>-1</sup>). The diastereomeric ratios (dr) of the products were determined by integration of signal in the <sup>1</sup>H-NMR. Chemical yields refer to pure isolated substances.

## Experimental procedures

### General procedure A: Fluoro-Cyclization

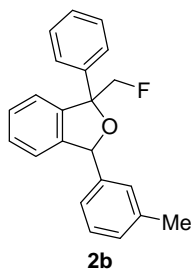
To a screw-cap test tube was added the substrate (1 equiv) and Selectfluor (1.1 equiv). The vessel was evacuated and refilled with a N<sub>2</sub> atmosphere 3 times before the addition of MeCN (1 mL/mmol). The reaction was stirred overnight at room temperature before being quenched with aqueous NH<sub>4</sub>Cl. The aqueous layer was extracted with EtOAc (×3) and the combined organics were washed with brine, dried (Na<sub>2</sub>SO<sub>4</sub>) and concentrated *in vacuo* to yield the crude product. Purification by column chromatography on silica gel gave the title compound.

#### 1-(Fluoromethyl)-1,3-diphenyl-1,3-dihydroisobenzofuran 2a



As for general procedure A, reaction of phenyl(2-(1-phenylvinyl)phenyl)methanol (56 mg, 0.196 mmol, 1 equiv) and Selectfluor (83 mg, 0.23 mmol, 1.1 equiv) gave after column chromatography on silica gel eluting with 20:1 hexane:EtOAc the title compound (54 mg, 0.178 mmol, 91%) as a colourless oil and as a 2:1 mixture of diastereoisomers;  $\nu_{\max}$  (neat)/cm<sup>-1</sup> 3035, 2859, 2329, 1600, 1489, 1454, 1272, 1132, 1075, 1011, 926, 888, 752; Characterized as a mixture of two diastereoisomers:  $\delta_{\text{H}}$  (600 MHz, CDCl<sub>3</sub>) 4.82–4.96 (4H, m, 2 × CH<sub>2</sub>F), 6.15 (1H, s, CHAr from major dias.), 6.39 (1H, s, CHAr from minor dias.), 6.94–7.65 (28H, m, ArCH);  $\delta_{\text{C}}$  (150 MHz, CDCl<sub>3</sub>) 84.6, 86.2, 86.5 (d,  $J$  = 182.8, CH<sub>2</sub>F from major dias.), 87.2 (d,  $J$  = 181.6, CH<sub>2</sub>F from minor dias.), 89.8 (d,  $J$  = 18.8, CCH<sub>2</sub>F from minor dias.), 89.8 (d,  $J$  = 19.1, CCH<sub>2</sub>F from major dias.), 122.4, 122.8, 122.8, 126.1, 126.2, 127.8, 128.0, 128.1, 128.1, 128.2, 128.5, 128.6, 128.7, 128.7, 128.8, 128.8, 140.2, 140.2, 140.3, 140.3, 140.5, 140.5, 140.9, 140.9, 141.3, 141.4, 143.0, 143.5;  $\delta_{\text{F}}$  (564 MHz, CDCl<sub>3</sub>) -222.1 (t,  $J$  = 47.6, CH<sub>2</sub>F from minor dias.), -220.4 (t,  $J$  = 47.8, CH<sub>2</sub>F from major dias.);  $m/z$  (EI) 271 (M-CH<sub>2</sub>F, 100), 193 (32), 165 (23); HRMS for C<sub>21</sub>H<sub>17</sub>OFNa calculated for [M+Na]<sup>+</sup>: 327.11556, found 327.11548.

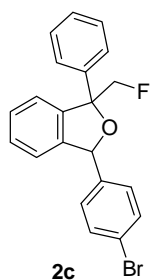
#### 1-(Fluoromethyl)-1-phenyl-3-*m*-tolyl-1,3-dihydroisobenzofuran 2b



As for general procedure A, reaction of (2-(1-phenylvinyl)phenyl)(*m*-tolyl)methanol (64 mg, 0.213 mmol, 1 equiv) and Selectfluor (83 mg, 0.23 mmol, 1.1 equiv) gave after column chromatography on silica gel eluting with 20:1 hexane:EtOAc the title compound

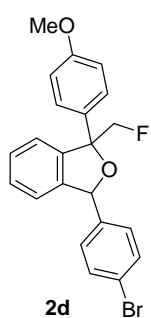
(51 mg, 0.160 mmol, 75%) as a colourless oil and as a 2:1 mixture of diastereoisomers;  $\nu_{\max}$  (neat)/ $\text{cm}^{-1}$  3031, 2946, 2865, 1957, 1663, 1604, 1488, 1455, 1381, 1327, 1268, 1155, 1133, 1073, 1027, 933, 910, 884, 762, 729, 699, 651, 582, 502; Characterized as a mixture of two diastereoisomers:  $\delta_{\text{H}}$  (600 MHz,  $\text{CDCl}_3$ ) 2.30 (3H, s,  $\text{ArCH}_3$  from minor dias.), 2.36 (3H, s,  $\text{ArCH}_3$  from minor dias.), 4.81-4.96 (4H, m,  $2 \times \text{CH}_2\text{F}$ ), 6.11 (1H, s,  $\text{CHAr}$  from major dias.), 6.35 (1H, s,  $\text{CHAr}$  from minor dias.), 6.95-7.64 (26H, m,  $\text{ArCH}$ );  $\delta_{\text{C}}$  (150 MHz,  $\text{CDCl}_3$ ) 21.5, 21.6, 84.6, 86.3, 86.5 (d,  $J = 183.0$ ,  $\text{CH}_2\text{F}$  from major dias.), 87.2 (d,  $J = 181.5$ ,  $\text{CH}_2\text{F}$  from minor dias.), 89.7 (d,  $J = 21.1$ ,  $\text{CCH}_2\text{F}$  from minor dias.), 89.8 (d,  $J = 21.9$ ,  $\text{CCH}_2\text{F}$  from major dias.), 122.4, 122.8, 122.8, 125.0, 125.2, 126.2, 126.2, 127.9, 128.1, 128.1, 128.2, 128.5, 128.5 ( $\times 2$ ), 128.6 ( $\times 2$ ), 128.6, 128.7 ( $\times 2$ ), 128.8, 128.9, 129.2, 129.4, 138.3, 138.5, 140.2, 140.2, 140.3, 141.1, 141.3, 143.0, 143.5;  $\delta_{\text{F}}$  (564 MHz,  $\text{CDCl}_3$ ) -222.2 (t,  $J = 47.6$ ,  $\text{CH}_2\text{F}$  from minor dias.), -220.4 (t,  $J = 47.8$ ,  $\text{CH}_2\text{F}$  from major dias.);  $m/z$  (ESI) 319 ( $\text{M}+\text{Na}$ , 24), 357 (100); HRMS for  $\text{C}_{22}\text{H}_{19}\text{OFK}$  calculated for  $[\text{M}+\text{K}]^+$ : 357.10515, found 357.10501.

### 3-(4-bromophenyl)-1-(fluoromethyl)-1-phenyl-1,3-dihydroisobenzofuran 2c



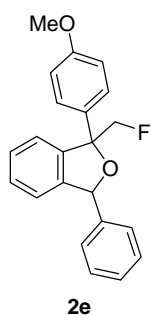
As for general procedure A, reaction of 3-(4-bromophenyl)(2-(1-phenylvinyl)phenyl)methanol (60 mg, 0.164 mmol, 1 equiv) and Selectfluor (76 mg, 0.21 mmol, 1.1 equiv) gave after column chromatography on silica gel eluting with 30:1 hexane:EtOAc the title compound (53 mg, 0.138 mmol, 84%) as a colourless oil and as a 2:1 mixture of diastereoisomers;  $\nu_{\max}$  (neat)/ $\text{cm}^{-1}$  3364, 3056, 1647, 1608, 1489, 1444, 1376, 1308, 1270, 1149, 1021, 905, 769, 705; Characterized as a mixture of two diastereoisomers:  $\delta_{\text{H}}$  (600 MHz,  $\text{CDCl}_3$ ) 4.71-4.86 (4H, m,  $2 \times \text{CH}_2\text{F}$ ), 6.02 (1H, s,  $\text{CHAr}$  from major dias.), 6.26 (1H, s,  $\text{CHAr}$  from minor dias.), 6.83-7.53 (26H, m,  $\text{ArCH}$ );  $\delta_{\text{C}}$  (150 MHz,  $\text{CDCl}_3$ ) 83.9, 85.7, 86.3 (d,  $J = 183.0$ ,  $\text{CH}_2\text{F}$  from major dias.), 87.2 (d,  $J = 181.8$ ,  $\text{CH}_2\text{F}$  from minor dias.), 90.0 (d,  $J = 18.4$ ,  $\text{CCH}_2\text{F}$  from minor dias.), 90.1 (d,  $J = 18.7$ ,  $\text{CCH}_2\text{F}$  from major dias.), 122.5, 122.6, 122.7, 122.7, 122.9, 126.1, 126.1, 128.2, 128.3, 128.3, 128.3, 128.7 ( $\times 2$ ), 128.8, 128.9, 129.5, 129.8, 131.8, 131.9, 139.9, 139.9, 140.1, 140.4, 140.6, 140.7, 140.7, 142.5, 143.0;  $\delta_{\text{F}}$  (564 MHz,  $\text{CDCl}_3$ ) -222.1 (t,  $J = 47.5$ ,  $\text{CH}_2\text{F}$  from minor dias.), -220.1 (t,  $J = 47.8$ ,  $\text{CH}_2\text{F}$  from major dias.);  $m/z$  (CI) 349 ( $\text{M}-\text{CH}_2\text{F}$ , 100), 351 ( $\text{M}-\text{CH}_2\text{F}$ , 100), 270 (37).

### 3-(4-Bromophenyl)-1-(fluoromethyl)-1-(4-methoxyphenyl)-1,3-dihydroisobenzofuran 2d



As for general procedure A, reaction of (4-bromophenyl)(2-(1-(4-methoxyphenyl)vinyl)phenyl)methanol (75 mg, 0.190 mmol, 1 equiv) and Selectfluor (74 mg, 0.21 mmol, 1.1 equiv) gave after column chromatography on silica gel eluting with 10:1 hexane:EtOAc the title compound (55 mg, 0.133 mmol, 70%) as a yellow oil and as a 2:1 mixture of diastereoisomers;  $\nu_{\max}$  (neat)/ $\text{cm}^{-1}$  3073, 2948, 2838, 2077, 1608, 1510, 1486, 1459, 1407, 1298, 1248, 1177, 1131, 1074, 1006, 906, 873, 826, 737, 679; Characterized as a mixture of two diastereoisomers:  $\delta_{\text{H}}$  (400 MHz,  $\text{CDCl}_3$ ) 3.80 (3H, s,  $\text{OCH}_3$  from major dias.), 3.81 (3H, s,  $\text{OCH}_3$  from major dias.), 4.74-4.94 (4H, m,  $2 \times \text{CH}_2\text{F}$ ), 6.06 (1H, s,  $\text{CHAr}$  from major dias.), 6.31 (1H, s,  $\text{CHAr}$  from minor dias.), 6.89-7.53 (24H, m,  $\text{ArCH}$ );  $\delta_{\text{C}}$  (100 MHz,  $\text{CDCl}_3$ ) 55.4, 55.4, 83.7, 85.4, 86.3 (d,  $J = 183.1$ ,  $\text{CH}_2\text{F}$  from major dias.), 87.1 (d,  $J = 181.8$ ,  $\text{CH}_2\text{F}$  from minor dias.), 89.8 (d,  $J = 18.9$ ,  $\text{CCH}_2\text{F}$  from minor dias.), 89.9 (d,  $J = 19.2$ ,  $\text{CCH}_2\text{F}$  from major dias.), 114.0 ( $\times 2$ ), 122.4, 122.5, 122.6, 122.6, 122.7, 123.0, 127.5 ( $\times 2$ ), 128.1, 128.3, 128.7, 128.9, 129.5 ( $\times 2$ ), 129.6 ( $\times 2$ ), 131.8, 131.9 ( $\times 2$ ), 140.3, 140.4, 140.5, 140.7, 143.0, 159.5, 159.6;  $\delta_{\text{F}}$  (376 MHz,  $\text{CDCl}_3$ ) -221.7 (t,  $J = 47.6$ ,  $\text{CH}_2\text{F}$  from minor dias.), -219.4 (t,  $J = 47.9$ ,  $\text{CH}_2\text{F}$  from major dias.);  $m/z$  (CI) 413 ( $\text{M}^+$ , 5), 256 (100), 305 (61);

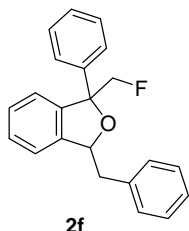
### 1-(Fluoromethyl)-1-(4-methoxyphenyl)-3-phenyl-1,3-dihydroisobenzofuran 2e



As for general procedure A, reaction of 3 (2-(1-(4-methoxyphenyl)vinyl)phenyl)(phenyl)methanol (64 mg, 0.203 mmol, 1 equiv) and Selectfluor (79 mg, 0.22 mmol, 1.1 equiv) gave after column chromatography on silica gel eluting with 10:1 hexane:EtOAc the title compound (59 mg, 0.177 mmol, 87%) as a colourless oil and as a 1.5:1 mixture of diastereoisomers;  $\nu_{\max}$  (neat)/ $\text{cm}^{-1}$  3033, 2944, 2840, 1608, 1510, 1456, 1298, 1248, 1178, 1130, 1080, 1017, 933, 830, 754, 700; Characterized as a mixture of two diastereoisomers:  $\delta_{\text{H}}$  (600 MHz,  $\text{CDCl}_3$ ) 3.79 (3H, s,  $\text{OCH}_3$  from major dias.), 3.80 (3H, s,  $\text{OCH}_3$  from major dias.), 4.78-4.93 (4H, m,  $2 \times \text{CH}_2\text{F}$ ), 6.11 (1H, s,  $\text{CHAr}$  from major dias.), 6.34 (1H, s,  $\text{CHAr}$  from minor dias.), 6.89-7.53 (26H, m,  $\text{ArCH}$ );  $\delta_{\text{C}}$  (150 MHz,  $\text{CDCl}_3$ ) 55.4, 55.4, 84.4, 86.1, 86.4 (d,  $J = 183.0$ ,  $\text{CH}_2\text{F}$  from major dias.), 87.1 (d,  $J = 181.6$ ,  $\text{CH}_2\text{F}$  from minor dias.), 89.6 (d,  $J = 19.5$ ,  $\text{CCH}_2\text{F}$  from major and minor dias.), 114.0 ( $\times 2$ ), 122.4, 122.7, 122.8, 122.9, 127.6 ( $\times 2$ ), 127.8, 127.9, 128.0, 128.1, 128.4, 128.5, 128.6, 128.6, 128.7, 128.7, 128.8 ( $\times 2$ ), 140.4, 140.7,

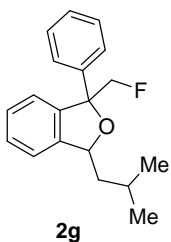
141.3, 141.6, 143.1, 143.5, 159.4, 159.5;  $\delta_F$  (564 MHz,  $CDCl_3$ ) -222.7 (t,  $J$  = 47.6,  $CH_2F$  from minor dias.), -219.7 (t,  $J$  = 47.9,  $CH_2F$  from major dias.);  $m/z$  (CI) 334 (M, 37), 224 (100), 254 (82), 299 (63), 316 (57), 163 (51).

### 3-Benzyl-1-(fluoromethyl)-1-phenyl-1,3-dihydroisobenzofuran 2f



As for general procedure A, reaction of 2-phenyl-1-(2-(1-phenylvinyl)phenyl)ethanol (59 mg, 0.196 mmol, 1 equiv) and Selectfluor (77 mg, 0.22 mmol, 1.1 equiv) gave after column chromatography on silica gel eluting with 20:1 hexane:EtOAc the title compound (45 mg, 0.141 mmol, 72%) as a colourless oil and as a 2:1 mixture of diastereoisomers;  $\nu_{max}$  (neat)/ $cm^{-1}$  3062, 3030, 2943, 2858, 1956, 1810, 1601, 1494, 1454, 1380, 1276, 1133, 1032, 945, 913, 753, 699, 650, 542; Characterized as a mixture of two diastereoisomers:  $\delta_H$  (600 MHz,  $CDCl_3$ ) 3.02 (1H, dd,  $J$  = 13.9, 6.1,  $CH_aH_bPh$  from minor dias.), 3.16 (1H, dd,  $J$  = 14.0, 5.8,  $CH_aH_bPh$  from major dias.), 3.21 (1H, dd,  $J$  = 13.9, 7.2,  $CH_aH_bPh$  from minor dias.), 3.30 (1H, dd,  $J$  = 14.0, 6.9,  $CH_aH_bPh$  from major dias.), 4.61-4.82 (4H, m, 2  $\times$   $CH_2F$ ), 5.62 (1H, t,  $J$  = 6.3,  $CHCH_2Ph$  from major dias.), 5.68 (1H, t,  $J$  = 6.7,  $CHCH_2Ph$  from minor dias.), 6.95-7.56 (28H, m, ArCH);  $\delta_C$  (150 MHz,  $CDCl_3$ ) 43.1, 43.6, 83.5, 84.4, 86.7 (d,  $J$  = 181.4,  $CH_2F$  from major dias.), 87.0 (d,  $J$  = 182.0,  $CH_2F$  from minor dias.), 89.2 (d,  $J$  = 19.0,  $CCH_2F$  from minor dias.), 89.2 (d,  $J$  = 19.1,  $CCH_2F$  from major dias.), 122.0, 122.1, 122.7, 123.0, 125.9, 126.1, 126.6, 126.6, 127.9, 128.0 ( $\times 2$ ), 128.3, 128.4 ( $\times 2$ ), 128.4, 128.5, 128.6, 129.8, 130.0 ( $\times 2$ ), 137.7, 137.8, 140.5, 140.9, 141.3, 141.4, 142.3, 142.5;  $\delta_F$  (564 MHz,  $CDCl_3$ ) -222.1 (t,  $J$  = 47.6,  $CH_2F$  from minor dias.), -221.8 (t,  $J$  = 47.7,  $CH_2F$  from major dias.);  $m/z$  (ESI) 319 (M+H, 4), 357 (100), 341 (76), 208 (44), 336 (28); HRMS for  $C_{22}H_{19}OFNa$  calculated for  $[M+Na]^+$ : 341.13121, found 341.13126.

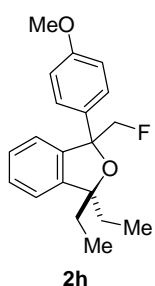
### 1-(Fluoromethyl)-3-isobutyl-1-phenyl-1,3-dihydroisobenzofuran 2g



As for general procedure A, reaction of 3-methyl-1-(2-(1-phenylvinyl)phenyl)butan-1-ol (75 mg, 0.282 mmol, 1 equiv) and Selectfluor (110 mg, 0.31 mmol, 1.1 equiv) gave after column chromatography on silica gel eluting with 20:1 hexane:EtOAc the title compound (62 mg, 0.218 mmol, 77%) as a colourless oil and as a 2:1 mixture of diastereoisomers;  $\nu_{max}$  (neat)/ $cm^{-1}$  3063, 3032, 2955, 2871, 1601, 1459, 1370, 1333, 1274, 1132, 1061, 1033, 983, 751, 699, 649,

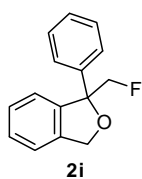
596, 541; Characterized as a mixture of two diastereoisomers:  $\delta_{\text{H}}$  (600 MHz,  $\text{CDCl}_3$ ) 1.02-1.10 (12H, m,  $4 \times \text{CH}_3$ ), 1.59-1.69 (2H, m,  $\text{CH}_2$  from minor dias.), 1.72-1.81 (2H, m,  $\text{CH}_2$  from minor dias.), 2.10-2.19 (2H, m,  $4 \times \text{CH}$ ), 4.68-4.4.85 (4H, m,  $2 \times \text{CH}_2\text{F}$ ), 5.36 (1H, dd,  $J = 9.1, 3.5$ ,  $\text{CHAr}$  from major dias.), 5.49 (1H, dd,  $J = 9.5, 3.7$ ,  $\text{CHAr}$  from minor dias.), 7.17-7.62 (18H, m,  $\text{ArCH}$ );  $\delta_{\text{C}}$  (150 MHz,  $\text{CDCl}_3$ ) 22.2, 22.3, 23.8, 23.8, 25.3 ( $\times 2$ ), 46.0, 46.7, 81.0, 82.0, 86.8 (d,  $J = 181.8$ ,  $\text{CH}_2\text{F}$  from major dias.), 87.0 (d,  $J = 181.8$ ,  $\text{CH}_2\text{F}$  from minor dias.), 88.9 (d,  $J = 19.2$ ,  $\text{CCH}_2\text{F}$  from minor dias.), 89.0 (d,  $J = 18.0$ ,  $\text{CCH}_2\text{F}$  from major dias.), 121.4, 121.5, 122.6, 122.9, 126.0, 127.7, 127.7, 127.9, 128.4, 128.5, 128.5, 140.4, 140.8, 141.2, 141.9, 141.9, 143.8, 143.8, 143.9, 143.9;  $\delta_{\text{F}}$  (564 MHz,  $\text{CDCl}_3$ ) -222.0 (t,  $J = 47.7$ ,  $\text{CH}_2\text{F}$  from minor dias.), -221.6 (t,  $J = 47.7$ ,  $\text{CH}_2\text{F}$  from major dias.);  $m/z$  (EI) 251 (M- $\text{CH}_2\text{F}$ , 100), 194 (30), 227 (28); HRMS for  $\text{C}_{19}\text{H}_{21}\text{OFNa}$  calculated for  $[\text{M}+\text{Na}]^+$ : 307.14686, found 307.14618.

### 1,1-Diethyl-3-(fluoromethyl)-3-(4-methoxyphenyl)-1,3-dihydroisobenzofuran 2h



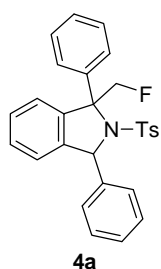
As for general procedure A, reaction of 3-(2-(1-(4-methoxyphenyl)vinyl)phenyl)pentan-3-ol (63 mg, 0.213 mmol, 1 equiv) and Selectfluor (83 mg, 0.23 mmol, 1.1 equiv) gave after column chromatography on silica gel eluting with 30:1 hexane:EtOAc the title compound (55 mg, 0.175 mmol, 82%) as a colourless oil and a mixture of rotamers;  $\nu_{\text{max}}$  (neat)/ $\text{cm}^{-1}$  2959, 2873, 2838, 2075, 1609, 1509, 1457, 1370, 1299, 1248, 1175, 1081, 1027, 960, 912, 829, 758, 709; Characterized as a mixture of two rotamers:  $\delta_{\text{H}}$  (400 MHz,  $\text{CDCl}_3$ ) 0.77 (3H, t,  $J = 7.4$ ,  $\text{CH}_2\text{CH}_3$ ), 0.91 (3H, t,  $J = 7.4$ ,  $\text{CH}_2\text{CH}_3$ ), 1.17-1.96 (4H, m,  $2 \times \text{CH}_2\text{CH}_3$ ), 3.79 (3H, s,  $\text{OCH}_3$  from 1 rotamer), 3.80 (3H, s,  $\text{OCH}_3$  from 1 rotamer), 4.55-4.77 (2H, m,  $\text{CH}_2\text{F}$ ), 6.86-7.61 (8H, m,  $\text{ArCH}$ );  $\delta_{\text{C}}$  (100 MHz,  $\text{CDCl}_3$ ) 14.5, 14.6, 17.3, 17.6, 27.6, 28.7, 44.4, 44.7, 55.2 ( $\times 2$ ), 87.1 (d,  $J = 182.6$ ,  $\text{CH}_2\text{F}$  for 1 rotamer), 87.3 (d,  $J = 183.1$ ,  $\text{CH}_2\text{F}$  for 1 rotamer), 87.7 (d,  $J = 19.4$ ,  $\text{CCH}_2\text{F}$  from 1 rotamer), 88.1 (d,  $J = 18.2$ ,  $\text{CCH}_2\text{F}$  from 1 rotamer), 113.5 ( $\times 2$ ), 121.1, 121.3, 122.8, 123.1, 127.4 ( $\times 2$ ), 127.5 ( $\times 2$ ), 128.4 ( $\times 2$ ), 133.6, 134.2, 139.2, 139.9, 146.7, 147.4, 159.0, 159.1;  $\delta_{\text{F}}$  (376 MHz,  $\text{CDCl}_3$ ) -219.8 (t,  $J = 47.9$ ,  $\text{CH}_2\text{F}$  from 1 rotamer), -218.8 (t,  $J = 48.0$ ,  $\text{CH}_2\text{F}$  from 1 rotamer);  $m/z$  (CI) 314 ( $\text{M}^+$ , 5), 280 (100);

### 1-(Fluoromethyl)-1-phenyl-1,3-dihydroisobenzofuran 2i



As for general procedure A, reaction of (2-(1-phenylvinyl)phenyl)methanol (45 mg, 0.214 mmol, 1 equiv) and Selectfluor (84 mg, 0.24 mmol, 1.1 equiv) gave after column chromatography on silica gel eluting with 10:1 hexane:EtOAc the title compound (38 mg, 0.167 mmol, 78%) as a colourless oil;  $\nu_{\max}$  (neat)/ $\text{cm}^{-1}$  3077, 3030, 2944, 2870, 2320, 2096, 1598, 1457, 1358, 1255, 1205, 1132, 1074, 1019, 919, 872, 755, 729, 695;  $\delta_{\text{H}}$  (600 MHz,  $\text{CDCl}_3$ ) 4.76 (1H, dd,  $J = 23.4, 9.8$ ,  $\text{CH}_a\text{H}_b\text{F}$ ), 4.84 (1H, dd,  $J = 22.6, 9.8$ ,  $\text{CH}_a\text{H}_b\text{F}$ ), 5.21 (1H, d,  $J = 12.2$ ,  $\text{CH}_a\text{H}_b\text{O}$ ), 5.27 (1H, d,  $J = 12.2$ ,  $\text{CH}_a\text{H}_b\text{O}$ ), 6.62 (7H, m, Ar-CH), 7.55 (2H, d,  $J = 7.3$ , Ar-CH);  $\delta_{\text{C}}$  (150 MHz,  $\text{CDCl}_3$ ) 72.6, 86.5 (d,  $J = 181.5$ ,  $\text{CH}_2\text{F}$ ), 90.0 (d,  $J = 19.0$ ,  $\text{CCH}_2\text{F}$ ), 121.4, 122.7, 125.9, 127.7, 128.1, 128.5, 128.6, 139.9, 140.7 (d,  $J = 2.8$ , ArC), 140.4 (d,  $J = 3.0$ , ArC);  $\delta_{\text{F}}$  (376 MHz,  $\text{CDCl}_3$ ) -222.7 (t,  $J = 47.6$ ,  $\text{CH}_2\text{F}$ );  $m/z$  (EI) 251 (M+Na, 5), 413 (100), 394 (18); HRMS for  $\text{C}_{15}\text{H}_{13}\text{OFNa}$  calculated for  $[\text{M}+\text{Na}]^+$ : 251.08426, found 251.08295.

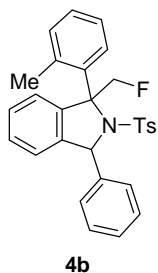
### 1-(Fluoromethyl)-1,3-diphenyl-2-tosylisoindoline 4a



As for general procedure A, reaction of 4-methyl-N-(phenyl(2-(1-phenylvinyl)phenyl)methyl)benzenesulfonamide (74 mg, 0.169 mmol, 1 equiv) and Selectfluor (66 mg, 0.19 mmol, 1.1 equiv) gave after column chromatography on silica gel eluting with 9:1 hexane:EtOAc the title compound (59 mg, 0.129 mmol, 77%) as a colourless oil and as a 1.2:1 mixture of diastereoisomers;  $\nu_{\max}$  (neat)/ $\text{cm}^{-1}$  3038, 2918, 1598, 1489, 1455, 1339, 1157, 1091, 1016, 912, 813, 737, 681; Characterized as a mixture of two diastereoisomers:  $\delta_{\text{H}}$  (600 MHz,  $\text{CDCl}_3$ ) 2.18 (3H, s,  $\text{CH}_3$ ), 2.28 (3H, s,  $\text{CH}_3$ ), 5.54-5.80 (4H, m,  $2 \times \text{CH}_2\text{F}$ ), 6.00 (1H, s, CHNTs), 6.22 (1H, s, CHNTs), 6.24 (2H, d,  $J = 8.3$ ,  $2 \times$  Ar-CH from Ts), 6.61 (2H, d,  $J = 8.3$ ,  $2 \times$  Ar-CH from Ts), 6.79-6.94 (6H, m, Ar-CH), 7.02-7.12 (8H, m, Ar-CH), 7.20-7.26 (10H, m, Ar-CH), 7.34-7.47 (8H, m, Ar-CH);  $\delta_{\text{C}}$  (150 MHz,  $\text{CDCl}_3$ ) 21.4, 21.5, 70.1, 70.3, 76.1 (d,  $J = 18.9$ ,  $\text{CCH}_2\text{F}$  from major dias.), 76.2 (d,  $J = 19.0$ ,  $\text{CCH}_2\text{F}$  from minor dias.), 85.7 (d,  $J = 177.2$ ,  $\text{CH}_2\text{F}$  from minor dias.), 86.5 (d,  $J = 176.6$ ,  $\text{CH}_2\text{F}$  from major dias.), 123.4, 123.4, 123.4, 123.5, 123.8, 123.9, 126.8, 127.5, 128.0, 128.0, 128.1 ( $\times 2$ ), 128.1, 128.2, 128.3, 128.3, 128.4, 128.4, 128.5, 128.8, 128.8, 129.0, 129.9, 136.8, 138.8, 139.4, 139.6, 139.6, 140.1, 140.5, 141.5, 141.5, 141.7, 141.9, 142.1, 142.6;  $\delta_{\text{F}}$  (564 MHz,  $\text{CDCl}_3$ ) -223.3 (t,  $J = 46.6$ ,  $\text{CH}_2\text{F}$  from major dias.), -221.9 (t,  $J = 46.9$ ,  $\text{CH}_2\text{F}$  from minor dias.);  $m/z$  (EI) 424 (M- $\text{CH}_2\text{F}$ , 42), 154 (100), 91 (95), 217 (59).

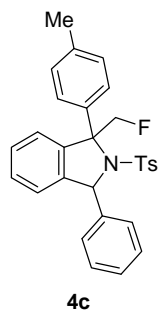


### 1-(Fluoromethyl)-3-phenyl-1-o-tolyl-2-tosylisoindoline 4b



As for general procedure A, reaction of 4-methyl-N-(phenyl(2-(1-o-tolylvinyl)phenyl)methyl)benzenesulfonamide (43 mg, 0.0948 mmol, 1 equiv) and Selectfluor (40 mg, 0.11 mmol, 1.2 equiv) gave after column chromatography on silica gel eluting with 8:1 hexane:EtOAc the title compound (36 mg, 0.076 mmol, 81%) as a yellow oil and as a 1.2:1 mixture of diastereoisomers;  $\nu_{\max}$  (neat)/ $\text{cm}^{-1}$  3065, 3034, 2925, 1598, 1491, 1457, 1342, 1287, 1159, 1091, 1019, 910, 871, 812, 732, 700, 670; Characterized as a mixture of two diastereoisomers:  $\delta_{\text{H}}$  (600 MHz,  $\text{CDCl}_3$ ) 0.97 (3H, s,  $\text{CH}_3$ ), 1.61 (3H, s,  $\text{CH}_3$ ), 2.21 (3H, s,  $\text{CH}_3$ ), 2.32 (3H, s,  $\text{CH}_3$ ), 5.28-5.83 (4H, m,  $2 \times \text{CH}_2\text{F}$ ), 5.98 (1H, s,  $\text{CHNTs}$ ), 6.20 (2H, d,  $J = 8.3$ ,  $2 \times \text{Ar-CH}$  from Ts), 6.33 (1H, s,  $\text{CHNTs}$ ), 6.66 (2H, d,  $J = 8.0$ ,  $2 \times \text{Ar-CH}$  from Ts), 6.74-7.01 (10H, m,  $\text{Ar-CH}$ ), 6.20-7.38 (16H, m,  $\text{Ar-CH}$ ), 7.50 (2H, d,  $J = 7.2$ ,  $2 \times \text{Ar-CH}$ ), 7.65-7.70 (2H, m,  $\text{Ar-CH}$ );  $\delta_{\text{C}}$  (150 MHz,  $\text{CDCl}_3$ ) 20.1, 21.5, 21.6, 22.2, 70.2, 70.2, 75.8 (d,  $J = 17.4$ ,  $\text{CCH}_2\text{F}$  from major dias.), 76.0 (d,  $J = 19.8$ ,  $\text{CCH}_2\text{F}$  from minor dias.), 87.0 (d,  $J = 178.2$ ,  $\text{CH}_2\text{F}$  from major dias.), 87.4 (d,  $J = 180.5$ ,  $\text{CH}_2\text{F}$  from minor dias.), 122.9, 123.2, 123.5, 123.5, 123.8, 125.8, 125.9, 126.6, 127.5, 128.1, 128.2, 128.2, 128.3, 128.3, 128.4, 128.4, 128.6, 128.7, 128.7, 128.8, 128.9, 129.4, 129.8, 131.7, 131.8, 132.7, 133.0, 134.8, 135.6, 136.4, 137.9, 138.6, 138.9, 139.1, 140.5, 141.0, 141.4, 142.2, 142.3, 142.8;  $\delta_{\text{F}}$  (564 MHz,  $\text{CDCl}_3$ ) -220.4 (t,  $J = 46.5$ ,  $\text{CH}_2\text{F}$  from 1 diastereoisomer), -215.4 (t,  $J = 47.0$ ,  $\text{CH}_2\text{F}$  from 1 diastereoisomer);  $m/z$  (CI) 472 ( $\text{M}+\text{H}$ , 5), 316 (100), 452 (61), 296 (49); HRMS for  $\text{C}_{29}\text{H}_{26}\text{O}_2\text{NFNaS}$  calculated for  $[\text{M}+\text{Na}]^+$ : 494.15605, found 494.15601.

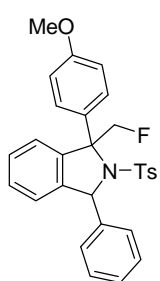
### 1-(Fluoromethyl)-3-phenyl-1-p-tolyl-2-tosylisoindoline 4c



As for general procedure A, reaction of 4-methyl-N-(phenyl(2-(1-p-tolylvinyl)phenyl)methyl)benzenesulfonamide (36 mg, 0.0795 mmol, 1 equiv) and Selectfluor (34 mg, 0.10 mmol, 1.2 equiv) gave after column chromatography on silica gel eluting with 8:1 hexane:EtOAc the title compound (30 mg, 0.0637 mmol, 80%) as a yellow oil and as a 1.2:1 mixture of diastereoisomers;  $\nu_{\max}$  (neat)/ $\text{cm}^{-1}$  3033, 2920, 1599, 1457, 1339, 1157, 1091, 1022, 912, 814, 732, 699; Characterized as a mixture of two diastereoisomers:  $\delta_{\text{H}}$  (600 MHz,  $\text{CDCl}_3$ ) 2.19 (3H, s,  $\text{CH}_3$ ), 2.28 (3H, s,  $\text{CH}_3$ ), 2.33 (3H, s,  $\text{CH}_3$ ), 2.42 (3H, s,  $\text{CH}_3$ ), 5.52-5.77 (4H, m,  $2 \times \text{CH}_2\text{F}$ ), 6.02 (1H, s,  $\text{CHNTs}$ ), 6.20 (1H, s,  $\text{CHNTs}$ ), 6.29 (2H, d,  $J = 8.3$ ,  $2 \times \text{Ar-CH}$  from Ts),

6.62 (2H, d,  $J = 8.3$ ,  $2 \times \text{Ar-CH}$  from Ts), 6.78-7.03 (12H, m, Ar-CH), 7.10-7.35 (18H, m, Ar-CH);  $\delta_{\text{C}}$  (150 MHz,  $\text{CDCl}_3$ ) 21.3, 21.3, 21.4, 21.5, 70.1, 70.3, 76.1 (d,  $J = 18.9$ ,  $\text{CCH}_2\text{F}$  from major dias.), 76.1 (d,  $J = 19.0$ ,  $\text{CCH}_2\text{F}$  from minor dias.), 85.7 (d,  $J = 177.0$ ,  $\text{CH}_2\text{F}$  from major dias.), 86.6 (d,  $J = 176.5$ ,  $\text{CH}_2\text{F}$  from minor dias.), 123.3 ( $\times 2$ ), 123.5, 123.8, 126.9, 127.5, 127.9 ( $\times 2$ ), 128.1, 128.1, 128.2, 128.2, 128.3, 128.3, 128.5, 128.7 ( $\times 2$ ), 128.7, 128.9, 129.0, 129.1, 129.9, 132.8, 136.7, 137.1, 137.2, 137.9, 138.3, 138.9, 139.5, 140.4, 141.6, 141.8, 141.9, 142.2, 142.5;  $\delta_{\text{F}}$  (564 MHz,  $\text{CDCl}_3$ ) -223.4 (t,  $J = 46.6$ ,  $\text{CH}_2\text{F}$  from 1 diastereoisomer), -222.0 (t,  $J = 47.0$ ,  $\text{CH}_2\text{F}$  from 1 diastereoisomer);  $m/z$  (EI) 471 ( $\text{M}^+$ , 3), 439 (100); HRMS for  $\text{C}_{29}\text{H}_{26}\text{O}_2\text{NFNaS}$  calculated for  $[\text{M}+\text{Na}]^+$ : 494.15605, found 494.15561.

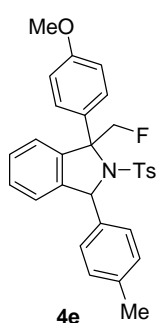
#### 1-(Fluoromethyl)-1-(4-methoxyphenyl)-3-phenyl-2-tosylisoindoline 4d



**4d**

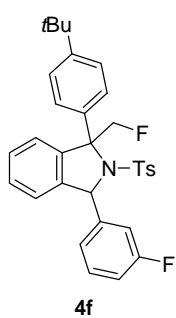
As for general procedure A, reaction of N-((2-(1-(4-methoxyphenyl)vinyl)phenyl)(phenyl)methyl)-4-methylbenzenesulfonamide (40 mg, 0.0853 mmol, 1 equiv) and Selectfluor (33 mg, 0.09 mmol, 1.1 equiv) gave after column chromatography on silica gel eluting with 8:1 hexane:EtOAc the title compound (33 mg, 0.0678 mmol, 79%) as a yellow oil and as a 1.2:1 mixture of diastereoisomers;  $\nu_{\text{max}}$  (neat)/ $\text{cm}^{-1}$  3067, 2927, 1606, 1513, 1458, 1340, 1253, 1157, 1090, 1023, 912, 838, 812, 732, 700, 671; Characterized as a mixture of two diastereoisomers:  $\delta_{\text{H}}$  (600 MHz,  $\text{CDCl}_3$ ) 2.19 (3H, s,  $\text{CH}_3$ ), 2.29 (3H, s,  $\text{CH}_3$ ), 3.80 (3H, s,  $\text{OCH}_3$ ), 3.88 (3H, s,  $\text{OCH}_3$ ), 5.51-5.76 (4H, m,  $2 \times \text{CH}_2\text{F}$ ), 5.98 (1H, s,  $\text{CHNTs}$ ), 6.19 (1H, s,  $\text{CHNTs}$ ), 6.29 (2H, d,  $J = 8.2$ ,  $2 \times \text{ArCH}$ ), 6.63 (2H, d,  $J = 8.2$ ,  $2 \times \text{ArCH}$ ), 6.70 (2H, d,  $J = 8.7$ ,  $2 \times \text{ArCH}$ ), 6.79 (2H, d,  $J = 7.5$ ,  $2 \times \text{ArCH}$ ), 6.85 (2H, d,  $J = 7.5$ ,  $2 \times \text{ArCH}$ ), 6.90-7.38 (24H, m, ArCH);  $\delta_{\text{C}}$  (150 MHz,  $\text{CDCl}_3$ ) 21.4, 21.5, 55.4, 55.6, 70.0, 70.2, 75.9 (d,  $J = 18.8$ ,  $\text{CCH}_2\text{F}$  from major dias.), 75.9 (d,  $J = 19.7$ ,  $\text{CCH}_2\text{F}$  from minor dias.), 85.7 (d,  $J = 177.1$ ,  $\text{CH}_2\text{F}$  from major dias.), 86.4 (d,  $J = 176.8$ ,  $\text{CH}_2\text{F}$  from minor dias.), 113.5, 113.7, 123.4, 123.5, 123.8, 126.6, 126.8, 127.3, 127.5, 127.7, 127.8, 127.9, 128.1, 128.1, 128.2, 128.3, 128.3, 128.5, 128.7, 128.8, 129.5, 129.6, 129.9, 130.4, 137.0, 139.0, 139.5, 140.4, 141.5, 141.6, 141.9, 142.0, 142.2, 142.52, 159.3, 159.6;  $\delta_{\text{F}}$  (564 MHz,  $\text{CDCl}_3$ ) -223.0 (t,  $J = 46.6$ ,  $\text{CH}_2\text{F}$  from 1 diastereoisomer), -221.2 (t,  $J = 47.0$ ,  $\text{CH}_2\text{F}$  from 1 diastereoisomer);  $m/z$  (EI) 487 ( $\text{M}^+$ , 5), 454 (100); HRMS for  $\text{C}_{29}\text{H}_{26}\text{O}_3\text{NFNaS}$  calculated for  $[\text{M}+\text{Na}]^+$ : 510.15096, found 510.15036.

### 1-(Fluoromethyl)-1-(4-methoxyphenyl)-3-p-tolyl-2-tosylisoindoline 4e



As for general procedure A, reaction of N-((2-(1-(4-methoxyphenyl)vinyl)phenyl)(p-tolyl)methyl)-4-methylbenzenesulfonamide (35 mg, 0.0725 mmol, 1 equiv) and Selectfluor (31 mg, 0.09 mmol, 1.2 equiv) gave after column chromatography on silica gel eluting with 8:1 hexane:EtOAc the title compound (28 mg, 0.0559 mmol, 77%) as a yellow oil and as a 1.2:1 mixture of diastereoisomers;  $\nu_{\max}$  (neat)/ $\text{cm}^{-1}$  3022, 2928, 1739, 1606, 1512, 1458, 1338, 1251, 1157, 1088, 1020, 913, 836, 726, 668; Characterized as a mixture of two diastereoisomers:  $\delta_{\text{H}}$  (600 MHz,  $\text{CDCl}_3$ ) 2.20 (3H, s,  $\text{CH}_3$ ), 2.30 (6H, s,  $2 \times \text{CH}_3$ ), 2.32 (3H, s,  $\text{CH}_3$ ), 3.80 (3H, s,  $\text{OCH}_3$ ), 3.87 (3H, s,  $\text{OCH}_3$ ), 5.50-5.76 (4H, m,  $2 \times \text{CH}_2\text{F}$ ), 5.94 (1H, s,  $\text{CHNTs}$ ), 6.15 (1H, s,  $\text{CHNTs}$ ), 6.32 (2H, d,  $J = 8.3$ ,  $2 \times \text{ArCH}$ ), 6.63 (2H, d,  $J = 8.3$ ,  $2 \times \text{ArCH}$ ), 6.63 (2H, d,  $J = 9.0$ ,  $2 \times \text{ArCH}$ ), 6.80 (2H, d,  $J = 7.3$ ,  $2 \times \text{ArCH}$ ), 6.86 (2H, d,  $J = 7.3$ ,  $2 \times \text{ArCH}$ ), 6.89 (12H, m,  $\text{ArCH}$ ), 7.02 (2H, d,  $J = 7.3$ ,  $2 \times \text{ArCH}$ ), 7.07 (2H, d,  $J = 7.3$ ,  $2 \times \text{ArCH}$ ), 7.18-7.24 (4H, m,  $\text{ArCH}$ ), 7.37 (2H, d,  $J = 8.8$ ,  $2 \times \text{ArCH}$ );  $\delta_{\text{C}}$  (150 MHz,  $\text{CDCl}_3$ ) 21.3, 21.3, 21.4, 21.5, 55.4, 55.5, 69.7, 70.0, 75.7 (d,  $J = 15.9$ ,  $\text{CCH}_2\text{F}$  from major dias.), 75.8 (d,  $J = 18.9$ ,  $\text{CCH}_2\text{F}$  from minor dias.), 85.8 (d,  $J = 177.4$ ,  $\text{CH}_2\text{F}$  from major dias.), 86.5 (d,  $J = 176.8$ ,  $\text{CH}_2\text{F}$  from minor dias.), 113.5, 113.7, 123.4, 123.5, 123.5, 123.9, 126.9, 127.5, 128.0 ( $\times 2$ ), 128.2, 128.7, 128.7, 128.7, 128.9, 129.2, 129.6, 129.8, 130.4, 131.8, 131.9, 133.7, 136.5, 137.1, 137.7, 137.9, 139.0, 139.1, 140.5, 141.6, 141.6, 141.8, 142.1, 142.4, 159.2, 159.6;  $\delta_{\text{F}}$  (376 MHz,  $\text{CDCl}_3$ ) -222.7 (t,  $J = 46.6$ ,  $\text{CH}_2\text{F}$  from 1 diastereoisomer), -221.0 (t,  $J = 47.1$ ,  $\text{CH}_2\text{F}$  from 1 diastereoisomer);  $m/z$  (EI) 501 ( $\text{M}^+$ , 5), 468 (100); HRMS for  $\text{C}_{30}\text{H}_{28}\text{O}_3\text{NFNaS}$  calculated for  $[\text{M}+\text{Na}]^+$ : 524.16661, found 524.16559.

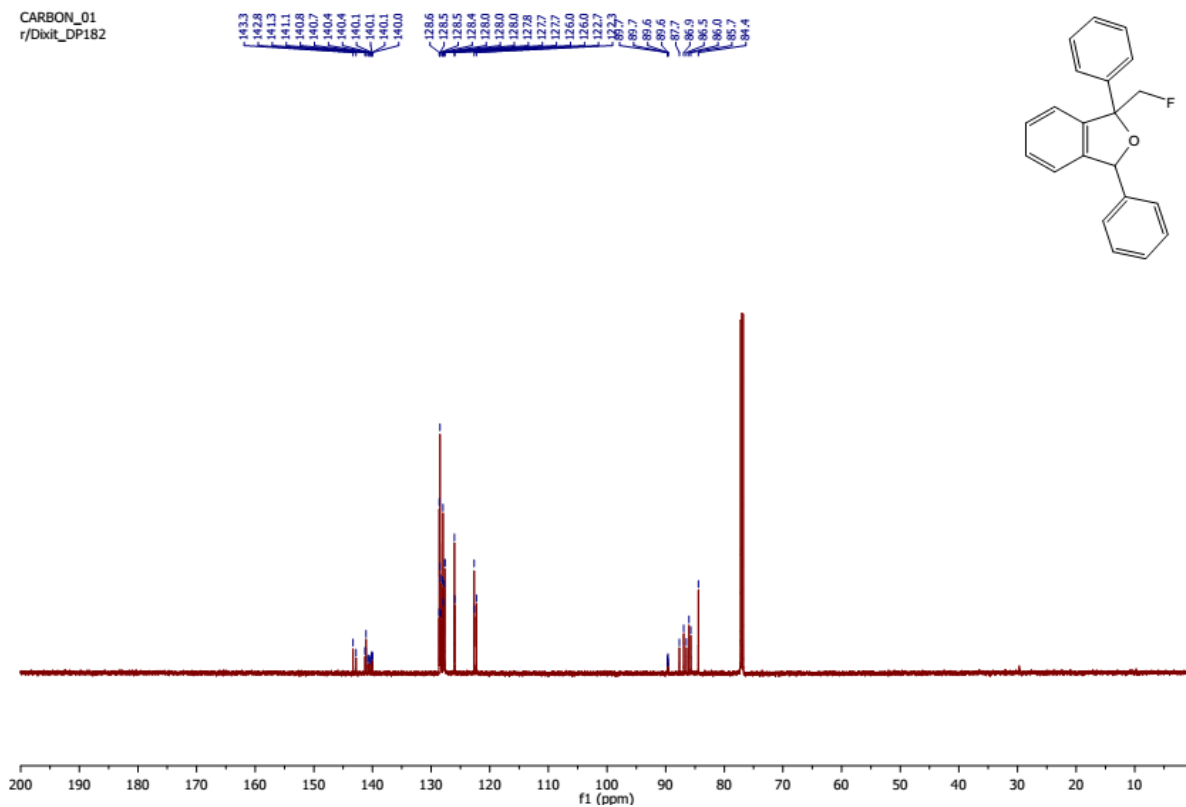
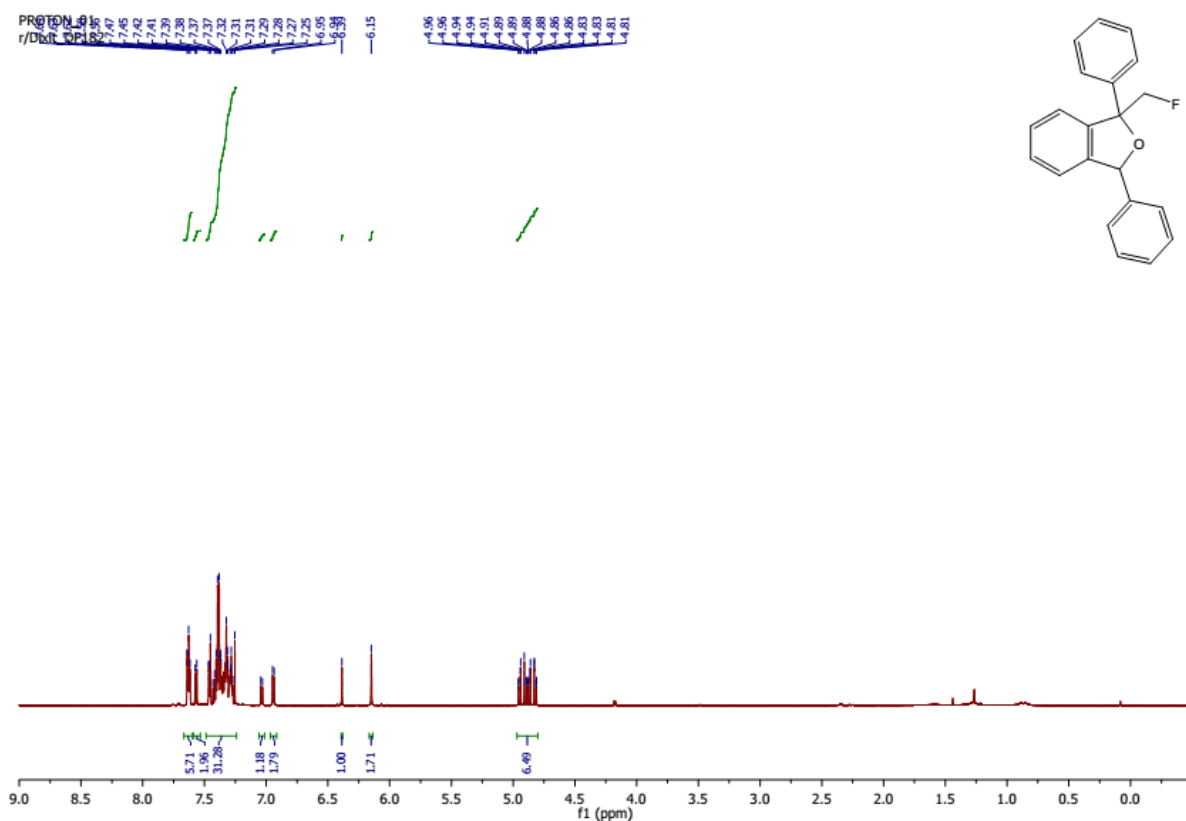
### 1-(4-Tert-butylphenyl)-1-(fluoromethyl)-3-(3-fluorophenyl)-2-tosylisoindoline 4f



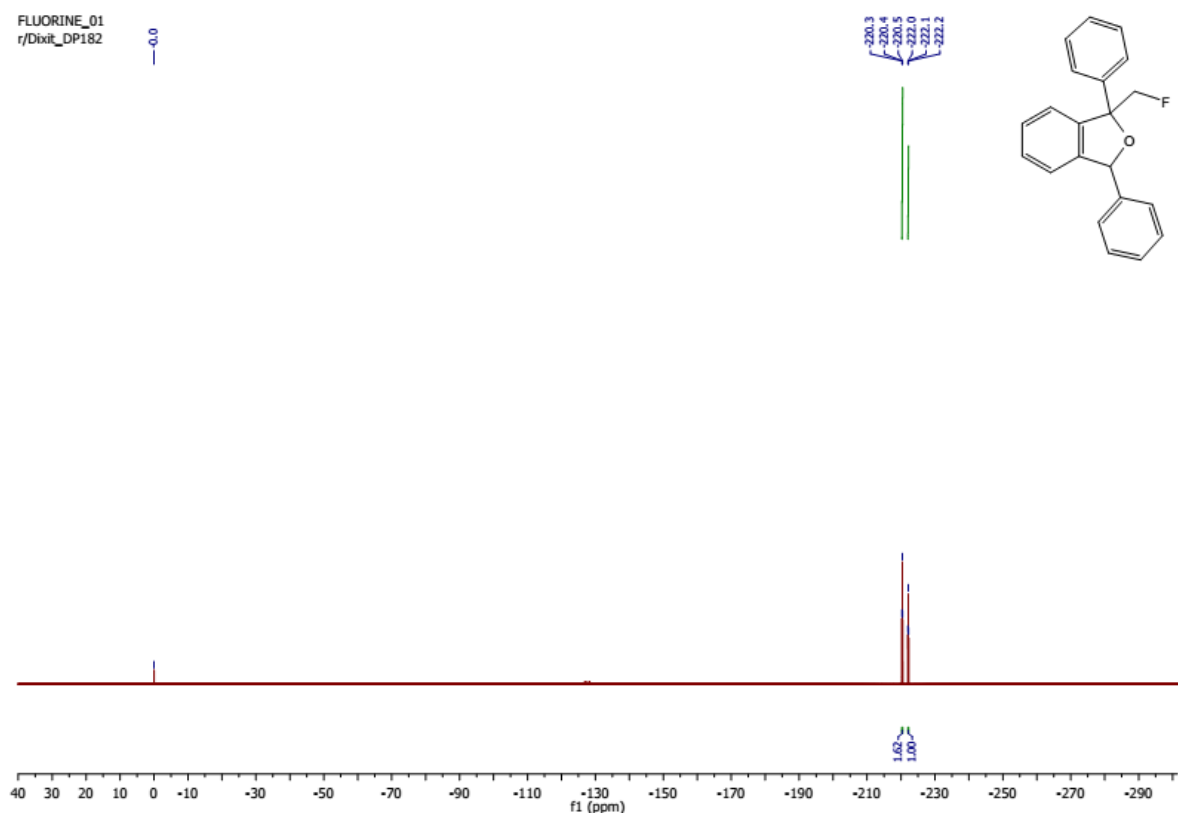
As for general procedure A, reaction of N-((2-(1-(4-tert-butylphenyl)vinyl)phenyl)(3-fluorophenyl)methyl)-4-methylbenzenesulfonamide (44 mg, 0.0857 mmol, 1 equiv) and Selectfluor (36 mg, 0.10 mmol, 1.2 equiv) gave after column chromatography on silica gel eluting with 8:1 hexane:EtOAc the title compound (43 mg, 0.009 mmol, 94%) as a yellow oil and as a 1.2:1 mixture of diastereoisomers;  $\nu_{\max}$  (neat)/ $\text{cm}^{-1}$  3040, 2960, 2870, 1596, 1485, 1456, 1343, 1264, 1158, 1090, 1022, 948, 911, 885, 840, 811, 784, 727, 668; Characterized as a mixture of two diastereoisomers:  $\delta_{\text{H}}$  (600 MHz,  $\text{CDCl}_3$ ) 1.32 (9H, s,  $3 \times \text{CH}_3$  from tBu), 1.40

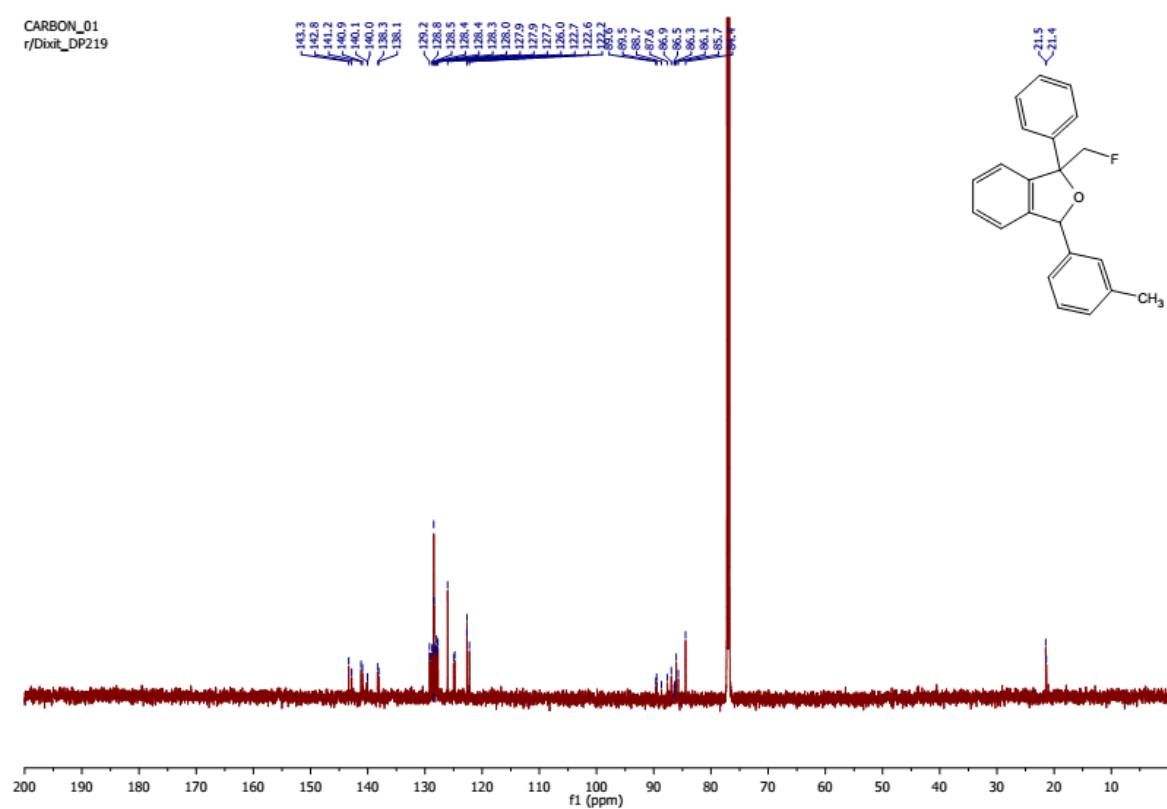
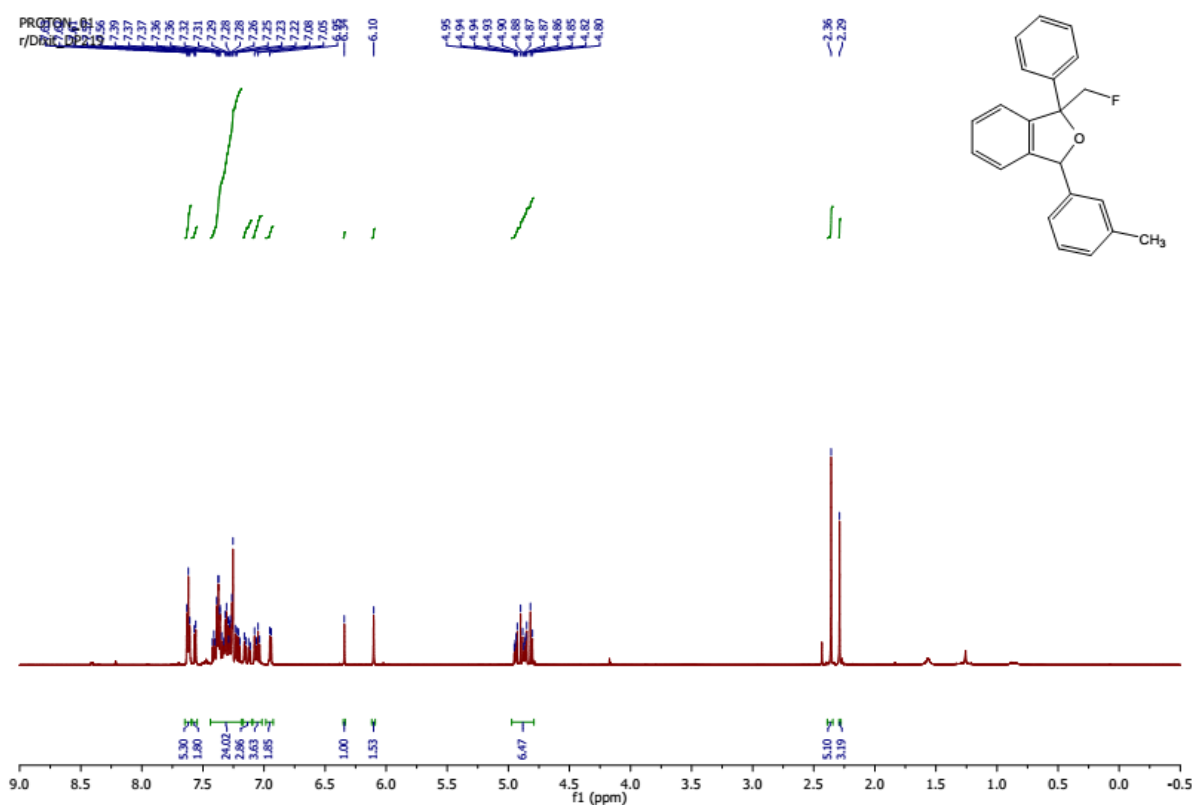
(9H, s, 3 × CH<sub>3</sub> from tBu), 2.19 (3H, s, CH<sub>3</sub>), 2.29 (3H, s, CH<sub>3</sub>), 5.48-5.75 (4H, m, 2 × CH<sub>2</sub>F), 5.94 (1H, s, CHNTs), 6.20 (1H, s, CHNTs), 6.22 (2H, d, *J* = 8.3, 2 × Ar-CH from Ts), 6.62 (2H, d, *J* = 8.3, 2 × Ar-CH from Ts), 6.80-7.29 (24H, m, Ar-CH), 7.36 (2H, d, *J* = 8.4, 2 × Ar-CH), 7.43 (2H, d, *J* = 8.4, 2 × Ar-CH); δ<sub>C</sub> (150 MHz, CDCl<sub>3</sub>) 21.4, 21.5, 31.5, 31.5, 34.7, 34.8, 69.5, 69.6, 76.0 (d, *J* = 18.9, CCH<sub>2</sub>F from major dias.), 76.1 (d, *J* = 18.9, CCH<sub>2</sub>F from minor dias.), 85.7 (d, *J* = 176.8, CH<sub>2</sub>F from major dias.), 86.5 (d, *J* = 176.3, CH<sub>2</sub>F from minor dias.), 114.9, 115.0, 115.2, 116.3, 116.4, 123.2, 123.4, 123.5, 123.6, 123.9, 125.2, 125.4, 125.6, 126.7, 127.5, 127.9, 128.2, 128.5, 128.8, 128.9, 128.9, 129.7, 129.7, 129.9, 130.0, 136.1, 136.3, 136.7, 138.9, 139.8, 141.0, 141.5, 142.0, 142.1, 142.2, 142.7, 144.7, 144.8, 151.1, 151.8, 162.8 (d, *J* = 246.4, ArCF), 163.0 (d, *J* = 245.8, ArCF); δ<sub>F</sub> (564 MHz, CDCl<sub>3</sub>) -224.2 (t, *J* = 46.5, CH<sub>2</sub>F from 1 diastereoisomer), -222.2 (t, *J* = 46.9, CH<sub>2</sub>F from 1 diastereoisomer), -114.0 (dd, *J* = 14.9, 8.9, Ar-CF from 1 diastereoisomer), -113.4 (dd, *J* = 14.8, 8.9, Ar-CF from 1 diastereoisomer); *m/z* (CI) 531 (M+H, 5), 398 (100), 376 (84), 512 (72), 328 (48), 498 (45); HRMS for C<sub>32</sub>H<sub>31</sub>O<sub>2</sub>NF<sub>2</sub>NaS calculated for [M+Na]<sup>+</sup>: 554.19358, found 554.19360.

# $^1\text{H}$ NMR, $^{13}\text{C}$ NMR and $^{19}\text{F}$ NMR Spectra of new compounds

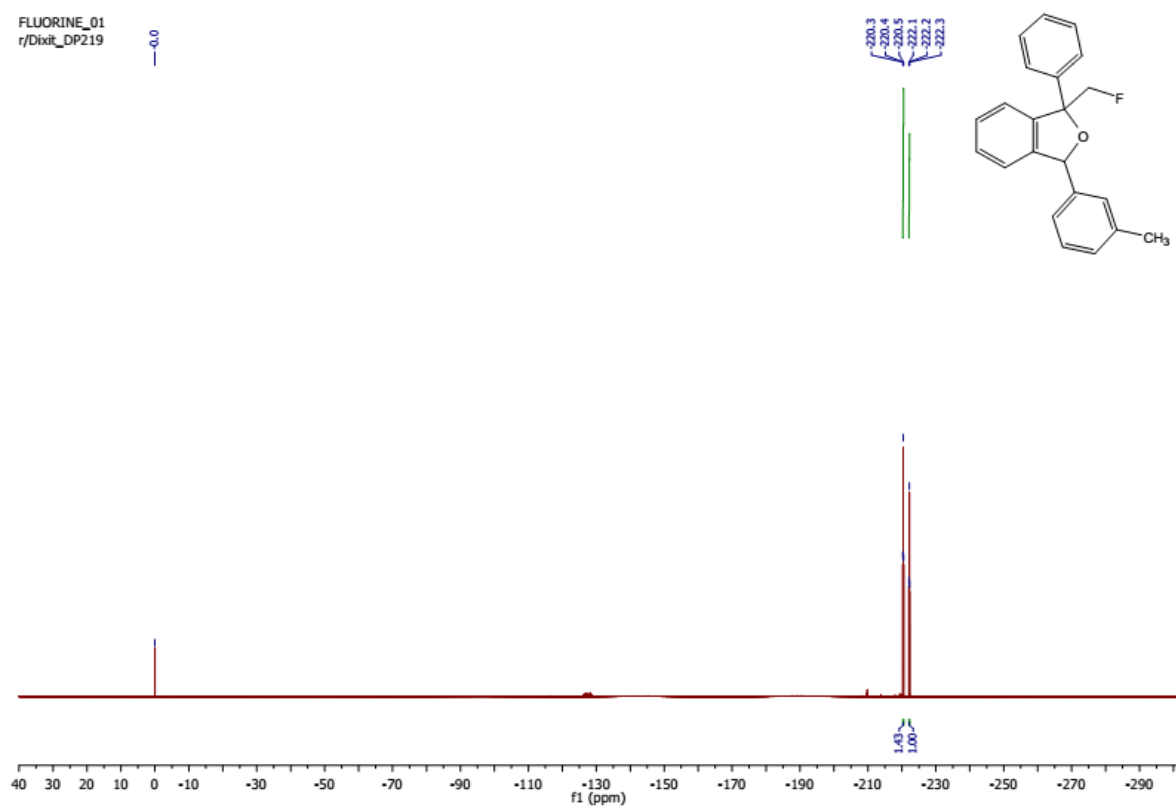


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r/Dxit\_DP182

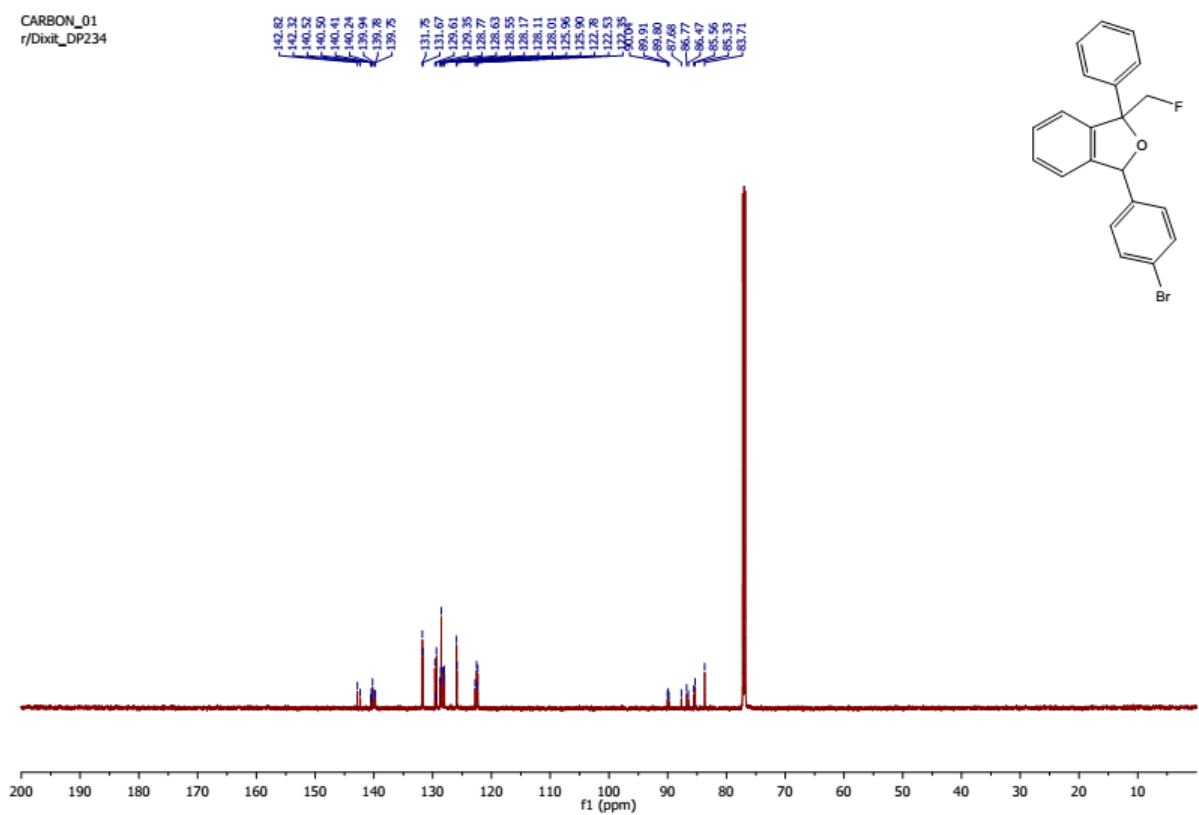
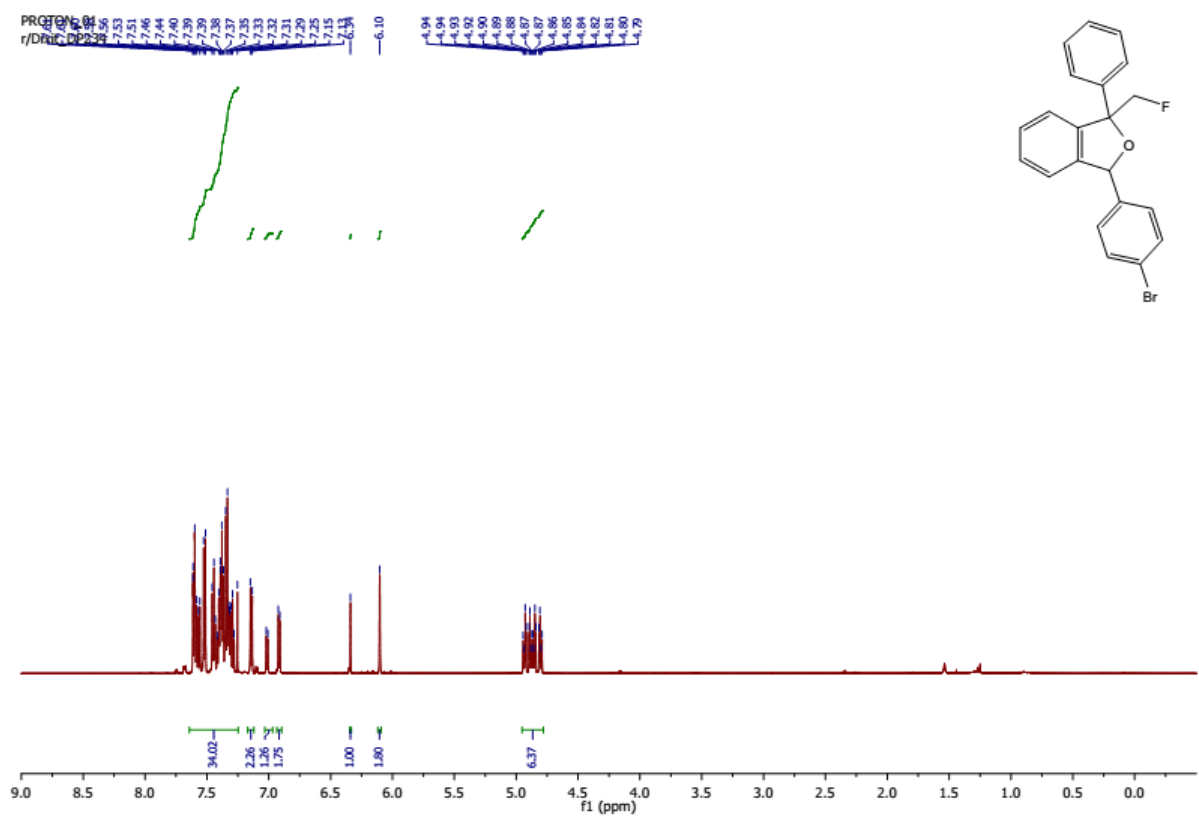




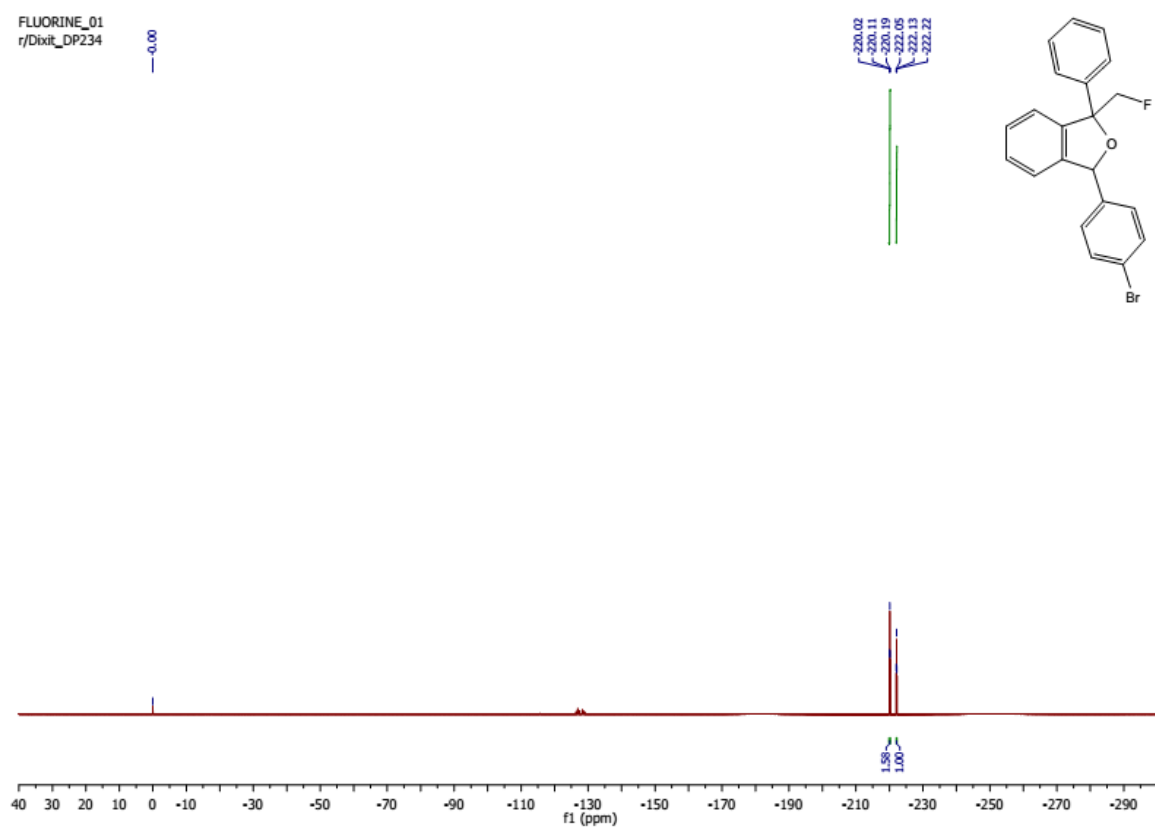
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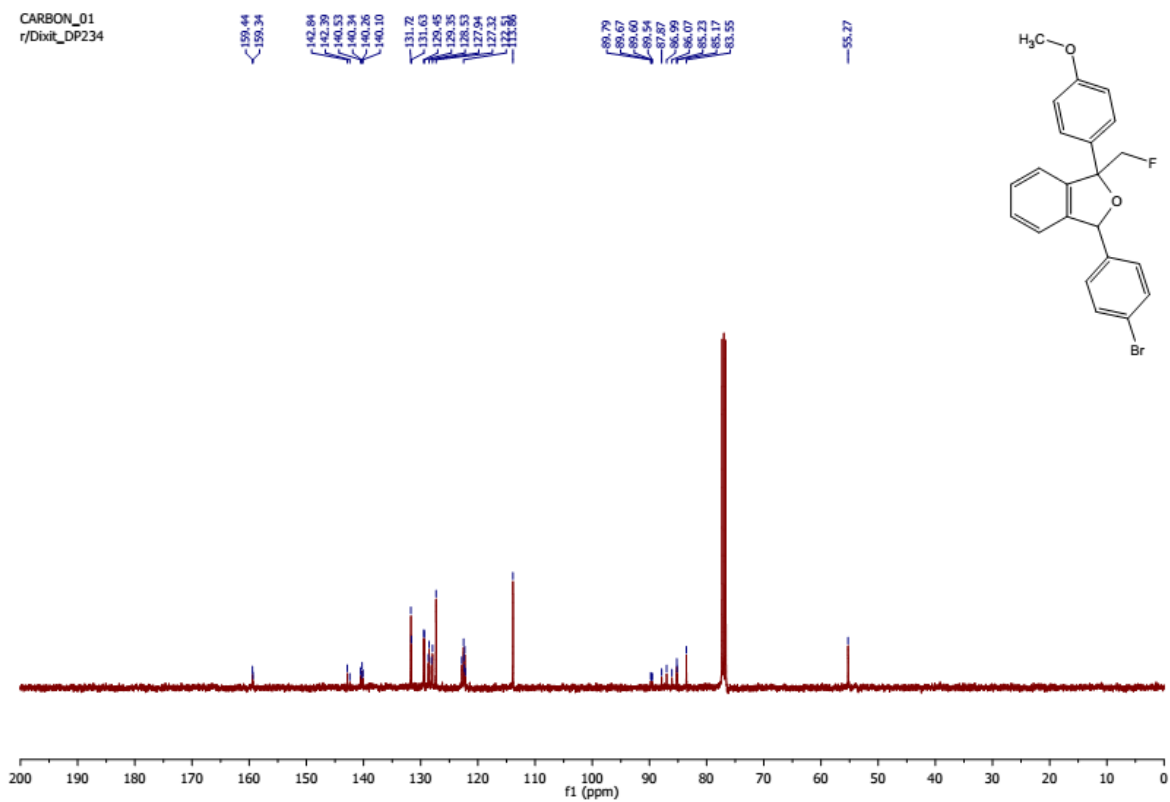
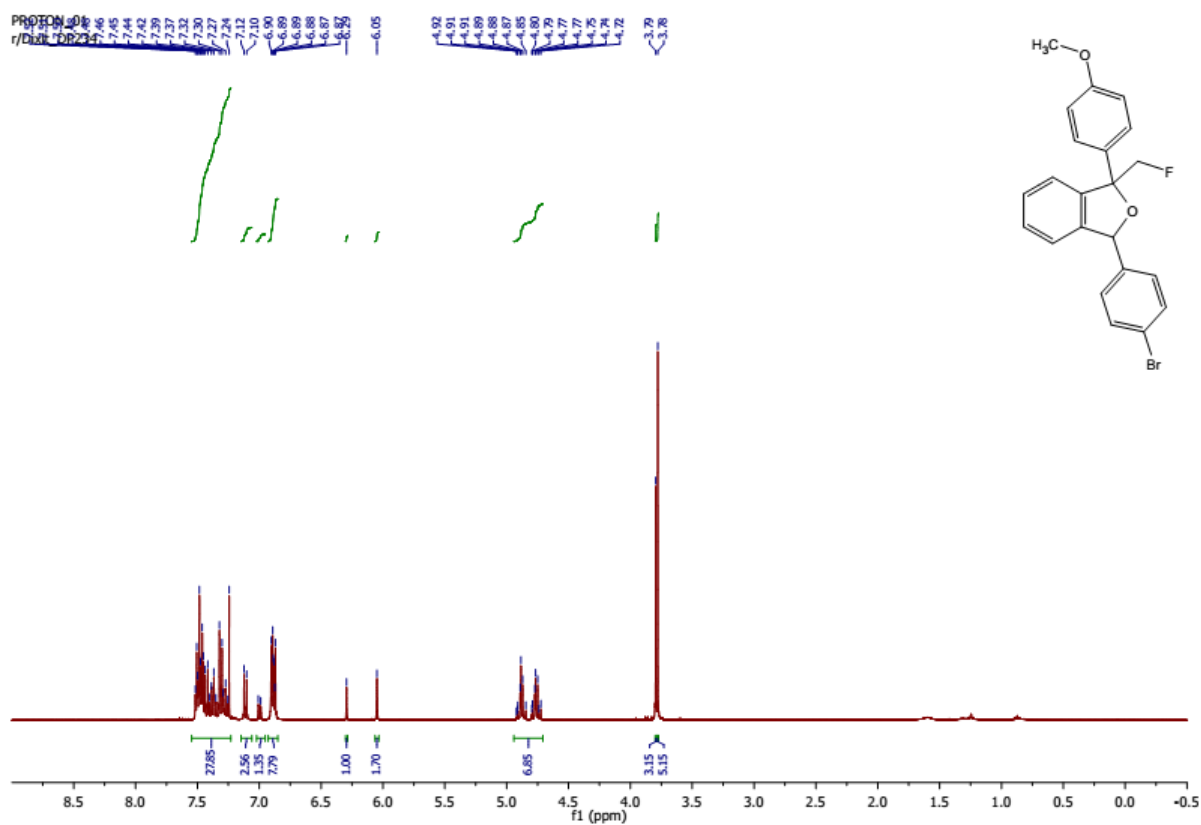




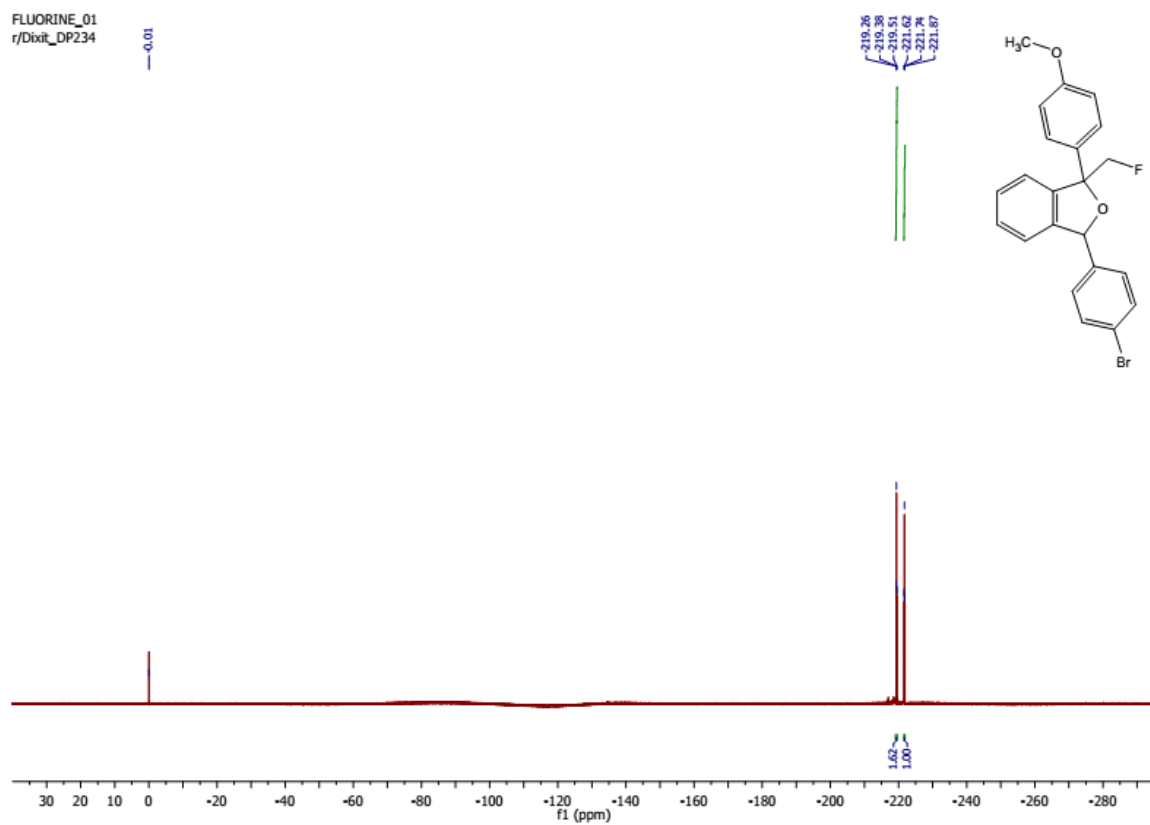


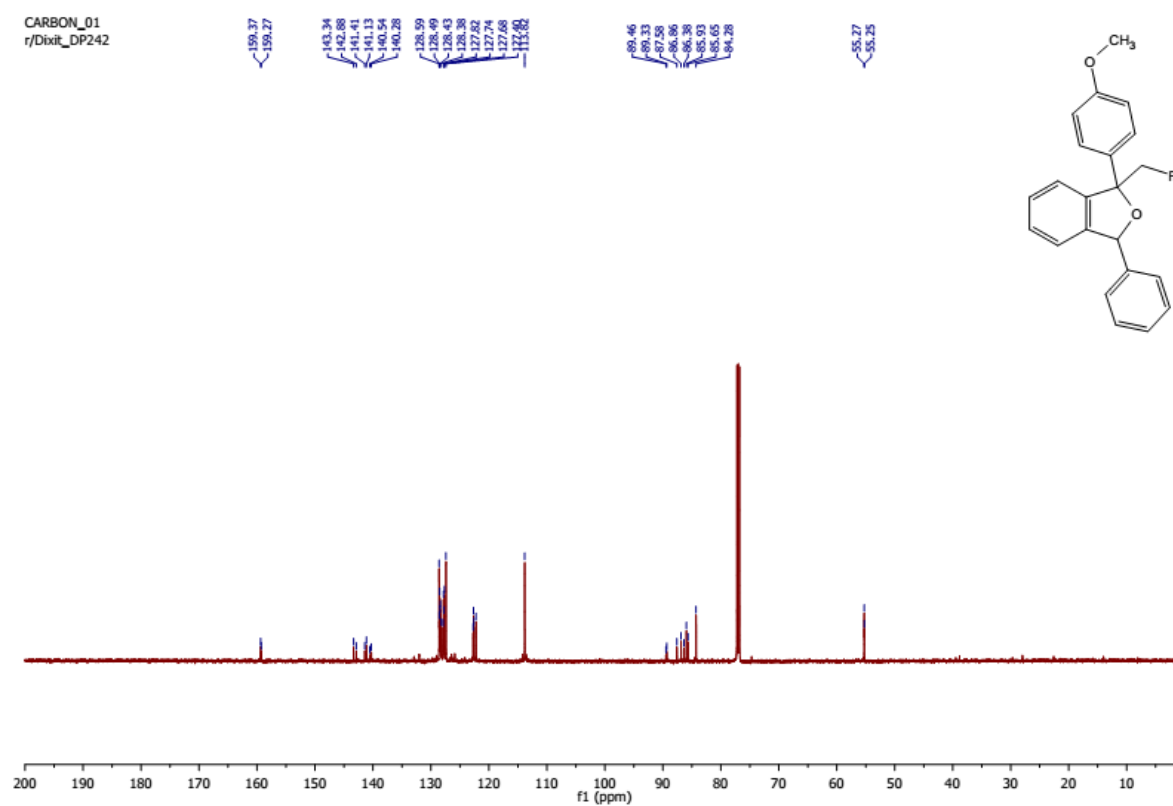
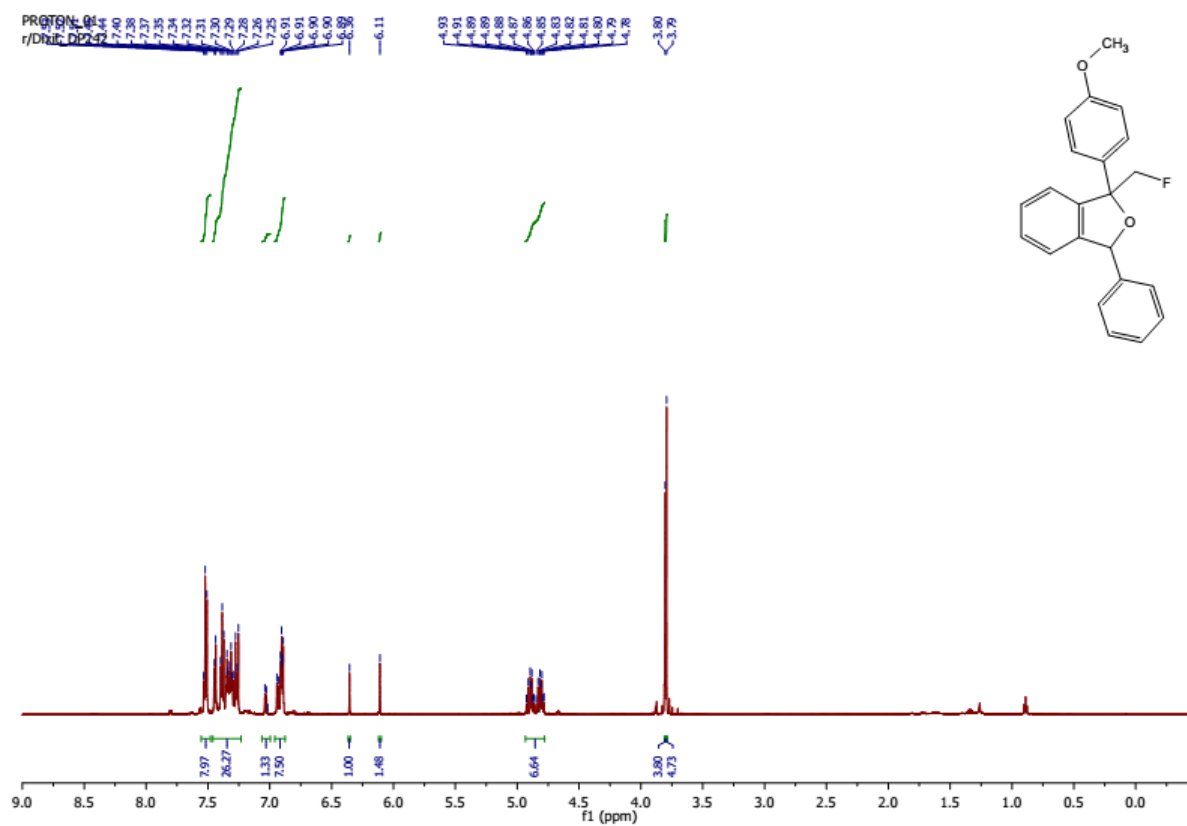
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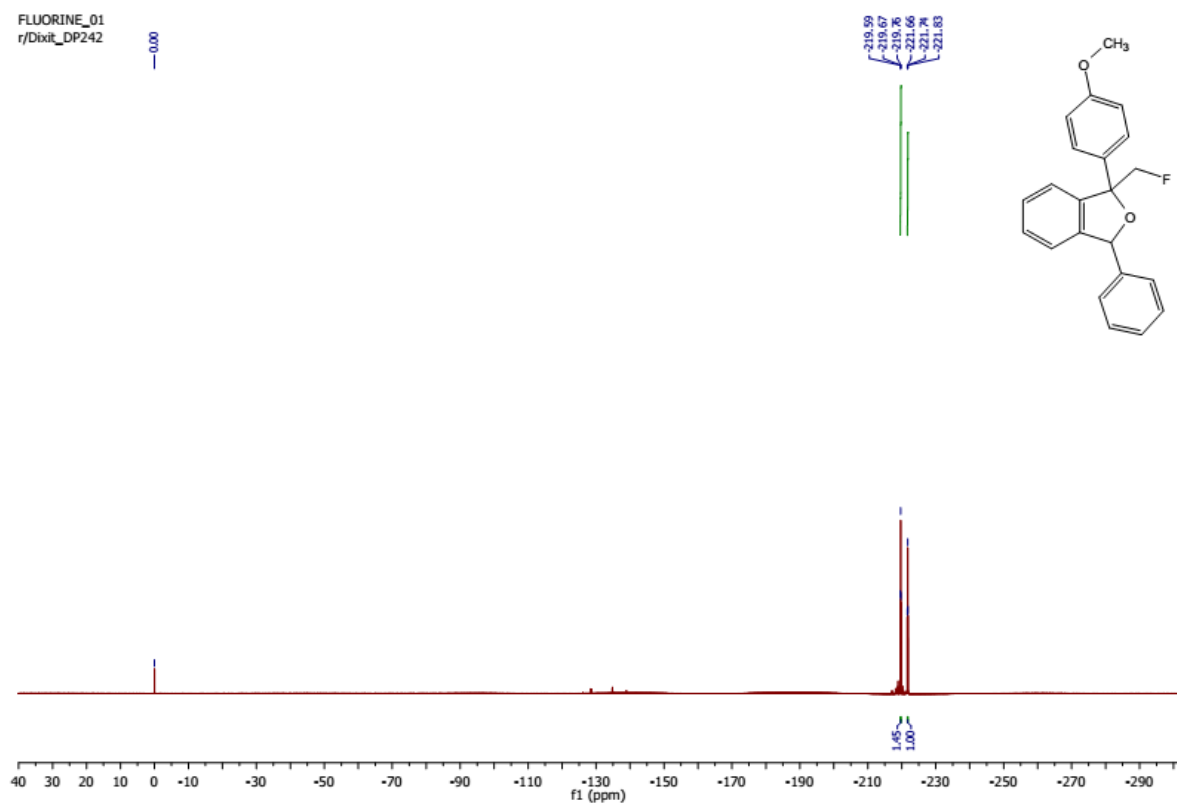


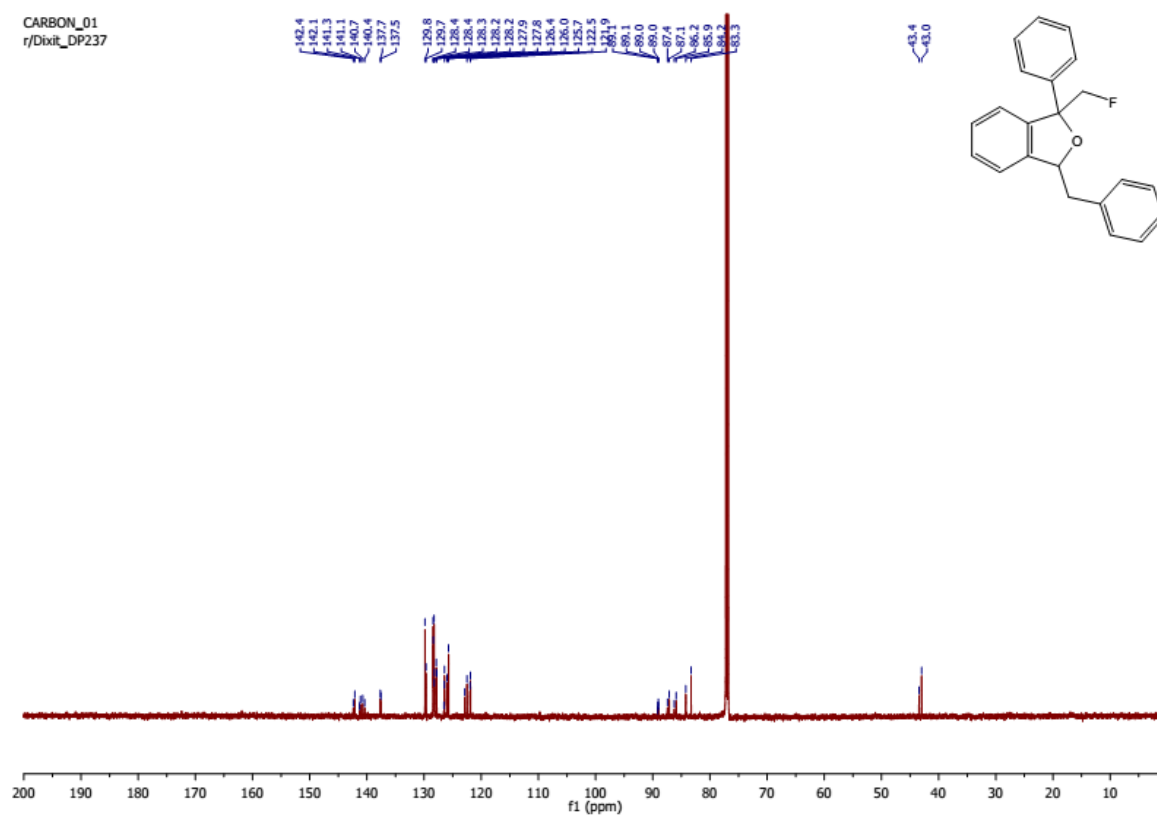
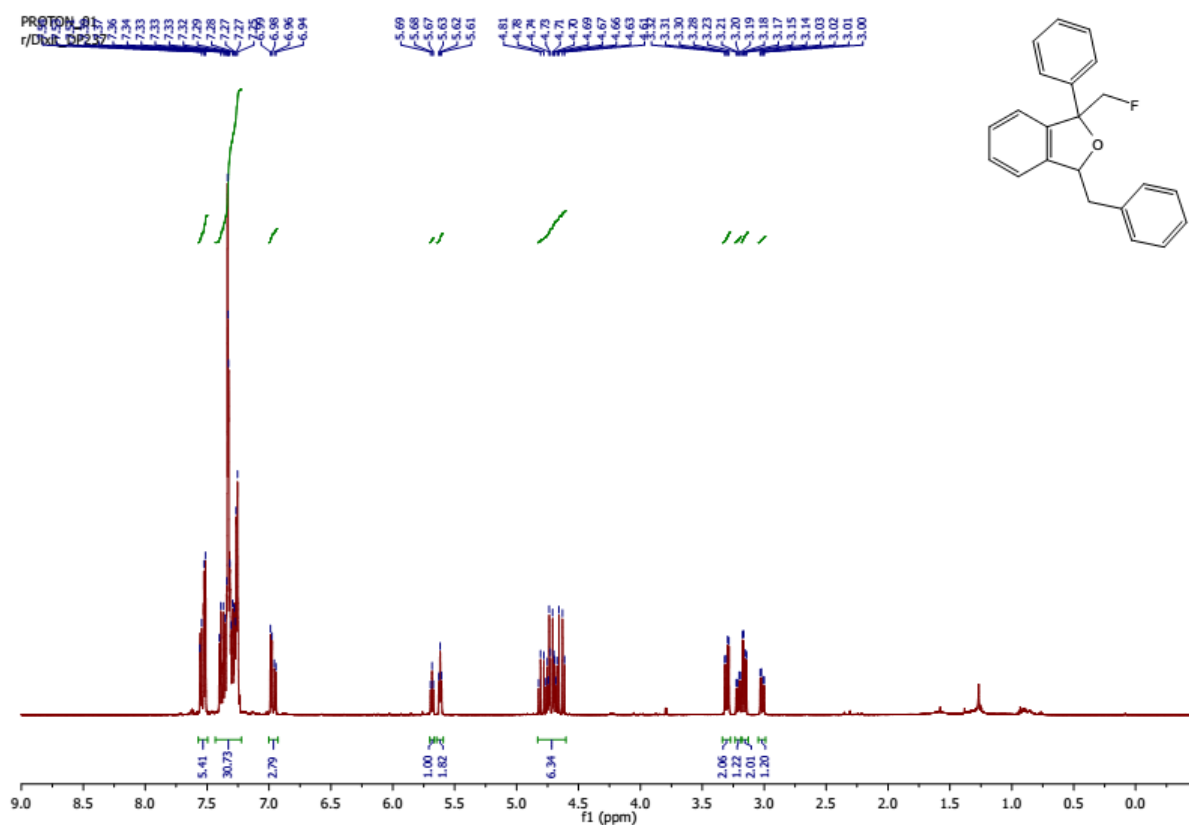
FLUORINE\_01  
r/Dxit\_DP234





FLUORINE\_01  
r/Dixit\_DP242

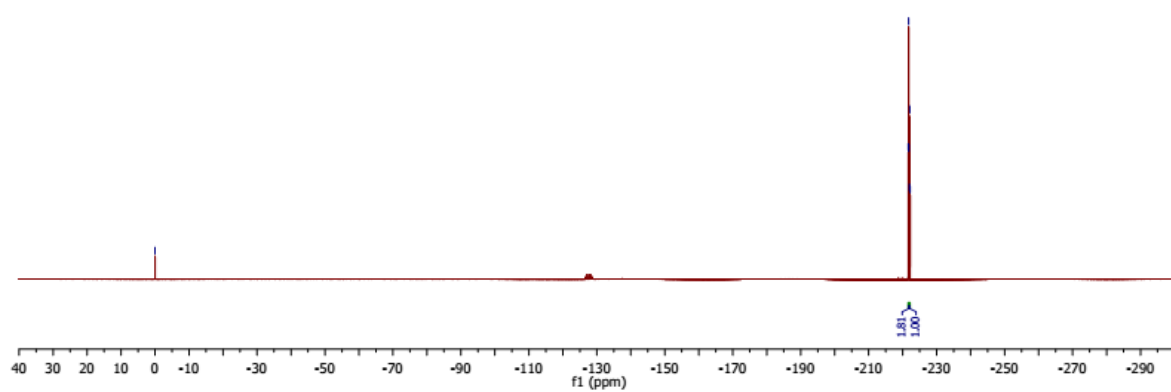
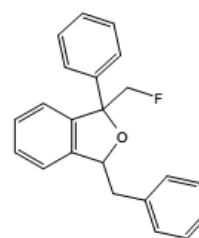




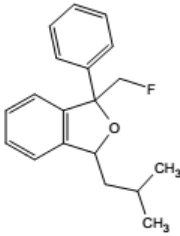
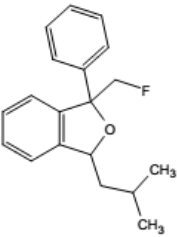
FLUORINE\_01  
r/Divit\_DP237

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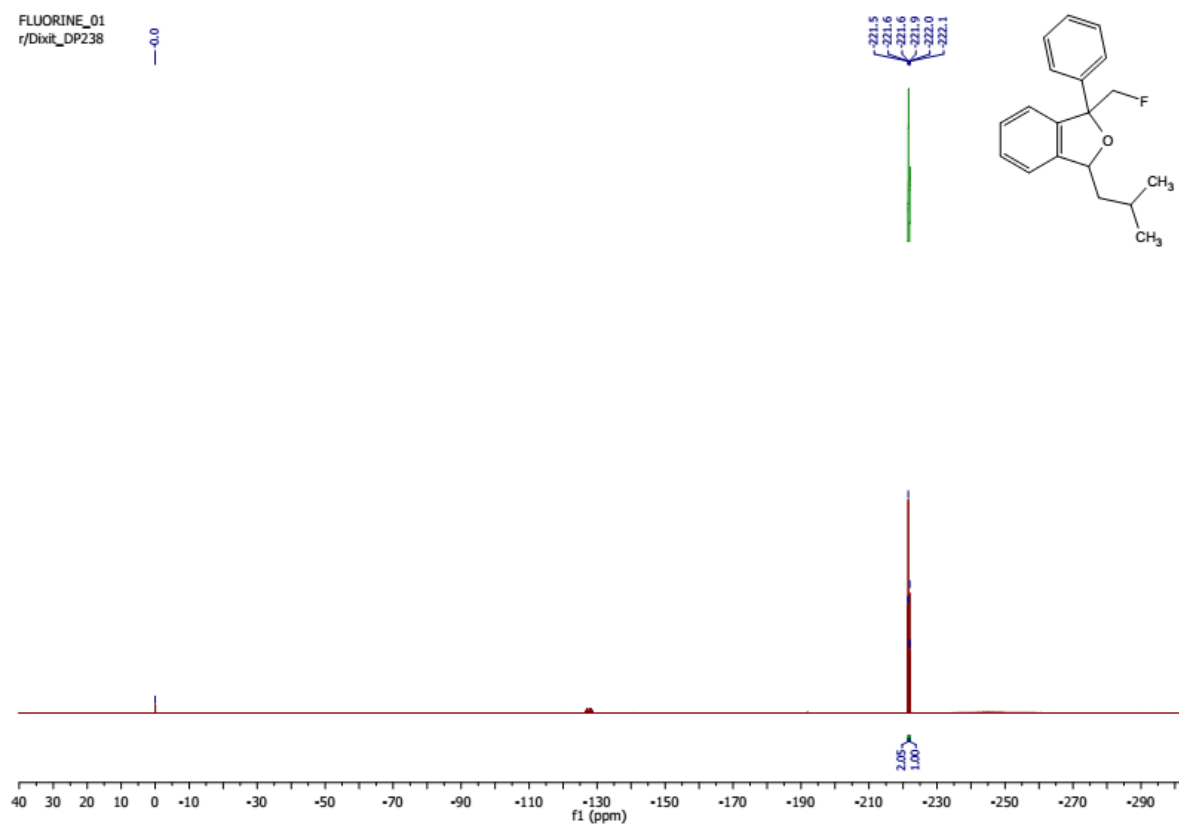
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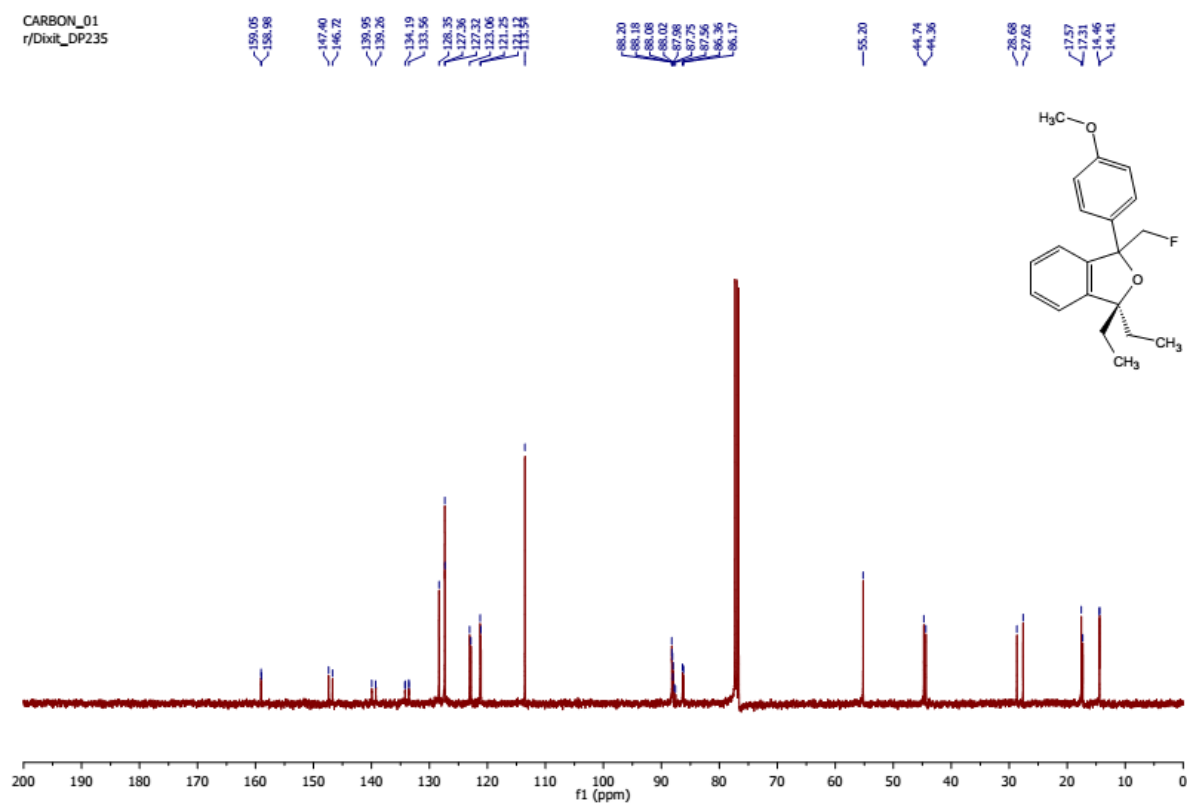
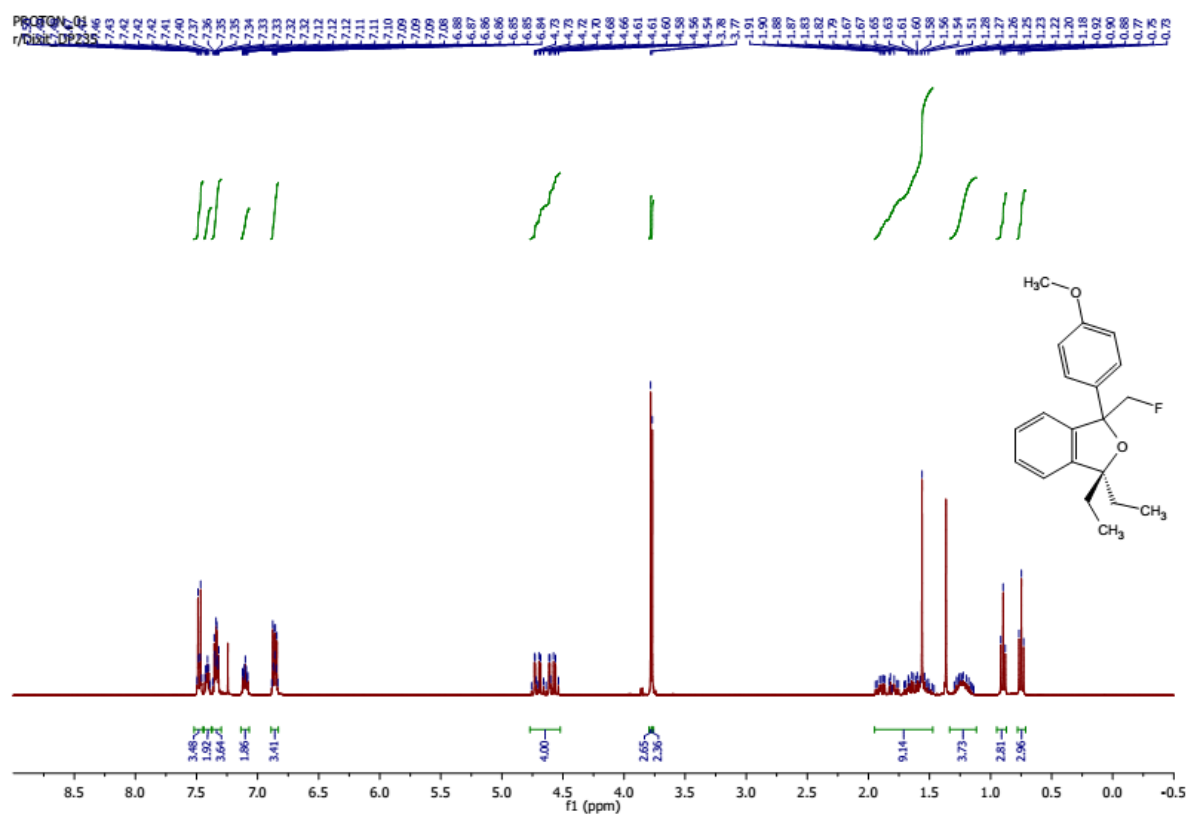




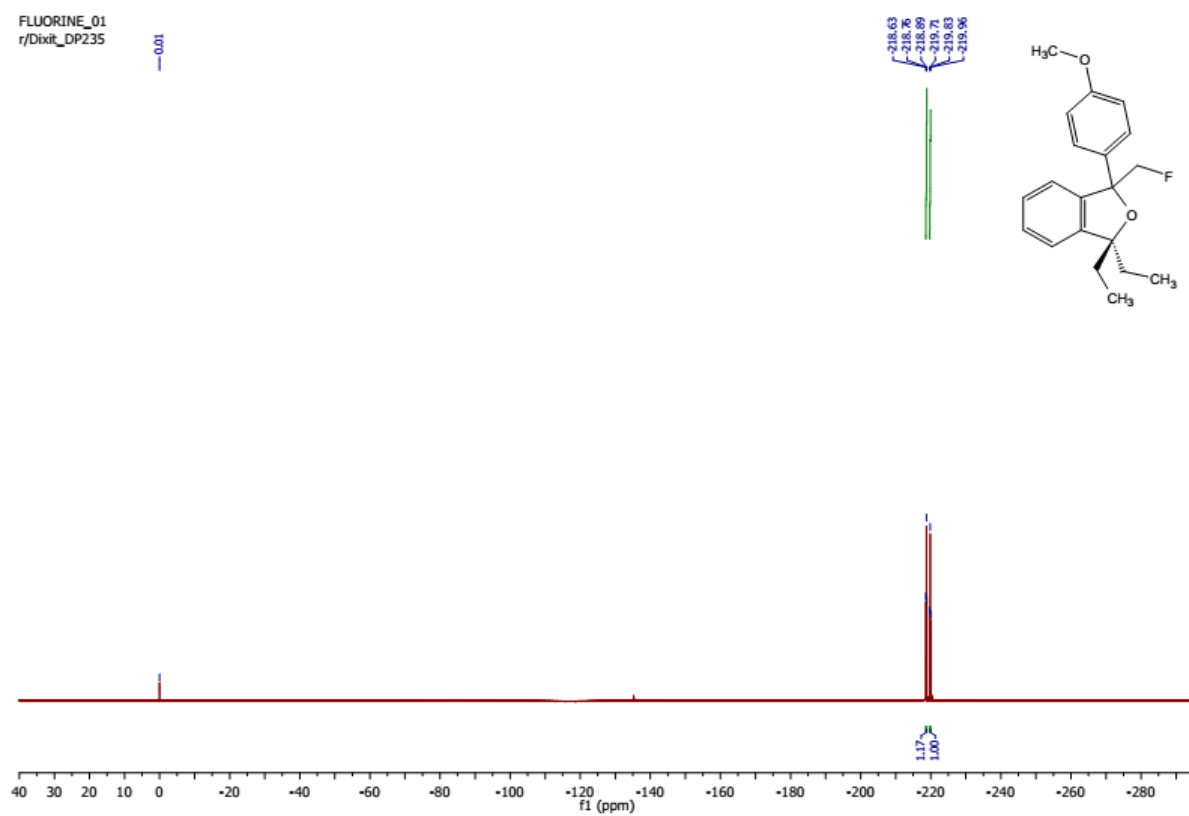


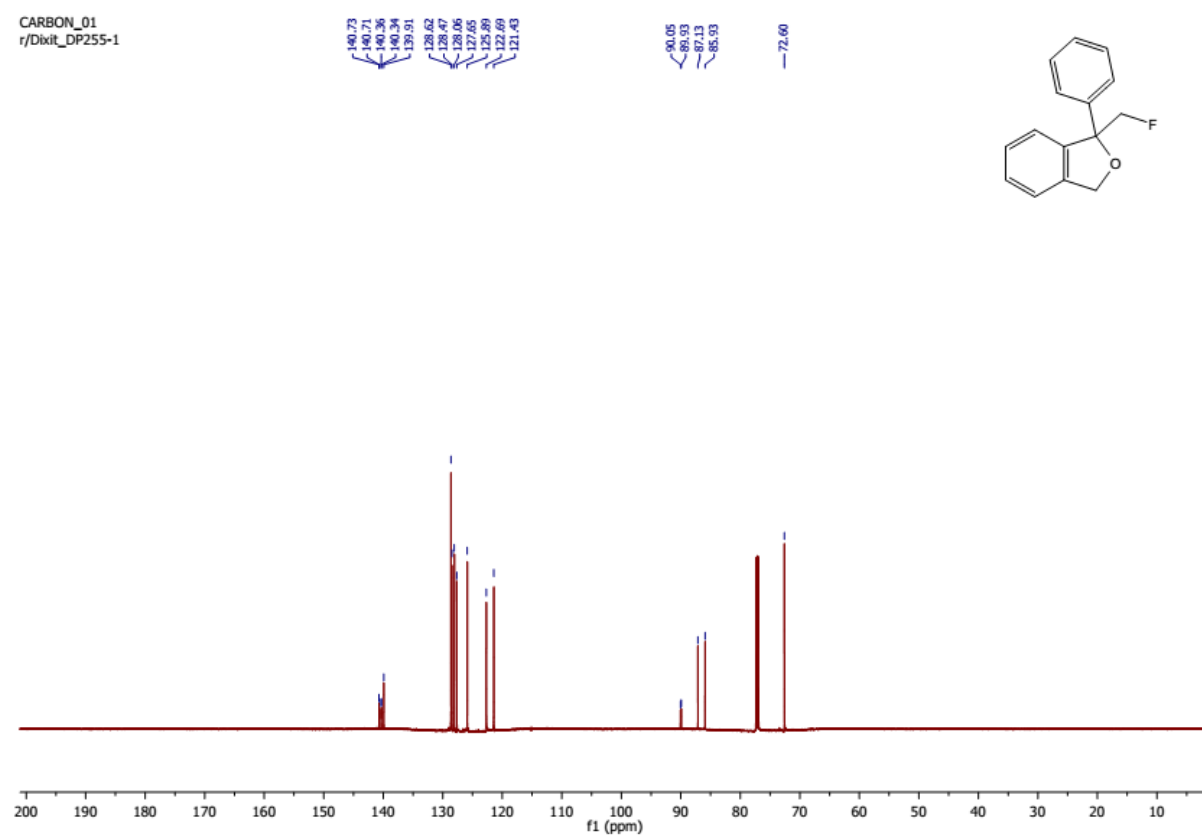
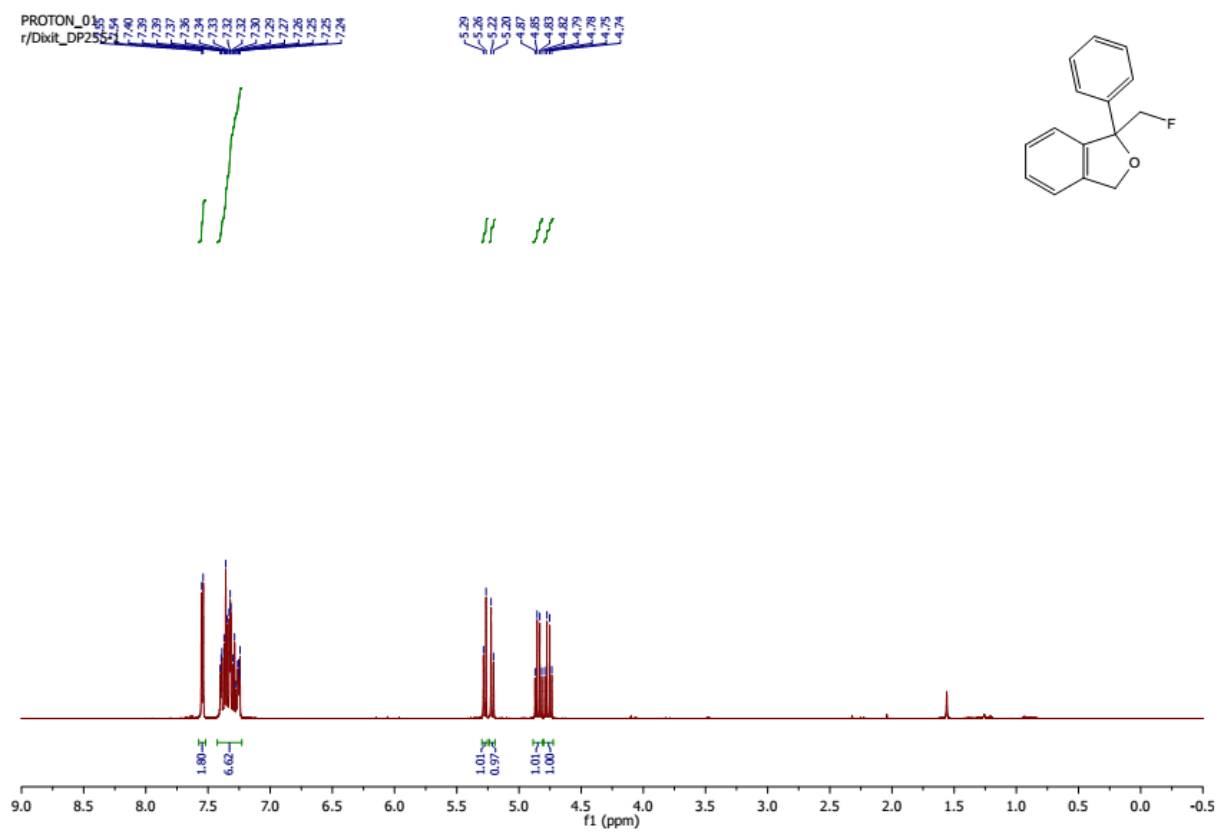
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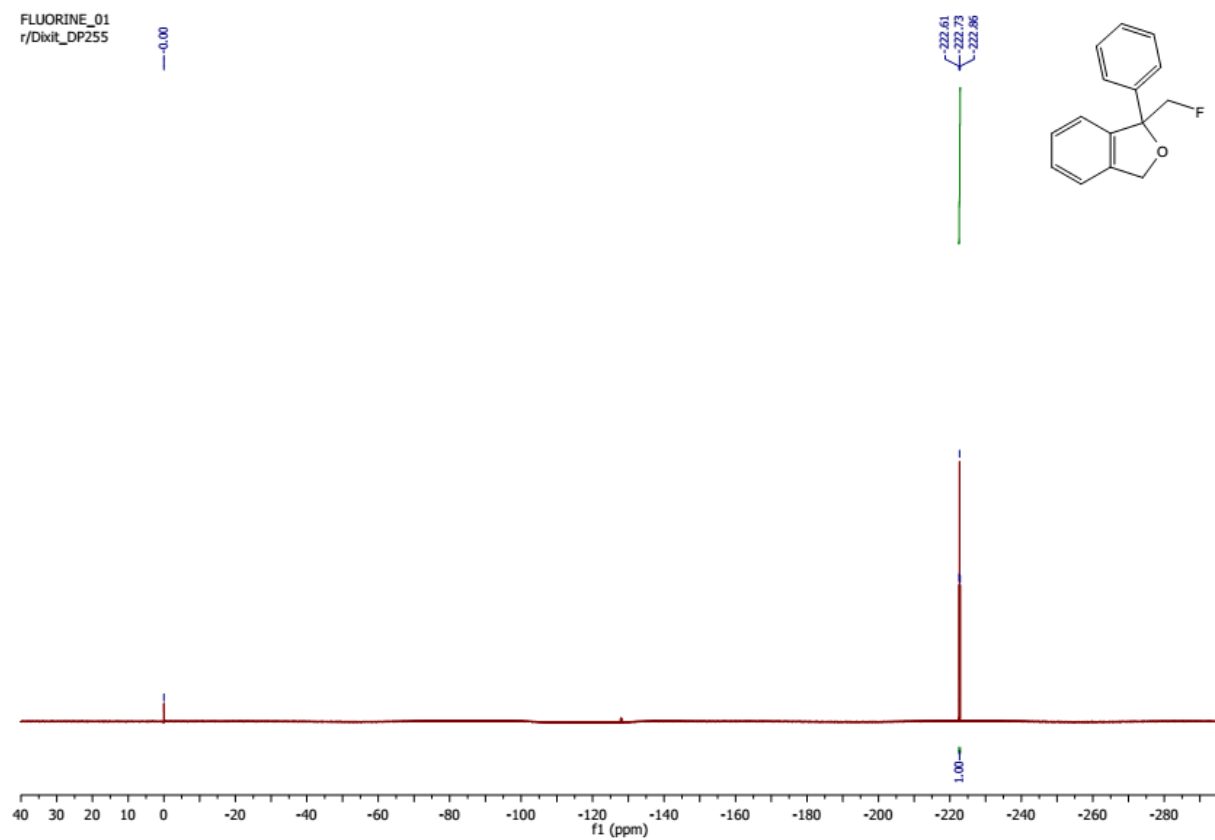


FLUORINE\_01  
r/Dioxit\_DP235





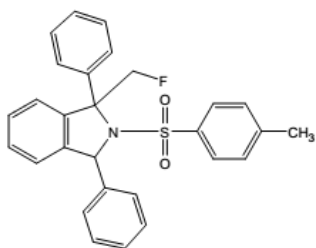
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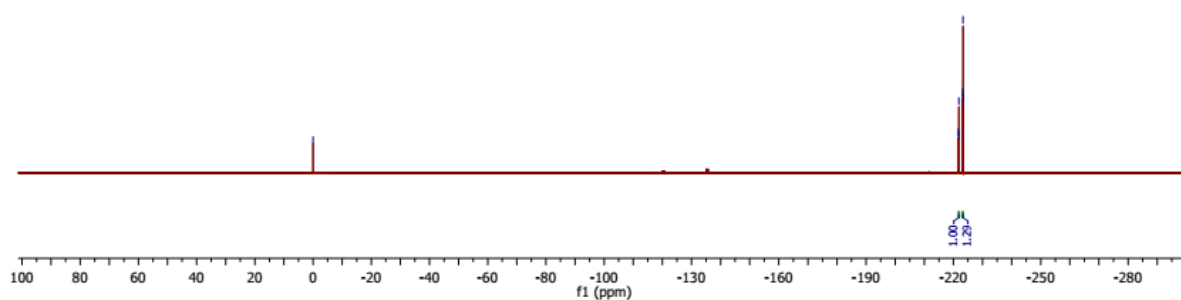


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r/Dixit\_DP313

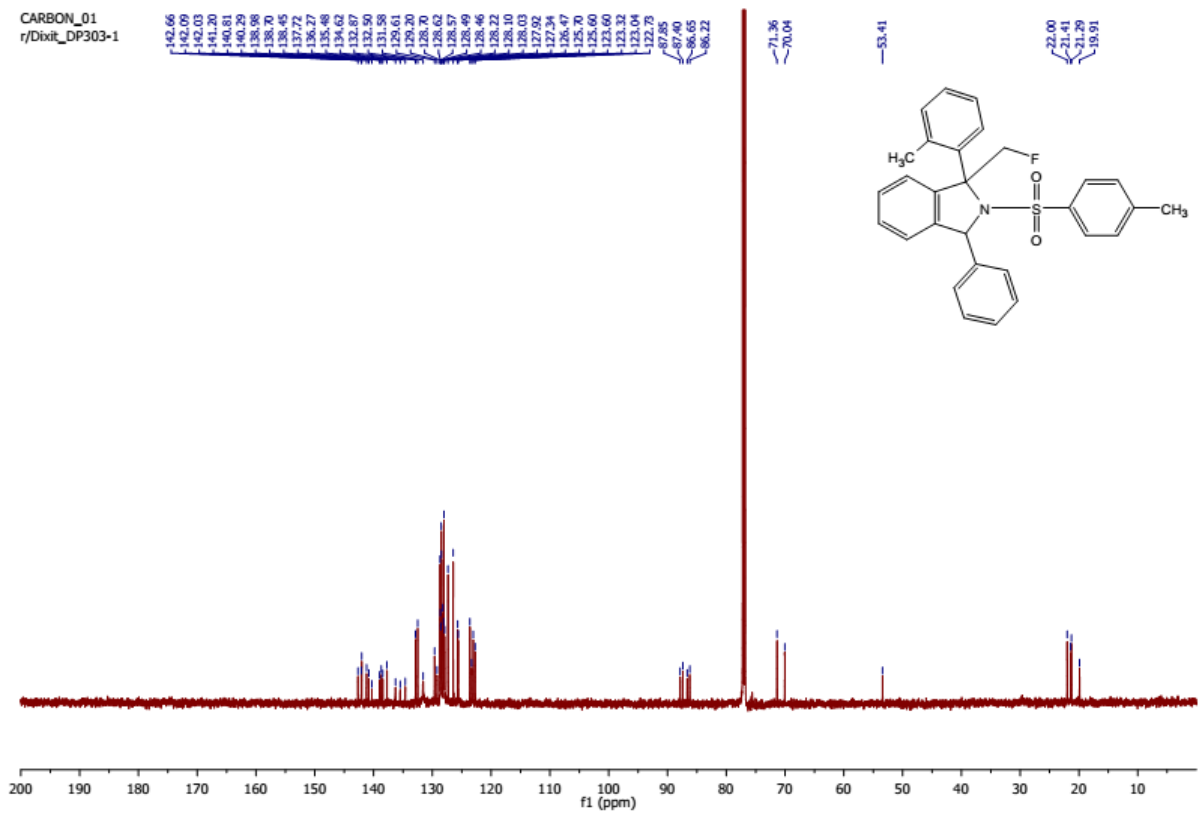
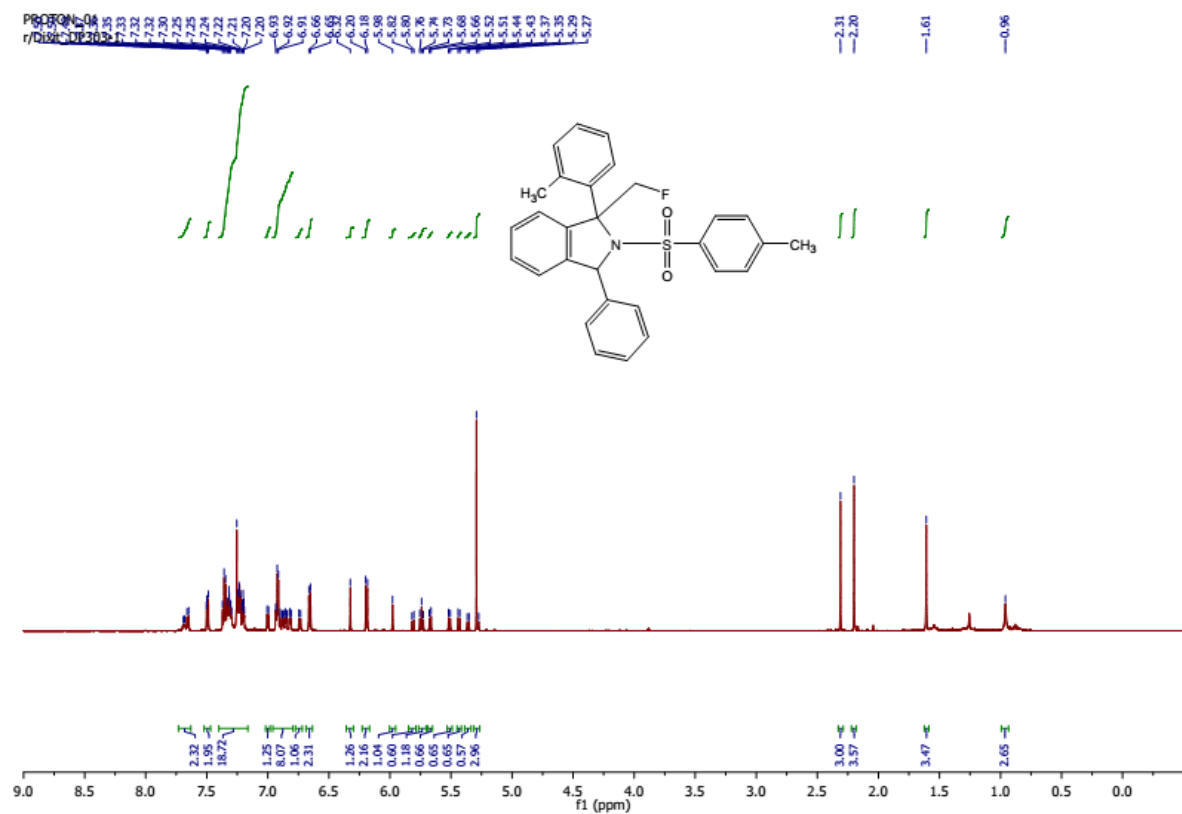
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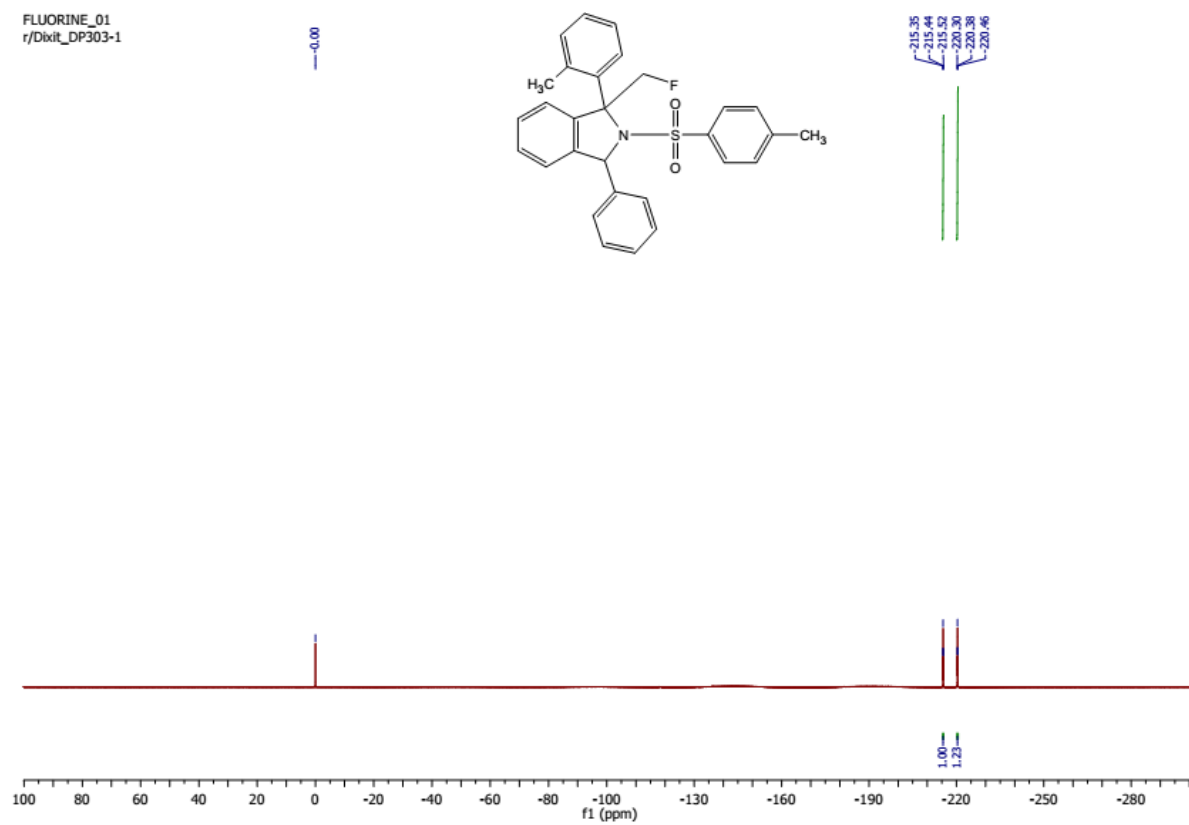
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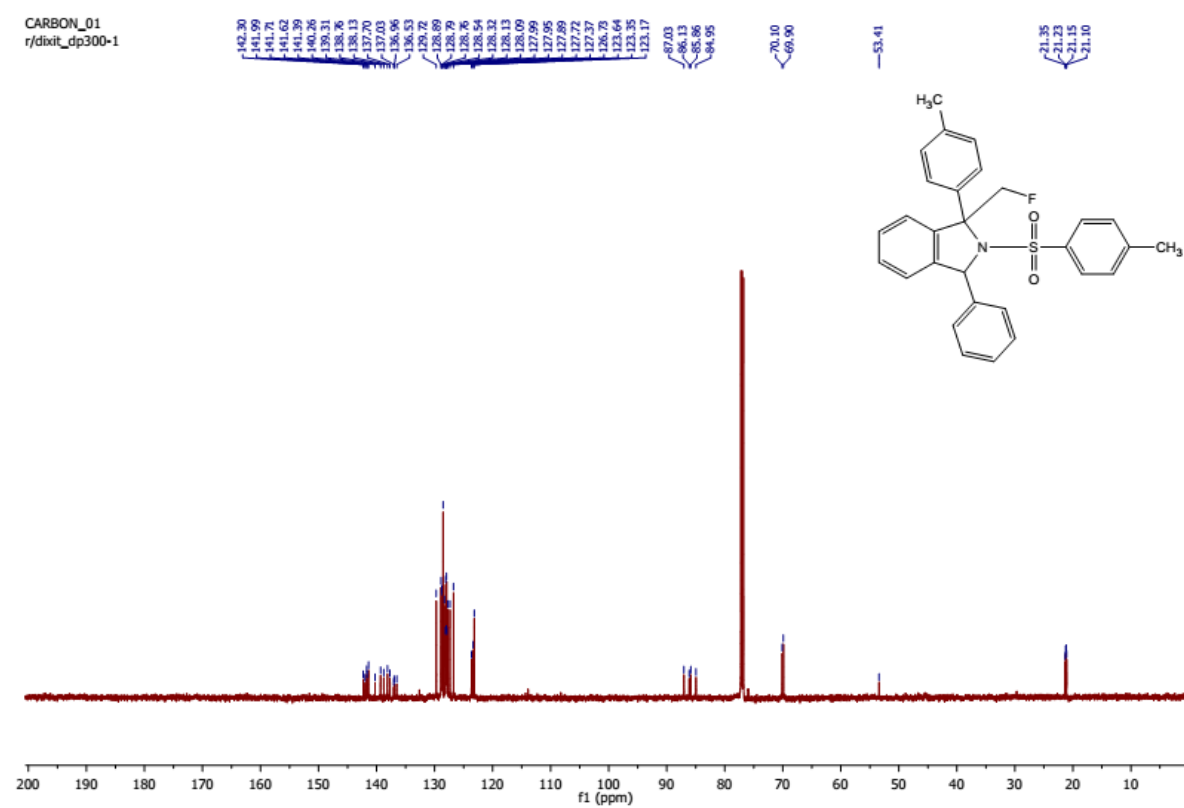
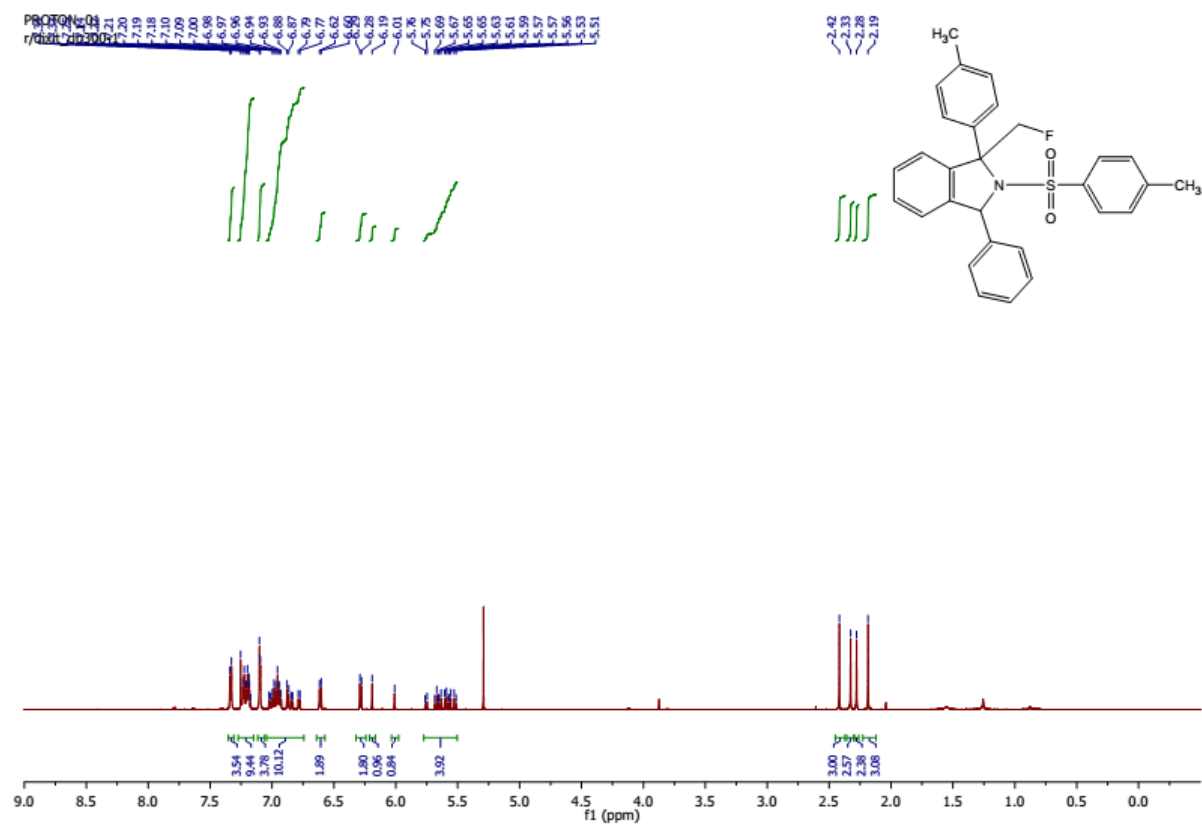






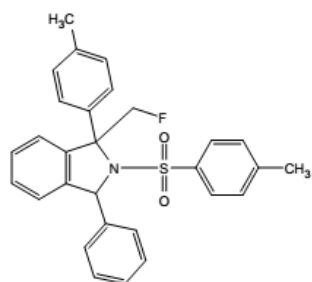
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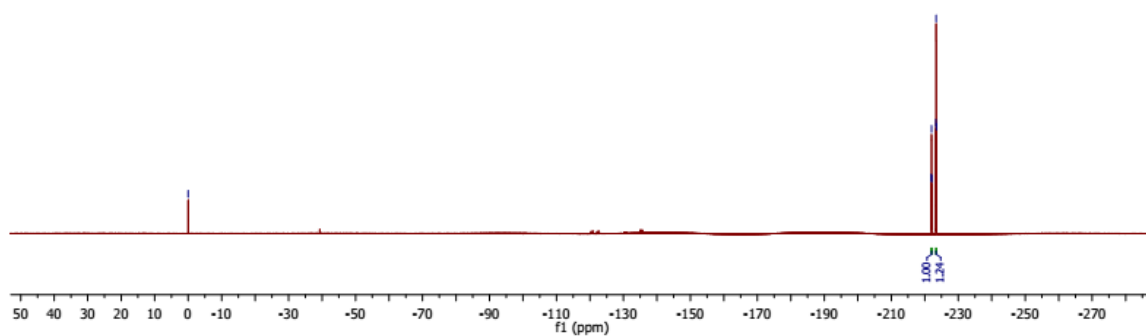


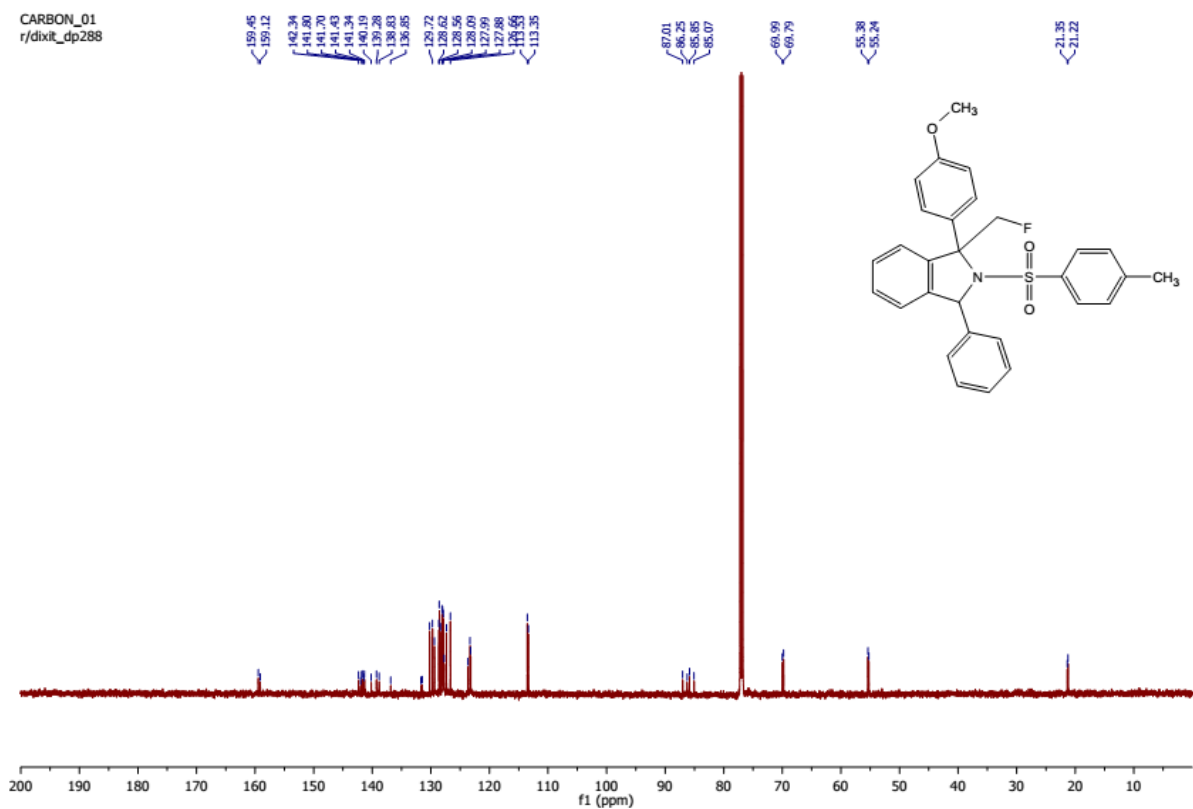
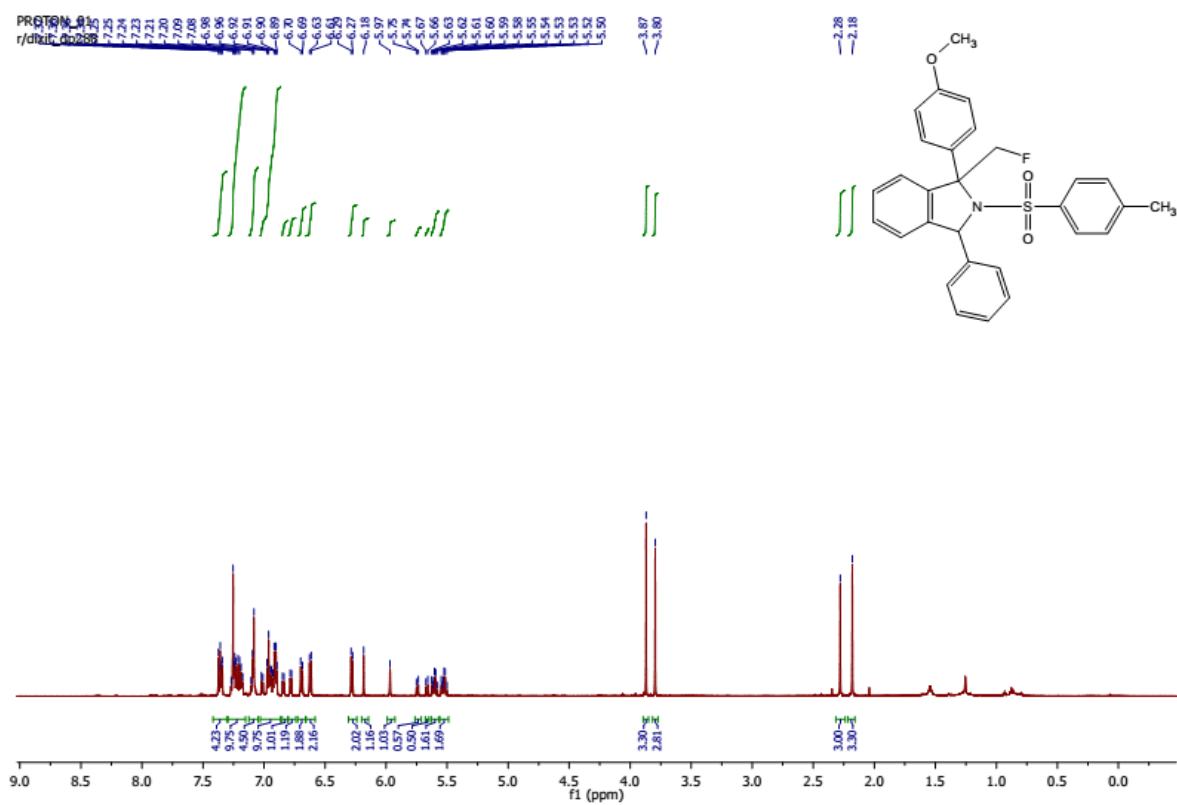
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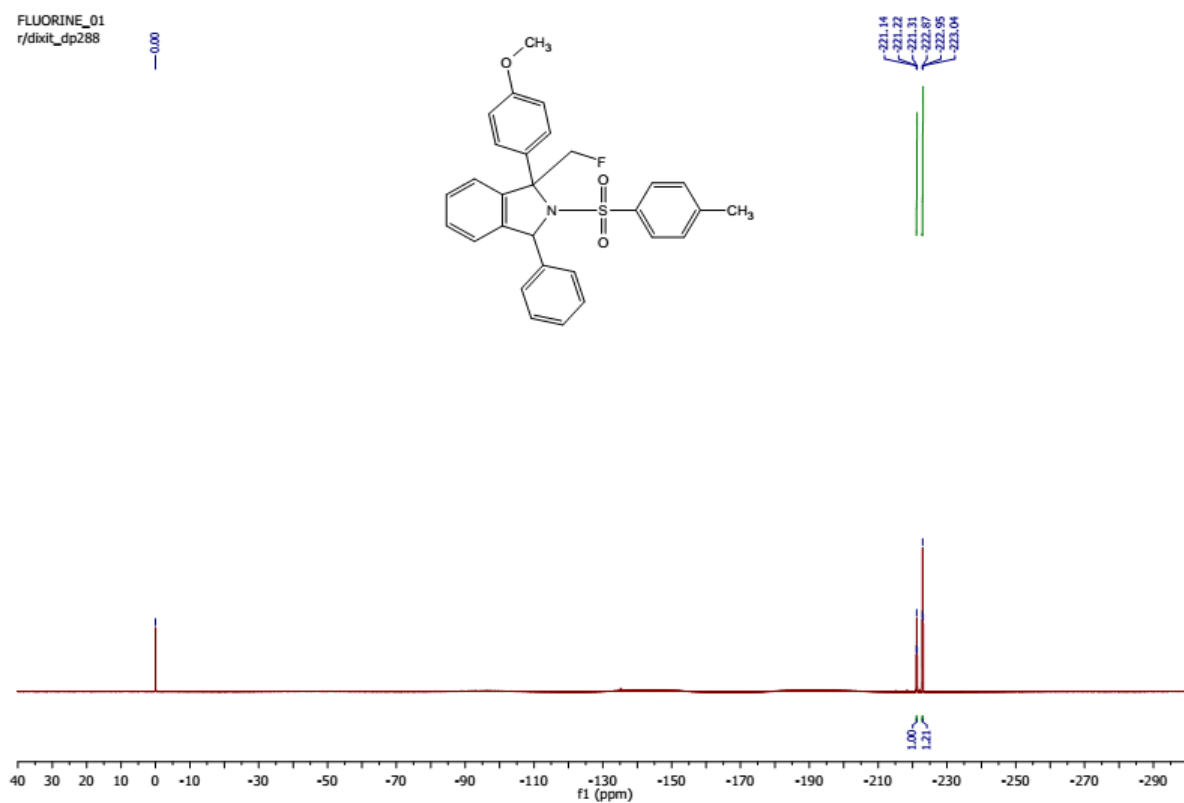


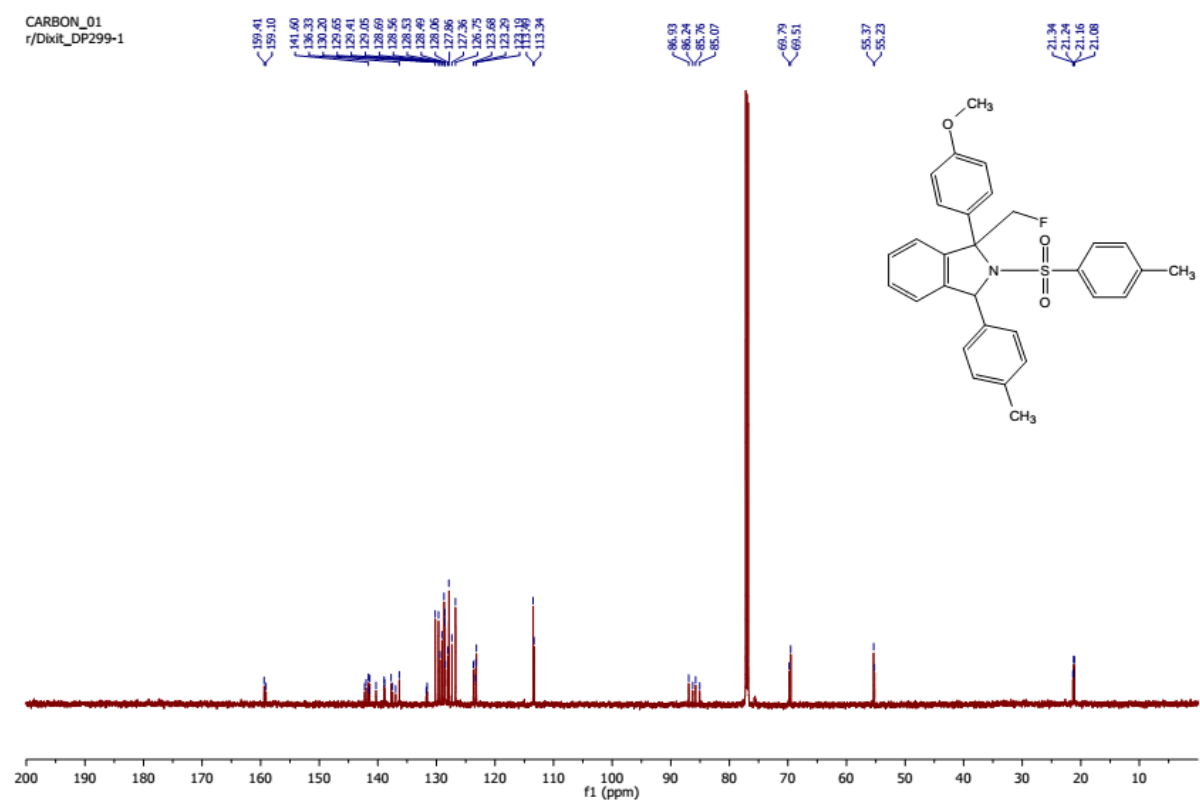
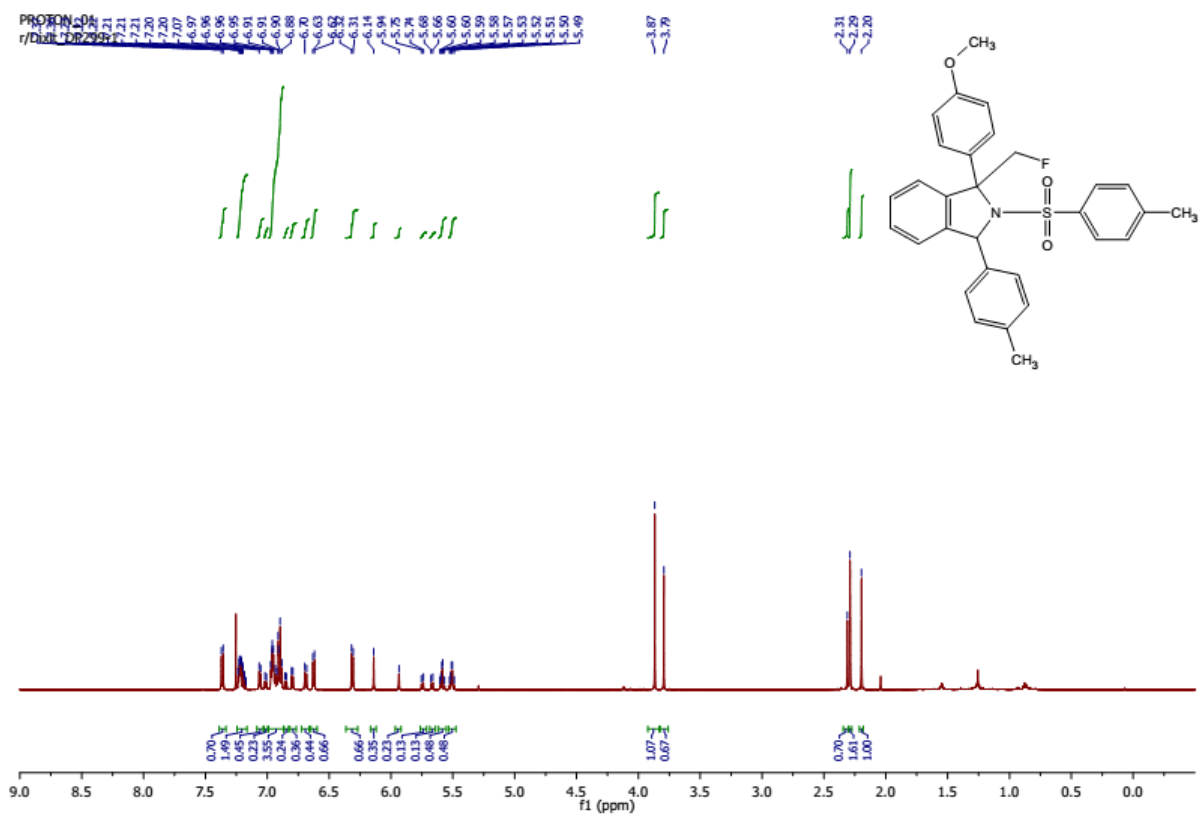
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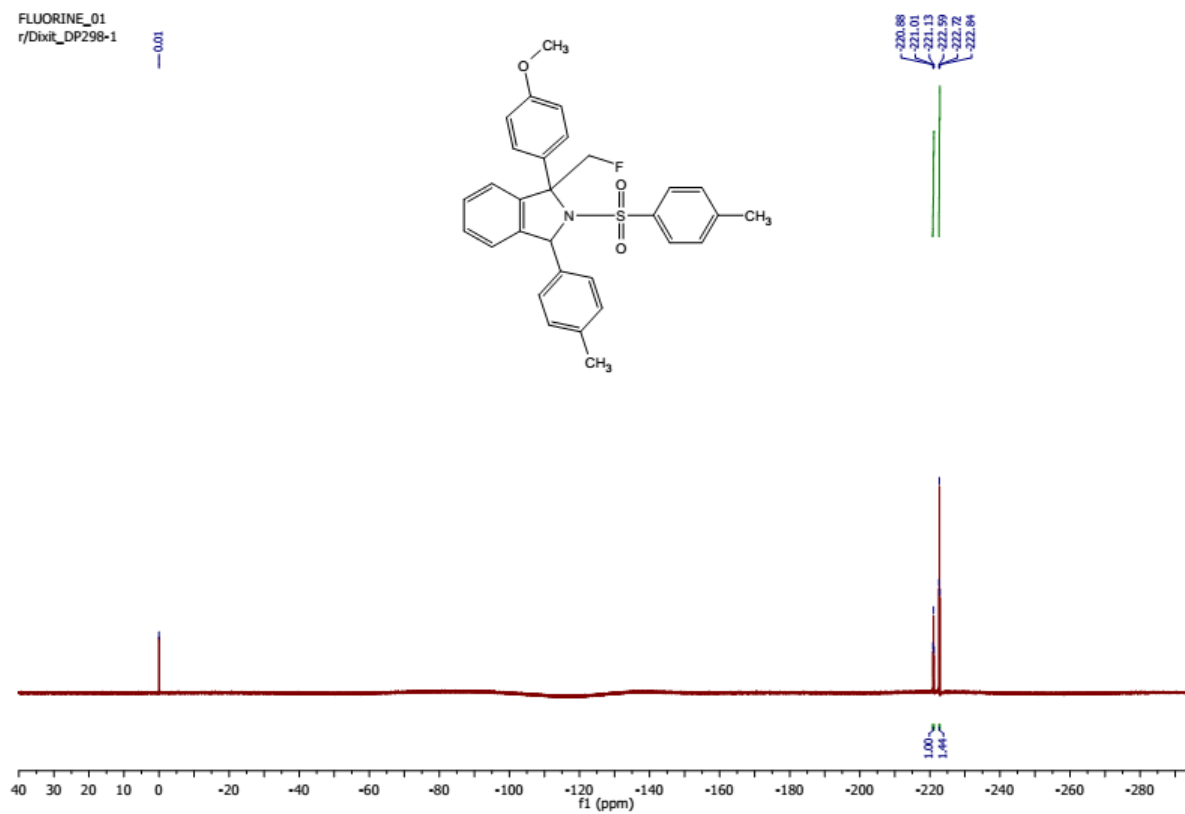


FLUORINE\_01  
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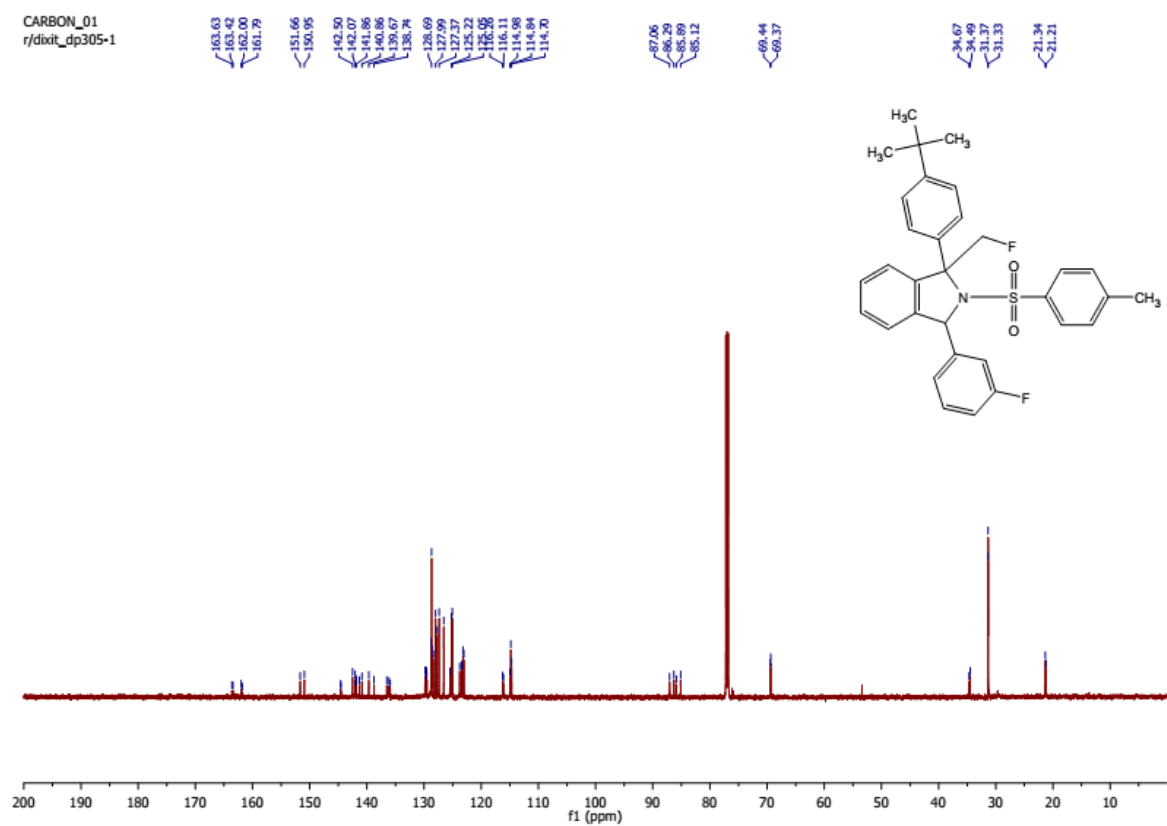
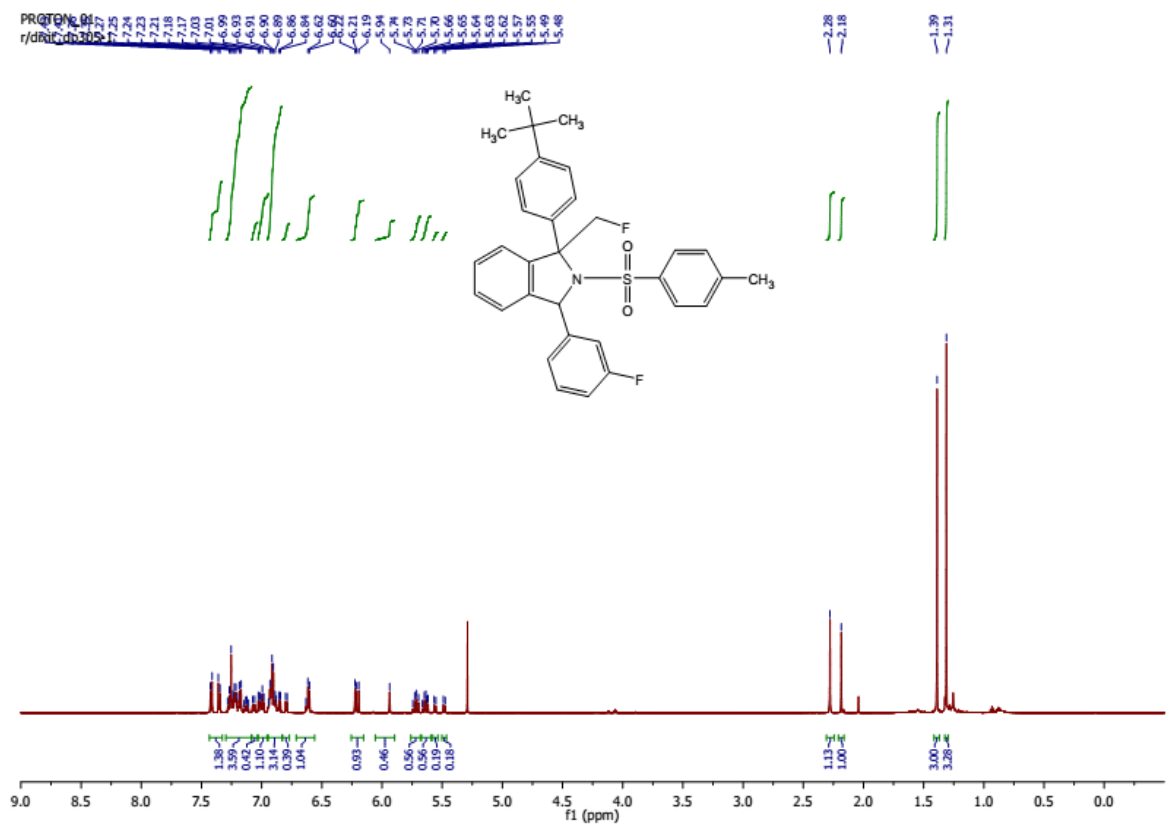




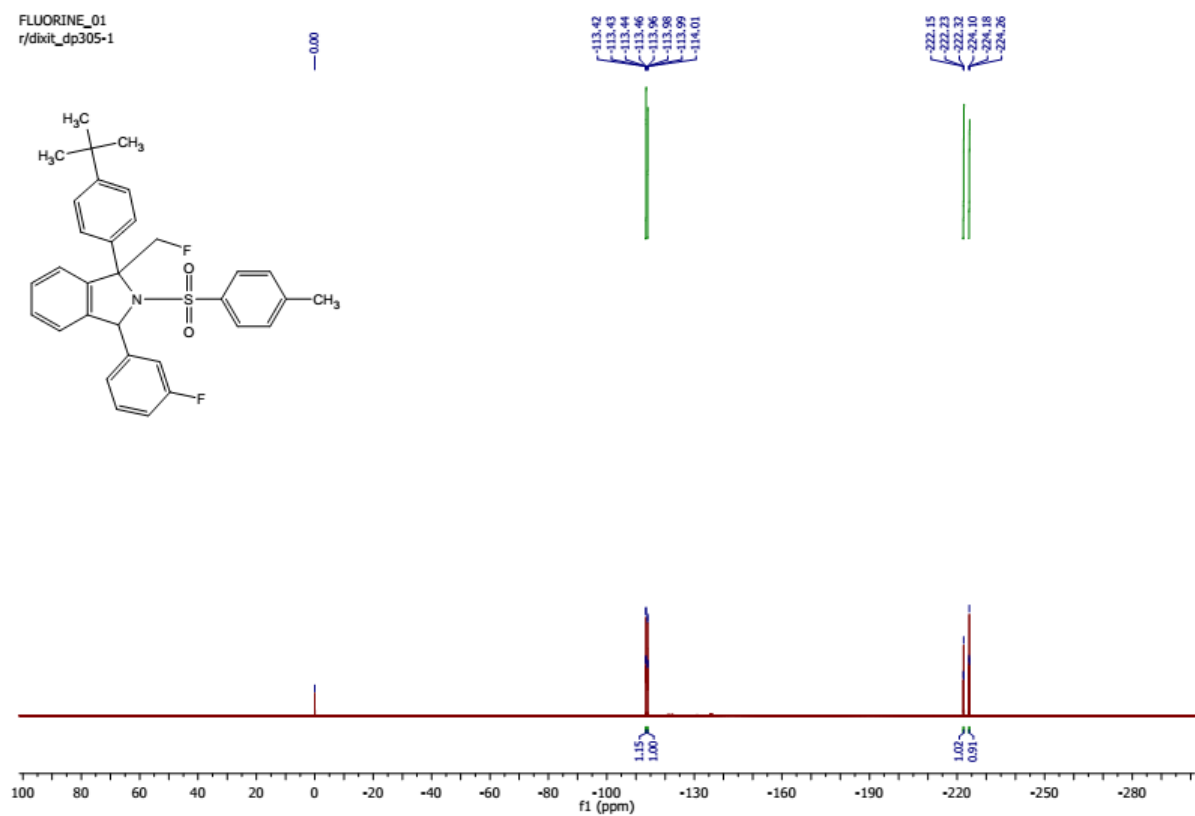
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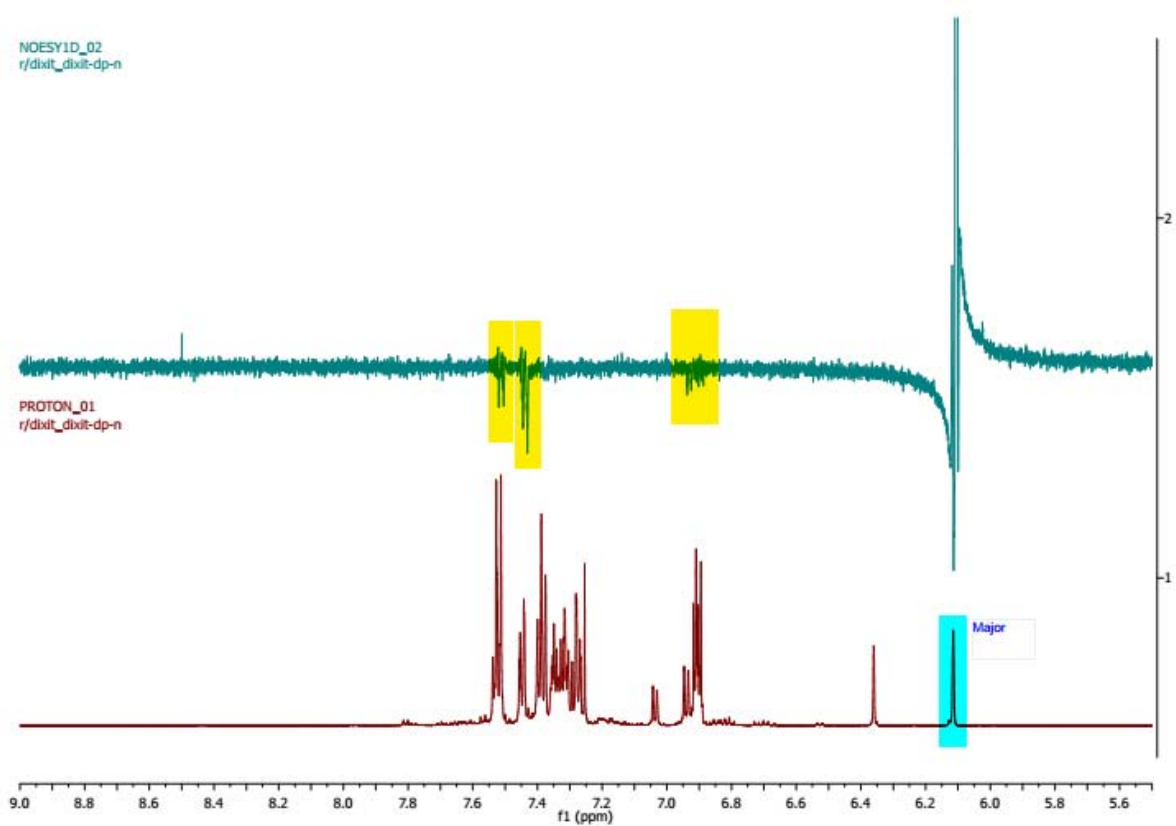
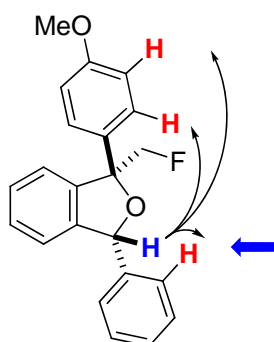


FLUORINE\_01  
r/dixit\_dp305-1



## NOE Studies

Major diastereoisomer:



Minor diastereoisomer:

