Supporting Information
For

2-Aryl-Perfluorobenzoxazoles: Synthesis, Fluorescence Properties and Synthetic Application in Cubic Platinum Nanoparticles

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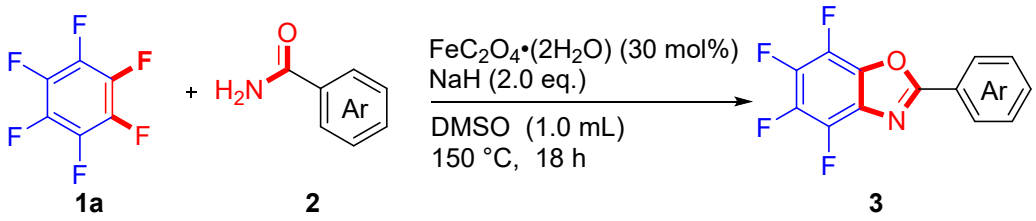
Contents

1. General information

All reagents were purchased from commercial suppliers and used as received unless otherwise noted. The reaction of the product was observed by 254 nm ultraviolet radiation, and further analyzed by GC-MS. Finally, the product was separated and purified by column chromatography. Proton, carbon and fluorine nuclear magnetic.resonance spectrum (^{1}H, ^{13}C and ^{19}F NMR) were recorded on a Bruker-400 (400 MHz for ^{1}H NMR, 101 MHz for ^{13}C NMR and 376 MHz for ^{19}F NMR) spectrometer with solvent resonance as the internal standard (^{1}H NMR, $CDCl_3$ at 7.26 ppm, DMSO at 2.50 ppm; ^{13}C NMR, $CDCl_3$ at 77.00 ppm, DMSO at 39.52 ppm. The chemical shift of the ^{1}H NMR spectrum is reported as δ, in parts per million (ppm), downfield of $(CH_3)_4Si$ (δ 0.0) and relative to the signal of $(CH_3)_4Si$ (δ 0.00, Singlet). Chemical shifts, multiplets (s = singlet, d = doublet, t = triplet, q = quadruple, m = multiplet) and coupling constants (*J*) have been reported in Hertz.

2. Experimental section

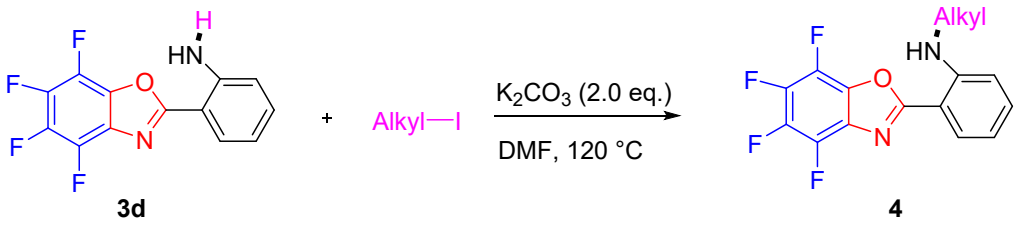
2.1 General procedure for the synthesis of perfluorobenzoxazole compounds 3a – 3x



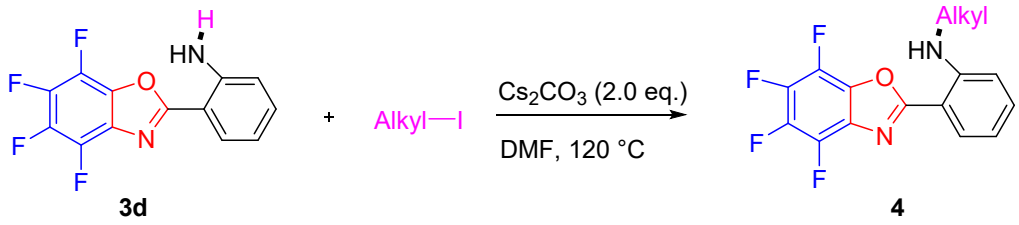
Weight **1a** (22.3 mg, 0.12 mmol), **2** (0.1 mmol), $FeC_2O_4 \cdot (2H_2O)$ (5.4 mg, 30 mol%), NaH (4.8 mg, 0.2 mmol) in a 10.0 mL reaction tube equipped with a magnetic stir bar in the glove box, and then inject 1.0 mL of anhydrous DMSO. The reaction solution was heated to 150 °C and stirred for 18 hours under nitrogen. After the reaction finished, the reaction mixture was cooled to room temperature, and the aqueous phase was extracted 3 times with ethylacetate. The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel and eluted with petroleum ether to obtain crude compound **3**. The crude product was separated by GPC (gel permeation chromatography) to obtain the main compound.

2.2 Procedure for preparation of compound 4

The general process 1



The general process 2



The general process 1: The mixture of **3d** (56.4 mg, 0.2 mmol), Alkyl iodide (0.4 mmol), K_2CO_3 (55.2 mg, 0.4 mmol) were added in the Schlenk tube of 10.0 mL equipped with a magnetic stir bar, then inject 2.0 mL of anhydrous DMF. The reaction solution was heated to 120 °C and stirred for 12 hours under nitrogen. After the reaction finished, the reaction mixture was cooled to room temperature and extracted with ethylacetate (3 × 5.0 mL). The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel and eluted with petroleum ether / ethylacetate (100:1, v/v) to afford the compound **4**. The crude product was separated by GPC gel permeation chromatography to obtain the main compound **4**.

The general process 2: The mixture of **3d** (56.4 mg, 0.2 mmol), Alkyl iodide (0.4 mmol), Cs_2CO_3 (112.4mg, 0.4 mmol) were added in the Schlenk tube of 10.0 mL equipped with a magnetic stir bar, then inject 2.0 mL of anhydrous DMF. The reaction solution was heated to 120 °C and stirred for 12 hours under nitrogen. After the reaction finished, the reaction mixture was cooled to room temperature and extracted with ethylacetate (3 × 5.0 mL), The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel and eluted with petroleum ether / ethylacetate (100:1, v/v) to afford the

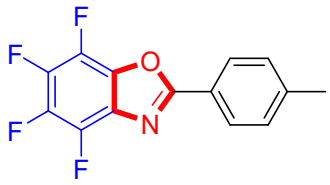
compound **4**. The crude product was separated by GPC (gel permeation chromatography) to obtain the main compound **4**.

3. Analysis data for product

3.1 Analysis Data for product 3a – 3x

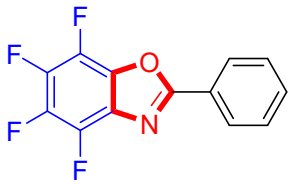
Because of the magnetic properties of fluorine nucleus, the exact assignment of all carbons bearing fluorine were not possible due to the large C-F spin-spin splitting.

4,5,6,7-tetrafluoro-2-(*p*-tolyl)benzo[*d*]oxazole (**3a**)



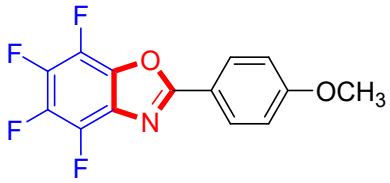
The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 72% yield. MP: 168 - 170 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 7.8 Hz, 2H), 7.35 (d, J = 7.8 Hz, 2H), 2.45 (s, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -151.31 – -151.84 (m), -158.81 – -159.16 (m), -159.84 (t, J = 20.0 Hz), -161.80 (t, J = 19.9 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.3, 143.6, 129.9, 128.0, 122.6, 21.7. HRMS-ESI (m/z): calcd for $C_{14}H_8NOF_4$, [M+H]: 282.0542; found 282.0539.

4,5,6,7-tetrafluoro-2-phenylbenzo[*d*]oxazole (**3b**)



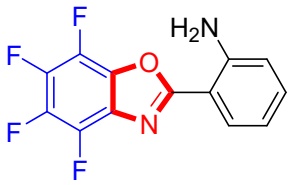
The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 73% yield. MP: 105 - 107 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 7.6 Hz, 2H), 7.62 -7.53 (m, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -150.54 – -151.72 (m), -158.39 – -159.02 (m), -159.34 (t, J = 19.9 Hz), -161.53 (t, J = 19.8 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.0, 132.7, 129.1, 128.1, 125.4. HRMS-ESI (m/z): calcd for $C_{13}H_6NOF_4$, [M+H]: 268.0386; found 268.0382.

4,5,6,7-tetrafluoro-2-(4-methoxyphenyl)benzo[*d*]oxazole (**3c**)



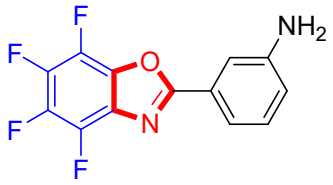
The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 60% yield. MP: 125 - 127 °C. ^{1}H NMR (400 MHz, DMSO) δ 8.14 (d, *J* = 8.0 Hz, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 3.88 (s, 3H). ^{19}F NMR (376 MHz, DMSO) δ -153.08 – 153.18 (m), -159.05 – -159.18 (m), -161.45 (t, *J* = 21.4 Hz), -163.14 (t, *J* = 21.2 Hz). ^{13}C NMR (101 MHz, DMSO) δ 165.2, 163.5, 130.3, 117.3, 115.4, 56.1. HRMS-ESI (m/z): calcd for $C_{14}H_8NO_2F_4$, [M+H]: 298.0491; found, 298.0493.

2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**3d**)



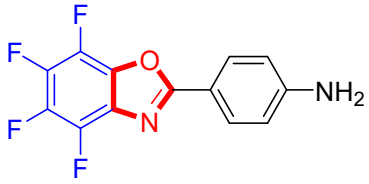
The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 72% yield. MP: 213 - 215 °C. ^{1}H NMR (400 MHz, DMSO) δ 7.90 (s, 1H), 7.38 (s, 1H), 7.11 (s, 2H), 6.98 (s, 1H), 6.74 (s, 1H). ^{19}F NMR (376 MHz, DMSO) δ -153.42 (t, *J* = 17.5 Hz), -159.43 (t, *J* = 17.0 Hz), -161.68 (t, *J* = 20.8 Hz), -163.27 (t, *J* = 20.4 Hz). ^{13}C NMR (101 MHz, DMSO) δ 165.3, 149.7, 134.2, 128.7, 116.8, 116.1, 104.8. HRMS-ESI (m/z): calcd for $C_{13}H_7N_2OF_4$, [M+H]: 283.0495; found, 283 .0494.

3-(4,5,6,7-tetrafluoro-5,6-dihydrobenzo[*d*]oxazol-2-yl)aniline (**3e**)



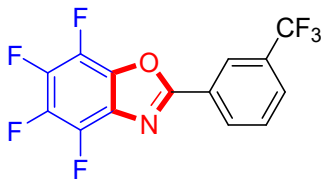
The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 64% yield. MP: 184 - 186 °C. ^{1}H NMR (400 MHz, DMSO) δ 7.41 (s, 1H), 7.31 (d, *J* = 7.6 Hz, 1H), 7.25 (t, *J* = 7.8 Hz, 1H), 6.87 – 6.78 (m, 1H), 5.59 (s, 2H). ^{19}F NMR (376 MHz, DMSO) δ -152.89 – -152.99 (m), -159.01 – -159.11 (m), -160.97 (t, *J* = 21.5 Hz), -163.02 (t, *J* = 21.3 Hz). ^{13}C NMR (101 MHz, DMSO) δ 165.8, 150.0, 130.4, 125.5, 118.7, 115.3, 112.6. HRMS-ESI (m/z): calcd for $C_{13}H_7N_2OF_4$, [M+H]: 283.0495; found, 283.0494.

4-(4,5,6,7-tetrafluoro-5,6-dihydrobenzo[*d*]oxazol-2-yl)aniline (**3f**)



The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 56% yield. MP: 190 - 192 °C.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 7.9 Hz, 2H), 6.76 (d, *J* = 8.0 Hz, 2H), 4.16 (s, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -152.13 – -153.26 (m), -159.24 – -159.91 (m), -161.33 (t, *J* = 20.0 Hz), -162.52 (t, *J* = 20.0 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.5, 150.7, 130.0, 114.6. One carbon was lost due to overlap. HRMS-ESI (m/z): calcd for $C_{13}H_7N_2OF_4$, [M+H]: 283.0495; found, 283.0493.

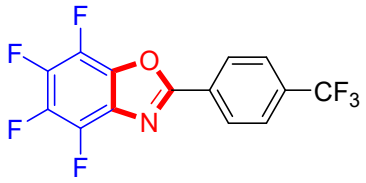
4,5,6,7-tetrafluoro-2-(3-(trifluoromethyl)phenyl)benzo[*d*]oxazole(**3g**)



The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 73% yield. MP: 89 - 91 °C. ^{1}H NMR (400

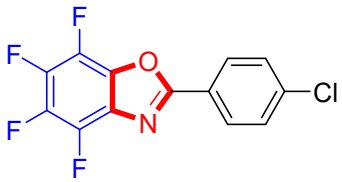
MHz, DMSO) δ 8.52 (d, *J* = 7.8 Hz, 1H), 8.44 (s, 1H), 8.10 (d, *J* = 7.7 Hz, 1H), 7.91 (t, *J* = 7.8 Hz, 1H). ^{19}F NMR (376 MHz, DMSO) δ -61.57 (s), -152.15 (dd, *J* = 21.0, 16.4 Hz), -158.50 (dd, *J* = 21.3, 16.4 Hz), -159.38 (t, *J* = 21.3 Hz), -162.07 (t, *J* = 21.1 Hz). ^{13}C NMR (101 MHz, DMSO) δ 131.8, 131.0, 125.8, 124.0 (q, *J* = 3.7 Hz). HRMS-ESI (m/z): calcd for $C_{14}H_5NOF_7$, [M+H]: 336.0259; found, 336.0258.

4,5,6,7-tetrafluoro-2-(4-(trifluoromethyl)phenyl)benzo[*d*]oxazole (**3h**)



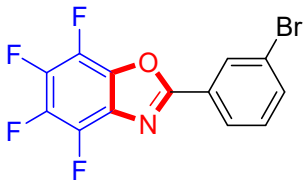
The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 75% yield. MP: 104 - 106 °C. ^{1}H NMR (400 MHz, DMSO) δ 8.37 (d, *J* = 7.9 Hz, 2H), 7.98 (d, *J* = 8.0 Hz, 2H). ^{19}F NMR (376 MHz, DMSO) δ -61.90 (s), -152.02 – 152.11 (m), -158.29 – -158.80 (m), -159.27 (t, *J* = 21.2 Hz), -162.10 (t, *J* = 21.0 Hz). ^{13}C NMR (101 MHz, DMSO) δ 163.58 (s), 132.85 (q, *J* = 32.4 Hz), 129.06 (s), 128.78 (s), 126.84 (q, *J* = 3.7 Hz), 124.1 (q, *J* = 273.7 Hz). HRMS-ESI (m/z): calcd for $C_{14}H_5NOF_7$, [M+H]: 336.0259; found 336.0264.

2-(4-chlorophenyl)-4,5,6,7-tetrafluorobenzo[*d*]oxazole (**3i**)



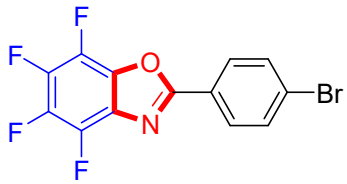
The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 79% yield. MP: 124 - 126 °C. ^{1}H NMR (400 MHz, DMSO) δ 8.22 (d, *J* = 7.9 Hz, 2H), 7.72 (d, *J* = 7.9 Hz, 2H). ^{19}F NMR (376 MHz, DMSO) δ -152.38 – 152.49 (m), -157.95 – -158.99 (m), -159.98 (t, *J* = 21.3 Hz), -162.41 (t, *J* = 21.2 Hz). ^{13}C NMR (101 MHz, DMSO) δ 164.2, 138.5, 130.2, 130.1, 124.1. HRMS-ESI (m/z): calcd for $C_{13}H_5NOF_4Cl$, [M+H]: 301.9996; found, 301.9999.

2-(3-bromophenyl)-4,5,6,7-tetrafluorobenzo[*d*]oxazole（**3j**）



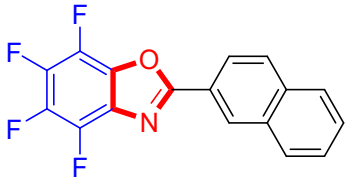
The compound was prepared according to the procedure A. The title compound was obtained as a white solid, 71% yield. MP: 109 - 111 °C. ^{1}H NMR (400 MHz, DMSO) δ 8.23 (s, 1H), 8.14 (d, *J* = 7.8 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 1H). ^{19}F NMR (376 MHz, DMSO) δ -152.16 – 152.26 (m), -158.26 – -158.74 (m), -159.58 (t, *J* = 21.3 Hz), -162.19 (t, *J* = 21.2 Hz). ^{13}C NMR (101 MHz, DMSO) δ 163.5, 136.2, 132.2, 130.4, 127.3, 123.0. One carbon was lost due to overlap. HRMS-ESI (m/z): calcd for $C_{13}H_5NOF_4Br$, [M+H]: 345.9491; found, 345.9493.

2-(4-bromophenyl)-4,5,6,7-tetrafluorobenzo[*d*]oxazole (**3k**)



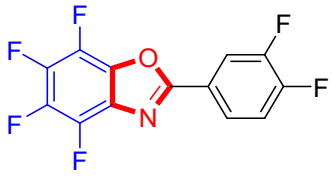
The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 76% yield. MP: 152 - 153 °C. ^{1}H NMR (400 MHz, DMSO) δ 8.15 (d, *J* = 7.7 Hz, 2H), 7.86 (d, *J* = 7.8 Hz, 2H). ^{19}F NMR (376 MHz, DMSO) δ -152.37 – -152.47 (m), -158.43 – -158.94 (m), -159.94 (t, *J* = 21.4 Hz), -162.39 (t, *J* = 21.2 Hz). ^{13}C NMR (101 MHz, DMSO) δ 163.8, 132.6, 129.7, 127.0, 123.9. HRMS-ESI (m/z): calcd for $C_{13}H_5NOF_4Br$, [M+H]: 345.9491; found 345.9490.

4,5,6,7-tetrafluoro-2-(naphthalen-2-yl)benzo[*d*]oxazole (**3l**)



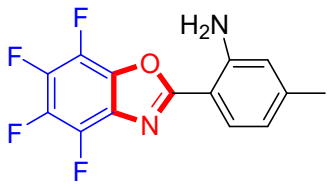
The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 69% yield. MP: 235 - 237 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (s, 1H), 8.30 (d, J = 8.6 Hz, 1H), 8.06 – 7.98 (m, 2H), 7.93 (d, J = 7.8 Hz, 1H), 7.69 – 7.55 (m, 2H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -150.84 – -151.47 (m), -158.47 – -158.96 (m), -159.24 (t, J = 19.9 Hz), -161.43 (t, J = 19.8 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.2, 132.8, 129.2, 129.1, 129.0, 128.6, 128.0, 127.3, 123.8, 122.6. HRMS-ESI (m/z): calcd for $C_{17}H_8NOF_4$, [M+H]: 318.0542; found 318.0544.

2-(3,4-difluorophenyl)-4,5,6,7-tetrafluorobenzo[*d*]oxazole (**3m**)



The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 63% yield. MP: 90 - 92 °C. ^{1}H NMR (400 MHz, DMSO) δ 8.29 – 8.19 (m, 1H), 8.07 (s, 1H), 7.72 (q, 9.0 Hz, 1H). ^{19}F NMR (376 MHz, DMSO) δ -130.94 – -131.03 (m), -135.52 – -136.88 (m), -152.23 – -152.33 (m), -157.34 – -158.95 (m), -159.77 (t, J = 21.3 Hz), -162.29 (t, J = 21.1 Hz). ^{13}C NMR (101 MHz, DMSO) δ 162.7, 152.4 (dd, J = 254.0, 12.3 Hz), 149.7 (dd, J = 234.4, 14.0 Hz), 125.6 (dd, J = 7.8, 3.6 Hz), 122.1 (dd, J = 6.8, 3.4 Hz), 119.1 (d, J = 18.2 Hz), 117.2 (d, J = 19.9 Hz). HRMS-ESI (m/z): calcd for $C_{13}H_4NOF_6$, [M+H]: 304.0197; found, 304.0197.

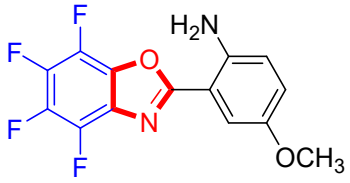
5-methyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**3n**)



The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 65% yield. MP: 195 - 197 °C. ^{1}H NMR (400 MHz, DMSO) δ 7.70 (d, J = 8.2 Hz, 1H), 6.96 (s, 2H), 6.70 (s, 1H), 6.50 (d, J = 8.2 Hz, 1H), 2.24 (s, 3H). ^{19}F NMR (376 MHz, DMSO) δ -153.63 – 153.73 (m), -158.83 – -

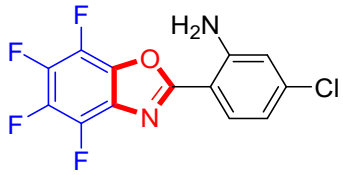
160.41 (m), -162.20 (t, J = 21.4 Hz), -163.54 (t, J = 21.2 Hz). ^{13}C NMR (101 MHz, DMSO) δ 164.9, 149.2, 144.1, 128.1, 117.2, 116.0, 102.1, 21.3. HRMS-ESI (m/z): calcd for $C_{14}H_9N_2OF_4$, [M+H]: 297.0651; found, 297.0649.

4-methoxy-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**3o**)



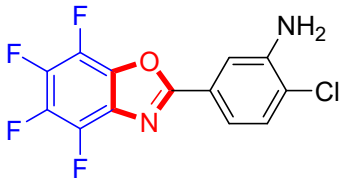
The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 62% yield. MP: 71 - 72 °C. ^{1}H NMR (400 MHz, DMSO) δ 7.26 (s, 1H), 7.04 (d, J = 9.0 Hz, 1H), 6.90 (d, J = 9.0 Hz, 1H), 6.74 (s, 2H), 3.75 (s, 3H). ^{19}F NMR (376 MHz, DMSO) δ -153.43 (dd, J = 21.0, 16.1 Hz), -158.80 – -159.52 (m), -161.66 (t, J = 21.5 Hz), -163.21 (t, J = 21.2 Hz). ^{13}C NMR (101 MHz, DMSO) δ 164.7, 149.7, 144.3, 123.4, 118.2, 109.3, 103.8, 55.5. HRMS-ESI (m/z): calcd for $C_{14}H_9N_2O_2F_4$, [M+H]: 313.0600; found 313.0602.

5-chloro-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**3p**)



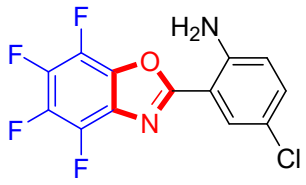
The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 71% yield. MP: 181 - 182 °C. ^{1}H NMR (400 MHz, DMSO) δ 7.77 (s, 1H), 7.18 (s, 2H), 6.92 (s, 1H), 6.64 (s, 1H). ^{19}F NMR (376 MHz, DMSO) δ -152.81 – -153.53 (m), -159.05 – -159.61 (m), -161.23 (t, J = 20.8 Hz), -163.01 (t, J = 20.8 Hz). ^{13}C NMR (101 MHz, DMSO) δ 163.9, 149.8, 138.3, 130.0, 115.6, 114.9, 103.4. HRMS-ESI (m/z): calcd for $C_{13}H_6N_2OF_4Cl$, [M+H]: 317.0105; found, 317.0104.

2-chloro-5-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**3q**)



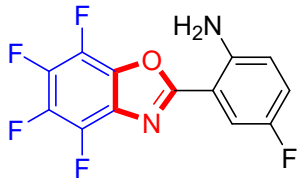
The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 62% yield. MP: 205 - 207 °C. ^{1}H NMR (400 MHz, DMSO) δ 7.67 (s, 1H), 7.44 (d, *J* = 8.2 Hz, 1H), 7.34 (d, *J* = 8.2 Hz, 1H), 5.83 (s, 2H). ^{19}F NMR (376 MHz, DMSO) δ -152.79 (dd, *J* = 21.0, 16.3 Hz), -158.19 – -159.40 (m), -160.58 (t, *J* = 21.4 Hz), -162.78 (t, *J* = 21.1 Hz). ^{13}C NMR (101 MHz, DMSO) δ 164.4, 145.6, 130.2, 123.9, 121.5, 115.6, 113.7. HRMS-ESI (m/z): calcd for $C_{13}H_6N_2OF_4Cl$, [M+H]: 317.0105; found, 317.0107.

4-chloro-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**3r**)



The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 76% yield. MP: 182 - 184 °C. ^{1}H NMR (400 MHz, DMSO) δ 7.75 (s, 1H), 7.33 (d, *J* = 9.0 Hz, 1H), 7.17 (s, 2H), 6.95 (d, *J* = 8.9 Hz, 1H). ^{19}F NMR (376 MHz, DMSO) δ -153.01 (dd, *J* = 21.0, 16.1 Hz), -158.79 – -159.46 (m), -160.88 (t, *J* = 21.4 Hz), -162.80 (t, *J* = 21.2 Hz). ^{13}C NMR (101 MHz, DMSO) δ 163.5, 147.9, 133.4, 126.8, 118.8, 118.3, 105.2. HRMS-ESI (m/z): calcd for $C_{13}H_6N_2OF_4Cl$, [M+H]: 317.0105; found, 317.0105.

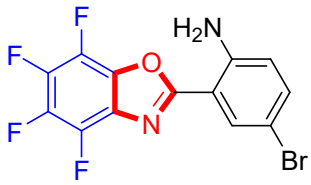
4-fluoro-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**3s**)



The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 60% yield. MP: 179 - 181 °C.^{1}H NMR (400

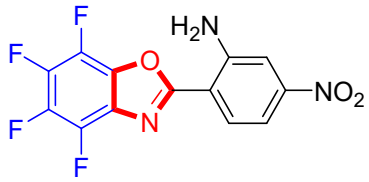
MHz, DMSO) δ 7.50 (d, J = 9.3 Hz, 1H), 7.23 (t, J = 7.7 Hz, 1H), 6.93 (s, 3H). ^{19}F NMR (376 MHz, DMSO) δ -127.27 – -129.70 (m), -153.13 (dd, J = 21.0, 16.1 Hz), -158.99 – -159.35 (m), -161.05 (t, J = 21.3 Hz), -162.93 (t, J = 21.1 Hz). ^{13}C NMR (101 MHz, DMSO) δ 163.8, 152.9 (d, J = 231.8 Hz), 146.1, 121.9 (d, J = 23.5 Hz), 118.0 (d, J = 7.4 Hz), 112.5 (d, J = 24.3 Hz), 103.7 (d, J = 8.1 Hz). HRMS-ESI (m/z): calcd for $C_{13}H_6N_2OF_5$, [M+H]: 301.0400; found, 301.0398.

4-bromo-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**3t**)



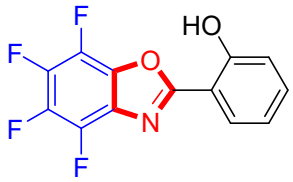
The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 64% yield. MP: 190 - 192 °C. ^{1}H NMR (400 MHz, DMSO) δ 7.90 – 7.64 (m, 1H), 7.48 – 7.28 (m, 1H), 7.13 (s, 2H), 6.84 (d, J = 8.5 Hz, 1H). ^{19}F NMR (376 MHz, DMSO) δ -152.95 (dd, J = 20.7, 16.4 Hz), -158.62 – -159.30 (m), -160.83 (t, J = 21.3 Hz), -162.74 (t, J = 21.1 Hz). ^{13}C NMR (101 MHz, DMSO) δ 163.2, 148.1, 135.9, 129.5, 118.4, 105.6. One carbon was lost due to overlap. HRMS-ESI (m/z): calcd for $C_{13}H_6N_2OF_4Br$, [M+H]: 360.9600; found, 360.9601.

5-nitro-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**3u**)



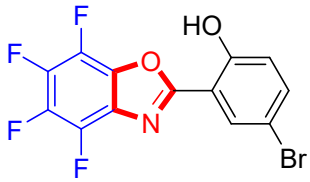
The compound was prepared according to the procedure mentioned above. The title compound was obtained as a yellow solid, 58% yield. MP: 202 - 204 °C. ^{1}H NMR (400 MHz, DMSO) δ 8.13 (d, J = 8.8 Hz, 1H), 7.80 (s, 1H), 7.54 (s, 2H), 7.42 (d, J = 8.6 Hz, 1H). ^{19}F NMR (376 MHz, DMSO) δ -152.36 (dd, J = 21.0, 16.3 Hz), -158.45 – -159.16 (m), -159.88 (t, J = 21.4 Hz), -162.38 (t, J = 21.1 Hz). ^{13}C NMR (101 MHz, DMSO) δ 163.1, 150.3, 149.3, 130.4, 110.6, 109.1. One carbon was lost due to overlap. HRMS-ESI (m/z): calcd for $C_{13}H_6N_3O_3F_4$, [M+H]: 328.0345; found, 328.0344.

2-(perfluorobenzo[*d*]oxazol-2-yl)phenol (**3v**)



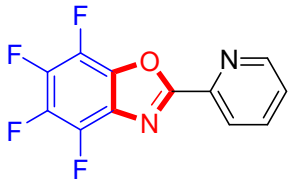
The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 59% yield. MP: 222 - 224 °C. ^{1}H NMR (400 MHz, DMSO) δ 10.92 (s, 1H), 7.81 (d, *J* = 7.6 Hz, 1H), 7.68 (t, *J* = 7.6 Hz, 1H), 7.44 – 7.37 (m, 2H). ^{19}F NMR (376 MHz, DMSO) δ -150.15 (dd, *J* = 23.2, 6.8 Hz), -158.66 (dd, *J* = 23.2, 6.8 Hz), -161.73 (t, *J* = 23.0 Hz), -162.43 (t, *J* = 22.9 Hz). ^{13}C NMR (101 MHz, DMSO) δ 164.9, 158.1, 135.0, 132.0, 126.7, 125.1, 120.4. HRMS-ESI (m/z): calcd for $C_{13}H_6NO_2F_4$, [M+H]: 284.0335; found, 284.0331.

4-bromo-2-(perfluorobenzo[*d*]oxazol-2-yl)phenol (**3w**)



The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 54% yield. MP: 226 - 228 °C. ^{1}H NMR (400 MHz, DMSO) δ 11.06 (s, 1H), 8.03 – 7.73 (m, 2H), 7.35 (d, *J* = 8.5 Hz, 1H). ^{19}F NMR (376 MHz, DMSO) δ -149.84 (dd, *J* = 23.1, 6.7 Hz), -158.29 (dd, *J* = 23.2, 6.8 Hz), -161.37 (t, *J* = 23.0 Hz), -162.04 (t, *J* = 23.0 Hz). ^{13}C NMR (101 MHz, DMSO) δ 163.5, 157.2, 137.4, 134.1, 127.2, 122.9, 118.5. HRMS-ESI (m/z): calcd for $C_{13}H_5NO_2F_4Br$, [M+H]: 361.9440; found, 361.9450.

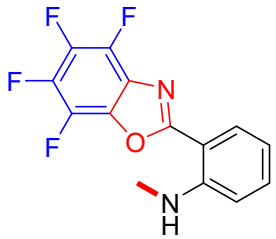
4,5,6,7-tetrafluoro-2-(pyridin-2-yl)benzo[*d*]oxazole (**3x**)



The compound was prepared according to the procedure mentioned above. The title compound was obtained as a white solid, 51% yield. MP: 101 - 103 °C. ^{1}H NMR (400 MHz, DMSO) δ 8.21 (s, 2H), 7.71 (s, 2H). ^{13}C NMR (101 MHz, DMSO) δ 163.7, 156.7, 138.0, 129.7, 129.6, 123.6. ^{19}F NMR (376 MHz, DMSO) δ -152.23 – -152.55 (m), -158.56 – -159.03 (m), -160.00 (t, J = 20.1 Hz), -162.43 (t, J = 20.6 Hz). HRMS-ESI (m/z): calcd for $C_{12}H_5N_2OF_4$, [M+H]: 269.0338; found, 269.0339.

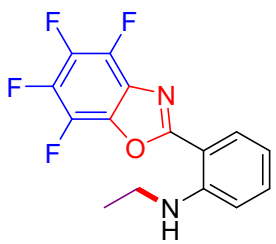
3.2 Analysis data for product 4a – 4l

N-methyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline **(4a)**



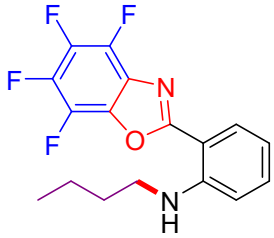
The representative **general procedure 1** mentioned above was followed. The title compound was obtained as a white solid, 56% yield. MP: 212 - 215 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, J = 8.0 Hz, 1H), 7.93 (s, 1H), 7.43 (t, J = 7.7 Hz, 1H), 6.92 – 6.44 (m, 2H), 3.07 (d, J = 3.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -152.17 – -152.31 (m), -158.82 – -159.55 (m), -160.51 (t, J = 20.1 Hz), -162.24 (t, J = 19.9 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.2, 149.5, 134.2, 129.3, 115.3, 110.8, 106.1, 29.8. HRMS-ESI (m/z): calcd for $C_{14}H_9N_2OF_4$, [M+H]: 297.0651; found 297.0657.

N-ethyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4b**)



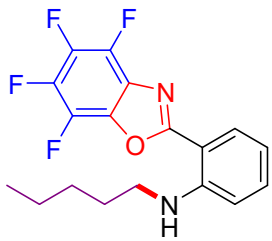
The representative **general procedure 1** mentioned above was followed. The title compound was obtained as a white solid, 60% yield. MP: 159 - 161 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.9 Hz, 1H), 7.92 (s, 1H), 7.39 (t, *J* = 7.7 Hz, 1H), 6.78 (d, *J* = 8.5 Hz, 1H), 6.71 (t, *J* = 7.4 Hz, 1H), 3.63 – 3.00 (m, 2H), 1.41 (t, *J* = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -151.87 – -153.49 (m), -158.98 – -159.75 (m), -160.65 (t, *J* = 20.1 Hz), -162.38 (t, *J* = 19.9 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.2, 148.6, 134.1, 129.3, 115.1, 111.2, 105.8, 37.6, 14.5. HRMS-ESI (m/z): calcd for $C_{15}H_{11}N_2OF_4$, [M+H]: 311.0808; found 311.0815.

N-butyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4c**)



The representative **general procedure 2** mentioned above was followed. The title compound was obtained as a white solid, 48% yield. MP: 98 - 100 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 7.8 Hz, 2H), 7.39 (t, *J* = 7.7 Hz, 1H), 6.79 (d, *J* = 8.5 Hz, 1H), 6.71 (t, *J* = 7.4 Hz, 1H), 3.33 (dd, *J* = 12.1, 6.0 Hz, 2H), 1.85 – 1.68 (m, 2H), 1.55 (d, *J* = 7.5 Hz, 2H), 1.02 (t, *J* = 7.2 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -151.94 – -153.04 (m), -158.74 – -159.88 (m), -160.68 (t, *J* = 20.1 Hz), -162.40 (t, *J* = 19.9 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.3, 148.8, 134.1, 129.3, 115.0, 111.2, 105.8, 42.8, 31.1, 20.3, 13.8. HRMS-ESI (m/z):calcd for $C_{17}H_{15}N_2OF_4$, [M+H]: 339.1121; found, 339.1123.

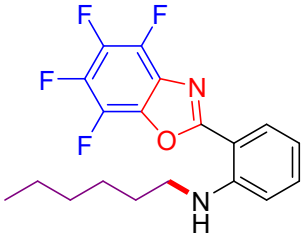
N-pentyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4d**)



The representative **general procedure 2** mentioned above was followed. The title

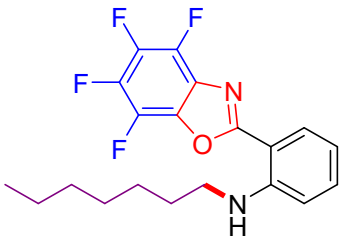
compound was obtained as a white solid, 44% yield. MP: 71 - 73 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, J = 7.6 Hz, 2H), 7.38 (t, J = 7.7 Hz, 1H), 6.77 (d, J = 8.5 Hz, 1H), 6.70 (t, J = 7.5 Hz, 1H), 3.31 (dd, J = 11.7, 5.6 Hz, 2H), 1.87 – 1.72 (m, 2H), 1.54 – 1.42 (m, 4H), 0.96 (t, J = 6.9 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -152.02 – -152.83 (m), -159.00 – -159.90 (m), -160.71 (t, J = 20.1 Hz), -162.42 (t, J = 19.9 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.3, 148.8, 134.0, 129.3, 115.0, 111.2, 105.8, 43.0, 29.4, 28.8, 22.5, 14.0. HRMS-ESI (m/z): calcd for $C_{18}H_{17}N_2OF_4$, [M+H]: 353.1277; found, 353.1277 .

N-hexyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4e**)



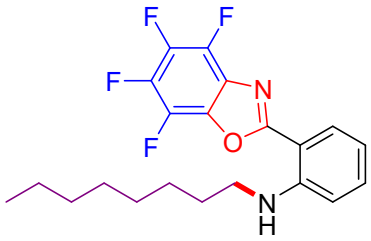
The representative **general procedure 2** mentioned above was followed. The title compound was obtained as a white solid, 41% yield. MP: 66 - 68 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, J = 7.6 Hz, 2H), 7.39 (t, J = 7.7 Hz, 1H), 6.78 (d, J = 8.5 Hz, 1H), 6.71 (t, J = 7.4 Hz, 1H), 3.63 – 3.08 (m, 2H), 1.87 – 1.71 (m, 2H), 1.60 – 1.48 (m, 2H), 1.38 (s, 4H), 0.91 (t, J = 11.4 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -152.22 – -153.13 (m), -158.42 – -159.68 (m), -160.69 (t, J = 20.1 Hz), -162.39 (t, J = 19.9 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.3, 148.8, 134.1, 129.3, 115.0, 111.2, 105.8, 43.0, 31.6, 29.0, 26.8, 22.6, 14.0. HRMS-ESI (m/z): calcd for $C_{19}H_{19}N_2OF_4$, [M+H]: 367.1434; found, 367.1431.

N-heptyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4f**)



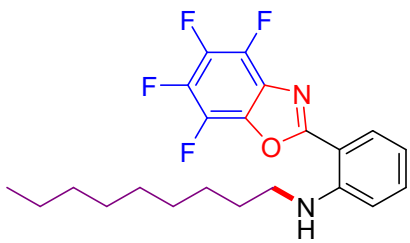
The compound was prepared according to the procedure B. The title compound was obtained as a white solid, 46% yield. MP: 70 - 72 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 – 7.82 (m, 2H), 7.39 – 7.30 (m, 1H), 6.71 (d, *J* = 8.5 Hz, 1H), 6.69 – 6.63 (m, 1H), 3.29 – 3.24 (m, 2H), 1.85 – 1.68 (m, 2H), 1.52 – 1.47 (m, 2H), 1.44 – 1.22 (m, 6H), 1.04 – 0.80 (m, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -152.66 (dd, *J* = 19.8, 16.6 Hz), -159.42 – -159.52 (m), -160.82 (dd, *J* = 26.1, 14.4 Hz), -162.16 – -163.33 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.1 (d, *J* = 2.4 Hz), 148.6, 133.9, 129.1, 114.9, 111.1, 105.6, 43.0, 31.8, 29.1, 29.0, 27.2, 22.6, 14.0. HRMS-ESI (m/z): calcd for $C_{20}H_{21}N_2OF_4$, [M+H]: 381.1590; found, 381.1583.

N-octyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4g**)



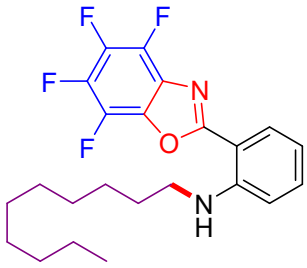
The representative **general procedure 2** mentioned above was followed. The title compound was obtained as a white solid, 50% yield. MP: 73 - 74 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (dd, *J* = 7.9, 1.4 Hz, 2H), 7.40 (dd, *J* = 11.4, 4.2 Hz, 1H), 6.79 (d, *J* = 8.5 Hz, 1H), 6.72 (t, *J* = 7.5 Hz, 1H), 3.32 (dd, *J* = 12.1, 6.9 Hz, 2H), 1.86 – 1.70 (m, 2H), 1.55 – 1.46 (m, 2H), 1.45 – 1.19 (m, 8H), 0.89 (t, *J* = 6.8 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -152.45 (dd, *J* = 19.8, 16.6 Hz), -159.01 – -159.87 (m), -160.63 (t, *J* = 20.1 Hz), -162.36 (t, *J* = 20.0 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.3, 148.8, 134.1, 129.3, 115.0, 111.2, 105.8, 43.0, 31.8, 29.4, 29.3, 29.0, 27.2, 22.6, 14.1. HRMS-ESI(m/z): calcd for $C_{21}H_{23}N_2OF_4$, [M+H]: 395.1747; found, 395.1751.

N-nonyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4h**)



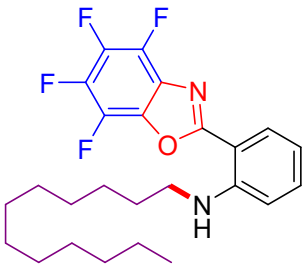
The representative **general procedure 2** mentioned above was followed. The title compound was obtained as a white solid, 43% yield. MP: 79 - 80 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 6.7 Hz, 2H), 7.40 (t, *J* = 7.8 Hz, 1H), 6.79 (d, *J* = 8.5 Hz, 1H), 6.72 (t, *J* = 7.5 Hz, 1H), 3.32 (dd, *J* = 12.1, 6.8 Hz, 2H), 1.85 – 1.73 (m, 2H), 1.50 (dd, *J* = 15.3, 7.5 Hz, 2H), 1.34 – 1.21 (m, 10H), 0.88 (t, *J* = 6.6 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -152.46 (dd, *J* = 19.7, 16.6 Hz), -158.86 – -159.84 (m), -160.66 (t, *J* = 20.1 Hz), -161.48 – -162.65 (m). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.3, 148.8, 134.1, 129.3, 115.0, 111.2, 105.8, 43.0, 31.9, 29.6, 29.4, 29.3, 29.0, 27.2, 22.7, 14.1. HRMS-ESI (m/z): calcd for $C_{22}H_{25}N_2OF_4$, [M+H]: 409.1903; found, 409.1907.

N-decyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4i**)



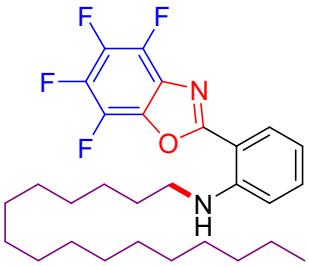
The representative **general procedure 2** mentioned above was followed. The title compound was obtained as a white solid, 46% yield. MP: 74 - 76 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (dd, *J* = 7.9, 1.4 Hz, 2H), 7.40 (t, *J* = 7.2 Hz, 1H), 6.80 (d, *J* = 8.6 Hz, 1H), 6.72 (t, *J* = 7.5 Hz, 1H), 3.32 (dd, *J* = 12.1, 6.9 Hz, 2H), 1.84 – 1.73 (m, 2H), 1.55 – 1.45 (m, 2H), 1.28 (d, *J* = 11.8 Hz, 12H), 0.88 (t, *J* = 6.8 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -152.42 (dd, *J* = 19.9, 16.6 Hz), -158.38 – -159.94 (m), -160.63 (t, *J* = 20.1 Hz), -162.35 (t, *J* = 20.0 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.3, 148.8, 134.1, 129.3, 115.0, 111.2, 105.8, 43.0, 31.9, 29.6, 29.6, 29.4, 29.3, 29.0, 27.2, 22.7, 14.1. HRMS-ESI (m/z): calcd for $C_{23}H_{27}N_2OF_4$, [M+H]: 423.2060; found, 423.2060.

N-dodecyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4j**)



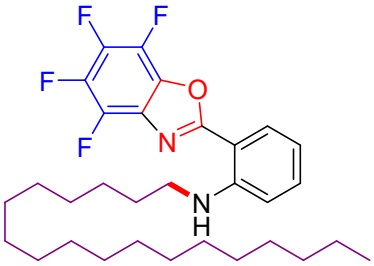
The representative **general procedure 2** mentioned above was followed. The title compound was obtained as a white solid, 47% yield. MP: 77 - 78 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 7.2 Hz, 2H), 7.42 (t, *J* = 7.7 Hz, 1H), 6.82 (d, *J* = 8.5 Hz, 1H), 6.74 (t, *J* = 7.4 Hz, 1H), 3.35 (d, *J* = 5.7 Hz, 2H), 1.85 – 1.80 (m, 2H), 1.54 – 1.50 (m, 2H), 1.29 (s, 16H), 0.90 (d, *J* = 6.6 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -152.00 – -153.21 (m), -159.13 – -159.68 (m), -160.68 (t, *J* = 20.1 Hz), -162.38 (t, *J* = 19.9 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.3, 148.8, 134.1, 129.3, 115.0, 111.3, 105.9, 43.0, 31.9, 29.7, 29.6, 29.5, 29.4, 29.3, 29.1, 27.2, 22.7, 14.1. One carbon was lost due to overlap. HRMS-ESI (m/z): calcd for $C_{25}H_{31}N_2OF_4$, [M+H]: 451.2373; found, 451.2371.

N-hexadecyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4k**)



The representative **general procedure 2** mentioned above was followed. The title compound was obtained as a white solid, 50% yield. MP: 66 - 68 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 7.5 Hz, 2H), 7.42 (t, *J* = 7.5 Hz, 1H), 6.82 (d, *J* = 8.5 Hz, 1H), 6.75 (t, *J* = 7.4 Hz, 1H), 3.35 (dd, *J* = 11.6, 5.9 Hz, 2H), 1.85 –1.78 (m, 2H), 1.62 – 1.47 (m, 6H), 1.28 (s, 20H), 0.90 (t, *J* = 6.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -151.73 – -152.77 (m), -159.04 – -159.79 (m), -160.68 (t, *J* = 20.1 Hz), -162.37 (t, *J* = 19.9 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.3, 148.8, 134.1, 129.3, 115.0, 111.2, 105.8, 43.0, 32.2, 31.9, 29.8, 29.7, 29.6, 29.5, 29.4, 29.3, 29.2, 29.1, 29.0, 28.9, 27.2, 22.7, 14.1. HRMS-ESI (m/z): calcd for $C_{29}H_{39}N_2OF_4$, [M+H]: 507.2999; found, 507.2996.

N-octadecyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4l**)



The representative **general procedure 2** mentioned above was followed. The title compound was obtained as a white solid, 47% yield. MP: 66 - 68 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, J = 6.8 Hz, 2H), 7.40 (t, J = 7.4 Hz, 1H), 6.79 (d, J = 8.4 Hz, 1H), 6.72 (t, J = 6.9 Hz, 1H), 3.32 (d, J = 4.8 Hz, 2H), 2.50 (t, J = 6.8 Hz, 1H), 1.78 (d, J = 6.7 Hz, 2H), 1.53 (d, J = 15.6 Hz, 3H), 1.25 (s, 26H), 0.87 (d, J = 6.0 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -151.84 – -153.17 (m), -158.88 – -159.72 (m), -160.66 (t, J = 20.1 Hz), -162.36 (t, J = 19.9 Hz). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.3, 148.8, 134.1, 129.3, 115.0, 111.3, 105.8, 43.0, 32.2, 31.9, 29.9, 29.8, 29.7, 29.6, 29.5, 29.4, 29.3, 29.2, 29.1, 29.0, 28.9, 27.2, 22.7, 14.1. One carbon was lost due to overlap. HRMS-ESI (m/z): calcd for $C_{31}H_{43}N_2OF_4$, [M+H]: 535.3312; found, 535.3315.

4. X−ray Information of 3c （CCDC 2076932）

Table 1 Crystal data and structure refinement for **3c**.

Identification code	**3c**
Empirical formula	$C_{14}H_7F_4NO_2$
Formula weight	297.21
Temperature/K	149.99(10)
Crystal system	triclinic
Space group	P-1
a/Å	5.9650(6)
b/Å	7.5856(11)
c/Å	13.5287(15)
α/°	82.212(11)
β/°	82.531(9)
γ/°	88.960(10)
Volume/Å^3	601.36(13)
Z	2
ρ_{calc}g/cm^3	1.641
μ/mm^{-1}	0.152
F(000)	300.0
Crystal size/mm^3	0.14 × 0.12 × 0.11
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/	5.42 to 49.994
Index ranges	-4 ≤ h ≤ 7, -9 ≤ k ≤ 8, -15 ≤ l ≤ 16
Reflections collected	3832
Independent reflections	2113 [R_{int} = 0.0219, R_{sigma} = 0.0424]
Data/restraints/parameters	2113/7/191
Goodness-of-fit on F^2	1.079
Final R indexes [I>=2σ (I)]	R_1 = 0.0417, wR_2 = 0.0957
Final R indexes [all data]	R_1 = 0.0586, wR_2 = 0.1060
Largest diff. peak/hole / e Å^{-3}	0.16/-0.22

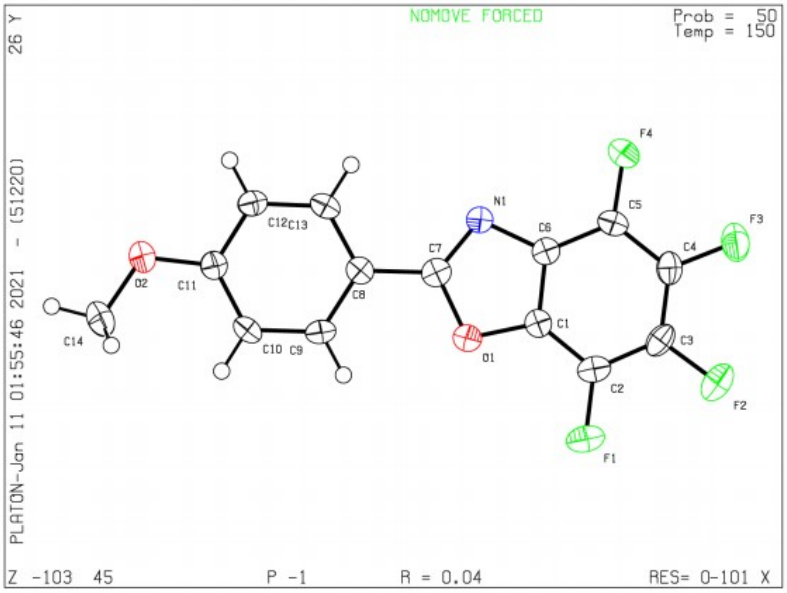


Figure S1. The Ellipsoid Contour % Probability Levels of **3c** is 50%

5. Fluorescence Spectra of Solvents Screening, Absorption of 3a – 3u, 4a – 4l

5.1 The fluorescence emission spectra of solvents screening 3d

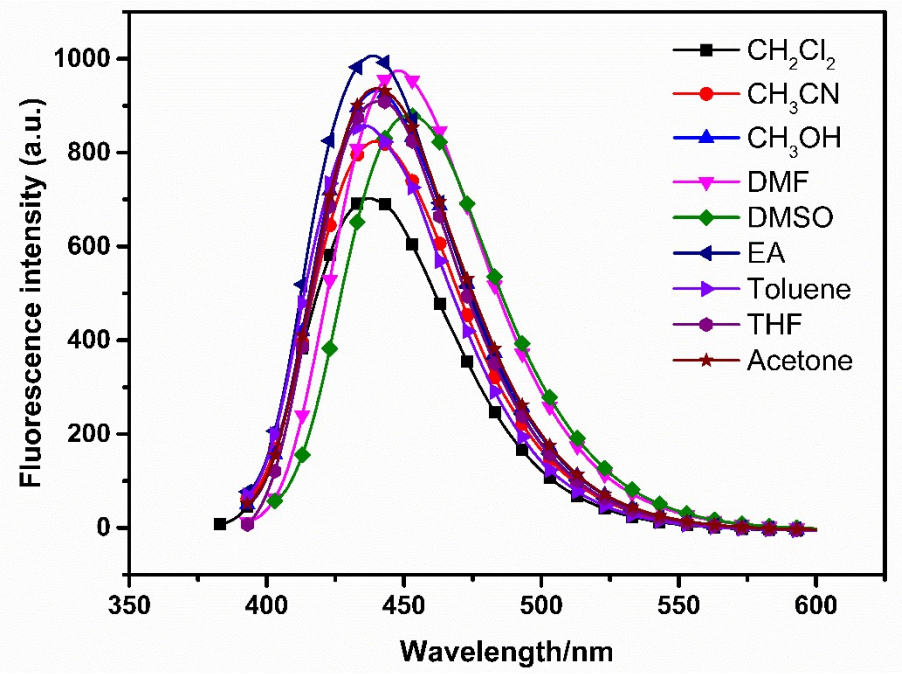
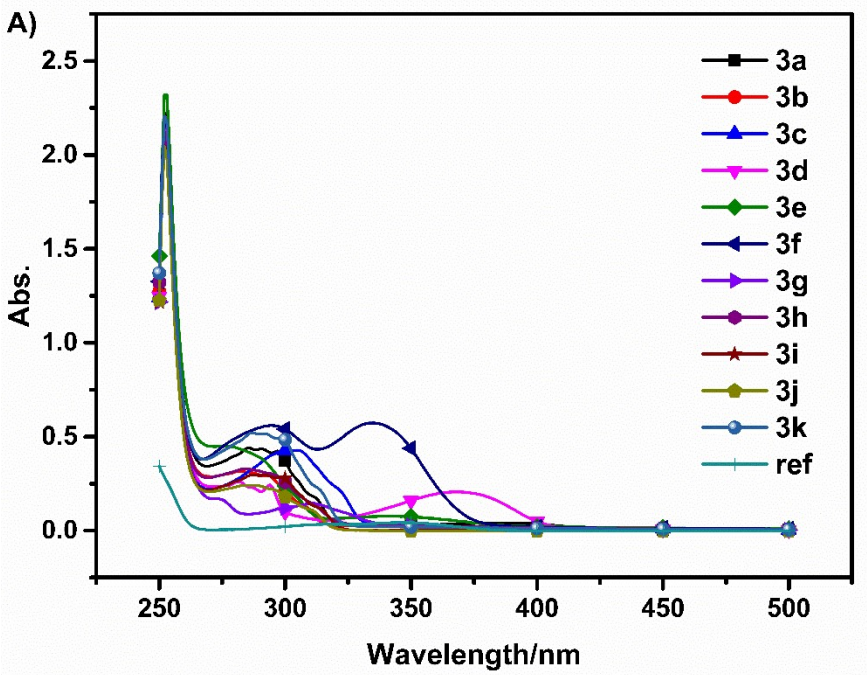


Figure S2 The Fluorescence Emission Spectra of **3d** in CH_2Cl_2, CH_3CN, CH_3OH , DMF, DMSO, EA, Toluene, THF and Acetone at a concentration 12.5 μmol/L.

Compound **3d** were choosed as the sample to screen solvents, such as CH_2Cl_2, CH_3CN, CH_3OH , DMF, DMSO, EA, Toluene, THF and Acetone in 12.5 μmol/L. We found that EA is the best solvent for fluorescence emission. The data of the fluorescence emission was tested by HITACHI F7000 at room temperature.

5.2 Absorption of 3a – 3u, 4a – 4l



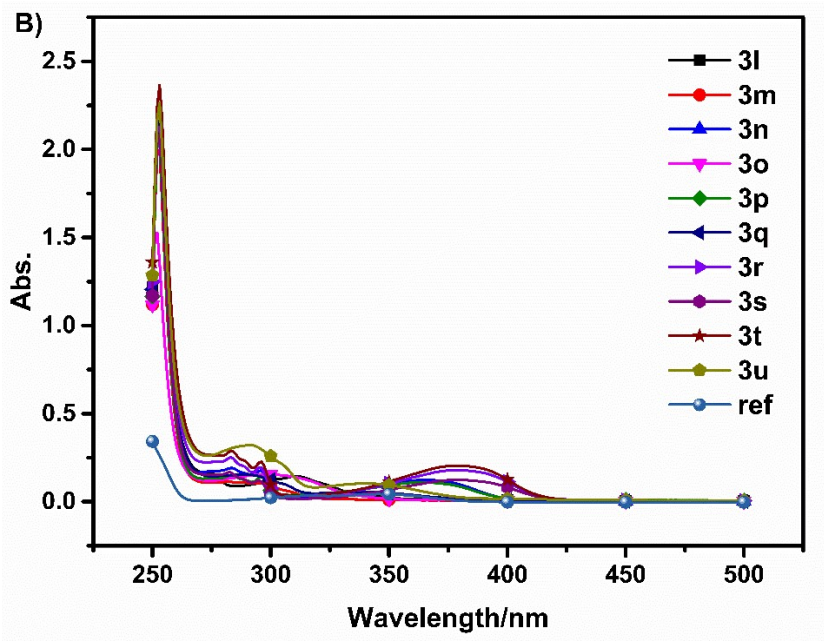


Figure S3. The UV Absorption Spectra of **3a – 3u** (12.5 μmol/L solution in EA)

The data was tested by SHIMADZU UV 2000 at room temperature.

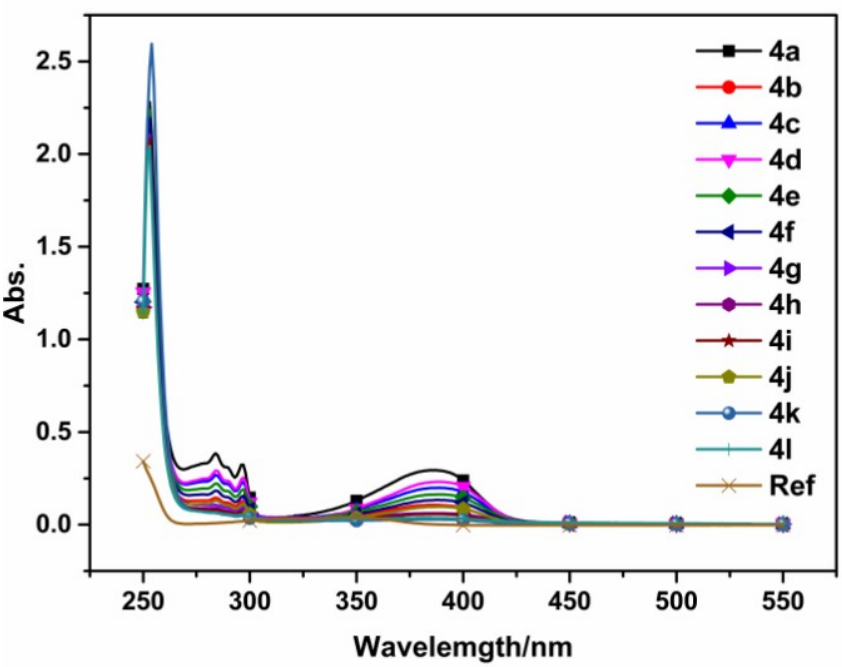


Figure S4. The UV Absorption Spectra of **4a – 4l** (12.5 μmol/L solution in EA) The data was tested by SHIMADZU UV 2000 at room temperature.

5.3 The Fluorescence Emission Spectra of 3a – 3u, 4a – 4l

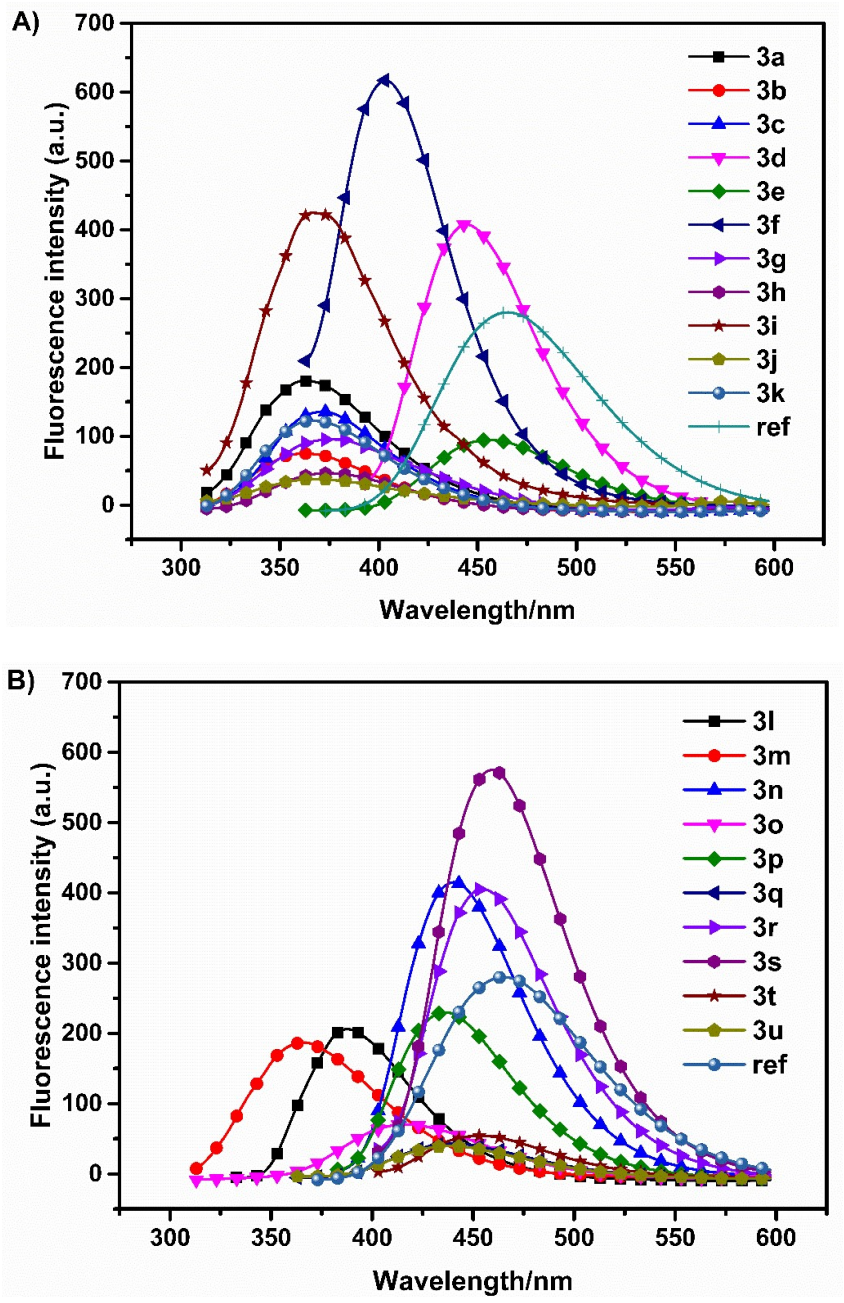


Figure S5. The Fluorescence Emission Spectra of **3a – 3u**

We controlled the UV absorbance of **3a** – **3u** between 0.025 and 0.050 in EA for fluorescence quantum yield by SHIMADZU UV 2000 at room temperature. Next, we tested the data of fluorescence emission when excited at their maximum absorption wavelength by HITACHI F7000.

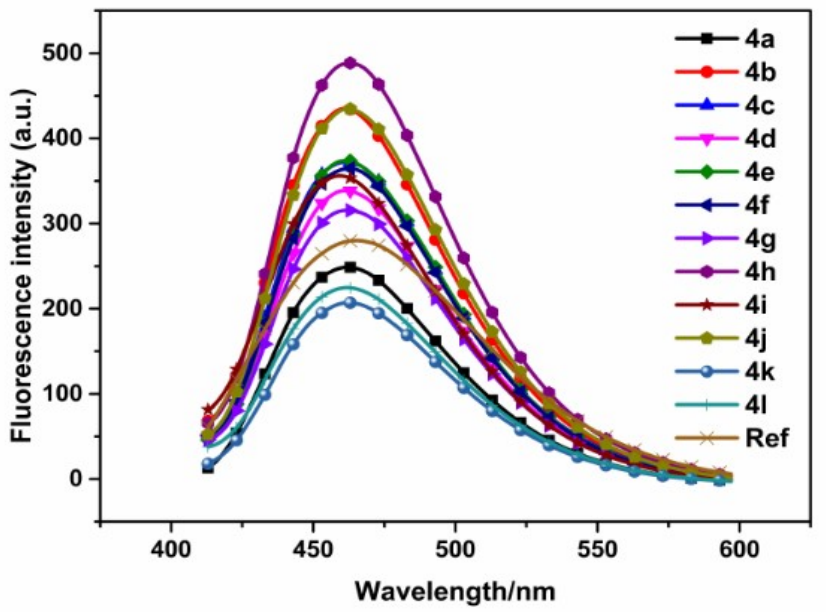


Figure S6. The Fluorescence Emission Spectra of **4a – 4l**

We controlled the UV absorbance of **4a** – **4l** between 0.025 and 0.050 in EA for fluorescence quantum yield by SHIMADZU UV 2000 at room temperature. Next, we tested the data of fluorescence emission when excited at their maximum absorption wavelength by HITACHI F7000.

6. Optical data table 3a – 3u, 4a – 4l

6.1 The measured photophysical properties of 3a – 3u

Table S2. the Measured Photophysical Properties of **3a – 3u**

Compound	Abs.	λmax(nm)	Emission(nm)	Fluorescent Area	Φ_F(%)
3a	0.044	286	362	13307.92	29
3b	0.048	281	362	5046.75	10
3c	0.032	296	372	8618.78	26
3d	0.03	370	444	30650.11	99
3e	0.041	343	456	7078.79	17
3f	0.052	334	403	44735.56	83
3g	0.048	283	375	8262.31	17
3h	0.053	284	374	2937.43	5
3i	0.043	287	366	35258.74	79
3j	0.049	284	366	3335.17	7
3k	0.046	287	367	8822.08	19
3l	0.043	310	388	12359.34	28
3m	0.051	283	367	14558.67	28
3n	0.049	363	440	30482.20	60
3o	0.05	293	415	4962.12	10
3p	0.037	363	436	16217.65	42
3q	0.051	338	440	2615.98	5
3r	0.05	377	454	31092.74	60
3s	0.047	379	459	45030.85	93
3t	0.049	378	453	3544.35	7
3u	0.05	341	438	2358.99	5
Ref	0.044	345	465	26380.63	54.6

6.2 The measured photophysical properties of 4a – 4l

Table S3. the Measured Photophysical Properties of **4a – 4l**

Compound	Abs.	λ_{max}(nm)	Emission(nm)	Fluorescent Area	Φ_F (%)
4a	0.042	378	462	18608.72	43
4b	0.05	384	461	33349.11	64
4c	0.048	385	462	28689.65	58
4d	0.044	385	462	25895.9	57
4e	0.045	384	461	28489.16	61
4f	0.051	384	462	27997.76	53
4g	0.047	385	462	24382.84	50
4h	0.054	389	462	38035.11	68
4i	0.047	384	459	27571.52	57
4j	0.043	389	462	33518.23	75
4k	0.03	380	462	15657.16	50
4l	0.033	384	462	17239.47	50
Ref	0.044	345	465	26380.63	54.6

The calculation formula of quantum yield as follows:

$$\Phi_s = \frac{F_S A_r n_s^2}{F_r A_s n_r^2} \Phi_r$$

In formula,s and r represent sample and reference respectively, F is the relative integrated fluorescence intensity, A is the absorbance,and n is the refractive index of the solvent.

7. Preparation and characterization of platinum nanomaterials of compound 4l and CTAB

7.1 General preparation process of platinum nanomaterials of compound 4l

Experimental process: Weigh $Pt(acac)_2$ (5.0 mg) and **4l** (26.2 mg) into a 30.0 mL reaction flask, then add 4.0 mL oleylamine, cap the bottle and sonicate it in an ultrasonic machine for 30 min until a uniform solution is formed (the ultrasonic temperature is controlled below 25 °C). After sonication is uniform, weigh 5.0 mg of tungsten hexacarbonyl into the reaction flask, tighten the cap and shake it lightly for a few times, then put it in a 165 °C oil bath for 2 h.

7.2 General preparation process of platinum nanomaterials of CTAB

Experimental process: Weigh $Pt(acac)_2$ (10.0 mg) and CTAB (75.0 mg) into a 30.0 mL reaction flask, add 4.0 mL oleylamine and close the cap, then sonicate in an ultrasonic machine for 30 min until a uniform solution is formed (the ultrasonic temperature is controlled below 25 °C). After sonication is uniform, weigh 10.0 mg tungsten hexacarbonyl into the reaction flask, tighten the cap and shake it lightly for a few times, then put it in a 165 ° C oil bath for 2 h.

7.3 Transimission Electron Microscopic (TEM) characterization of platinum nanomaterials of compound 4l and CTAB

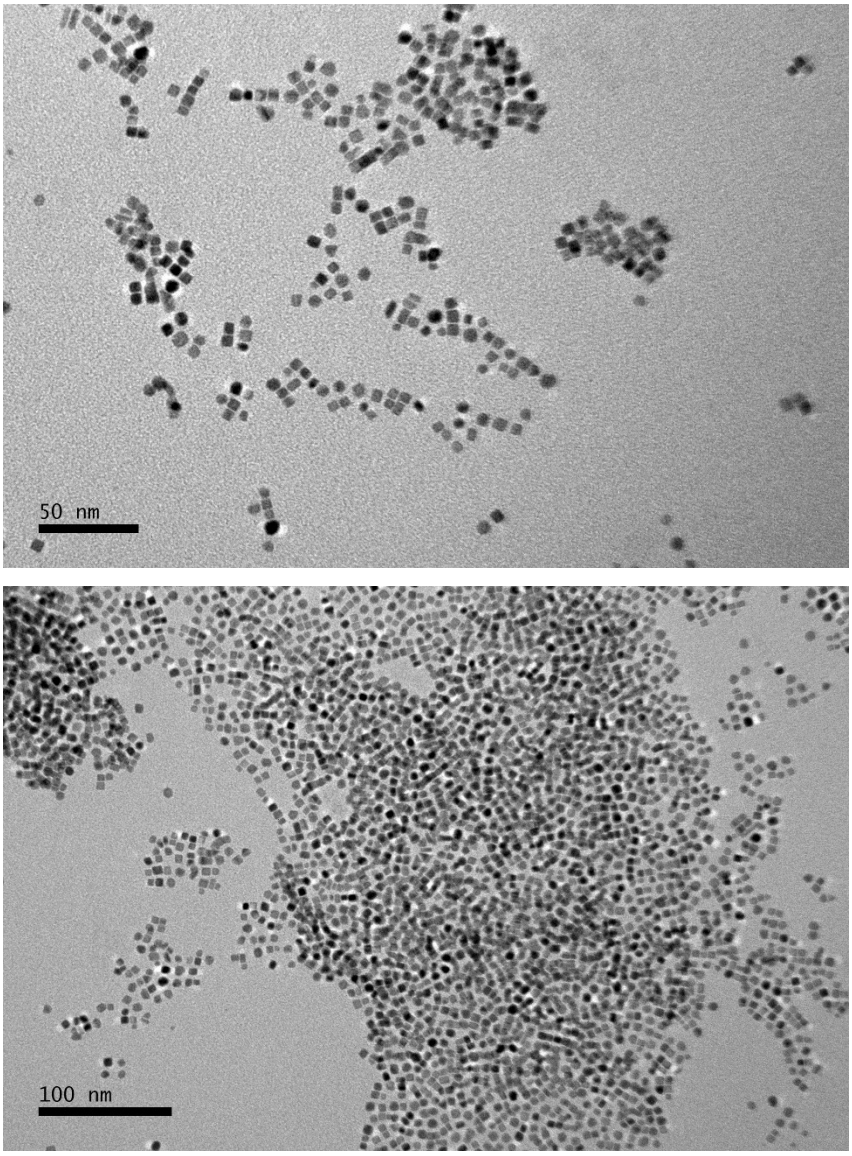


Figure S7 TEM images of uniform cubic platinum nanoparticles (**4l**)

TEM sample preparation: Take 0.3 mL of the original solution into a 1.5 mL centrifuge tube, add 0.9 mL of n-hexane, sonicate for 5 min and centrifuge at 13000 r/min for 5 min to obtain a black precipitate. After the first centrifugation, remove the supernatant with a pipette, then add hexane:ethanol (2:1), sonicate for 5 min and then centrifuge at the same speed. Perform the above operation again and disperse the sample in hexane. Next, the transmission electron microscope (TEM) test of uniform cubic platinum (**4l)** nanoparticles was carried out on the JEM-2100 Plus instrument.

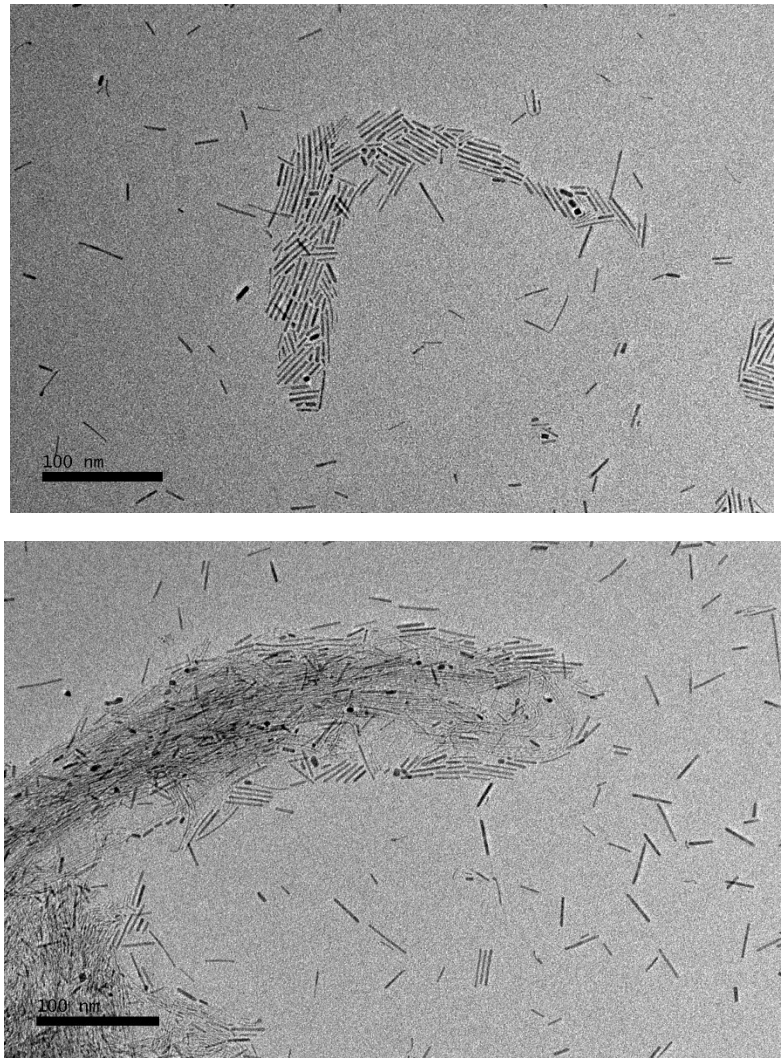


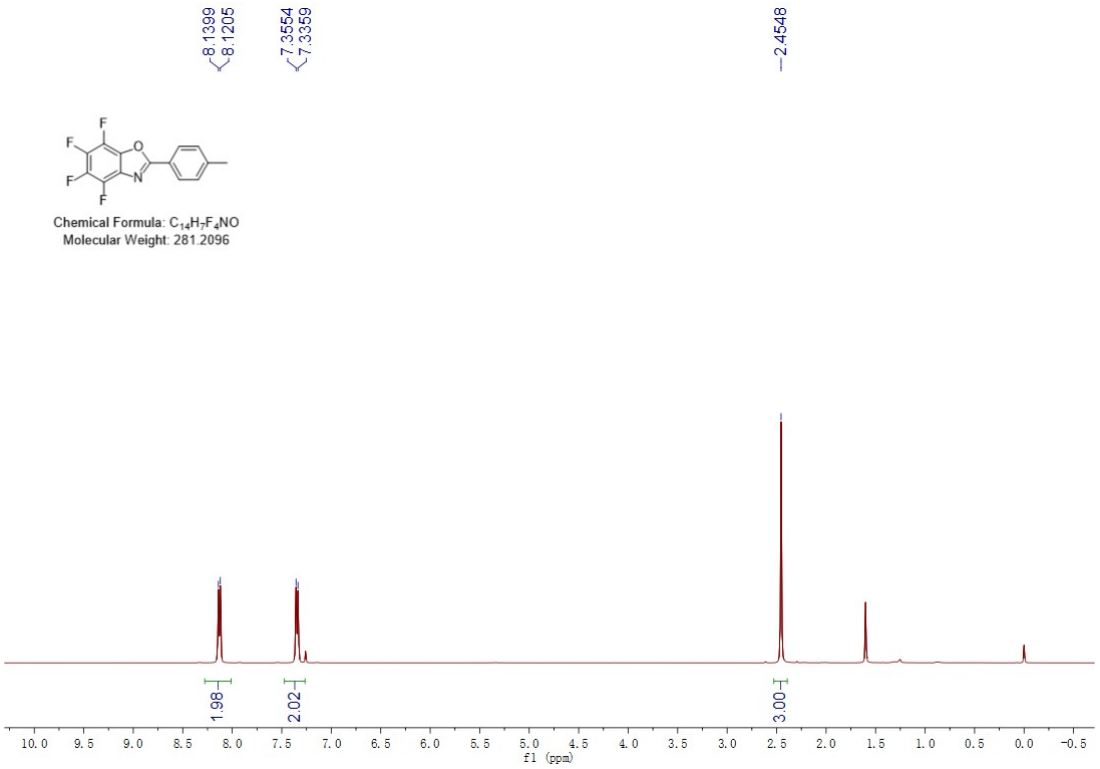
Figure S8 TEM images of platinum nanowire (CTAB)

TEM sample preparation: Take 0.3 mL of the original solution into a 1.5 mL centrifuge tube, add 0.9 mL of n-hexane, sonicate for 5 min and centrifuge at 13000 r/min for 5 min to obtain a black precipitate. After the first centrifugation, remove the supernatant with a pipette, then add hexane:ethanol (2:1), sonicate for 5 min and then centrifuge at the same speed. Perform the above operation again and disperse the sample in hexane. Next, the transmission electron microscope (TEM) test of platinum nanowires (CTAB) was carried out on the JEM-2100 Plus instrument.

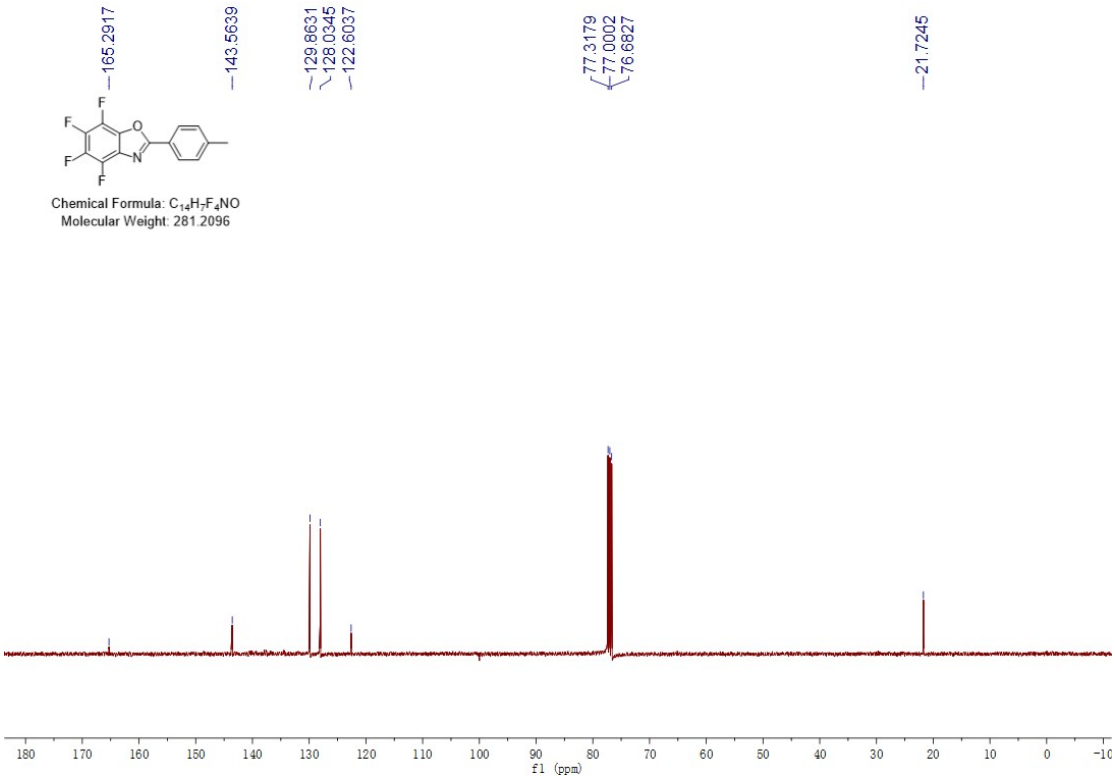
8. ^{1}H, ^{13}C, ^{19}F NMR and HRMS spectra for the compound

4,5,6,7-tetrafluoro-2-(*p*-tolyl)benzo[*d*]oxazole (**3a**)

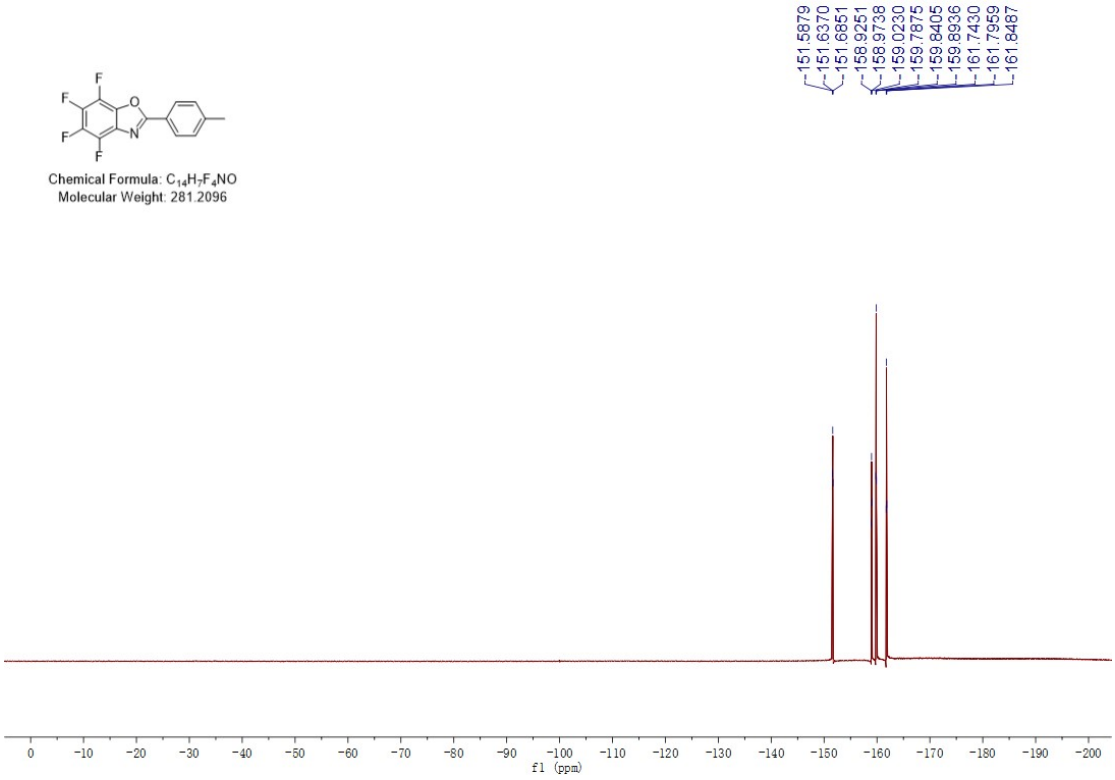
^{1}H NMR (400 MHz, $CDCl_3$)



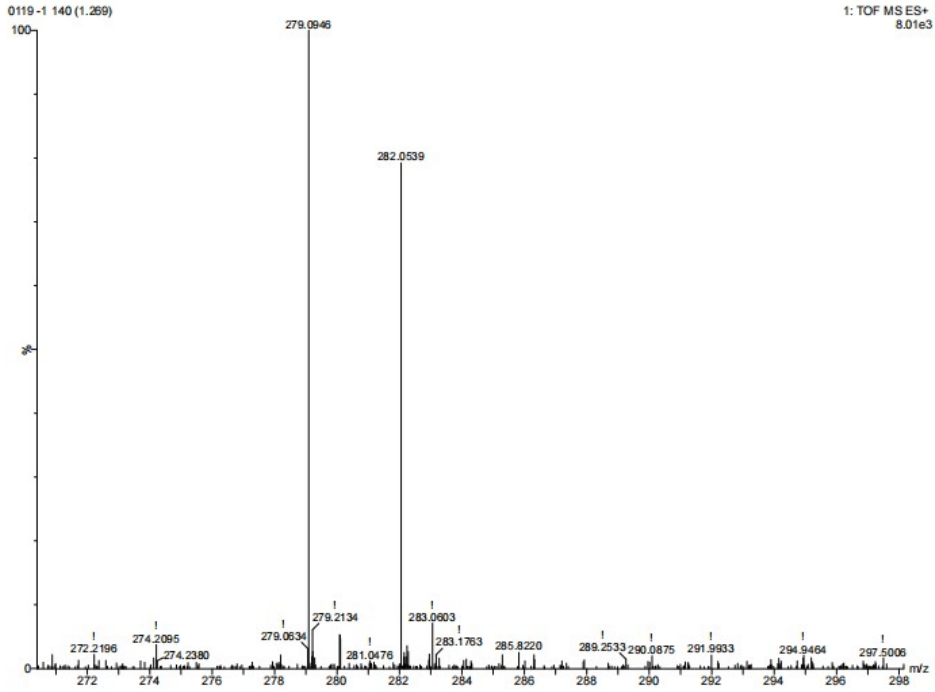
^{13}C NMR (101 MHz, $CDCl_3$)



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

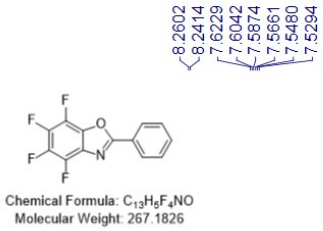


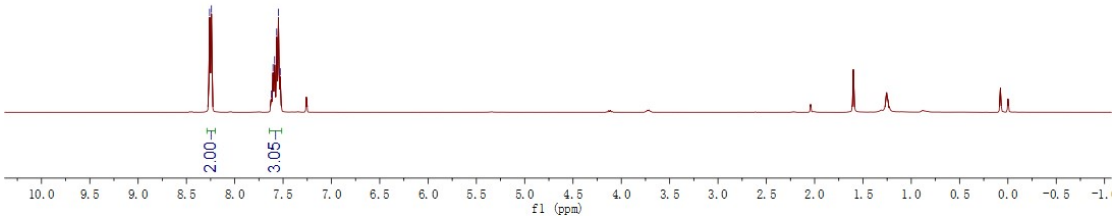
HRMS spectra



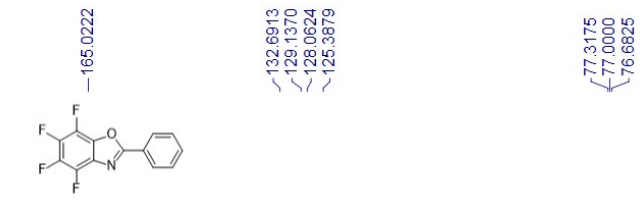
4,5,6,7-tetrafluoro-2-phenylbenzo[*d*]oxazole (**3b**)

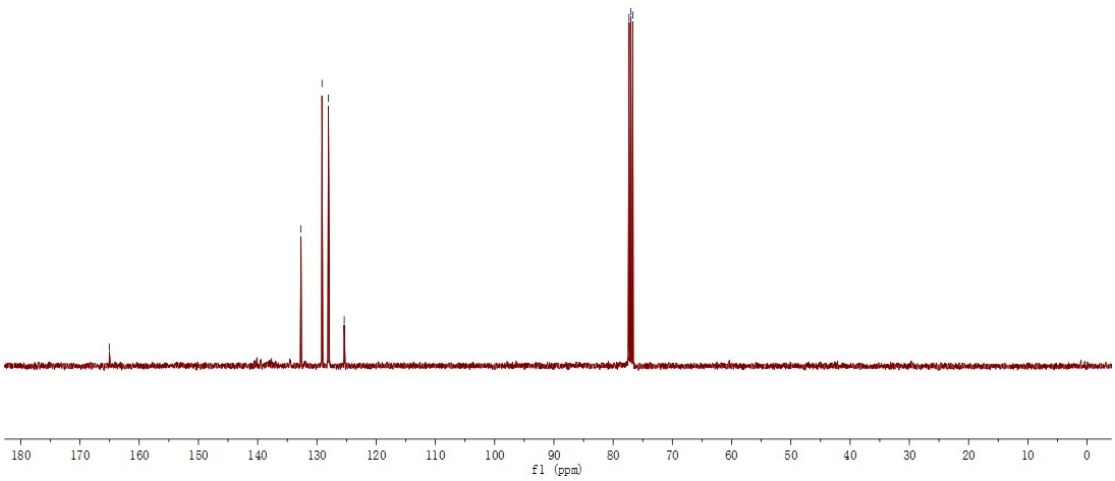
^{1}HNMR (400 MHz, $CDCl_3$)



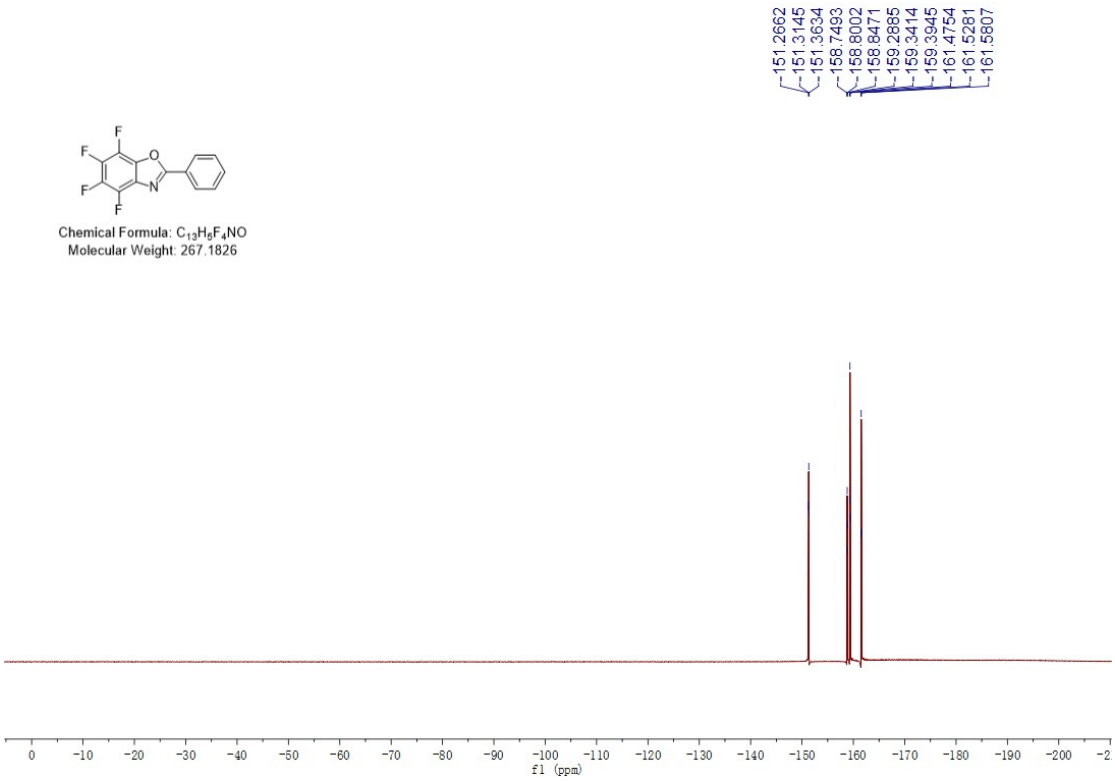


^{13}C NMR (101 MHz, $CDCl_3$)

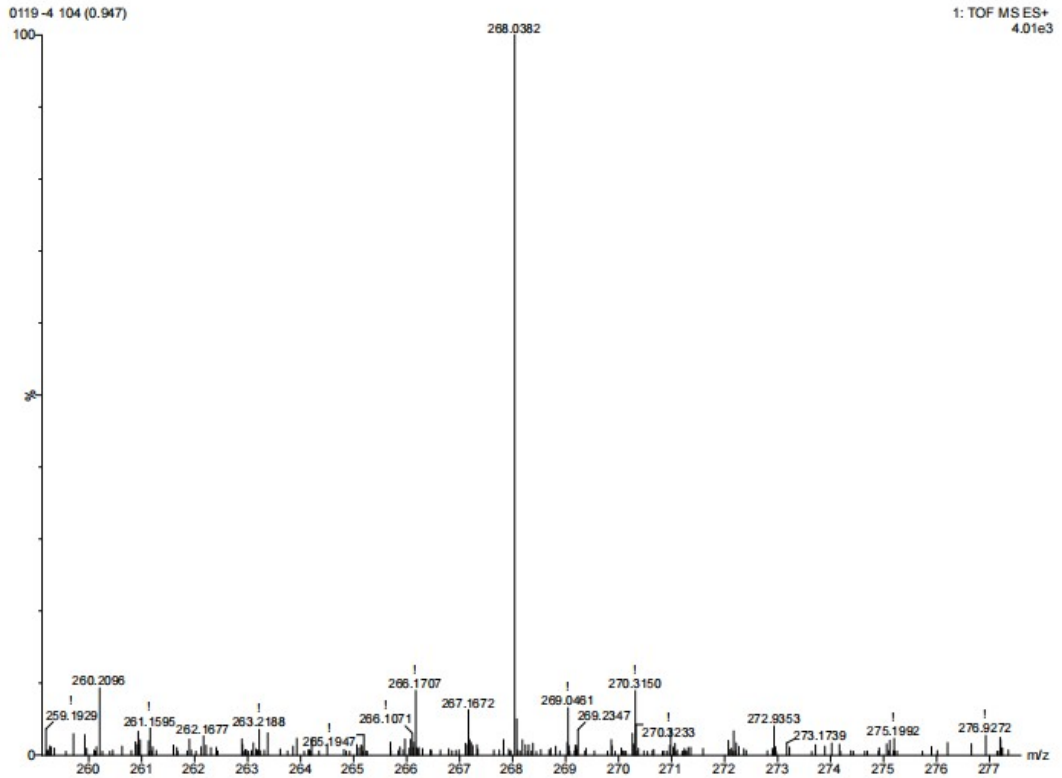




^{19}F NMR (376 MHz, $CDCl_3$)

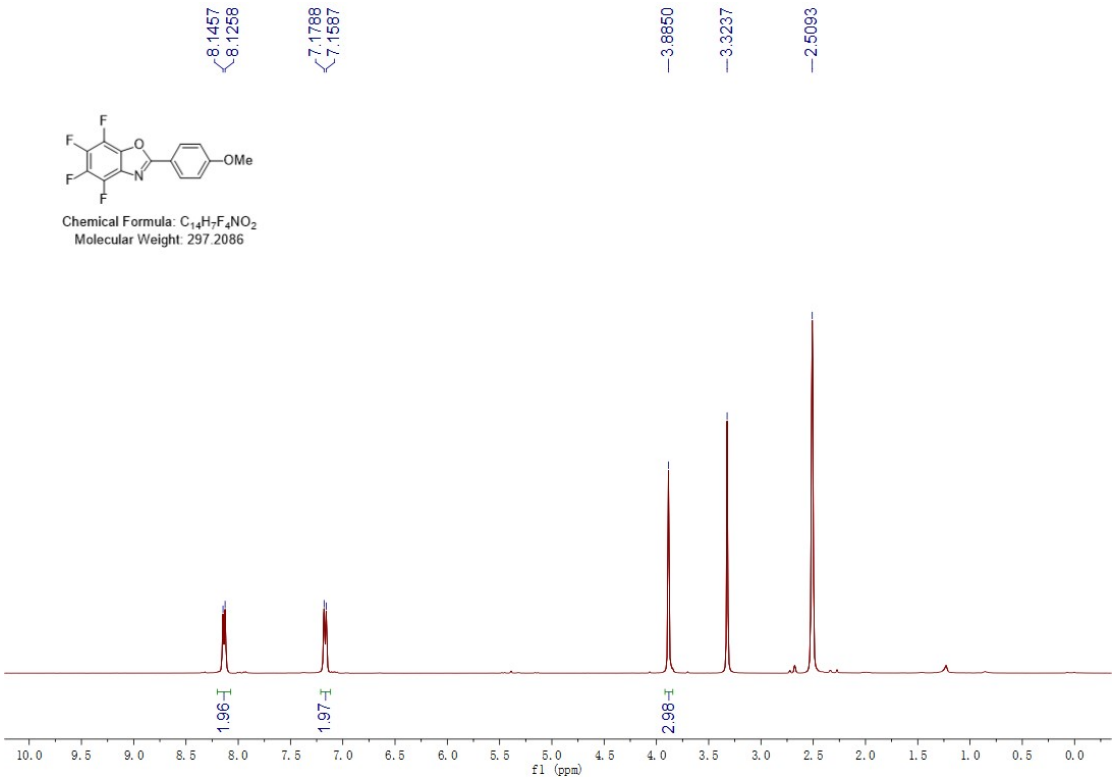


HRMS spectra

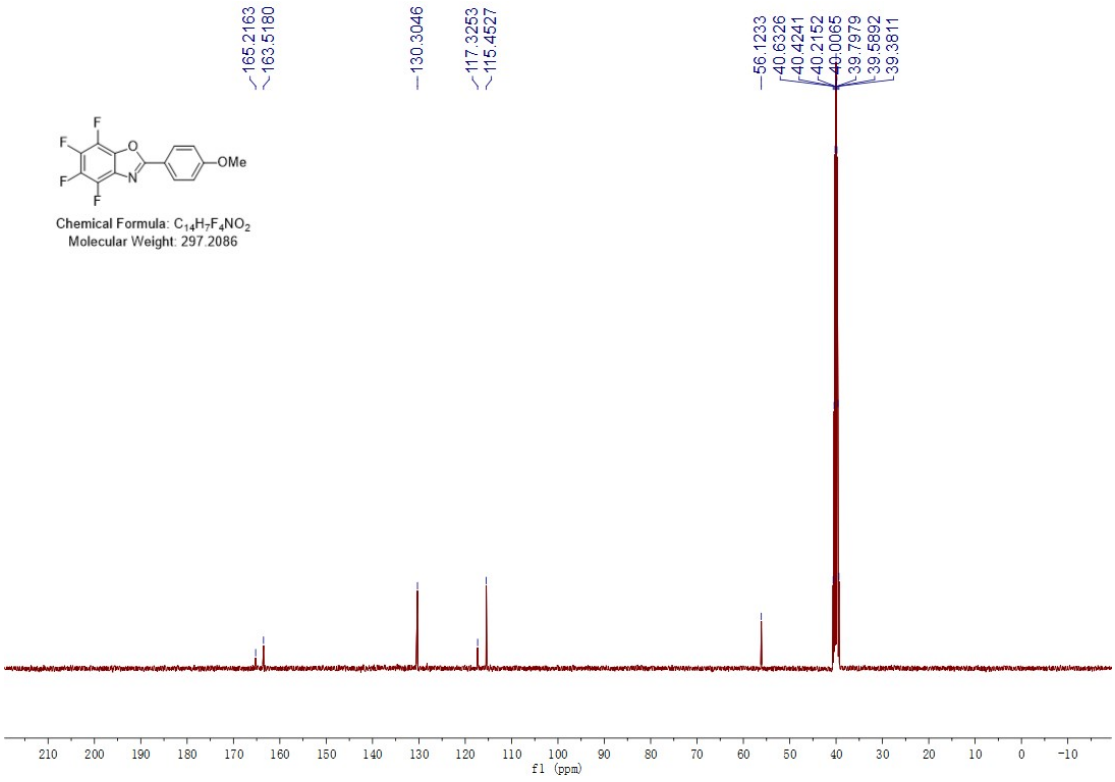


4,5,6,7-tetrafluoro-2-(4-methoxyphenyl)benzo[*d*]oxazole (**3c**)

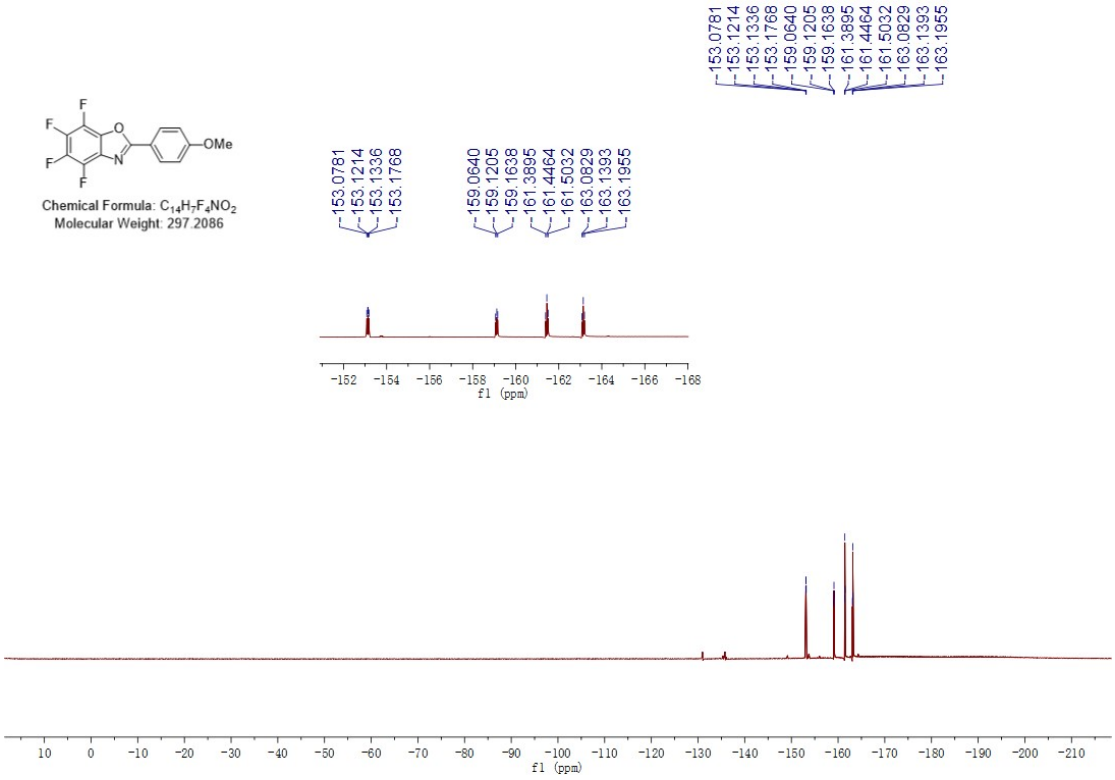
^{1}H NMR (400 MHz, DMSO)



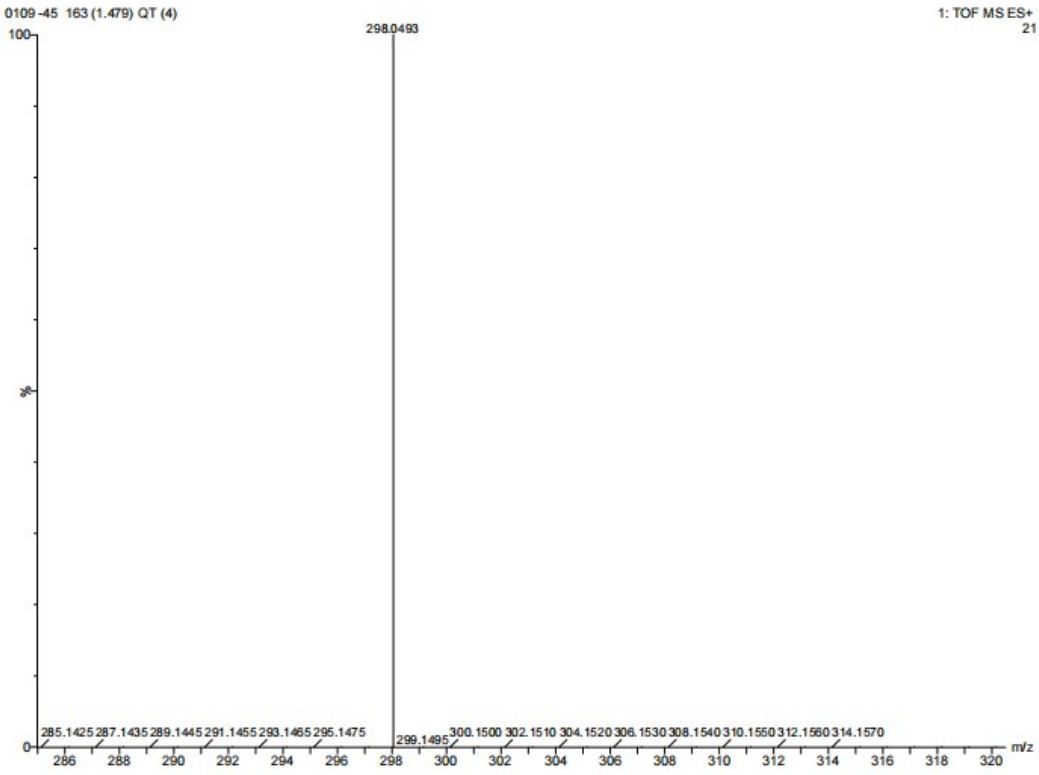
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

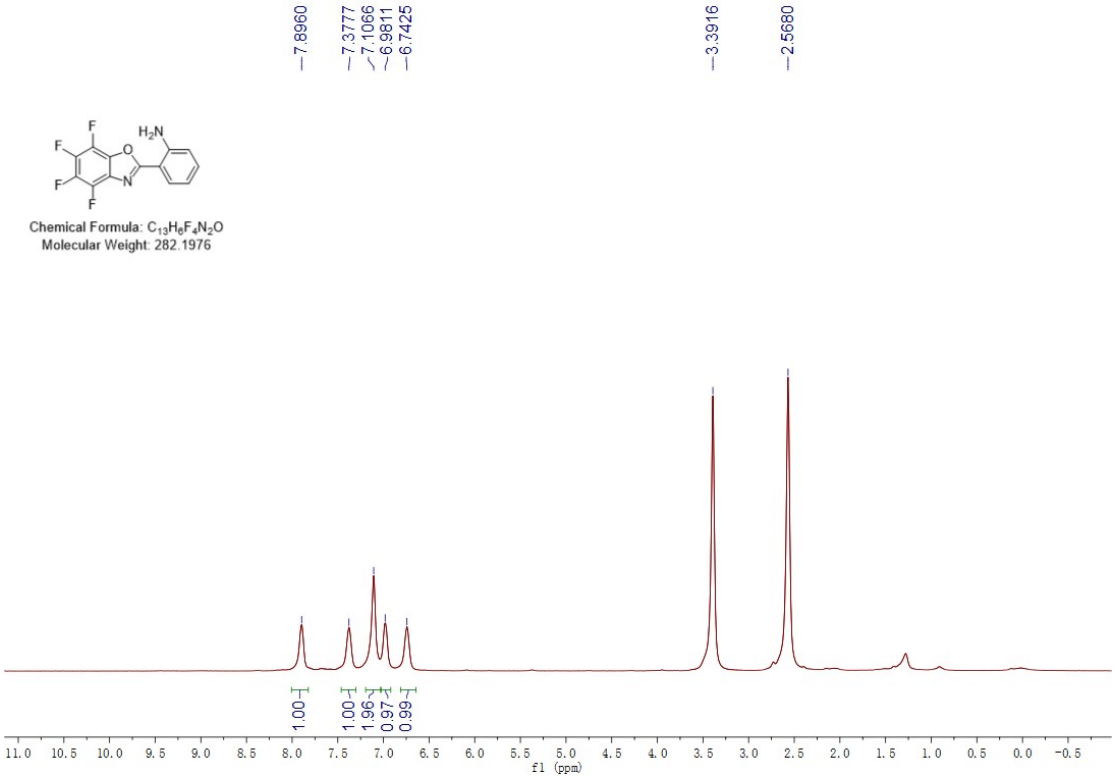


HRMS spectra

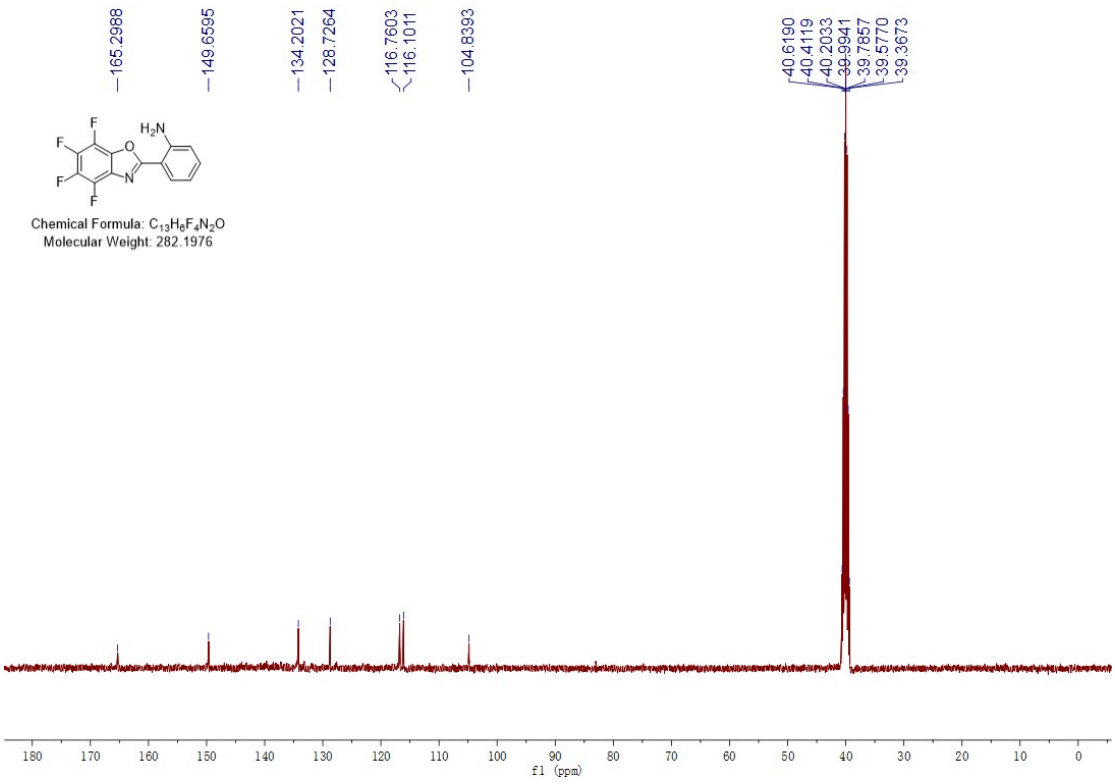


2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**3d**)

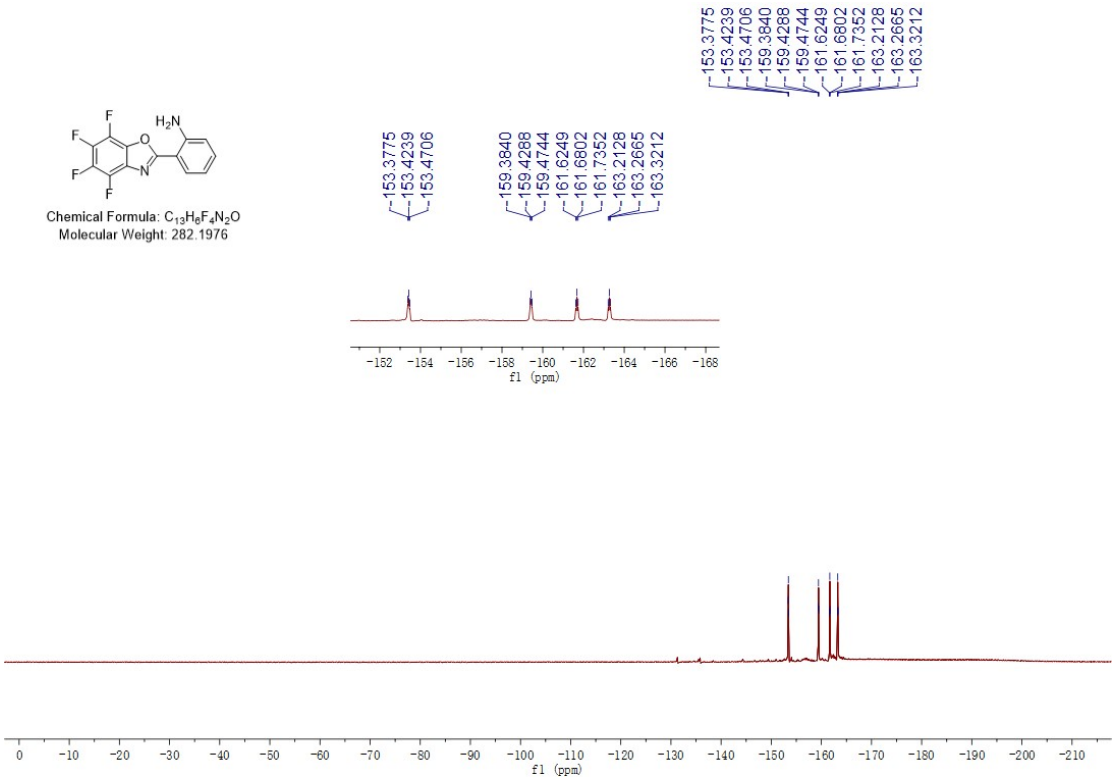
^{1}H NMR (400 MHz, DMSO)



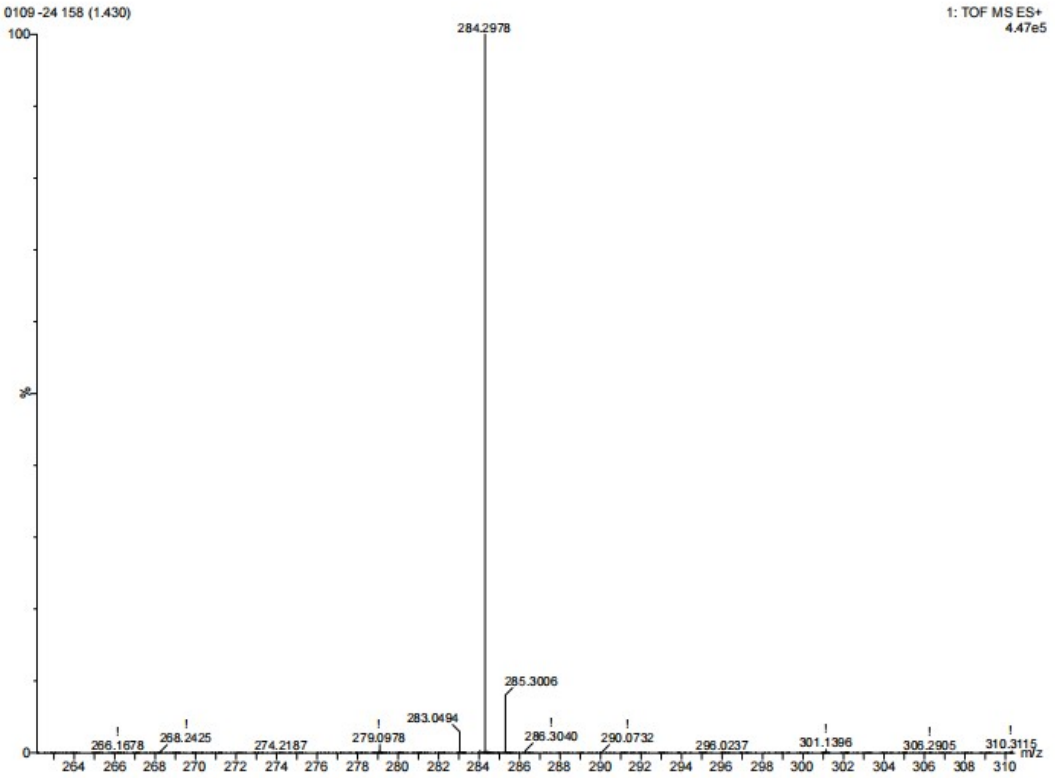
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

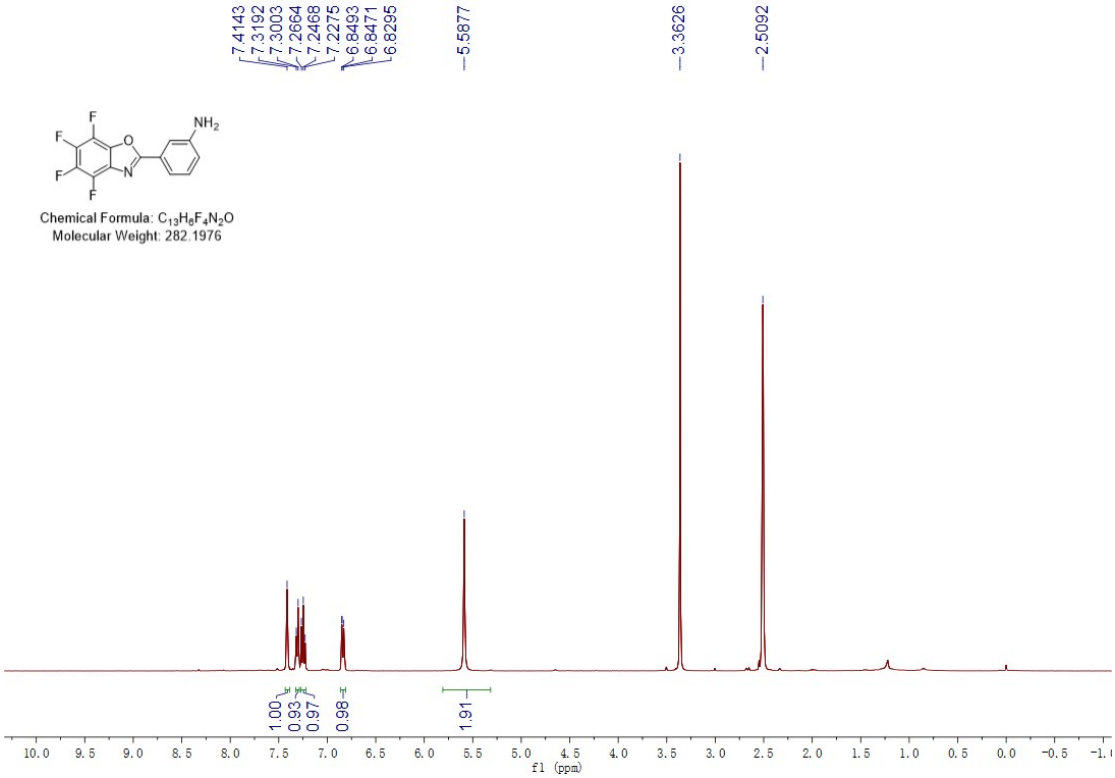


HRMS spectra

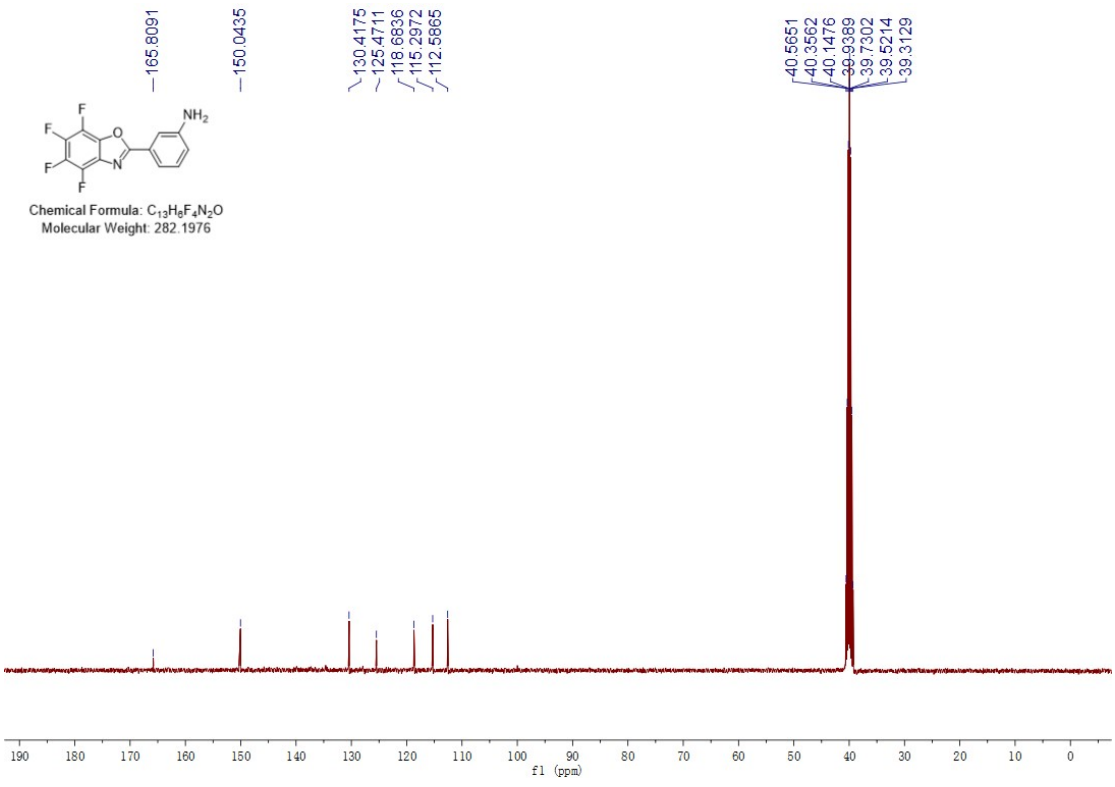


3-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**3e**)

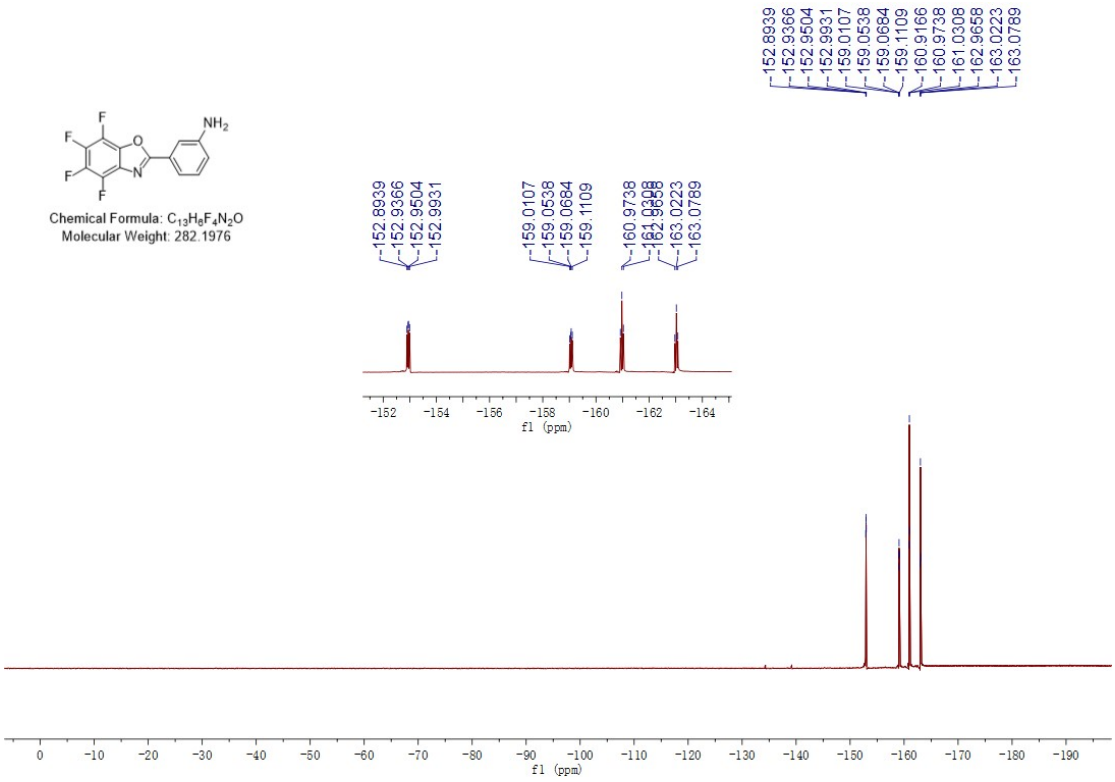
^{1}H NMR (400 MHz, DMSO)



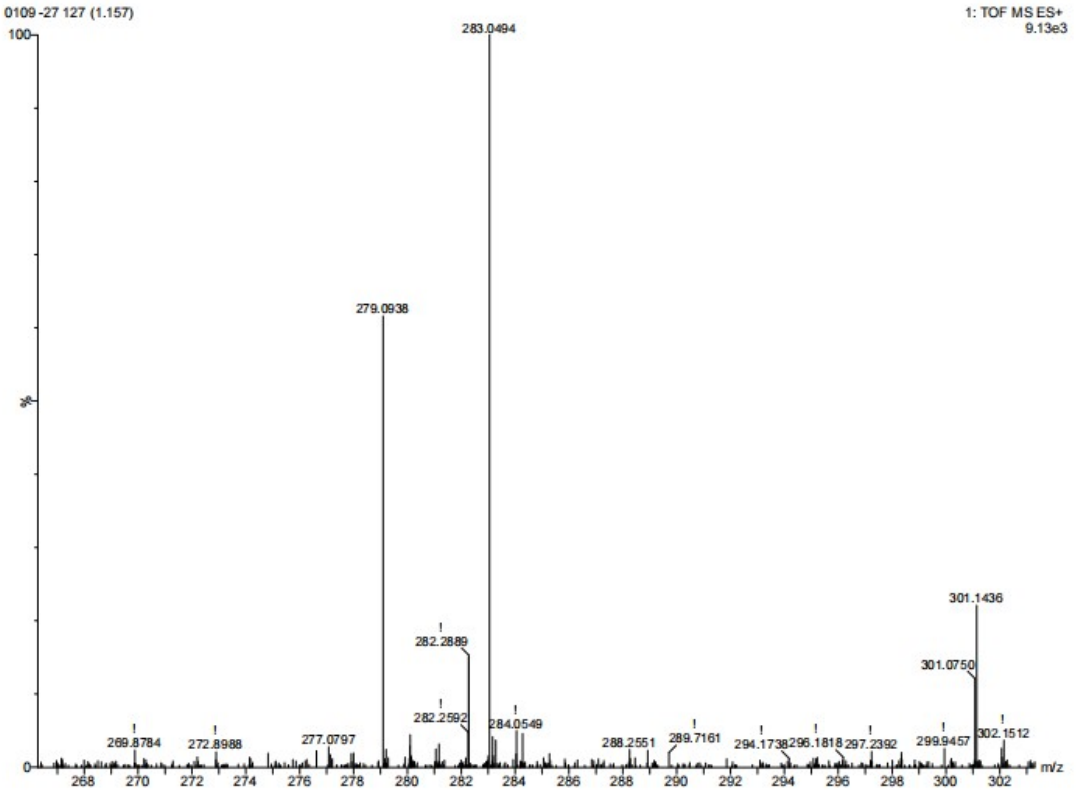
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

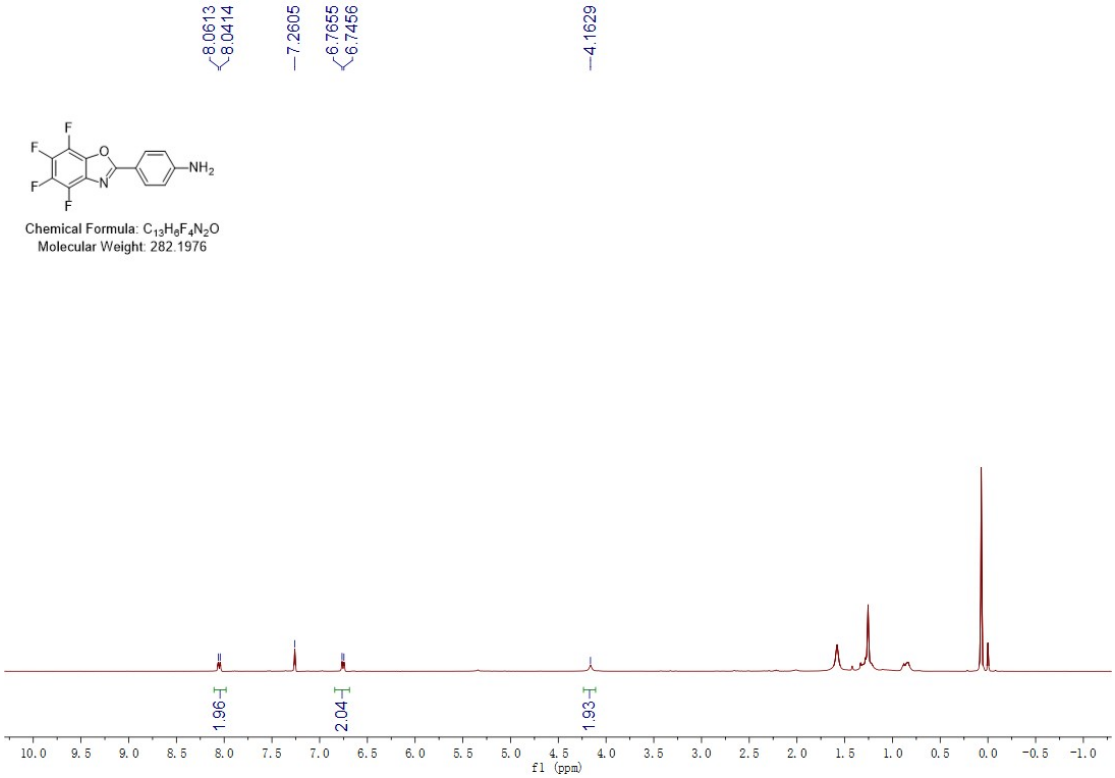


HRMS spectra

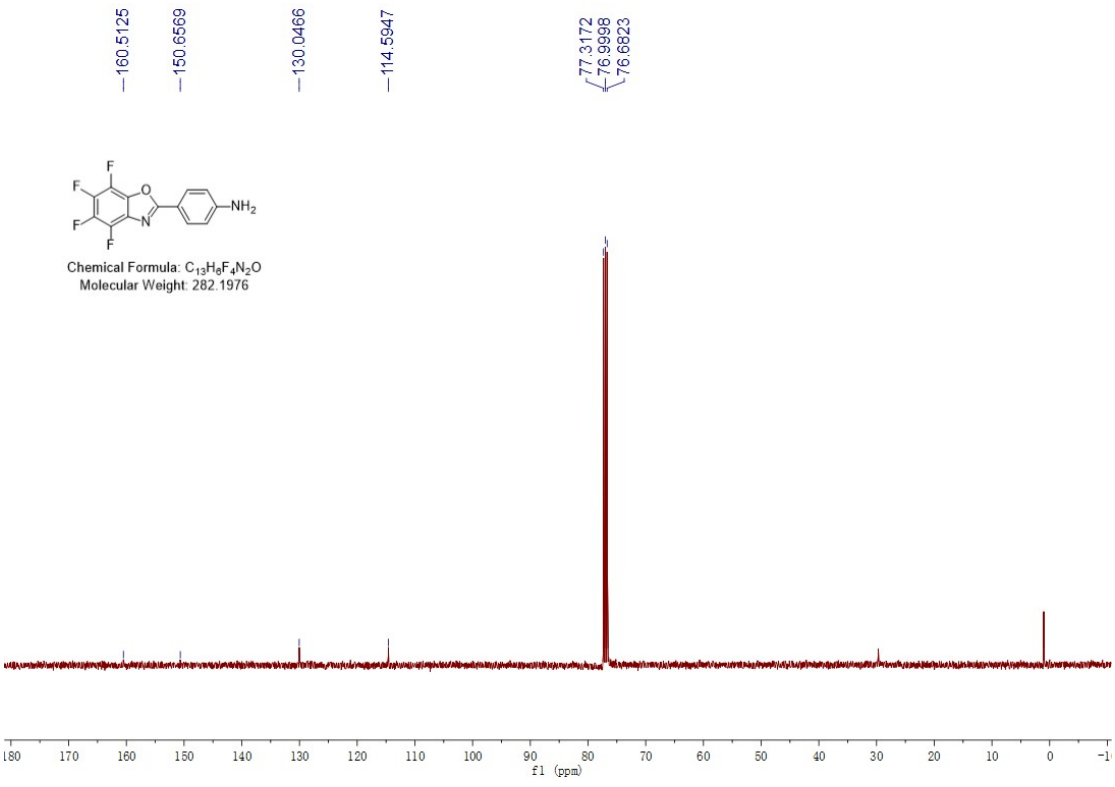


2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**3f**)

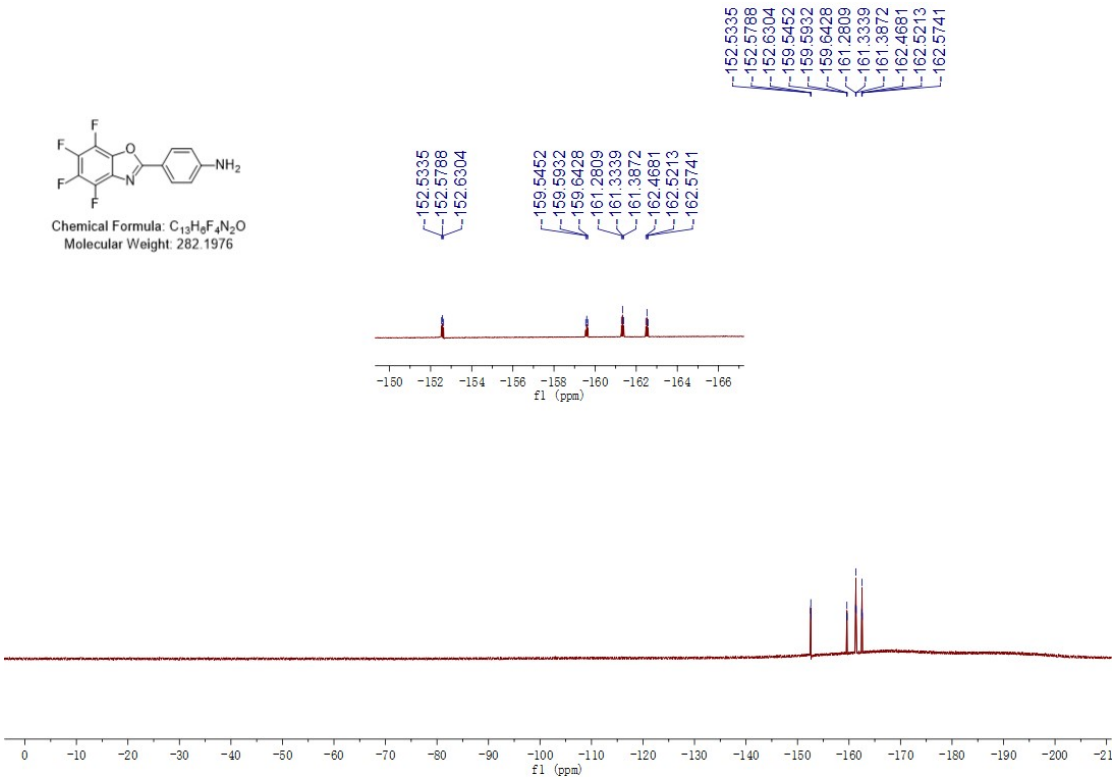
^{1}H NMR (400 MHz, DMSO)



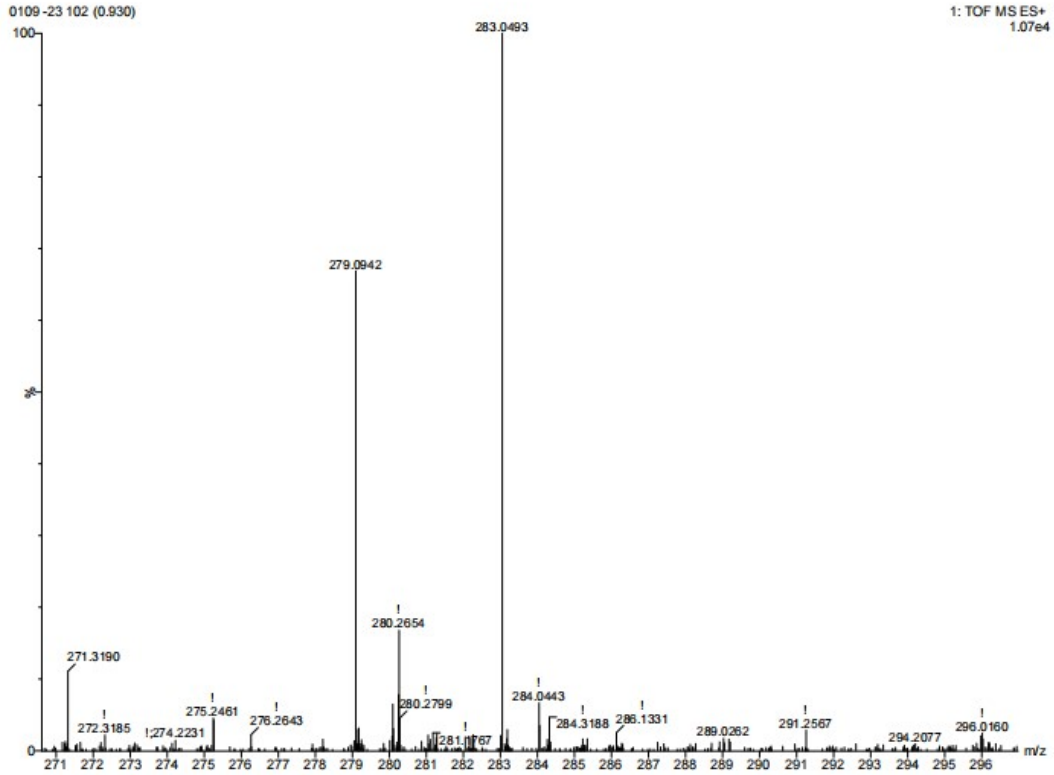
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

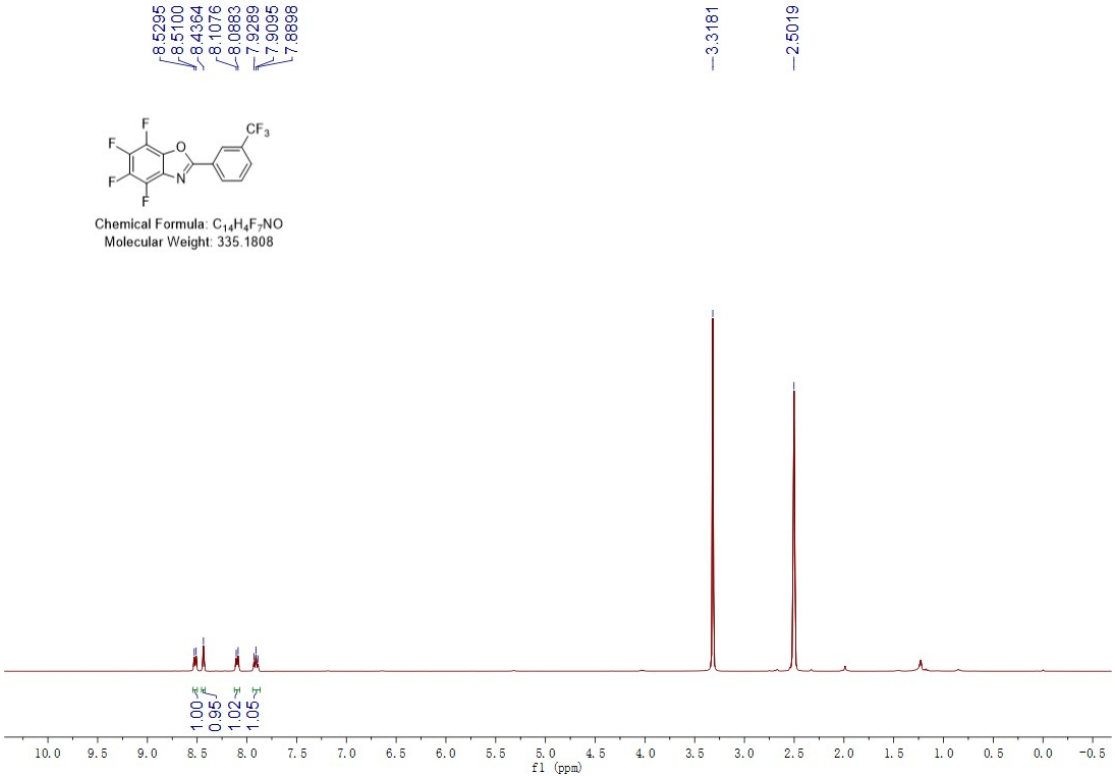


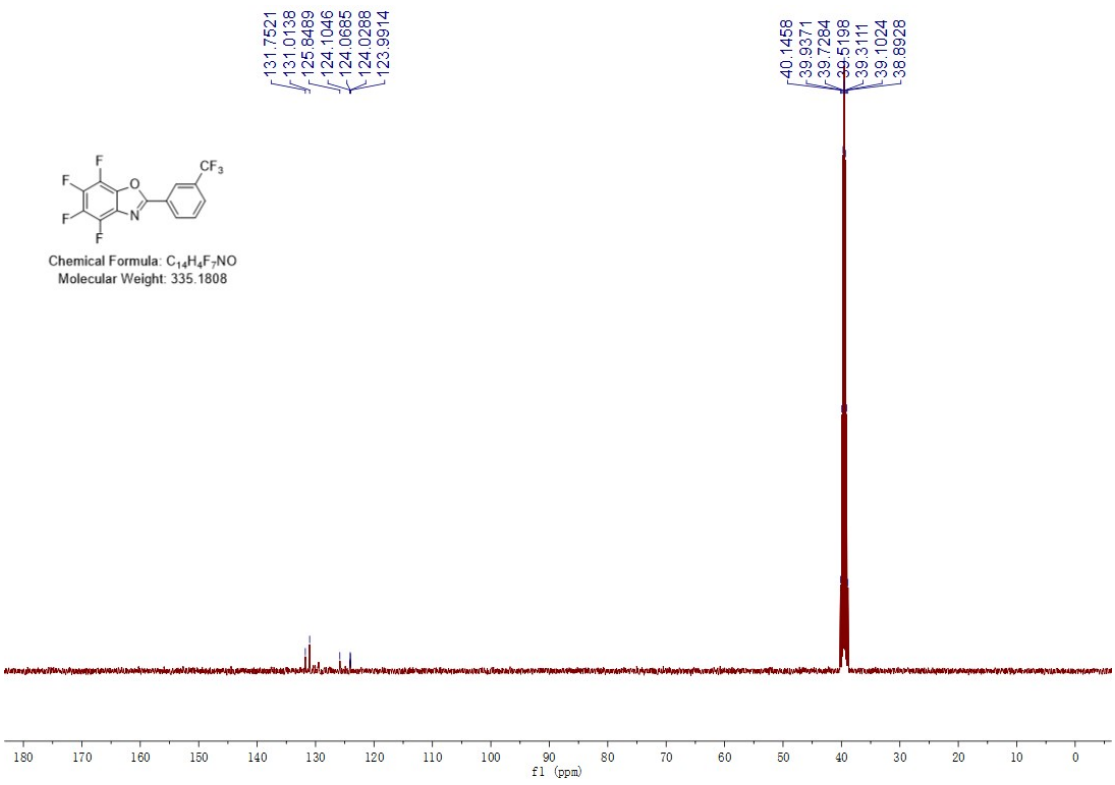
HRMS spectra



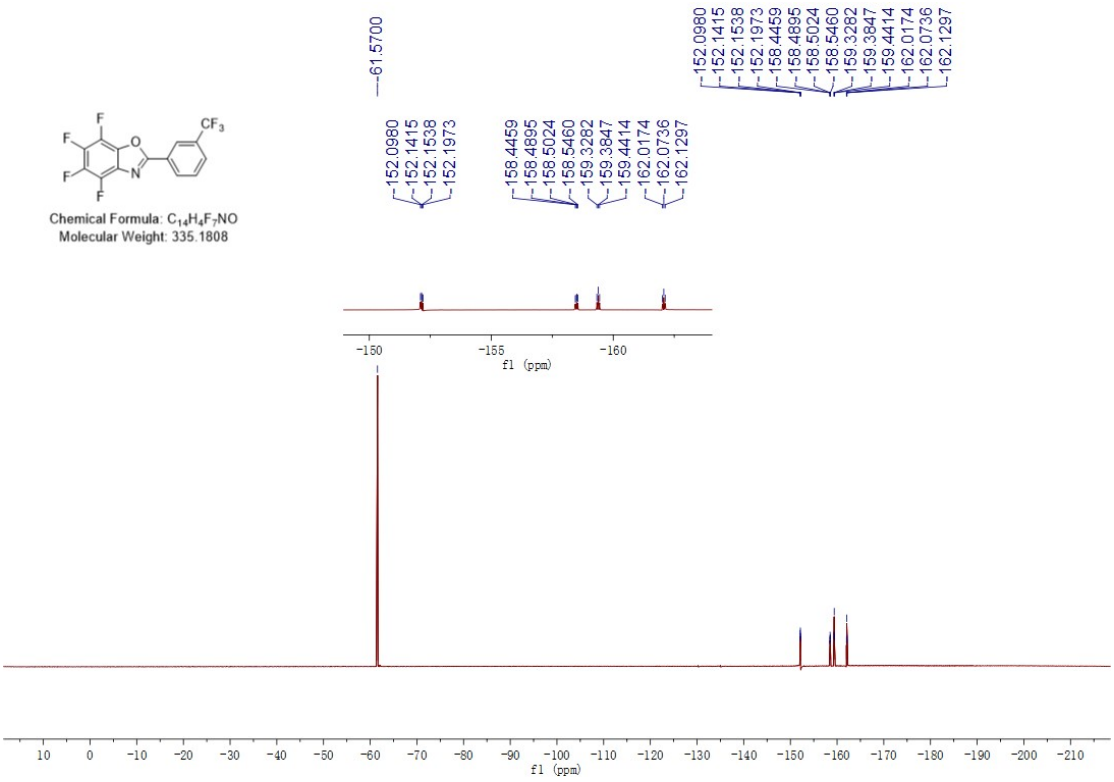
4,5,6,7-tetrafluoro-2-(3-(trifluoromethyl)phenyl)benzo[*d*]oxazole(**3g**)

^{1}H NMR (400 MHz, DMSO)

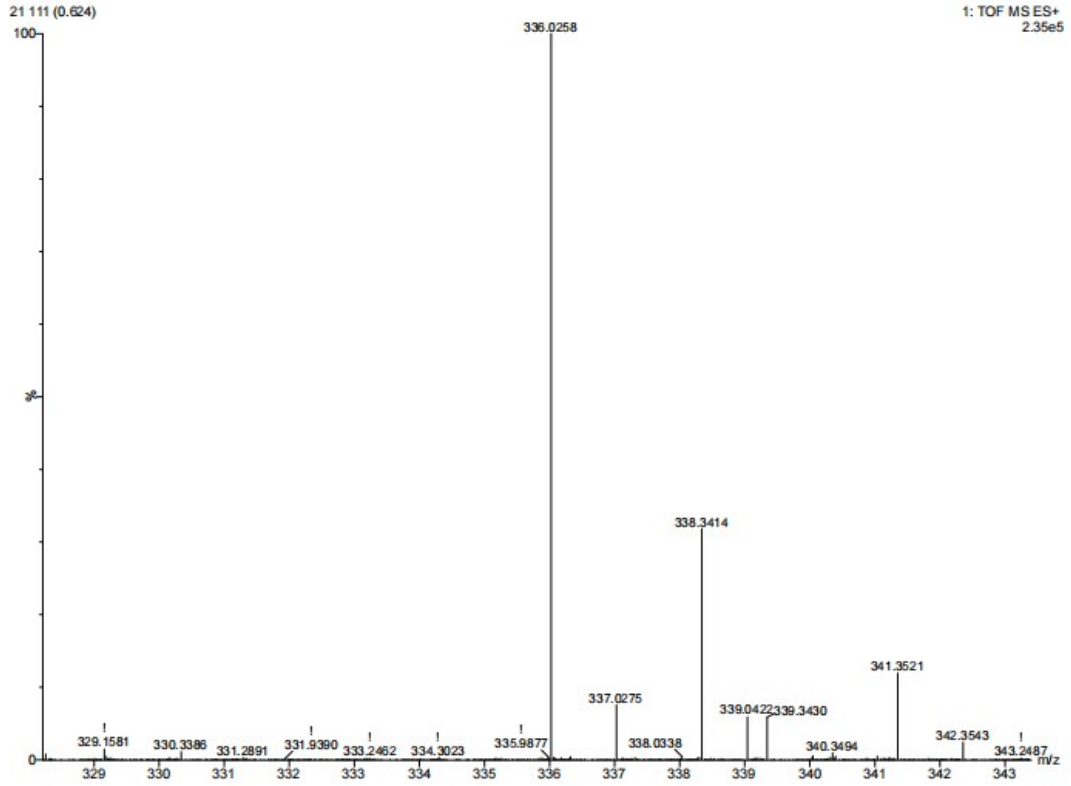




^{19}F NMR (376 MHz, DMSO)

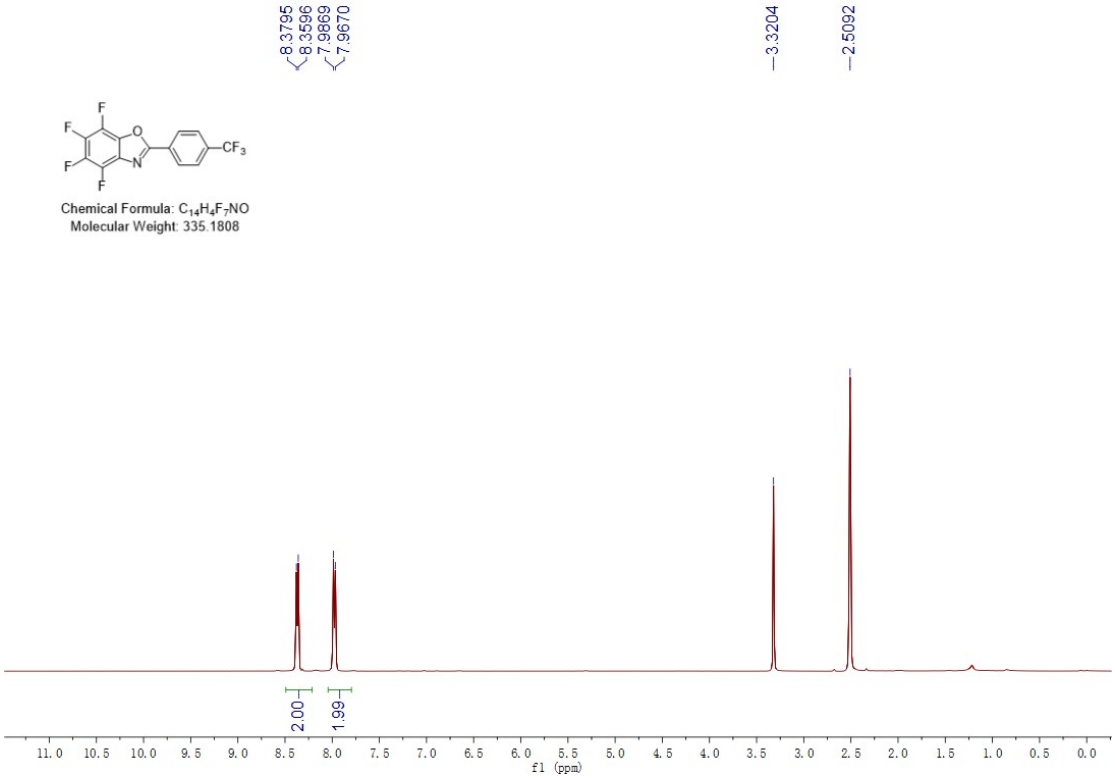


HRMS spectra

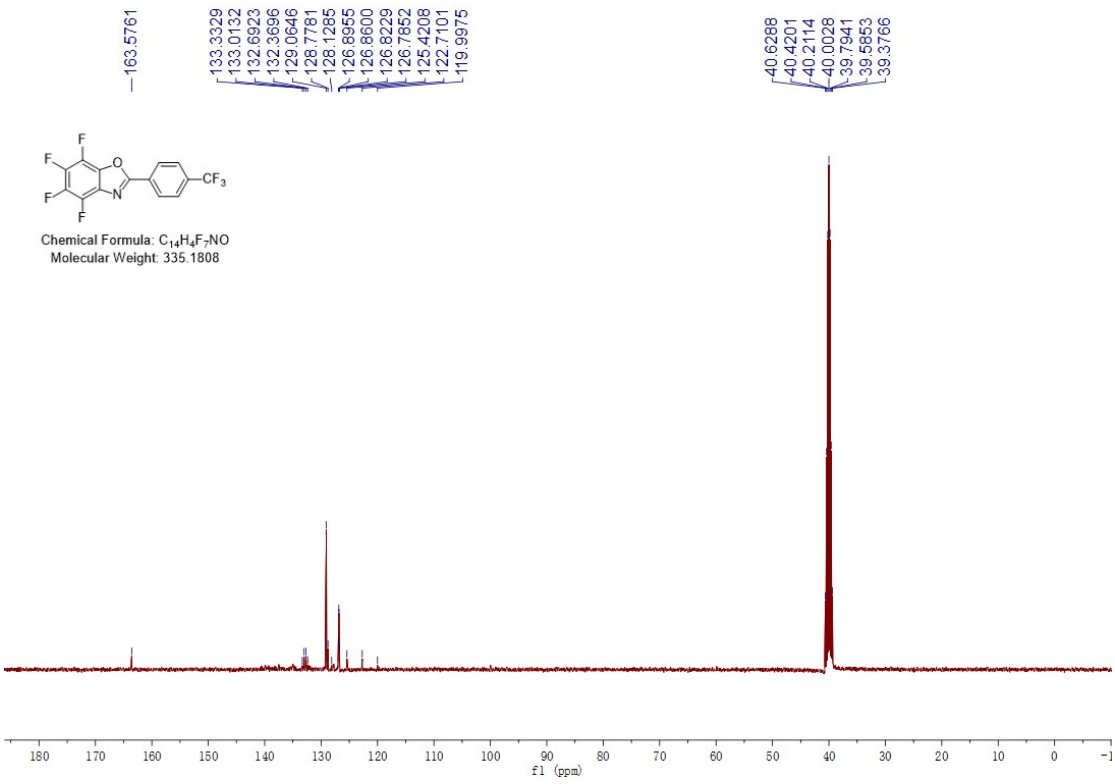


4,5,6,7-tetrafluoro-2-(4-(trifluoromethyl)phenyl)benzo[*d*]oxazole (**3h**)

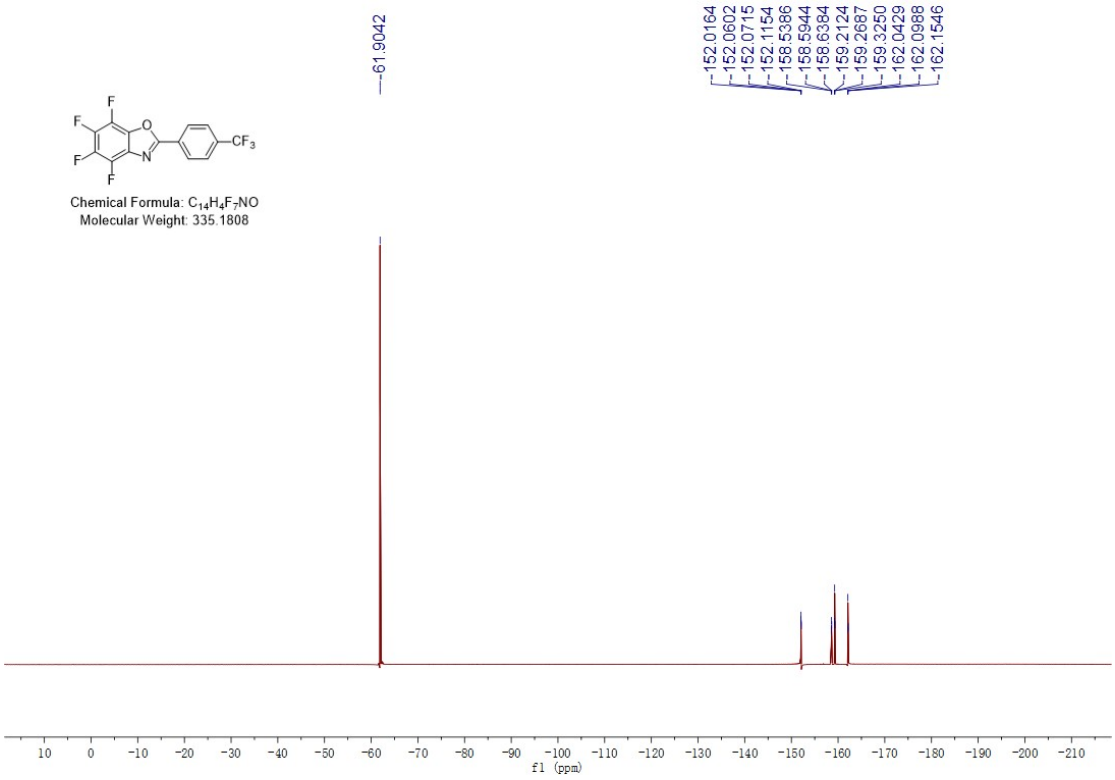
^{1}H NMR (400 MHz, DMSO)



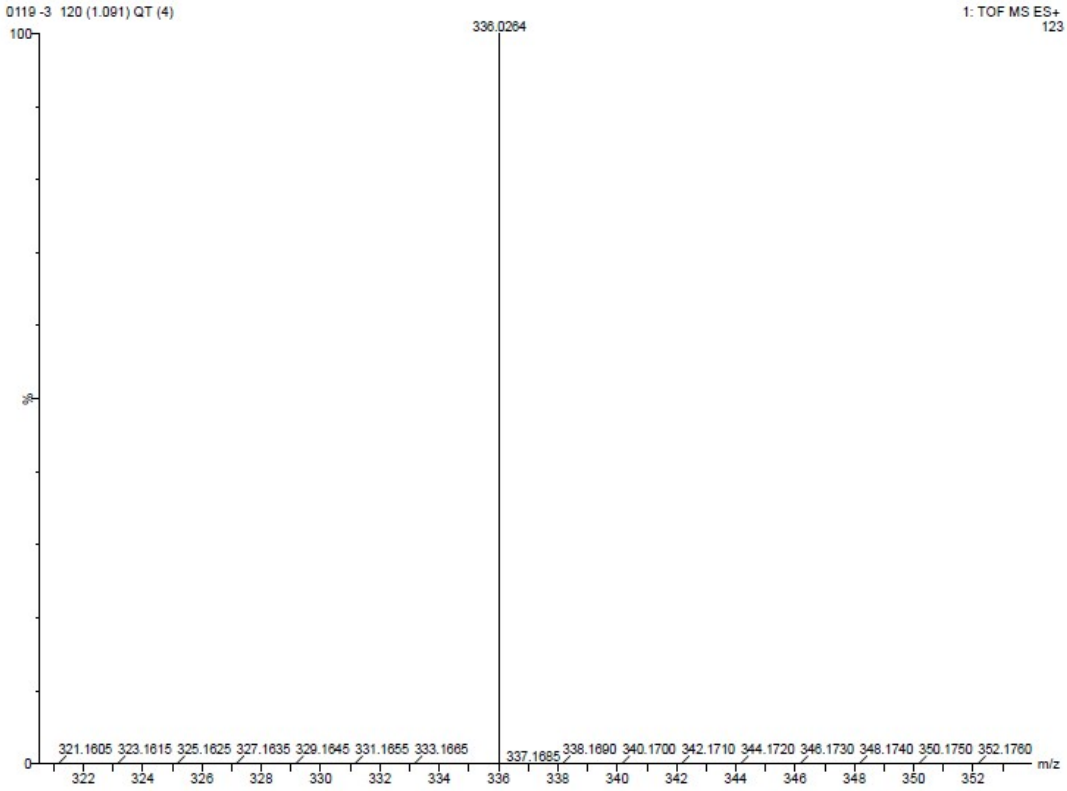
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

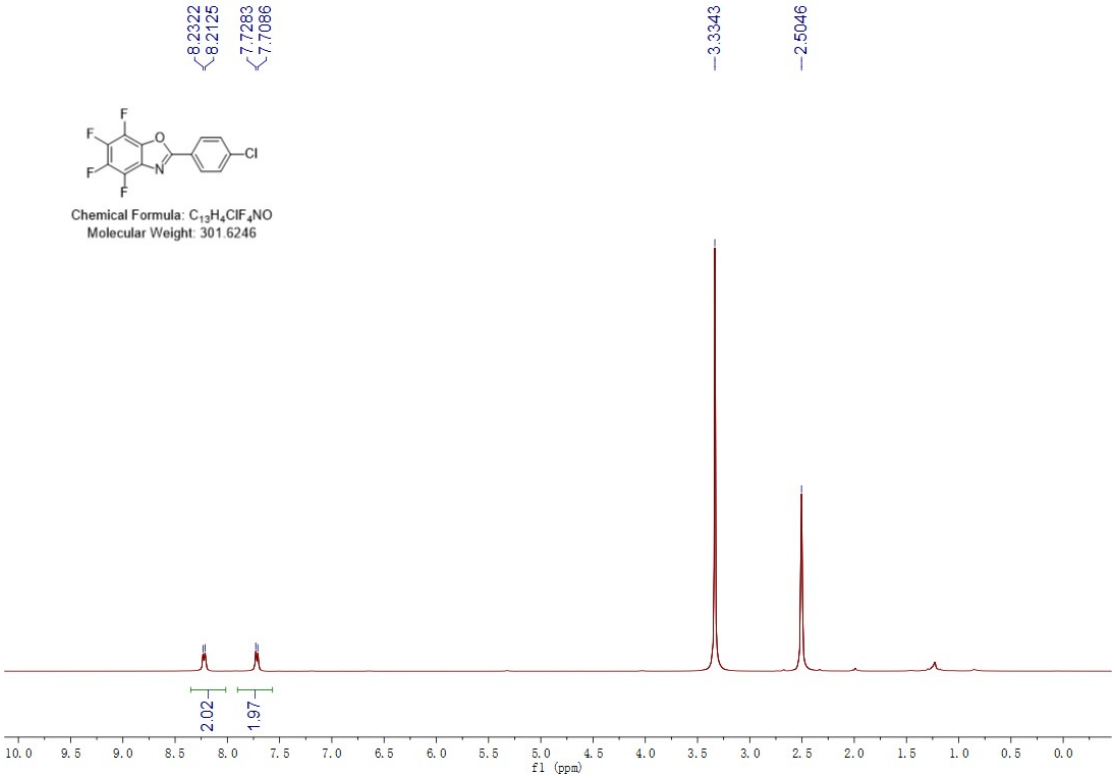


HRMS spectra

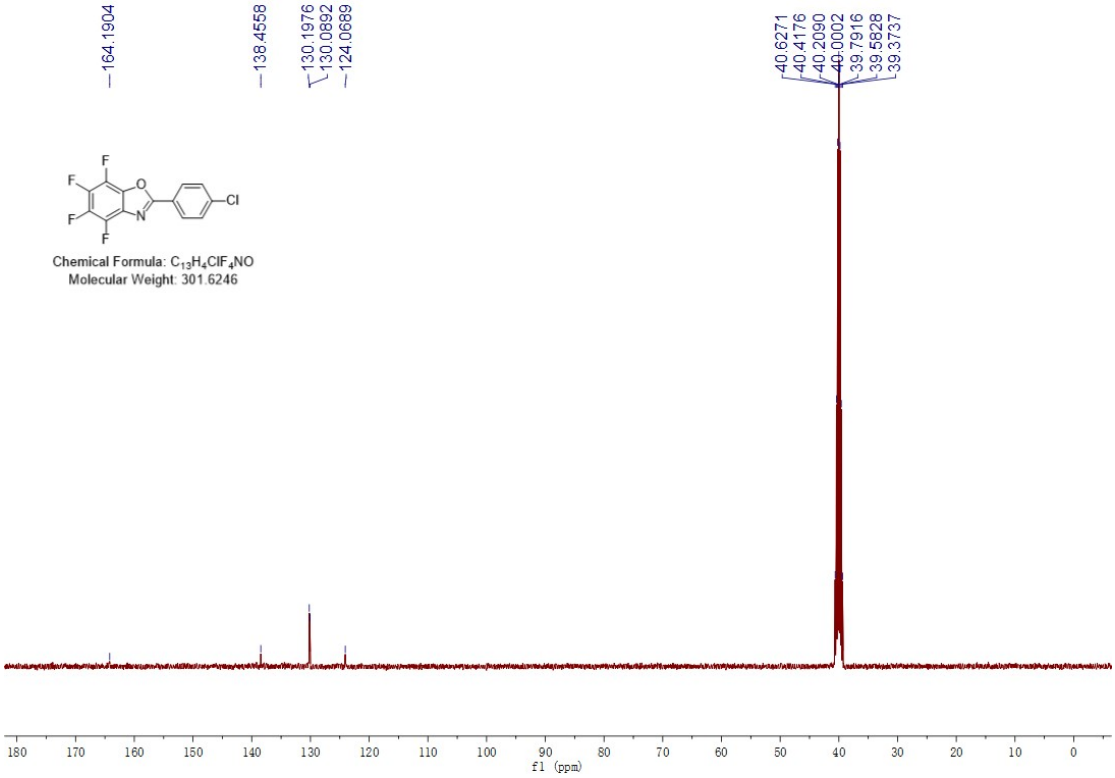


2-(4-chlorophenyl)-4,5,6,7-tetrafluorobenzo[*d*]oxazole(**3i**)

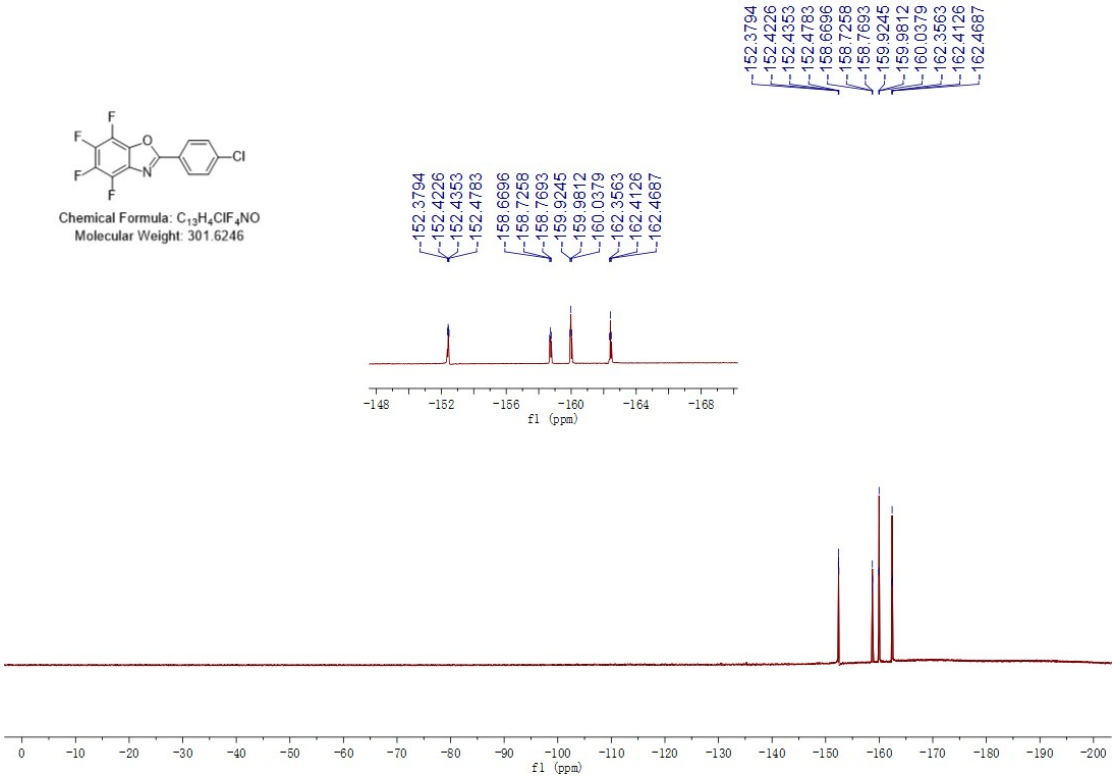
^{1}H NMR (400 MHz, DMSO)



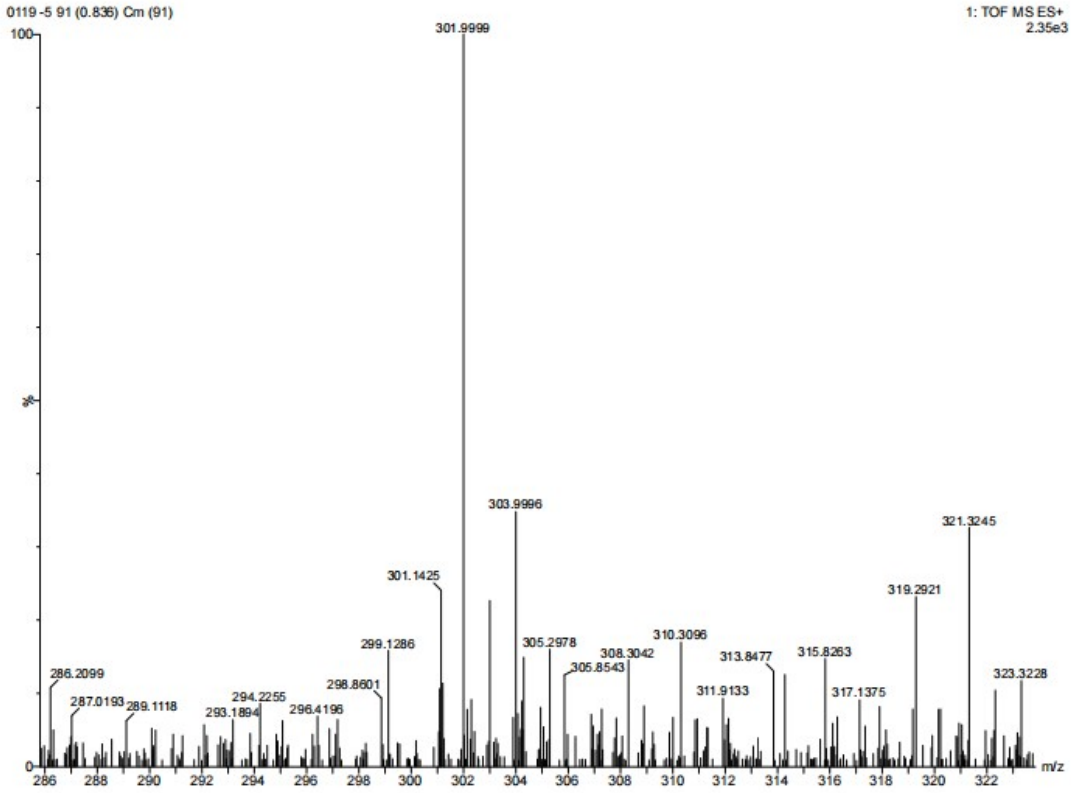
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

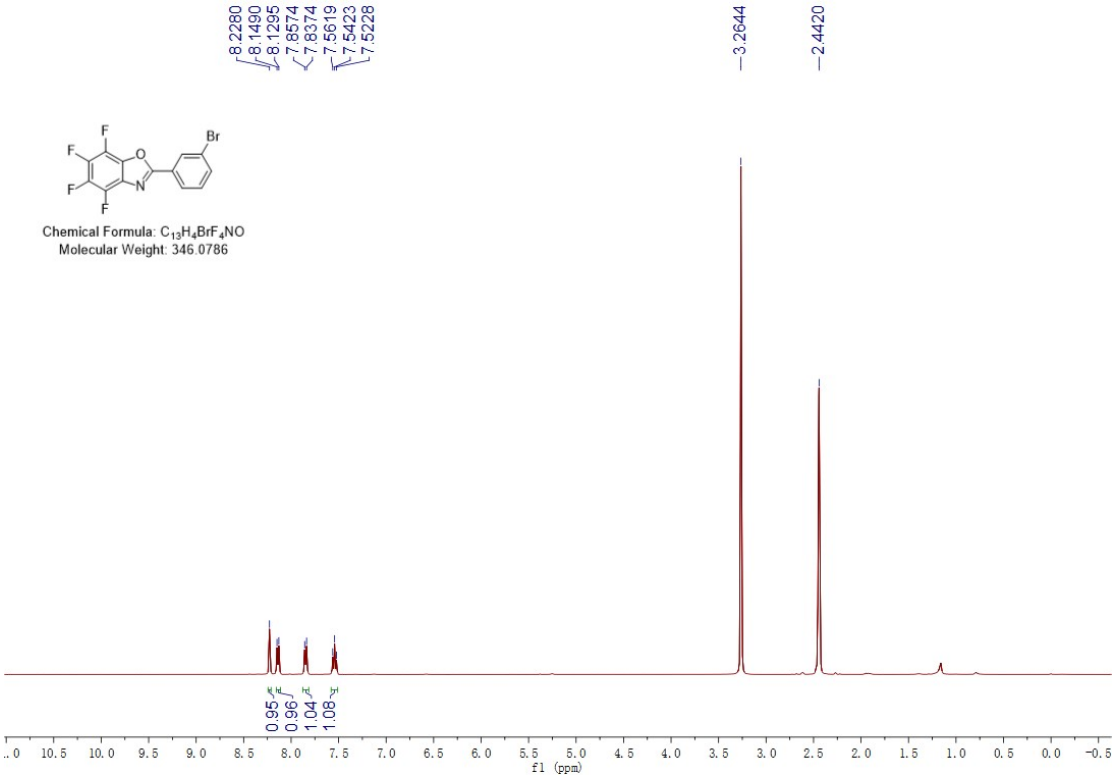


HRMS spectra

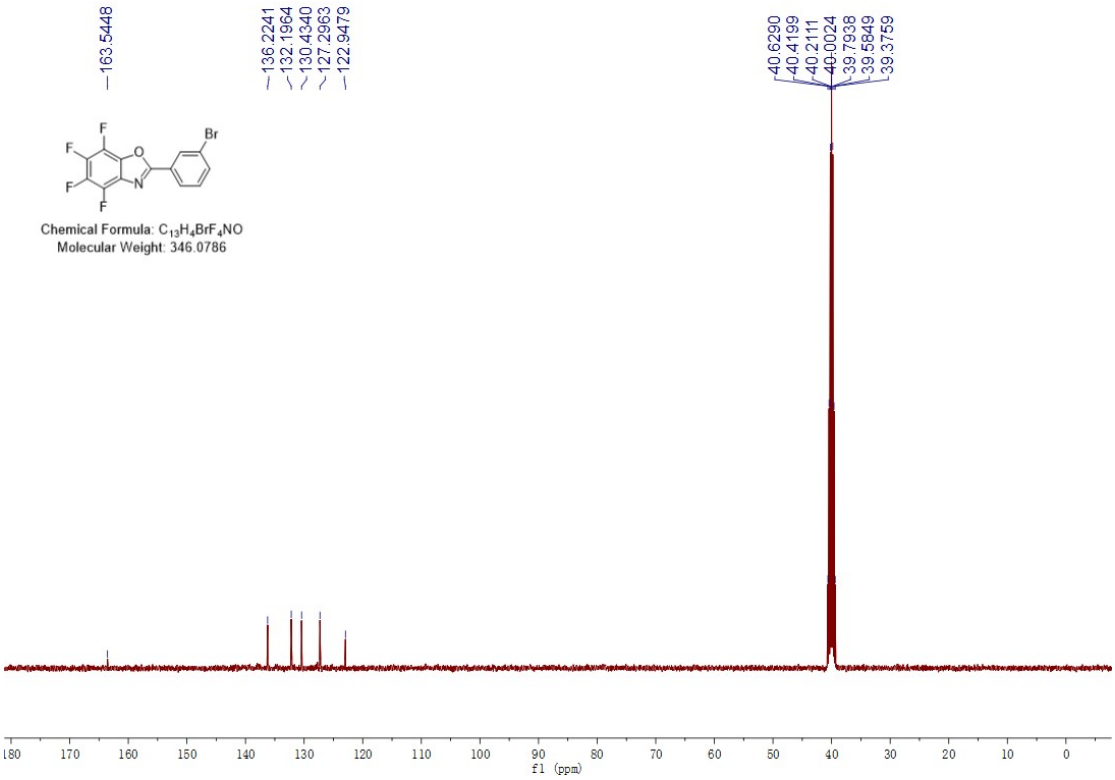


2-(3-bromophenyl)-4,5,6,7-tetrafluorobenzo[*d*]oxazole (**3j**)

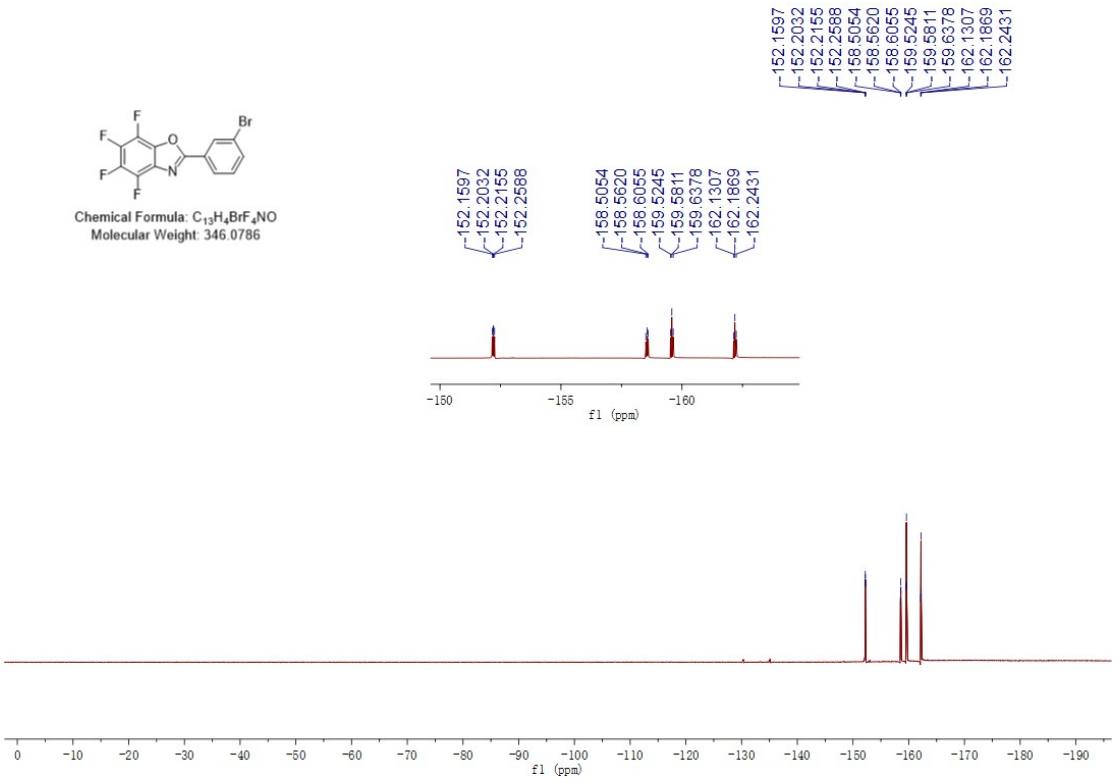
^{1}H NMR (400 MHz, DMSO)



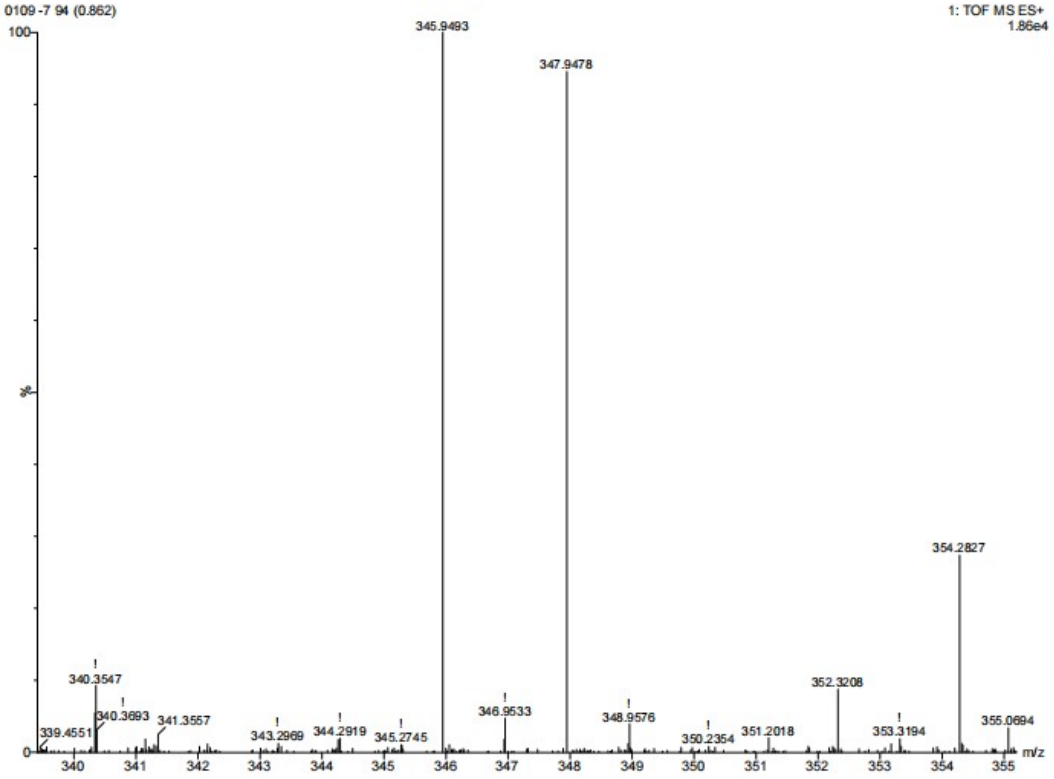
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

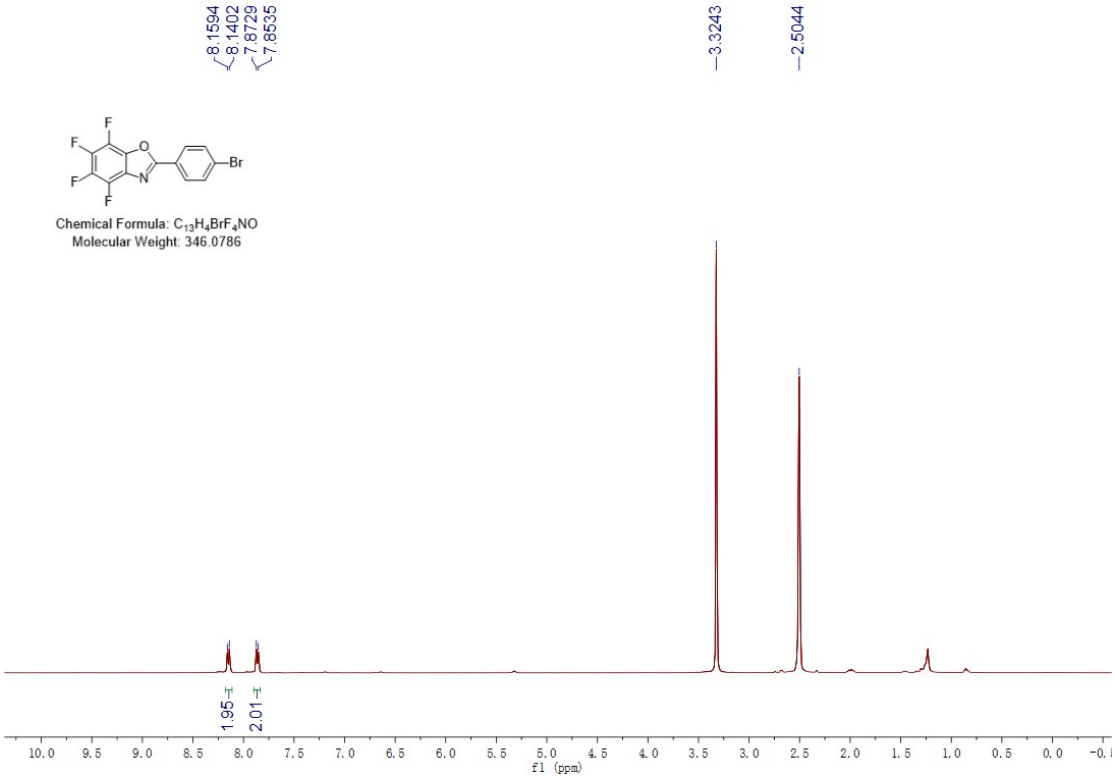


HRMS spectra

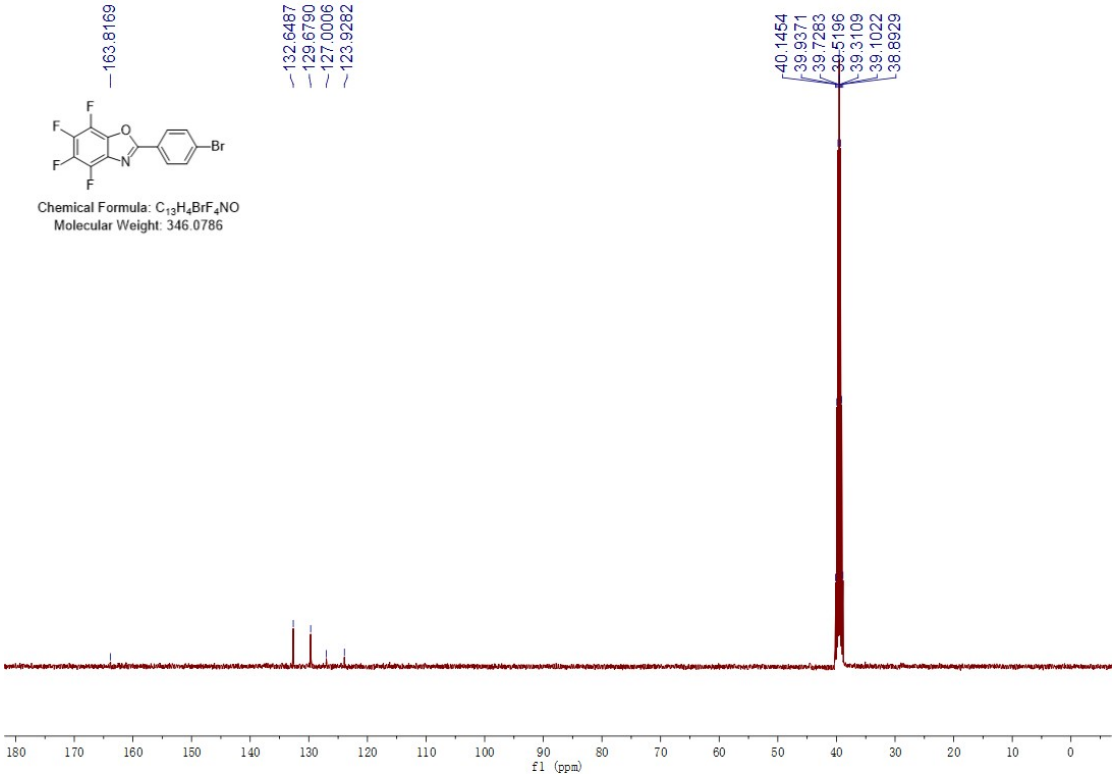


2-(4-bromophenyl)-4,5,6,7-tetrafluorobenzo[*d*]oxazole (**3k**)

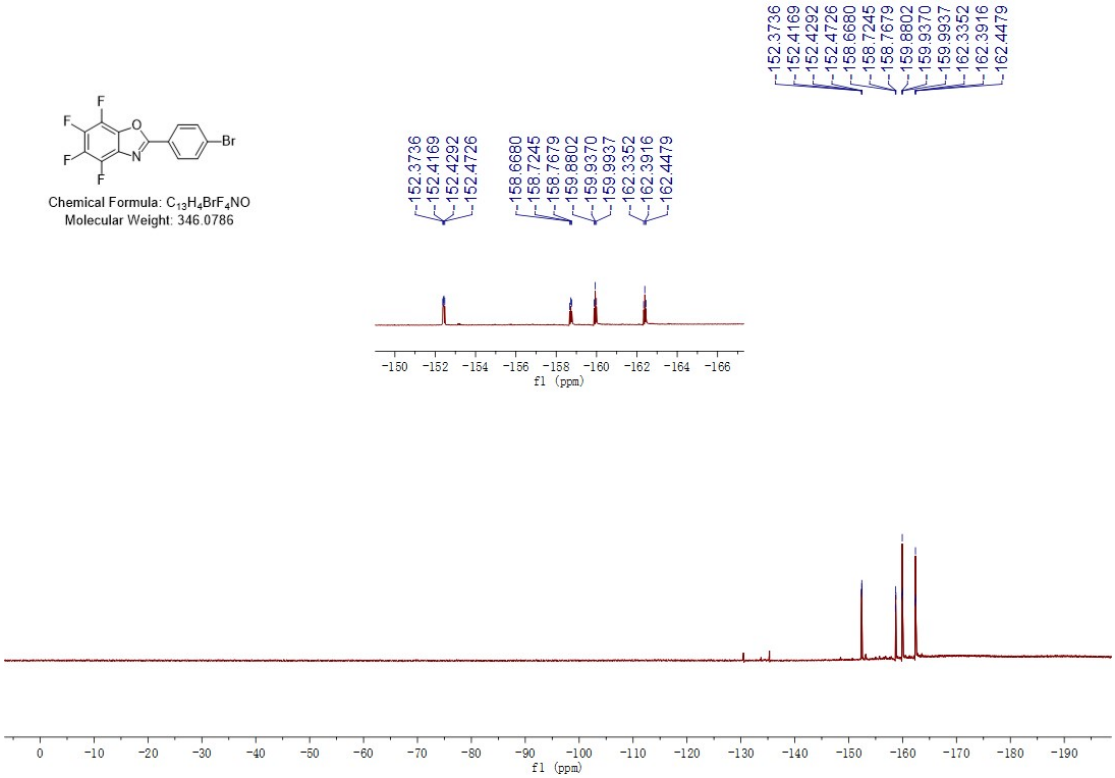
^{1}H NMR (400 MHz, DMSO)



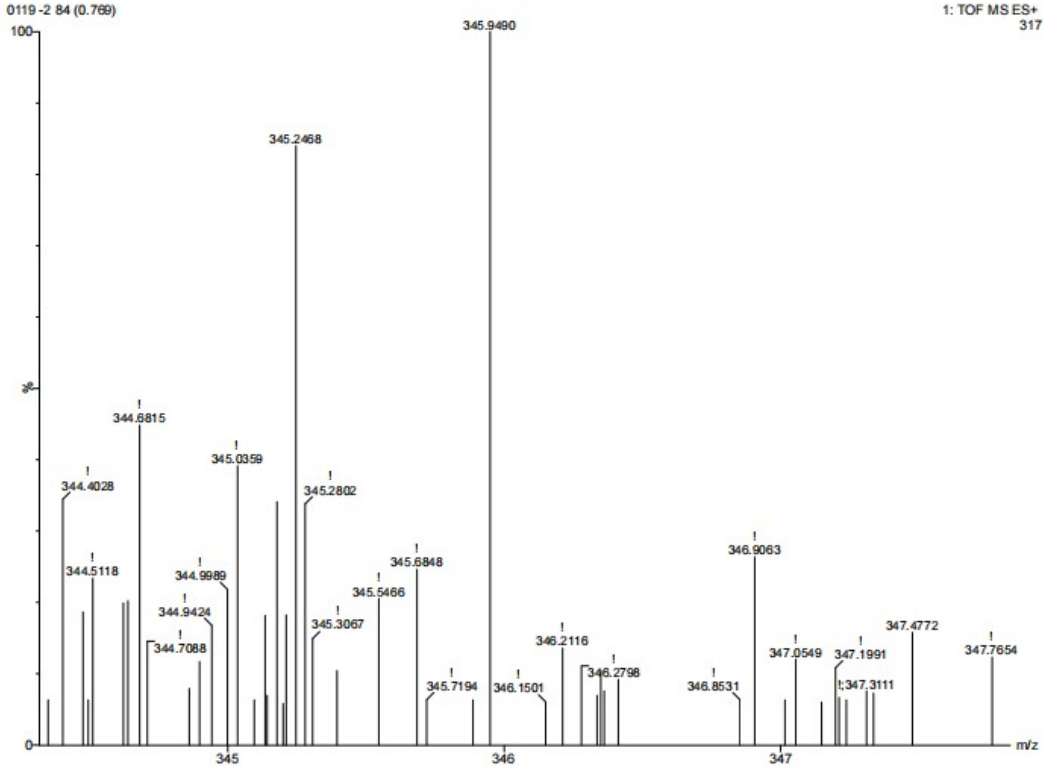
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

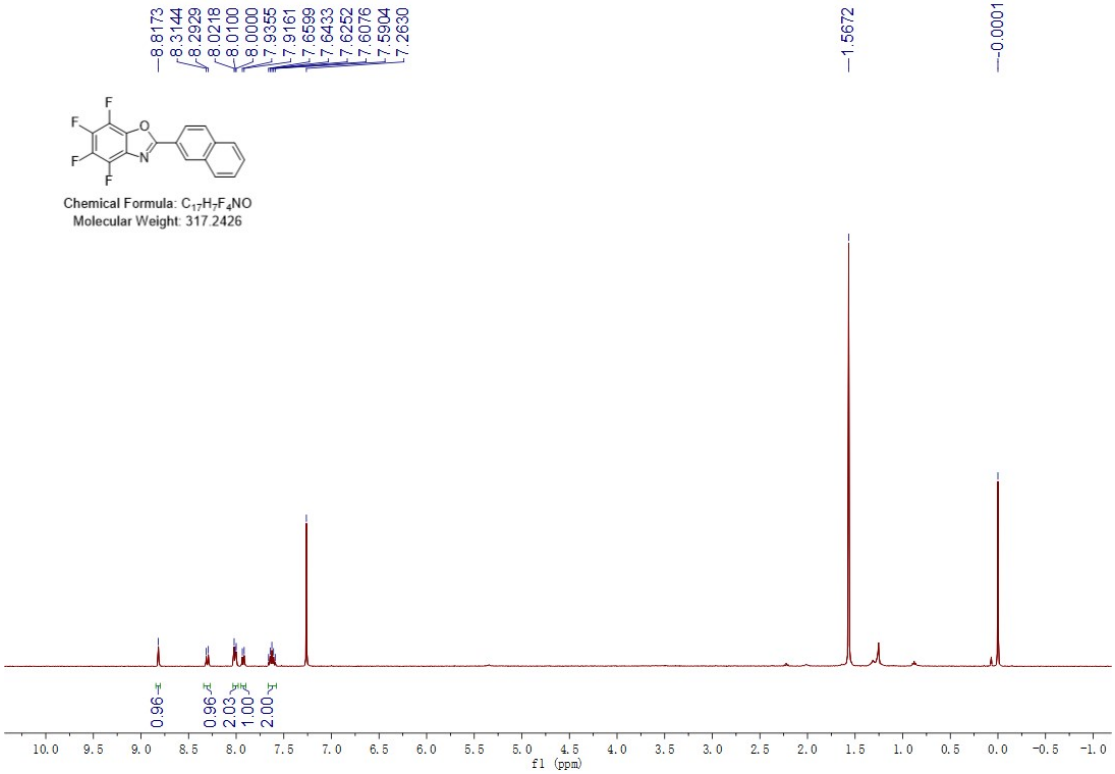


HRMS spectra

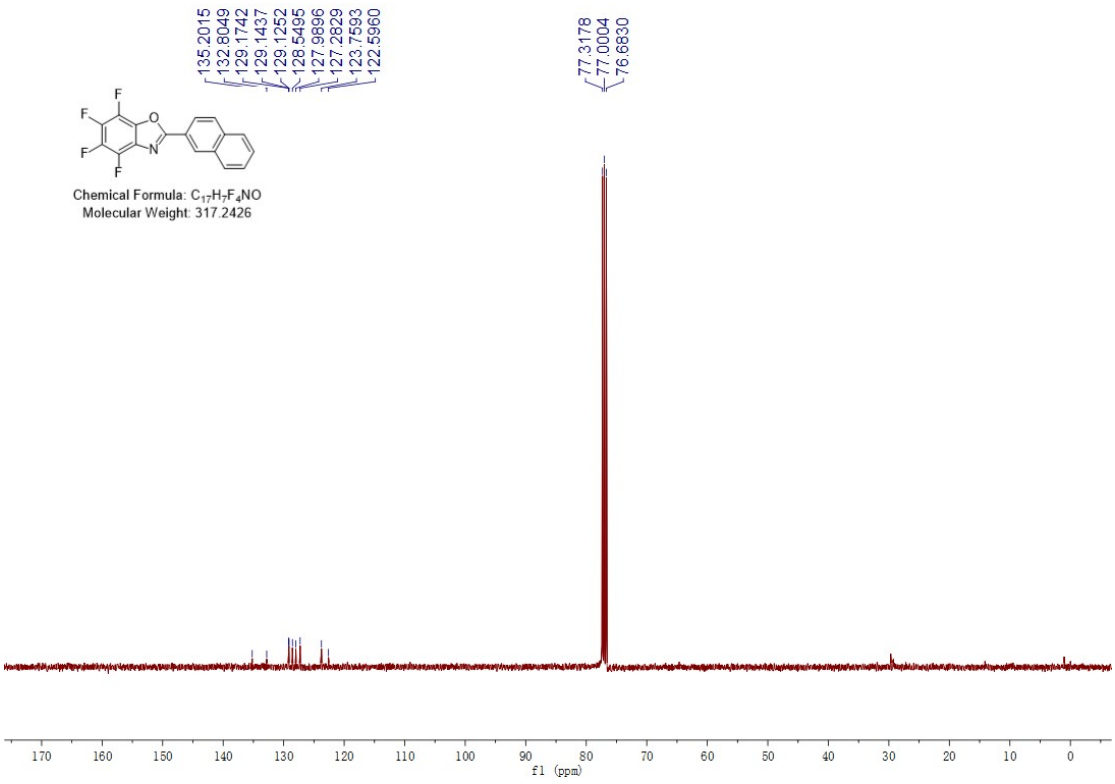


4,5,6,7-tetrafluoro-2-(naphthalen-2-yl)benzo[*d*]oxazole (**3l**)

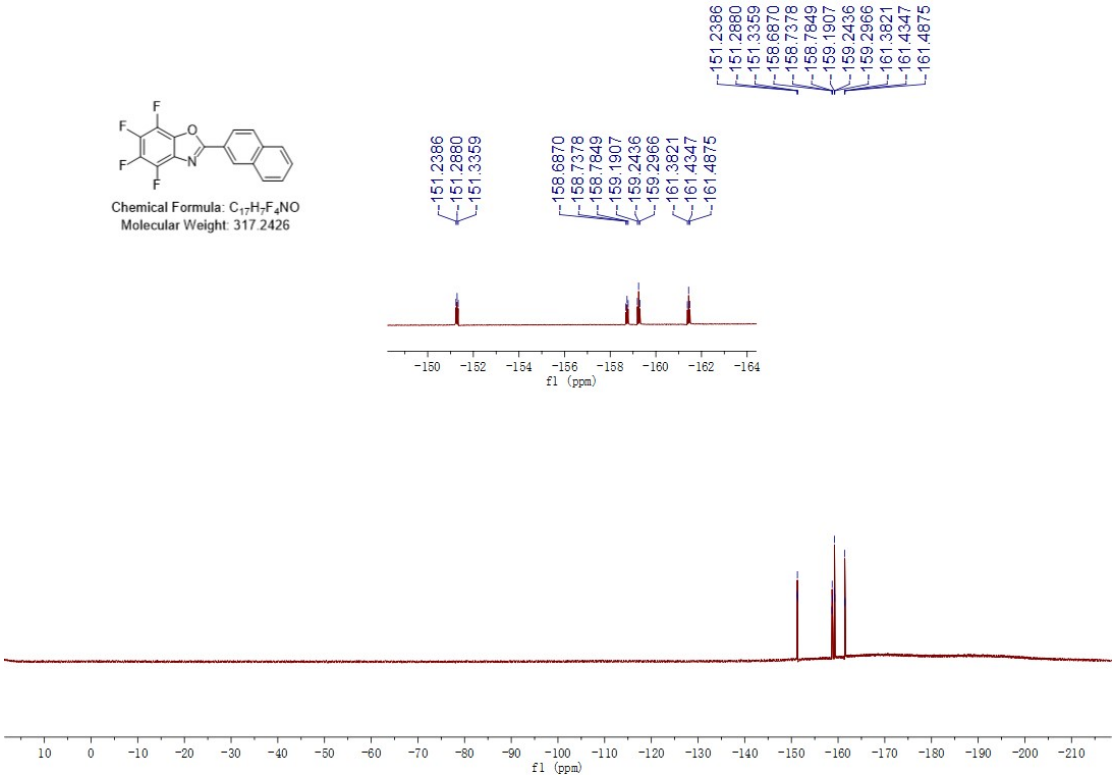
^{1}H NMR (400 MHz, DMSO)



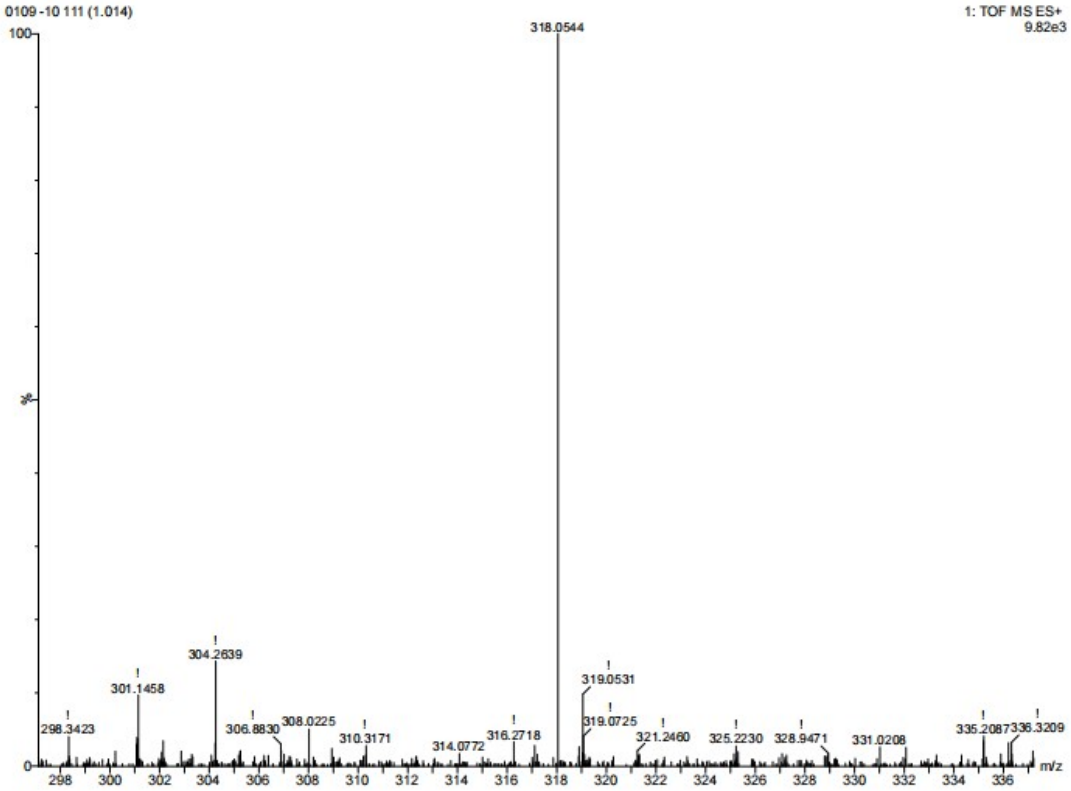
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

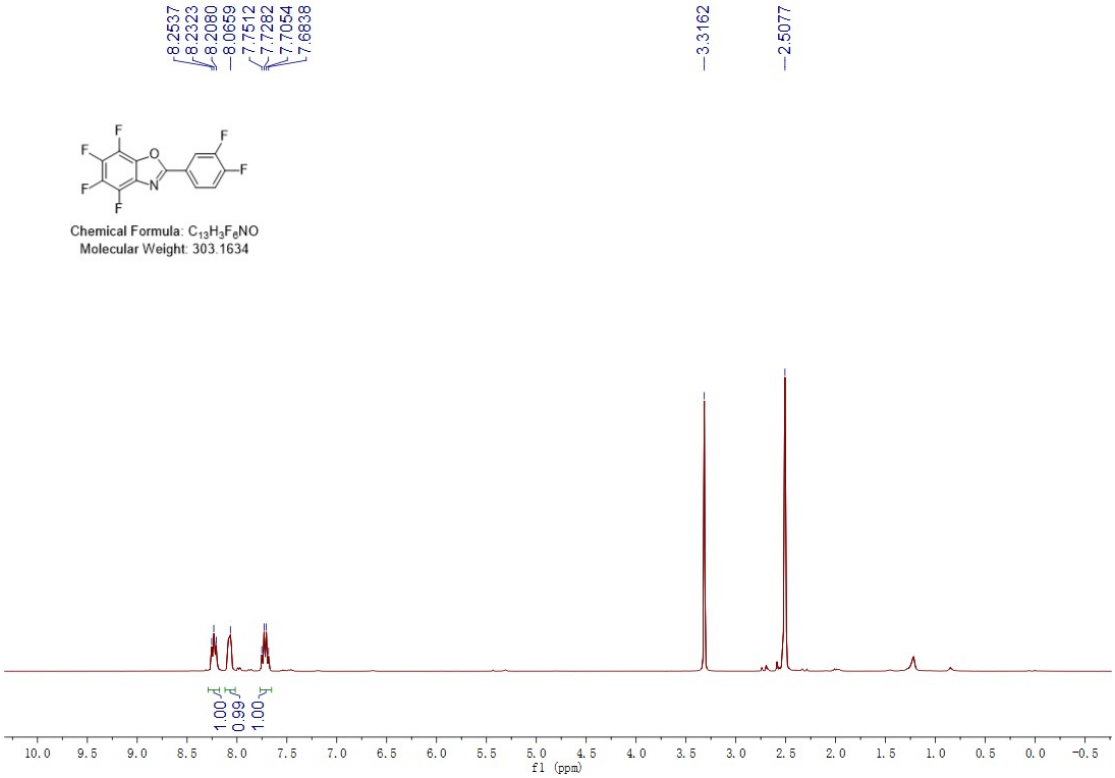


HRMS spectra

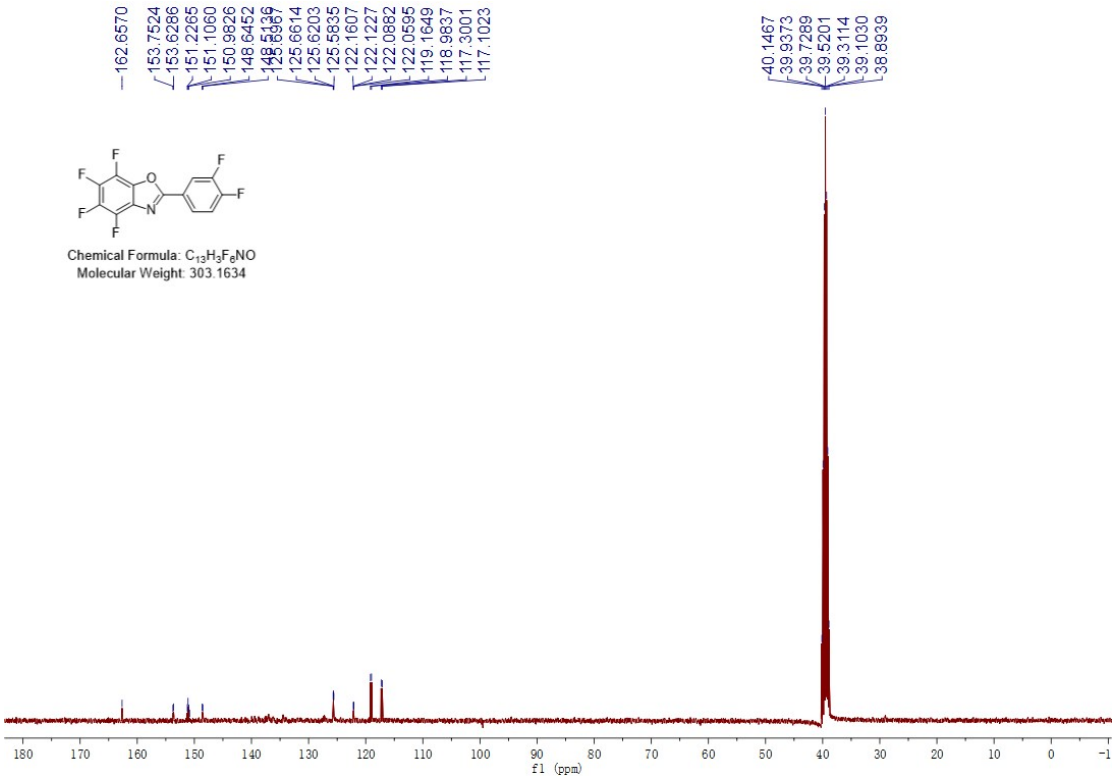


2-(3,4-difluorophenyl)-4,5,6,7-tetrafluorobenzo[*d*]oxazole (**3m**)

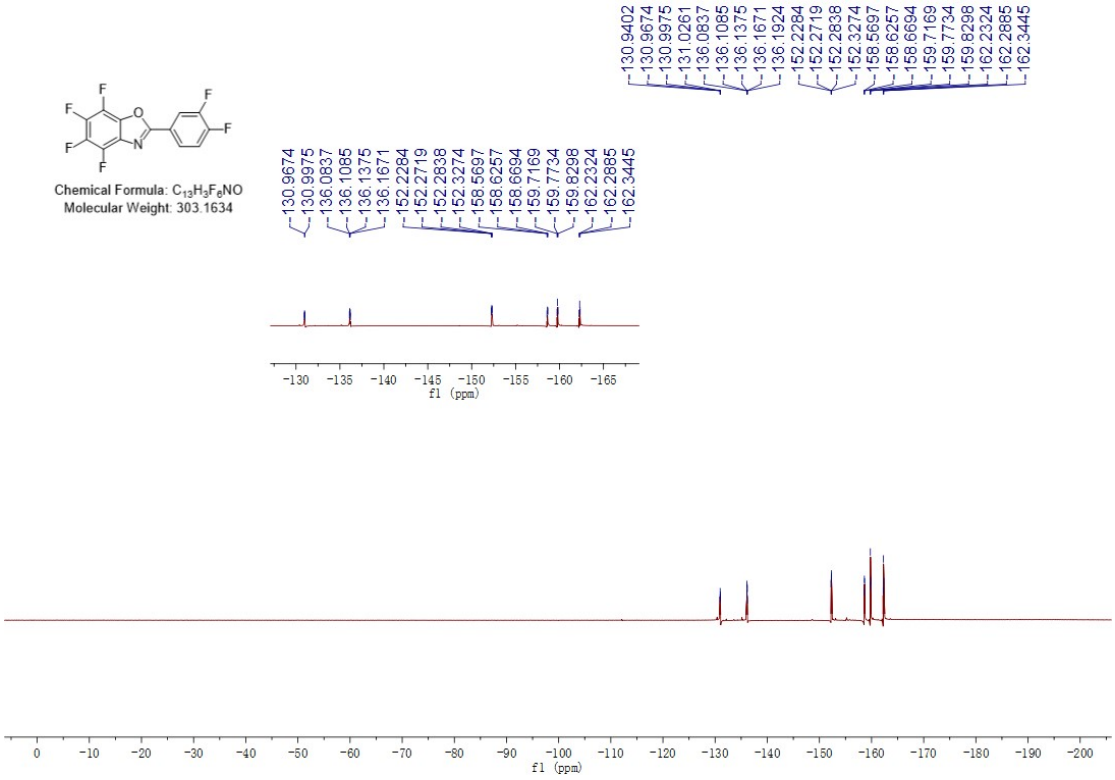
^{1}H NMR (400 MHz, DMSO)



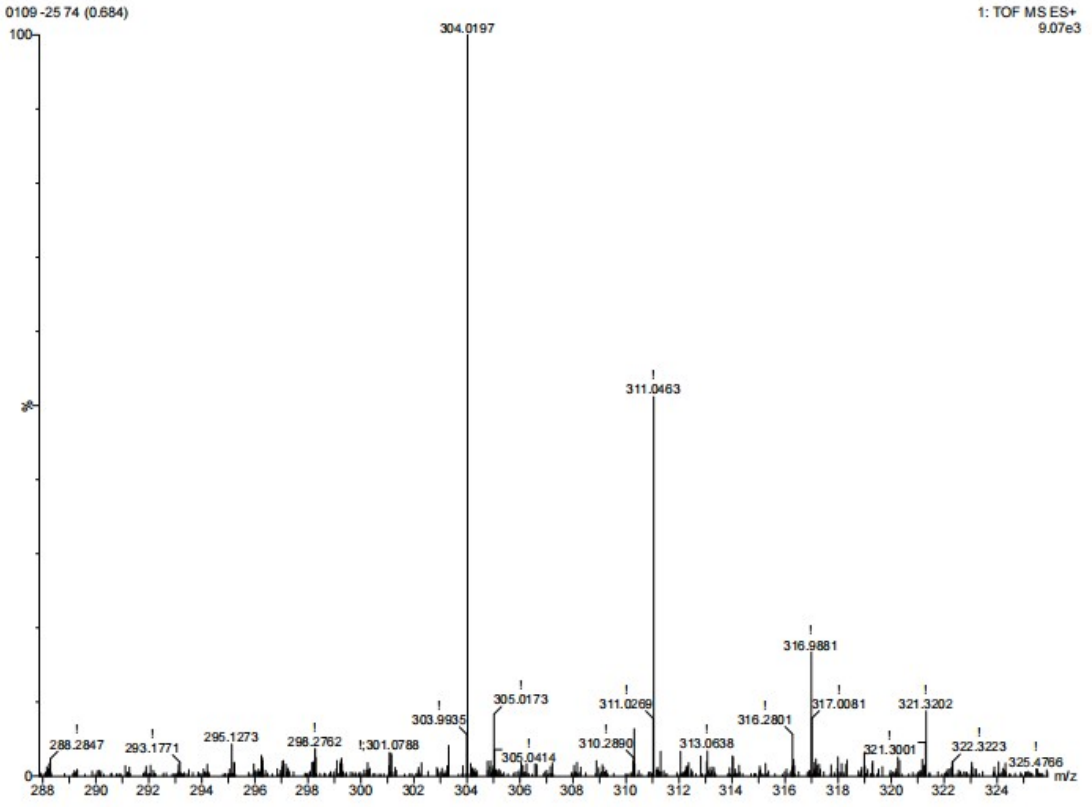
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

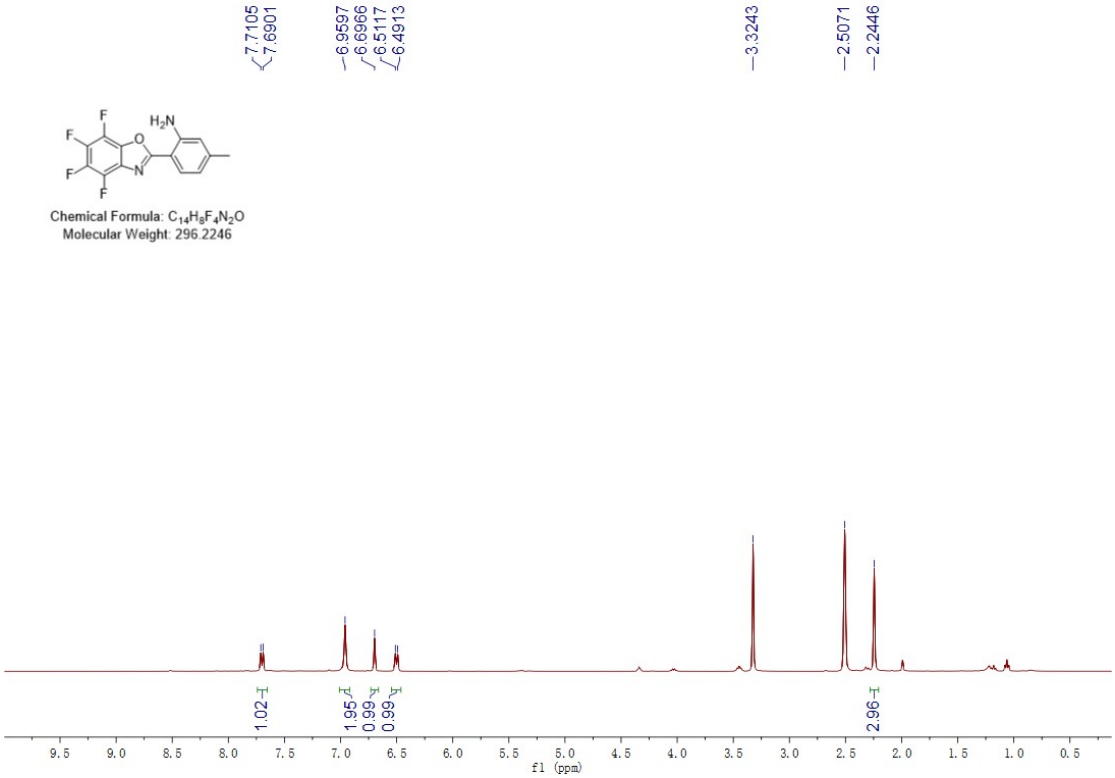


HRMS spectra

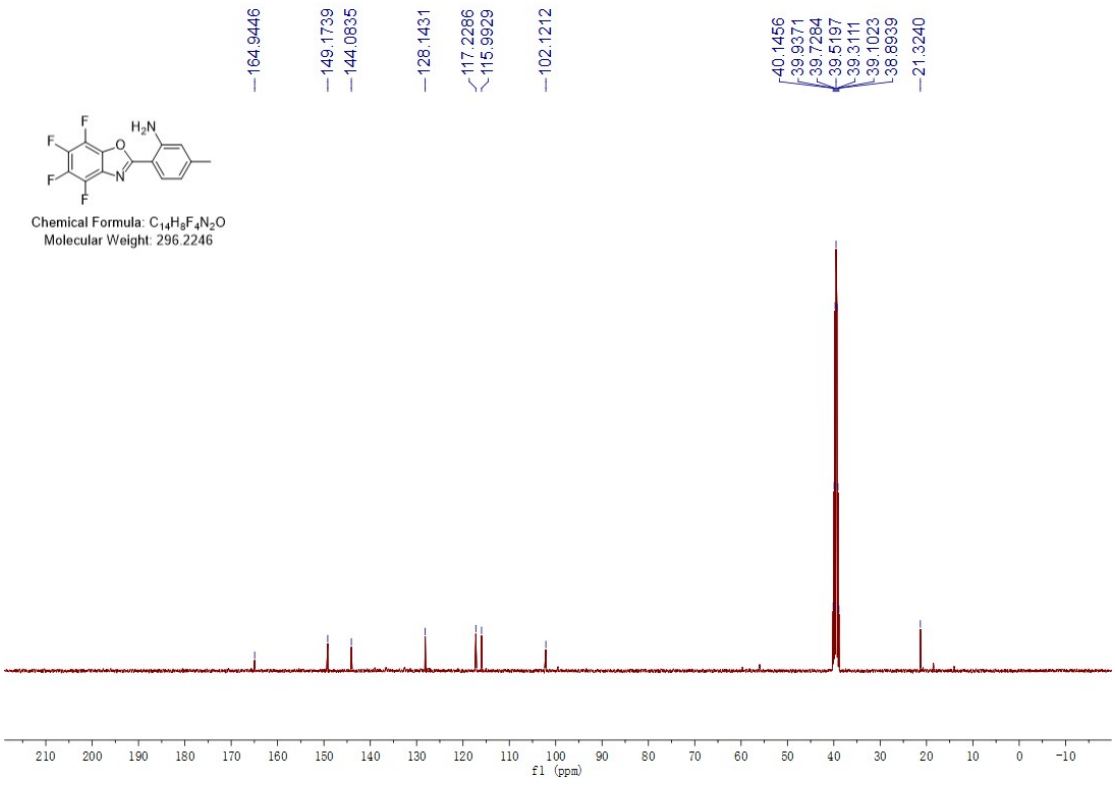


2-methyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**3n**)

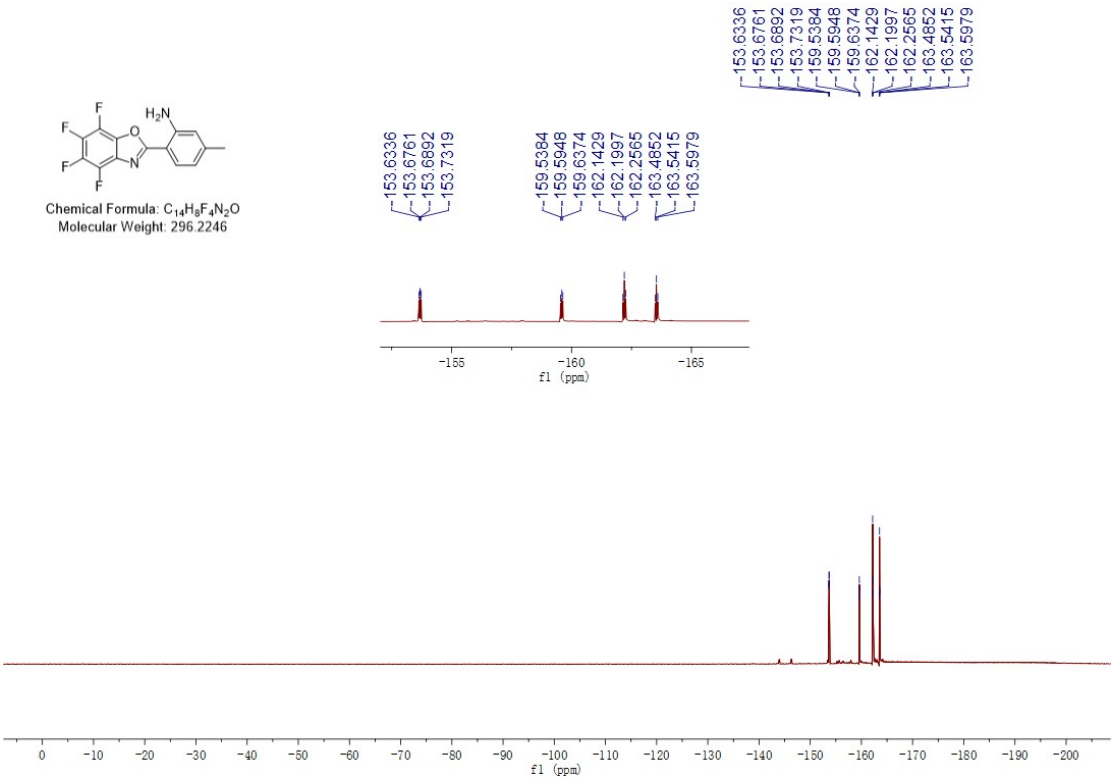
^{1}H NMR (400 MHz, DMSO)



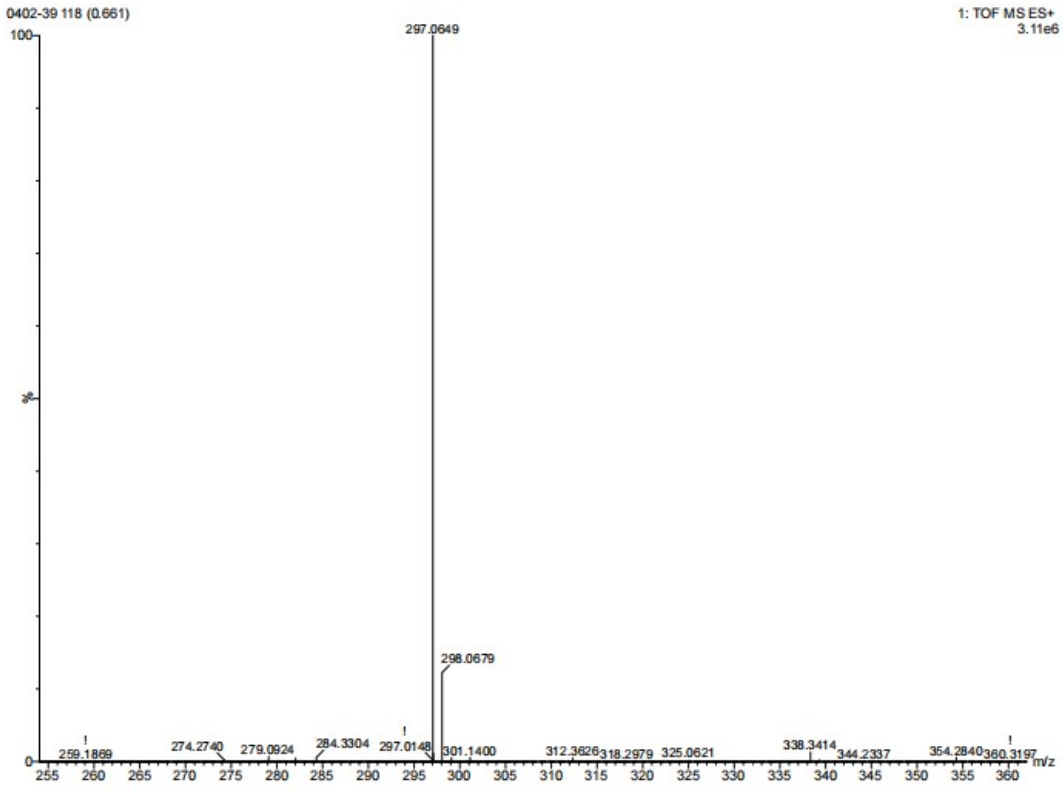
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

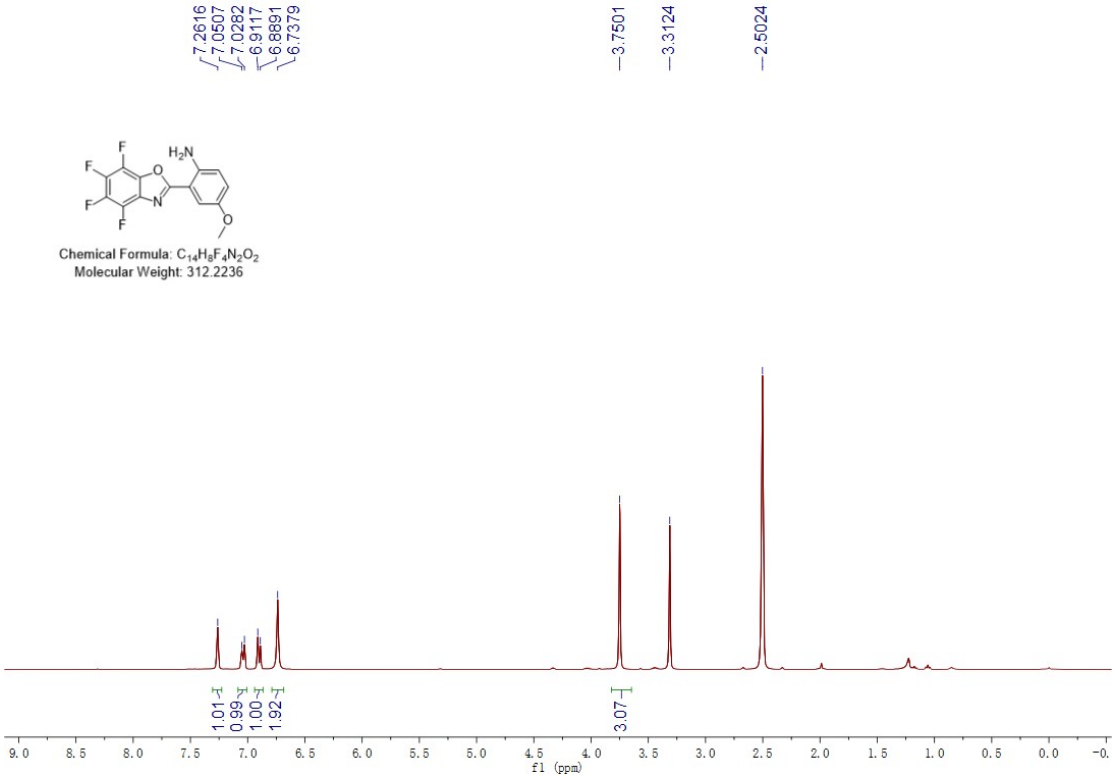


HRMS spectra

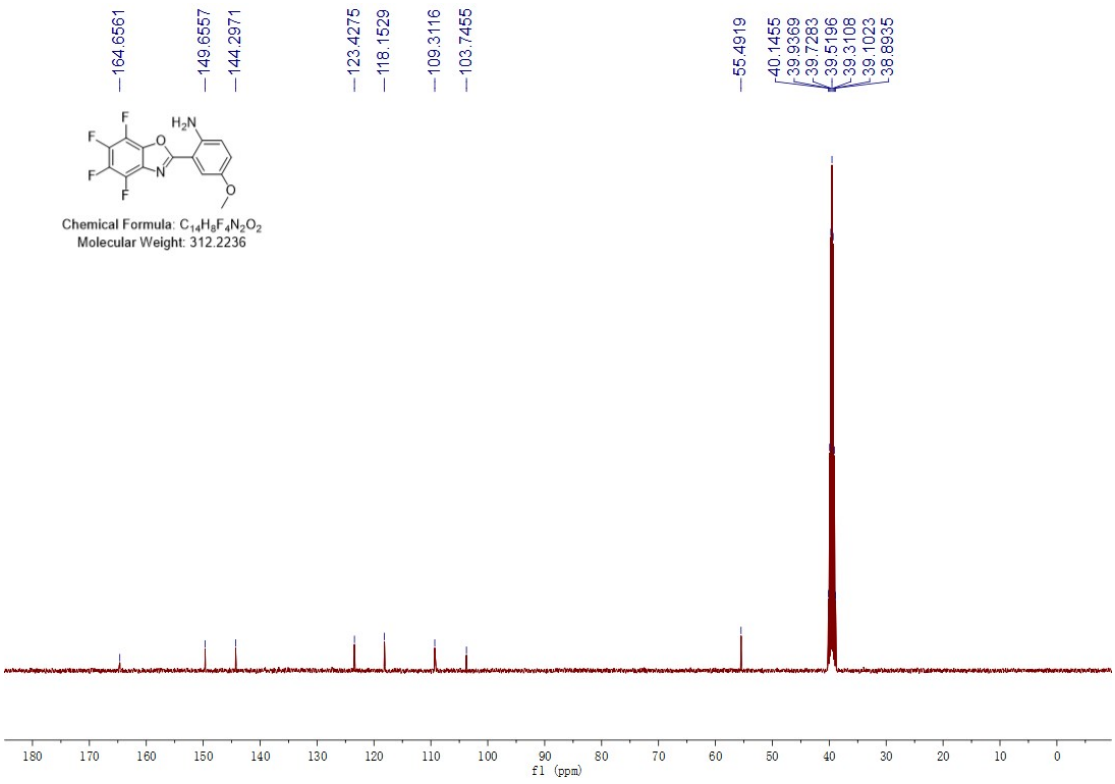


2-methoxy-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**3o**)

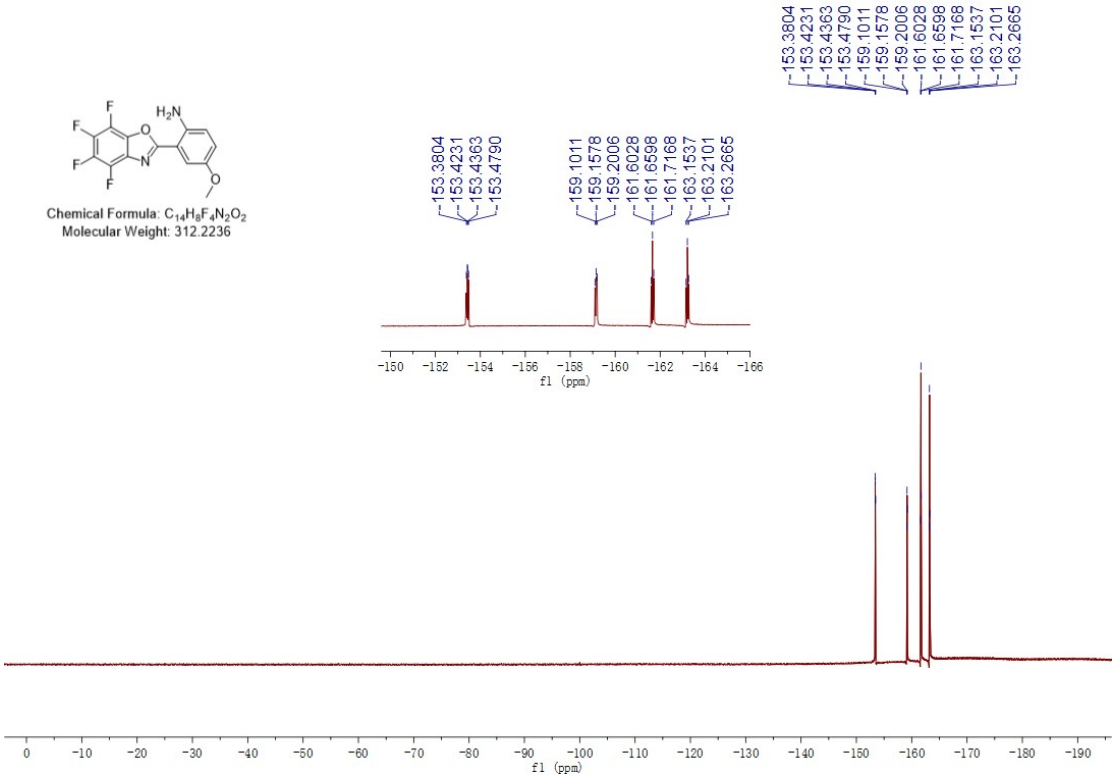
^{1}H NMR (400 MHz, DMSO)



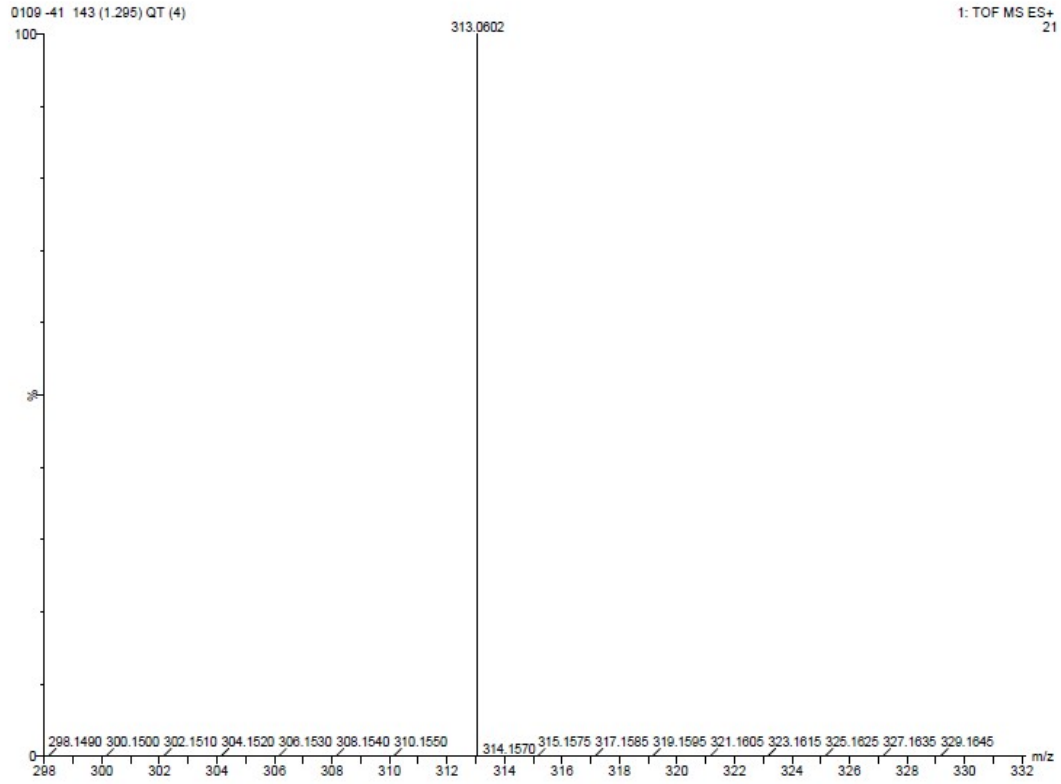
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

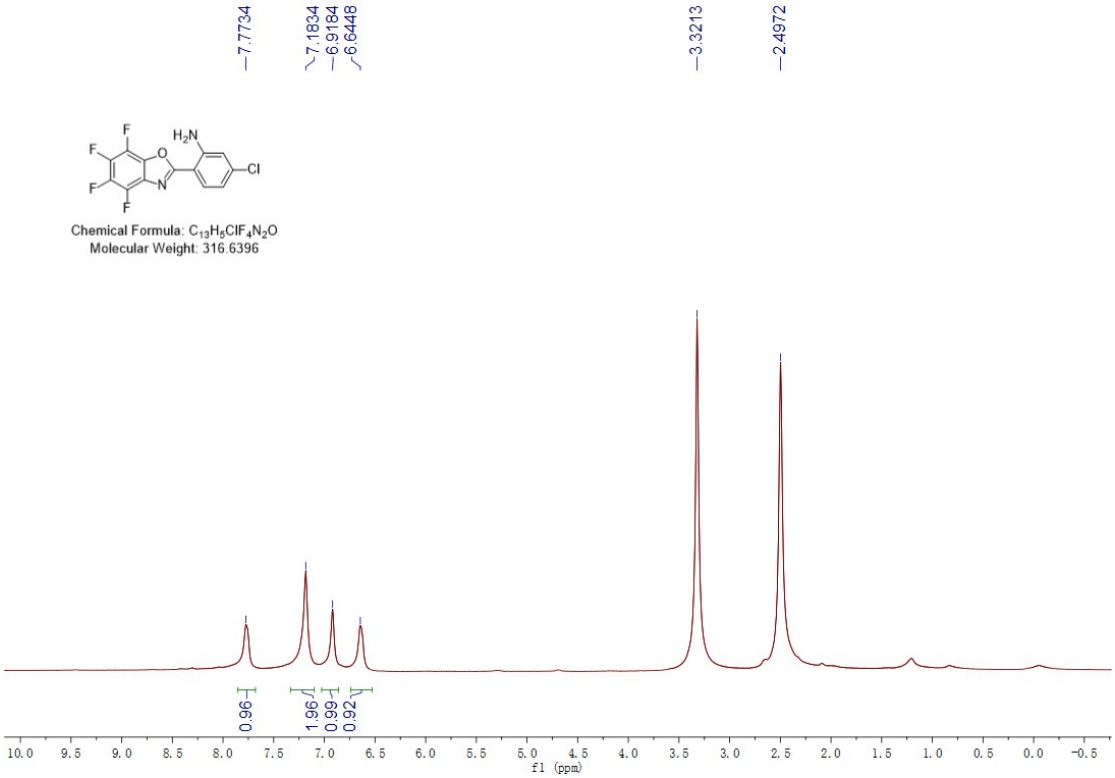


HRMS spectra

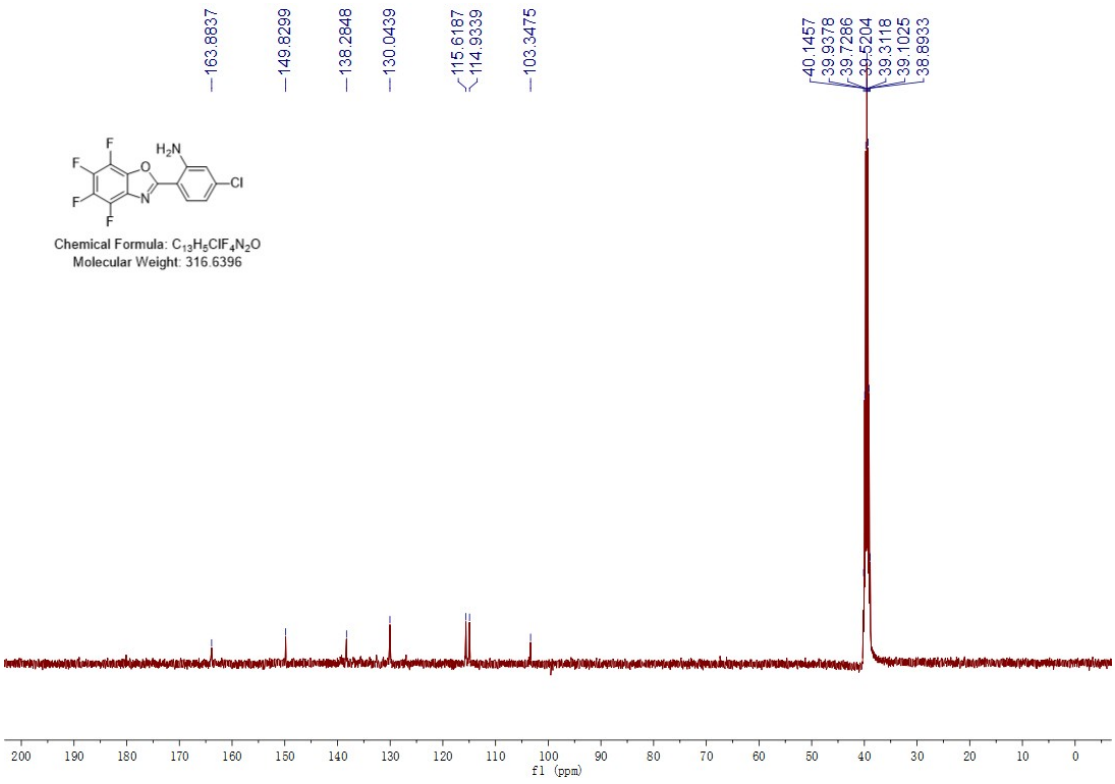


2-chloro-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**3p**)

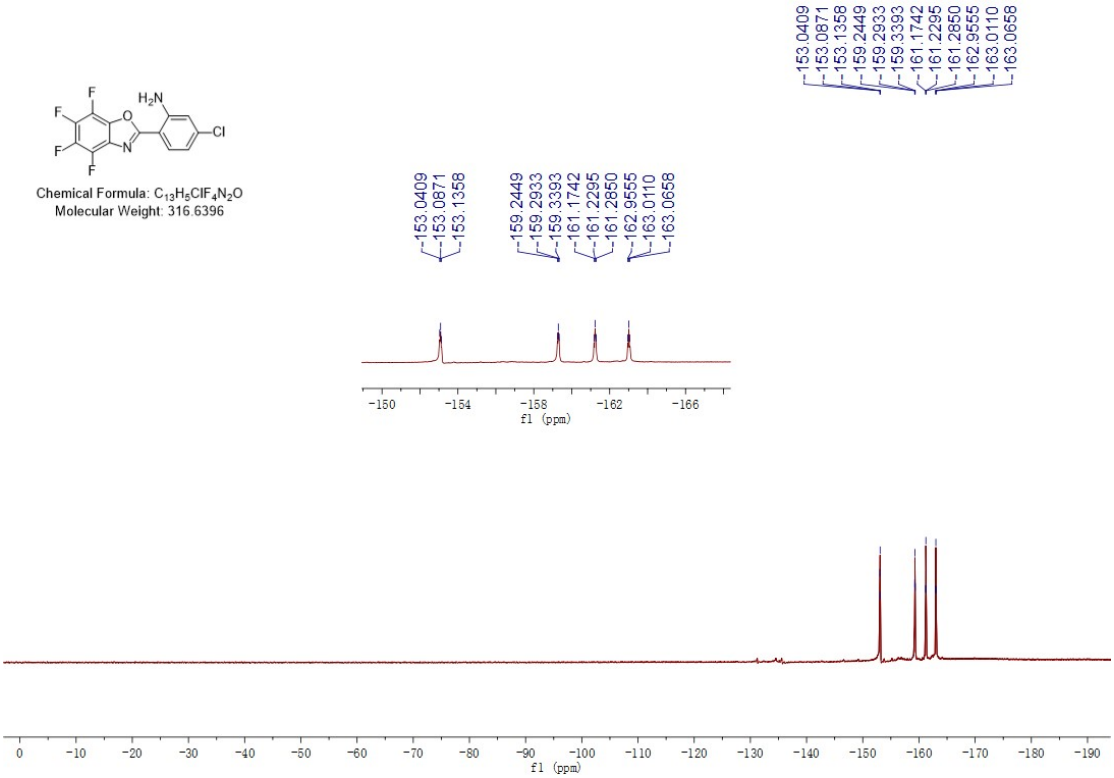
^{1}H NMR (400 MHz, DMSO)



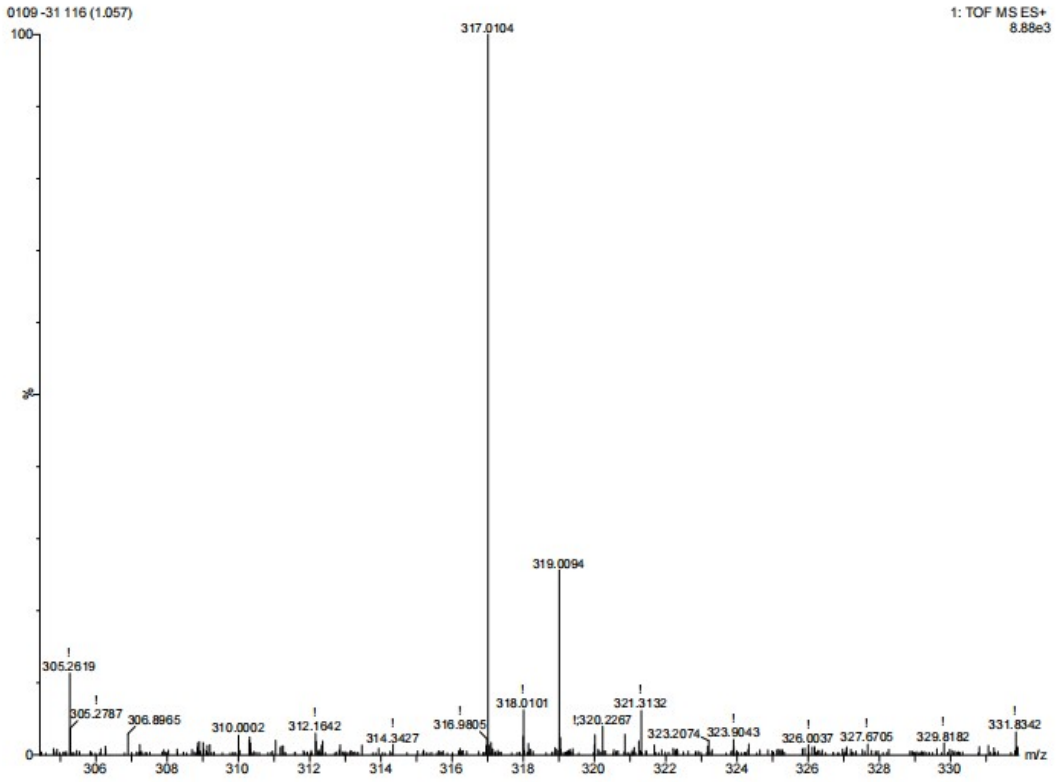
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

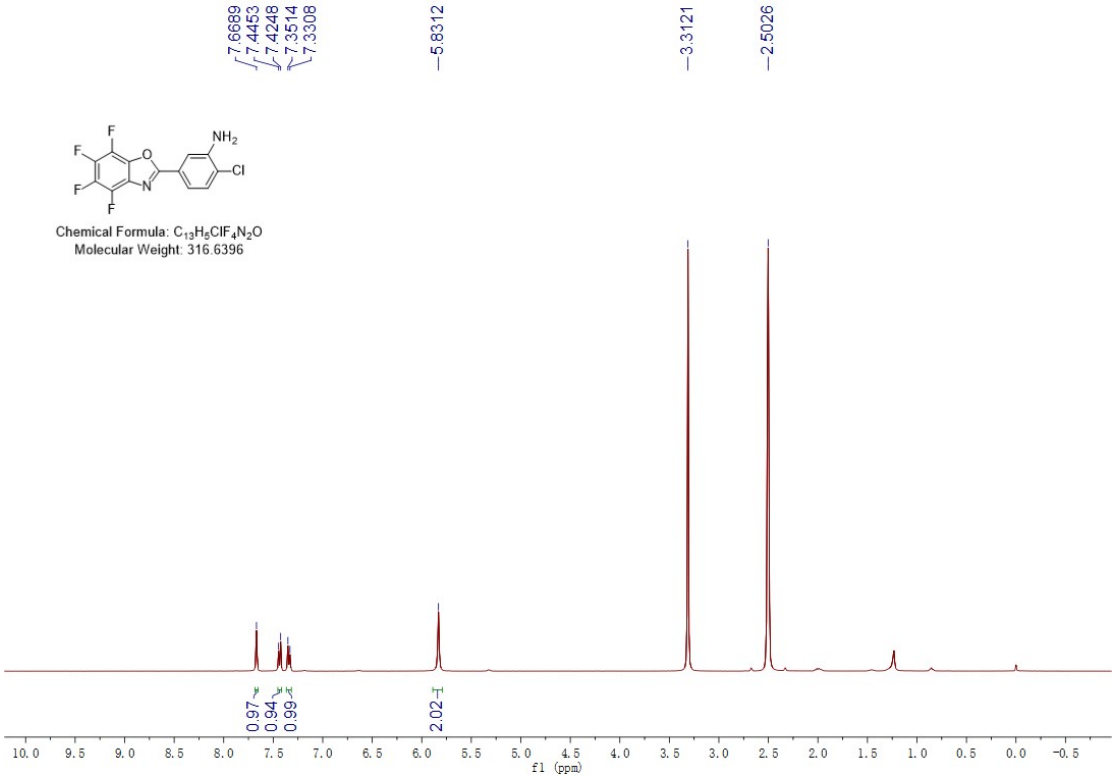


HRMS spectra

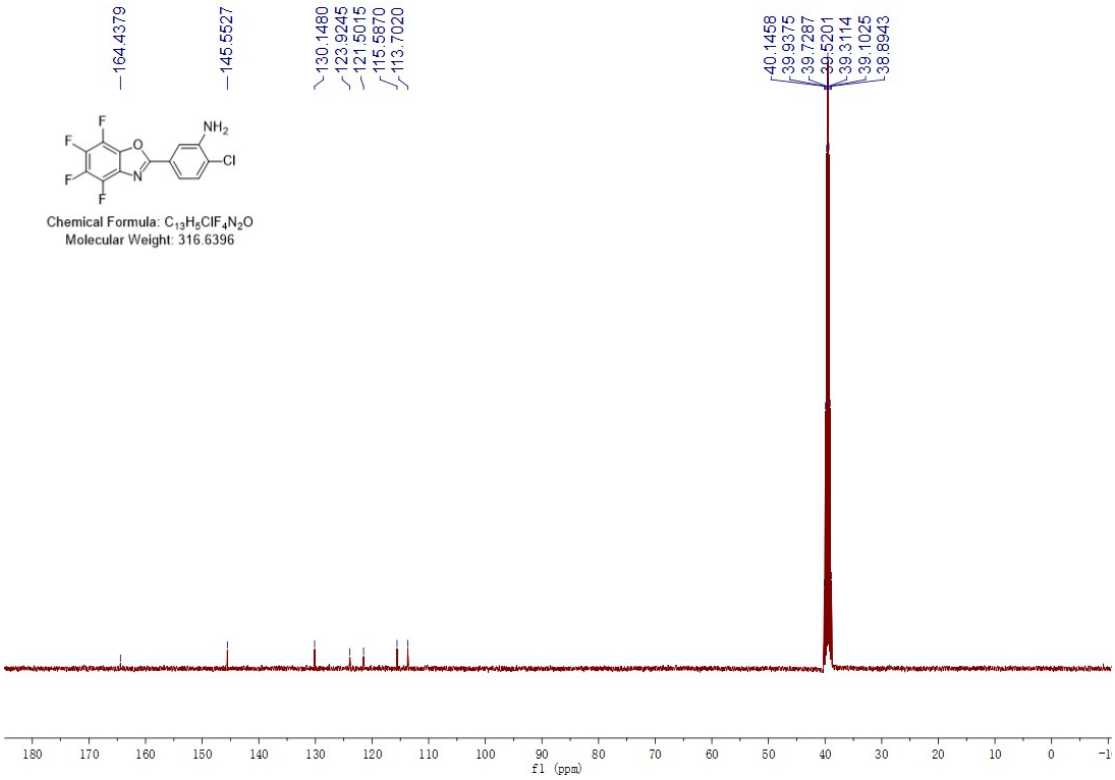


2-chloro-5-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**3q**)

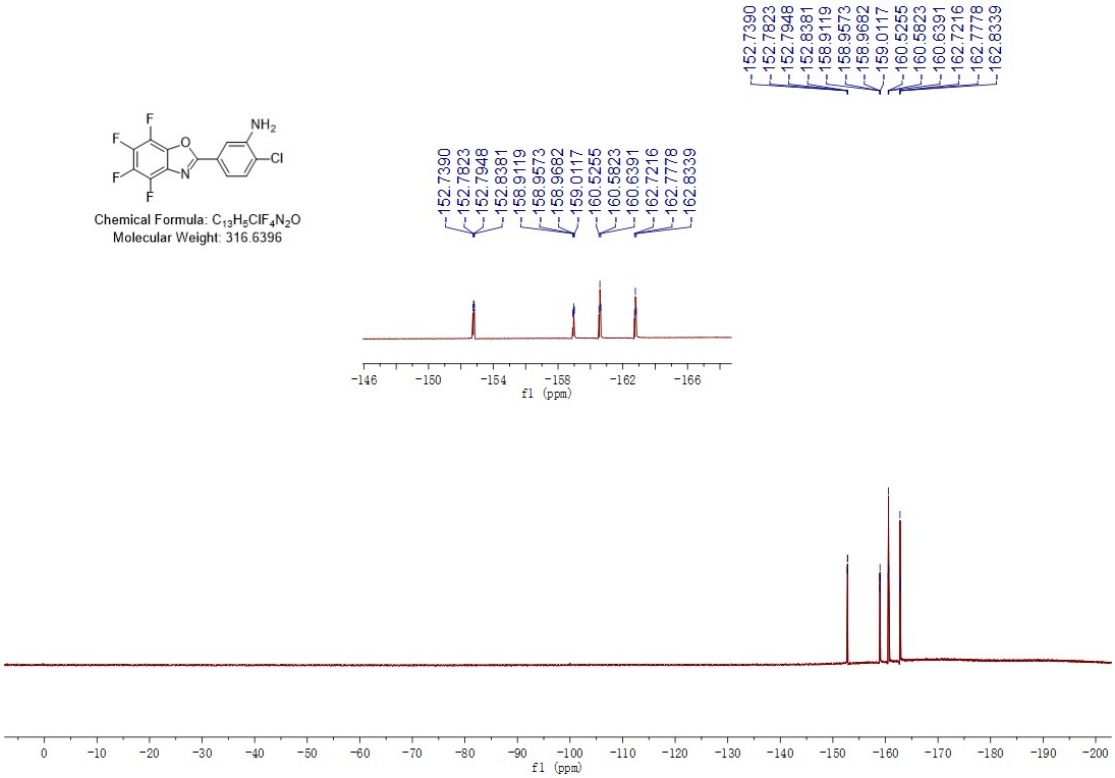
^{1}H NMR (400 MHz, DMSO)



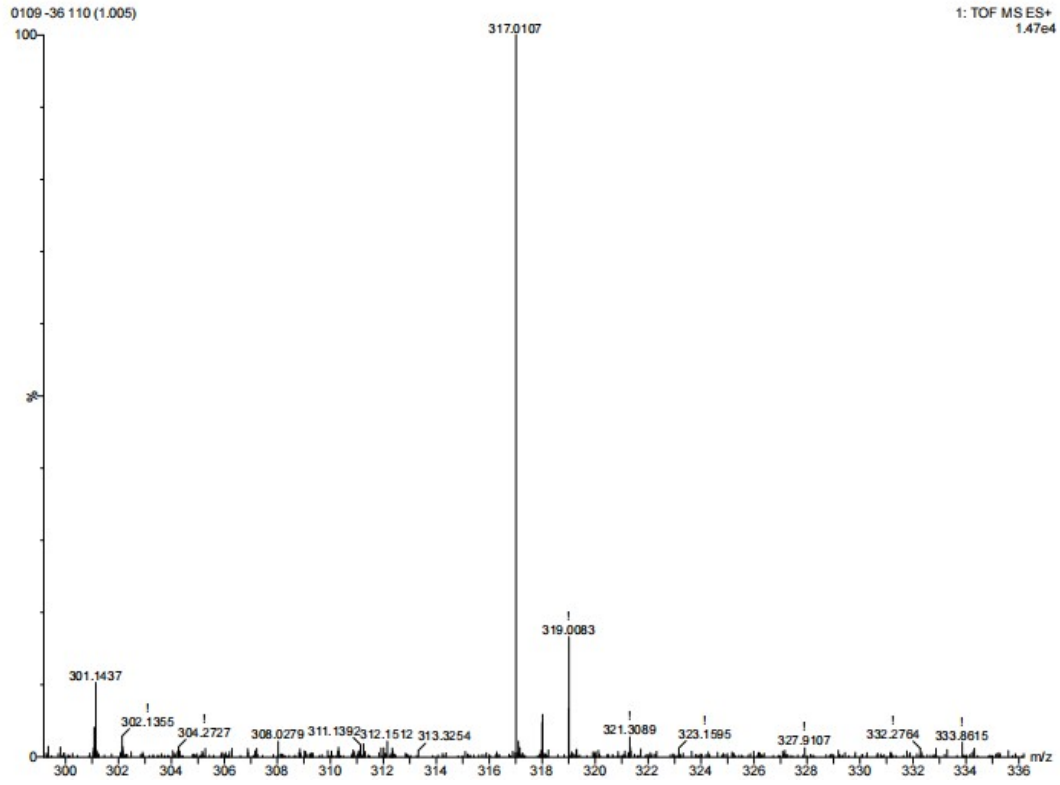
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

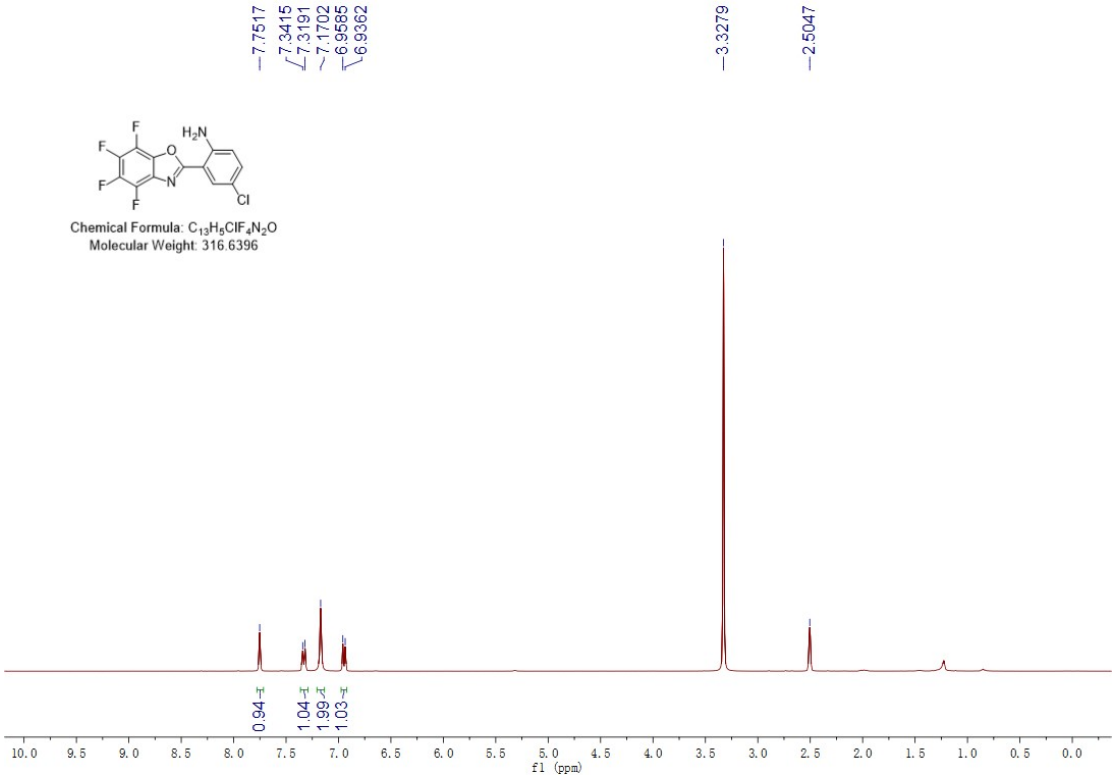


HRMS spectra

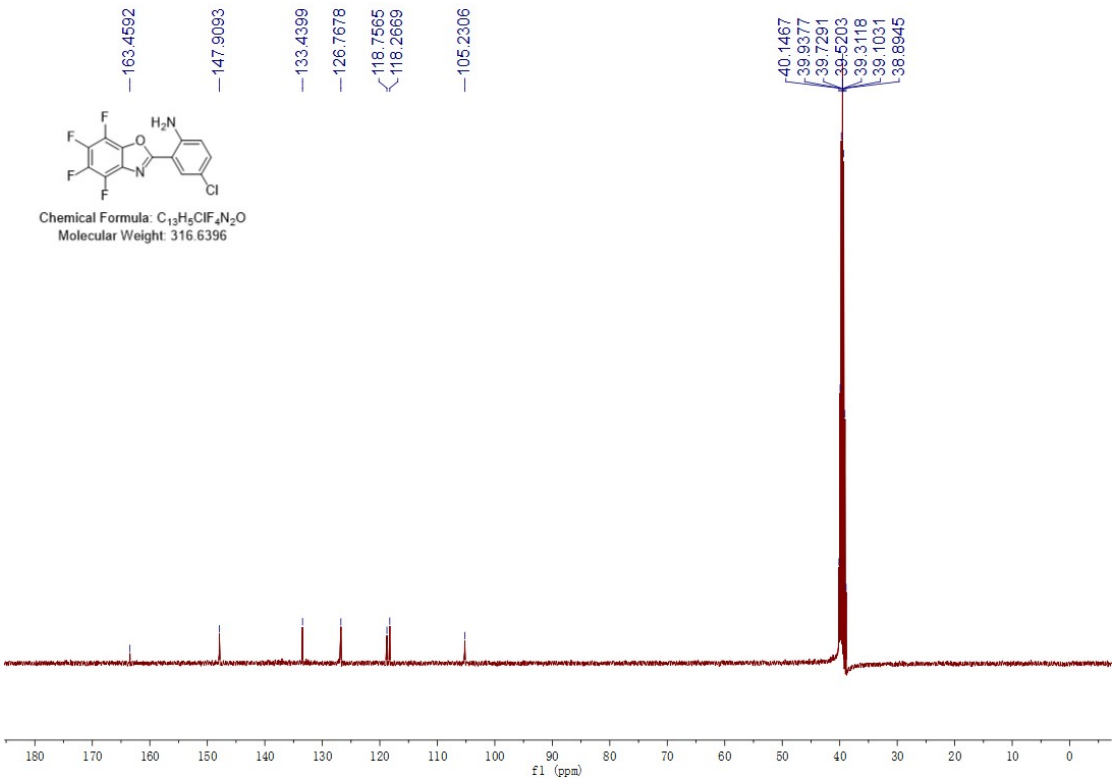


2-chloro-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**3r**)

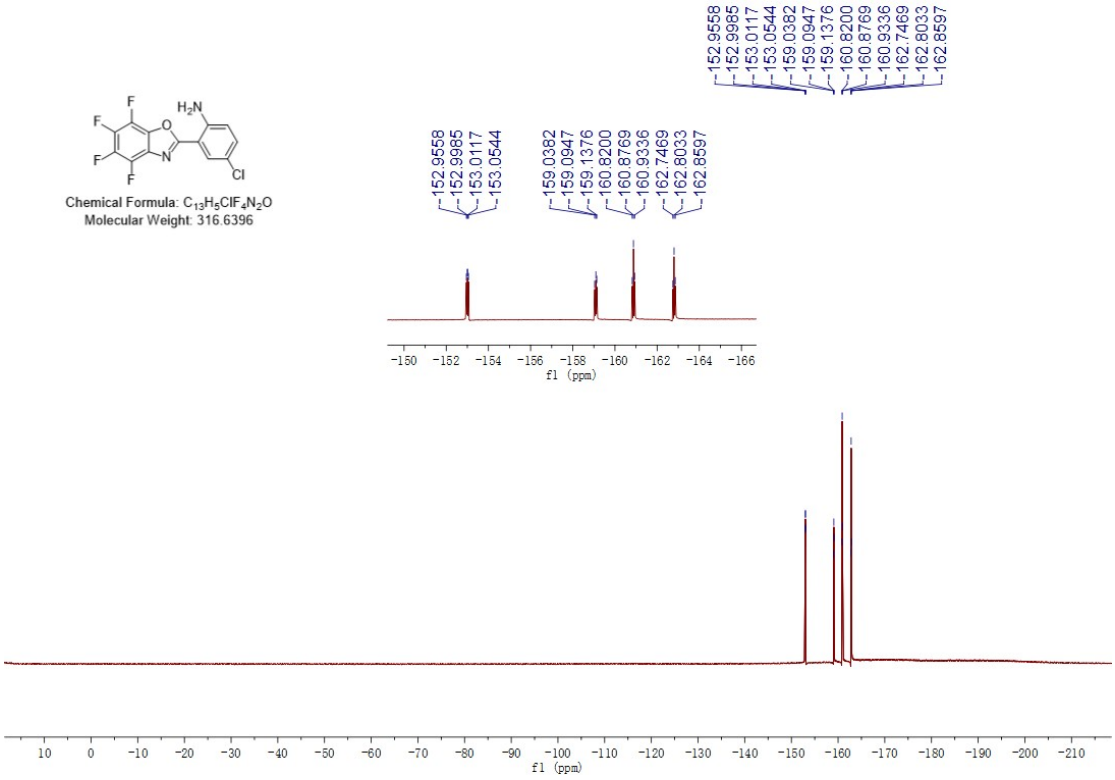
^{1}H NMR (400 MHz, DMSO)



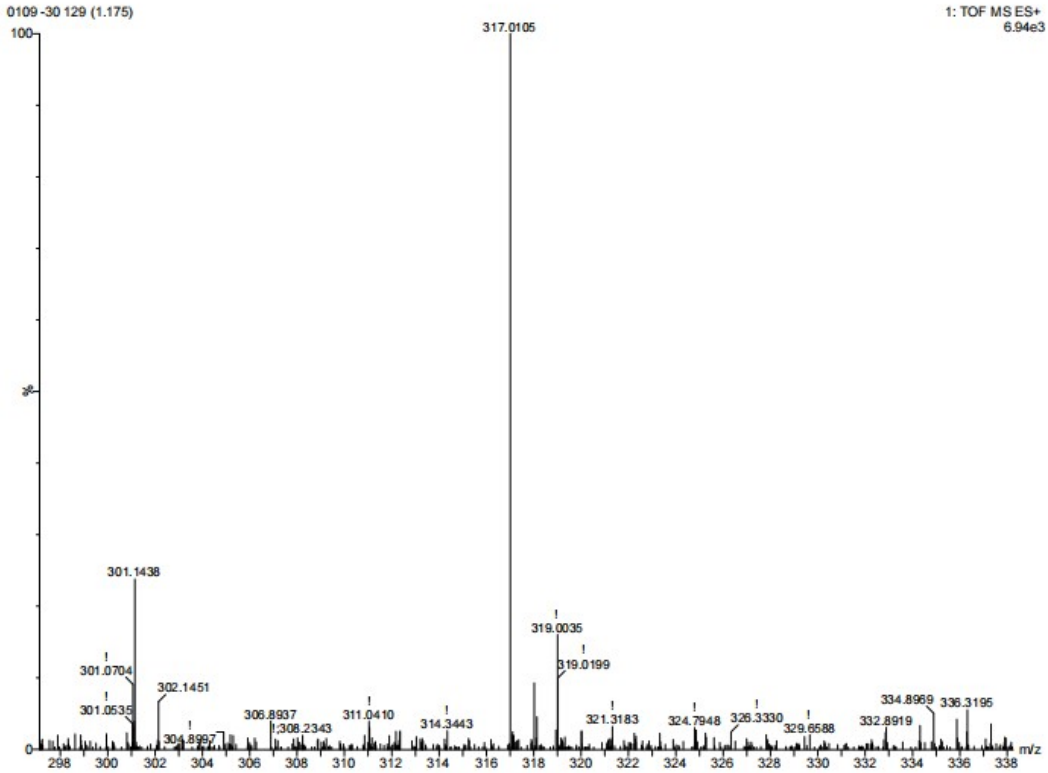
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

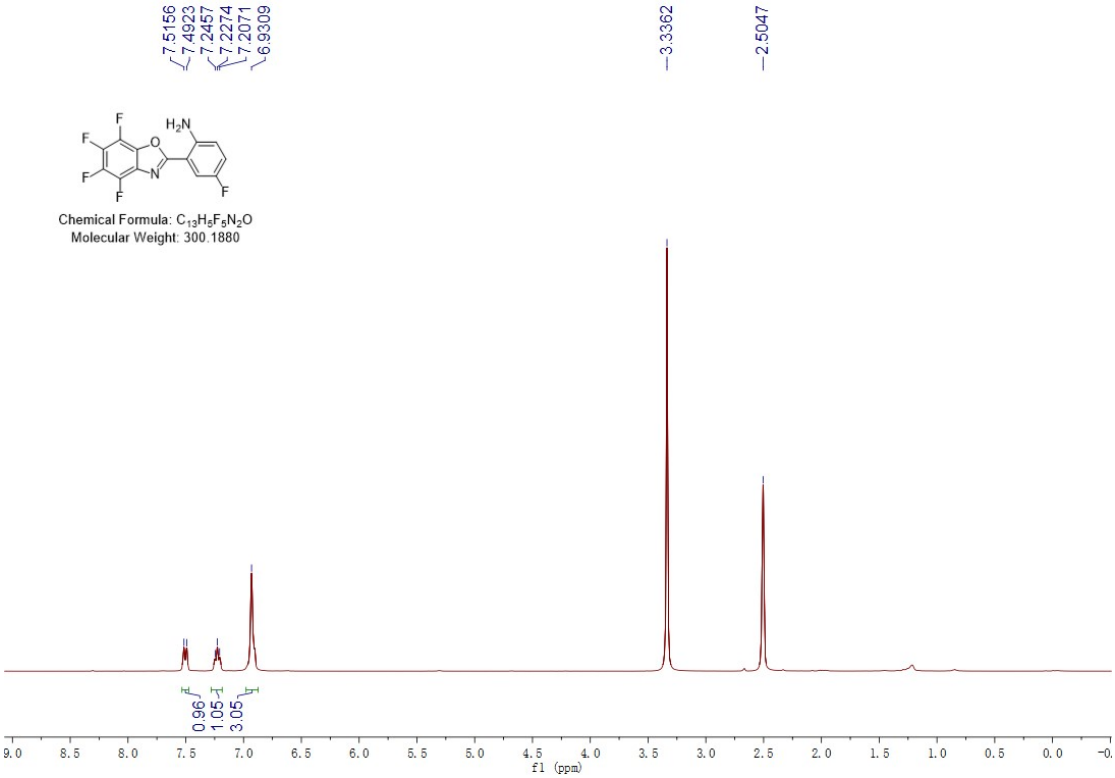


HRMS spectra

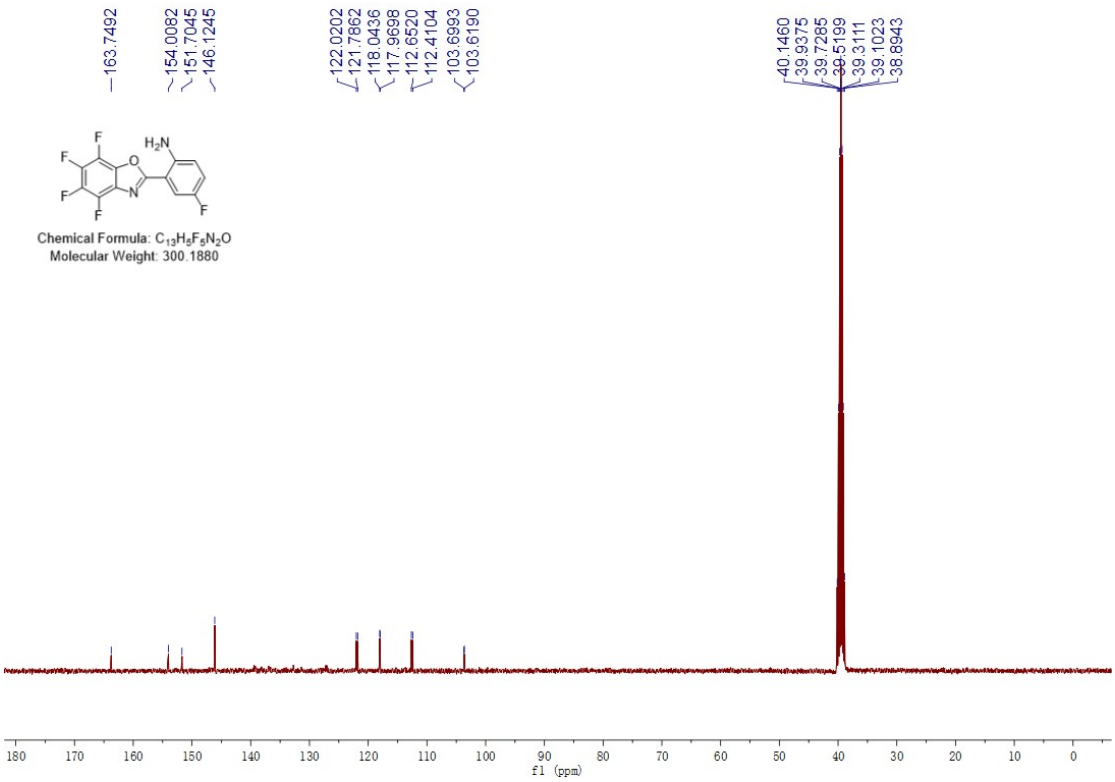


2-fluoro-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**3s**)

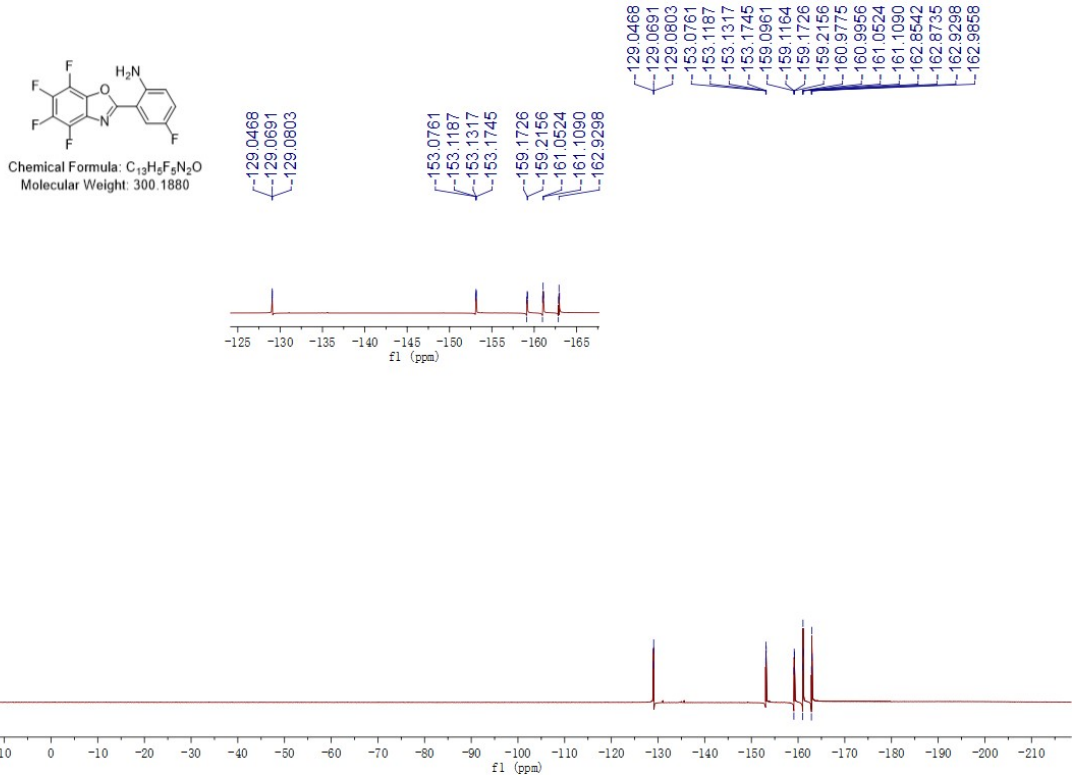
^{1}H NMR (400 MHz, DMSO)



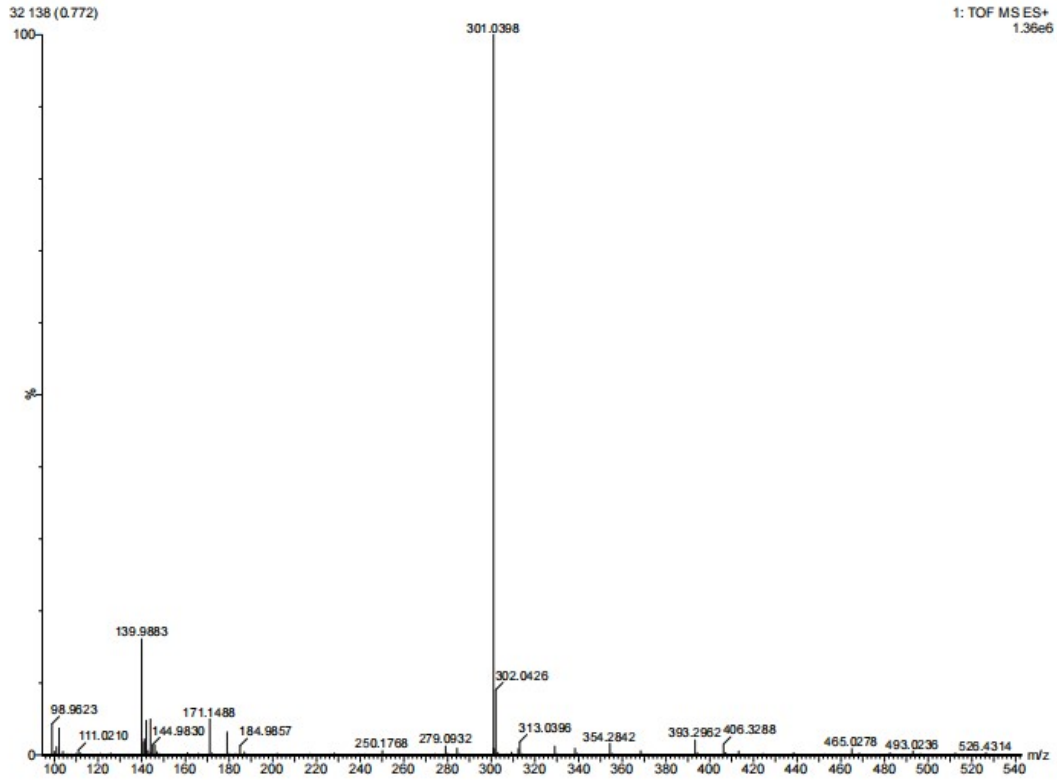
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

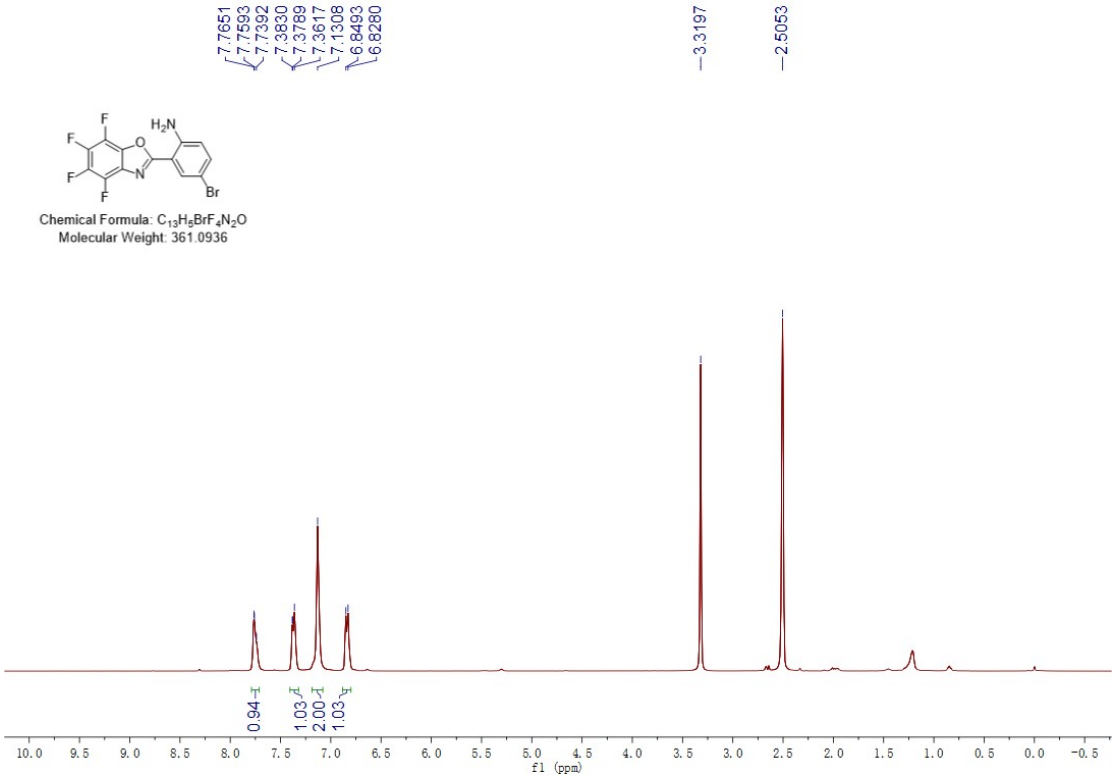


HRMS spectra

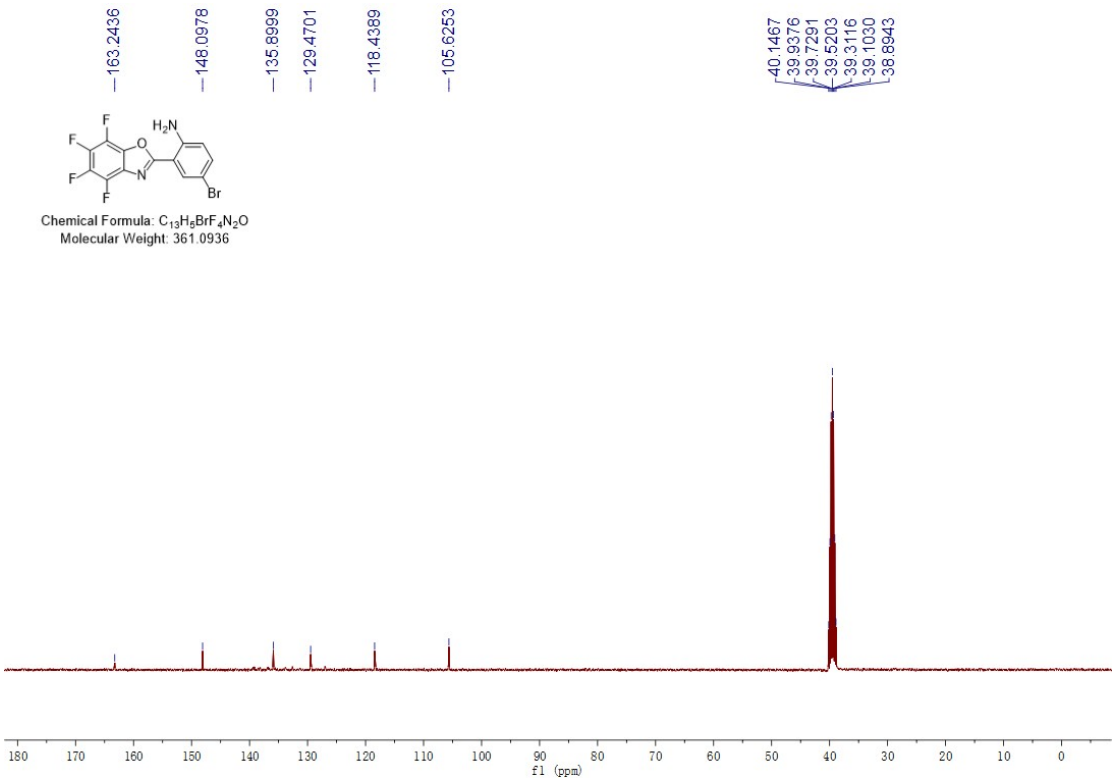


2-bromo-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**3t**)

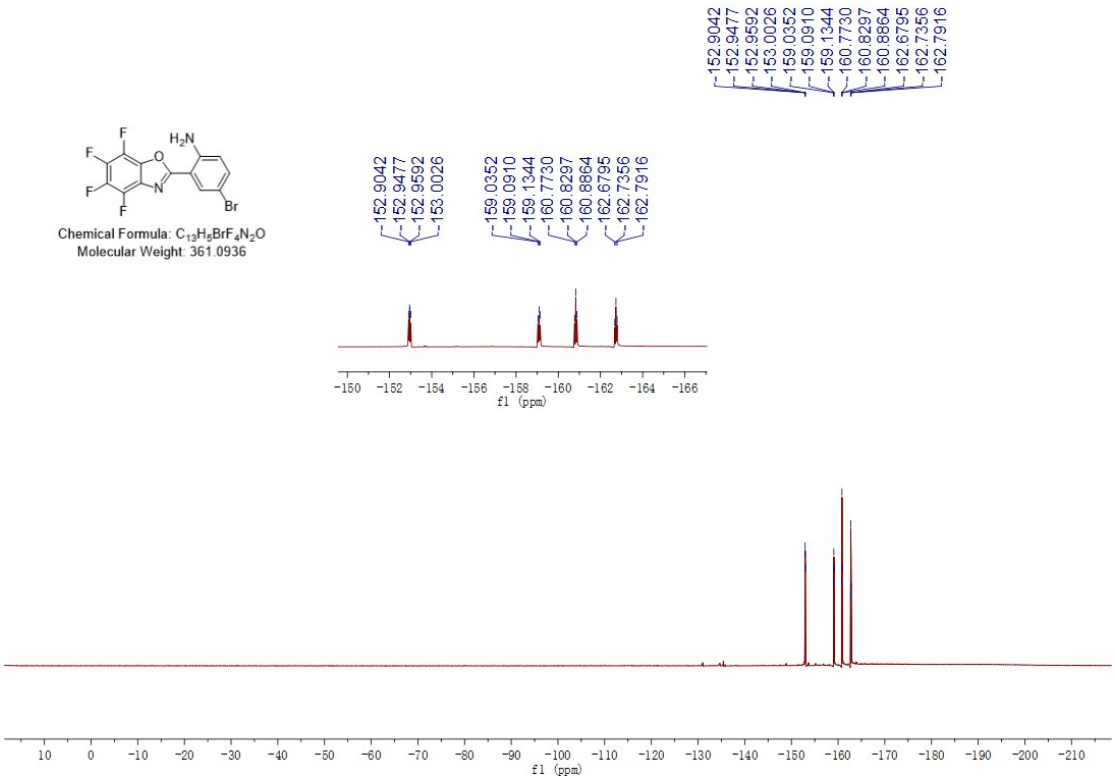
^{1}H NMR (400 MHz, DMSO)



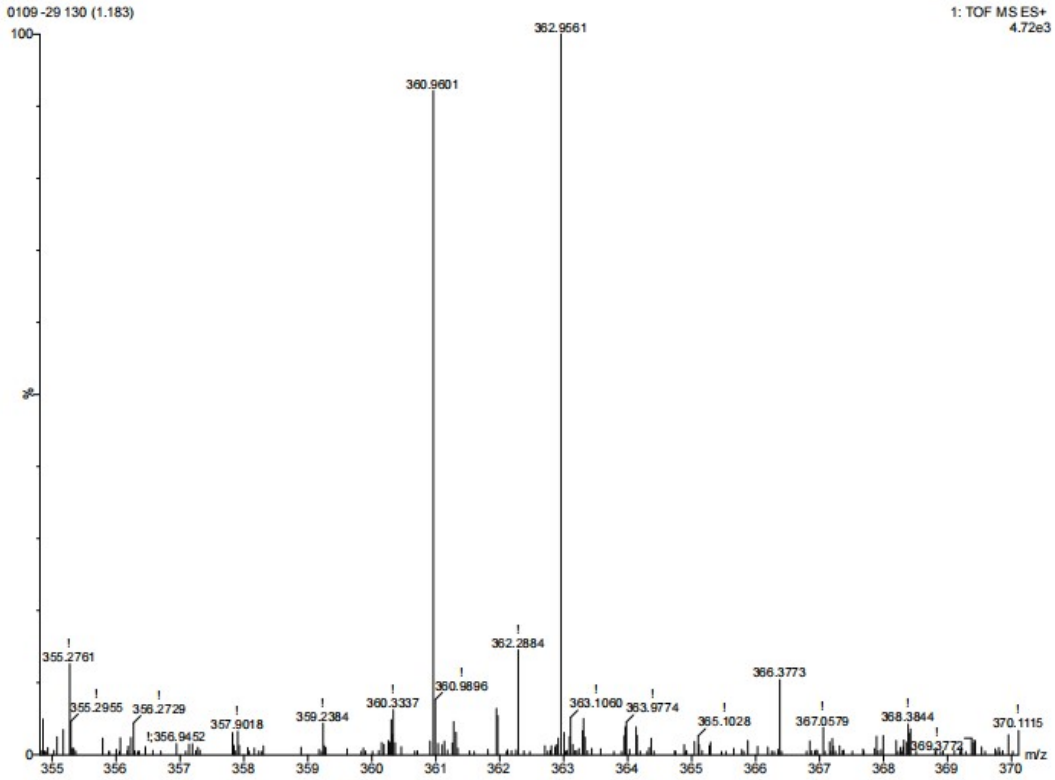
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

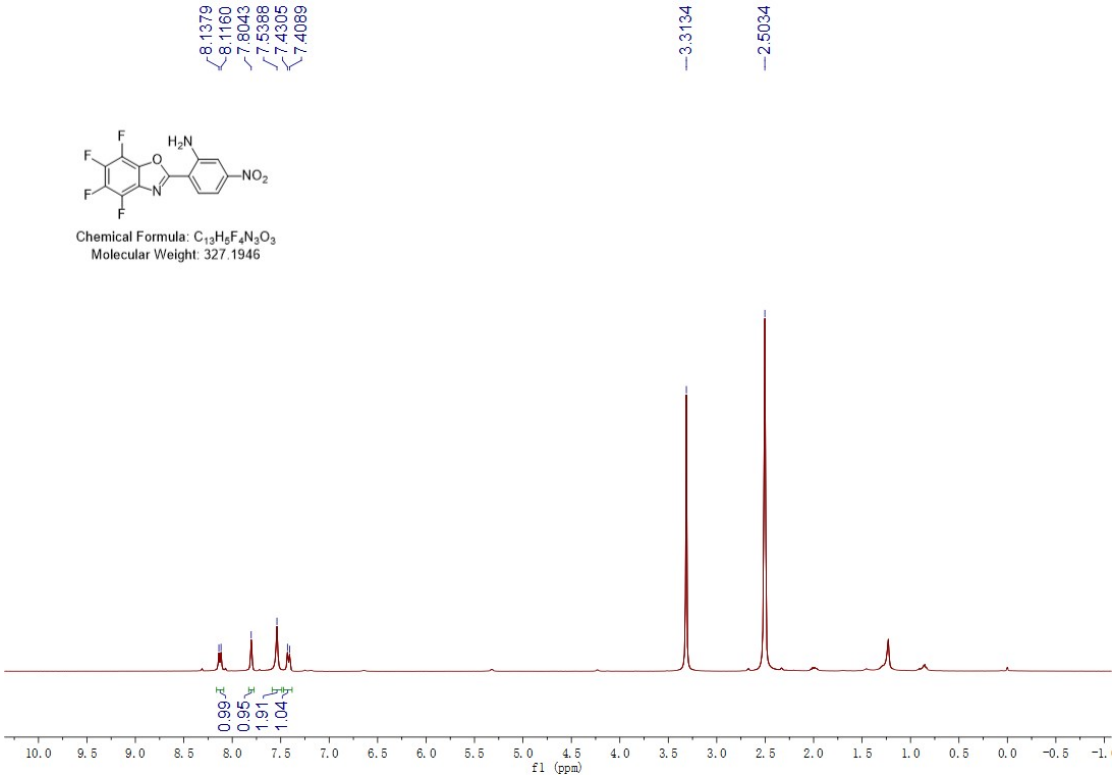


HRMS spectra

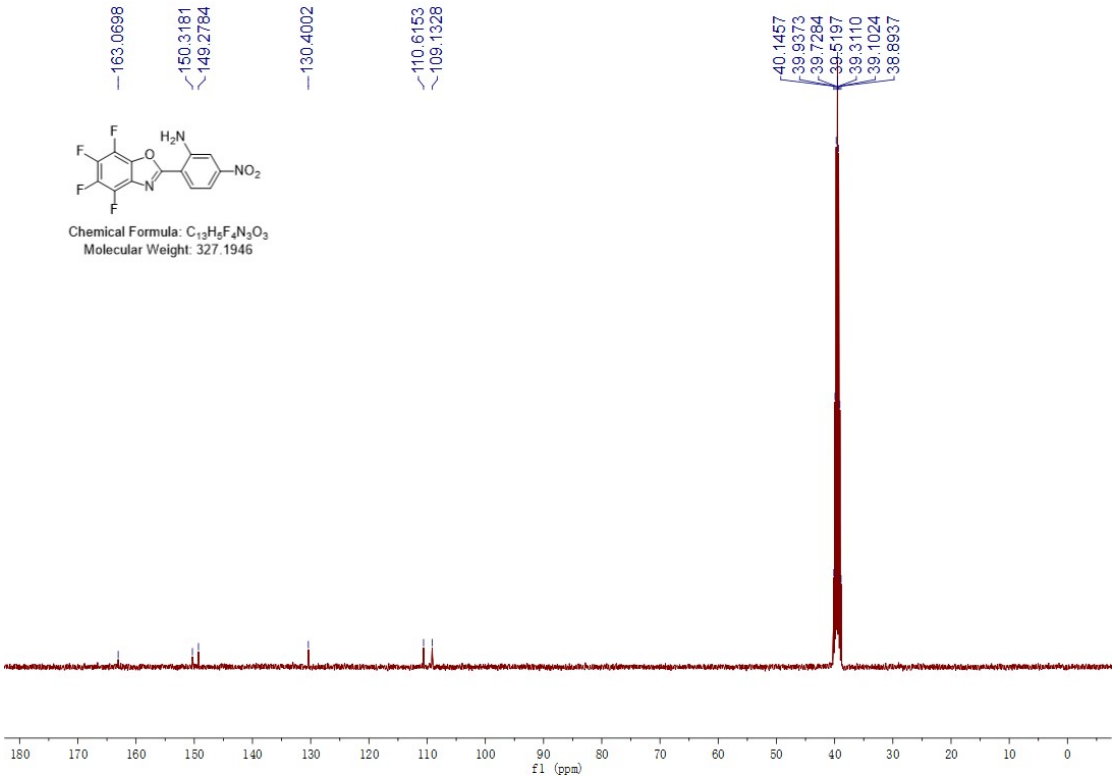


2-nitro-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**3u**)

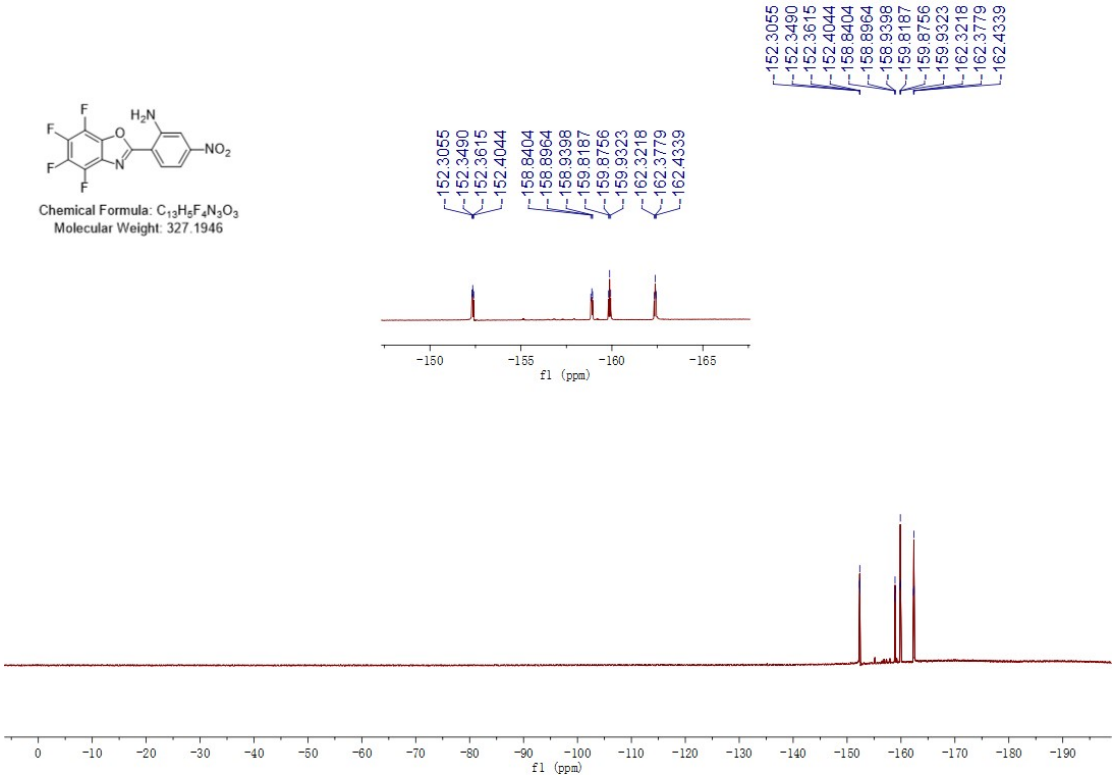
^{1}H NMR (400 MHz, DMSO)



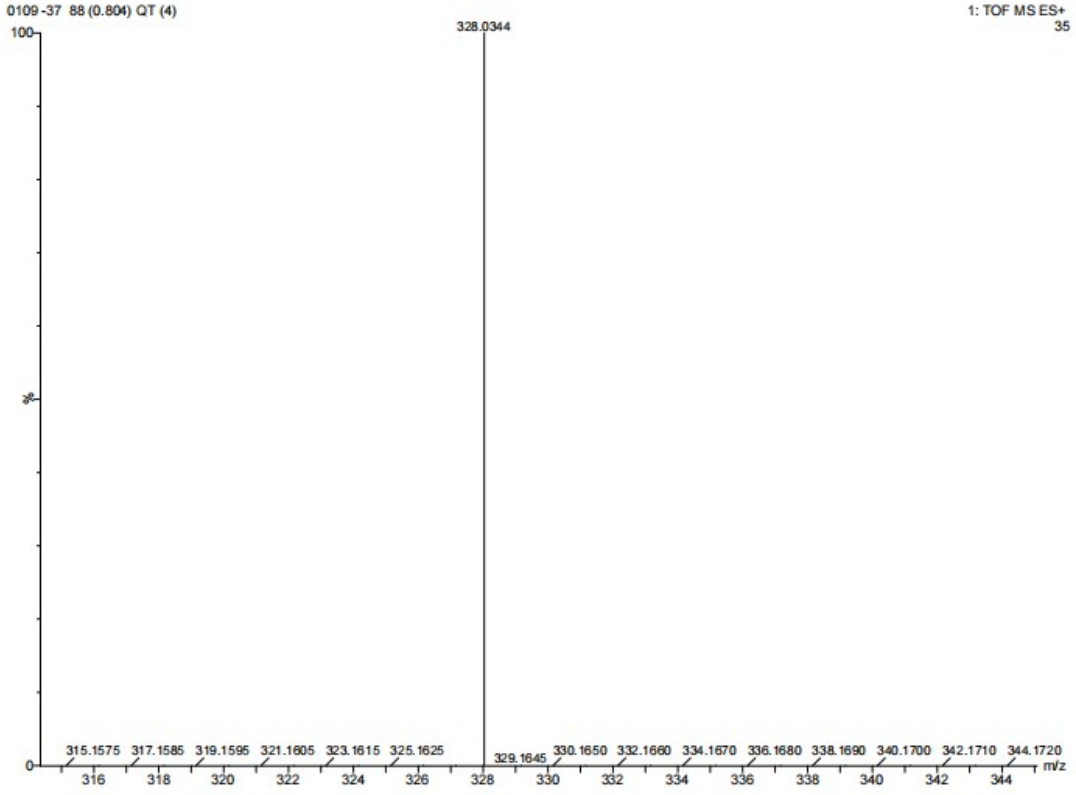
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

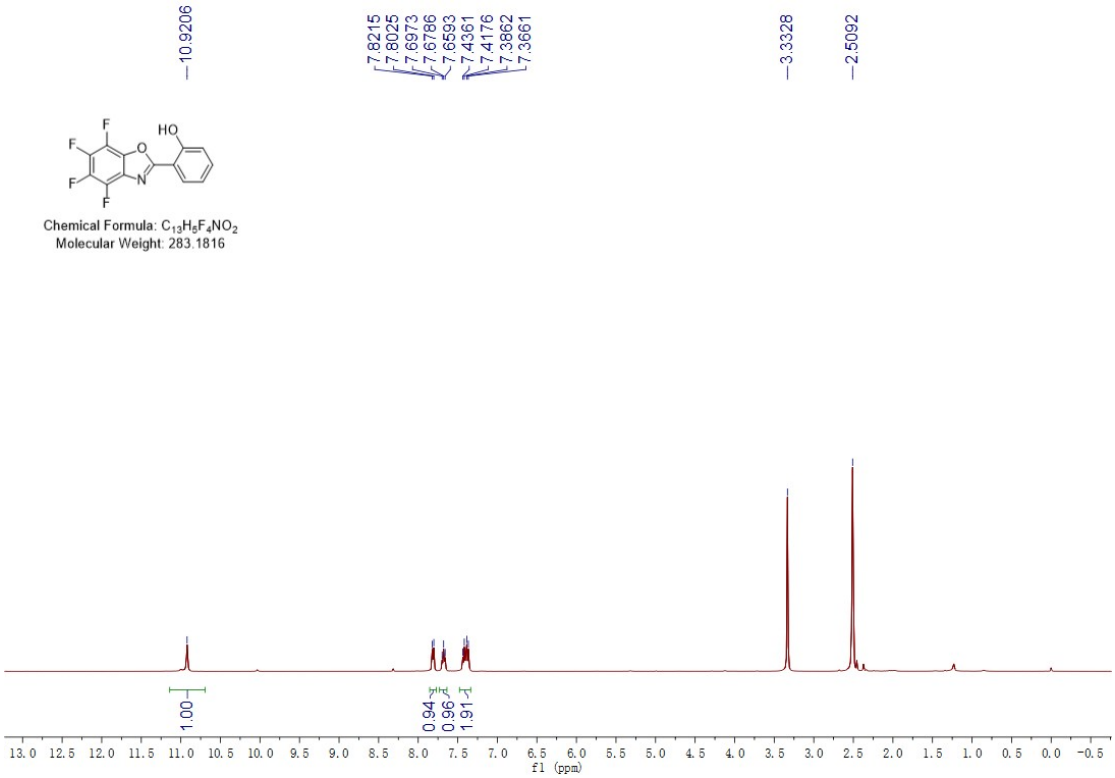


HRMS spectra

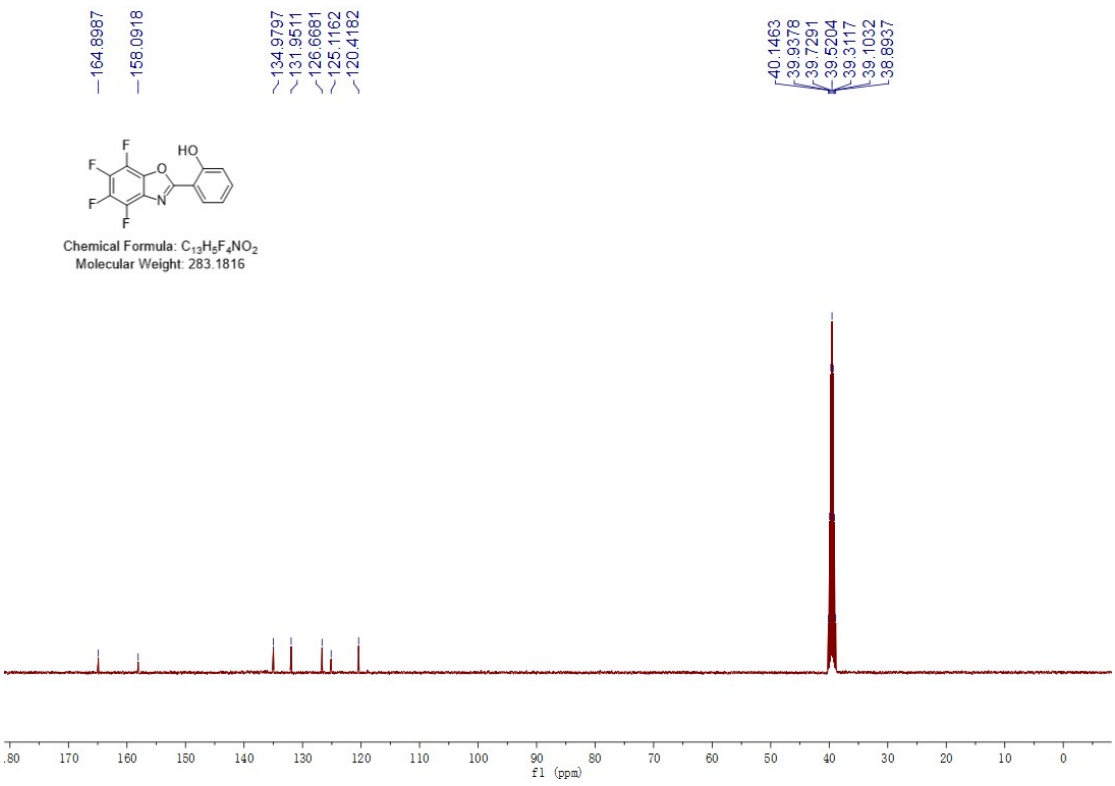


2-(perfluorobenzo[*d*]oxazol-2-yl)phenol (**3v**)

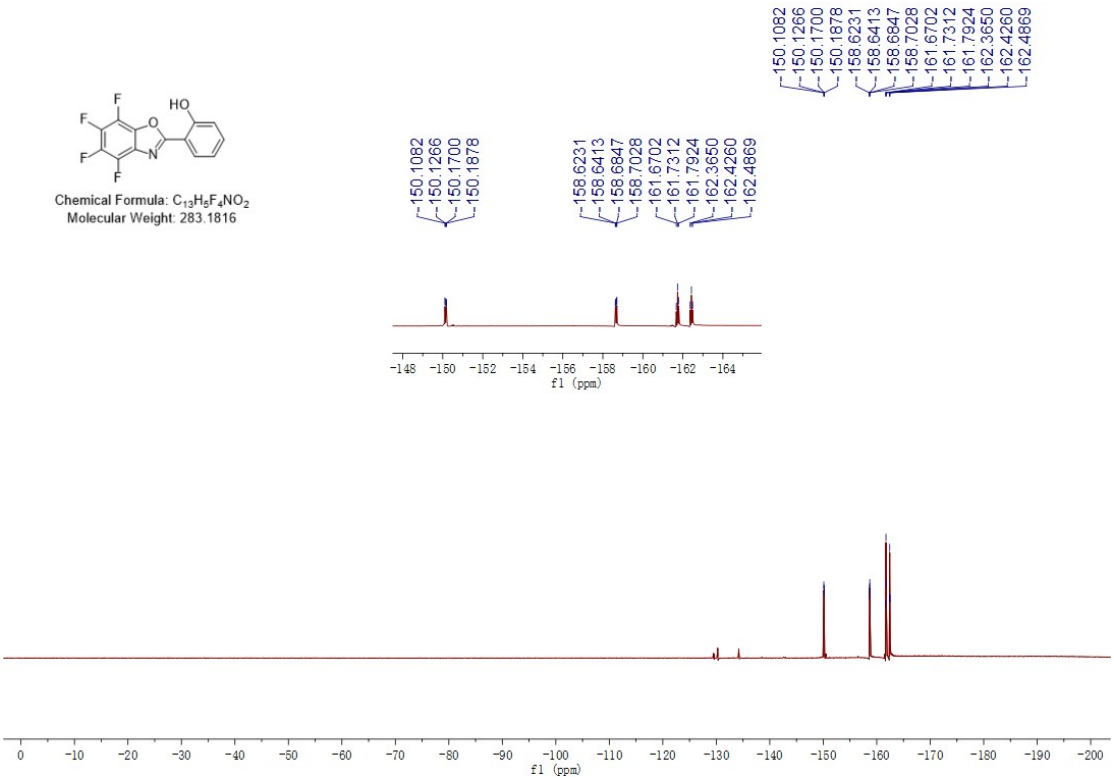
^{1}H NMR (400 MHz, DMSO)



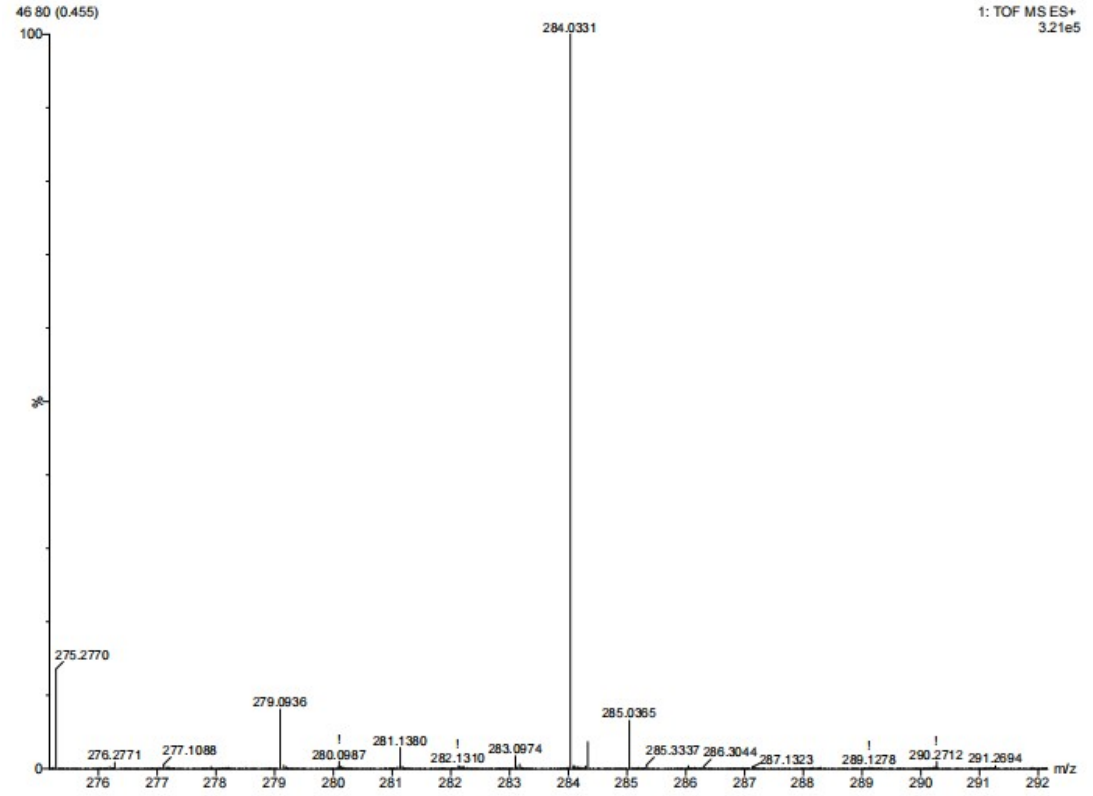
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

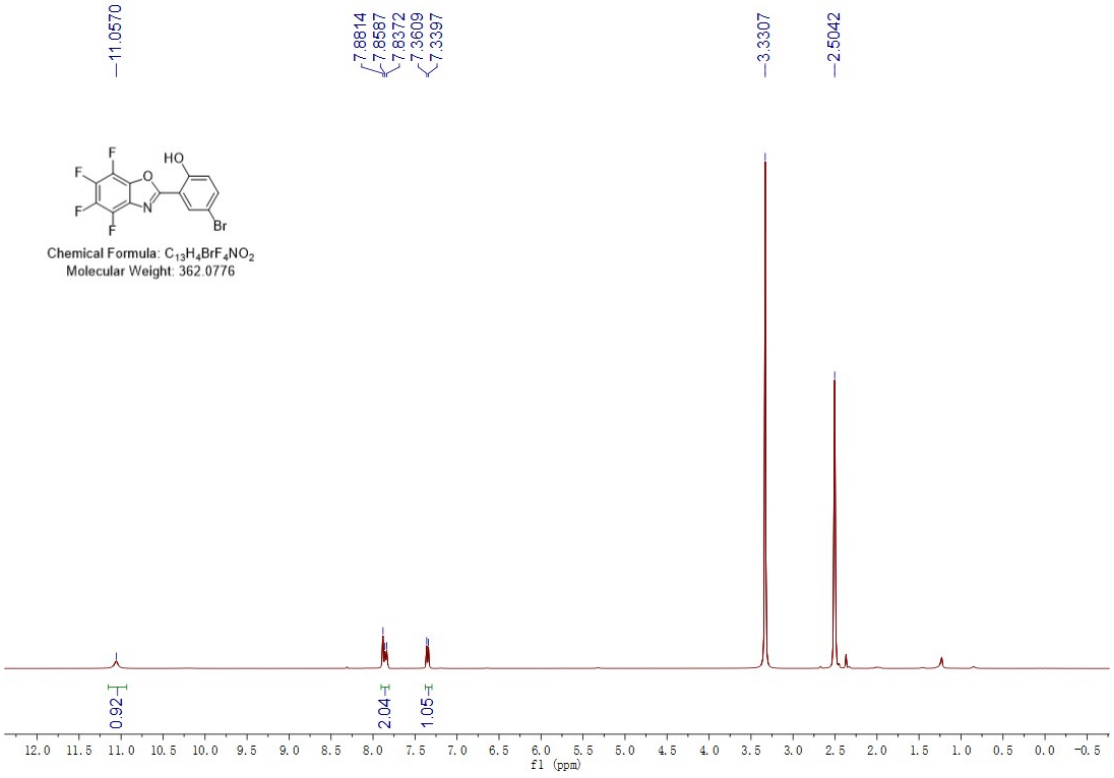


HRMS spectra

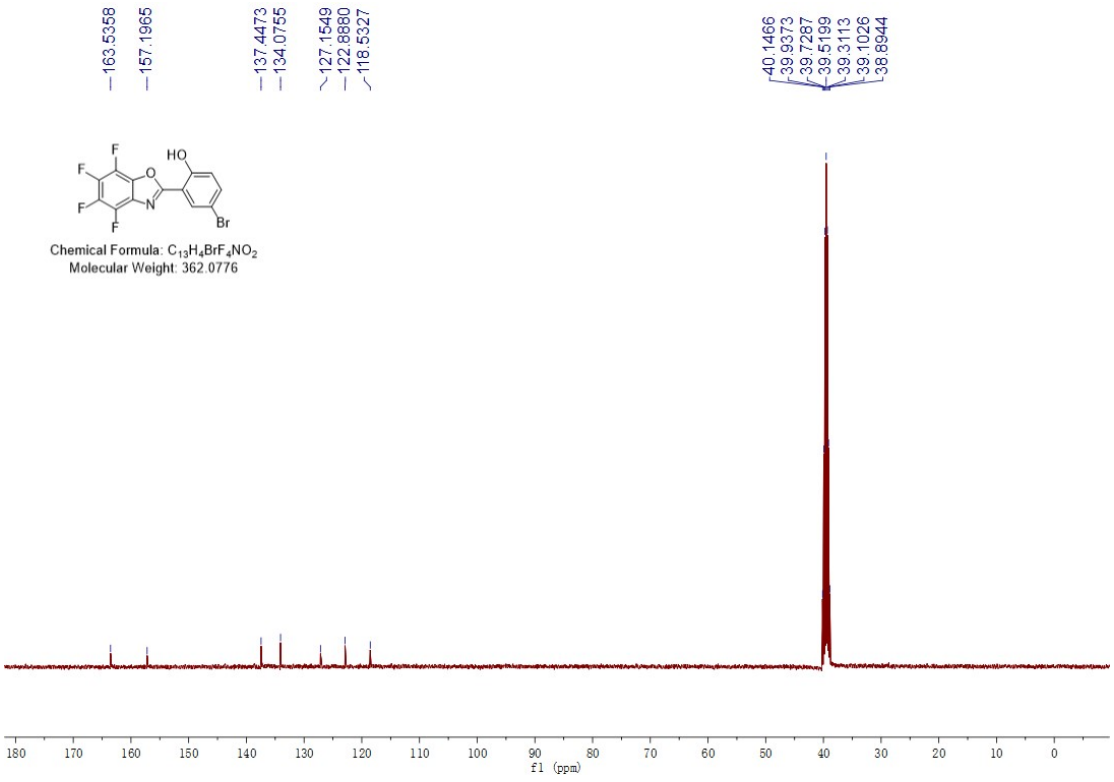


2-bromo-2-(perfluorobenzo[*d*]oxazol-2-yl)phenol (**3w**)

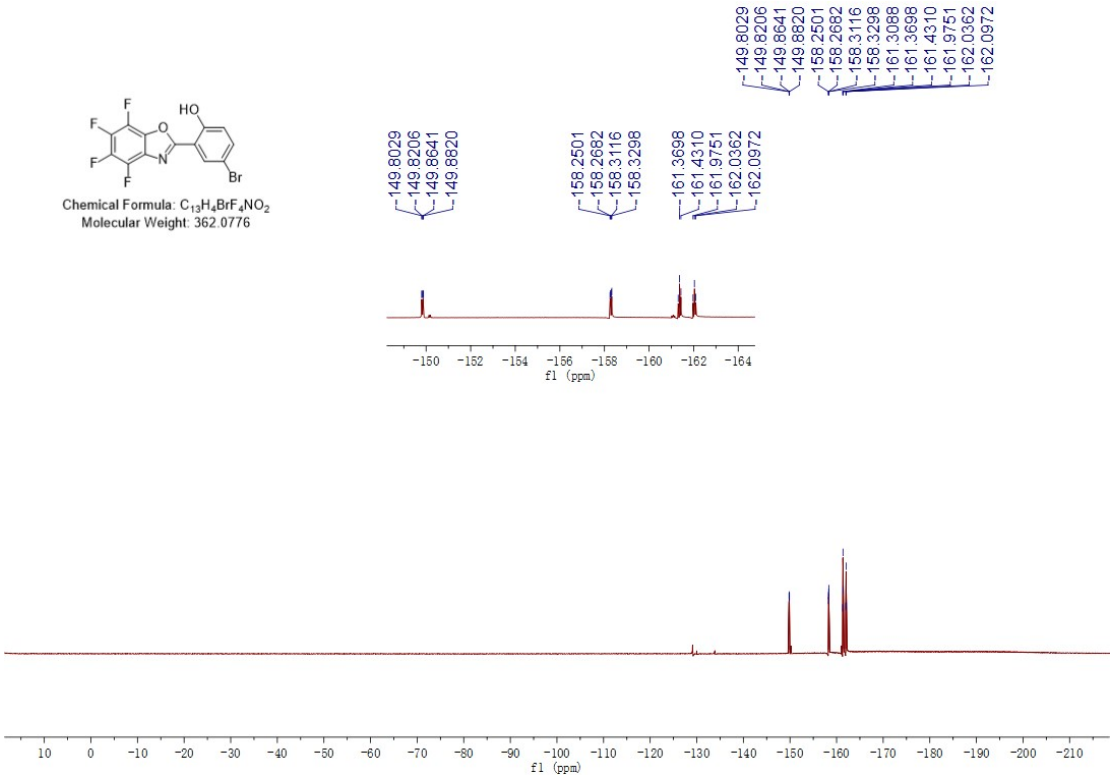
^{1}H NMR (400 MHz, DMSO)



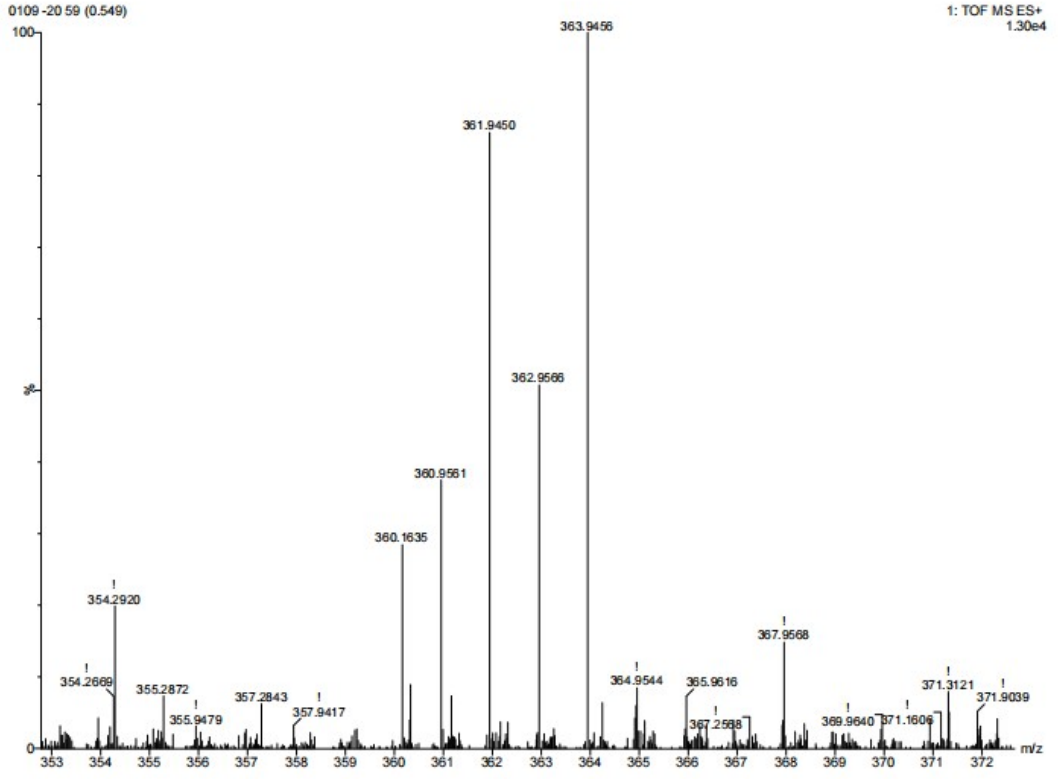
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

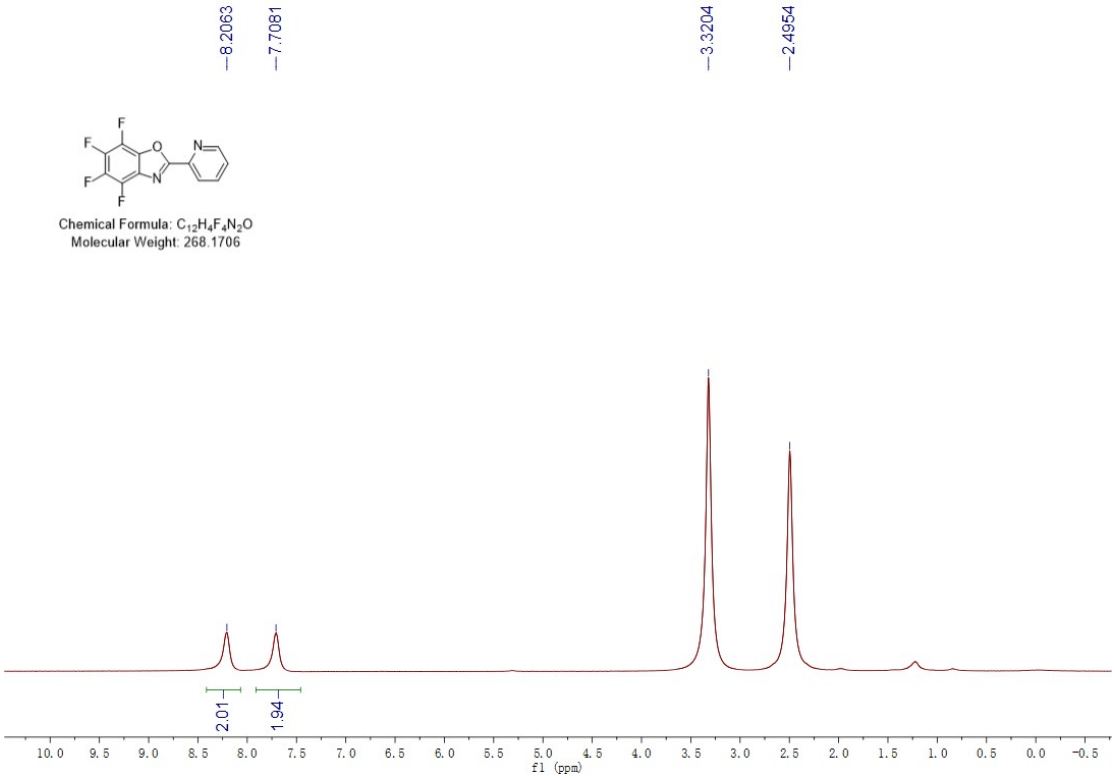


HRMS spectra

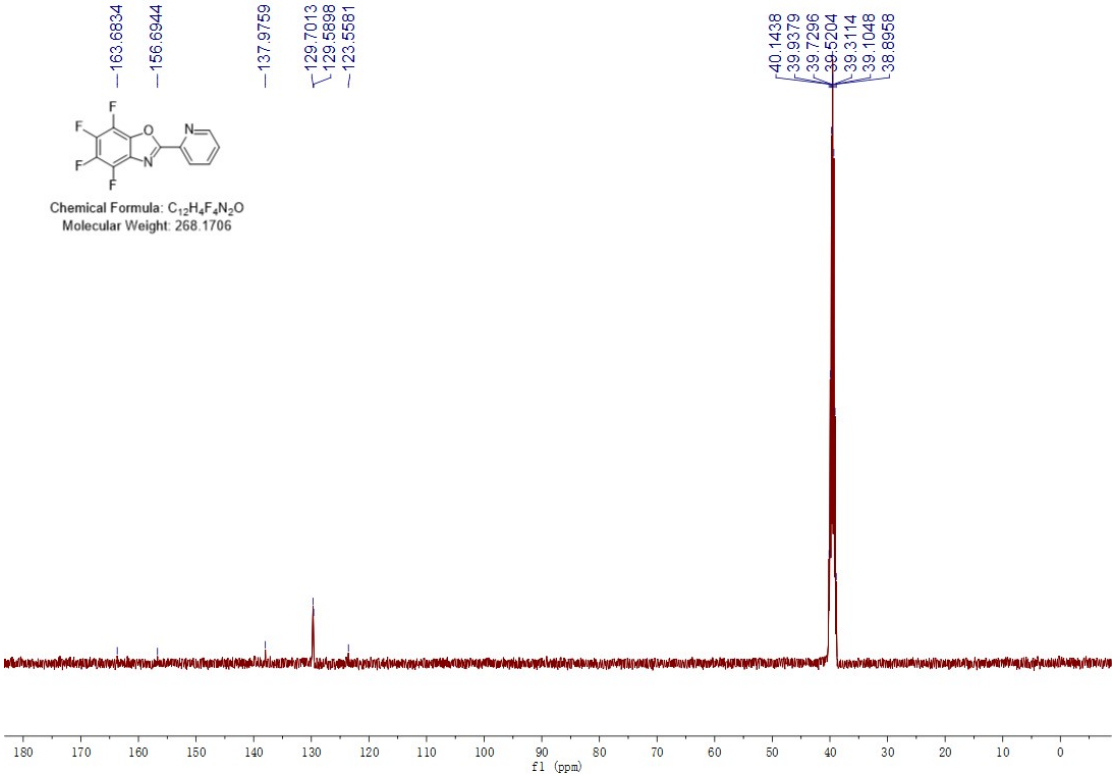


4,5,6,7-tetrafluoro-2-(pyridin-2-yl)benzo[*d*]oxazole (**3x**)

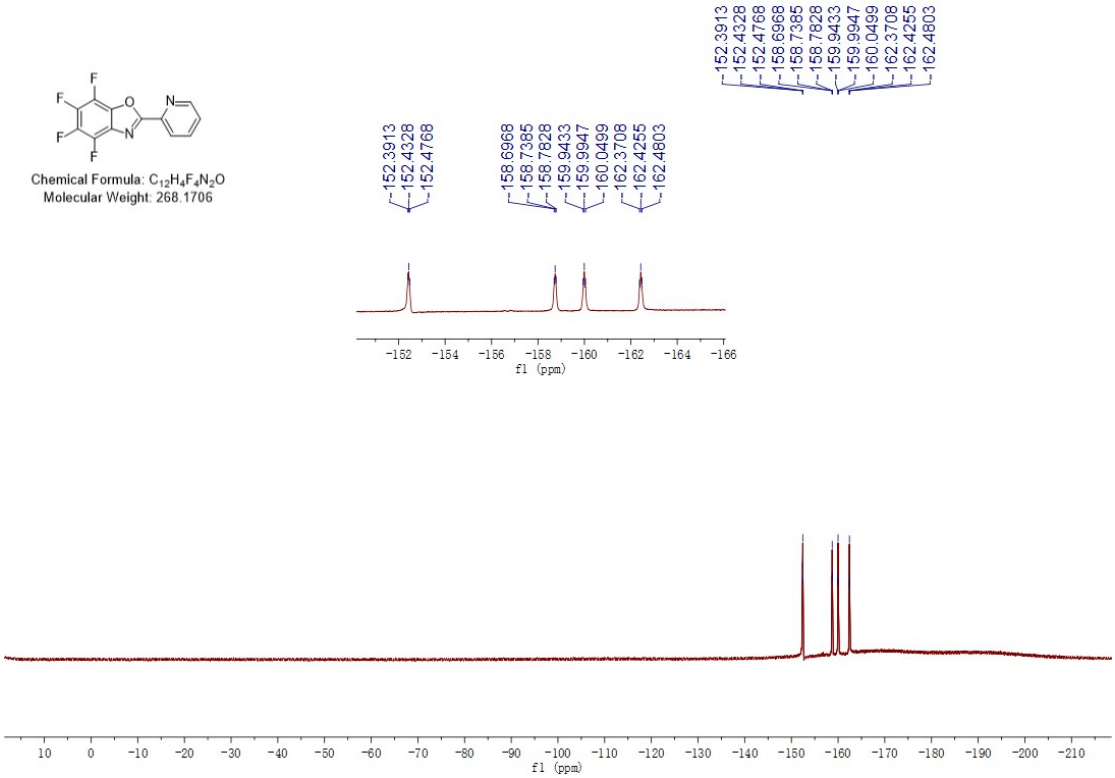
^{1}H NMR (400 MHz, DMSO)



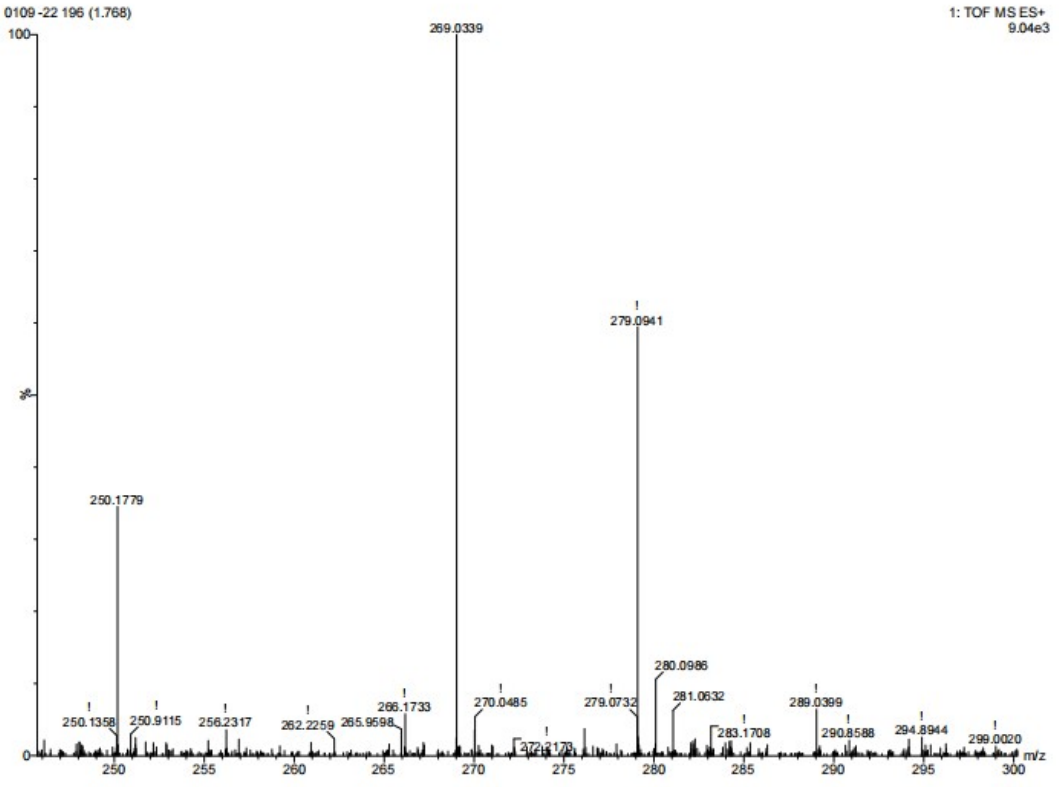
^{13}C NMR (101 MHz, DMSO)



^{19}F NMR (376 MHz, DMSO)

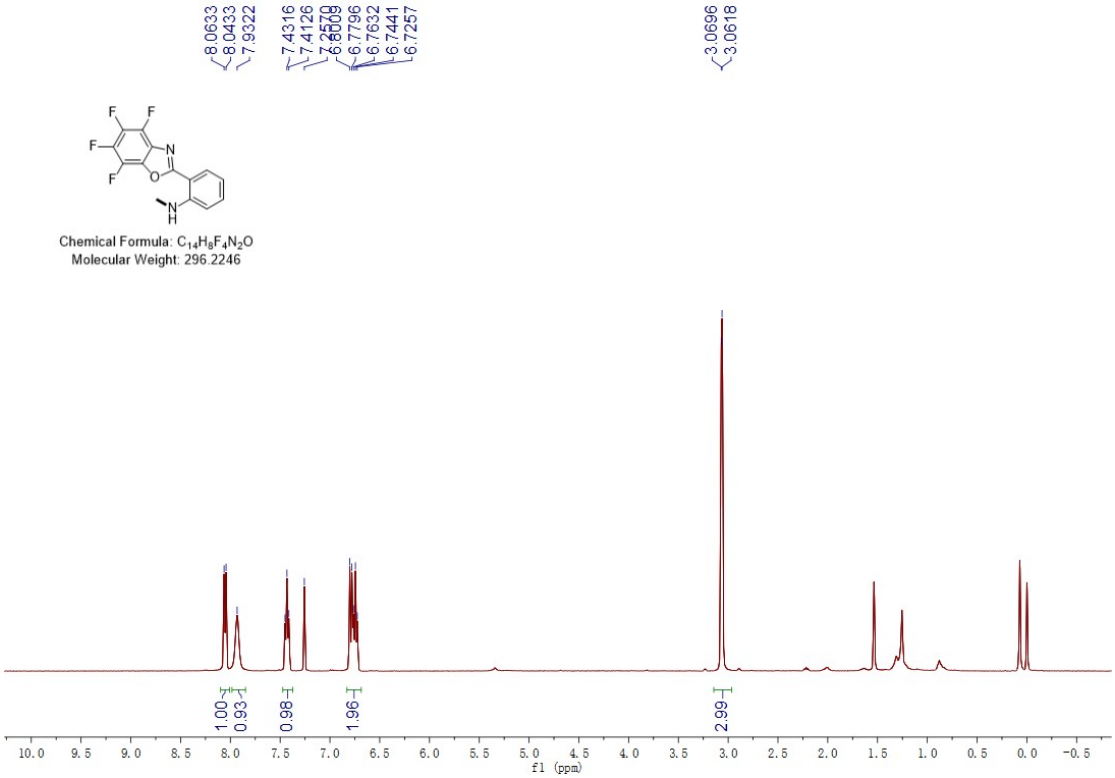


HRMS spectra

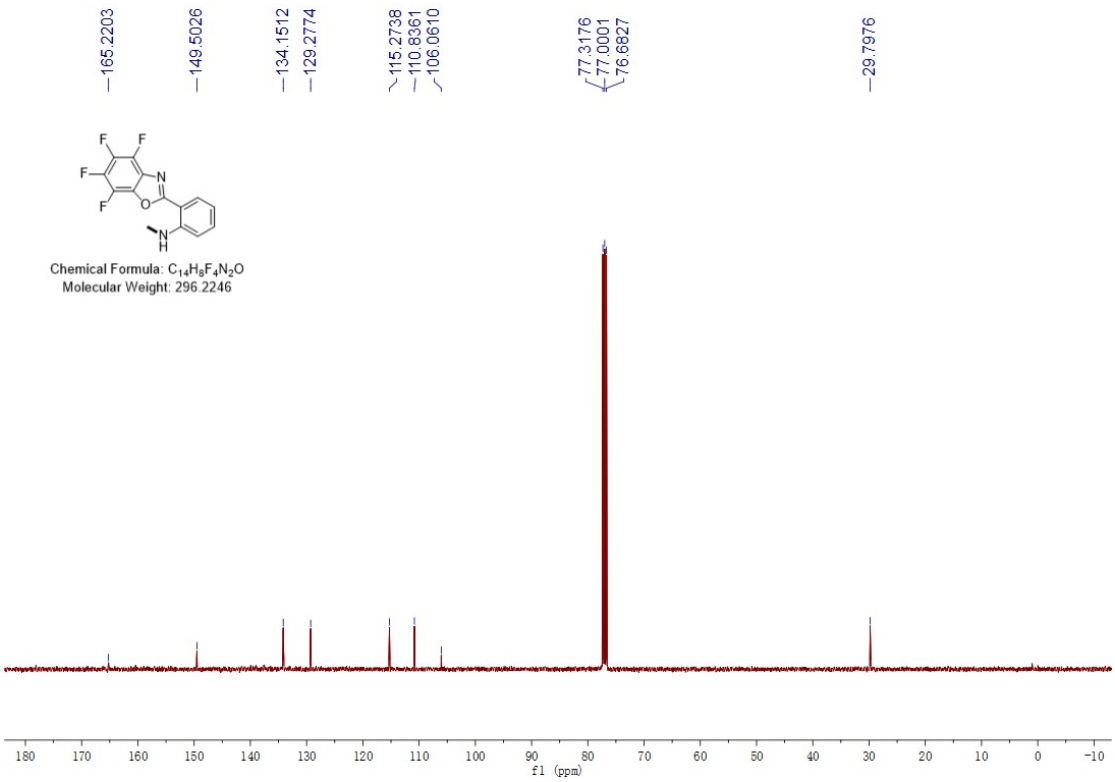


N-methyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4a**)

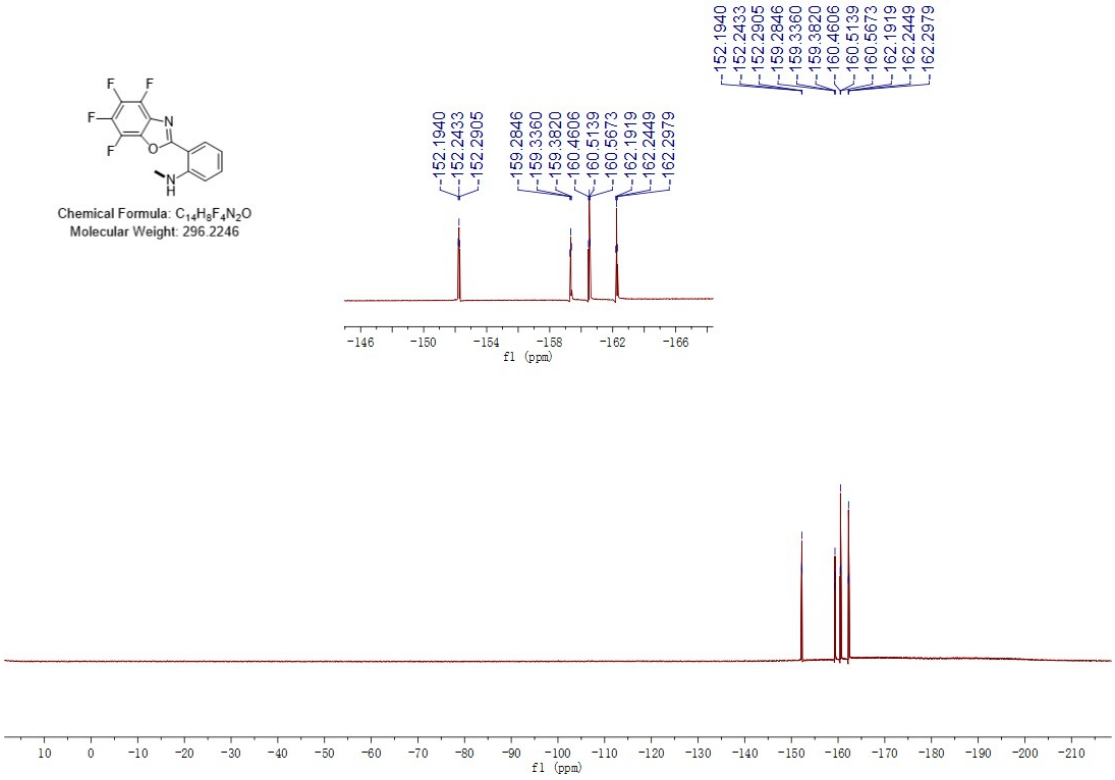
^{1}H NMR(400 MHz, $CDCl_3$)



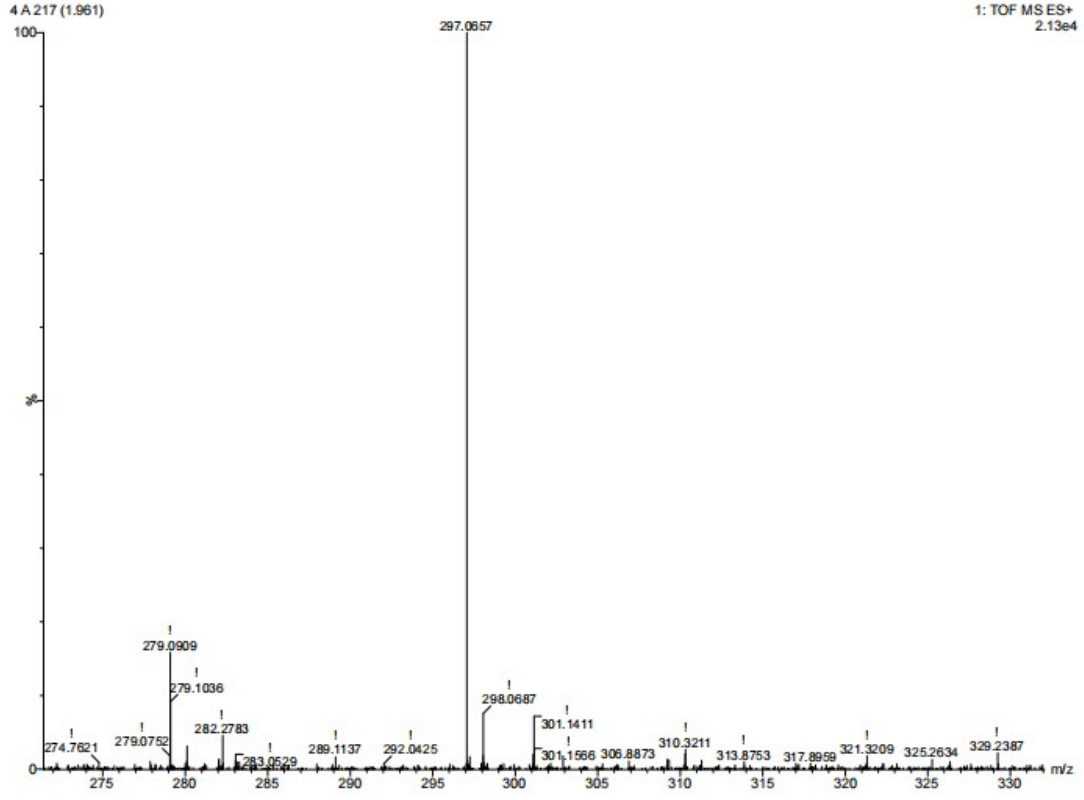
^{13}C NMR (101 MHz, $CDCl_3$)



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

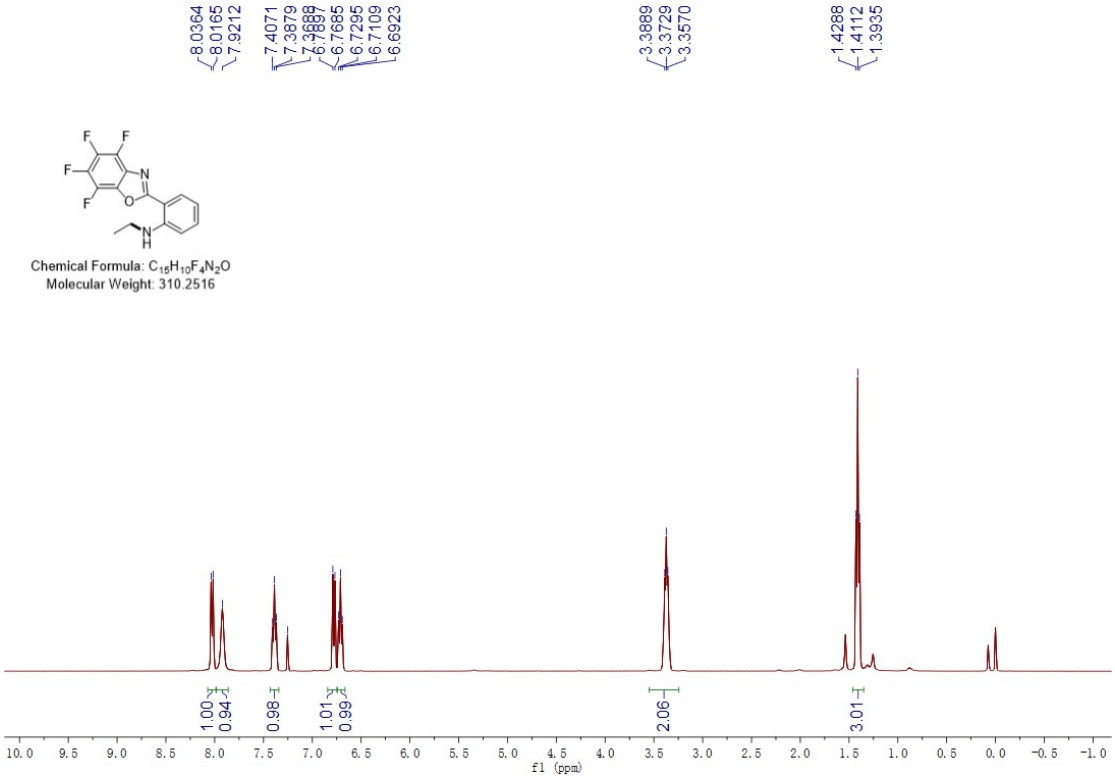


HRMS spectra

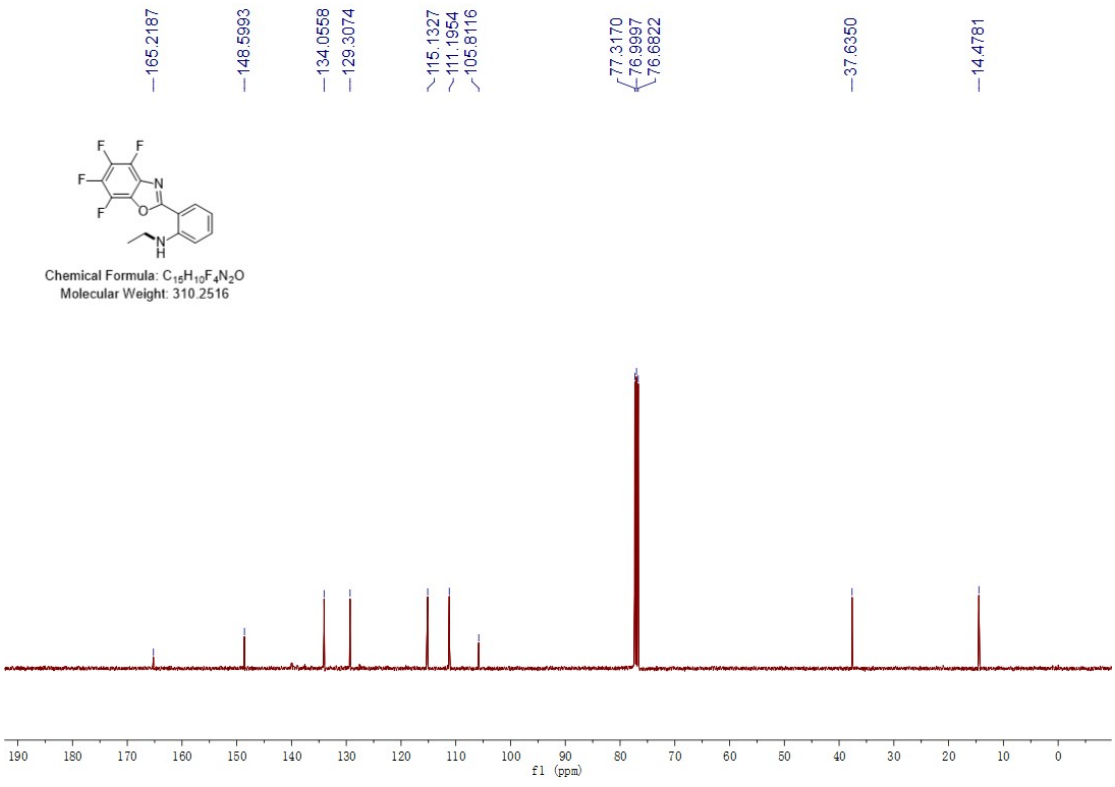


N-ethyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline(**4b**)

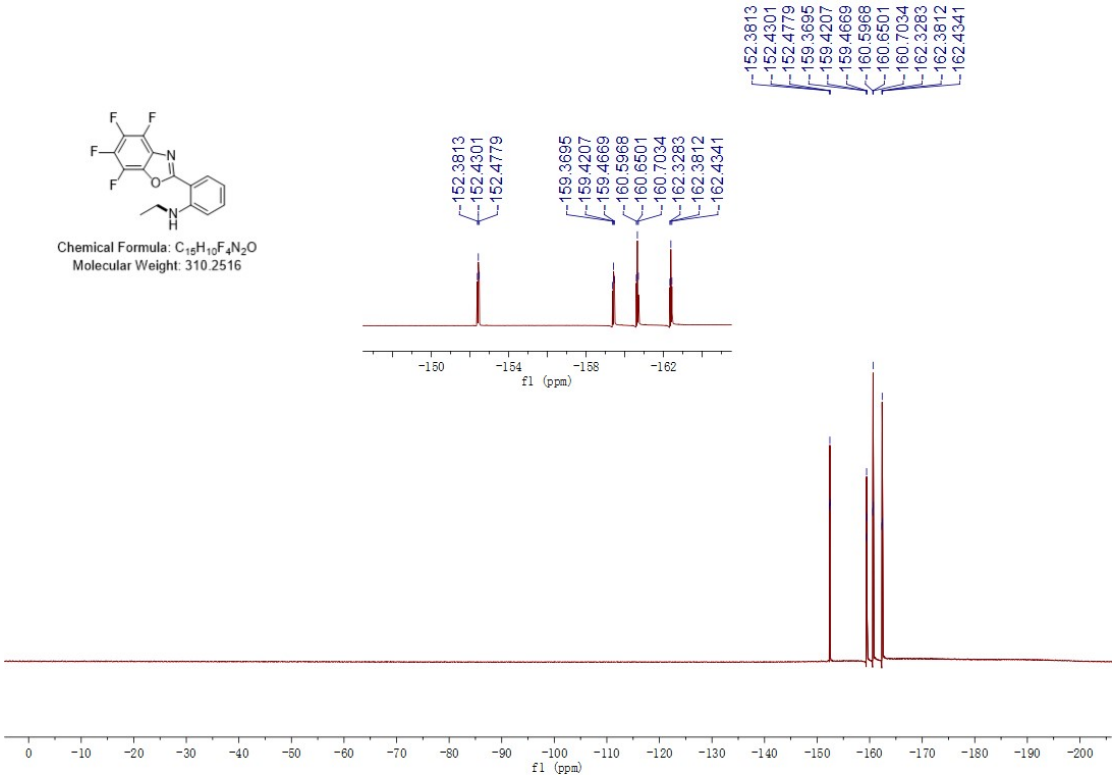
^{1}H NMR(400MHz, $CDCl_3$)



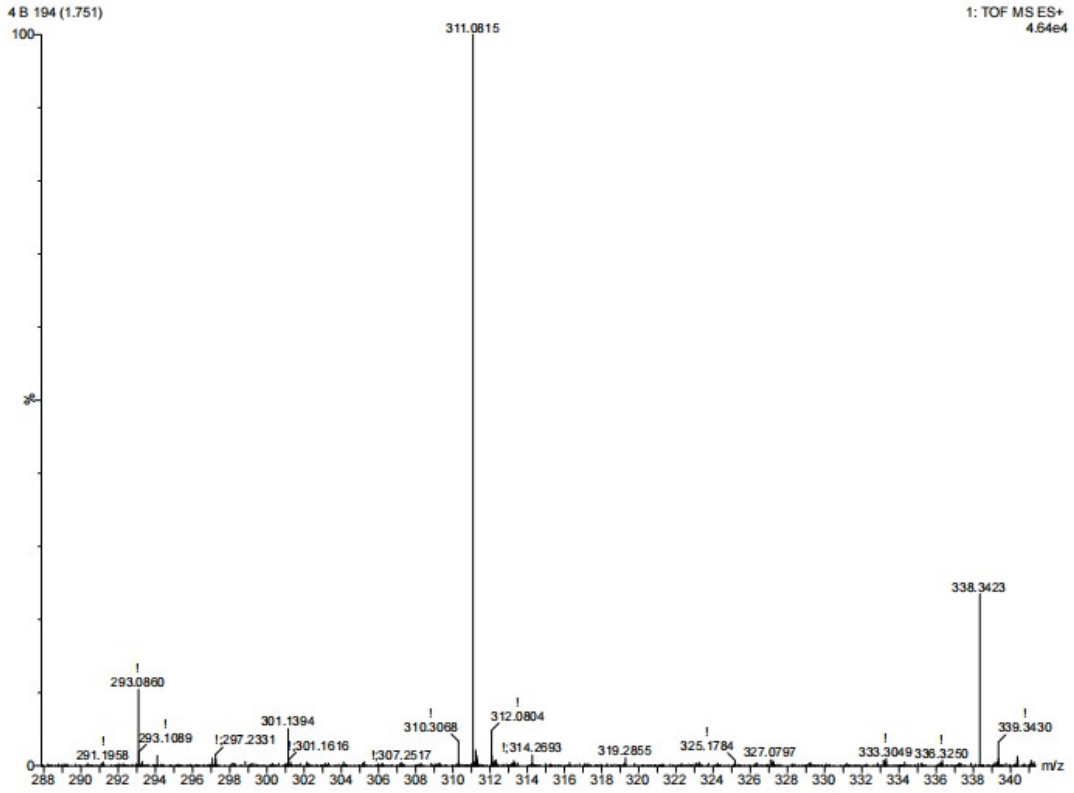
^{13}C NMR (101 MHz, $CDCl_3$)



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

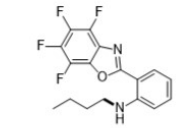


HRMS spectra

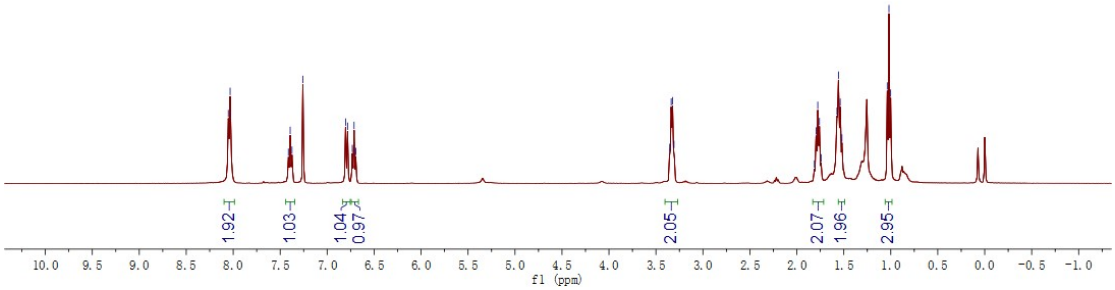


N-butyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4c**)

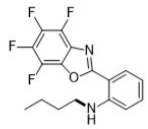
^{1}H NMR (400 MHz, CDCl3)



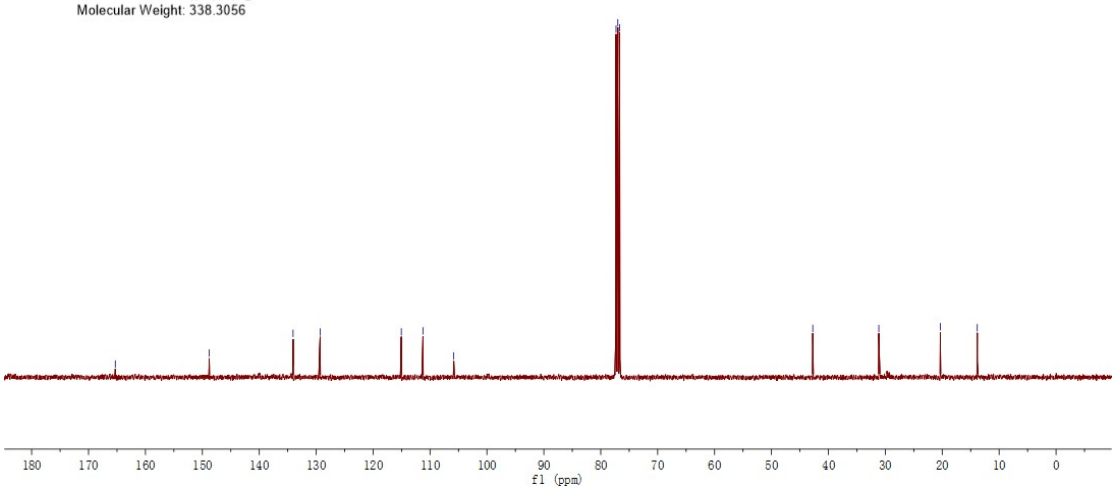
Chemical Formula: $C_{17}H_{14}F_4N_2O$
Molecular Weight: 338.3056



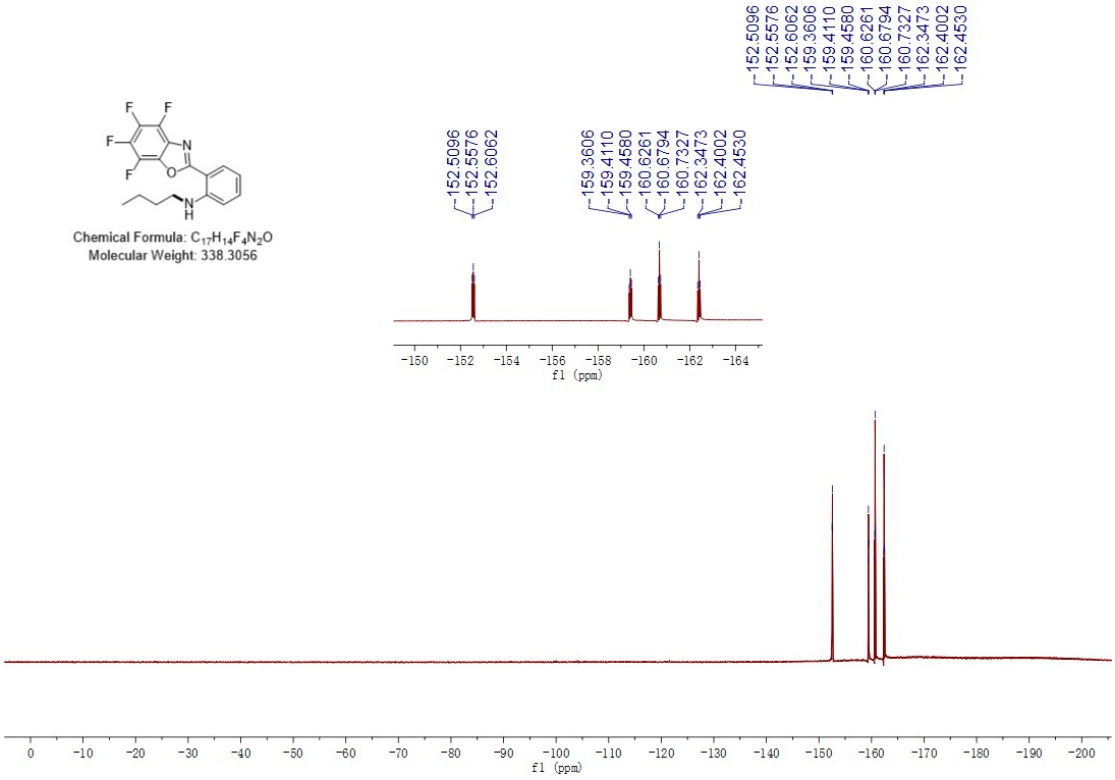
^{13}C NMR (101 MHz, $CDCl_3$)



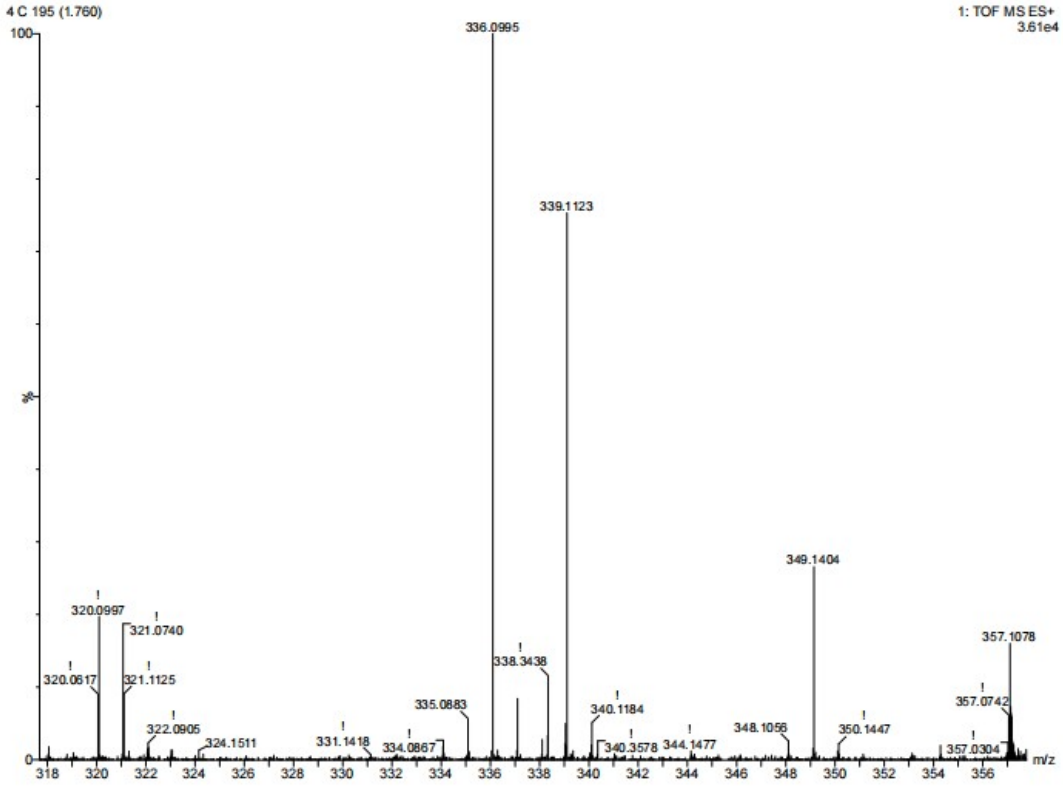
Chemical Formula: $C_{17}H_{14}F_4N_2O$
Molecular Weight: 338.3056



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

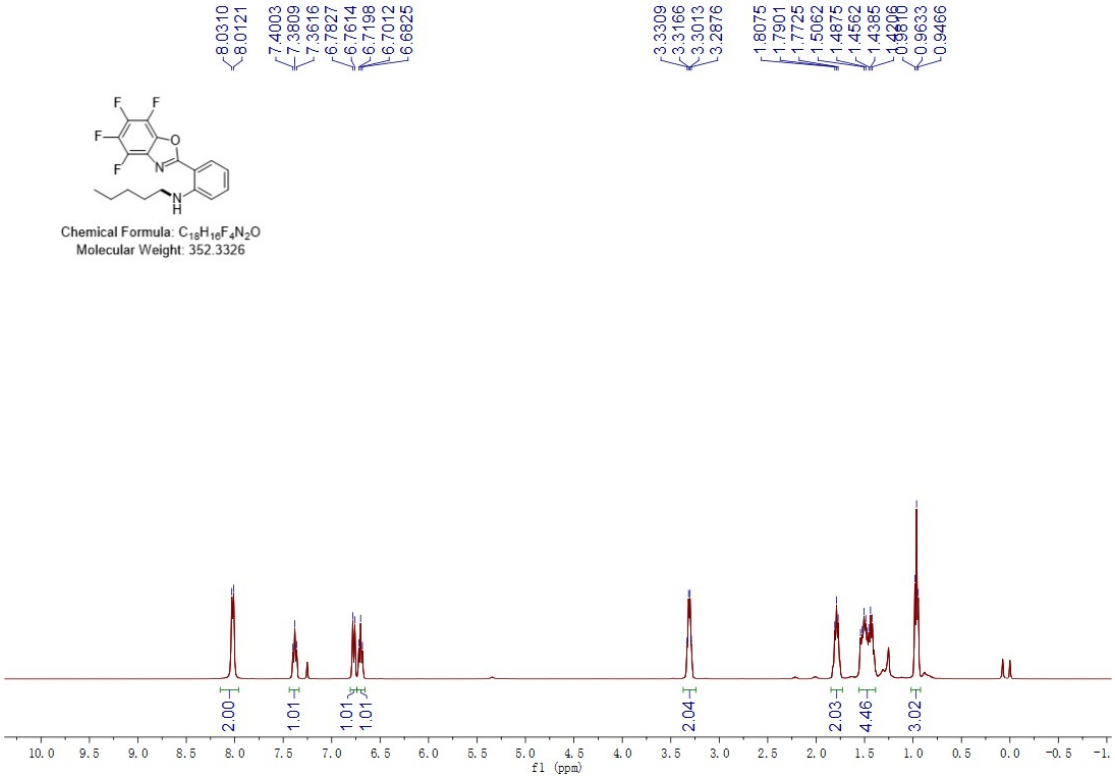


HRMS spectra

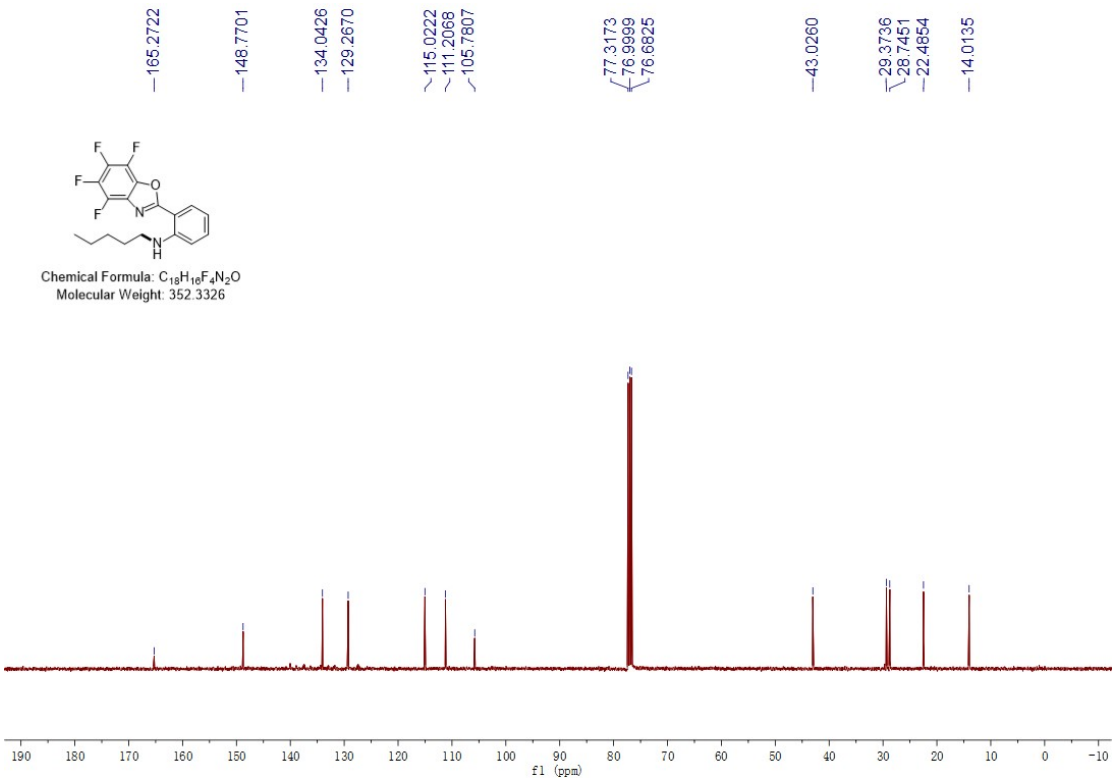


N-pentyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4d**)

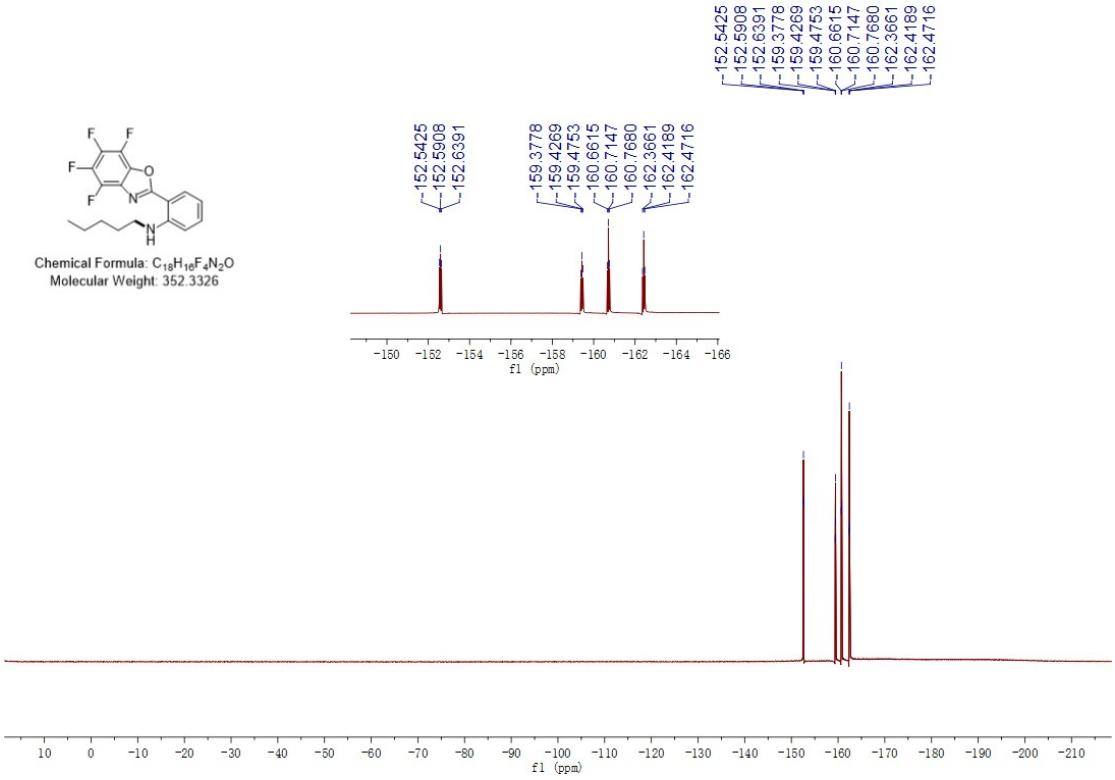
^{1}H NMR (400 MHz, $CDCl_3$)

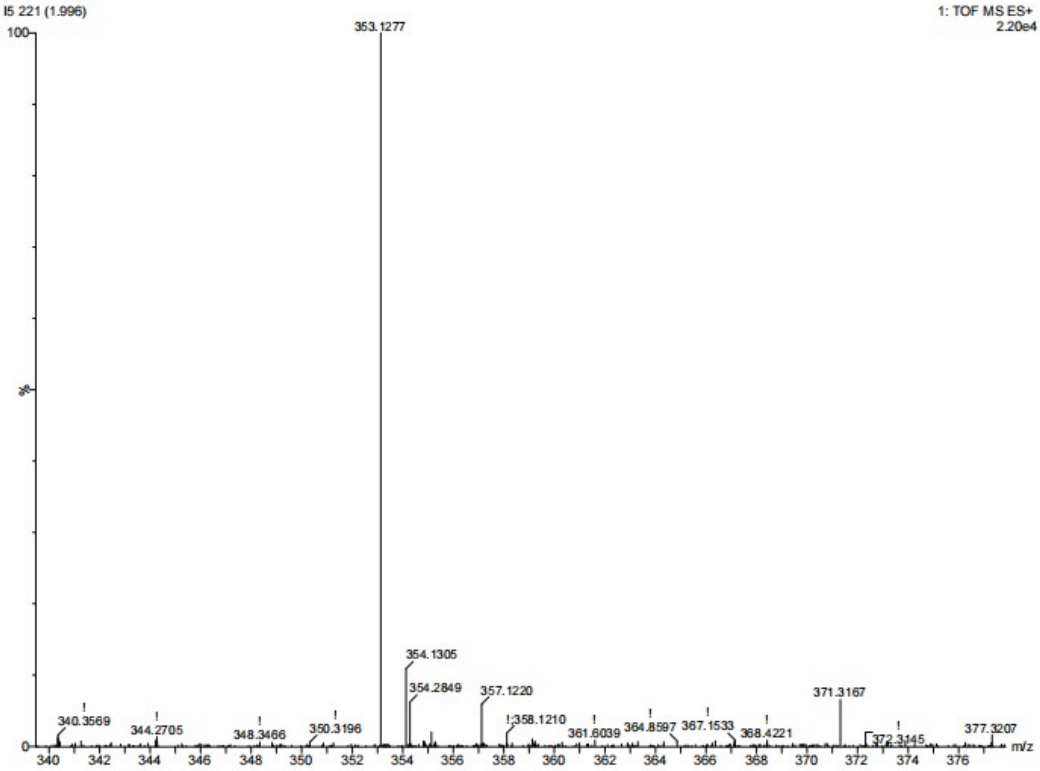


^{13}C NMR (101 MHz, $CDCl_3$)



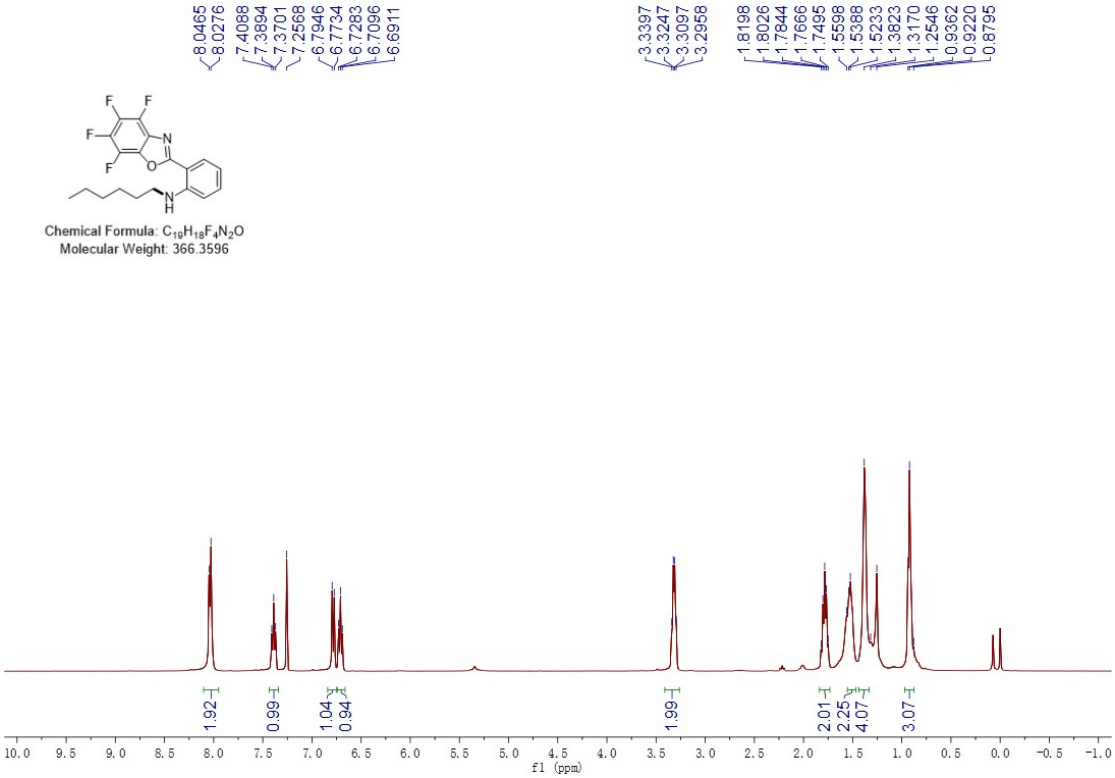
^{19}F NMR (376 MHz, $CDCl_3$)



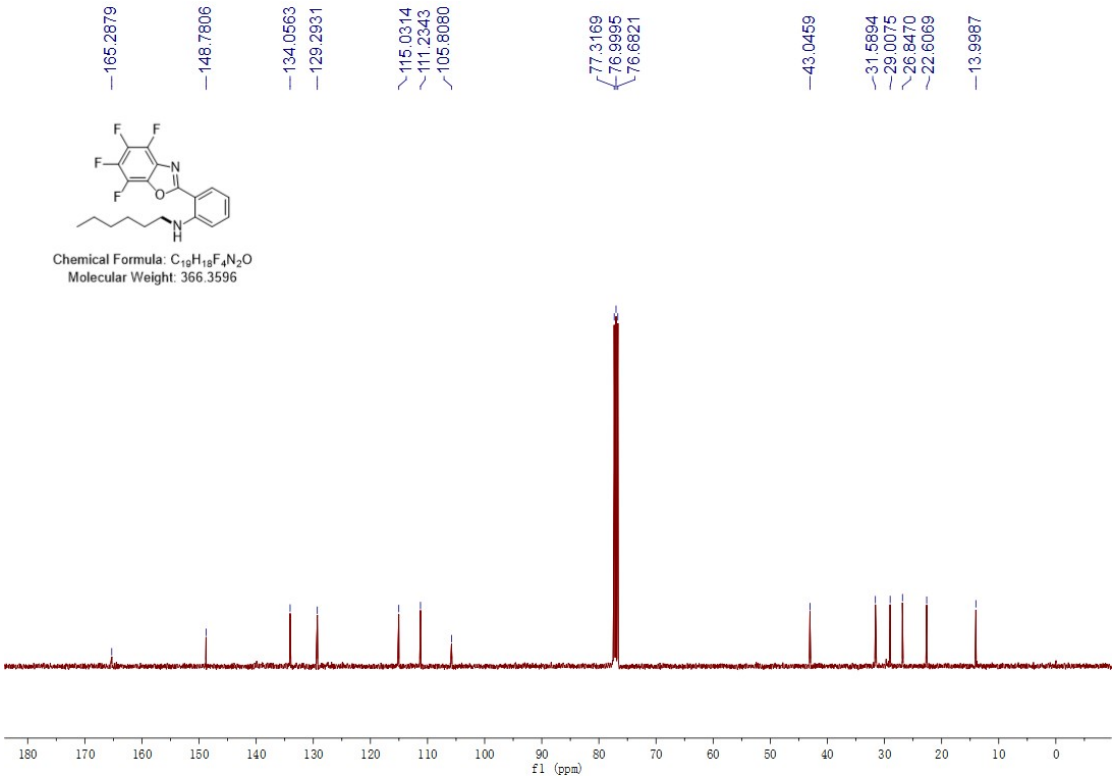


N-hexyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4e**)

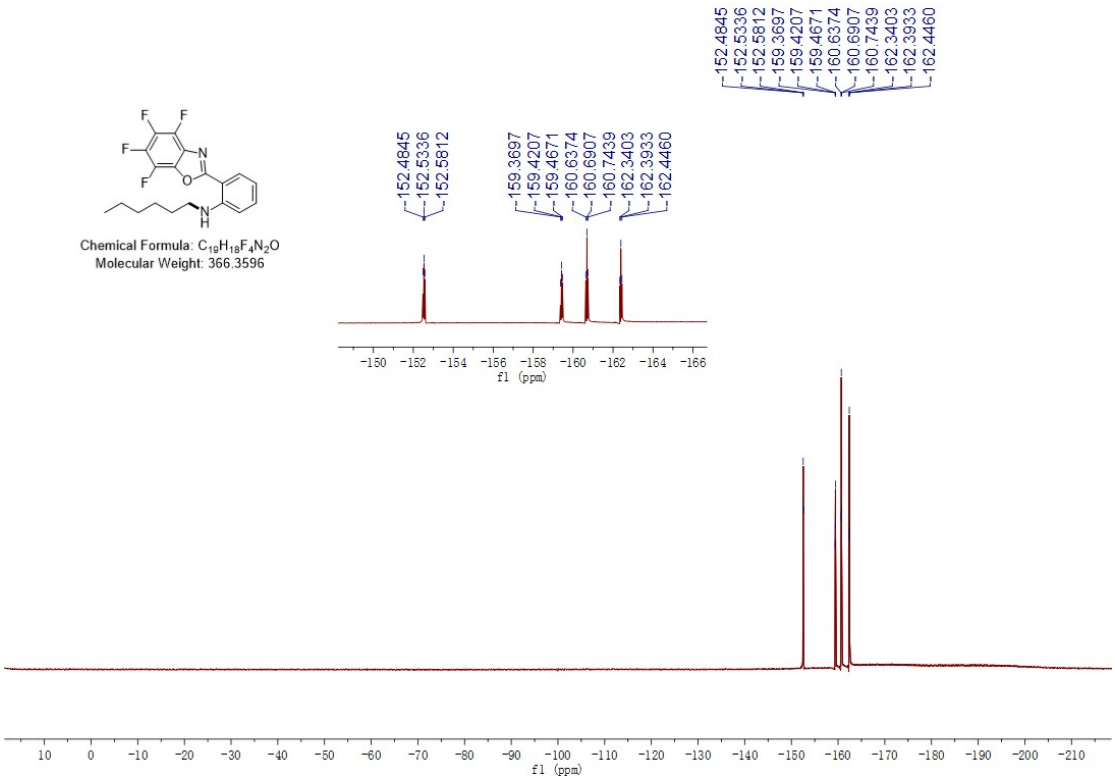
^{1}H NMR (400 MHz, $CDCl_3$)



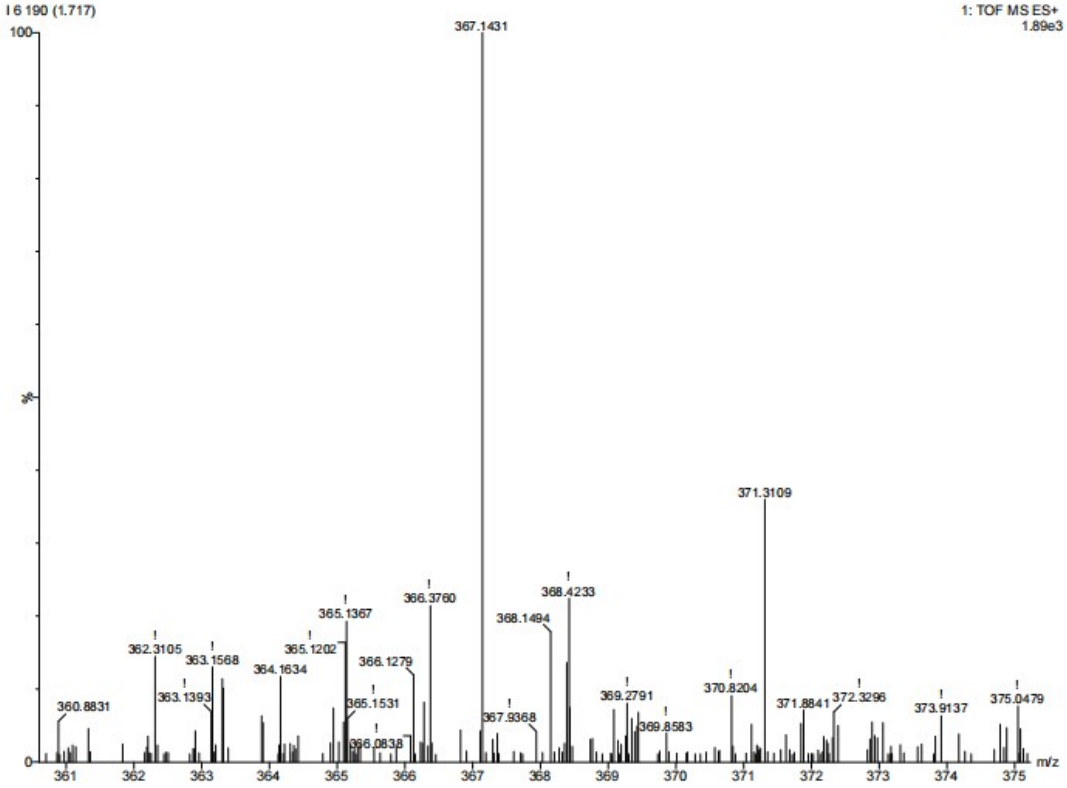
^{13}C NMR (101 MHz, $CDCl_3$)



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

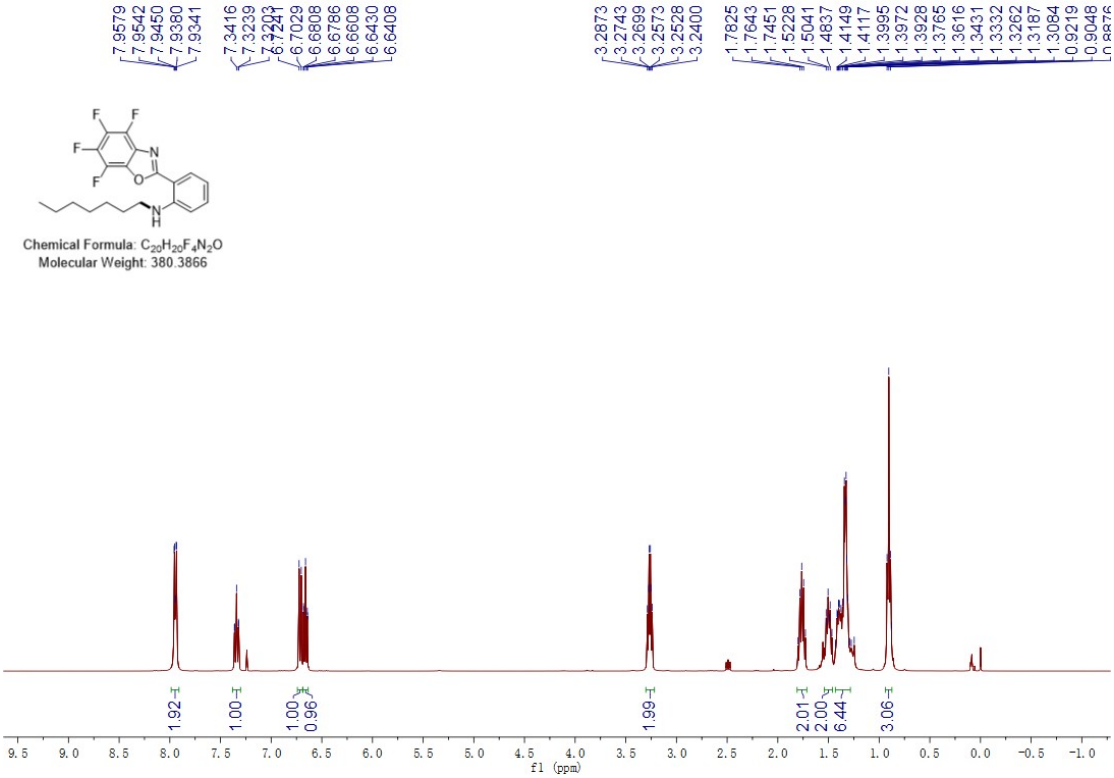


HRMS spectra



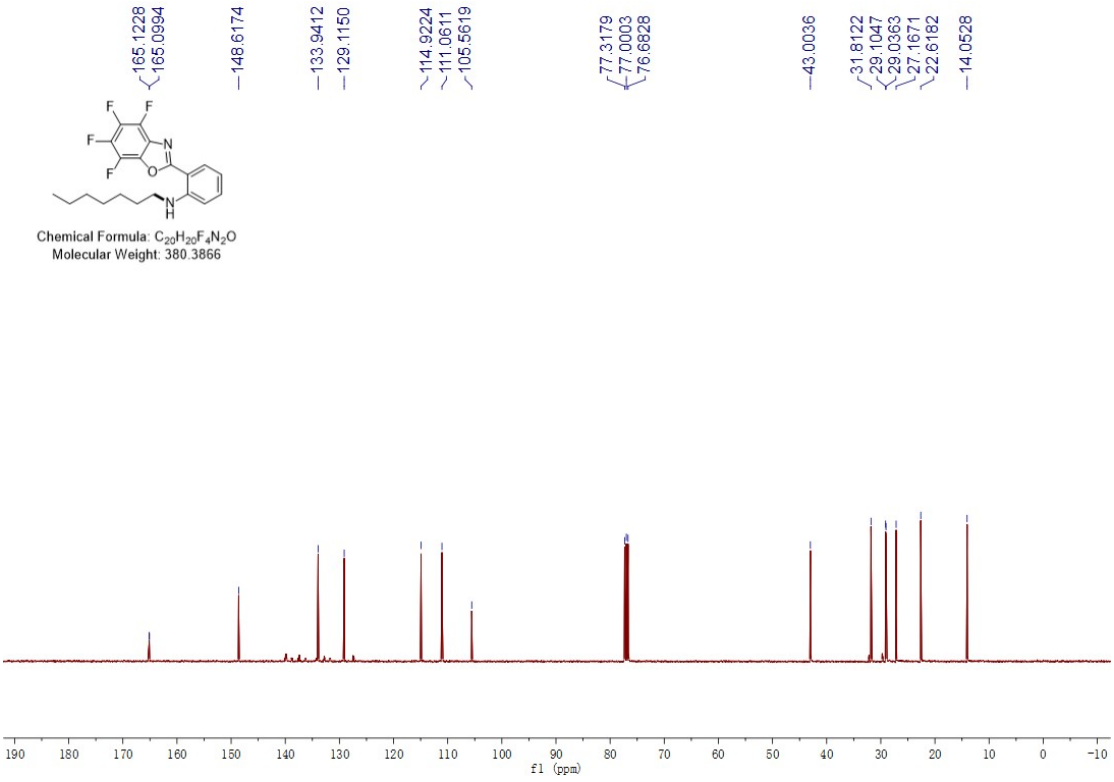
N-heptyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4f**)

^{1}H NMR (400 MHz, CDCl3)



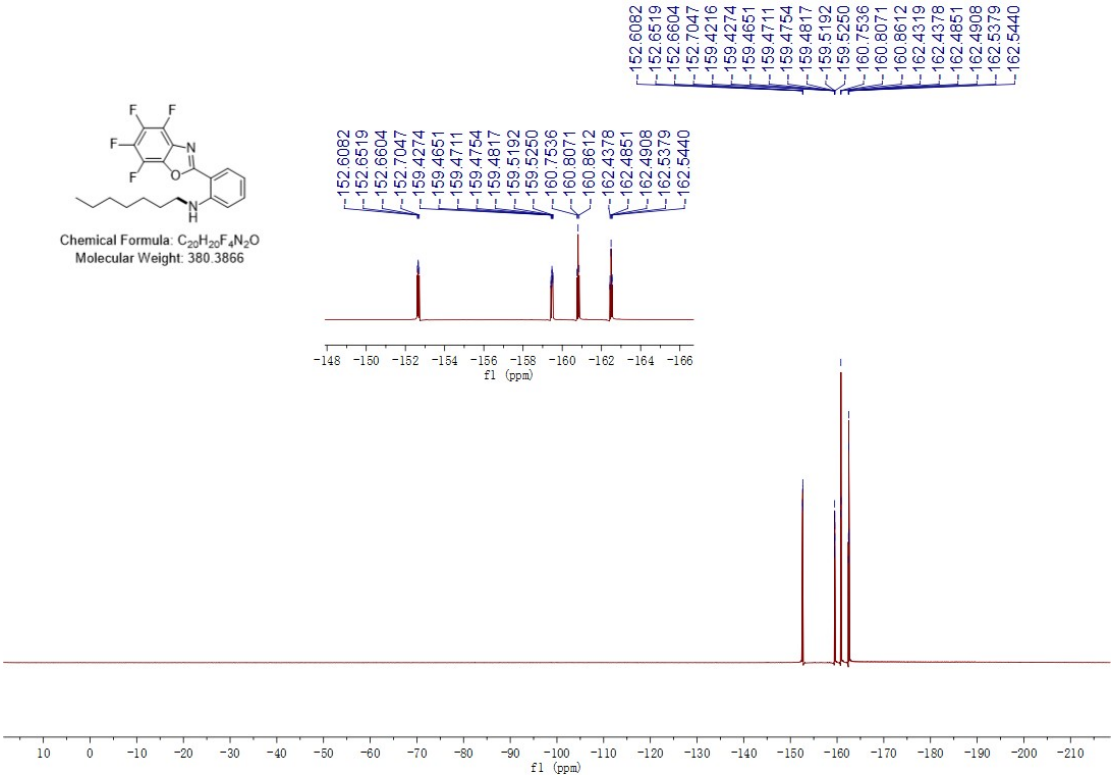
Chemical Formula: $C_{20}H_{20}F_4N_2O$
Molecular Weight: 380.3866

^{13}C NMR (101 MHz, $CDCl_3$)

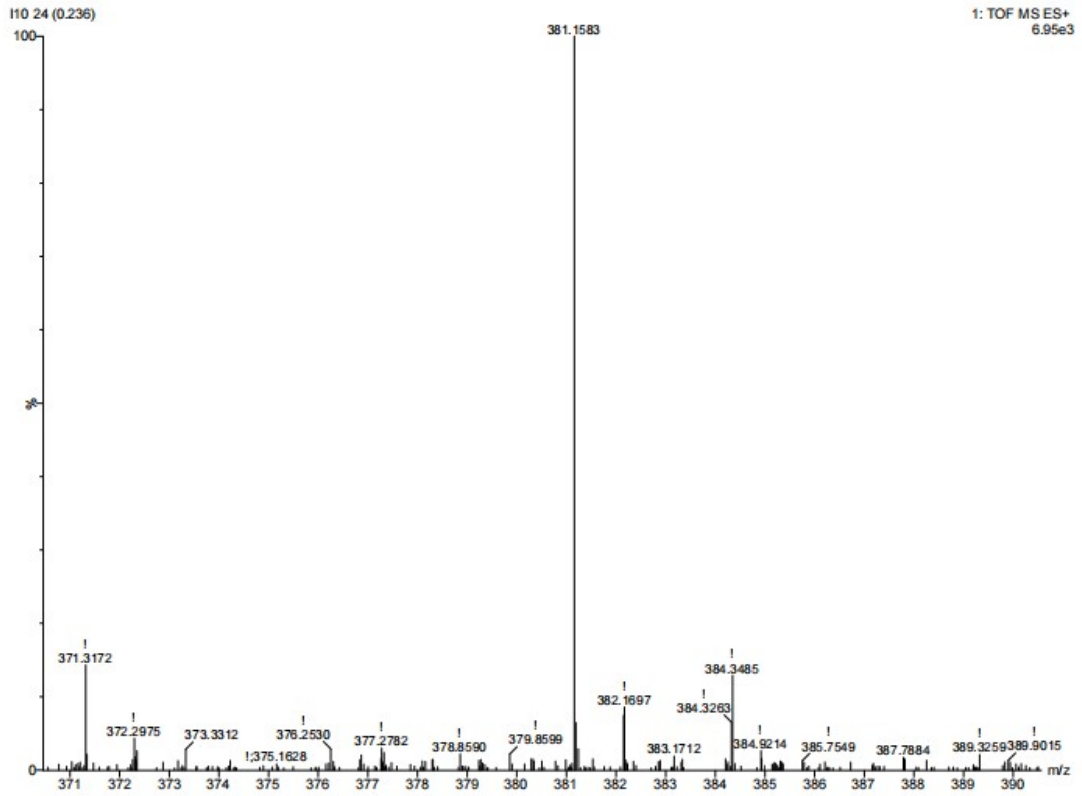


Chemical Formula: $C_{20}H_{20}F_4N_2O$
Molecular Weight: 380.3866

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

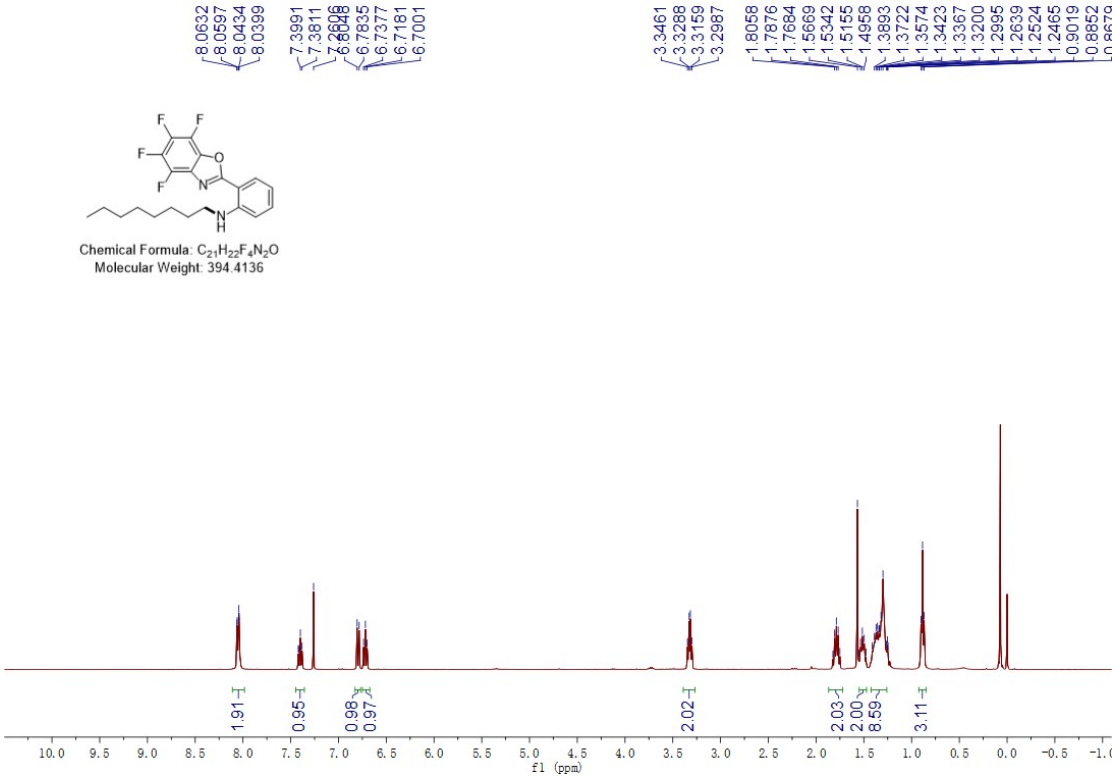


HRMS spectra

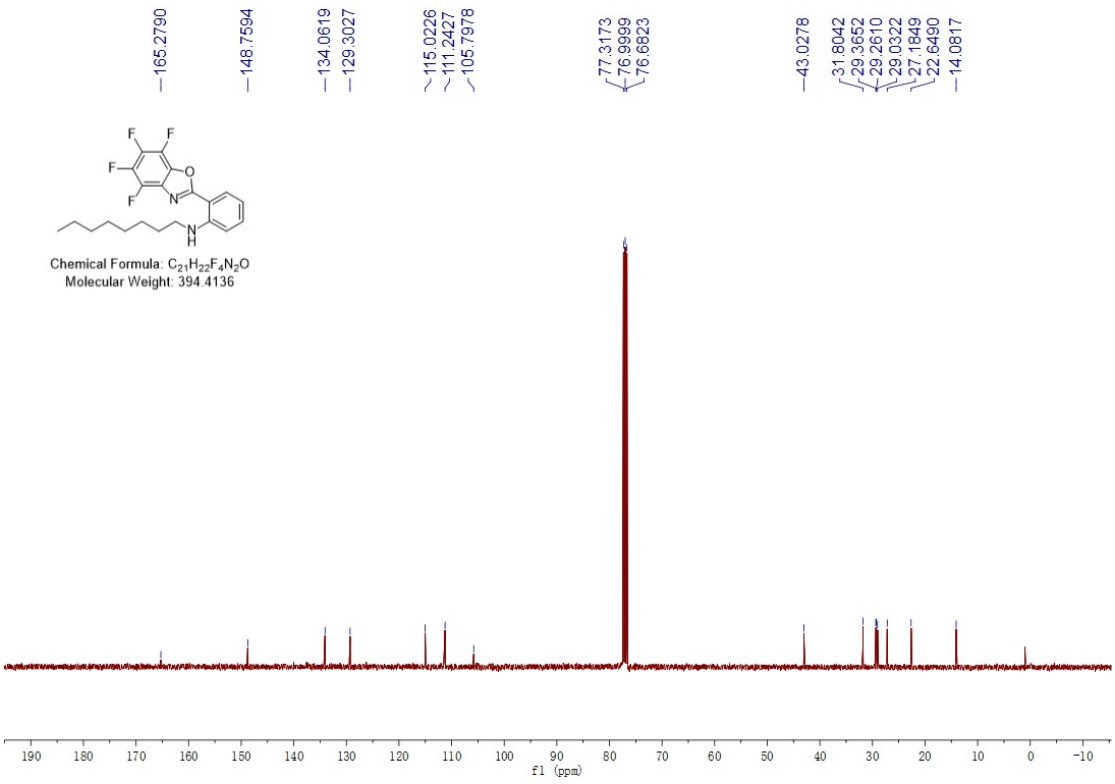


N-octyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4g**)

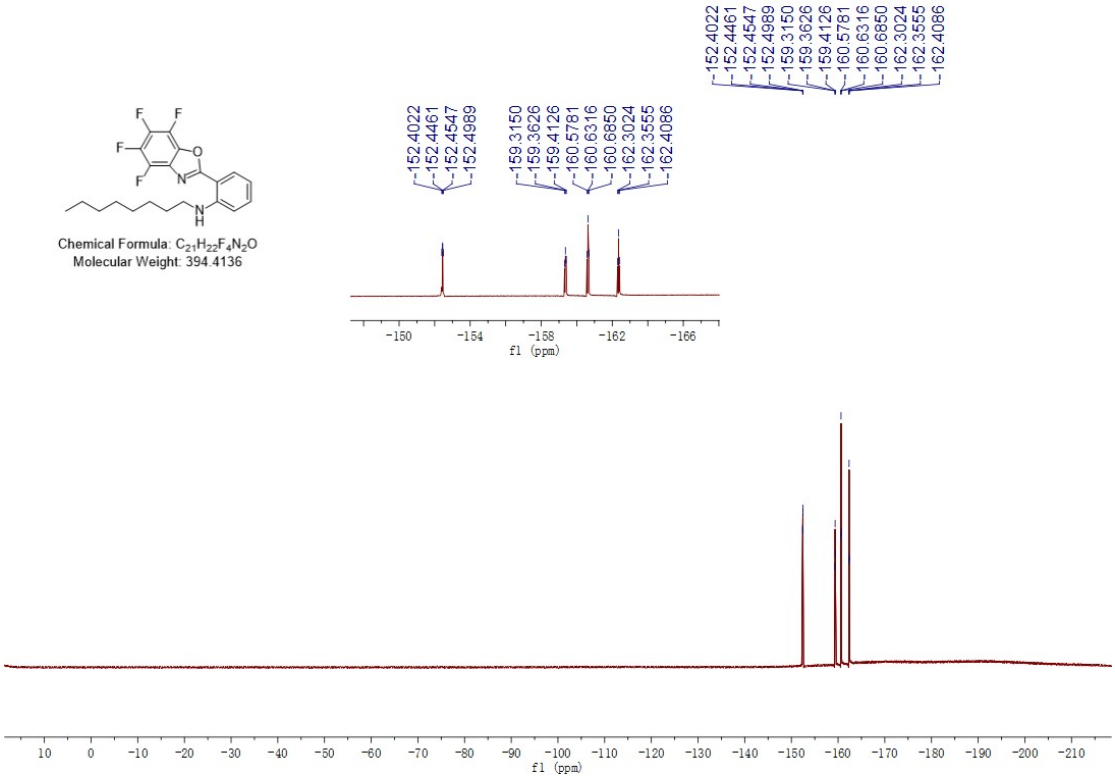
^{1}H NMR (400 MHz, $CDCl_3$)



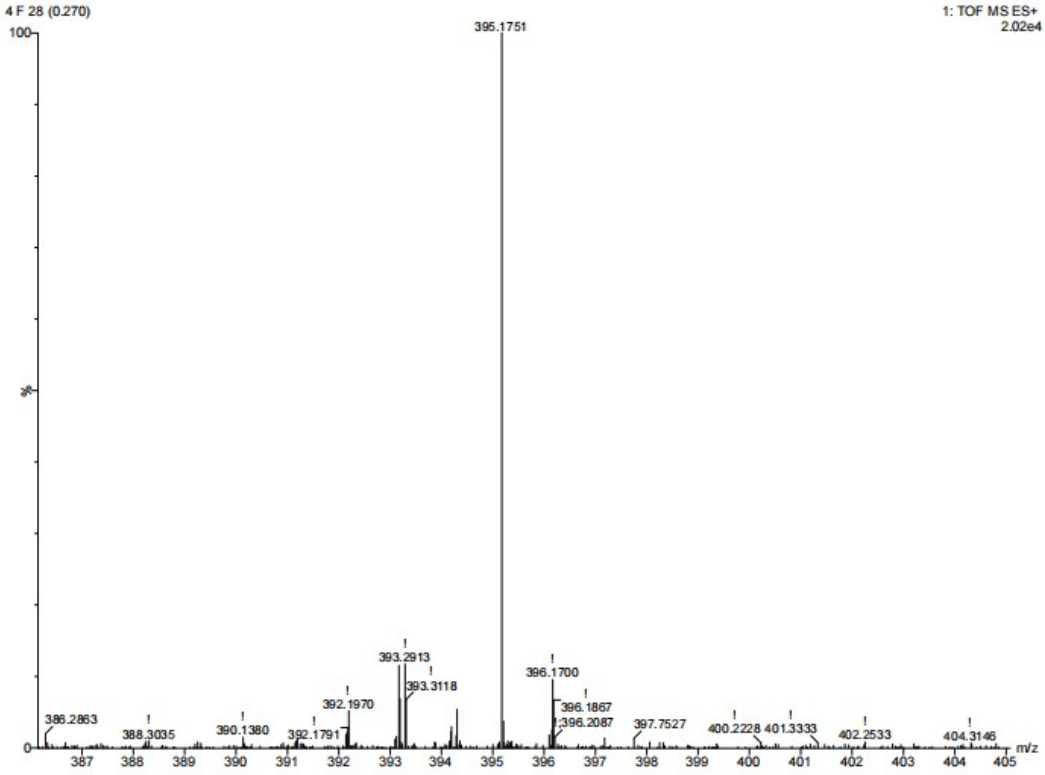
^{13}C NMR (101MHz, $CDCl_3$)



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

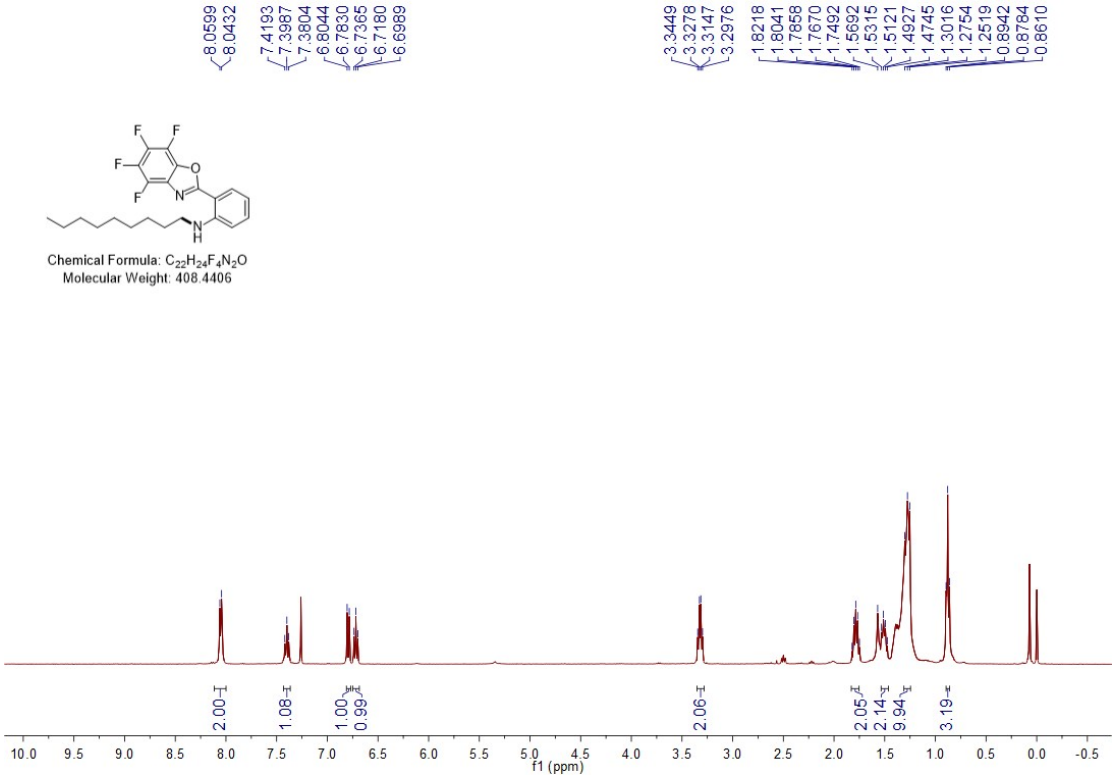


HRMS spectra

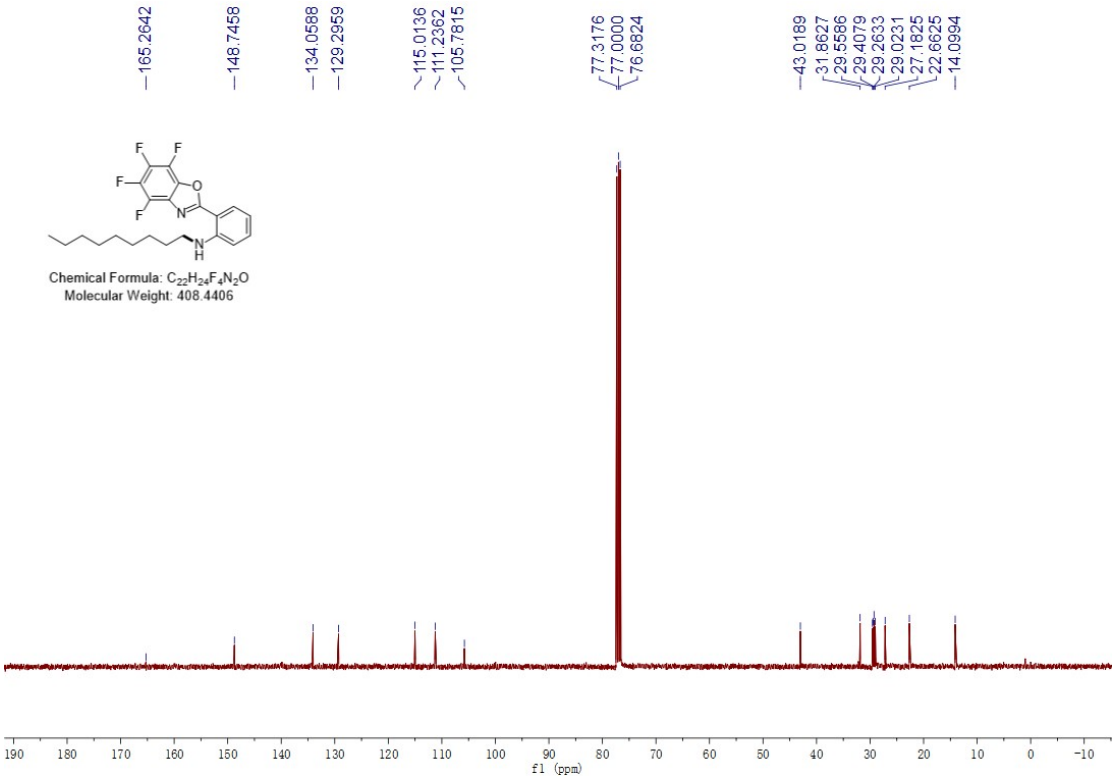


N-nonyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4h**)

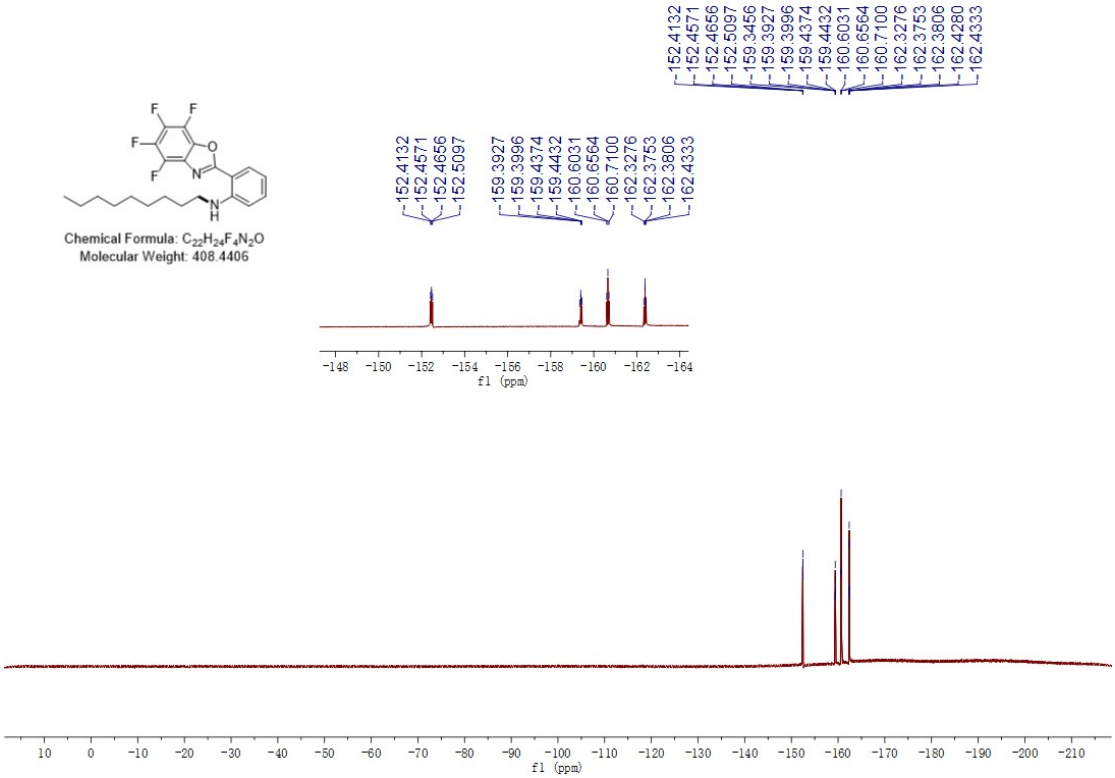
^{1}H NMR (400 MHz, $CDCl_3$)



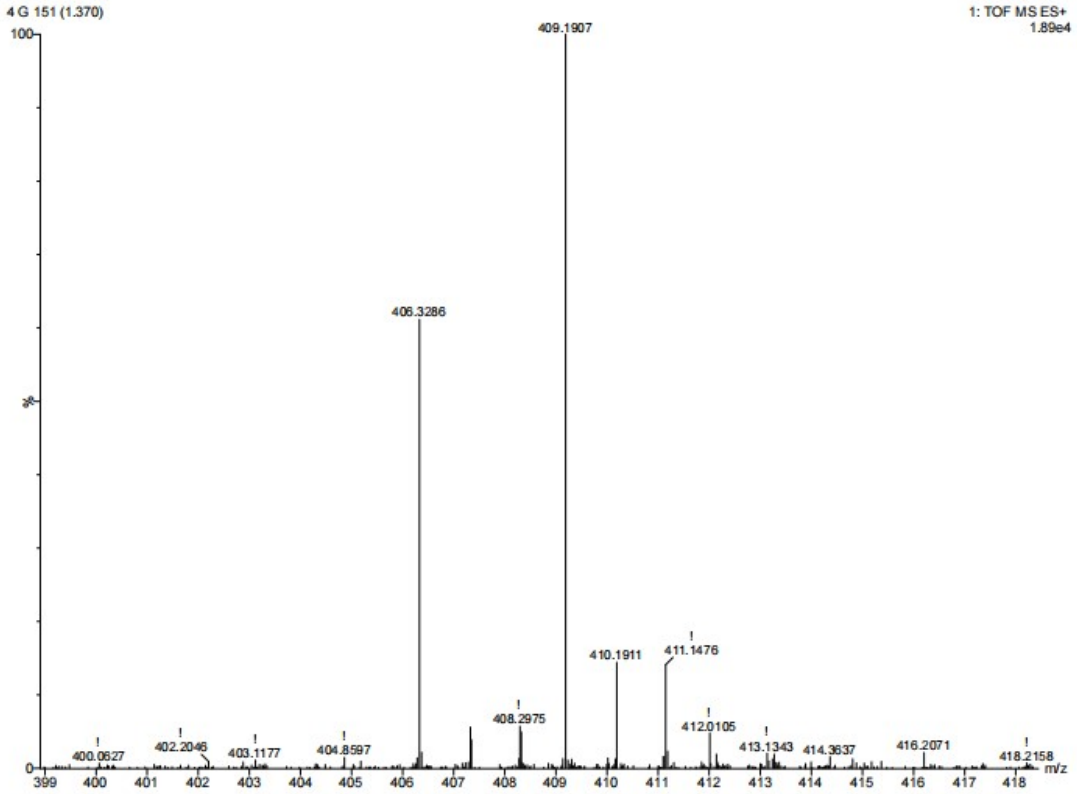
^{13}C NMR (101MHz, $CDCl_3$)



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

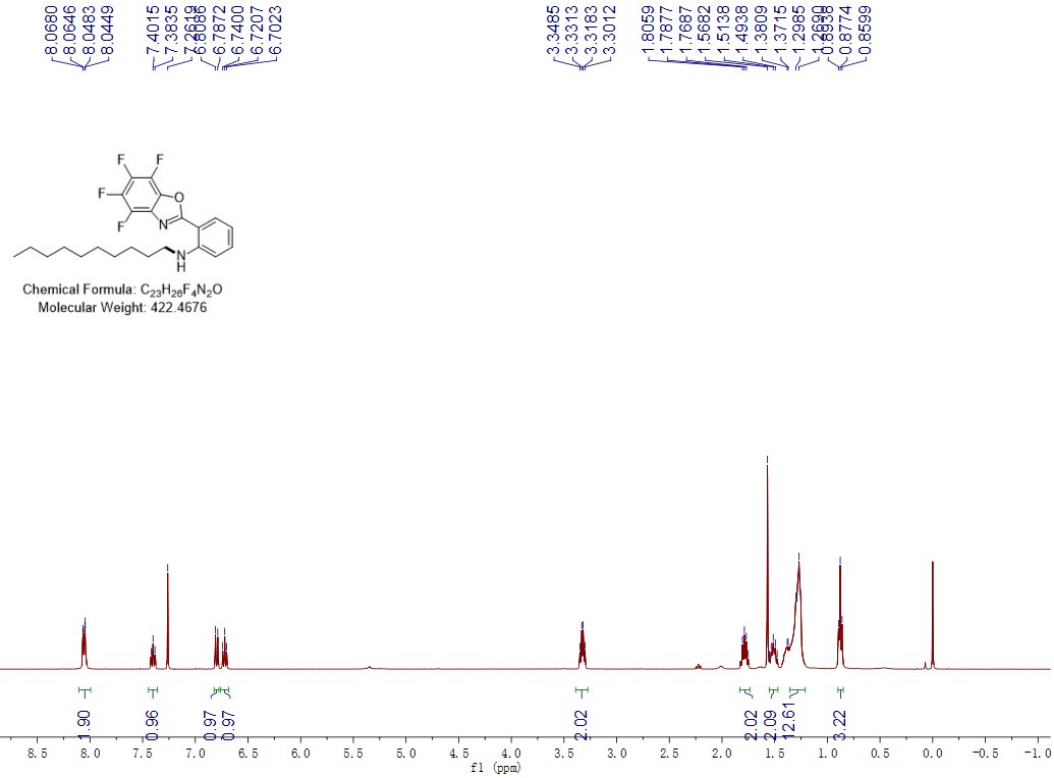


HRMS spectra

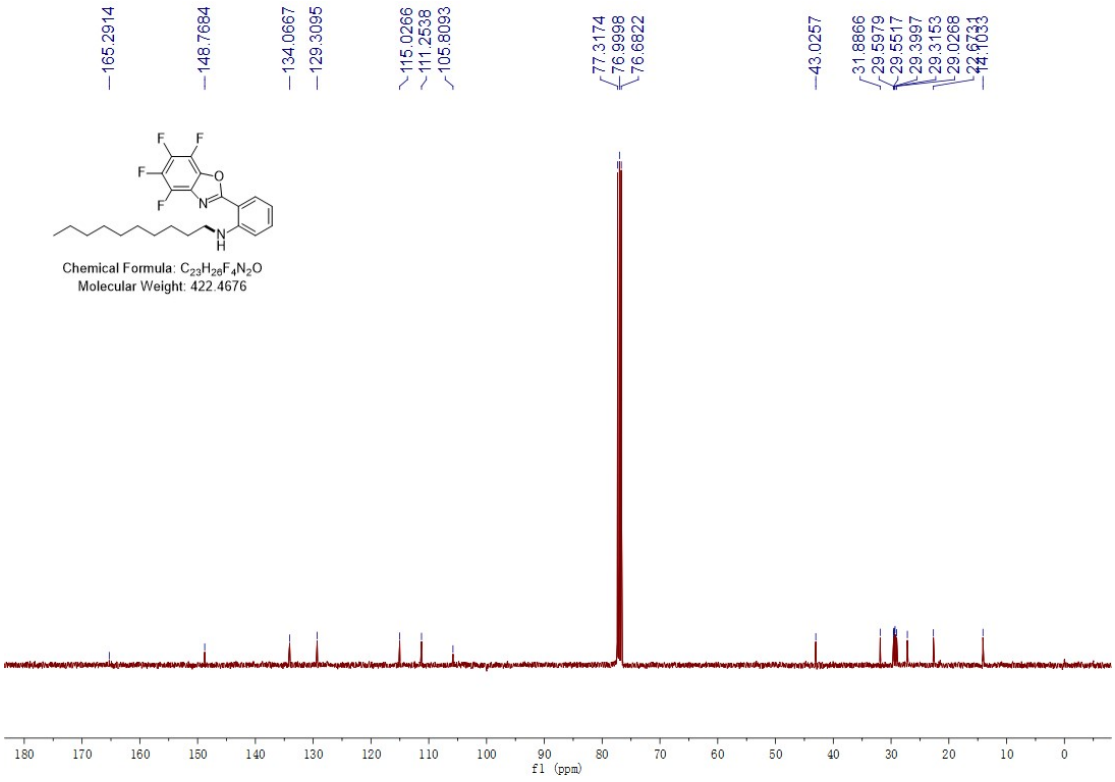


N-decyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4i**)

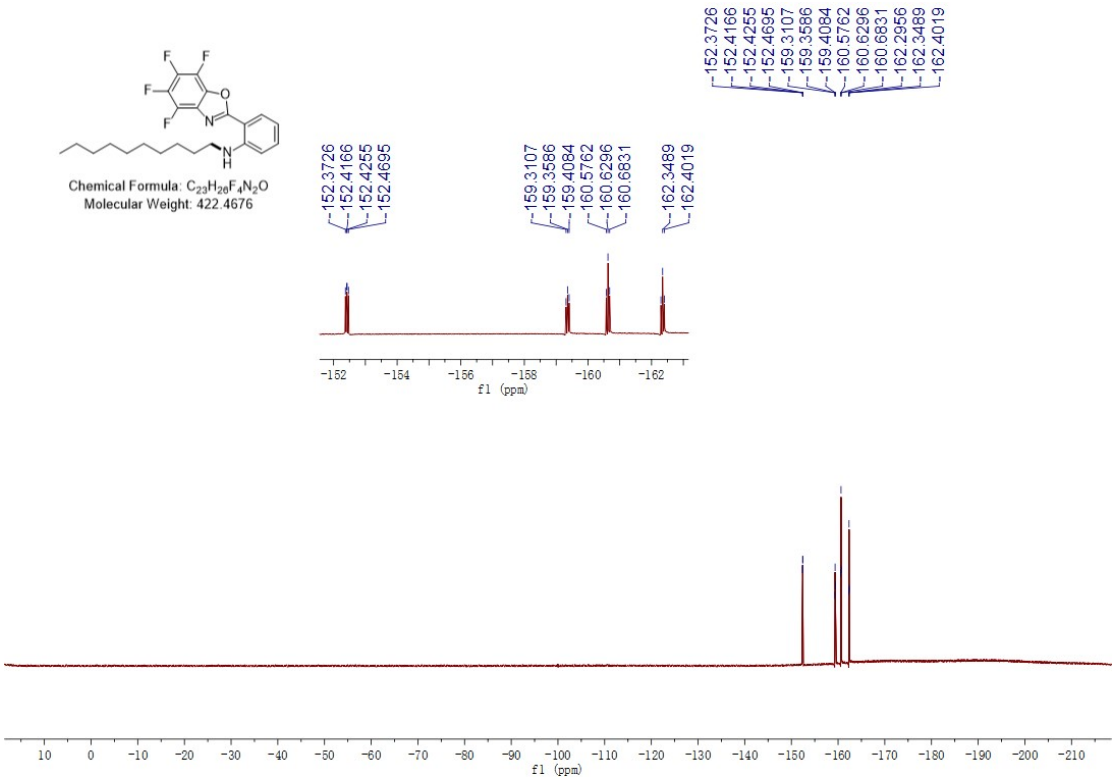
^{1}H NMR (400 MHz, $CDCl_3$)



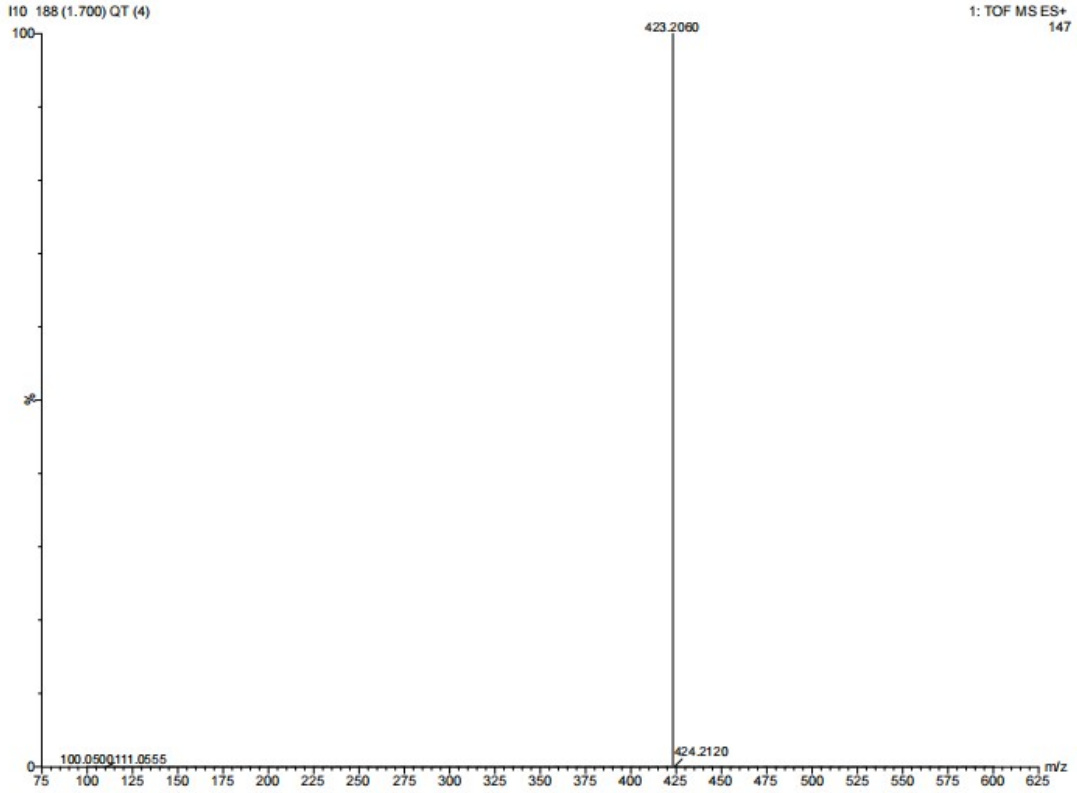
^{13}C NMR (101 MHz, $CDCl_3$)



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

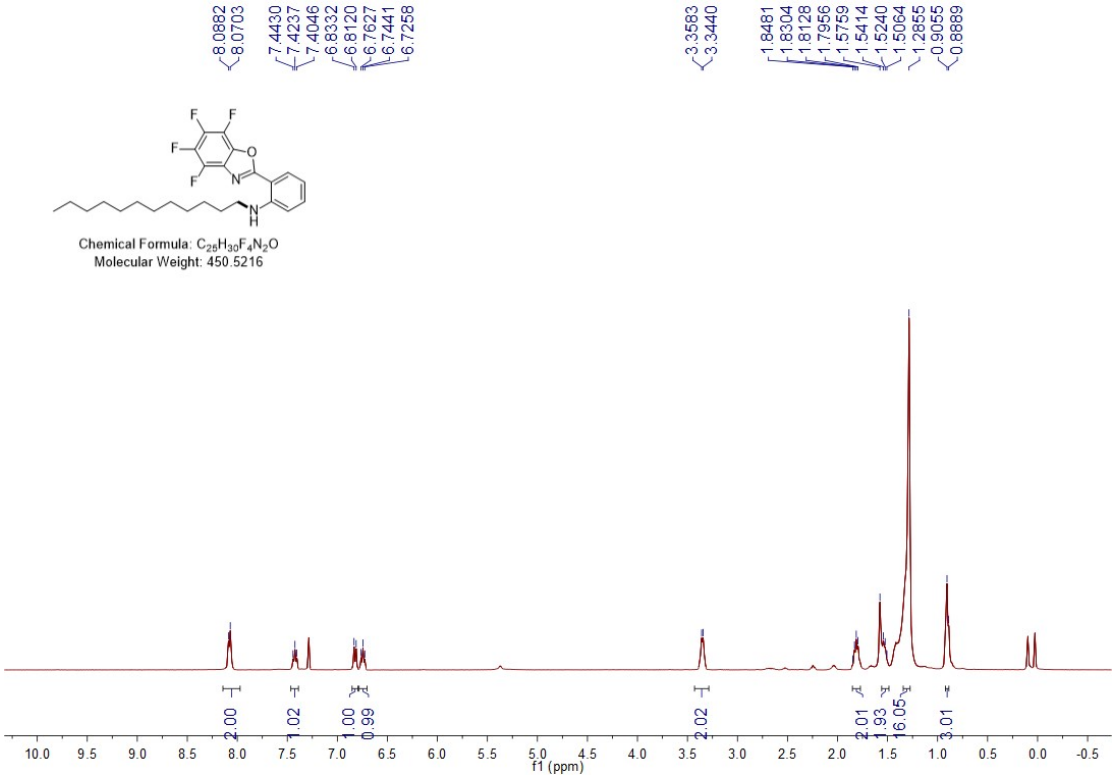


HRMS spectra

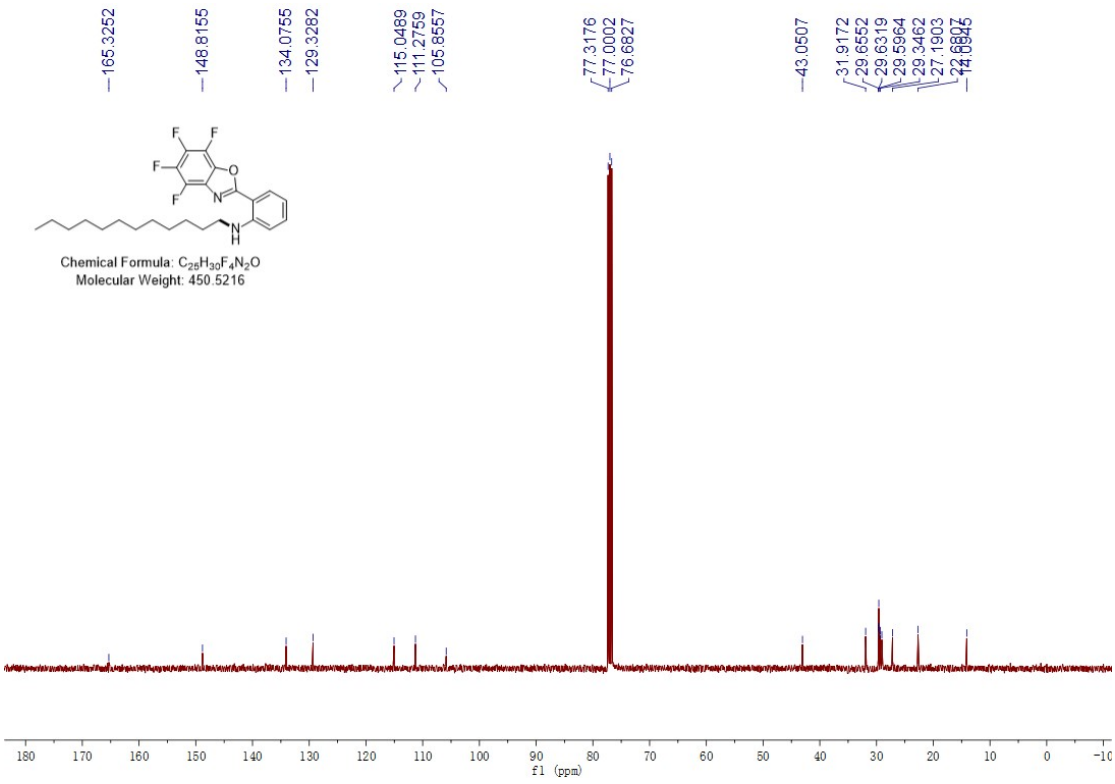


N-dodecyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4j**)

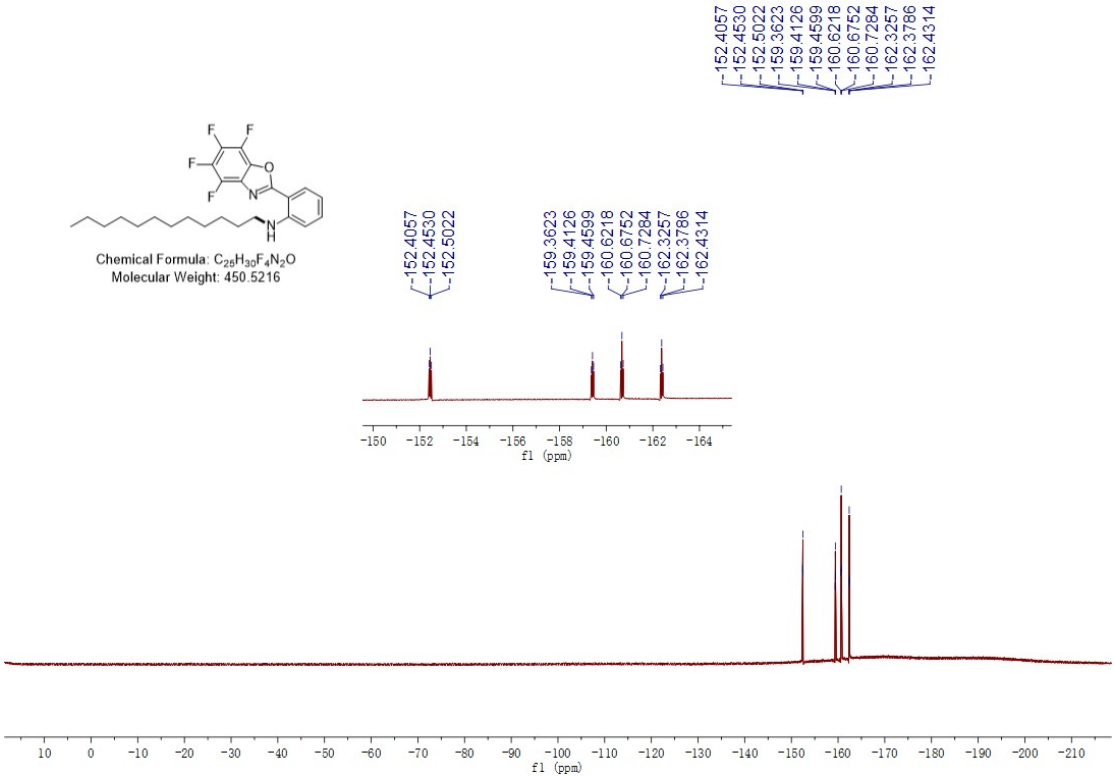
^{1}H NMR (400 MHz, $CDCl_3$)



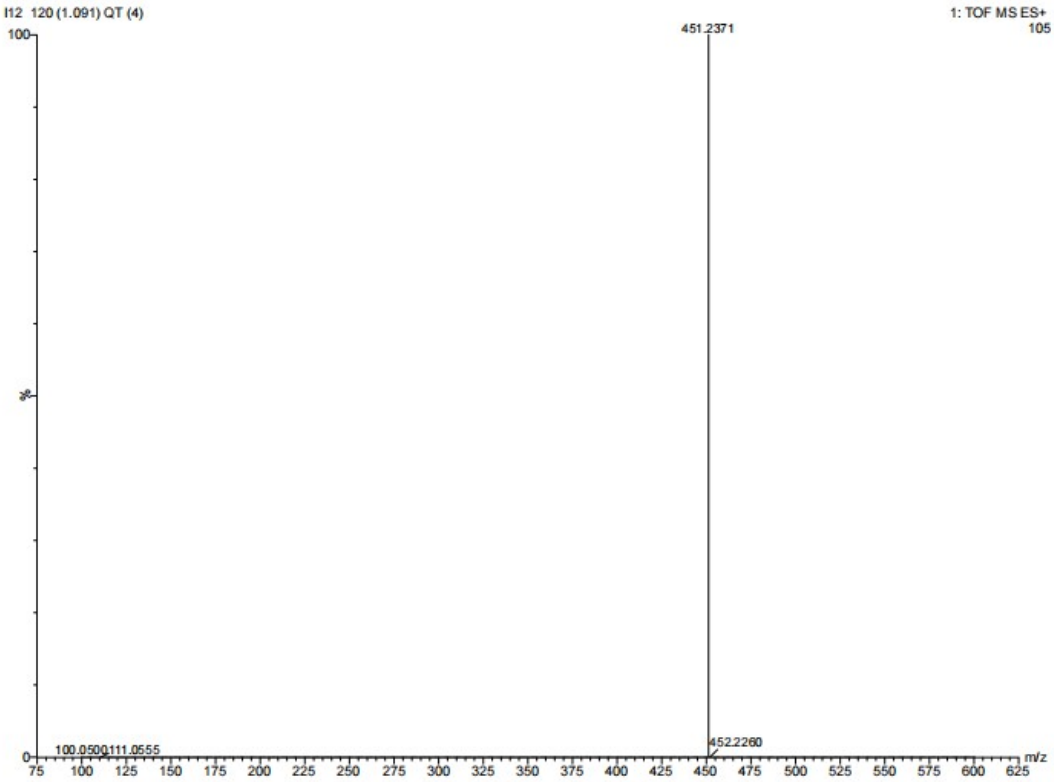
^{13}C NMR (101 MHz, $CDCl_3$)



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

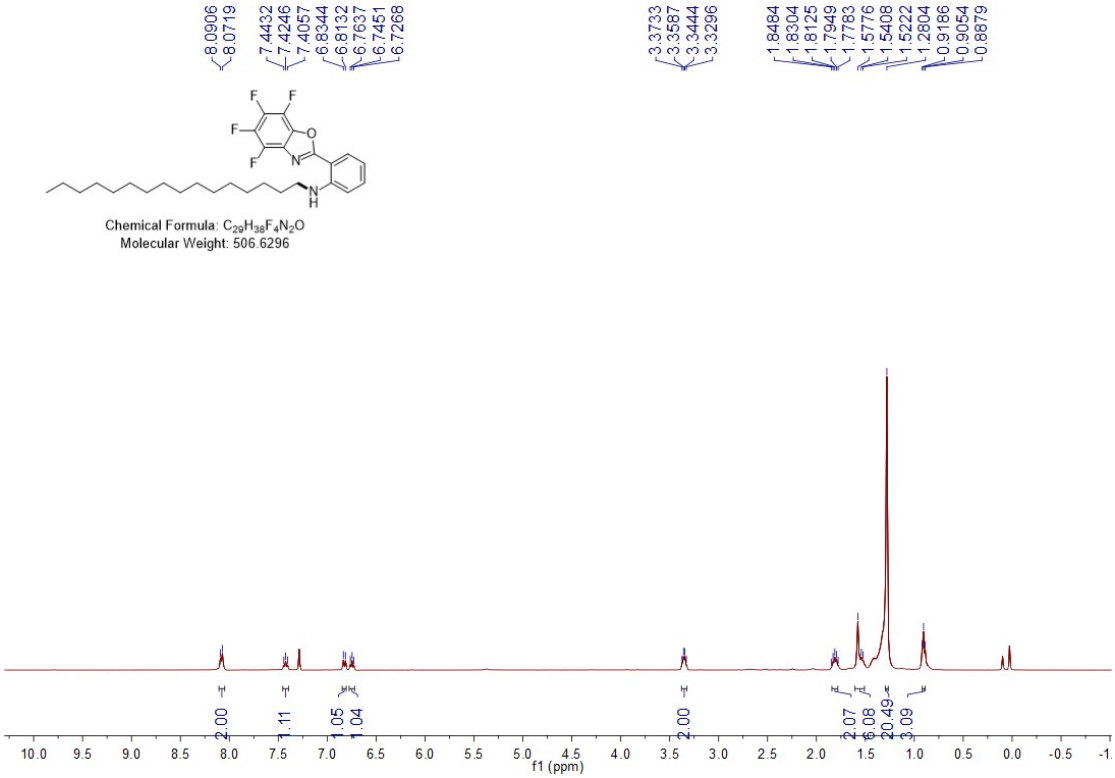


HRMS spectra

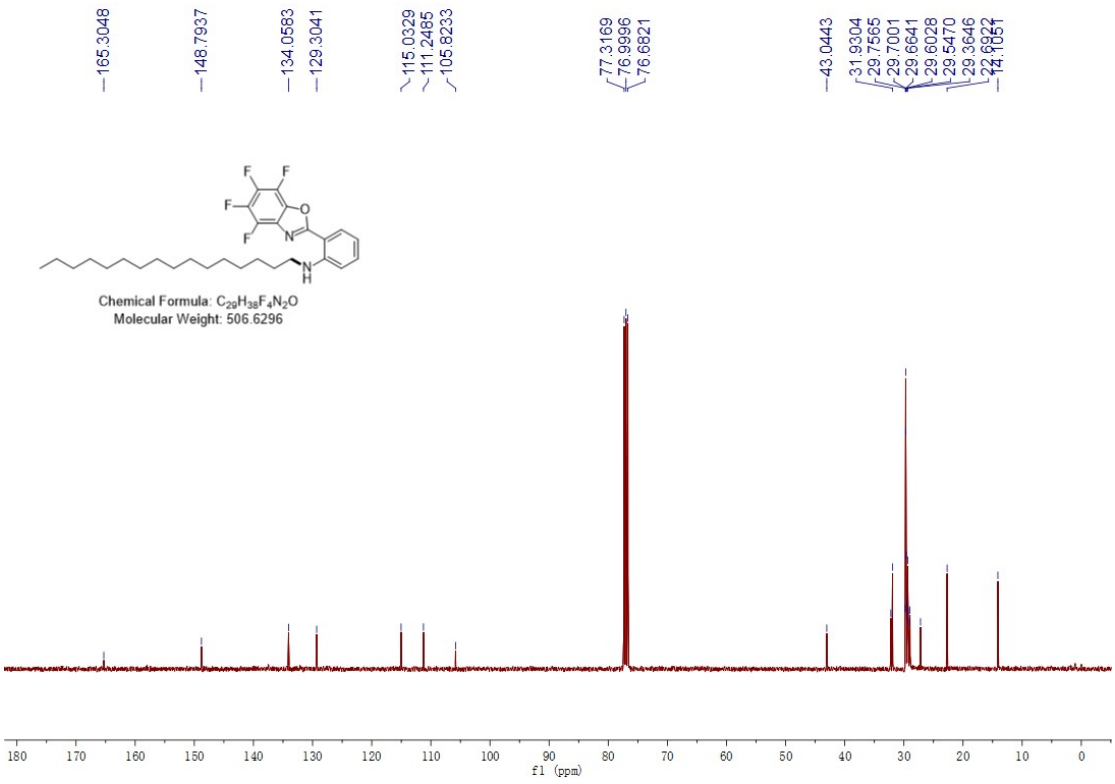


N-hexadecyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4k**)

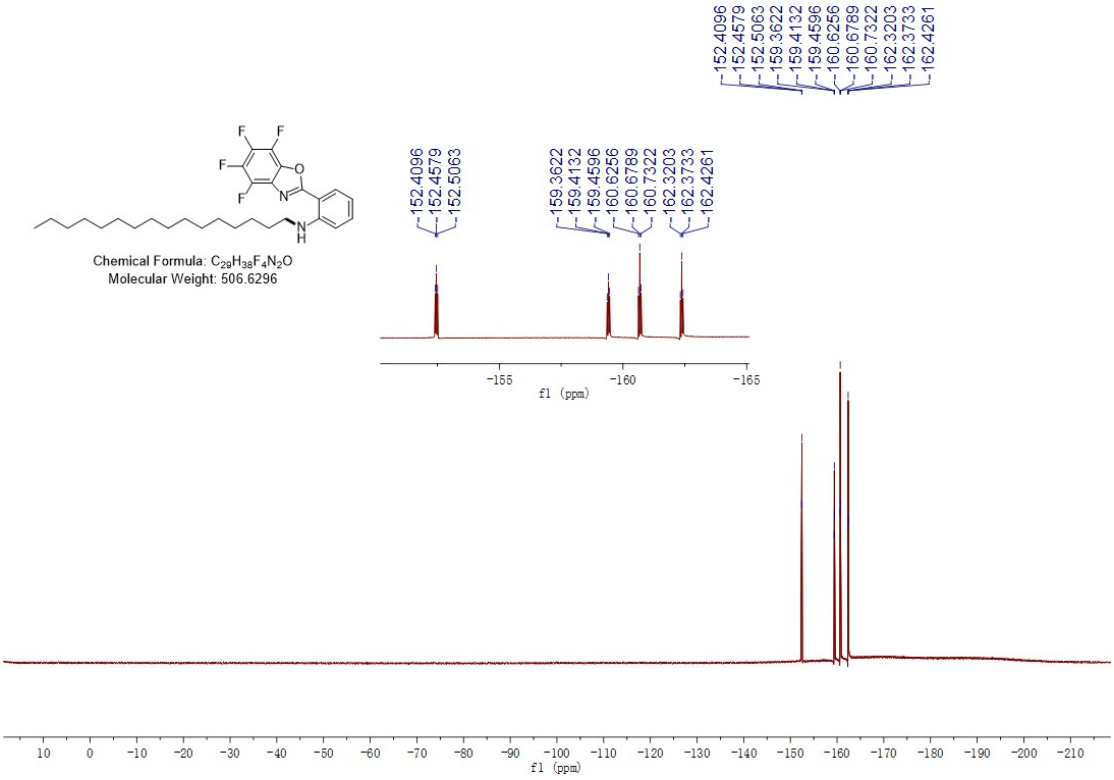
^{1}H NMR (400 MHz, $CDCl_3$)



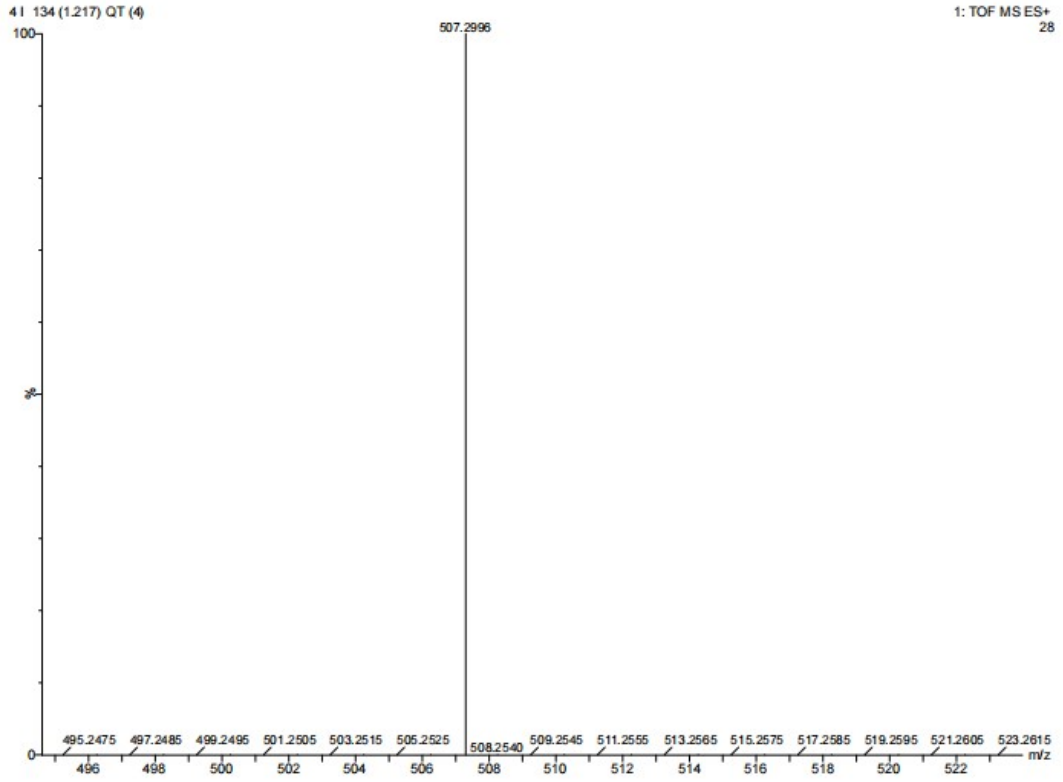
^{13}C NMR (101 MHz, $CDCl_3$)



^{19}F NNMR (376 MHz, $CDCl_3$)

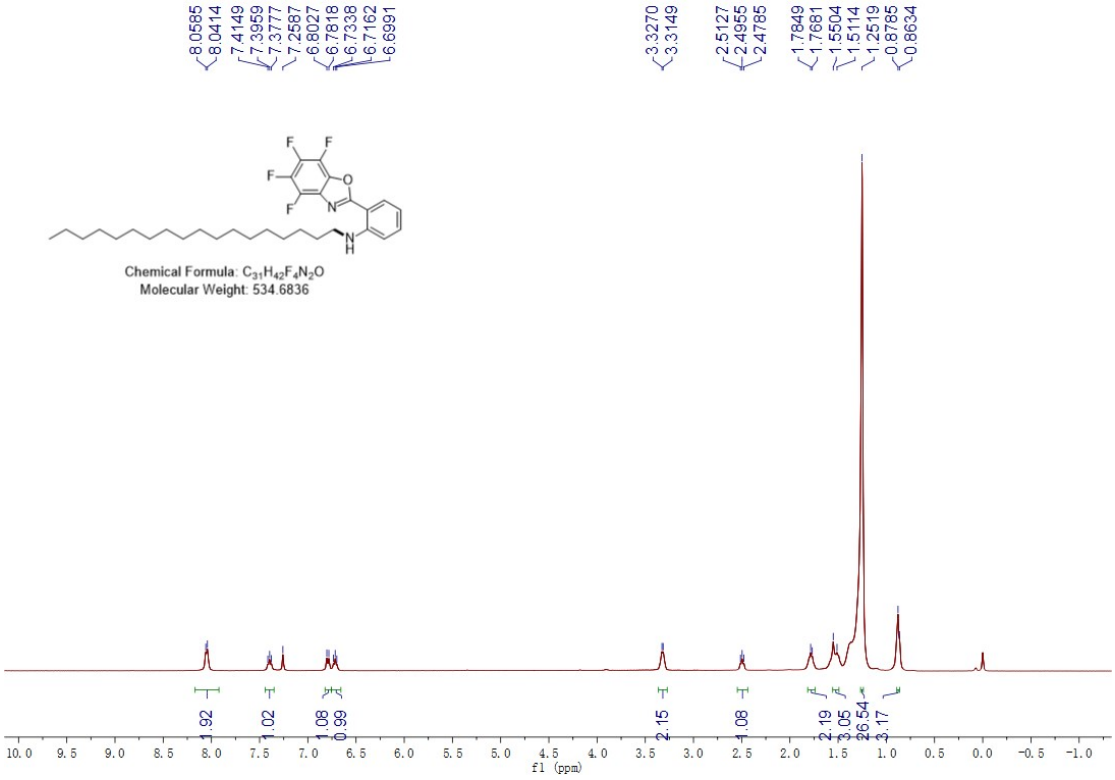


HRMS spectra

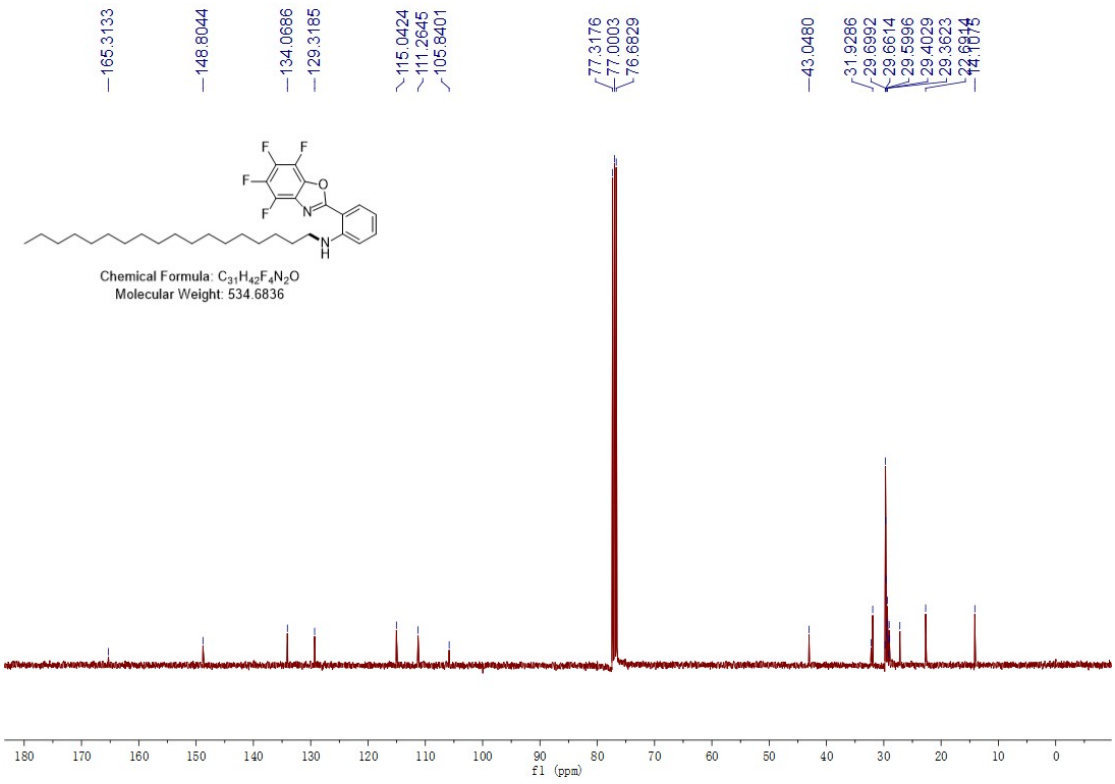


N-octadecyl-2-(perfluorobenzo[*d*]oxazol-2-yl)aniline (**4l**)

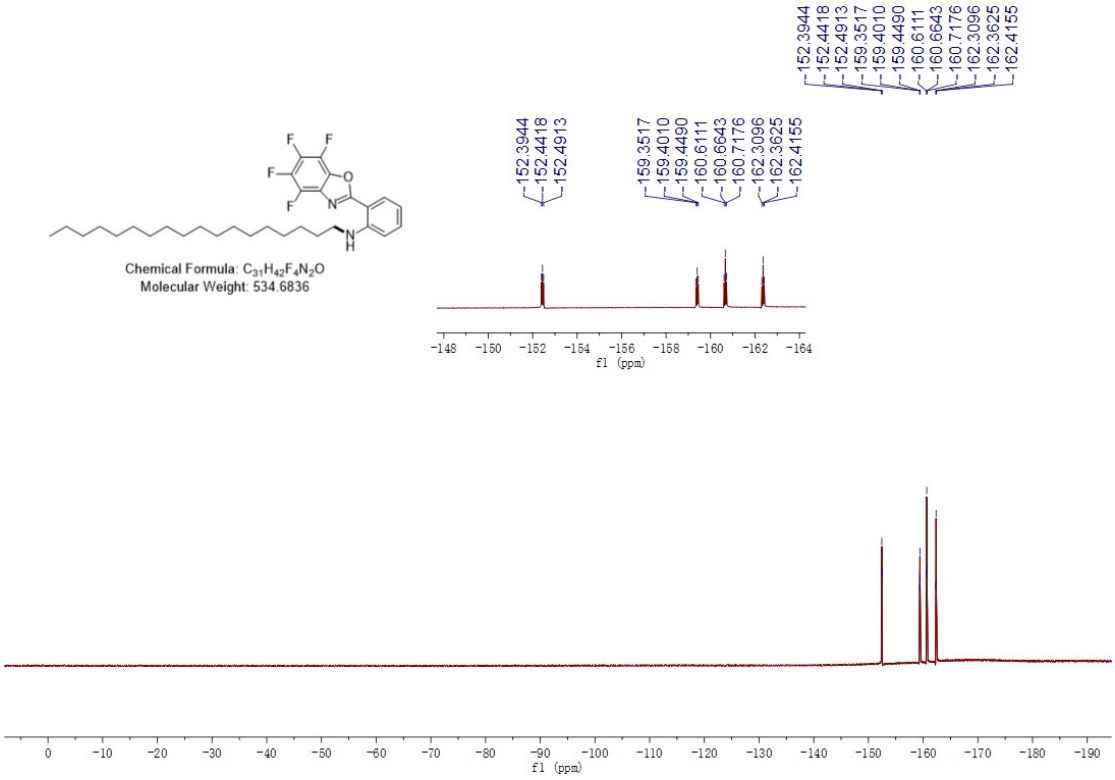
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (101 MHz, $CDCl_3$)



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



HRMS spectra