Intermolecular Fluoroamination of Allenes Towards Substituted Vinyl Fluorides

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Materials and methods. All reactions were performed in flame dried glassware. Dioxane was distilled from sodium prior to use. All other chemicals were obtained from commercial sources and used directly without further purification. Yields refer to chromatographically pure material. Reactions were monitored by thin-layer chromatography (TLC) performed on 0.25 mm Merck TLC Silica gel $60F_{254}$, precoated on aluminium sheets using UV light as a visualizing agent. Merck silica gel (particle size 100-200 and 230-400 mesh) was used for flash column chromatography.

NMR spectra were recorded on Bruker Avance 500 (^{1}H: 500 MHz, ^{13}C: 125 MHz) or 400 (^{1}H: 400 MHz, ^{13}C: 100 MHz) NMR spectrometers in $CDCl_3$ having TMS 0.03% as internal standard. ^{19}F were recorded $PhCF_3$ as reference standard. Mass spectrometric data were obtained using WATERS-Q-TOF Premier-ESI-MS.

The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublet, ddd = doublet of a doublet of doublet, m = multiplet.

The crystal structures of **4a**, **6c**, and **6i'** have been deposited in the CCDC with the deposition numbers 2003624, 2003625, and 2002738 respectively.

Synthesis of Precursors

Diaryl allenes[1], triazoles[2] and tetrazoles[3] were synthesized by the using the procedures reported in the literature.

General procedure for Aminofluorination (A) :

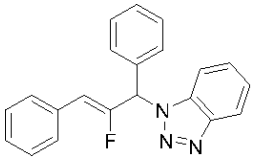
1,3-diphenylpropa-1,2-diene was taken in a reaction vial and nitromethane solvent (0.5 mL/0.1 mmol of allene) was added followed by selectfluor and the nucleophile. The reaction mixture was stirred at room temperature for 15h. After completion of the reaction (as monitored by TLC analysis), the reaction mixture was poured in a separating funnel and extracted with EtOAc (x3). The combined organic layers was

collected, washed with brine and dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by using column chromatography on silica gel (solvent system - EtOAc/ petroleum ether).

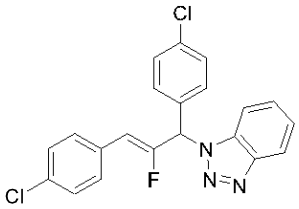
Procedure for Control Experiments with TEMPO & BHT (B):

1,3-diphenylpropa-1,2-diene (161 mg, 840 µmol) was taken in reaction vial and nitromethane (4mL) was added followed by selectfluor (238 mg, 672 µmol), nucleophile (40 mg, 336 µmol) and TEMPO or BHT (5 equiv). The reaction mixture was stirred at room temperature for 24h, after which no formation of the vinylfluoride product was observed.

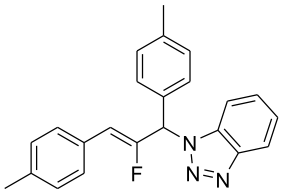
Characterization Data of Products



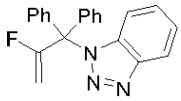
(*Z*)-1-(2-fluoro-1,3-diphenylallyl)-1*H*-benzo[*d*][1,2,3]triazole (4a) : According to the general procedure, benzotriazole **1a** (40 mg 336 µmol), selectfluor (238 mg, 671 µmol) and diphenyl allene (161 mg, 840 µmol) provided **4a** as a yellow solid (93 mg, 84%) after flash column chromatography (10% ethyl acetate in petroleum ether); R_f = 0.50 (20% ethyl acetate in petroleum ether) ; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.05-8.00 (m, 1H), 7.43-7.42 (m, 2H), 7.32 – 7.26 (m, 8H), 7.25 – 7.18 (m, 3H), 6.88 (d, *J* = 14.9 Hz, 1H), 5.79 (d, *J* = 37.9 Hz, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 154.6 (d, *J* = 270.4 Hz), 146.5, 134.1, 132.7, 131.8 (d, *J* = 2.7 Hz), 129.2, 129.1, 128.7, 128.4, 127.8, 127.7, 124.2, 120.3, 112.4 (d, *J* = 6.3 Hz), 110.9 (d, *J* = 2.2 Hz), 65.3 (d, *J* = 28.8 Hz) ; ^{19}F NMR (373 MHz, Chloroform-*d*) δ -108.94 (d, *J* = 32.2 Hz) ; HRMS calculated for $C_{21}H_{17}FN_3^+$ $[M+H]^+$: 330.1407; found 330.1404; IR (liquid): 3373, 3061, 1954, 1691, 1600, 1450,1159, 748 cm^{-1}.



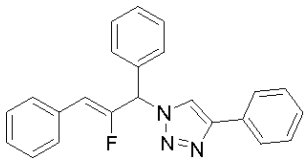
(*Z*)-1-(1,3-bis(4-chlorophenyl)-2-fluoroallyl)-1*H*-benzo[*d*][1,2,3]triazole (4b): According to the general procedure, benzotriazole **1a** (40 mg, 336 µmol), selectfluor (238 mg, 671µmol) and diaryl allene (219 mg, 840 µmol) provided **4b** as a yellow oil (91 mg, 68%) after flash column chromatography (10% ethyl acetate in petroleum ether); R_f = 0.50 (20% ethyl acetate in petroleum ether), ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.05 – 8.03 (m, 1H), 7.37 – 7.30 (m, 5H), 7.25 – 7.19 (m, 6H), 6.81 (d, *J* = 14.5 Hz, 1H), 5.74 (d, *J* = 37.3 Hz, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 154.6 (d, *J* = 271.3 Hz), 146.6, 135.5, 134.3 (d, *J* = 3.4 Hz), 132.6, 132.5, 130.5, 130.4, 130.2, 130.1, 129.6, 129.2, 129.0, 128.1, 124.5, 120.5, 111.5 (d, *J* = 6.2 Hz), 110.5 (d, *J* = 2.7 Hz), 64.5 (d, *J* = 29.2 Hz); ^{19}F NMR (373 MHz, Chloroform-*d*) δ -102.29 – -117.60 (m); HRMS calculated for $C_{21}H_{15}Cl_2FN_3^+$ $[M+H]^+$: 398.0627; found 398.0628; IR (liquid): 3063, 2925, 1906,1690, 1161, 745 cm^{-1}.



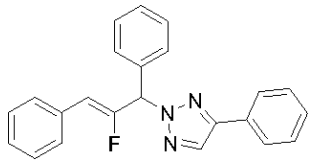
(*Z*)-1-(2-fluoro-1,3-dip-tolylallyl)-1*H* benzo[*d*][1,2,3]triazole (4c) : According to the general procedure, benzotriazole **1a** (40 mg 336 µmol), selectfluor (238 mg, 671 µmol) and diaryl allene (185 mg, 840 µmol) provided **4c** as a yellow oil (97 mg, 80%) after flash column chromatography (10% ethyl acetate in petroleum ether); R_f = 0.57 (20% ethyl acetate in petroleum ether), ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.01 (d, *J* = 8.3 Hz, 1H), 7.31 (d, *J* = 8.2 Hz, 2H), 7.30 – 7.22 (m, 3H), 7.18 – 7.07 (m, 4H), 7.05 (d, *J* = 7.7 Hz, 2H), 6.83 (d, *J* = 14.7 Hz, 1H), 5.74 (d, *J* = 38.2 Hz, 1H), 2.27 (s, 3H), 2.26 (s, 3H).); ^{13}C NMR (125 MHz, Chloroform-*d*) δ 154.2 (d, *J* = 269.2 Hz), 146.6, 139.1, 138.3, 132.8, 131.4, 129.9, 129.4, 129.1, 129.1, 127.7, 124.1, 120.3, 112.1 (d, *J* = 6.3 Hz), 111.0, 65.2 (d, *J* = 28.9 Hz), 21.4, 21.3; ^{19}F NMR (373 MHz, Chloroform-*d*) δ -109.86 (d, *J* = 34.6 Hz); HRMS calculated for $C_{23}H_{21}FN_3^+$ $[M+H]^+$: 358.1720 ; found 358.1724; IR (liquid): 3293, 3027, 2857, 1910, 1688, 1450, 1110, 745 cm^1.



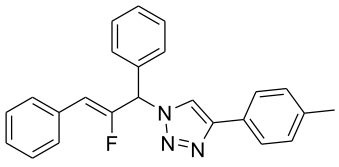
1-(2-fluoro-1,1-diphenylallyl)-1*H*-benzo[d][1,2,3]triazole (4d) : According to the general procedure, benzotriazole **1a** (40 mg, 336µmol), selectfluor (238 mg, 672 µmol) and 1,1-diphenylallene (161 mg, 839 µmol) provided **4d** as a white solid (46 mg, 41%) after flash column chromatography (10 % ethyl acetate in petroleum ether); R_f = 0.47 (20% ethyl acetate in petroleum); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 (d, *J* = 8.3 Hz, 1H), 7.39 (dd, *J* = 5.1, 2.5 Hz, 4H), 7.36 – 7.27 (m, 4H), 7.23 – 7.15 (m, 5H), 5.42 (d, *J* = 19.1 Hz, 2H) ; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 149.8 (d, *J* = 262.1 Hz), 146.2, 137.0 (d, *J* = 6.8 Hz), 136.0, 133.4, 130.5, 129.8, 129.8, 129.1, 128.6, 128.3, 128.2, 127.8, 124.2, 120.2, 109.7, 47.6 (d, *J* = 28.7 Hz); ^{19}F NMR (373 MHz, Chloroform-*d*) δ -112.7 (t, *J* = 19.8 Hz); HRMS calculated for $C_{21}H_{17}FN_3^+$ $[M+H]^+$: 330.1407; found 330.1418; IR (liquid): 3058, 2963, 1956, 1666, 1157, 764 cm^{-1}.



(*Z*)-1-(2-fluoro-1,3-diphenylallyl)-4-phenyl-1*H*-1,2,3-triazole (6a) : According to the general procedure, 5-phenyl-*1H*-1,2,3-triazole **5a** (40 mg, 276 µmol), selectfluor (195 mg, 551 µmol) and diaryl allene (132 mg, 689 µmol) provided **6a** as a creamish solid (61 mg, 62%) after flash column chromatography (10% ethyl acetate in petroleum ether); R_f = 0.50 (20% ethyl acetate in petroleum ether), ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.81 – 7.75 (m, 2H), 7.44 (d, *J* = 7.2 Hz, 2H), 7.37 – 7.20 (m, 12H), 6.62 (d, *J* = 16.6 Hz, 1H), 5.79 (d, *J* = 38.0 Hz, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 154.1 (d, *J* = 269.1 Hz), 148.2, 134.7, 131.7, 129.3, 129.2, 128.9, 128.8, 128.5, 127.5, 125.9, 119.5, 112.4 (d, *J* = 6.1 Hz), 66.1 (d, *J* = 28.6 Hz); ^{19}F NMR (373 MHz, Chloroform-*d*) δ -112.44 (d, *J* = 35.5 Hz); HRMS calculated for $C_{23}H_{19}FN_3^+$ $[M+H]^+$: 356.1563; found 356.1567; IR (liquid): 3063, 2924, 1955, 1689, 1451, 1156, 763 cm^{-1}.

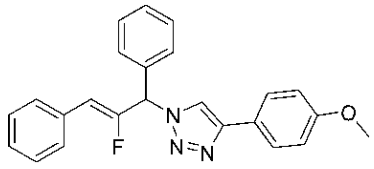


(*Z*)-2-(2-fluoro-1,3-diphenylallyl)-4-phenyl-2*H*-1,2,3-triazole (6a') : According to the general procedure, 5-phenyl-1H-1,2,3-triazole **5a** (40 mg, 276 µmol), selectfluor (195 mg, 551 µmol) and diaryl allene (132 mg, 689 µmol) provided **6a'** as a yellow oil (20 mg, 20%) after flash column chromatography (20% DCM in petroleum ether); R_f = 0.40 (5% ethyl acetate in petroleum ether), ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89 (s, 1H), 7.74 (d, *J* = 8.5 Hz, 2H), 7.44 – 7.19 (m, 13H), 6.55 (d, *J* = 9.5 Hz, 1H), 5.59 (d, *J* = 37.9 Hz, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 155.5 (d, *J* = 269.7 Hz), 148.5, 134.9, 132.3, 131.9, 130.2, 129.2, 129.1, 129.0, 128.7, 128.6, 128.2, 128.1, 126.2, 111.7 (d, *J* = 6.5 Hz), 70.1 (d, *J* = 29.8 Hz); ^{19}F NMR (373 MHz, Chloroform-*d*) δ -109.37 (d, *J* = 43.6 Hz); HRMS calculated for $C_{23}H_{19}FN_3^+$ $[M+H]^+$: 356.1563; found 356.1560. IR (liquid): 3064, 2853, 1602, 1432, 972, 754 cm^{-1}.

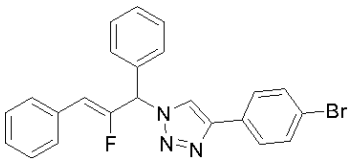


(*Z*)-1-(2-fluoro-1,3-diphenylallyl)-4-*p*-tolyl-1*H*-1,2,3-triazole (6b) : According to the general procedure, triazole **5b** (40 mg, 251µmol), selectfluor (178 mg, 503 µmol) and diaryl allene (121 mg, 628 µmol) provided **6b** as a white solid (66 mg, 71%) after flash column chromatography (8% ethyl acetate in petroleum ether); R_f = 0.60 (20% ethyl acetate in petroleum ether); ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.76 (s, 1H), 7.66 (d, *J* = 8.1 Hz, 2H), 7.45 (d, *J* = 7.3 Hz, 2H), 7.35 (d, *J* = 7.1 Hz, 3H), 7.27 (dt, *J* = 13.9, 6.2 Hz, 5H), 7.15 (d, *J* = 7.9 Hz, 2H), 6.62 (d, *J* = 16.5 Hz, 1H), 5.78 (d, *J* = 37.9 Hz, 1H), 2.30 (s, 3H) ; ^{13}C NMR (125 MHz, Chloroform-*d*) δ 154.2 (d, *J* = 269.1 Hz), 148.3, 138.3, 134.8, 131.8, 129.7, 129.4, 129.4, 129.3, 129.2, 128.8, 128.6, 127.6, 125.8, 119.0, 112.4 (d, *J* = 6.1 Hz), 66.1 (d, *J* = 28.7 Hz), 21.4; ^{19}F NMR (373 MHz, Chloroform-*d*) δ -112.4(dd, *J* = 39.5, 17.2 Hz); HRMS calculated for

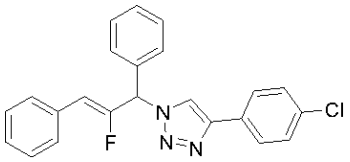
$C_{24}H_{21}FN_3^+$ [M+H]$^+$: 370.1720; found 370.1722. IR (liquid): 3029, 2924, 1688, 1496, 1450, 1039, 694 cm^{-1}.



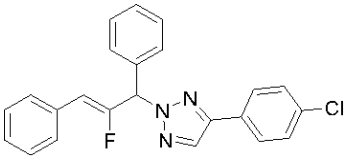
(*Z*)-1-(2-fluoro-1,3-diphenylallyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (6c) : According to the general procedure, triazole **5c** (40 mg, 228µmol), selectfluor (162 mg, 457 µmol) and diaryl allene (110 mg, 571 µmol) provided **6c** as a white solid (62 mg, 71%) after flash column chromatography (10 % ethyl acetate in petroleum ether); R_f = 0.38 (20% ethyl acetate in petroleum ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.71 (d, *J* = 2.1 Hz, 3H), 7.45 (d, *J* = 7.5 Hz, 2H), 7.38 – 7.31 (m, 3H), 7.26 (dq, *J* = 12.8, 7.4 Hz, 5H), 6.87 (d, *J* = 8.7 Hz, 2H), 6.61 (d, *J* = 16.5 Hz, 1H), 5.78 (d, *J* = 38.0 Hz, 1H), 3.76 (s, 3H); ^{13}C NMR (125 MHz, Chloroform-*d*) δ 159.9, 154.2 (d, *J* = 269.0 Hz), 148.1, 134.8, 131.8, 129.4 (d, *J* = 4.3 Hz), 129.3, 129.2, 128.8, 128.5, 127.6, 127.3, 123.2, 118.6, 114.4, 112.3 (d, *J* = 6.2 Hz), 66.1 (d, *J* = 28.6 Hz), 55.5 ; ^{19}F NMR (373 MHz, Chloroform-*d*) δ -111.6 (d, *J* = 26.6 Hz) ; HRMS calculated for $C_{24}H_{21}FN_3O^+$ [M+H] $^+$: 386.1669; found 386.1663; IR (liquid): 3032, 2838, 1615, 1496, 721 cm^{-1}.



(*Z*)-4-(4-bromophenyl)-1-(2-fluoro-1,3-diphenylallyl)-1*H*-1,2,3-triazole (6d) : According to the general procedure, triazole **5d** (40 mg, 179 µmol), selectfluor (126 mg, 357 µmol) and diaryl allene (86 mg, 446 µmol) provided **6d** as a white solid (57 mg, 74%) after flash column chromatography (10 % ethyl acetate in petroleum ether); R_f = 0.56 (20% ethyl acetate in petroleum ; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80 (s, 1H), 7.65 (d, *J* = 8.3 Hz, 2H), 7.51 – 7.42 (m, 4H), 7.35 – 7.27 (m, 5H), 7.25 – 7.23 (m, 3H), 6.62 (d, *J* = 17.0 Hz, 1H), 5.80 (d, *J* = 38.0 Hz, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 153.9 (d, *J* = 268.8 Hz), 147.2, 134.6, 132.1, 131.6, 129.5, 129.4, 129.3, 129.2, 128.8, 128.6, 127.5, 127.5, 122.4, 119.5 (d, *J* = 2.1 Hz), 112.6 (d, *J* = 6.3 Hz), 66.2 (d, *J* = 28.3 Hz); ^{19}F NMR (373 MHz, Chloroform-*d*) δ -112.7 (dd, *J* = 38.8, 16.7 Hz).; HRMS calculated for $C_{23}H_{18}BrFN_3^+$ [M+H] $^+$: 434.0668; found 434.0668; IR (liquid): 3031, 2923, 1954, 1903, 1602, 1450, 1232, 1131, 755 cm^{-1}.

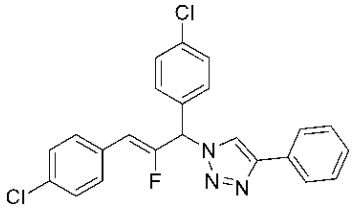


(*Z*)-4-(4-chlorophenyl)-1-(2-fluoro-1,3-diphenylallyl)-1*H*-1,2,3-triazole (6e) : According to the general procedure, triazole **5e** (40 mg, 223 µmol), selectfluor (158 mg, 445 µmol) and diaryl allene (107 mg, 557 µmol) provided **6e** as a white solid (58 mg, 67%) after flash column chromatography (10% ethyl acetate in petroleum ether); R_f = 0.55 (20% ethyl acetate in petroleum ; ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.79 (s, 1H), 7.70 (d, *J* = 8.5 Hz, 2H), 7.44 (d, *J* = 7.5 Hz, 2H), 7.36 – 7.32 (m, 3H), 7.33 – 7.19 (m, 7H), 6.61 (d, *J* = 16.8 Hz, 1H), 5.79 (d, *J* = 38.0 Hz, 1H).; ^{13}C NMR (125 MHz, Chloroform-*d*) δ 154.0 (d, *J* = 268.8 Hz), 147.2, 134.6, 134.2, 132.2 – 130.9 (m), 129.5, 129.4, 129.3, 129.2, 129.0, 128.8, 128.6, 127.5, 127.2, 119.5, 112.6 (d, *J* = 6.2 Hz), 66.2 (d, *J* = 28.4 Hz) ; ^{19}F NMR (373 MHz, Chloroform-*d*) δ -111.8 – -112.0 (m) HRMS calculated for $C_{23}H_{18}ClFN_3^+$ [M+H] $^+$: 390.1173; found 390.1171 ; IR (liquid): 3381, 3029, 1601, 1450, 1153, 754, 695 cm^{-1}.

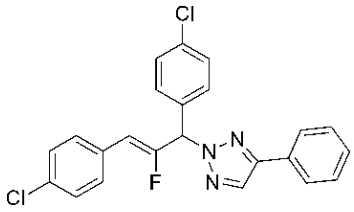


(*Z*)-4-(4-chlorophenyl)-2-(2-fluoro-1,3-diphenylallyl)-2*H*-1,2,3-triazole (6e') : According to the general procedure, triazole **5e** (40 mg, 223 µmol), selectfluor (158 mg, 445 µmol) and diaryl allene (107 mg, 557 µmol) provided **6e'** as a yellow oil (18 mg, 20%) after flash column chromatography (20% DCM in petroleum ether); R_f = 0.40 (5 % ethyl acetate in petroleum ether); ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.86 (s, 1H), 7.67 (d, *J* = 8.6 Hz, 2H), 7.44 – 7.22 (m, 12H),

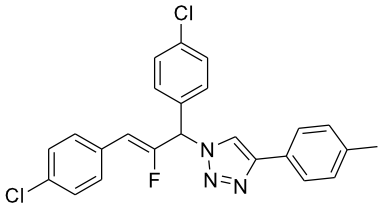
6.54 (d, *J* = 9.6 Hz, 1H), 5.59 (d, *J* = 37.9 Hz, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 155.3 (d, *J* = 269.8 Hz), 147.5, 134.8, 134.6, 131.9, 129.3, 129.2, 129.2, 129.0, 128.8, 128.6, 128.2, 128.2, 128.2, 127.5, 111.9 (d, *J* = 6.4 Hz), 70.3 (d, *J* = 29.7 Hz) ; ^{19}F NMR (373 MHz, Chloroform-*d*) δ -109.5 (d, *J* = 36.9 Hz); HRMS calculated for $C_{23}H_{18}ClFN_3^+$ [M+H] $^+$: 390.1173; found 390.1176; IR (liquid): 3363, 2921, 1600, 1452, 1260, 1093, 696 cm^{-1}.



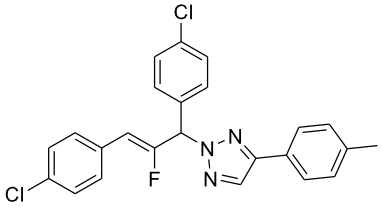
(*Z*)-1-(1,3-bis(4-chlorophenyl)-2-fluoroallyl)-4-phenyl-1*H*-1,2,3-triazole (6f): According to the general procedure, triazole **5a** (40 mg, 276µmol), selectfluor (195 mg, 551µmol) and diaryl allene (180 mg, 689 µmol) provided **6f** as a yellow solid (76 mg, 65%) after flash column chromatography (60% DCM in petroleum ether); R_f = 0.52 (20% ethyl acetate in petroleum ether); ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.9 – 7.8 (m, 1H), 7.72 (d, *J* = 8.1 Hz, 1H), 7.43 (dd, *J* = 18.5, 8.7 Hz, 6H), 7.32 (d, *J* = 8.5 Hz, 3H), 7.29 – 7.18 (m, 3H), 6.63 (d, *J* = 16.3 Hz, 1H), 5.82 (d, *J* = 37.4 Hz, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 154.0 (d, *J* = 269.4 Hz), 148.4, 138.5, 135.7, 132.9, 130.5, 130.4, 130.2, 129.6, 129.0, 129.0, 128.9, 128.6, 125.9, 119.3, 111.0 (d, *J* = 6.4 Hz), 65.4 (d, *J* = 28.5 Hz) ; ^{19}F NMR (373 MHz, Chloroform-*d*) δ -111.3 (q, *J* = 28.4, 23.9 Hz); HRMS calculated for $C_{23}H_{17}Cl_2FN_3^+$ [M+H] $^+$: 424.0784, found 424.0789; IR (liquid): 3064, 2925, 1904, 1432, 1135, 754 cm^{-1}.



(*Z*)-2-(1,3-bis(4-chlorophenyl)-2-fluoroallyl)-4-phenyl-2*H*-1,2,3-triazole (6f'): According to the general procedure, triazole **5a** (40 mg, 276µmol), selectfluor (195 mg, 551µmol) and diaryl allene (180 mg, 689 µmol) provided **6f'** as a yellow oil (18 mg, 15%) after flash column chromatography (20% DCM in petroleum ether); R_f = 0.38 (5% ethyl acetate in petroleum ether); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89 (s, 1H), 7.73 (d, *J* = 7.2 Hz, 2H), 7.38 – 7.29 (m, 9H), 7.23 – 7.21 (m, 2H), 6.50 (d, *J* = 9.2 Hz, 1H), 5.53 (d, *J* = 37.3 Hz, 1H); ^{13}C NMR (125 MHz, Chloroform-*d*) δ 155.5 (d, *J* = 270.3 Hz), 148.8, 135.4, 134.0, 133.2, 132.2, 130.5, 130.4, 130.0, 129.7, 129.3, 129.1, 128.9, 128.9, 126.2, 110.7 (d, *J* = 6.3 Hz), 69.3 (d, *J* = 30.4 Hz).^{19}F NMR (373 MHz, Chloroform-*d*) δ -108.1 (d, *J* = 37.4 Hz); HRMS calculated for $C_{23}H_{17}Cl_2FN_3^+$ [M+H] $^+$: 424.0784, found 424.0784; IR (liquid) 2920, 2850, 1727, 1492, 1092, 800 cm^{-1}.

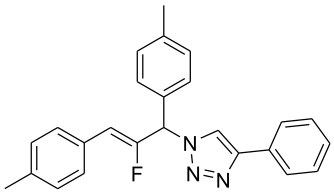


(*Z*)-1-(1,3-bis(4-chlorophenyl)-2-fluoroallyl)-4-p-tolyl-1*H*-1,2,3-triazole (6g) : According to the general procedure, triazole **5b** (40 mg, 251µmol), selectfluor (178 mg, 503 µmol) and diaryl allene (164 mg, 628 µmol) provided **6g** as a yellow solid (62 mg, 71%) after flash column chromatography (10% ethyl acetate in petroleum ether); R_f = 0.52 (20% ethyl acetate in petroleum ether); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.72 (d, *J* = 0.8 Hz, 1H), 7.66 (d, *J* = 8.1 Hz, 2H), 7.36 (dd, *J* = 15.6, 8.6 Hz, 3H), 7.26 (d, *J* = 8.6 Hz, 2H), 7.18 (dd, *J* = 12.8, 8.2 Hz, 5H), 6.56 (d, *J* = 16.3 Hz, 1H), 5.74 (d, *J* = 37.4 Hz, 1H), 2.31 (s, 3H); ^{13}C NMR (125 MHz, Chloroform-*d*) δ 154.2(d, *J* = 269.8 Hz), 148.6, 138.5, 135.7, 134.5, 133.2, 130.5, 130.5, 129.7, 129.7, 129.0, 129.0, 127.4, 125.9, 118.9, 111.6, 65.4 (d, *J* = 29.0 Hz), 21.5 ;^{19}F NMR (373 MHz, Chloroform-*d*) δ -112.0 (d, *J* = 17.2 Hz) ; HRMS calculated for $C_{24}H_{19}Cl_2FN_3^+$ [M+H]$^+$: 438.0940; found 438.0949; IR (liquid): 2960, 1905, 1455, 754 cm^{-1}.

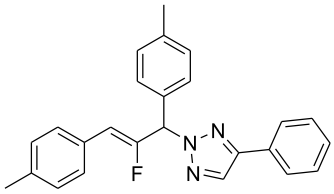


(*Z*)-2-(1,3-bis(4-chlorophenyl)-2-fluoroallyl)-4-p-tolyl-2*H*-1,2,3-triazole (6g') : According to the general procedure, triazole **5b** (40 mg, 251 µmol), selectfluor (178 mg, 503 µmol) and diaryl allene (164 mg, 628 µmol) provided **6g'** as a yellow oil (20 mg, 18%) after flash column chromatography (20% DCM in petroleum ether); R_f = 0.47 (5% ethyl acetate

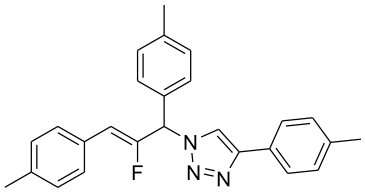
in petroleum ether); ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.85 (s, 1H), 7.61 (d, *J* = 8.1 Hz, 2H), 7.36 – 7.31 (m, 6H), 7.22 (d, *J* = 8.6 Hz, 2H), 7.16 (d, *J* = 7.9 Hz, 2H), 6.49 (d, *J* = 9.2 Hz, 1H), 5.53 (d, *J* = 37.3 Hz, 1H), 2.31 (s, 3H) ; ^{19}F NMR (373 MHz, Chloroform-*d*) δ -108.0 (d, *J* = 36.4 Hz) ;HRMS calculated for $C_{24}H_{19}Cl_2FN_3^+$ [M+H]$^+$: 438.0940; found 438.0947; IR (liquid) : 2924, 1900, 1690, 754 cm^{-1}.



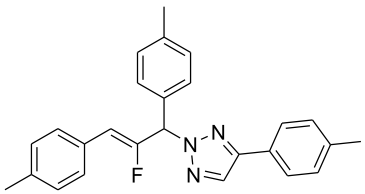
(*Z*)-1-(2-fluoro-1,3-dip-tolylallyl)-4-phenyl-1*H*-1,2,3-triazole (6h) : According to the general procedure, triazole **5a** (40 mg, 276 µmol), selectfluor (195 mg, 551µmol) and diaryl allene (152 mg, 689 µmol) provided **6h** as a yellow oil (28 mg, 26%) after flash column chromatography (10% ethyl acetate in petroleum ether); R_f = 0.55 (20% ethyl acetate in petroleum ether); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.77 (d, *J* = 8.6 Hz, 3H), 7.38 – 7.30 (m, 4H), 7.25 (t, *J* = 7.3 Hz, 1H), 7.14 (s, 4H), 7.08 (d, *J* = 7.9 Hz, 2H), 6.57 (d, *J* = 16.3 Hz, 1H), 5.73 (d, *J* = 38.3 Hz, 1H), 2.30 (s, 3H), 2.27 (s, 3H) ^{13}C NMR (125 MHz, Chloroform-*d*) δ 153.8 (d, *J* = 267.8 Hz), 148.1, 139.4, 138.5, 131.9, 130.6, 130.0, 129.5, 129.2, 129.1, 129.0, 128.4, 127.5, 125.9, 119.4, 112.0 (d, *J* = 6.4 Hz), 66.0 (d, *J* = 28.7 Hz), 21.4, 21.3 ; ^{19}F NMR (373 MHz, Chloroform-*d*) δ -113.4 (dd, *J* = 36.9, 14.9 Hz); HRMS calculated for $C_{25}H_{23}FN_3^+$ [M+H] $^+$: 384.1876, found 384.1870; IR (liquid): 3028, 2922, 1688, 1513, 764 cm^{-1}.



(*Z*)-2-(2-fluoro-1,3-dip-tolylallyl)-4-phenyl-2*H*-1,2,3-triazole (6h') : According to the general procedure, triazole **5a** (40 mg, 276µmol), selectfluor (195 mg, 551 µmol) and diaryl allene (152 mg, 689 µmol) provided **6h'** as a white solid (66 mg, 62 %) after flash column chromatography (2.5% ethyl acetate in petroleum ether); R_f = 0.44 (5% ethyl acetate in petroleum ether); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.87 (s, 1H), 7.73 (d, *J* = 7.3 Hz, 2H), 7.38 – 7.25 (m, 7H), 7.13 (d, *J* = 8.0 Hz, 2H), 7.04 (d, *J* = 8.0 Hz, 2H), 6.50 (d, *J* = 9.3 Hz, 1H), 5.55 (d, *J* = 38.2 Hz, 1H), 2.29 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (125 MHz, Chloroform-*d*) δ 155.1 (d, *J* = 268.5 Hz), 148.4, 139.0, 138.0, 132.1, 131.8, 130.4, 129.7, 129.3, 129.1, 129.0, 129.0, 128.7, 128.2, 126.2, 111.3, 70.0 (d, *J* = 30.1 Hz), 21.4, 21.4 ; ^{19}F NMR (373 MHz, Chloroform-*d*) δ -110.5 (d, *J* = 47.5 Hz). ; HRMS calculated for $C_{25}H_{23}FN_3^+$ [M+H] $^+$: 384.1876, found 384.1877; IR (liquid) : 2919, 1689, 1458, 1135, 768 cm^{-1}.

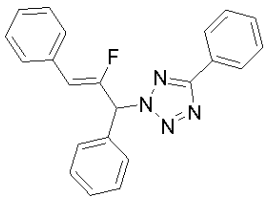


(*Z*)-1-(2-fluoro-1,3-dip-tolylallyl)-4-*p*-tolyl-1*H*-1,2,3-triazole (6i) : According to the general procedure, triazole **5b** (40 mg, 251µmol) and selectfluor (178 mg, 503µmol) and Diaryl allene (138 mg, 628 µmol) provided **6i** as a yellow oil (28 mg, 28%) after flash column chromatography (10 % ethyl acetate in petroleum ether); R_f = 0.51 (20% ethyl acetate in petroleum ether) ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 (s, 1H), 7.66 (d, *J* = 8.1 Hz, 2H), 7.34 (d, *J* = 8.2 Hz, 2H), 7.15 (d, *J* = 6.9 Hz, 6H), 7.09 (d, *J* = 8.1 Hz, 2H), 6.57 (d, *J* = 16.2 Hz, 1H), 5.73 (d, *J* = 38.3 Hz, 1H), 2.30 (s, 3H), 2.28 (s, 3H), 2.25 (s, 3H) ; ^{13}C NMR (125 MHz, Chloroform-*d*) δ 153.8 (d, *J* = 267.6 Hz), 148.2, 139.4, 138.5, 138.3, 131.9, 130.0, 129.6, 129.5, 129.1, 129.1, 127.8, 127.5, 125.8, 119.0, 112.1 – 111.7 (m), 65.9 (d, *J* = 28.5 Hz), 21.5, 21.3 ; ^{19}F NMR (373 MHz, Chloroform-*d*) δ -113.2 (d, *J* = 28.7 Hz) ; HRMS calculated for $C_{26}H_{25}FN_3^+$ [M+H] $^+$: 398.2033; found 398.2035; IR (liquid) : 3064, 2850, 1602, 1451, 1116, 726 cm.$^{-1}$

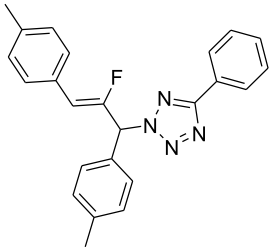


(*Z*)-2-(2-fluoro-1,3-dip-tolylallyl)-4-*p*-tolyl-2*H*-1,2,3-triazole (6i') : According to the general procedure, triazole **5b** (40 mg, 251µmol) and selectfluor (178 mg, 503 µmol) and Diaryl allene (138 mg, 628 µmol) provided **6i'** as a cream coloured solid (62 mg, 62%) after flash column chromatography (2.5% ethyl acetate in petroleum ether); R_f = 0.46 (5% ethyl acetate in petroleum ether); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 (s, 1H), 7.62 (d, *J* = 7.9 Hz, 2H), 7.29 (dd, *J* = 11.0, 8.2 Hz, 4H), 7.13 (t, *J* = 7.3 Hz, 4H), 7.04 (d, *J* = 7.9 Hz,

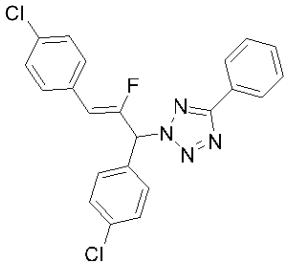
2H), 6.48 (d, *J* = 9.3 Hz, 1H), 5.54 (d, *J* = 38.2 Hz, 1H), 2.30 (s, 3H), 2.28 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 155.2 (d, *J* = 268.9 Hz), 148.4, 139.0, 138.6, 137.9, 132.2, 132.1, 131.7, 129.6, 129.3, 129.1, 129.0, 128.2, 127.5, 126.1, 111.3 (d, *J* = 6.6 Hz), 69.9 (d, *J* = 30.0 Hz), 21.5, 21.4, 21.4; ^{19}F NMR (373 MHz, Chloroform-*d*) δ -110.3 (d, *J* = 36.9 Hz); HRMS calculated for $C_{26}H_{25}FN_3^+$ [M+H] $^+$: 398.2033; found 398.2037; IR (liquid) : 3027, 2921, 1907, 1513, 1135, 819 cm^{-1}.



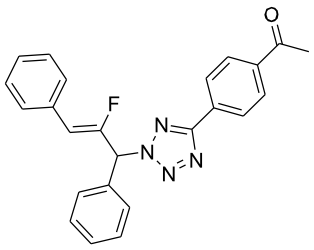
(*Z*)-2-(2-fluoro-1,3-diphenylallyl)-5-phenyl-2*H*-tetrazole (8a) : According to the general procedure, tetrazole **7a** (40 mg, 274 µmol), selectfluor (194 mg, 547 µmol) and diaryl allene (132 mg, 684 µmol) provided **8a** as a yellow solid (82 mg, 84%) after flash column chromatography (2.5 % ethyl acetate in petroleum ether); R_f = 0.38 (5% ethyl acetate in petroleum ether); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.18 – 8.00 (m, 2H), 7.47 – 7.31 (m, 10H), 7.29 – 7.16 (m, 3H), 6.77 (d, *J* = 9.6 Hz, 1H), 5.67 (d, *J* = 37.4 Hz, 1H) ; ^{13}C NMR (100 MHz, Chloroform-*d*) δ 165.6, 153.9 (d, *J* = 269.7 Hz), 133.3, 131.8, 130.6, 129.7, 129.3, 129.2, 129.0, 128.7, 128.5, 128.3, 127.3, 127.2, 112.7 (d, *J* = 6.3 Hz), 69.0 (d, *J* = 29.7 Hz) ; ^{19}F NMR (373 MHz, Chloroform-*d*) δ -110.5 (d, *J* = 38.7 Hz) ; HRMS calculated for $C_{22}H_{17}NaFN_4^+$ [M+Na]$^+$: 379.1335; found 379.1336; IR (liquid): 3032, 1956, 1689, 1466, 1135, 732 cm^{-1}.



(*Z*)-2-(2-fluoro-1,3-dip-tolylallyl)-5-phenyl-2*H*-tetrazole (8b) : According to the general procedure, tetrazole **7a** (40 mg, 274 µmol), selectfluor (194 mg, 547 µmol) and diaryl allene (151 mg, 684 µmol) provided **8b** as a yellow solid (92 mg, 87%) after flash column chromatography (2.5 % ethyl acetate in petroleum ether); R_f = 0.43 (5% ethyl acetate in petroleum ether), ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.10 (dd, *J* = 7.5, 2.1 Hz, 2H), 7.42 – 7.36 (m, 3H), 7.31 (dd, *J* = 11.8, 8.2 Hz, 4H), 7.15 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 8.0 Hz, 2H), 6.72 (d, *J* = 9.4 Hz, 1H), 5.64 (d, *J* = 37.7 Hz, 1H), 2.29 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 165.5, 153.5 (d, *J* = 268.6 Hz), 139.7, 138.4, 130.5, 129.9, 129.4, 129.2, 129.1, 129.0, 129.0, 128.3, 127.4, 127.2, 112.4 (d, *J* = 6.5 Hz), 68.9 (d, *J* = 29.6 Hz), 21.4, 21.4 ; ^{19}F NMR (373 MHz, Chloroform-*d*) δ -110.8 (d, *J* = 37.6 Hz); HRMS calculated for $C_{24}H_{22}FN_4^+$ [M+H] $^+$: 385.1828; found 385.1829; IR (liquid): 3030, 2922, 1908, 1690, 1449, 1134, 732 cm^{-1}.

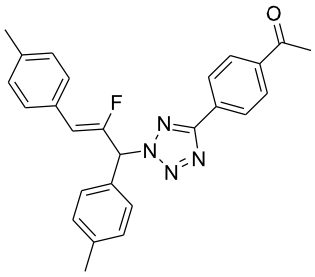


(*Z*)-2-(1,3-bis(4-chlorophenyl)-2-fluoroallyl)-5-phenyl-2*H*-tetrazole (8c) : According to the general procedure, tetrazole **7a** (40 mg, 274 µmol), selectfluor (194 mg, 547 µmol) and diaryl allene (179 mg, 684 µmol) provided **8c** as a yellow oil (90 mg, 77%) after flash column chromatography (2.5 % ethyl acetate in petroleum ether); R_f = 0.40 (5% ethyl acetate in petroleum ether); ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.12 – 8.07 (m, 2H), 7.43 – 7.38 (m, 5H), 7.34 (dd, *J* = 8.7, 2.0 Hz, 4H), 7.23-7.21 (m, 2H), 6.73 (d, *J* = 9.6 Hz, 1H), 5.63 (d, *J* = 36.8 Hz, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) 165.7, 153.8 (d, *J* = 270.5 Hz), 136.0, 135.2 – 133.7 (m), 131.5 (d, *J* = 2.5 Hz), 130.8, 130.5 (d, *J* = 7.6 Hz), 130.1 (d, *J* = 2.6 Hz), 129.8, 129.6, 129.0, 129.0, 127.1, 111.7 (d, *J* = 6.3 Hz), 68.1 (d, *J* = 30.0 Hz); ^{19}F NMR (373 MHz, Chloroform-*d*) δ -110.1 (d, *J* = 29.4 Hz); HRMS calculated for $C_{44}H_{31}Cl_4F_2N_8^+$ [2M+H] $^+$: 849.1394; found 849.1393; IR (liquid): 3383, 2962, 1693, 1450, 1139, 758 cm^{-1}.

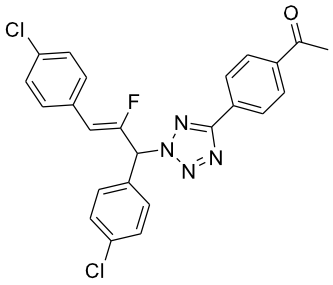


(*Z*)-1-(4-(2-(2-fluoro-1,3-diphenylallyl)-2*H*-tetrazol-5-yl)phenyl)ethanone (8d) : According to the general procedure, tetrazole **7b** (40 mg, 213 µmol), selectfluor (151 mg, 425 µmol) and diaryl allene (102 mg, 531 µmol) provided **4p** as a white solid (81 mg, 95%) after flash column chromatography (2.5 % ethyl acetate in petroleum ether); R_f = 0.26 (5% ethyl

acetate in petroleum; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.21 (d, *J* = 8.4 Hz, 2H), 7.99 (d, *J* = 8.4 Hz, 2H), 7.49 – 7.33 (m, 7H), 7.32 – 7.12 (m, 3H), 6.80 (d, *J* = 9.7 Hz, 1H), 5.69 (d, *J* = 37.4 Hz, 1H), 2.56 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 197.6, 164.6, 153.7 (d, *J* = 269.5 Hz), 138.5, 133.1, 131.8 (d, *J* = 2.6 Hz), 131.5, 129.8, 129.3, 129.2, 129.0, 128.7, 128.6, 128.3, 127.3, 112.9 (d, *J* = 6.0 Hz), 69.2 (d, *J* = 29.3 Hz), 26.9; ^{19}F NMR (373 MHz, Chloroform-*d*) δ -110.7 (d, *J* = 38.3 Hz) ; HRMS calculated for $C_{24}H_{18}FN_4O^+$ [M-H] $^+$: 397.1465; found 397.1461 ; IR (liquid): 3029, 2850, 1954, 1423,763 cm^{-1}.



(*Z*)-1-(4-(2-(2-fluoro-1,3-dip-tolylallyl)-2*H*-tetrazol-5-yl)phenyl)ethanone (8e) : According to the general procedure, tetrazole **7b** (40 mg, 213 µmol), selectfluor (151 mg, 425µmol) and diaryl allene (117 mg, 531µmol) provided **4q** as a yellow oil (72 mg, 80%) after flash column chromatography (2.5 % ethyl acetate in petroleum ether); R_f = 0.40 (5% ethyl acetate in petroleum; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.22 (d, *J* = 8.4 Hz, 2H), 8.00 (d, *J* = 8.4 Hz, 2H), 7.33 (dd, *J* = 9.9, 8.2 Hz, 4H), 7.17 (s, 2H), 7.07 (d, *J* = 8.0 Hz, 2H), 6.75 (d, *J* = 9.4 Hz, 1H), 5.66 (d, *J* = 37.7 Hz, 1H), 2.58 (s, 3H), 2.32 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 197.7, 164.5, 153.3 (d, *J* = 268.3 Hz), 139.9, 138.5, 138.4, 131.6, 130.3, 130.0, 129.4, 129.2, 129.1, 129.0, 128.3, 127.3, 112.6 (d, *J* = 6.3 Hz), 69.1 (d, *J* = 29.2 Hz), 26.9, 21.4, 21.4; ^{19}F NMR (373 MHz, Chloroform-*d*) δ -111.8 (dd, *J* = 38.6, 10.6 Hz) ; HRMS calculated for $C_{26}H_{22}FN_4O^+$ [M-H]$^+$: 425.1772; found 425.1774; IR (liquid): 2963, 1687, 1418, 1261, 800, 762 cm^{-1}.



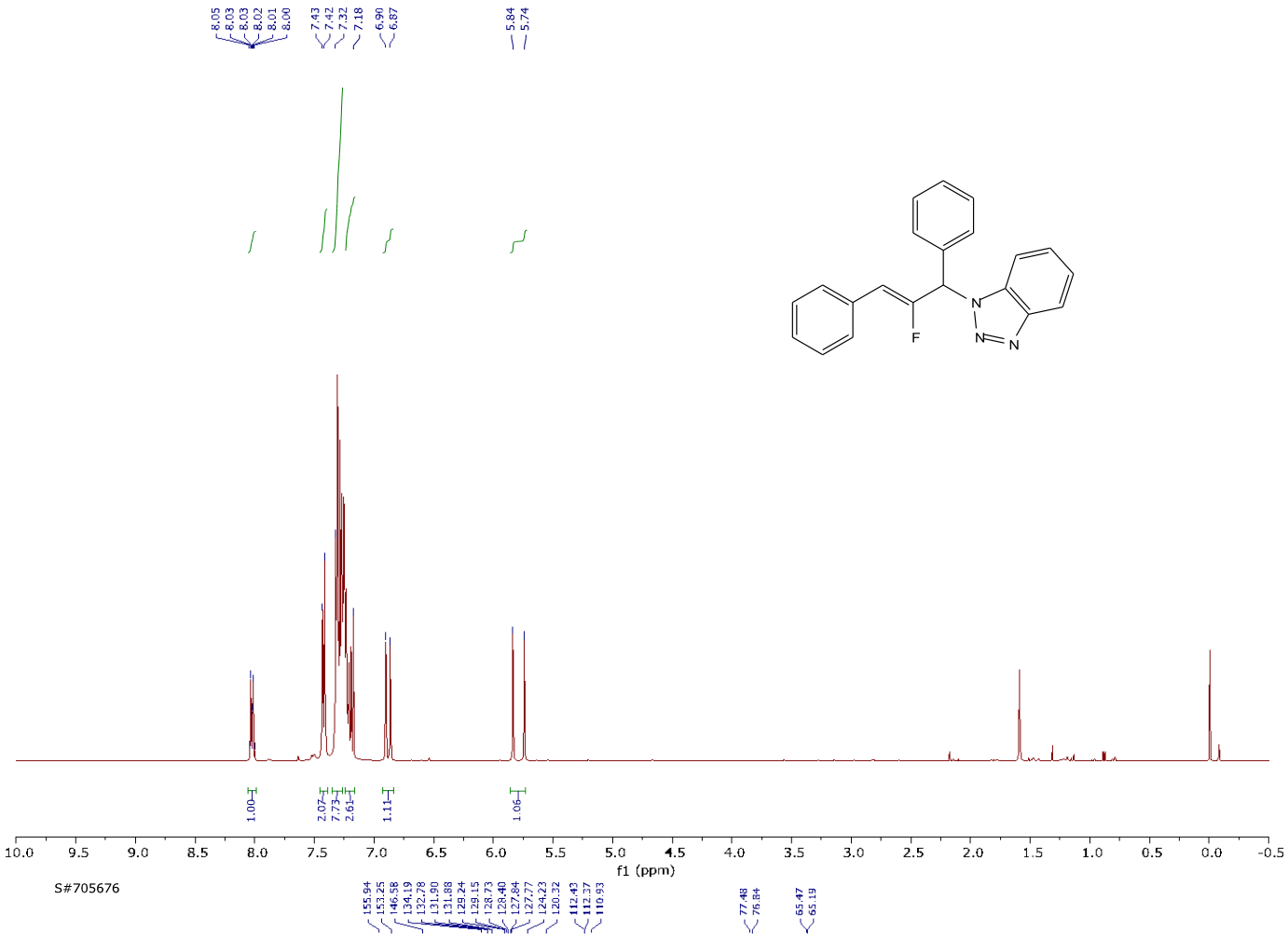
(*Z*)-1-(4-(2-(1,3-bis(4-chlorophenyl)-2-fluoroallyl)-2*H*-tetrazol-5-yl)phenyl)ethanone (8f) : According to the general procedure, tetrazole **7b** (40 mg, 213µmol), selectfluor (151 mg, 425 µmol) and diaryl allene (139 mg, 531 µmol) provided **8f** as a yellow oil (90 mg, 90%) after flash column chromatography (2.5 % ethyl acetate in petroleum ether); R_f = 0.26 (5 % ethyl acetate in petroleum); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.21 (d, *J* = 8.4 Hz, 2H), 8.00 (d, *J* = 8.4 Hz, 2H), 7.37 (dd, *J* = 13.3, 8.4 Hz, 6H), 7.21 (d, *J* = 17.6 Hz, 2H), 6.76 (d, *J* = 9.7 Hz, 1H), 5.65 (d, *J* = 36.8 Hz, 1H), 2.58 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 197.6, 164.8, 153.6 (d, *J* = 270.7 Hz), 138.6, 136.2, 134.5, 131.4, 131.2, 130.6, 130.5, 130.0, 129.8, 129.7, 129.0, 127.3, 111.9 (d, *J* = 6.2 Hz), 68.4 (d, *J* = 29.6 Hz), 26.9; ^{19}F NMR (373 MHz, Chloroform-*d*) δ -109.6 (d, *J* = 36.7 Hz) ; HRMS calculated for $C_{48}H_{35}Cl_4F_2N_8O_2^+$ [2M+H]$^+$: 933.1605; found 933.1608; IR (liquid): 3355, 2925, 2185, 1907, 1466, 1150, 748 cm^{-1}.

References

[1] M. L. Hossain, F. Ye, Y. Zhang, J. Wang, *The Journal of Organic Chemistry* **2013**, *78*, 1236-1241.

[2] a) S. Jana, A. Chakraborty, V. Z. Shirinian, A. Hajra, *Adv. Synth. Catal.* **2018**, *360*, 2402-2408; b) X.-J. Quan, Z.-H. Ren, Y.-Y. Wang, Z.-H. Guan, *Org. Lett.* **2014**, *16*, 5728-5731.

[3] a) D. Amantini, R. Beleggia, F. Fringuelli, F. Pizzo, L. Vaccaro, *The Journal of Organic Chemistry* **2004**, *69*, 2896-2898; b) B. Das, C. R. Reddy, D. N. Kumar, M. Krishnaiah, R. Narender, *Synlett* **2010**, *2010*, 391-394.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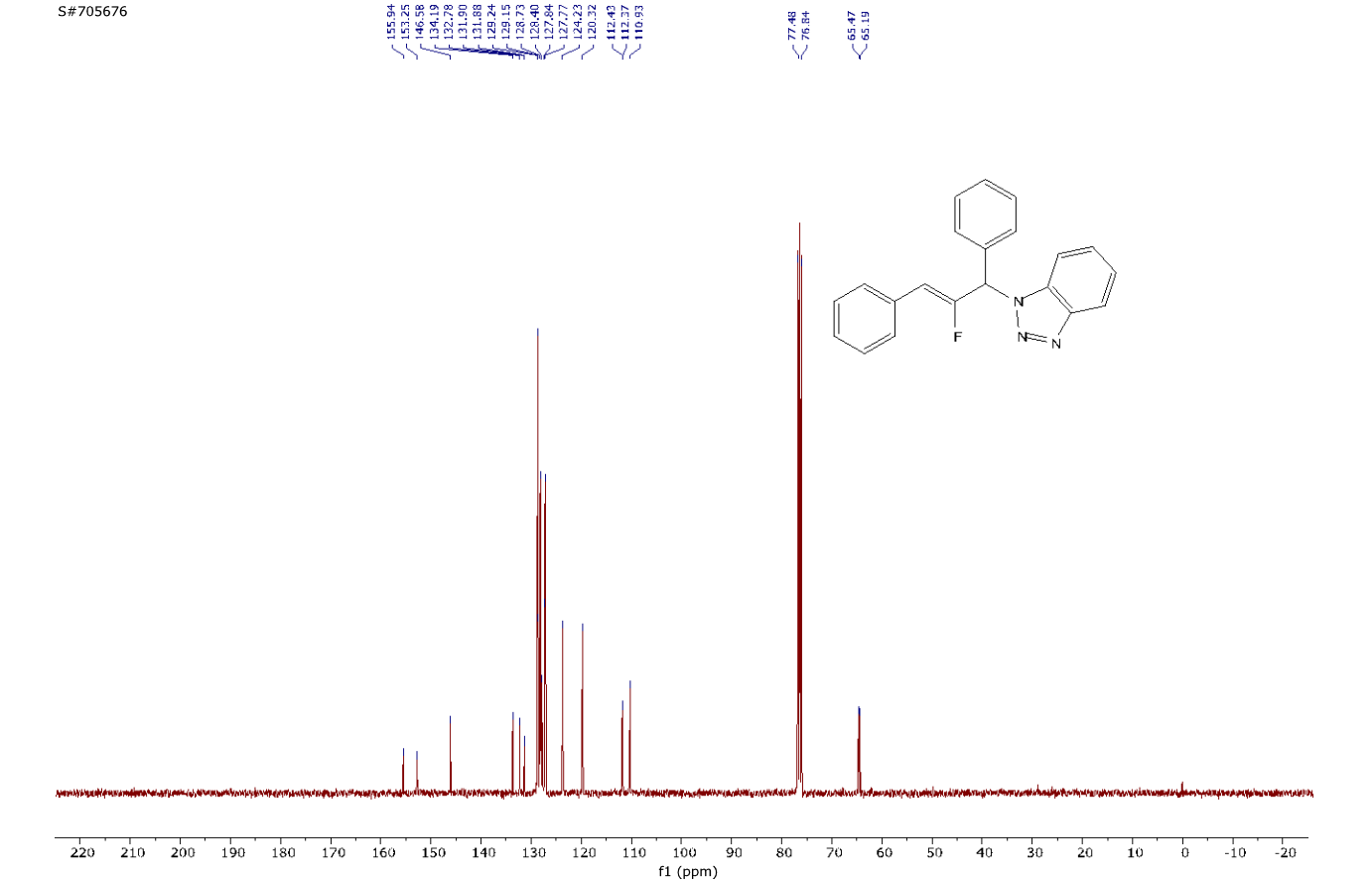
8.03
8.03
8.02
8.01
8.00
7.43
7.42
7.32
7.18
6.90
6.87
5.84
5.74
F
N
N
N
1.00
2.07
7.73
2.61
1.11
1.06
f1 (ppm)

S#705676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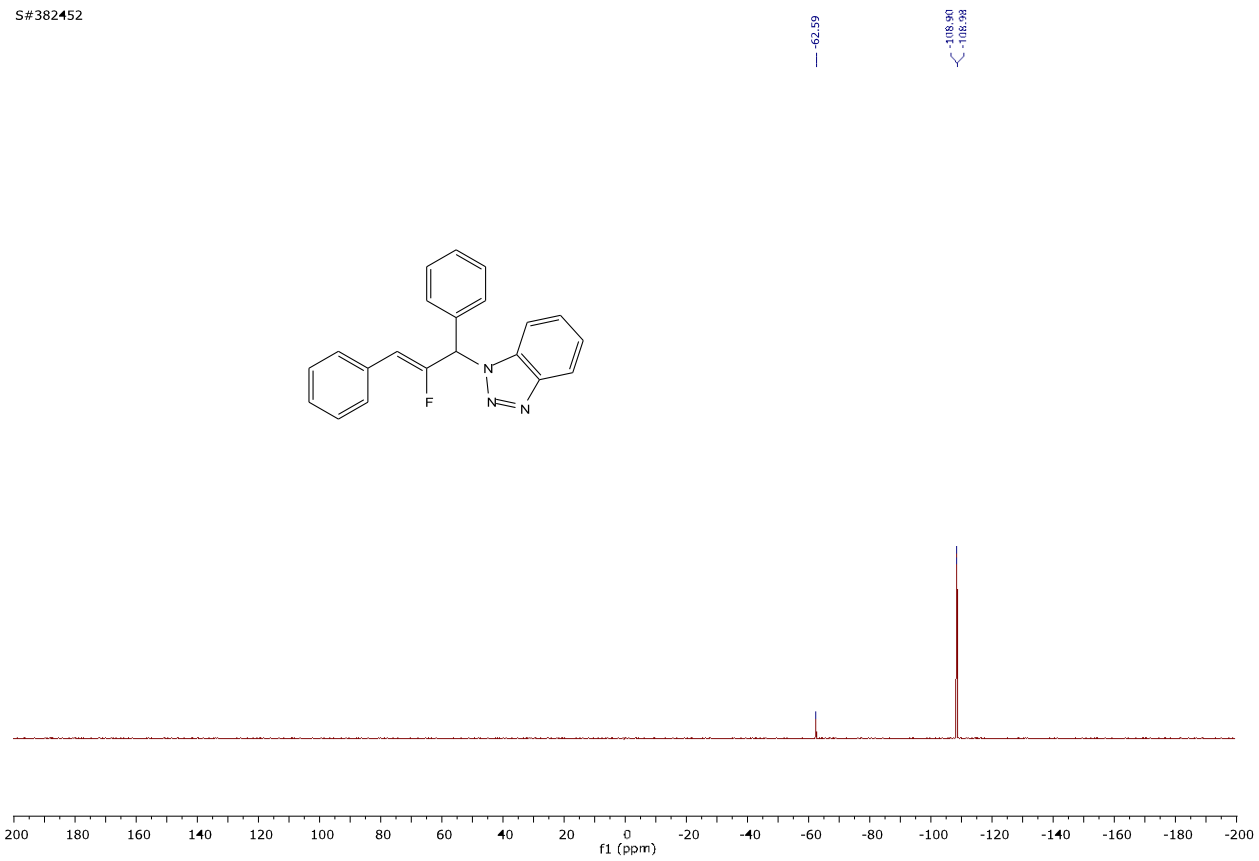
153.25
146.58
134.19
132.78
131.90
131.88
129.24
129.15
128.73
128.40
127.84
127.77
124.23
120.32
112.43
112.37
110.93
77.48
76.84
65.47
65.19
F
N
N
N
f1 (ppm)

S#382452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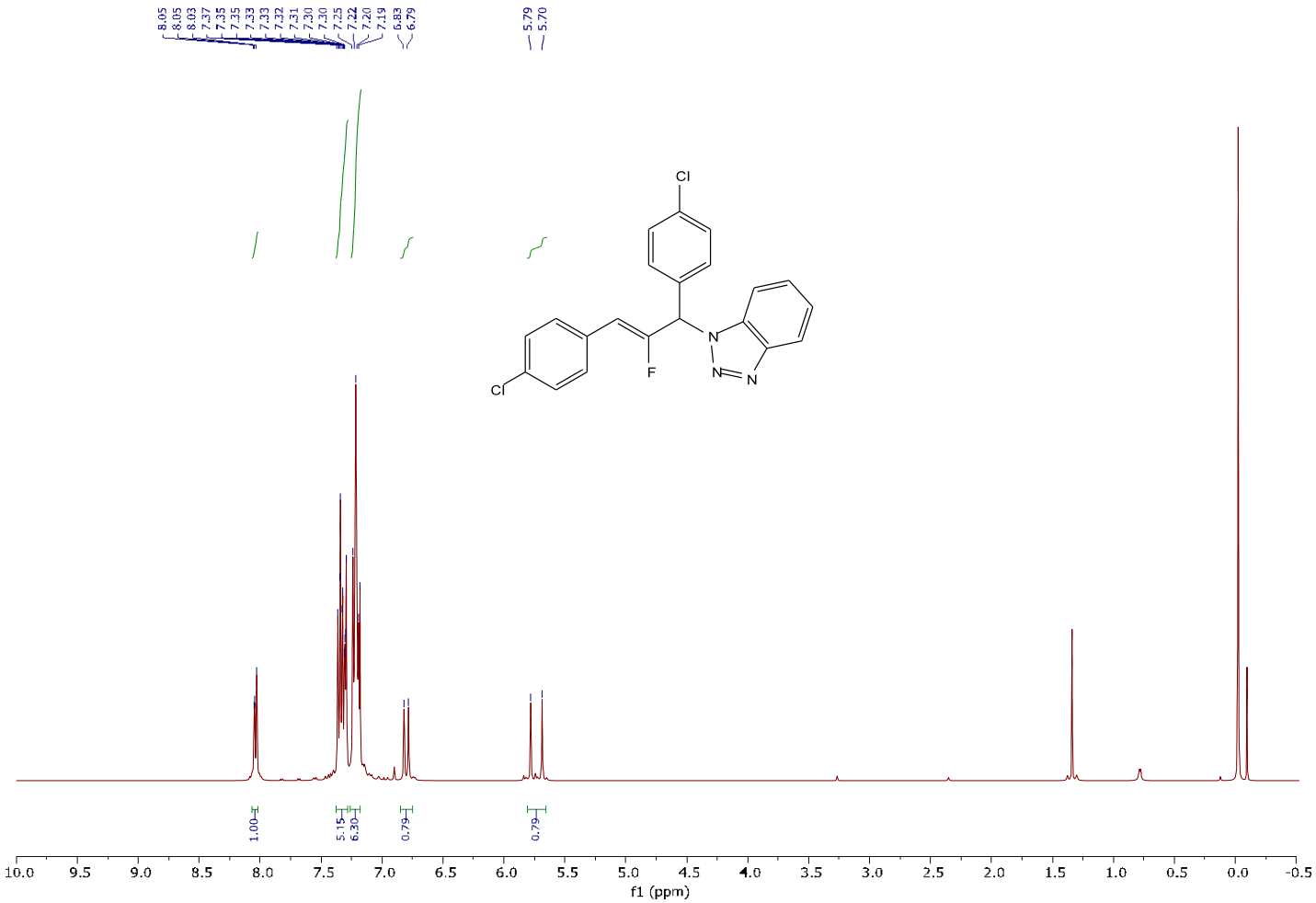
-108.90
-108.98
F
N
N
N
200
180
160
140
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)


8.05
8.05
8.03
7.37
7.35
7.35
7.33
7.33
7.32
7.31
7.30
7.30
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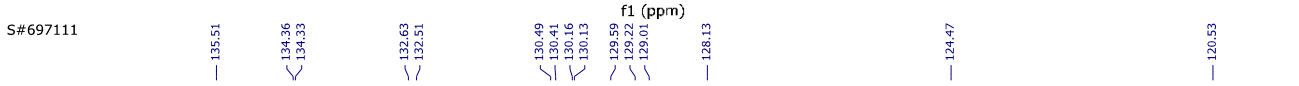
7.22
7.20
7.19
6.83
6.79
5.79
5.70
Cl
Cl
F
N
N
N
1.00
5.15
6.30
0.79
0.79
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

S#697111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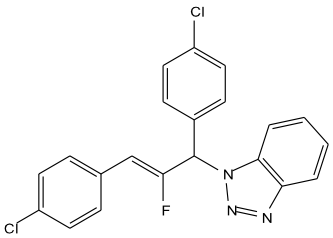
134.36
134.33
132.63
132.51
130.49
130.41
130.16
130.13
129.59
129.22
129.01
128.13
124.47
120.53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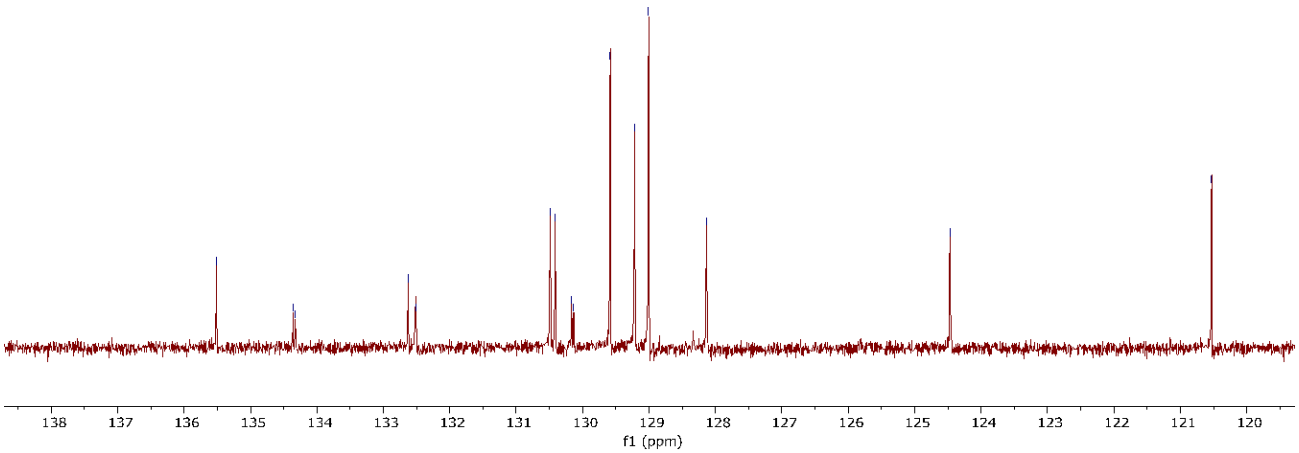
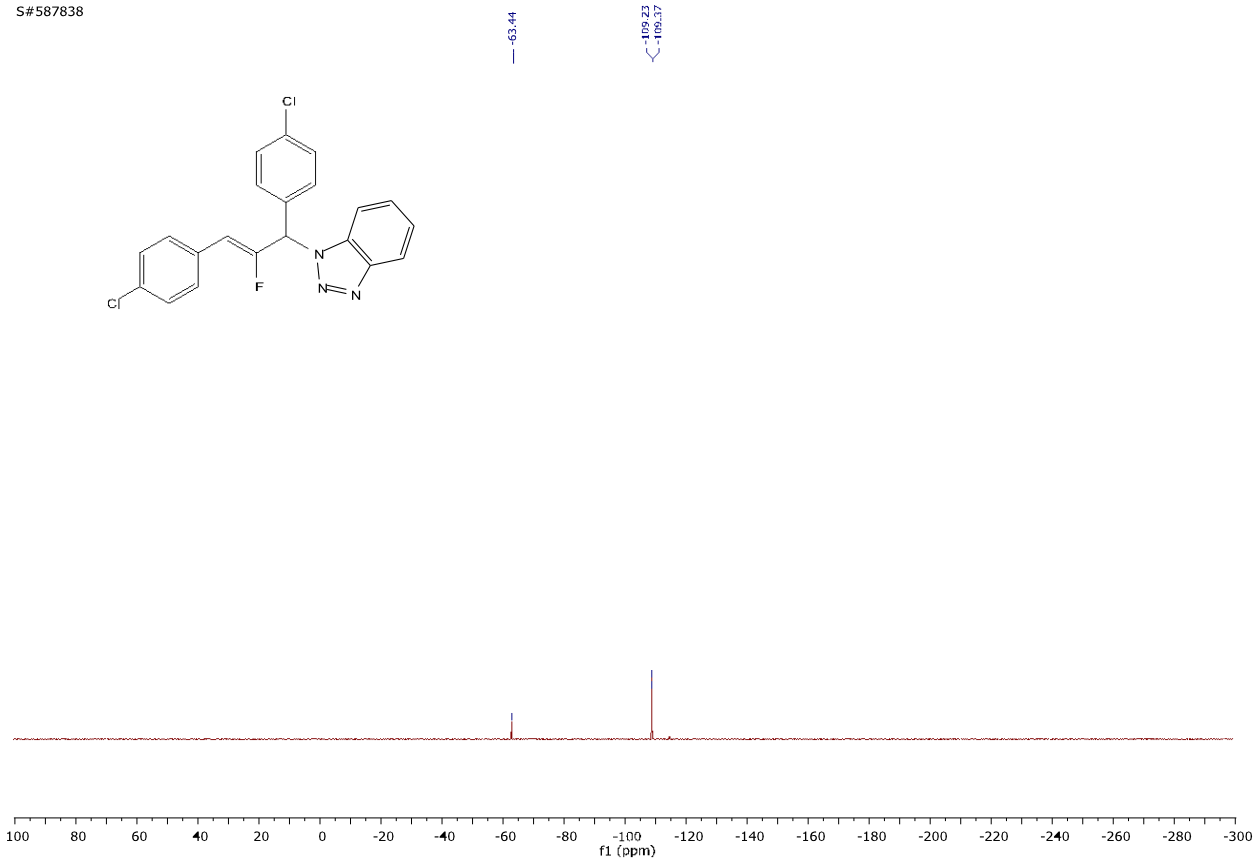
Cl
F
N
N
N


138
137
136
135
134
133
132
131
130
129
128
127
126
125
124
123
122
121
120
f1 (ppm)

S#587838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-109.37
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Cl
F
N
N
N
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
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-260
-280
-300
f1 (ppm)

S#458261
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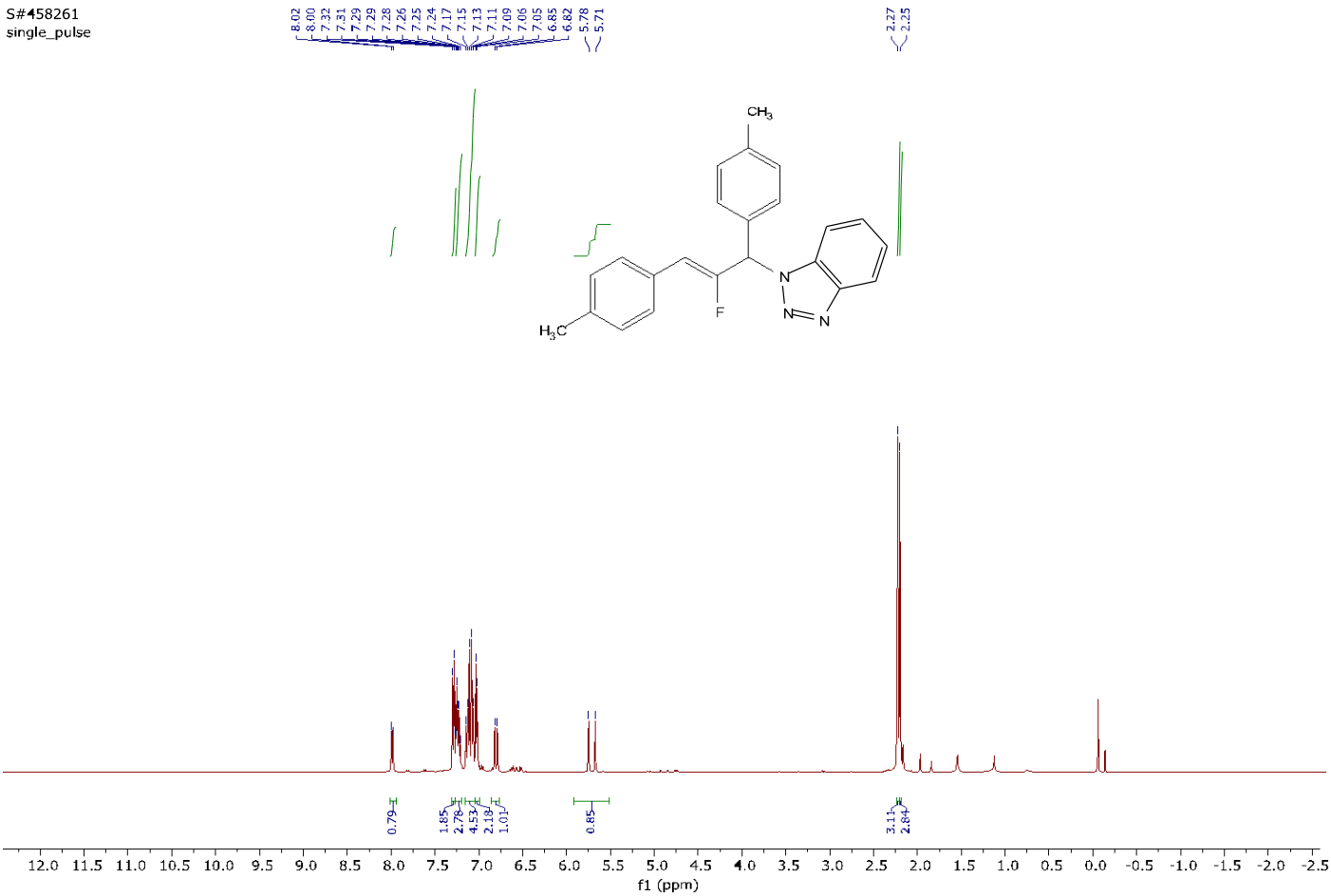

S#848515
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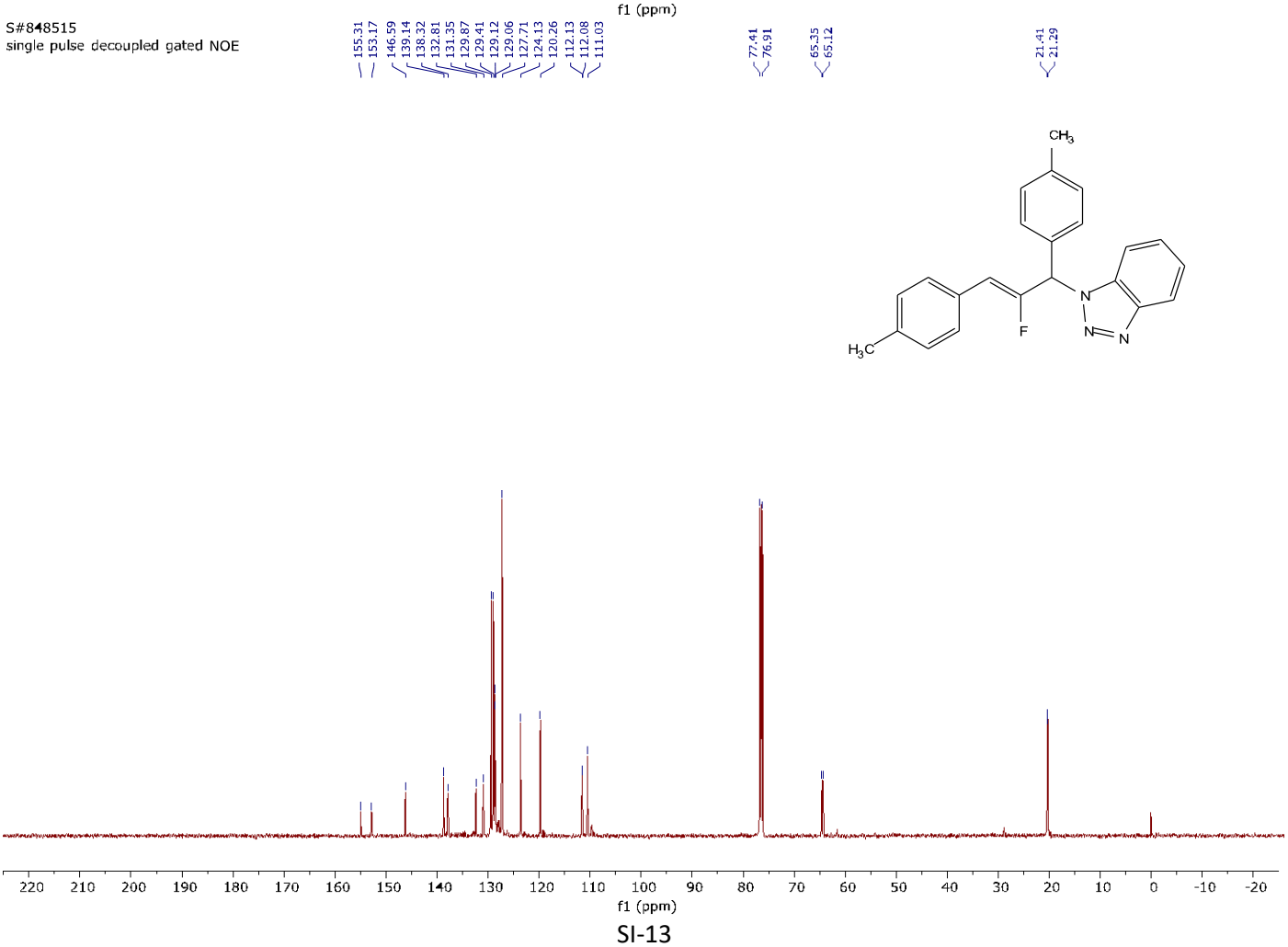

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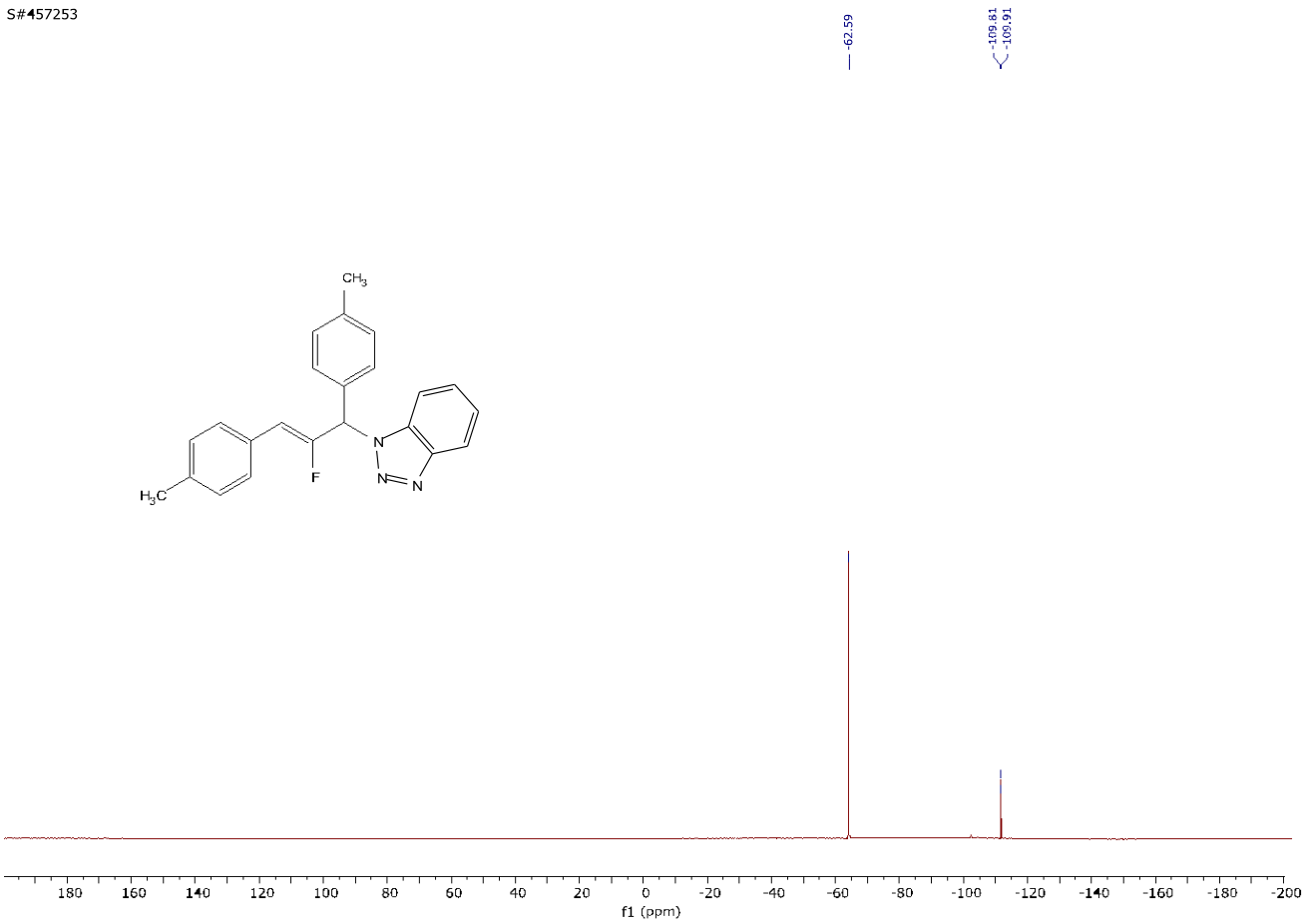
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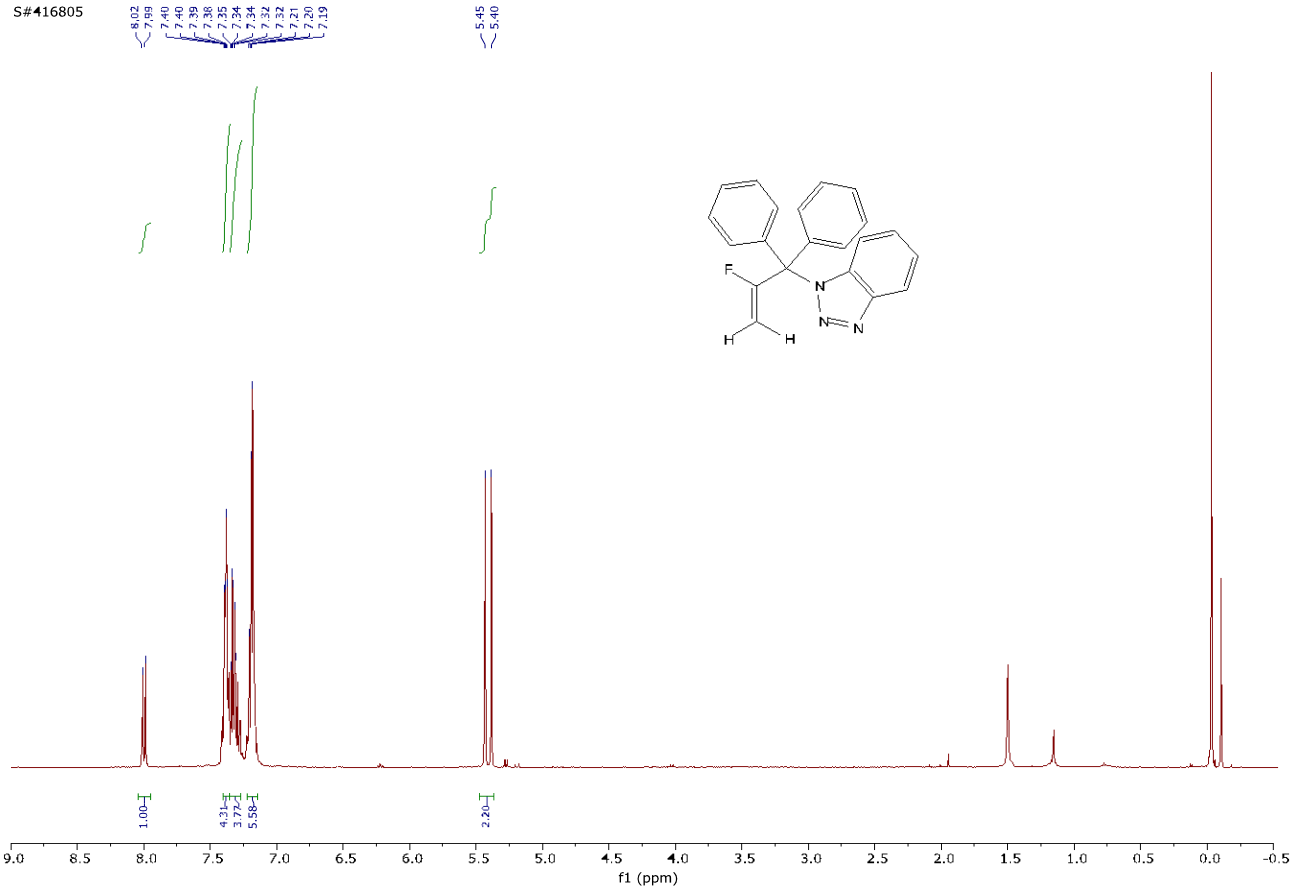
H3C
F
N
N
N
180
160
140
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)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7.35
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7.34
7.32
7.32
7.21
7.20
7.19
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F
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N
N
H
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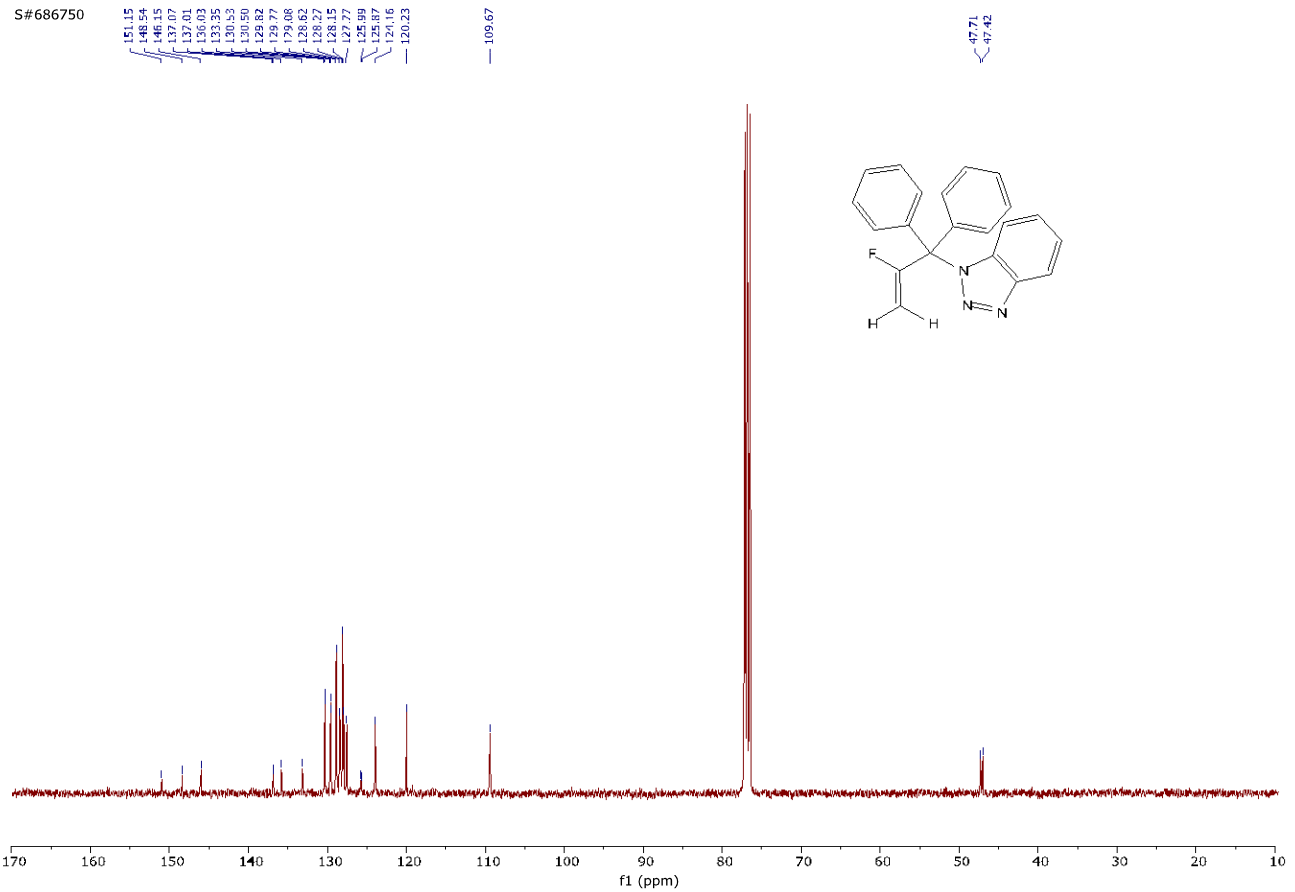
2.20
f1 (ppm)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137.01
136.02
133.35
130.53
130.50
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128.27
128.15
127.77
125.99
125.87
124.16
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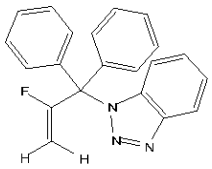
47.42
F
N
N
N
H
H
f1 (ppm)

S#447146


F
N
N
N
H
H

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-112.71
-112.77
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80
60
40
20
0
-20
-40
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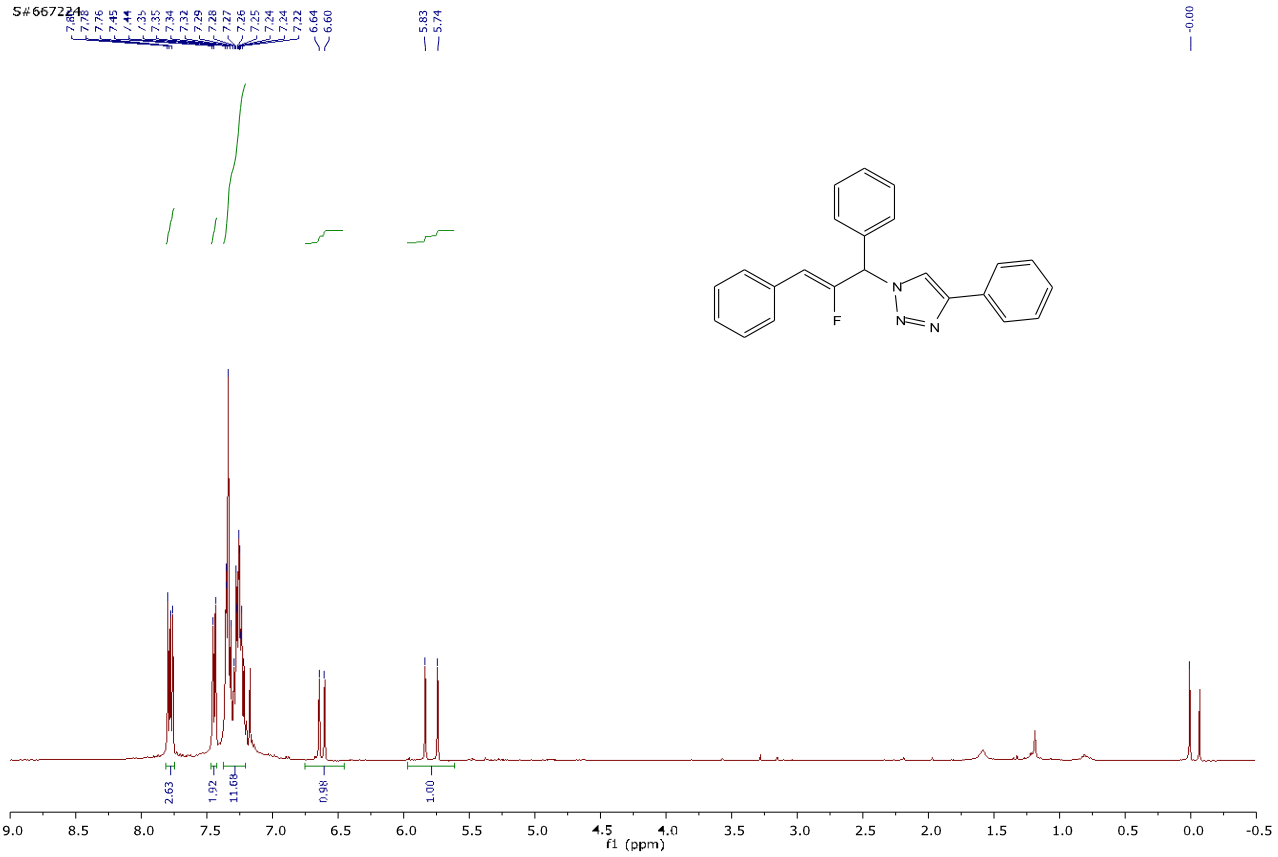
-180
-200
-220
-240
-260
-280
-300
f1 (ppm)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7.28
7.27
7.26
7.25
7.24
7.24
7.22
6.64
6.60
5.83
5.74
-0.00
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N
N
N
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11.68
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1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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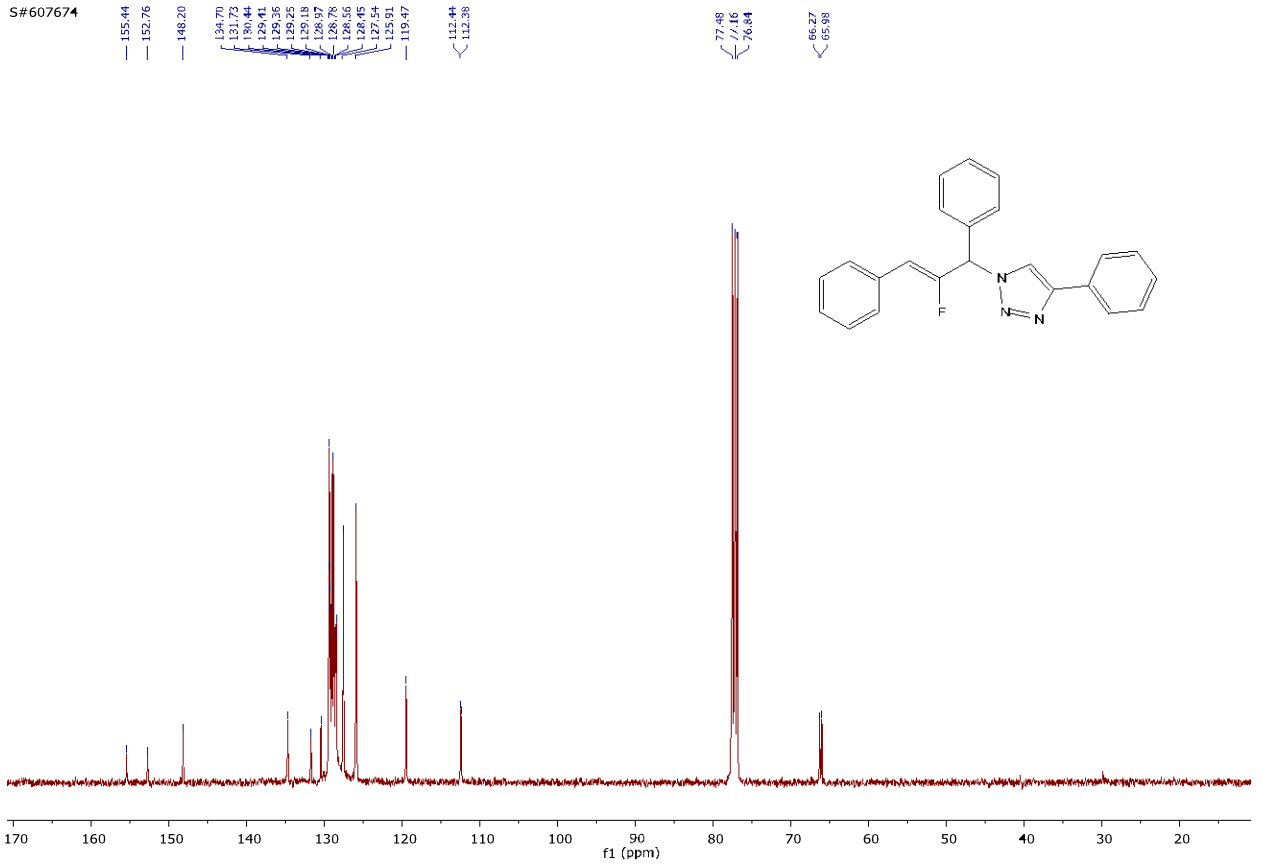
-0.5
f1 (ppm)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128.78
128.56
128.45
127.54
125.91
119.47
112.44
112.38
77.48
77.16
76.84
66.27
65.98
F
N
N
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)


S#434767
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-112.39
-112.49
A (d)
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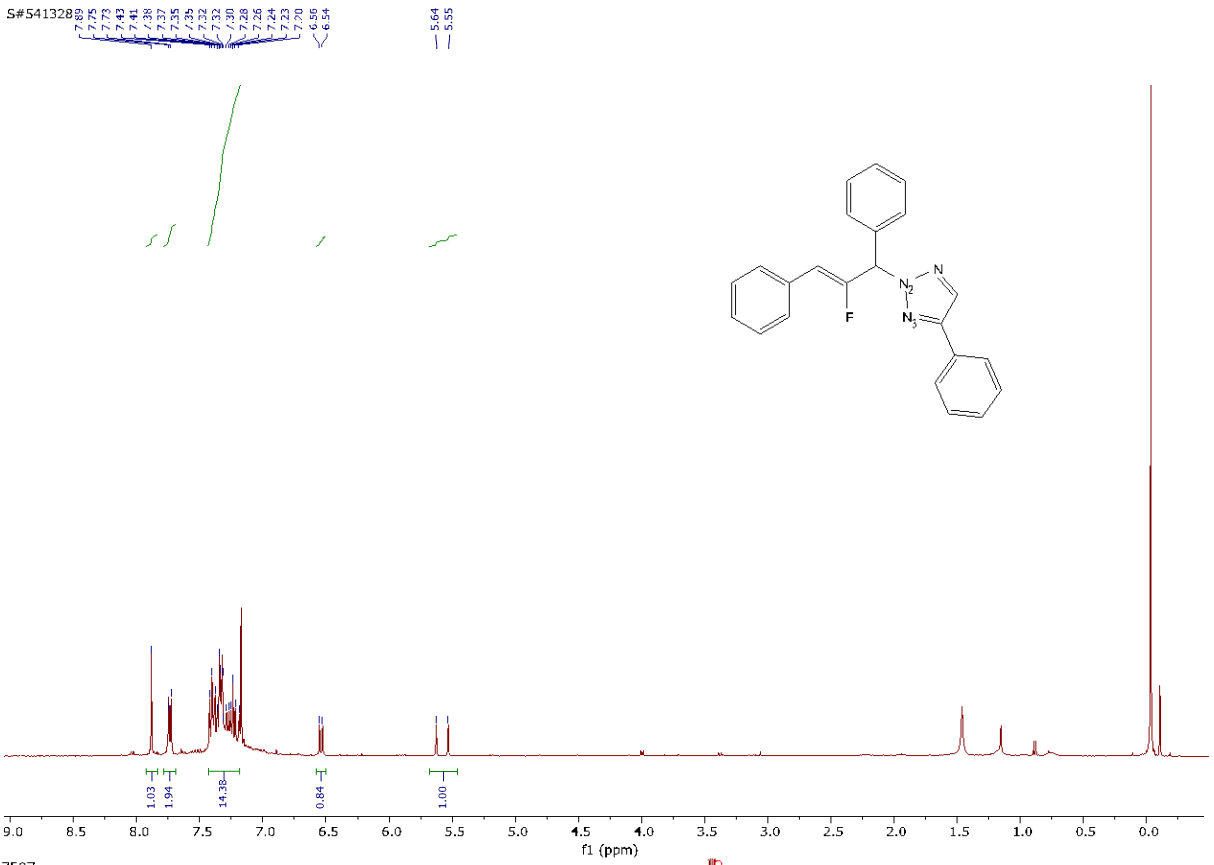
f1 (ppm)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7.23
7.70
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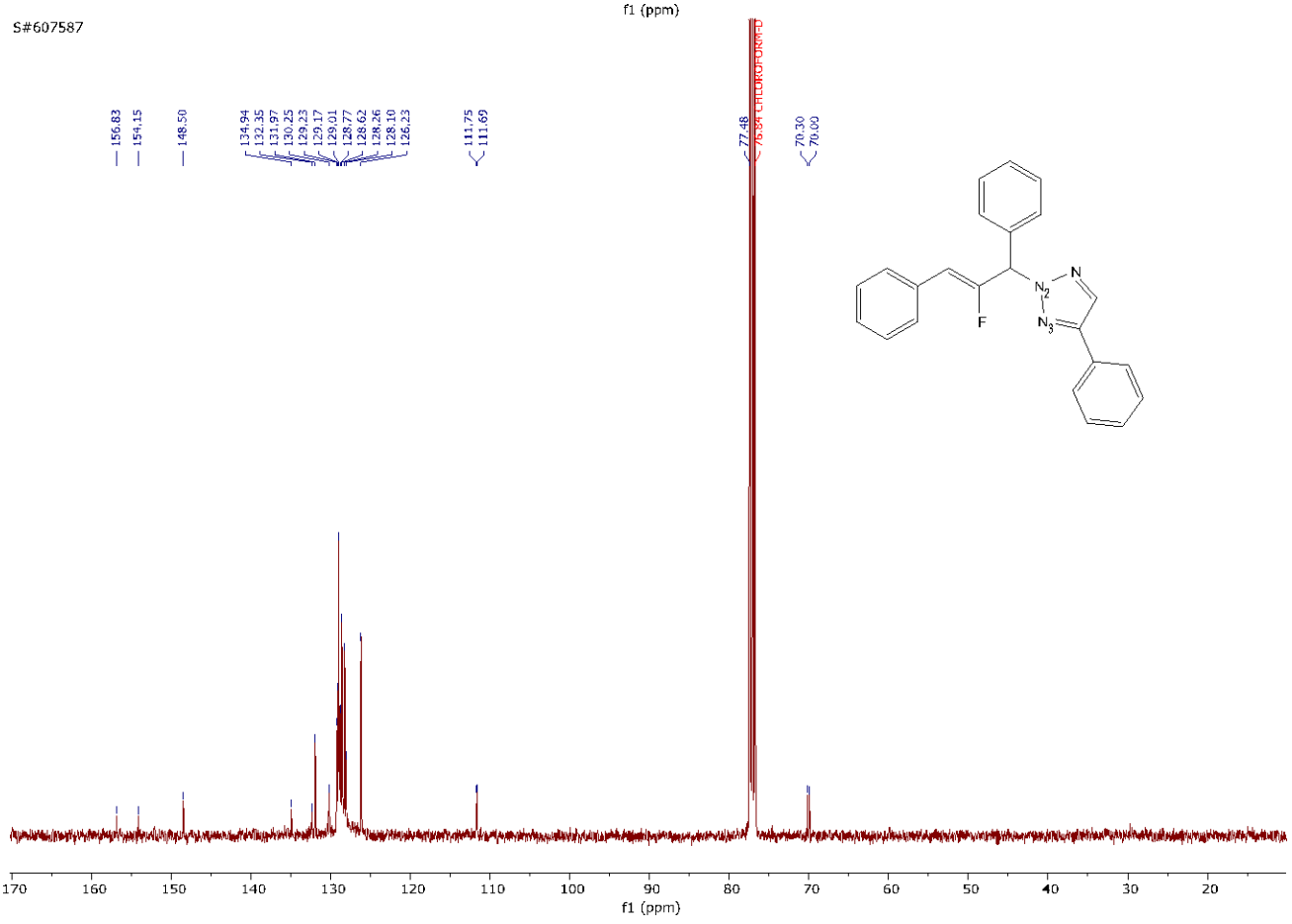
1.00
f1 (ppm)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128.26
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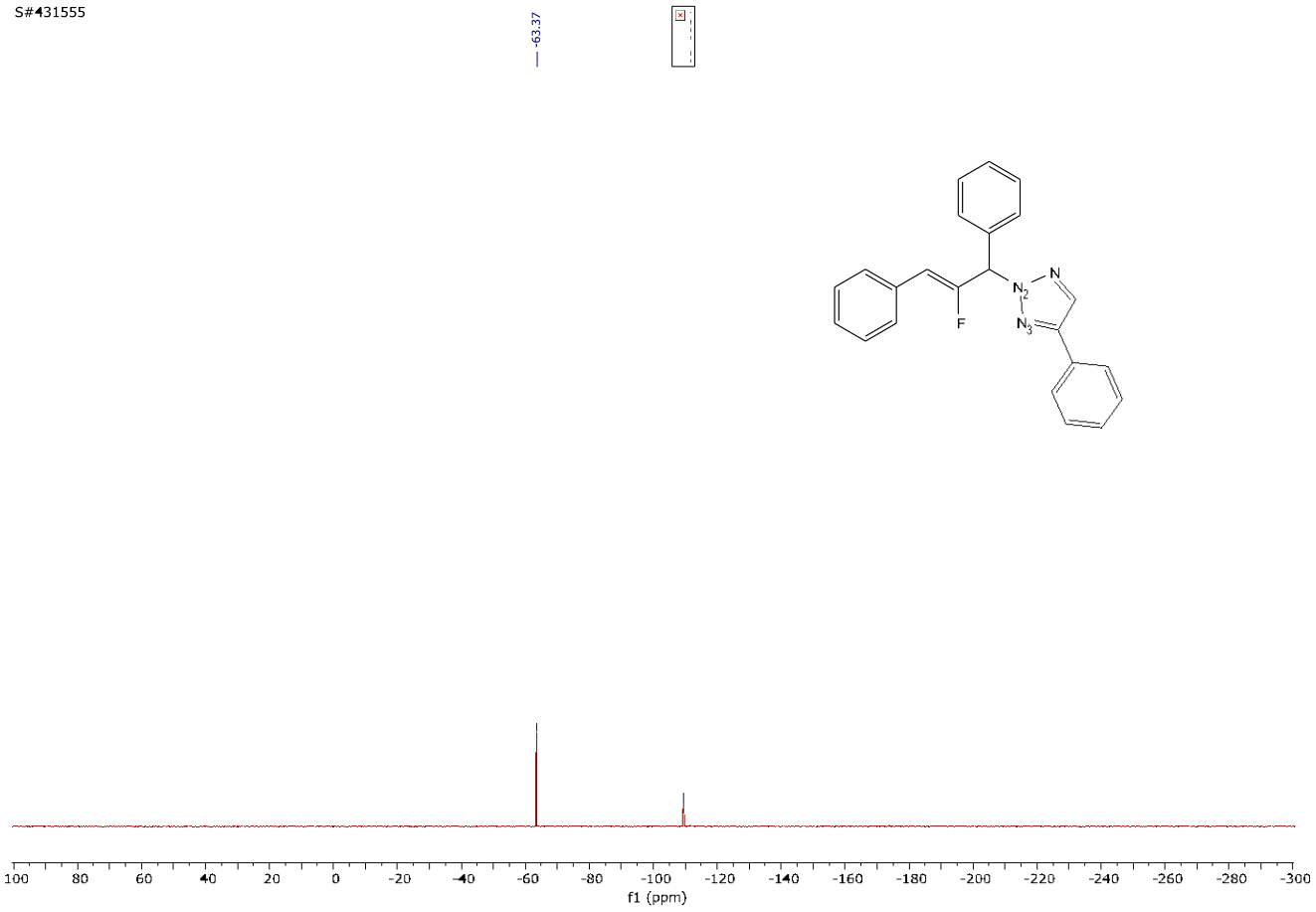
N
N2
N3
f1 (ppm)

S#431555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N3
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0
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-100
-120
-140
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-200
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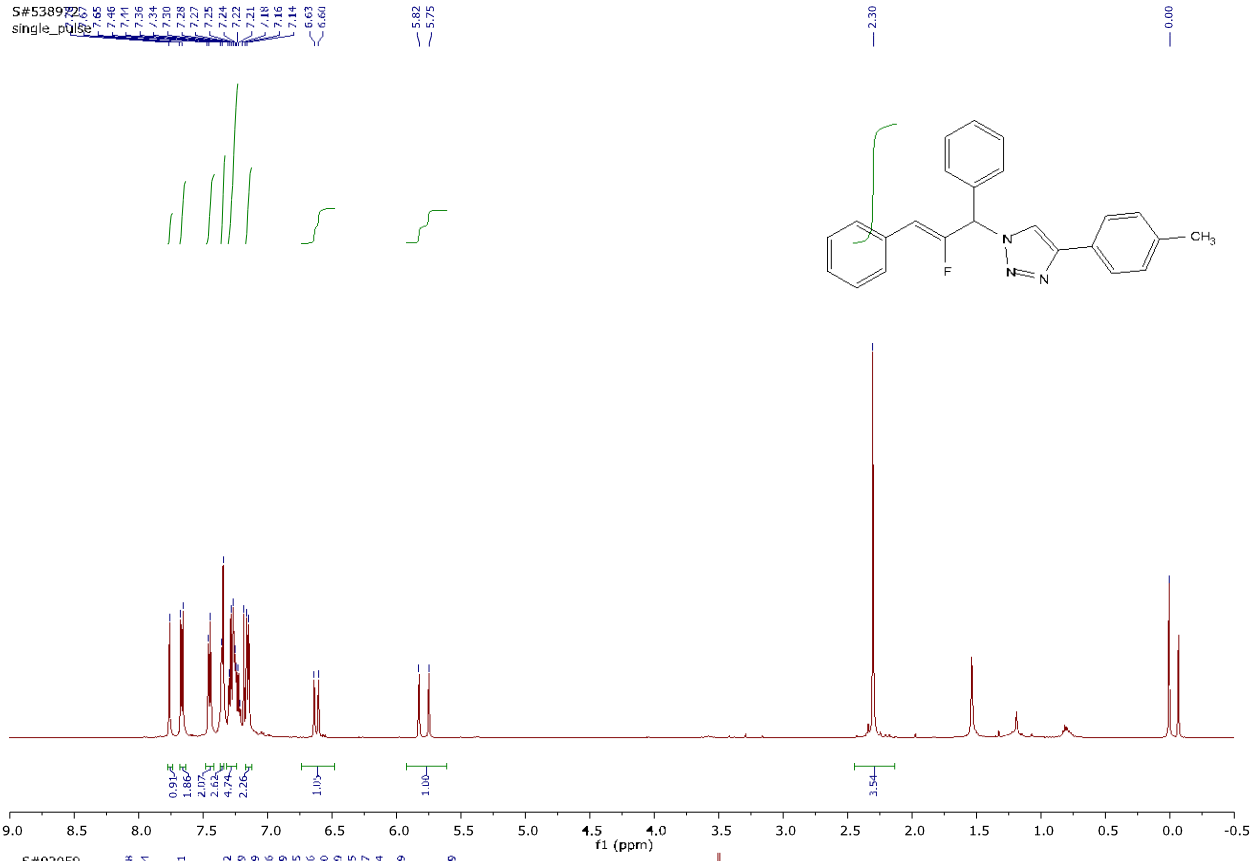
-240
-260
-280
-300
f1 (ppm)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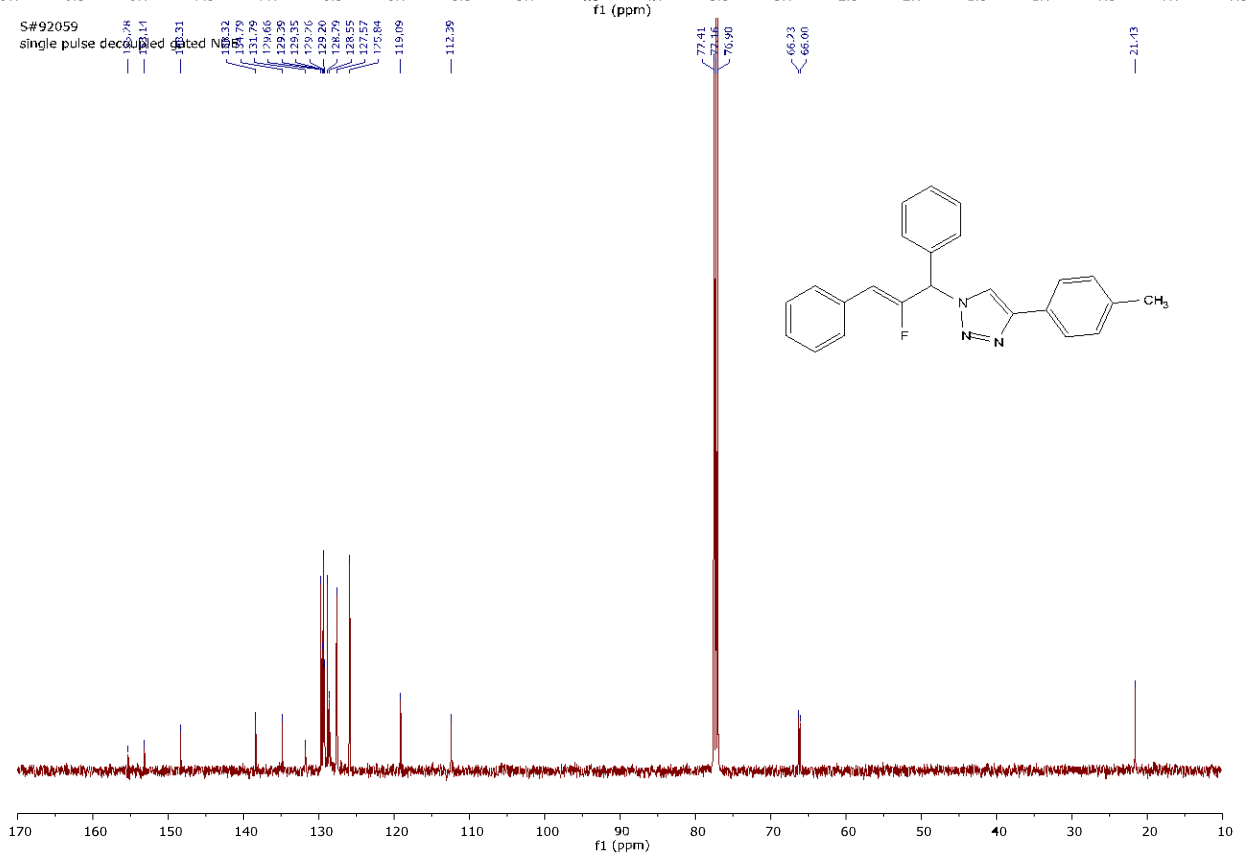
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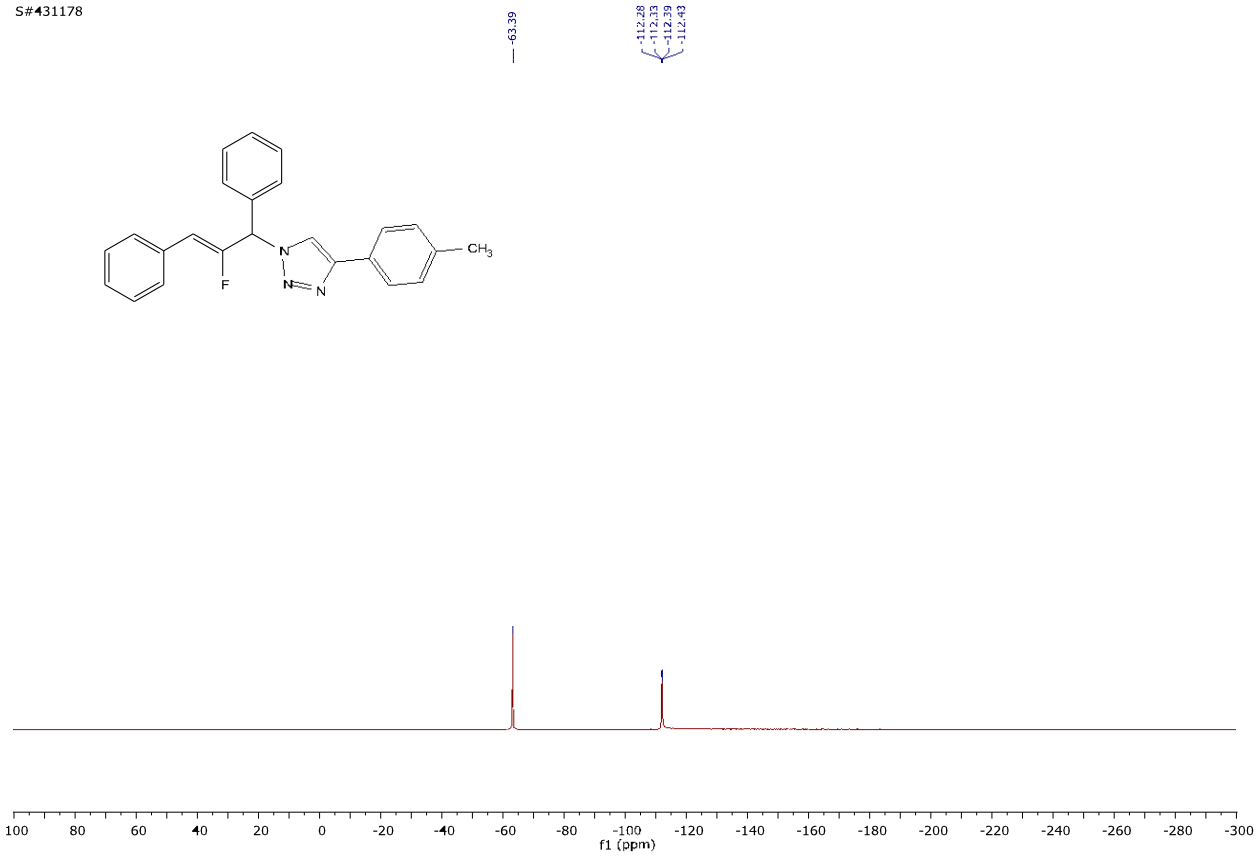
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CH3
F
N
N
N
100
80
60
40
20
0
-20
-40
-60
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-140
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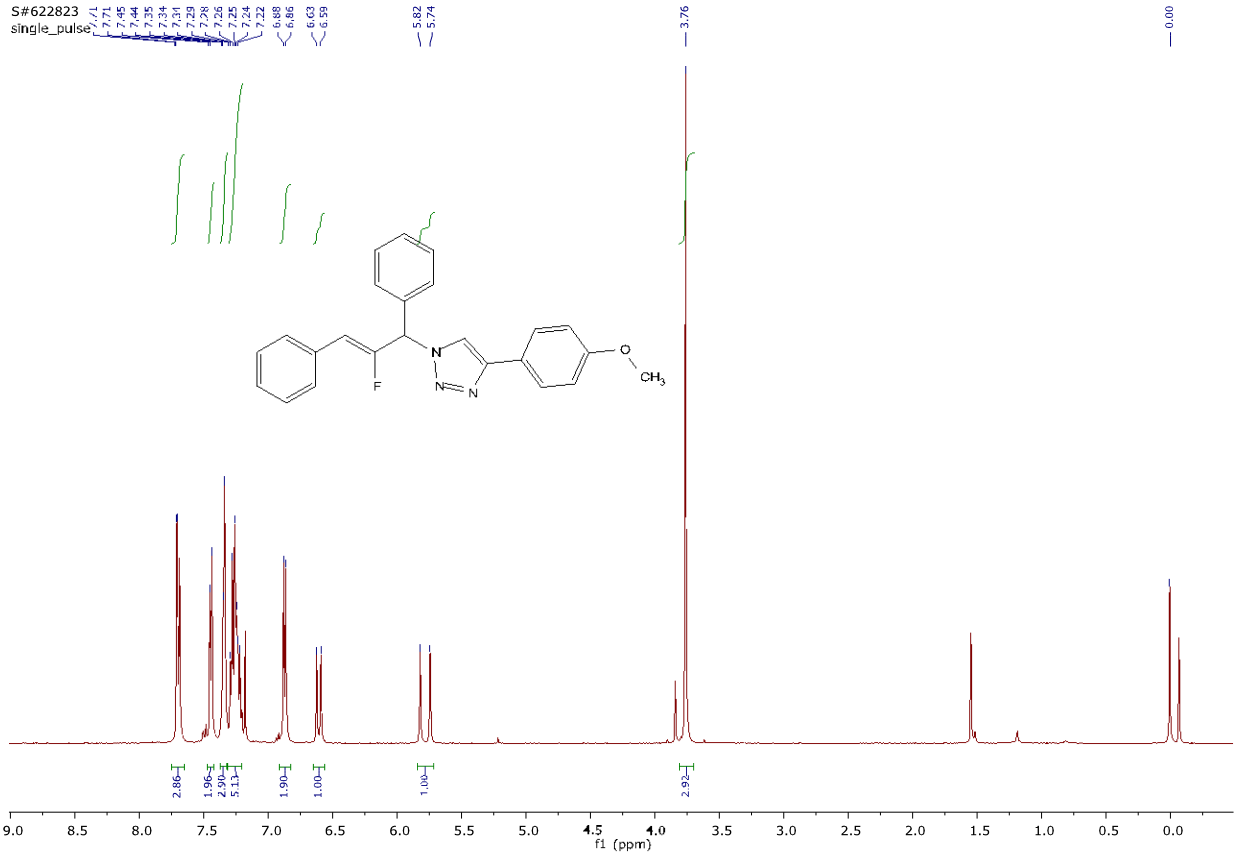
-200
-220
-240
-260
-280
-300
f1 (ppm)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7.29
7.28
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7.25
7.24
7.22
6.88
6.86
6.63
6.59
5.82
5.74
3.76
0.00
F
N
N
N
O
CH3
2.86
1.96
2.90
5.13
1.90
1.00
1.00
2.92
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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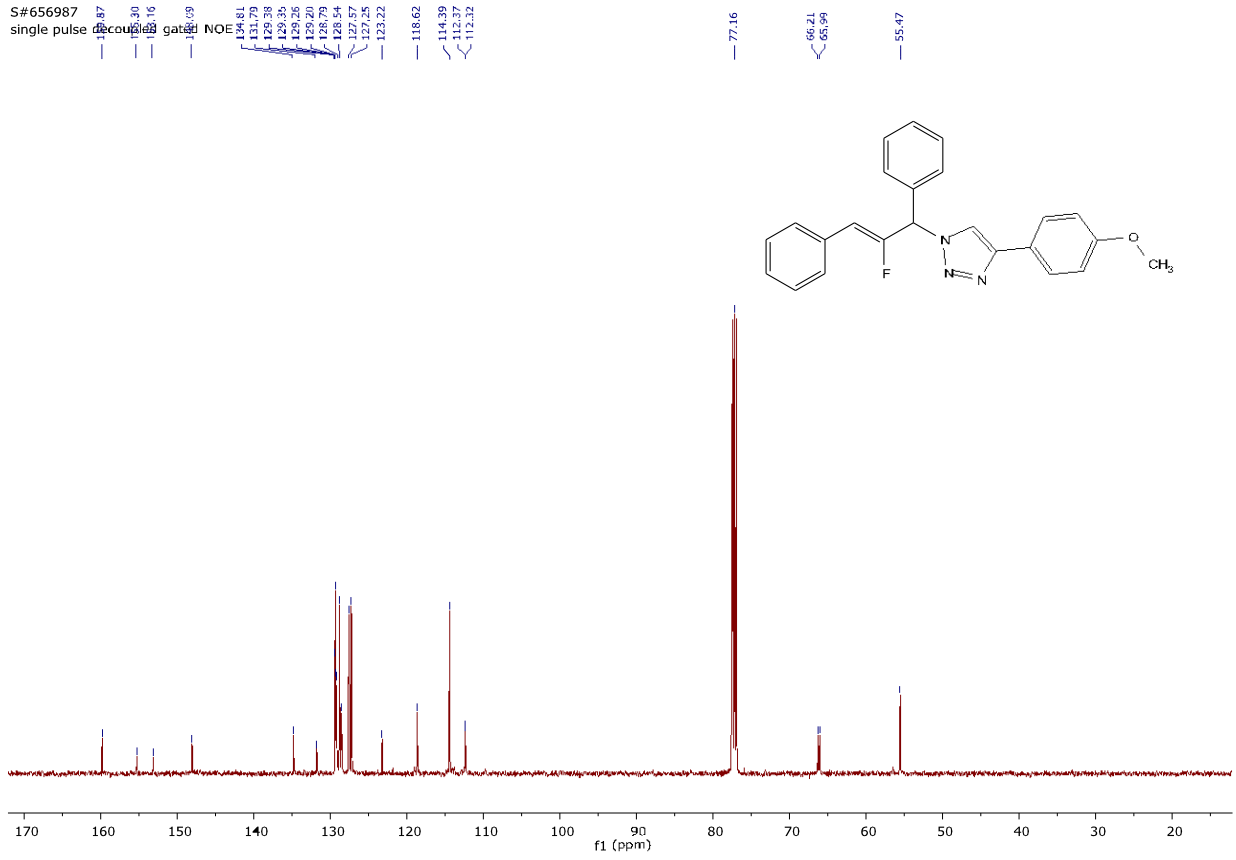
0.0
f1 (ppm)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single pulse decoupled gated NOE
137.87
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129.20
128.79
128.54
127.57
127.25
123.22
118.62
114.39
112.37
112.32
77.16
66.21
65.99
55.47
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N
N
N
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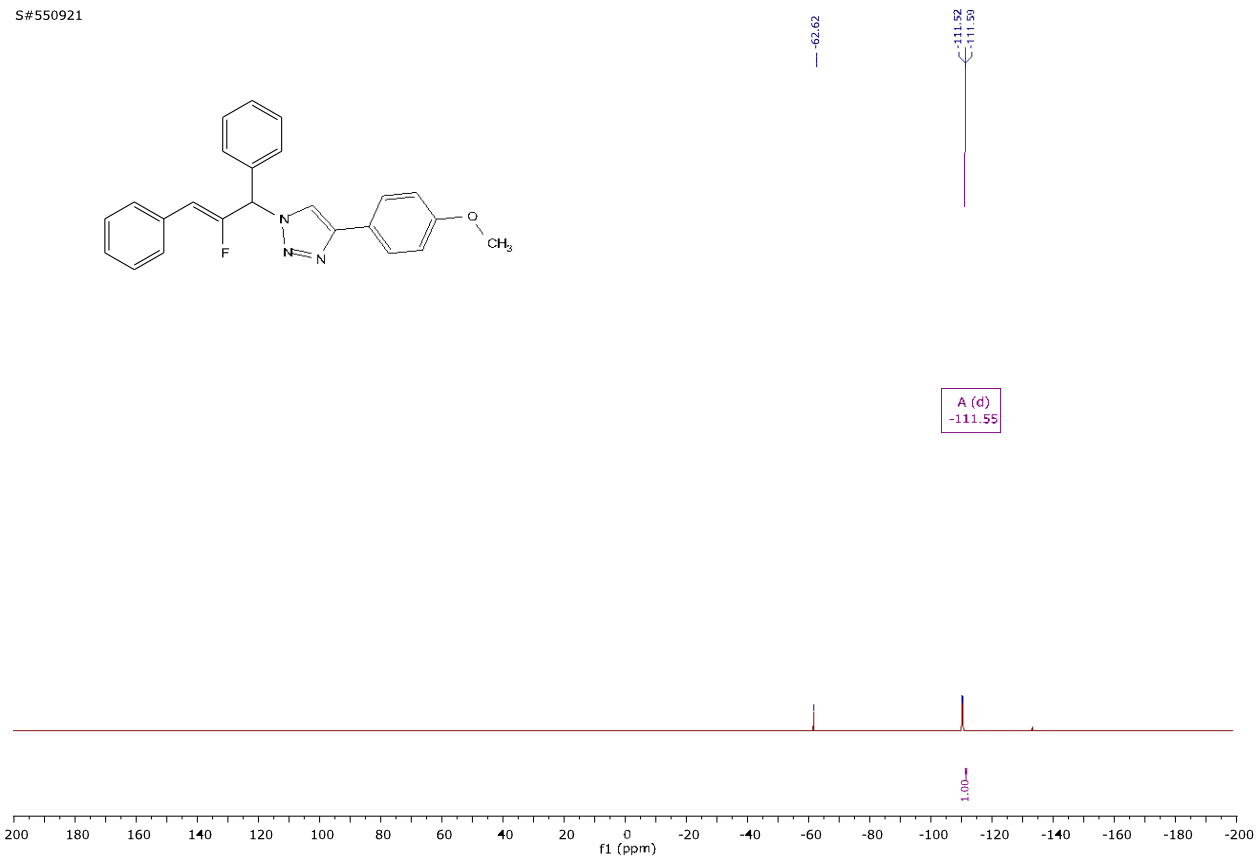
80
70
60
50
40
30
20
f1 (ppm)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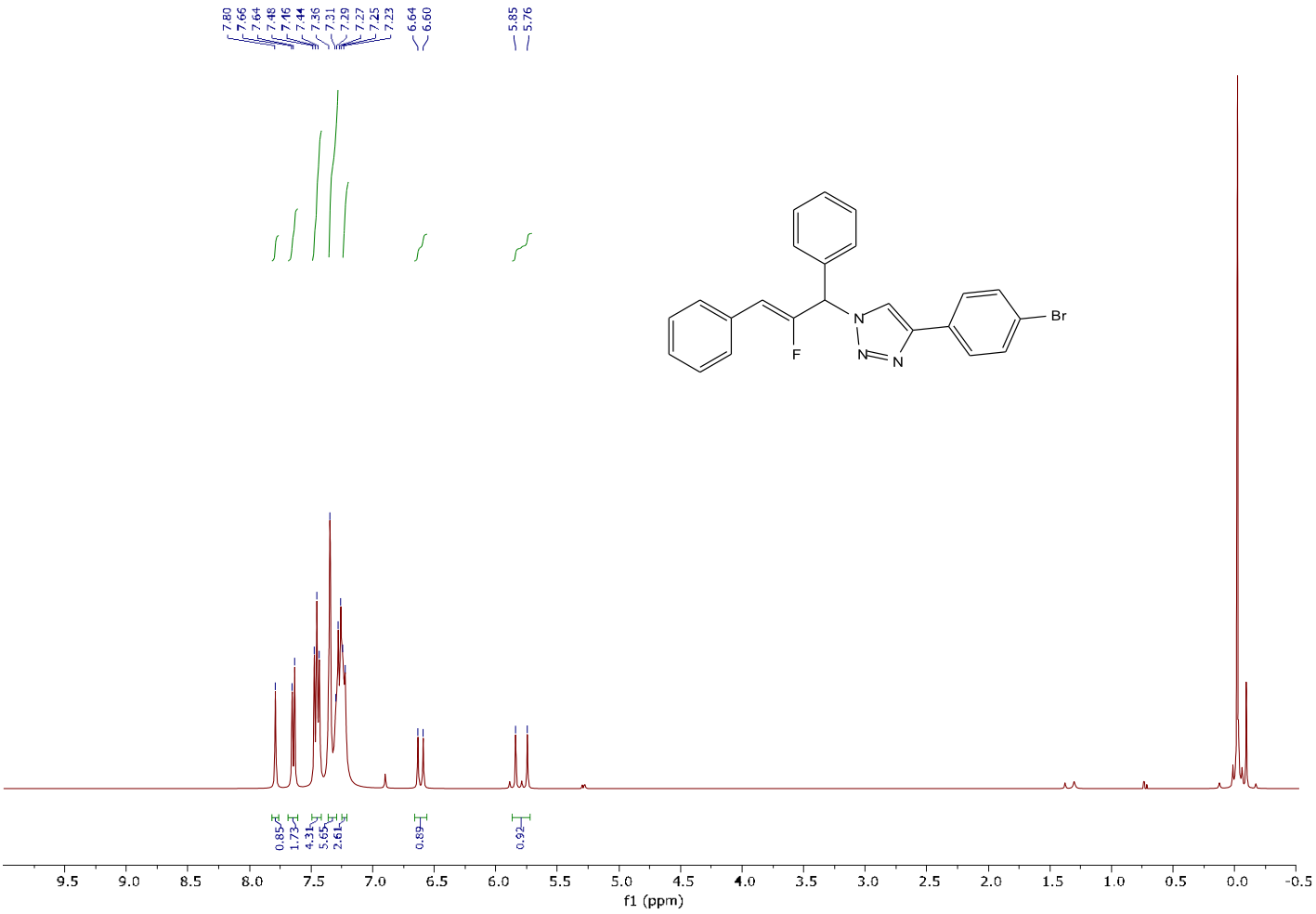
-111.52
-111.59
A (d)
-111.55
1.00
200
180
160
140
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)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7.66
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7.46
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7.31
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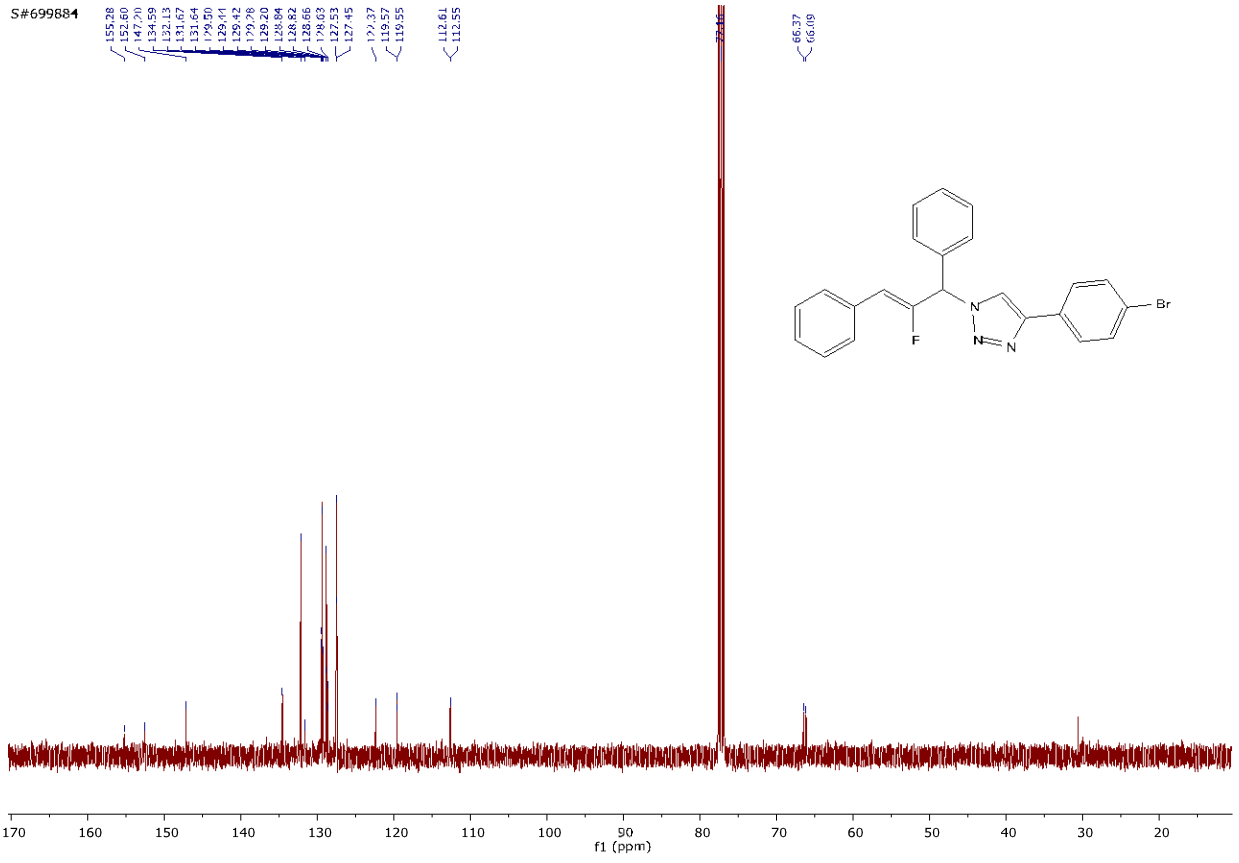
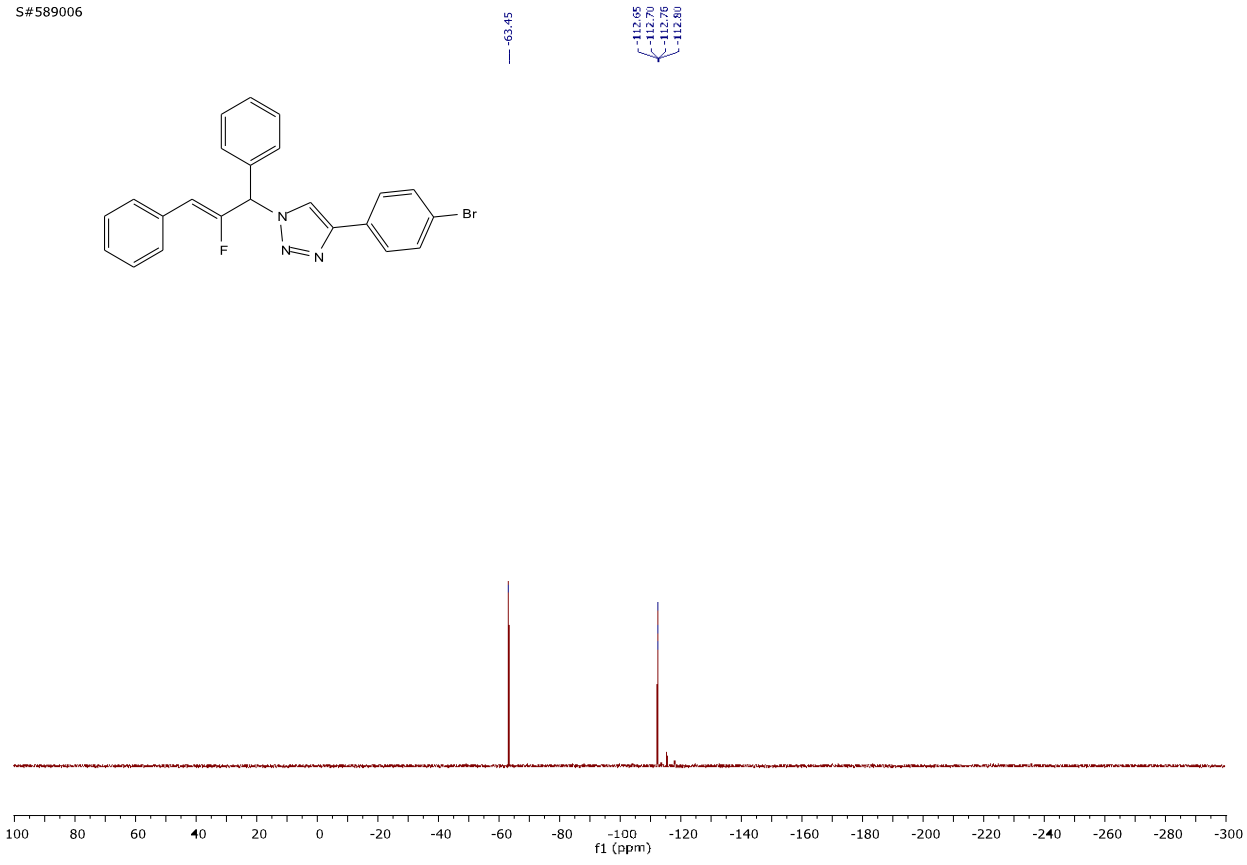
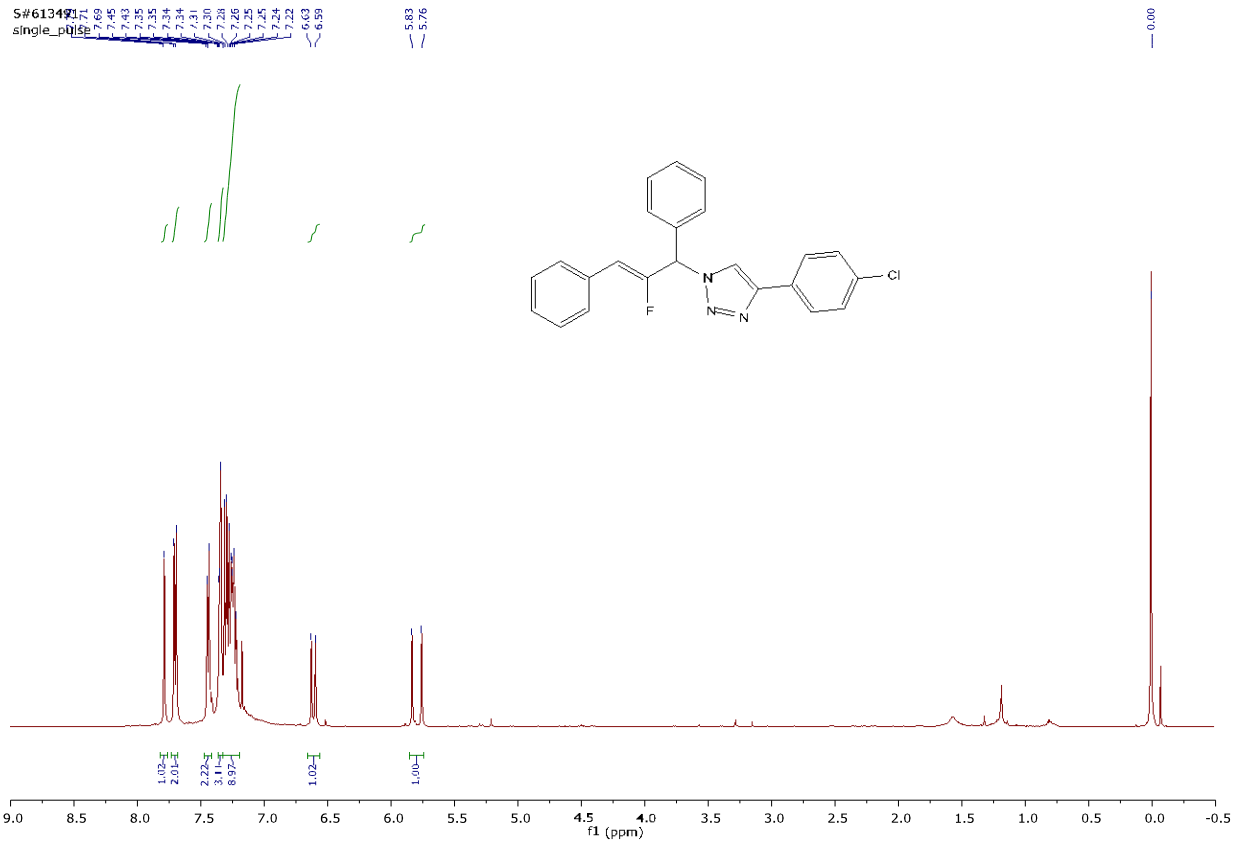
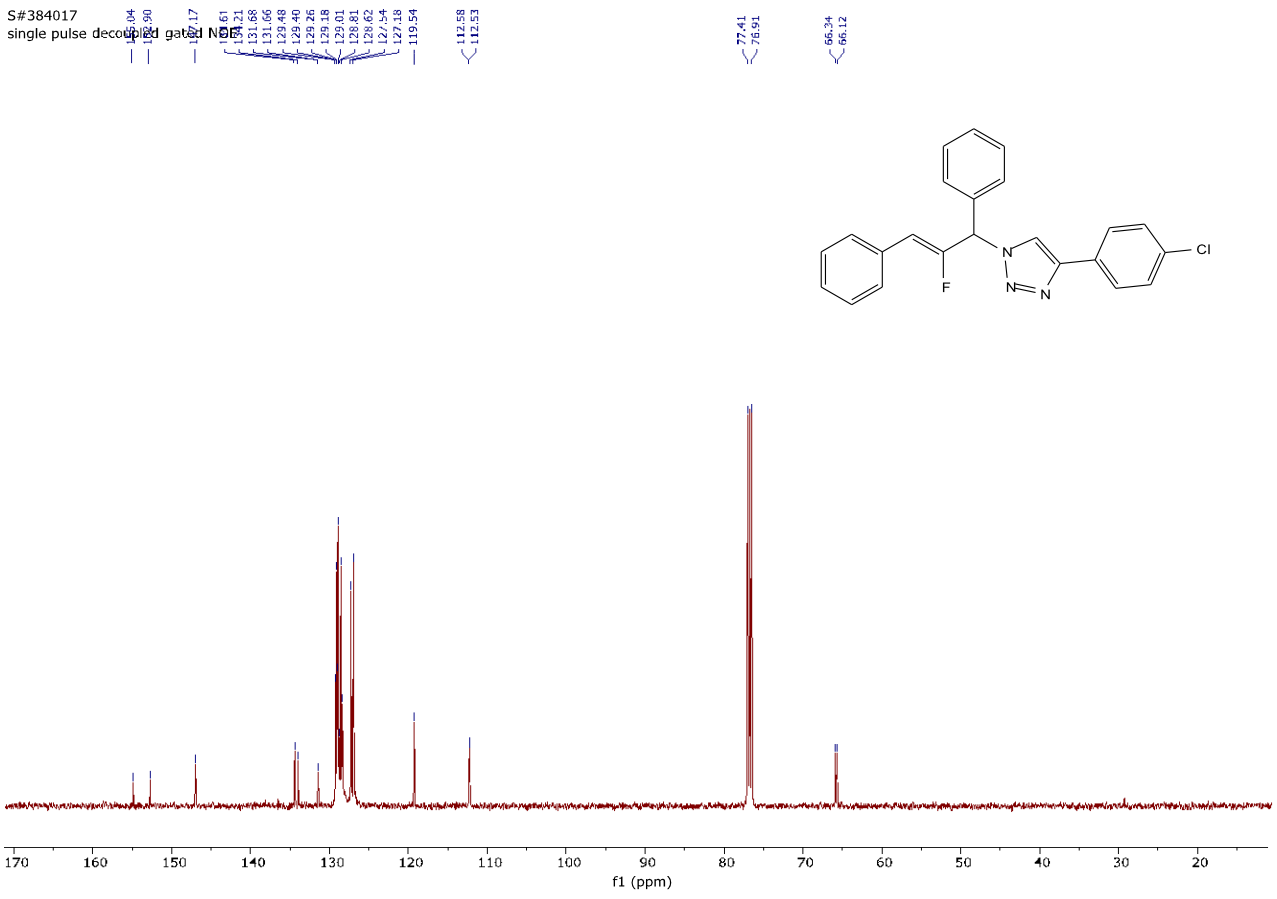
7.27
7.25
7.23
6.64
6.60
5.85
5.76
Br
F
N
N
N
0.85
1.73
4.31
5.65
2.61
0.69
0.92
f1 (ppm)

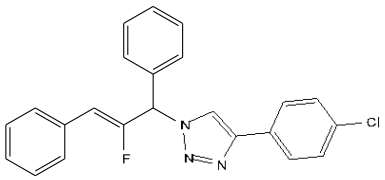

S#699884
155.28
152.60
147.20
134.59
132.13
131.67
131.64
129.50
129.41
129.42
129.28
129.20
128.84
128.82
128.66
128.63
127.53
127.45
122.37
119.57
119.55
112.61
112.55
77.16
66.37
66.09
Br
F
N
N
N
f1 (ppm)


S#589006
-63.45
-112.65
-112.70
-112.76
-112.80
Br
F
N
N
N
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-300
f1 (ppm)

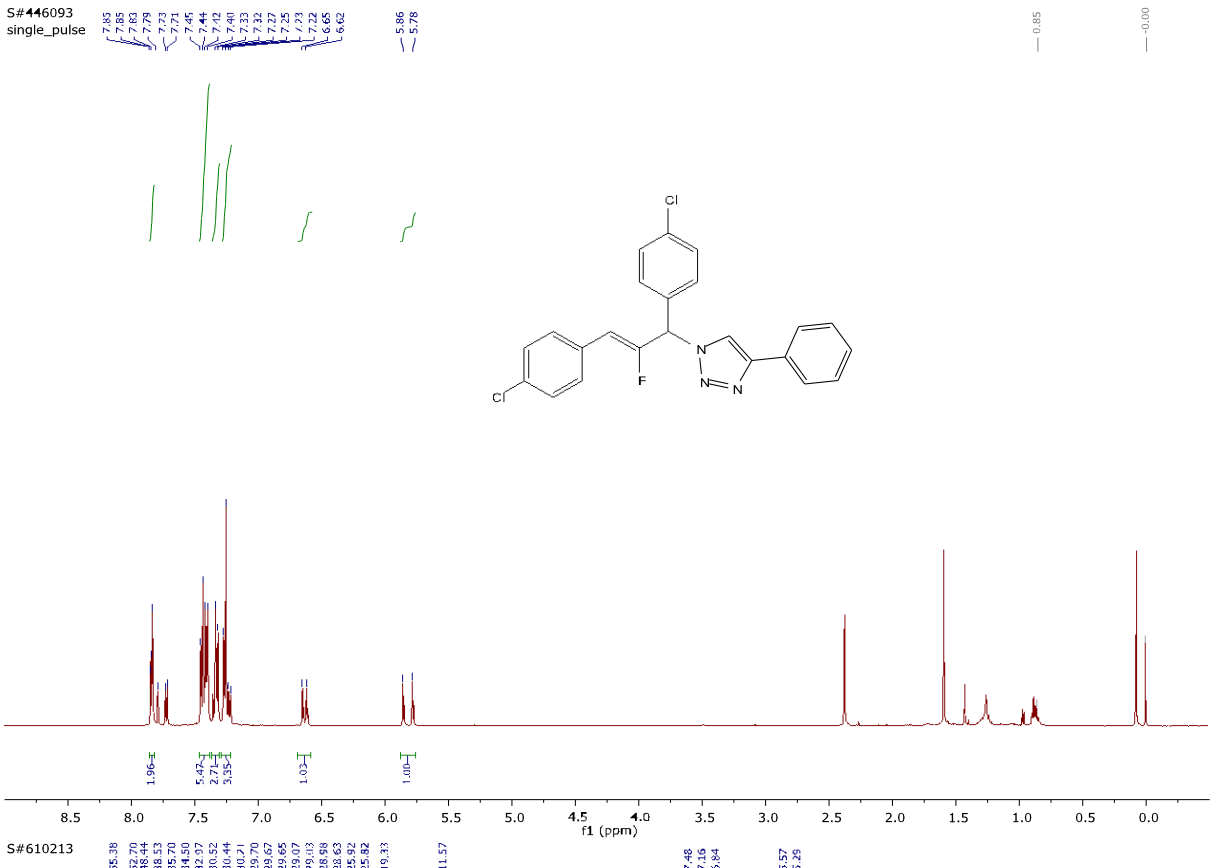

S#61349
single_pulse
7.71
7.69
7.45
7.43
7.35
7.35
7.34
7.34
7.31
7.30
7.28
7.26
7.25
7.25
7.24
7.22
6.63
6.59
5.83
5.76
0.00
Cl
F
N
N
N
1.02
2.01
2.22
3.11
8.97
1.02
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

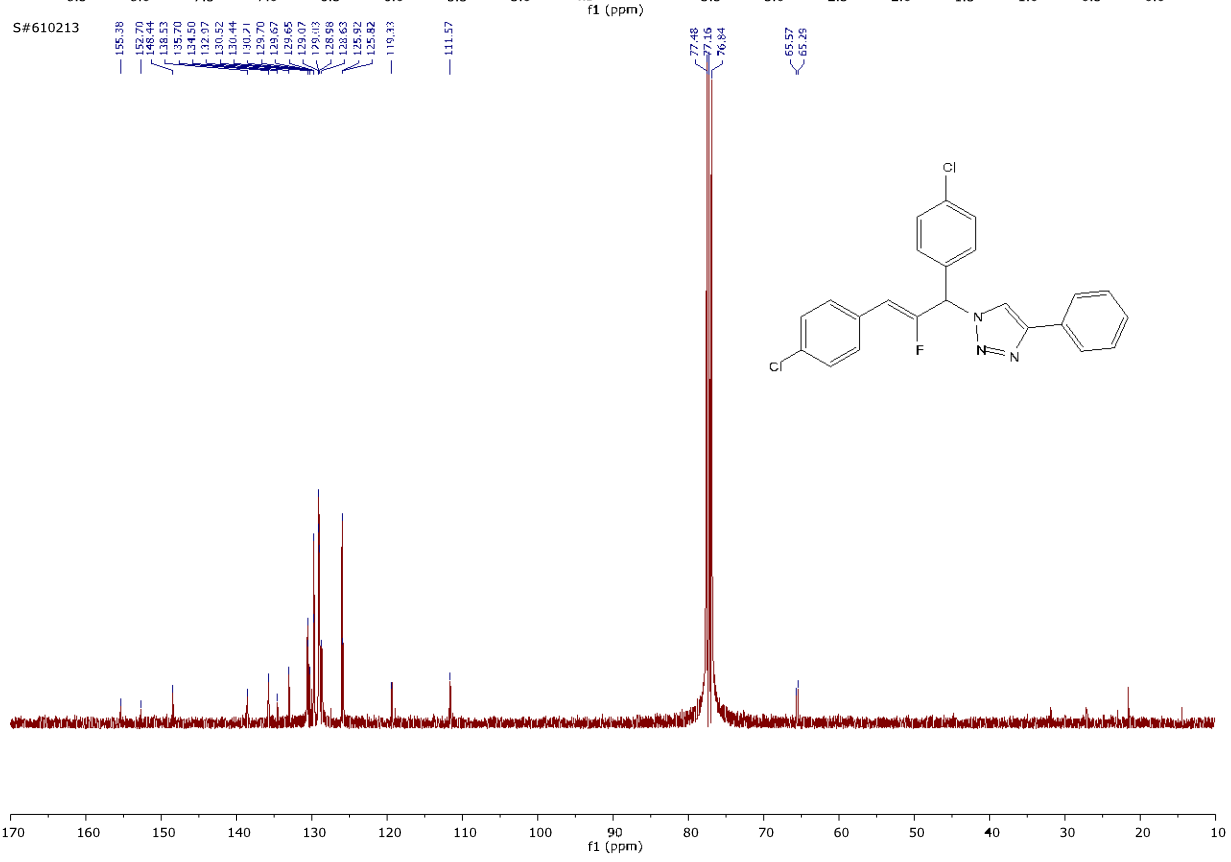

S#384017
single pulse decoupled gated NOE
163.04
162.90
147.17
135.61
134.21
131.68
131.66
129.48
129.40
129.26
129.18
129.01
128.81
128.62
127.54
127.18
119.54
112.58
112.53
77.41
76.91
66.24
66.12
Cl
F
N
N
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

S#606274

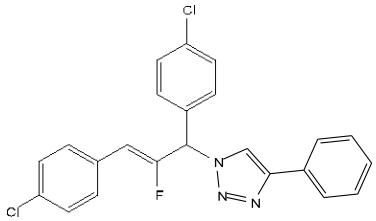

F
N
N
N
Cl

-62.59
-111.80
-111.86
-111.95
200
180
160
140
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

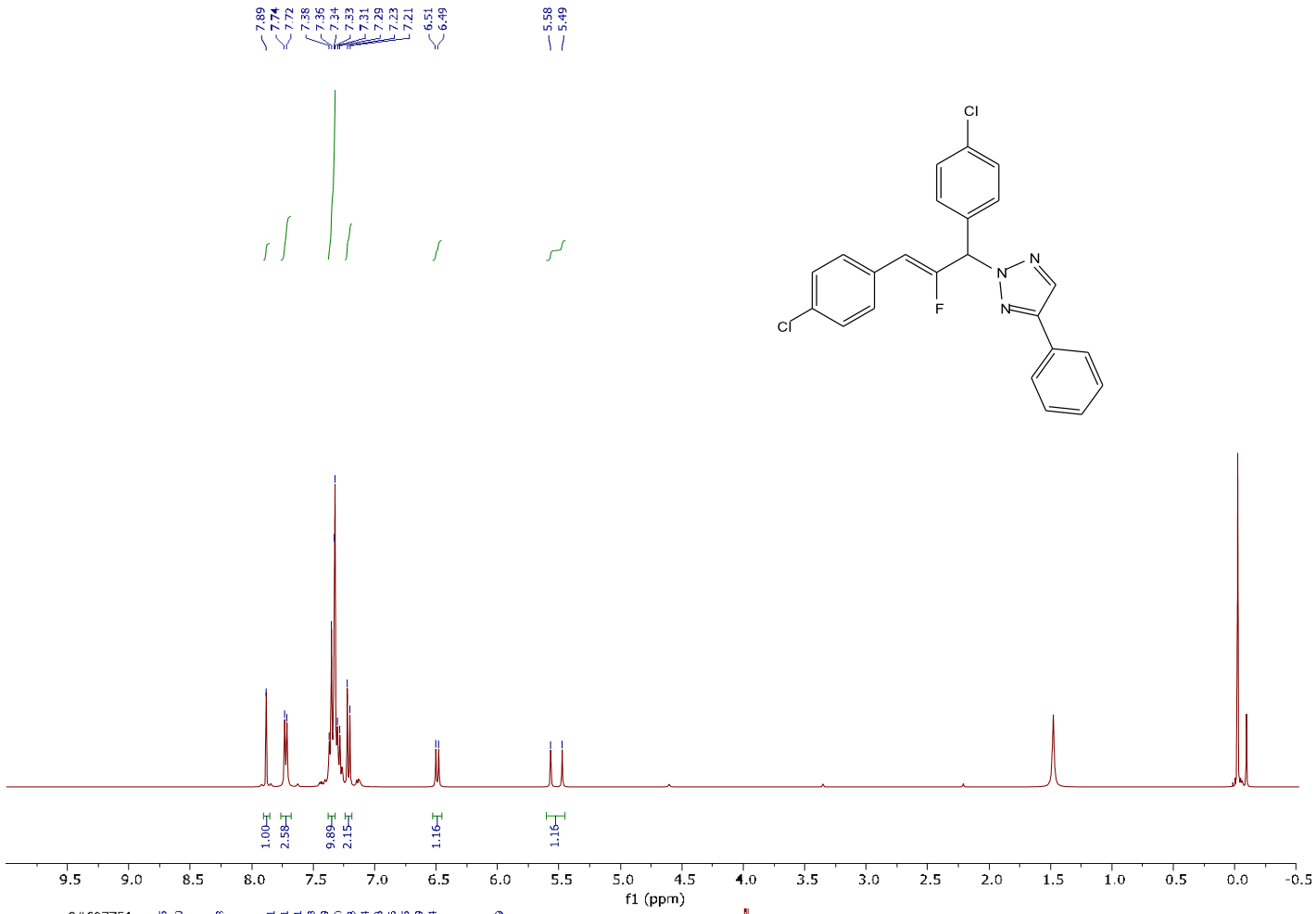

S#446093
single_pulse
7.85
7.83
7.79
7.73
7.71
7.45
7.44
7.42
7.40
7.33
7.32
7.27
7.25
7.23
7.22
6.65
6.62
5.86
5.78
0.85
0.00
Cl
Cl
F
N
N
N
1.96
5.42
2.71
3.35
1.03
1.00
f1 (ppm)

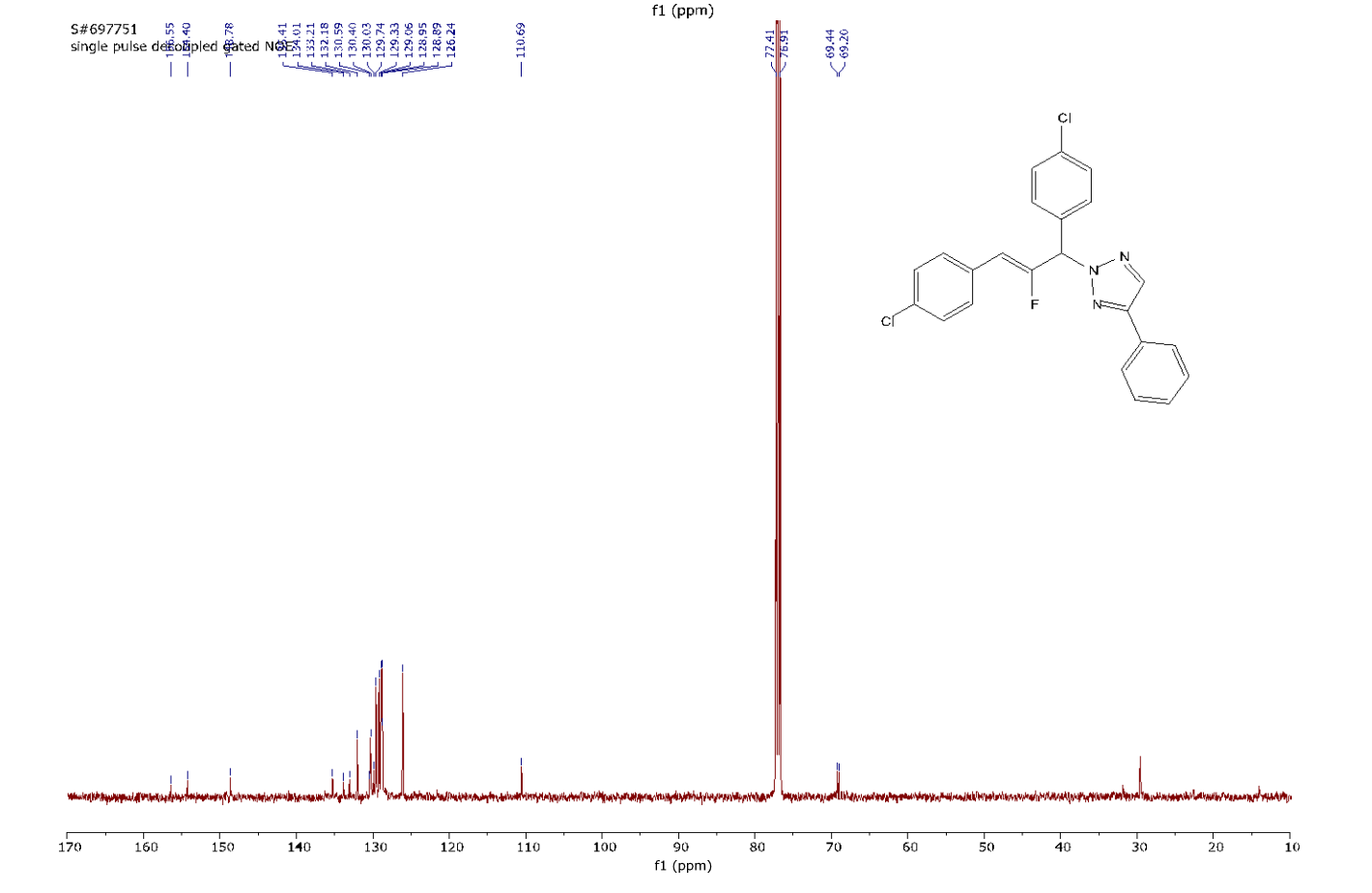

S#610213
155.38
152.70
148.44
138.53
135.70
134.50
132.97
130.52
130.44
130.21
129.70
129.67
129.65
129.07
128.98
128.63
125.92
125.82
119.33
111.57
77.48
77.16
76.84
65.57
65.29
Cl
Cl
F
N
N
N
f1 (ppm)

S#550386

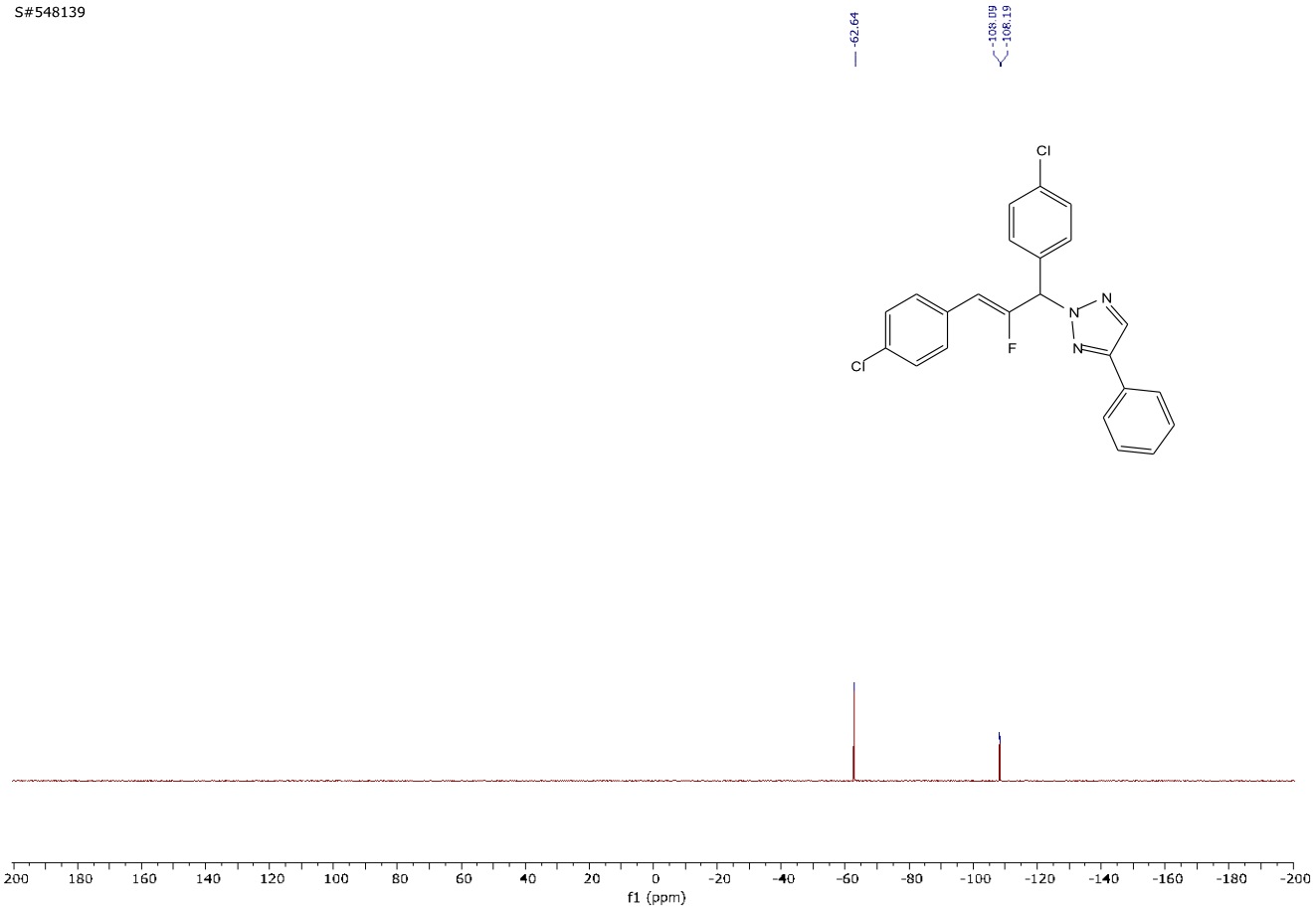

Cl
Cl
F
N
N
N

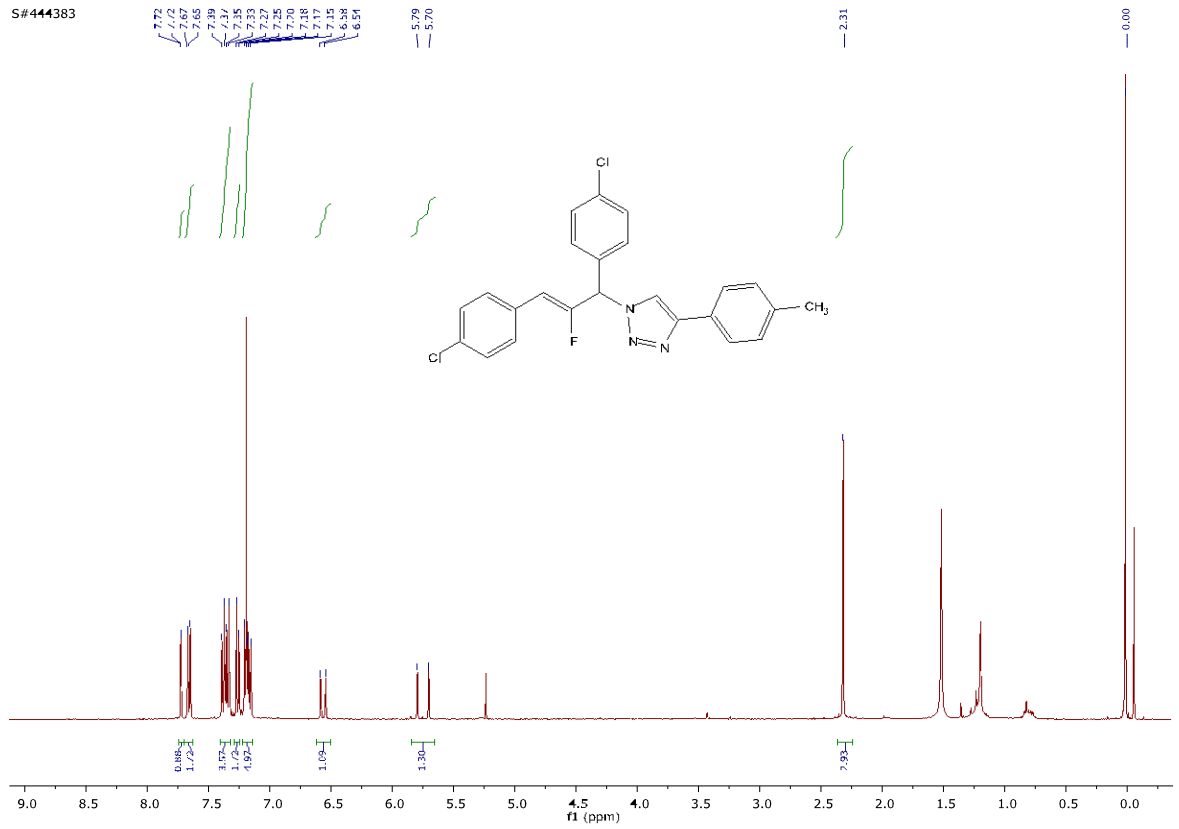
-62.62
-111.13
-111.22
-111.31
-111.37
200
180
160
140
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

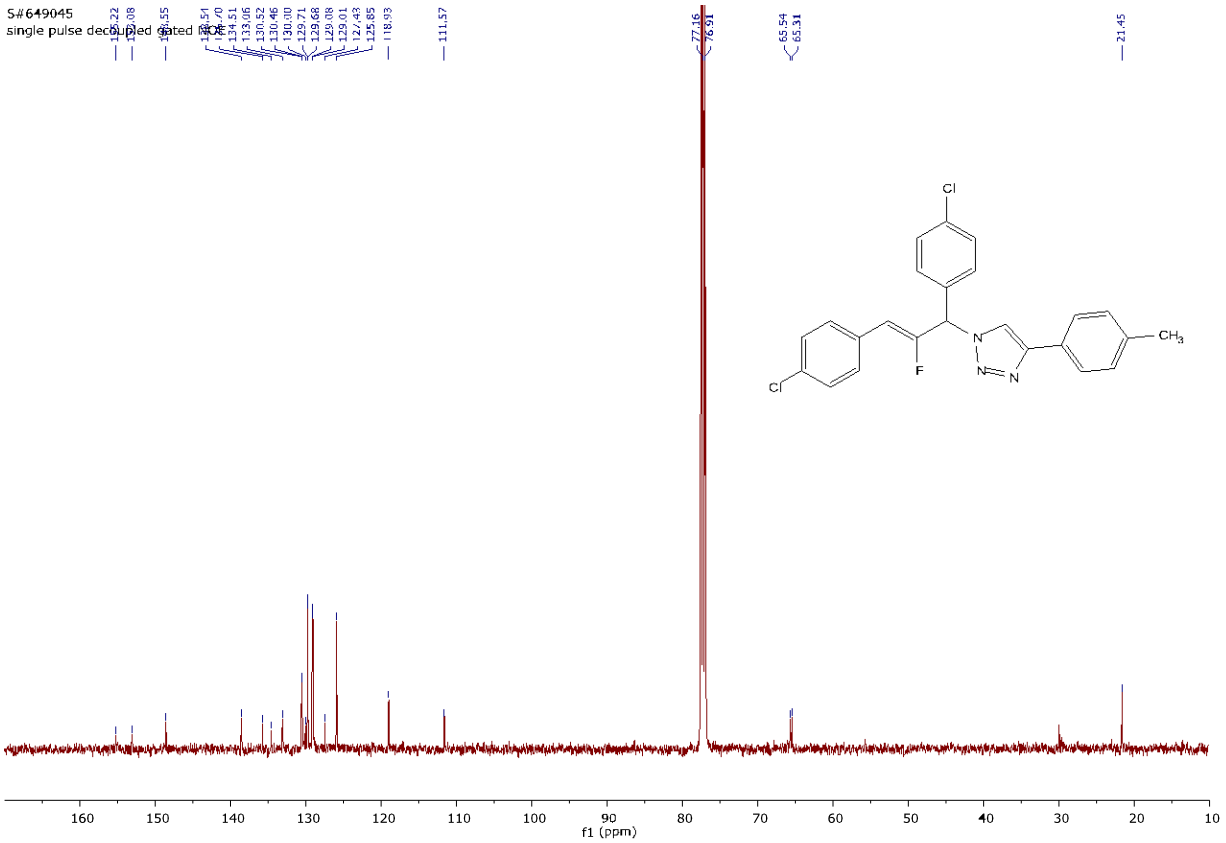

7.89
7.74
7.72
7.38
7.36
7.34
7.33
7.31
7.29
7.23
7.21
6.51
6.49
5.58
5.49
Cl
Cl
F
N
N
N
1.00
2.58
9.89
2.15
1.16
1.16
f1 (ppm)

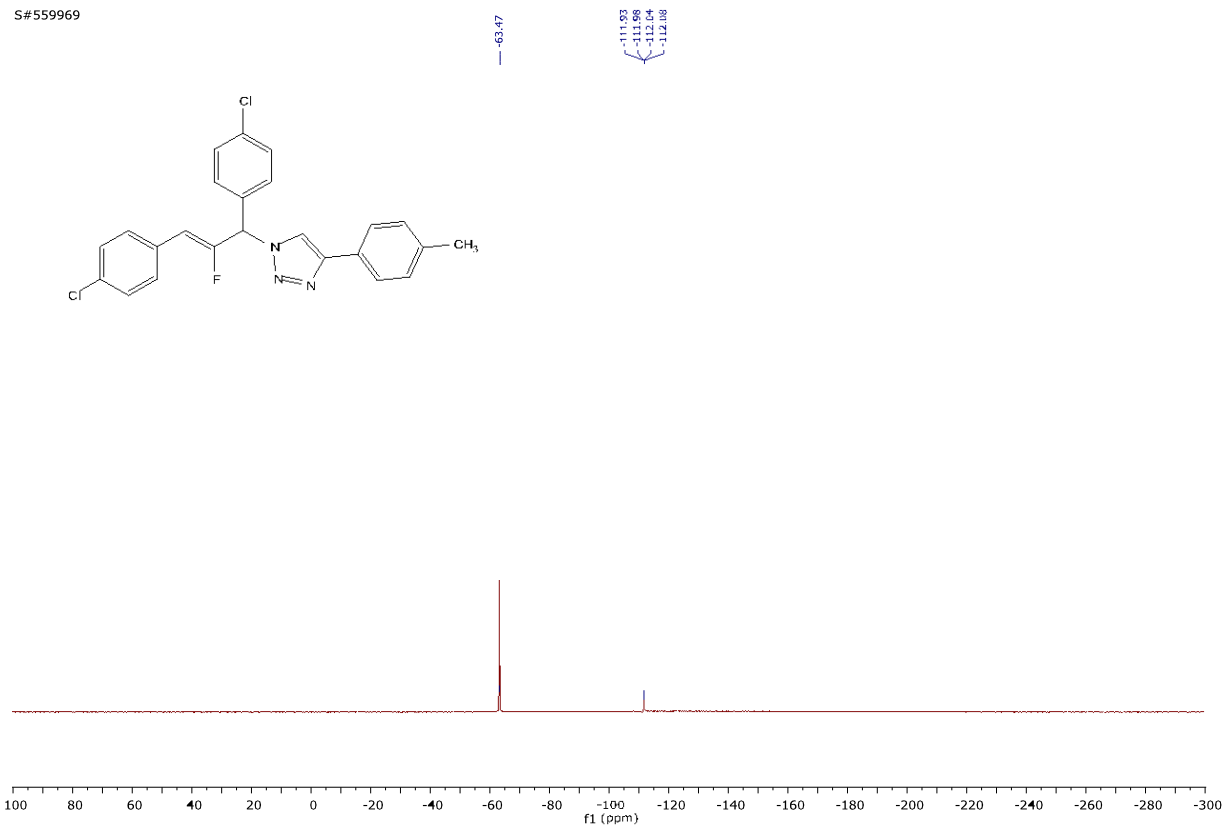

S#697751
single pulse decoupled gated NOE
160.55
157.40
150.78
134.41
134.01
133.21
132.18
130.59
130.40
130.03
129.74
129.33
129.06
128.95
126.89
126.24
110.69
77.41
76.91
69.44
69.20
Cl
Cl
F
N
N
N
f1 (ppm)

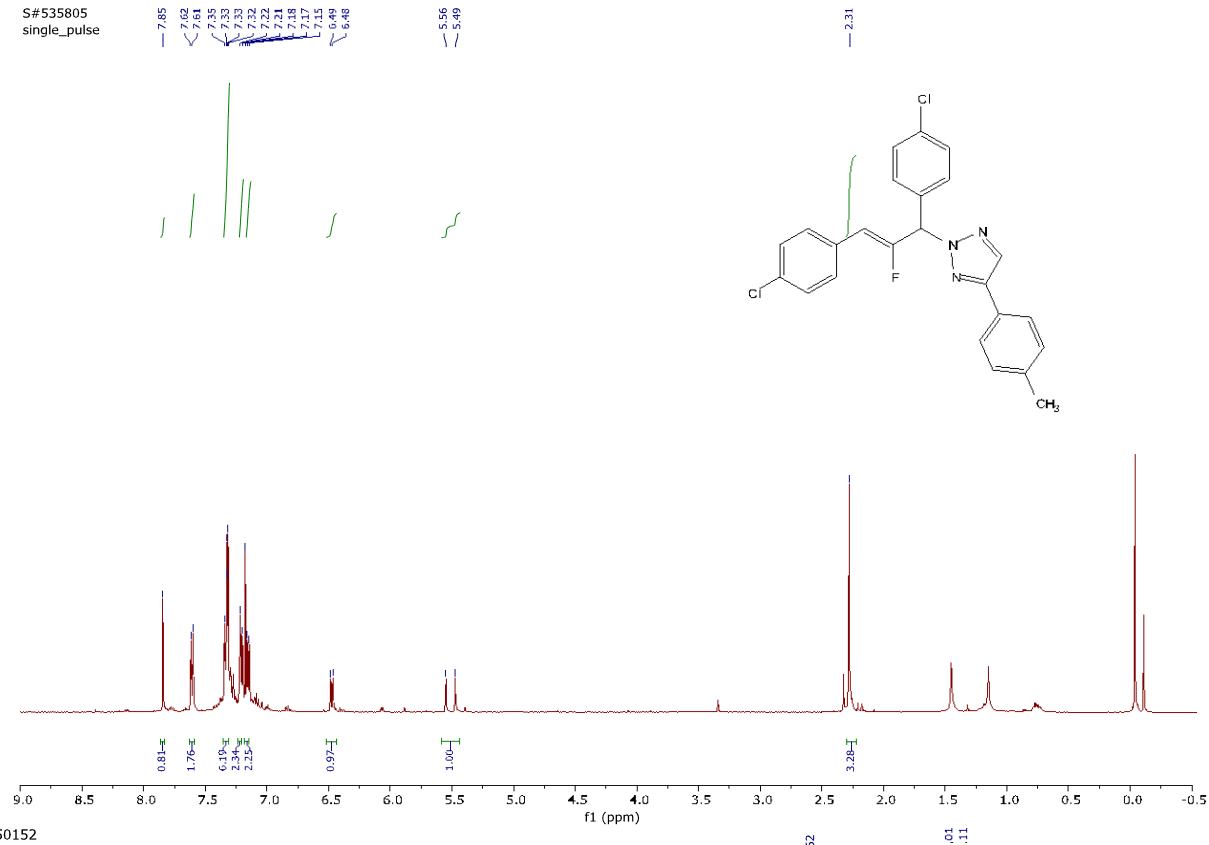
S#548139

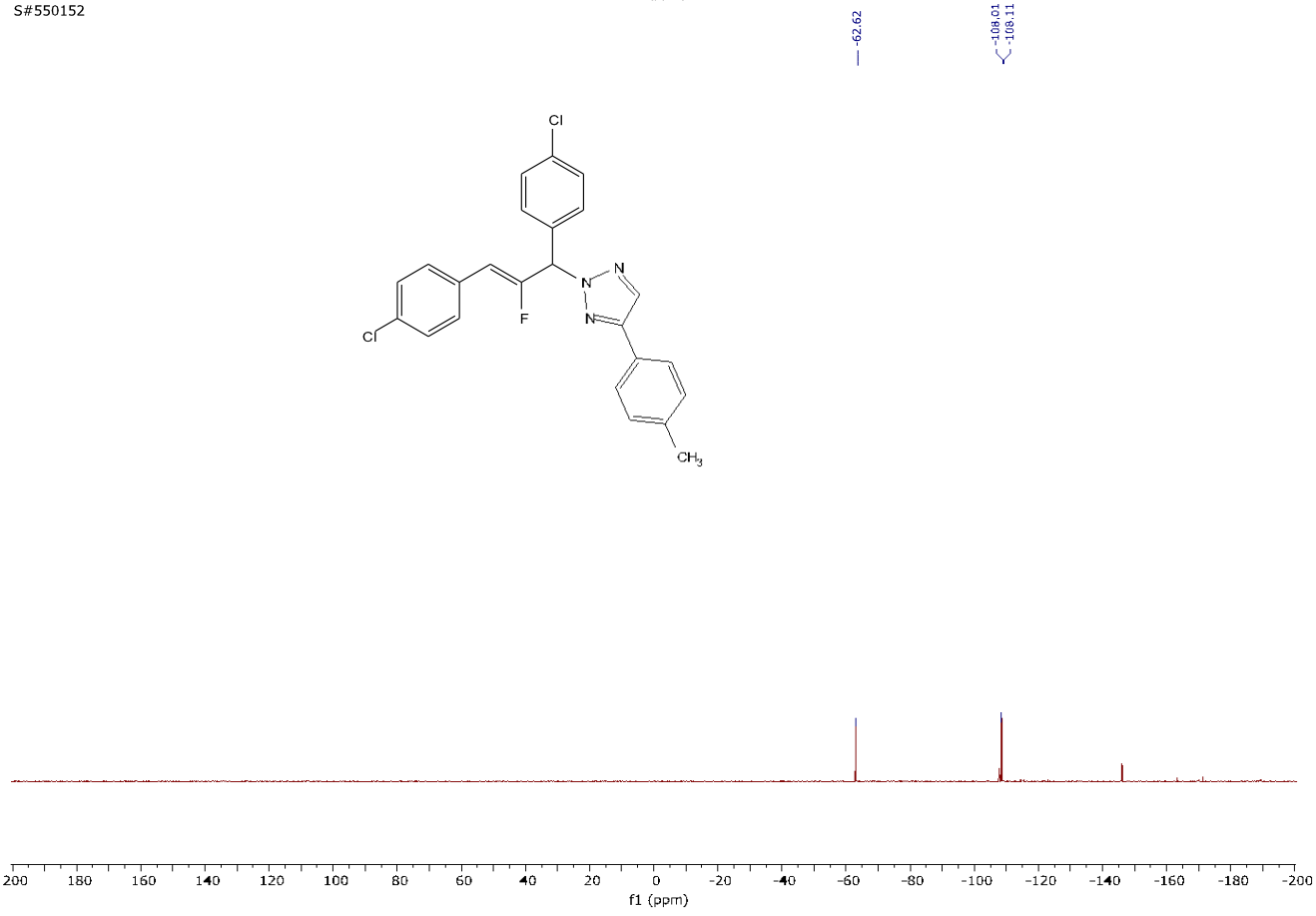

-62.64
-108.09
-108.19
Cl
Cl
F
N
N
N
200
180
160
140
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

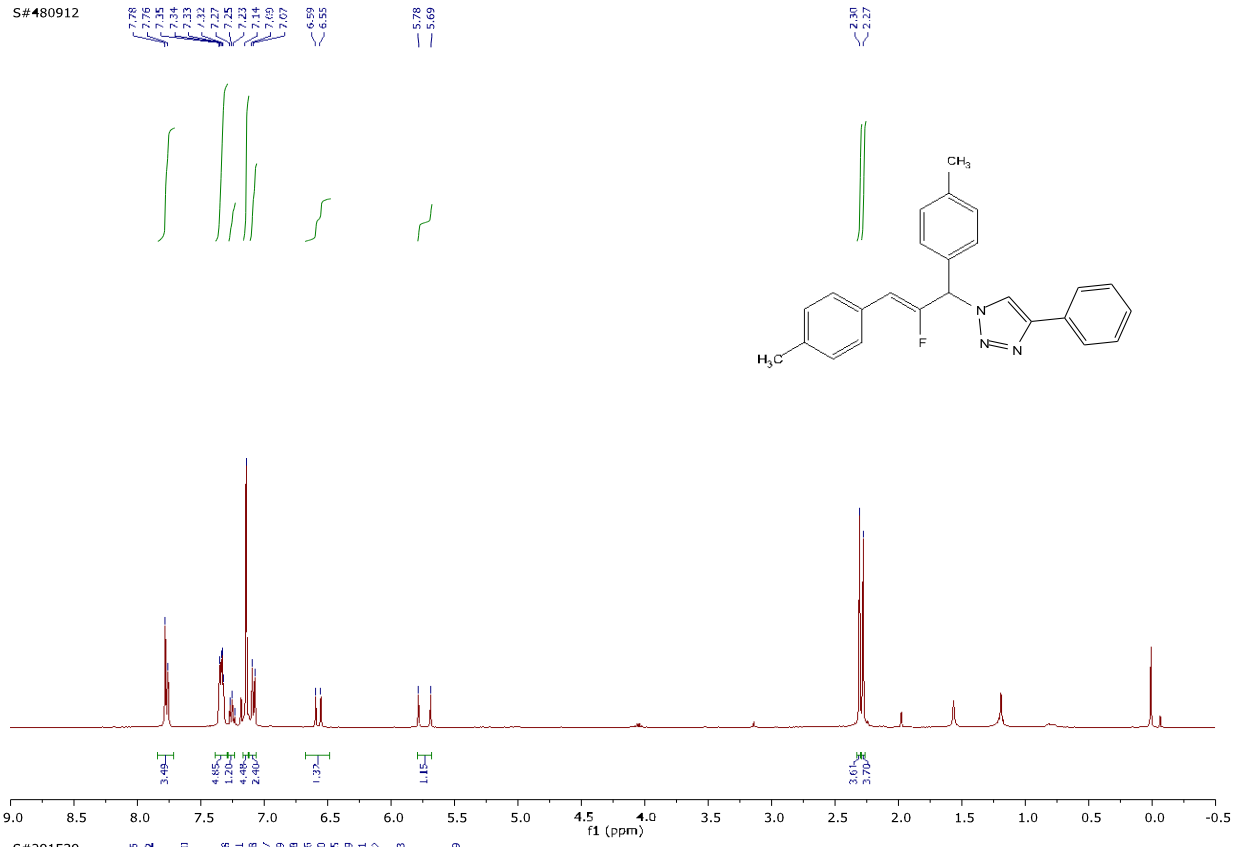

S#444383
7.72
7.67
7.65
7.39
7.35
7.33
7.27
7.25
7.20
7.18
7.17
7.15
6.54
6.51
5.79
5.70
2.31
0.00
Cl
Cl
F
N
N
N
CH3
0.88
1.72
3.07
1.72
4.92
1.09
1.30
7.93
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

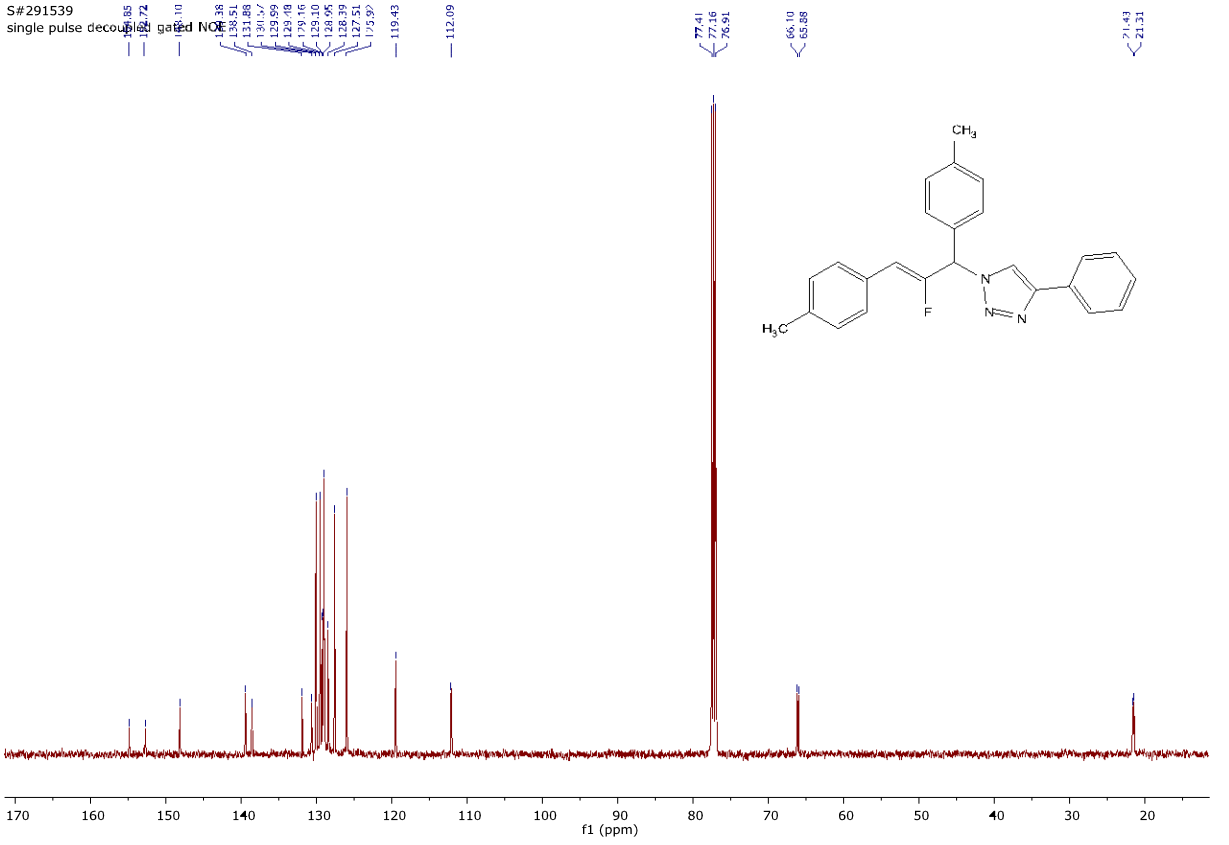

S#649045
single pulse decoupled gated
142.22
142.08
136.55
135.51
135.40
134.51
133.06
130.52
130.46
130.00
129.71
129.68
129.08
129.01
127.43
125.85
118.93
111.57
77.16
76.91
65.54
65.31
21.45
Cl
Cl
F
N
N
N
CH3
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

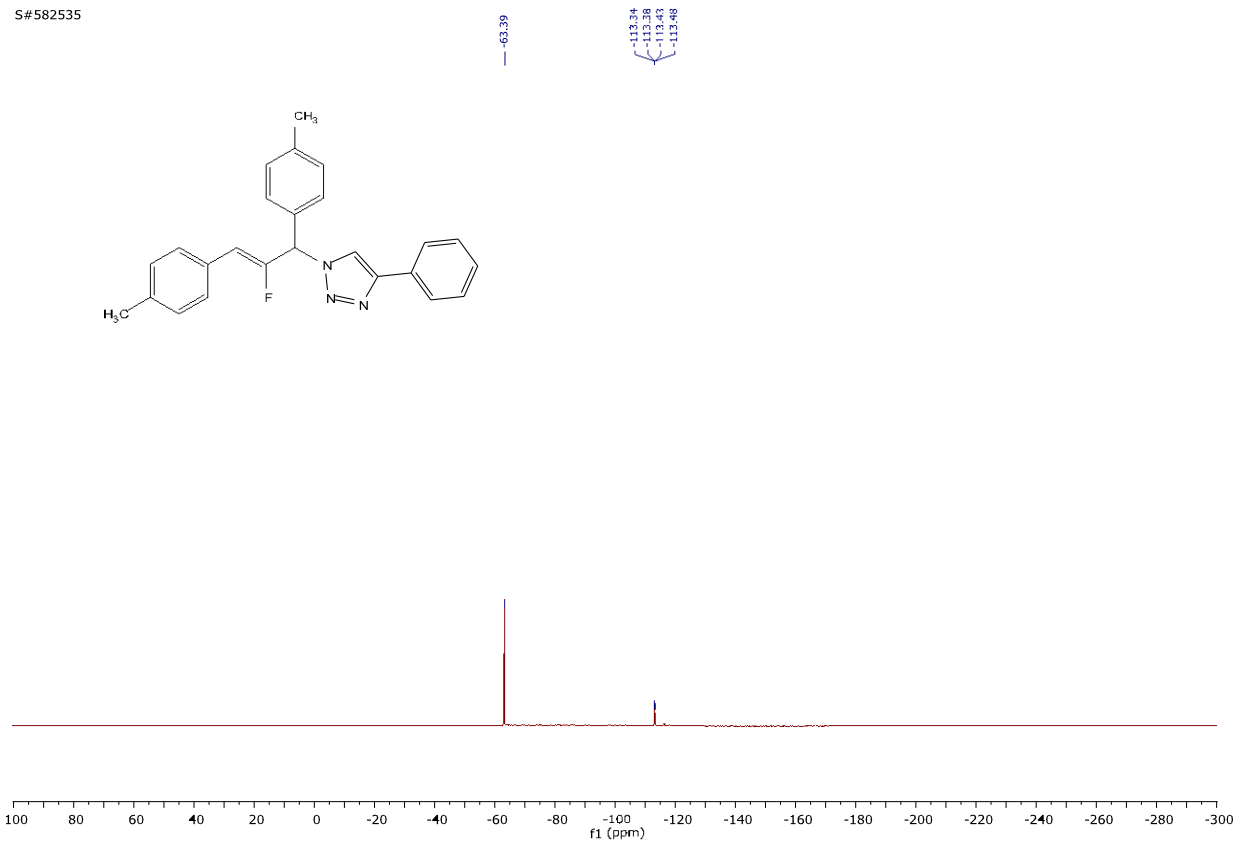

S#559969
-63.47
-111.93
-111.98
-112.04
-112.08
Cl
F
Cl
N
N
N
CH3
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-300
f1 (ppm)

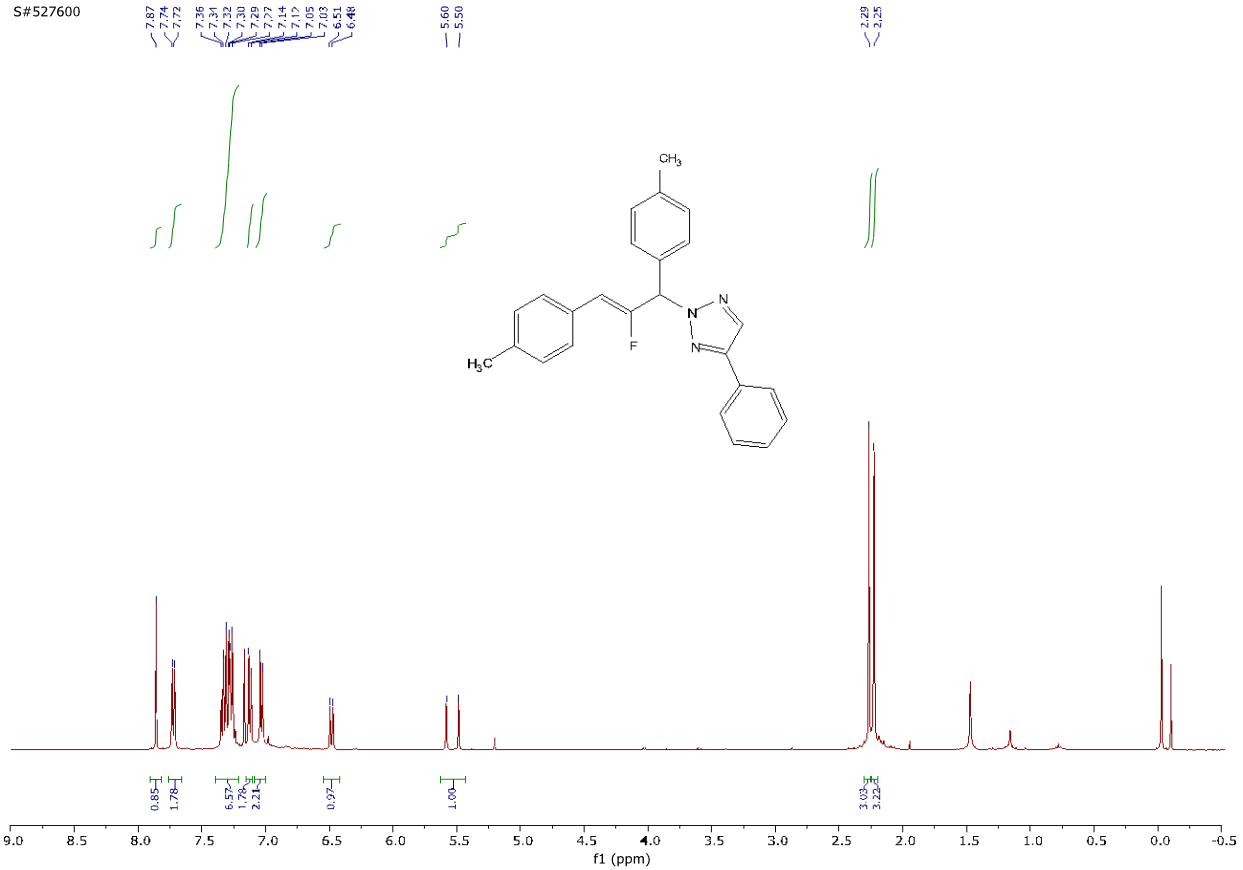

S#535805
single_pulse
7.85
7.62
7.61
7.35
7.33
7.33
7.32
7.22
7.21
7.18
7.17
7.15
6.49
6.48
5.56
5.49
2.31
Cl
Cl
F
N
N
N
CH3
0.81
1.76
6.19
2.34
2.25
0.97
1.00
3.28
f1 (ppm)

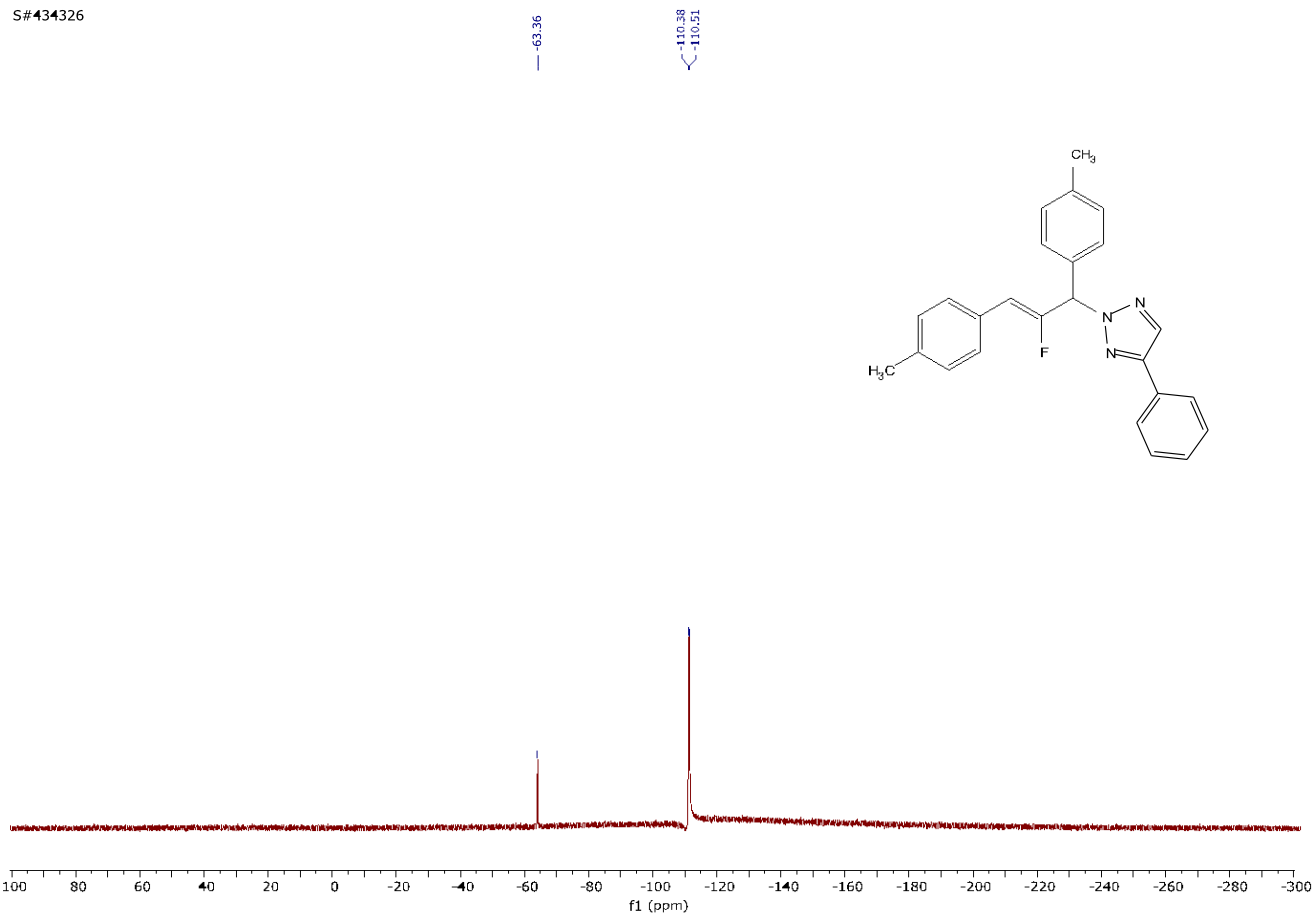

S#550152
-62.62
-108.01
-108.11
Cl
Cl
F
N
N
N
CH3
f1 (ppm)

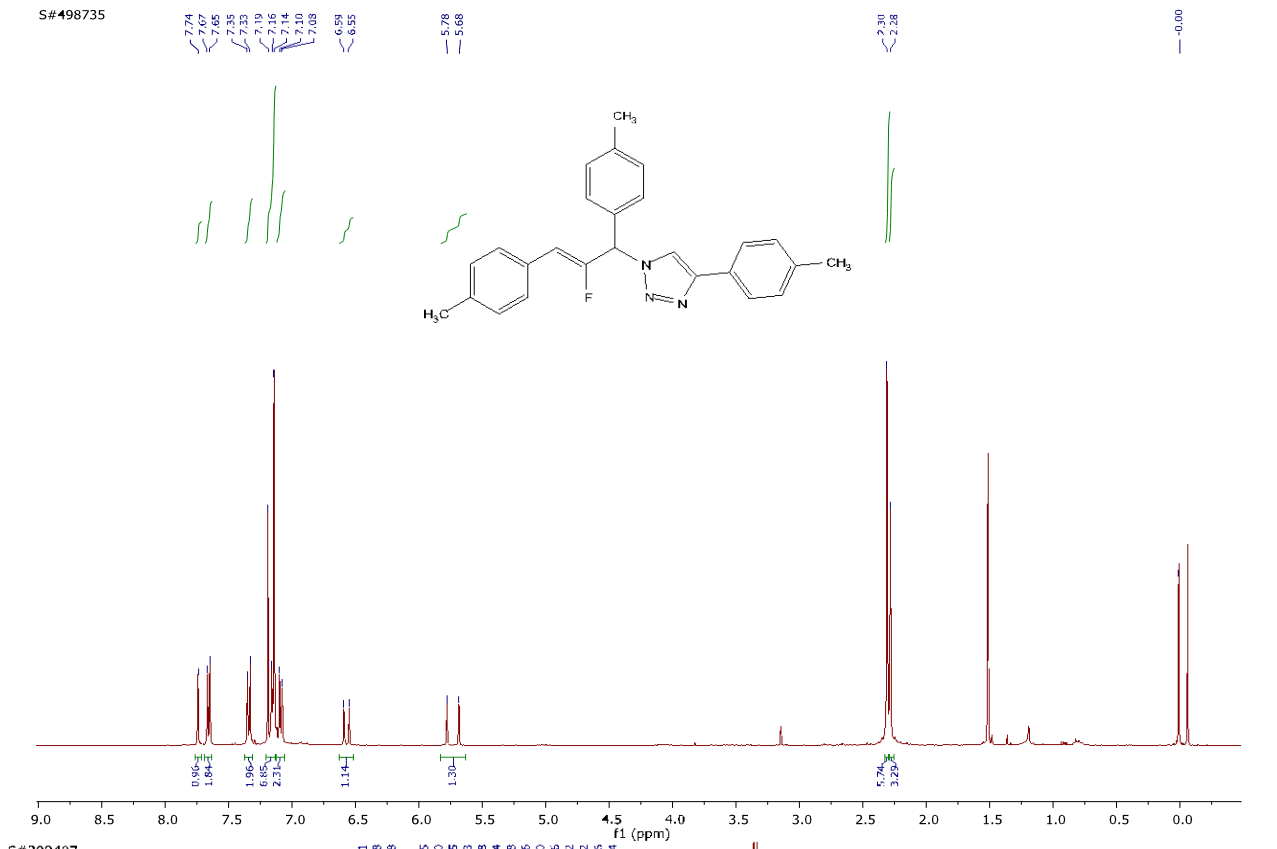

S#480912
f1 (ppm)

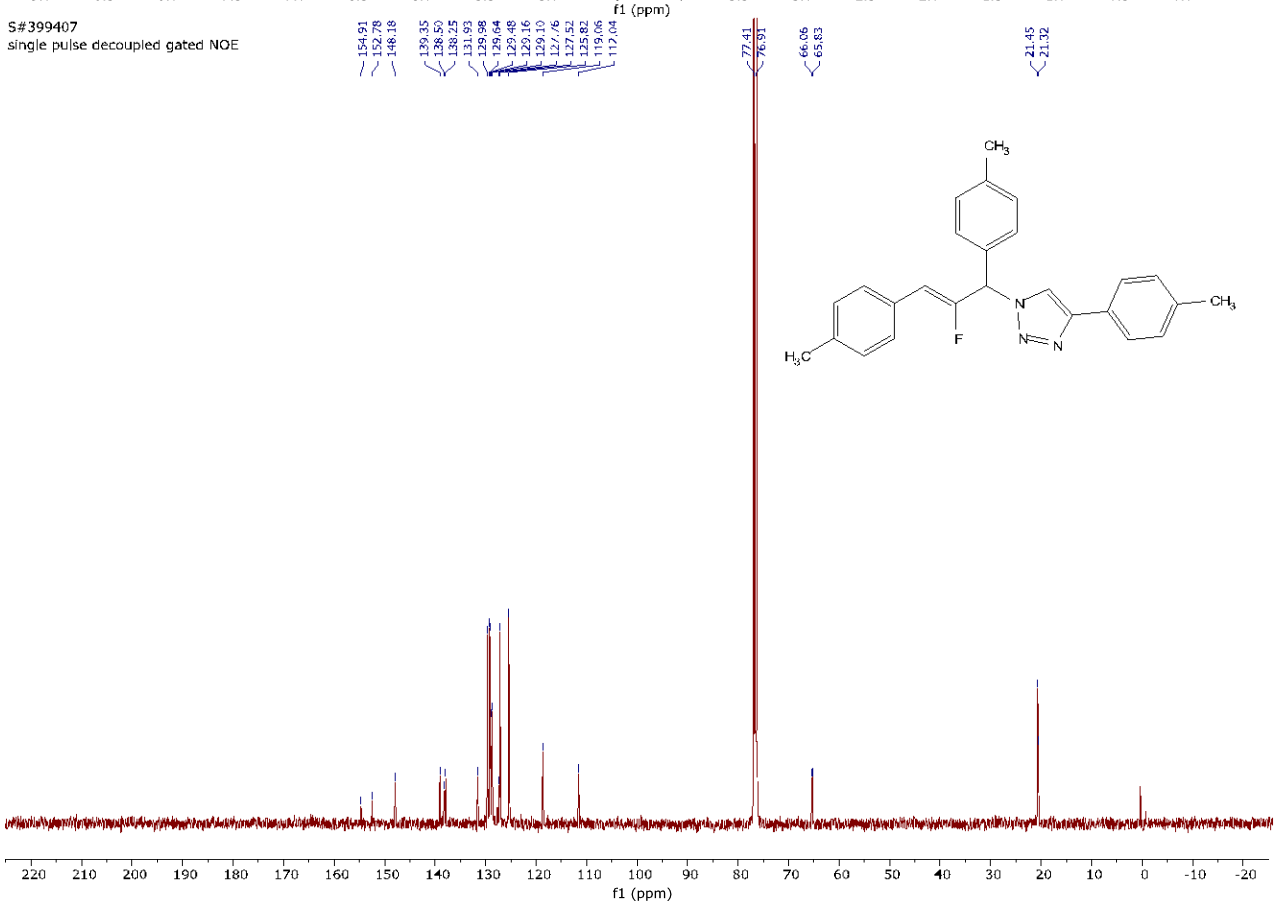

S#291539
single pulse decoupled gated NOE
f1 (ppm)

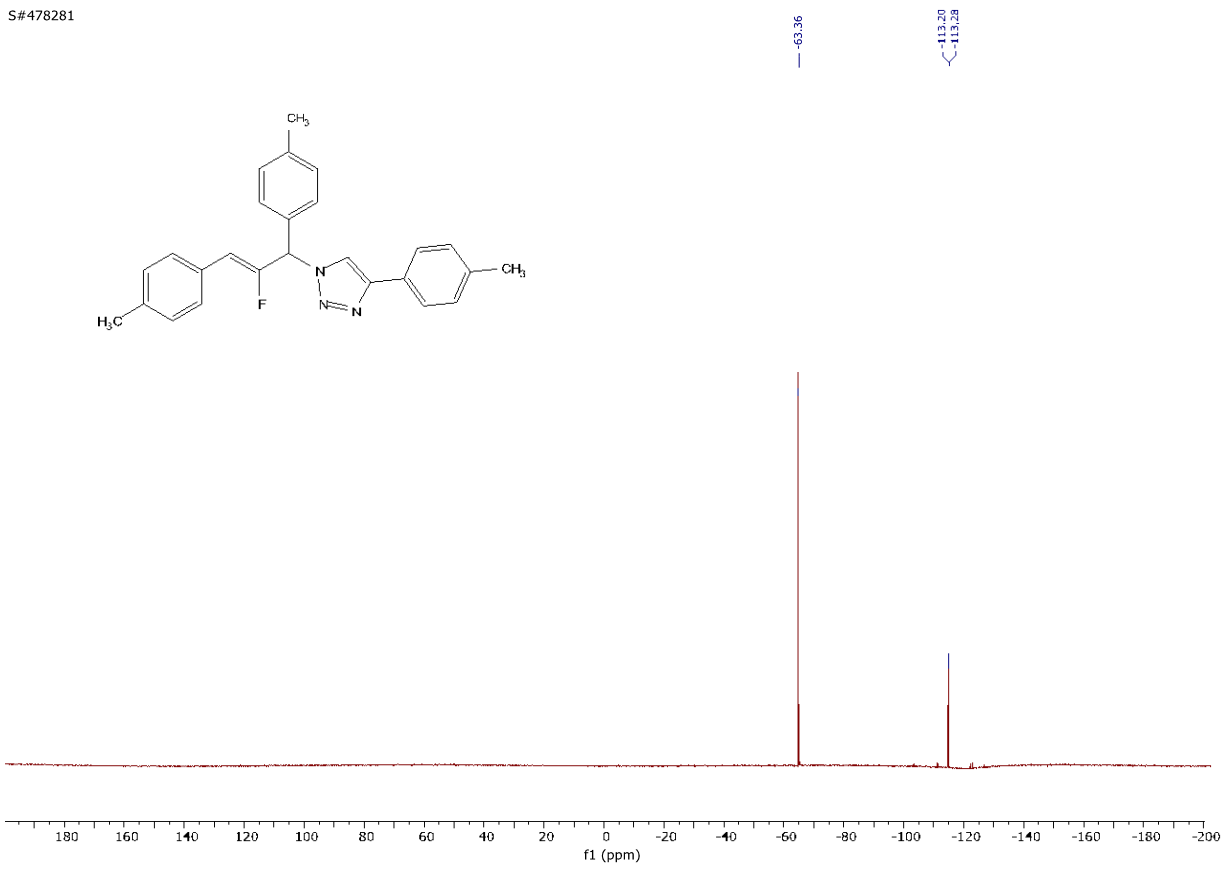

S#582535
-63.39
-113.34
-113.38
-113.43
-113.48
CH3
H3C
F
N
N
N
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-300
f1 (ppm)


S#527600
7.87
7.74
7.72
7.36
7.31
7.32
7.30
7.29
7.27
7.14
7.12
7.05
7.03
6.51
6.48
5.60
5.50
2.29
2.25
CH3
H3C
F
N
N
N
0.85
1.78
6.57
1.78
2.21
0.97
1.00
3.03
3.22
f1 (ppm)

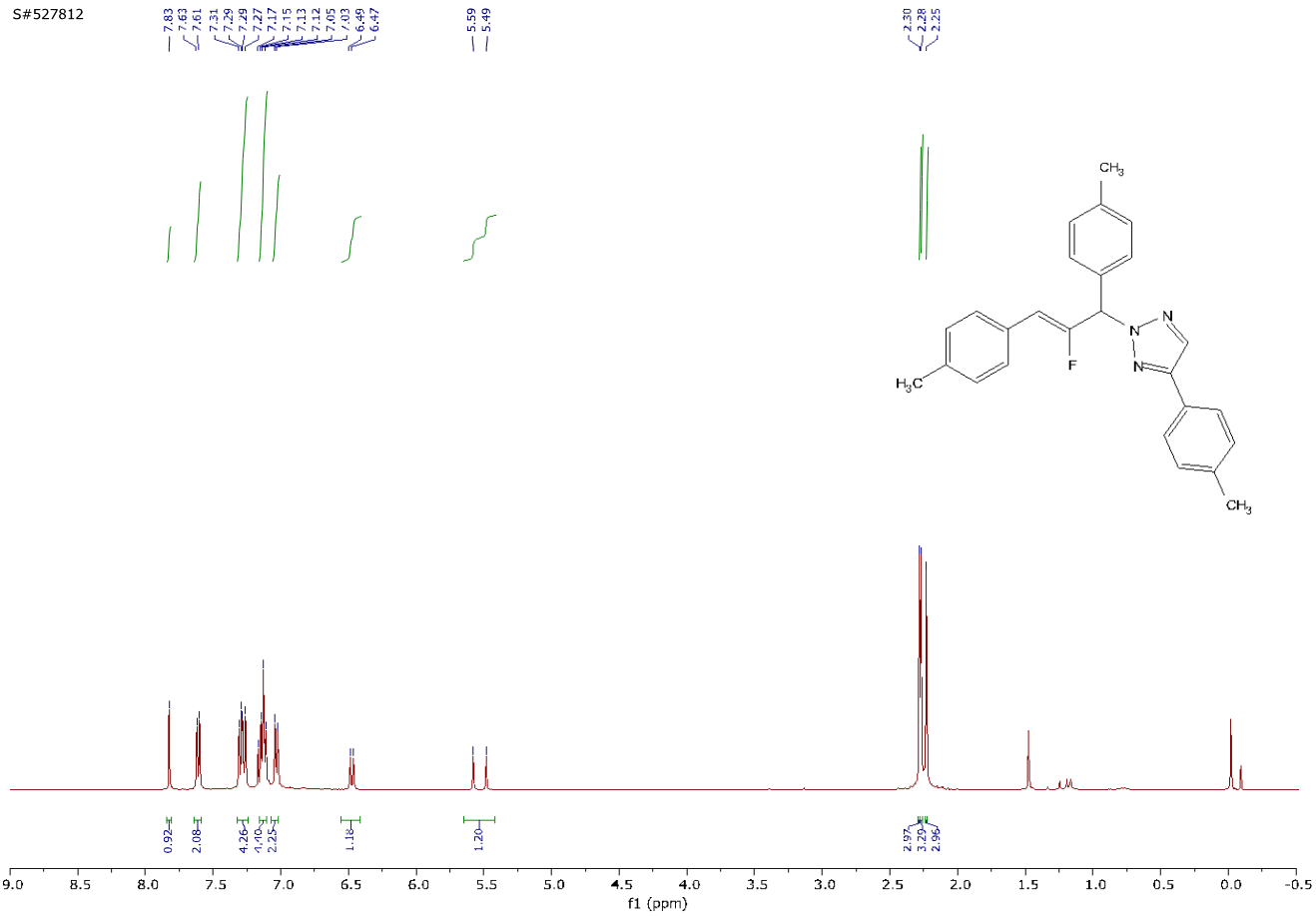

S#434326
-63.36
-110.38
-110.51
CH3
H3C
F
N
N
N
f1 (ppm)


S#498735
7.74
7.67
7.65
7.35
7.33
7.19
7.16
7.14
7.10
7.08
6.59
6.55
5.78
5.68
2.31
2.28
-0.00
CH3
H3C
F
N
N=N
CH3
0.96
1.64
1.96
6.85
2.31
1.14
1.30
5.74
3.29
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

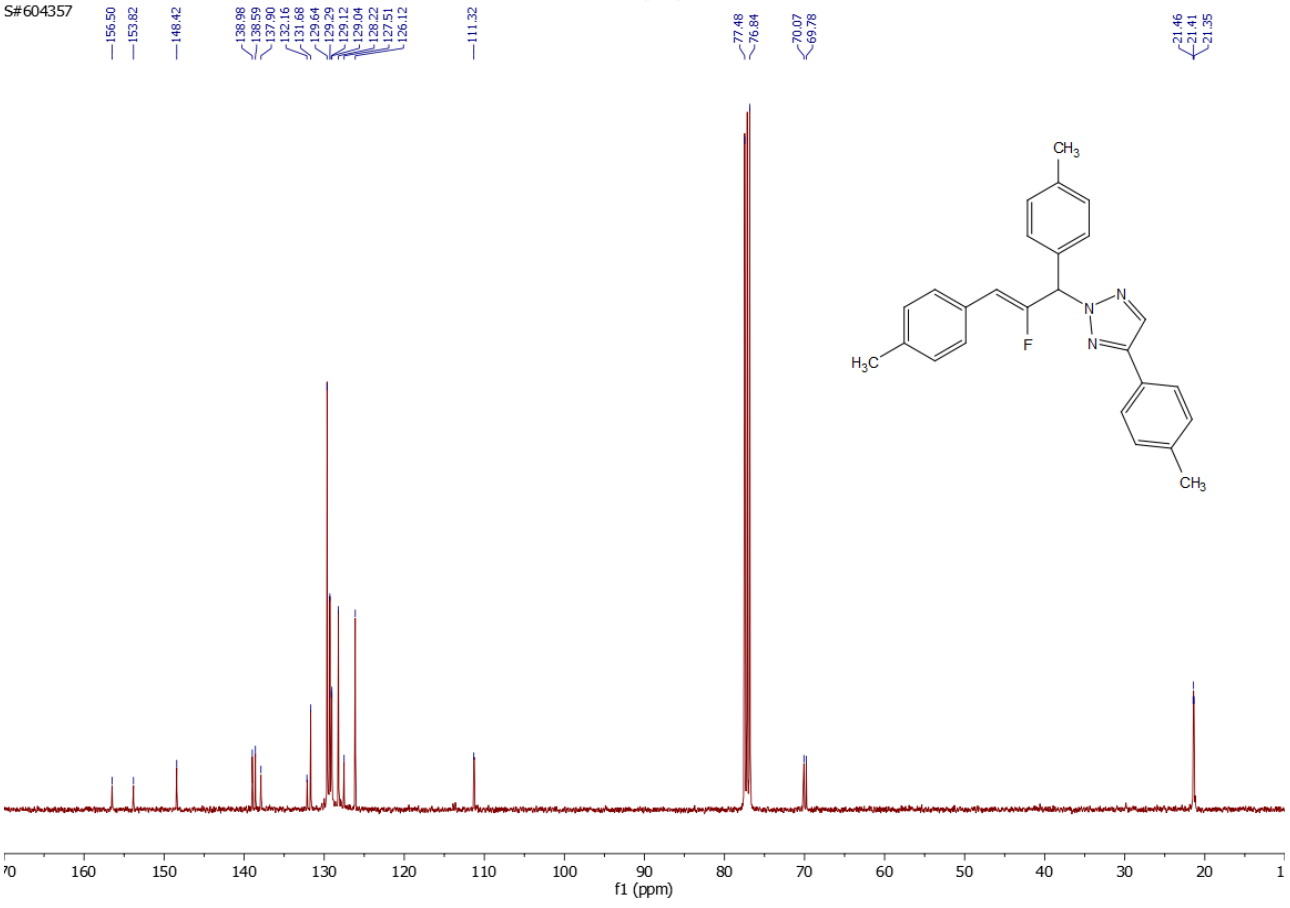

S#399407
single pulse decoupled gated NOE
154.91
152.78
148.18
139.35
138.50
138.25
131.93
129.98
129.64
129.48
129.16
129.10
127.46
127.52
125.82
119.06
112.04
77.41
76.91
66.06
65.83
21.45
21.32
CH3
H3C
F
N
N=N
CH3
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

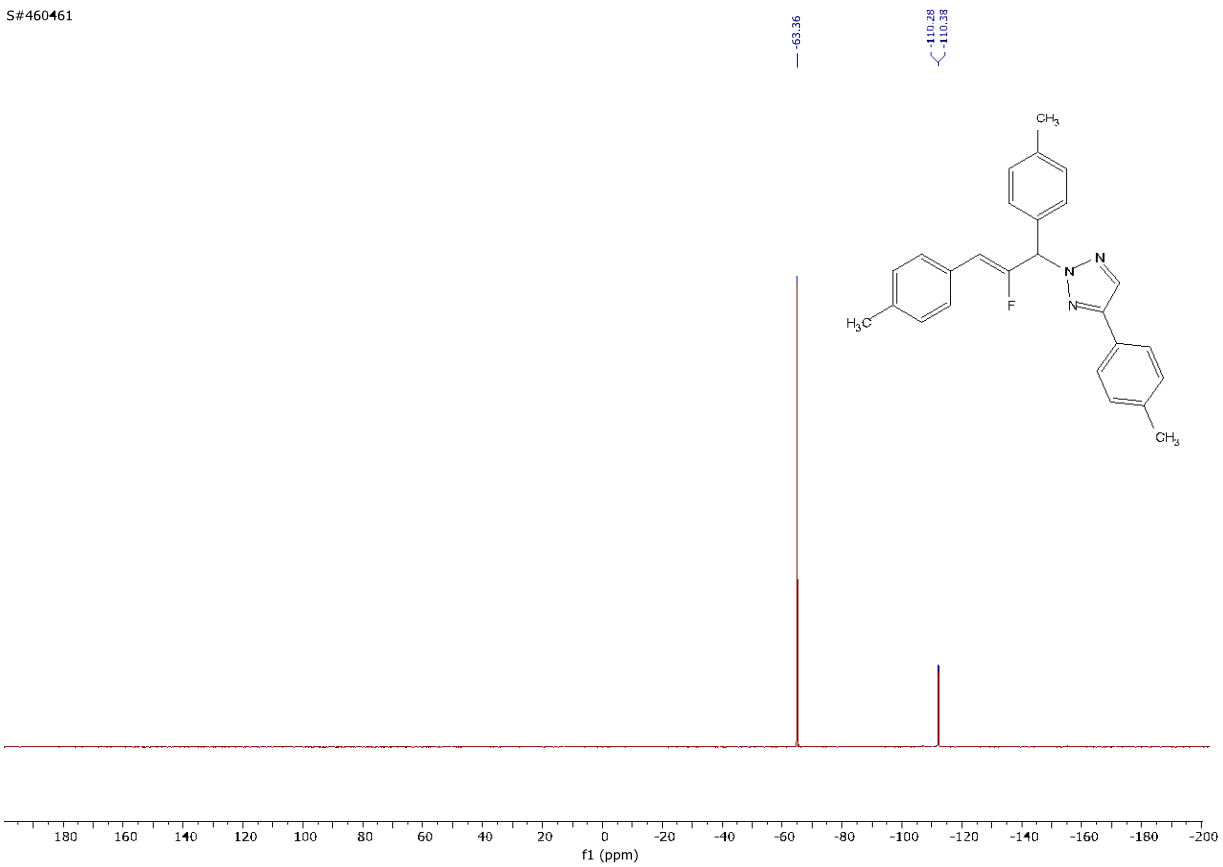

S#478281
-63.36
-113.20
-113.28
CH3
CH3
H3C
F
N
N
N
180
160
140
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

S#527812

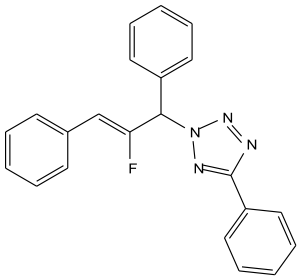


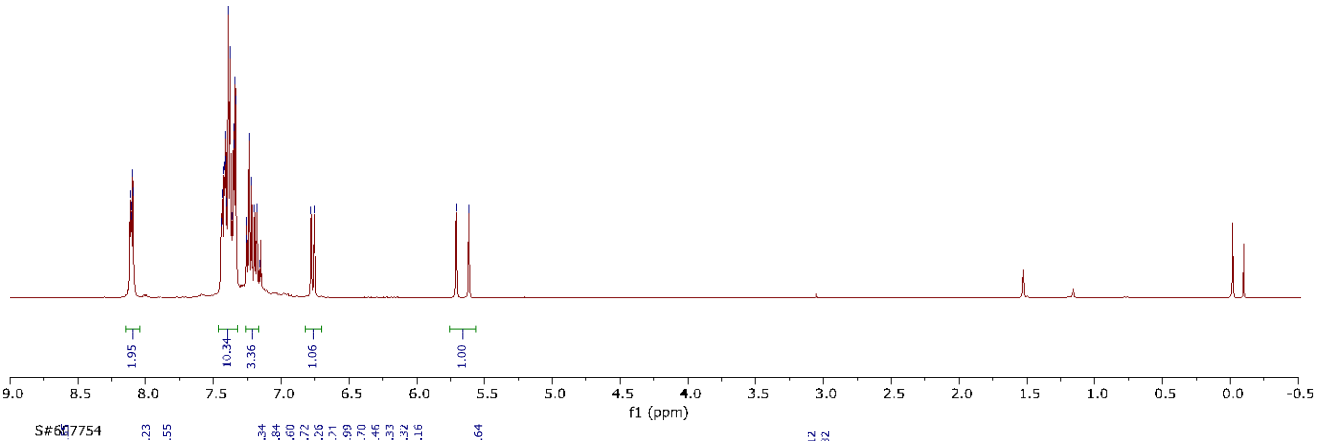
S#604357



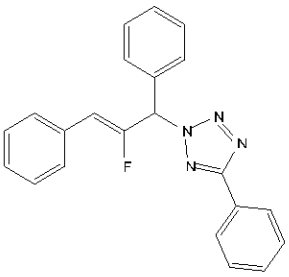

S#460461
-63.36
-110.28
-110.38
CH3
H3C
F
N
N
N
CH3
180
160
140
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

S#672575

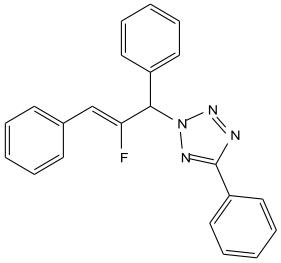




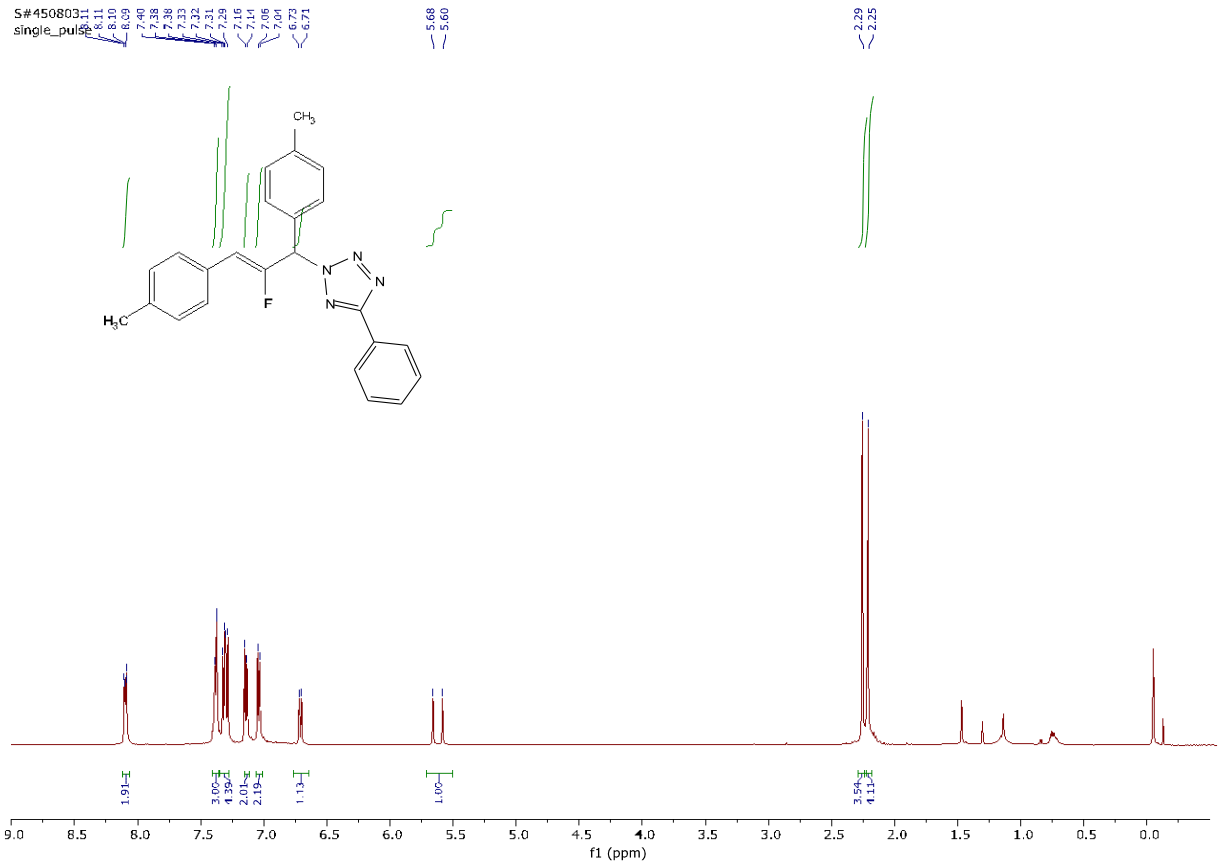
S#677754



S#434639


F
N
N
N
N

-63.36
-110.46
-110.57
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-300
f1 (ppm)


S#4508031
single_pulse
8.11
8.10
8.09
7.40
7.38
7.38
7.33
7.32
7.31
7.29
7.16
7.14
7.06
7.04
6.73
6.71
5.68
5.60
2.29
2.25
CH3
N
N
N
F
H3C
1.91
3.00
4.39
2.01
2.19
1.13
1.00
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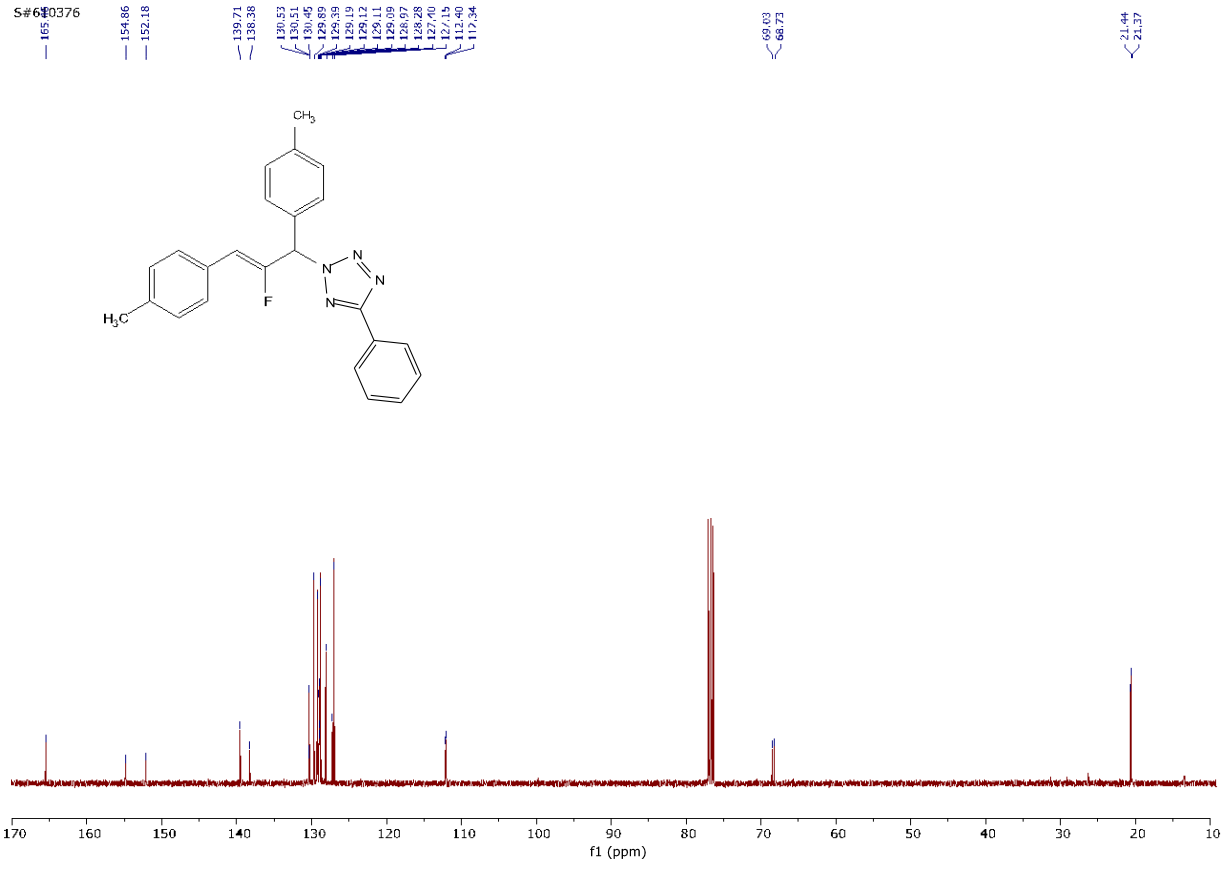
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129.11
129.09
128.97
128.28
127.40
127.15
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113.34
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68.73
21.44
21.37
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N
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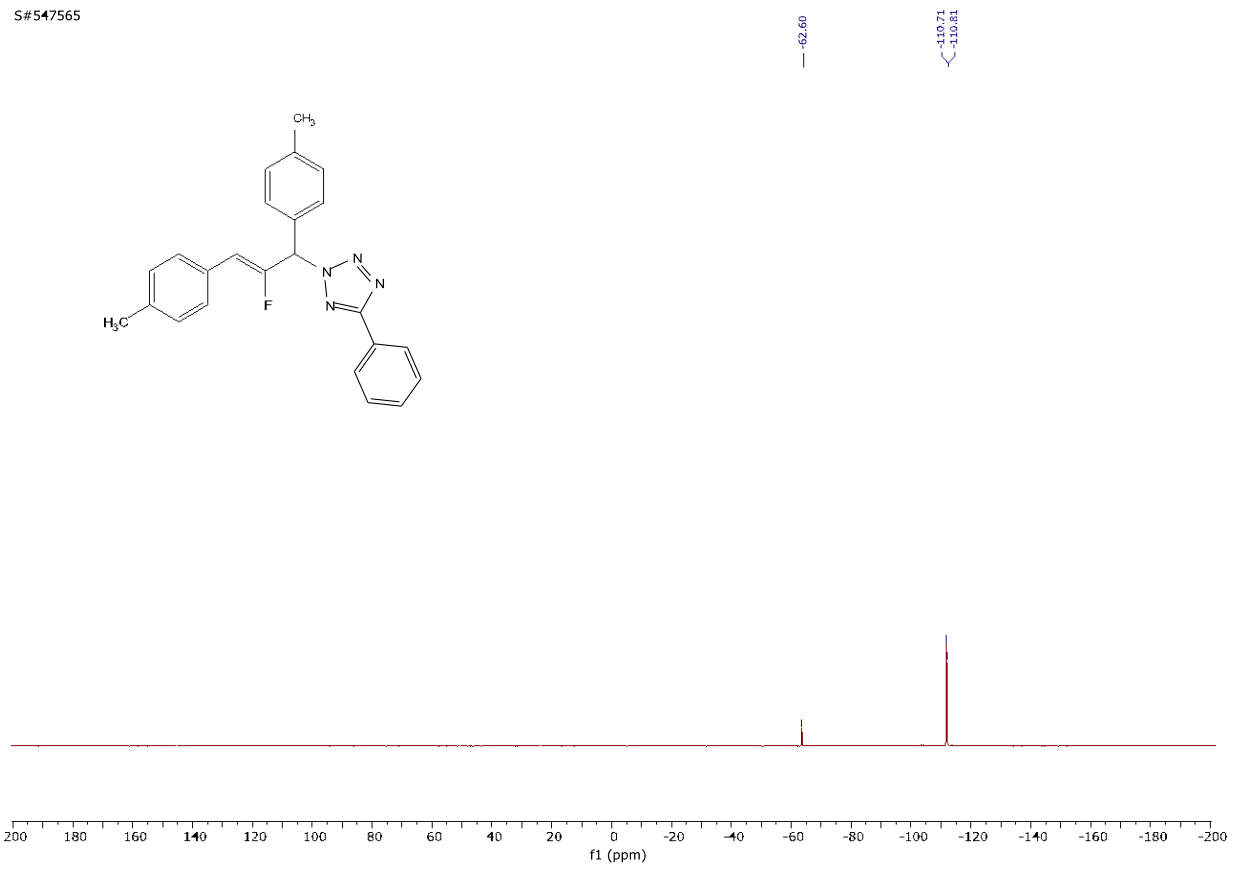
N
F
H3C
f1 (ppm)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140
120
100
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-40
-60
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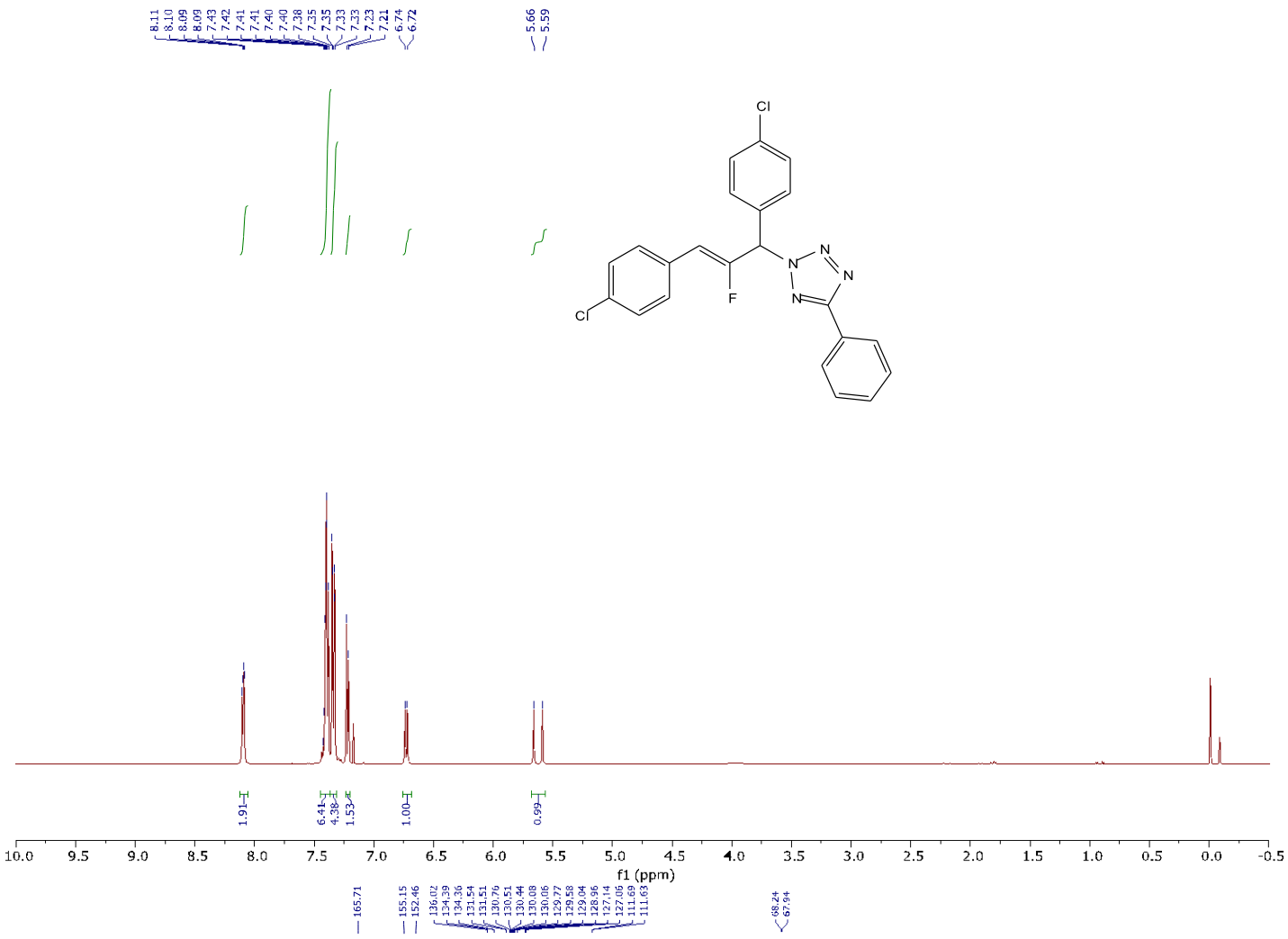
-100
-120
-140
-160
-180
-200
f1 (ppm)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8.09
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7.42
7.41
7.41
7.40
7.40
7.38
7.35
7.35
7.33
7.33
7.23
7.21
6.74
6.72
5.66
5.59
Cl
N
N
N
F
Cl
1.91
6.41
4.38
1.53
1.00
0.99
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

165.71
155.15
152.46
136.02
134.39
134.36
131.54
131.51
130.76
130.51
130.44
130.08
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129.58
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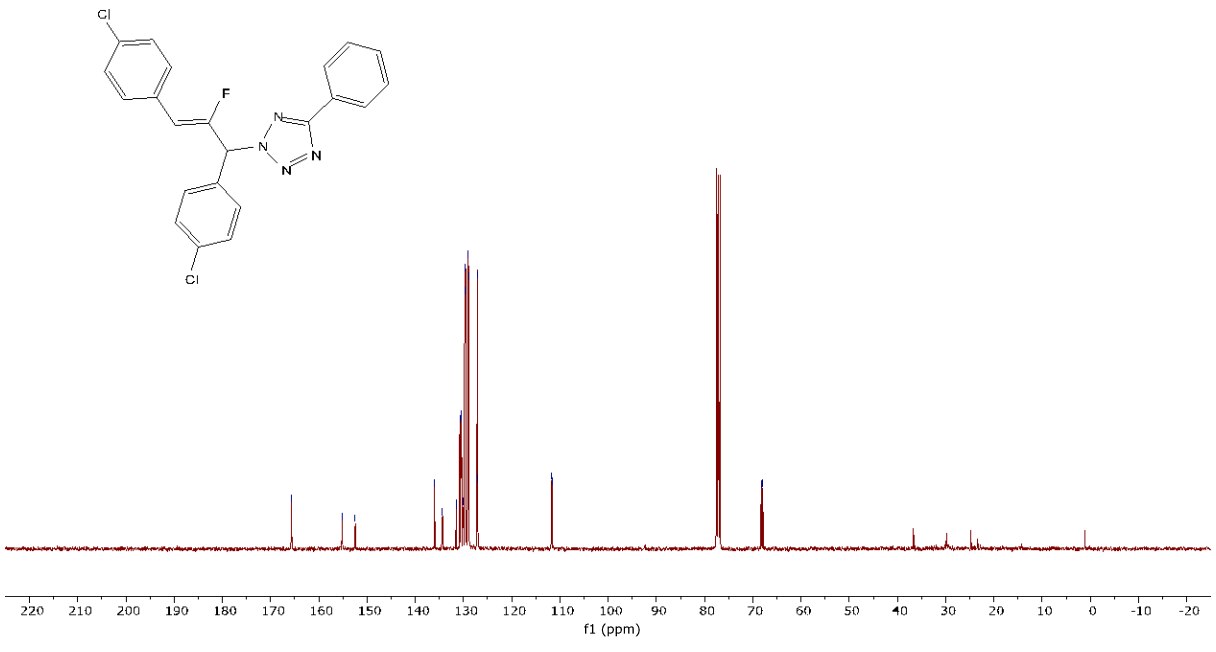
128.96
127.14
127.06
111.69
111.63
68.24
67.94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F
N
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N
Cl
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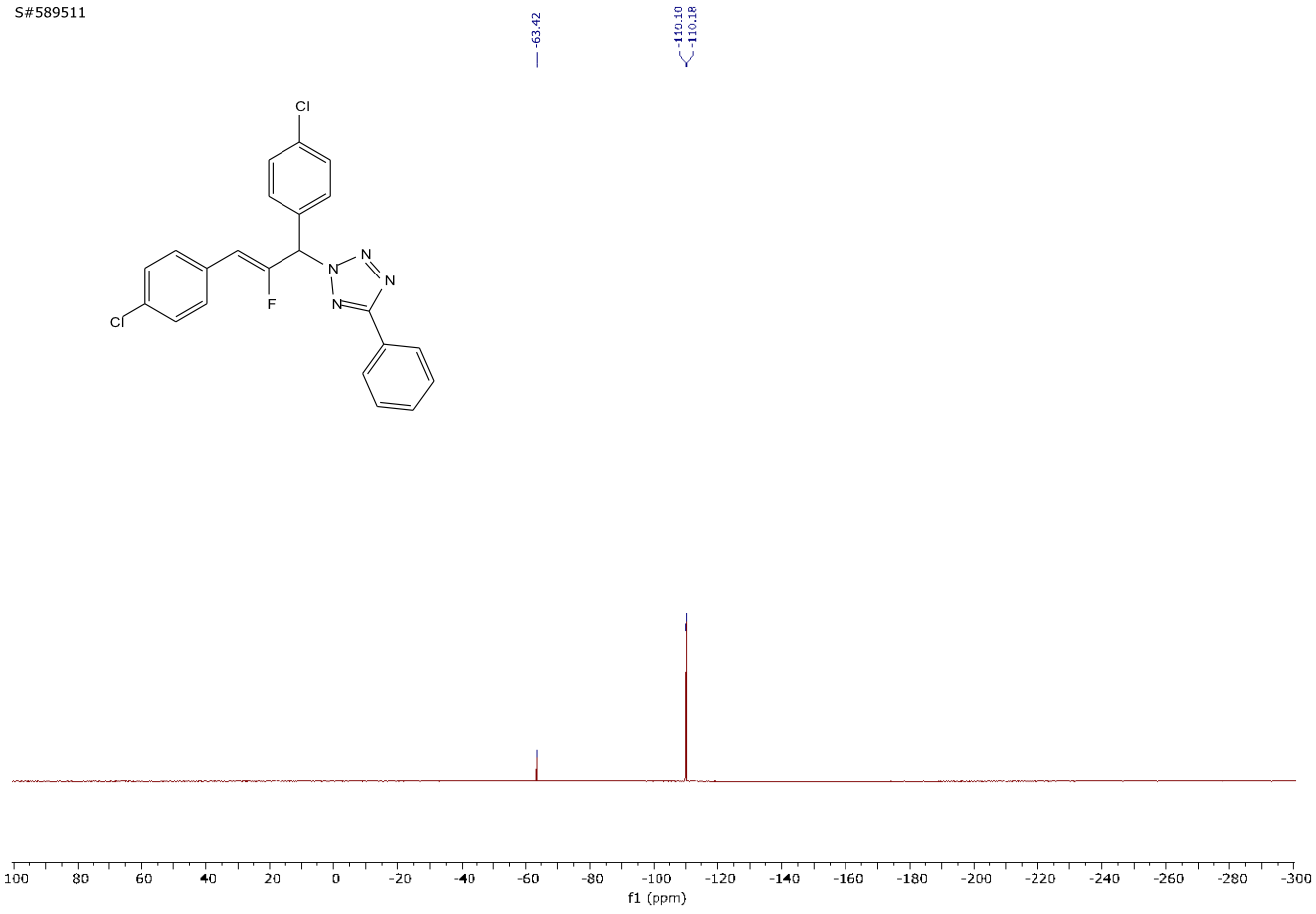
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

S#589511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Cl
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N
N
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40
20
0
-20
-40
-60
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-120
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-200
-220
-240
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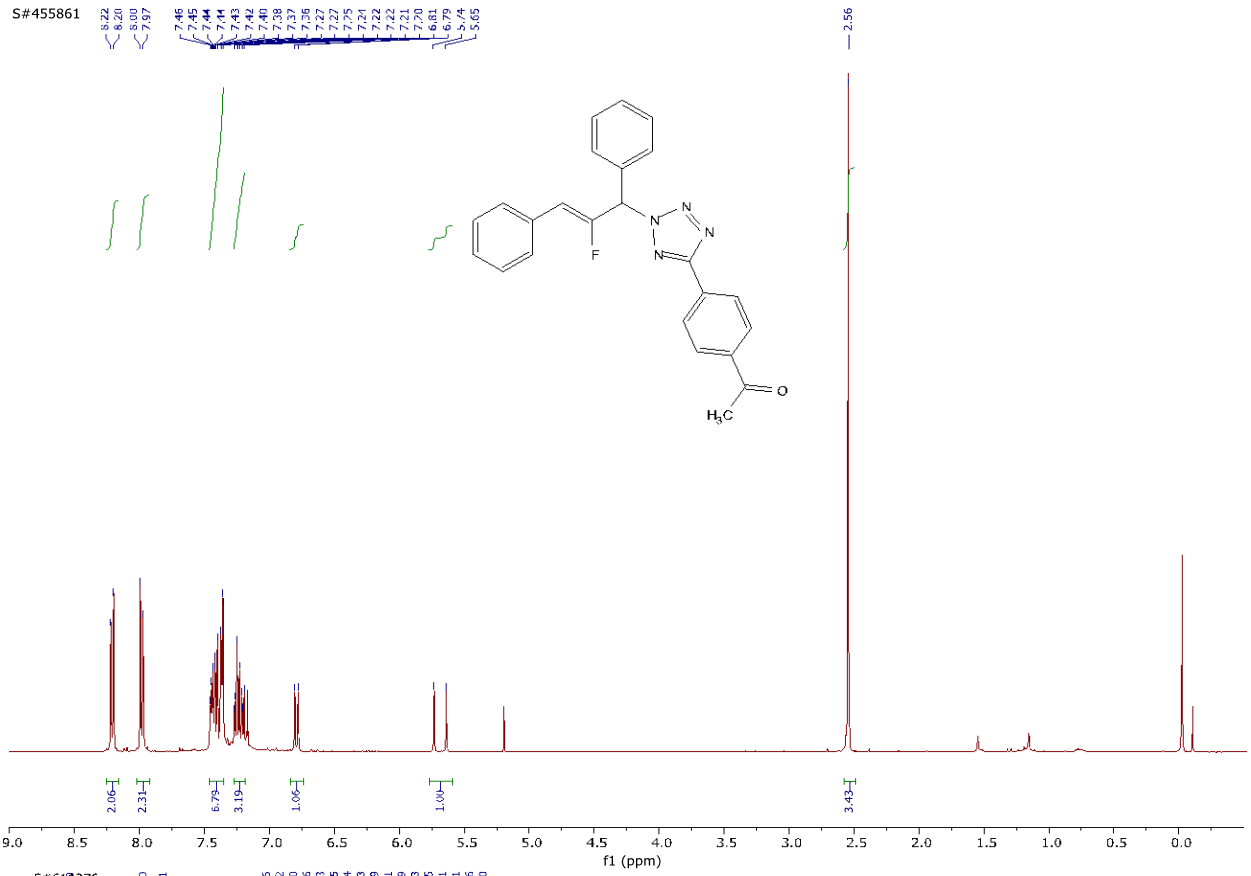
f1 (ppm)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7.37
7.36
7.27
7.27
7.25
7.24
7.22
7.22
7.21
7.20
6.81
6.79
5.74
5.65
2.56
F
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H3C
2.06
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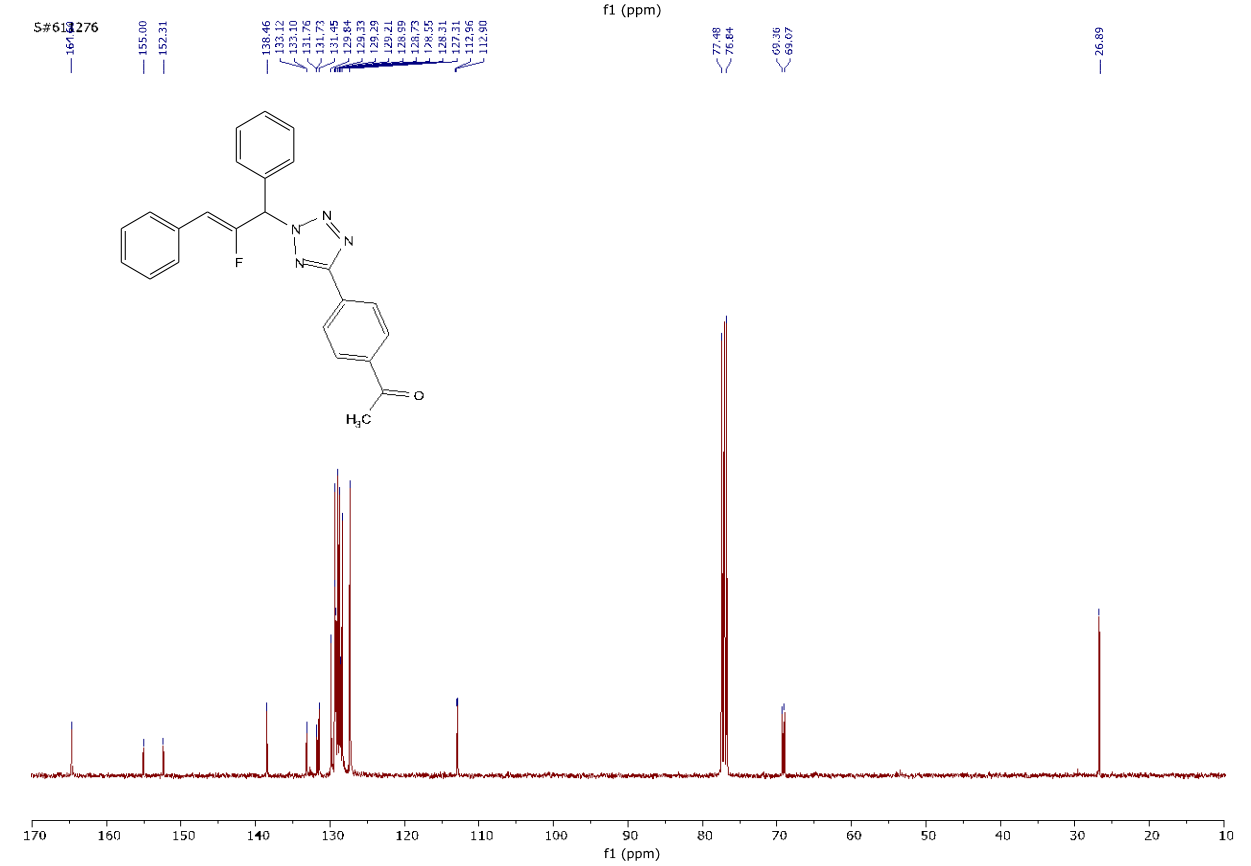
3.19
1.06
1.00
3.43
f1 (ppm)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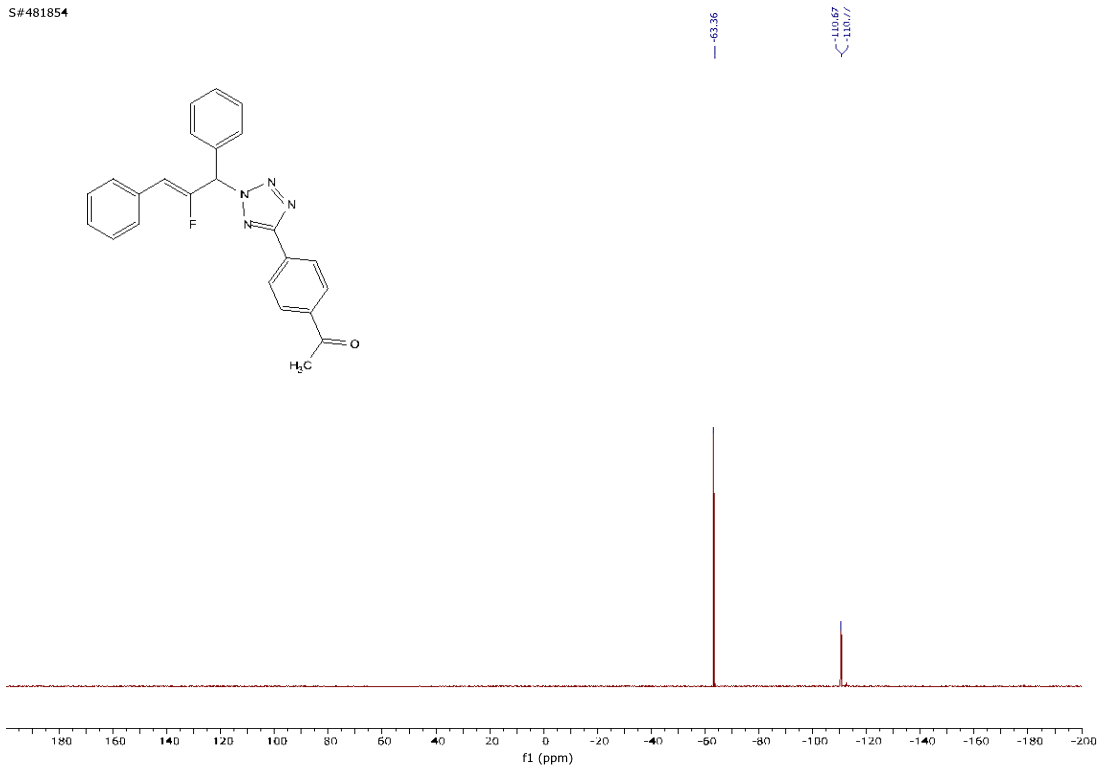
129.33
129.29
129.21
128.99
128.73
126.55
128.31
127.31
112.96
112.90
77.48
76.84
69.36
69.07
26.89
F
N
N
N
N
O
H3C
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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-110.77
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N
O
H3C
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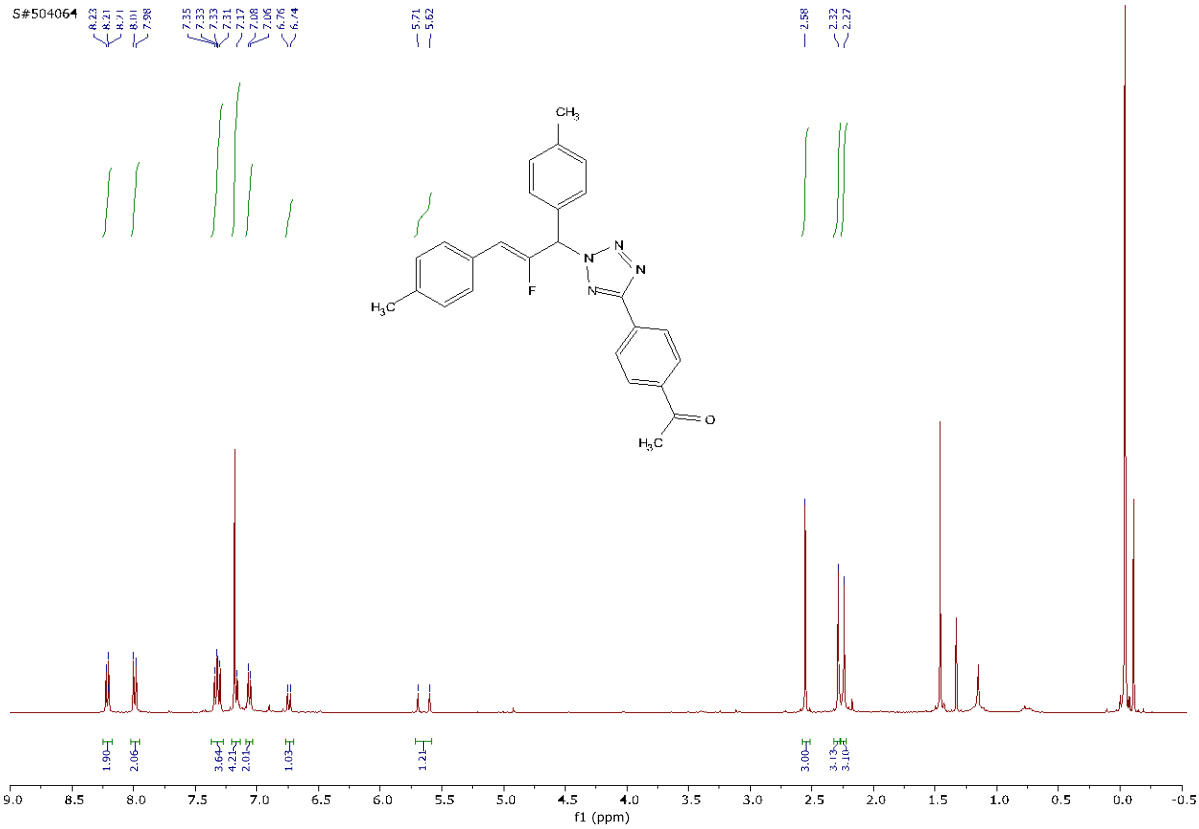
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)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7.17
7.08
7.06
6.76
6.74
5.71
5.62
2.58
2.32
2.27
CH3
N
N
N
F
H3C
O
H3C
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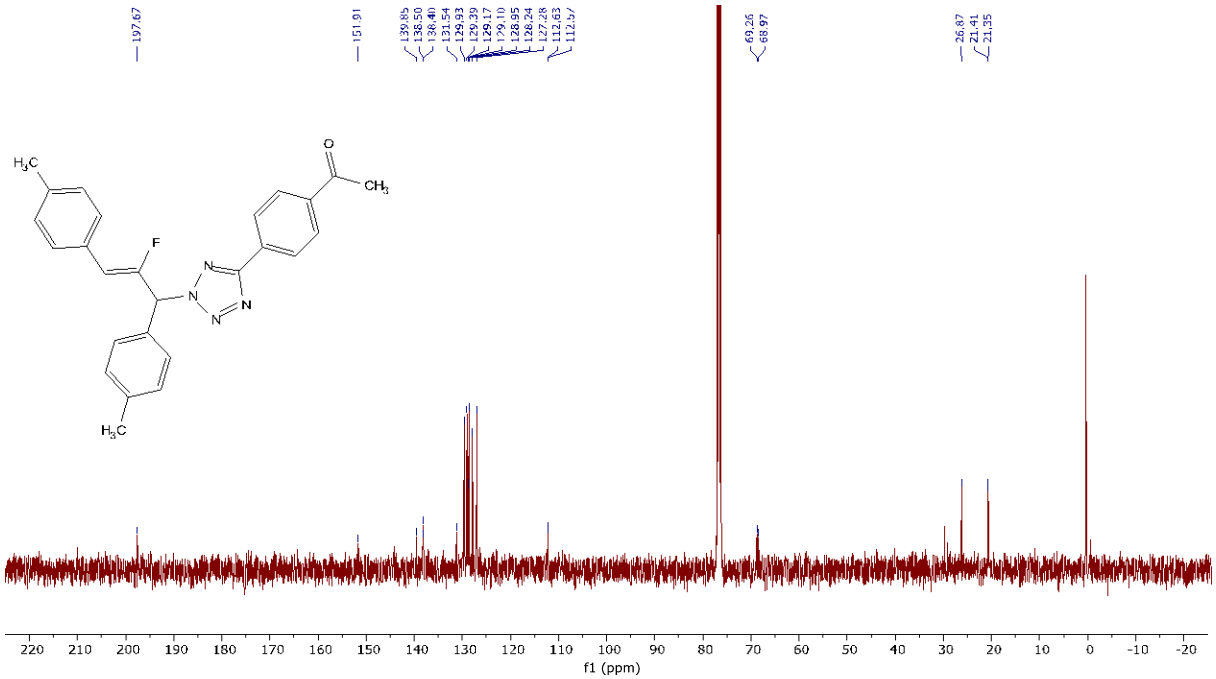
3.64
4.23
2.01
1.03
1.21
3.00
3.13
3.10
f1 (ppm)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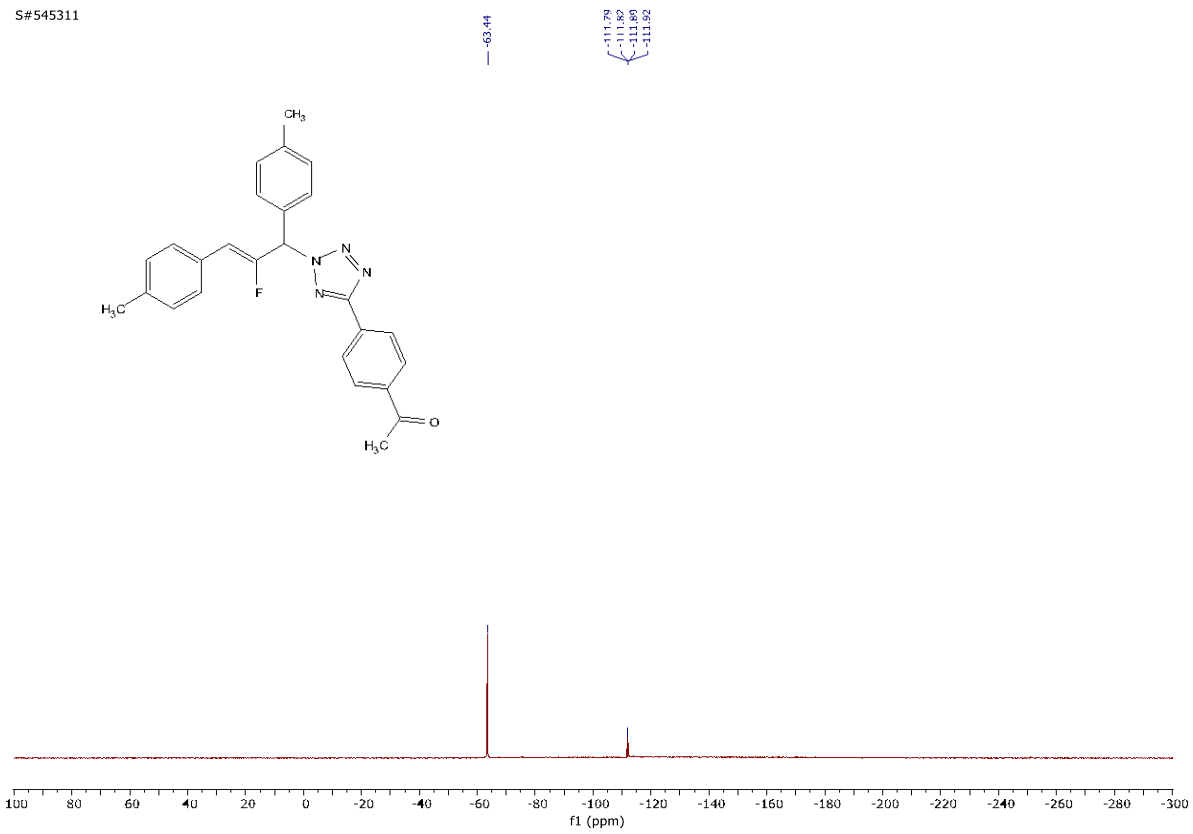
129.93
129.39
129.17
129.10
128.65
128.24
127.28
117.65
112.57
69.26
68.97
26.87
21.41
21.35
H3C
O
CH3
F
N
N
N
H3C
f1 (ppm)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-111.89
-111.92
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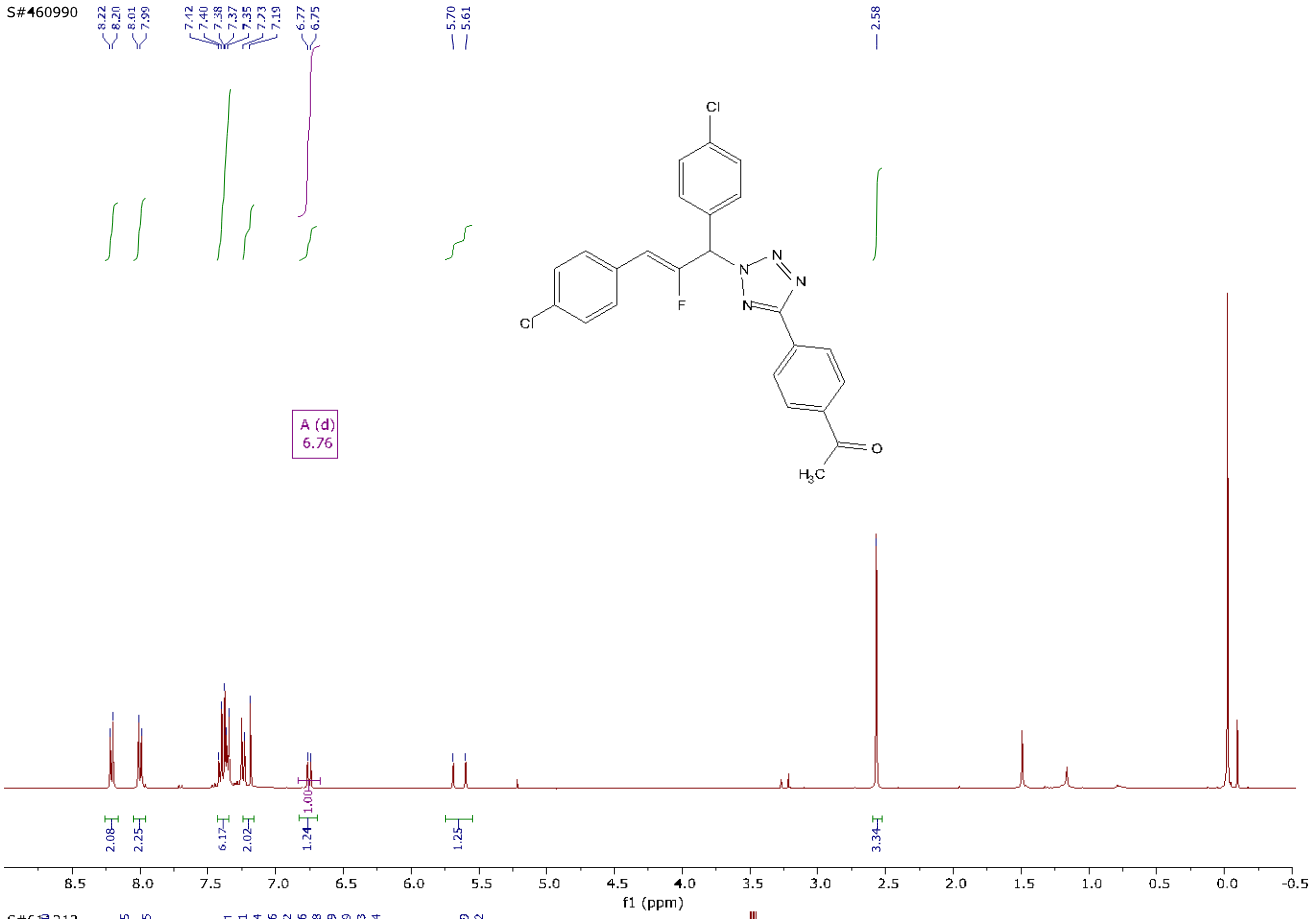
H3C
F
N
N
N
N
O
H3C
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-300
f1 (ppm)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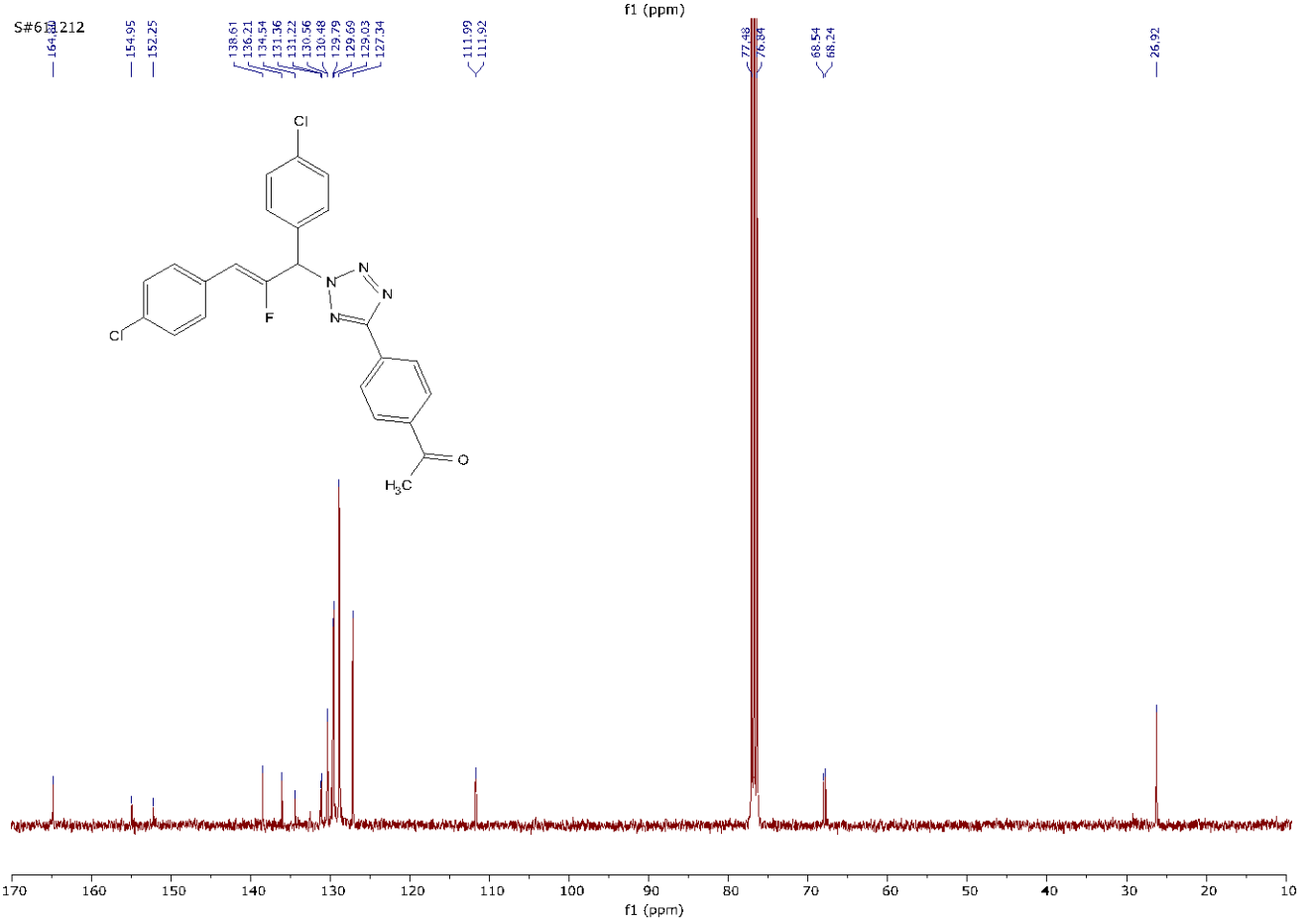
7.33
7.19
6.77
6.75
5.70
5.61
2.58
A (d)
6.76
Cl
Cl
F
N
N
N
O
H3C
2.08
2.25
6.17
2.02
1.24
1.00
1.25
3.34
f1 (ppm)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130.56
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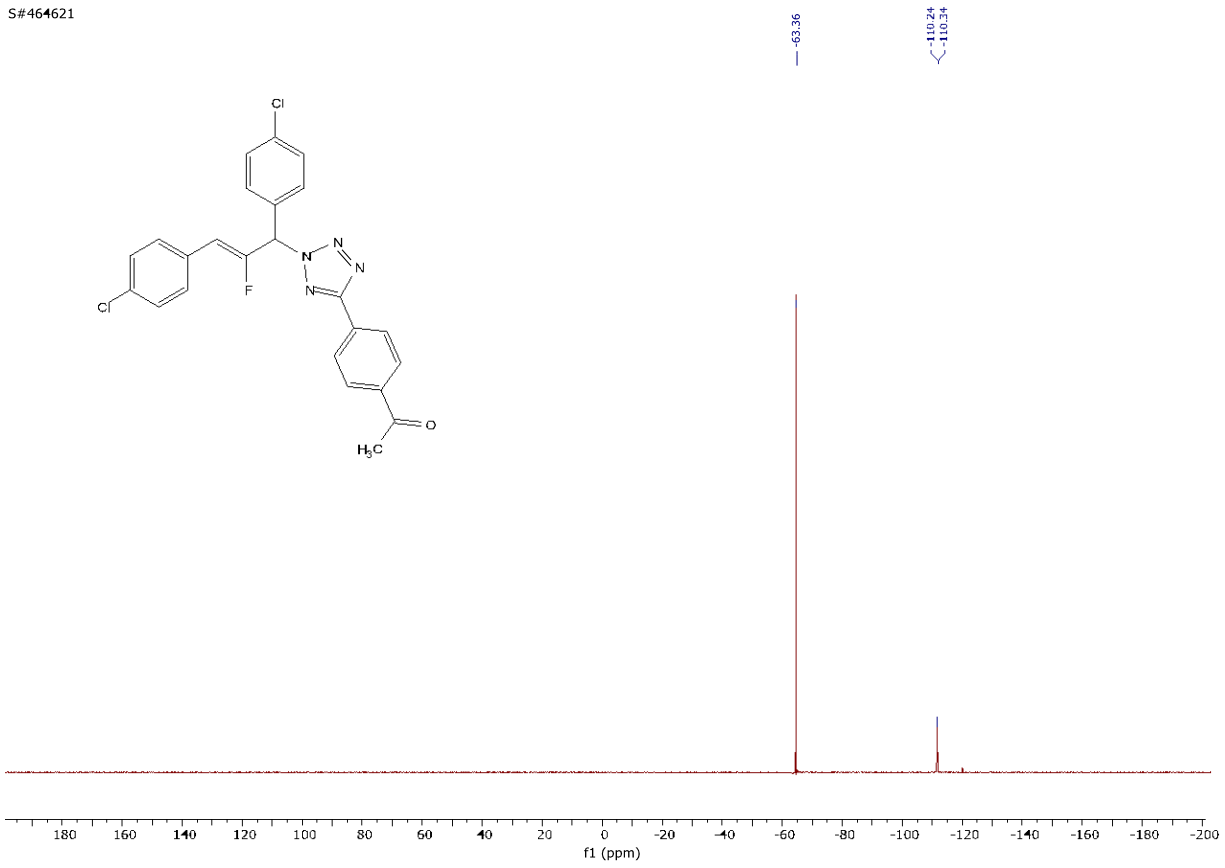
129.69
129.03
127.34
111.99
111.92
77.48
76.84
68.54
68.24
26.92
Cl
Cl
F
N
N
N
O
H3C
f1 (ppm)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-110.34
Cl
Cl
F
N
N
N
O
H3C
180
160
140
120
100
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
f1 (ppm)

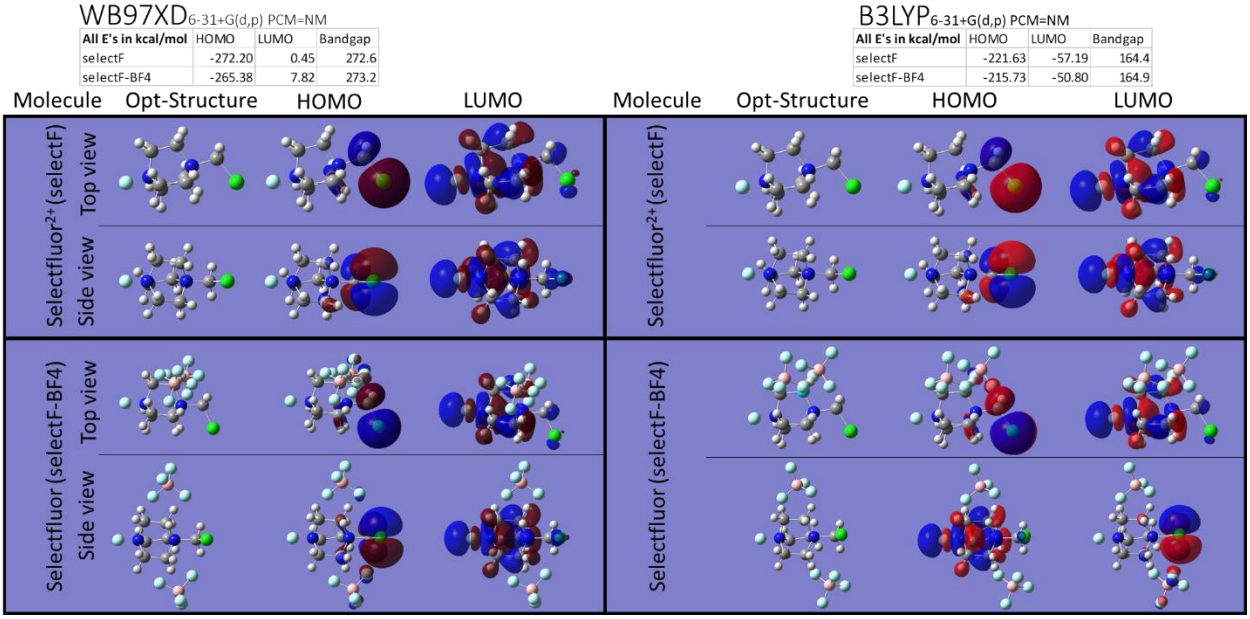


Figure S1. Frontier orbital analysis for Selectfluor with and without the counter ions. The left and right penal shows calculated frontier orbitals at wB97xd/6-31+G(d,p) and B3LYP/6-31+G(d,p) level of theory with the implicit solvation of nitromethane. The top tables show the energies (in kcal/mol) of frontier orbitals and the HOMO-LUMO gap.

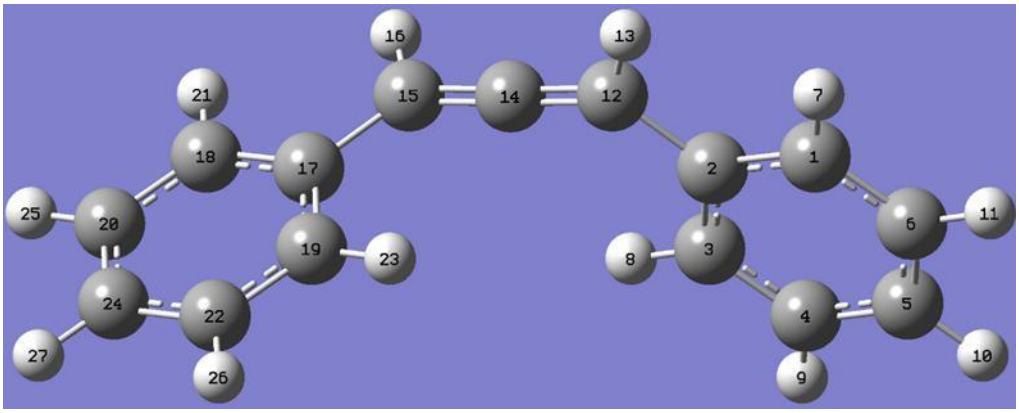


Figure S2. Atom numbering for diphenylallene (DPA) to be used in Table S1.

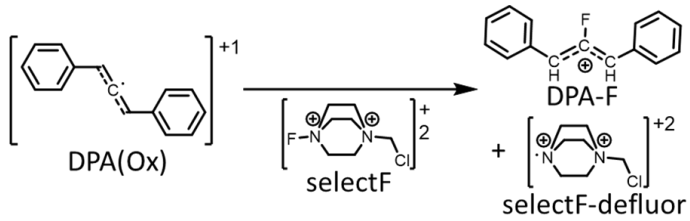
Table S1. Calculated NBO charge and spin values (in a.u.) for diphenylallene (DPA) and oxidized DPA using B3LYP and wB97xd functionals with 6-31+G(d,p) basis sets and implicit solvation of nitromethane. Refer to Figure S2 for atom numbering.

		DPA (B3LYP)	Oxidized DPA (B3LYP)		DPA (wB97XD)	Oxidized DPA (wB97XD)	
Atom type	Number	Natural Charge	Natural Charge	Natural spin	Natural Charge	Natural Charge	Natural spin
C	1	-0.232	-0.178	0.05	-0.24	-0.219	-0.009
C	2	-0.077	-0.078	0.063	-0.079	-0.098	0.03
C	3	-0.23	-0.177	0.062	-0.237	-0.221	-0.007
C	4	-0.246	-0.243	-0.027	-0.252	-0.248	0.005
C	5	-0.253	-0.163	0.114	-0.26	-0.237	-0.008
C	6	-0.247	-0.241	-0.019	-0.252	-0.249	0.005
H	7	0.252	0.269	-0.001	0.259	0.267	0
H	8	0.254	0.267	-0.002	0.26	0.263	0
H	9	0.256	0.272	0.001	0.262	0.268	0
H	10	0.255	0.269	-0.003	0.261	0.267	0
H	11	0.256	0.272	0.001	0.262	0.268	0
C	12	-0.309	-0.188	0.048	-0.306	-0.267	-0.05
H	13	0.27	0.311	0.018	0.276	0.324	0.028
C	14	0.098	0.228	0.394	0.1	0.239	0.378
C	15	-0.298	-0.205	0.048	-0.317	-0.213	0.056
H	16	0.268	0.309	0.018	0.277	0.305	0
C	17	-0.08	-0.071	0.063	-0.076	0.003	0.153
C	18	-0.232	-0.178	0.05	-0.24	-0.154	0.124
C	19	-0.23	-0.177	0.062	-0.237	-0.146	0.146
C	20	-0.247	-0.24	-0.019	-0.252	-0.249	-0.059
H	21	0.252	0.269	-0.001	0.259	0.285	-0.004
C	22	-0.246	-0.243	-0.027	-0.252	-0.257	-0.076
H	23	0.254	0.267	-0.002	0.26	0.284	-0.005
C	24	-0.253	-0.163	0.114	-0.26	-0.078	0.299
H	25	0.256	0.272	0.001	0.262	0.289	0.001
H	26	0.256	0.272	0.001	0.262	0.289	0.002
H	27	0.255	0.269	-0.003	0.261	0.283	-0.009

Figure S3. Reaction energetics (free energies) for various steps in the proposed reaction mechanisms. Level of theories are provided in the description.

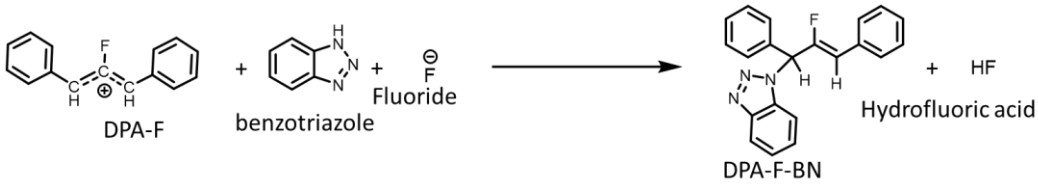
WB97XD/6-31+G(d,p) PCM=NM	
Molecule	**Free Energy (kcal/mol)**
DPA	-363083.49
DPA(Ox)	-362939.45
selectF	-592459.47
selectF(Red)	-592586.13
ΔG Prod - React	**17.37**

B3LYP/6-31+G(d,p) PCM=NM	
Molecule	**Free Energy (kcal/mol)**
DPA	-363217.35
DPA(Ox)	-363077.67
selectF	-592549.27
selectF(Red)	-592680.95
ΔG Prod - React	**8.00**



WB97XD/6-31+G(d,p) PCM=NM	
Molecule	**Free Energy (kcal/mol)**
DPA(Ox)	-362939.45
selectF	-592459.47
selectF-defluor	-529832.46
DPA-F	-425601.90
ΔG Prod - React	**-35.44**

B3LYP/6-31+G(d,p) PCM=NM	
Molecule	**Free Energy (kcal/mol)**
DPA(Ox)	-363077.67
selectF	-592549.27
selectF-defluor	-529908.20
DPA-F	-425753.47
ΔG Prod - React	**-34.72**



WB97XD/6-31+G(d,p) PCM=NM	
Molecule	**Free Energy (kcal/mol)**
DPA-F	-425601.90
benzotriazole	-248346.54
Fluoride	-62726.42
DPA-F-BN	-673717.02
HF	-63020.94
ΔG Prod - React	**-63.10**

B3LYP/6-31+G(d,p) PCM=NM	
Molecule	**Free Energy (kcal/mol)**
DPA-F	-425753.47
benzotriazole	-248433.77
Fluoride	-62746.48
DPA-F-BN	-673942.31
HF	-63037.98
ΔG Prod - React	**-46.57**

Coordinates of Optimized Geometries

b3lyp-benzotriazole

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	-2.111938	-0.692378	0.000023
2	6	0	-2.090638	0.728310	0.000126
3	6	0	-0.903882	1.447910	0.000152
4	6	0	0.278807	0.689504	0.000073
5	6	0	0.271637	-0.721284	-0.000059
6	6	0	-0.941352	-1.435347	-0.000065
7	1	0	-3.070674	-1.201252	0.000031
8	1	0	-3.033965	1.265698	0.000161
9	1	0	-0.891492	2.532176	0.000184
10	1	0	-0.951217	-2.520292	-0.000175
11	7	0	1.579371	-1.163725	-0.000112
12	7	0	2.364430	-0.128100	-0.000082
13	7	0	1.608753	0.995353	-0.000054
14	1	0	2.063659	1.898678	0.000035

b3lyp-Ox-benzotriazole

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	-2.110787	-0.706035	0.000035
2	6	0	-2.132147	0.691377	0.000120
3	6	0	-0.946120	1.432068	0.000119
4	6	0	0.273605	0.686556	0.000031
5	6	0	0.297012	-0.727065	-0.000055
6	6	0	-0.878567	-1.452204	-0.000052
7	1	0	-3.044989	-1.256139	0.000032
8	1	0	-3.082718	1.211078	0.000189
9	1	0	-0.943929	2.515914	0.000188
10	1	0	-0.886809	-2.536572	-0.000124
11	7	0	1.626465	-1.136081	-0.000149
12	7	0	2.375164	-0.098273	-0.000095
13	7	0	1.562192	1.029668	0.000023
14	1	0	1.993725	1.950344	0.000077

wb97xd-benzotriazole

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	-2.104398	-0.690982	-0.000012
2	6	0	-2.082299	0.728023	0.000014
3	6	0	-0.901320	1.444135	0.000028
4	6	0	0.278676	0.684066	0.000010
5	6	0	0.271019	-0.717175	-0.000017

6	6	0	-0.939701	-1.431391	-0.000029
7	1	0	-3.063162	-1.198551	-0.000011
8	1	0	-3.025236	1.264959	0.000021
9	1	0	-0.886372	2.527645	0.000039
10	1	0	-0.949267	-2.515755	-0.000047
11	7	0	1.576040	-1.158040	-0.000005
12	7	0	2.352795	-0.126457	-0.000004
13	7	0	1.604573	0.988940	0.000018
14	1	0	2.058313	1.890549	-0.000026

wb97xd-Ox-benzotriazole

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	-2.101270	-0.706076	0.000029
2	6	0	-2.126155	0.688483	0.000049
3	6	0	-0.947877	1.427828	-0.000056
4	6	0	0.272648	0.682451	-0.000201
5	6	0	0.298101	-0.725612	-0.000131
6	6	0	-0.870085	-1.450850	0.000084
7	1	0	-3.033997	-1.257409	-0.000055
8	1	0	-3.078131	1.203947	0.000114
9	1	0	-0.944217	2.510915	-0.000037
10	1	0	-0.877691	-2.534528	0.000234
11	7	0	1.626038	-1.128435	-0.000307
12	7	0	2.362505	-0.092055	0.000401
13	7	0	1.554222	1.025457	0.000047
14	1	0	1.982515	1.944955	0.000122

b3lyp-diphenylallene

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	-3.539860	0.607837	-0.948127
2	6	0	-2.348696	0.475451	-0.212757
3	6	0	-2.313422	-0.447755	0.849717
4	6	0	-3.436357	-1.212270	1.163572
5	6	0	-4.618223	-1.072458	0.423908
6	6	0	-4.664821	-0.159192	-0.633214
7	1	0	-3.582472	1.316923	-1.770871
8	1	0	-1.401310	-0.561840	1.428757
9	1	0	-3.391459	-1.919535	1.986904
10	1	0	-5.491194	-1.669362	0.670767
11	1	0	-5.575589	-0.041903	-1.213413
12	6	0	-1.182200	1.307300	-0.578492
13	1	0	-1.334427	1.992209	-1.415089
14	6	0	0.000000	1.296672	-0.000046
15	6	0	1.182199	1.307340	0.578399
16	1	0	1.334427	1.992310	1.414947
17	6	0	2.348696	0.475466	0.212723
18	6	0	3.539858	0.607902	0.948087
19	6	0	2.313424	-0.447812	-0.849689
20	6	0	4.664819	-0.159149	0.633229

21	1	0	3.582469	1.317044	1.770782
22	6	0	3.436360	-1.212349	-1.163489
23	1	0	1.401313	-0.561936	-1.428723
24	6	0	4.618224	-1.072486	-0.423832
25	1	0	5.575587	-0.041821	1.213421
26	1	0	3.391463	-1.919669	-1.986773
27	1	0	5.491195	-1.669407	-0.670649

b3lyp-diphenylallene

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	-3.539860	0.607837	-0.948127
2	6	0	-2.348696	0.475451	-0.212757
3	6	0	-2.313422	-0.447755	0.849717
4	6	0	-3.436357	-1.212270	1.163572
5	6	0	-4.618223	-1.072458	0.423908
6	6	0	-4.664821	-0.159192	-0.633214
7	1	0	-3.582472	1.316923	-1.770871
8	1	0	-1.401310	-0.561840	1.428757
9	1	0	-3.391459	-1.919535	1.986904
10	1	0	-5.491194	-1.669362	0.670767
11	1	0	-5.575589	-0.041903	-1.213413
12	6	0	-1.182200	1.307300	-0.578492
13	1	0	-1.334427	1.992209	-1.415089
14	6	0	0.000000	1.296672	-0.000046
15	6	0	1.182199	1.307340	0.578399
16	1	0	1.334427	1.992310	1.414947
17	6	0	2.348696	0.475466	0.212723
18	6	0	3.539858	0.607902	0.948087
19	6	0	2.313424	-0.447812	-0.849689
20	6	0	4.664819	-0.159149	0.633229
21	1	0	3.582469	1.317044	1.770782
22	6	0	3.436360	-1.212349	-1.163489
23	1	0	1.401313	-0.561936	-1.428723
24	6	0	4.618224	-1.072486	-0.423832
25	1	0	5.575587	-0.041821	1.213421
26	1	0	3.391463	-1.919669	-1.986773
27	1	0	5.491195	-1.669407	-0.670649

wb97xd-diphenylallene

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	-3.515653	0.613054	0.916273
2	6	0	-2.308364	0.498029	0.216984
3	6	0	-2.214752	-0.443495	-0.817882
4	6	0	-3.303259	-1.245318	-1.143645
5	6	0	-4.504324	-1.122751	-0.441491
6	6	0	-4.606299	-0.191209	0.589665
7	1	0	-3.600869	1.337984	1.721299
8	1	0	-1.282449	-0.545302	-1.366665
9	1	0	-3.215340	-1.969954	-1.947263
10	1	0	-5.352346	-1.750043	-0.697274
11	1	0	-5.535211	-0.088439	1.141924
12	6	0	-1.170396	1.365724	0.592224
13	1	0	-1.331040	2.042937	1.431137
14	6	0	-0.000001	1.376174	-0.000009
15	6	0	1.170393	1.365716	-0.592243

16	1	0	1.331036	2.042916	-1.431167
17	6	0	2.308364	0.498028	-0.216990
18	6	0	3.515645	0.613030	-0.916296
19	6	0	2.214761	-0.443465	0.817905
20	6	0	4.606291	-0.191228	-0.589679
21	1	0	3.600854	1.337936	-1.721344
22	6	0	3.303269	-1.245282	1.143677
23	1	0	1.282464	-0.545252	1.366702
24	6	0	4.504326	-1.122739	0.441505
25	1	0	5.535198	-0.088477	-1.141951
26	1	0	3.215358	-1.969894	1.947318
27	1	0	5.352349	-1.750027	0.697296

wb97xd-diphenylallene

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	-3.515653	0.613054	0.916273
2	6	0	-2.308364	0.498029	0.216984
3	6	0	-2.214752	-0.443495	-0.817882
4	6	0	-3.303259	-1.245318	-1.143645
5	6	0	-4.504324	-1.122751	-0.441491
6	6	0	-4.606299	-0.191209	0.589665
7	1	0	-3.600869	1.337984	1.721299
8	1	0	-1.282449	-0.545302	-1.366665
9	1	0	-3.215340	-1.969954	-1.947263
10	1	0	-5.352346	-1.750043	-0.697274
11	1	0	-5.535211	-0.088439	1.141924
12	6	0	-1.170396	1.365724	0.592224
13	1	0	-1.331040	2.042937	1.431137
14	6	0	-0.000001	1.376174	-0.000009
15	6	0	1.170393	1.365716	-0.592243
16	1	0	1.331036	2.042916	-1.431167
17	6	0	2.308364	0.498028	-0.216990
18	6	0	3.515645	0.613030	-0.916296
19	6	0	2.214761	-0.443465	0.817905
20	6	0	4.606291	-0.191228	-0.589679
21	1	0	3.600854	1.337936	-1.721344
22	6	0	3.303269	-1.245282	1.143677
23	1	0	1.282464	-0.545252	1.366702
24	6	0	4.504326	-1.122739	0.441505
25	1	0	5.535198	-0.088477	-1.141951
26	1	0	3.215358	-1.969894	1.947318
27	1	0	5.352349	-1.750027	0.697296

b3lyp-Selectfluor-salt

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	-1.695147	1.126070	1.446350
2	6	0	-1.069663	1.817727	0.211306
3	6	0	0.045494	-0.347653	-0.188345
4	6	0	-0.278045	-0.896357	1.218439
5	1	0	-1.720196	1.688442	-0.653023
6	1	0	-0.887785	2.875964	0.385309
7	1	0	-2.504929	0.447451	1.180481
8	1	0	-0.783552	-0.506929	-0.877513
9	1	0	0.959850	-0.808430	-0.558600
10	1	0	0.569230	-1.404704	1.677456
11	1	0	-1.157231	-1.539397	1.193632
12	1	0	-2.021265	1.849865	2.191879
13	7	0	-0.617451	0.288149	2.078720
14	7	0	0.265442	1.161942	-0.103406

15	6	0	0.602486	1.111141	2.376661
16	1	0	0.271056	1.989071	2.929742
17	1	0	1.264028	0.507065	2.995884
18	6	0	1.253140	1.455329	1.016724
19	1	0	2.141008	0.856473	0.816547
20	1	0	1.509342	2.512483	0.976259
21	6	0	0.820159	1.601534	-1.449459
22	1	0	0.118481	1.275386	-2.214107
23	1	0	1.792418	1.125205	-1.561861
24	17	0	1.014175	3.365627	-1.566031
25	9	0	-1.116418	-0.195986	3.298831
26	5	0	3.732636	-1.584202	-0.392105
27	9	0	2.586174	-2.240538	0.122858
28	9	0	3.364364	-0.237349	-0.701233
29	9	0	4.751705	-1.574799	0.574034
30	9	0	4.167702	-2.226432	-1.561860
31	5	0	-3.791075	-1.160405	-0.913809
32	9	0	-2.900715	-0.209511	-1.490834
33	9	0	-5.085940	-0.621258	-0.864179
34	9	0	-3.774685	-2.341536	-1.670063
35	9	0	-3.337265	-1.432364	0.409419

b3lyp-Red-Selectfluor-salt

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	1.020201	2.927056	0.149463
2	6	0	1.204242	1.589368	0.928479
3	6	0	-0.136888	0.507954	-0.857562
4	6	0	-0.413727	1.895311	-1.511568
5	1	0	2.082267	1.040359	0.588832
6	1	0	1.256048	1.747287	2.003996
7	1	0	1.767977	3.032913	-0.636227
8	1	0	0.806325	0.077983	-1.194060
9	1	0	-0.956717	-0.190053	-1.030370
10	1	0	-1.415317	1.939484	-1.938638
11	1	0	0.316896	2.110227	-2.291181
12	1	0	1.086015	3.782870	0.820700
13	7	0	-0.304487	2.905422	-0.463879
14	7	0	-0.007361	0.703591	0.658014
15	6	0	-1.373818	2.796085	0.524108
16	1	0	-1.249090	3.587028	1.263342
17	1	0	-2.333563	2.924341	0.024069
18	6	0	-1.270116	1.384352	1.175245
19	1	0	-2.103940	0.734872	0.908876
20	1	0	-1.189326	1.444414	2.259426
21	6	0	0.158585	-0.677138	1.253094
22	1	0	1.042440	-1.133469	0.808691
23	1	0	-0.752245	-1.233354	1.038934
24	17	0	0.385435	-0.643559	3.028177
25	9	0	-0.546004	4.720612	-1.365101
26	5	0	-3.499012	-1.903127	-0.577375
27	9	0	-2.744493	-1.394851	-1.662463
28	9	0	-2.902172	-1.456366	0.636155
29	9	0	-4.820392	-1.422315	-0.649916
30	9	0	-3.492464	-3.310198	-0.609568
31	5	0	3.671916	-1.504480	-0.727210
32	9	0	2.834425	-2.167156	0.205931
33	9	0	4.945693	-1.304978	-0.161989
34	9	0	3.777280	-2.274538	-1.900449
35	9	0	3.090058	-0.244363	-1.038040

wb97xd-Selectfluor-salt

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	-1.494404	-1.107573	1.516803
2	6	0	-1.209093	0.396429	1.360793
3	6	0	-0.001748	-0.276351	-0.680740
4	6	0	0.035387	-1.761775	-0.293361
5	1	0	-2.021425	0.877130	0.818045
6	1	0	-1.070798	0.884891	2.323511
7	1	0	-2.262023	-1.455121	0.826185
8	1	0	-0.927568	-0.017756	-1.191324

9	1	0	0.862742	-0.027795	-1.295123
10	1	0	1.012953	-2.208236	-0.466908
11	1	0	-0.753146	-2.318721	-0.796757
12	1	0	-1.750986	-1.365139	2.542635
13	7	0	-0.231983	-1.829575	1.172600
14	7	0	0.064430	0.573907	0.571900
15	6	0	0.929830	-1.300611	1.947951
16	1	0	0.649610	-1.315497	2.999625
17	1	0	1.769392	-1.970795	1.771401
18	6	0	1.222904	0.116003	1.418999
19	1	0	2.115265	0.134148	0.797992
20	1	0	1.340108	0.813638	2.245945
21	6	0	0.243659	1.995916	0.102773
22	1	0	-0.586409	2.215142	-0.567028
23	1	0	1.203197	2.042886	-0.410502
24	17	0	0.232307	3.154329	1.436121
25	9	0	-0.396804	-3.159703	1.515894
26	5	0	3.759738	-0.115604	-1.107688
27	9	0	3.044447	-1.318415	-0.862951
28	9	0	2.822176	0.869759	-1.526460
29	9	0	4.349955	0.309159	0.095566
30	9	0	4.720922	-0.316206	-2.096535
31	5	0	-3.690101	0.089387	-1.157490
32	9	0	-2.779493	1.165719	-1.345821
33	9	0	-4.193673	0.154652	0.156763
34	9	0	-4.718763	0.157065	-2.093042
35	9	0	-2.967062	-1.124678	-1.303043

wb97xd-Red-Selectfluor-salt

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	1.243670	2.284101	0.675129
2	6	0	1.194873	0.894989	1.356448
3	6	0	0.063983	0.188953	-0.719776
4	6	0	-0.170500	1.648656	-1.171851
5	1	0	2.087075	0.308253	1.141566
6	1	0	1.050024	0.970696	2.433055
7	1	0	2.036913	2.326955	-0.070257
8	1	0	1.047638	-0.178121	-1.008071
9	1	0	-0.711774	-0.475802	-1.097529
10	1	0	-1.171260	1.777915	-1.581997
11	1	0	0.570431	1.947946	-1.912210
12	1	0	1.393154	3.073851	1.410137
13	7	0	-0.034716	2.484458	0.009730
14	7	0	0.005145	0.143170	0.799160
15	6	0	-1.160466	2.327334	0.916869
16	1	0	-0.982650	2.935134	1.803463
17	1	0	-2.068556	2.671903	0.423538
18	6	0	-1.264637	0.820605	1.261852
19	1	0	-2.092886	0.337198	0.746542
20	1	0	-1.358163	0.659153	2.334450
21	6	0	0.030089	-1.309123	1.173222
22	1	0	0.941497	-1.734650	0.755343
23	1	0	-0.866787	-1.767944	0.759525
24	17	0	0.049266	-1.564290	2.929332
25	9	0	-0.065707	4.394658	-0.605357
26	5	0	-3.555455	-1.065225	-0.938014
27	9	0	-3.102392	0.171418	-1.456280
28	9	0	-2.434410	-1.925862	-0.794352
29	9	0	-4.126823	-0.848951	0.331093
30	9	0	-4.489300	-1.640749	-1.806281
31	5	0	3.564709	-1.024254	-0.957547
32	9	0	3.084679	-1.548832	0.272984
33	9	0	4.904265	-1.386349	-1.137634
34	9	0	2.770140	-1.526626	-2.005583
35	9	0	3.440267	0.384778	-0.917701

b3lyp-Selectfluor-dication

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	-1.266314	-0.670795	1.301483

2	6	0	0.267227	-0.514456	1.174302
3	6	0	-0.284817	1.656799	0.127330
4	6	0	-1.762296	1.285849	-0.132908
5	1	0	0.681595	-0.071083	2.078685
6	1	0	0.759780	-1.465781	0.985629
7	1	0	-1.698540	-0.054950	2.088001
8	1	0	-0.134536	2.050460	1.131451
9	1	0	0.054678	2.390977	-0.602284
10	1	0	-2.101520	1.547143	-1.134260
11	1	0	-2.423234	1.726618	0.612221
12	1	0	-1.552987	-1.711712	1.444355
13	7	0	-1.862177	-0.208555	-0.000426
14	7	0	0.578220	0.403615	-0.001761
15	6	0	-1.211756	-0.899096	-1.167556
16	1	0	-1.221076	-1.967717	-0.957911
17	1	0	-1.813196	-0.690410	-2.051120
18	6	0	0.212063	-0.311677	-1.295863
19	1	0	0.283381	0.418012	-2.102057
20	1	0	0.936073	-1.107347	-1.463395
21	6	0	2.035552	0.850044	-0.012612
22	1	0	2.198435	1.459355	0.873707
23	1	0	2.188808	1.425508	-0.922562
24	17	0	3.168698	-0.514571	0.004075
25	9	0	-3.219532	-0.549643	0.000057

b3lyp-Red-Selectfluor-dication

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	1.240710	-0.690645	-1.237588
2	6	0	-0.301465	-0.467899	-1.211874
3	6	0	0.184028	1.685344	-0.069522
4	6	0	1.691018	1.309320	0.056637
5	1	0	-0.654925	0.056321	-2.099587
6	1	0	-0.849616	-1.402120	-1.104060
7	1	0	1.702646	-0.176587	-2.079949
8	1	0	-0.043943	2.161474	-1.022880
9	1	0	-0.142553	2.330637	0.745999
10	1	0	2.106917	1.654561	1.002863
11	1	0	2.266224	1.737150	-0.764111
12	1	0	1.477503	-1.752845	-1.295566
13	7	0	1.786453	-0.145969	0.002237
14	7	0	-0.645784	0.398776	-0.001856
15	6	0	1.215217	-0.782901	1.185494
16	1	0	1.309101	-1.863317	1.081776
17	1	0	1.767822	-0.460816	2.067888
18	6	0	-0.277972	-0.348771	1.278323
19	1	0	-0.459382	0.337087	2.105974
20	1	0	-0.945200	-1.204329	1.364547
21	6	0	-2.101301	0.810887	-0.004234
22	1	0	-2.281098	1.395859	-0.903941
23	1	0	-2.281181	1.400195	0.891850
24	17	0	-3.222256	-0.574952	0.001557
25	9	0	3.768881	-0.588973	-0.000374

wb97xd-Selectfluor-dication

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	-1.192429	-0.910597	-1.145204
2	6	0	0.208038	-0.291699	-1.292028
3	6	0	0.266669	-0.524317	1.153958
4	6	0	-1.260826	-0.648680	1.300087
5	1	0	0.943887	-1.070139	-1.486207
6	1	0	0.251252	0.450357	-2.088927
7	1	0	-1.170167	-1.973047	-0.905789
8	1	0	0.732968	-1.482925	0.935990
9	1	0	0.702187	-0.112798	2.063240
10	1	0	-1.674652	-0.009787	2.077792
11	1	0	-1.561795	-1.680875	1.469592
12	1	0	-1.800084	-0.742921	-2.032330
13	7	0	-1.852814	-0.209053	-0.000792
14	7	0	0.574154	0.403659	-0.000565
15	6	0	-1.748080	1.274867	-0.151338
16	1	0	-2.060070	1.524108	-1.164417
17	1	0	-2.424580	1.728945	0.570710
18	6	0	-0.283607	1.643971	0.141453
19	1	0	-0.151120	2.019379	1.155194
20	1	0	0.063183	2.394722	-0.567333
21	6	0	2.019593	0.846929	-0.008706
22	1	0	2.183702	1.454901	0.878672
23	1	0	2.174727	1.427550	-0.915443
24	17	0	3.141265	-0.512477	0.003434
25	9	0	-3.190720	-0.546717	-0.003216

wb97xd-Red-Selectfluor-dication

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	1.235038	-0.647328	-1.251183
2	6	0	-0.305865	-0.504564	-1.174553
3	6	0	0.186932	1.666350	-0.117550
4	6	0	1.675889	1.299913	0.099577
5	1	0	-0.720427	-0.050561	-2.074425
6	1	0	-0.796587	-1.459914	-0.996256
7	1	0	1.654625	-0.064784	-2.070154
8	1	0	0.003090	2.072670	-1.111967
9	1	0	-0.170379	2.372361	0.631853
10	1	0	2.028611	1.611777	1.081904
11	1	0	2.300884	1.758663	-0.665479
12	1	0	1.519301	-1.691371	-1.375838
13	7	0	1.777954	-0.146966	0.001916
14	7	0	-0.638852	0.395379	-0.000250
15	6	0	1.195685	-0.813613	1.155951
16	1	0	1.238558	-1.890159	0.996441
17	1	0	1.772141	-0.563843	2.045880
18	6	0	-0.263111	-0.310028	1.287740
19	1	0	-0.380136	0.416373	2.092165
20	1	0	-0.962042	-1.131335	1.438260
21	6	0	-2.082682	0.808267	0.001865
22	1	0	-2.262340	1.402891	-0.891724
23	1	0	-2.258742	1.394180	0.901453

24	17	0	-3.194761	-0.567886	-0.000770
25	9	0	3.724371	-0.583973	-0.001307

b3lyp-Red-Selectfluor-defluorinated

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	1.558026	-0.920371	-1.251767
2	6	0	0.027088	-0.542534	-1.206525
3	6	0	0.742680	1.556735	-0.076515
4	6	0	2.219410	1.024360	0.069102
5	1	0	-0.258424	-0.003913	-2.108897
6	1	0	-0.593562	-1.427614	-1.086774
7	1	0	2.064416	-0.434092	-2.083832
8	1	0	0.590543	2.045871	-1.037356
9	1	0	0.504606	2.241829	0.735920
10	1	0	2.657018	1.312257	1.023483
11	1	0	2.833509	1.380767	-0.757537
12	1	0	1.681638	-2.001819	-1.305007
13	7	0	2.079408	-0.417491	0.003853
14	7	0	-0.214155	0.365564	-0.002112
15	6	0	1.510219	-1.032528	1.187744
16	1	0	1.472404	-2.112637	1.058666
17	1	0	2.095116	-0.769695	2.069190
18	6	0	0.064431	-0.410670	1.282157
19	1	0	-0.016646	0.287279	2.113540
20	1	0	-0.681750	-1.196740	1.379217
21	6	0	-1.631291	0.932996	-0.004870
22	1	0	-1.741526	1.534313	-0.904380
23	1	0	-1.741640	1.540118	0.890786
24	17	0	-2.874462	-0.334139	0.000284

wb97xd-Red-Selectfluor-defluorinated

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	1.547965	-0.908197	-1.250529
2	6	0	0.018515	-0.568119	-1.179273
3	6	0	0.739170	1.541905	-0.113264
4	6	0	2.202856	1.017603	0.083820
5	1	0	-0.302766	-0.069012	-2.092082
6	1	0	-0.577351	-1.463816	-1.017490
7	1	0	2.037712	-0.395754	-2.076451
8	1	0	0.606193	1.992982	-1.095318
9	1	0	0.489364	2.263436	0.663059
10	1	0	2.605366	1.296952	1.055033
11	1	0	2.846439	1.379205	-0.716818
12	1	0	1.693863	-1.985418	-1.323640
13	7	0	2.063301	-0.417300	0.005720
14	7	0	-0.212122	0.364033	-0.005822
15	6	0	1.489514	-1.034150	1.178528
16	1	0	1.424165	-2.110115	1.033851
17	1	0	2.085340	-0.800148	2.059970
18	6	0	0.071738	-0.374836	1.286031

19	1	0	0.026576	0.349500	2.097649
20	1	0	-0.690425	-1.138704	1.426490
21	6	0	-1.617087	0.928501	-0.011580
22	1	0	-1.729374	1.525906	-0.913940
23	1	0	-1.726575	1.543380	0.879219
24	17	0	-2.850753	-0.331281	0.003458

wb97xd-Red-Selectfluor-defluorinated

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	1.547965	-0.908197	-1.250529
2	6	0	0.018515	-0.568119	-1.179273
3	6	0	0.739170	1.541905	-0.113264
4	6	0	2.202856	1.017603	0.083820
5	1	0	-0.302766	-0.069012	-2.092082
6	1	0	-0.577351	-1.463816	-1.017490
7	1	0	2.037712	-0.395754	-2.076451
8	1	0	0.606193	1.992982	-1.095318
9	1	0	0.489364	2.263436	0.663059
10	1	0	2.605366	1.296952	1.055033
11	1	0	2.846439	1.379205	-0.716818
12	1	0	1.693863	-1.985418	-1.323640
13	7	0	2.063301	-0.417300	0.005720
14	7	0	-0.212122	0.364033	-0.005822
15	6	0	1.489514	-1.034150	1.178528
16	1	0	1.424165	-2.110115	1.033851
17	1	0	2.085340	-0.800148	2.059970
18	6	0	0.071738	-0.374836	1.286031
19	1	0	0.026576	0.349500	2.097649
20	1	0	-0.690425	-1.138704	1.426490
21	6	0	-1.617087	0.928501	-0.011580
22	1	0	-1.729374	1.525906	-0.913940
23	1	0	-1.726575	1.543380	0.879219
24	17	0	-2.850753	-0.331281	0.003458

wb97xd-diphenylallene-F (DPA-F)

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	2.919794	0.029644	-0.672842
2	6	0	1.764518	0.433477	0.033915
3	6	0	1.208335	-0.432478	1.003126
4	6	0	1.765077	-1.678184	1.215611
5	6	0	2.873494	-2.088405	0.463491
6	6	0	3.452013	-1.235050	-0.476480
7	1	0	3.371977	0.707197	-1.389998
8	1	0	0.367432	-0.109138	1.605605
9	1	0	1.348646	-2.335103	1.970606
10	1	0	3.299493	-3.072057	0.630566
11	1	0	4.322253	-1.551307	-1.039784
12	6	0	1.255002	1.740408	-0.234064
13	1	0	1.973832	2.461395	-0.620491
14	6	0	-0.000004	2.287842	0.000000
15	6	0	-1.255009	1.740409	0.234064
16	1	0	-1.973841	2.461396	0.620489

17	6	0	-1.764522	0.433476	-0.033916
18	6	0	-2.919796	0.029638	0.672842
19	6	0	-1.208336	-0.432475	-1.003128
20	6	0	-3.452008	-1.235059	0.476481
21	1	0	-3.371982	0.707189	1.389998
22	6	0	-1.765072	-1.678185	-1.215612
23	1	0	-0.367436	-0.109131	-1.605607
24	6	0	-2.873486	-2.088412	-0.463490
25	1	0	-4.322246	-1.551320	1.039785
26	1	0	-1.348639	-2.335102	-1.970608
27	1	0	-3.299479	-3.072066	-0.630564
28	9	0	-0.000002	3.648685	0.000002

b3lyp-diphenylallene-F-benzotriazole (DPA-F-BN)

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z
1	6	0	-2.337287	2.124134	-0.858047
2	6	0	-1.050921	1.801804	-0.399708
3	6	0	-0.404327	2.675857	0.481881
4	6	0	-1.036573	3.849640	0.906342
5	6	0	-2.319396	4.162246	0.451640
6	6	0	-2.967826	3.295378	-0.434841
7	1	0	-2.849348	1.459553	-1.547932
8	1	0	0.594394	2.451534	0.841659
9	1	0	-0.522903	4.515529	1.593304
10	1	0	-2.810158	5.072574	0.782635
11	1	0	-3.963620	3.530630	-0.798524
12	6	0	-0.357089	0.547257	-0.942617
13	1	0	-0.123909	0.710415	-1.998591
14	6	0	0.940500	0.184806	-0.270167
15	6	0	2.151112	0.173557	-0.841211
16	1	0	2.152386	0.462423	-1.888786
17	6	0	3.466879	-0.154607	-0.278961
18	6	0	4.584833	-0.034523	-1.130631
19	6	0	3.684165	-0.581576	1.048608
20	6	0	5.871898	-0.326096	-0.678773
21	1	0	4.437770	0.291771	-2.156691
22	6	0	4.973389	-0.872745	1.496674
23	1	0	2.849175	-0.687626	1.729185
24	6	0	6.072242	-0.747168	0.639567
25	1	0	6.715734	-0.225061	-1.354882
26	1	0	5.119512	-1.200529	2.521830
27	1	0	7.072370	-0.975745	0.995531
28	6	0	-3.810242	-2.818978	1.383700
29	6	0	-3.213441	-1.698673	2.020291
30	6	0	-2.330247	-0.856481	1.359697
31	6	0	-2.053634	-1.171169	0.017118
32	6	0	-2.643701	-2.280948	-0.623713
33	6	0	-3.537093	-3.125988	0.060167
34	1	0	-4.493293	-3.442971	1.951270
35	1	0	-3.456405	-1.495520	3.058748
36	1	0	-1.878370	-0.007281	1.856877
37	1	0	-3.987789	-3.978795	-0.436683
38	7	0	-2.190260	-2.326566	-1.925392
39	7	0	-1.377759	-1.333714	-2.110799
40	7	0	-1.272467	-0.609591	-0.961859
41	9	0	0.769821	-0.162907	1.043922