Advanced Synthesis & Catalysis

Supporting Information

A Metal-Free Synthesis of *N*-Aryl Oxazolidin-2-Ones by the One-Pot Reaction of Carbon Dioxide with *N*-Aryl Aziridines

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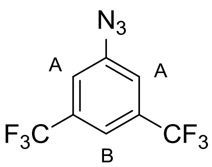
1. General methods

Unless otherwise specified, all the reactions were carried out under nitrogen atmosphere employing standard Schlenk techniques and magnetic stirring. THF and benzene were distilled over sodium and benzophenone and kept under nitrogen. Styrene and α-methyl styrene were distilled over calcium hydride and kept under nitrogen. *Meso*-tetraphenylporphyrin ($TPPH_2$) was synthesized following Lindsey's procedure.[1] All the other starting materials were commercial products used as received. NMR spectra were recorded at room temperature either on a Bruker Avance 300-DRX, operating at 300 MHz for ^{1}H, at 75 MHz for ^{13}C and at 282 MHz for ^{19}F or on a Bruker Avance 400-DRX spectrometers, operating at 400 MHz for ^{1}H and at 100 MHz for ^{13}C and at 376 MHz for ^{19}F. Chemical shifts (ppm) are reported relative to TMS. The ^{1}H NMR signals of the compounds described in the following were attributed by 2D NMR techniques. Assignments of the resonances in ^{13}C NMR were made by using the APT pulse sequence, HSQC and HMBC techniques. Infrared spectra were recorded on a Varian Scimitar FTS 1000 spectrophotometer. UV/Vis spectra were recorded on an Agilent 8453E instrument. Elemental analyses, mass spectra and melting points were recorded in the analytical laboratories of Milan University.

2. Synthesis of aryl azides

General procedure: all the reactions were performed in air. The desired aniline (99.8 mmol) was dissolved in a water solution of HCl 18.5% (100 mL). The so-obtained mixture was cooled to 0°C in an ice bath and 25 mL of a sodium nitrite (104.0 mmol) water solution were added dropwise. The reaction mixture was stirred for 2 hours and then urea (11.0 mmol) was added in one portion. 30 mL of a sodium azide (103.0 mmol) water solution were added dropwise in about 30 minutes, under vigorous stirring. The reaction was stirred for 30 minutes at 0°C and for additional 3 hours at room temperature. The aqueous phase was extracted by diethyl ether (3 x 50 mL) and the so-obtained organic phase was dried over Na_2SO_4, filtered and the solvent was removed under reduced pressure.

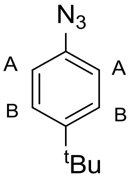
2.1 Synthesis of 3,5-*bis*-(trifluoromethyl) phenylazide



3,5-*Bis*-(trifluoromethyl)aniline was used as starting material and the product was obtained as an orange oil (21.13 g, 83% yield). The collected analytical data were in accordance with those reported in literature.[2]

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.64 (s, 1H, H_B), 7.44 ppm (s, 2H, H_A).

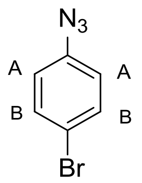
2.2 Synthesis of 4-*tert*-butylphenylazide



4-*Tert*-butyl phenylaniline was used as starting material and the product was obtained as a red oil (16.01 g, 92% yield). The collected analytical data were in accordance with those reported in literature.[2]

^{1}H NMR: (300 MHz, $CDCl_3$): δ 7.37 (d, *J* = 7.2, Hz 2H, H_B), 6.98 (d, *J* = 7.2 Hz, 2H, H_A), 1.32 ppm (s, 9H, H_{tBu}).

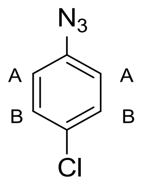
2.3 Synthesis of 4-bromophenylazide



4-Bromophenyl aniline was used as starting material and the product was obtained as a pale brown solid (16.41 g, 83% yield). The collected analytical data were in accordance with those reported in literature.[3]

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46 (d, J = 8.8 Hz, 2H, H_B), 6.90 ppm (d, J = 8.8 Hz, 2H, H_A).

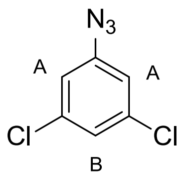
2.4 Synthesis of 4-chlorophenylazide



4-Chlorophenyl aniline was used as starting material and the product was obtained as an opalescent yellow oil (13.49 g, 88% yield). The collected analytical data were in accordance with those reported in literature.[3]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, J = 8.7 Hz, 2H, H_B), 6.96 ppm (d, J = 8.7 Hz, 2H, H_A).

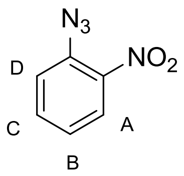
2.5 Synthesis of 3,5-dichlorophenylazide



3,5-Dichlorophenyl aniline was used as starting material and the product was obtained as a light brown solid (16.52 g, 88% yield). The collected analytical data were in accordance with those reported in literature.[4]

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.13 (s, 1H, H_B), 6.91 ppm (s, 2H, H_A).

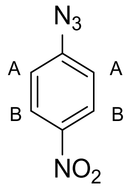
2.6 Synthesis of 2-nitrophenylazide



2-Nitrophenyl aniline was used as starting material and the product was obtained as a yellow powder (13.76 g, 84% yield). The collected analytical data were in accordance with those reported in literature.[2]

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 - 7.84 (m, 1H, H_A), 7.63 (pst, J = 7.8 Hz, 1H, H_C), 7.40 - 7.25 (m, 1H, H_D), 7.26 ppm (pst, J = 7.8 Hz, 1H, H_B).

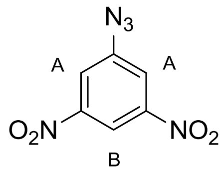
2.7 Synthesis of 4-nitrophenylazide



4-Nitrophenyl aniline was used as starting material and the product was obtained as a yellow powder (14.25 g, 87% yield). The collected analytical data were in accordance with those reported in literature.[2]

^{1}H NMR (300 MHz, C_6D_6) δ 7.62 (d, *J* = 9.1 Hz, 2H, H_B), 6.15 ppm (d, *J* = 9.1 Hz, 2H, H_A).

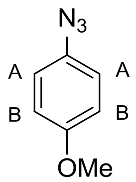
2.8 Synthesis of 3,5-dinitrophenylazide



3,5-Dinitrophenyl aniline was used as starting material and the product was obtained as a yellow powder (18.58 g, 89% yield). The collected analytical data were in accordance with those reported in literature.[5]

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.80 (s, 1H, H_B), 8.19 ppm (s, 2H, H_A).

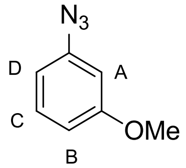
2.9 Synthesis of 4-methoxyphenylazide



4-Methoxyphenyl aniline was used as starting material and the product was obtained as a dark red oil (10.12 g, 68% yield). The collected analytical data were in accordance with those reported in literature.[2]

^{1}H NMR (400 MHz, C_6D_6) δ 6.80 (d, *J* = 8.5 Hz, 2H, H_B), 6.68 (d, *J* = 8.5 Hz, 2H, H_A), 3.35 ppm (s, 3H, H_{OMe}).

2.10 Synthesis of 3-methoxyphenylazide



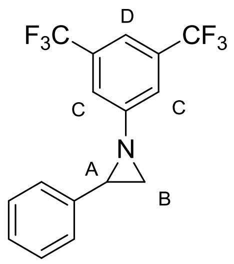
3-Methoxyphenyl aniline was used as starting material and the product was obtained as a red oil (9.23 g, 62 % yield). The collected analytical data were in accordance with those reported in literature.[6]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (pst, *J* = 8.1 Hz, 1H, H_C), 6.78 - 6.64 (m, 2H, H_{B+D}), 6.61 - 6.55 (m, 1H, H_A), 3.83 ppm (s, 3H, H_{OMe}).

3. Synthesis of *N*-aryl aziridines

General procedure: In a Schlenk flask Ru(TPP)(CO) (0.25 g, 3.37 x 10^{-2} mmol), the desired styrene (8.40 mmol) and aryl azide (1.68 mmol) were refluxed in benzene (50 mL). The reaction mixture was dried *in vacuo* and purified by flash-chromatography (silica gel, *n*- hexane/ethyl acetate 9:1, 0.5% of triethylamine was added in order to deactivate the silica).

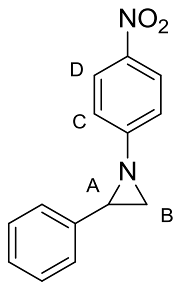
3.1 Synthesis of 1-(3,5-*bis*-trifluoromethylphenyl)-2-phenylaziridine (1)



3,5-*Bis*-trifluoromethylphenylazide and styrene were refluxed for 1 hour. The product was obtained as a purple-brown solid (0.55 g, 99 % yield). The collected analytical data were in accordance with those reported in literature.[5]

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.49 (s, 1H, H_D), 7.44 (s, 2H, H_C), 7.39 - 7.36 (m, 5H, H_{Ph}), 3.24 (dd, *J* = 6.6, 3.3 Hz, 1H, H_A), 2.57 (d, *J* = 6.6 Hz, 1H, H_B), 2.54 ppm (d, *J* = 3.3 Hz, 1H, $H_{B'}$).

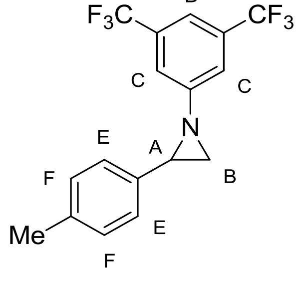
3.2 Synthesis of 1-(4-nitrophenyl)-2-phenyilaziridine (3)



4-Nitrophenylazide and styrene were refluxed for 1 hour. The product was obtained as a yellow oil (0.38 g, 93% yield). The collected analytical data were in accordance with those reported in literature [5]

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 9.0 Hz, 2H, H_D), 7.40 - 7.32 (m, 5H, H_{Ph}), 7.10 (d, *J* = 9.0 Hz, 2H, H_C), 3.25 (dd, *J* = 6.4, 2.6 Hz, 1H, H_A), 2.58 (d, *J* = 6.4 Hz, 1H, H_B), 2.55 ppm(d, *J* = 2.6 Hz, 1H, $H_{B'}$).

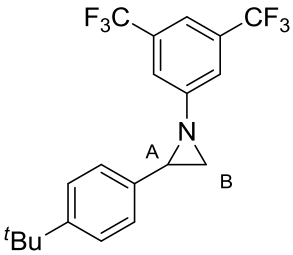
3.3 Synthesis of 1-(3,5-*bis*-(trifluoromethyl)phenyl)-2-(4-methylphenyl) aziridine (5)



3,5-*Bis*-trifluoromethylphenylazide and 4-methylstyrene were refluxed for 4 hours. The product was obtained as a purple-brown solid (0.58 g, 98% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.49 (s, 1H, H_D), 7.44 (s, 2H, H_C), 7.29 (d, *J* = 8.0 Hz, 2H, H_F), 7.21 (d, *J* = 8.0 Hz, 2H, H_E), 3.21 (dd, *J* = 6.4, 3.6 Hz, 1H, H_A), 2.55 (d, *J* = 6.4 Hz, 1H, H_B), 2.53 (d, *J* = 3.6 Hz, 1H, $H_{B'}$), 2.39 ppm (s, 3H, H_{Me}). ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.28 (C), 138.12 (C), 135.24 (C), 132.82 (q, *J* = 33.3 Hz, two overlapping CF_3), 129.75 (two overlapping CH), 126.42 (two overlapping CH), 125.42 (C), 121.81 (C), 121.05 (two overlapping CH), 116.30, (CH), 42.35 (CH), 38.27 (CH_2), 21.51 ppm (CH_3). ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.32 ppm (s). LR-MS (ESI): m/z ($C_{17}H_{13}F_6N$) calcd 345.10, found $[M+H]^+$ 346.25. Elemental Analysis calcd. for $C_{17}H_{13}F_6N$: C (59.13), H (3.79), N (4.06), found: C (58.83), H (3.55), N (4.14). UV-Vis λ_{max} (DCM)/nm (log ε): 248 (4.35). IR ν_{max} (DCM)/cm^{-1}: 1004, 1136, 1179, 1244, 1391, 1465, 1613, 3685. M.P.: 66-67 °C

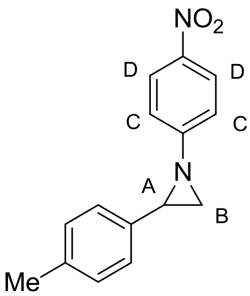
3.4 Synthesis of 1-(3,5-*bis*-(trifluoromethyl)phenyl)-2-(4-*tert*-butylphenyl) aziridine (7)



3,5-*Bis*-trifluoromethylphenylazide and 4-*tert*-butyl styrene were refluxed for 4 hours. The product was obtained as a brown oil (0.62 g, 95% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 - 7.32 (m, 7H, H_{Ar}), 3.23 (dd, *J* = 6.0, 3.2 Hz, 1H, H_A), 2.57 - 2.55 (m, 2H, H_B), 1.36 ppm (s, 9H, H_{tBu}). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.90 (C), 151.08 (C), 134.84 (C), 132.41 (q, *J* = 33.3 Hz, two overlapping CF_3), 126.87 (CH), 125.73 (CH), 124.58 (C), 121.87 (C), 120.70 (CH), 115.90 (CH), 112.97 (C), 112.35 (CH), 41.88 (CH), 37.88 (CH_2), 34.60 (C), 31.33 ppm (three overlapping CH_3). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.98 ppm (s). LR-MS (ESI): m/z ($C_{20}H_{19}F_6N$) calcd 387.14, found $[M+H]^+$ 388.27. Elemental Analysis calcd. for ($C_{20}H_{19}F_6N$): C (62.01), H (4.94), N (3.62), found: C (62.27), H (5.33), N (3.54). UV-Vis λ_{max} (DCM)/nm (log ε): 249 (4.26). IR ν_{max} (DCM)/cm^{-1}: 947, 1002, 1135, 1180, 1376, 1391, 1466, 1614, 1616.

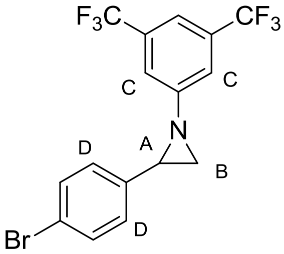
3.5 Synthesis of 1-(4-nitrophenyl)-2-(4-methylphenyl) aziridine (9)



4-Nitrophenylazide and 4-methyl styrene were refluxed for 2 hours. The product was obtained as a yellow powder (0.38 g, 90% yield). The collected analytical data were in accordance with those reported in literature.[5]

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.14 (d, *J* = 9.0 Hz, 2H, H_D), 7.26 - 7.20 (m, 4H, H_{Ar}), 7.09 (d, *J* = 9.0 Hz, 2H, H_C), 3.21 (dd, *J* = 6.3, 3.3 Hz, 1H, H_A), 2.56 - 2.52 (m, 2H, H_B), 2.37 ppm (s, 3H, H_{Me}).

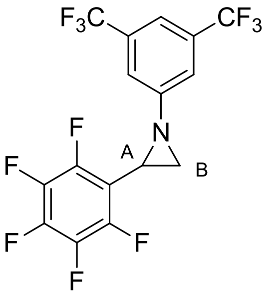
3.6 Synthesis of 1-(3,5-*bis*-(trifluoromethyl)phenyl)-2-(4-bromophenyl) aziridine (11)



3,5-*Bis*-trifluoromethylphenylazide and 4-bromostyrene were refluxed for 3 hours. The product was obtained as a brown oil. (0.53 g, 77% yield). The collected analytical data were in accordance with those reported in literature.[7]

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52-7.49 (m, 3H, H_{Ar}), 7.41 (s, 2H, H_C), 7.27 - 7.25 (m, 2H, H_D), 3.19 (dd, *J* = 4.8, 2.6 Hz, 1H, H_A) 2.56 (dd, *J* = 4.8, 0.6 Hz, 1H, H_B), 2.48 ppm (dd, *J* = 2.6, 0.6 Hz, 1H, $H_{B'}$).

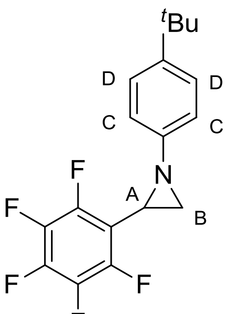
3.7 Synthesis of 1-(3,5-*bis*-(trifluoromethyl)phenyl)-2-(2,3,4,5,6-pentafluorophenyl) aziridine (13)



3,5-*Bis*-trifluoromethylphenylazide and 2,3,4,5,6-pentafluoro styrene were refluxed for 4 hours. The product was obtained as a purple-brown solid (0.69 g, 97% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 (s, 3H, H_{Ar}), 3.29 (dd, *J* = 6.3, 3.6 Hz, 1H, H_A), 2.96 (d, *J* = 3.6 Hz, 1H, H_B), 2.63 ppm (d, *J* = 6.6 Hz, 1H, $H_{B'}$). ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.05 (C), 148.13 (m, C-F), 144.83 (m, C-F), 143.29 (m, C-F), 139.90 (m, C- F), 136.39 (m, C-F), 133.10 (q, *J* = 33.4 Hz, two overlapping CF_3), 128.88 (C), 125.27 (C), 121.65 (C), 121.10 (CH), 117.23 (CH), 34.36 (CH), 32.81 ppm (CH_2). ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.49 (s, 6F, F_{CF3}), -143.14 (d, *J* = 20.3 Hz, 2F, F_o), -153.88 - -154.06 (m, 1F, F_p), -161.86 - -162.01 (m, 2F, F_m). LR-MS (ESI): m/z ($C_{16}H_6F_{11}N$) calcd 421.03, found $[M+H]^+$ 422.25. Elemental Analysis calcd. for ($C_{16}H_6F_{11}N$): C (45.62), H (1.44), N (3.33), found: C (45.44), H (1.68), N (3.42). UV-Vis λ_{max} (DCM)/nm (log ε): 248 (4.35). IR ν_{max} (DCM)/cm^{-1}: 1138, 1182, 1395,1465, 1502, 1525,1607, 3599, 3685. M.P.: 96-97 °C

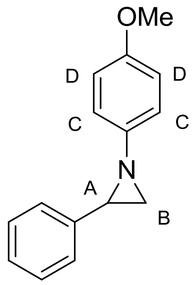
3.8 Synthesis of 1-(4-*tert*-butylphenyl)-2-(2,3,4,5,6-pentafluorophenyl) aziridine (15)



4-*Tert*-butylphenylazide and 2,3,4,5,6-pentafluoro styrene were refluxed for 24 hours. The product was obtained as a brown oil (0.33 g, 57% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32 (d, *J* = 8.7 Hz, 2H, H_D), 7.08 (d, *J* = 8.7 Hz, 2H, H_C), 3.13 (dd, *J* = 6.3 , 3.3 Hz, 1H, H_A), 2.80 (d, *J* = 3.3 Hz, 1H, H_B), 2.49 (d, *J* = 6.3 Hz, 1H, $H_{B'}$), 1.31 ppm (s, 9H, H_{tBu}). ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.15 (C), 148.25 (m, C-F), 146.55 (C), 144.79 (m, C-F), 142.83 (m, C-F), 139.47 (m, C-F), 136.28 (m, C-F), 126.42 (CH), 126.37 (CH) 122.83 (CH) 120.50 (CH), 34.67 (C), 34.10 (CH_2), 32.27 (CH), 31.82 ppm (three overlapping CH_3). One quaternary carbon was not detected. ^{19}F NMR (282 MHz, $CDCl_3$) δ -143.02 (dd, *J* = 22.1, 8.0 Hz, 2F, F_o), -155.20 - -155.35 (m, 1F, F_p), - 162.62 - -162.72 ppm (m, $2F_m$). LR-MS (ESI): m/z ($C_{18}H_{16}F_5N$) calcd 341.12, found $[M+H]^+$ 342.05. Elemental Analysis calcd. for ($C_{18}H_{16}F_5N$): C (63.34), H (4.72), N (4.10), found: C (62.97), H (4.76), N (4.08). UV-Vis λ_{max} (DCM)/nm (log ε): 233 (3.14). IR ν_{max} (DCM)/cm^{-1}: 909, 915, 920, 1244, 1500, 1523, 1606, 3686.

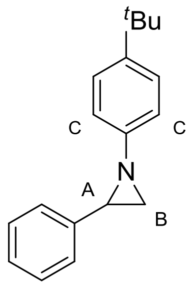
3.9 Synthesis of 1-(4-methoxyphenyl)-2-phenylaziridine (17)



4-Methoxyphenylazide and styrene were refluxed for 6 hours. The product was obtained as an orange oil (0.28 g, 65% yield). The collected analytical data were in accordance with those reported in literature.[5]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 - 7.28 (m, 5H, H_{Ph}), 6.95 (d, *J* = 8.8 Hz, 2H, H_D), 6.77 (d, *J* = 8.8 Hz, 2H, H_C), 3.73 (s, 3H, H_{OMe}), 3.01 – 2.98 (m, 1H, H_A), 2.37 (d, *J* = 6.3 Hz, 1H, H_B), 2.33 ppm (d, *J* = 2.4 Hz, 1H, $H_{B'}$).

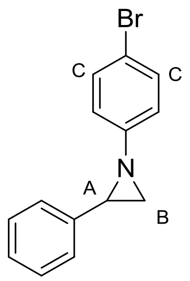
3.10 Synthesis of 1-(4-*tert*-butylphenyl)-2-phenylaziridine (19)



4-*tert*-butylphenylazide and styrene were refluxed for 4 hours. The product was obtained as a brown oil (0.36 g, 84% yield). The collected analytical data were in accordance with those reported in literature.[5]

^{1}H NMR: (400 MHz, $CDCl_3$) δ 7.43 - 7.30 (m, 7H, H_{Ar}), 7.03 (d, *J* = 8.4 Hz, 2H, H_C) 3.12 (dd, *J* = 8.8, 4.4 Hz, 1H, H_A), 2.48 (d, *J* = 8.8 Hz, 1H, H_B), 2.41 (d, *J* = 4.4 Hz, 1H, $H_{B'}$), 1.35 ppm (s, 9H, H_{tBu}).

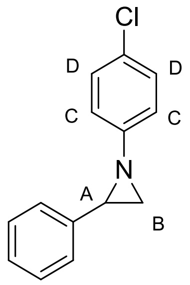
3.11 Synthesis of 1-(4-bromophenyl)-2-phenylaziridine (21)



4-Bromophenylazide and styrene were refluxed for 3 hours. The product was obtained as a light brown solid (0.41 g, 97% yield). The collected analytical data were in accordance with those reported in literature.[5]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 - 7.32 (m, 7H, H_{Ar}), 6.91 (d, J = 11.2 Hz, 2H, H_C), 3.07 (dd, J = 8.0, 4.4 Hz, 1H, H_A), 2.42 - 2.40 ppm (m, 2H, H_B).

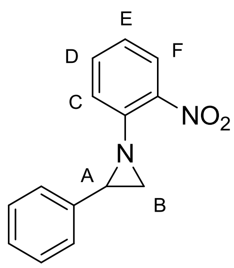
3.12 Synthesis of 1-(4-chlorophenyl)-2-phenylaziridine (23)



4-Chlorophenylazide and styrene were refluxed for 3 hours. The product was obtained as a brown oil (0.35 g, 90% yield). The collected analytical data were in accordance with those reported in literature.[5]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 - 7.36 (m, 5H, H_{Ph}), 7.20 (d, J = 8.8 Hz, 2H, H_C), 6.97 (d, J = 8.8 Hz, 2H, H_D), 3.08 (dd, J = 6.4, 3.6 Hz, 1H, H_A), 2.44 - 2.41 ppm (m, 2H, H_B).

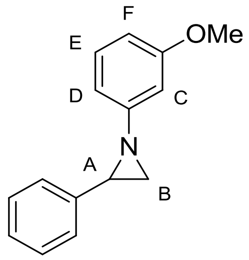
3.13 Synthesis of 1-(2-nitrophenyl)-2-phenylaziridine (25)



2-Nitrophenylazide and styrene were refluxed for 4 hours. The product was obtained as a yellow oil (0.38 g, 95% yield). The collected analytical data were in accordance with those reported in literature.[5]

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.93 (d, J = 8.1 Hz, 1H, H_F), 7.46 (pst, J = 7.5, Hz 1H, H_D), 7.35 - 7.24 (m, 5H, H_{Ar}), 7.19 – 7.16 (m, 1H, H_C), 7.06 (pst, J = 7.8 Hz, 1H, H_E), 3.32 (dd, J = 6.2, 3.5 Hz, 1H, H_A), 2.66 (d, J = 3.5 Hz, 1H, H_B), 2.47 ppm (d, J = 6.2 Hz, 1H, $H_{B'}$).

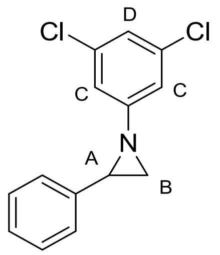
3.14 Synthesis of 1-(3-methoxyphenyl)-2-phenylaziridine (27)



3-Methoxyphenylazide and styrene were used, the mixture was refluxed for 72 hours. The product was obtained as a brown oil (0.16 g, 43% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 - 7.24 (m, 5H, H_{Ph}), 7.14 (pst, *J* = 8.0 Hz, 1H, H_E), 6.64 (ddd, *J* = 7.9, 2.1, 1.0 Hz, 1H, H_D), 6.60 (pst, *J* = 2.2 Hz, 1H, H_C), 6.53 (ddd, *J* = 8.3, 2.5, 1.0 Hz, 1H, H_F), 3.76 (s, 3H, H_{OMe}), 3.09 (dd, *J* = 6.5, 3.3 Hz, 1H, H_A), 2.45 (dd, *J* = 6.5, 1.2 Hz, 1H, H_B), 2.37 ppm (dd, *J* = 3.3, 1.2 Hz, 1H, $H_{B'}$).

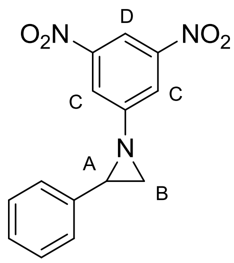
3.15 Synthesis of 1-(3,5-dichlorophenyl)-2-phenylaziridine (28)



3,5-Dichorophenylazide and styrene were refluxed for 4 hours. The product was obtained as a brown oil (0.43 g, 96% yield). The collected analytical data were in accordance with those reported in literature.[5]

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40 - 7.31 (m, 5H, H_{Ph}), 6.98 (s, 1H, H_D), 6.93 (s, 2H, H_C), 3.14 (dd, *J* = 6.4, 3.4 Hz, 1H, H_A), 2.48 (d, *J* = 6.4 Hz, 1H, H_B), 2.43 ppm (d, *J* = 3.4 Hz, 1H, $H_{B'}$).

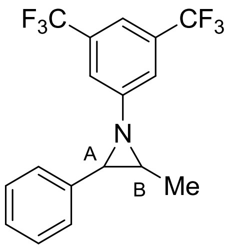
3.16 Synthesis of 1-(3,5-dinitrophenyl)-2-phenylaziridine (30)



3,5-Dinitrophenylazide and styrene were refluxed 4 hours. The product was obtained as a dark yellow powder (0.45 g, 94% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.64 (t, *J* = 2.0 Hz, 1H, H_D), 8.15 (d, *J* = 2.0 Hz, 2H, H_C), 7.42 - 7.36 (m, 5H, H_{Ph}), 3.36 (dd, *J* = 6.6, 3.6 Hz, 1H, H_A), 2.68 (d, *J* = 6.6 Hz, 1H, H_B), 2.66 ppm (d, *J* = 3.6 Hz, 1H, $H_{B'}$). ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.87 (C), 149.00 (C), 136.87 (two overlapping C), 128.83 (two overlapping CH), 128.28 (CH), 126.15 (two overlapping CH), 120.74 (two overlapping CH) 112.39 (CH), 42.71 (CH), 38.46 ppm (CH_2). LR-MS (ESI): m/z ($C_{14}H_{11}N_3O_4$) calcd 285.07, found $[M+H]^+$ 286.08. Elemental Analysis calcd. for ($C_{14}H_{11}N_3O_4$): C (58.95), H (3.89), N (14.73), found: C (58.73), H (3.62), N (14.71). UV-Vis λ_{max} (DCM)/nm (log ε): 233 (4.40). IR ν_{max} (DCM)/cm^{-1}: 1009, 1078, 1137, 1172, 1255, 1346, 1394, 1464, 1543, 1605, 1712. M.P.: 125-126°C

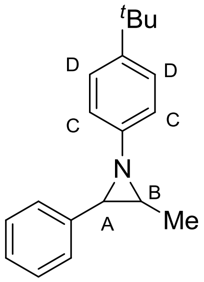
3.17 Synthesis of 1-(3,5-*bis*-trifluoromethylphenyl)-2-phenyl-3-methyl aziridine (32)



3,5-*Bis*-trifluoromethylphenylazide and *trans*-β-methyl styrene were refluxed for 4 hours. The product was obtained as a brown oil (0.36 g, 62% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45 - 7.30 (m, 8H, H_{Ar}), 3.06 (d, *J* = 2.7 Hz, 1H, H_A), 2.77 – 2.70 (m, 1H, H_B), 1.29 ppm (d, *J* = 5.7 Hz, 3H, H_{Me}). ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.67 (C), 137.59 (C), 132.62 (q, *J* = 33.1 Hz, two overlapping CF_3), 129.00 (two overlapping CH), 128.21 (CH), 126.76 (two overlapping CH), 125.48 (C), 121.11 (CH), 121.07 (CH), 115.77 (CH), 48.90 (CH), 44.64 (CH), 15.43 ppm (three overlapping CH_3). One quaternary carbon not detected. ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.34 ppm (s). LR-MS (ESI): m/z ($C_{14}H_{11}F_6N$) calcd 345.10, found $[M+H]^+$ 346.30. Elemental Analysis calcd. for ($C_{14}H_{11}F_6N$): C (59.13), H (3.79), N (4.06), found: C (58.75), H (3.84), N (4.03). UV-Vis λ_{max} (DCM)/nm (log ε): 251 (4.18). IR ν_{max} (DCM)/cm^{-1}: 1003, 1040, 1136, 1179, 1385, 1465, 1612, 3599.

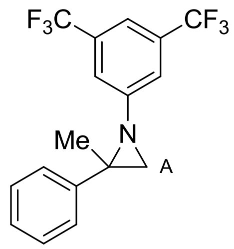
3.18 Synthesis of 1-(4-*tert*-butylphenyl)-2-phenyl-3-methyl aziridine (34)



4-*Tert*-butylphenylazide and *trans*-β-methyl styrene were refluxed for 12 hours. The product was obtained as a brown oil (0.21 g, 48% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33 – 7.31 (m, 5H, H_{Ph}), 7.25 - 7.22 (m, 2H, H_D), 6.86 (d, *J* = 8.4 Hz, 2H, H_C), 2.90 (d, *J* = 2.7 Hz, 1H, H_A), 2.56 (qd, *J* = 5.7, 2.7 Hz 1H, H_B), 1.28 (s, 9H, H_{tBu}), 1.21 ppm (d, *J* = 5.7 Hz, 1H, H_{Me}). ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.14 (C), 145.11 (C), 139.76 (C), 128.73 (CH), 127.48 (CH), 126.79 (CH), 126.03 (two overlapping CH), 120.78 (two overlapping CH), 48.09 (CH), 44.15 (CH), 34.56 (C) 31.91 (three overlapping CH_3), 15.16 ppm (CH_3). LR-MS (ESI): m/z ($C_{19}H_{23}N$) calcd 265.18, found $[M+H]^+$ 266.27. Elemental Analysis calcd. for ($C_{19}H_{23}N$): C (85.99), H (8.74), N (5.27), found: C (85.97), H (9.02), N (5.01). UV-Vis λ_{max} (DCM)/nm (log ε): 246 (4.16). IR ν_{max} (DCM)/cm^{-1}: 909, 913, 918, 923, 927, 933, 939, 1255, 1417, 1510, 1517, 1605, 3599, 3686.

3.19 Synthesis of 1-(3,5-bis(trifluoromethyl)phenyl)-2-methyl-2-phenylaziridine (36)



3,5-*Bis*-trifluoromethylphenylazide and α-methyl styrene were refluxed for 1 hour. The product was obtained as a brown oil (0.57 g, 99% yield). The collected analytical data were in accordance with those reported in literature.[5]

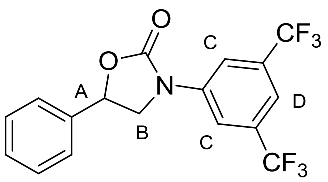
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.29 (m, 8H, H_{Ar}), 2.65 (s, 1H, H_A), 2.38 (s, 1H, $H_{A'}$), 1.45 ppm (s, 3H, H_{Me}).

4. Synthesis of *N*-aryl oxazolidin-2-ones

General procedure for synthesizing 2a/2b (Table 1): in a 25.0 mL glass liner equipped with a screw cap and glass wool, the catalyst (3.75 x 10^{-3} mmol), the co-catalyst (5.2 mg, 1.88 x 10^{-2} mmol) and the aziridine (3.75 x 10^{-1} mmol) were dissolved in the opportune solvent (3.30 mL). The reaction mixture was cooled to -78°C and the vessel was transferred into a stainless-steel autoclave; three vacuum-nitrogen cycles were performed and 1.2 MPa CO_2 was charged at room temperature. The autoclave was placed in a preheated oil bath at 100°C and stirred for 15 h, then it was cooled at room temperature and slowly vented. The solvent was evaporated to dryness and the crude analyzed by ^{1}H NMR spectroscopy by using 2,4-dinitrotoluene as the internal standard.

Optimization of the catalytic conditions: the general procedure reported for synthesizing **2a**/**2b** (Table 1) was repeated by varying the following experimental conditions:
a) the aziridine concentration at 1.2 MPa CO_2, 100°C for 15 h: [**1**] = 0.075 M, 30% yield; [**1**] = 0.16 M, 45% yield; [**1**] = 0.33 M, 58% yield; [**1**] = 0.66 M, 69 % yield; [**1**] = 1.00 M, 80% yield; [**1**] = 1.50 M, 86% yield; [**1**] = 2.0 M, 89 % yield.
b) the CO_2 pressure at 1.5 M of aziridine, 100°C for 15 h: CO_2 pressure = 0.1 MPa, 56% yield; CO_2 pressure = 0.4 MPa, 57% yield; CO_2 pressure = 0.6 MPa, 74% yield; CO_2 pressure = 1.2 MPa 86% yield; CO_2 pressure = 1.8 MPa, 75% yield.
c) the reaction temperature at 1.5 M of aziridine, 1.2 MPa CO_2 for 15 h: T = 25°C, 8% yield; T = 50°C, 9% yield; T = 75°C, 32% yield; T = 100°C, 70% yield; T = 125°C, 99% yield; T = 150°C, 99% yield.

4.1 Synthesis of 3-(3,5-*bis*-(trifluoromethyl)phenyl-5-phenyloxazalidin-2-one (2)

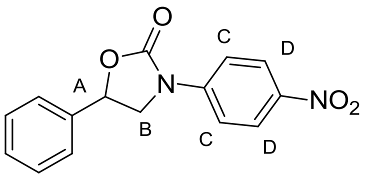


The product was obtained starting from aziridine **1** and following the general procedure. The product was obtained as a brown oil (0.14 g, 99% yield). The collected analytical data were in accordance with those reported in literature.[8]

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 2H, H_C), 7.64 (s, 1H, H_D), 7.45 - 7.41 (m, 5H, H_{Ph}), 5.72 (pst, *J* = 8.0 Hz, 1H, H_A), 4.47 (pst, *J* = 8.8 Hz, 1H, H_B), 4.03 ppm (pst, *J* = 7.6 Hz, 1H, $H_{B'}$). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.49 (C=O), 140.02 (C), 137.55 (C), 132.92 (q, *J* = 33.7, two overlapping CF_3), 129.85 (CH), 129.57 (two overlapping CH), 125.96 (two overlapping CH), 124.73 (C), 122.02 (C), 117.97 (CH), 117.94 (CH), 117.58 (CH), 74.69 (CH), 52.68 ppm (CH_2). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.97 ppm (s). LR-MS (ESI): m/z ($C_{17}H_{11}F_6NO_2$) calcd 375.07, found $[M+H]^+$ 376.11. Elemental

Analysis calcd. for ($C_{17}H_{11}F_6NO_2$): C (54.41), H (2.95), N (3.73), found: C (54.09), H (3.25), N (3.61). UV-Vis λ_{max} (DCM)/nm (log ε): 244 (4.22). IR ν_{max} (DCM)/cm^{-1}:1140 1184, 1403, 1476, 1764 (C=O), 2976.

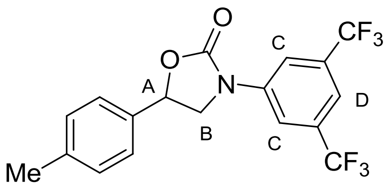
4.2 Synthesis of 3-(4-nitrophenyl)-5-phenyloxazalidin-2-one (4)



The product was obtained starting from aziridine **3** and following the general procedure. The product was obtained as a dark yellow solid (0.11 g, 99% yield). The collected analytical data were in accordance with those reported in literature.[9]

^{1}H NMR (400 MHz, $CDCl_3$) 8.27 - 8.24 (m, 2H, H_D), 7.74 (d, J = 9.3 Hz, 2H, H_C), 7.46 - 7.42 (m, 5H, H_{Ph}) 5.71 (pst, J = 8.2 Hz, 1H, H_A), 4.47 (pst, J = 8.8 Hz, 1H, H_B), 4.03 ppm (dd, J = 8.8, 7.6 Hz, 1H, $H_{B'}$). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.05 (C=O), 143.65 (C), 143.41 (C), 137.23 (C), 129.53 (CH), 129.24 (two overlapping CH), 125.66 (two overlapping CH), 125.02 (two overlapping CH), 117.55 (two overlapping CH), 74.30 (CH), 52.42 ppm (CH_2). LR-MS (ESI): m/z ($C_{15}H_{12}N_2O_4$) calcd 284.08, found $[M+H]^+$ 285.02. Elemental Analysis calcd. for ($C_{15}H_{12}N_2O_4$): C (63.38), H (4.25), N (9.85), found: C (63.01), H (4.29), N (9.80). UV-Vis λ_{max} (DCM)/nm (log ε): 317 (4.28). IR ν_{max} (DCM)/cm^{-1}:1143, 1205, 1220, 1298, 1333, 1344, 1369, 1395, 1417, 1482, 1503, 1520, 1599, 1764 (C=O). M.P. 163-164 °C

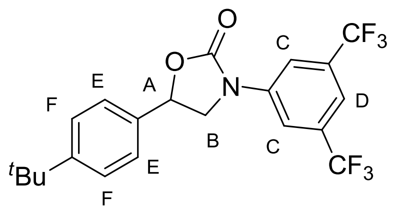
4.3 Synthesis of 3-(3,5-bis-(trifluoromethyl)phenyl-5-(4-methylphenyl)oxazalidin-2-one (6)



The product was obtained starting from aziridine **5** and following the general procedure. The product was obtained as a brown oil (0.13 g, 90% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05 (s, 2H, H_C), 7.64 (s, 1H, H_D), 7.35 - 7.24 (m, 4H, H_{Ar}), 5.68 (pst, J = 8.1 Hz, 1H, H_A), 4.43 (pst, J = 8.7 Hz, 1H, H_B), 4.01 (pst, J = 8.1 Hz, 1H, $H_{B'}$), 2.38 ppm (s, 3H, H_{Me}). ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.20 (C=O), 139.72 (C), 134.12 (C), 132.80 (q, J = 33.4 Hz, two overlapping CF_3), 129.86 (two overlapping CH), 125.69 (two overlapping CH), 124.85 (C), 121.23 (C), 117.62 (two overlapping CH), 117.16 (CH), 74.40 (CH), 52.38 (CH_2), 21.22 ppm (CH_3). ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.26 ppm (s). LR-MS (ESI): m/z ($C_{18}H_{13}F_6NO_2$) calcd 389.09, found $[M+H]^+$ 390.13. Elemental Analysis calcd. for ($C_{18}H_{13}F_6NO_2$): C (55.53), H (3.37), N (3.60), found: C (55.17), H (3.42), N (3.57). UV-Vis λ_{max} (DCM)/nm (log ε): 244 (4.17). IR ν_{max} (DCM)/cm^{-1}: 1141, 1185, 1246, 1403, 1476, 1763 (C=O).

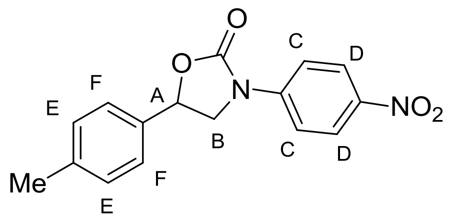
4.4 Synthesis of 3-(3,5-*bis*-(trifluoromethyl)phenyl)-5-(4-*tert*-butylphenyl)oxazalidin-2-one (8)



The product was obtained starting from aziridine **7** and following the general procedure. The product was obtained as a brown oil (0.14 g, 84 % yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05 (s, 2H, H_C), 7.64 (s, 1H, H_D), 7.47 (d, *J* = 8.4 Hz, 2H, H_F), 7.36 (d, *J* = 8.4 Hz, 2H, H_E), 5.70 (pst, *J* = 7.7 Hz, 1H, H_A), 4.44 (pst, *J* = 8.6 Hz, 1H, H_B), 4.03 (dd, *J* = 8.6, 7.7 Hz, 1H, $H_{B'}$), 1.33 ppm (s, 9H, H_{tBu}). ^{13}C NMR (75 MHz, $CDCl_3$) 140.12 (C), 134.52 (C) 132.95 (q, *J* = 33.7 Hz, two overlapping CF_3), 126.54 (two overlapping CH), 125.86 (two overlapping CH), 125.24 (C), 121.62 (C), 117.95 (two overlapping CH), 117.58 (CH), 74.70 (CH), 52.73 (CH_2), 35.15 (C), 31.62 ppm (three overlapping CH_3). C=O was not detected. ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.27 ppm (s). LR-MS (ESI): m/z ($C_{21}H_{19}F_6NO_2$) calcd 431.16, found $[M+Na]^+$ 454.16 Elemental Analysis calcd. for ($C_{21}H_{19}F_6NO_2$): C (58.47), H (4.44), N (3.25), found: C (58.17), H (4.47), N (3.23). UV-Vis λ_{max} (DCM)/nm (log ε): 245 (3.90). IR ν_{max} (DCM)/cm^{-1}: 895, 922, 1136, 1183, 1245, 1420, 1476, 1609, 1762 (C=O).

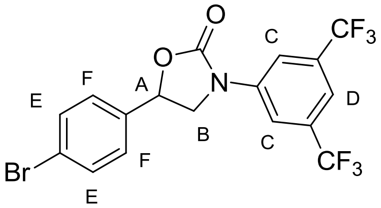
4.5 Synthesis of 3-(4-nitrophenyl)-5-(4-methylphenyl)oxazalidin-2-one (10)



The product was obtained starting from aziridine **9** and following the general procedure. The product was obtained as a brown solid (0.10 g, 90% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 9.2 Hz, 2H, H_D), 7.77 (d, *J* = 9.2 Hz, 2H, H_C), 7.35 (d, *J* = 8.0 Hz, 2H, H_F), 7.29 (d, *J* = 8.0 Hz, 2H, H_E), 5.71 (pst, *J* = 8.0 Hz, 1H, H_A), 4.47 (pst, *J* = 8.8 Hz, 1H, H_B), 4.05 - 4.03 (m, 1H, $H_{B'}$), 2.42 ppm (s, 3H, H_{Me}). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.73 (C), 143.34 (C), 139.61 (C), 134.14 (C), 129.86 (two overlapping CH), 125.78 (two overlapping CH), 125.00 (two overlapping CH), 117.53 (two overlapping CH), 74.41 (CH), 52.42 (CH_2), 21.24 ppm (CH_3). C=O was not detected. LR-MS (ESI): m/z ($C_{16}H_{14}N_2O_4$) calcd 298.10, found $[M+H]^+$ 299.00. Elemental Analysis calcd. for ($C_{16}H_{14}N_2O_4$): C (64.42), H (4.73), N (9.39), found: C (64.04), H (4.77), N (9.33). UV-Vis λ_{max} (DCM)/nm (log ε): 320 (4.72). IR ν_{max} (DCM)/cm^{-1}:1113, 1143, 1311, 1331, 1393, 1422, 1503, 1519, 1598, 1764 (C=O). M.P. 103-104 °C.

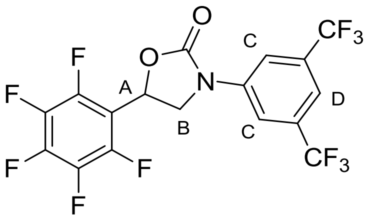
4.6 Synthesis of 3-(3,5-*bis*-(trifluoromethyl)phenyl)-5-(4-bromophenyl)oxazalidin-2-one (12)



The product was obtained starting from aziridine **11** and following the general procedure. The product was obtained as a brown oil (0.17 g, 99% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 2H, H_C), 7.65 (s, 1H, H_D), 7.60 - 7.57 (m, 2H, H_E), 7.31 (d, *J* = 8.4 Hz, 2H, H_F), 5.68 (pst, *J* = 8.0 Hz, 1H, H_A), 4.48 (pst, *J* = 8.8 Hz, 1H, H_B), 3.99 ppm (dd, *J* = 8.4, 7.2 Hz, 1H, $H_{B'}$). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.88 (C=O), 139.48 (C), 136.20 (C), 132.47 (q, *J* = 33.8 Hz, two overlapping CF_3), 132.44 (two overlapping CH), 127.27 (two overlapping CH), 124.34 (C), 123.64 (C), 121.63 (C), 117.62 (two overlapping CH), 117.43 (CH), 73.66 (CH), 52.16 ppm (CH_2). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.95 ppm (s). LR-MS (ESI): m/z ($C_{17}H_{10}BrF_6NO_2$) calcd 452.98, found $[M+H]^+$ 454.08. Elemental Analysis calcd. for ($C_{17}H_{10}BrF_6NO_2$): C (44.96), H (2.22), N (3.08), found: C (44.74), H (2.26), N (3.05). UV-Vis λ_{max} (DCM)/nm (log ε): 241 (4.04). IR ν_{max} (DCM)/cm^{-1}: 917, 1142, 1185, 1476, 1622, 1767 (C=O).

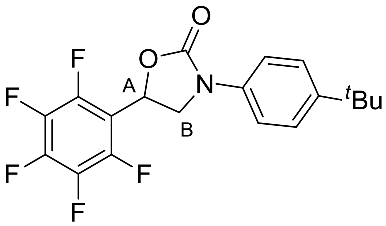
4.7 Synthesis of 3-(3,5-*bis*-(trifluoromethyl)phenyl)-5-(2,3,4,5,6-pentafluorophenyl)oxazalidin-2-one (14)



The product was obtained starting from aziridine **13** and following the general procedure. The product was obtained as a brown oil (0.11 g, 64% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 2H, H_C), 7.69 (s, 1H, H_D), 6.06 (dd, *J* = 9.6, 7.2 Hz, 1H, H_A), 4.55 (pst, *J* = 9.4 Hz, 1H, H_B), 4.24 - 4.20 ppm (m, 1H, $H_{B'}$). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.91 (C=O), 139.09 (C), 132.98 (q, *J* = 33.6 Hz, two overlapping CF_3), 124.30 (m, two overlapping C-F), 121.58 (C-F), 117.70 (two overlapping CH), 112.79 (CH), 64.44 (CH), 49.71 ppm (CH_2). Three quaternary carbon were not detected. ^{19}F NMR (282 MHz, $CDCl_3$) δ -63.32 (s, 6F, F_{CF3}), -142.64 (d, *J* = 15.3 Hz, 2F, F_o), -149.66 (t, *J* = 20.5 Hz, 1F, F_p), -159.69 - -159.81 ppm (m, 2F, F_m). LR-MS (ESI): m/z ($C_{17}H_6F_6NO_2$) calcd 465.02, found $[M+H]^+$ 466.11. Elemental Analysis calcd. for ($C_{17}H_6F_6NO_2$): C (43.89), H (1.30), N (3.01), found: C (43.65), H (1.35), N (2.99). UV-Vis λ_{max} (DCM)/nm (log ε): 242 (3.68). IR ν_{max} (DCM)/cm^{-1}: 1422, 1511, 1604, 1774 (C=O), 3057.

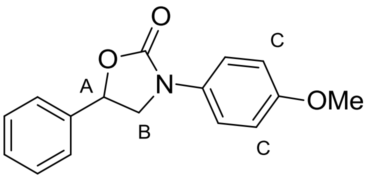
4.8 Synthesis of 3-(4-*tert*-butylphenyl-5-(2,3,4,5,6-pentafluorophenyl)oxazalidin-2-one (16)



The product was obtained starting from aziridine **15** and following the general procedure. The product was obtained as a brown oil (0.12 g, 79% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.49 - 7.41 (m, 4H, H_{Ar}), 5.97 (dd, *J* = 9.6, 6.9 Hz, 1H, H_A), 4.44 (pst, *J* = 9.3 Hz, 1H, H_B), 4.15- 4.09 (m, 1H, $H_{B'}$), 1.33 ppm (s, 9H, H_{tBu}). ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.04 (C=O), 148.27 (C), 144.24 (C), 135.36 (C), 126.52 (two overlapping CH), 118.96 (two overlapping CH), 64.65 (CH), 50.69 (CH_2), 34.79 (C), 31.69 ppm (three overlapping CH_3). Five C-F quaternary carbons were not detected. ^{19}F NMR (282 MHz, $CDCl_3$) δ -142.65 (dd, *J* = 21.9, 10.1 Hz, 1F, F_o), -150.95 (pst, *J* = 20.5 Hz, 1F, F_p), -160.42 - -160.56 ppm (m, 1F, F_m). LR-MS (ESI): m/z ($C_{19}H_{16}F_5NO_2$) calcd 385.11, found $[M+Na]^+$ 408.22. Elemental Analysis calcd. for ($C_{17}H_6F_6NO_2$): C (59.22), H (4.19), N (3.64), found: C (58.88), H (4.23), N (3.61). UV-Vis λ_{max} (DCM)/nm (log ε): 240 (4.26). IR ν_{max} (DCM)/cm^{-1}: 978, 1135, 1230, 1308, 1379, 1511, 1765 (C=O).

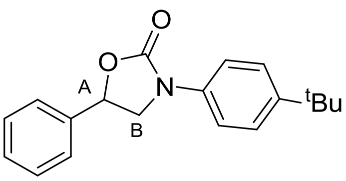
4.9 Synthesis of 3-(4-methoxyphenyl)-5-phenyloxazalidin-2-one (18)



The product was obtained starting from aziridine **17** and following the general procedure. The product was obtained as brown syrup (0.02 g, 20% yield). The collected analytical data were in accordance with those reported in literature.[9]

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47 - 7.41 (m, 7H, H_{Ar}), 6.92 (d, *J* = 9.0 Hz, 2H, H_C), 5.66-5.60 (m, 1H, H_A), 4.35 (pst, *J* = 8.8 Hz, 1H, H_B), 3.96 - 3.90 (m, 1H, $H_{B'}$), 3.80 ppm (s, 3H, H_{OMe}). ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.91 (C), 155.41 (C=O), 138.69 (C), 131.75 (C), 129.43 (three overlapping CH), 126.06 (two overlapping CH), 120.77 (two overlapping CH), 114.76 (two overlapping CH), 74.40 (CH), 55.92 (CH_2), 53.65 ppm (CH_3). LR-MS (ESI): m/z ($C_{16}H_{15}NO_3$) calcd 269.11, found $[M+H]^+$ 269.95. Elemental Analysis calcd. for ($C_{16}H_{15}NO_3$): C (71.36), H (5.61), N (5.20), found: C (71.00), H (5.64), N (5.17). UV-Vis λ_{max} (DCM)/nm (log ε): 244 (3.97). IR ν_{max} (DCM)/cm^{-1}: 1420, 1514, 1647, 1754 (C=O).

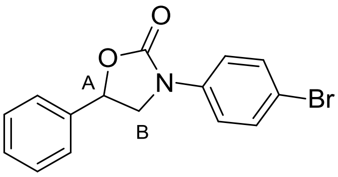
4.10 Synthesis of 3-(4-*tert*-butylphenyl)-5-phenyloxazalidin-2-one (20)



The product was obtained starting from aziridine **19** following the general procedure. The product was obtained as a brown oil (0.06 g, 54% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 - 7.39 (m, 9H, H_{Ar}), 5.63 (dd, *J* = 8.4, 7.2 Hz, 1H, H_A), 4.37 (pst, *J* = 8.8 Hz 1H, H_B), 3.97 - 3.93 (m, 1H, $H_{B'}$), 1.31 ppm (s, 9H, H_{tBu}). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.85 (C=O), 147.26 (C), 138.26 (C), 135.55 (C), 129.10 (two overlapping CH), 129.05 (two overlapping CH), 125.99 (two overlapping CH), 125.71 (CH), 118.19 (two overlapping CH), 74.07 (CH), 52.84 (CH_2), 34.36 (C), 31.34 (three overlapping CH_3). LR-MS (ESI): m/z ($C_{19}H_{21}NO_2$) calcd 295.16, found $[M+H]^+$ 296.07. Elemental Analysis calcd. for ($C_{19}H_{21}NO_2$): C (77.26), H (7.17), N (4.74), found: C (76.92), H (7.19), N (4.72). UV-Vis λ_{max} (DCM)/nm (log ε): 241 (4.19). IR ν_{max} (DCM)/cm^{-1}: 906, 915, 1276, 1420, 1518, 1756 (C=O).

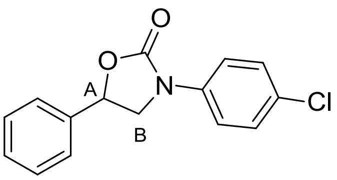
4.11 Synthesis of 3-(4-bromophenyl)-5-phenyloxazalidin-2-one (22)



The product was obtained starting from aziridine **21** following the general procedure. The product was obtained as a dark yellow solid (0.06 g, 50% yield). The collected analytical data were in accordance with those reported in literature.[9]

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.51 - 7.39 (m, 9H, H_{Ar}), 5.65 (pst, *J* = 8.1 Hz, 1H, H_A), 4.35 (pst, *J* = 8.7 Hz, 1H, H_B), 3.93 ppm (pst, *J* = 7.8 Hz, 1H, $H_{B'}$). ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.86 (C=O), 138.24 (C), 137.69 (C), 132.47 (two overlapping CH), 129.64 (CH), 129.56 (CH), 129.51 (CH) 126.05 (two overlapping CH), 120.15 (two overlapping CH), 117.43 (C), 74.46 (CH), 52.96 ppm (CH_2). LR-MS (ESI): m/z ($C_{15}H_{12}BrNO_2$) calcd 317.01, found $[M+H]^+$ 318.30. Elemental Analysis calcd. for ($C_{15}H_{12}BrNO_2$): C (56.62), H (3.80), N (4.40), found: C (56.31), H (3.86), N (4.38). UV-Vis λ_{max} (DCM)/nm (log ε): 247 (4.28). IR ν_{max} (DCM)/cm^{-1}: 1077, 1140, 1369, 1397, 1418, 1493, 1758 (C=O). M.P.: 102-105 °C

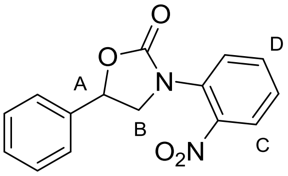
4.12 Synthesis of 3-(4-clorophenyl)-5-phenyloxazalidin-2-one (24)



The product was obtained starting from aziridine **23** following the general procedure. The product was obtained as a cream solid (0.07 g, 72% yield). The collected analytical data were in accordance with those reported in literature.[9]

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 - 7.33 (m, 9H, H_{Ar}), 5.65 (pst, *J* = 8.7 Hz 1H, H_A), 4.36 (pst, *J* = 8.8 Hz, 1H, H_B), 3.94 ppm (dd, *J* = 8.7, 7.5 Hz, 1H, $H_{B'}$). ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.91 (C=O), 138.26 (C), 137.17 (C), 129.63 (CH), 129.53 (two overlapping CH), 129.51 (two overlapping CH), 126.04 (two overlapping CH), 119.83(two overlapping CH), 74.45 (CH), 53.04 ppm (CH_2). One quaternary carbon was not detected. LR-MS (ESI): m/z ($C_{15}H_{12}ClNO_2$) calcd 273.06, found $[M+H]^+$ 274.27. Elemental Analysis calcd. for ($C_{15}H_{12}ClNO_2$): C (65.82), H (4.42), N (5.12), found: C (65.46), H (4.46), N (5.09). UV-Vis λ_{max} (DCM)/nm (log ε): 245 (4.16). IR ν_{max} (DCM)/cm^{-1}: 1096, 1142, 1223, 1368, 1398, 1420, 1496, 1599, 1758 (C=O). M.P.: 111-112 °C.

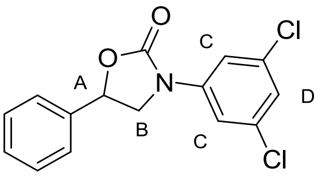
4.13 Synthesis of 3-(2-nitrophenyl)-5-phenyloxazalidin-2-one (26)



The product was obtained starting from aziridine **25** and following the general procedure. The product was obtained as a cream solid (0.06 g, 60% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05 (dd, *J* = 8.1, 1.5 Hz, 1H, H_C), 7.67 - 7.64 (m, 1H, H_D), 7.52 - 7.41 (m, 7H, H_{Ar}), 5.76 (pst, *J* = 8.2 Hz, 1H, H_A), 4.39 (pst, *J* = 8.6 Hz, 1H, H_B), 4.01 ppm (pst, *J* = 8.1 Hz, 1H, $H_{B'}$). ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.92 (C), 134.34 (CH), 131.71 (C), 129.71 (CH), 129.48 (two overlapping CH), 128.56 (CH), 128.33 (CH), 126.43 (two overlapping CH), 76.25 (CH), 55.20 ppm (CH_2). Two quaternary carbons were not detected. LR-MS (ESI): m/z ($C_{15}H_{12}N_2O_4$) calcd 284.08, found $[M+Na]^+$ 307.08. Elemental Analysis calcd. for ($C_{15}H_{12}N_2O_4$): C (63.38), H (4.25), N (9.85), found: C (63.04), H (4.29), N (9.80). UV-Vis λ_{max} (DCM)/nm (log ε): 231 (3.75). IR ν_{max} (DCM)/cm^{-1}: 1015, 1095, 1276, 1422, 1535, 1607, 1765 (C=O). M.P.: 145-146 °C.

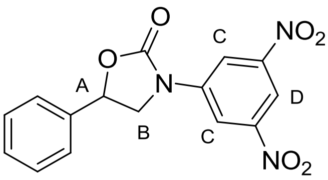
4.14 Synthesis of 3-(3,5-diclorophenyl)-5-phenyloxazalidin-2-one (29)



The product was obtained starting from aziridine **28** and following the general procedure. The product was obtained as a brown oil (0.11 g, 93% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 (d, *J* = 1.5 Hz, 2H, H_C), 7.44 - 7.42 (m, 5H, H_{Ph}),7.14 - 7.13 (m, 1H, H_D), 5.66 (pst, *J* = 8.0 Hz, 1H, H_A), 4.35 (pst, *J* = 8.8 Hz, 1H, H_B), 3.92 ppm (dd, *J* = 8.7, 7.5 Hz, 1H, $H_{B'}$). ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.47 (C=O), 140.35 (C), 137.84 (C), 135.95 (two overlapping C), 129.79 (CH), 129.58 (two overlapping CH), 126.01 (two overlapping CH), 124.42 (CH), 116.76 (two overlapping CH), 74.56 (CH), 52.81 ppm (CH_2). LR-MS (ESI): m/z ($C_{15}H_{12}Cl_2NO_2$) calcd 307.02, found $[M+Na]^+$ 330.30. Elemental Analysis calcd. for ($C_{15}H_{12}ClNO_2$): C (58.46), H (3.60), N (4.55), found: C (58.12), H (3.64), N (4.51). UV-Vis λ_{max} (DCM)/nm (log ε): 245 (3.16). IR ν_{max} (DCM)/cm^{-1}: 1148, 1208, 1366, 1392, 1426, 1455, 1569, 1493, 1763 (C=O).

4.15 Synthesis of 3-(3,5-dinitrophenyl-5-phenyloxazalidin-2-one (31)

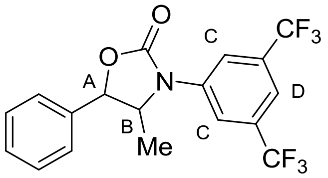


The product was obtained starting from aziridine **30** and following the general procedure. The product was obtained as a brown oil (0.04 g, 30% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81 - 8.80 (m, 3H, H_{C+D}), 7.50 - 7.43 (m, 5H, H_{Ph}), 5.79 (pst, *J* = 8.0 Hz, 1H, H_A), 4.55 (pst, *J* = 8.8 Hz, 1H, H_B), 4.13 - 4.08 ppm (m, 1H, $H_{B'}$). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.55 (C), 136.70 (C), 129.75 (CH), 129.35 (two overlapping CH), 125.58 (two overlapping CH), 117.30 (two overlapping CH), 113.72 (C), 113.32 (CH) 107.80 (C), 74.54 (CH), 52.40 ppm (CH_2). C=O was not detected. LR-MS (ESI): m/z ($C_{15}H_{12}N_3O_6$) calcd 329.06, found $[M+H]^+$ 329.94. Elemental Analysis calcd. for ($C_{15}H_{12}N_2O_4$): C (54.72), H (3.37), N (12.76), found: C (54.47), H (3.40), N (12.70).

UV-Vis λ_{max} (DCM)/nm (log ε): 232 (4.34). IR ν_{max} (DCM)/cm^{-1}: 1158, 1206, 1347, 1395, 1423, 1478, 1547, 1768 (C=O).

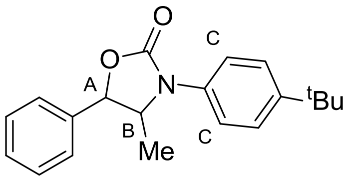
4.16 Synthesis of 3-(3,5-*bis*-(trifluoromethyl)phenyl)-4-methyl-5-phenyloxazalidin-2-one (33)



The product was obtained starting from aziridine **32** and following the general procedure. The product was obtained as a brown oil (0.08 g, 52% yield).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.92 (s, 2H, H_C), 7.68 (s, 1H, H_D), 7.47 - 7.40 (m, 5H, H_{Ph}), 5.19 (d, *J* = 6.3 Hz, 1H, H_A), 4.41 (psp, *J* = 6.1 Hz, 1H, H_B), 1.51 ppm (d, *J* = 6.3 Hz, 3H, H_{Me}). ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.85 (C=O), 138.87 (C), 137.29 (C), 133.06 (q, *J* = 33.7 Hz, two overlapping CF_3), 129.94 (CH), 129.63 (CH), 126.29 (CH), 126.09 (CH), 125.17 (C), 121.56 (C), 121.20 (CH), 118.61 (CH), 82.57 (CH), 60.13 (CH), 18.23 (CH_3). ^{19}F NMR (276 MHz, $CDCl_3$) δ -63.27 ppm (s). LR-MS (ESI): m/z ($C_{18}H_{13}F_6NO_2$) calcd 389.09, found $[M+H]^+$ 390.12. Elemental Analysis calcd. for ($C_{18}H_{13}F_6NO_2$): C (55.53), H (3.37), N (3.60), found: C (55.32), H (3.40), N (3.57). UV-Vis λ_{max} (DCM)/nm (log ε): 244 (3.87). IR ν_{max} (DCM)/cm^{-1}: 1158, 1206, 1347, 1395, 1423, 1478, 1547, 1768 (C=O).

4.17 Synthesis of 3-(4-*tert*-butylphenyl)-4-methyl-5-phenyloxazalidin-2-one (35)

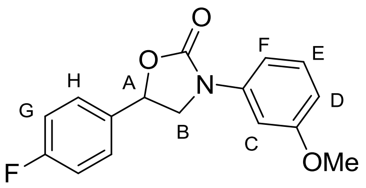


The product was obtained starting from aziridine **34** and following the general procedure. The product was obtained as a brown oil (0.03 g, 28% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 - 7.40 (m, 7H, H_{Ar}), 7.30 (d, *J* = 8.8 Hz, 2H, H_C), 5.11 (d, *J* = 6.8 Hz, 1H, H_A), 4.27 (psp, *J* = 6.4 Hz, 1H, H_B), 1.42 (d, *J* = 6.0 Hz, 3H, H_{Me}), 1.32 (s, 9H, H_{tBu}). ^{13}C NMR (100 MHz, $CDCl_3$) δ 129.11 (CH), 129.01 (two overlapping CH), 126.11 (two overlapping CH), 125.86 (two overlapping CH), 122.23(two overlapping CH), 82.19 (CH), 60.55 (CH), 31.32 (three overlapping CH_3), 18.11 (CH_3). Quaternary carbons were not detected. LR-MS (ESI): m/z ($C_{20}H_{23}NO_2$) calcd 309.17, found $[M+H]^+$ 310.00. Elemental Analysis calcd. for ($C_{20}H_{26}NO_2$): C (77.64), H (7.49), N (4.23), found: C (77.82), H (7.86), N (4.02). UV-Vis λ_{max} (DCM)/nm (log ε): 240 (4.30). IR ν_{max} (DCM)/cm^{-1}: 1369, 1394, 1519, 1607, 1753 (C=O).

5. Synthesis of *N*-aryl oxazolidin-2-ones by the two-step procedure

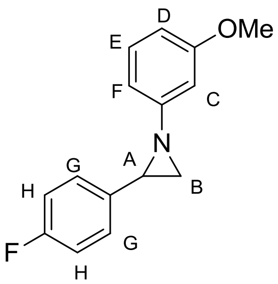
5.1 Synthesis of 3-(3-methoxyphenyl)-5-(4-fluorophenyl)oxazalidin-2-one (37a)



The product was obtained starting from 1-(3-methoxyphenyl)-2-phenyl aziridine and following the general procedure. The product was obtained as a yellowish oil (0.03 g, 35% yield). The collected analytical data were in accordance with those reported in literature.[10]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 - 7.40 (m, 2H, H_G), 7.30 - 7.27 (m, 2H, H_H), 7.15 - 7.13 (m, 2H, H_{E+F}), 7.03 (ddd, *J* = 8.3, 2.2, 0.8 Hz, 1H, H_C), 6.71 (ddd, *J* = 8.4, 2.5, 0.8 Hz, 1H, H_D), 5.61 (pst, *J* = 8.0 Hz, 1H, H_A), 4.36 (pst, *J* = 8.8 Hz, 1H, H_B), 3.92 (dd, *J* = 8.8, 7.6 Hz, 1H, $H_{B'}$), 3.83 ppm (s, 1H, H_{OMe}).

^{1}H NMR data of 1-(3-methoxyphenyl)-2-(4-fluorophenyl) aziridine



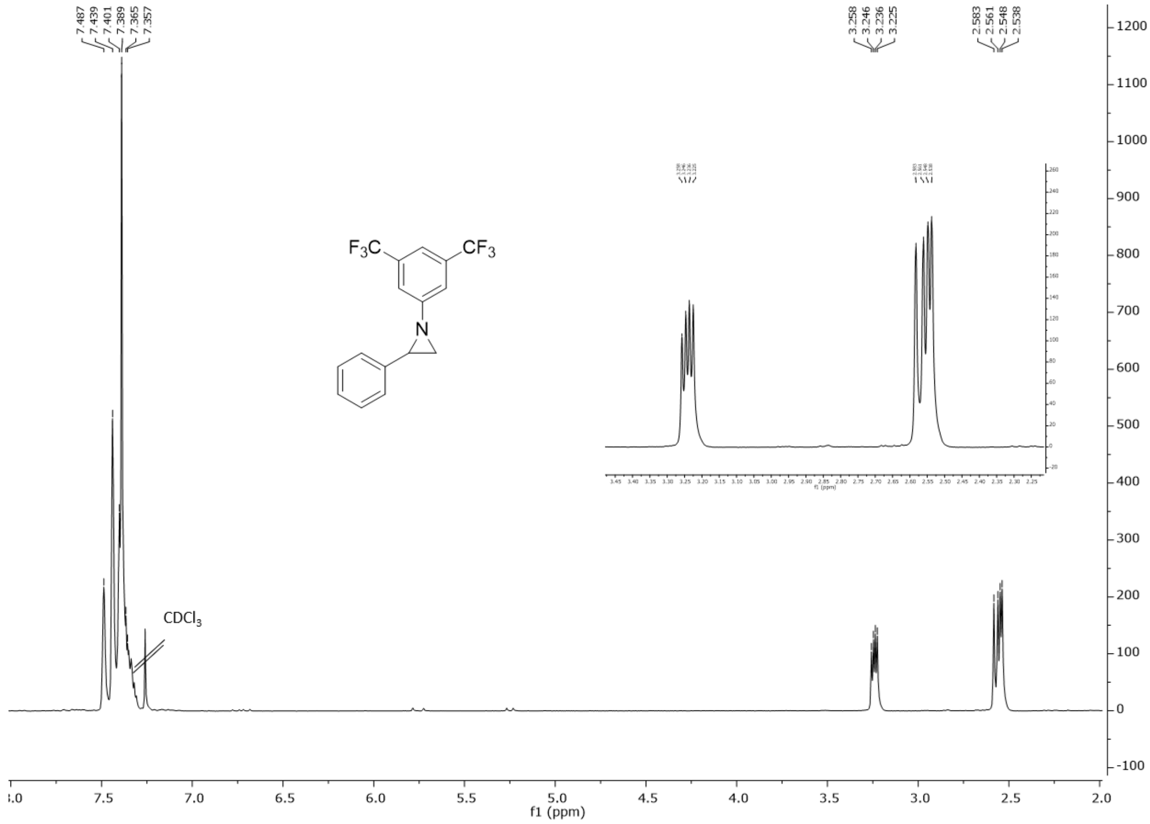
3-Methoxyphenylazide and 4-fluorostyrene were refluxed for 72 hours. (0.15 g, 37% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (m, 2H, H_H), 7.17 (pst, *J* = 8.0 Hz, 1H, H_E), 7.05 (m, 2H, H_G), 6.73 – 6.63 (m, 1H, H_F), 6.61 (s, 1H, H_C), 6.59 – 6.53 (m, 1H, H_D), 3.79 (s, 3H, H_{OMe}), 3.10 (dd, *J* = 6.3, 3.3 Hz, 1H, H_A), 2.46 (psd, *J* = 6.4 Hz, 1H, H_B), 2.35 ppm (psd, *J* = 3.2 Hz, 1H, $H_{B'}$).

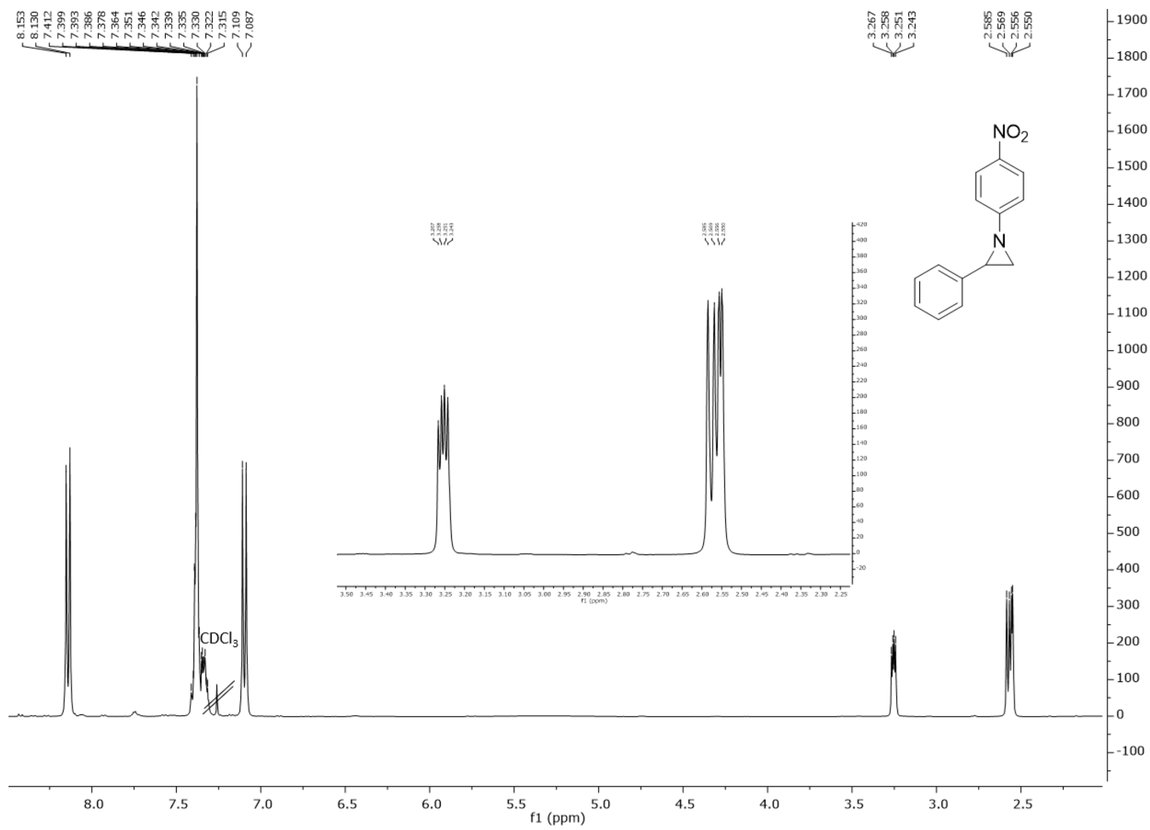
6. ^{1}H, ^{13}C and ^{19}F NMR spectra of reported compounds

6.1 NMR spectra of aziridines

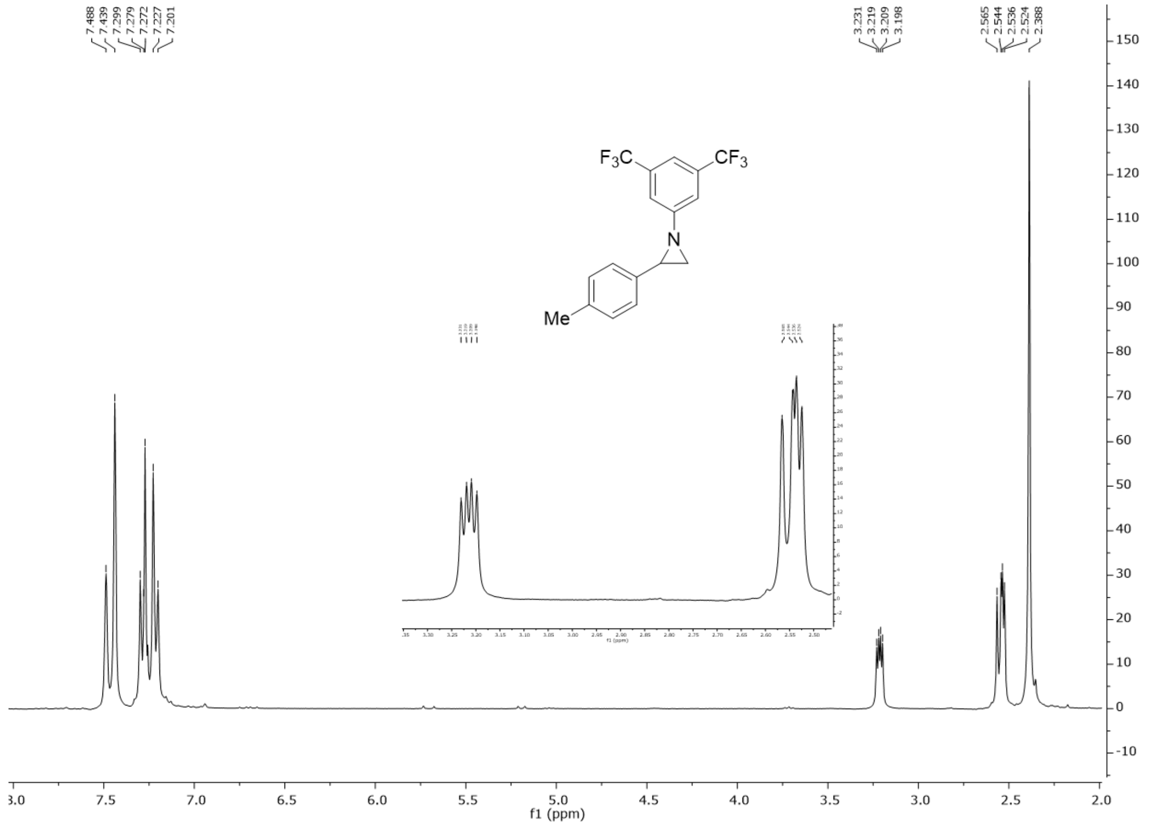
Compound (1): ^{1}H NMR (300 MHz, $CDCl_3$)



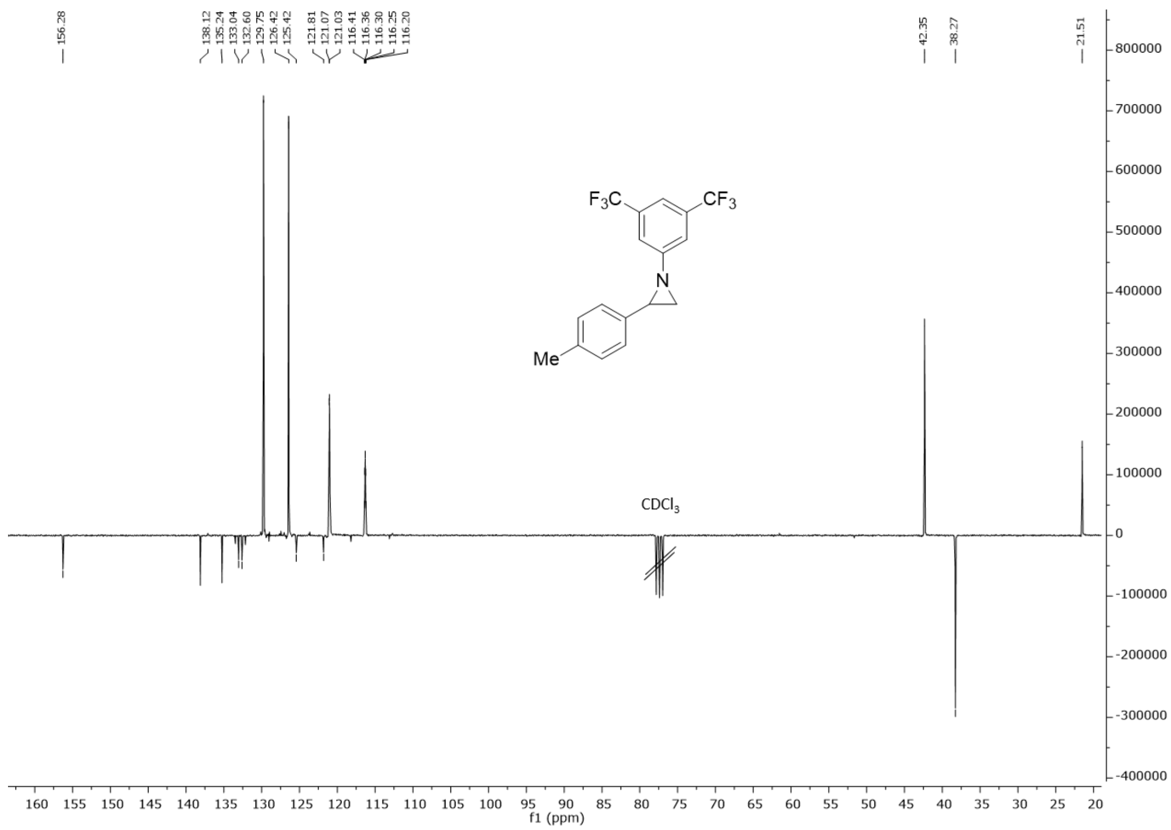
Compound (3): ^{1}H NMR (400 MHz, $CDCl_3$)



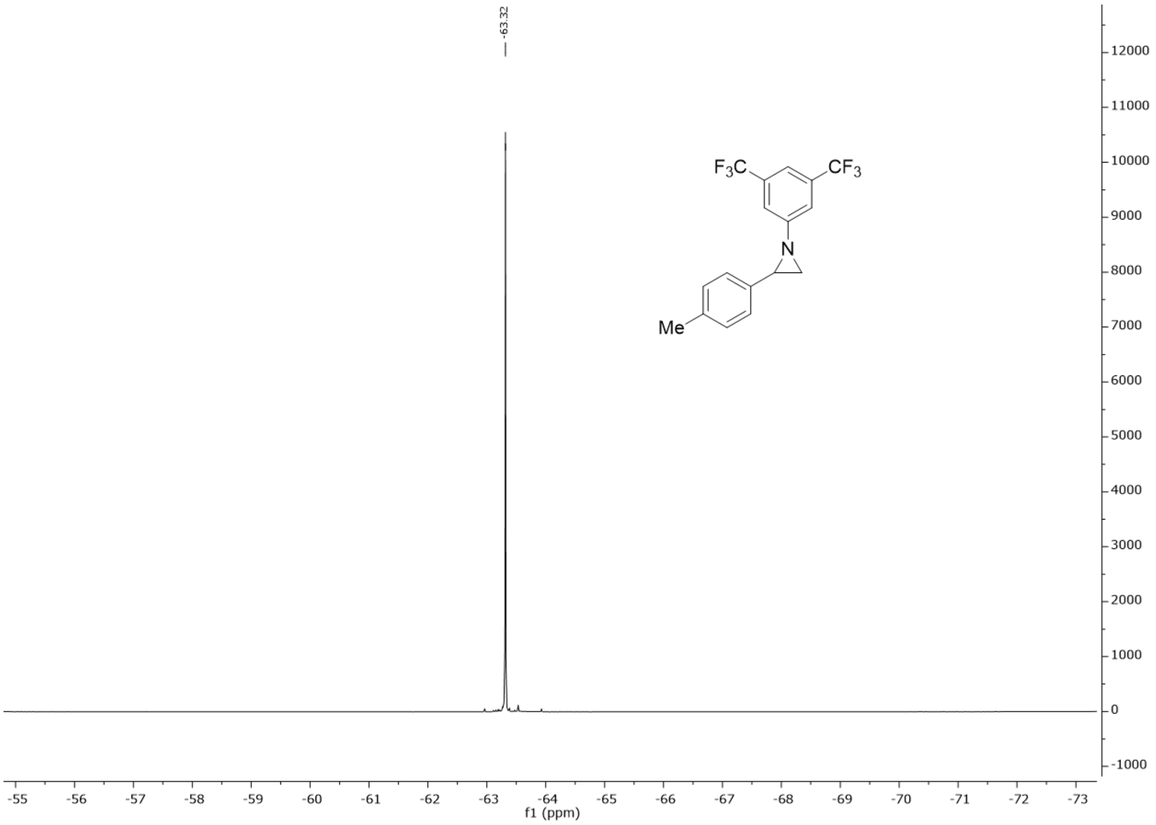
Compound (5): ^{1}H NMR (300 MHz, $CDCl_3$)



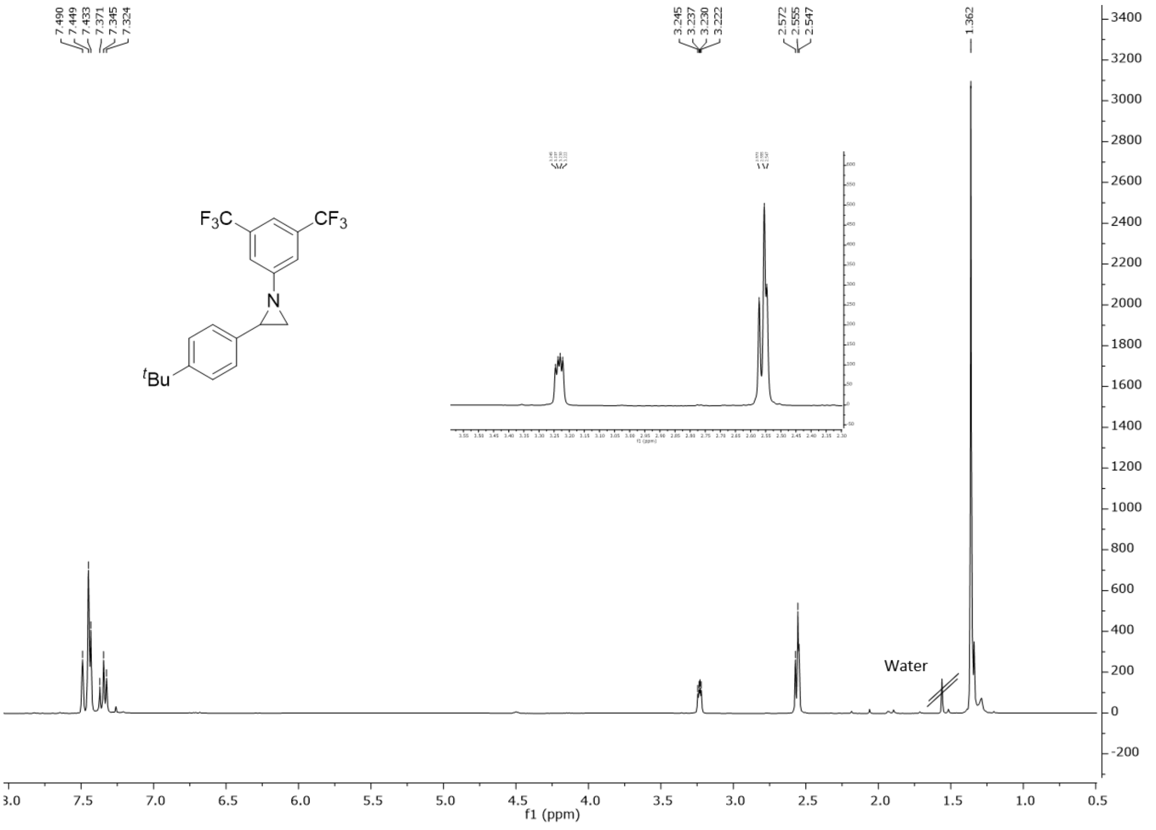
Compound (5): ^{13}C NMR (75 MHz, $CDCl_3$)



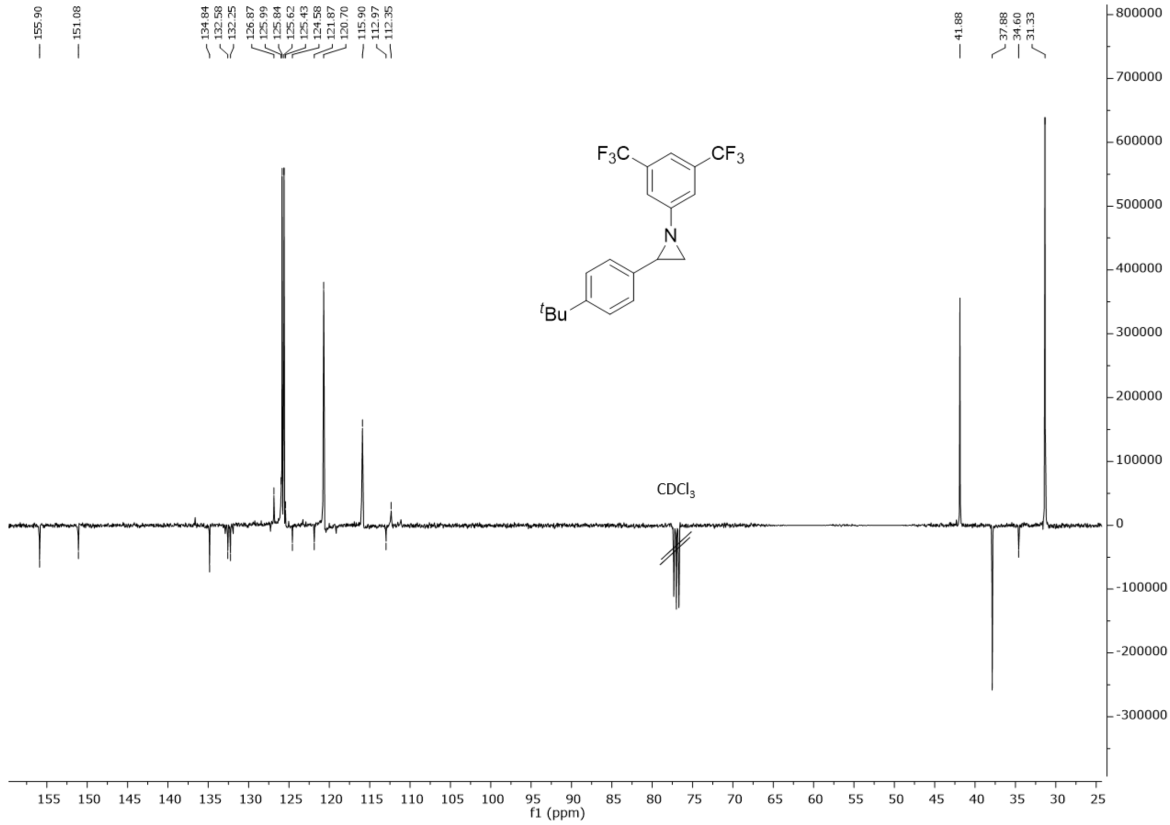
Compound (5): ^{19}F NMR (282 MHz, CDCl$_3$)



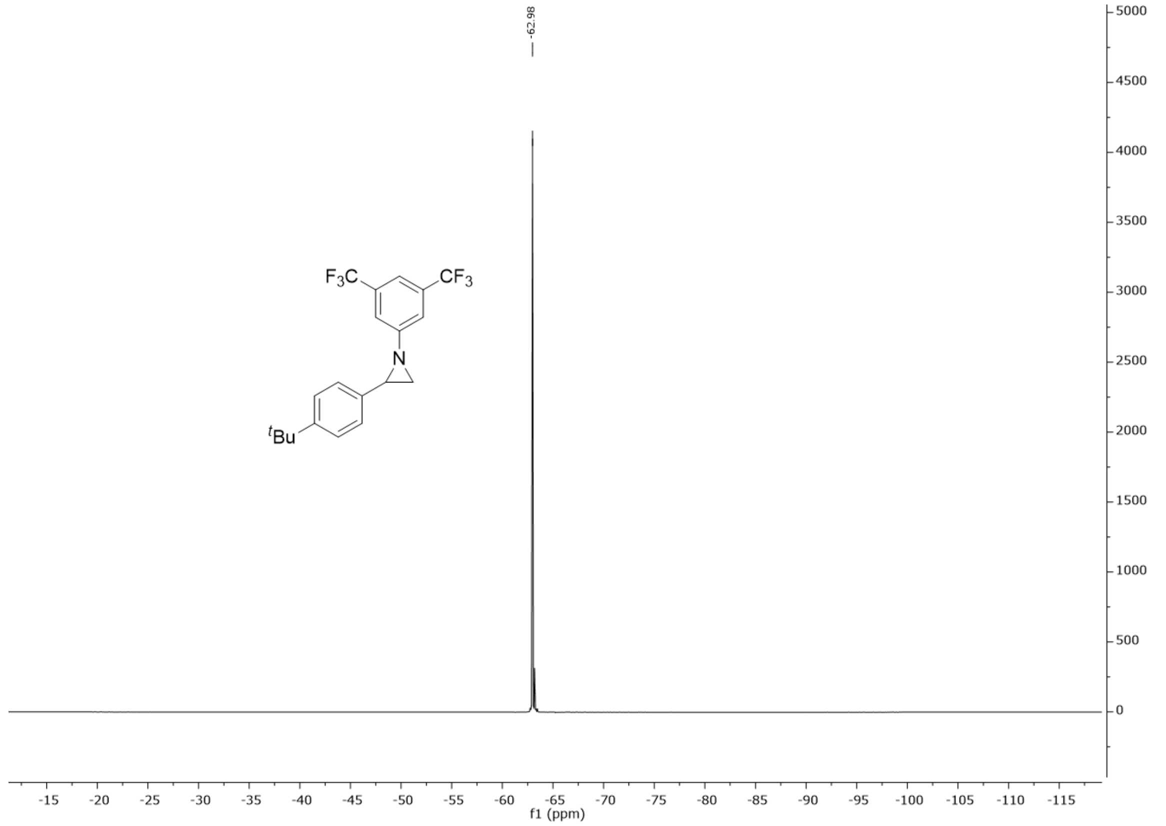
Compound (7): ^{1}H NMR (400 MHz, CDCl$_3$)



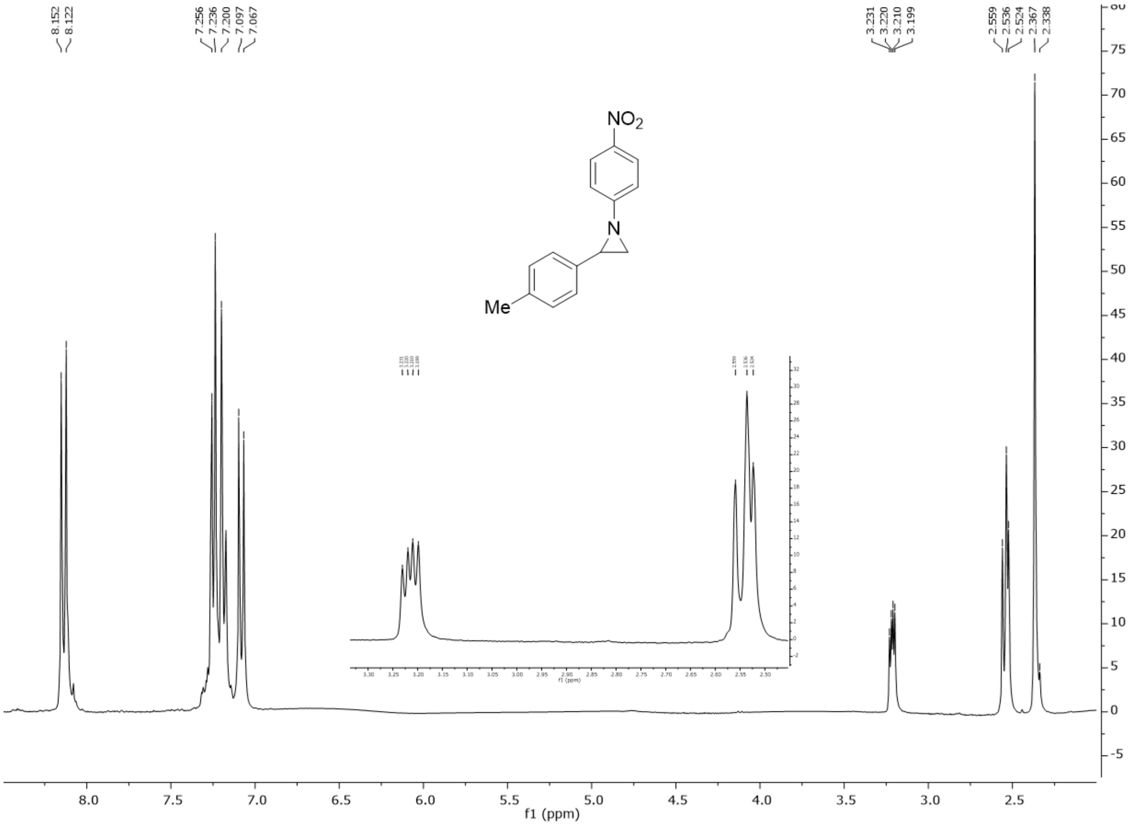
Compound (7): ^{13}C NMR (100 MHz, $CDCl_3$)



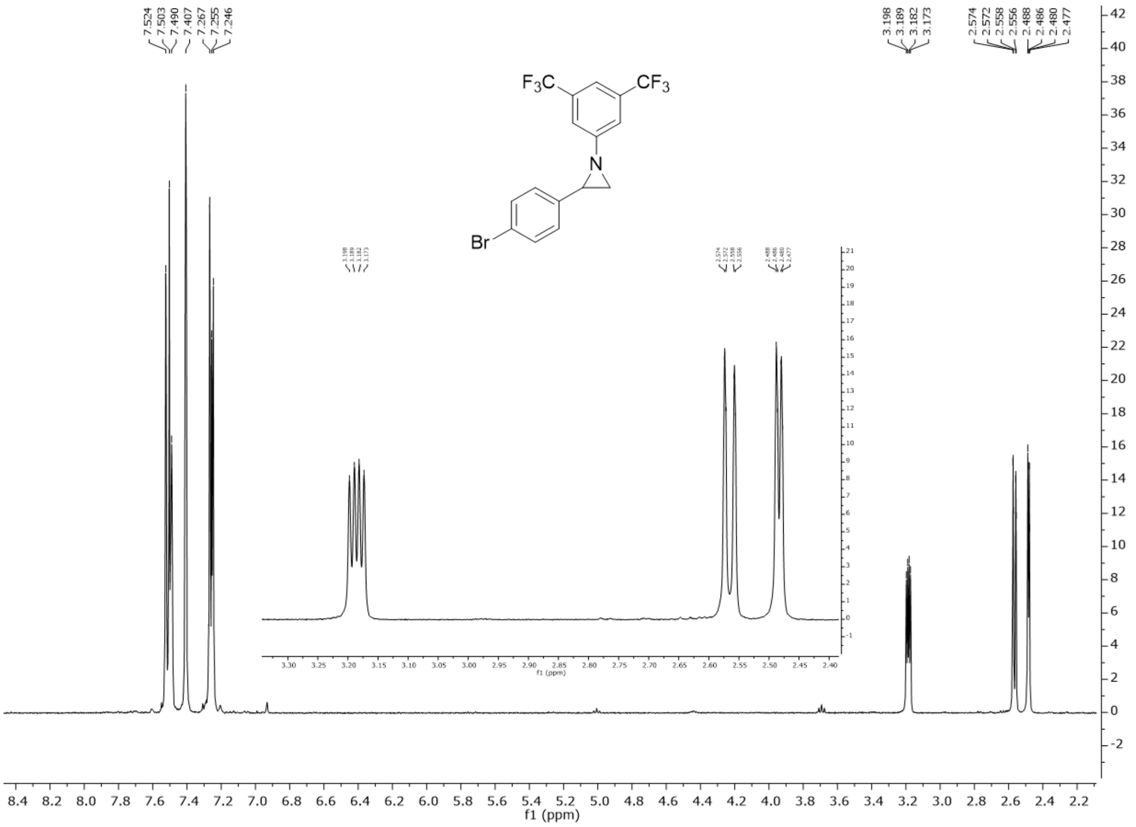
Compound (7): ^{19}F NMR (376 MHz, $CDCl_3$)



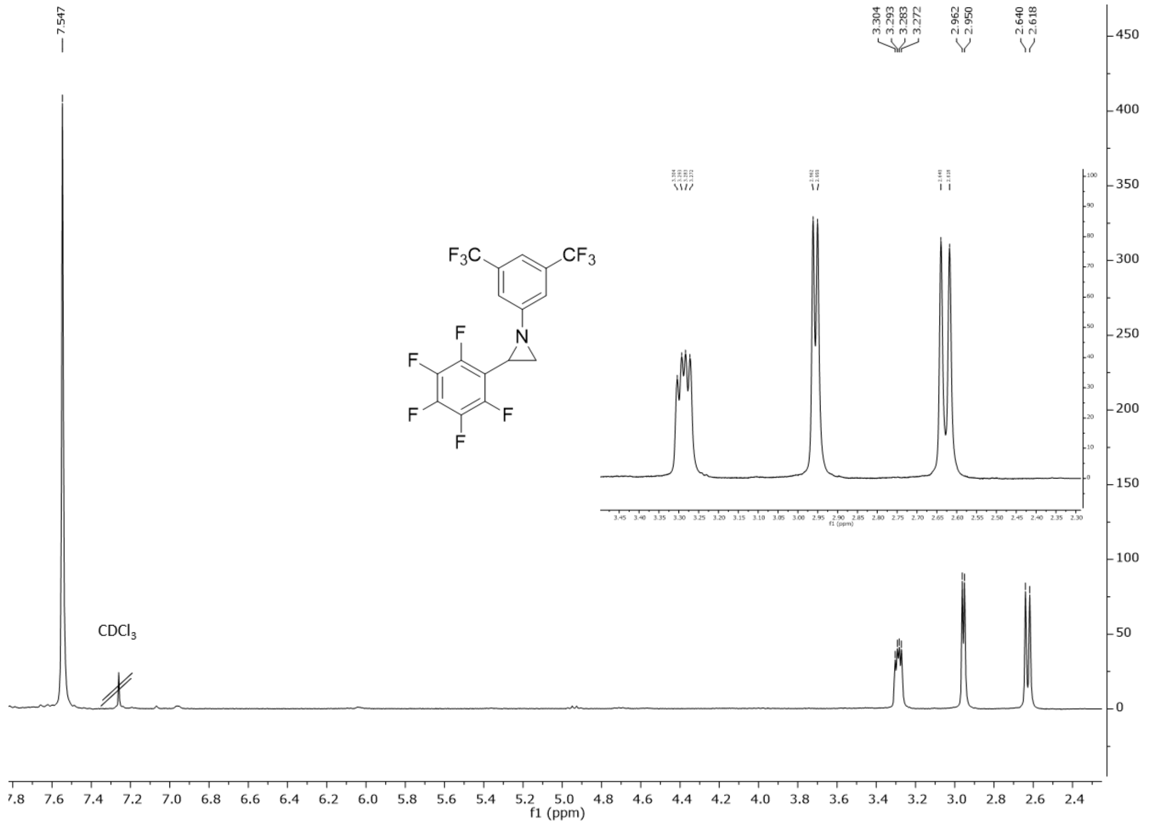
Compound (9): ^{1}H NMR (300 MHz, $CDCl_3$)



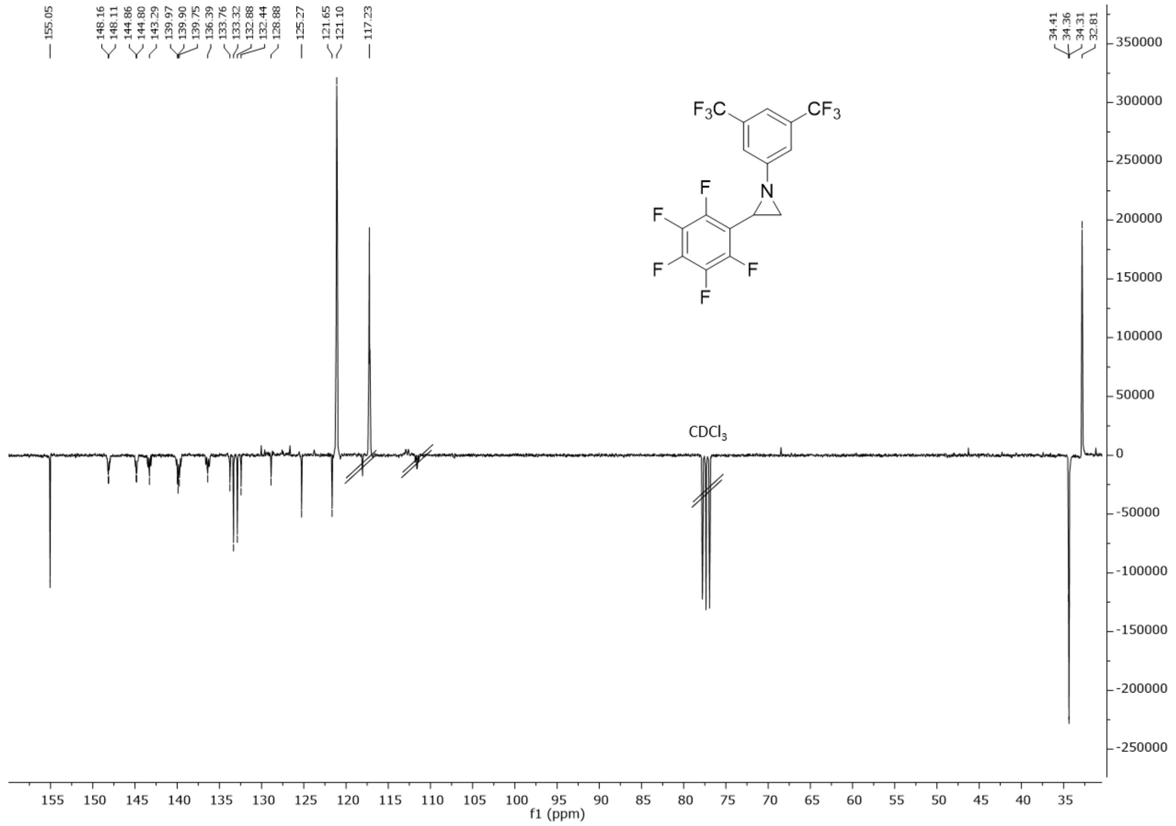
Compound (11): ^{1}H NMR (300 MHz, $CDCl_3$)



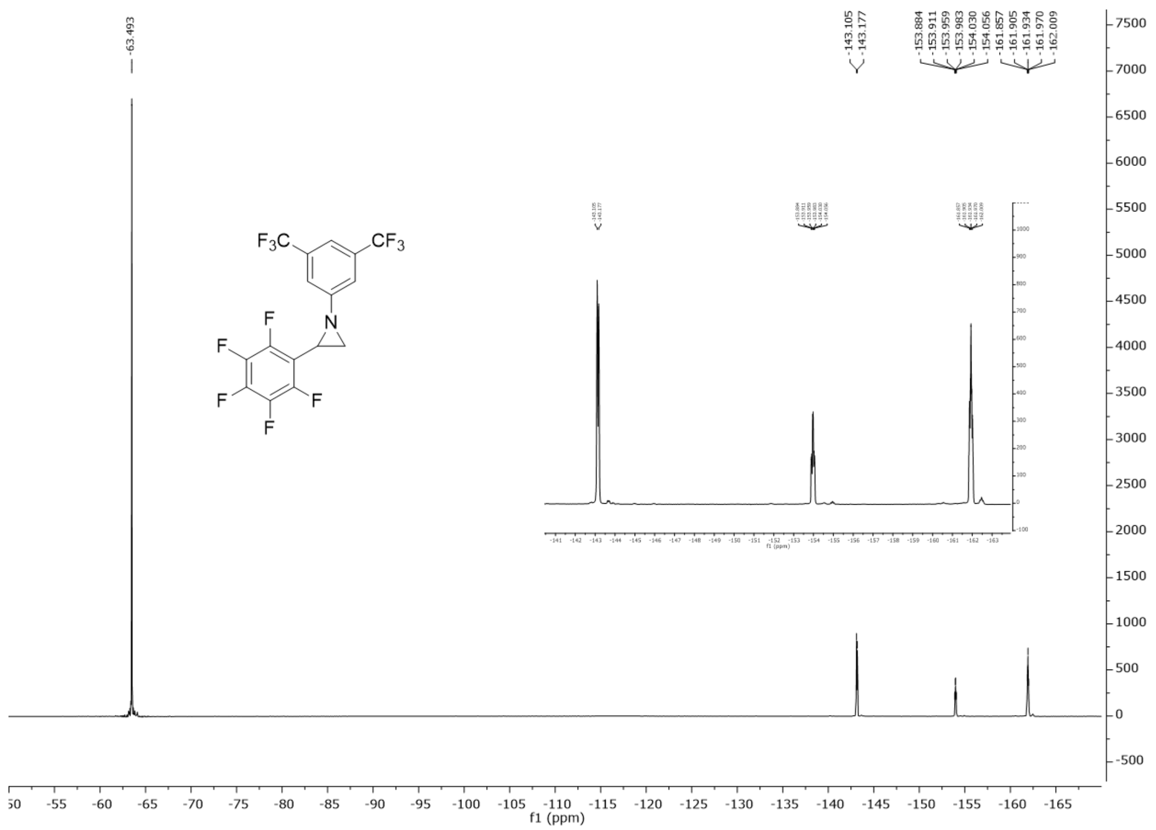
Compound (13): ^{1}H NMR (300 MHz, $CDCl_3$)



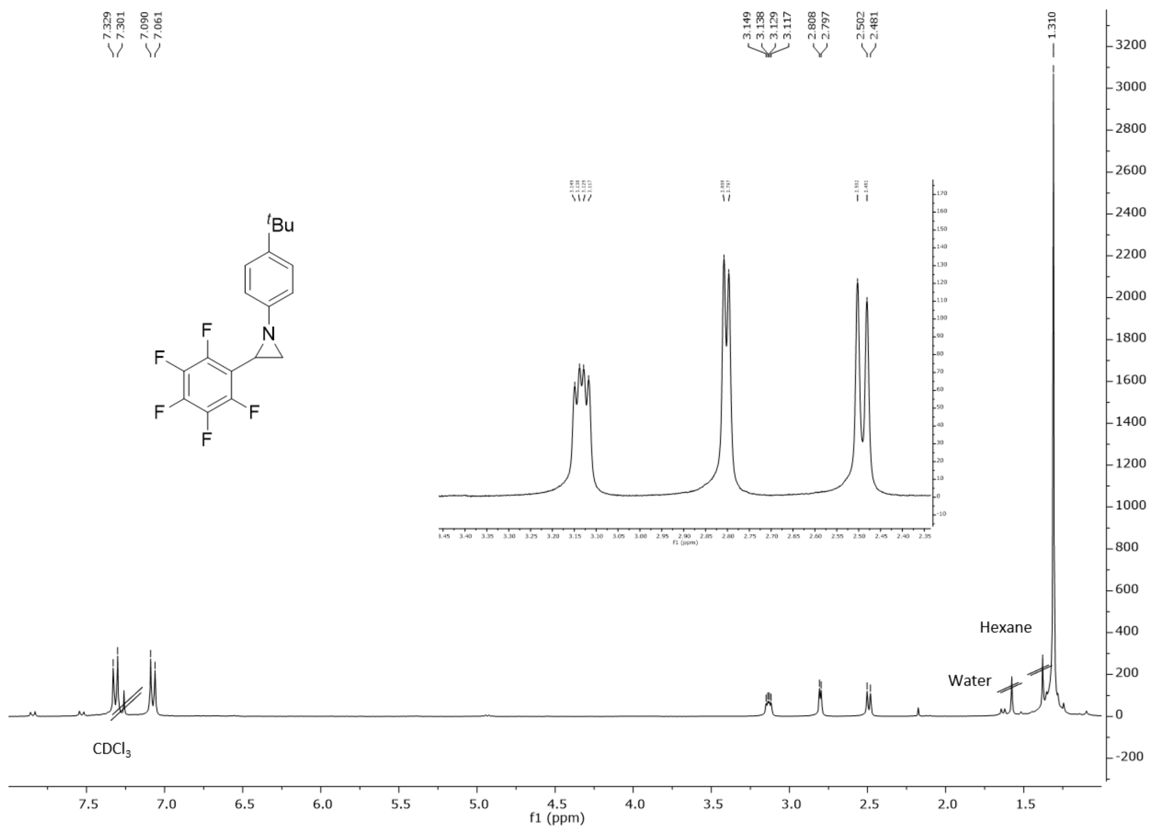
Compound (13): ^{13}C NMR (75 MHz, $CDCl_3$)



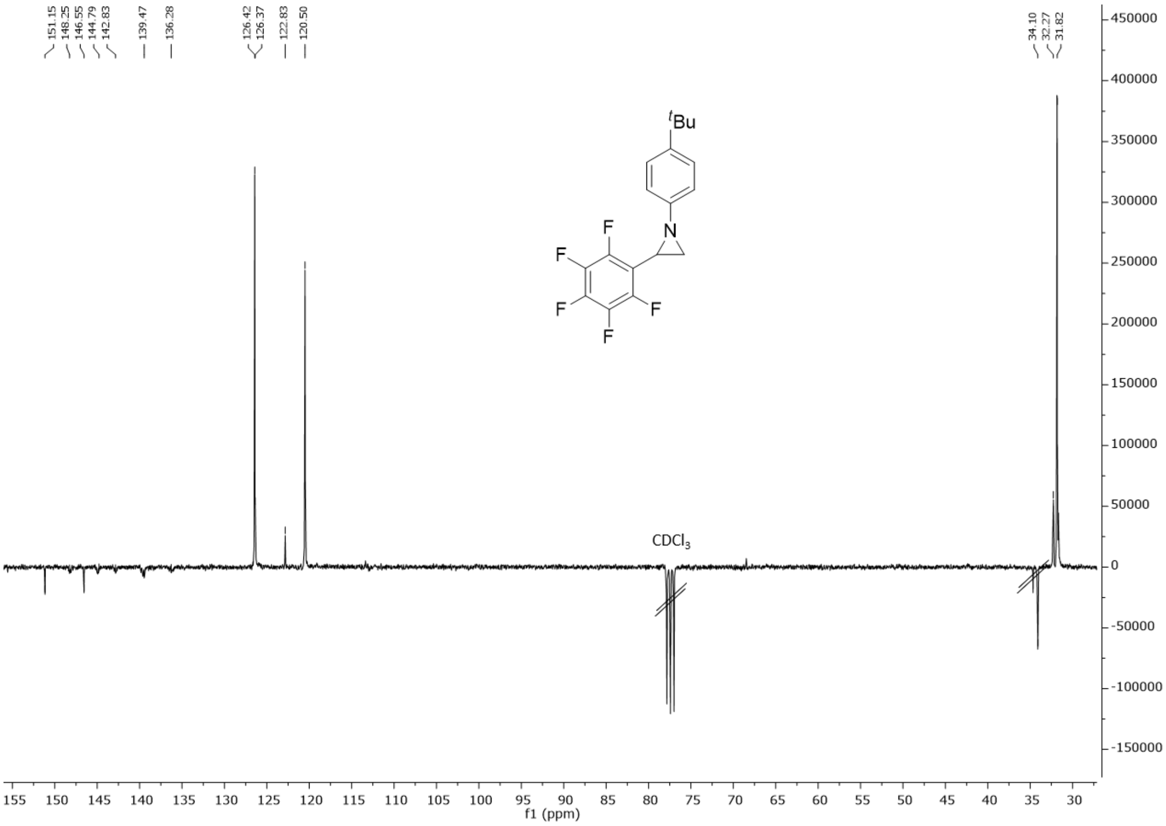
Compound (13): ^{19}F NMR (282 MHz, $CDCl_3$)



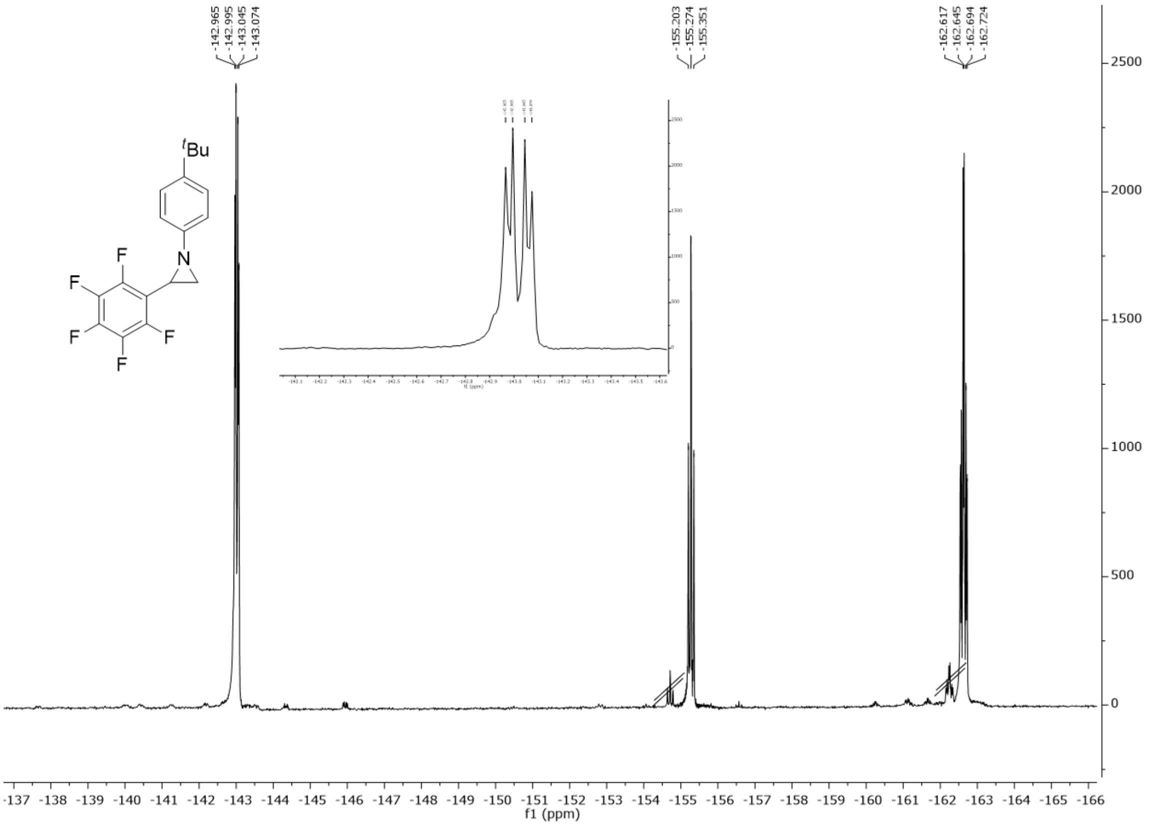
Compound (15): ^{1}H NMR (300 MHz, $CDCl_3$)



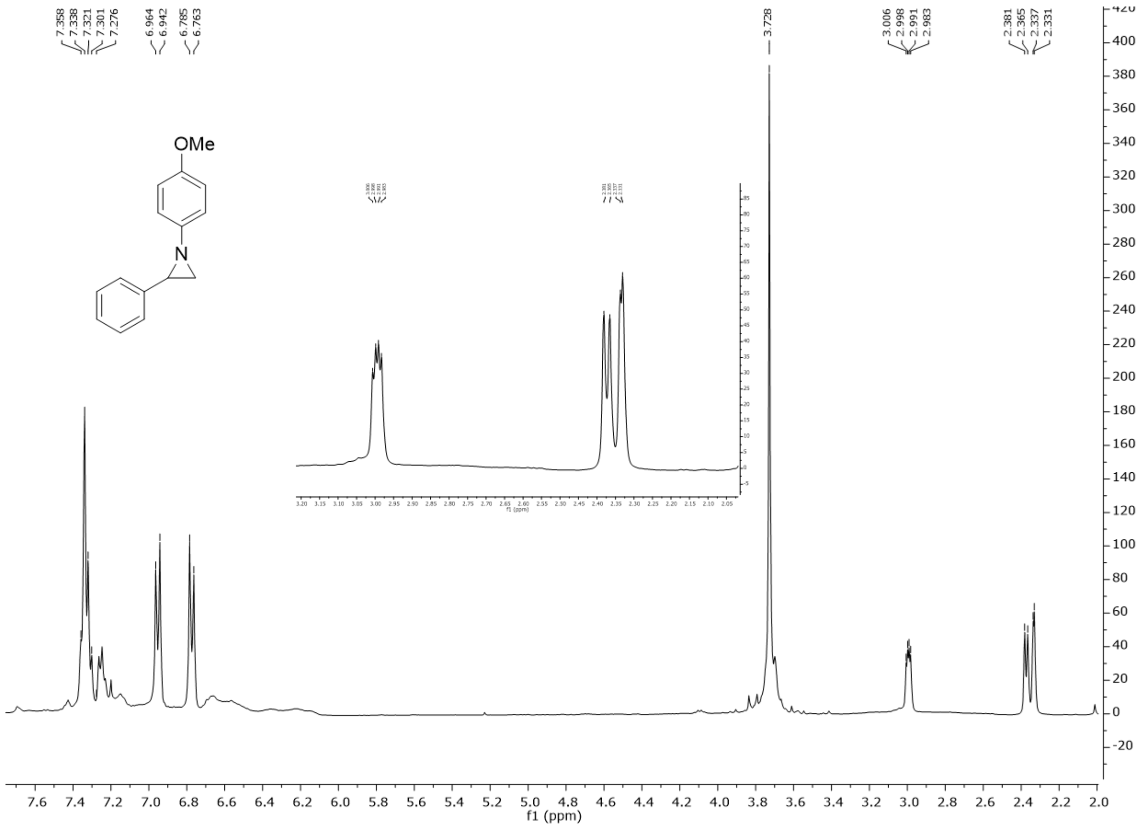
Compound (15): ^{13}C NMR (75 MHz, $CDCl_3$)



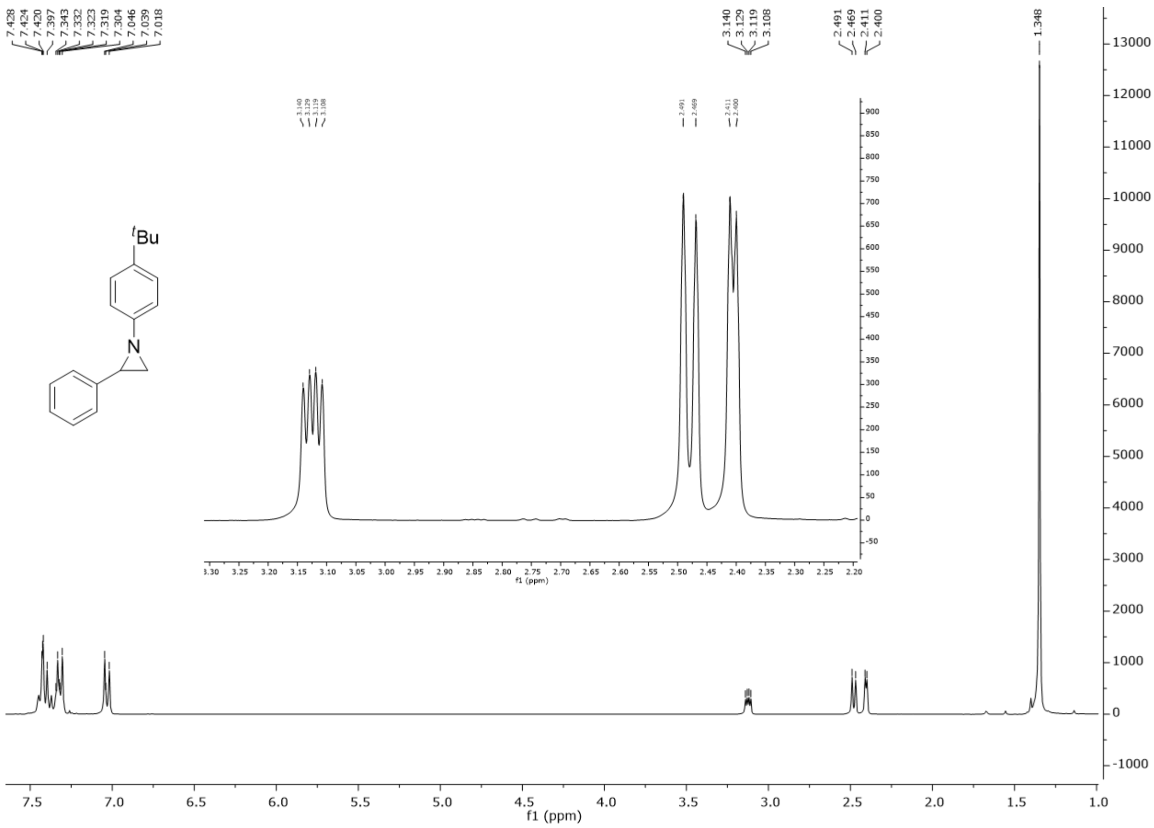
Compound (15): ^{19}F NMR (282 MHz, $CDCl_3$)



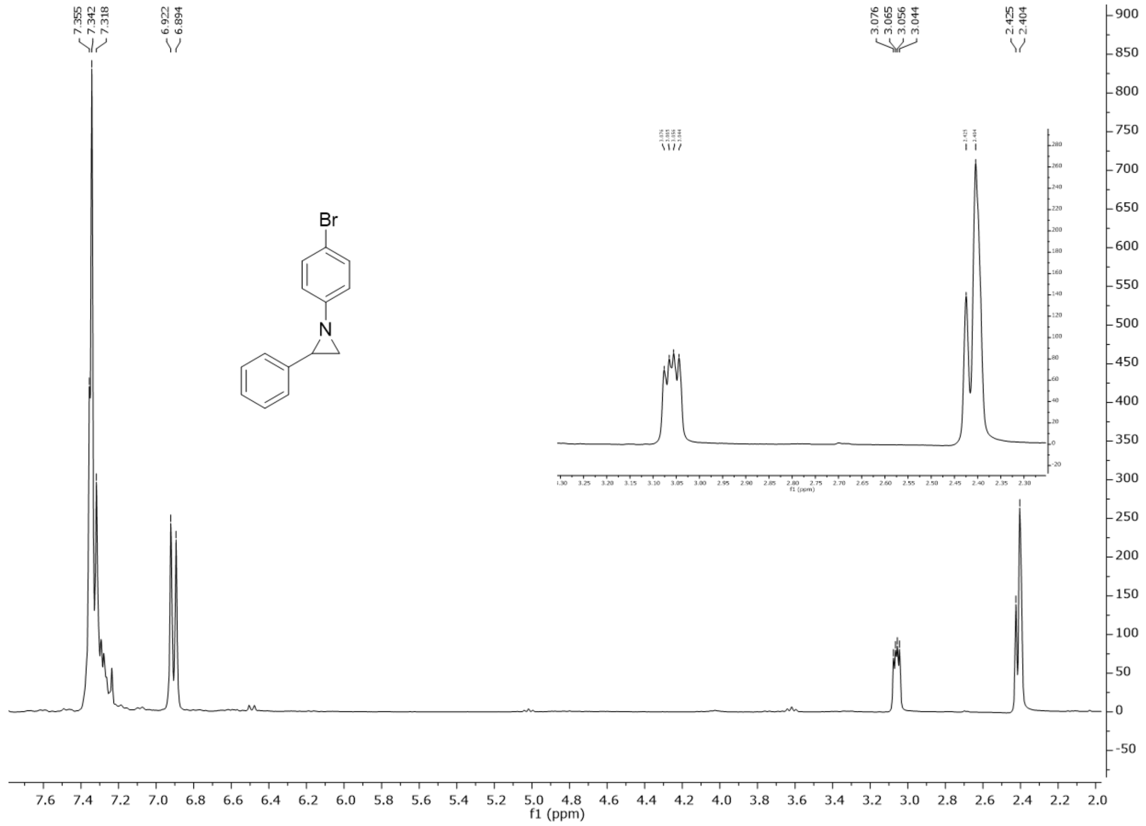
Compound (17): ^{1}H NMR (400 MHz, $CDCl_3$)



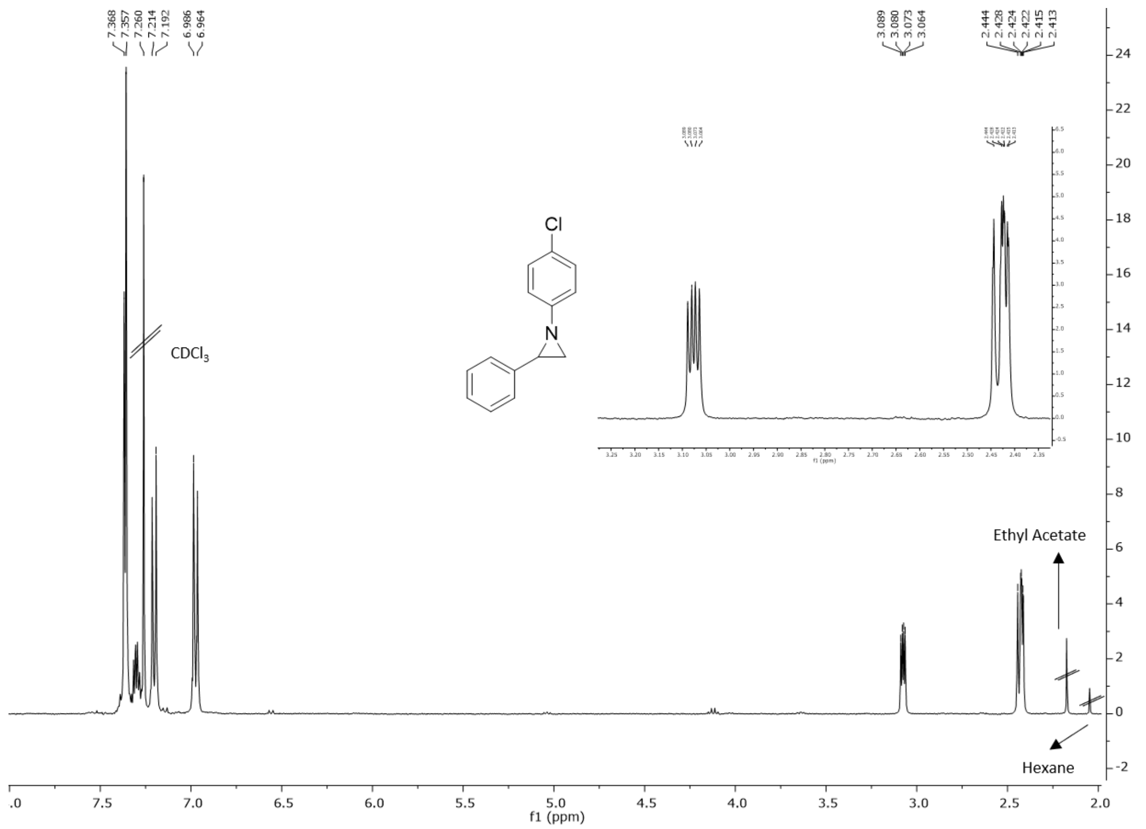
Compound (19): ^{1}H NMR (400 MHz, $CDCl_3$)



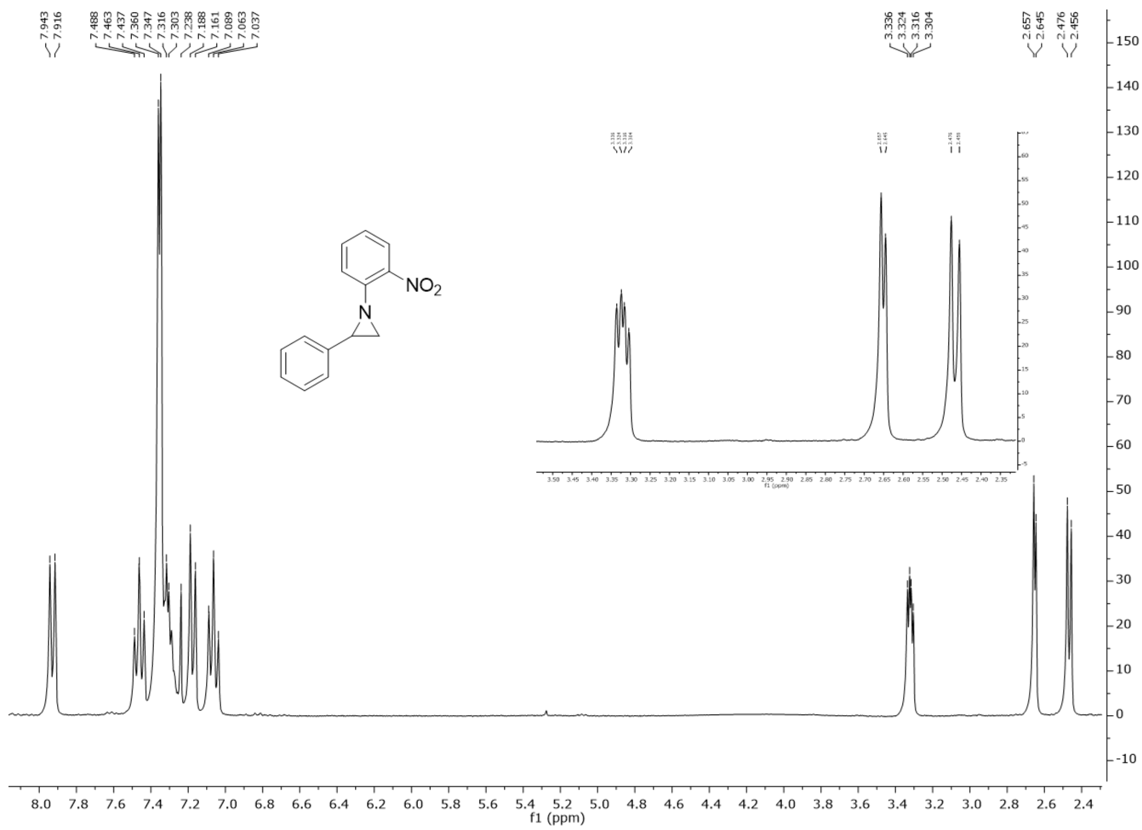
Compound (21): ^{1}H NMR (400 MHz, $CDCl_3$)



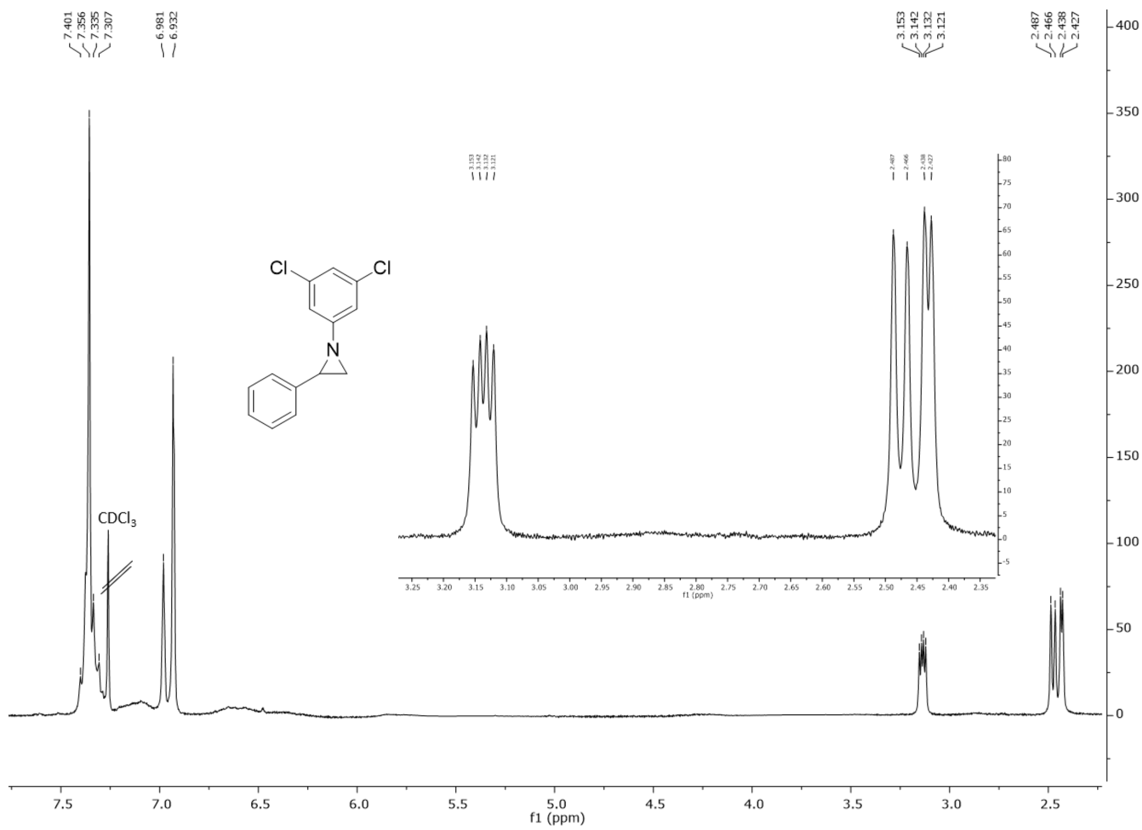
Compound (23): ^{1}H NMR (400 MHz, $CDCl_3$)



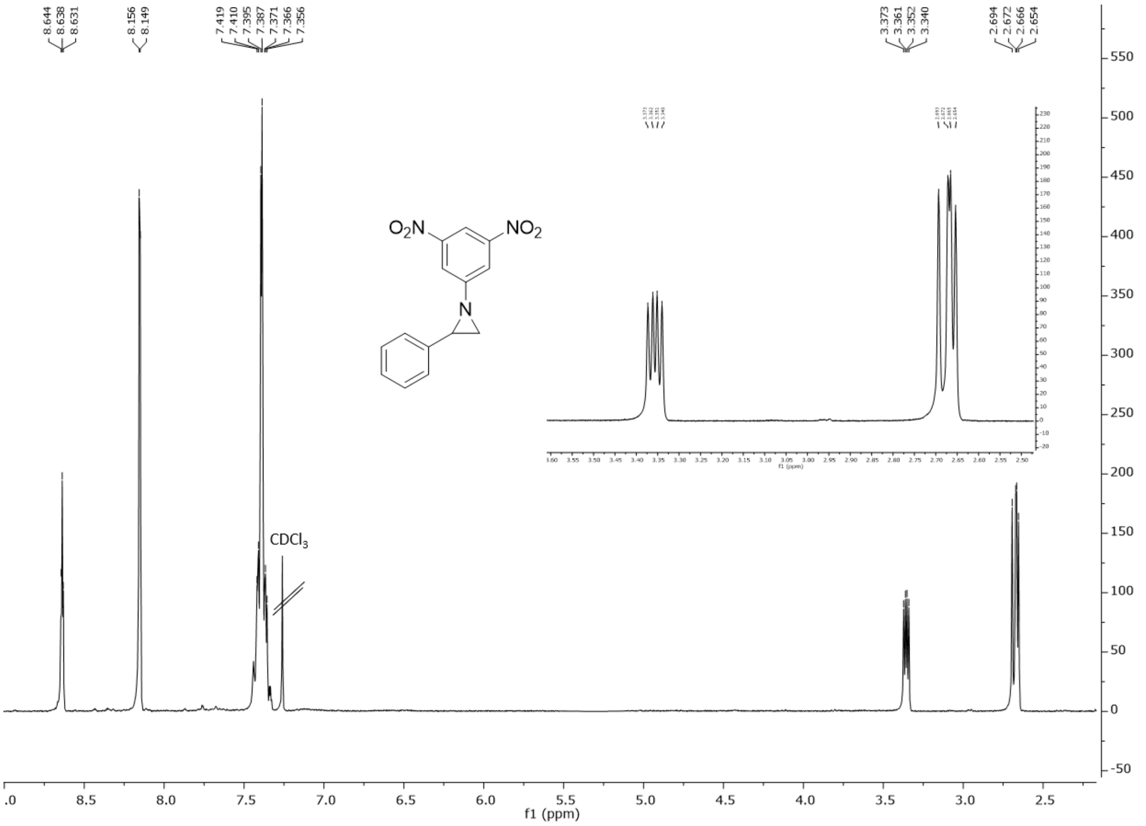
Compound (25): ^{1}H NMR (300 MHz, $CDCl_3$)



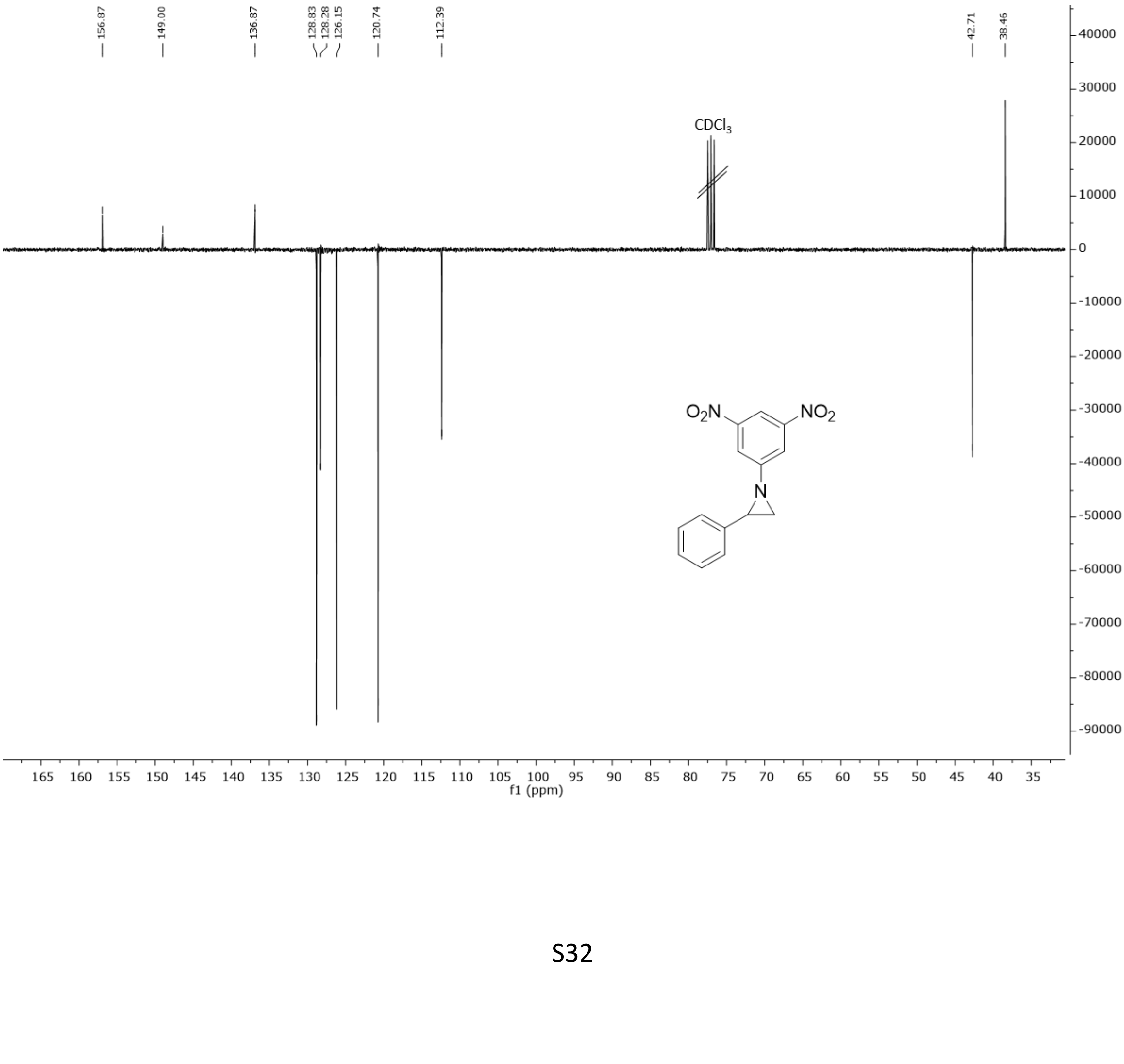
Compound (28): ^{1}H NMR (300 MHz, $CDCl_3$)



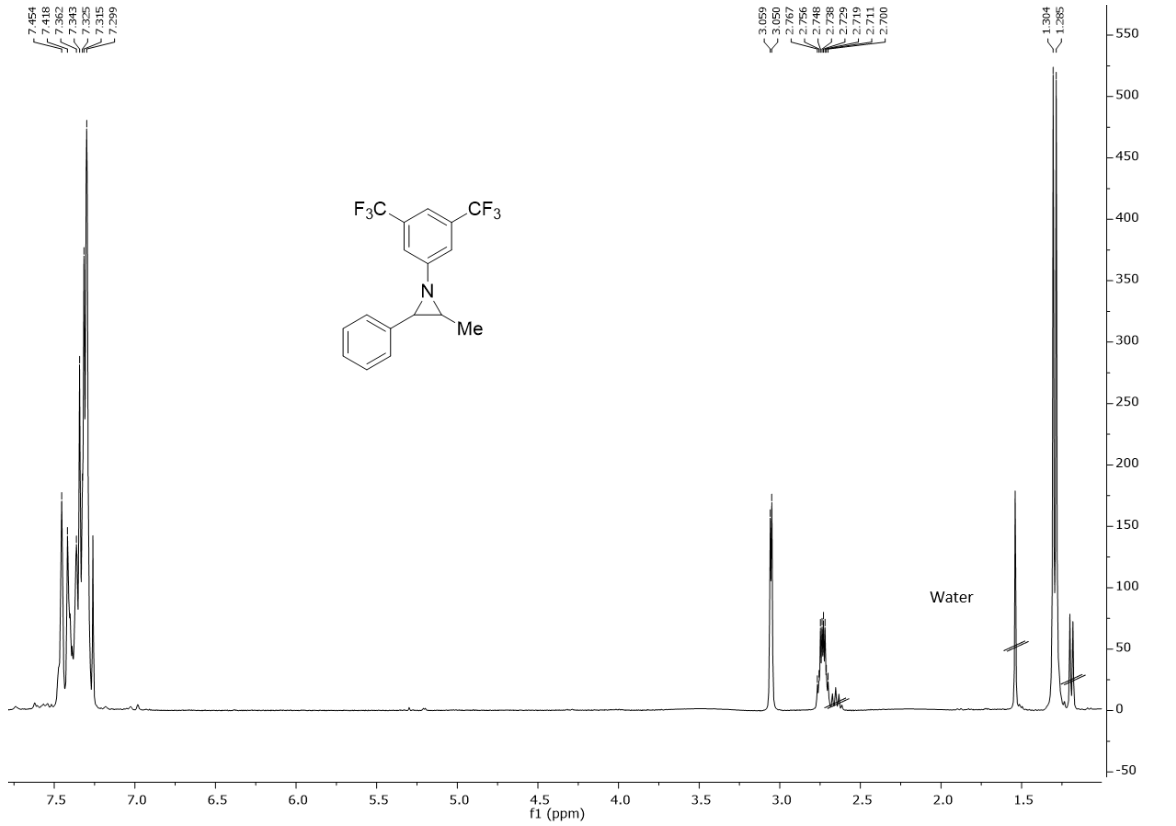
Compound (30): ^{1}H NMR (300 MHz, $CDCl_3$)



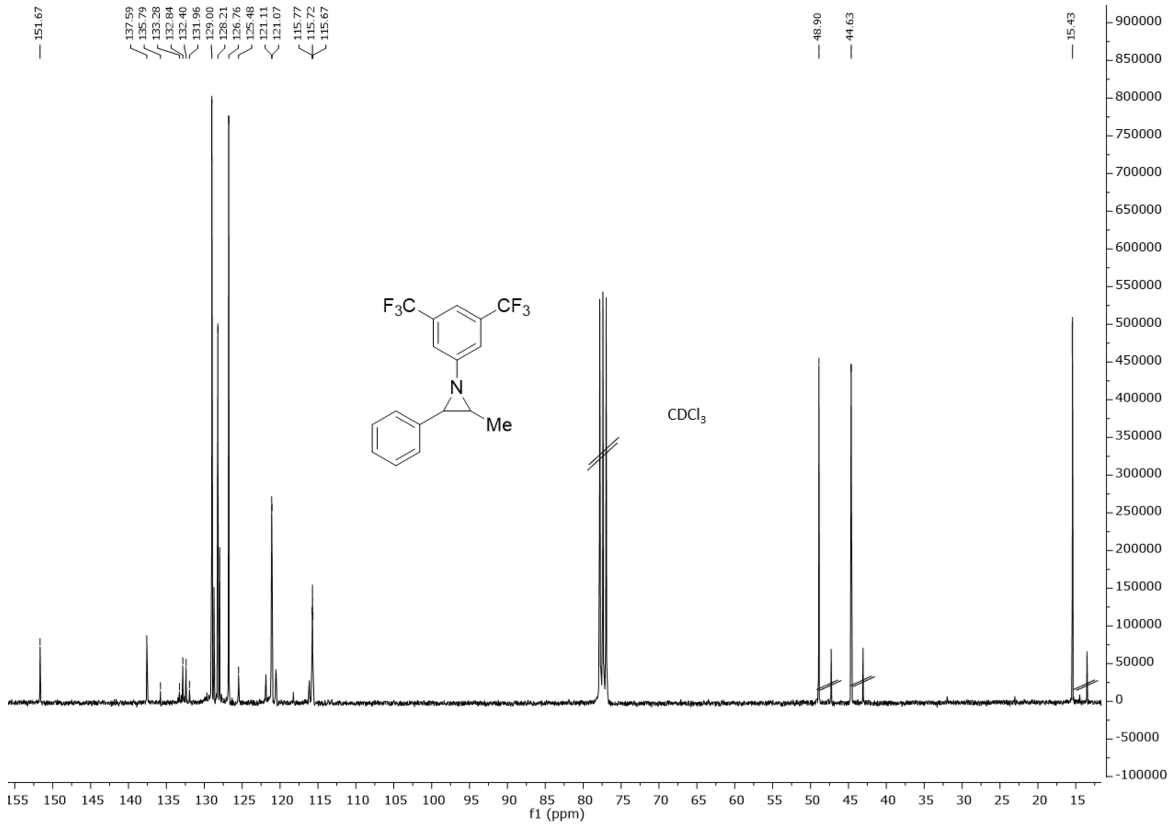
Compound (30): ^{13}C NMR (75 MHz, $CDCl_3$)



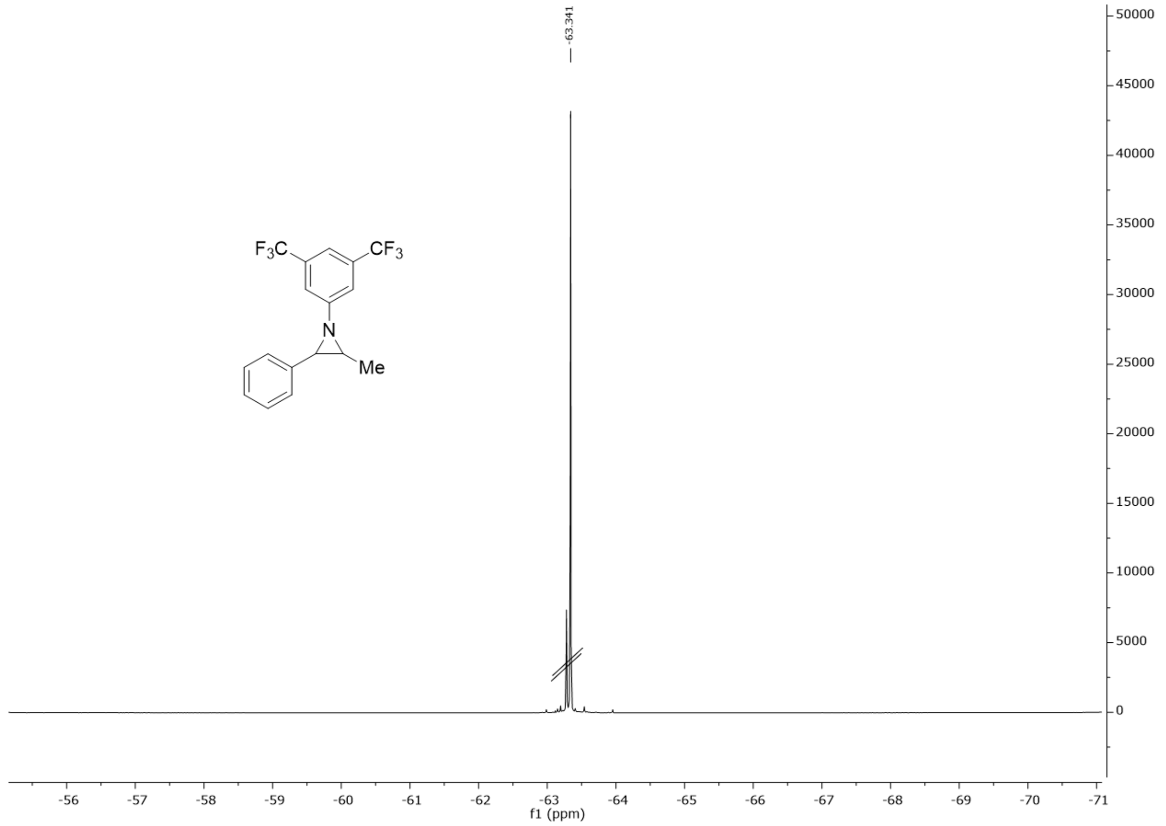
Compound (32): ^{1}H NMR (300 MHz, $CDCl_3$)



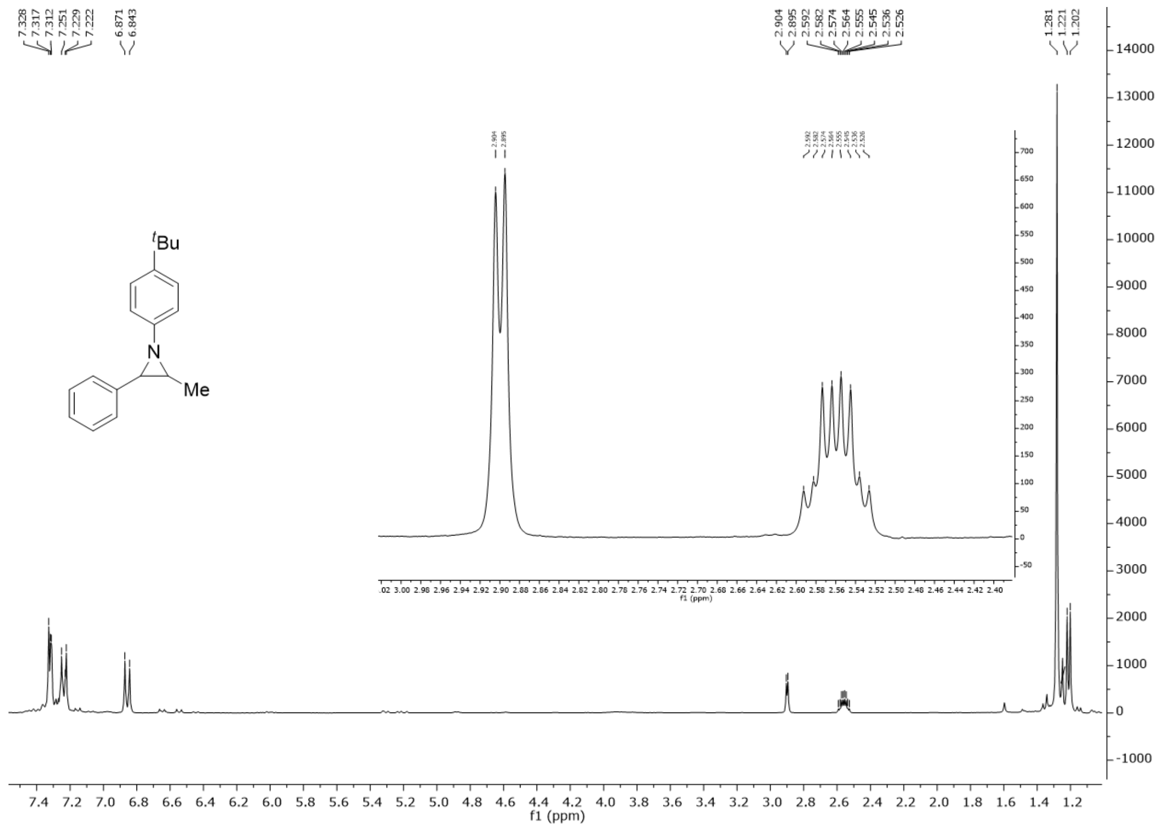
Compound (32): ^{13}C NMR (75 MHz, $CDCl_3$)



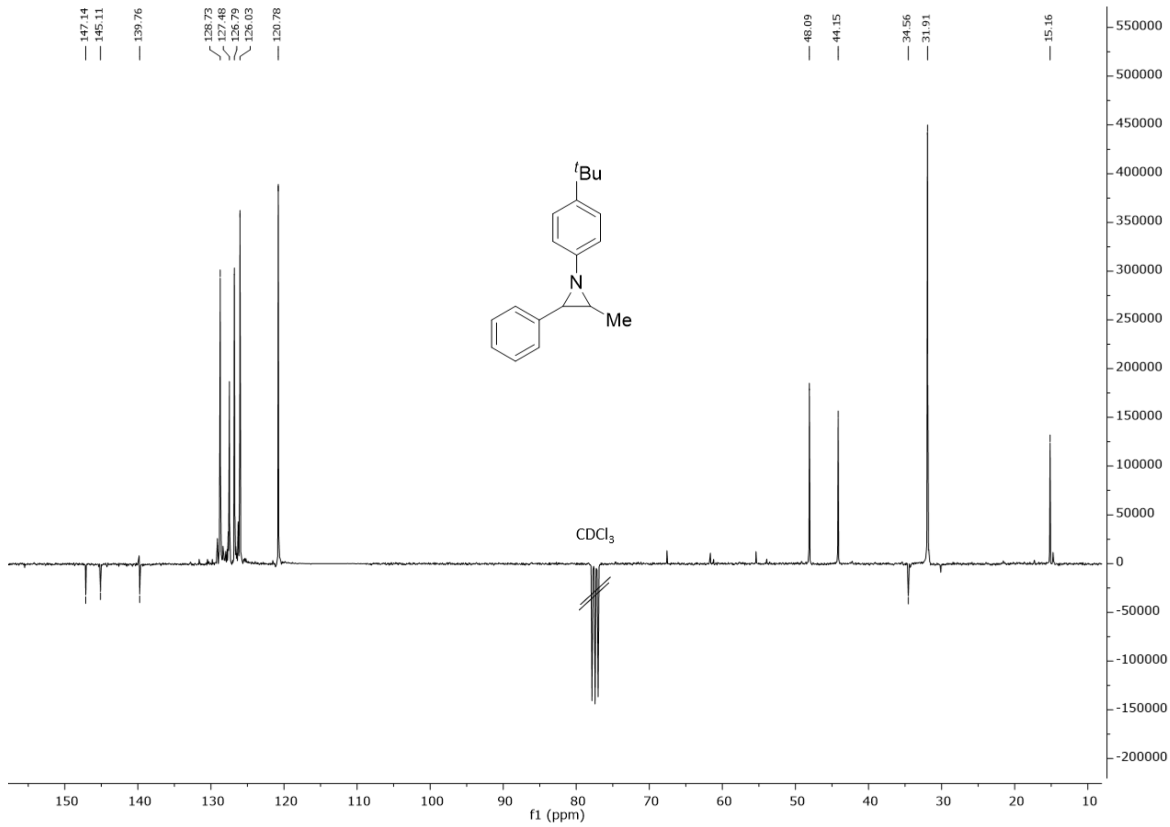
Compound (32): ^{19}F NMR (282 MHz, $CDCl_3$)



Compound (34): ^{1}H NMR (300 MHz, $CDCl_3$)

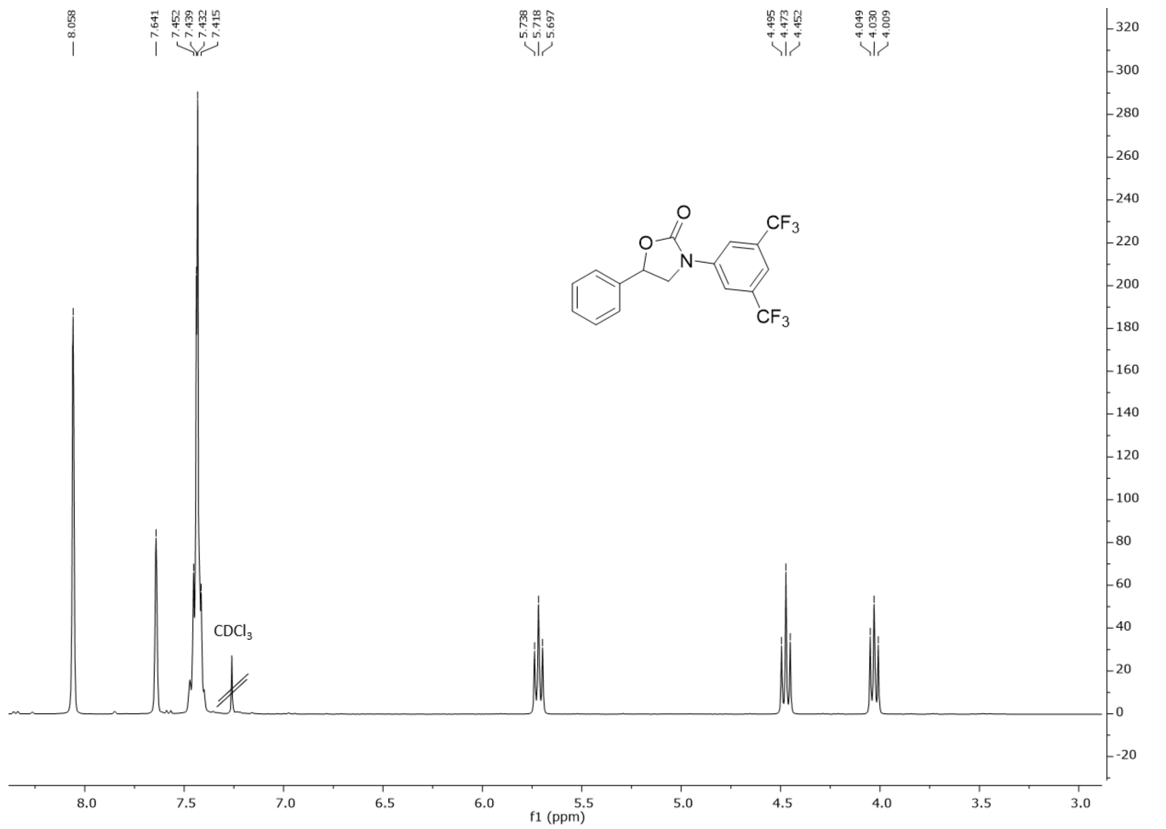


Compound (34): ^{13}C NMR (75 MHz, $CDCl_3$)

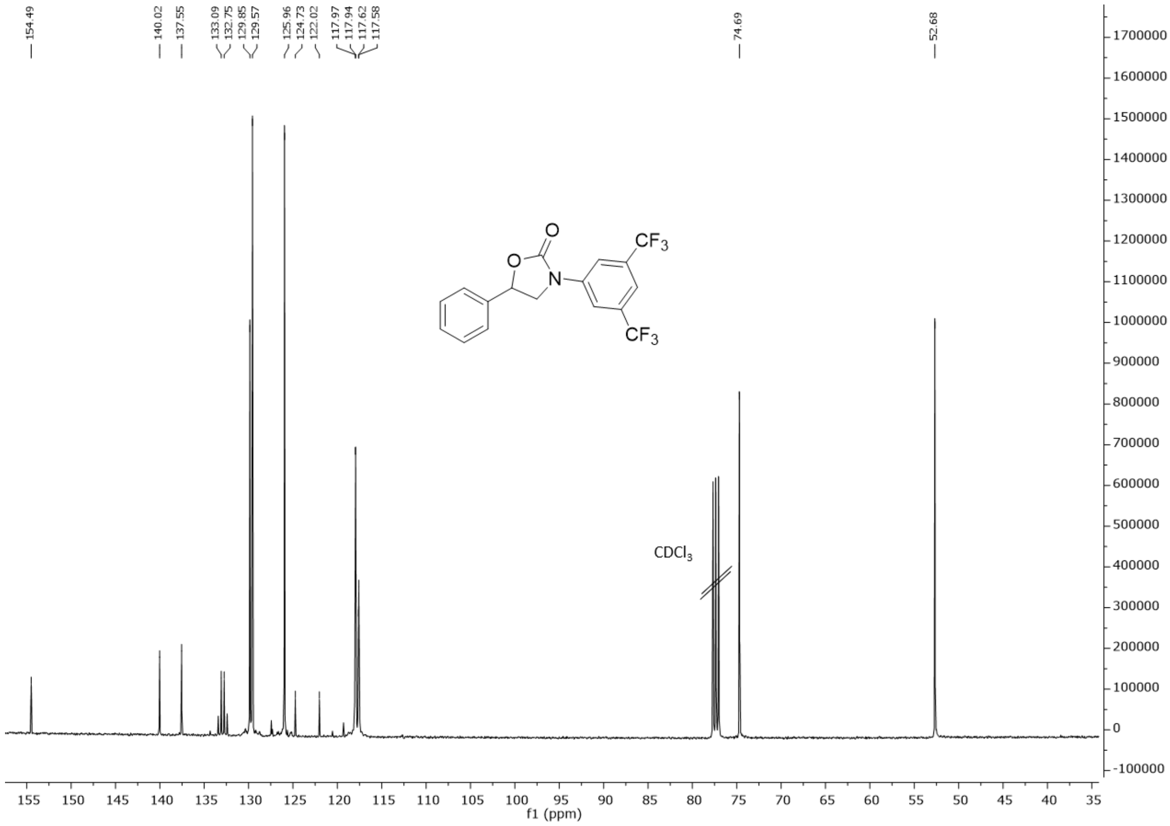


6.2 NMR spectra of oxazolidinones

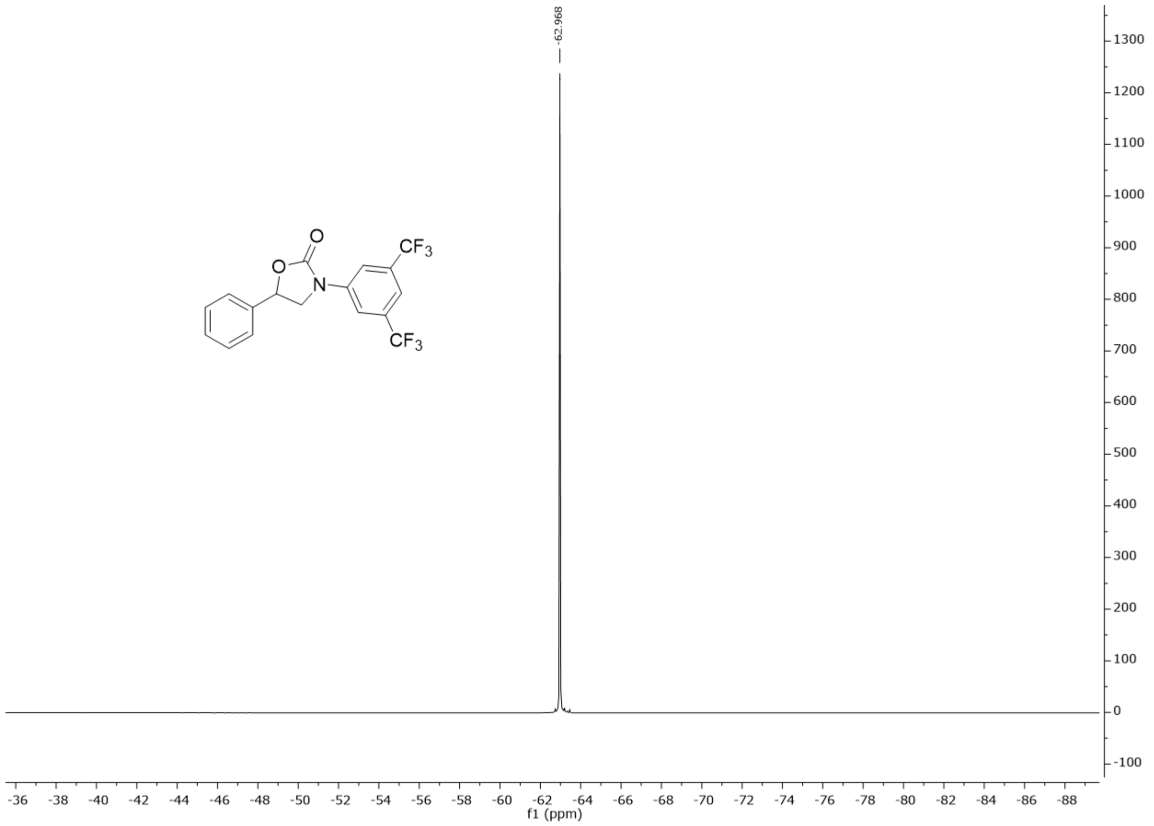
Compound (2a): ^{1}H NMR (400 MHz, $CDCl_3$)



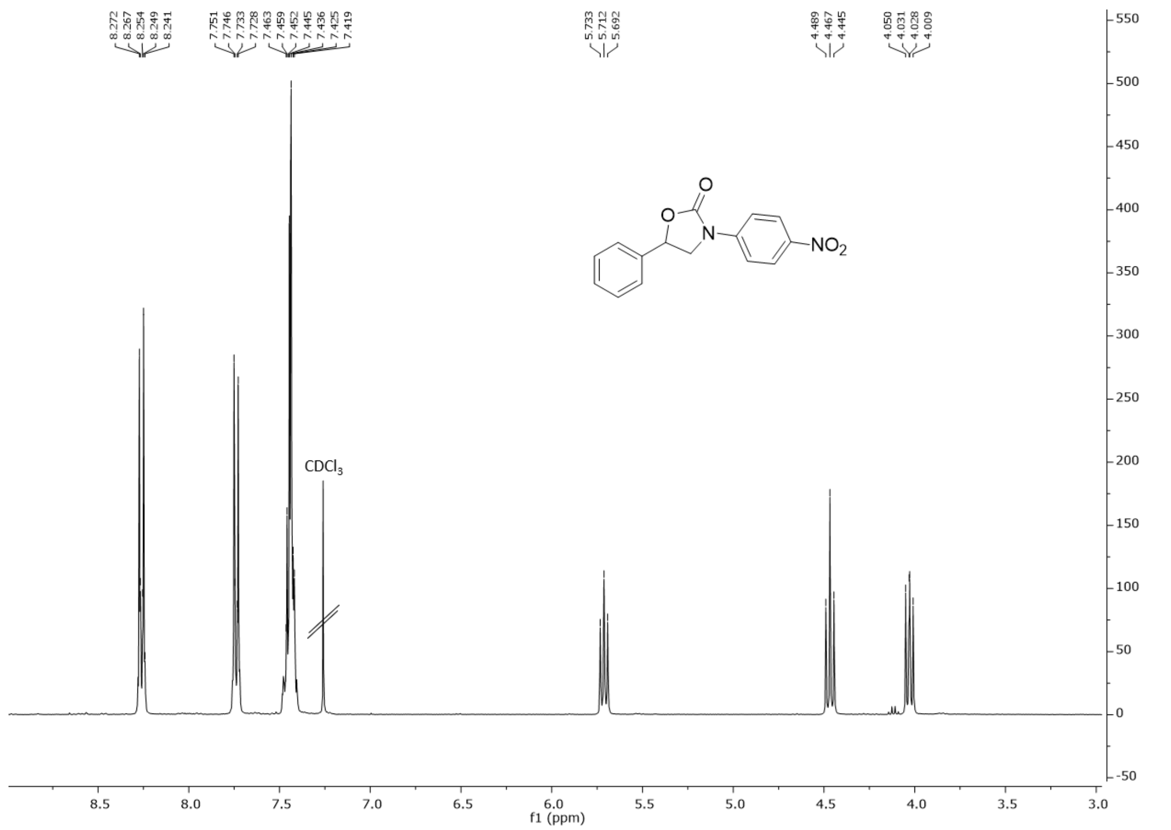
Compound (2a): ^{13}C NMR (100 MHz, CDCl$_3$)



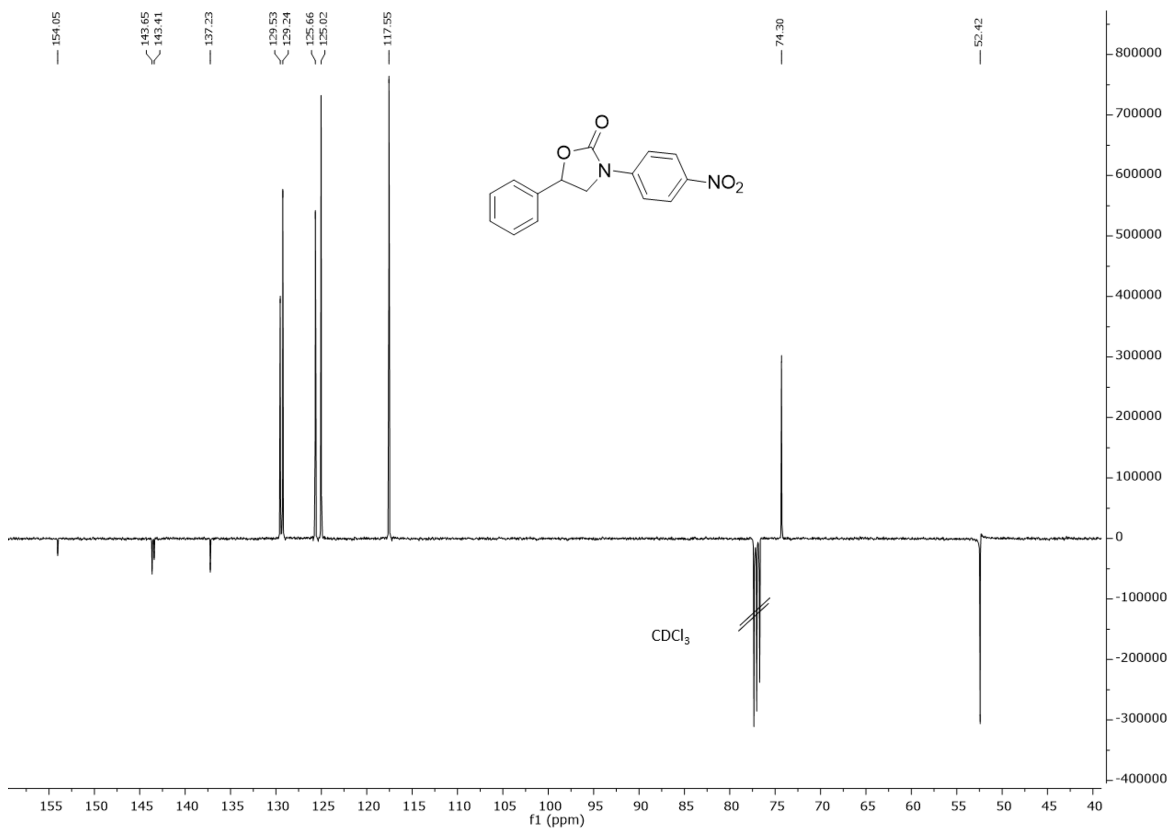
Compound (2a): ^{19}F NMR (376 MHz, CDCl$_3$)



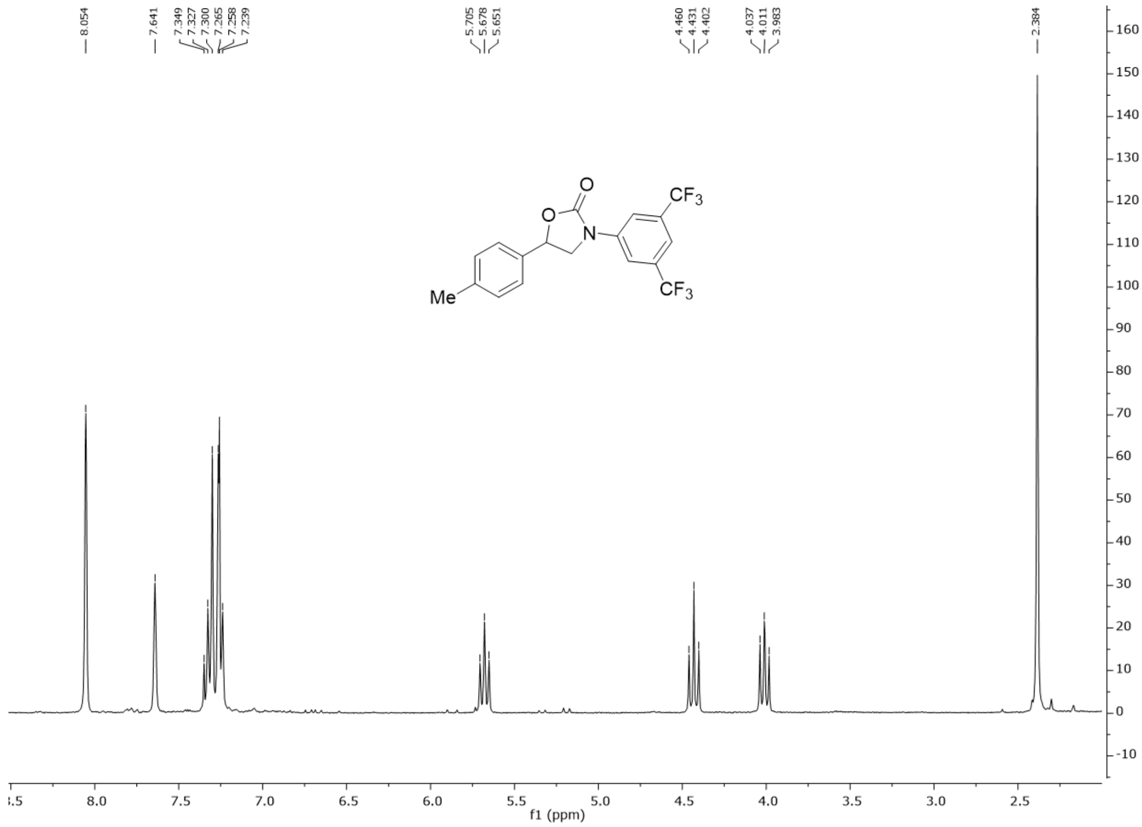
Compound (4a): ^{1}H NMR (400 MHz, $CDCl_3$)



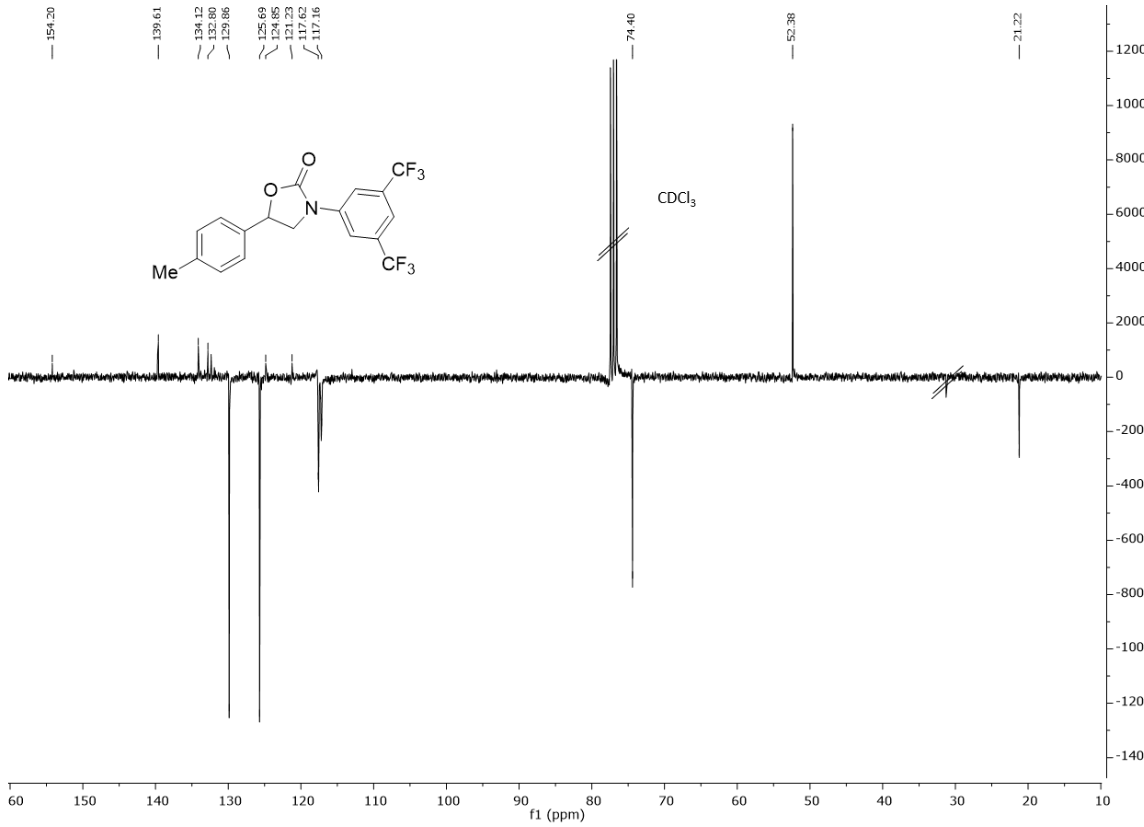
Compound (4a): ^{13}C NMR (100 MHz, $CDCl_3$)



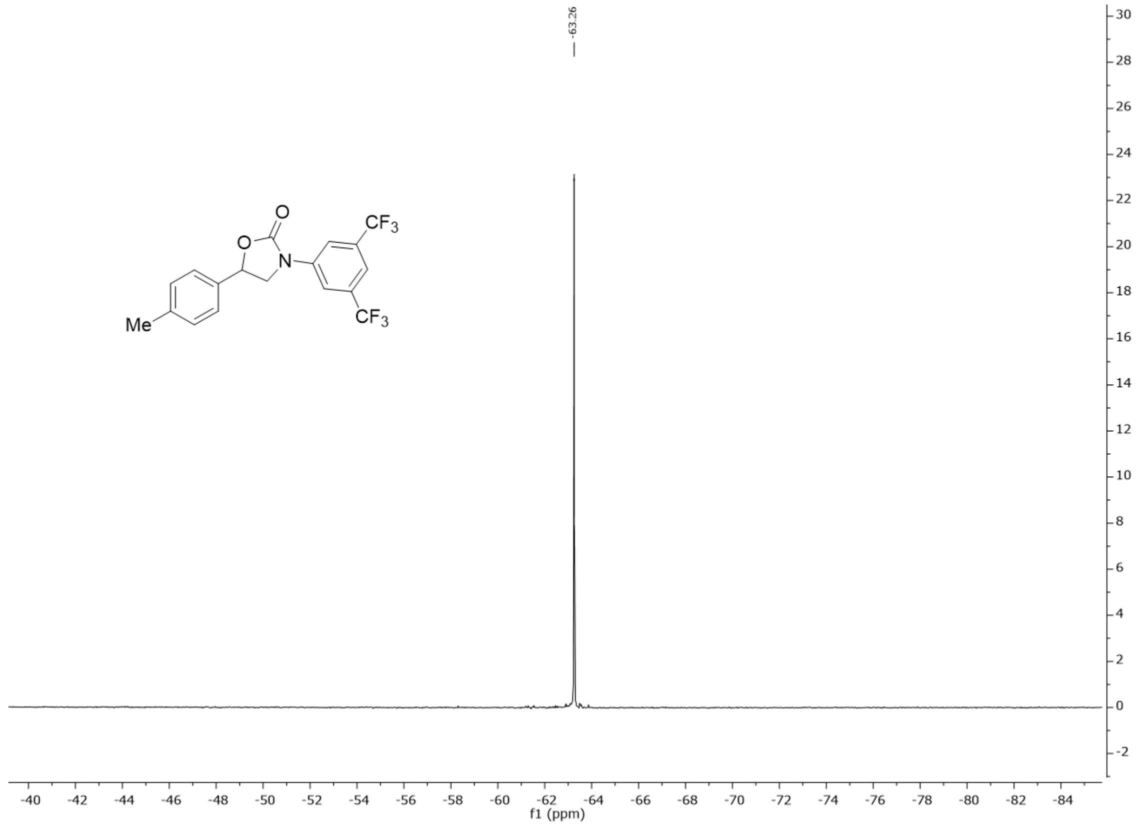
Compound (6a): ^{1}H NMR (300 MHz, $CDCl_3$)



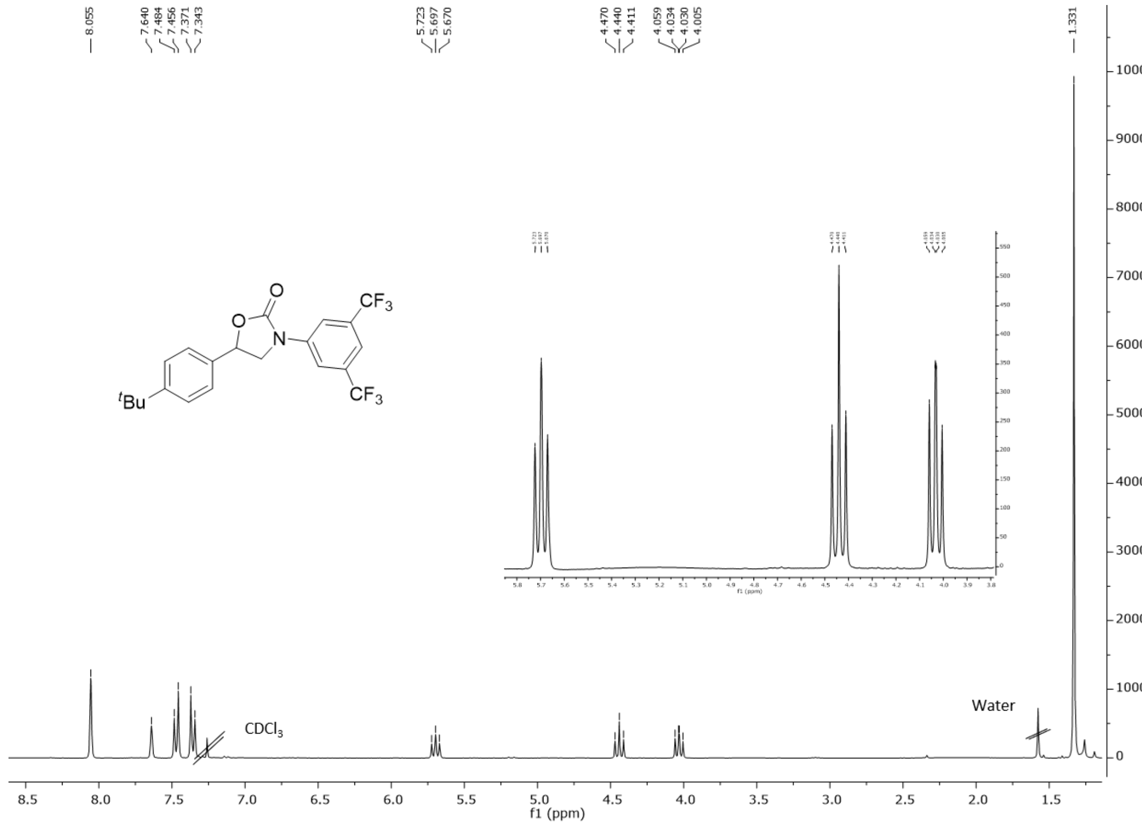
Compound (6a): ^{13}C NMR (75 MHz, $CDCl_3$)



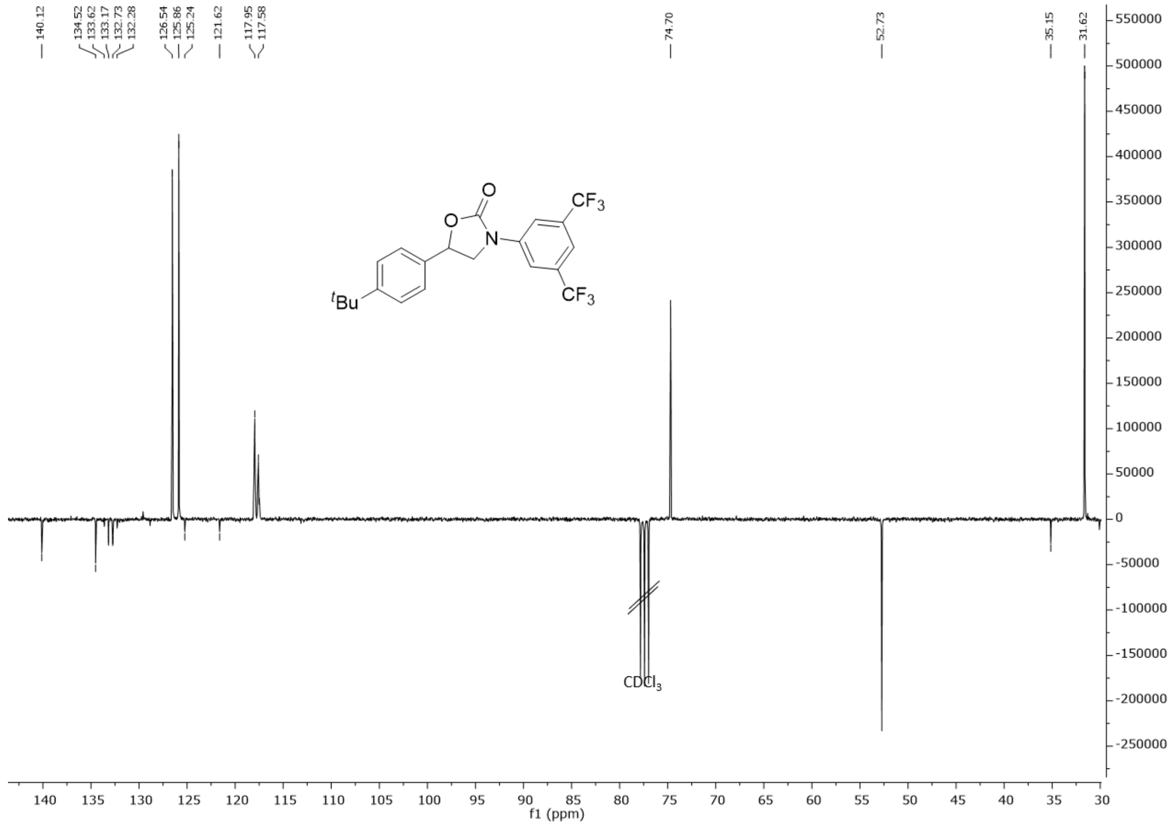
Compound (6a): ^{19}F NMR (282 MHz, $CDCl_3$)



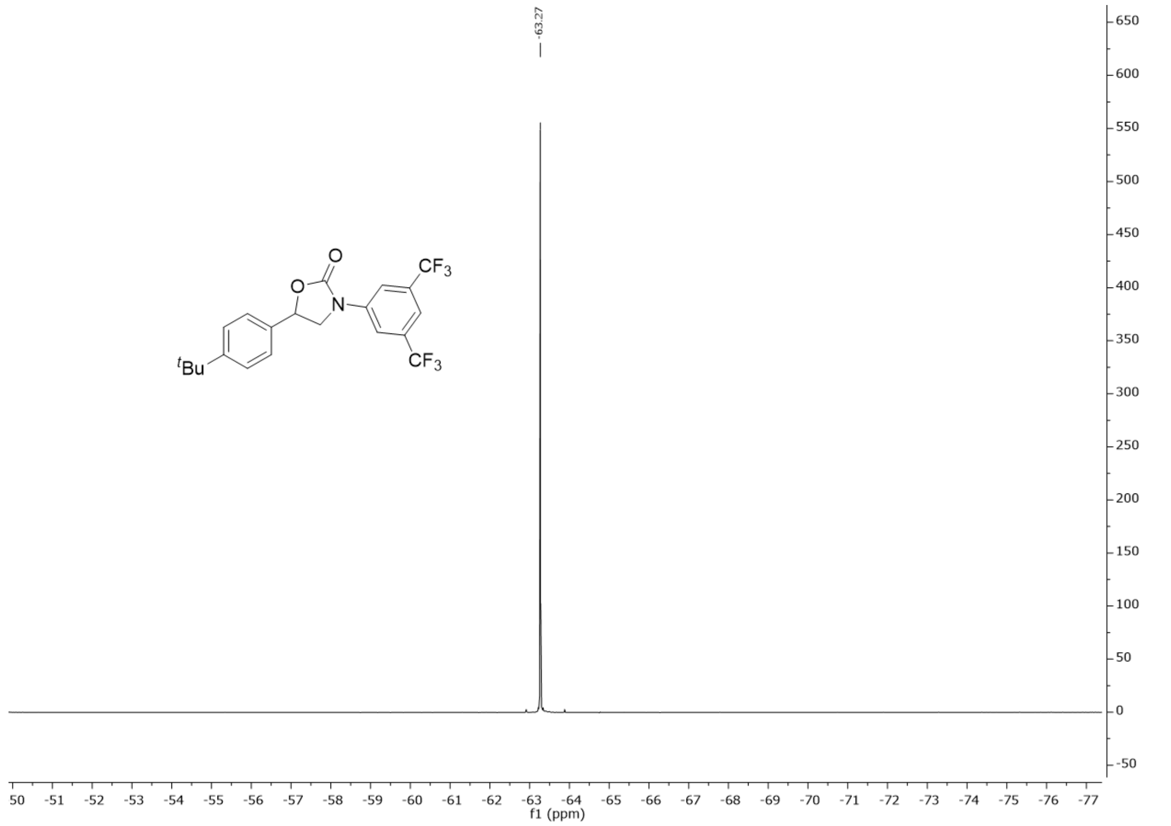
Compound (8a): ^{1}H NMR (300 MHz, $CDCl_3$)



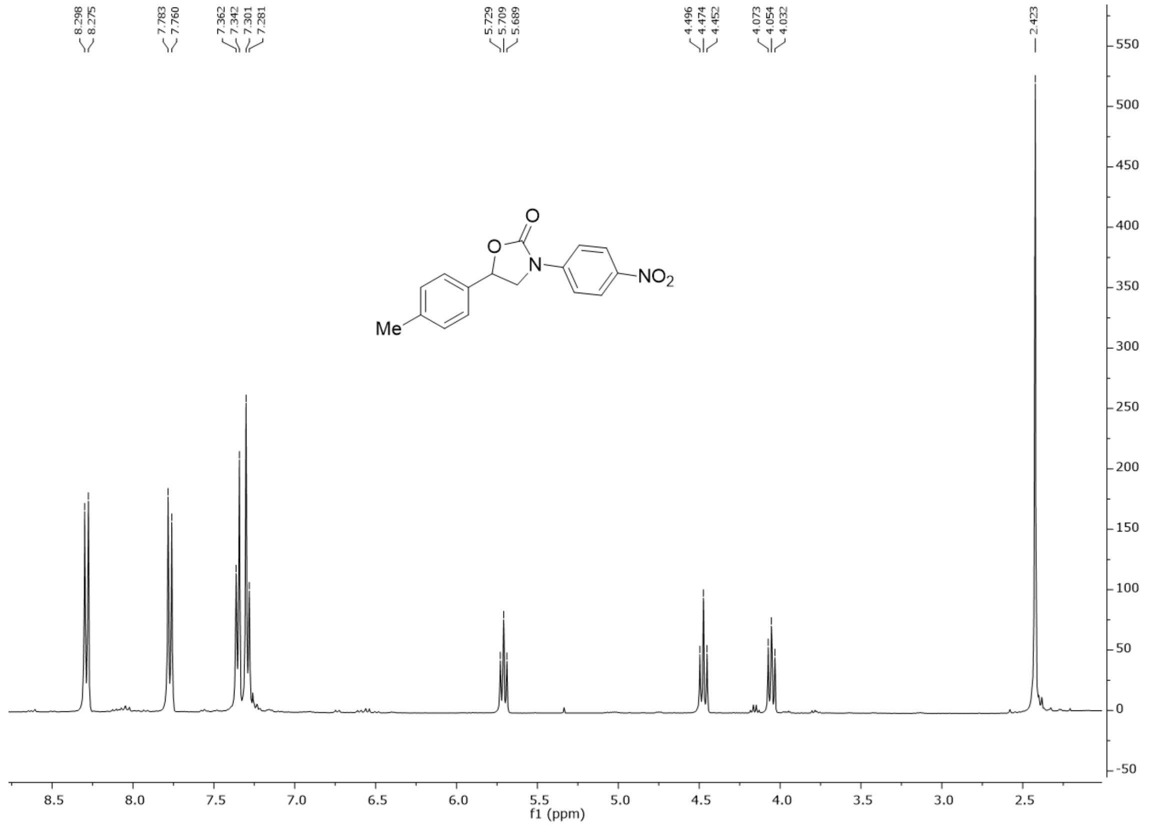
Compound (8a): ^{13}C NMR (75 MHz, $CDCl_3$)



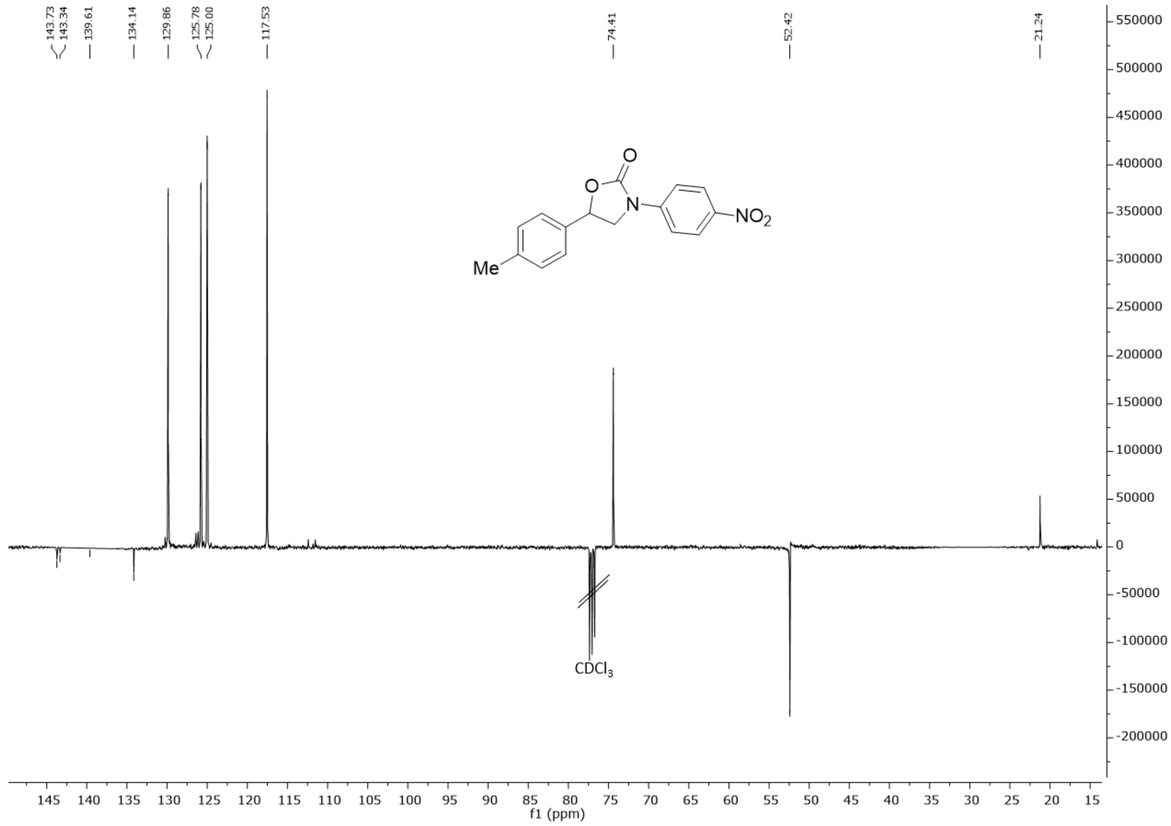
Compound (8a): ^{19}F NMR (282 MHz, $CDCl_3$)



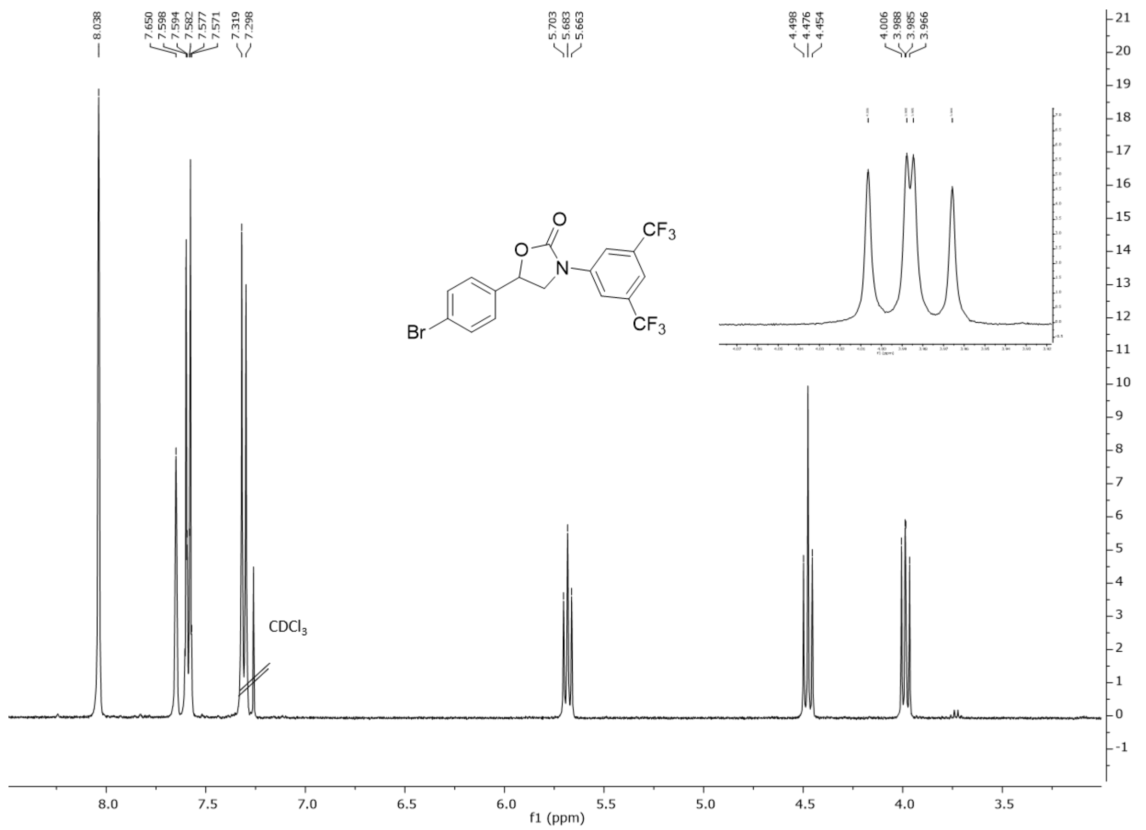
Compound (10a): ^{1}H NMR (400 MHz, $CDCl_3$)



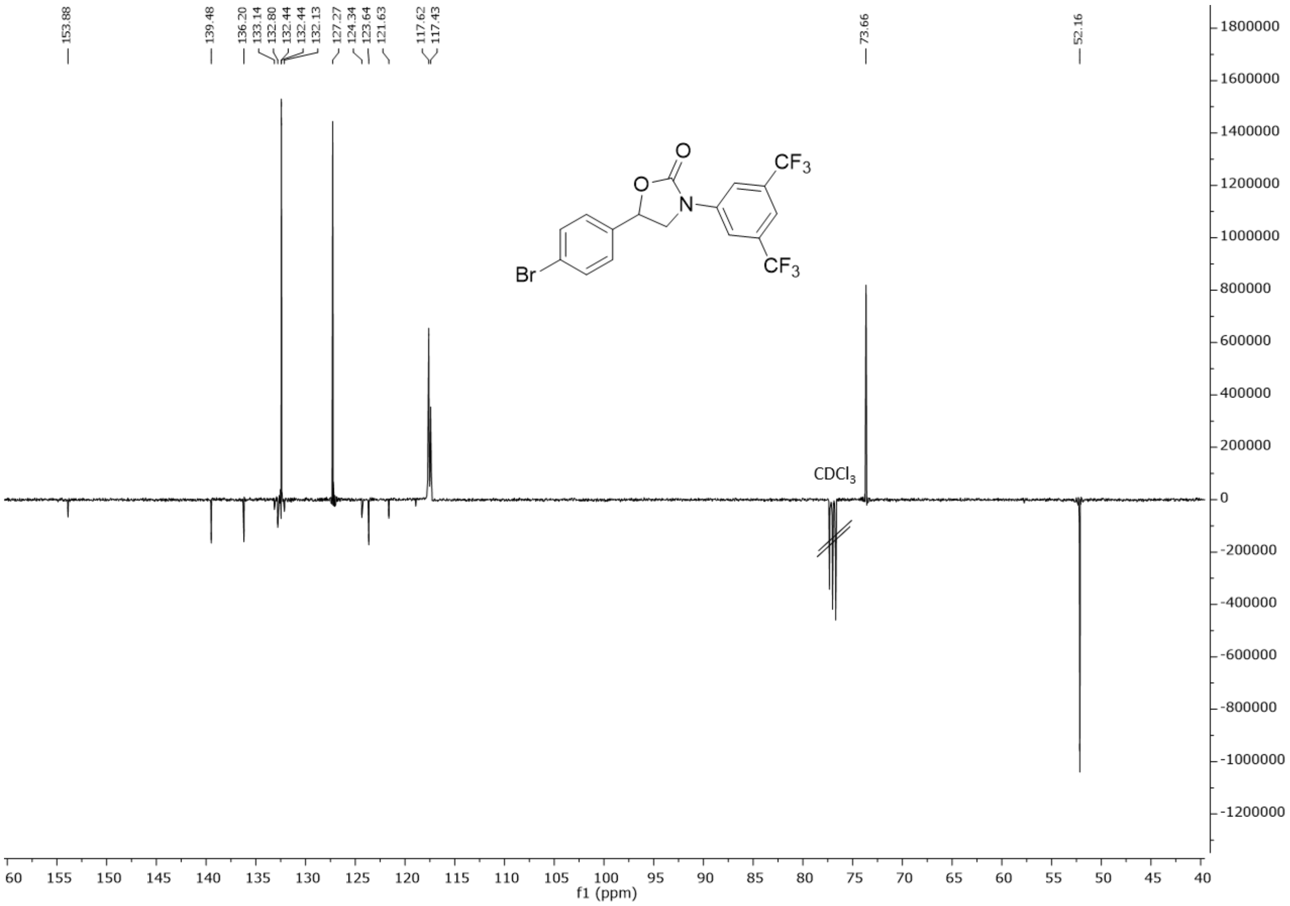
Compound (10a): ^{13}C NMR (100 MHz, $CDCl_3$)



Compound (12a): ^{1}H NMR (400 MHz, $CDCl_3$)

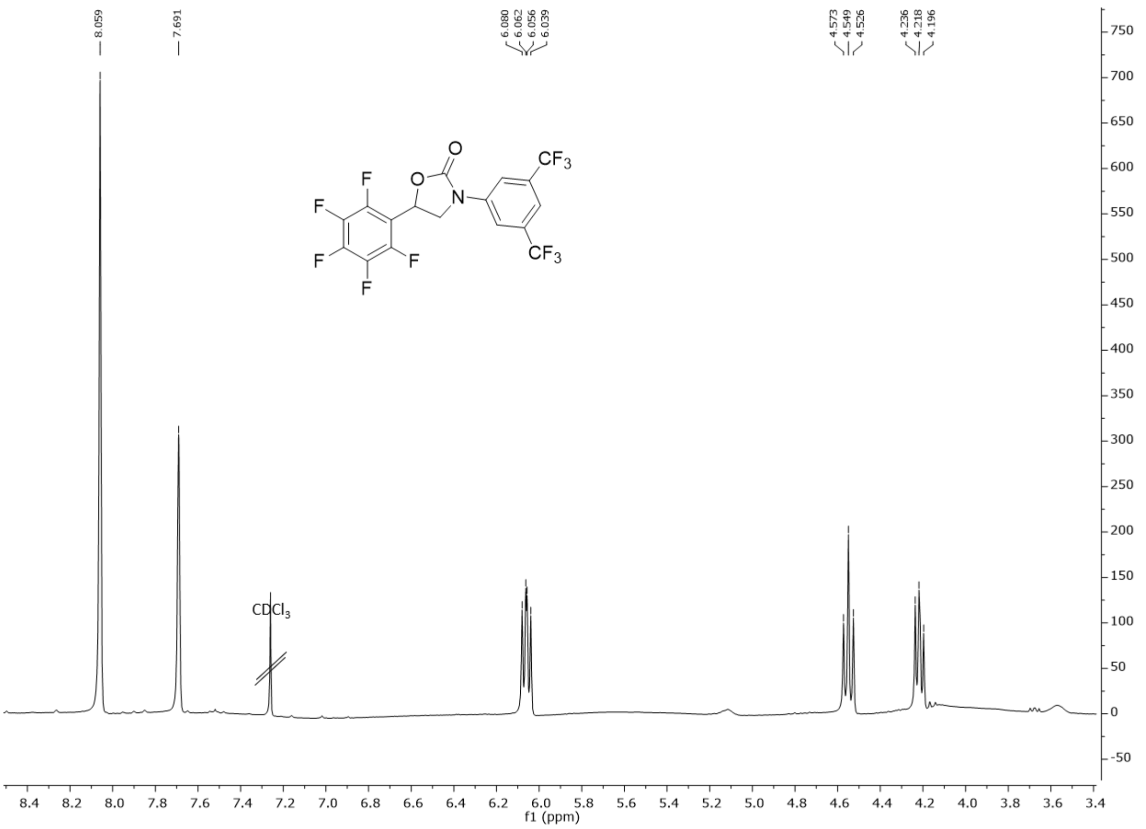


Compound (12a): ^{13}C NMR (100 MHz, $CDCl_3$)

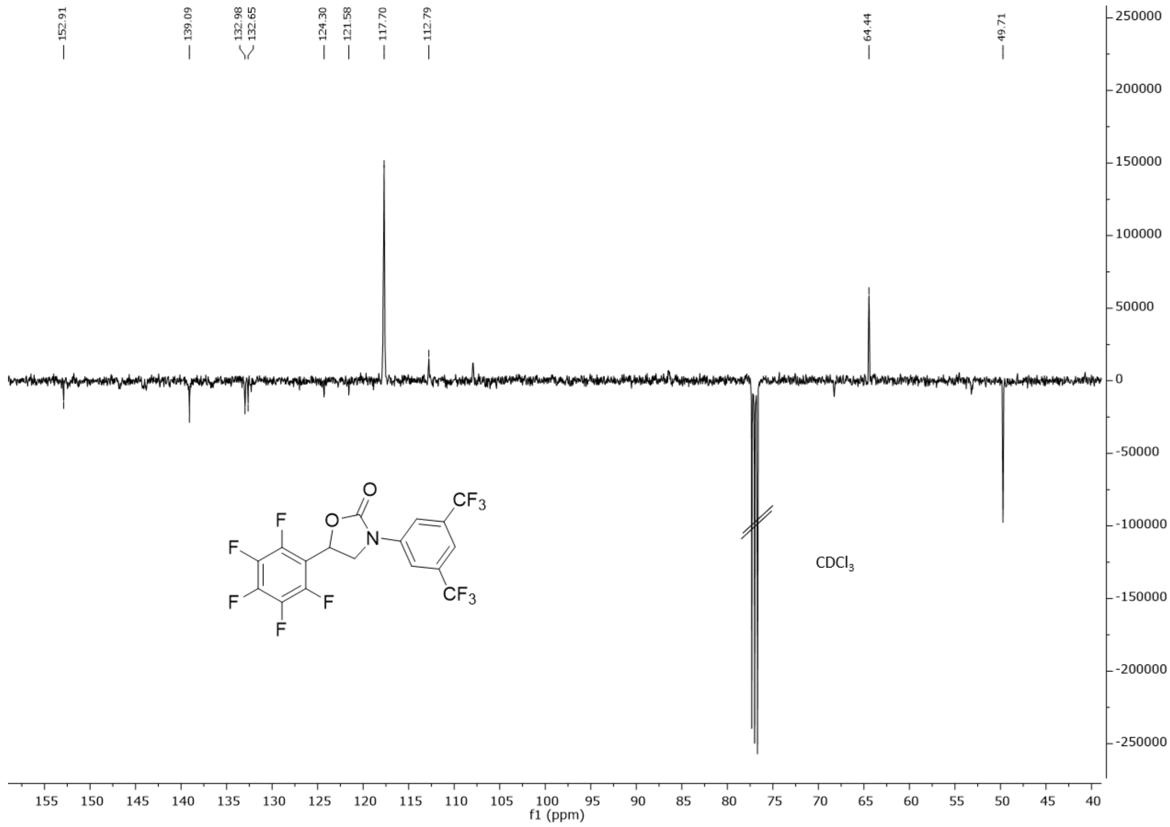


Compound (12a): ^{19}F NMR (376 MHz, $CDCl_3$)

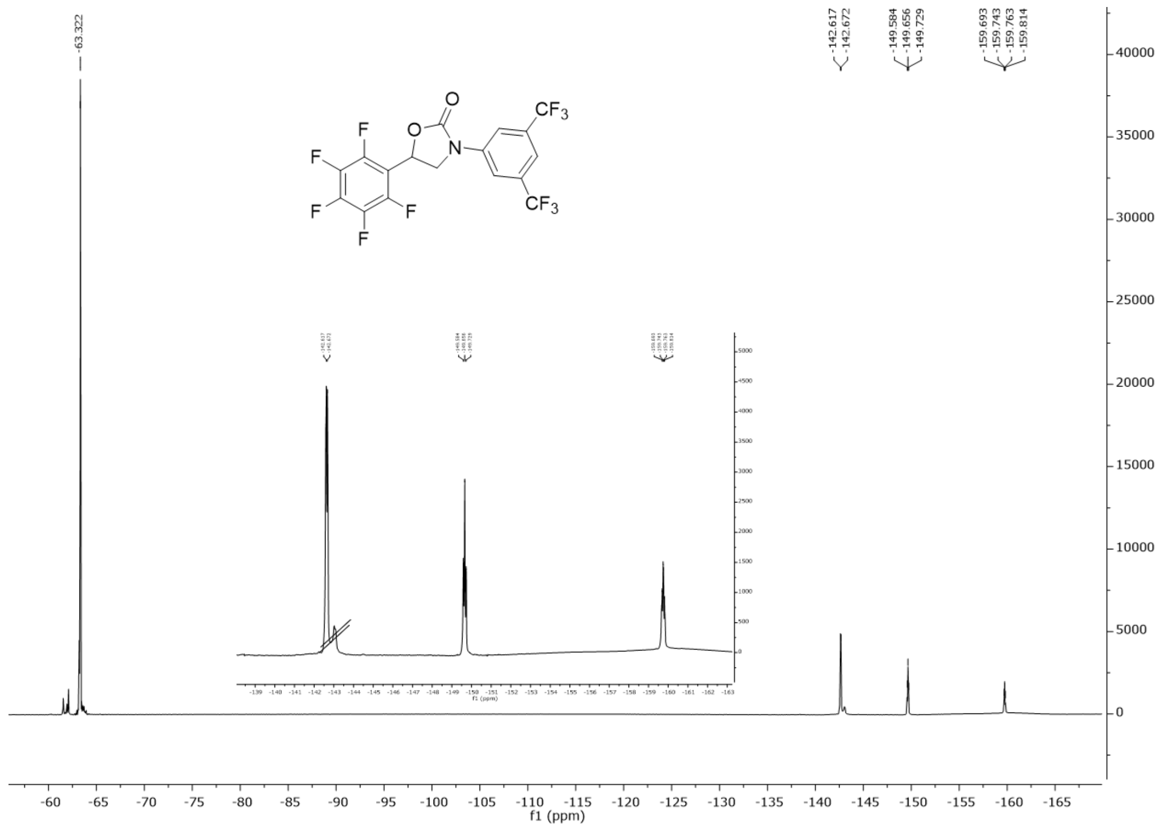
Compound (14a): ^{1}H NMR (400 MHz, $CDCl_3$)



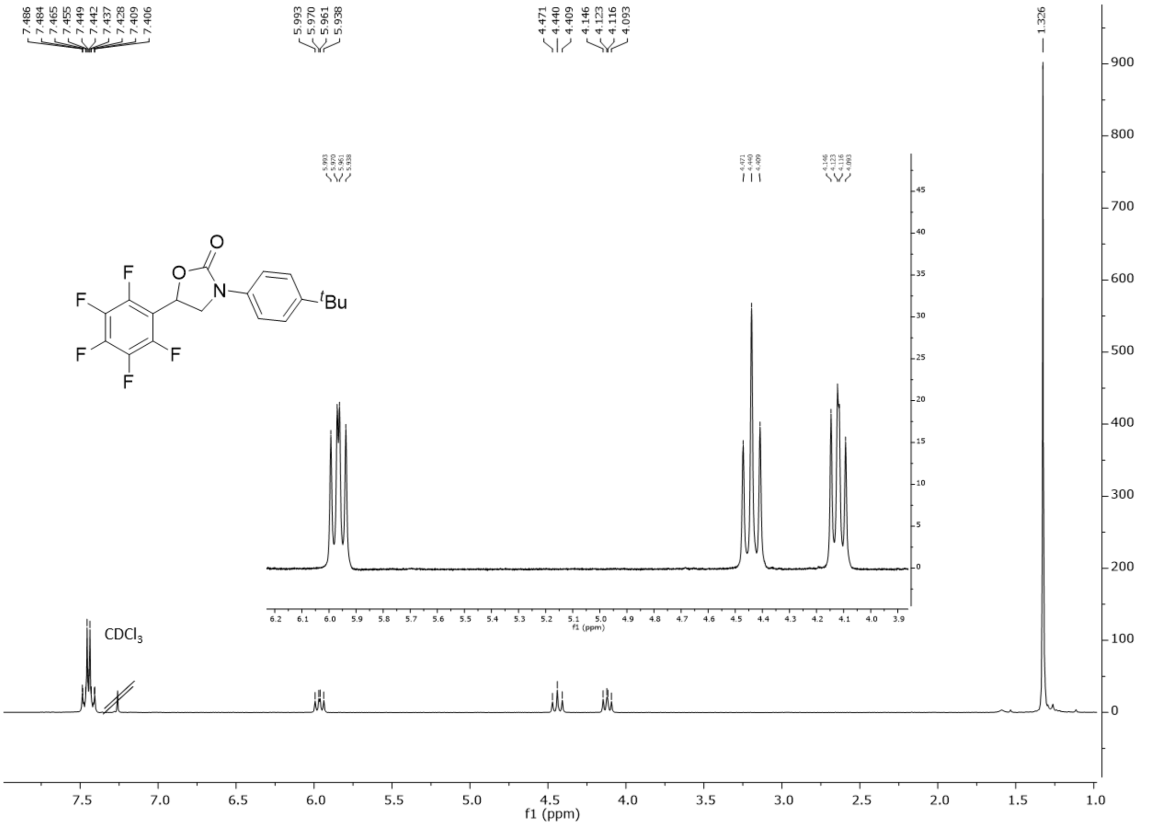
Compound (14a): ^{13}C NMR (100 MHz, $CDCl_3$)



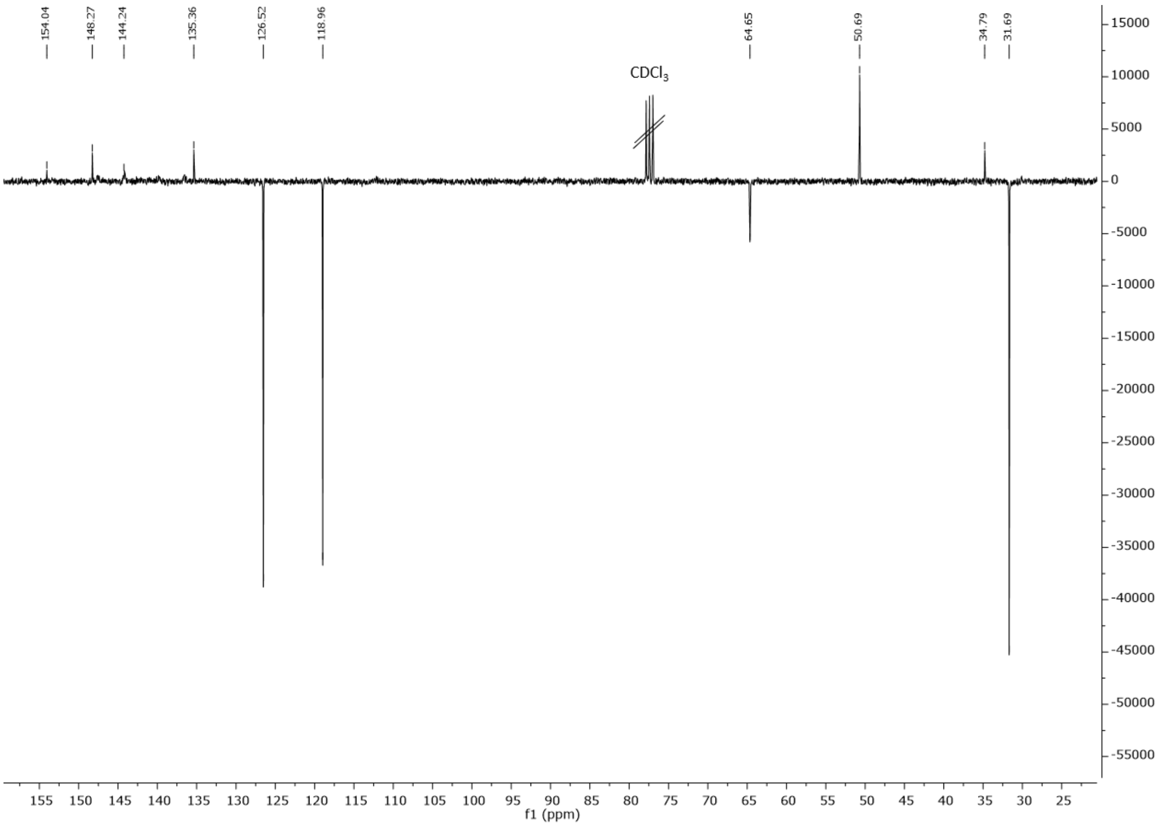
Compound (14a): ^{19}F NMR (376 MHz, $CDCl_3$)



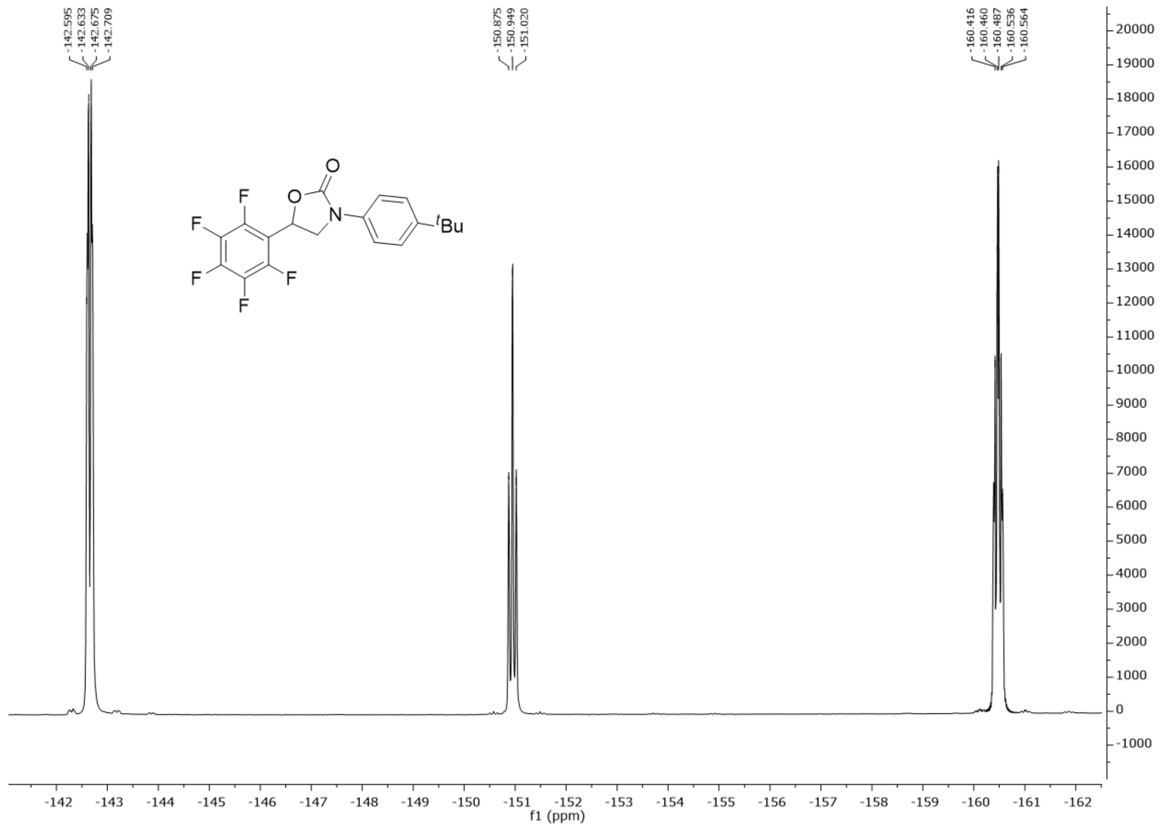
Compound (16a): ^{1}H NMR (300 MHz, $CDCl_3$)



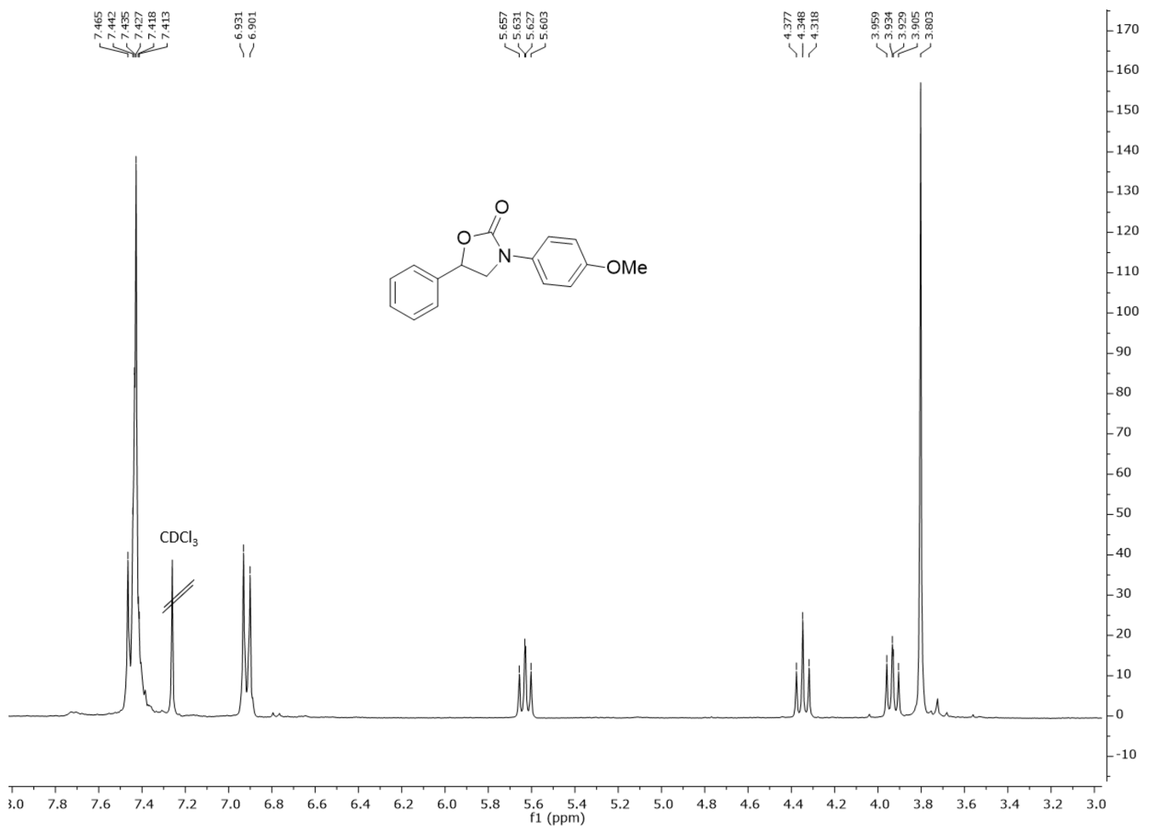
Compound (16a): ^{13}C NMR (75 MHz, $CDCl_3$)



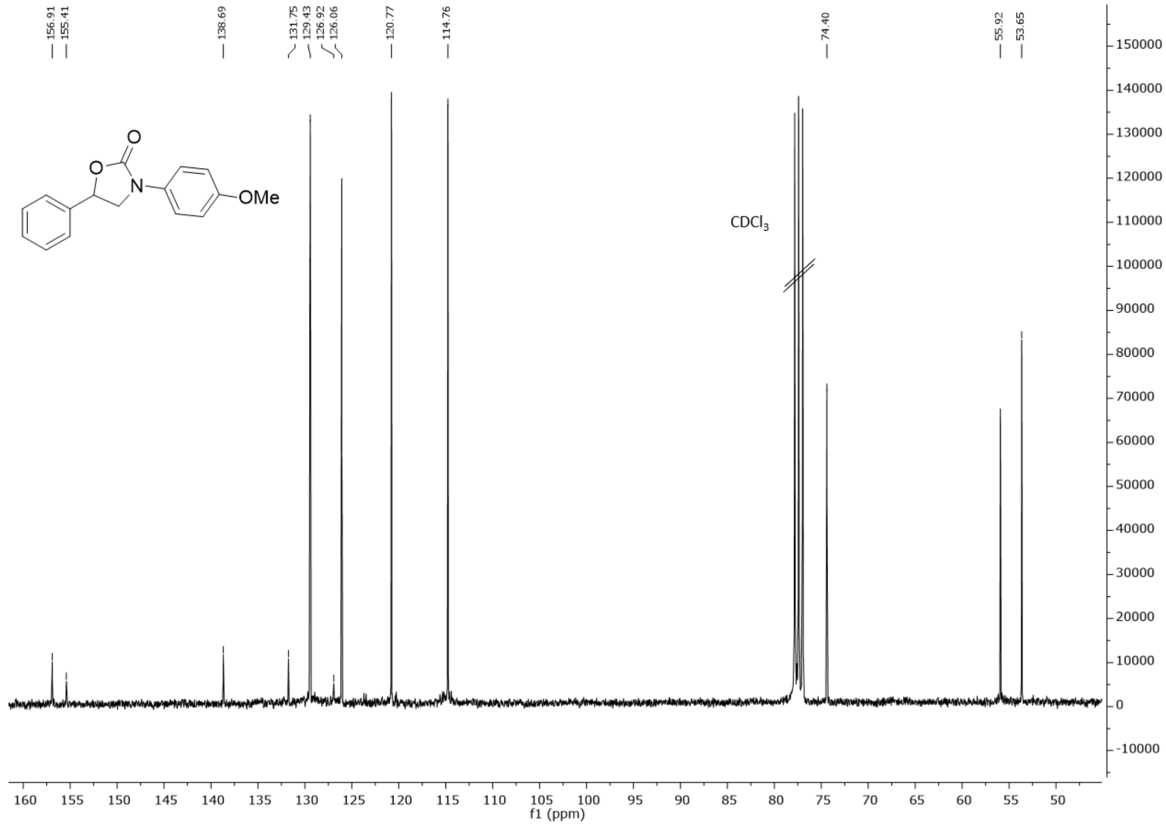
Compound (16a): ^{19}F NMR (282 MHz, $CDCl_3$)



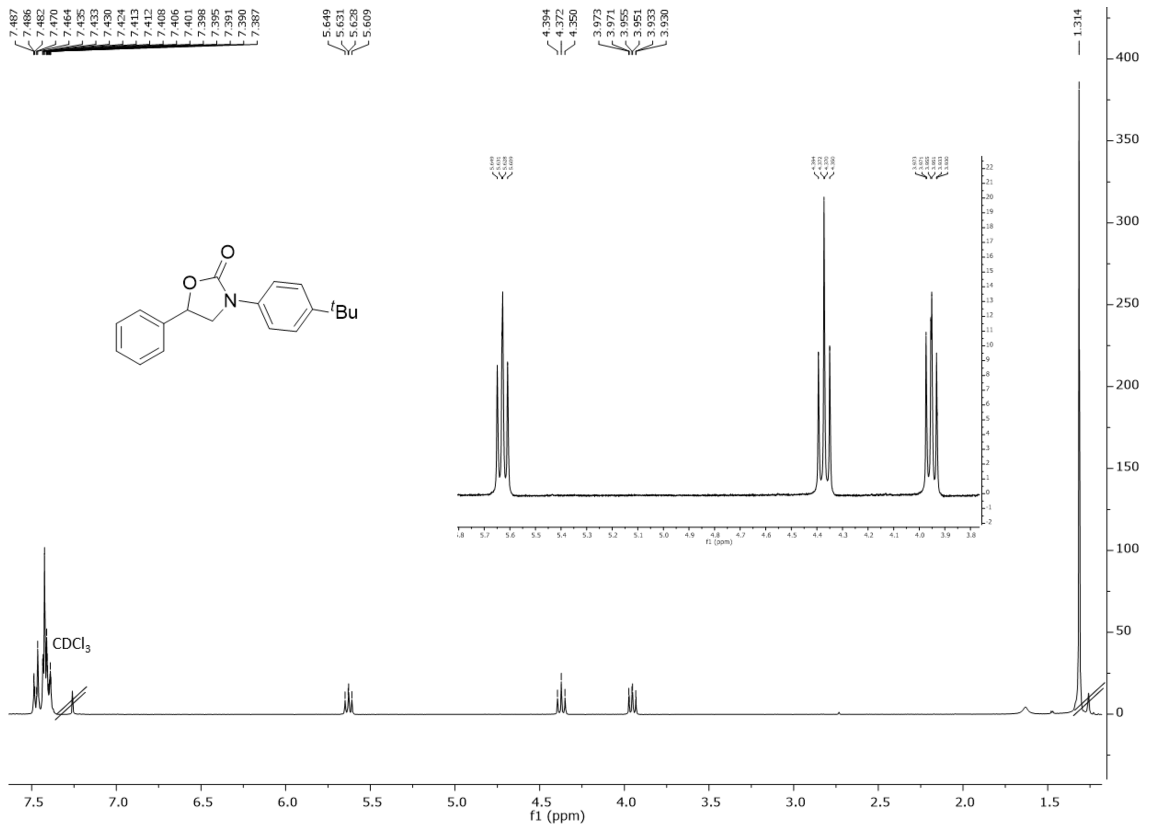
Compound (18a): ^{1}H NMR (300 MHz, $CDCl_3$)



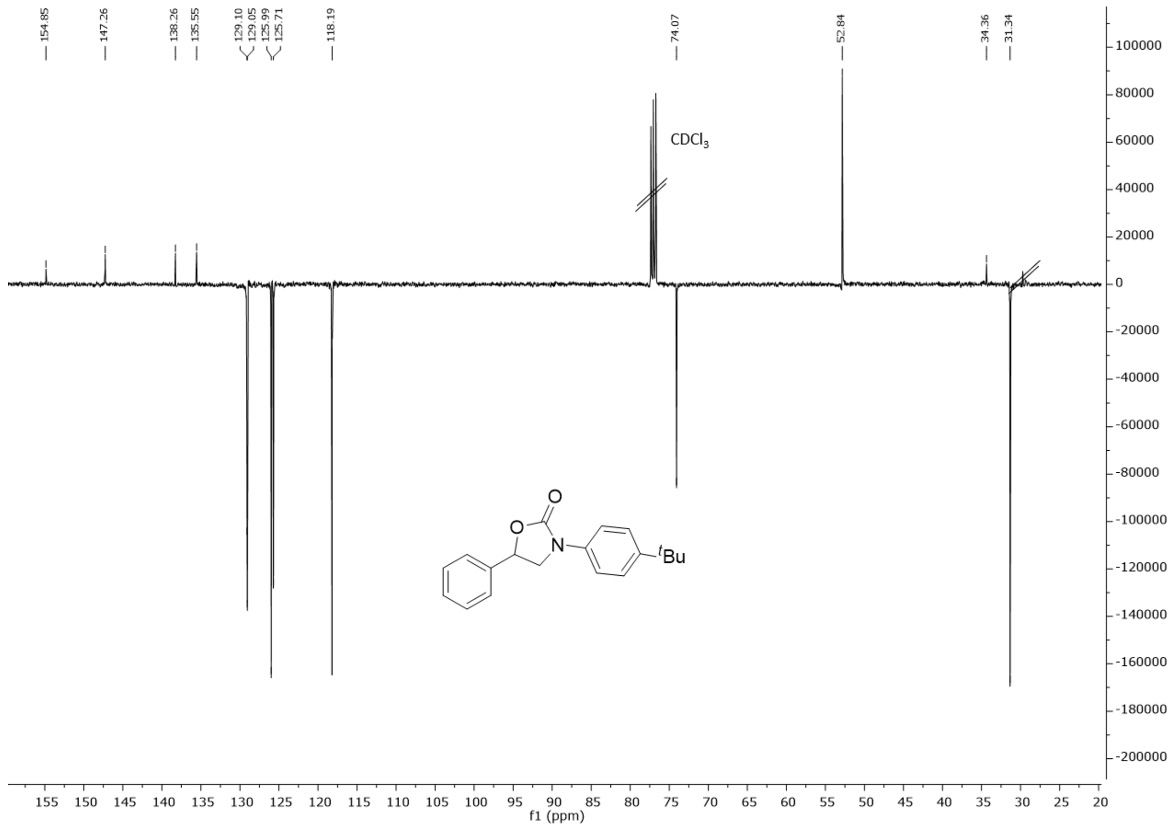
Compound (18a): ^{13}C NMR (75 MHz, $CDCl_3$)



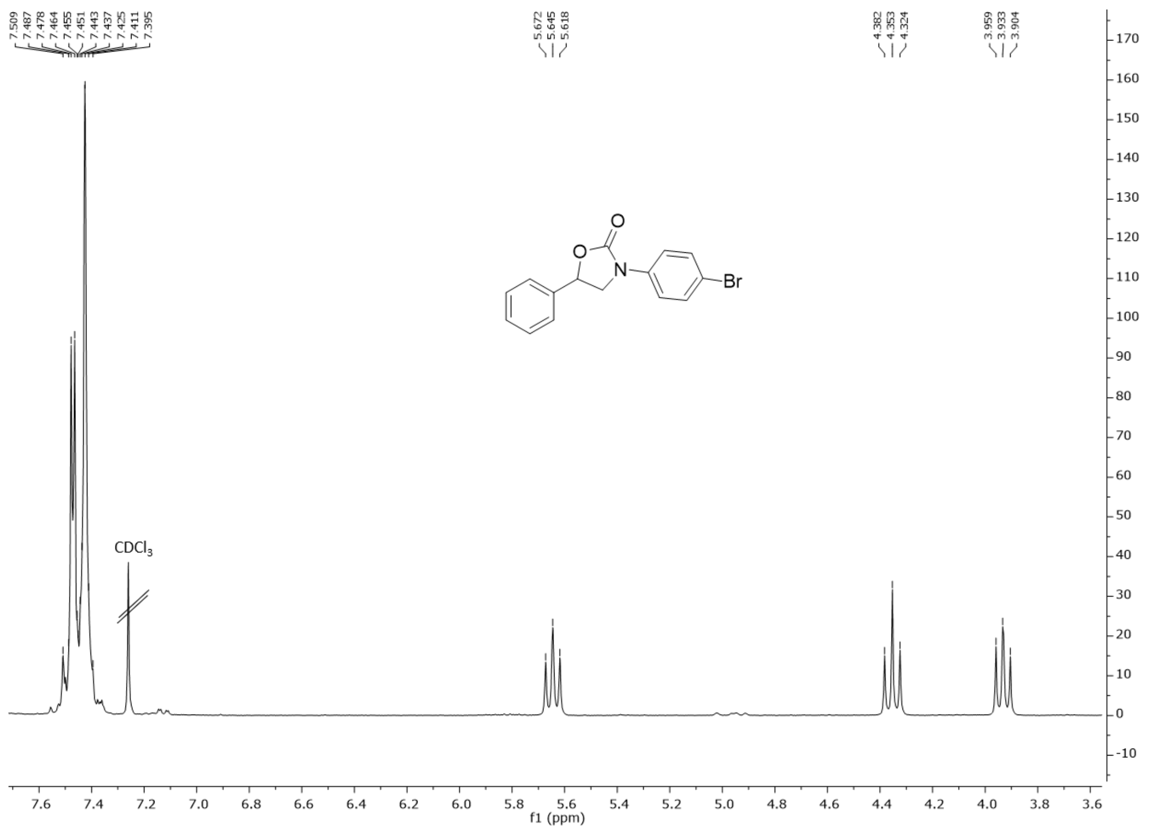
Compound (20a): ^{1}H NMR (400 MHz, $CDCl_3$)



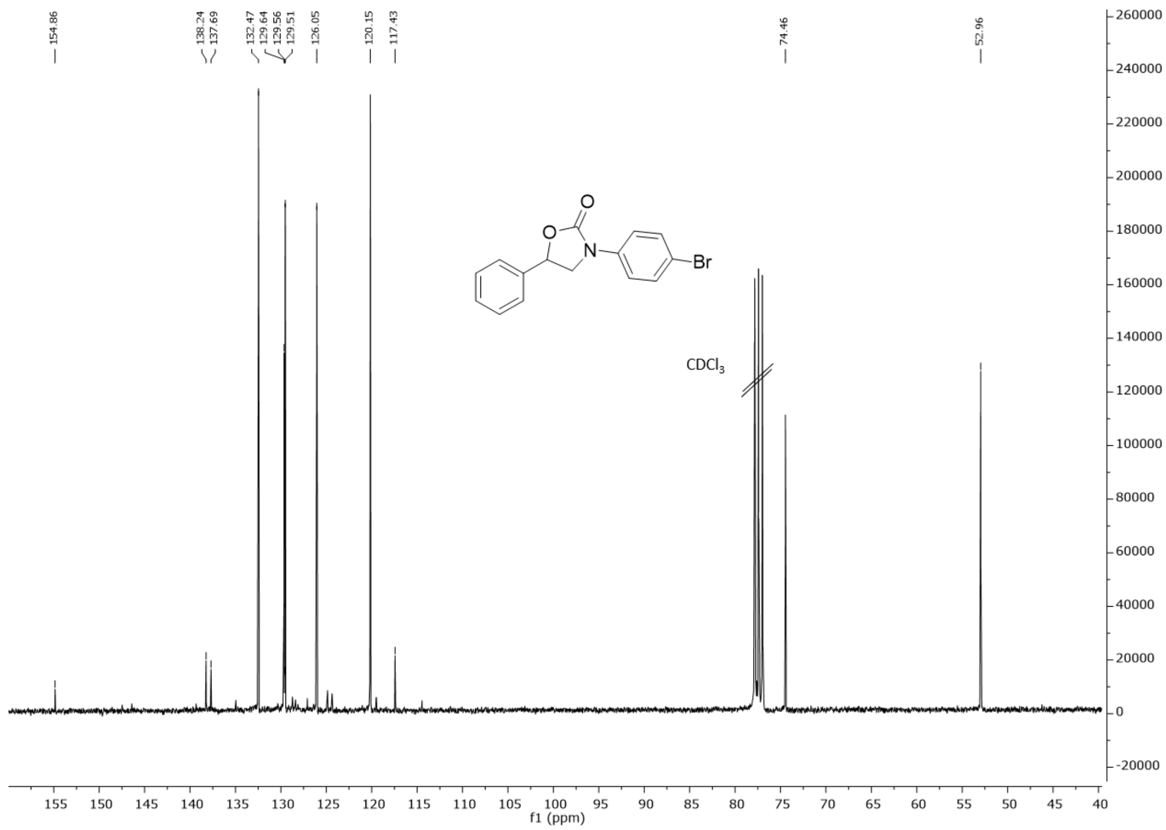
Compound (20a): ^{13}C NMR (100 MHz, $CDCl_3$)



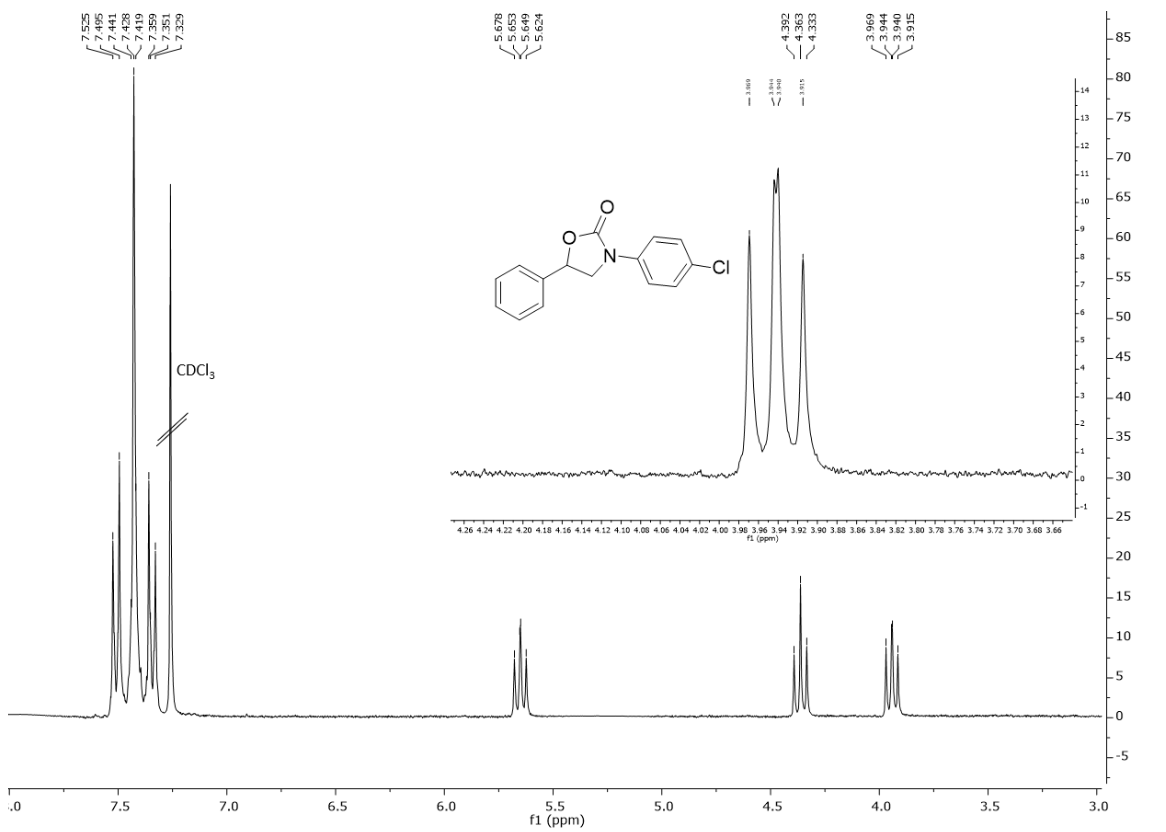
Compound (22a): ^{1}H NMR (300 MHz, $CDCl_3$)



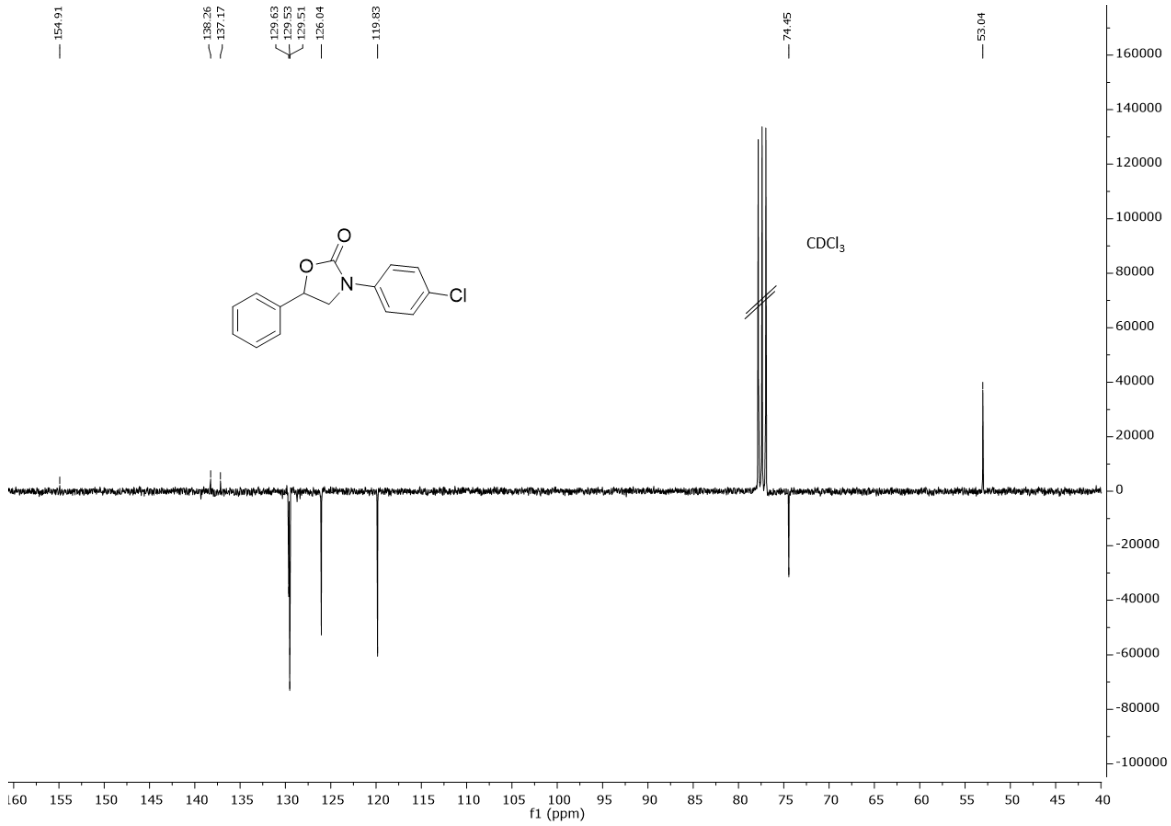
Compound (22a): ^{13}C NMR (75 MHz, $CDCl_3$)



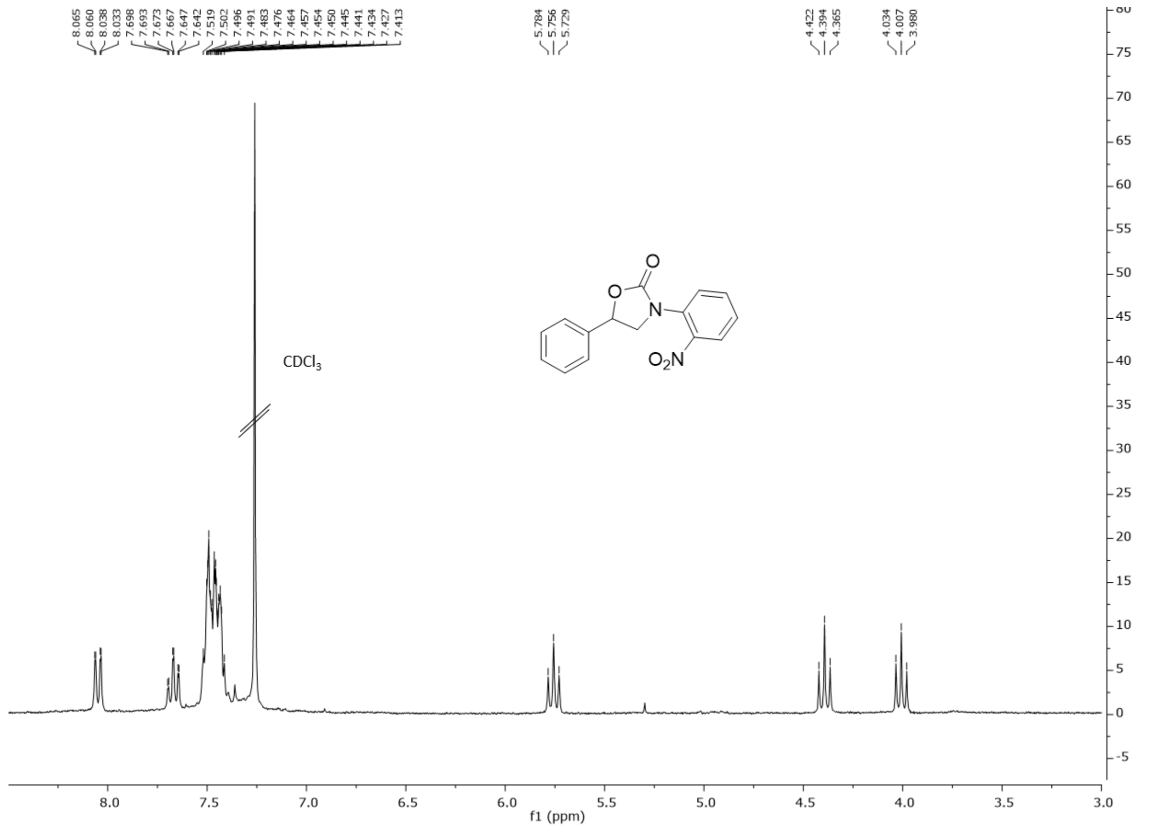
Compound (24a): ^{1}H NMR (300 MHz, $CDCl_3$)



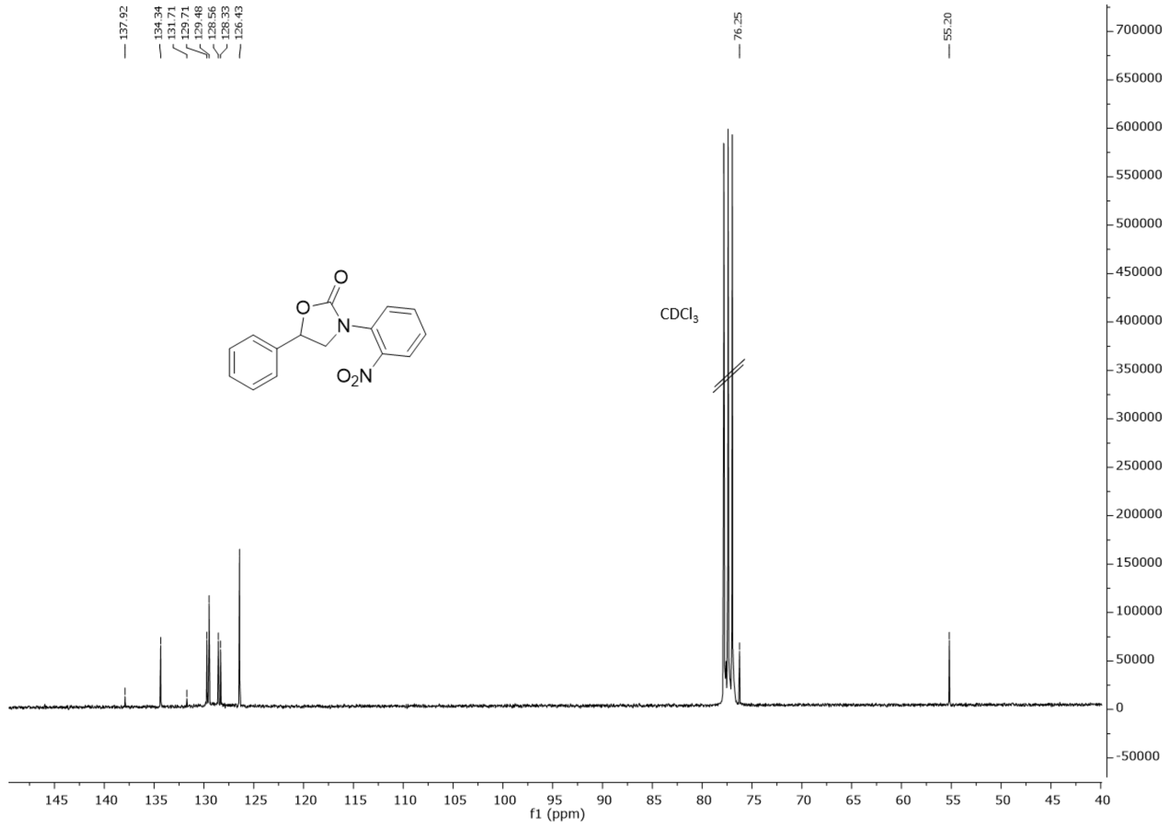
Compound (24a): ^{13}C NMR (75 MHz, $CDCl_3$)



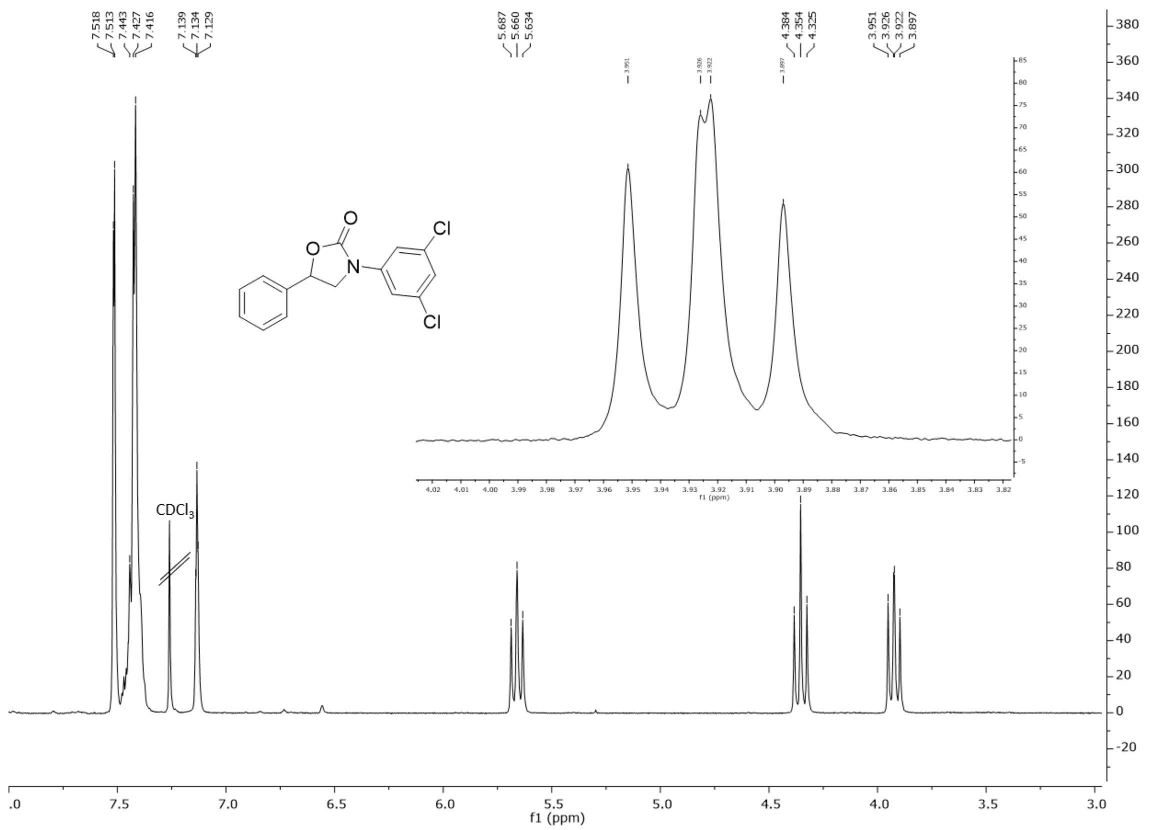
Compound (26a): ^{1}H NMR (300 MHz, $CDCl_3$)



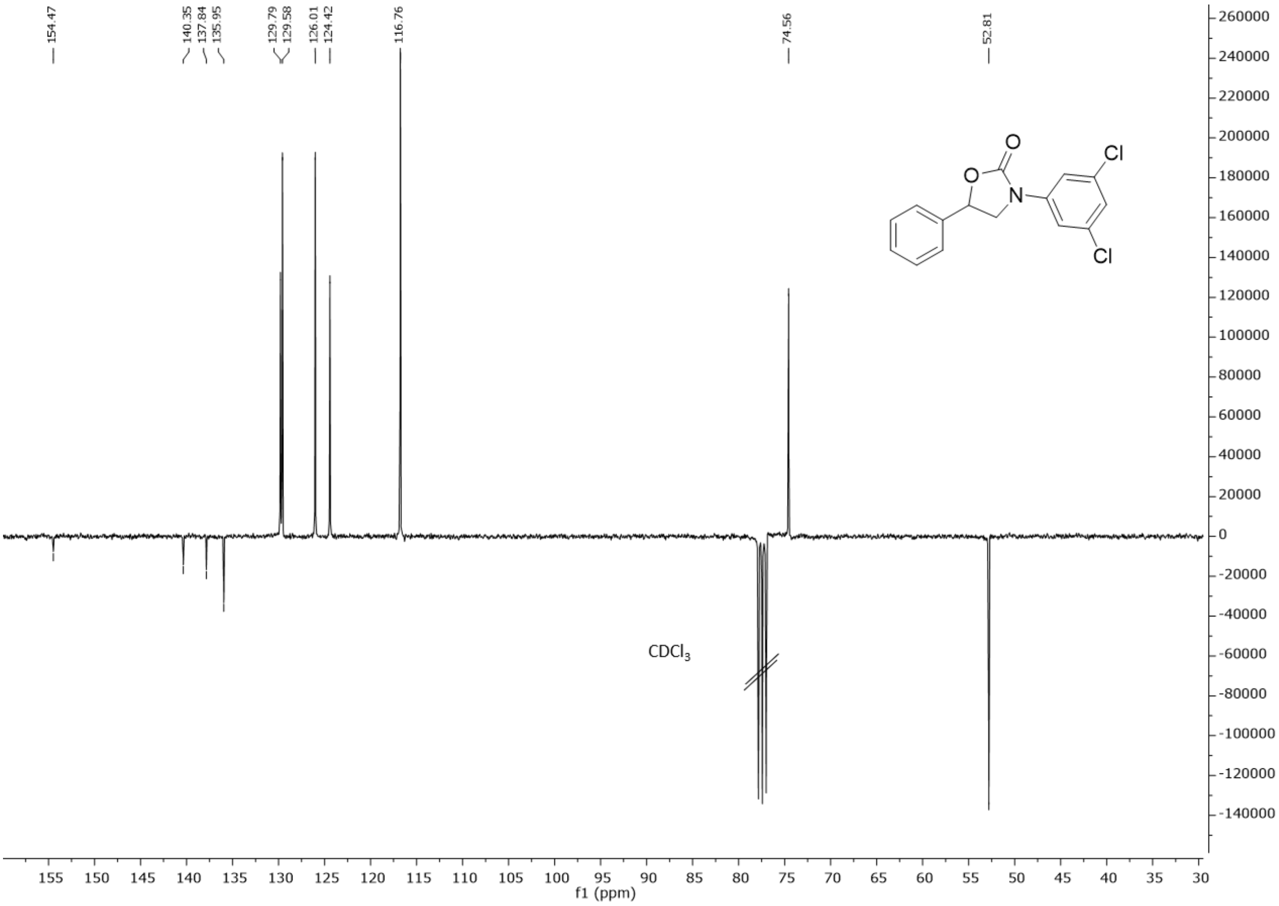
Compound (26a): ^{13}C NMR (75 MHz, $CDCl_3$)



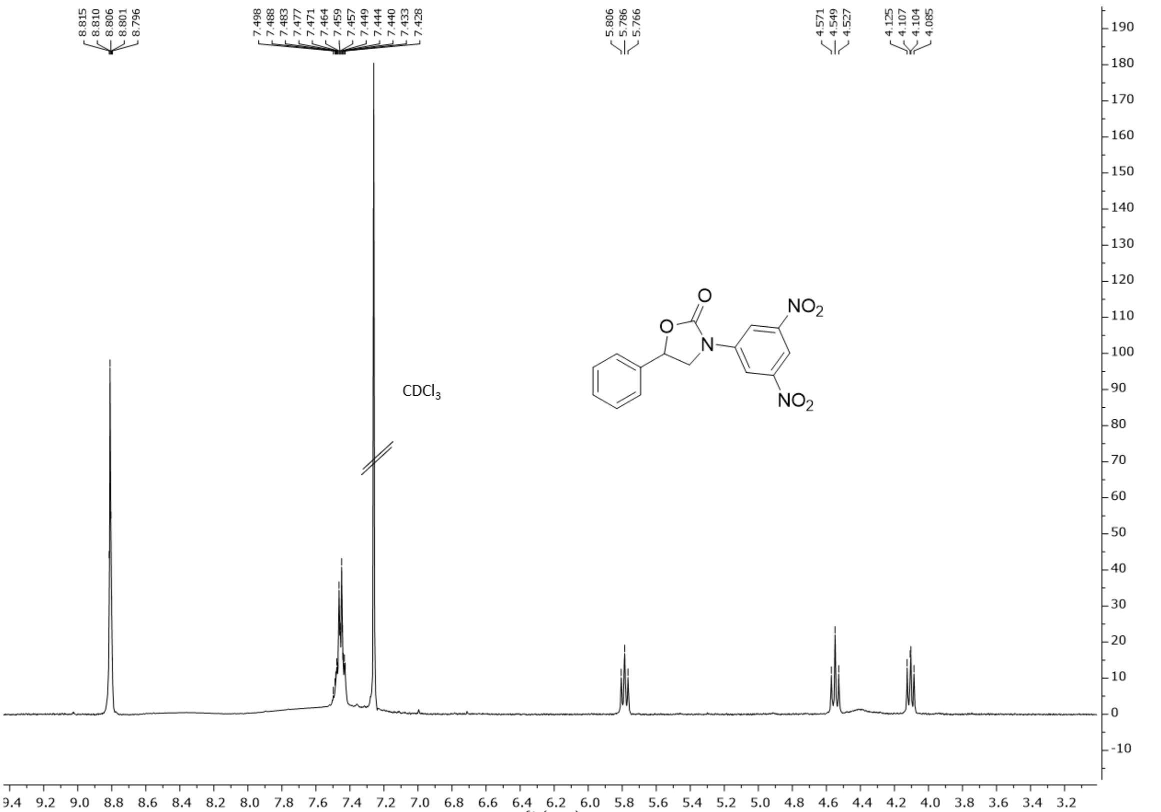
Compound (29a): ^{1}H NMR (300 MHz, $CDCl_3$)



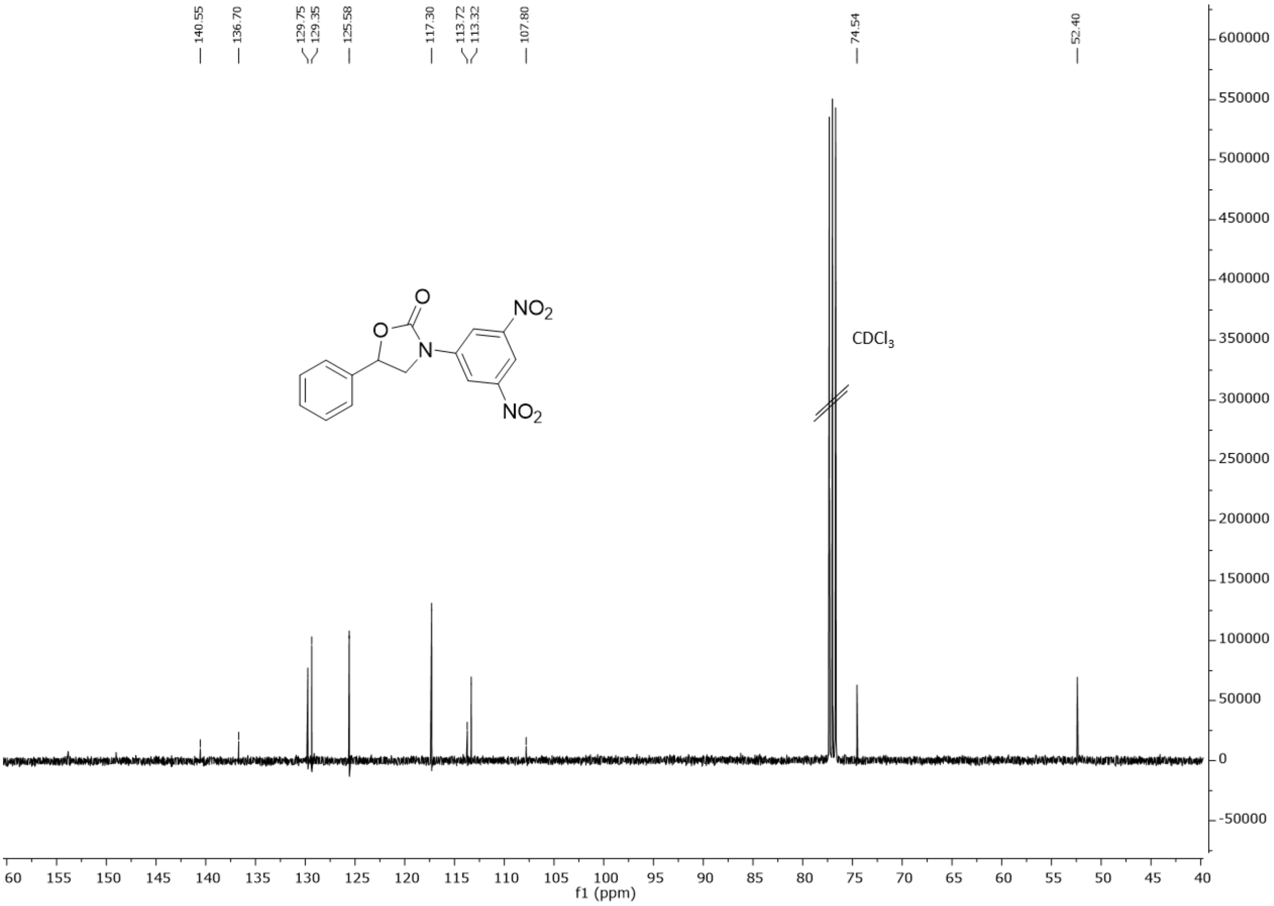
Compound (29a): ^{13}C NMR (75 MHz, $CDCl_3$)



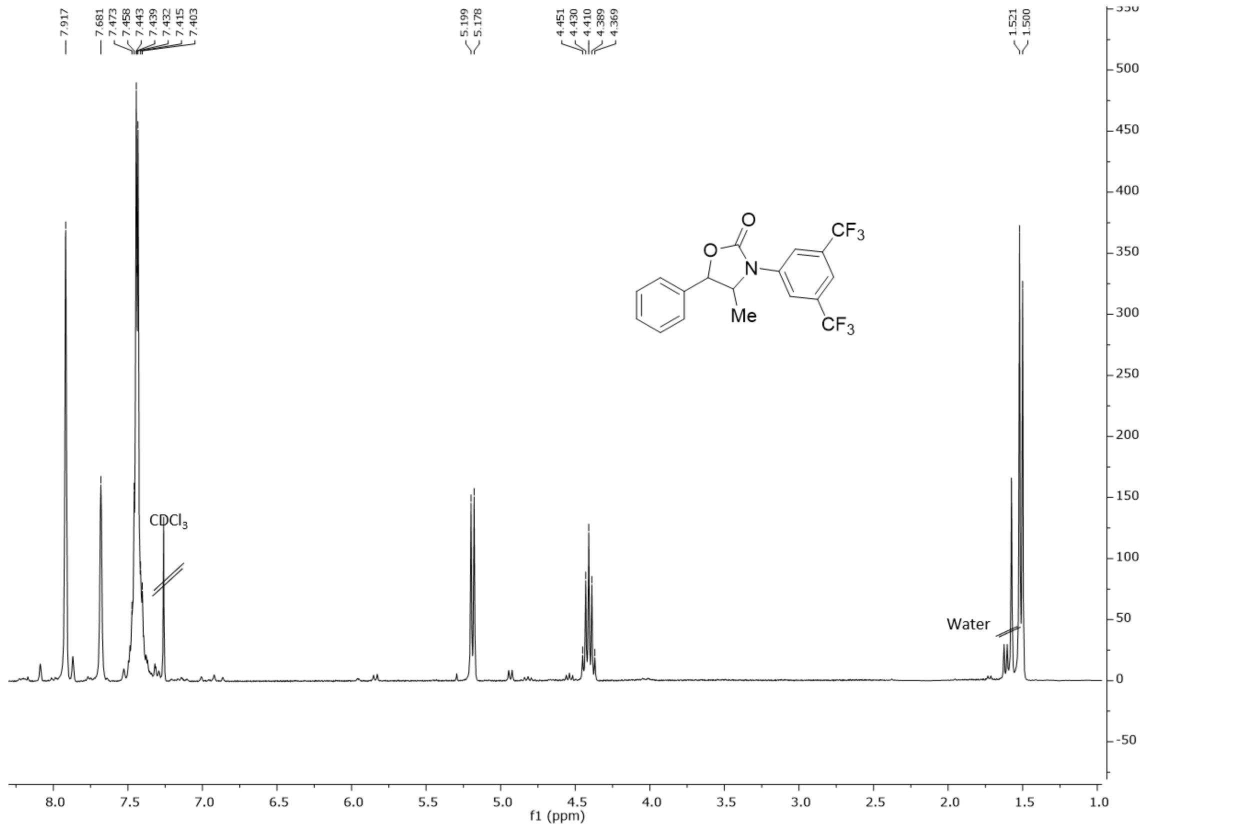
Compound (31a): ^{1}H NMR (400 MHz, $CDCl_3$)



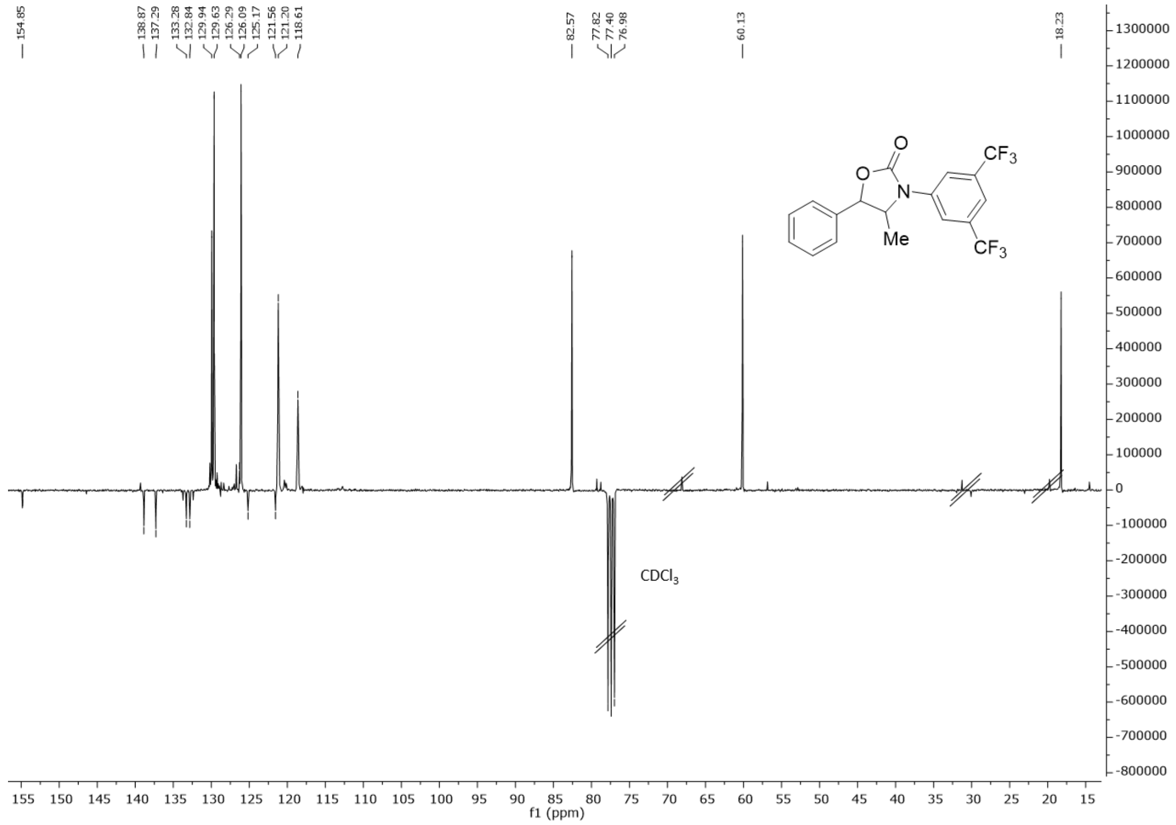
Compound (31a): ^{13}C NMR (100 MHz, $CDCl_3$)



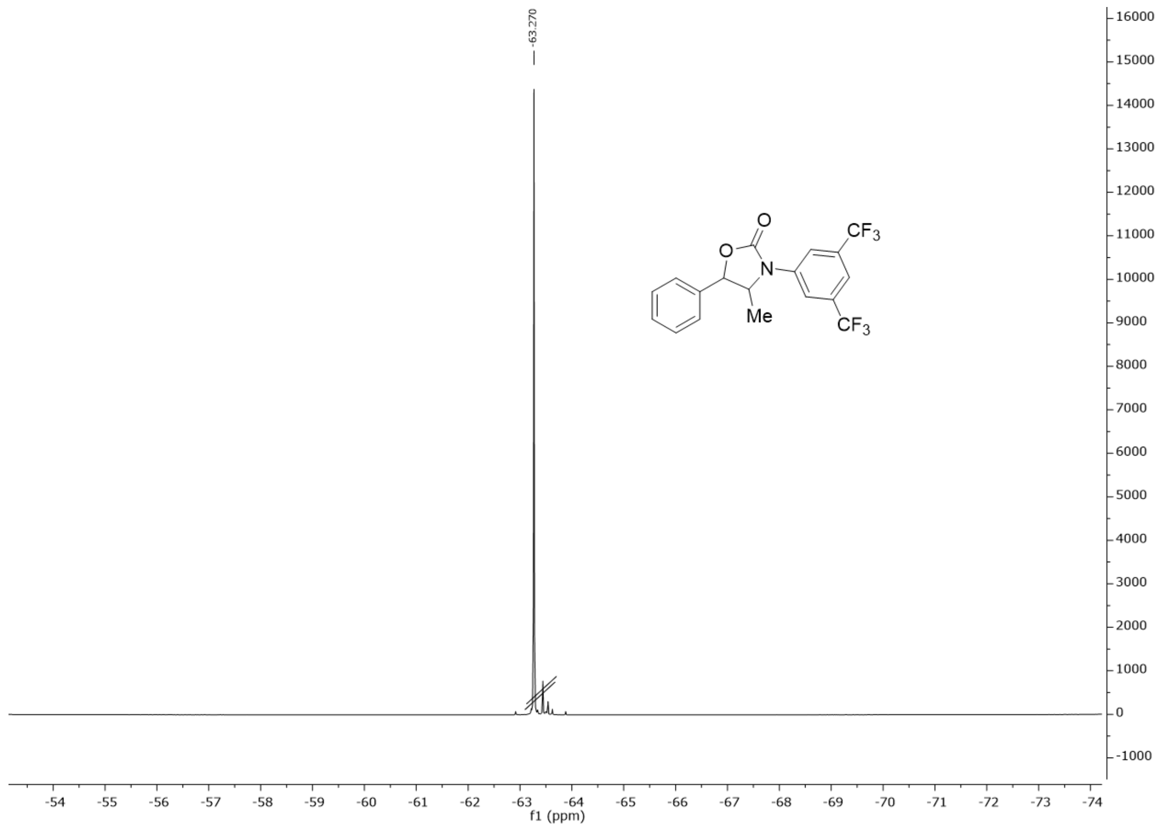
Compound (33a): ^{1}H NMR (300 MHz, $CDCl_3$)



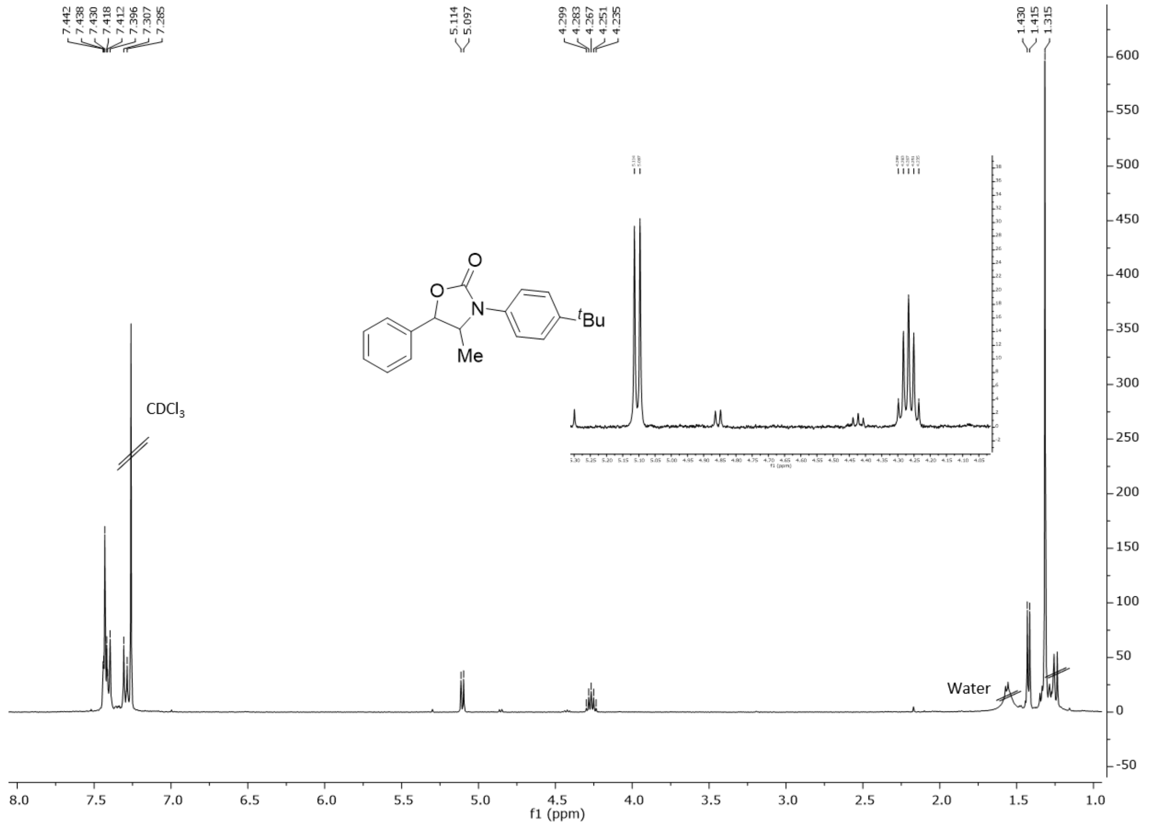
Compound (33a): ^{13}C NMR (75 MHz, $CDCl_3$)



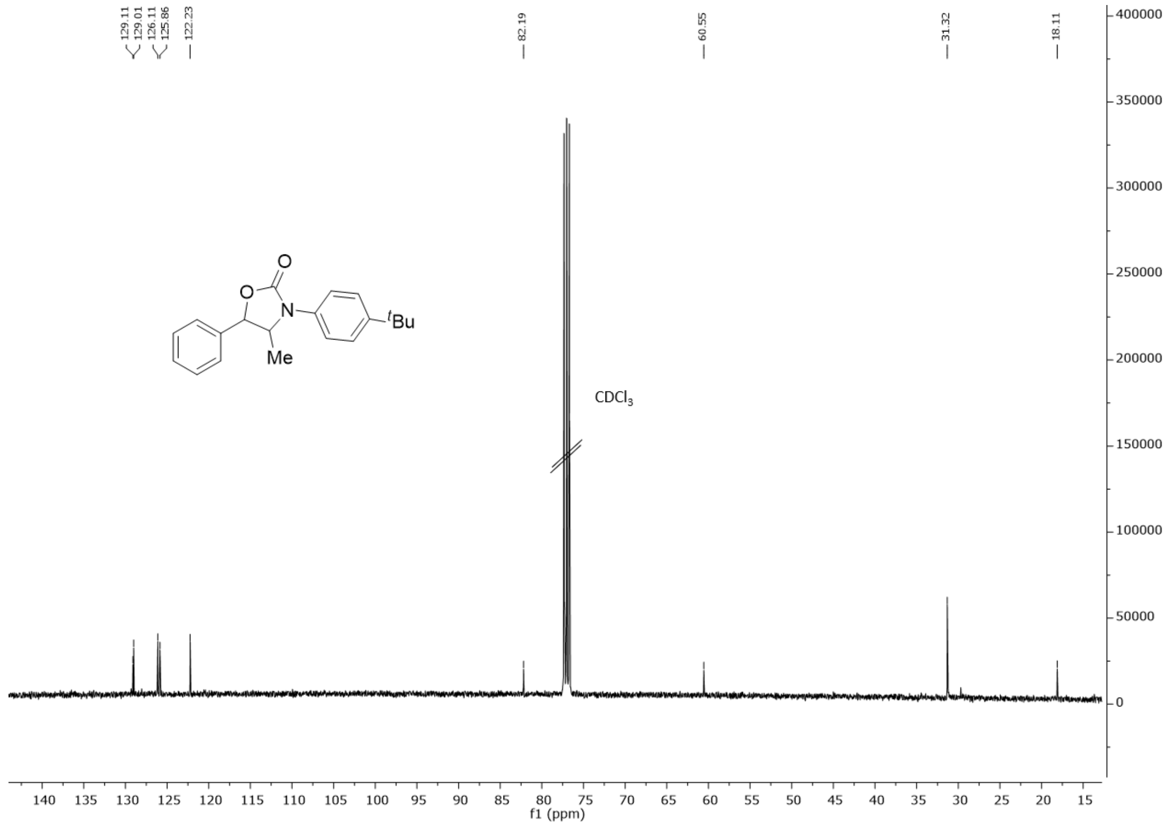
Compound (33a): ^{19}F NMR (282 MHz, $CDCl_3$)



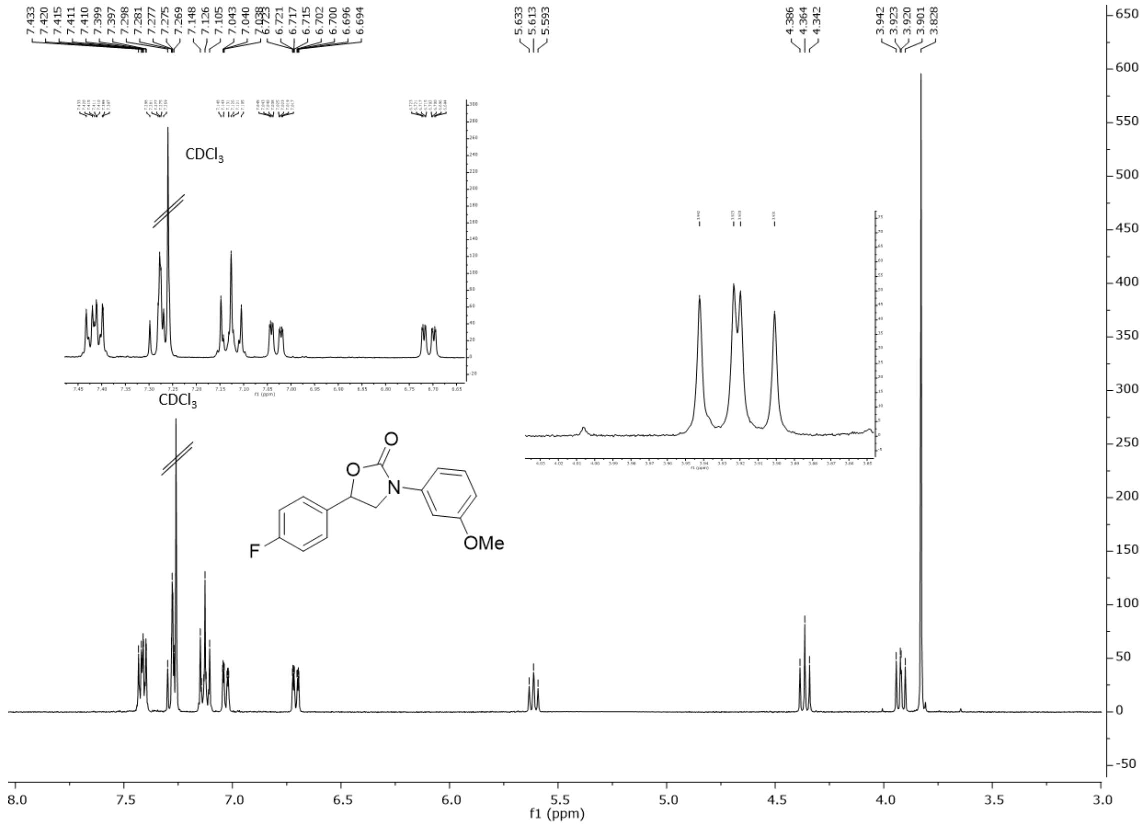
Compound (35a): ^{1}H NMR (400 MHz, $CDCl_3$)



Compound (35a): ^{13}C NMR (100 MHz, $CDCl_3$)



Compound (36a): ^{1}H NMR (400 MHz, $CDCl_3$)



7. Computational Data

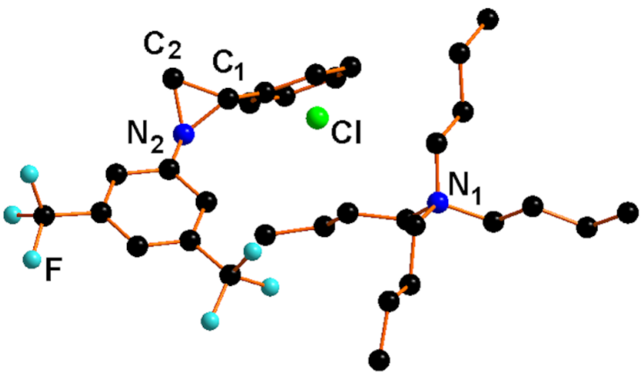


Figure S1. Optimized structure of the adduct **40** between TBACl and aziridine **1.** Hydrogen atoms are omitted for clarity.

Cartesian coordinates and free energies of all the structures optimized in the computational analysis (B97D level of theory).

Compound TPPH$_2$

Cartesian Coordinates

N 0.000337 -2.124710 -0.031618
N 2.050608 0.000307 0.017518
C 2.473703 2.453839 -0.010806
C -2.473683 -2.453831 -0.010690
C 2.877743 1.094046 -0.085174
H 1.350580 -5.114563 0.350969
C 0.690528 -4.263104 0.230041
C 4.266531 -0.682604 -0.295396
C 2.878088 -1.093164 -0.085158
C 1.137632 -2.906587 0.056010
H 5.108530 1.352601 -0.442758
C -0.689173 -4.263318 0.230085
C 2.474465 -2.453081 -0.010746
C 4.266318 0.683911 -0.295383
C -1.136715 -2.906942 0.056083
H 5.108958 -1.351023 -0.442774
H -1.348932 -5.114996 0.351056
C -2.877709 -1.094034 -0.085126
N -2.050594 -0.000304 0.017633
C 1.136731 2.906948 0.055899
N -0.000319 2.124723 -0.031831
C -1.137609 2.906595 0.055916
C -0.690502 4.263100 0.229944
C 0.689201 4.263322 0.229894
H 1.348963 5.115004 0.350819
H -1.350539 5.114559 0.350930
C -2.474437 2.453082 -0.010798
C -2.878052 1.093166 -0.085167
C -4.266464 0.682599 -0.295596
C -4.266250 -0.683907 -0.295584
H -5.108437 -1.352595 -0.443121
H 0.000183 -1.109489 -0.094656
H -0.000168 1.109495 -0.094740
C 3.538170 -3.504808 0.002707
C 4.504480 -3.531477 1.032982
C 3.596155 -4.487482 -1.010537
C 5.503951 -4.518043 1.050996
H 4.461445 -2.778083 1.820354
C 4.598047 -5.471878 -0.995881
H 2.857734 -4.467311 -1.812999
C 5.554544 -5.491040 0.035854
H 6.239378 -4.528246 1.857024
H 4.633508 -6.219264 -1.790104
H 6.331935 -6.256497 0.048385
C 3.537086 3.505877 0.002735
C 4.503348 3.532799 1.033048
C 3.594849 4.488574 -1.010491
C 5.502537 4.519643 1.051124
H 4.460499 2.779372 1.820397
C 4.596468 5.473251 -0.995783
H 2.856488 4.468201 -1.812999
C 5.552908 5.492671 0.035999
H 6.237929 4.530037 1.857182
H 4.631763 6.220647 -1.790003
H 6.330087 6.258342 0.048575
C -3.537079 -3.505856 0.002776
C -4.503540 -3.532620 1.032912
C -3.594709 -4.488664 -1.010353
C -5.502761 -4.519433 1.050934
H -4.460821 -2.779090 1.820170

C -4.596358 -5.473309 -0.995700
H -2.856228 -4.468392 -1.812756
C -5.552976 -5.492586 0.035921
H -6.238295 -4.529705 1.856864
H -4.631543 -6.220789 -1.789846
H -6.330176 -6.258237 0.048453
H -5.108852 1.351017 -0.443161
C -3.538149 3.504780 0.002703
C -3.596173 4.487517 -1.010467
C -4.504470 3.531347 1.032970
C -4.598108 5.471868 -0.995762
H -2.857781 4.467396 -1.812952
C -5.503968 4.517879 1.051057
H -4.461400 2.777908 1.820294
C -5.554602 5.490938 0.035977
H -4.633613 6.219285 -1.789955
H -6.239388 4.528011 1.857093
H -6.332017 6.256370 0.048556

Free Energy= -1911.893838

Compound 1-(3,5-*bis*-trifluoromethylphenyl)-2-phenylaziridine (1)

Cartesian Coordinates

N -0.244537 0.340537 0.921491
C 0.694239 0.907619 1.887792
C 0.806767 -0.545336 1.505333
C -1.605376 0.181446 1.223178
C -2.349009 1.244971 1.780219
C -2.255563 -1.029027 0.909595
C -3.721658 1.086726 2.008998
H -1.848169 2.178435 2.028390
C -3.628438 -1.169904 1.161675
H -1.680426 -1.853381 0.492630
C -4.380063 -0.120758 1.710276
H -5.443591 -0.235811 1.903020
C -4.270397 -2.499071 0.831562
C -4.539098 2.205003 2.616091
H 0.312190 1.137557 2.887647
H 1.412929 1.626491 1.485932
H 1.573965 -0.810317 0.772889
C 0.455635 -1.660176 2.439399
C -0.384861 -1.486201 3.561028
C 0.946787 -2.951632 2.152863
C -0.722068 -2.577770 4.375827
H -0.787105 -0.501428 3.796257
C 0.615322 -4.044788 2.971115
H 1.590217 -3.096708 1.282696
C -0.223702 -3.861277 4.084411
H -1.375429 -2.426110 5.236237
H 1.006535 -5.035737 2.736083
H -0.488286 -4.708792 4.718313
F -4.173616 -2.792154 -0.507142
F -3.657168 -3.535272 1.492251
F -5.594751 -2.555129 1.152406
F -5.041207 1.853835 3.846641
F -3.832054 3.357634 2.795168
F -5.625716 2.522227 1.839629

Free Energy= -1269.20668

Compound TBACl

Cartesian Coordinates

Cl 2.167162 -7.610589 8.973934
N 0.669908 -3.646539 8.249511
C -0.197215 -2.395496 8.412300
H -0.696717 -2.249064 7.448050
H 0.501574 -1.563529 8.556483
C 3.467225 -4.072028 5.540629

H 2.811182 -3.857751 4.680162
H 4.002719 -3.136664 5.775607
C 2.603601 -4.483776 6.749489
H 2.064142 -5.411549 6.514764
H 3.256765 -4.702946 7.605311
C -0.997702 -4.841234 6.662600
H -1.672897 -3.972186 6.641722
H -0.331307 -4.769159 5.790111
C 1.628623 -3.359835 7.090026
H 0.992019 -3.122126 6.229998
H 2.169061 -2.447206 7.365748
C -2.009378 -1.109441 9.578142
H -1.305615 -0.270382 9.706918
H -2.509328 -0.962814 8.606291
C 1.443310 -3.962168 9.536259
H 0.680802 -4.189487 10.290153
H 1.984971 -4.892118 9.331223
C 4.110142 -4.447279 11.077865
H 4.649796 -4.688579 12.006230
H 4.851996 -4.148795 10.319132
H 3.615710 -5.364919 10.725395
C 3.101166 -3.307602 11.318611
H 3.626084 -2.433407 11.734188
H 2.354971 -3.616797 12.069975
C -1.836615 -6.130576 6.541266
H -2.508565 -6.208229 7.411990
H -1.164003 -7.002888 6.577305
C -3.052299 -1.094558 10.709379
H -3.608510 -0.145168 10.720558
H -2.565281 -1.219204 11.689614
H -3.775992 -1.915418 10.582657
C -0.188296 -4.885423 7.956837
H 0.504080 -5.736365 7.964226
H -0.849675 -4.994721 8.823415
C -2.659587 -6.156079 5.241627
H -3.253350 -7.079736 5.168877
H -1.999061 -6.102675 4.361444
H -3.350989 -5.299042 5.200411
C 4.477426 -5.170783 5.165700
H 5.088097 -4.868054 4.301556
H 3.956217 -6.106568 4.909251
H 5.153577 -5.381133 6.009366
C -1.219399 -2.434118 9.547342
H -0.718705 -2.574288 10.516568
H -1.925224 -3.266401 9.411414
C 2.370100 -2.853110 10.033501
H 1.795232 -1.940777 10.250186
H 3.123153 -2.603324 9.270886

Free Energy= -1145.537115

Compound CO_2

Cartesian Coordinates
C 0.000000 0.000000 0.000000
O 1.177628 0.000000 0.000000
O -1.177628 0.000000 0.000000

Free Energy= -188.491026

Adduct 38a between $TPPH_2$ and CO_2

Cartesian Coordinates
N -0.119562 2.127401 -0.237033
N -2.145729 -0.016128 -0.173656
C -2.544735 -2.472888 -0.202246
C 2.350690 2.480754 -0.281162
C -2.962368 -1.117221 -0.278154
H -1.486222 5.095114 0.245913
C -0.822093 4.252845 0.088644
C -4.371063 0.646828 -0.460096
C -2.985361 1.069248 -0.255091
C -1.261301 2.896546 -0.105467
H -5.192756 -1.395537 -0.623744
C 0.557174 4.266277 0.052909
C -2.594972 2.431801 -0.158192
C -4.356492 -0.719572 -0.475663
C 1.012102 2.918671 -0.163568
H -5.221523 1.308001 -0.593372
H 1.212671 5.120898 0.176121
C 2.764439 1.126458 -0.383916
N 1.951116 0.026194 -0.250490
C -1.202773 -2.912093 -0.140269
N -0.074992 -2.121780 -0.256907
C 1.070173 -2.888313 -0.150753
C 0.638741 -4.244792 0.059555
C -0.740811 -4.259657 0.063199

H -1.391316 -5.114849 0.207271
H 1.308423 -5.085735 0.199316
C 2.401071 -2.421606 -0.238232
C 2.787455 -1.059977 -0.357155
C 4.164381 -0.638681 -0.609417
C 4.149311 0.727988 -0.629249
H 4.980109 1.403517 -0.807046
H -0.112535 1.113750 -0.320874
H -0.085555 -1.106937 -0.321475
C -3.669106 3.470723 -0.100587
C -4.623080 3.453852 0.941642
C -3.750577 4.484746 -1.080958
C -5.632596 4.428173 1.003719
H -4.562436 2.676512 1.704169
C -4.762423 5.457216 -1.022046
H -3.022654 4.498114 -1.893071
C -5.706089 5.432793 0.021360
H -6.357884 4.404289 1.818594
H -4.815727 6.229261 -1.791280
H -6.491138 6.189010 0.068096
C -3.596873 -3.535135 -0.170948
C -4.561156 -3.556614 0.861581
C -3.645342 -4.534742 -1.168176
C -5.549257 -4.553948 0.897188
H -4.524965 -2.790924 1.637289
C -4.636042 -5.529913 -1.136008
H -2.908476 -4.518946 -1.972179
C -5.590614 -5.543366 -0.102379
H -6.282964 -4.559811 1.704787
H -4.664315 -6.290205 -1.918154
H -6.359215 -6.317307 -0.076285
C 3.404181 3.541981 -0.281247
C 4.405967 3.553701 0.715051
C 3.416783 4.549213 -1.271706
C 5.396205 4.549550 0.721437
H 4.396388 2.781353 1.484793
C 4.409649 5.542738 -1.268810
H 2.650600 4.540547 -2.047939
C 5.401919 5.546783 -0.271250
H 6.159528 4.548226 1.501178
H 4.410272 6.308968 -2.045719
H 6.172334 6.319345 -0.267803
H 5.009483 -1.301046 -0.768460
C 3.479665 -3.456157 -0.192985
C 4.454033 -3.423302 0.829724
C 3.545818 -4.480076 -1.163947
C 5.468944 -4.392517 0.882015
H 4.404789 -2.637095 1.584043
C 4.563427 -5.447059 -1.115213
H 2.801922 -4.504887 -1.961210
C 5.527382 -5.407300 -0.090986
H 6.210347 -4.356817 1.681833
H 4.605449 -6.226742 -1.877478
H 6.316853 -6.159384 -0.052053
C 1.608142 -0.158665 2.763669
O 0.514512 -0.587808 2.686949
O 2.699746 0.267448 2.884954

Free Energy= -2100.379219

Adduct 38b between TPPH$_2$ and TBACl

Cartesian Coordinates

Cl 5.747578 -0.615775 1.282222
N 8.025618 -0.042499 -2.345751
C 9.242083 0.275316 -3.226015
H 8.995191 1.191127 -3.773947
H 9.304337 -0.537167 -3.958786
C 4.325769 -0.661164 -3.419434
H 4.205151 0.385202 -3.741060
H 4.462437 -1.254933 -4.331713
C 5.574630 -0.780339 -2.531289
H 5.418802 -0.198778 -1.612614
H 5.696551 -1.827593 -2.216508
C 7.188892 2.393547 -2.092677
H 7.804288 2.668460 -2.962203
H 6.164682 2.227155 -2.456240
C 6.832972 -0.315744 -3.269916
H 6.659155 0.615534 -3.817304
H 7.171701 -1.060857 -3.996024
C 11.706328 0.813840 -3.408900
H 11.826595 0.034660 -4.172957
H 11.440370 1.743721 -3.932541
C 8.300133 -1.267380 -1.467478
H 9.104870 -0.976297 -0.783140
H 7.397939 -1.412431 -0.861902
C 9.220201 -5.007208 -2.033741
H 9.333457 -5.850769 -1.336209
H 10.169139 -4.884341 -2.579103
H 8.441538 -5.268727 -2.767812
C 8.848404 -3.716194 -1.283572
C 7.177576 3.574945 -1.102449
H 8.202869 3.746593 -0.734516

H 6.562082 3.310629 -0.227036
C 13.031882 0.996663 -2.651579
H 13.850137 1.249490 -3.343125
H 13.309463 0.069984 -2.124178
H 12.950158 1.802661 -1.905042
C 7.712945 1.131719 -1.403813
H 6.992237 0.753816 -0.668703
H 8.644745 1.337393 -0.867577
C 6.636301 4.855748 -1.762126
H 6.638327 5.697490 -1.053056
H 5.605901 4.706503 -2.119854
H 7.254116 5.132648 -2.631003
C 3.060580 -1.135975 -2.686636
H 2.173913 -1.043127 -3.332576
H 2.889492 -0.543038 -1.774253
H 3.158983 -2.192381 -2.389663
C 10.561197 0.421874 -2.460606
H 10.822845 -0.525974 -1.968571
H 10.479929 1.189333 -1.677979
C 8.674087 -2.527433 -2.248180
H 9.609747 -2.374054 -2.806538
H 7.895778 -2.778855 -2.983890
N 6.464771 0.521548 -6.444593
N 8.667131 2.450144 -6.298087
N 10.669978 0.322484 -6.543524
N 8.459244 -1.604523 -6.322033
C 5.623855 -0.560305 -6.621801
C 4.290187 -0.030879 -6.719553
C 4.358976 1.335599 -6.549529
C 5.736709 1.691889 -6.342120
C 6.253020 2.969522 -6.027599
C 7.634131 3.293046 -5.958857
C 8.139824 4.604490 -5.556380
C 9.497033 4.556660 -5.713592
C 9.807247 3.208262 -6.185097
C 11.130613 2.764250 -6.449497
C 11.508067 1.417468 -6.638880
C 12.840491 0.901227 -6.798616
C 12.778908 -0.474463 -6.715649
C 11.400736 -0.850433 -6.546827
C 10.887238 -2.150072 -6.346726
C 9.512109 -2.486713 -6.255251
C 9.037140 -3.868995 -6.217746
C 7.674994 -3.808788 -6.300468
C 7.329737 -2.389610 -6.370984
C 6.002495 -1.919244 -6.546236
H 3.400812 -0.634608 -6.857051
H 3.537223 2.042472 -6.548516
H 7.538266 5.432657 -5.196701
H 10.223367 5.336512 -5.507388
H 13.725499 1.513686 -6.926335
H 13.604617 -1.175326 -6.757187
H 9.666285 -4.752229 -6.173202
H 6.971228 -4.633995 -6.337508
H 7.474922 0.453803 -6.351387
H 9.662430 0.377667 -6.417150
C 5.252314 4.041546 -5.742960
C 5.233508 5.236198 -6.497104
C 4.306534 3.877697 -4.705878
C 4.295056 6.242867 -6.218189
H 5.953188 5.365227 -7.306051
C 3.370651 4.884735 -4.423683
H 4.317700 2.962414 -4.114192
C 3.362299 6.071542 -5.178753
H 4.290354 7.157272 -6.813342
H 2.655233 4.745111 -3.611920
H 2.635593 6.855187 -4.959858
C 12.219169 3.788594 -6.455210
C 12.191201 4.848886 -7.388101
C 13.275106 3.732544 -5.518620
C 13.201248 5.824897 -7.391077
H 11.377257 4.897979 -8.112499
C 14.282047 4.711169 -5.517250
H 13.294546 2.928059 -4.784253
C 14.249623 5.759395 -6.454981
H 13.169609 6.633580 -8.122796
H 15.086125 4.657726 -4.781695
H 15.032613 6.519062 -6.455055
C 11.887698 -3.257707 -6.235300
C 12.695857 -3.625923 -7.331611
C 12.029448 -3.953843 -5.015744
C 13.628546 -4.669781 -7.210090
H 12.582849 -3.097648 -8.279242
C 12.961105 -4.997446 -4.893038
H 11.406582 -3.670772 -4.166814
C 13.764403 -5.357969 -5.990445
H 14.243178 -4.948012 -8.067560
H 13.060480 -5.524805 -3.942995
H 14.488166 -6.168852 -5.896737
C 4.892184 -2.920874 -6.588241
C 4.089645 -3.068370 -7.739668
C 4.615560 -3.717344 -5.455071
C 3.032095 -3.993133 -7.757761
H 4.301800 -2.459695 -8.619664
C 3.557464 -4.640151 -5.471896
H 5.228084 -3.602584 -4.560472
C 2.761625 -4.780014 -6.623416
H 2.422728 -4.099909 -8.656460
H 3.352490 -5.243050 -4.586019
H 1.938256 -5.495535 -6.636703
H 7.911480 -3.865204 -0.722580
H 9.628924 -3.474094 -0.543173

Free Energy= -3057.442998

Adduct 38c between $TPPH_2$ and 1

Cartesian Coordinates
N -0.125862 -2.189124 -0.230604
N 2.174843 -0.379563 0.074985
C 2.908981 1.984040 0.355233
C -2.626790 -2.192123 -0.250717
C 3.137811 0.595707 0.166629
H 0.800925 -5.354638 -0.044699
C 0.264682 -4.415437 -0.119296
C 4.307864 -1.327828 -0.088677
C 2.862760 -1.560508 -0.052482
C 0.893450 -3.122953 -0.168786
H 5.410777 0.577758 0.055673
C -1.101683 -4.229600 -0.157635
C 2.279700 -2.853032 -0.127974
C 4.479570 0.020183 0.048436
C -1.359650 -2.816649 -0.230056
H 5.070246 -2.089488 -0.217791
H -1.873407 -4.990134 -0.119835
C -2.856521 -0.794517 -0.171287
N -1.888809 0.163745 0.016092
C 1.644997 2.610390 0.409308
N 0.420589 1.997952 0.231087
C -0.604896 2.901089 0.435931
C 0.013481 4.169261 0.721135
C 1.379001 3.993845 0.701718
H 2.142252 4.738437 0.896160
H -0.529444 5.079615 0.939610
C -1.988904 2.621022 0.400759
C -2.568286 1.349164 0.146963
C -4.008413 1.146479 -0.011789
C -4.187812 -0.192628 -0.218572
H -5.118341 -0.723216 -0.393031
H 0.016200 -1.181341 -0.225355
H 0.299902 0.988865 0.183708
C 3.189602 -4.040140 -0.140411
C 4.058792 -4.289218 0.944956
C 3.192024 -4.934409 -1.233644
C 4.911514 -5.405232 0.936672
H 4.056312 -3.604898 1.794210
C 4.046555 -6.049147 -1.244399
H 2.527499 -4.744566 -2.077497
C 4.908722 -6.288512 -0.158638
H 5.573539 -5.586236 1.784940
H 4.041770 -6.726086 -2.100161
H 5.572074 -7.154659 -0.165934
C 4.096252 2.873282 0.552317
C 4.949514 2.684741 1.660764
C 4.377072 3.919554 -0.353426
C 6.056626 3.523774 1.862903
H 4.733707 1.883915 2.366521
C 5.487391 4.756976 -0.155320
H 3.724623 4.067028 -1.215074
C 6.329719 4.562830 0.955005
H 6.697466 3.371080 2.732383
H 5.694986 5.557323 -0.867376
H 7.189640 5.215861 1.111481
C -3.813557 -3.100721 -0.316311
C -4.746533 -3.137217 0.743605
C -4.014430 -3.943386 -1.431358
C -5.857378 -3.994815 0.687897
H -4.590311 -2.496270 1.611962
C -5.127168 -4.798891 -1.489593
H -3.297732 -3.917475 -2.253261
C -6.052022 -4.827247 -0.429705
H -6.566607 -4.015599 1.516846
H -5.272635 -5.438734 -2.361391
H -6.915681 -5.492418 -0.473746
H -4.763905 1.925195 0.014888
C -2.914928 3.757203 0.696908
C -3.780552 3.682861 1.810390
C -2.943480 4.913809 -0.112230
C -4.651281 4.741628 2.111473
H -3.758507 2.795094 2.442928
C -3.815630 5.973332 0.187197
H -2.285437 4.973141 -0.980048
C -4.670988 5.891470 1.301563
H -5.305491 4.671730 2.981907
H -3.830123 6.858467 -0.450713
H -5.345909 6.716076 1.535857
N 0.563785 0.332958 2.752903
C 0.817625 -1.021411 3.223944
C -0.591890 -0.574865 2.922245
C 0.810959 1.469442 3.516743
C 2.097997 1.673449 4.064532
C -0.175400 2.467373 3.674128
C 2.388350 2.867510 4.732761
H 2.852644 0.897937 3.953267
C 0.129792 3.641278 4.377639
H -1.168338 2.306947 3.264289
C 1.412206 3.867133 4.900194
H 1.642456 4.783634 5.437962
C -0.941773 4.695433 4.547183
C 3.753748 3.106916 5.333747
H 1.106209 -1.142344 4.273523
H 1.328151 -1.673152 2.510047

H -1.007389 -0.871244 1.959424
C -1.632522 -0.301859 3.958532
C -1.332511 -0.111331 5.323271
C -2.965129 -0.139635 3.521426
C -2.346601 0.226518 6.233936
H -0.305832 -0.213532 5.675306
C -3.980379 0.197138 4.431349
H -3.196870 -0.263457 2.462868
C -3.673817 0.381931 5.791760
H -2.100081 0.373696 7.286575
H -5.005204 0.320973 4.077148
H -4.459199 0.648706 6.500516
F -1.016706 5.538858 3.464089
F -2.187037 4.150531 4.698714
F -0.726010 5.495530 5.637607
F 3.695272 3.207871 6.704671
F 4.651408 2.116129 5.054607
F 4.308766 4.281675 4.892716

Free Energy= -3181.106196

Adduct 39 between 38b and 1

Cartesian Coordinates

N	2.766898	-1.865202	1.727500
N	1.166399	0.308999	2.787500
C	0.599201	2.707100	2.497100
C	4.627097	-2.265204	0.135800
C	0.456800	1.433200	3.117500
H	1.092395	-4.689201	2.013300
C	1.785796	-3.896901	1.759000
C	-0.383701	-0.179000	4.465000
C	0.618399	-0.704301	3.539800
C	1.757297	-2.581601	2.337100
H	-1.171799	1.882101	4.633200
C	2.795996	-3.933302	0.818400
C	0.840398	-2.086201	3.297700
C	-0.511000	1.152600	4.174400
C	3.454097	-2.654803	0.822000
H	-0.923901	-0.753199	5.210600
H	3.057695	-4.763202	0.173500
C	5.214698	-0.970404	0.236900
N	4.569399	0.156996	0.667900
C	1.734702	3.101799	1.755600
N	2.865201	2.327398	1.569000
C	3.851202	3.046397	0.925600
C	3.300403	4.347197	0.659000
C	2.004603	4.372098	1.138600
H	1.296003	5.188999	1.076700
H	3.828203	5.138497	0.138500
C	5.130401	2.560996	0.556300
C	5.469700	1.184096	0.499400
C	6.764400	0.670294	0.058700
C	6.594999	-0.674105	-0.138400
H	7.327298	-1.401206	-0.476400
H	2.951399	-0.876002	1.875400
H	2.930400	1.345098	1.825000
C	0.006197	-3.105100	3.998700
C	-1.406003	-3.034799	3.991000
C	0.623396	-4.192301	4.661900
C	-2.177504	-4.017798	4.629300
H	-1.894903	-2.217798	3.465600
C	-0.147505	-5.175200	5.301900
H	1.712096	-4.255001	4.677400
C	-1.552205	-5.092399	5.286700
H	-3.266104	-3.949397	4.601200
H	0.347294	-6.002200	5.813200
H	-2.152306	-5.858298	5.780200
C	-0.537098	3.663800	2.611700
C	-1.826198	3.243201	2.206600
C	-0.371997	4.983400	3.088500
C	-2.917497	4.122502	2.259600
H	-1.960199	2.227402	1.836400
C	-1.465396	5.862601	3.146300
H	0.612104	5.310099	3.425700
C	-2.739896	5.436902	2.728000
H	-3.899098	3.784503	1.926200
H	-1.323595	6.876701	3.522700
H	-3.586696	6.123503	2.768200
C	5.286397	-3.257004	-0.757700
C	5.582497	-2.894005	-2.093700
C	5.615195	-4.561605	-0.324300
C	6.175096	-3.811605	-2.973800
H	5.329398	-1.891904	-2.439400
C	6.207595	-5.480605	-1.204800
H	5.417295	-4.845504	0.709400
C	6.485795	-5.111005	-2.533900
H	6.383496	-3.515405	-4.002900
H	6.458294	-6.481805	-0.851100
H	6.942494	-5.827506	-3.218000
H	7.663700	1.258794	-0.092100
C	6.123102	3.584795	0.118700
C	6.751902	3.506394	-1.145400
C	6.433803	4.676895	0.962400
C	7.667903	4.488894	-1.552400
H	6.507201	2.679795	-1.810000

C	7.353904	5.657094	0.558200
H	5.955803	4.743695	1.940500
C	7.973604	5.567193	-0.701900
H	8.136203	4.415693	-2.535100
H	7.587905	6.487194	1.226500
H	8.686204	6.330293	-1.018200
C	-4.528103	-2.734596	-1.696700
C	-5.947003	-3.261695	-1.645500
N	-5.524503	-2.155295	-0.787200
H	-6.143604	-4.205495	-1.129600
H	-6.605903	-3.022195	-2.486700
C	-3.383504	-3.494697	-1.101600
C	-3.369504	-3.890597	0.251400
C	-2.300204	-3.847098	-1.932400
C	-2.288505	-4.622398	0.768900
H	-4.199604	-3.600297	0.895700
C	-1.230805	-4.599699	-1.420300
H	-2.298604	-3.519898	-2.973700
C	-1.218605	-4.985599	-0.068700
H	-2.276505	-4.898198	1.824100
H	-0.405805	-4.878800	-2.073500
H	-0.379905	-5.559500	0.326200
C	-6.017801	-0.852595	-0.964800
C	-5.141001	0.228204	-1.198100
C	-7.395201	-0.604494	-0.795400
C	-5.642000	1.537505	-1.198000
H	-4.087701	0.034703	-1.385400
C	-7.877400	0.712806	-0.824400
H	-8.072902	-1.439893	-0.624100
C	-7.010999	1.800506	-1.018500
H	-7.387498	2.819606	-1.026100
C	-9.365600	0.931308	-0.672700
C	-4.688099	2.684904	-1.441300
F	-3.448599	2.444703	-0.910200
F	-9.888901	0.210008	0.370600
F	-10.054000	0.530408	-1.794400
F	-9.699899	2.236808	-0.456900
F	-5.125198	3.862104	-0.896500
F	-4.497198	2.926004	-2.778900
Cl	-2.820901	-0.501498	-4.144400
N	0.729999	0.128799	-1.744300
C	2.216000	0.476698	-1.589900
C	2.986500	0.556698	-2.910600
H	2.652899	-0.276002	-0.928300
H	2.255700	1.424498	-1.046900
C	4.402300	1.113196	-2.688500
H	3.062999	-0.442903	-3.363100

H	2.464400	1.201798	-3.632400
C	5.192000	1.197996	-4.004700
H	4.330401	2.108696	-2.224200
H	4.939100	0.471296	-1.978700
H	6.204901	1.593995	-3.834200
H	5.290899	0.200896	-4.463100
H	4.684001	1.855696	-4.728000
C	0.182499	-0.182700	-0.350600
C	-1.334201	-0.380999	-0.278500
H	0.490600	0.647100	0.294200
H	0.718298	-1.072901	-0.005400
C	-1.725601	-0.720699	1.172800
H	-1.845400	0.541202	-0.582700
H	-1.667102	-1.182499	-0.951300
C	-3.231401	-0.598197	1.443900
H	-1.377802	-1.738499	1.401200
H	-1.196801	-0.041599	1.850100
H	-3.454701	-0.839997	2.495100
H	-3.576200	0.429903	1.255800
H	-3.814802	-1.276397	0.810800
C	-0.035200	1.302000	-2.370600
C	-0.108899	2.563900	-1.509400
H	-1.036600	0.918201	-2.601600
H	0.461300	1.509800	-3.324500
C	-0.795998	3.697701	-2.296600
H	-0.681199	2.369101	-0.592600
H	0.888402	2.908399	-1.201200
C	-1.006797	4.942801	-1.417000
H	-0.177598	3.954100	-3.172900
H	-1.763798	3.342401	-2.679400
H	-1.509996	5.743501	-1.980000
H	-1.622497	4.697101	-0.538400
H	-0.041396	5.330900	-1.055800
C	0.553898	-1.079800	-2.670500
C	1.318297	-2.331301	-2.230100
H	0.893899	-0.742201	-3.656200
H	-0.524902	-1.256700	-2.747000
C	1.415196	-3.340101	-3.390100
H	2.339998	-2.083402	-1.912100
H	0.818897	-2.805301	-1.373800
C	2.229795	-4.584202	-2.993600
H	0.402796	-3.628700	-3.715900
H	1.893797	-2.847102	-4.252800
H	2.287195	-5.300202	-3.827300
H	3.254196	-4.298703	-2.710800
H	1.775795	-5.099001	-2.132400
H	-4.268003	-2.137697	-2.578400

Free Energy= -4326.651111

Adduct 40 between TBACl and 1

Cartesian Coordinates

C 1.541734 2.662097 -0.674336
C 2.888325 3.297790 -0.939057
N 2.738934 2.268743 0.089237
H 3.080681 4.307594 -0.566156
H 3.407649 3.017103 -1.861419
C 0.453546 3.389687 0.050227

C 0.707542 4.115197 1.232509
C -0.853692 3.364769 -0.475433
C -0.328489 4.806244 1.879028
H 1.715240 4.115480 1.649611
C -1.888107 4.068097 0.165286
H -1.048584 2.782120 -1.377964
C -1.630973 4.788423 1.345041
H -0.121597 5.356594 2.798465
H -2.891644 4.058378 -0.257535
H -2.437016 5.328675 1.844132
C 3.316406 0.997399 -0.062419
C 2.525857 -0.168865 0.020019
C 4.714637 0.879689 -0.198982
C 3.145038 -1.426853 0.014854
H 1.443562 -0.080989 0.073124
C 5.310200 -0.390512 -0.221286
H 5.324070 1.779450 -0.272548
C 4.538796 -1.558093 -0.110786
H 5.006913 -2.538238 -0.120309
C 6.808687 -0.473477 -0.406039
C 2.283431 -2.667406 0.086535
F 1.195885 -2.497097 0.903520
F 7.480373 0.387036 0.425039
F 7.180038 -0.132048 -1.685873
F 7.312290 -1.720397 -0.173394
F 2.960780 -3.757470 0.560181
F 1.789911 -3.022577 -1.143978
Cl -0.335701 0.059205 -2.564819
N -3.437459 -0.706495 0.303177
C -4.832236 -1.140500 0.757504
C -5.733705 -1.709430 -0.336203
H -5.287707 -0.251680 1.209772
H -4.677201 -1.876451 1.553910
C -7.107349 -2.077416 0.260686
H -5.877829 -0.973502 -1.140765
H -5.284057 -2.608262 -0.782944
C -8.057371 -2.650064 -0.805570
H -6.966543 -2.812861 1.070087
H -7.555579 -1.179369 0.717629
H -9.031777 -2.911257 -0.366053
H -8.228311 -1.916073 -1.609088
H -7.630489 -3.558321 -1.259936
C -2.745225 -0.109893 1.532058
C -1.253284 0.194277 1.395393
H -2.900096 -0.834216 2.340988
H -3.309928 0.796377 1.778993
C -0.790270 0.935434 2.670721
H -0.690441 -0.742846 1.289841
H -1.044849 0.808415 0.509979
C 0.739449 0.967673 2.820738
H -1.186052 1.962831 2.646383
H -1.227085 0.440766 3.555748
H 1.025287 1.502973 3.739374
H 1.146736 -0.053589 2.877813
H 1.211098 1.482434 1.975123
C -2.637051 -1.889115 -0.255353
C -2.363055 -3.024992 0.728454
H -1.705412 -1.456856 -0.642168
H -3.209504 -2.254201 -1.115266
C -1.620654 -4.162955 -0.002919
H -1.747745 -2.670840 1.568415
H -3.298580 -3.424788 1.147179
C -1.217679 -5.293115 0.959514
H -2.271648 -4.560101 -0.799236
H -0.724792 -3.755346 -0.493256
H -0.694418 -6.099137 0.423186
H -0.545763 -4.911019 1.744167
H -2.104233 -5.726134 1.450382
C -3.523563 0.324139 -0.830539
C -4.410104 1.539308 -0.566866
H -3.897573 -0.230228 -1.698964
H -2.489927 0.610794 -1.054608
C -4.421823 2.435325 -1.822354
H -5.443853 1.235146 -0.345530
H -4.042004 2.122135 0.289526
C -5.349698 3.649366 -1.649456
H -3.394931 2.766919 -2.044735
H -4.751893 1.837785 -2.687769
H -5.337092 4.285557 -2.547003
H -6.386422 3.321027 -1.473202
H -5.042856 4.269389 -0.791926
H 1.191365 1.945748 -1.425705

Free Energy= -2414.738215

Transition state 39_{TS}
Imaginary Frequency at -110.1 cm^{-1}
Cartesian Coordinates

N	2.161804	-1.449796	2.011501
N	0.511798	0.967500	1.890801
C	0.389792	3.305500	1.058501
C	4.384106	-2.281991	1.250901

C	-0.126105	2.173699	1.744601
H	0.215110	-4.093501	2.349801
C	1.030908	-3.399899	2.183201
C	-1.614302	0.883595	2.855601
C	-0.398000	0.147498	2.515201
C	0.929205	-1.976199	2.352301
H	-2.139107	2.981494	2.412701
C	2.300109	-3.687896	1.724401
C	-0.232997	-1.248902	2.707201
C	-1.447705	2.148095	2.363701
C	3.032806	-2.455694	1.628401
H	-2.468201	0.489093	3.392901
H	2.697611	-4.659295	1.456001
C	5.044603	-1.027789	1.135001
N	4.423300	0.195009	1.088601
C	1.733492	3.463103	0.652301
N	2.764594	2.574505	0.903201
C	3.971793	3.101308	0.487001
C	3.677990	4.371108	-0.121699
C	2.316489	4.582704	-0.035699
H	1.755587	5.430403	-0.412199
H	4.419788	5.016309	-0.579399
C	5.236994	2.477711	0.584401
C	5.434698	1.109012	0.903001
C	6.740699	0.448615	0.898301
C	6.494302	-0.890586	1.020301
H	7.213004	-1.704384	1.061101
H	2.378601	-0.457895	1.944201
H	2.637896	1.660805	1.332001
C	-1.365595	-2.048004	3.264201
C	-2.634495	-2.056207	2.647301
C	-1.167393	-2.838504	4.421201
C	-3.684593	-2.818510	3.178101
H	-2.801796	-1.481508	1.737101
C	-2.218891	-3.599206	4.957401
H	-0.188093	-2.840402	4.901601
C	-3.482991	-3.588009	4.337601
H	-4.641193	-2.804112	2.654501
H	-2.051890	-4.195506	5.856001
H	-4.300690	-4.181111	4.751001
C	-0.558010	4.410098	0.731601
C	-1.698409	4.140395	-0.058199
C	-0.334113	5.730498	1.179601
C	-2.594412	5.167093	-0.392899
H	-1.872807	3.125294	-0.412999
C	-1.233816	6.756996	0.849401
H	0.537686	5.942900	1.799501
C	-2.365815	6.478493	0.060701
H	-3.469411	4.940791	-1.004099
H	-1.054718	7.769996	1.212901
H	-3.063317	7.276792	-0.197099
C	5.165009	-3.506289	0.921801
C	5.801309	-3.608287	-0.336999
C	5.273711	-4.585789	1.826701
C	6.526412	-4.758286	-0.682899
H	5.713007	-2.783788	-1.044699
C	5.999214	-5.736987	1.481301
H	4.801111	-4.510590	2.806601
C	6.626514	-5.828485	0.225001
H	7.002912	-4.821985	-1.662299
H	6.079916	-6.558187	2.195101
H	7.187216	-6.724984	-0.043299
H	7.702098	0.942717	0.807701
C	6.416292	3.333914	0.244701
C	7.282093	3.006216	-0.821899
C	6.669490	4.509015	0.988001
C	8.376791	3.828319	-1.134399
H	7.089995	2.111116	-1.409199
C	7.767288	5.329017	0.679901
H	6.005889	4.768013	1.814001
C	8.624089	4.992019	-0.383899
H	9.031592	3.562220	-1.965699
H	7.953786	6.227218	1.270601
H	9.475387	5.630021	-0.625499
C	-5.060293	-2.920513	-1.387099
C	-6.147393	-2.989316	-0.364999
N	-5.606795	-2.014214	0.573601
H	-6.211090	-3.978716	0.112501
H	-7.133393	-2.748318	-0.800299
C	-3.751291	-3.552210	-1.211399
C	-2.785992	-3.432208	-2.243699
C	-3.410690	-4.286309	-0.048799
C	-1.531690	-4.039905	-2.125699
H	-3.044993	-2.877308	-3.145599
C	-2.138888	-4.861606	0.082401
H	-4.122789	-4.351711	0.771001
C	-1.195688	-4.749604	-0.957099
H	-0.814390	-3.965003	-2.943699
H	-1.883287	-5.398106	0.997301
H	-0.211387	-5.207902	-0.857999
C	-5.913998	-0.703215	0.372401
C	-5.496800	0.221786	1.390501
C	-6.597399	-0.142917	-0.757699
C	-5.735203	1.589185	1.270801
H	-4.988399	-0.180213	2.264301
C	-6.801003	1.239783	-0.861599
H	-6.927298	-0.788517	-1.569299
C	-6.377305	2.134184	0.136501
H	-6.542607	3.204483	0.044001
C	-7.402504	1.794781	-2.130899
C	-5.358606	2.539386	2.380301
F	-6.472007	3.103484	2.967301
F	-8.303502	0.946479	-2.715999
F	-6.434205	2.037984	-3.085999
F	-8.053107	2.986680	-1.943499
F	-4.604208	3.596588	1.925301
F	-4.641204	1.956488	3.387101
H	-5.060395	-2.018113	-1.997799
Cl	-6.023990	-4.134215	-3.272799
N	1.523002	-0.576197	-2.210199
C	2.955001	-0.160194	-1.868199
C	3.978501	-0.342692	-2.991099

H 3.246602 -0.741593 -0.989199
H 2.897098 0.882606 -1.541799
C 5.271999 0.426011 -2.627399
H 4.208504 -1.412791 -3.100199
H 3.585000 0.003707 -3.958499
C 6.538801 -0.251586 -3.171799
H 5.198397 1.454911 -3.014499
H 5.322499 0.516512 -1.533899
H 7.443500 0.300317 -2.873899
H 6.624503 -1.279285 -2.785099
H 6.518001 -0.302086 -4.272099
C 0.736902 -0.535699 -0.893999
C -0.760898 -0.823403 -1.021199
H 0.916499 0.448901 -0.456299
H 1.228503 -1.262898 -0.247999
C -1.633201 0.441895 -1.037799
H -0.978196 -1.441903 -1.901599
H -1.047596 -1.442804 -0.159399
C -3.104600 0.099092 -1.295499
H -1.529302 0.942095 -0.065699
H -1.274002 1.151496 -1.800999
H -3.747602 0.984590 -1.205499
H -3.234899 -0.322709 -2.304899
H -3.462798 -0.649209 -0.575499
C 0.903699 0.375201 -3.235399
C 0.992196 1.860101 -2.871299
H -0.141600 0.057999 -3.324299
H 1.401800 0.172902 -4.191399
C 0.044094 2.693699 -3.752999
H 0.722796 2.021701 -1.817999
H 2.021195 2.223304 -3.005699
C 0.107290 4.187199 -3.386899
H 0.310594 2.550300 -4.813199
H -0.986905 2.321897 -3.628999
H -0.566211 4.777698 -4.025999
H -0.190610 4.340198 -2.338699
H 1.130489 4.575602 -3.512799
C 1.500205 -1.985898 -2.809699
C 1.954908 -3.087696 -1.851199
H 2.137105 -1.947296 -3.699699
H 0.473205 -2.162000 -3.146899
C 2.211411 -4.401896 -2.612499
H 2.877807 -2.799394 -1.328399
H 1.187608 -3.259198 -1.083499
C 2.694613 -5.514695 -1.665299
H 1.286811 -4.721698 -3.120099
H 2.959910 -4.227294 -3.403099
H 2.875716 -6.448194 -2.218699
H 3.627913 -5.220793 -1.161699
H 1.940314 -5.718896 -0.889199

Free Energy= -4326.613631

Adduct 41

Cartesian Coordinates

N -2.240800 -1.365700 -2.076500
N -0.566200 1.050100 -1.882300
C -0.388600 3.361900 -0.992700
C -4.473500 -2.186500 -1.344400
C 0.086400 2.247900 -1.739300
H -0.286500 -4.009600 -2.354500
C -1.105000 -3.314900 -2.206700
C 1.518800 0.970400 -2.935500
C 0.316800 0.234900 -2.553400
C -1.003300 -1.894000 -2.391400
H 2.076700 3.055000 -2.477200
C -2.383800 -3.601300 -1.771400
C 0.160400 -1.164400 -2.731600
C 1.381900 2.225600 -2.412000
C -3.117500 -2.367900 -1.700000
H 2.348900 0.576400 -3.510200
H -2.786300 -4.570900 -1.503000
C -5.108800 -0.921900 -1.204600
N -4.463900 0.282600 -1.083500
C -1.725000 3.522000 -0.562100
N -2.770400 2.662000 -0.850900
C -3.964200 3.165500 -0.371000
C -3.649300 4.403400 0.289400
C -2.288000 4.609000 0.191900
H -1.716800 5.430900 0.606200
H -4.376700 5.029000 0.794300
C -5.237100 2.555600 -0.477000
C -5.456500 1.208400 -0.868200
C -6.776600 0.586000 -0.948600
C -6.557900 -0.752000 -1.132800
H -7.292200 -1.545400 -1.234500
H -2.447600 -0.372600 -2.006200
H -2.662100 1.766700 -1.321300
C 1.322200 -1.963200 -3.216400
C 2.570400 -1.893800 -2.558800
C 1.185300 -2.830300 -4.325400
C 3.658400 -2.663800 -2.995400
H 2.683100 -1.243800 -1.691500
C 2.273400 -3.598300 -4.768800
H 0.225400 -2.887800 -4.840400
C 3.511700 -3.517100 -4.103700
H 4.596800 -2.599700 -2.438300
H 2.155100 -4.255300 -5.632100
H 4.355500 -4.119300 -4.445400
C 0.602300 4.410200 -0.615600
C 1.784000 4.032300 0.065500
C 0.398100 5.776200 -0.913400
C 2.730600 4.994100 0.447200

H 1.947600 2.981200 0.300100
C 1.347000 6.739100 -0.533600
H -0.497400 6.075600 -1.458600
C 2.514200 6.351800 0.151000
H 3.633800 4.681800 0.973400
H 1.179400 7.788700 -0.779700
H 3.250600 7.101200 0.444900
C -5.276100 -3.411500 -1.062000
C -5.929200 -3.549700 0.185100
C -5.386600 -4.457800 -2.005300
C -6.663800 -4.707100 0.485200
H -5.845900 -2.749500 0.920900
C -6.124600 -5.614500 -1.707100
H -4.900200 -4.352900 -2.975500
C -6.762600 -5.744800 -0.459700
H -7.152300 -4.801000 1.456200
H -6.205700 -6.409800 -2.449500
H -7.333000 -6.645200 -0.227400
H -7.728000 1.101600 -0.866100
C -6.405600 3.392600 -0.071700
C -7.279300 2.974500 0.957700
C -6.647800 4.633800 -0.704000
C -8.368200 3.772900 1.341700
H -7.093400 2.026800 1.460200
C -7.739700 5.430700 -0.323900
H -5.980500 4.963200 -1.501400
C -8.603500 5.003100 0.701200
H -9.028100 3.436500 2.143000
H -7.916900 6.381400 -0.829000
H -9.450700 5.622900 0.998200
C 5.292200 -2.896700 1.713500
C 6.319800 -2.912400 0.561900
N 5.904500 -2.061200 -0.535400
H 6.412300 -3.951400 0.203000
H 7.304100 -2.632400 0.991000
C 3.943600 -3.538200 1.472400
C 2.997800 -3.588300 2.522100
C 3.583800 -4.072800 0.218400
C 1.744200 -4.185900 2.335300
H 3.260300 -3.174200 3.496500
C 2.312500 -4.641100 0.020700
H 4.278400 -4.005100 -0.614900
C 1.390300 -4.710200 1.078300
H 1.045500 -4.239100 3.171300
H 2.048300 -5.027600 -0.964600
H 0.410100 -5.164200 0.926600
C 6.066000 -0.734300 -0.381500
C 5.678000 0.122500 -1.480600
C 6.575700 -0.043800 0.783900
C 5.726200 1.509700 -1.385800
H 5.316400 -0.353900 -2.390100
C 6.602600 1.355300 0.848100
H 6.910700 -0.612600 1.648400
C 6.170600 2.169900 -0.214100
H 6.187400 3.254200 -0.145900
C 6.990700 2.018400 2.145100
C 5.369700 2.364900 -2.573300
F 4.717200 1.693400 -3.571600
F 7.871700 1.283300 2.895400
F 5.892000 2.232600 2.961500
F 7.566900 3.253100 1.972700
F 6.488200 2.925200 -3.161100
F 4.565300 3.430700 -2.233800
H 5.160200 -1.879000 2.097200
Cl 6.120500 -3.768600 3.233700
N -1.421500 -0.860000 2.013100
C -2.845300 -0.474700 1.605000
C -3.857200 -0.498000 2.749000
H -3.133900 -1.161800 0.805300
H -2.774700 0.517600 1.152100
C -5.201600 0.095900 2.291600
H -4.017200 -1.530900 3.093700
H -3.488300 0.081100 3.608900
C -6.265300 0.009300 3.398200
H -5.045600 1.143400 1.993100
H -5.553800 -0.432900 1.395000
H -7.224300 0.432200 3.062300
H -6.440700 -1.039800 3.686300
H -5.944200 0.560100 4.296700
C -0.589800 -0.905900 0.722000
C 0.924500 -1.078800 0.907200
H -0.814600 0.014900 0.174000
H -1.017600 -1.731200 0.152100
C 1.725700 0.230900 0.802100
H 1.160200 -1.585800 1.852900
H 1.273000 -1.772300 0.129300
C 3.216400 0.008100 1.082300
H 1.591000 0.643200 -0.207500
H 1.328500 0.979600 1.501800
H 3.804800 0.914700 0.885500
H 3.374500 -0.285500 2.132500
H 3.618700 -0.796300 0.452500
C -0.848500 0.160600 2.997600
C -0.989400 1.623500 2.568700
H 0.203500 -0.113200 3.133000
H -1.360700 -0.006100 3.951700
C -0.109600 2.515400 3.466500
H -0.696000 1.758000 1.518000
H -2.037500 1.944000 2.657400
C -0.306300 4.010600 3.166300
H -0.346800 2.311200 4.524000
H 0.948100 2.239900 3.319500
H 0.328400 4.627600 3.820200
H -0.042800 4.234300 2.123000
H -1.356000 4.304200 3.324900
C -1.407700 -2.229500 2.701400
C -2.042200 -3.365700 1.896600
H -1.934500 -2.094800 3.653100
H -0.357800 -2.447100 2.922300
C -2.081800 -4.664300 2.724600
H -3.071600 -3.111200 1.609800
H -1.481500 -3.552100 0.970800

C -2.731300 -5.808800 1.925600
H -1.059900 -4.948100 3.022000
H -2.647700 -4.485900 3.653900
H -2.769500 -6.734000 2.519700
H -3.758600 -5.542300 1.630800
H -2.159600 -6.014600 1.006600

Free Energy= -4326.623681

Adduct 42

Cartesian Coordinates

N	-3.028002	-1.718593	-1.822701
N	-1.008596	0.344001	-2.121301
C	-0.512789	2.763299	-2.050101
C	-5.487402	-1.960186	-1.476901
C	-0.263092	1.438199	-2.493201
H	-1.715611	-4.729497	-1.505501
C	-2.362808	-3.864495	-1.587801
C	0.931602	-0.337605	-3.227601
C	-0.276099	-0.745201	-2.514101
C	-1.908904	-2.531296	-1.871901
H	1.651008	1.694493	-3.692901
C	-3.737608	-3.827391	-1.446501
C	-0.611803	-2.100900	-2.235001
C	0.923006	1.030395	-3.241301
C	-4.166304	-2.463490	-1.594101
H	1.664800	-1.006507	-3.664901
H	-4.401310	-4.656989	-1.229301
C	-5.795898	-0.598385	-1.224001
N	-4.856396	0.368012	-0.944601
C	-1.632587	3.139203	-1.267801
N	-2.780990	2.397206	-1.078001
C	-3.667988	3.065809	-0.252801
C	-3.008684	4.276807	0.155299
C	-1.783984	4.332703	-0.481001
H	-1.031582	5.109201	-0.400001
H	-3.422882	5.000208	0.846599
C	-4.987589	2.645913	0.028099
C	-5.561792	1.439014	-0.465801
C	-6.998893	1.183218	-0.510901
C	-7.146697	-0.078781	-1.022001
H	-8.070299	-0.610778	-1.226201
H	-2.994299	-0.705393	-1.903601
H	-2.948792	1.470107	-1.460801
C	0.472794	-3.115903	-2.324501
C	1.684495	-2.894307	-1.627501
C	0.336891	-4.297803	-3.088501
C	2.730292	-3.827210	-1.682401
H	1.797497	-1.985107	-1.036901
C	1.380988	-5.234706	-3.143701
H	-0.579910	-4.466000	-3.654301
C	2.577689	-5.003310	-2.439801
H	3.658093	-3.630113	-1.145701
H	1.264385	-6.137306	-3.745701
H	3.389386	-5.730912	-2.487001
C	0.480115	3.838496	-2.339101
C	1.845914	3.699092	-2.001001
C	0.052318	5.040898	-2.950101
C	2.756817	4.731890	-2.271201
H	2.186711	2.785991	-1.515801
C	0.964921	6.070895	-3.226301
H	-0.998782	5.154001	-3.218101
C	2.321421	5.919291	-2.886601
H	3.802717	4.616987	-1.992501
H	0.618124	6.986596	-3.707601
H	3.033023	6.719089	-3.096501
C	-6.582305	-2.970983	-1.541701
C	-7.546206	-3.088680	-0.513801
C	-6.656408	-3.858383	-2.641701
C	-8.557109	-4.059777	-0.586001
H	-7.489704	-2.424780	0.346299
C	-7.669611	-4.826780	-2.716701
H	-5.919308	-3.774285	-3.441001
C	-8.623911	-4.931677	-1.688101
H	-9.286509	-4.139375	0.221499
H	-7.715313	-5.495579	-3.577501
H	-9.410113	-5.685974	-1.743901
H	-7.774691	1.884721	-0.218801
C	-5.828886	3.509415	0.902399
C	-6.433488	2.945717	2.051199
C	-6.031882	4.882216	0.634899
C	-7.205286	3.735219	2.916999
H	-6.278091	1.888416	2.266099
C	-6.804880	5.672318	1.500399
H	-5.592481	5.321314	-0.260901
C	-7.390482	5.103220	2.646599
H	-7.653887	3.284820	3.803699
H	-6.955877	6.729318	1.276199
H	-7.988080	5.719421	3.319799
C	6.085902	-0.585120	3.117599
C	7.235701	-0.889023	2.133299
N	6.693400	-1.240922	0.818199
H	7.822498	-1.741225	2.486299
H	7.913203	-0.025325	2.071899
C	5.107998	-1.708617	3.342899

C	3.731899	-1.411113	3.413299
C	5.528994	-3.048018	3.476099
C	2.790196	-2.435610	3.595799
H	3.402502	-0.376212	3.313399
C	4.587091	-4.072316	3.654399
H	6.587194	-3.294021	3.408099
C	3.213892	-3.770412	3.712399
H	1.729197	-2.192307	3.644899
H	4.923588	-5.106417	3.738799
H	2.483090	-4.569509	3.843999
C	6.272703	-0.230321	-0.039901
C	5.808202	-0.499019	-1.361401
C	6.336807	1.140479	0.344299
C	5.432405	0.540682	-2.216701
H	5.735999	-1.529419	-1.691001
C	5.975710	2.162880	-0.543601
H	6.672807	1.430378	1.334199
C	5.508509	1.892082	-1.836701
H	5.213211	2.688183	-2.513601
C	5.999314	3.587580	-0.044001
C	5.017104	0.193483	-3.628201
F	6.107004	0.074380	-4.463101
F	7.012615	3.826877	0.844499
F	4.832015	3.916984	0.611699
F	6.137717	4.502380	-1.054601
F	4.209207	1.144986	-4.193301
F	4.343500	-0.994415	-3.710401
H	5.543204	0.318882	2.821199
Cl	6.884703	-0.076622	4.753499
N	-1.792898	-0.493397	2.251099
C	-3.198799	-0.704693	1.671499
C	-4.280900	-0.995790	2.714499
H	-3.110301	-1.521893	0.949799
H	-3.440396	0.194608	1.098299
C	-5.622301	-1.306586	2.030099
H	-4.001202	-1.850790	3.347799
H	-4.417597	-0.127089	3.374899
C	-6.727401	-1.607282	3.055599
H	-5.918898	-0.451585	1.408799
H	-5.491503	-2.163186	1.352299
H	-7.683402	-1.822580	2.554299
H	-6.462604	-2.477883	3.676599
H	-6.882699	-0.745582	3.724699
C	-0.893997	0.011601	1.115799
C	0.583104	0.147996	1.488899
H	-1.317594	0.967102	0.792899
H	-1.023299	-0.689099	0.285899
C	1.372506	0.763094	0.320899
H	0.713206	0.784496	2.376499
H	1.011101	-0.836705	1.724799
C	2.879806	0.807289	0.602299
H	1.187804	0.178694	-0.588801
H	0.987709	1.775195	0.125499
H	3.425307	1.231188	-0.250401
H	3.102507	1.423389	1.487699
H	3.274303	-0.203412	0.781999
C	-1.837595	0.524503	3.395899
C	-2.407491	1.891605	3.010399
H	-0.811895	0.617200	3.766999
H	-2.434597	0.058005	4.187599
C	-2.616489	2.760906	4.265699
H	-1.727590	2.411703	2.320799
H	-3.371391	1.782508	2.495099
C	-3.164284	4.153007	3.903299
H	-3.317390	2.248608	4.945799
H	-1.660588	2.861603	4.806299
H	-3.320483	4.761008	4.807299
H	-2.459783	4.686805	3.246799
H	-4.125585	4.067010	3.374099
C	-1.244702	-1.807398	2.816599
C	-0.961005	-2.896899	1.780099
H	-1.971103	-2.148996	3.561199
H	-0.325301	-1.538501	3.348499
C	-0.477209	-4.182301	2.479399
H	-1.855406	-3.131597	1.186399
H	-0.182804	-2.564602	1.079799
C	-0.045012	-5.247602	1.456699
H	0.369192	-3.940003	3.140099
H	-1.282810	-4.574598	3.121699
H	0.313585	-6.156603	1.962499
H	-0.888413	-5.525699	0.805399
H	0.764989	-4.864704	0.816599
C	6.676495	-2.718622	0.475999
O	5.727294	-3.108819	-0.248801
O	7.617193	-3.375424	0.986699

Free Energy= -4515.1174173

Transition state 42$_{TS}$
Imaginary frequency at -151 cm^{-1}
Cartesian Coordinates

N	-2.866067	-0.978626	-2.359506
C	-1.724430	-1.682634	-2.700630
C	-3.966592	-1.811171	-2.328375
H	-2.871847	0.014911	-2.142390
N	-0.940484	1.189634	-2.172461
C	-0.237382	2.369417	-2.221148
C	-0.164002	0.275309	-2.837837
C	-0.531479	3.513853	-1.433882
C	-1.649767	3.625871	-0.572083
C	0.442287	4.646771	-1.403889
C	-5.299381	-1.429875	-2.023693
C	-5.647059	-0.211774	-1.384180
C	-6.363101	-2.423639	-2.349905
C	0.970982	2.223070	-3.031673
C	-2.119201	-3.058736	-2.829407
C	-3.483760	-3.133499	-2.620503
C	1.034231	0.903244	-3.389641
C	-0.455933	-1.111068	-2.956479
C	0.638780	-2.025672	-3.389815
N	-4.734933	0.683007	-0.873664
C	-7.008909	0.177045	-1.025255
C	-5.463830	1.561233	-0.117511
N	-2.752022	2.794513	-0.551638
C	-1.841521	4.581160	0.487756
C	-3.639668	3.185346	0.435837
H	-2.886392	1.987123	-1.155352
C	-3.028271	4.285217	1.128269
C	-4.920923	2.637372	0.642613
C	-5.759141	3.230717	1.720727
C	-6.891842	1.264306	-0.200877
C	1.849232	-2.083235	-2.658055
C	0.488279	-2.849971	-4.528045
C	2.875425	-2.960179	-3.046693
C	1.517643	-3.717752	-4.923816
C	2.710523	-3.775719	-4.181711
C	1.793193	4.436725	-1.044883
C	0.019840	5.960502	-1.710719
C	2.699769	5.507042	-0.999423
C	0.927100	7.031865	-1.670752
C	2.270112	6.809034	-1.314530
C	-7.296708	-2.859631	-1.380823
C	-6.443856	-2.967281	-3.654617
C	-8.279373	-3.807921	-1.705481
C	-7.428728	-3.912460	-3.980943
C	-8.349631	-4.338582	-3.006414
C	-6.305631	2.389179	2.718913
C	-6.032184	4.615130	1.774987
C	-7.096811	2.919367	3.749076
C	-6.821259	5.146800	2.807657
C	-7.352360	4.301924	3.800273
C	4.087222	-2.334802	2.581278

C	5.364288	-1.617183	2.151004
C	4.015339	-3.517451	3.446055
N	5.498024	-1.631040	0.683771
C	5.967471	-0.495728	0.007429
C	5.281494	-2.989489	0.207741
C	2.805949	-4.251727	3.455392
C	5.072471	-3.934185	4.286575
C	2.656552	-5.382874	4.261702
C	4.922690	-5.069168	5.097254
C	3.719044	-5.798582	5.087615
C	5.532398	-0.242436	-1.319149
C	6.775956	0.469425	0.641811
C	5.872390	0.948720	-1.956376
C	7.095479	1.672829	-0.016061
C	6.651570	1.934492	-1.315944
C	5.310043	1.264308	-3.322696
C	7.930032	2.682849	0.734825
F	9.144135	2.164549	1.118062
F	7.309527	3.092268	1.891733
F	8.191659	3.810132	0.011281
F	6.274013	1.723356	-4.185566
F	4.355047	2.255505	-3.258322
F	4.718255	0.193826	-3.926235
N	-1.645422	-0.950426	1.906466
C	-3.063767	-1.075140	1.326375
C	-0.822406	-0.124025	0.911603
C	-1.691757	-0.262621	3.272815
C	-1.010087	-2.336154	2.106419
C	-4.109752	-1.629140	2.293790
C	-5.459502	-1.808776	1.579454
C	-6.526324	-2.390594	2.521995
C	0.632205	0.073717	1.323491
C	1.327667	1.060428	0.372399
C	2.838177	1.132250	0.623590
C	-2.268673	1.153296	3.239358
C	-2.516764	1.675778	4.666895
C	-2.985486	3.141068	4.650751
C	-0.690692	-3.090744	0.809179
C	-0.485087	-4.601544	1.059472
C	-0.079834	-5.320629	-0.239309
O	5.690340	-3.308547	-0.934645
O	4.683398	-3.720103	1.063577
Cl	3.206247	-0.797592	4.086507
H	1.677084	3.011329	-3.272604
H	-1.443027	-3.874905	-3.053285
H	-4.107272	-4.020093	-2.643917
H	1.796071	0.402899	-3.980062
H	-7.919065	-0.316544	-1.350960
H	-1.131359	5.359120	0.744248
H	-3.451960	4.782051	1.993551
H	-7.683767	1.834462	0.275497

H	1.970737	-1.450043	-1.778132
H	-0.433657	-2.792963	-5.107288
H	3.811305	-3.018896	-2.488902
H	1.389610	-4.341299	-5.810042
H	3.511930	-4.451195	-4.485173
H	2.123672	3.434014	-0.787240
H	-1.020506	6.133011	-1.989376
H	3.736850	5.322861	-0.712352
H	0.586343	8.038189	-1.919037
H	2.974106	7.641838	-1.282278
H	-7.243700	-2.458991	-0.370926
H	-5.734468	-2.633470	-4.412624
H	-8.984848	-4.135785	-0.940436
H	-7.478848	-4.312163	-4.994840
H	-9.113724	-5.075336	-3.258219
H	-6.095169	1.320135	2.686024
H	-5.636899	5.267300	0.995259
H	-7.504325	2.256506	4.513948
H	-7.028647	6.217523	2.831350
H	-7.965135	4.716581	4.601889
H	3.243548	-2.181594	1.915612
H	6.248381	-2.056369	2.636296
H	5.285626	-0.574045	2.468131
H	1.979679	-3.938825	2.817496
H	6.007465	-3.376852	4.319527
H	1.712113	-5.930015	4.252860
H	5.745377	-5.383420	5.740749
H	3.608113	-6.678369	5.722886
H	4.892426	-0.963243	-1.815169
H	7.154670	0.296027	1.646889
H	6.896507	2.867519	-1.817436
H	-2.967872	-1.713287	0.444519
H	-3.347428	-0.084282	0.960003
H	-1.347842	0.828893	0.797785
H	-0.886741	-0.647709	-0.046376
H	-0.665122	-0.261078	3.653348
H	-2.280091	-0.921812	3.921305
H	-1.711289	-2.900062	2.730801
H	-0.099778	-2.164023	2.692483
H	-3.791996	-2.599416	2.703240
H	-4.253094	-0.942453	3.140673
H	-5.802088	-0.838339	1.195873
H	-5.328664	-2.465158	0.706153
H	-7.490410	-2.506837	2.003540
H	-6.220329	-3.378242	2.902233
H	-6.683996	-1.725767	3.386438
H	0.722488	0.445859	2.349852
H	1.156945	-0.890463	1.287012
H	1.117184	0.763218	-0.660718
H	0.887857	2.060083	0.507743
H	3.339845	1.740226	-0.143391
H	3.058286	1.567059	1.610214
H	3.286866	0.133455	0.591233
H	-1.573698	1.831306	2.723538
H	-3.217606	1.179961	2.686139
H	-3.274758	1.041422	5.156245
H	-1.591356	1.585862	5.259458
H	-3.174911	3.505761	5.671612
H	-2.216916	3.783178	4.192737
H	-3.911100	3.254127	4.065180
H	-1.520037	-2.996713	0.093784
H	0.204462	-2.665356	0.332733
H	0.283304	-4.793071	1.826831
H	-1.426887	-5.023942	1.446366
H	0.011371	-6.405103	-0.077793
H	-0.830356	-5.148924	-1.026180
H	0.887471	-4.942480	-0.605136

Free Energy= -4515.09939497

Compound 2a

Cartesian Coordinates

C 0.329835 -1.303894 -0.804502
C 1.717369 -1.885608 -0.443627
C 1.121632 -0.322076 1.185227
N 0.218218 -0.179321 0.133598
H -0.475683 -2.034491 -0.634914
H 1.684337 -2.976608 -0.356169
C -0.813612 0.773656 0.048604
C -1.887020 0.545766 -0.838724
C -0.783669 1.971706 0.797360
C -2.909826 1.498530 -0.963159
H -1.934863 -0.364522 -1.430683
C -1.821994 2.902208 0.657222
H 0.041497 2.168747 1.473571
C -2.899818 2.683409 -0.215382
H -3.696491 3.414673 -0.314810
O 1.210629 0.343331 2.207038
O 1.950714 -1.373589 0.923510
H 0.291128 -0.948754 -1.841797
C 2.851000 -1.458019 -1.349432
C 3.004992 -0.107703 -1.729785

C 3.776083 -2.415437 -1.805437
C 4.072571 0.275762 -2.555415
H 2.292094 0.641602 -1.382346
C 4.844123 -2.033331 -2.636849
H 3.657446 -3.459844 -1.510377
C 4.994242 -0.686872 -3.011055
H 4.185322 1.321400 -2.844825
H 5.554212 -2.783151 -2.988105
H 5.822273 -0.387354 -3.655038
C -1.763740 4.154605 1.507678
C -4.049610 1.188137 -1.909838
F -4.807590 0.135592 -1.456224
F -3.596085 0.823487 -3.151973
F -4.899159 2.237867 -2.088854
F -2.680584 5.094931 1.138984
F -1.995951 3.872707 2.831578
F -0.533124 4.754256 1.453247

Free Energy = -1457.7012180

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