Electronic Supplementary Material (ESI) for Green Chemistry.

Visible-light-induced direct perfluoroalkylation/heteroarylation of [1.1.1]propellane to diverse bicyclo[1.1.1]pentanes (BCPs) under metal and photocatalyst-free conditions

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Supporting Information

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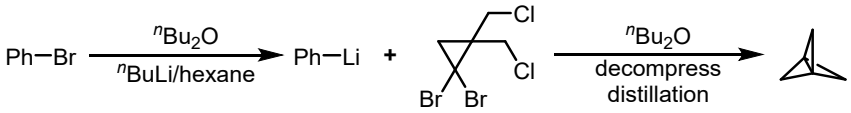
General Information

All reagents and deuterated solvents were commercially available and used without further purification. All products were separated by silica gel (200-300 mesh) column chromatography with petroleum ether (PE) (60-90°C) and ethyl acetate (EA). ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on a Bruker Advance 500 spectrometer at ambient temperature with $CDCl_3$ as solvent and tetramethylsilane (TMS) as the internal standard. Analytical thin layer chromatography (TLC) was performed on Merk precoated TLC (silica gel 60 F254) plates. Compounds for HRMS were analyzed by positive mode electrospray ionization (ESI) using Agilent 6530 QTOF mass spectrometer.

1. Experimental Section

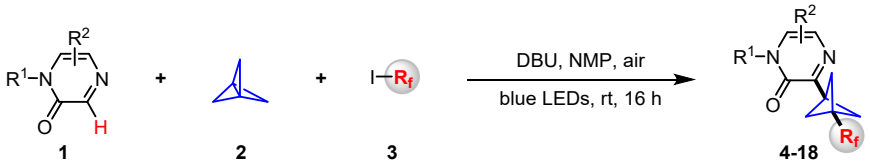
1.1 Preparation of the solution of [1.1.1]propellane in hexane



A 150 ml three-neck round bottom flask equipped with a magnetic stirring bar was charged with bromobenzene (100 mmol, 1.0 equiv.) and anhydrous $^{n}Bu_2O$ (20 mL). Then the reaction mixture was cooled down to -30 °C and ^{n}BuLi (100 mmol, 1.0 equiv., 2.5 M in hexane) was added dropwise. After the addition was completed, the reaction mixture was allowed to warm to room temperature, and stirred at room temperature for 1 h. The reaction mixture was used in the next step directly.

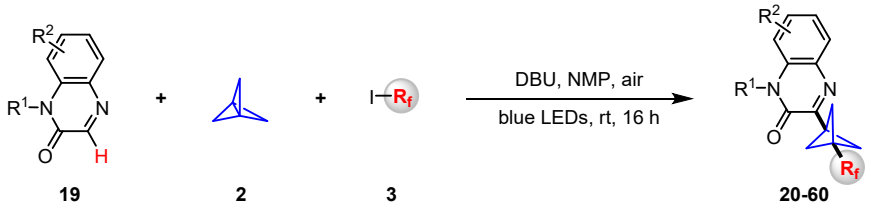
A solution of the above prepared PhLi in $^{n}Bu_2O$/hexane (65 mL) was added dropwise to a suspension of 1,1-dibromo-2,2-bis(chloromethyl)cyclopropane (45.0 mmol) in anhydrous $^{n}Bu_2O$ (20 mL) at -20 °C. After the addition was completed, the reaction mixture was allowed to warm to 0 °C and stirred for 2 h, then the addition funnel was swapped out for a distillation head with attached 100 mL round bottom flask in a bath (liquid nitrogen). A vacuum was slowly applied to the system and the distillate collected, while maintaining the reaction/distillation flask below 0 °C. Approximately 30 mL of distillate was collected. The concentration of [1.1.1]propellane (0.4-0.6 M) was measured by ^{1}H NMR using dichloromethane as the standard.

1.2 General procedure for multi-component reaction of pyrazinones with [1.1.1]propellane and perfluoroalkyl iodine



A mixture of pyrazinones (**1**) (0.2 mmol), [1.1.1]propellane (**2**) (0.5 mmol), perfluoroalkyl iodine (**3**) (0.4 mmol), DBU (0.4 mmol) and NMP (0.5 mL) in a 10-mL test tube was stirred under the irradiation of blue LED (10 W) for 16 h. After completing the reaction as indicated by TLC, a saturated NH_4Cl solution was added to the mixture. The mixture was then extracted with DCM, and the collected organic layer was washed with brine, and dried with $MgSO_4$. The solvent was removed *in vacuo*, and the obtained residue was further purified by silica gel column chromatography (200-300 mesh silica gel).

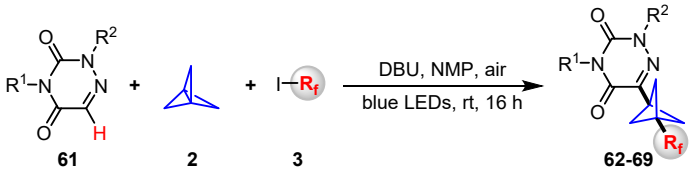
1.3 General procedure for multi-component reaction of quinoxalinones with [1.1.1]propellane and perfluoroalkyl iodine



19 2 3 20-60

A mixture of quinoxalinones (**19**) (0.2 mmol), [1.1.1]propellane (**2**) (0.5 mmol), perfluoroalkyl iodine (**3**) (0.4 mmol), DBU (0.4 mmol) and NMP (0.5 mL) in a 10-mL test tube was stirred under the irradiation of blue LED (10 W) for 16 h. After completing the reaction as indicated by TLC, a saturated NH_4Cl solution was added to the mixture. The mixture was then extracted with DCM, and the collected organic layer was washed with brine, and dried with $MgSO_4$. The solvent was removed *in vacuo*, and the obtained residue was further purified by silica gel column chromatography (200-300 mesh silica gel).

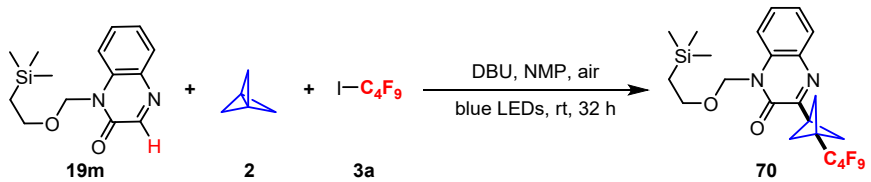
1.4 General procedure for multi-component reaction of azauracils with [1.1.1]propellane and perfluoroalkyl iodine



61 2 3 62-69

A mixture of azauracils (**61**) (0.2 mmol), [1.1.1]propellane (**2**) (0.5 mmol), perfluoroalkyl iodine (**3**) (0.4 mmol), DBU (0.4 mmol) and NMP (0.5 mL) in a 10-mL test tube was stirred under the irradiation of blue LED (10 W) for 16 h. After completing the reaction as indicated by TLC, a saturated NH_4Cl solution was added to the mixture. The mixture was then extracted with DCM, and the collected organic layer was washed with brine, and dried with $MgSO_4$. The solvent was removed *in vacuo*, and the obtained residue was further purified by silica gel column chromatography (200-300 mesh silica gel).

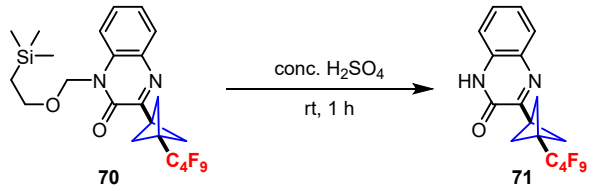
1.5 General procedure for large-scale multi-component reaction of quinoxalinone (19m) with [1.1.1]propellane and perfluorobutyl iodine



19m 2 3a 70

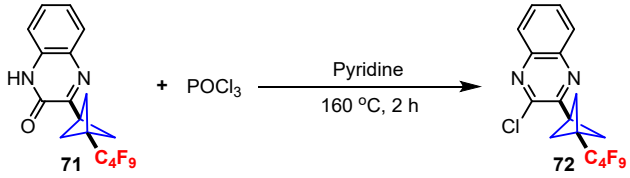
A mixture of quinoxalinones (**19m**) (2 mmol), [1.1.1]propellane (**2**) (5 mmol), perfluoroalkyl iodine (**3**) (4 mmol), DBU (4 mmol) and NMP (5 mL) in a 50-mL test tube was stirred under the irradiation of blue LED (10 W) for 32 h. After completing the reaction as indicated by TLC, a saturated NH_4Cl solution was added to the mixture. The mixture was then extracted with DCM, and the collected organic layer was washed with brine, and dried with $MgSO_4$. The solvent was removed *in vacuo*, and the obtained residue was further purified by silica gel column chromatography (200-300 mesh silica gel).

1.6 General procedure for the hydrolysis of compound 70



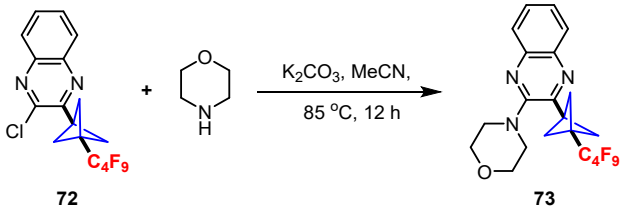
A mixture of compound (**70**) (2 mmol) and conc. H_2SO_4 (5 mL) in a 25-mL flask was stirred at room temperature for 1 h. After reaction completion confirmed by TLC, the reaction mixture was dropwise added to ice water (25 mL). The mixture was then extracted with DCM, and the collected organic layer was washed with a saturated $NaHCO_3$ solution, brine, and dried with $MgSO_4$. The solvent was removed *in vacuo*, and the obtained residue was further purified by silica gel column chromatography (200-300 mesh silica gel).

1.7 General procedure for the chlorination of compound 71



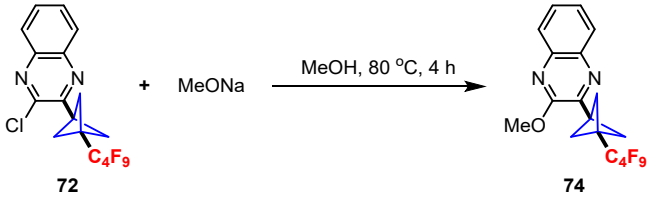
A mixture of compound (**71**) (2 mmol), $POCl_3$ (2.5 mmol) and pyridine (2 mmol) in a 15-mL pressure tube was stirred at 160 °C in an oil bath for 2 h. After reaction completion confirmed by TLC, a saturated $NaHCO_3$ solution was added to the residue. The mixture was then extracted with DCM, and the collected organic layer was washed with brine, and dried with $MgSO_4$. The solvent was removed *in vacuo*, and the obtained residue was further purified by silica gel column chromatography (200-300 mesh silica gel).

1.8 General procedure for amination of compound 72



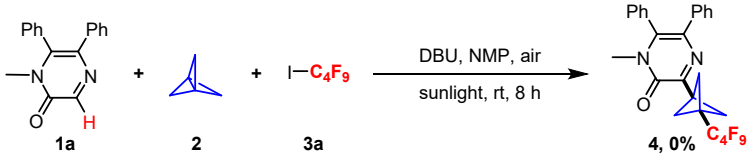
A mixture of compound (**72**) (0.2 mmol), morpholine (1.5 equiv), K_2CO_3 (1.5 equiv) and MeCN (1.5 mL) in a 15-mL pressure tube was stirred at 85 °C in an oil bath for 12 h. After completion of the reaction as indicated by TLC, a saturated $NaHCO_3$ solution was added to the residue. The mixture was then extracted with DCM, and the collected organic layer was washed with brine and dried with $MgSO_4$. The solvent was removed *in vacuo*, and the obtained residue was further purified by silica gel column chromatography (200-300 mesh silica gel).

1.9 General procedure for methoxylation of compound 72



A mixture of compound (**72**) (0.2 mmol), MeONa (3.0 equiv) and MeOH (2.0 mL) in a 15-mL pressure tube was stirred at 80 °C in an oil bath for 4 h. After completion of the reaction as indicated by TLC, a saturated $NaHCO_3$ solution was added to the residue. The mixture was then extracted with DCM, and the collected organic layer was washed with brine, and dried with $MgSO_4$. The solvent was removed *in vacuo*, and the obtained residue was further purified by silica gel column chromatography (200-300 mesh silica gel).

1.10 General procedure for sunlight-induced multi-component reaction of pyrazinone with [1.1.1]propellane and perfluorobutyl iodine



A mixture of pyrazinones (**1a**) (0.2 mmol), [1.1.1]propellane (**2**) (0.5 mmol), perfluorobutyl iodine (**3a**) (0.4 mmol), DBU (0.4 mmol) and NMP (0.5 mL) in a 10-mL test tube was stirred under the irradiation of sunlight for 8 h. It was found that no corresponding product (**4**) was generated.

1.11 Visible light irradiation On/Off experiment

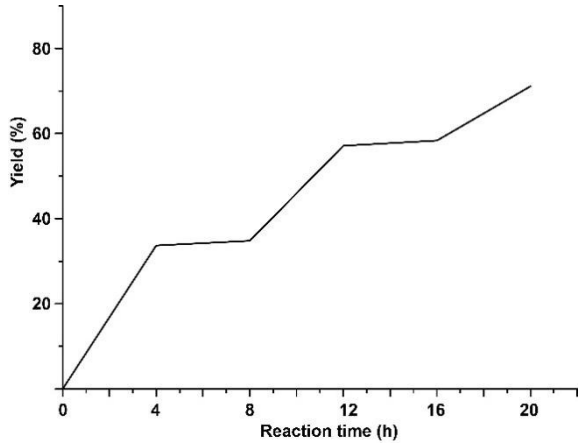
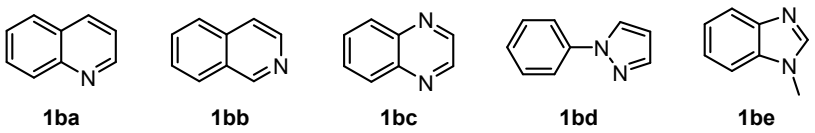


Figure S1. Visible light irradiation On/Off experiment

The results of LEDs irradiation On/Off experiments demonstrate that the continuous irradiation of LEDs is indispensable for the multi-component reaction.

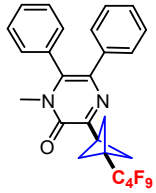
To expand the substrate scope, we tested some other heteroarenes, such as quinoline (**1ba**), isoquinoline (**1bb**), quinoxaline (**1bc**), 1-phenylpyrazole (**1bd**), and 1-methylbenzimidazole (**1be**). Unfortunately, the substrates above were not compatible with this method.



Scheme S1. Ineffective heteroarenes for the multi-component reaction

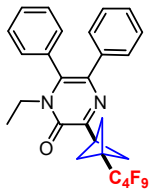
2 Characterization of Products

1-Methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-5,6-diphenylpyrazin-2(1*H*)-one (4)



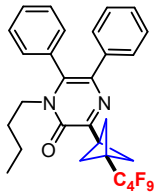
Obtained as a light yellow solid (74 mg, 68% yield); M. P. = 146-147 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (dd, J = 4.8, 2.3 Hz, 3H), 7.20 (dd, J = 7.3, 2.1 Hz, 2H), 7.13 (s, 5H), 3.30 (s, 3H), 2.55 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 151.6, 138.0, 137.6, 132.7, 132.5, 130.0, 129.6, 129.3, 129.2, 127.8, 127.1, 51.0, 41.8, 37.9 (t, J = 37.8 Hz), 33.7, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.03 – -81.09 (m), -115.64 – -117.48 (m), -121.42 – -122.98 (m), -125.32 – -126.91 (m); HRMS (ESI+): Calculated for $C_{26}H_{19}F_9N_2O$: $[M+H]^+$ 547.1426, Found 547.1427.

1-Ethyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-5,6-diphenylpyrazin-2(1*H*)-one (5)



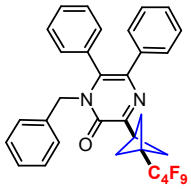
Obtained as a yellow liquid (73 mg, 65% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 (dd, J = 9.2, 6.3 Hz, 3H), 7.19 – 7.15 (m, 2H), 7.04 (s, 5H), 3.79 (d, J = 7.1 Hz, 2H), 2.48 (s, 6H), 1.09 (dd, J = 9.3, 4.8 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.6, 152.0, 137.8, 137.7, 132.8, 132.3, 130.1, 129.5, 129.3, 128.9, 127.7, 127.0, 51.1, 41.2, 37.9 (t, J = 31.5 Hz), 29.7, 13.6, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.99 – -81.08 (m), -116.51 – -116.58 (m), -122.29 – -122.34 (m), -125.83 – -126.05 (m); HRMS (ESI+): Calculated for $C_{27}H_{21}F_9N_2O$: $[M+H]^+$ 561.1583, Found 561.1591.

1-Butyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-5,6-diphenylpyrazin-2(1*H*)-one (6)



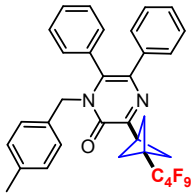
Obtained as a yellow liquid (78 mg, 66% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 – 7.36 (m, 3H), 7.22 (dd, J = 7.9, 1.5 Hz, 2H), 7.12 (s, 5H), 3.81 – 3.72 (m, 2H), 2.55 (s, 6H), 1.59 (s, 2H), 1.14 (dd, J = 14.8, 7.4 Hz, 2H), 0.73 (t, J = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.8, 151.9, 137.9, 137.7, 132.8, 132.2, 130.2, 129.5, 129.3, 128.8, 127.7, 127.0, 51.0, 45.9, 37.9 (t, J = 31.5 Hz), 30.2, 29.7, 20.0, 13.3, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.03 – -81.08 (m), -116.53 – -116.59 (m), -122.29 – -122.33 (m), -125.97 – -126.04 (m); HRMS (ESI+): Calculated for $C_{29}H_{25}F_9N_2O$: $[M+H]^+$ 589.1896, Found 589.1895.

1-Benzyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-5,6-diphenylpyrazin-2(1*H*)-one (7)



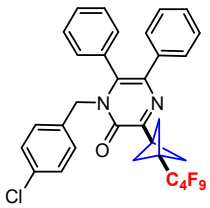
Obtained as a light yellow solid (75 mg, 60% yield); M. P. = 89-90 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (t, J = 7.5 Hz, 1H), 7.24 (d, J = 8.7 Hz, 5H), 7.11 (d, J = 1.9 Hz, 5H), 6.99 (d, J = 7.3 Hz, 2H), 6.85 (dd, J = 6.3, 2.7 Hz, 2H), 5.11 (s, 2H), 2.58 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.0, 152.5, 137.9, 137.5, 136.0, 132.9, 131.9, 130.5, 129.5, 129.3, 128.6, 128.5, 127.7, 127.5, 127.2, 127.1, 51.1, 48.7, 41.9, 37.9 (t, J = 31.5 Hz), ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.03 – -81.07 (m), -116.50 – -116.59 (m), -122.29 – -122.31 (m), -126.00 – -126.04 (m); HRMS (ESI+): Calculated for $C_{32}H_{23}F_9N_2O$: $[M+H]^+$ 623.1739, Found 623.174.

1-(4-Methylbenzyl)-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-5,6-diphenylpyrazin-2(1*H*)-one (8)



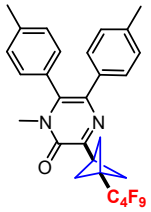
Obtained as a yellow liquid (79 mg, 62% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 (t, J = 7.5 Hz, 1H), 7.25 (t, J = 7.7 Hz, 2H), 7.10 (d, J = 1.4 Hz, 5H), 7.01 (dd, J = 7.3, 4.0 Hz, 4H), 6.75 (d, J = 8.0 Hz, 2H), 5.06 (s, 2H), 2.57 (s, 6H), 2.28 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.0, 152.4, 138.0, 137.6, 137.3, 133.0, 132.9, 132.0, 130.5, 129.5, 129.3, 129.2, 128.6, 127.7, 127.2, 127.0, 51.1, 48.5, 41.9, 37.9 (t, J = 31.5 Hz), 21.1, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.03 – -81.07 (m), -116.52 – -116.56 (m), -122.28 – -122.31 (m), -125.97– -126.03 (m); HRMS (ESI+): Calculated for $C_{33}H_{25}F_9N_2O$: $[M+H]^+$637.1896, Found 637.1888.

1-(4-Chlorobenzyl)-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-5,6-diphenylpyrazin-2(1*H*)-one (9)



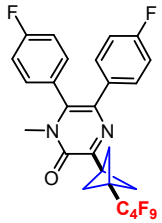
Obtained as a light yellow solid (72 mg, 55% yield); M. P. = 145-146 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (t, J = 7.5 Hz, 1H), 7.28 – 7.24 (m, 2H), 7.19 – 7.14 (m, 2H), 7.14 – 7.06 (m, 5H), 6.99 (d, J = 7.2 Hz, 2H), 6.79 (d, J = 8.4 Hz, 2H), 5.06 (s, 2H), 2.57 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.0, 152.6, 137.6, 137.4, 134.5, 133.5, 133.1, 131.8, 130.5, 129.7, 129.3, 128.8, 128.8, 128.7, 127.7, 127.1, 51.1, 48.1, 41.9, 37.9 (t, J = 31.5 Hz), ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.03 – 81.07(m), -116.51 – -116.57 (m), -122.27 – -122.31 (m), -125.96 – -126.03 (m); HRMS (ESI+): Calculated for $C_{32}H_{22}ClF_9N_2O$: $[M+H]^+$ 657.135, Found 657.1346.

1-Methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-5,6-di-p-tolylpyrazin-2(1*H*)-one (10)



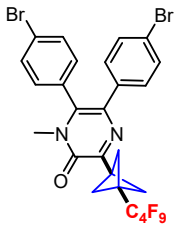
Obtained as a light yellow solid (76 mg, 66% yield); M. P. = 168-169 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.20 (d, J = 7.8 Hz, 2H), 7.05 (dd, J = 17.1, 8.0 Hz, 4H), 6.94 (d, J = 8.0 Hz, 2H), 3.28 (s, 3H), 2.54 (s, 6H), 2.38 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.4, 151.2, 139.6, 137.8, 136.7, 134.9, 132.7, 129.8, 129.8, 129.7, 129.1, 128.5, 51.0, 41.8, 37.9 (t, J = 31.5 Hz), 33.6, 21.4, 21.1, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.03 – -81.08 (m), -116.49 – -116.56 (m), -122.29 – -122.31 (m), -125.99 – -126.05 (m); HRMS (ESI+): Calculated for $C_{28}H_{23}F_9N_2O$: $[M+H]^+$ 575.1739, Found 575.1734.

5,6-Bis(4-fluorophenyl)-1-methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)pyrazin-2(1*H*)-one (11)



Obtained as a light yellow solid (58 mg, 50% yield); M. P. = 116-117°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.20 – 7.15 (m, 2H), 7.12 (d, J = 8.4 Hz, 2H), 7.09 – 7.04 (m, 2H), 6.84 (t, J = 8.6 Hz, 2H), 3.29 (s, 3H), 2.54 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.2 (d, J = 252.0 Hz), 161.9 (d, J = 247.0 Hz), 158.0, 155.2, 152.1, 136.9, 133.5 (d, J = 2.5 Hz), 132.0 (d, J = 7.6 Hz), 131.0 (d, J = 7.6 Hz), 128.4 (d, J = 2.5 Hz), 116.6 (d, J = 21.4 Hz), 114.9 (d, J = 21.4 Hz), 51.0, 41.8, 37.9 (t, J = 31.5 Hz), 33.6, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.06 – -81.92 (m), -109.63 (s), -114.65 (s), -115.57 – -117.62 (m), -122.27 – -122.94 (m), -125.57 – -126.96 (m); HRMS (ESI+): Calculated for $C_{26}H_{17}F_{11}N_2O$: $[M+H]^+$ 583.1238, Found 583.1238.

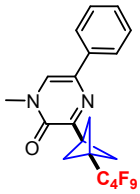
5,6-Bis(4-bromophenyl)-1-methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)pyrazin-2(1*H*)-one (12)



Obtained as a light yellow solid (69 mg, 49% yield); M. P. = 134-135 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 (d, J = 8.4 Hz, 2H), 7.31 – 7.28 (m, 2H), 7.07 (d, J = 8.4 Hz, 2H), 7.00 – 6.97 (m, 2H), 3.28 (s, 3H), 2.53 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.1, 152.3, 136.9, 136.3, 132.7, 131.5, 131.5, 131.1, 131.0, 130.9, 124.4, 121.6, 51.0, 41.7, 37.9 (t, J = 31.5 Hz), 33.7, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.03 – -81.09 (m), -116.55 – -116.61 (m), -122.27 – -

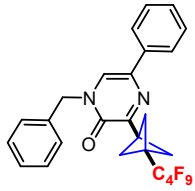
122.33 (m), -125.99 – -126.06 (m); HRMS (ESI+): Calculated for $C_{26}H_{17}Br_2F_9N_2O$: $[M+H]^+$ 702.9637, Found 702.9597.

1-Methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-5-phenylpyrazin-2(1*H*)-one (13)



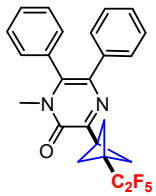
Obtained as a yellow liquid (37 mg, 39% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 – 7.71 (m, 2H), 7.50 (s, 1H), 7.43 (dd, J = 10.5, 4.8 Hz, 2H), 7.34 (t, J = 7.4 Hz, 1H), 3.59 (s, 3H), 2.53 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.2, 153.2, 135.5, 132.6, 128.9, 128.1, 125.2, 124.9, 51.0, 41.8, 37.9 (t, J = 31.5 Hz), 37.4, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.06 (t, J = 10.0 Hz), -116.52 – -116.62 (m), -122.27 – -122.35 (m), -125.49 – -126.08 (m); HRMS (ESI+): Calculated for $C_{20}H_{15}F_9N_2O$: $[M+H]^+$ 471.1113, Found 471.1114.

1-Benzyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-5-phenylpyrazin-2(1*H*)-one (14)



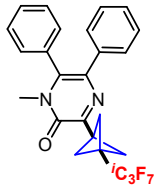
Obtained as a yellow liquid (35 mg, 32% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 – 7.67 (m, 2H), 7.45 (s, 1H), 7.39 (s, 2H), 7.38 (s, 2H), 7.36 (dd, J = 6.5, 3.0 Hz, 3H), 7.32 (d, J = 7.4 Hz, 1H), 5.13 (s, 2H), 2.54 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.7, 153.8, 135.5, 134.8, 132.7, 129.2, 128.8, 128.7, 128.5, 128.1, 124.9, 123.7, 52.1, 51.1, 41.9, 37.9 (t, J = 30.2 Hz), ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.02 – -81.07 (m), -116.54 – -116.60 (m), -122.30 – -122.33 (m), -125.97 – -126.04 (m); HRMS (ESI+): Calculated for $C_{26}H_{19}F_9N_2O$: $[M+H]^+$ 547.1426, Found 547.1424.

1-Methyl-3-(3-(perfluoroethyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (15)



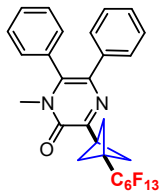
Obtained as a yellow liquid (55 mg, 62% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (t, J = 5.8 Hz, 3H), 7.19 (dd, J = 7.5, 1.8 Hz, 2H), 7.13 (s, 5H), 3.30 (s, 3H), 2.51 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.3, 151.6, 138.0, 137.6, 132.7, 132.5, 130.0, 129.6, 129.3, 129.2, 127.7, 127.1, 50.6, 41.5, 37.0 (t, J = 30.2 Hz), 33.7, ^{13}C NMR for C_2F_5 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -82.65, -120.86; HRMS (ESI+): Calculated for $C_{24}H_{19}F_5N_2O$: $[M+H]^+$ 447.149, Found 447.1493.

1-Methyl-3-(3-(perfluoroisopropyl)bicyclo[1.1.1]pentan-1-yl)-5,6-diphenylpyrazin-2(1*H*)-one (16)



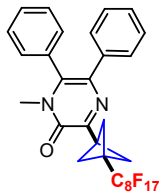
Obtained as a light yellow solid (66 mg, 67% yield); M. P. = 175-176 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (d, J = 6.8 Hz, 3H), 7.19 (dd, J = 7.5, 1.8 Hz, 2H), 7.12 (s, 5H), 3.30 (s, 3H), 2.57 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.3, 151.4, 138.0, 137.6, 132.7, 132.5, 130.0, 130.0, 129.3, 129.2, 127.7, 127.1, 52.0, 41.7, 36.5 (d, J = 26.5 Hz), 33.7, ^{13}C NMR for $^{i}C_3F_7$ could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -74.62 (d, J = 8.8 Hz), -183.26 – -183.29 (m); HRMS (ESI+): Calculated for $C_{25}H_{19}F_7N_2O$: $[M+H]^+$ 497.1458, Found 497.1456.

1-Methyl-3-(3-(perfluorohexyl)bicyclo[1.1.1]pentan-1-yl)-5,6-diphenylpyrazin-2(1*H*)-one (17)



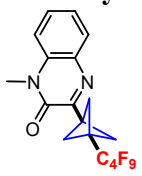
Obtained as a light yellow solid (93 mg, 72% yield); M. P. = 125-126 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (dt, J = 5.6, 2.9 Hz, 3H), 7.20 (dd, J = 7.3, 2.1 Hz, 2H), 7.13 (s, 5H), 3.30 (s, 3H), 2.55 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 151.6, 138.0, 137.6, 132.7, 132.5, 130.0, 129.6, 129.3, 129.2, 127.8, 127.1, 51.0, 41.8, 38.0 (t, J = 31.5 Hz), 33.7, ^{13}C NMR for C_6F_{13} could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.78 – -80.83 (m), -116.30 – -116.37 (m), -121.30 – -121.36 (m), -121.87 – -121.93 (m), -122.92 (s), -126.08 – -126.16 (m); HRMS (ESI+): Calculated for $C_{28}H_{19}F_{13}N_2O$: $[M+H]^+$ 647.1363, Found 647.1363.

1-Methyl-3-(3-(perfluorooctyl)bicyclo[1.1.1]pentan-1-yl)-5,6-diphenylpyrazin-2(1*H*)-one (18)



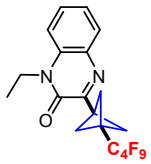
Obtained as a light yellow solid (104 mg, 70% yield); M. P. = 159-160 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (d, J = 6.7 Hz, 3H), 7.20 (dd, J = 7.5, 1.7 Hz, 2H), 7.13 (s, 5H), 3.30 (s, 3H), 2.55 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.3, 151.6, 138.0, 137.6, 132.7, 132.5, 130.0, 129.6, 129.3, 129.2, 127.7, 127.1, 51.0, 41.8, 38.0 (t, J = 31.5 Hz), 33.7, ^{13}C NMR for C_8F_{17} could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.74 – -80.78 (m), -116.29 – -116.36 (m), -121.24 – -121.28 (m), -121.64 – -121.68 (m), -121.89 – -121.92 (m), -122.68 – -122,73 (m), -126.07 – -126.11 (m); HRMS (ESI+): Calculated for $C_{30}H_{19}F_{17}N_2O$: $[M+H]^+$ 747.1299, Found 747.1299.

1-Methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (20)



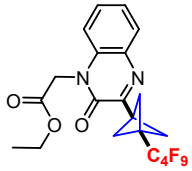
Obtained as a light yellow solid (71 mg, 80% yield); M. P. = 70-71 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (dd, J = 8.0, 1.3 Hz, 1H), 7.59 – 7.52 (m, 1H), 7.38 – 7.33 (m, 1H), 7.30 (d, J = 8.4 Hz, 1H), 3.67 (s, 3H), 2.56 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.8, 154.5, 133.5, 132.7, 130.5, 130.2, 123.7, 113.6, 51.2, 42.1, 38.0 (t, J = 31.5 Hz), 28.6, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.07 – -81.12 (m), -116.60 – -116.67 (m), -122.29 – -122.35 (m), -126.01 – -126.08 (m); HRMS (ESI+): Calculated for $C_{18}H_{13}F_9N_2O$: $[M+H]^+$ 445.0957, Found 445.0957.

1-Ethyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (21)



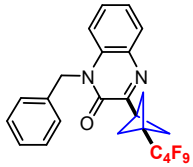
Obtained as a yellow liquid (75 mg, 82% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 – 7.84 (m, 1H), 7.57 – 7.52 (m, 1H), 7.33 (td, J = 8.7, 1.6 Hz, 2H), 4.29 (q, J = 7.2 Hz, 2H), 2.56 (s, 6H), 1.38 (t, J = 7.2 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.8, 154.0, 133.0, 132.4, 130.5, 130.4, 123.5, 113.5, 51.2, 42.0, 37.9 (t, J = 31.5 Hz), 37.0, 12.4, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.05 – -81.11 (m), -116.60 – -116.66 (m), -122.30 – -122.36 (m), -125.99 – -126.06 (m); HRMS (ESI+): Calculated for $C_{19}H_{15}F_9N_2O$: $[M+H]^+$ 459.1113, Found 459.1105.

Ethyl-2-(3-(3-(perfluorobutyl)-2-oxoquinoxalin-1(2*H*)-yl)acetate (22)



Obtained as a light yellow solid (77 mg, 75% yield); M. P. = 88-89 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (dd, J = 8.0, 1.4 Hz, 1H), 7.55 – 7.48 (m, 1H), 7.39 – 7.31 (m, 1H), 7.05 (d, J = 8.4 Hz, 1H), 4.99 (s, 2H), 4.26 (d, J = 7.1 Hz, 2H), 2.55 (s, 6H), 1.28 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.0, 154.7, 154.0, 132.8, 132.6, 130.6, 130.5, 124.0, 113.1, 62.2, 51.3, 43.1, 41.9, 37.9 (t, J = 31.5 Hz), 14.1, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.04 – -81.10 (m), -116.60 – -116.67 (m), -122.29 – -122.35 (m), -125.99 – -126.06 (m); HRMS (ESI+): Calculated for $C_{21}H_{17}F_9N_2O_3$: $[M+H]^+$ 517.1168, Found 517.117.

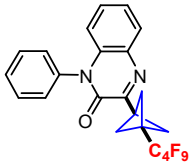
1-Benzyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (23)



Obtained as a light yellow solid (75 mg, 72% yield); M. P. = 93-94 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (dd, J = 8.0, 1.3 Hz, 1H), 7.47 – 7.39 (m, 1H), 7.30 (ddd, J = 7.4, 6.4, 5.3 Hz, 4H), 7.23 (t, J =

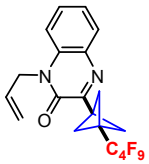
8.1 Hz, 3H), 5.46 (s, 2H), 2.59 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.0, 154.5, 135.1, 133.0, 132.9, 130.5, 130.3, 129.0, 127.8, 126.9, 123.8, 114.5, 51.3, 45.6, 42.1, 37.9 (t, J = 31.5 Hz), ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.05 (ddd, J = 13.6, 8.4, 3.4 Hz), -115.59 – -117.55 (m), -122.30 (dd, J = 18.2, 8.3 Hz), -124.69 – -126.96 (m); HRMS (ESI+): Calculated for $C_{24}H_{17}F_9N_2O$: $[M+H]^+$ 521.127, Found 521.1266.

3-(3-(Perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-1-phenylquinoxalin-2(1*H*)-one (24)



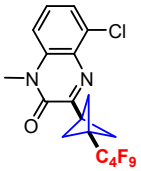
Obtained as a yellow liquid (68 mg, 67% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.90 (dd, J = 7.6, 1.7 Hz, 1H), 7.63 (t, J = 7.5 Hz, 2H), 7.56 (t, J = 7.4 Hz, 1H), 7.36 – 7.29 (m, 4H), 6.70 (dd, J = 7.9, 1.5 Hz, 1H), 2.58 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.6, 154.2, 135.4, 134.3, 132.6, 130.4, 130.1, 129.8, 129.6, 128.2, 123.9, 115.5, 51.4, 42.0, 37.9 (t, J = 31.5 Hz), ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.54 – -81.57 (m), -115.71 – -117.36 (m), -121.72 – -122.99 (m), -125.52 – -126.07 (m); HRMS (ESI+): Calculated for $C_{23}H_{15}F_9N_2O$: $[M+H]^+$ 507.1113, Found 507.1121.

1-Allyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (25)



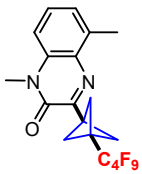
Obtained as a yellow liquid (59 mg, 63% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (dd, J = 8.0, 1.2 Hz, 1H), 7.54 – 7.50 (m, 1H), 7.33 (dd, J = 11.2, 4.0 Hz, 1H), 7.28 (d, J = 8.4 Hz, 1H), 5.93 (ddd, J = 22.3, 10.4, 5.2 Hz, 1H), 5.28 (d, J = 10.5 Hz, 1H), 5.18 (d, J = 17.3 Hz, 1H), 4.87 (d, J = 5.1 Hz, 2H), 2.56 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.9, 154.0, 132.9, 132.7, 130.5, 130.4, 130.3, 123.7, 118.3, 114.2, 51.3, 44.2, 42.0, 37.9 (t, J = 31.5 Hz), ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.07 – -81.12 (m), -116.61 – -116.68 (m), -122.30 – -122.35 (m), -126.00 – -126.07 (m); HRMS (ESI+): Calculated for $C_{20}H_{15}F_9N_2O$: $[M+H]^+$ 471.1113, Found 471.1107.

5-Chloro-1-methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (26)



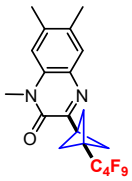
Obtained as a light yellow solid (71 mg, 74% yield); M. P. = 81-82 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 – 7.41 (m, 2H), 7.22 (dd, J = 7.7, 1.8 Hz, 1H), 3.68 (s, 3H), 2.58 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.2, 154.1, 135.2, 135.0, 130.4, 129.4, 124.7, 112.5, 51.3, 42.2, 38.0 (t, J = 31.5 Hz), 29.1, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.04 – -81.08 (m), -116.60 – -116.66 (m), -122.29 – -122.31 (m), -125.99 – -126.06 (m); HRMS (ESI+): Calculated for $C_{18}H_{12}ClF_9N_2O$: $[M+H]^+$ 479.0567, Found 479.0563.

1,5-Dimethyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (27)



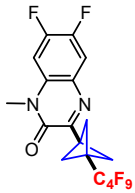
Obtained as a light yellow solid (72 mg, 79% yield); M. P. = 133-134 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 – 7.40 (m, 1H), 7.20 (d, *J* = 7.4 Hz, 1H), 7.13 (d, *J* = 8.4 Hz, 1H), 3.66 (s, 3H), 2.67 (s, 3H), 2.54 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.4, 152.8, 139.1, 133.6, 131.3, 130.2, 125.0, 111.5, 51.1, 42.3, 37.8 (t, *J* = 31.5 Hz), 28.7, 17.2, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.07 (t, *J* = 9.9 Hz), -115.92 – -116.63 (m), -121.72 – -122.32 (m), -125.77 – -126.52 (m); HRMS (ESI+): Calculated for $C_{19}H_{15}F_9N_2O$: $[M+H]^+$ 459.1113, Found 459.111.

1,6,7-Trimethyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (28)



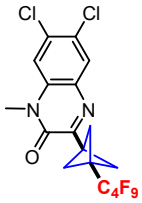
Obtained as a yellow liquid (77 mg, 82% yield); ^{1}H NMR (500 MHz, $CDCl_3$) *δ* 7.61 (s, 1H), 7.06 (s, 1H), 3.65 (s, 3H), 2.54 (s, 6H), 2.42 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) *δ* 154.6, 153.5, 140.4, 132.7, 131.5, 131.2, 130.2, 114.2, 51.1, 42.1, 37.8 (t, *J* = 31.5 Hz), 28.5, 20.6, 19.1, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) *δ* -81.04 – -81.10 (m), -116.57 – -116.63 (m), -122.28 – -122.32 (m), -125.99 – -126.06 (m); HRMS (ESI+): Calculated for $C_{20}H_{17}F_9N_2O$: $[M+H]^+$ 473.1270, Found 473.1271.

6,7-Difluoro-1-methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (29)



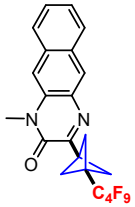
Obtained as a light yellow solid (61 mg, 64% yield); M. P. = 89-90 °C; ^{1}H NMR (500 MHz, $CDCl_3$) *δ* 7.65 (dd, *J* = 10.0, 8.3 Hz, 1H), 7.09 (dd, *J* = 11.2, 7.0 Hz, 1H), 3.62 (s, 3H), 2.52 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) *δ* 155.3 (d, *J* = 3.5 Hz), 154.0, 151.5 (dd, *J* = 254.1, 14.4 Hz), 146.7 (dd, *J* = 247.5, 14.0 Hz), 130.8 (d, *J* = 8.9 Hz), 129.0 (dd, *J* = 9.3, 2.9 Hz), 117.8 (dd, *J* = 18.0, 2.0 Hz), 102.3 (d, *J* = 23.1 Hz), 51.2, 41.9, 37.8 (t, *J* = 31.5 Hz), 29.1, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) *δ* -81.15 – -81.19 (m), -116.71 – -116.77 (m), -122.34 – -122.39 (m), -126.08 – -126.15 (m), -130.17 (d, *J* = 22.4 Hz), -141.91 (d, *J* = 22.4 Hz); HRMS (ESI+): Calculated for $C_{18}H_{11}F_{11}N_2O$: $[M+H]^+$ 481.0768, Found 481.0768.

6,7-Dichloro-1-methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (30)



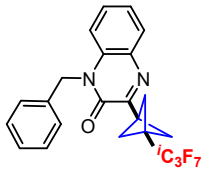
Obtained as a light yellow solid (71 mg, 69% yield); M. P. = 94-95 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.38 (s, 1H), 3.62 (s, 3H), 2.53 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.3, 153.8, 134.6, 132.9, 131.8, 131.0, 127.6, 115.2, 51.3, 42.0, 37.9 (t, J = 31.5 Hz), 28.9, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.05 – -81.09 (m), -116.65 – -116.71 (m), -122.29 – -122.33 (m), -126.01 – -126.07 (m); HRMS (ESI+): Calculated for $C_{18}H_{11}Cl_2F_9N_2O$: $[M+H]^+$ 513.0177, Found 513.0172.

1-Methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)benzo[g]quinoxalin-2(1*H*)-one (31)



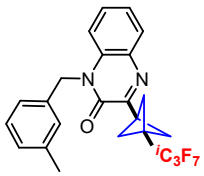
Obtained as a light yellow solid (56 mg, 57% yield); M. P. = 126-127 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.96 (d, J = 8.2 Hz, 1H), 7.90 (d, J = 8.3 Hz, 1H), 7.61 – 7.55 (m, 2H), 7.52 – 7.46 (m, 1H), 3.73 (s, 3H), 2.59 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.4, 154.3, 133.8, 132.0, 131.8, 129.8, 129.5, 128.5, 128.1, 127.2, 125.4, 110.0, 51.4, 42.2, 37.9 (t, J = 31.5 Hz), 28.6, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.02 – -81.07 (m), -116.57 – -116.63 (m), -122.26 – -122.29 (m), -125.97 – -126.04 (m); HRMS (ESI+): Calculated for $C_{22}H_{15}F_9N_2O$: $[M+Na]^+$ 517.0933, Found 517.094.

1-Benzyl-3-(3-(perfluoroisopropyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (32)



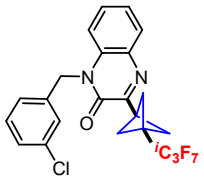
Obtained as a light yellow solid (66 mg, 70% yield); M. P. = 129-130 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (dd, J = 8.0, 1.4 Hz, 1H), 7.43 (ddd, J = 8.6, 7.4, 1.5 Hz, 1H), 7.34 – 7.29 (m, 3H), 7.26 – 7.17 (m, 4H), 5.46 (s, 2H), 2.61 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.9, 154.5, 135.1, 133.0, 132.9, 130.5, 130.3, 129.0, 127.8, 126.9, 123.8, 114.5, 52.3, 45.6, 42.0, 36.5 (d, J = 25.2 Hz), ^{13}C NMR for $^{i}C_3F_7$ could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -74.62 (d, J = 8.7 Hz), -183.34 – -183.54 (m); HRMS (ESI+): Calculated for $C_{23}H_{17}F_7N_2O$: $[M+H]^+$ 471.1302, Found 471.1306.

3-(3-(Perfluoroisopropyl)bicyclo[1.1.1]pentan-1-yl)-1-(3-methylbenzyl)quinoxalin-2(1*H*)-one (33)



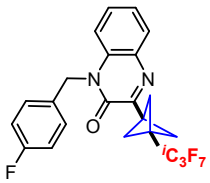
Obtained as a light yellow solid (69 mg, 71% yield); M. P. = 131-132 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (dd, J = 8.0, 1.3 Hz, 1H), 7.43 (ddd, J = 8.6, 7.4, 1.5 Hz, 1H), 7.33 – 7.27 (m, 1H), 7.27 – 7.23 (m, 1H), 7.19 (t, J = 7.6 Hz, 1H), 7.07 (d, J = 7.6 Hz, 1H), 7.05 – 6.97 (m, 2H), 5.41 (s, 2H), 2.61 (s, 6H), 2.30 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.9, 154.6, 138.8, 135.0, 133.0, 130.5, 130.3, 128.9, 128.8, 128.6, 127.5, 123.9, 123.8, 114.5, 52.3, 45.6, 42.0, 36.5 (d, J = 25.2 Hz), 21.4, ^{13}C NMR for $^{i}C_3F_7$ could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -74.62 (d, J = 8.7 Hz), -183.34 – -183.54 (m); HRMS (ESI+): Calculated for $C_{24}H_{19}F_7N_2O$: $[M+H]^+$ 485.1458, Found 485.1459.

1-(3-Chlorobenzyl)-3-(3-(perfluoroisopropyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (34)



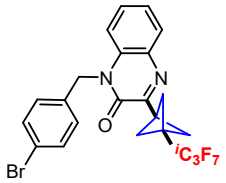
Obtained as a light yellow solid (61 mg, 61 % yield); M. P. = 154-155 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (dd, J = 8.0, 1.4 Hz, 1H), 7.49 – 7.43 (m, 1H), 7.35 – 7.30 (m, 1H), 7.25 (dt, J = 8.0, 2.6 Hz, 2H), 7.20 (dd, J = 19.6, 11.9 Hz, 2H), 7.11 (dd, J = 5.7, 2.8 Hz, 1H), 5.42 (s, 2H), 2.61 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.8, 154.4, 137.2, 135.0, 133.0, 132.7, 130.6, 130.5, 130.3, 128.1, 126.9, 125.0, 124.0, 114.2, 52.4, 45.1, 42.0, 36.5 (d, J = 25.2 Hz), ^{13}C NMR for $^{i}C_3F_7$ could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -74.62 (d, J = 8.7 Hz), -183.33 – -183.54 (m); HRMS (ESI+): Calculated for $C_{23}H_{16}ClF_7N_2O$: $[M+Na]^+$ 527.0732, Found 527.0733.

1-(4-Fluorobenzyl)-3-(3-(perfluoroisopropyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (35)



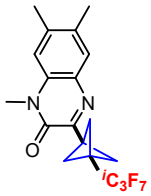
Obtained as a light yellow solid (63 mg, 65% yield); M. P. = 112-113 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (dd, J = 8.0, 1.4 Hz, 1H), 7.50 – 7.41 (m, 1H), 7.32 (dd, J = 11.2, 4.1 Hz, 1H), 7.26 – 7.12 (m, 3H), 7.00 (dd, J = 9.6, 7.7 Hz, 2H), 5.41 (s, 2H), 2.61 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.3 (d, J = 247.0 Hz), 154.9, 154.5, 133.0, 132.7, 130.9 (d, J = 3.2 Hz), 130.9, 130.8, 128.7 (d, J = 8.2 Hz), 123.9, 116.0 (d, J = 21.7 Hz), 114.2, 52.3, 45.0, 42.0, 36.5 (d, J = 25.4 Hz), ^{13}C NMR for $^{i}C_3F_7$ could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -74.62 (d, J = 8.9 Hz), -114.18 – -114.24 (m), -183.36 – -183.44 (m); HRMS (ESI+): Calculated for $C_{23}H_{16}F_8N_2O$: $[M+H]^+$ 489.1208, Found 489.1203.

1-(4-Bromobenzyl)-3-(3-(perfluoroisopropyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (36)



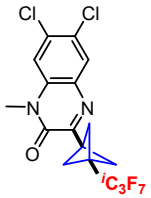
Obtained as a light yellow solid (64 mg, 58% yield); M. P. = 173-174 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (dd, J = 8.0, 1.2 Hz, 1H), 7.48 – 7.41 (m, 3H), 7.32 (t, J = 7.3 Hz, 1H), 7.19 (d, J = 8.3 Hz, 1H), 7.11 (d, J = 8.4 Hz, 2H), 5.39 (s, 2H), 2.60 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.8, 154.4, 134.2, 133.0, 132.7, 132.1, 130.6, 130.5, 128.7, 124.0, 121.8, 114.2, 52.3 (d, J = 3.4 Hz), 45.1, 42.0, 36.5 (d, J = 25.4 Hz), ^{13}C NMR for $^{i}C_3F_7$ could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -74.62 (d, J = 8.8 Hz), -183.35 – -183.43 (m); HRMS (ESI+): Calculated for $C_{23}H_{16}BrF_7N_2O$: $[M+H]^+$ 571.0226, Found 571.0226.

3-(3-(Perfluoroisopropyl)bicyclo[1.1.1]pentan-1-yl)-1,6,7-trimethylquinoxalin-2(1*H*)-one (37)



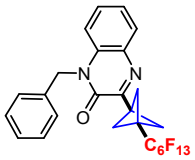
Obtained as a light yellow solid (66 mg, 78% yield); M. P. = 146-147 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (s, 1H), 7.06 (s, 1H), 3.64 (s, 3H), 2.56 (s, 6H), 2.42 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.6, 153.4, 140.4, 132.7, 131.5, 131.2, 130.2, 114.2, 52.1, 42.0, 36.4 (d, J = 25.2 Hz), 28.5, 20.6, 19.1, ^{13}C NMR for $^{i}C_3F_7$ could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -74.63 (d, J = 8.8 Hz), -183.42 – -183.45 (m); HRMS (ESI+): Calculated for $C_{19}H_{17}F_7N_2O$: $[M+H]^+$ 423.1302, Found 423.1301.

6,7-Dichloro-3-(3-(perfluoroisopropyl)bicyclo[1.1.1]pentan-1-yl)-1-methylquinoxalin-2(1*H*)-one (38)



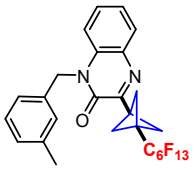
Obtained as a light yellow solid (58 mg, 63% yield); M. P. = 131-132 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.38 (s, 1H), 3.62 (s, 3H), 2.55 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.2, 153.8, 134.6, 132.8, 131.8, 130.9, 127.6, 115.2, 52.3, 41.9, 36.6 (d, J = 25.4 Hz), 28.9, ^{13}C NMR for $^{i}C_3F_7$ could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -74.63 (d, J = 8.8 Hz), -183.42 – -183.45 (m); HRMS (ESI+): Calculated for $C_{17}H_{11}Cl_2F_7N_2O$: $[M+H]^+$ 463.0209, Found 463.021.

1-Benzyl-3-(3-(perfluorohexyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (39)



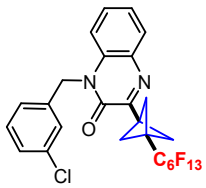
Obtained as a light yellow solid (93 mg, 75% yield); M. P. = 97-98 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (dd, J = 8.0, 1.4 Hz, 1H), 7.43 (ddd, J = 8.6, 7.4, 1.5 Hz, 1H), 7.34 – 7.27 (m, 4H), 7.25 – 7.21 (m, 3H), 5.46 (s, 2H), 2.59 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.0, 154.5, 135.1, 133.0, 132.9, 130.5, 130.3, 129.0, 127.8, 126.9, 123.8, 114.5, 51.3, 45.6, 42.1, 38.0 (t, J = 31.5 Hz), ^{13}C NMR for C_6F_{13} could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.76 – -80.81 (m), -116.37 – -116.43 (m), -121.32 – -121.36 (m), -121.84 – -121.92 (m), -122.87 – -122.92 (m), -126.09 – -126.13 (m); HRMS (ESI+): Calculated for $C_{26}H_{17}F_{13}N_2O$: $[M+H]^+$ 621.1206, Found 621.1207.

1-(3-Methylbenzyl)-3-(3-(perfluorohexyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (40)



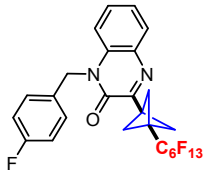
Obtained as a light yellow solid (87 mg, 69% yield); M. P. = 95-96 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 (d, J = 7.9 Hz, 1H), 7.34 (t, J = 7.8 Hz, 1H), 7.21 (t, J = 7.6 Hz, 1H), 7.18 – 7.15 (m, 1H), 7.11 (t, J = 7.6 Hz, 1H), 6.99 (d, J = 7.6 Hz, 1H), 6.97 – 6.90 (m, 2H), 5.34 (s, 2H), 2.52 (s, 6H), 2.22 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.0, 154.5, 138.8, 135.0, 133.0, 133.0, 130.4, 130.3, 128.9, 128.6, 127.4, 123.8, 123.3, 114.5, 51.3, 45.6, 42.1, 38.0 (t, J = 31.5 Hz), 21.4, ^{13}C NMR for C_6F_{13} could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.82 (t, J = 10.5 Hz), -116.35 – -117.14 (m), -121.28 – -121.75 (m), -121.84 – -121.94 (m), -122.88 – -122.95 (m), -125.52 – -126.16 (m); HRMS (ESI+): Calculated for $C_{27}H_{19}F_{13}N_2O$: $[M+H]^+$ 635.1363, Found 635.1363.

1-(3-Chlorobenzyl)-3-(3-(perfluorohexyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (41)



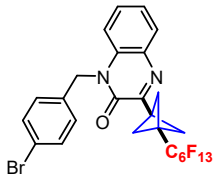
Obtained as a light yellow solid (77 mg, 59% yield); M. P. = 93-94 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (dd, J = 8.0, 1.4 Hz, 1H), 7.45 (ddd, J = 8.6, 7.4, 1.5 Hz, 1H), 7.35 – 7.30 (m, 1H), 7.25 (td, J = 4.5, 1.9 Hz, 2H), 7.19 (dd, J = 9.4, 8.7 Hz, 2H), 7.14 – 7.08 (m, 1H), 5.42 (s, 2H), 2.59 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.0, 154.4, 137.2, 135.0, 133.0, 132.7, 130.6, 130.5, 130.3, 128.1, 126.9, 125.0, 124.0, 114.2, 51.4, 45.1, 42.0, 38.0 (t, J = 31.5 Hz), ^{13}C NMR for C_6F_{13} could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.78 – -80.82 (m), -116.37 – -116.45 (m), -121.31 – -121.37 (m), -121.86 – -121.92 (m), -122.91 – -122.92 (m), -126.08 – -126.16 (m); HRMS (ESI+): Calculated for $C_{26}H_{16}ClF_{13}N_2O$: $[M+H]^+$ 655.0816, Found 655.0815.

1-(4-Fluorobenzyl)-3-(3-(perfluorohexyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (42)



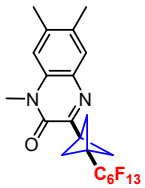
Obtained as a light yellow solid (89 mg, 70% yield); M. P. = 79 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (dd, J = 8.0, 1.4 Hz, 1H), 7.45 (ddd, J = 8.6, 7.4, 1.5 Hz, 1H), 7.35 – 7.29 (m, 1H), 7.23 (dd, J = 8.5, 4.8 Hz, 3H), 7.04 – 6.98 (m, 2H), 5.42 (s, 2H), 2.59 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.3 (d, J = 247.0 Hz), 155.0, 154.5, 133.0, 132.7, 130.9 (d, J = 3.3 Hz), 130.5, 130.4, 128.7 (d, J = 8.2 Hz), 123.9, 115.9 (d, J = 21.7 Hz), 114.2, 51.3, 45.0, 42.1, 38.0 (t, J = 30.4 Hz), ^{13}C NMR for C_6F_{13} could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.78 – -80.82 (m), -114.22 – -114.26 (m), -116.38 – -116.45 (m), -121.31 – -121.38 (m), -121.87 – -121.92 (m), -122.91 (s), -126.10 – -126.15 (m); HRMS (ESI+): Calculated for $C_{26}H_{16}F_{14}N_2O$: $[M+H]^+$ 639.1112, Found 639.1117.

1-(4-Bromobenzyl)-3-(3-(perfluorohexyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (43)



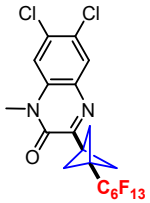
Obtained as a light yellow solid (93 mg, 67% yield); M. P. = 155-156 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (dd, J = 8.0, 1.4 Hz, 1H), 7.48 – 7.39 (m, 3H), 7.36 – 7.29 (m, 1H), 7.18 (d, J = 8.4 Hz, 1H), 7.11 (d, J = 8.5 Hz, 2H), 5.40 (s, 2H), 2.59 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.0, 154.4, 134.2, 133.0, 132.7, 132.1, 130.5, 130.5, 128.7, 124.0, 121.8, 114.2, 51.3, 45.1, 42.0, 38.0 (t, J = 30.4 Hz), ^{13}C NMR for C_6F_{13} could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.79 – -80.84 (m), -116.39 – -116.45 (m), -121.32– -121.38 (m), -121.88 – -121.94 (m), -122.89 – -122.95 (m), -126.10 – -126.17 (m); HRMS (ESI+): Calculated for $C_{26}H_{16}BrF_{13}N_2O$: $[M+H]^+$ 699.0311, Found 699.0308.

1,6,7-Trimethyl-3-(3-(perfluorohexyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (44)



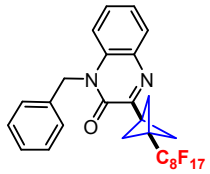
Obtained as a light yellow solid (91 mg, 80% yield); M. P. = 114-115 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (s, 1H), 7.06 (s, 1H), 3.65 (s, 3H), 2.54 (s, 6H), 2.42 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.6, 153.5, 140.4, 132.7, 131.5, 131.2, 130.2, 114.2, 51.2, 42.1, 37.9 (t, J = 30.4 Hz), 28.5, 20.6, 19.1, ^{13}C NMR for C_6F_{13} could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.77 – -80.81 (m), -116.37 – -116.41 (m), -121.31 – -121.35 (m), -121.89 – -121.92 (m), -122.91 – -122.94 (m), -126.09 – -126.12 (m); HRMS (ESI+): Calculated for $C_{22}H_{17}F_{13}N_2O$: $[M+H]^+$ 573.1206, Found 573.1205.

6,7-Dichloro-1-methyl-3-(3-(perfluorohexyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (45)



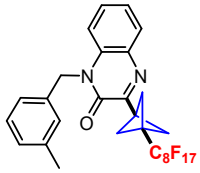
Obtained as a light yellow solid (84 mg, 69% yield); M. P. = 130-131 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 (s, 1H), 7.39 (s, 1H), 3.63 (s, 3H), 2.54 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.3, 153.9, 134.6, 132.9, 131.8, 131.0, 127.6, 115.2, 51.3, 42.0, 38.0 (t, J = 30.4 Hz), 28.9, ^{13}C NMR for C_6F_{13} could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.77 – -80.82 (m), -116.44 – -116.51 (m), -121.30 – -121.34 (m), -121.88 – -121.95 (m), -122.91 – -122.94 (m), -126.11 – -126.14 (m); HRMS (ESI+): Calculated for $C_{20}H_{11}Cl_2F_{13}N_2O$: $[M+H]^+$ 613.0114, Found 613.0121.

1-Benzyl-3-(3-(perfluorooctyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (46)



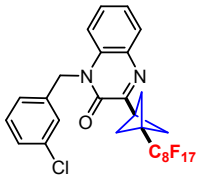
Obtained as a light yellow solid (112 mg, 78% yield); M. P. = 89-90 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (dd, J = 8.0, 1.3 Hz, 1H), 7.45 – 7.39 (m, 1H), 7.34 – 7.27 (m, 4H), 7.23 (d, J = 7.2 Hz, 3H), 5.46 (s, 2H), 2.59 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.0, 154.5, 135.1, 133.0, 132.9, 130.4, 130.3, 129.0, 127.8, 126.9, 123.8, 114.5, 51.3, 45.6, 42.1, 38.0 (t, J = 30.2 Hz), ^{13}C NMR for C_8F_{17} could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.78 – -80.83 (m), -116.36 – -116.44 (m), -121.25 – -121.31 (m), -121.63 – -121.68 (m), -121.92 – -121.97 (m), -122.72 – -122.75 (m), -123.52 – -123.56 (m), -126.12 – -126.116 (m); HRMS (ESI+): Calculated for $C_{28}H_{17}F_{17}N_2O$: $[M+H]^+$ 721.1142, Found 721.1134.

3-(3-(Perfluorooctyl)bicyclo[1.1.1]pentan-1-yl)-1-(3-methylbenzyl)quinoxalin-2(1*H*)-one (47)



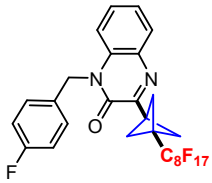
Obtained as a light yellow solid (110 mg, 75% yield); M. P. = 99-100 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (dd, J = 8.0, 1.4 Hz, 1H), 7.42 (ddd, J = 8.6, 7.5, 1.5 Hz, 1H), 7.31 – 7.27 (m, 1H), 7.25 (dd, J = 5.5, 2.9 Hz, 1H), 7.19 (t, J = 7.6 Hz, 1H), 7.07 (d, J = 7.6 Hz, 1H), 7.05 – 6.96 (m, 2H), 5.42 (s, 2H), 2.60 (s, 6H), 2.30 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.0, 154.5, 138.8, 135.1, 133.0, 133.0, 130.4, 130.3, 128.8, 128.6, 127.4, 123.8, 123.7, 114.5, 51.3, 45.6, 42.1, 38.0 (t, J = 30.2 Hz), 21.4, ^{13}C NMR for C_8F_{17} could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.83 (t, J = 10.8 Hz), -116.35 – -116.46 (m), -121.26 – -121.29 (m), -121.65 – -121.70 (m), -121.93 – -121.96 (m), -122.78 – -122.93 (m), -125.45 – -126.17 (m); HRMS (ESI+): Calculated for $C_{29}H_{19}F_{17}N_2O$: $[M+H]^+$ 735.1299, Found 735.1298.

1-(3-Chlorobenzyl)-3-(3-(perfluorooctyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (48)



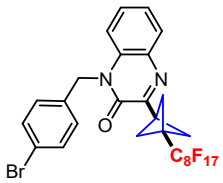
Obtained as a light yellow solid (90 mg, 60% yield); M. P. = 81-82 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (dd, J = 8.0, 1.1 Hz, 1H), 7.48 – 7.41 (m, 1H), 7.32 (t, J = 7.6 Hz, 1H), 7.25 (dd, J = 4.4, 2.7 Hz, 2H), 7.23 – 7.16 (m, 2H), 7.11 (t, J = 3.5 Hz, 1H), 5.42 (s, 2H), 2.59 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.0, 154.4, 137.2, 135.0, 133.0, 132.7, 130.6, 130.5, 130.3, 128.1, 126.9, 125.0, 124.0, 114.2, 51.3, 45.1, 42.0, 38.0 (t, J = 30.2 Hz), ^{13}C NMR for C_8F_{17} could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.84 (t, J = 10.7 Hz), -116.38 – -117.08 (m), -121.28 – -121.30 (m), -121.68 – -121.70 (m), -121.93 – -121.96 (m), -122.74 – -122.76 (m), -126.14 – -126.17 (m); HRMS (ESI+): Calculated for $C_{28}H_{16}ClF_{17}N_2O$: $[M+H]^+$ 755.0752, Found 755.0748.

1-(4-Fluorobenzyl)-3-(3-(perfluorooctyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (49)



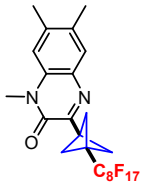
Obtained as a light yellow solid (100 mg, 68% yield); M. P. = 88-89 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (d, J = 7.4 Hz, 1H), 7.44 (t, J = 7.4 Hz, 1H), 7.30 (t, J = 7.5 Hz, 1H), 7.26 – 7.20 (m, 3H), 6.99 (t, J = 8.6 Hz, 2H), 5.41 (s, 2H), 2.60 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.2, 161.3, 155.0, 154.4, 133.0, 132.7, 130.9 (d, J = 3.2 Hz), 130.4, 128.7 (d, J = 8.2 Hz), 123.8, 115.9 (d, J = 21.7 Hz), 114.2, 51.3, 44.9, 42.0, 38.0 (t, J = 30.3 Hz), ^{13}C NMR for C_8F_{17} could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.02 – -81.06 (m), -116.51 – -116.58 (m), -121.35 – -121.38 (m), -121.77 – -121.80 (m), -122.05 – -122.08 (m), -122.86 – -122.89 (m), -126.29 – -126.31 (m); HRMS (ESI+): Calculated for $C_{28}H_{16}F_{18}N_2O$: $[M+H]^+$ 739.1048, Found 739.1041.

1-(4-Bromobenzyl)-3-(3-(perfluorooctyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (50)



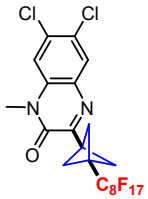
Obtained as a light yellow solid (102 mg, 64% yield); M. P. = 126-127 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (d, J = 7.9 Hz, 1H), 7.44 (t, J = 5.9 Hz, 3H), 7.32 (t, J = 7.6 Hz, 1H), 7.18 (d, J = 8.4 Hz, 1H), 7.11 (d, J = 8.3 Hz, 2H), 5.40 (s, 2H), 2.58 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.0, 154.4, 134.2, 133.0, 132.7, 132.1, 130.5, 130.5, 128.7, 123.9, 121.8, 114.2, 51.33, 45.05, 42.03, 38.0 (t, J = 30.3 Hz), ^{13}C NMR for C_8F_{17} could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.78 (t, J = 10.8 Hz), -116.35 – -116.45 (m), -121.24 – -121.31 (m), -121.62 – -121.68 (m), -121.88 – -121.96 (m), -122.67 – -122.74 (m), -125.57 – -126.80 (m); HRMS (ESI+): Calculated for $C_{28}H_{16}BrF_{17}N_2O$: $[M+H]^+$ 799.0247, Found 799.0245.

3-(3-(Perfluorooctyl)bicyclo[1.1.1]pentan-1-yl)-1,6,7-trimethylquinoxalin-2(1*H*)-one (51)



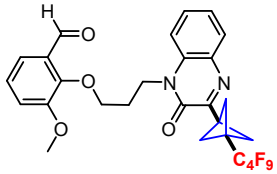
Obtained as a light yellow solid (105 mg, 78% yield); M. P. = 83-84 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (s, 1H), 7.05 (s, 1H), 3.64 (s, 3H), 2.54 (s, 6H), 2.41 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.6, 153.5, 140.4, 132.7, 131.5, 131.2, 130.2, 114.2, 51.2, 42.1, 37.9 (t, J = 30.2 Hz), 28.5, 20.6, 19.1, ^{13}C NMR for C_8F_{17} could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.73 – -80.78 (m), -116.34 – -116.41 (m), 121.26 (d, J = 6.8 Hz), -121.66 (d, J = 5.5 Hz), -121.93 (d, J = 9.3 Hz), -122.71 (s), -126.06 – -126.12 (m); HRMS (ESI+): Calculated for $C_{24}H_{17}F_{17}N_2O$: $[M+H]^+$ 673.1142, Found 673.1149.

6,7-Dichloro-3-(3-(perfluorooctyl)bicyclo[1.1.1]pentan-1-yl)-1-methylquinoxalin-2(1*H*)-one (52)



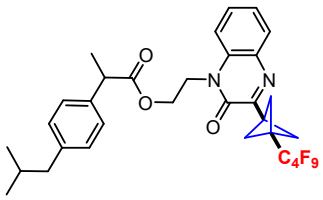
Obtained as a light yellow solid (104 mg, 73% yield); M. P. = 128-129 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 (s, 1H), 7.39 (s, 1H), 3.63 (s, 3H), 2.54 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.3, 153.8, 134.6, 132.9, 131.8, 131.0, 127.6, 115.1, 51.3, 42.0, 38.1 (t, J = 30.2 Hz), 28.9, ^{13}C NMR for C_8F_{17} could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.77 – -80.82 (m), -116.47 – -116.51 (m), -121.25 – -121.27 (m), -121.68 – -121.70 (m), -121.94 – -121.96 (m), -123.66 – -123.76 (m), -126.12 – -126.14 (m); HRMS (ESI+): Calculated for $C_{22}H_{11}Cl_2F_{17}N_2O$: $[M+H]^+$ 713.005, Found 713.0047.

3-Methoxy-2-(3-(3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-2-oxoquinoxalin-1(2*H*)-yl)propoxy)benzaldehyde (53)



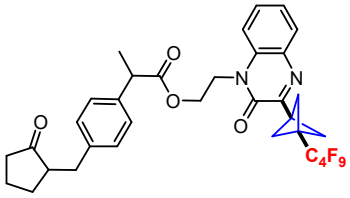
Obtained as a light yellow solid (86 mg, 69% yield); M. P. = 99-100 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.46 (s, 1H), 7.87 (d, J = 7.8 Hz, 1H), 7.56 (t, J = 7.5 Hz, 1H), 7.48 (d, J = 8.3 Hz, 1H), 7.45 – 7.42 (m, 1H), 7.35 (t, J = 7.5 Hz, 1H), 7.17 (d, J = 4.4 Hz, 2H), 4.57 – 4.50 (m, 2H), 4.28 (t, J = 5.7 Hz, 2H), 3.88 (s, 3H), 2.56 (s, 6H), 2.26 (td, J = 11.6, 5.8 Hz, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 189.9, 154.7, 154.3, 152.9, 151.2, 133.0, 132.6, 130.7, 130.4, 129.9, 124.4, 123.7, 119.7, 118.0, 113.7, 72.2, 56.0, 51.3, 42.0, 39.6, 37.9 (t, J = 30.2 Hz), 28.0, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.06 (t, J = 9.9 Hz), -116.57 – -116.66 (m), -122.11 – -122.35 (m), -125.48 – -126.07 (m); HRMS (ESI+): Calculated for $C_{28}H_{23}F_9N_2O_4$: $[M+H]^+$ 623.1587, Found 623.1586.

2-(3-(3-(Perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-2-oxoquinoxalin-1(2*H*)-yl)ethyl 2-(4-isobutylphenyl)propanoate (54)



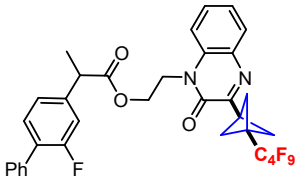
Obtained as a light yellow solid (103 mg, 78% yield); M. P. = 80-81 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (dd, J = 7.9, 0.9 Hz, 1H), 7.51 – 7.45 (m, 1H), 7.38 – 7.31 (m, 2H), 7.09 (d, J = 8.1 Hz, 2H), 7.05 (d, J = 8.1 Hz, 2H), 4.53 – 4.47 (m, 1H), 4.46 – 4.36 (m, 3H), 3.59 (q, J = 7.1 Hz, 1H), 2.55 (s, 6H), 2.44 (d, J = 7.2 Hz, 2H), 1.84 (dt, J = 13.5, 6.8 Hz, 1H), 1.42 (d, J = 7.2 Hz, 3H), 0.90 (d, J = 6.6 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 174.7, 154.6, 154.3, 140.7, 137.2, 133.0, 132.9, 130.5, 130.4, 129.4, 127.1, 123.8, 113.8, 61.0, 51.2, 45.1, 45.0, 41.9, 40.6, 37.9 (t, J = 30.2 Hz), 30.2, 22.4, 18.3, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.08 (t, J = 9.9 Hz), -115.53 – -116.68 (m), -121.39 – -122.89 (m), -125.25 – -126.08 (m); HRMS (ESI+): Calculated for $C_{32}H_{31}F_9N_2O_3$: $[M+H]^+$ 663.2264, Found 663.2265.

2-(3-(3-(Perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-2-oxoquinoxalin-1(2H)-yl)ethyl 2-(4-((2-oxocyclopentyl)methyl)phenyl)propanoate (55)



Obtained as a yellow liquid (102 mg, 73% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (dd, J = 7.9, 1.1 Hz, 1H), 7.51 – 7.44 (m, 1H), 7.34 (dd, J = 15.6, 7.8 Hz, 2H), 7.08 (q, J = 8.3 Hz, 4H), 4.52 – 4.34 (m, 4H), 3.59 (q, J = 7.1 Hz, 1H), 3.11 (dd, J = 13.9, 2.6 Hz, 1H), 2.54 (s, 6H), 2.48 (dd, J = 11.8, 4.8 Hz, 1H), 2.38 – 2.29 (m, 2H), 2.13 – 2.05 (m, 2H), 1.96 (d, J = 6.5 Hz, 1H), 1.78 – 1.70 (m, 1H), 1.58 – 1.50 (m, 1H), 1.41 (d, J = 7.2 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 220.09, 174.5, 154.6, 154.3, 139.1, 137.8, 132.9, 132.9, 130.5, 130.4, 129.2, 127.4, 123.8, 113.7, 61.0, 51.2, 50.9, 45.0, 41.9, 40.5, 38.1, 37. 9 (t, J = 30.2 Hz), 35.2, 29.3, 20.5, 18.3, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.51 – -81.75 (m), -115.67 – -117.56 (m), -121.36 – -123.00 (m), -125.38 – -126.96 (m); HRMS (ESI+): Calculated for $C_{34}H_{31}F_9N_2O_4$: $[M+H]^+$ 703.2213, Found 703.2214.

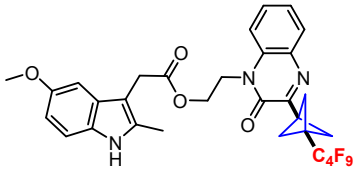
2-(3-(3-(Perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-2-oxoquinoxalin-1(2*H*)-yl)ethyl 2-(2-fluoro-[1,1'-biphenyl]-4-yl)propanoate (56)



Obtained as a yellow liquid (98 mg, 70% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (dd, J = 8.0, 1.3 Hz, 1H), 7.56 – 7.52 (m, 2H), 7.47 (ddd, J = 17.2, 11.8, 4.6 Hz, 3H), 7.41 – 7.29 (m, 4H), 7.07 – 6.92 (m, 2H), 4.59 – 4.39 (m, 4H), 3.65 (q, J = 7.1 Hz, 1H), 2.56 (s, 6H), 1.47 (d, J = 7.2 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 173.9, 159.6 (d, J = 249.5 Hz), 154.6, 154.3, 141.2 (d, J = 7.6 Hz), 135.3, 132.9 (d, J = 10.1 Hz), 130.8 (d, J = 3.8 Hz), 130.5, 130.4, 128.9 (d, J = 2.5 Hz), 128.5, 128.0, 127.9, 127.8, 123.8, 123.4 (d, J = 3.8 Hz), 115.2 (d, J = 23.9 Hz), 113.7, 61.3, 51.2, 44.9, 41.9, 40.6, 37.9 (t,

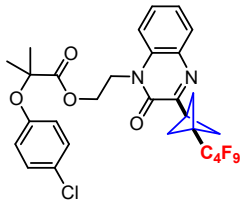
J = 30.2 Hz), 18.2, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.70 – -81.49 (m), -116.25 – -116.93 (m), -117.24 (s), -121.90 – -122.80 (m), -125.56 – -126.42 (m); HRMS (ESI+): Calculated for $C_{34}H_{26}F_{10}N_2O_3$: $[M+H]^+$ 701.1857, Found 701.1855.

2-(3-(3-(Perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-2-oxoquinoxalin-1(2H)-yl)ethyl 2-(5-methoxy-2-methyl-1*H*-indol-3-yl)acetate (57)



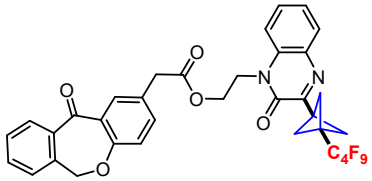
Obtained as a yellow liquid (86 mg, 64% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (dd, J = 7.9, 1.3 Hz, 1H), 7.78 (s, 1H), 7.39 (ddd, J = 8.4, 7.1, 1.4 Hz, 1H), 7.34 – 7.27 (m, 2H), 7.12 (d, J = 8.7 Hz, 1H), 6.90 (d, J = 2.3 Hz, 1H), 6.77 (dd, J = 8.7, 2.4 Hz, 1H), 4.44 (t, J = 4.0 Hz, 4H), 3.82 (s, 3H), 3.59 (s, 2H), 2.56 (s, 6H), 2.26 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.9, 154.6, 154.3, 154.2, 133.6, 132.9, 132.8, 130.5, 130.4, 130.1, 128.8, 123.8, 113.6, 111.0, 110.9, 103.7, 100.4, 60.9, 55.9, 51.3, 41.9, 40.7, 37.9 (t, J = 30.2 Hz), 30.3, 11.7, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.38 – -81.77 (m), -115.60 – -117.58 (m), -121.32 – -123.02 (m), -125.32 – -127.25 (m); HRMS (ESI+): Calculated for $C_{31}H_{26}F_9N_3O_4$: $[M+H]^+$ 676.1852, Found 676.1857.

2-(3-(3-(Perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-2-oxoquinoxalin-1(2*H*)-yl)ethyl 2-(4-chlorophenoxy)-2-methylpropanoate (58)



Obtained as a yellow liquid (100 mg, 75% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (d, J = 7.3 Hz, 1H), 7.49 (t, J = 7.3 Hz, 1H), 7.33 (dd, J = 12.5, 5.3 Hz, 2H), 7.06 (d, J = 8.9 Hz, 2H), 6.59 (d, J = 8.8 Hz, 2H), 4.49 (s, 4H), 2.54 (s, 6H), 1.48 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 173.9, 154.5, 154.2, 153.7, 132.8, 132.7, 130.5, 130.4, 129.0, 127.3, 123.9, 120.1, 113.7, 79.3, 61.9, 51.2, 41.9, 40.4, 37.9 (t, J = 30.2 Hz), 25.2, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.08 – -81.22 (m), -116.65 – -116.79 (m), -122.32 – -122.36 (m), -126.05 – -126.11 (m); HRMS (ESI+): Calculated for $C_{29}H_{24}ClF_9N_2O_4$: $[M+H]^+$ 671.1354, Found 671.1355.

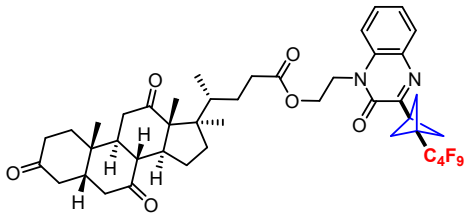
2-(3-(3-(Perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-2-oxoquinoxalin-1(2*H*)-yl)ethyl 2-(11-oxo-6,11-dihydrodibenzo[*b*,*e*]oxepin-2-yl)acetate (59)



Obtained as a yellow liquid (107 mg, 74% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03 (d, J = 2.1 Hz, 1H), 7.89 (d, J = 7.6 Hz, 1H), 7.83 (dd, J = 8.0, 1.0 Hz, 1H), 7.56 (dd, J = 10.7, 4.2 Hz, 1H), 7.53 – 7.46 (m, 2H), 7.38 (t, J = 8.0 Hz, 2H), 7.31 (dd, J = 11.2, 4.6 Hz, 2H), 6.98 (d, J = 8.4 Hz, 1H), 5.18 (s, 2H), 4.48 (dd, J = 8.8, 4.3 Hz, 4H), 3.56 (s, 2H), 2.55 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ

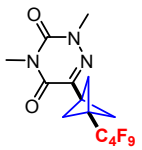
190.7, 171.4, 160.6, 154.6, 154.3, 140.4, 136.2, 135.5, 133.0, 132.9, 132.8, 132.5, 130.6, 130.5, 129.5, 129.3, 127.9, 127.1, 125.2, 123.9, 121.2, 113.6, 73.6, 61.2, 51.3, 41.9, 40.6, 40.0, 37.9 (t, J = 30.2 Hz), ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.41 – -81.73 (m), -116.55 – -116.65 (m), -122.26 – -122.32 (m), -125.95 – -126.07 (m); HRMS (ESI+): Calculated for $C_{35}H_{25}F_9N_2O_5$: $[M+H]^+$ 725.1693, Found 725.1692.

2-(3-(3-(Perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-2-oxoquinoxalin-1(2*H*)-yl)ethyl (*R*)-4-((5*S*,8*R*,9*S*,10*S*,13*S*,14*S*,17*R*)-10,13,17-trimethyl-3,7,12-trioxohexadecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)pentanoate (60)



Obtained as a light yellow solid (105 mg, 60% yield); M. P. = 189-190 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (dd, J = 8.0, 1.2 Hz, 1H), 7.58 – 7.51 (m, 1H), 7.43 (d, J = 8.3 Hz, 1H), 7.34 (t, J = 7.6 Hz, 1H), 4.48 (t, J = 5.4 Hz, 2H), 4.41 (t, J = 5.7 Hz, 2H), 2.88 (dd, J = 31.5, 18.4 Hz, 3H), 2.54 (s, 6H), 2.30 (dd, J = 22.9, 11.7 Hz, 5H), 2.24 (d, J = 11.8 Hz, 2H), 2.15 (dd, J = 26.3, 14.5 Hz, 4H), 2.02 (d, J = 9.9 Hz, 1H), 1.98 – 1.90 (m, 3H), 1.82 (t, J = 11.1 Hz, 1H), 1.75 – 1.70 (m, 1H), 1.59 (dd, J = 19.1, 9.5 Hz, 1H), 1.39 (s, 3H), 1.33 – 1.23 (m, 5H), 1.03 (s, 3H), 0.78 (d, J = 6.6 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 211.9, 209.0, 208.7, 173.9, 154.6, 154.3, 133.0, 132.9, 130.5, 130.5, 123.8, 113.7, 60.5, 56.8, 51.7, 51.2, 51.1, 49.0, 46.8, 45.5, 45.5, 45.0, 42.8, 41.9, 40.7, 38.6, 37.9 (t, J = 30.2 Hz), 36.5, 36.0, 35.4, 35.3, 31.2, 30.2, 27.6, 25.1, 21.9, 18.6, 11.8, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.26 – -81.80 (m), -115.52 – -117.63 (m), -121.26 – -123.02 (m), -125.24 – -127.00 (m); HRMS (ESI+): Calculated for $C_{44}H_{49}F_9N_2O_6$: $[M+H]^+$ 873.352, Found 873.352.

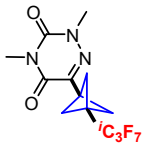
2,4-Dimethyl-6-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-1,2,4-triazine 3,5(2*H*,4*H*)-dione (62)



Obtained as a light yellow solid (70 mg, 82% yield); M. P. = 98-99 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.61 (d, J = 1.1 Hz, 3H), 3.32 (d, J = 1.1 Hz, 3H), 2.39 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.8, 149.2, 139.9, 51.0, 39.6, 38.8, 38.2 (t, J = 30.2 Hz), 26.9, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.47 – -81.55 (m), -116.60 – -116.73 (m), -122.30 – -122.39 (m), -125.42 – -126.13 (m); HRMS (ESI+): Calculated for $C_{14}H_{12}F_9N_3O_2$: $[M+H]^+$ 426.0859, Found 426.0866.

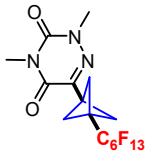
2,4-Dimethyl-6-(3-(perfluoroisopropyl)bicyclo[1.1.1]pentan-1-yl)-1,2,4-triazine 3,5(2*H*,4*H*)-

dione (63)



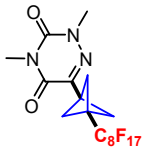
Obtained as a light yellow solid (60 mg, 80% yield); M. P. = 77-78 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.61 (s, 3H), 3.32 (s, 3H), 2.41 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.8, 149.2, 139.8, 52.0, 39.6, 38.7, 36.8 (d, J = 25.2 Hz), 26.9, ^{13}C NMR for C_3F_7 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -74.69 (d, J = 8.7 Hz), -183.27 – -183.45 (m); HRMS (ESI+): Calculated for $C_{13}H_{12}F_7N_3O_2$: $[M+H]^+$ 376.0891, Found 376.0889.

2,4-Dimethyl-6-(3-(perfluorohexyl)bicyclo[1.1.1]pentan-1-yl)-1,2,4-triazine 3,5(2*H*,4*H*)-dione (64)



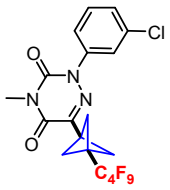
Obtained as a light yellow solid (78 mg, 74% yield); M. P. = 59-60 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.62 (s, 3H), 3.32 (s, 3H), 2.40 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.8, 149.2, 139.9, 51.0, 39.6, 38.8, 38.3 (t, J = 30.2 Hz), 26.9, ^{13}C NMR for C_6F_{13} could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.17 – -81.51 (m), -116.48 (dd, J = 20.6, 10.2 Hz), -121.38 (dd, J = 19.2, 11.6 Hz), -121.97 (dd, J = 16.6, 10.5 Hz), -122.98 (dd, J = 19.4, 12.7 Hz), -126.13 – -126.24 (m); HRMS (ESI+): Calculated for $C_{16}H_{12}F_{13}N_3O_2$: $[M+H]^+$ 526.0795, Found 526.0798.

2,4-Dimethyl-6-(3-(perfluorooctyl)bicyclo[1.1.1]pentan-1-yl)-1,2,4-triazine 3,5(2*H*,4*H*)-dione (65)



Obtained as a light yellow solid (97 mg, 78% yield); M. P. = 99-100 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.61 (s, 3H), 3.32 (s, 3H), 2.40 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.8, 149.2, 139.9, 51.0, 39.6, 38.8, 38.3 (t, J = 30.2 Hz), 26.9, ^{13}C NMR for C_8F_{17} could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.84 (t, J = 10.8 Hz), -116.43 – -116.51 (m), -122.29 – -122.33 (m), -122.72 – -122.75 (m), -121.96 – -122.00 (m), -122.74 – -122.78 (m), -126.14 – -126.17 (m); HRMS (ESI+): Calculated for $C_{18}H_{12}F_{17}N_3O_2$: $[M+H]^+$ 626.0731, Found 626.0730.

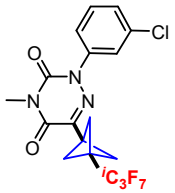
2-(3-Chlorophenyl)-4-methyl-6-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (66)



Obtained as a light yellow solid (73 mg, 70% yield); M. P. = 164-165 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45 (d, J = 5.1 Hz, 2H), 7.26 (d, J = 2.5 Hz, 1H), 7.18 – 7.09 (m, 1H), 3.67 (s, 3H), 2.42 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.2, 148.5, 140.9, 135.2, 133.6, 130.5, 129.8, 128.4, 126.2, 51.1,

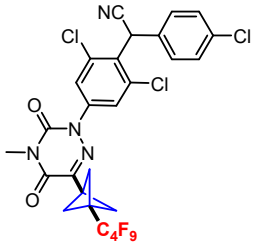
39.7, 38.8, 38.3 (t, J = 30.2 Hz), ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.04 – -81.63 (m), -115.79 – -116.69 (m), -122.29 – -122.35 (m), -125.99 – -126.10 (m); HRMS (ESI+): Calculated for $C_{19}H_{13}ClF_9N_3O_2$: $[M+H]^+$ 522.0625, Found 522.0627.

2-(3-Chlorophenyl)-4-methyl-6-(3-(perfluoroisopropyl)bicyclo[1.1.1]pentan-1-yl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (67)



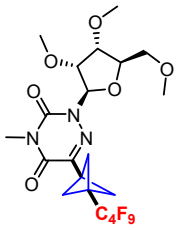
Obtained as a light yellow solid (68 mg, 72% yield); M. P. = 204-205 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 – 7.40 (m, 2H), 7.26 (d, J = 4.5 Hz, 1H), 7.17 – 7.09 (m, 1H), 3.66 (s, 3H), 2.44 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.2, 148.5, 140.8, 135.1, 133.6, 130.5, 129.8, 128.3, 126.2, 52.1, 39.7, 38.7, 36.9 (d, J = 25.2 Hz), ^{13}C NMR for $^{i}C_3F_7$ could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -74.69 (d, J = 8.8 Hz), -183.32 – -183.40 (m); HRMS (ESI+): Calculated for $C_{18}H_{13}ClF_7N_3O_2$: $[M+H]^+$ 472.0657, Found 472.0655.

2-(4-Chlorophenyl)-2-(2,6-dichloro-4-(4-methyl-6-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-3,5-dioxo-4,5-dihydro-1,2,4-triazin-2(3H)-yl)phenyl)acetonitrile (68)



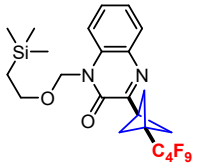
Obtained as a yellow liquid (92 mg, 65% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.79 (d, J = 8.5 Hz, 2H), 7.68 (s, 2H), 7.48 (d, J = 8.6 Hz, 2H), 3.42 (s, 3H), 2.49 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.6, 154.8, 148.1, 142.2, 141.7, 141.2, 136.4, 133.6, 132.1, 131.0, 129.5, 124.1, 51.2, 38.8, 38.4 (t, J = 30.2 Hz), 29.7, 27.4, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.01 – -81.72 (m), -116.61 – -117.08 (m), -122.22 – -122.28 (m), -125.99 – -126.05 (m); HRMS (ESI+): Calculated for $C_{27}H_{16}Cl_3F_9N_4O_2$: $[M+H]^+$ 705.0268, Found 705.026.

2-(3,4-Dimethoxy-5-(methoxymethyl)tetrahydrofuran-2-yl)-4-methyl-6-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (69)



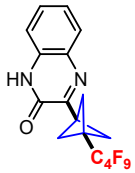
Obtained as a yellow liquid (81 mg, 69% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.29 (d, J = 3.0 Hz, 1H), 4.21 (d, J = 3.8 Hz, 1H), 4.15 (dd, J = 5.1, 3.1 Hz, 1H), 4.02 (d, J = 5.5 Hz, 1H), 3.58 (d, J = 3.6 Hz, 1H), 3.53 (d, J = 5.5 Hz, 1H), 3.49 (s, 3H), 3.48 (s, 3H), 3.38 (s, 3H), 3.31 (s, 3H), 2.42 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.1, 148.8, 140.9, 89.1, 81.0, 80.6, 79.1, 72.6, 59.3, 58.4, 58.3, 51.0, 39.0, 38.4 (t, J = 30.2 Hz), 27.0, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.62 – -81.59 (m), -116.59 – -116.67 (m), -122.19 – -122.25 (m), -125.99 – -126.09 (m); HRMS (ESI+): Calculated for $C_{21}H_{24}F_9N_3O_6$: $[M+H]^+$ 608.1414, Found 608.1413.

3-(3-(Perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-1-((2(trimethylsilyl)ethoxy)methyl)quinoxalin-2(1*H*)-one (70)



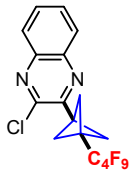
Obtained as a yellow liquid (806 mg, 72% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, J = 8.0 Hz, 1H), 7.54 – 7.51 (m, 2H), 7.34 (dd, J = 4.9, 3.4 Hz, 1H), 5.68 (s, 2H), 3.71 – 3.65 (m, 2H), 2.55 (s, 6H), 0.97 – 0.93 (m, 2H), -0.03 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.4, 156.0, 134.2, 133.7, 131.9, 131.5, 125.6, 116.4, 72.6, 68.5, 52.7, 43.5, 39.3 (t, J = 31.5 Hz), 19.4, 0.0, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.44 – -81.74 (m), -116.62 – -116.69 (m), -122.28 – -122.87 (m), -126.00 – -126.07 (m); HRMS (ESI+): Calculated for $C_{23}H_{25}F_9N_2O_2Si$: $[M+Na]^+$ 583.1434, Found 583.1432.

3-(3-(Perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (71)



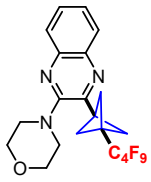
Obtained as a light yellow solid (774 mg, 90% yield); M. P.= 219-220 °C; ^{1}H NMR (500 MHz, Acetone) δ 11.22 (s, 1H), 7.77 (d, J = 7.9 Hz, 1H), 7.53 (t, J = 7.3 Hz, 1H), 7.39 (d, J = 8.0 Hz, 1H), 7.32 (t, J = 7.6 Hz, 1H), 2.55 (s, 6H); ^{13}C NMR (126 MHz, Acetone) δ 155.9, 154.3, 132.5, 132.2, 130.2, 128.9, 123.3, 115.2, 50.8, 41.7, 37.5 (t, J = 31.5 Hz), ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, Acetone) δ -81.95 (t, J = 10.1 Hz), -116.90 – -116.97 (m), -122.78 – -122.85 (m), -126.65 – -126.71 (m); HRMS (ESI+): Calculated for $C_{17}H_{11}F_9N_2O$: $[M+H]^+$ 431.08, Found 431.0808.

2-Chloro-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (72)



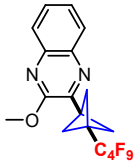
Obtained as a light yellow solid (798 mg, 89% yield); M. P.= 62-63 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 – 8.04 (m, 1H), 8.02 – 7.96 (m, 1H), 7.80 – 7.72 (m, 2H), 2.67 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 149.9, 146.2, 141.3, 140.8, 130.9, 130.3, 129.0, 128.1, 51.5, 42.5, 38.0 (t, J = 31.5 Hz), ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.08 (t, J = 3.5 Hz), -115.69 – -117.43 (m), -121.59 – -122.97 (m), -125.24 – -126.85 (m); HRMS (ESI+): Calculated for $C_{17}H_{10}ClF_9N_2$: $[M+H]^+$ 449.0462, Found 449.0463.

4-(3-(3-(Perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2-yl)morpholine (73)



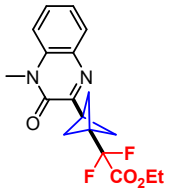
Obtained as a light yellow solid (95 mg, 95% yield); M. P.= 67-68 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96 (d, J = 8.2 Hz, 1H), 7.87 (d, J = 8.1 Hz, 1H), 7.64 (dd, J = 11.1, 4.1 Hz, 1H), 7.59 (dd, J = 11.0, 4.0 Hz, 1H), 3.98 – 3.88 (m, 4H), 3.33 – 3.22 (m, 4H), 2.58 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.2, 148.5, 140.2, 139.4, 129.8, 128.5, 127.8, 127.6, 66.7, 52.1, 51.4, 37.4 (t, J = 31.5 Hz), 29.7, ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.52 – -81.07 (m), -116.32 – -116.38 (m), -122.17 – -122.23 (m), -125.94 – -126.06 (m); HRMS (ESI+): Calculated for $C_{21}H_{18}F_9N_3O$: $[M+H]^+$ 500.1379, Found 500.1377.

2-Methoxy-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxaline (74)



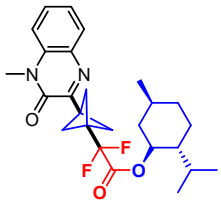
Obtained as a colourless liquid (79 mg, 89% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 (d, J = 8.1 Hz, 1H), 7.81 (d, J = 7.9 Hz, 1H), 7.66 – 7.58 (m, 1H), 7.57 – 7.47 (m, 1H), 4.11 (s, 3H), 2.54 (s, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.8, 145.4, 140.2, 138.5, 129.7, 128.7, 126.8, 126.6, 53.7, 51.2, 41.1, 37.97 (t, J = 31.5 Hz), ^{13}C NMR for C_4F_9 could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -81.07 (t, J = 10.0 Hz), -115.44 – -117.60 (m), -122.29 (dd, J = 18.2, 8.2 Hz), -125.02 – -127.00 (m); HRMS (ESI+): Calculated for $C_{18}H_{13}F_9N_2O$: $[M+H]^+$ 445.0957, Found 445.0959.

Ethyl 2,2-difluoro-2-(3-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[1.1.1]pentan-1-yl)acetate (75)



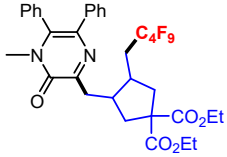
Obtained as a light yellow liquid (46 mg, 66% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (d, J = 8.0 Hz, 1H), 7.54 (t, J = 7.8 Hz, 1H), 7.34 (t, J = 7.6 Hz, 1H), 7.29 (d, J = 8.4 Hz, 1H), 4.36 (q, J = 7.1 Hz, 2H), 3.66 (s, 3H), 2.43 (s, 6H), 1.37 (t, J = 7.1 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.3 (t, J = 34.0 Hz), 155.3, 154.5, 133.4, 132.8, 130.4, 130.2, 123.7, 113.6, 112.2 (t, J = 250.7 Hz), 62.8, 50.5 (t, J = 3.8 Hz), 41.5, 39.2 (t, J = 31.5 Hz), 28.6, 14.2; ^{19}F NMR (471 MHz, $CDCl_3$) δ -111.55; HRMS (ESI+): Calculated for $C_{18}H_{18}F_2N_2O_3$: $[M+H]^+$ 349.1358, Found 349.1359.

(1*R*,2*R*,5*S*)-2-Isopropyl-5-methylcyclohexyl-2,2-difluoro-2-(3-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[1.1.1]pentan-1-yl)acetate (77)



Obtained as a light yellow liquid (73 mg, 80% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (d, J = 7.8 Hz, 1H), 7.55 (t, J = 7.6 Hz, 1H), 7.35 (t, J = 7.5 Hz, 1H), 7.30 (d, J = 8.3 Hz, 1H), 4.86 (td, J = 10.9, 4.3 Hz, 1H), 3.67 (s, 3H), 2.44 (s, 6H), 2.07 (d, J = 11.4 Hz, 1H), 1.96 – 1.87 (m, 1H), 1.74 – 1.69 (m, 2H), 1.57 – 1.49 (m, 2H), 1.15 – 1.06 (m, 2H), 0.93 (t, J = 6.9 Hz, 6H), 0.88 (d, J = 13.0 Hz, 1H), 0.79 (d, J = 6.9 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ163.0 (t, J = 34.0 Hz), 155.4, 154.5, 133.5, 132.8, 130.4, 130.2, 123.7, 113.6, 112.2 (t, J = 250.7 Hz), 77.5, 50.5, 46.8, 40.6, 39.3 (t, J = 31.5 Hz), 34.0, 31.5, 29.7, 28.6, 26.1, 23.3, 22.0, 20.7, 16.1; ^{19}F NMR (471 MHz, $CDCl_3$) δ -111.05 (qd, J = 261.6, 5.2 Hz); HRMS (ESI+): Calculated for $C_{26}H_{32}F_2N_2O_3$: $[M+H]^+$ 459.2454, Found 459.2455.

Diethyl-3-((4-methyl-3-oxo-5,6-diphenyl-3,4-dihydropyrazin-2-yl)methyl)-4-(perfluorobutyl)cyclopentane-1,1-dicarboxylate (81)

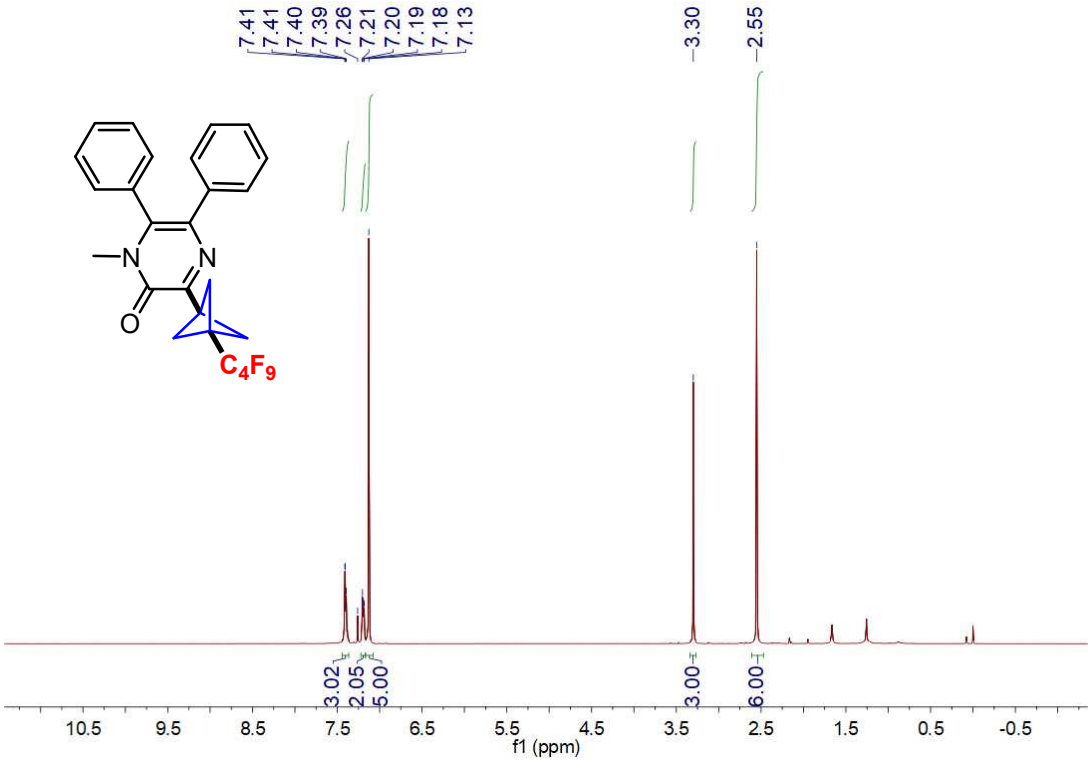


Obtained as a light yellow liquid (79 mg, 55% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 – 7.37 (m, 3H), 7.21 (dd, J = 8.8, 5.9 Hz, 2H), 7.11 (s, 5H), 4.21 – 4.12 (m, 4H), 3.31 (s, 3H), 2.97 – 2.95 (m, 1H), 2.89 – 2.81 (m, 1H), 2.61 – 2.54 (m, 2H), 2.36 – 2.25 (m, 2H), 1.22 (ddd, J = 15.8, 9.6, 5.1 Hz, 10H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.5, 172.5, 155.7, 155.7, 137.8, 136.7, 132.6, 132.4, 130.1, 129.5, 129.3, 129.1, 127.7, 126.9, 61.7, 61.6, 58.7, 39.5, 39.0, 38.7, 34.8, 34.0, 33.0, 29.7, 14.0, 13.9, ^{13}C NMR for C_8F_{17} could not be assigned; ^{19}F NMR (471 MHz, $CDCl_3$) δ -80.00 – -80.04 (m), -

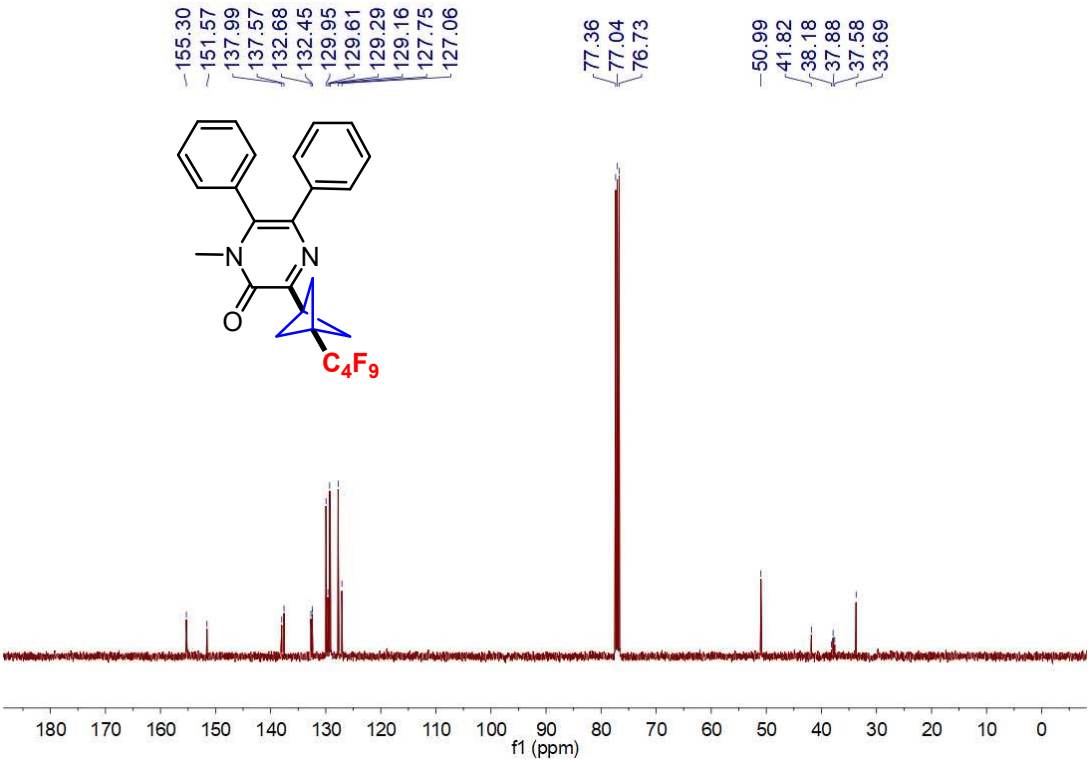
114.16 – -114.28 (m), -124.29 – -124.68 (m), -125.85 – -125.95 (m); HRMS (ESI+): Calculated for $C_{34}H_{33}F_9N_2O_5$: $[M+Na]^+$ 743.2138, Found 743.2142.

3 Copies of ^1H, ^{13}C and ^{19}F NMR Spectra

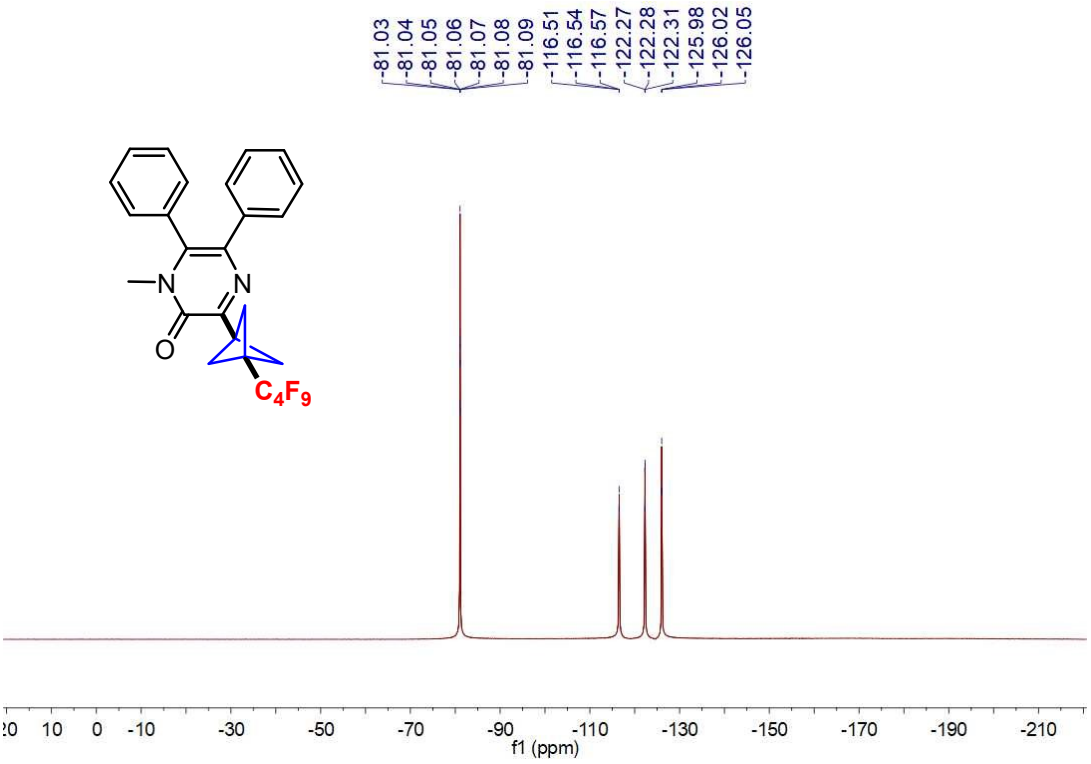
4 ^1H NMR (500 MHz, $CDCl_3$)



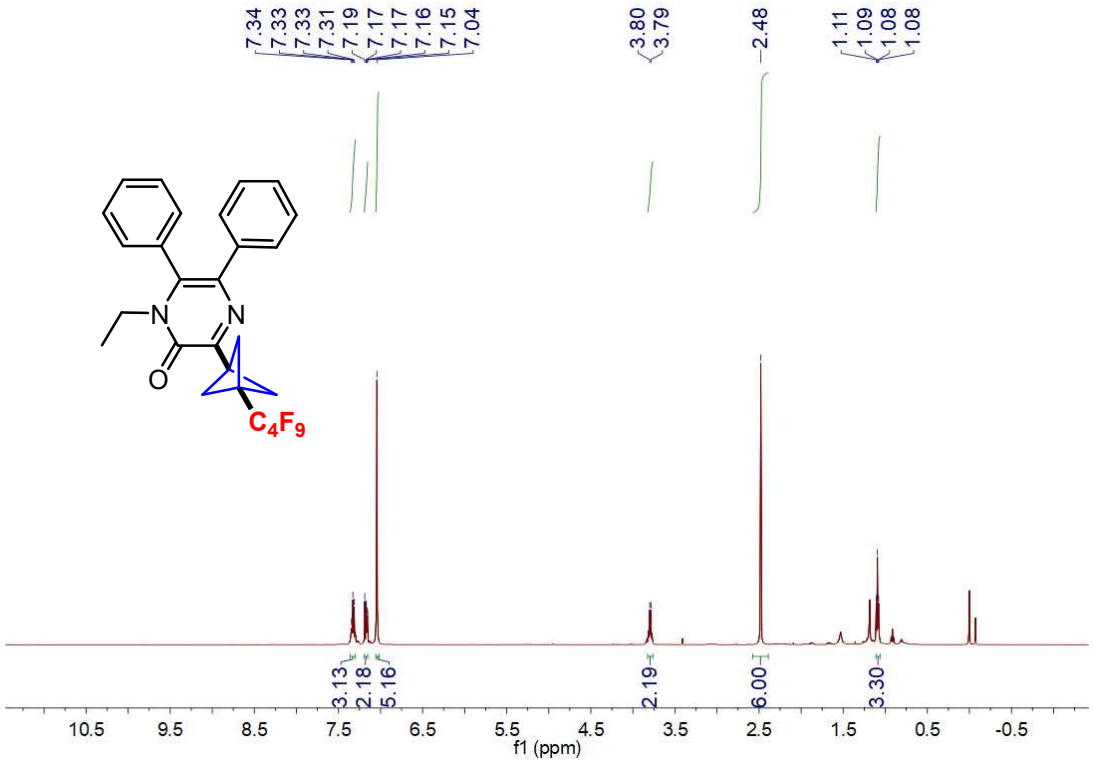
4 ^{13}C NMR (126 MHz, $CDCl_3$)



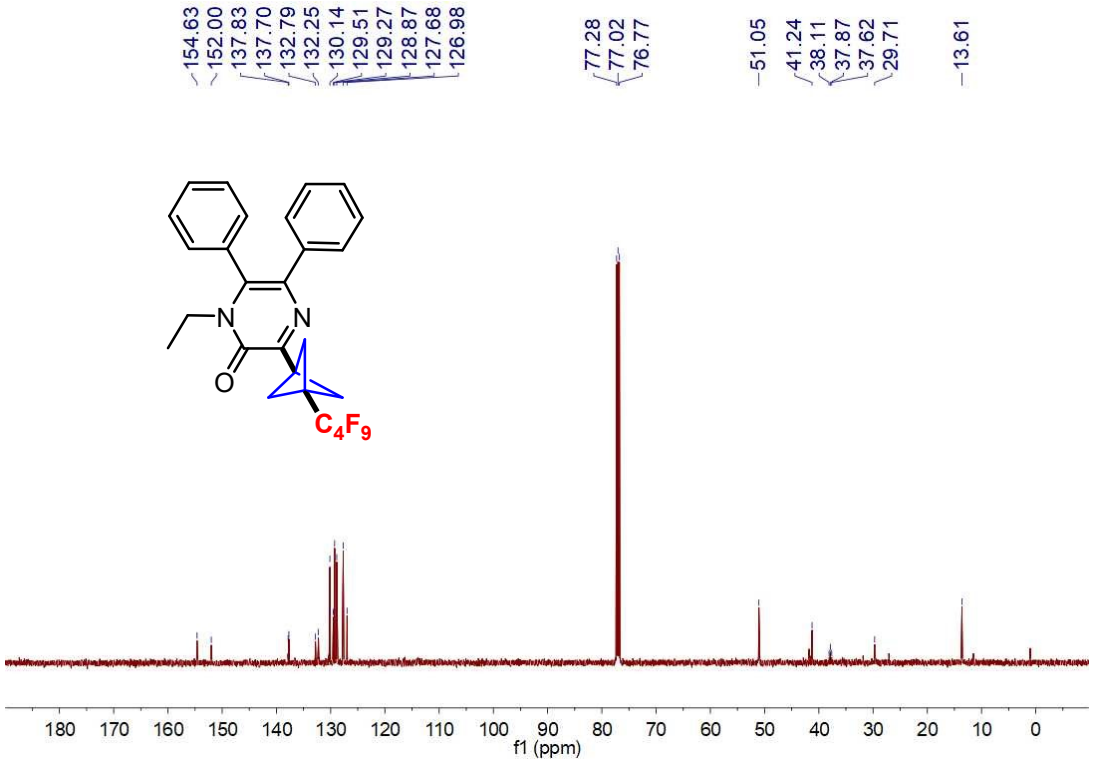
4 ^{19}F NMR (471 MHz, $CDCl_3$)



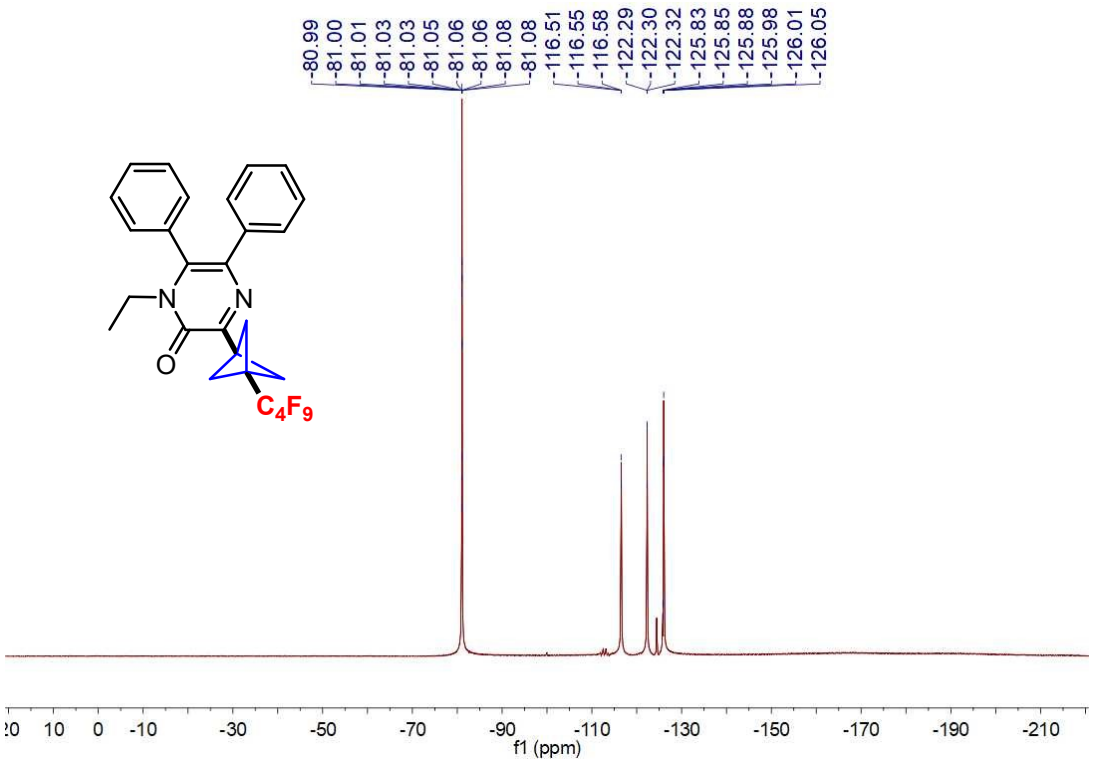
5 ^{1}H NMR (500 MHz, $CDCl_3$)



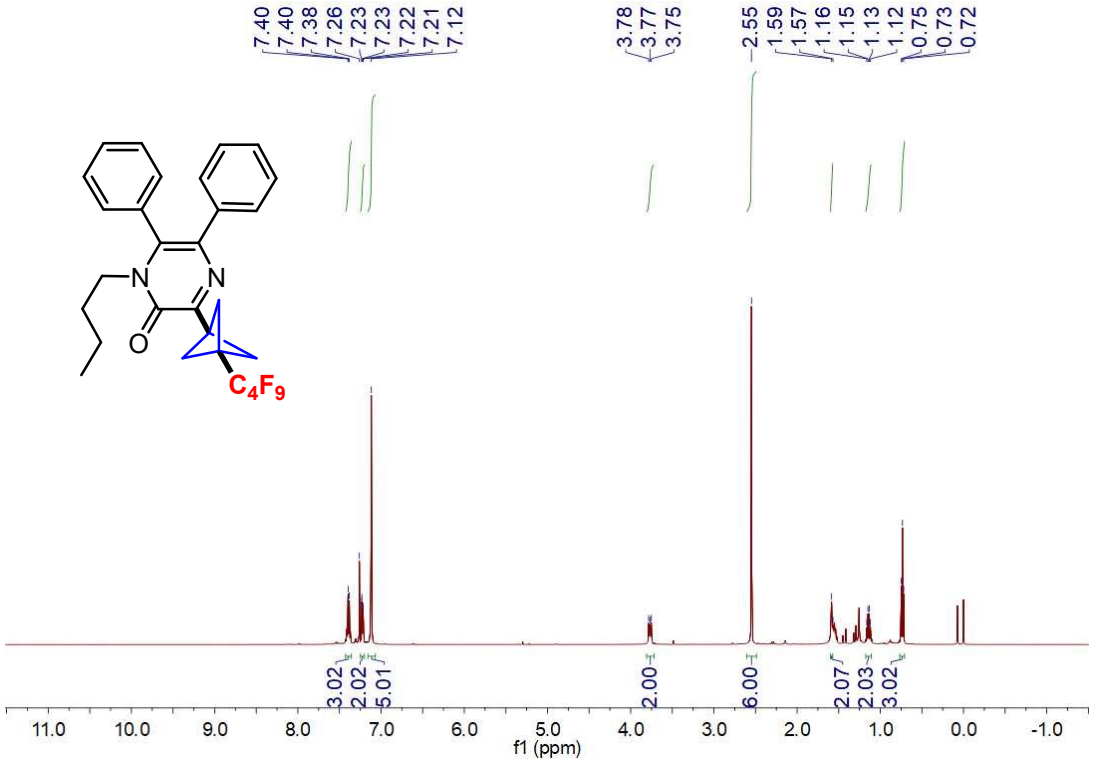
5 ^{13}C NMR (126 MHz, $CDCl_3$)



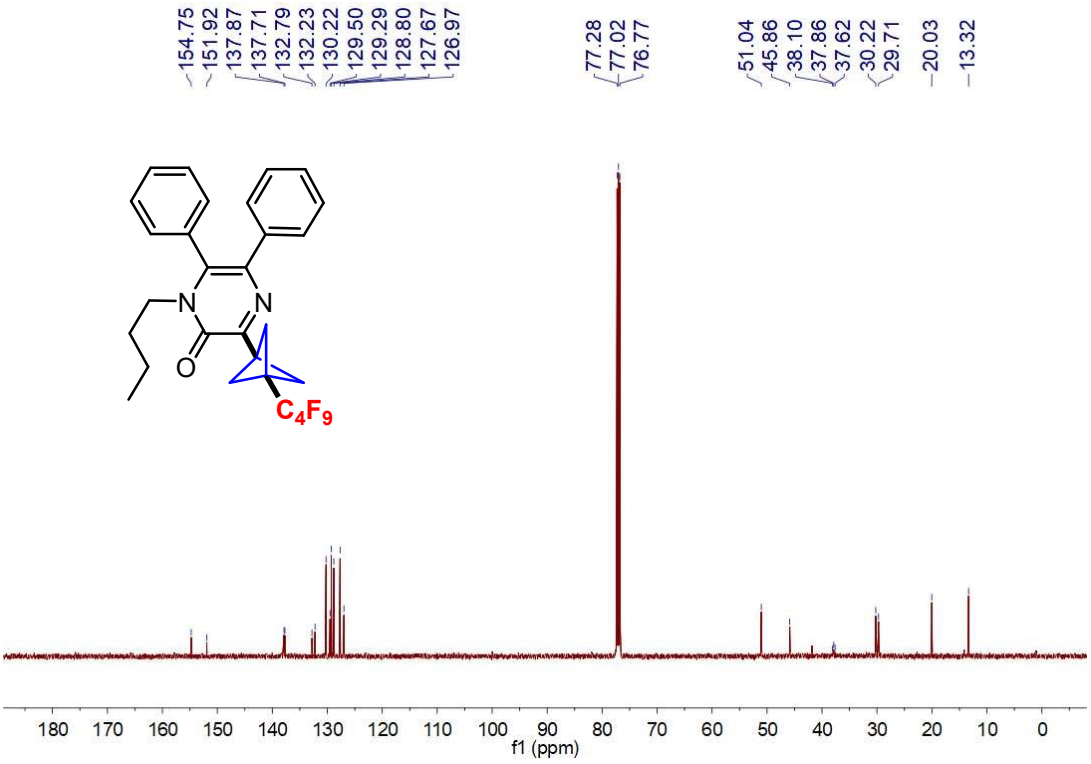
5 ^{19}F NMR (471 MHz, $CDCl_3$)



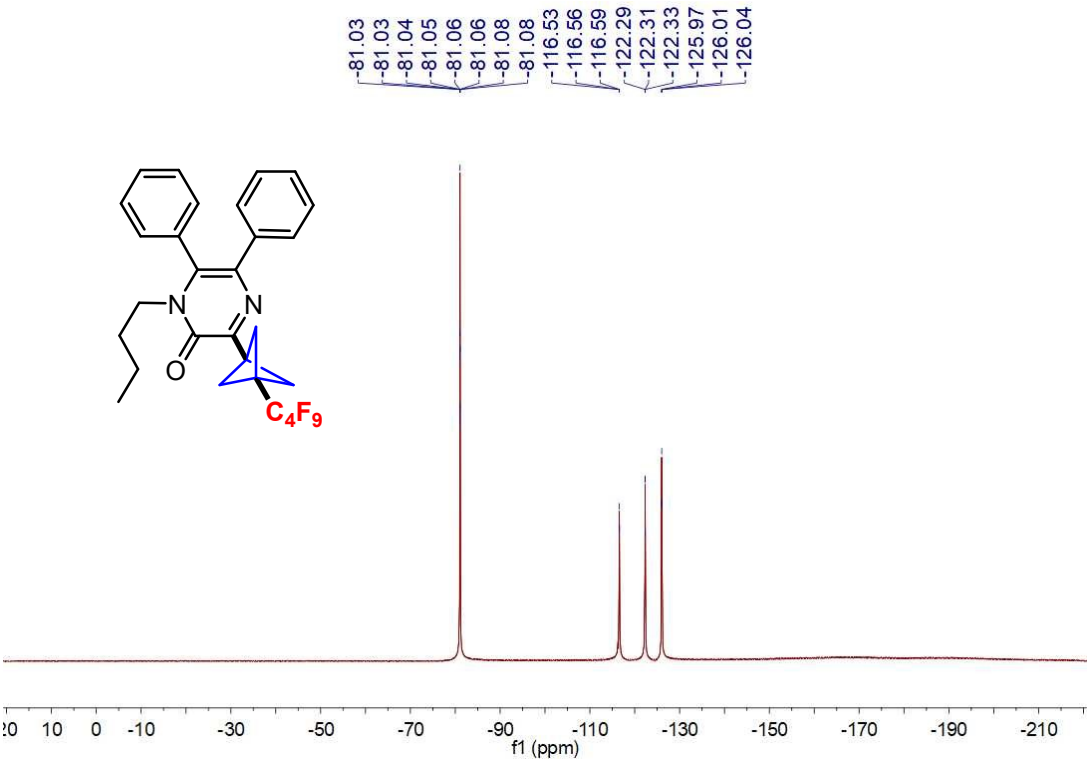
6 ^{1}H NMR (500 MHz, $CDCl_3$)



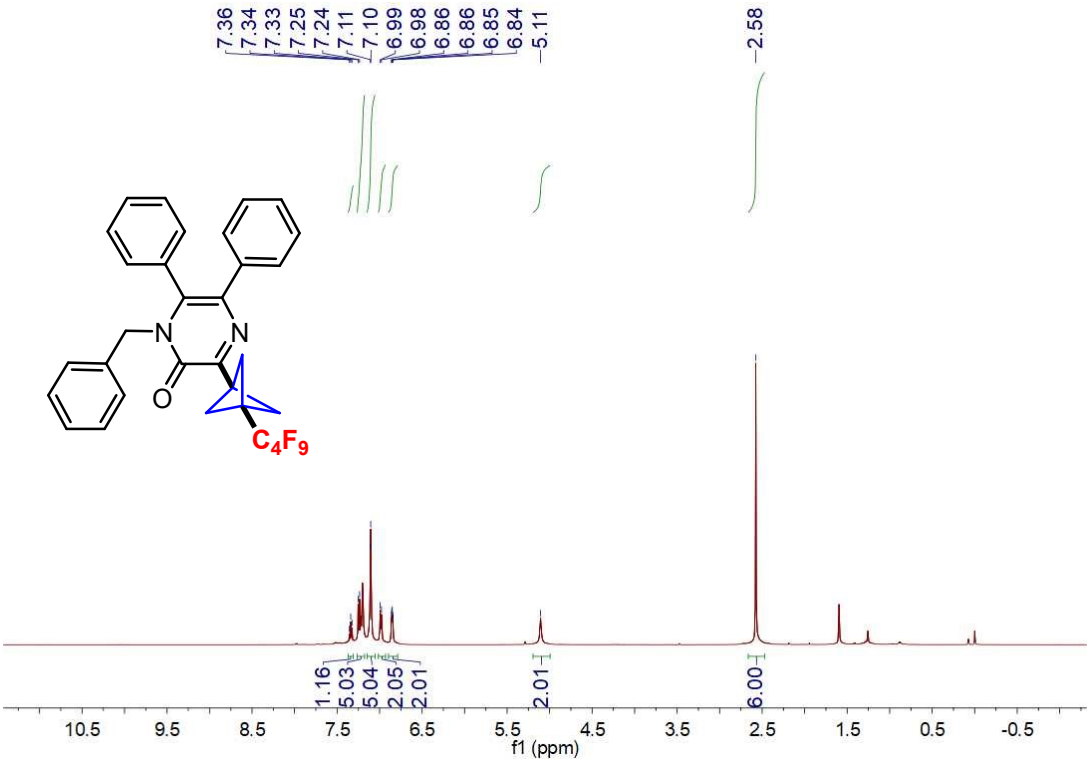
6 ^{13}C NMR (126 MHz, $CDCl_3$)



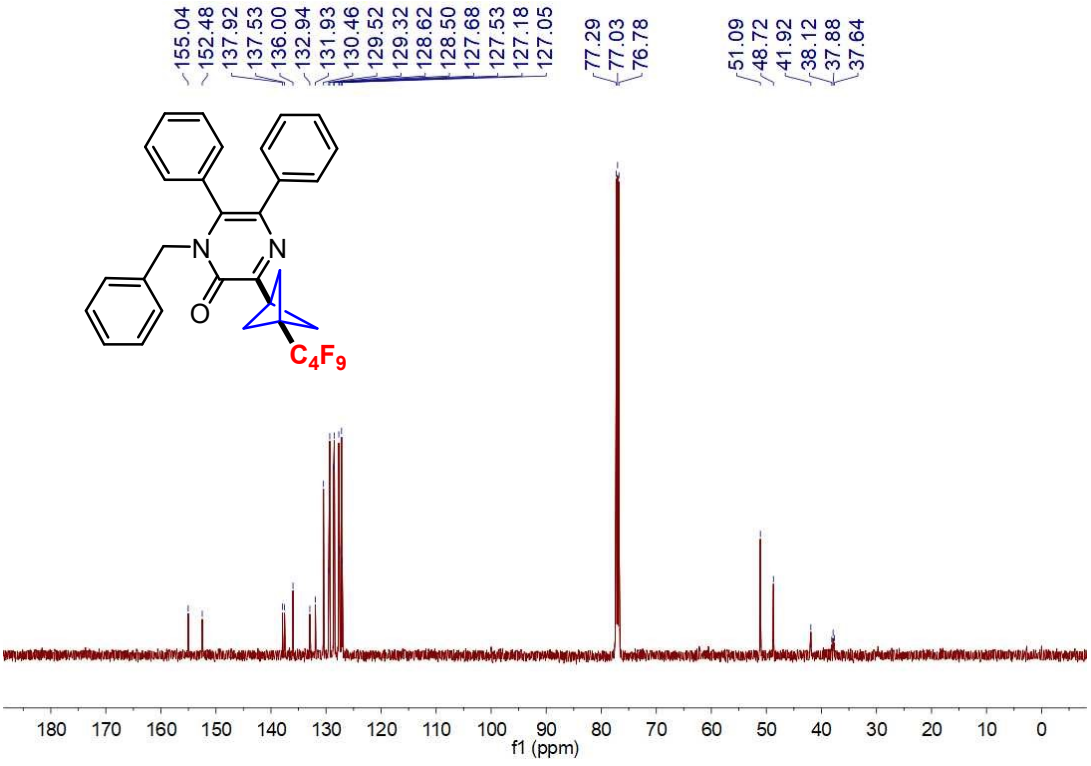
6 ^{19}F NMR (471 MHz, $CDCl_3$)



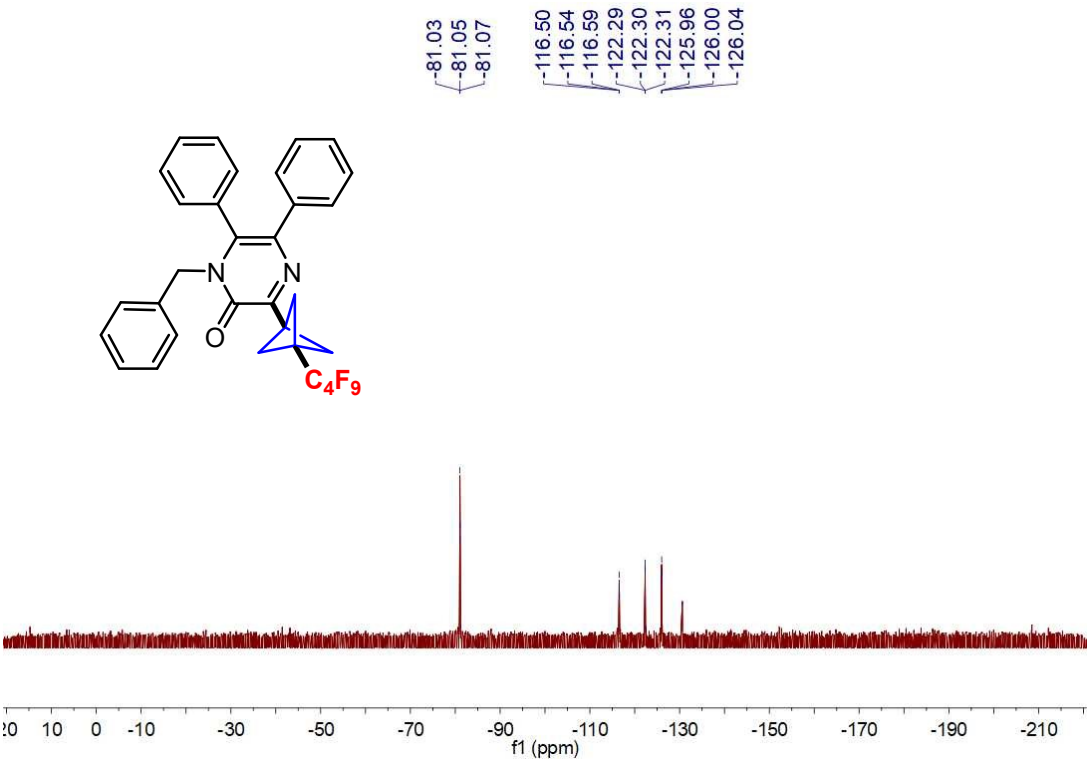
7 ^{1}H NMR (500 MHz, $CDCl_3$)



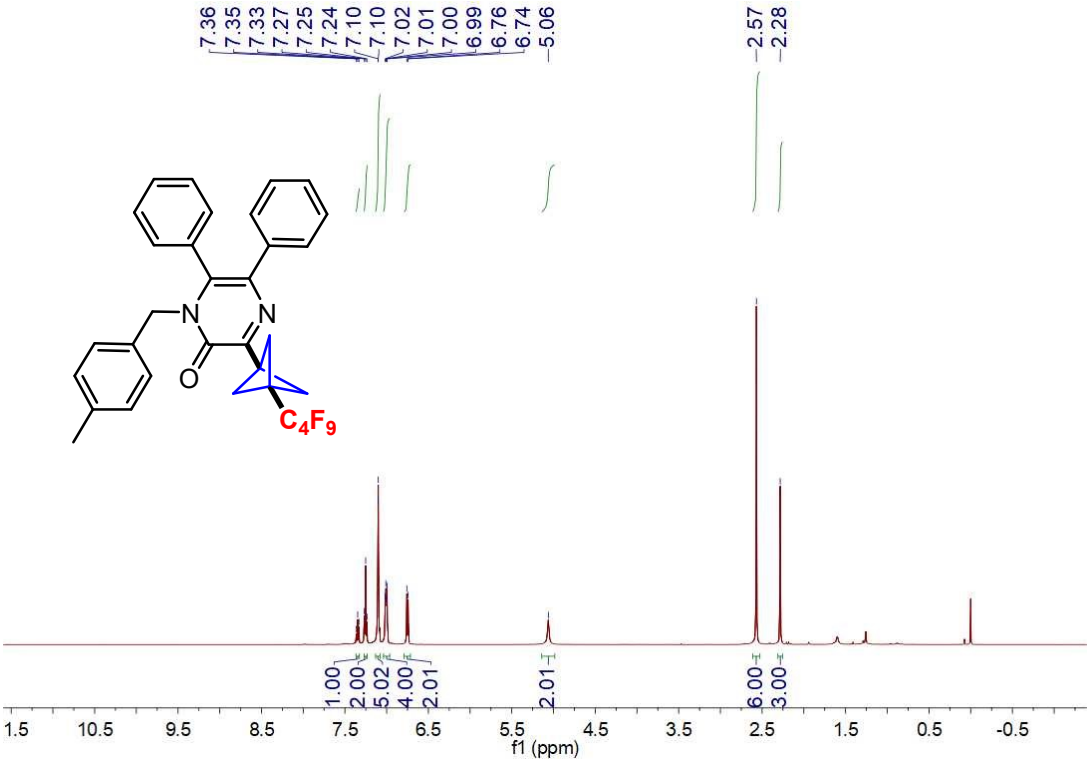
7 ^{13}C NMR (126 MHz, $CDCl_3$)



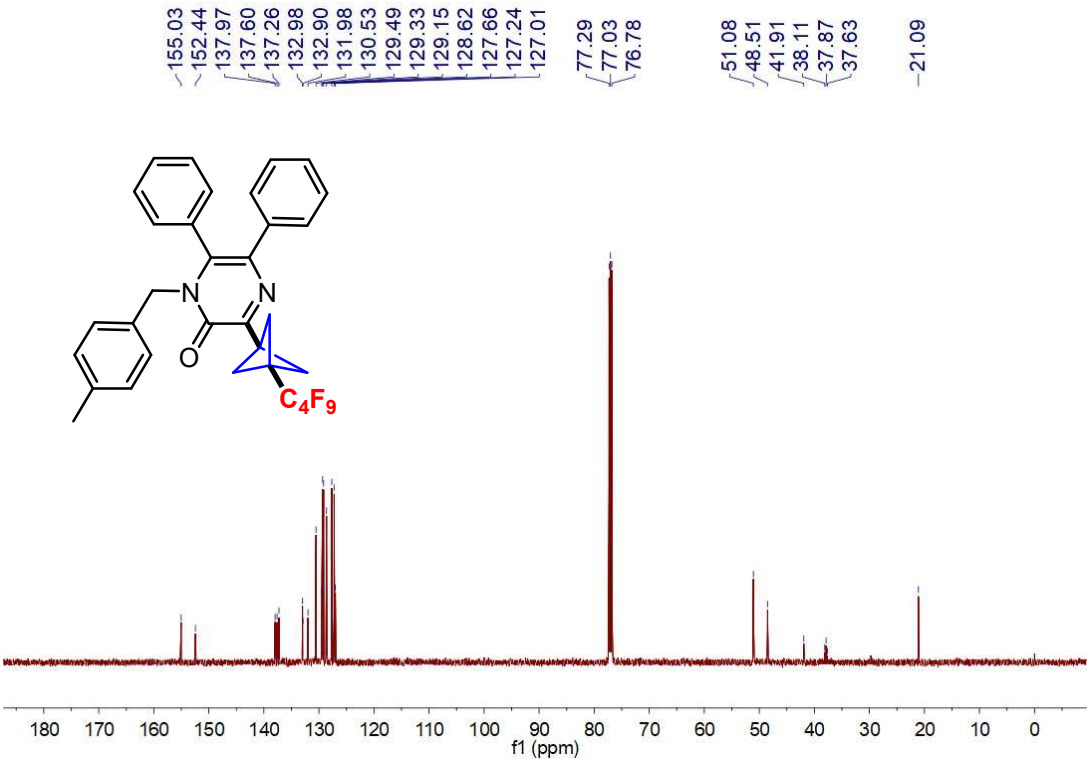
7 ^{19}F NMR (471 MHz, $CDCl_3$)



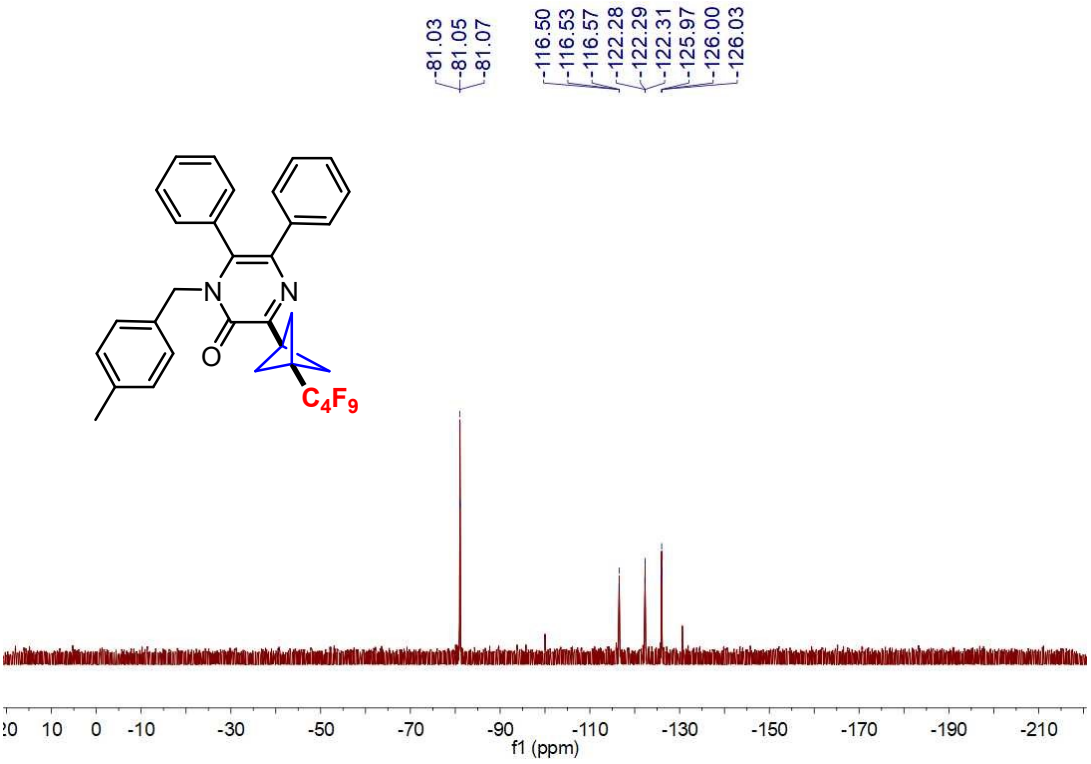
8 ^{1}H NMR (500 MHz, $CDCl_3$)



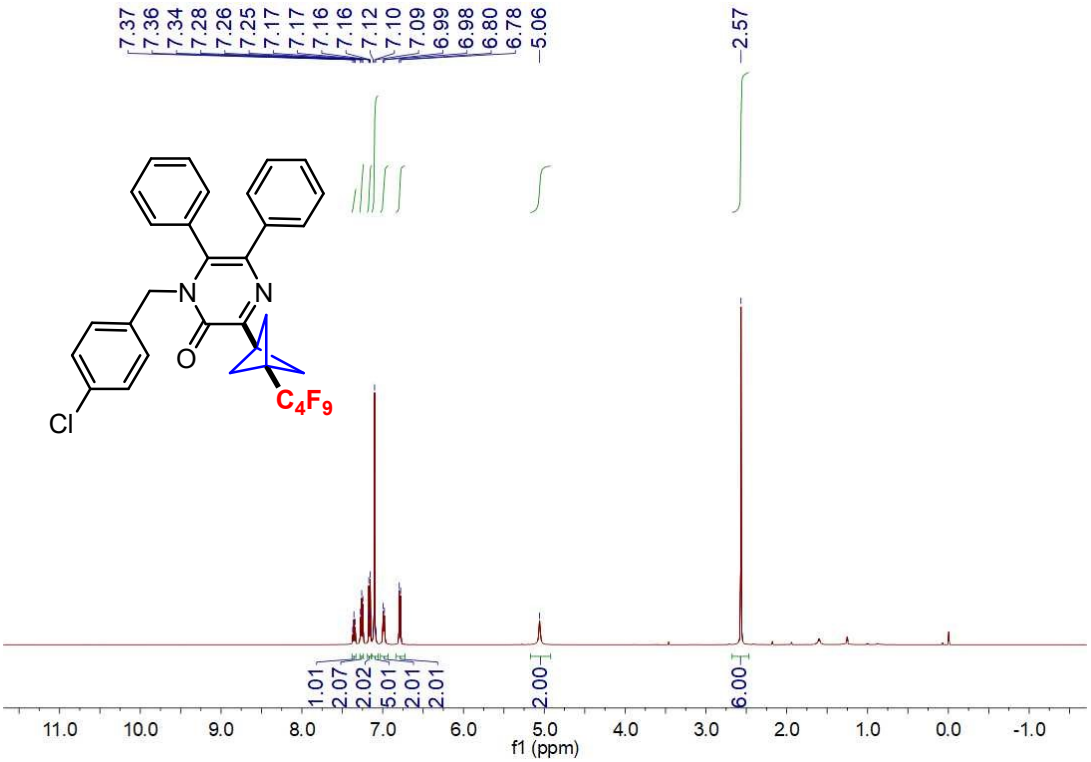
8 ^{13}C NMR (126 MHz, $CDCl_3$)



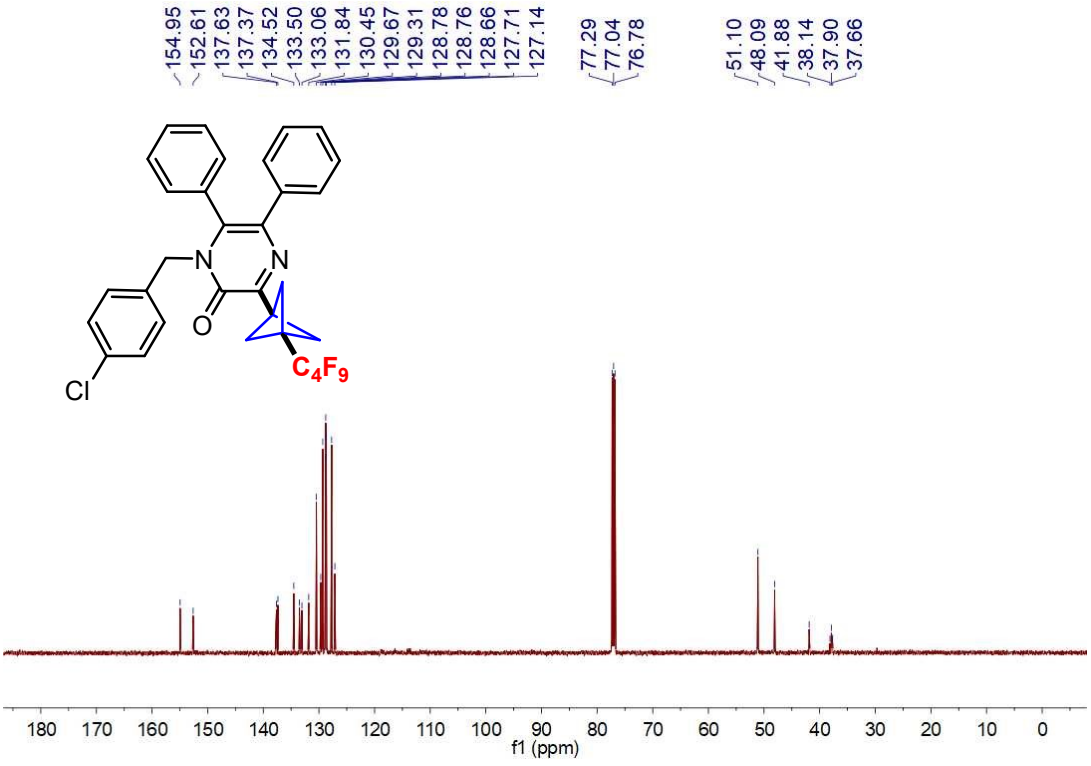
8 ^{19}F NMR (471 MHz, $CDCl_3$)



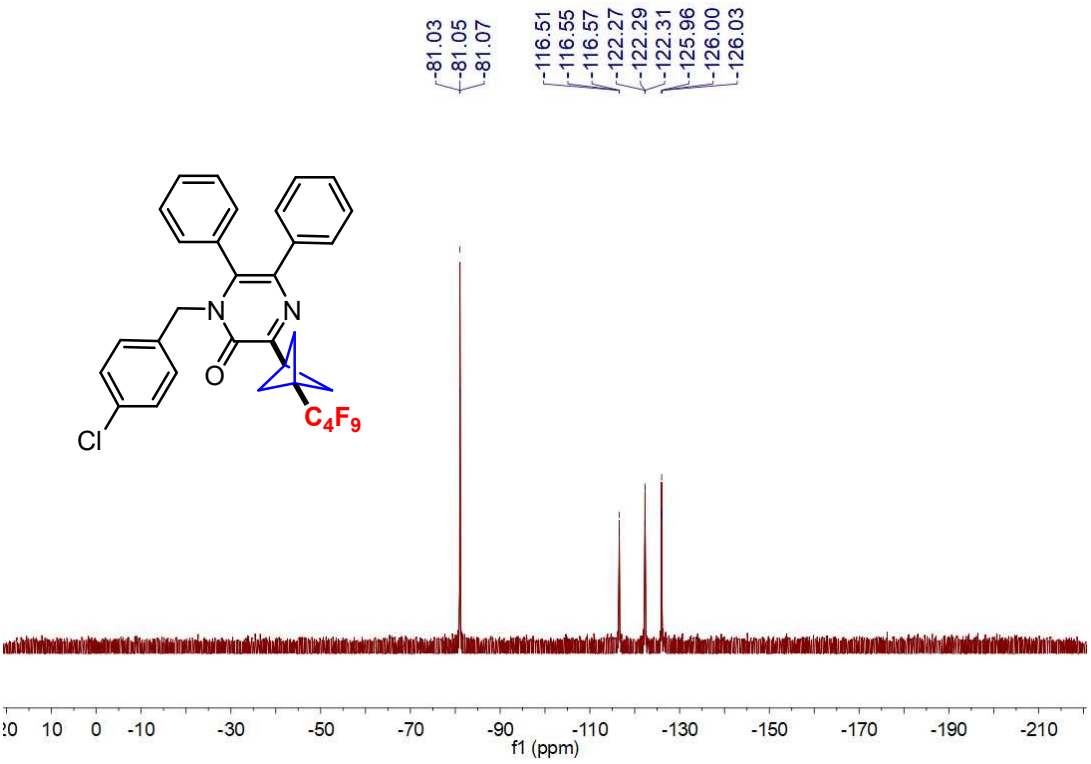
9 ^{1}H NMR (500 MHz, $CDCl_3$)



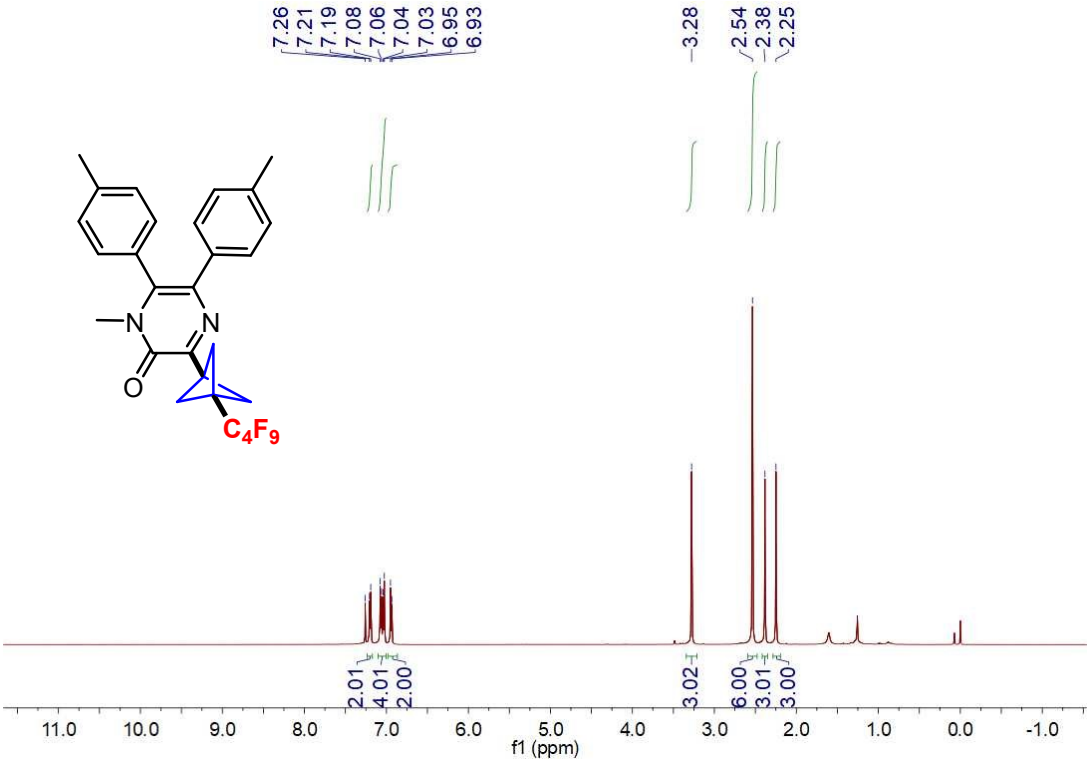
9 ^{13}C NMR (126 MHz, $CDCl_3$)



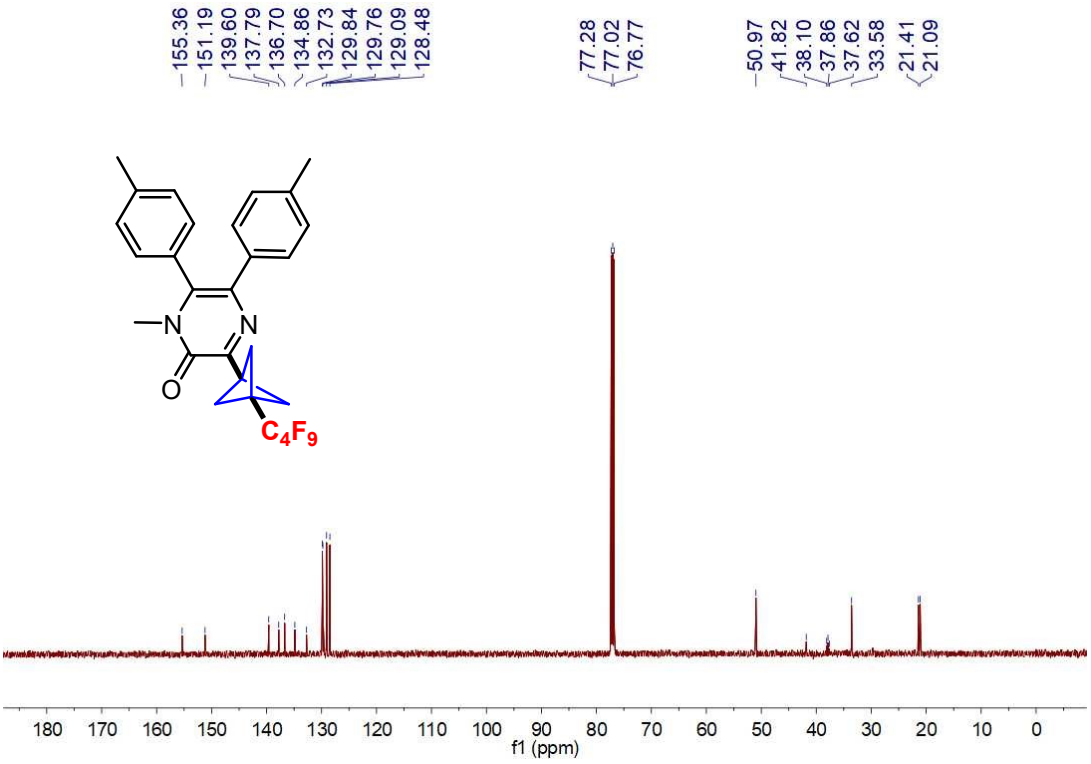
9 ^{19}F NMR (471 MHz, $CDCl_3$)



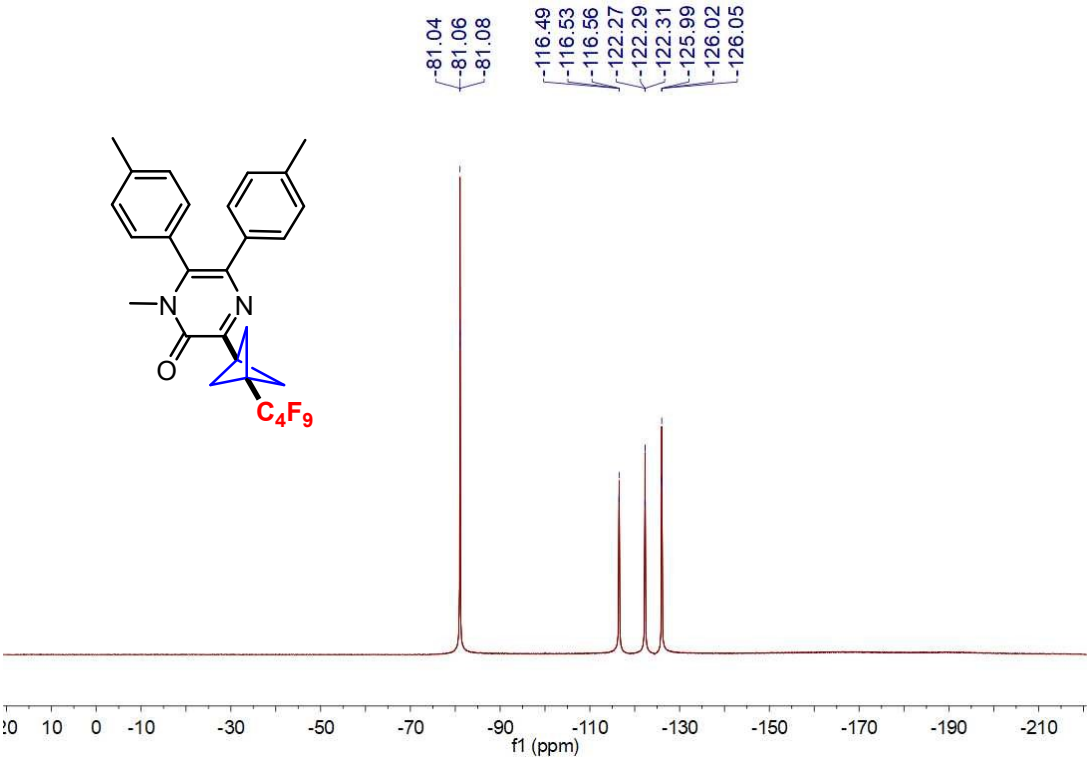
10 ^{1}H NMR (500 MHz, $CDCl_3$)



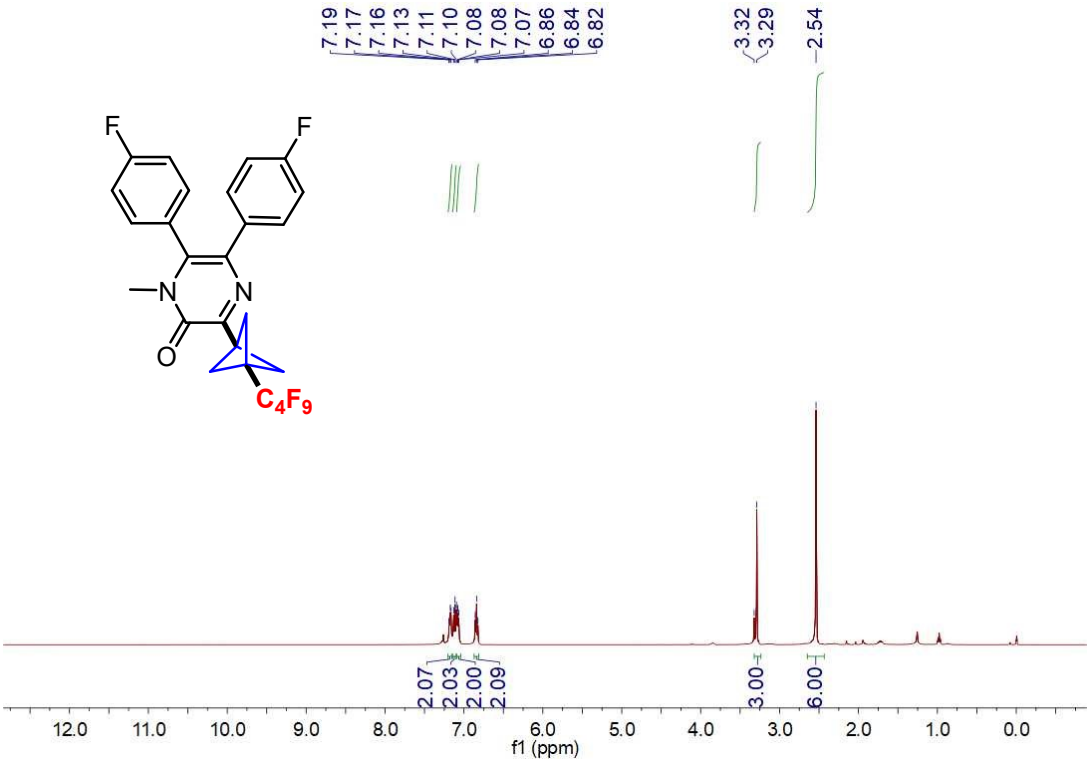
10 ^{13}C NMR (126 MHz, $CDCl_3$)



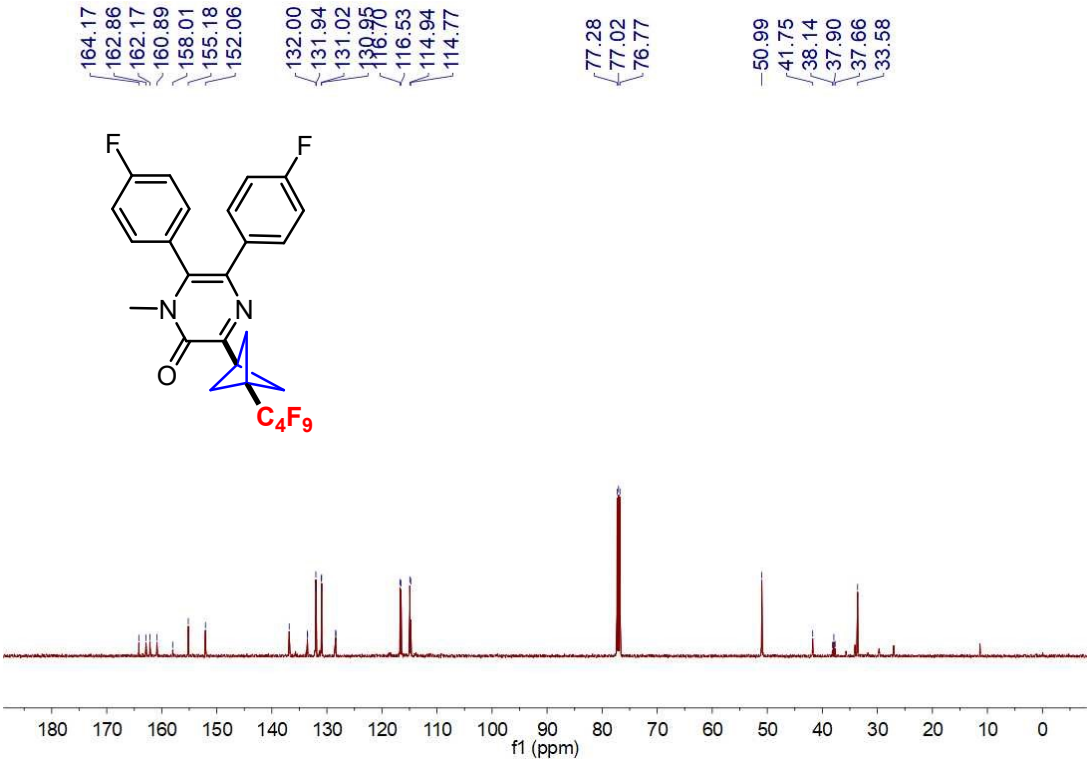
10 ^{19}F NMR (471 MHz, $CDCl_3$)



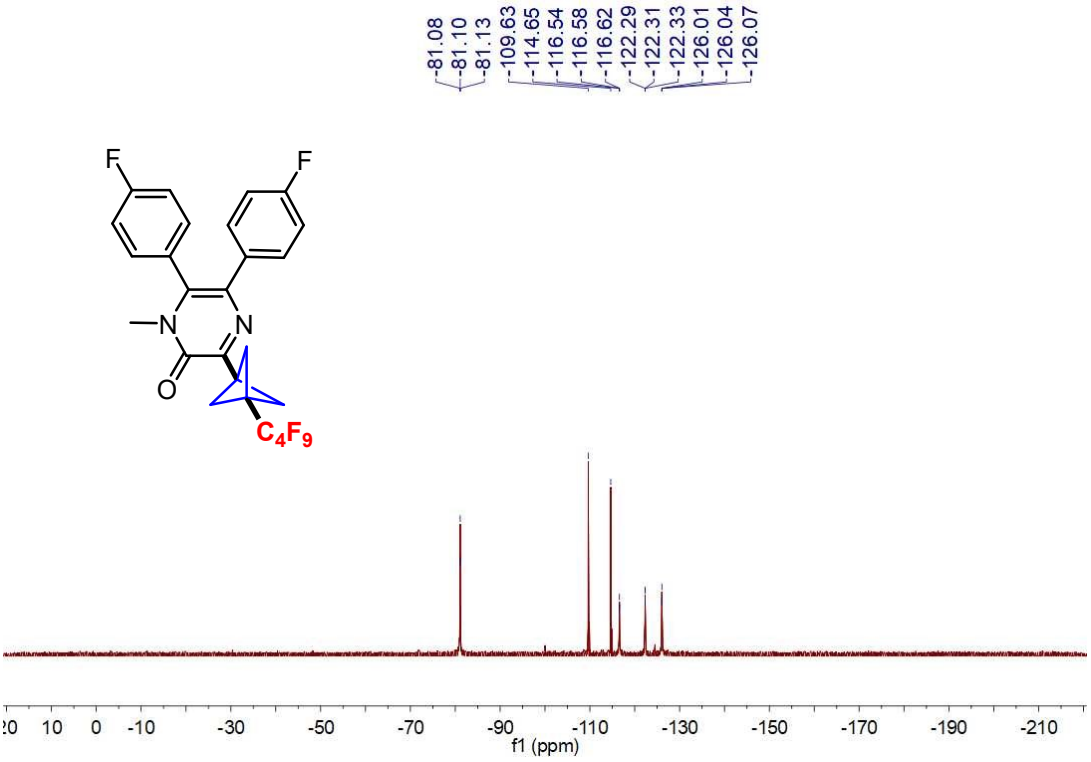
11 ^{1}H NMR (500 MHz, $CDCl_3$)



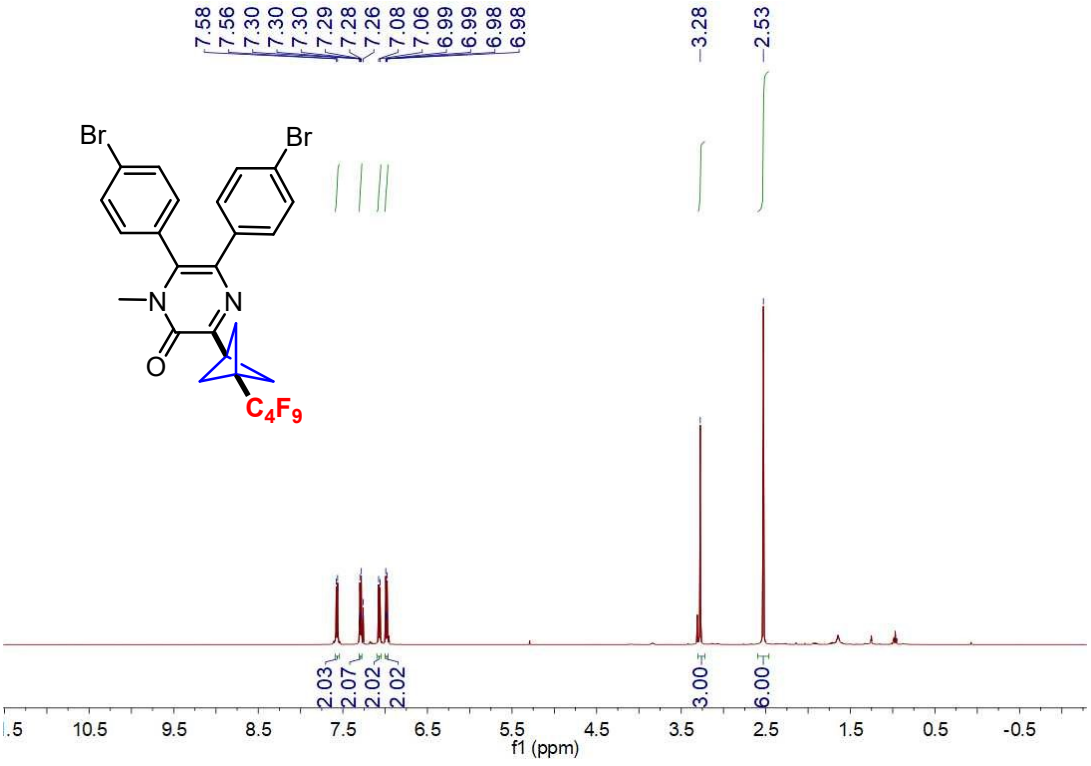
11 ^{13}C NMR (126 MHz, $CDCl_3$)



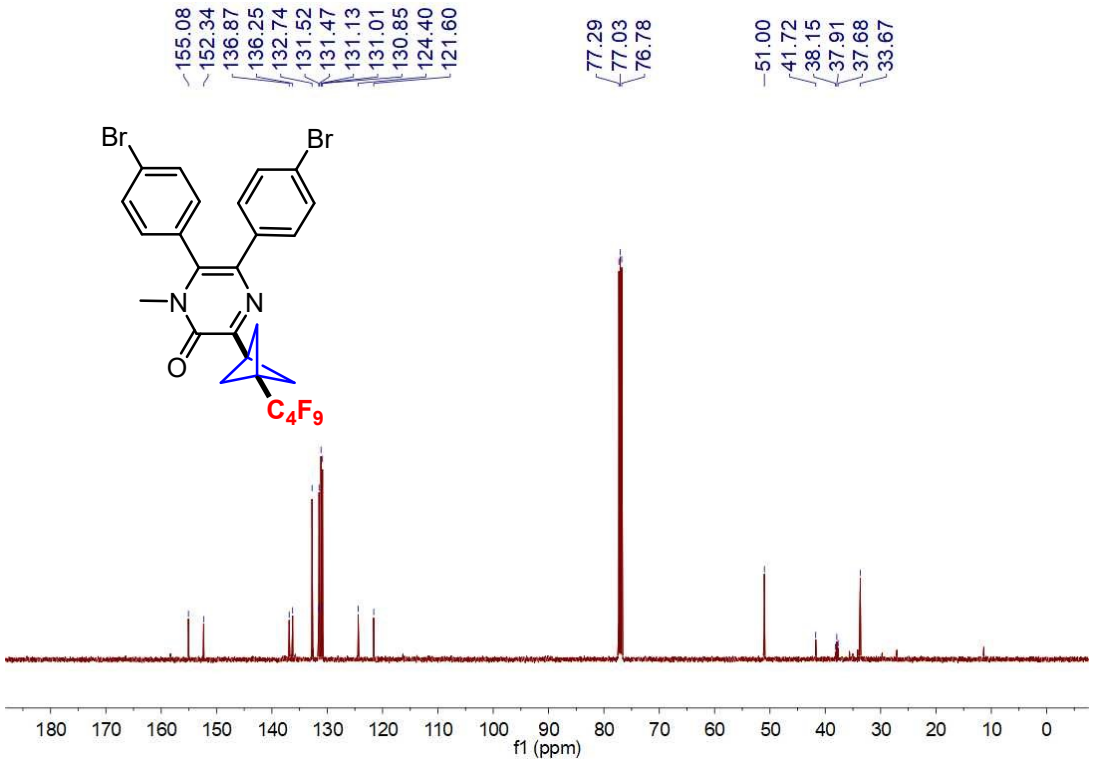
11 ^{19}F NMR (471 MHz, $CDCl_3$)



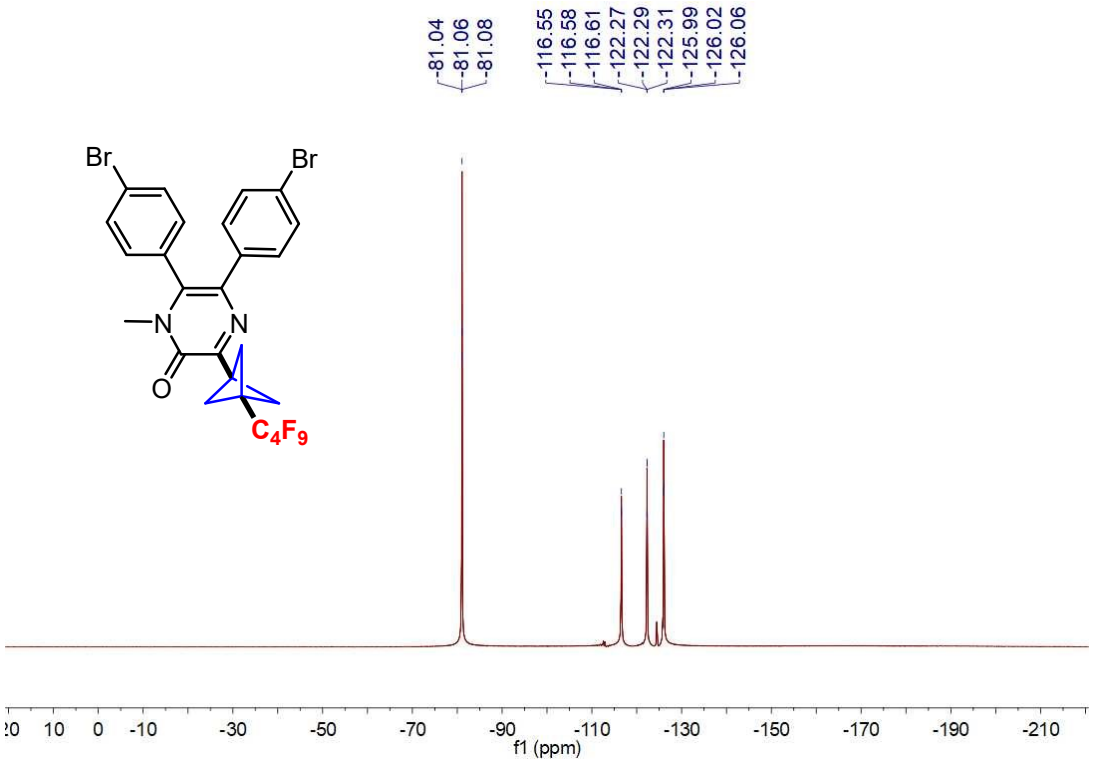
12 ^{1}H NMR (500 MHz, $CDCl_3$)



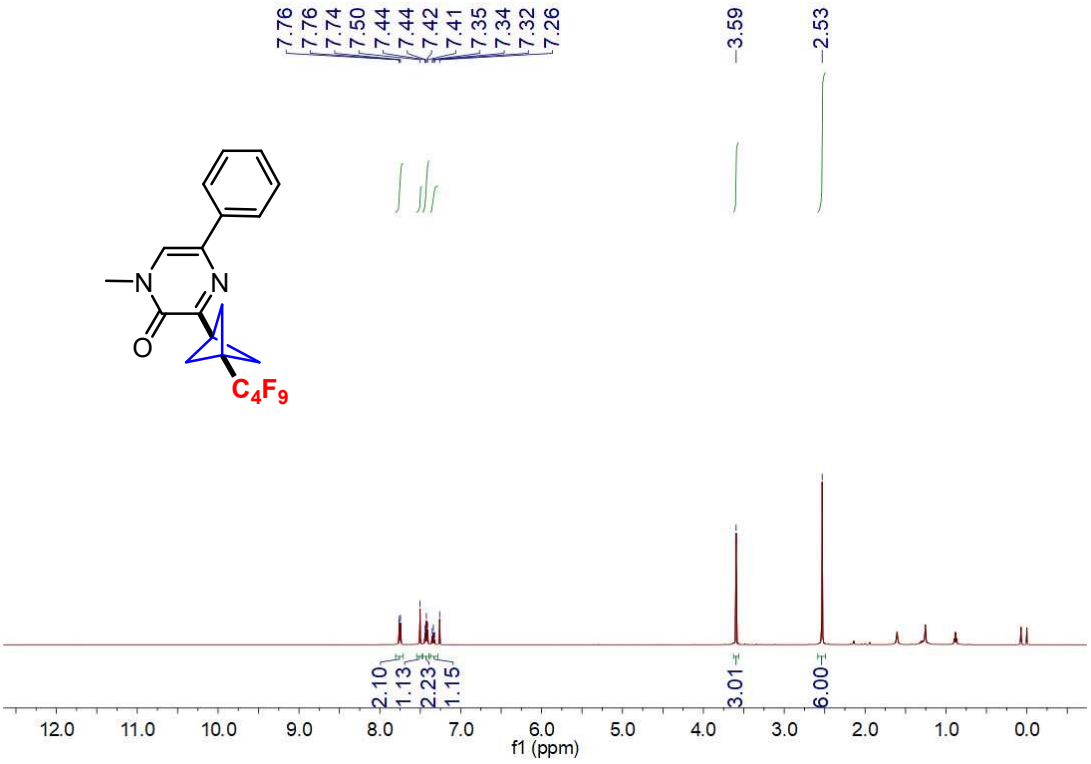
12 ^{13}C NMR (126 MHz, $CDCl_3$)



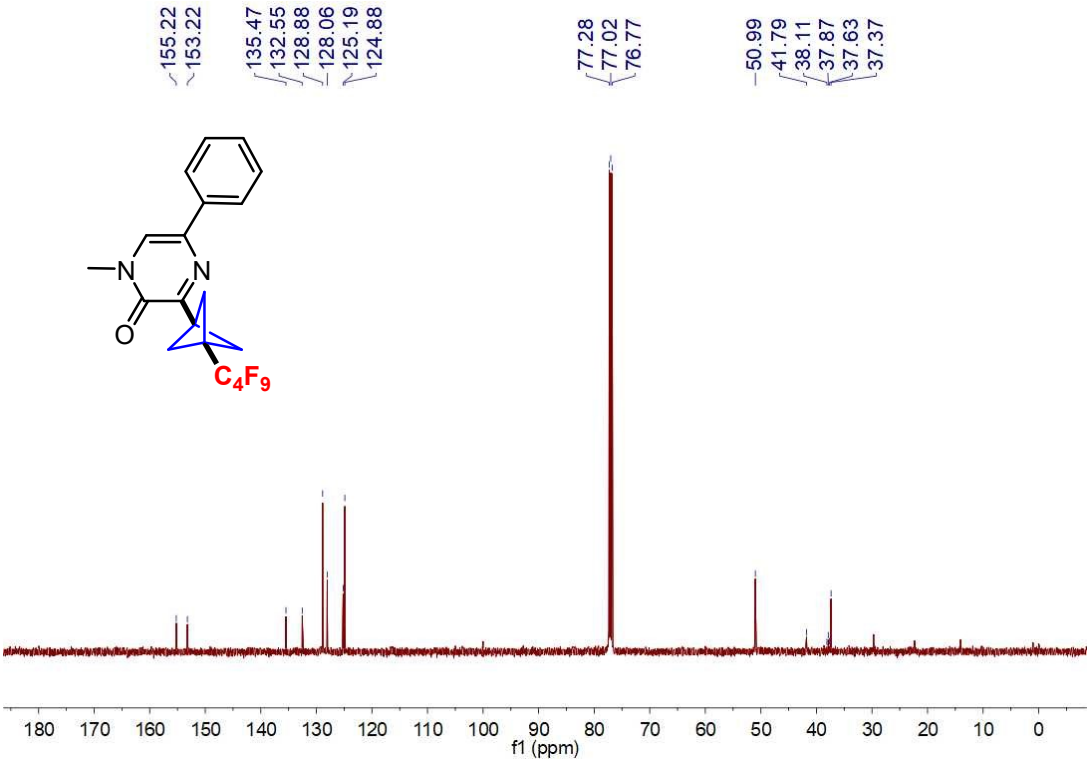
12 ^{19}F NMR (471 MHz, $CDCl_3$)



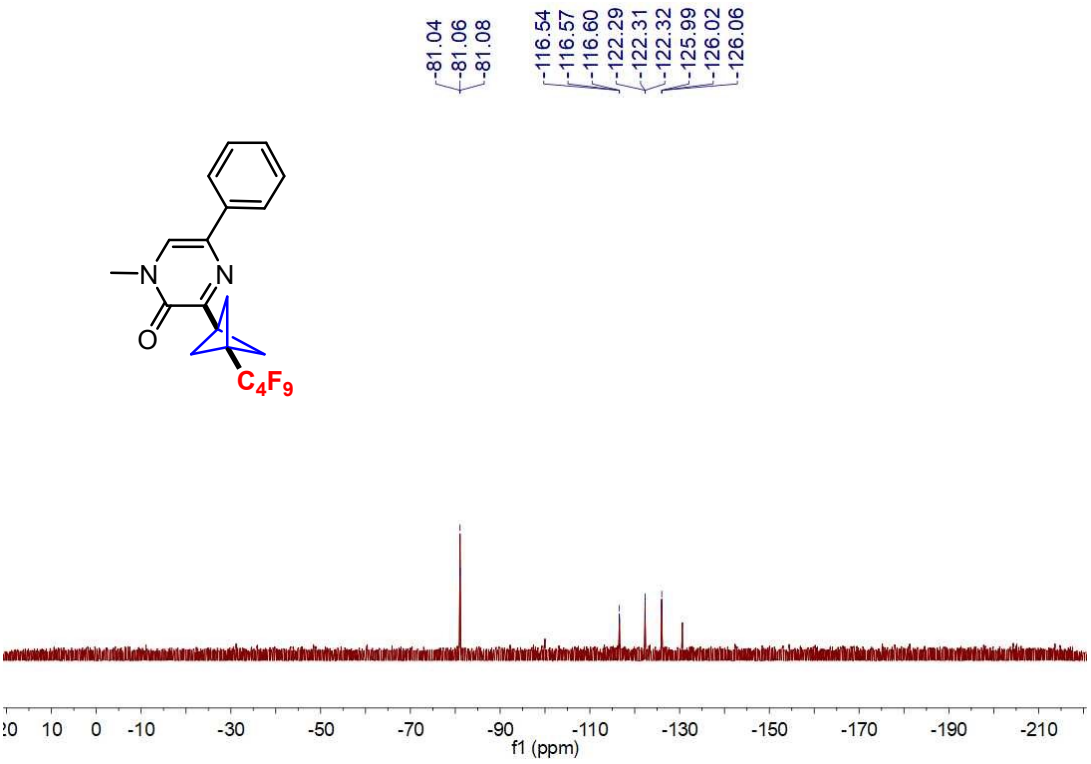
13 ^{1}H NMR (500 MHz, $CDCl_3$)



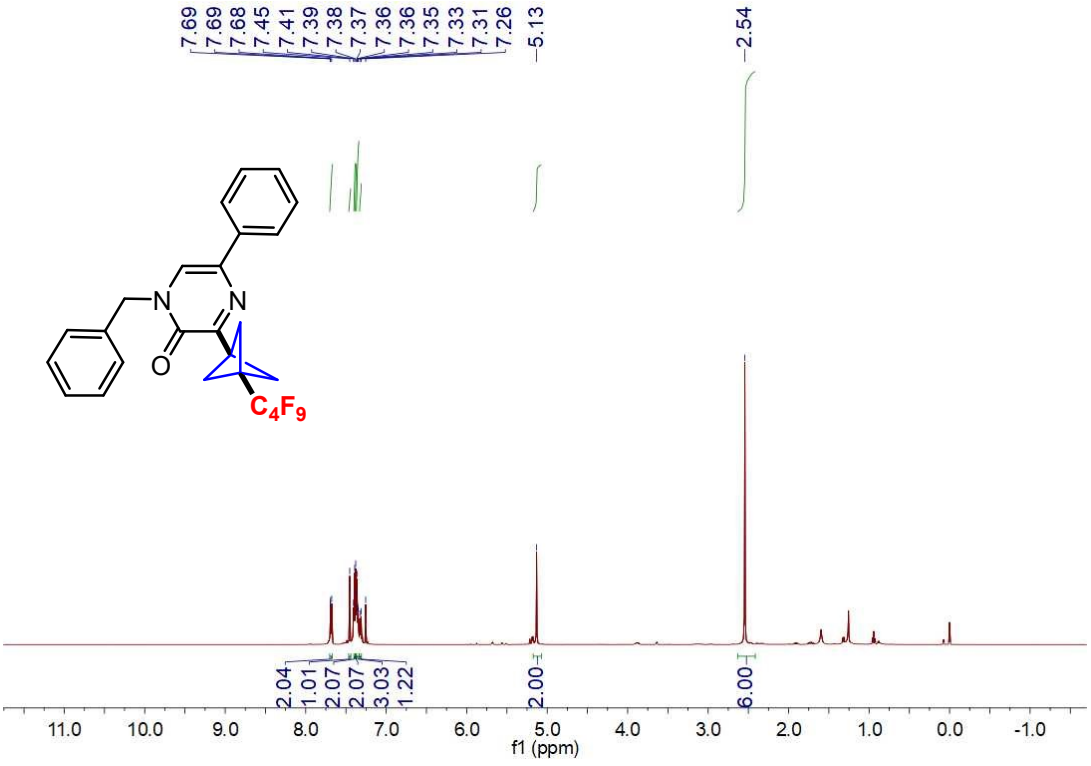
13 ^{13}C NMR (126 MHz, $CDCl_3$)



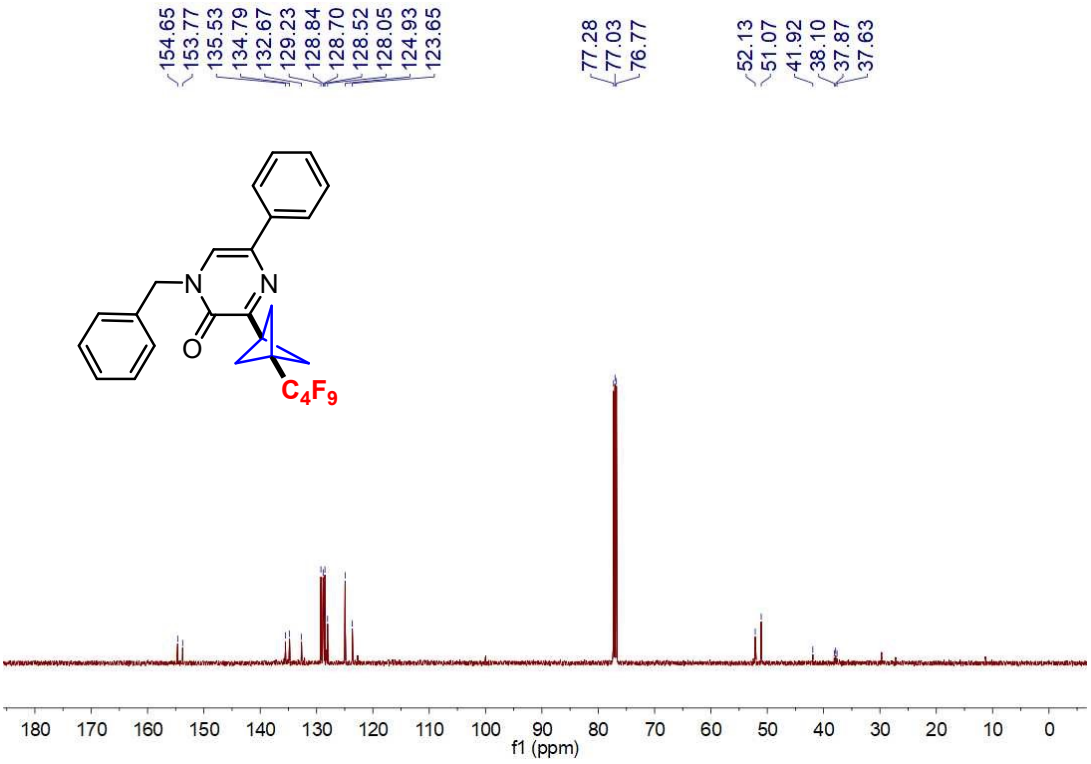
13 ^{19}F NMR (471 MHz, $CDCl_3$)



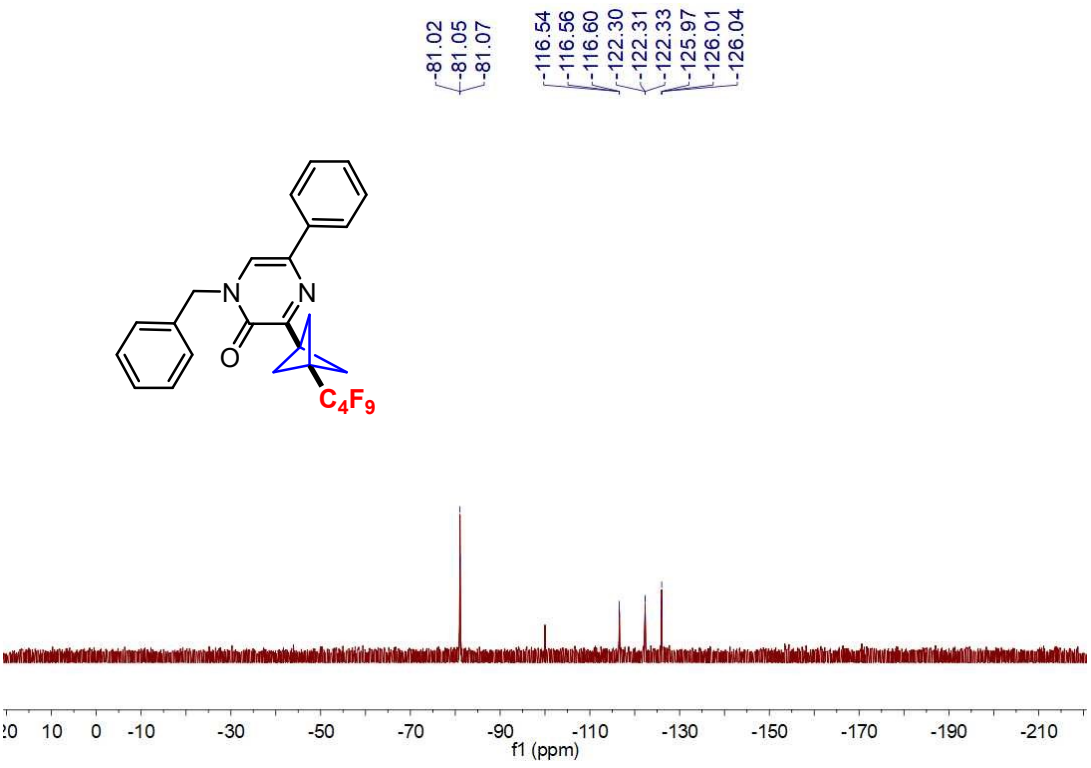
14 ^{1}H NMR (500 MHz, $CDCl_3$)



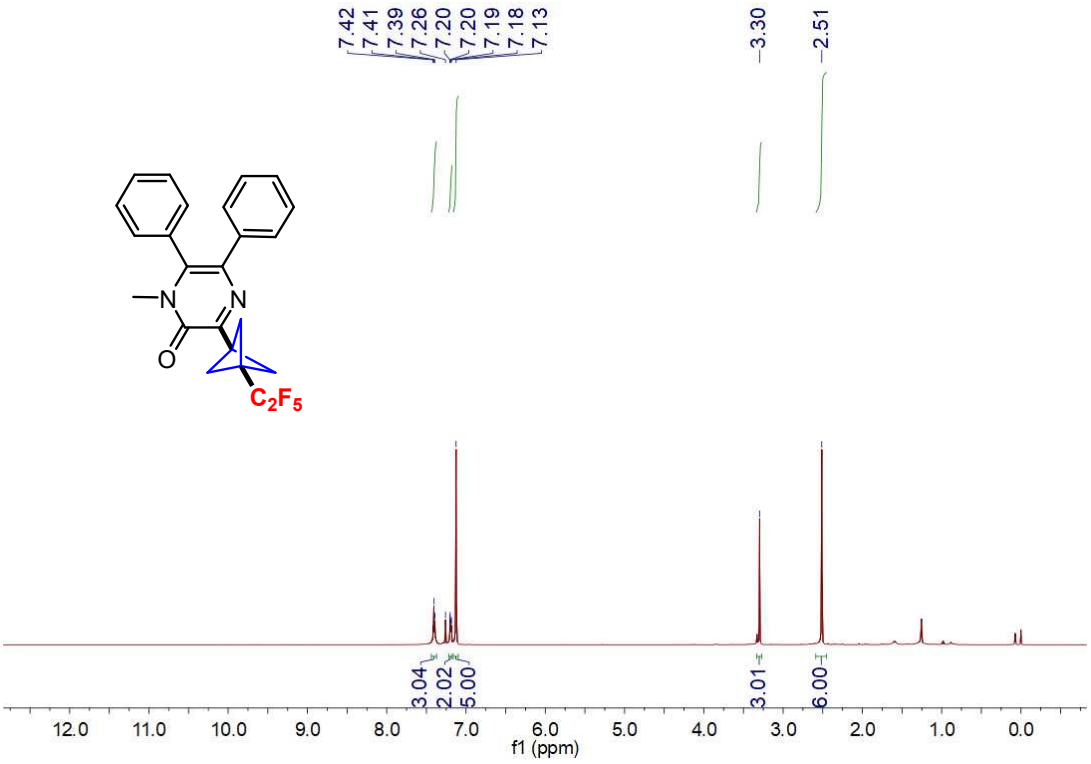
14 ^{13}C NMR (126 MHz, $CDCl_3$)



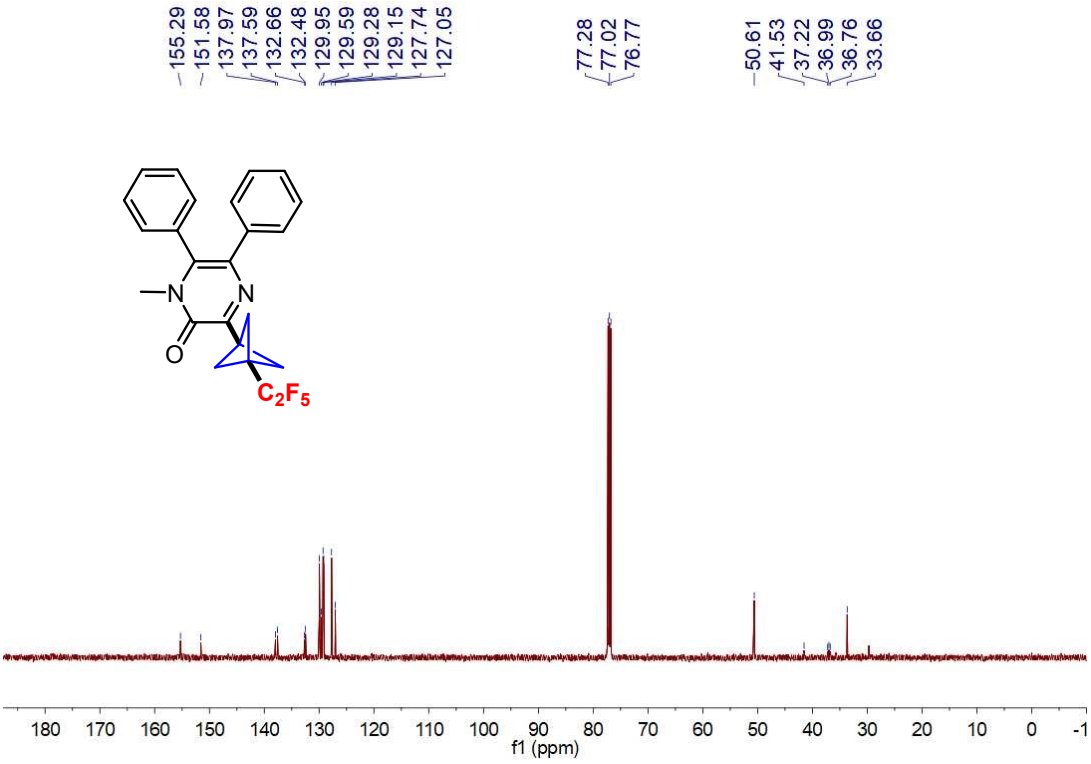
14 ^{19}F NMR (471 MHz, $CDCl_3$)



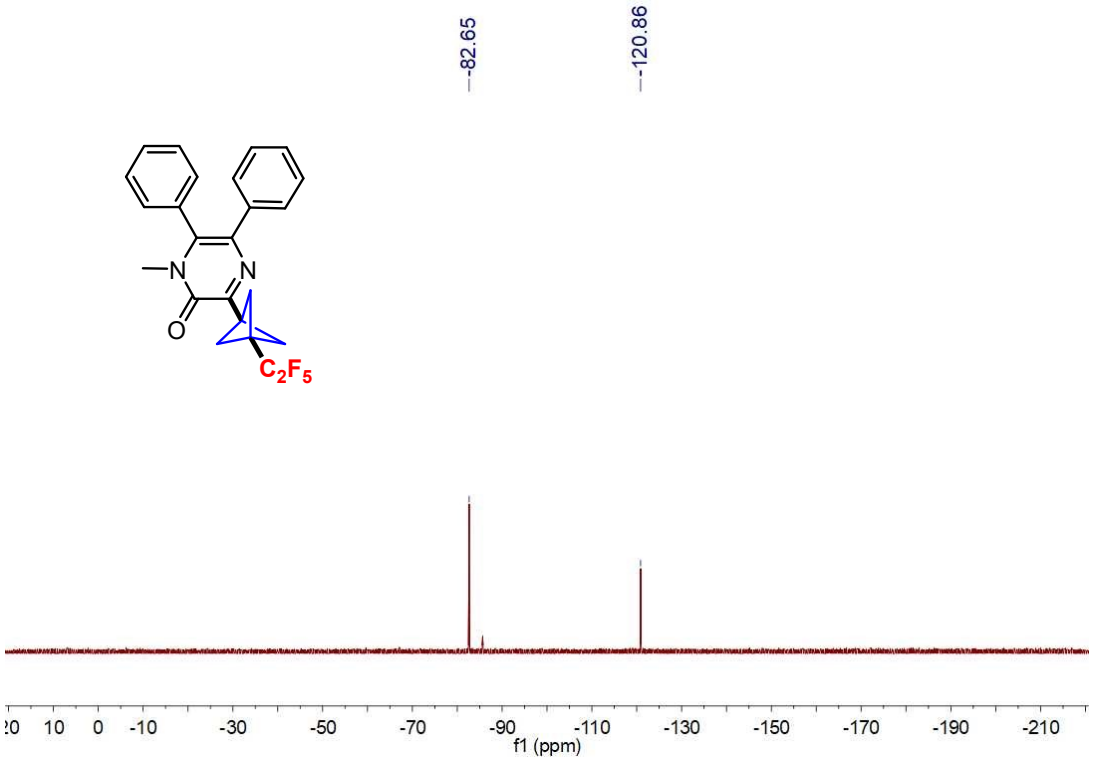
15 ^{1}H NMR (500 MHz, $CDCl_3$)



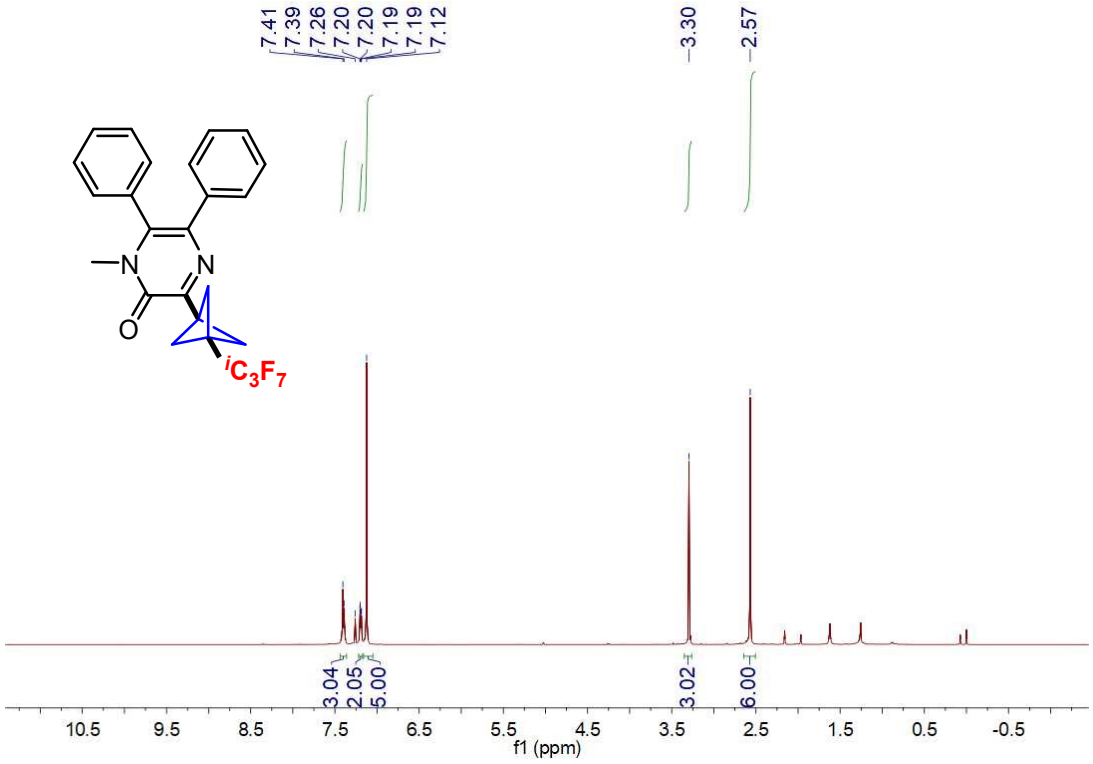
15 ^{13}C NMR (126 MHz, $CDCl_3$)



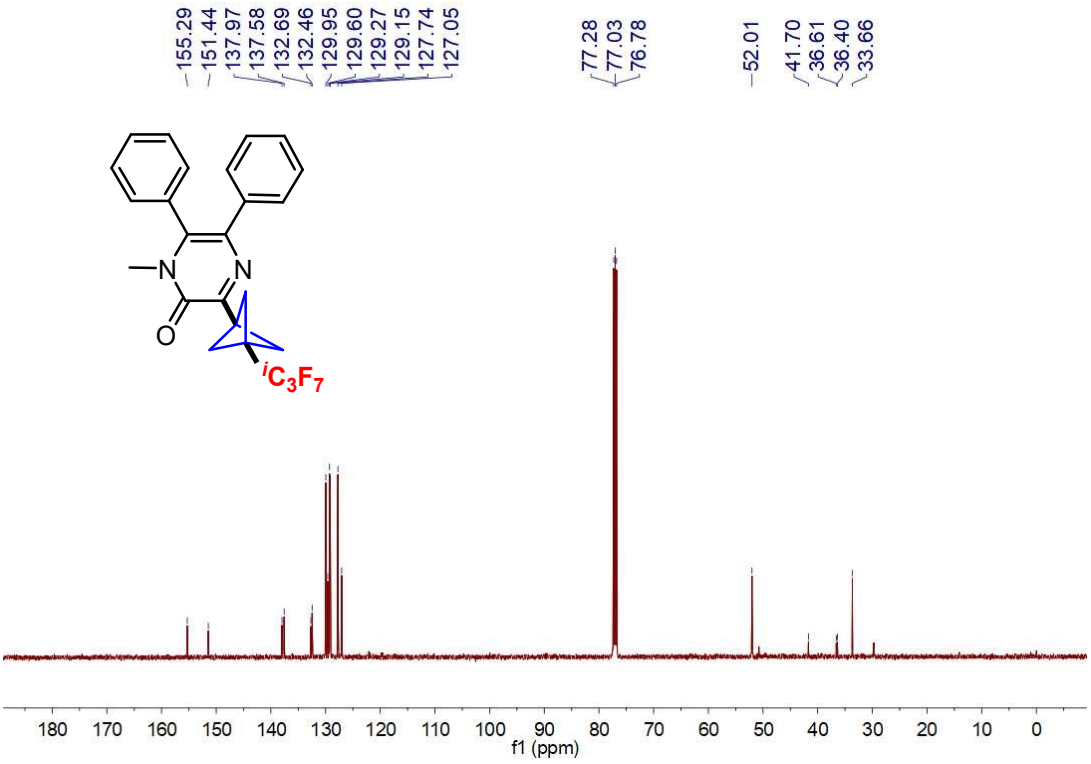
15 ^{19}F NMR (471 MHz, $CDCl_3$)



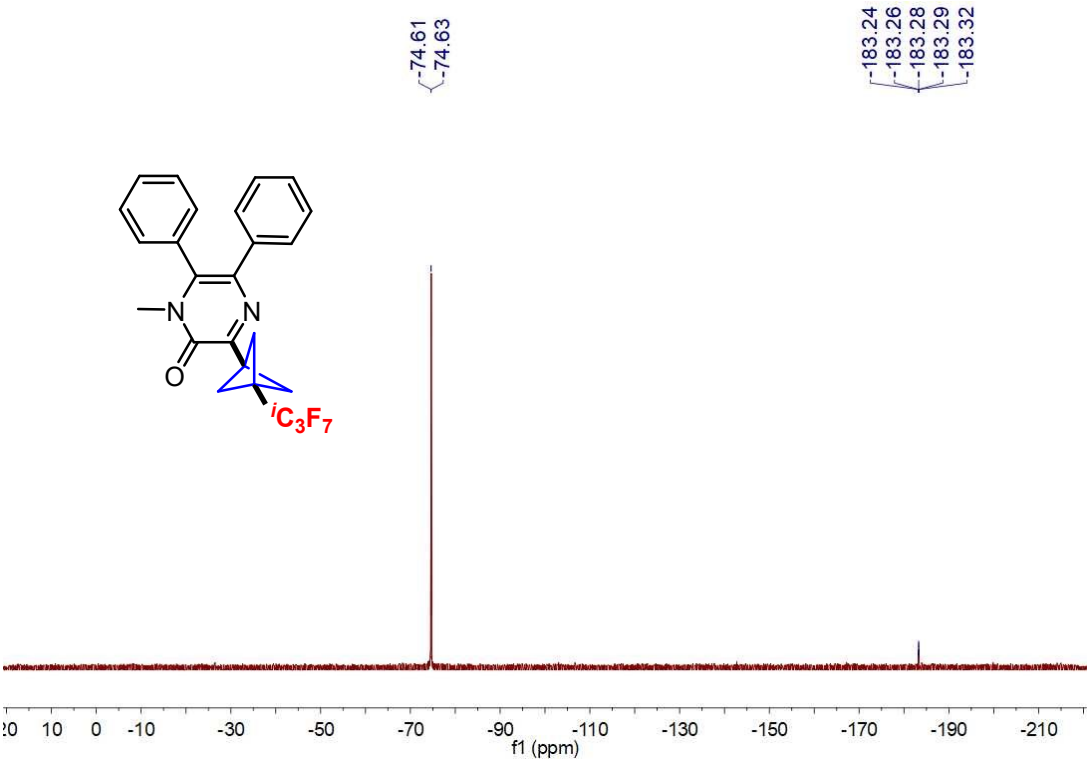
16 ^{1}H NMR (500 MHz, $CDCl_3$)



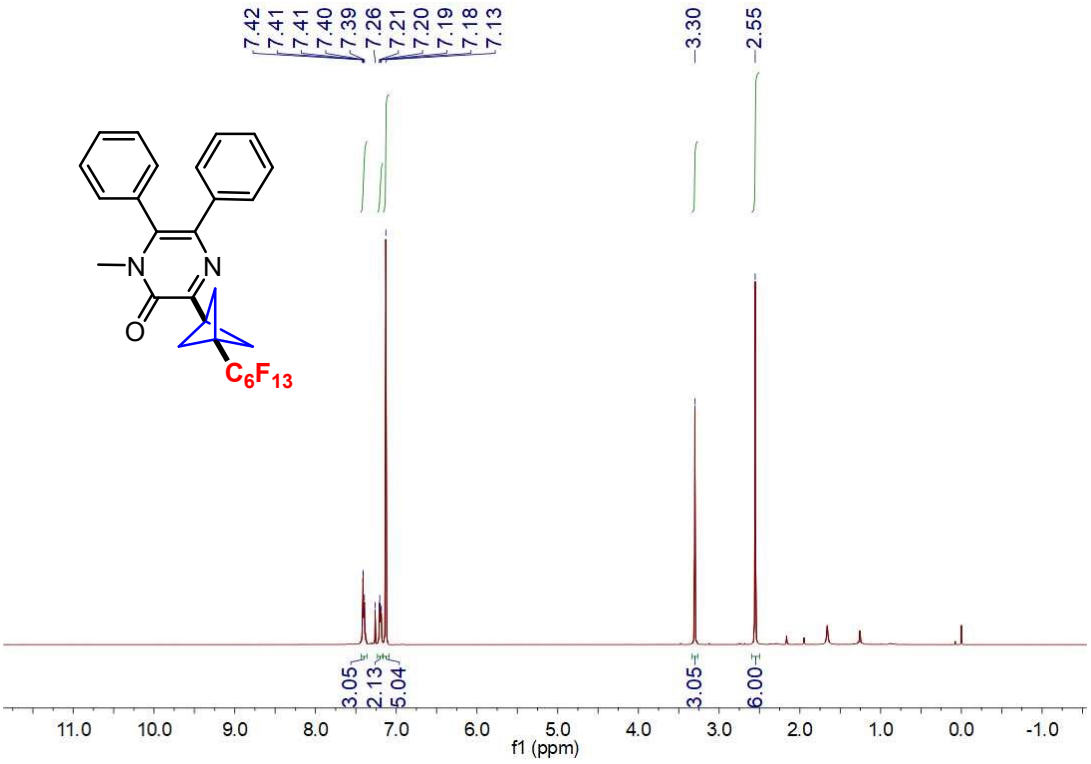
16 ^{13}C NMR (126 MHz, $CDCl_3$)



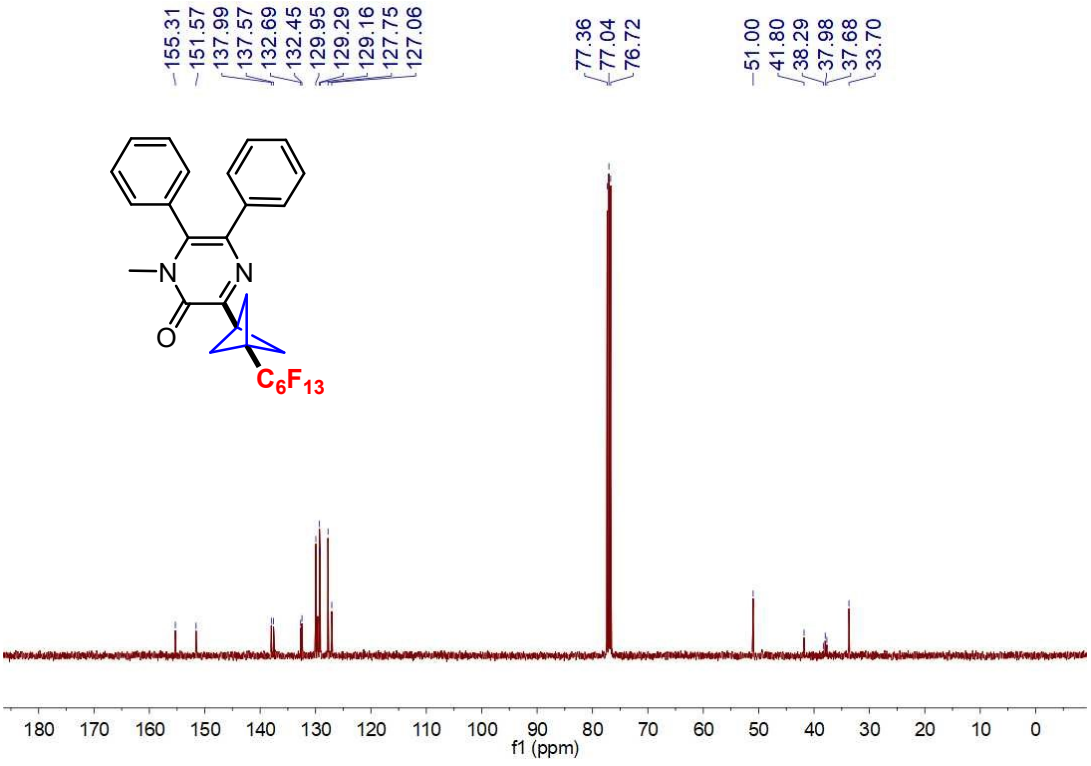
16 ^{19}F NMR (471 MHz, $CDCl_3$)



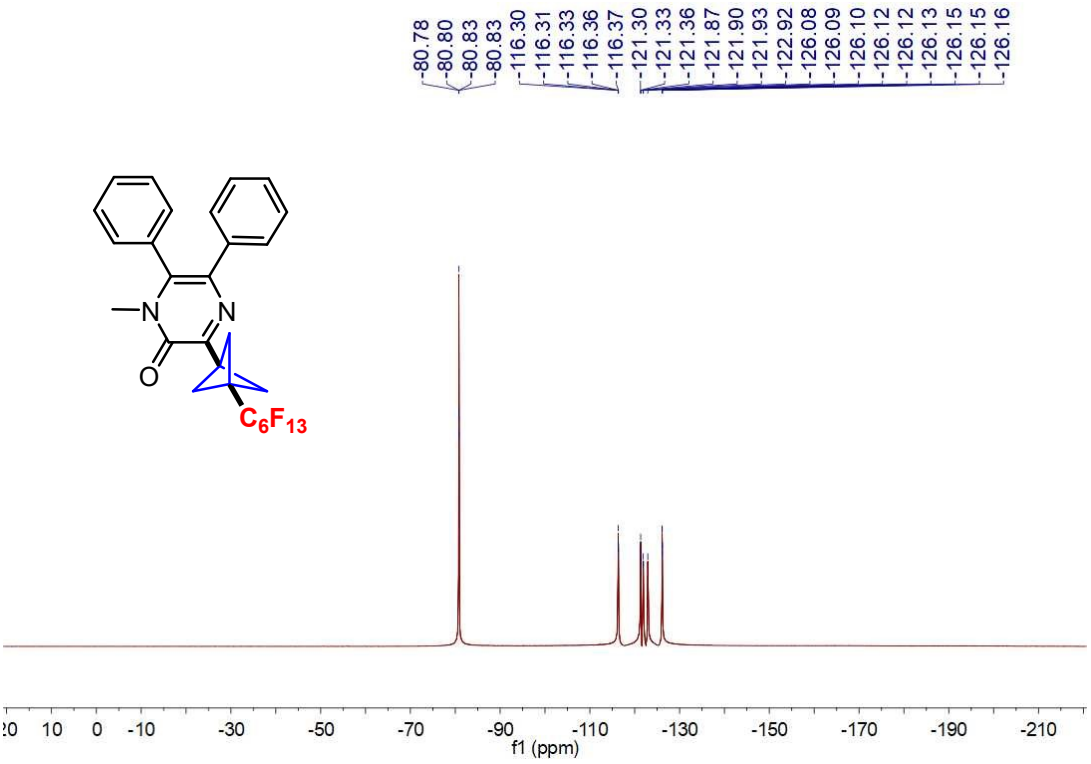
17 ^{1}H NMR (500 MHz, $CDCl_3$)



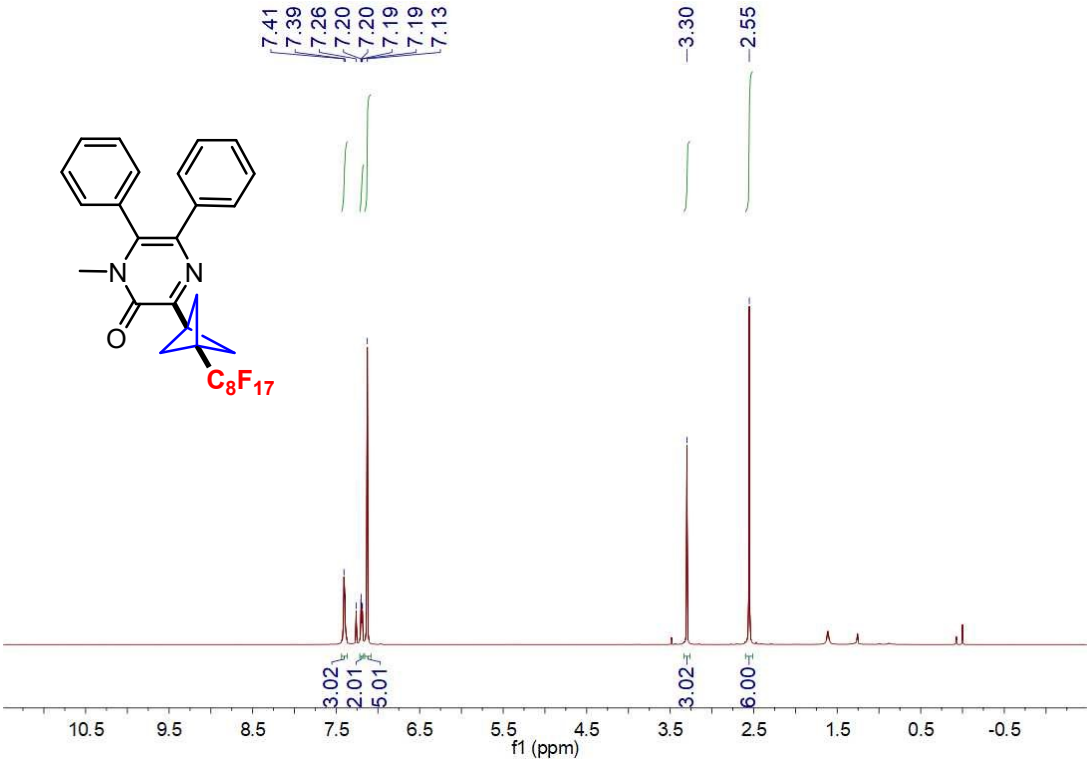
17 ^{13}C NMR (126 MHz, $CDCl_3$)



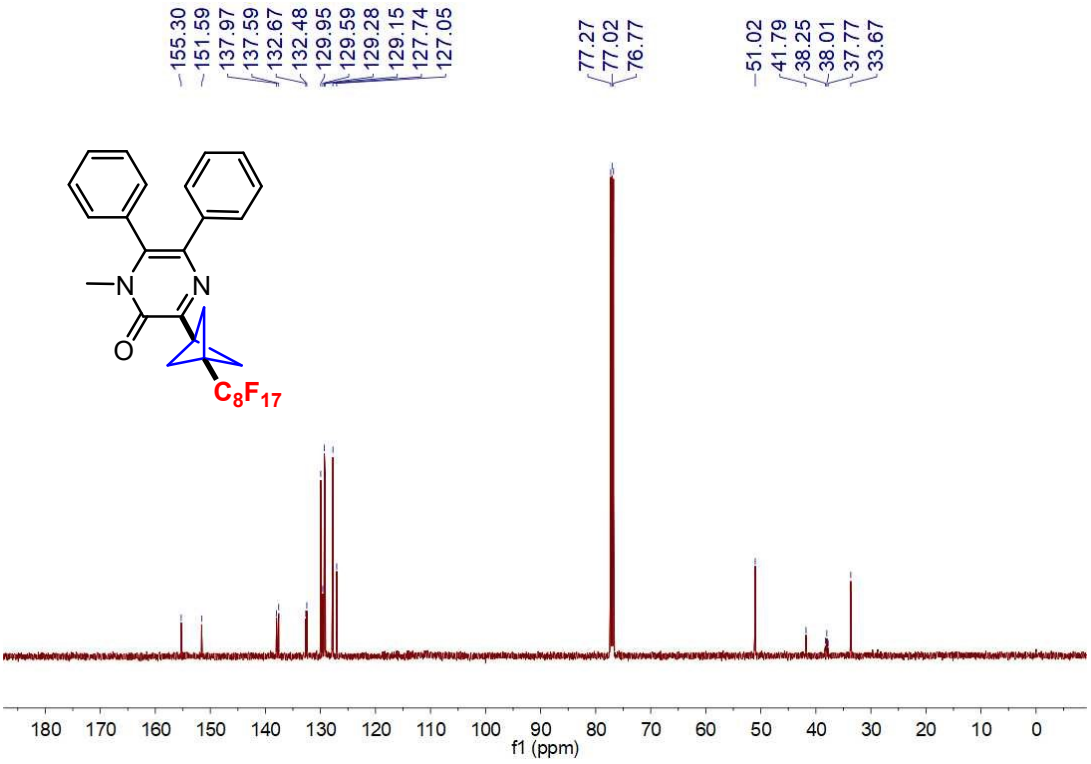
17 ^{19}F NMR (471 MHz, $CDCl_3$)



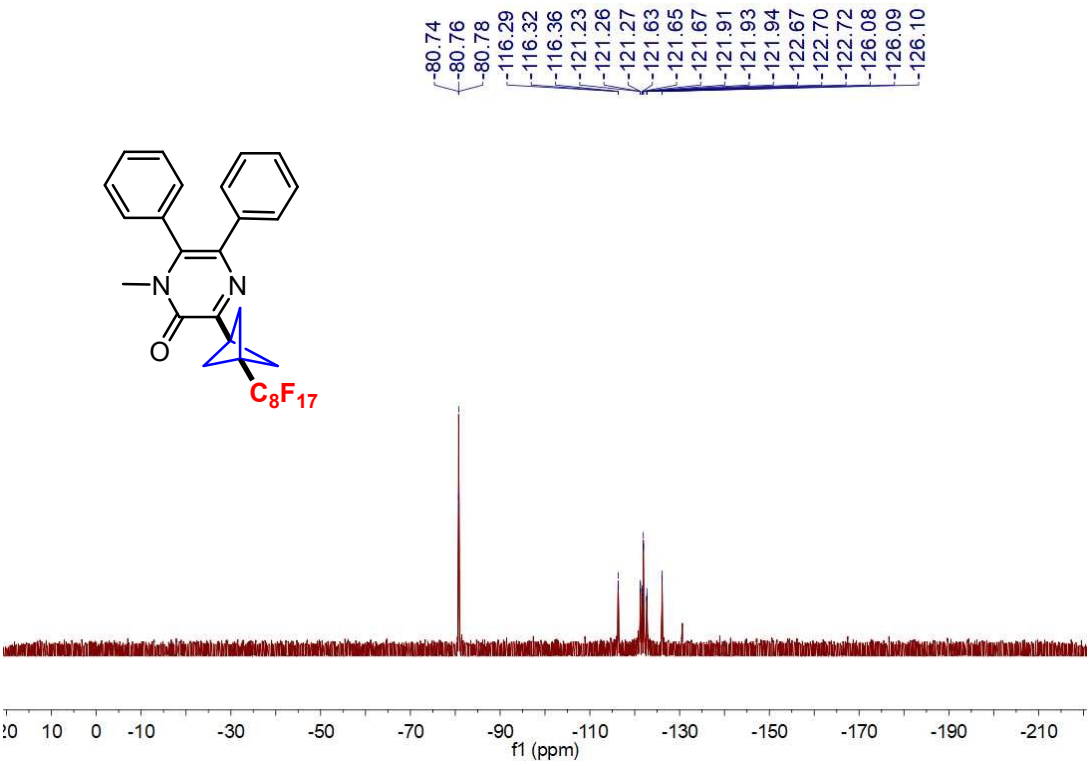
18 ^{1}H NMR (500 MHz, $CDCl_3$)



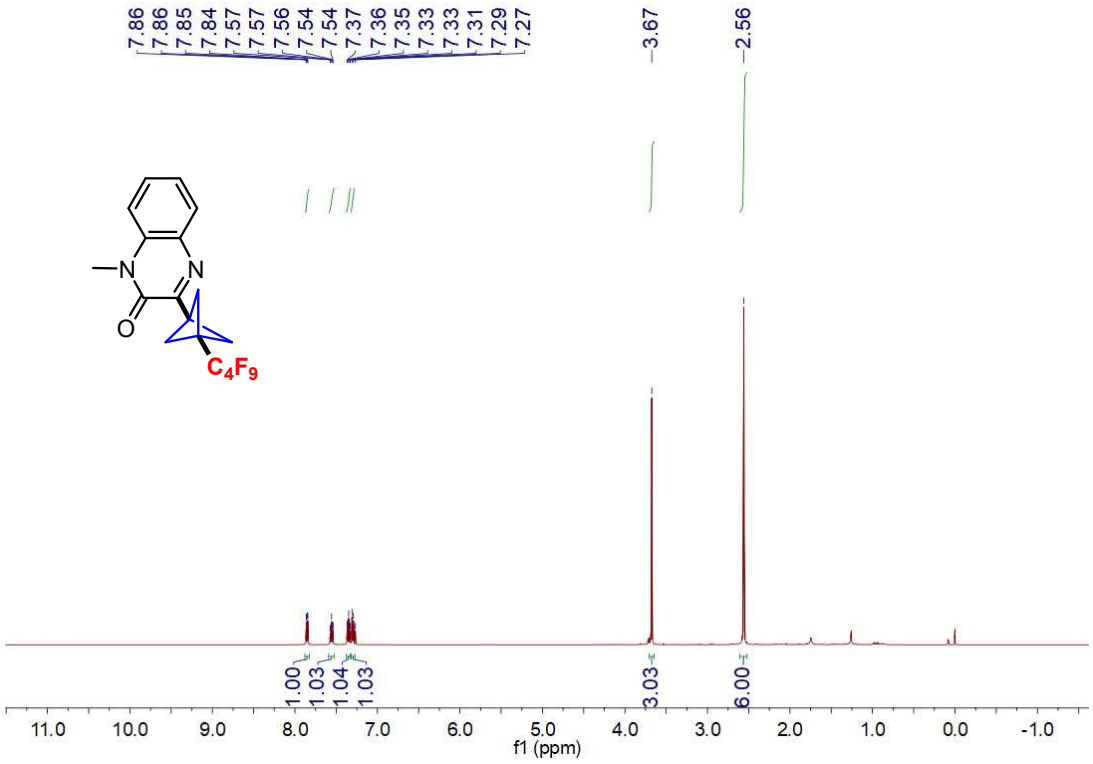
18 ^{13}C NMR (126 MHz, $CDCl_3$)



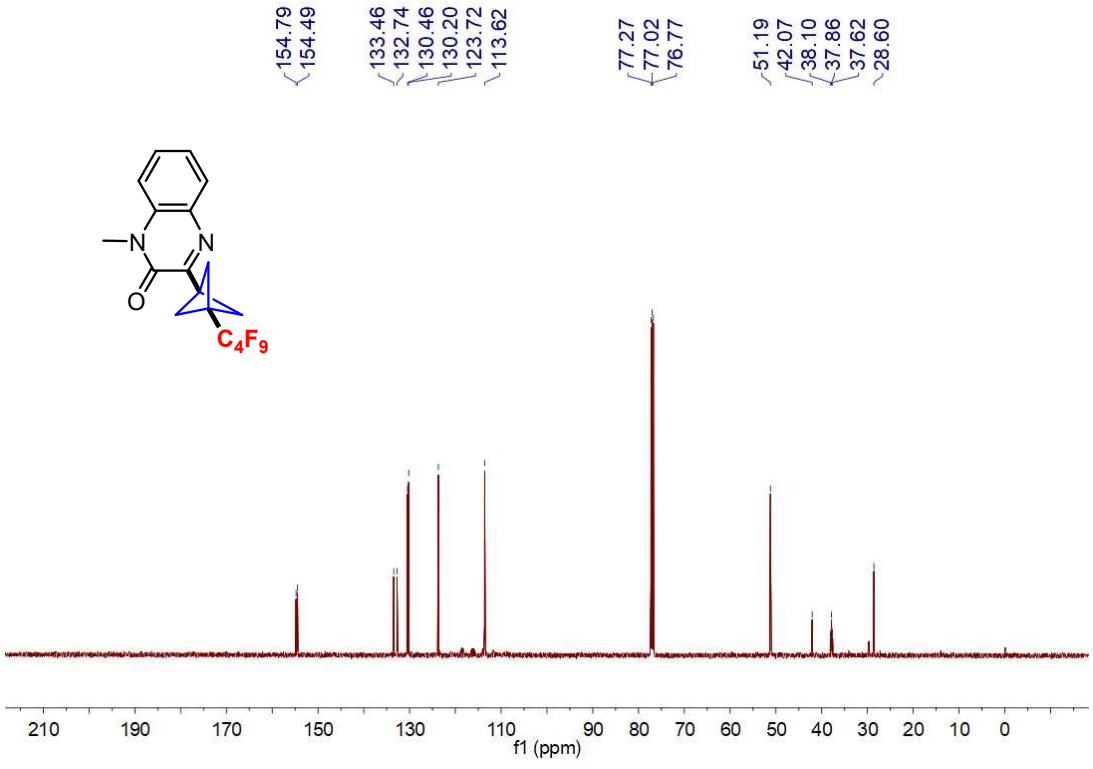
18 ^{19}F NMR (471 MHz, $CDCl_3$)



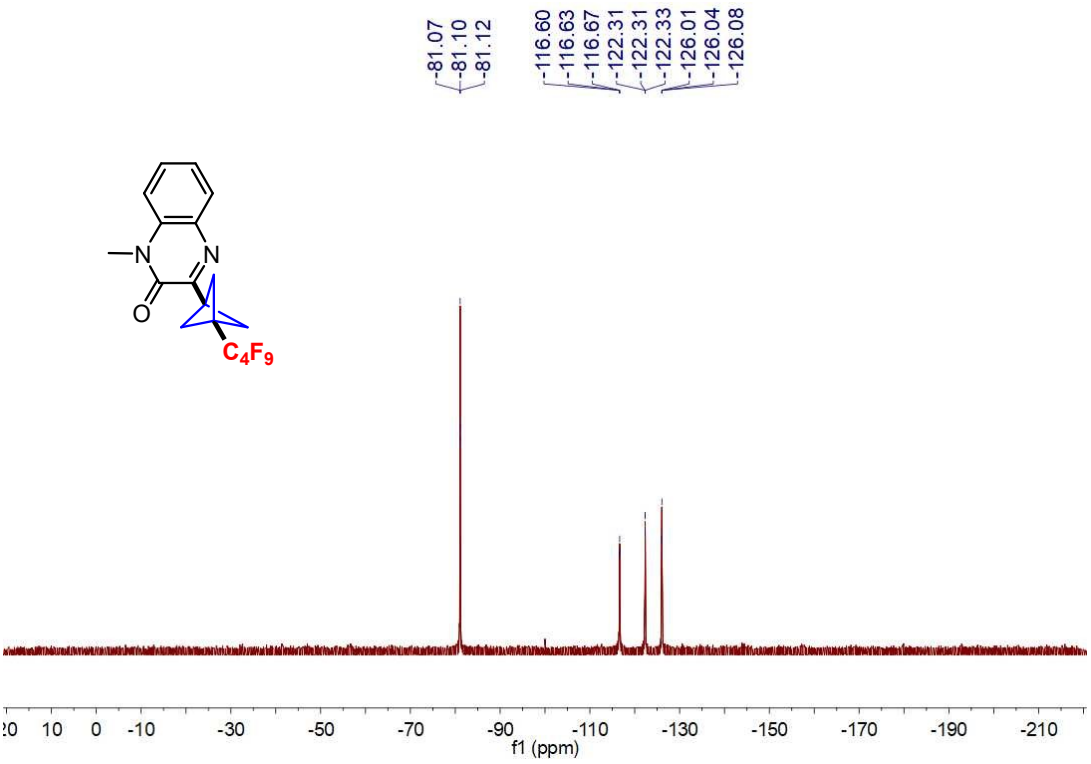
20 ^{1}H NMR (500 MHz, $CDCl_3$)



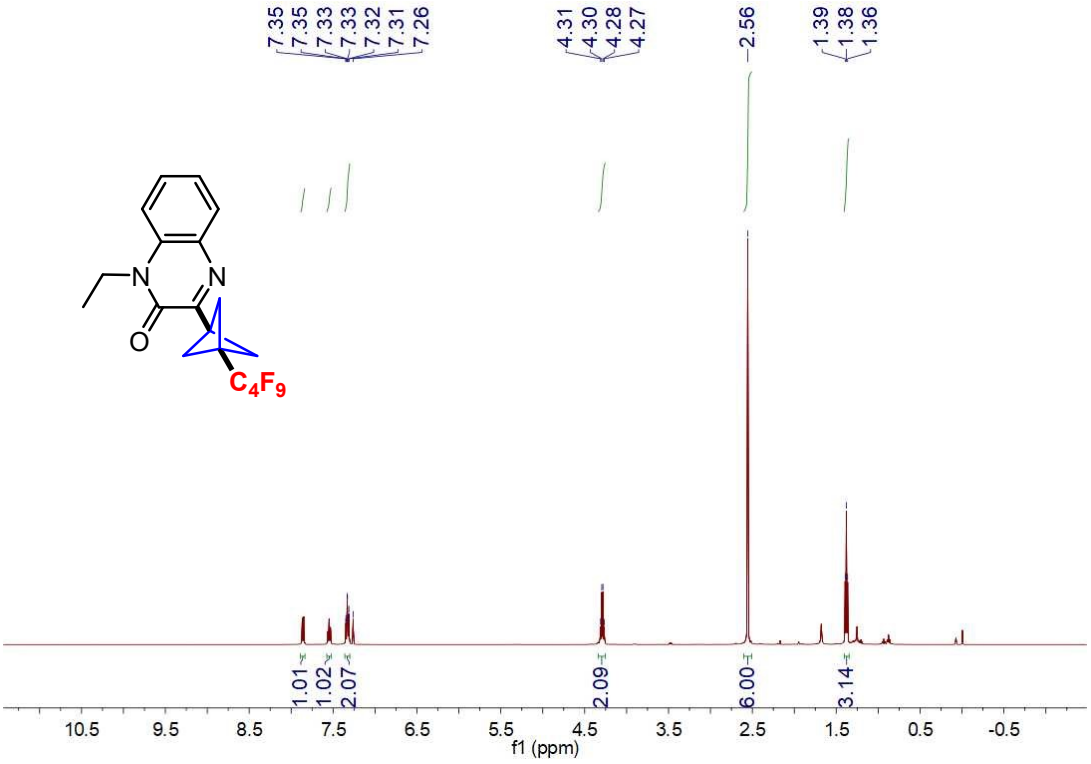
20 ^{13}C NMR (126 MHz, $CDCl_3$)



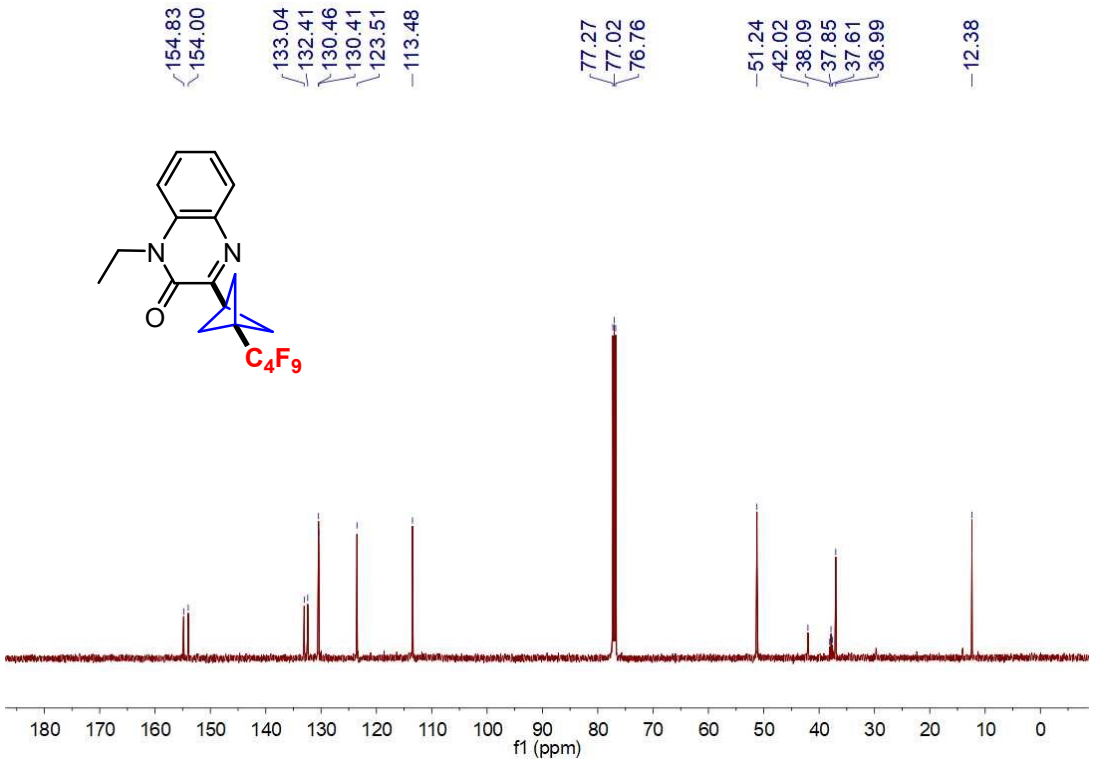
20 ^{19}F NMR (471 MHz, $CDCl_3$)



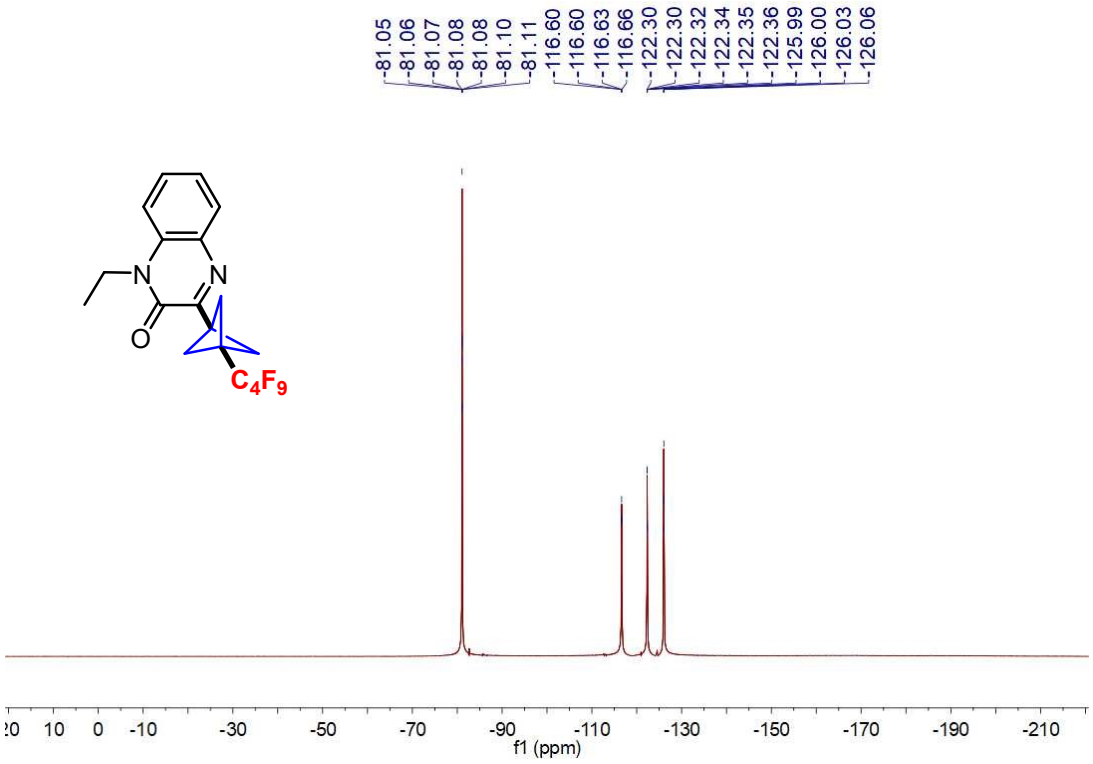
21 ^{1}H NMR (500 MHz, $CDCl_3$)



21 ^{13}C NMR (126 MHz, $CDCl_3$)



21 ^{19}F NMR (471 MHz, $CDCl_3$)



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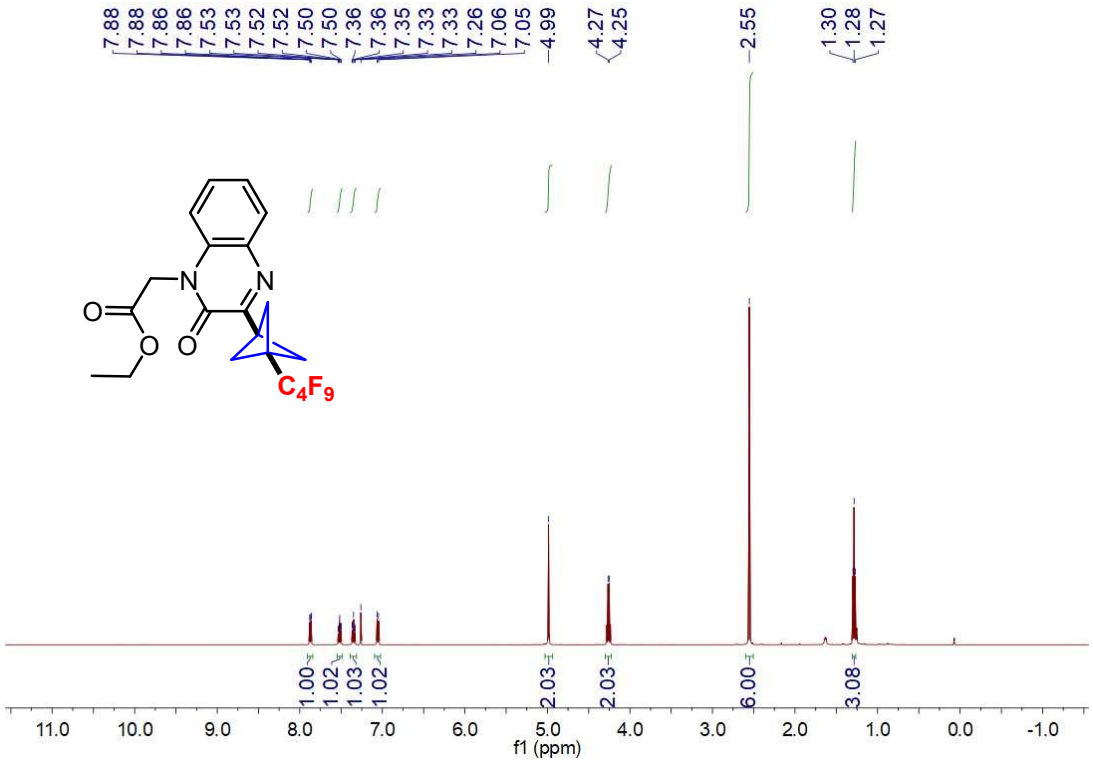
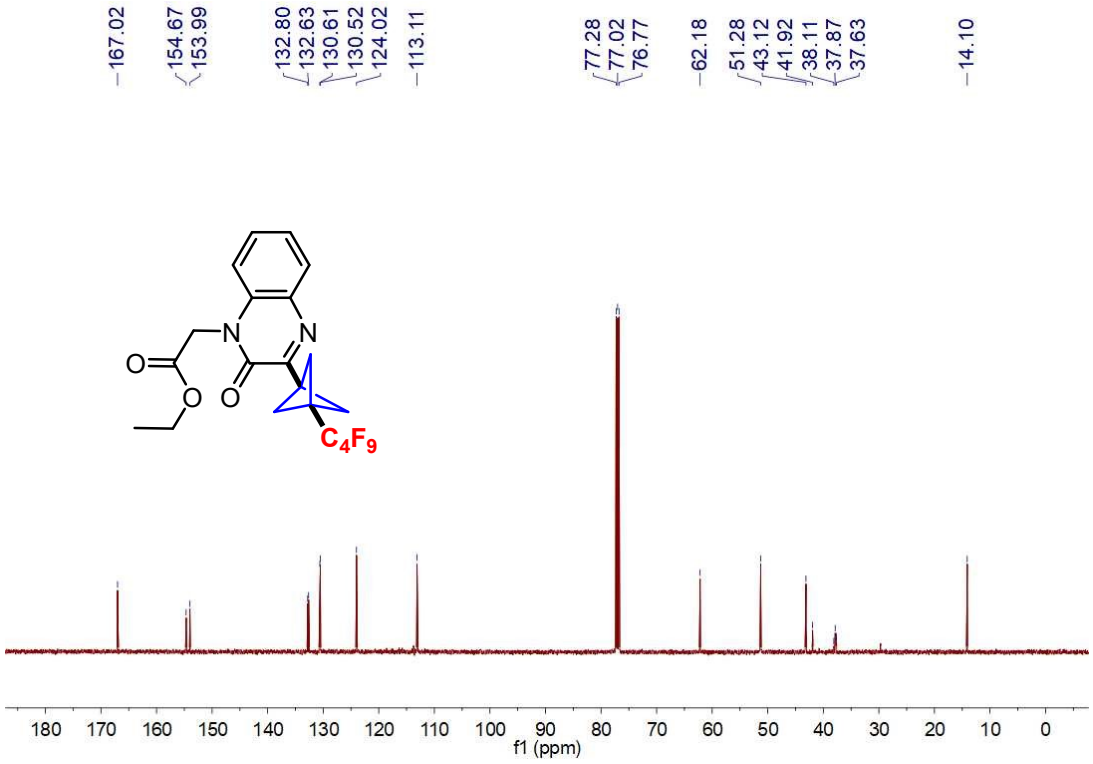
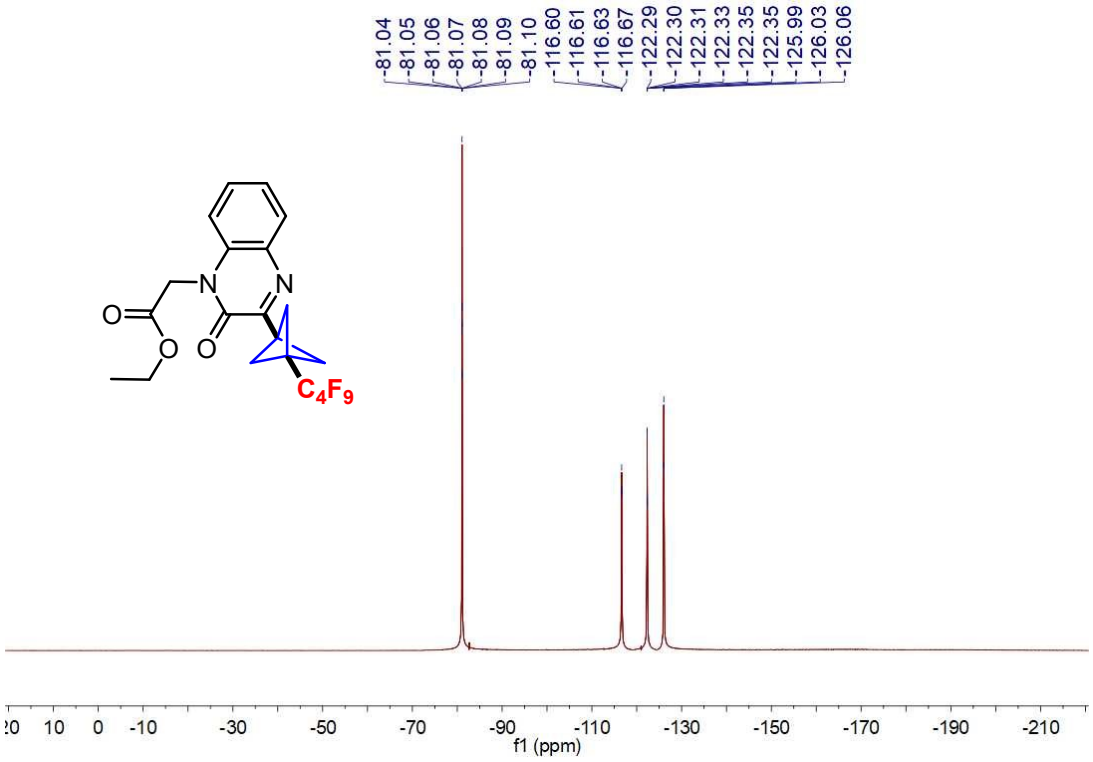


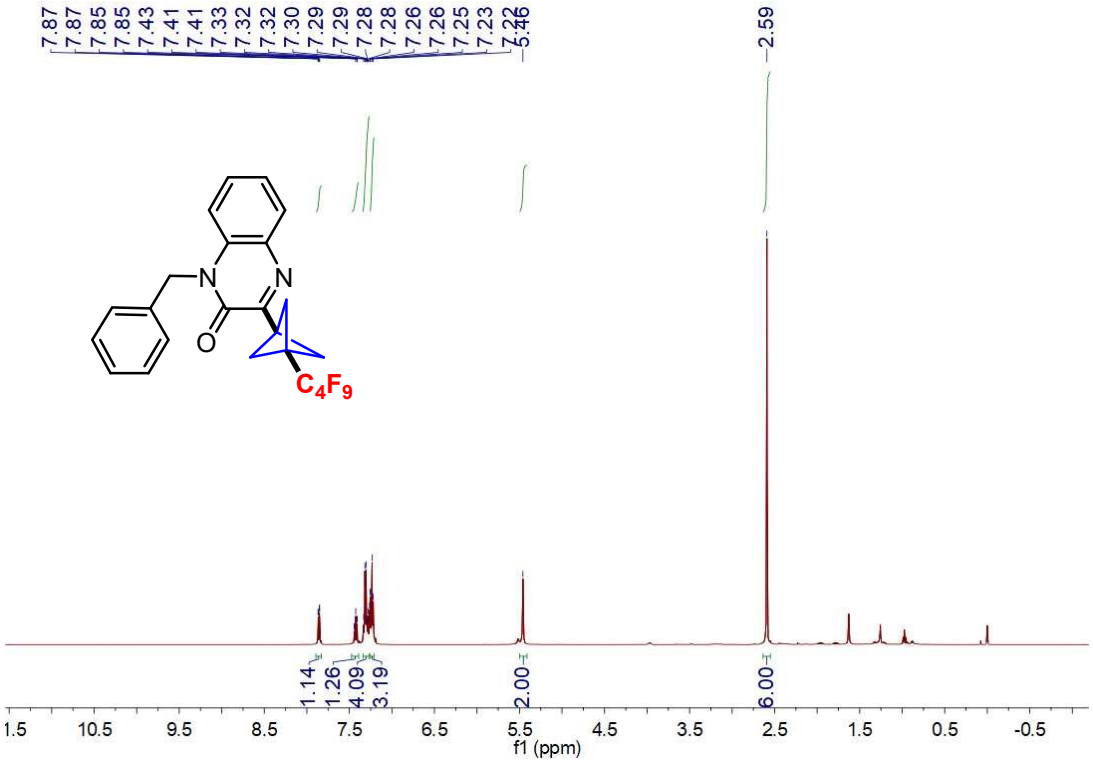
22 ^{13}C NMR (126 MHz, $CDCl_3$)



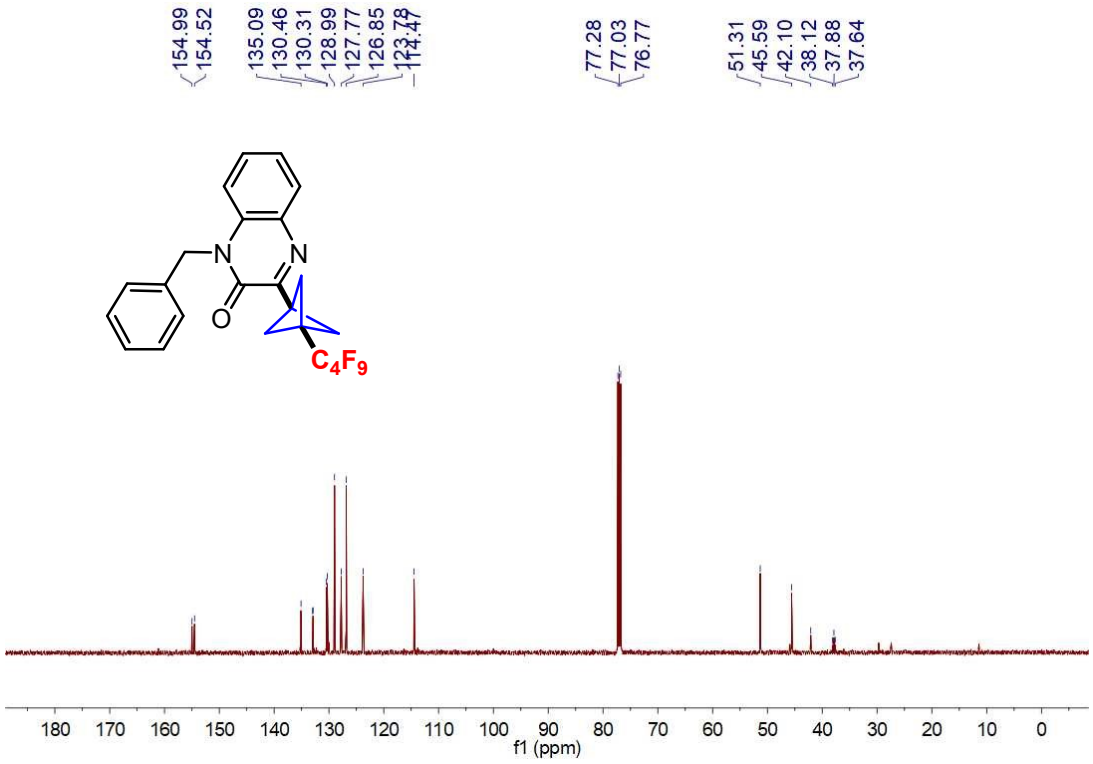
22 ^{19}F NMR (471 MHz, $CDCl_3$)



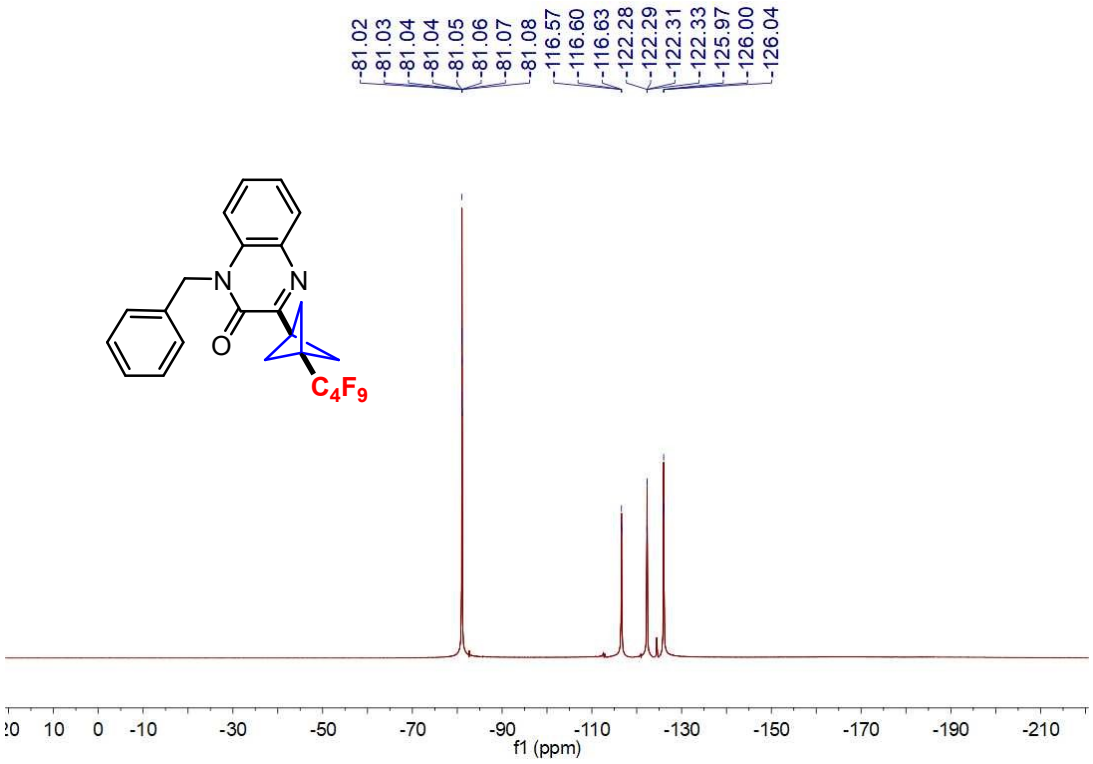
23 ^{1}H NMR (500 MHz, $CDCl_3$)



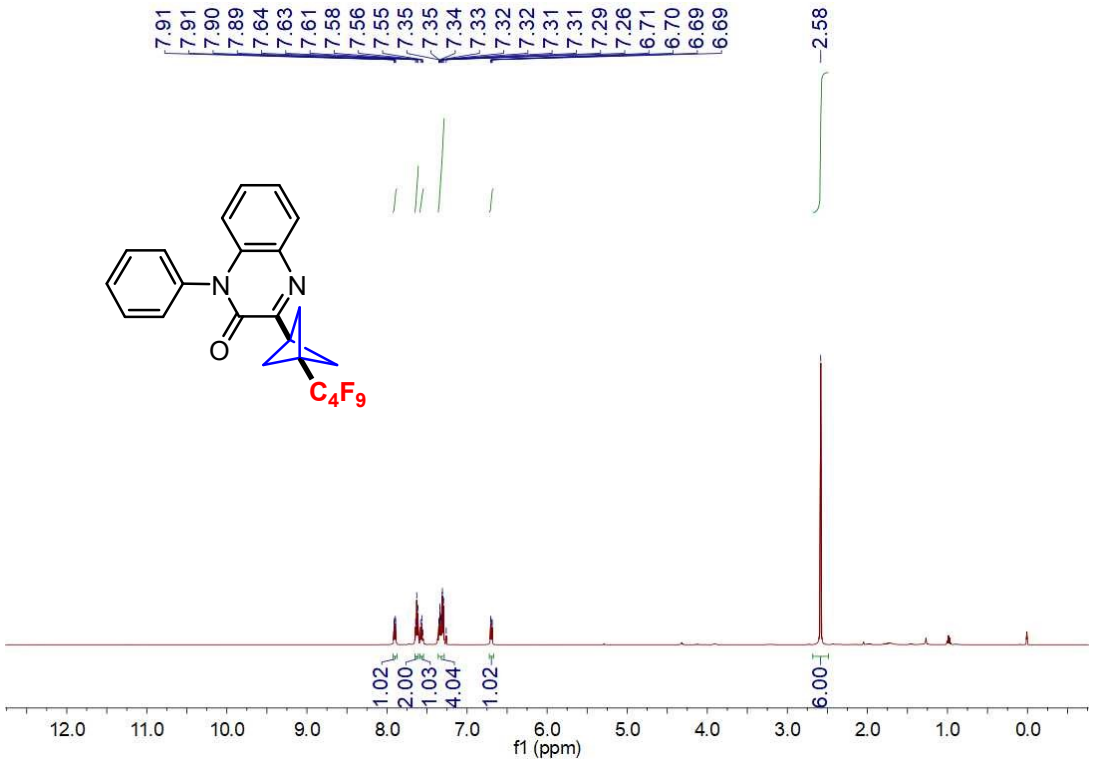
23 ^{13}C NMR (126 MHz, $CDCl_3$)



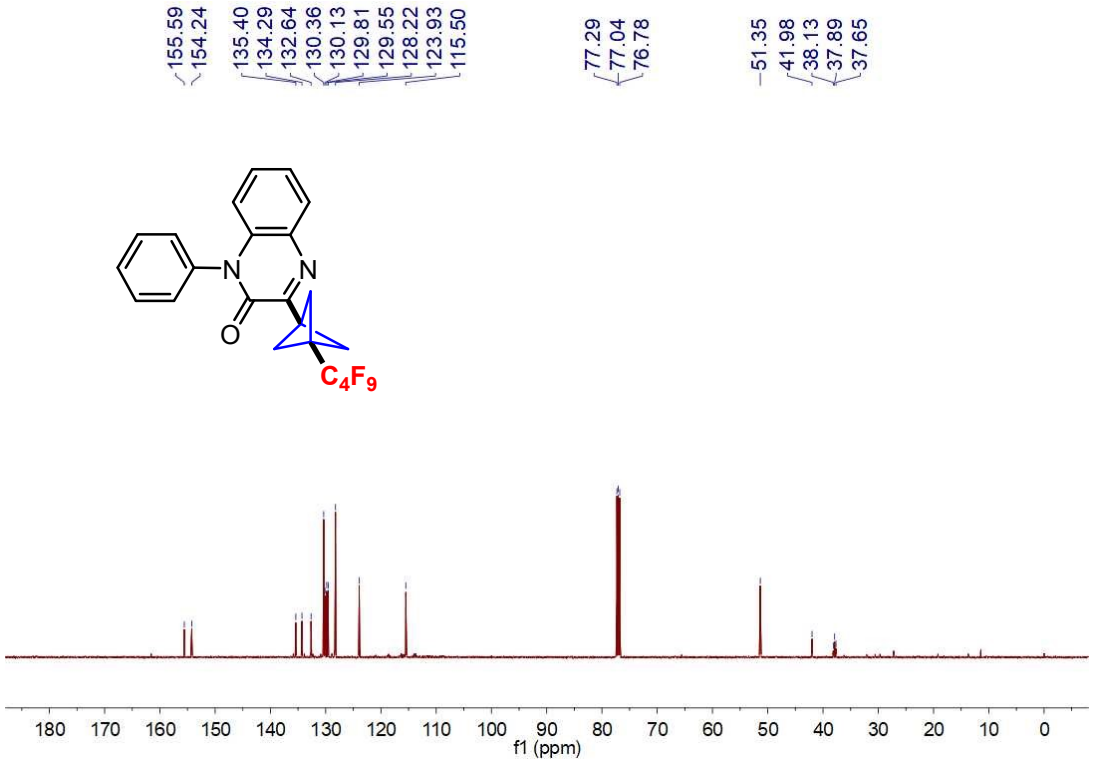
23 ^{19}F NMR (471 MHz, $CDCl_3$)



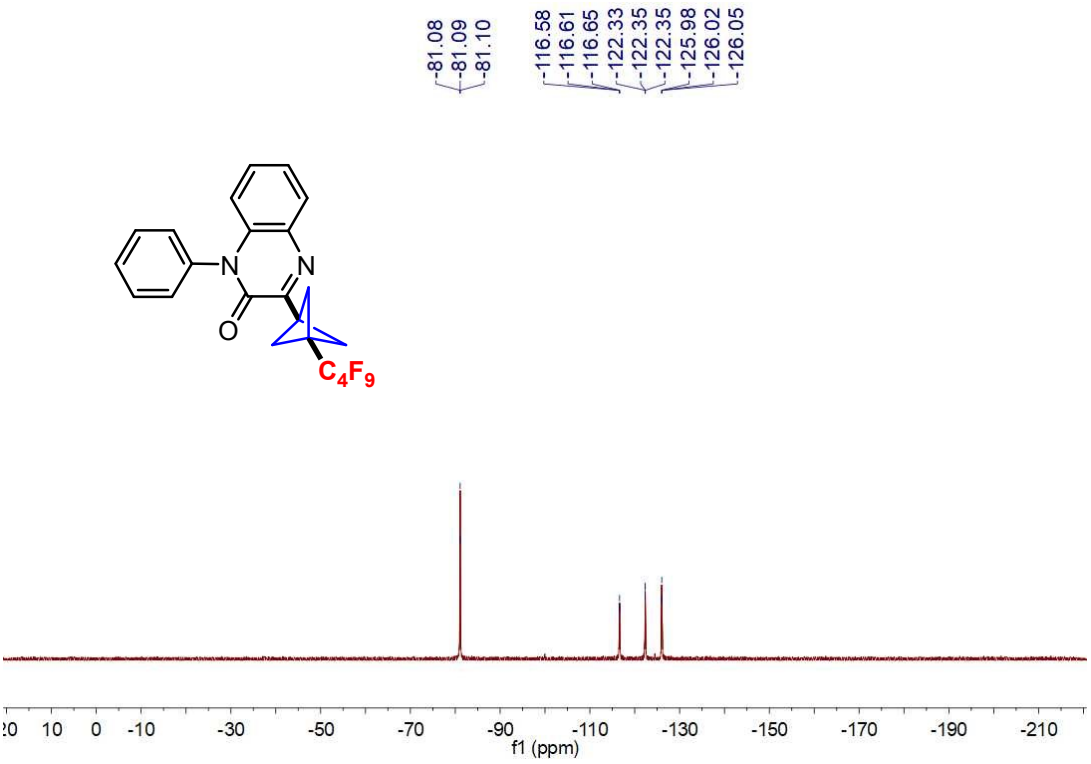
24 ^{1}H NMR (500 MHz, $CDCl_3$)



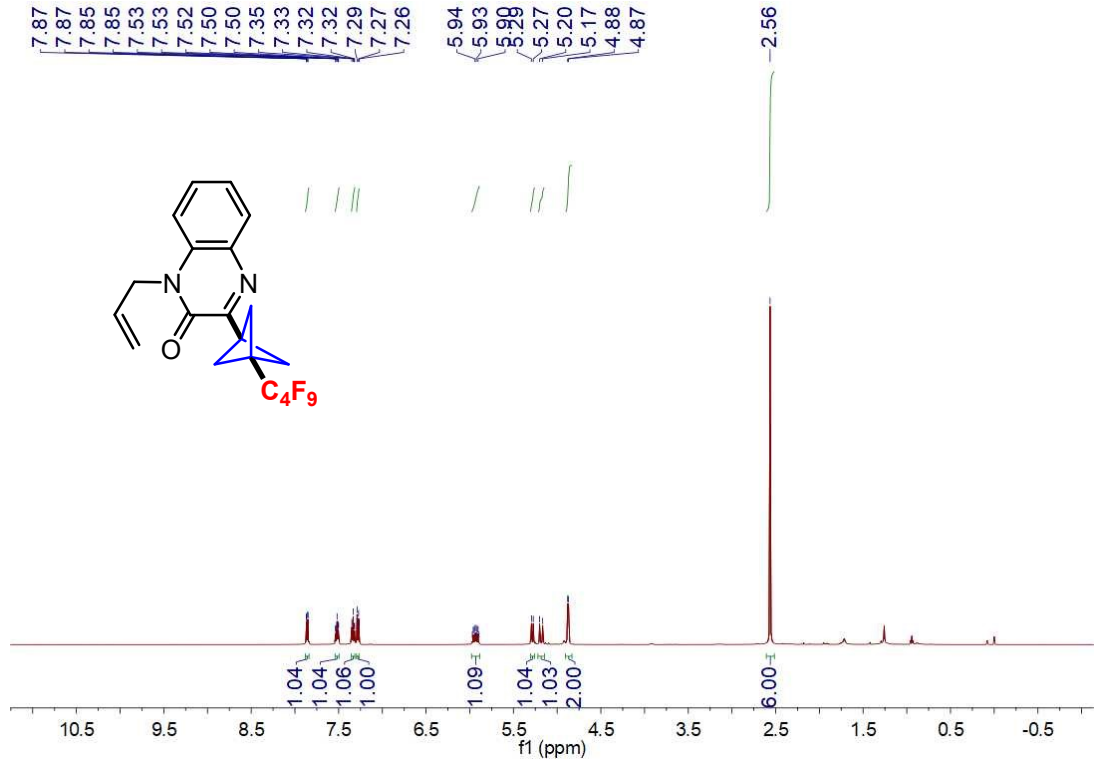
24 ^{13}C NMR (126 MHz, $CDCl_3$)



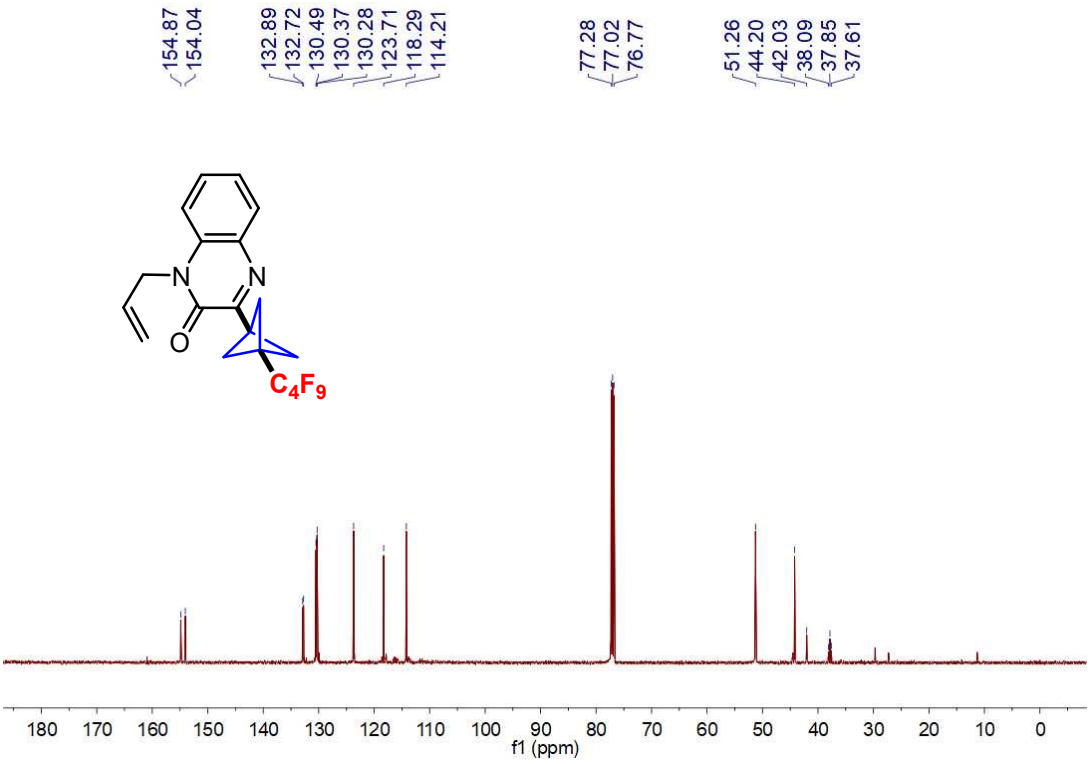
24 ^{19}F NMR (471 MHz, $CDCl_3$)



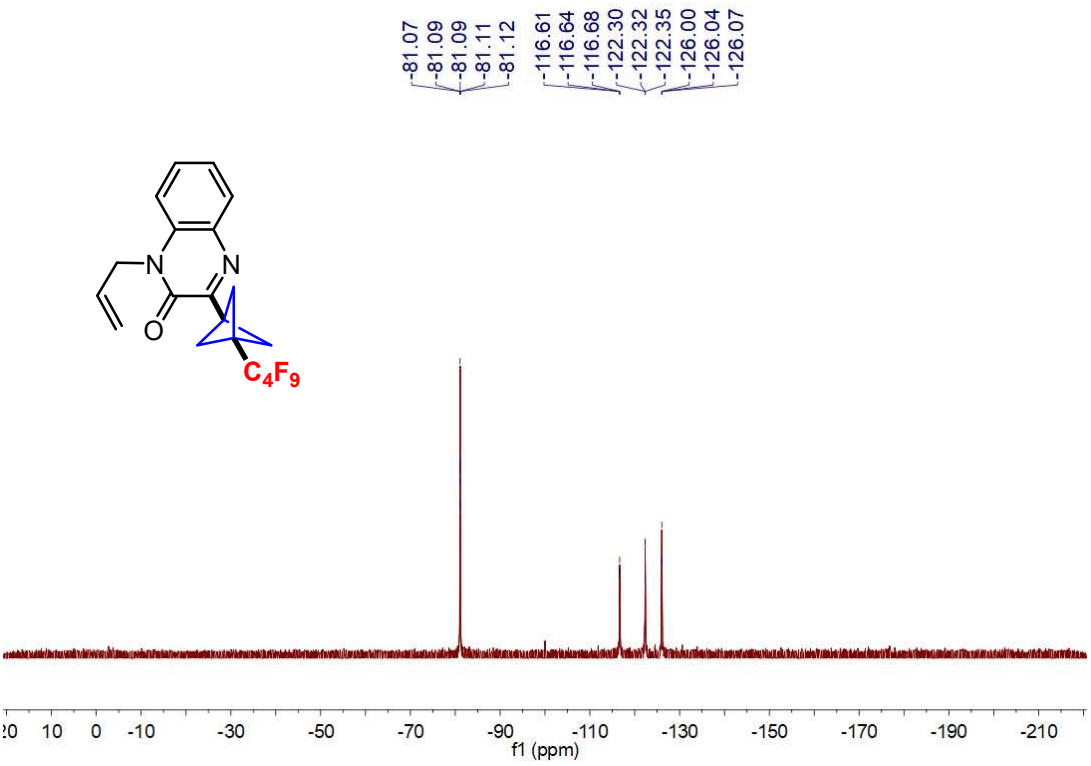
25 ^{1}H NMR (500 MHz, $CDCl_3$)



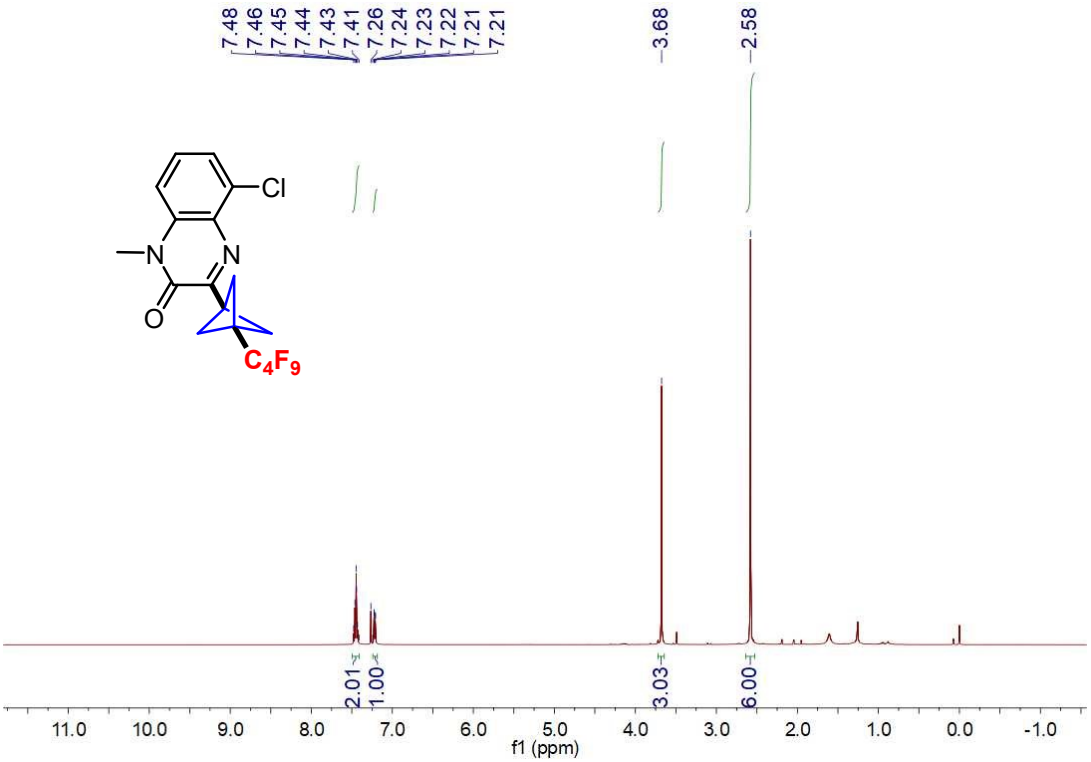
25 ^{13}C NMR (126 MHz, $CDCl_3$)



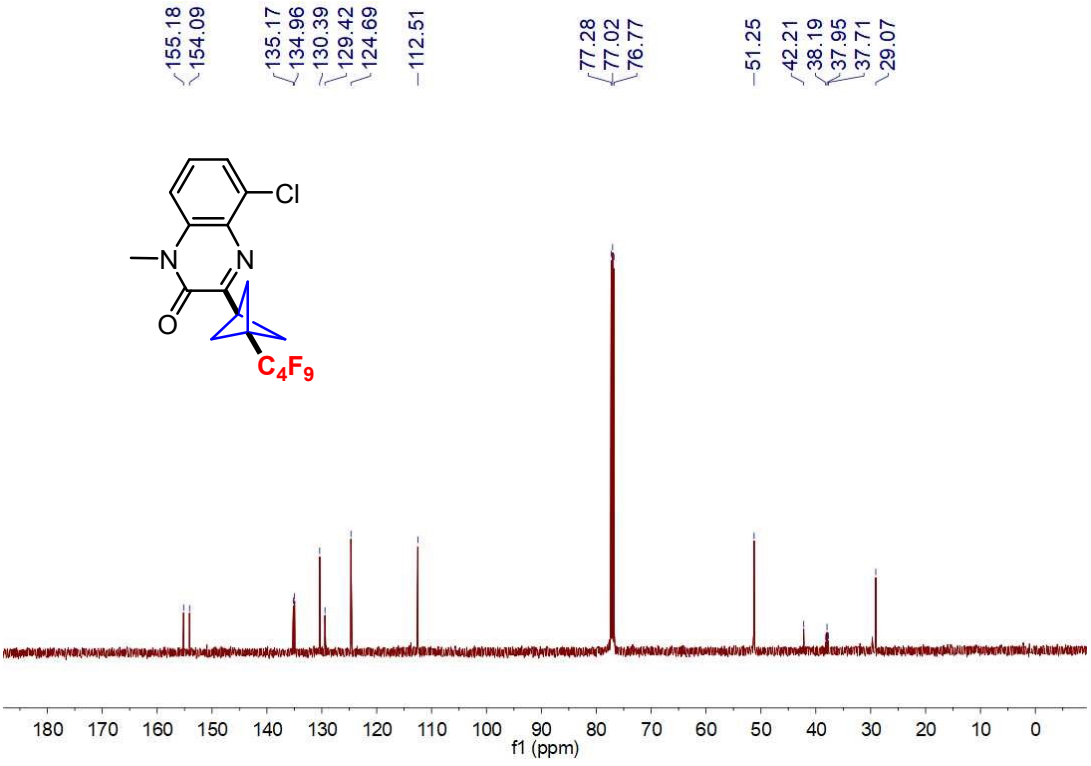
25 ^{19}F NMR (471 MHz, $CDCl_3$)



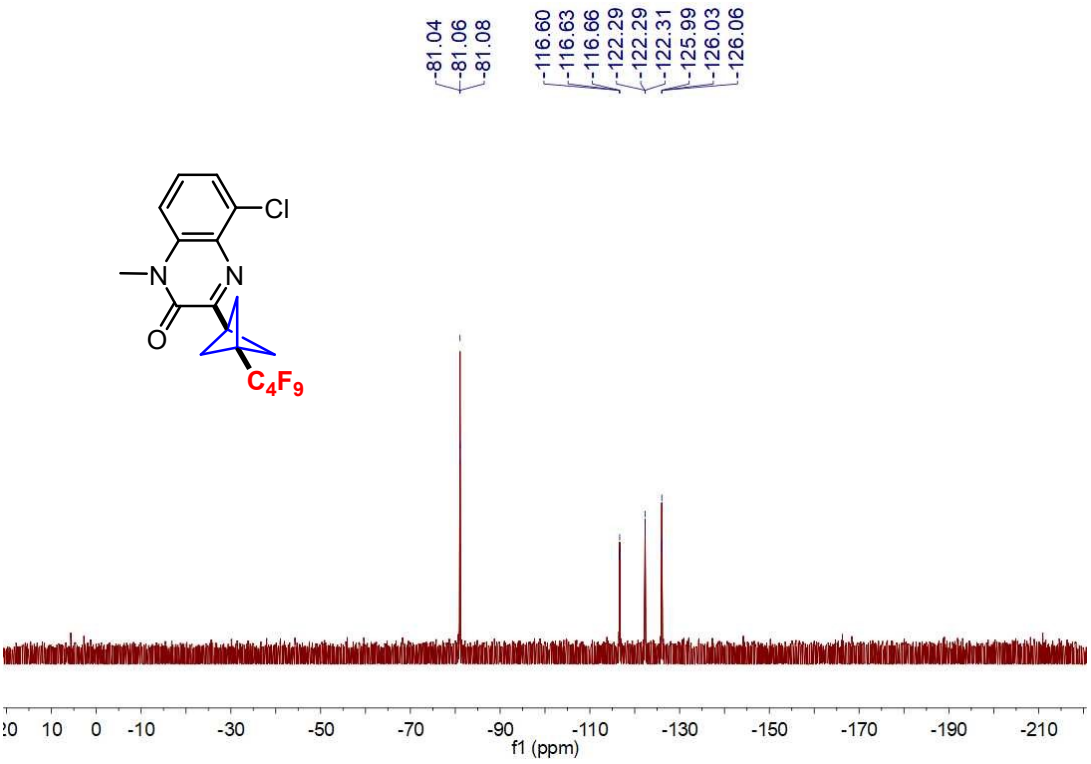
26 ^{1}H NMR (500 MHz, $CDCl_3$)



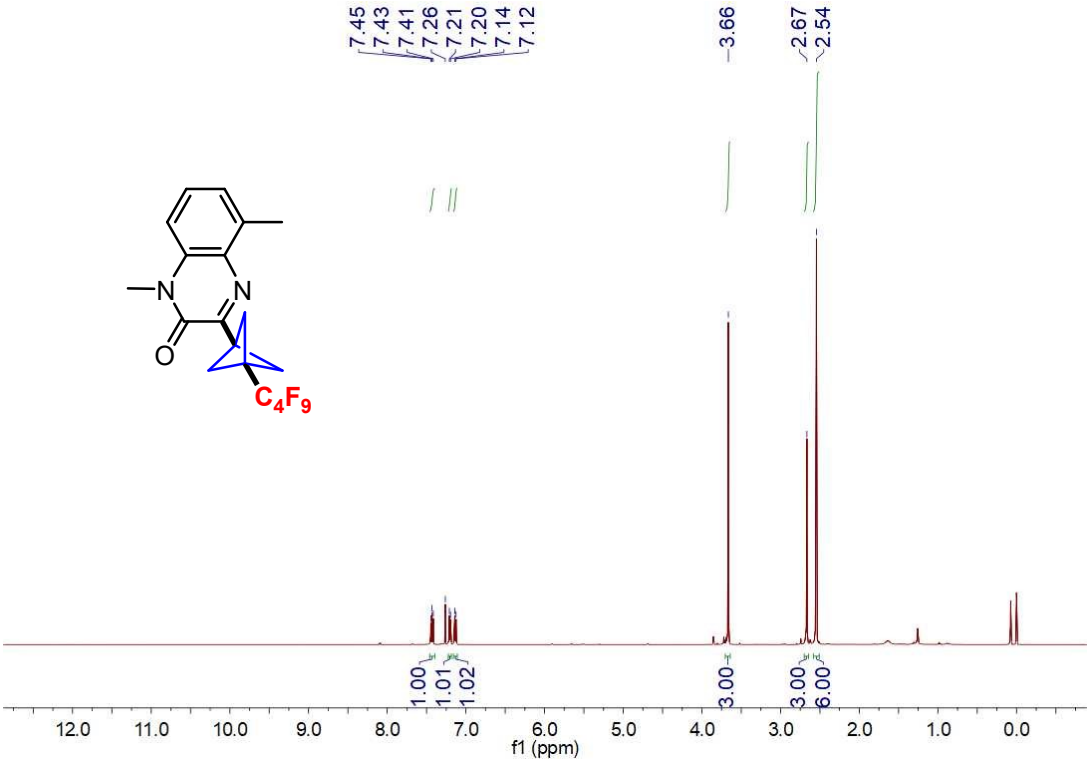
26 ^{13}C NMR (126 MHz, $CDCl_3$)



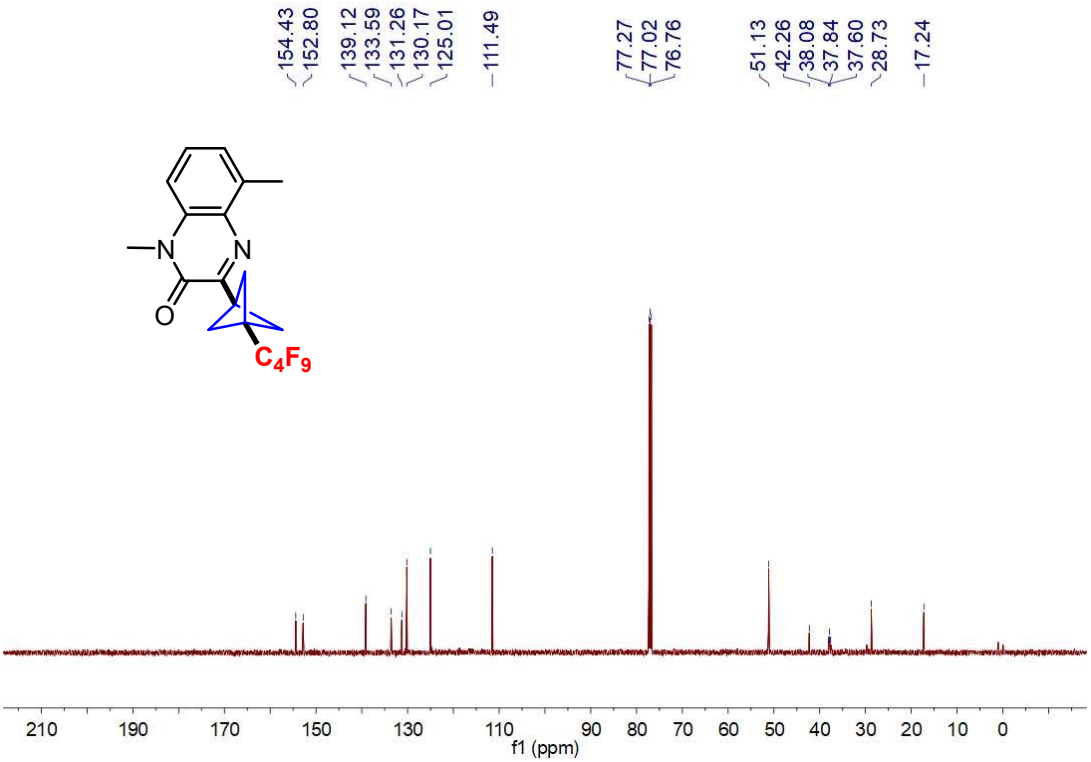
26 ^{19}F NMR (471 MHz, $CDCl_3$)



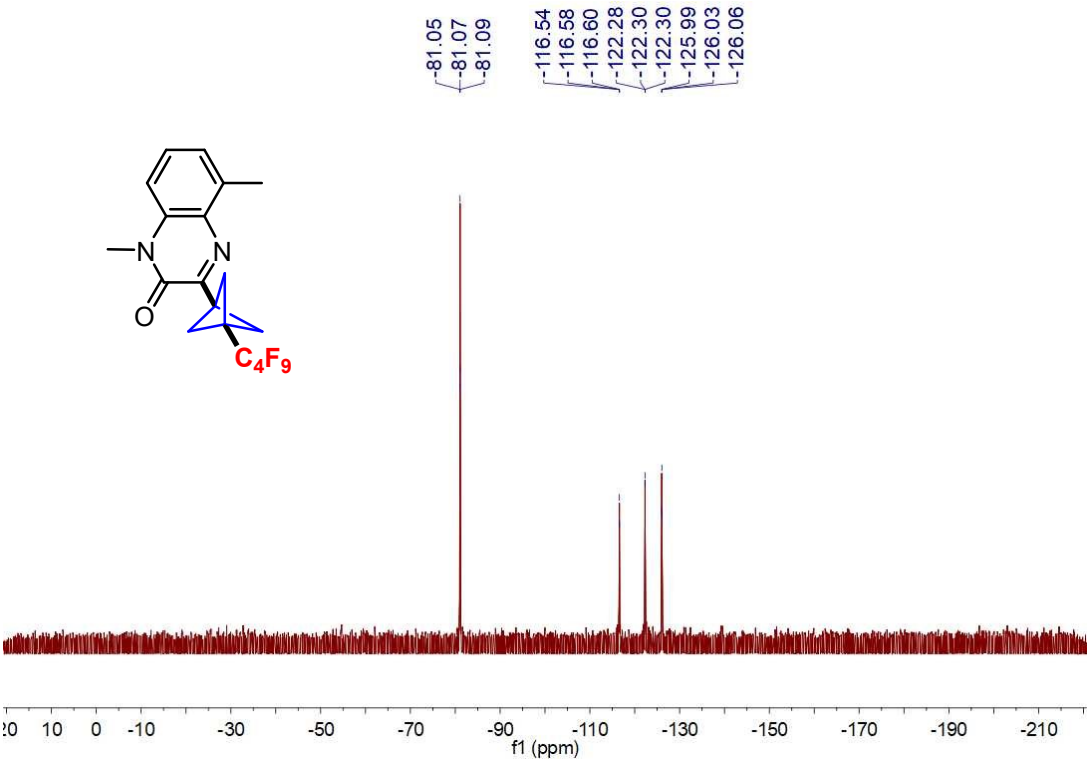
27 ^{1}H NMR (500 MHz, $CDCl_3$)



27 ^{13}C NMR (126 MHz, $CDCl_3$)



27 ^{19}F NMR (471 MHz, $CDCl_3$)



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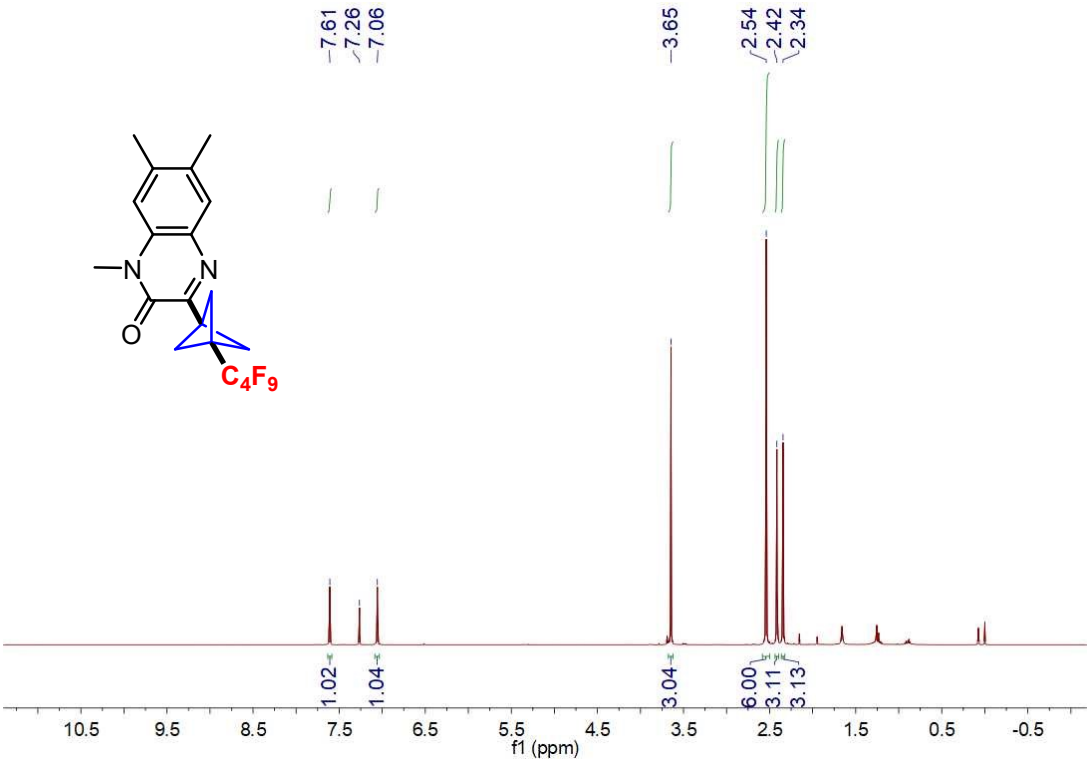
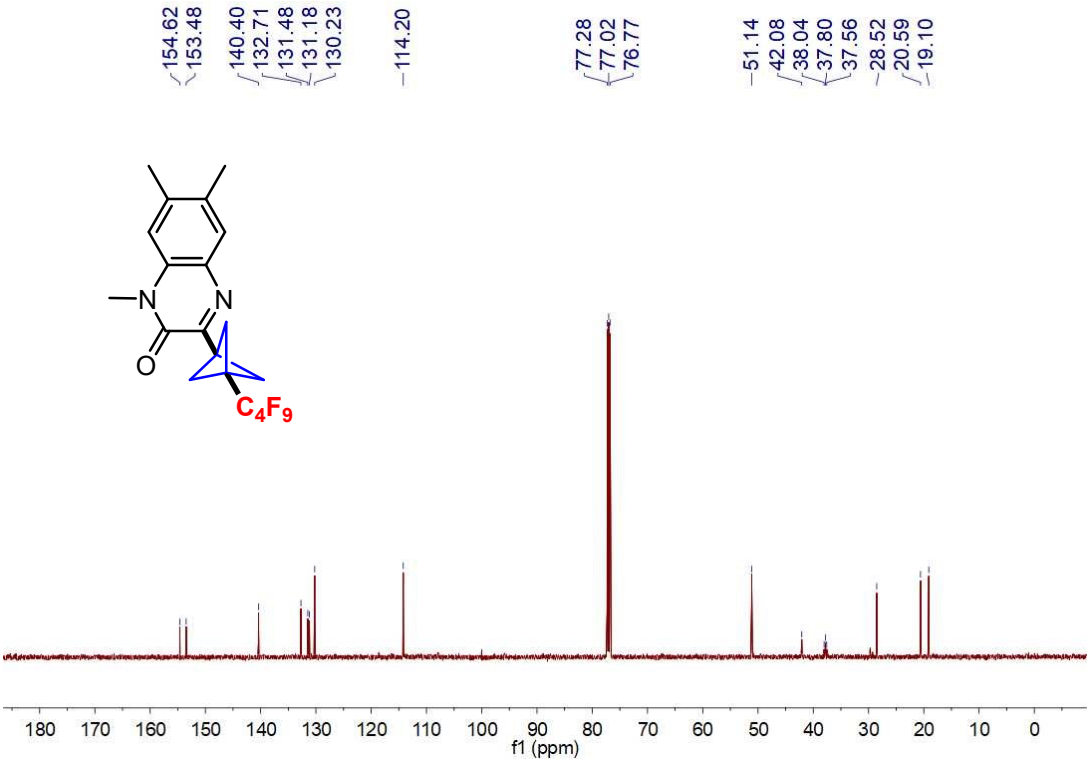
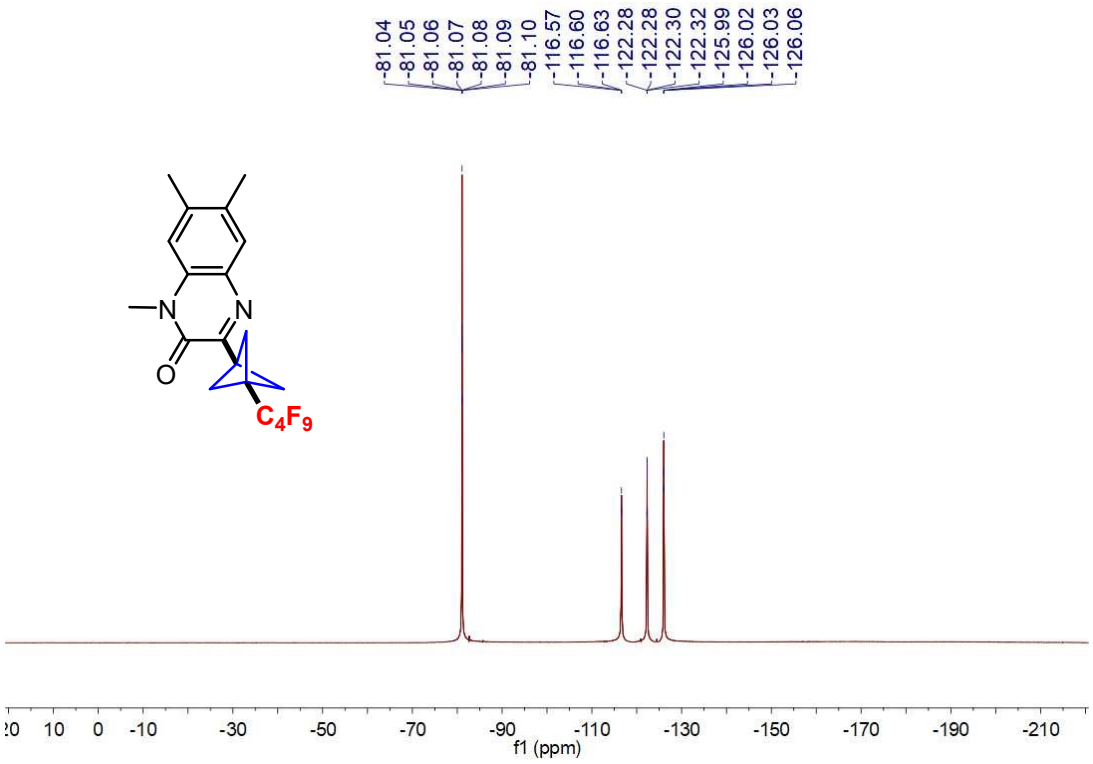


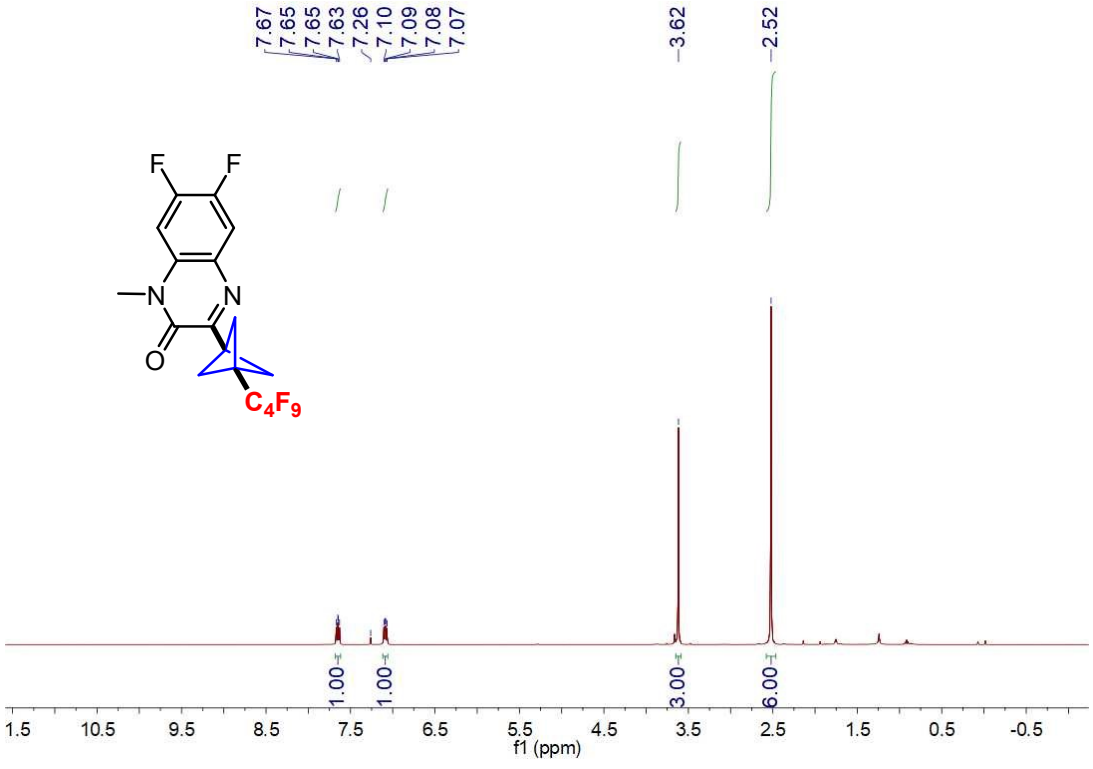
28 ^{13}C NMR (126 MHz, $CDCl_3$)



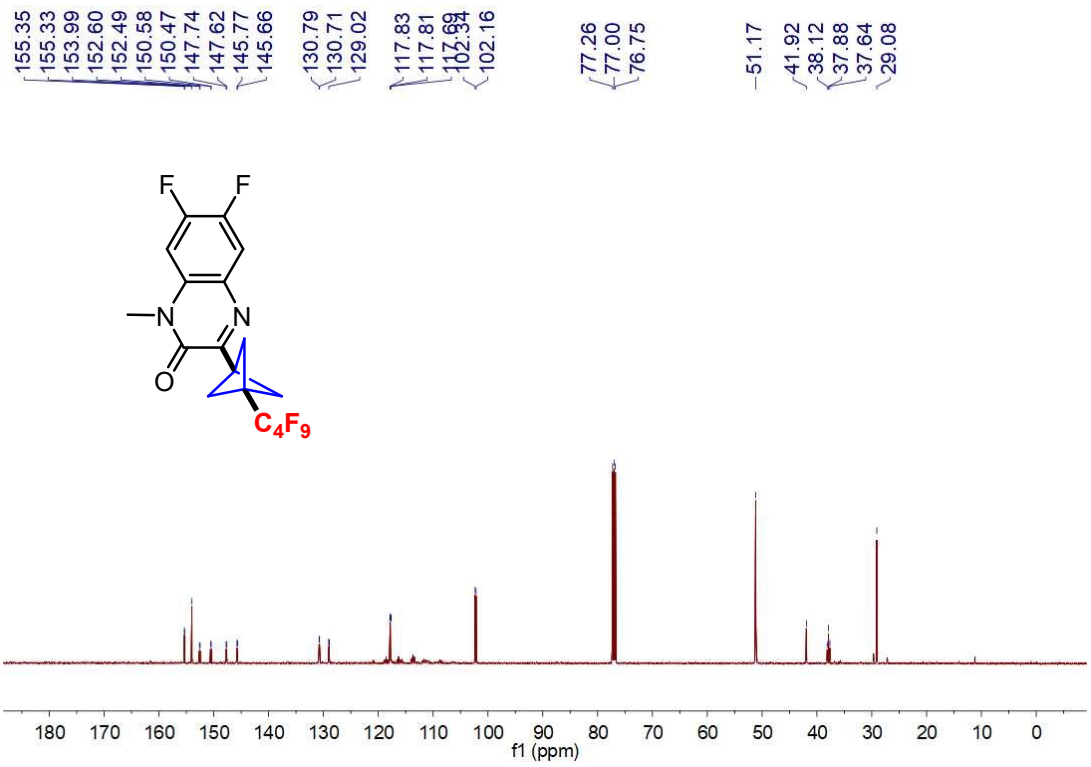
28 ^{19}F NMR (471 MHz, $CDCl_3$)



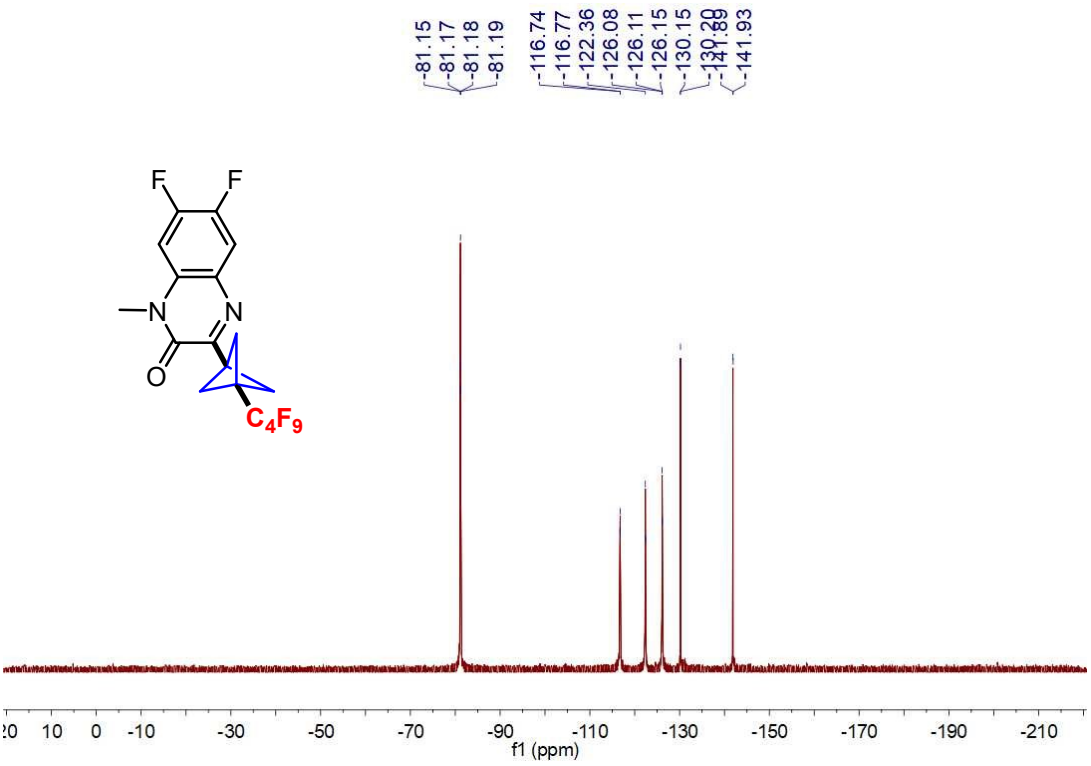
29 ^{1}H NMR (500 MHz, $CDCl_3$)



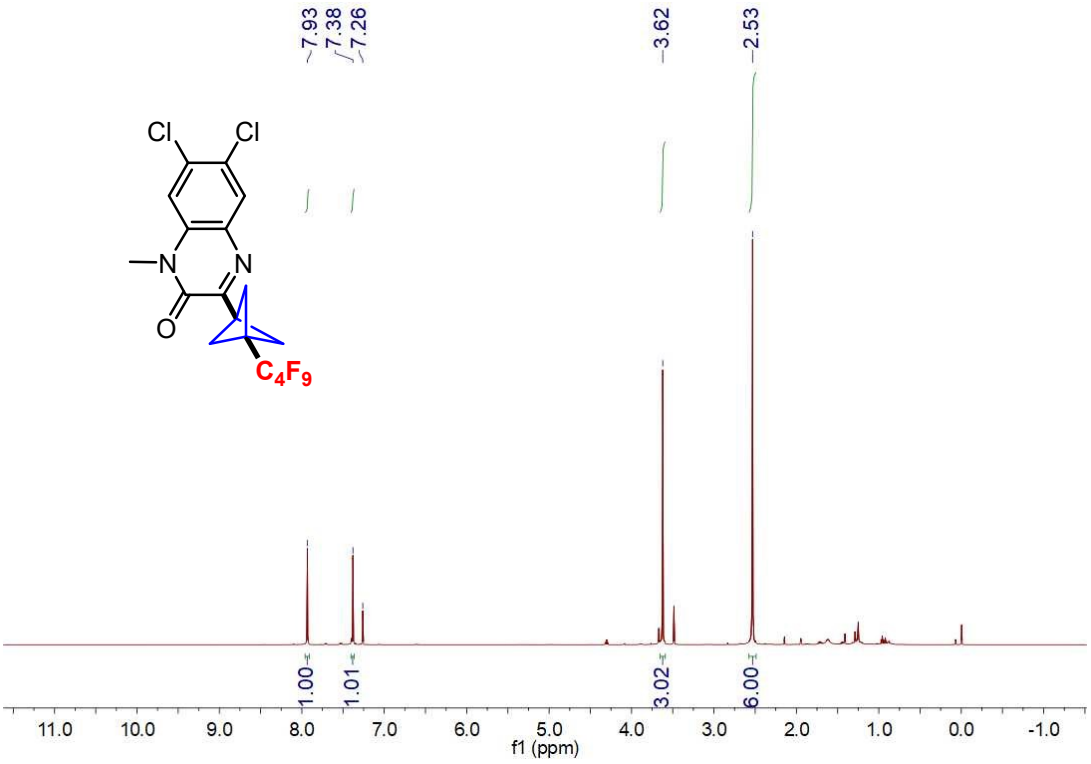
29 ^{13}C NMR (126 MHz, $CDCl_3$)



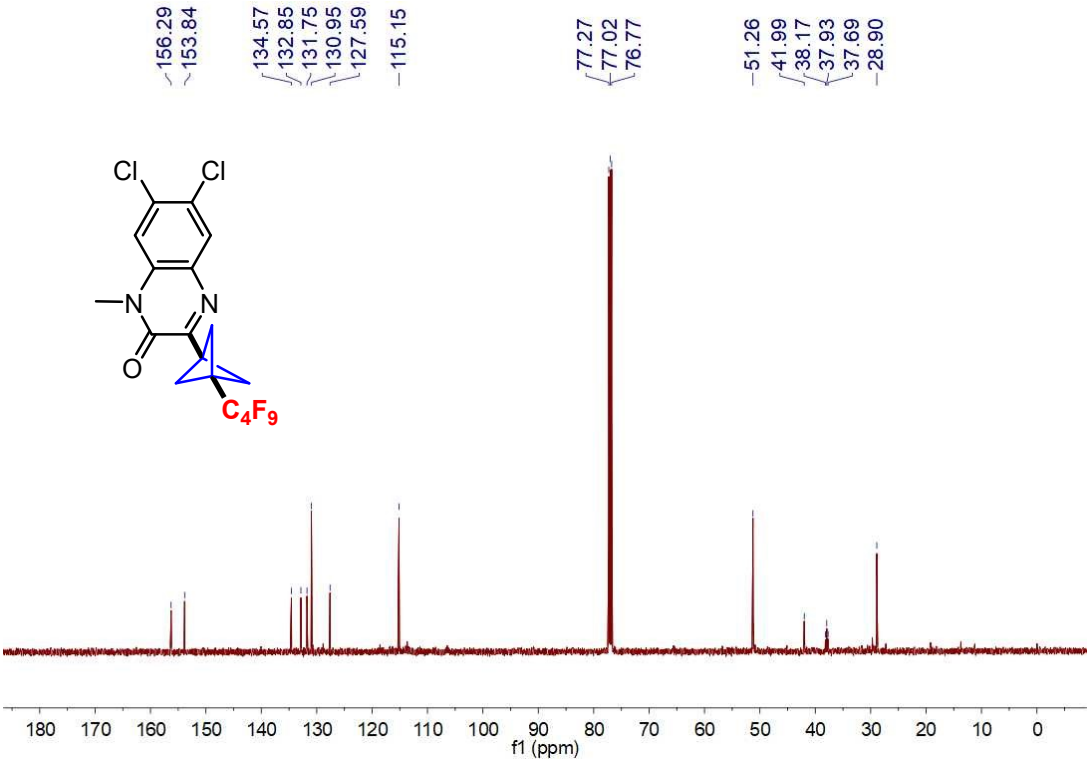
29 ^{19}F NMR (471 MHz, $CDCl_3$)



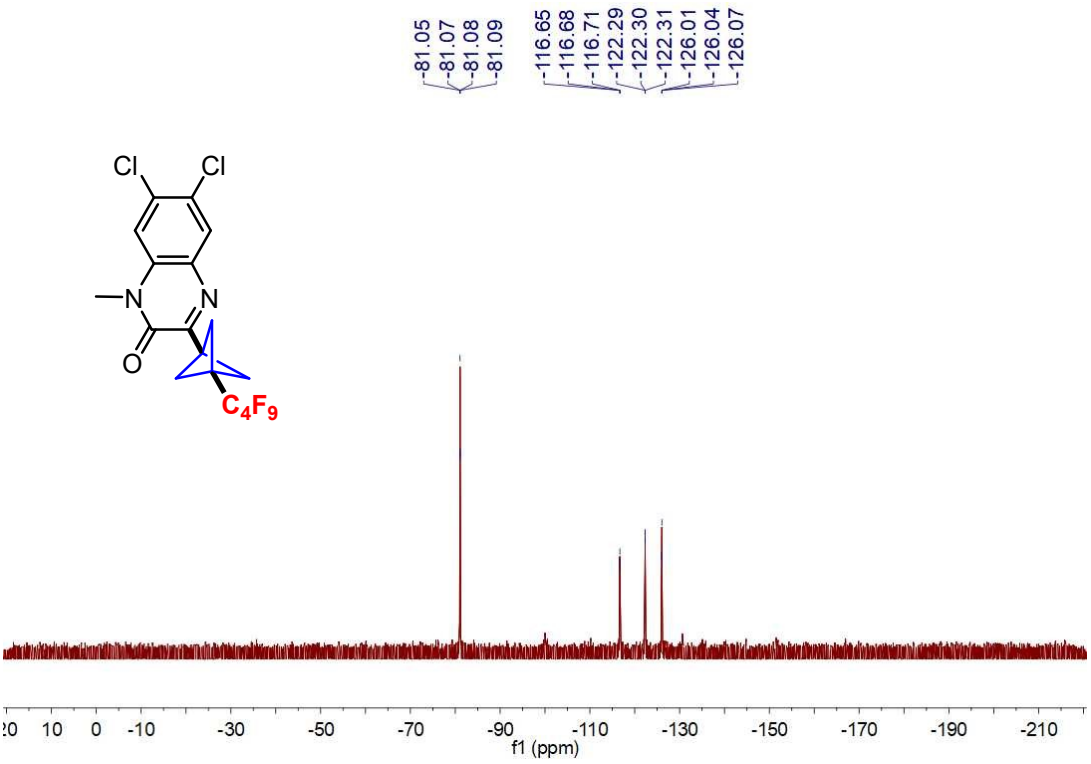
30 ^{1}H NMR (500 MHz, $CDCl_3$)



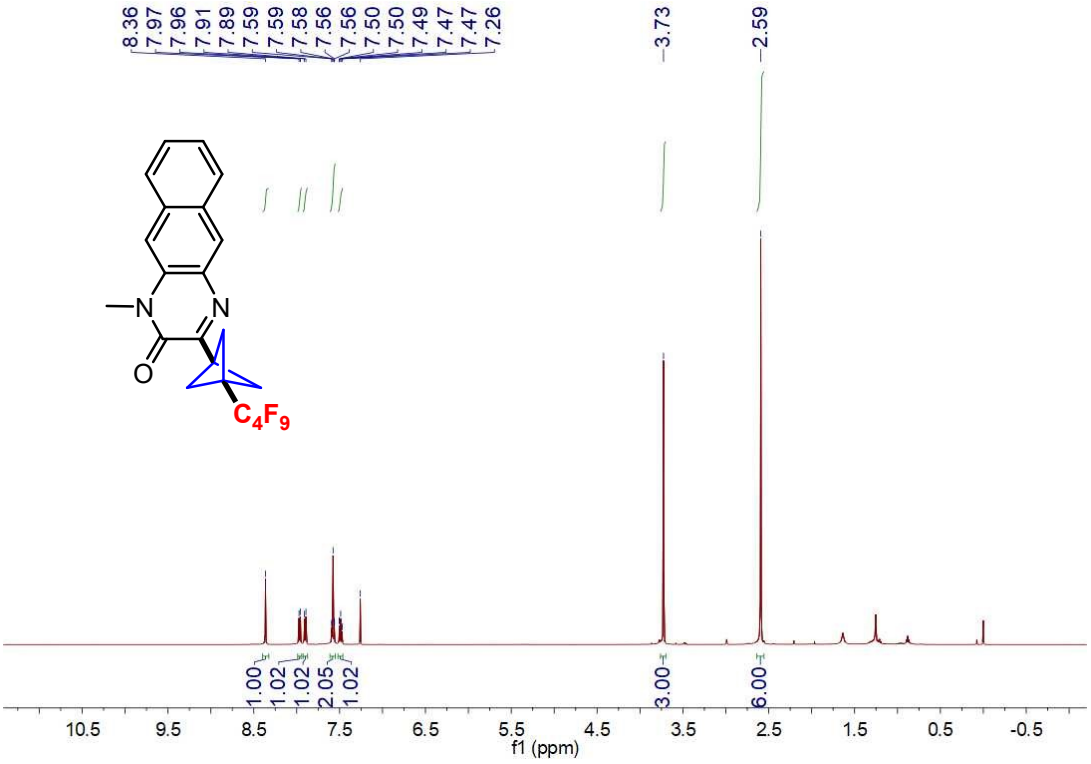
30 ^{13}C NMR (126 MHz, $CDCl_3$)



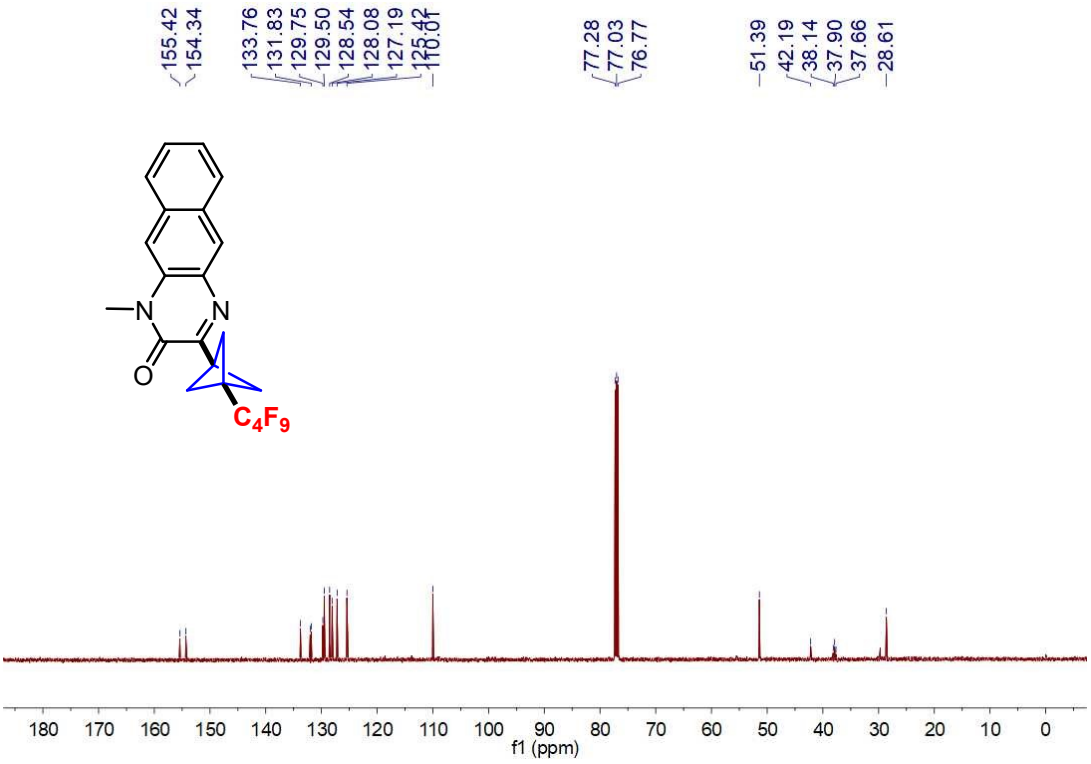
30 ^{19}F NMR (471 MHz, $CDCl_3$)



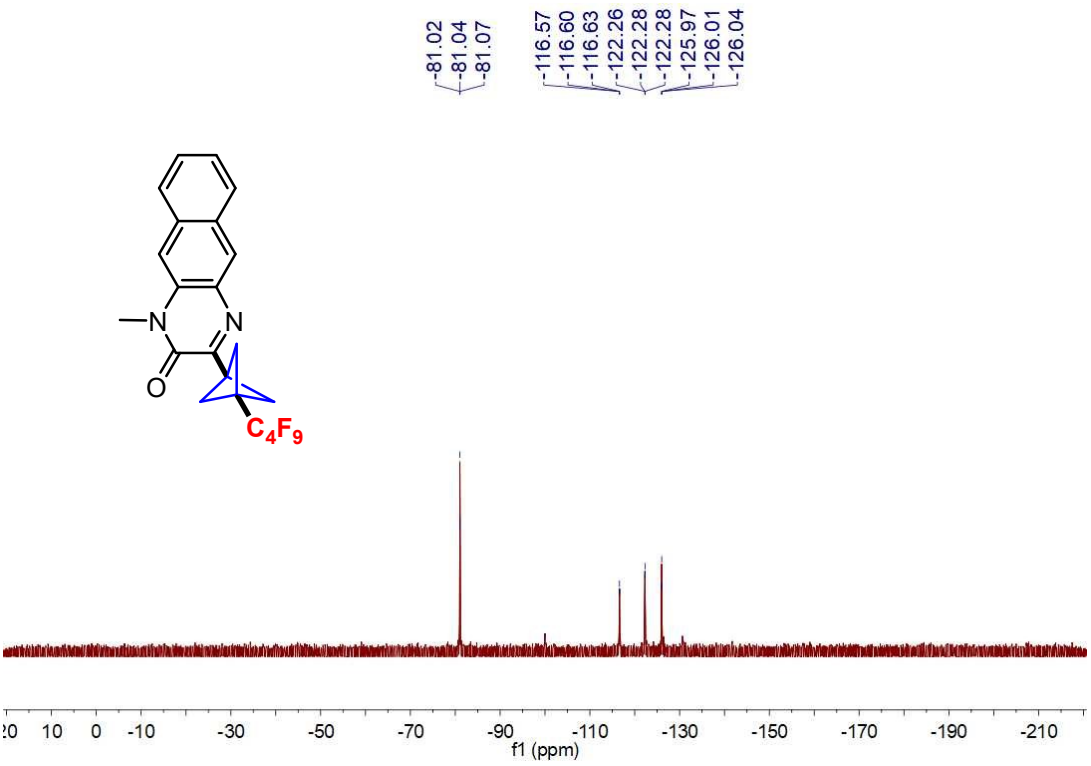
31 ^{1}H NMR (500 MHz, $CDCl_3$)



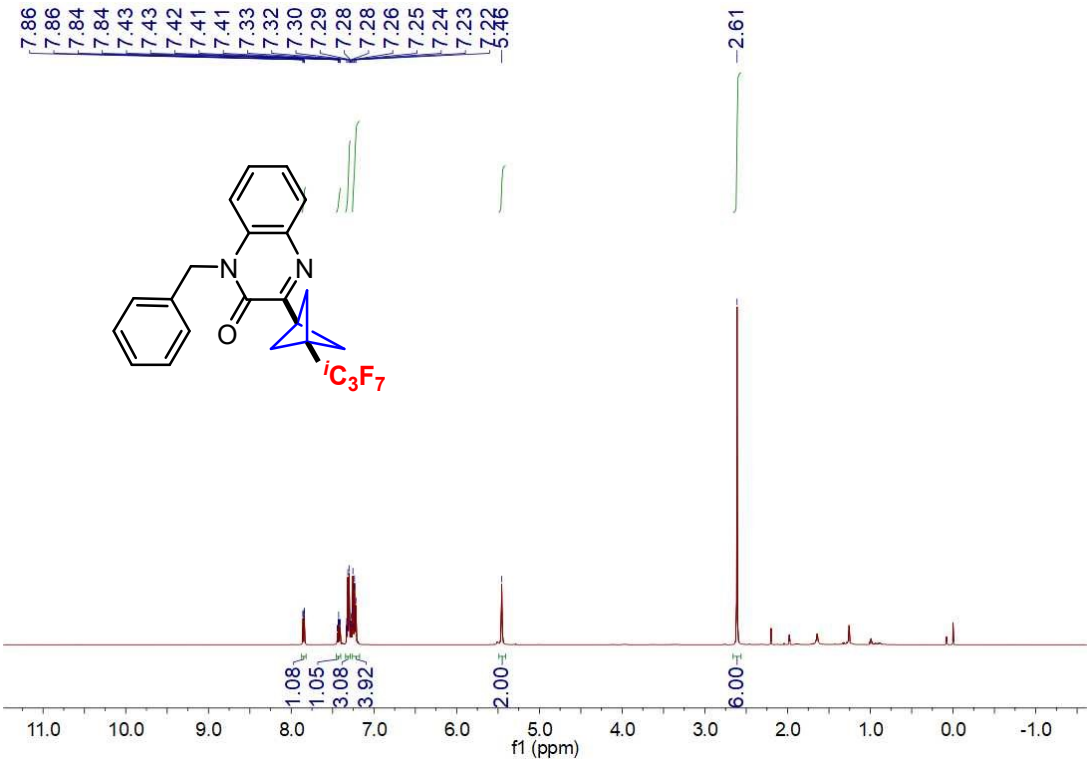
31 ^{13}C NMR (126 MHz, $CDCl_3$)



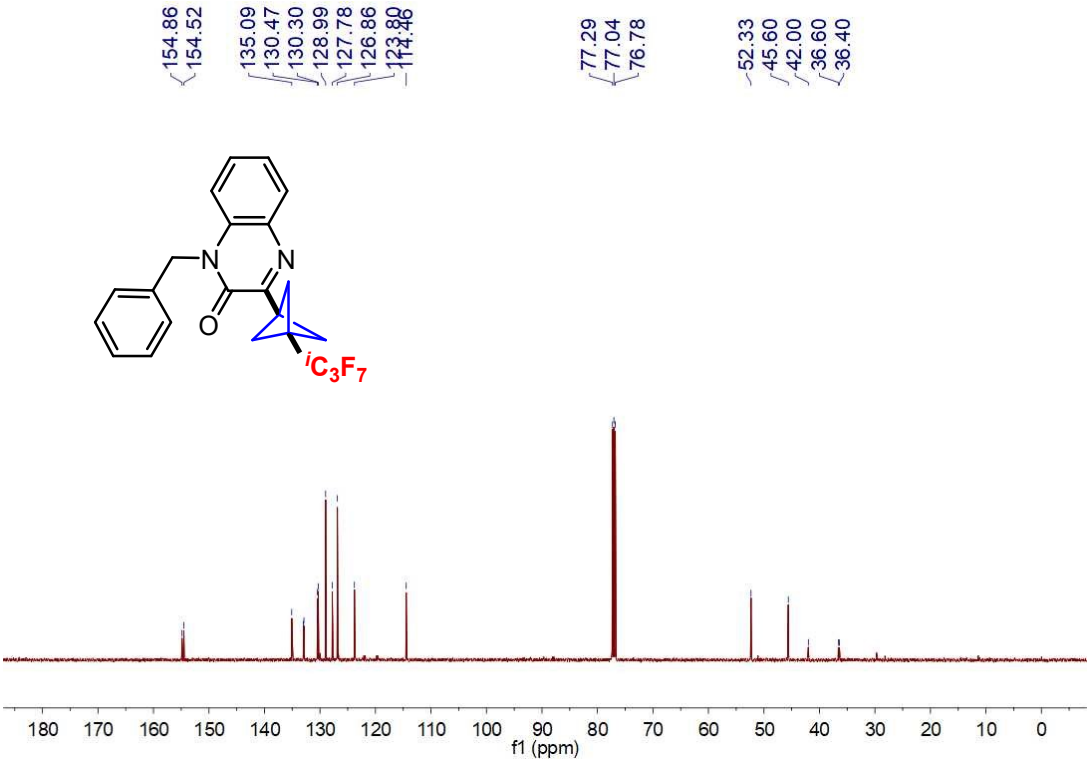
31 ^{19}F NMR (471 MHz, $CDCl_3$)



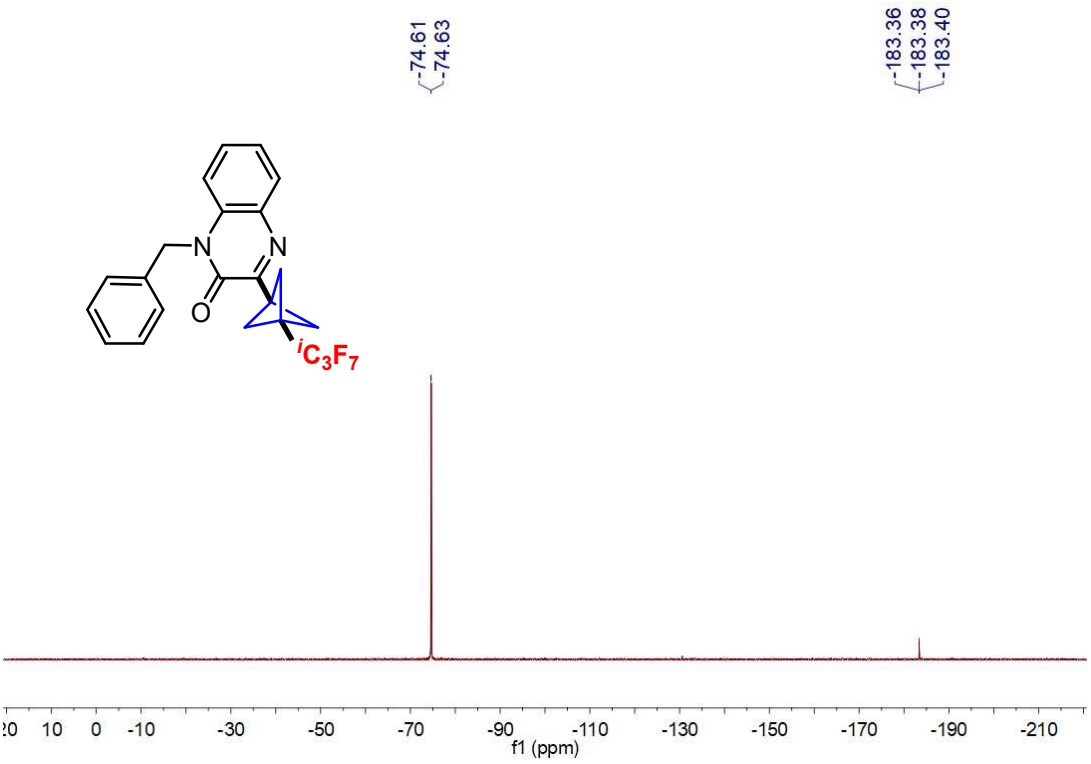
32 ^{1}H NMR (500 MHz, $CDCl_3$)



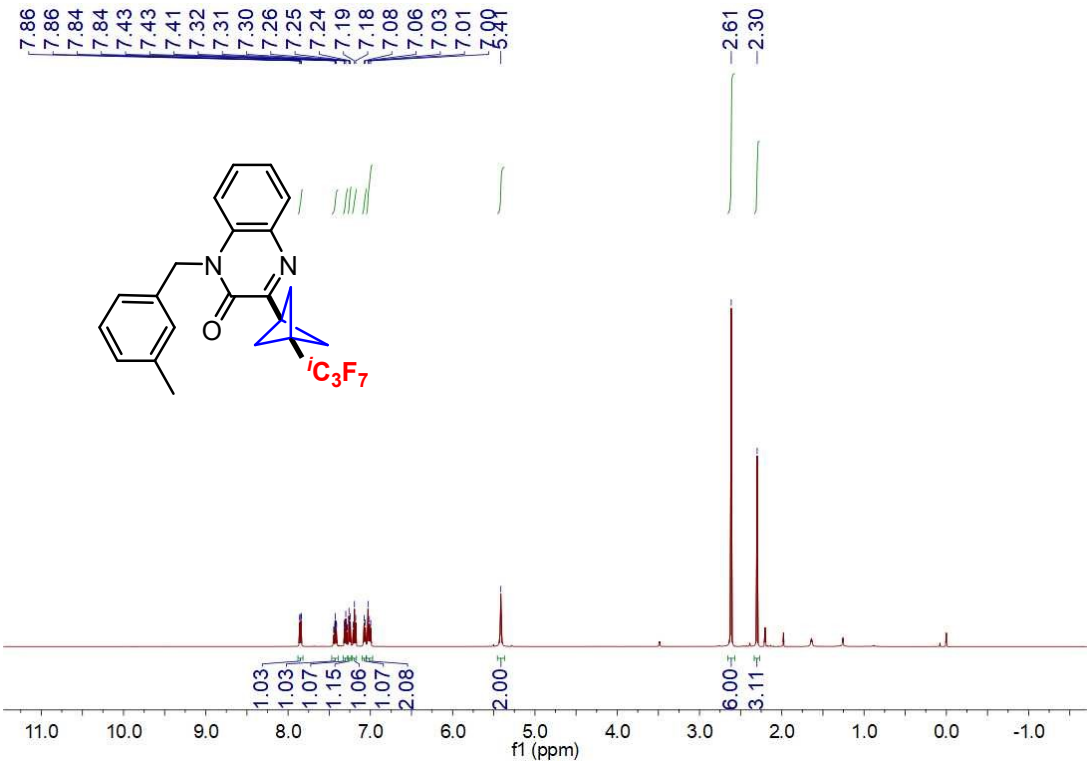
32 ^{13}C NMR (126 MHz, $CDCl_3$)



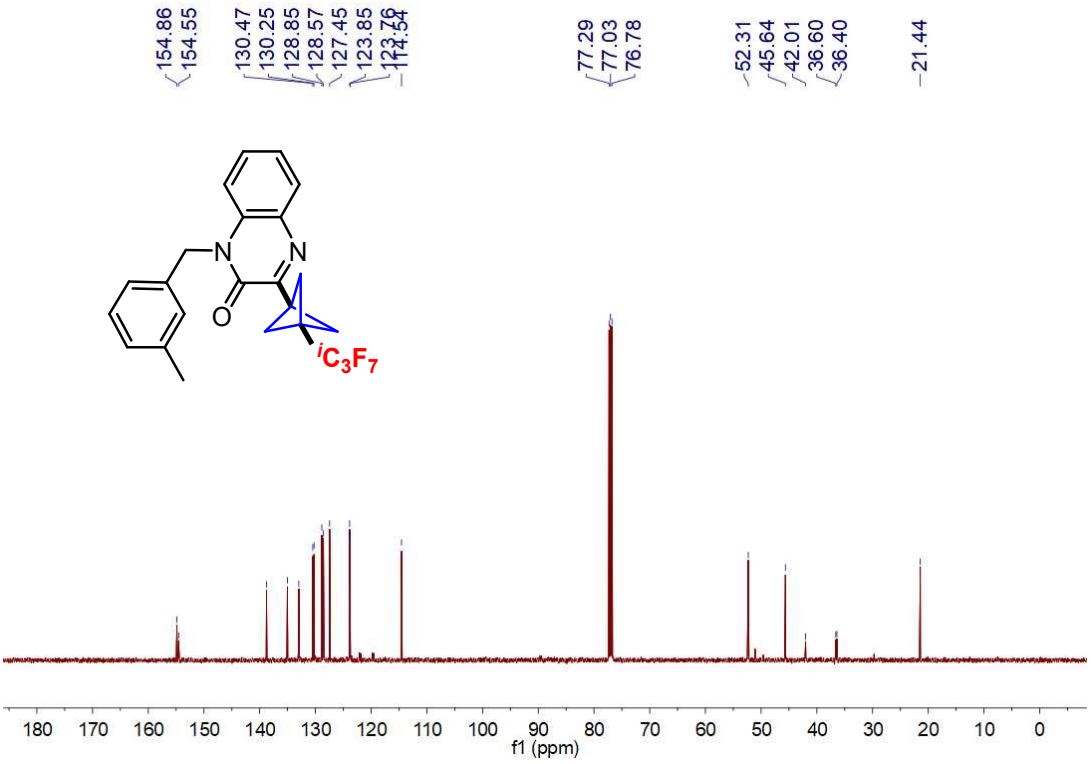
32 ^{19}F NMR (471 MHz, $CDCl_3$)



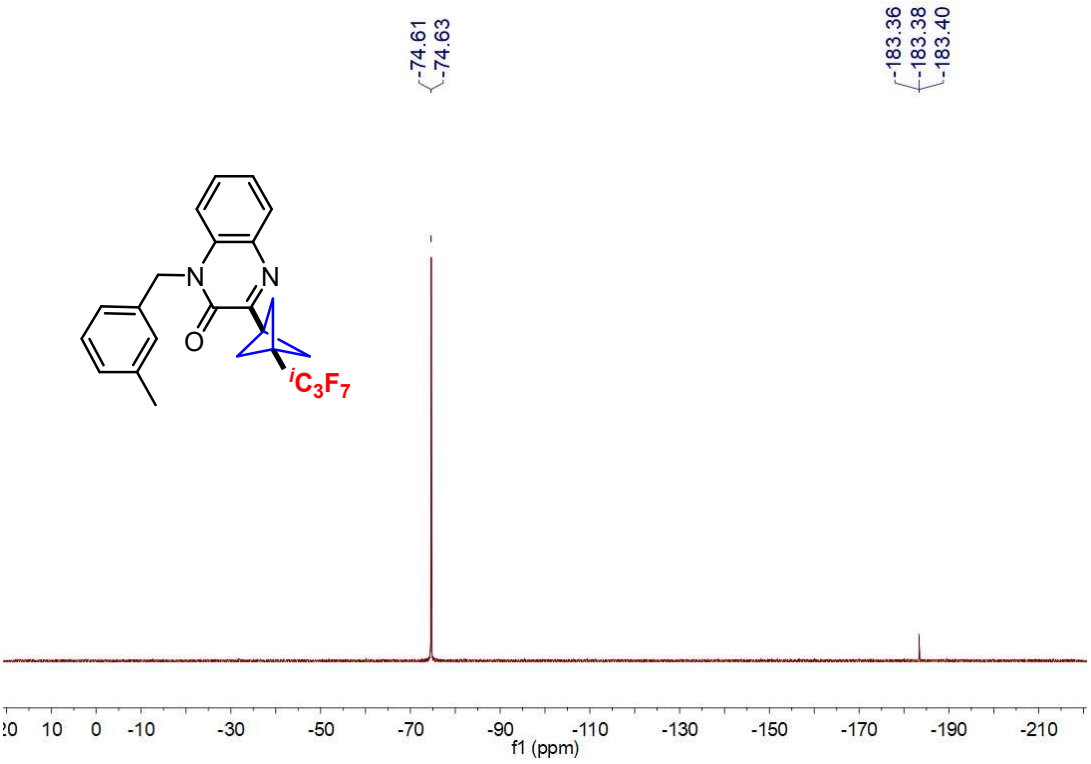
33 ^{1}H NMR (500 MHz, $CDCl_3$)



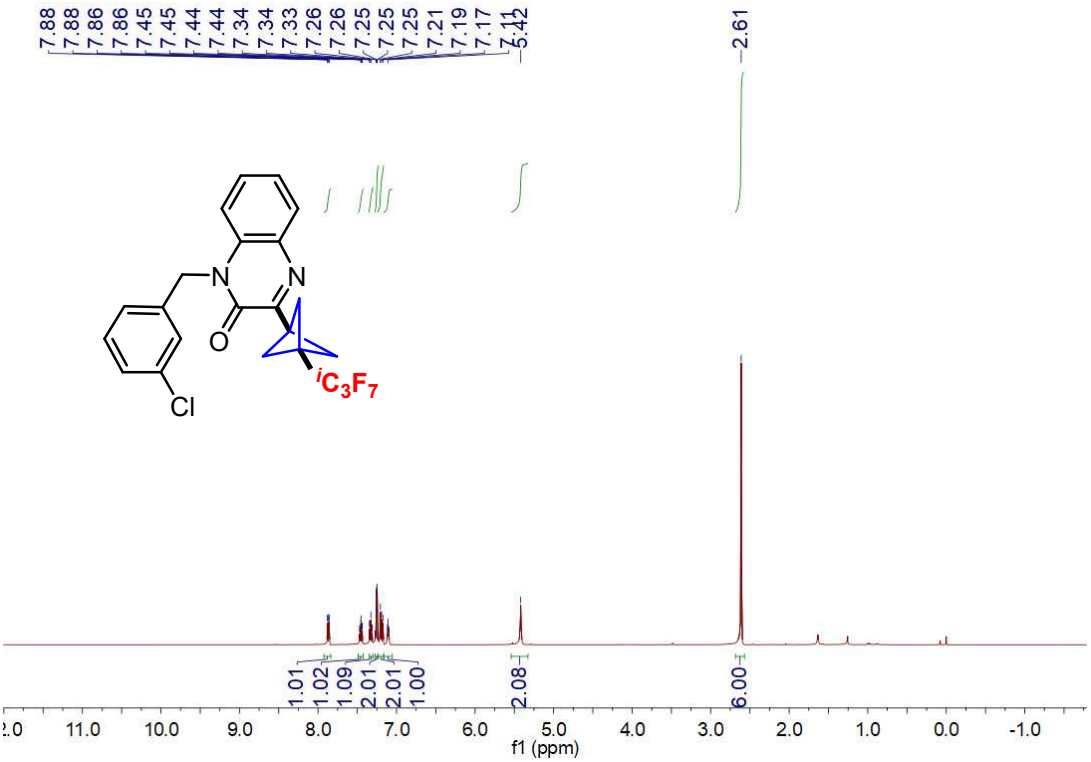
33 ^{13}C NMR (126 MHz, $CDCl_3$)



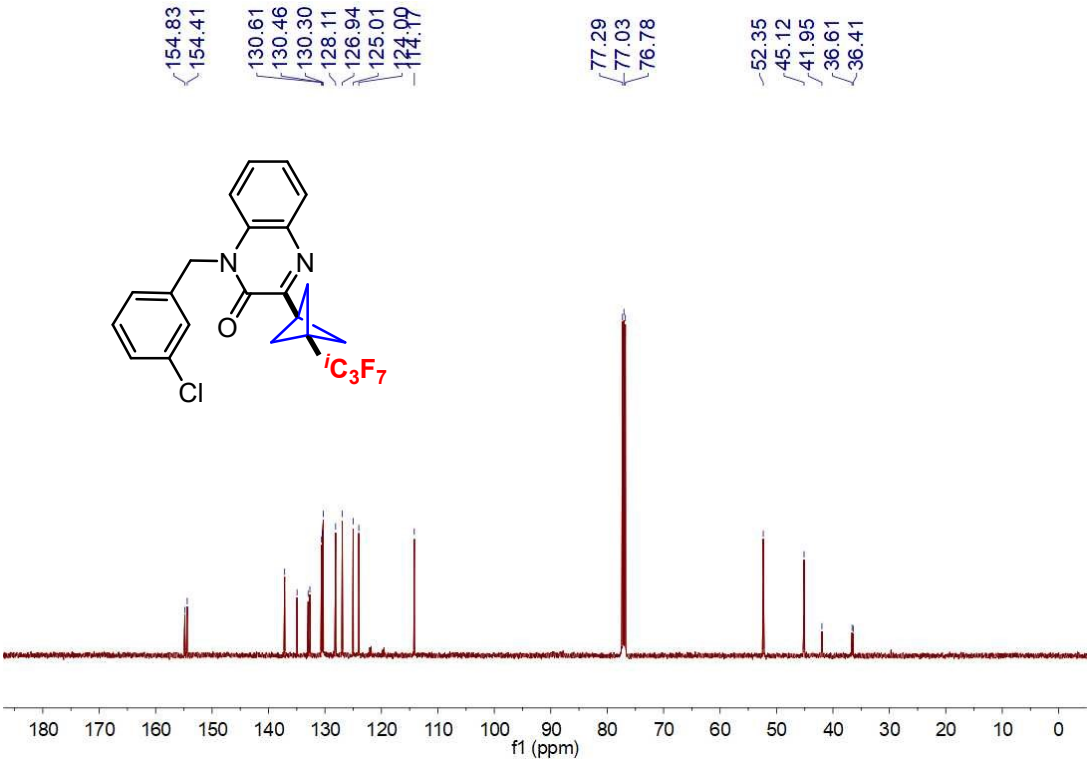
33 ^{19}F NMR (471 MHz, $CDCl_3$)



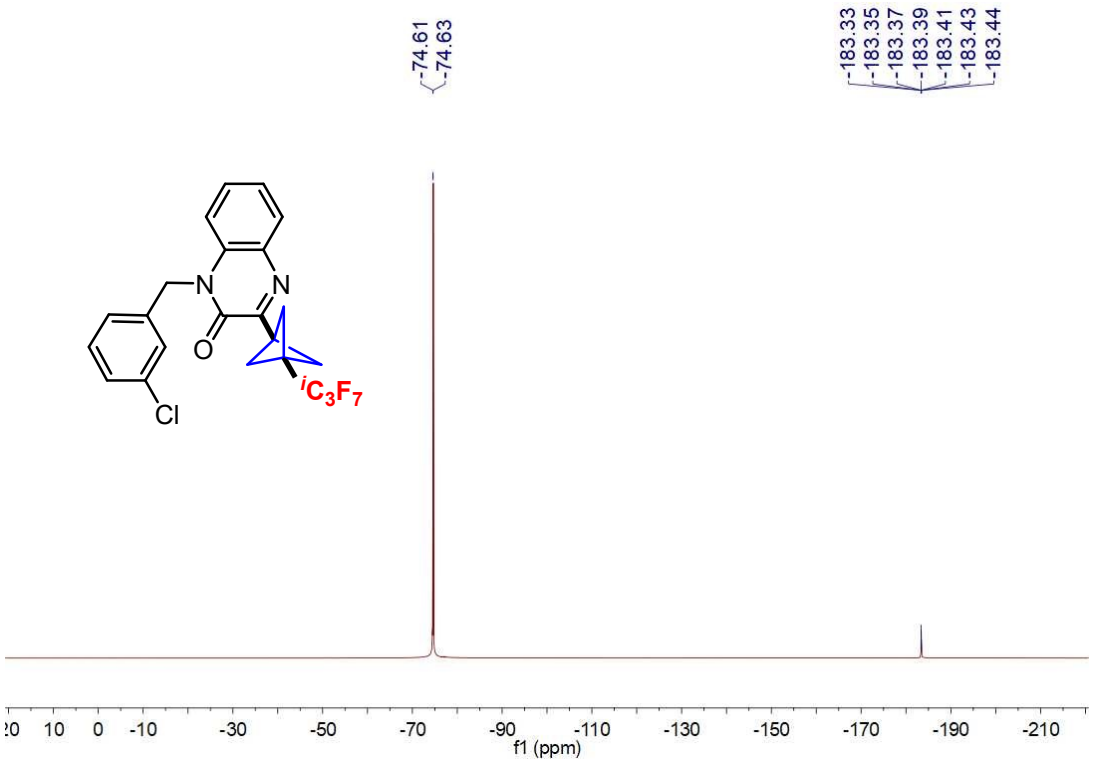
34 ^{1}H NMR (500 MHz, $CDCl_3$)



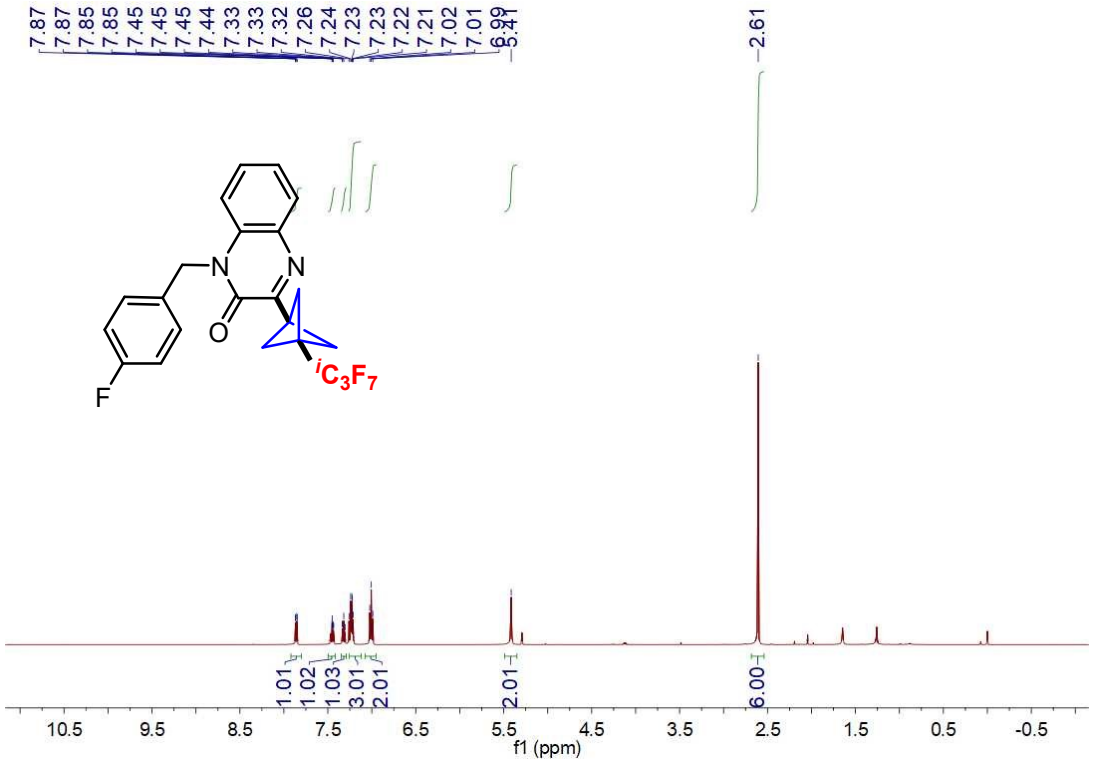
34 ^{13}C NMR (126 MHz, $CDCl_3$)



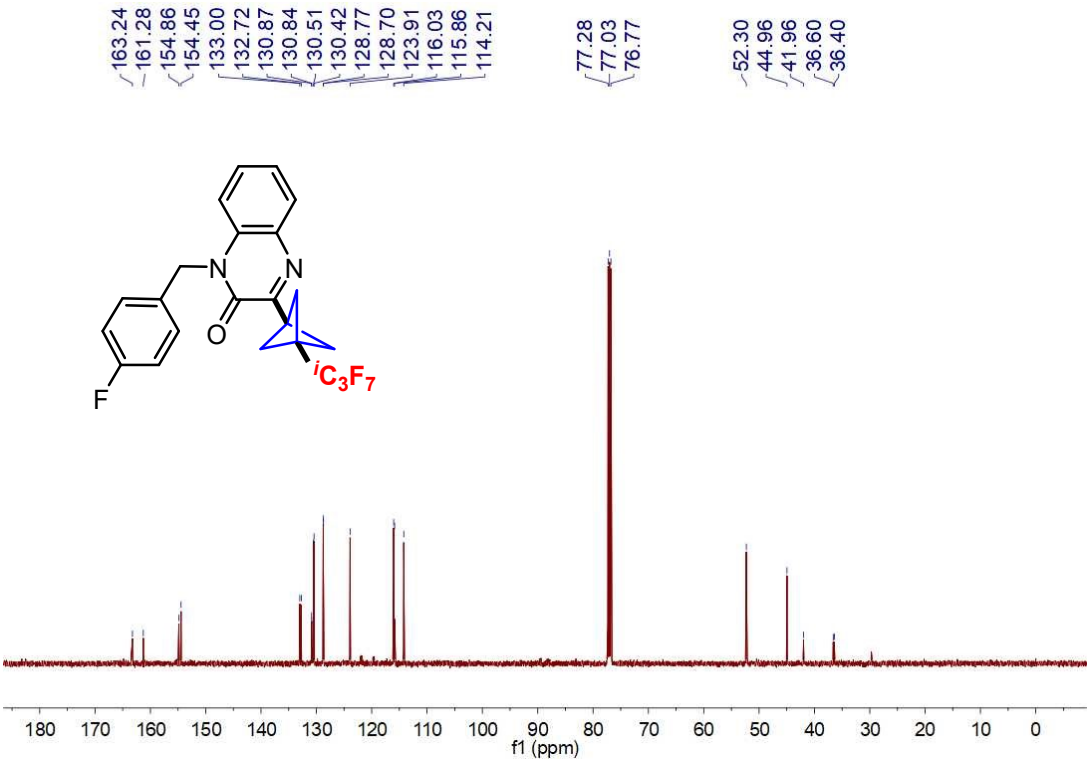
34 ^{19}F NMR (471 MHz, $CDCl_3$)



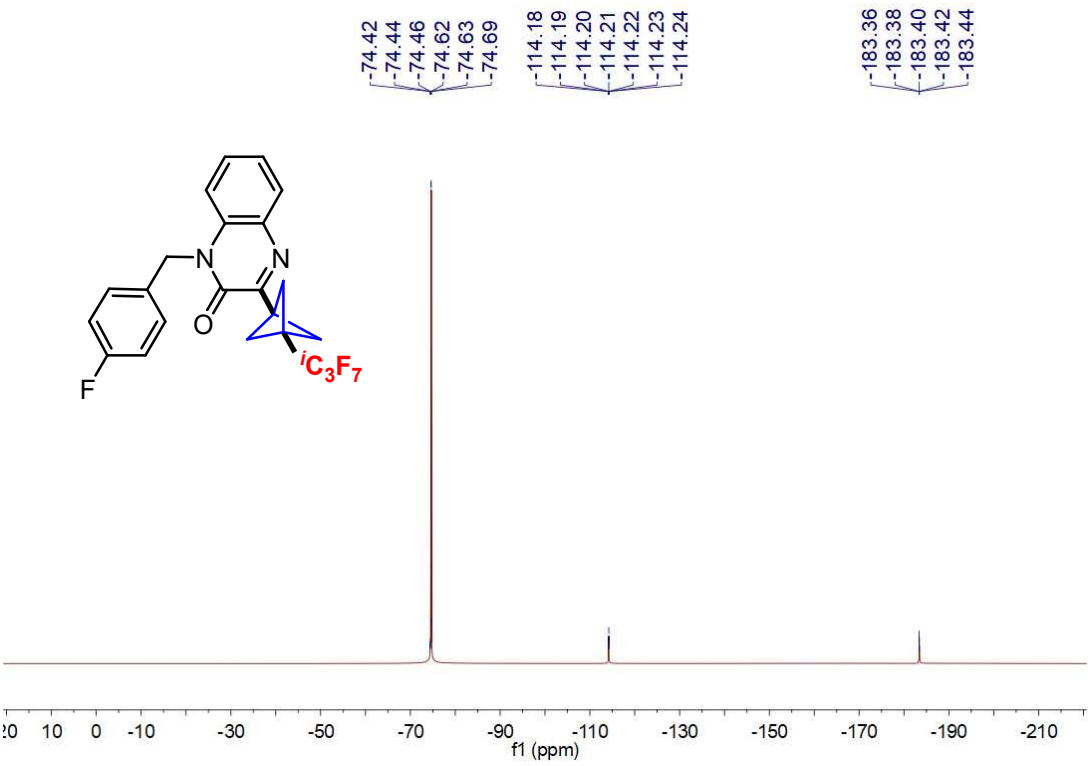
35 ^{1}H NMR (500 MHz, $CDCl_3$)



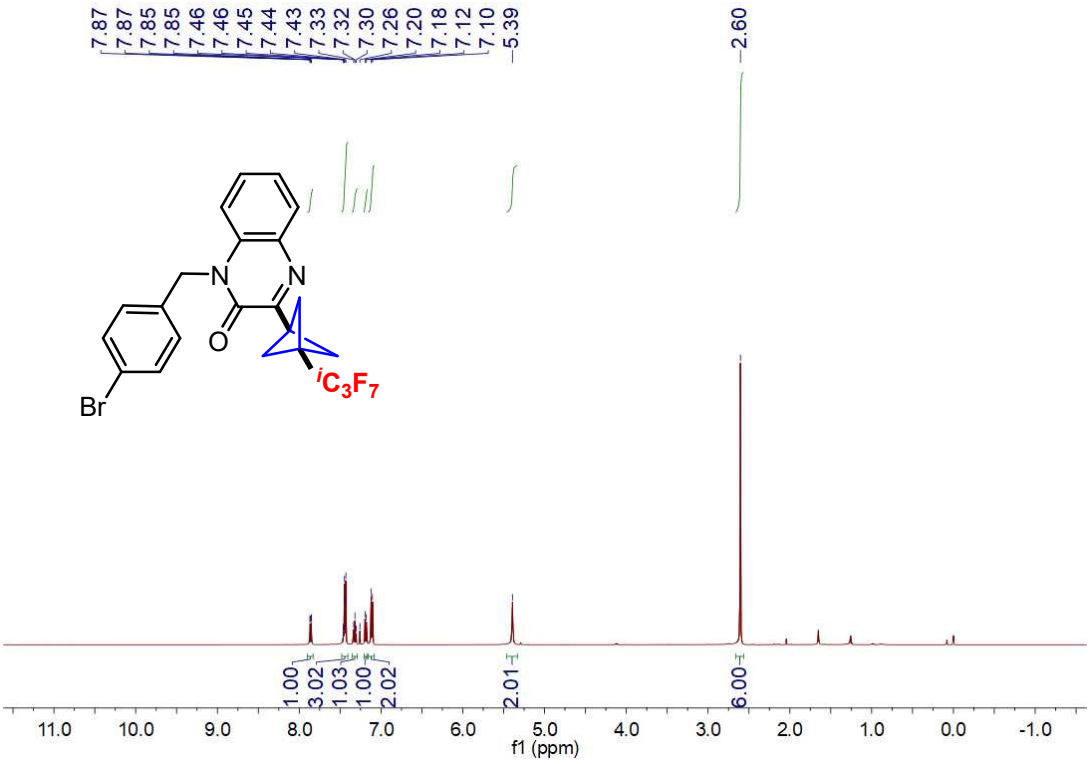
35 ^{13}C NMR (126 MHz, $CDCl_3$)



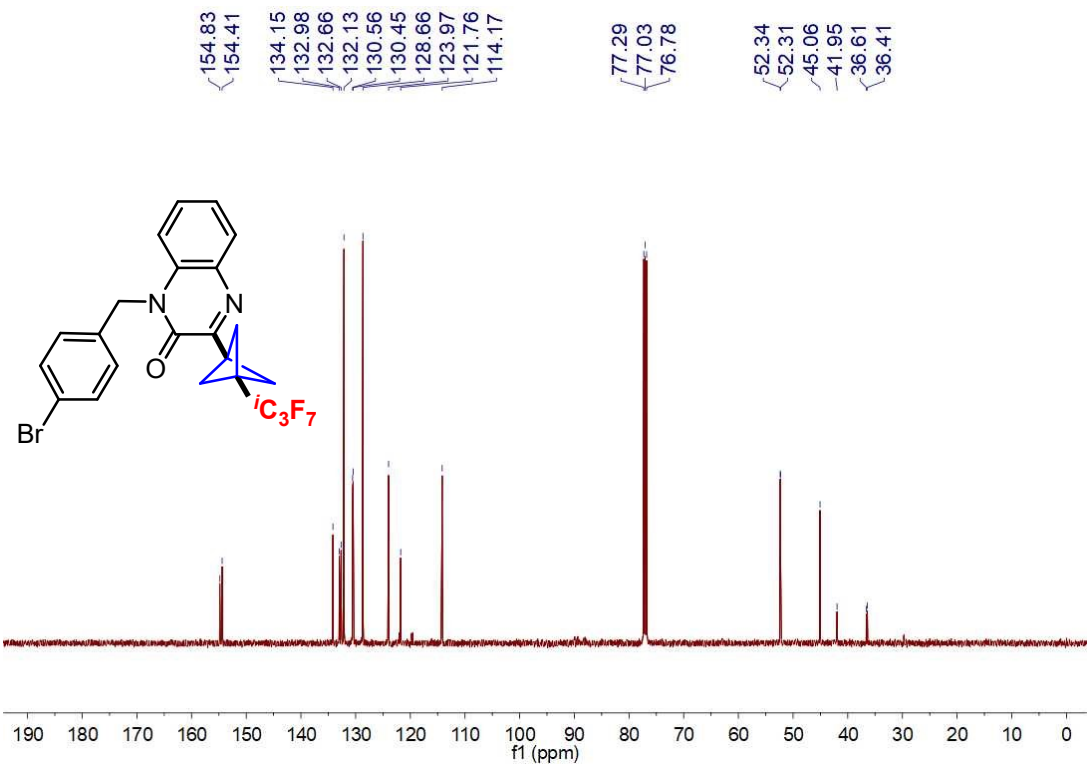
35 ^{19}F NMR (471 MHz, $CDCl_3$)



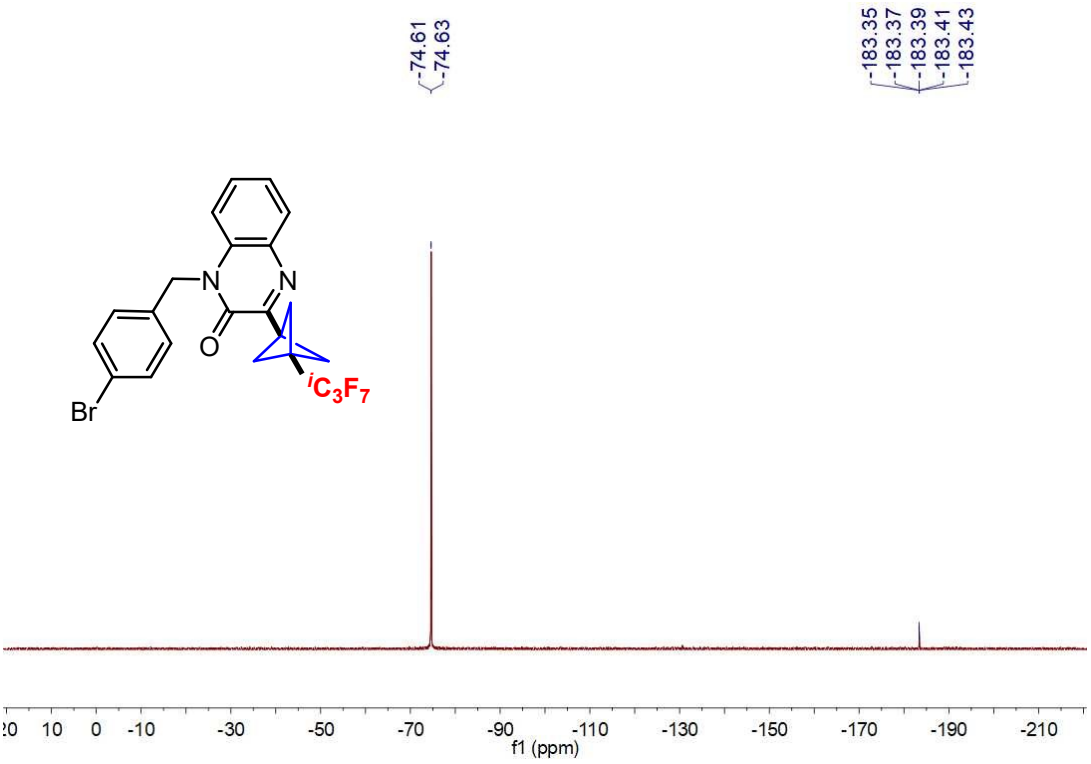
36 ^{1}H NMR (500 MHz, $CDCl_3$)



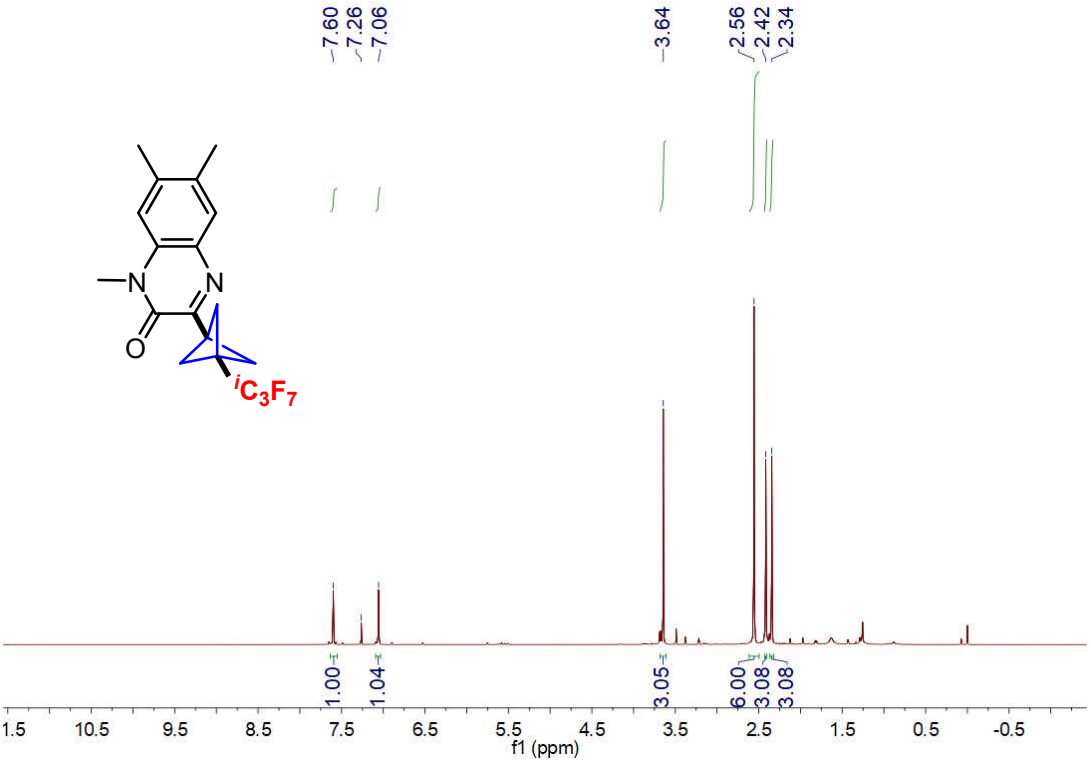
36 ^{13}C NMR (126 MHz, $CDCl_3$)



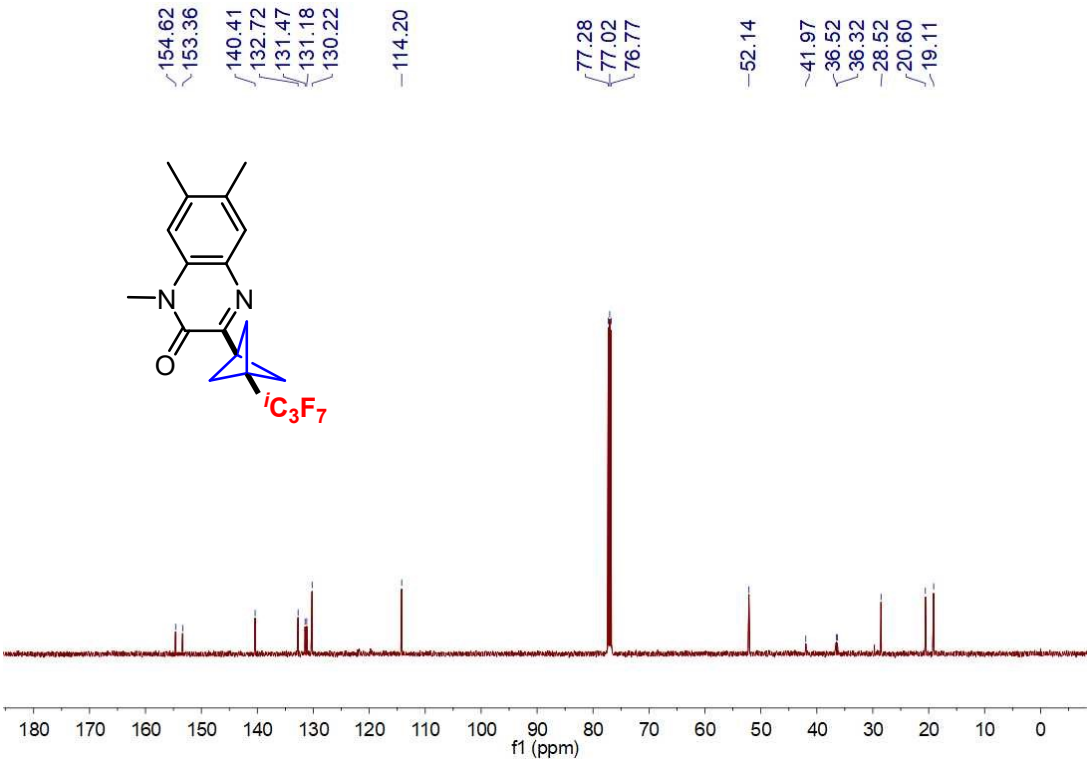
36 ^{19}F NMR (471 MHz, $CDCl_3$)



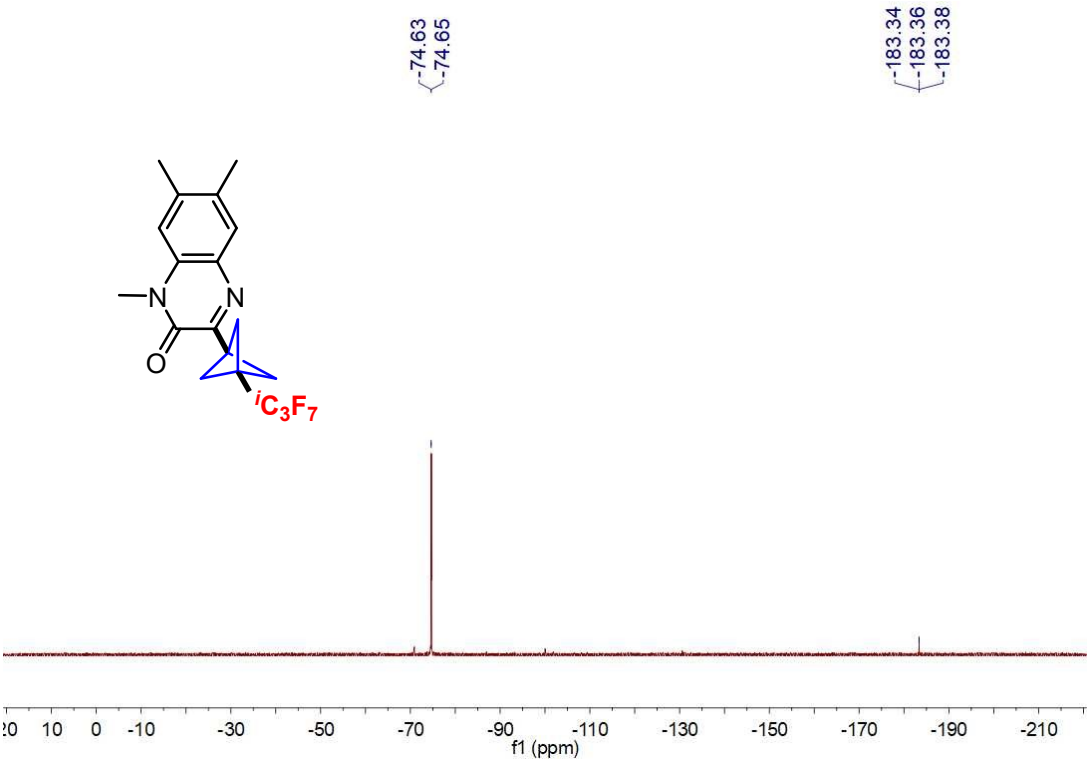
37 ^{1}H NMR (500 MHz, $CDCl_3$)



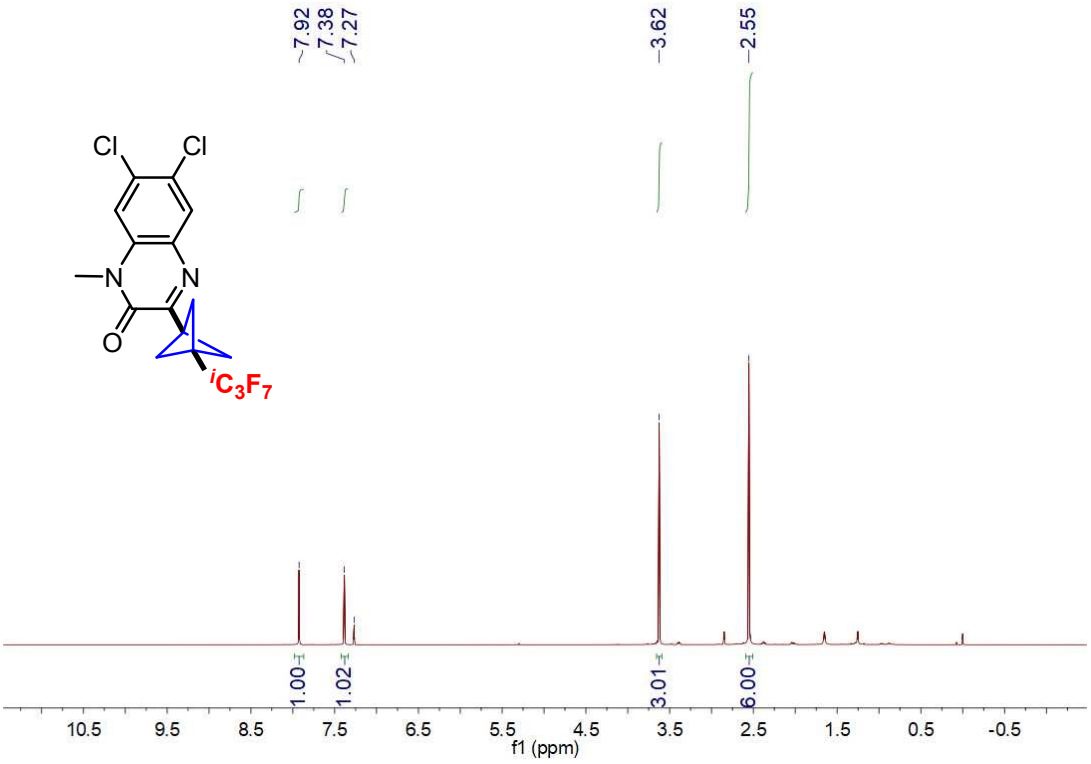
37 ^{13}C NMR (126 MHz, $CDCl_3$)



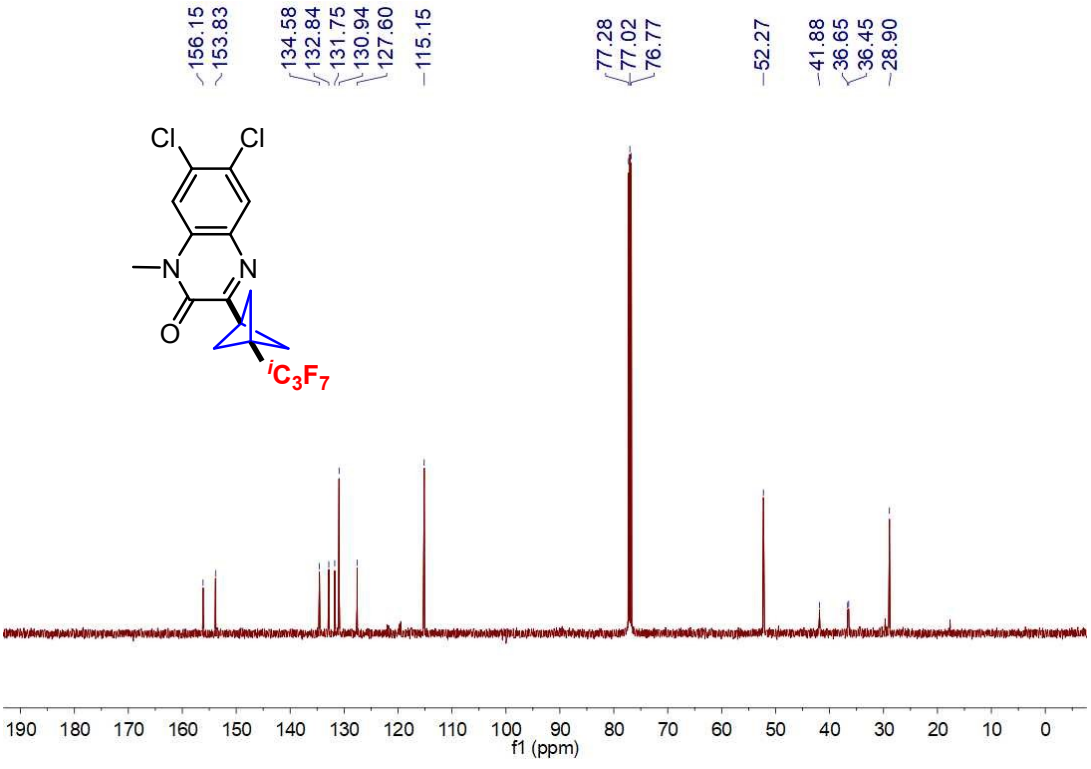
37 ^{19}F NMR (471 MHz, $CDCl_3$)



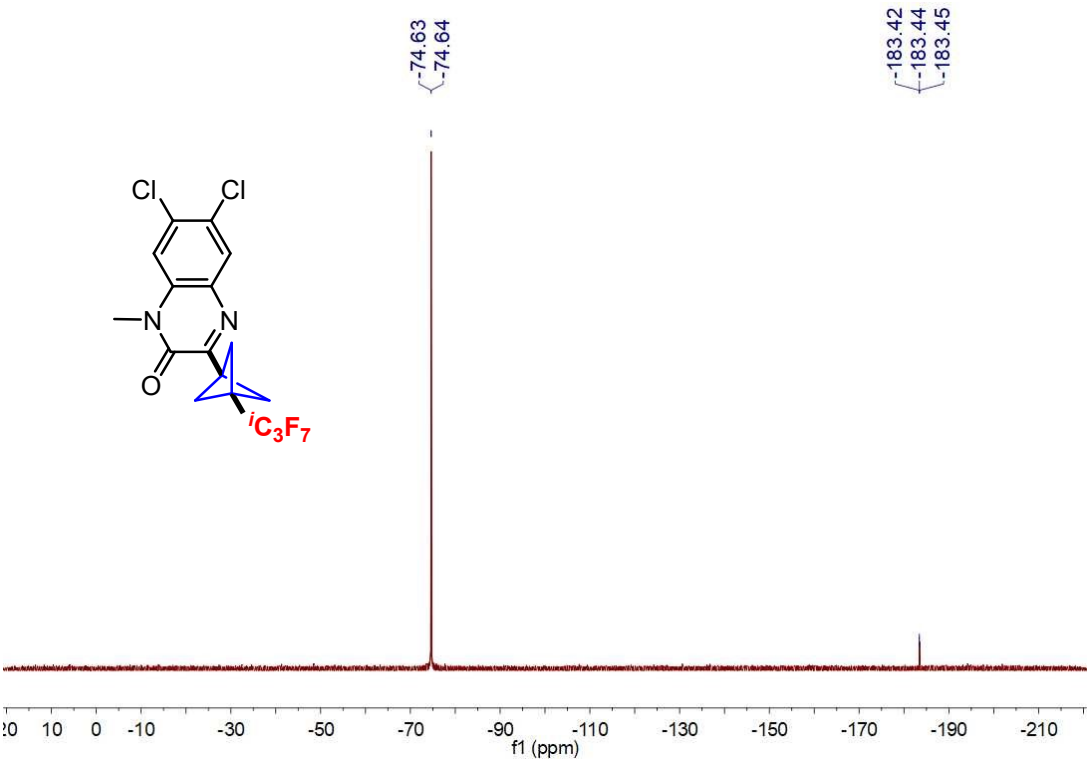
38 ^{1}H NMR (500 MHz, $CDCl_3$)



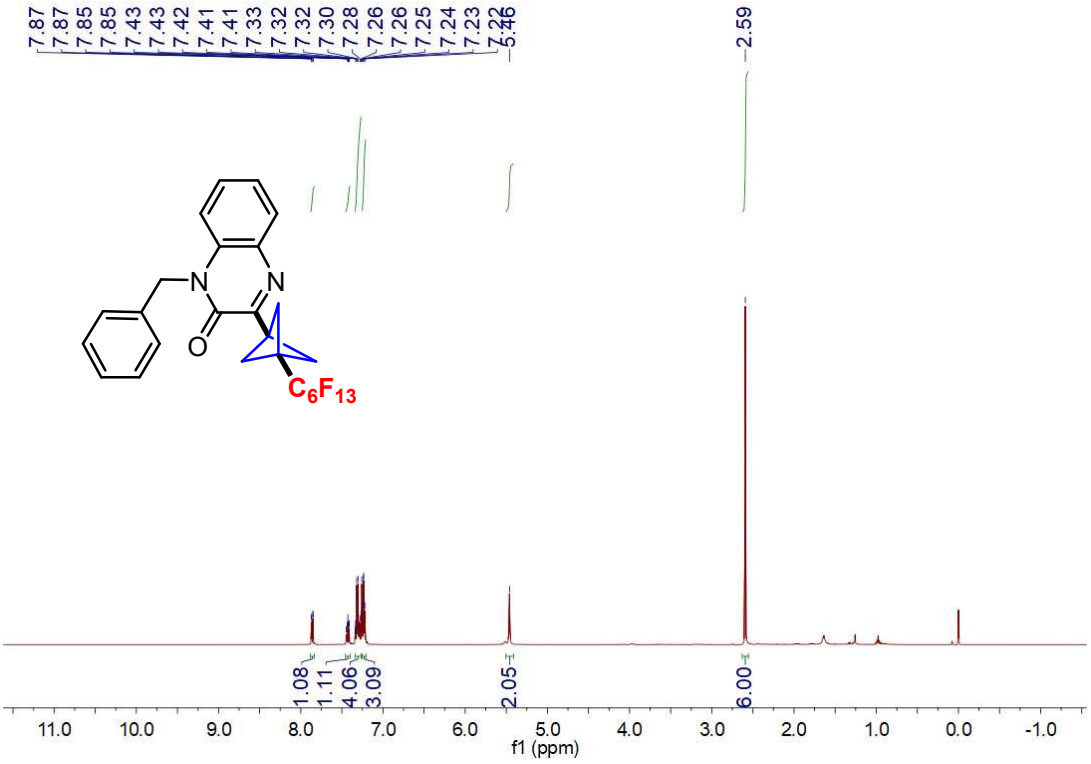
38 ^{13}C NMR (126 MHz, $CDCl_3$)



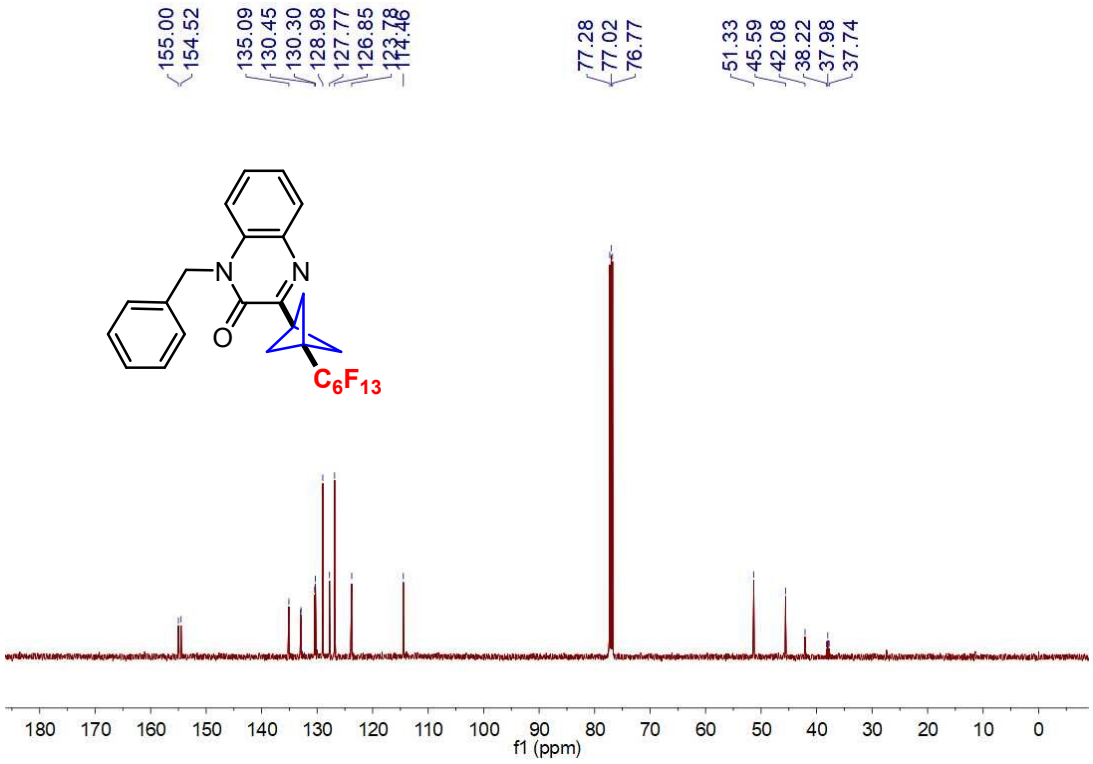
38 ^{19}F NMR (471 MHz, $CDCl_3$)



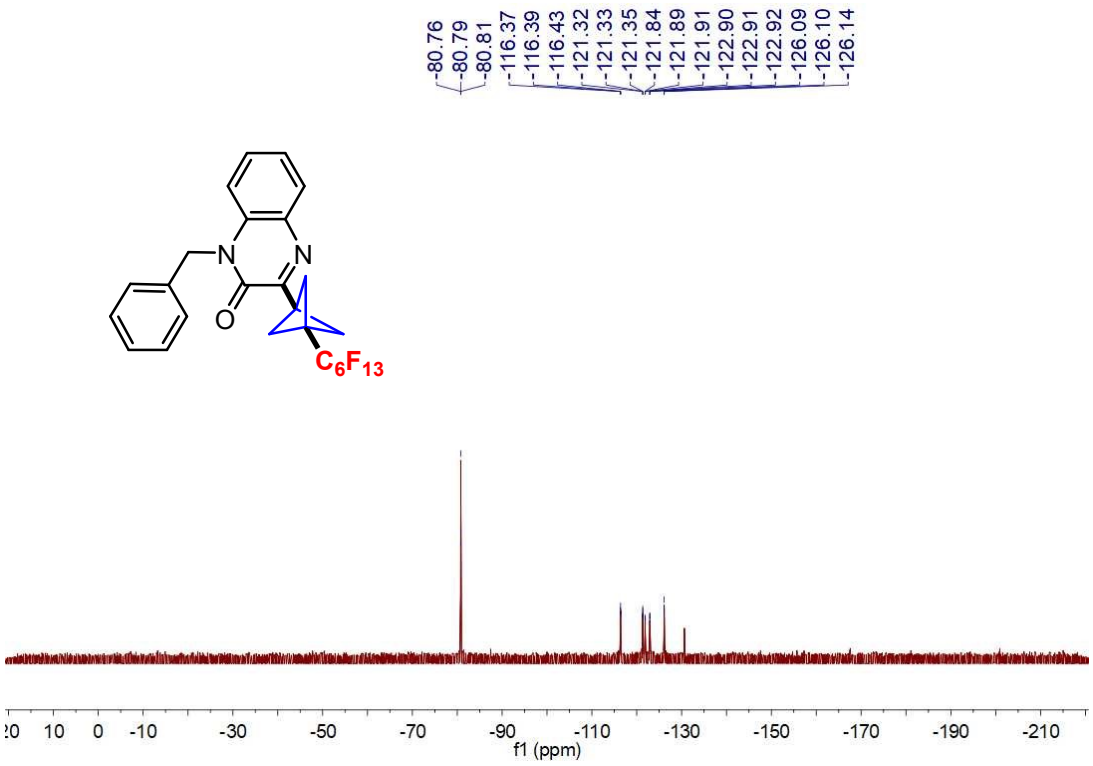
39 ^{1}H NMR (500 MHz, $CDCl_3$)



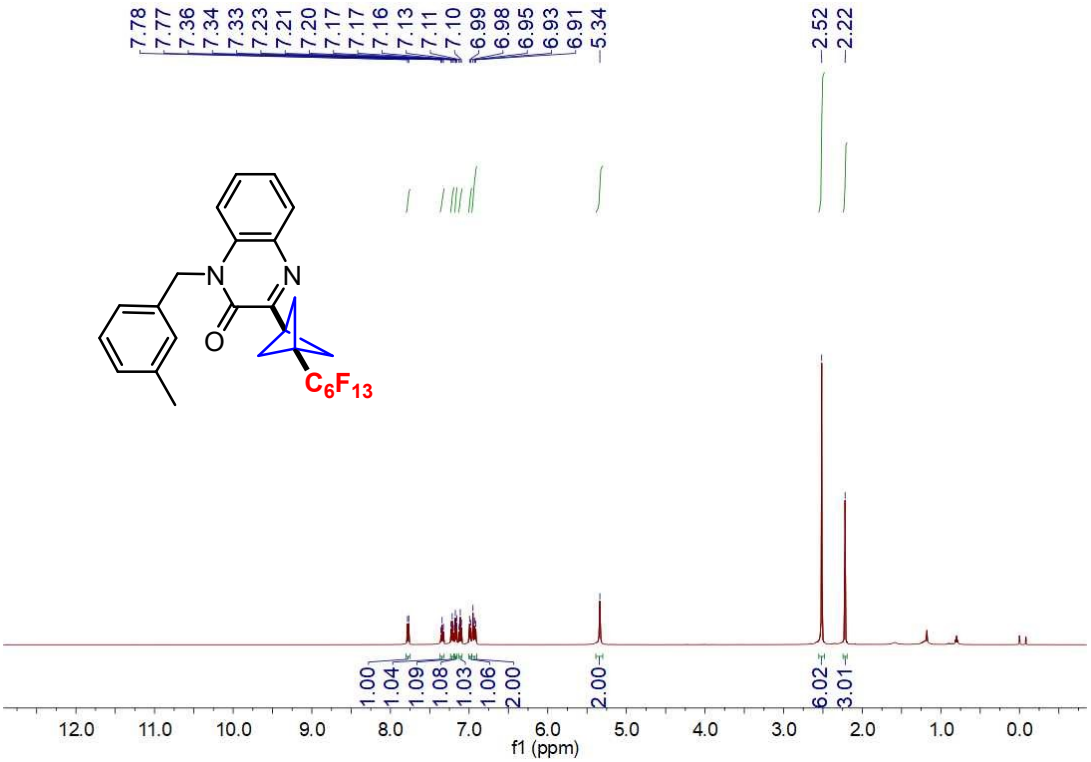
39 ^{13}C NMR (126 MHz, $CDCl_3$)



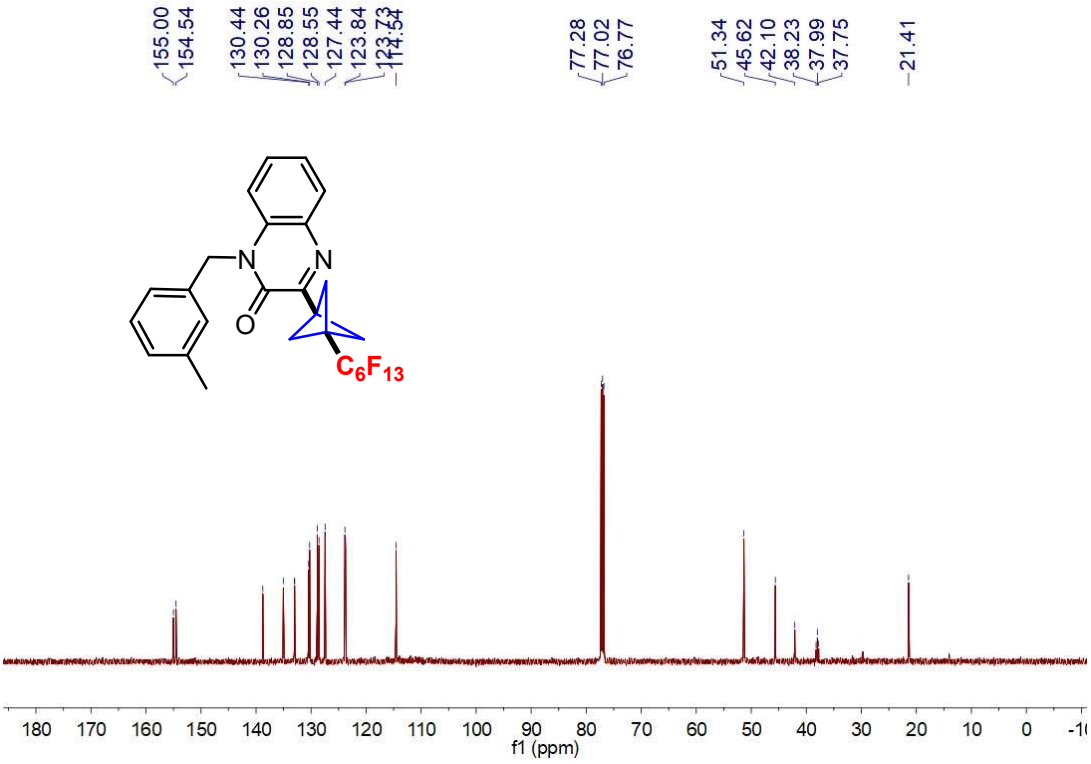
39 ^{19}F NMR (471 MHz, $CDCl_3$)



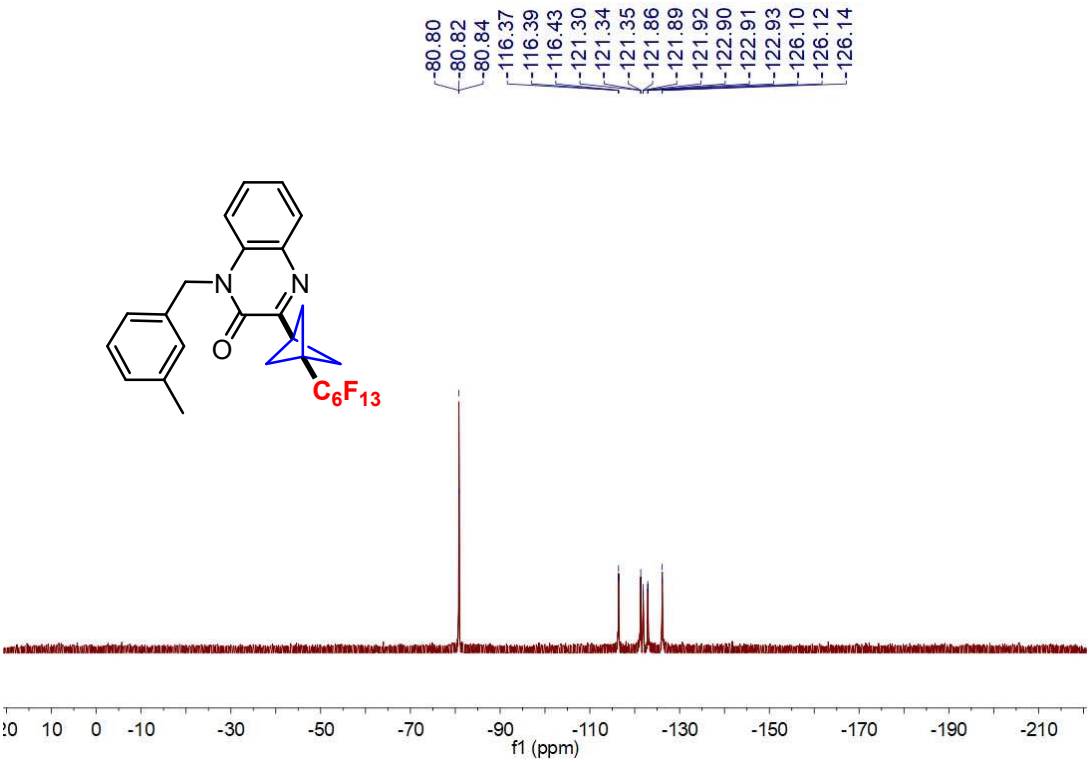
40 ^{1}H NMR (500 MHz, $CDCl_3$)



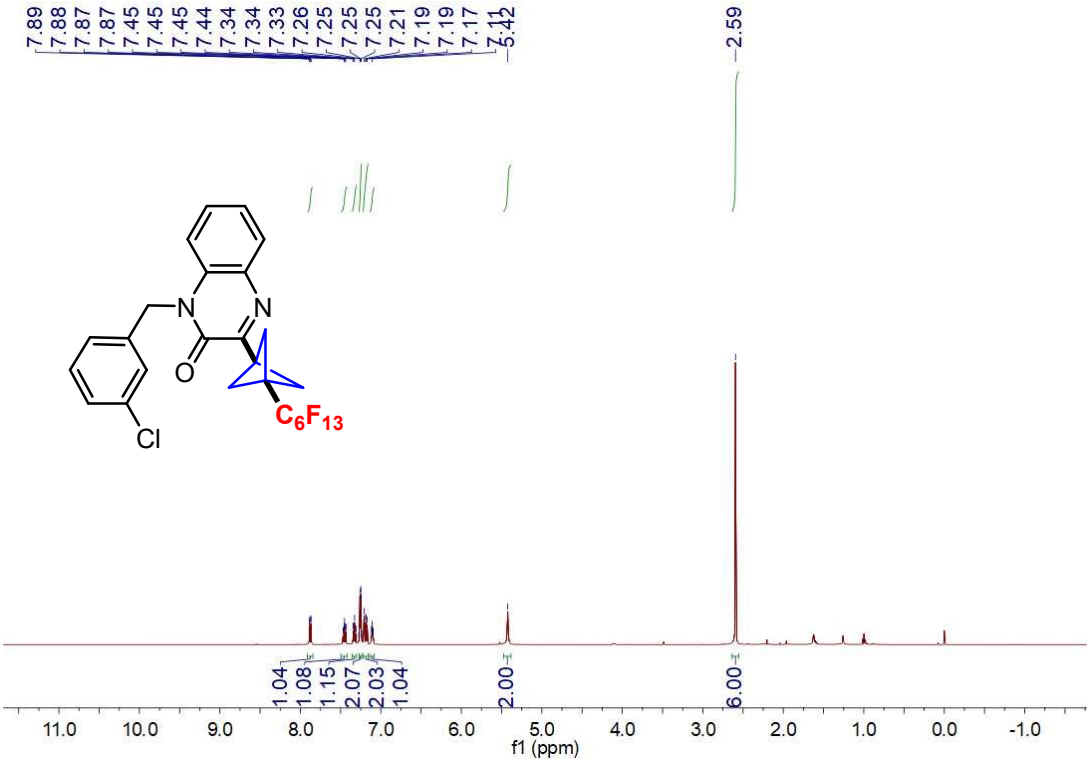
40 ^{13}C NMR (126 MHz, $CDCl_3$)



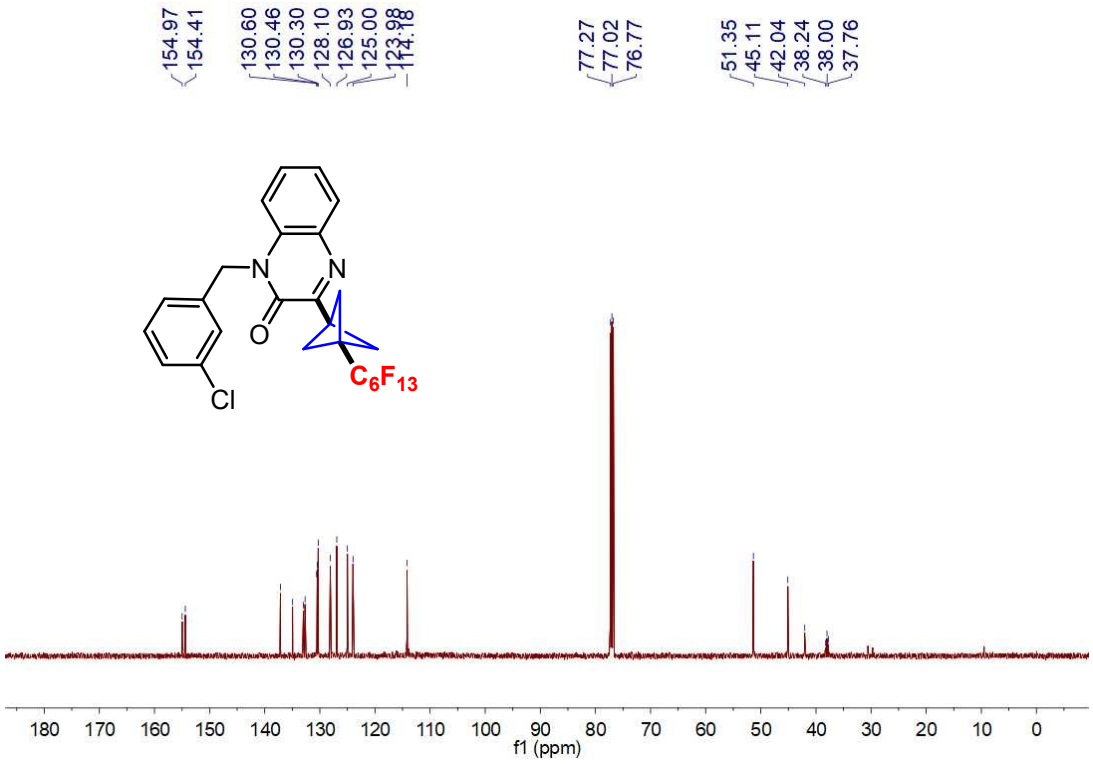
40 ^{19}F NMR (471 MHz, $CDCl_3$)



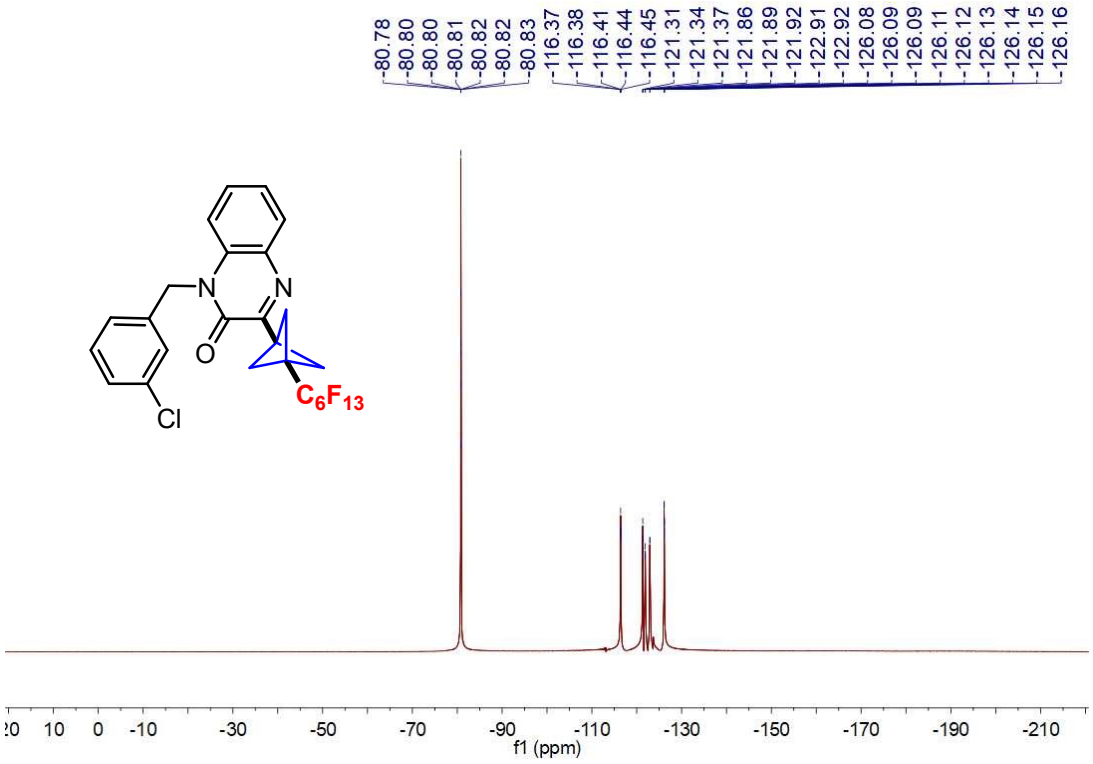
41 ^{1}H NMR (500 MHz, $CDCl_3$)



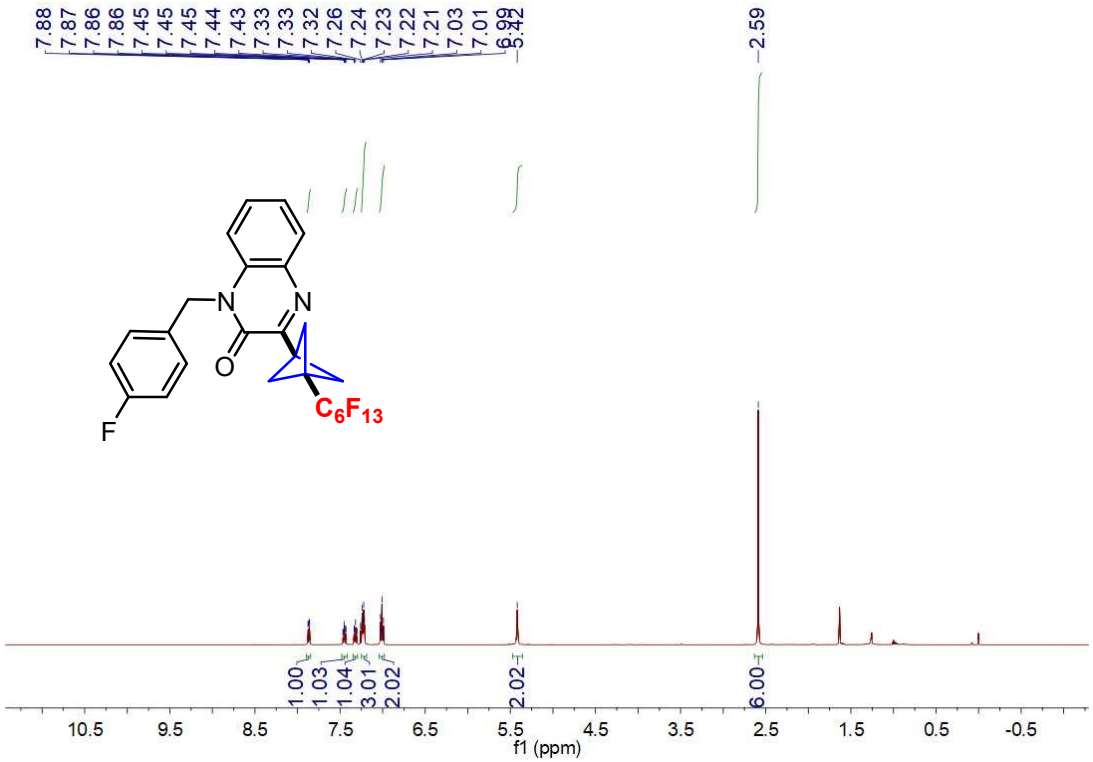
41 ^{13}C NMR (126 MHz, $CDCl_3$)



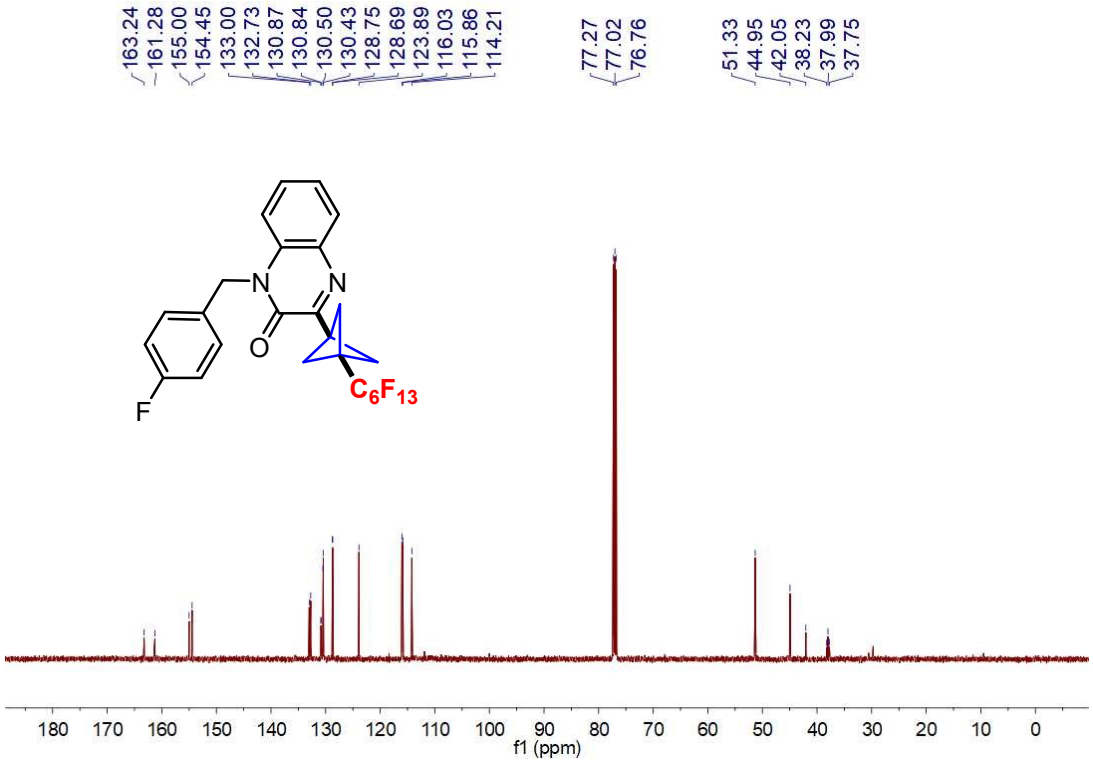
41 ^{19}F NMR (471 MHz, $CDCl_3$)



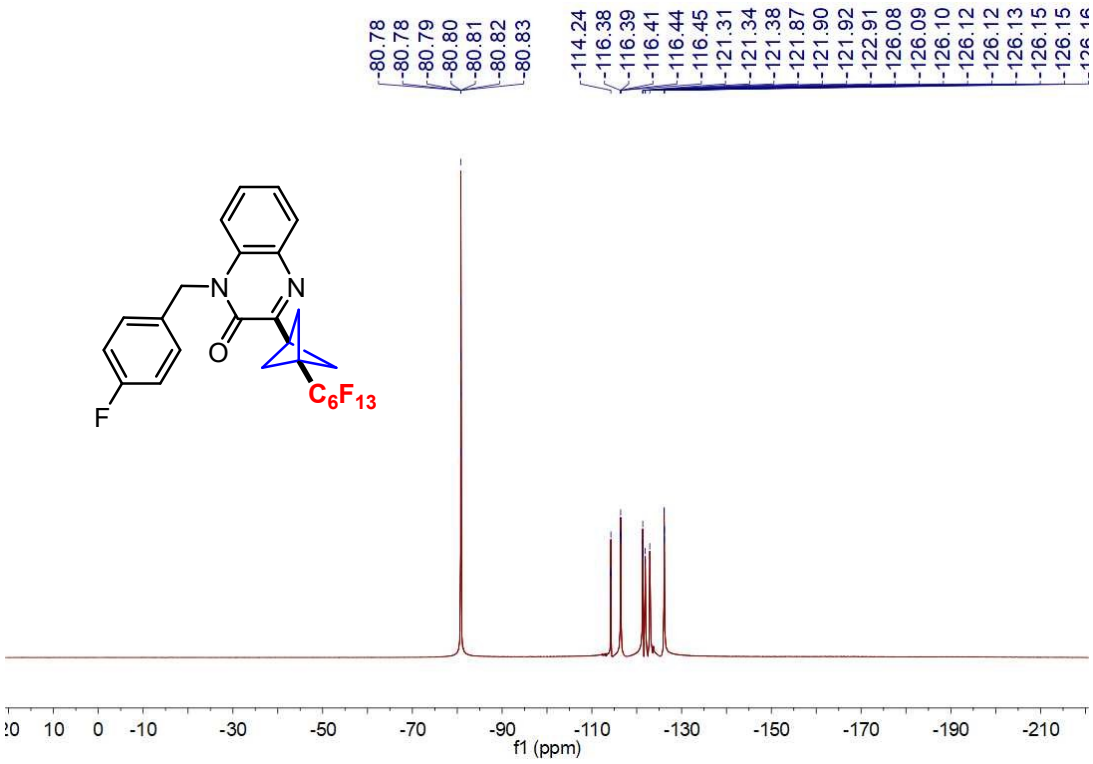
42 ^{1}H NMR (500 MHz, $CDCl_3$)



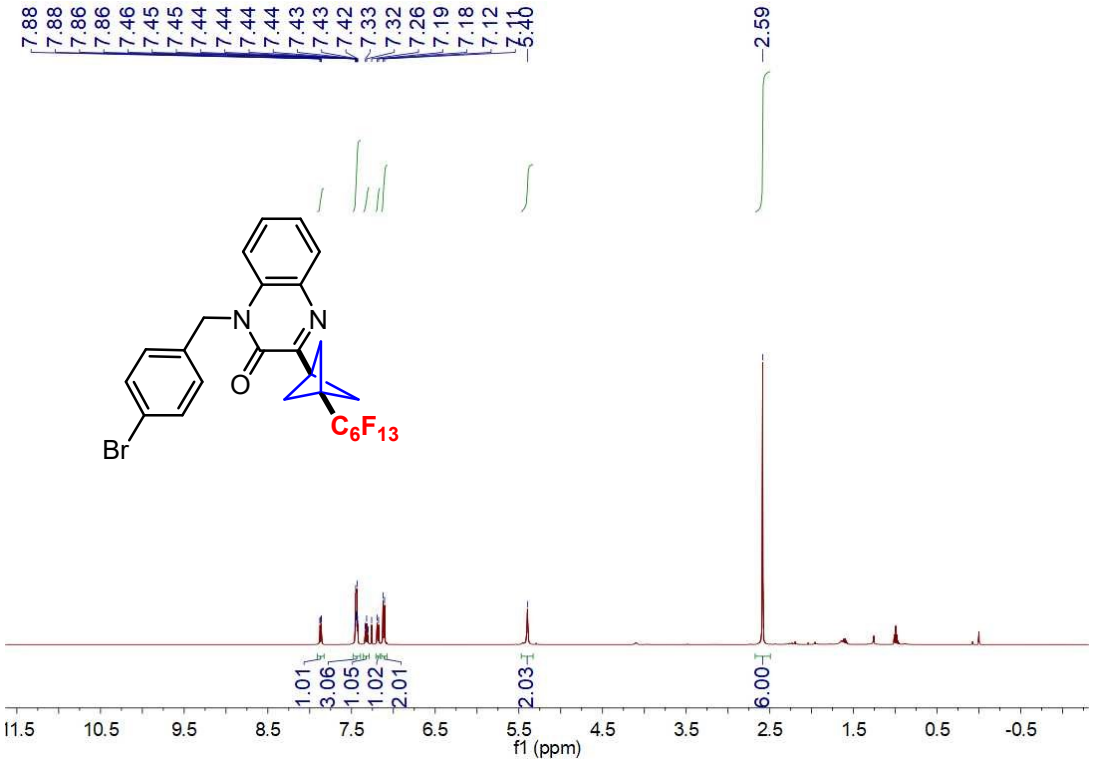
42 ^{13}C NMR (126 MHz, $CDCl_3$)



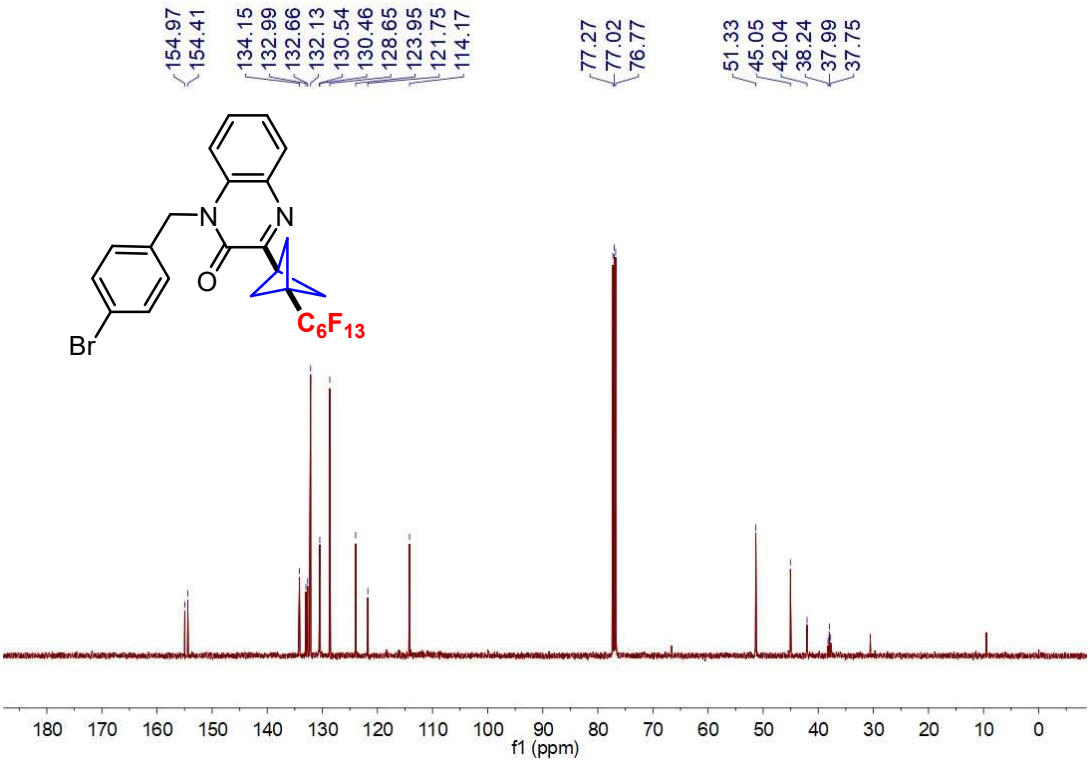
42 ^{19}F NMR (471 MHz, $CDCl_3$)



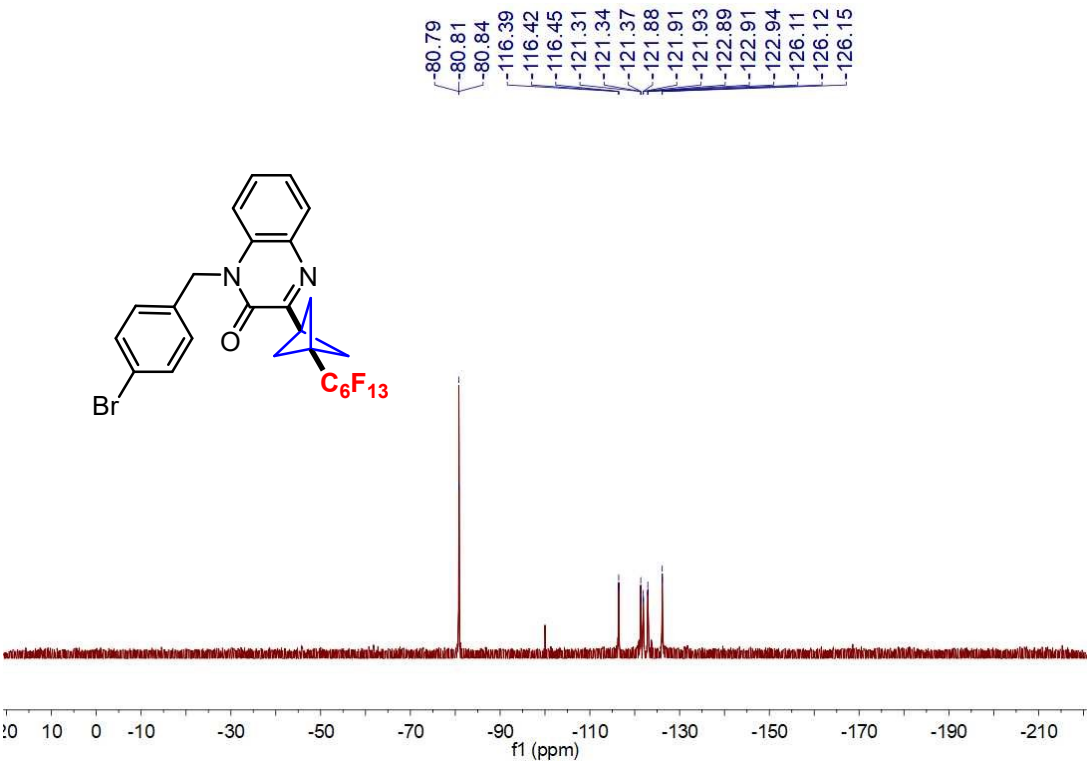
43 ^{1}H NMR (500 MHz, $CDCl_3$)



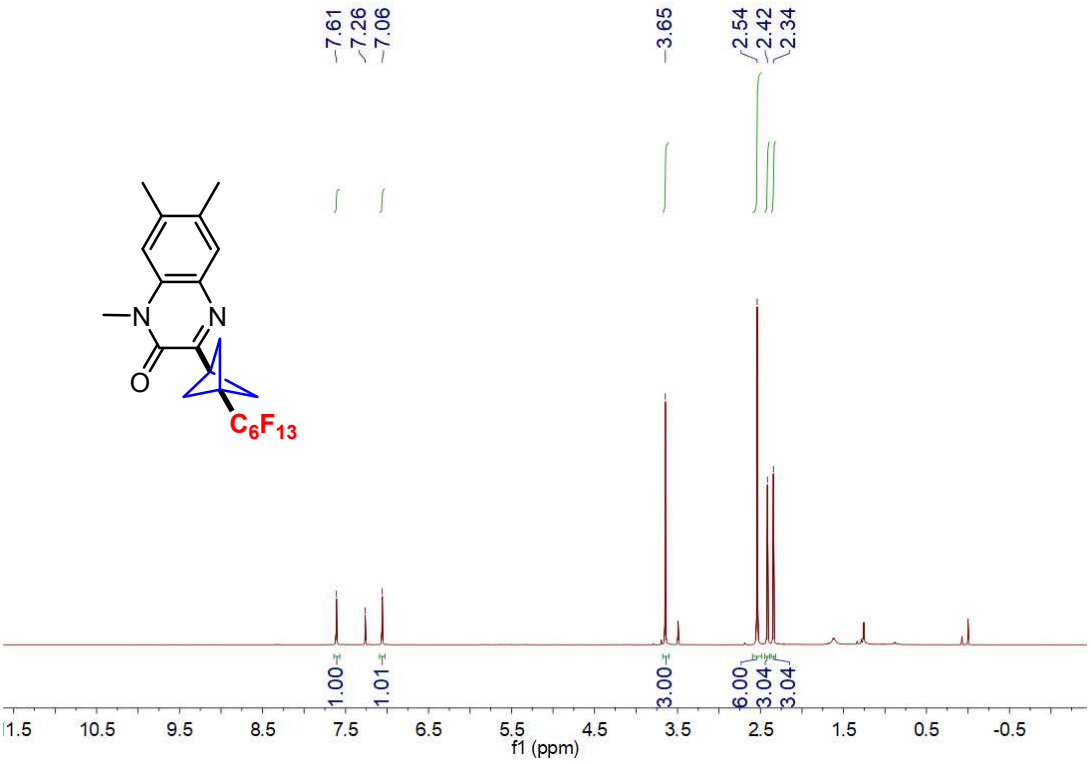
43 ^{13}C NMR (126 MHz, $CDCl_3$)



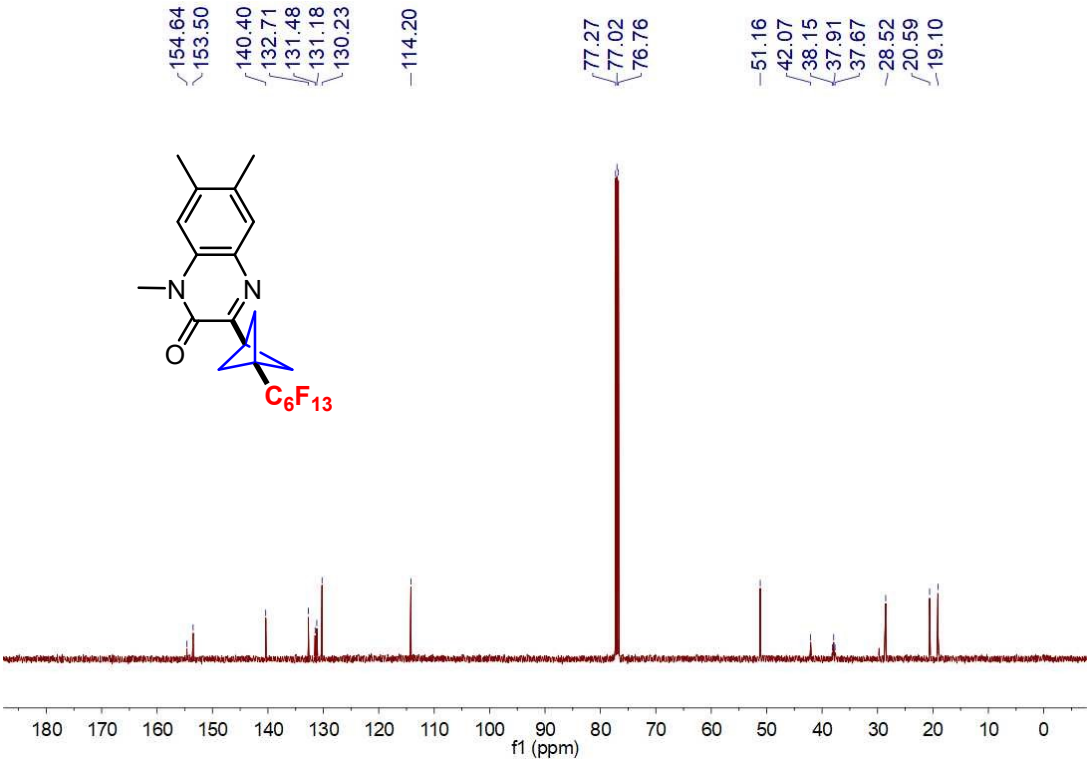
43 ^{19}F NMR (471 MHz, $CDCl_3$)



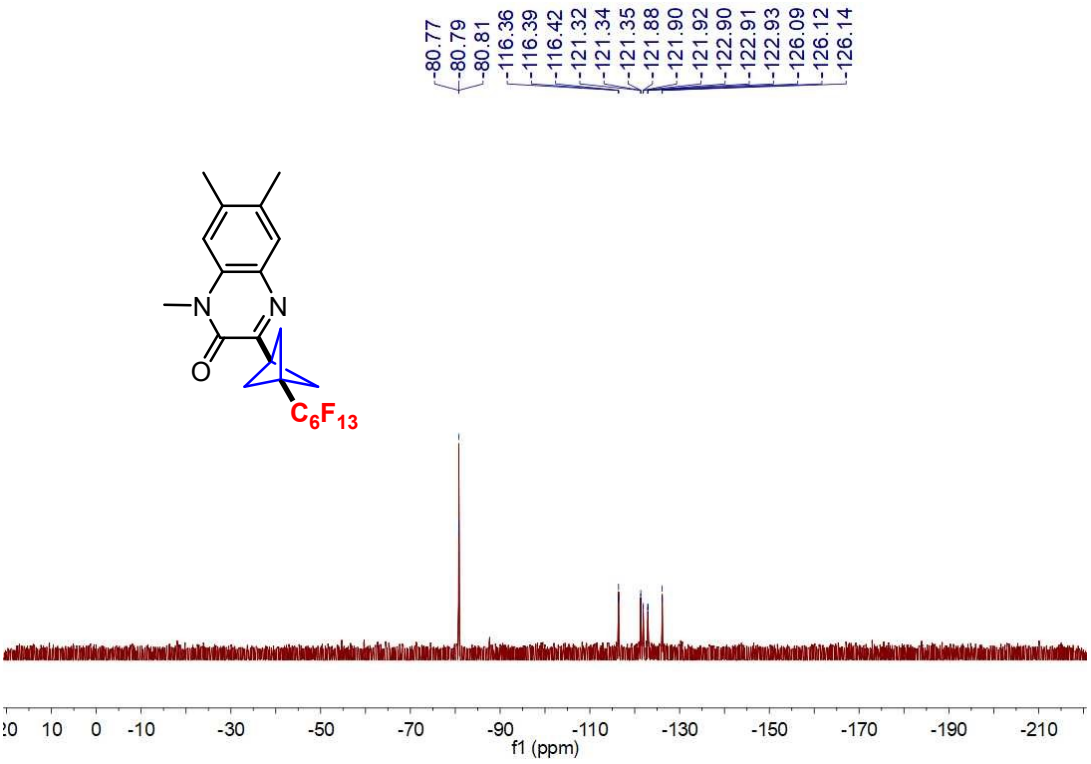
44 ^{1}H NMR (500 MHz, $CDCl_3$)



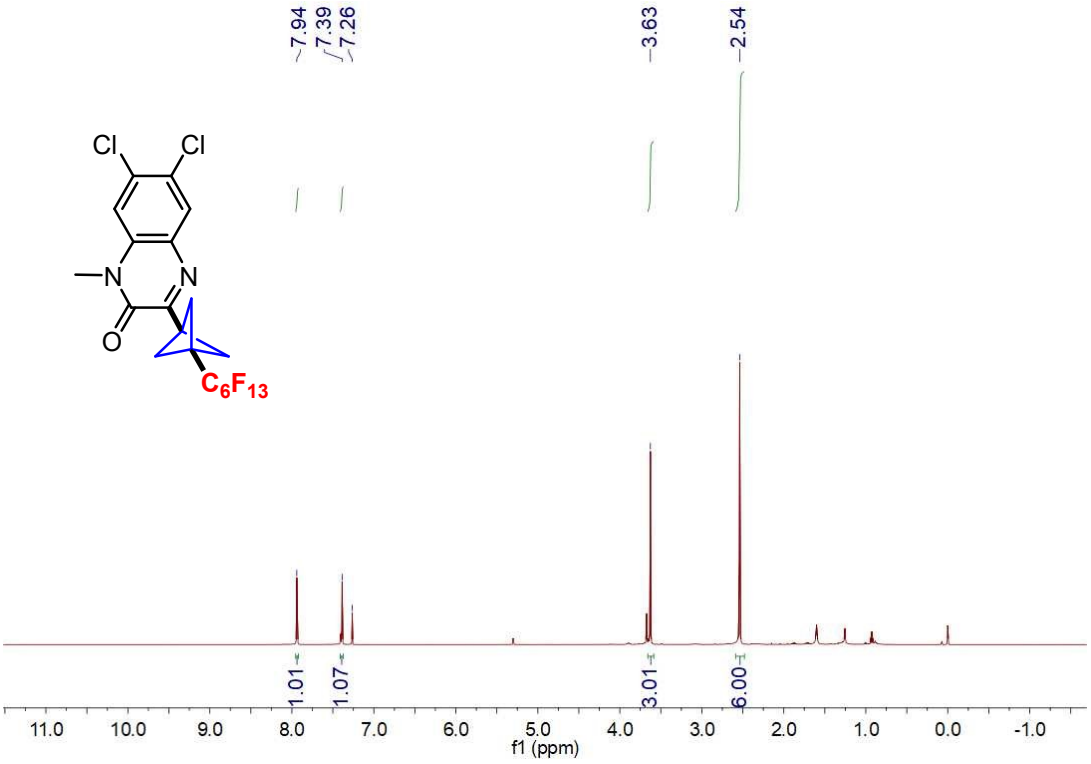
44 ^{13}C NMR (126 MHz, $CDCl_3$)



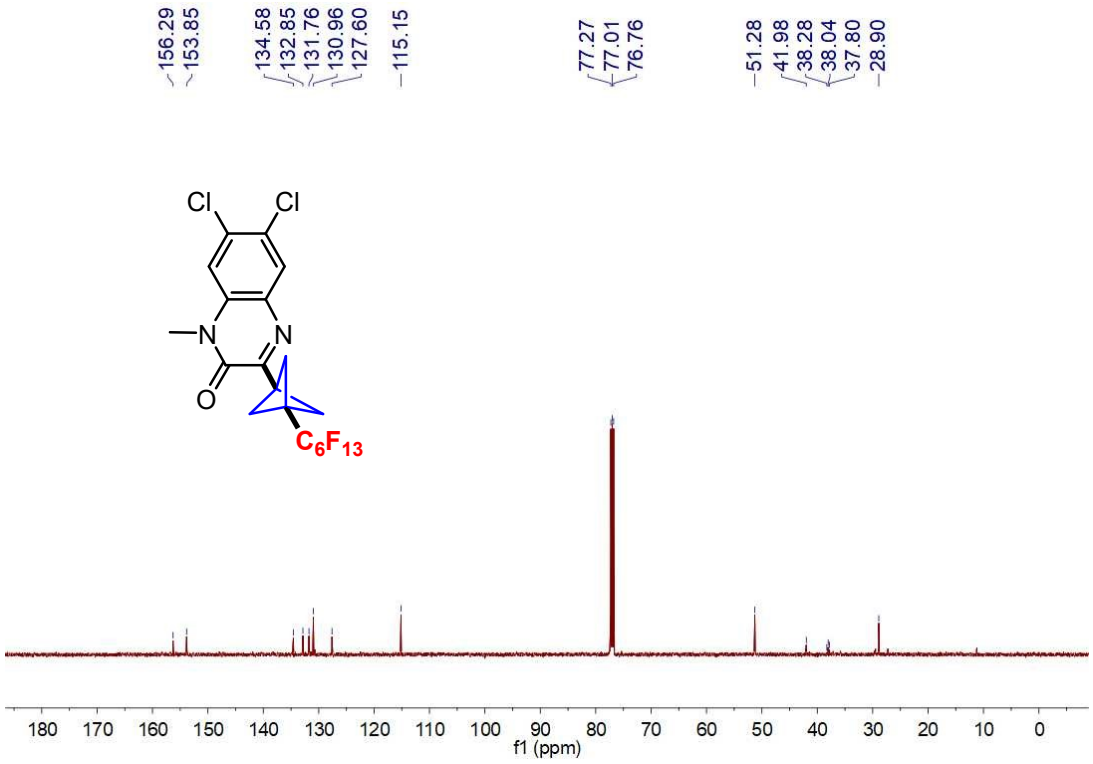
44 ^{19}F NMR (471 MHz, $CDCl_3$)



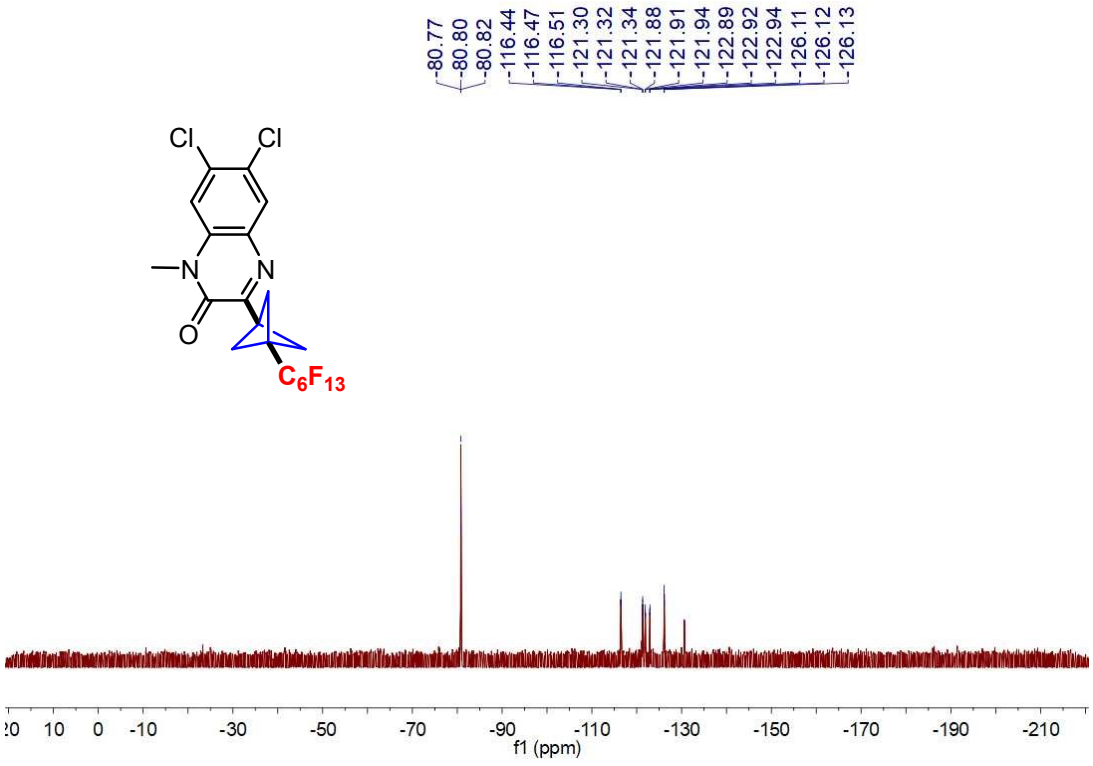
45 ^{1}H NMR (500 MHz, $CDCl_3$)



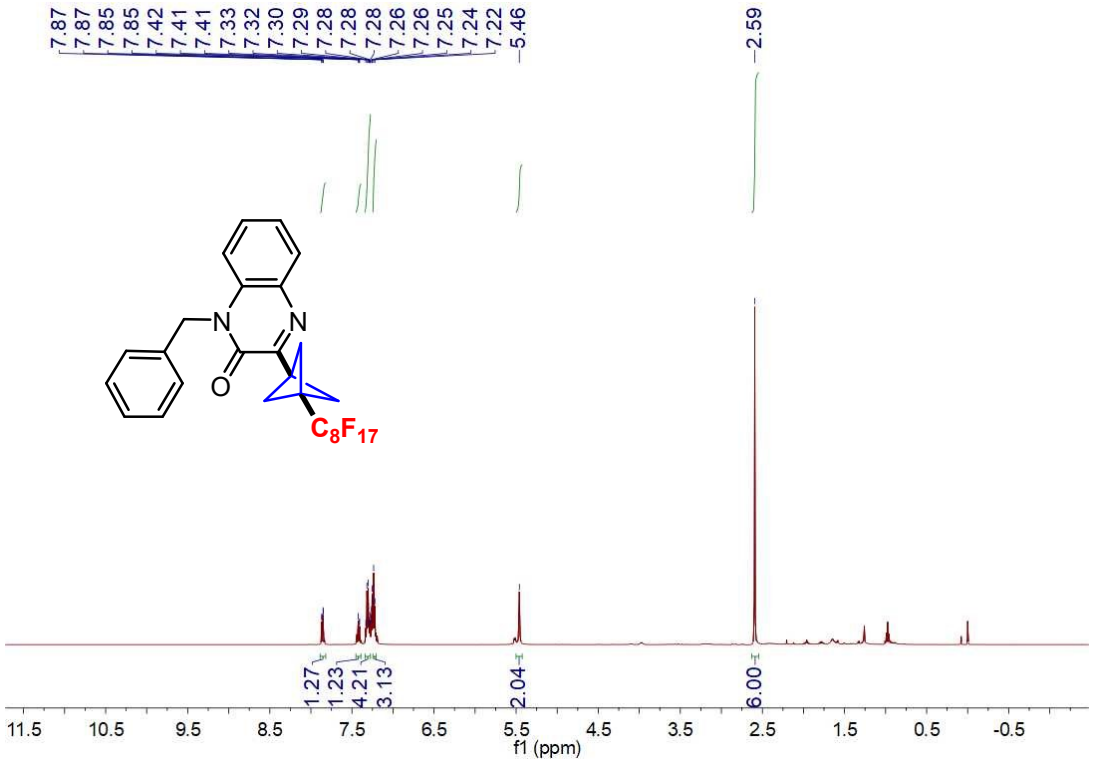
45 ^{13}C NMR (126 MHz, $CDCl_3$)



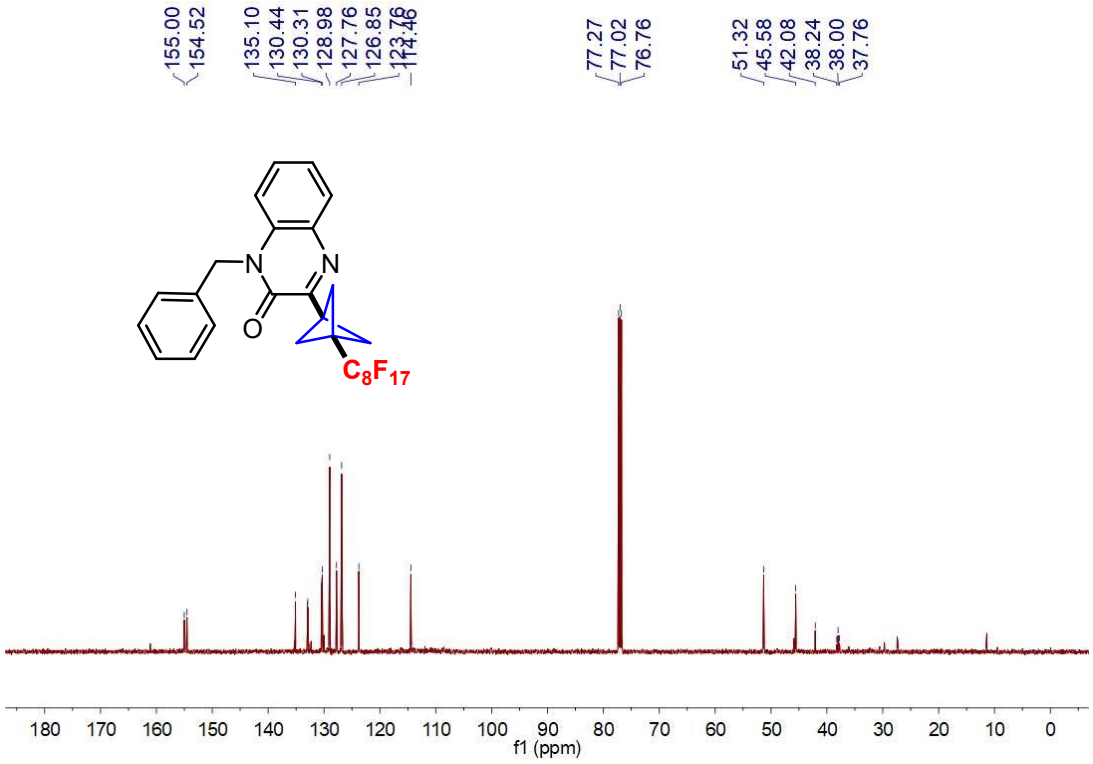
45 ^{19}F NMR(471 MHz, $CDCl_3$)



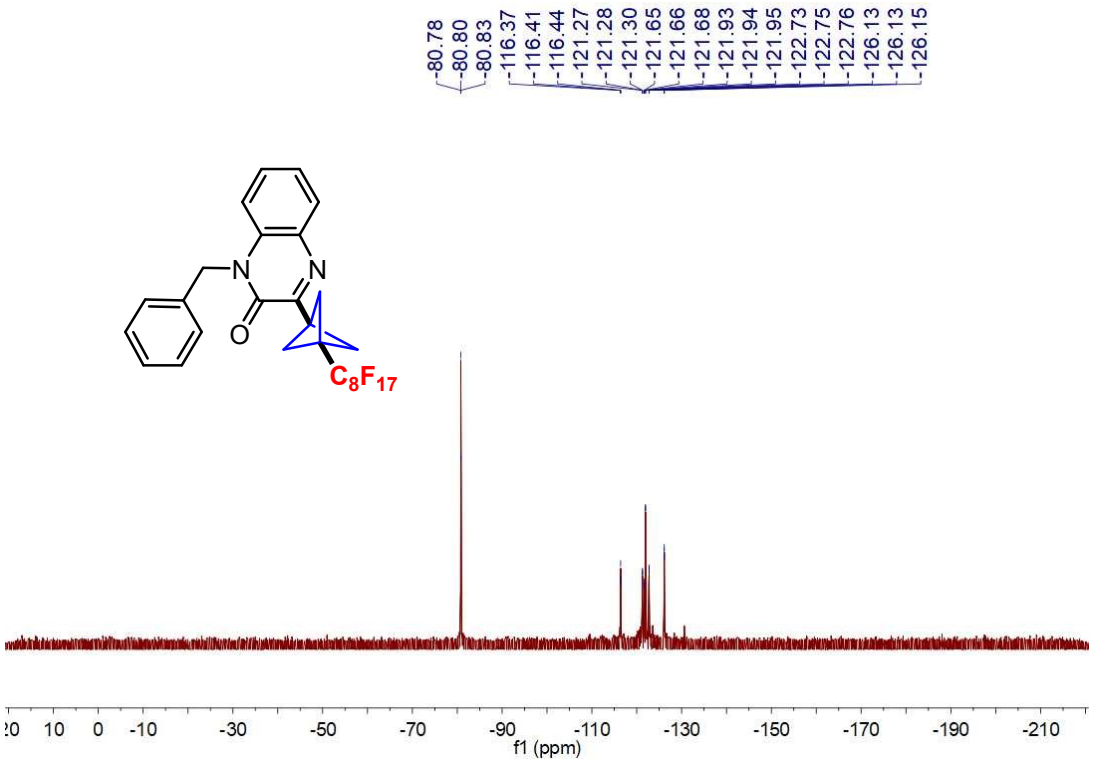
46 ^{1}H NMR (500 MHz, $CDCl_3$)



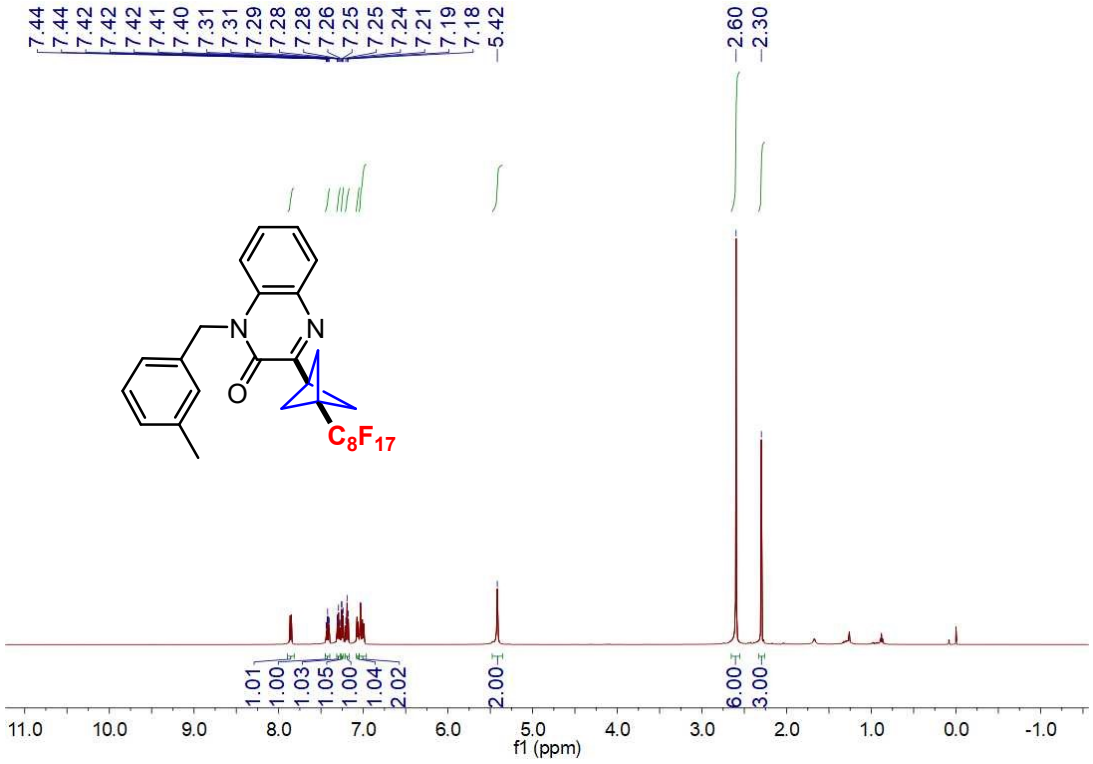
46 ^{13}C NMR (126 MHz, $CDCl_3$)



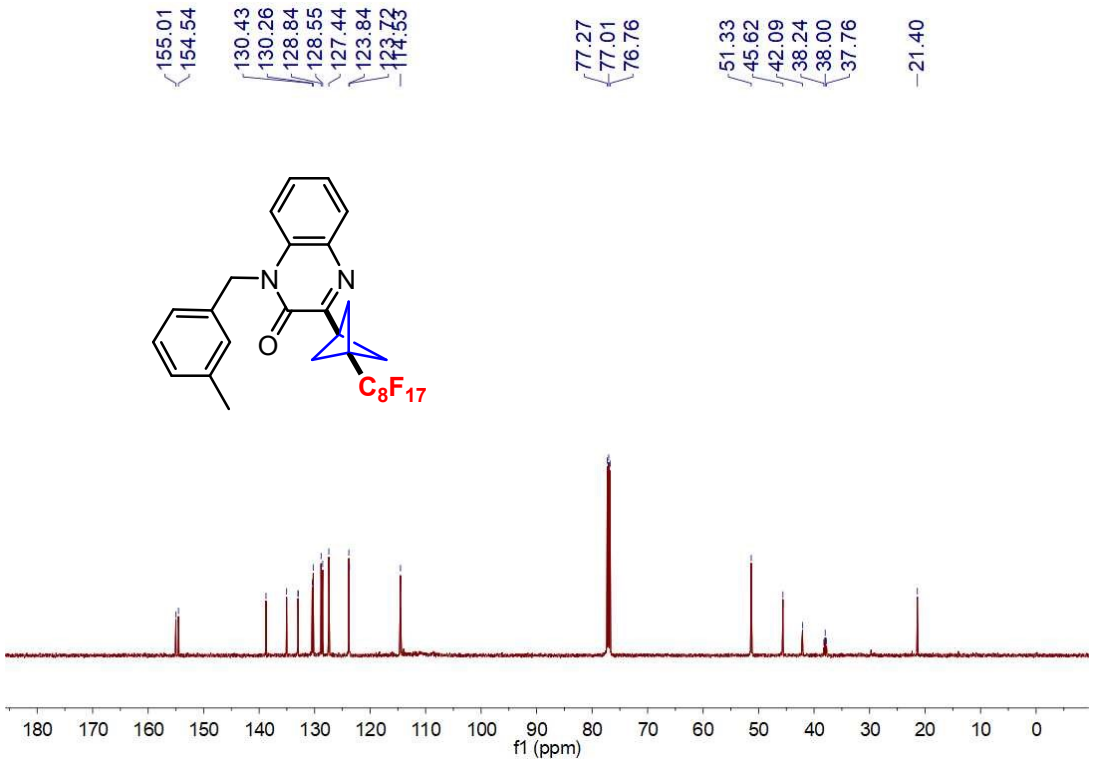
46 ^{19}F NMR (471 MHz, $CDCl_3$)



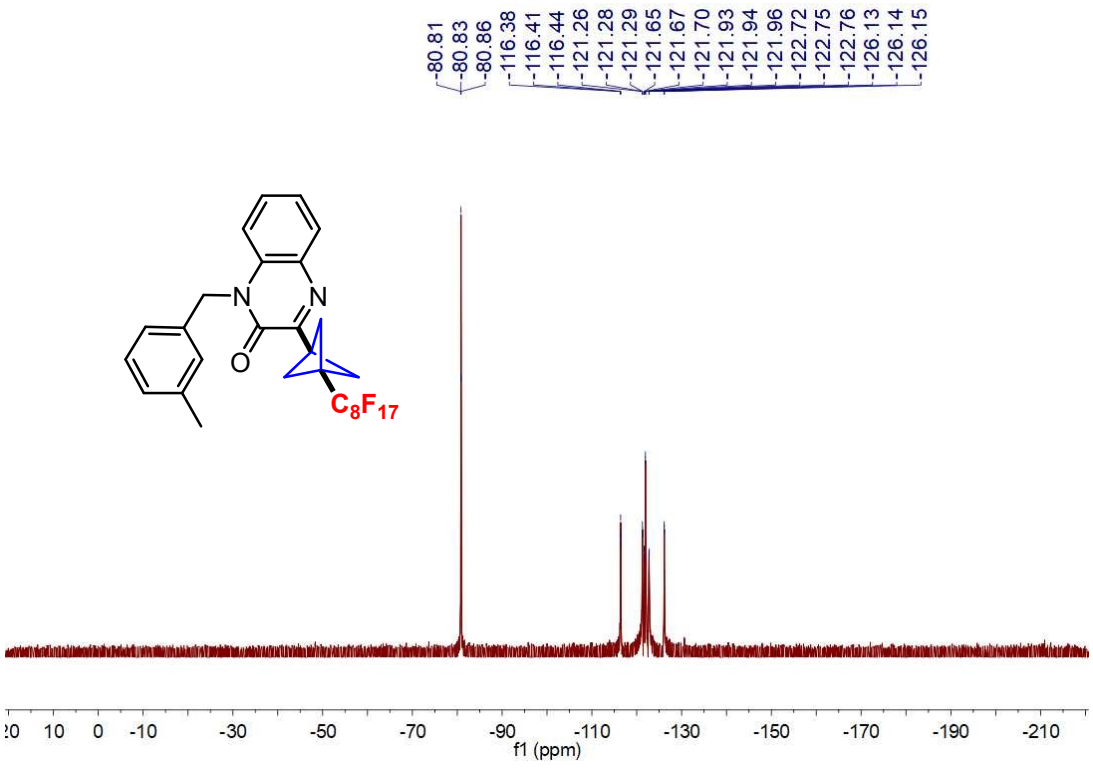
47 ^{1}H NMR (500 MHz, $CDCl_3$)



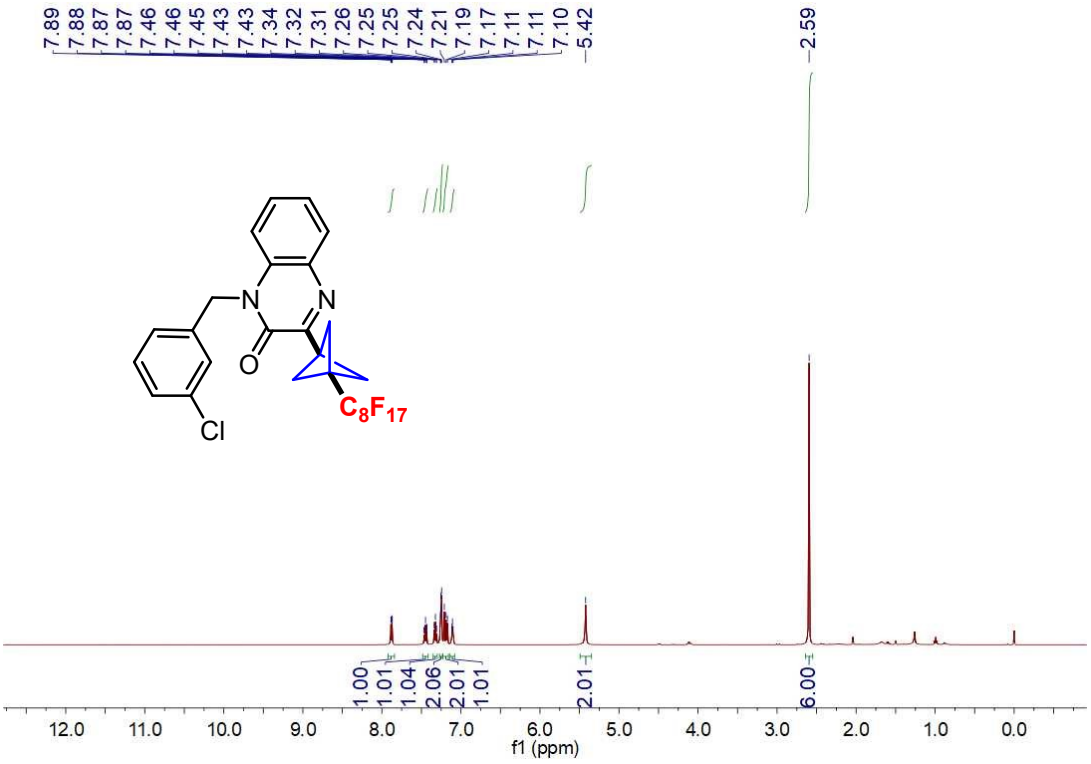
47 ^{13}C NMR (126 MHz, $CDCl_3$)



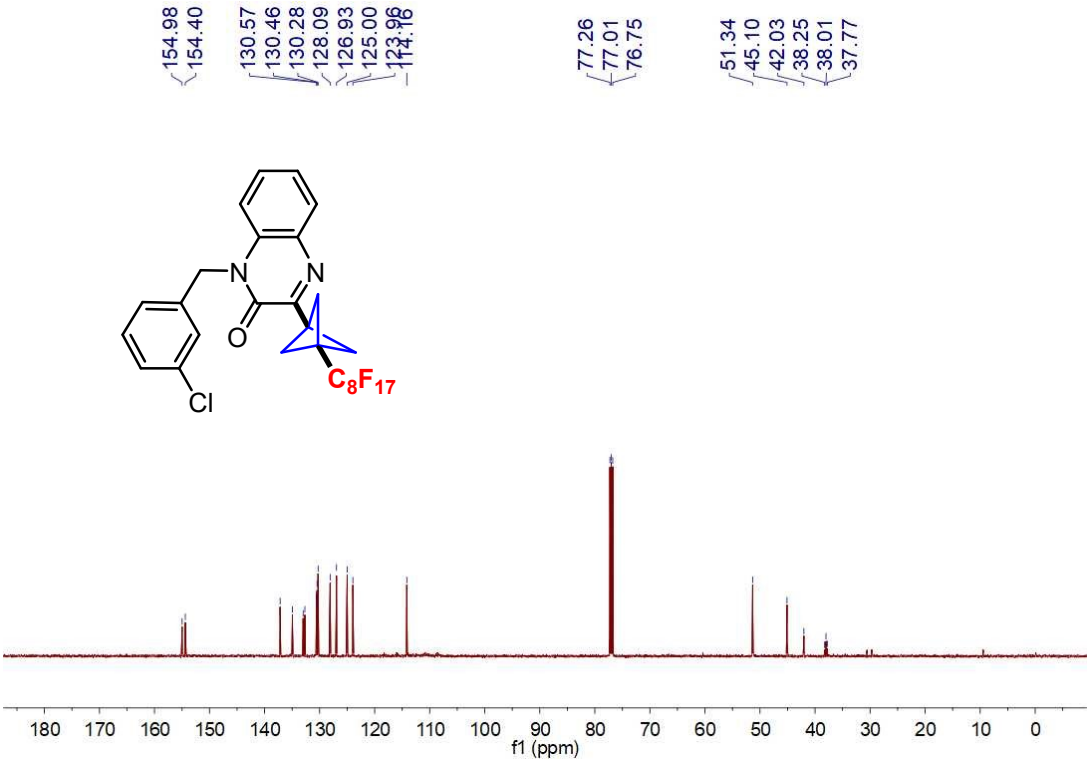
47 ^{19}F NMR (471 MHz, $CDCl_3$)



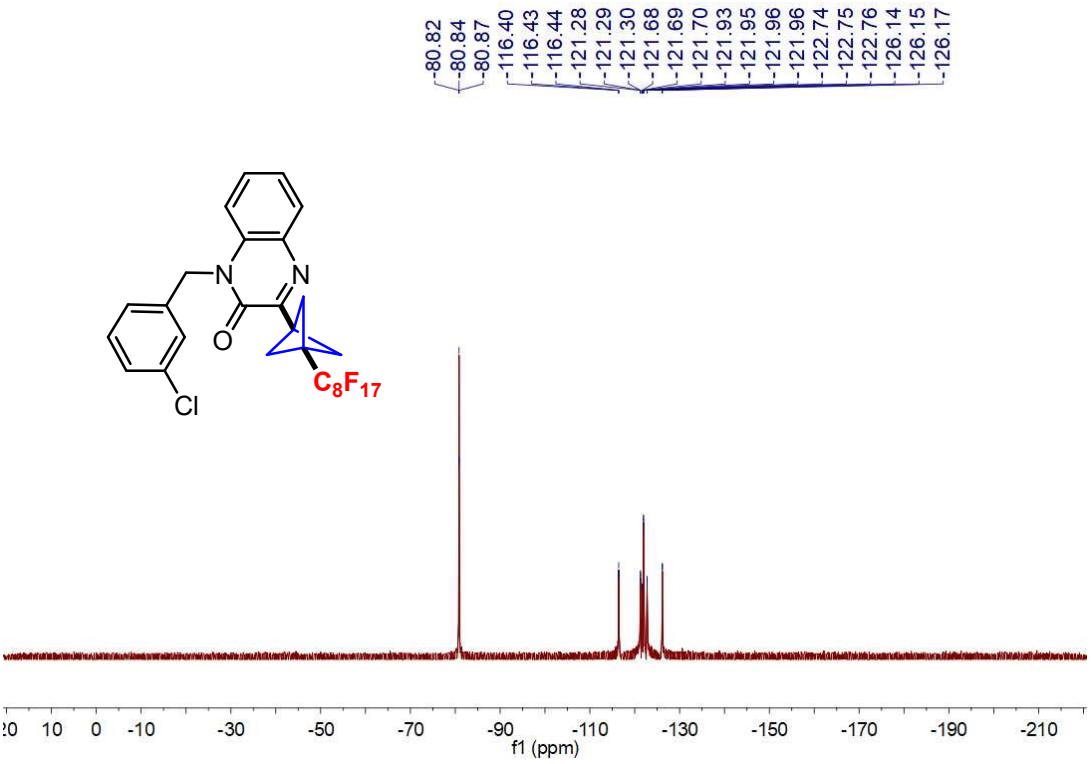
48 ^{1}H NMR (500 MHz, $CDCl_3$)



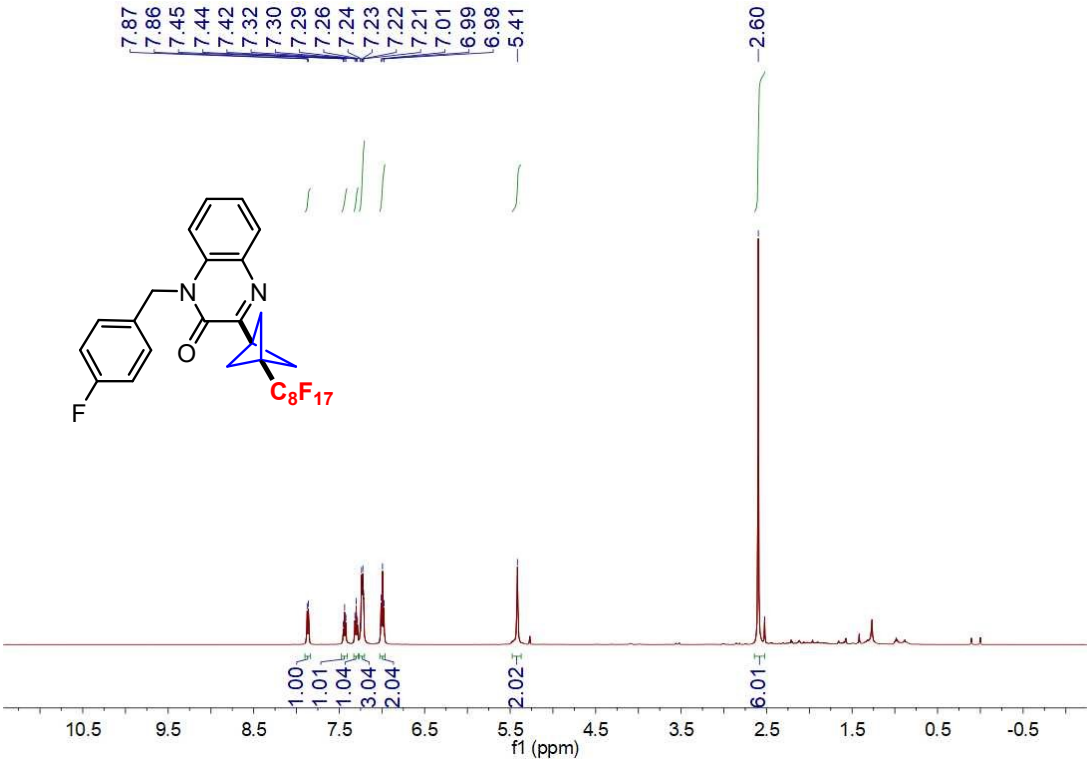
48 ^{13}C NMR (126 MHz, $CDCl_3$)



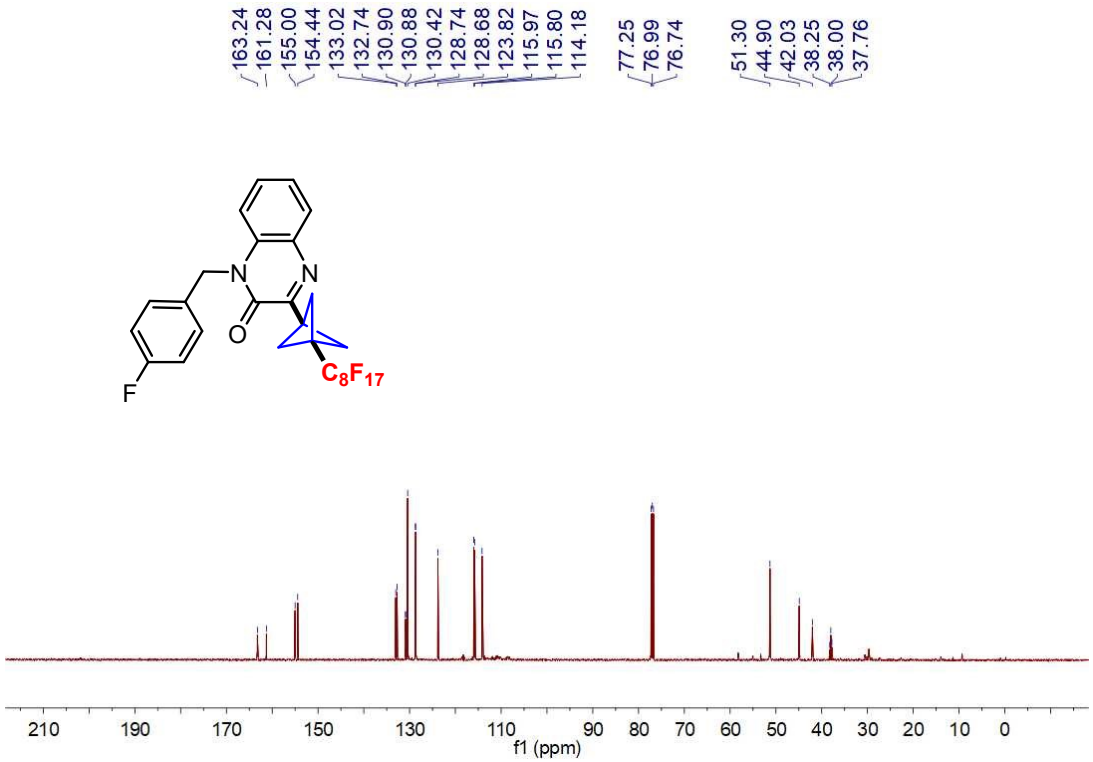
48 ^{19}F NMR (471 MHz, $CDCl_3$)



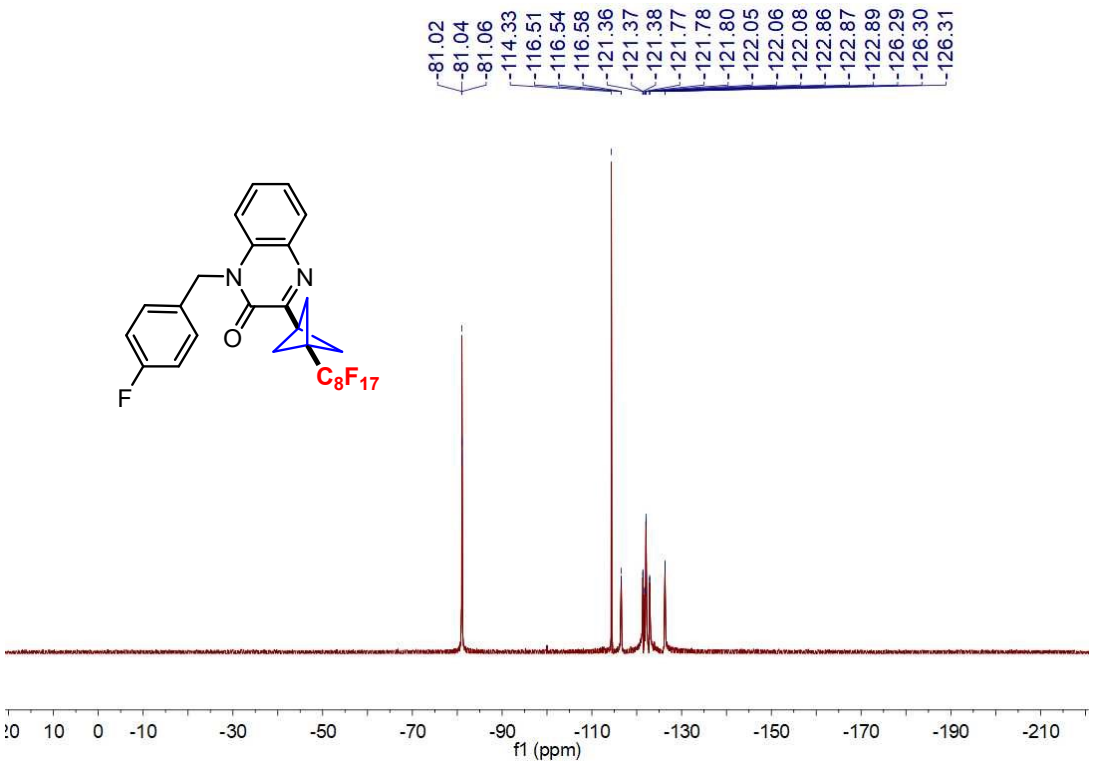
49 ^{1}H NMR (500 MHz, $CDCl_3$)



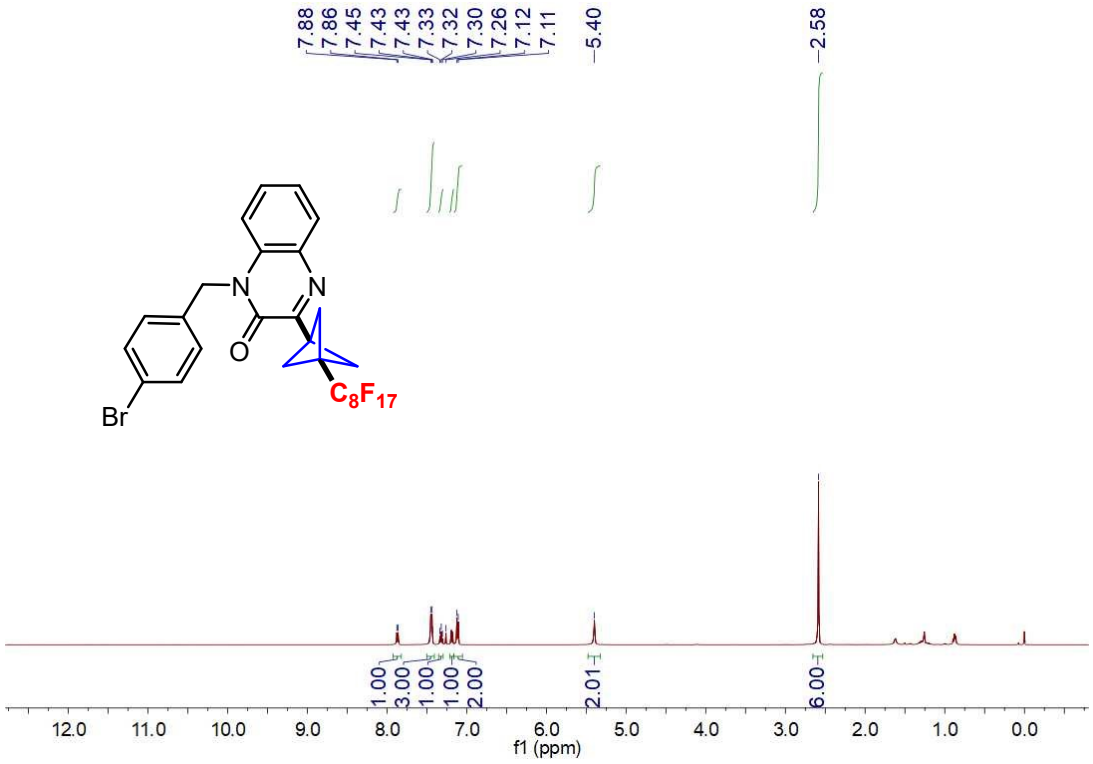
49 ^{13}C NMR (126 MHz, $CDCl_3$)



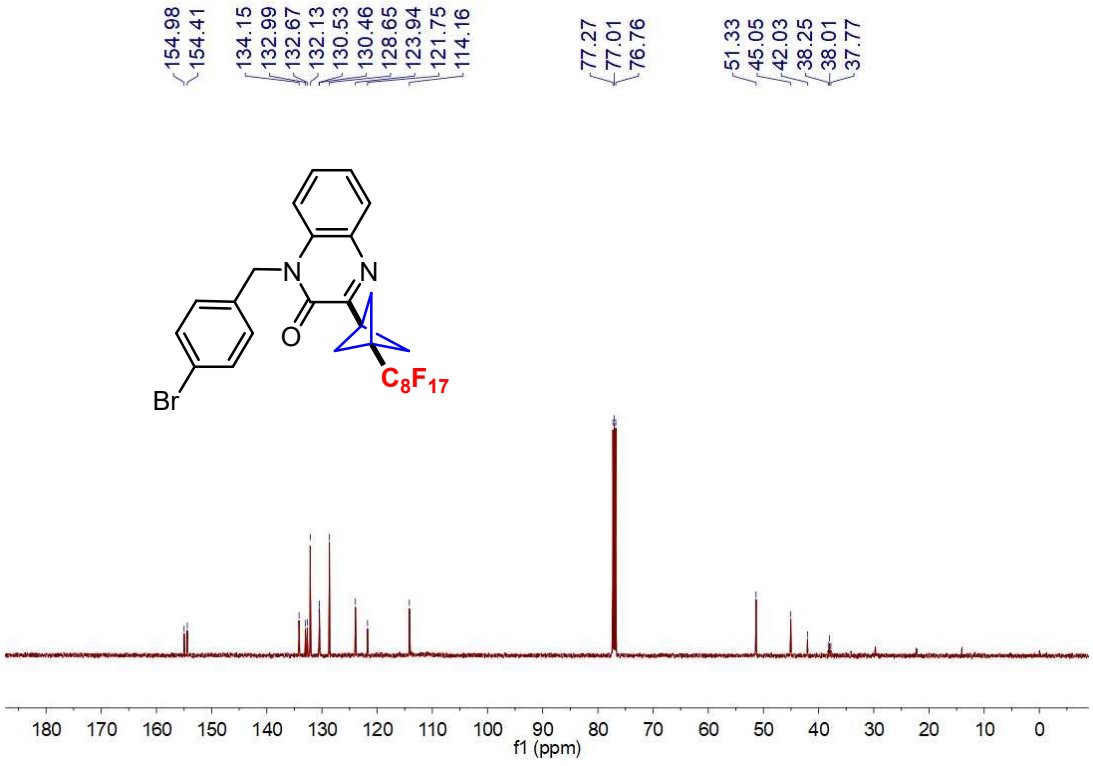
49 ^{19}F NMR (471 MHz, $CDCl_3$)



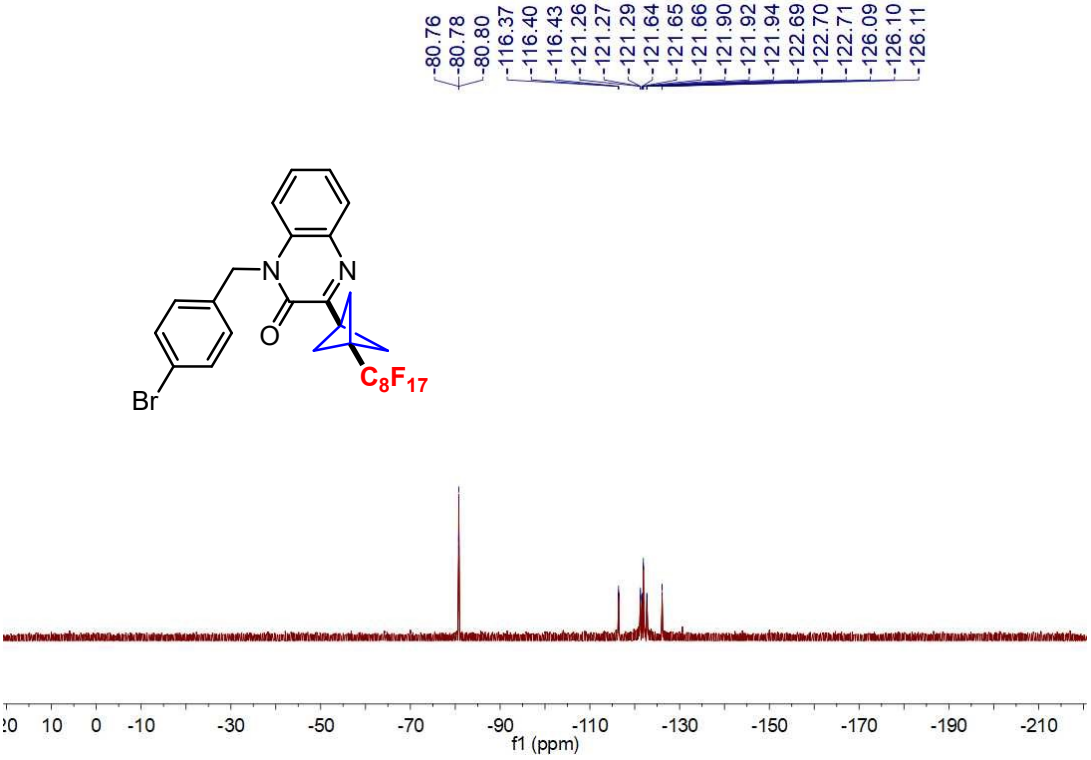
50 ^{1}H NMR (500 MHz, $CDCl_3$)



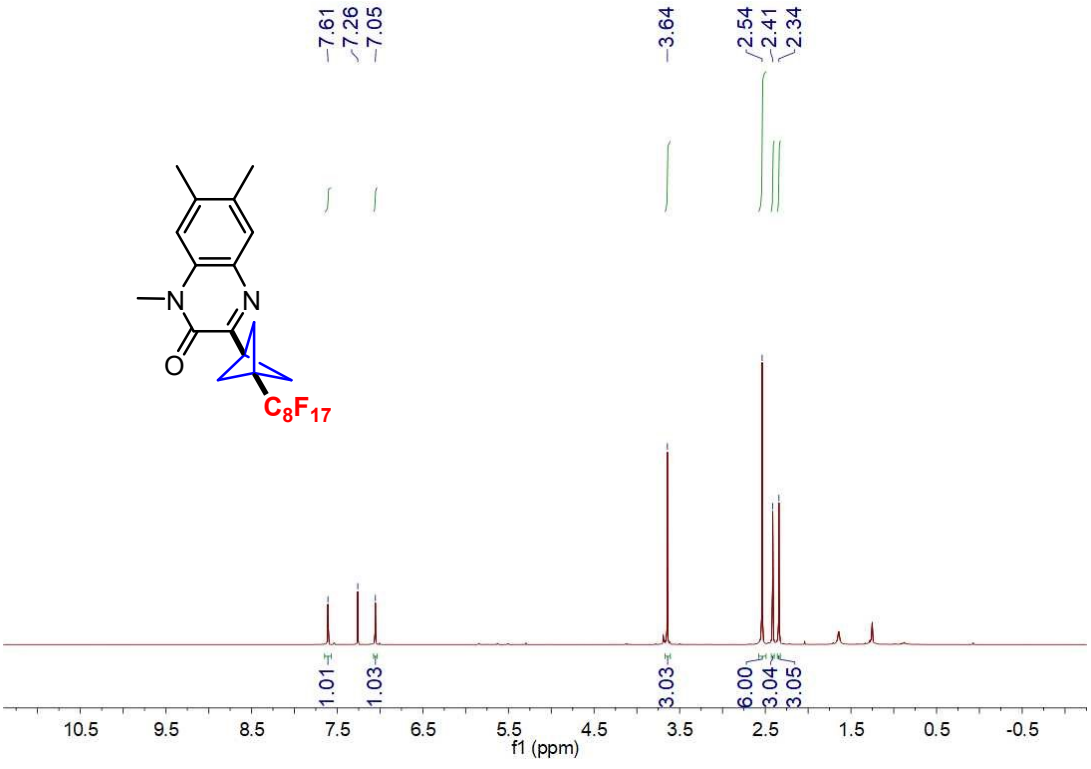
50 ^{13}C NMR (126 MHz, $CDCl_3$)



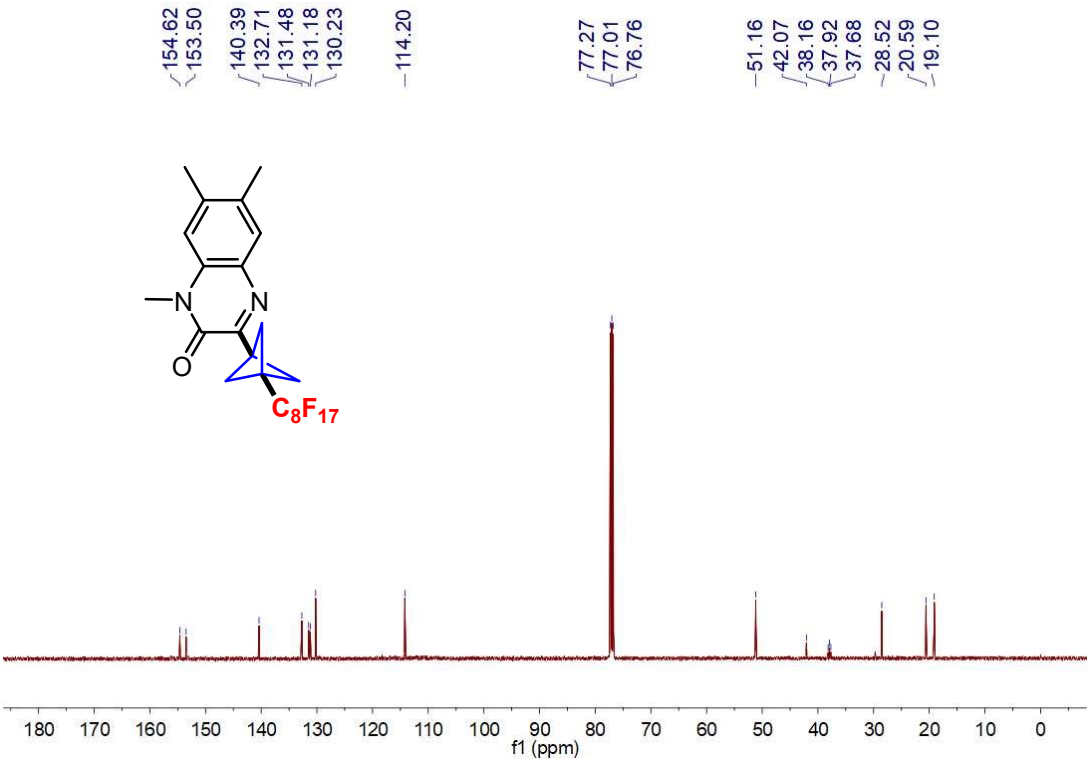
50 ^{19}F NMR (471 MHz, $CDCl_3$)



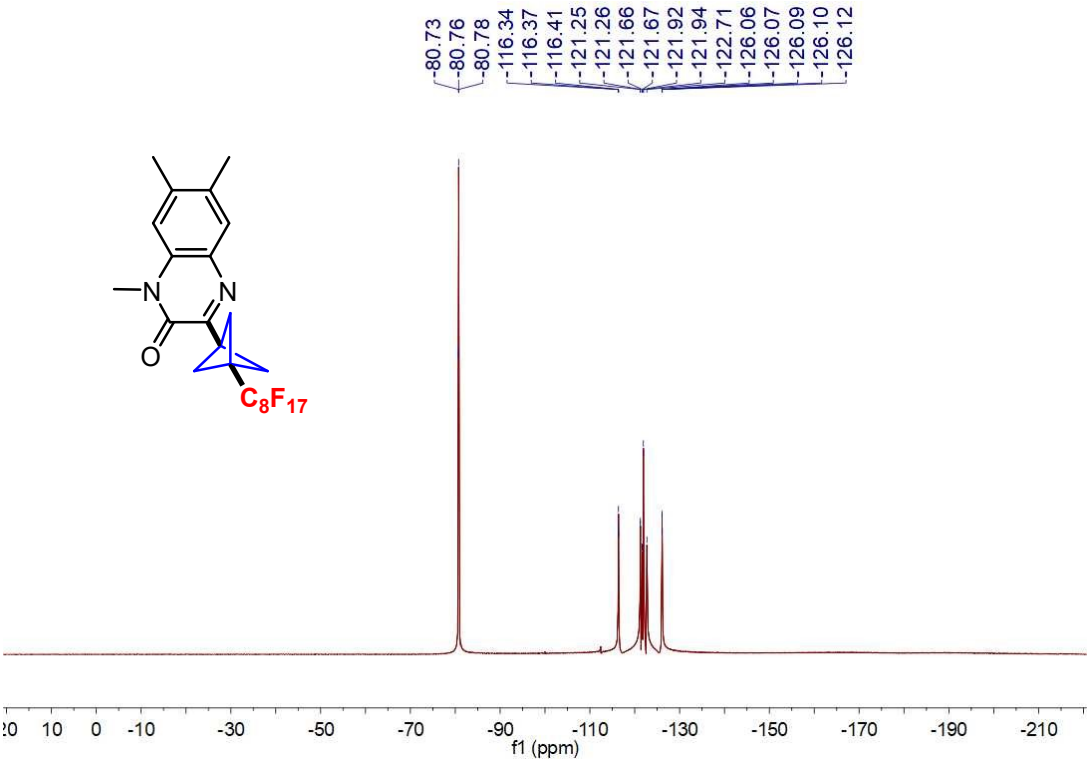
51 ^{1}H NMR (500 MHz, $CDCl_3$)



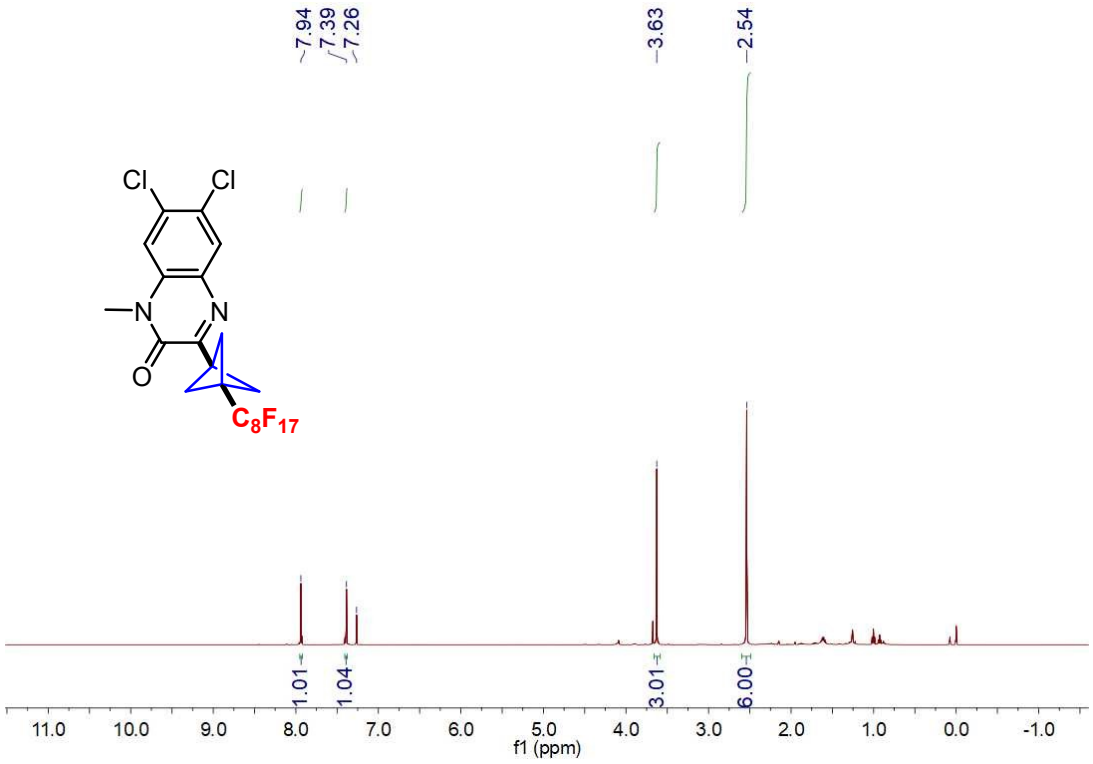
51 ^{13}C NMR (126 MHz, $CDCl_3$)



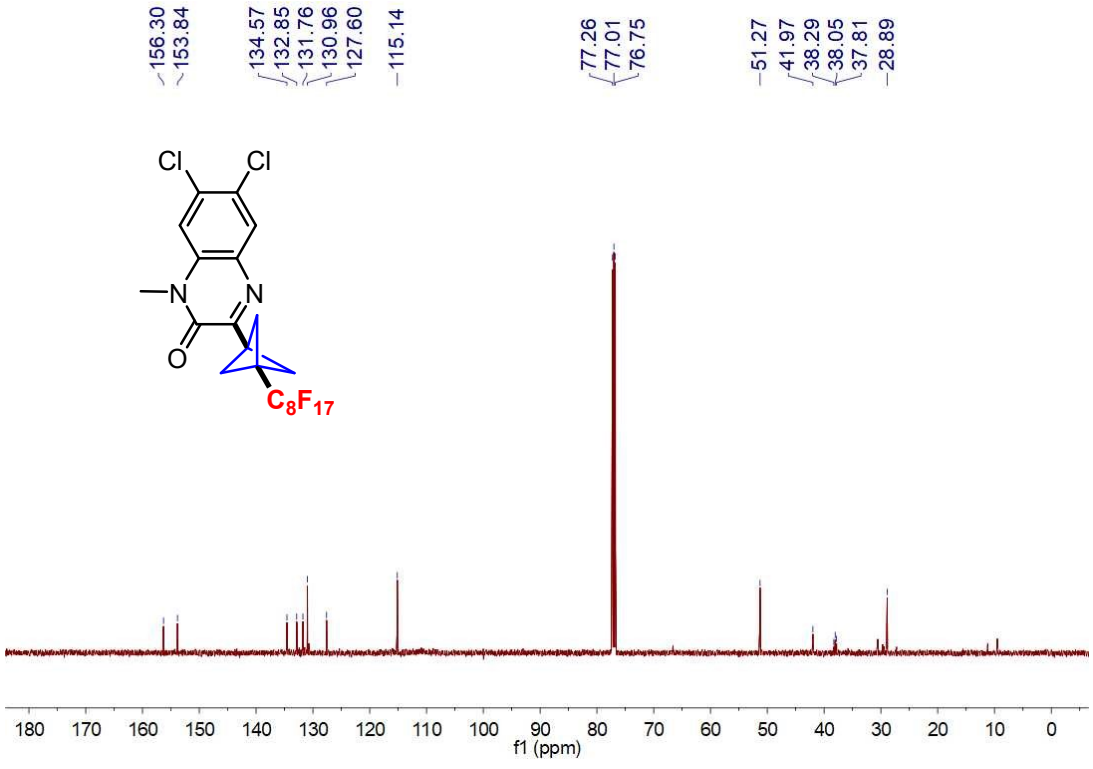
51 ^{19}F NMR (471 MHz, $CDCl_3$)



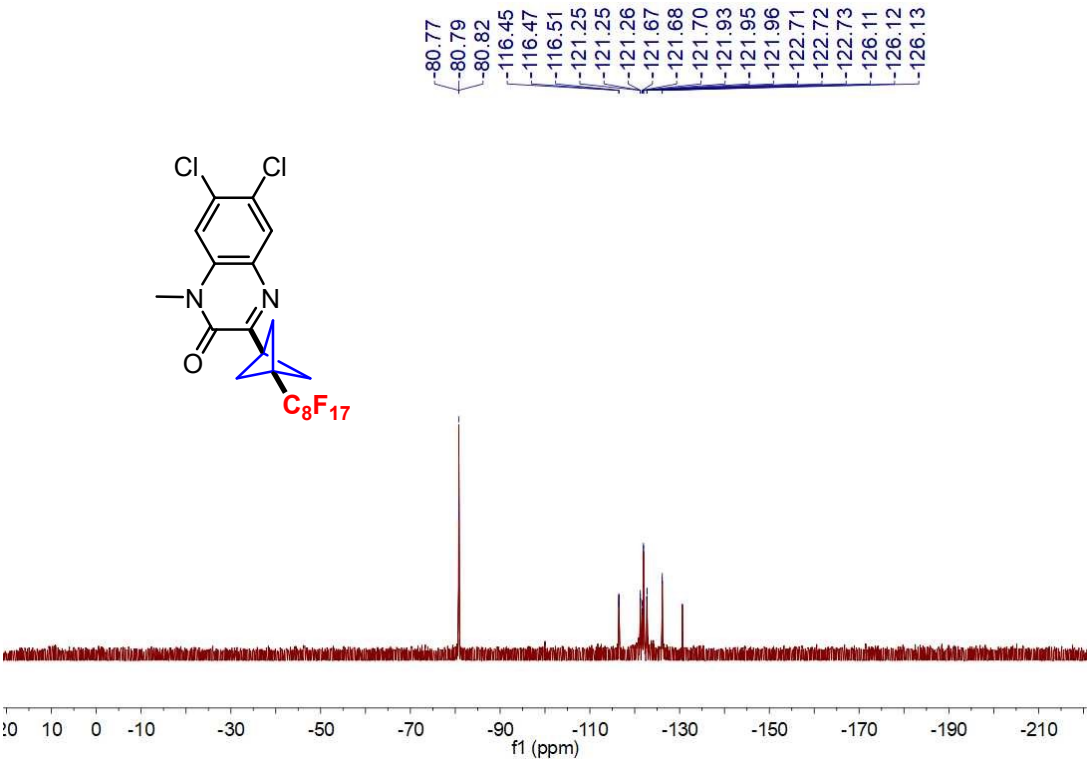
52 ^{1}H NMR (500 MHz, $CDCl_3$)



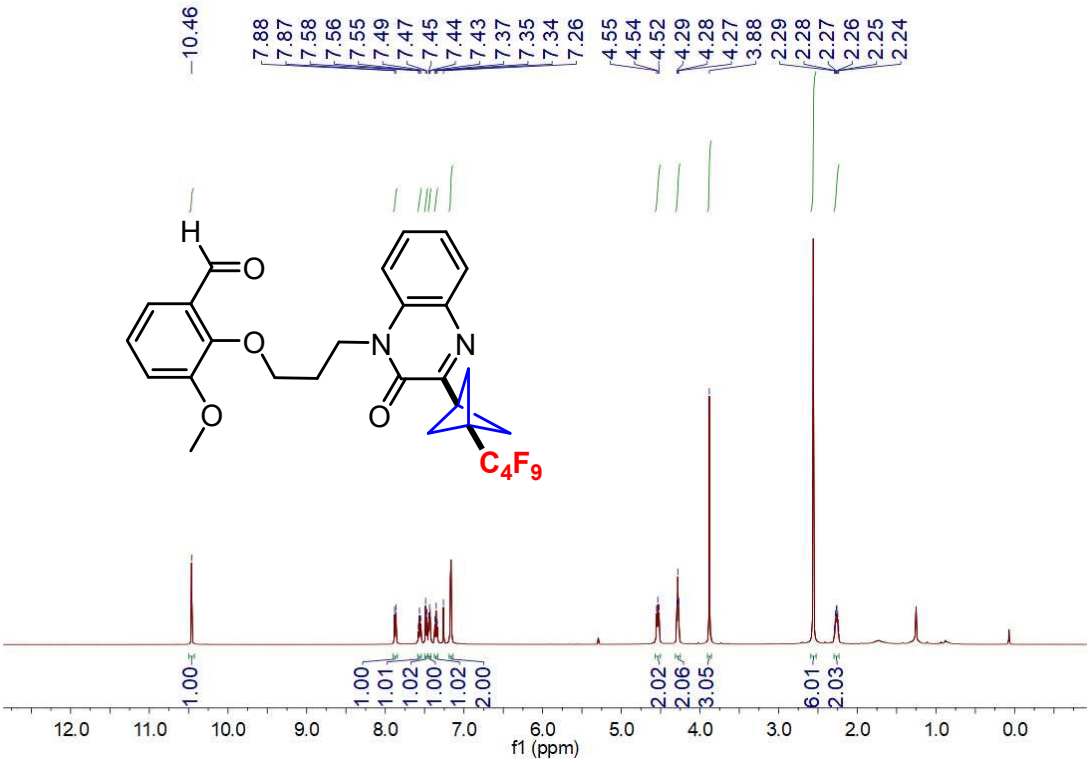
52 ^{13}C NMR (126 MHz, $CDCl_3$)



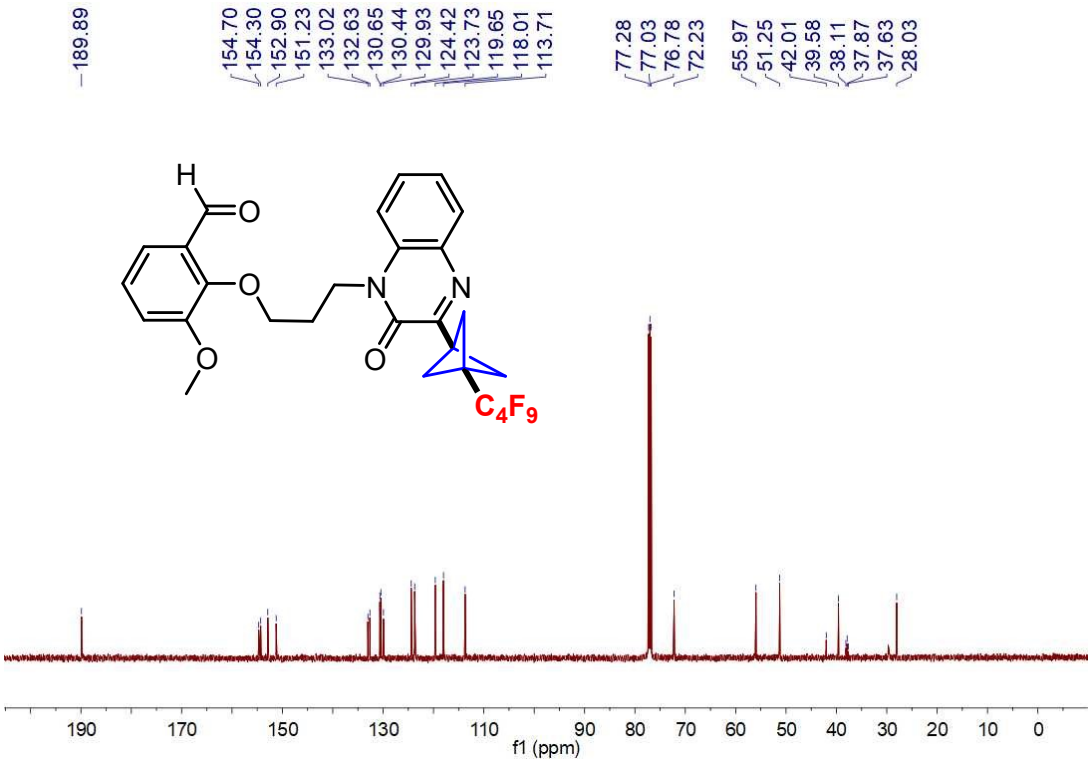
52 ^{19}F NMR (471 MHz, $CDCl_3$)



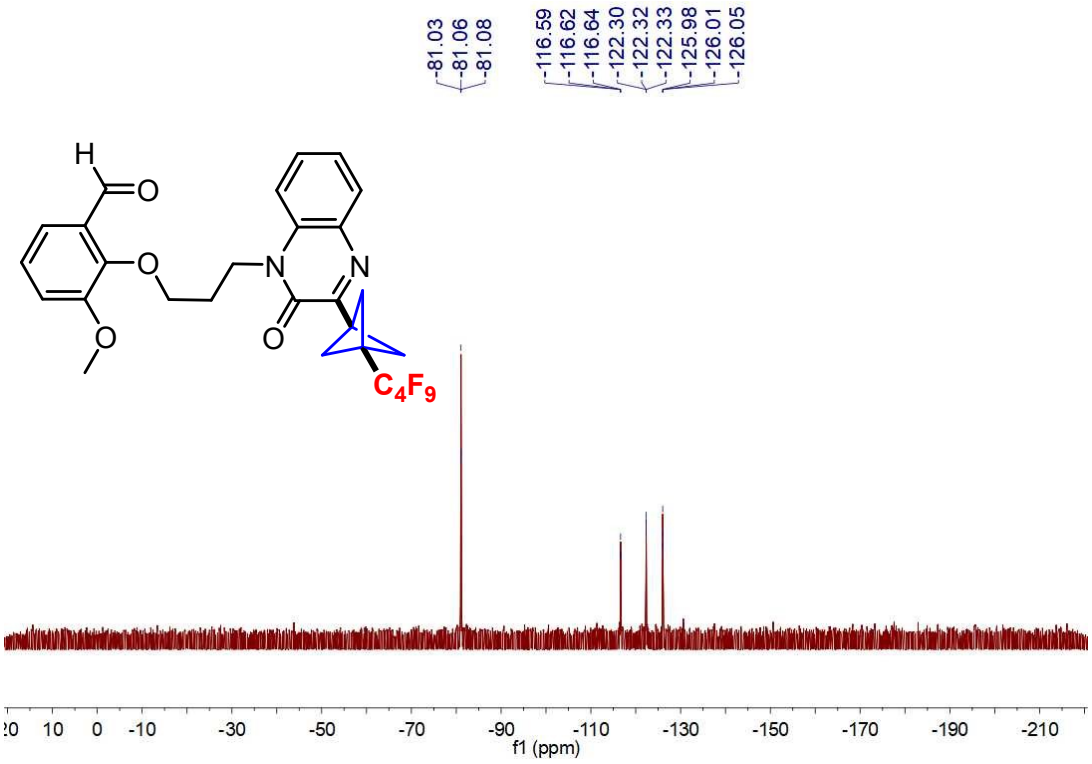
53 ^{1}H NMR (500 MHz, $CDCl_3$)



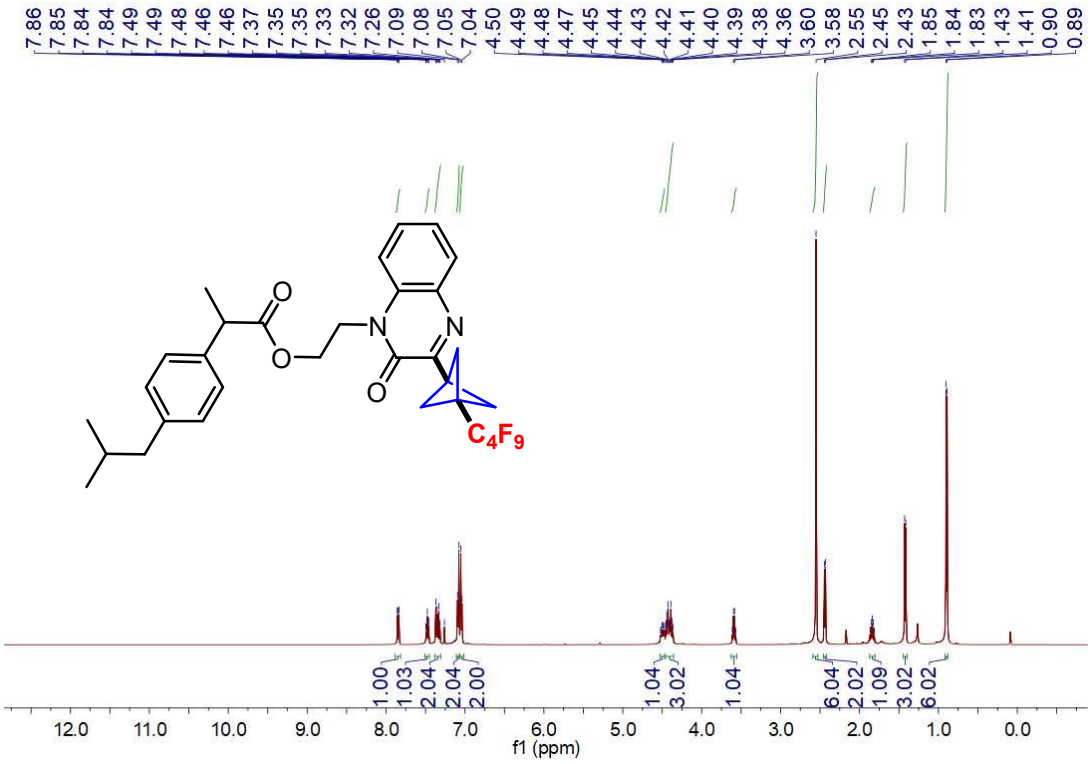
53 ^{13}C NMR (126 MHz, $CDCl_3$)



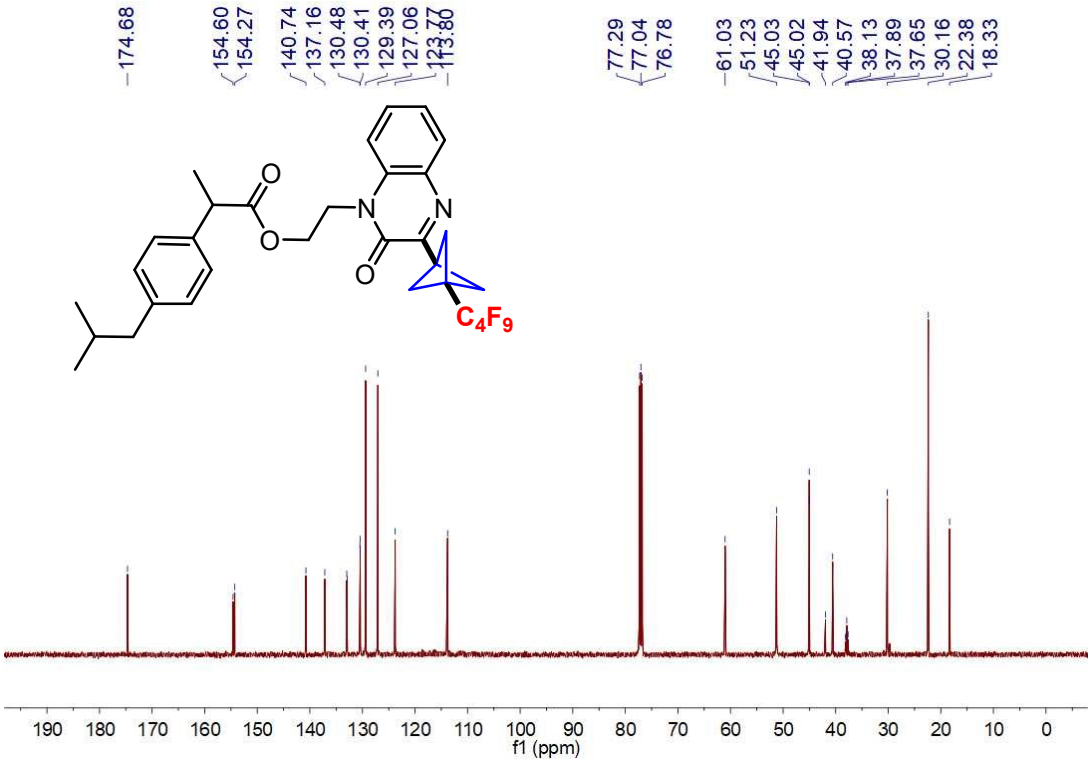
53 ^{19}F NMR (471 MHz, $CDCl_3$)



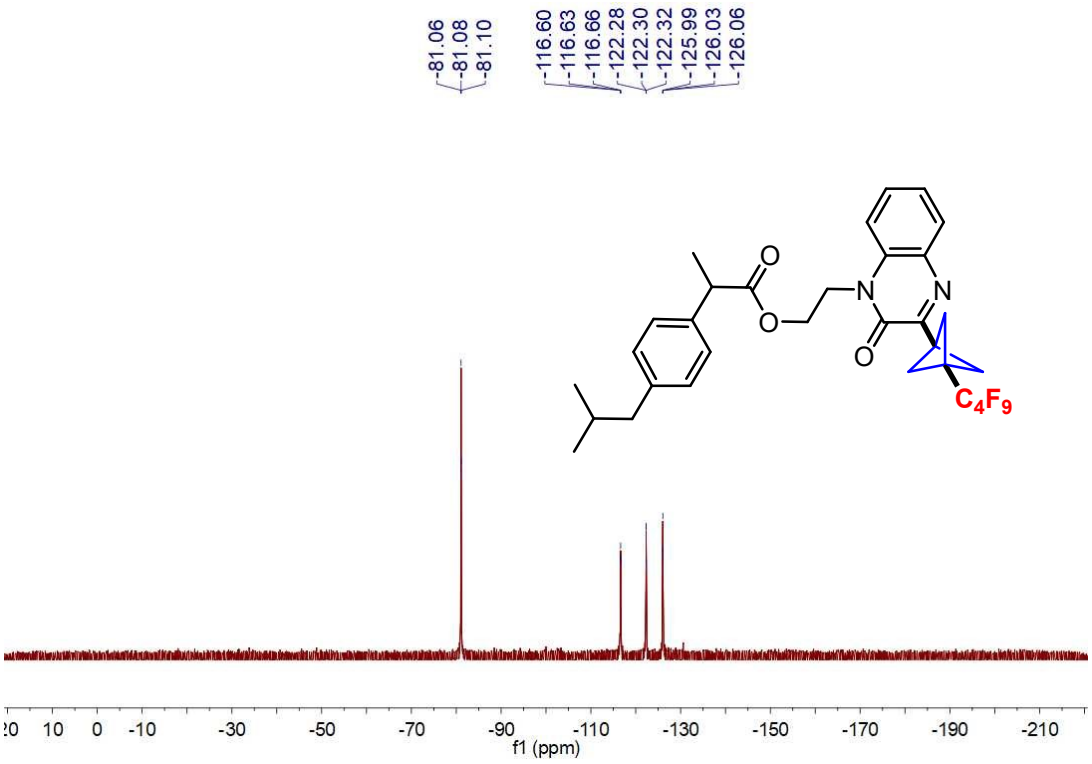
54 ^{1}H NMR (500 MHz, $CDCl_3$)



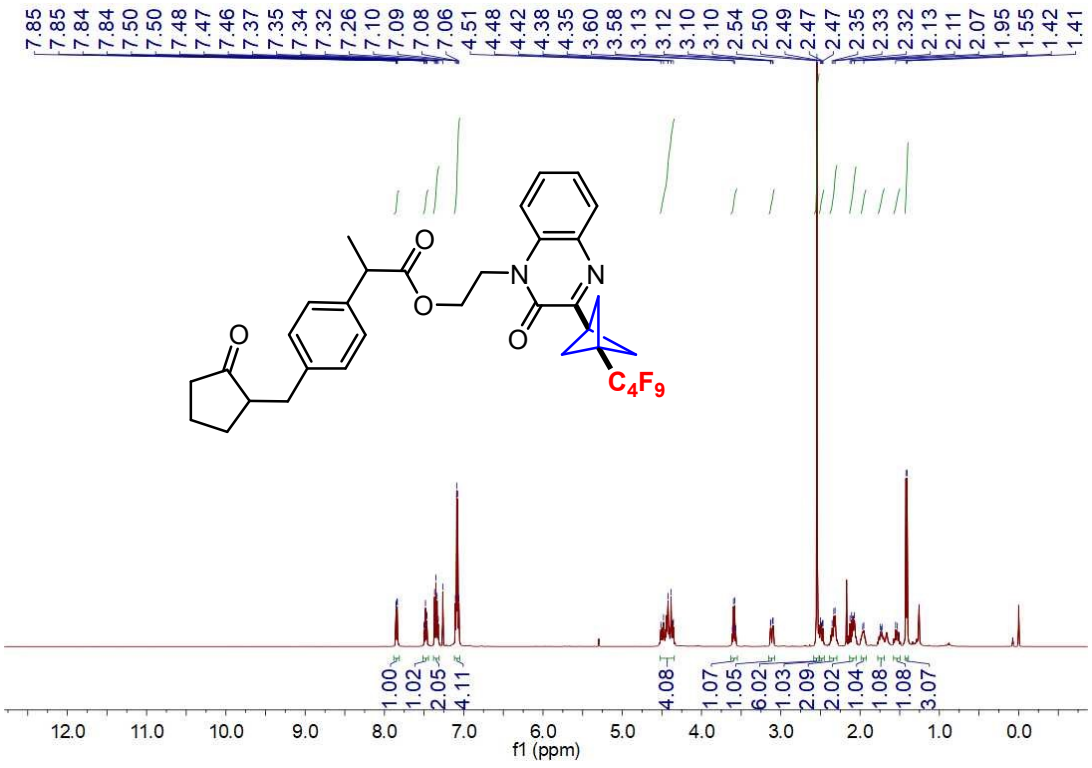
54 ^{13}C NMR (126 MHz, $CDCl_3$)



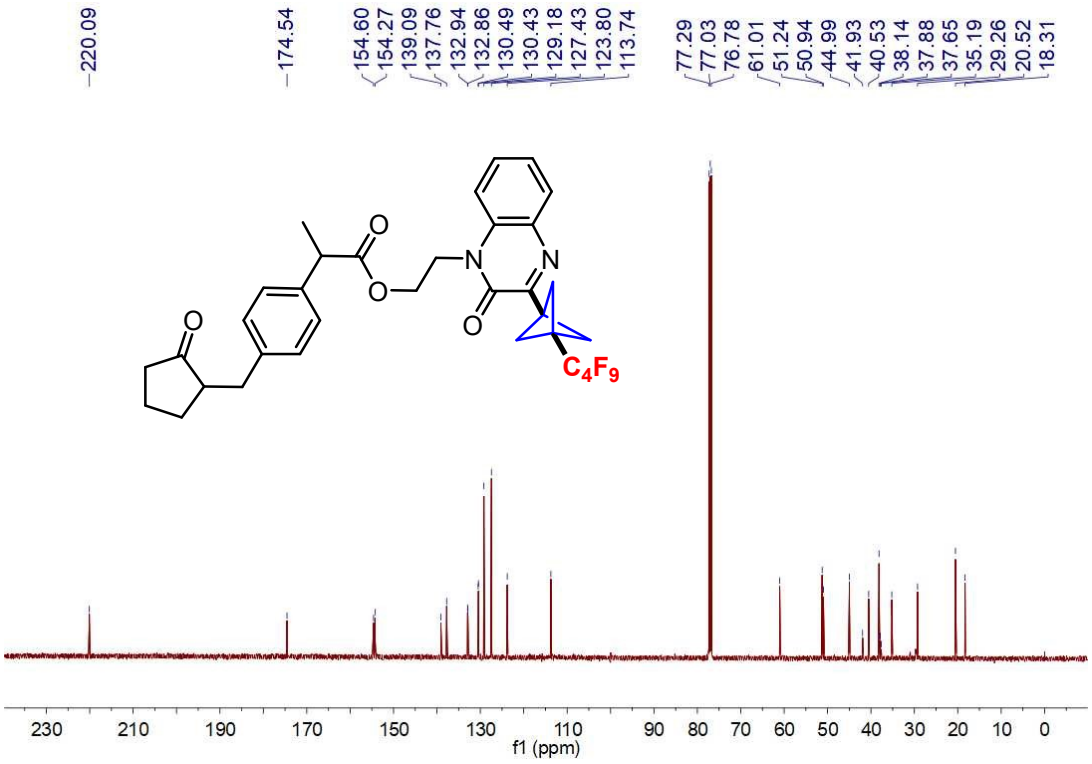
54 ^{19}F NMR (471 MHz, $CDCl_3$)



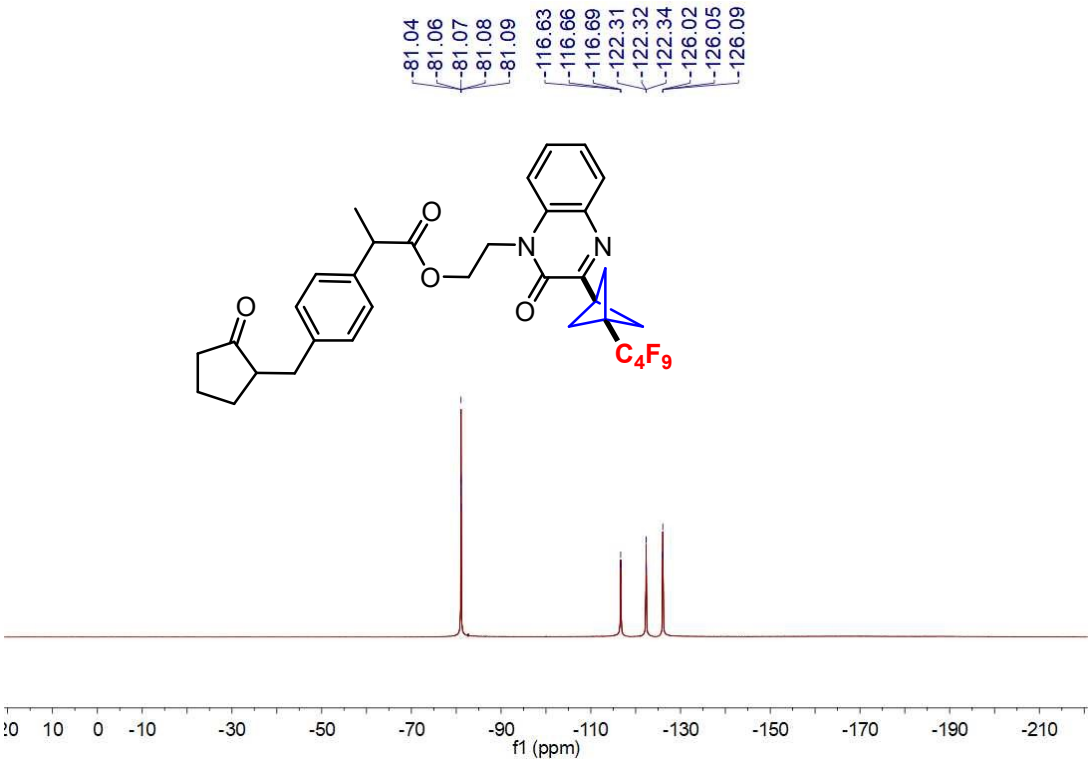
55 ^{1}H NMR (500 MHz, $CDCl_3$)



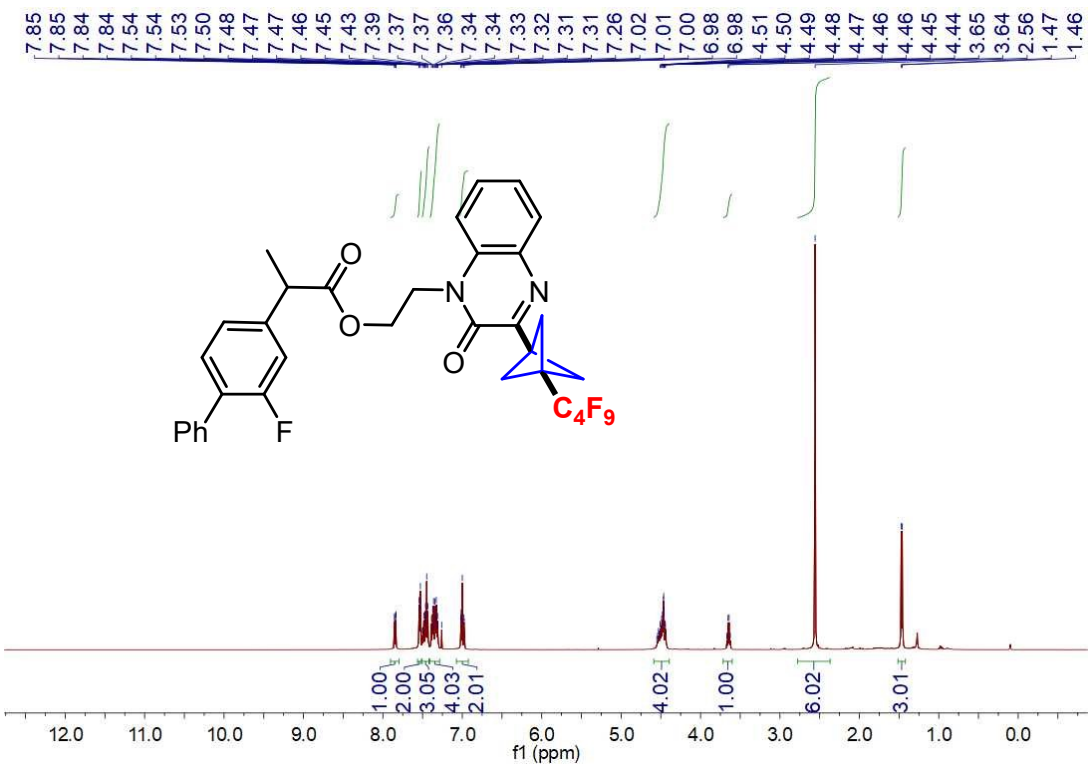
55 ^{13}C NMR (126 MHz, $CDCl_3$)



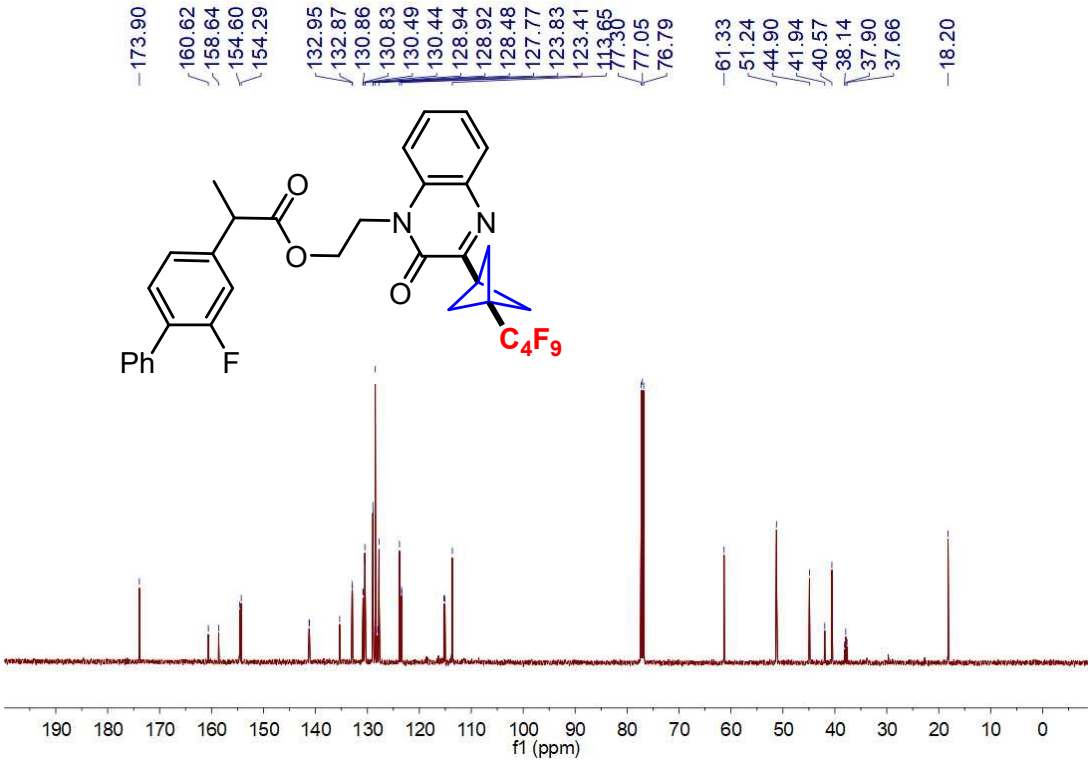
55 ^{19}F NMR (471 MHz, $CDCl_3$)



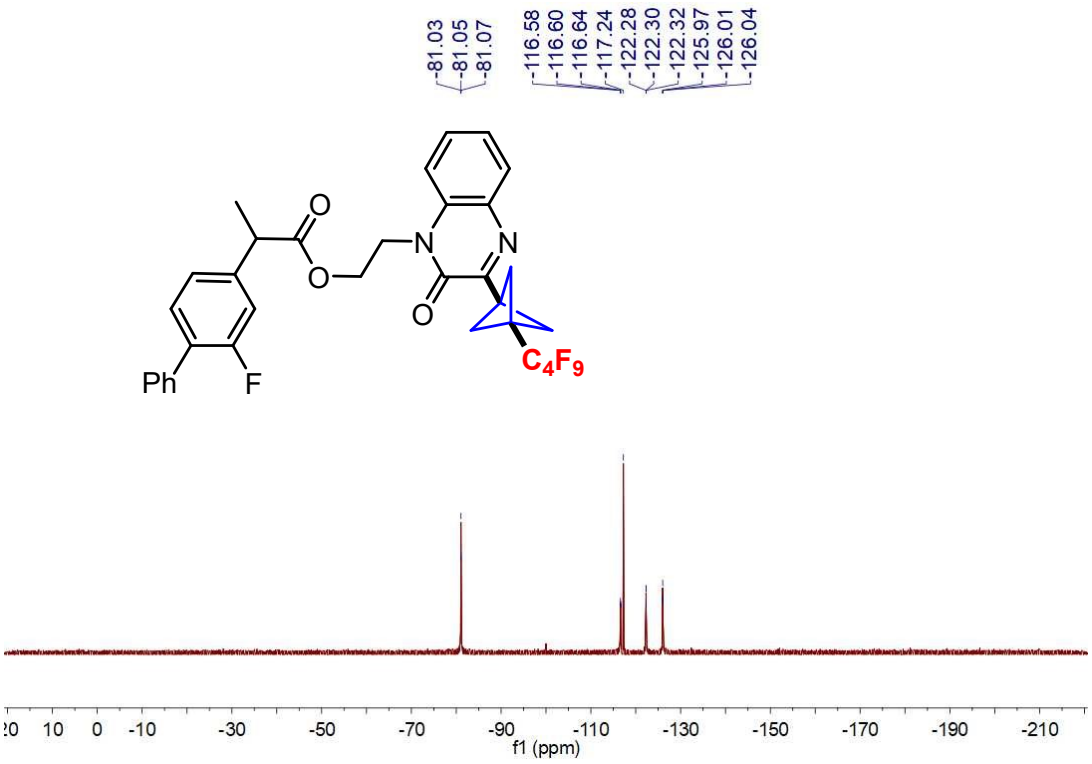
56 ^{1}H NMR (500 MHz, $CDCl_3$)



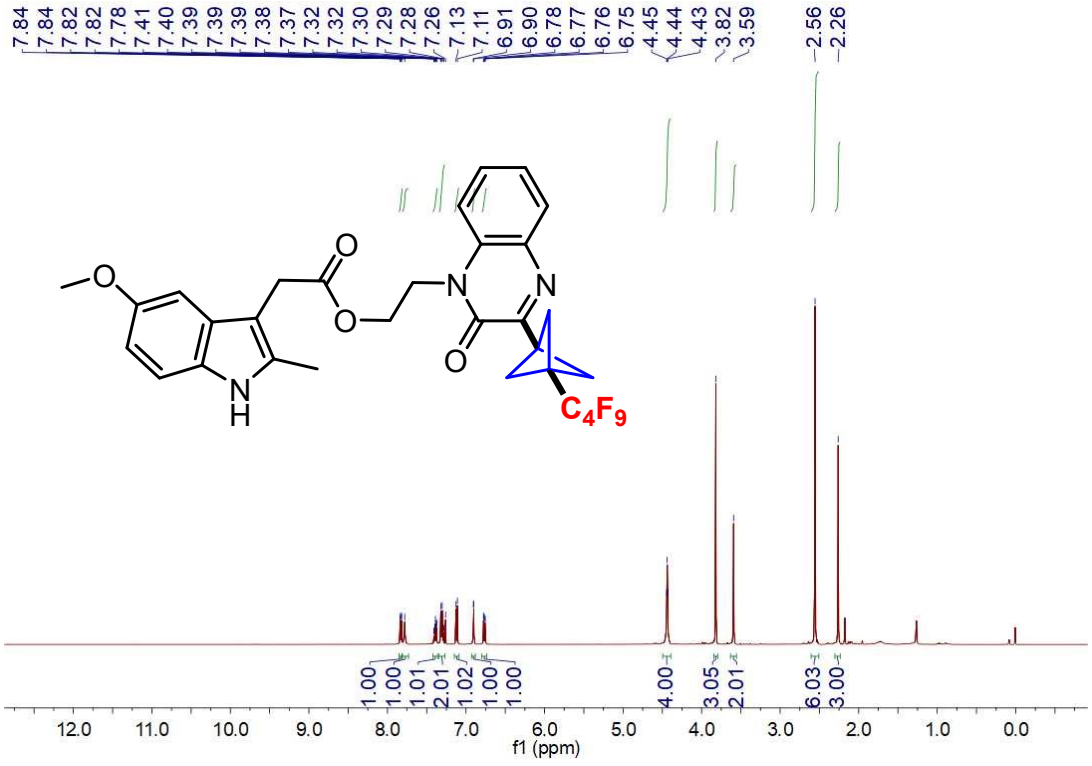
56 ^{13}C NMR (126 MHz, $CDCl_3$)



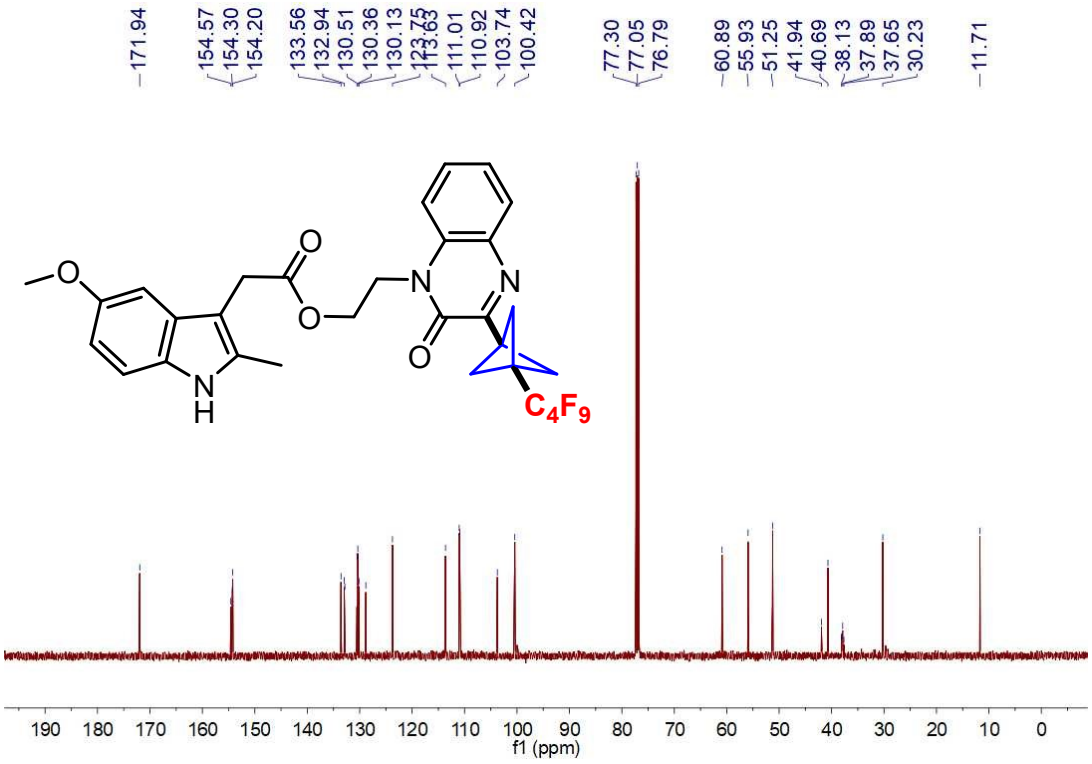
56 ^{19}F NMR (471 MHz, $CDCl_3$)



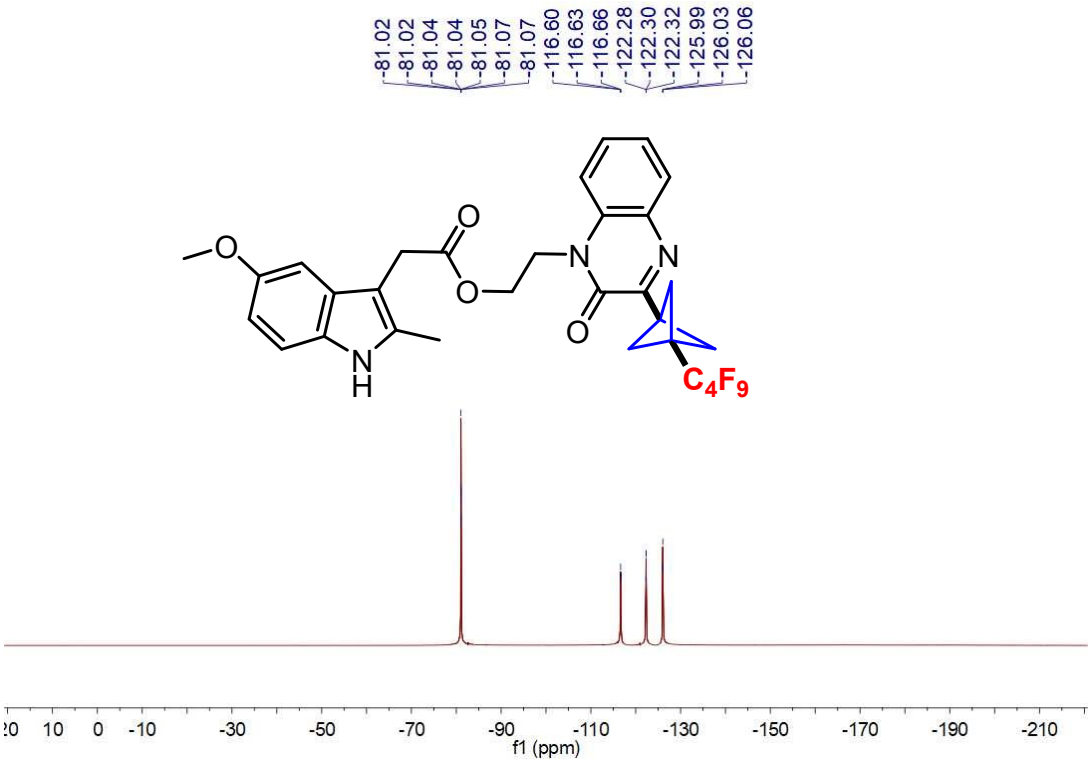
57 ^{1}H NMR (500 MHz, $CDCl_3$)



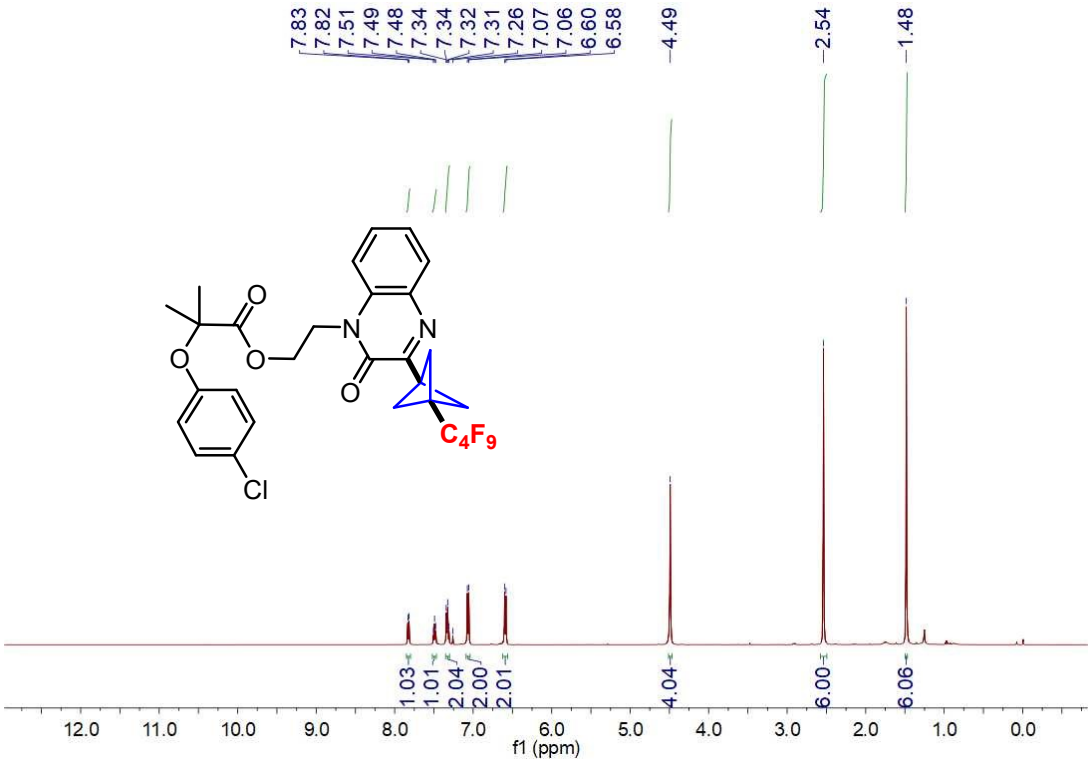
57 ^{13}C NMR (126 MHz, $CDCl_3$)



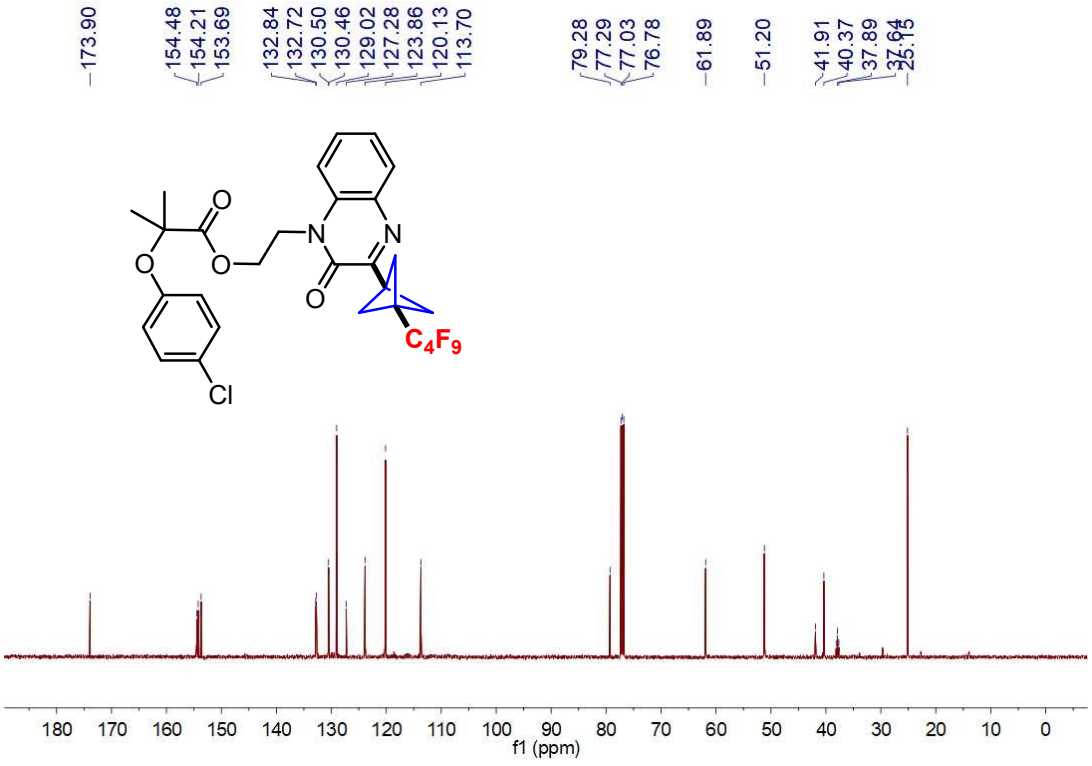
57 ^{19}F NMR (471 MHz, $CDCl_3$)



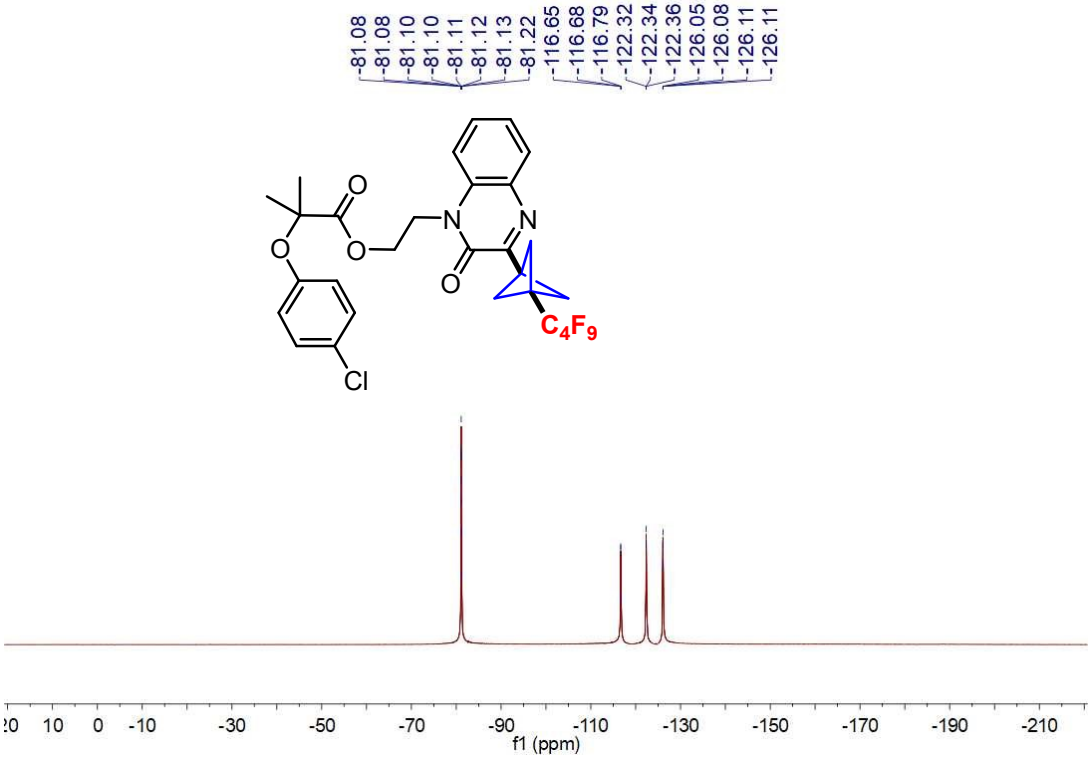
58 ^{1}H NMR (500 MHz, $CDCl_3$)



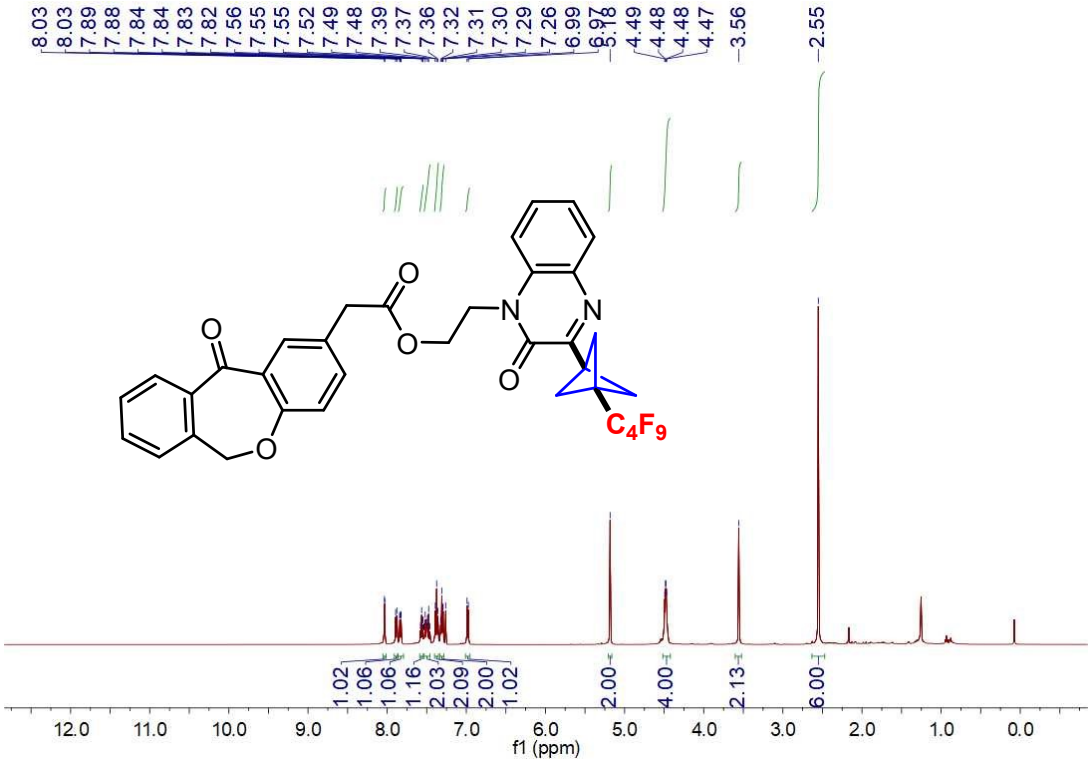
58 ^{13}C NMR (126 MHz, $CDCl_3$)



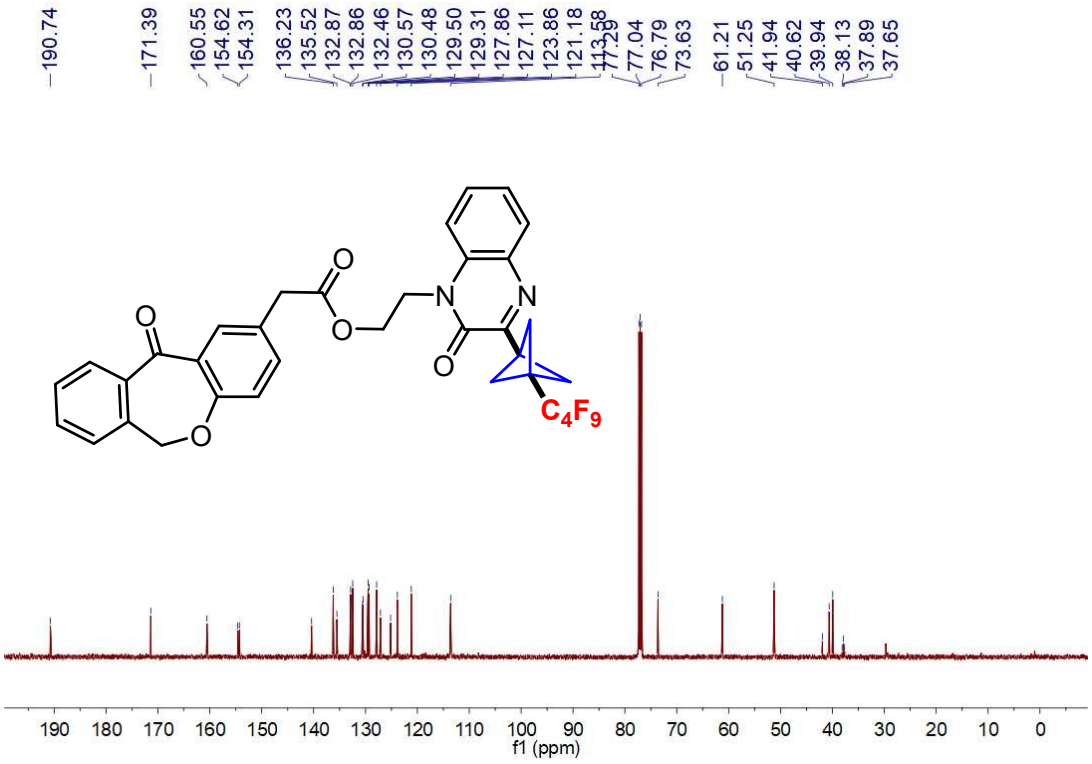
58 ^{19}F NMR (471 MHz, $CDCl_3$)



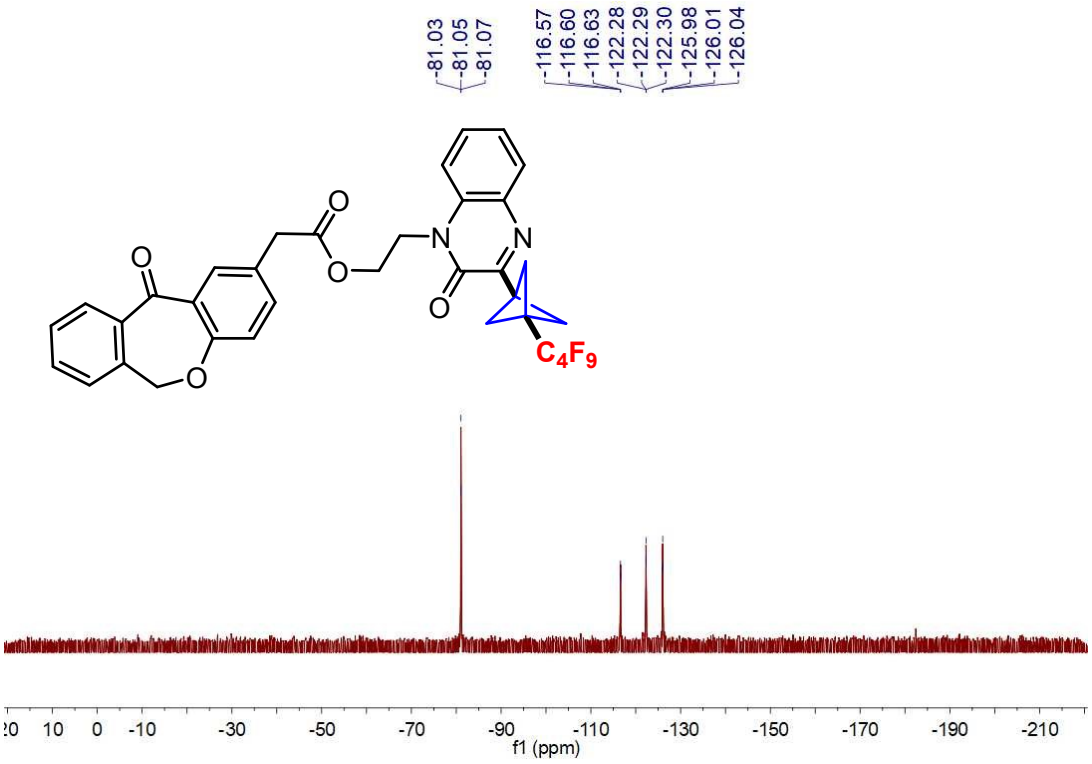
59 ^{1}H NMR (500 MHz, $CDCl_3$)



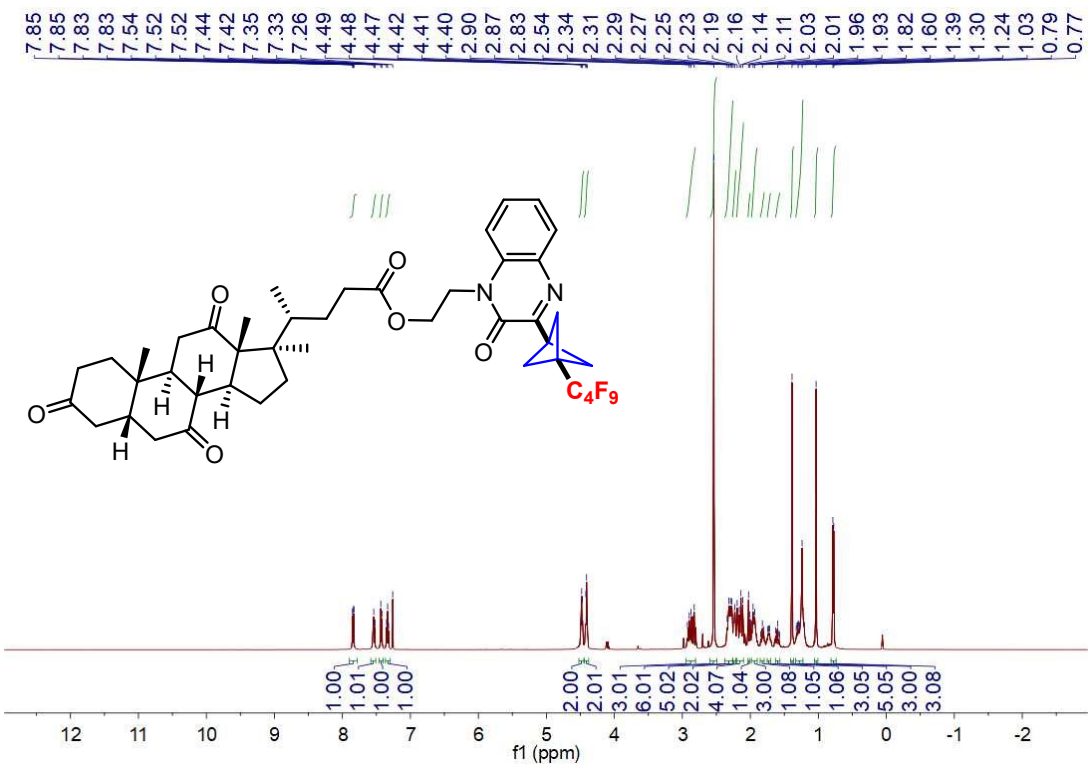
59 ^{13}C NMR (126 MHz, $CDCl_3$)



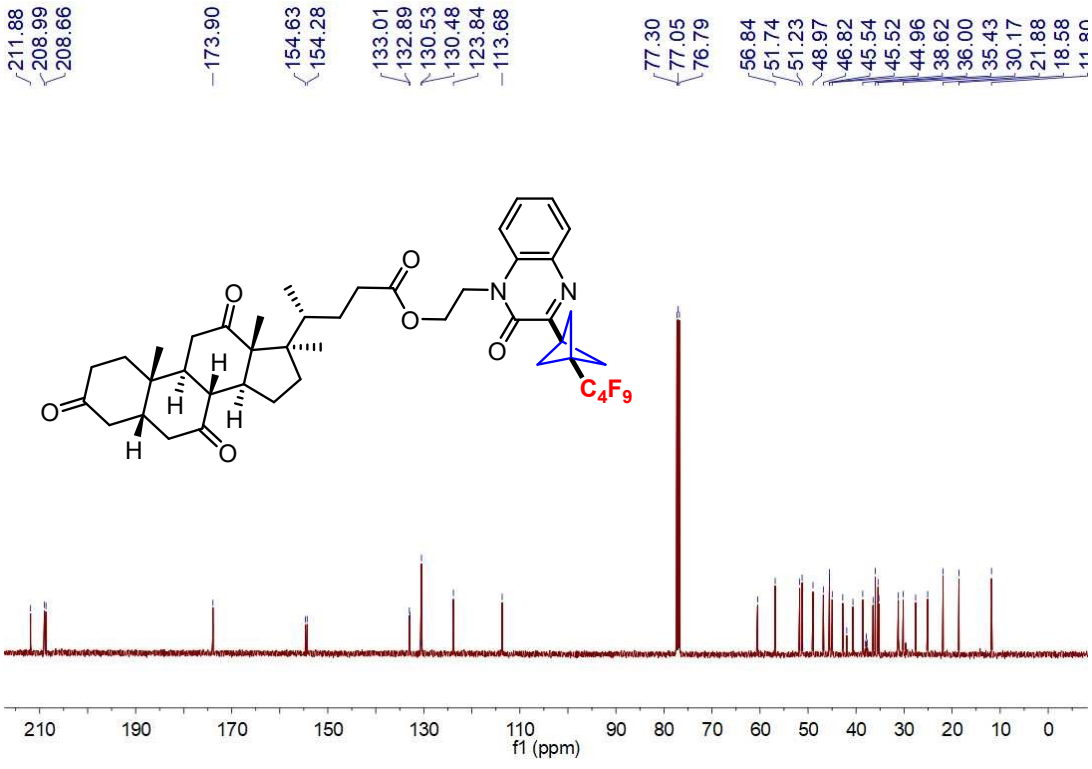
59 ^{19}F NMR (471 MHz, $CDCl_3$)



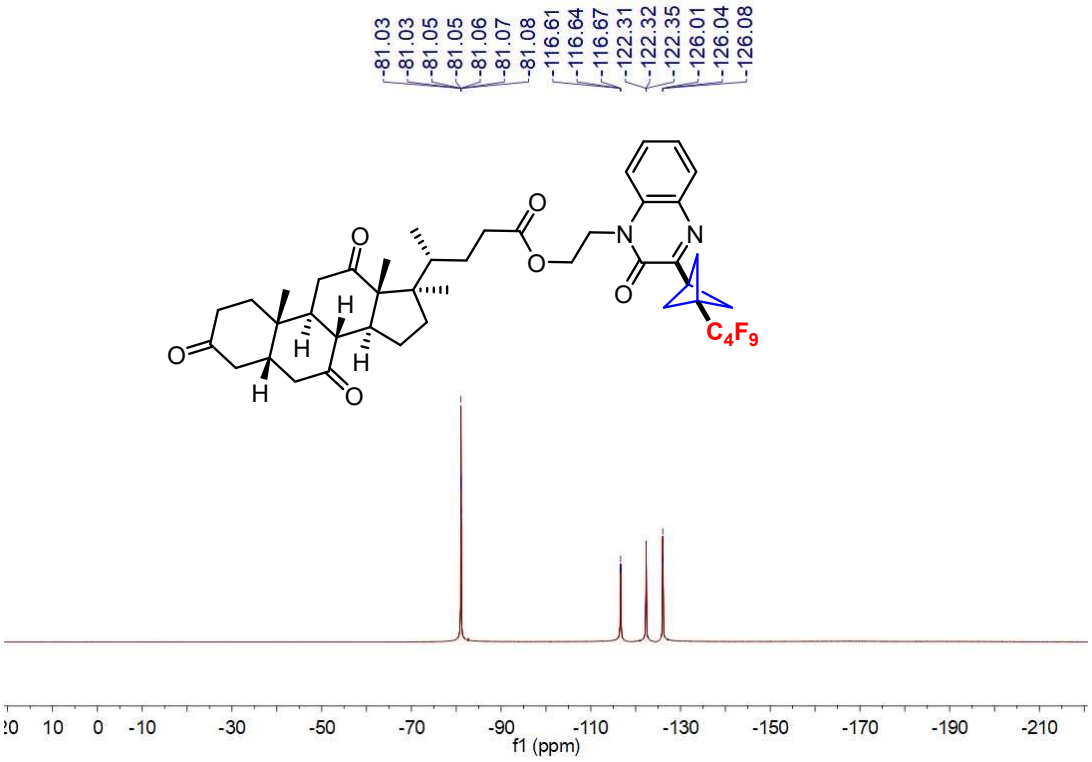
60 ^{1}H NMR (500 MHz, $CDCl_3$)



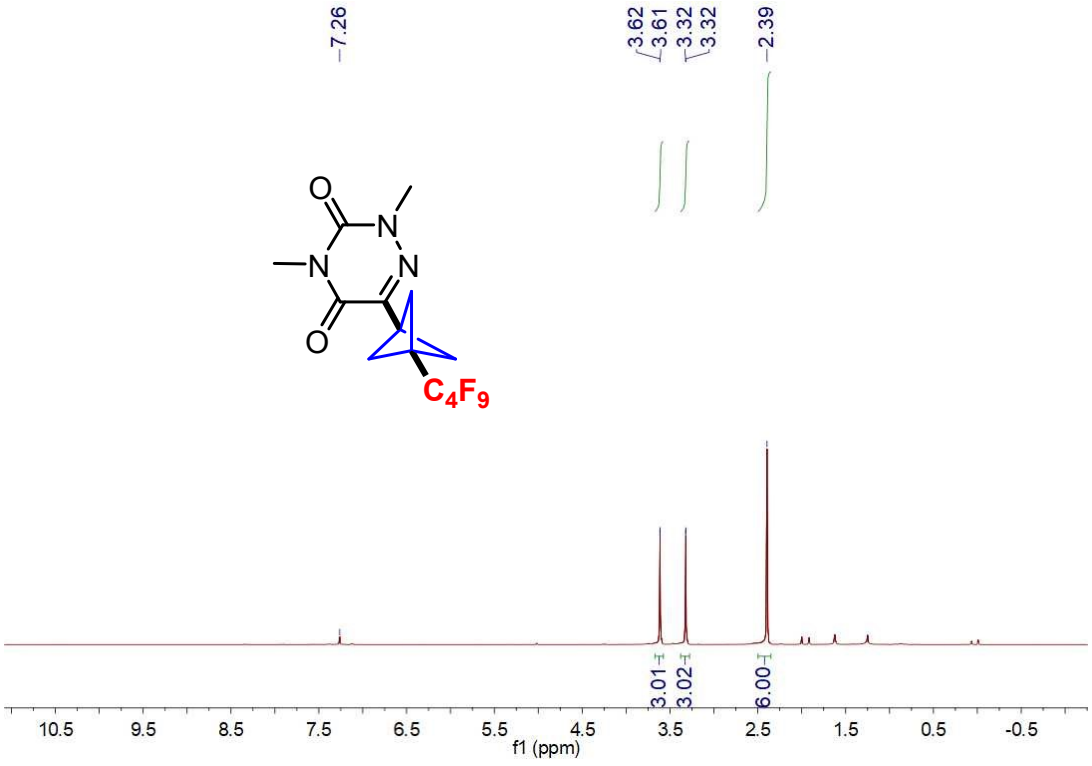
60 ^{13}C NMR (126 MHz, $CDCl_3$)



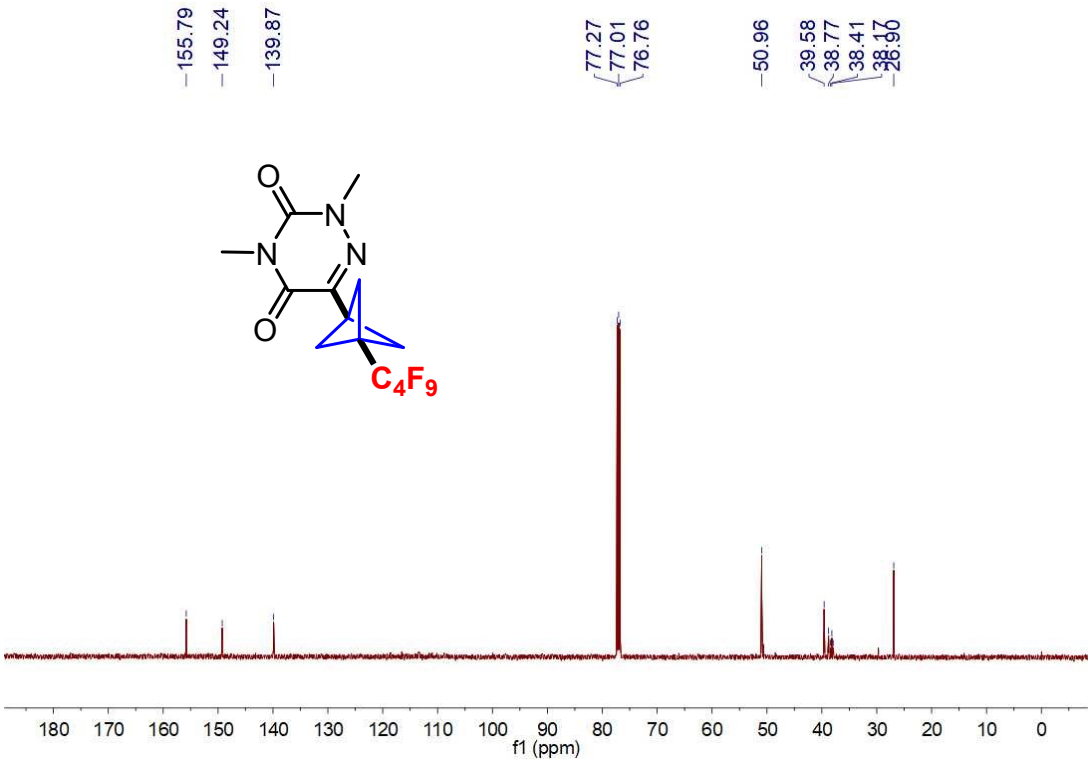
60 ^{19}F NMR (471 MHz, $CDCl_3$)



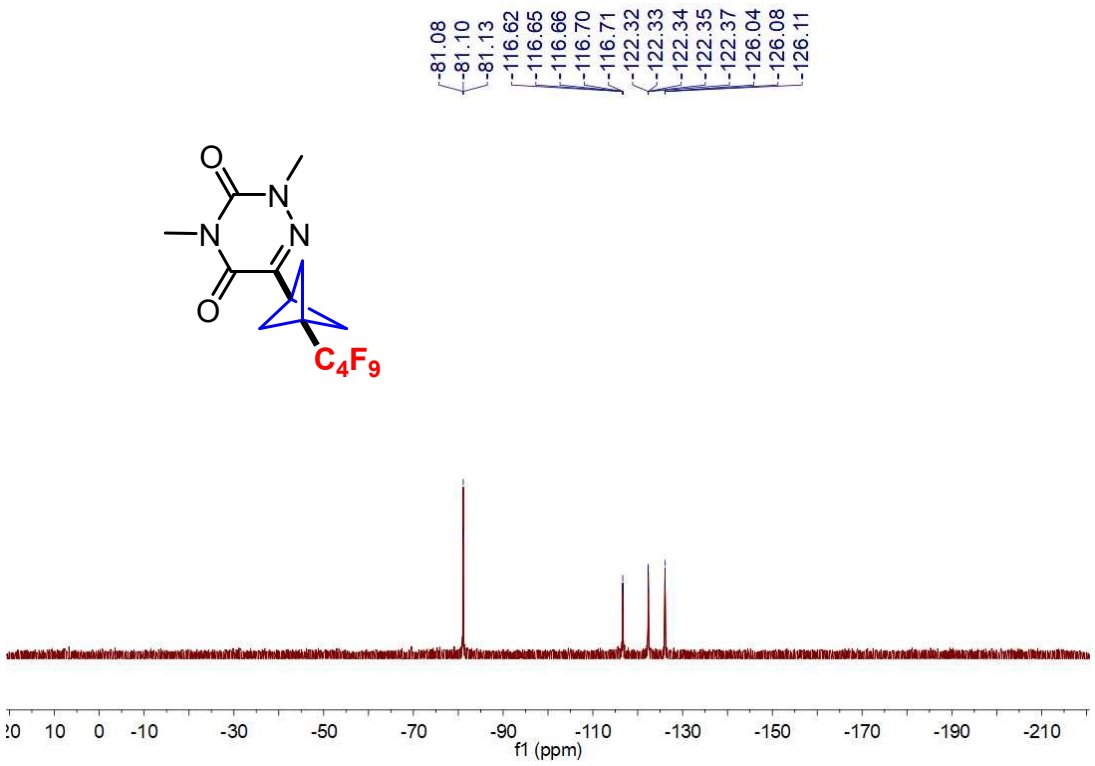
62 ^{1}H NMR (500 MHz, $CDCl_3$)



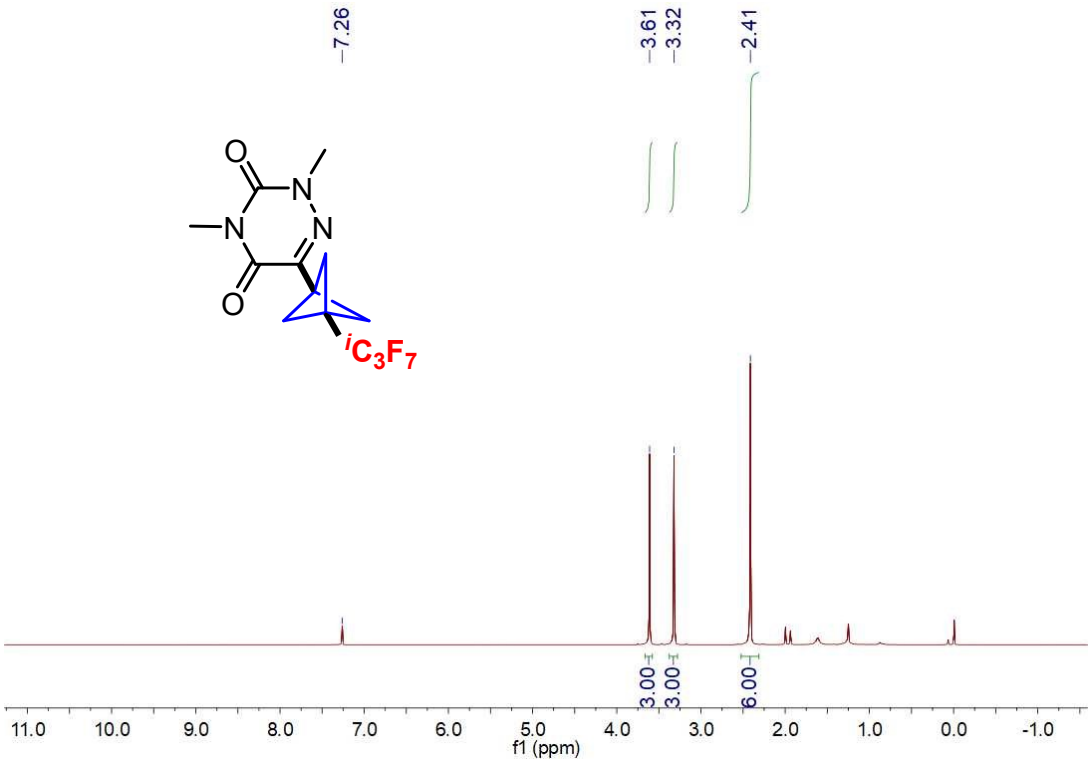
62 ^{13}C NMR (126 MHz, $CDCl_3$)



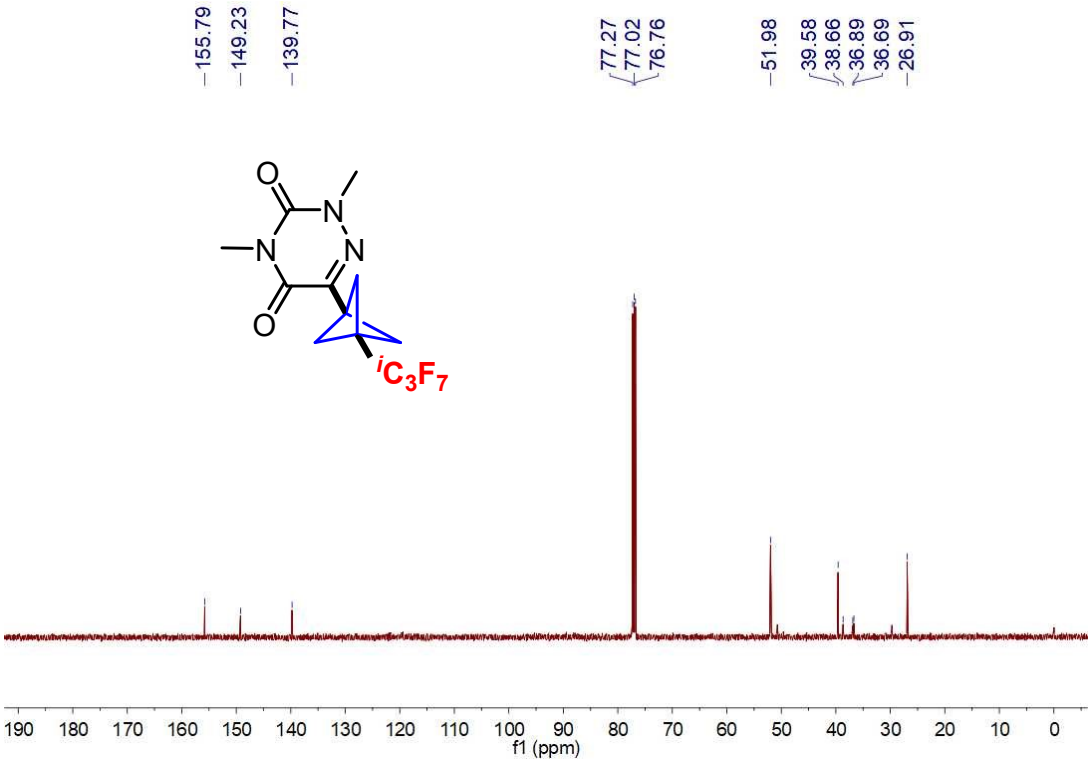
62 ^{19}F NMR (471 MHz, $CDCl_3$)



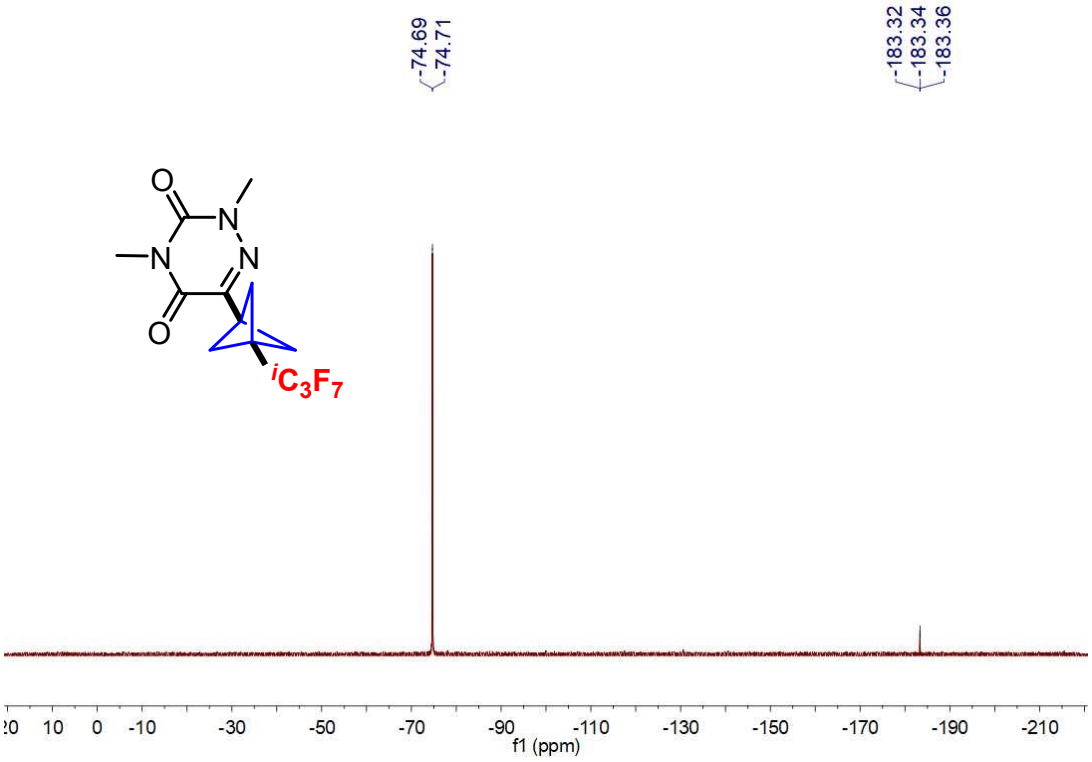
63 ^{1}H NMR (500 MHz, $CDCl_3$)



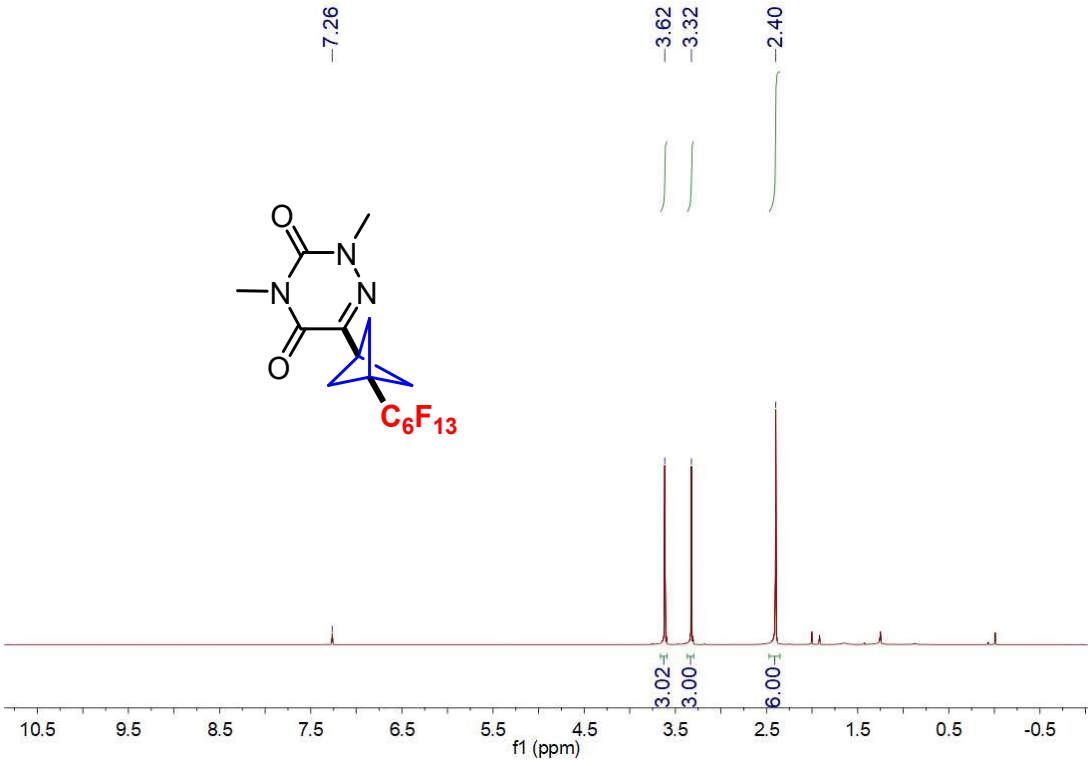
63 ^{13}C NMR (126 MHz, $CDCl_3$)



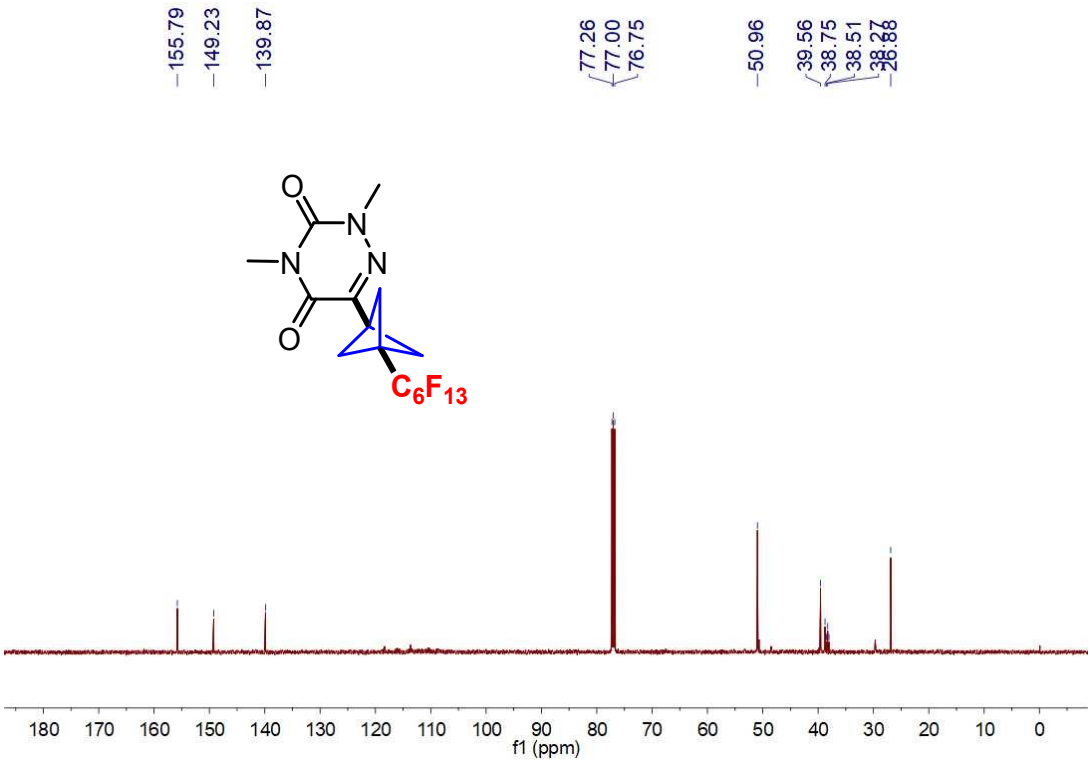
63 ^{19}F NMR (471 MHz, $CDCl_3$)



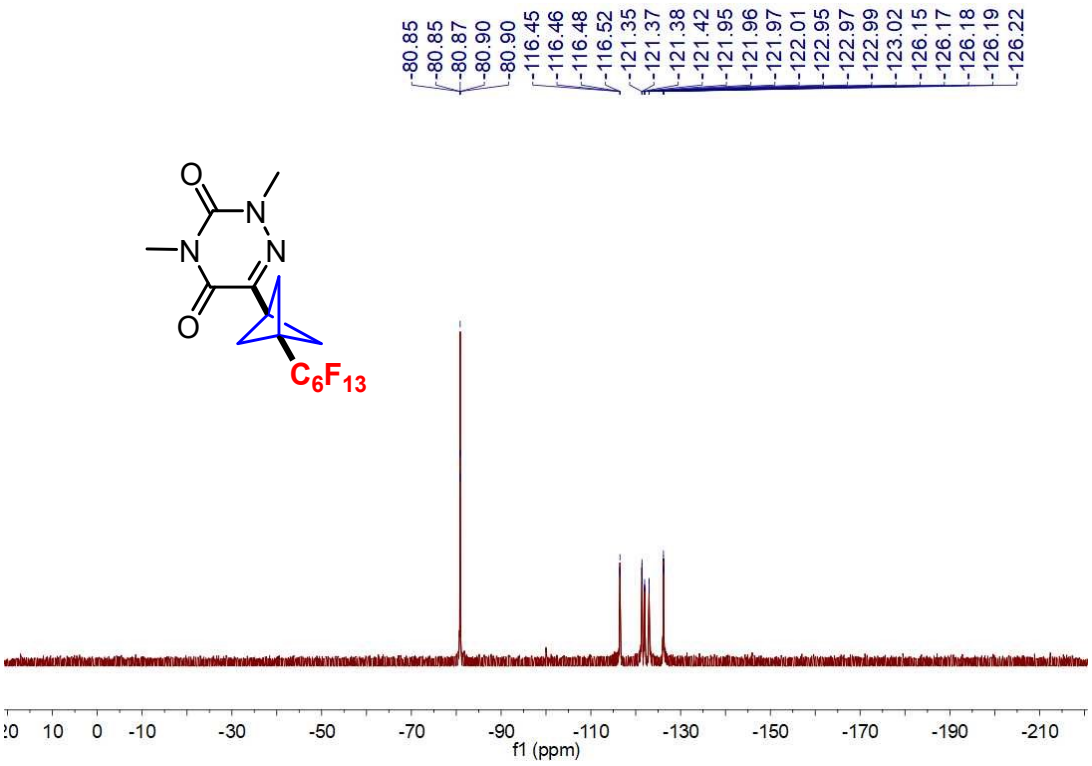
64 ^{1}H NMR (500 MHz, $CDCl_3$)



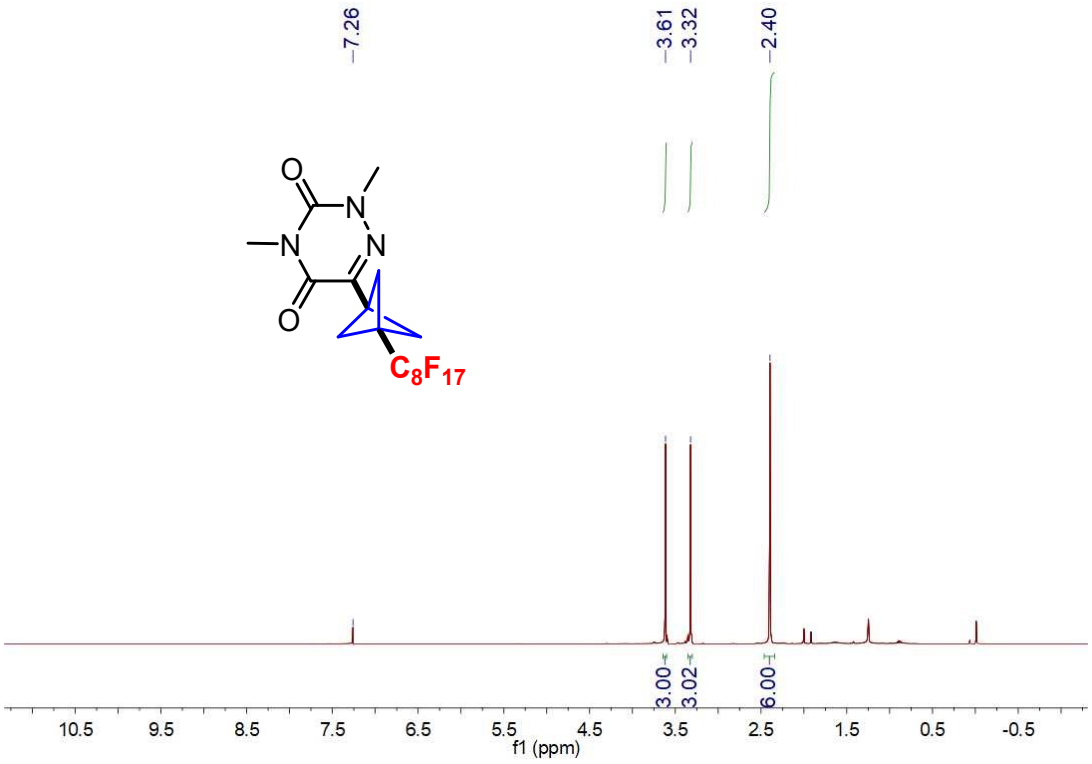
64 ^{13}C NMR (126 MHz, $CDCl_3$)



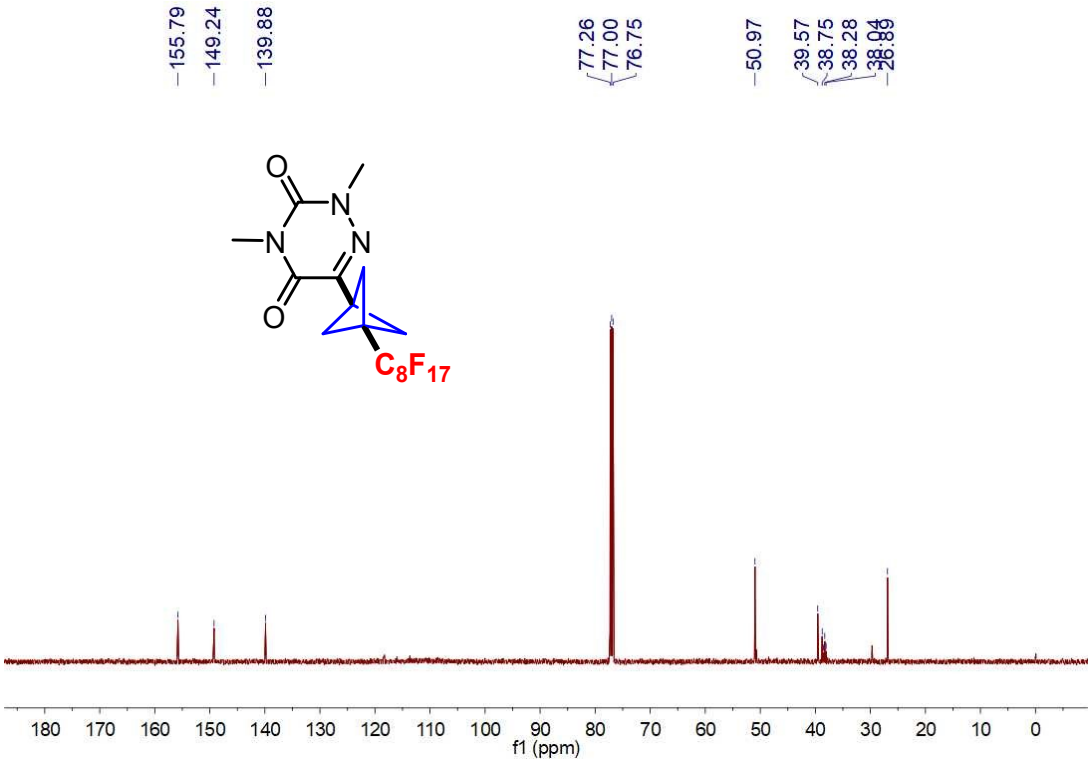
64 ^{19}F NMR (471 MHz, $CDCl_3$)



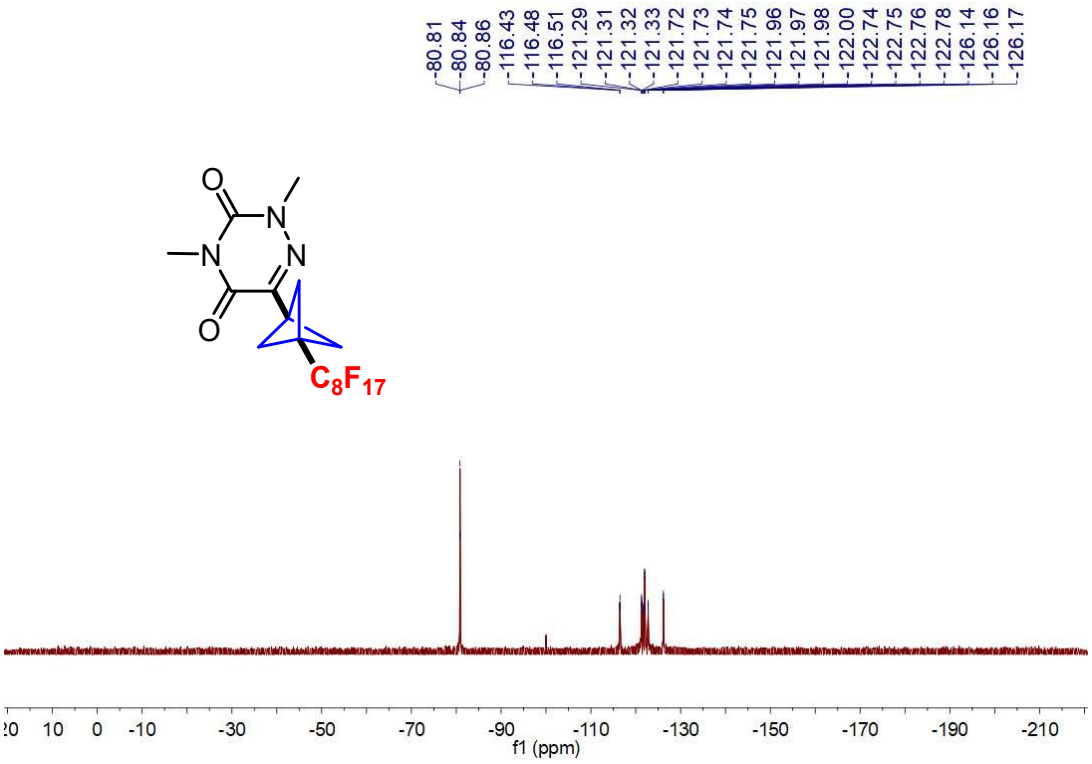
65 ^{1}H NMR (500 MHz, $CDCl_3$)



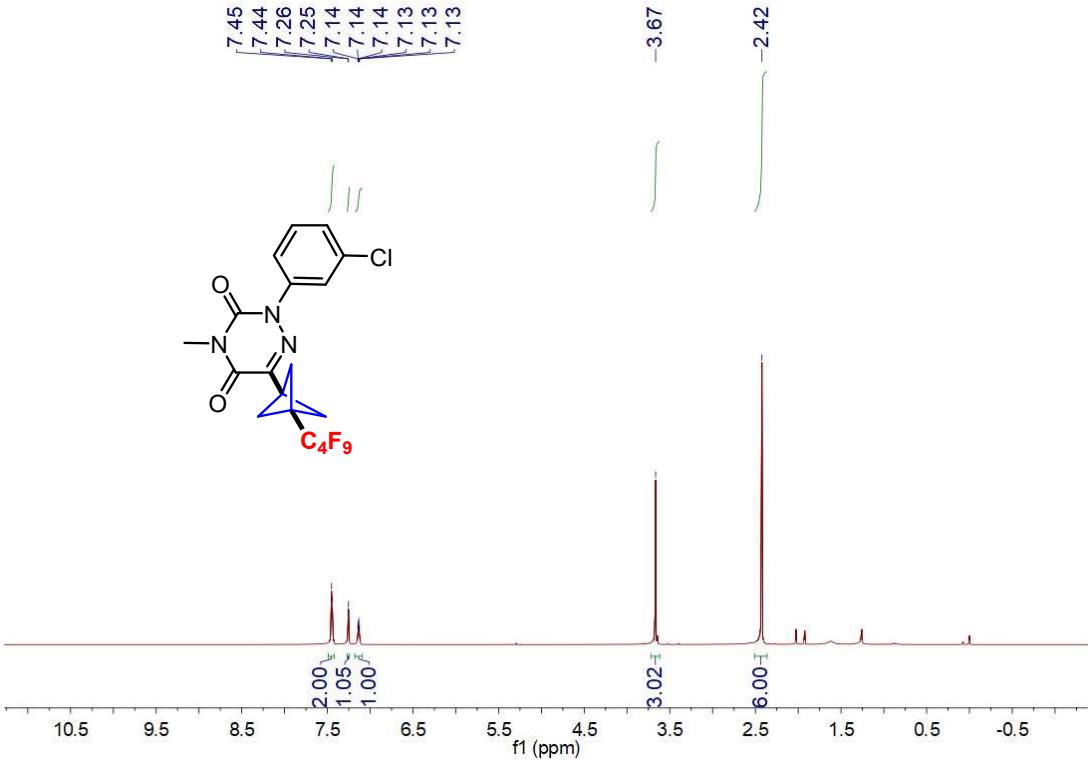
65 ^{13}C NMR (126 MHz, $CDCl_3$)



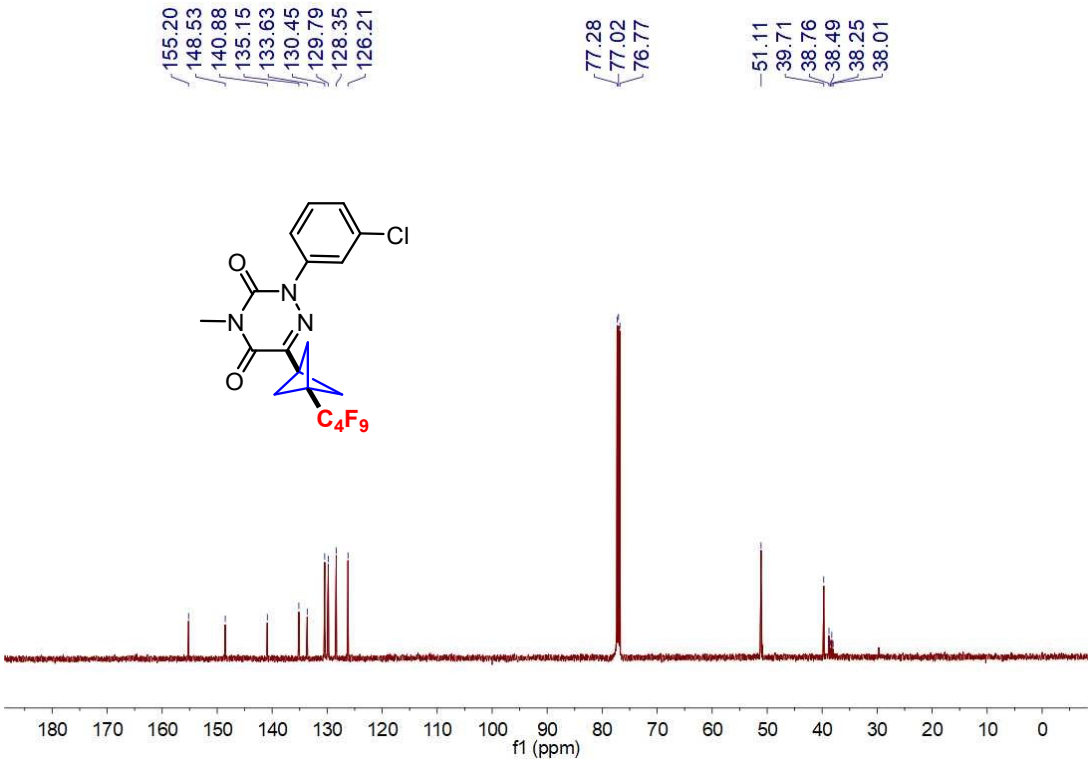
65 ^{19}F NMR (471 MHz, $CDCl_3$)



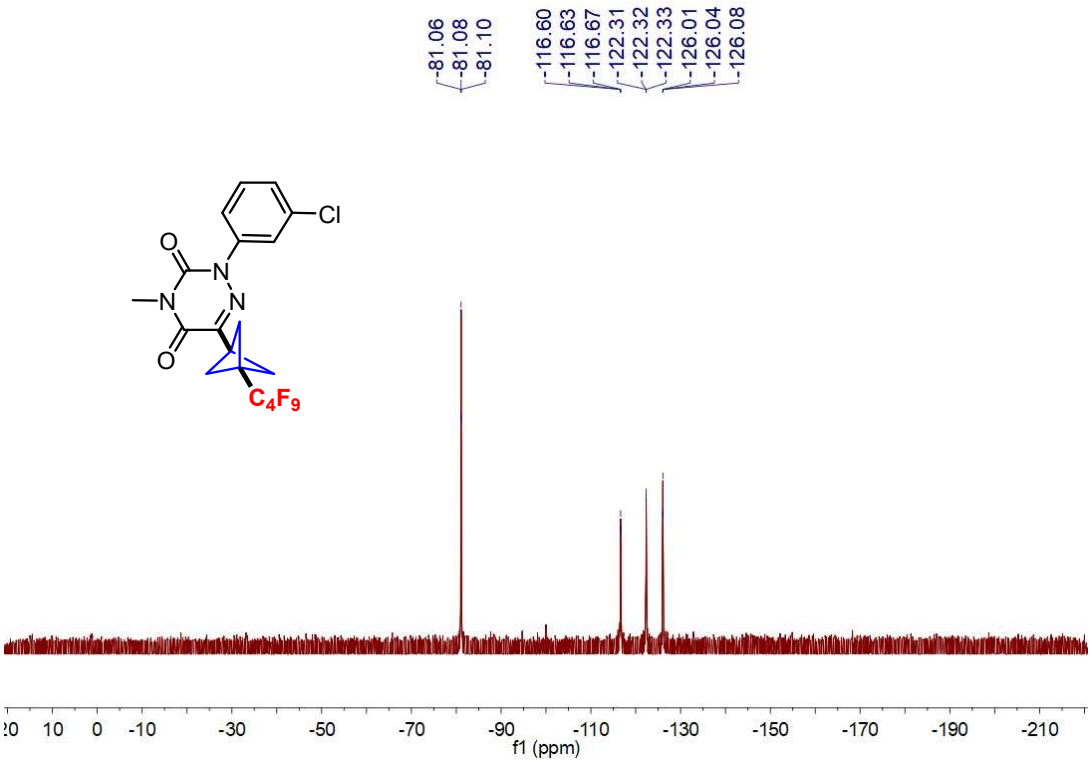
66 ^{1}H NMR (500 MHz, $CDCl_3$)



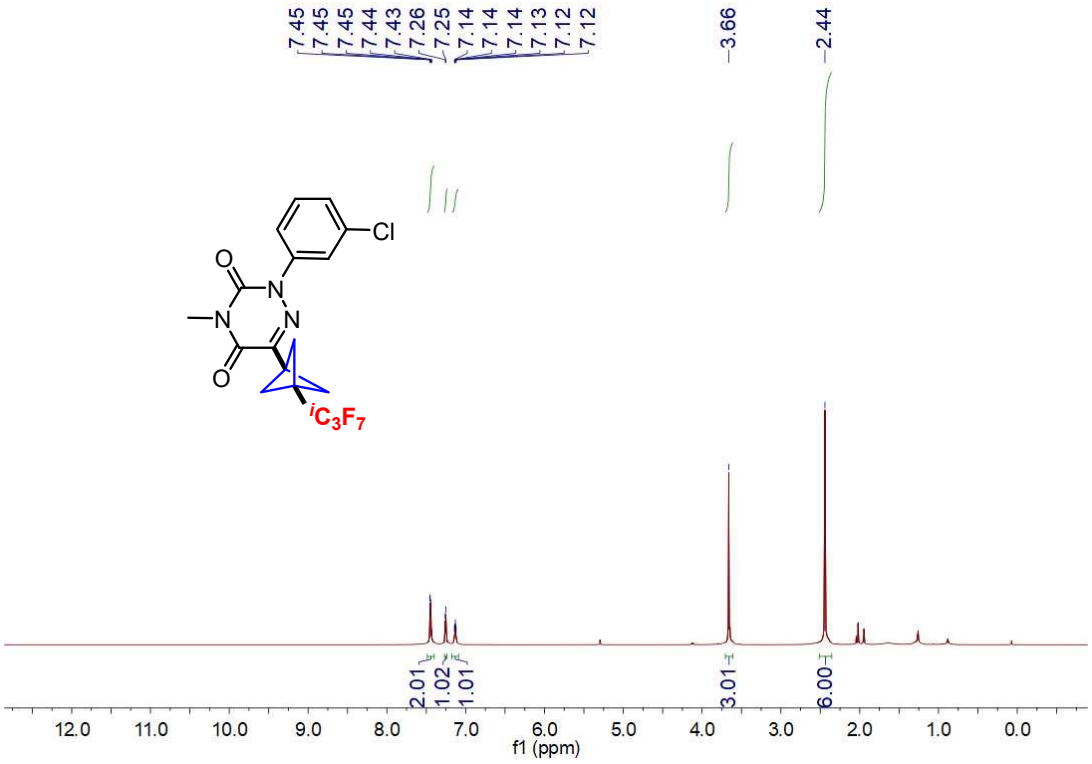
66 ^{13}C NMR (126 MHz, $CDCl_3$)



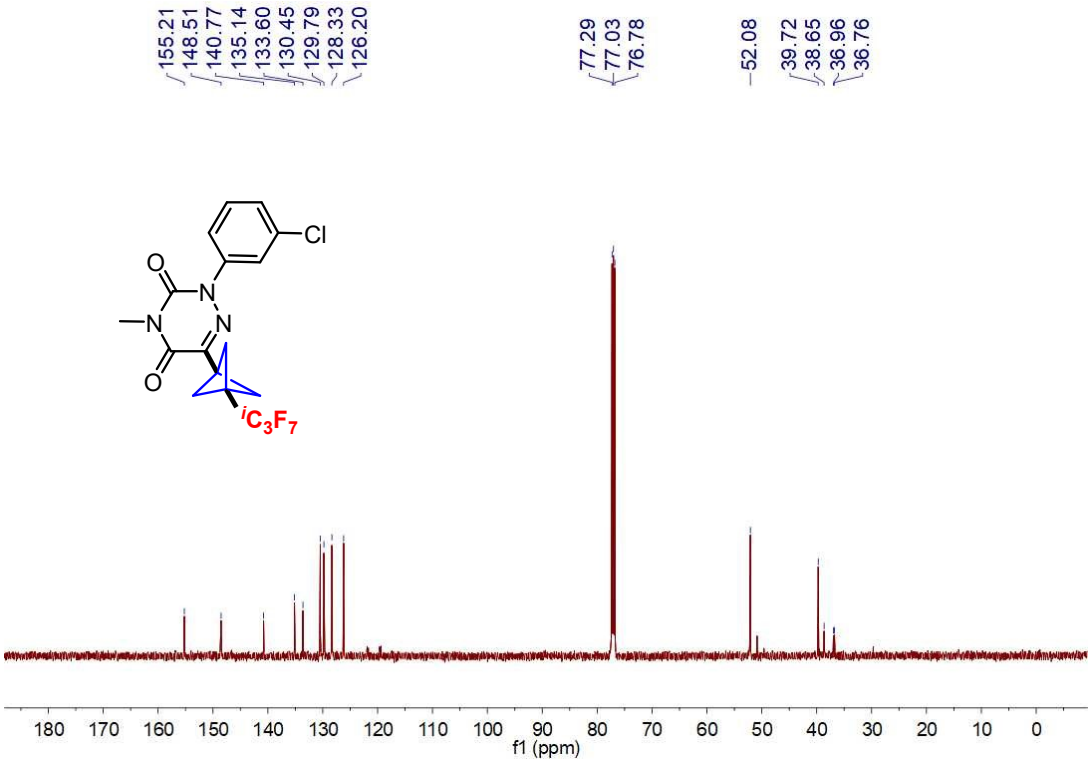
66 ^{19}F NMR (471 MHz, $CDCl_3$)



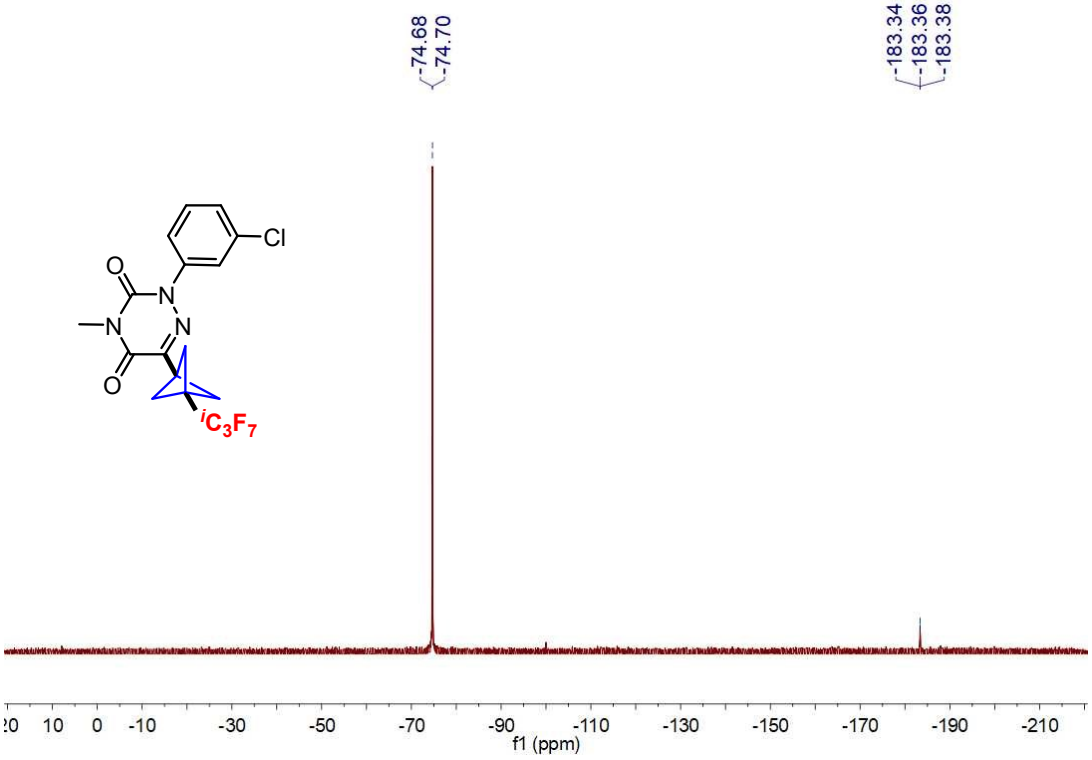
67 ^{1}H NMR (500 MHz, $CDCl_3$)



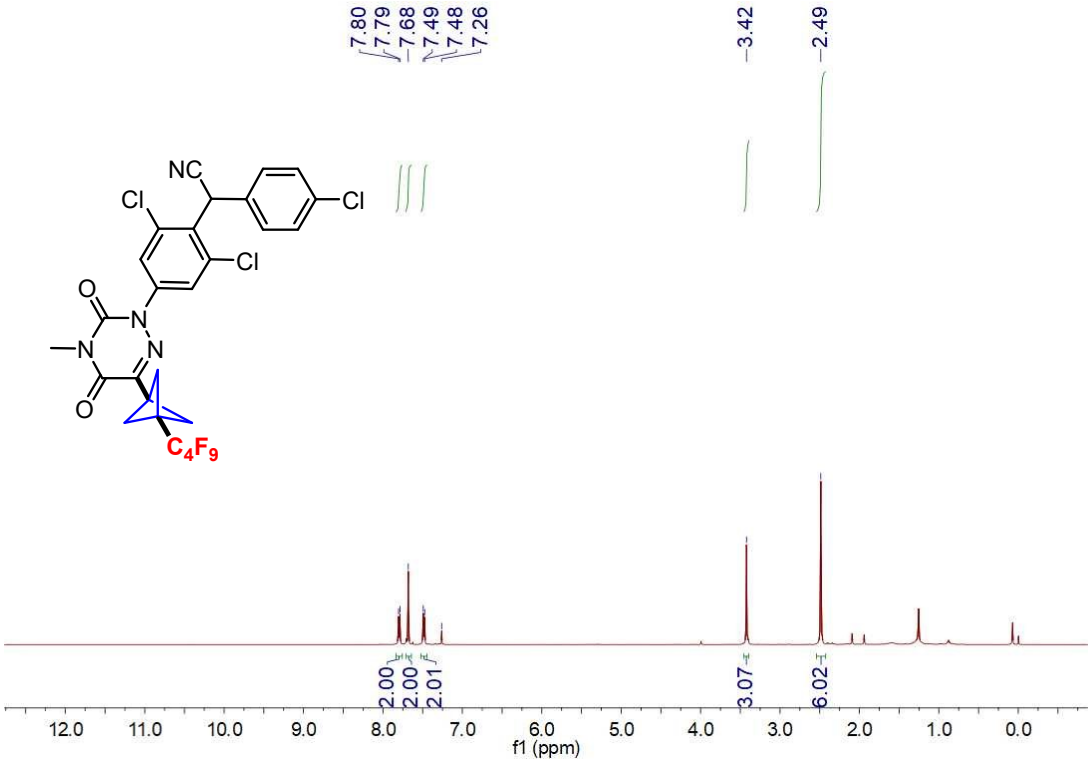
67 ^{13}C NMR (126 MHz, $CDCl_3$)



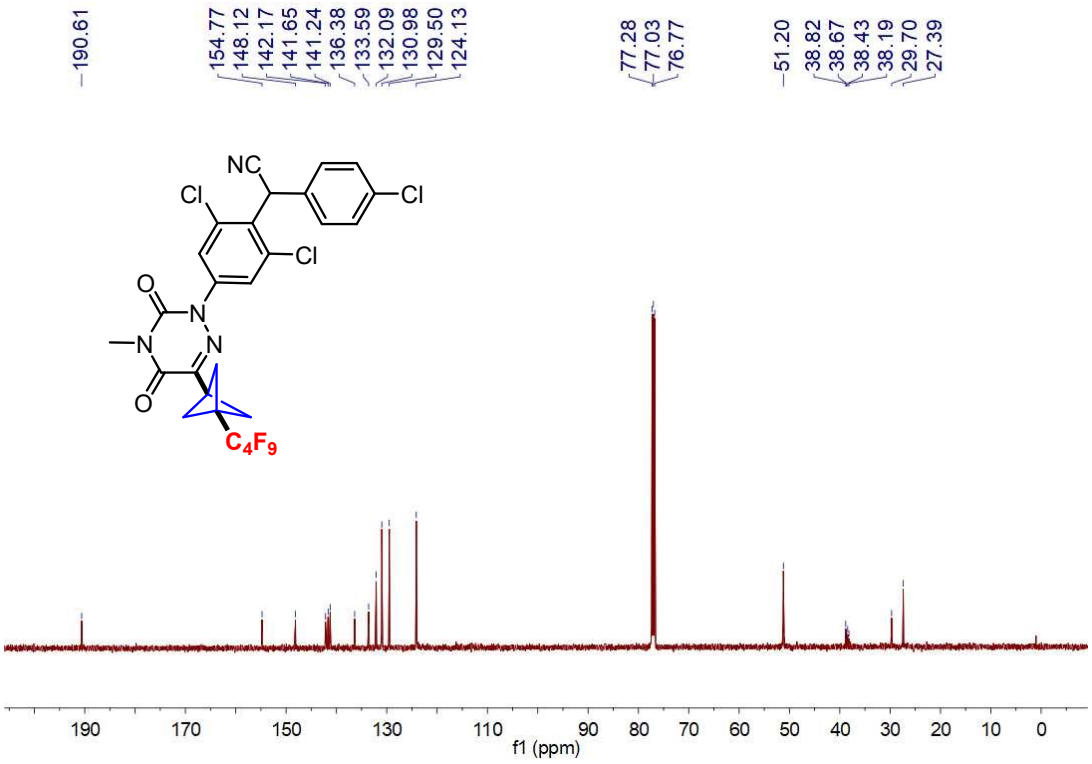
67 ^{19}F NMR (471 MHz, $CDCl_3$)



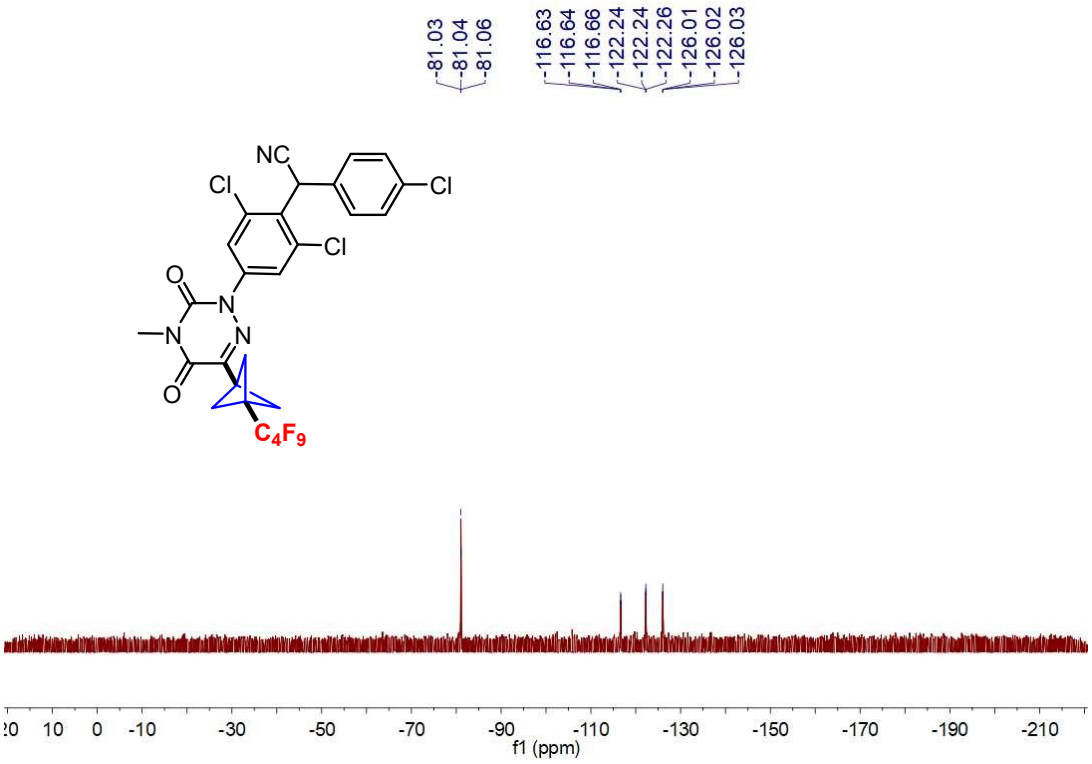
68 ^{1}H NMR (500 MHz, $CDCl_3$)



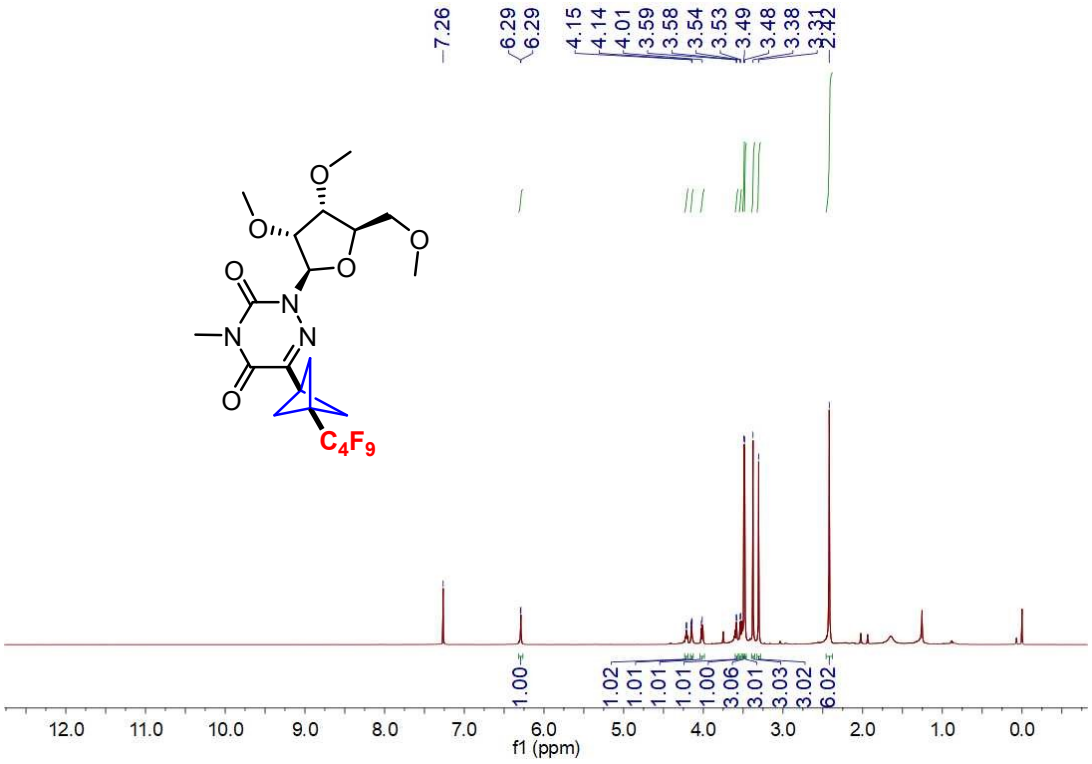
68 ^{13}C NMR (126 MHz, $CDCl_3$)



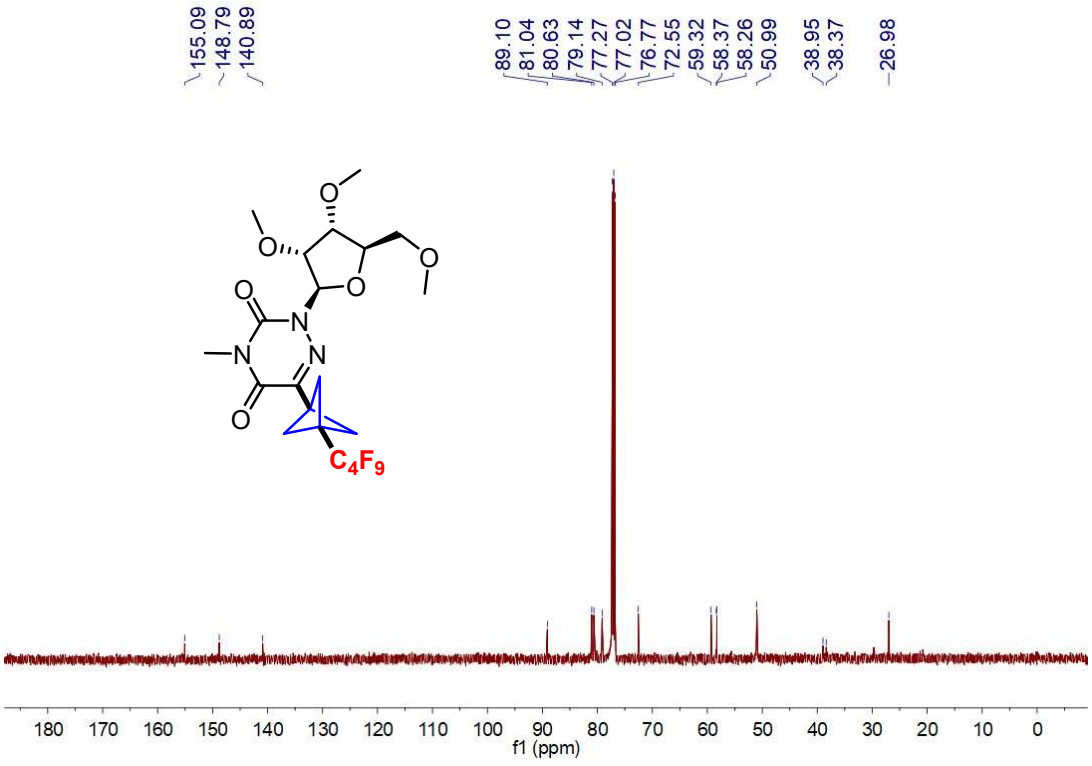
68 ^{19}F NMR (471 MHz, $CDCl_3$)



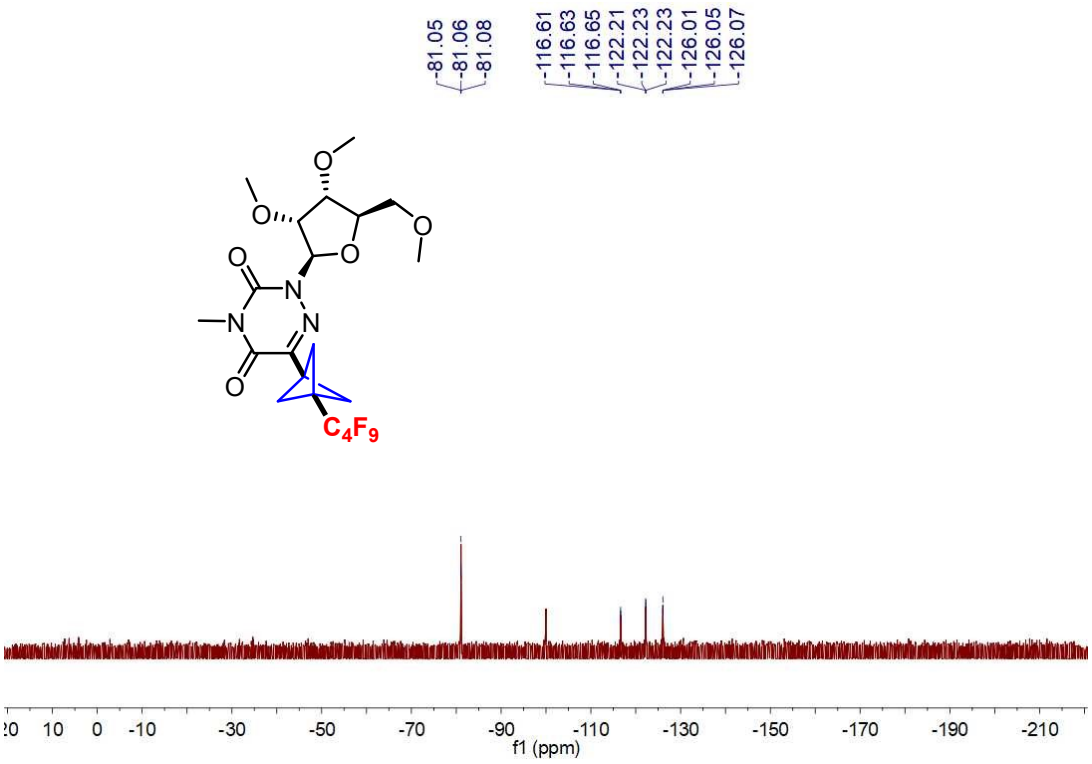
69 ^{1}H NMR (500 MHz, $CDCl_3$)



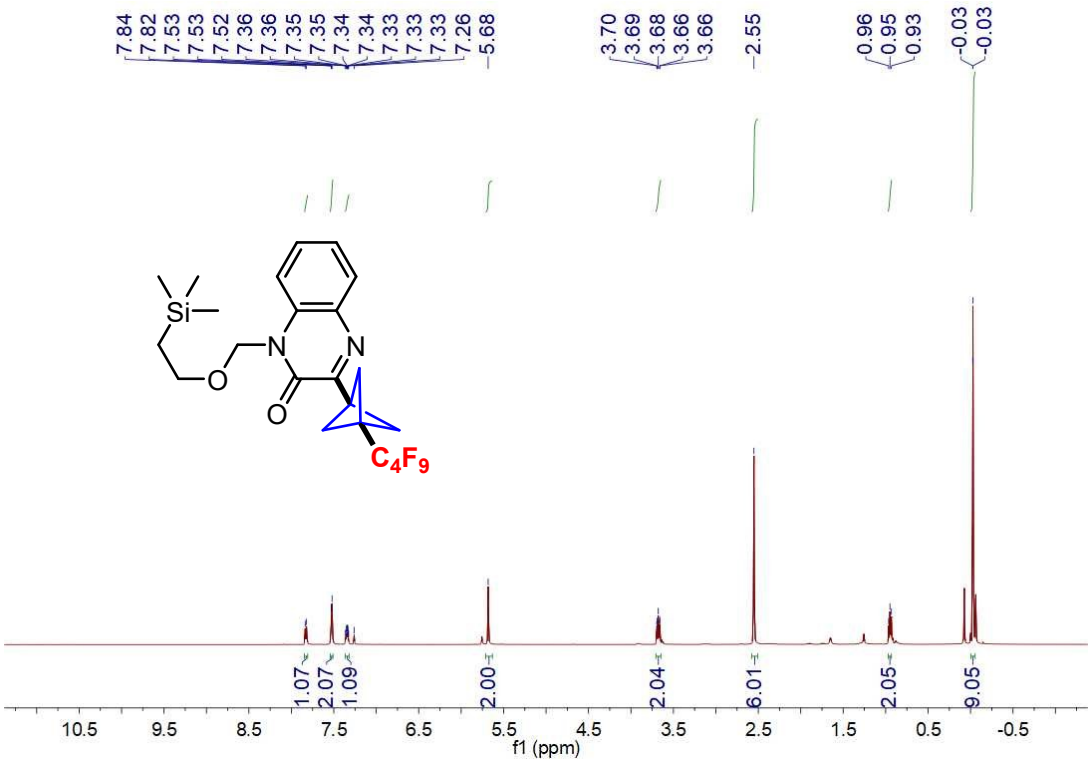
69 ^{13}C NMR (126 MHz, $CDCl_3$)



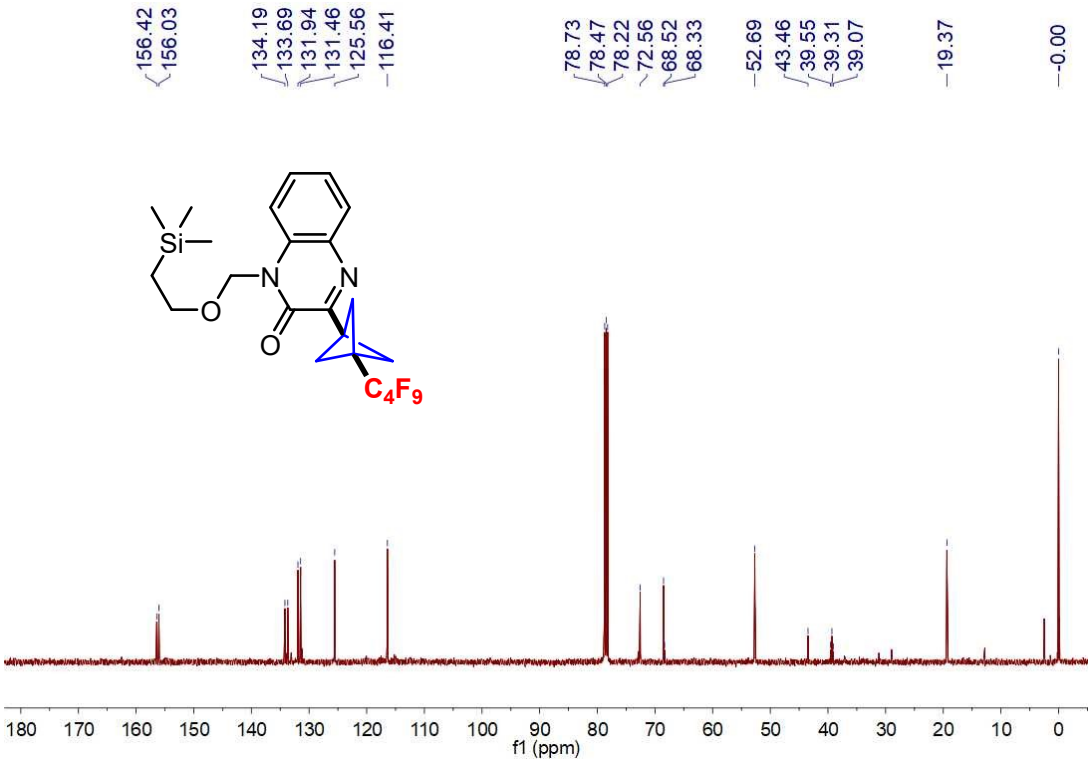
69 ^{19}F NMR (471 MHz, $CDCl_3$)



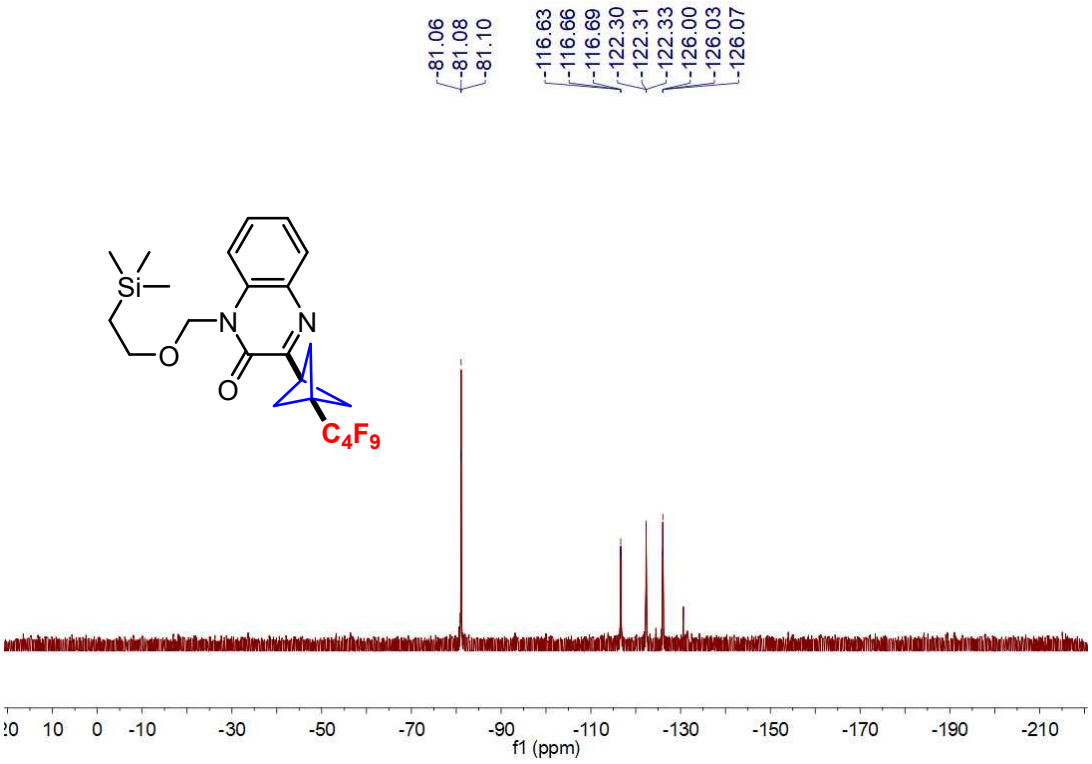
70 ^{1}H NMR (500 MHz, $CDCl_3$)



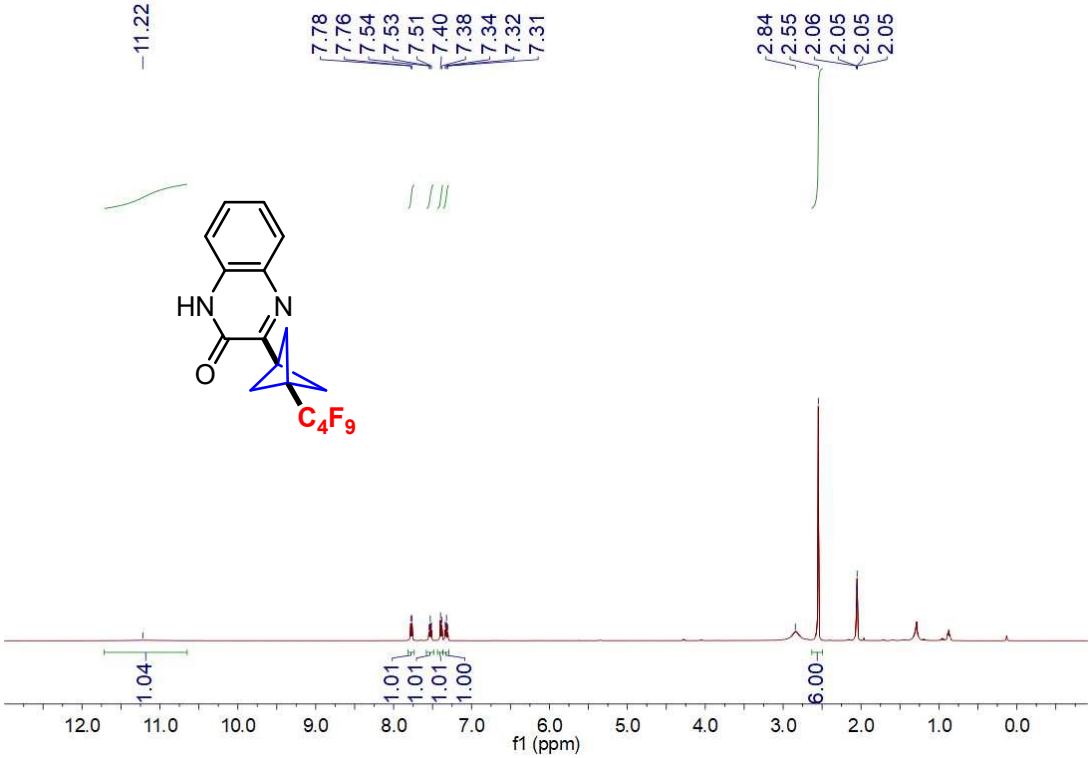
70 ^{13}C NMR (126 MHz, $CDCl_3$)



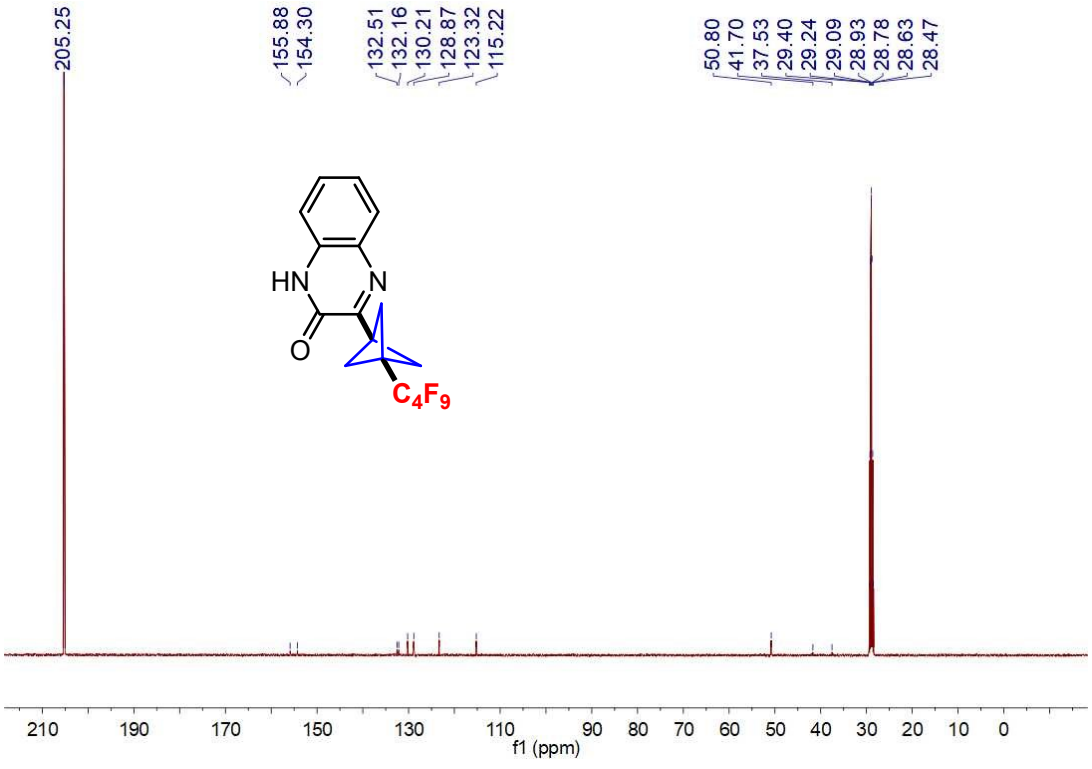
70 ^{19}F NMR (471 MHz, $CDCl_3$)



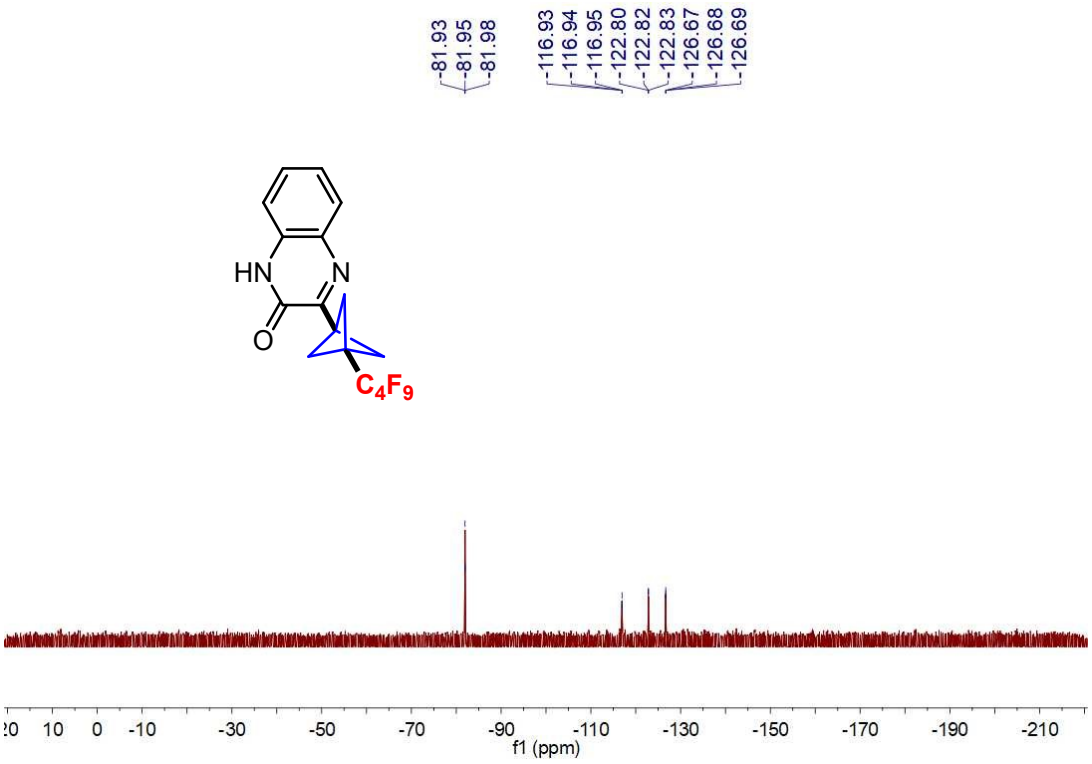
71 ^{1}H NMR (500 MHz, $CDCl_3$)



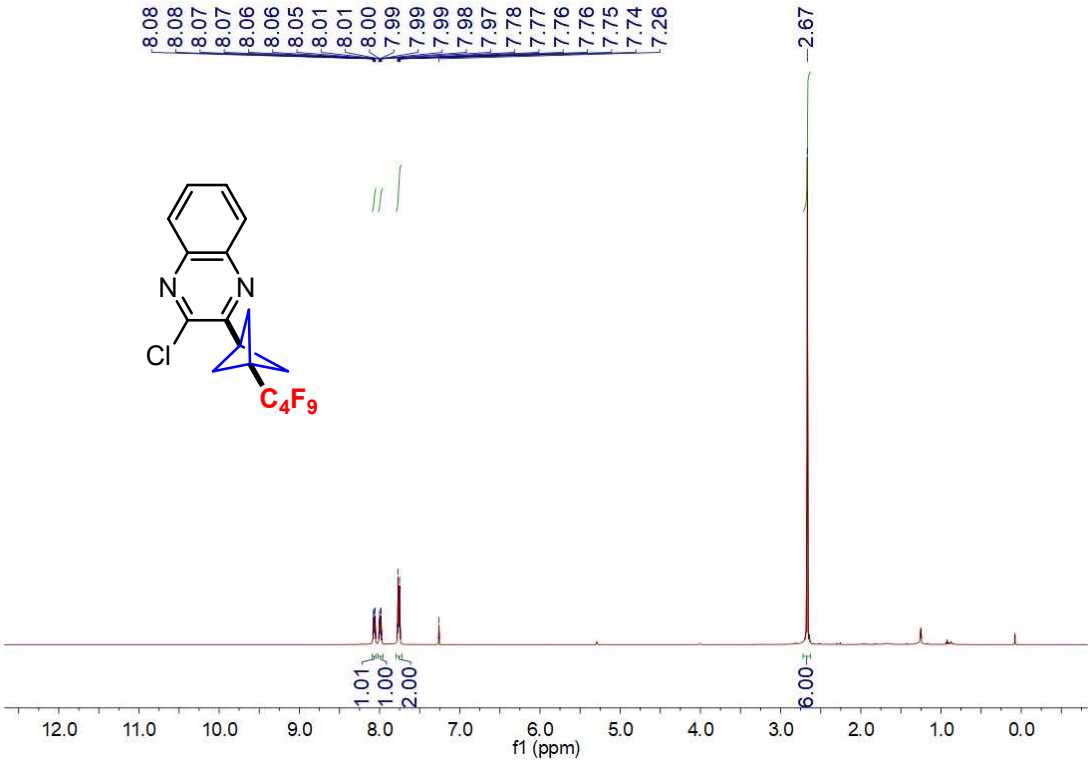
71 ^{13}C NMR (126 MHz, $CDCl_3$)



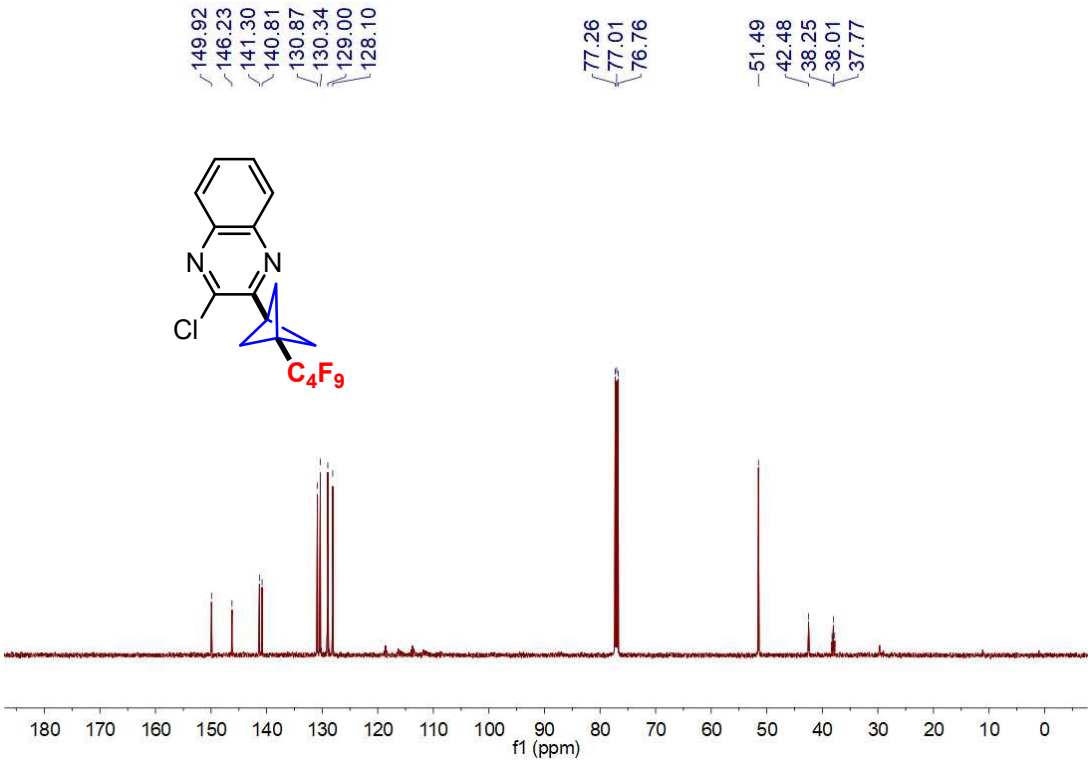
71 ^{19}F NMR (471 MHz, $CDCl_3$)



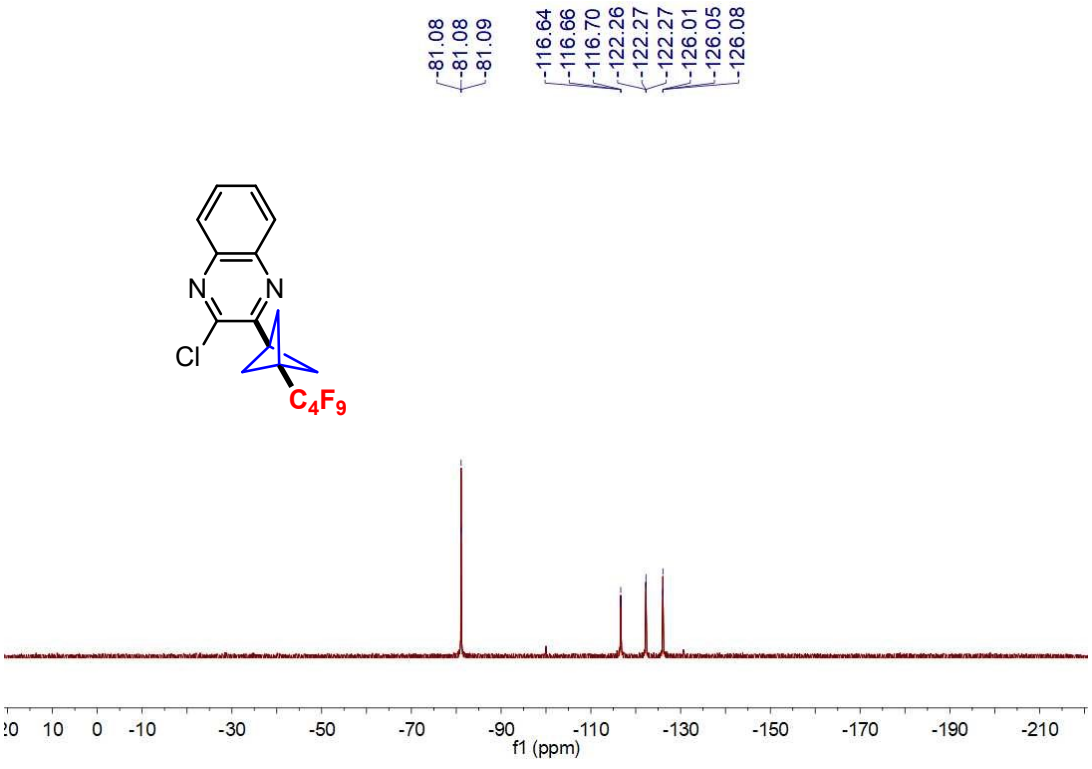
72 ^{1}H NMR (500 MHz, $CDCl_3$)



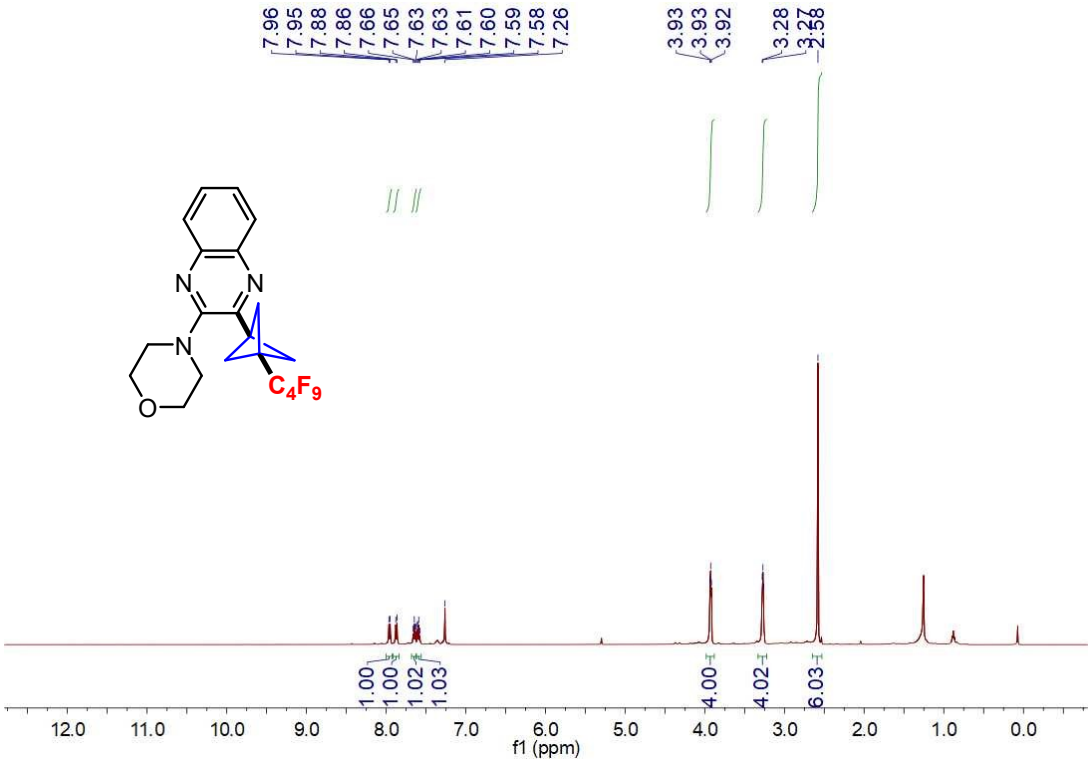
72 ^{13}C NMR (126 MHz, $CDCl_3$)



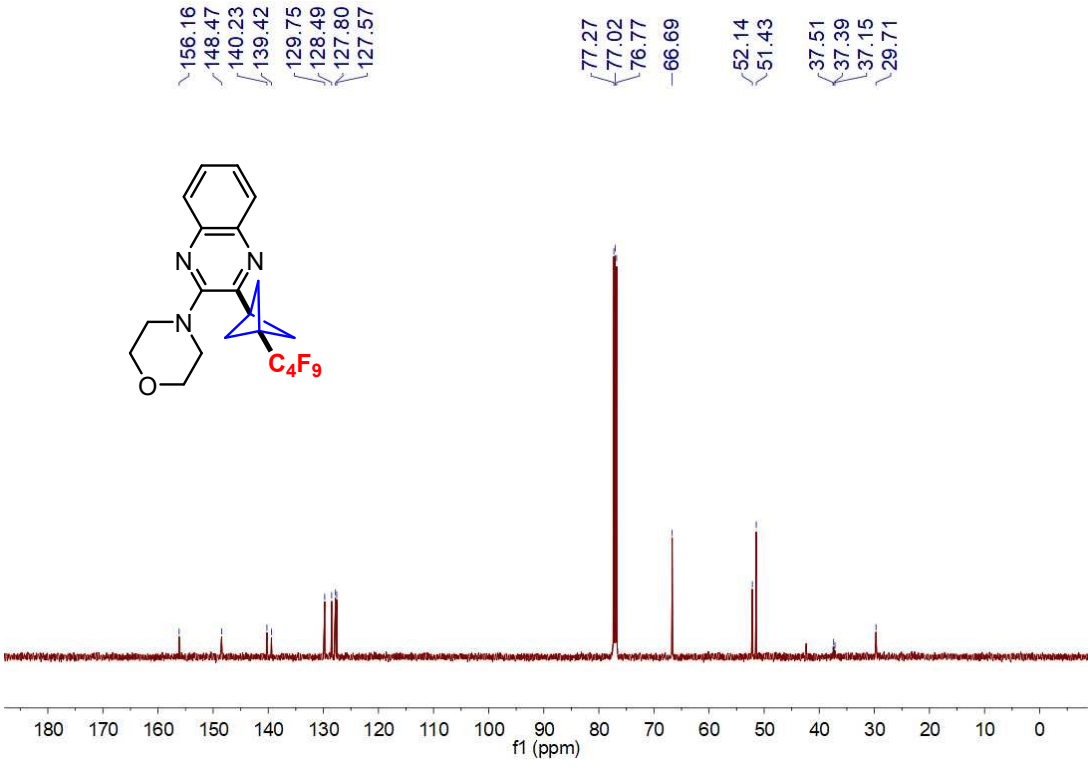
72 ^{19}F NMR (471 MHz, $CDCl_3$)



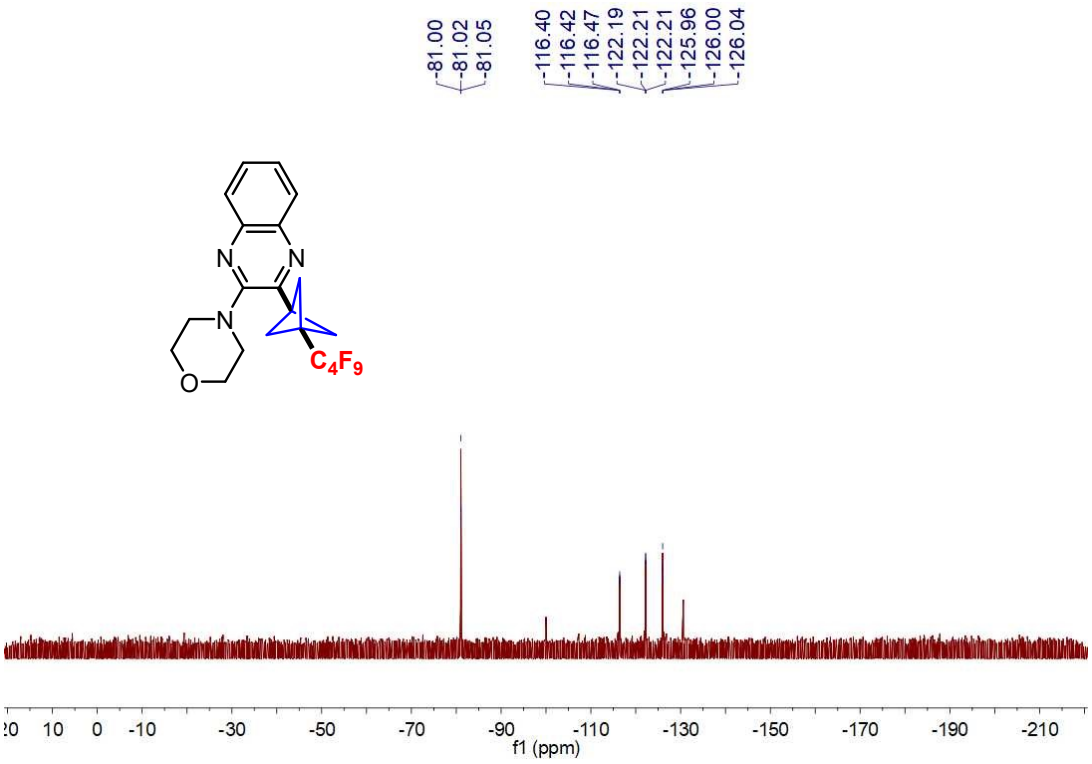
73 ^{1}H NMR (500 MHz, $CDCl_3$)



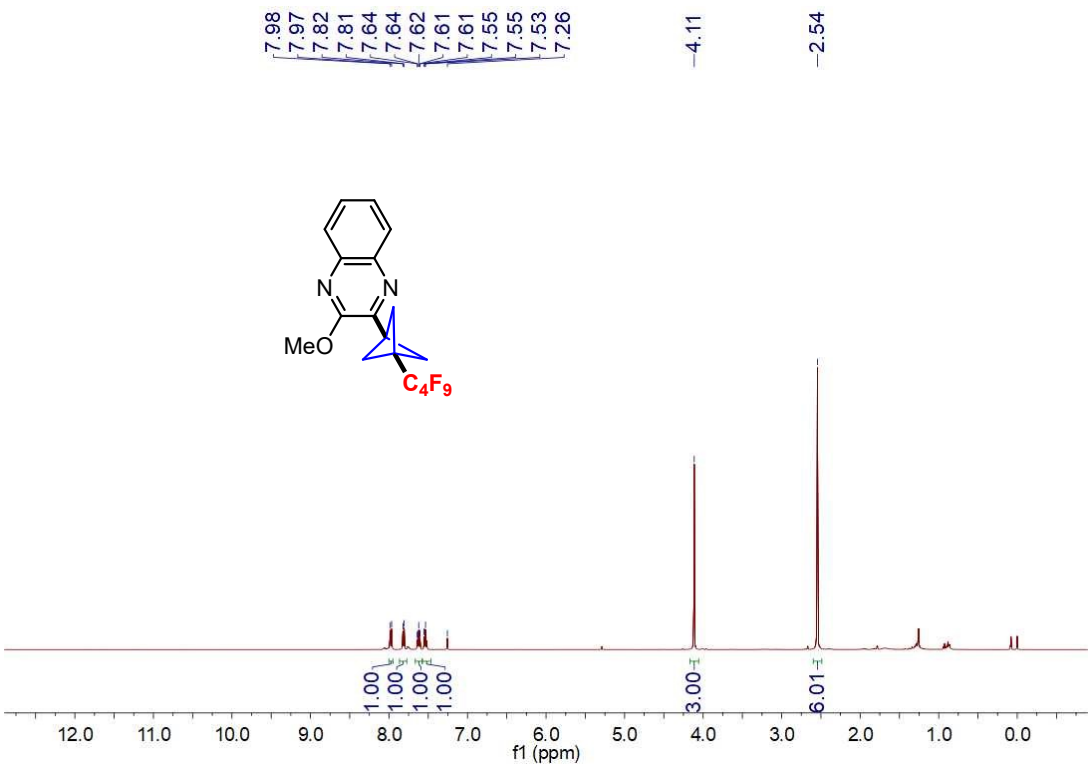
73 ^{13}C NMR (126 MHz, $CDCl_3$)



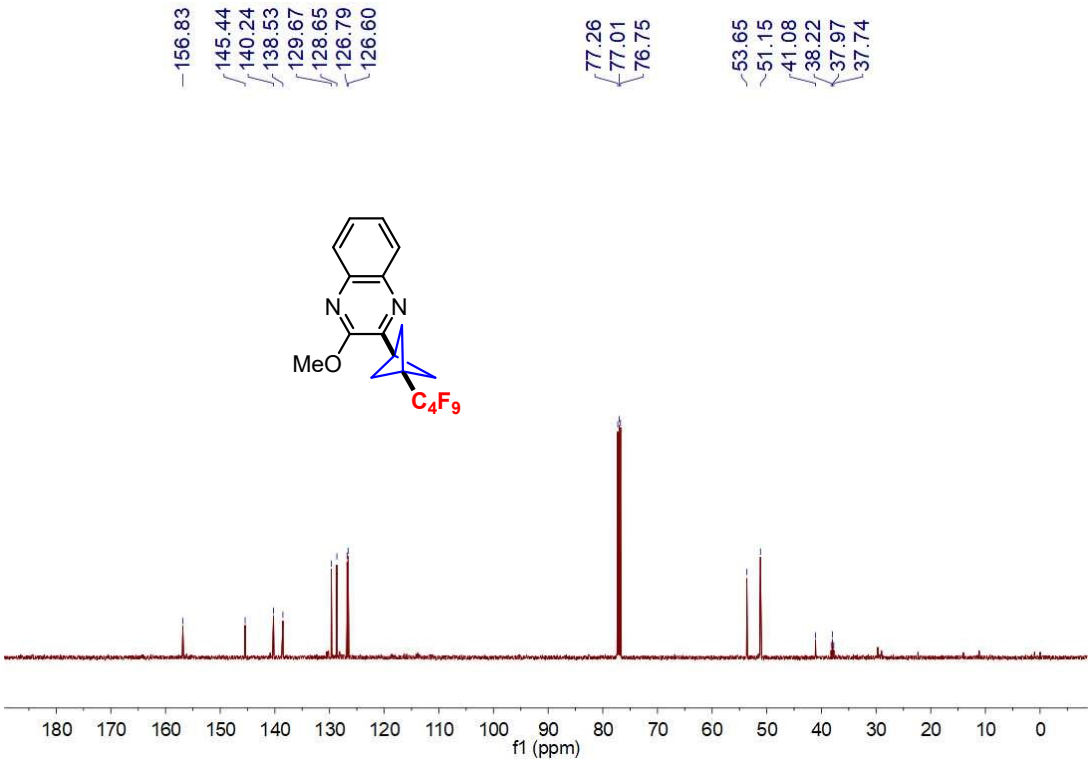
73 ^{19}F NMR (471 MHz, $CDCl_3$)



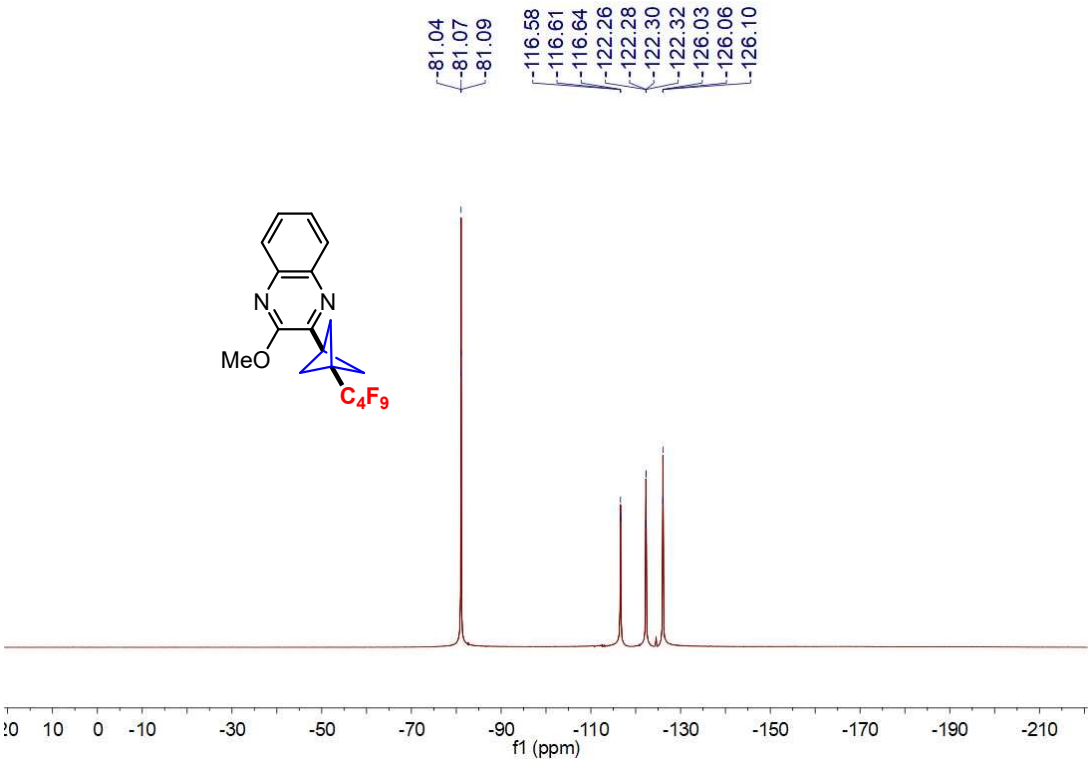
74 ^{1}H NMR (500 MHz, $CDCl_3$)



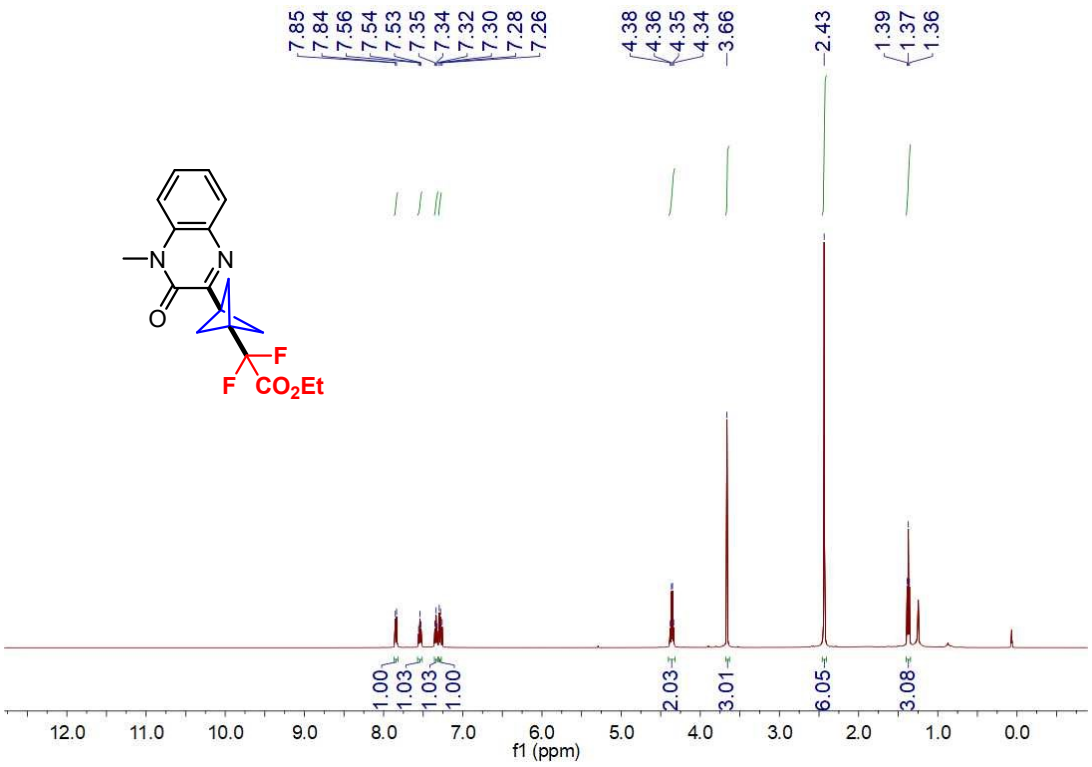
74 ^{13}C NMR (126 MHz, $CDCl_3$)



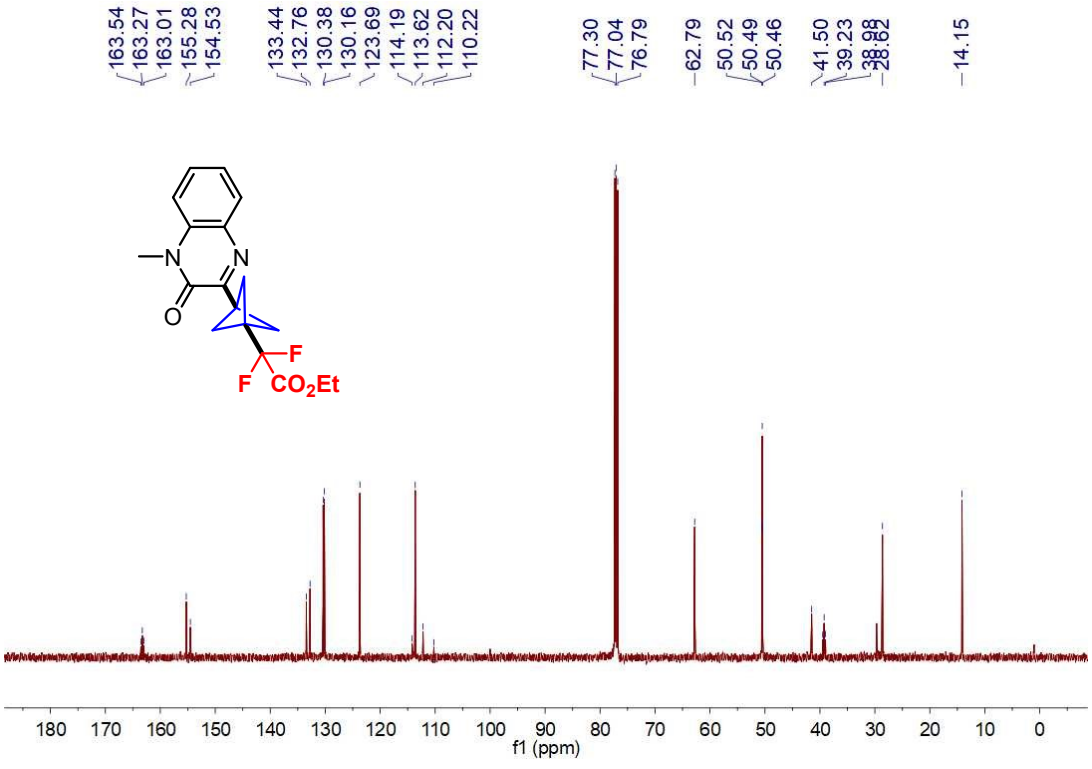
74 ^{19}F NMR (471 MHz, $CDCl_3$)



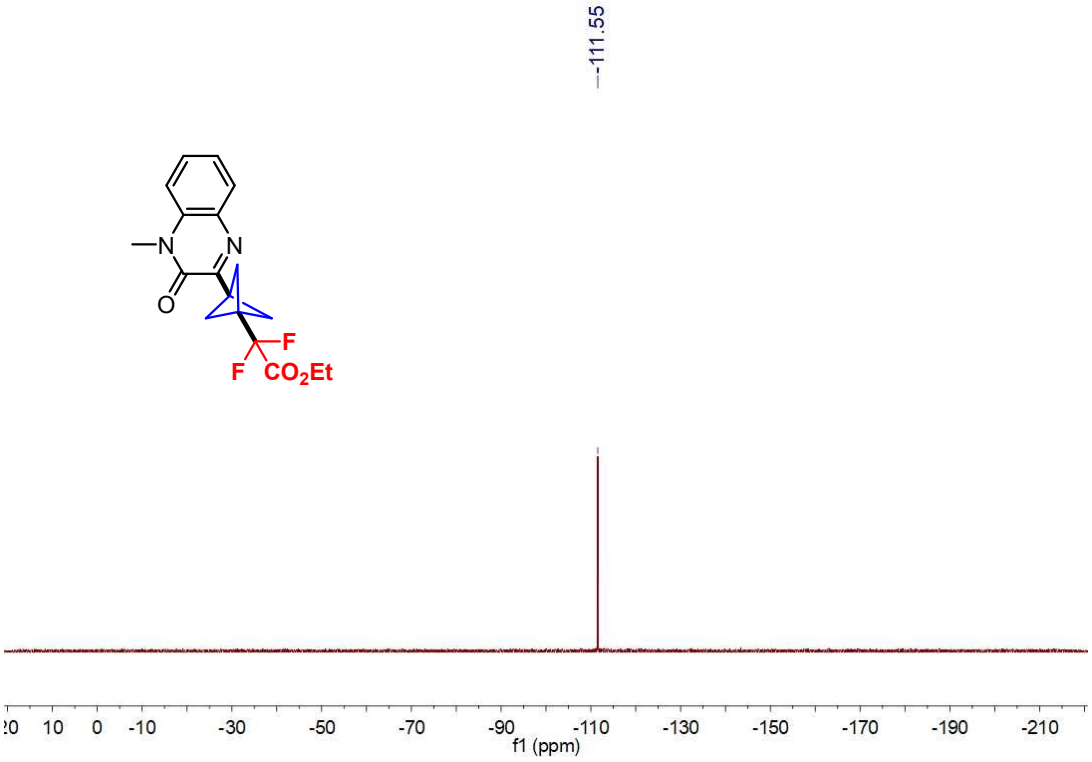
75 ^{1}H NMR (500 MHz, $CDCl_3$)



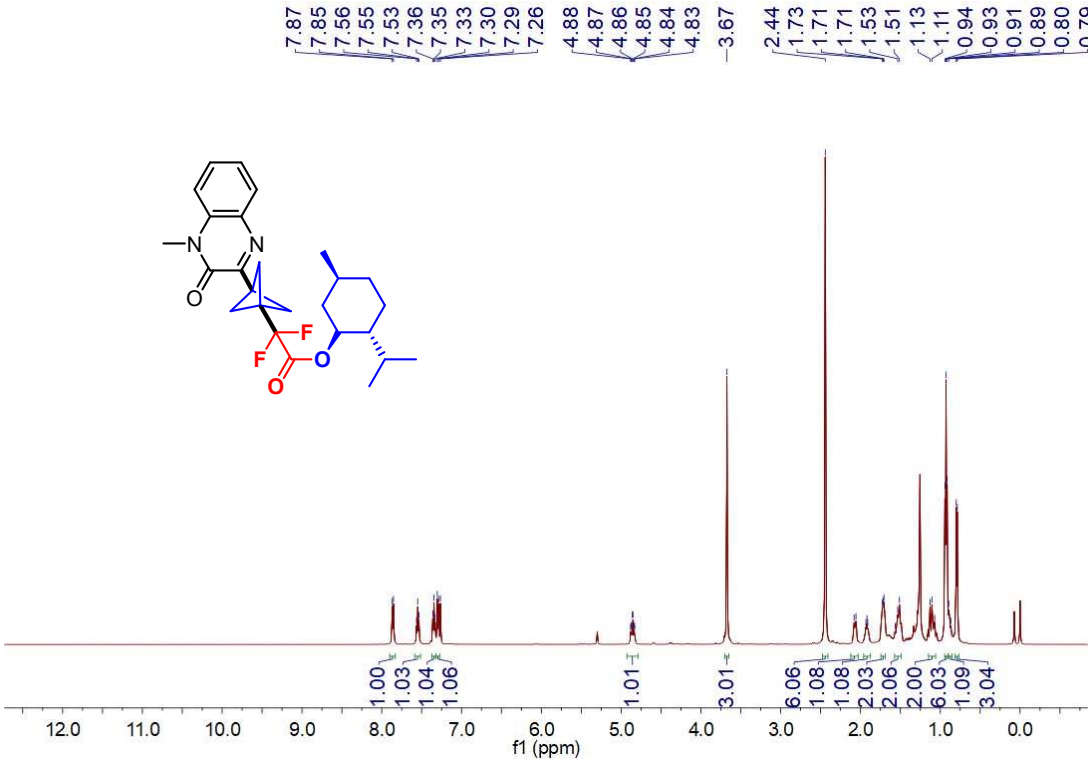
75 ^{13}C NMR (126 MHz, $CDCl_3$)



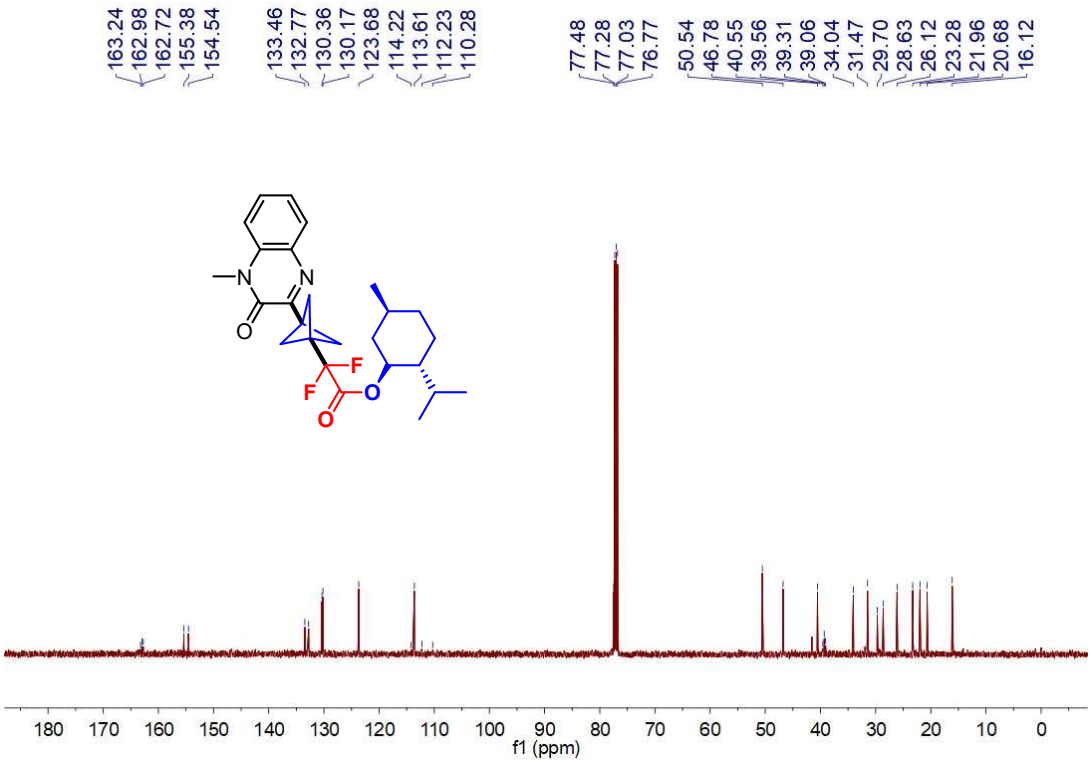
75 ^{19}F NMR (471 MHz, $CDCl_3$)



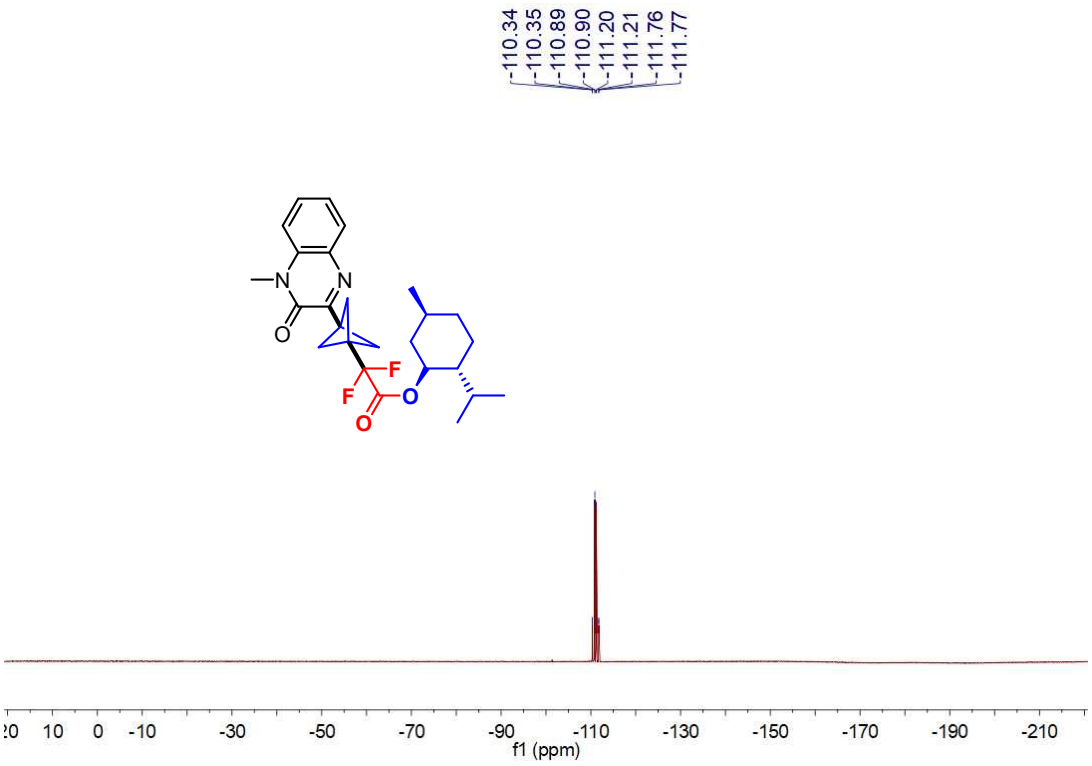
77 ^{1}H NMR (500 MHz, $CDCl_3$)



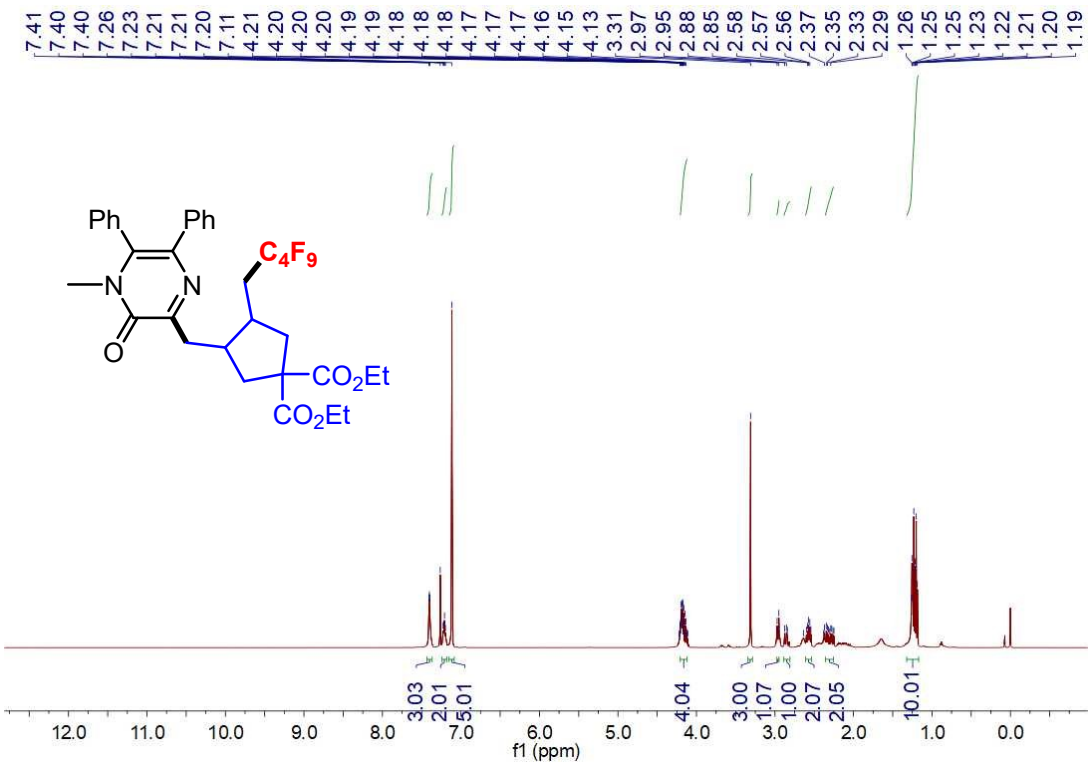
77 ^{13}C NMR (126 MHz, $CDCl_3$)



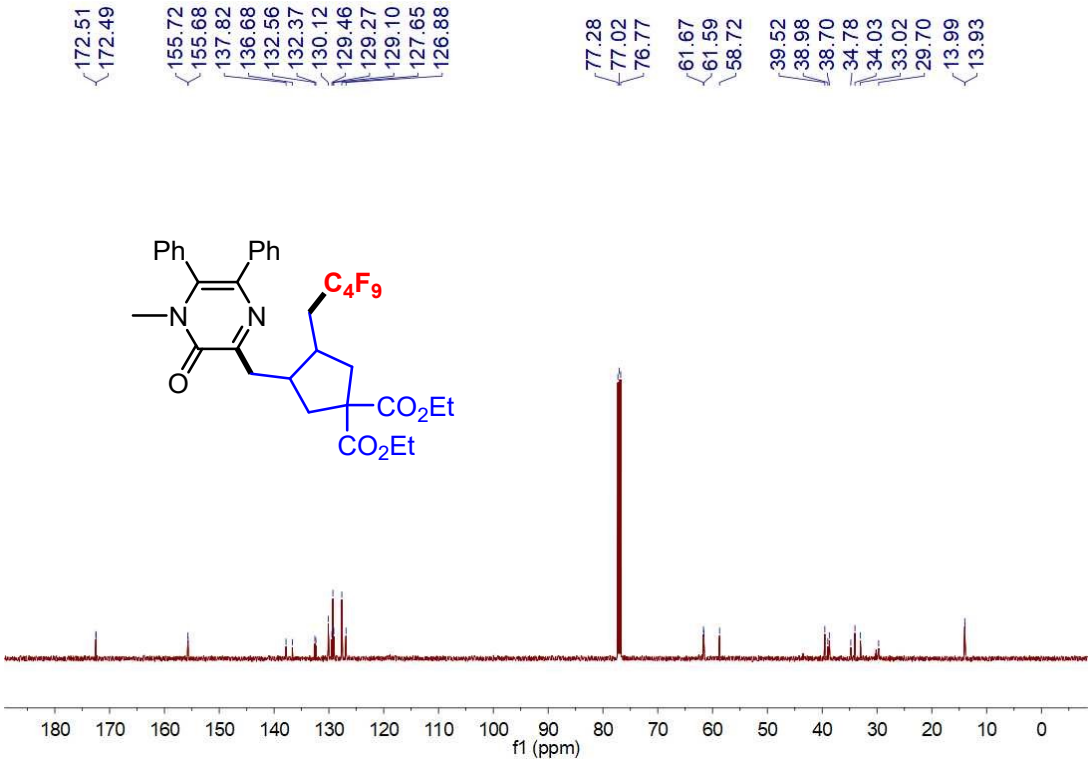
77 ^{19}F NMR (471 MHz, $CDCl_3$)



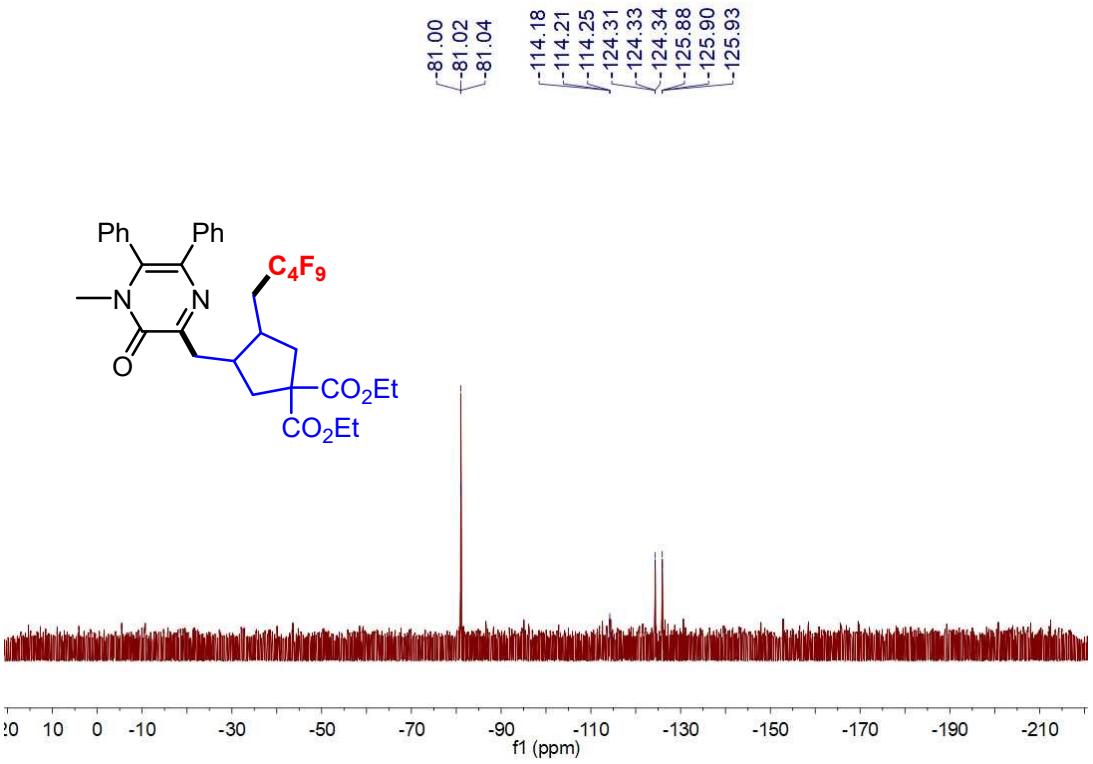
81 ^{1}H NMR (500 MHz, $CDCl_3$)



81 ^{13}C NMR (126 MHz, $CDCl_3$)



81 ^{19}F NMR (471 MHz, $CDCl_3$)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Ph
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CO2Et
CO2Et
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f1 (ppm)