Supporting Information

for

Palladium-catalyzed Regioselective Azidation of Allylic C-H Bond under Atmospheric Pressure of Dioxygen **

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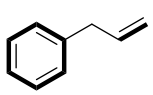
General procedure and compound's characterization

Experimental Procedure and Spectral data

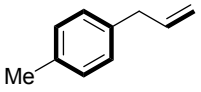
General Considerations.

^{1}H NMR spectra were recorded in $CDCl_3$ at 400 MHz and ^{13}C NMR spectra were recorded in $CDCl_3$ at 100 MHz respectively, and the chemical shifts (d) were referenced to TMS. GC–MS was obtained using electron ionization . HRMS was carried out on a MAT 95XP (Thermo). IR spectra were obtained as potassium bromide pellets or as liquid films between two potassium bromide pellets with a Brucker Vector 22 spectrometer. TLC was performed using commercially prepared 100-400 mesh silica gel plates (GF_{254}), and visualization was effected at 254 nm.

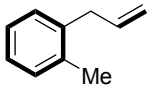
Substrates.



1a



1b



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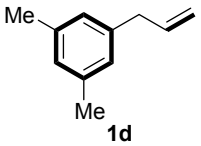

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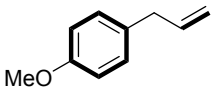
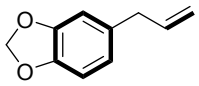
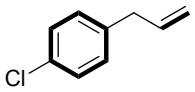


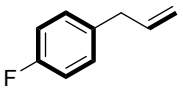
1e



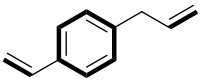
1f



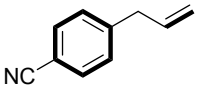
1g



1h



1i



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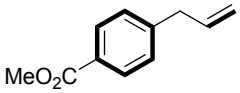

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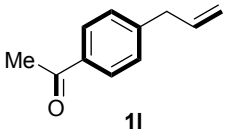
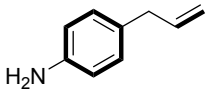


1l



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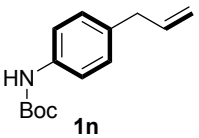
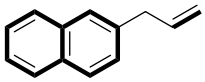
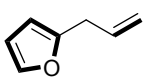


1n



1o



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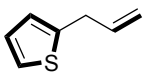
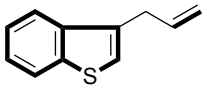
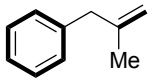


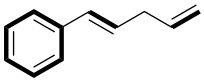
1q



1r



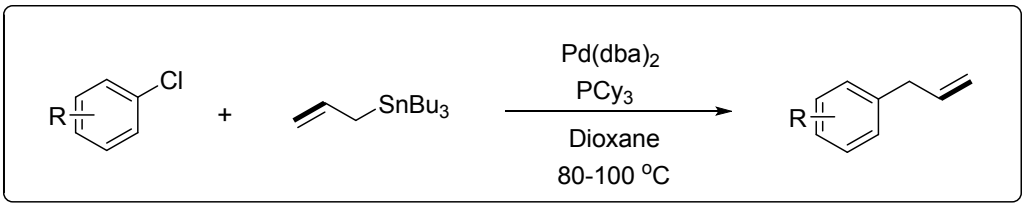
1s



1t

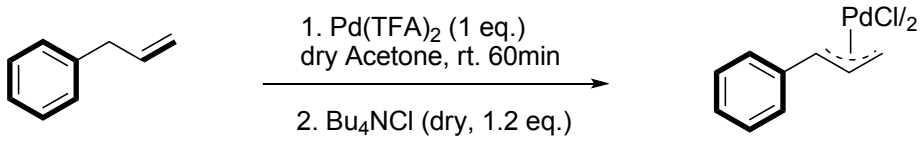
Substrates **1a**, **1e** and **1s** were purchased from Aldrich.

Substrates **1i-1n** were synthesized through Stille reaction[1]: An oven-dried 10 mL Schlenk flask under argon atmosphere was charged with $Pd(dba)_2$ (34.5 mg, 0.060 mmol, 0.03 equiv), PCy_3 (33.7 mg, 0.12 mmol, 0.06 equiv), CsF (668 mg, 4.40 mmol, 2.2 equiv), aryl halide (2.00 mmol, 1 equiv), and a stir bar. Allyltributyltin (644 μL, 2.10 mmol, 1.05 equiv) and dioxane (2 mL, 1.0M) were added via syringe. The mixture was stirred and heated to 80-100°C. Conversion was monitored by GC. When complete consumption of aryl halide was observed (8-24 h), the reaction was cooled to room temperature. The reaction mixture was diluted with saturated aqueous NH_4Cl (40 mL) and extracted with diethyl ether (2 x 40 mL). The combined organics were dried over $MgSO_4$. The mixture was filtered and concentrated for further purification.



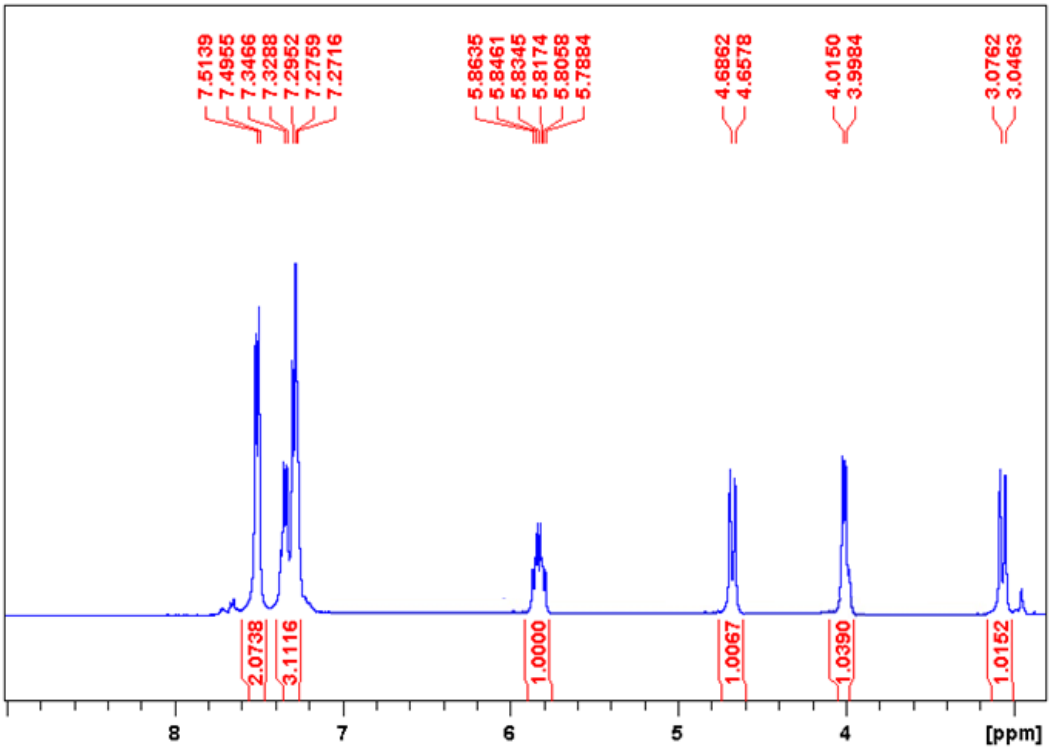
Other substrates were synthesized through Grignard reaction: The aryl bromide was reacted with magnesium in THF using I_2 as initiator. After finishing the reaction, the combined organics added to the THF solution of allyl bromide with magnetic stirring. After 1 hour, NH_4Cl (aq.) was added to the reaction mixture, washing with water and then concentrated for further purification.

Synthesis of complex 6 [2]:

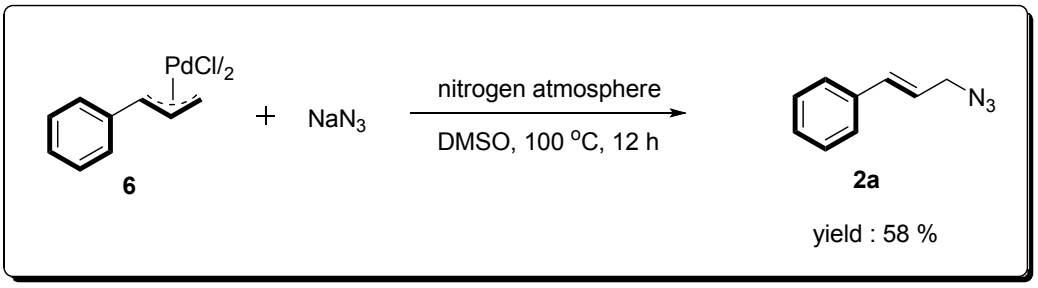


Bis[chloro(1,2,3-trihapto-allylbenzene)palladium(II)], was synthesized using a literature procedure[1] with 41% yield. The ^1H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, 2H),

7.27-7.34 (m, 3H), 5.78-5.86 (m, 1H), 4.67 (d, J = 11.2 Hz, 1H), 4.0 (d, J = 6.8 Hz, 1H), 3.05 (d, J = 12.0 Hz, 1H). Spectral data match those of the reported compound. [1]



Reaction of complex 6 with NaN_3 in DMSO under nitrogen atmosphere.



The palladium complex **6** (0.25 mmol) in DMSO (1 mL) was added to a glass vial which have DMSO (1 mL) and NaN_3 (0.75 mmol). The mixture was heated in an oil bath (100 °C) under nitrogen atmosphere for 12 hours, After cooling down to room temperature, 5 mL of ethyl acetate was added and removal of DMSO with brine, the combined organics evaporated under reduced pressure and then concentrated for further purification to afford the allylic azide **2a** in 58 % isolated yield.

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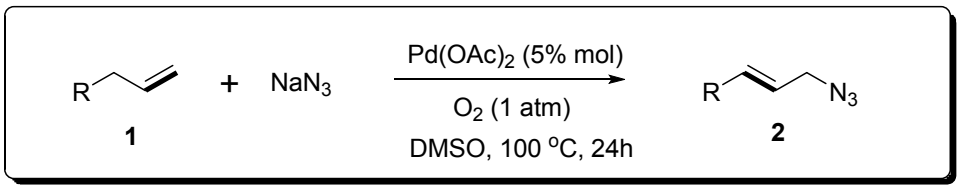
[1] A. J. Young, M. C. White, *J. Am. Chem. Soc.* **2008**, *130*, 14090.

[2] B. M. Trost, P. J. Metzner, *J. Am. Chem. Soc.*, **1980**, *102*, 3572–3577.

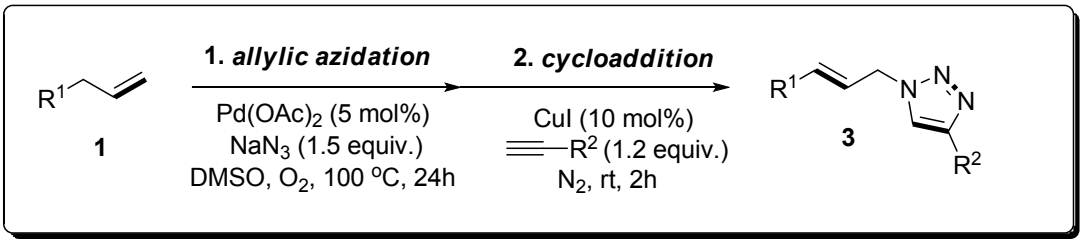
Palladium-Catalyzed Regioselective Azidation of Allylic C-H Bond

Typical procedure for Pd-catalyzed allylic azidation of alkenes to form allylic azides (Table 1):



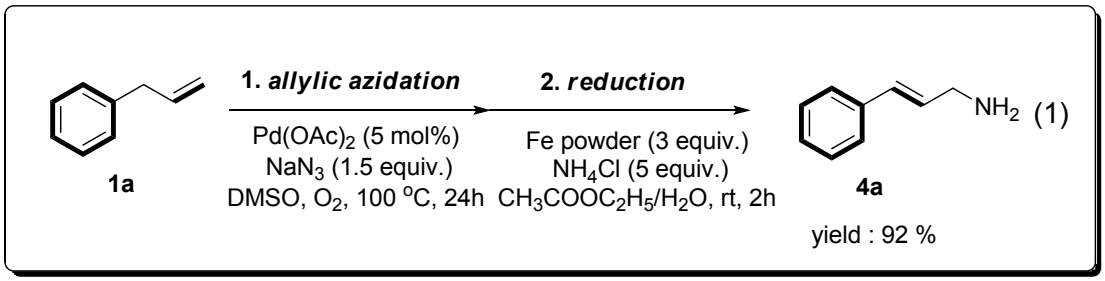
$Pd(OAc)_2$ (0.025 mmol, 6 mg) was mixed with DMSO (2.5 mL) in a glass vial or round-bottom flask equipped with a magnetic stirring bar. Then, alkene (0.5 mmol) was added. The mixture was stirred under an dioxygen atmosphere (1 atm) at 100 °C for 24 h. After cooling down to room temperature, 5 mL of ethyl acetate was added and removal of the DMSO with brine, the residue was purified by flash chromatography on silica gel to obtain the desired product 2a using light petroleum ether/ethyl acetate(20:1, v/v) as eluent, which furnished the allylic azide.

Typical procedure for the one pot, two-step synthesis of triazoles from alkenes (Table 2):



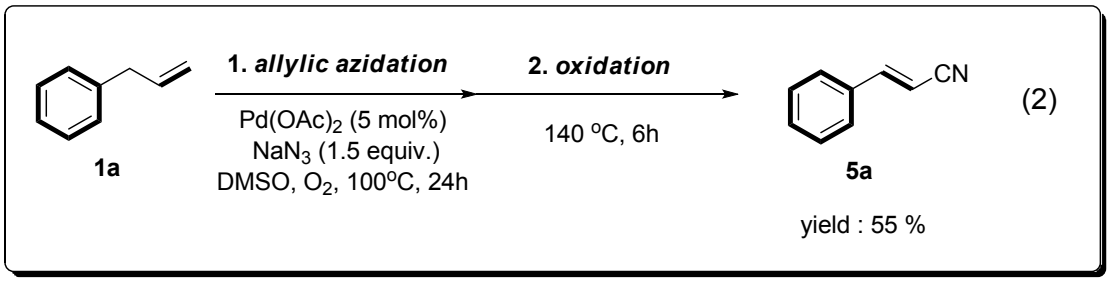
The crude allylic azide was prepared as described above. The residue was mixed CuI (0.05 mmol, 9.5 mg) with alkyne (0.6 mmol), the mixture was stirred under an nitrogen atmosphere at 80 °C for 2h. After cooling down to room temperature, 5 mL of ethyl acetate was added and removal of the DMSO with brine, the residue was purified by flash chromatography on silica gel to obtain the desired product 3a using light petroleum ether/ethyl acetate(5:1, v/v) as eluent, which furnished the 1,2,3-triazole.

Typical procedure for one pot, two-step synthesis of allylic amine 4a [Eq. (1)]:



The crude allylic azide was prepared as described above. Then, removal of DMSO with brine and concentrated. The residue was mixed Fe powder (3 equiv.), NH_4Cl (5 equiv.), with ethyl acetate/water(*v*/*v* = 2:1, 3 mL). The mixture was stirred at room temperature for 2h. Then 5 mL of ethyl acetate was added, wash with Na_2CO_3 (aq.) and concentrated, the residue was purified by flash chromatography on silica gel to obtain the desired products **4a** using light petroleum ether/ethyl acetate (1:2, v/v) as eluent.

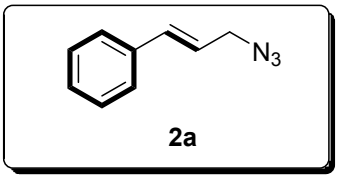
Typical procedure for one pot, two-step synthesis of alkenyl nitrile 5a [Eq. (2)]::



$Pd(OAc)_2$ (0.025 mmol, 6 mg) was mixed with DMSO (2.5 mL) in a glass vial or round-bottom flask equipped with a magnetic stirring bar. Then, allylbenzene (0.5 mmol) was added. The mixture was stirred under an dioxygen atmosphere (1 atm) at 100 °C for 24 h. Then the mixture was stirred at 140 °C for 6 h. After cooling down to room temperature, 5 mL of ethyl acetate was added and removal of the DMSO with

brine, the residue was purified by flash chromatography on silica gel to obtain the alkenyl nitrile 5a using light petroleum ether/ethyl acetate(10:1, v/v) as eluent.

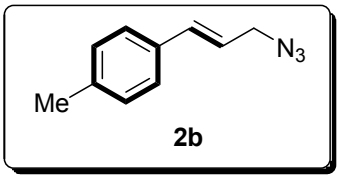
Characterization data for all prepared compounds:



2a

(*E*)-(3-Azidoprop-1-enyl)benzene (2a) [3]

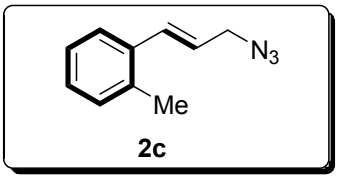
IR (KBr, cm^{-1}):ν 2098, 1446, 1239, cm^{-1}; MS (EI) m/z: 159.08; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.24–7.41 (m, 5H), 6.64 (d, *J*=15.6 Hz, 1H), 6.21-6.27 (m, 1H), 3.93 (d, *J*=6.4 Hz, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=136.0, 134.6, 128.7, 128.2, 126.7, 122.4, 53.0 ppm.



2b

(*E*)- (3-Azidoprop-1-enyl)-4-methylbenzene (2b) [3]

IR (KBr, cm^{-1}):ν 2100, 1512, 1239, cm^{-1}; MS (EI) m/z: 173.09; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.21 (d, *J*=8.0 Hz, 2H), 7.11 (d, *J*=8.0 Hz, 2H), 6.53 (d, *J*=15.6 Hz, 1H), 6.06-6.14 (m, 1H), 3.84 (d, *J*=6.4 Hz, 2H), 3.26 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=138.1, 134.6, 133.2, 129.4, 126.6, 121.3, 53.1, 21.2 ppm.

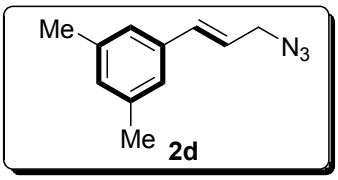


2c

(*E*)- (3-Azidoprop-1-enyl)-2-methylbenzene (2c)

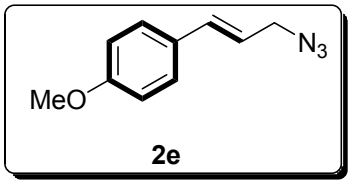
IR (KBr, cm^{-1}):ν 2105, 1515, 1240, 965, cm^{-1}; MS (EI) m/z: 173.10; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.48 (t, 1H), 7.21-7.28 (m, 3H), 6.90 (d, *J*=15.6 Hz, 1H), 6.12-

6.19 (m, 1H), 3.99 (d, *J*=6.4 Hz, 2H), 2.41 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=135.6, 135.3, 132.7, 130.4, 128.1, 126.2, 126.0, 123.7, 53.2, 19.8 ppm; HRMS EI (m/z): calcd for $C_{10}H_{11}N_3$, 173.0953; found, 173.0947.



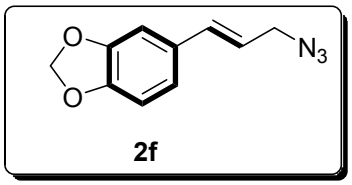
(*E*)- (3-Azidoprop-1-enyl)-3,5-dimethylbenzene (2d)

IR (KBr, cm^{-1}):ν 2101, 1515, 1240, 965, 619cm^{-1}; MS (EI) m/z: 187.10; ^{1}H NMR (400 MHz, $CDCl_3$): δ= 7.01 (s, 1H), 6.97 (s, 2H), 6.62 (d, *J*=15.6 Hz, 1H), 6.24-6.29 (m, 1H), 3.96 (d, *J*=6.4 Hz, 2H), 2.36 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=138.2, 135.9, 134.9, 129.9, 124.6, 121.9, 53.1, 21.2 ppm; HRMS EI (m/z): calcd for $C_{11}H_{13}N_3$, 187.1109; found, 187.1106.



(*E*)- (3-Azidoprop-1-enyl)-4-methoxylbenzene (2e) [4]

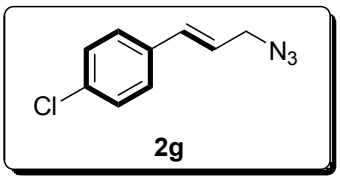
IR (KBr, cm^{-1}): 2919, 2837, 1599, 1491, 1243, cm^{-1}; MS (EI) m/z: 189.09; ^{1}H NMR (400 MHz, $CDCl_3$): δ= 7.37 (d, *J*=8.8 Hz, 2H), 6.90 (d, *J*=8.8 Hz, 2H), 6.62 (d, *J*=15.6 Hz, 1H), 6.11-6.17 (m, 1H), 3.94 (d, *J*=6.4 Hz, 2H), 384 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=159.7, 134.2, 128.8, 127.9, 120.1, 114.1, 55.3, 53.2 ppm.



(*E*)-5-(3-Azidoprop-1-enyl)benzo[*d*][1,3]dioxole (2f)

IR (KBr, cm^{-1}): 2922, 2838, 1610, 1495, 1234, cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ= 6.93 (s, 1H), 6.83 (d, *J*=8.0 Hz, 1H), 6.76 (d, *J*=8.0 Hz, 1H), 6.54 (d, *J*=15.6 Hz,

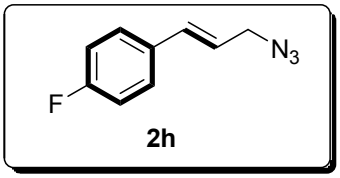
1H), 6.02-6.08 (m, 1H), 5.96 (s, 2H), 3.90 (d, *J*=6.4 Hz, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=148.1, 147.7, 134.2, 130.4, 121.5, 120.5, 108.3, 105.8, 101.2, 53.1 ppm; HRMS EI (m/z): calcd for $C_{10}H_9N_3O_2$, 203.0695; found, 203.0693.



2g

(*E*)-(3-Azidoprop-1-enyl)-4-chlorobenzene (2g)

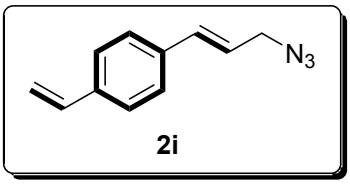
IR (KBr, cm^{-1}): 2919, 2837, 1599, 1491, 1243, cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ= 7.28-7.34 (m, 4H), 6.59 (d, *J*=15.6 Hz, 1H), 6.17-6.25 (m, 1H), 3.94 (d, *J*=6.4 Hz, 2H), ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=134.5, 133.9, 133.2, 128.9, 127.8, 123.2, 52.9 ppm. HRMS EI (m/z): calcd for $C_9H_8ClN_3$, 193.0407; found, 193.0411.



2h

(*E*)-(3-Azidoprop-1-enyl)-4-fluorobenzene (2h) [3]

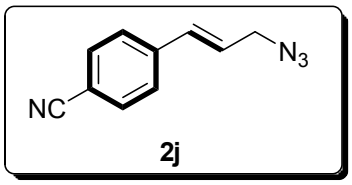
IR (KBr, cm^{-1}): 2919, 2837, 2099, 1446, 1239, 693, cm^{-1}; MS (EI) m/z: 177.09; ^{1}H NMR (400 MHz, $CDCl_3$): δ= 7.37 (t, 2H), 7.02 (t, 2H), 6.61 (d, *J*=15.6 Hz, 1H), 6.11-6.19 (m, 1H), 3.93 (d, *J*=6.4 Hz, 2H), ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=162.6 (d, $J_{C\text{-}F}$ = 246.4 Hz), 133.3, 132.2 (d, $J_{C\text{-}F}$ = 3.3 Hz), 128.2(d, $J_{C\text{-}F}$ = 8.1 Hz), 122.2 (d, $J_{C\text{-}F}$ = 2.1 Hz), 115.6 (d, $J_{C\text{-}F}$ = 21.6 Hz), 52.9 ppm.



2i

(*E*)-1-(3-azidoprop-1-enyl)-4-vinylbenzene (2i)

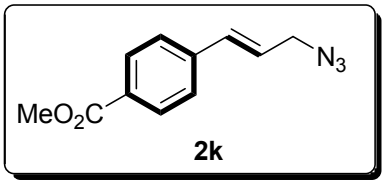
IR (KBr, cm^{-1}): 2913, 2847, 2012, 1446, 1240, cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.38-7.43 (m, 4H), 6.74 (dd, *J*=17.6, 10.8 Hz, 1H), 6.66 (d, *J*=15.6 Hz, 1H), 6.23-6.31 (m, 1H), 5.79 (d, *J*=17.6 Hz, 1H), 5.29 (d, *J*=10.8 Hz, 1H), 3.98 (d, *J*=6.4 Hz, 2H), ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=137.5, 136.3, 135.5, 134.1, 126.8, 126.5, 122.3, 114.1, 53.1 ppm. HRMS EI (m/z): calcd for $C_{11}H_{11}N_3$, 185.0952; found, 185.0953.



2j

(*E*)-4-(3-azidoprop-1-enyl)benzonitrile (2j)

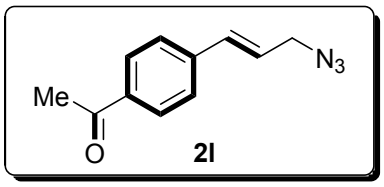
IR (KBr, cm^{-1}): 2925, 2833, 2532, 2010, 1442, 1240, 690, cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.56 (d, *J*=8.0 Hz, 2H), 7.39 (d, *J*=8.0 Hz, 2H), 6.36 (d, *J*=15.6 Hz, 1H), 5.91-5.99 (m, 1H), 4.09 (d, *J*=6.4 Hz, 2H), ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=142.4, 132.3, 130.2, 129.8, 126.3, 119.1, 109.9, 53.8 ppm. HRMS EI (m/z): calcd for $C_{10}H_8N_4$, 184.0745; found, 184.0749.



2k

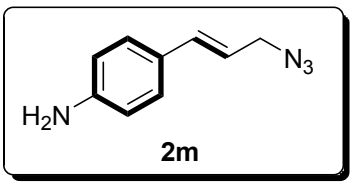
(*E*)-methyl 4-(3-azidoprop-1-enyl)benzoate (2k)

IR (KBr, cm^{-1}): 2919, 2837, 2099, 1446, 1239, 1185, 693, cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.95 (d, *J*=8.0 Hz, 2H), 7.36 (d, *J*=8.0 Hz, 2H), 6.37 (d, *J*=15.6 Hz, 1H), 5.92-5.99 (m, 1H), 4.10 (d, *J*=5.2 Hz, 2H), 3.90 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=167.0, 142.4, 130.4, 129.9, 129.6, 128.8, 125.7, 53.9, 52.0 ppm. HRMS EI (m/z): calcd for $C_{11}H_{11}N_3O_2$, 217.0847; found, 217.0851.



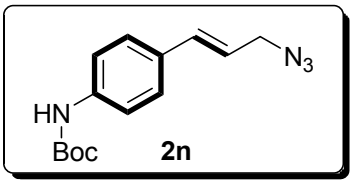
(*E*)-1-(4-(3-azidoprop-1-enyl)phenyl)ethanone (2l)

IR (KBr, cm^{-1}): 2920, 2838, 2011, 1694, 1446, 1239, 690, cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.88 (d, *J*=8.0 Hz, 2H), 7.39 (d, *J*=8.0 Hz, 2H), 6.39 (d, *J*=15.6 Hz, 1H), 5.89-5.99 (m, 1H), 4.09 (d, *J*=6.4 Hz, 2H), 2.57 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=197.6, 142.6, 135.4, 130.3, 129.1, 128.7, 125.8, 53.9, 26.5 ppm. HRMS EI (m/z): calcd for $C_{11}H_{11}N_3O$, 201.0899; found, 201.0902.



(*E*)-4-(3-azidoprop-1-enyl)aniline (2m)

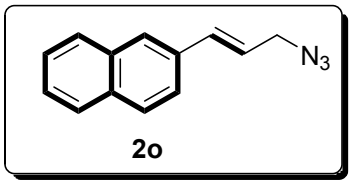
IR (KBr, cm^{-1}): 3405, 3350, 2919, 2837, 2010, 1436, 1223, 693, cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.50 (d, *J*=8.8 Hz, 2H), 6.38 (d, *J*=15.6 Hz, 1H), 7.30 (d, *J*=8.8 Hz, 2H), 5.97-6.04 (m, 1H), 3.91 (d, *J*=7.2 Hz, 2H), 3.52 (br, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=146.4, 130.1, 129.4, 126.5, 122.4, 115.3, 54.1 ppm. HRMS EI (m/z): calcd for $C_9H_{10}N_4$, 174.0902; found, 174.0905.



(*E*)-*tert*-butyl 4-(3-azidoprop-1-enyl)phenylcarbamate (2n)

IR (KBr, cm^{-1}): 3456, 2946, 2835, 2010, 1446, 1242, 691, cm^{-1};^1H NMR (400 MHz, $CDCl_3$): δ= 7.74 (d, *J*=12 Hz, 2H), 7.47 (d, *J*=12 Hz, 2H), 6.62 (br, 1H), 6.36 (d, *J*=15.6 Hz, 1H), 5.88-5.96 (m, 1H), 3.91 (d, *J*=6.4 Hz, 2H), 1.38 (s, 9H) ppm; ^{13}C

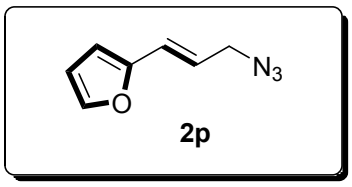
NMR (100 MHz, $CDCl_3$): δ=152.9, 137.5, 130.4, 128.9, 128.8, 119.7, 118.7, 60.3, 54.1, 28.3 ppm. HRMS EI (m/z): calcd for $C_{14}H_{18}N_4O_2$, 274.1435; found, 274.1430.



2o

(*E*)-2-(3-Azidoprop-1-enyl)naphthalene (2o)

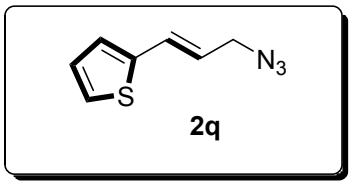
IR (KBr, cm^{-1}):ν 2938, 2840, 2098, 1446, 1239, cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.76-7.79 (m, 3H), 7.72 (s, 1H), 7.57 (d, 1H), 7.43-7.45 (m, 2H), 6.76 (d, *J*=15.6 Hz, 1H), 6.28-6.36 (m, 1H), 3.95 (d, *J*=6.4 Hz, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=134.6, 133.5, 133.4, 133.3, 128.4, 128.1, 127.7, 126.9, 126.4, 126.2, 123.5, 122.8 ppm; HRMS EI (m/z): calcd for $C_{13}H_{11}N_3$, 209.2953; found, 209.2958.



2p

(*E*)-2-(3-Azidoprop-1-enyl)furan (2p)

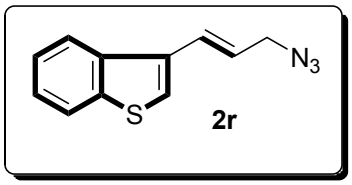
IR (KBr, cm^{-1}):ν 2098, 1446, 1239, cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.39 (s, 1H), 6.48 (d, *J*=15.6 Hz, 1H), 6.41 (t, *J*=3.2, 2.0 Hz, 1H), 6.32 (d, *J*=3.2 Hz, 2H), 6.16-6.23 (m, 1H), 3.94 (d, *J*=6.4 Hz, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=151.6, 142.5, 122.4, 120.9, 111.4, 109.0, 52.7 ppm; HRMS EI (m/z): calcd for $C_7H_7N_3O$, 149.0589; found, 149.0581.



2q

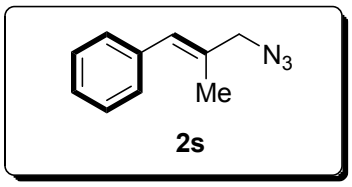
(*E*)-2-(3-Azidoprop-1-enyl)thiophene (2q)

IR (KBr, cm^{-1}):ν 2099, 1442, 1240, cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ=7.25 (s, 1H), 6.68-6.19 (m, 2H), 6.77 (d, *J*=15.6 Hz, 1H), 6.03-6.10 (m, 1H), 3.91 (d, *J*=6.4 Hz, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=140.9, 127.5, 127.5, 126.6, 125.0, 121.9, 52.8 ppm; HRMS EI (m/z): calcd for $C_7H_7N_3S$, 165.0361; found, 165.0360.



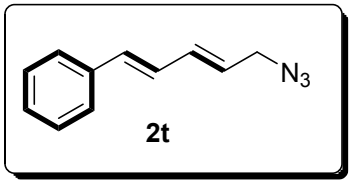
(*E*)-2-(3-Azidoprop-1-enyl)benzo[*b*]thiophene (2r)

IR (KBr, cm^{-1}):ν 2098, 1444, 1239, cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ= 7.85-7.91 (m, 2H), 7.47 (s, 1H), 7.35-7.44 (m, 2H), 6.91 (d, *J*=15.6 Hz, 1H), 6.27-6.34 (m, 1H), 4.01 (d, *J*=6.4 Hz, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=140.5, 137.5, 132.8, 126.8, 124.6, 124.4, 124.1, 123.2, 123.0, 121.9, 53.2 ppm; HRMS EI (m/z): calcd for $C_{11}H_9N_3S$, 215.0517; found, 215.0513.



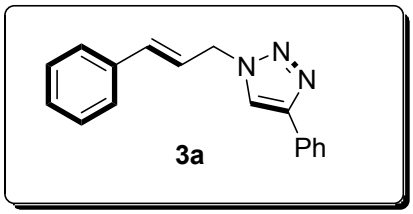
(*E*)-(3-azido-2-methylprop-1-enyl)benzene (2s)

IR (KBr, cm^{-1}):ν 2010, 1446, 1240, cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ= 7.11-7.28 (m, 5H), 6.45 (s, 1H), 3.80 (s, 2H), 1.87 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=132.5, 129.1, 129.0, 128.5, 128.2, 126.9, 59.7, 16.3 ppm; HRMS EI (m/z): calcd for $C_{10}H_{11}N_3$, 173.0953; found, 173.0947.



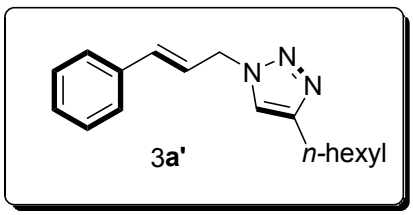
((1*E*,3*E*)-5-azidopenta-1,3-dienyl)benzene (2t)

IR (KBr, cm^{-1}):ν 2098, 1602, 1446, 1239, cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ= 7.24-7.39 (m, 5H), 6.78 (dd, *J*=15.6, 10.4 Hz, 1H), 6.60 (d, *J*=15.6 Hz, 1H), 6.45 (dd, *J*=14.8, 10.4 Hz, 1H), 5.79-5.87 (m, 1H), 3.86 (d, *J*=6.8 Hz, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=136.8, 134.9, 134.0, 128.7, 127.9, 127.4, 126.5, 126.0, 52.8 ppm; HRMS EI (m/z): calcd for $C_{11}H_{11}N_3$, 185.0953; found, 185.0954.



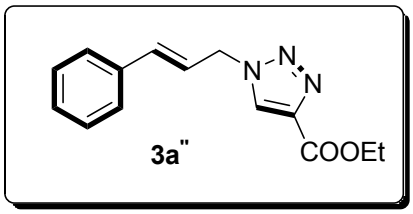
1-cinnamyl-4-phenyl-1*H*-1,2,3-triazole (3a) [5]

IR (KBr, cm^{-1}):ν 3451, 1642, 1103, 620; mp = 124.5-127.7 °C; MS (EI) m/z: 261.32; ^{1}H NMR (400 MHz, $CDCl_3$): δ= 7.81–7.84 (m, 3H), 7.28–7.42 (m, 8H), 6.68 (d, *J*=16 Hz, 1H), 6.33-6.41 (m, 1H), 5.16 (d, *J*=6.4 Hz, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=148.1, 135.5, 135.4, 130.6, 128.8, 128.8, 128.7, 128.2, 126.7, 125.7, 121.9, 119.4, 52.4 ppm;



(*E*)-4-hexyl-1-(3-p-tolylallyl)-1*H*-1,2,3-triazole (3a')

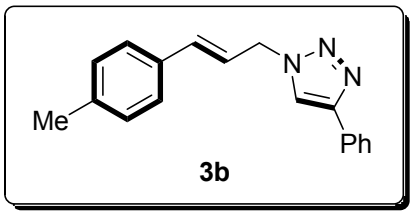
IR (KBr, cm^{-1}):ν 3455, 1654, 1121, 722; mp = 127.3-130.2 °C; MS (EI) m/z: 269.19; ^{1}H NMR (400 MHz, $CDCl_3$): δ= 7.28–7.40 (m, 6H), 6.64 (d, *J*=16 Hz, 1H), 6.30-6.37 (m, 1H), 5.16 (dd, *J*=6.8, 1.2 Hz, 2H), 2.72 (t, *J*=7.6, 7.6 Hz, 2H), 1.65-1.68 (m, 2H), 1.28-1.32 (m, 6H), 0.89 (t, *J*=6.8, 6.8 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=148.8, 135.6, 135.0, 128.7, 128.5, 126.9, 122.3, 120.4, 52.2, 31.6, 29.4, 29.0, 25.7, 22.5, 14.1 ppm; HRMS EI (m/z): calcd for $C_{17}H_{23}N_3$, 269.1892; found, 269.1890.



3a"

Ethyl 1-cinnamyl-1*H*-1,2,3-triazole-4-carboxylate (3a'')

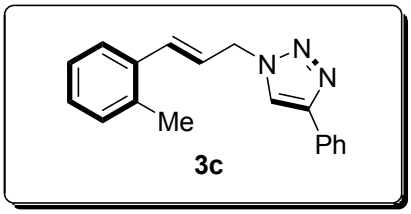
IR (KBr, cm^{-1}):ν 3447, 2362, 2335, 1629, 1106, 620; MS (EI) m/z: 257.12; ^{1}H NMR (400 MHz, $CDCl_3$): δ= 8.18 (s, 1H), 7.28–7.40 (m, 5H), 6.69 (d, *J*=16 Hz, 1H), 6.31-6.36 (m, 1H), 5.18 (d, *J*=6.4 Hz, 2H), 4.39 (q, 2H), 1.38 (t, *J*=7.2, 7.2 Hz,3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=160.5, 140.2, 136.0, 13.0, 128.6, 128.5, 127.1, 126.5, 120.8, 61.0, 52.3, 14.1 ppm; HRMS EI (m/z): calcd for $C_{14}H_{15}N_3O_2$, 257.1164; found, 257.1161.



3b

(*E*)-4-phenyl-1-(3-*p*-tolylallyl)-1*H*-1,2,3-triazole (3b)

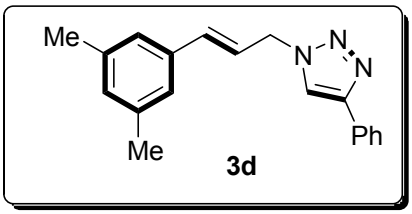
IR (KBr, cm^{-1}):ν 3452, 2361, 1639, 1104, 621; mp = 128.6-138.4 ^{o}C; MS (EI) m/z: 275.14; ^{1}H NMR (400 MHz, $CDCl_3$): δ= 7.80–7.84 (m, 3H), 7.41 (d, 2H), 7.28–7.35 (m, 3H), 7.14 (d, 2H), 6.67 (d, *J*=15.6 Hz, 1H), 6.28-6.36 (m, 1H), 5.15 (d, *J*=6.0 Hz, 2H), 2.34 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=148.1, 138.6, 135.5, 132.7, 130.6, 129.5, 128.8, 128.2, 126.7, 125.7, 120.8, 119.4, 52.5, 21.3 ppm; HRMS EI (m/z): calcd for $C_{18}H_{17}N_3$, 275.1422; found, 275.1420.



3c

(*E*)-4-phenyl-1-(3-*o*-tolylallyl)-1*H*-1,2,3-triazole (3c)

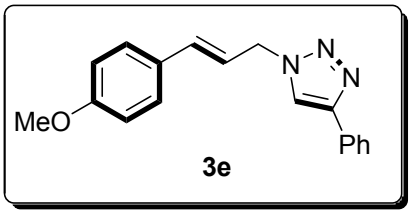
IR (KBr, cm^{-1}):ν 3450, 2361, 1640, 1107, 621; mp = 130.1-131.4 °C; MS (EI) m/z: 275.14; ^{1}H NMR (400 MHz, $CDCl_3$): δ= 7.81–7.84 (m, 3H), 7.16-7.44 (m, 8H), 6.95 (d, *J*=16 Hz, 1H), 6.24-6.32 (m, 1H), 5.20 (d, *J*=6.4 Hz, 2H), 2.37 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=148.1, 135.8, 134.6, 133.4, 130.6, 130.5, 128.9, 128.5, 128.2, 126.3, 125.9, 125.7, 123.2, 119.3, 52.7, 19.8 ppm; HRMS EI (m/z): calcd for $C_{18}H_{17}N_3$, 275.1422; found, 275.1420.



3d

(*E*)-1-(3-(3,5-dimethylphenyl)allyl)-4-phenyl-1*H*-1,2,3-triazole (3d)

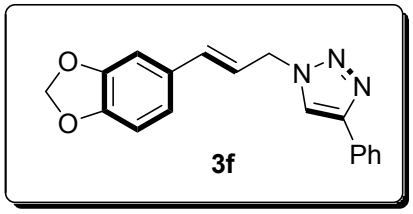
IR (KBr, cm^{-1}):ν 3448, 2362, 1640, 1103, 620; mp = 128.3-130.4 °C; MS (EI) m/z: 289.15; ^{1}H NMR (400 MHz, $CDCl_3$): δ= 7.83–7.87 (m, 3H), 7.33–7.46 (m, 3H), 7.05 (s, 2H), 6.97 (s, 1H), 6.68 (d, *J*=15.6 Hz, 1H), 6.33-6.41 (m, 1H), 5.16 (d, *J*=6.4 Hz, 2H) , 2.34 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=148.1, 138.3, 135.7, 135.4, 130.7, 130.3, 128.9, 128.1, 125.7, 124.7, 121.5, 119.4, 52.5, 21.2 ppm; HRMS EI (m/z): calcd for $C_{19}H_{19}N_3$, 289.1579; found, 289.1572.



3e

(*E*)-1-(3-(4-methoxyphenyl)allyl)-4-phenyl-1*H*-1,2,3-triazole (3e)

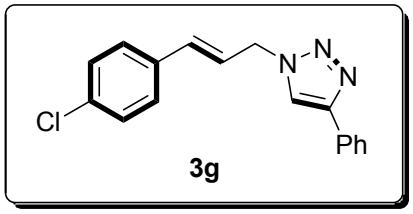
IR (KBr, cm^{-1}):ν 3450, 2361, 1641, 1105, 621; mp = 148.7-151.2 °C; MS (EI) m/z: 291.14; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.79–7.83 (m, 3H), 7.30–7.42 (m, 5H), 6.85 (d, 2H), 6.63 (d, *J*=15.6 Hz, 1H), 6.18-6.25 (m, 1H), 5.11 (d, *J*=6.8 Hz, 2H), 3.79 (s 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=159.9, 148.0, 135.0, 130.6, 128.8, 128.2, 128.1, 128.0, 125.7, 119.5, 119.3, 114.1, 55.3, 52.5 ppm; HRMS EI (m/z): calcd for $C_{18}H_{17}N_3O$, 291.1372; found, 291.1377.



3f

(*E*)-1-(3-(benzo[*d*][1,3]dioxol-5-yl)allyl)-4-phenyl-1*H*-1,2,3-triazole (3f)

IR (KBr, cm^{-1}):ν 3448, 2360, 1636, 1103, 619; mp = 143.1-144.3 °C; MS (EI) m/z: 305.11; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.72–7.76 (m, 3H), 7.25–7.36 (m, 3H), 6.85 (s, 1H), 6.76 (d, 1H), 6.69 (d, 1H), 6.54 (d, *J*=15.6 Hz, 1H), 6.11-6.17 (m, 1H), 5.89 (s, 2H), 5.07 (d, *J*=6.8 Hz, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=148.2, 148.1, 148.1, 135.2, 130.6, 129.9, 128.8, 128.2, 125.7, 121.8, 120.0, 119.3, 108.4, 105.8, 101.3, 52.5 ppm; HRMS EI (m/z): calcd for $C_{18}H_{15}N_3O_2$, 305.1164; found, 305.1165.

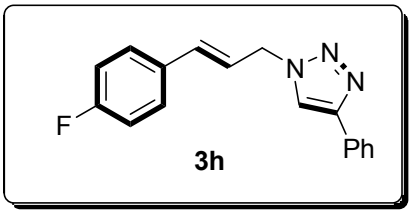


3g

(*E*)-1-(3-(4-chlorophenyl)allyl)-4-phenyl-1*H*-1,2,3-triazole (3g)

IR (KBr, cm^{-1}):ν 3450, 2361, 1640, 1103, 620; mp = 128.7-129.6 °C; MS (EI) m/z: 295.1; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.80–7.84 (m, 3H), 7.30–7.43 (m, 7H), 6.62 (d, *J*=16 Hz, 1H), 6.32-6.39 (m, 1H), 5.16 (d, *J*=6.8 Hz, 2H) ppm; ^{13}C NMR (100

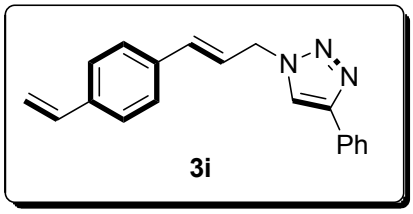
MHz, $CDCl_3$): δ=148.2, 134.3, 134.0, 130.5, 129.0, 128.9, 128.2, 127.9, 125.7, 122.7, 119.4, 52.3 ppm; HRMS EI (m/z): calcd for $C_{17}H_{14}ClN_3$, 295.0876; found, 295.0871.



3h

(*E*)-1-(3-(4-fluorophenyl)allyl)-4-phenyl-1*H*-1,2,3-triazole (3h)

IR (KBr, cm^{-1}):ν 3453, 2361, 1641, 1103, 622; mp = 124.5-126.7 °C; MS (EI) m/z: 279.1; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.81–7.84 (m, 3H), 7.32–7.43 (m, 5H), 7.02 (t, 2H), 6.68 (d, *J*=15.6 Hz, 1H), 6.25-6.33 (m, 1H), 5.15 (d, *J*=6.4 Hz, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=162.8 (d, J_{C-F} = 247.0 Hz),148.1, 134.1, 131.7 (d, J_{C-F} = 3.2 Hz), 130.6, 128.8, 128.4 (d, J_{C-F} = 8.1 Hz), 128.2, 125.7, 121.7 (d, J_{C-F} = 2.1 Hz), 119.4, 115.7 (d, J_{C-F} = 21.6 Hz), 52.3 ppm; HRMS EI (m/z): calcd for $C_{17}H_{14}FN_3$, 279.1172; found, 279.1154.

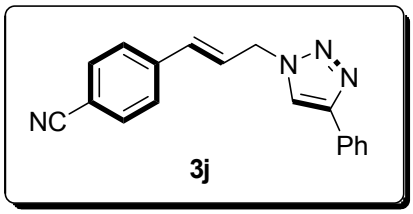


3i

(*E*)-4-phenyl-1-(3-(4-vinylphenyl)allyl)-1H-1,2,3-triazole (3i)

IR (KBr, cm^{-1}):ν 3447, 2362, 1103, 619; mp = 150.7-153.6 °C; MS (EI) m/z: 287.1; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.81–7.92 (m, 3H), 7.32–7.41 (m, 7H), 6.69 (dd, *J*=17.6, 10.8 Hz, 1H), 6.67 (d, *J*=15.6 Hz, 1H), 6.33-6.41 (m, 1H), 5.76 (d, *J*=17.6 Hz, 1H), 5.26 (d, *J*=10.8 Hz, 1H), 5.17 (dd, *J*=6.8, 1.0 Hz, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=148.1, 137.9, 136.2, 135.0, 134.9, 130.6, 128.9, 128.2, 126.9, 126.6,

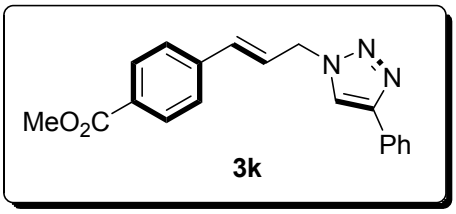
125.7, 121.8, 119.4, 114.4, 52.5 ppm; HRMS EI (m/z): calcd for $C_{19}H_{17}N_3$, 287.1420; found, 287.1422.



3j

(*E*)-4-(3-(4-phenyl-1H-1,2,3-triazol-1-yl)prop-1-enyl)benzonitrile (3j)

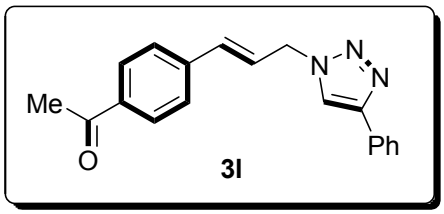
IR (KBr, cm^{-1}):ν 3450, 2363, 1629, 1101, 620; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.79–7.83 (m, 3H), 7.56 (d, *J*=18 Hz, 2H), 7.30–7.37 (m, 5H), 6.37 (d, *J*=15.6 Hz, 1H), 5.96-6.02 (m, 1H), 5.29 (d, *J*=6.8 Hz, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=148.2, 143.5, 132.8, 131.7, 131.2, 129.4, 128.8, 127.6, 126.4, 125.8, 120.3, 118.9, 109.7, 53.1 ppm; HRMS EI (m/z): calcd for $C_{18}H_{14}N_4$, 286.1215.; found, 286.1218.



3k

(*E*)-methyl 4-(3-(4-phenyl-1H-1,2,3-triazol-1-yl)prop-1-enyl)benzoate (3k)

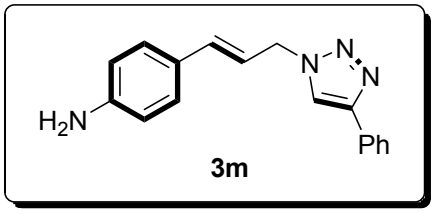
IR (KBr, cm^{-1}):ν 3451, 2360, 1640, 1210, 1103, 618; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.96 (d, 2H), 7.85–7.89 (m, 3H), 7.34–7.40 (m, 5H), 6.44 (d, *J*=16 Hz, 1H), 6.01-6.04 (m, 1H), 5.36 (d, *J*=7.6 Hz, 2H), 3.90 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=167.0, 148.5, 142.4, 130.9, 130.3, 129.9, 129.6, 128.7, 128.4, 128.3, 128.2, 125.7, 125.6, 52.9, 51.9 ppm; HRMS EI (m/z): calcd for $C_{19}H_{17}N_3O_2$, 319.1320; found, 319.1321.



3l

(*E*)-1-(4-(3-(4-phenyl-1H-1,2,3-triazol-1-yl)prop-1-enyl)phenyl)ethanone (3l)

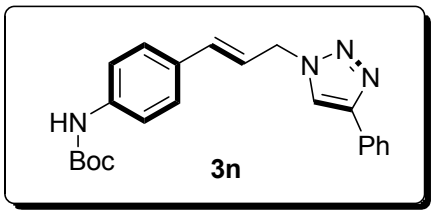
IR (KBr, cm^{-1}):ν 3450, 2362, 1694, 1640, 1103, 620; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.77–7.86 (m, 5H), 7.40–7.49 (m, 5H), 6.52 (d, *J*=15.6 Hz, 1H), 5.97-6.04 (m, 1H), 5.24 (d, *J*=6.4 Hz, 2H), 2.62 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=197.7, 148.3, 142.7, 135.4, 130.9, 130.3, 129.1, 128.6, 128.3, 128.1, 125.8, 125.6, 119.9, 53.3, 26.5 ppm; HRMS EI (m/z): calcd for $C_{19}H_{17}N_3O$, 303.1375; found, 303.1372.



3m

(*E*)-4-(3-(4-phenyl-1H-1,2,3-triazol-1-yl)prop-1-enyl)aniline (3m)

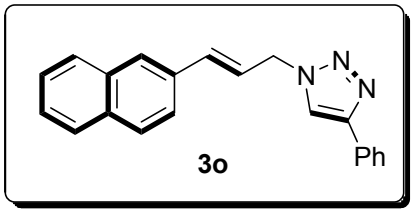
IR (KBr, cm^{-1}):ν 3448, 3310, 2362, 1638, 1112, 619^1H NMR (400 MHz, $CDCl_3$): δ= 7.70–7.73 (m, 3H), 7.30–7.51 (m, 5H), 6.31 (d, *J*=15.6 Hz, 1H), 6.30 (d, 2H) 6.08-6.15 (m, 1H), 5.13 (d, *J*=6.4 Hz, 2H), 3.59 (br, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=148.0, 146.5, 135.8, 130.5, 128.9, 128.8, 128.2, 127.0, 125.7, 122.7, 119.4, 116.5, 53.5 ppm; HRMS EI (m/z): calcd for $C_{17}H_{16}N_4$, 276.1371; found, 276.1375.



3n

(*E*)-*tert*-butyl 4-(3-(4-phenyl-1H-1,2,3-triazol-1-yl)prop-1-enyl)phenylcarbamate (3n)

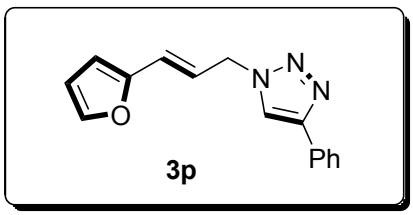
IR (KBr, cm^{-1}):ν 3448, 2362, 1640, 1301, 1103, 620; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.71–7.80 (m, 5H), 7.28–7.43 (m, 5H), 6.63 (br, 1H), 6.52 (d, *J*=16 Hz, 1H), 5.97-6.05 (m, 1H), 5.13 (d, *J*=6.4 Hz, 2H), 1.38 (s, 9H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ= 153.2, 148.1, 137.2, 130.6, 130.4, 128.8, 128.7, 128.6, 128.2, 125.7, 119.9, 119.5, 119.3, 60.4, 52.7, 29.2 ppm; HRMS EI (m/z): calcd for $C_{22}H_{24}N_4O_2$, 376.1894; found, 376.1899.



3o

(*E*)-1-(3-(naphthalen-2-yl)allyl)-4-phenyl-1*H*-1,2,3-triazole (3o)

IR (KBr, cm^{-1}):ν 3451, 2361, 1641, 1103, 620; mp = 128.6-130.8 °C; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.77–7.84 (m, 7H), 7.33–7.60 (m, 8H), 6.85 (d, *J*=15.6 Hz, 1H), 6.47-6.55 (m, 1H), 5.24 (d, *J*=6.4 Hz, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=148.2, 135.5, 133.4, 133.4, 132.9, 131.7, 130.6, 128.8, 128.5, 128.2, 128.1, 127.7, 127.2, 126.6, 126.4, 125.8, 123.3, 122.2, 52.5; HRMS EI (m/z): calcd for $C_{21}H_{17}N_3$, 311.1422; found, 311.1429.

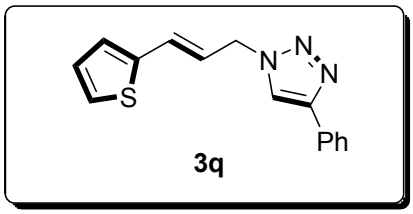


3p

(*E*)-1-(3-(furan-2-yl)allyl)-4-phenyl-1*H*-1,2,3-triazole (3p)

IR (KBr, cm^{-1}):ν 3444, 2362, 1634, 1105, 620; mp = 107.6-108.5 °C; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.82–7.84 (m, 3H), 7.32–7.44 (m, 4H), 6.47 (d, *J*=15.6 Hz, 1H), 6.40 (d, *J*=1.2 Hz, 1H), 6.29-6.39 (m, 2H), 5.16 (dd, *J*=6.4, 0.8 Hz, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=151.1, 148.1, 142.8, 130.6, 128.8, 128.2, 125.7, 123.3,

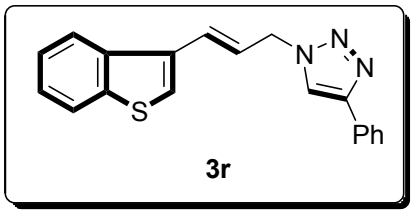
120.2, 119.4, 111.5, 109.8, 52.1; HRMS EI (m/z): calcd for $C_{15}H_{13}N_3O$, 251.1059; found, 251.1050.



3q

(*E*)-4-phenyl-1-(3-(thiophen-2-yl)allyl)-1*H*-1,2,3-triazole (3q)

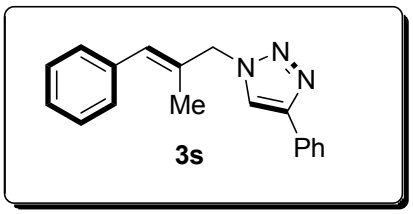
IR (KBr, cm^{-1}):ν 3450, 2361, 1641, 1104, 621; mp = 145.3-147.1 °C; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.39–7.43 (m, 3H), 7.20–7.34 (m, 3H), 7.02 (d, 1H), 6.97-6.99 (m, 2H), 6.80 (d, *J*=15.6 Hz, 1H), 6.17-6.24 (m, 1H), 5.14 (dd, *J*=6.8, 1.2 Hz, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=148.1, 140.3, 130.6, 128.8, 128.5, 128.2, 127.6, 127.2, 125.8, 125.6, 121.1, 119.4, 52.1; HRMS EI (m/z): calcd for $C_{15}H_{13}N_3S$, 267.0830; found, 267.0818.



3r

(*E*)-1-(3-(benzo[*b*]thiophen-3-yl)allyl)-4-phenyl-1*H*-1,2,3-triazole (3r)

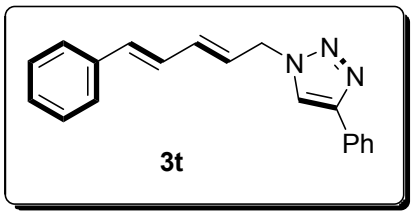
IR (KBr, cm^{-1}):ν 3450, 2361, 1640, 1103, 620; mp = 152.3-154.4 °C; MS (EI) m/z: 289.15;^1H NMR (400 MHz, $CDCl_3$): δ= 7.43–7.44 (m, 3H), 7.42 (s, 1H), 7.34–7.41 (m, 5H), 7.00 (d, *J*=16 Hz, 1H), 6.44-6.52 (m, 1H), 5.24 (dd, *J*=6.8, 1.2 Hz, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=148.2, 140.5, 137.2, 132.2, 130.6, 128.9, 128.2, 127.7, 125.8, 124.8, 124.6, 124.0, 123.4, 123.0, 121.8, 119.3, 52.7 ppm; HRMS EI (m/z): calcd for $C_{19}H_{15}N_3S$, 317.0987; found, 317.0983.



3s

(*E*)-1-(2-methyl-3-phenylallyl)-4-phenyl-1H-1,2,3-triazole (3s)

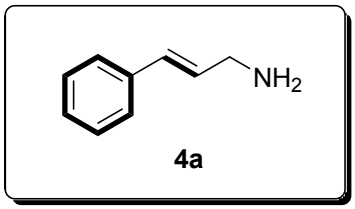
IR (KBr, cm^{-1}):ν 3449, 2361, 1640, 1103, 621; ^1H NMR (400 MHz, $CDCl_3$): δ= 7.83–7.86 (m, 3H), 7.30–7.44 (m, 8H), 6.57 (s, 1H), 5.09 (s, 2H), 1.86 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ=148.2, 136.3, 132.0, 130.2, 129.0, 128.9, 128.7, 128.4, 128.2, 127.3, 125.7, 58.9, 15.7 ppm. HRMS EI (m/z): calcd for $C_{18}H_{17}N_3$, 275.1422; found, 275.1420.



3t

4-phenyl-1-((2*E*,4*E*)-5-phenylpenta-2,4-dienyl)-1*H*-1,2,3-triazole (3t)

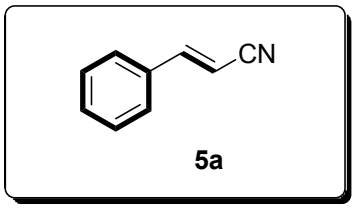
IR (KBr, cm^{-1}):ν 3451, 2363, 1636, 1103, 620; mp = 132.5-133.7 °C; ^1H NMR ($CDCl_3$, 400 MHz) δ= 7.39–7.42 (m, 3H), 7.30–7.34 (m, 8H), 6.79 (dd, *J*=15.6, 10.4 Hz, 1H), 6.63 (d, *J*=15.6 Hz, 1H), 6.47 (dd, *J*=14.8, 10.4 Hz, 1H), 5.93-6.00 (m, 1H), 5.11 (d, *J*=6.4 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 148.1, 136.6, 135.6, 134.9, 130.6, 128.8, 128.7, 128.2, 126.9, 126.6, 125.7, 125.3, 119.3, 52.2 ppm; HRMS EI (m/z): calcd for $C_{19}H_{117}N_3$, 287.1422; found, 287.1419.



4a

(*E*)-3-Phenylprop-2-enamine (4a) [6]

^{1}H NMR ($CDCl_3$, 400 MHz) δ= 7.19-7.37 (m, 5H), 6.50 (d, *J* = 16 Hz, 1H), 6.27-6.34 (m, 1H), 3.47 (d, *J* = 6.0 Hz, 1 H), 1.80 (br, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ= 137.2, 131.0, 129.6, 128.6, 127.3, 126.2, 44.2 ppm.



5a

(*E*)-3-Phenyl-2-propenenitrile (5a) [7]

^{1}H NMR ($CDCl_3$, 400 MHz) δ= 7.38-7.46 (m, 6H), 5.88 (d, *J* = 16.4 Hz ,1 H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 150.6, 133.6, 131.2, 129.1, 127.4, 118.1, 96.4 ppm.

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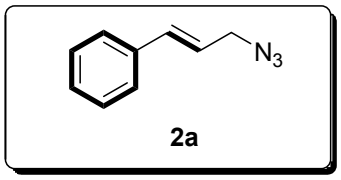
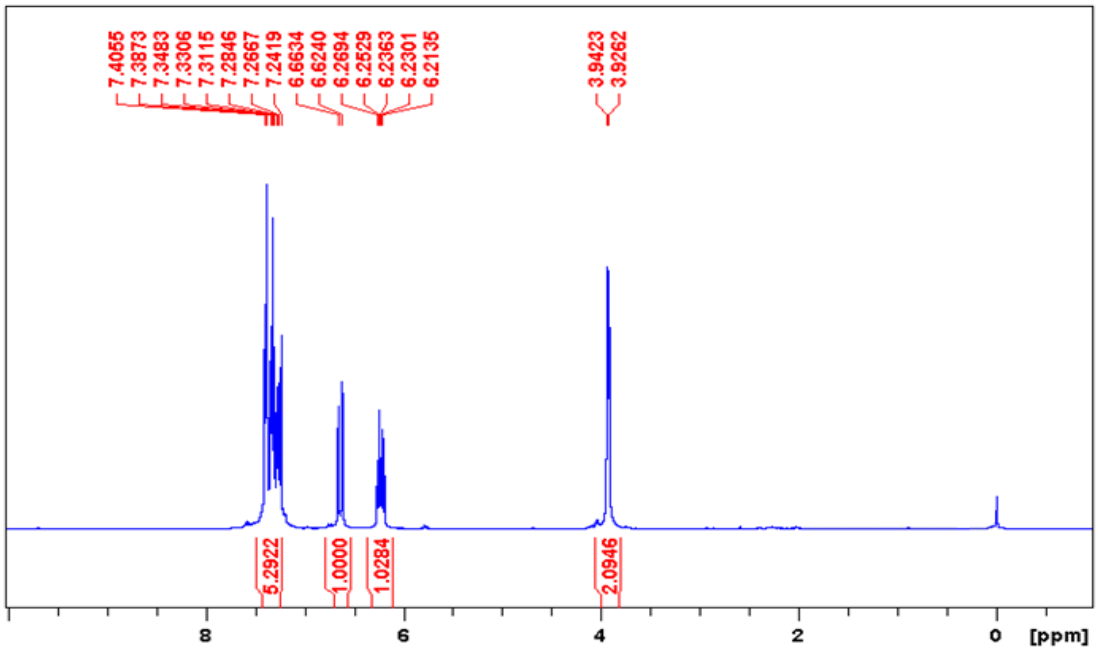
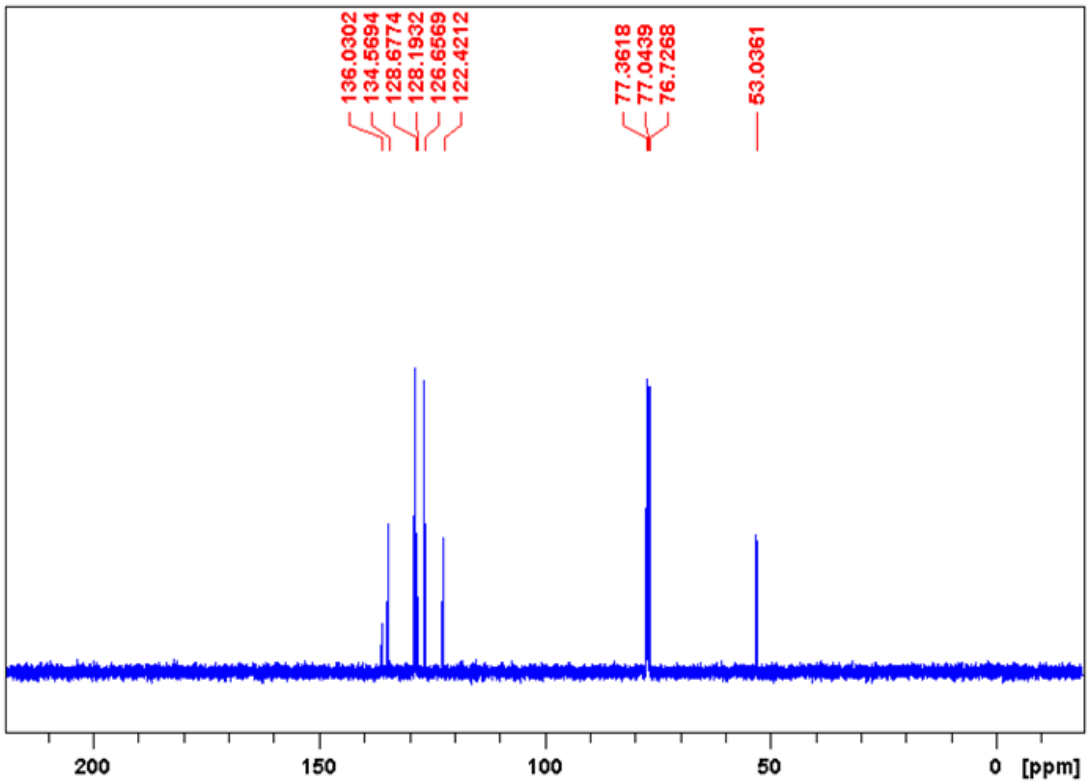
NMR Spectra



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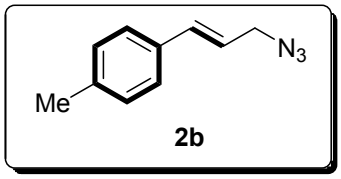
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Me

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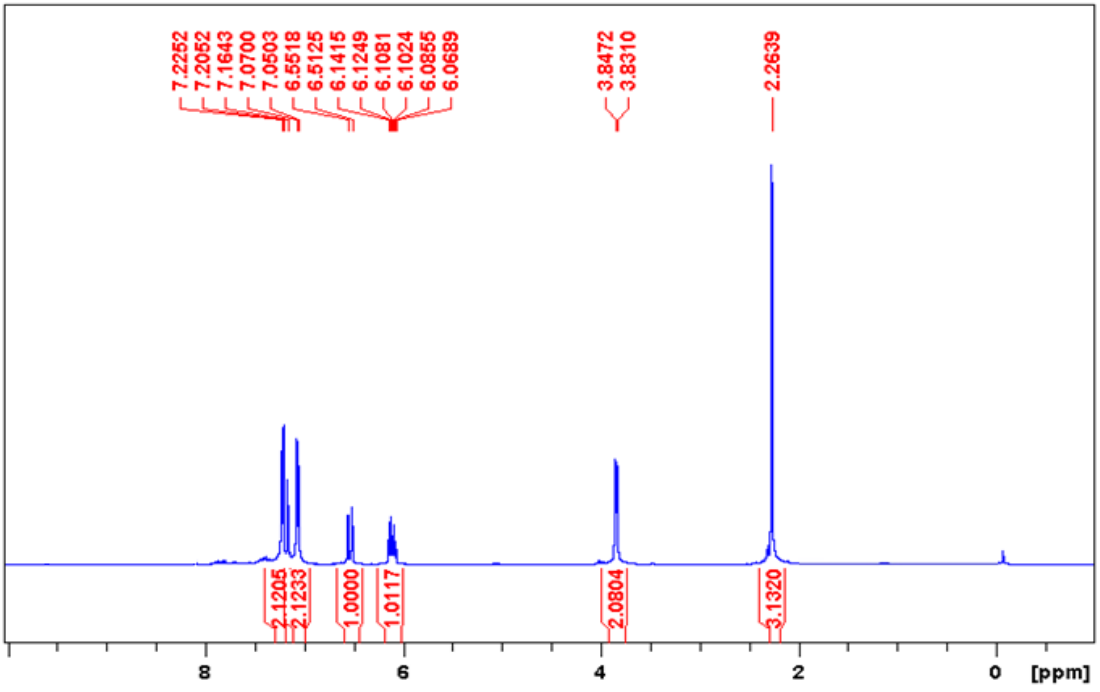
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6.0855
6.0689
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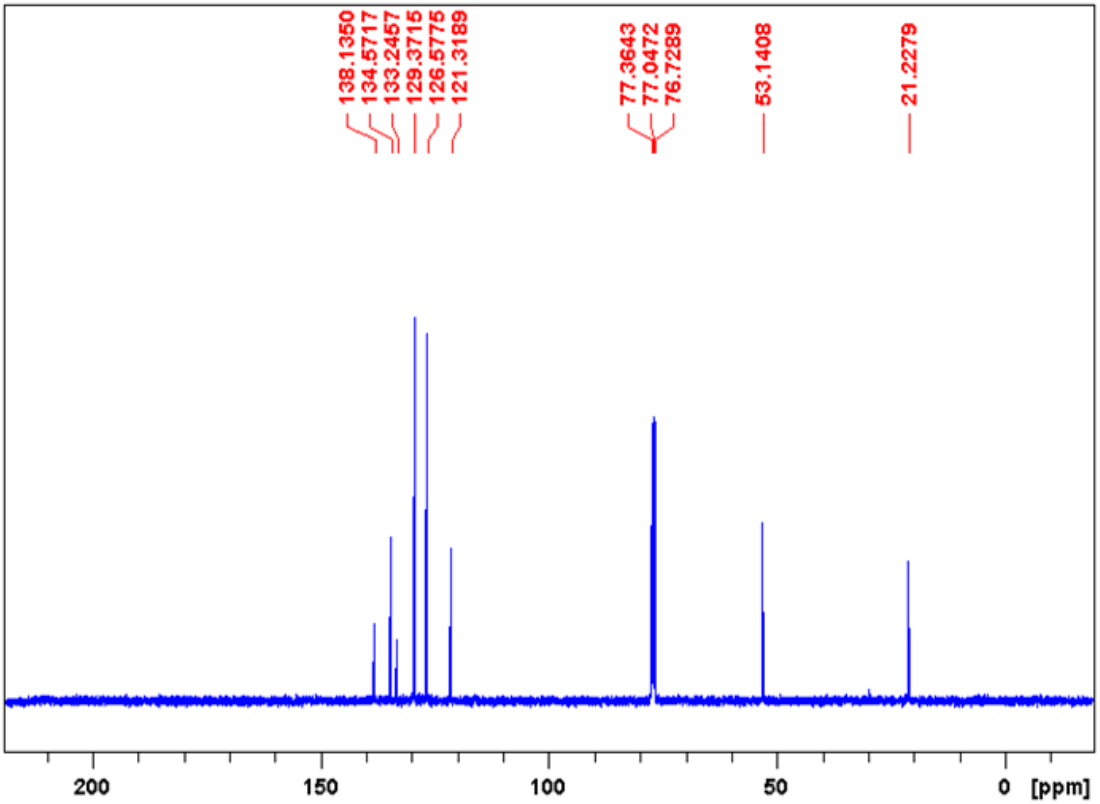
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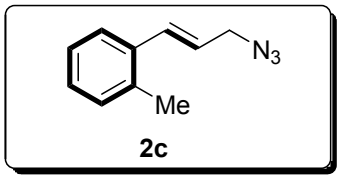
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Me

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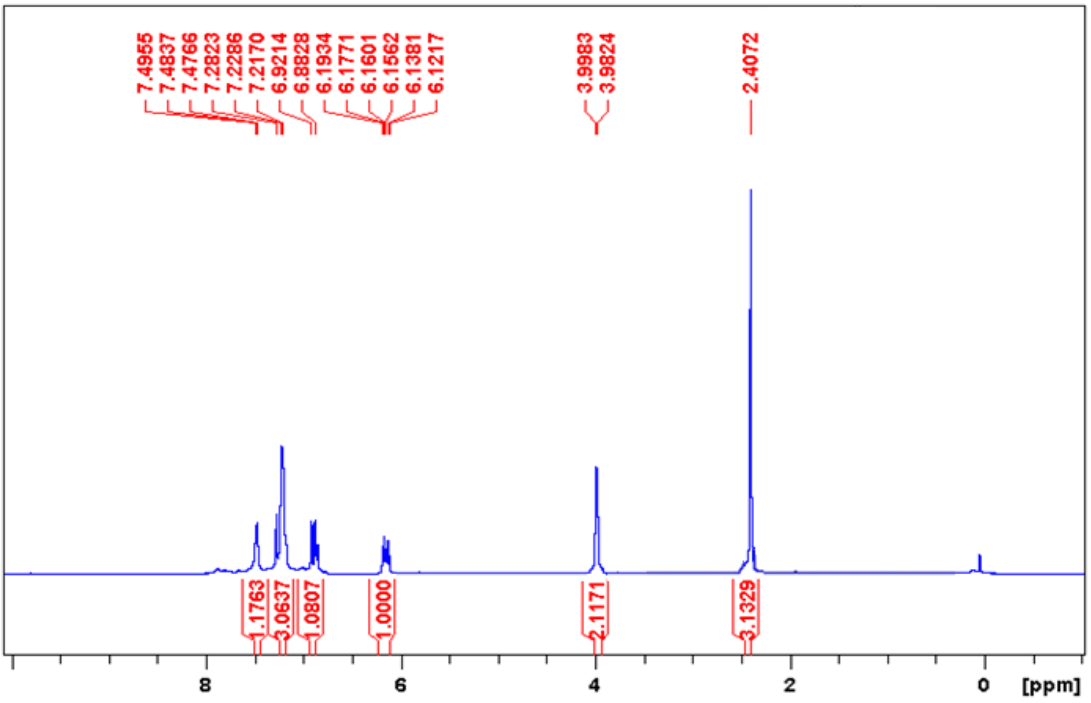
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7.2286
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6.1934
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6.1601
6.1562
6.1381
6.1217
3.9983
3.9824
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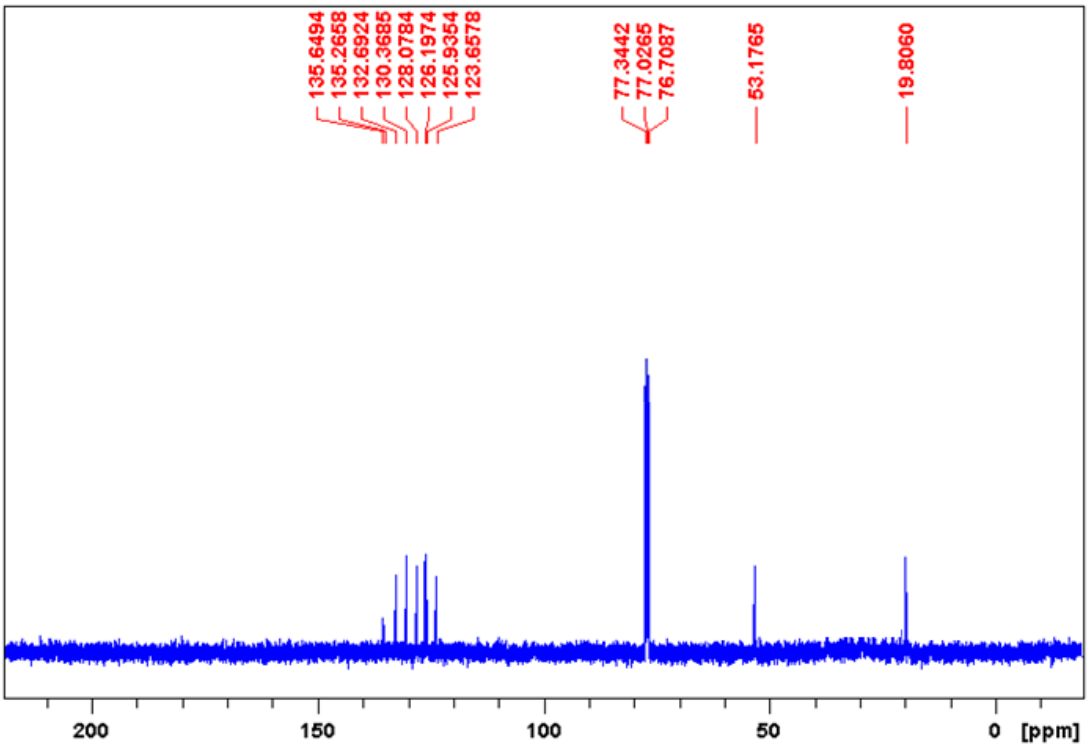
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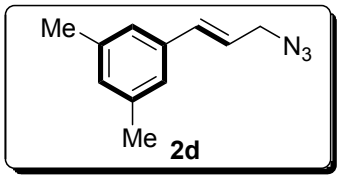
Me
N3
Me
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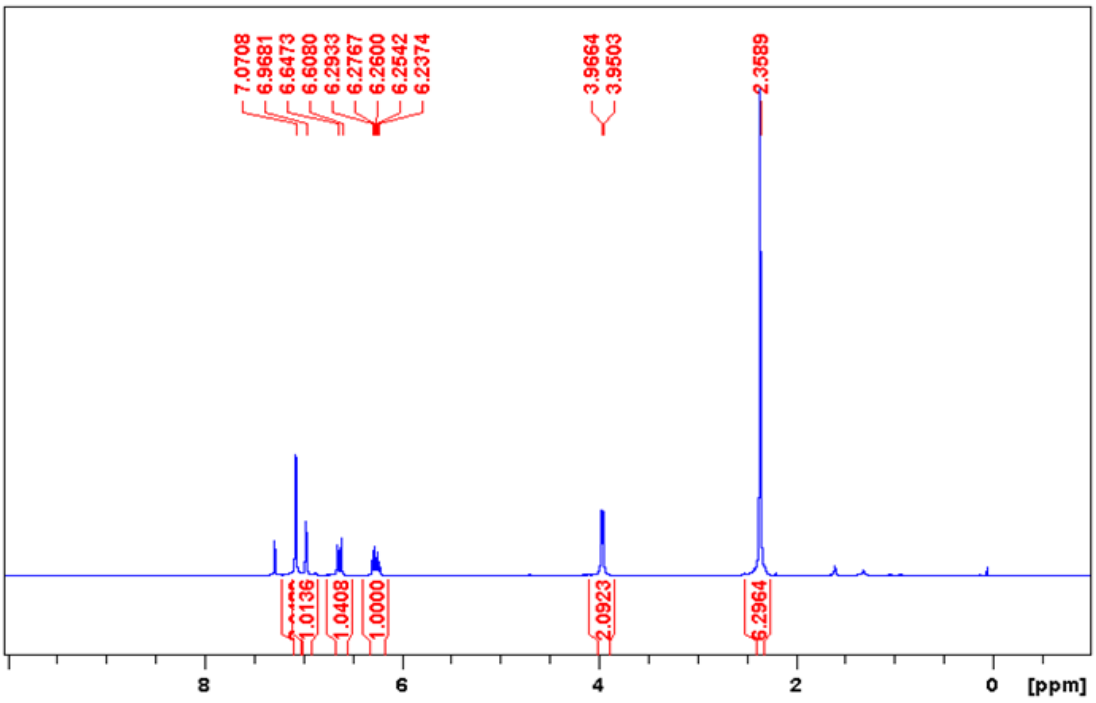
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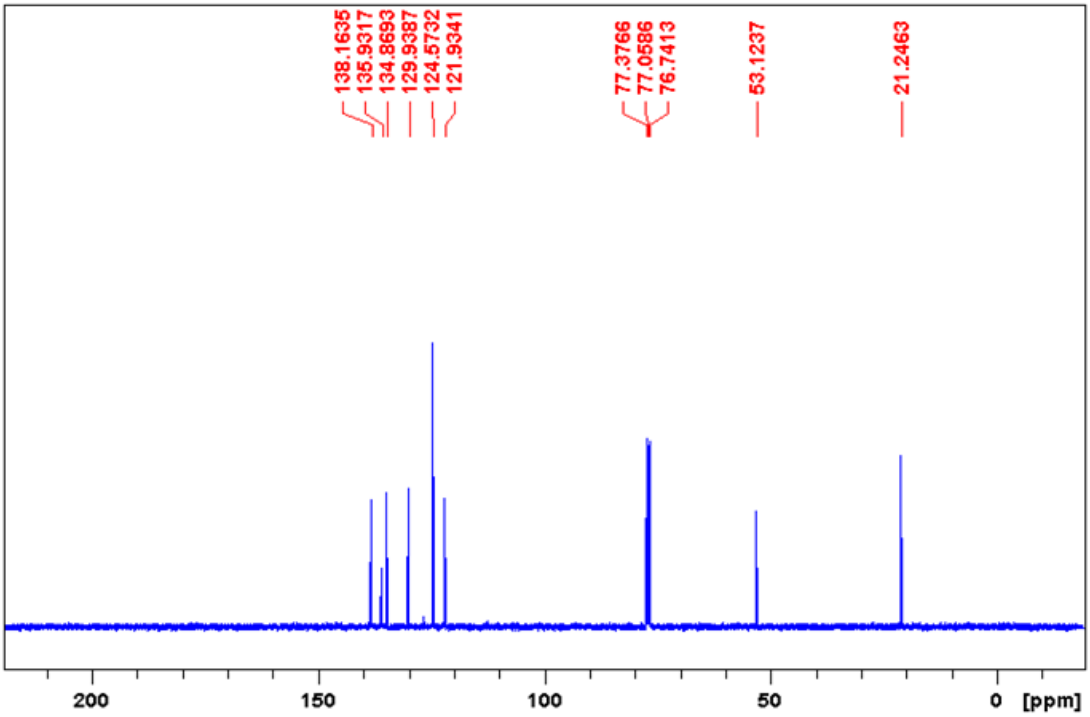
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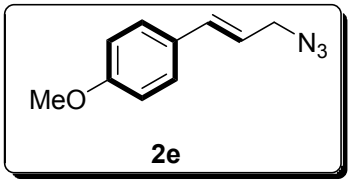
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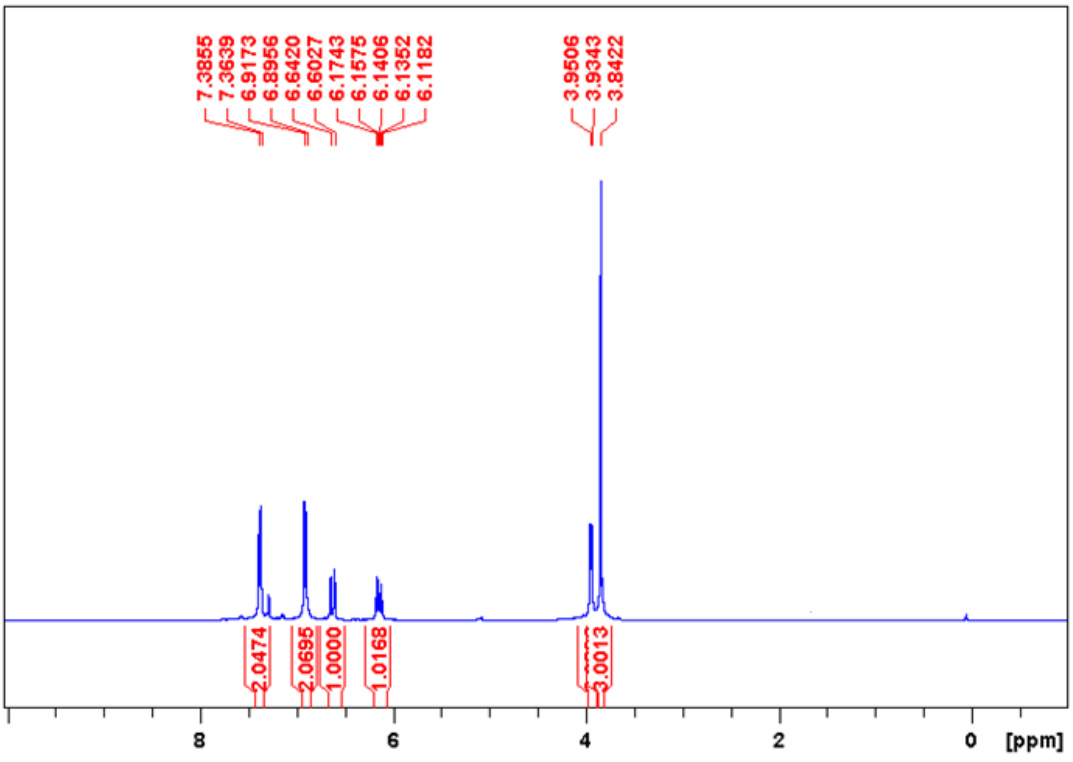
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6.6027
6.1743
6.1575
6.1406
6.1352
6.1182
3.9506
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3.0013
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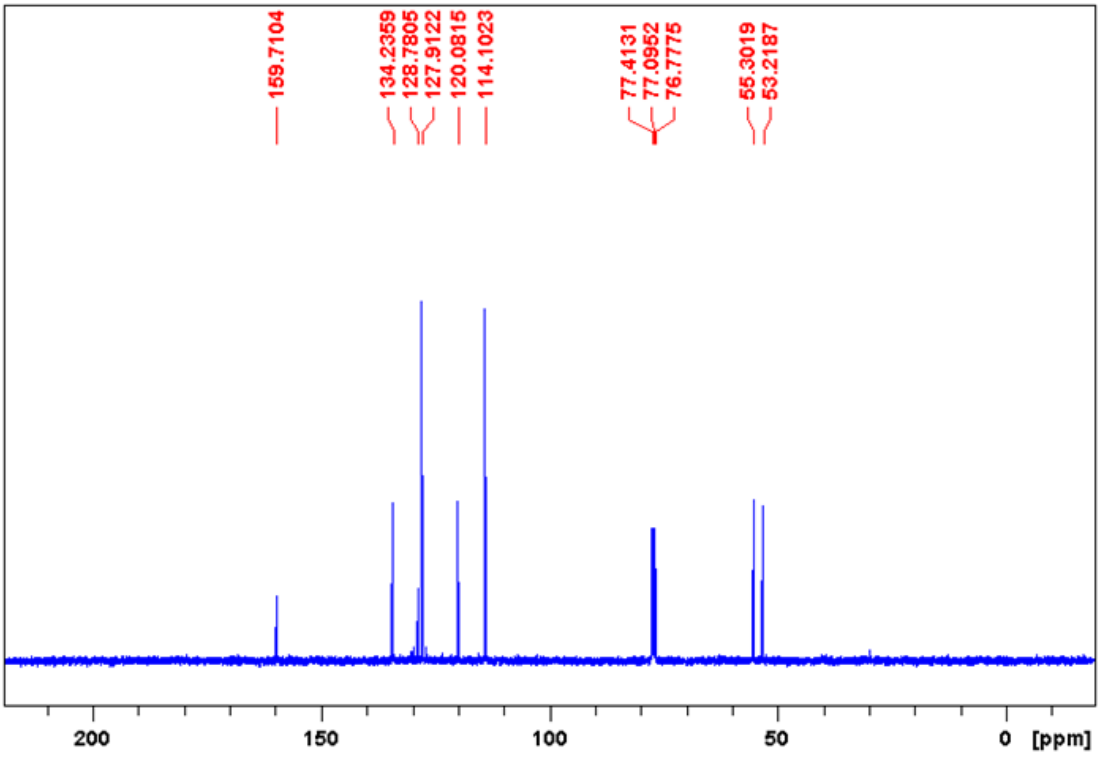
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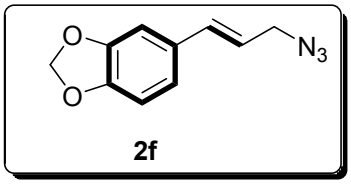
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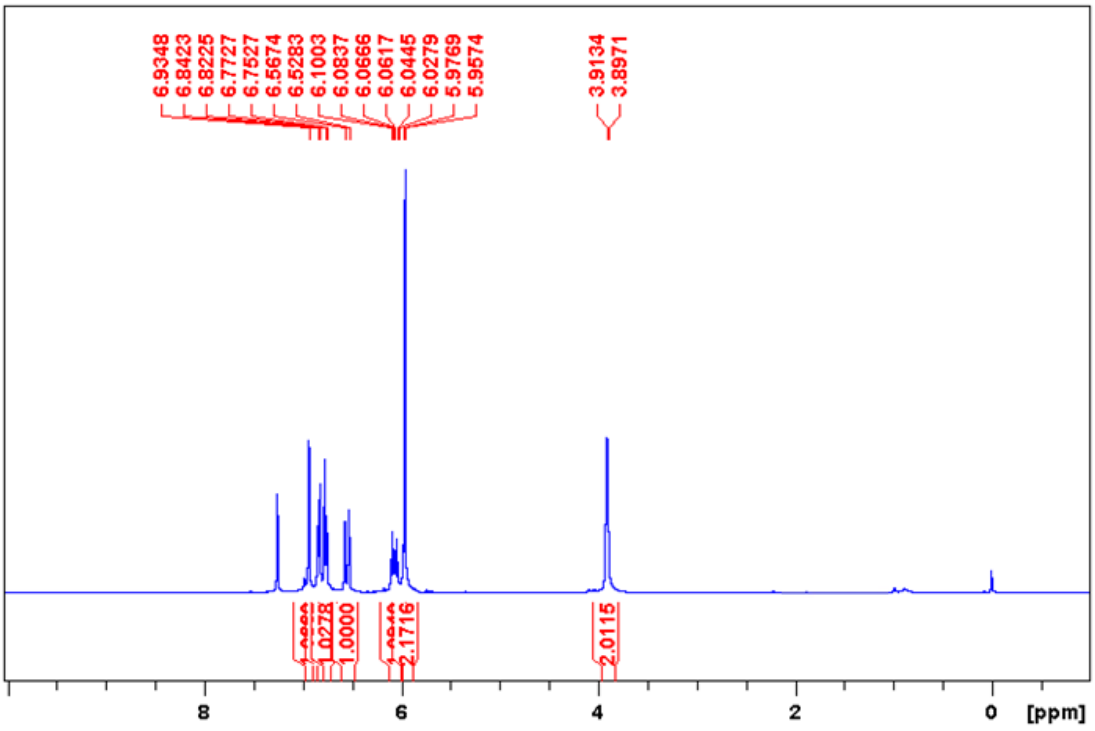
O
N3

2f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6.5283
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6.0837
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5.9769
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2.0115
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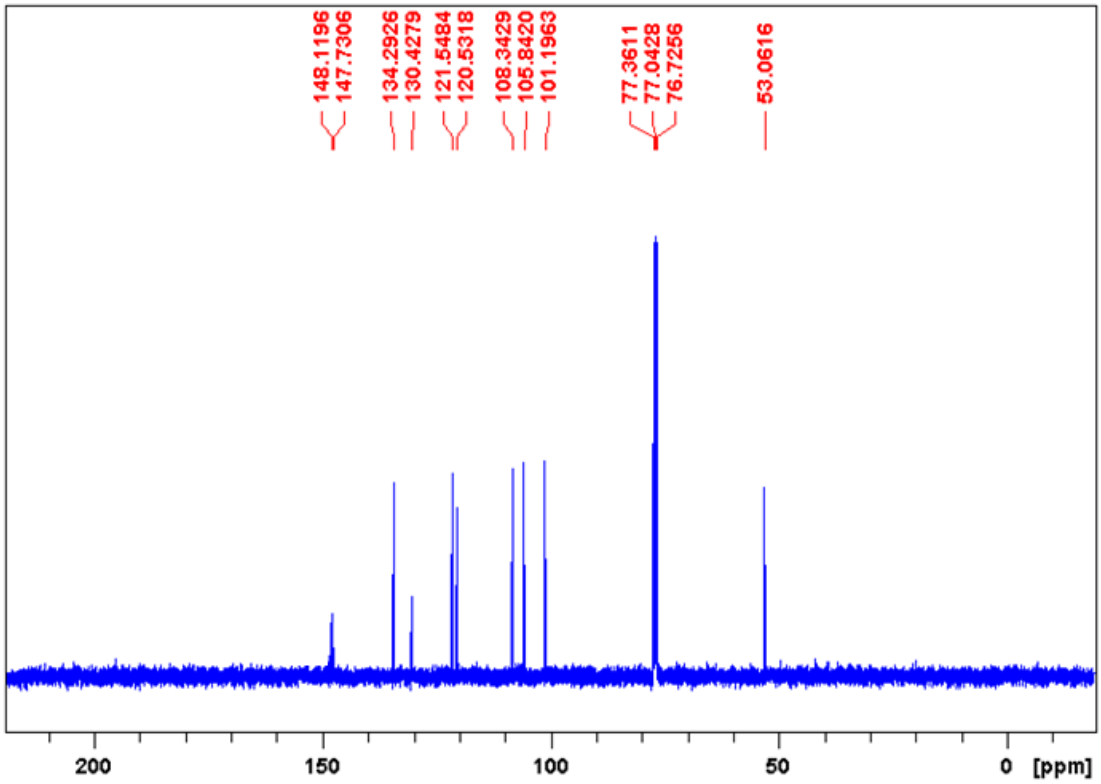
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130.4279
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120.5318
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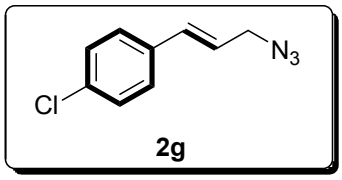
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Cl

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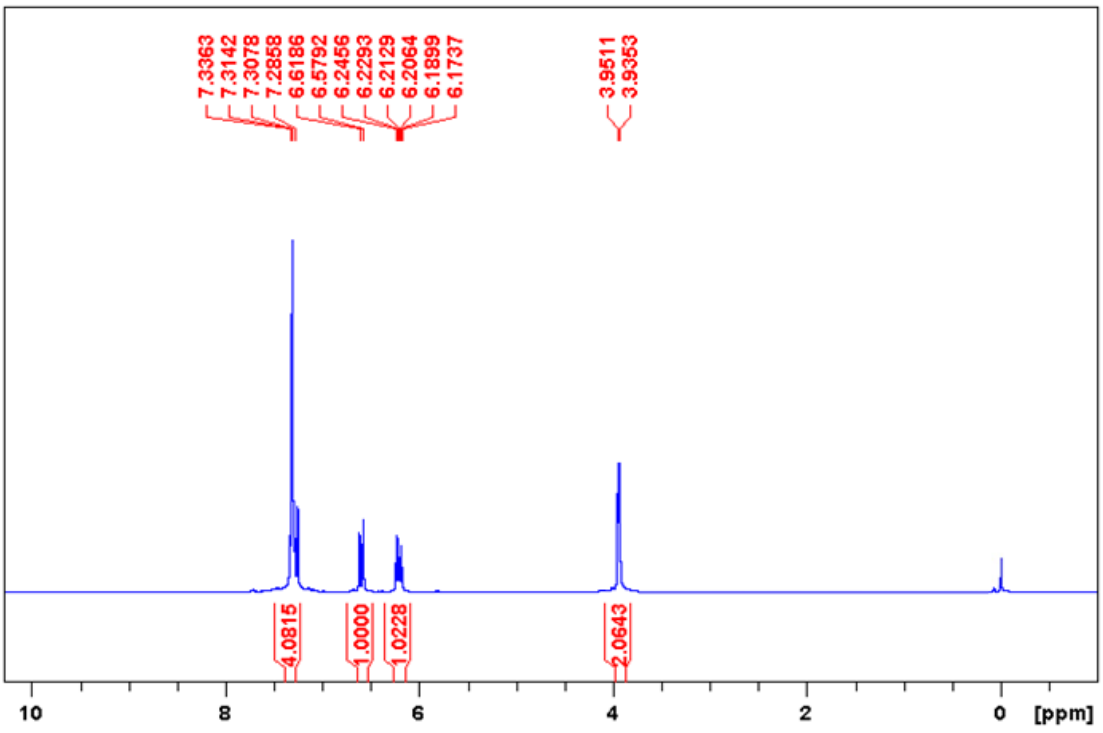
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6.2129
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6.1899
6.1737
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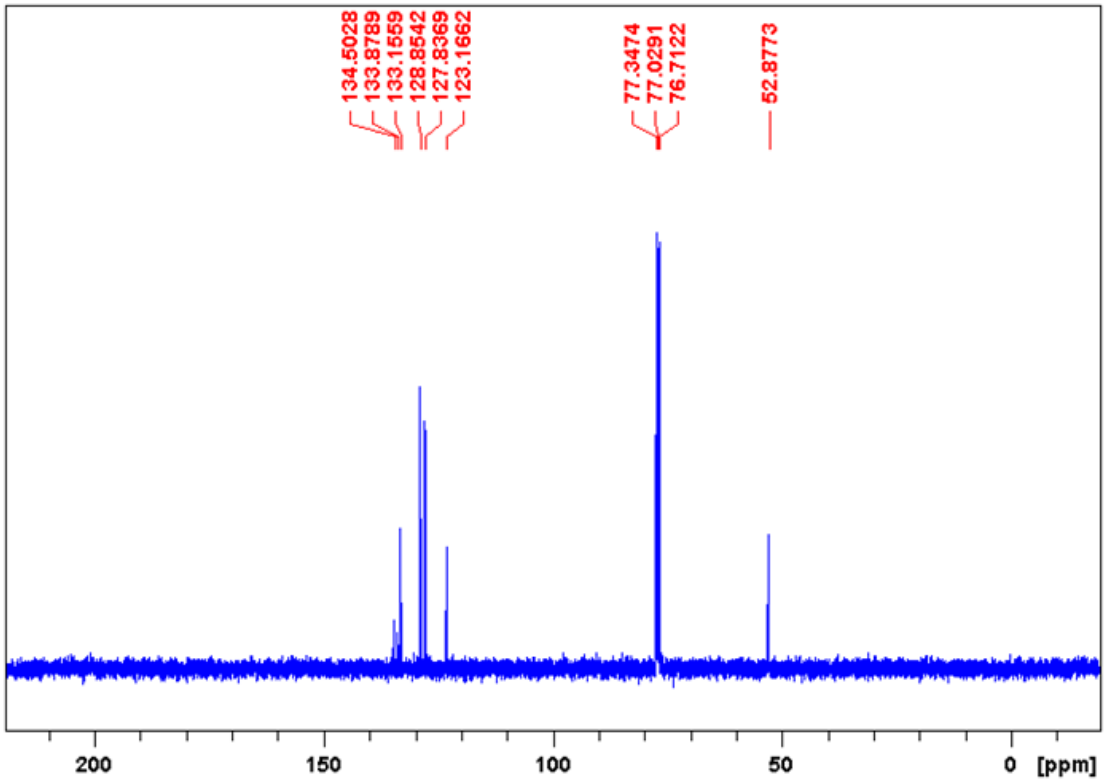
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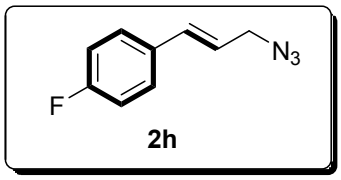
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F

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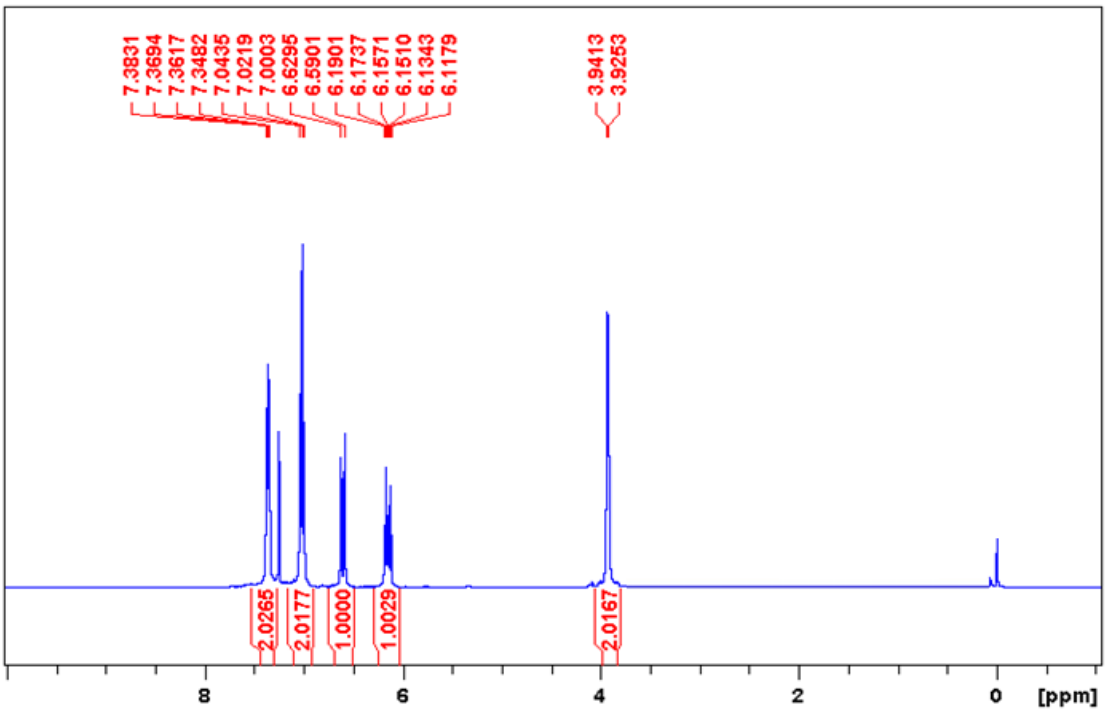
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7.0003
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6.1901
6.1737
6.1571
6.1510
6.1343
6.1179
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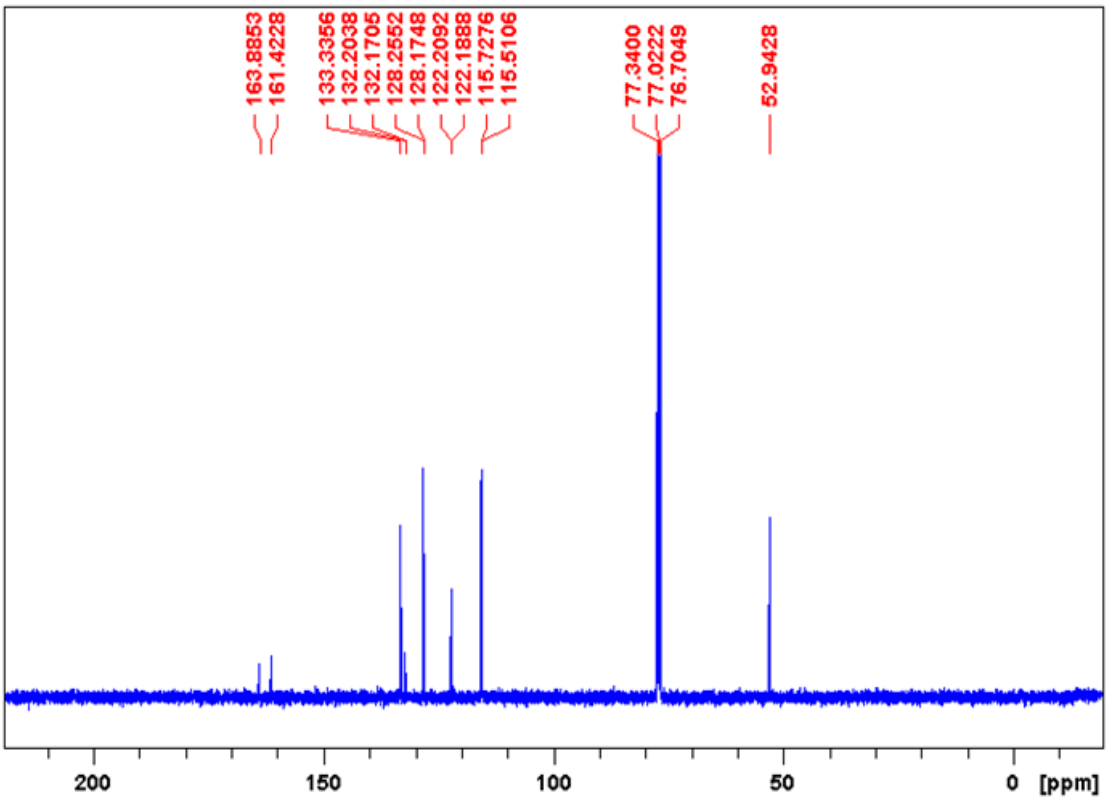
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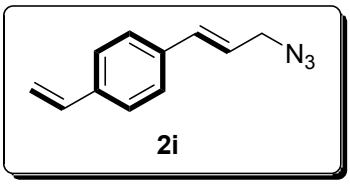
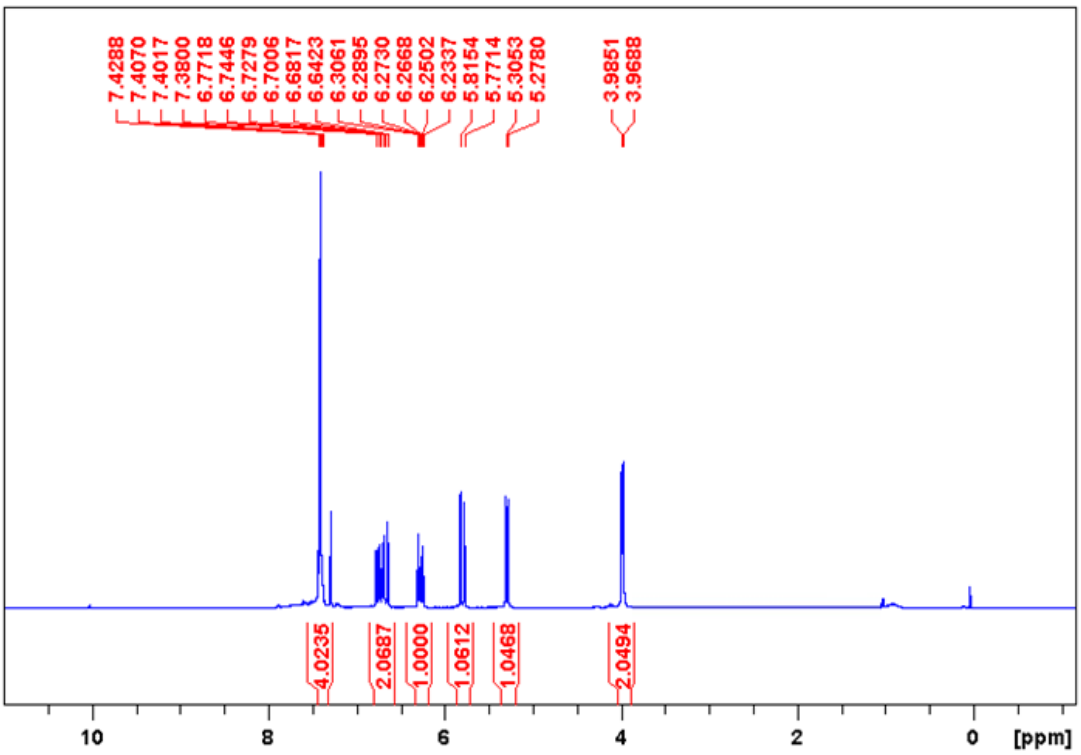

N3

2i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6.7279
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6.6817
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6.2895
6.2730
6.2668
6.2502
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5.7714
5.3053
5.2780
3.9851
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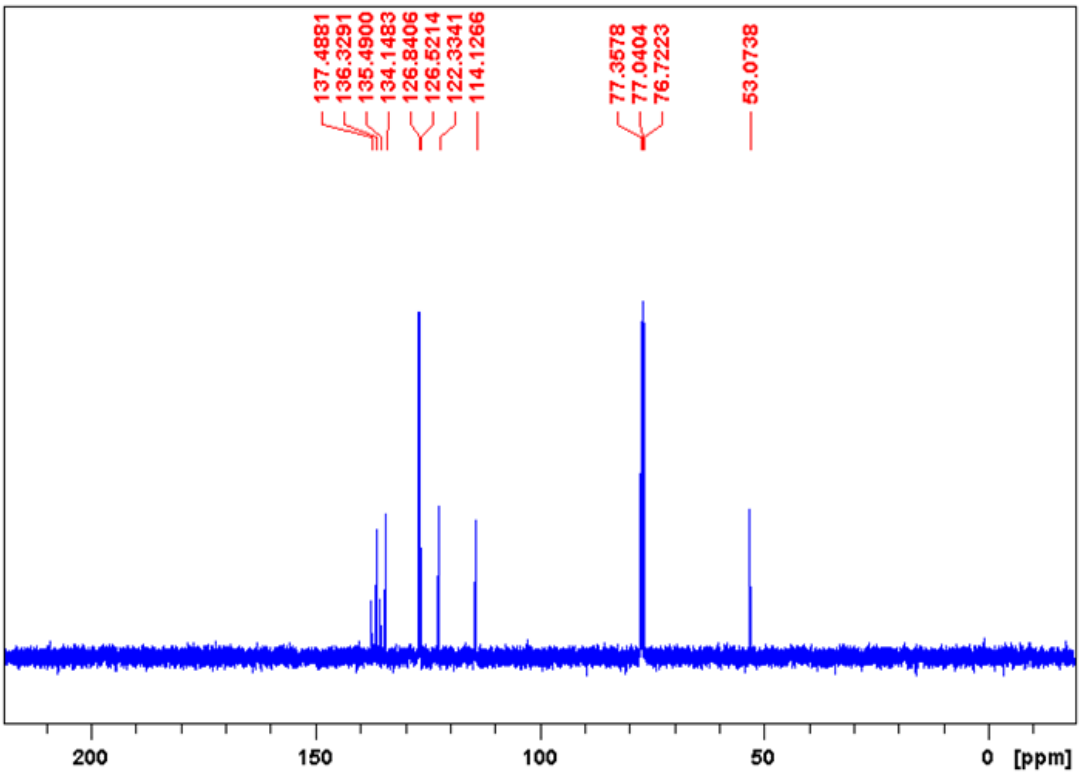
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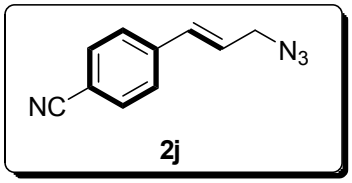
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NC

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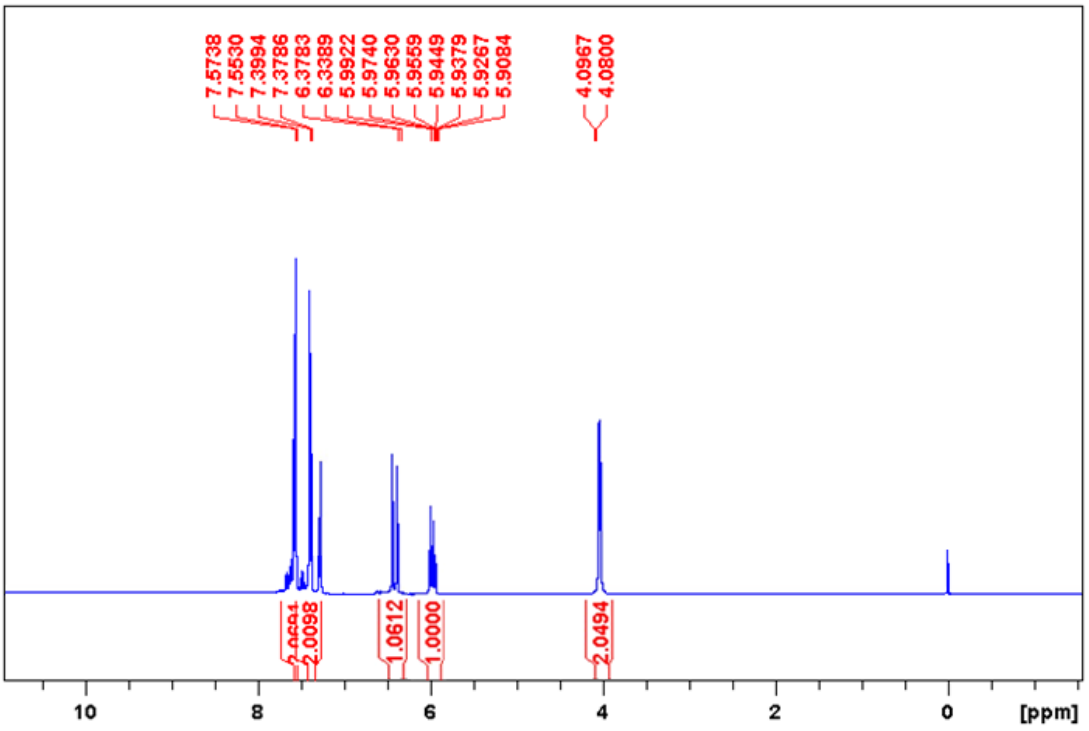
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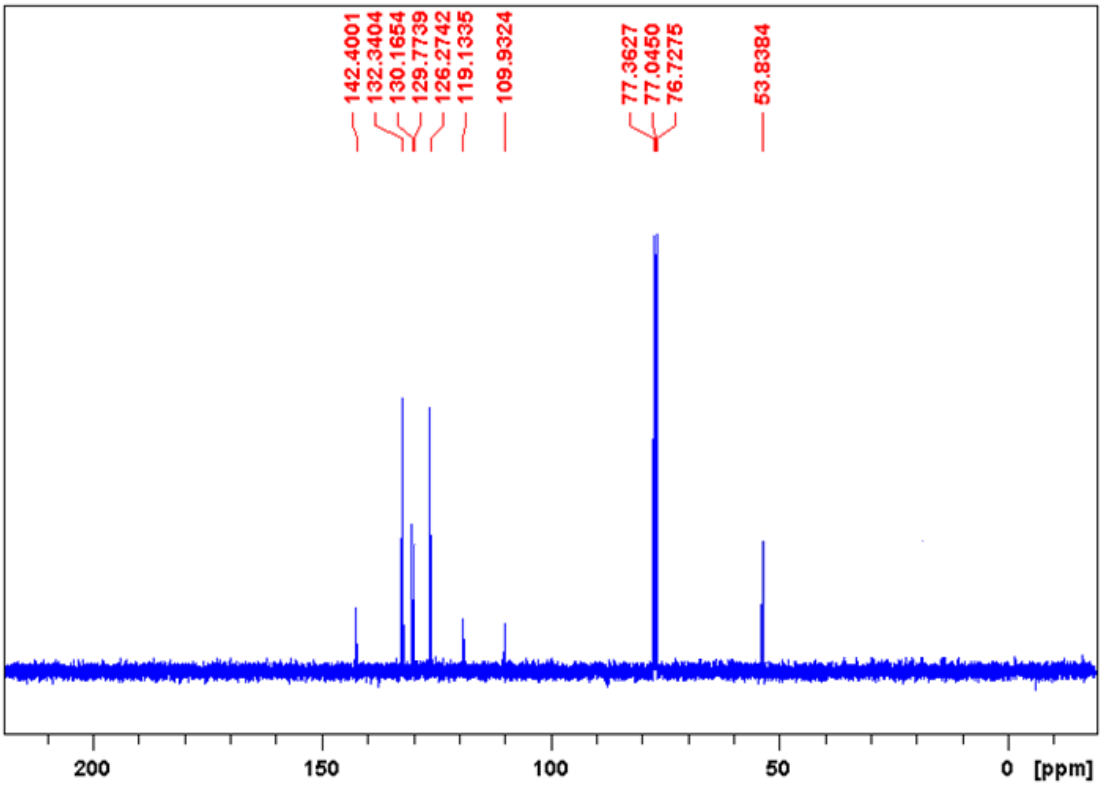
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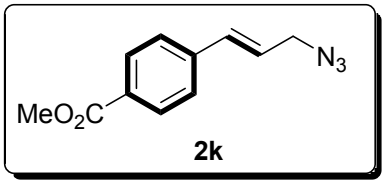
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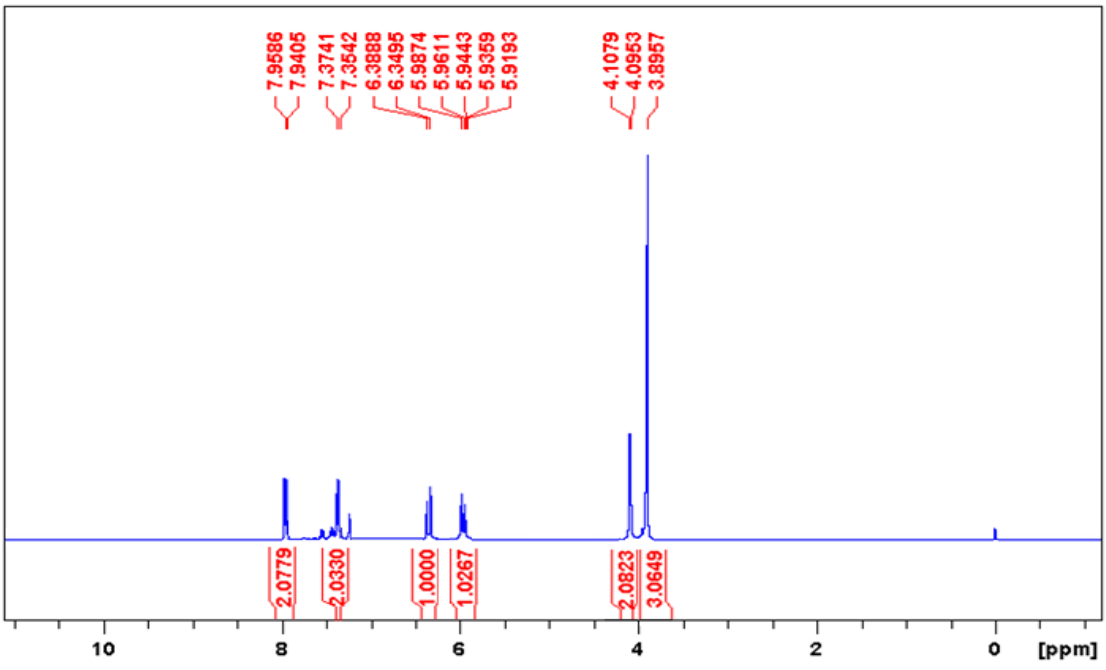
MeO2C

2k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4.0953
3.8957
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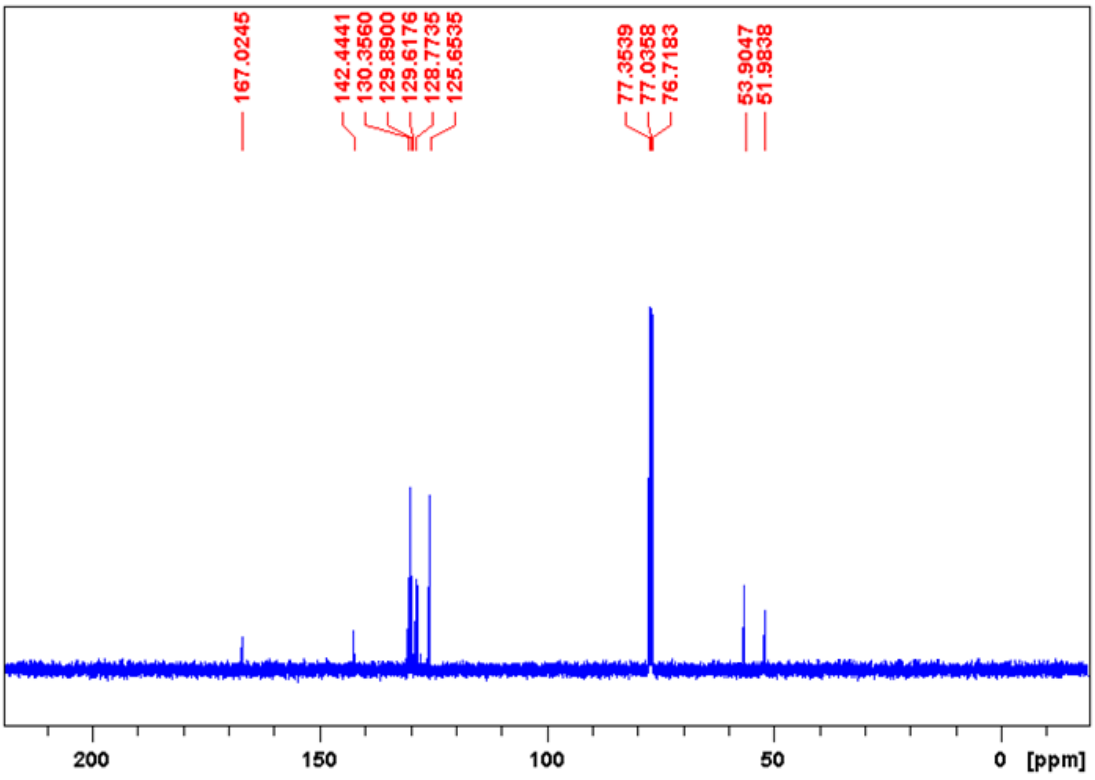
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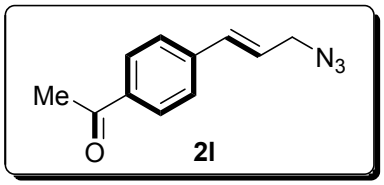
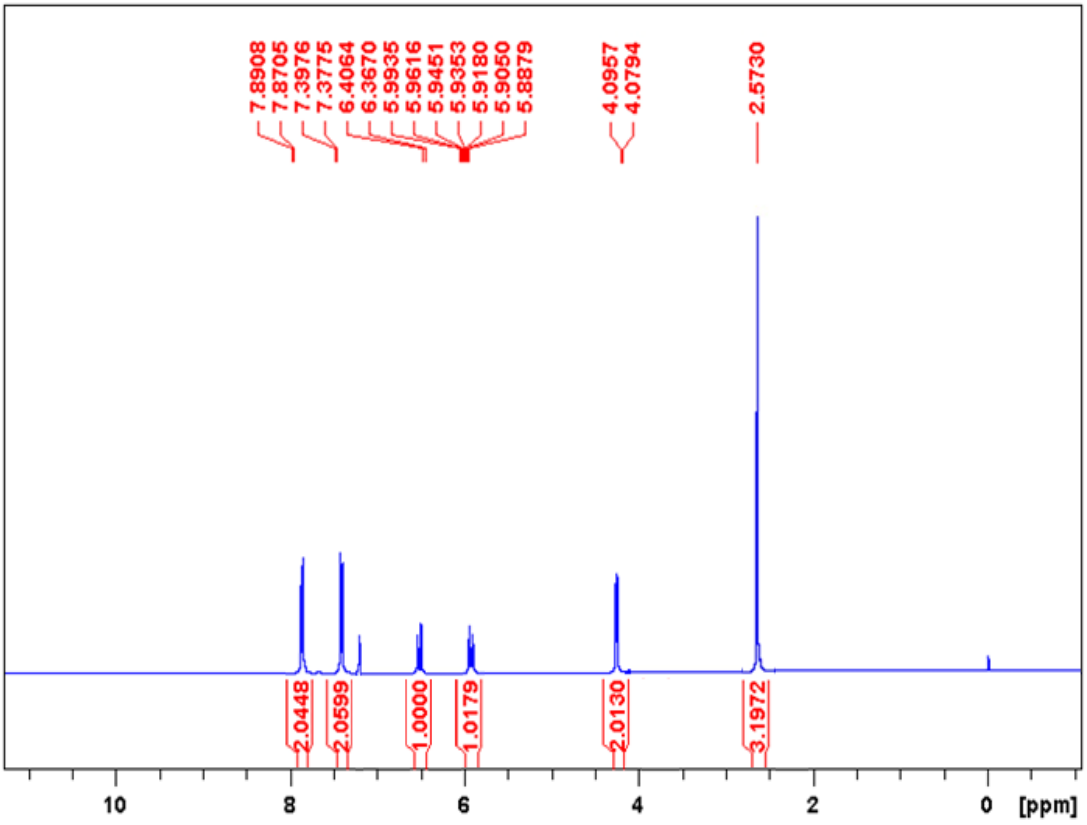

Me
O
N3

2l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5.9050
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4.0794
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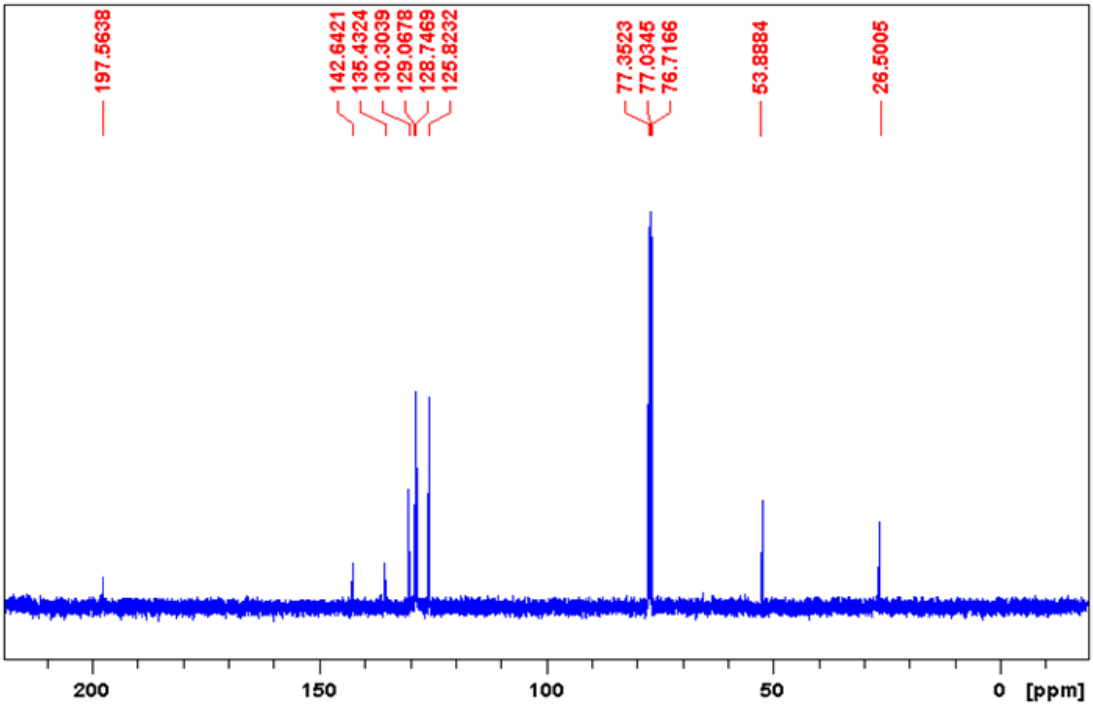
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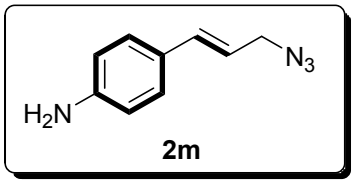
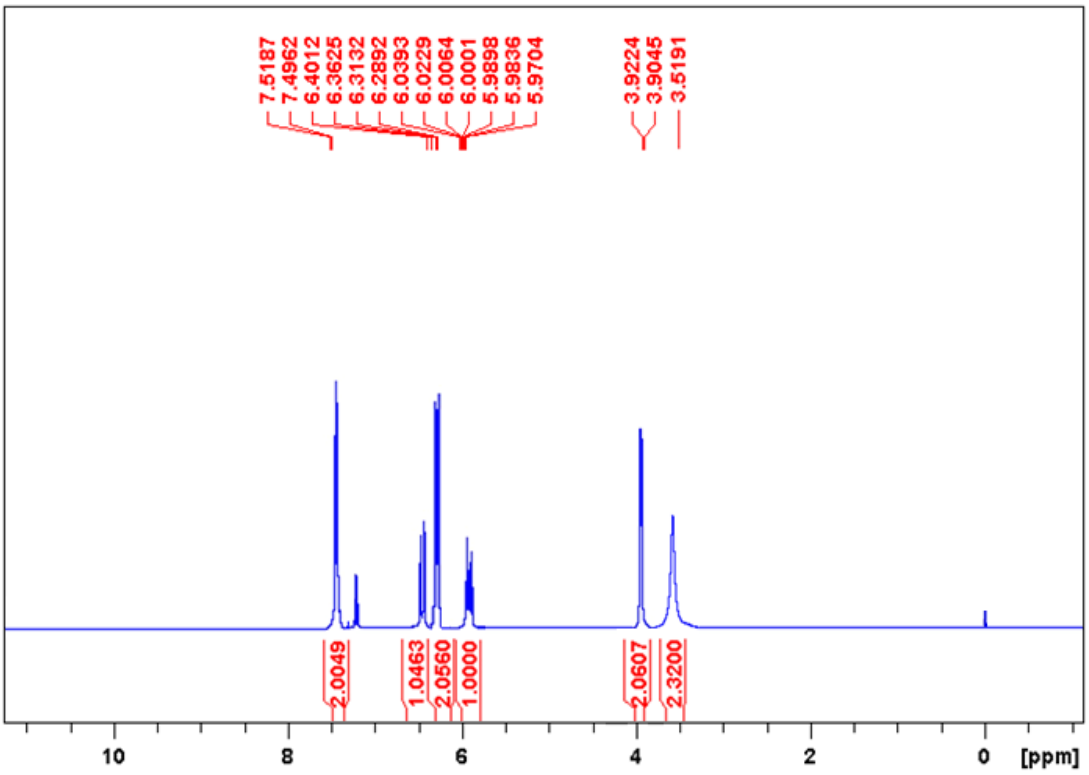

H_2N
N_3

2m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3.9045
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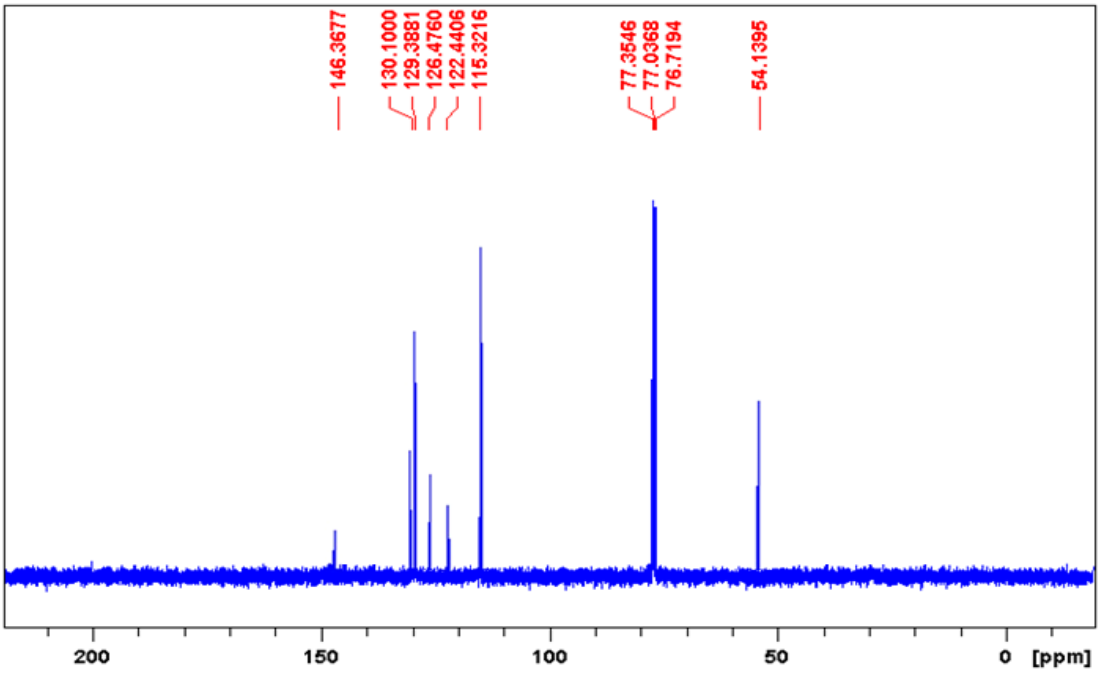
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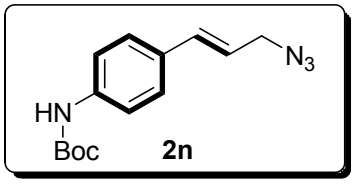
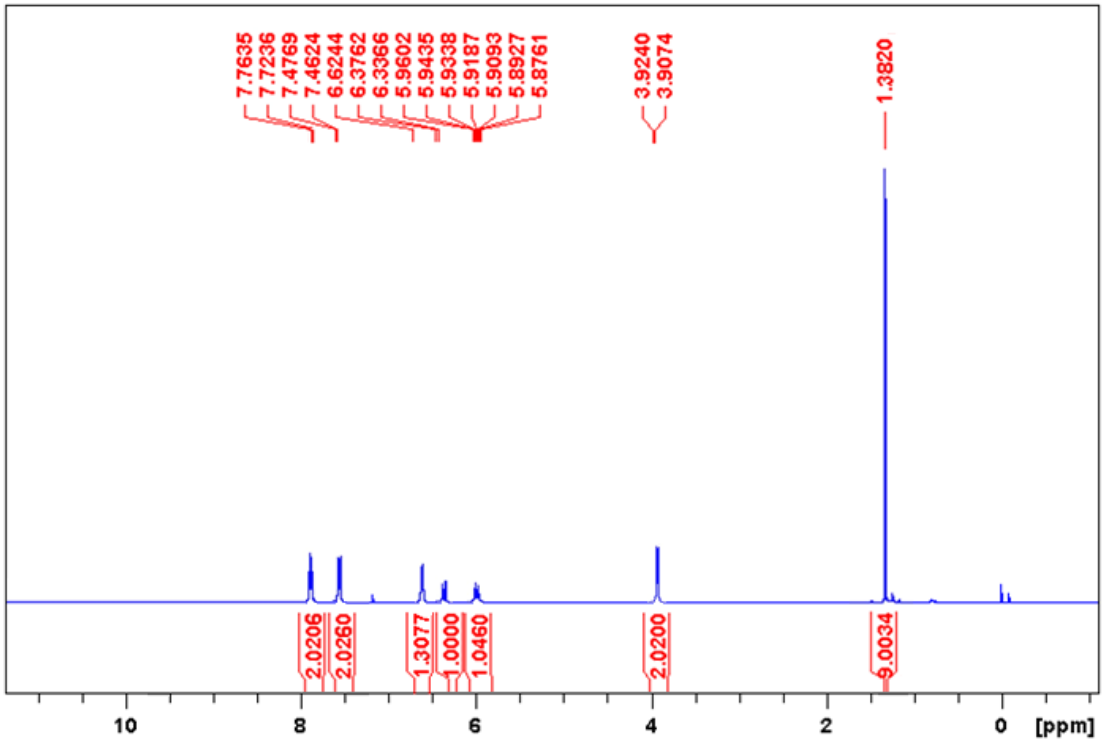

HN
Boc
N3

2n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3.9074
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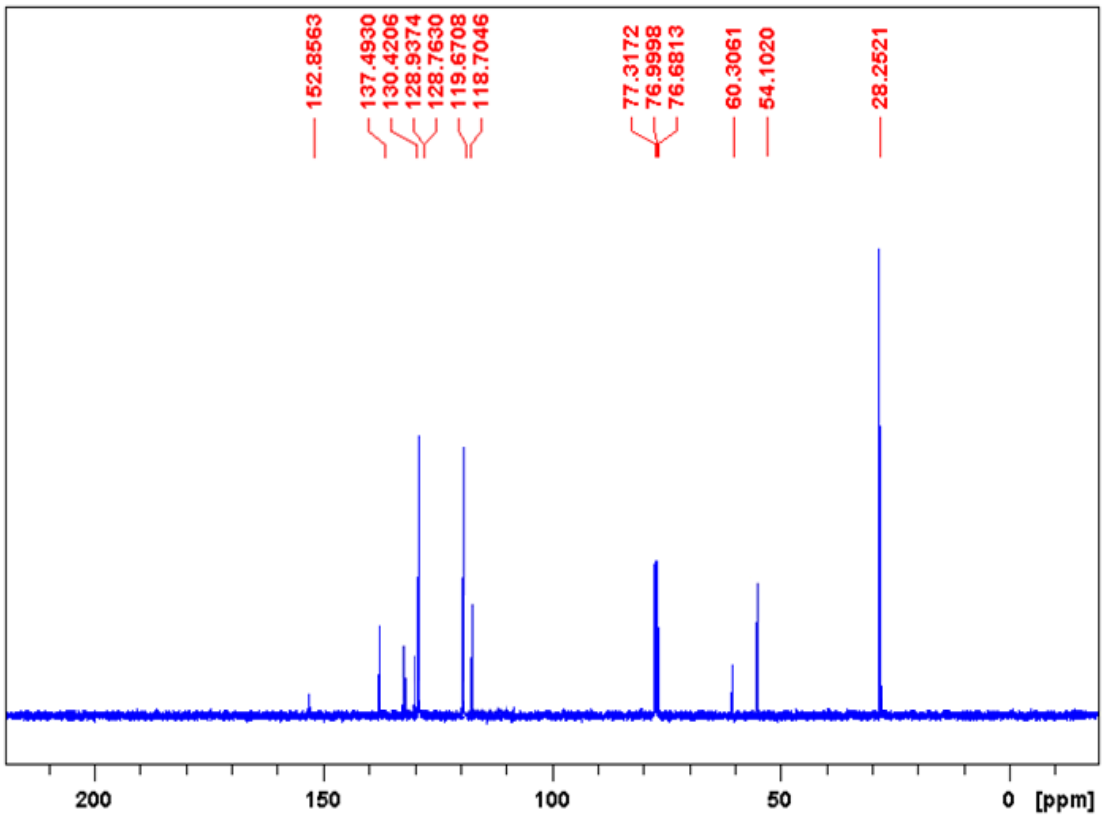
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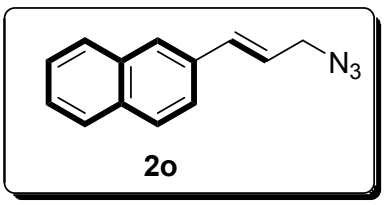
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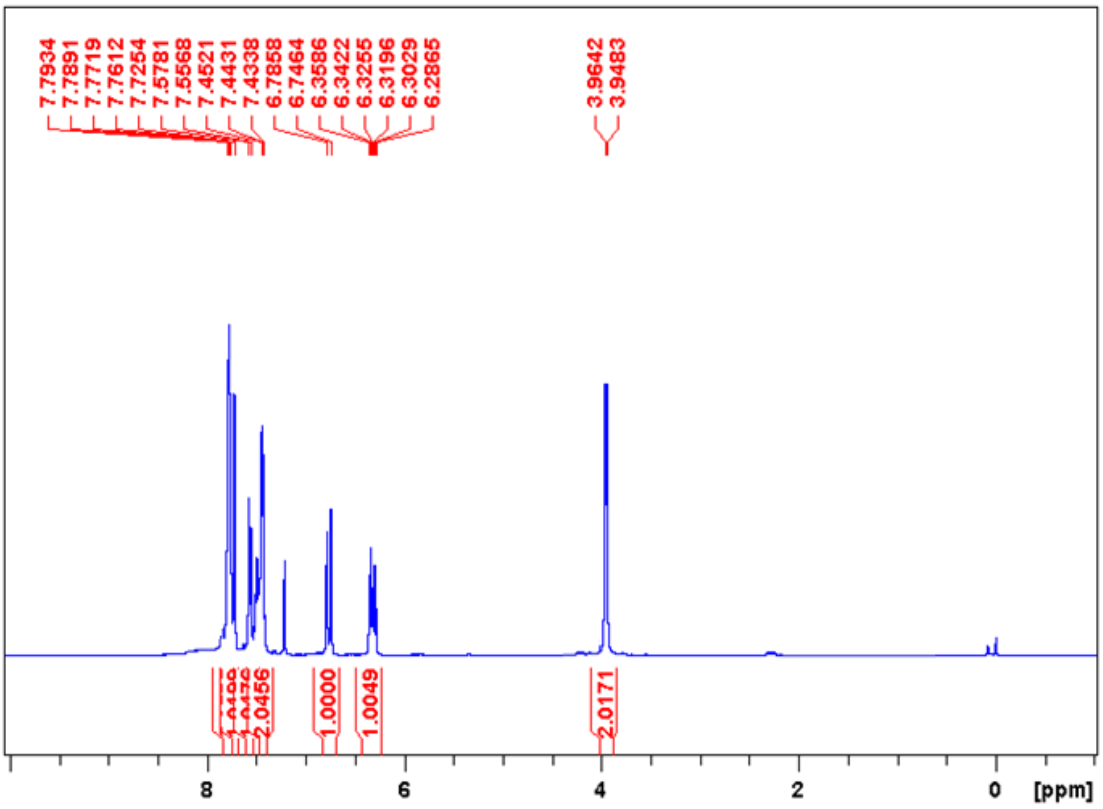
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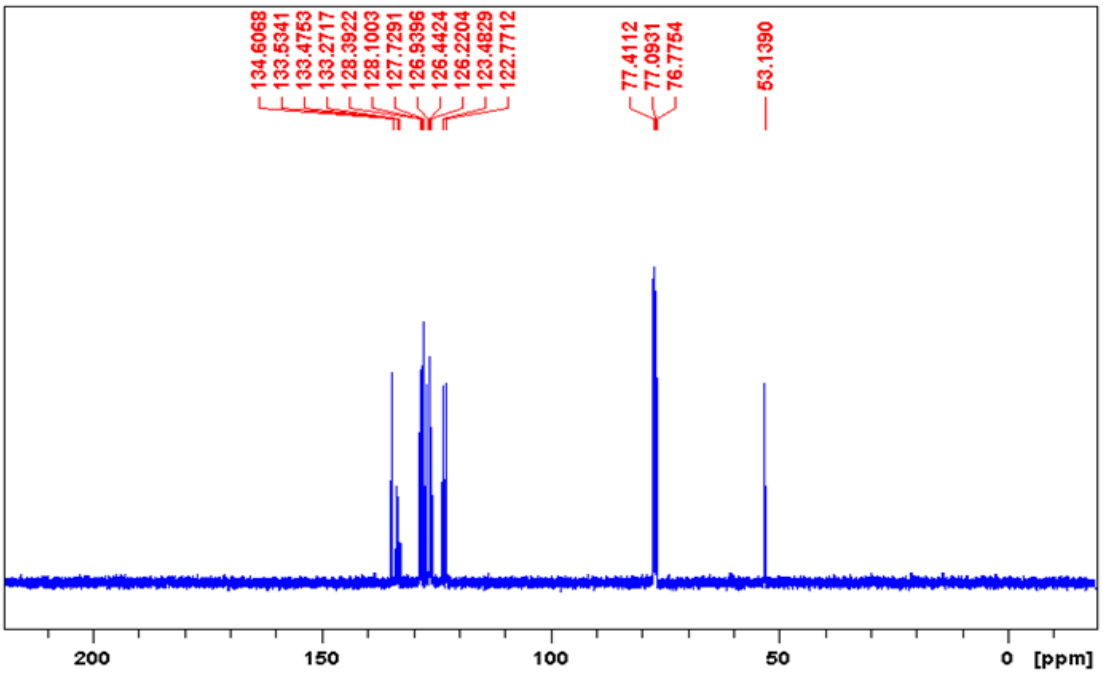
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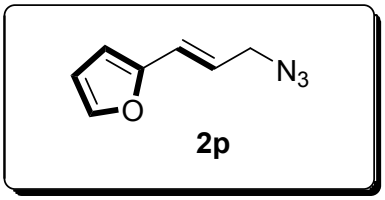
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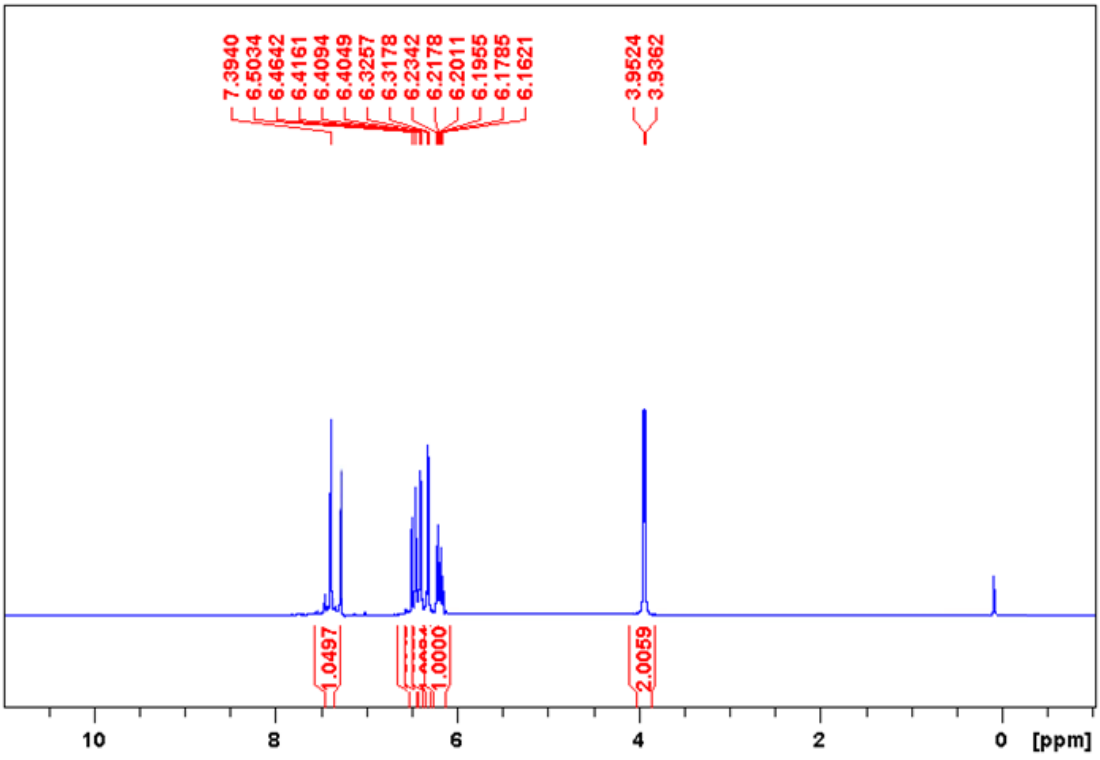
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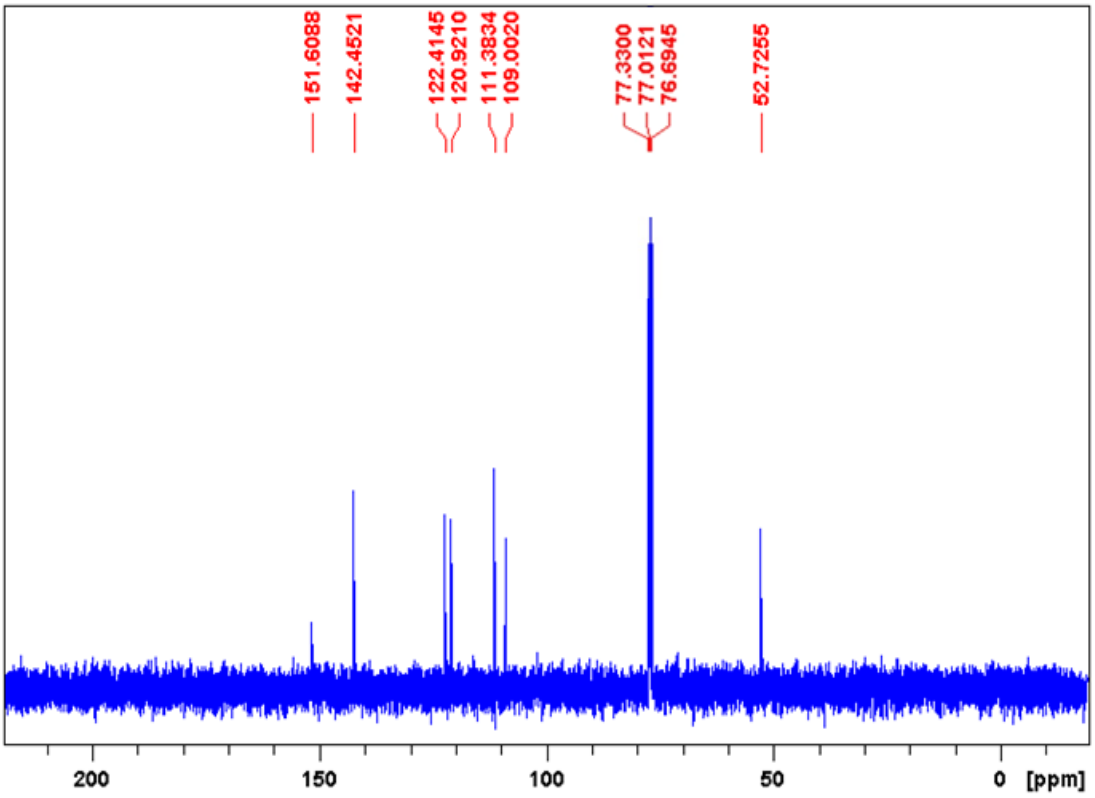
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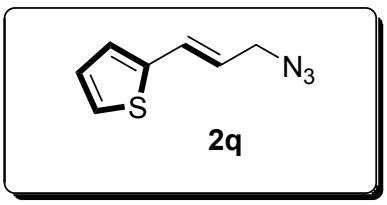
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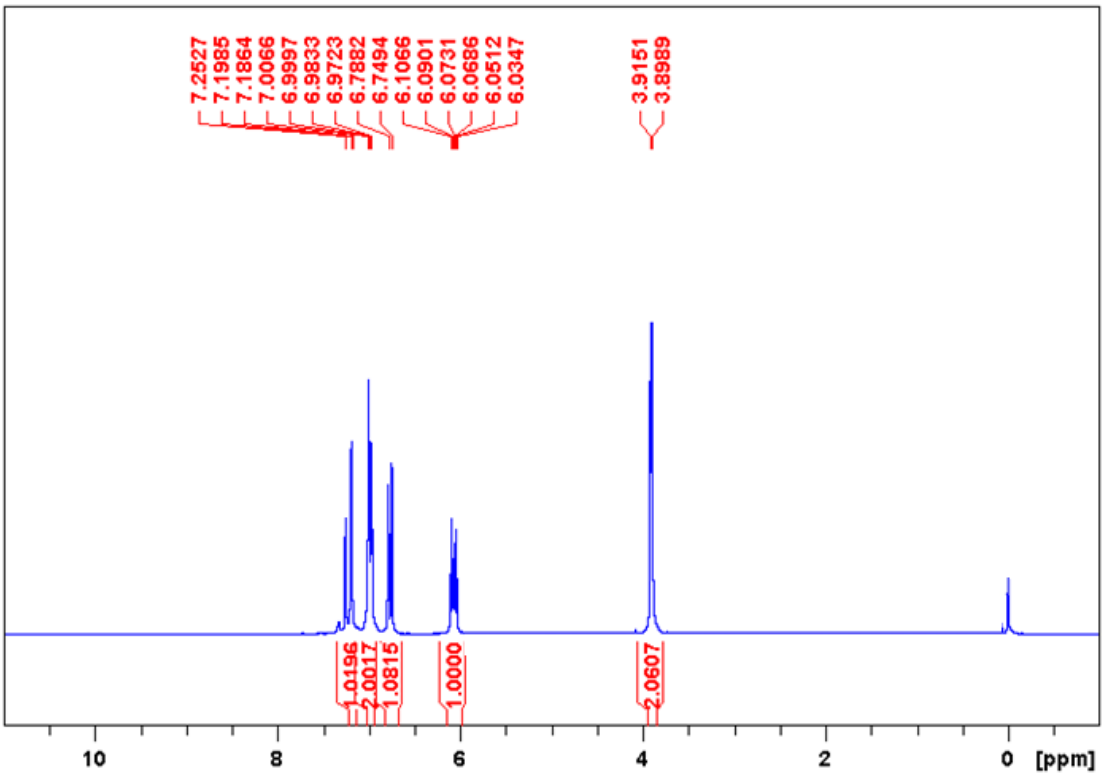
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6.1066
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6.0731
6.0686
6.0512
6.0347
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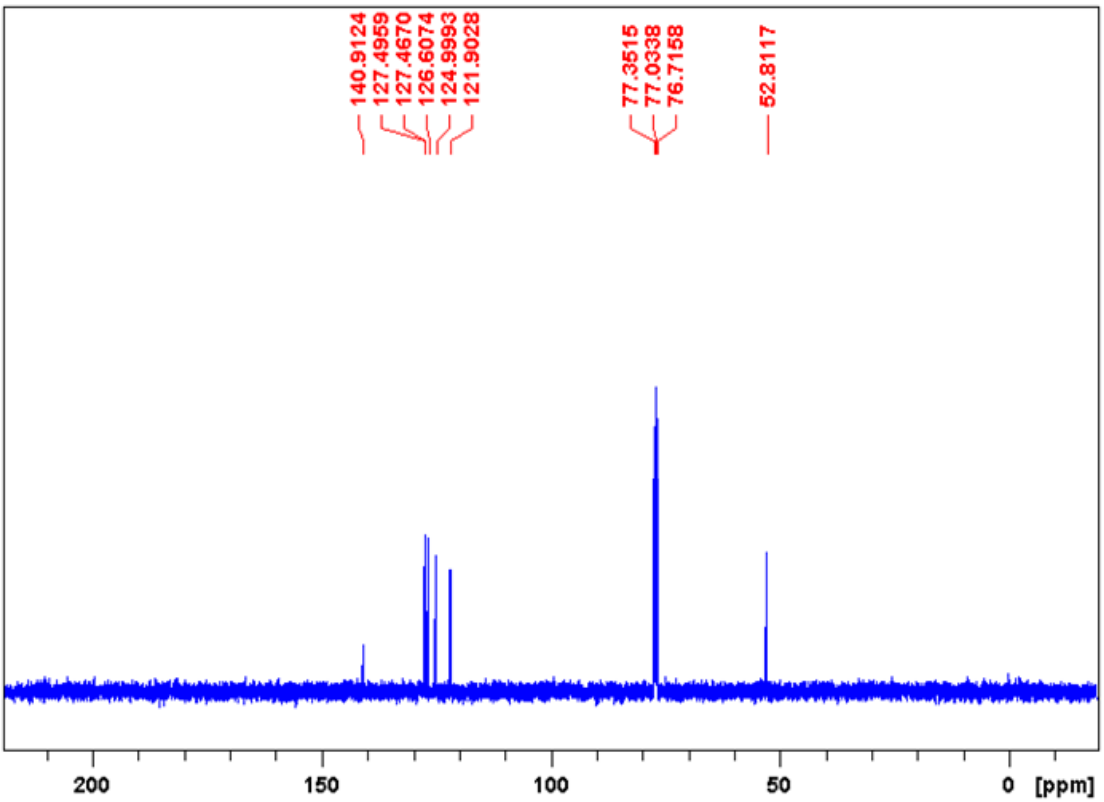
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76.7158
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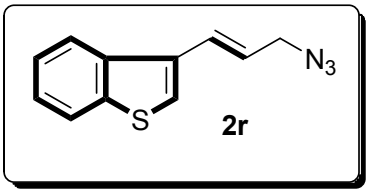
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S
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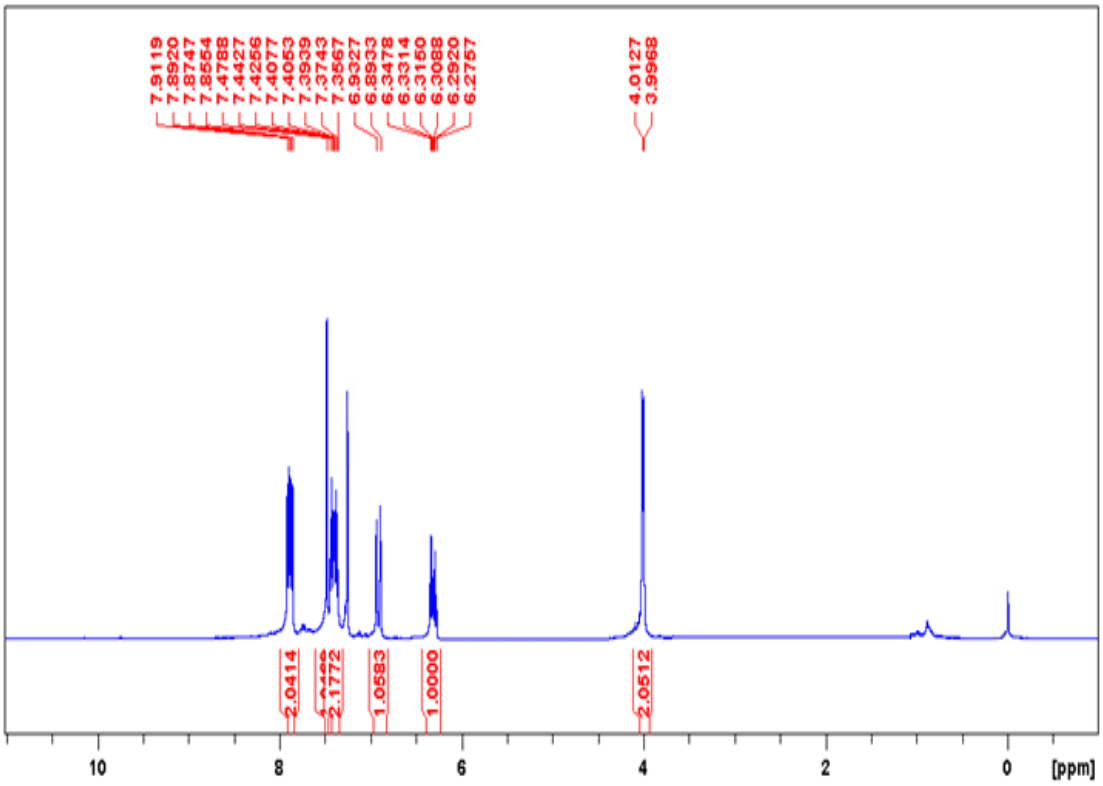
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7.4053
7.3939
7.3743
7.3567
6.9327
6.8933
6.3478
6.3314
6.3150
6.3088
6.2920
6.2757
4.0127
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1.0000
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2
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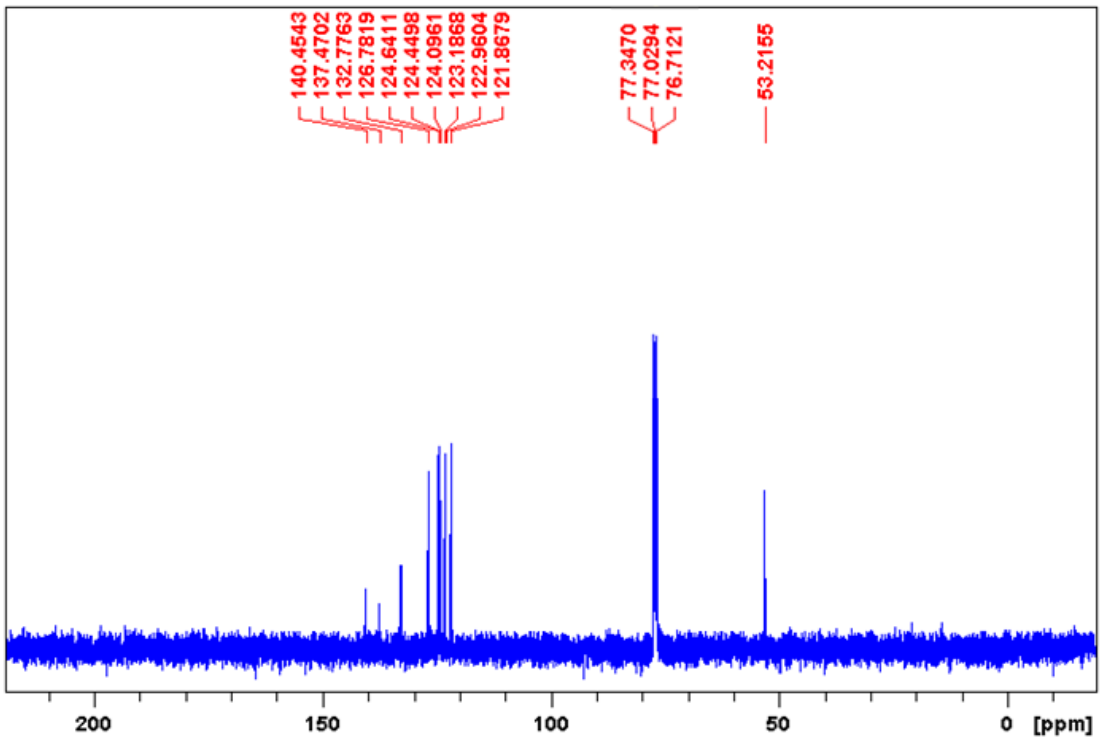
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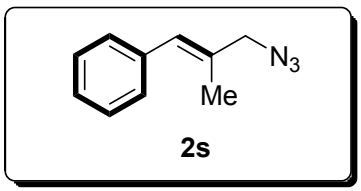
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Me

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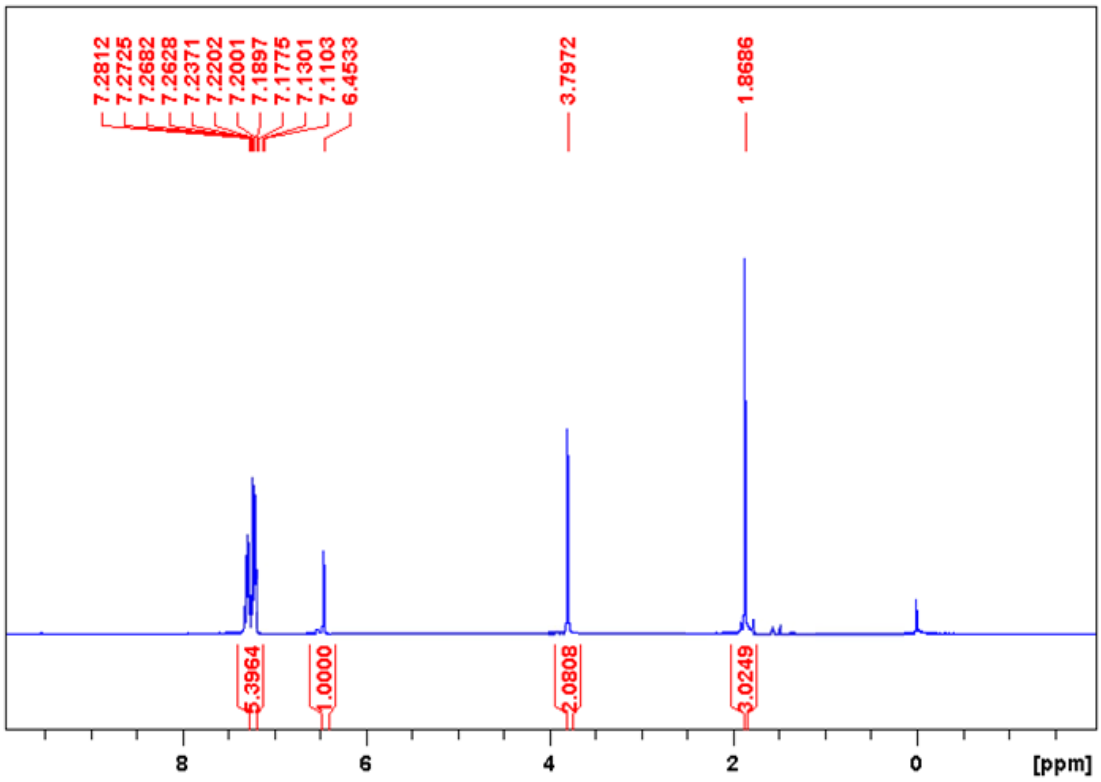
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7.2371
7.2202
7.2001
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7.1103
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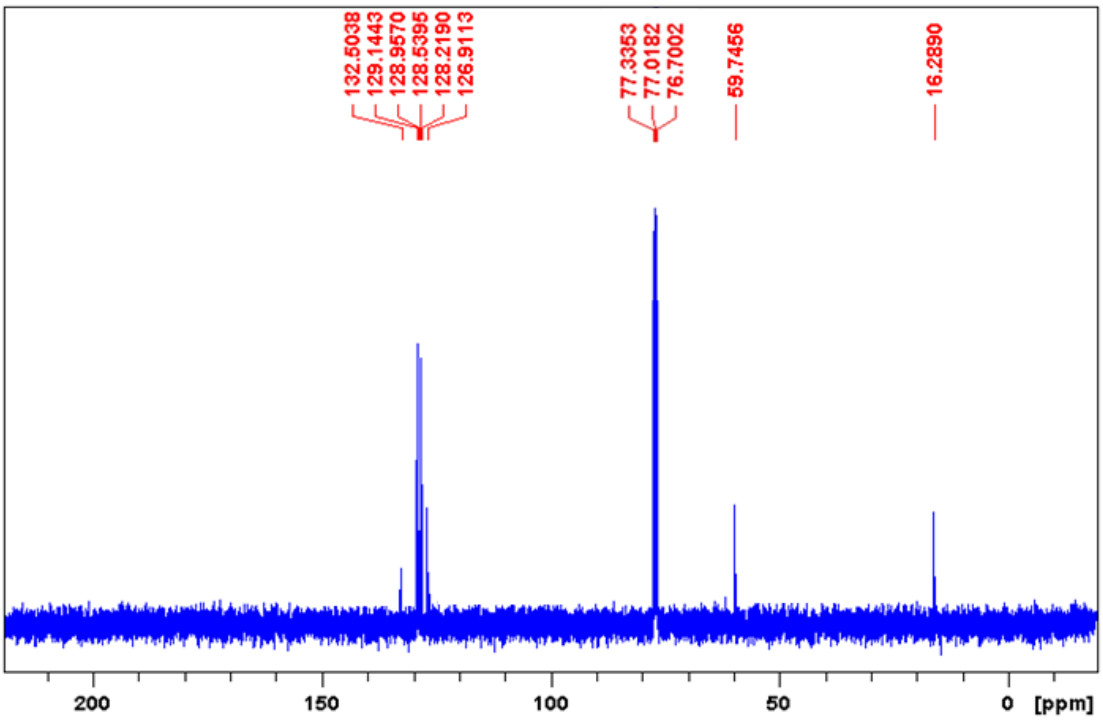
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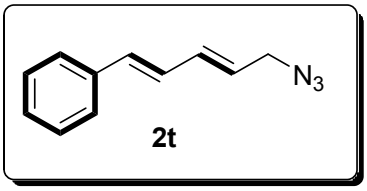
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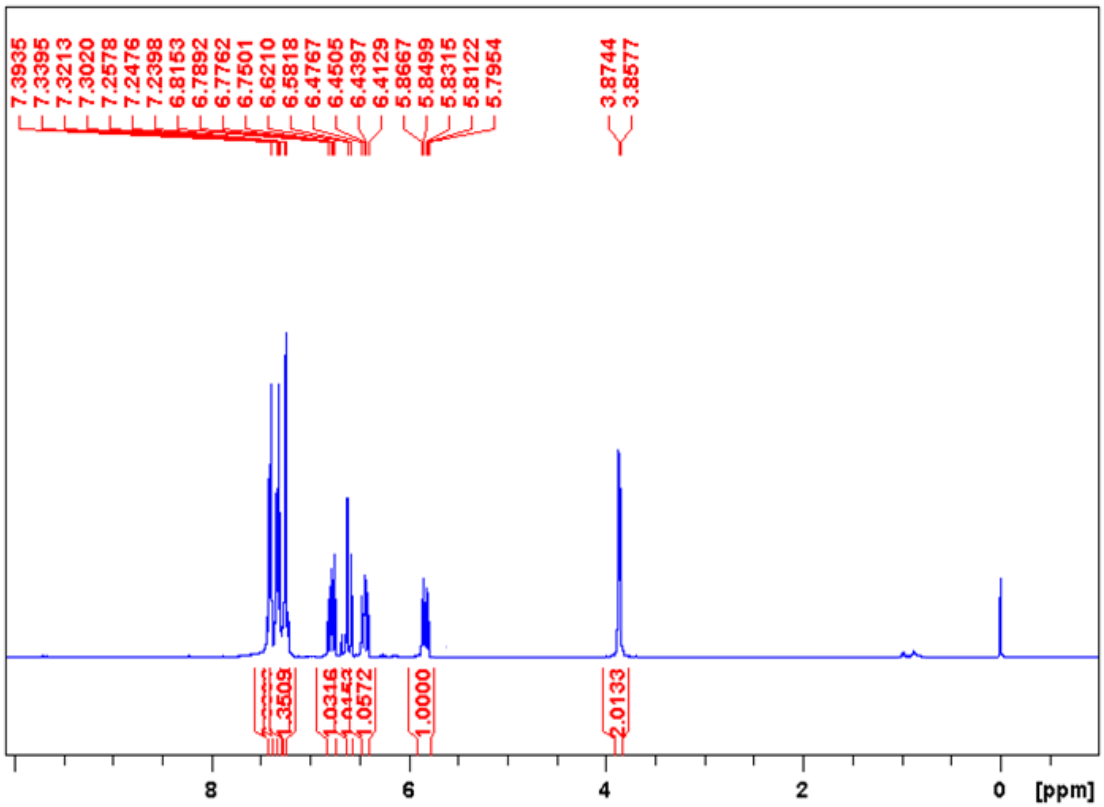
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6.7892
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6.7501
6.6210
6.5818
6.4767
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6.4397
6.4129
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5.8122
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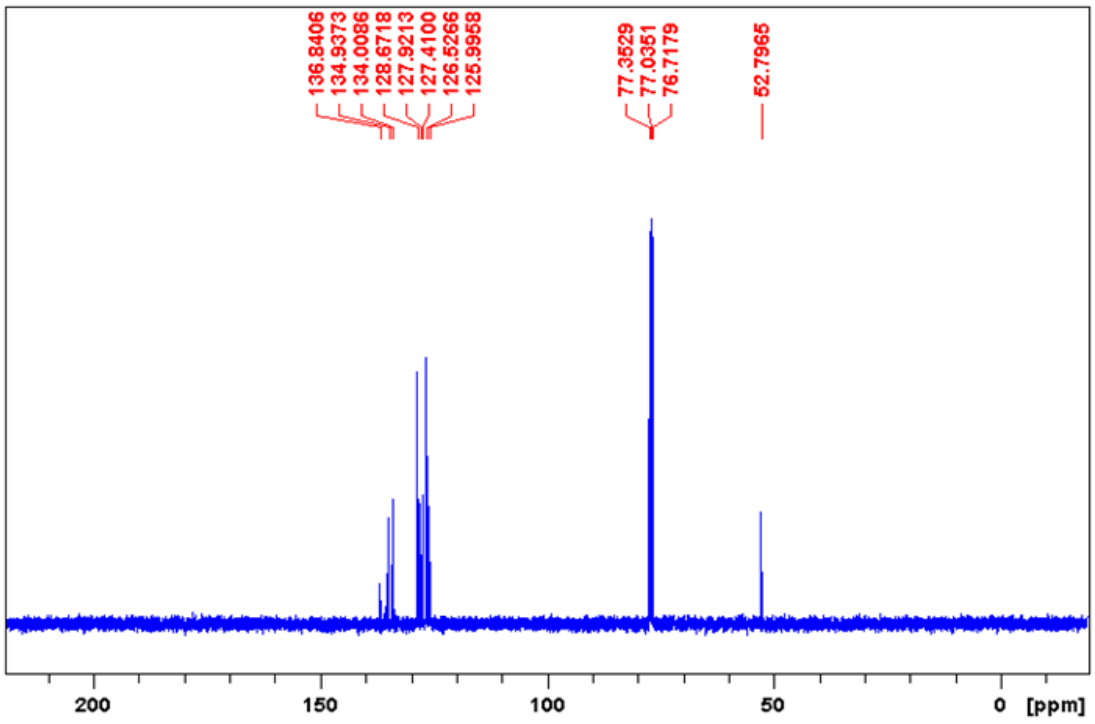
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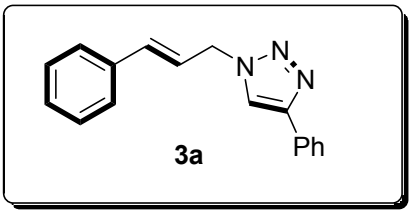
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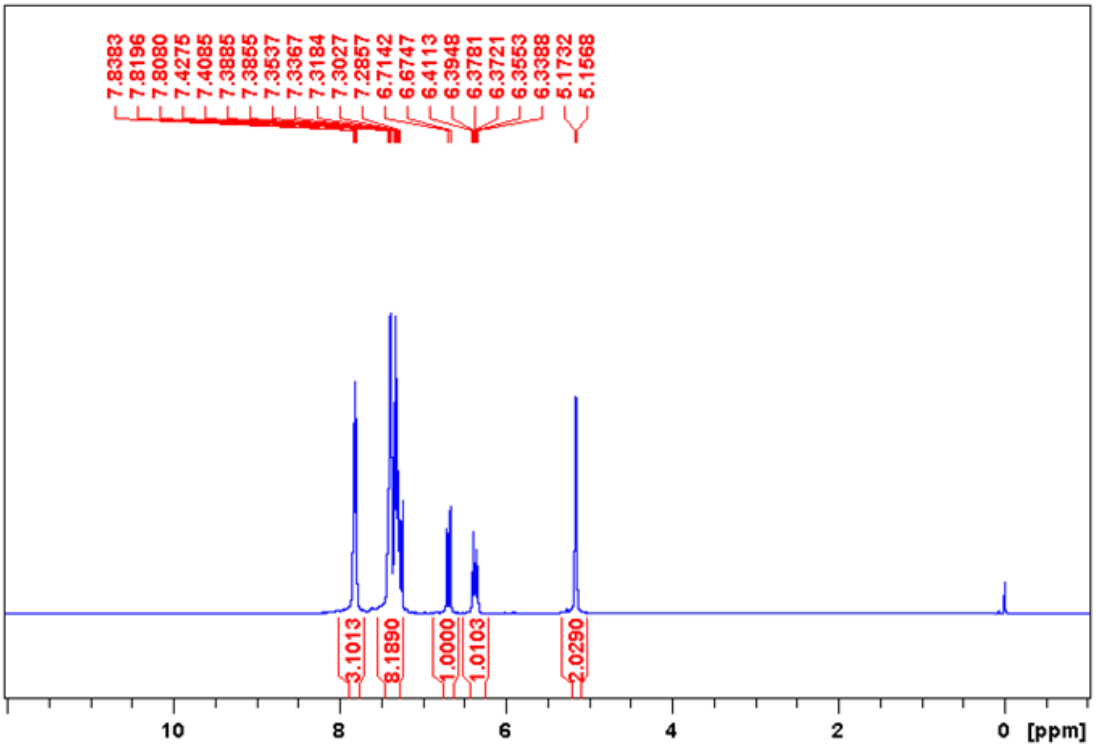
N
N
Ph

3a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7.3885
7.3855
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7.3367
7.3184
7.3027
7.2857
6.7142
6.6747
6.4113
6.3948
6.3781
6.3721
6.3553
6.3388
5.1732
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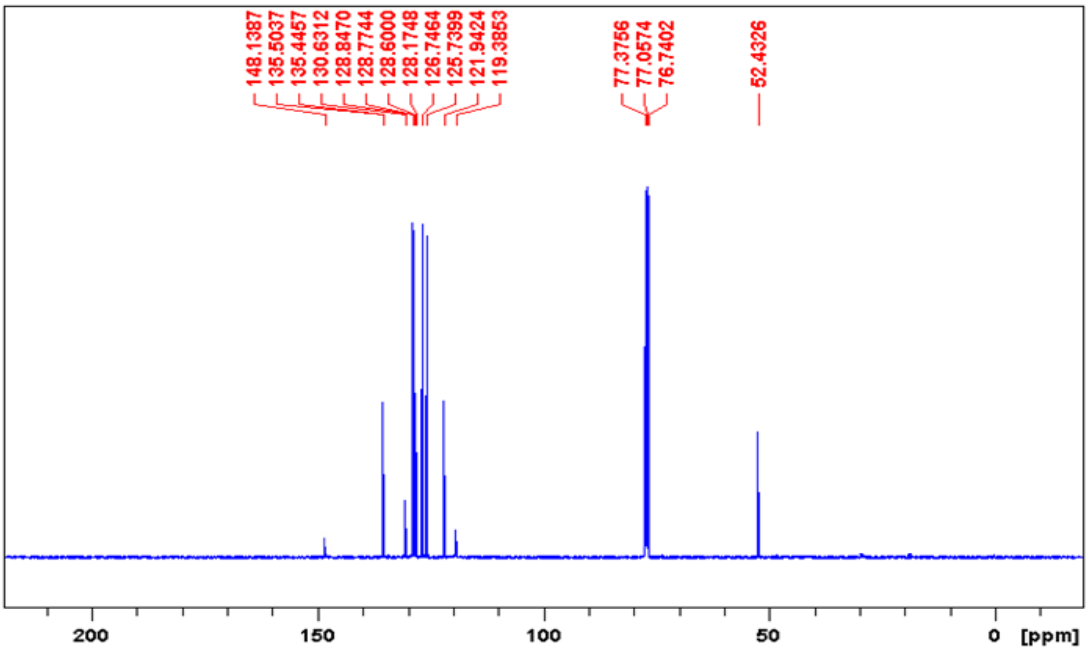
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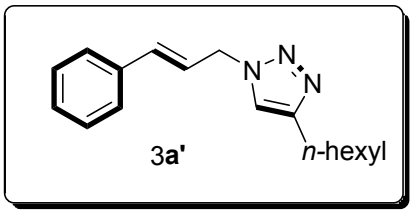
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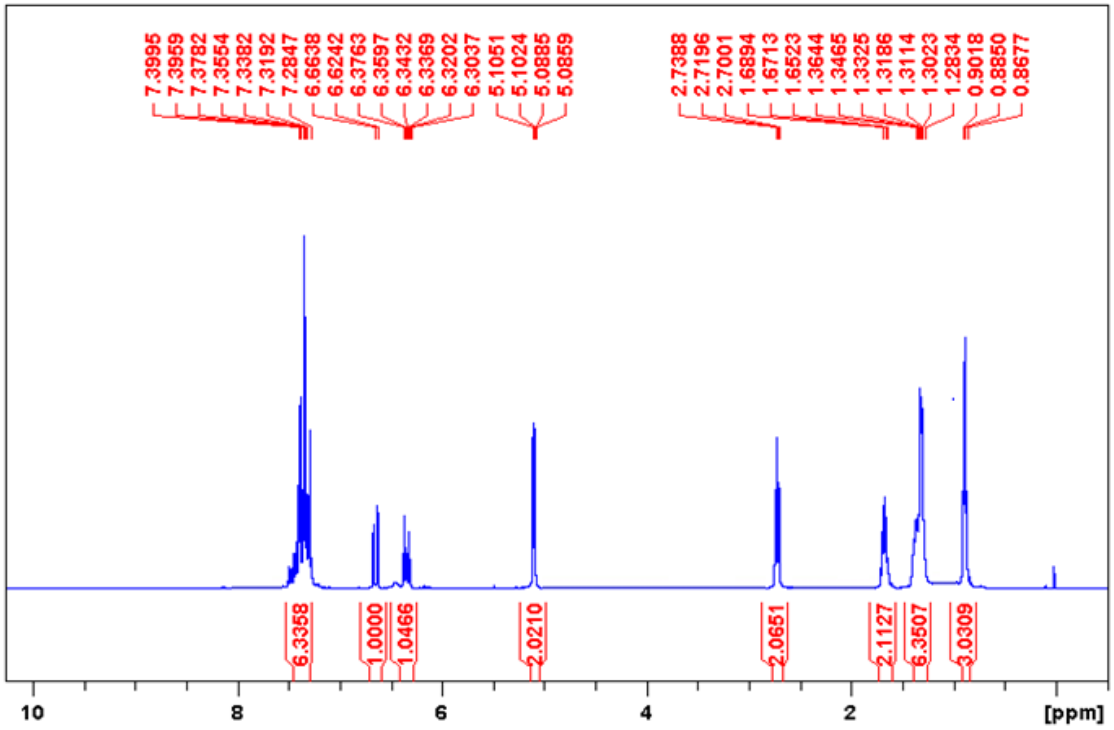
n-hexyl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1.6713
1.6523
1.3644
1.3465
1.3325
1.3186
1.3114
1.3023
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0.8850
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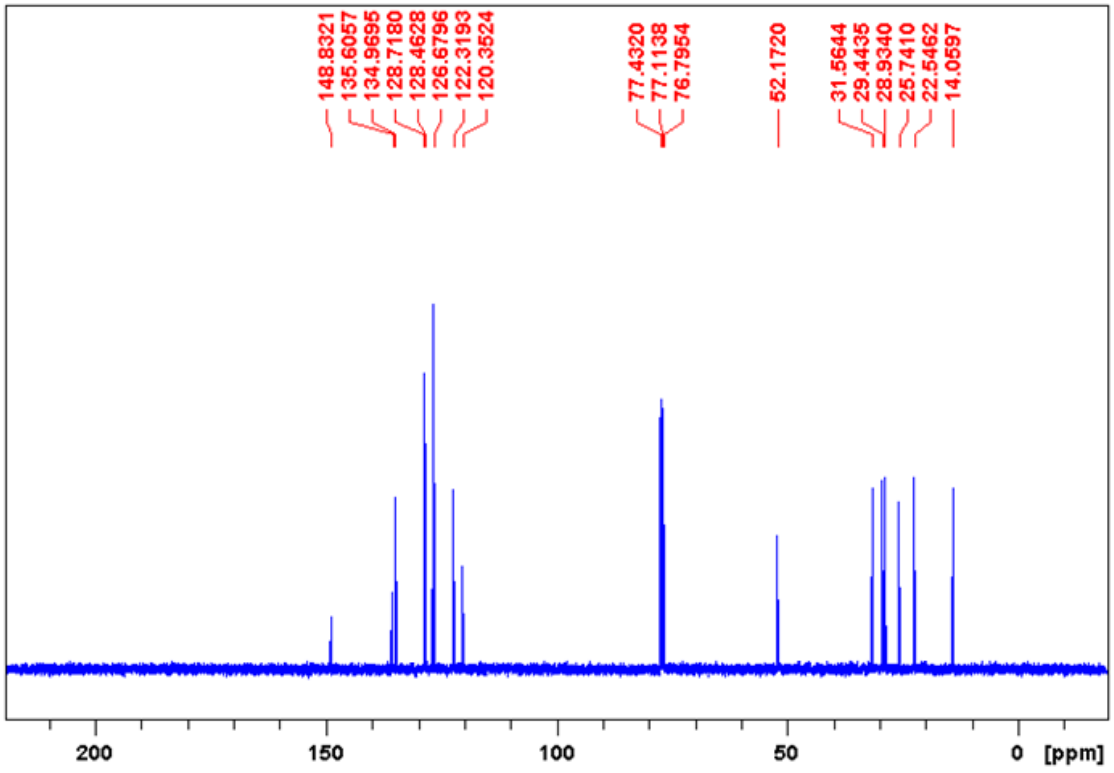
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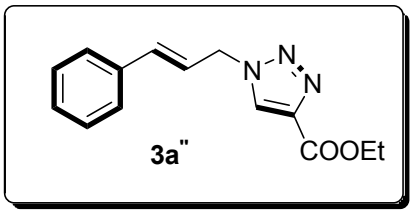
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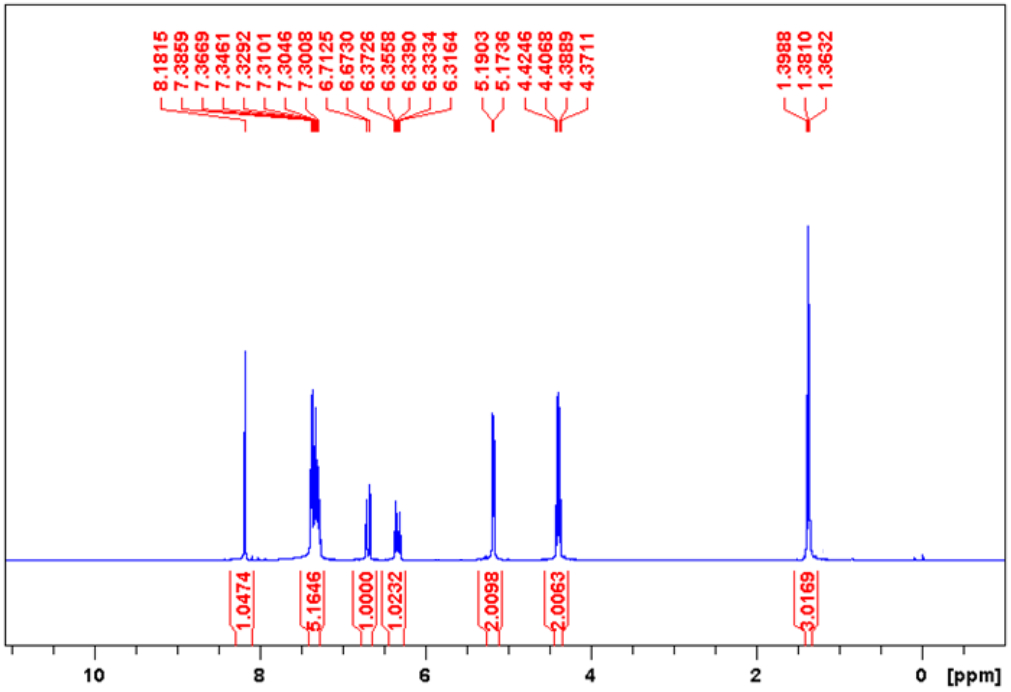
COOEt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6.3558
6.3390
6.3334
6.3164
5.1903
5.1736
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4.4068
4.3889
4.3711
1.3988
1.3810
1.3632
1.0474
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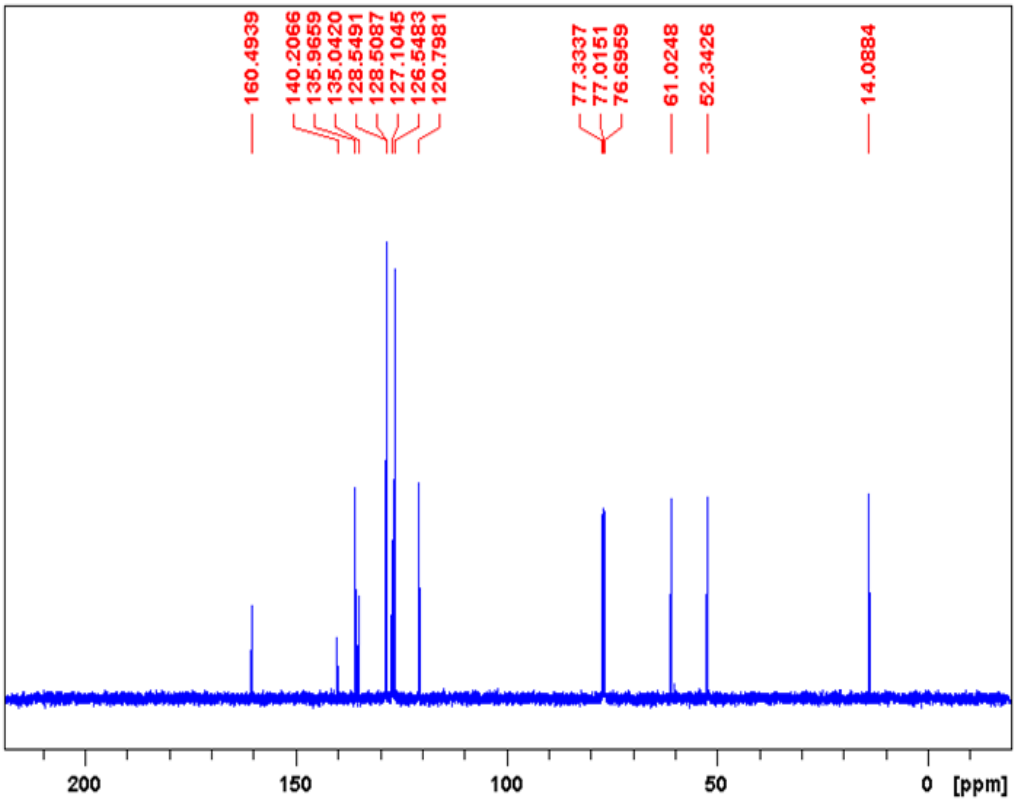
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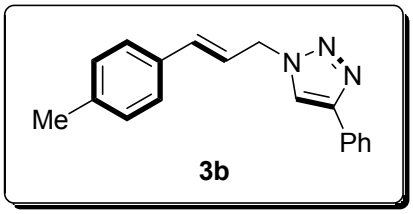
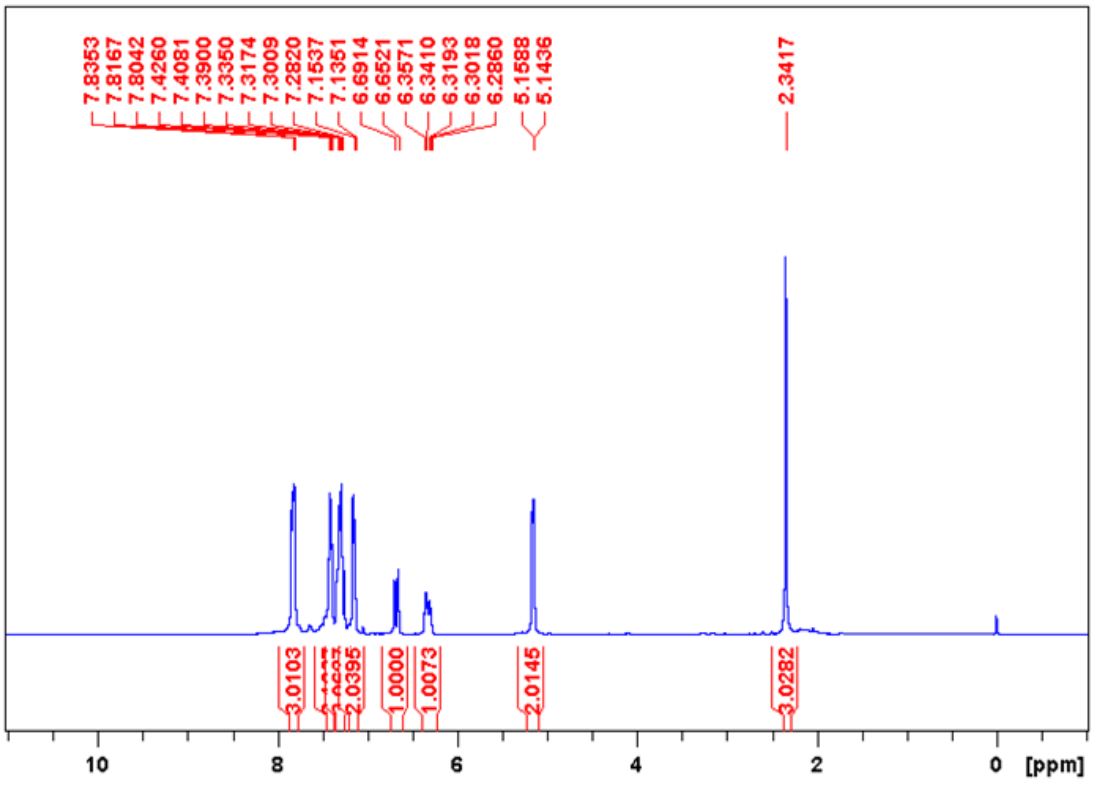

Me
N
N
N
Ph

3b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6.6521
6.3571
6.3410
6.3193
6.3018
6.2860
5.1588
5.1436
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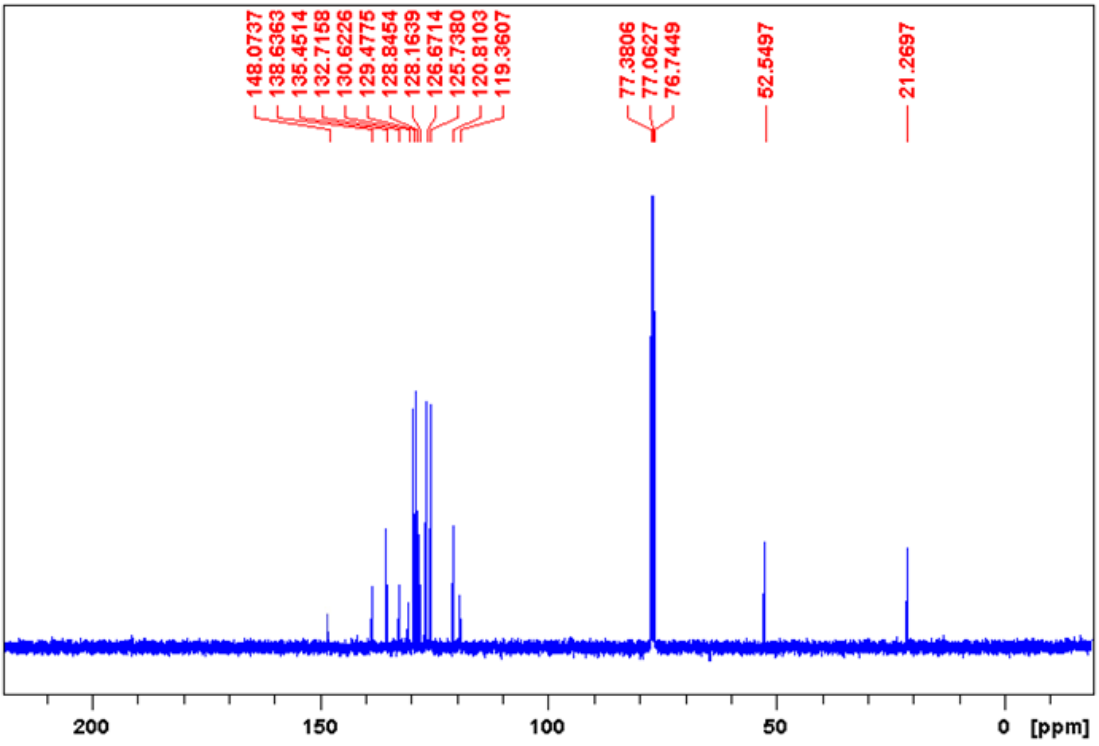
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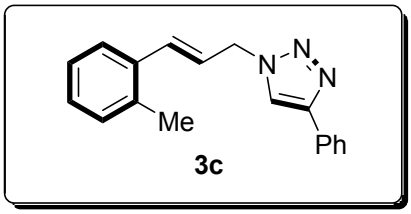
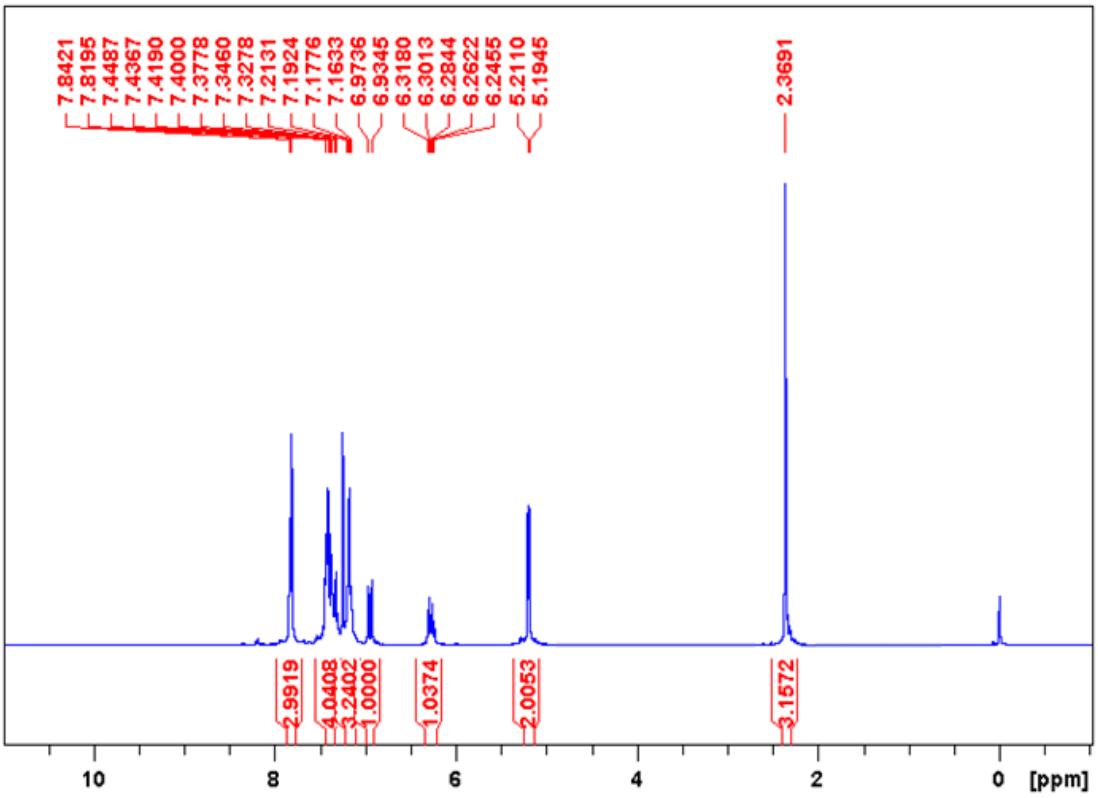

Me
Ph
3c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7.1776
7.1633
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6.9345
6.3180
6.3013
6.2844
6.2622
6.2455
5.2110
5.1945
2.3691
2.9919
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1.0374
2.0053
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4
2
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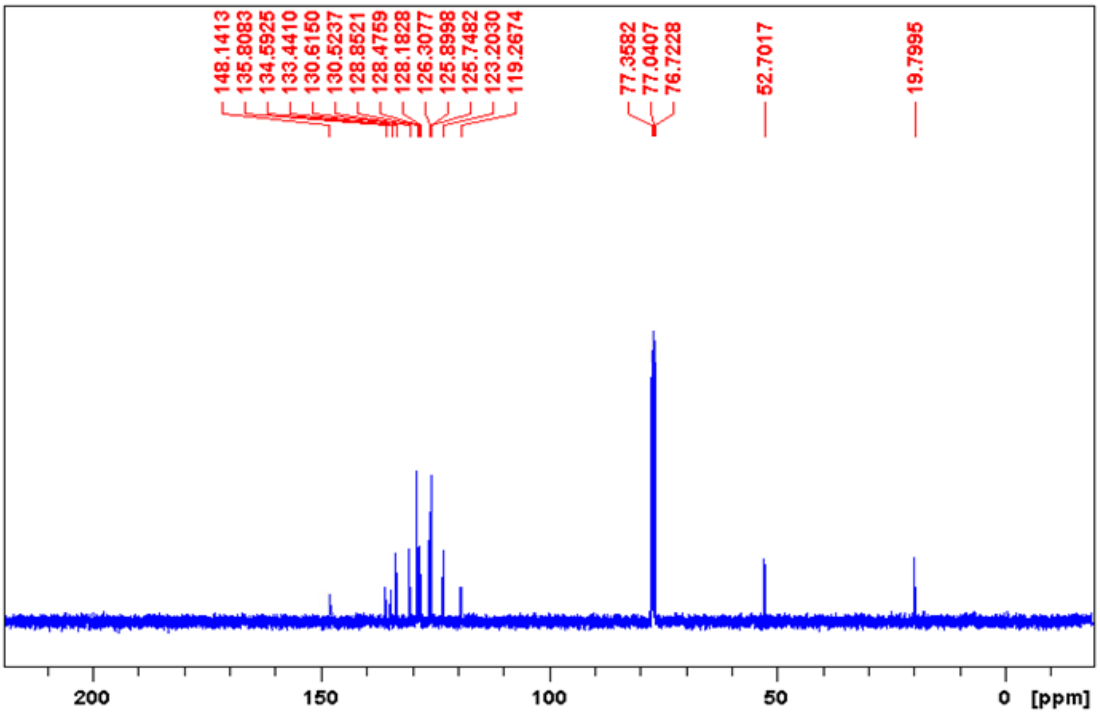
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128.1828
126.3077
125.8998
125.7482
123.2030
119.2674
77.3582
77.0407
76.7228
52.7017
19.7995
200
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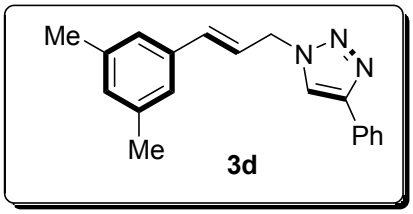
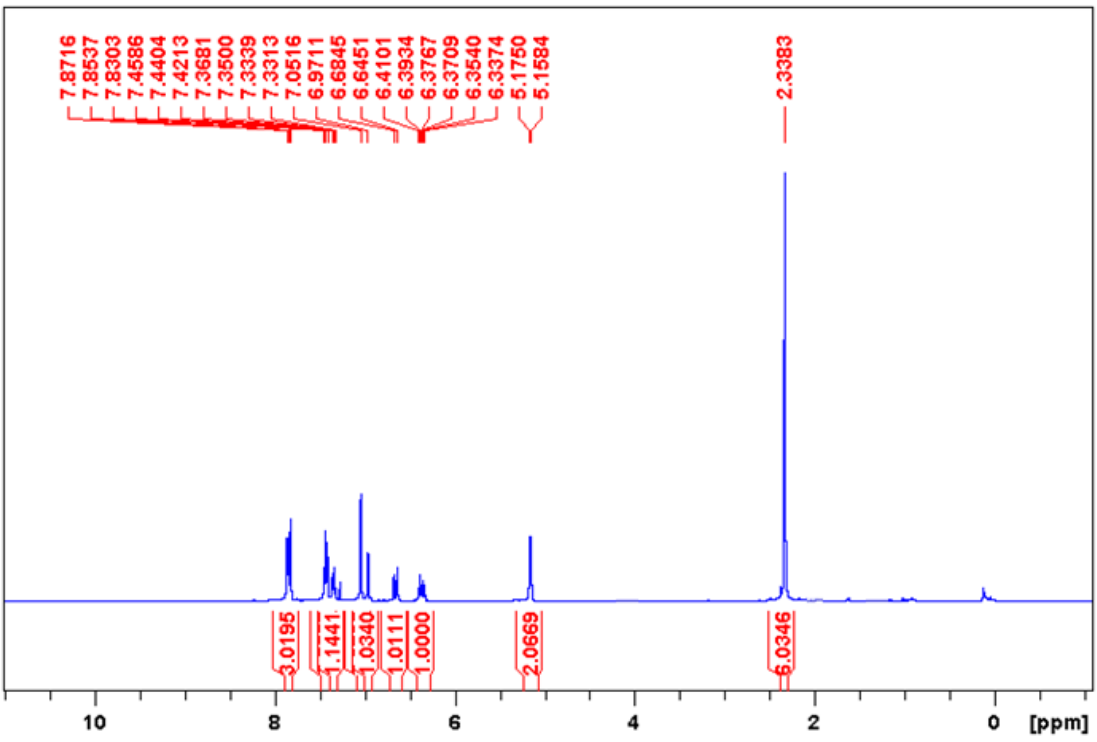
100
50
0
[ppm]


Me
Me
N
N
N
Ph

3d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6.9711
6.6845
6.6451
6.4101
6.3934
6.3767
6.3709
6.3540
6.3374
5.1750
5.1584
2.3383
3.0195
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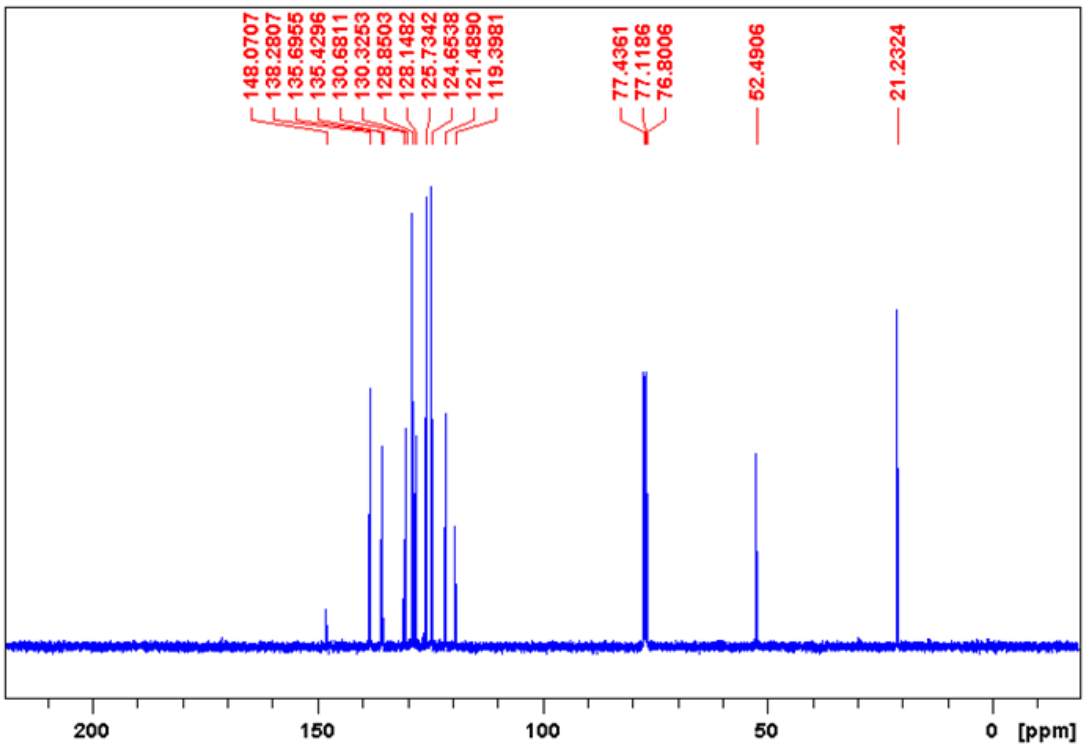
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125.7342
124.6538
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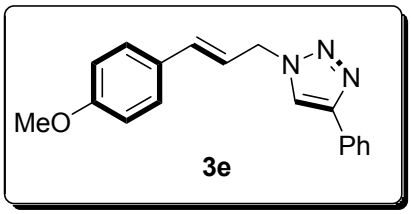
MeO
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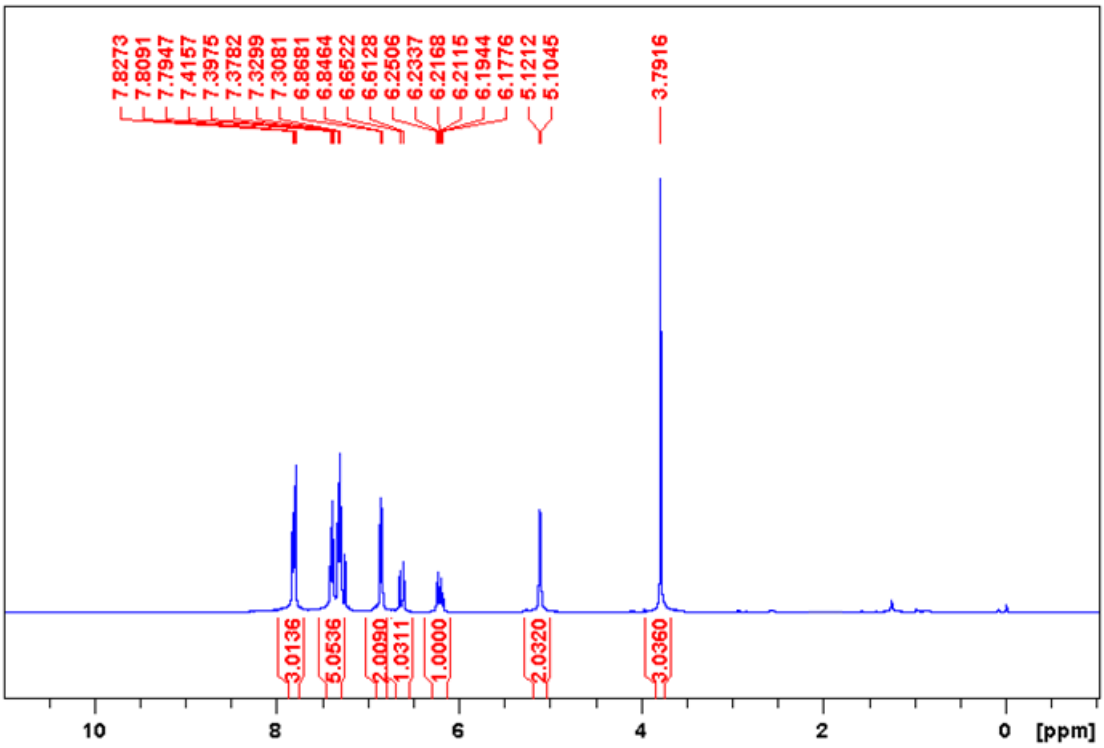
N
N
Ph

3e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6.6128
6.2506
6.2337
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6.2115
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5.1045
3.7916
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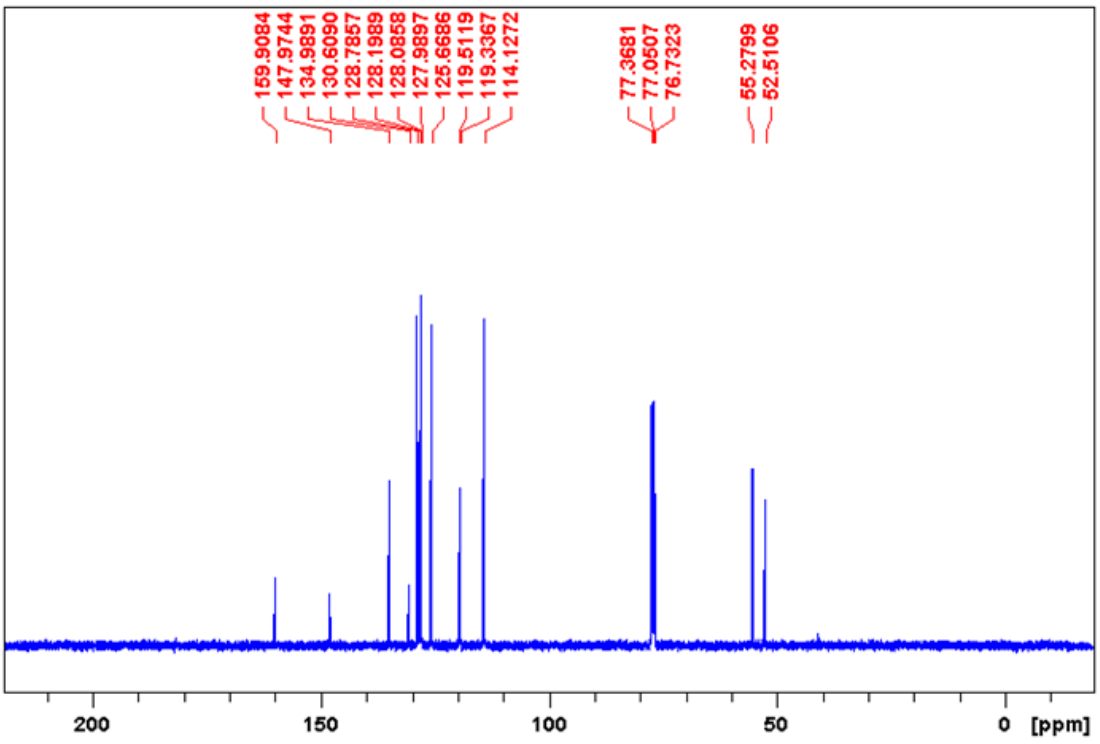
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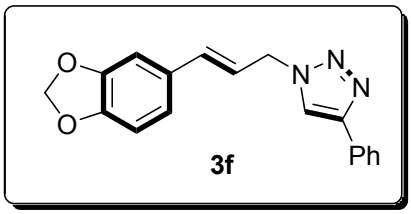
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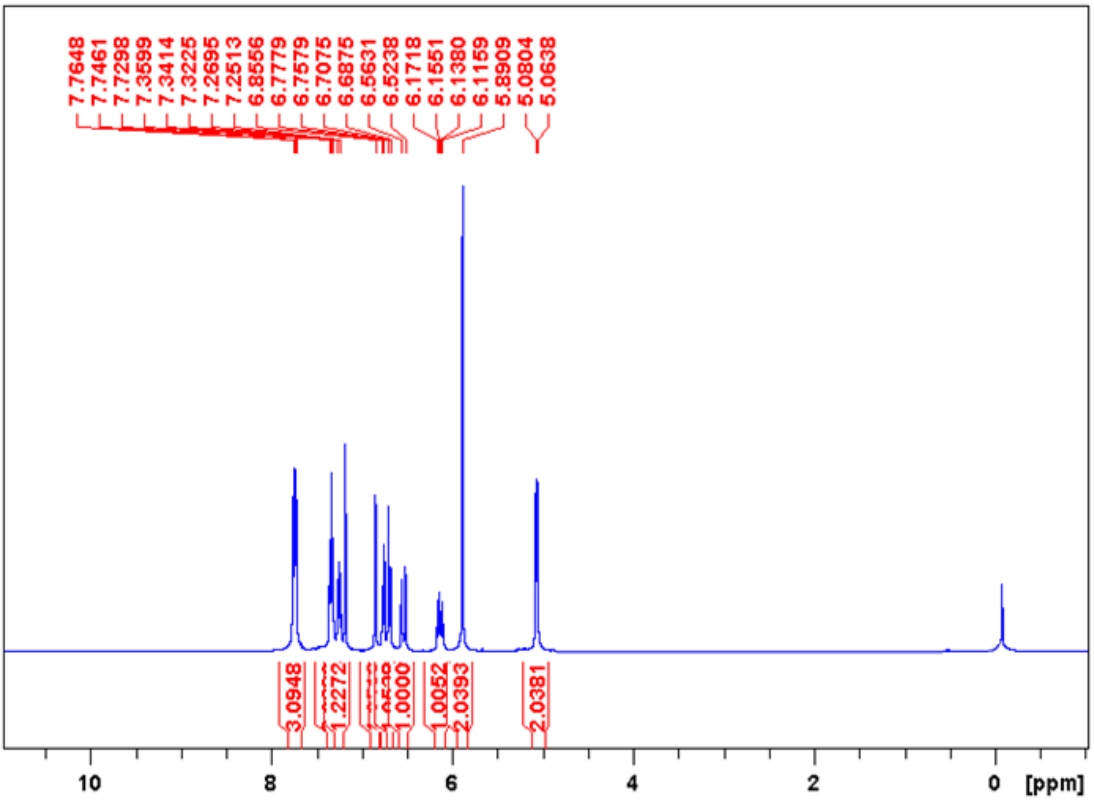
O
N
N
N
Ph

3f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6.7579
6.7075
6.6875
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6.1718
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6.1159
5.8909
5.0804
5.0638
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2.0381
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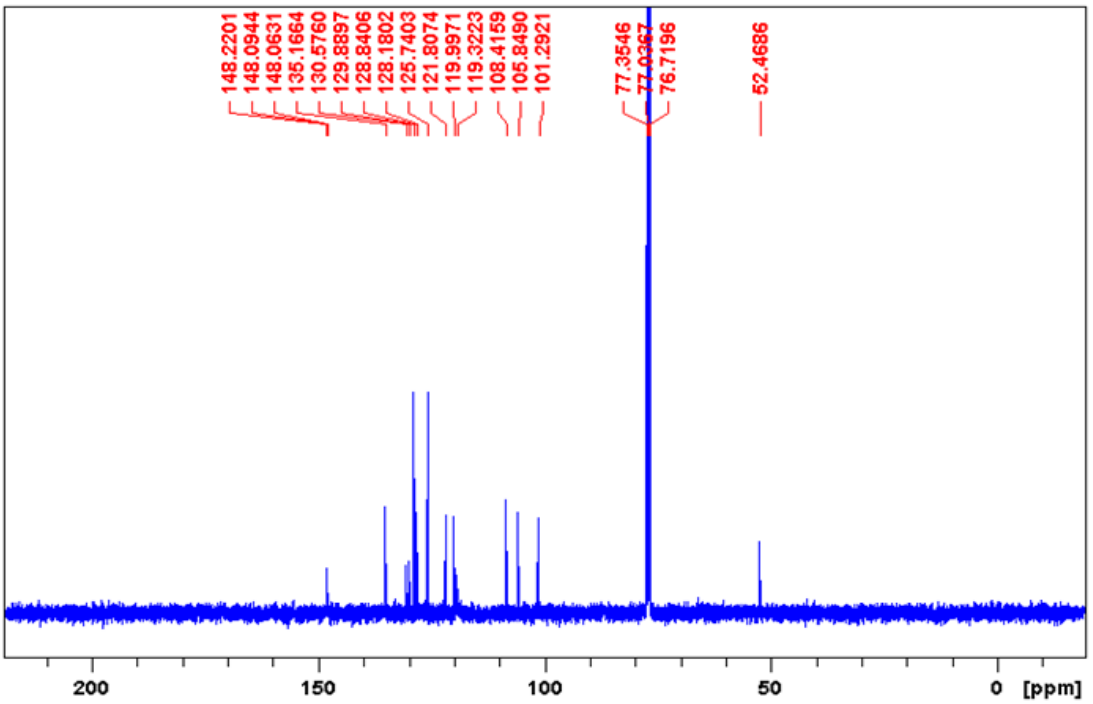
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129.8897
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125.7403
121.8074
119.9971
119.3223
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101.2921
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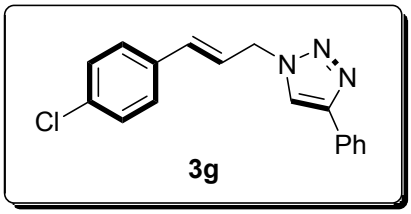
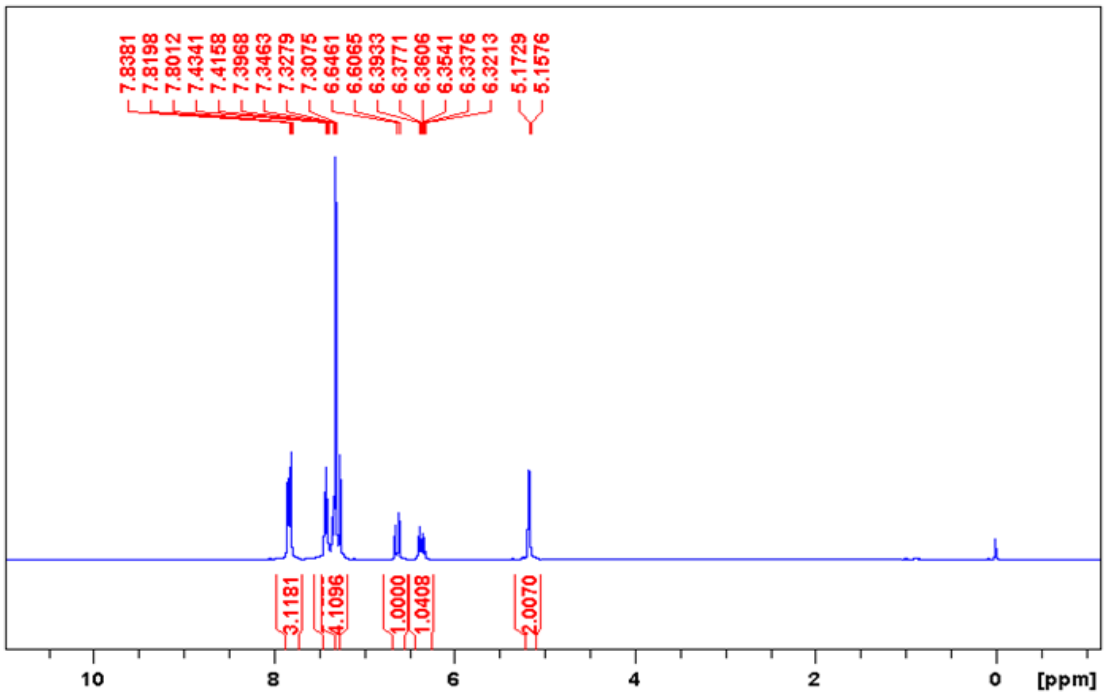

Cl
N
N
N
Ph

3g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7.8012
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7.4158
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7.3075
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6.6065
6.3933
6.3771
6.3606
6.3541
6.3376
6.3213
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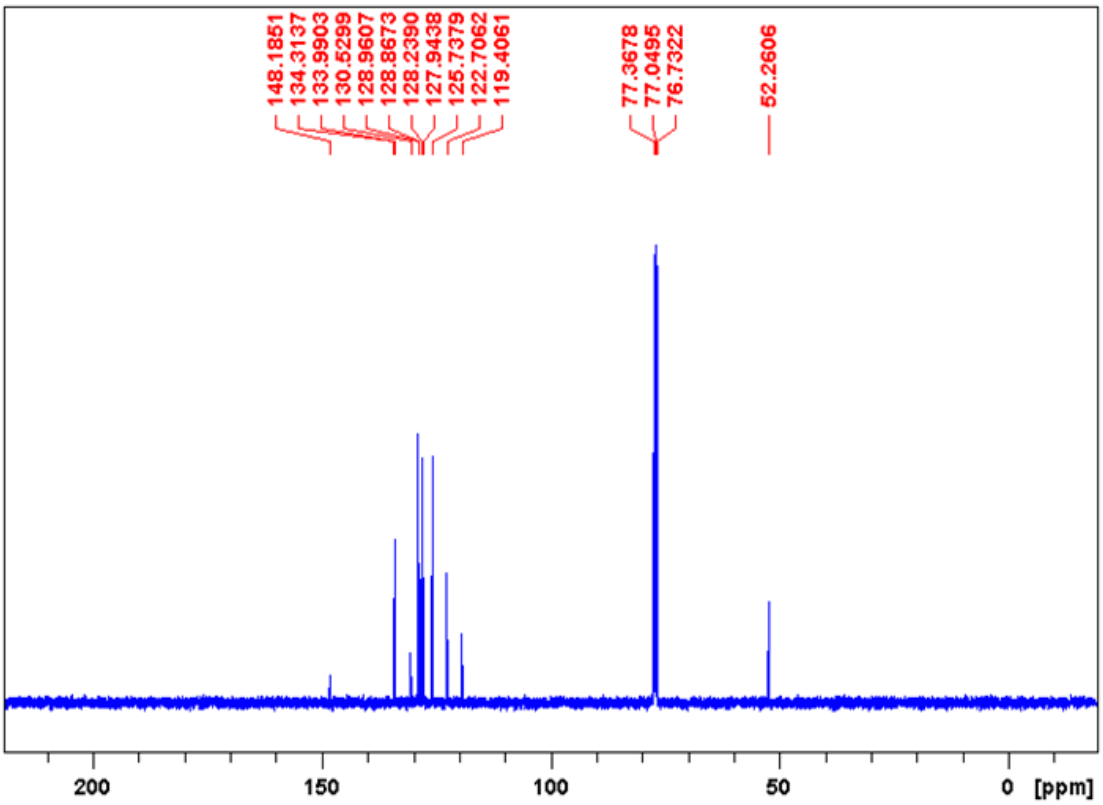
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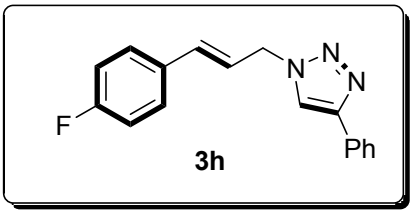
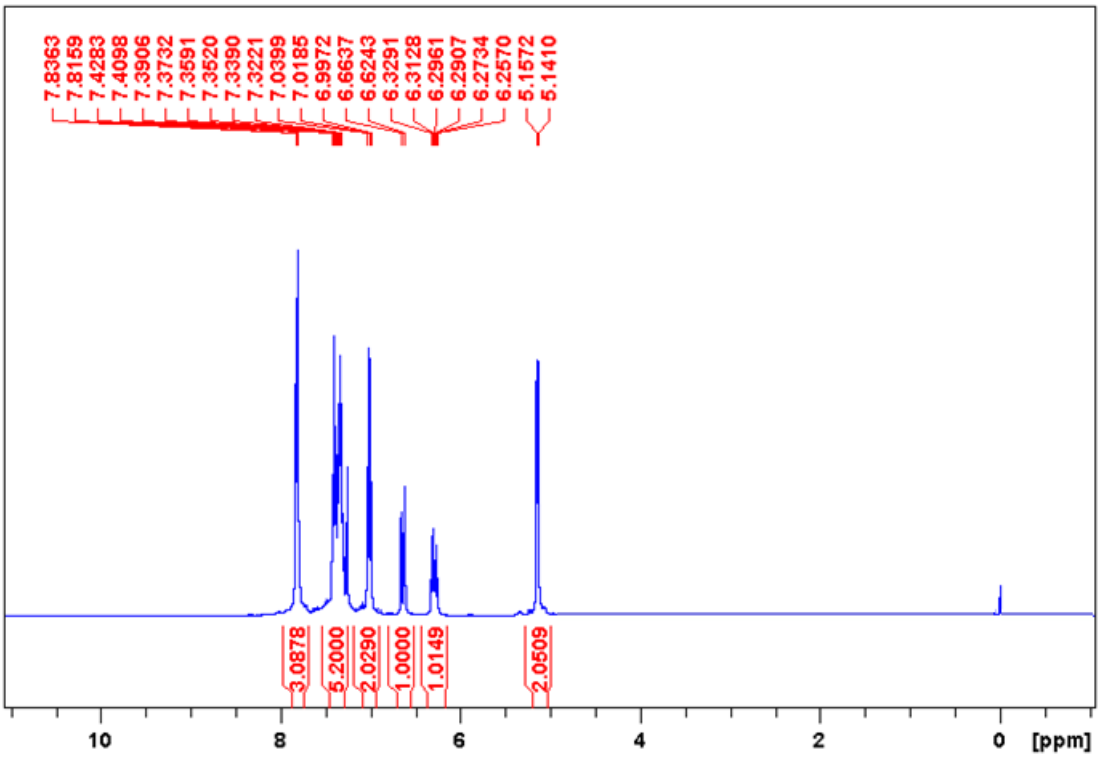

F
N
N
N
Ph

3h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7.3390
7.3221
7.0399
7.0185
6.9972
6.6637
6.6243
6.3291
6.3128
6.2961
6.2907
6.2734
6.2570
5.1572
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2.0509
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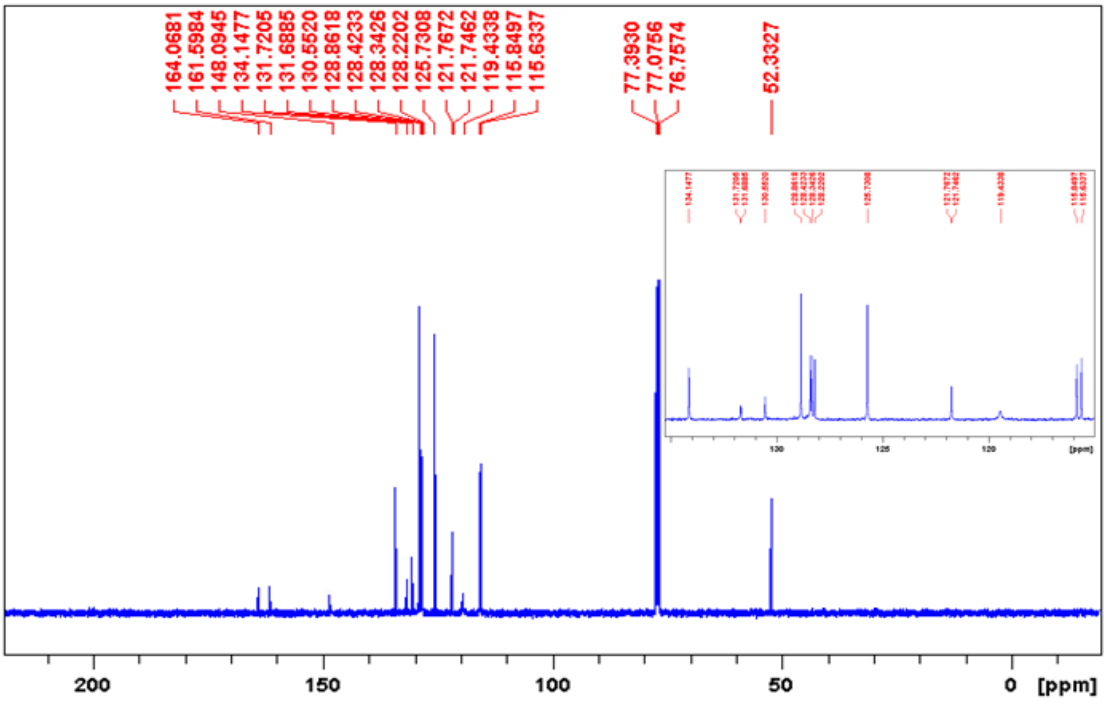
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121.7462
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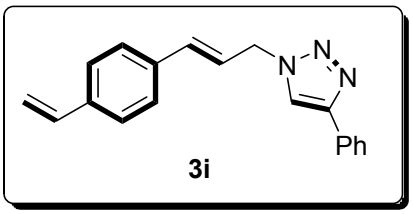
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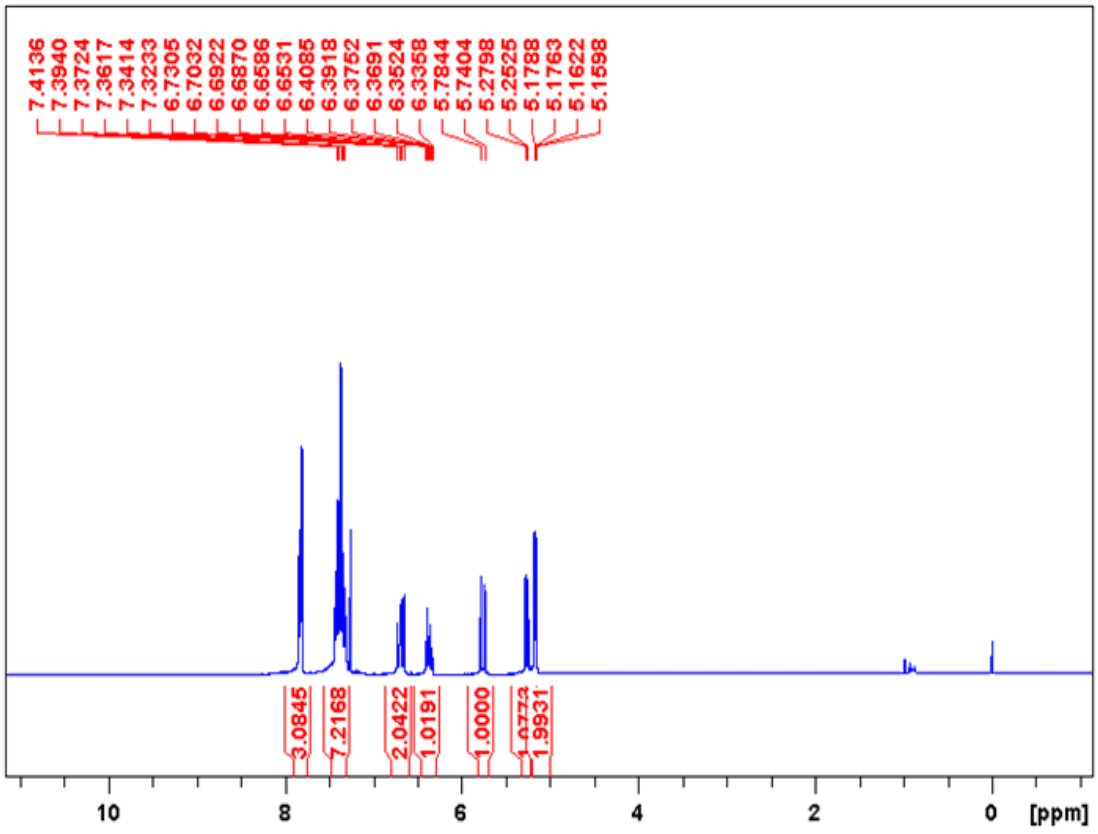
N
N
Ph

3i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6.6531
6.4085
6.3918
6.3752
6.3691
6.3524
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5.7404
5.2798
5.2525
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5.1763
5.1622
5.1598
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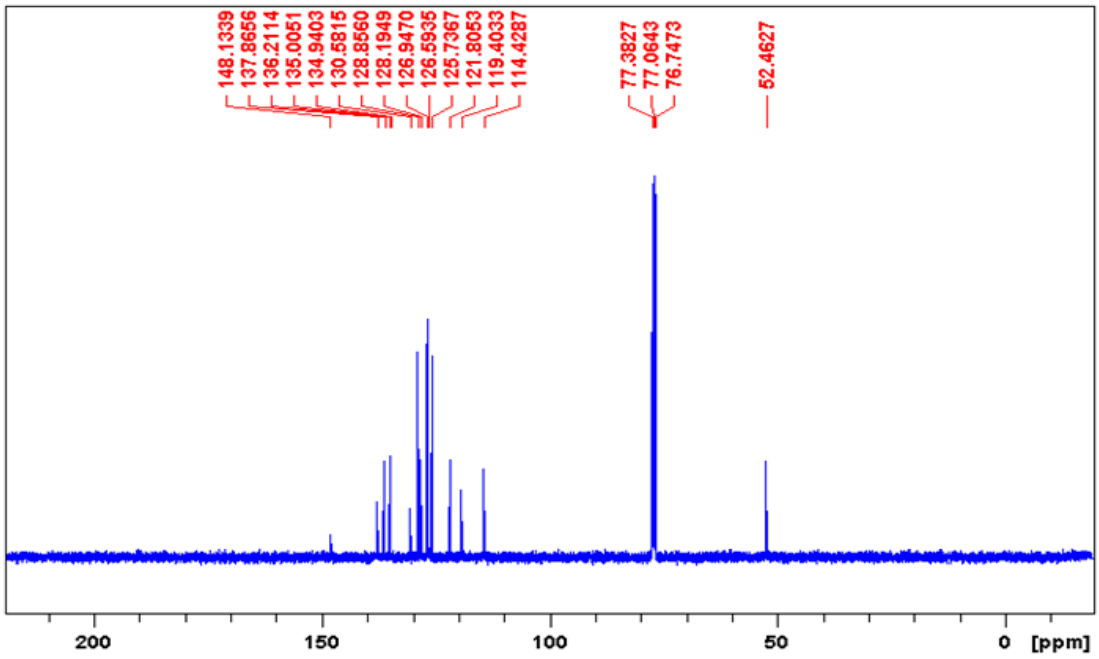
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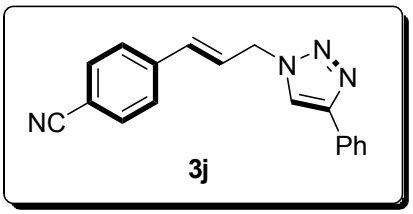
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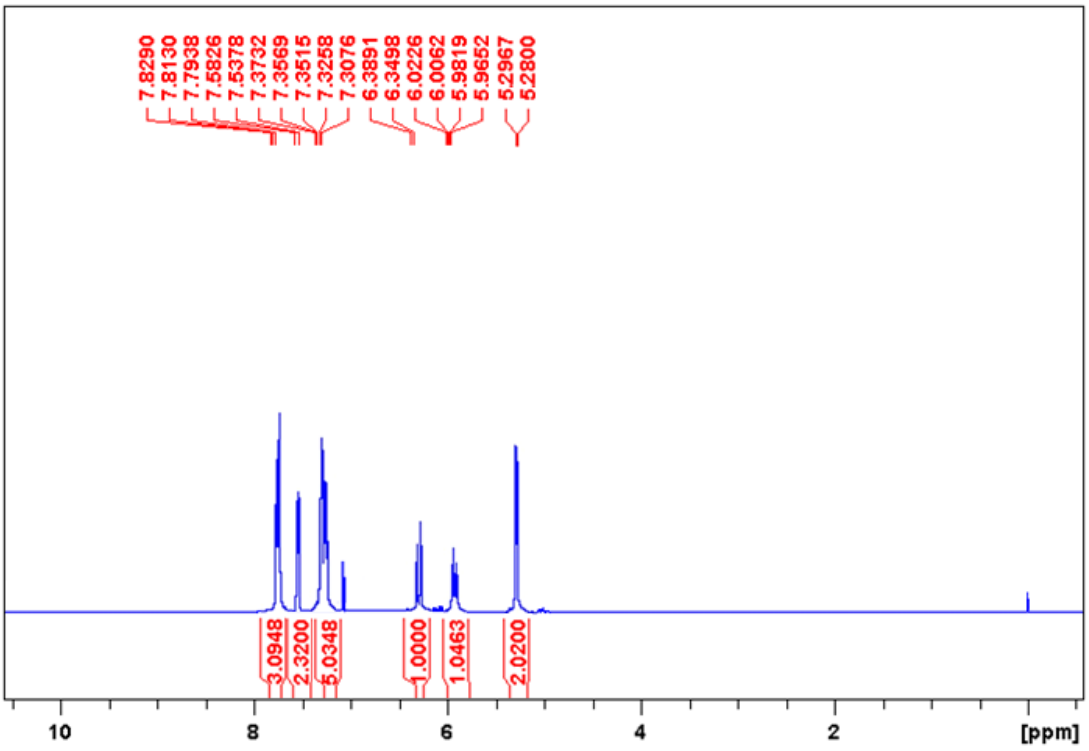
N
N
N
Ph

3j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7.3732
7.3569
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7.3258
7.3076
6.3891
6.3498
6.0226
6.0062
5.9819
5.9652
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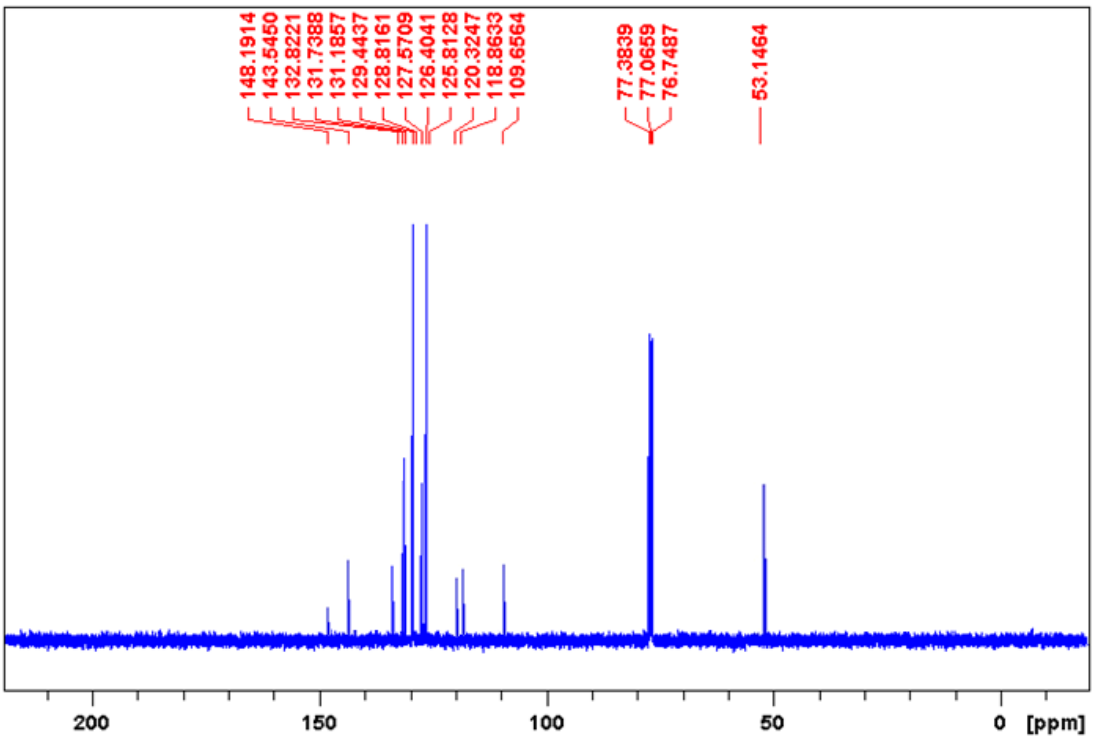
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125.8128
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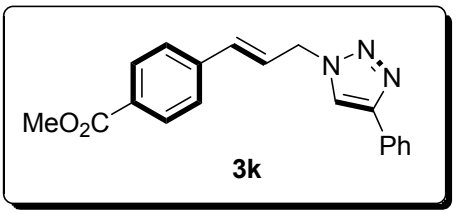
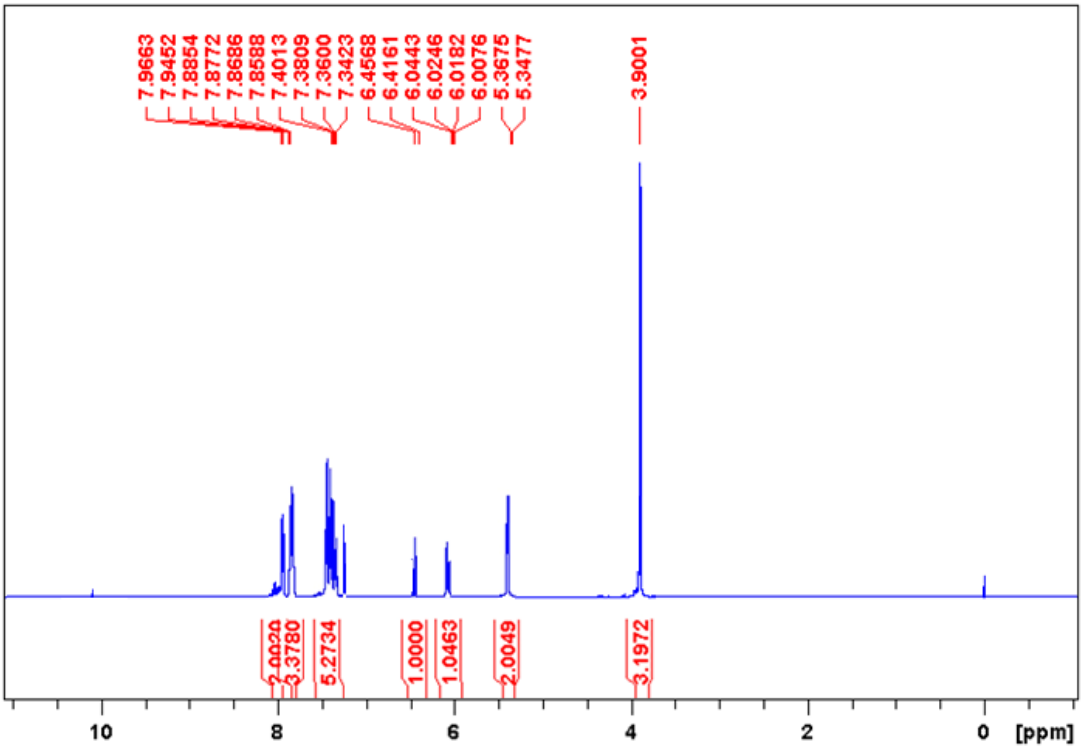

MeO2C
N
N
N
Ph

3k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7.3423
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6.4161
6.0443
6.0246
6.0182
6.0076
5.3675
5.3477
3.9001
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2.0049
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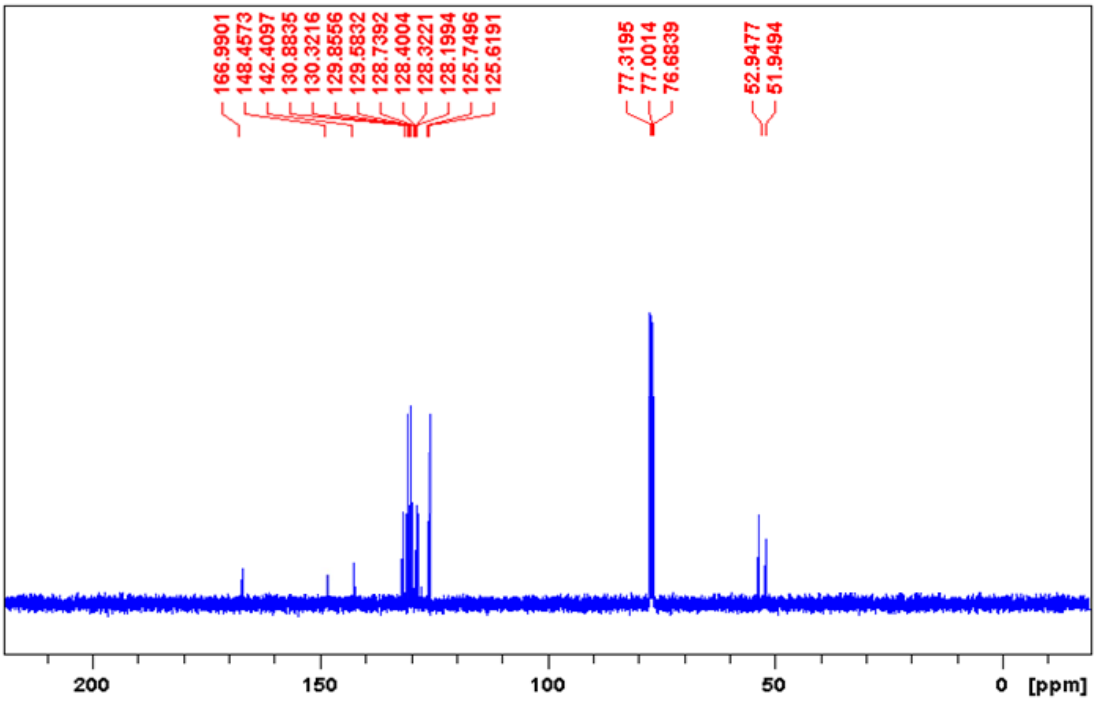
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128.1994
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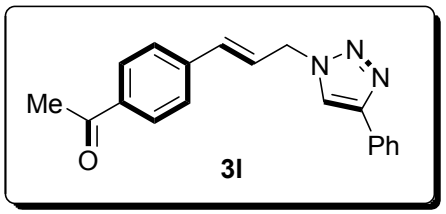
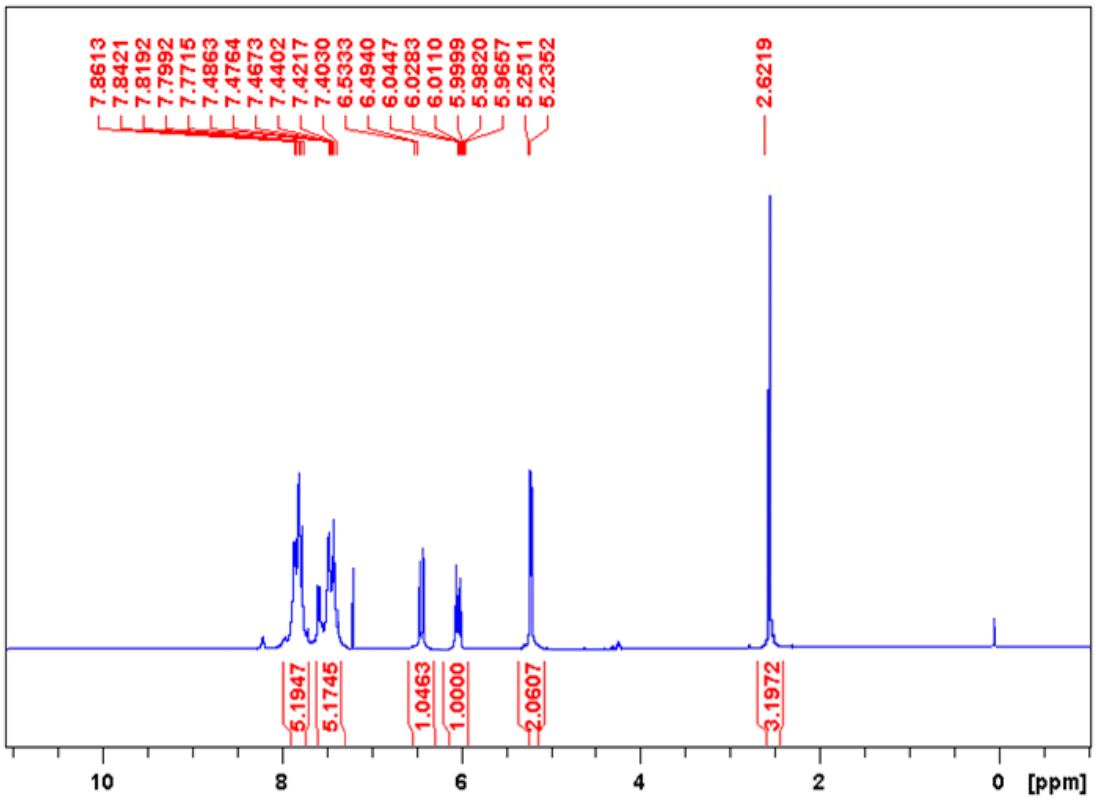

Me
O
N
N
N
Ph

3l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7.4030
6.5333
6.4940
6.0447
6.0283
6.0110
5.9999
5.9820
5.9657
5.2511
5.2352
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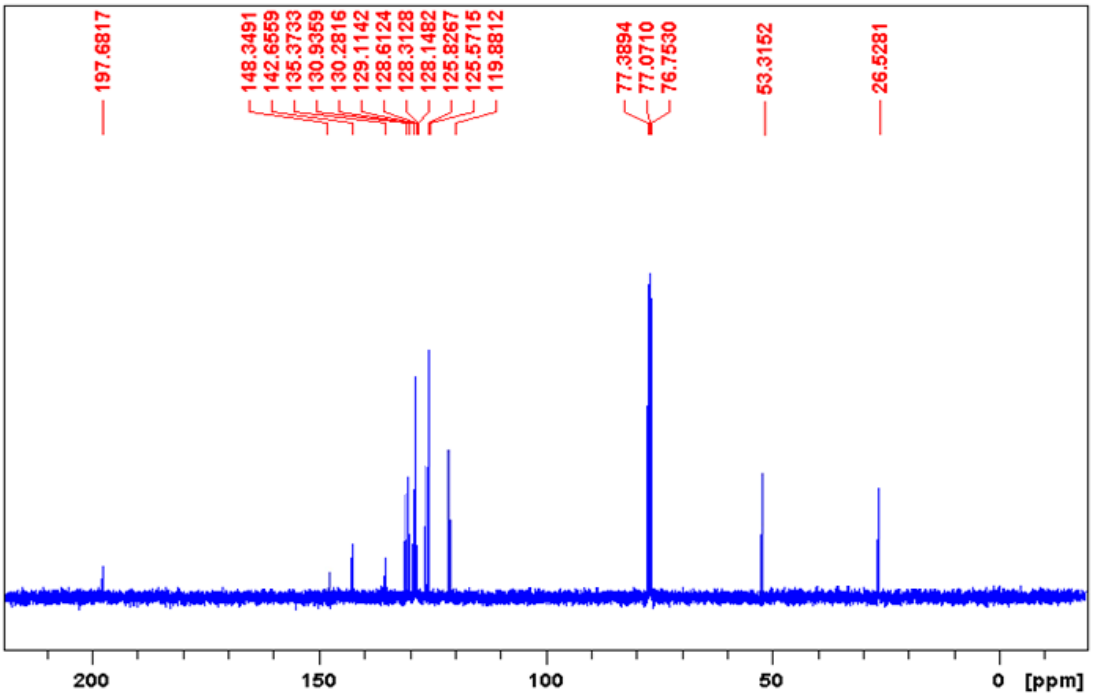
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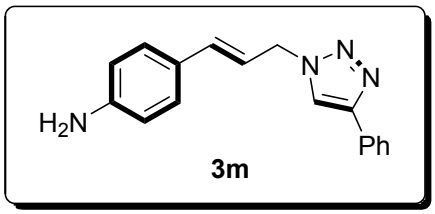
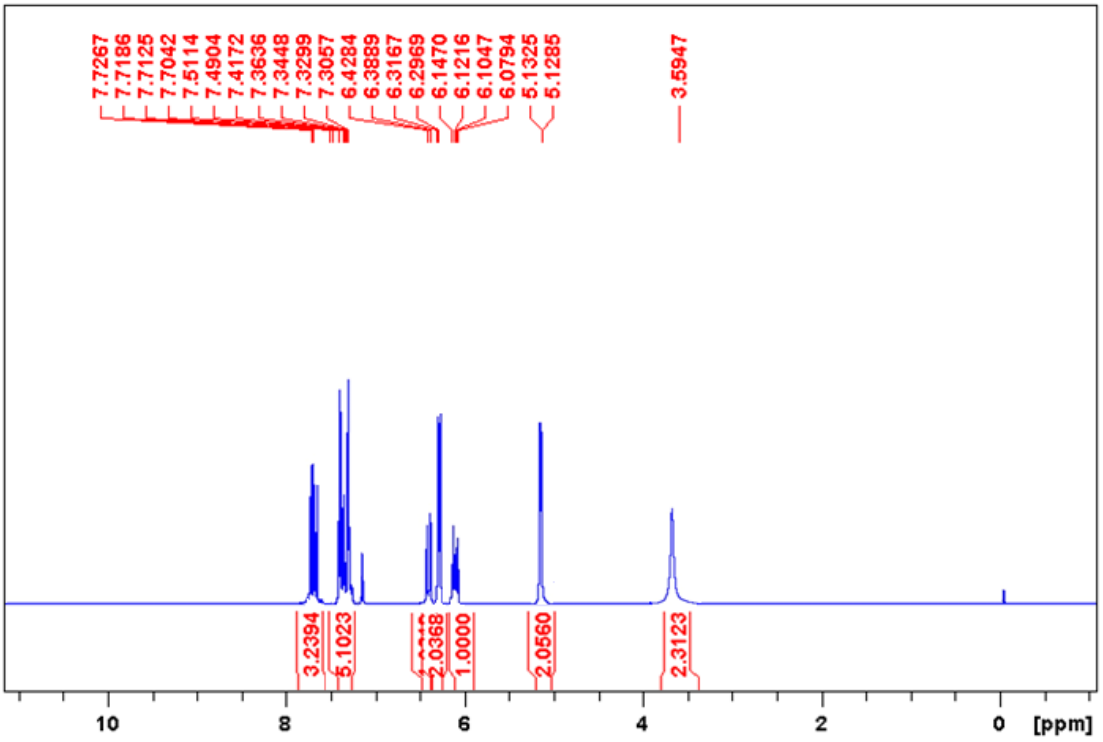

H2N
N
N
N
Ph

3m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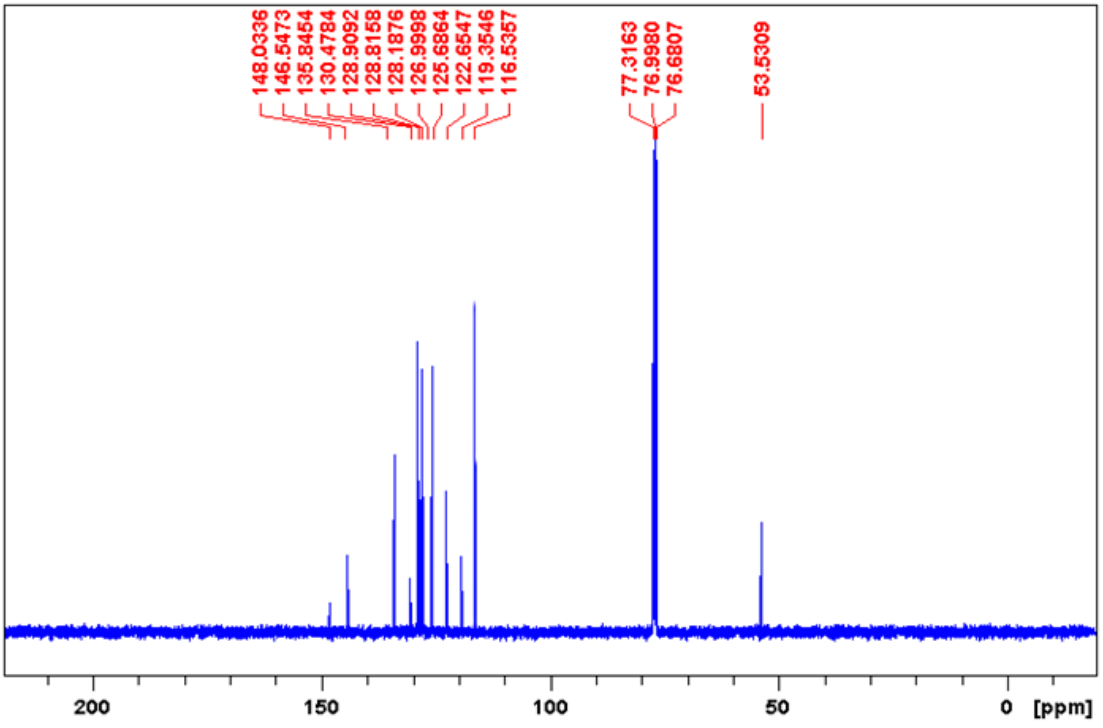
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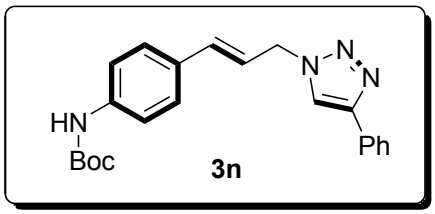
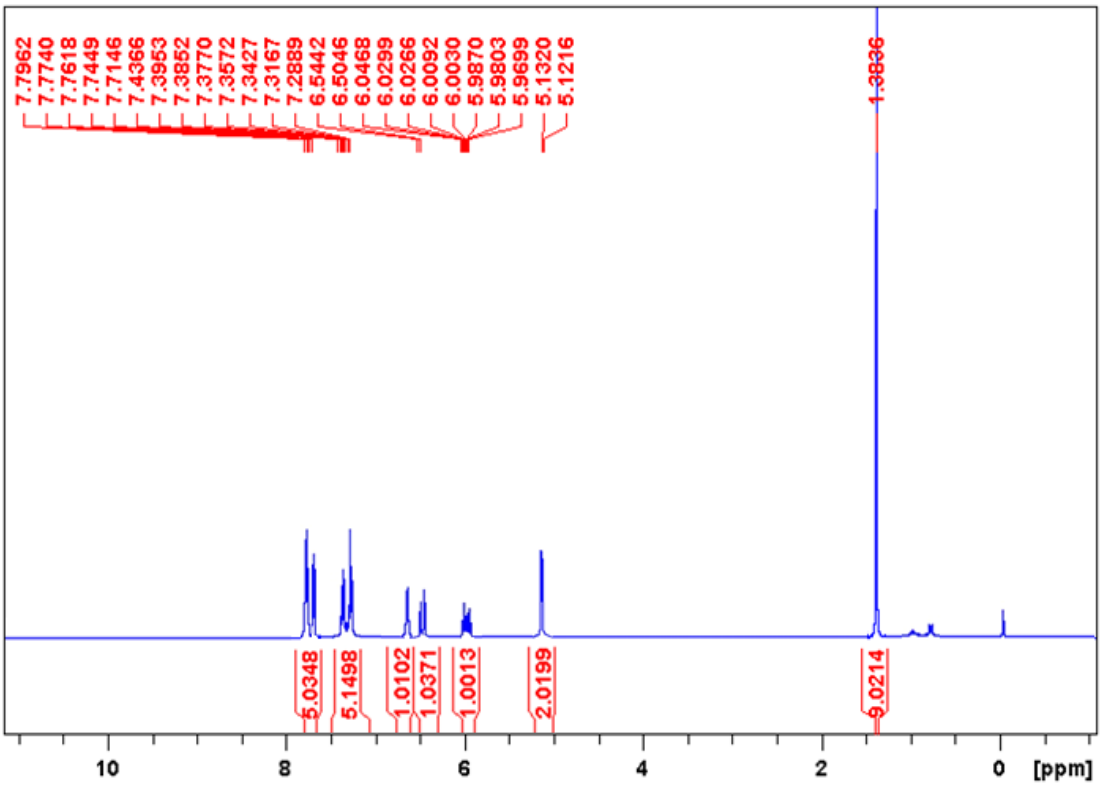

HN
Boc
N
N
N
Ph

3n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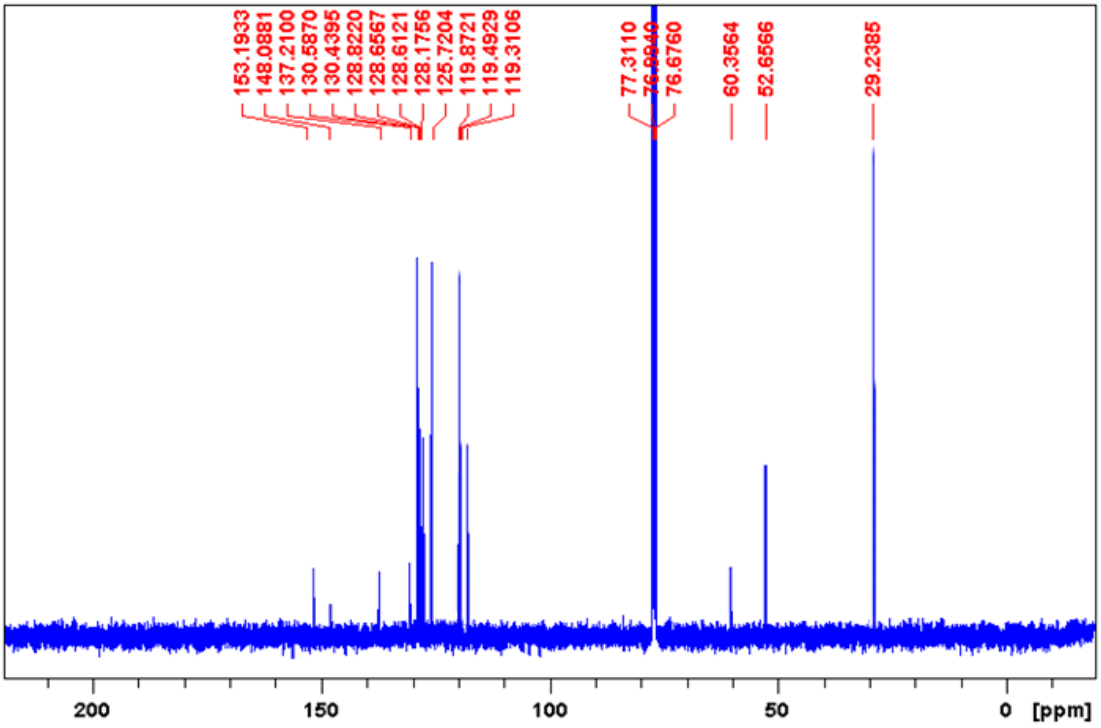
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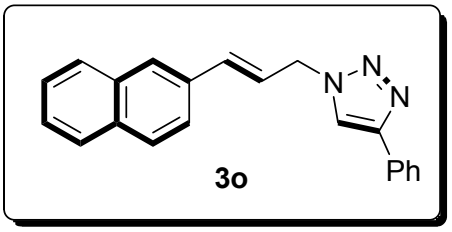
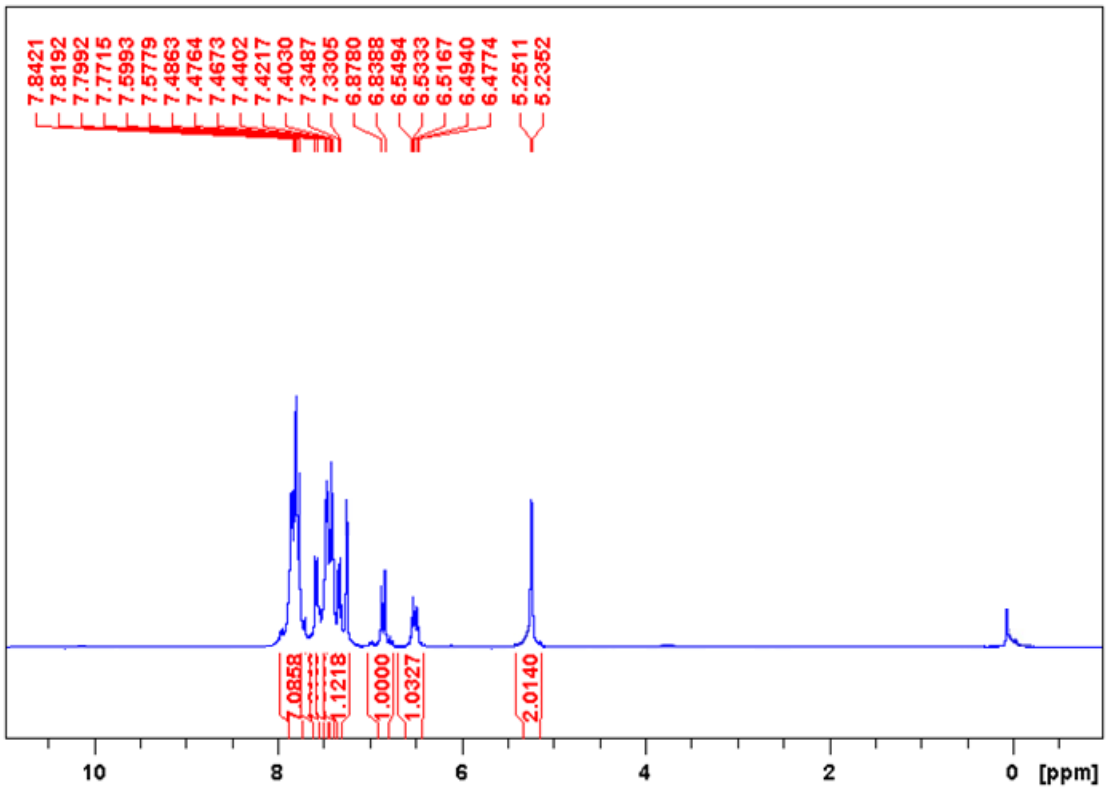

N
N
N
Ph

3o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7.4030
7.3487
7.3305
6.8780
6.8388
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6.5167
6.4940
6.4774
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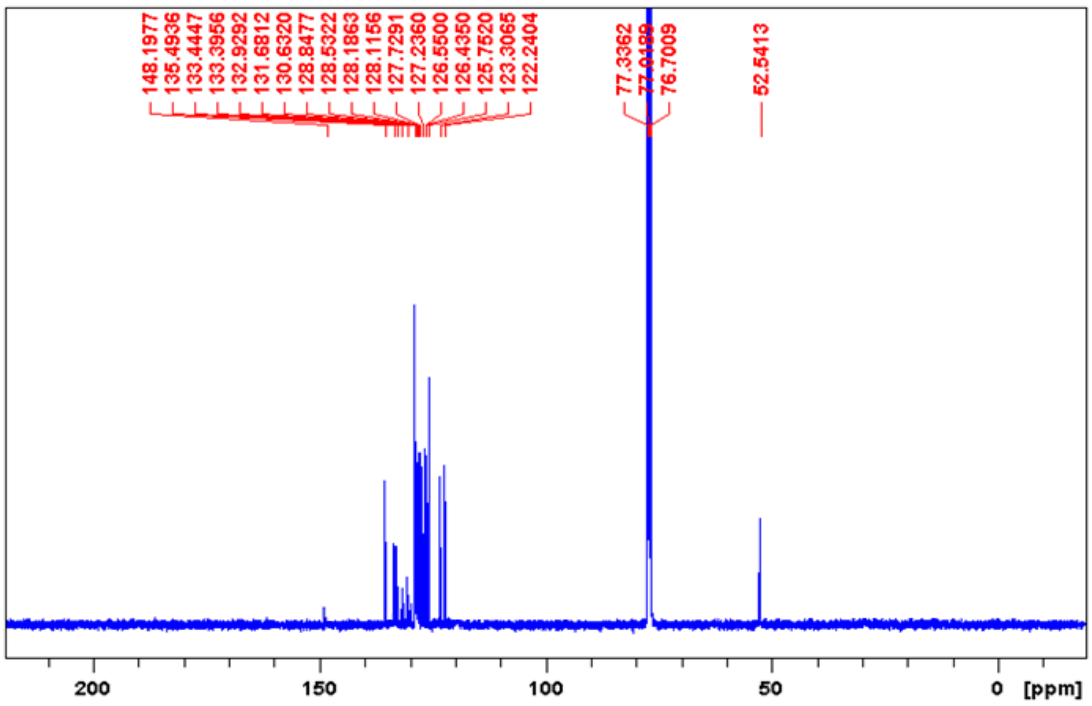
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127.7291
127.2360
126.5500
126.4350
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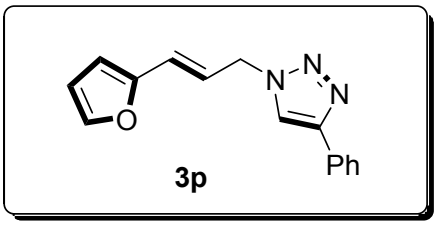
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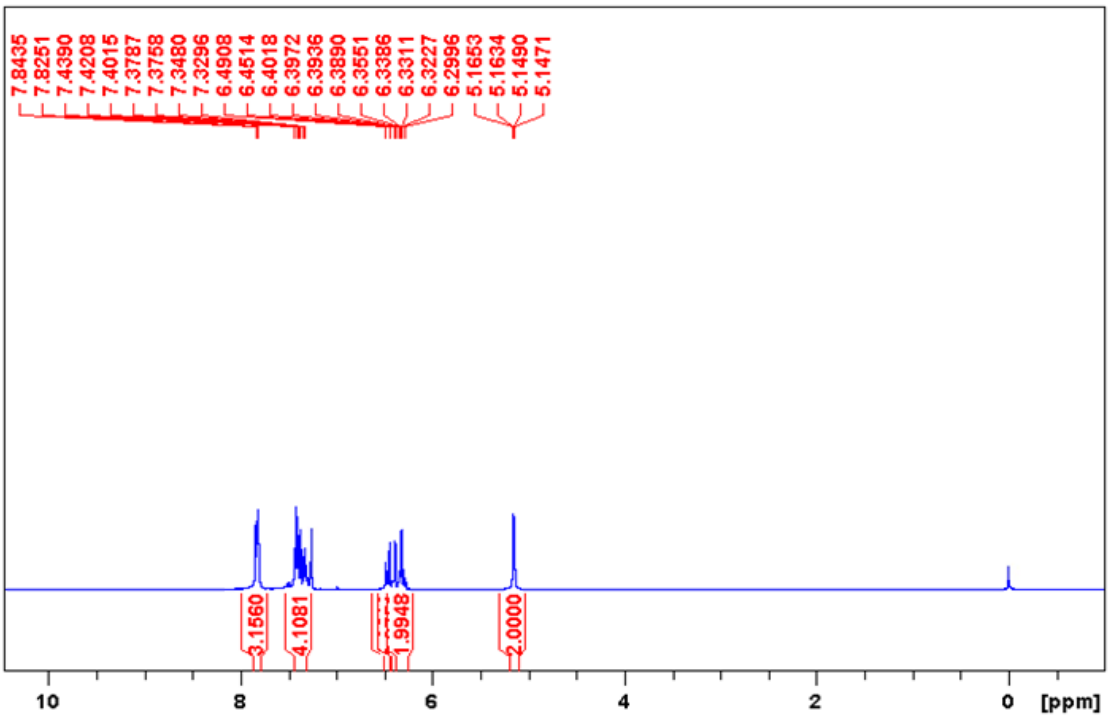
N
N
N
Ph

3p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6.4018
6.3972
6.3936
6.3890
6.3551
6.3386
6.3311
6.3227
6.2996
5.1653
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0
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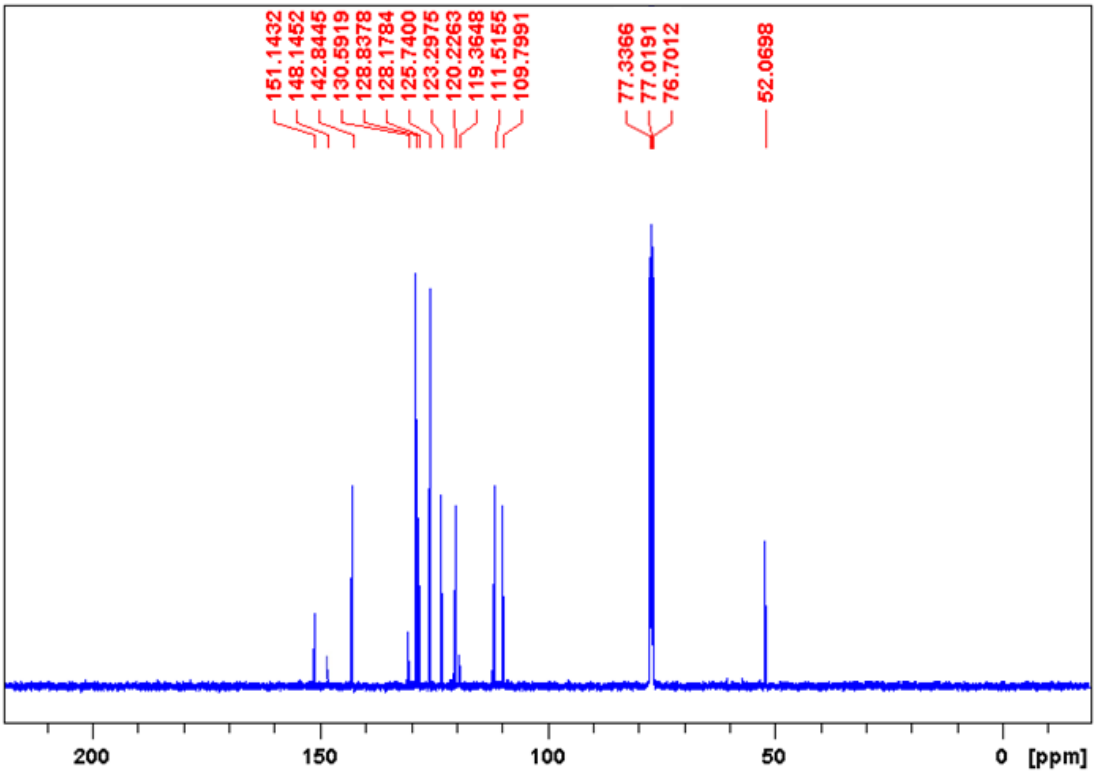
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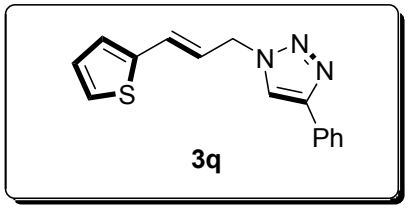
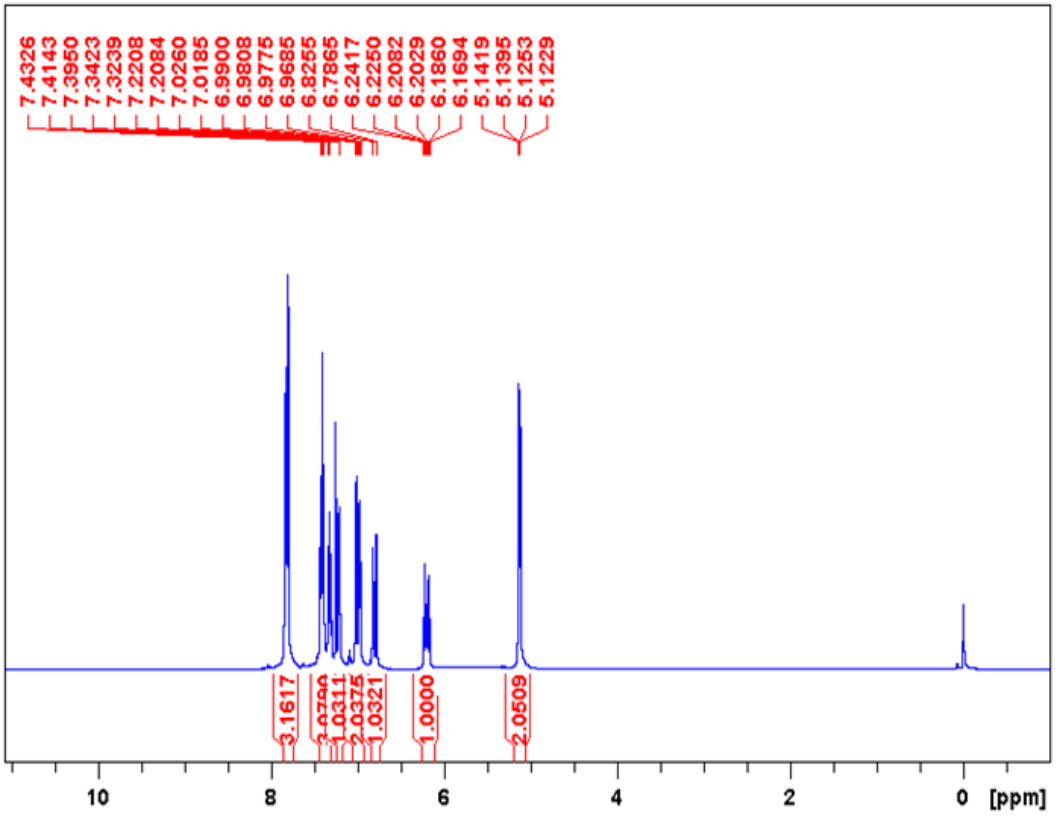

S
N
N
N
Ph

3q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6.9808
6.9775
6.9685
6.8255
6.7865
6.2417
6.2250
6.2082
6.2029
6.1860
6.1694
5.1419
5.1395
5.1253
5.1229
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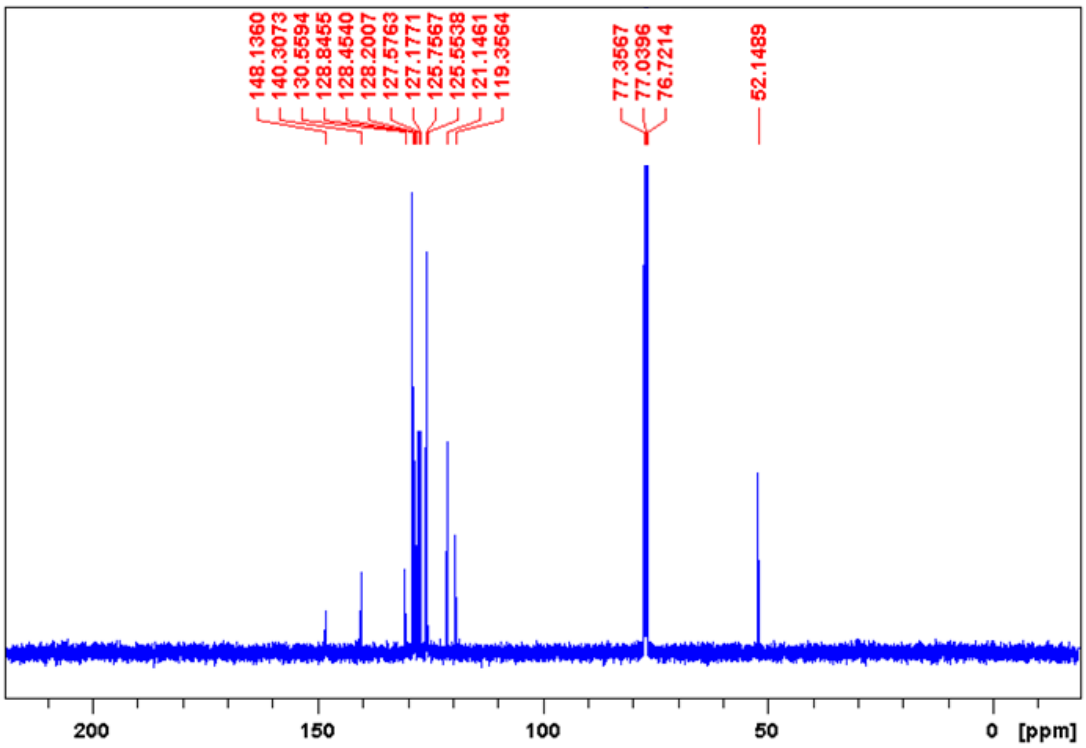
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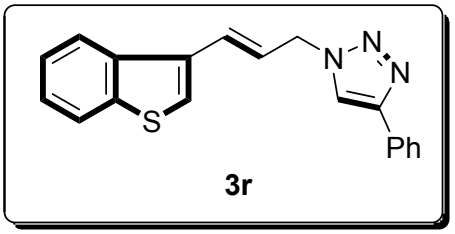
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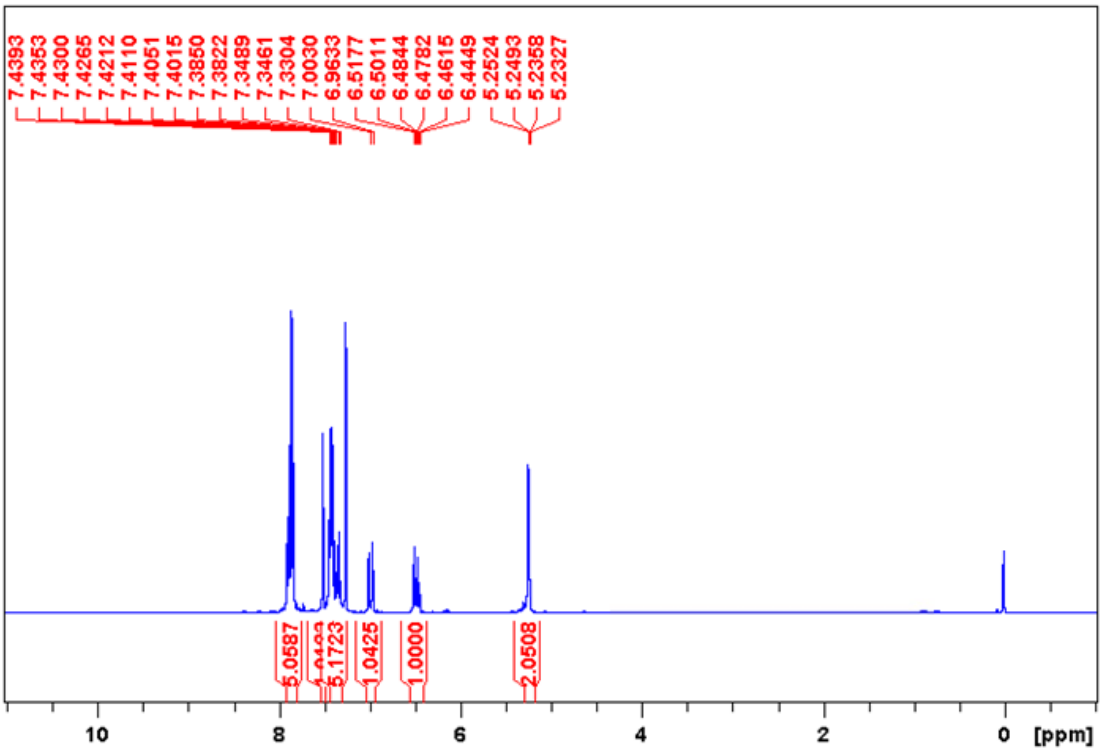
N
N
S
Ph

3r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7.4212
7.4110
7.4051
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7.3850
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7.3304
7.0030
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6.5177
6.5011
6.4844
6.4782
6.4615
6.4449
5.2524
5.2493
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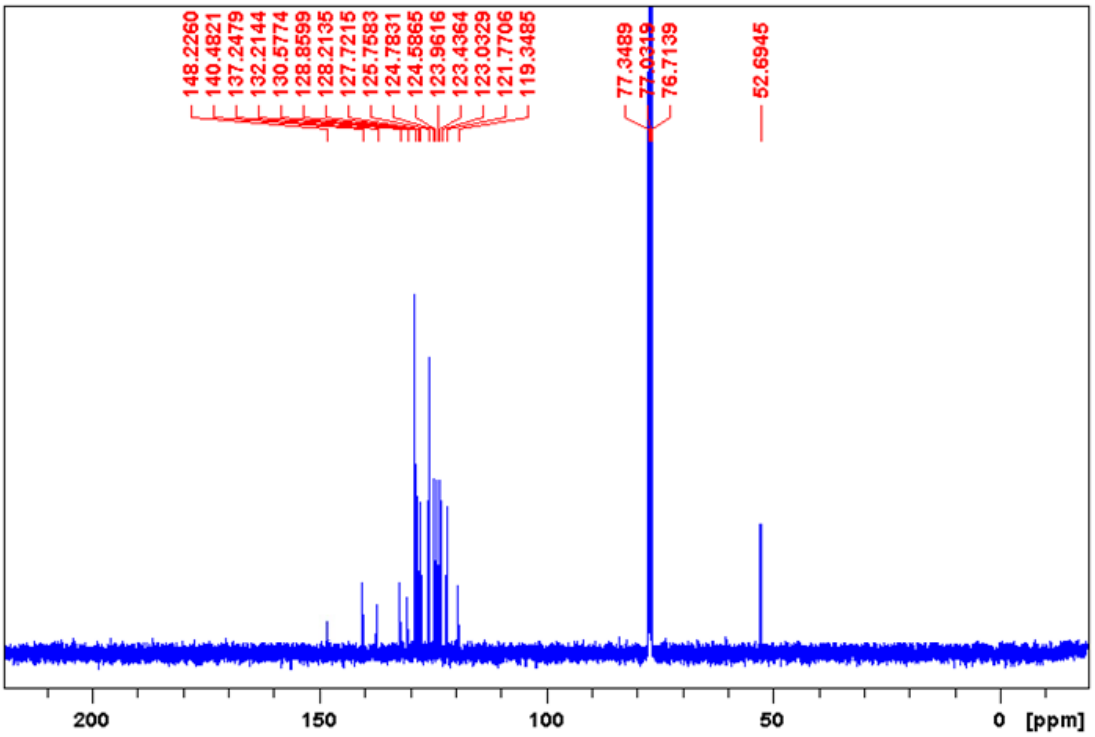
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125.7583
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123.9616
123.4364
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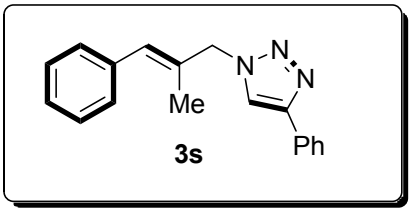
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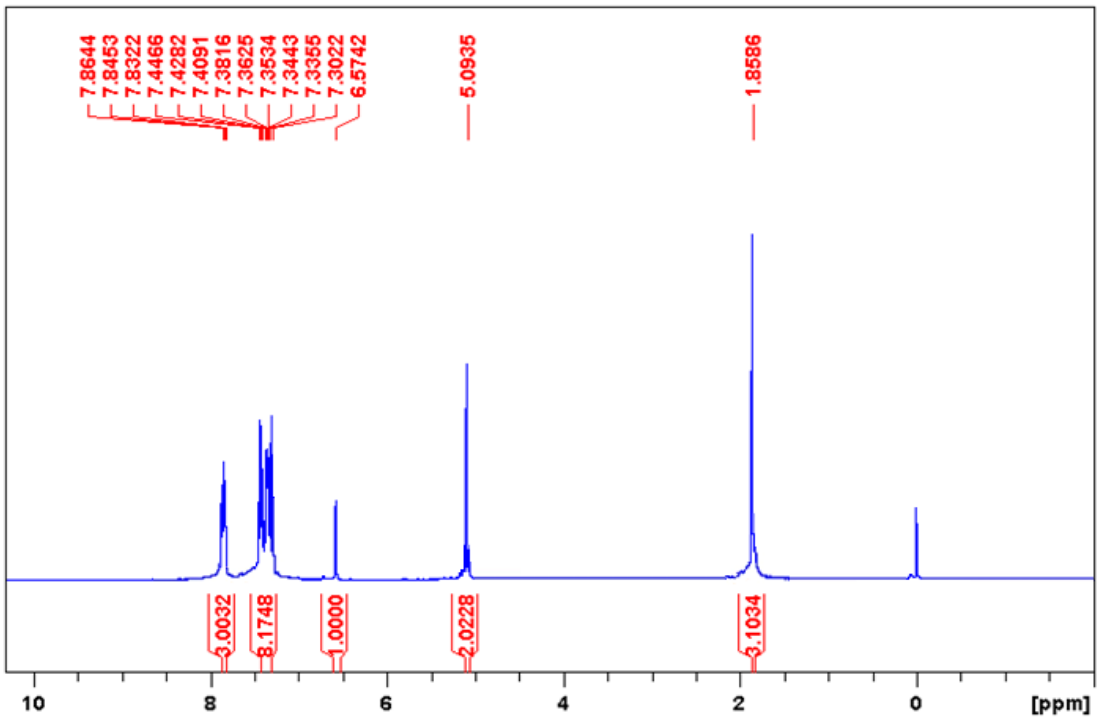
N
N
Me
Ph

3s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6.5742
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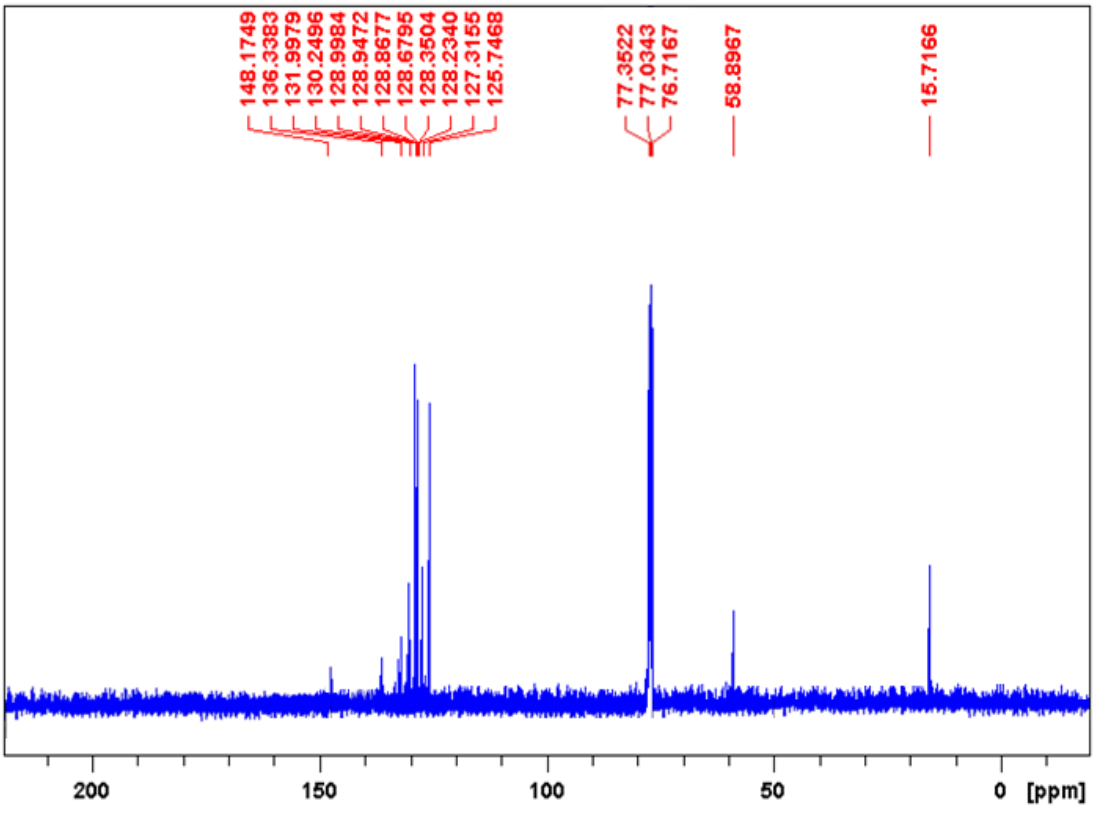
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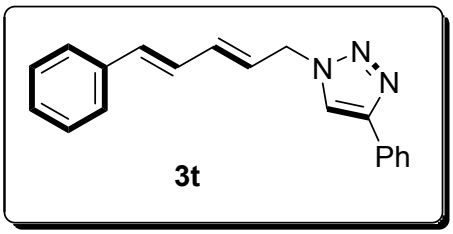
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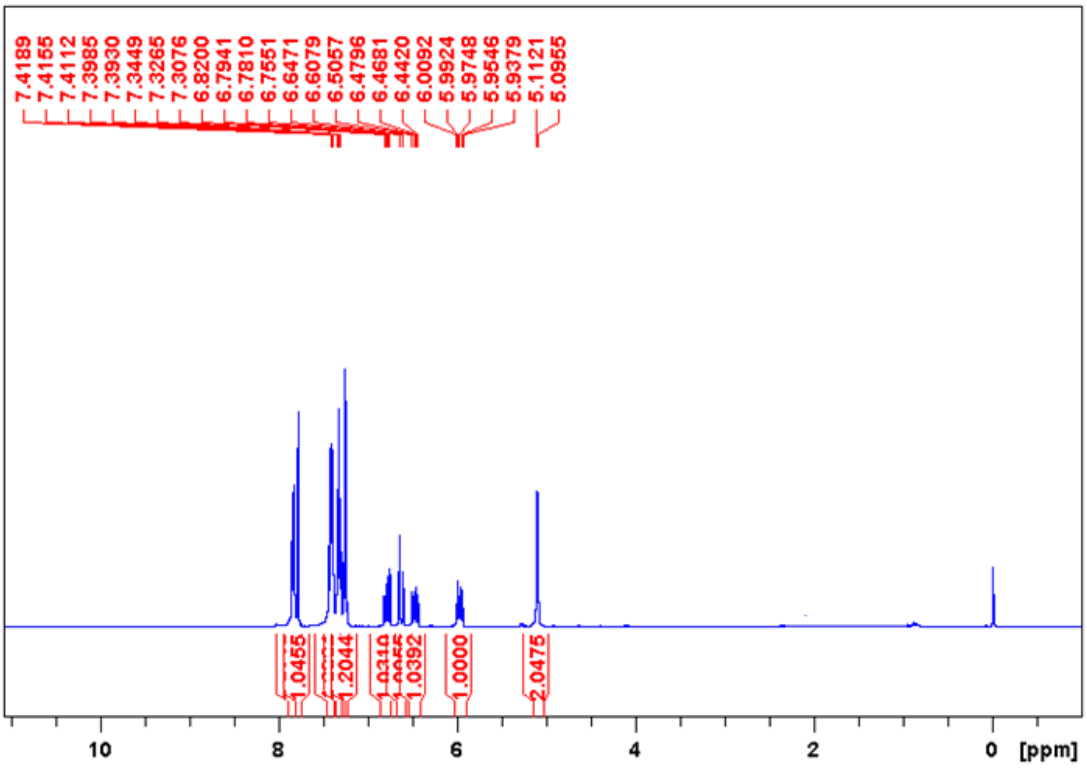
N
N
Ph

3t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7.3930
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6.7810
6.7551
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6.6079
6.5057
6.4796
6.4681
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5.9924
5.9748
5.9546
5.9379
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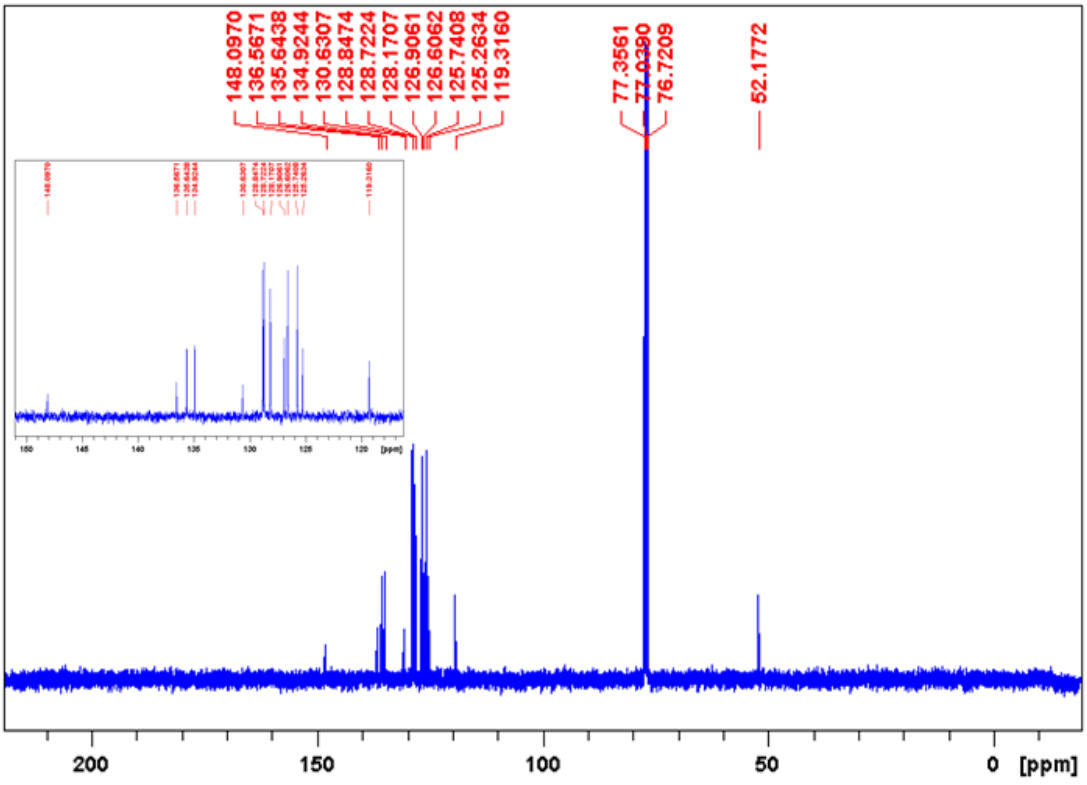
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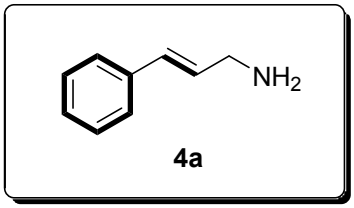
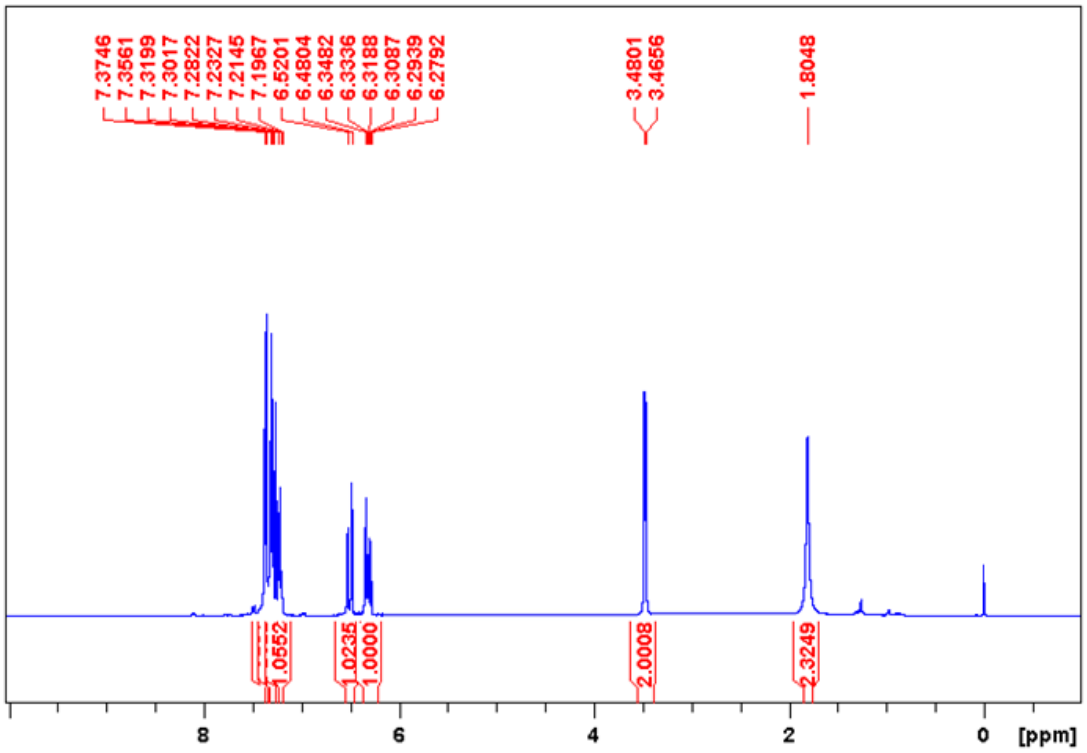

NH2

4a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7.2145
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6.3482
6.3336
6.3188
6.3087
6.2939
6.2792
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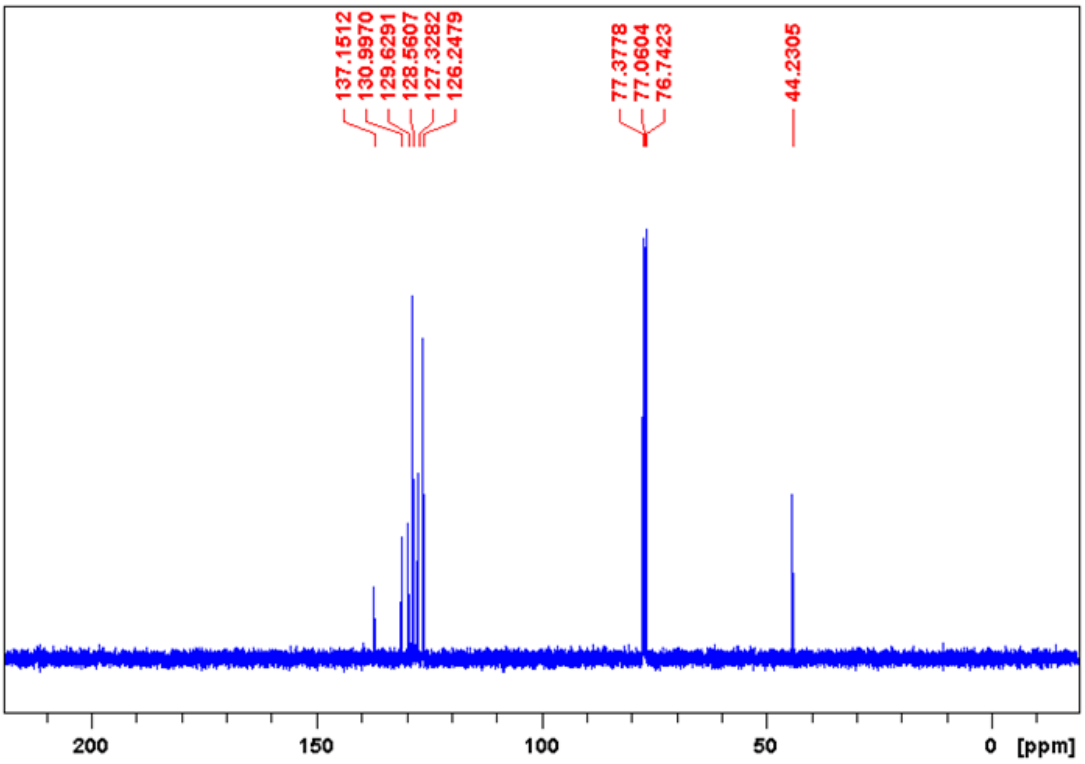
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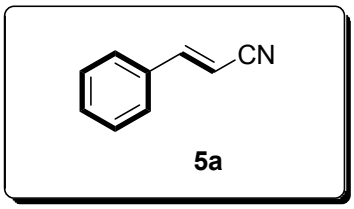
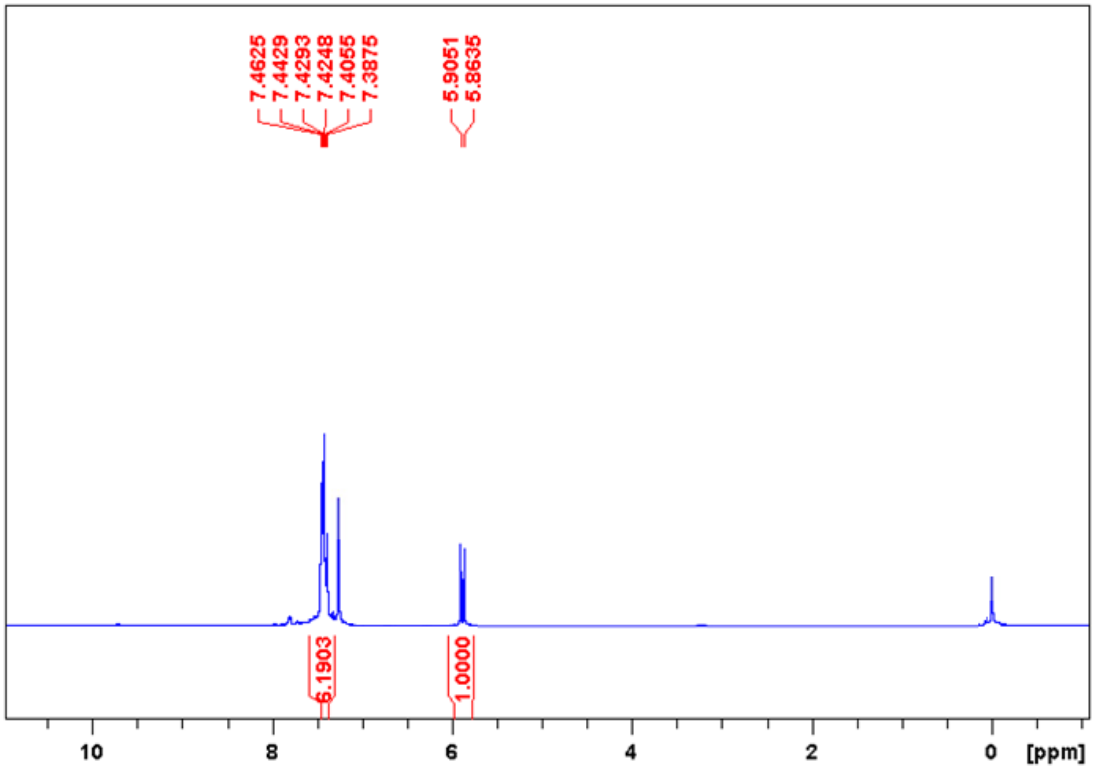

CN

5a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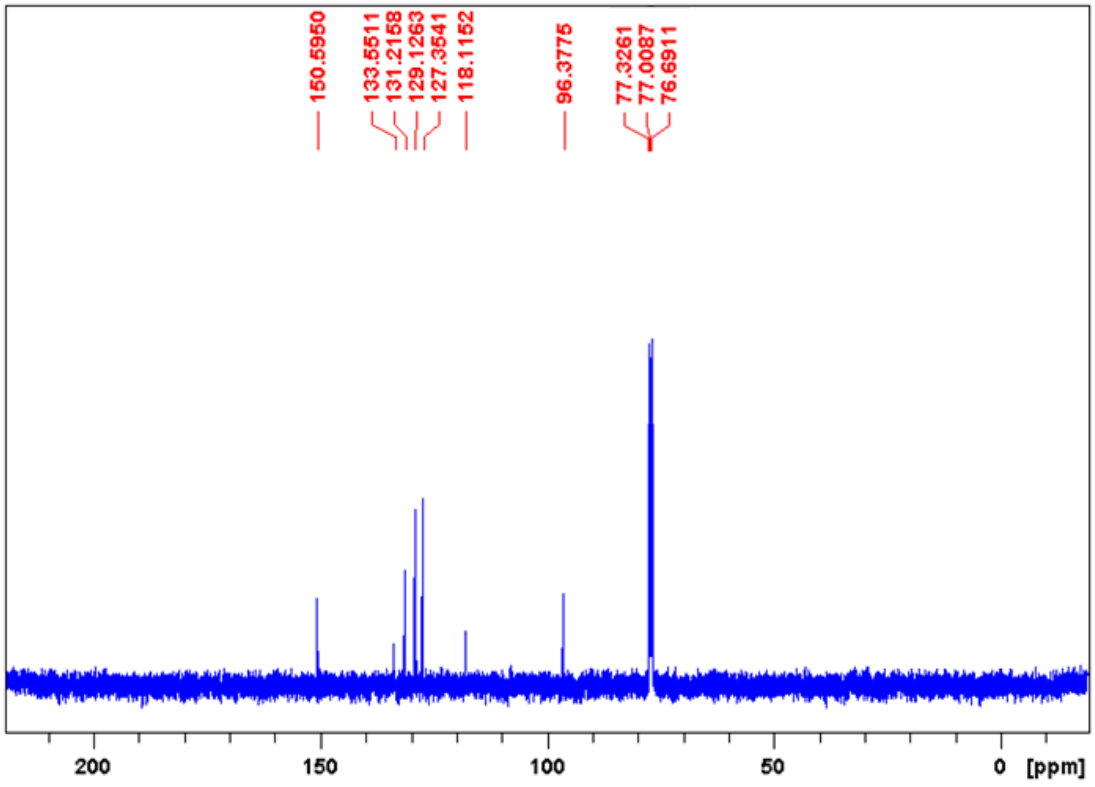
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50
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