Electronic Supplementary Information

A soluble iron(II)-phthalocyanine-catalyzed intramolecular C(sp^3)–H amination with alkyl azides

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Table of Contents

General information

All catalytic reactions were performed using the standard Schlenk technique under an argon (Ar) atmosphere. Reagents obtained commercially were used without further purification unless indicated otherwise. Anhydrous toluene and dichloromethane (DCM) were freshly distilled with Na/benzophenone and CaH_2, respectively. Dry 1,2-dichloroethane (DCE), chlorobenzene, benzene, dimethylformamide (DMF) were purchased from J&K and were used directly. ^1H, ^{13}C NMR and ^{19}F spectra were measured on either a Bruker DPX-500 or DPX-400 spectrometer. Chemical shifts (δ) are reported in ppm, and coupling constants (*J*) are in Hertz (Hz). ^1H NMR and ^{13}C NMR chemical shifts were determined relative to internal standard tetramethylsilane (TMS). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. All reactions were monitored by thin-layer chromatography (TLC) or ^1H NMR. Flash column chromatography was carried out using 300–400 mesh silica gel. High-resolution mass spectra were recorded using a Q Exactive mass spectrometer (Thermo Fisher Scientific, USA).

Synthesis of iron complexes

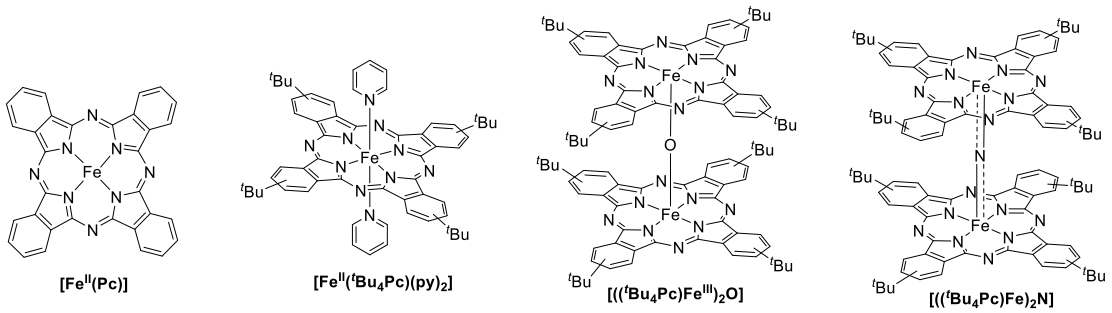


Fig. S1 The structures of iron phthalocyanine complexes.

$[Fe^{II}(Pc)]$ was purchased from Energy Chemical, and was used directly. $[Fe^{II}(^tBu_4Pc)(py)_2]$,[1] $[((^tBu_4Pc)Fe^{III})_2O]$[2] and $[((^tBu_4Pc)Fe)_2N]$[3] are known compounds, and were synthesized according to literatures (these three complexes were produced as isomeric mixtures, which were not separable). The UV-visible spectrum of $[Fe^{II}(^tBu_4Pc)(py)_2]$ is consistent with reported data.[1a,1c,4] ^1H NMR (400 MHz, benzene-d_6) δ 9.90 – 9.84 (m, 4H), 9.67 (dd, *J* = 8.0, 2.9 Hz, 4H), 8.00 – 7.93 (m, 4H), 4.60 (t, *J* = 7.5 Hz, 2H), 3.81 (t, *J* = 7.0 Hz, 4H), 2.43 (d, *J* = 5.4 Hz, 4H), 1.61 – 1.49 (m, 36H). HRMS (ESI) m/z: $[M - (py)_2]^+$ calcd. for $[C_{48}H_{48}N_8Fe]^+$: 792.3351, found 792.3387.

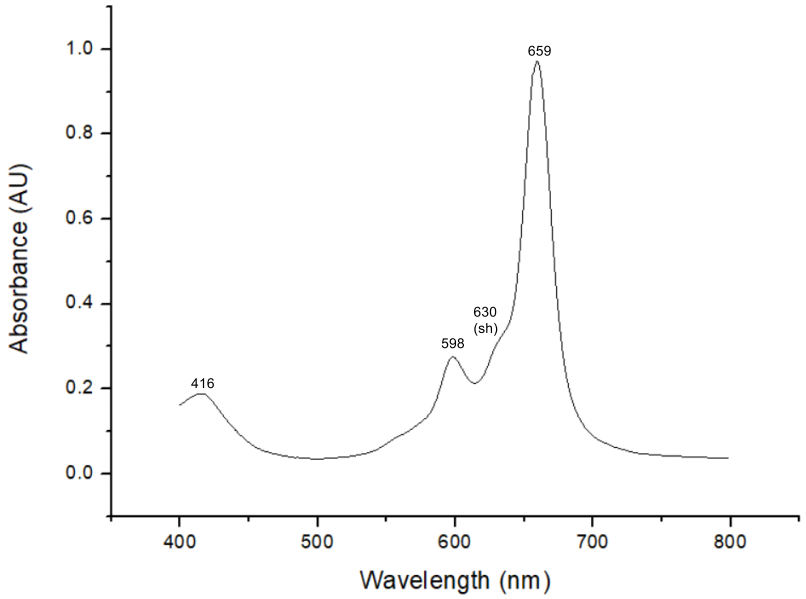


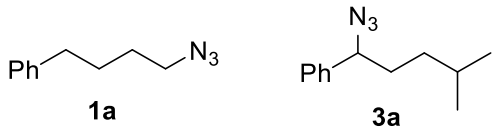
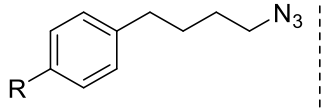
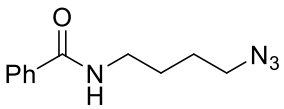
Fig. S2 UV-visible spectrum of [Fe^{II}(^{t}Bu$_4$Pc)(py)$_2$] in pyridine.

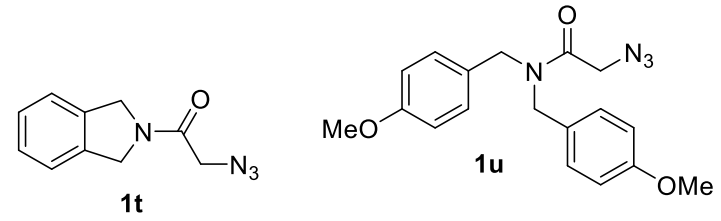
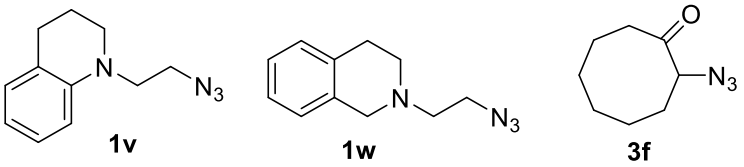
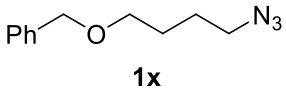
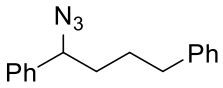
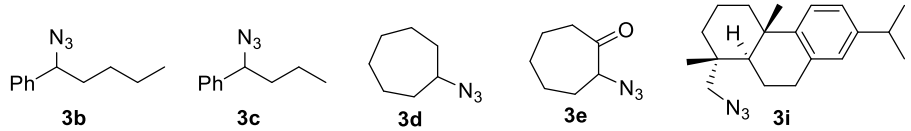
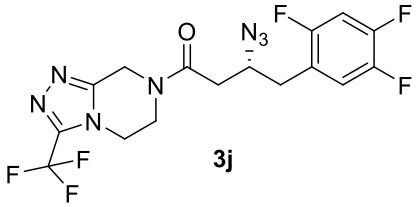
Synthesis of substrates

CAUTION: Organic azides are potentially explosive and should be handled with care. While we did not encounter any problems during handling these compounds, proper precautions should be taken during the whole process. Once isolated, these azides were stored in a -20 ºC freezer.

Alkyl azides reported in the literature were prepared according to the literature procedure and listed in Table S1. The detailed synthetic procedures and characterizations for the new azides were described below.

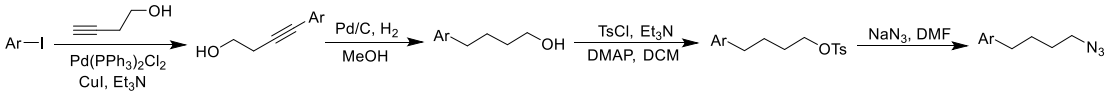
Table S1 Azides reported in the literature.

Azides	References
 **1a** **3a**	Ref. 5
 R = Me, **1b**; R = OMe, **1c** R = *N*,*N*-dimethyl, **1d**; R = F, **1f** R = Cl, **1g**	Ref. 6
 **1s**	Ref. 7

 **1t** **1u**	Ref. 8
 **1v** **1w** **3f**	Ref. 9
 **1x**	Ref. 10
 **1z**	Ref. 11
 **3b** **3c** **3d** **3e** **3i**	Ref. 12
 **3j**	Ref. 13

Synthesis of alkyl azides and their precursors

General procedure A for the synthesis of alkyl azides



Step 1:[14] To a solution of aryl iodide (1.0 equiv.), $PdCl_2(PPh_3)_2$ (0.05-0.1 equiv.), CuI (0.15-0.3 equiv.) in Et_3N (0.25 M) was added but-3-yn-1-ol (1.3 equiv.) and the mixture was stirred at room temperature under Ar atmosphere. After completion, the resulting mixture was concentrated under reduced pressure and the residue was subjected to column chromatography on silica gel to give the desired coupling product.

Step 2: To a solution of the above unsaturated substrate containing triple bond (5 mmol) in MeOH (0.1 M) was added 10% Pd/C (100 mg). Then the mixture was stirred vigorously under H_2 atmosphere (1 atm) overnight. Upon completion, the reaction mixture was filtered through celite and washed with ethyl acetate (EA). After

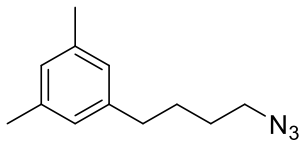
removal of the solvent, the residue was used for the next step directly.

Step 3: To a stirring solution of primary alcohol (1 equiv.) in anhydrous DCM (0.25 M), Et_3N (1.5 equiv.) and 4-dimethylaminopyridine (DMAP, 0.1 equiv.) were added. 4-Toluenesulfonyl chloride (TsCl, 1.2 equiv.) was added at 0 °C. Then, the reaction mixture was allowed to warm up to room temperature (rt) and stirred overnight. The mixture was quenched with water once completion. The aqueous phase was extracted three times with DCM. The combined organic phase was washed with sat. aq. $NaHCO_3$ and brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by silica column chromatography to give the corresponding tosylate.

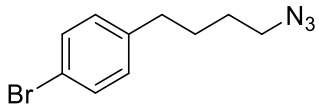
Step 4: To a stirring solution of tosylate (1 equiv.) in DMF (0.5 M) was added sodium azide (1.5 equiv.), and the reaction was heated at 80 °C overnight. After completion of the reaction, water was added and the mixture was extracted with Et_2O three times. The combined organic phase was washed with water and brine, respectively, and dried over Na_2SO_4. After removal of the solvent under reduced pressure, the residue was purified by silica column chromatography to give the desired azide.

General procedure B for the synthesis of alkyl alcohols from the reduction of carboxylic ester

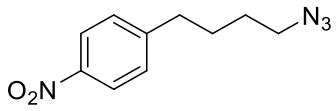
To a solution of alkyl carboxylic ester (5 mmol, 1 equiv.) in tetrahydrofuran (THF, 0.5 M) was added $LiAlH_4$ (375 mg, 10 mmol, 2 equiv.) portionwise at 0 °C under Ar atmosphere. Then the solution was stirred at rt for 24 h. After that, a solution of NaOH (10% in water) was added carefully until a white solid precipitated. After filtration over $MgSO_4$ and evaporation of the solvent the crude alcohol was directly used for the next step without further purification.



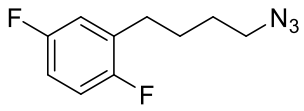
1-(4-Azidobutyl)-3,5-dimethylbenzene (1e): Synthesized following the general procedure A from 1-iodo-3,5-dimethylbenzene and obtained as a colorless oil (46% yield over four steps). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.90 (s, 1H), 6.86 (s, 2H), 3.33 (t, *J* = 6.6 Hz, 2H), 2.63 (t, *J* = 7.3 Hz, 2H), 2.36 (s, 6H), 1.79 – 1.65 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.8, 137.9, 127.6, 126.3, 51.4, 35.3, 28.5, 21.3. HRMS (ESI) m/z: $[M - N_2 + H]^+$ calcd. for $[C_{12}H_{18}N]^+$: 176.1434, found 176.1434.



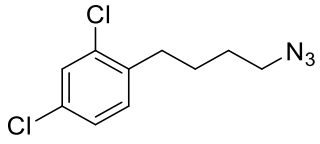
1-(4-Azidobutyl)-4-bromobenzene (1h): Synthesized following the general procedure A (steps 3 and 4) from 4-(4-bromophenyl)butan-1-ol and obtained as a colorless oil (78% yield over two steps). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.3 Hz, 2H), 7.05 (d, *J* = 8.4 Hz, 2H), 3.28 (t, *J* = 6.6 Hz, 2H), 2.59 (t, *J* = 7.4 Hz, 2H), 1.72 – 1.65 (m, 2H), 1.64 – 1.58 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.8, 131.4, 130.1, 119.7, 51.3, 34.8, 28.4, 28.3. HRMS (ESI) m/z: $[M - N_2 + H]^+$ calcd. for $[C_{10}H_{13}NBr]^+$: 226.0226, found 226.0222.



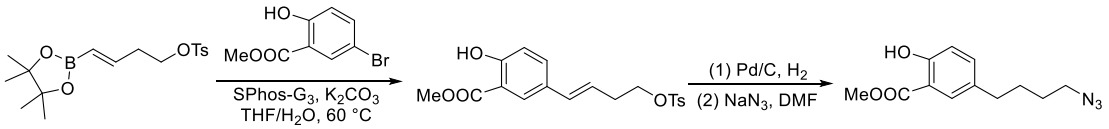
1-(4-Azidobutyl)-4-nitrobenzene (1i): Synthesized following the general procedure A (steps 3 and 4) from 4-(4-nitrophenyl)butan-1-ol and obtained as a light yellow oil (77% yield over two steps). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.7 Hz, 2H), 7.34 (d, *J* = 8.6 Hz, 2H), 3.32 (t, *J* = 6.6 Hz, 2H), 2.76 (t, *J* = 7.6 Hz, 2H), 1.80 – 1.70 (m, 2H), 1.69 – 1.60 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.7, 146.4, 129.2, 123.7, 51.2, 35.3, 28.4, 28.0. HRMS (ESI) m/z: $[M - N_2 + H]^+$ calcd. for $[C_{10}H_{13}N_2O_2]^+$: 193.0972, found 193.0971.



2-(4-Azidobutyl)-1,4-difluorobenzene (1j): Synthesized following the general procedure A and obtained as a colorless oil (30% yield over four steps). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.96 (td, *J* = 9.0, 4.6 Hz, 1H), 6.91 – 6.81 (m, 2H), 3.30 (t, *J* = 6.5 Hz, 2H), 2.65 (t, *J* = 7.0 Hz, 2H), 1.75 – 1.59 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ158.6 (dd, *J* = 241.6, 2.4 Hz), 157.0 (dd, *J* = 240.2, 2.4 Hz), 130.3 (dd, *J* = 18.8, 7.6 Hz), 116.7 (dd, *J* = 23.6, 5.4 Hz), 116.1 (dd, *J* = 25.4, 8.8 Hz), 113.9 (dd, *J* = 24.0, 8.5 Hz), 51.2, 28.5, 28.4, 27.0. ^{19}F NMR (376 MHz, $CDCl_3$) δ -119.62 (d, *J* = 17.6 Hz), -125.03 (d, *J* = 17.6 Hz). HRMS (EI) m/z: $[M - N_2 - H]^+$ calcd. for $[C_{10}H_{10}F_2N]^+$: 182.0781, found 182.0776.

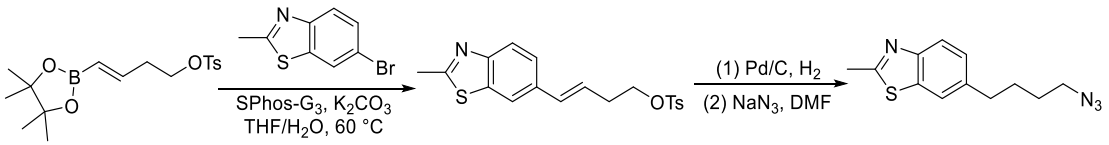


1-(4-Azidobutyl)-2,4-dichlorobenzene (1k): Synthesized following the general procedure A from 2,4-dichloro-1-iodobenzene and obtained as a colorless oil (45% yield over four steps). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 2.0 Hz, 1H), 7.18 (dd, *J* = 8.2, 2.0 Hz, 1H), 7.14 (d, *J* = 8.2 Hz, 1H), 3.32 (t, *J* = 6.4 Hz, 2H), 2.73 (t, *J* = 7.3 Hz, 2H), 1.74 – 1.62 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.1, 134.5, 132.3, 131.1, 129.2, 127.1, 51.2, 32.5, 28.5, 26.8. HRMS (ESI) m/z: $[M - N_2 + H]^+$ calcd. for $[C_{10}H_{12}Cl_2N]^+$: 216.0341, found 216.0342.



Methyl (*E*)-2-hydroxy-5-(4-(tosyloxy)but-1-en-1-yl)benzoate: Synthesized following the reported general procedure for the Suzuki-Miyaura coupling reactions[15] to provide the desired compound as a colorless oil (77% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.72 (s, 1H), 7.78 (d, *J* = 8.3 Hz, 2H), 7.73 (d, *J* = 2.1 Hz, 1H), 7.39 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.30 (d, *J* = 8.4 Hz, 2H), 6.91 (d, *J* = 8.6 Hz, 1H), 6.30 (d, *J* = 15.9 Hz, 1H), 5.89 (dt, *J* = 15.8, 7.0 Hz, 1H), 4.12 (t, *J* = 6.5 Hz, 2H), 3.95 (s, 3H), 2.53 (q, *J* = 6.5 Hz, 2H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.4, 160.9, 144.8, 133.1, 133.0, 131.8, 129.8, 128.5, 127.9, 127.5, 122.7, 117.8, 112.2, 69.7, 52.4, 32.4, 21.6. HRMS (ESI) m/z: $[M + H]^+$ calcd. for $[C_{19}H_{21}O_6S]^+$ 377.1053, found 377.1054.

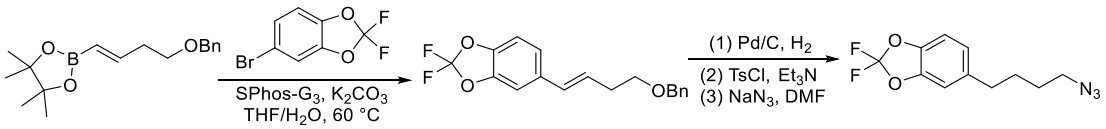
Methyl 5-(4-azidobutyl)-2-hydroxybenzoate (1l): Synthesized following the general procedure A (steps 2 and 4), and obtained as a colorless oil (28% yield over two steps). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.60 (s, 1H), 7.62 (d, *J* = 2.2 Hz, 1H), 7.25 (dd, *J* = 8.5, 2.3 Hz, 1H), 6.89 (d, *J* = 8.5 Hz, 1H), 3.92 (s, 3H), 3.26 (t, *J* = 6.5 Hz, 2H), 2.55 (t, *J* = 7.3 Hz, 2H), 1.71 – 1.55 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.5, 159.9, 135.9, 132.5, 129.1, 117.5, 112.0, 52.2, 51.3, 34.3, 28.5, 28.3. HRMS (ESI) m/z: $[M - N_2 + H]^+$ calcd. for $[C_{12}H_{16}NO_3]^+$: 222.1125, found 222.1123.



(*E*)-4-(2-Methylbenzo[*d*]thiazol-6-yl)but-3-en-1-yl 4-methylbenzenesulfonate: Synthesized following the reported general procedure for the Suzuki-Miyaura coupling reactions[15] using 6-bromo-2-methylbenzo[*d*]thiazole (600 mg, 2.6 mmol, 1.0

equiv.), (*E*)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)but-3-en-1-yl 4-methylbenzenesulfonate[16] (1.21 g, 3.45 mmol, 1.3 equiv.), SPhos-G3 (99 mg, 0.132 mmol, 0.05 equiv.), and K_2CO_3 (1.09 g, 7.89 mmol, 3.0 equiv.) in THF/H_2O = 3:1 (0.3 M) at 60 °C for 6 h. The crude residue was purified by column chromatography to provide the desired compound as a colorless oil (600 mg, ~ 45% yield, the yield was calculated after deducting pinacol residue according to ^{1}H NMR ratios). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (dd, *J* = 8.4, 3.3 Hz, 1H), 7.76 – 7.70 (m, 2H), 7.61 (d, *J* = 2.7 Hz, 1H), 7.33 – 7.27 (m, 1H), 7.25 – 7.19 (m, 2H), 6.40 (d, *J* = 15.8 Hz, 1H), 6.05 – 5.91 (m, 1H), 4.11 (t, *J* = 6.4 Hz, 2H), 2.76 (s, 3H), 2.57 – 2.47 (m, 2H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.2, 152.6, 144.8, 136.1, 133.9, 132.9, 132.6, 129.8, 127.9, 124.5, 124.2, 122.1, 118.9, 69.6, 32.5, 21.6, 20.1. HRMS (ESI) m/z: [M + H]$^+$ calcd. for $[C_{19}H_{20}NO_3S_2]^+$: 374.0879, found 374.0876.

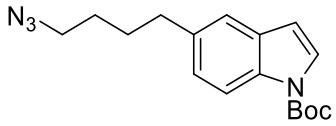
6-(4-Azidobutyl)-2-methylbenzo[*d*]thiazole (1m): Synthesized following the general procedure A (steps 2 and 4), and obtained as a colorless oil (97% yield over two steps). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.3 Hz, 1H), 7.49 (s, 1H), 7.14 (dd, *J* = 8.3, 1.4 Hz, 1H), 3.15 (t, *J* = 6.7 Hz, 2H), 2.69 (s, 3H), 2.62 (t, *J* = 7.5 Hz, 2H), 1.68 – 1.56 (m, 2H), 1.55 – 1.46 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.0, 151.8, 138.7, 135.9, 126.6, 122.0, 120.6, 51.2, 35.2, 28.6, 28.4, 20.0. HRMS (ESI) m/z: [M + H]$^+$ calcd. for $[C_{12}H_{15}N_4S]^+$: 247.1012, found 247.1009.



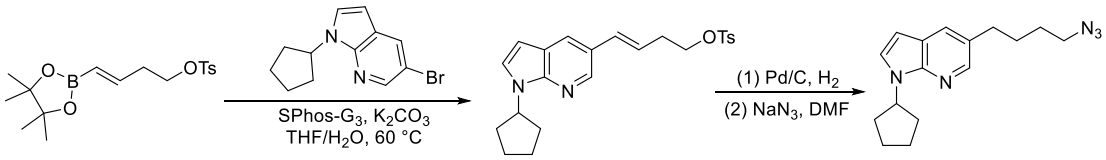
(*E*)-5-(4-(Benzyloxy)but-1-en-1-yl)-2,2-difluorobenzo[*d*][1,3]dioxole: Synthesized following the reported general procedure for the Suzuki-Miyaura coupling reactions[15] using 5-bromo-2,2-difluorobenzo[*d*][1,3]dioxol (600 mg, 2.53 mmol, 1.0 equiv.), (*E*)-2-(4-(benzyloxy)but-1-en-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane[16] (947 mg, 3.29 mmol, 1.3 equiv.), SPhos-G3 (94.8 mg, 0.126 mmol, 0.05 equiv.) and K_2CO_3 (1.047 g, 7.59 mmol, 3.0 equiv.) in THF/H_2O = 3:1 (0.3 M) at 60 °C for 6 h. The crude residue was purified by column chromatography to provide the desired compound (668 mg, 83% yield) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.28 (m, 5H), 7.09 (d, *J* = 1.5 Hz, 1H), 7.00 (dd, *J* = 8.3, 1.5 Hz, 1H), 6.97 (d, *J* = 8.2 Hz, 1H), 6.42 (d, *J* = 15.9 Hz, 1H), 6.17 (dt, *J* = 15.9, 6.9 Hz, 1H), 4.57 (s, 2H), 3.62 (t, *J* = 6.6 Hz, 2H), 2.59 – 2.50 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.3, 142.9, 138.5, 134.4, 131.8 (t, *J* = 254.8 Hz), 130.5, 128.6, 127.9, 127.8, 127.8, 122.0, 109.4, 106.6, 73.2, 69.7, 33.5. ^{19}F NMR (376 MHz, $CDCl_3$) δ -50.24.

5-(4-Azidobutyl)-2,2-difluorobenzo[*d*][1,3]dioxole (1n): Synthesized following the general procedure A (steps 2, 3 and 4), and obtained as a colorless oil (21% yield over

three steps). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (d, *J* = 8.1 Hz, 1H), 6.91 – 6.84 (m, 2H), 3.29 (t, *J* = 6.6 Hz, 2H), 2.64 (t, *J* = 7.4 Hz, 2H), 1.75 – 1.56 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.8, 142.0, 138.1, 131.7 (t, *J* = 254.1 Hz), 123.2, 109.5, 109.1, 51.2, 35.1, 28.6, 28.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -50.12. HRMS (ESI) m/z: [M – N_2 + H]$^+$ calcd. for $[C_{11}H_{12}F_2NO_2]^+$: 228.0831, found 228.0829.



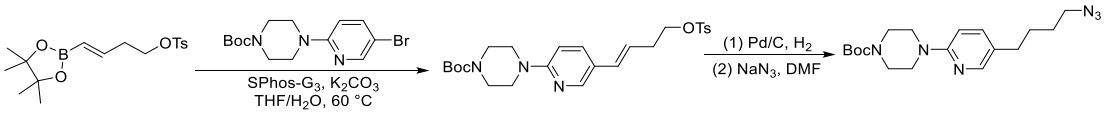
***tert*-Butyl 5-(4-azidobutyl)-1*H*-indole-1-carboxylate (1o):** Synthesized following the general procedure A from *tert*-butyl 5-iodo-1*H*-indole-1-carboxylate[17] and obtained as a colorless oil (68% yield over four steps). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.1 Hz, 1H), 7.56 (d, *J* = 3.4 Hz, 1H), 7.34 (s, 1H), 7.12 (d, *J* = 8.4 Hz, 1H), 6.50 (d, *J* = 3.6 Hz, 1H), 3.27 (t, *J* = 6.8 Hz, 2H), 2.73 (t, *J* = 7.4 Hz, 2H), 1.83 – 1.70 (m, 2H), 1.66 (s, 9H), 1.65 – 1.53 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.9, 136.3, 133.8, 130.9, 126.2, 125.0, 120.4, 115.1, 107.2, 83.6, 51.5, 35.3, 29.0, 28.5, 28.3. HRMS (ESI) m/z: [M – N_2 + H]$^+$ calcd. for $[C_{17}H_{23}N_2O_2]^+$: 287.1754, found 287.1752.



(*E*)-4-(1-Cyclopentyl-1H-pyrrolo[2,3-*b*]pyridin-5-yl)but-3-en-1-yl 4-methylbenzenesulfonate: Synthesized following the reported general procedure for the Suzuki-Miyaura coupling reactions[15] from 5-bromo-1-cyclopentyl-1*H*-pyrrolo[2,3-*b*]pyridine[18] to provide the desired compound as a colorless oil (46% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 2.0 Hz, 1H), 7.82 – 7.74 (m, 3H), 7.29 – 7.26 (m, 2H), 7.25 (s, 1H), 6.47 (d, *J* = 15.9 Hz, 1H), 6.41 (d, *J* = 3.6 Hz, 1H), 5.95 (dt, *J* = 15.9, 7.0 Hz, 1H), 5.31 – 5.20 (m, 1H), 4.15 (t, *J* = 6.6 Hz, 2H), 2.60 – 2.51 (m, 2H), 2.35 (s, 3H), 2.27 – 2.17 (m, 2H), 1.96 – 1.67 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.3, 144.8, 141.8, 133.1, 131.3, 129.8, 127.9, 125.7, 125.3, 125.1, 122.3, 120.6, 99.7, 69.9, 55.0, 32.9, 32.6, 24.1, 21.6. HRMS (ESI) m/z: [M + H]$^+$ calcd. for $[C_{23}H_{27}N_2O_3S]^+$: 411.1737, found 411.1740.

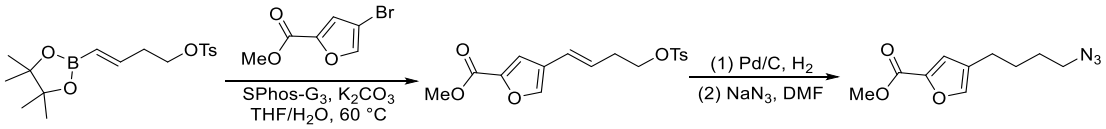
5-(4-Azidobutyl)-1-cyclopentyl-1*H*-pyrrolo[2,3-b]pyridine (1p): Synthesized following the general procedure A (steps 2 and 4) and obtained as a colorless oil (69% yield over two steps). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 1.9 Hz, 1H), 7.66 (d, *J* = 1.9 Hz, 1H), 7.24 (d, *J* = 3.5 Hz, 1H), 6.37 (d, *J* = 3.5 Hz, 1H), 5.35 – 5.18 (m,

1H), 3.23 (t, *J* = 6.7 Hz, 2H), 2.69 (t, *J* = 7.4 Hz, 2H), 2.28 – 2.13 (m, 2H), 1.89 – 1.79 (m, 4H), 1.78 – 1.65 (m, 4H), 1.64 – 1.56 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.7, 143.1, 128.6, 128.0, 125.1, 120.6, 99.0, 54.9, 51.3, 32.9, 32.6, 29.1, 28.3, 24.1. HRMS (ESI) m/z: $[M + H]^+$ calcd. for $[C_{16}H_{22}N_5]^+$: 284.1870, found 284.1867.



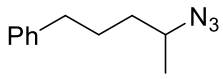
***tert*-Butyl (*E*)-4-(5-(4-(tosyloxy)but-1-en-1-yl)pyridin-2-yl)piperazine-1-carboxylate:** Synthesized following the reported general procedure for the Suzuki-Miyaura coupling reactions[15] to provide the desired compound as a colorless oil (39% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 2.2 Hz, 1H), 7.78 (d, *J* = 8.3 Hz, 2H), 7.48 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.31 (d, *J* = 8.1 Hz, 2H), 6.60 (d, *J* = 8.8 Hz, 1H), 6.27 (d, *J* = 15.9 Hz, 1H), 5.83 (dt, *J* = 15.8, 7.0 Hz, 1H), 4.12 (t, *J* = 6.6 Hz, 2H), 3.53 (s, 8H), 2.53 (q, *J* = 6.3 Hz, 2H), 2.43 (s, 3H), 1.49 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.5, 154.8, 146.6, 144.8, 134.4, 133.1, 129.8, 129.8, 127.9, 122.9, 121.5, 107.0, 80.0, 69.8, 45.1, 45.1, 32.6, 28.4, 21.7. HRMS (ESI) m/z: $[M + H]^+$ calcd. for $[C_{25}H_{34}N_3O_5S]^+$: 488.2214, found 488.2214.

***tert*-Butyl 4-(5-(4-azidobutyl)pyridin-2-yl)piperazine-1-carboxylate (1q):** Synthesized following the general procedure A (steps 2 and 4), and obtained as a colorless oil (40% yield over two steps). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 1.8 Hz, 1H), 7.33 (dd, *J* = 8.5, 2.2 Hz, 1H), 6.61 (d, *J* = 8.6 Hz, 1H), 3.57 – 3.51 (m, 4H), 3.50 – 3.44 (m, 4H), 3.27 (t, *J* = 6.3 Hz, 2H), 2.52 (t, *J* = 6.9 Hz, 2H), 1.68 – 1.57 (m, 4H), 1.48 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.1, 154.8, 147.4, 137.7 126.6, 107.2, 79.8, 51.2, 45.4, 31.4, 28.4, 28.4, 28.2. HRMS (ESI) m/z: $[M + H]^+$ calcd. for $[C_{18}H_{29}N_6O_2]^+$: 361.2347, found 361.2343.

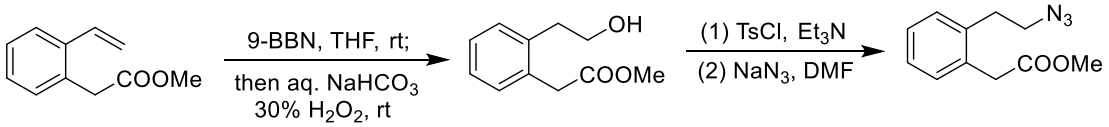


Methyl (*E*)-4-(4-(tosyloxy)but-1-en-1-yl)furan-2-carboxylate: Synthesized following the reported general procedure for the Suzuki-Miyaura coupling reactions[15] to provide the desired compound as a colorless oil (44% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.3 Hz, 2H), 7.46 (s, 1H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.17 (s, 1H), 6.21 (d, *J* = 15.9 Hz, 1H), 5.80 (dt, *J* = 15.8, 7.0 Hz, 1H), 4.11 (t, *J* = 6.4 Hz, 2H), 3.90 (s, 3H), 2.51 (q, *J* = 6.4 Hz, 2H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 144.9, 144.9, 143.1, 133.0, 129.9, 127.9, 125.7, 121.7, 115.3, 69.3, 52.0, 32.3, 21.6. HRMS (ESI) m/z: $[M + H]^+$ calcd. for $[C_{17}H_{19}O_6S]^+$: 351.0897, found 351.0894.

Methyl 4-(4-azidobutyl)furan-2-carboxylate (1r): Synthesized following the general procedure A (steps 2 and 4) and obtained as a colorless oil (53% yield over two steps). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (s, 1H), 6.98 (s, 1H), 3.79 (s, 3H), 3.21 (t, *J* = 6.1 Hz, 2H), 2.39 (t, *J* = 6.8 Hz, 2H), 1.60 – 1.50 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 144.5, 142.9, 126.9, 118.8, 51.7, 51.1, 28.2, 26.8, 24.0. HRMS (ESI) m/z: $[M - N_2 + H]^+$ calcd. for $[C_{10}H_{14}NO_3]^+$: 196.0968, found 196.0968.

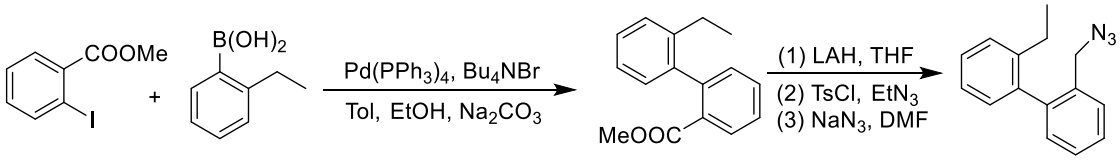


(4-Azidopentyl)benzene (1y): Synthesized following the general procedure A (steps 3 and 4) from 5-phenylpentan-2-ol[19] and obtained as a colorless oil (58% yield over two steps). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.24 (m, 2H), 7.22 – 7.14 (m, 3H), 3.50 – 3.38 (m, 1H), 2.62 (t, *J* = 7.6 Hz, 2H), 1.82 – 1.62 (m, 2H), 1.59 – 1.45 (m, 2H), 1.24 (d, *J* = 6.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.0, 128.4, 125.9, 57.9, 35.8, 35.6, 27.9, 19.5. HRMS (ESI) m/z: $[M - N_2 + H]^+$ calcd. for $[C_{11}H_{16}N]^+$: 162.1277, found 162.1277.



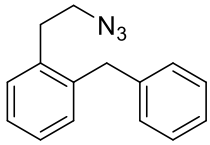
Methyl 2-(2-(2-hydroxyethyl)phenyl)acetate: Synthesized following the reported procedure.[20] To a flask containing methyl 2-(2-vinylphenyl)acetate[21] (1.19 g, 6.75 mmol) was added 9-BBN (0.5 M solution in THF, 27 mL, 13.5 mmol), and the solution was stirred at rt for several hours until completion. The resultant mixture was cooled to 0 °C and treated with saturated aqueous $NaHCO_3$ (27 mL) and 30% H_2O_2 (10 mL). After being stirred at rt overnight, the resultant mixture was extracted with EtOAc, washed with saturated aqueous Na_2SO_3 and brine, dried over Na_2SO_4, filtered, and concentrated under reduced pressure. Purification of the residue by silica gel flash chromatography gave alcohol (824 mg, 63% yield) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.17 (m, 4H), 3.81 (t, *J* = 6.7 Hz, 2H), 3.71 (s, 2H), 3.68 (s, 3H), 2.90 (t, *J* = 6.7 Hz, 2H), 2.13 (br s, 1H).

Methyl 2-(2-(2-azidoethyl)phenyl)acetate (3g): Synthesized following the general procedure A (steps 3 and 4) and obtained as a colorless oil (86% yield over two steps). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 – 7.19 (m, 4H), 3.70 (s, 3H), 3.69 (s, 2H), 3.50 (t, *J* = 7.4 Hz, 2H), 2.94 (t, *J* = 7.4 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.9, 136.6, 132.7, 131.0, 129.9, 127.8, 127.3, 52.2, 51.9, 38.6, 32.3. HRMS (ESI) m/z: $[M + Na]^+$ calcd. for $[C_{11}H_{13}N_3NaO_2]^+$: 242.0900, found 242.0901.



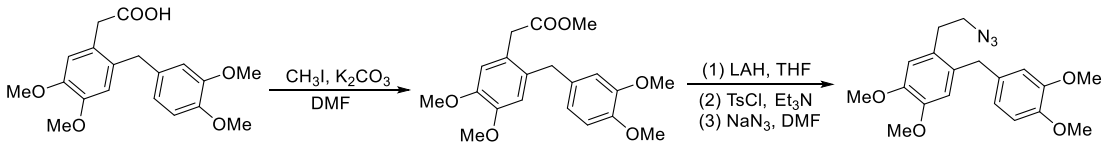
Methyl 2'-ethyl-[1,1'-biphenyl]-2-carboxylate : A mixture of methyl 2-iodobenzoate (524 mg, 2 mmol), (2-ethylphenyl)boronic acid (450 mg, 3 mmol, 1.5 equiv.), toluene (15 mL), ethanol (6 mL) and 2 M Na_2CO_3 (2 mL, 4 mmol, 2 equiv.) was degassed, then $Pd(PPh_3)_4$ (115.5 mg, 0.1 mmol, 0.05 equiv.) and Bu_4NBr (32 mg, 0.1 mmol, 0.05 equiv.) were added under Ar. The mixture was heated at 95 °C for 4 h, then stirred overnight at rt. The reaction was diluted with water and extracted with EA. The combined extract was washed with brine, dried over anhydrous Na_2SO_4, filtered and evaporated. The residue was purified by silica gel chromatography to provide the desired product as a colorless oil (388 mg, 81% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.53 (td, *J* = 7.6, 1.4 Hz, 1H), 7.42 (td, *J* = 7.6, 1.3 Hz, 1H), 7.35 – 7.26 (m, 3H), 7.19 (td, *J* = 7.1, 2.1 Hz, 1H), 7.05 (d, *J* = 8.0 Hz, 1H), 3.59 (s, 3H), 2.49 – 2.31 (m, 2H), 1.03 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.8, 142.8, 141.2, 140.9, 131.4, 131.2, 130.0, 128.7, 127.8, 127.5, 127.1, 125.1, 51.8, 26.2, 14.9. HRMS (ESI) m/z: $[M + H]^+$ calcd. for $[C_{16}H_{17}O_2]^+$: 241.1223, found 241.1221.

2-(Azidomethyl)-2'-ethyl-1,1'-biphenyl (3h): Synthesized following the general procedures B and A (steps 3 and 4), and obtained as a colorless oil (56% yield over three steps). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 (d, *J* = 7.4 Hz, 1H), 7.42 – 7.31 (m, 4H), 7.26 – 7.19 (m, 2H), 7.10 (d, *J* = 7.3 Hz, 1H), 4.12 (d, *J* = 13.7 Hz, 1H), 4.08 (d, *J* = 13.8 Hz, 1H), 2.46 – 2.26 (m, 2H), 1.04 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 141.9, 141.2, 139.0, 133.5, 130.2, 129.7, 128.8, 128.4, 128.1, 127.9, 127.8, 125.6, 52.5, 26.2, 15.2. HRMS (ESI) m/z: $[M - N_2 + H]^+$ calcd. for $[C_{15}H_{16}N]^+$: 210.1277, found 210.1277.



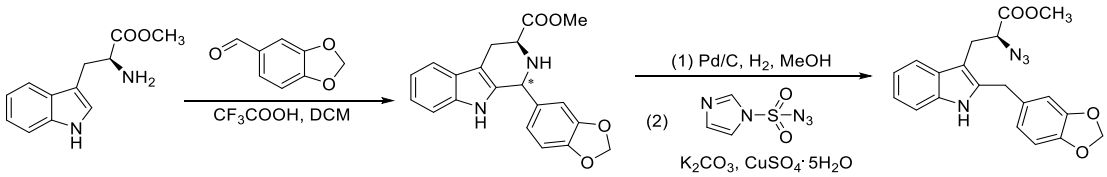
1-(2-Azidoethyl)-2-benzylbenzene (3k): Synthesized following the general procedure A (steps 3 and 4) from 2-(2-benzylphenyl)ethan-1-ol[22] and obtained as a colorless oil (87% yield over two steps). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.24 (m, 2H), 7.24 – 7.14 (m, 5H), 7.11 (d, *J* = 7.0 Hz, 2H), 4.04 (s, 2H), 3.22 (t, *J* = 7.6 Hz, 2H), 2.86 (t, *J* = 7.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.6, 138.8, 136.4, 131.0, 130.0, 128.6, 128.6, 127.1, 126.2, 51.8, 39.2, 32.3. HRMS (ESI) m/z: $[M + H]^+$

calcd. for $[C_{15}H_{16}N_3]^+$: 238.1339, found 238.1336.



Methyl 2-(2-(3,4-dimethoxybenzyl)-4,5-dimethoxyphenyl)acetate: To a stirred mixture of 2-(2-(3,4-dimethoxybenzyl)-4,5-dimethoxyphenyl)acetic acid[23] (2.5 g, 7.22 mmol, 1.0 equiv.) and K_2CO_3 (3 g, 21.7 mmol, 3.0 equiv.) in DMF (20 mL), methyl iodide (0.9 mL, 14.44 mmol, 2.0 equiv.) was added at room temperature, and then the reaction mixture was stirred at room temperature for 5 h. After completion, the mixture was diluted by 100 mL H_2O. The aqueous layer was extracted three times with EA. The combined organic layer was washed twice with brine, dried over Na_2SO_4, and evaporated. The residue was purified by silica gel flash chromatography to give the desired compound as an off-white solid (2.4 g, ~ 77% yield, the yield was calculated after deducting DMF residue according to ^{1}H NMR ratios). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.79 – 6.76 (m, 2H), 6.67 – 6.63 (m, 2H), 6.61 (d, *J* = 8.3 Hz, 1H), 3.93 (s, 2H), 3.88 (s, 3H), 3.85 (s, 3H), 3.81 (s, 3H), 3.80 (s, 3H), 3.62 (s, 3H), 3.54 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.2, 148.9, 148.1, 147.4, 147.3, 133.0, 131.6, 124.8, 120.5, 113.9, 113.7, 111.9, 111.2, 56.0, 55.9, 55.8, 52.0, 38.2, 38.1. HRMS (ESI) m/z: $[M + Na]^+$ calcd. for $[C_{20}H_{24}O_6Na]^+$: 383.1465, found 383.1466.

1-(2-Azidoethyl)-2-(3,4-dimethoxybenzyl)-4,5-dimethoxybenzene (3l): Synthesized following the general procedures B and A (steps 3 and 4) and obtained as a colorless oil (58% yield over three steps). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.77 (d, *J* = 8.2 Hz, 1H), 6.72 (s, 1H), 6.68 (s, 1H), 6.65 (d, *J* = 1.8 Hz, 1H), 6.61 (dd, *J* = 8.2, 1.8 Hz, 1H), 3.92 (s, 2H), 3.87 (s, 3H), 3.83 (s, 3H), 3.81 (s, 3H), 3.80 (s, 3H), 3.23 (t, *J* = 7.5 Hz, 2H), 2.81 (t, *J* = 7.5 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.0, 147.7, 147.6, 147.4, 133.4, 131.1, 128.4, 120.4, 114.0, 113.3, 111.8, 111.3, 56.0, 55.9, 55.9, 55.8, 51.9, 38.2, 32.1. HRMS (ESI) m/z: $[M + Na]^+$ calcd. for $[C_{19}H_{23}N_3O_4Na]^+$: 380.1581, found 380.1580.

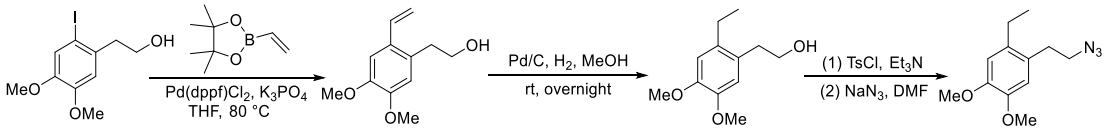


Methyl (*S*)-1-(benzo[*d*][1,3]dioxol-5-yl)-2,3,4,9-tetrahydro-1*H*-1λ^3-pyrido[3,4-*b*]indole-3-carboxylate: Trifluoroacetic acid (1.02 g, 8.93 mmol, 1.5 equiv.) was added to a solution of (*S*)-tryptophan methyl ester[24] (1.3 g, 5.96 mmol, 1.0 equiv.) and

benzo[*d*][1,3]dioxole-5-carbaldehyde (1.08 g, 7.15 mmol, 1.2 equiv.) in DCM (20 mL). The reaction mixture was stirred for 1 day at room temperature and then evaporated. The obtained residue was triturated with a 5% K_2CO_3 aqueous solution (30 mL) and extracted with DCM. The organic layer was dried over $MgSO_4$ and evaporated to dryness under reduced pressure. The residue was purified by column chromatography to afford the desired product as isomers (76% yield). The isolated ratio of the two isomers is nearly 1:1. **Isomer a** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.50 (m, 2H), 7.24 – 7.19 (m, 1H), 7.18 – 7.09 (m, 2H), 6.87 (dd, *J* = 7.8, 1.7 Hz, 1H), 6.82 (d, *J* = 1.7 Hz, 1H), 6.79 (d, *J* = 7.9 Hz, 1H), 5.94 (s, 2H), 5.15 (t, *J* = 2.1 Hz, 1H), 3.94 (dd, *J* = 11.1, 4.2 Hz, 1H), 3.81 (s, 3H), 3.21 (ddd, *J* = 15.0, 4.2, 1.8 Hz, 1H), 2.99 (ddd, *J* = 15.0, 11.1, 2.5 Hz, 1H). 2.43 (br s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.3, 148.3, 148.0, 136.3, 134.9, 134.8, 127.3, 122.1, 119.8, 118.4, 111.1, 109.0, 108.9, 108.5, 101.4, 58.6, 57.0, 52.4, 25.8. HRMS (ESI) m/z: $[M + H]^+$ calcd. for $[C_{20}H_{19}N_2O_4]^+$: 351.1339, found 351.1333. **Isomer b** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 – 7.73 (m, 1H), 7.55 (d, *J* = 7.3 Hz, 1H), 7.22 (d, *J* = 7.4 Hz, 1H), 7.19 – 7.09 (m, 2H), 6.78 – 6.67 (m, 3H), 5.90 (s, 2H), 5.31 – 5.25 (m, 1H), 3.96 (t, *J* = 6.0 Hz, 1H), 3.71 (s, 3H), 3.25 (dd, *J* = 15.4, 5.4 Hz, 1H), 3.10 (dd, *J* = 15.3, 6.7 Hz, 1H), 2.37 (br s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.2, 148.1, 147.4, 136.2, 136.1, 133.3, 127.0, 122.0, 121.7, 119.5, 118.3, 111.0, 108.7, 108.3, 108.1, 101.2, 54.7, 52.5, 52.1, 24.7. HRMS (ESI) m/z: $[M + H]^+$ calcd. for $[C_{20}H_{19}N_2O_4]^+$: 351.1339, found 351.1331.

Methyl (*S*)-2-azido-3-(2-(benzo[*d*][1,3]dioxol-5-ylmethyl)-1*H*-indol-3-yl)propanoate (3m): Step 1. To a solution of the above isomers (600 mg, 1.72 mmol) in MeOH (50 mL) was added 10% Pd/C (60 mg). The resulting solution was stirred at 50 °C under atmospheric pressure of hydrogen for 3 days. The solution was concentrated to dryness. The residue was purified by column chromatography to afford methyl (*S*)-2-amino-3-(2-(benzo[*d*][1,3]dioxol-5-ylmethyl)-1*H*-indol-3-yl)propanoate as an off-white solid (450 mg, 74% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.57 (d, *J* = 7.2 Hz, 1H), 7.20 (d, *J* = 7.5 Hz, 1H), 7.16 – 7.07 (m, 2H), 6.73 (d, *J* = 8.2 Hz, 1H), 6.67 – 6.61 (m, 2H), 5.90 (s, 2H), 4.01 (s, 2H), 3.83 (dd, *J* = 7.9, 5.2 Hz, 1H), 3.70 (s, 3H), 3.30 (dd, *J* = 14.3, 5.1 Hz, 1H), 3.04 (dd, *J* = 14.3, 8.1 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.9, 148.0, 146.4, 135.6, 135.3, 132.3, 128.5, 121.6, 121.5, 119.5, 118.4, 110.7, 109.1, 108.4, 107.6, 101.0, 55.4, 52.1, 32.0, 30.1. HRMS (ESI) m/z: $[M + H]^+$ calcd. for $[C_{20}H_{21}N_2O_4]^+$: 353.1496, found 353.1489. Step 2. Synthesized following the reported procedures,[25] and the desired azide was afforded as a brown oil (68% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (s, 1H), 7.56 – 7.49 (m, 1H), 7.23 – 7.18 (m, 1H), 7.15 – 7.07 (m, 2H), 6.74 (d, *J* = 7.7 Hz, 1H), 6.69 – 6.62 (1d + 1s, *J* = 7.8 Hz, 1+1H), 5.89 (s, 2H), 4.17 (dd, *J* = 8.5, 5.5

Hz, 1H), 4.03 (s, 2H), 3.73 (s, 3H), 3.36 (dd, *J* = 14.6, 5.5 Hz, 1H), 3.15 (dd, *J* = 14.6, 8.5 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.9, 148.1, 146.5, 135.6, 135.5, 132.0, 128.1, 121.8, 121.7, 119.7, 118.0, 110.8, 109.2, 108.5, 106.5, 101.1, 62.7, 52.7, 32.0, 27.2. HRMS (ESI) m/z: [M + H]$^+$ calcd. for $[C_{20}H_{19}N_4O_4]^+$: 379.1401, found 379.1395.

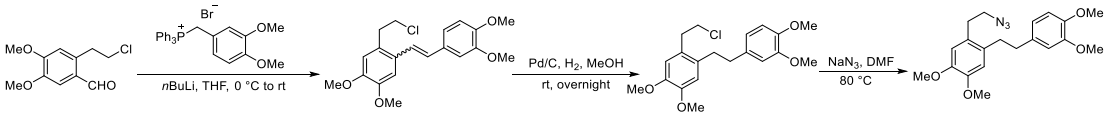


2-(4,5-Dimethoxy-2-vinylphenyl)ethan-1-ol: Synthesized following the reported procedure[26] from 2-(2-iodo-4,5-dimethoxyphenyl)ethan-1-ol[27]. To a solution of vinylboronic acid pinacol cyclic ester (274 mg, 1.78 mmol, 2.2 equiv.) in THF (10 mL) was added H_2O (0.3 mL), $PdCl_2$(dppf) (11.8 mg, 0.016 mmol, 0.02 equiv.), K_3PO_4 (515 mg, 2.4 mmol, 3 equiv.) in sequence. The resulting suspension was stirred for 15 min and then added 2-(2-iodo-4,5-dimethoxyphenyl)ethan-1-ol (250 mg, 0.811 mmol). The reaction mixture was warmed to 80 °C and stirred overnight and then was diluted with H_2O (20 mL). The organic layer was collected, and the aqueous layer was further extracted with EA (3×20 mL). The combined organic layer was washed with NaCl (saturated aq., 50 mL), dried over Na_2SO_4, filtered and concentrated in vacuo. The residue was subjected to purification by column chromatography on silica gel to afford desired product as a yellow oil (157 mg, ~ 80% yield, the yield was calculated after deducting pinacol residue according to ^{1}H NMR ratios). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.01 (s, 1H), 6.92 (dd, *J* = 17.3, 10.9 Hz, 1H), 6.68 (s, 1H), 5.54 (d, *J* = 17.3 Hz, 1H), 5.19 (d, *J* = 11.0 Hz, 1H), 3.86 (s, 3H), 3.84 (s, 3H), 3.73 (t, *J* = 7.2 Hz, 2H), 2.92 (br, 1H), 2.88 (t, *J* = 7.1 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.6, 147.5, 133.7, 128.9, 128.5, 113.4, 113.1, 108.4, 63.0, 55.7 (55.7, overlap), 35.8. HRMS (ESI) m/z: [M + H]$^+$ calcd. for $[C_{12}H_{17}O_3]^+$: 209.1172, found 209.1170.

2-(2-Ethyl-4,5-dimethoxyphenyl)ethan-1-ol: Synthesized following the general procedure A (step 2) and the desired product was afforded as a yellow oil (69% yield) after flash chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.73 – 6.66 (m, 2H), 3.83 (s, 3H), 3.82 (s, 3H), 3.76 (t, *J* = 7.2 Hz, 2H), 2.96 (br, 1H), 2.82 (t, *J* = 7.2 Hz, 2H), 2.59 (q, *J* = 7.5 Hz, 2H), 1.19 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.5, 146.8, 134.8, 127.8, 113.4, 112.2, 63.4, 55.9, 55.9, 35.5, 25.3, 15.9. HRMS (ESI) m/z: [M + H]$^+$ calcd. for $[C_{12}H_{19}O_3]^+$: 211.1329, found 211.1325.

1-(2-Azidoethyl)-2-ethyl-4,5-dimethoxybenzene (3n): Synthesized following the general procedure A (steps 3 and 4) from and obtained as a colorless oil (59% yield over two steps). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.70 (s, 1H), 6.67 (s, 1H), 3.85 (s, 3H),

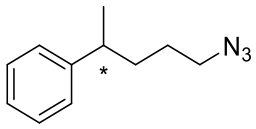
3.84 (s, 3H), 3.42 (t, *J* = 7.5 Hz, 2H), 2.85 (t, *J* = 7.5 Hz, 2H), 2.59 (q, *J* = 7.6 Hz, 2H), 1.21 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.9, 147.1, 134.6, 127.2, 113.0, 112.2, 56.0, 55.9, 52.3, 31.8, 25.3, 15.8. HRMS (ESI) m/z: $[M - N_2 + H]^+$ calcd. for $[C_{12}H_{18}NO_2]^+$: 208.1332, found 208.1330.



1-(2-Chloroethyl)-2-(3,4-dimethoxystyryl)-4,5-dimethoxybenzene: Synthesized following the reported procedures[28] from 2-(2-chloroethyl)-4,5-dimethoxybenzaldehyde[29] and obtained as a pink solid (69% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.76 (s, 1H), 6.75 – 6.69 (m, 3H), 6.65 (s, 1H), 6.55 (s, 2H), 3.89 (s, 3H), 3.84 (s, 3H), 3.66 (s, 3H), 3.63 (t, *J* = 7.4 Hz, 2H), 3.56 (s, 3H), 3.02 (t, *J* = 7.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.4, 148.2, 148.0, 130.9, 129.7, 129.6, 128.6, 126.6, 122.4, 113.4, 112.7, 111.7, 110.8, 100.1, 56.1, 56.0, 55.9, 55.6, 44.6, 36.9.

1-(2-Chloroethyl)-2-(3,4-dimethoxyphenethyl)-4,5-dimethoxybenzene:
Synthesized following the general procedure A (step 2) and the desired product was obtained as a white solid (82% yield) after flash chromatography. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.79 (d, *J* = 8.1 Hz, 1H), 6.69 (dd, *J* = 8.1, 2.0 Hz, 1H), 6.67 (s, 1H), 6.63 (s, 2H), 3.86 (s, 3H+3H), 3.83 (s, 3H), 3.82 (s, 3H), 3.56 (t, *J* = 7.8 Hz, 2H), 2.96 (t, *J* = 7.9 Hz, 2H), 2.88 – 2.77 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.0, 148.0, 147.6, 147.4, 134.2, 132.2, 128.0, 120.5, 113.1, 113.0, 112.1, 111.5, 56.2, 56.2, 56.1, 56.0, 44.7, 37.7, 36.0, 34.7. HRMS (ESI) m/z: $[M + Na]^+$ calcd. for $[C_{20}H_{25}ClO_4Na]^+$: 387.1334, found 387.1327.

1-(2-Azidoethyl)-2-(3,4-dimethoxyphenethyl)-4,5-dimethoxybenzene (3o):
Synthesized following the last step in the general procedure A (the tosylate was replaced by alkyl chloride) and obtained as a white solid (93% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.79 (d, *J* = 8.1 Hz, 1H), 6.69 (dd, *J* = 8.3, 1.8 Hz, 1H), 6.66 (s, 1H), 6.63 (s, 1H), 6.61 (d, *J* = 2.0 Hz, 1H), 3.86 (s, 3H), 3.86 (s, 3H), 3.82 (s, 3H + 3H), 3.35 (t, *J* = 7.5 Hz, 2H), 2.88 – 2.80 (m, 4H), 2.77 (t, *J* = 7.5 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.8, 147.7, 147.4, 147.3, 134.1, 132.0, 127.7, 120.4, 112.9, 112.8, 111.9, 111.3, 56.0, 56.0, 55.9, 55.8, 52.3, 37.6, 34.5, 31.8. HRMS (ESI) m/z: $[M + Na]^+$ calcd. for $[C_{20}H_{25}N_3O_4Na]^+$: 394.1737, found 394.1732.



1-(2-Azidoethyl)-2-benzylbenzene (3p) and (*S*)-(5-azidopentan-2-yl)benzene (*S*-3p): Synthesized following the general procedure A from 4-phenylpentan-1-ol and (*S*)-4-phenylpentan-1-ol respectively[30] and obtained as a colorless oil (71% yield over two steps). ^{1}H NMR (400 MHz, $CDCl_3$) δ7.30 (t, *J* = 7.3 Hz, 2H), 7.24 – 7.13 (m, 3H), 3.21 (t, *J* = 6.8 Hz, 2H), 2.76 – 2.63 (m, 1H), 1.70 – 1.61 (m, 2H), 1.59 – 1.41 (m, 2H), 1.26 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.8, 128.5, 126.9, 126.1, 51.6, 39.7, 35.3, 27.1, 22.4. Characterization data are consistent with the literature values.[5] (*S*)-(5-azidopentan-2-yl)benzene was determined to be 98% ee by chiral HPLC analysis (CHIRALCEL OD-H, Hexane, 0.9 mL/min, 210 nm, tr (minor) = 11.4 min, tr (major) = 12.1 min).

General procedure for catalytic C–H amination

General procedure for iron-catalyzed intramolecular C–H amination of alkyl azides

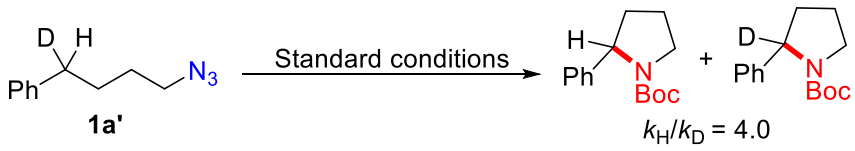
An oven-dried Schlenk tube was charged with organic azides (0.2 mmol, 1.0 equiv.), Boc_2O (2.0 equiv), iron catalyst (1-3 mol %), and dry toluene (2.0 mL) under Ar. The mixture was refluxed vigorously (130 °C) until full completion detected by TLC (usually completed within 6 h). The reaction mixture was cooled to room temperature and concentrated, and the residue was purified by silica gel column chromatography to give the corresponding products.

Large-scale reaction of iron-catalyzed intramolecular C–H amination of alkyl azides

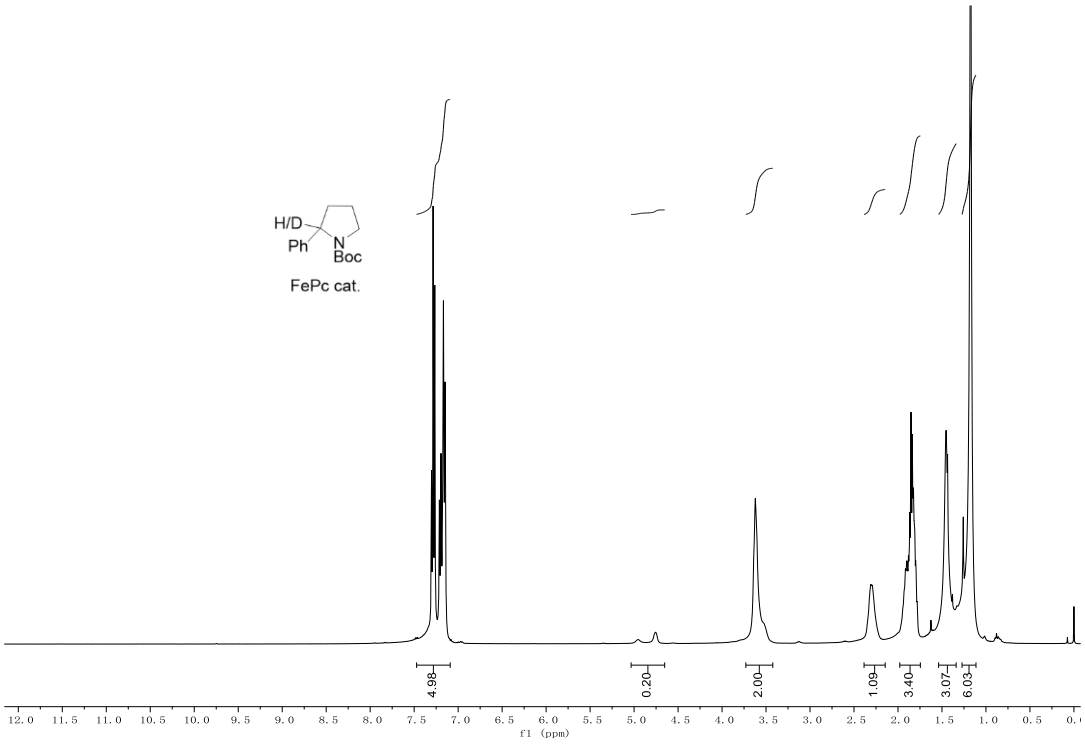
An oven-dried Schlenk flask was charged with azide (6 mmol for **1a**; 3 mmol for **3d**), Boc_2O (2.0 equiv), iron catalyst (0.5 mol % for **1a**; 3 mol % for **3d**), and dry toluene (18 mL for **1a**; 15 mL for **3d**) under Ar. The reaction mixture was refluxed vigorously (130 °C) for indicated time, and then cooled to room temperature and concentrated, and the residue was purified by silica gel column chromatography to give the corresponding products.

Mechanistic studies

(a) Kinetic isotope effect

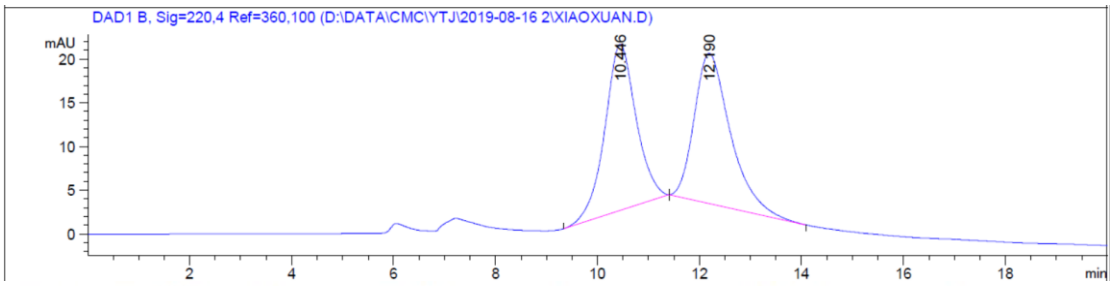


Monodeuterated azide **1a′** was prepared according to the reported literature procedure,[12] and it was reacted under the standard conditions. The ratios of k_H/k_D were determined by ^{1}H NMR integration of the methine proton in product against the methylene protons at the 2- and 4- positions, respectively. Below are shown the ^{1}H NMR analysis results.

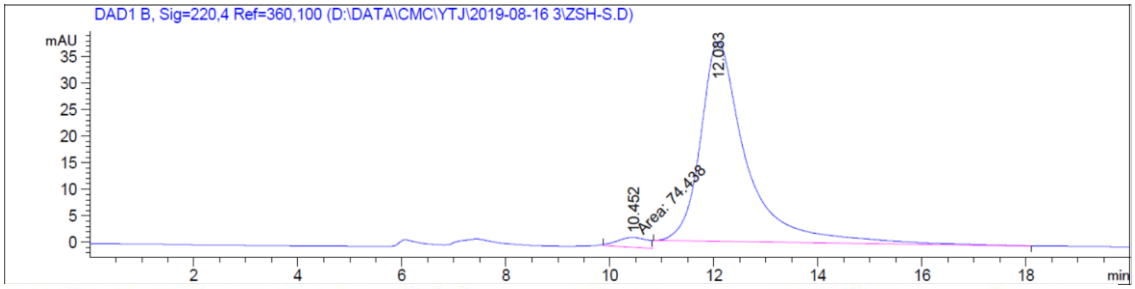


(b) Analysis of stereochemistry

(*S*)-(5-Azidopentan-2-yl)benzene (***S*-3p**) was treated under the catalytic conditions, and the product was determined to be 94% ee by chiral HPLC analysis (CHIRALCEL OJ-H, 1% IPA in hexane, 0.5 mL/min, 220 nm, tr (minor) = 10.3-10.5 min, tr (major) = 11.8-12.1 min).



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.446	BB	0.6341	811.26819	19.00231	48.8866
2	12.190	BBA	0.7400	848.22205	17.17933	51.1134



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.452	MM	0.6614	74.43803	1.87578	3.1215
2	12.083	BB	0.8842	2310.28516	37.63496	96.8785

(c) Procedures for the effect of radical scavengers (TEMPO)

The procedures are similar to the above intramolecular C–H amination but TEMPO (5 equiv.) was added.

(d) Proposed mechanism

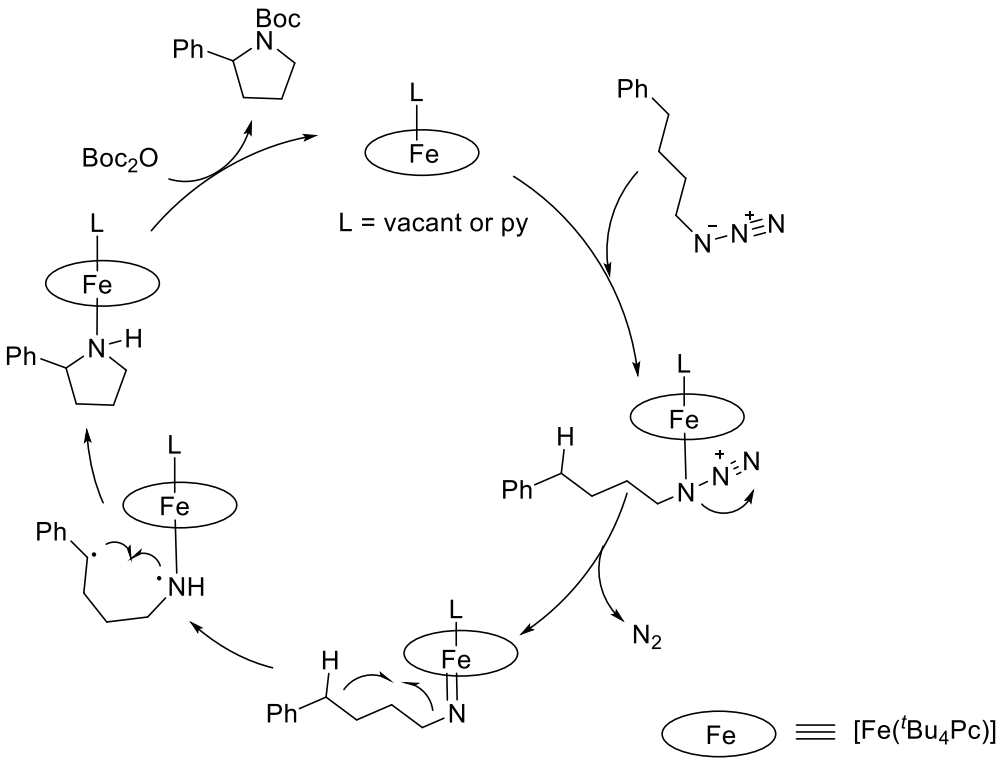
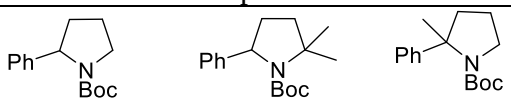


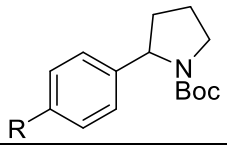
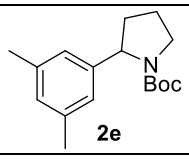
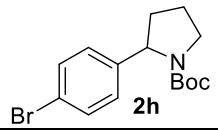
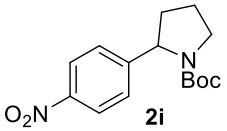
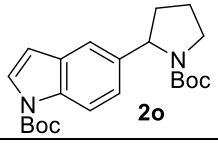
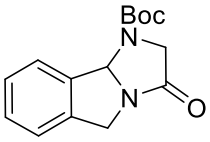
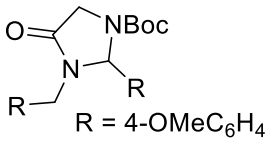
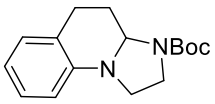
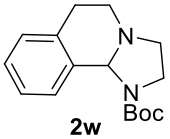
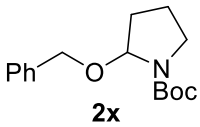
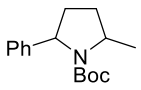
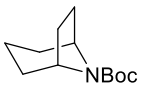
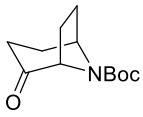
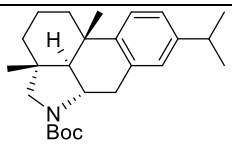
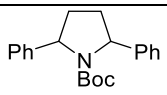
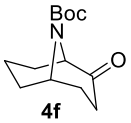
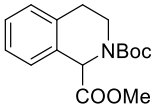
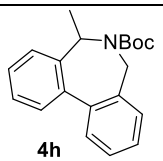
Fig. S3 Proposed mechanism for [Fe(^{t}Bu$_4$Pc)(py)$_2$]-catalyzed C–H amination using substrate **1a** as an example (charges of the species are omitted).

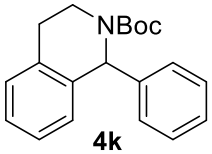
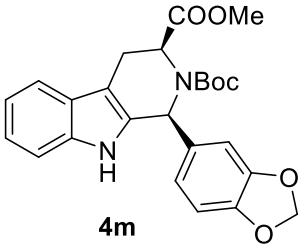
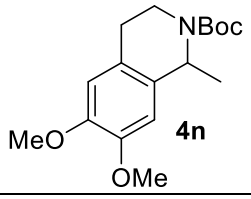
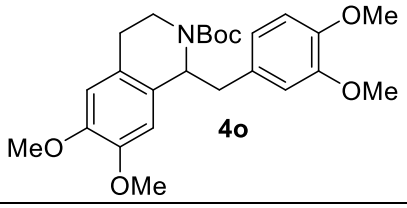
We propose that the catalytic cycle might be initiated by thermally driven dissociation of pyridine ligand(s) from [Fe(^{t}Bu$_4$Pc)(py)$_2$] to give [Fe(^{t}Bu$_4$Pc)(L)] (L = vacant or py) which binds an alkyl azide to give [Fe(^{t}Bu$_4$Pc)(L)(N$_3$R)], with subsequent azide decomposition affording Fe(Pc)-imido species. Intramolecular hydrogen atom abstraction (HAA) of the Fe(Pc)-imido species followed by a fast radical rebound results in cyclization to give the cyclic amine product (Fig. S3).

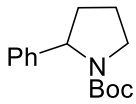
Products reported in the literature

Table S2 Reported products in the literature (for each compound, a ^{1}H NMR spectrum was given to verify the product's purity).

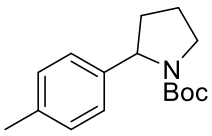
Compounds	References
 **2a** & **4c** **4a** **4p**	Ref. 5

 R = Me, **2b**; R = OMe, **2c** R = *N*,*N*-dimethyl, **2d**; R = F, **2f** R = Cl, **2g**	Ref. 6
 **2e**	Ref. 31
 **2h**  **2i**	Ref. 32
 **2o**	Ref. 33
 **2t**  **2u**	Ref. 8
 **2v**  **2w**	Ref. 9
 **2x**	Ref. 34
 **2y** & **4b**  **4d**  **4e**  **4i**	Ref. 12
 **2z**	Ref. 11
 **4f**	Ref. 9
 **4g**	Ref. 35
 **4h**	Ref. 36

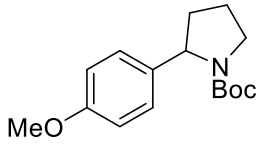
 **4k**	Ref. 37
 **4m**	Ref. 38
 **4n**  **4o**	Ref. 39



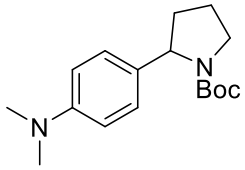
***tert*-Butyl 2-phenylpyrrolidine-1-carboxylate (2a and 4c):** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.25 (m, 2H), 7.23 – 7.12 (m, 3H), 5.05 – 4.64 (br m, 1H), 3.74 – 3.40 (br m, 2H), 2.42 – 2.19 (m, 1H), 1.97 – 1.77 (m, 3H), 1.52 – 1.12 (br m, 3H + 6H).



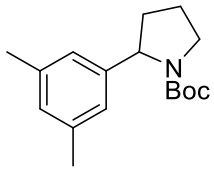
***tert*-Butyl 2-(*p*-tolyl)pyrrolidine-1-carboxylate (2b):** ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.13 – 7.00 (m, 4H), 4.97 – 4.62 (br m, 1H), 3.69 – 3.43 (br m, 2H), 2.37 – 2.24 (s+m, 3+1H), 1.92 – 1.74 (br m, 3H), 1.50 – 1.14 (br m, 3H + 6H).



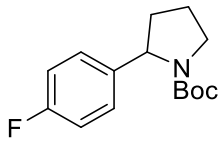
***tert*-Butyl 2-(4-methoxyphenyl)pyrrolidine-1-carboxylate (2c):** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.08 (d, *J* = 8.0 Hz, 2H), 6.83 (d, *J* = 8.6 Hz, 2H), 4.98 – 4.65 (br m, 1H), 3.78 (s, 3H), 3.60 (br m, 2H), 2.34 – 2.13 (br m, 1H), 1.95 – 1.70 (m, 3H), 1.50 – 1.15 (br m, 3H + 6H).



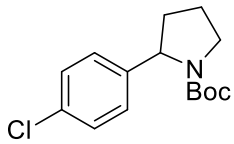
***tert*-Butyl 2-(4-(dimethylamino)phenyl)pyrrolidine-1-carboxylate (2d):** ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.08 – 6.97 (m, 2H), 6.68 (d, *J* = 8.3 Hz, 2H), 4.98 – 4.61 (br m, 1H), 3.66 – 3.41 (br m, 2H), 2.91 (s, 6H), 2.30 – 2.16 (br m, 1H), 1.95 – 1.86 (m, 1H), 1.85 – 1.77 (m, 2H), 1.51 – 1.17 (br m, 3H + 6H).



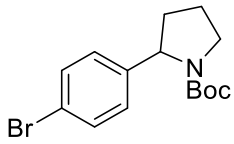
***tert*-Butyl 2-(3,5-dimethylphenyl)pyrrolidine-1-carboxylate (2e):** ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.83 (s, 1H), 6.76 (s, 2H), 4.96 – 4.56 (br m, 1H), 3.64 – 3.44 (br m, 2H), 2.28 (s, 6H), 1.98 – 1.87 (m, 1H), 1.86 – 1.70 (m, 3H), 1.50 – 1.14 (br m, 3H + 6H).



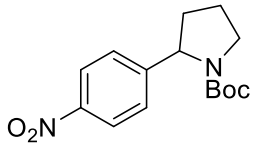
***tert*-Butyl 2-(4-fluorophenyl)pyrrolidine-1-carboxylate (2f):** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13 (dd, *J* = 8.3, 5.6 Hz, 2H), 7.02 – 6.93 (m, 2H), 5.02 – 4.65 (br m, 1H), 3.65 – 3.47 (br m, 2H), 2.36 – 2.23 (br m, 1H), 1.93 – 1.76 (br m, 3H), 1.52 – 1.11 (br m, 3H + 6H).



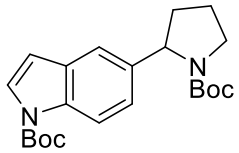
***tert*-Butyl 2-(4-chlorophenyl)pyrrolidine-1-carboxylate (2g):** ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26 (d, *J* = 8.3 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 4.99 – 4.62 (br m, 1H), 3.66 – 3.45 (br m, 2H), 2.34 – 2.22 (br m, 1H), 1.91 – 1.82 (m, 2H), 1.80 – 1.72 (m, 1H), 1.49 – 1.16 (br m, 3H + 6H).



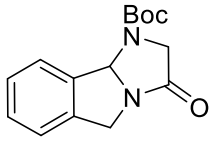
***tert*-Butyl 2-(4-bromophenyl)pyrrolidine-1-carboxylate (2h):** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.4 Hz, 2H), 7.05 (d, *J* = 8.1 Hz, 2H), 4.98 – 4.63 (br m, 1H), 3.72 – 3.43 (br m, 2H), 2.39 – 2.22 (br m, 1H), 1.93 – 1.82 (m, 2H), 1.81 – 1.72 (m, 1H), 1.48 – 1.17 (m, 3H + 6H).



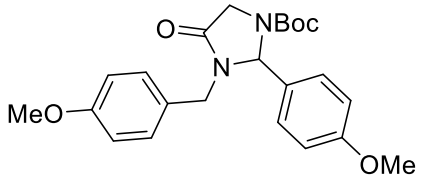
***tert*-Butyl 2-(4-nitrophenyl)pyrrolidine-1-carboxylate (2i):** ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.17 (d, *J* = 7.9 Hz, 2H), 7.35 (d, *J* = 8.5 Hz, 2H), 5.07 – 4.76 (br m, 1H), 3.75 – 3.49 (br m, 2H), 2.47 – 2.32 (br m, 1H), 1.95 – 1.86 (m, 2H), 1.84 – 1.77 (m, 1H), 1.48 – 1.14 (br m, 3H + 6H).



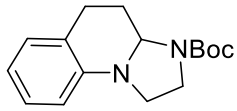
***tert*-Butyl 5-(1-(*tert*-butoxycarbonyl)pyrrolidin-2-yl)-1H-indole-1-carboxylate (2o):** ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 (br s, 1H), 7.57 (s, 1H), 7.33 (s, 1H), 7.12 (d, *J* = 8.7 Hz, 1H), 6.51 (d, *J* = 3.7 Hz, 1H), 5.10 – 4.81 (br m, 1H), 3.74 – 3.50 (br m, 2H), 2.39 – 2.22 (br m, 1H), 1.98 – 1.90 (m, 1H), 1.88 – 1.82 (m, 2H), 1.66 (s, 9H), 1.46 and 1.17 (2s, 3H + 6H).



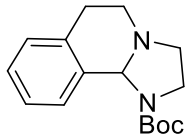
***tert*-Butyl 3-oxo-2,3,5,9b-tetrahydro-1*H*-imidazo[2,1-*a*]isoindole-1-carboxylate (2t):** ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.90 – 7.55 (br m, 1H), 7.43 – 7.19 (m, 3H), 6.52 – 6.33 (br m, 1H), 5.05 (d, *J* = 14.8 Hz, 1H), 4.40 – 4.15 (br m, 2H), 3.82 (d, *J* = 16.2 Hz, 1H), 1.66 – 1.50 (br m, 9H).



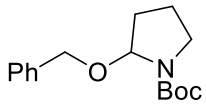
***tert*-Butyl 3-(4-methoxybenzyl)-2-(4-methoxyphenyl)-4-oxoimidazolidine-1-carboxylate (2u):** ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.21 (d, *J* = 7.5 Hz, 1H), 7.12 (d, *J* = 7.9 Hz, 1H), 7.08 (d, *J* = 7.9 Hz, 2H), 6.91 (d, *J* = 8.3 Hz, 2H), 6.89 – 6.82 (m, 2H), 5.74 – 5.41 (br m, 1H), 5.02 (d, *J* = 14.8 Hz, 1H), 4.29 – 4.14 (m, 2H), 3.84 (s, 3H), 3.81 (s, 3H), 3.38 – 3.23 (m, 1H), 1.39 – 1.16 (s + s, 4H + 5H).



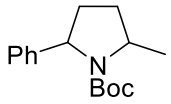
***tert*-Butyl 1,2,4,5-tetrahydroimidazo[1,2-*a*]quinoline-3(3a*H*)-carboxylate (2v):** ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.09 (t, *J* = 7.7 Hz, 1H), 7.02 (d, *J* = 7.4 Hz, 1H), 6.69 (t, *J* = 7.4 Hz, 1H), 6.57 (d, *J* = 8.1 Hz, 1H), 4.68 (d, *J* = 8.3 Hz, 1H), 3.76 (br s, 1H), 3.54 – 3.43 (m, 3H), 2.90 (td, *J* = 15.2, 13.1, 5.4 Hz, 1H), 2.83 – 2.75 (m, 1H), 2.71 – 2.47 (br m, 1H), 1.50 (s, 9H), 1.46 – 1.39 (m, 1H).



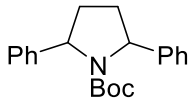
***tert*-Butyl 2,3,6,10b-tetrahydroimidazo[2,1-*a*]isoquinoline-1(5*H*)-carboxylate (2w):** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (s, 1H), 7.25 – 7.14 (m, 2H), 7.06 (d, *J* = 7.0 Hz, 1H), 5.79 (s, 1H), 3.66 (q, *J* = 9.2 Hz, 1H), 3.42 (td, *J* = 13.1, 12.5, 4.6 Hz, 1H), 3.33 (t, *J* = 8.7 Hz, 1H), 3.23 – 3.13 (m, 1H), 3.03 (dq, *J* = 11.4, 7.1, 5.8 Hz, 3H), 2.54 (d, *J* = 16.6 Hz, 1H), 1.53 (s, 9H).



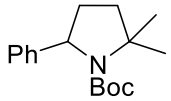
***tert*-Butyl 2-(benzyloxy)pyrrolidine-1-carboxylate (2x):** ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 – 7.23 (m, 5H), 5.53 – 5.23 (m, 1H), 4.78 – 4.43 (m, 2H), 3.70 – 3.22 (m, 2H), 2.24 – 2.05 (m, 1H), 2.03 – 1.93 (m, 1H), 1.92 – 1.83 (m, 1H), 1.83 – 1.73 (m, 1H), 1.48 (s, 9H).



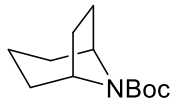
***tert*-Butyl 2-methyl-5-phenylpyrrolidine-1-carboxylate (2y and 4b):** ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 (t, *J* = 7.5 Hz, 2H), 7.25 – 7.16 (m, 3H), 5.00 – 4.59 (br m, 1H), 4.31 – 3.91 (br m, 1H), 2.46 – 2.18 (m, 1H), 2.17 – 1.97 (m, 1H), 1.92 – 1.82 (m, 1H), 1.74 – 1.53 (m, 1H), 1.52 – 1.09 (m, 3H + 3H + 6H).



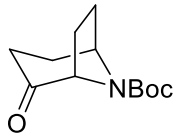
***tert*-Butyl 2,5-diphenylpyrrolidine-1-carboxylate (2z):** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.32 (m, 8H), 7.32 – 7.25 (m, 2H), 5.39 – 4.78 (br m, 2H), 2.47 – 2.30 (m, 2H), 2.21 – 1.99 (br m, 2H), 1.27 (s, 9H).



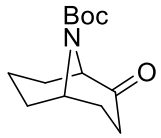
***tert*-Butyl 2,2-dimethyl-5-phenylpyrrolidine-1-carboxylate (4a):** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.26 (m, 2H), 7.25 – 7.14 (m, 3H), 5.12 – 4.79 (br m, 1H), 2.38 – 2.20 (br m, 1H), 1.97 – 1.79 (br m, 1H), 1.75 – 1.67 (m, 2H), 1.65 – 1.57 (m, 2H), 1.51 – 1.08 (br m, 7H + 1H + 5H).



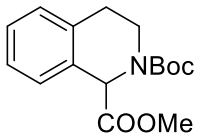
***tert*-Butyl-8-azabicyclo[3.2.1]octane-8-carboxylate (4d):** ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.21 (br s, 1H), 4.11 (br s, 1H), 1.98 – 1.88 (m, 2H), 1.83 – 1.69 (m, 3H), 1.68 – 1.62 (m, 2H), 1.47 (s, 9H), 1.44 (br s, 1H), 1.43 – 1.37 (br m, 2H).



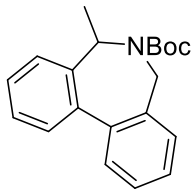
***tert*-Butyl-2-oxo-8-azabicyclo[3.2.1]octane-8-carboxylate (4e):** ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.59 (br s, 1H), 4.05 (br s, 1H), 2.66 (dd, *J* = 17.9, 7.4 Hz, 1H), 2.26 – 2.16 (m, 1H), 1.98 (br s, 1H), 1.82 – 1.76 (m, 1H), 1.74 – 1.62 (m, 4H), 1.49 (s, 9H).



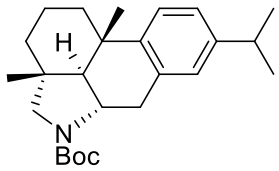
***tert*-Butyl-2-oxo-9-azabicyclo[3.3.1]nonane-9-carboxylate (4f):** ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.72 – 4.53 (br m, 1H), 4.17 – 3.96 (m, 1H), 2.82 – 2.66 (m, 1H), 2.46 – 2.18 (m, 1H), 2.16 – 2.06 (m, 1H), 2.00 – 1.68 (m, 4H), 1.62 – 1.54 (m, 1H), 1.52 – 1.46 (m, 9H), 1.29 – 1.21 (m, 1H), 1.09 – 0.93 (m, 1H).



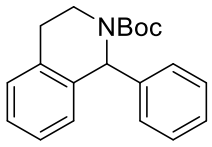
2-(*tert*-Butyl) 1-methyl 3,4-dihydroisoquinoline-1,2(1*H*)-dicarboxylate (4g): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.43 (m, 1H), 7.33 – 7.11 (m, 3H), 5.72 – 5.33 (br m, 1H), 3.94 – 3.76 (m, 2H), 3.71 (s, 3H), 3.10 – 2.92 (m, 1H), 2.91 – 2.76 (m, 1H), 1.69 – 1.37 (m, 9H).



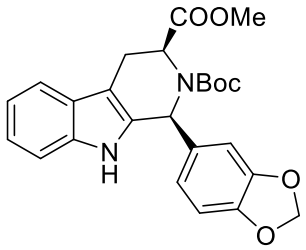
***tert*-Butyl 5-methyl-5,7-dihydro-6*H*-dibenzo[*c*,*e*]azepine-6-carboxylate (4h):** ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 – 7.47 (m, 2H), 7.47 – 7.42 (m, 2H), 7.41 – 7.30 (m, 4H), 5.37 – 4.74 (br m, 2H), 3.72 (br s, 1H), 1.53 (s, 9H), 0.86 (d, *J* = 6.9 Hz, 3H).



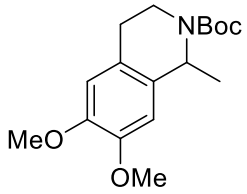
***tert*-Butyl (3a*R*,3a1*R*,5a*S*,10b*S*)-8-isopropyl-3a,10b-dimethyl-2,3,3a,3a1,4,5a,6,10b-octahydrodibenzo[*cd*,*f*]indole-5(1*H*)-carboxylate (4i):** ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.14 (t, *J* = 8.3 Hz, 1H), 7.04 (t, *J* = 8.0 Hz, 1H), 6.95 (d, *J* = 14.7 Hz, 1H), 3.85 – 3.50 (m, 2H), 3.51 – 3.34 (m, 1H), 2.95 (t, *J* = 9.0 Hz, 1H), 2.83 (dp, *J* = 9.2, 6.9 Hz, 1H), 2.70 (dd, *J* = 16.2, 9.3 Hz, 1H), 2.23 – 2.15 (m, 2H), 1.90 – 1.69 (m, 3H), 1.57 – 1.48 (m, 10H), 1.25 – 1.17 (m, 1H + 9H), 1.09 (s, 3H).



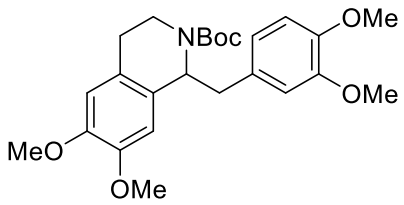
***tert*-Butyl 1-phenyl-3,4-dihydroisoquinoline-2(1*H*)-carboxylate (4k):** ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.25 (m, 2H), 7.24 – 7.13 (m, 6H), 7.05 (s, 1H), 6.58 – 6.06 (br m, 1H), 4.23 – 3.80 (br m, 1H), 3.27 – 3.16 (m, 1H), 2.96 (br s, 1H), 2.83 – 2.67 (br m, 1H), 1.49 (s, 9H).



2-(*tert*-Butyl) 3-methyl (1*S*,3*S*)-1-(benzo[*d*][1,3]dioxol-5-yl)-1,3,4,9-tetrahydro-2*H*-pyrido[3,4-*b*]indole-2,3-dicarboxylate (4m): ^{1}H NMR (500 MHz, DMSO-d_6, 70 ℃) δ 10.65 (br s, 1H), 7.51 (d, *J* = 7.8 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.11 – 7.06 (m, 1H), 7.04 – 6.99 (m, 1H), 6.80 (d, *J* = 8.1 Hz, 1H), 6.79 – 6.78 (m, 1H), 6.68 (dd, *J* = 8.1, 1.5 Hz, 1H), 6.34 (s, 1H), 5.96 (s, 2H), 5.22 – 5.16 (m, 1H), 3.32 (dd, *J* = 15.7, 2.9 Hz, 1H), 3.23 (s, 3H), 3.06 – 2.98 (m, 1H), 1.49 (s, 9H).

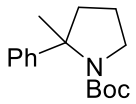


***tert*-Butyl 6,7-dimethoxy-1-methyl-3,4-dihydroisoquinoline-2(1*H*)-carboxylate (4n):** ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.59 (s, 2H), 5.29 – 4.89 (br m, 1H), 4.28 – 3.97 (br m, 1H), 3.86 (s, 3H), 3.85 (s, 3H), 3.30 – 3.05 (br m, 1H), 2.93 – 2.75 (br m, 1H), 2.68 – 2.57 (br m, 1H), 1.70 – 1.46 (m, 1H + 8H), 1.42 (d, *J* = 6.7 Hz, 3H).



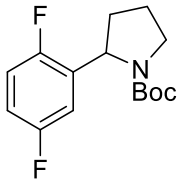
***tert*-Butyl 1-(3,4-dimethoxybenzyl)-6,7-dimethoxy-3,4-dihydroisoquinoline-**

2(1*H*)-carboxylate (4o): ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.82 – 6.70 (m, 1H), 6.66 – 6.55 (m, 3H), 6.36 – 6.17 (br m, 1H), 5.28 – 4.99 (m, 1H), 4.19 – 3.83 (m, 1H + 3H + 3H), 3.83 – 3.77 (br m, 3H), 3.74 – 3.61 (br m, 3H), 3.37 – 3.17 (m, 1H), 3.11 – 2.95 (m, 1H), 2.94 – 2.67 (m, 2H), 2.65 – 2.46 (m, 1H), 1.47 – 1.31 (m, 9H).

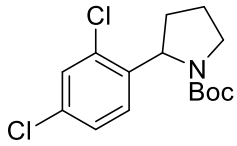


***tert*-Butyl 2-methyl-2-phenylpyrrolidine-1-carboxylate (4p):** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.13 (m, 5H), 3.75 – 3.54 (m, 2H), 2.13 – 1.98 (m, 2H), 1.92 – 1.79 (m, 2H), 1.75 (s, 3H), 1.49 – 1.08 (s, 2H + 7H).

Characterization data of new products

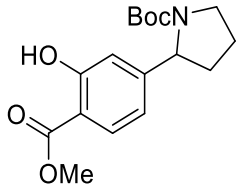


***tert*-Butyl 2-(2,5-difluorophenyl)pyrrolidine-1-carboxylate (2j)**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.06 – 6.70 (m, 3H), 5.26 – 4.89 (br m, 1H), 3.73 – 3.40 (br m, 2H), 2.45 – 2.22 (m, 1H), 1.98 – 1.77 (m, 3H), 1.47 and 1.23 (br s + s, 3H + 6H). ^{13}C NMR (125 MHz, $CDCl_3$) (minor rotamer was shown in the parentheses) δ 158.7 (d, J = 242.3 Hz), 155.6 (d, J = 240.5 Hz), 154.2 (154.3), 134.26 – 132.22 (m), 116.64 – 115.78 (m), 114.57 – 113.88 (m), 113.82 – 112.87 (m), 79.6 (79.7), 55.2 (55.3), 46.9 (47.2), 34.3 (33.3), 28.1 (28.5), 23.3 (23.6). ^{19}F NMR (376 MHz, $CDCl_3$) δ -119.21 (d, J = 17.9 Hz), -119.29 – -119.38 (m), -124.63 – -124.73 (m), -125.83 (d, J = 17.8 Hz). HRMS (ESI) m/z: $[M+Na]^+$ calcd. for $[C_{15}H_{19}F_2NO_2Na]^+$: 306.1276, found 306.1274.

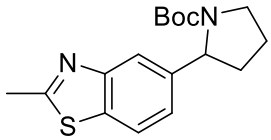


***tert*-Butyl 2-(2,4-dichlorophenyl)pyrrolidine-1-carboxylate (2k)**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 (s, 1H), 7.13 (d, J = 8.0 Hz, 1H), 7.00 (dd, J = 28.3, 8.2 Hz, 1H), 5.16 – 5.00 (br m, 1H), 3.60 – 3.39 (br m, 2H), 2.35 – 2.23 (m, 1H), 1.85 – 1.75 (m, 2H), 1.73 – 1.67 (m, 1H), 1.39 and 1.14 (br s + s, 3H + 6H). ^{13}C NMR (125 MHz, $CDCl_3$) (minor rotamer was shown in the parentheses) ^{13}C NMR (126 MHz, Chloroform-*d*) δ 154.3, 140.9 (139.8), 132.6 (132.8), 132.4, 129.6 (129.6), 129.1,

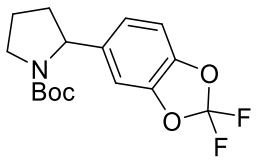
126.9 (127.3), 79.6 (79.7), 58.3, 47.1 (47.5), 33.9 (32.7), 28.1 (28.5), 23.0 (23.3). HRMS (ESI) m/z: $[M+Na]^+$ calcd. for $[C_{15}H_{19}Cl_2NO_2Na]^+$: 338.0685, found 338.0684.



***tert*-Butyl 2-(3-hydroxy-4-(methoxycarbonyl)phenyl)pyrrolidine-1-carboxylate (2l):** ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.66 (br s, 1H), 7.64 (s, 1H), 7.28 (d, *J* = 7.8 Hz, 1H), 6.93 (d, *J* = 8.6 Hz, 1H), 4.98 – 4.54 (br m, 1H), 3.94 (s, 3H), 3.69 – 3.47 (br m, 2H), 2.36 – 2.23 (br m, 1H), 1.94 – 1.84 (m, 2H), 1.83 – 1.74 (m, 1H), 1.50 – 1.15 (br m, 3H + 6H). ^{13}C NMR (125 MHz, $CDCl_3$) (minor rotamer was shown in the parentheses) δ 170.5, 160.3, 154.6, 135.8 (134.8), 133.2 (133.0), 126.6, 117.3 (117.6), 111.8 (112.0), 79.4, 60.5 (60.0), 52.3 (52.2), 47.0 (47.3), 35.9 (34.8), 28.2 (28.4), 23.2 (23.5). HRMS (ESI) m/z: $[M + H]^+$ calcd. for $[C_{17}H_{24}NO_5]^+$: 322.1649, found 322.1647.

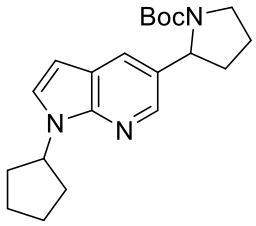


***tert*-Butyl 2-(2-methylbenzo[*d*]thiazol-5-yl)pyrrolidine-1-carboxylate (2m):** ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.4 Hz, 1H), 7.61 (s, 1H), 7.26 (d, *J* = 8.5 Hz, 1H), 5.14 – 4.80 (br m, 1H), 3.74 – 3.51 (br m, 2H), 2.82 (s, 3H), 2.43 – 2.28 (br m, 1H), 1.98 – 1.83 (br m, 3H), 1.50 – 1.07 (br m, 3H + 6H). ^{13}C NMR (125 MHz, $CDCl_3$) (minor rotamer was shown in the parentheses) δ 166.6 (166.4), 154.6, 152.2 (152.3), 142.2 (141.2), 135.7 (135.8), 124.0 (123.7), 122.0 (122.2), 118.0, 79.4, 61.3 (60.7), 47.1 (47.5), 36.2 (35.1), 28.2 (28.5), 23.2 (23.5), 20.13. HRMS (ESI) m/z: $[M + H]^+$ calcd. for $[C_{17}H_{23}N_2O_2S]^+$: 319.1475, found 319.1471.

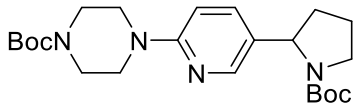


***tert*-Butyl 2-(2,2-difluorobenzo[*d*][1,3]dioxol-5-yl)pyrrolidine-1-carboxylate (2n):** ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.98 (d, *J* = 8.4 Hz, 1H), 6.93 – 6.86 (m, 2H), 4.99 – 4.69 (br m, 1H), 3.70 – 3.45 (br m, 2H), 2.39 – 2.23 (br m, 1H), 1.93 – 1.83 (br m, 2H), 1.83 – 1.72 (br m, 1H), 1.52 – 1.17 (br m, 3H + 6H). ^{13}C NMR (125 MHz,

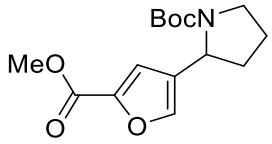
$CDCl_3$) (minor rotamer was shown in the parentheses) δ 154.4 (154.5), 143.8 (143.9), 142.3 (142.4), 141.7 (140.7), 131.65 (t, *J* = 254.4 Hz), 120.4, 108.9 (109.2), 106.8, 79.6 (79.7), 60.98 (60.5), 47.1 (47.4), 36.1 (35.1), 28.2 (28.5), 23.0 (23.5). ^{19}F NMR (376 MHz, $CDCl_3$) δ -49.88 (d, *J* = 11.3 Hz), -50.17 (d, *J* = 9.1 Hz). HRMS (ESI) m/z: $[M + Na]^+$ calcd. for $[C_{16}H_{19}F_2NO_4Na]^+$: 350.1174, found 350.1172.



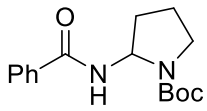
***tert*-Butyl 2-(1-cyclopentyl-1*H*-pyrrolo[2,3-*b*]pyridin-5-yl)pyrrolidine-1-carboxylate (2p):** ^1H NMR (500 MHz, $CDCl_3$) δ 8.17 (s, 1H), 7.68 (d, *J* = 1.8 Hz, 1H), 7.29 (s, 1H), 6.41 (d, *J* = 3.6 Hz, 1H), 5.32 – 5.22 (br m, 1H), 5.16 – 4.86 (br m, 1H), 3.74 – 3.48 (br m, 2H), 2.43 – 2.31 (br m, 1H), 2.30 – 2.18 (br m, 2H), 1.93 – 1.84 (br m, 6H), 1.82 – 1.71 (br m, 3H), 1.50 – 1.15 (br m, 3H + 6H). ^{13}C NMR (125 MHz, $CDCl_3$) (minor rotamer was shown in the parentheses) δ 154.6 (154.6), 147.0, 141.2 (140.7), 132.2 (131.3), 125.4 (125.5), 125.3 (125.2), 120.3 (120.5), 99.2 (99.3), 79.3, 59.5 (59.1), 54.9, 47.0 (47.4), 36.3 (35.3), 32.9 (32.9), 28.3 (28.6), 24.1, 23.1 (23.4). HRMS (ESI) m/z: $[M + H]^+$ calcd. for $[C_{21}H_{30}N_3O_2]^+$: 356.2333, found 356.2329.



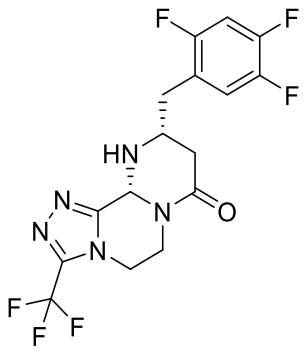
***tert*-Butyl 4-(5-(1-(*tert*-butoxycarbonyl)pyrrolidin-2-yl)pyridin-2-yl)piperazine-1-carboxylate (2q):** ^1H NMR (500 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.33 (d, *J* = 8.2 Hz, 1H), 6.61 (d, *J* = 8.7 Hz, 1H), 4.93 – 4.62 (br m, 1H), 3.62 – 3.45 (m, 10H), 2.34 – 2.19 (br m, 1H), 1.94 – 1.83 (br m, 2H), 1.82 – 1.75 (br m, 1H), 1.48 (s, 9H), 1.47 – 1.22 (m, 3H + 6H). ^{13}C NMR (125 MHz, $CDCl_3$) (minor rotamer was shown in the parentheses) δ 158.5, 154.8, 154.5, 145.7 (145.1), 135.1 (135.5), 130.0, (129.0), 106.9 (107.1), 79.9, 79.4, 58.6 (58.2), 46.9 (47.1), 45.4, 43.8, 42.9, 35.7 (34.5), 28.4 (28.3), 23.2 (23.5). HRMS (ESI) m/z: $[M + H]^+$ calcd. for $[C_{23}H_{37}N_4O_4]^+$: 433.2809, found 433.2807.



***tert*-Butyl 2-(5-(methoxycarbonyl)furan-3-yl)pyrrolidine-1-carboxylate (2r):** ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 – 7.36 (m, 1H), 7.08 (s, 1H), 5.00 – 4.65 (br m, 1H), 3.89 (s, 3H), 3.59 – 3.34 (br m, 2H), 2.30 – 2.12 (br m, 1H), 1.95 – 1.85 (m, 3H), 1.53 – 1.33 (br m, 4H + 5H). ^{13}C NMR (125 MHz, $CDCl_3$) (minor rotamer was shown in the parentheses) δ 159.1, 154.3 (154.5), 144.6, 142.7 (142.9), 131.01 (130.4), 116.9 (117.2), 79.7, 52.8 (52.4), 51.9, 46.2 (46.5), 33.9 (32.6), 28.4, 23.2 (24.0). HRMS (ESI) m/z: $[M + Na]^+$ calcd. for $[C_{15}H_{21}NO_5Na]^+$: 318.1312, found 318.1310.

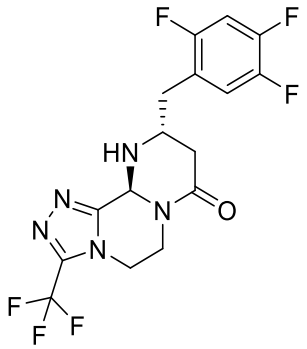


***tert*-Butyl 2-benzamidopyrrolidine-1-carboxylate (2s):** ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.32 (m, 5H), 5.67 – 5.03 (br, m, 2H), 3.82 – 3.24 (br, m, 2H), 2.42 – 1.70 (br, m, 4H), 1.54 – 1.26 (br m, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) (minor rotamer was shown in the parentheses) δ 171.1 (170.0), 154.9 (153.2), 136.5, 130.1, 128.3, 127.3 (126.7), 79.7, 66.7 (66.1), 50.0 (45.9), 34.5 (30.7), 28.3, 24.5 (21.3). HRMS (ESI): m/z: M^+ calcd. for $C_{16}H_{22}N_2O_3$: 290.1630, found 290.1629.

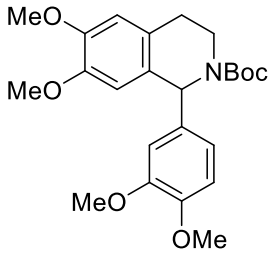


(10*R*,11a*R*)-10-(2,4,5-Trifluorobenzyl)-3-(trifluoromethyl)-5,6,9,10,11,11a-hexahydro-8*H*-[1,2,4]triazolo[3',4':3,4]pyrazino[1,2-*a*]pyrimidin-8-one (4j): ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.13 (q, *J* = 8.8 Hz, 1H), 6.94 (q, *J* = 9.4 Hz, 1H), 5.70 (d, *J* = 8.6 Hz, 1H), 5.14 (dd, *J* = 14.3, 4.0 Hz, 1H), 4.22 (dd, *J* = 12.6, 4.0 Hz, 1H), 4.12 (td, *J* = 12.3, 4.3 Hz, 1H), 3.55 – 3.43 (m, 1H), 3.18 – 3.08 (m, 1H), 2.99 (dd, *J* = 13.9, 6.1 Hz, 1H), 2.92 (t, *J* = 8.9 Hz, 1H), 2.85 (dd, *J* = 13.9, 7.2 Hz, 1H), 2.48 (dd, *J* = 17.2, 3.3 Hz, 1H), 2.25 (dd, *J* = 17.2, 11.8 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.0, 156.1 (ddd, *J* = 244.6, 9.3, 2.4 Hz), 151.4, 149.1 (dt, *J* = 250.8, 13.4 Hz), 146.7 (ddd, *J* = 245.4, 12.5, 3.5 Hz), 143.9 (q, *J* = 40.1 Hz), 120.2 (dt, *J* = 18.3, 4.6 Hz),

119.0 (dd, *J* = 19.0, 5.6 Hz), 118.0 (q, *J* = 270.8 Hz), 105.7 (dd, *J* = 28.6, 20.8 Hz), 67.1, 51.3, 43.4, 38.1, 35.9, 34.4. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.16, -118.56 – -118.68 (m), -134.84 – -135.00 (m), -142.23 – -142.44 (m). HRMS (ESI) m/z: $[M + H]^+$ calcd. for $[C_{16}H_{14}F_6N_5O]^+$: 406.1097, found 406.1096.



(10*R*,11a*S*)-10-(2,4,5-Trifluorobenzyl)-3-(trifluoromethyl)-5,6,9,10,11,11a-hexahydro-8*H*-[1,2,4]triazolo[3',4':3,4]pyrazino[1,2-*a*]pyrimidin-8-one (4j′): ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.17 (q, *J* = 8.7 Hz, 1H), 6.93 (td, *J* = 9.6, 6.6 Hz, 1H), 5.77 (s, 1H), 5.06 (d, *J* = 13.6 Hz, 1H), 4.15 (d, *J* = 6.1 Hz, 2H), 3.32 – 3.19 (m, 2H), 2.95 (dd, *J* = 14.1, 6.3 Hz, 1H), 2.82 (dd, *J* = 14.1, 6.7 Hz, 1H), 2.73 – 2.52 (m, 1H), 2.43 (dd, *J* = 16.7, 3.3 Hz, 1H), 2.27 (dd, *J* = 16.7, 10.5 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.7, 156.1 (ddd, *J* = 244.1, 9.0, 2.4 Hz), 152.8, 149.1 (dt, *J* = 251.3, 13.4 Hz), 146.8 (ddd, *J* = 245.4, 12.2, 3.2 Hz), 144.8 (q, *J* = 39.4 Hz), 119.8 (dt, *J* = 18.3, 4.7 Hz), 118.9 (dd, *J* = 19.2, 5.8 Hz), 118.0 (q, *J* = 270.4 Hz), 105.7 (dd, *J* = 28.7, 20.7 Hz), 66.8, 49.4, 42.8, 38.5, 38.3, 33.4. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.43, -118.32 – -118.44 (m), -134.68 – -134.83 (m), -141.99 – -142.29 (m). HRMS (ESI) m/z: $[M + H]^+$ calcd. for $[C_{16}H_{14}F_6N_5O]^+$: 406.1097, found 406.1088.



***tert*-Butyl 1-(3,4-dimethoxyphenyl)-6,7-dimethoxy-3,4-dihydroisoquinoline-2(1*H*)-carboxylate (4l):**[40] ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.96 (s, 1H), 6.74 (d, *J* = 8.2 Hz, 1H), 6.68 (s, 1H), 6.61 (d, *J* = 6.7 Hz, 1H), 6.52 (s, 1H), 6.43 – 6.05 (br m, 1H), 4.22 – 3.94 (br m, 1H), 3.89 (s, 3H), 3.85 (s, 3H), 3.83 (s, 3H), 3.77 (s, 3H), 3.12 – 3.00 (br m, 1H), 2.99 – 2.86 (br m, 1H), 2.73 – 2.60 (br m, 1H), 1.52 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) (minor rotamer was shown in the parentheses) δ 154.7

(154.3), 148.7, 148.2, 147.9, 147.3, 135.8, 127.3, 127.1, 120.8, 111.8, 111.2, 111.1, 110.3, 79.9, 57.1, 55.9, 55.8, 55.8, 55.8, 37.8 (36.5), 28.6, 28.1. HRMS (ESI) m/z: $[M + H]^+$ calcd. for $[C_{24}H_{32}NO_6]^+$: 430.2224, found 430.2224.

X-ray crystal structure determination

Diffraction-quality crystals of **4j** and **4j'** were obtained by slow evaporation of their $CDCl_3$ solution in the NMR tube. The X-ray diffraction data were collected on a Bruker D8 (for **4j**) and Bruker SMART APEX2 (for **4j'**) diffractometer with monochromated Mo-Kα radiation (the crystals were quickly mounted in a glass fiber and measured at a temperature of 100 K). The structure was solved by direct methods (Olex2) and refined with the XL refinement package using least squares minimization. All non-hydrogen atoms were refined anisotropically and hydrogen atoms by a riding model (Olex2). The crystallographic data and structure refinement parameters are depicted in Table S3. CCDC 2102181 (**4j**), and CCDC 2102171 (**4j'**) contain the supplementary crystallographic data for this paper. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S3 Crystallographic data and structure refinement parameters.

Compound	**4j**	**4j'**
Empirical formula	$C_{16}H_{13}F_6N_5O$	
Formula weight	405.31	
Temperature/K	100.0	
Crystal system	triclinic	orthorhombic
Space group	P1	$P2_12_12$
a/Å	4.6849(8)	26.094(2)
b/Å	5.6677(10)	6.5624(5)
c/Å	15.258(3)	9.4316(7)
α/°	98.838(6)	90
β/°	91.269(6)	90
γ/°	93.319(6)	90
Volume/$Å^3$	399.46(12)	1615.1(2)
Z	1	4
$\rho_{calc}g/cm^3$	1.685	1.667
μ/mm^{-1}	0.158	0.156
F(000)	206.0	824.0
Crystal size/mm^3	0.28 × 0.28 × 0.24	0.42 × 0.41 × 0.36
Radiation	MoKα (λ = 0.71073)	
2Θ range for data collection/°	5.406 to 55.12	4.318 to 55.02
Index ranges	$-6 \le h \le 5, -7 \le k \le 7, -19$	$-25 \le h \le 33, -8 \le k \le 8,$

	≤ l ≤ 19	-8 ≤ l ≤ 12
Reflections collected	6666	13312
Independent reflections	3455 [R_{int} = 0.0598, R_{sigma} = 0.0752]	3691 [R_{int} = 0.0334, R_{sigma} = 0.0305]
Data/restraints/parameters	3455/3/253	3691/0/261
Goodness-of-fit on F^2	1.030	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0377, wR_2 = 0.0906	R_1 = 0.0436, wR_2 = 0.1090
Final R indexes [all data]	R_1 = 0.0490, wR_2 = 0.0949	R_1 = 0.0475, wR_2 = 0.1117
Largest diff. peak/hole / e $Å^{-3}$	0.22/-0.20	0.91/-0.45
Flack parameter	-0.3(5)	0.0(2)

Computational details

DFT calculations were performed using the B3LYP functional[41] as implemented in Gaussian 09.[42] The def2-SVP basis set was used for all atoms. Geometry optimizations were carried out with Grimme's D3 dispersion correction.[43] The solvent effect was considered through the polarizable continuum model (PCM).[44] Frequency calculations were performed to ensure that they are minimum energy structures by the absence of imaginary frequency. Spin-density plots were generated using Multiwfn.[45]

Cartesian coordinates

[Fe(^{t}Bu$_4$Pc)(py)(NR)]

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[Fe(^{t}Bu$_4$Pc)(NR)]

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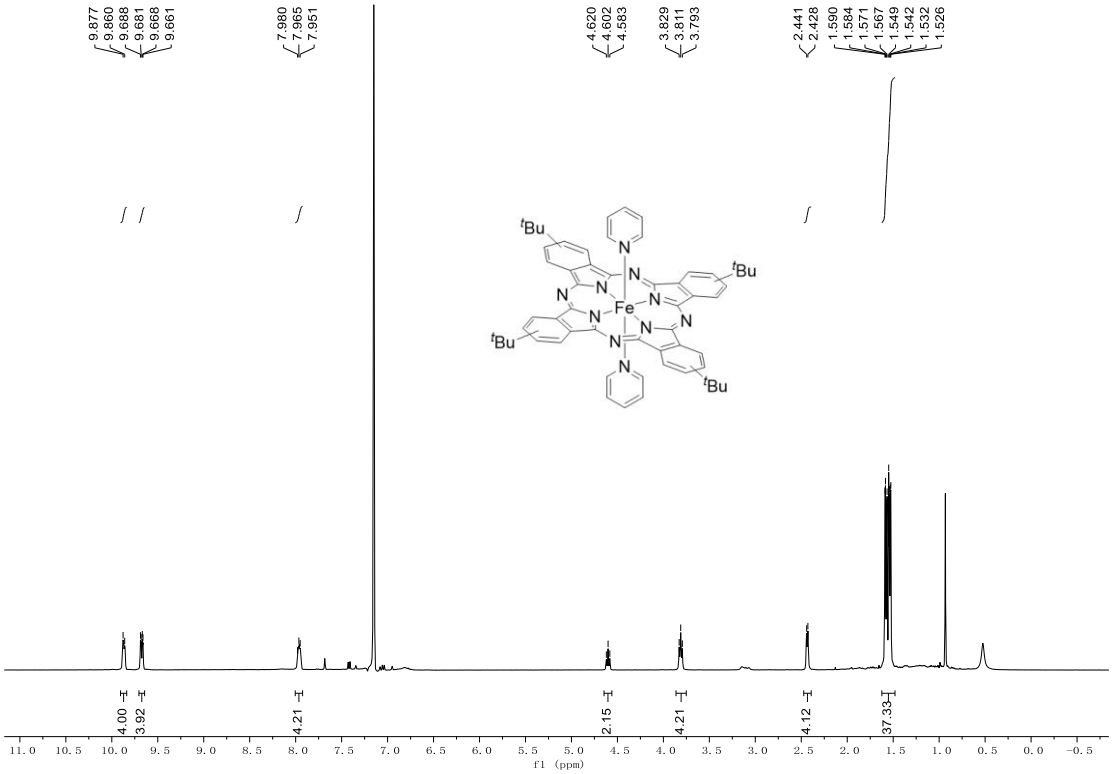
NMR spectra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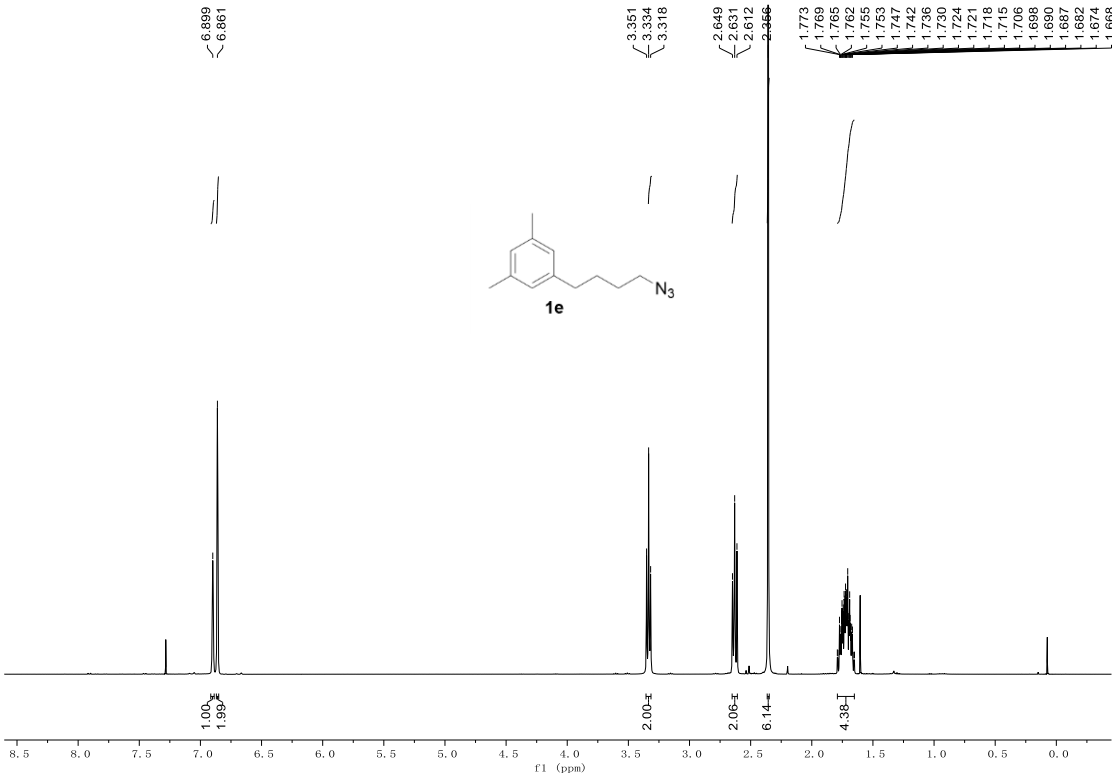
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1.690
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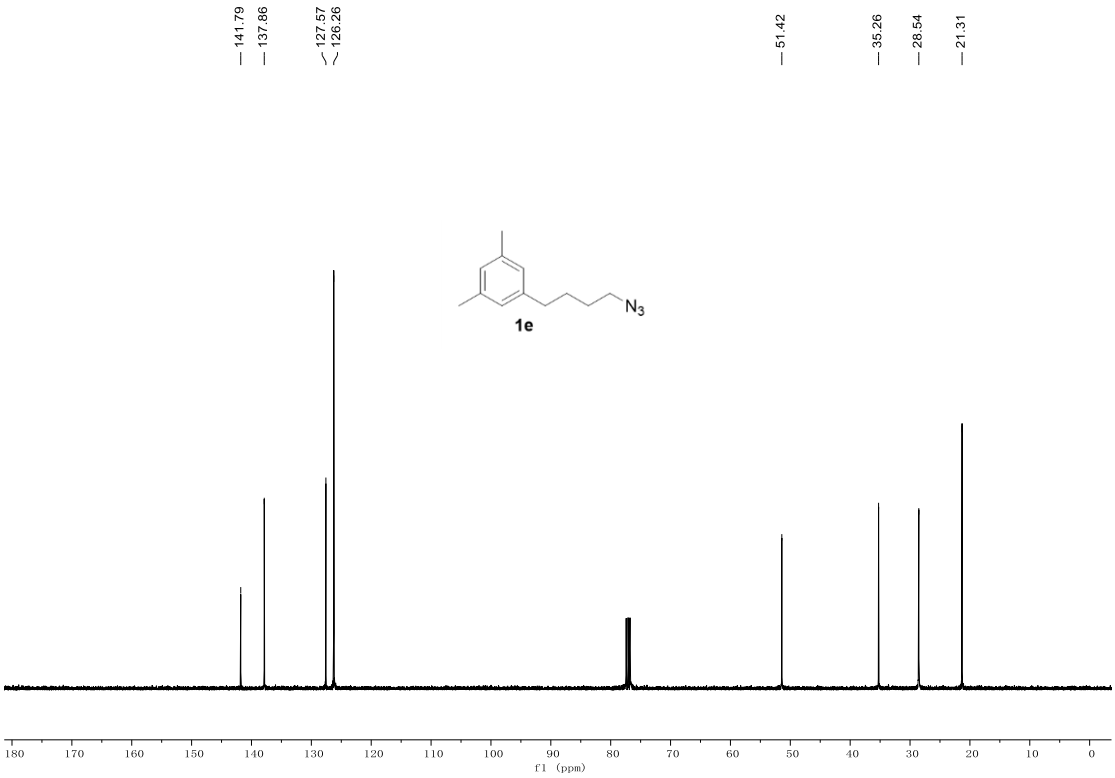
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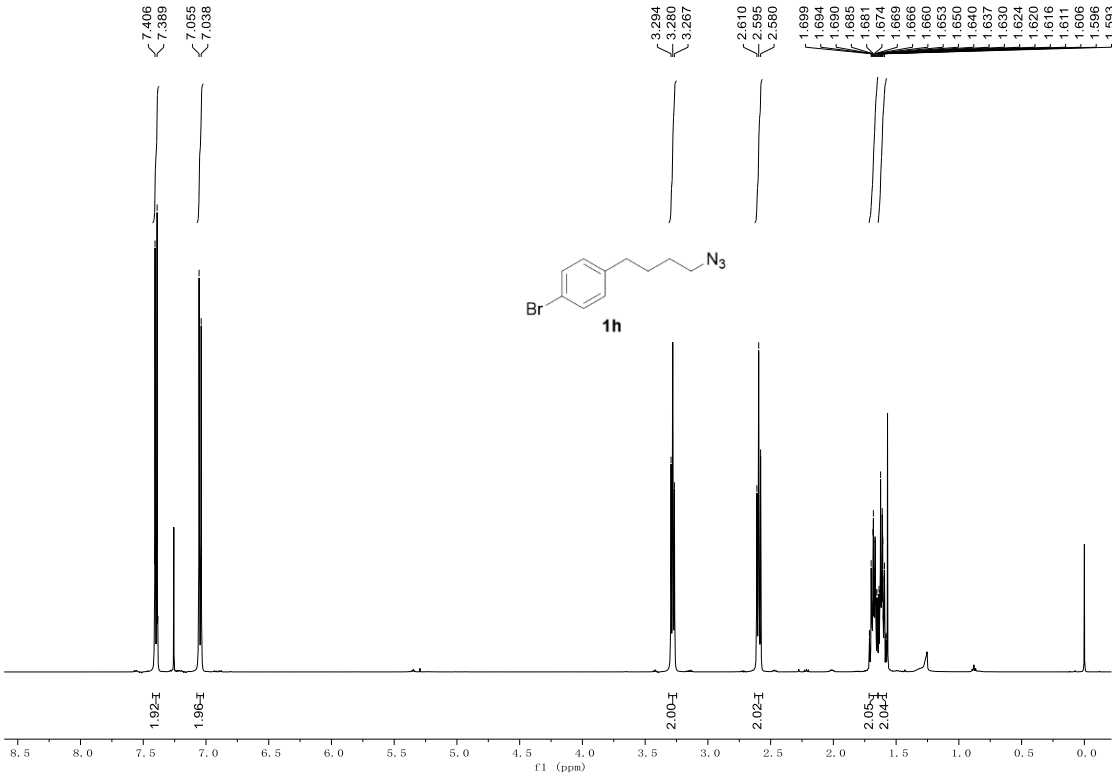
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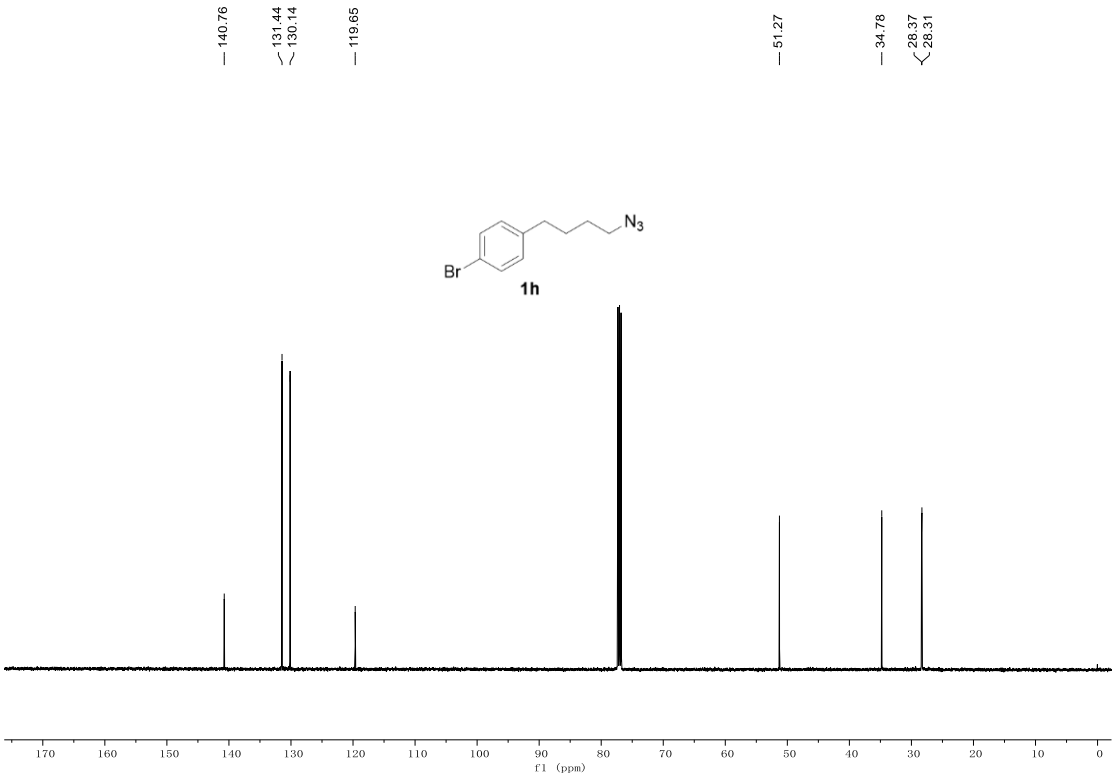
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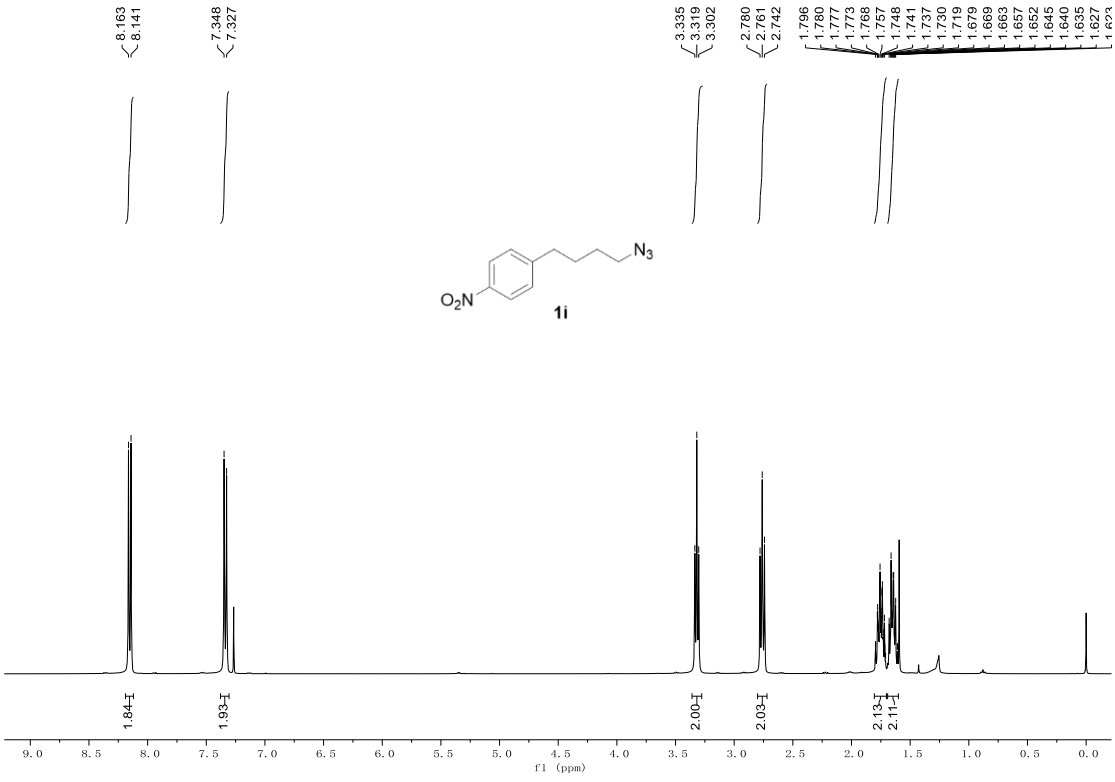
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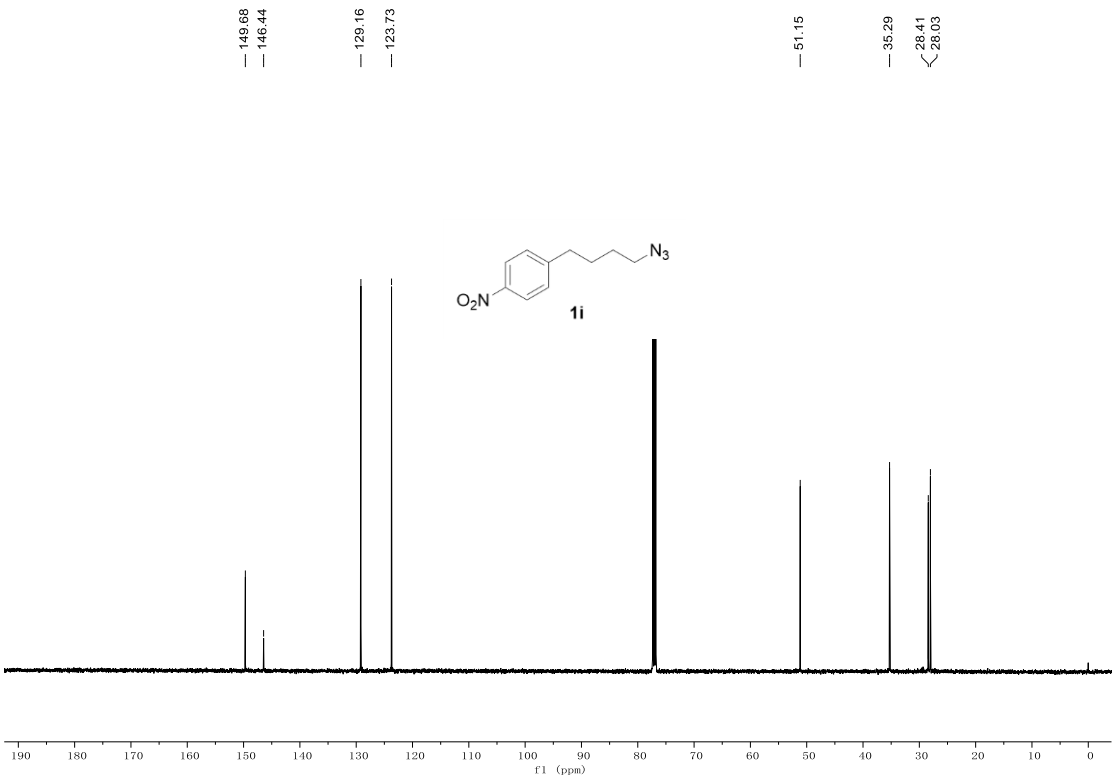
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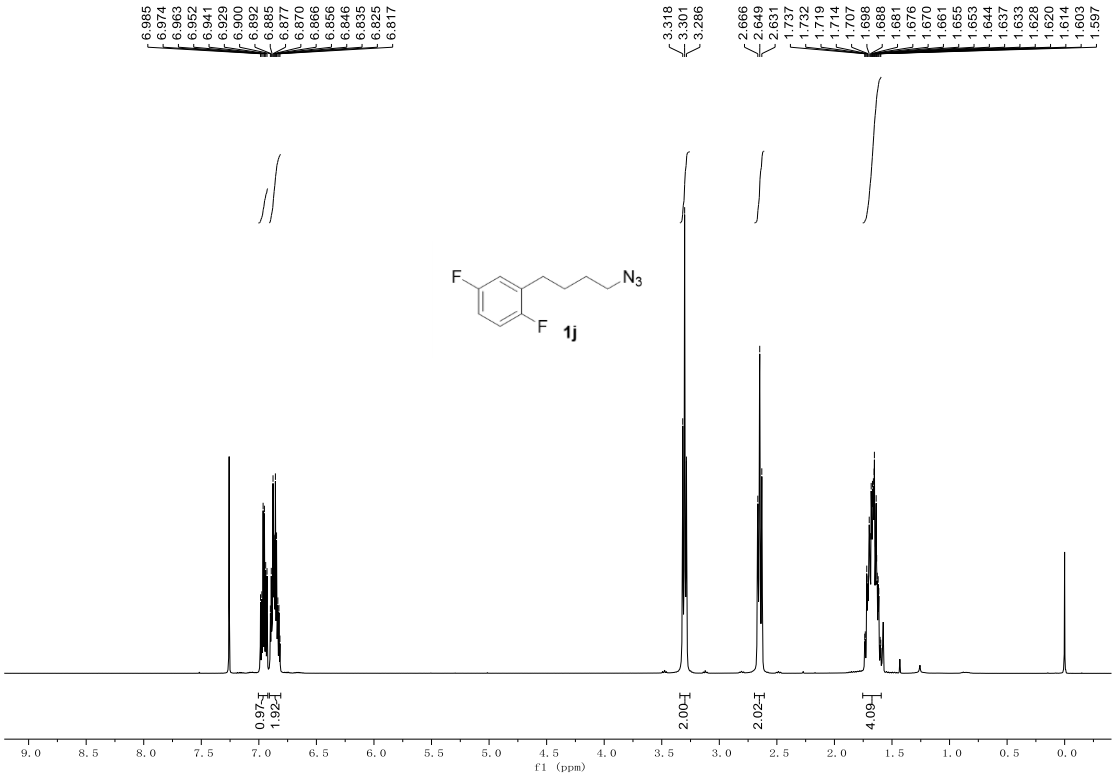
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N_3
F
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2.02
4.09
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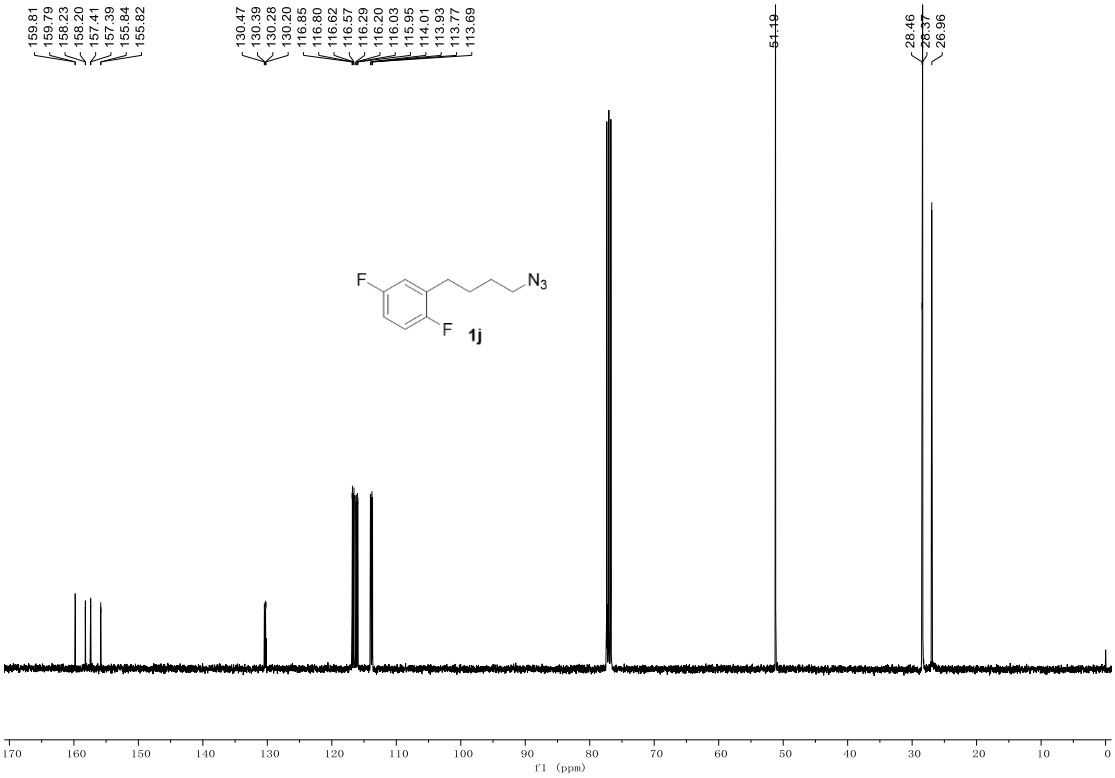
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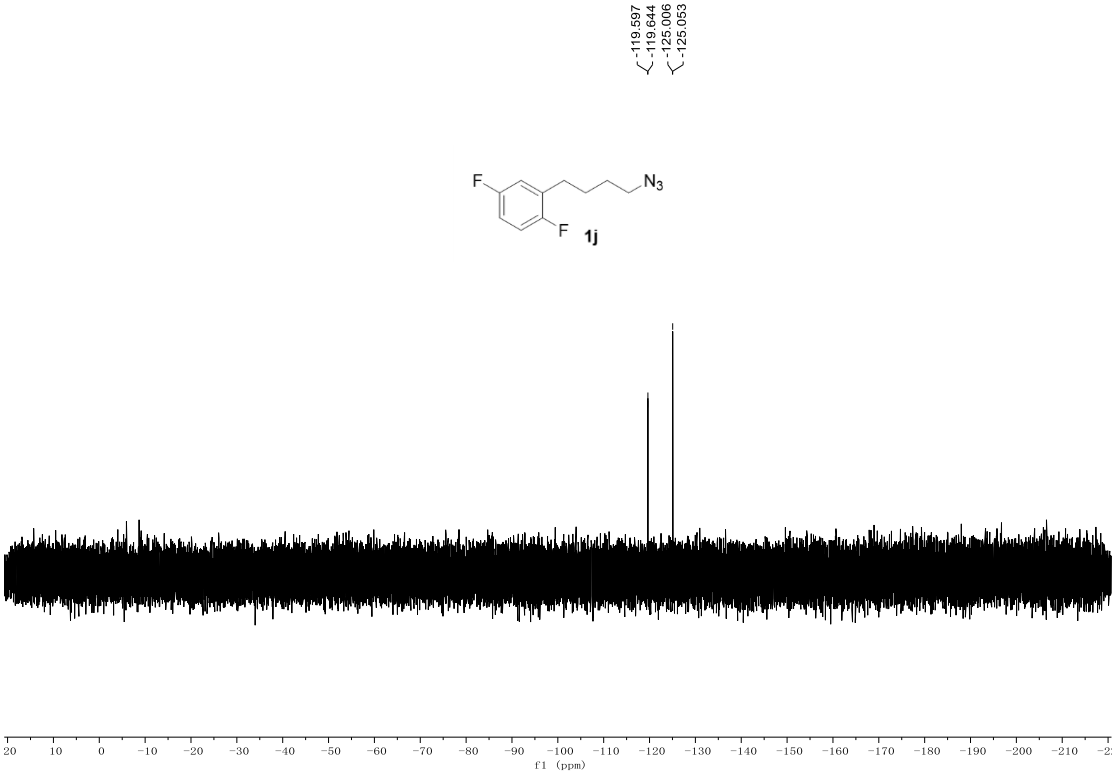
F
1j
f1 (ppm)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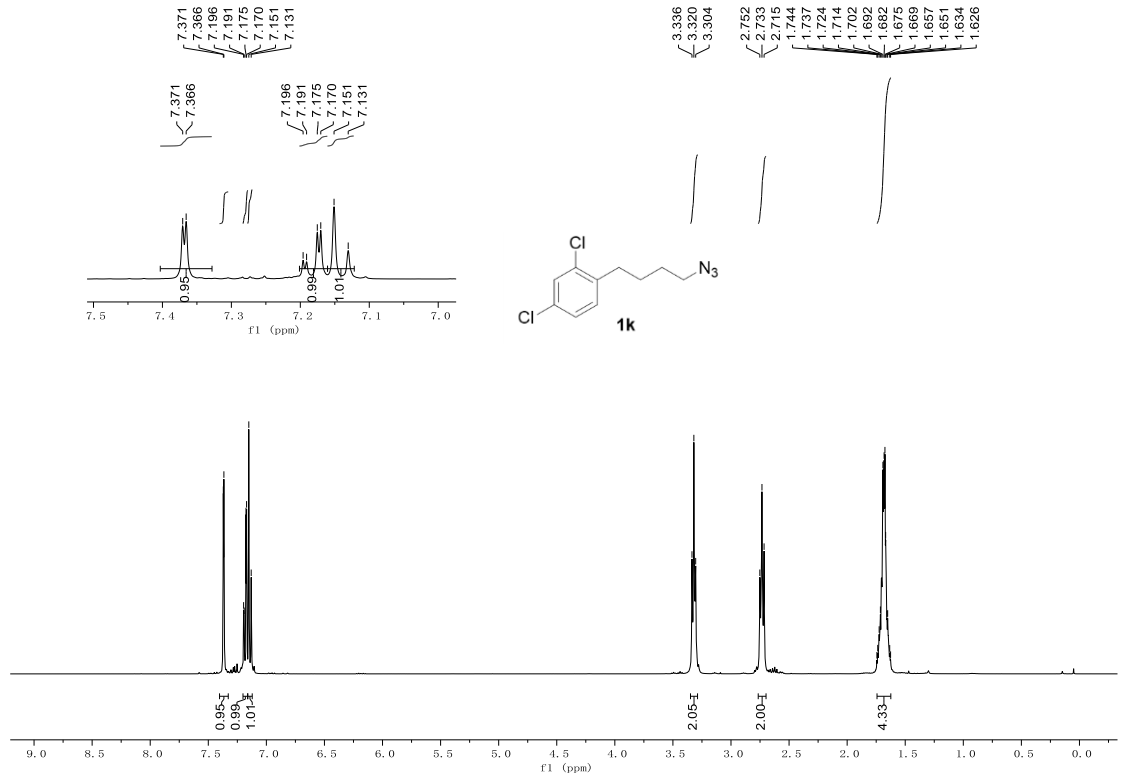
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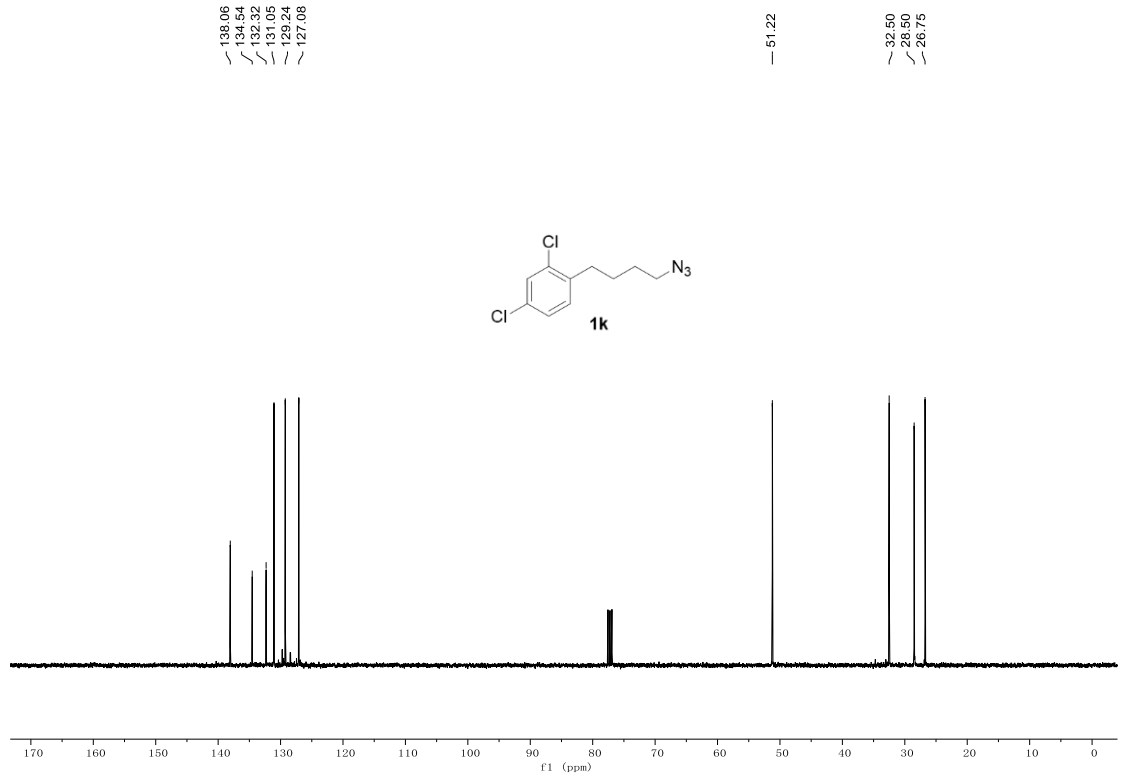
Cl
N3
Cl
1k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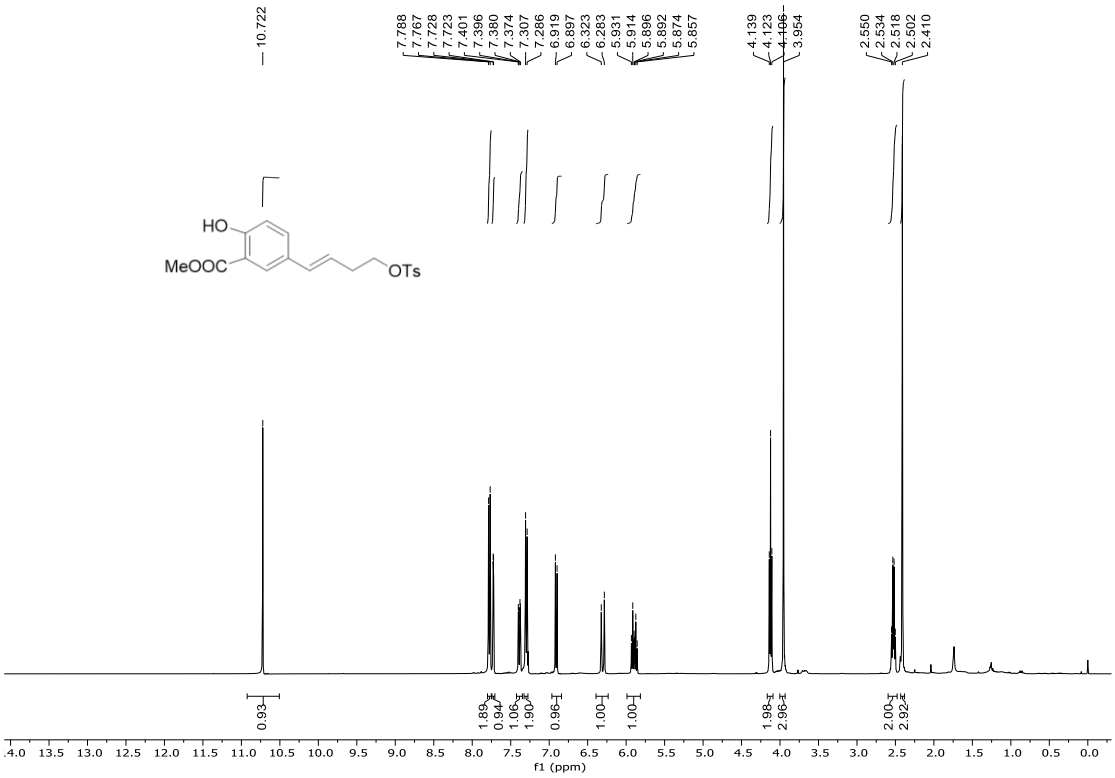
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3.954
2.550
2.534
2.518
2.502
2.410
HO
MeOOC
OTs
0.93
1.89
0.94
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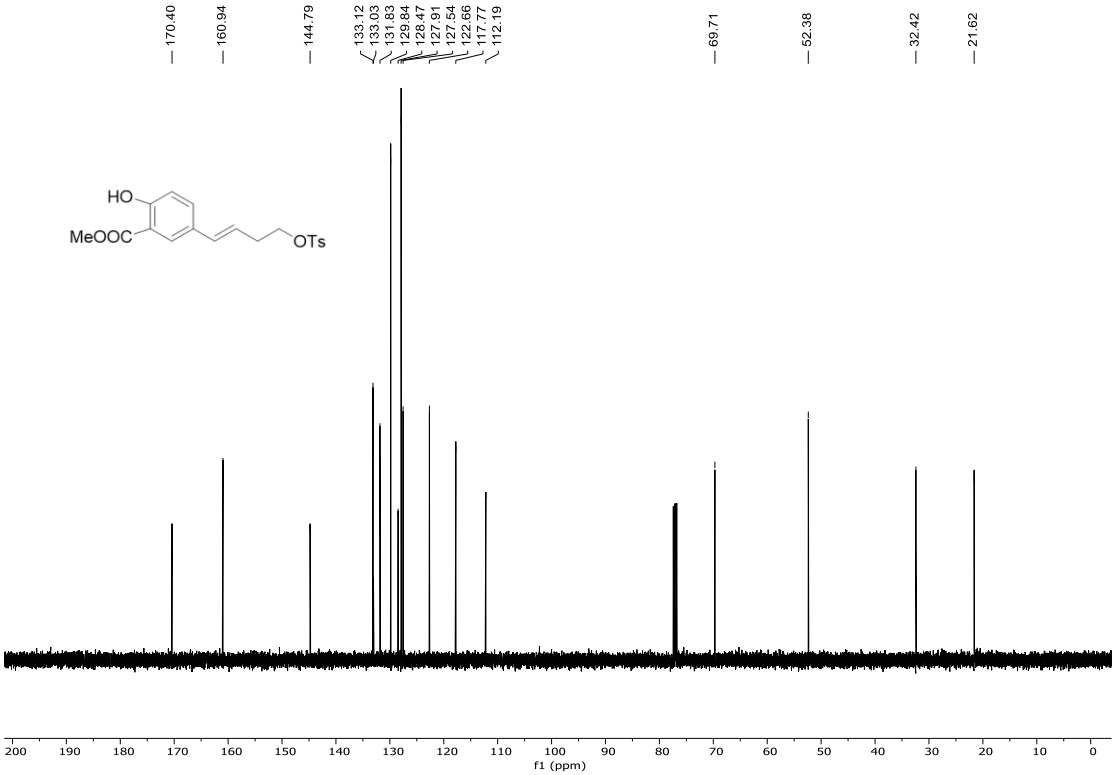
1.90
0.96
1.00
1.00
1.98
2.96
2.00
2.92
f1 (ppm)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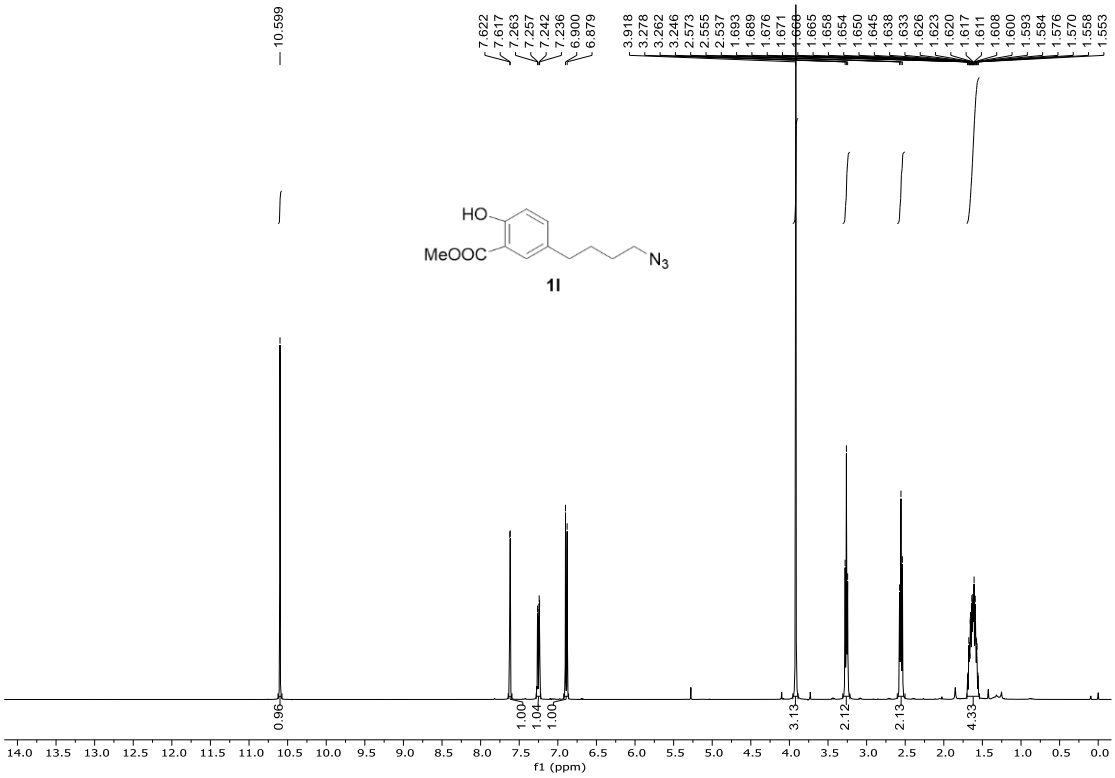
144.79
133.12
133.03
131.83
129.84
128.47
127.91
127.54
122.66
117.77
112.19
69.71
52.38
32.42
21.62
HO
MeOOC
OTs
f1 (ppm)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7.236
6.900
6.879
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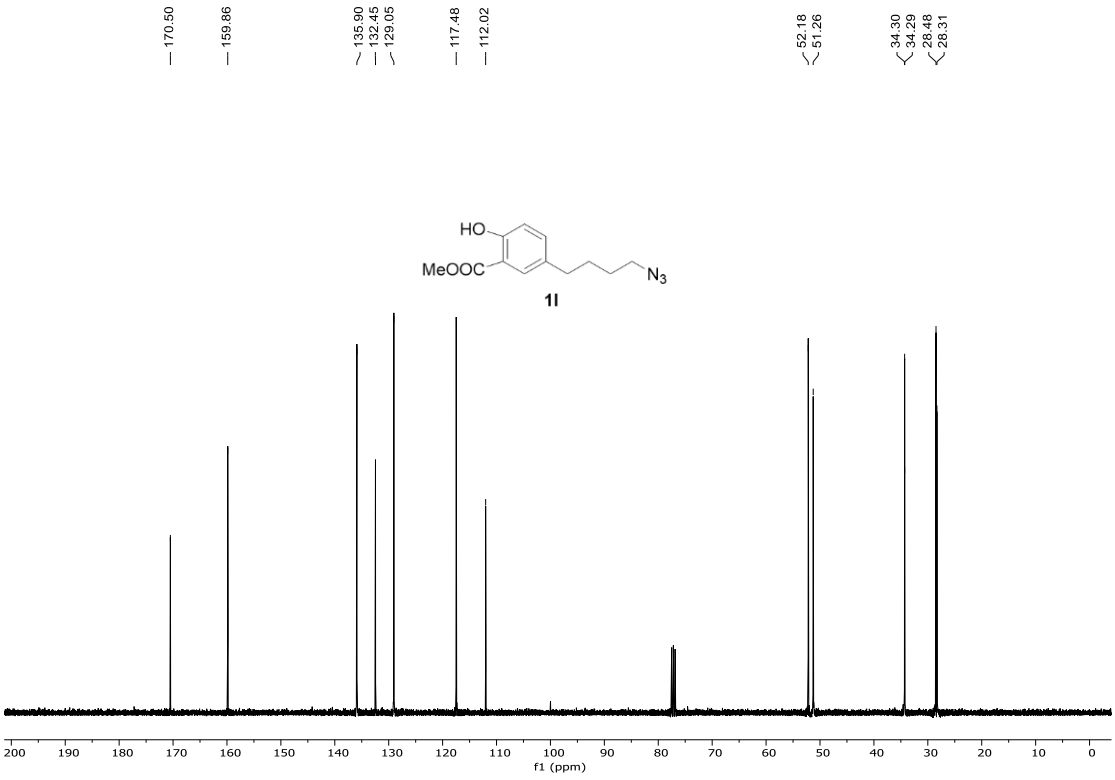
3.278
3.262
3.246
2.573
2.555
2.537
1.693
1.689
1.676
1.671
1.668
1.665
1.658
1.654
1.650
1.645
1.638
1.633
1.626
1.623
1.620
1.617
1.611
1.608
1.600
1.593
1.584
1.576
1.570
1.558
1.553
HO
MeOOC
N3
1l
0.96
1.00
1.04
1.00
3.13
2.12
2.13
4.33
f1 (ppm)


170.50
159.86
135.90
132.45
129.05
117.48
112.02
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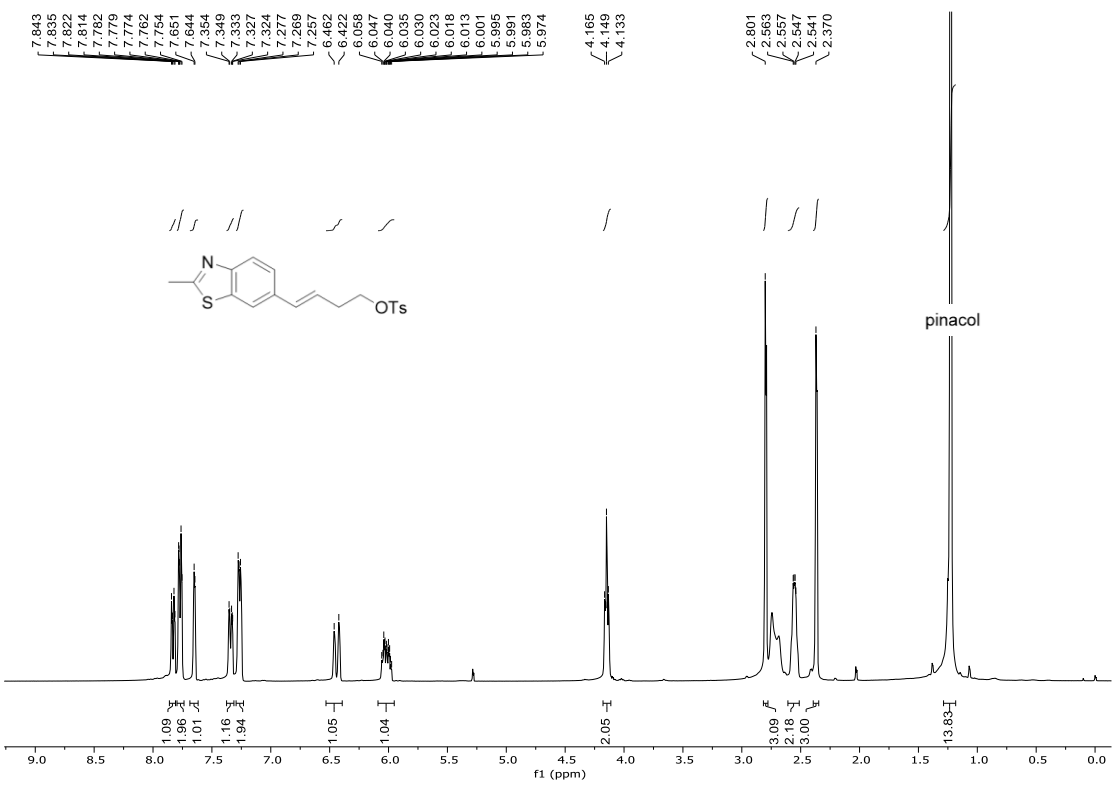
51.26
34.30
34.29
28.48
28.31
HO
MeOOC
N3
1l
f1 (ppm)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7.762
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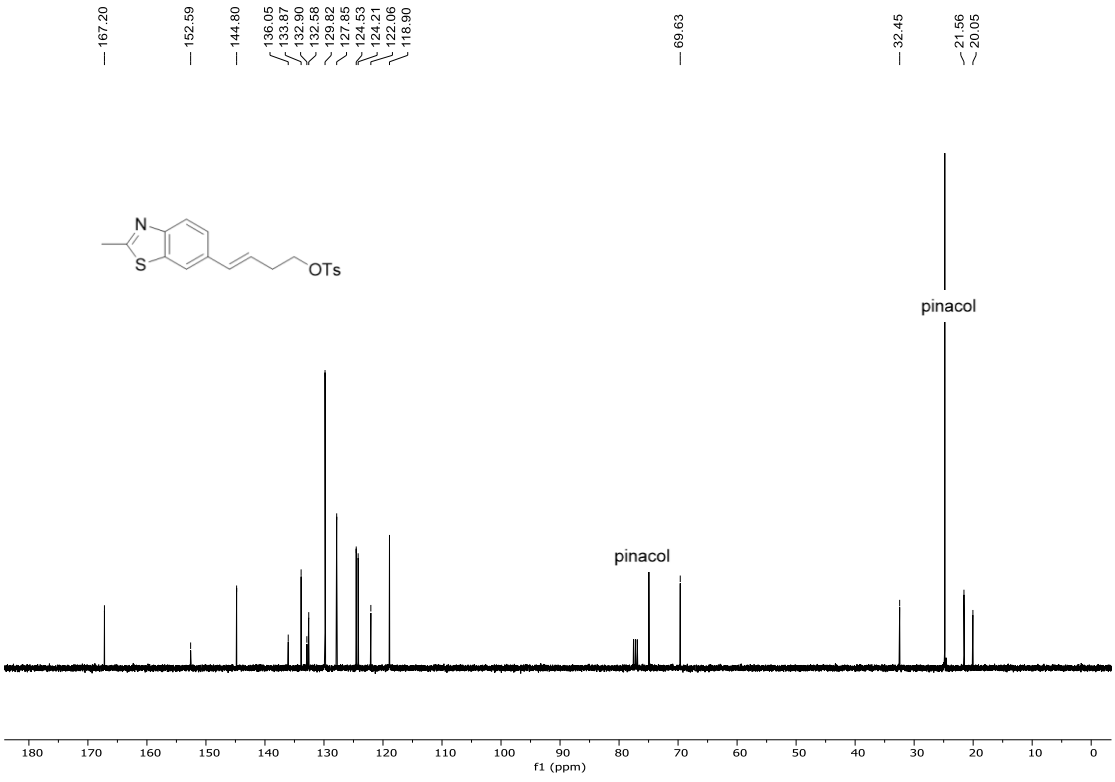
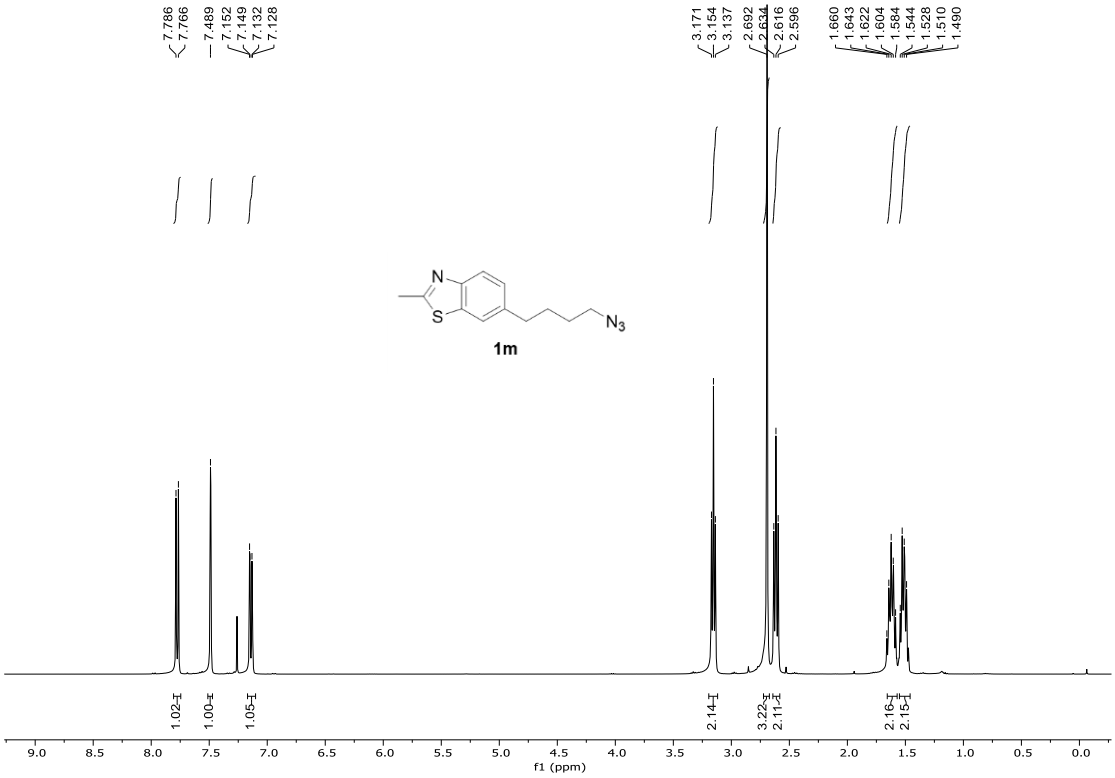
7.651
7.644
7.354
7.349
7.333
7.327
7.324
7.277
7.269
7.257
6.462
6.422
6.058
6.047
6.040
6.035
6.030
6.023
6.018
6.013
6.001
5.995
5.991
5.983
5.974
4.165
4.149
4.133
2.801
2.563
2.557
2.547
2.541
2.370
N
S
OTs
pinacol
1.09
1.96
1.01
1.16
1.94
1.05
1.04
2.05
3.09
2.18
3.00
13.83
f1 (ppm)


167.20
152.59
144.80
136.05
133.87
132.90
132.58
129.82
127.85
124.53
124.21
122.06
118.90
69.63
32.45
21.56
20.05
N
S
OTs
pinacol
pinacol
f1 (ppm)


7.786
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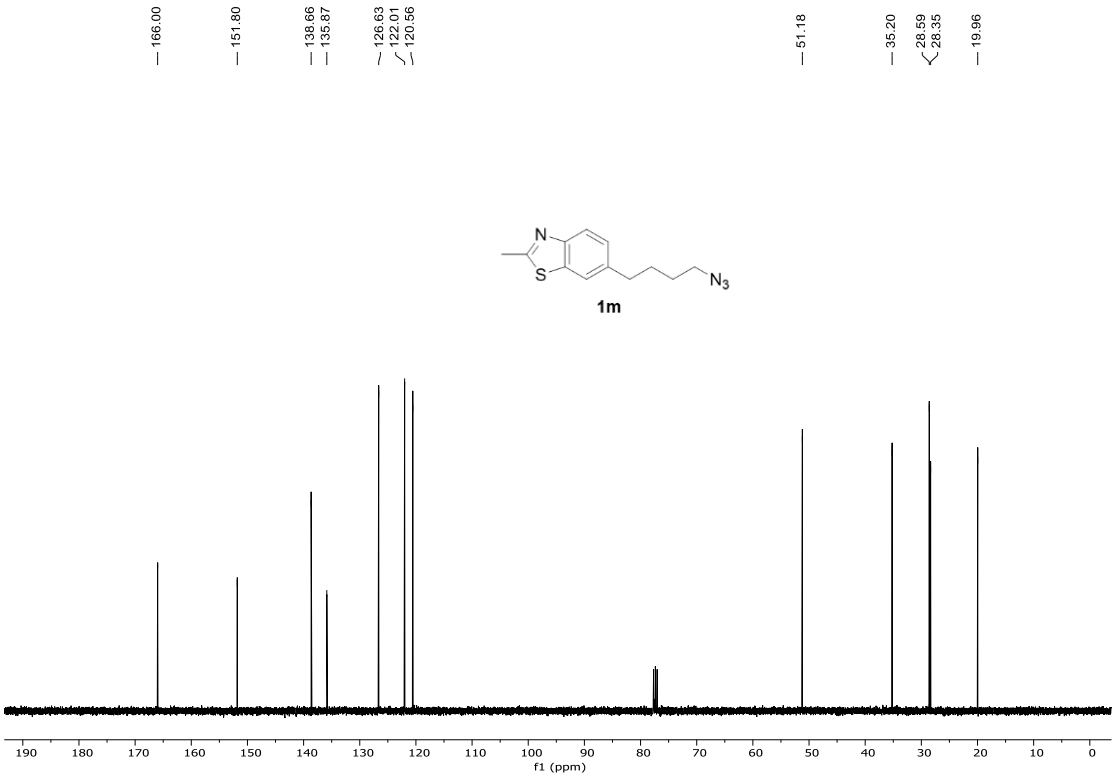
7.489
7.152
7.149
7.132
7.128
3.171
3.154
3.137
2.692
2.634
2.616
2.596
1.660
1.643
1.622
1.604
1.584
1.544
1.528
1.510
1.490
1.02
1.00
1.05
2.14
3.22
2.11
2.16
2.15
f1 (ppm)

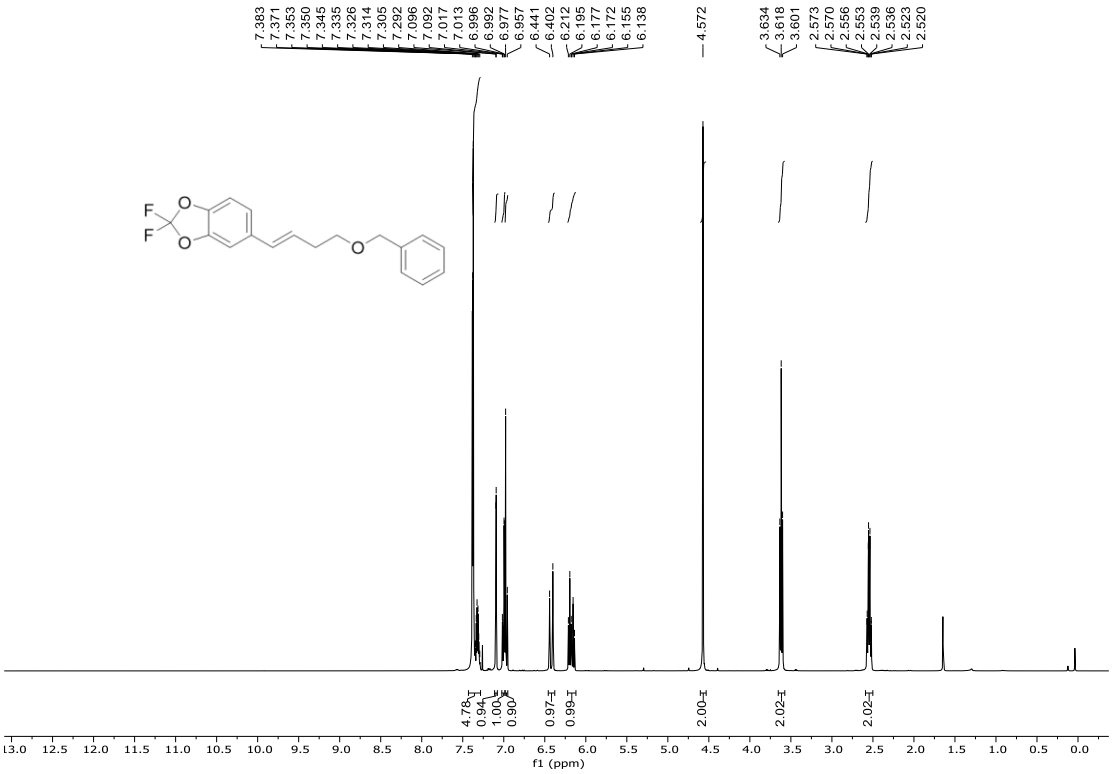
N
S
N3

1m


166.00
151.80
138.66
135.87
126.63
122.01
120.56
51.18
35.20
28.59
28.35
19.96
f1 (ppm)

N
S
N3

1m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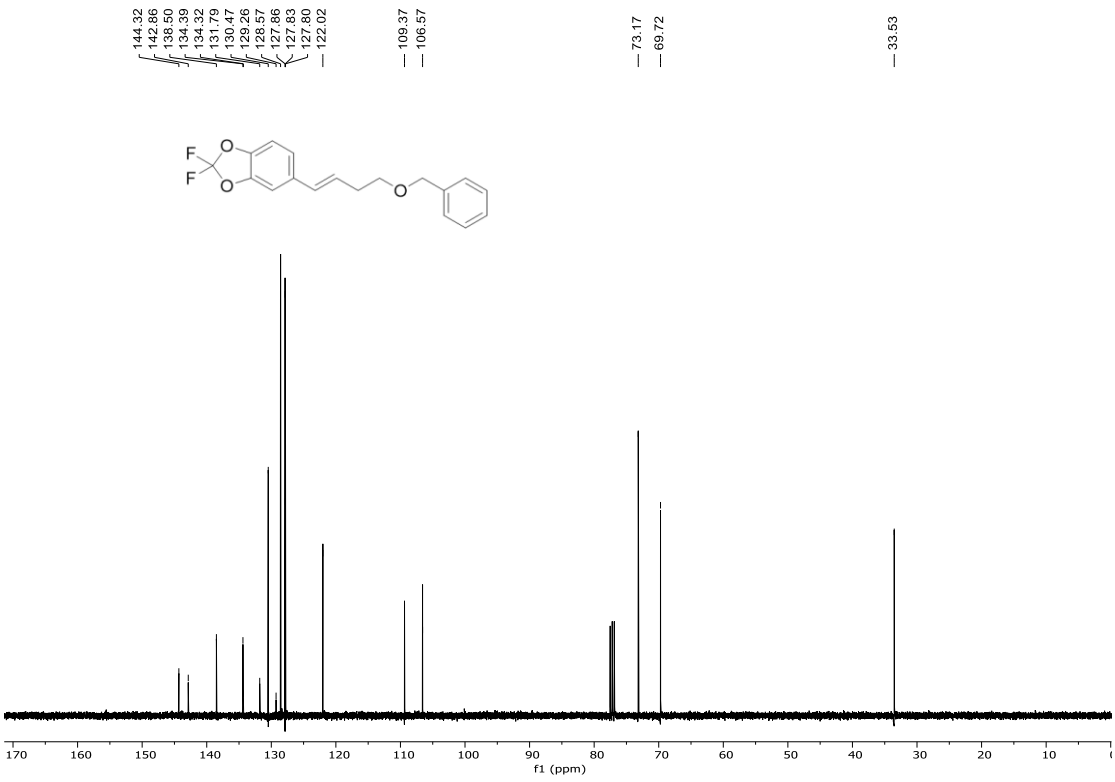
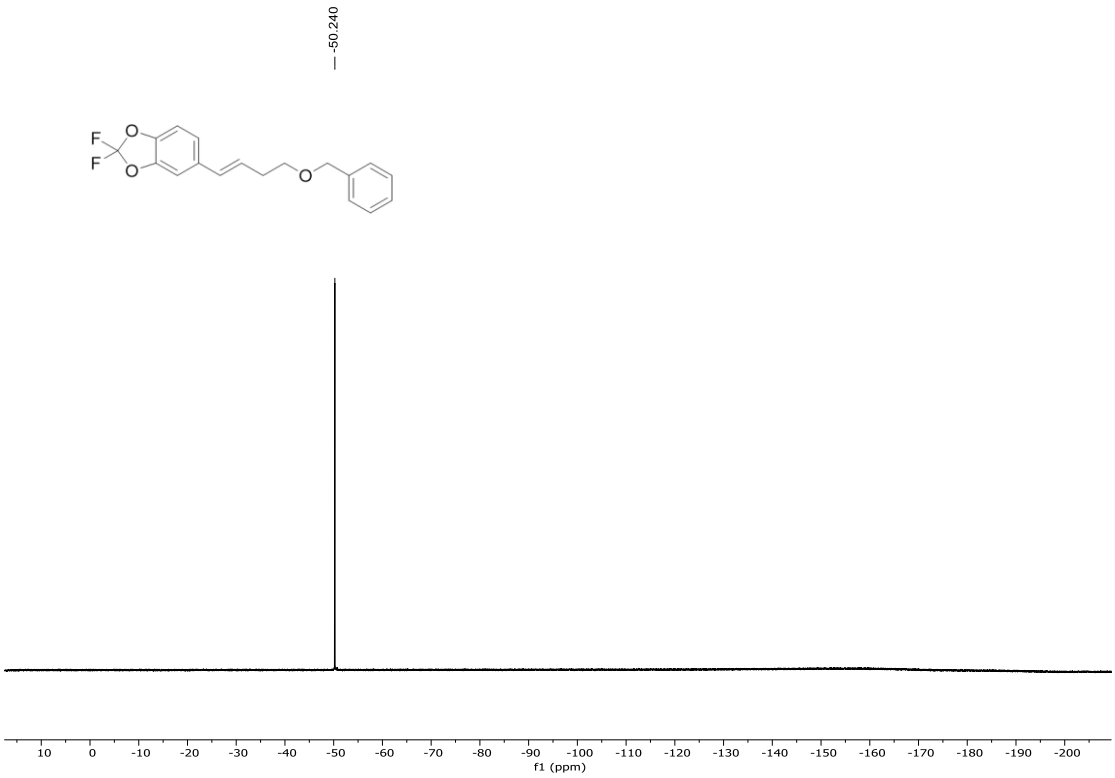
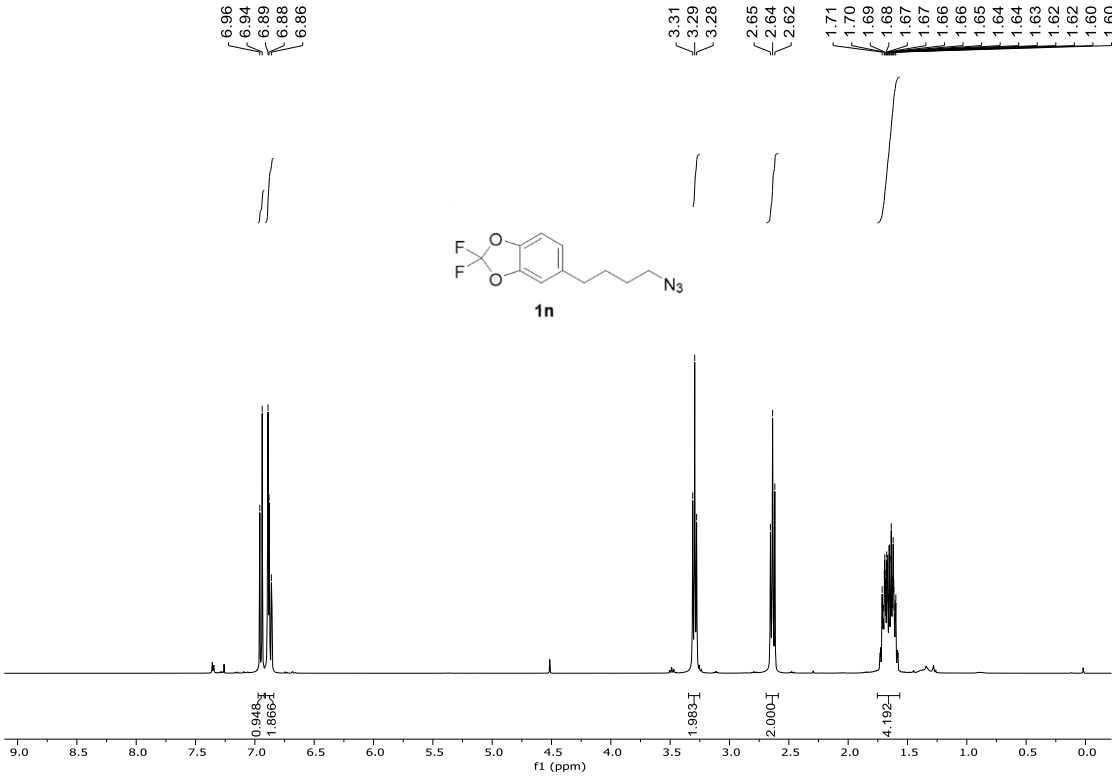
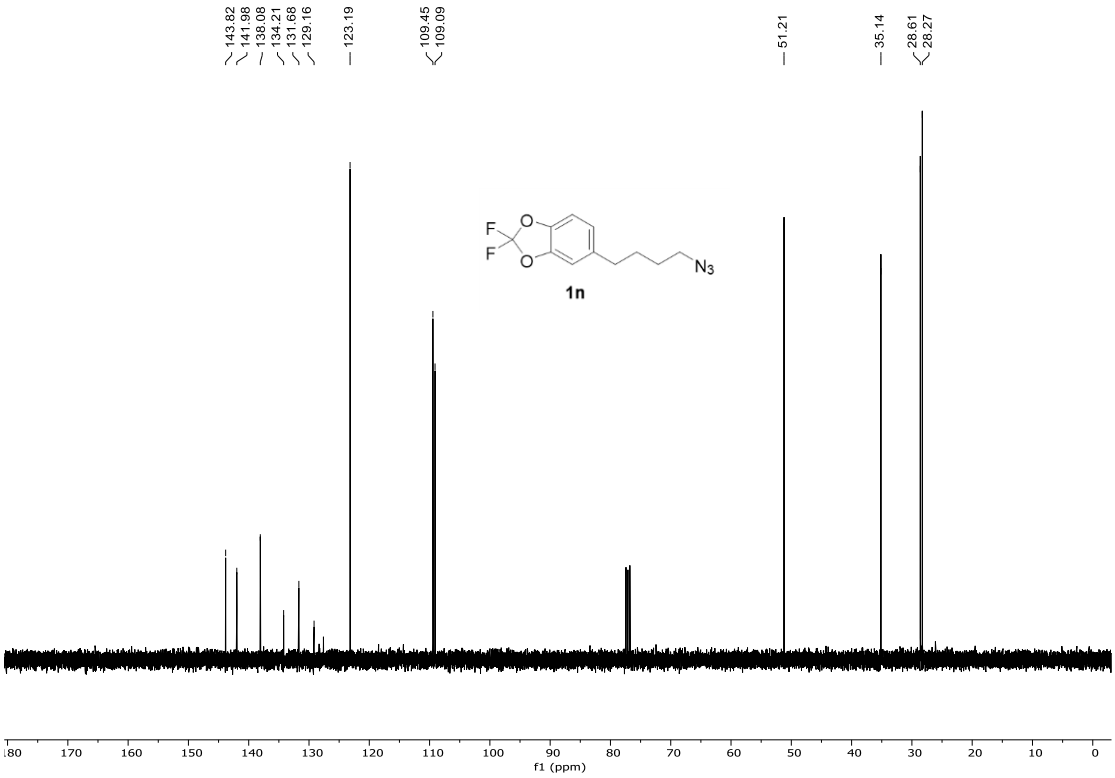
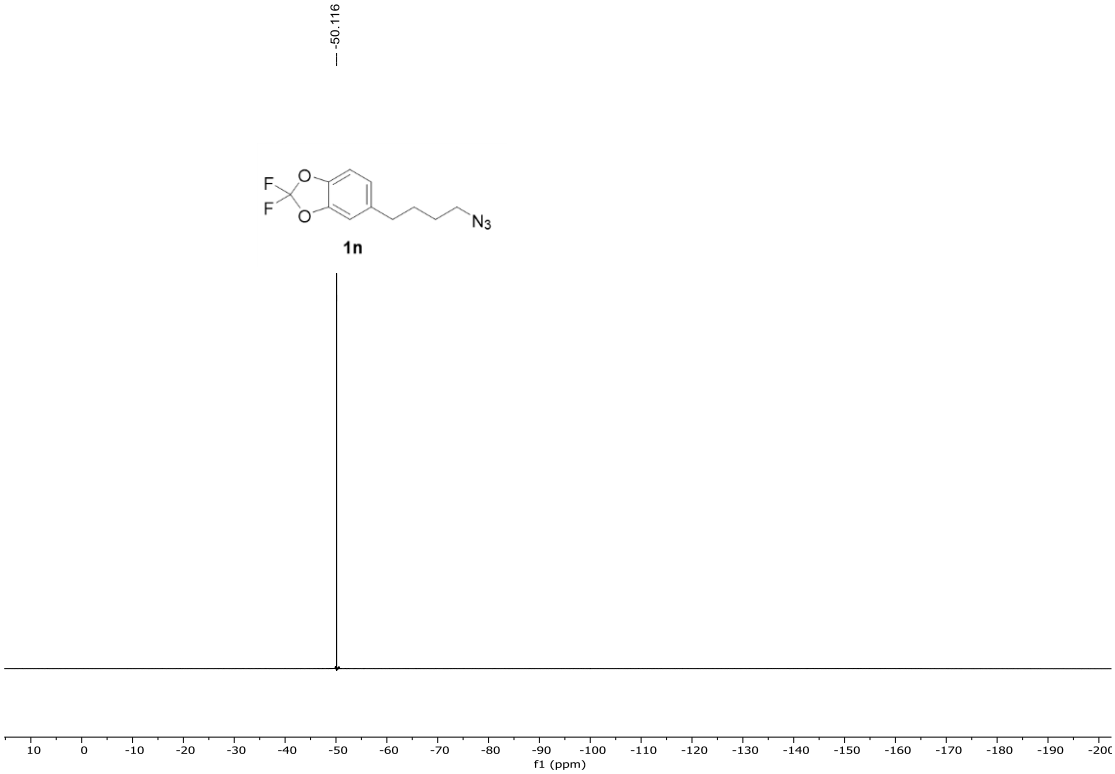
7.353
7.350
7.345
7.335
7.326
7.314
7.305
7.292
7.096
7.092
7.017
7.013
6.996
6.992
6.977
6.957
6.441
6.402
6.212
6.195
6.177
6.172
6.155
6.138
4.572
3.634
3.618
3.601
2.573
2.570
2.556
2.553
2.539
2.536
2.523
2.520
F
F
O
O
O
4.78
0.94
1.00
0.90
0.97
0.99
2.00
2.02
2.02
f1 (ppm)

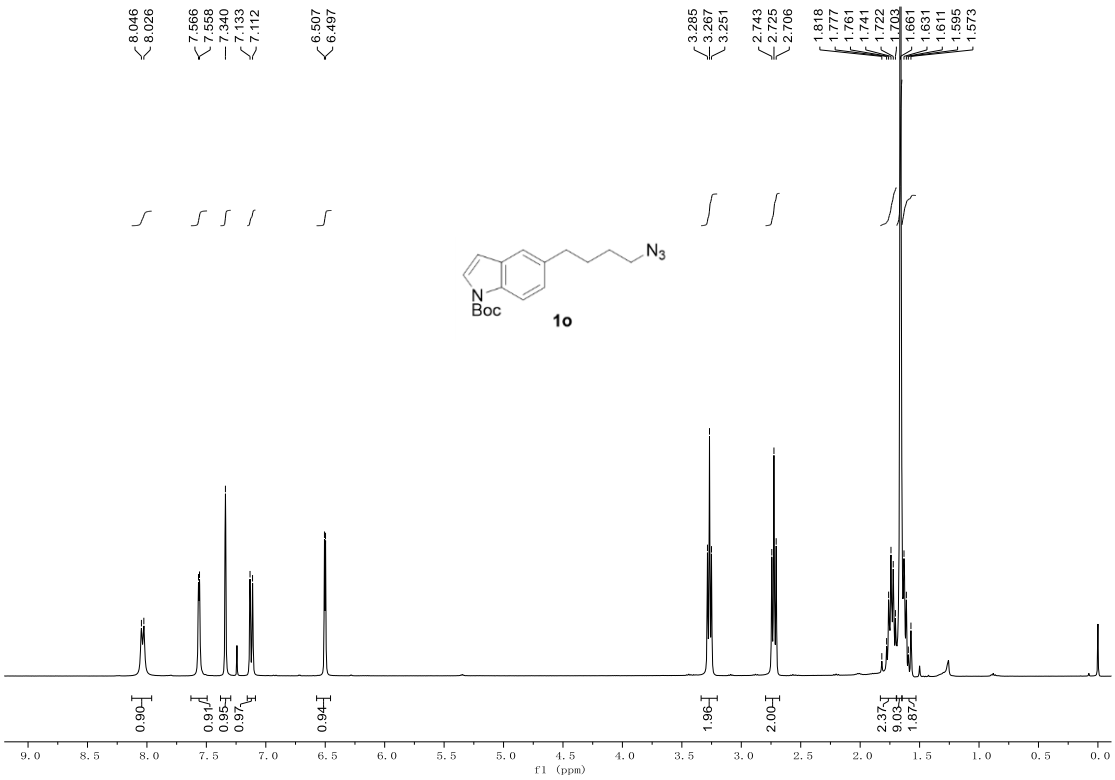

144.32
142.86
138.50
134.39
134.32
131.79
130.47
129.26
128.57
127.86
127.83
127.80
122.02
109.37
106.57
73.17
69.72
33.53
F
F
O
O
O
f1 (ppm)


-50.240
F
F
O
O
O
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


6.96
6.94
6.89
6.88
6.86
3.31
3.29
3.28
2.65
2.64
2.62
1.71
1.70
1.69
1.68
1.67
1.67
1.66
1.66
1.65
1.64
1.64
1.63
1.62
1.62
1.60
F
F
O
O
O
N3
1n
0.946
1.866
1.983
2.000
4.192
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


143.82
141.98
138.08
134.21
131.68
129.16
123.19
109.45
109.09
51.21
35.14
28.61
28.27
F
F
O
O
N3
1n
f1 (ppm)


-50.116
F
F
O
O
N3
1n
f1 (ppm)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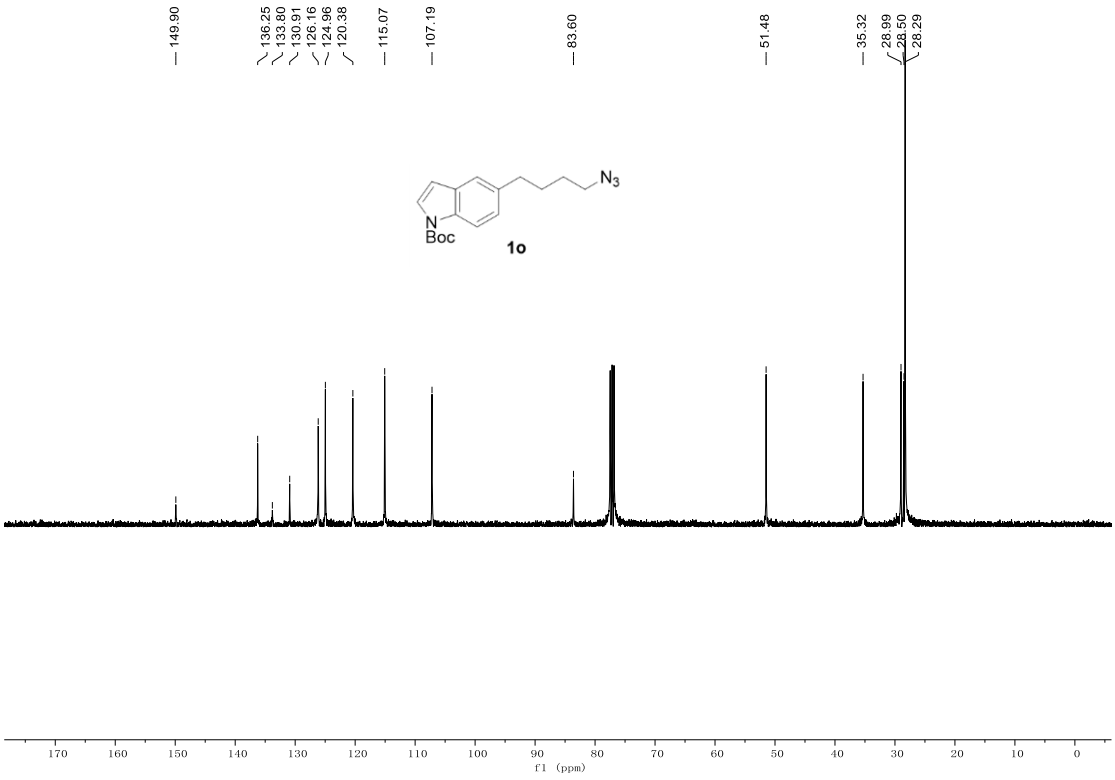
8.026
7.566
7.558
7.340
7.133
7.112
6.507
6.497
3.285
3.267
3.251
2.743
2.725
2.706
1.818
1.777
1.761
1.741
1.722
1.703
1.661
1.631
1.611
1.595
1.573
N3
N
Boc
1o
0.90
0.91
0.95
0.97
0.94
1.96
2.00
2.37
9.03
1.87
f1 (ppm)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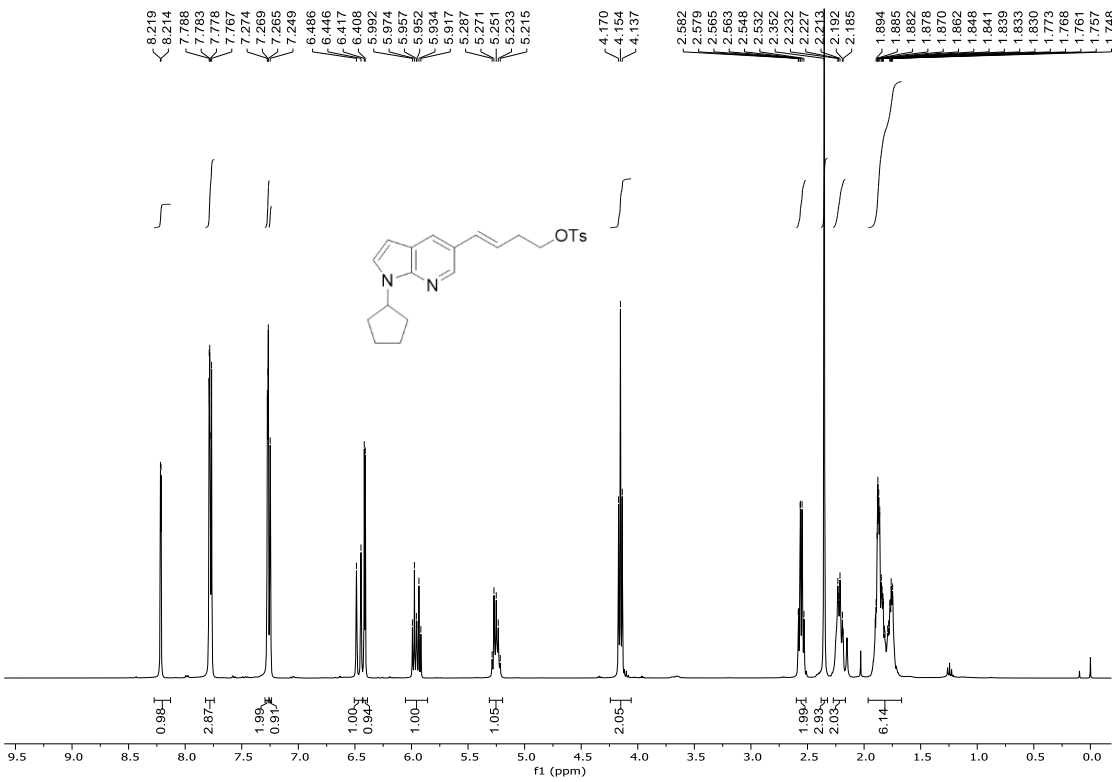
136.25
133.80
130.91
126.16
124.96
120.38
115.07
107.19
83.60
51.48
35.32
28.99
28.50
28.29
N3
N
Boc
1o
f1 (ppm)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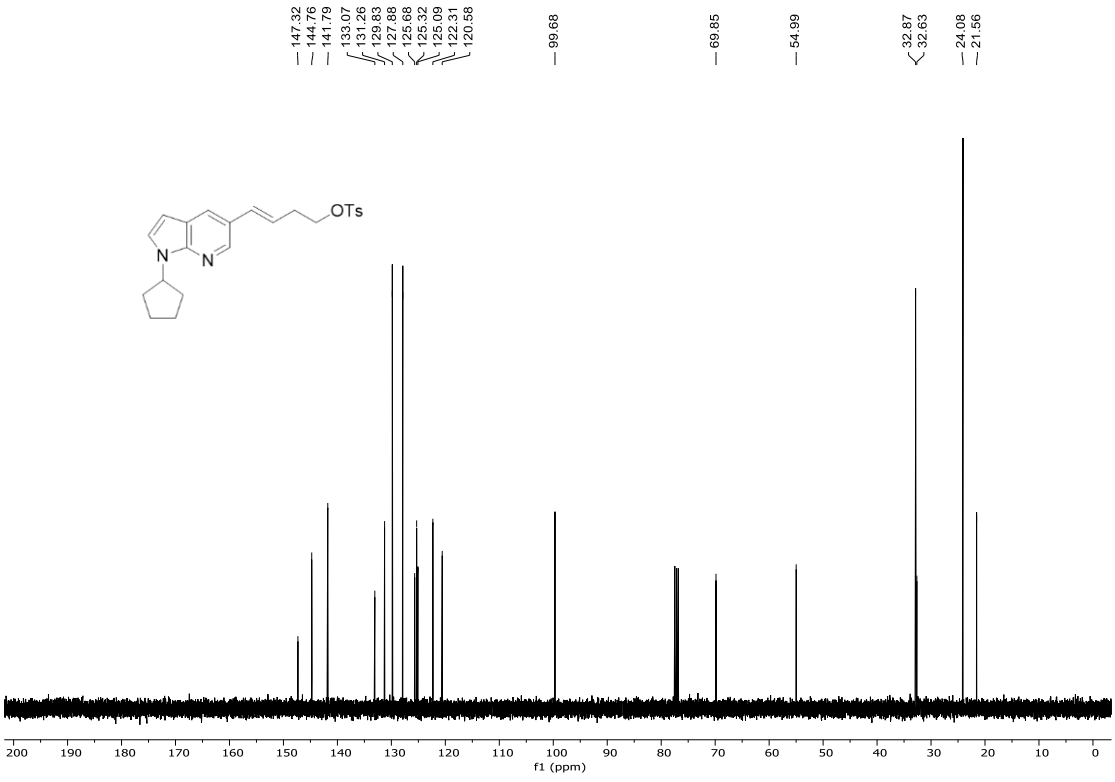
7.767
7.274
7.269
7.265
7.249
6.486
6.446
6.417
6.408
5.992
5.974
5.957
5.952
5.934
5.917
5.287
5.271
5.251
5.233
5.215
4.170
4.154
4.137
2.582
2.579
2.565
2.563
2.548
2.532
2.352
2.232
2.227
2.213
2.192
2.185
1.894
1.885
1.882
1.878
1.870
1.862
1.848
1.841
1.839
1.833
1.830
1.773
1.768
1.761
1.757
OTs
N
N
0.98
2.87
1.99
0.91
1.00
0.94
1.00
1.05
2.05
1.99
2.93
2.03
6.14
f1 (ppm)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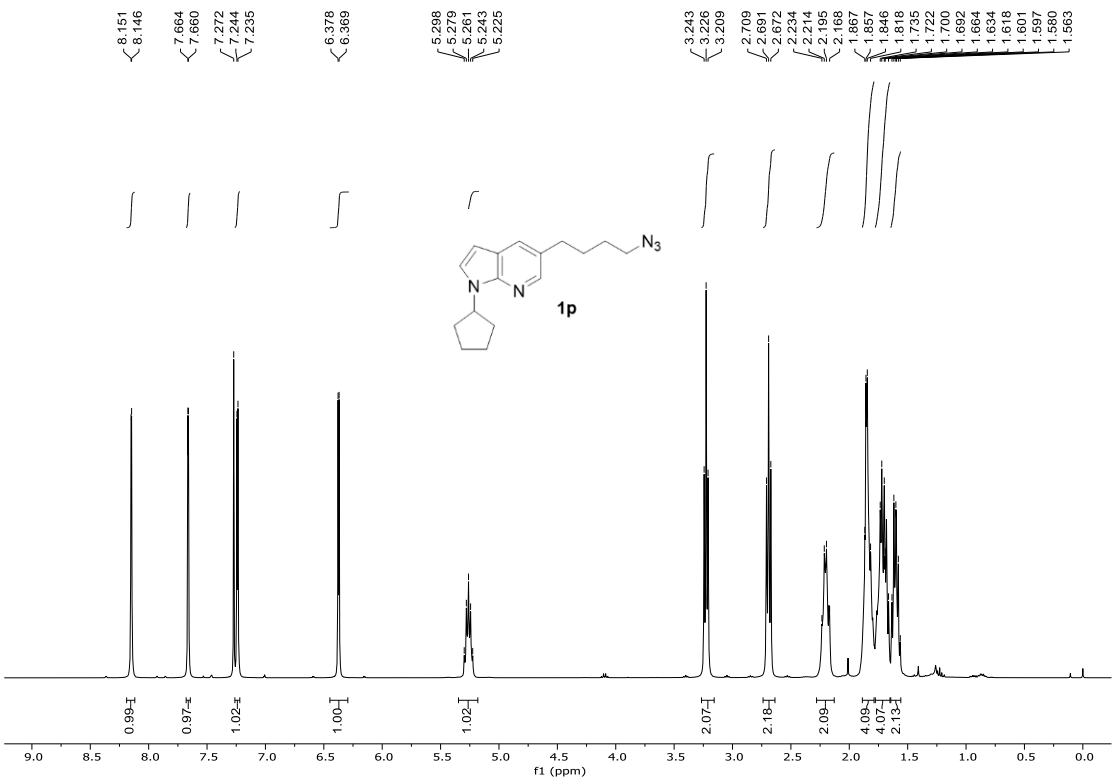
141.79
133.07
131.26
129.83
127.88
125.68
125.32
125.09
122.31
120.58
99.68
69.85
54.99
32.87
32.63
24.08
21.56
OTs
N
N
f1 (ppm)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6.378
6.369
5.298
5.279
5.261
5.243
5.225
3.243
3.226
3.209
2.709
2.691
2.672
2.234
2.214
2.195
2.168
1.867
1.857
1.846
1.818
1.735
1.722
1.700
1.692
1.664
1.634
1.618
1.601
1.597
1.580
1.563
N3
N
N
1p
0.99
0.97
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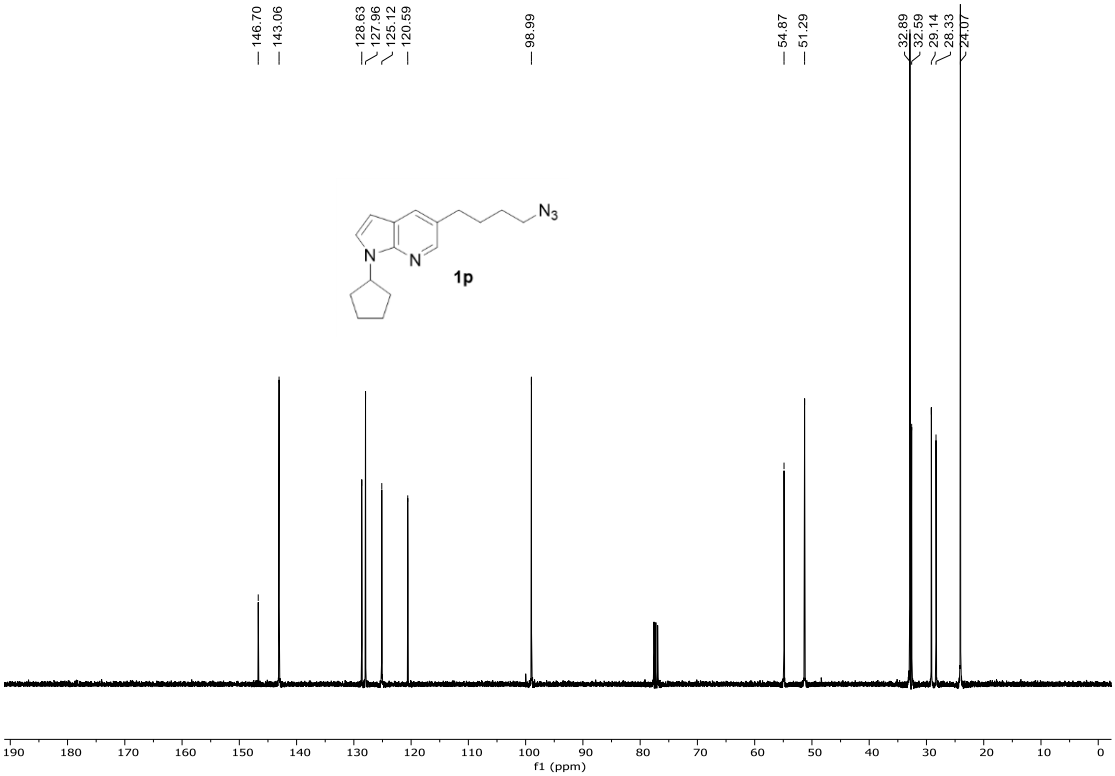
1.00
1.02
2.07
2.18
2.09
4.09
4.07
2.13
f1 (ppm)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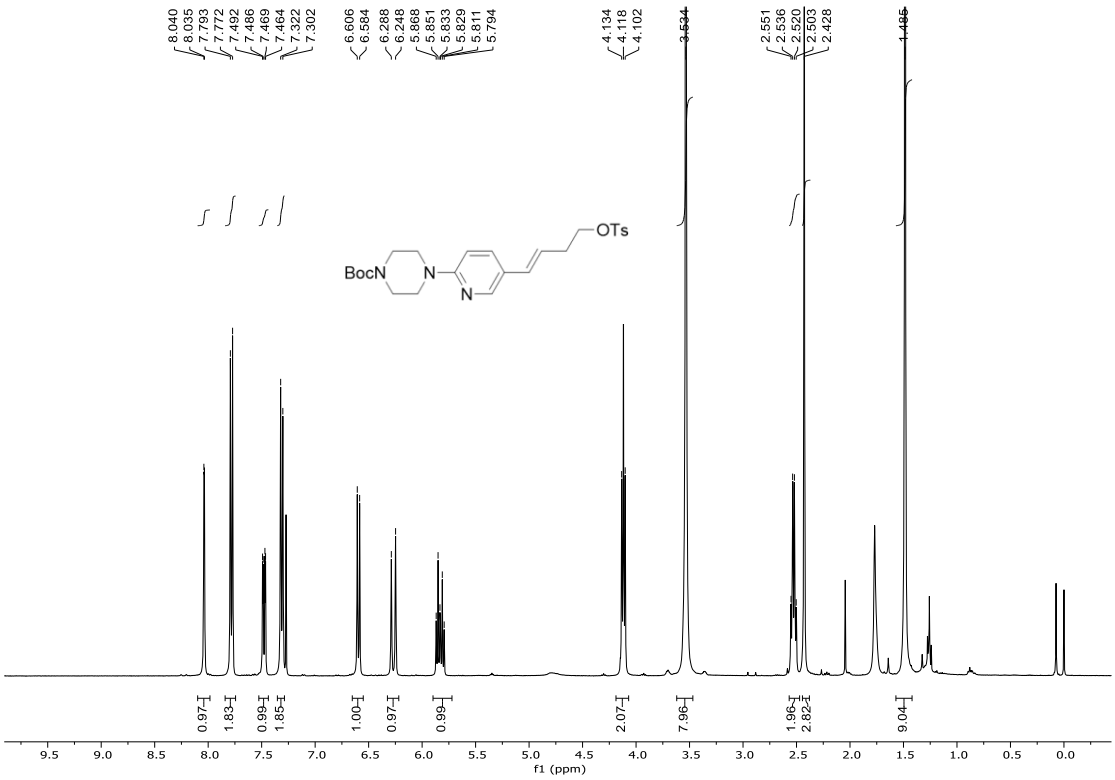
128.63
127.96
125.12
120.59
98.99
54.87
51.29
32.89
32.59
29.14
28.33
24.07
N3
N
N
1p
f1 (ppm)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7.464
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7.302
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6.584
6.288
6.248
5.868
5.851
5.833
5.829
5.811
5.794
4.134
4.118
4.102
3.534
2.551
2.536
2.520
2.503
2.428
1.486
OTs
BocN
N
N
0.97
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0.99
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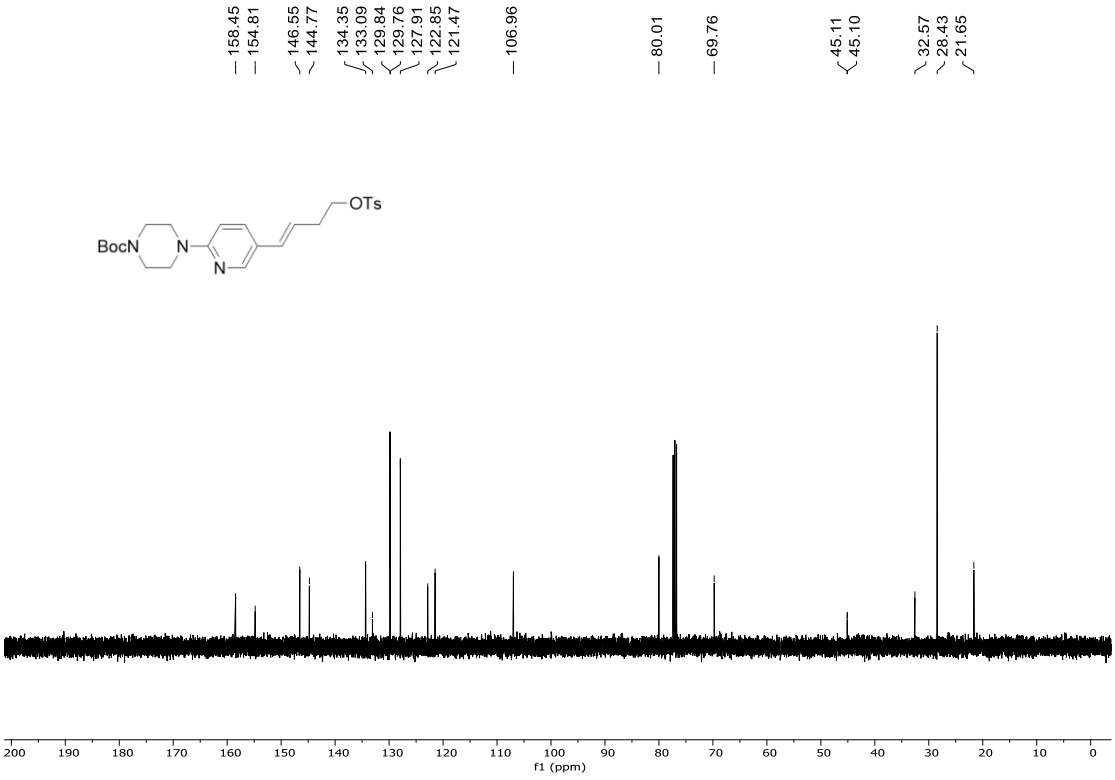
1.00
0.97
0.99
2.07
7.96
1.96
2.82
9.04
f1 (ppm)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144.77
134.35
133.09
129.84
129.76
127.91
122.85
121.47
106.96
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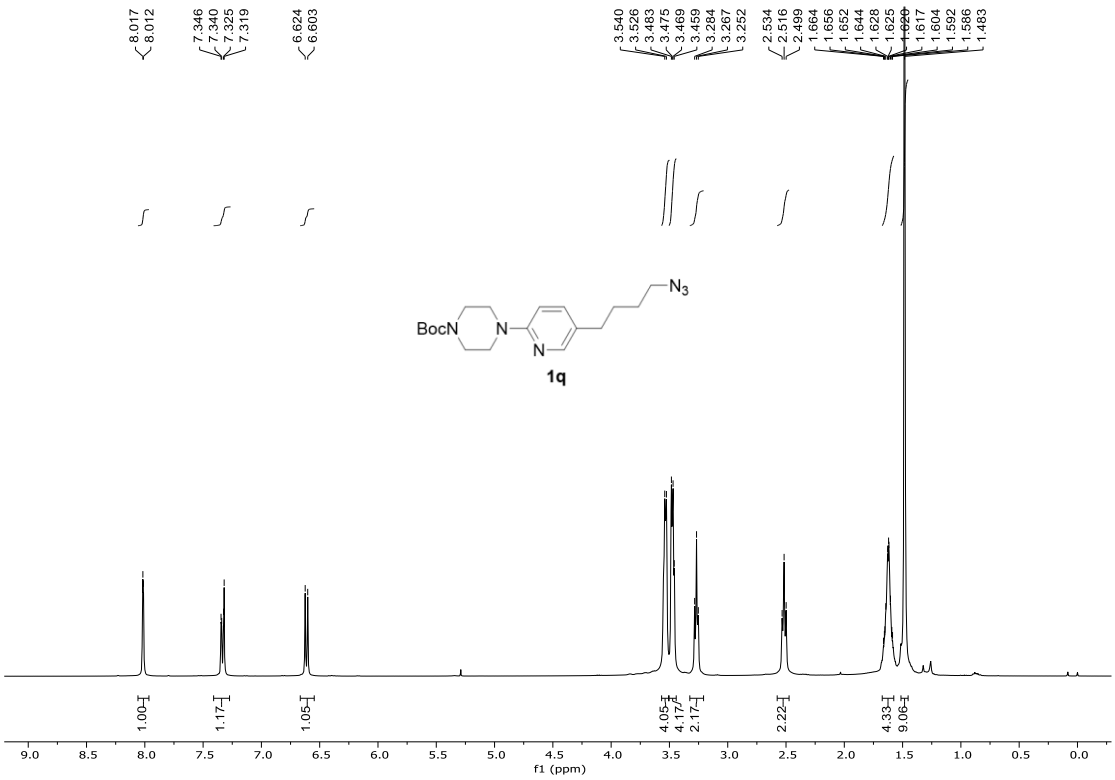
45.11
45.10
32.57
28.43
21.65
OTs
BocN
N
N
f1 (ppm)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6.603
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3.526
3.483
3.475
3.469
3.459
3.284
3.267
3.252
2.534
2.516
2.499
1.664
1.656
1.652
1.644
1.628
1.625
1.620
1.617
1.604
1.592
1.586
1.483
BocN
N
N
N3
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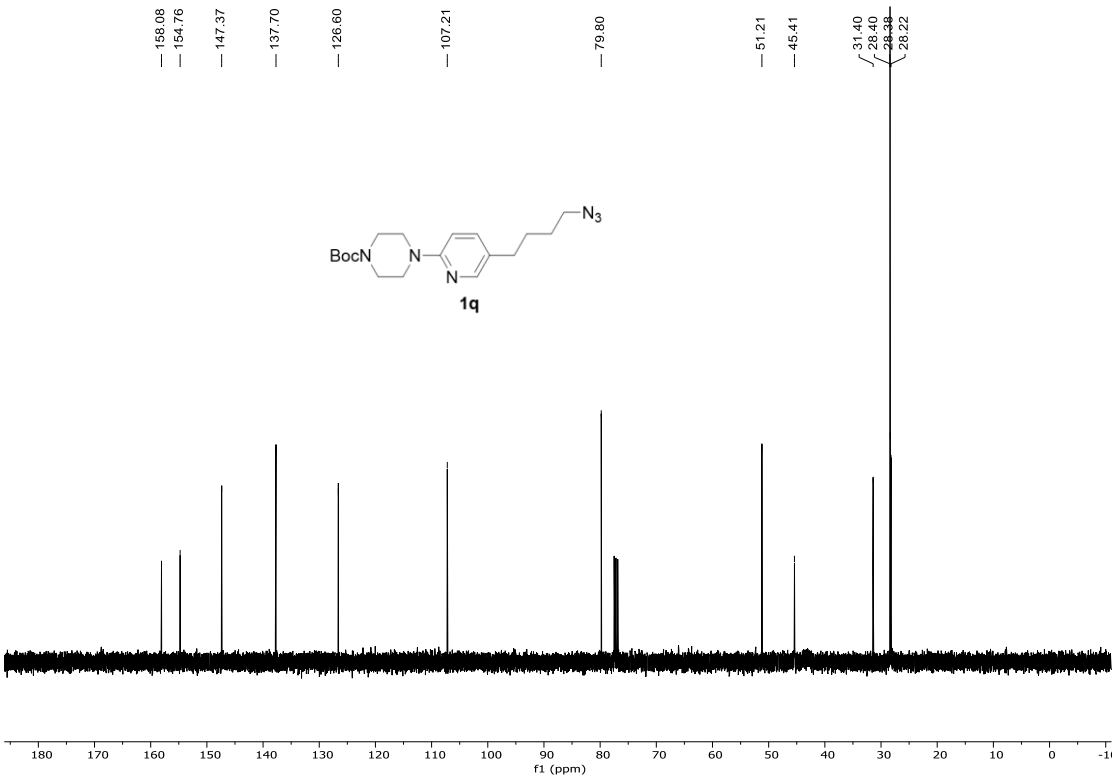
1.17
1.05
4.05
4.17
2.17
2.22
4.33
9.06
f1 (ppm)


158.08
154.76
147.37
137.70
126.60
107.21
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51.21
45.41
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28.38
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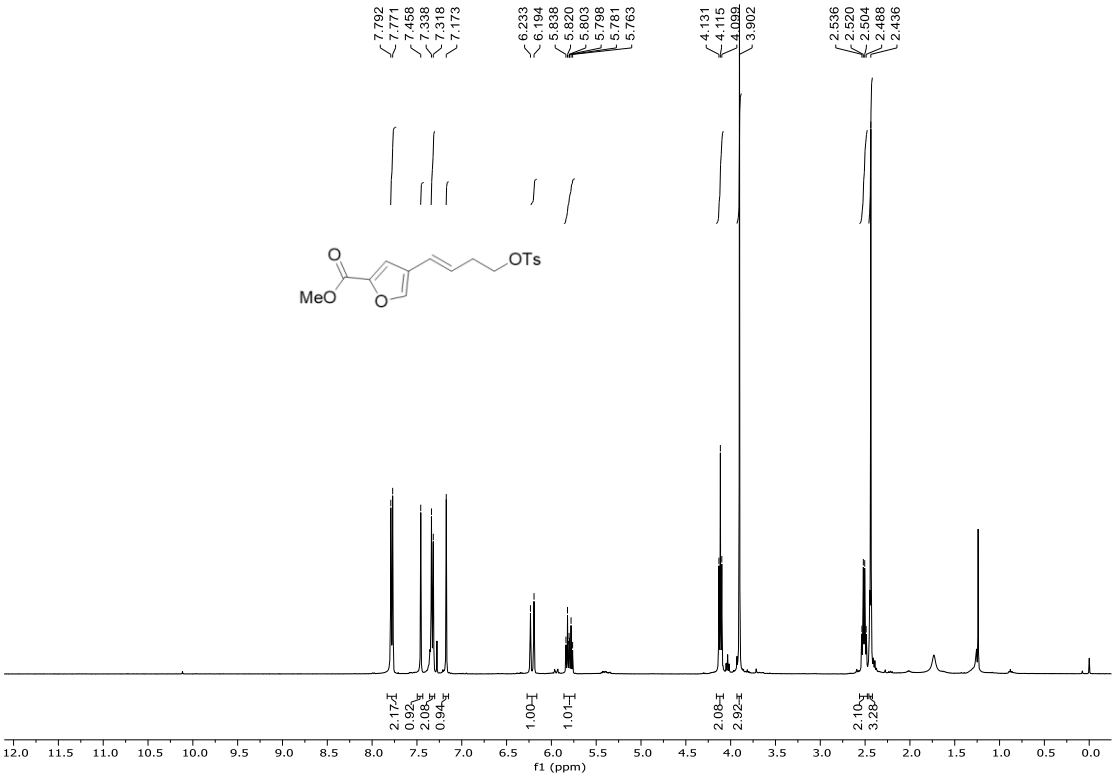
BocN
N
N
N3
1q
f1 (ppm)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6.194
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5.820
5.803
5.798
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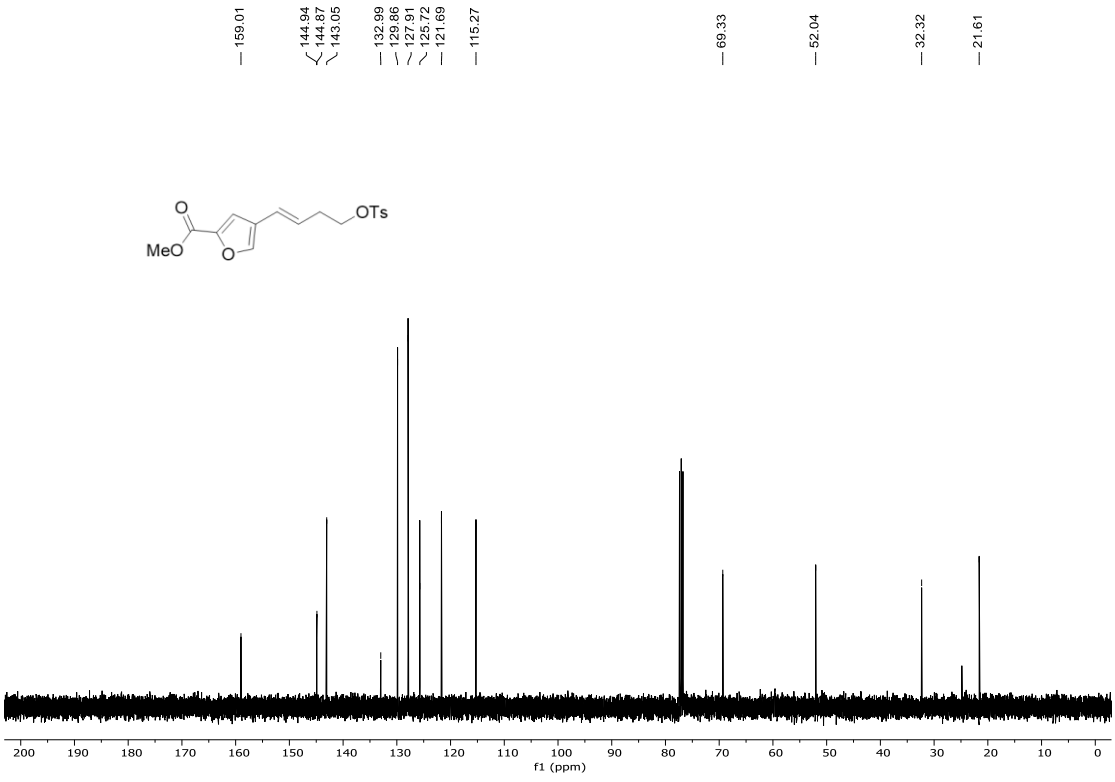
5.763
4.131
4.115
4.099
3.902
2.536
2.520
2.504
2.488
2.436
O
MeO
O
OTs
2.17
0.92
2.08
0.94
1.00
1.01
2.08
2.92
2.10
3.28
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


159.01
144.94
144.87
143.05
132.99
129.86
127.91
125.72
121.69
115.27
69.33
52.04
32.32
21.61
O
MeO
O
OTs
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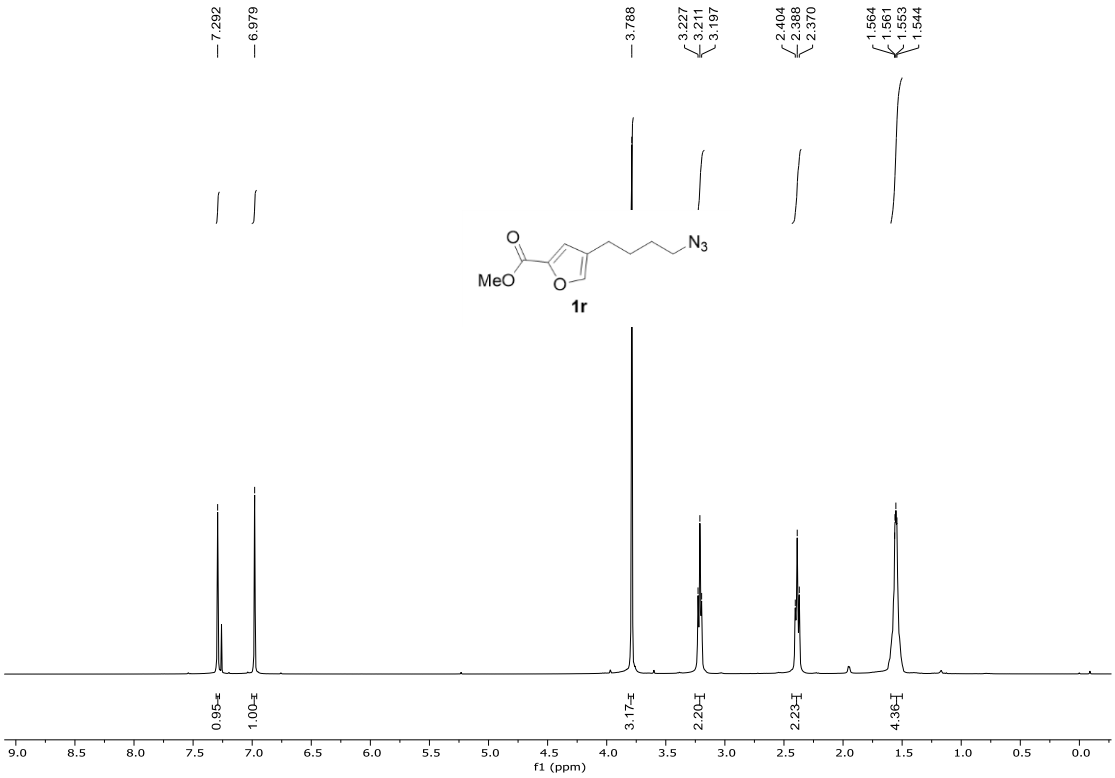
f1 (ppm)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6.979
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3.227
3.211
3.197
2.404
2.388
2.370
1.564
1.561
1.553
1.544
MeO
O
O
N3
1r
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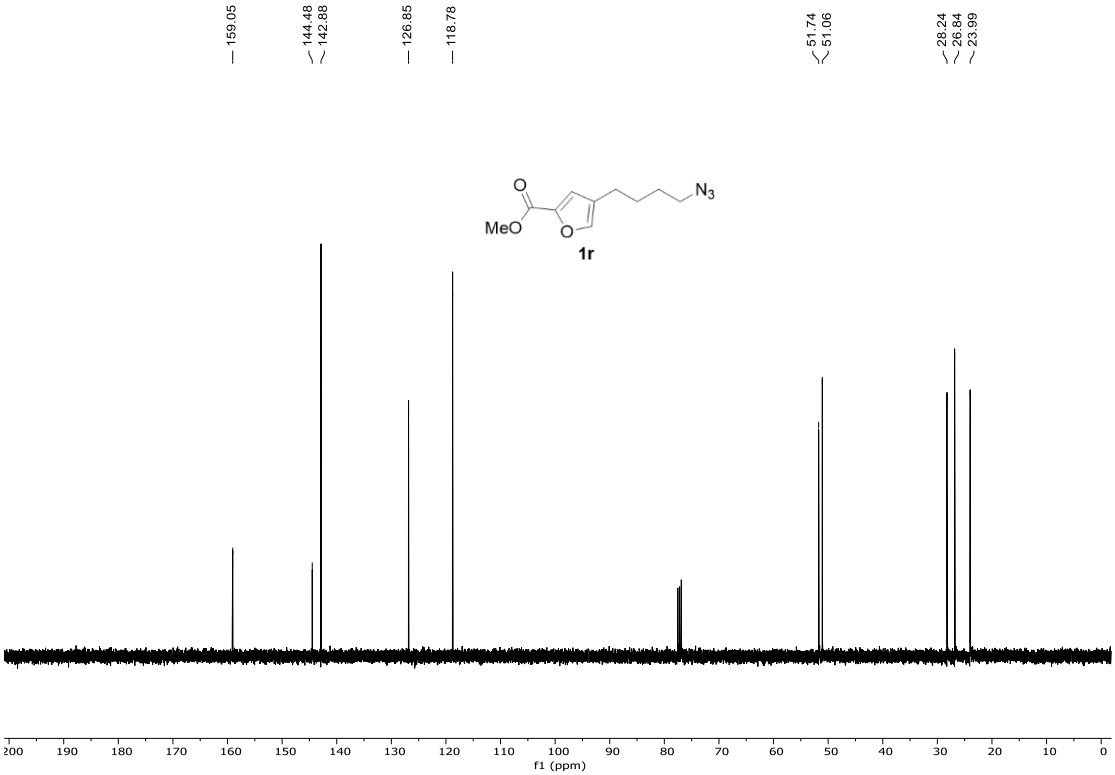
1.00
3.17
2.20
2.23
4.36
f1 (ppm)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144.48
142.88
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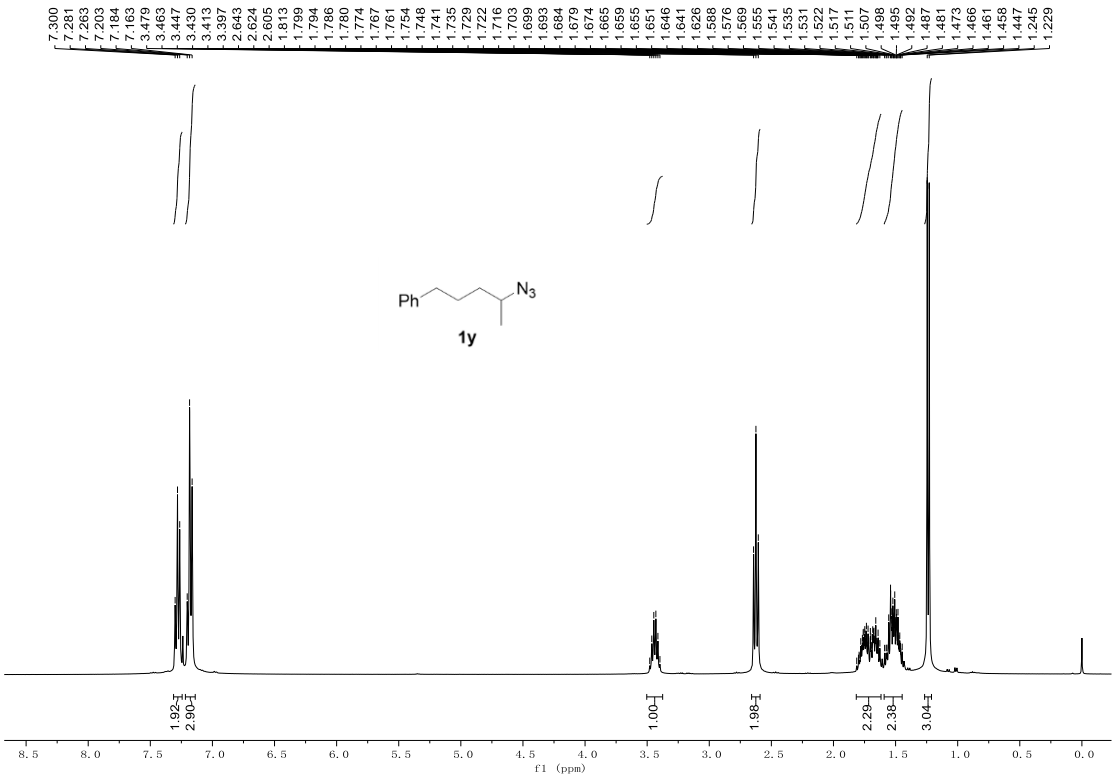
51.74
51.06
28.24
26.84
23.99
MeO
O
O
N3
1r
f1 (ppm)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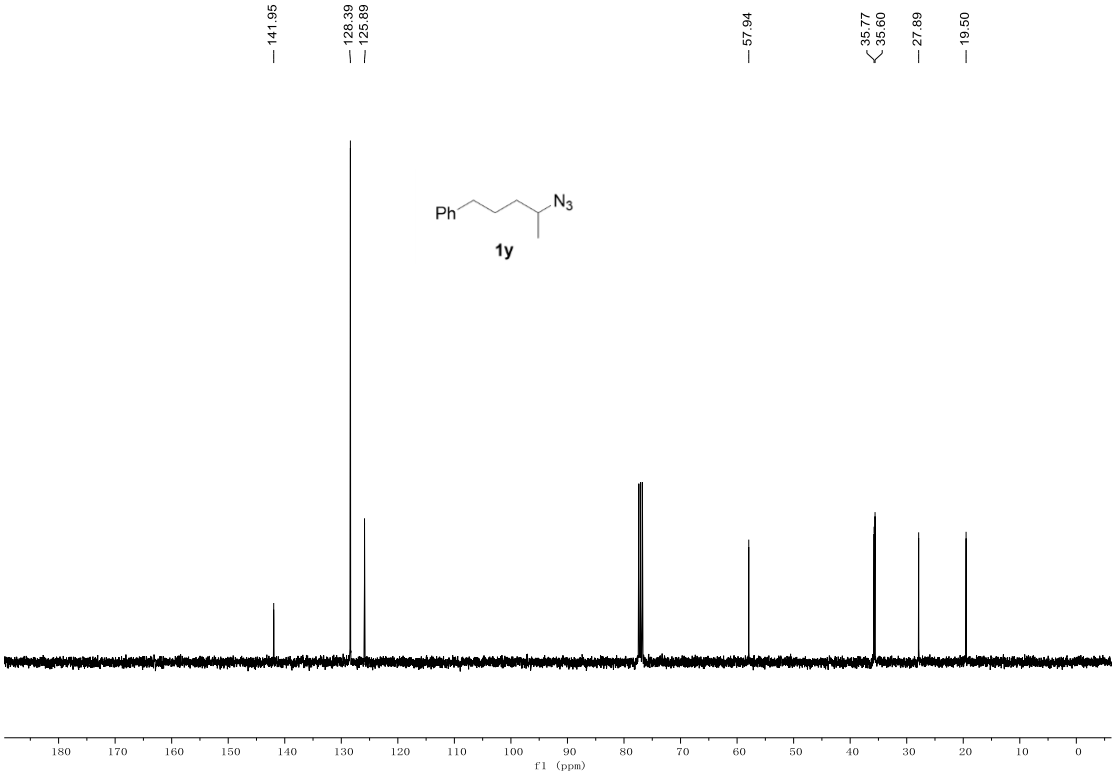
7.203
7.184
7.163
3.479
3.463
3.447
3.430
3.413
3.397
2.643
2.624
2.605
1.813
1.799
1.794
1.786
1.780
1.774
1.767
1.761
1.754
1.748
1.741
1.735
1.729
1.722
1.716
1.703
1.699
1.693
1.684
1.679
1.674
1.665
1.659
1.655
1.651
1.646
1.641
1.626
1.588
1.576
1.569
1.555
1.541
1.535
1.531
1.522
1.517
1.511
1.507
1.498
1.495
1.492
1.487
1.481
1.473
1.466
1.461
1.458
1.447
1.245
1.229
Ph
N3
1y
1.92
2.90
1.00
1.98
2.29
2.38
3.04
f1 (ppm)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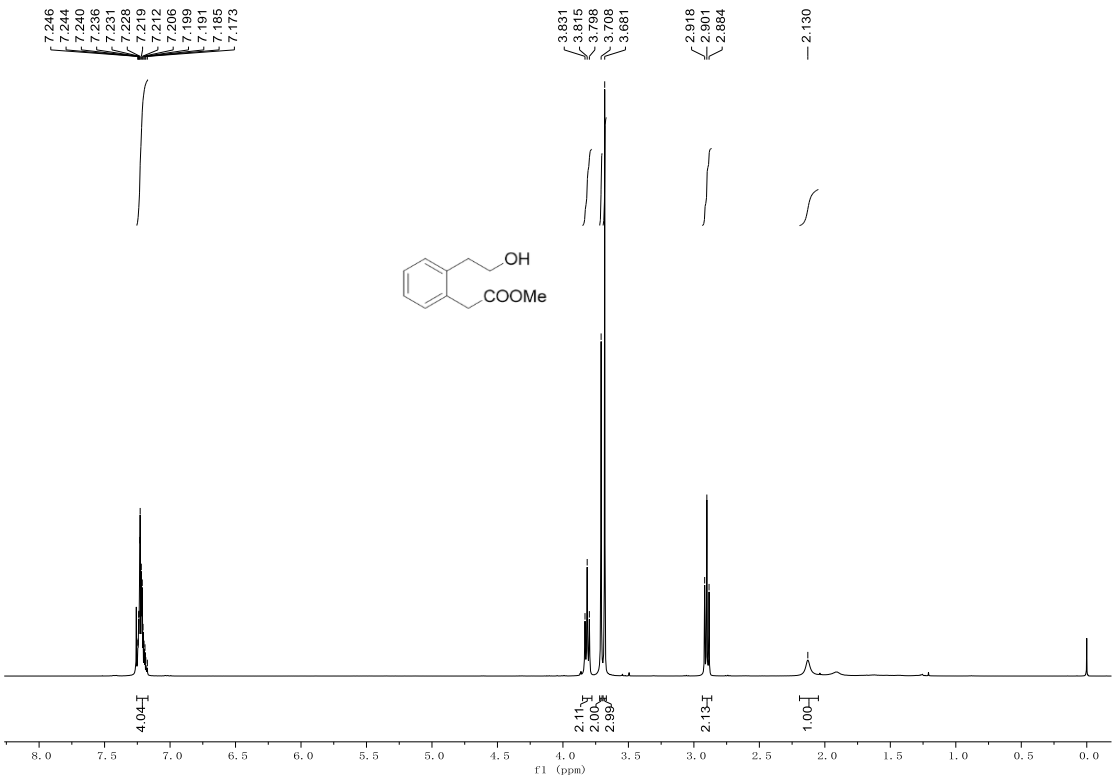
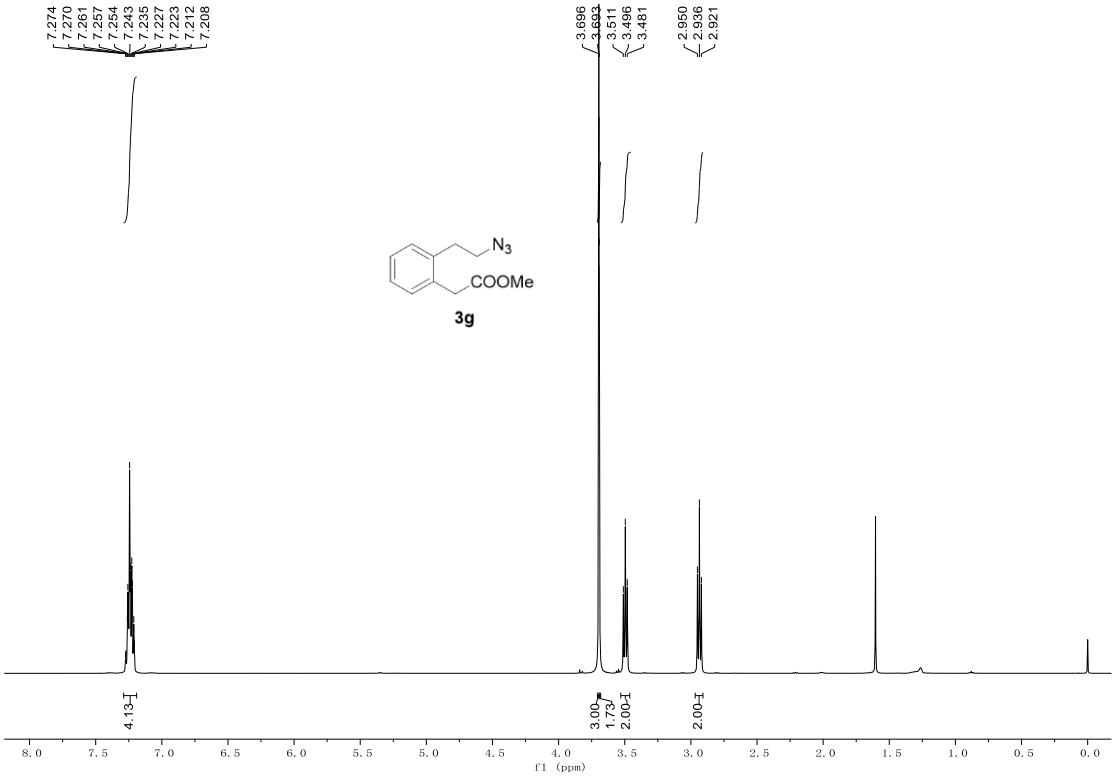
57.94
35.77
35.60
27.89
19.50
Ph
N3
1y
f1 (ppm)


7.246
7.244
7.240
7.236
7.231
7.228
7.219
7.212
7.206
7.199
7.191
7.185
7.173
3.831
3.815
3.798
3.708
3.681
2.918
2.901
2.884
2.130
OH
COOMe
4.04
2.11
2.00
2.99
2.13
1.00
f1 (ppm)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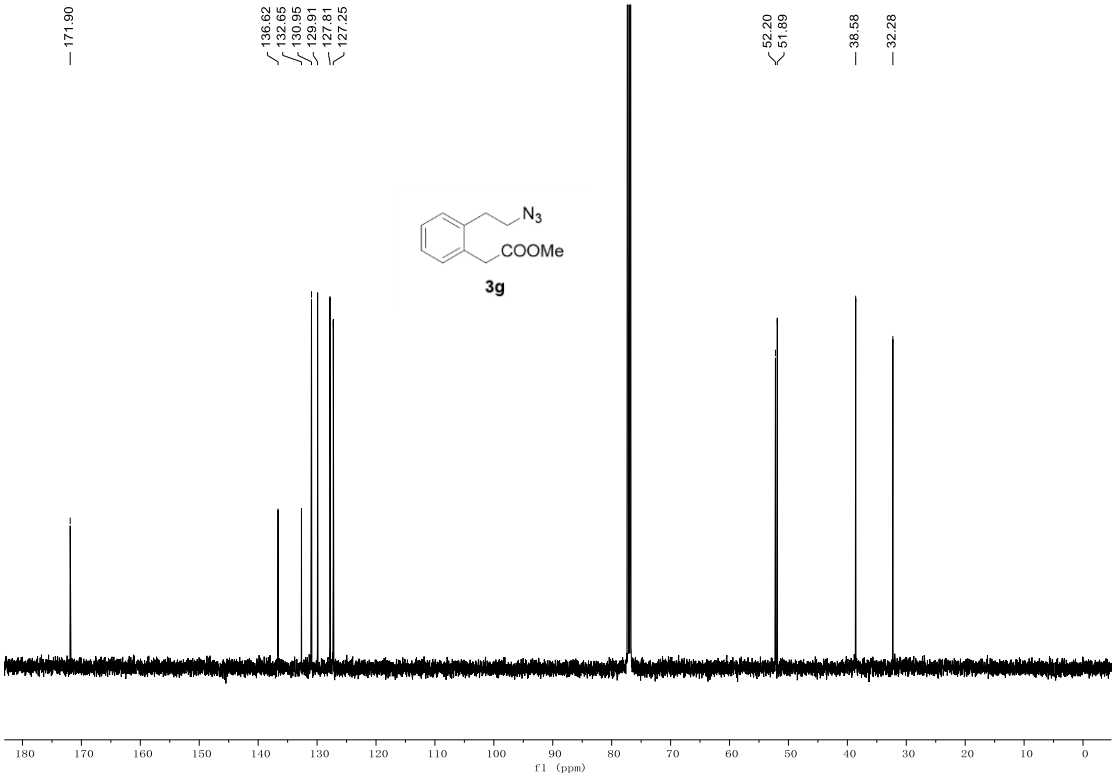
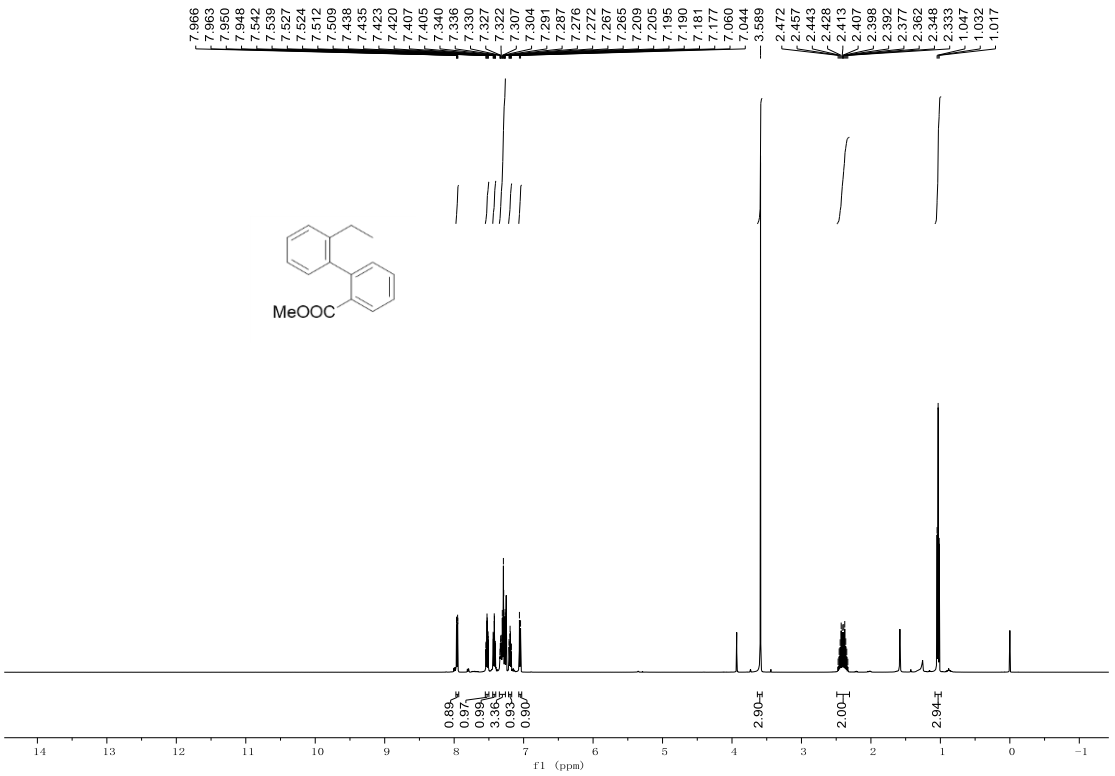
7.270
7.261
7.257
7.254
7.243
7.235
7.227
7.223
7.212
7.208
3.696
3.693
3.511
3.496
3.481
2.950
2.936
2.921
N3
COOMe
4.13
3.00
1.73
2.00
2.00
f1 (ppm)

3g


171.90
136.62
132.65
130.95
129.91
127.81
127.25
52.20
51.89
38.58
32.28
N3
COOMe
3g
f1 (ppm)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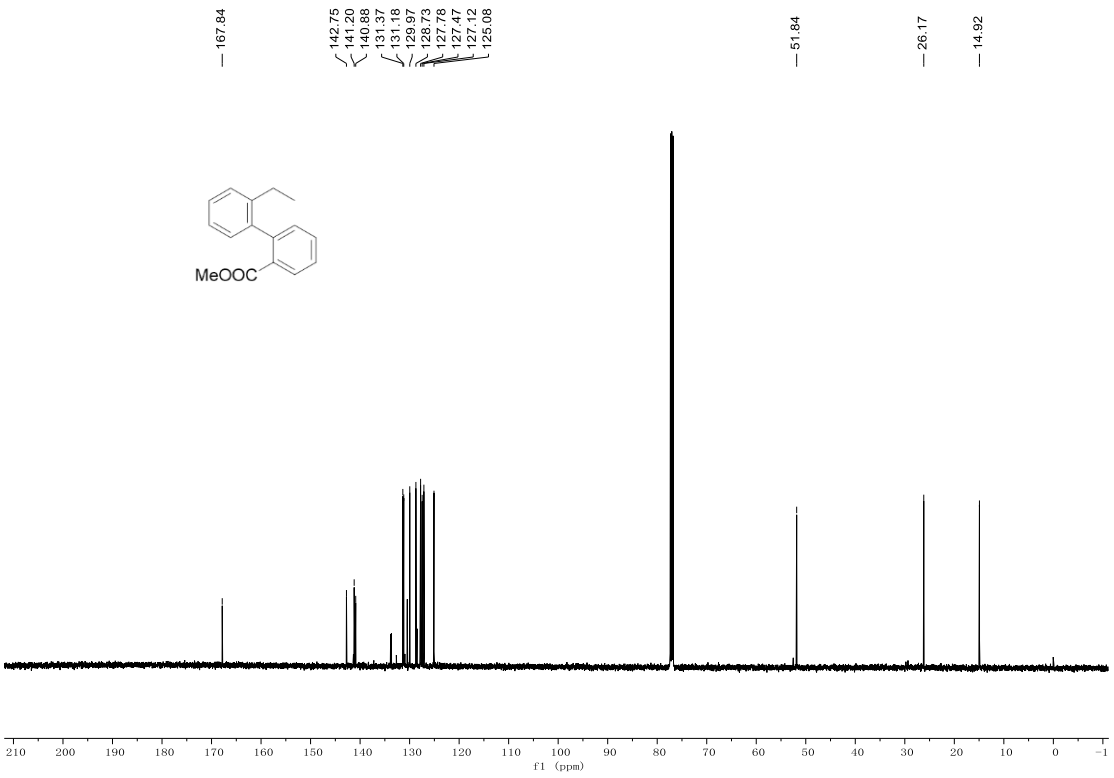
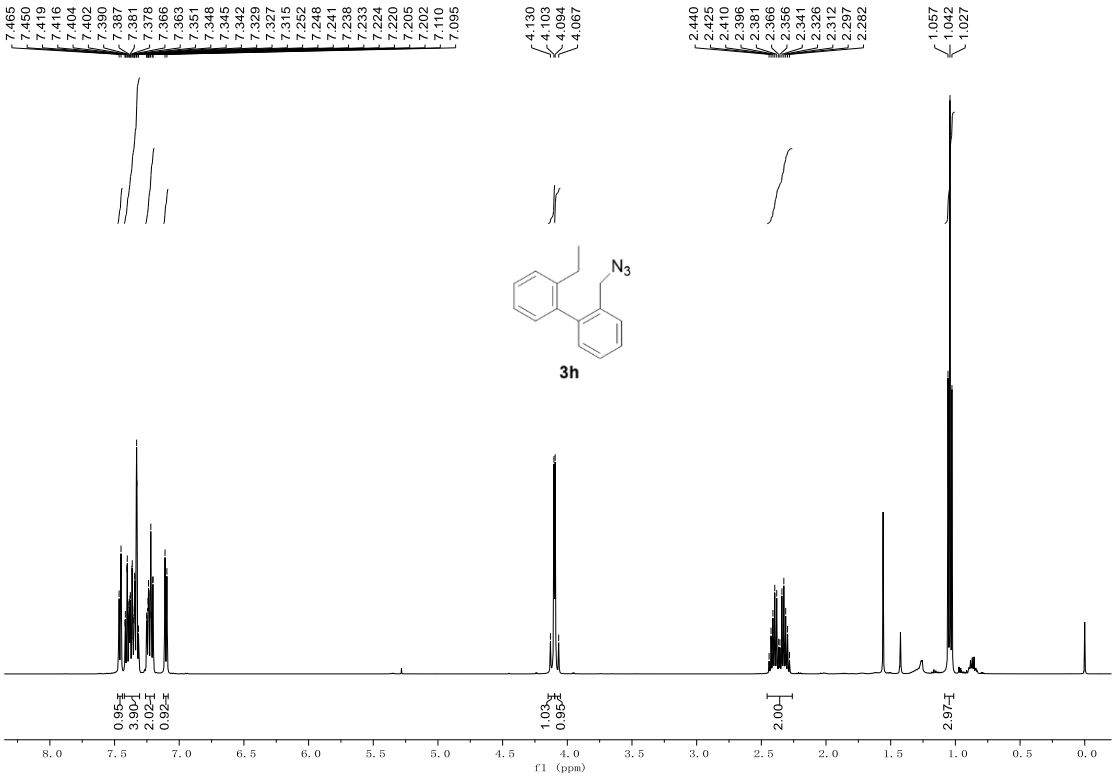
7.963
7.950
7.948
7.542
7.539
7.527
7.524
7.512
7.509
7.438
7.435
7.423
7.420
7.407
7.405
7.340
7.336
7.330
7.327
7.322
7.307
7.304
7.291
7.287
7.276
7.272
7.267
7.265
7.209
7.205
7.195
7.190
7.181
7.177
7.060
7.044
3.589
2.472
2.457
2.443
2.428
2.413
2.407
2.398
2.392
2.377
2.362
2.348
2.333
1.047
1.032
1.017
MeOOC
0.89
0.97
0.99
3.36
0.93
0.90
2.90
2.00
2.94
f1 (ppm)


167.84
142.75
141.20
140.88
131.37
131.18
129.97
128.73
127.78
127.47
127.12
125.08
51.84
26.17
14.92
MeOOC
f1 (ppm)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7.450
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7.416
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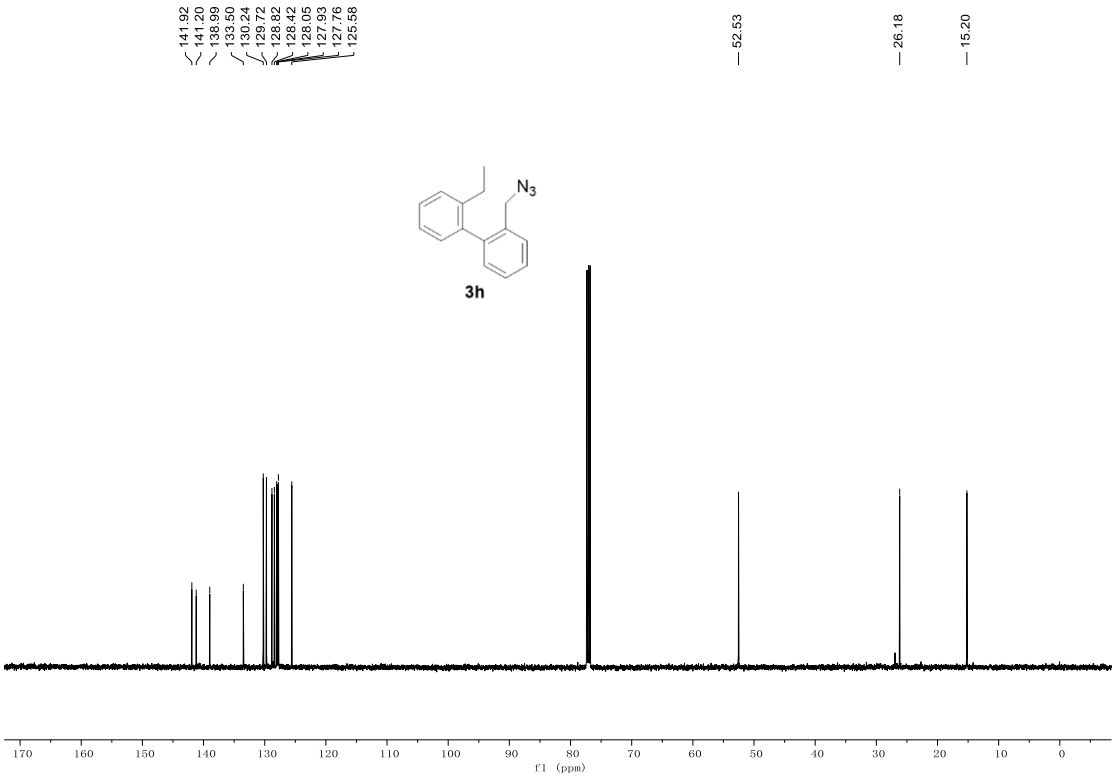
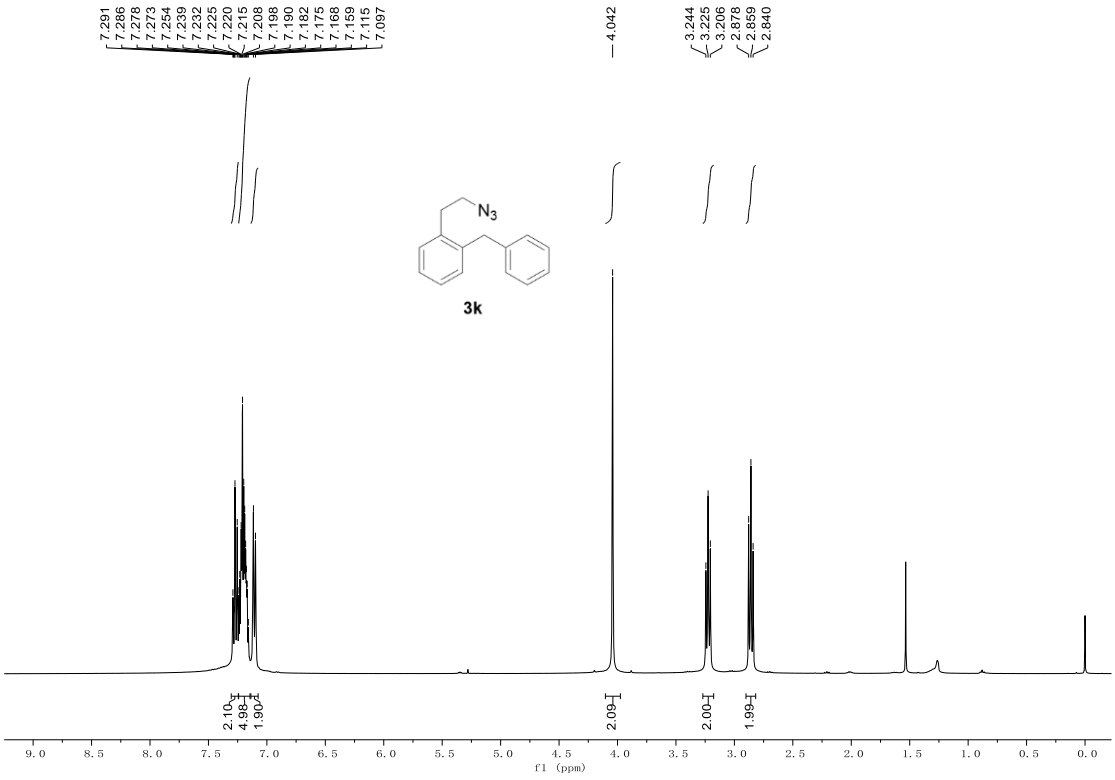
7.402
7.390
7.387
7.381
7.378
7.366
7.363
7.351
7.348
7.345
7.342
7.329
7.327
7.315
7.252
7.248
7.241
7.238
7.233
7.224
7.220
7.205
7.202
7.110
7.095
4.130
4.103
4.094
4.067
2.440
2.425
2.410
2.396
2.381
2.366
2.356
2.341
2.326
2.312
2.297
2.282
1.057
1.042
1.027
N3
3h
0.95
3.90
2.02
0.92
1.03
0.95
2.00
2.97
f1 (ppm)


141.92
141.20
138.99
133.50
130.24
129.72
128.82
128.42
128.05
127.93
127.76
125.58
52.53
26.18
15.20
N3
3h
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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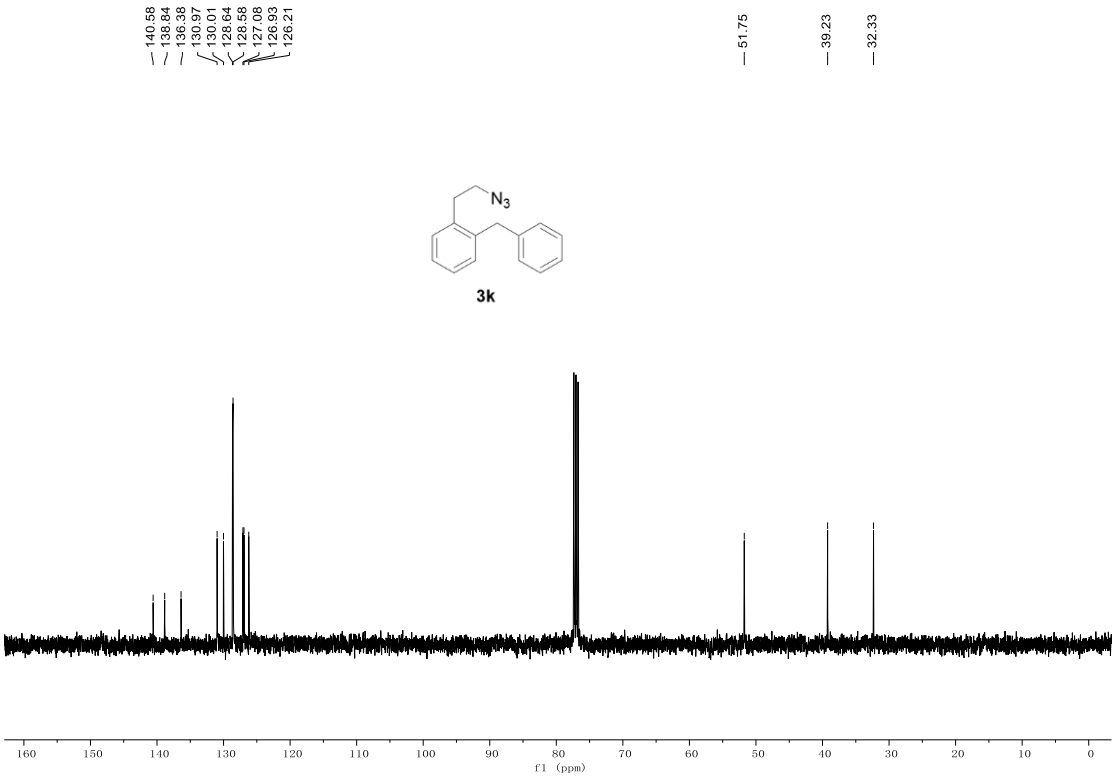
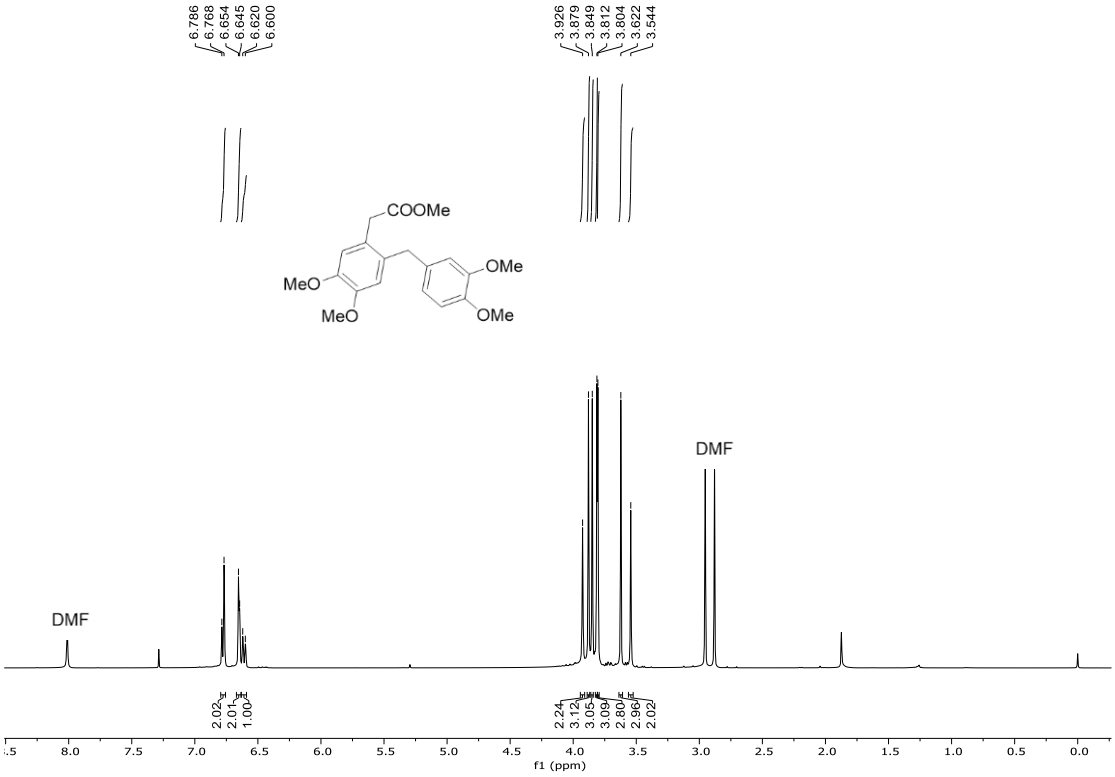
7.278
7.273
7.254
7.239
7.232
7.225
7.220
7.215
7.208
7.198
7.190
7.182
7.175
7.168
7.159
7.115
7.097
4.042
3.244
3.225
3.206
2.878
2.859
2.840
N3
3k
2.10
4.98
1.90
2.09
2.00
1.99
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


140.58
138.84
136.38
130.97
130.01
128.64
128.58
127.08
126.93
126.21
51.75
39.23
32.33
N3
3k
f1 (ppm)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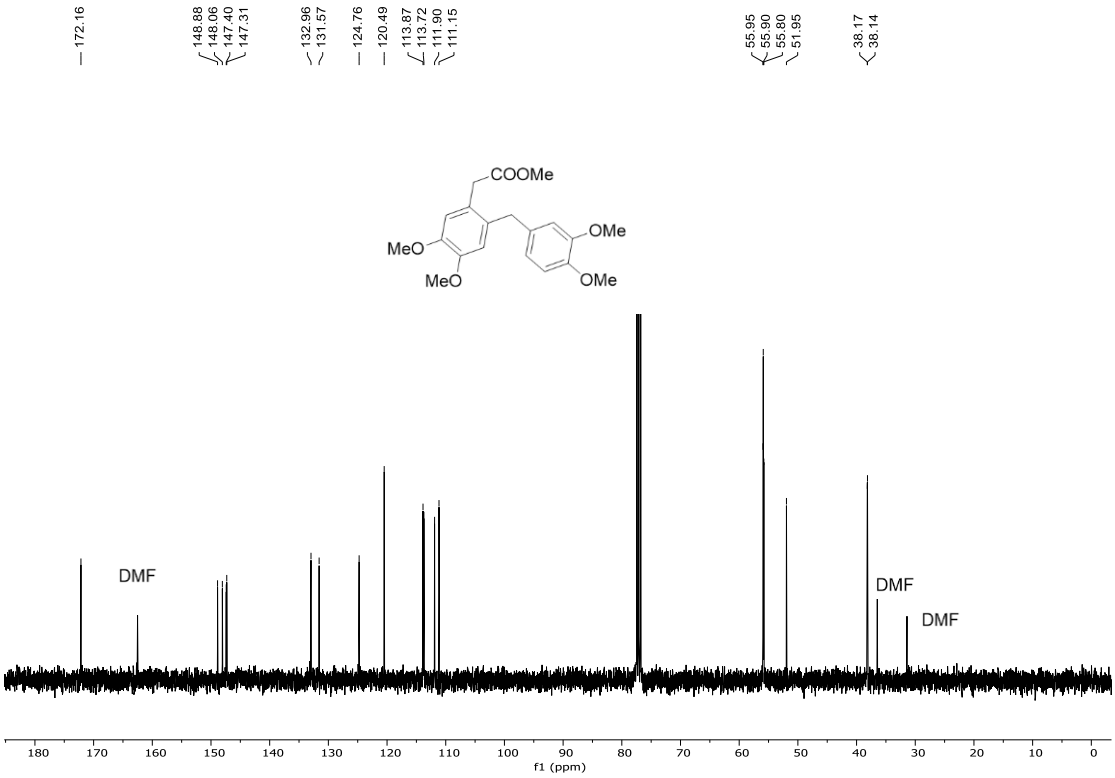
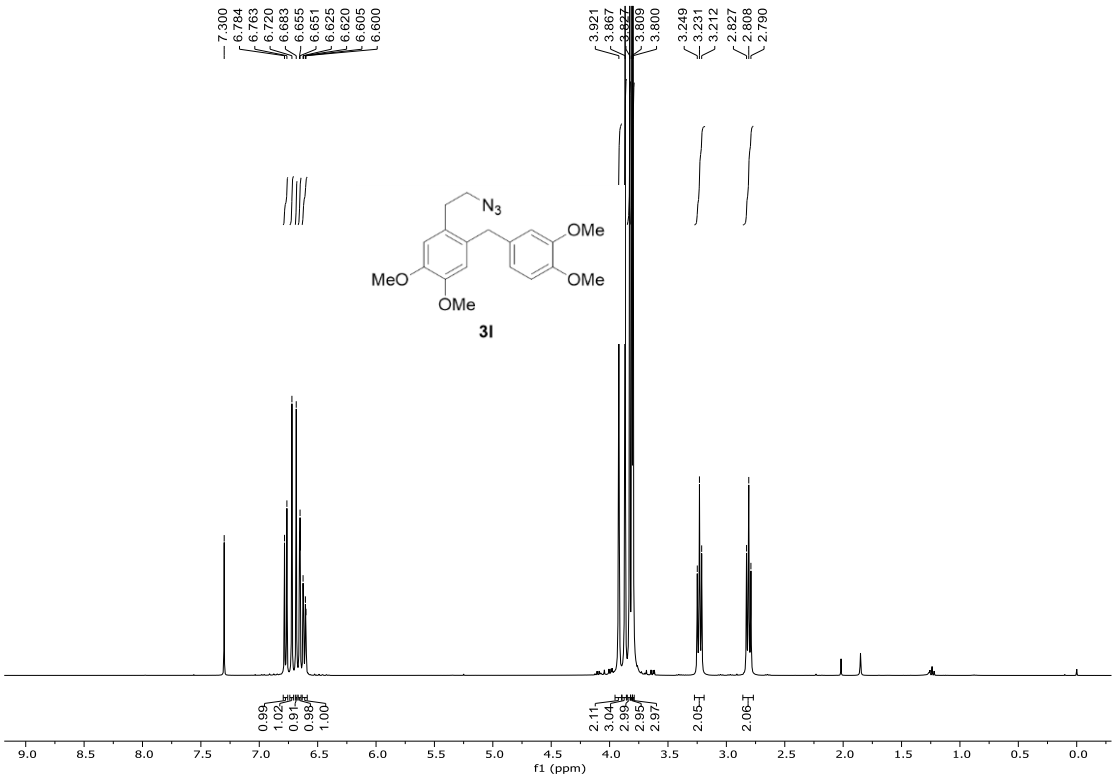
6.768
6.654
6.645
6.620
6.600
3.926
3.879
3.849
3.812
3.804
3.622
3.544
COOMe
MeO
MeO
OMe
OMe
DMF
DMF
2.02
2.01
1.00
2.24
3.12
3.05
3.09
2.80
2.98
2.02
f1 (ppm)


172.16
148.88
148.06
147.40
147.31
132.96
131.57
124.76
120.49
113.87
113.72
111.90
111.15
55.95
55.90
55.80
51.95
38.17
38.14
COOMe
MeO
OMe
MeO
OMe
DMF
DMF
DMF
f1 (ppm)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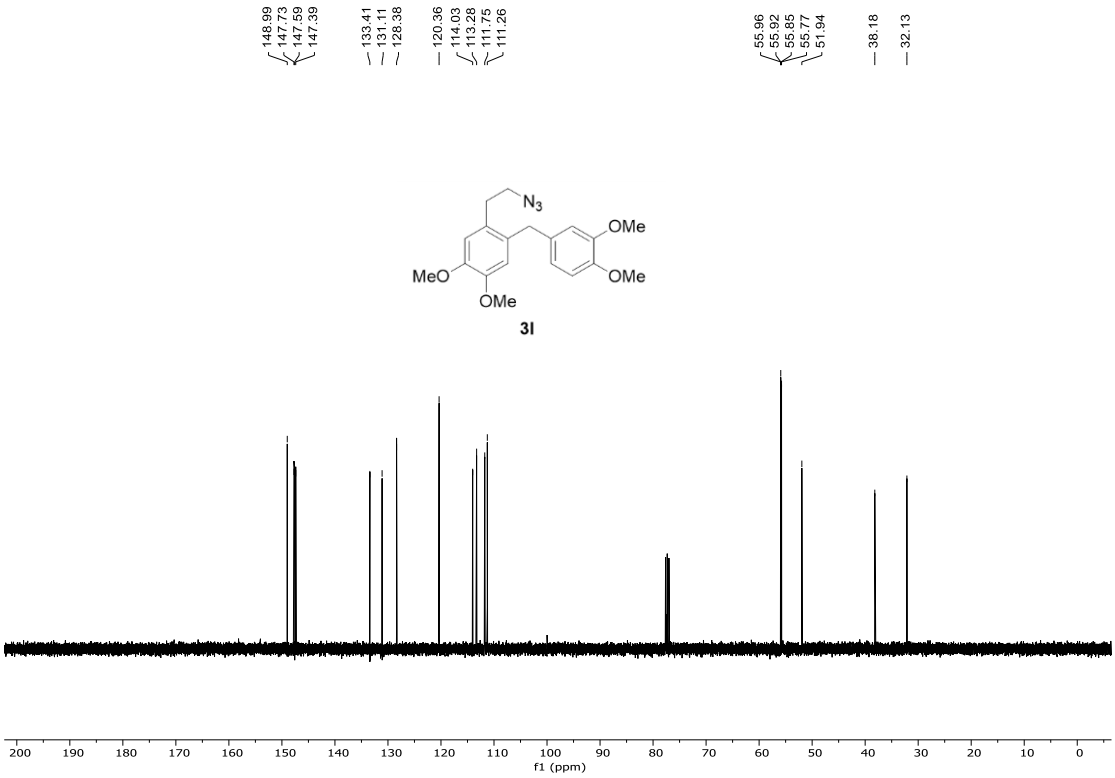
6.784
6.763
6.720
6.683
6.655
6.651
6.625
6.620
6.605
6.600
3.921
3.867
3.822
3.809
3.800
3.249
3.231
3.212
2.827
2.808
2.790
N3
OMe
MeO
OMe
OMe
3l
0.99
1.02
0.91
0.98
1.00
2.11
3.04
2.99
2.95
2.97
2.05
2.06
f1 (ppm)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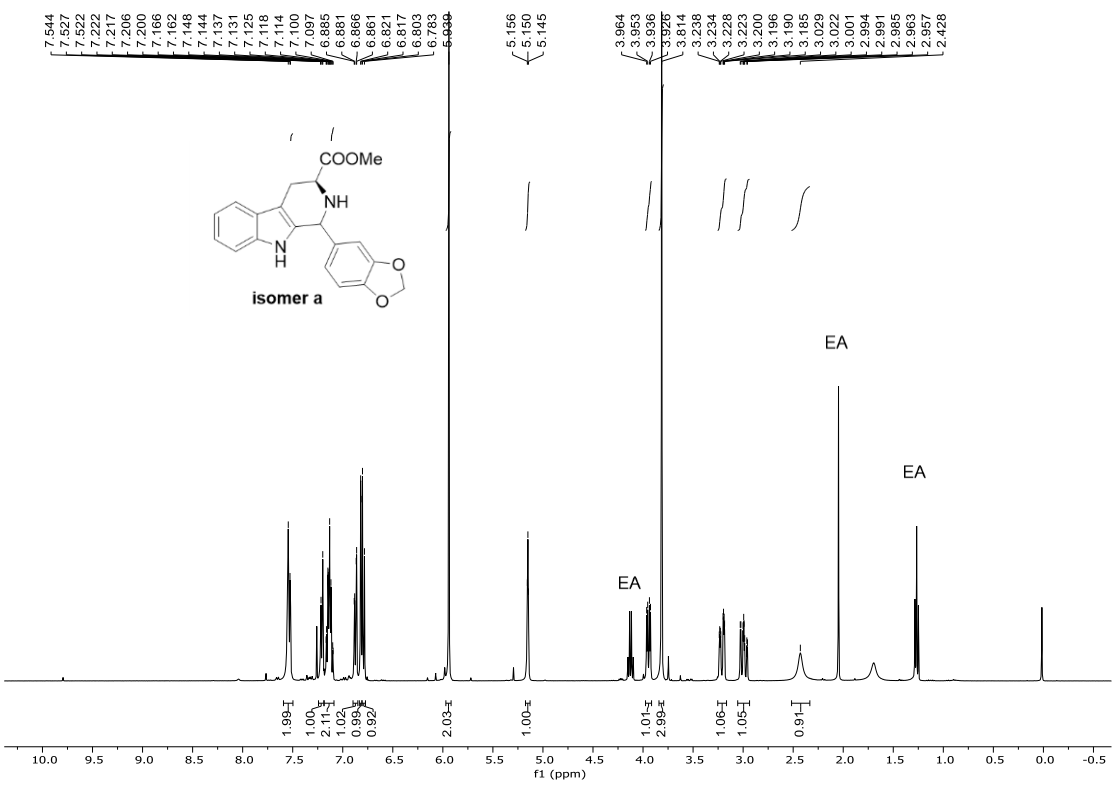
147.73
147.59
147.39
133.41
131.11
128.38
120.36
114.03
113.28
111.75
111.26
55.96
55.92
55.85
55.77
51.94
38.18
32.13
N3
OMe
MeO
OMe
OMe
3l
f1 (ppm)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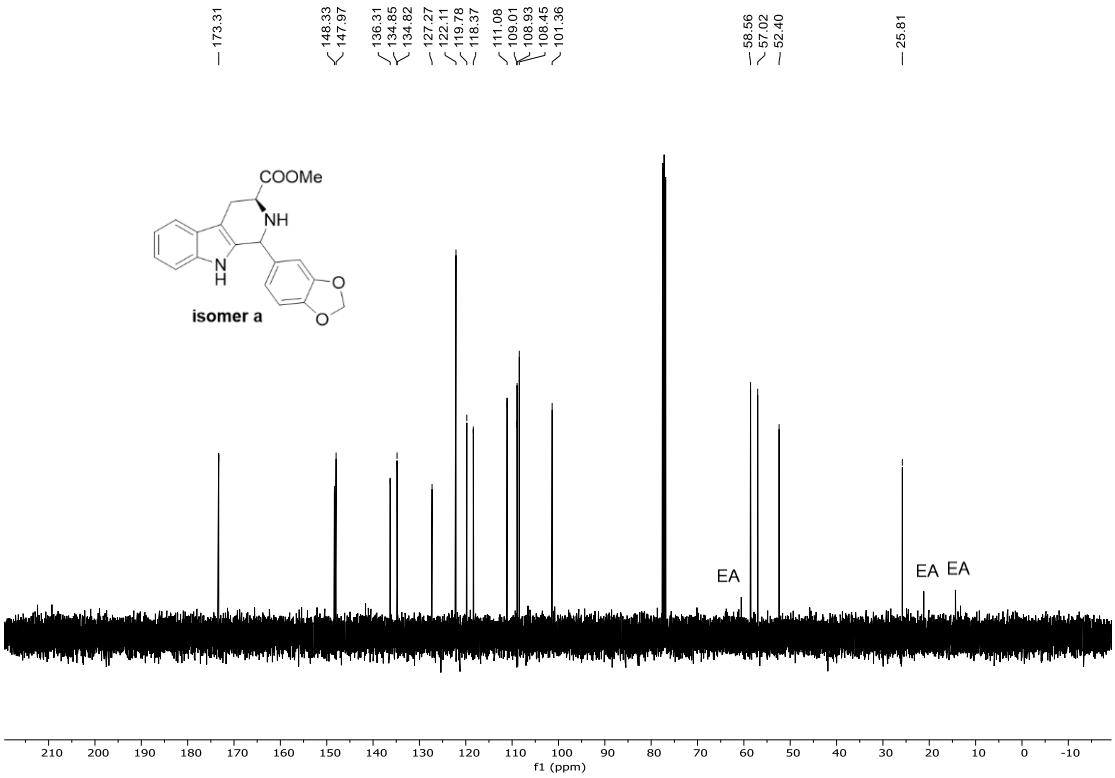
7.522
7.222
7.217
7.206
7.200
7.166
7.162
7.148
7.144
7.137
7.131
7.125
7.118
7.114
7.100
7.097
6.885
6.881
6.866
6.861
6.821
6.817
6.803
6.783
5.030
5.156
5.150
5.145
3.964
3.953
3.936
3.926
3.814
3.238
3.234
3.228
3.223
3.200
3.196
3.190
3.185
3.029
3.022
3.001
2.994
2.991
2.985
2.963
2.957
2.428
COOMe
NH
N
H
O
O
isomer a
EA
EA
EA
1.99
1.00
2.11
1.02
0.93
0.92
2.03
1.00
1.01
2.99
1.06
1.05
0.91
f1 (ppm)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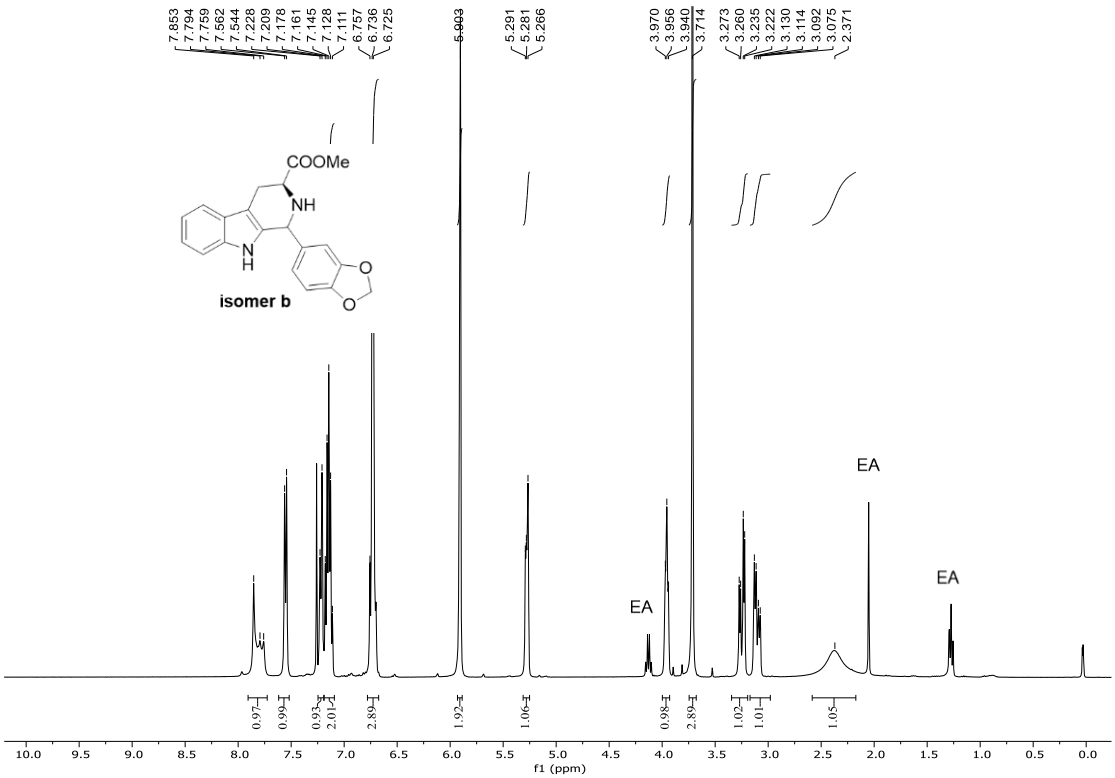
147.97
136.31
134.85
134.82
127.27
122.11
119.78
118.37
111.08
109.01
108.93
108.45
101.36
58.56
57.02
52.40
25.81
COOMe
NH
N
H
O
O
isomer a
EA
EA
EA
f1 (ppm)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7.544
7.228
7.209
7.178
7.161
7.145
7.128
7.111
6.757
6.736
6.725
5.903
5.291
5.281
5.266
3.970
3.956
3.940
3.714
3.273
3.260
3.235
3.222
3.130
3.114
3.092
3.075
2.371
COOMe
NH
N
H
O
O
isomer b
EA
EA
EA
0.97
0.99
0.93
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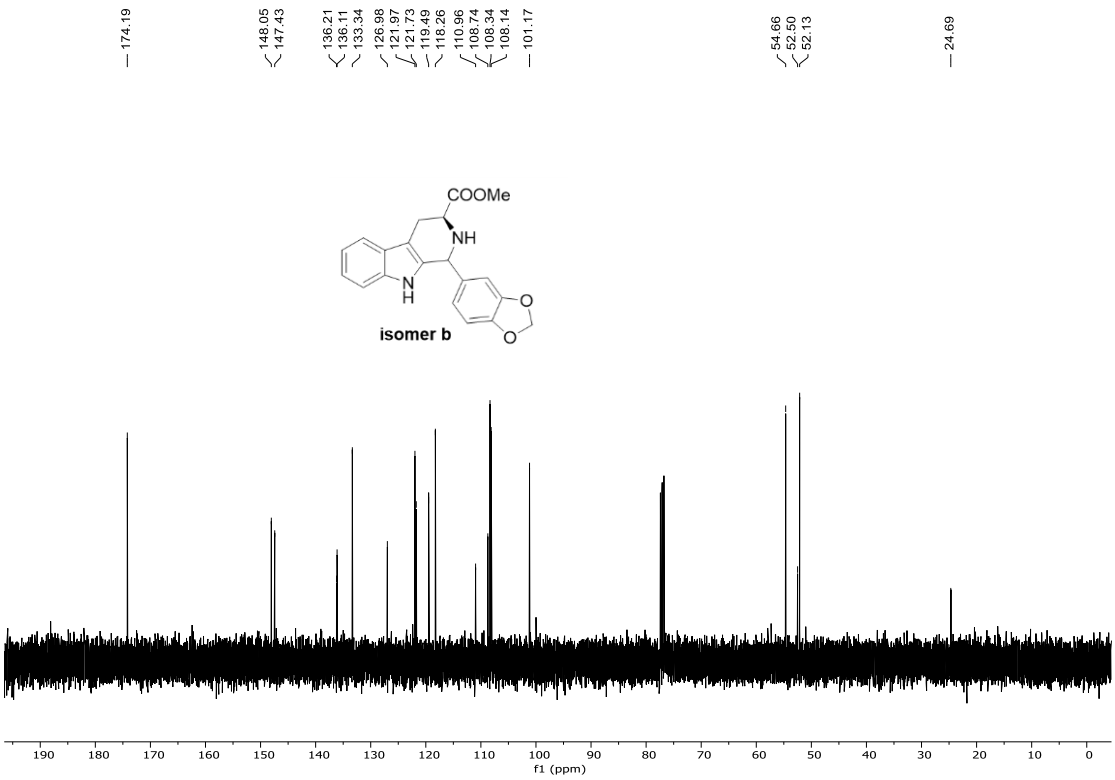
2.89
1.92
1.06
0.98
2.89
1.02
1.01
1.05
f1 (ppm)


174.19
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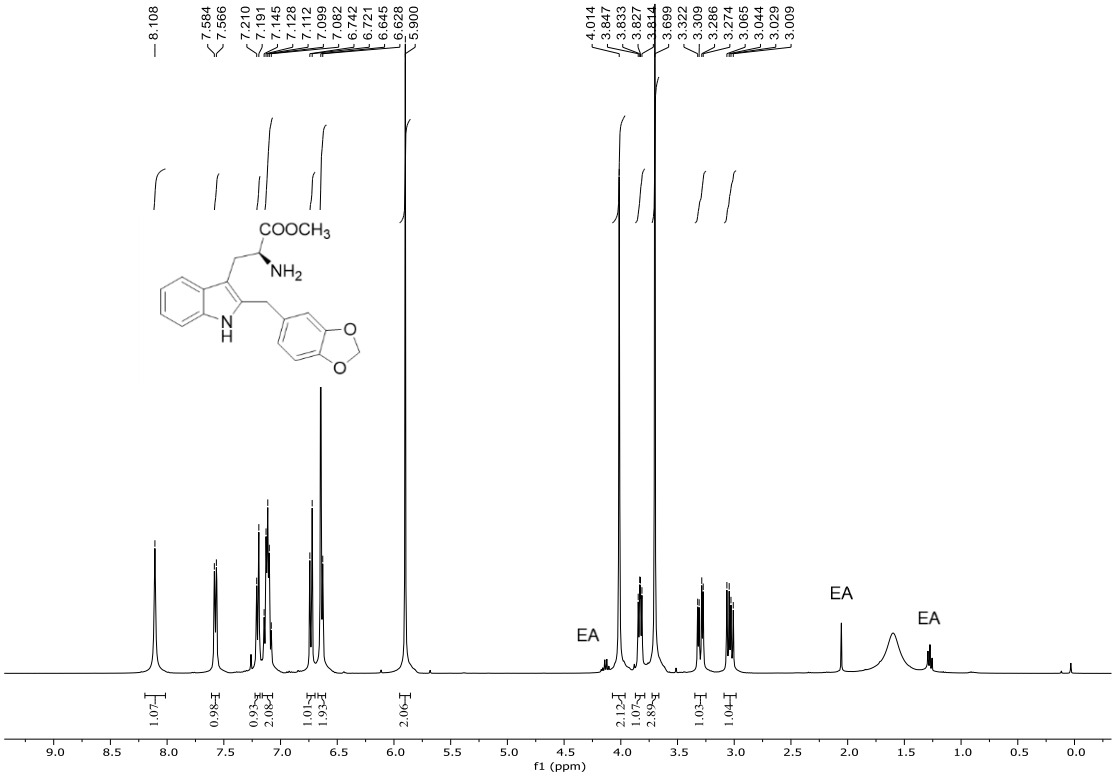
147.43
136.21
136.11
133.34
126.98
121.97
121.73
119.49
118.26
110.96
108.74
108.34
108.14
101.17
54.66
52.50
52.13
24.69
COOMe
NH
N
H
O
O
isomer b
f1 (ppm)


8.108
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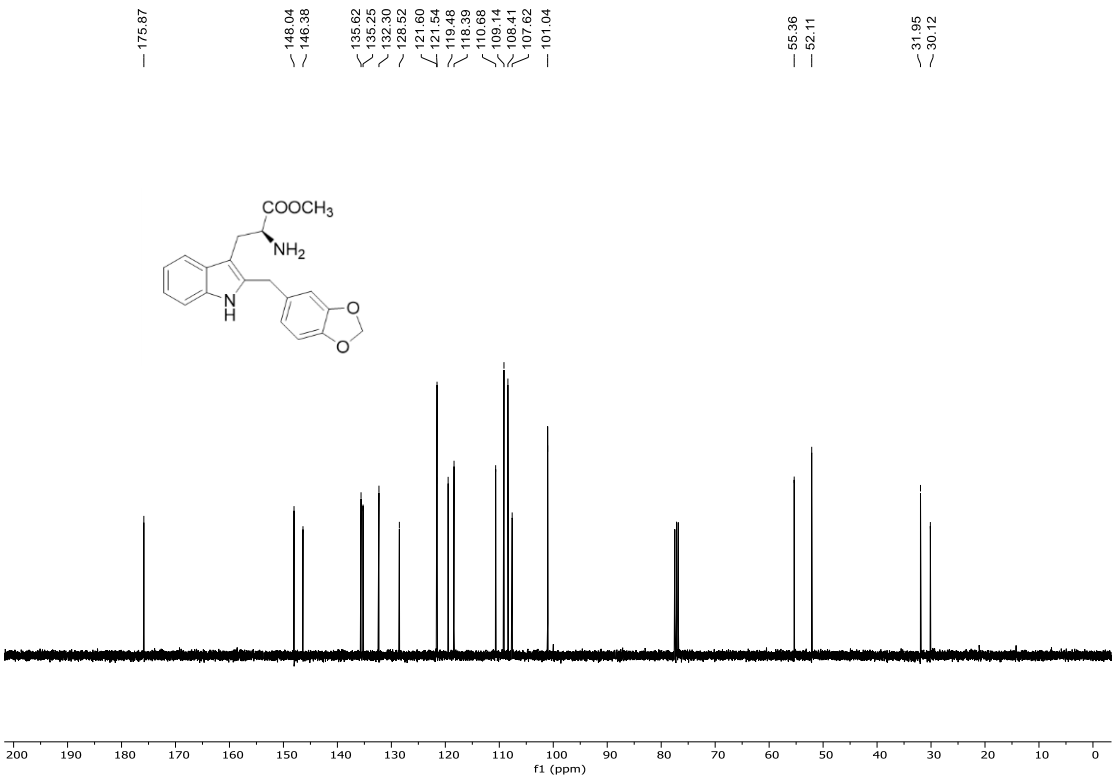
7.566
7.210
7.191
7.145
7.128
7.112
7.099
7.082
6.742
6.721
6.645
6.628
5.900
4.014
3.847
3.833
3.827
3.814
3.699
3.322
3.309
3.286
3.274
3.065
3.044
3.029
3.009
COOCH3
NH2
N
H
O
O
EA
EA
EA
1.07
0.96
0.93
2.08
1.01
1.93
2.06
2.12
1.07
2.89
1.03
1.04
f1 (ppm)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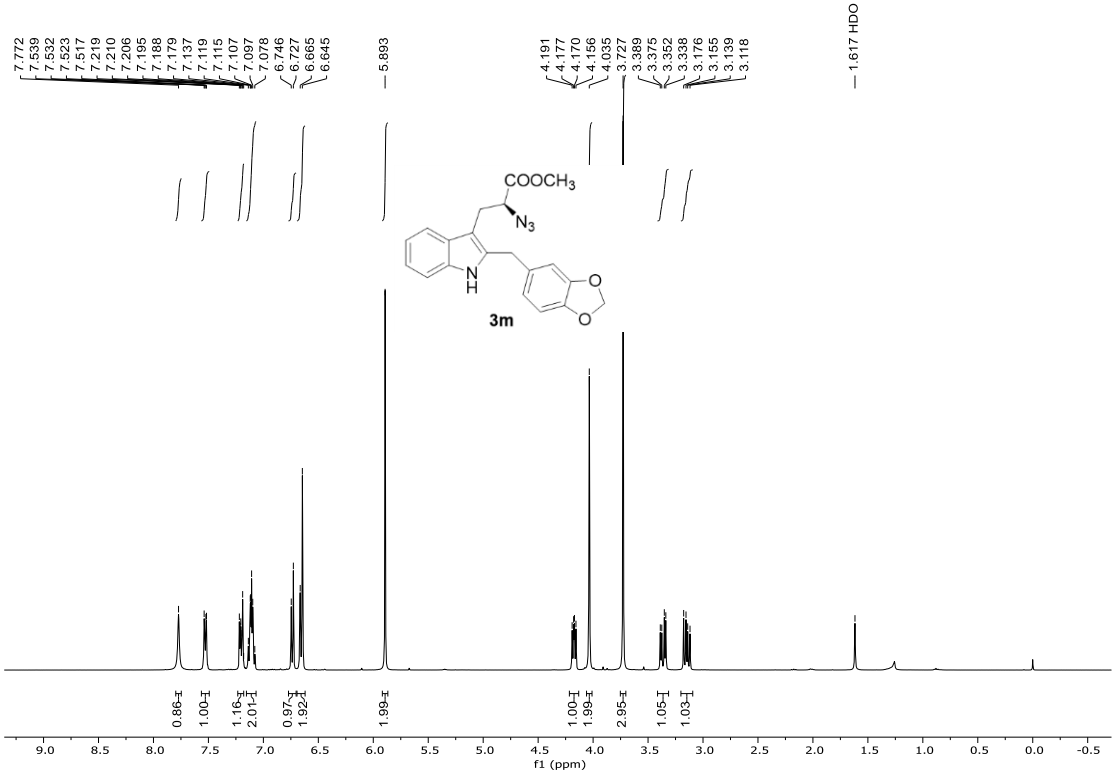
135.25
132.30
128.52
121.60
121.54
119.48
118.39
110.68
109.14
108.41
107.62
101.04
55.36
52.11
31.95
30.12
COOCH3
NH2
N
H
O
O
f1 (ppm)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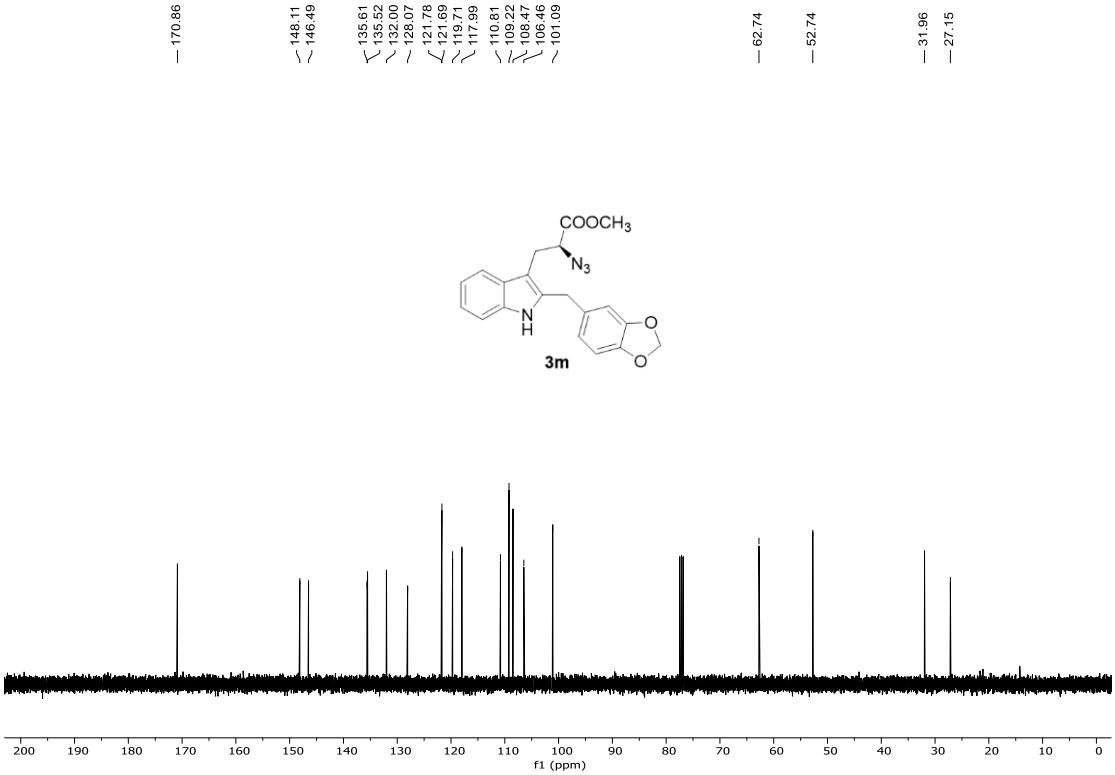
7.523
7.517
7.219
7.210
7.206
7.195
7.188
7.179
7.137
7.119
7.115
7.107
7.097
7.078
6.746
6.727
6.665
6.645
5.893
4.191
4.177
4.170
4.156
4.035
3.727
3.389
3.375
3.352
3.338
3.176
3.155
3.139
3.118
1.617 HDO
COOCH3
N3
N
H
O
O
3m
0.86
1.00
1.16
2.01
0.97
1.92
1.99
1.00
1.99
2.95
1.05
1.03
f1 (ppm)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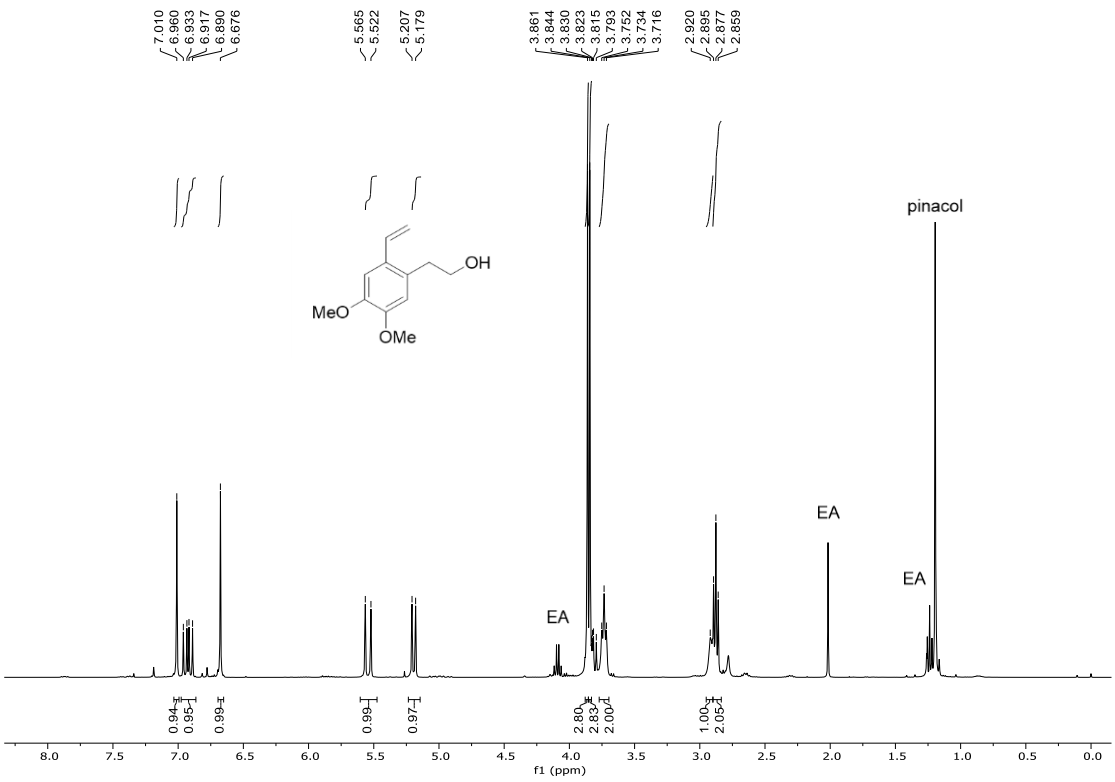
146.49
135.61
135.52
132.00
128.07
121.78
121.69
119.71
117.99
110.81
109.22
108.47
106.46
101.09
62.74
52.74
31.96
27.15
COOCH3
N3
N
H
O
O
3m
f1 (ppm)


7.010
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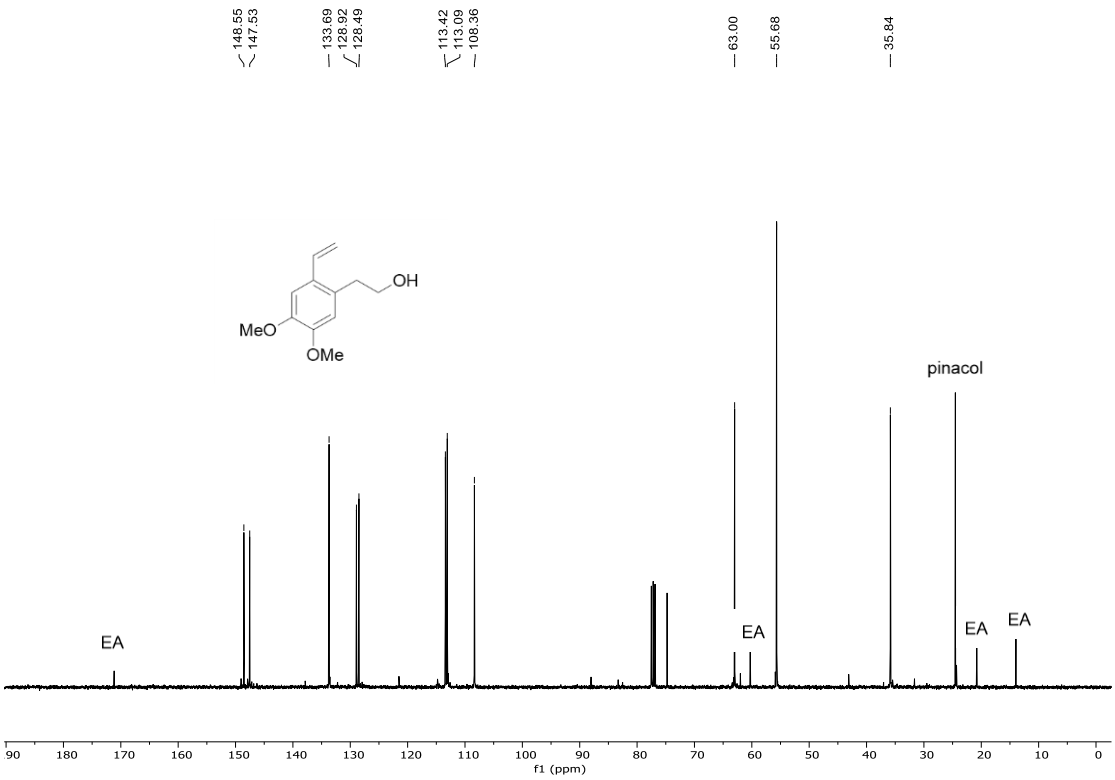
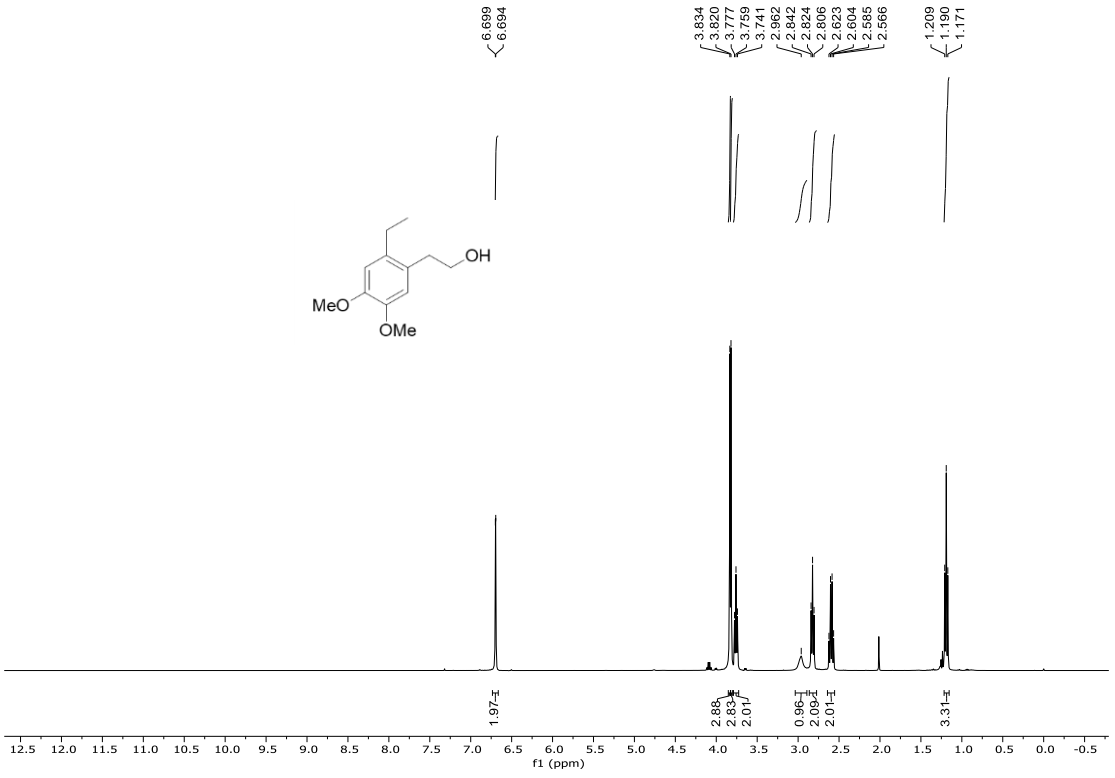
6.933
6.917
6.890
6.676
5.565
5.522
5.207
5.179
3.861
3.844
3.830
3.823
3.815
3.793
3.752
3.734
3.716
2.920
2.895
2.877
2.859
OH
MeO
OMe
pinacol
EA
EA
EA
0.94
0.95
0.99
0.99
0.97
2.80
2.83
2.00
1.00
2.05
f1 (ppm)


148.55
147.53
133.69
128.92
128.49
113.42
113.09
108.36
63.00
55.68
35.84
OH
MeO
OMe
pinacol
EA
EA
EA
EA
f1 (ppm)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3.777
3.759
3.741
2.962
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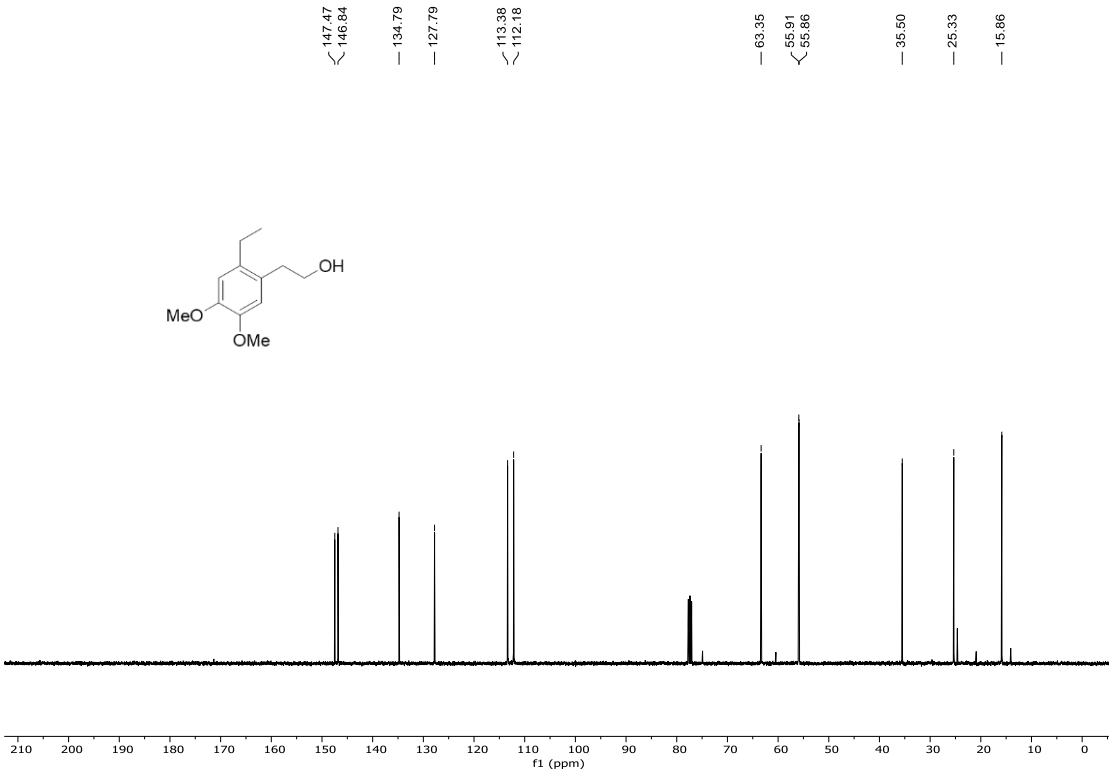
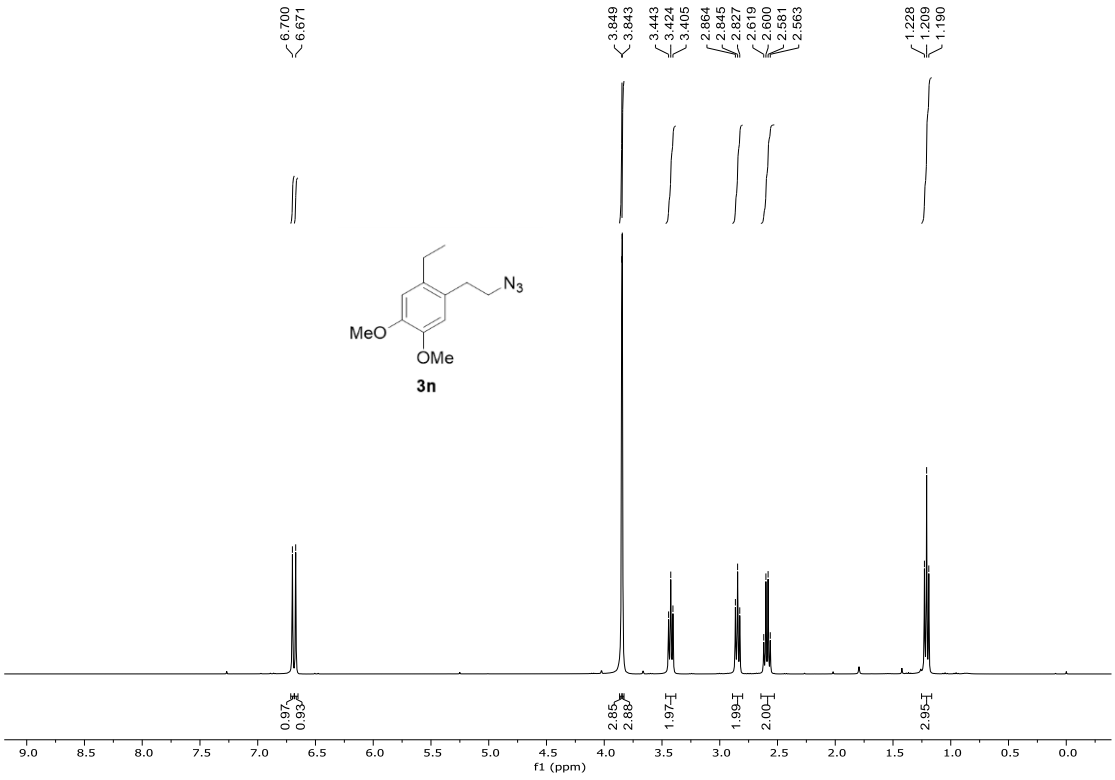
2.824
2.806
2.623
2.604
2.585
2.566
1.209
1.190
1.171
OH
MeO
OMe
1.97
2.88
2.83
2.01
0.96
2.09
2.01
3.31
f1 (ppm)


147.47
146.84
134.79
127.79
113.38
112.18
63.35
55.91
55.86
35.50
25.33
15.86
OH
MeO
OMe
f1 (ppm)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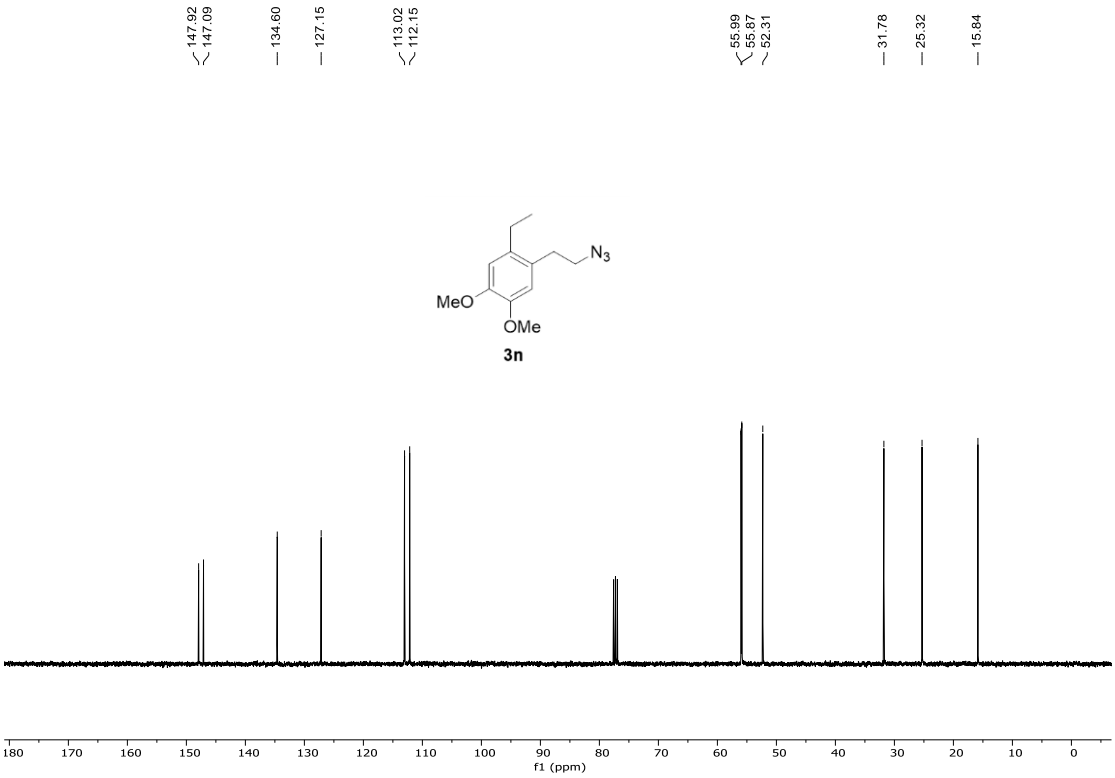
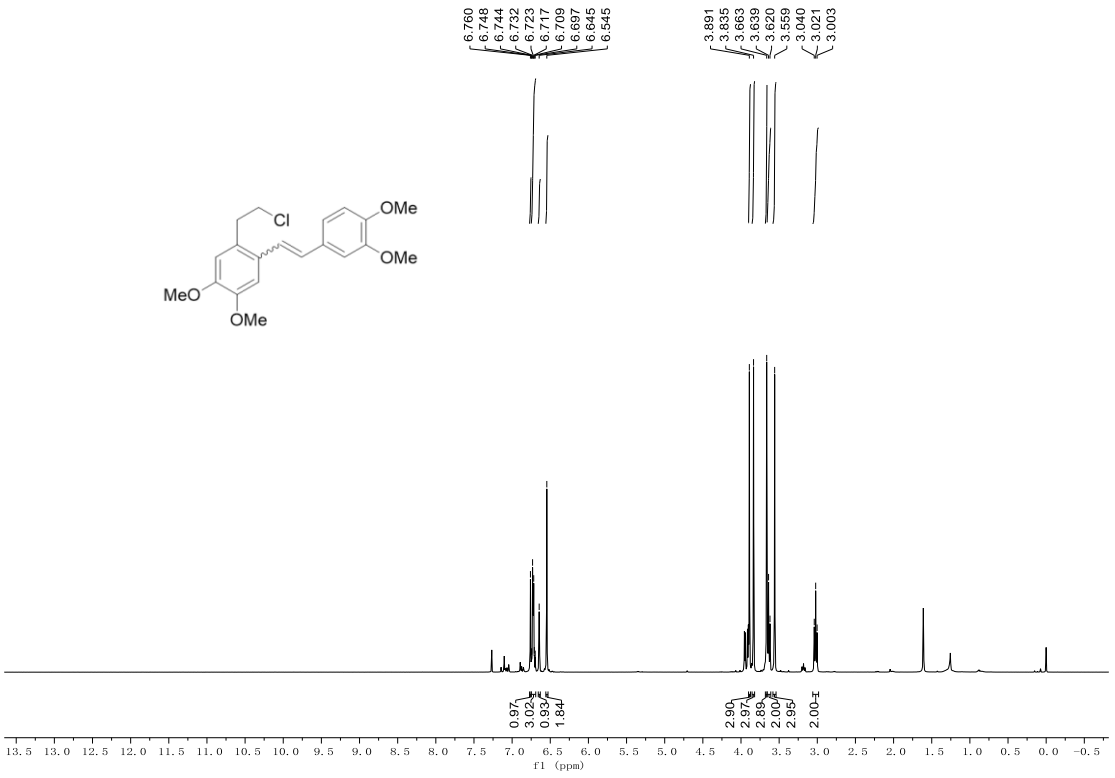
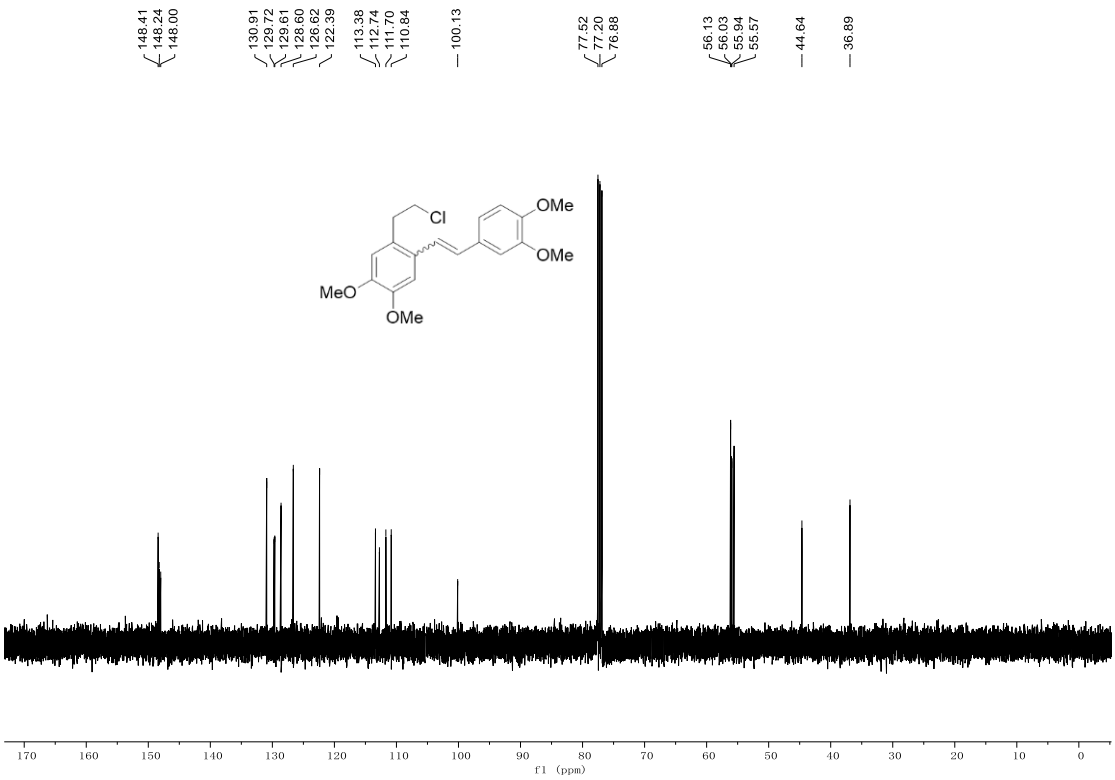
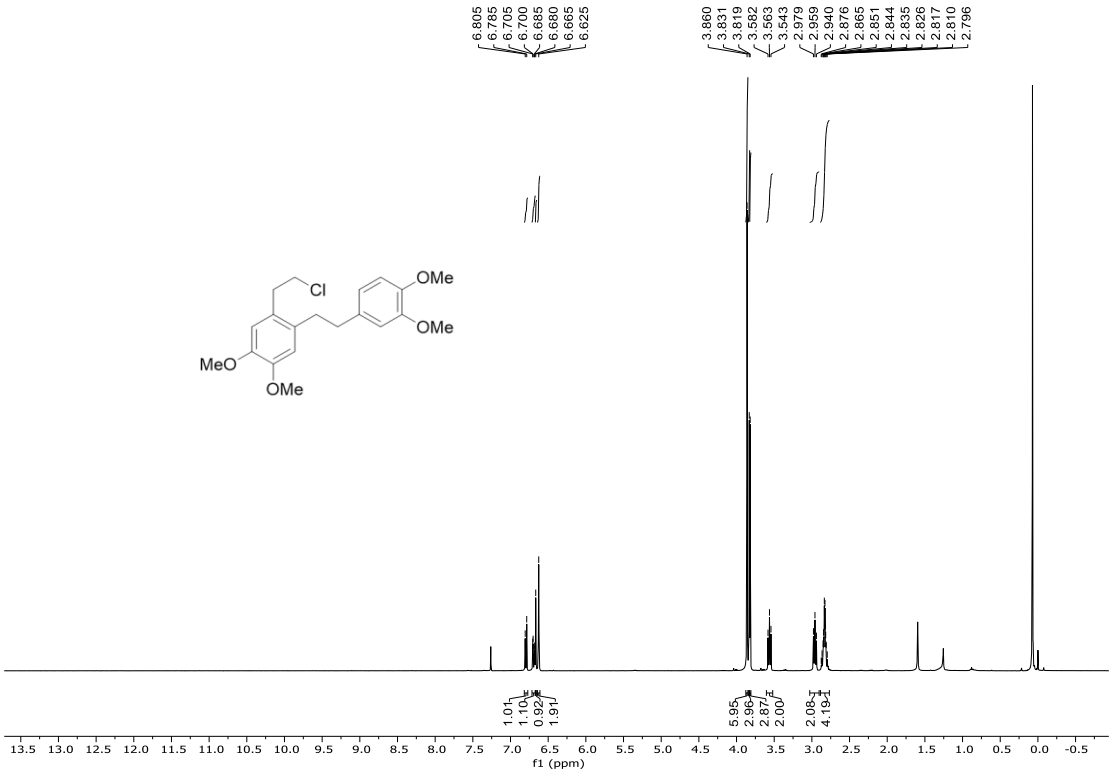
6.671
3.849
3.843
3.443
3.424
3.405
2.864
2.845
2.827
2.619
2.600
2.581
2.563
1.228
1.209
1.190
N3
MeO
OMe
3n
0.97
0.93
2.85
2.88
1.97
1.99
2.00
2.95
f1 (ppm)

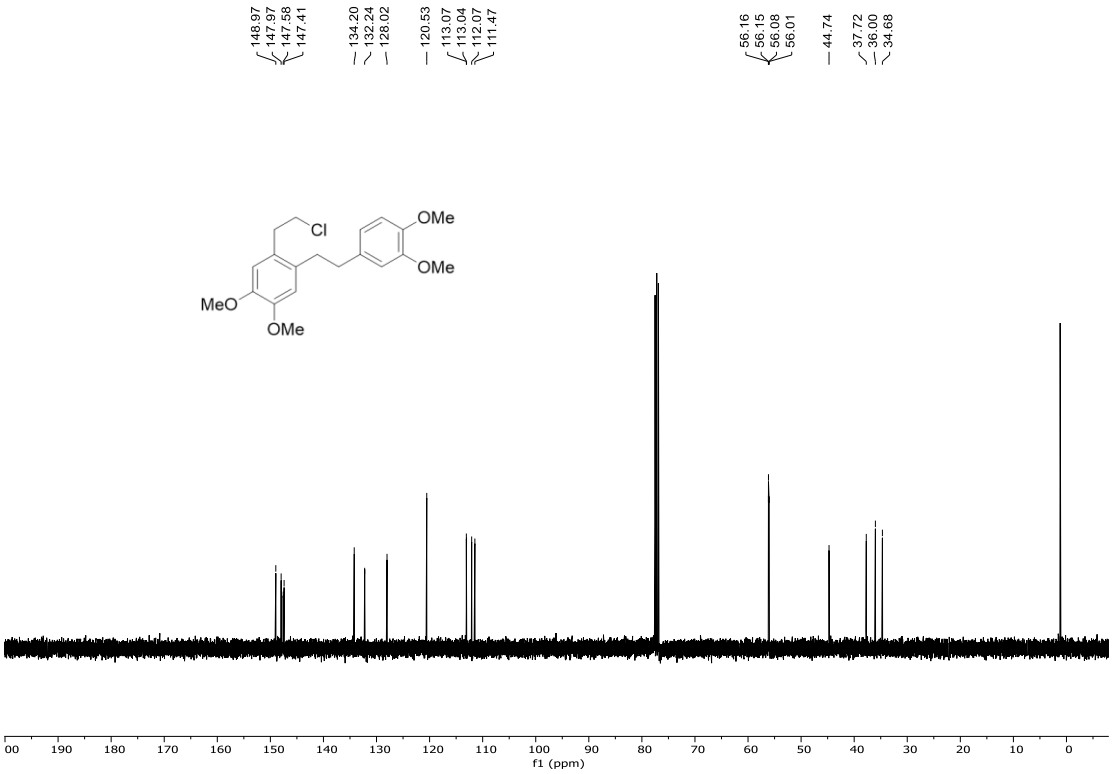

147.92
147.09
134.60
127.15
113.02
112.15
55.99
55.87
52.31
31.78
25.32
15.84
N3
MeO
OMe
f1 (ppm)

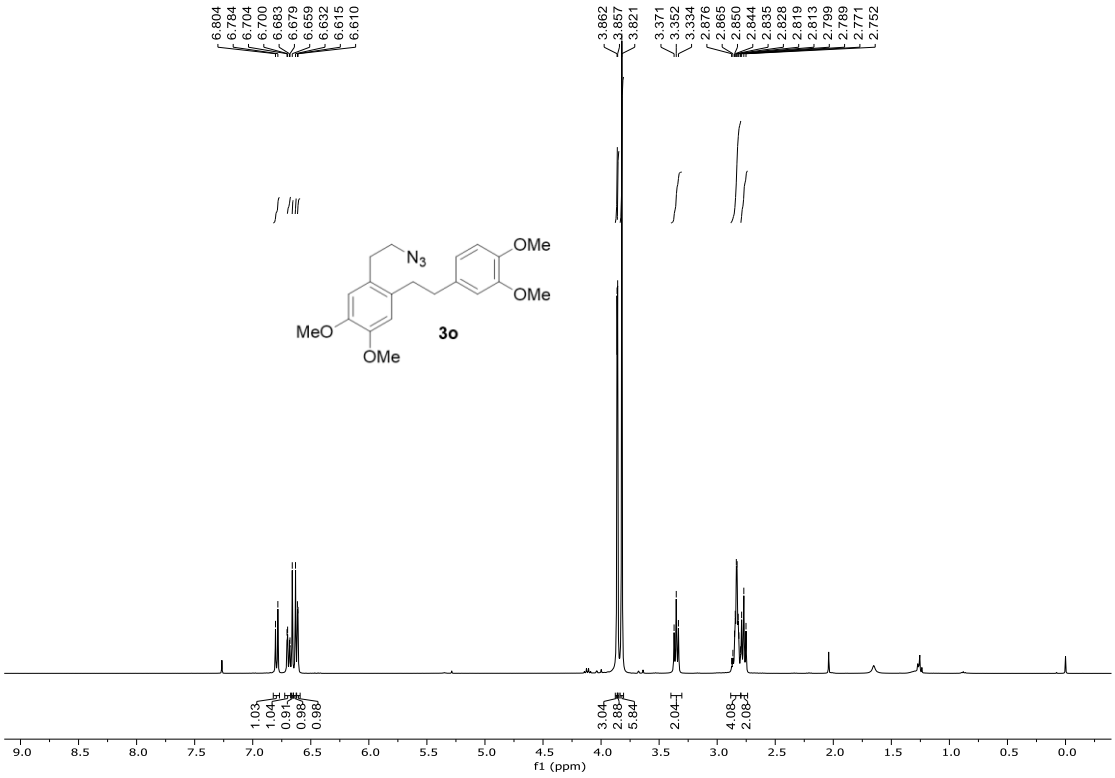
3n

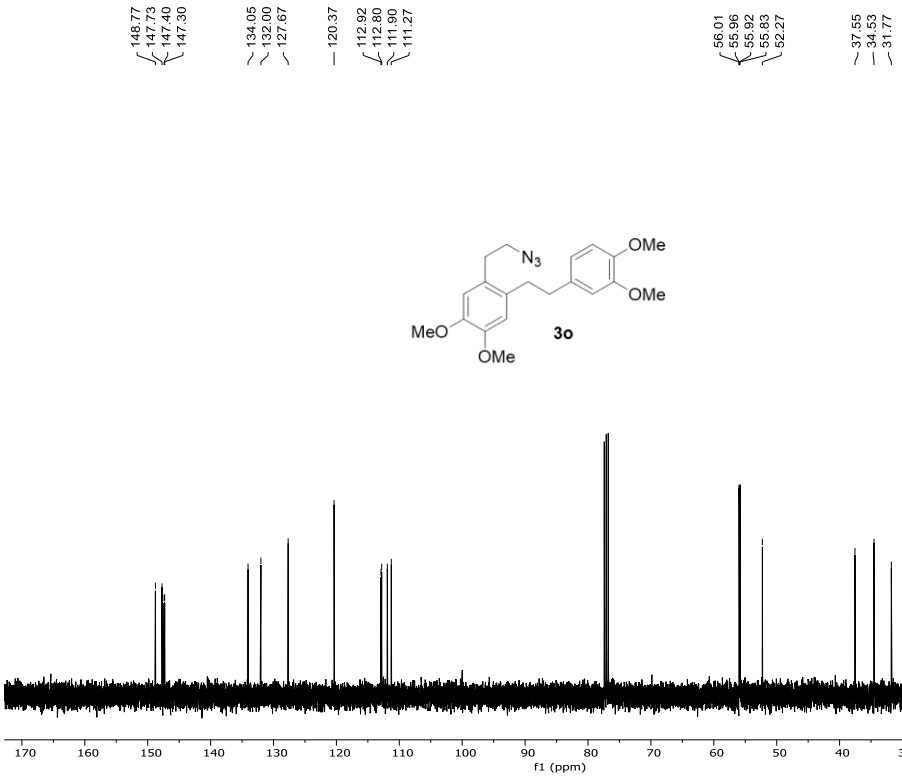

6.760
6.748
6.744
6.732
6.723
6.717
6.709
6.697
6.645
6.545
3.891
3.835
3.663
3.639
3.620
3.559
3.040
3.021
3.003
Cl
OMe
OMe
MeO
OMe
0.97
3.02
0.93
1.84
2.90
2.97
2.89
2.00
2.95
2.00
f1 (ppm)

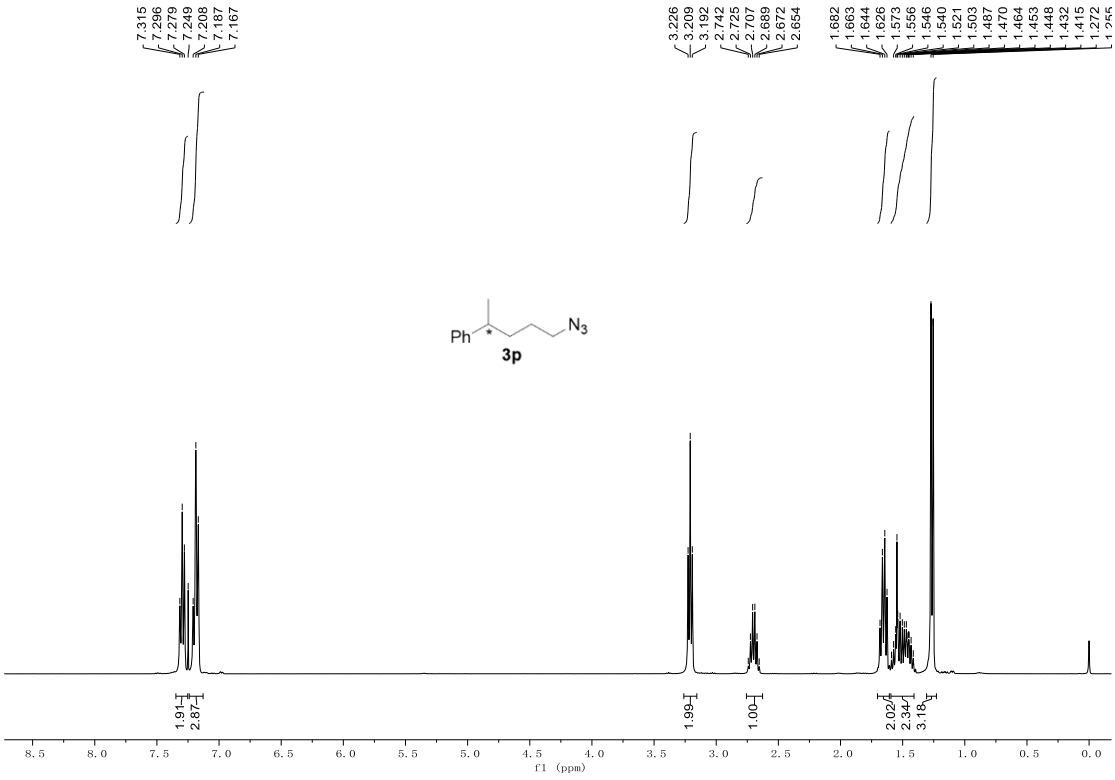

148.41
148.24
148.00
130.91
129.72
129.61
128.60
126.62
122.39
113.38
112.74
111.70
110.84
100.13
77.52
77.20
76.88
56.13
56.03
55.94
55.57
44.64
36.89
Cl
OMe
OMe
MeO
OMe
f1 (ppm)

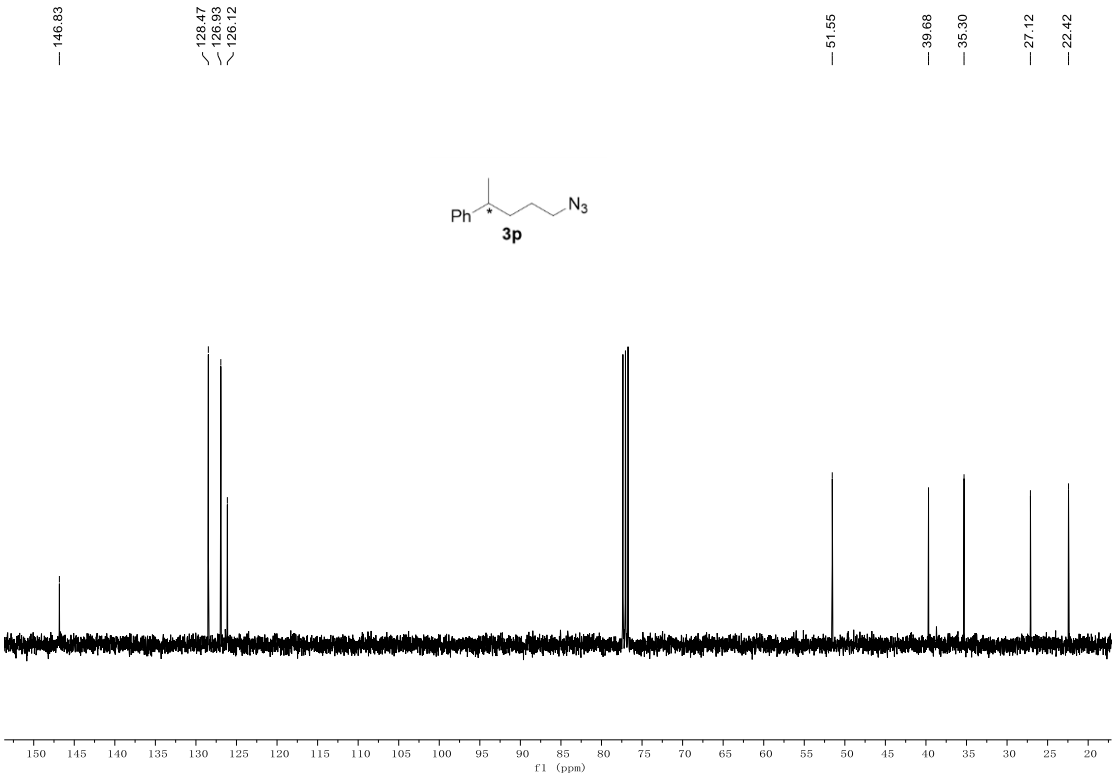

6.805
6.785
6.705
6.700
6.685
6.680
6.665
6.625
3.860
3.831
3.819
3.582
3.563
3.543
2.979
2.959
2.940
2.876
2.865
2.851
2.844
2.835
2.826
2.817
2.810
2.796
Cl
OMe
OMe
MeO
OMe
1.01
1.10
0.92
1.91
5.95
2.96
2.87
2.00
2.08
4.19
f1 (ppm)

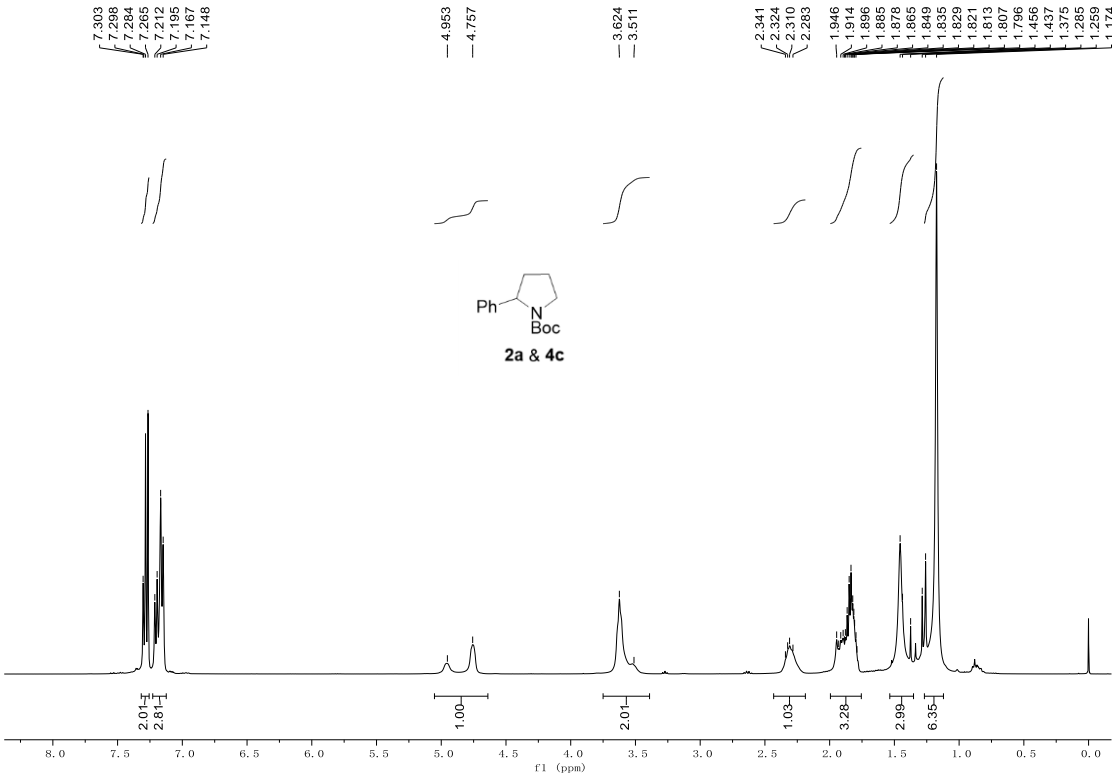

148.97
147.97
147.58
147.41
134.20
132.24
128.02
120.53
113.07
113.04
112.07
111.47
56.16
56.15
56.08
56.01
44.74
37.72
36.00
34.68
Cl
OMe
OMe
MeO
OMe
f1 (ppm)

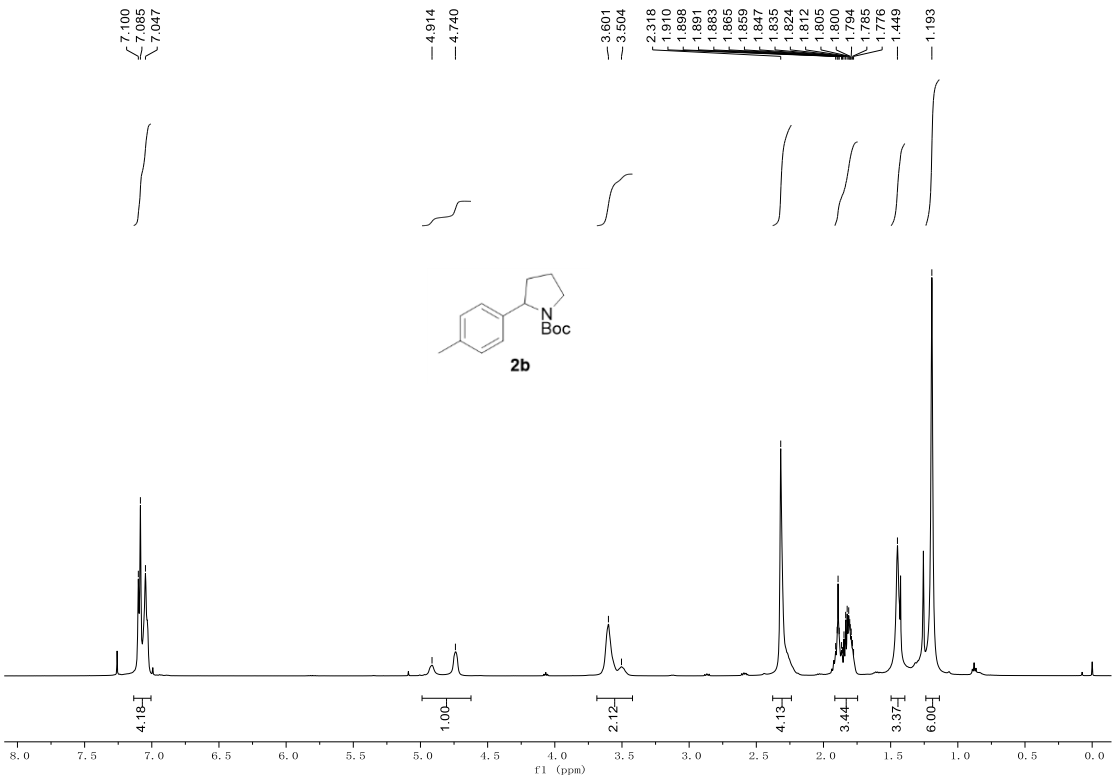

6.804
6.784
6.704
6.700
6.683
6.679
6.659
6.632
6.615
6.610
3.862
3.857
3.821
3.371
3.352
3.334
2.876
2.865
2.850
2.844
2.835
2.828
2.819
2.813
2.799
2.789
2.771
2.762
N3
OMe
OMe
MeO
OMe
3o
1.03
1.04
0.91
0.98
0.98
3.04
2.88
5.84
2.04
4.08
2.08
f1 (ppm)

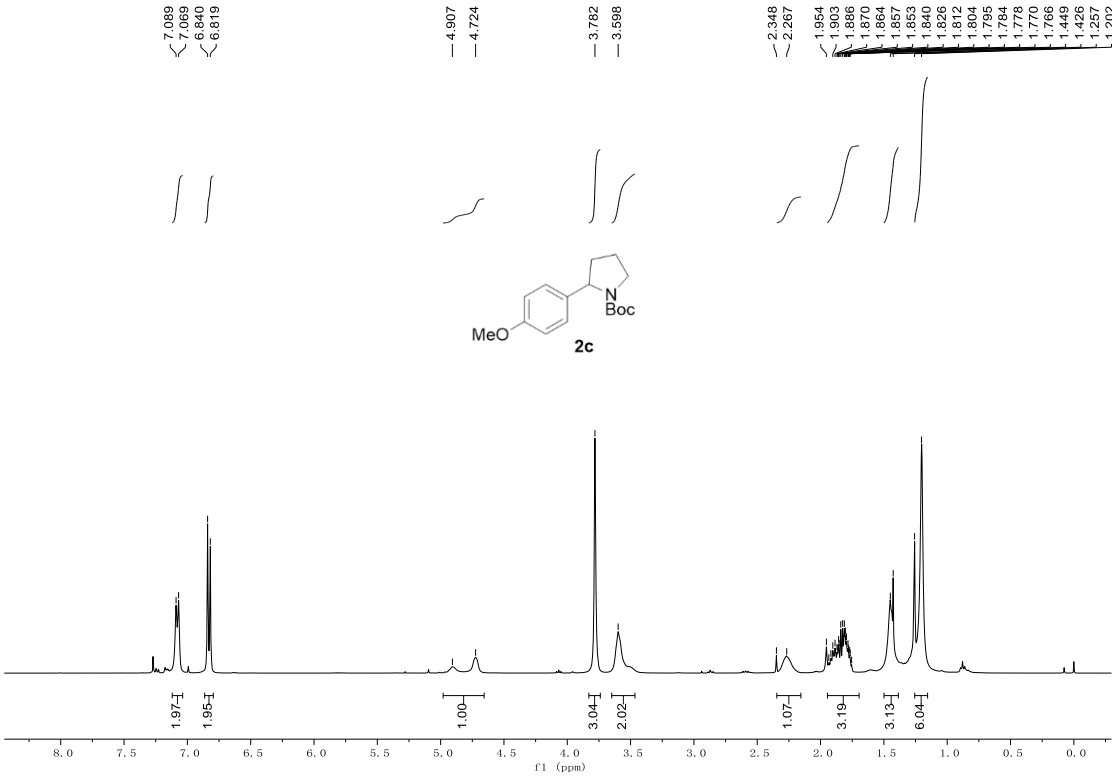

148.77
147.73
147.40
147.30
134.05
132.00
127.67
120.37
112.92
112.80
111.90
111.27
56.01
55.96
55.92
55.83
52.27
37.55
34.53
31.77
N3
OMe
OMe
MeO
OMe
3o
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

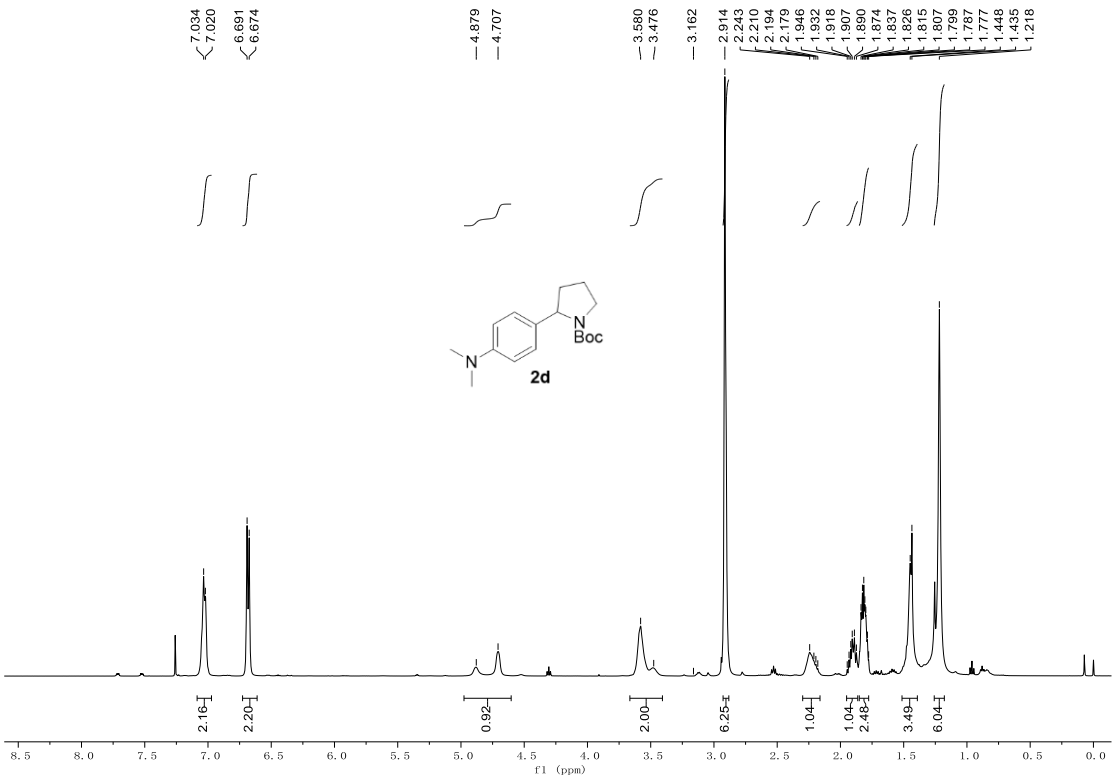

7.315
7.296
7.279
7.249
7.208
7.187
7.167
3.226
3.209
3.192
2.742
2.725
2.707
2.689
2.672
2.654
1.682
1.663
1.644
1.626
1.573
1.556
1.546
1.540
1.521
1.503
1.487
1.470
1.464
1.453
1.448
1.432
1.415
1.272
Ph
N3
3p
1.91
2.87
1.99
1.00
2.02
2.34
3.18
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

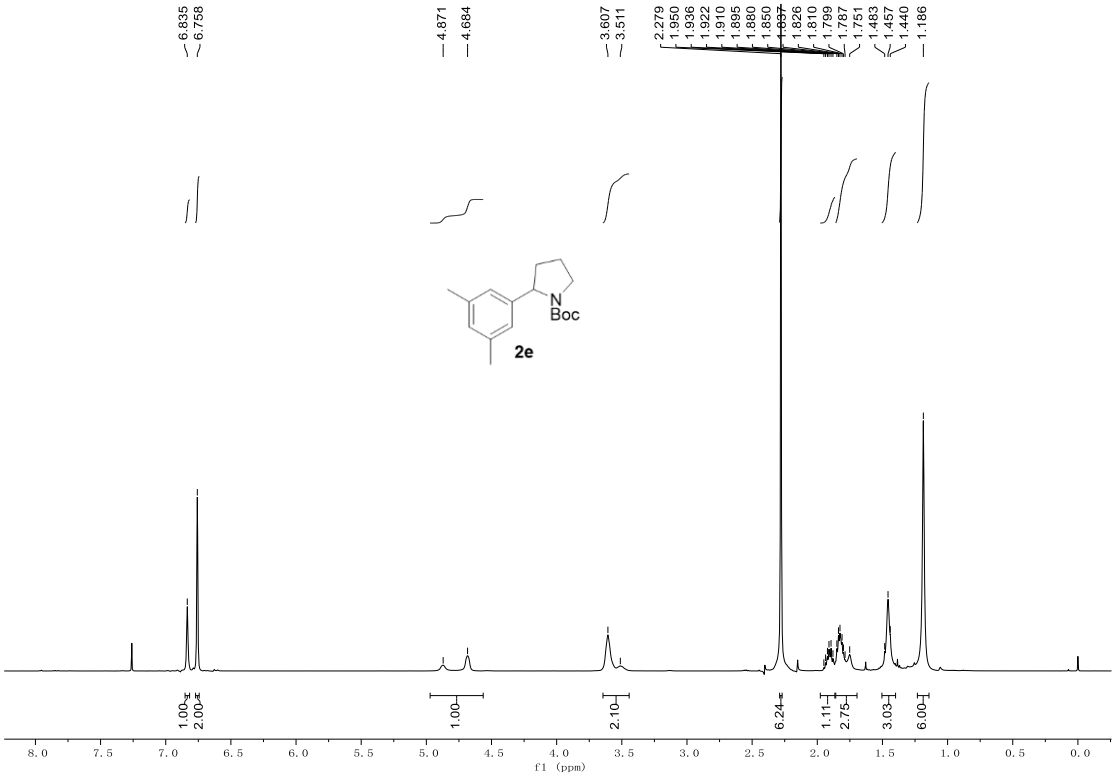

146.83
128.47
126.93
126.12
51.55
39.68
35.30
27.12
22.42
Ph
N3
3p
f1 (ppm)

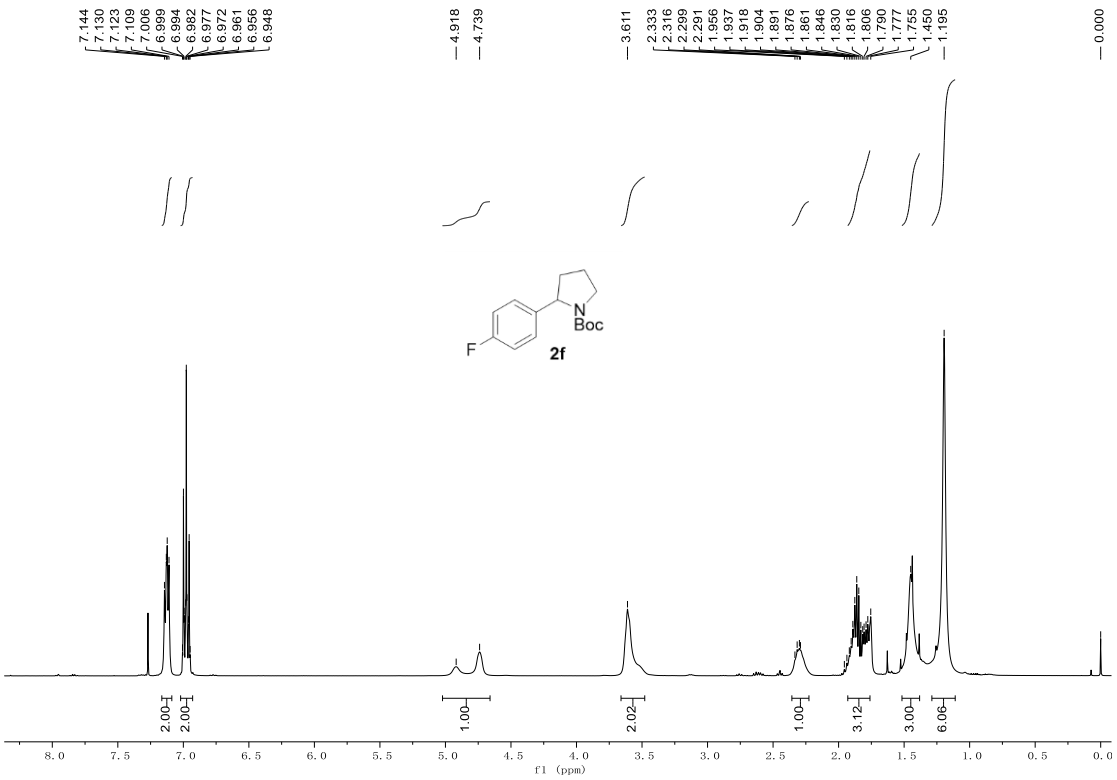

7.303
7.298
7.284
7.265
7.212
7.195
7.167
7.148
4.953
4.757
3.624
3.511
2.341
2.324
2.310
2.283
1.946
1.914
1.896
1.885
1.878
1.865
1.849
1.835
1.829
1.821
1.813
1.807
1.796
1.456
1.437
1.375
1.285
1.259
1.174
Ph
N
Boc
2a & 4c
2.01
2.81
1.00
2.01
1.03
3.28
2.99
6.35
f1 (ppm)

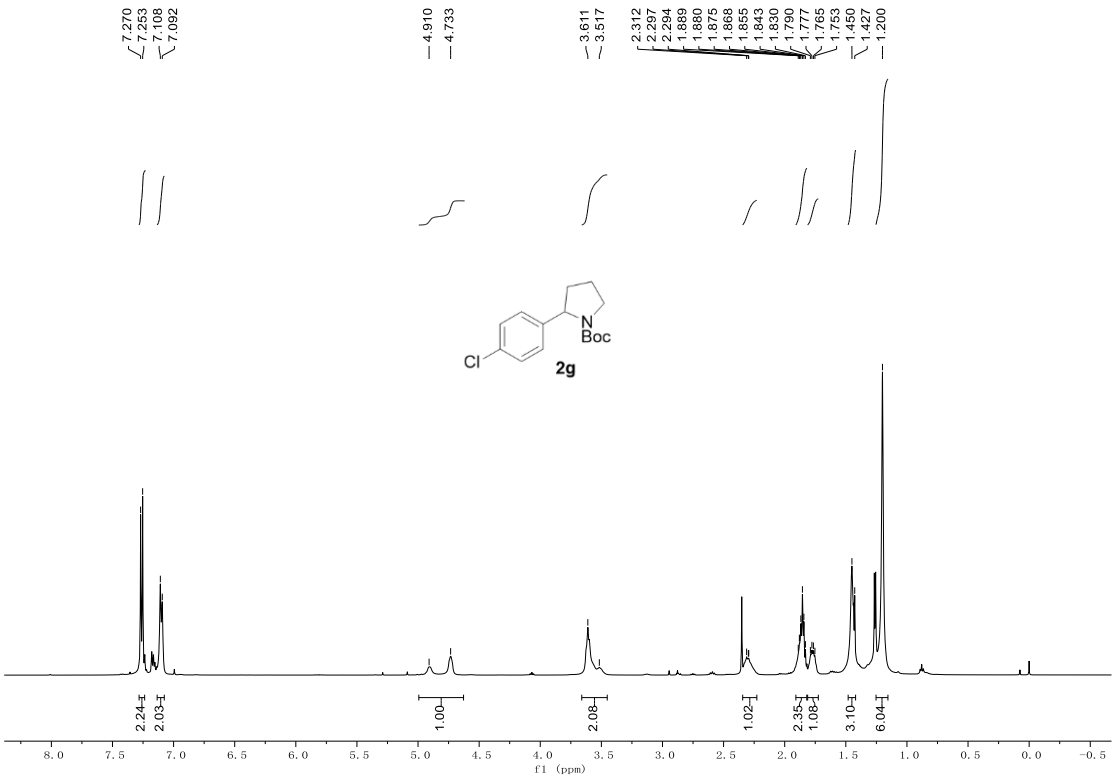

7.100
7.085
7.047
4.914
4.740
3.601
3.504
2.318
1.910
1.898
1.891
1.883
1.865
1.859
1.847
1.835
1.824
1.812
1.805
1.800
1.794
1.785
1.776
1.449
1.193
N
Boc
2b
4.18
1.00
2.12
4.13
3.44
3.37
6.00
f1 (ppm)

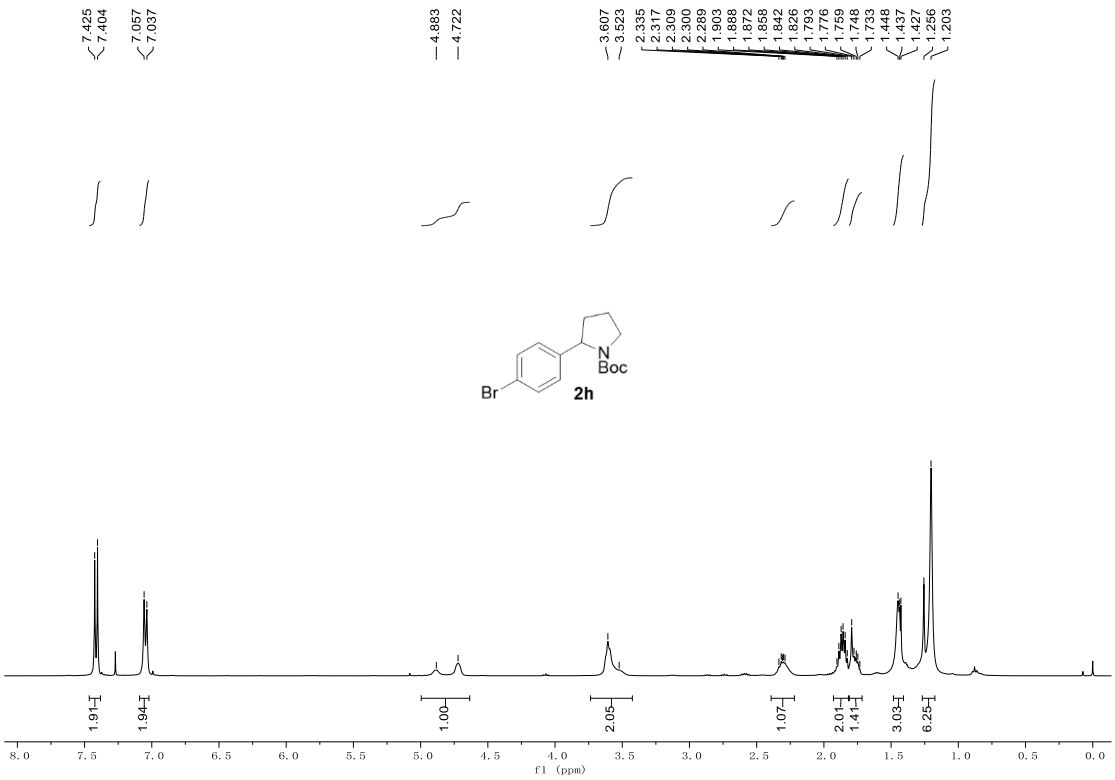

7.089
7.069
6.840
6.819
4.907
4.724
3.782
3.598
2.348
2.267
1.954
1.903
1.886
1.870
1.864
1.857
1.853
1.840
1.826
1.812
1.804
1.795
1.784
1.778
1.770
1.766
1.449
1.426
1.257
N
Boc
MeO
2c
1.97
1.95
1.00
3.04
2.02
1.07
3.19
3.13
6.04
f1 (ppm)


7.034
7.020
6.691
6.674
4.879
4.707
3.580
3.476
3.162
2.914
2.243
2.210
2.194
2.179
1.946
1.932
1.918
1.907
1.890
1.874
1.837
1.826
1.815
1.807
1.799
1.787
1.777
1.448
1.435
1.218
N
Boc
N
2d
2.16
2.20
0.92
2.00
6.25
1.04
1.04
2.48
3.49
6.04
f1 (ppm)


6.835
6.758
4.871
4.684
3.607
3.511
2.279
1.950
1.936
1.922
1.910
1.895
1.880
1.850
1.826
1.810
1.799
1.787
1.751
1.483
1.457
1.440
1.186
N
Boc
2e
1.00
2.00
1.00
2.10
6.24
1.11
2.75
3.03
6.00
f1 (ppm)


7.144
7.130
7.123
7.109
7.006
6.999
6.994
6.982
6.977
6.972
6.961
6.956
6.948
4.918
4.739
3.611
2.333
2.316
2.299
2.291
1.956
1.937
1.918
1.904
1.891
1.876
1.861
1.846
1.830
1.816
1.806
1.790
1.777
1.755
1.450
1.195
0.000
N
Boc
F
2f
2.00
2.00
1.00
2.02
1.00
3.12
3.00
6.06
f1 (ppm)


7.270
7.253
7.108
7.092
4.910
4.733
3.611
3.517
2.312
2.297
2.294
1.889
1.880
1.875
1.868
1.855
1.843
1.830
1.790
1.777
1.765
1.753
1.450
1.427
1.200
N
Boc
Cl
2g
2.24
2.03
1.00
2.08
1.02
2.35
1.08
3.10
6.04
f1 (ppm)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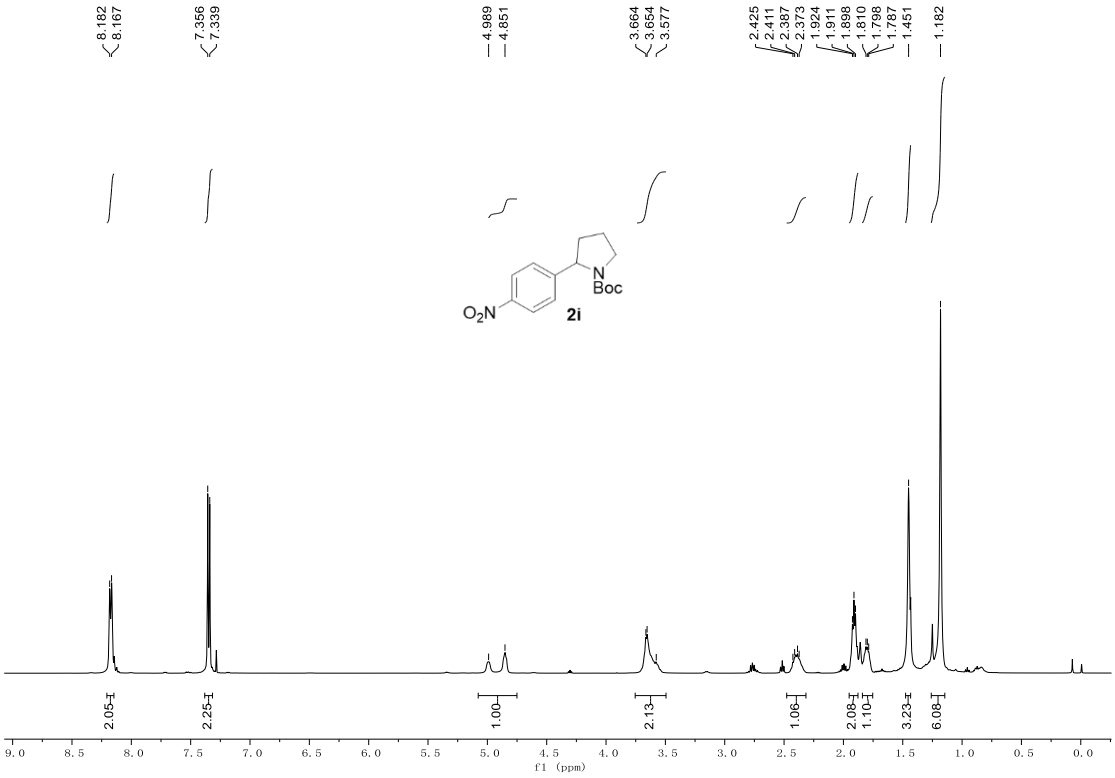
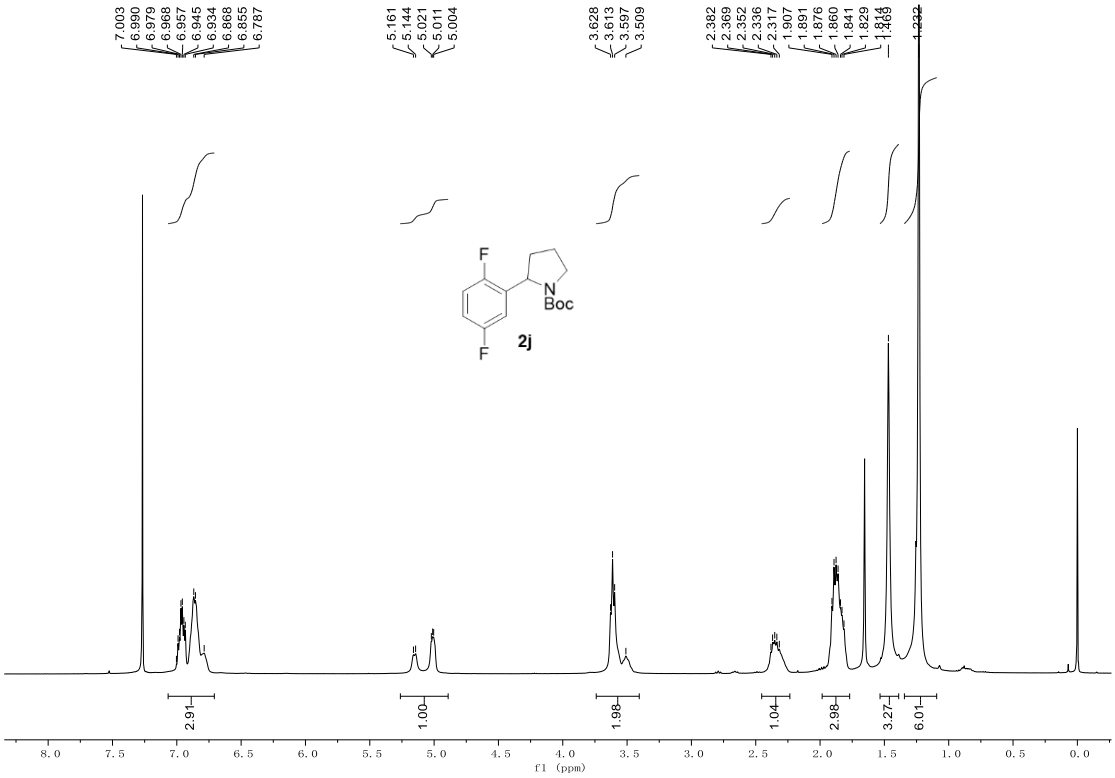
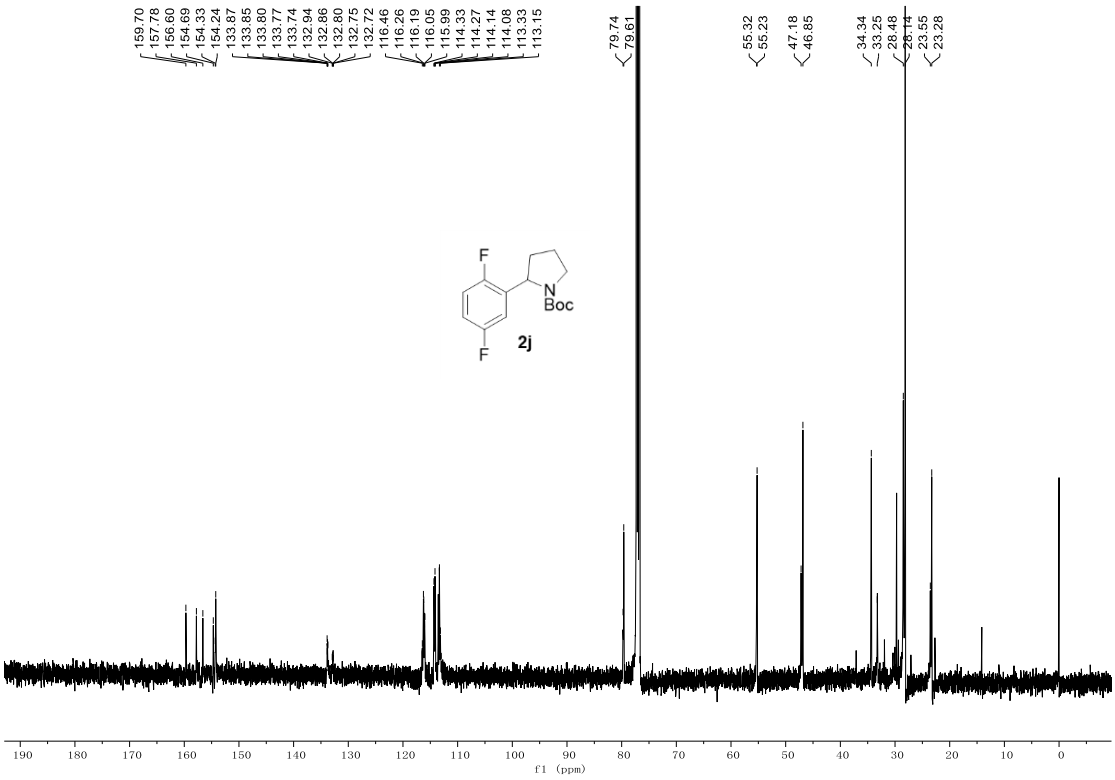
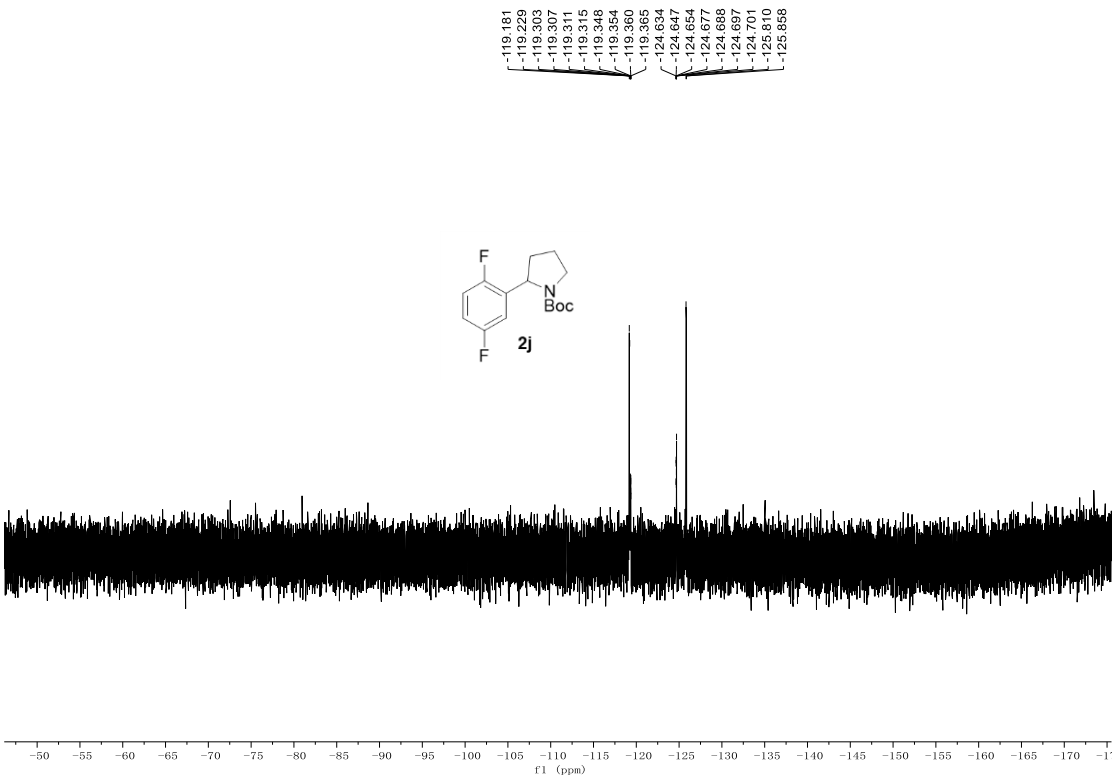
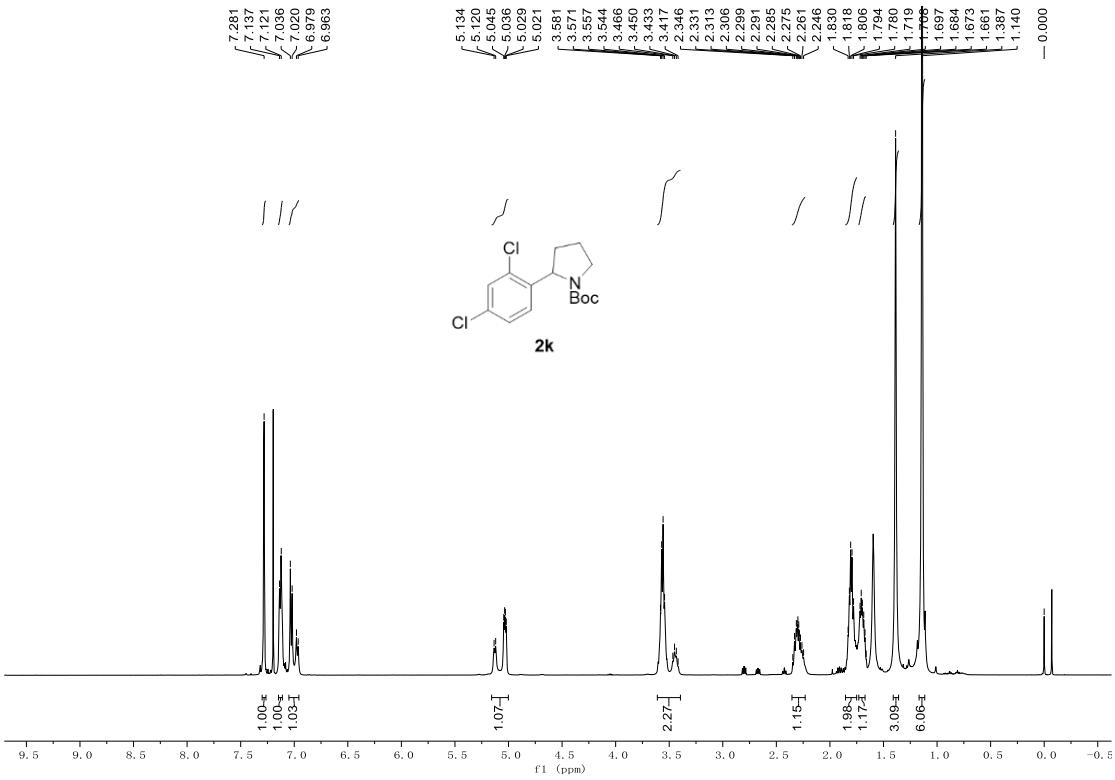
7.404
7.057
7.037
4.883
4.722
3.607
3.523
2.335
2.317
2.309
2.300
2.289
1.903
1.888
1.872
1.858
1.842
1.826
1.793
1.776
1.759
1.748
1.733
1.448
1.437
1.427
1.256
1.203
N
Boc
Br
2h
1.91
1.94
1.00
2.05
1.07
2.01
1.41
3.03
6.25
f1 (ppm)

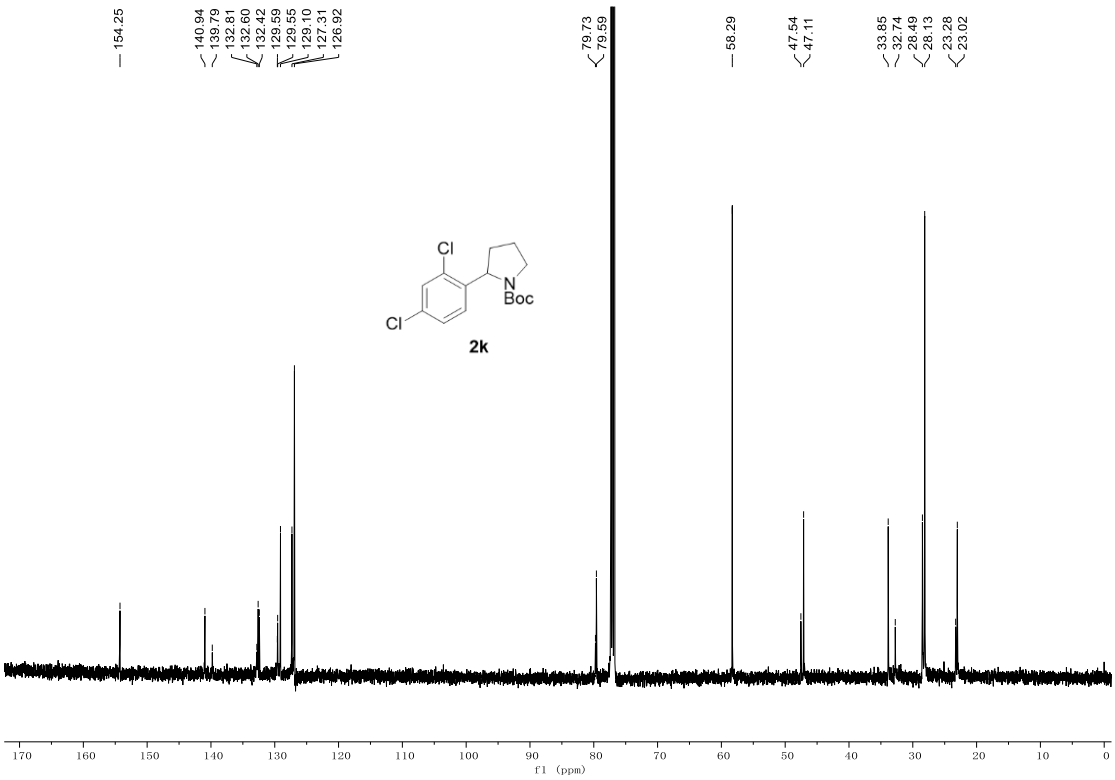

8.182
8.167
7.356
7.339
4.989
4.851
3.664
3.654
3.577
2.425
2.411
2.387
2.373
1.924
1.911
1.898
1.810
1.798
1.787
1.451
1.182
N
Boc
O2N
2i
2.05
2.25
1.00
2.13
1.06
2.08
1.10
3.23
6.08
f1 (ppm)

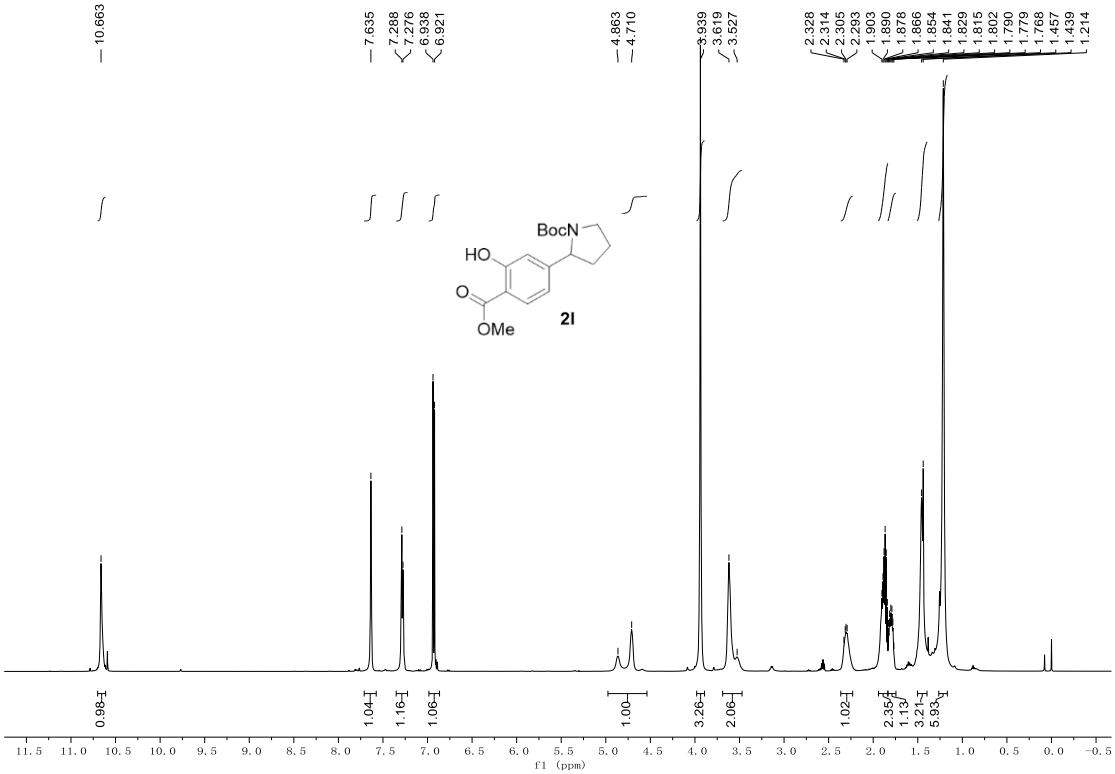

7.003
6.990
6.979
6.968
6.957
6.945
6.934
6.868
6.855
6.787
5.161
5.144
5.021
5.011
5.004
3.628
3.613
3.597
3.509
2.382
2.369
2.352
2.336
2.317
1.907
1.891
1.876
1.860
1.841
1.829
1.814
1.469
1.332
F
N
Boc
F
2j
2.91
1.00
1.98
1.04
2.98
3.27
6.01
f1 (ppm)

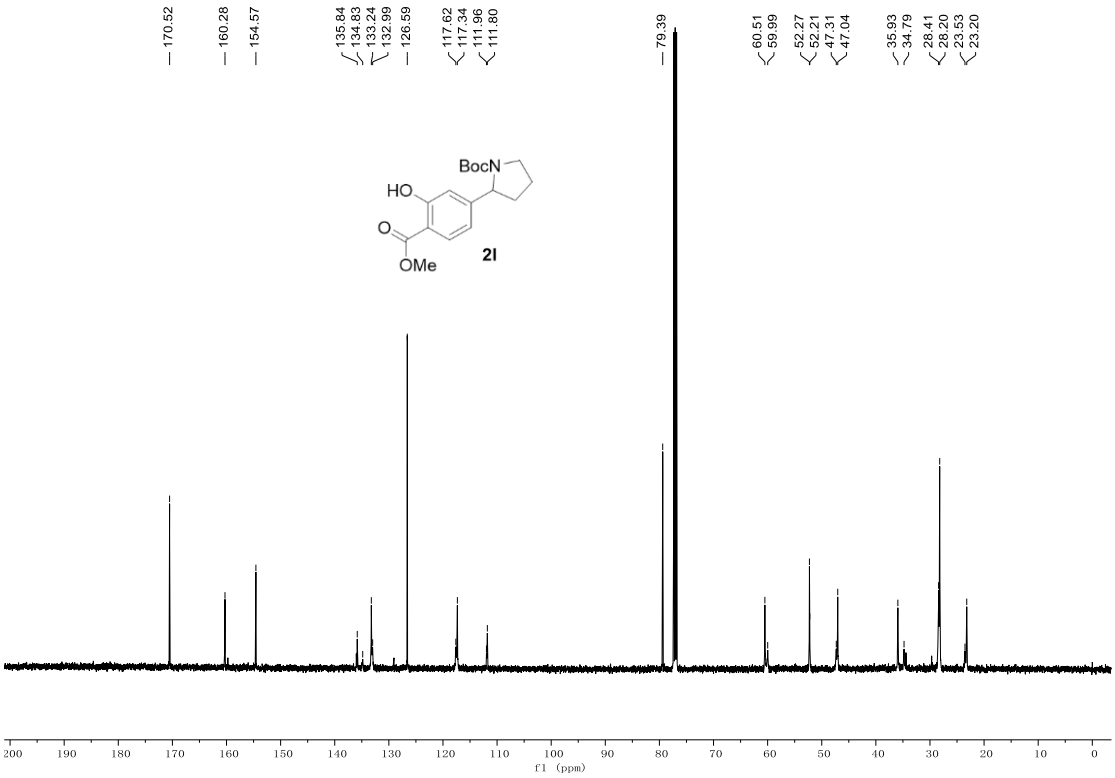

159.70
157.78
156.60
154.69
154.33
154.24
133.87
133.85
133.80
133.77
133.74
132.94
132.86
132.80
132.75
132.72
116.46
116.26
116.19
116.05
115.99
114.33
114.27
114.14
114.08
113.33
113.15
79.74
79.61
55.32
55.23
47.18
46.85
34.34
33.25
28.48
28.14
23.55
23.28
F
N
Boc
F
2j
f1 (ppm)


-119.181
-119.229
-119.303
-119.307
-119.311
-119.315
-119.348
-119.354
-119.360
-119.365
-124.634
-124.647
-124.654
-124.677
-124.688
-124.697
-124.701
-125.810
-125.858
F
N
Boc
F
2j
f1 (ppm)


7.281
7.137
7.121
7.036
7.020
6.979
6.963
5.134
5.120
5.045
5.036
5.029
5.021
3.581
3.571
3.557
3.544
3.466
3.450
3.433
3.417
2.346
2.331
2.313
2.306
2.299
2.291
2.285
2.275
2.261
2.246
1.830
1.818
1.806
1.794
1.780
1.719
1.708
1.697
1.684
1.673
1.661
1.387
1.140
0.000
Cl
N
Boc
Cl
2k
1.00
1.00
1.03
1.07
2.27
1.15
1.98
1.17
3.09
6.06
f1 (ppm)


154.25
140.94
139.79
132.81
132.60
132.42
129.59
129.55
129.10
127.31
126.92
79.73
79.59
58.29
47.54
47.11
33.85
32.74
28.49
28.13
23.28
23.02
Cl
Cl
N
Boc
2k
f1 (ppm)


10.663
7.635
7.288
7.276
6.938
6.921
4.863
4.710
3.939
3.619
3.527
2.328
2.314
2.305
2.293
1.903
1.890
1.878
1.866
1.854
1.841
1.829
1.815
1.802
1.790
1.779
1.768
1.457
1.439
1.214
BocN
HO
O
OMe
2l
0.98
1.04
1.16
1.06
1.00
3.26
2.06
1.02
2.35
1.13
3.21
5.93
f1 (ppm)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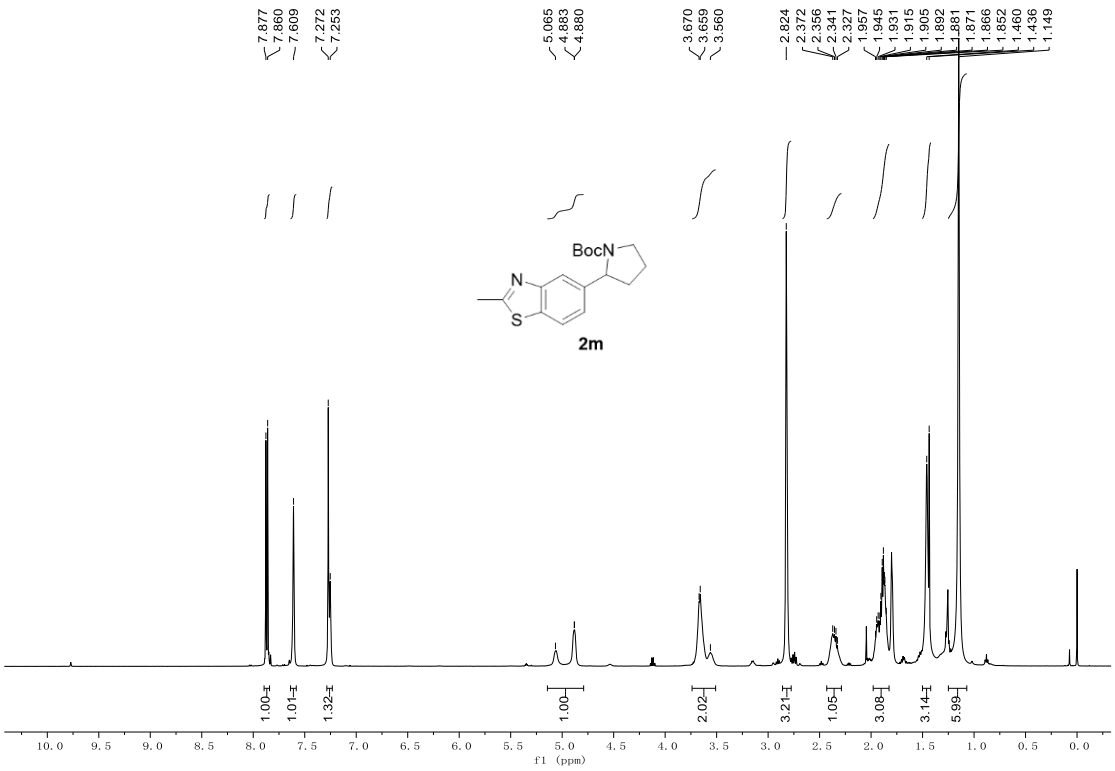
135.84
134.83
133.24
132.99
126.59
117.62
117.34
111.96
111.80
79.39
60.51
59.99
52.27
52.21
47.31
47.04
35.93
34.79
28.41
28.20
23.53
23.20
BocN
HO
O
OMe
2l
f1 (ppm)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7.609
7.272
7.253
5.065
4.883
4.880
3.670
3.659
3.560
2.824
2.372
2.356
2.341
2.327
1.957
1.945
1.931
1.915
1.905
1.892
1.881
1.871
1.866
1.852
1.460
1.436
1.149
BocN
N
S
2m
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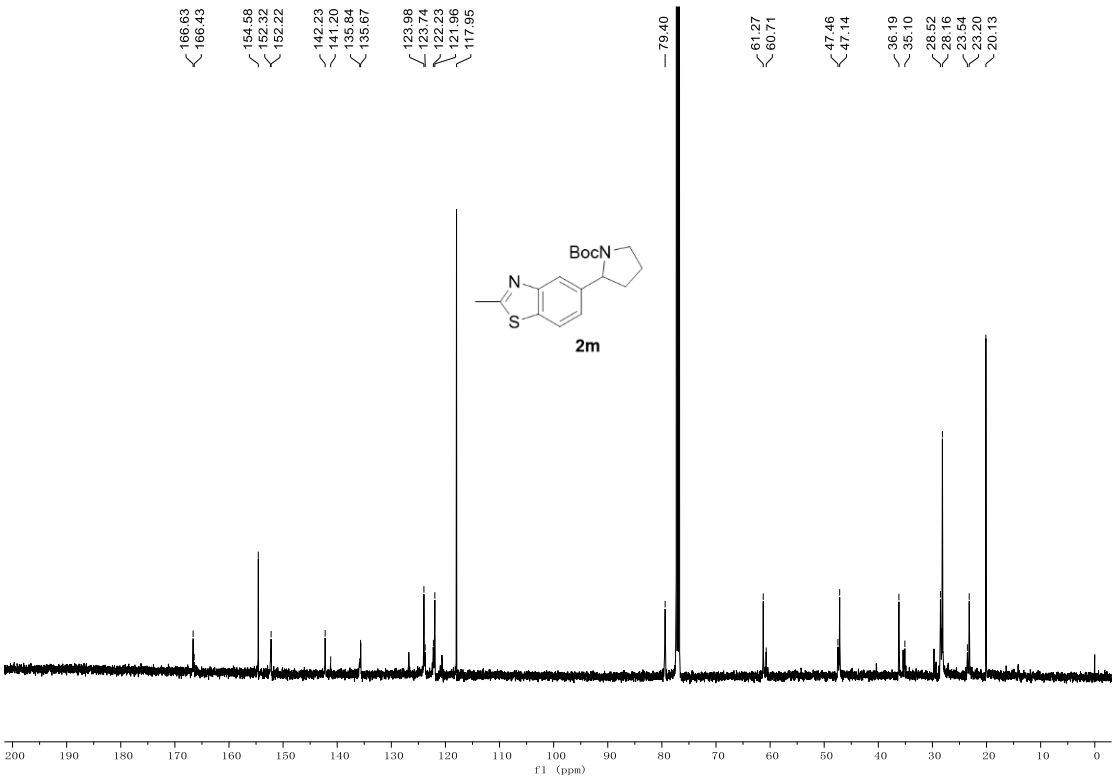
1.01
1.32
1.00
2.02
3.21
1.05
3.08
3.14
5.99
f1 (ppm)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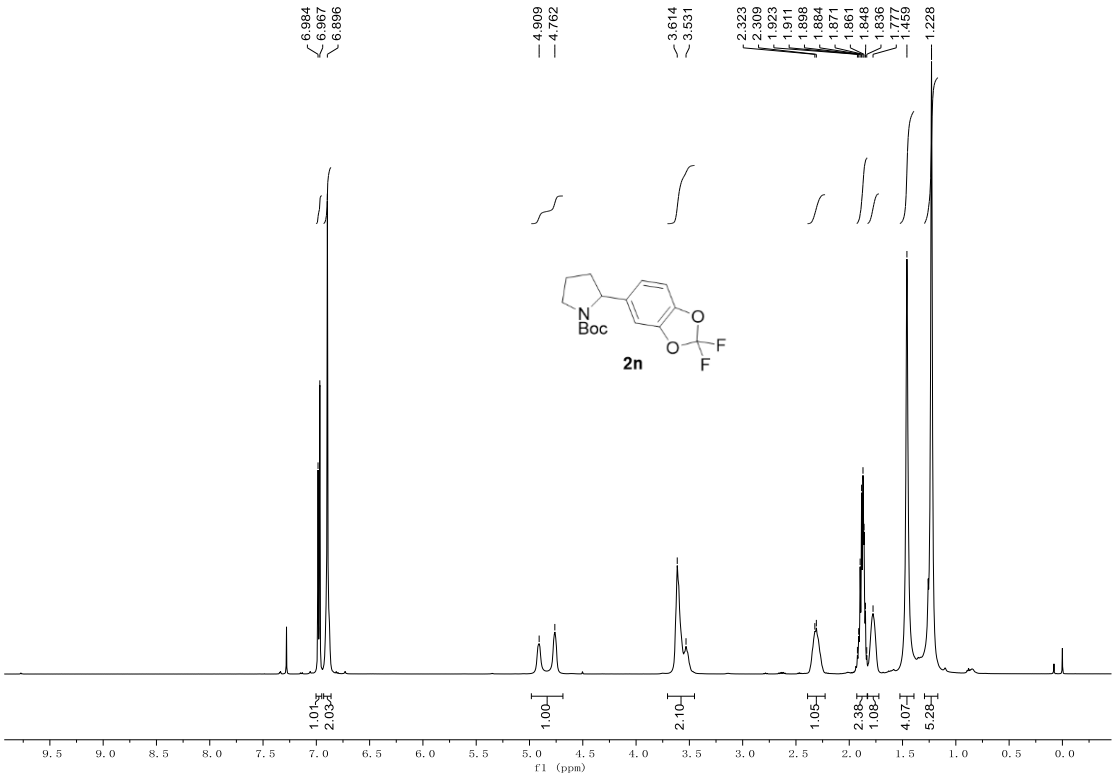
166.43
154.58
152.32
152.22
142.23
141.20
135.84
135.67
123.98
123.74
122.23
121.96
117.95
79.40
61.27
60.71
47.46
47.14
36.19
35.10
28.52
28.16
23.54
23.20
20.13
BocN
N
S
2m
f1 (ppm)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6.896
4.909
4.762
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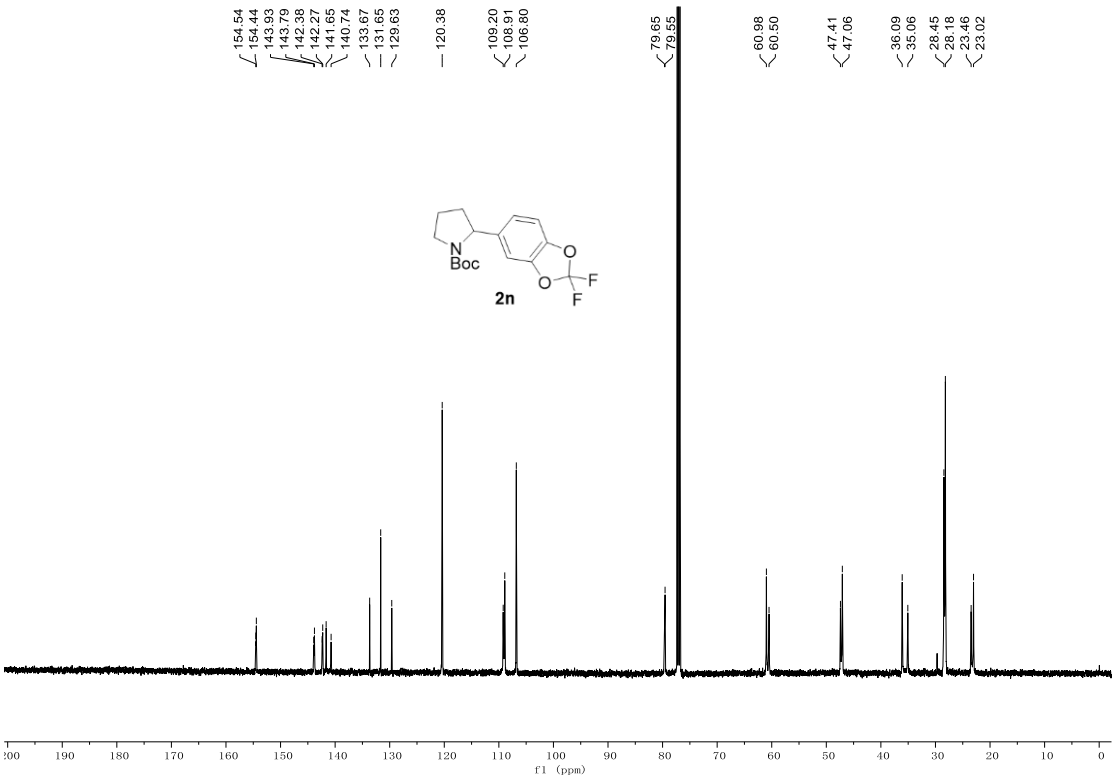
3.531
2.323
2.309
1.923
1.911
1.898
1.884
1.871
1.861
1.848
1.836
1.777
1.459
1.228
N
Boc
O
O
F
F
2n
1.01
2.03
1.00
2.10
1.05
2.38
1.08
4.07
5.28
f1 (ppm)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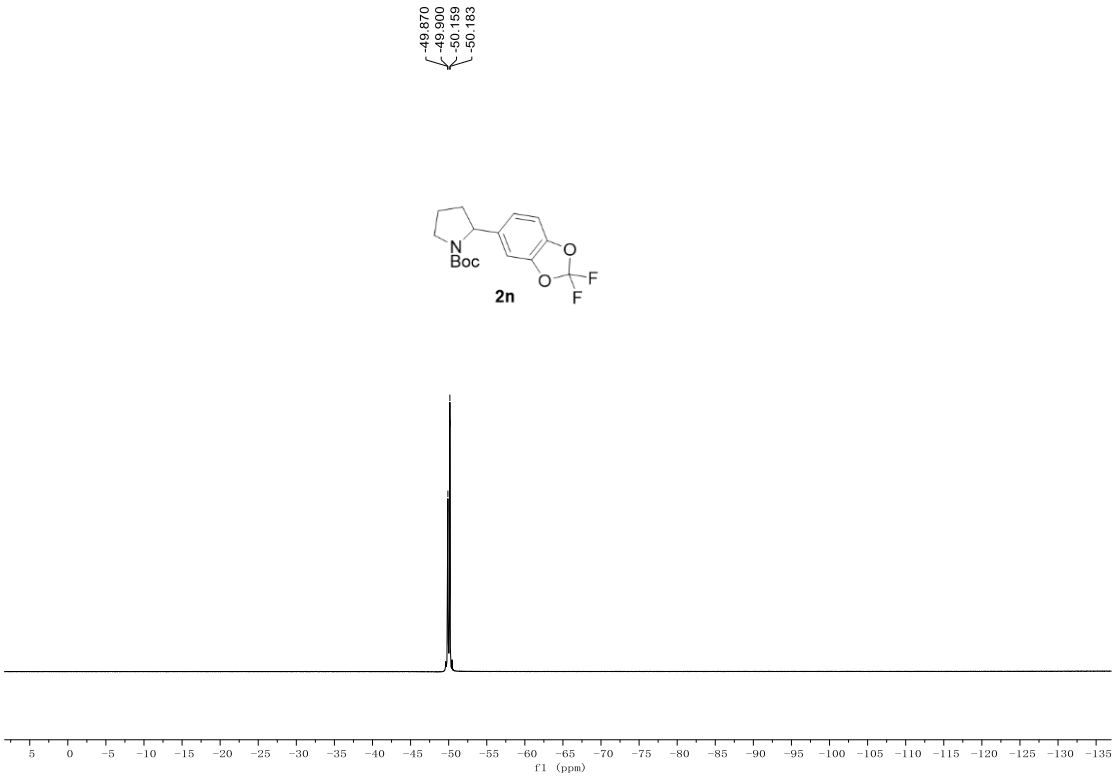
154.44
143.93
143.79
142.38
142.27
141.65
140.74
133.67
131.65
129.63
120.38
109.20
108.91
106.80
79.65
79.55
60.98
60.50
47.41
47.06
36.09
35.06
28.45
28.18
23.46
23.02
N
Boc
O
O
F
F
2n
f1 (ppm)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-50.159
-50.183
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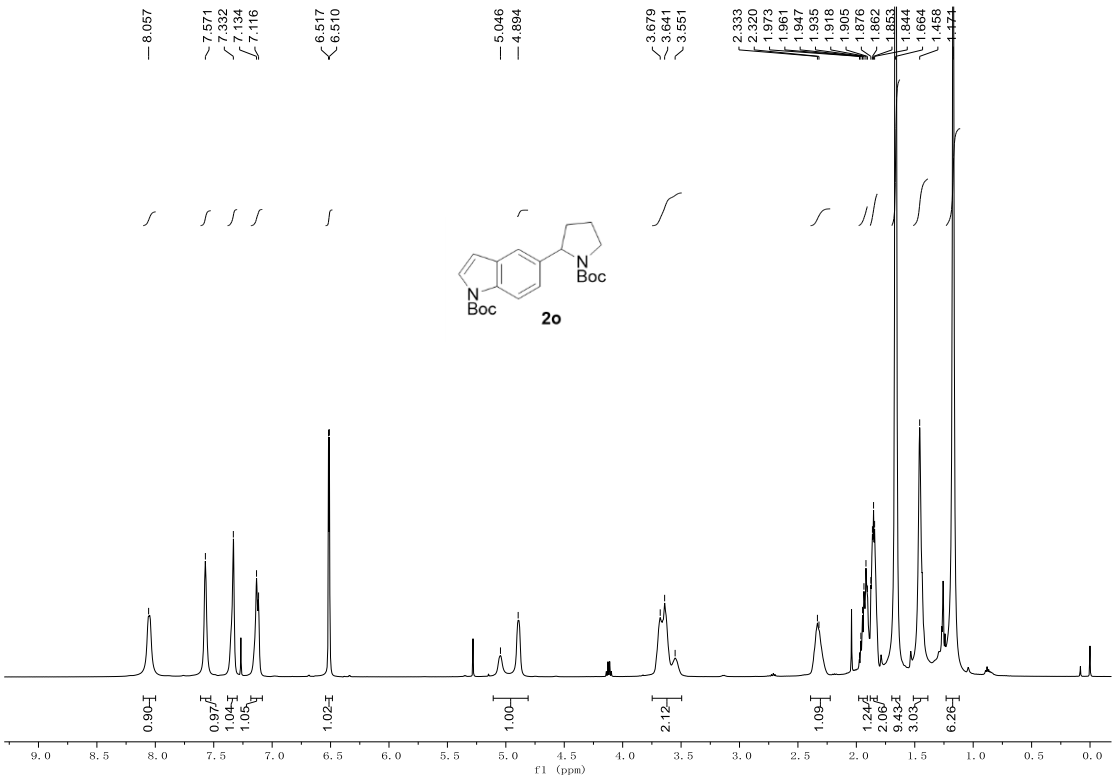
Boc
O
O
F
F
2n
f1 (ppm)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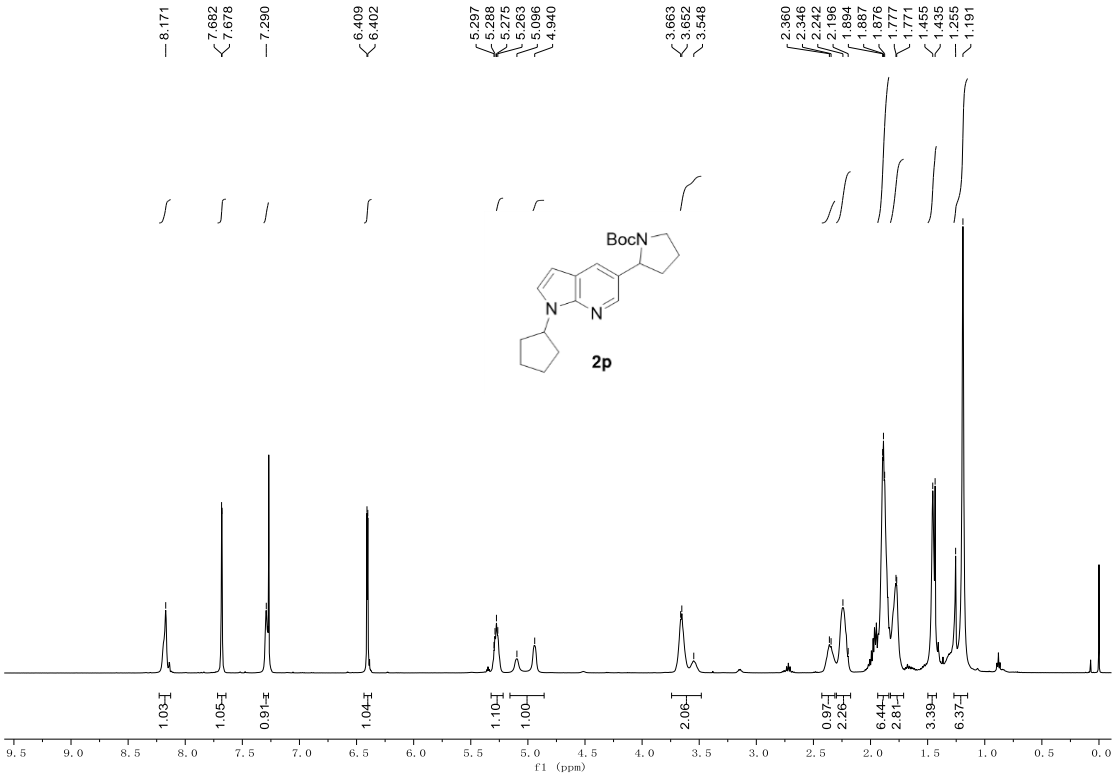
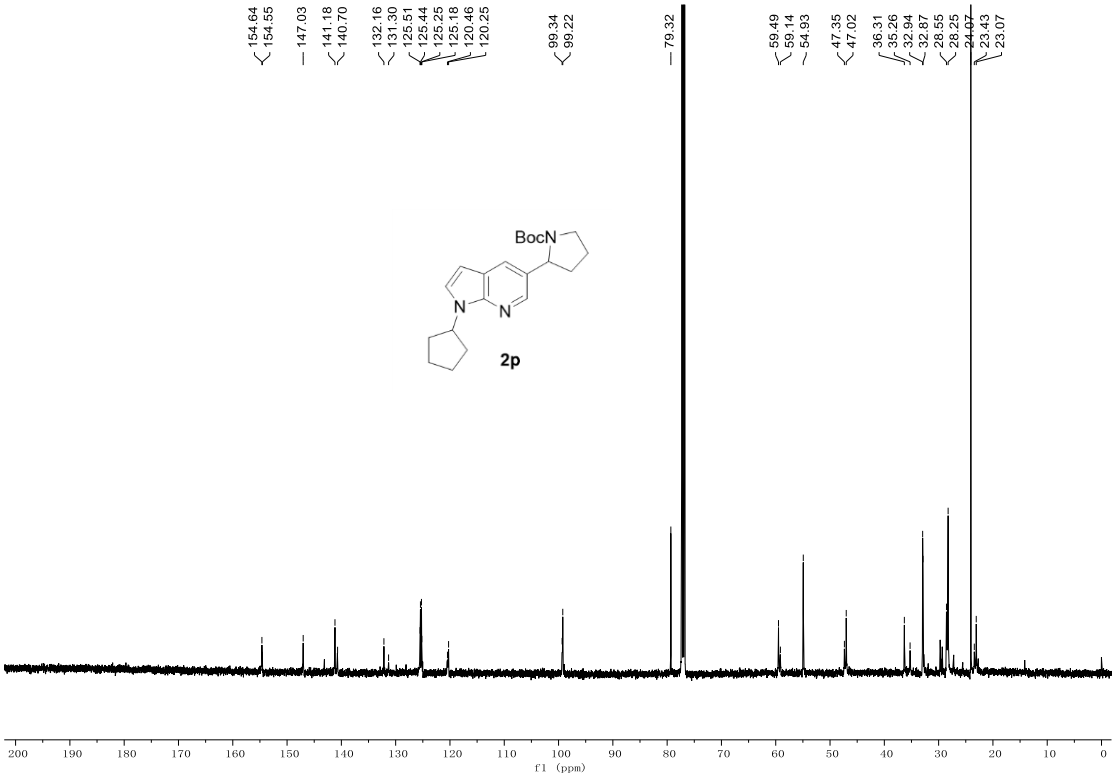
7.571
7.332
7.134
7.116
6.517
6.510
5.046
4.894
3.679
3.641
3.551
2.333
2.320
1.973
1.961
1.947
1.935
1.918
1.905
1.876
1.862
1.853
1.844
1.664
1.458
1.174
N
Boc
N
Boc
2o
0.90
0.97
1.04
1.05
1.02
1.00
2.12
1.09
1.24
2.06
9.43
3.03
6.26
f1 (ppm)


8.171
7.682
7.678
7.290
6.409
6.402
5.297
5.288
5.275
5.263
5.096
4.940
3.663
3.652
3.548
2.360
2.346
2.242
2.196
1.894
1.887
1.876
1.777
1.771
1.455
1.435
1.255
1.191
BocN
N
N
2p
1.03
1.05
0.91
1.04
1.10
1.00
2.06
0.97
2.26
6.44
2.81
3.39
6.37
f1 (ppm)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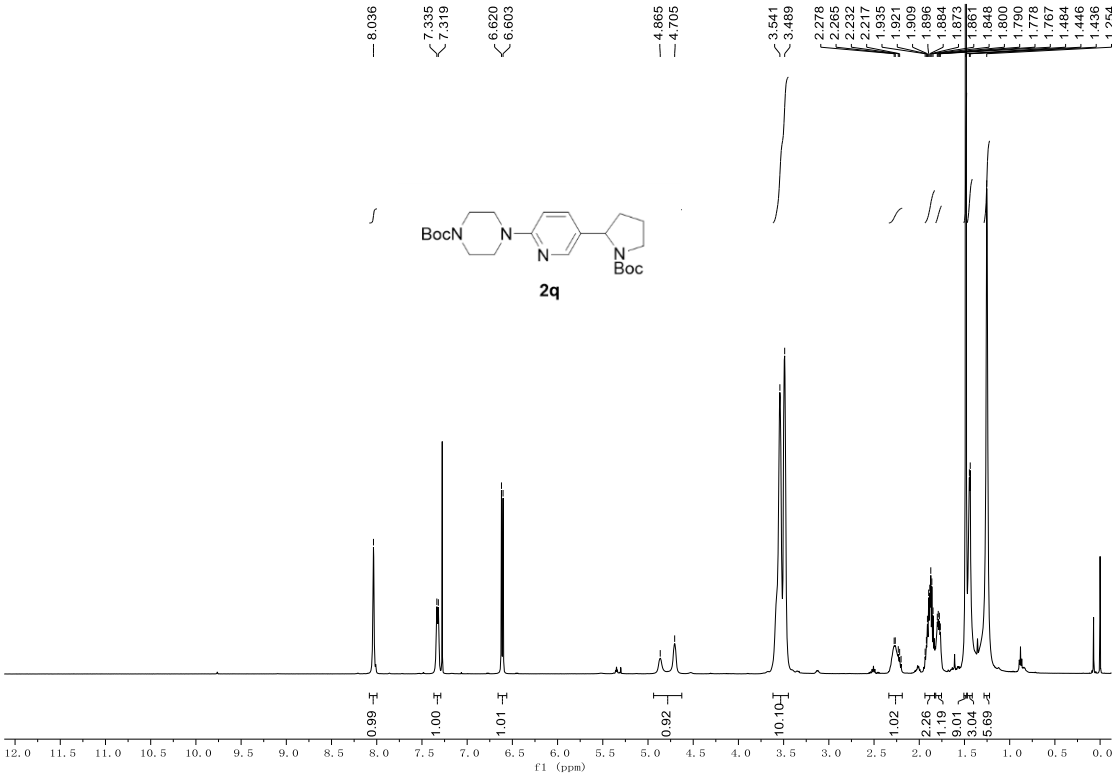
154.55
147.03
141.18
140.70
132.16
131.30
125.51
125.44
125.25
125.18
120.46
120.25
99.34
99.22
79.32
59.49
59.14
54.93
47.35
47.02
36.31
35.26
32.94
32.87
28.55
28.25
24.07
23.43
23.07
BocN
N
N
2p
f1 (ppm)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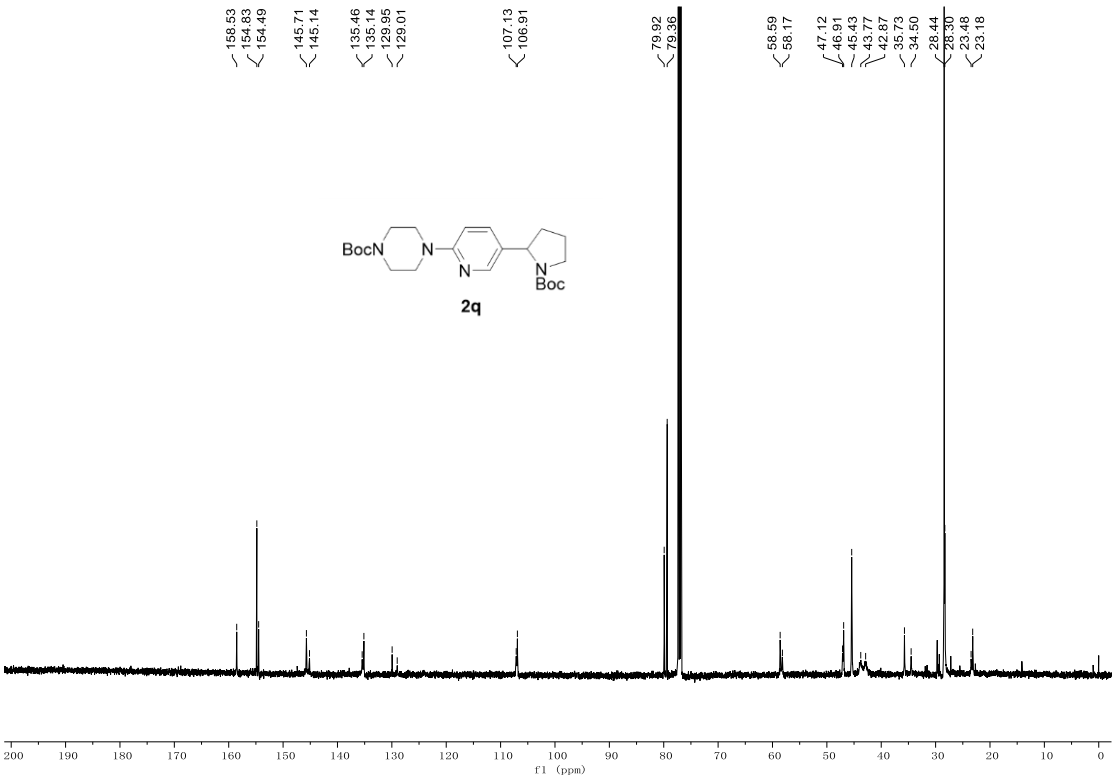
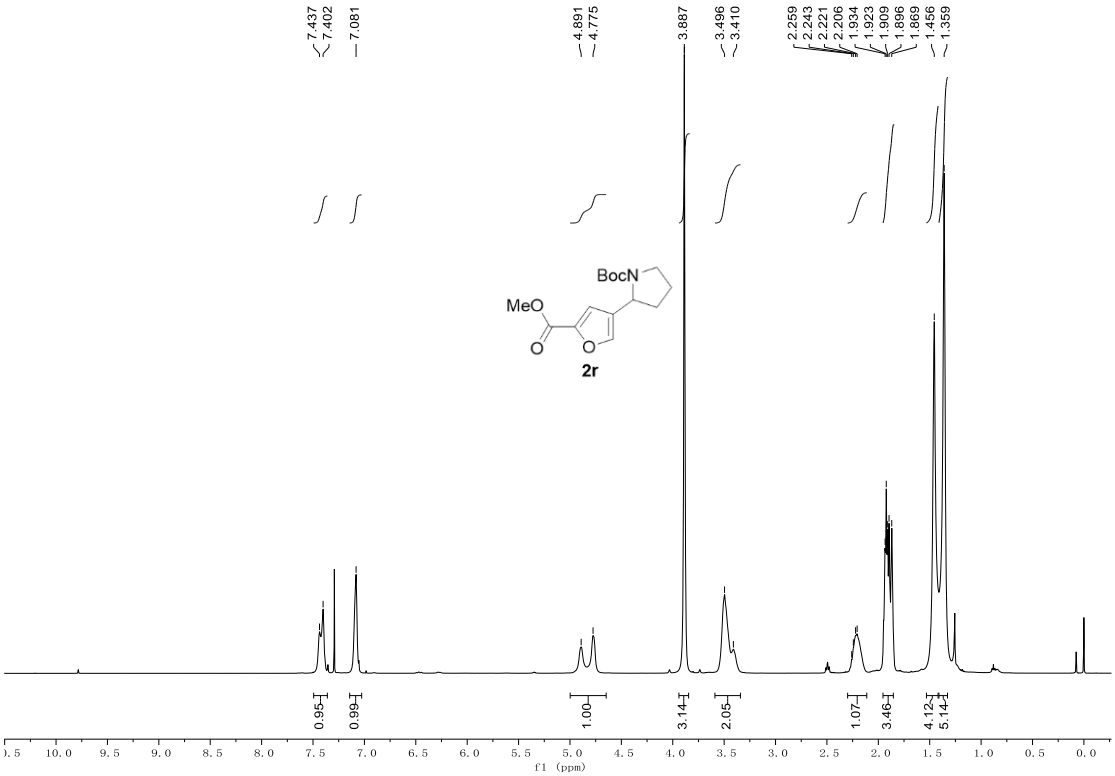
7.335
7.319
6.620
6.603
4.865
4.705
3.541
3.489
2.278
2.265
2.232
2.217
1.935
1.921
1.909
1.896
1.884
1.873
1.861
1.848
1.800
1.790
1.778
1.767
1.484
1.446
1.436
BocN
N
N
N
Boc
2q
0.99
1.00
1.01
0.92
10.10
1.02
2.26
1.19
9.01
3.04
5.69
f1 (ppm)


158.53
154.83
154.49
145.71
145.14
135.46
135.14
129.95
129.01
107.13
106.91
79.92
79.36
58.59
58.17
47.12
46.91
45.43
43.77
42.87
35.73
34.50
28.44
28.30
23.48
23.18
BocN
N
N
N
Boc
2q
f1 (ppm)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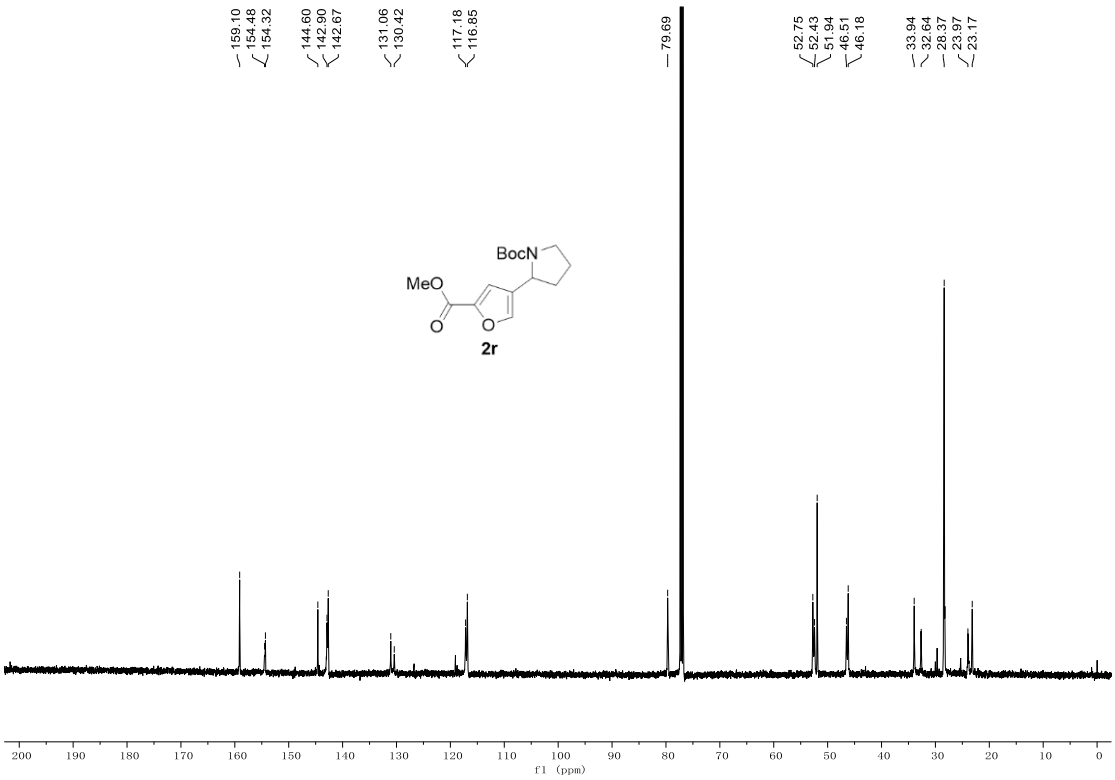
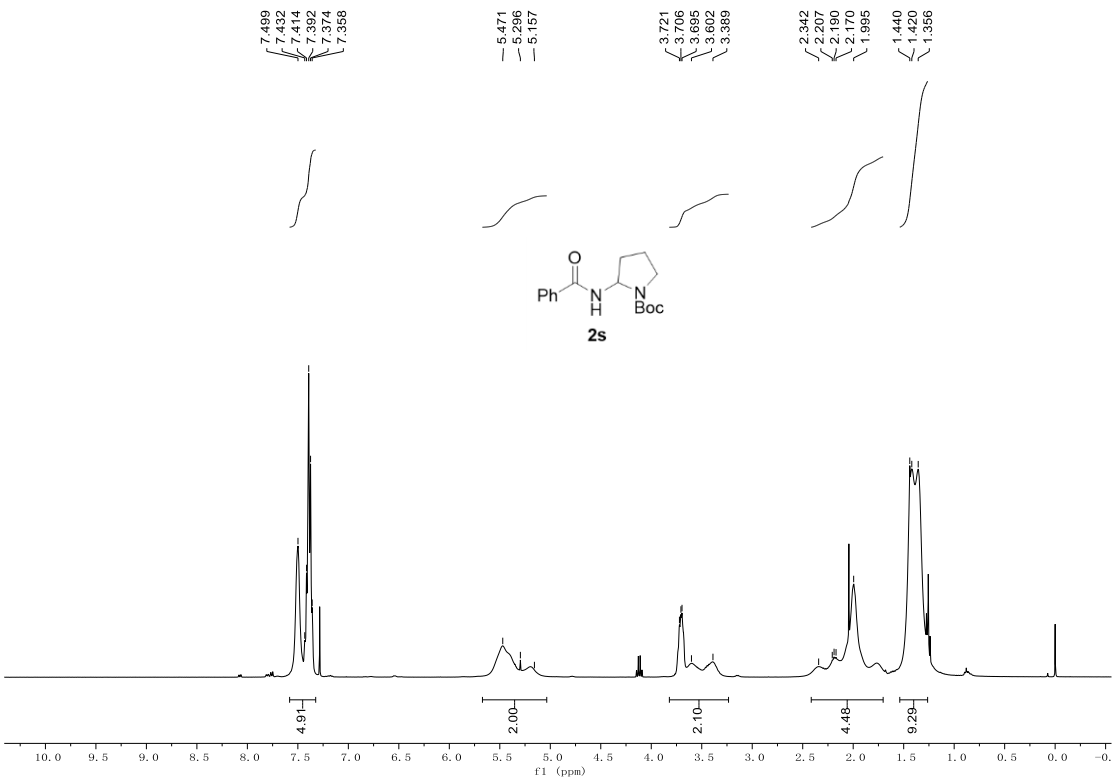
4.891
4.775
3.887
3.496
3.410
2.259
2.243
2.221
2.206
1.934
1.923
1.909
1.896
1.869
1.456
1.359
BocN
MeO
O
O
2r
0.95
0.99
1.00
3.14
2.05
1.07
3.46
4.12
5.14
f1 (ppm)


159.10
154.48
154.32
144.60
142.90
142.67
131.06
130.42
117.18
116.85
79.69
52.75
52.43
51.94
46.51
46.18
33.94
32.64
28.37
23.97
23.17
BocN
MeO
O
O
2r
f1 (ppm)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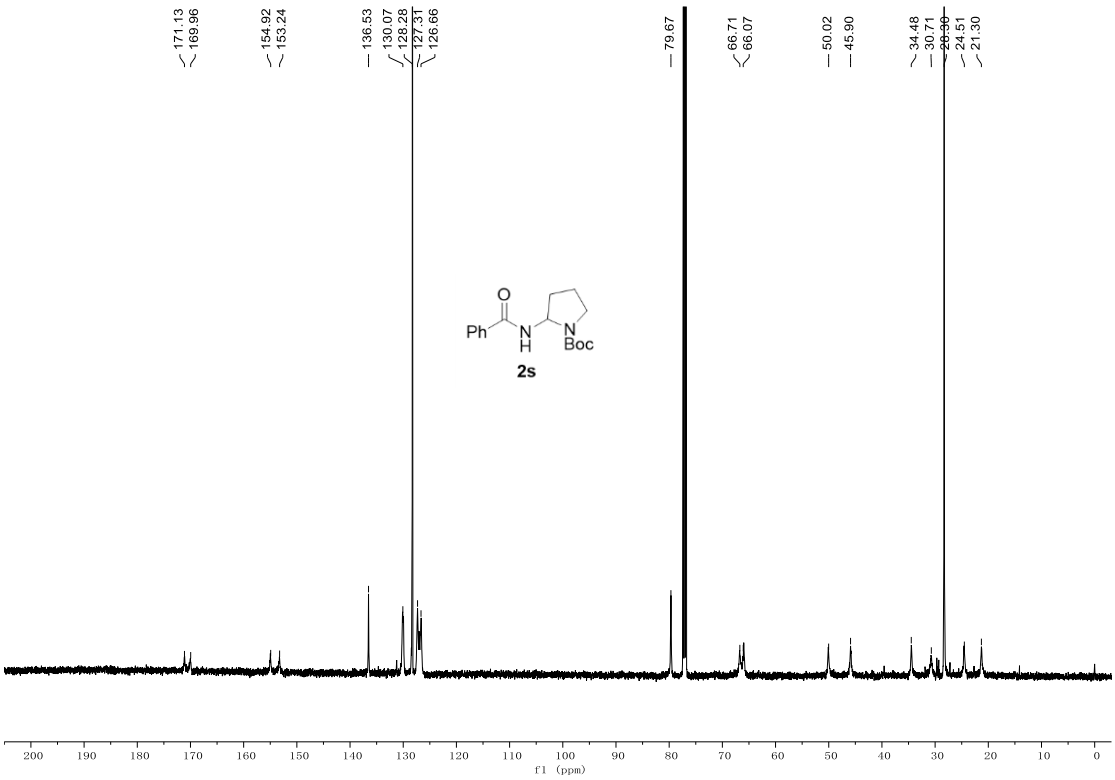
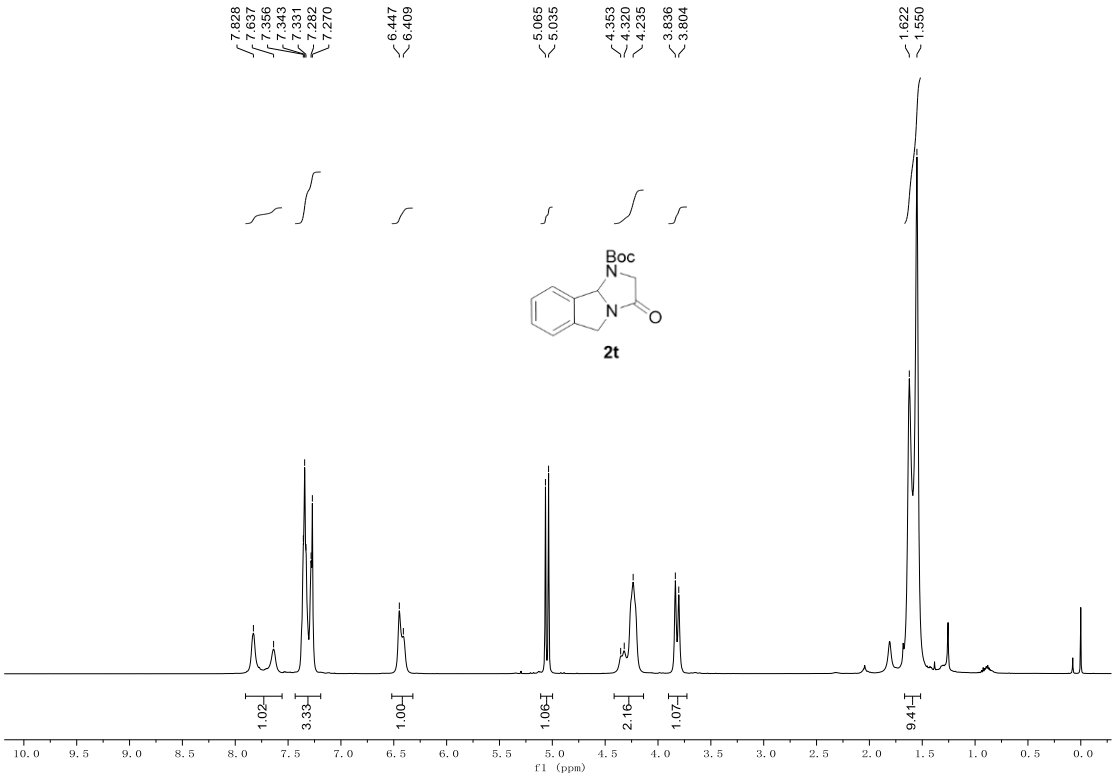
7.414
7.392
7.374
7.358
5.471
5.296
5.157
3.721
3.706
3.695
3.602
3.389
2.342
2.207
2.190
2.170
1.995
1.440
1.420
1.356
Ph
O
N
H
N
Boc
2s
4.91
2.00
2.10
4.48
9.29
f1 (ppm)


171.13
169.96
154.92
153.24
136.53
130.07
128.28
127.31
126.66
79.67
66.71
66.07
50.02
45.90
34.48
30.71
28.30
24.51
21.30
Ph
N
H
O
N
Boc
2s
f1 (ppm)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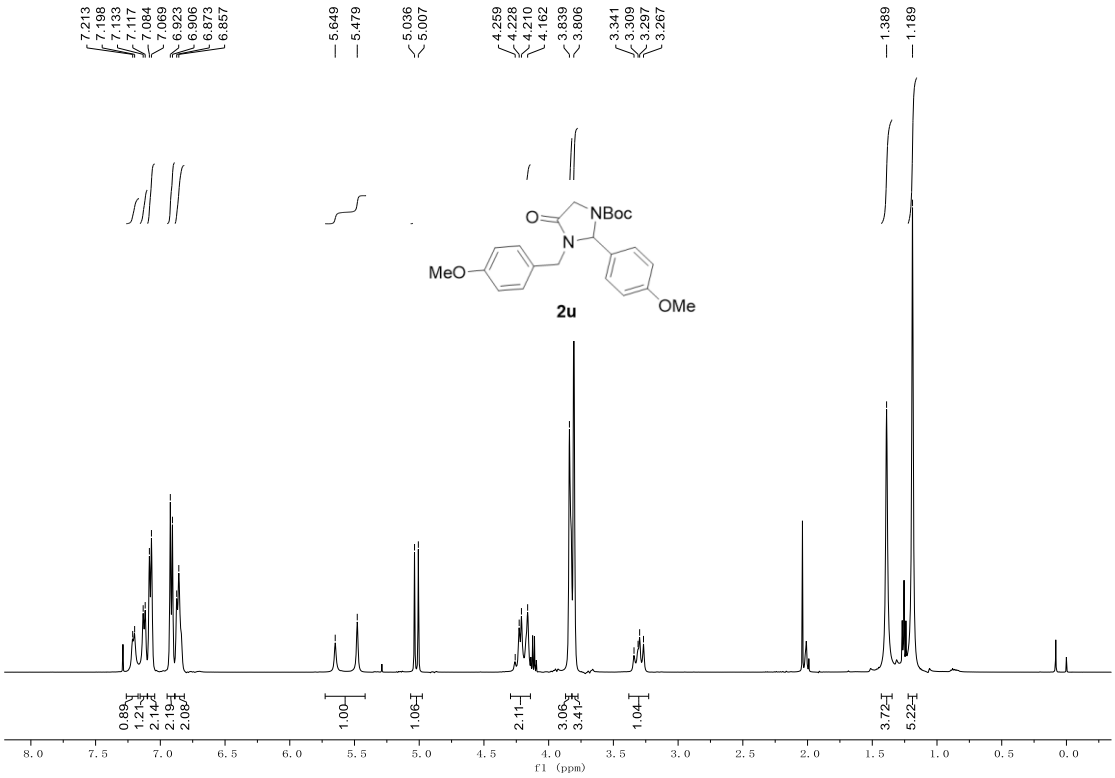
7.282
7.270
6.447
6.409
5.065
5.035
4.353
4.320
4.235
3.836
3.804
1.622
1.550
Boc
N
N
O
2t
1.02
3.33
1.00
1.06
2.16
1.07
9.41
f1 (ppm)


7.213
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7.133
7.117
7.084
7.069
6.923
6.906
6.873
6.857
5.649
5.479
5.036
5.007
4.259
4.228
4.210
4.162
3.839
3.806
3.341
3.309
3.297
3.267
1.389
1.189
NBoc
O
N
MeO
OMe
2u
0.89
1.21
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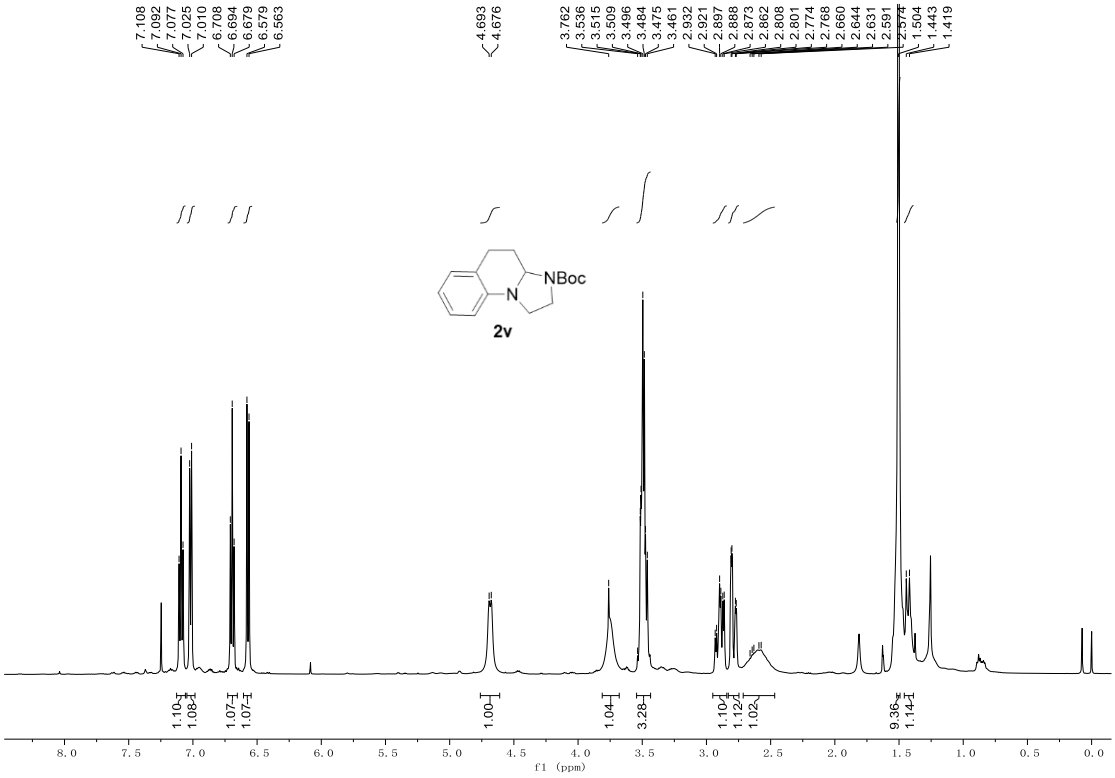
1.00
1.06
2.11
3.06
3.41
1.04
3.72
5.22
f1 (ppm)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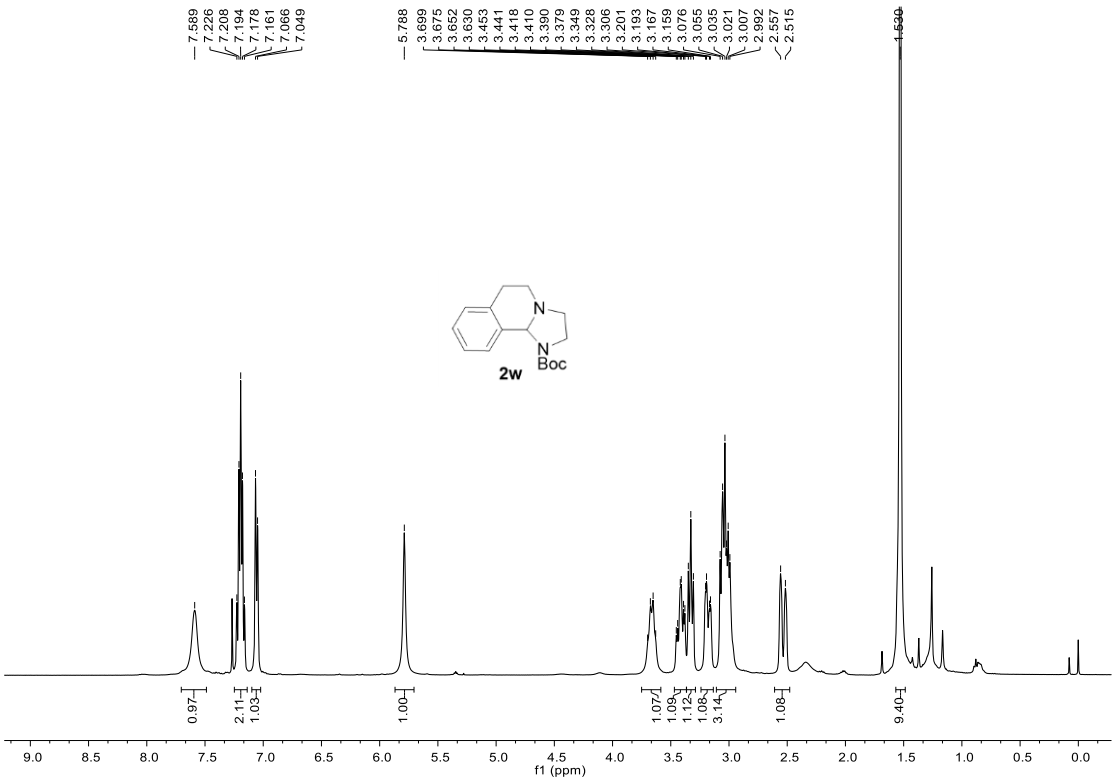
6.679
6.579
6.563
4.693
4.676
3.762
3.536
3.515
3.509
3.496
3.484
3.475
3.461
2.932
2.921
2.897
2.888
2.873
2.862
2.808
2.801
2.774
2.768
2.660
2.644
2.631
2.591
1.504
1.443
1.419
NBoc
N
2v
1.10
1.08
1.07
1.07
1.00
1.04
3.28
1.10
1.12
1.02
9.36
1.14
f1 (ppm)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7.194
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7.161
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7.049
5.788
3.699
3.675
3.652
3.630
3.453
3.441
3.418
3.410
3.390
3.379
3.349
3.328
3.306
3.201
3.193
3.167
3.159
3.076
3.055
3.035
3.021
3.007
2.992
2.557
2.515
1.530
N
N
Boc
2w
0.97
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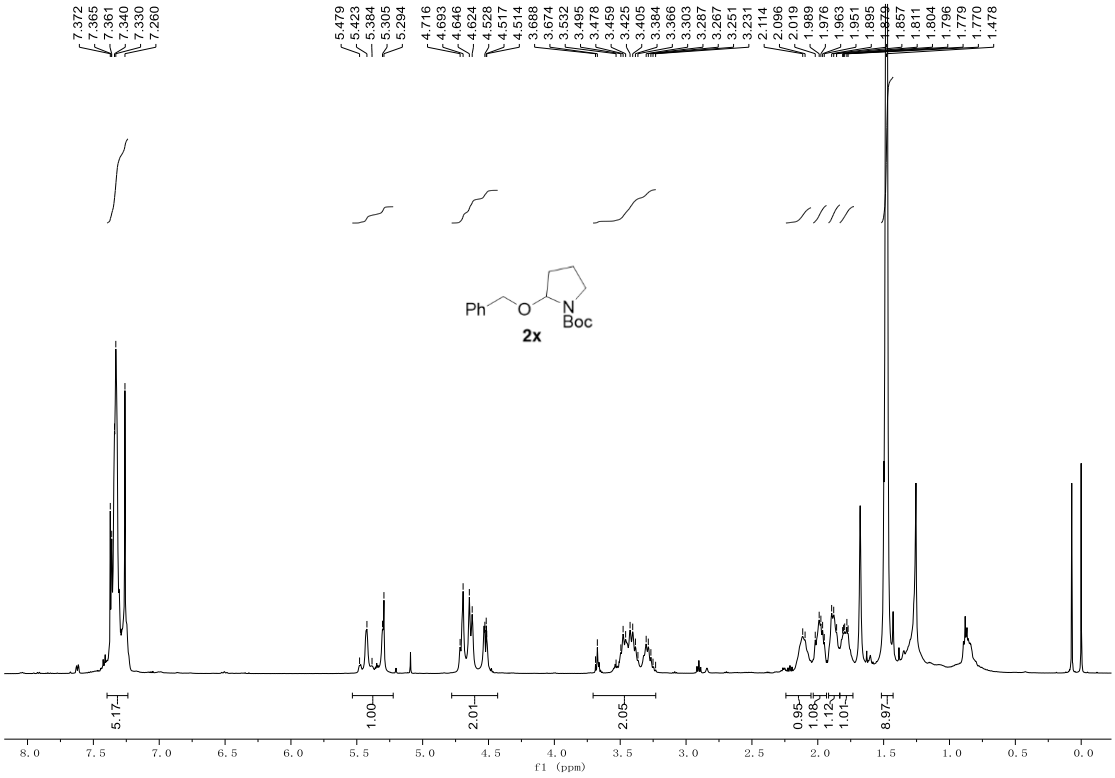
1.00
1.07
1.09
1.12
1.06
3.14
1.08
9.40
f1 (ppm)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7.260
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5.423
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5.305
5.294
4.716
4.693
4.646
4.624
4.528
4.517
4.514
3.688
3.674
3.532
3.495
3.478
3.459
3.425
3.405
3.384
3.366
3.303
3.287
3.267
3.251
3.231
2.114
2.096
2.019
1.989
1.976
1.963
1.951
1.895
1.873
1.857
1.811
1.804
1.796
1.779
1.770
1.478
Ph
O
N
Boc
2x
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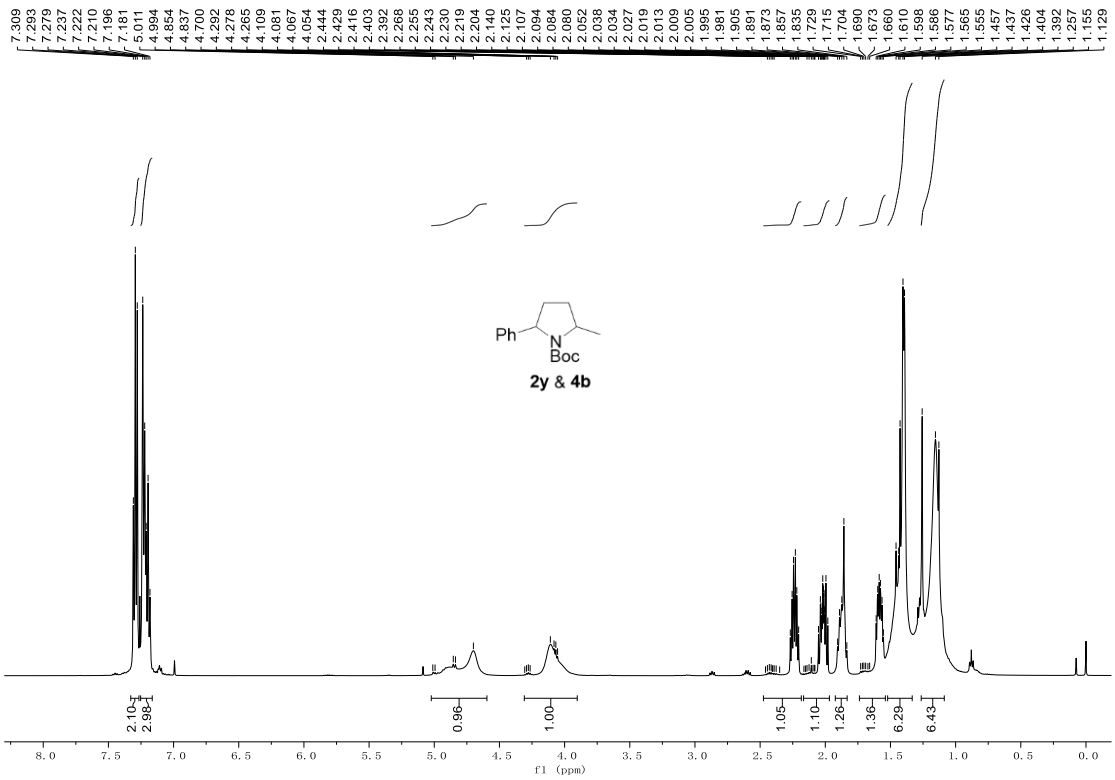
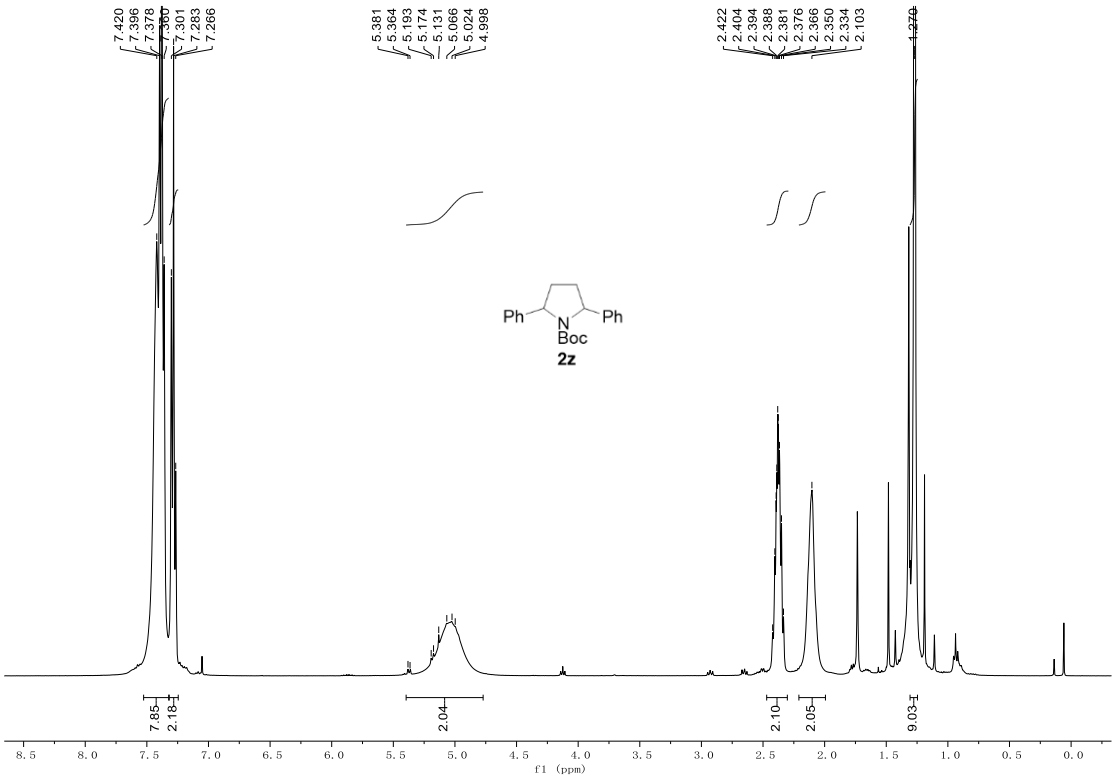
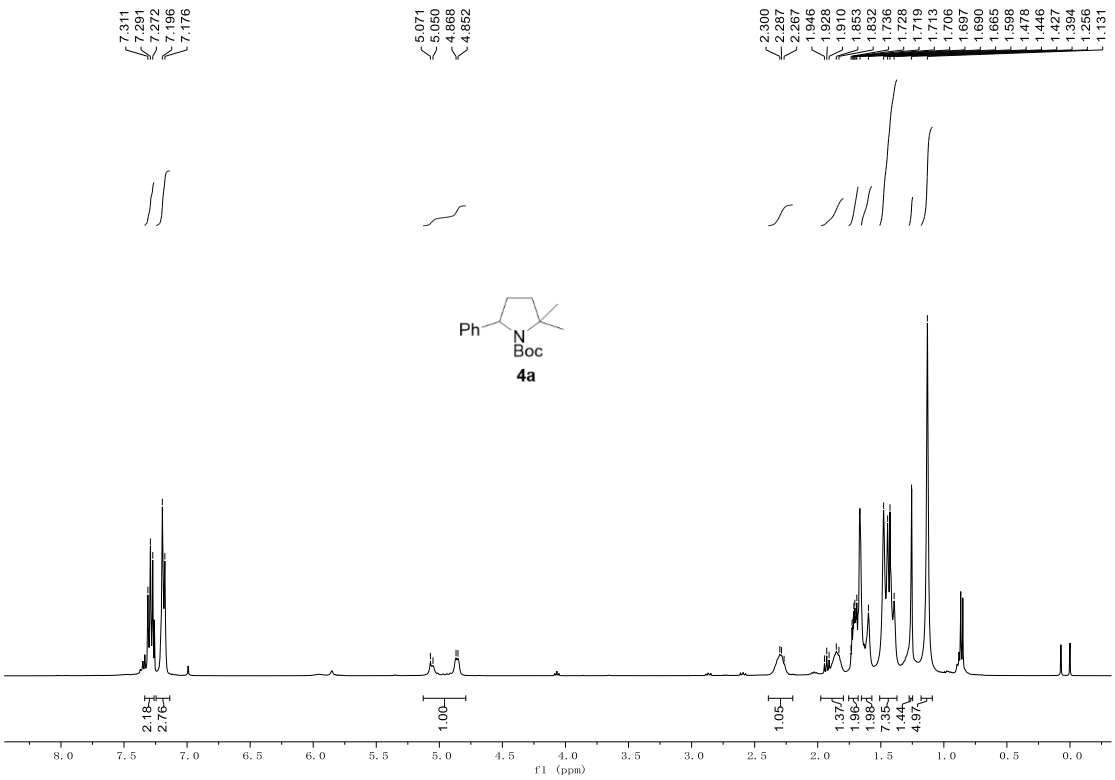
1.00
2.01
2.05
0.95
1.08
1.12
1.01
8.97
f1 (ppm)


Ph
N
Boc
2y & 4b
f1 (ppm)


Ph
Ph
N
Boc
2z
f1 (ppm)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7.196
7.176
5.071
5.050
4.868
4.852
2.300
2.287
2.267
1.946
1.928
1.910
1.853
1.832
1.736
1.728
1.719
1.713
1.706
1.697
1.690
1.665
1.598
1.478
1.446
1.427
1.394
1.256
1.131
Ph
N
Boc
4a
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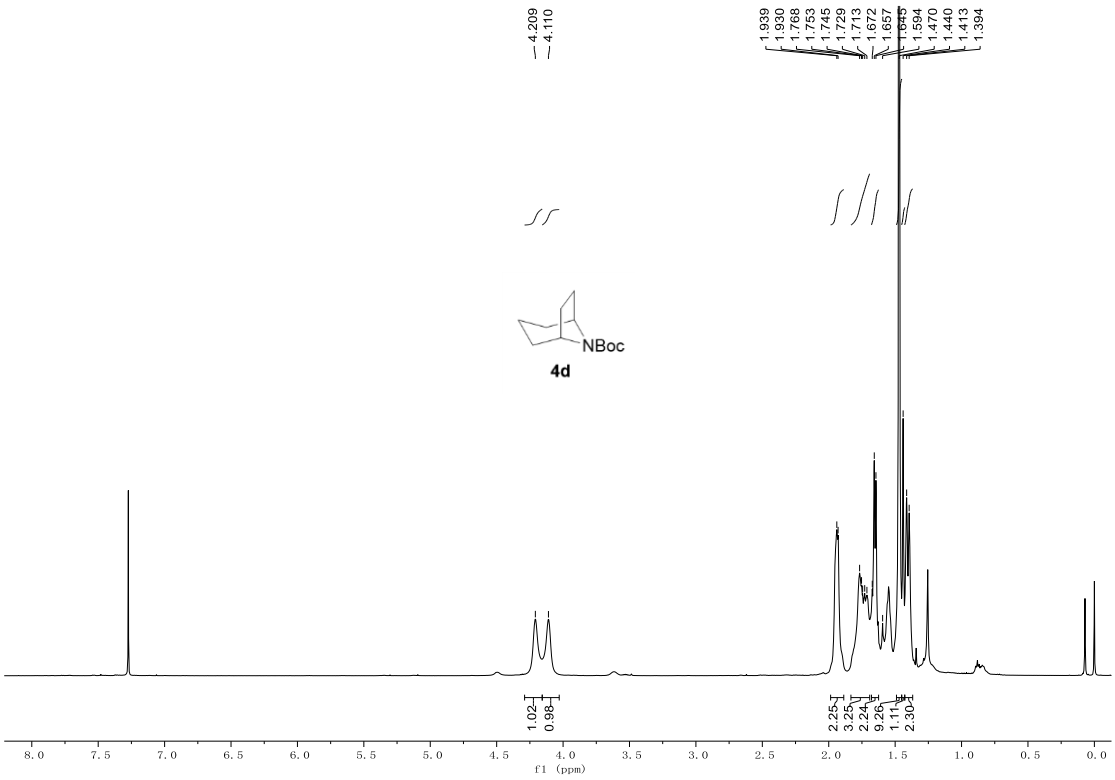
1.00
1.05
1.37
1.96
1.98
7.35
1.44
4.97
f1 (ppm)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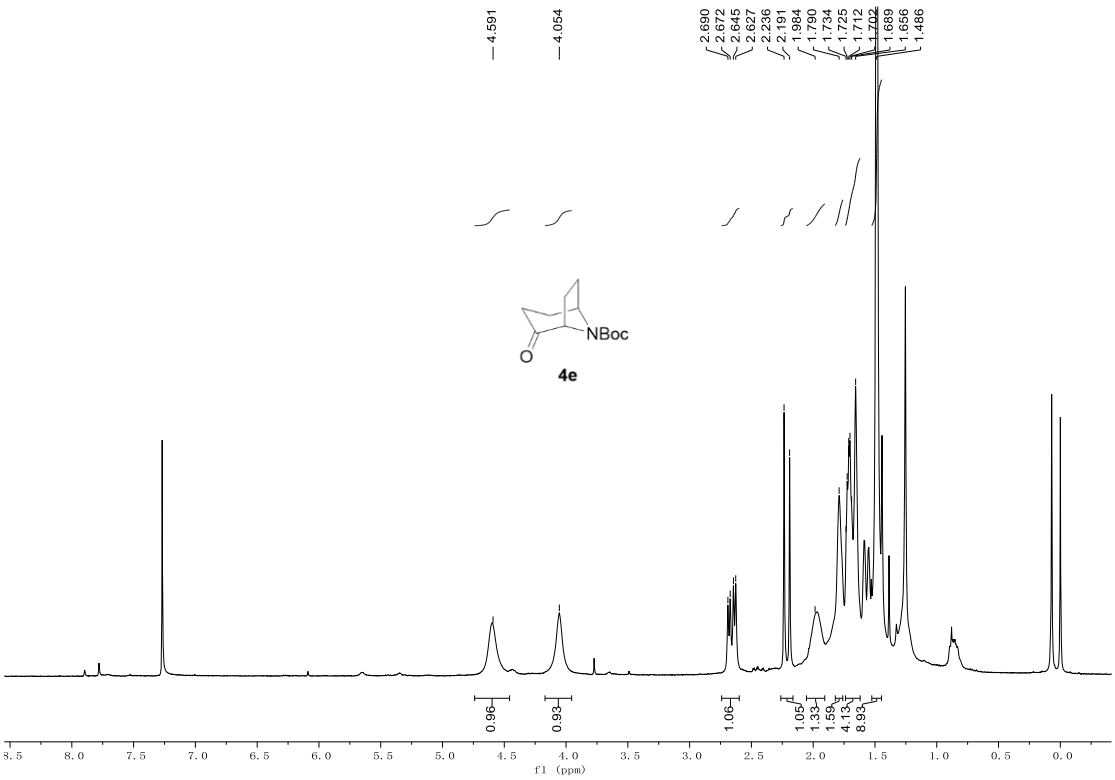
1.729
1.713
1.672
1.657
1.645
1.594
1.470
1.440
1.413
1.394
NBoc
4d
1.02
0.98
2.25
3.25
2.24
9.26
1.11
2.30
f1 (ppm)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4.054
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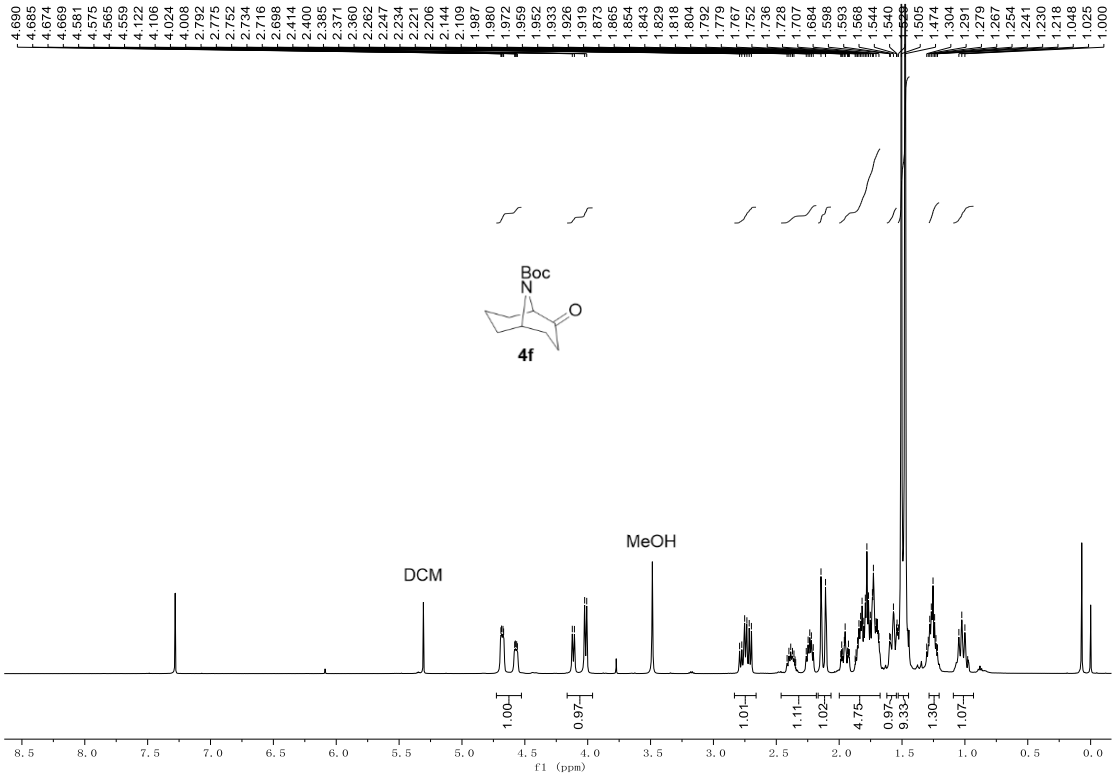
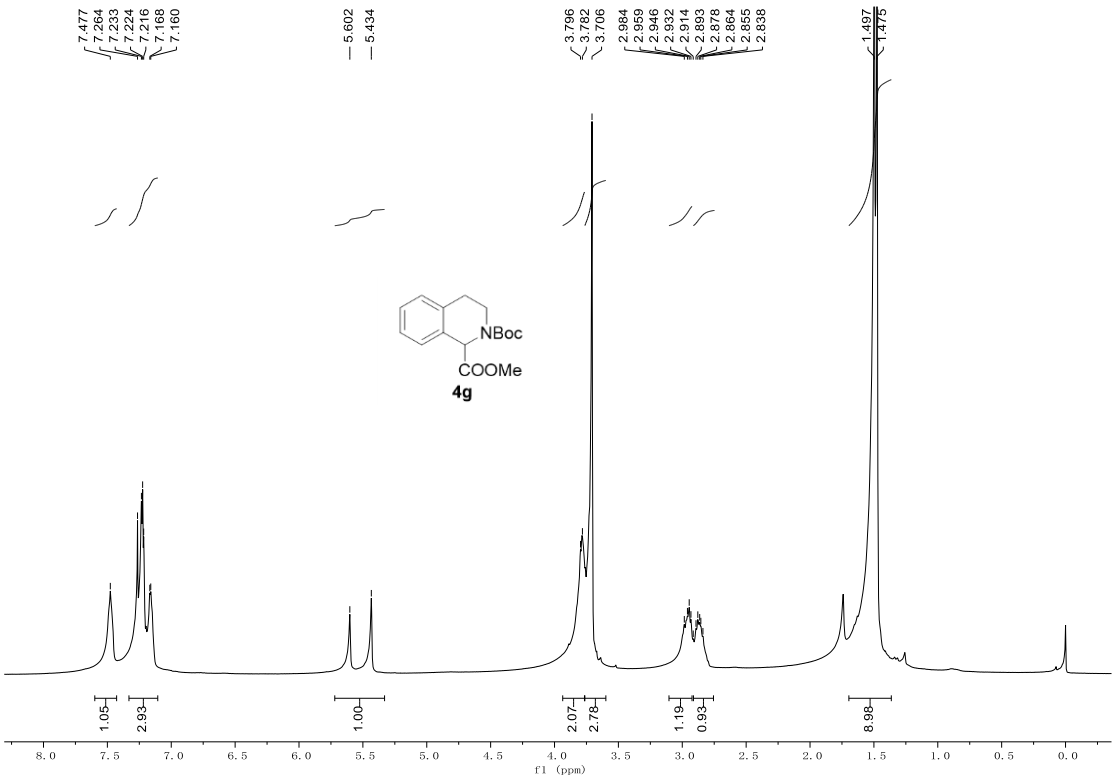
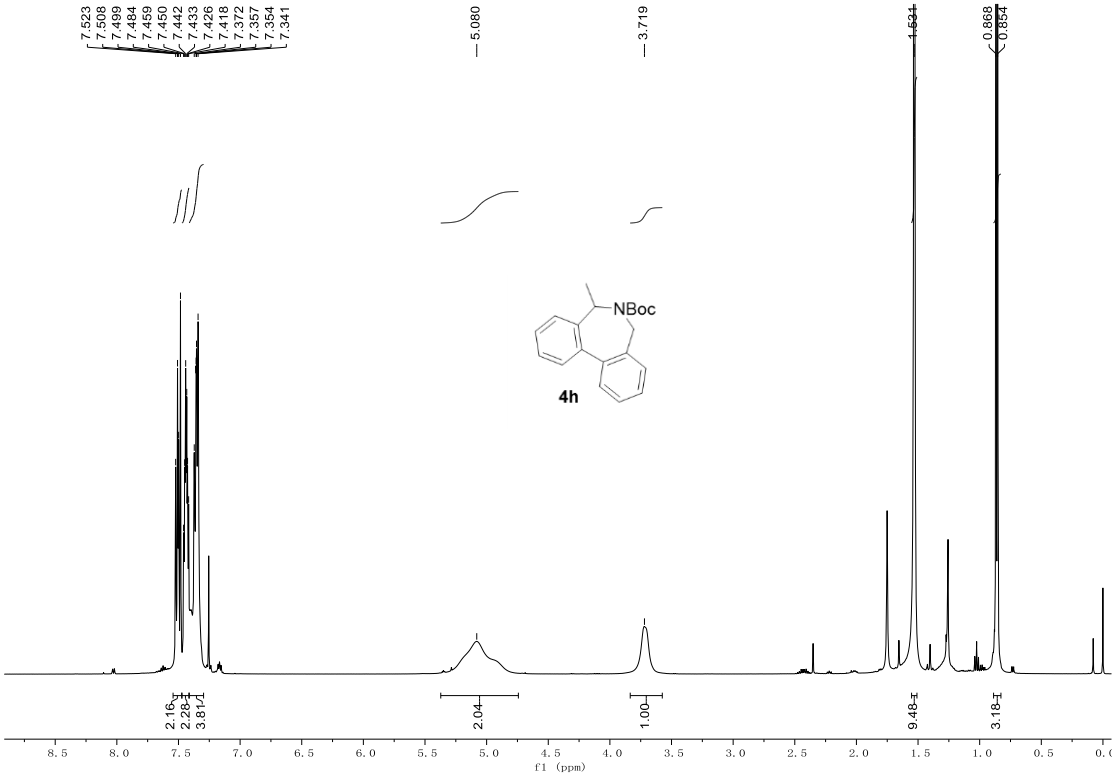
2.672
2.645
2.627
2.236
2.191
1.984
1.790
1.734
1.725
1.712
1.702
1.689
1.656
1.486
NBoc
O
4e
0.96
0.93
1.06
1.05
1.33
1.59
4.13
8.93
f1 (ppm)


Boc
N
O
4f
DCM
MeOH
1.00
0.97
1.01
1.11
1.02
4.75
0.97
9.33
1.30
1.07
f1 (ppm)


7.477
7.264
7.233
7.224
7.216
7.168
7.160
5.602
5.434
3.796
3.782
3.706
2.984
2.959
2.946
2.932
2.914
2.893
2.878
2.864
2.855
2.838
1.497
1.475
NBoc
COOMe
4g
1.05
2.93
1.00
2.07
2.78
1.19
0.93
8.98
f1 (ppm)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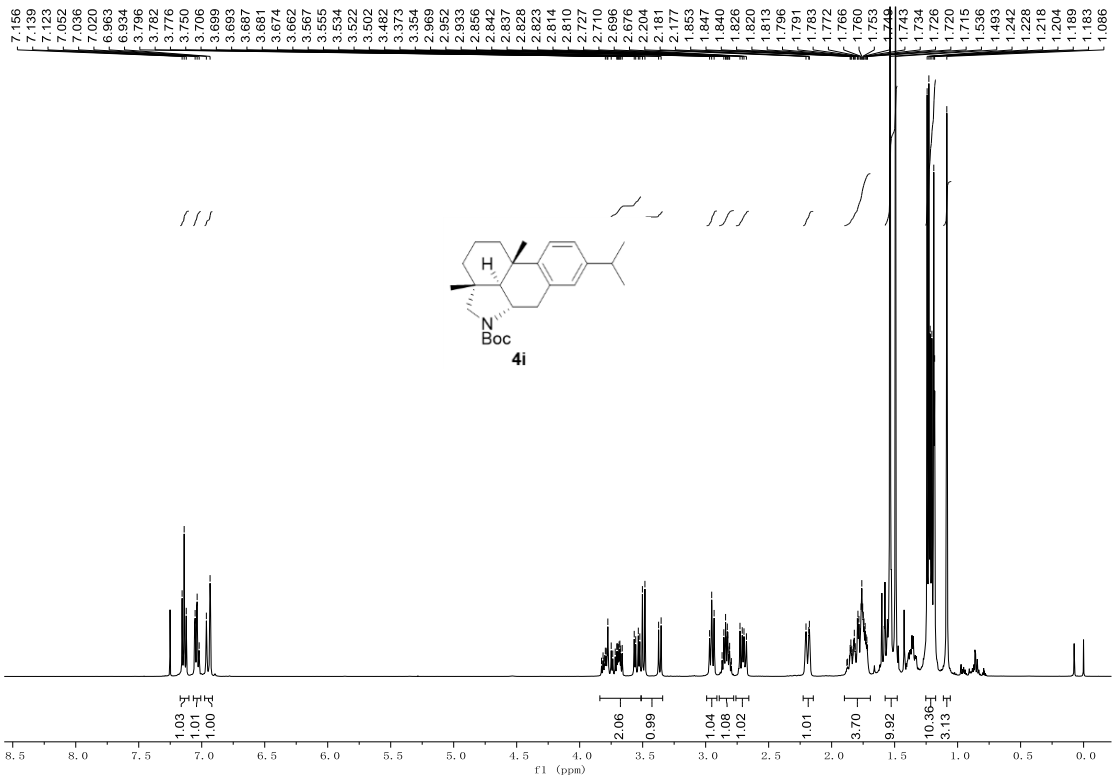
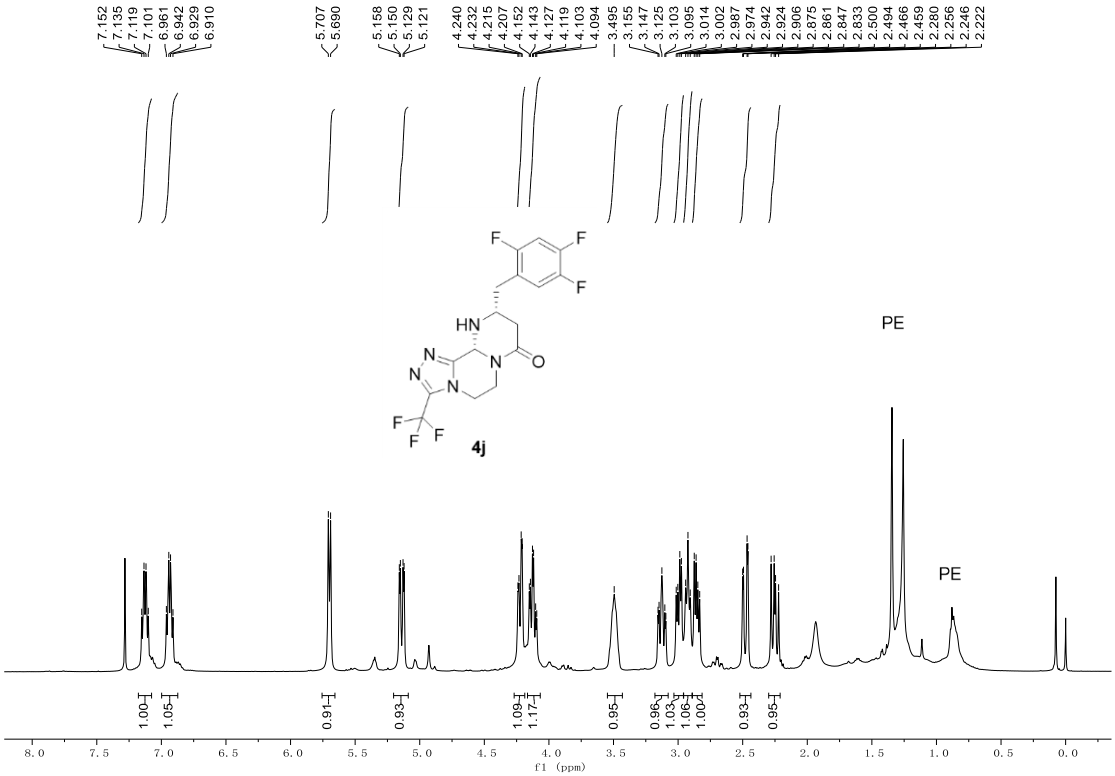
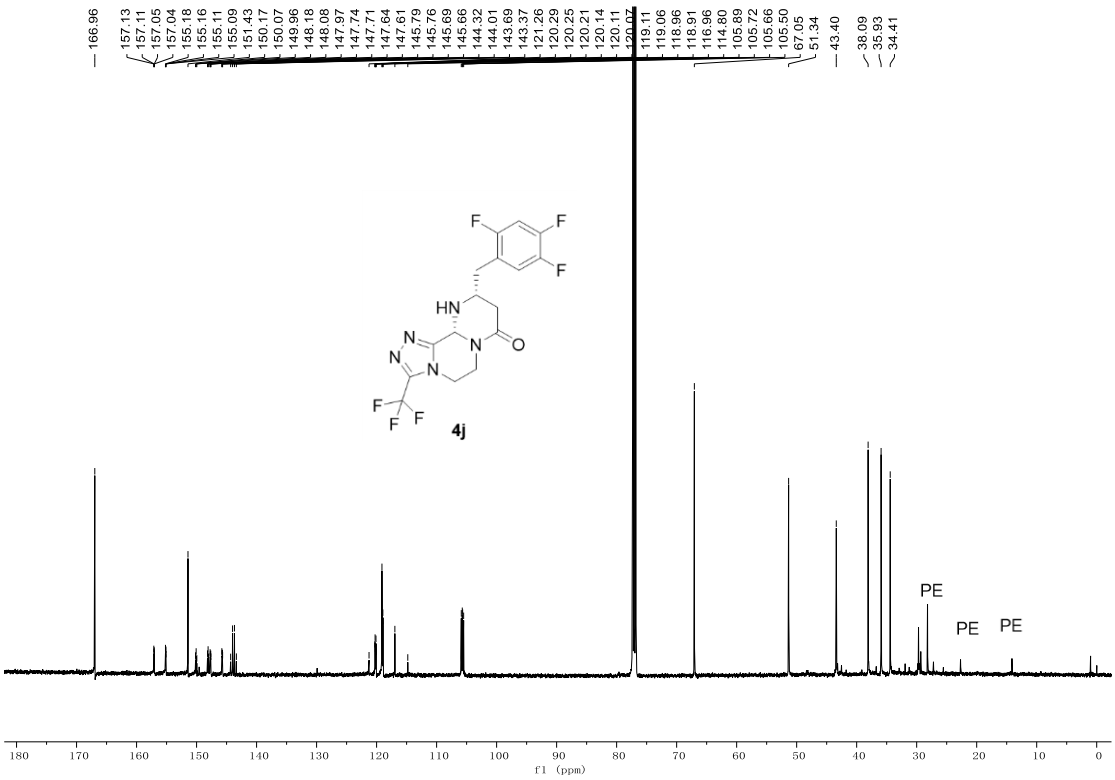
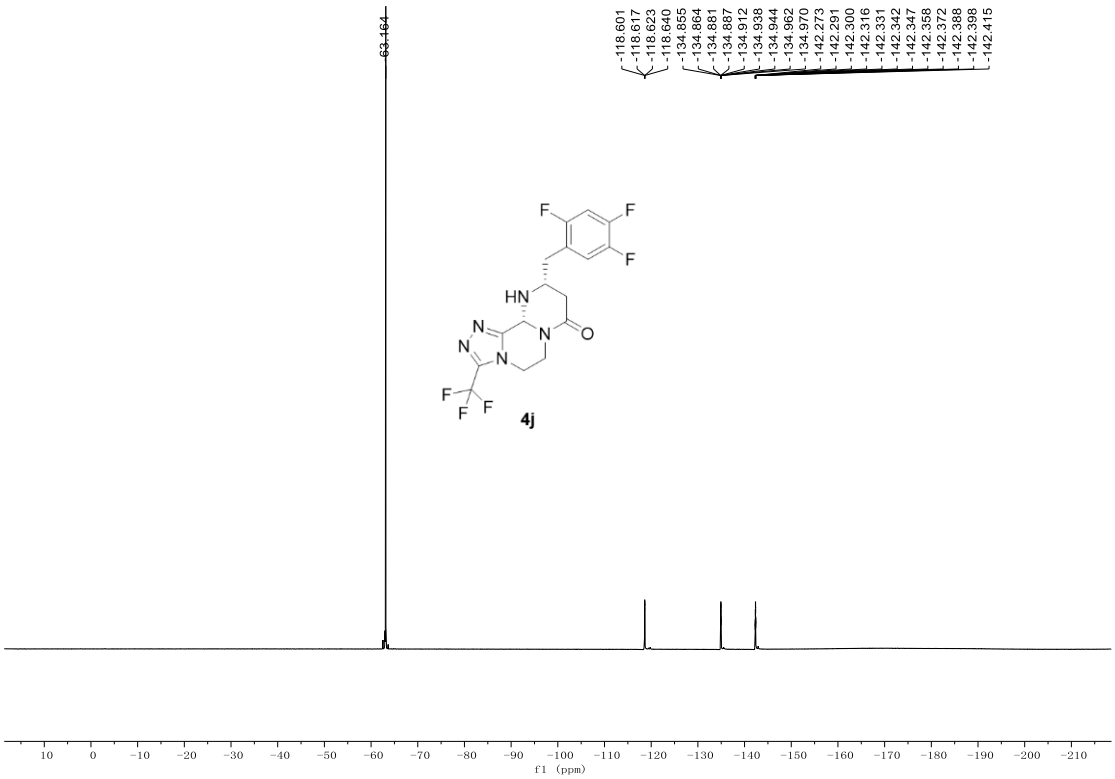
7.508
7.499
7.484
7.459
7.450
7.442
7.433
7.426
7.418
7.372
7.357
7.354
7.341
5.080
3.719
1.531
0.868
0.854
NBoc
4h
2.16
2.26
3.81
2.04
1.00
9.48
3.18
f1 (ppm)


H
N
Boc
4i
f1 (ppm)


F
F
F
HN
N
N
N
O
F
F
F
4j
PE
PE
f1 (ppm)


166.96
157.13
157.11
157.05
157.04
155.18
155.16
155.11
155.09
151.43
150.17
150.07
149.96
148.18
148.08
147.97
147.74
147.71
147.64
147.61
145.79
145.76
145.69
145.66
144.32
144.01
143.69
143.37
121.26
120.29
120.25
120.21
120.14
120.11
120.07
119.11
119.06
118.96
118.91
116.96
114.80
105.89
105.72
105.66
105.50
67.05
51.34
43.40
38.09
35.93
34.41
PE
PE
PE
4j
f1 (ppm)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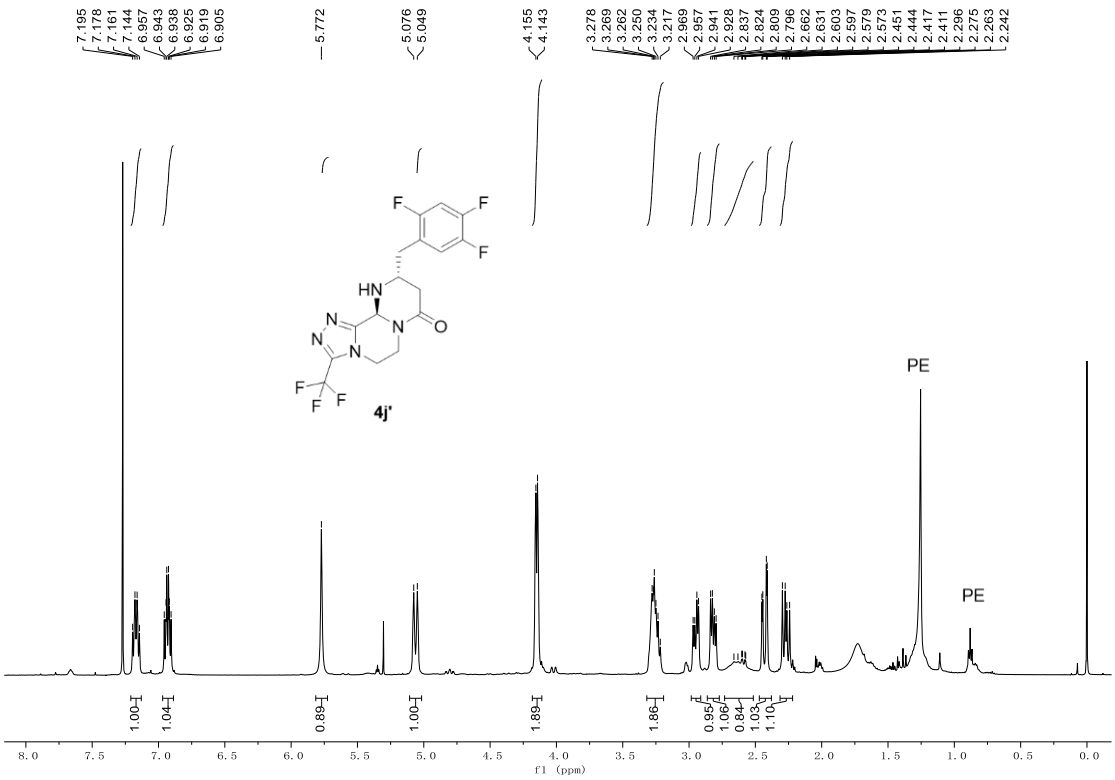
-118.617
-118.623
-118.640
-134.855
-134.864
-134.881
-134.887
-134.912
-134.938
-134.944
-134.962
-134.970
-142.273
-142.291
-142.300
-142.316
-142.331
-142.342
-142.347
-142.358
-142.372
-142.388
-142.398
-142.415
4j
f1 (ppm)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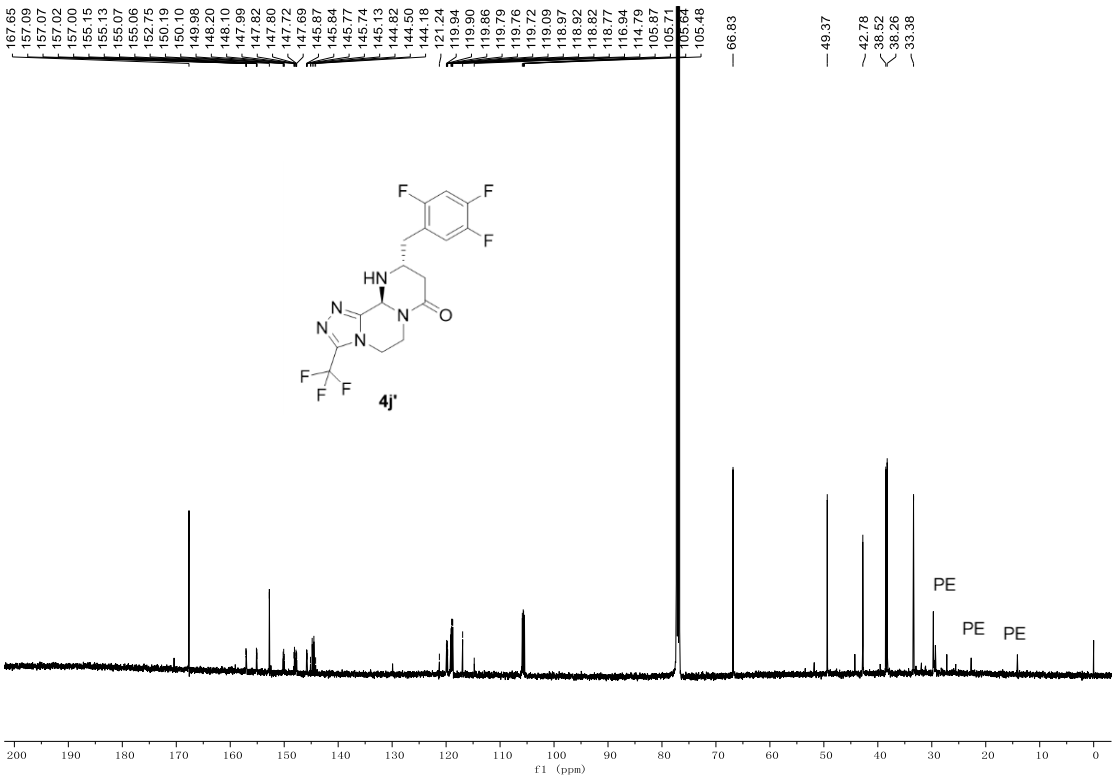
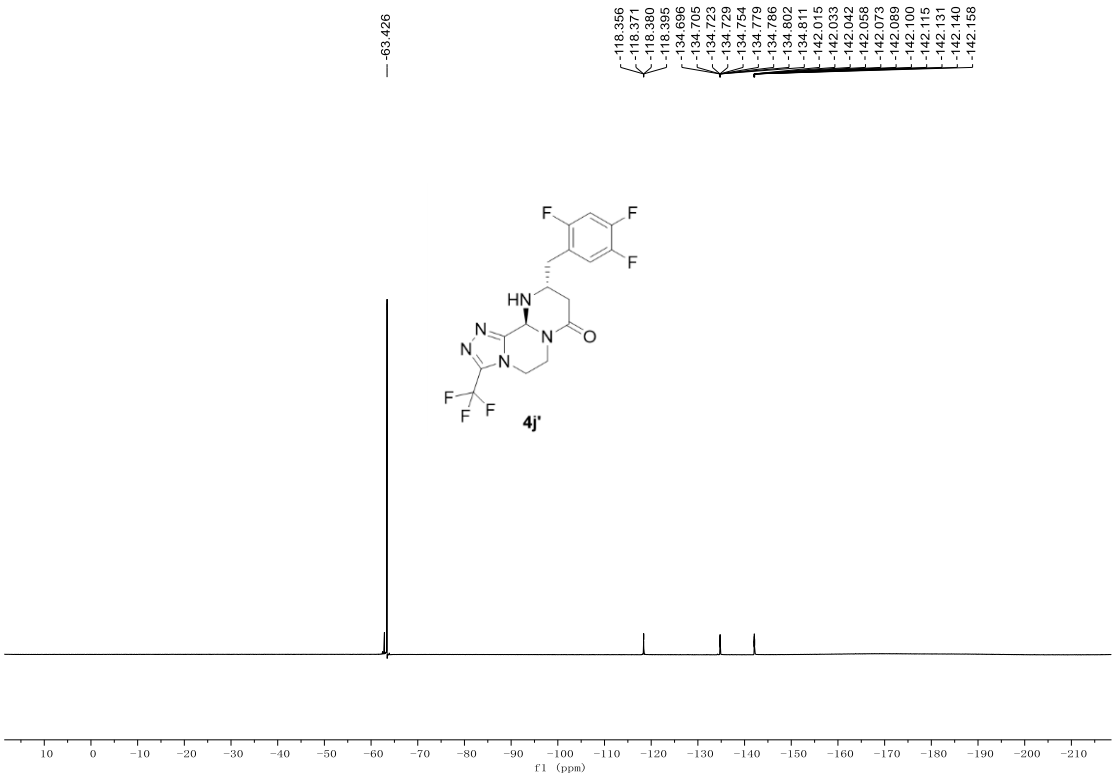
7.178
7.161
7.144
6.957
6.943
6.938
6.925
6.919
6.905
5.772
5.076
5.049
4.155
4.143
3.278
3.269
3.262
3.250
3.234
3.217
2.969
2.957
2.941
2.928
2.837
2.824
2.809
2.796
2.662
2.631
2.603
2.597
2.579
2.573
2.451
2.444
2.417
2.411
2.296
2.275
2.263
2.242
HN
N
N
N
O
F
F
F
F
F
F
4j'
PE
PE
1.00
1.04
0.89
1.00
1.89
1.86
0.95
1.06
0.84
1.03
1.10
f1 (ppm)


167.65
157.09
157.07
157.02
157.00
155.15
155.13
155.07
155.06
152.75
150.19
150.10
149.98
148.20
148.10
147.99
147.82
147.80
147.72
147.69
145.87
145.84
145.77
145.74
145.13
144.82
144.50
144.18
121.24
119.94
119.90
119.86
119.79
119.76
119.72
119.09
118.97
118.92
118.82
118.77
116.94
114.79
105.87
105.71
105.64
105.48
66.83
49.37
42.78
38.52
38.26
33.38
HN
N
N
N
O
F
F
F
F
F
F
4j'
PE
PE
PE
f1 (ppm)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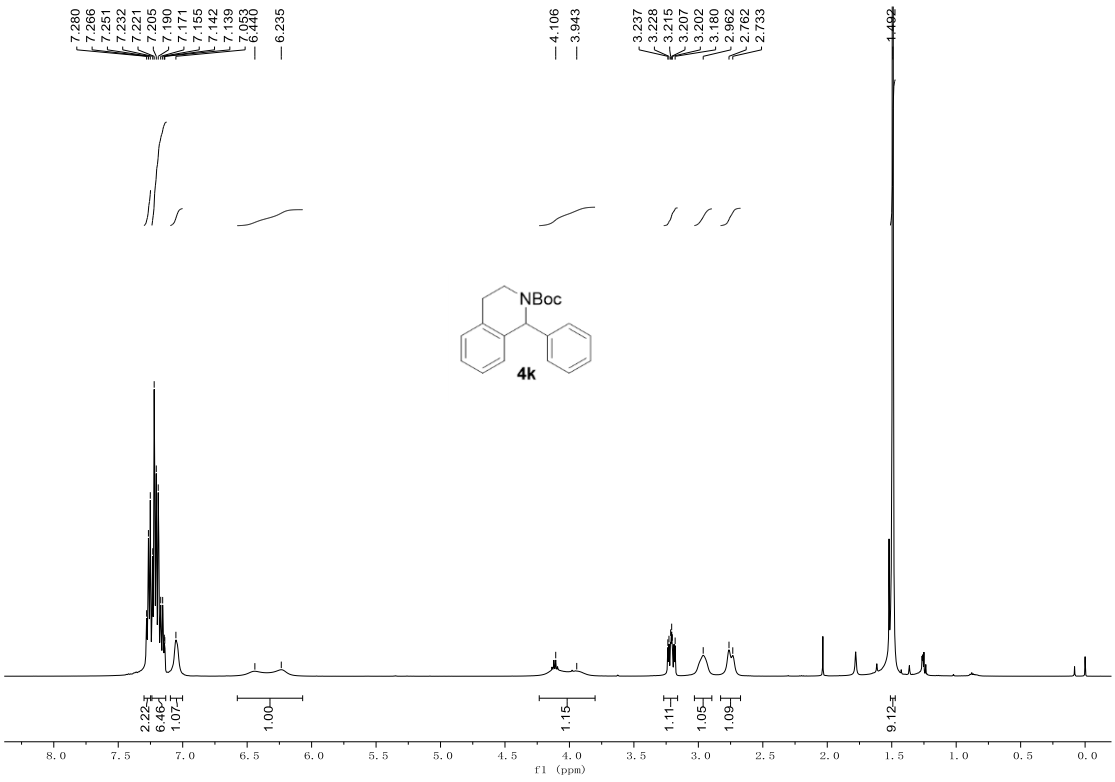
-118.371
-118.380
-118.395
-134.696
-134.705
-134.723
-134.729
-134.754
-134.779
-134.786
-134.802
-134.811
-142.015
-142.033
-142.042
-142.058
-142.073
-142.089
-142.100
-142.115
-142.131
-142.140
-142.158
F
F
F
HN
N
N
N
N
O
F
F
F
4j'
f1 (ppm)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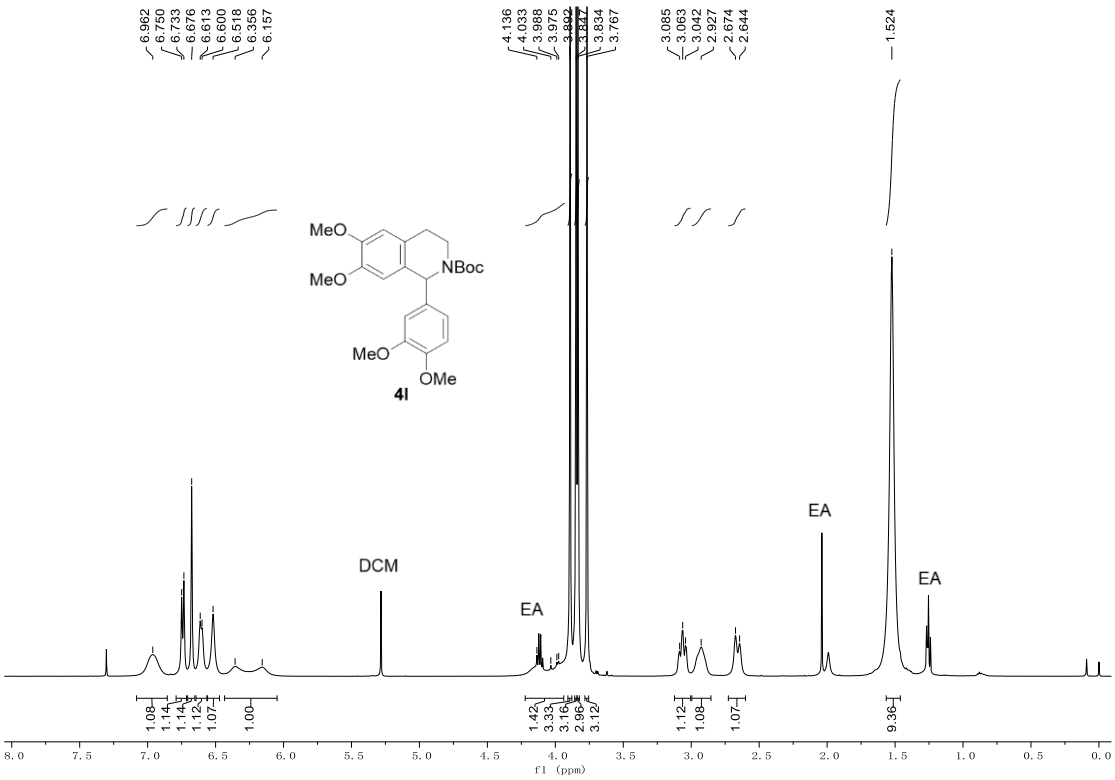
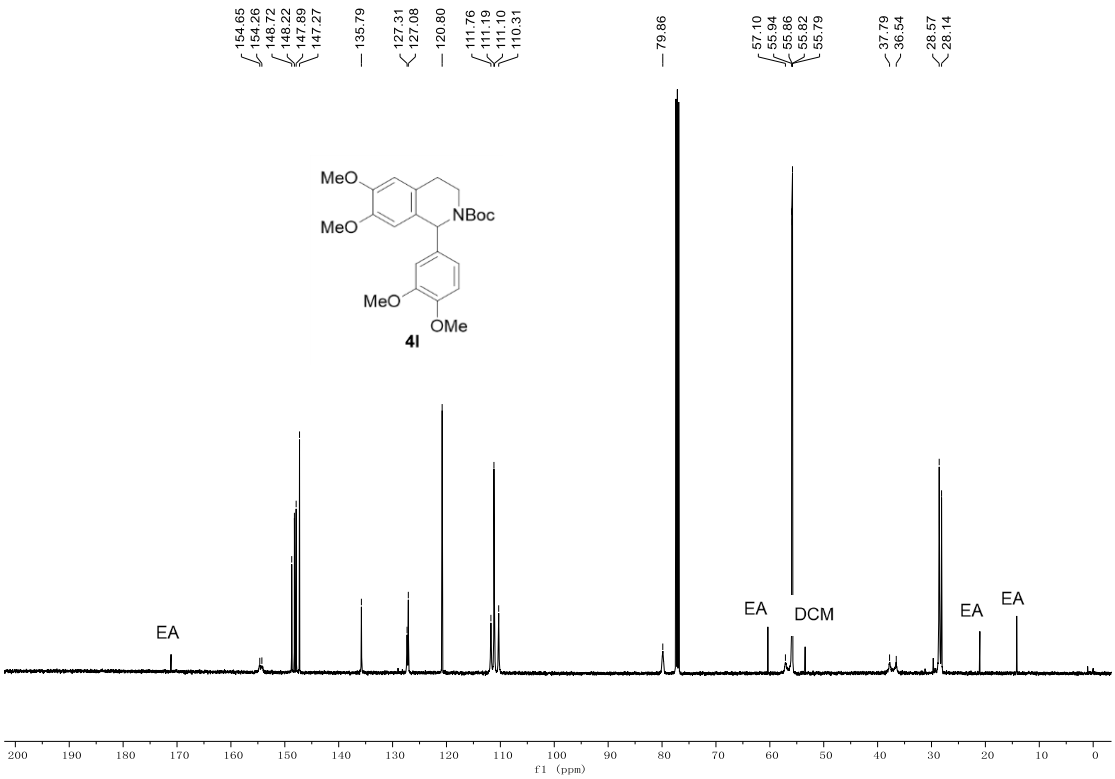
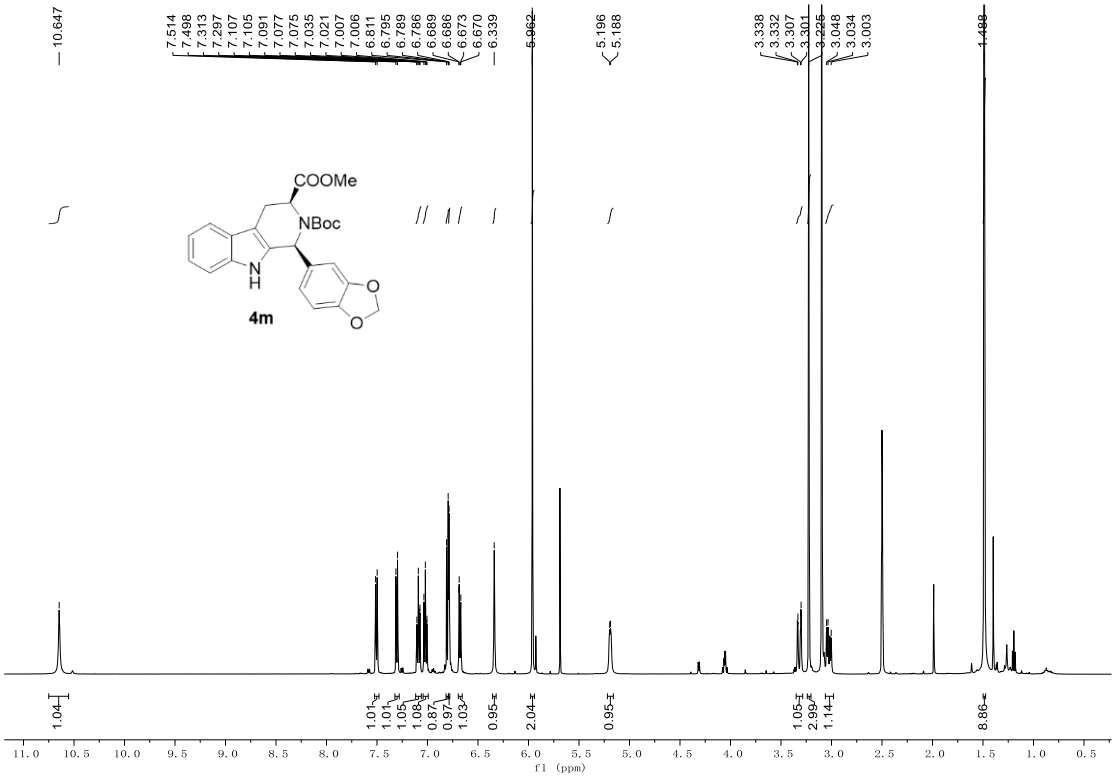
7.266
7.251
7.232
7.221
7.205
7.190
7.171
7.155
7.142
7.139
7.053
6.440
6.235
4.106
3.943
3.237
3.228
3.215
3.207
3.202
3.180
2.962
2.782
2.733
1.492
NBoc
4k
2.22
6.46
1.07
1.00
1.15
1.11
1.05
1.09
9.12
f1 (ppm)


6.962
6.750
6.733
6.676
6.613
6.600
6.518
6.356
6.157
4.136
4.033
3.988
3.975
3.834
3.767
3.085
3.063
3.042
2.927
2.674
2.644
1.524
MeO
MeO
NBoc
MeO
OMe
4l
DCM
EA
EA
EA
1.08
1.14
1.14
1.12
1.07
1.00
1.42
3.33
3.16
2.96
3.12
1.12
1.08
1.07
9.36
f1 (ppm)


154.65
154.26
148.72
148.22
147.89
147.27
135.79
127.31
127.08
120.80
111.76
111.19
111.10
110.31
79.86
57.10
55.94
55.86
55.82
55.79
37.79
36.54
28.57
28.14
MeO
MeO
NBoc
MeO
OMe
4l
EA
EA
DCM
EA
EA
f1 (ppm)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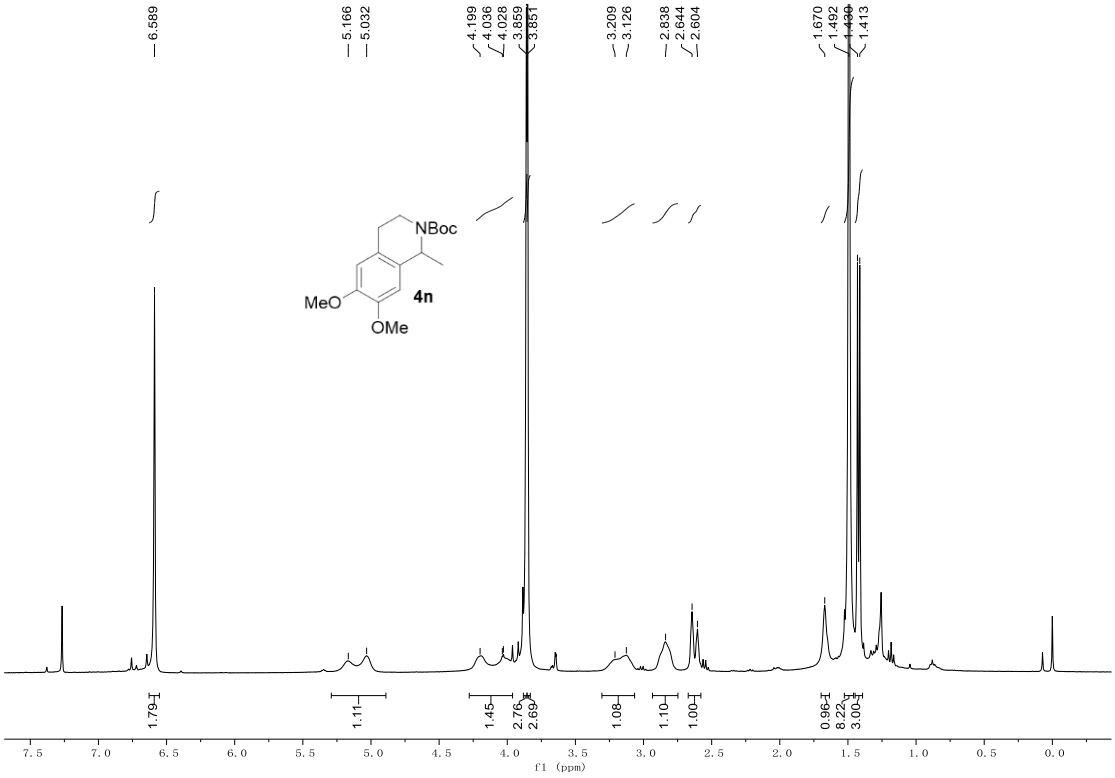
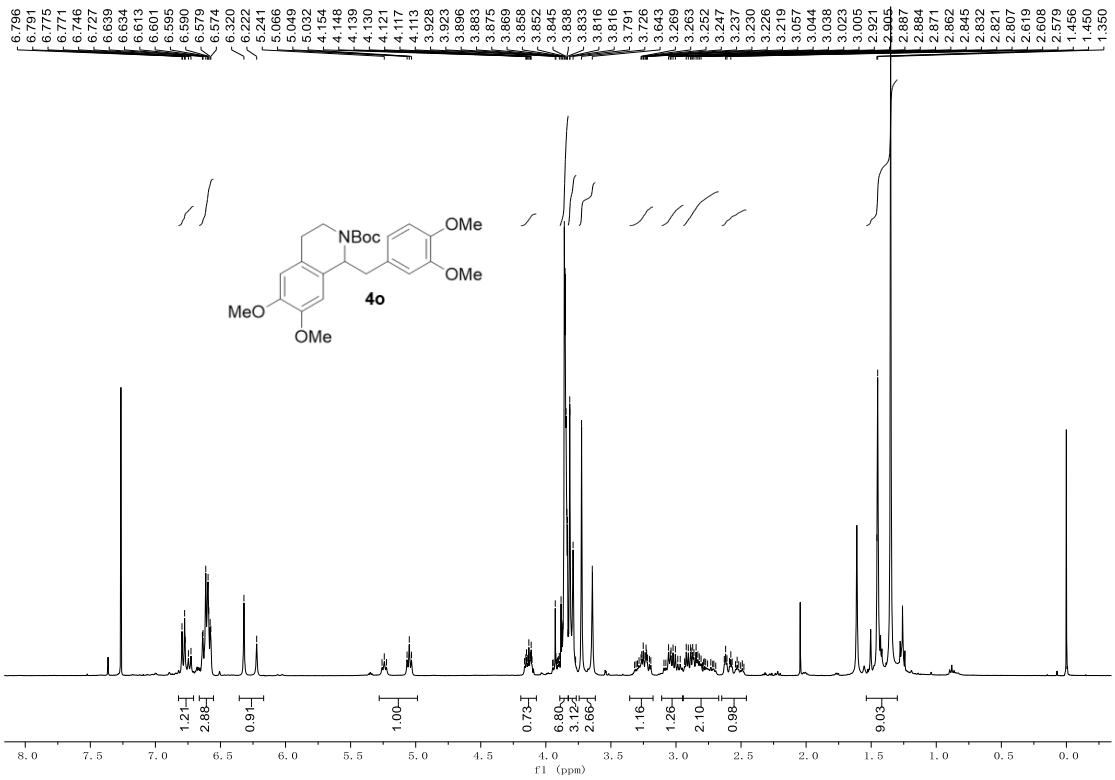
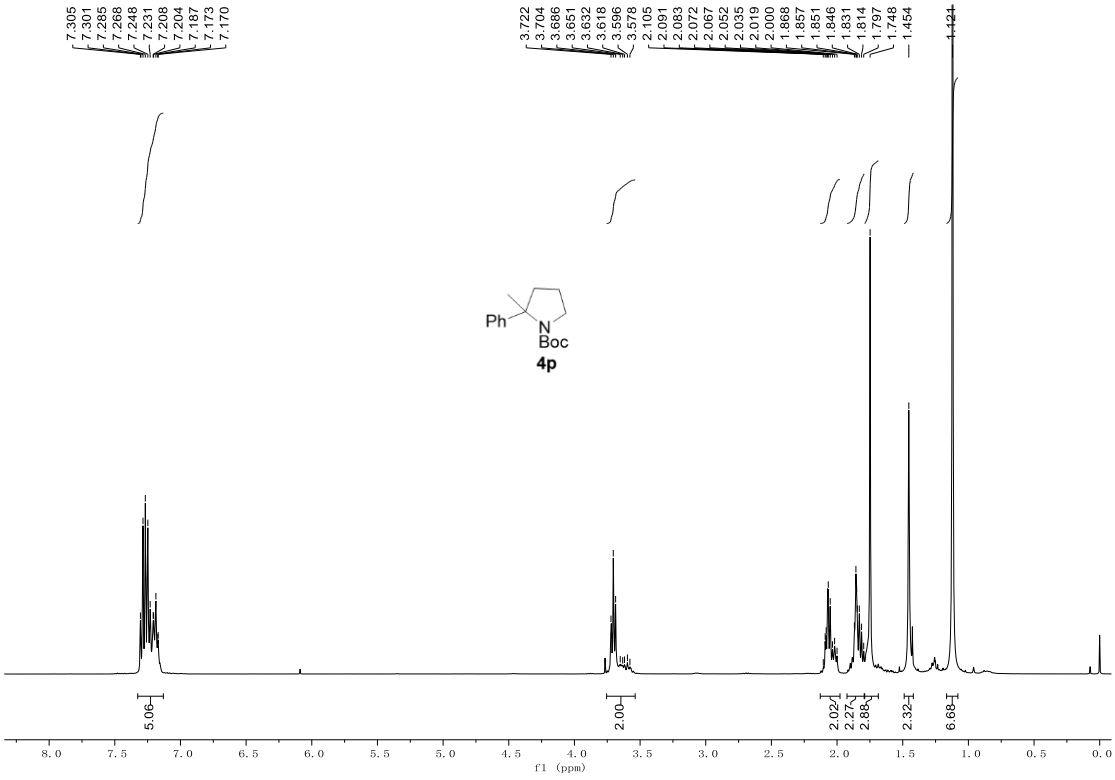
7.498
7.313
7.297
7.107
7.105
7.091
7.077
7.075
7.035
7.021
7.007
7.006
6.811
6.795
6.789
6.786
6.689
6.686
6.673
6.670
6.339
5.082
5.196
5.188
3.338
3.332
3.307
3.301
3.226
3.048
3.034
3.003
1.498
COOMe
NBoc
N
H
O
O
4m
1.04
1.01
1.01
1.05
1.08
0.87
0.97
1.03
0.95
2.04
0.95
1.05
2.99
1.14
8.86
f1 (ppm)


6.589
5.166
5.032
4.199
4.036
4.028
3.859
3.851
3.209
3.126
2.838
2.644
2.604
1.670
1.492
1.430
1.413
NBoc
MeO
OMe
4n
1.79
1.11
1.45
2.76
2.69
1.08
1.10
1.00
0.96
8.22
3.00
f1 (ppm)


NBoc
OMe
OMe
MeO
OMe
4o
f1 (ppm)


Ph
N
Boc
4p
f1 (ppm)