Electronic Supplementary Material (ESI) for RSC Advances.

DMSO-allyl bromide: A mild and efficient reagent for atom economic one-pot N-allylation and bromination of 2°-aryl amines, 2-aryl aminoamides, indoles and 7-aza indoles

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1. General remarks

All the reactions were carried out in oven-dried glassware. Progress of reactions was monitored by Thin Layer Chromatography (TLC) while purification of crude compounds was done by column chromatography using Silica gel (Mesh size 100-200). The NMR spectra were recorded on Bruker-400 MHz NMR spectrometer (400 MHz for ^{1}H NMR and 100 MHz for ^{13}C NMR) with $CDCl_3$ or $(CD_3)_2SO$ as the solvent and TMS as internal reference. Integrals are in accordance with assignments; Coupling constants were reported in Hertz (Hz). All ^{13}C spectra are proton-decoupled. Multiplicity is indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), br s (broad singlet). FTIR spectra were recorded on a Perkin-Elmer RX-IFT-IR and absorbencies are reported in cm^{-1}. HRMS analyses were recorded using Q-T of Micro mass spectrometer (different mass analyses based on availability of instruments). Yields refer to quantities obtained after chromatography.

2. Experimental procedures

a. General experimental procedure (A) for the preparation of compounds 3a-r/ 4a:

To a stirred solution of **1** (1 equiv.) and KOH (2 equiv.) in DMSO, alkyl halide (**2a**) (2.5 equiv.) was added and stirred for 12 h at 70 °C. The reaction was quenched with cold water upon completion. The crude was extracted with ethyl acetate washed with dil. HCl and distilled water. The combined organic layer was dried over anhydrous Na_2SO_4. Solvent was removed under vacuum and crude was purified by silica gel column chromatography to afford pure *N*-allylated-brominated derivatives (**3a-r**) and brominated derivatives (**4a**).

b. General procedure (B) for synthesis of compounds10a-b&10a'-b'

A mixture of compound **3a** (1 equiv.), aryl boronic acids **9a-b** (2.5 equiv.), $Pd(dppf)Cl_2$.DCM (0.2 equiv.), and K_2CO_3 (1.5 equiv.) in 4 mL of dioxane-MeOH (3:1) was microwave irradiated (power mode) at 100 W for 10 min. After completion of the reaction (TLC), the solvent was removed *in vacuo*, and the residue was extracted with EtOAc and washed with HCl (0.25 M, 20 mL) followed by saturated brine. The organic layer was dried over anhydrous Na_2SO_4 and purified through a silica gel column chromatography by gradient elution using EtOAc:hexane to afford compounds **10a-b** in very good yields along with **10a'-b'**.

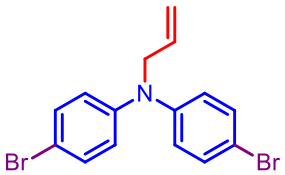
c. General Procedure (C) for synthesis of compound 11a

To a solution of RCM substrate **(3e')** in toluene, 3mol% of Grubbs II catalyst was added and stirred at RT for 3min. After completion of the reaction, the solvent was removed under reduced pressure and residue was purified by silica gel column chromatography using EtOAc:hexane as eluent to afford pure **11a** in good yields.

3. Spectroscopic data of synthesized new compounds

N-allyl-4-bromo-N-(4-bromophenyl)aniline (**3a);**

Following the general procedure **(A)**, reaction of compound **1a** (200 mg, 1.183 mmol, 1 equiv.), allyl bromide **2a** (0.2mL, 2.957 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (132 mg, 2.366 mmol, 2 equiv.) afforded compound **3a.**



3a

Colourless liquid: 310mg, 71% yield;

R_f (5% EtOAc-Hexane):0.40;

FTIR (KBr) ν_{max}: 3338, 3087, 2881, 1895, 1654, 1581, 1487, 1377, 1315, 1175, 1010, 819, 768, 720cm^{-1};

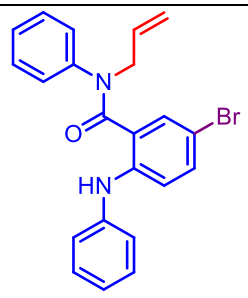
^{1}H NMR (400 MHz, $CDCl_3$):δ 7.37 – 7.35 (m, 2H), 7.34 – 7.32 (m, 2H), 6.91 – 6.89 (m, 2H), 6.88 (d, *J* = 3.2 Hz, 2H), 5.88 (ddt, *J* = 17.2, 10.3, 4.8 Hz, 1H), 5.26 – 5.16 (m, 2H), 4.30 (dt, *J* = 4.7, 1.8 Hz, 2H);

^{13}C NMR ($CDCl_3$/TMS, 100 MHz): δ 54.9, 114.2, 117, 122.5, 132.4, 133.5, 146.6;

HRMS-ESI: Calcd. for $C_{15}H_{13}Br_2N$ $[M+H]^+$*m/z*: 369.9316; Found 369.9316.

N-allyl-5-bromo-N-phenyl-2-(phenylamino)benzamide (**3b**):

Following the general procedure **(A)**, reaction of compound **1b** (100 mg, 0.347 mmol, 1equiv.), allyl bromide **2a** (0.07 mL, 0.868 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (38 mg, 0.694 mmol, 2 equiv.) afforded compound **3b.**



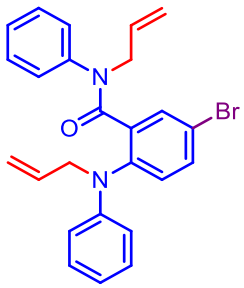
3b

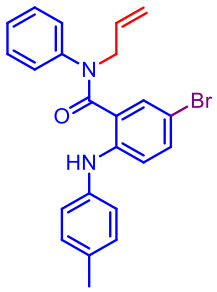
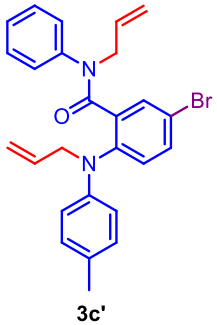
Colourless liquid: 94mg, 66% yield;

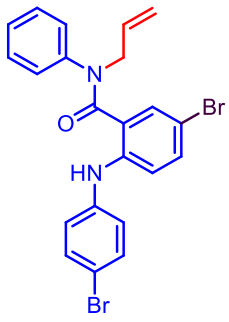
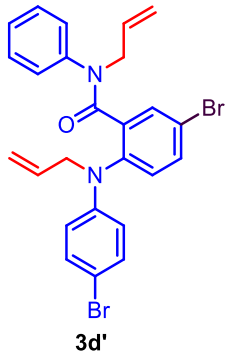
R_f (5% EtOAc-Hexane): 0.43;

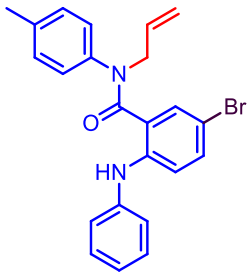
FTIR (KBr) ν_{max}: 3264, 3066, 2921, 2853, 1871, 1644, 1593, 1494, 1443, 1376, 1326, 1246, 1182, 1129, 1075, 993, 914, 813, 754 cm^{-1};

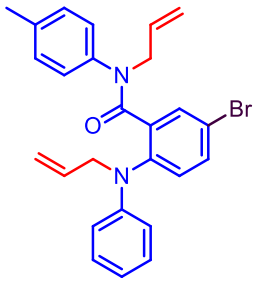
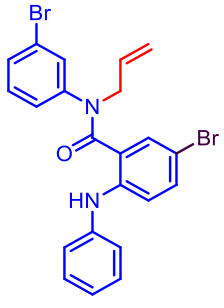
^{1}H NMR (400 MHz, $CDCl_3$): δ 9.74 (s, 1H), 8.20 (dd, *J* = 7.8,

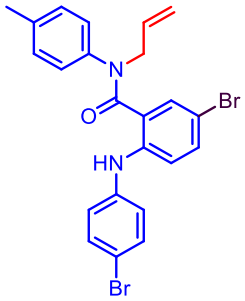
	1.6 Hz, 1H), 7.45 (td, *J* = 7.7, 1.7 Hz, 1H), 7.38 (dd, *J* = 7.7, 1.1 Hz, 1H), 7.33 (d, *J*= 8.5 Hz, 2H), 7.30 – 7.25 (m, 2H), 7.21 (dd, *J* = 13.8, 5.5 Hz, 2H), 7.09 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.02 (t, *J*= 7.4 Hz, 1H), 6.68 – 6.61 (m, 2H), 5.92 – 5.80 (m, 1H), 5.21 – 5.09 (m, 2H), 4.15 (d, *J* = 6.0 Hz, 2H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 56.1, 112.8, 117.9, 119.6, 120.1, 120.4, 124.4, 127.7, 129.1, 129.2, 129.5, 130.0, 132.0, 132.1, 132.3, 132.5, 133.0, 138.0, 145.3, 147.2, 163.7; **HRMS-ESI**: Calcd. for$C_{22}H_{19}BrN_2O[M+Na]^+$*m/z*: 429.0578; Found 429.0583.
N-allyl-2-(allyl(phenyl)amino)-5-bromo-N-phenylbenzamide (**3b')** Following the general procedure **(A)**, reaction of compound **1b** (100 mg, 0.347 mmol, 1 equiv.), allyl bromide **2a** (0.07 mL, 0.868 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (38 mg, 0.694 mmol, 2 equiv.) afforded compound **3b'.**	
 **3b'**	**Colourless liquid**: 52 mg, 33% yield; **R_f** (5% EtOAc-Hexane):0.42; **FTIR** (KBr) ν_{max}: 3134, 2924, 1647, 1490, 1400, 1074, 754cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.38 (dd, *J* = 7.5, 1.1 Hz, 1H), 7.15 – 6.98 (m, 7H), 6.88 (d, *J* = 8.0 Hz, 1H), 6.81 (d, *J* = 3.4 Hz, 2H), 6.18 (d, *J* = 8.8 Hz, 2H), 5.66 (dqd, *J* = 12.1, 10.3, 5.6 Hz, 2H), 5.13 – 4.96 (m, 4H), 4.26 (d, *J* = 6.0 Hz, 2H), 3.91 (s, 2H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 52.8, 54.6, 110.8, 117.4, 117.8, 125.3, 126.7, 127.2, 127.4, 128.8, 130.5, 130.8, 131.3, 133.2, 134.0, 134.6, 142.4, 144.1, 146.1, 169.3; **HRMS-ESI**: Calcd. for $C_{25}H_{23}BrN_2O[M+H]^+$*m/z*:447.1072; Found 447.1070.
N-allyl-5-bromo-N-phenyl-2-(p-tolylamino)benzamide (**3c**): Following the general procedure **(A)**, reaction of compound **1c** (100 mg, 0.331 mmol, 1equiv.), allyl bromide **2a** (0.07 mL, 0.827mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (37 mg, 0.662 mmol, 2 equiv.) afforded compound **3c.**	

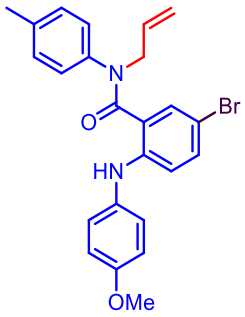
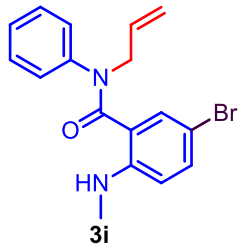
 **3c**	**Yellow liquid**:93 mg, 67% yield; **R_f** (15% EtOAc-Hexane): 0 .42; **FTIR** (KBr) ν_{max}: 3354, 3034, 2981, 2920, 2859, 181, 1791, 1632, 1577, 1512, 1489, 1302, 1224, 1137, 1105, 1034, 995, 966, 929, 812, 769, 698cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.49 (s, 1H), 7.35 (d, *J* = 1.1 Hz, 1H), 7.19 (s, 1H), 7.17 – 7.09 (m, 3H), 7.07 – 7.02 (m, 2H), 7.01 – 6.95 (m, 4H), 6.88 (d, *J* = 8.8 Hz, 1H), 5.90 (ddt, *J* = 16.2, 10.2, 6.0 Hz, 1H), 5.12 (ddd, *J* = 10.0, 7.9, 1.3 Hz, 2H), 4.44 (d, *J* = 6.0 Hz, 2H), 2.24 (s, 3H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 21.0, 53.0, 109.6, 117.2, 118.2, 120.4, 124.1, 127.1, 127.2, 127.3, 129.3, 130.1, 132.2, 132.3, 132.8, 133.0, 139.0, 143.0, 143.2, 169.2; **HRMS-ESI**: Calcd. for $C_{23}H_{21}BrN_2O[M+H]^+$*m/z*: 421.0916; Found 421.0913.
N-allyl-2-(allyl(p-tolyl)amino)-5-bromo-N-phenylbenzamide (**3c'**): Following the general procedure **(A)**, reaction of compound **1c** (100 mg, 0.331 mmol, 1 equiv.), allyl bromide **2a** (0.07 mL, 0.827mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (37 mg, 0.662 mmol, 2 equiv.) afforded compound **3c'.**	
 **3c'**	**Colourless liquid**: 52 mg, 34% yield; **R_f** (15% EtOAc-Hexane): 0.42; **FTIR** (KBr) ν_{max}: 3354, 3066, 3028, 2923, 2860, 1890, 1644, 1593, 1511, 1450, 1383, 1304, 1162, 1130, 1072, 921, 870, 813, 765, 698cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.35 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.13 – 6.94 (m, 5H), 6.84 (dt, *J* = 7.1, 5.5 Hz, 5H), 6.30 (d, *J* = 8.2 Hz, 1H), 5.72 (ddd, *J* = 22.0, 10.2, 5.0 Hz, 1H), 5.58 (tt, *J* = 10.4, 6.1 Hz, 1H), 5.11 – 4.92 (m, 4H), 4.23 (d, *J* = 5.9 Hz, 2H), 3.90 (s, 2H), 2.17 (s, 3H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 20.5, 52.5, 54.6, 116.9, 117.1, 117.4, 124.1, 126.2, 126.4, 127.3, 128.4, 128.6, 129.0, 130.1, 130.5, 133.5, 133.8, 134.5, 142.4, 144.5, 145.1, 169.6; **HRMS-ESI**: Calcd. for $C_{26}H_{25}BrN_2O[M+Na]^+$*m/z*: 483.1048;

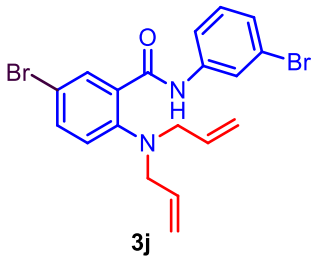
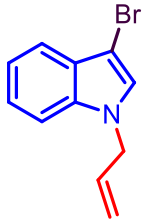
	Found 483.1046.
N-allyl-5-bromo-2-((4-bromophenyl)amino)-N-phenylbenzamide (**3d**): Following the general procedure **(A)**, reaction of compound **1d** (100 mg, 0.2724 mmol, 1equiv.), allyl bromide **2a** (0.06 mL, 0.681 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (30 mg, 0.544 mmol, 2 equiv.) afforded compound **3d.**	
 **3d**	**Colourless liquid**: 83 mg, 62% yield; **R_f** (10% EtOAc-Hexane): 0.44; **FTIR** (KBr) ν_{max}: 3482, 1633, 1583, 1500, 1399, 1262, 1074, 815, 698 cm^{-1} **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.43 (s, 1H), 7.34 – 7.30 (m, 2H), 7.19 (t, *J* = 3.8 Hz, 2H), 7.16 – 7.11 (m, 1H), 7.06 (dd, *J* = 8.8, 2.2 Hz, 1H), 7.01 (s, 1H), 6.98 (dd, *J* = 5.7, 4.3 Hz, 2H), 6.93 (d, *J* = 2.2 Hz, 1H), 6.90 – 6.84 (m, 2H), 5.87 (ddt, *J* = 16.3, 10.3, 6.0 Hz, 1H), 5.12 (ddd, *J* = 6.6, 4.5, 1.3 Hz, 2H), 4.42 (d, *J* = 6.0 Hz, 2H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz):δ 53.0, 11.1, 114.1, 118.1, 118.3, 120.8, 125.4, 127.2, 127.5, 129.4, 132.5, 132.5, 132.6, 133.2, 141.0, 141.7, 143.0, 169.0; **HRMS-ESI**: Calcd. for $C_{22}H_{18}Br_2N_2O[M+H]^+$*m/z*: 488.9864; Found 488.9849.
N-allyl-2-(allyl(4-bromophenyl)amino)-5-bromo-N-phenylbenzamide (**3d'**): Following the general procedure **(A)**, reaction of compound **1d** (100 mg, 0.2724 mmol, 1 equiv.), allyl bromide **2a**(0.06 mL, 0.681 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (30 mg, 0.544 mmol, 2 equiv.) afforded compound **3d'.**	
 **3d'**	**Colourless liquid**: 52 mg, 36% yield; **R_f** (10% EtOAc-Hexane): 0.44; **FTIR** (KBr) ν_{max}: 3418, 2995, 1644, 1589, 1491, 1452, 1384, 1307, 995, 923, 817, 765, 698cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.38 (d, *J* = 6.8 Hz, 1H), 7.12 (d, *J* = 7.3 Hz, 1H), 7.09 – 6.99 (m, 5H), 6.89 (d, *J* = 7.9 Hz, 1H), 6.82 (d, *J* = 3.1 Hz, 2H), 6.18 (d, *J* = 8.7 Hz, 2H), 5.68 (dddd, *J* = 22.9, 16.4, 11.0, 5.6 Hz, 2H), 5.11 – 4.97 (m, 4H),

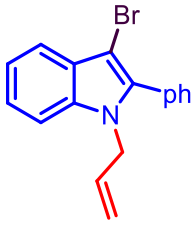
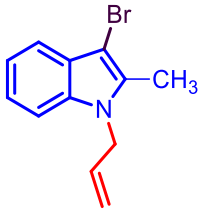
	4.27 (d, *J* = 5.9 Hz, 2H), 3.92 (s, 2H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz):δ 20.5, 52.5, 54.6, 116.9, 117.1, 117.4, 124.1, 126.2, 126.4, 127.3, 128.4, 128.6, 129.0, 130.1, 130.5, 133.5, 133.8, 134.5, 142.4, 144.5, 145.1, 169.6; **HRMS-ESI**: Calcd. for $C_{25}H_{22}Br_2N_2O[M+H]^+$ *m/z*: 529.0177; Found 529.0159.
N-allyl-5-bromo-2-(phenylamino)-N-(p-tolyl)benzamide (**3e**): Following the general procedure **(A)**, reaction of compound **1e** (150 mg, 0.496 mmol, 1 equiv.), allyl bromide **2a** (0.1 mL, 1.241 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (55 mg, 0.993 mmol, 2 equiv.) afforded compound **3e.**	
 **3e**	**Colourless Liquid**: 133mg, 64% yield; **R_f** (15% EtOAc-Hexane): 0.45; **FTIR** (KBr) ν_{max}: 3295, 3190, 3111, 3037, 2986, 2926, 1626, 1585, 1513, 1485, 1395, 1225, 1165, 1073, 1046, 1006, 974, 911, 817, 770, 742, 714 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ7.50 (s, 1H), 7.33 – 7.27 (m, 2H), 7.15 (d, *J* = 8.2 Hz, 1H), 7.02 – 6.96 (m, 1H), 6.92 (t, *J* = 9.3 Hz, 4H), 6.84 (d, *J* = 8.2 Hz, 3H), 6.48 (t, *J* = 7.4 Hz, 1H), 5.87 (ddt, *J* = 16.2, 10.3, 5.9 Hz, 1H), 5.15 – 5.06 (m, 2H), 4.41 (d, *J* = 5.9 Hz, 2H), 2.19 (s, 3H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ21.0, 52.0, 113.2, 116.8, 117.8, 119.5, 120.2, 124.3, 127.0, 129.7, 129.8, 130.1, 132.2, 133.0, 136.7, 140.6, 141.6, 142.3, 170.4; **HRMS-ESI**: Calcd. for $C_{23}H_{21}BrN_2O[M+H]^+$*m/z*: 421.0916; Found 421.0918.
N-allyl-2-(allyl(phenyl)amino)-5-bromo-N-(p-tolyl)benzamide (**3e'**): Following the general procedure **(A)**, reaction of compound **1e** (150 mg, 0.496 mmol, 1 equiv.), allyl bromide **2a** (0.1 mL, 1.241 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (55 mg, 0.993 mmol, 2 equiv.) afforded compound **3e'.**	

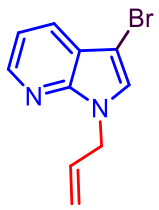
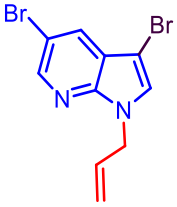
 **3e'**	**Colourless Liquid**: 73 mg, 31% yield; **R_f** (15% EtOAc-Hexane): 0.41; **FTIR** (KBr) ν_{max}: 3659, 3070, 3032, 2979, 2923, 2860, 1846, 1642, 1586, 1511, 1488, 1449, 1383, 1306, 1241, 1162, 1129, 994, 922, 818, 772, 723, 655cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.37 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.11 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.08 – 7.01 (m, 3H), 6.89 (d, *J* = 7.9 Hz, 1H), 6.77 (d, *J* = 8.1 Hz, 2H), 6.67 (d, *J* = 8.2 Hz, 2H), 6.16 (d, *J* = 8.9 Hz, 2H), 5.78 – 5.70 (m, 1H), 5.66 (ddd, *J* = 12.2, 9.5, 5.4 Hz, 1H), 5.12 – 5.04 (m, 2H), 5.04 – 4.97 (m, 2H), 4.26 (d, *J* = 6.1 Hz, 2H), 3.97 (d, *J* = 4.3 Hz, 2H), 2.16 (s, 3H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 21.0, 52.7, 54.6, 110.5, 117.3, 117.6, 117.7, 125.3, 127.0, 127.2, 127.5, 129.3, 130.1, 130.7, 131.5, 133.2, 133.6, 136.5, 139.6, 144.0, 146.1, 169.2; **HRMS-ESI**: Calcd. for $C_{26}H_{25}BrN_2O[M+Na]^+$ *m/z*: 483.1048; Found 483.1057.
N-allyl-5-bromo-N-(3-bromophenyl)-2-(phenylamino)benzamide **(3f):** Following the general procedure **(A)**, reaction of compound **1f** (150 mg, 0.408 mmol, 1 equiv.), allyl bromide **2a** (0.09 mL, 1.021 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (45 mg, 0.817 mmol, 2 equiv.) afforded compound **3f**.	
 **3f**	**Yellow Liquid**: 125 mg, 62% yield; **R_f** (10% EtOAc-Hexane): 0.42; **FTIR** (KBr) ν_{max}: 3342, 3069, 2925, 2855, 1876, 1638, 1583, 1506, 1454, 1375, 1309, 1225, 1164, 1072, 999, 876, 811, 753, 697cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$):δ 7.36 (s, 1H), 7.33 – 7.28 (m, 2H), 7.20 (d, *J* = 9.3 Hz, 1H), 7.15 (dd, *J* = 5.4, 3.3 Hz, 2H), 7.05 – 6.98 (m, 2H), 6.94 – 6.87 (m, 3H), 6.83 (dd, *J* = 7.7, 1.3 Hz, 1H), 6.56 – 6.49 (m, 1H), 5.86 (ddt, *J* = 16.2, 10.3, 5.9 Hz, 1H), 5.13 (ddd, *J* = 7.2, 5.0, 1.2 Hz, 2H), 4.41 (d, *J* = 5.9 Hz, 2H);

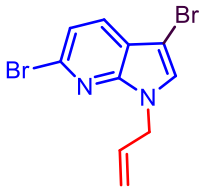
	^{13}C NMR ($CDCl_3$/TMS, 100 MHz): δ52.7, 113.5, 117.1, 118.2, 119.8, 120.4, 122.3, 123.9, 125.8, 129.5, 129.9, 130.1, 130.2, 130.6, 132.3, 132.6, 141.4, 142.4, 144.6, 170.4; **HRMS-ESI**: Calcd. for $C_{22}H_{18}Br_2N_2O[M+H]^+$ *m/z*: 484.9864; Found 484.9854.
N-allyl-5-bromo-2-((4-bromophenyl)amino)-N-(p-tolyl)benzamide (**3g**): Following the general procedure **(A)**, reaction of compound **1g** (100 mg, 0.263 mmol, 1 equiv.), allyl bromide **2a** (0.05 mL, 0.657 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (29 mg, 0.526 mmol, 2 equiv.) afforded compound **3g.**	
 **3g**	**ColourlessLiquid**: 107 mg, 81% yield; **R_f** (10% EtOAc-Hexane): 0.40; **FTIR** (KBr) ν_{max}: 3320, 3021, 2923, 2857, 2534, 1896, 1635, 1583, 1504, 1429, 1378, 1306, 1266 1224, 1176, 1073, 1003, 923, 814, 729, 641cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.37 (s, 1H), 7.33 – 7.29 (m, 2H), 7.06 (dd, *J* = 8.8, 2.3 Hz, 1H), 7.01 – 6.94 (m, 4H), 6.88 – 6.82 (m, 4H), 5.85 (ddt, *J* = 16.3, 10.3, 6.0 Hz, 1H), 5.14 – 5.07 (m, 2H), 4.38 (dt, *J* = 6.0, 1.3 Hz, 2H), 2.22 (s, 3H). **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 21.0, 53.0, 111.1, 113.9, 118.1, 118.2, 120.6, 125.7, 126.9, 129.9, 132.3, 132.4, 132.6, 132.9, 137.3, 140.1, 141.0, 141.5, 168.8; **HRMS-ESI**: Calcd. for $C_{23}H_{20}Br_2N_2O[M+H]^+$ *m/z*: 499.0021; Found 499.0000.
N-allyl-5-bromo-2-((4-methoxyphenyl)amino)-N-(p-tolyl)benzamide (**3h**): Following the general procedure **(A)**, reaction of compound **1h** (100 mg, 0.3008 mmol, 1 equiv.), allyl bromide **2a** (0.06 mL, 0.752 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (33 mg, 0.601 mmol, 2 equiv.) afforded compound **3h.**	

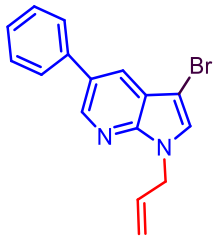
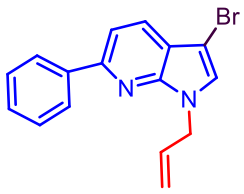
 **3h**	**Yellow liquid**: 75 mg, 55% yield; **R_f** (10% EtOAc-Hexane): 0.48; **FTIR** (KBr) ν_{max}: 3827, 3326, 3042, 3002, 2924, 2835, 2066, 1872, 1634, 1599, 1510, 1463, 1315, 1295, 1239, 1172, 1139, 1106, 999, 970, 929, 888, 819, 757, 718, 648 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.25 (s, 1H), 6.98 (dt, *J* = 4.6, 3.5 Hz, 5H), 6.92 – 6.87 (m, 3H), 6.83 – 6.79 (m, 2H), 6.77 (d, *J* = 8.9 Hz, 1H), 5.88 (ddt, *J* = 16.2, 10.2, 6.0 Hz, 1H), 5.16 – 5.08 (m, 2H), 4.40 (dt, *J* = 6.0, 1.3 Hz, 2H), 3.74 (s, 3H), 2.23 (s, 3H). **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 21.0, 53.0, 55.6, 108.9, 114.8, 116.1, 118.0, 123.2, 123.3, 126.8, 129.9, 132.2, 132.8, 132.9, 134.4, 137.0, 140.4, 144.2, 155.8, 169.3; **HRMS-ESI**: Calcd. for $C_{24}H_{23}BrN_2O_2[M+H]^+$ *m/z*: 451.1021; Found451.1009.
N-allyl-5-bromo-2-(methylamino)-N-phenylbenzamide (**3i**): Following the general procedure **(A)**, reaction of compound **1i** (100 mg, 0.441 mmol, 1 equiv.), allyl bromide **2a** (0.09 mL, 1.104 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (49 mg, 0.883 mmol, 2 equiv.) afforded compound **3i.**	
 **3i**	**Colourless Lquid**: 109mg, 71% yield; **R_f** (10% EtOAc-Hexane): 0.45; **FTIR** (KBr) ν_{max}: 3897, 3781, 3280, 3194, 3137, 3083, 2956, 2858, 2798, 1655, 1602, 1544, 1489, 1443, 1396, 1323, 1260, 1185, 1140, 980, 932, 898, 813, 759, 724 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 12.16 (s, 1H), 8.36 (d, *J* = 2.5 Hz, 1H), 7.60 (d, *J* = 7.6 Hz, 2H), 7.51 (dd, *J* = 8.5, 2.5 Hz, 1H), 7.30 (t, *J* = 7.9 Hz, 2H), 7.07 (dd, *J* = 15.9, 8.0 Hz,2H), 5.87 – 5.73 (m, 1H), 5.20 (dd, *J* = 11.4, 6.1 Hz, 2H), 3.54 (d, *J* = 6.7 Hz, 2H), 2.70 (s, 3H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 42.5, 61.0, 119.1, 120.1, 120.5, 123.8, 124.2, 129.2, 130.2, 132.8, 134.6, 135.2, 138.5, 150.2, 162.6; **HRMS-ESI**: Calcd. for $C_{17}H_{17}BrN_2O[M+H]^+$ *m/z*: 345.0603;

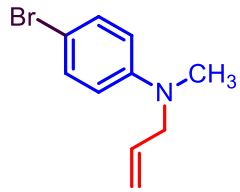
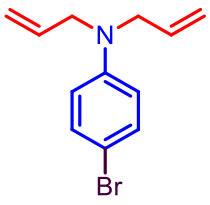
	Found 345.0602.
5-bromo-N-(3-bromophenyl)-2-(diallylamino)benzamide (**3j**): Following the general procedure **(A)**, reaction of compound **1j** (200 mg, 0.689 mmol, 1 equiv.), allyl bromide **2a** (0.1 mL, 1.723 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (77 mg, 1.378 mmol, 2 equiv.) afforded compound **3j.**	
 **3j**	**White powder**: 132 mg, 43% yield; **R_f** (10% EtOAc-Hexane): 0.48; **FTIR** (KBr) ν_{max}: 3705, 2924, 1667, 1589, 1541, 1474, 1421, 1254, 1032, 923, 769, 674 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ12.52 (s, 1H), 8.37 (d, *J* = 2.5 Hz, 1H), 7.87 (d, *J* = 1.7 Hz, 1H), 7.55 – 7.41 (m, 2 H), 7.20 – 7.13 (m, 2H), 7.07 (d, *J* = 8.5 Hz, 1H), 5.72 (ddt, *J* = 17.0, 10.3, 6.8 Hz, 2H), 5.19 – 5.09 (m, 4H), 3.59 (d, *J* = 6.8 Hz, 4H). **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 57.8, 118.4, 119.7, 120.8, 123.0, 122.9, 125.7, 127.1, 113.5, 113.8, 132.1, 134.6, 135.2, 139.8, 148.1, 162.6; **HRMS-ESI**: Calcd. for $C_{19}H_{18}Br_2N_2O[M+H]^+$ *m/z*: 452.9864; Found 452.9866.
1-allyl-3-bromo-1H-indole (**3k):** Following the general procedure **(A)**, reaction of compound **1k** (200 mg, 1.707 mmol, 1 equiv.), allyl bromide **2a** (0.4 mL, 4.268 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (191 mg, 3.414 mmol, 2 equiv.) afforded compound **3k.**	
 3k	**Yellow liquid**: 265mg, 66% yield; **R_f** (10% EtOAc-Hexane):0.40; **FTIR** (KBr) ν_{max}: 3118, 3056, 2985, 2919, 1645, 1611, 1516, 1459, 1417, 1387, 1322, 1253, 1200, 990, 793, 656cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.47 (d, *J* = 7.4 Hz, 1H), 7.18 – 7.05 (m, 3H), 6.96 (s, 1H), 5.81 (ddd, *J* = 22.4, 10.6, 5.5 Hz, 1H), 5.08 (dd, *J* = 10.2, 1.0 Hz, 1H), 4.97 (d, *J* = 17.1 Hz, 1H), 4.51 (d, *J* = 5.4 Hz, 2H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 49.05, 90.02, 109.91, 117.90, 119.44, 120.33, 122.75, 126.78, 127.52, 132..96,

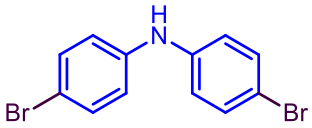
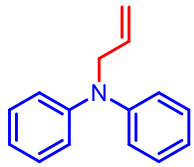
	135.75; **HRMS-ESI**: Calcd. for $C_{11}H_{10}BrN[M+Na]^+$ *m/z*: 257.1094; Found257.1054.
2-(allyl(phenyl)amino)-5-bromo-N-phenylbenzamide (**3l**): Following the general procedure **(A)**, reaction of compound **1l** (100 mg, 0.5174 mmol, 1 equiv.), allyl bromide **2a** (0.1 mL, 1.293 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (57 mg, 1.034 mmol, 2 equiv.) afforded compound **3l.**	
 3l	**Yellow Solid**: 89mg, 73% yield; **R_f** (10% EtOAc-Hexane): 0.43; **FTIR** (KBr) ν_{max}: 3076, 2979, 2923, 2325, 1960, 1895, 1818, 1768, 1680, 1643, 1603, 1454, 1419, 1386,1321, 1257, 1229, 1179, 1111, 1069, 985, 947, 831, 797, 698, 662, 576 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.68 (d, *J* = 7.6 Hz, 1H), 7.57 – 7.47 (m, 5H), 7.39 – 7.25 (m, 3H), 5.98 – 5.88 (m, 1H), 5.20 (d, *J* = 10.4 Hz, 1H), 4.97 (d, *J* = 17.2 Hz, 1H), 4.71 – 4.66 (m, 2H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 47.26, 90.80, 110.60, 116.87, 119.54, 120.83, 123.05, 127.55, 128.56, 128.94, 130.67, 133.45, 136.39, 138.05; **HRMS-ESI**: Calcd. for $C_{12}H_{12}BrNO[M+H]^+$ *m/z*: 314.0388; Found 314.0370.
1-allyl-3-bromo-2-methyl-1H-indole (**3m**): Following the general procedure **(A)**, reaction of compound **1m** (100 mg, 0.762 mmol, 1 equiv.), allyl bromide **2a** (0.2 mL, 1.90 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (85 mg, 1.52 mmol, 2 equiv.) afforded compound **3m.**	
 3m	**Yellow liquid**: 86 mg, 59% yield; **R_f** (7% EtOAc-Hexane): 0.42; **FTIR** (KBr) ν_{max}: 3398, 1643, 1463, 1383, 1332, 1263, 1197, 1084, 991, 923, 742, 547 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.57 – 7.53 (m, 1H), 7.29 – 7.17 (m, 3H), 5.94 (ddt, *J* = 17.1, 10.3, 4.7 Hz, 1H), 5.17 (ddd, *J* = 10.3, 2.7, 1.7 Hz, 1H), 4.88 (ddd, *J* = 17.1, 2.9, 1.9

	Hz, 1H), 4.76 – 4.71 (m, 2H), 2.44 (s, 3H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 10.97, 46.06, 89.82, 109.23, 116.55, 118.53, 120.15, 121.89, 127.03, 132.83, 133.89, 135.69; **HRMS-ESI**: Calcd. for $C_{18}H_{15}N_3O_2$ $[M+Na]^+$ *m/z*: 273.0003; Found 273.0031.
1-allyl-3-bromo-1H-pyrrolo[2,3-b]pyridine (**3n**): Following the general procedure **(A)**, reaction of compound **1n** (100 mg, 0.846 mmol, 1 equiv.), allyl bromide **2a** (0.2 mL, 2.116 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (94 mg, 1.692 mmol, 2 equiv.) afforded compound **3n.**	
 3n	**Colourless liquid**: 126mg, 63% yield; **R$_f$** (10% EtOAc-Hexane): 0.42; **FTIR** (KBr) ν_{max}: 3053, 2923, 1862, 1645, 1596, 1566, 1419, 1318, 1195, 1114, 991, 937, 792, 766, 672cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.26 (dd, *J* = 4.7, 1.4 Hz, 1H), 7.75 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.15 (s, 1H), 7.03 (dd, *J* = 7.9, 4.7 Hz, 1H), 5.92 (ddt, *J* = 16.9, 10.3, 5.6 Hz, 1H), 5.13 (dd, *J* = 10.2, 1.2 Hz, 1H), 5.07 – 5.00 (m, 1H), 4.80 (dt, *J* = 5.6, 1.5 Hz, 2H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 46.65, 88.35, 116.44, 117.95, 119.97, 126.71, 127.55, 133.23, 144.03, 146.36; **HRMS-ESI**: Calcd. for $C_{10}H_9BrN_2[M+H]^+$ *m/z*: 237.0027; Found 237.0030.
1-allyl-3,5-dibromo-1H-pyrrolo[2,3-b]pyridine (**3o**): Following the general procedure **(A)**, reaction of compound **1o** (70 mg, 0.355 mmol, 1equiv.), allyl bromide **2a** (0.07 mL, 0.887 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (39 mg, 0.710 mmol, 2 equiv.) afforded compound **3o.**	
	**White Solid**: 95 mg, 85% yield; **R$_f$** (10% EtOAc-Hexane): 0.44; **FTIR** (KBr) ν_{max}: 3123, 3072, 2926, 2854, 2188, 1852, 1811, 1746, 1738, 1710, 1641, 1589, 1463, 1410, 1379, 1334, 1298, 1193, 1136,965, 886, 799, 765, 686 cm^{-1};

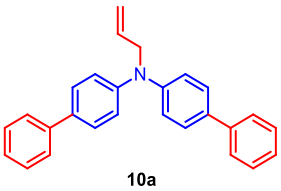
3o	**^{1}H NMR**(400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 2.1 Hz, 1H), 7.88 (d, *J* = 2.1 Hz, 1H), 7.16 (s, 1H), 5.91 (ddt, *J* = 17.0, 10.3, 5.7 Hz, 1H), 5.16 (ddd, *J* = 10.2, 2.4, 1.2 Hz, 1H), 5.05 (ddd, *J* = 17.0, 2.7, 1.5 Hz, 1H), 4.77 (dt, *J* = 5.7, 1.5 Hz, 2H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz):δ 46.89, 87.55, 112.38, 118.34, 121.35, 128.11, 129.65, 132.81, 144.68, 144.76; **HRMS-ESI**: Calcd. for $C_{10}H_8Br_2N_2[M+H]^+$ *m/z*: 314.9132; Found 314.9135.
1-allyl-3,6-dibromo-1H-pyrrolo[2,3-b]pyridine **(3p):** Following the general procedure **(A)**, reaction of compound **1p** (70 mg, 0.355 mmol, 1equiv.), allyl bromide **2a** (0.08 mL, 0.888 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (39 mg, 0.710 mmol, 2 equiv.) afforded compound **3p.**	
 3p	**White Solid**: 81 mg, 73% yield; **R_f** (15% EtOAc-Hexane): 0.42; **FTIR** (KBr) ν_{max}: 3886,3434, 3127, 3091, 3029, 2981, 2929, 2884, 2846, 2753, 2679, 2576, 2388, 2182, 1887, 1809, 1644, 1592, 1551, 15009, 1463, 13339, 1296, 1217, 1162, 1001, 934, 805, 757, 698cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.61 (d, *J* = 8.2 Hz, 1H), 7.20 (d, *J* = 8.2 Hz, 1H), 7.13 (s, 1H), 5.91 (ddt, *J* = 16.1, 10.2, 5.9 Hz, 1H), 5.15 (ddd, *J* = 18.2, 13.6, 1.2 Hz, 2H), 4.83 – 4.75 (m, 2H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 46.83, 88.83, 118.63, 120.29, 126.78, 129.72, 132.80, 136.02, 145.79; **HRMS-ESI**: Calcd. for $C_{10}H_8Br_2N_2[M+H]^+$ *m/z*: 314.9132; Found314.9134.
1-allyl-3-bromo-5-phenyl-1H-pyrrolo[2,3-b]pyridine (**3q**): Following the general procedure **(A)**, reaction of compound **1q** (70 mg, 0.360 mmol, 1 equiv.), allyl bromide **2a** (0.07 mL, 0.900 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (40 mg, 0.720 mmol, 2 equiv.) afforded compound **3q.**	

 3q	**Brown Solid**: 69 mg, 61% yield; **R_f** (7% EtOAc-Hexane): 0.45; **FTIR** (KBr) ν_{max}: 3433, 3115, 3062, 3028, 2925, 2854, 2605, 1954, 1895, 1856, 1730, 1643, 1602, 1555, 1474, 1446, 1350, 1328, 1244, 1196, 993, 970, 822, 766, 701, 659 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.51 (d, *J* = 2.0 Hz, 1H), 7.94 (d, *J* = 2.1 Hz, 1H), 7.56 (dd, *J* = 8.1, 1.0 Hz, 2H), 7.40 (dd, *J* = 10.4, 4.8 Hz, 2H), 7.30 (dt, *J* = 9.1, 4.2 Hz, 1H), 7.20 (s, 1H), 6.01 – 5.91 (m, 1H), 5.17 (dd, *J* = 10.2, 1.2 Hz, 1H), 5.09 (dd, *J* = 17.1, 1.2 Hz, 1H), 4.84 (dt, *J* = 5.6, 1.4 Hz, 2H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 46.83, 88.64, 118.08, 119.96, 125.92, 127.28, 127.42, 127.48, 129.00, 130.43, 133.18, 139.09, 143.48, 145.94; **HRMS-ESI**: Calcd. for $C_{16}H_{13}BrN_2[M+H]^+$ *m/z*: 313.0340; Found313.0341.
1-allyl-3-bromo-6-phenyl-1H-pyrrolo[2,3-b]pyridine (**3r**): Following the general procedure **(A)**, reaction of compound **1r** (50 mg, 0.257 mmol, 1 equiv.), allyl bromide **2a** (0.05 mL, 0.643 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (28 mg, 0.514 mmol, 2 equiv.) afforded compound **3r.**	
 3r	**Yellow Liquid**: 60 mg, 74% yield; **R_f** (7% EtOAc-Hexane): 0.41; **FTIR** (KBr) ν_{max}: 3123, 3061, 2924,1779, 1723, 1599, 1568, 1509, 1450, 1413, 1354, 1292, 1214, 1180, 1125, 1098, 1023, 995, 812, 756, 693cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.03 – 7.97 (m, 2H), 7.77 (d, J = 8.2 Hz, 1H), 7.51 (d, J = 8.3 Hz, 1H), 7.37 (dd, J = 10.3, 4.7 Hz, 2H), 7.30 (dd, J = 5.8, 1.6 Hz, 1H), 7.12 (s, 1H), 5.93 (ddt, J = 16.4, 10.5, 5.9 Hz, 1H), 5.17 – 5.10 (m, 2H), 4.85 (dd, J = 4.6, 1.3 Hz, 2H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 46.59, 88.43, 113.87, 118.26, 118.80, 126.94, 127.12, 128.03, 128.56, 128.72, 133.51, 139.88, 146.56, 152.00;

	HRMS-ESI: Calcd. for $C_{16}H_{13}BrN_2[M+H]^+$ *m/z*: 313.0340; Found 313.0332.
N-allyl-4-bromo-N-methylaniline (**3s);** Following the general procedure **(A)**, reaction of compound **1s** (100 mg, 0.9339 mmol, 1 equiv.), allyl bromide **2a** (0.2 mL, 2.334 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (104 mg, 1.867 mmol, 2 equiv.) afforded compound **3s.**	
 **3s**	**Yellow liquid**: 110 mg, 52% yield; **R_f** (10% EtOAc-Hexane):0.40; **^{1}H NMR** (400 MHz, $CDCl_3$):δ 7.23 – 7.17 (m, H), 6.52 – 6.47 (m, 2H), 5.74 (ddt, *J* = 15.4, 10.1, 3.2 Hz, 1H), 5.09 – 5.03 (m, 2H), 3.81 (dt, *J* = 4.9, 1.6 Hz, 2H), 2.84 (s, 3H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 37.12, 54.14, 107.20, 112.94, 115.30, 130.69, 132.11, 147.35;
N,N-diallyl-4-bromoaniline (**3t);** Following the general procedure **(A)**, reaction of compound **1t** (380 mg, 4.0803 mmol, 1 equiv.), allyl bromide **2a** (0.8 mL, 10.200 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (456 mg, 8.160 mmol, 2 equiv.) afforded compound **3t.**	
 **3t**	**Yellow liquid**: 635 mg, 62% yield; **R_f** (10% EtOAc-Hexane):0.40; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.25 – 7.15 (m, 2H), 6.72 – 6.63 (m, 2H), 5.89 – 5.75 (m, 2H), 5.20 – 5.10 (m, 4H), 3.92 – 3.81 (m, 4H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 52.12, 52.96, 112.44, 114.06, 116.06, 116.26, 116.40, 129.15, 131.79, 133.53, 134.15, 147.71, 148.79;
bis(4-bromophenyl)amine (**4a**): Following the general procedure **(A)**, reaction of compound **1a** (200 mg, 1.183 mmol, 1 equiv.), allyl bromide **2a** (0.2 mL, 2.954 mmol, 2.5 equiv.) in DMSO (3 mL) and KOH (132 mg, 2.366 mmol, 2 equiv.) afforded compound **4a.**	

 **4a**	**White Powder**: 120 mg, 31% yield; **R_f** (5% EtOAc-Hexane):0.40; **FTIR** (KBr) ν_{max}: 3414, 3061, 3027, 2922, 2854, 2804, 2727, 2539, 2100,1885, 1769, 1583, 1502, 1376, 1318, 1228, 1171, 1112, 1069, 1001, 927, 813, 690cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.38 – 7.36 (m, 2H), 7.36 – 7.34 (m, 2H), 6.92 (d, *J* = 2.2 Hz, 2H), 6.91 – 6.90 (m, 2H), 5.65 (s, 1H).; **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ113.5, 119.7, 132.5, 141.9; **HRMS-ESI;** Calcd for $C_{12}H_9Br_2N$ $[M+Na]^+$*m/z*:325.9180; Found 325.9194.
N-allyl-N-phenylaniline **(5a):** Following the general procedure **(A)**, reaction of compound **1a** (100 mg, 0.5915 mmol, 1 equiv.), allyl bromide **2a** (0.1mL, 1.477 mmol, 2.5 equiv.) in 1,4 dioxane (3 mL) and KOH (66 mg, 1.183 mmol, 2 equiv.) afforded compound **5a.**	
 **5a**	**Colourless liquid**:180 mg, 72% yield; **R_f** (7% EtOAc-Hexane):0.40; **FTIR** (KBr) ν_{max}: 3338, 3061, 2854, 2804, 2727, 2539, 2100,1885, 1769, 1583, 1502, 1487, 1376, 1318, 1069, 927, 813, 670 cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.36 – 7.30 (m, 4H), 7.11 (ddd, *J* = 8.6, 2.0, 1.0 Hz, 4H), 7.05 – 6.98 (m, 1H), 6.06 – 5.96 (m, 1H), 5.38 – 5.32 (m, 1H), 5.27 – 5.22 (m, 1H), 4.46 – 4.41 (m, 2H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 54.9, 116.5, 120.9, 121.4, 129.3, 134.4, 148.0; **HRMS-ESI;** Calcd for $C_{15}H_{15}N$ $[M+H]^+$ *m/z*: 210.1286; Found 210.1286.
N-([1,1'-biphenyl]-4-yl)-N-allyl-[1,1'-biphenyl]-4-amine **(10a):** Following the general procedure **(B)**, reaction of compound **3a** (100 mg, 0.2724 mmol, 1 equiv.) and phenyl boronic acid **9a** (82 mg, 0.681 mmol, 2.5 equiv.), Pd(dppf)Cl_2.DCM (38 mg, 0.544 mmol, 0.2 equiv.) and K_2CO_3 (56 mg, 0.4086 mmol, 1.5 equiv.) as base in	

dioxane:MeOH (3:1) solvent system was microwave (MW) irradiated (100 W) for 10 min afforded compound **10a**.



White powder:35 mg, 36% yield;

R_f(7% EtOAc-Hexane): 0.49;

FTIR (KBr) ν_{max}: 3402, 3032, 2983, 2913, 1880, 1600, 1519, 1486, 1429, 1374, 1349,1257, 1229, 1193, 1116, 1074, 1037, 985, 915, 823, 761, 692 cm^{-1};

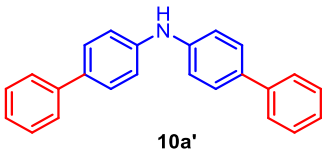
^{1}H NMR(400 MHz, $CDCl_3$): δ 7.50 (dd, *J* = 7.2, 0.7 Hz, 5H), 7.45 (d, *J* = 8.6 Hz, 4H), 7.34 (s, 3H), 7.25 – 7.21 (m, 2H), 7.09 – 7.06 (m, 4H), 5.96 – 5.86 (m, 1H), 5.25 (dd, *J* = 17.2, 1.5 Hz, 1H), 5.14 (dd, *J* = 10.4, 1.4 Hz, 1H), 4.39 – 4.35 (m, 2H);

^{13}C NMR($CDCl_3$/TMS, 100 MHz) δ 55.0, 117.0, 121.0, 121.1, 127.0, 128.0, 129.0, 134.2, 134.3, 141.0, 147.1;

HRMS-ESI: Calcd. For$C_{27}H_{23}N[M+H]^+$*m/z*: 362.1909; Found 362.1911;

di([1,1'-biphenyl]-4-yl)amine (**10a'**):

Following the general procedure **(B)**, reaction of compound **3a** (100 mg, 0.2724 mmol, 1 equiv.) and phenyl boronic acid **9a** (82 mg, 0.681 mmol, 2.5 equiv.), Pd(dppf)Cl_2.DCM (38 mg, 0.544 mmol, 0.2 equiv.) and K_2CO_3 (56 mg, 0.4086 mmol, 1.5 equiv.) as base in dioxane:MeOH (3:1) solvent system was microwave (MW) irradiated (100 W) for 10 min afforded compound **10a'**.



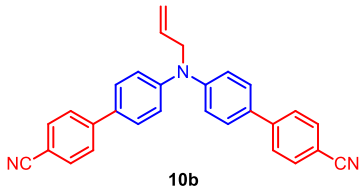
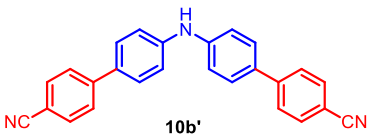
White powder: 53 mg, 61% yield;

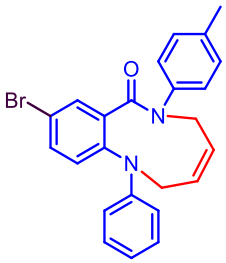
R_f (7% EtOAc-Hexane): 0.46;

FTIR (KBr) ν_{max}: 3422, 2923, 1607, 1529, 1491, 1319, 827, 758, 688 cm^{-1};

^{1}H NMR(400 MHz, $CDCl_3$) δ 7.52 (t, *J* = 1.6 Hz, 2H), 7.50 (d, *J* = 1.0 Hz, 2H), 7.49 – 7.47 (m, 2H), 7.46 – 7.44 (m, 2H), 7.37 (d, *J* = 1.8 Hz, 1H), 7.33 (d, *J* = 1.6 Hz, 2H), 7.24 (dt, *J* = 9.1, 4.2 Hz, 3H), 7.12 (s, 2H), 7.11 – 7.09 (m, 2H), 5.81 (s, 1H).

^{13}C NMR($CDCl_3$/TMS, 100 MHz): δ 118.2, 127.0, 127.8, 128.2, 128.9, 134.1, 141.0, 142.4;

	HRMS-ESI: Calcd. for $C_{24}H_{19}N$ $[M+H]^+$*m/z*: 322.1595; Found 322.1606;
4',4'''-(allylazanediyl)bis(([1,1'-biphenyl]-4-carbonitrile)) **(10b):** Following the general procedure **(B)**, reaction of compound **3a** (100 mg, 0.2724 mmol, 1 equiv.) and 4-Cyanophenyl phenyl boronic acid **9b** (100 mg, 0.681 mmol, 2.5 equiv.), Pd(dppf)Cl_2.DCM (38 mg, 0.544 mmol, 0.2 equiv.) and K_2CO_3 (56 mg, 0.4086 mmol, 1.5 equiv.) as base in dioxane:MeOH (3:1) solvent system was microwave (MW) irradiated (100 W) for 10 min afforded compound **10b**.	
 **10b**	**White powder**: 65 mg, 58% yield; **R_f** (7% EtOAc-Hexane): 0.39; **FTIR** (KBr) ν_{max}: 3414, 2923, 2525, 1952, 1691, 1597, 1265, 915, 823cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.71 (d, *J* = 1.9 Hz, 1H), 7.70 – 7.68 (m, 2H), 7.63 (t, *J* = 1.7 Hz, 3H), 7.61 (d, *J* = 1.7 Hz, 3H), 7.59 (d, *J* = 2.3 Hz, 2H), 7.57 (d, *J* = 0.8 Hz, 1H), 7.47 (d, *J* = 2.0 Hz, 1H), 7.45 (d, *J* = 2.1 Hz, 1H), 7.12 (d, *J* = 2.1 Hz, 1H), 7.10 (d, *J* = 2.1 Hz, 1H), 5.90 (ddt, *J* = 17.2, 10.3, 4.7 Hz, 1H), 5.24 (dd, *J* = 17.6, 1.8 Hz, 1H), 5.16 (dd, *J* = 10.4, 1.4 Hz, 1H), 4.44 – 4.35 (m, 2H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 54.8, 110.2, 112.5, 117.1, 118.5, 119.2, 121.2, 127.0, 128.0, 128.2, 132.2, 132.7, 133.0, 133.6, 143.6, 145.1, 148.0; **HRMS-ESI**: Calcd. for $C_{29}H_{21}N_3$$[M+H]^+$*m/z*:412.1814; Found 412.1814
4',4'''-azanediylbis(([1,1'-biphenyl]-4-carbonitrile)) **(10b'):** Following the general procedure **(B)**, reaction of compound **3a** (100 mg, 0.2724 mmol, 1 equiv.) and 4-Cyanophenyl phenyl boronic acid **9b** (100 mg, 0.681 mmol, 2.5 equiv.), Pd(dppf)Cl_2.DCM (38 mg, 0.544 mmol, 0.2 equiv.) and K_2CO_3 (56 mg, 0.4086 mmol, 1.5 equiv.) as base in dioxane:MeOH (3:1) solvent system was microwave (MW) irradiated (100 W) for 10 min afforded compound **10b'**.	
 **10b'**	**White powder**: 33mg, 34% yield; **R_f** (7% EtOAc-Hexane): 0.39; **FTIR** (KBr) ν_{max}: 3352, 3042, 2924, 2305, 2225, 1922, 1681,

	1597, 1526, 1492, 1334, 1284, 1183, 1121, 1006, 819, 546cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.66 (dt, *J* = 3.5, 1.0 Hz, 3H), 7.63 – 7.60 (m, 3H), 7.52 (ddd, *J* = 4.4, 3.5, 1.9 Hz, 3H), 7.44 – 7.33 (m, 5H), 1.18 (s, 1H); **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 111.1, 119.0, 127.4, 128.0, 128.8, 129.3, 132.7, 139.5, 145.8; **HRMS-ESI**: Calcd. for $C_{26}H_{17}N_3$ $[M+H]^+$ *m/z*: 371.1422; Found 371.1427.
(Z)-9-bromo-1-phenyl-6-(p-tolyl)-5,6-dihydro-1H-benzo[b][1,5]diazonin-7(2H)-one:**(11a):** Following the general procedure **(C)**, reaction of compound **(3e')** in toluene, 3mol% of Grubbs II catalyst was added and stirred at RT for 3min afforded compound **11a**.	
 11a	**White Solid**: 62 mg, 94% yield; **R_f** (30% EtOAc-Hexane): 0.39; **FTIR** (KBr) ν_{max}: 3418, 2922, 2854, 1636, 1489, 1454, 1398, 1226, 1078, 962, 790, 758, 514cm^{-1}; **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.61 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.54 (dd, *J* = 7.7, 6.1 Hz, 1H), 7.38 (td, *J* = 7.5, 1.0 Hz, 1H), 7.19 – 7.16 (m, 2H), 7.15 – 7.12 (m, 1H), 6.98 (d, *J* = 8.1 Hz, 2H), 6.50 (d, *J*= 8.3 Hz, 2H), 6.38 – 6.34 (m, 2H), 6.16 (dt, *J* = 9.9, 4.8 Hz, 1H), 5.49 (dd, *J* = 18.2, 8.1 Hz, 1H), 4.23 (d, *J* = 27.0 Hz, 3H), 3.88 (d, *J* = 15.7 Hz, 1H), 2.21 (s, 3H). **^{13}C NMR** ($CDCl_3$/TMS, 100 MHz): δ 21.2, 29.8, 30.4, 49.8, 51.3, 110.2, 114.8, 126.5, 127.9, 128.0, 128.4, 129.9, 130.3, 131.8, 132.7, 135.6, 136.8, 137.7, 143.0, 145.5, 168.8; **HRMS-ESI**: Calcd. for $C_{24}H_{21}BrN_2O[M+H]^+$ *m/z*: 435.0916; Found 435.0912.

4. Copies of NMR and HRMS Spectra

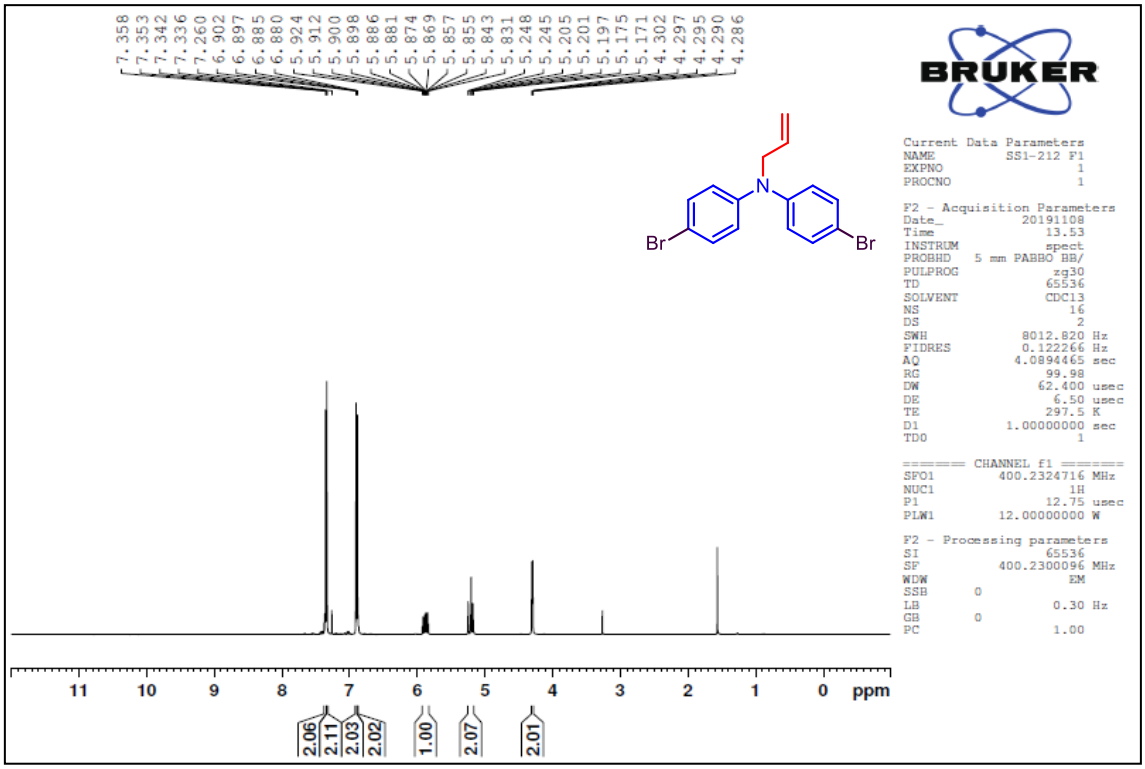


Figure 1. ^{1}H NMR spectrum of compound **3a**

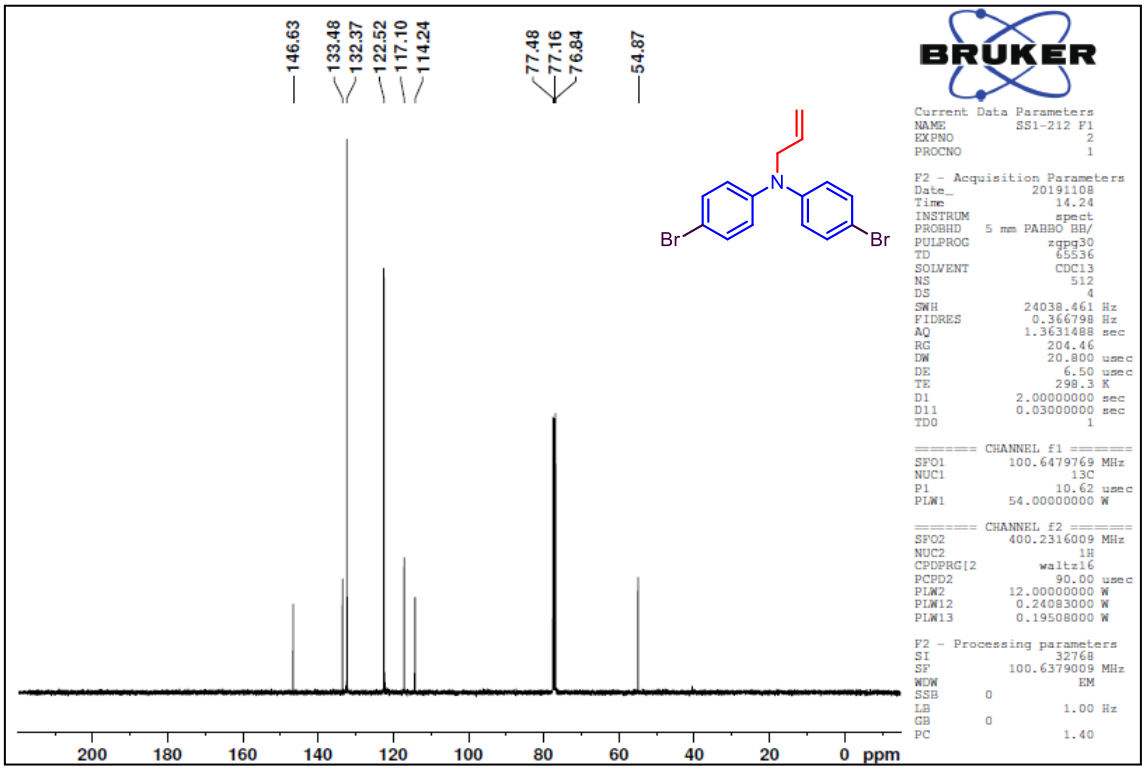


Figure 2. ^{13}C NMR spectrum of compound **3a**

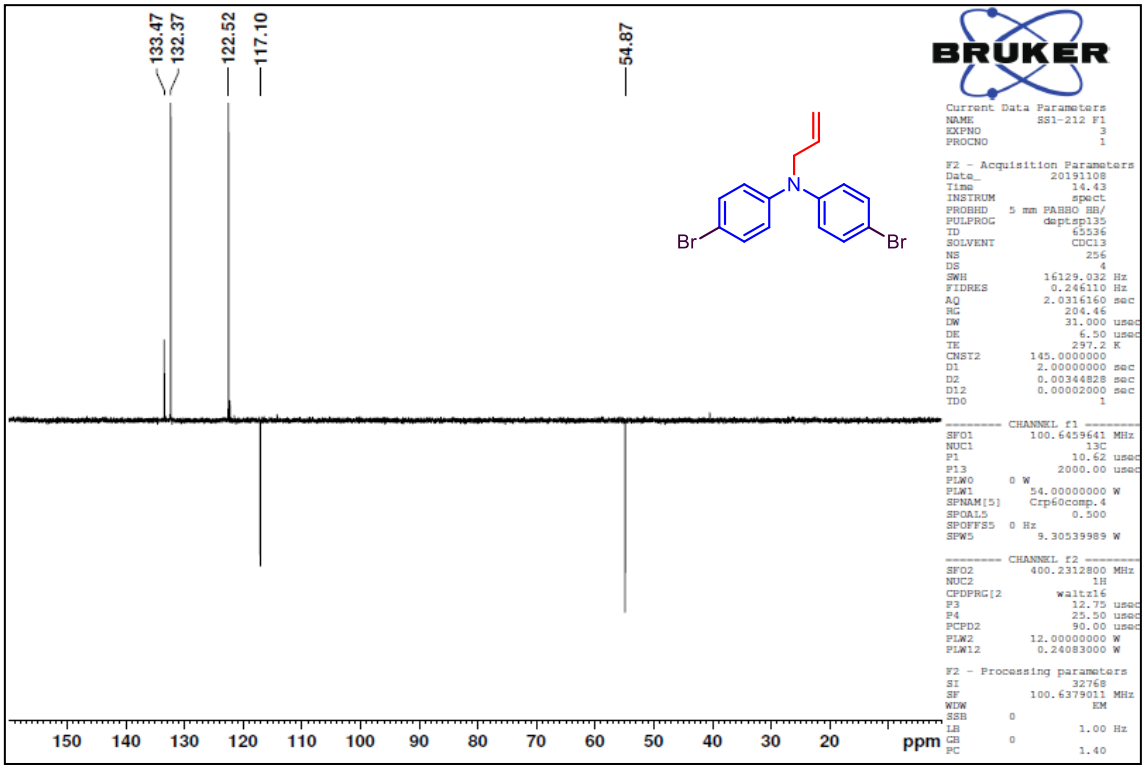


Figure 3. DEPT-135 NMR spectrum of compound **3a**

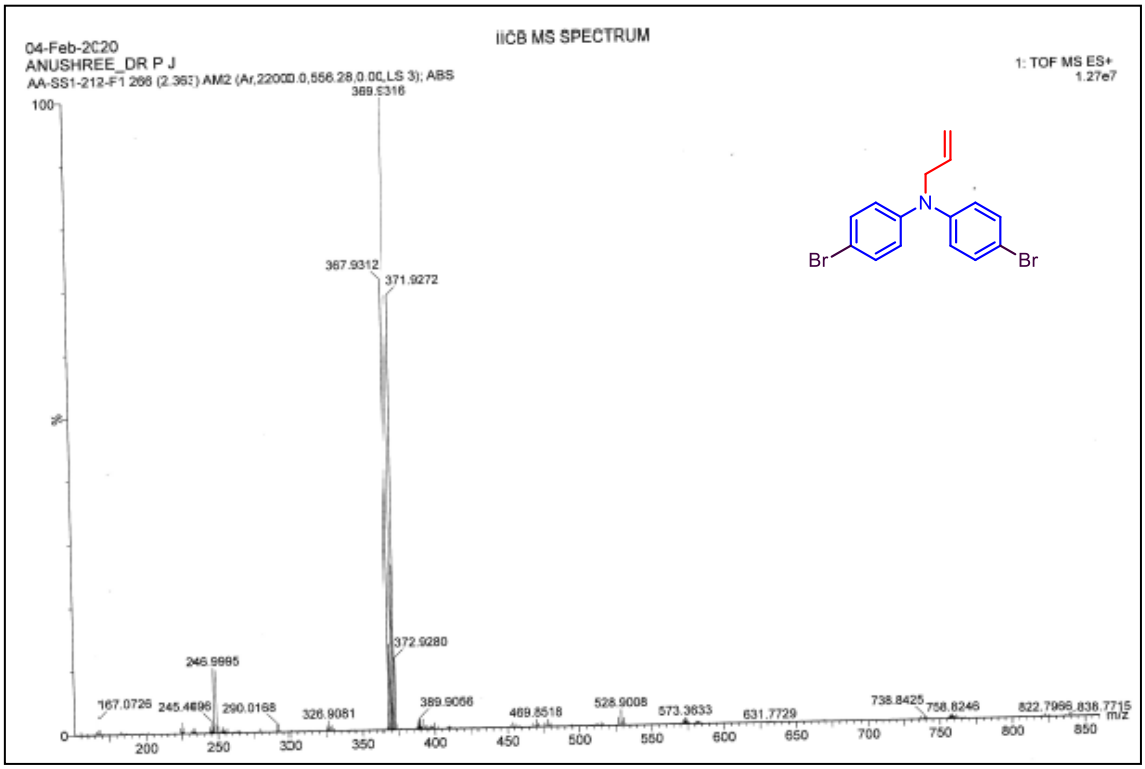


Figure 4. HRMS spectrum of compound **3a**

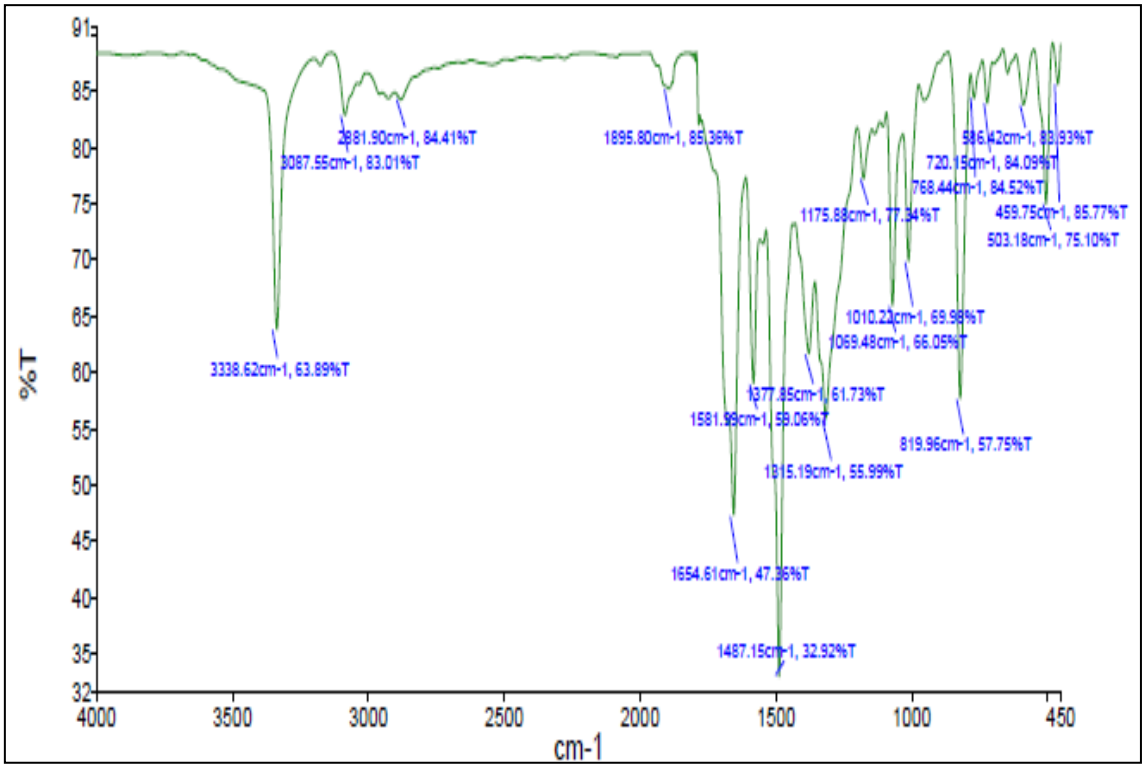


Figure 5. FTIR spectrum of compound **3a**

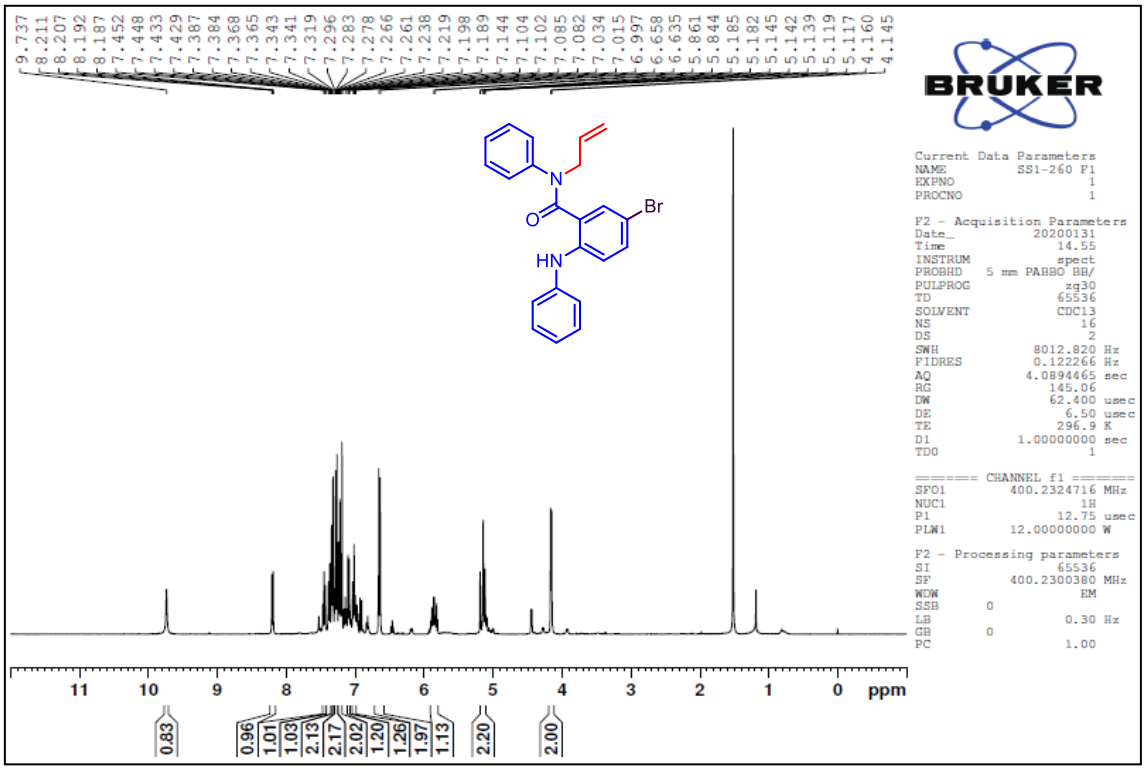


Figure 6. ^{1}H NMR spectrum of compound **3b**

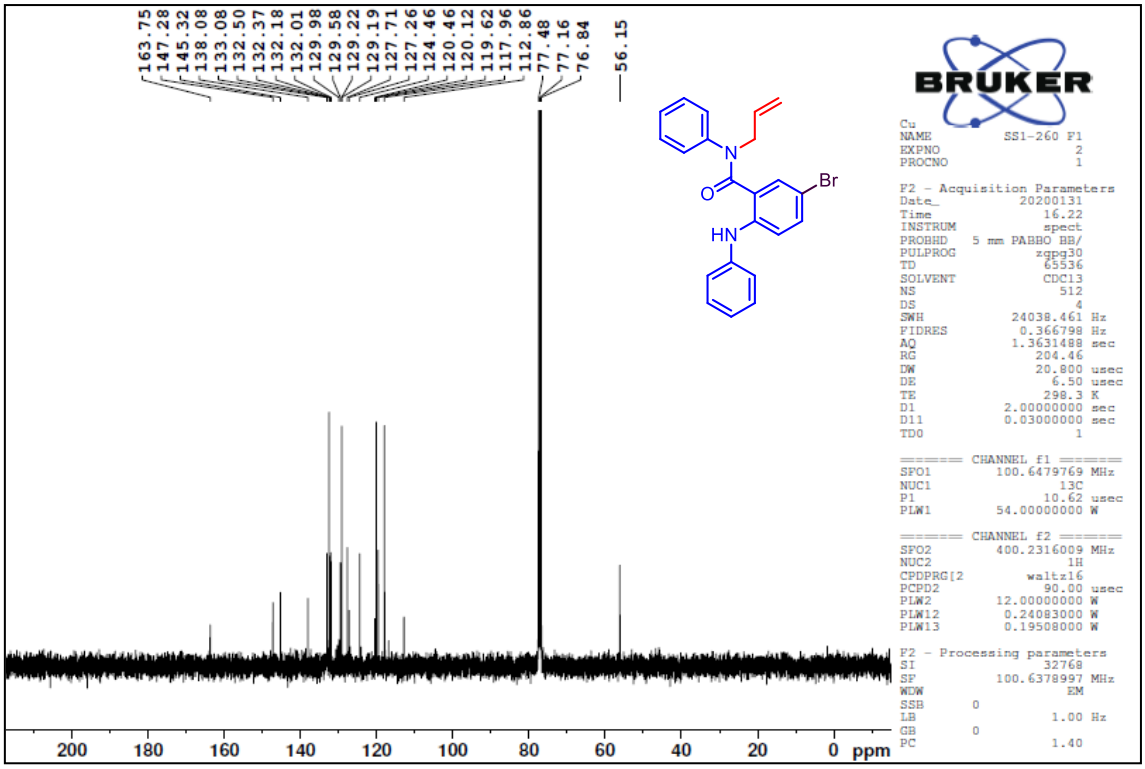


Figure 7. ^{13}C NMR spectrum of compound **3b**

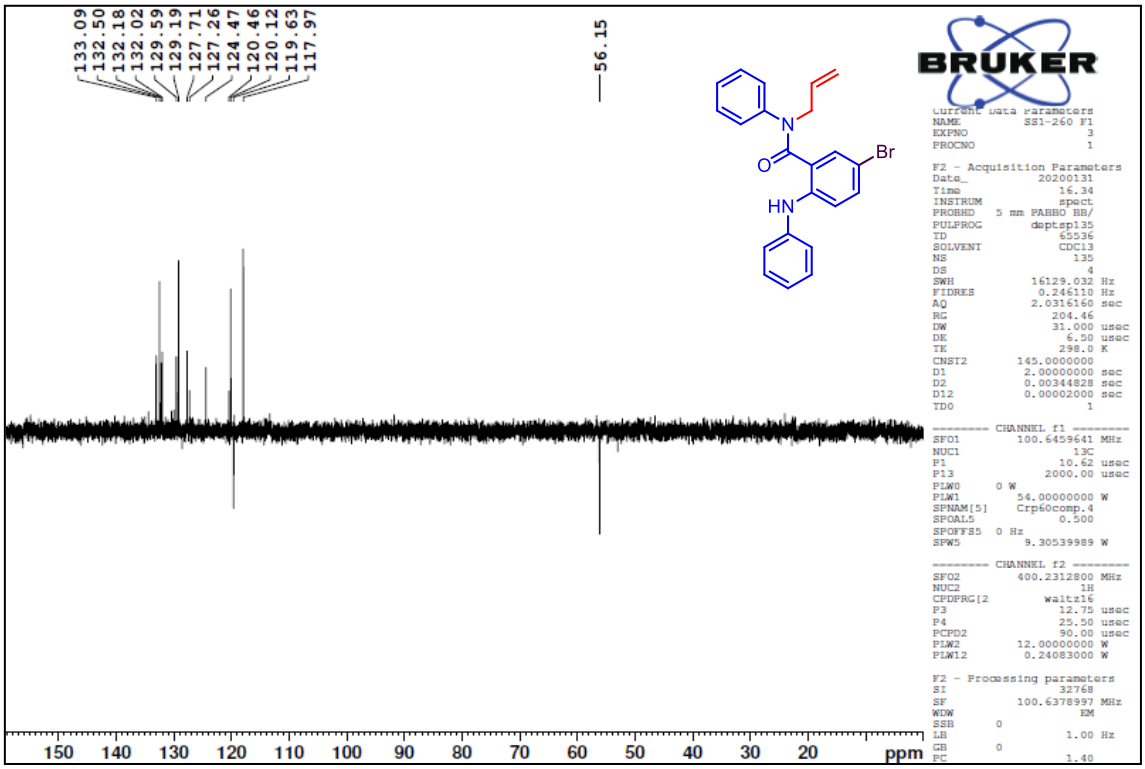


Figure 8. DEPT-135 NMR spectrum of compound **3b**

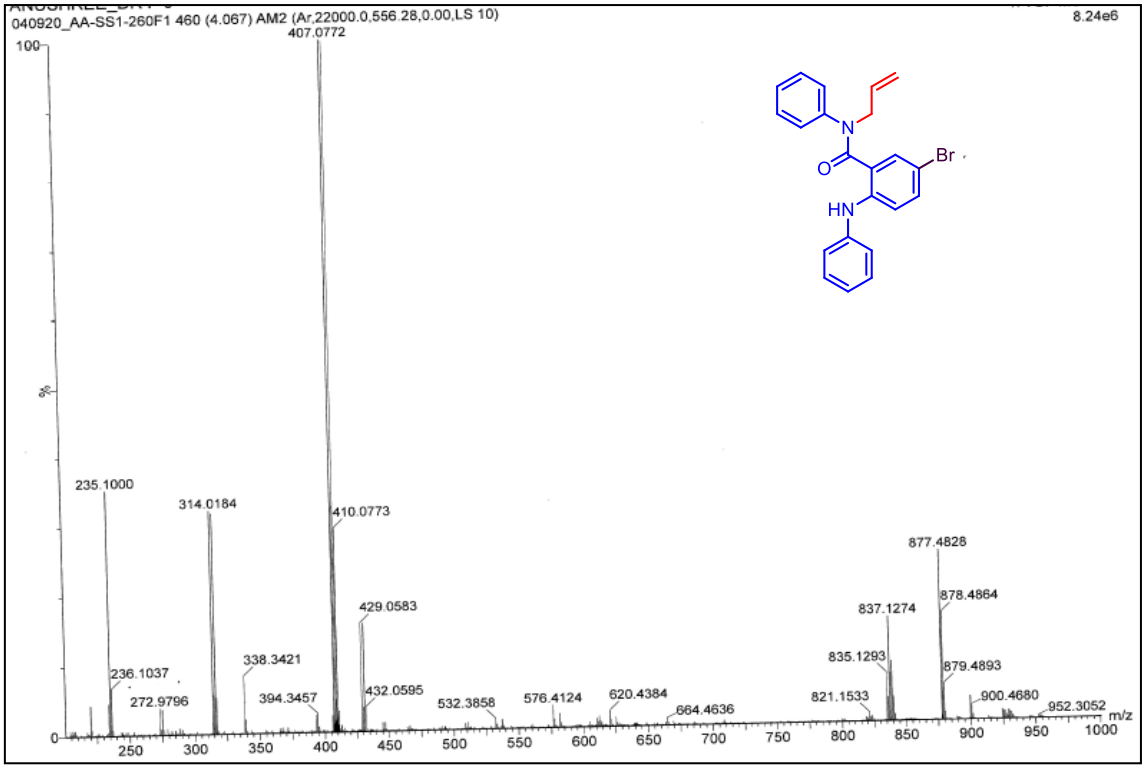


Figure 9. HRMS spectrum of compound **3b**

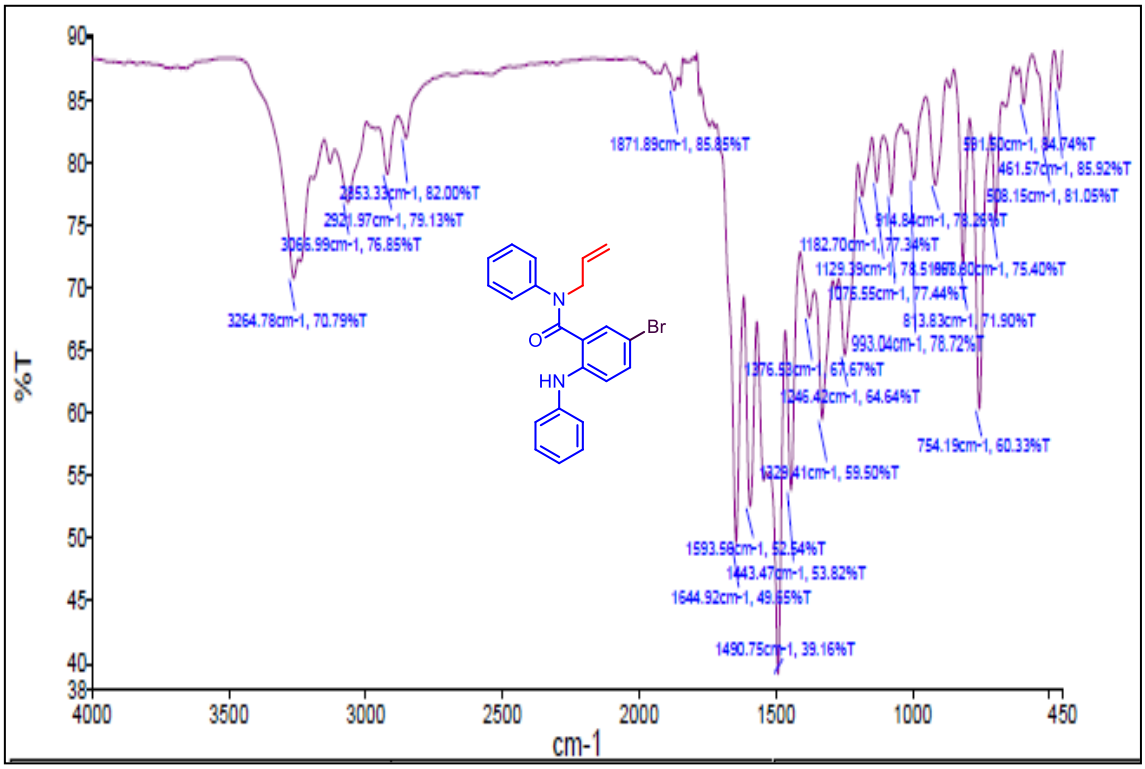


Figure 10. FTIR spectrum of compound **3b**

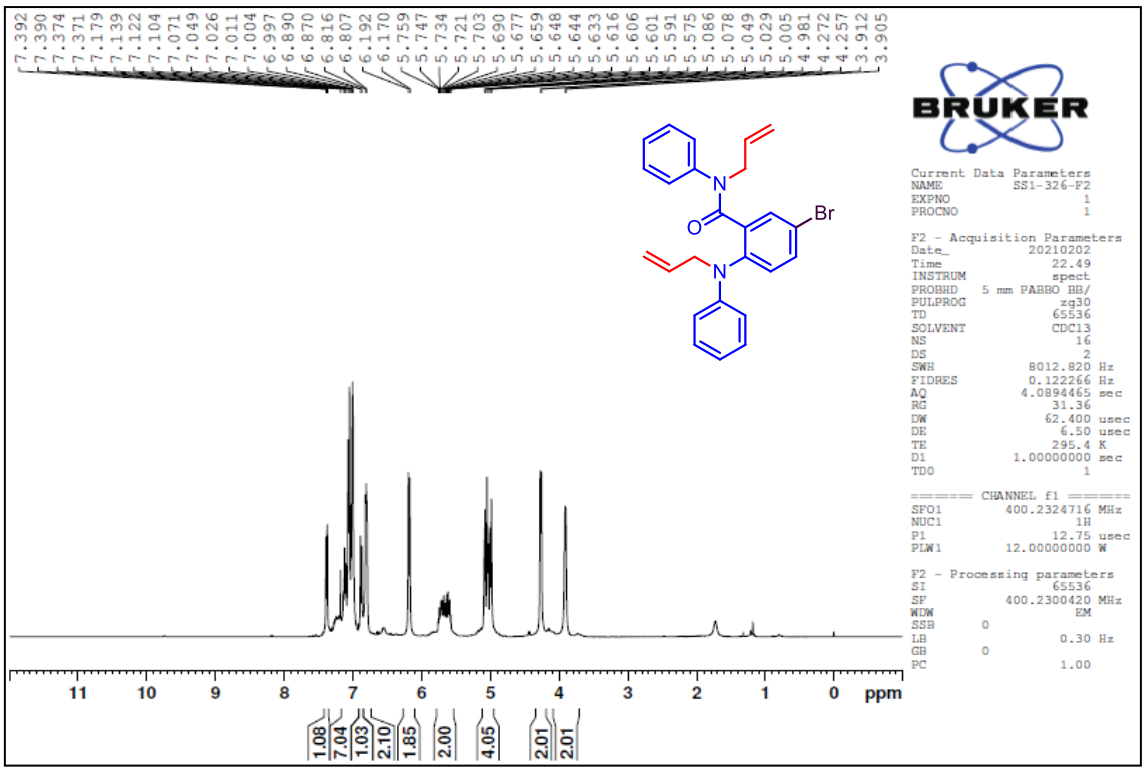


Figure 11. ^{1}H NMR spectrum of compound **3b'**

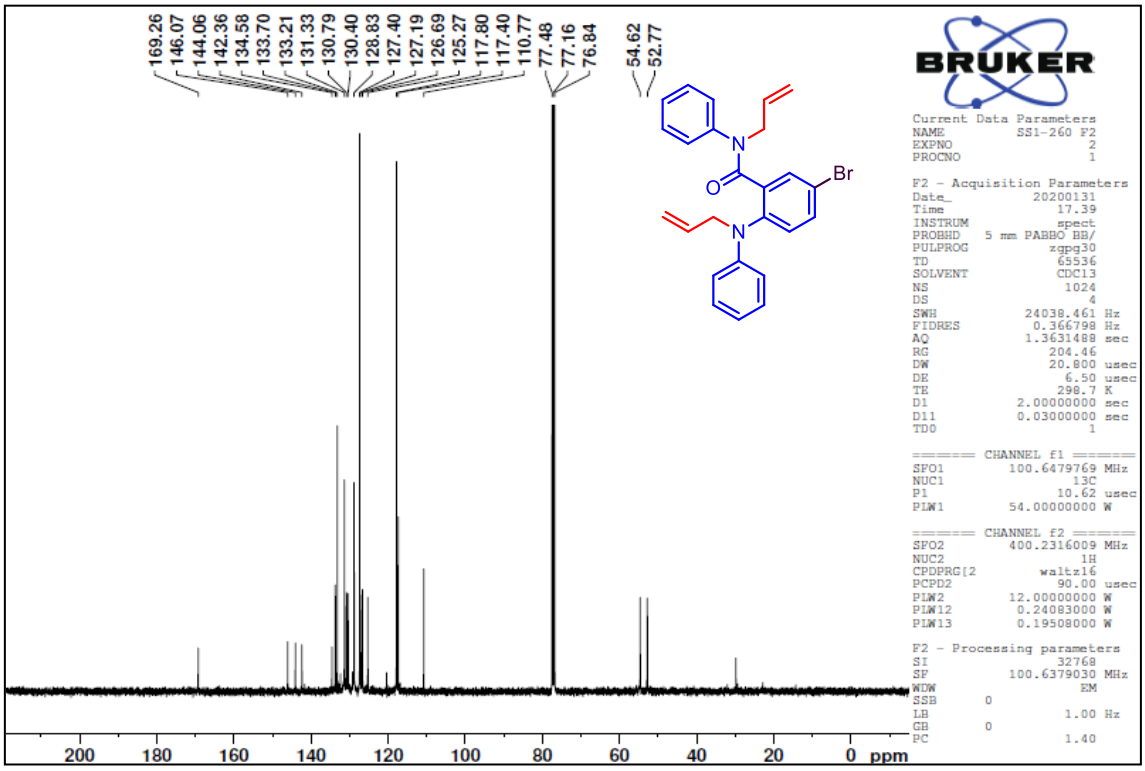


Figure 12. ^{13}C NMR spectrum of compound **3b'**

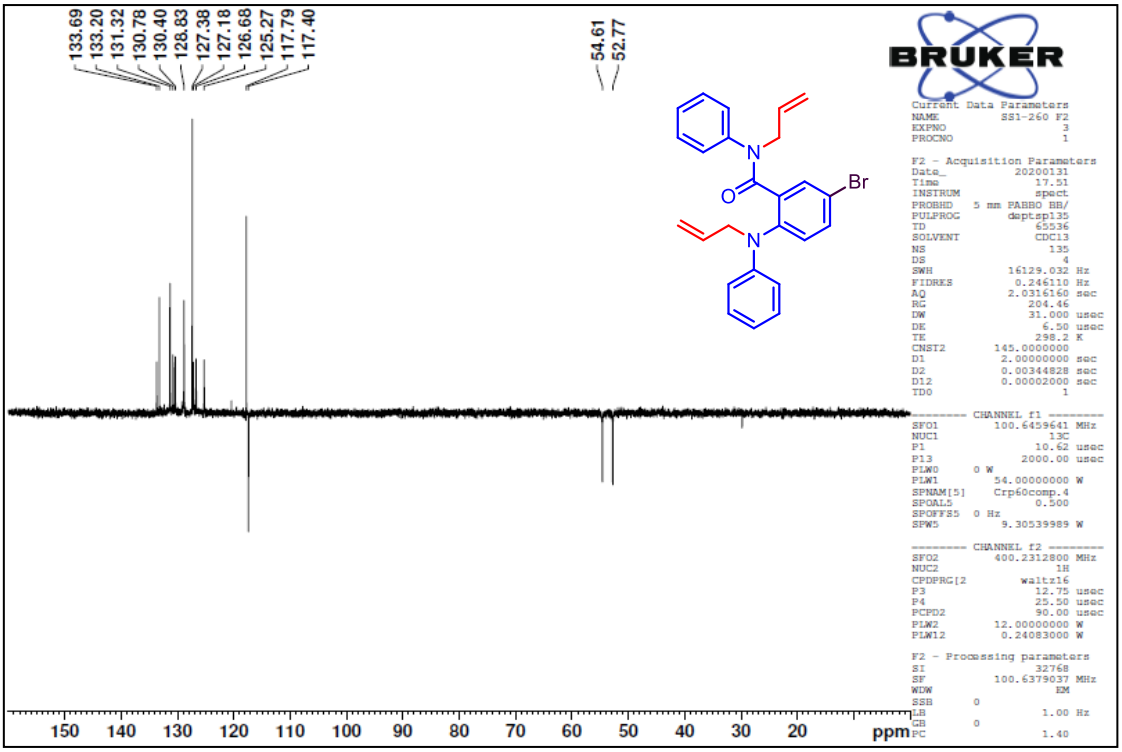


Figure 13. DEPT-135 NMR spectrum of compound **3b'**

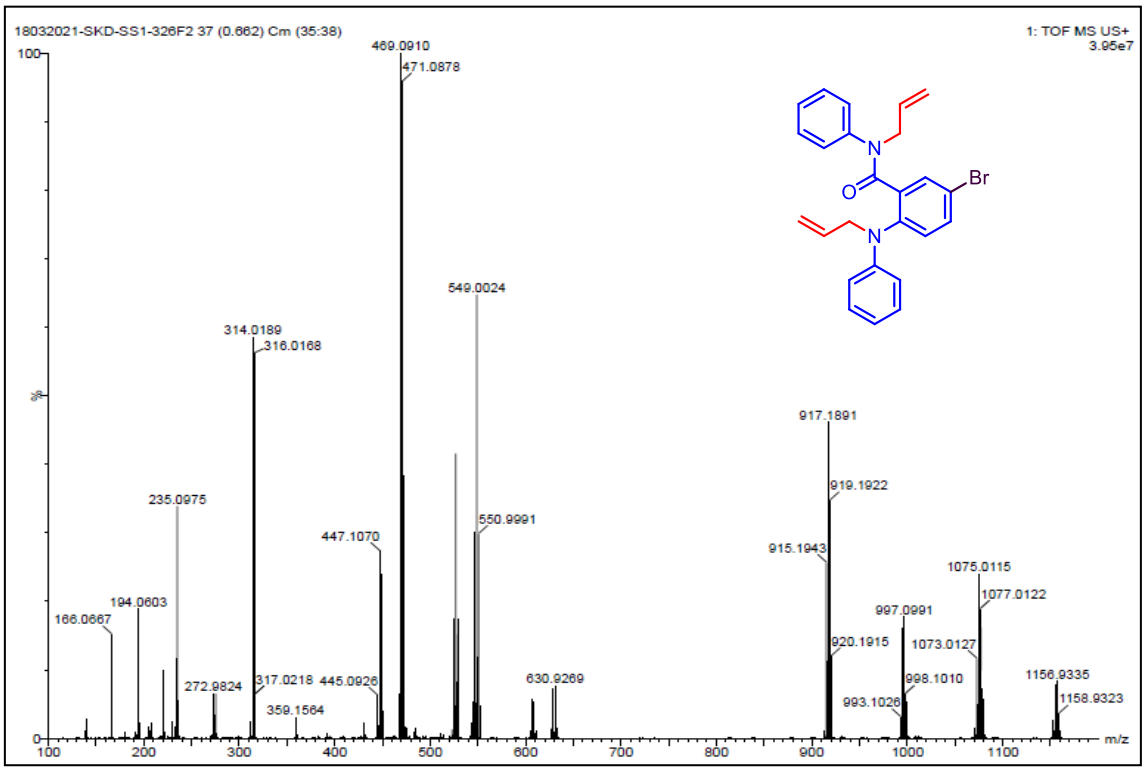


Figure 14. HRMS spectrum of compound **3b'**

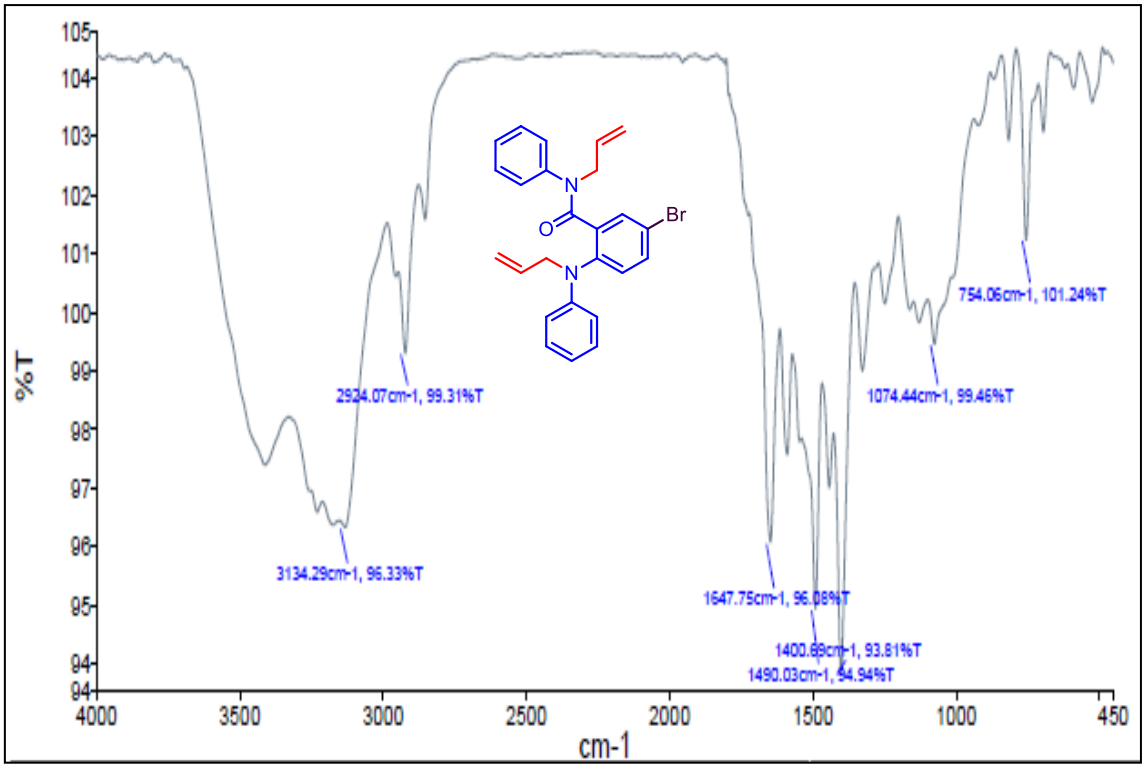


Figure 15. FTIR spectrum of compound **3b'**

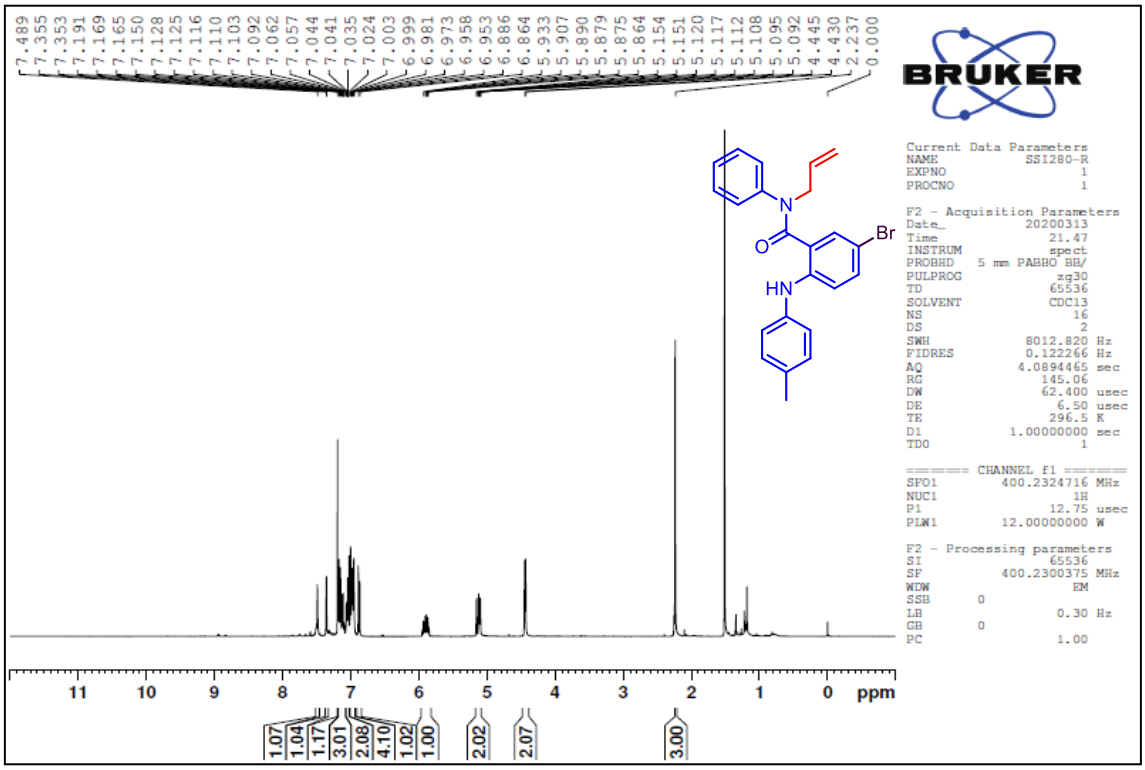


Figure 16. ^{1}H NMR spectrum of compound **3c**

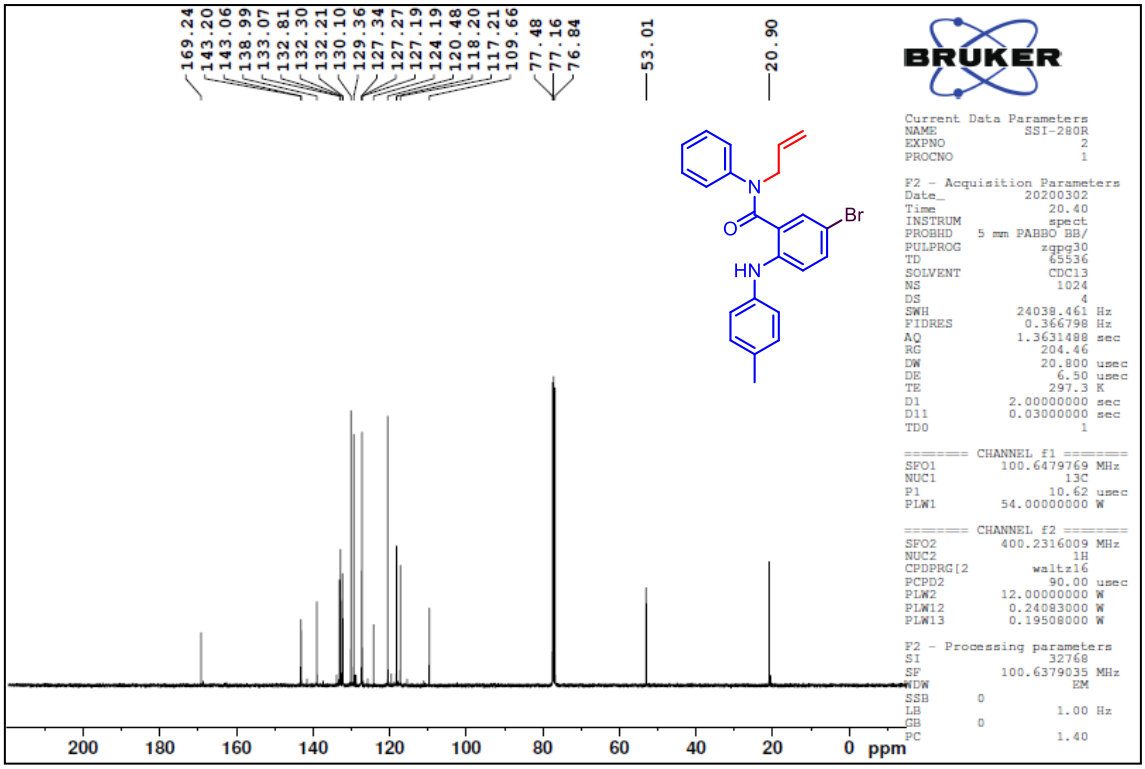


Figure 17. ^{13}C NMR spectrum of compound **3c**

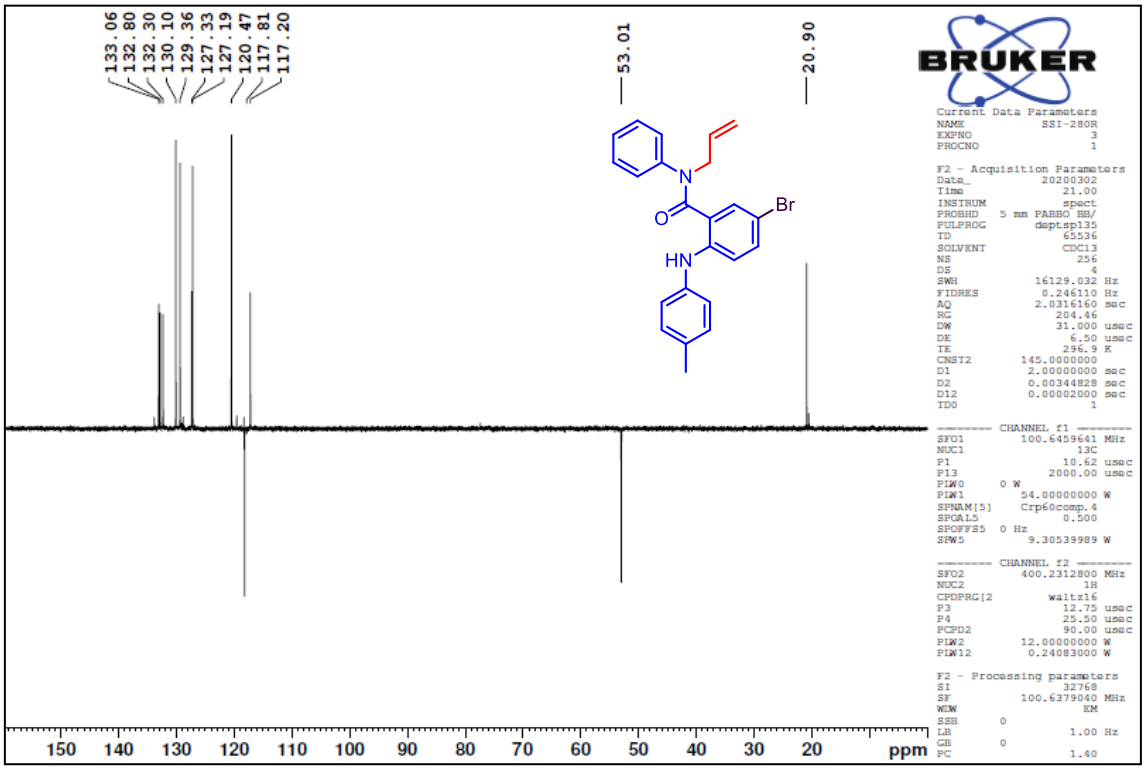


Figure 18. DEPT-135 NMR spectrum of compound **3c**

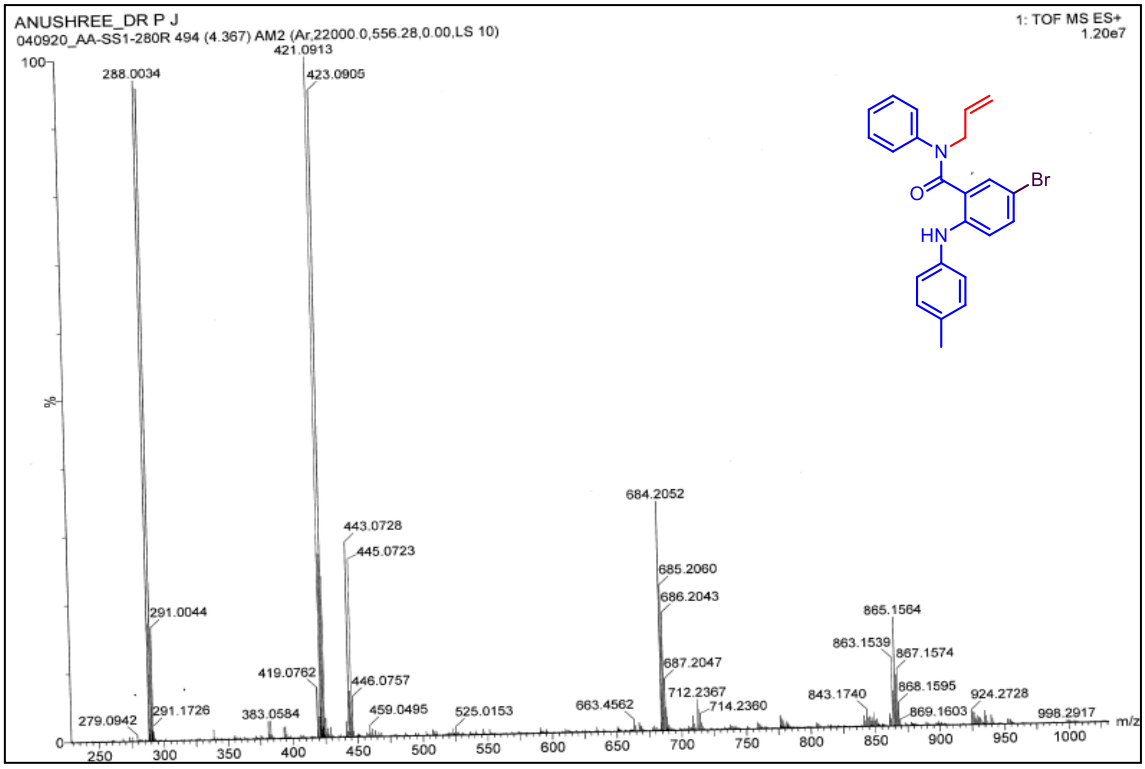


Figure 19. HRMS spectrum of compound **3c**

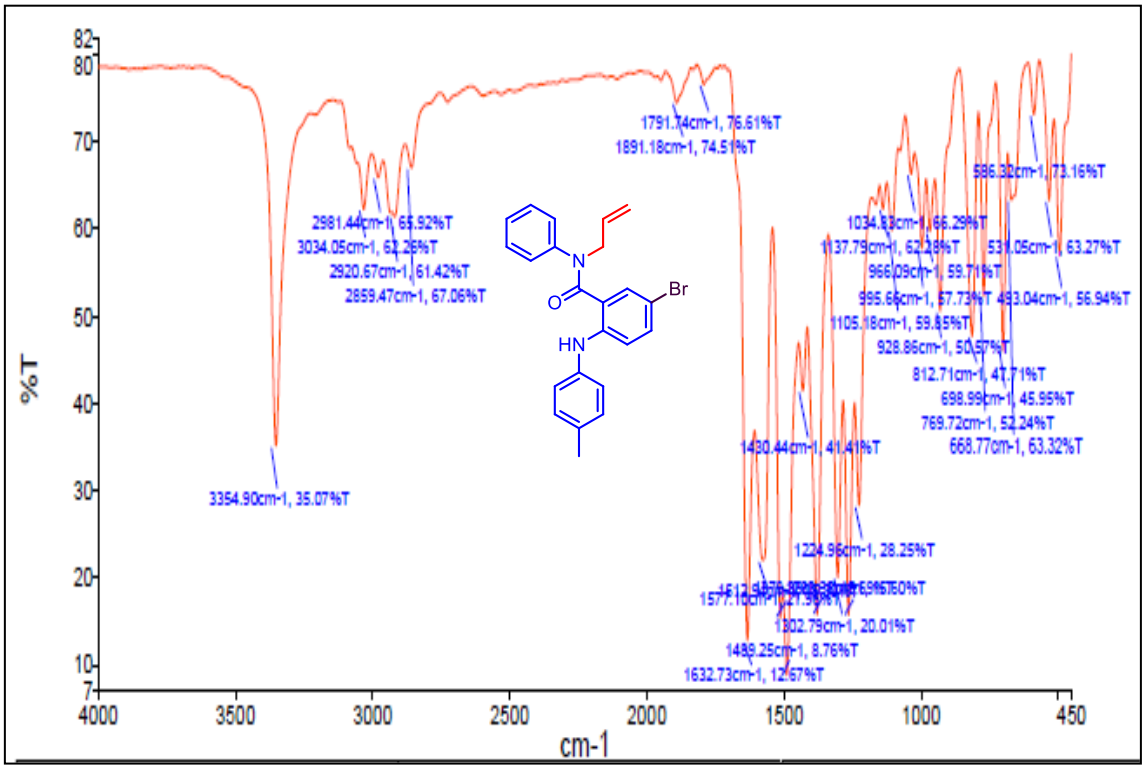


Figure 20. FTIR spectrum of compound **3c**

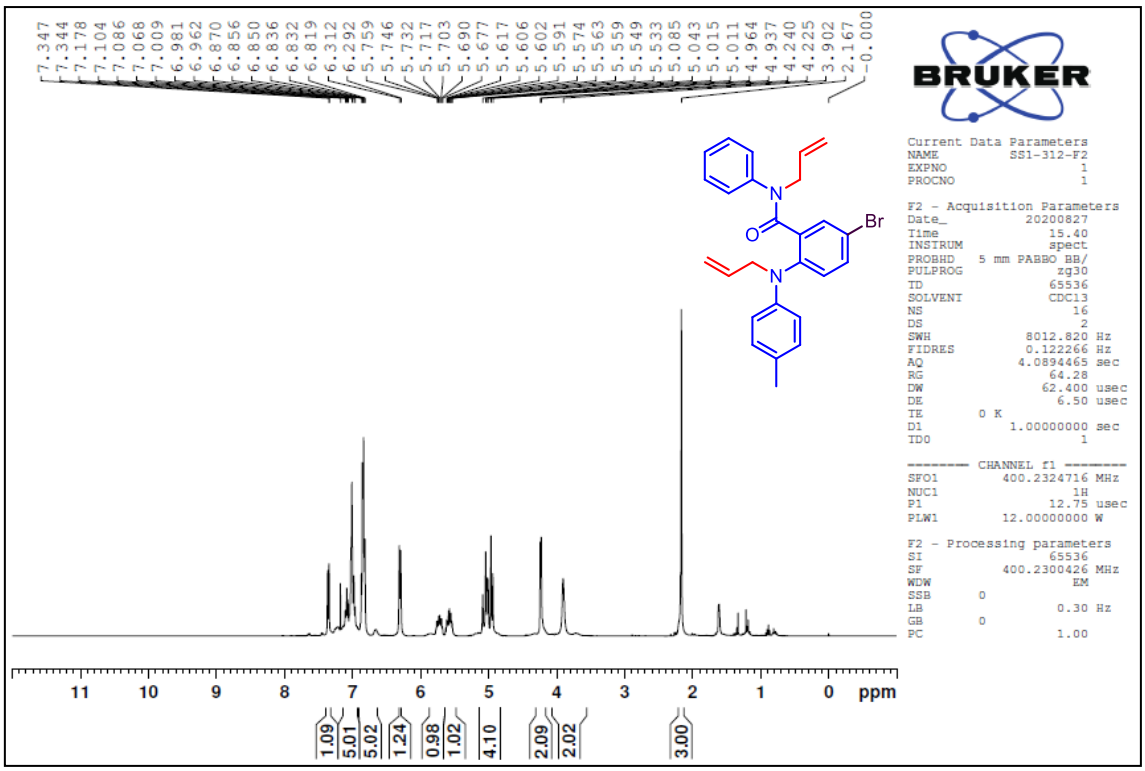


Figure 21. ^{1}H NMR spectrum of compound **3c'**

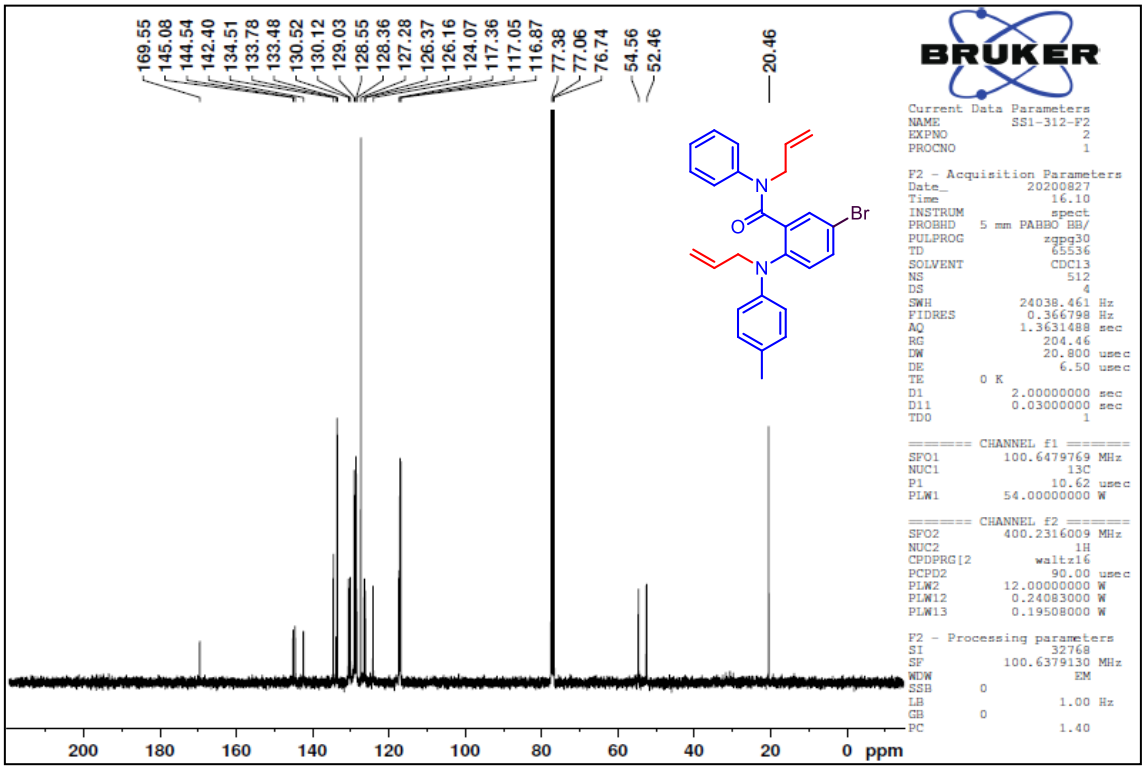


Figure 22. ^{13}C NMR spectrum of compound **3c'**

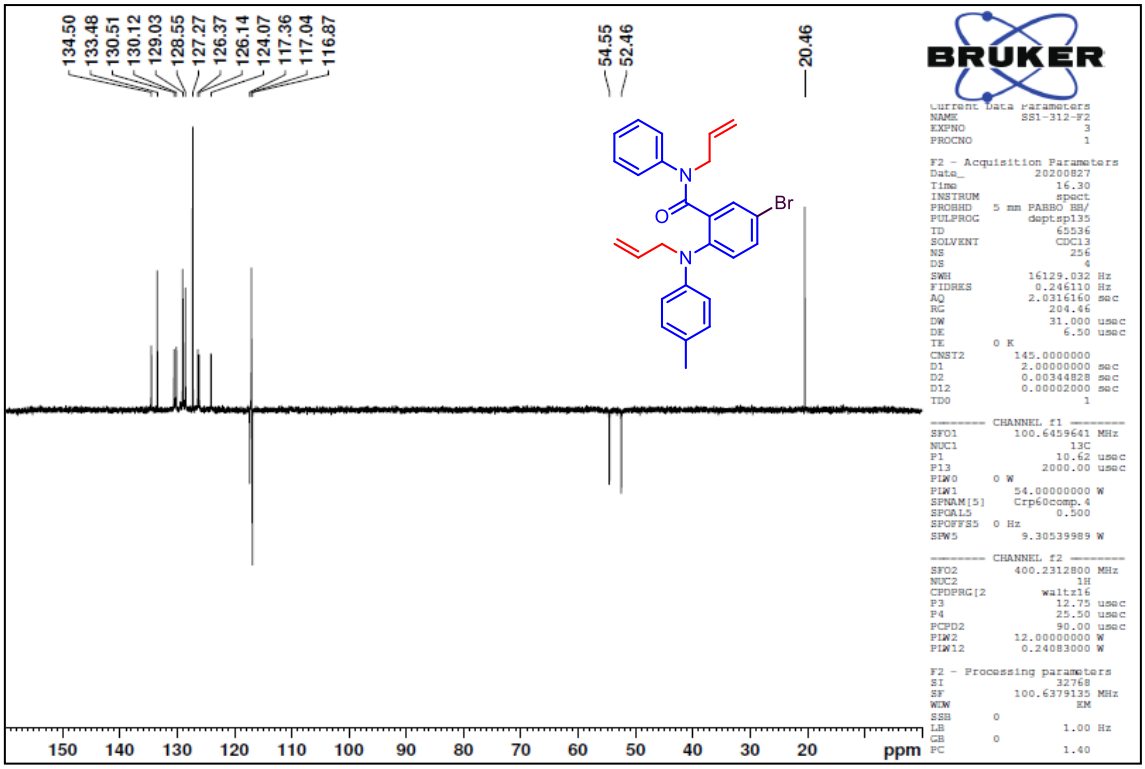


Figure 23. DEPT-135 NMR spectrum of compound **3c'**

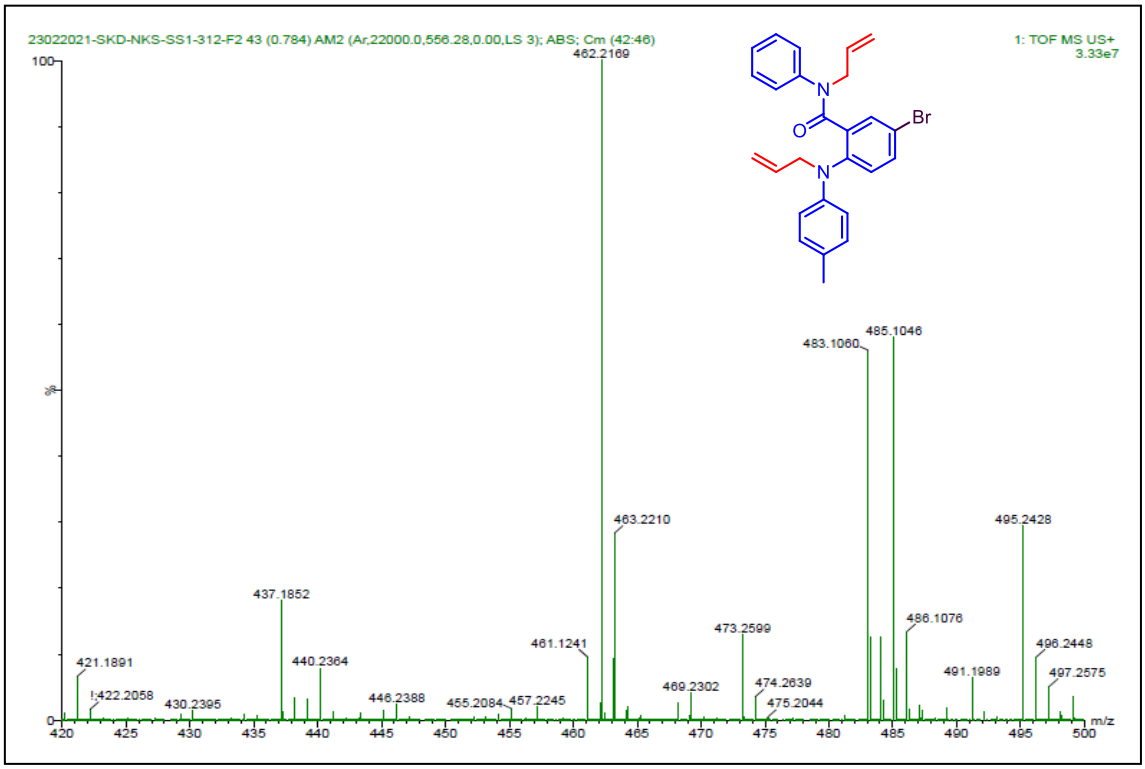


Figure 24. HRMS spectrum of compound **3c'**

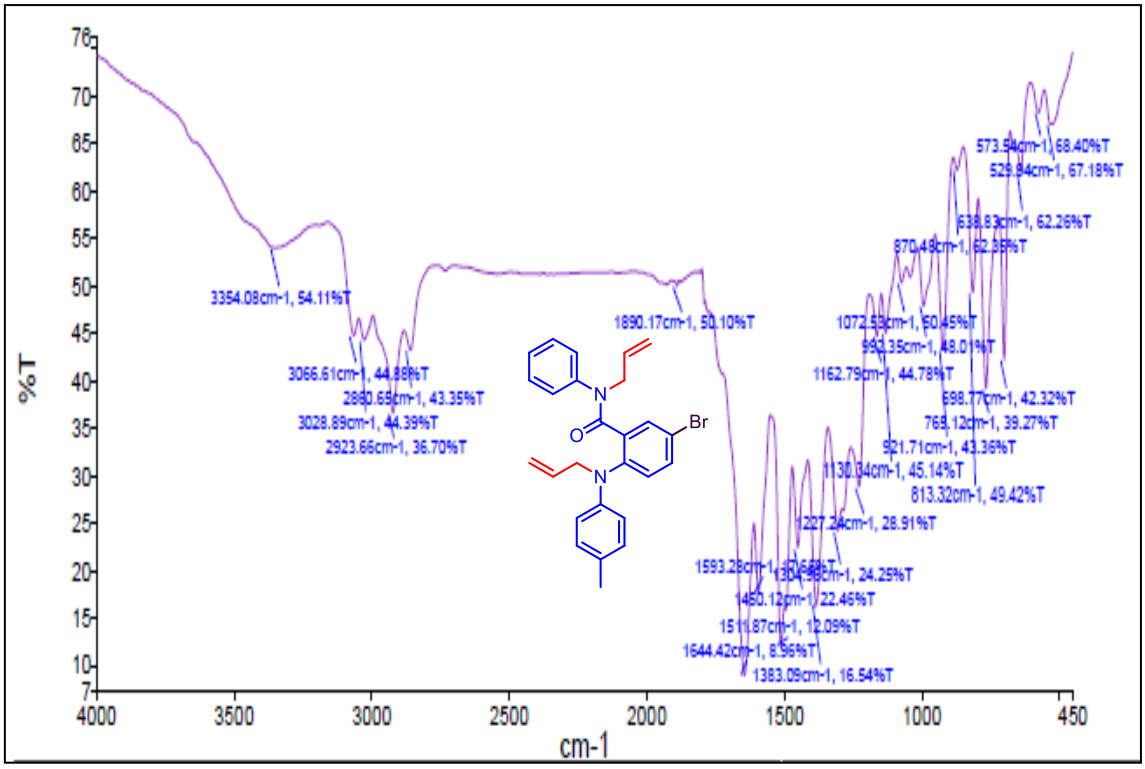


Figure 25. FTIR spectrum of compound **3c'**

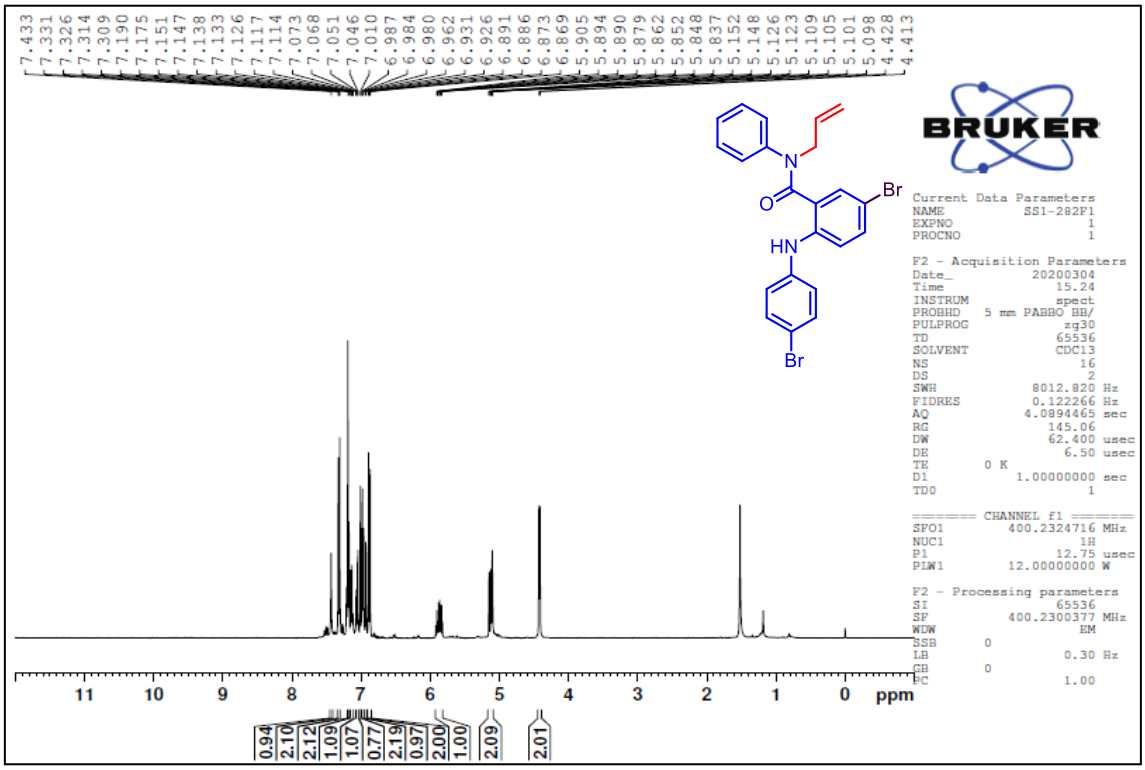


Figure 26. ^{1}H NMR spectrum of compound **3d**

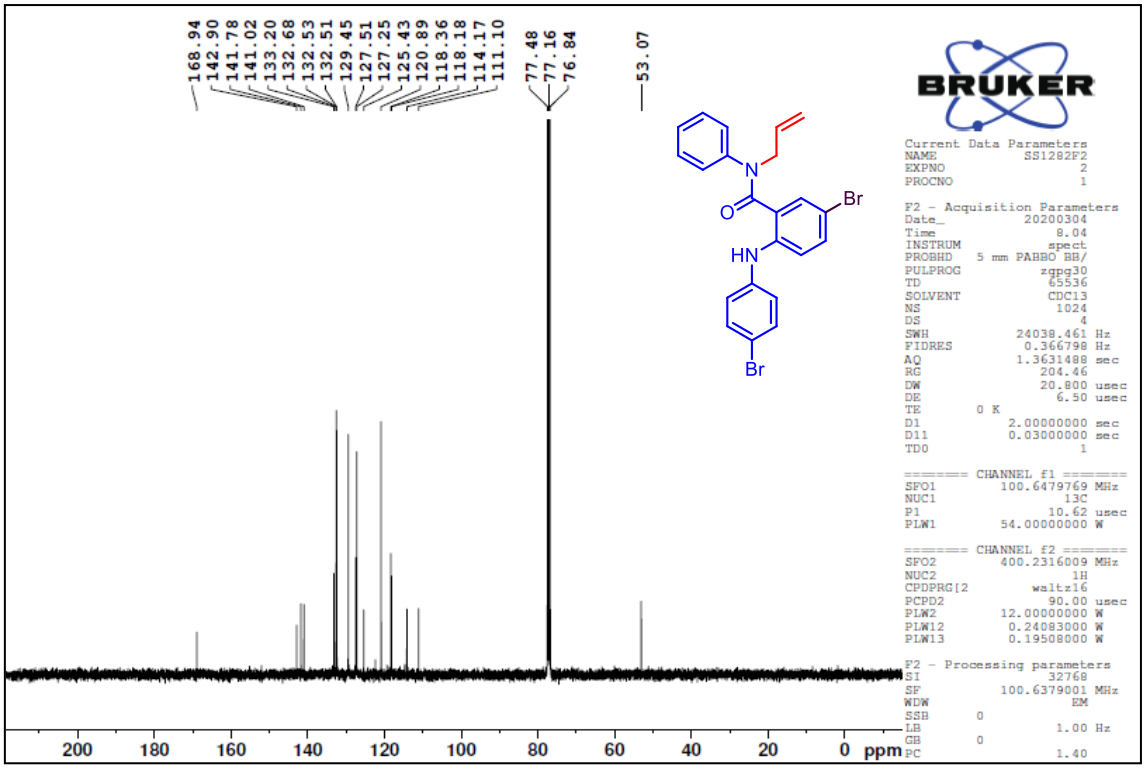


Figure 27. ^{13}CNMR spectrum of compound **3d**

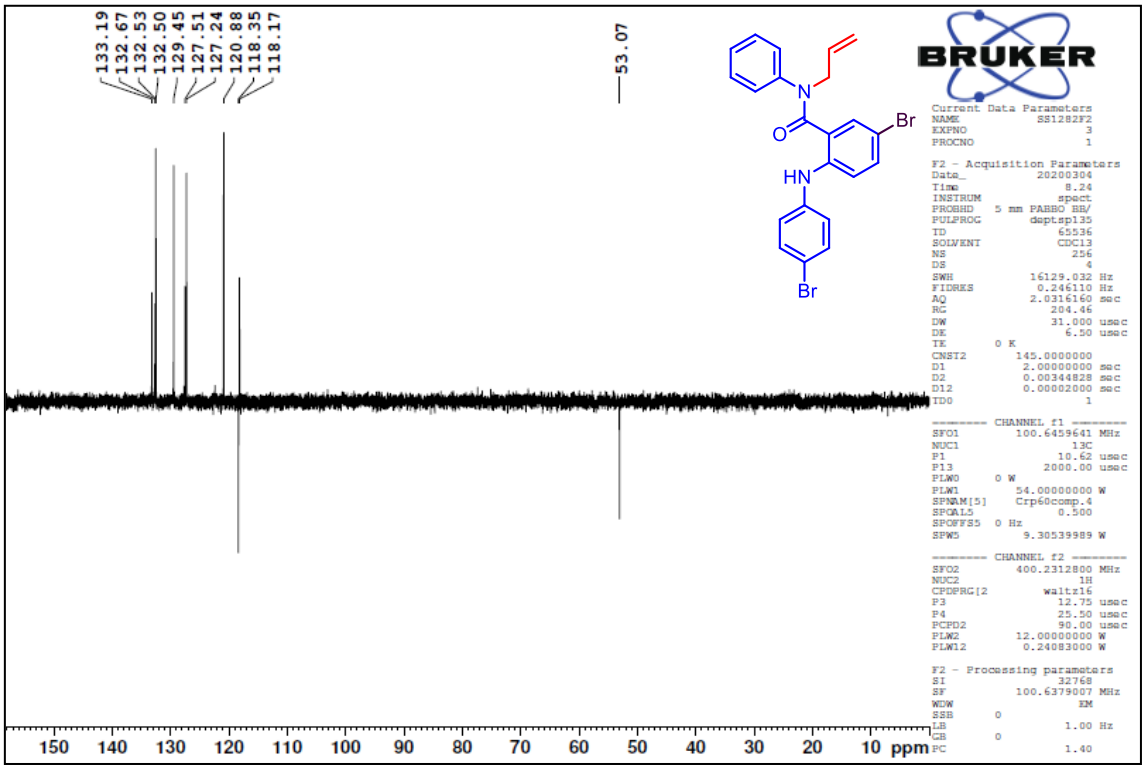


Figure 28. DEPT-135 NMR spectrum of compound **3d**

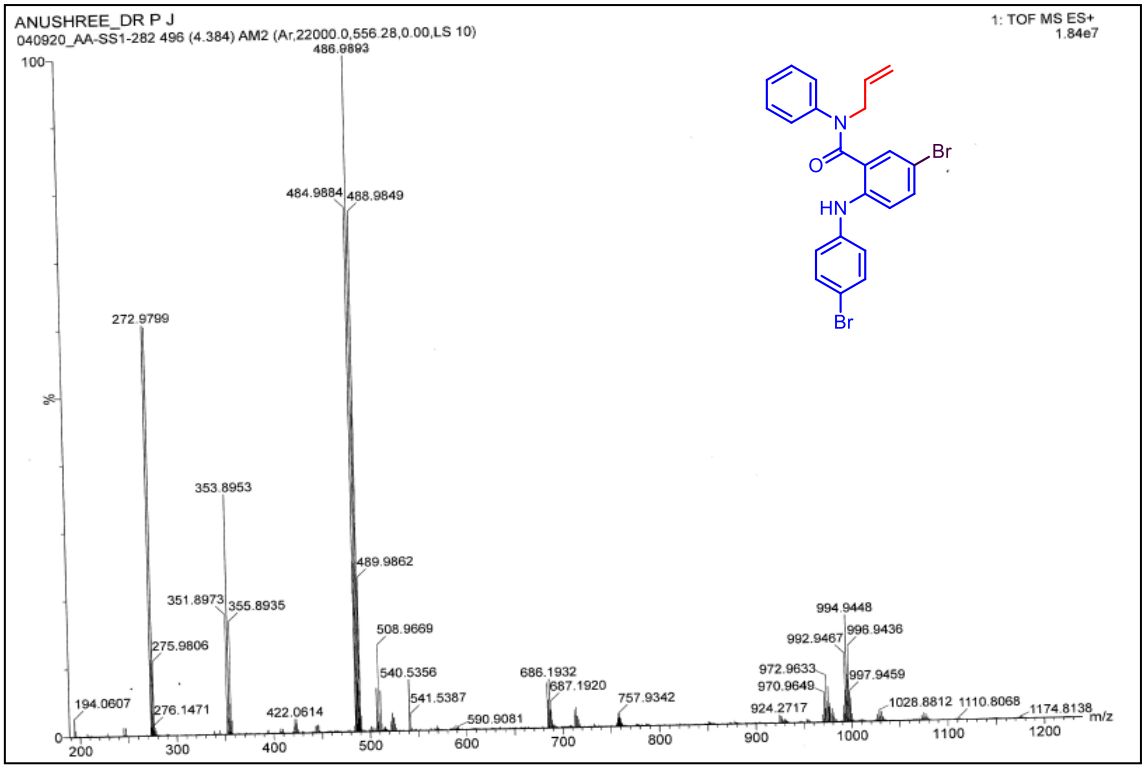


Figure 29. HRMS spectrum of compound **3d**

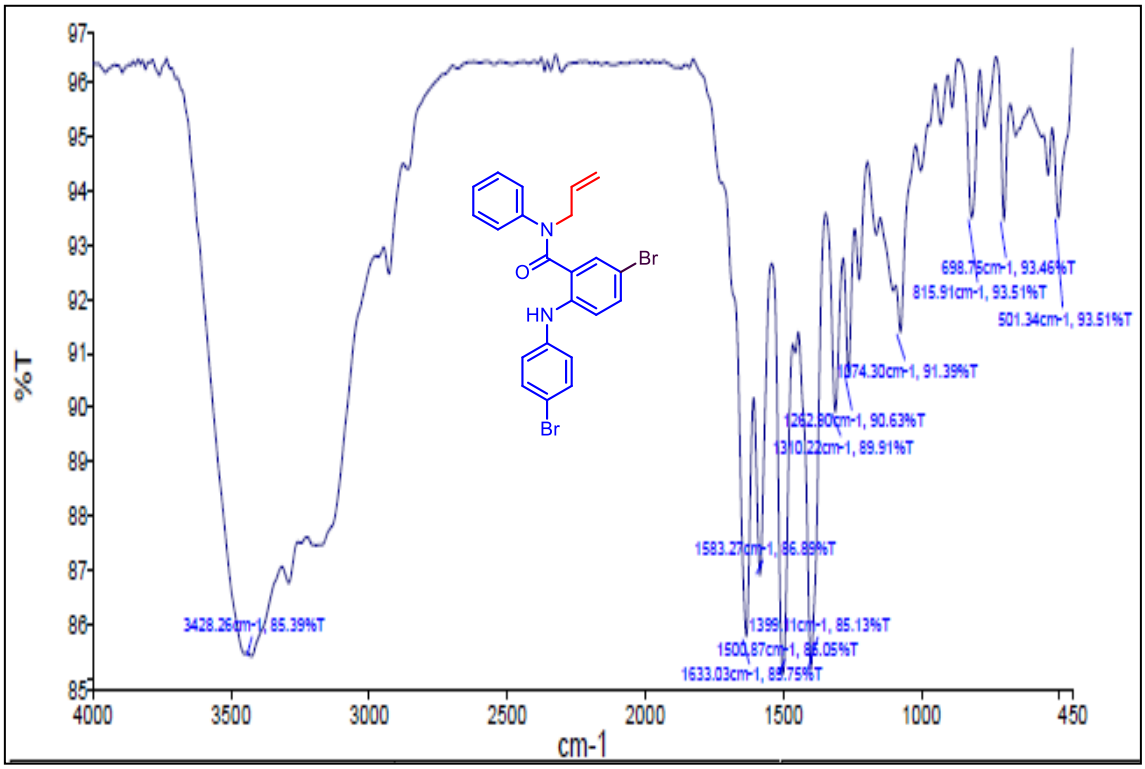


Figure 30. FTIR spectrum of compound **3d**

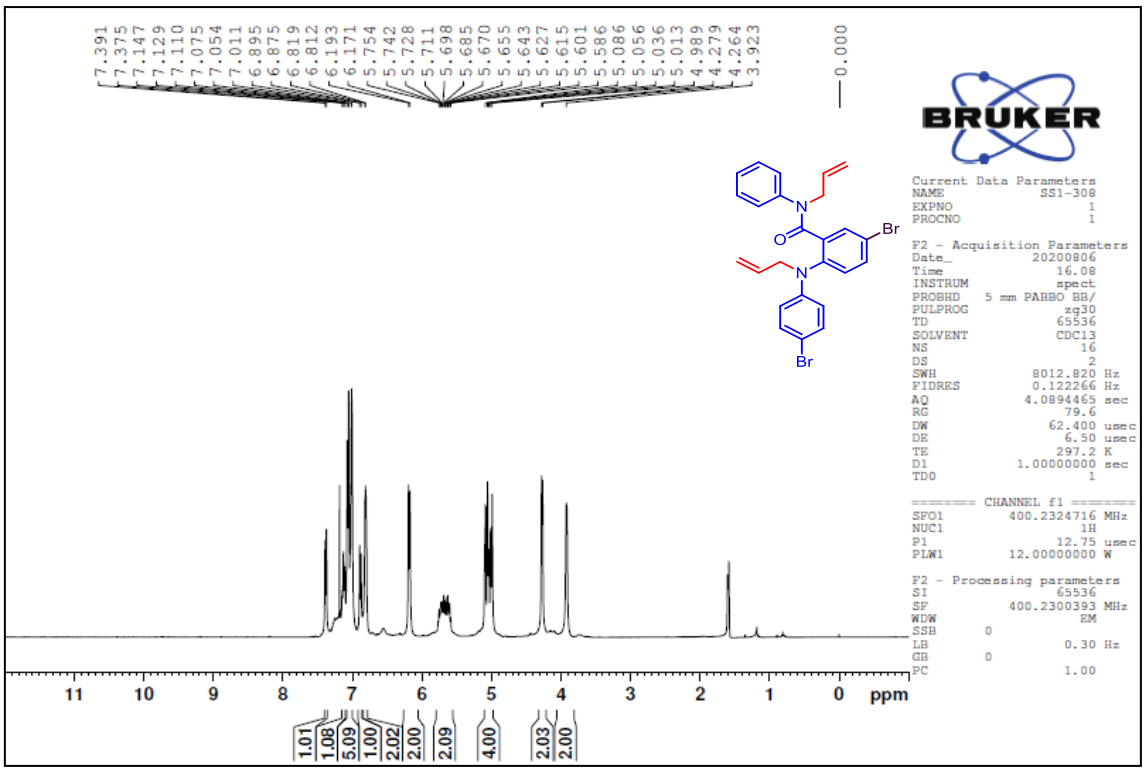


Figure 31. ^{1}H NMR spectrum of compound **3d'**

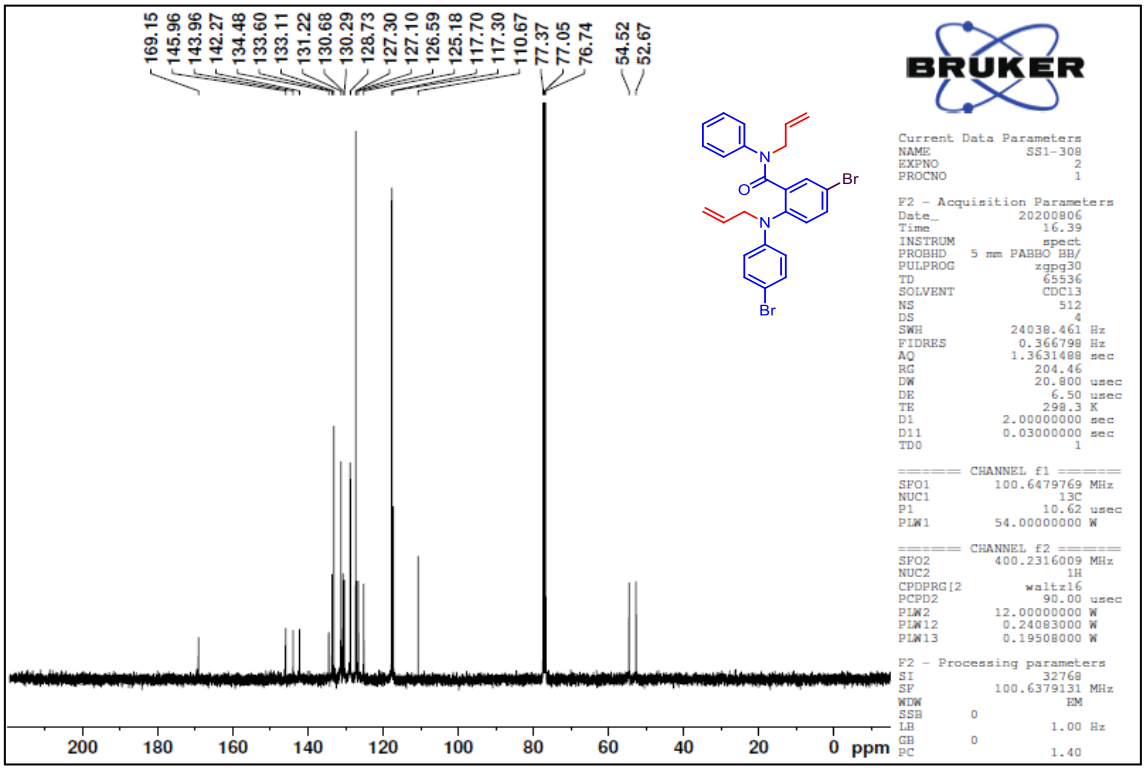


Figure 32. ^{13}C NMR spectrum of compound **3d'**

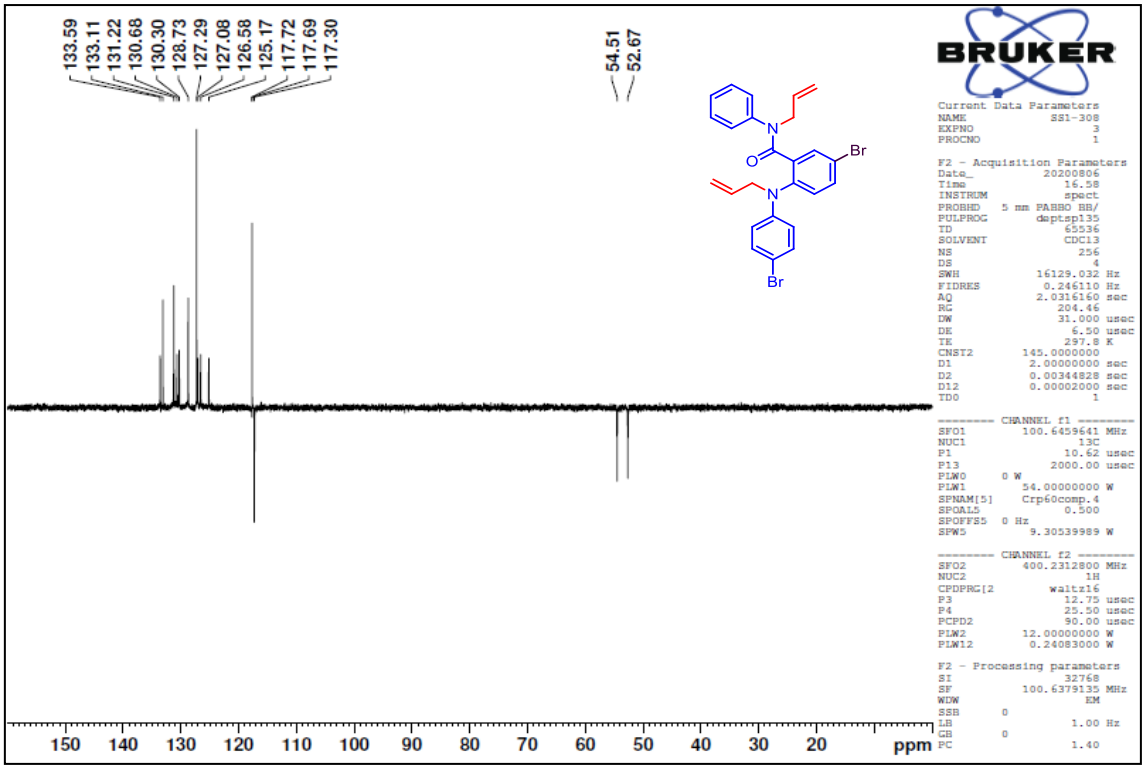


Figure 33. DEPT-135 NMR spectrum of compound **3d'**

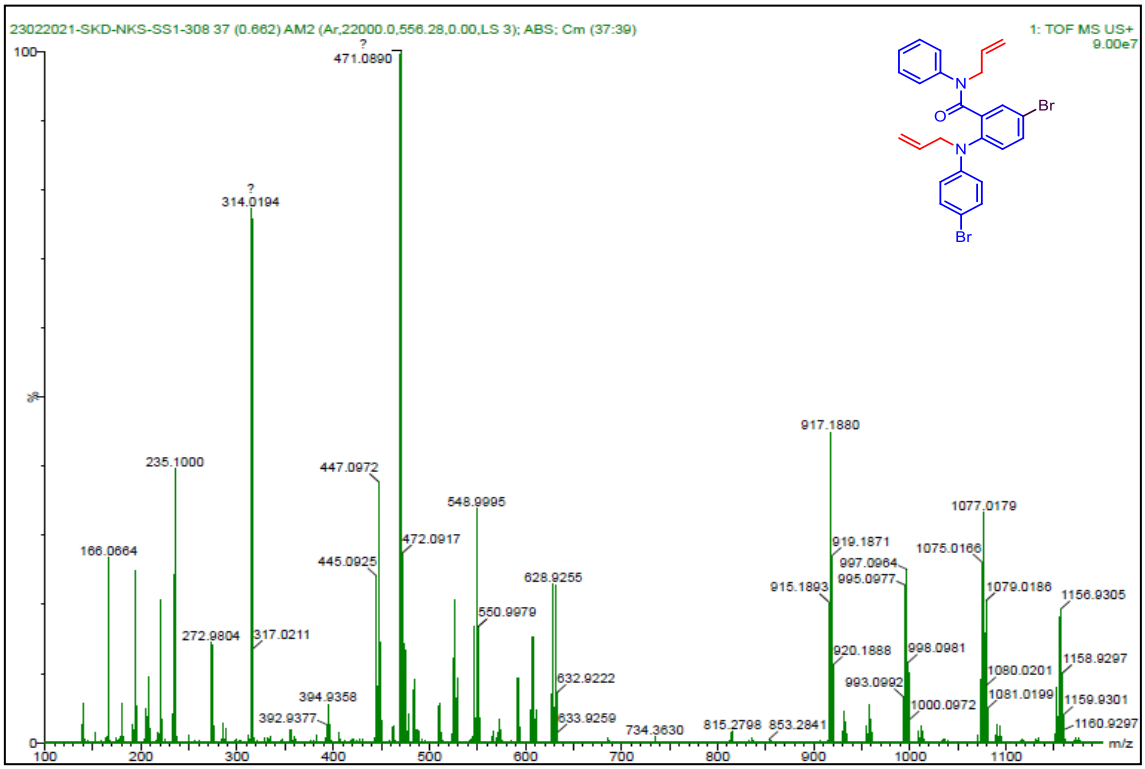


Figure 34. HRMS spectrum of compound **3d'**

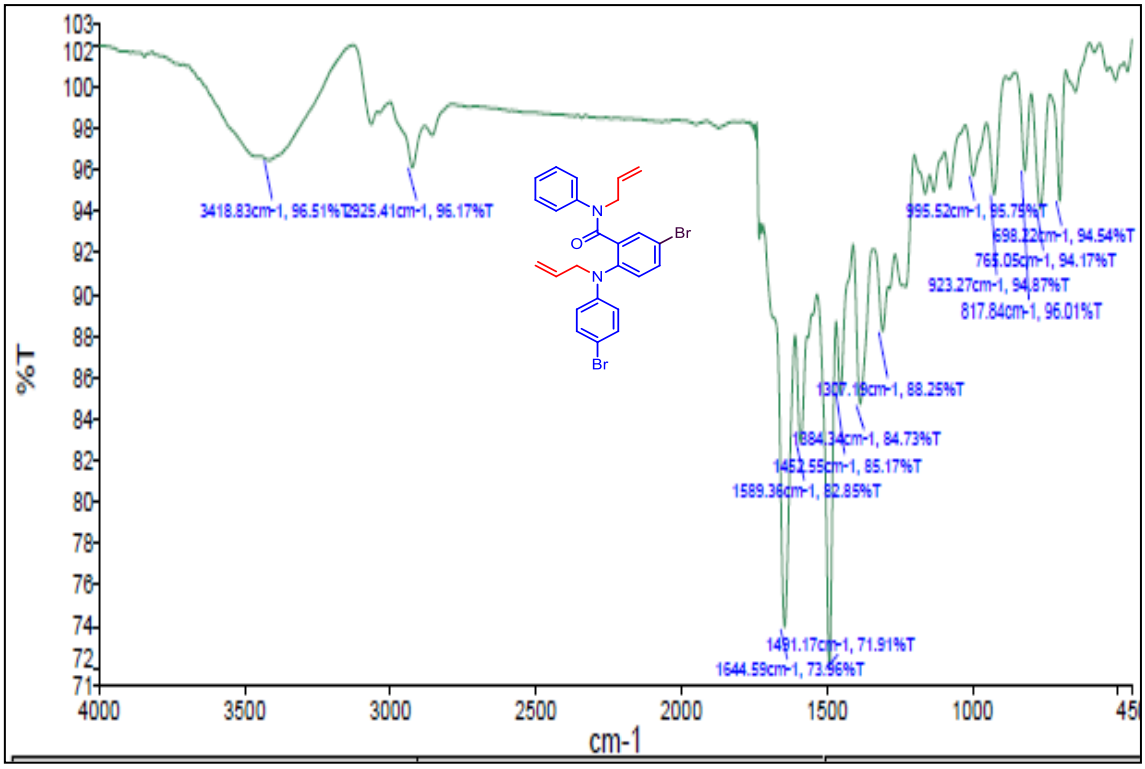


Figure 35. FTIR spectrum of compound **3d'**

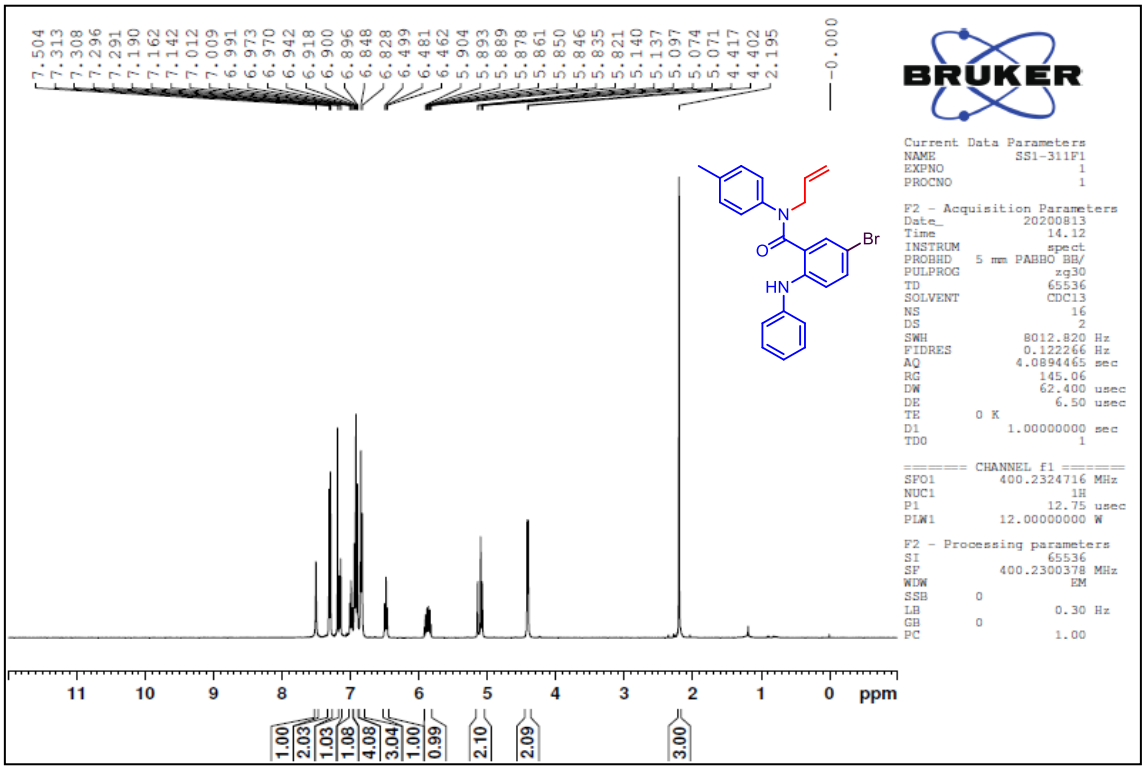


Figure 36. ^{1}H NMR spectrum of compound **3e**

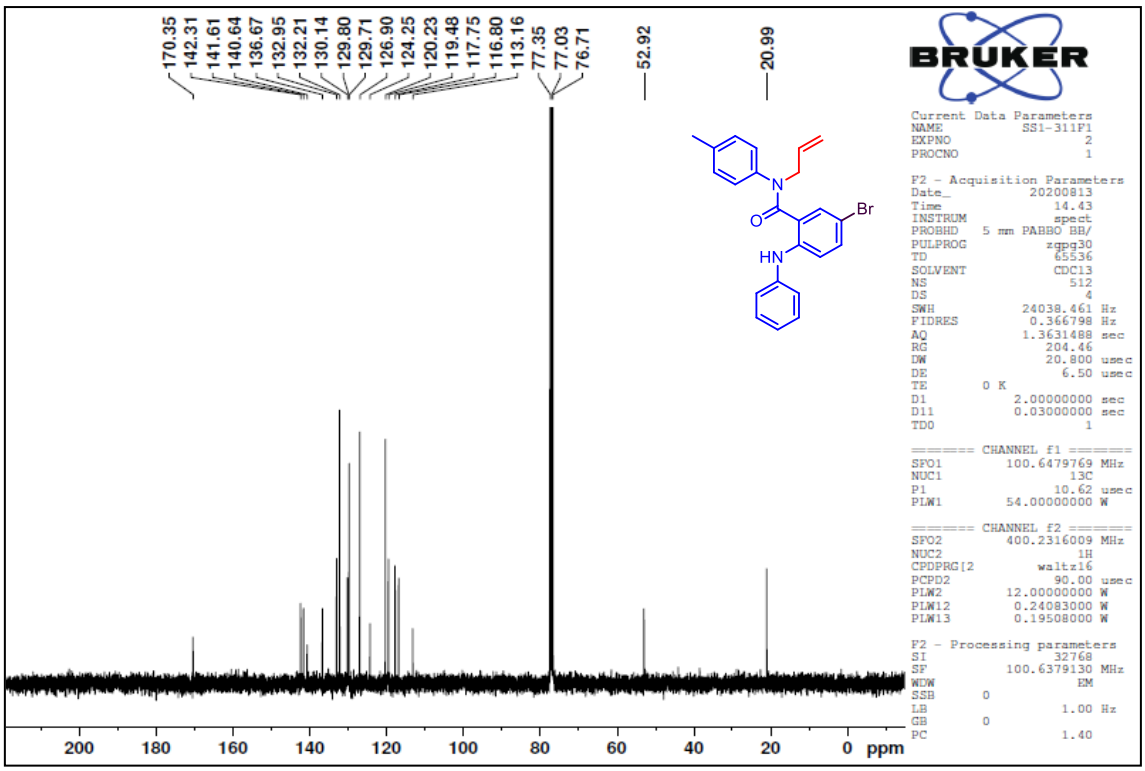


Figure 37. ^{13}C NMR spectrum of compound **3e**

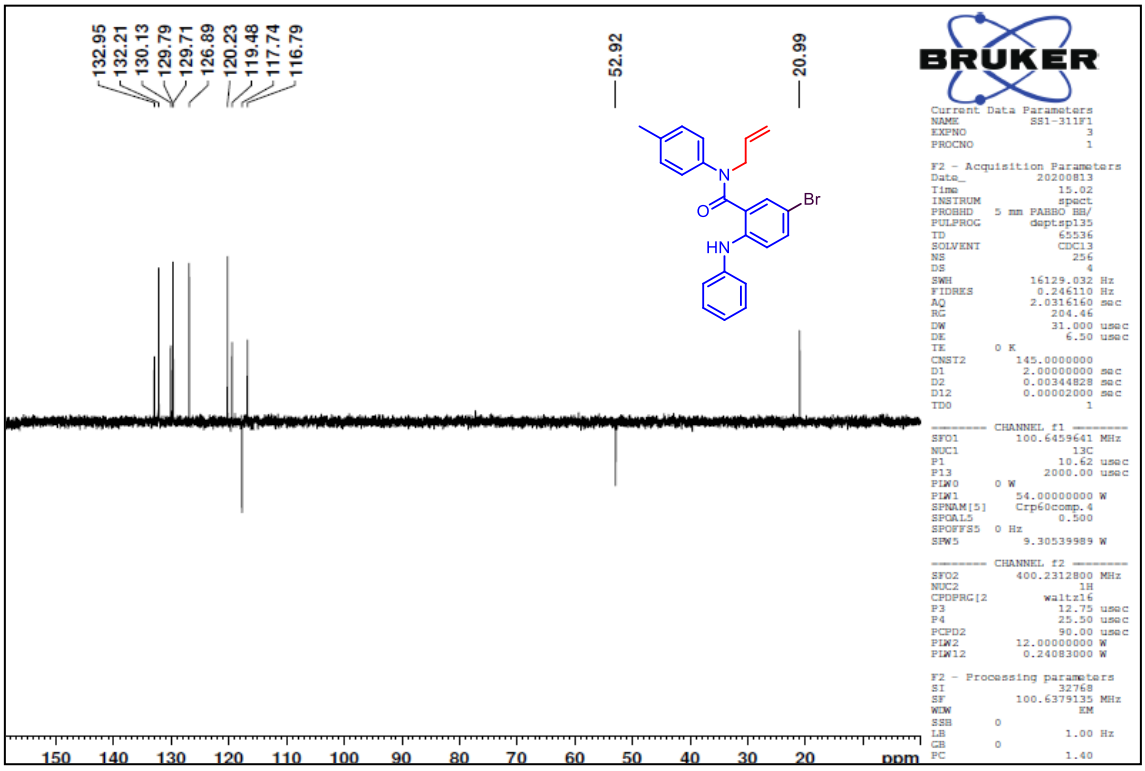


Figure 38. DEPT-135 NMR spectrum of compound **3e**

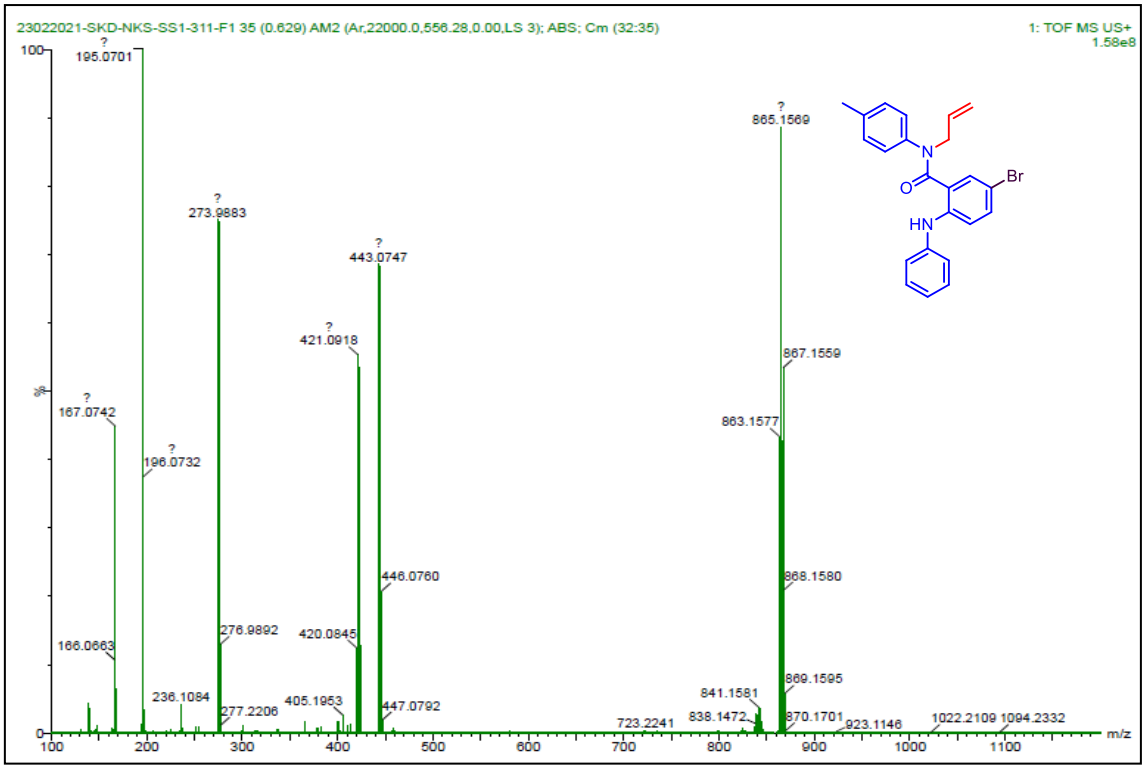


Figure 39. HRMS spectrum of compound **3e**

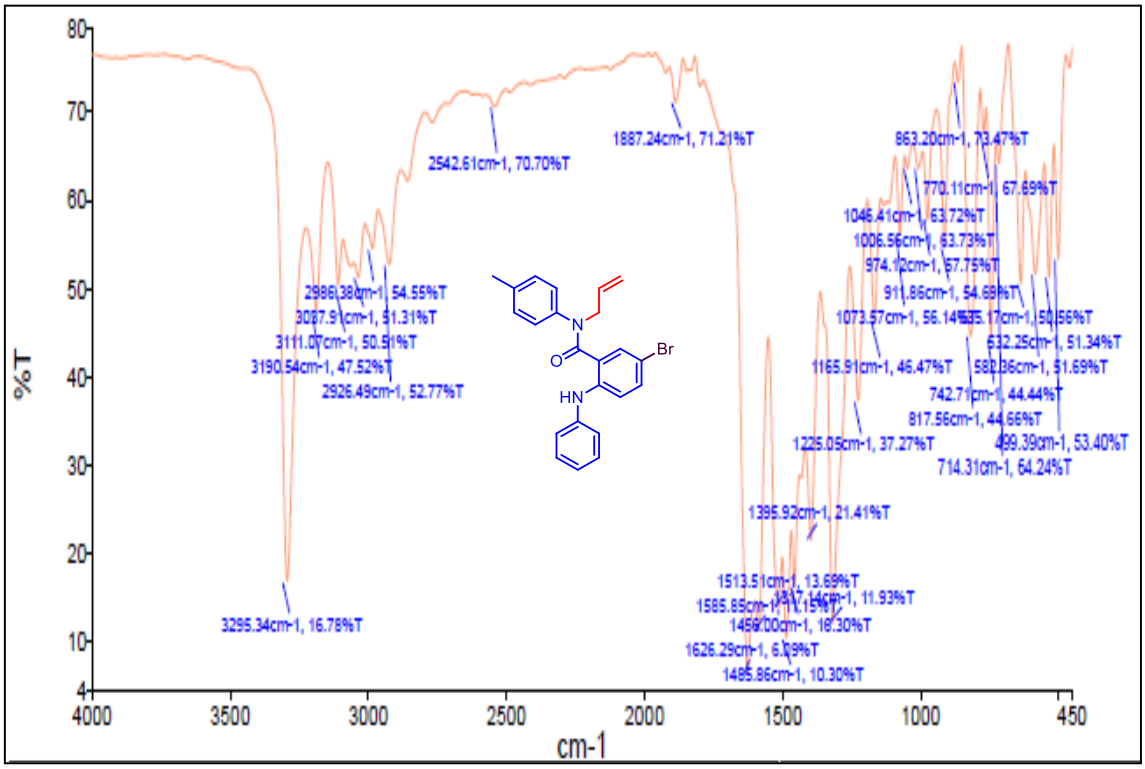


Figure 40. FTIR spectrum of compound **3e**

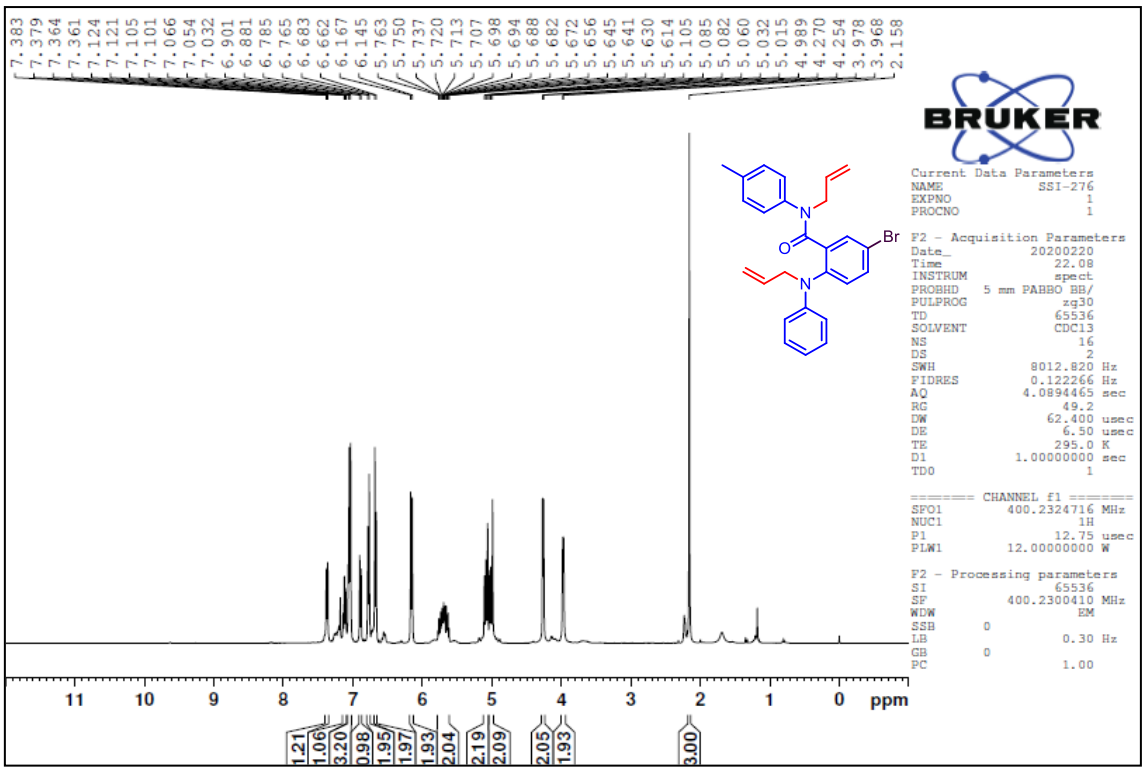


Figure 41.[1]H NMR spectrum of compound **3e'**

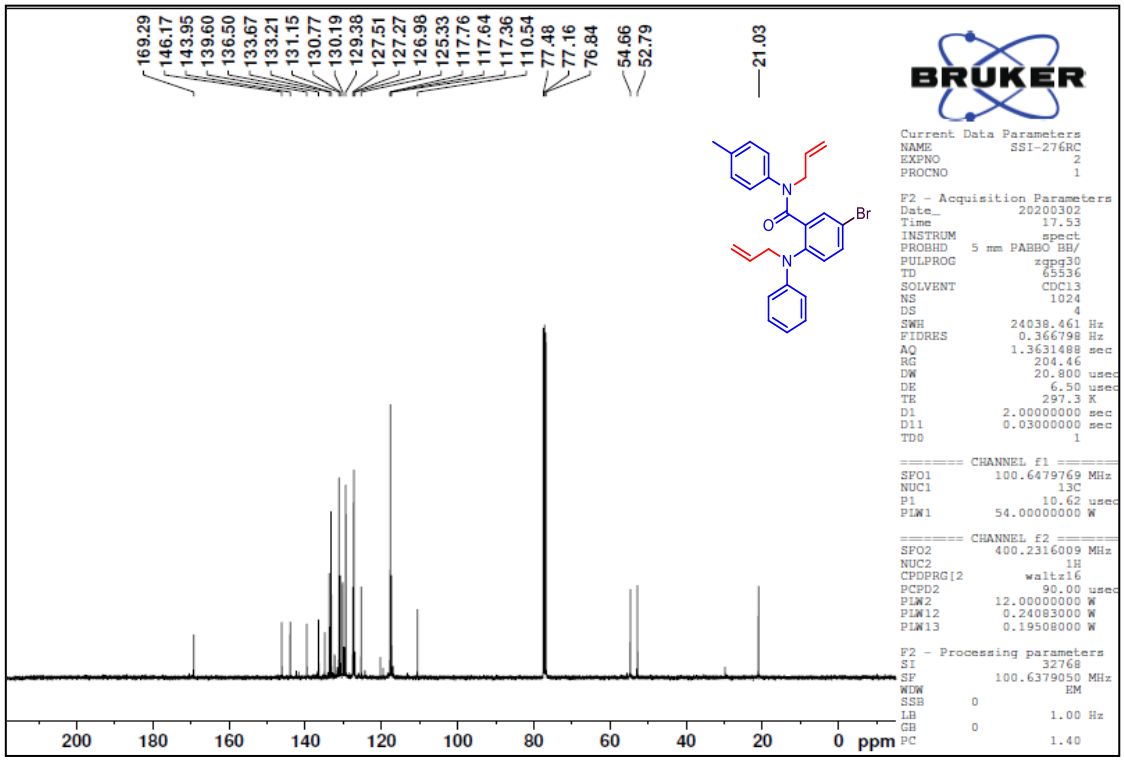


Figure 42. [13]CNMR spectrum of compound **3e'**

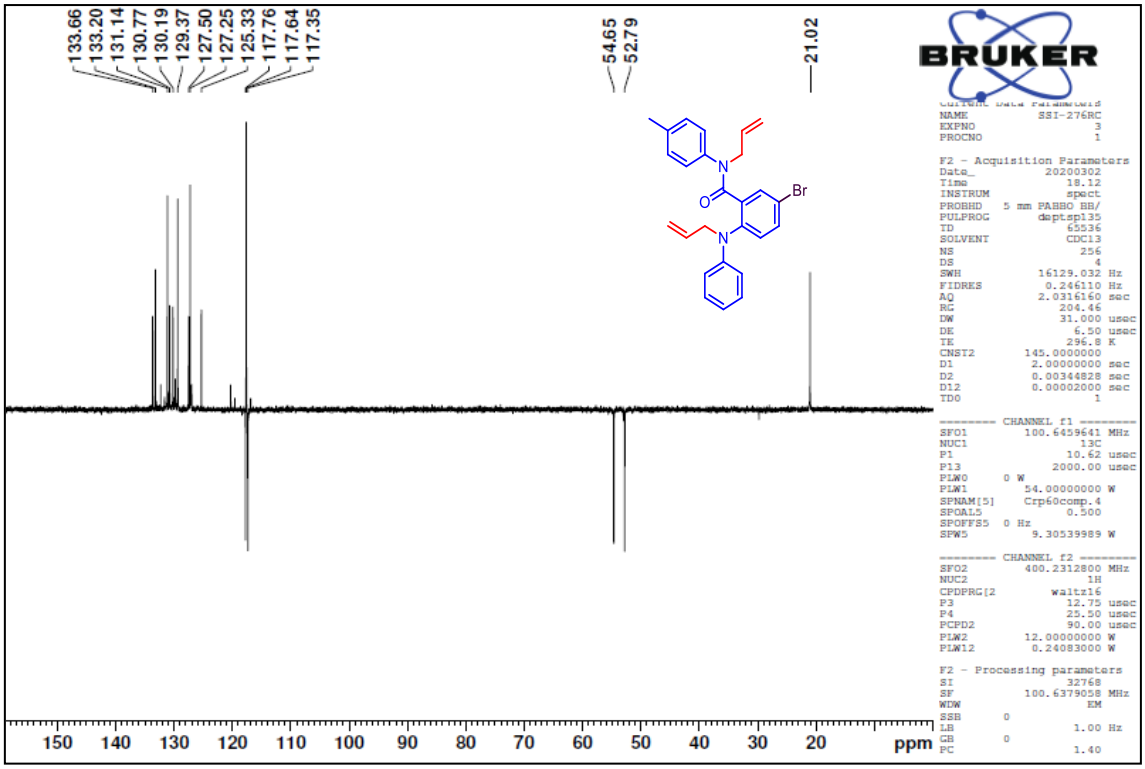


Figure 43. DEPT-135 NMR spectrum of compound **3e'**

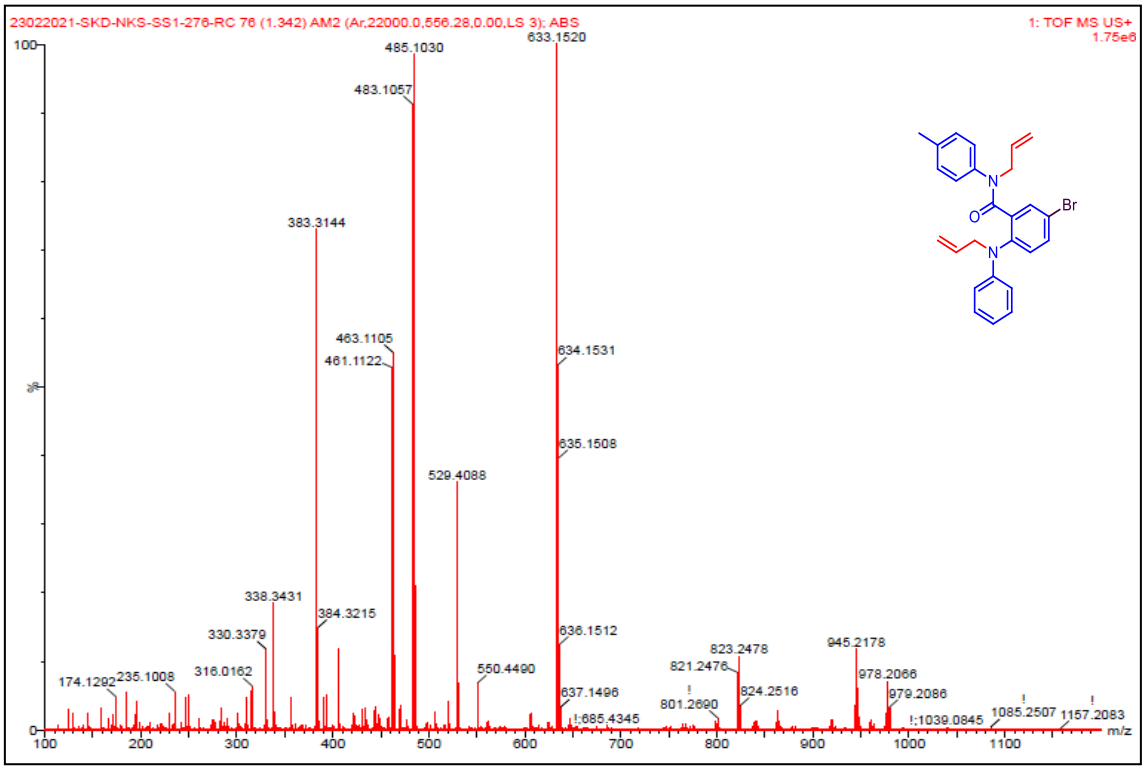


Figure 44. HRMS spectrum of compound **3e'**

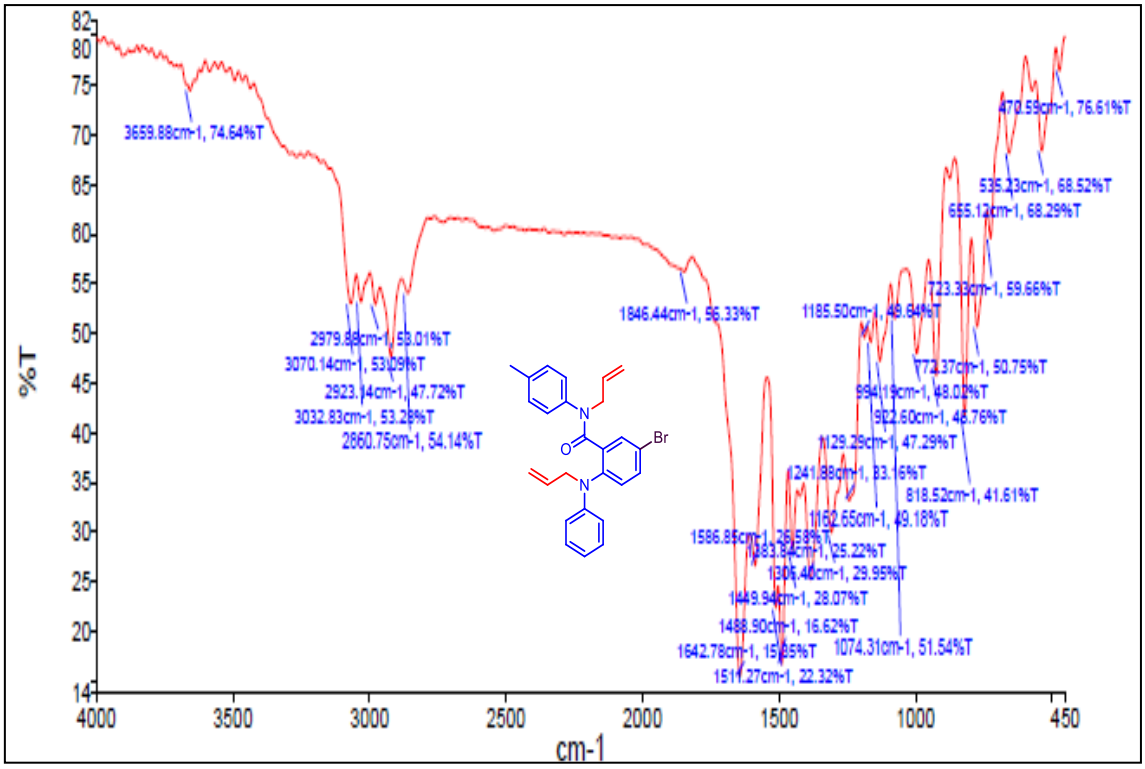


Figure 45. FTIR spectrum of compound **3e'**

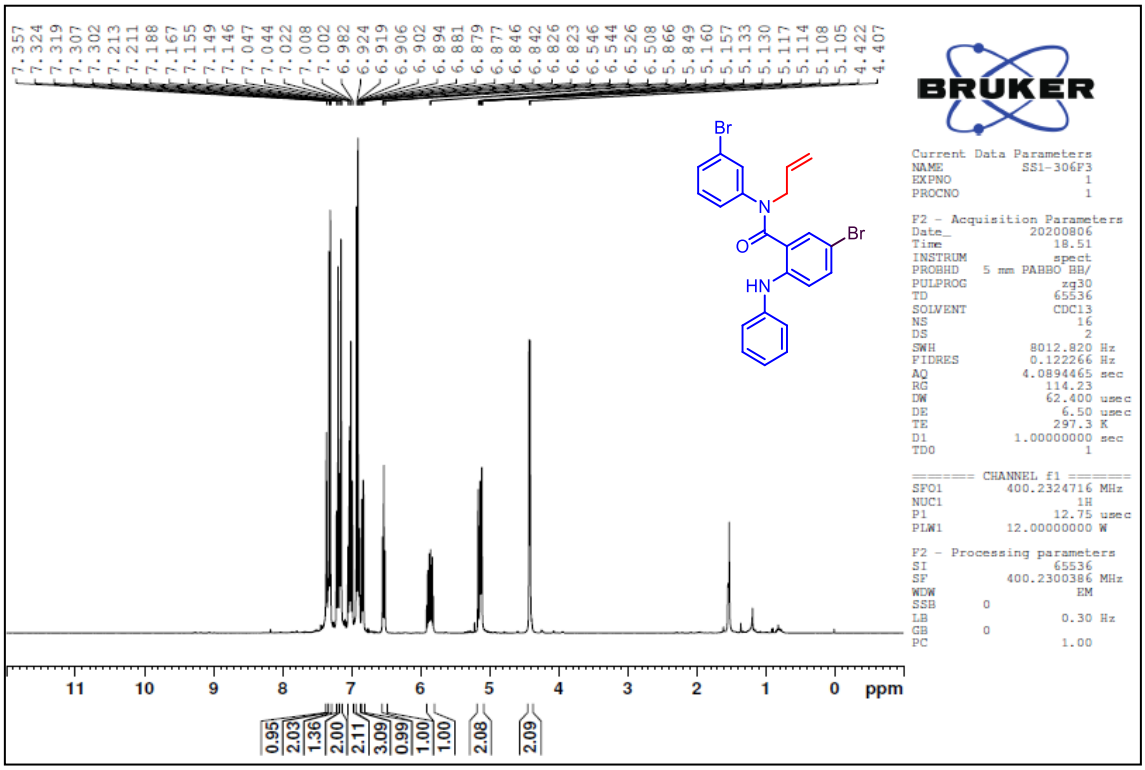


Figure 46. ^{1}H NMR spectrum of compound **3f**

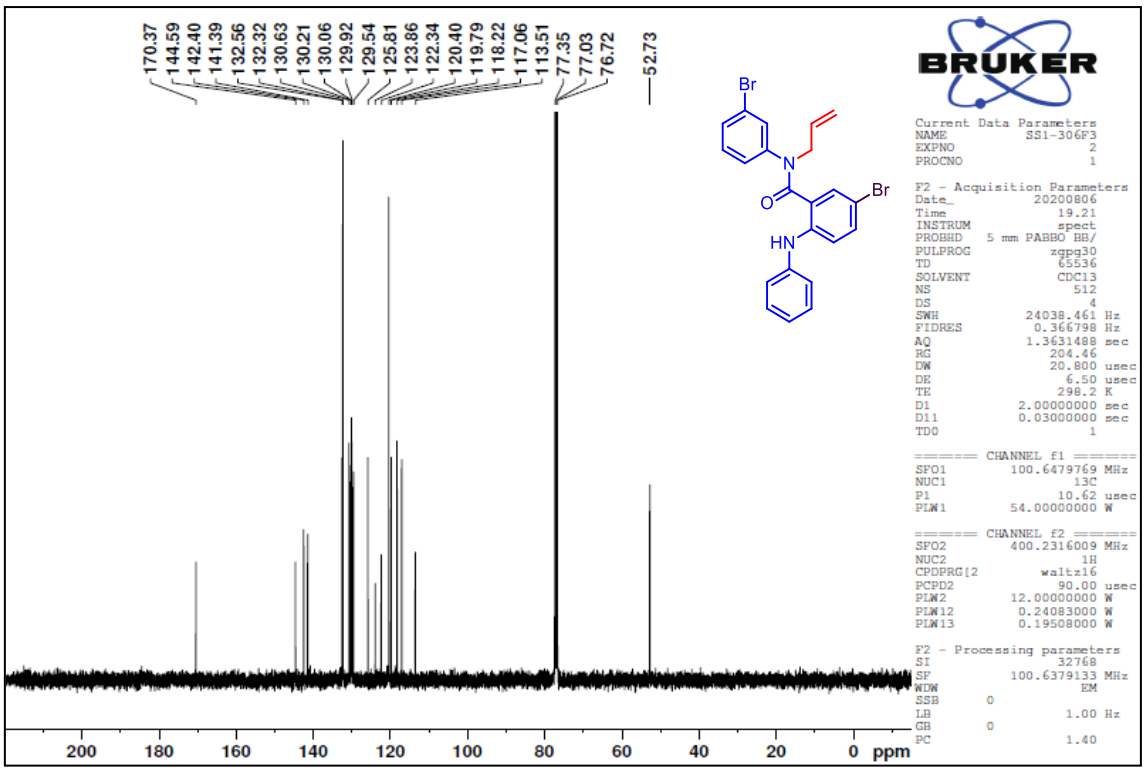


Figure 47. ^{13}CNMR spectrum of compound **3f**

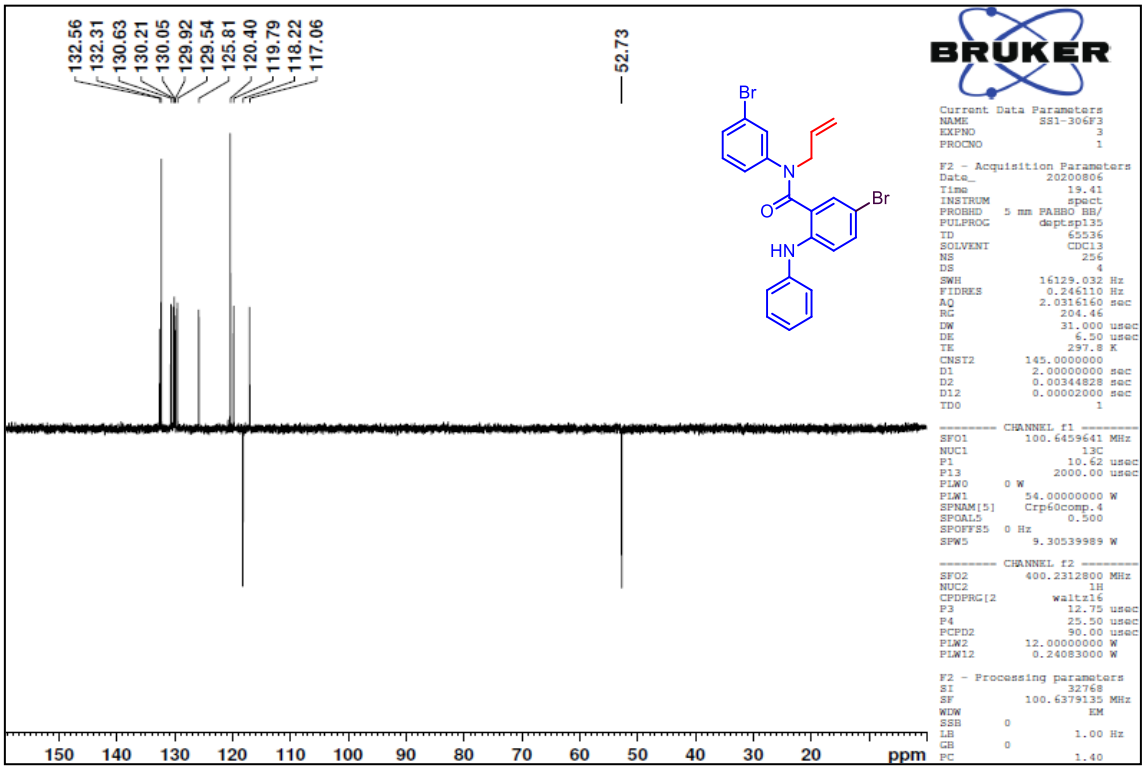


Figure 48. DEPT-135 NMR of spectrum of compound **3f**

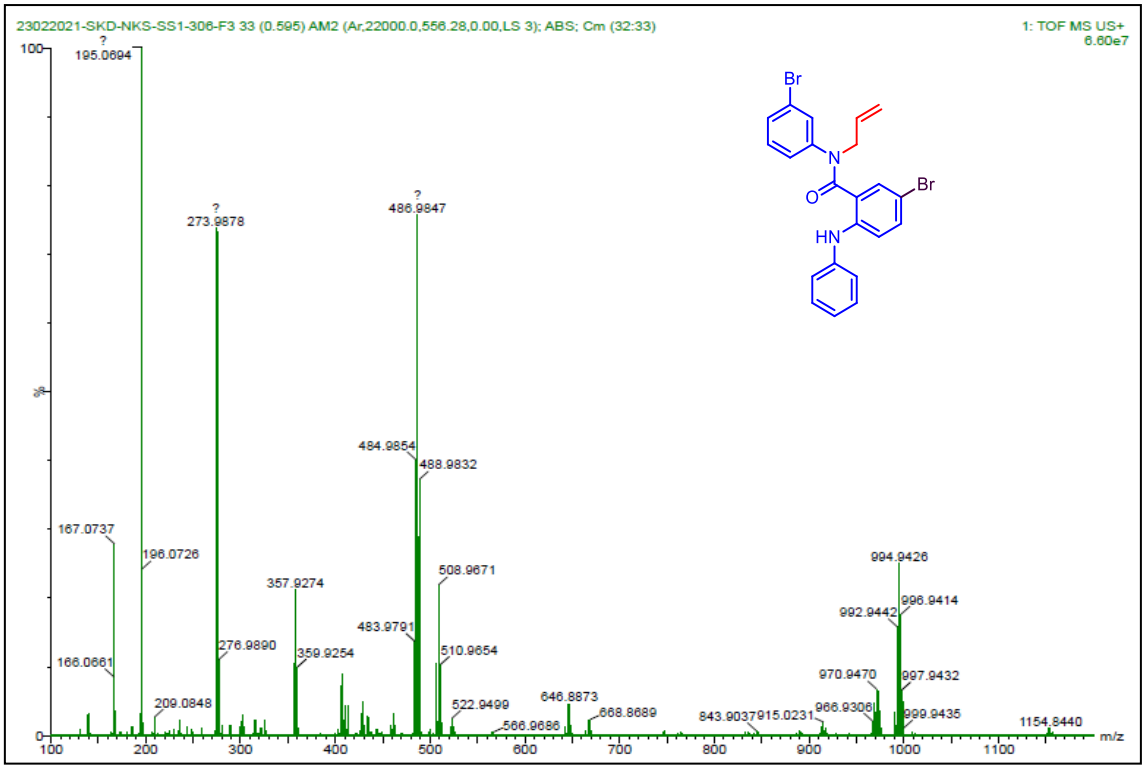


Figure 49. HRMS spectrum of compound **3f**

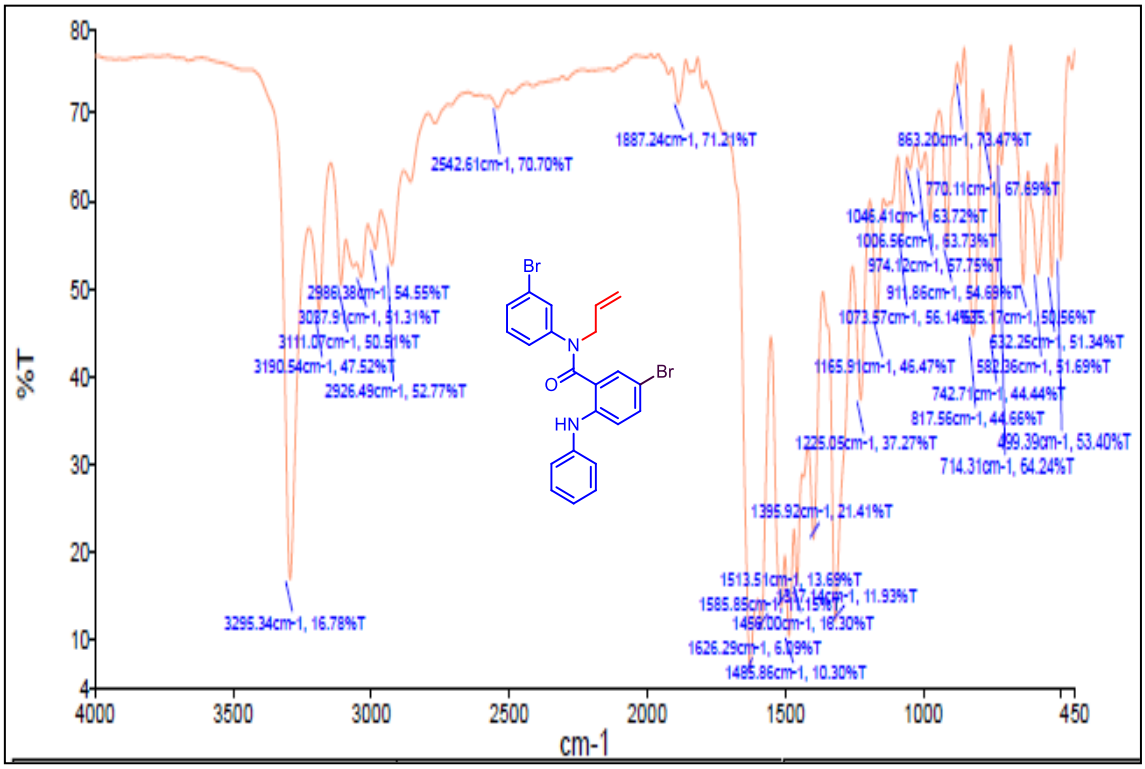


Figure 50. FTIR spectrum of compound **3f**

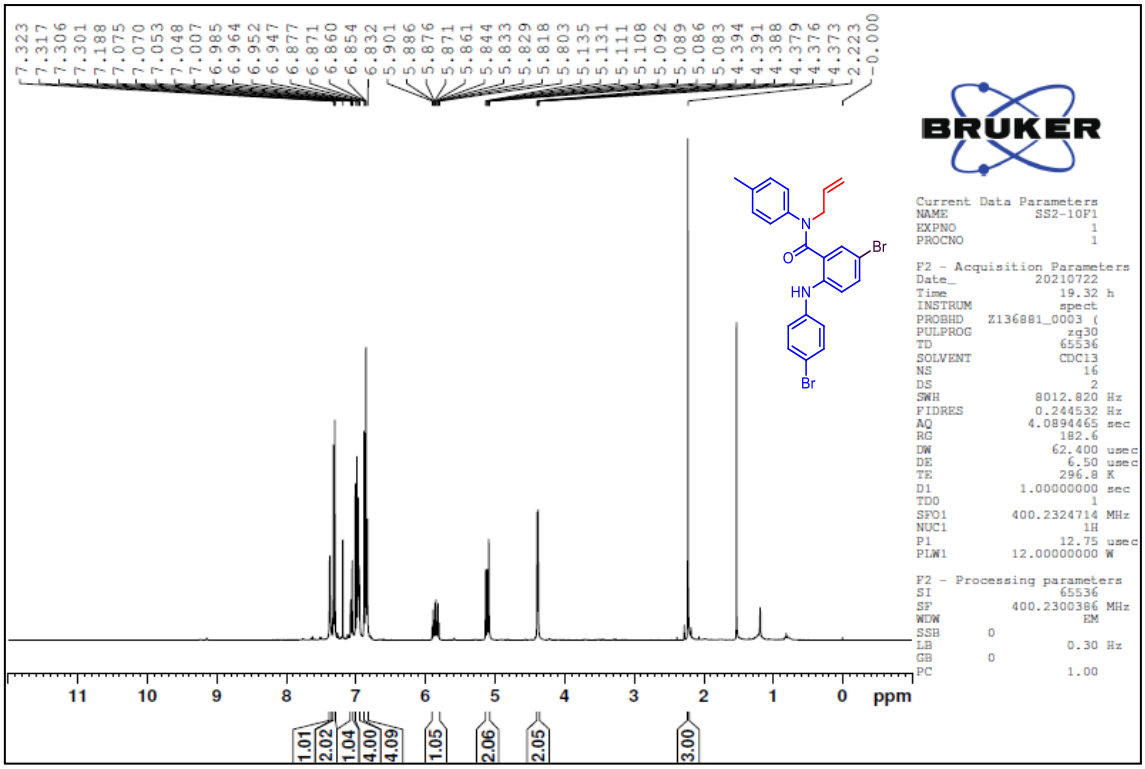


Figure 51. ^{1}H NMR spectrum of compound **3g**

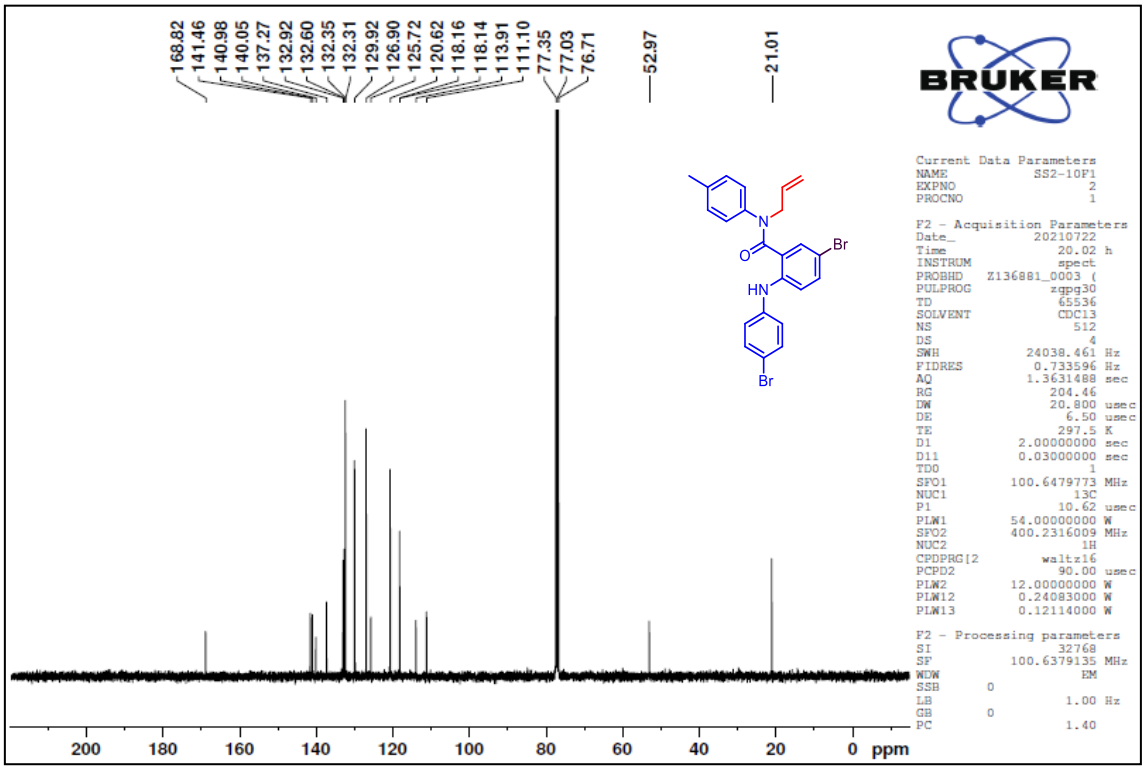


Figure 52. ^{13}C NMR spectrum of compound **3g**

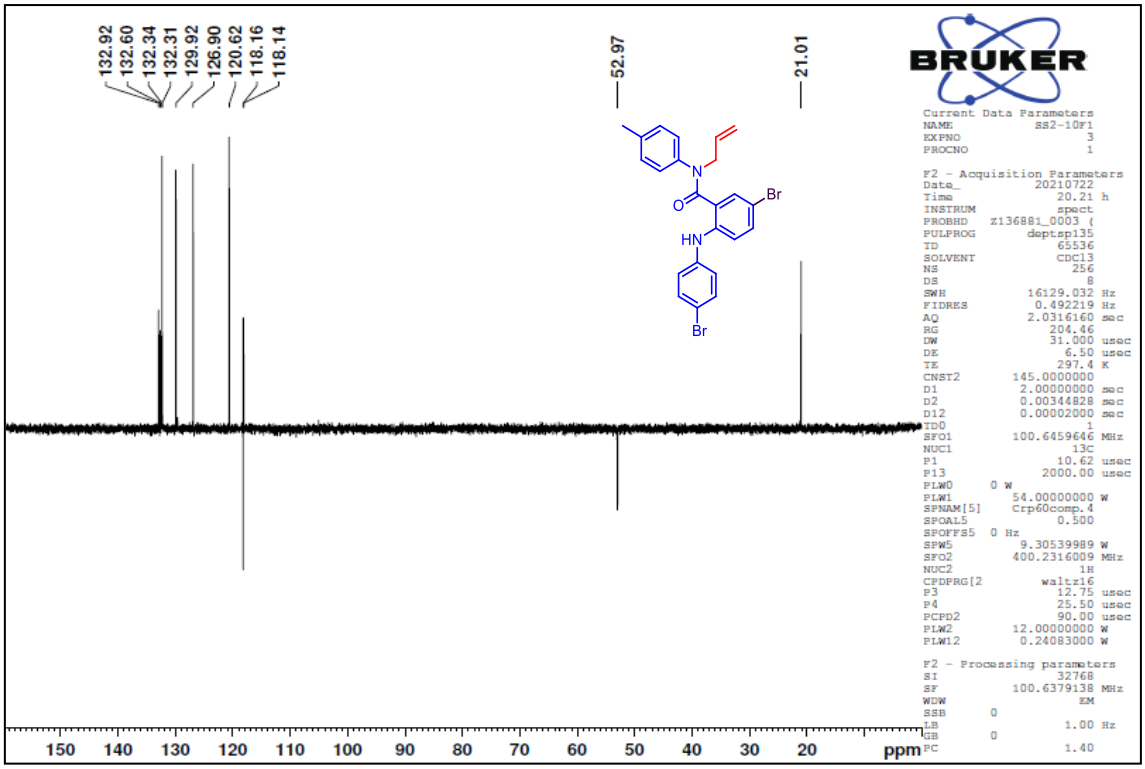


Figure 53. DEPT-135 NMR spectrum of compound **3g**

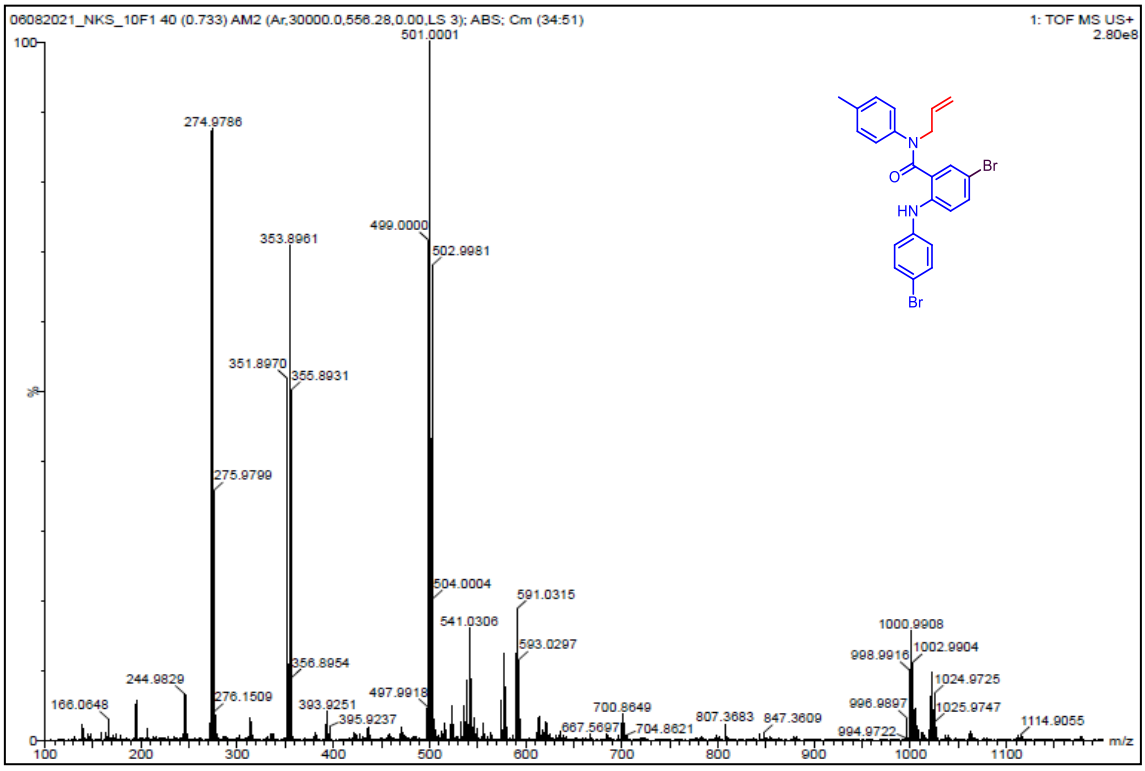


Figure 54. HRMS spectrum of compound **3g**

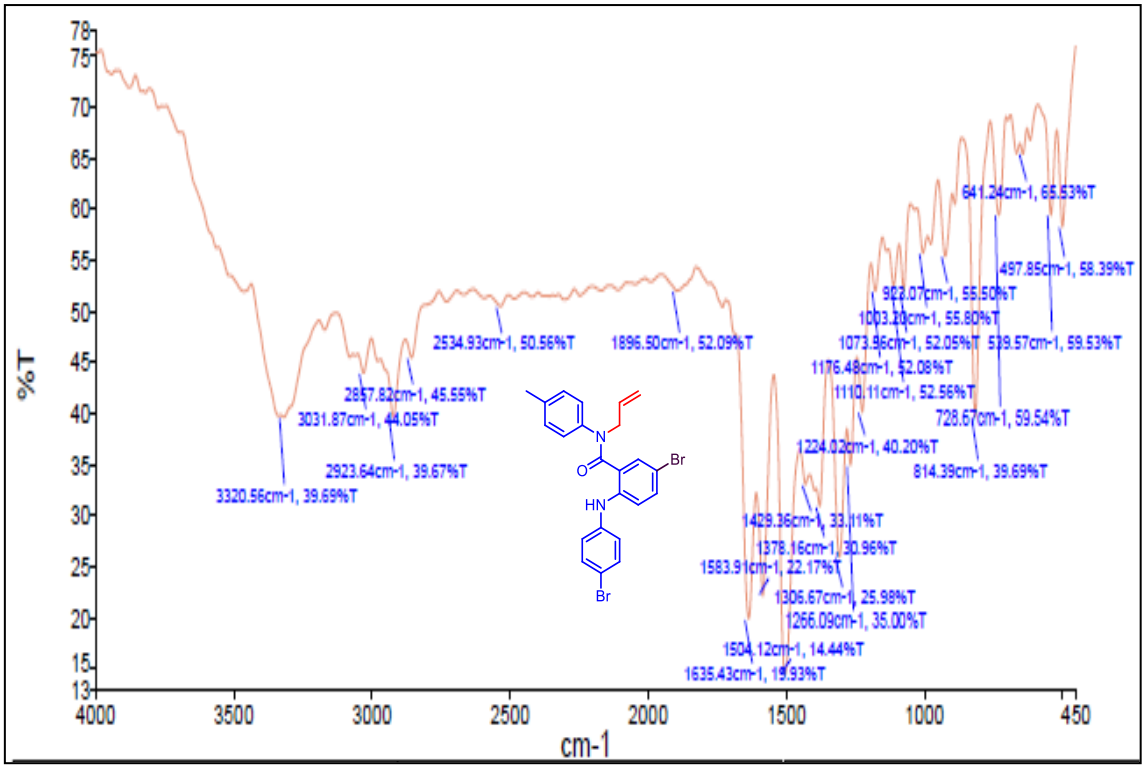


Figure 55. FTIR spectrum of compound **3g**

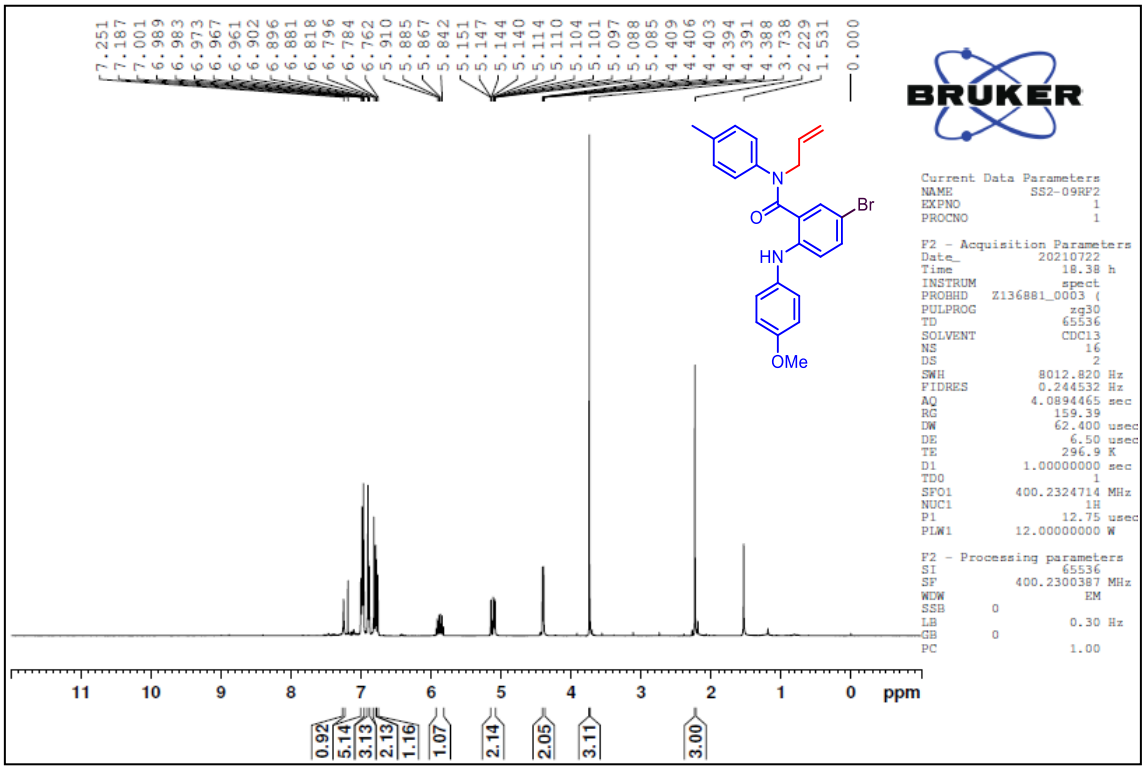


Figure 56. ^{1}H NMR spectrum of compound **3h**

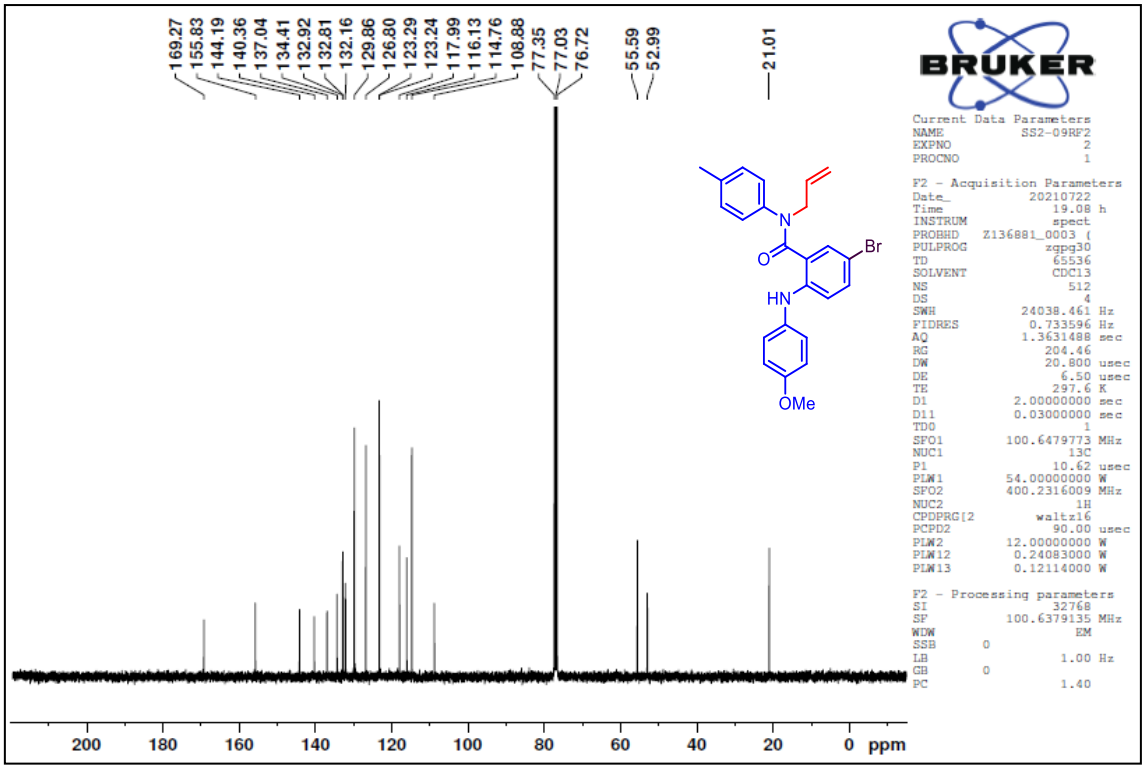


Figure 57. ^{13}C NMR spectrum of compound **3h**

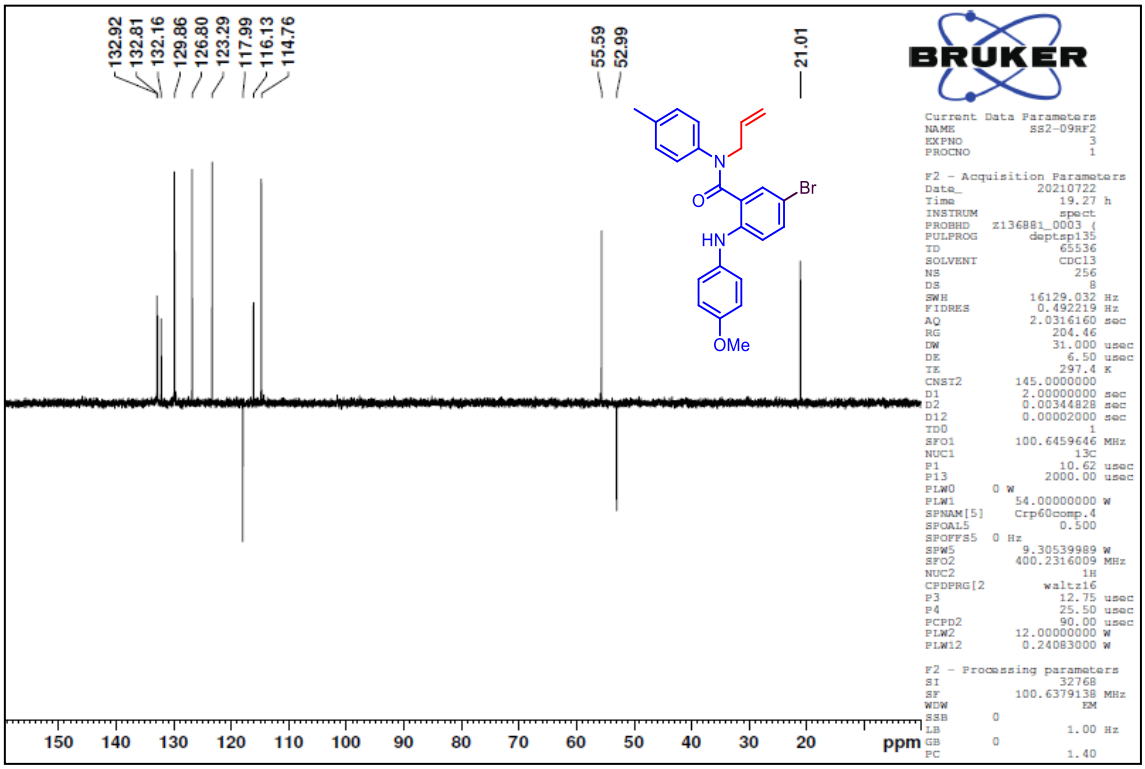


Figure 58. DEPT-135 NMR spectrum of compound **3h**

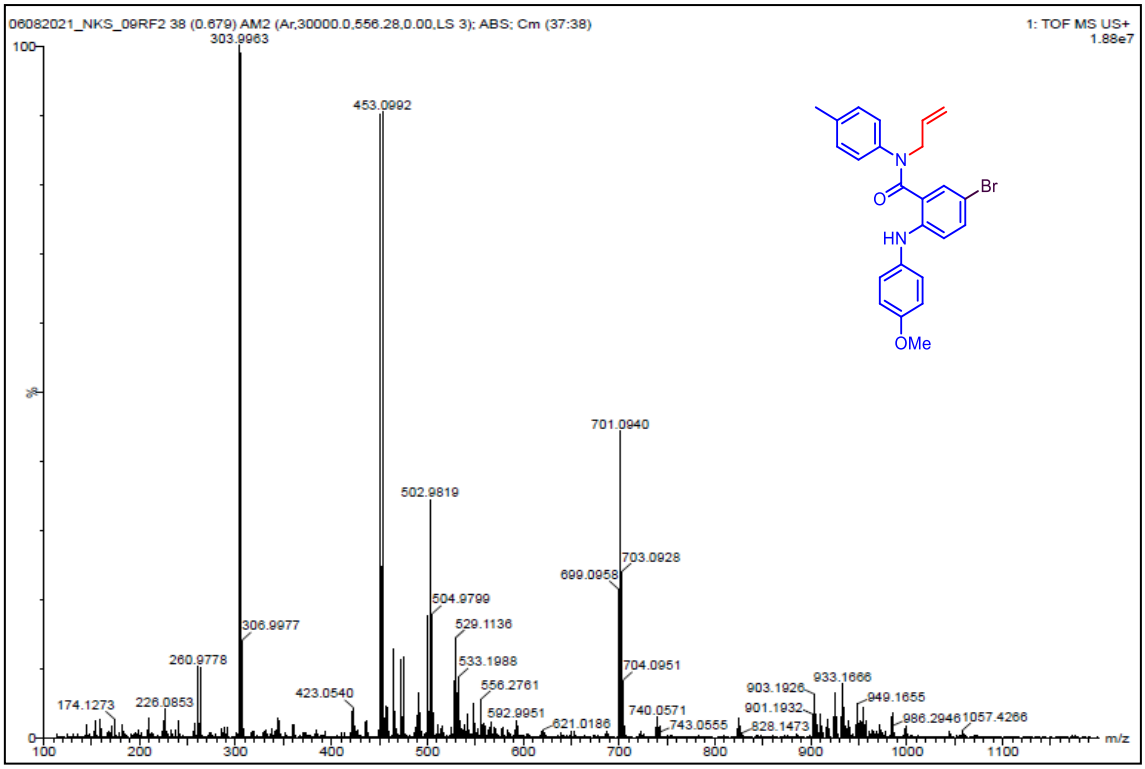


Figure 59. HRMS spectrum of compound **3h**

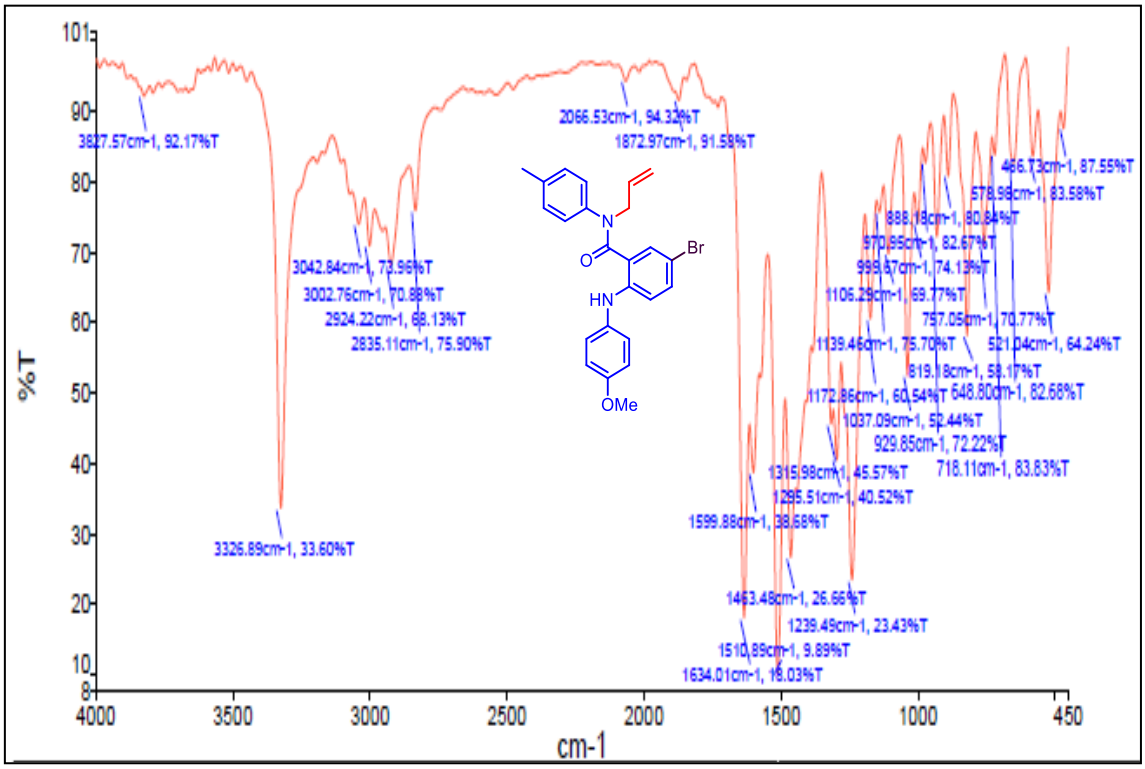


Figure 60. FTIR spectrum of compound **3h**

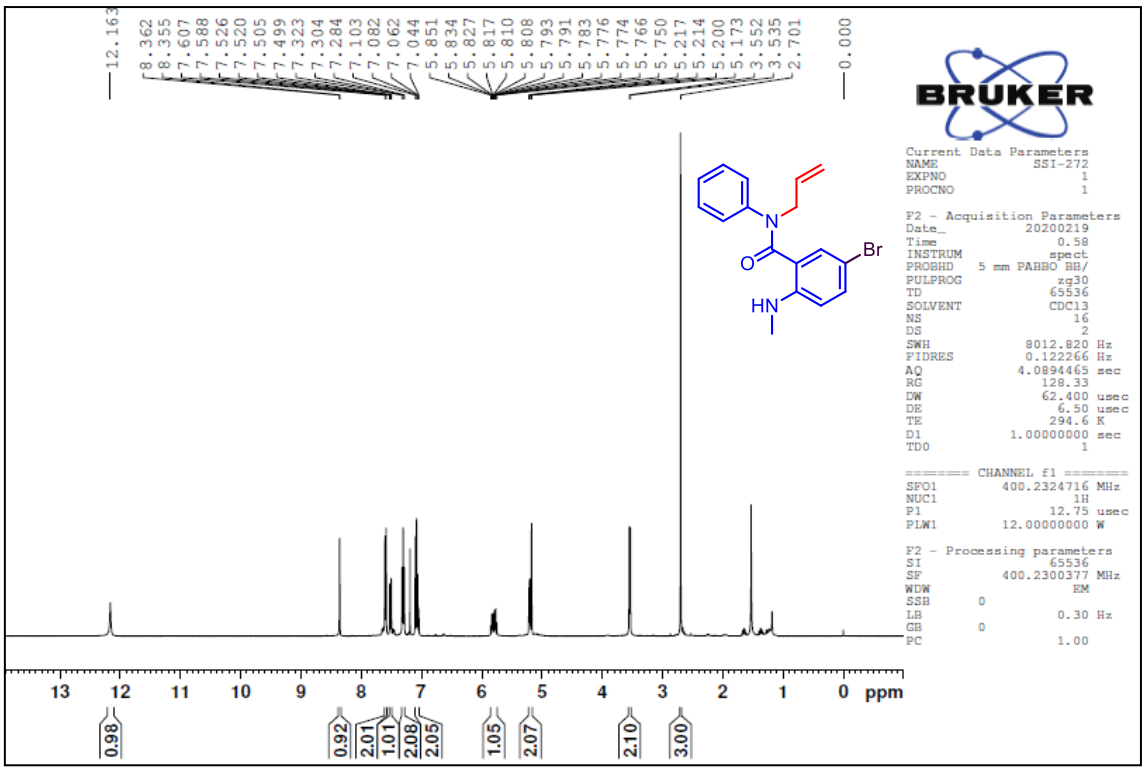


Figure 61. ^{1}H NMR spectrum of compound **3i**

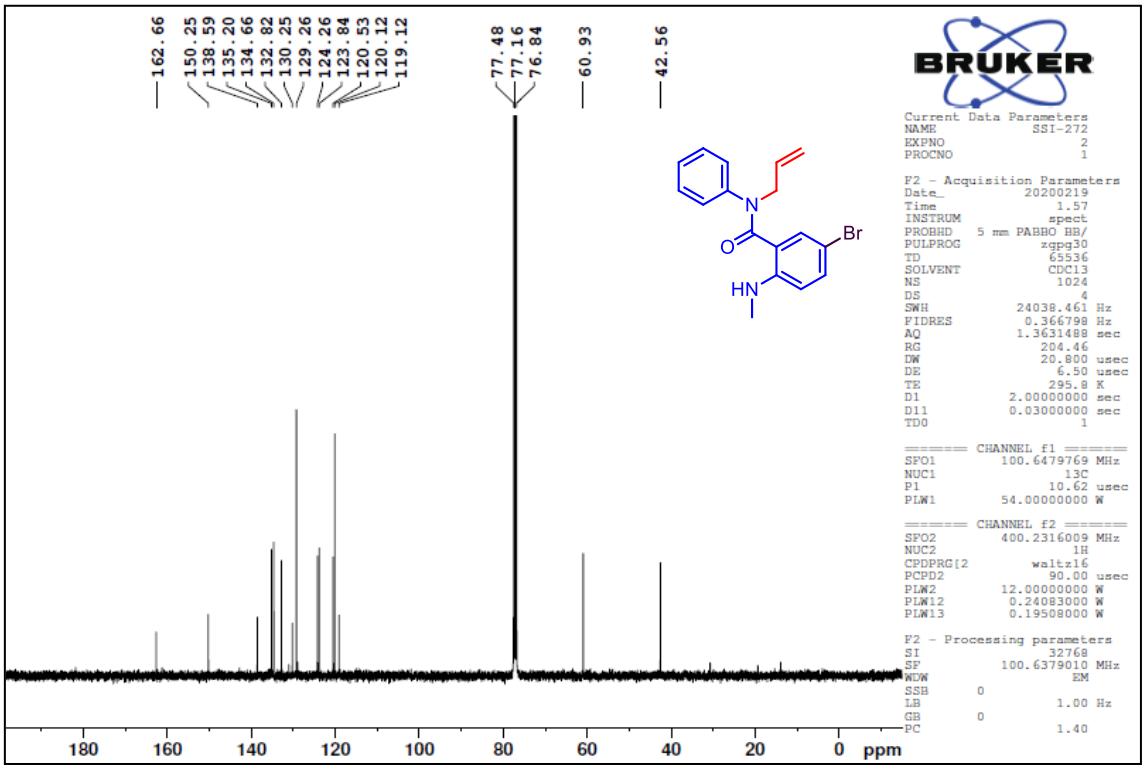


Figure 62. ^{13}C NMR spectrum of compound **3i**

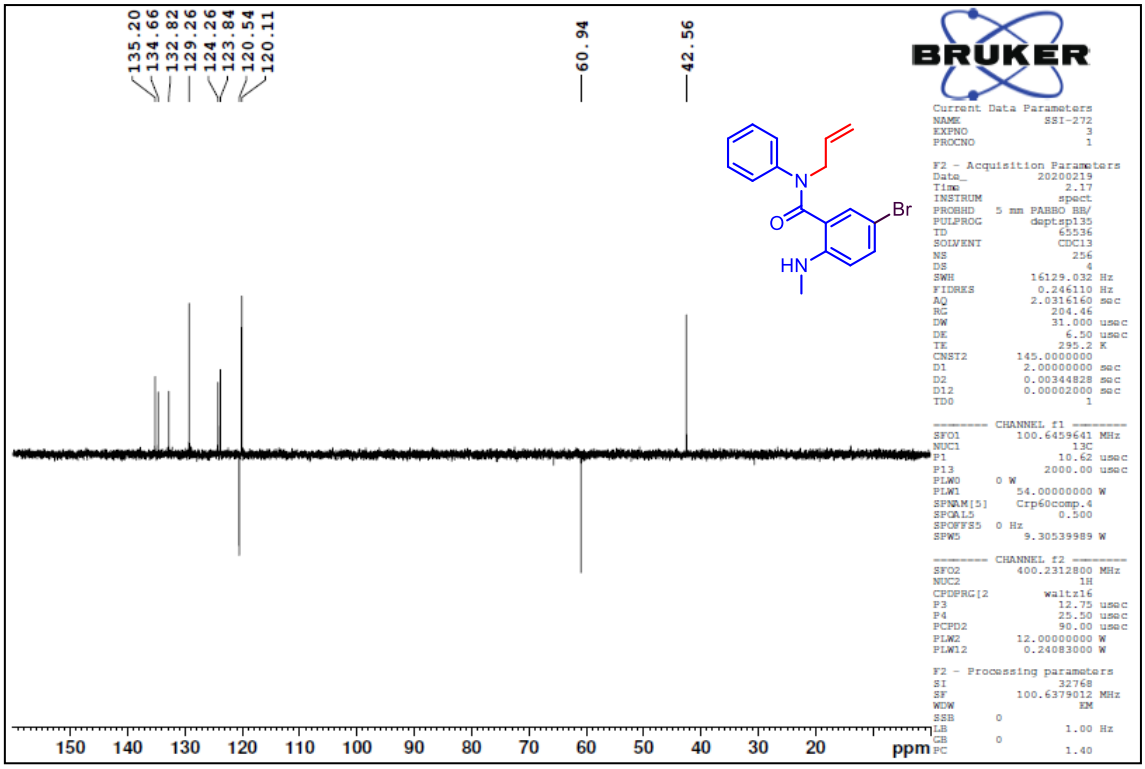


Figure 63. DEPT-135 NMR spectrum of compound **3i**

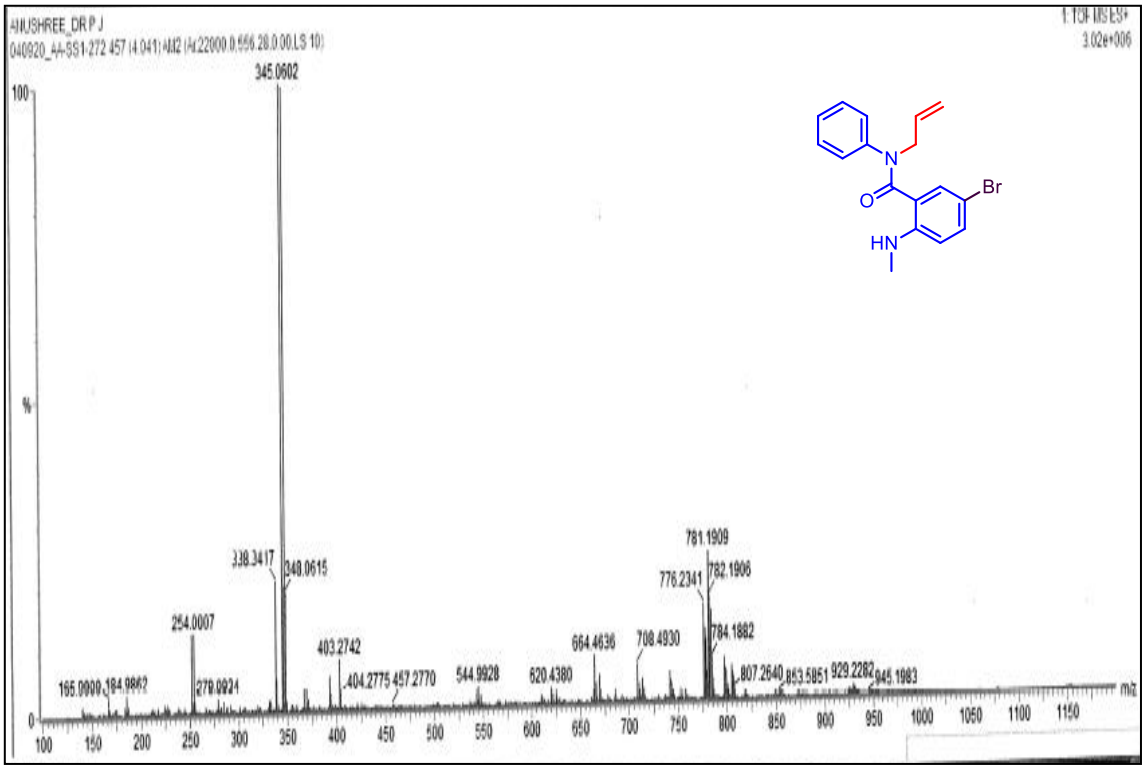


Figure 64. HRMS spectrum of compound **3i**

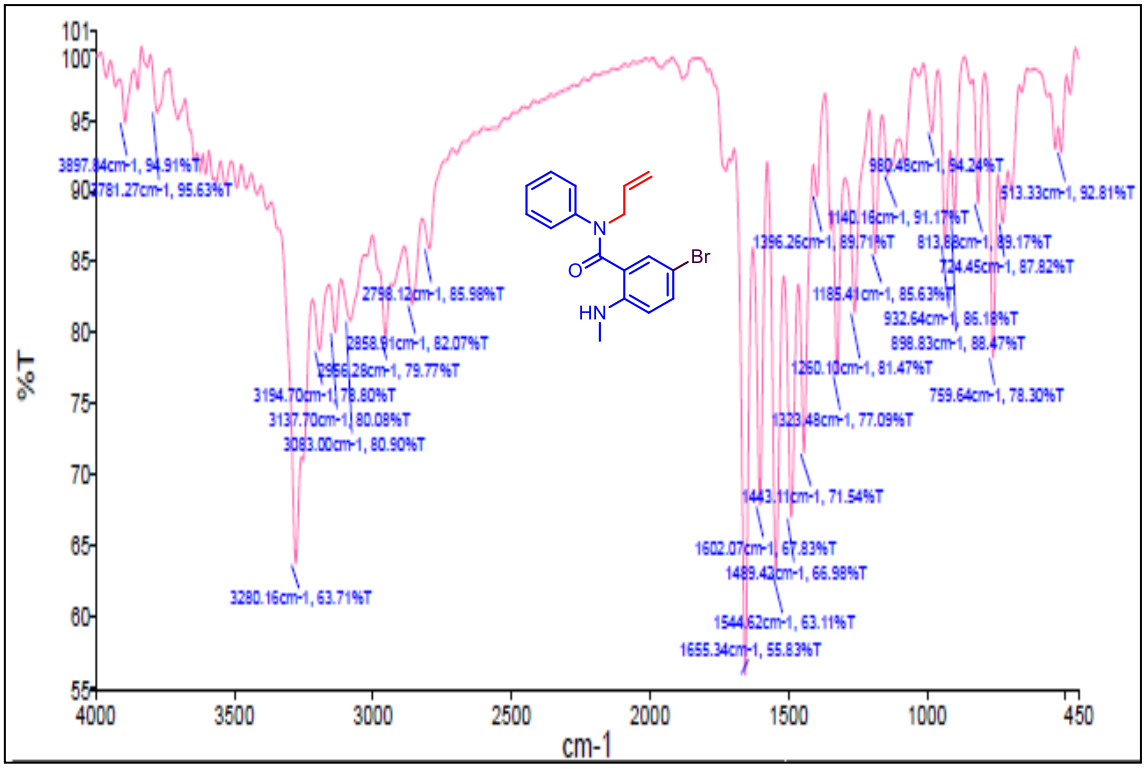


Figure 65. FTIR spectrum of compound **3i**

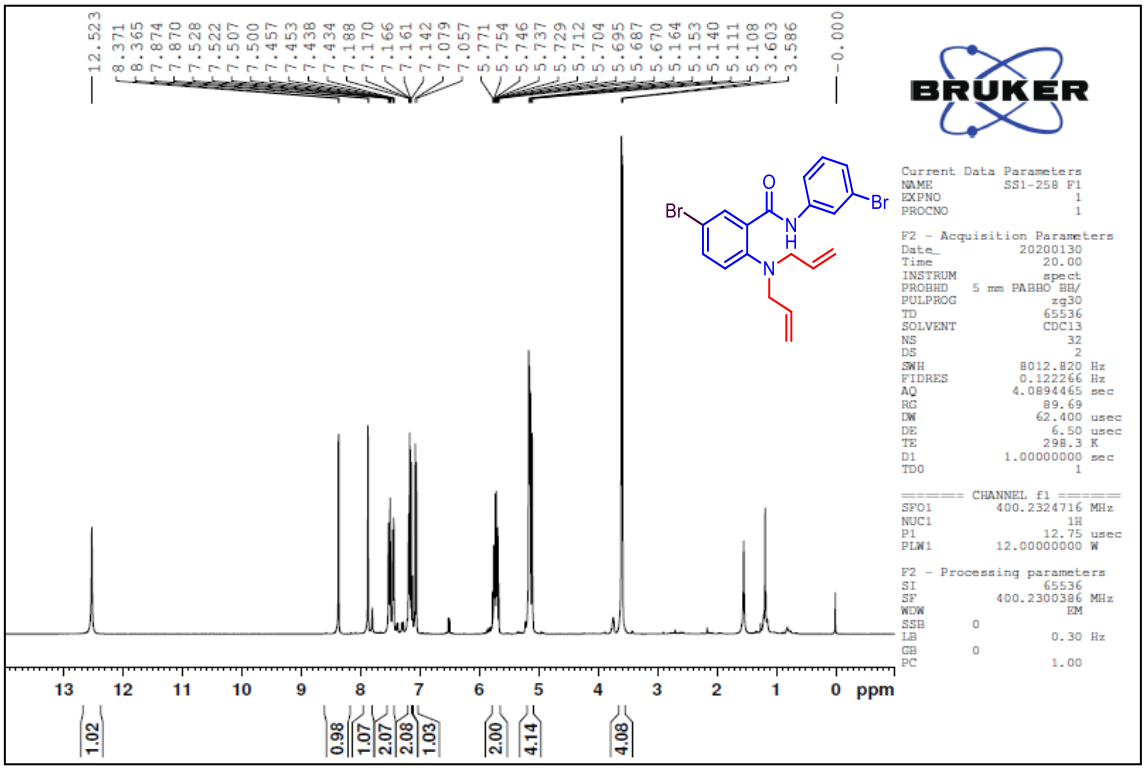


Figure 66. ^{1}H NMR spectrum of compound **3j**

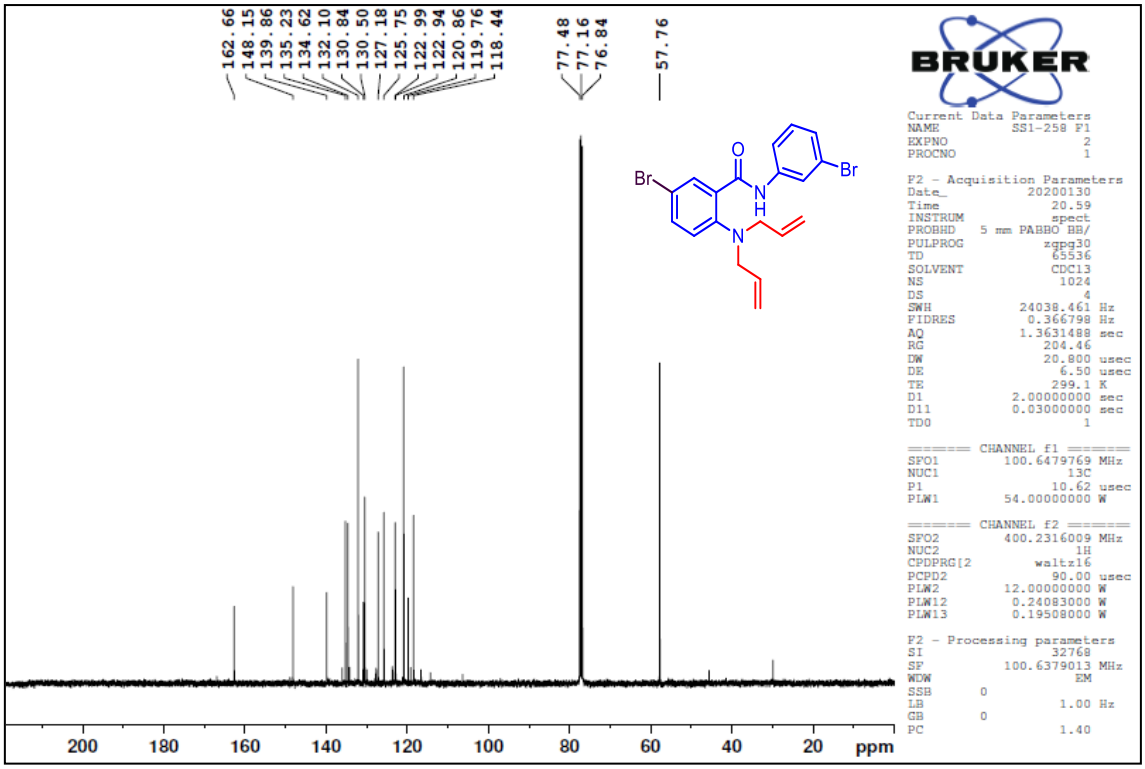


Figure 67. ^{13}C NMR spectrum of compound **3j**

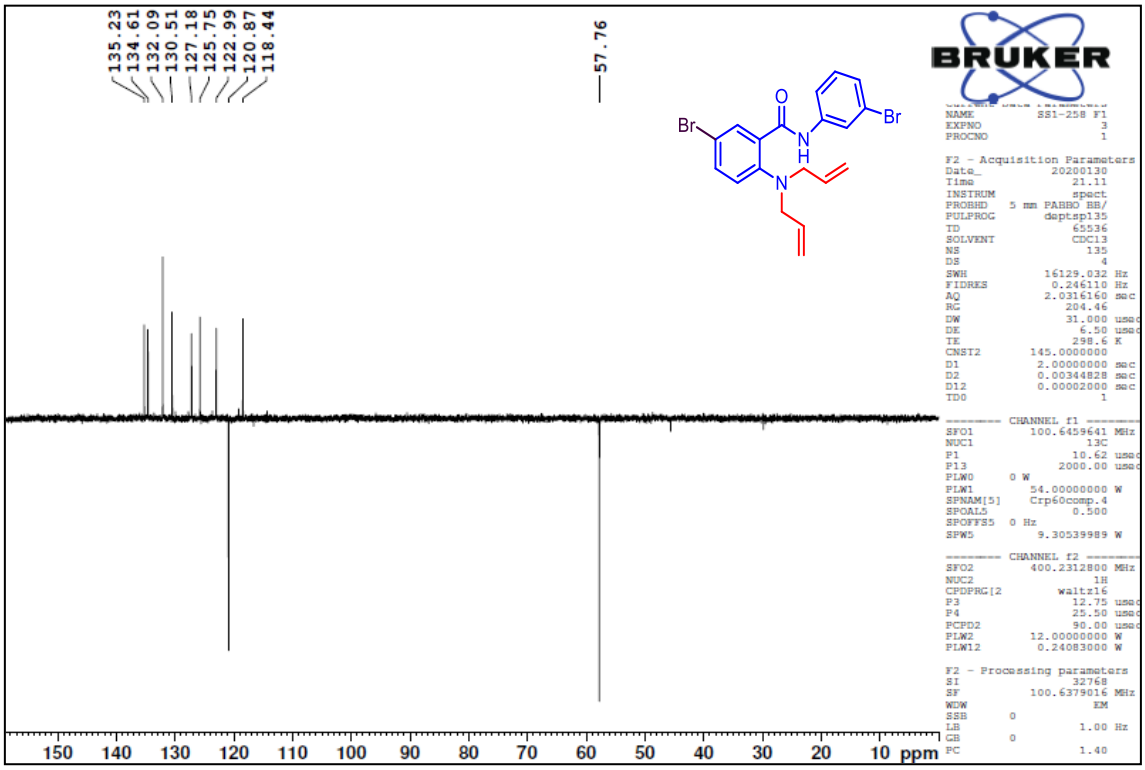


Figure 68. DEPT-135 NMR spectrum of compound **3j**

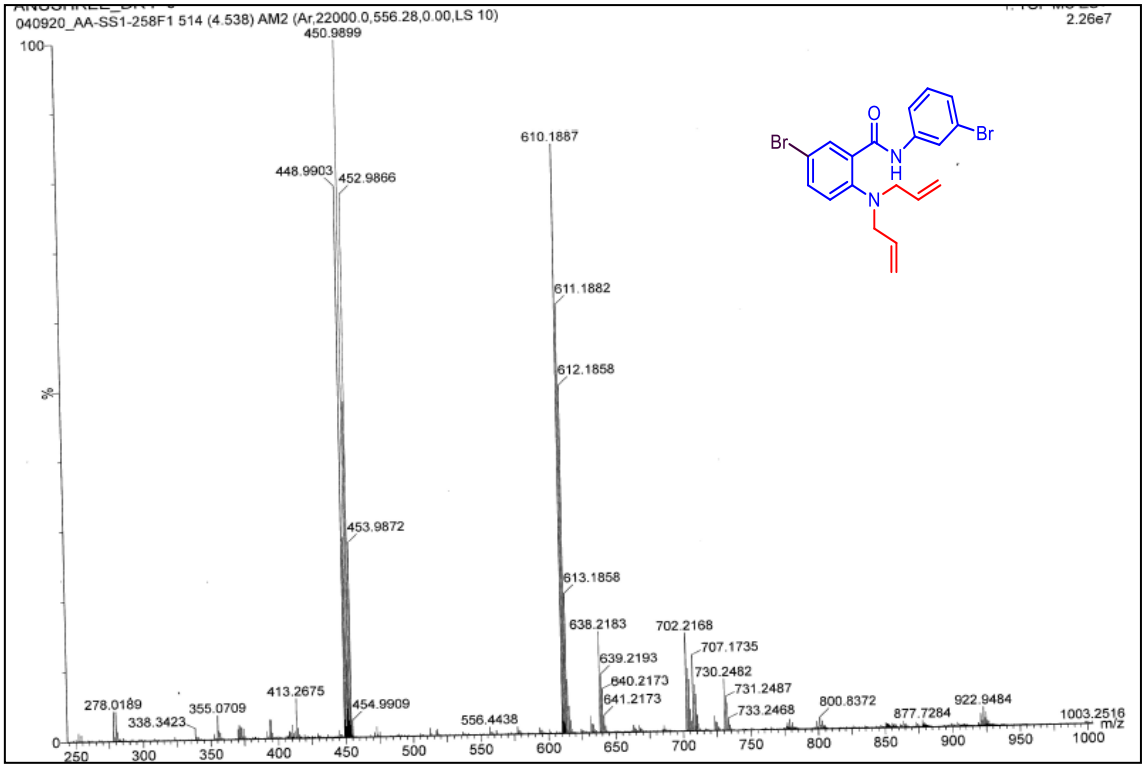


Figure 69. HRMS spectrum of compound **3j**

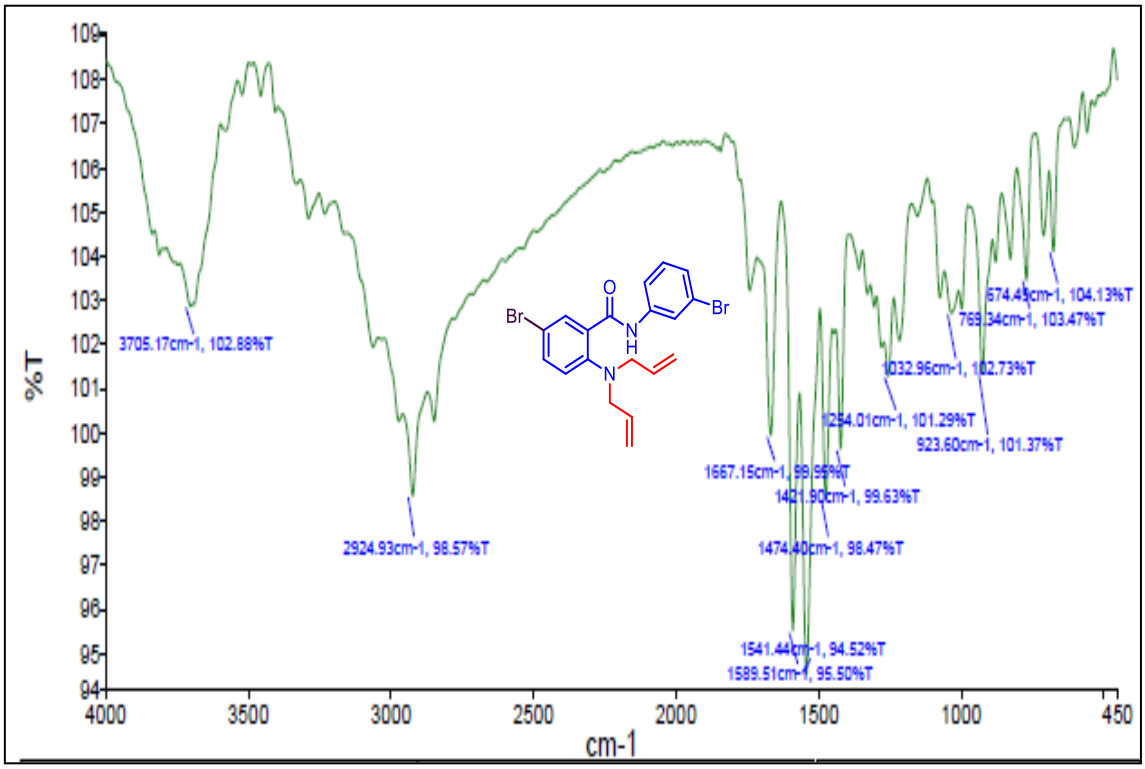


Figure 70. FTIR spectrum of compound **3j**

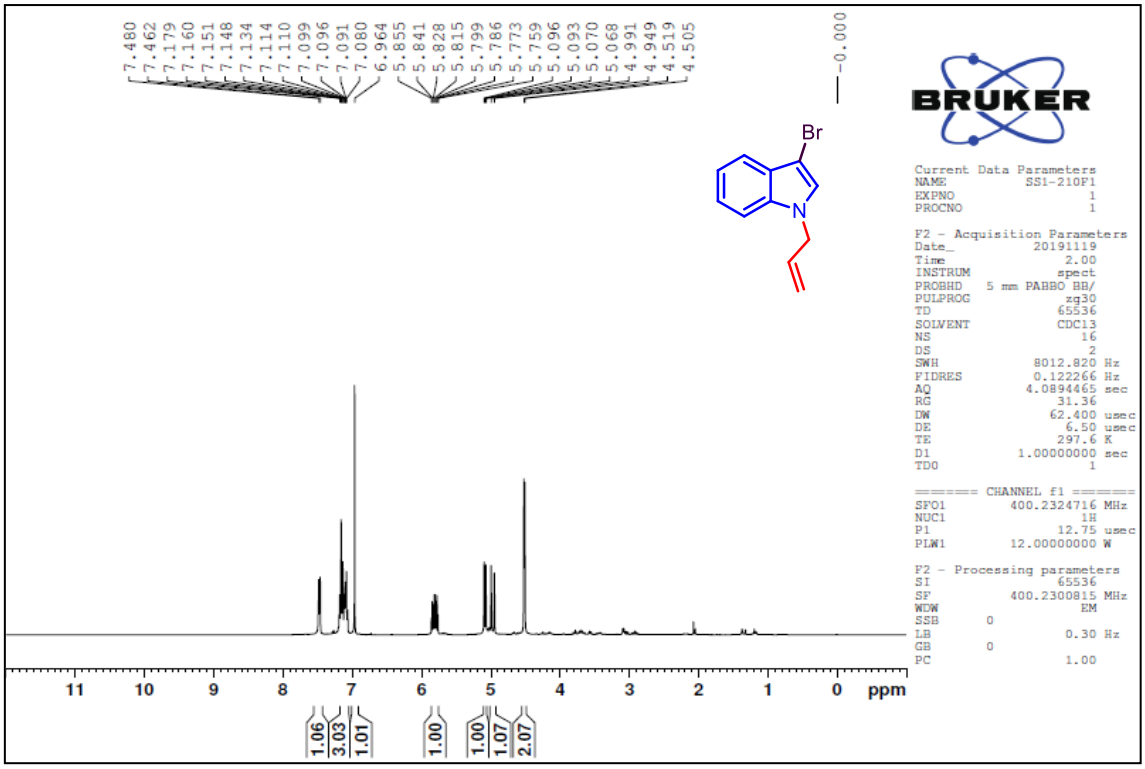


Figure 71.[1]H NMR spectrum of compound **3k**

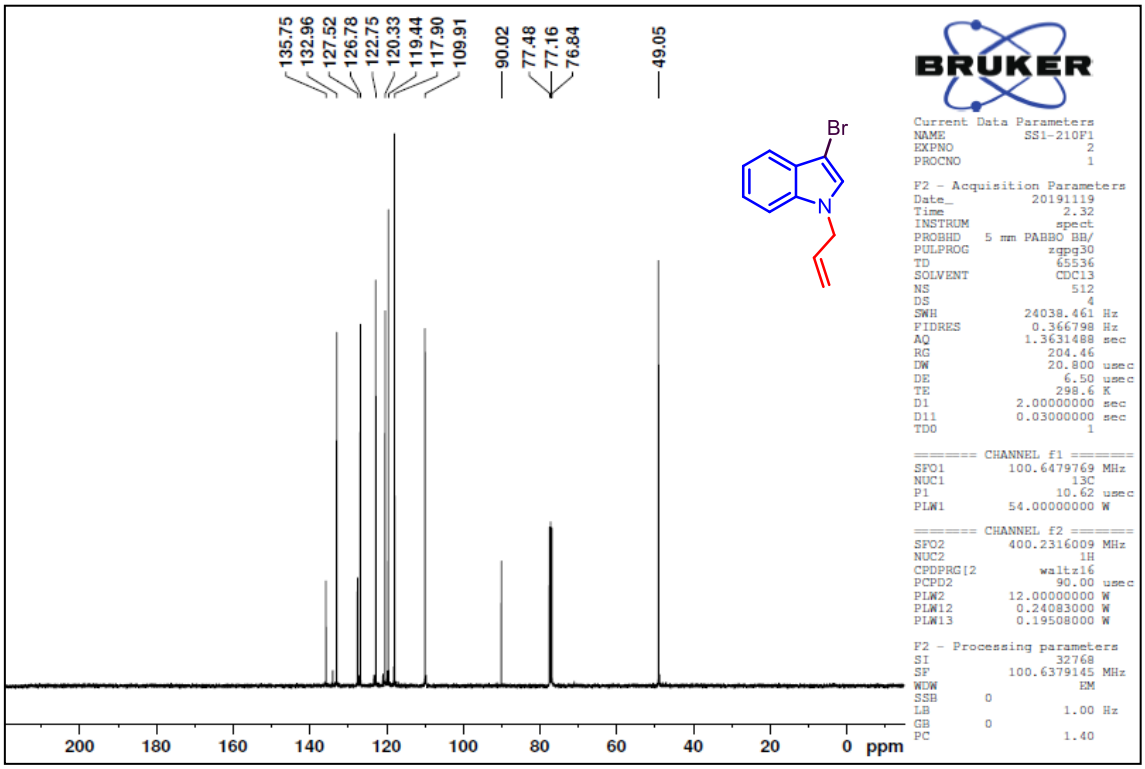


Figure 72.[13]C NMR spectrum of compound **3k**

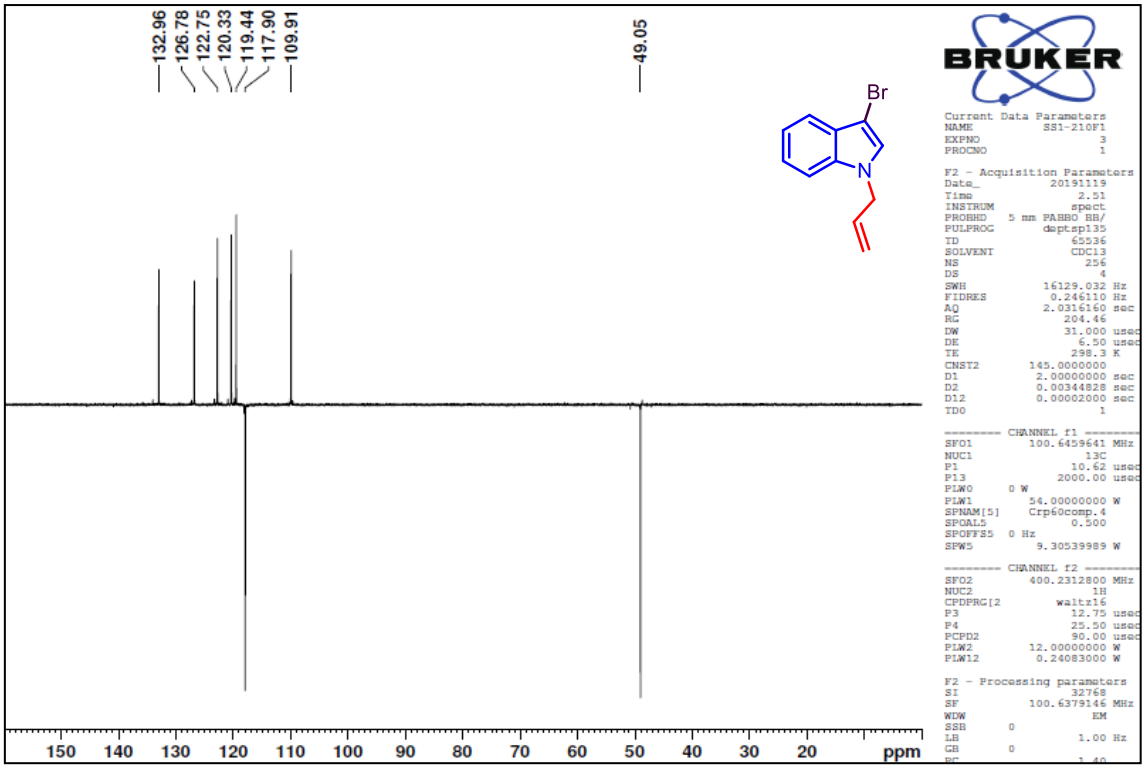


Figure 73. DEPT-135 NMR spectrum of compound **3k**

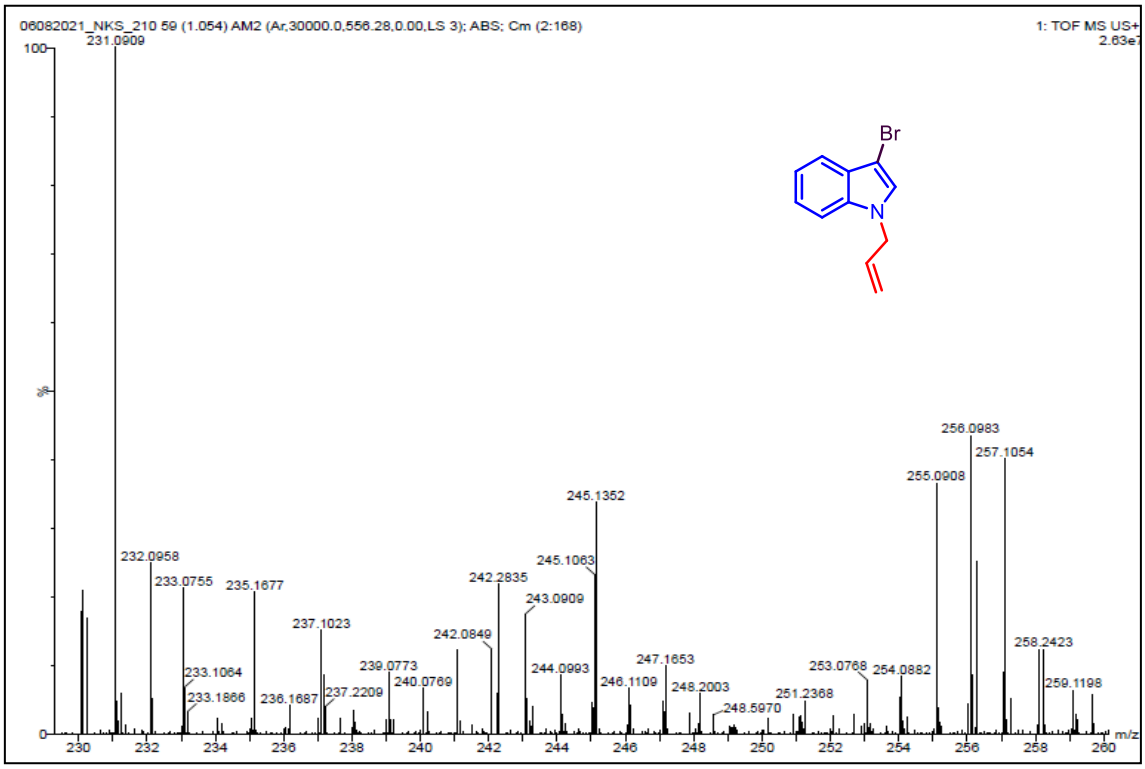


Figure 74. HRMS spectrum of compound **3k**

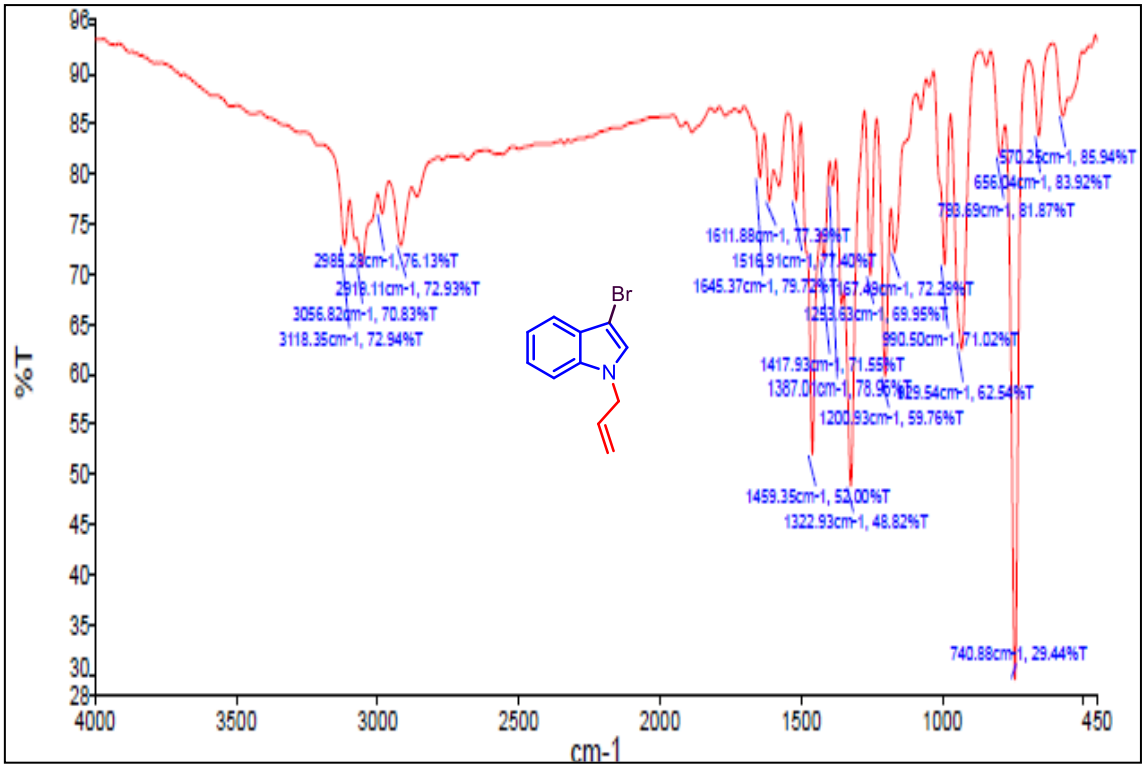


Figure 75. FTIR spectrum of compound **3k**

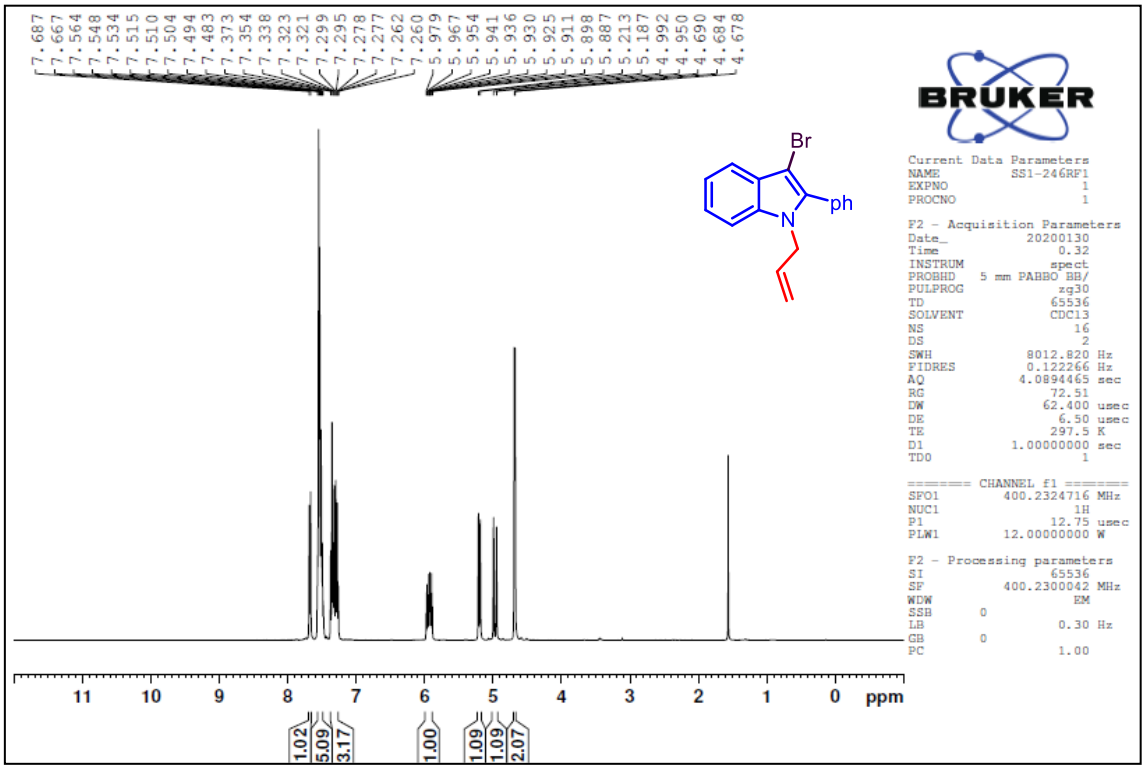


Figure 76. ^{1}H NMR spectrum of compound **3l**

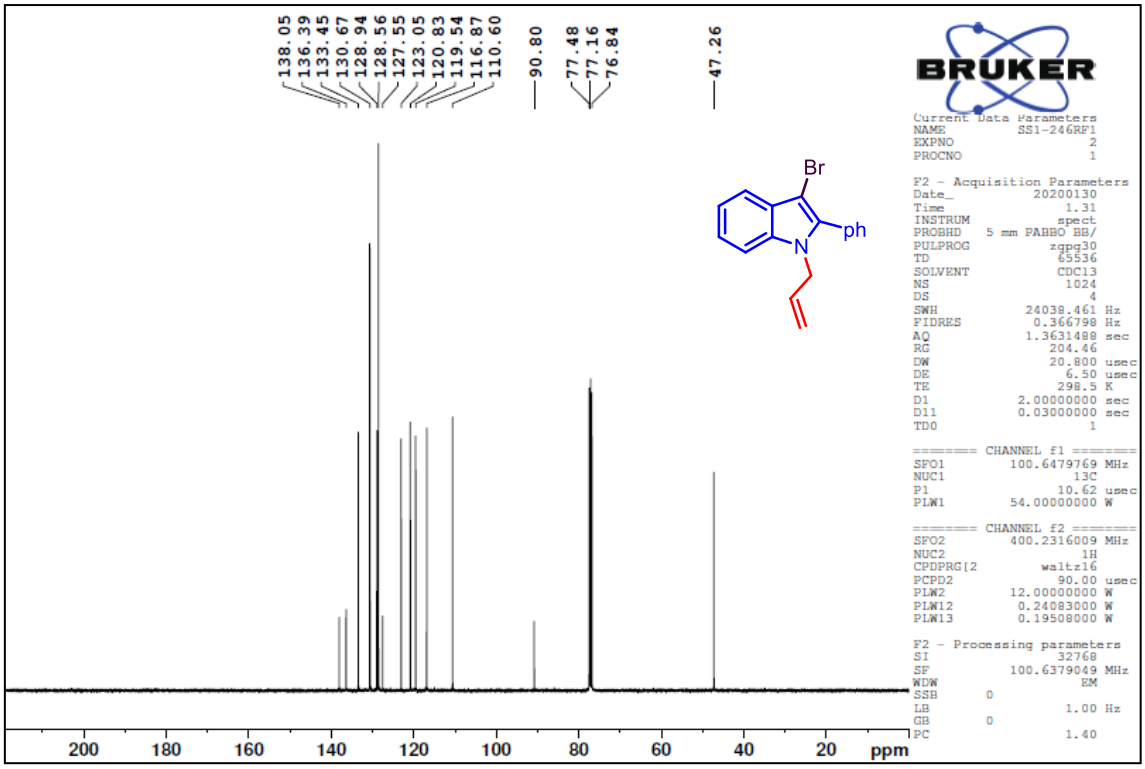


Figure 77. ^{13}C NMR spectrum of compound **3l**

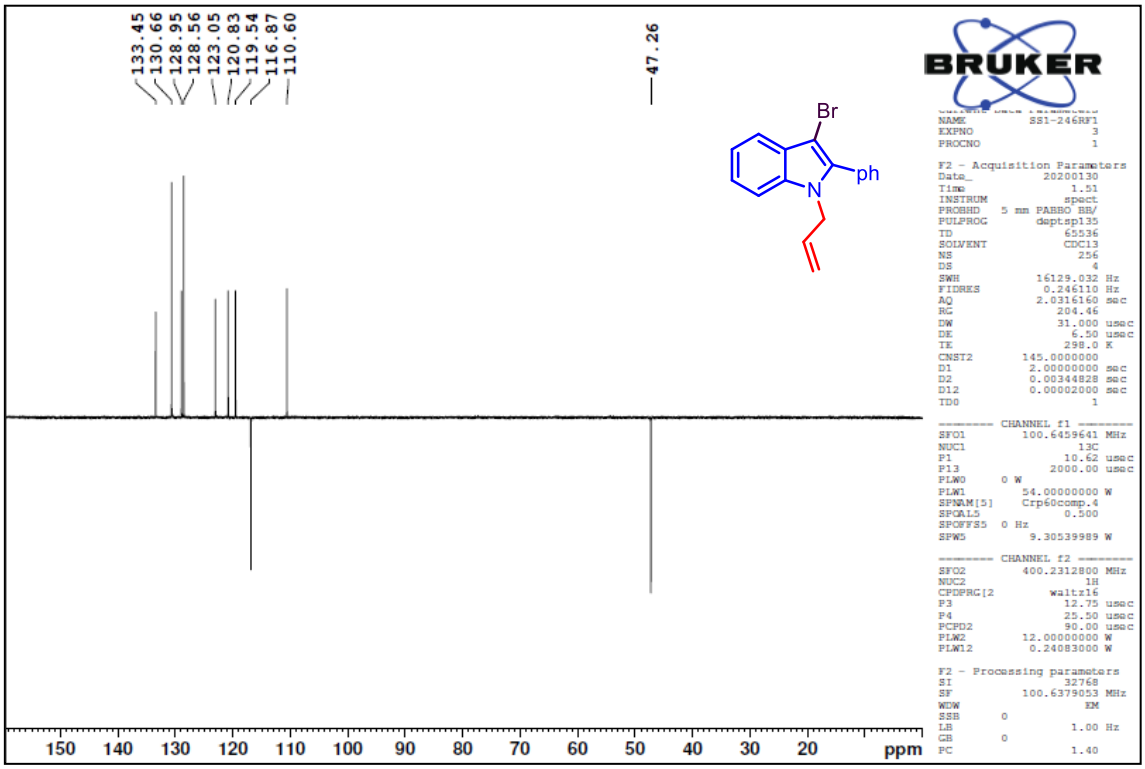


Figure 78. DEPT-135 NMR spectrum of compound **3l**

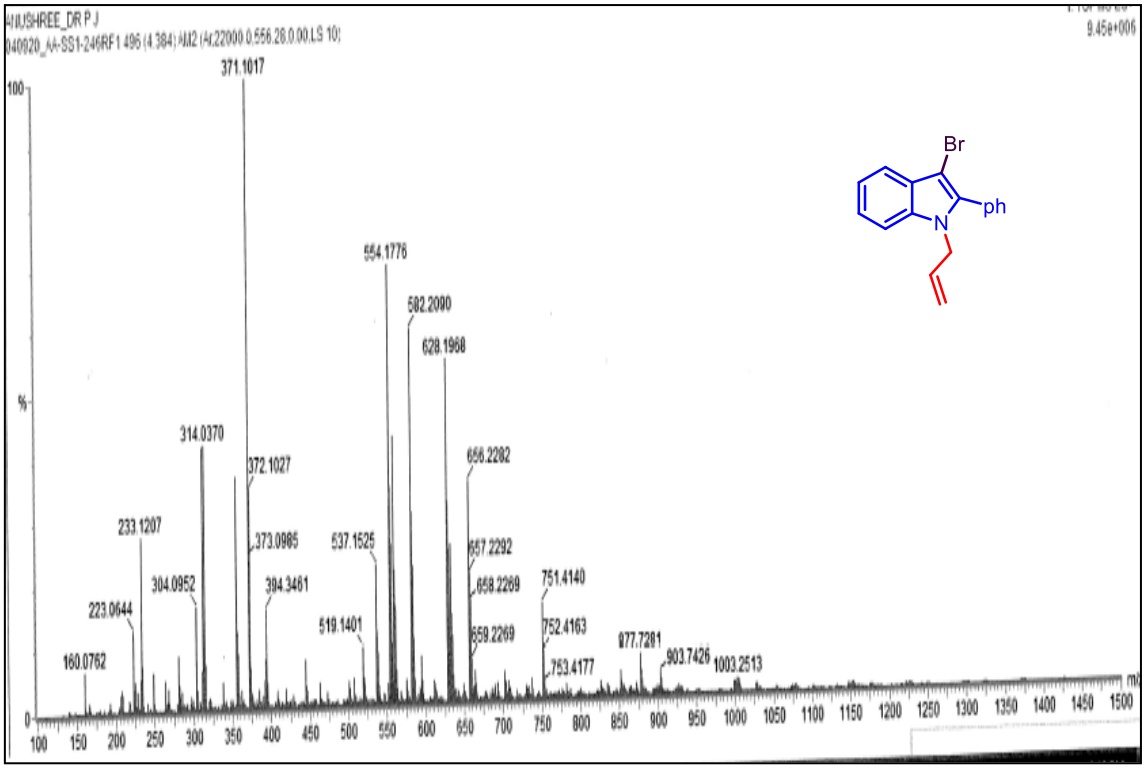


Figure 79. HRMS spectrum of compound **3l**

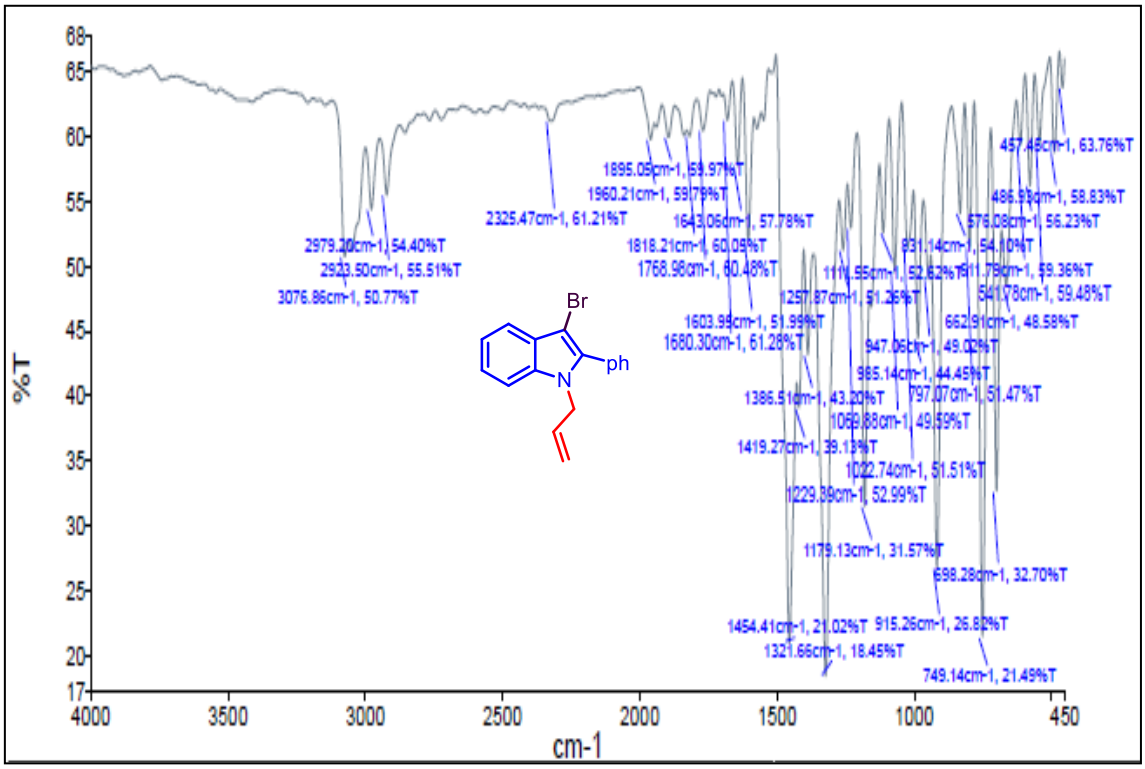


Figure 80. FTIR spectrum of compound **3l**

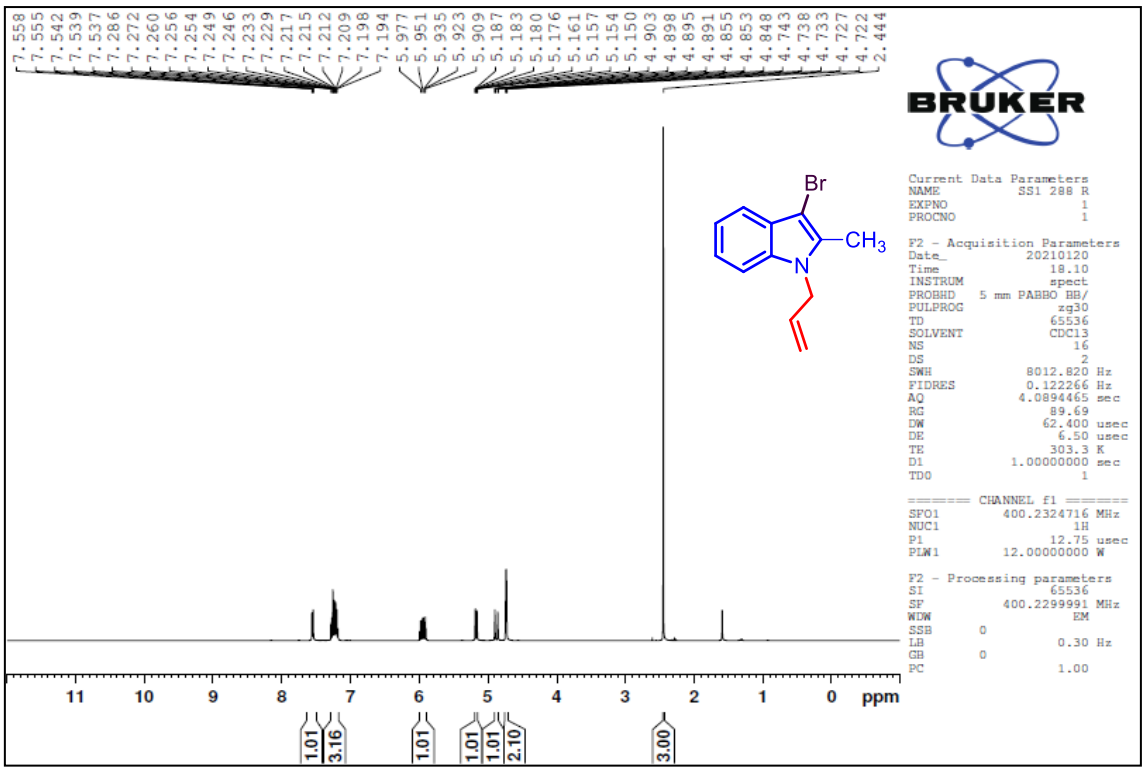


Figure 81.[1]H NMR spectrum of compound **3m**

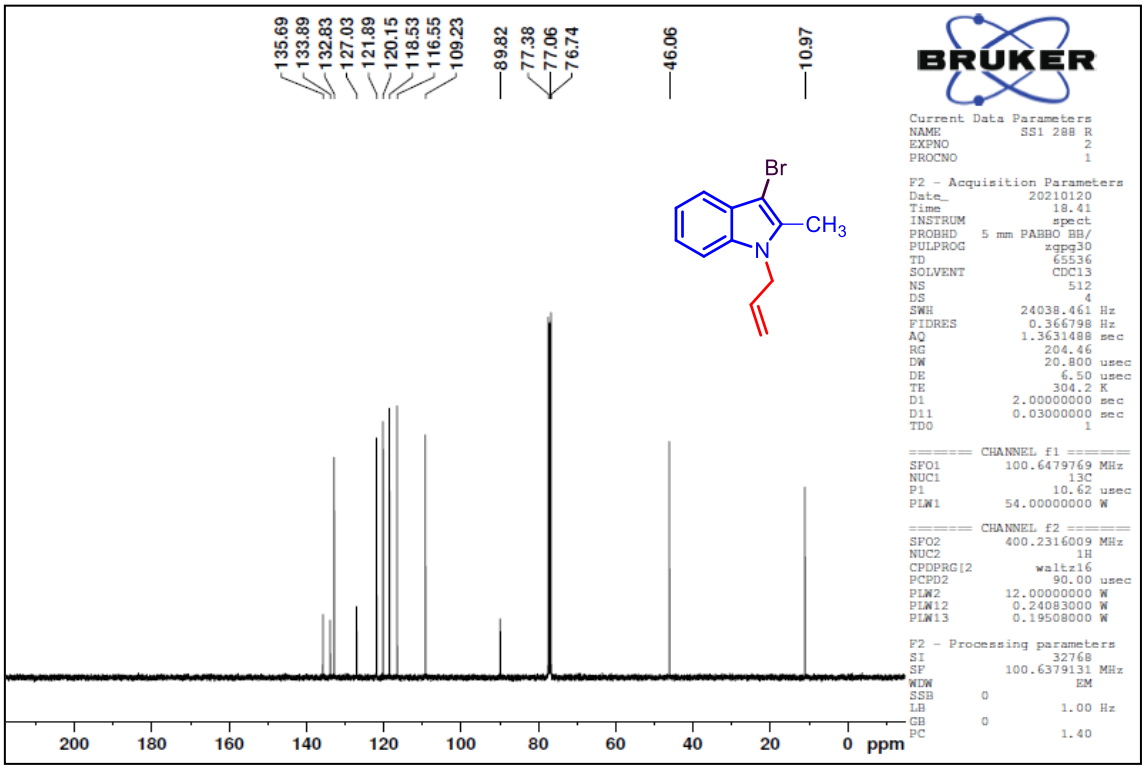


Figure 82.[13]CNMR spectrum of compound **3m**

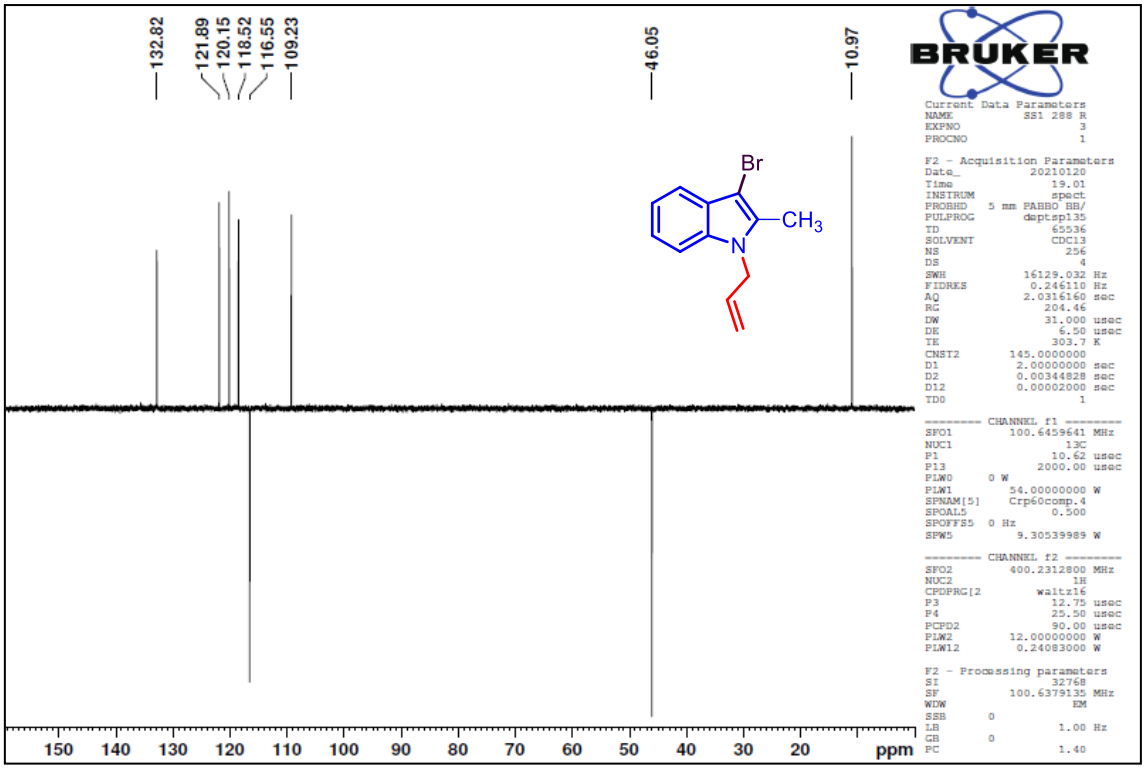


Figure 83. DEPT-135 NMR spectrum of compound **3m**

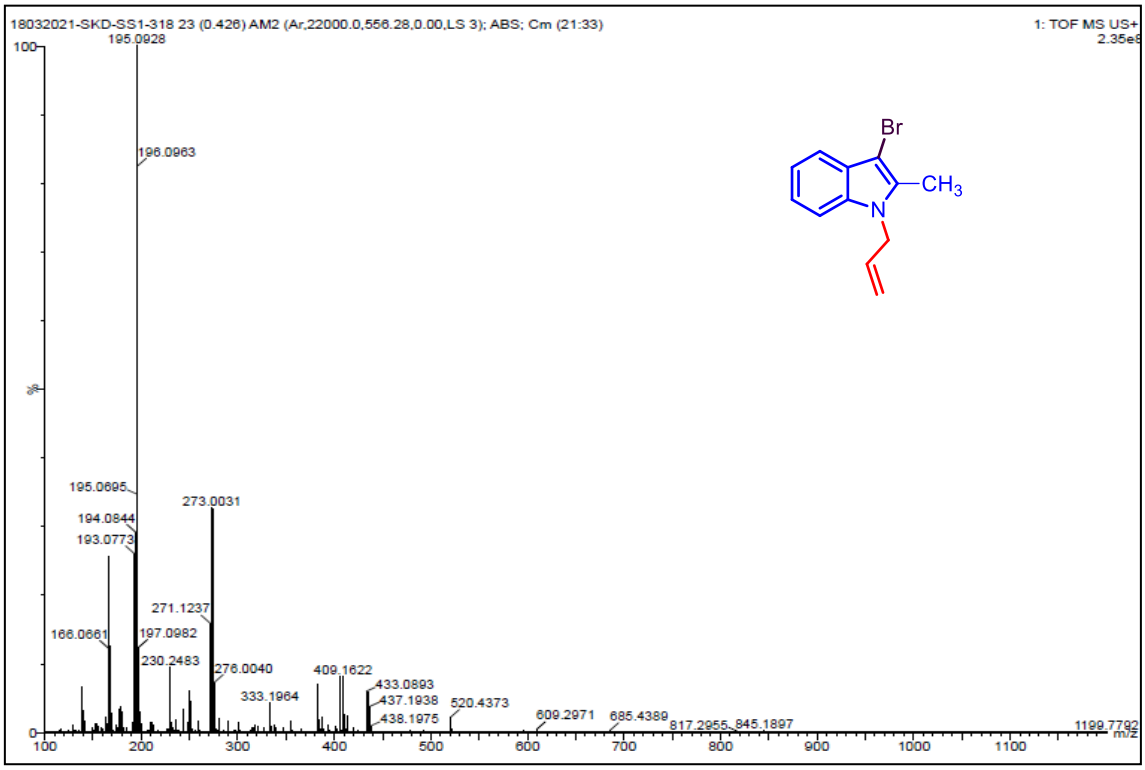


Figure 84. HRMS spectrum of compound **3m**

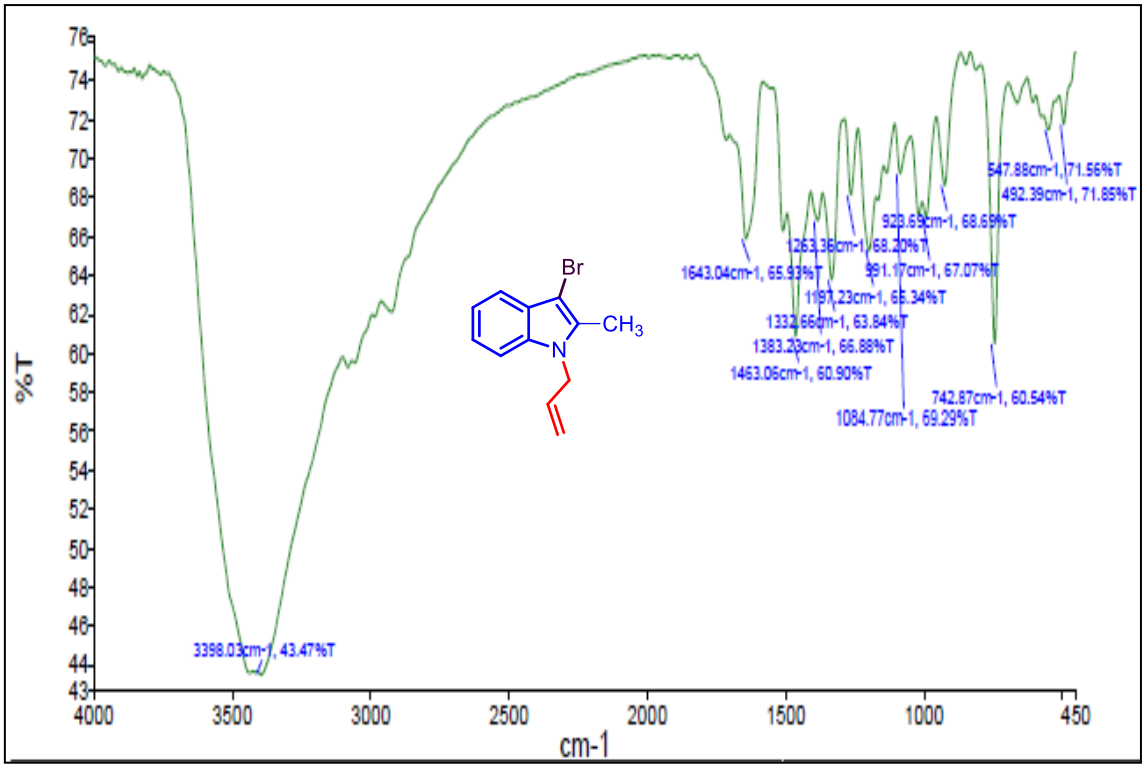


Figure 85. FTIR spectrum of compound **3m**

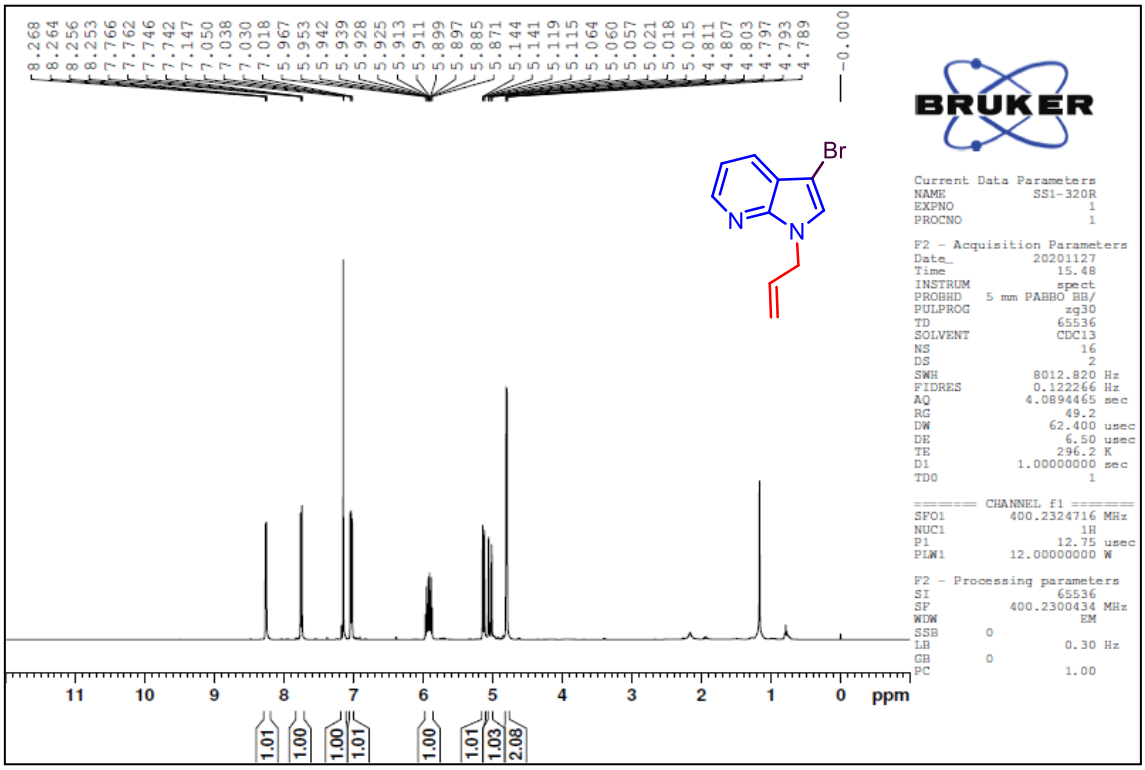


Figure 86. ^{1}H NMR spectrum of compound **3n**

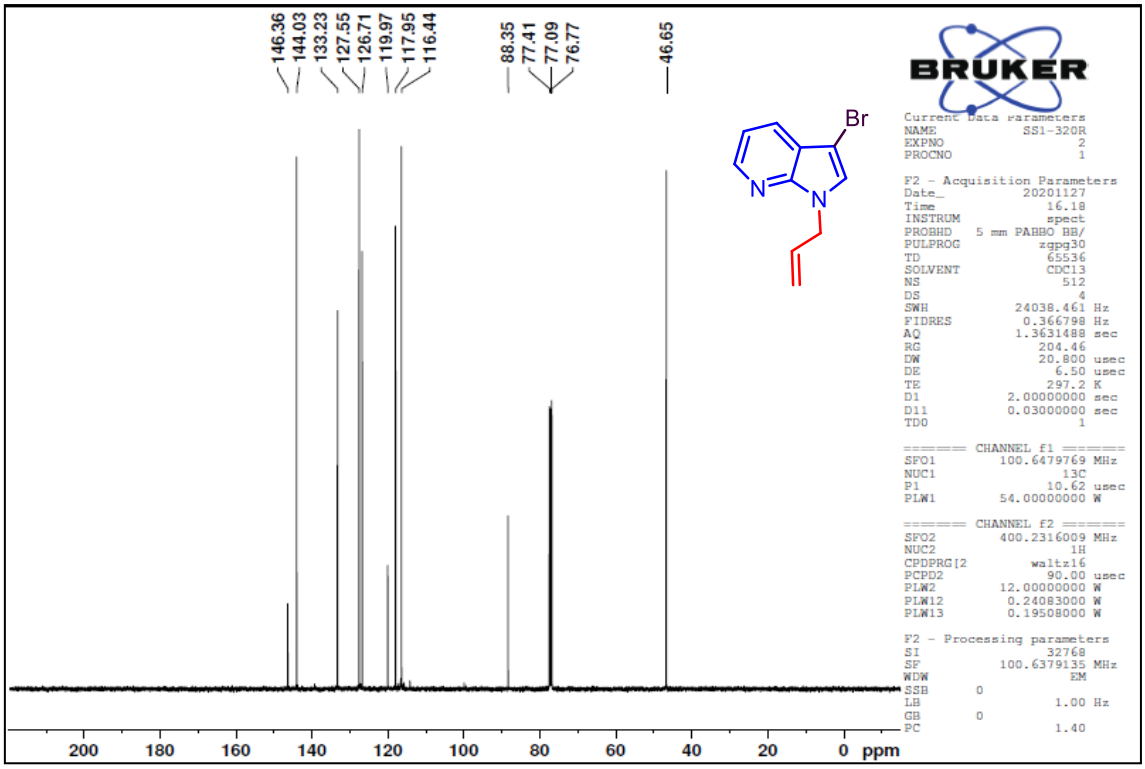


Figure 87. ^{13}C NMR spectrum of compound **3n**

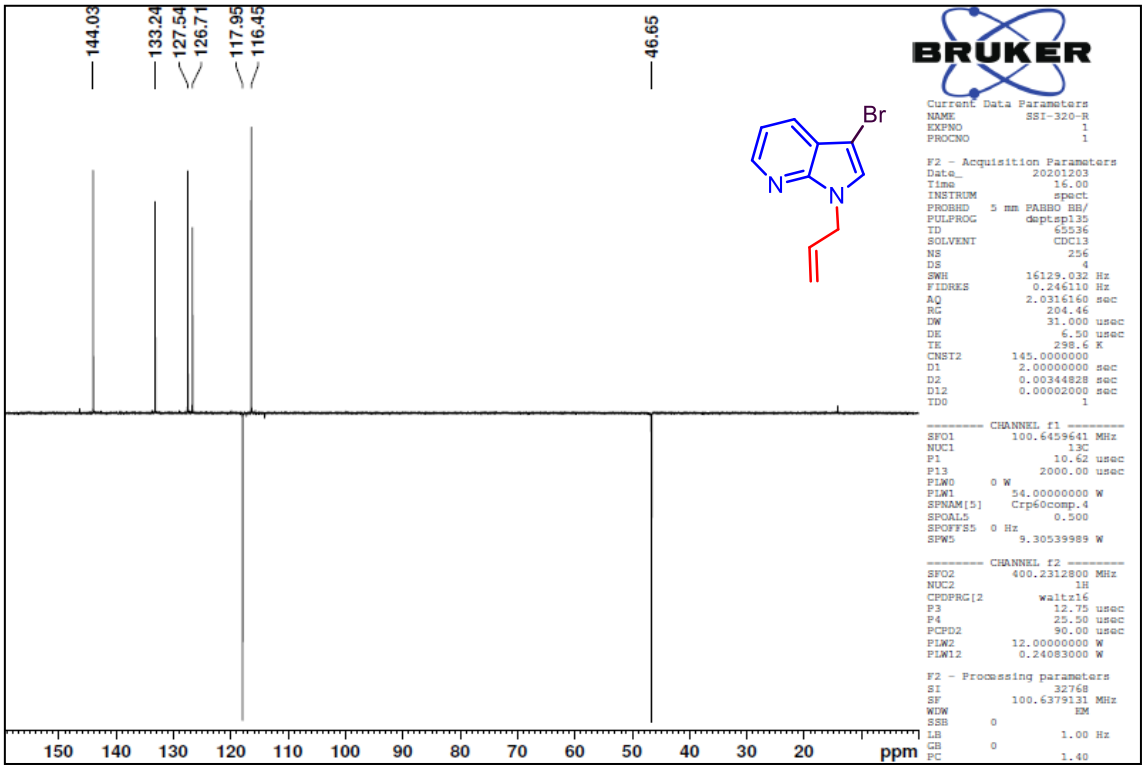


Figure 88. DEPT-135 NMR spectrum of compound **3n**

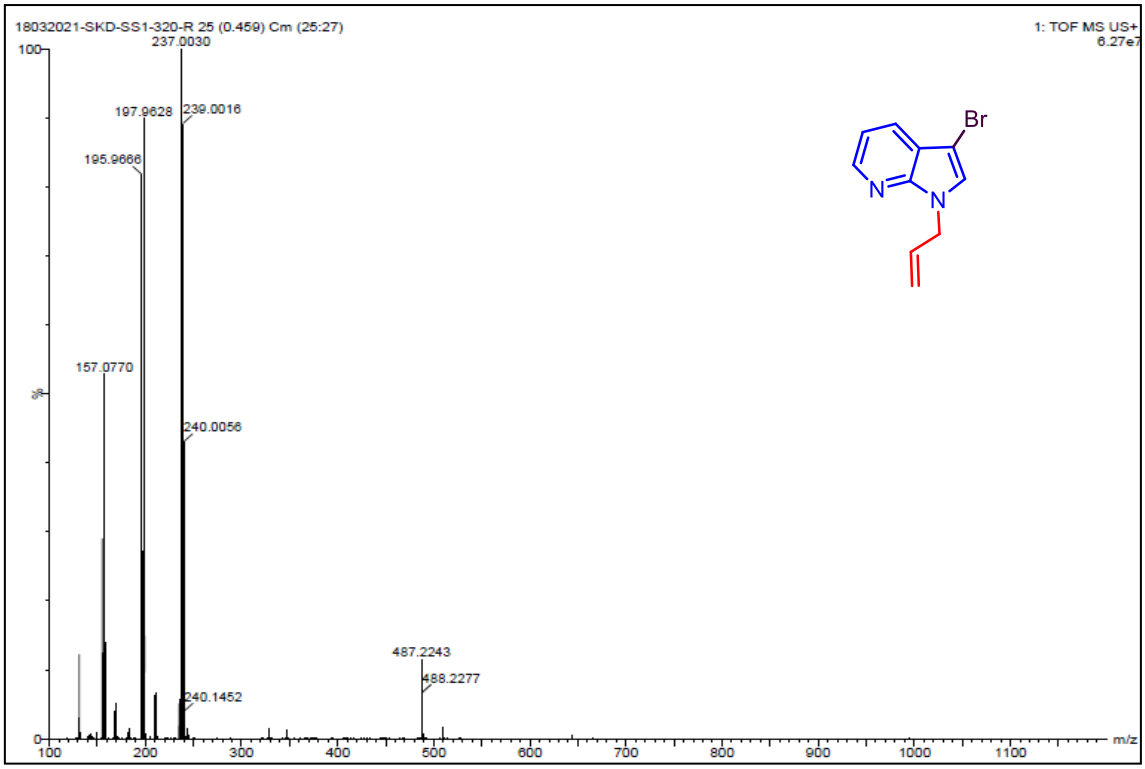


Figure 89. HRMS spectrum of compound **3n**

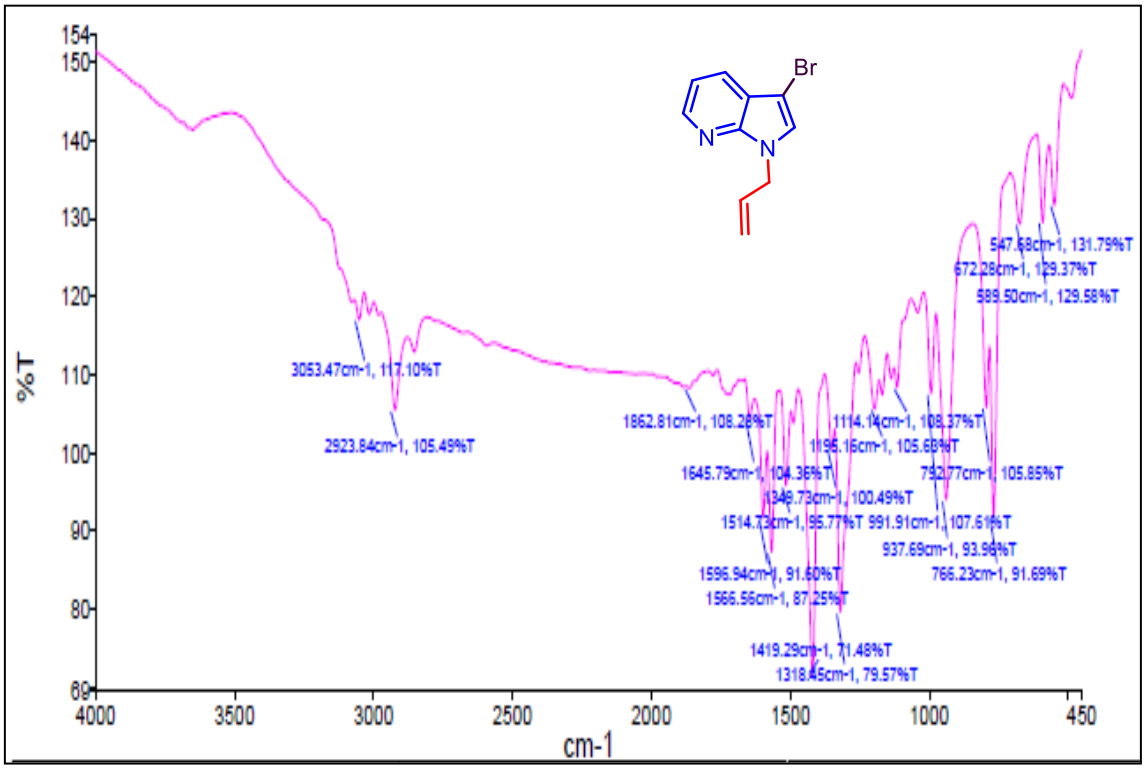


Figure 90. FTIR spectrum of compound **3n**

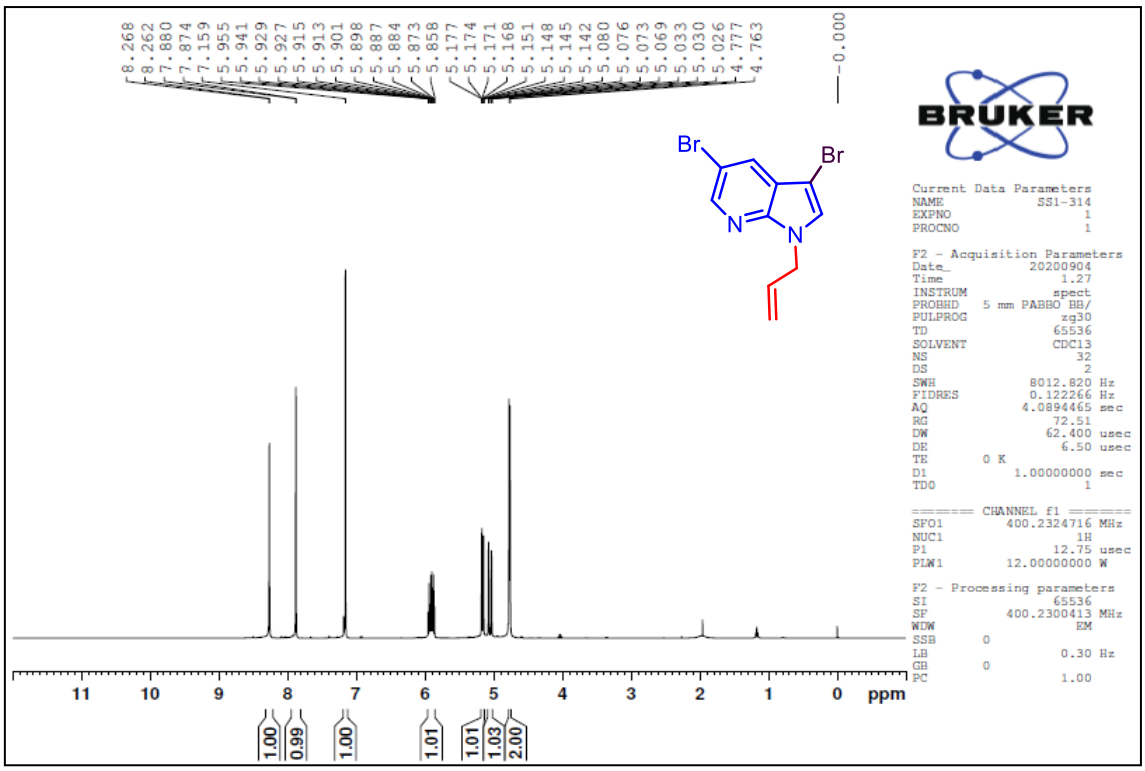


Figure 91.[1]H NMR spectrum of compound **3o**

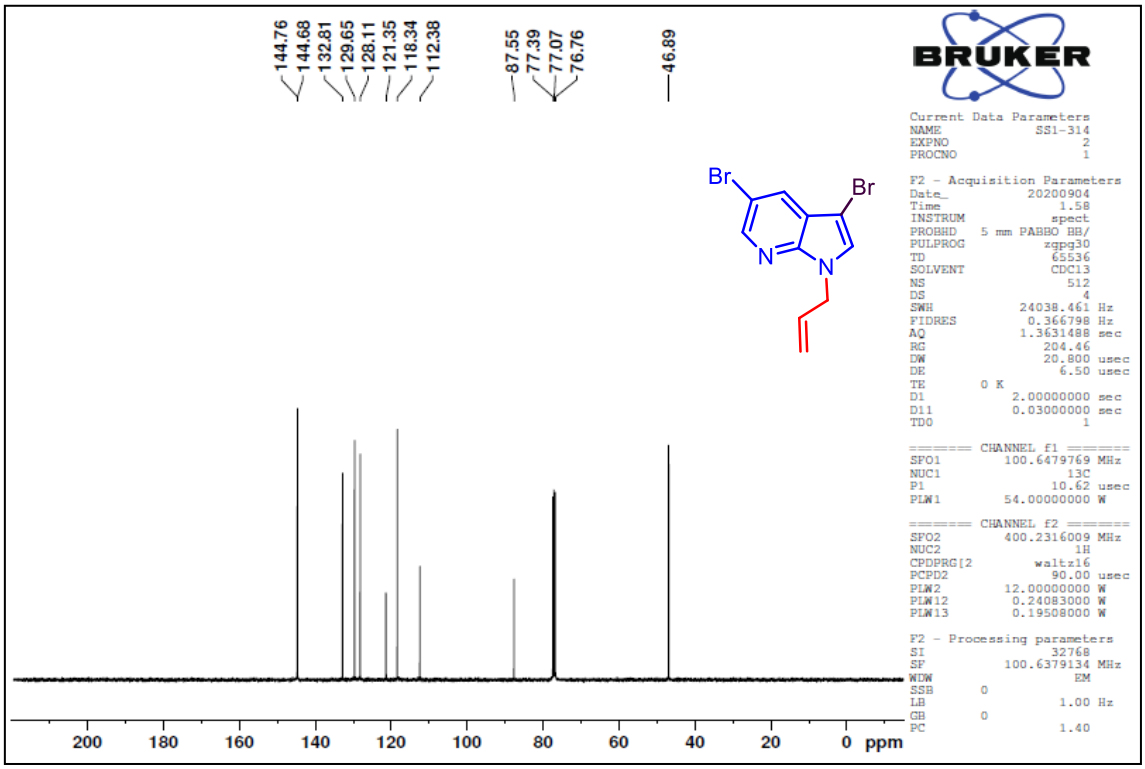


Figure 92. [13]C NMR spectrum of compound **3o**

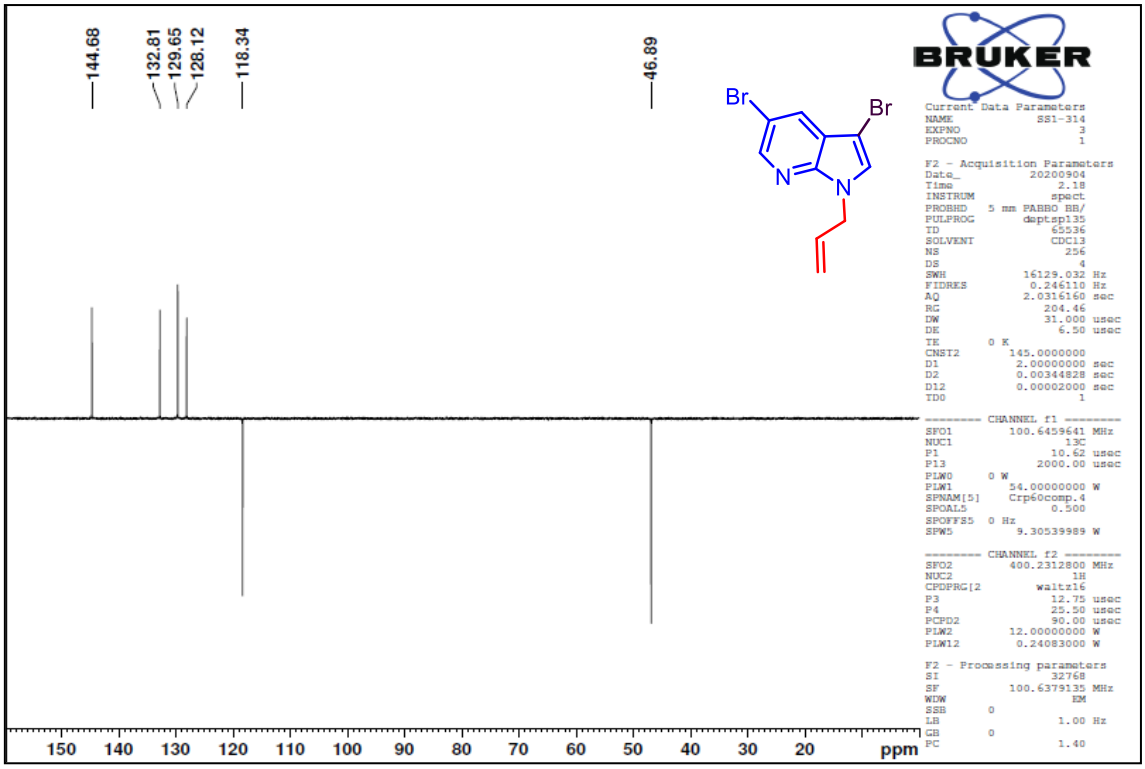


Figure 93. DEPT-135 NMR spectrum of compound **3o**

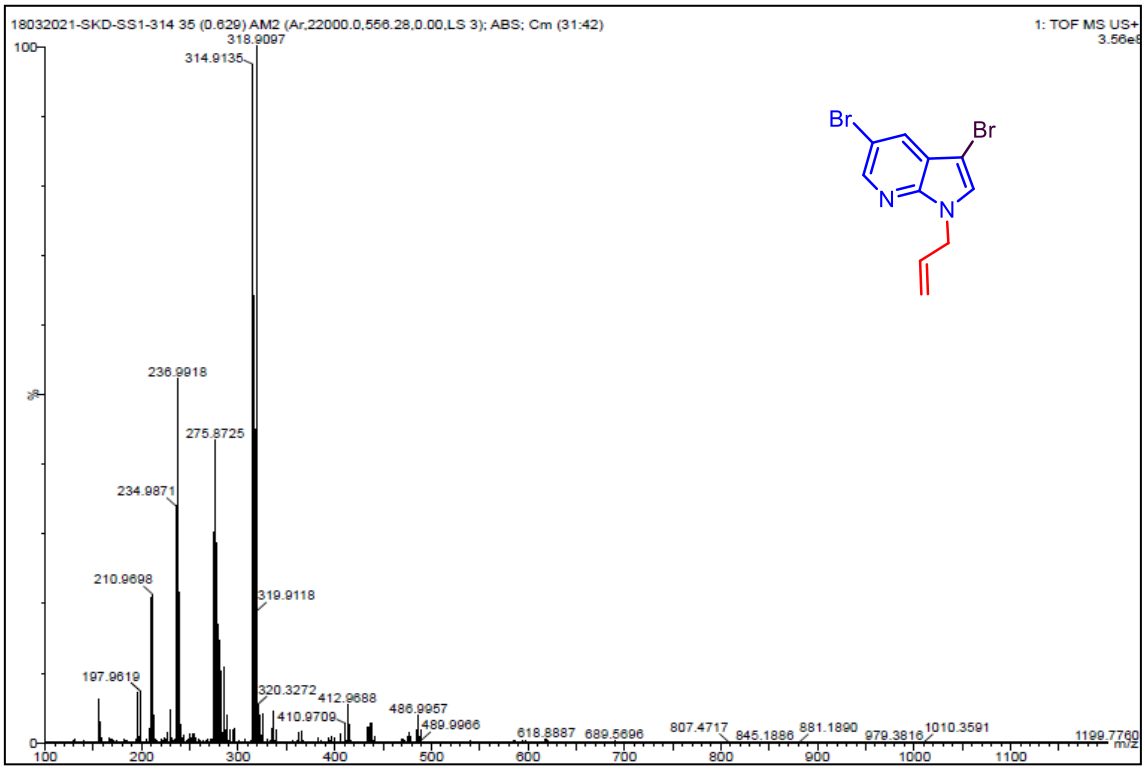


Figure 94. HRMS spectrum of compound **3o**

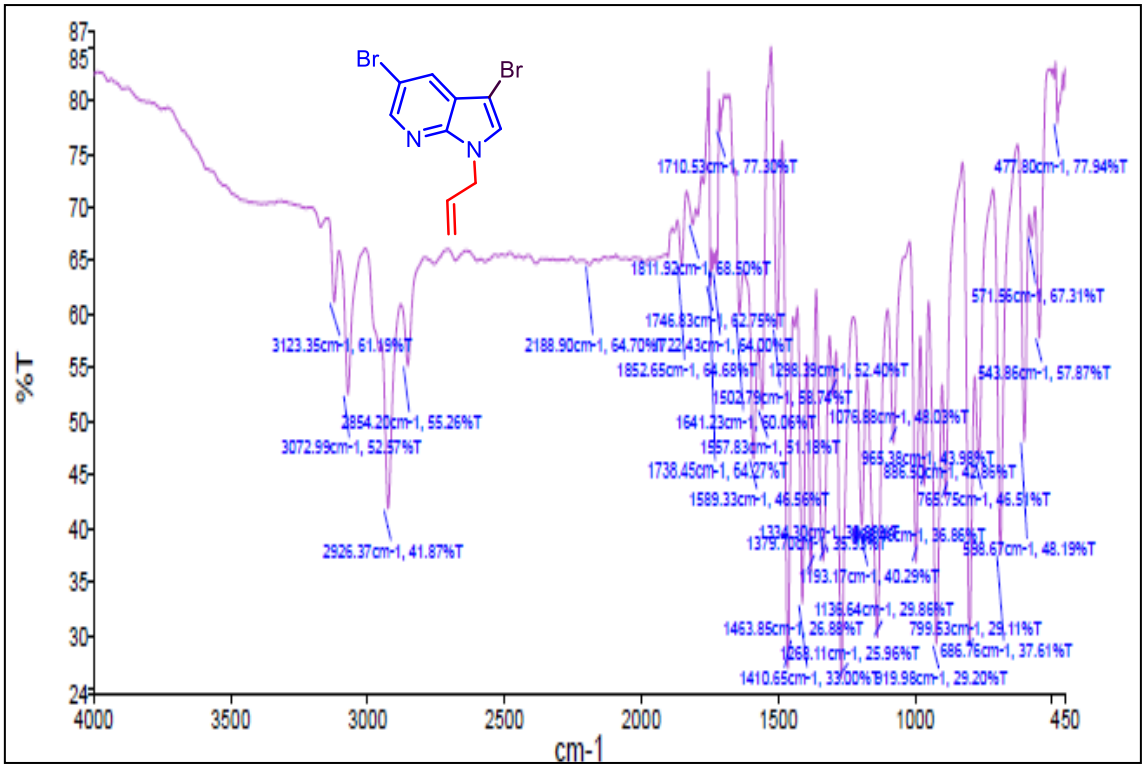


Figure 95. FTIR spectrum of compound **3o**

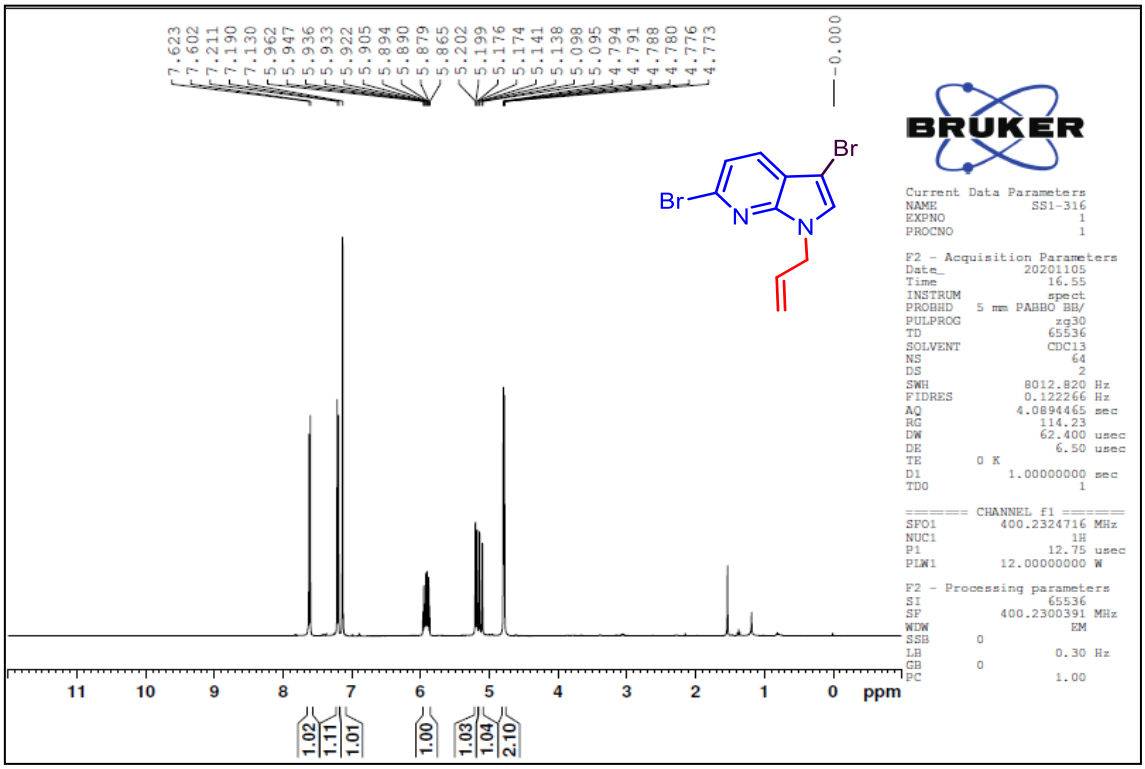


Figure 96. ^{1}H NMR spectrum of compound **3p**

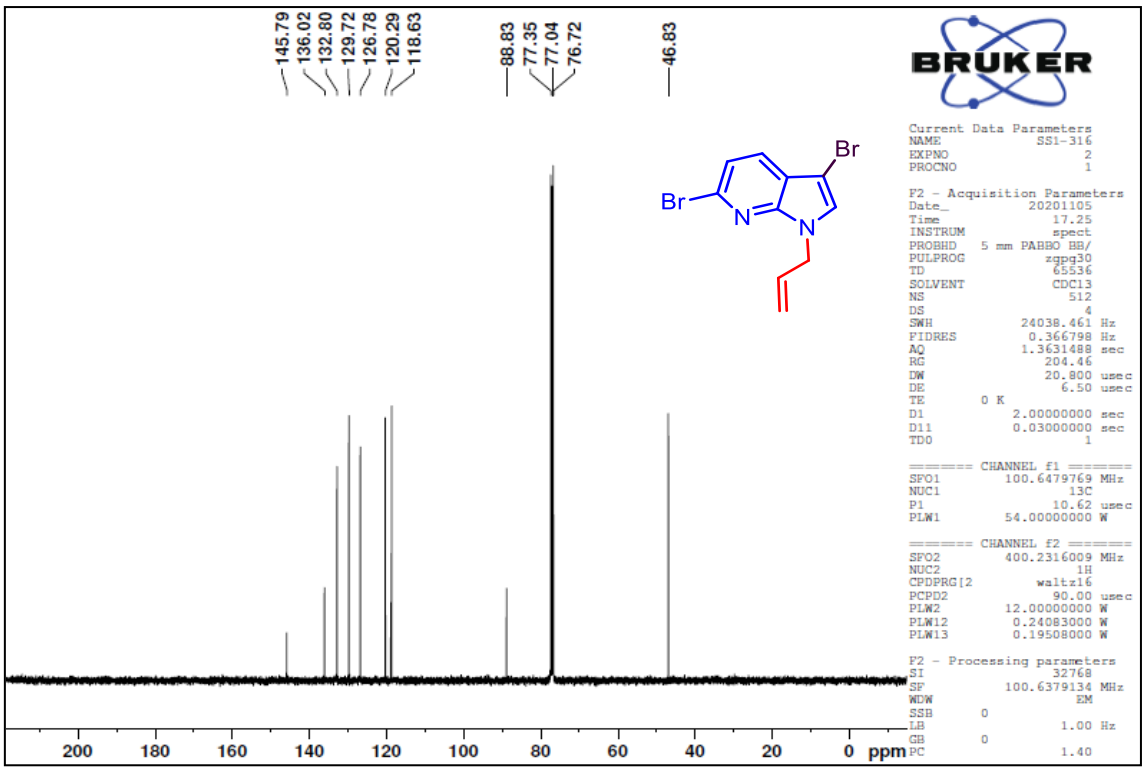


Figure 97. ^{13}C NMR spectrum of compound **3p**

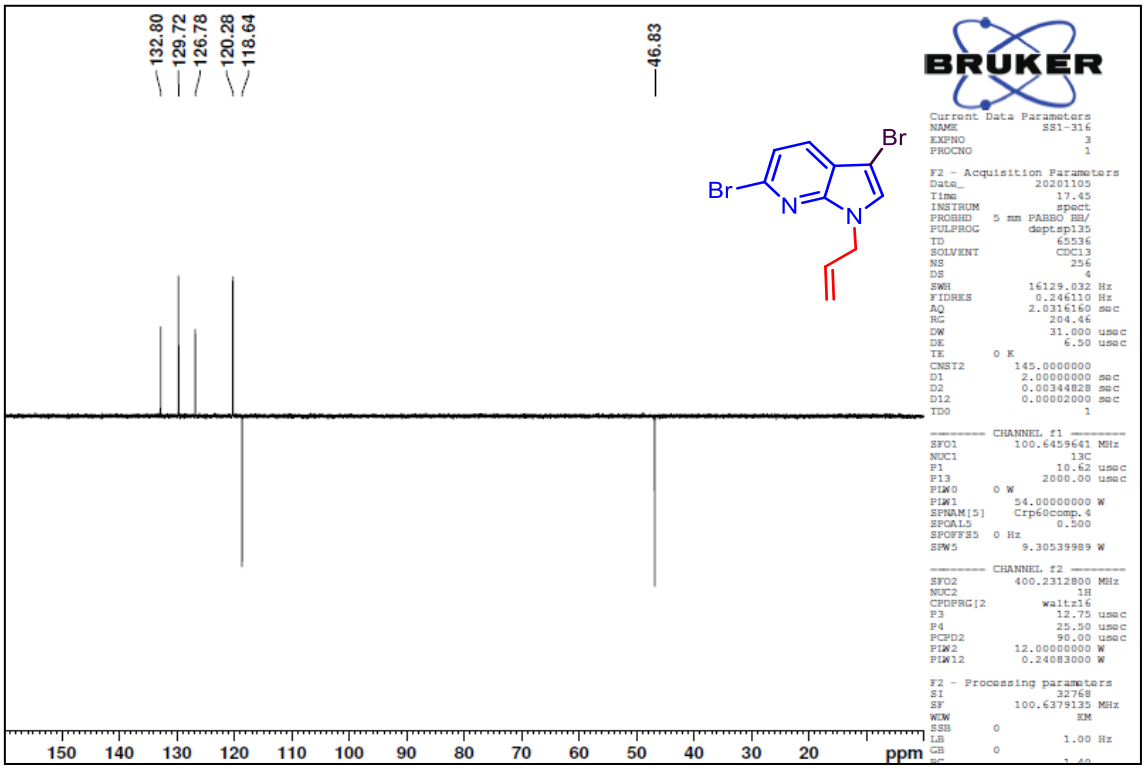


Figure 98. DEPT-135 NMR spectrum of compound **3p**

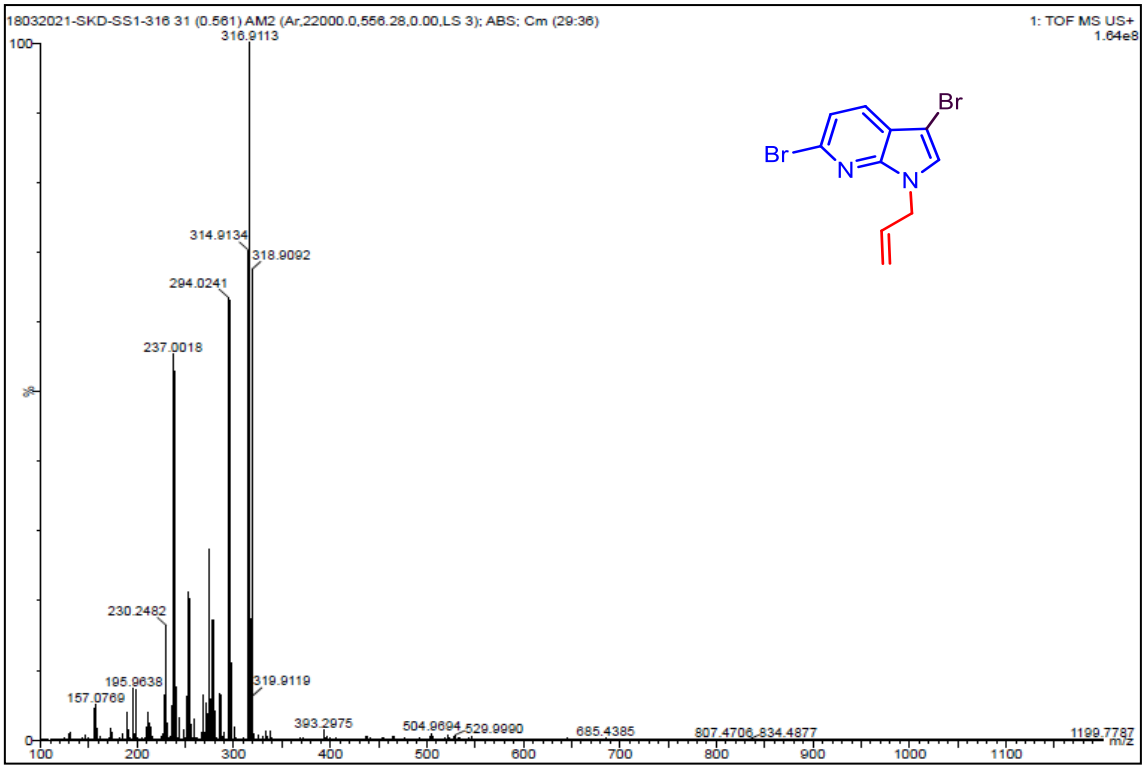


Figure 99. HRMS spectrum of compound **3p**

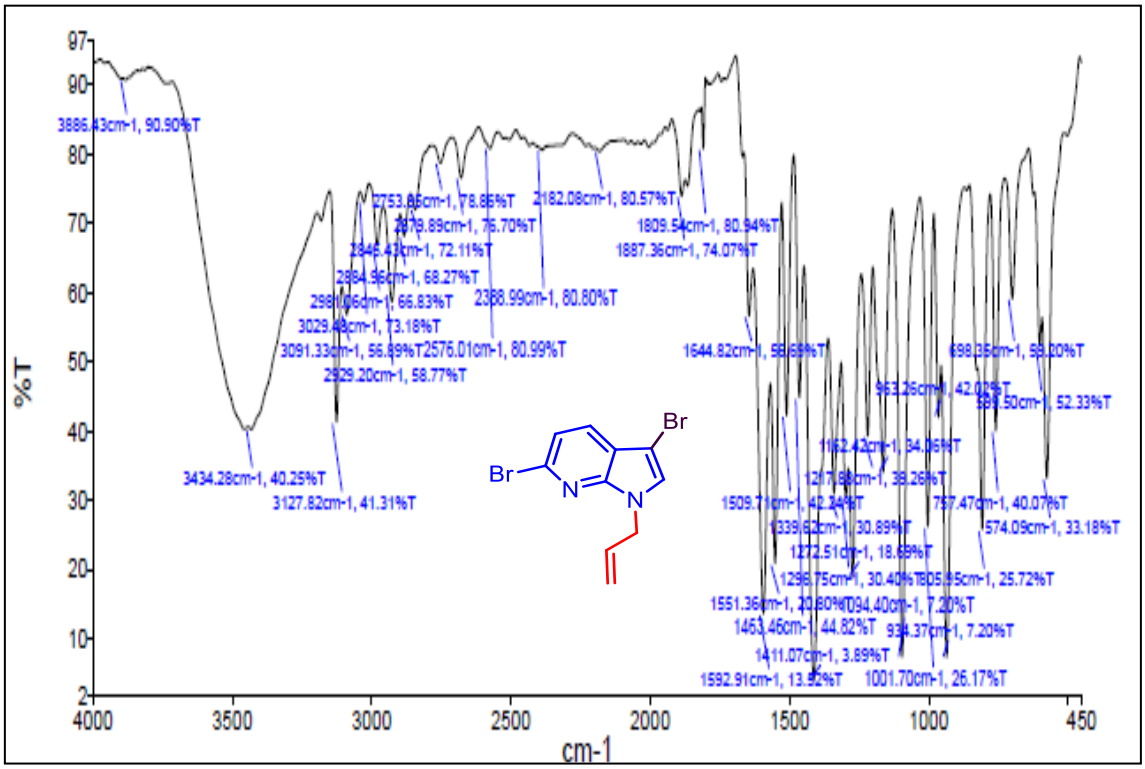


Figure 100. FTIR spectrum of compound **3p**

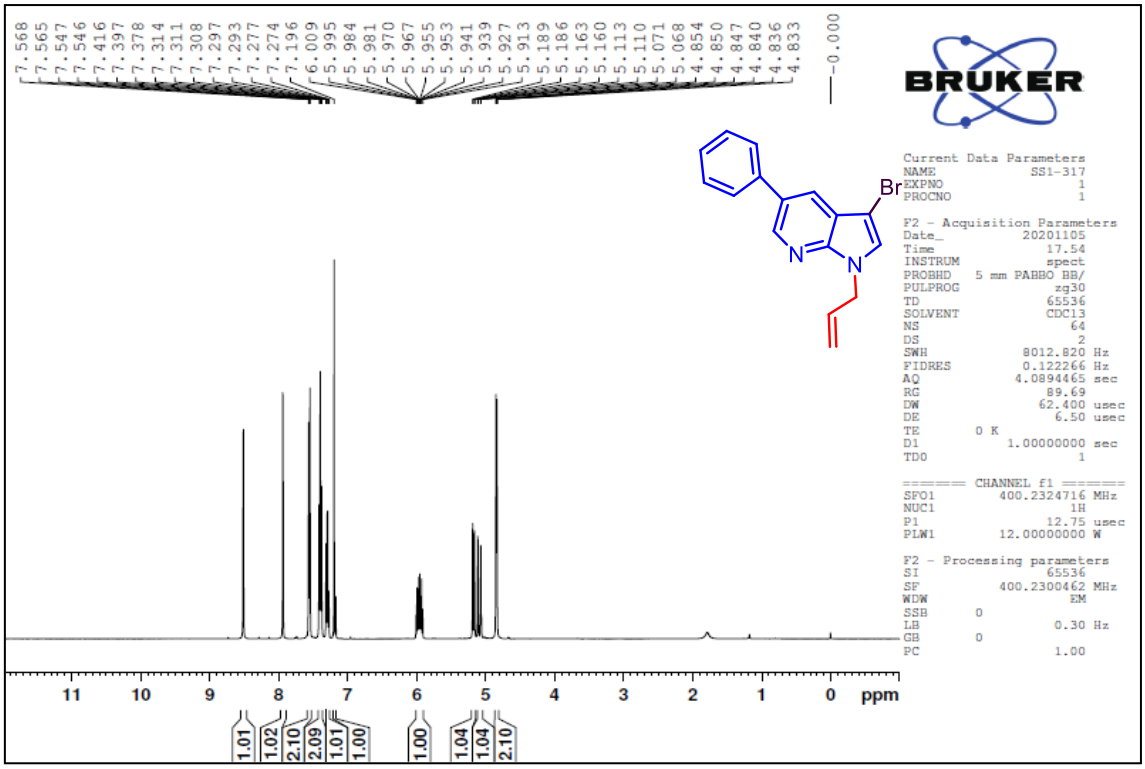


Figure 101.[1]H NMR spectrum of compound **3q**

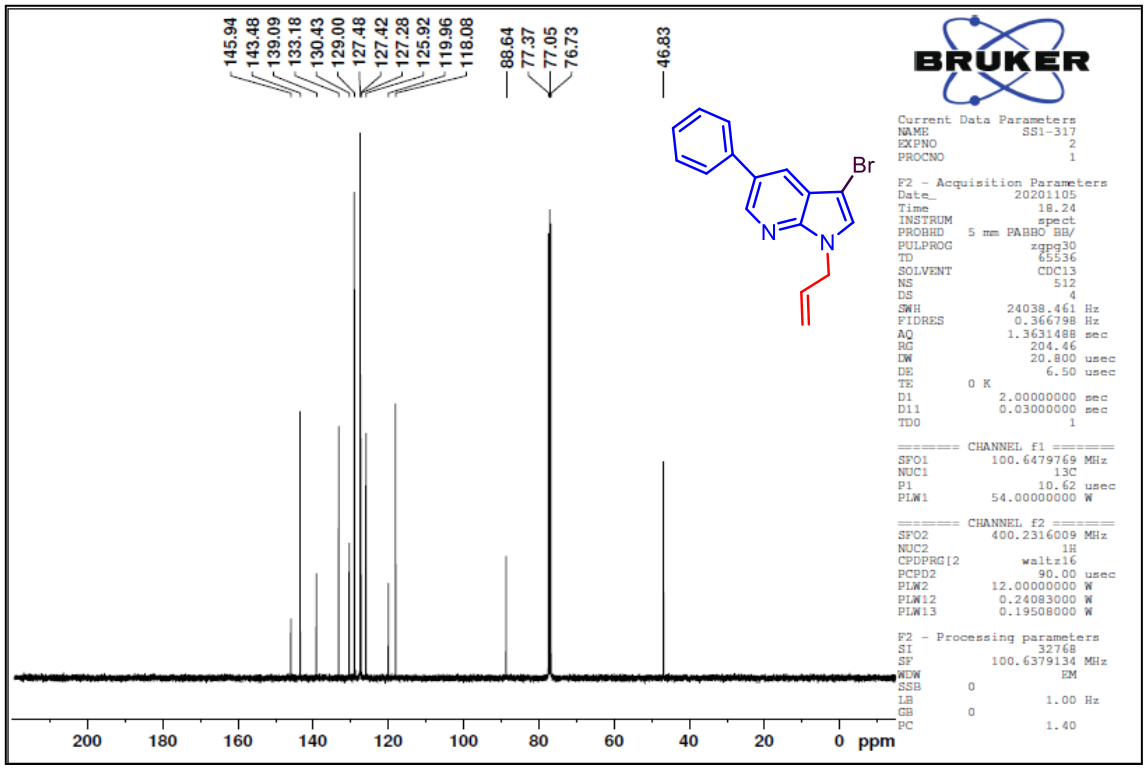


Figure 102.[13]C NMR spectrum of compound **3q**

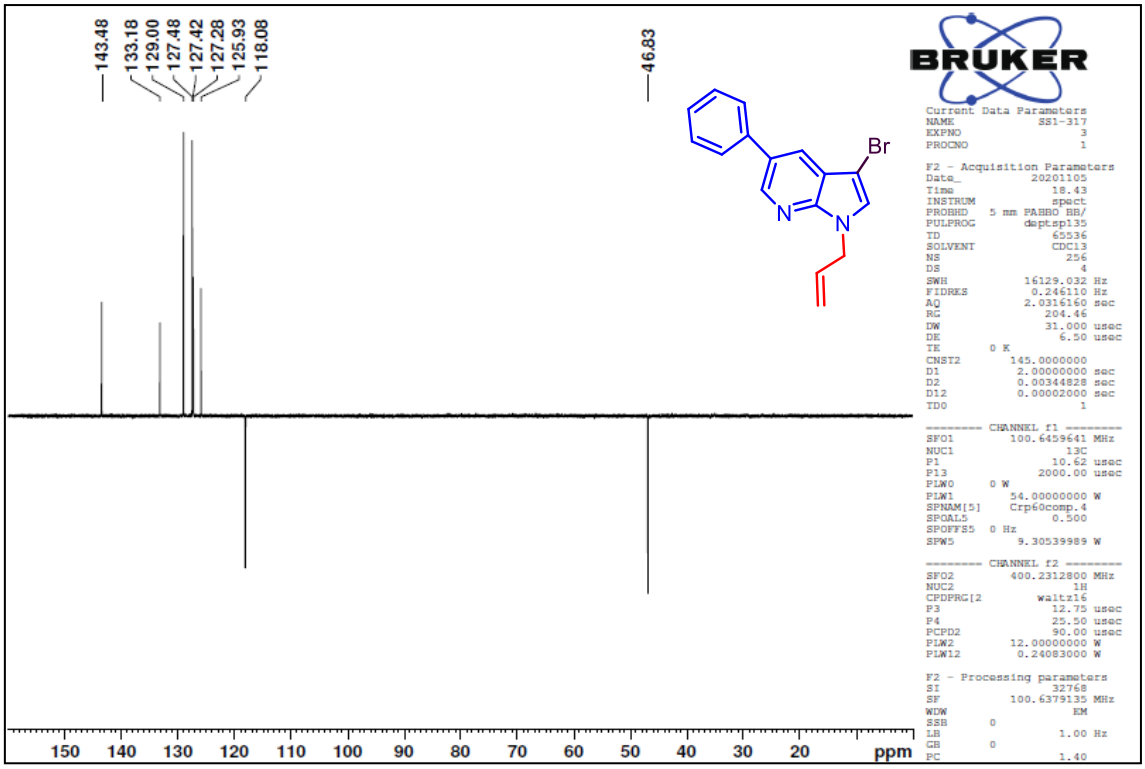


Figure 103. DEPT-135 NMR spectrum of compound **3q**

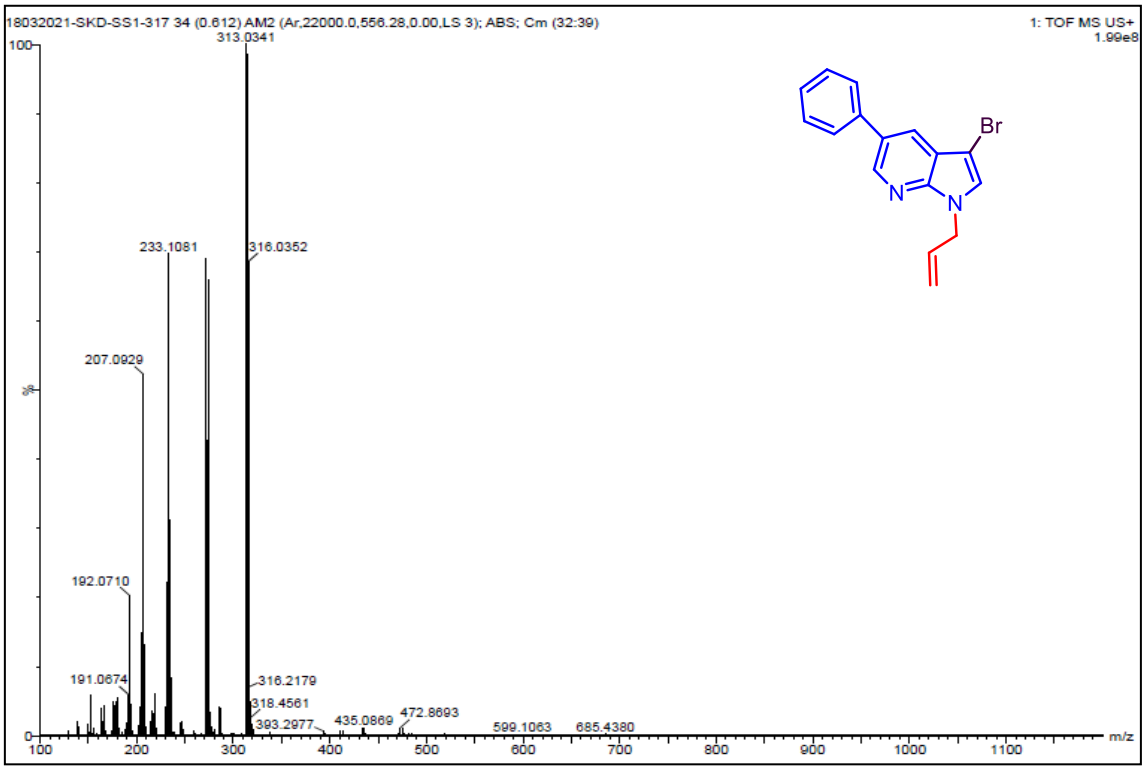


Figure 104. HRMS spectrum of compound **3q**

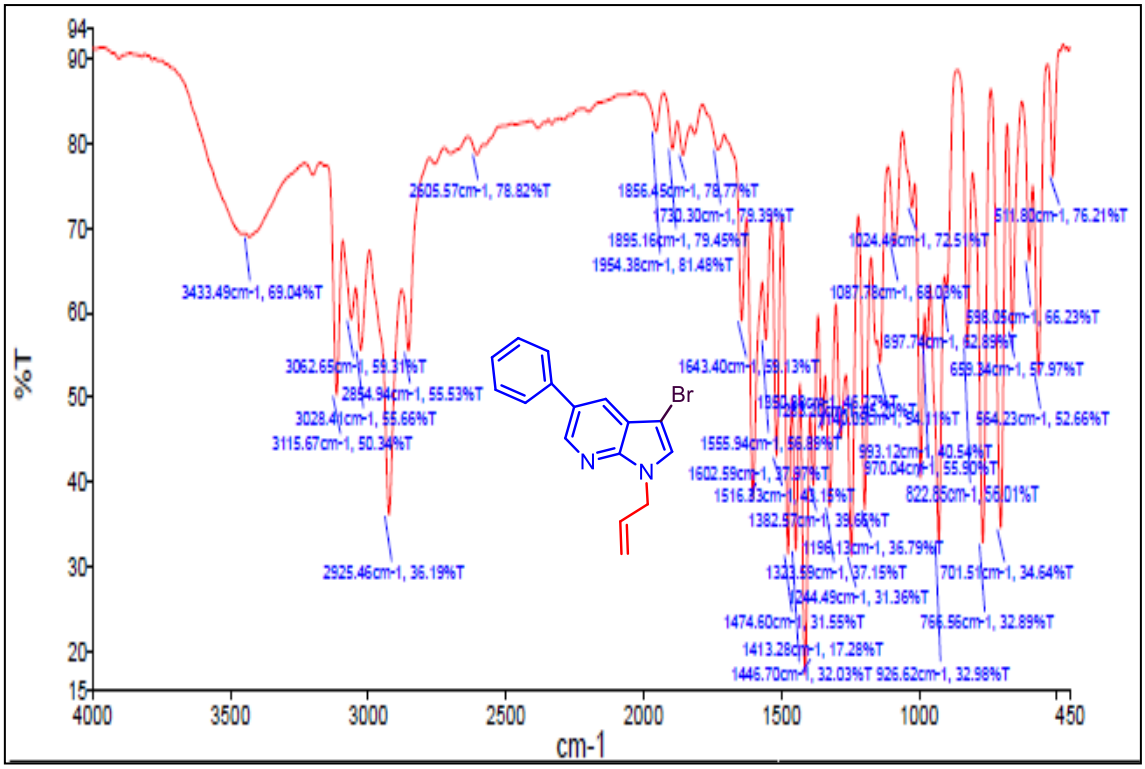


Figure 105. FTIR spectrum of compound **3q**

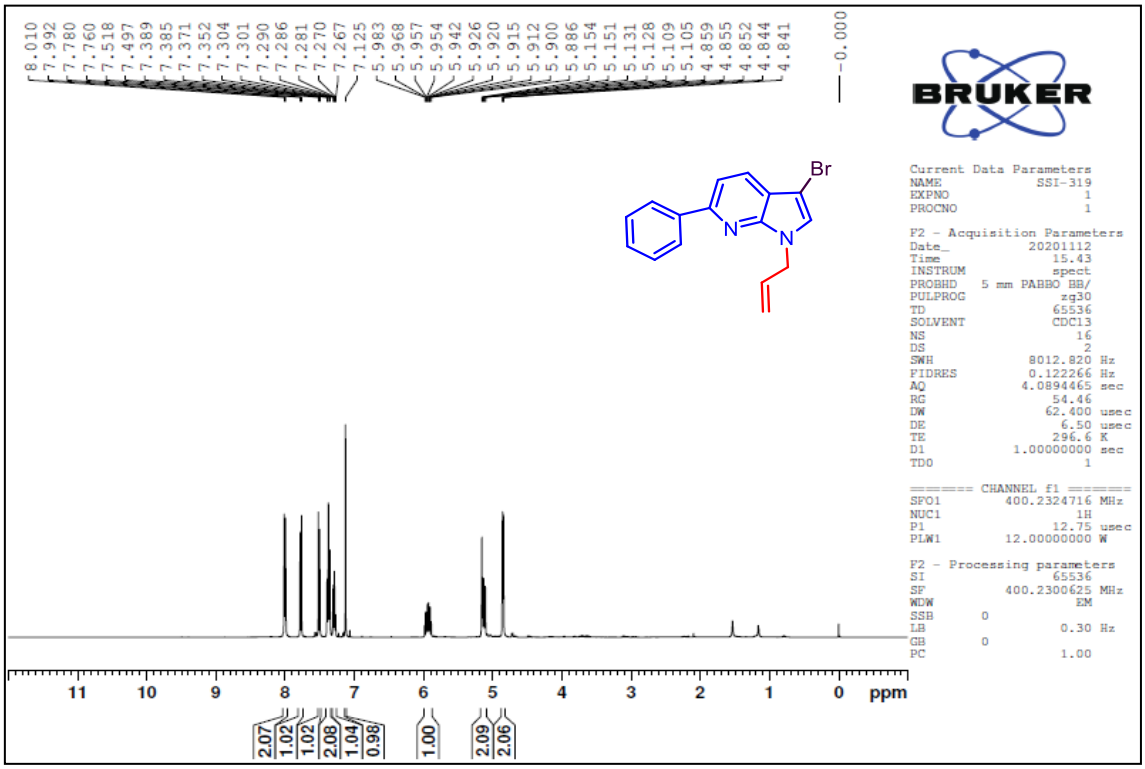


Figure 106. ^{1}H NMR spectrum of compound **3r**

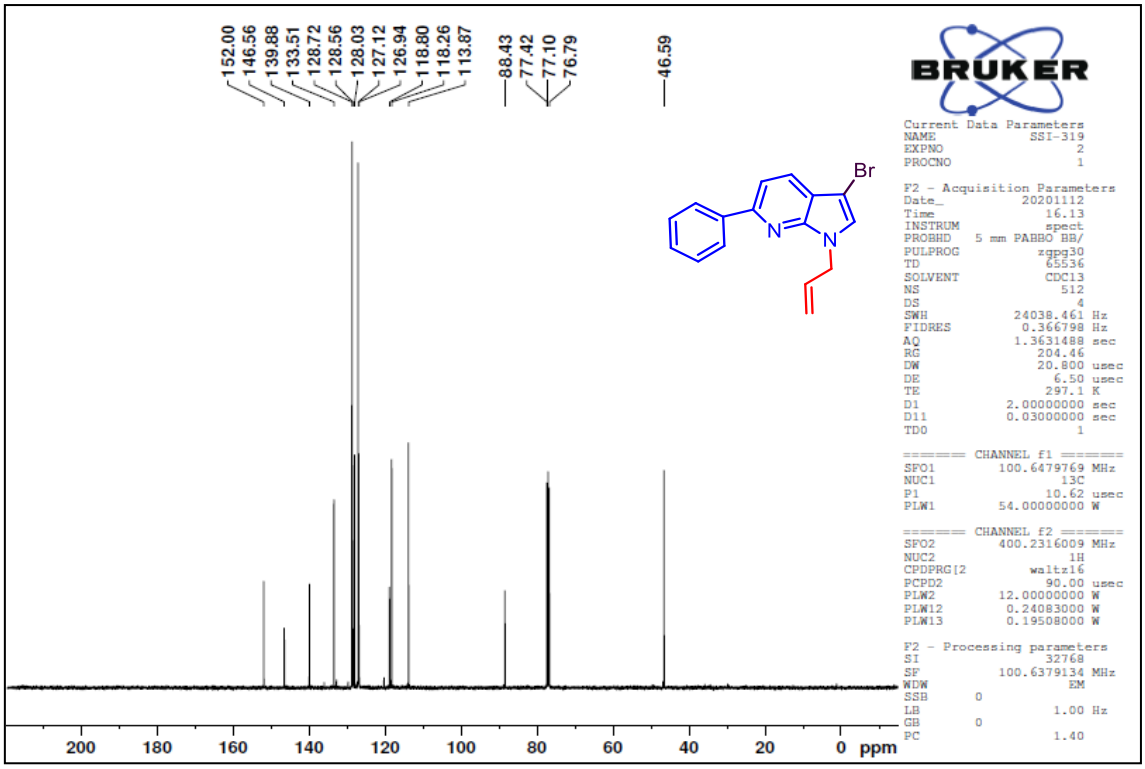


Figure 107. ^{13}C NMR spectrum of compound **3r**

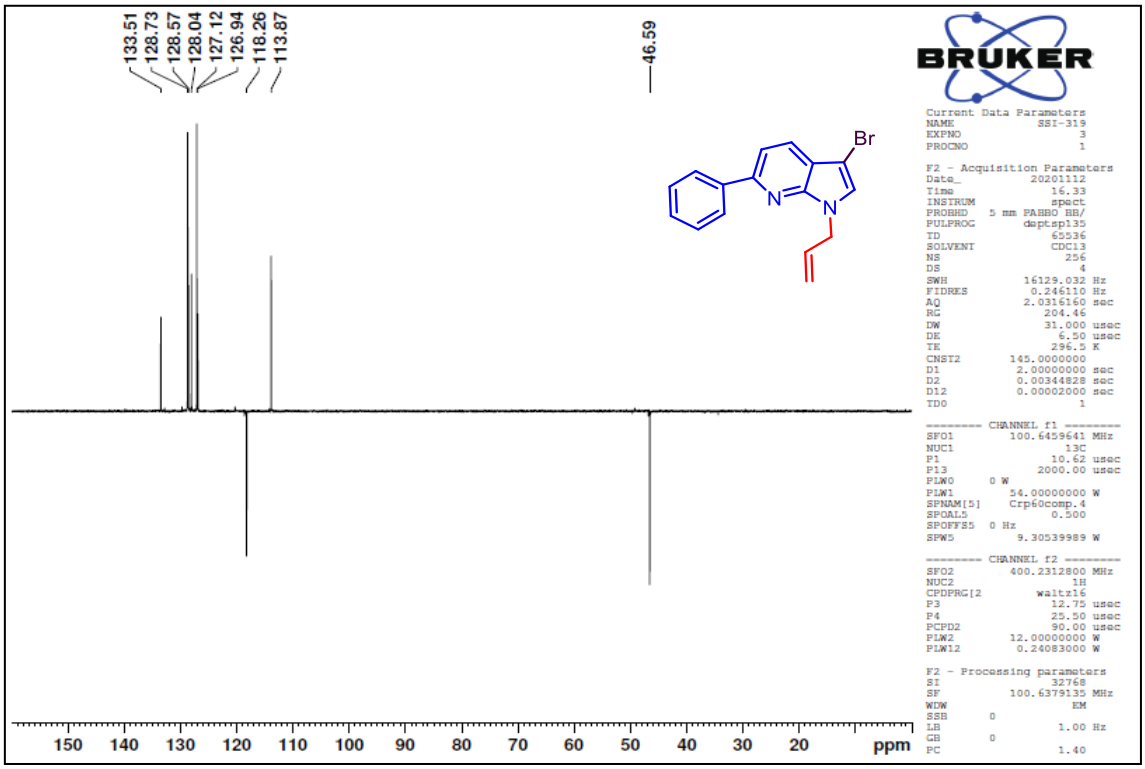


Figure 108. DEPT-135 NMR spectrum of compound **3r**

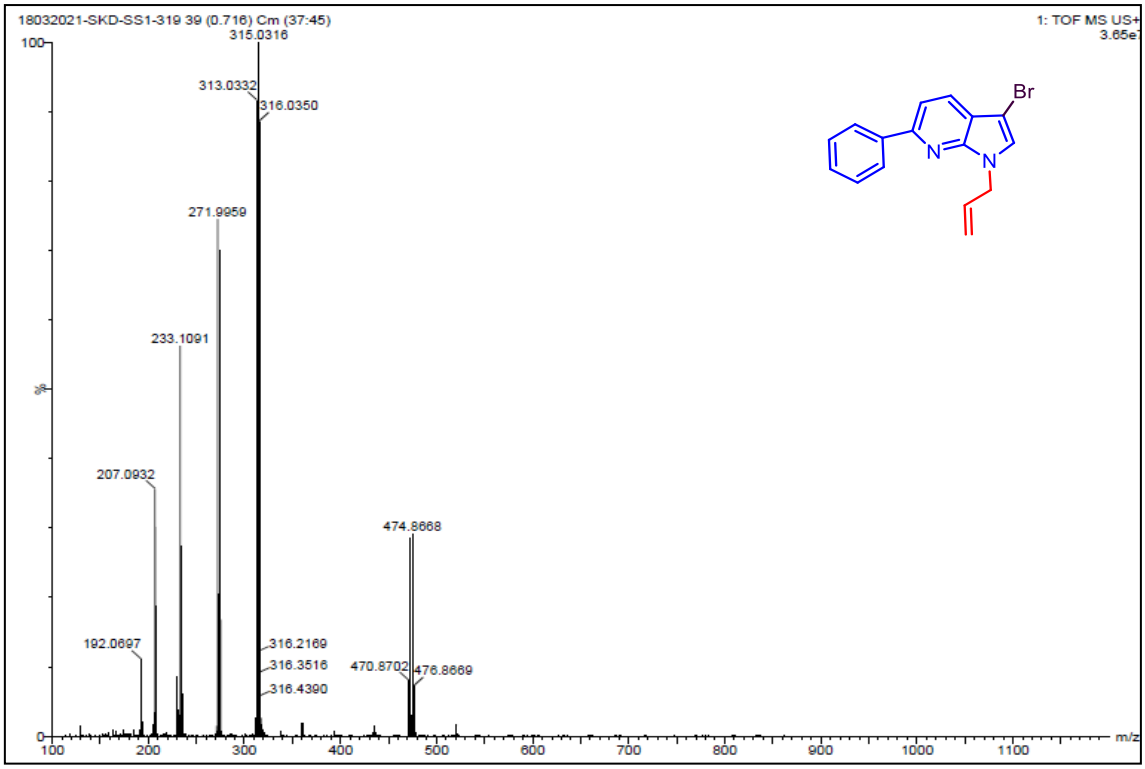


Figure 109. HRMS spectrum of compound **3r**

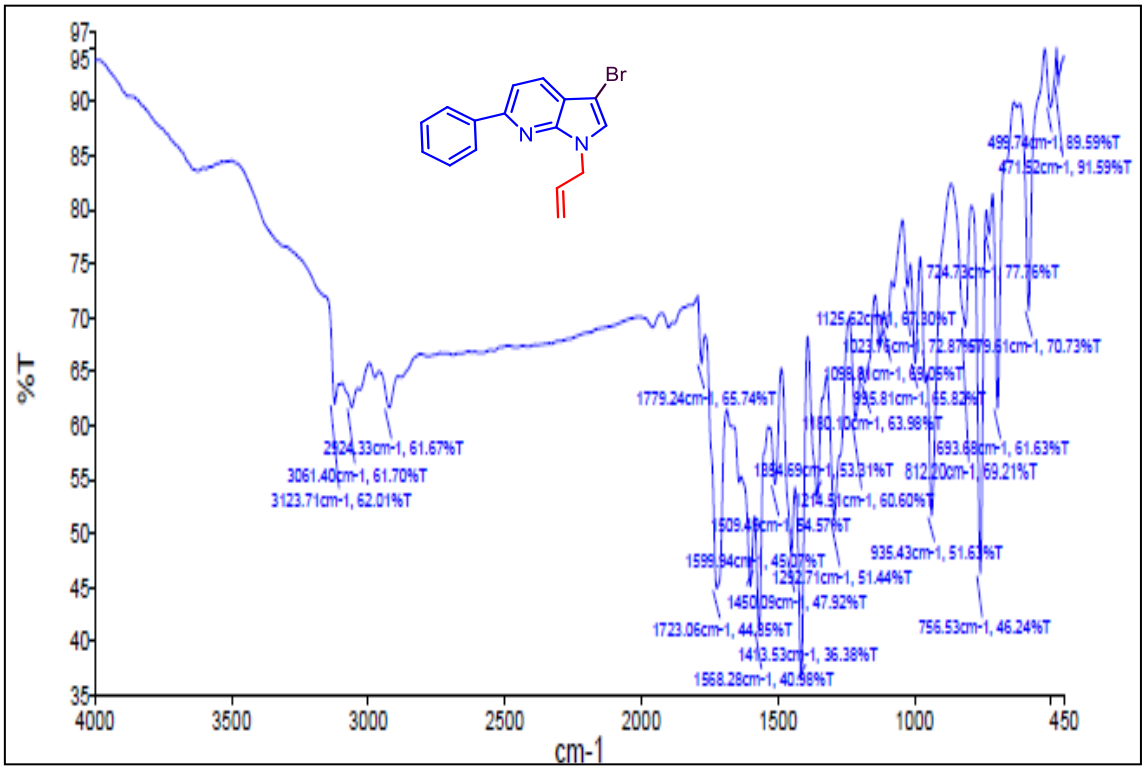


Figure 110. FTIR spectrum of compound **3r**

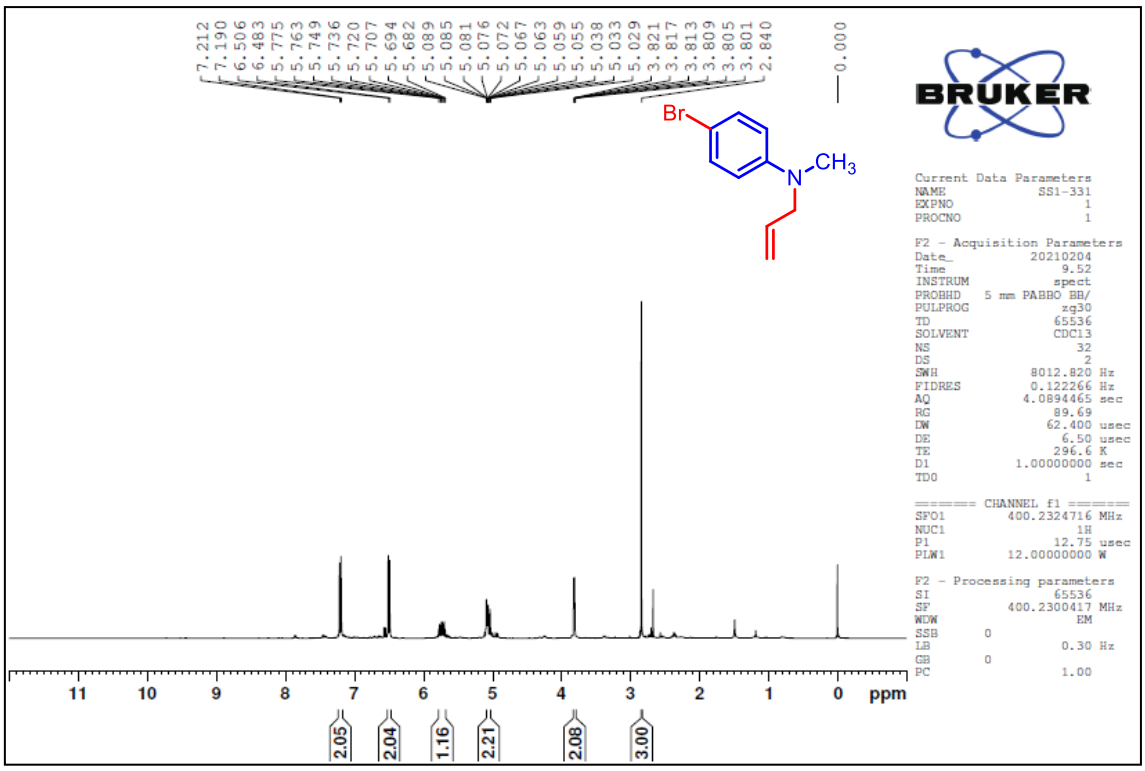


Figure 111. ^{1}H NMR spectrum of compound **3s**

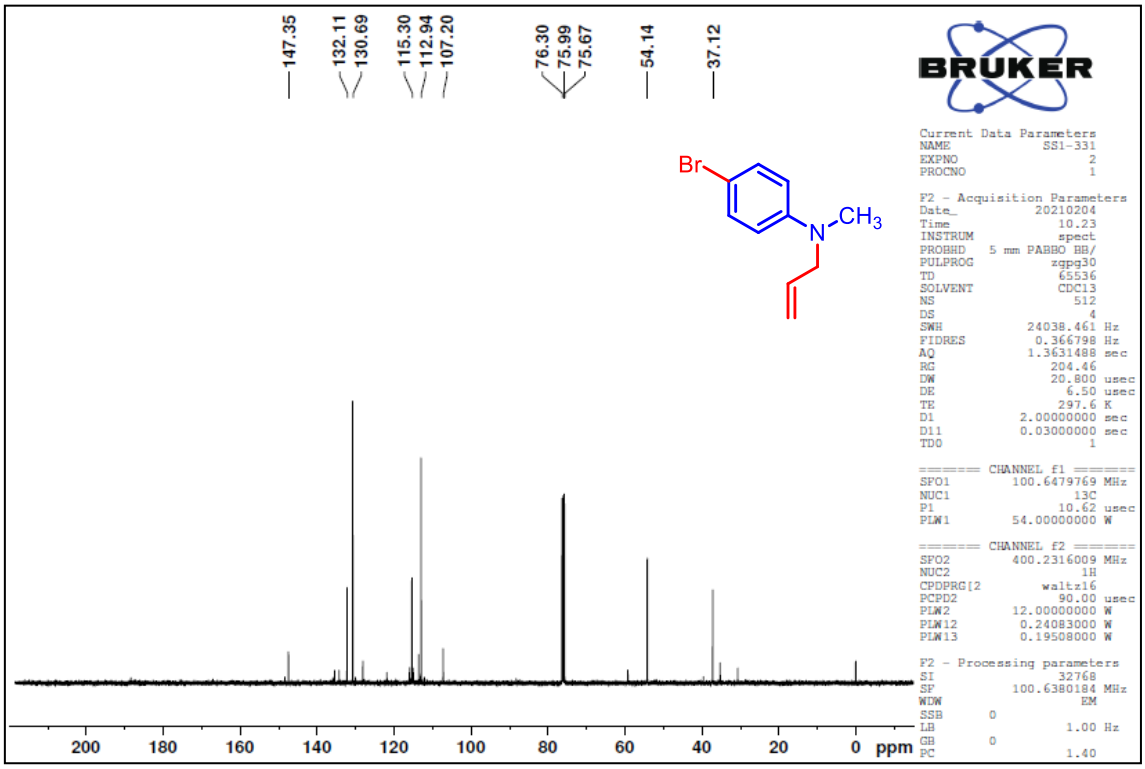


Figure 112. ^{13}C NMR spectrum of compound **3s**

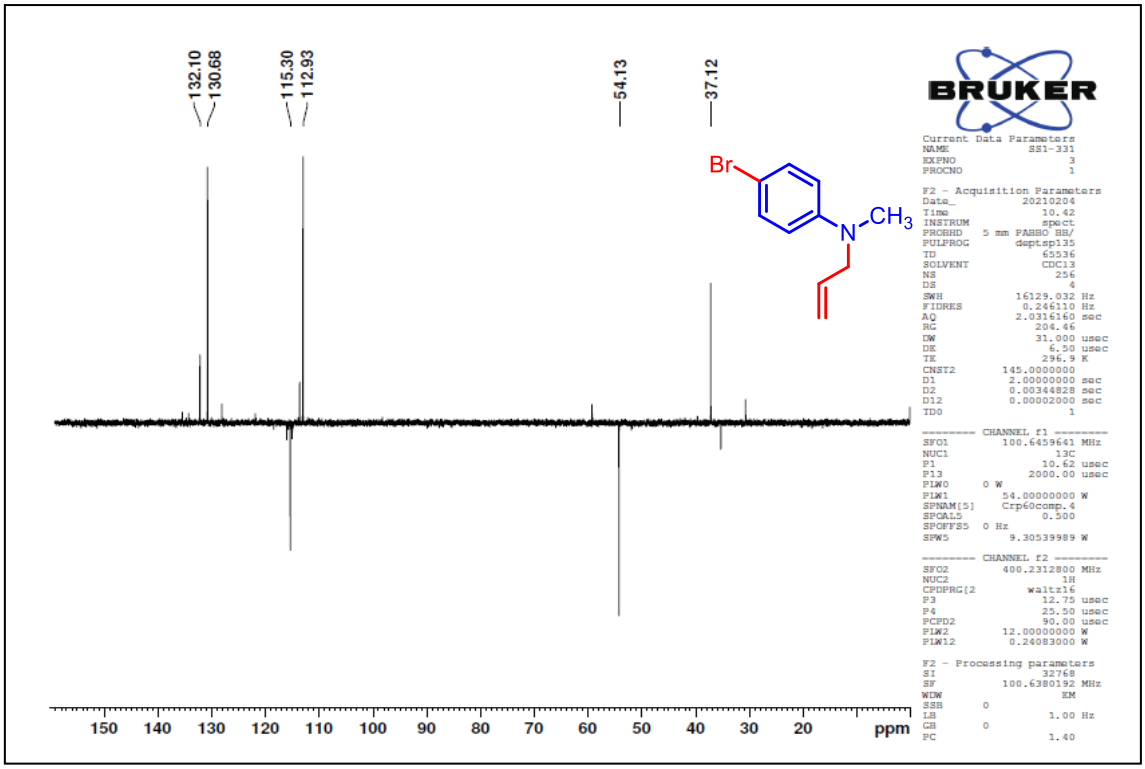


Figure 113. DEPT-135 NMR spectrum of compound **3s**

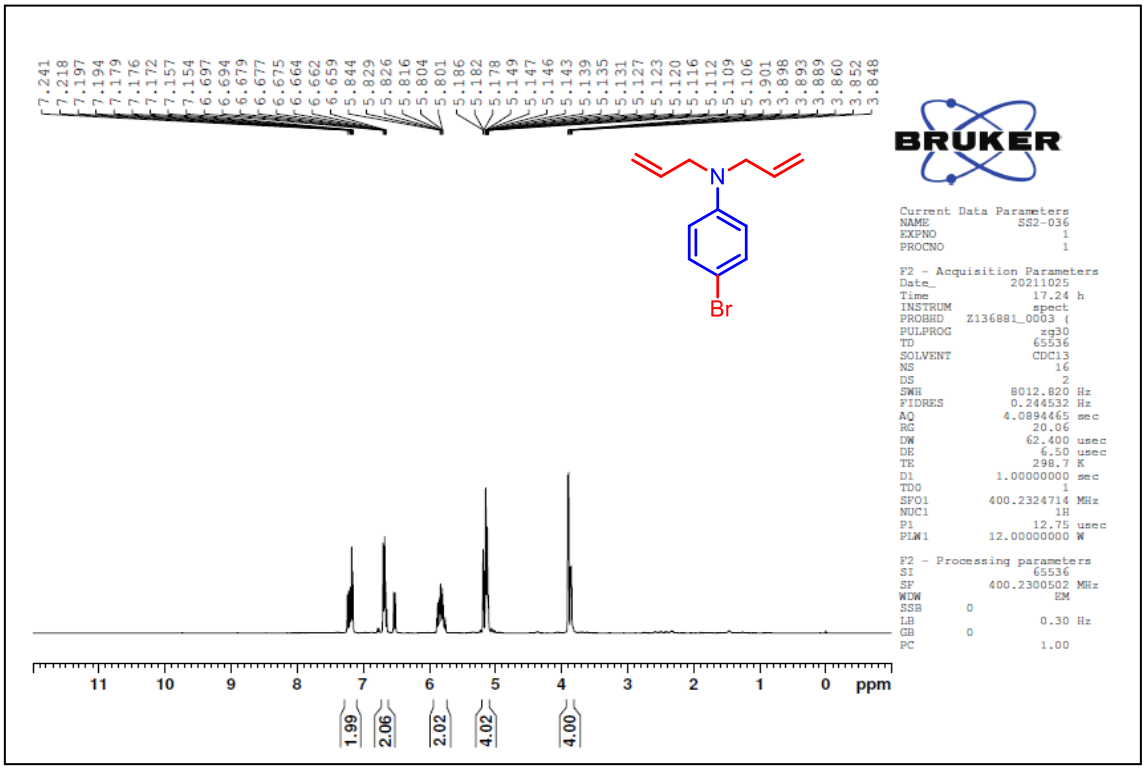


Figure 114. ^{1}H NMR spectrum of compound **3t**

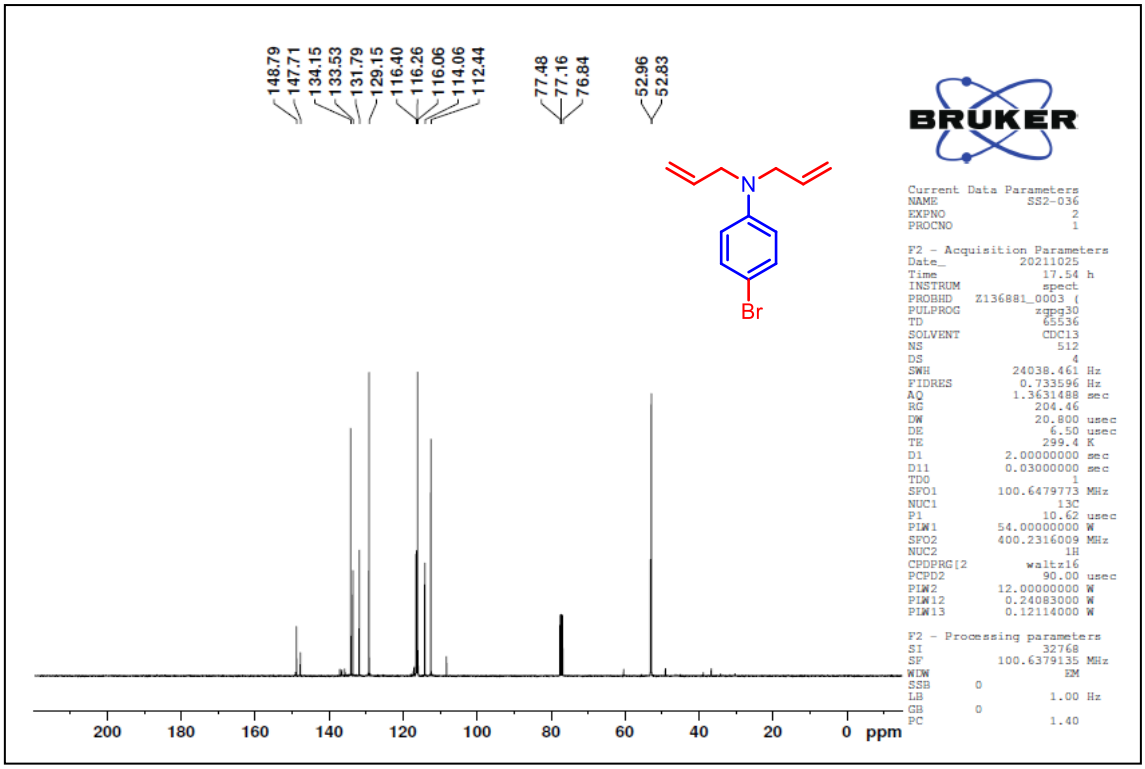


Figure 115. ^{13}C NMR spectrum of compound **3t**

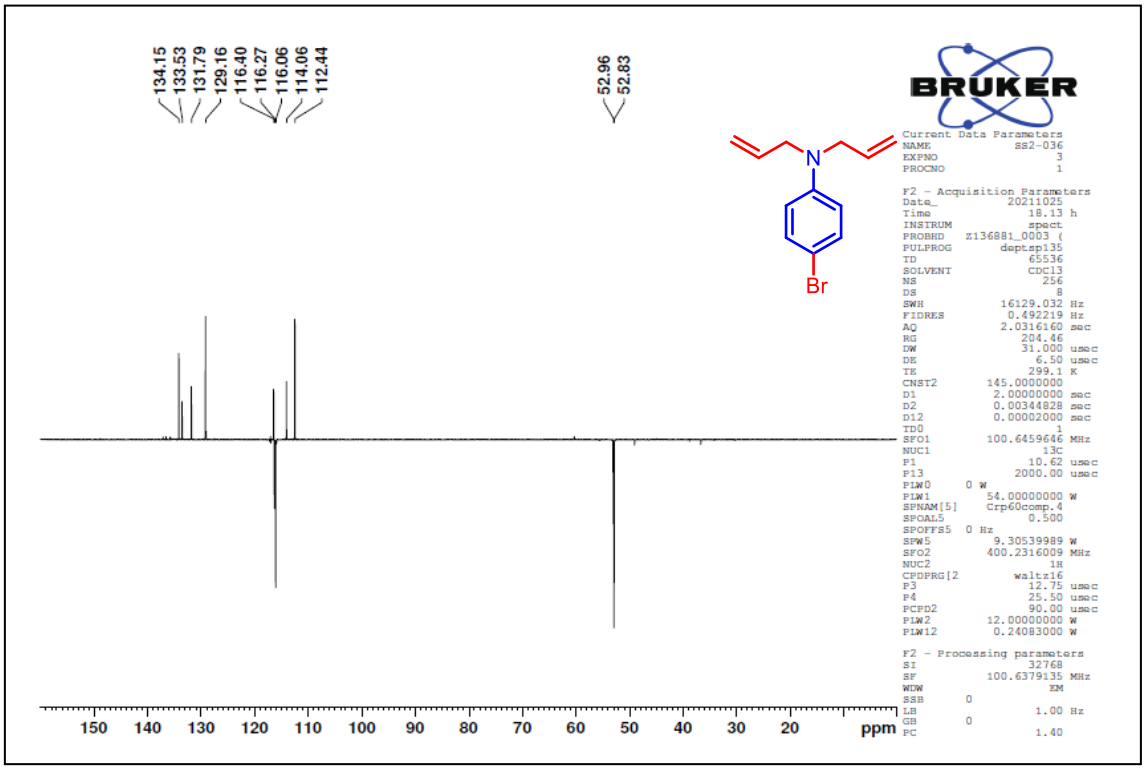


Figure 116. DEPT-135 NMR spectrum of compound **3t**

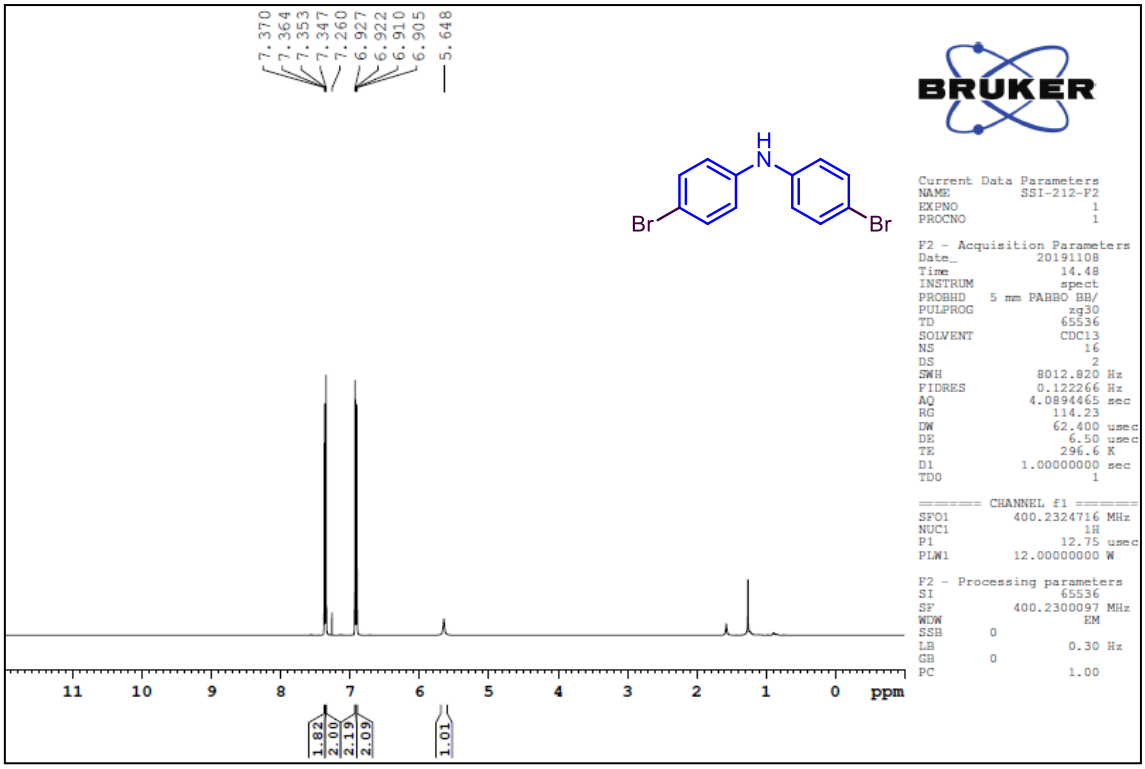


Figure 117. ^{1}H NMR spectrum of compound **4a**

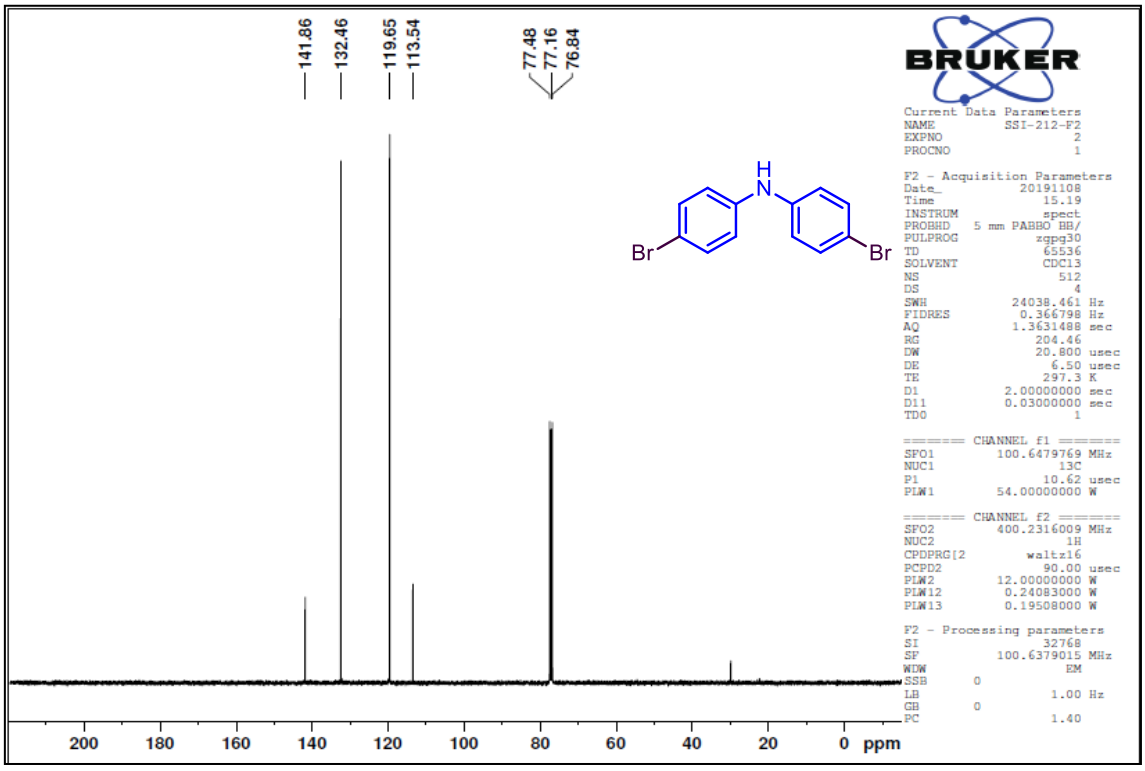


Figure 118. ^{13}C NMR spectrum of compound **4a**

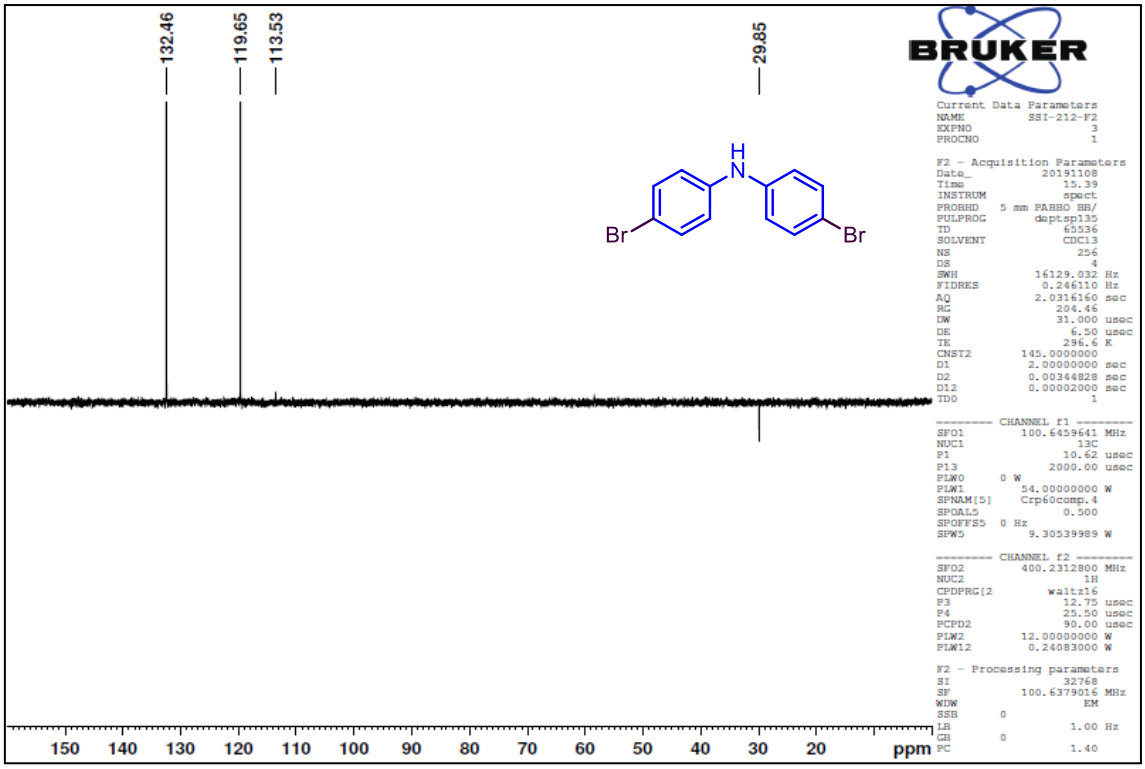


Figure 119. DEPT-135 NMR spectrum of compound **4a**

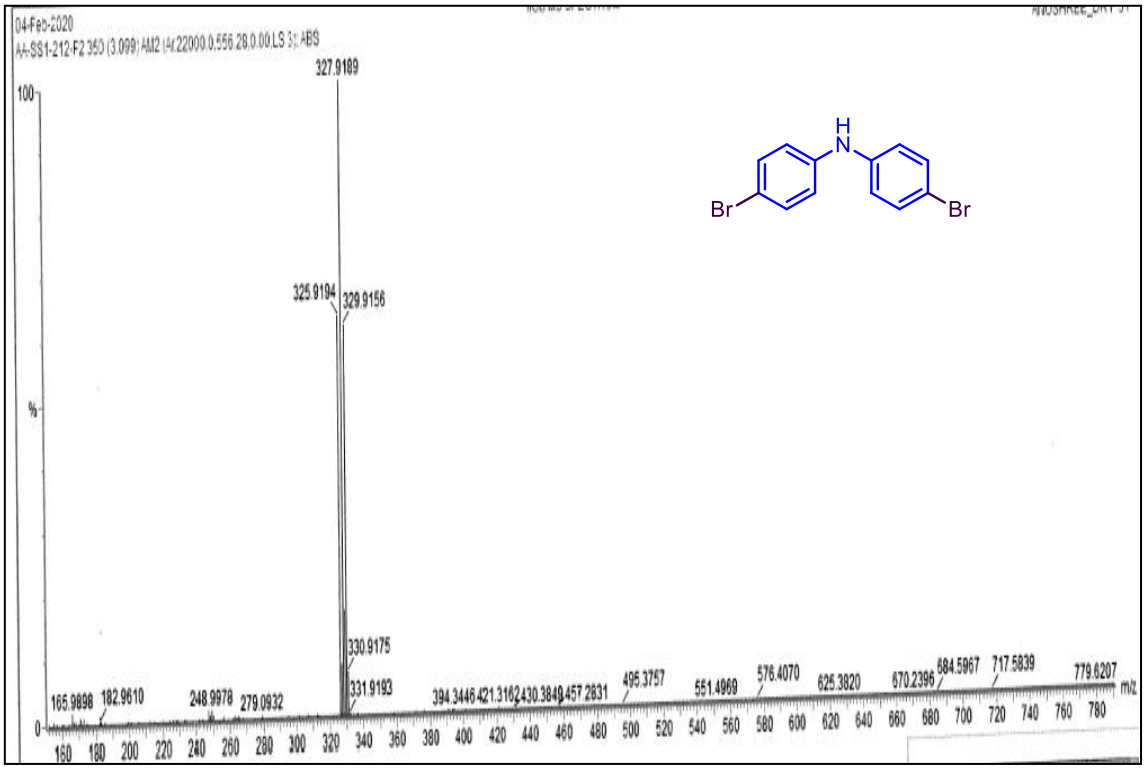


Figure 120. HRMS spectrum of compound **4a**

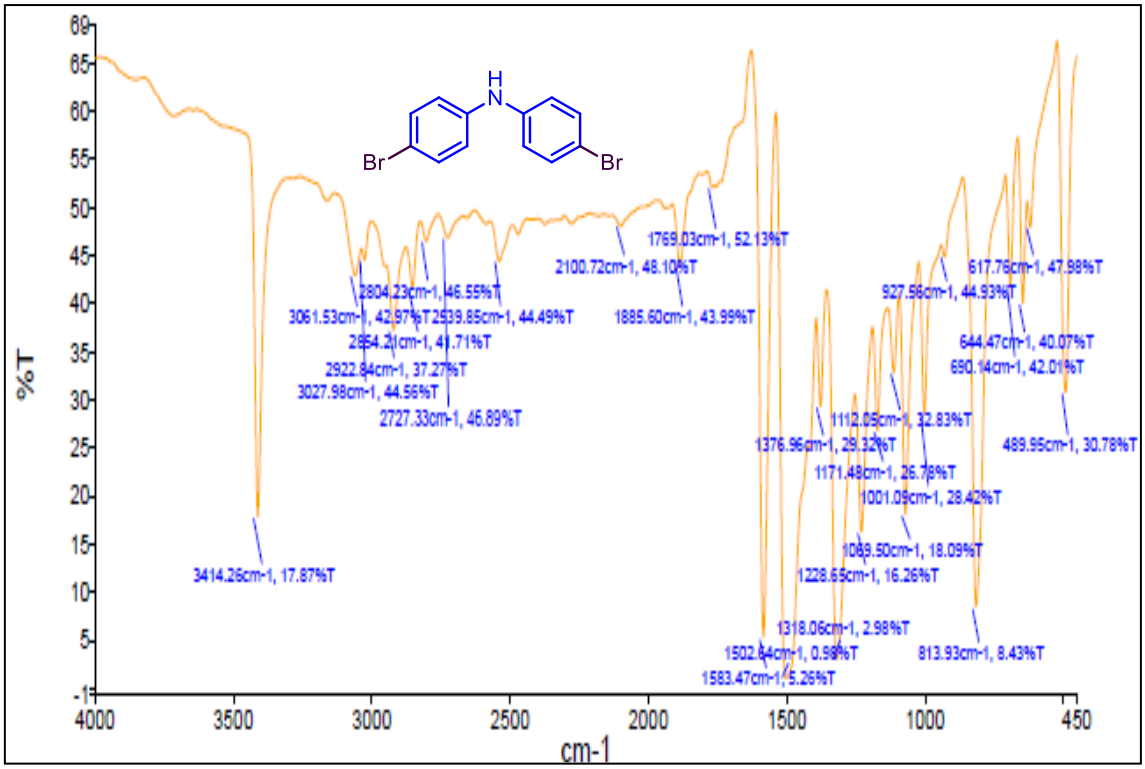


Figure 121. FTIR spectrum of compound **4a**

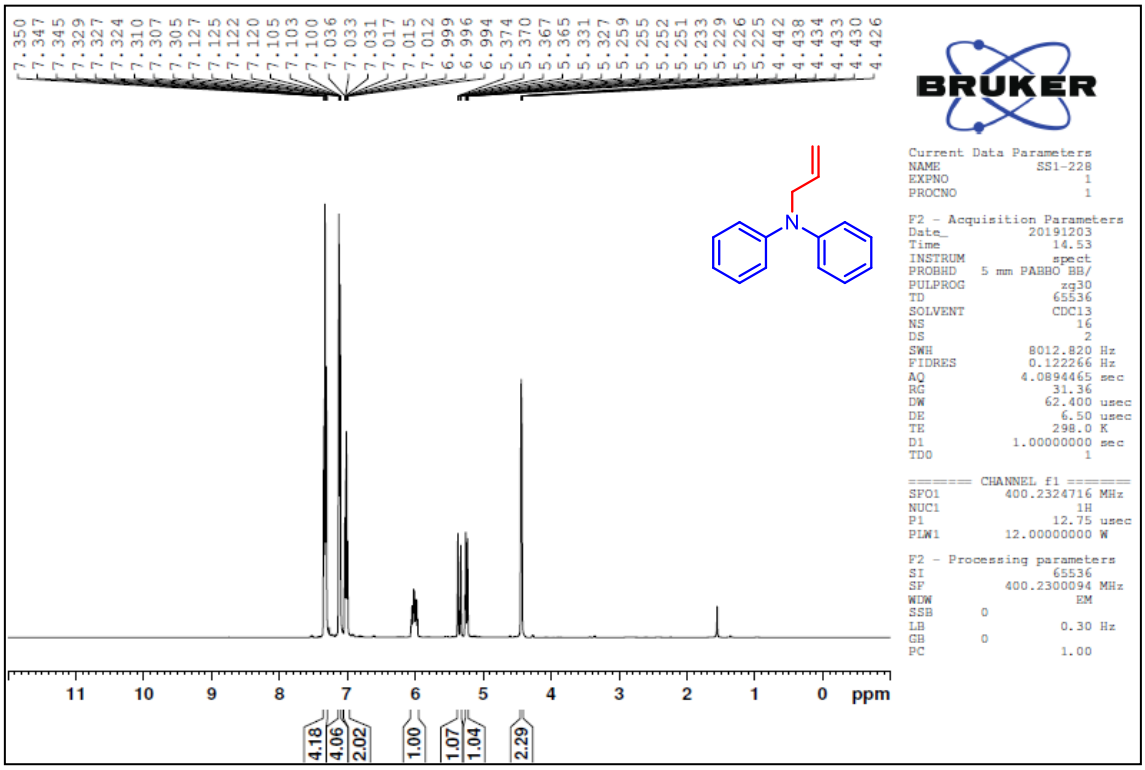


Figure 122. ^{1}H NMR spectrum of compound **5a**

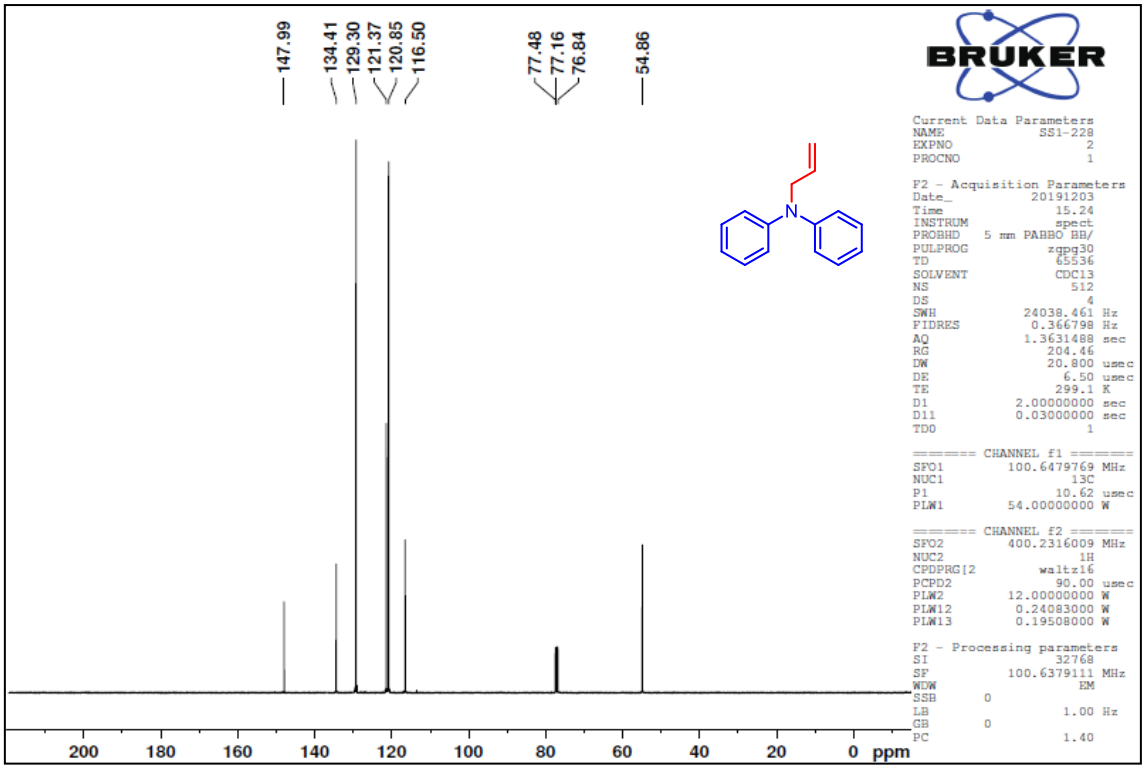


Figure 123. ^{13}C NMR spectrum of compound **5a**

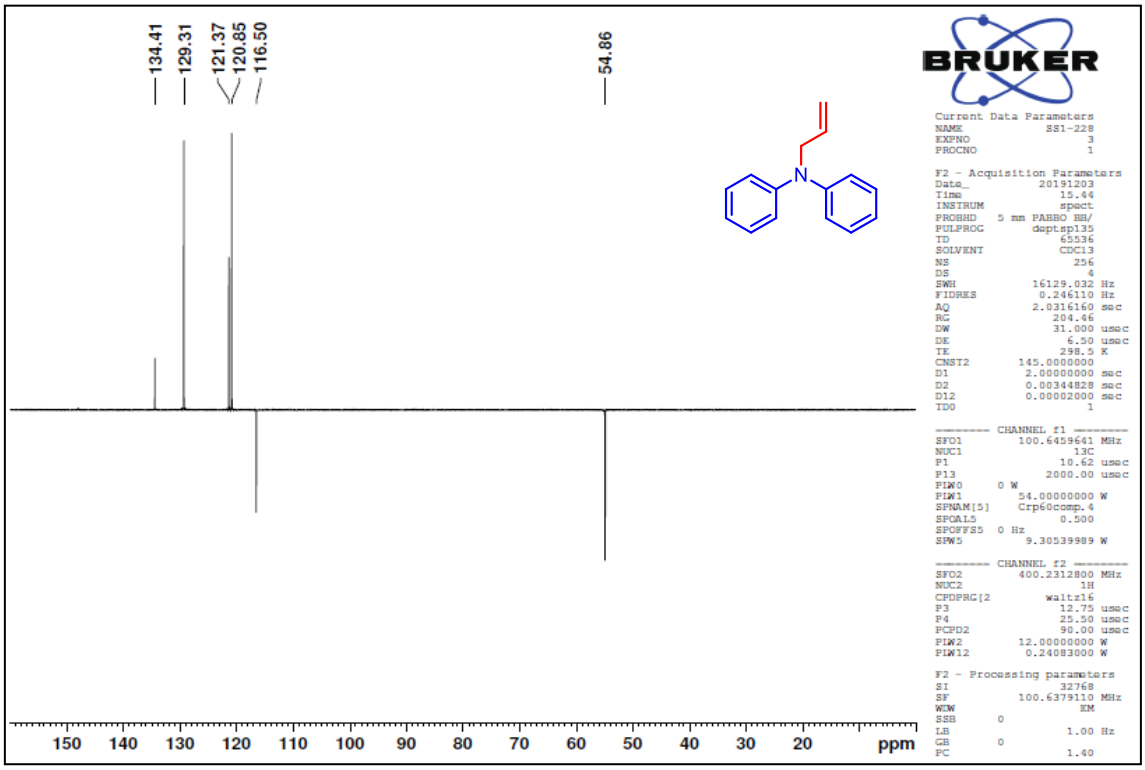


Figure 124. DEPT-135 NMR spectrum of compound **5a**

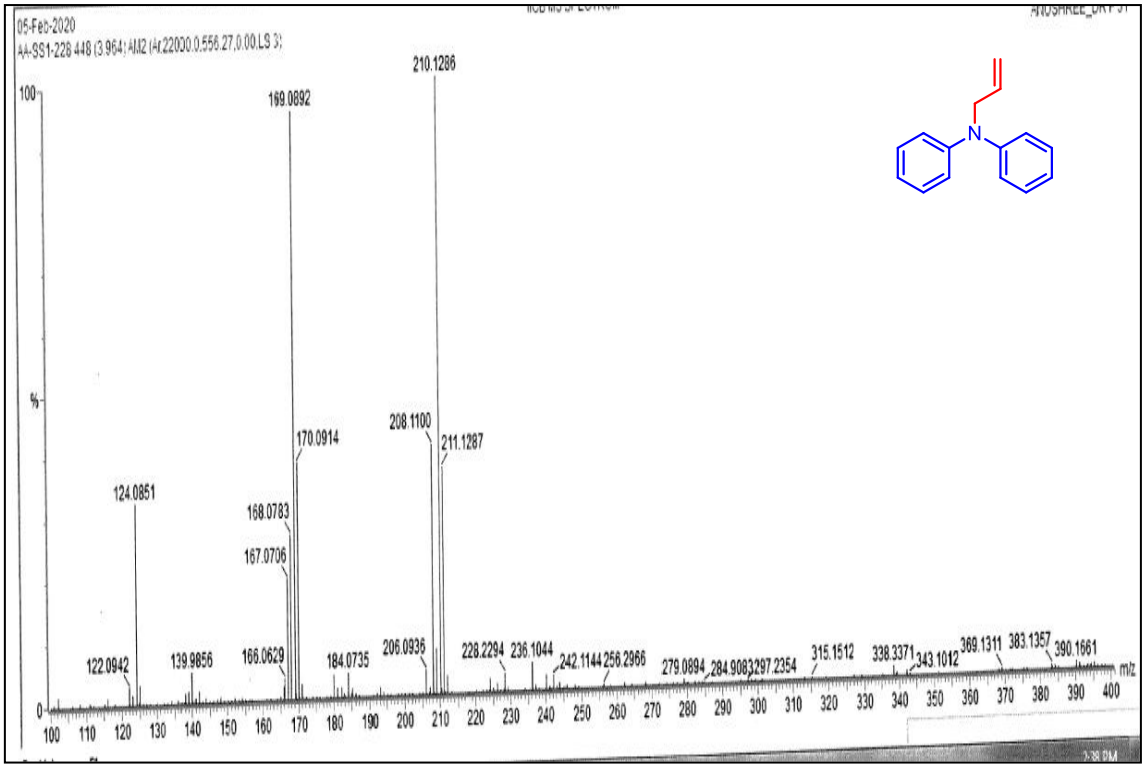


Figure 125. HRMS spectrum of compound **5a**

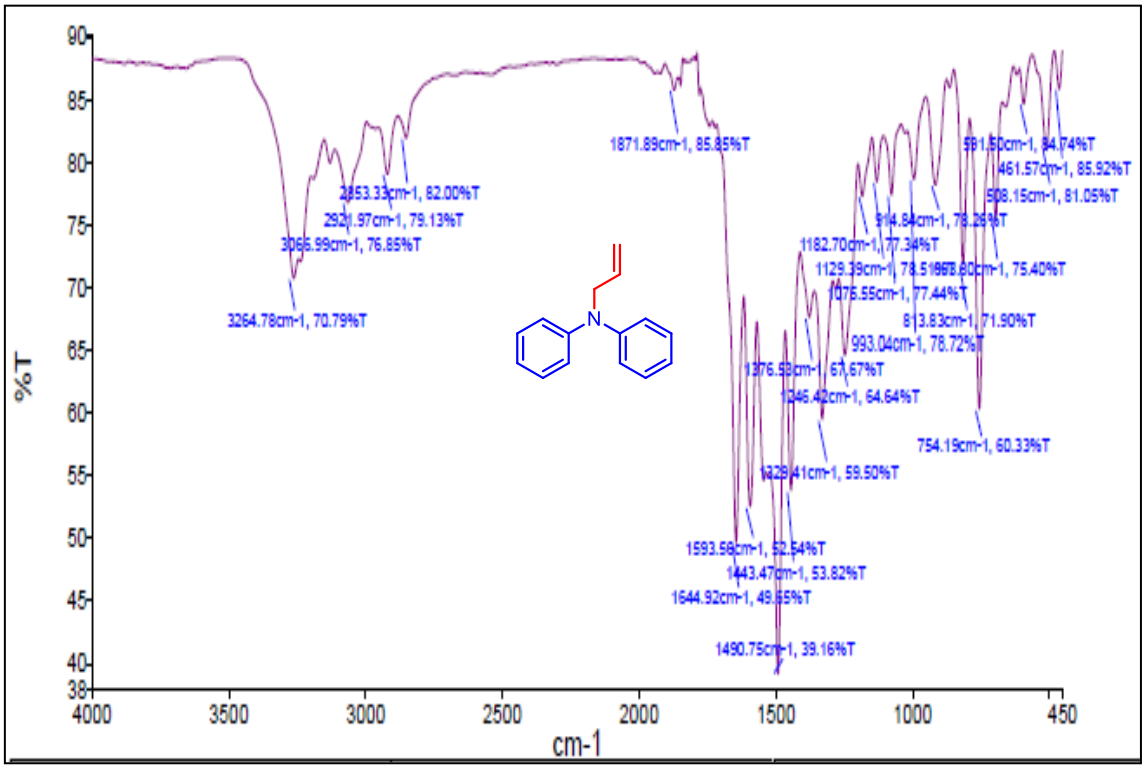


Figure 126. FTIR spectrum of compound **5a**

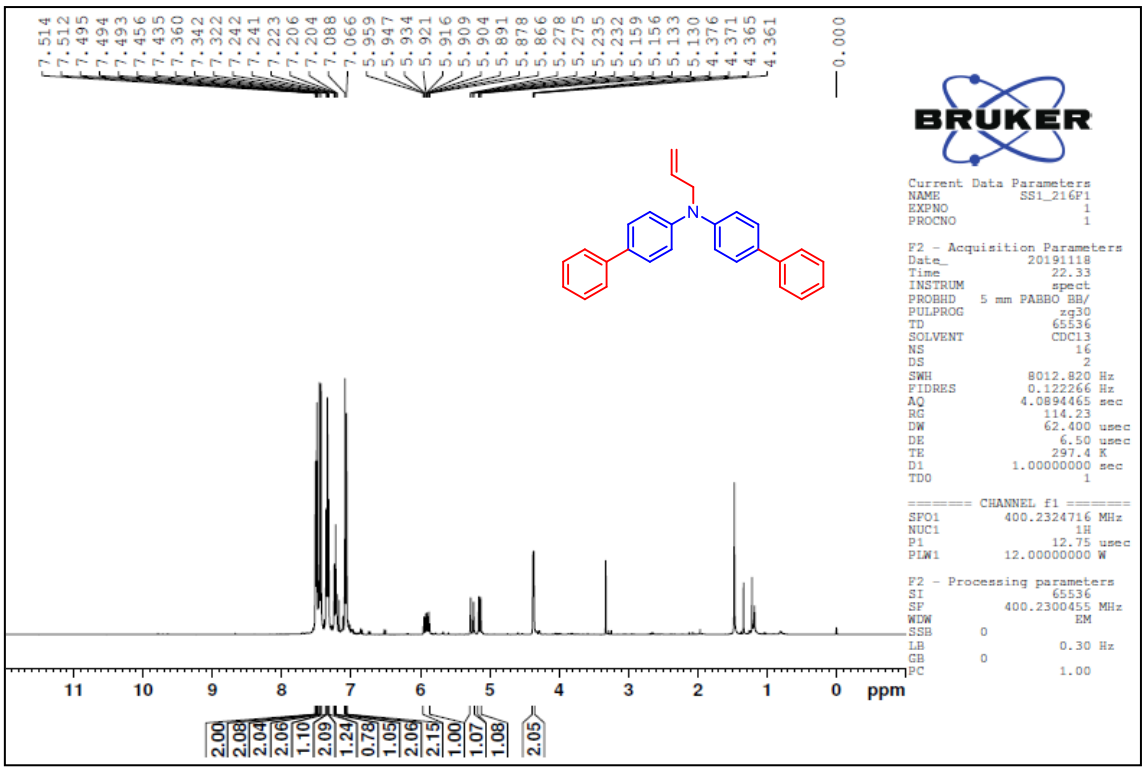


Figure 127.[1]H NMR spectrum of compound **10a**

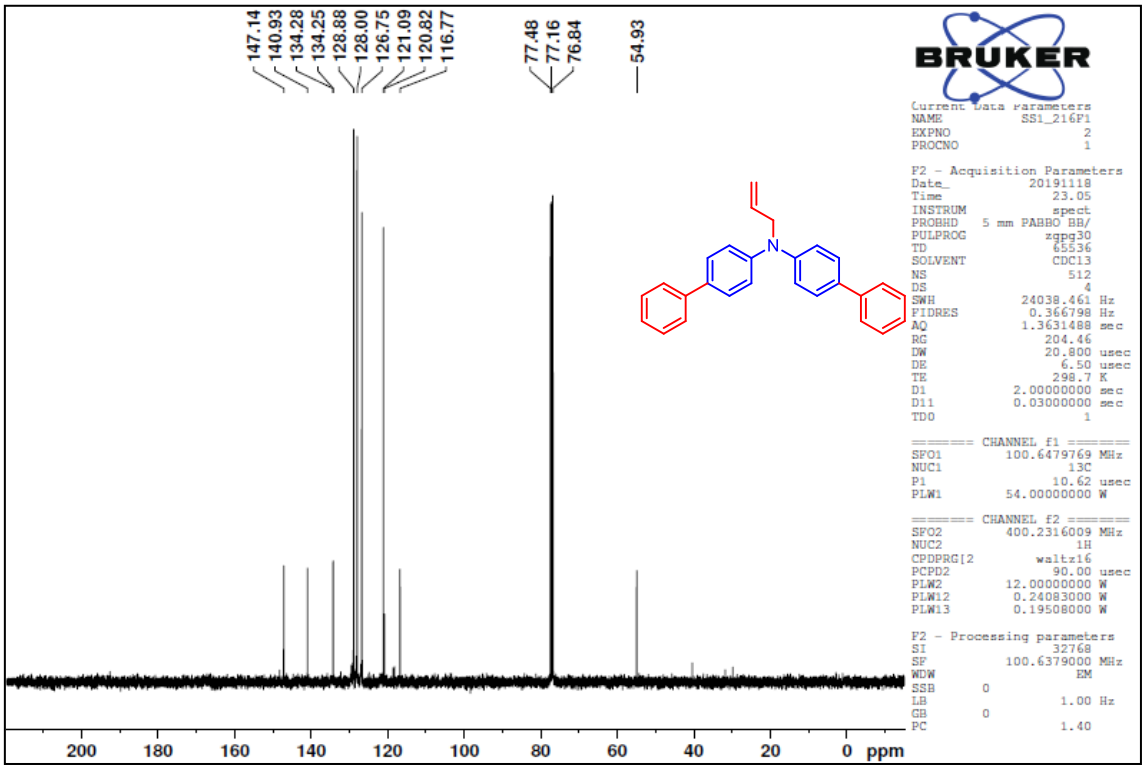


Figure 128.[13]C NMR spectrum of compound **10a**

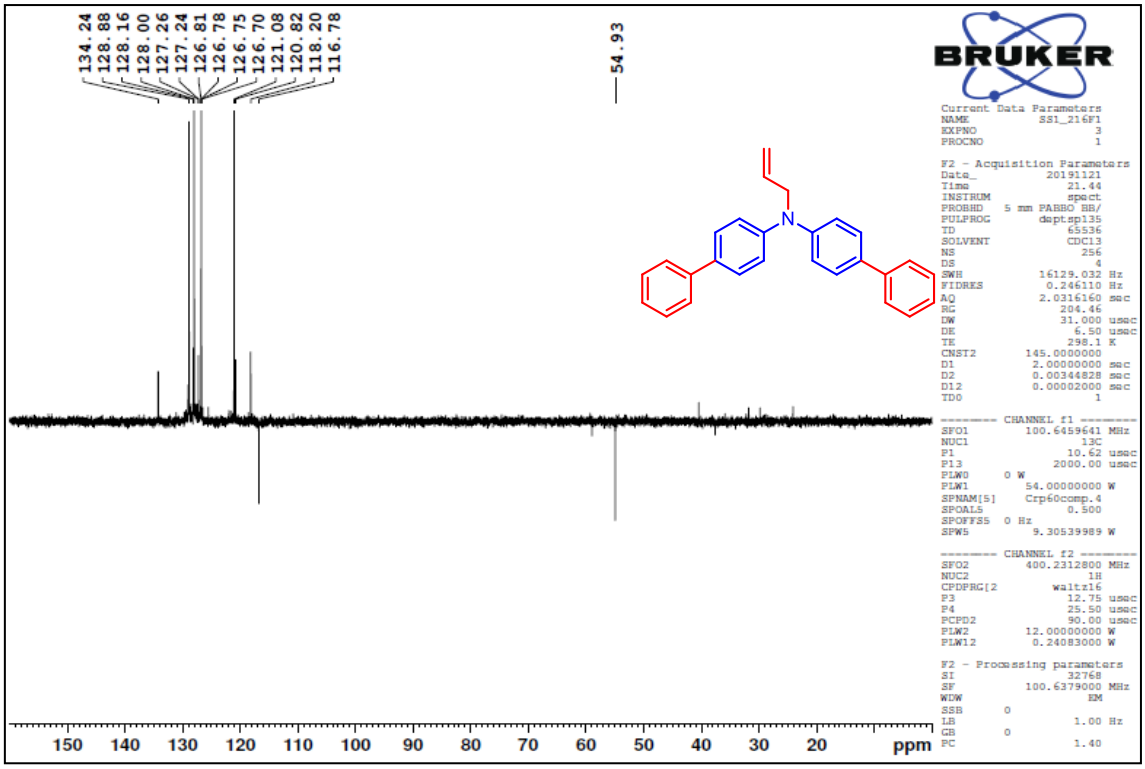


Figure 129. DEPT-135 NMR spectrum of compound **10a**

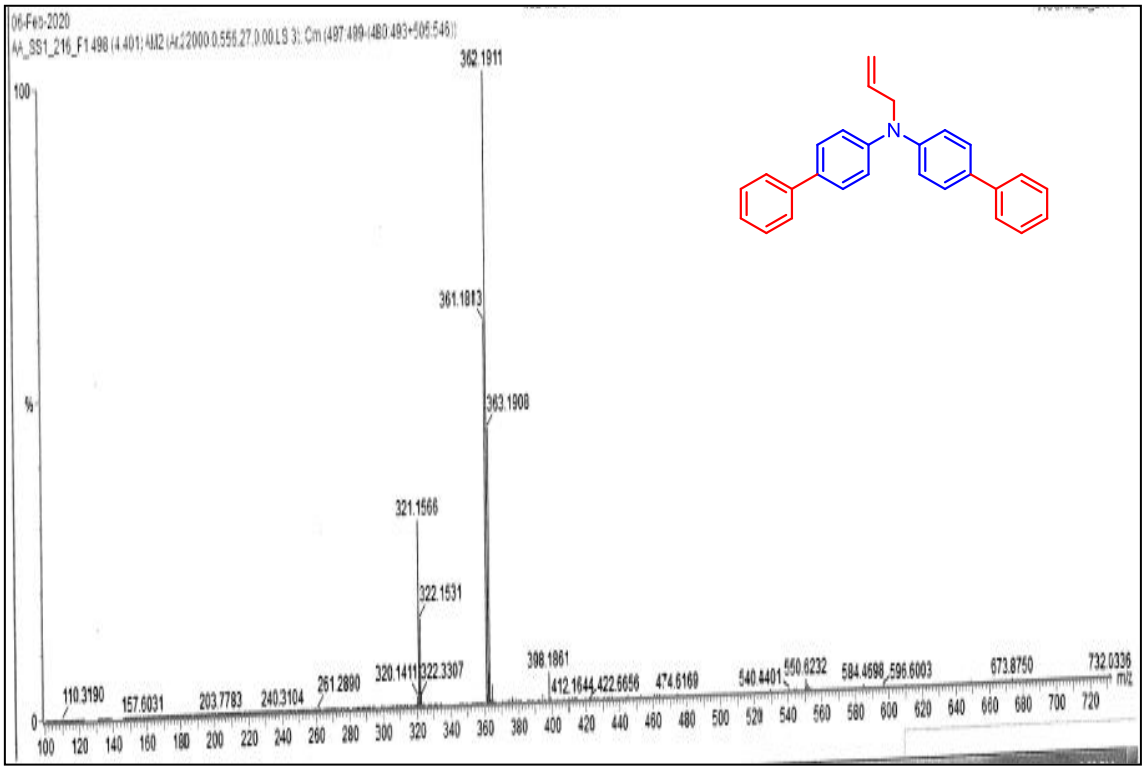


Figure 130. HRMS spectrum of compound **10a**

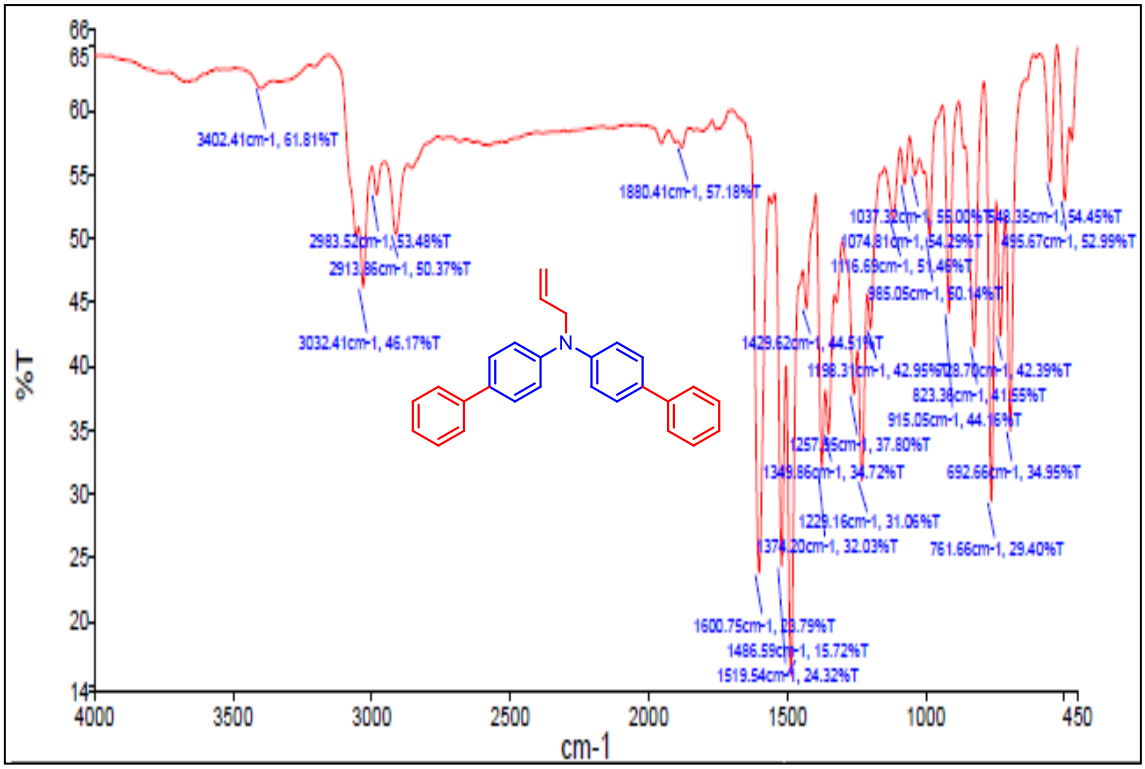


Figure 131. FTIR spectrum of compound **10a**

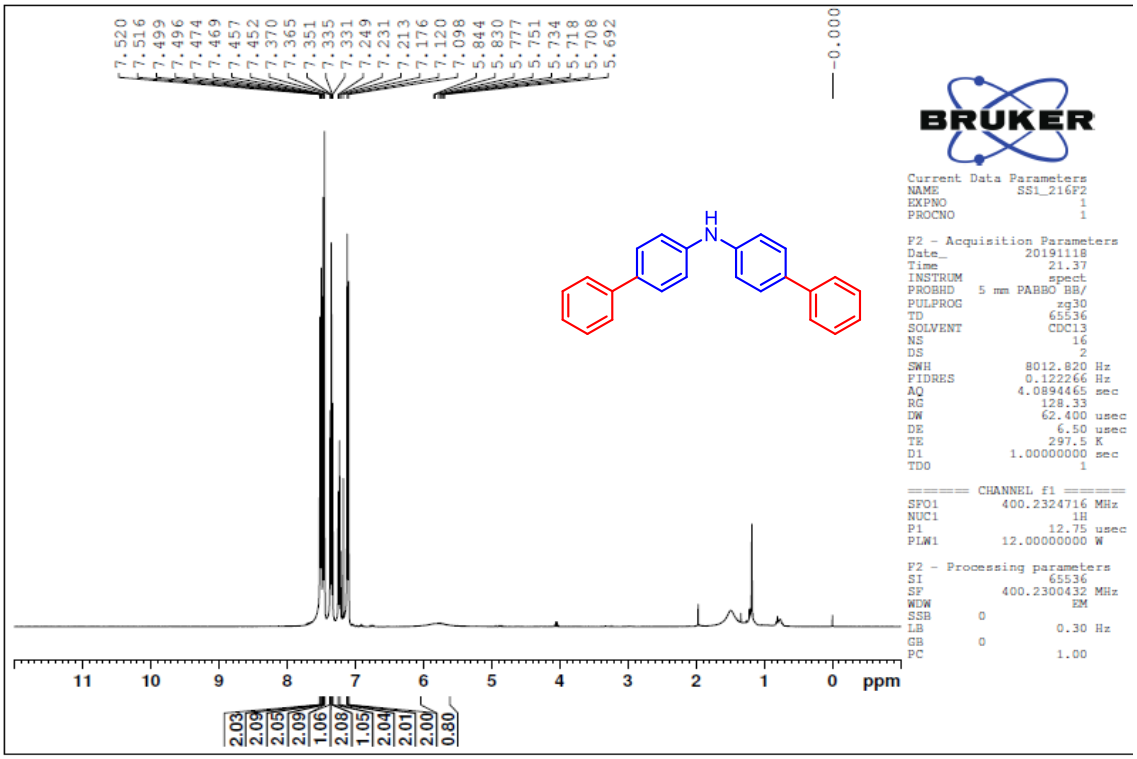


Figure 132. ^{1}H NMR spectrum of compound **10a'**

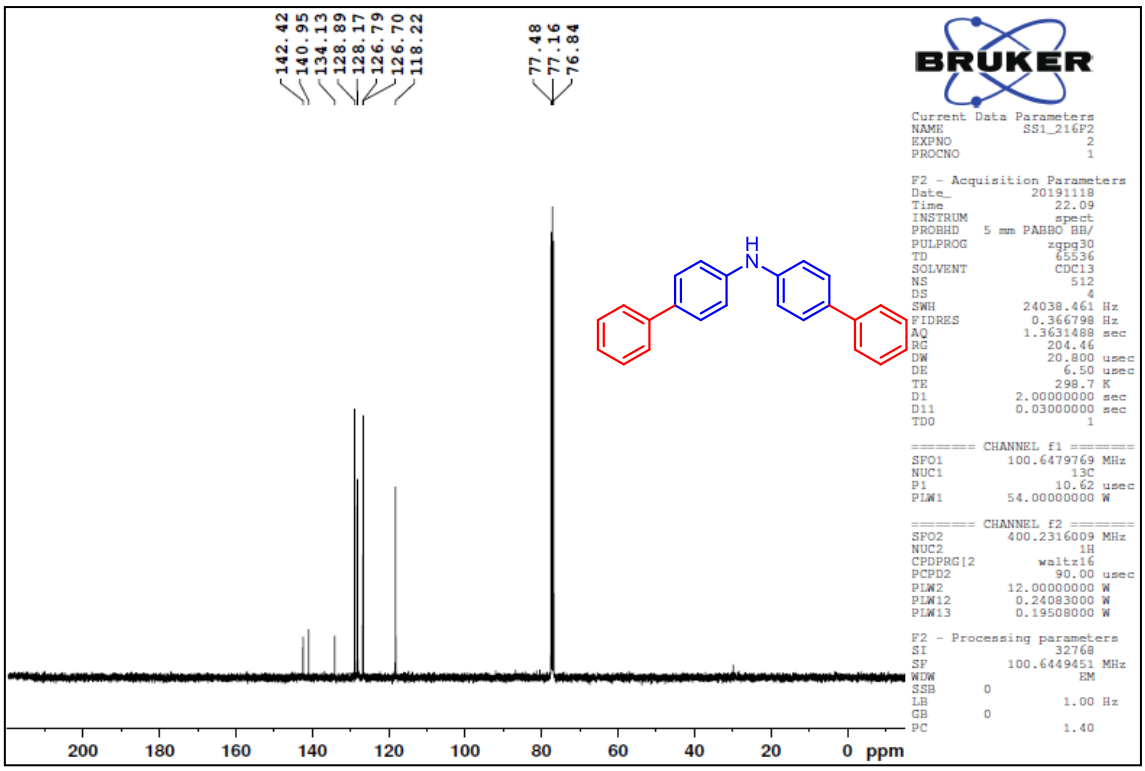


Figure 133. ^{13}C NMR spectrum of compound **10a'**

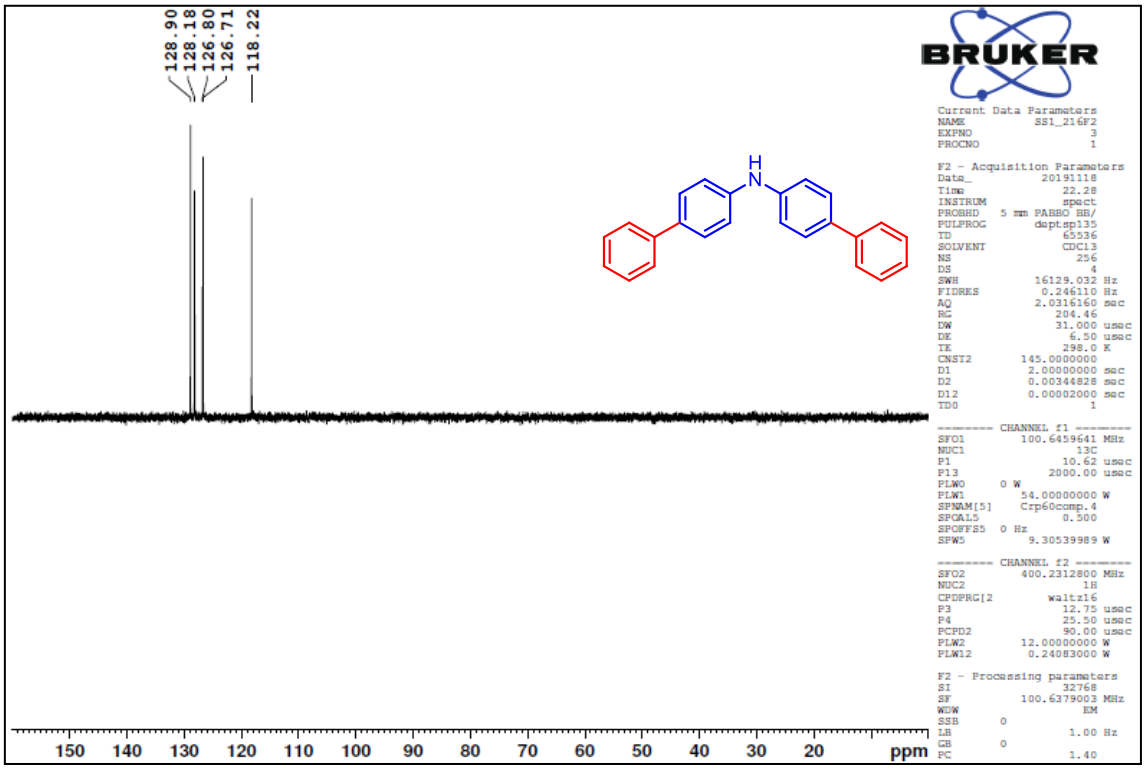


Figure 134. DEPT-135 NMR spectrum of compound **10a'**

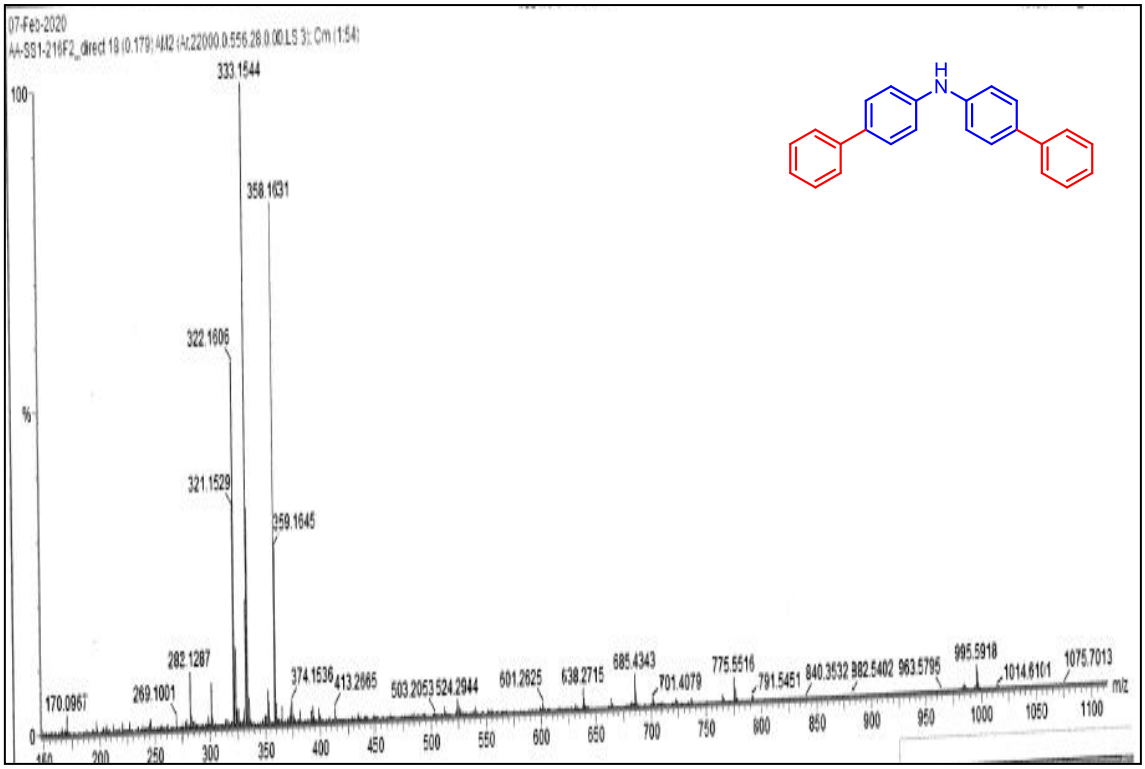


Figure 135. HRMS spectrum of compound **10a'**

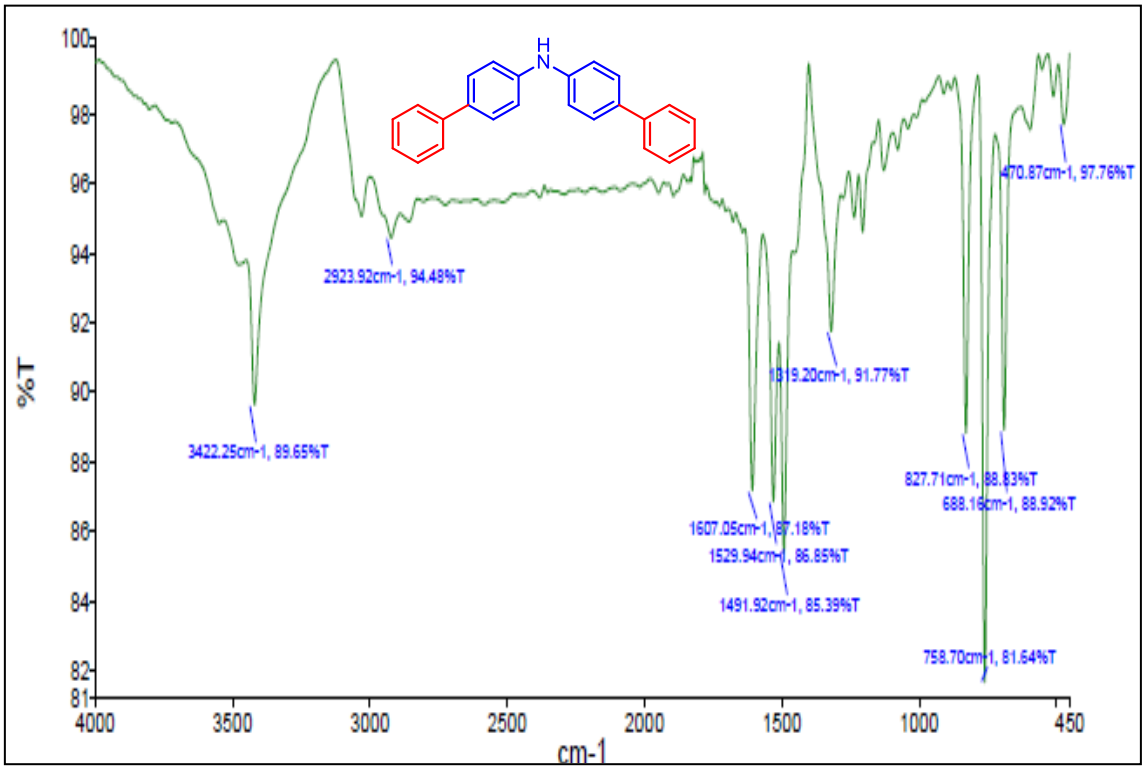


Figure 136. FTIR spectrum of compound **10a'**

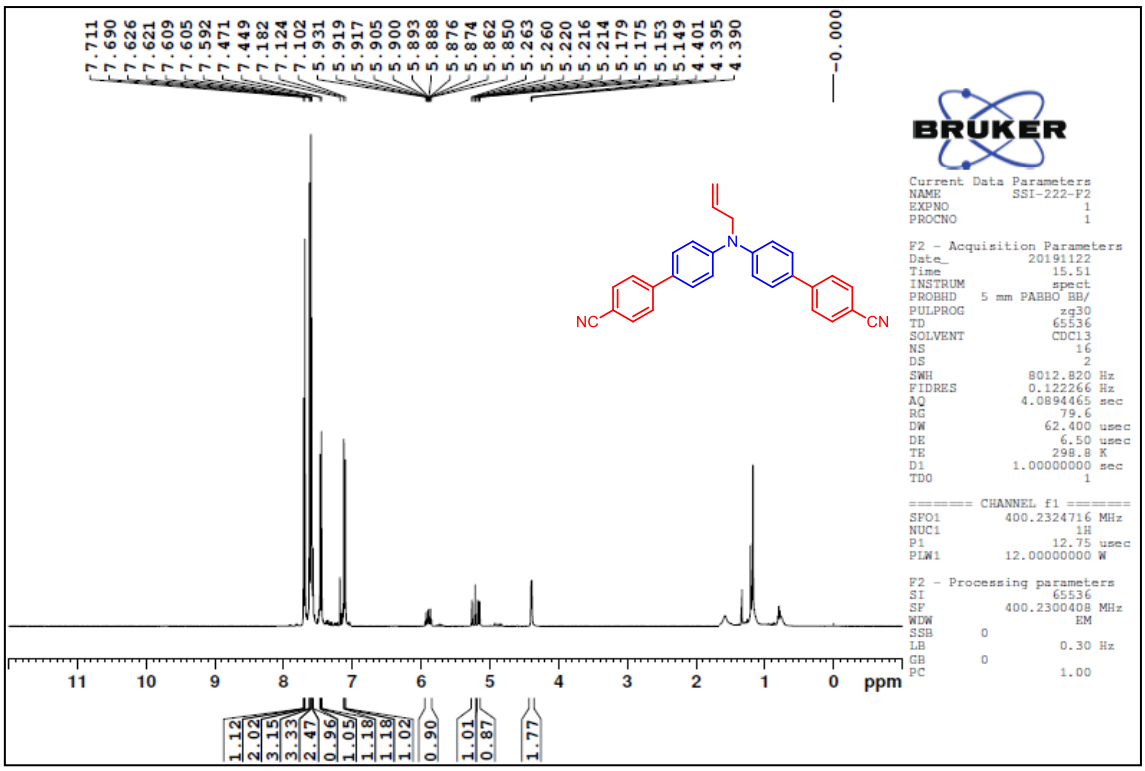


Figure 137. ^{1}H NMR spectrum of compound **10b**

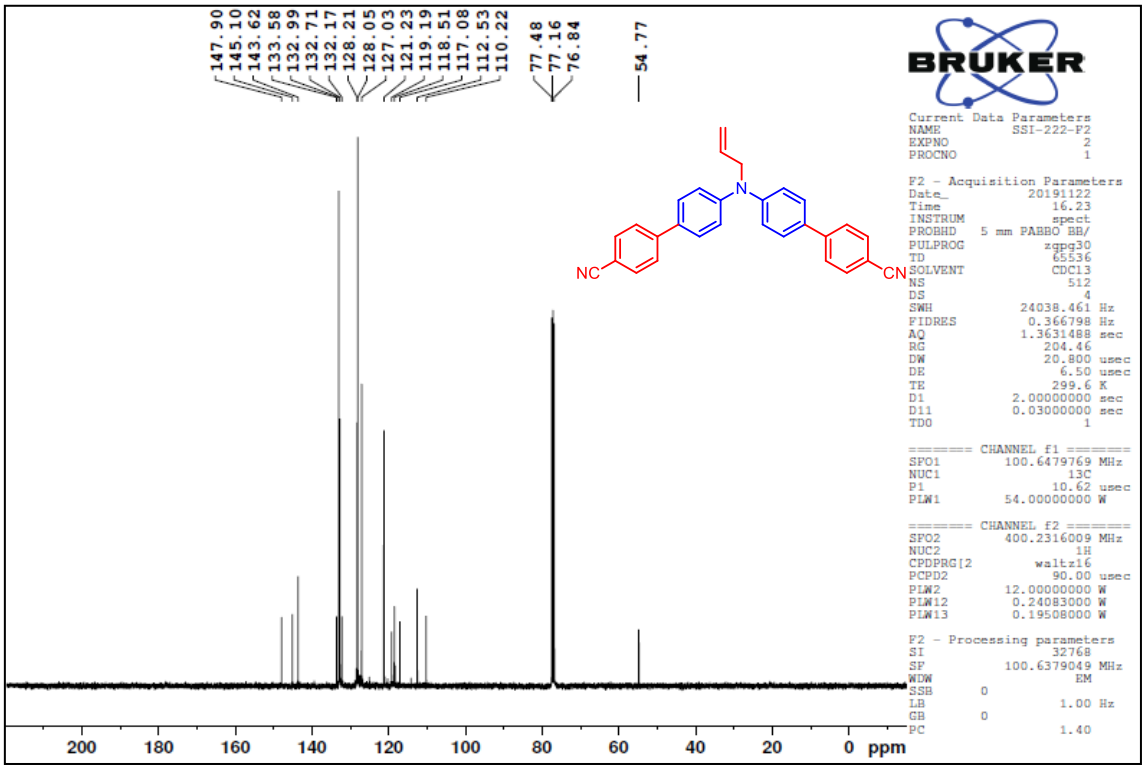


Figure 138. ^{13}C NMR spectrum of compound **10b**

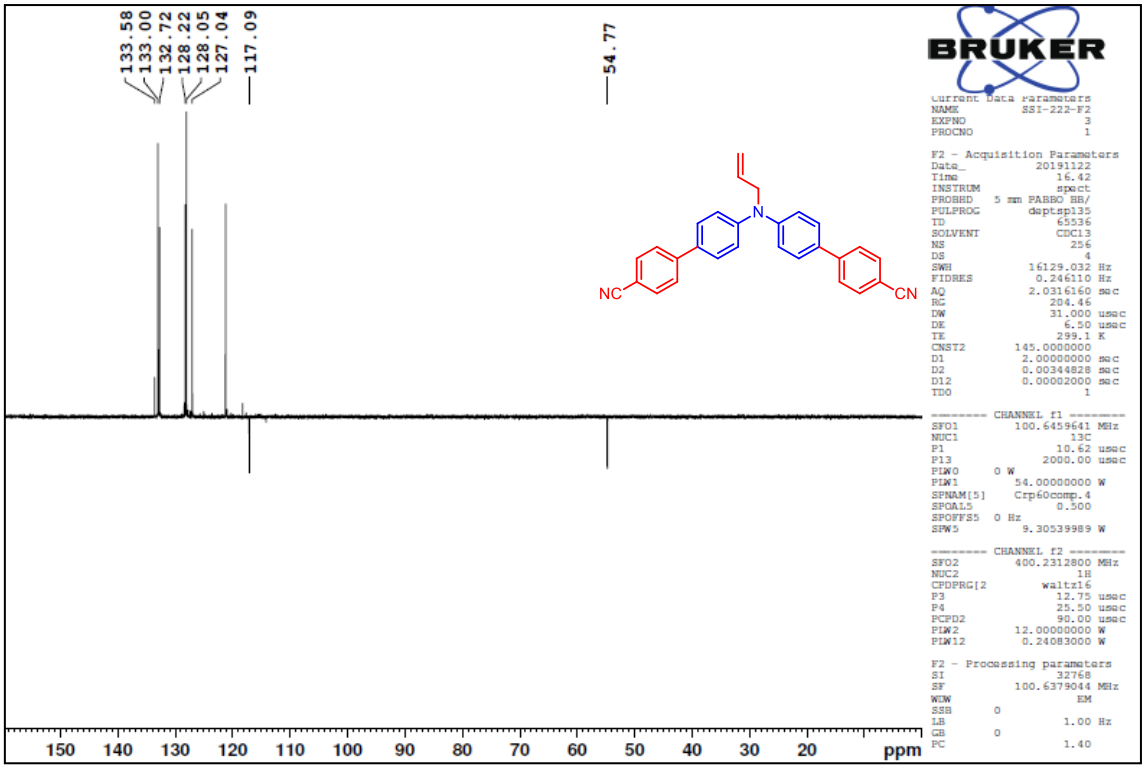


Figure 139. DEPT-135 NMR spectrum of compound **10b**

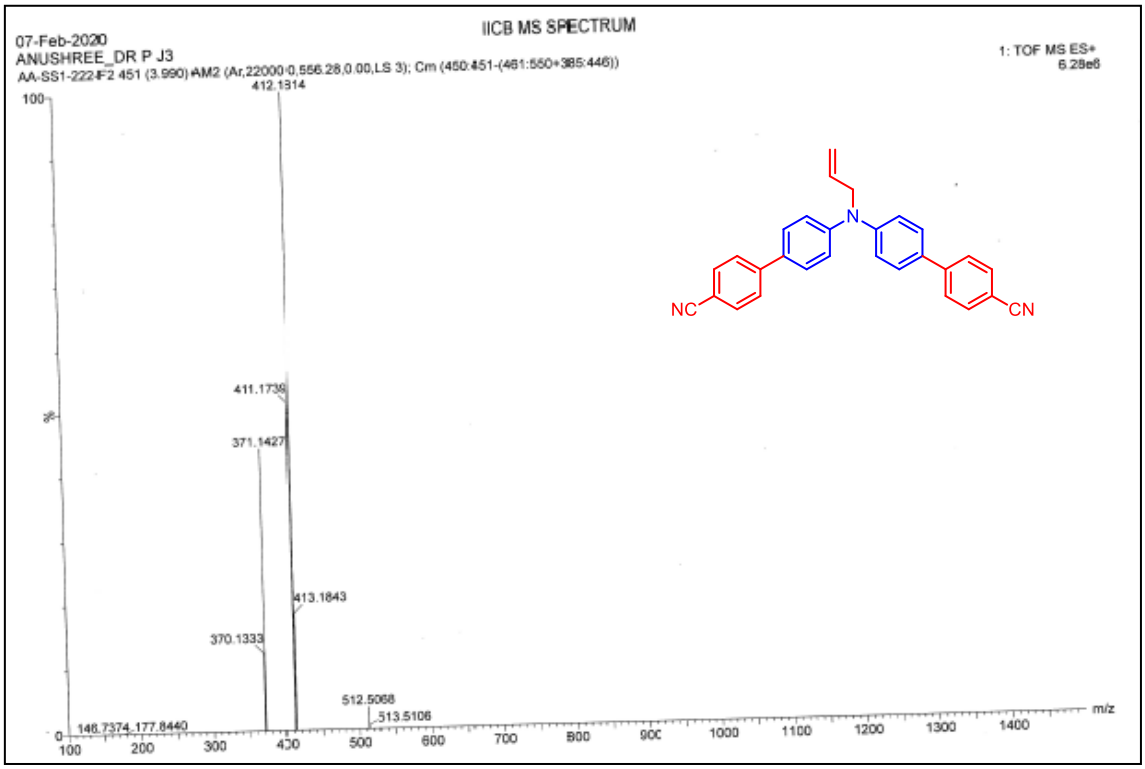


Figure 140. HRMS spectrum of compound **10b**

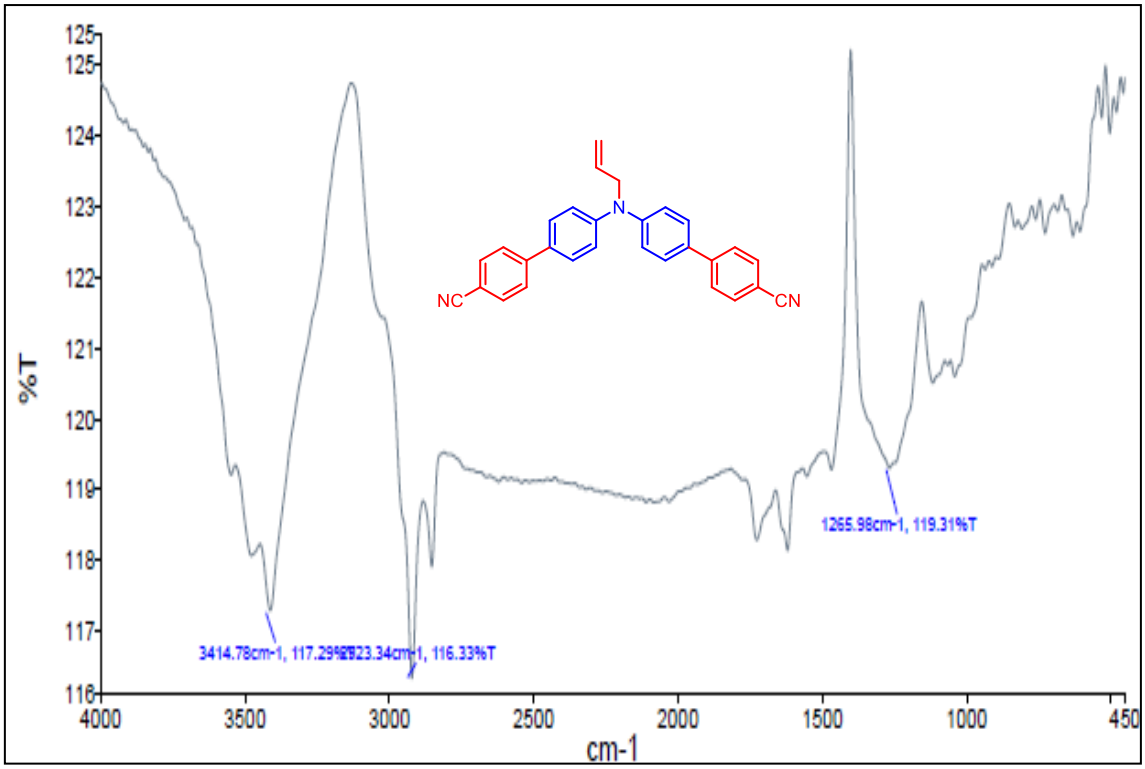


Figure 141. FTIR spectrum of compound **10b**

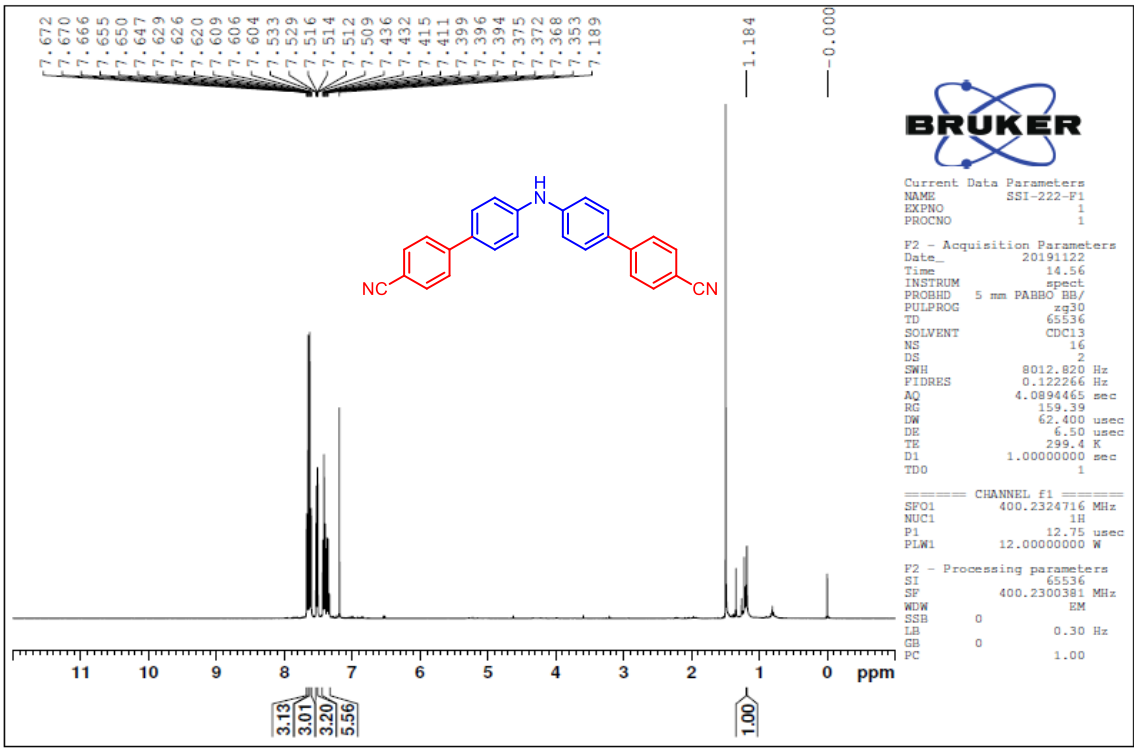


Figure 142. ^{1}H NMR spectrum of compound **10b'**

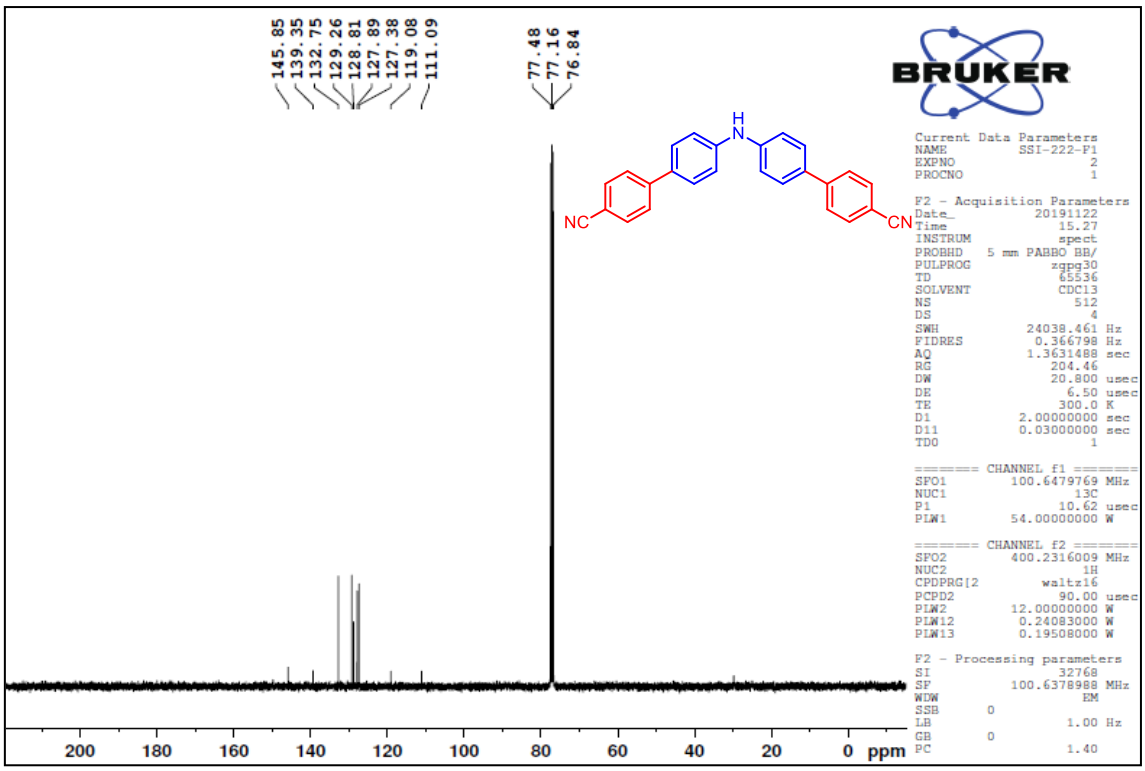


Figure 143. ^{13}C NMR spectrum of compound **10b'**

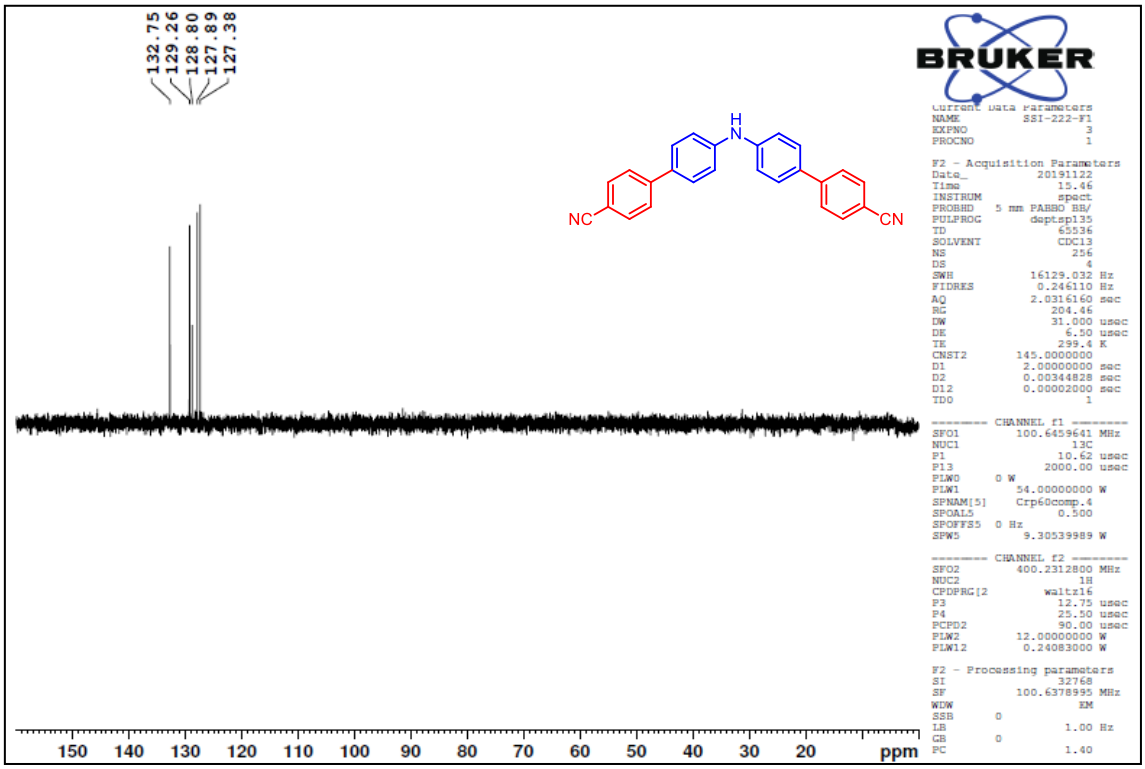


Figure 144. DEPT-135 NMR spectrum of compound **10b'**

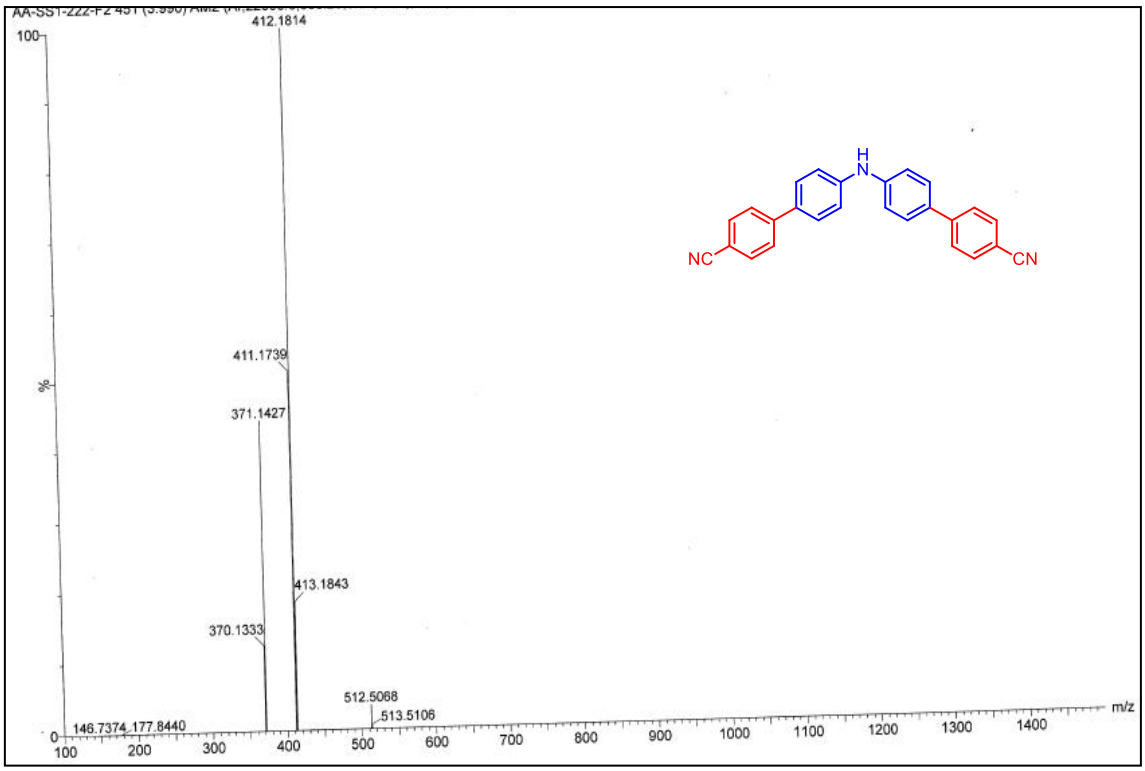


Figure 145. HRMS spectrum of compound **10b'**

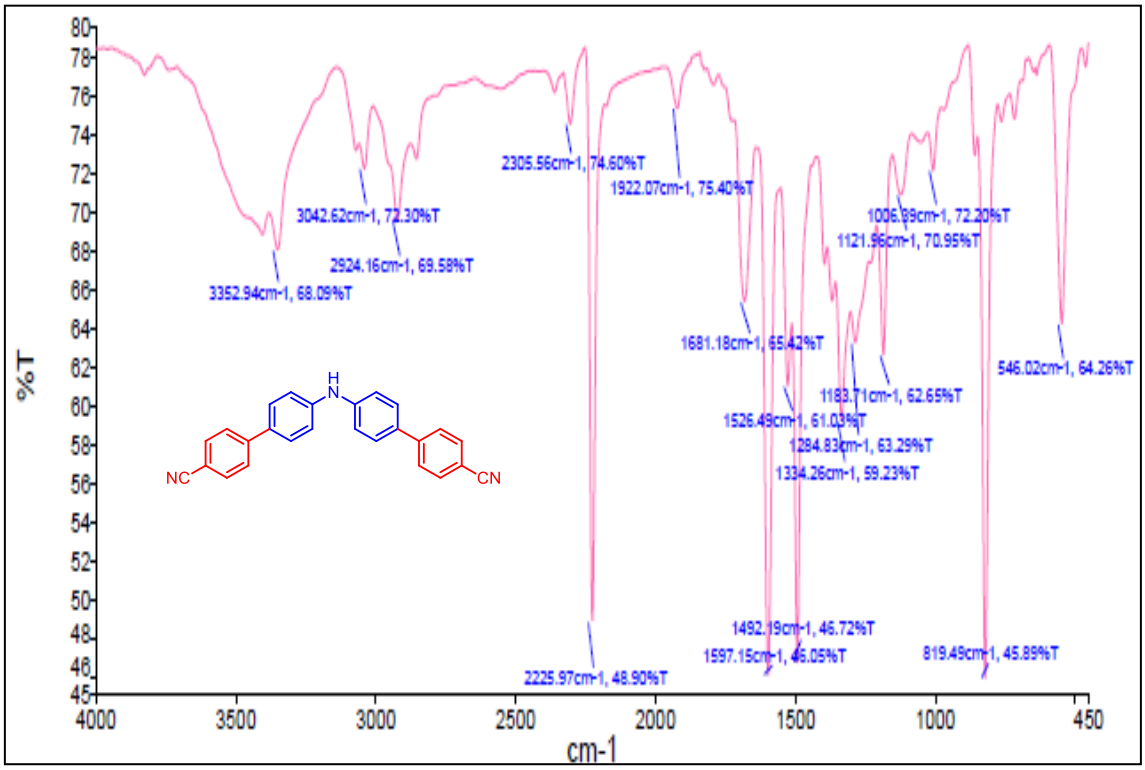


Figure 146. FTIR spectrum of compound **3b**

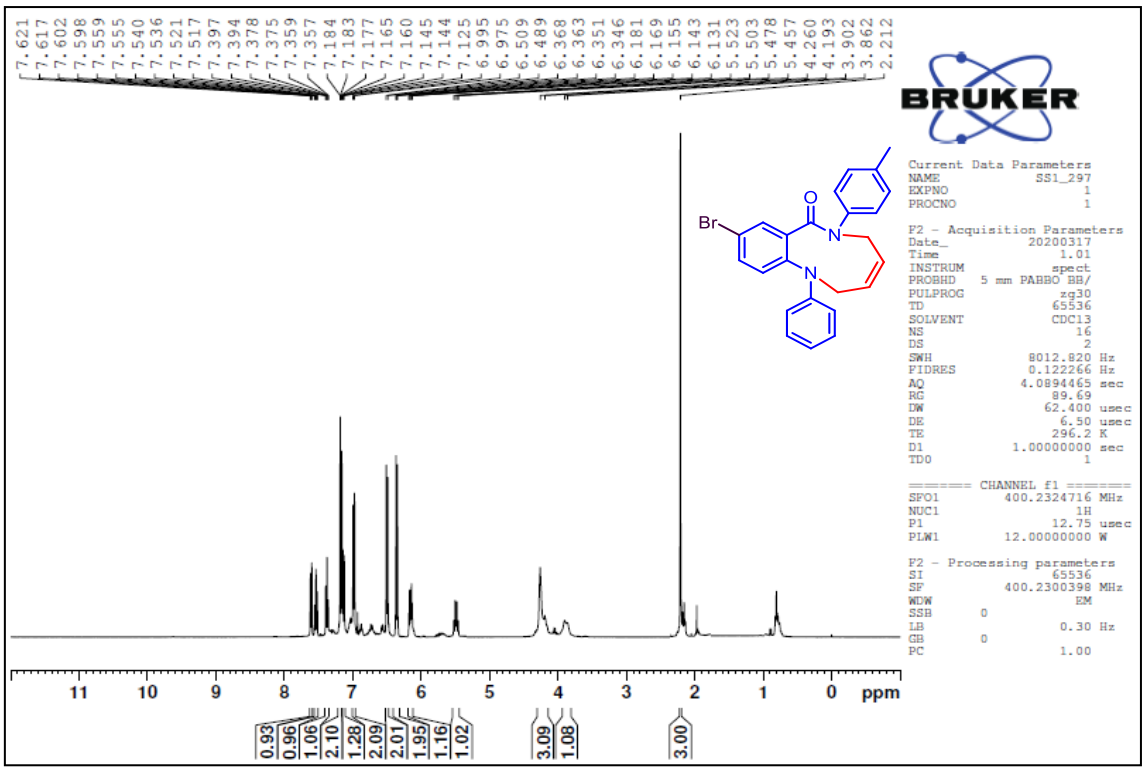


Figure 147. ^{1}H NMR spectrum of compound **11a**

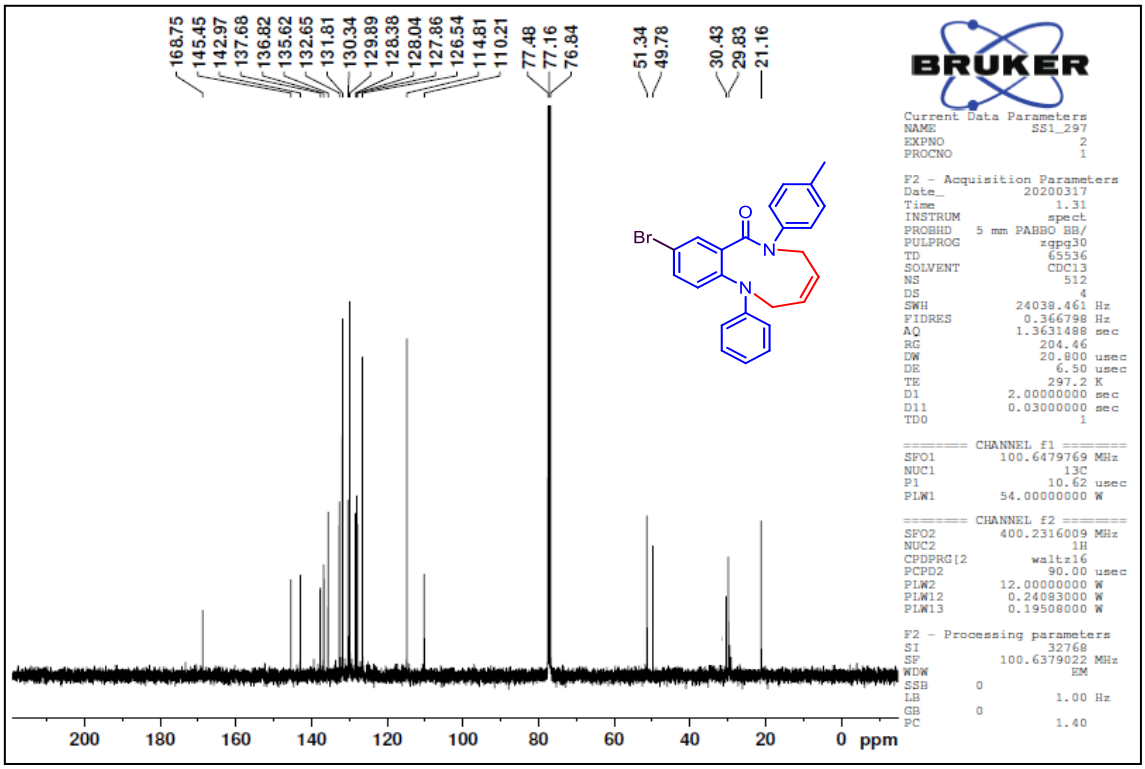


Figure 148. ^{13}C NMR spectrum of compound **11a**

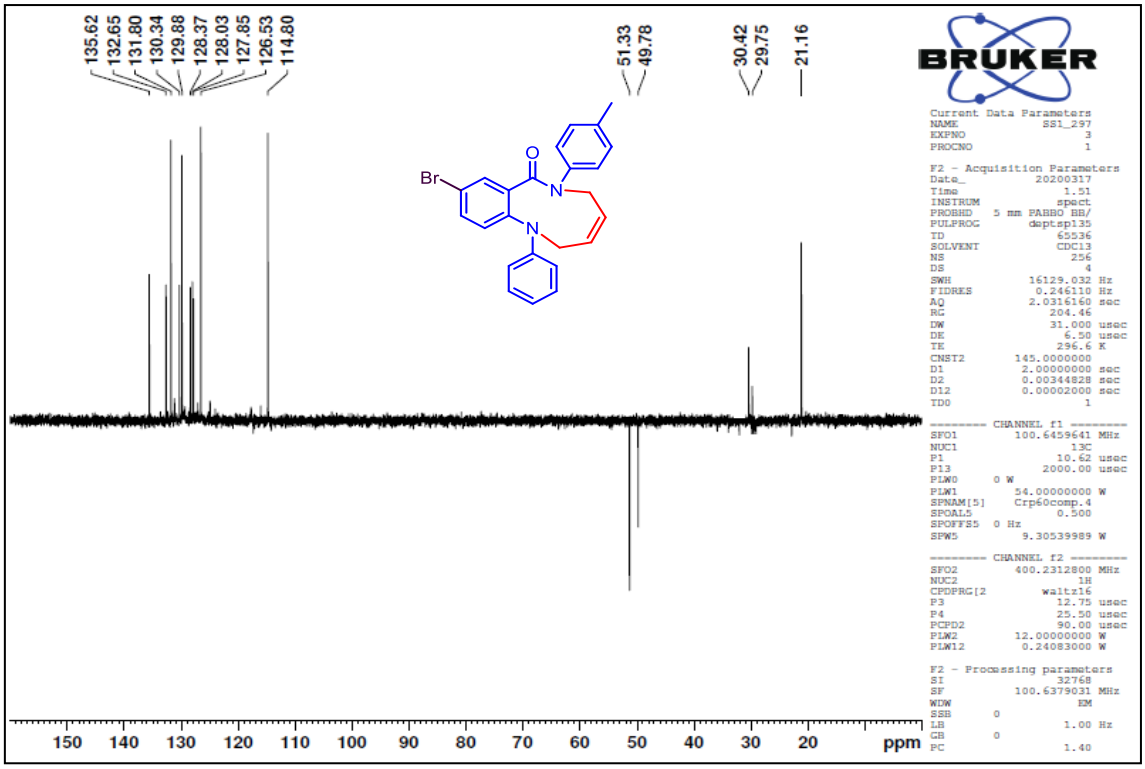


Figure 149. DEPT-135 NMR spectrum of compound **11a**

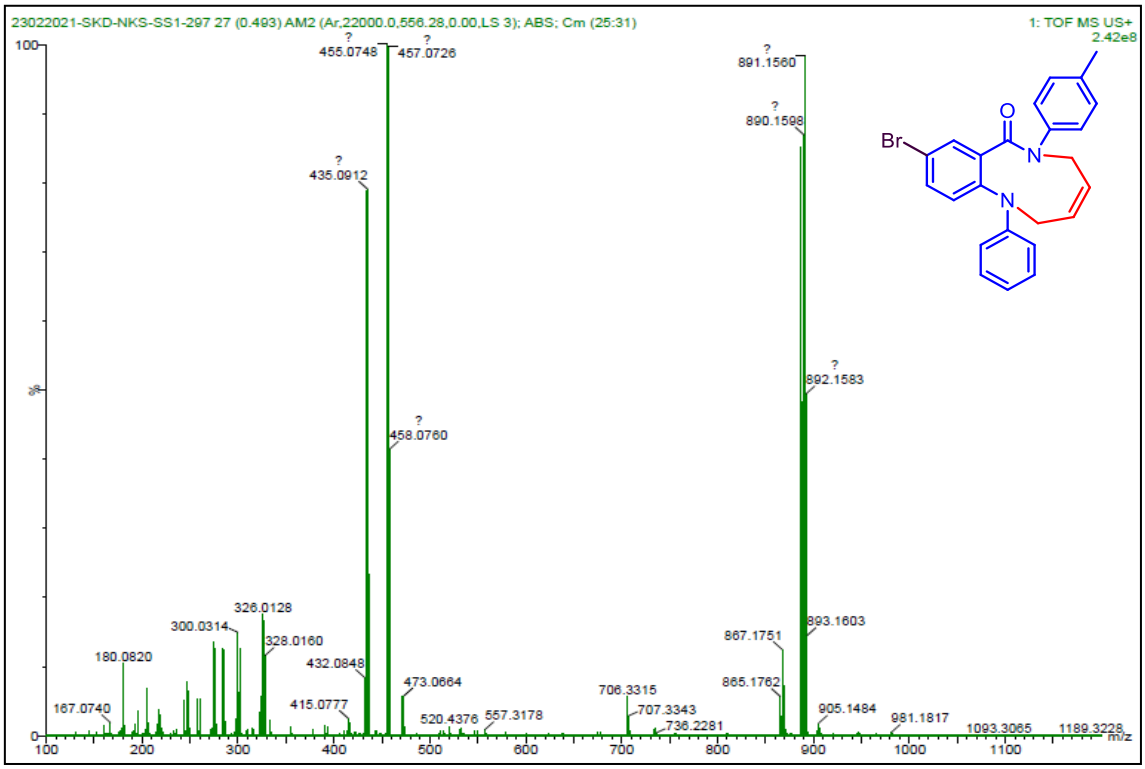


Figure 150. HRMS spectrum of compound **11a**

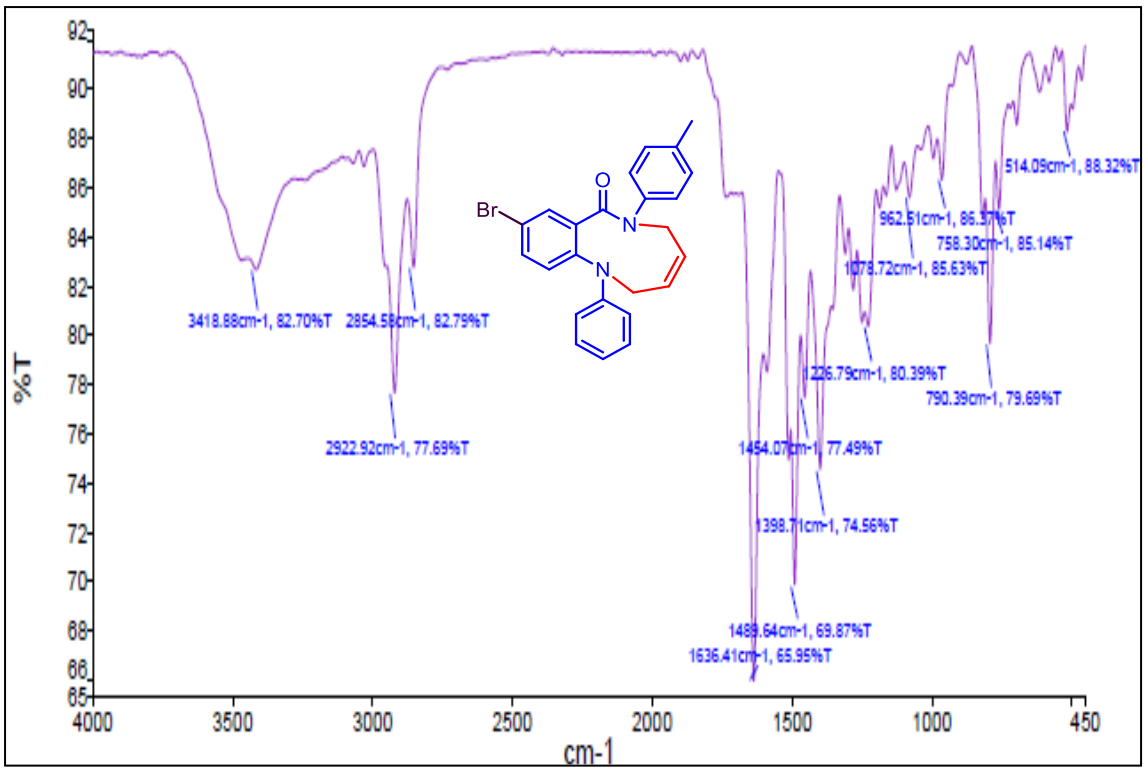
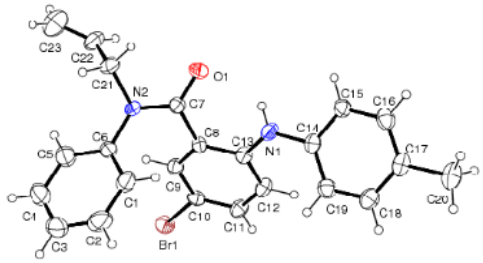


Figure 151. FTIR spectrum of compound **11a**



ORTEP diagram of compounds **3c** (CCDC-2101632)

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

Identification code	3c	
Empirical formula	C23 H21 Br N2 O	
Formula weight	421.33	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 10.519(3) Å	□= 90°.
	b = 9.117(2) Å	□= 90.312(7)°.
	c = 20.975(6) Å	□ = 90°.
Volume	2011.5(9) $Å^3$	
Z	4	
Density (calculated)	1.391 Mg/m^3	
Absorption coefficient	2.058 mm^{-1}	
F(000)	864	
Crystal size	0.200 x 0.180 x 0.150 mm^3	
Theta range for data collection	1.942 to 25.498°.	
Index ranges	-12<=h<=12, -11<=k<=11, -25<=l<=25	
Reflections collected	15037	
Independent reflections	3742 [R(int) = 0.0965]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.4182	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3742 / 0 / 248	
Goodness-of-fit on F^2	1.006	
Final R indices [I>2sigma(I)]	R1 = 0.0526, wR2 = 0.0890	
R indices (all data)	R1 = 0.1305, wR2 = 0.1110	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.421 and -0.417 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3c**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2030(5)	3703(5)	3002(2)	59(1)
C(2)	1531(7)	4485(8)	2488(3)	88(2)
C(3)	492(7)	5345(8)	2565(4)	98(3)
C(4)	-81(6)	5436(6)	3141(4)	85(2)
C(5)	403(5)	4677(5)	3658(3)	62(2)
C(6)	1461(4)	3812(4)	3586(2)	40(1)
C(7)	3135(4)	2838(5)	4313(2)	35(1)
C(8)	4031(4)	4058(4)	4154(2)	34(1)
C(9)	3638(4)	5509(4)	4239(2)	39(1)
C(10)	4485(5)	6655(4)	4166(2)	38(1)
C(11)	5728(5)	6374(5)	4016(2)	48(1)
C(12)	6140(4)	4940(5)	3934(2)	45(1)
C(13)	5294(4)	3782(4)	4008(2)	38(1)
C(14)	6771(4)	1793(4)	3637(2)	38(1)
C(15)	7288(4)	455(5)	3845(2)	46(1)
C(16)	8326(5)	-119(5)	3540(2)	53(1)
C(17)	8921(5)	568(6)	3040(2)	51(1)
C(18)	8397(5)	1862(5)	2832(2)	52(1)
C(19)	7352(5)	2449(5)	3115(2)	48(1)
C(20)	10124(5)	-39(6)	2749(2)	74(2)
C(21)	1015(5)	1836(5)	4365(2)	53(1)
C(22)	543(5)	2249(6)	5004(3)	69(2)
C(23)	-588(6)	2235(6)	5187(3)	94(2)
N(2)	1915(3)	2924(4)	4105(2)	39(1)
O(1)	3497(3)	1826(3)	4647(2)	53(1)
Br(1)	3940(1)	8611(1)	4299(1)	53(1)
N(1)	5687(4)	2319(4)	3934(2)	46(1)

Table 3. Bond lengths [Å] and angles [°] for **3c.**

C(1)-C(6)	1.371(6)
C(1)-C(2)	1.393(7)
C(1)-H(1)	0.9300
C(2)-C(3)	1.356(8)
C(2)-H(2)	0.9300
C(3)-C(4)	1.355(8)
C(3)-H(3)	0.9300
C(4)-C(5)	1.381(7)
C(4)-H(4)	0.9300
C(5)-C(6)	1.372(6)
C(5)-H(5)	0.9300
C(6)-N(2)	1.436(5)
C(7)-O(1)	1.218(4)
C(7)-N(2)	1.355(5)
C(7)-C(8)	1.498(6)
C(8)-C(13)	1.388(5)
C(8)-C(9)	1.397(5)
C(9)-C(10)	1.382(6)
C(9)-H(9)	0.9300
C(10)-C(11)	1.370(6)
C(10)-Br(1)	1.895(4)
C(11)-C(12)	1.389(5)
C(11)-H(11)	0.9300
C(12)-C(13)	1.391(5)
C(12)-H(12)	0.9300
C(13)-N(1)	1.405(5)
C(14)-N(1)	1.388(5)
C(14)-C(19)	1.392(6)
C(14)-C(15)	1.404(6)
C(15)-C(16)	1.371(6)
C(15)-H(15)	0.9300
C(16)-C(17)	1.376(6)
C(16)-H(16)	0.9300
C(17)-C(18)	1.373(6)
C(17)-C(20)	1.513(6)
C(18)-C(19)	1.361(6)

C(18)-H(18)	0.9300
C(19)-H(19)	0.9300
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(21)-N(2)	1.478(5)
C(21)-C(22)	1.480(6)
C(21)-H(21A)	0.9700
C(21)-H(21B)	0.9700
C(22)-C(23)	1.252(7)
C(22)-H(22)	0.9300
C(23)-H(23A)	0.9300
C(23)-H(23B)	0.9300
N(1)-H(1A)	0.85(4)
C(6)-C(1)-C(2)	119.4(5)
C(6)-C(1)-H(1)	120.3
C(2)-C(1)-H(1)	120.3
C(3)-C(2)-C(1)	120.2(6)
C(3)-C(2)-H(2)	119.9
C(1)-C(2)-H(2)	119.9
C(4)-C(3)-C(2)	120.4(6)
C(4)-C(3)-H(3)	119.8
C(2)-C(3)-H(3)	119.8
C(3)-C(4)-C(5)	120.3(6)
C(3)-C(4)-H(4)	119.8
C(5)-C(4)-H(4)	119.8
C(6)-C(5)-C(4)	119.9(5)
C(6)-C(5)-H(5)	120.1
C(4)-C(5)-H(5)	120.1
C(1)-C(6)-C(5)	119.8(5)
C(1)-C(6)-N(2)	119.4(4)
C(5)-C(6)-N(2)	120.5(4)
O(1)-C(7)-N(2)	121.4(4)
O(1)-C(7)-C(8)	119.8(4)
N(2)-C(7)-C(8)	118.7(4)
C(13)-C(8)-C(9)	119.0(4)
C(13)-C(8)-C(7)	121.2(4)
C(9)-C(8)-C(7)	119.2(4)

C(10)-C(9)-C(8)	120.7(4)
C(10)-C(9)-H(9)	119.7
C(8)-C(9)-H(9)	119.7
C(11)-C(10)-C(9)	120.1(4)
C(11)-C(10)-Br(1)	120.0(3)
C(9)-C(10)-Br(1)	120.0(4)
C(10)-C(11)-C(12)	120.2(4)
C(10)-C(11)-H(11)	119.9
C(12)-C(11)-H(11)	119.9
C(11)-C(12)-C(13)	120.0(4)
C(11)-C(12)-H(12)	120.0
C(13)-C(12)-H(12)	120.0
C(8)-C(13)-C(12)	120.0(4)
C(8)-C(13)-N(1)	118.7(4)
C(12)-C(13)-N(1)	121.3(4)
N(1)-C(14)-C(19)	124.7(4)
N(1)-C(14)-C(15)	118.6(4)
C(19)-C(14)-C(15)	116.6(4)
C(16)-C(15)-C(14)	119.7(4)
C(16)-C(15)-H(15)	120.2
C(14)-C(15)-H(15)	120.2
C(15)-C(16)-C(17)	123.2(5)
C(15)-C(16)-H(16)	118.4
C(17)-C(16)-H(16)	118.4
C(18)-C(17)-C(16)	116.7(4)
C(18)-C(17)-C(20)	121.5(5)
C(16)-C(17)-C(20)	121.8(5)
C(19)-C(18)-C(17)	121.6(5)
C(19)-C(18)-H(18)	119.2
C(17)-C(18)-H(18)	119.2
C(18)-C(19)-C(14)	122.1(4)
C(18)-C(19)-H(19)	118.9
C(14)-C(19)-H(19)	118.9
C(17)-C(20)-H(20A)	109.5
C(17)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(17)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5

H(20B)-C(20)-H(20C)	109.5
N(2)-C(21)-C(22)	112.5(4)
N(2)-C(21)-H(21A)	109.1
C(22)-C(21)-H(21A)	109.1
N(2)-C(21)-H(21B)	109.1
C(22)-C(21)-H(21B)	109.1
H(21A)-C(21)-H(21B)	107.8
C(23)-C(22)-C(21)	126.8(6)
C(23)-C(22)-H(22)	116.6
C(21)-C(22)-H(22)	116.6
C(22)-C(23)-H(23A)	120.0
C(22)-C(23)-H(23B)	120.0
H(23A)-C(23)-H(23B)	120.0
C(7)-N(2)-C(6)	126.0(4)
C(7)-N(2)-C(21)	116.7(4)
C(6)-N(2)-C(21)	116.5(4)
C(14)-N(1)-C(13)	128.4(4)
C(14)-N(1)-H(1A)	118(3)
C(13)-N(1)-H(1A)	111(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **3c**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	41(3)	84(4)	51(3)	2(3)	-2(3)	-9(3)
C(2)	66(5)	151(6)	47(4)	23(4)	-10(4)	-29(5)
C(3)	59(5)	126(6)	108(6)	62(5)	-34(5)	-31(4)
C(4)	64(5)	64(4)	125(6)	27(4)	-19(5)	6(3)
C(5)	53(4)	62(4)	72(4)	-1(3)	-1(3)	3(3)
C(6)	35(3)	35(3)	50(3)	3(2)	-6(3)	-8(2)
C(7)	34(3)	28(3)	44(3)	-3(2)	4(2)	-1(2)
C(8)	30(3)	34(3)	38(3)	-3(2)	-4(2)	6(2)
C(9)	35(3)	38(3)	44(3)	-1(2)	0(2)	2(2)
C(10)	46(3)	27(3)	40(3)	-1(2)	-1(2)	0(2)
C(11)	48(3)	40(3)	55(3)	-9(2)	6(3)	-11(3)

C(12)	32(3)	49(3)	54(3)	-10(2)	6(2)	-7(2)
C(13)	38(3)	32(3)	43(3)	-4(2)	1(2)	2(2)
C(14)	27(3)	44(3)	42(3)	-11(2)	-5(2)	-4(2)
C(15)	38(3)	44(3)	57(3)	2(2)	2(3)	4(2)
C(16)	46(4)	42(3)	71(4)	-7(3)	-5(3)	7(3)
C(17)	33(3)	63(4)	58(3)	-23(3)	2(3)	-1(3)
C(18)	49(4)	55(3)	50(3)	-11(3)	11(3)	0(3)
C(19)	48(4)	45(3)	51(3)	-1(2)	2(3)	7(3)
C(20)	49(4)	86(4)	88(4)	-21(3)	8(3)	13(3)
C(21)	45(3)	47(3)	66(4)	8(3)	5(3)	-15(2)
C(22)	45(4)	98(4)	64(4)	21(3)	9(3)	-15(3)
C(23)	86(6)	103(5)	94(5)	-19(4)	19(4)	-13(4)
N(2)	33(3)	38(2)	46(2)	7(2)	1(2)	-8(2)
O(1)	52(2)	34(2)	71(2)	14(2)	-2(2)	1(2)
Br(1)	60(1)	32(1)	67(1)	-2(1)	0(1)	0(1)
N(1)	37(3)	39(2)	63(3)	3(2)	15(2)	2(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **3c**.

	x	y	z	U(eq)
H(1)	2743	3112	2949	70
H(2)	1913	4418	2090	106
H(3)	170	5875	2222	117
H(4)	-804	6012	3188	101
H(5)	14	4752	4053	75
H(9)	2798	5705	4346	47
H(11)	6297	7147	3969	57
H(12)	6983	4755	3829	54
H(15)	6929	-39	4187	55
H(16)	8642	-1018	3678	64
H(18)	8764	2350	2490	62
H(19)	7014	3317	2954	58
H(20A)	10300	469	2358	112
H(20B)	10015	-1066	2663	112
H(20C)	10821	94	3040	112
H(21A)	1433	890	4392	63

H(21B)	298	1739	4075	63
H(22)	1150	2551	5300	83
H(23A)	-1231	1942	4909	113
H(23B)	-784	2517	5601	113
H(1A)	5310(40)	1760(40)	4199(19)	56

Table 6. Torsion angles [°] for**3c**.

C(6)-C(1)-C(2)-C(3)	-0.1(9)
C(1)-C(2)-C(3)-C(4)	-0.9(10)
C(2)-C(3)-C(4)-C(5)	1.3(10)
C(3)-C(4)-C(5)-C(6)	-0.8(9)
C(2)-C(1)-C(6)-C(5)	0.5(7)
C(2)-C(1)-C(6)-N(2)	175.4(4)
C(4)-C(5)-C(6)-C(1)	-0.1(7)
C(4)-C(5)-C(6)-N(2)	-175.0(4)
O(1)-C(7)-C(8)-C(13)	40.3(6)
N(2)-C(7)-C(8)-C(13)	-142.7(4)
O(1)-C(7)-C(8)-C(9)	-130.6(4)
N(2)-C(7)-C(8)-C(9)	46.4(6)
C(13)-C(8)-C(9)-C(10)	1.4(6)
C(7)-C(8)-C(9)-C(10)	172.6(4)
C(8)-C(9)-C(10)-C(11)	-0.8(6)
C(8)-C(9)-C(10)-Br(1)	-178.9(3)
C(9)-C(10)-C(11)-C(12)	0.3(7)
Br(1)-C(10)-C(11)-C(12)	178.4(3)
C(10)-C(11)-C(12)-C(13)	-0.5(7)
C(9)-C(8)-C(13)-C(12)	-1.6(6)
C(7)-C(8)-C(13)-C(12)	-172.6(4)
C(9)-C(8)-C(13)-N(1)	178.9(4)
C(7)-C(8)-C(13)-N(1)	8.0(6)
C(11)-C(12)-C(13)-C(8)	1.2(7)
C(11)-C(12)-C(13)-N(1)	-179.4(4)
N(1)-C(14)-C(15)-C(16)	177.1(4)
C(19)-C(14)-C(15)-C(16)	1.0(6)
C(14)-C(15)-C(16)-C(17)	1.5(7)
C(15)-C(16)-C(17)-C(18)	-2.6(7)
C(15)-C(16)-C(17)-C(20)	175.2(4)

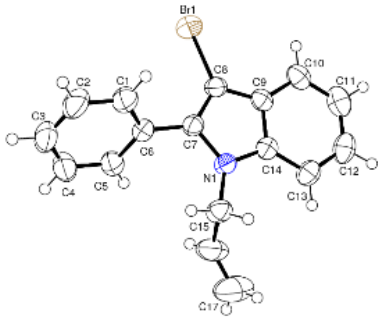
C(16)-C(17)-C(18)-C(19)	1.1(7)
C(20)-C(17)-C(18)-C(19)	-176.6(4)
C(17)-C(18)-C(19)-C(14)	1.4(7)
N(1)-C(14)-C(19)-C(18)	-178.3(4)
C(15)-C(14)-C(19)-C(18)	-2.5(6)
N(2)-C(21)-C(22)-C(23)	132.8(6)
O(1)-C(7)-N(2)-C(6)	-162.3(4)
C(8)-C(7)-N(2)-C(6)	20.8(6)
O(1)-C(7)-N(2)-C(21)	7.2(6)
C(8)-C(7)-N(2)-C(21)	-169.7(3)
C(1)-C(6)-N(2)-C(7)	53.1(6)
C(5)-C(6)-N(2)-C(7)	-132.0(5)
C(1)-C(6)-N(2)-C(21)	-116.3(5)
C(5)-C(6)-N(2)-C(21)	58.5(5)
C(22)-C(21)-N(2)-C(7)	81.2(5)
C(22)-C(21)-N(2)-C(6)	-108.4(5)
C(19)-C(14)-N(1)-C(13)	-32.5(7)
C(15)-C(14)-N(1)-C(13)	151.8(4)
C(8)-C(13)-N(1)-C(14)	161.8(4)
C(12)-C(13)-N(1)-C(14)	-17.6(7)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **3c**[Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...O(1)	0.85(4)	2.13(4)	2.790(5)	134(4)

Symmetry transformations used to generate equivalent atoms:



ORTEP diagram of compounds**3l** (CCDC-2045826)

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

Identification code	3l	
Empirical formula	C17 H14 Br N	
Formula weight	312.20	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P n a 21	
Unit cell dimensions	a = 8.2567(5) Å	□= 90°.
	b = 19.7843(11) Å	□= 90°.
	c = 8.8668(5) Å	□ = 90°.
Volume	1448.42(14) $Å^3$	
Z	4	
Density (calculated)	1.432 Mg/m^3	
Absorption coefficient	2.823 mm^{-1}	
F(000)	632	
Crystal size	0.200 x 0.200 x 0.180 mm^3	
Theta range for data collection	3.851 to 29.616°.	
Index ranges	-11<=h<=11, -27<=k<=27, -12<=l<=10	
Reflections collected	40196	
Independent reflections	3972 [R(int) = 0.0631]	
Completeness to theta = 25.242°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.4940	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3972 / 1 / 173	
Goodness-of-fit on F^2	1.022	
Final R indices [I>2sigma(I)]	R1 = 0.0372, wR2 = 0.0825	

R indices (all data)	R1 = 0.0587, wR2 = 0.0907
Absolute structure parameter	0.045(6)
Extinction coefficient	0.059(5)
Largest diff. peak and hole	0.338 and -0.343 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3)for **3l**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	653(6)	8115(2)	-4(5)	55(1)
C(2)	251(6)	7695(2)	1178(6)	68(1)
C(3)	822(7)	7809(2)	2589(6)	69(1)
C(4)	1810(6)	8358(3)	2859(5)	64(1)
C(5)	2228(5)	8786(2)	1696(4)	49(1)
C(6)	1655(4)	8669(2)	245(4)	41(1)
C(7)	2115(4)	9109(2)	-1024(4)	38(1)
C(8)	2907(4)	8957(2)	-2330(4)	41(1)
C(9)	3151(4)	9552(2)	-3185(4)	39(1)
C(10)	3867(4)	9703(2)	-4576(4)	50(1)
C(11)	3846(5)	10365(2)	-5069(5)	58(1)
C(12)	3128(5)	10875(2)	-4219(5)	57(1)
C(13)	2423(4)	10743(2)	-2835(6)	48(1)
C(14)	2443(4)	10077(2)	-2329(4)	38(1)
C(15)	794(4)	10172(2)	35(5)	49(1)
C(16)	1740(6)	10625(3)	1059(6)	70(1)
C(17)	1458(8)	11234(3)	1336(9)	101(2)
N(1)	1830(3)	9805(1)	-1020(3)	38(1)
Br(1)	3667(1)	8101(1)	-2899(1)	77(1)

Table 3. Bond lengths [Å] and angles [°] for **3l**.

C(1)-C(2)	1.378(6)
C(1)-C(6)	1.392(5)
C(1)-H(1)	0.9300
C(2)-C(3)	1.356(7)
C(2)-H(2)	0.9300
C(3)-C(4)	1.379(8)
C(3)-H(3)	0.9300
C(4)-C(5)	1.379(6)

C(4)-H(4)	0.9300
C(5)-C(6)	1.390(5)
C(5)-H(5)	0.9300
C(6)-C(7)	1.472(5)
C(7)-C(8)	1.363(5)
C(7)-N(1)	1.398(4)
C(8)-C(9)	1.415(5)
C(8)-Br(1)	1.876(3)
C(9)-C(10)	1.399(5)
C(9)-C(14)	1.412(5)
C(10)-C(11)	1.380(6)
C(10)-H(10)	0.9300
C(11)-C(12)	1.392(7)
C(11)-H(11)	0.9300
C(12)-C(13)	1.383(7)
C(12)-H(12)	0.9300
C(13)-C(14)	1.393(4)
C(13)-H(13)	0.9300
C(14)-N(1)	1.375(4)
C(15)-N(1)	1.461(4)
C(15)-C(16)	1.496(6)
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(16)-C(17)	1.250(7)
C(16)-H(16)	0.9300
C(17)-H(17A)	0.9300
C(17)-H(17B)	0.9300
C(2)-C(1)-C(6)	119.8(4)
C(2)-C(1)-H(1)	120.1
C(6)-C(1)-H(1)	120.1
C(3)-C(2)-C(1)	121.2(4)
C(3)-C(2)-H(2)	119.4
C(1)-C(2)-H(2)	119.4
C(2)-C(3)-C(4)	119.8(4)
C(2)-C(3)-H(3)	120.1
C(4)-C(3)-H(3)	120.1
C(5)-C(4)-C(3)	120.2(4)
C(5)-C(4)-H(4)	119.9

C(3)-C(4)-H(4)	119.9
C(4)-C(5)-C(6)	120.3(4)
C(4)-C(5)-H(5)	119.8
C(6)-C(5)-H(5)	119.8
C(5)-C(6)-C(1)	118.7(3)
C(5)-C(6)-C(7)	121.4(3)
C(1)-C(6)-C(7)	119.9(3)
C(8)-C(7)-N(1)	107.5(3)
C(8)-C(7)-C(6)	130.1(3)
N(1)-C(7)-C(6)	122.4(3)
C(7)-C(8)-C(9)	109.9(3)
C(7)-C(8)-Br(1)	126.0(3)
C(9)-C(8)-Br(1)	124.0(2)
C(10)-C(9)-C(14)	119.5(3)
C(10)-C(9)-C(8)	135.2(3)
C(14)-C(9)-C(8)	105.3(3)
C(11)-C(10)-C(9)	118.4(4)
C(11)-C(10)-H(10)	120.8
C(9)-C(10)-H(10)	120.8
C(10)-C(11)-C(12)	121.4(4)
C(10)-C(11)-H(11)	119.3
C(12)-C(11)-H(11)	119.3
C(13)-C(12)-C(11)	121.5(4)
C(13)-C(12)-H(12)	119.3
C(11)-C(12)-H(12)	119.3
C(12)-C(13)-C(14)	117.4(4)
C(12)-C(13)-H(13)	121.3
C(14)-C(13)-H(13)	121.3
N(1)-C(14)-C(13)	129.6(3)
N(1)-C(14)-C(9)	108.6(3)
C(13)-C(14)-C(9)	121.8(3)
N(1)-C(15)-C(16)	112.4(3)
N(1)-C(15)-H(15A)	109.1
C(16)-C(15)-H(15A)	109.1
N(1)-C(15)-H(15B)	109.1
C(16)-C(15)-H(15B)	109.1
H(15A)-C(15)-H(15B)	107.9
C(17)-C(16)-C(15)	126.8(5)

C(17)-C(16)-H(16)	116.6
C(15)-C(16)-H(16)	116.6
C(16)-C(17)-H(17A)	120.0
C(16)-C(17)-H(17B)	120.0
H(17A)-C(17)-H(17B)	120.0
C(14)-N(1)-C(7)	108.7(3)
C(14)-N(1)-C(15)	124.2(3)
C(7)-N(1)-C(15)	126.2(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **3l**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	66(2)	44(2)	55(2)	0(2)	-5(2)	-9(2)
C(2)	82(3)	41(2)	82(3)	10(2)	8(3)	-11(2)
C(3)	86(3)	54(2)	66(3)	21(2)	16(2)	2(2)
C(4)	75(3)	69(3)	47(2)	11(2)	1(2)	6(2)
C(5)	56(2)	48(2)	44(2)	2(1)	-3(2)	-2(2)
C(6)	45(2)	35(2)	43(2)	2(1)	-1(1)	3(1)
C(7)	41(2)	34(1)	39(2)	-1(1)	-6(1)	0(1)
C(8)	46(2)	38(2)	39(2)	-6(1)	-8(1)	7(1)
C(9)	34(2)	47(2)	36(2)	-2(1)	-7(1)	0(1)
C(10)	43(2)	65(2)	41(2)	-1(2)	1(2)	3(2)
C(11)	46(2)	77(3)	51(2)	13(2)	0(2)	-15(2)
C(12)	53(2)	51(2)	68(3)	19(2)	-4(2)	-11(2)
C(13)	46(2)	40(1)	58(2)	3(2)	-1(2)	-4(1)
C(14)	34(2)	39(2)	42(2)	0(1)	-5(1)	-2(1)
C(15)	45(2)	44(2)	57(2)	-2(2)	12(2)	6(2)
C(16)	75(3)	73(3)	62(3)	-25(2)	3(2)	17(2)
C(17)	112(5)	81(4)	111(5)	-43(4)	-12(4)	11(3)
N(1)	39(1)	33(1)	42(1)	-2(1)	4(1)	0(1)
Br(1)	122(1)	51(1)	58(1)	-5(1)	6(1)	31(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **3l**.

	x	y	z	U(eq)
H(1)	256	8027	-966	66
H(2)	-424	7326	1006	82
H(3)	548	7519	3373	82
H(4)	2195	8439	3827	76
H(5)	2897	9155	1883	59
H(10)	4344	9365	-5154	59
H(11)	4323	10472	-5988	70
H(12)	3121	11314	-4591	69
H(13)	1955	11086	-2265	58
H(15A)	189	9850	638	58
H(15B)	21	10441	-529	58
H(16)	2630	10435	1541	84
H(17A)	582	11449	883	122
H(17B)	2125	11472	1994	122

Table 6. Torsion angles [°] for **3l**.

C(6)-C(1)-C(2)-C(3)	-0.4(7)
C(1)-C(2)-C(3)-C(4)	0.6(8)
C(2)-C(3)-C(4)-C(5)	-0.5(8)
C(3)-C(4)-C(5)-C(6)	0.1(7)
C(4)-C(5)-C(6)-C(1)	0.1(6)
C(4)-C(5)-C(6)-C(7)	-178.4(4)
C(2)-C(1)-C(6)-C(5)	0.0(6)
C(2)-C(1)-C(6)-C(7)	178.5(4)
C(5)-C(6)-C(7)-C(8)	119.7(4)
C(1)-C(6)-C(7)-C(8)	-58.8(5)
C(5)-C(6)-C(7)-N(1)	-57.4(5)
C(1)-C(6)-C(7)-N(1)	124.1(4)
N(1)-C(7)-C(8)-C(9)	0.3(4)
C(6)-C(7)-C(8)-C(9)	-177.2(3)
N(1)-C(7)-C(8)-Br(1)	177.4(2)
C(6)-C(7)-C(8)-Br(1)	0.0(5)
C(7)-C(8)-C(9)-C(10)	-179.8(4)

Br(1)-C(8)-C(9)-C(10)	3.0(5)
C(7)-C(8)-C(9)-C(14)	-0.7(4)
Br(1)-C(8)-C(9)-C(14)	-177.9(2)
C(14)-C(9)-C(10)-C(11)	-0.3(5)
C(8)-C(9)-C(10)-C(11)	178.7(4)
C(9)-C(10)-C(11)-C(12)	-0.4(6)
C(10)-C(11)-C(12)-C(13)	0.9(6)
C(11)-C(12)-C(13)-C(14)	-0.7(6)
C(12)-C(13)-C(14)-N(1)	-179.5(3)
C(12)-C(13)-C(14)-C(9)	0.0(5)
C(10)-C(9)-C(14)-N(1)	-179.9(3)
C(8)-C(9)-C(14)-N(1)	0.8(3)
C(10)-C(9)-C(14)-C(13)	0.5(5)
C(8)-C(9)-C(14)-C(13)	-178.8(3)
N(1)-C(15)-C(16)-C(17)	130.9(6)
C(13)-C(14)-N(1)-C(7)	178.9(3)
C(9)-C(14)-N(1)-C(7)	-0.7(3)
C(13)-C(14)-N(1)-C(15)	9.4(5)
C(9)-C(14)-N(1)-C(15)	-170.2(3)
C(8)-C(7)-N(1)-C(14)	0.3(4)
C(6)-C(7)-N(1)-C(14)	177.9(3)
C(8)-C(7)-N(1)-C(15)	169.5(3)
C(6)-C(7)-N(1)-C(15)	-12.8(5)
C(16)-C(15)-N(1)-C(14)	-80.4(5)
C(16)-C(15)-N(1)-C(7)	112.0(4)

Symmetry transformations used to generate equivalent atoms: