Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting information

N,N'–dimethylurea as an efficient ligand for the synthesis of pharma-relevant motifs through Chan–Lam cross-coupling strategy

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Contents:

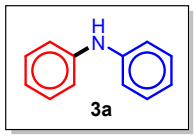
1. General information

All the chemicals used for the reactions were procured commercially and used without further purification. The progress of the reaction was monitored through thin layer chromatography on Merck Kieselgel Silica gel $60F_{254}$ plates using short wave UV light (λ=254 nm). The products were purified by column chromatography using Silica gel (60-120 mesh). The identification of the purified products was done by NMR spectroscopy. The ^{1}H and ^{13}C NMR spectra were recorded on a 400 MHz JEOL NMR spectrometer (400 MHz for ^{1}H and 100 MHz for ^{13}C spectroscopy). Chemical shifts for both ^{1}H (δ_H) and ^{13}C (δ_C) NMR are assigned in parts per million (ppm) using TMS (0 ppm) as the internal reference and $CDCl_3$ and DMSO-d_6 as solvent ($CDCl_3$: δ_H = 7.25 ppm and δ_C = 77.1 ppm; DMSO-d_6: δ_H = 2.5 ppm, DMSO-d_6 absorbed water = 3.3 ppm and δ_C = 40.0 ppm). The multiplicities of the signals are assigned as: s= singlet, d= doublet, t= triplet, q= quartet, m= multiplet and br= broad. Raw NMR data was processed using MestReNova software. Single crystal X-ray diffractions were collected on a Bruker SMART APEX-II CCD diffractometer using Mo Kα (λ =0.71073 Å) radiation.

2. ^{1}H and ^{13}C NMR spectral analysis of the *N*-aryl derivatives.

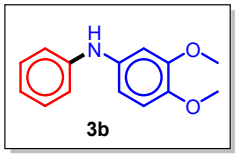
*^{1}H and ^{13}C NMR spectral analysis of N-arylamines (**3**)*

Diphenylamine (**3a**) [1]



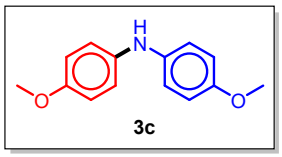
Synthesized as per the general experimental procedure **A**; obtained as a colourless solid, Yield: (101 mg, 80%); mp 55-56 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 6.78 (d, J = 8 Hz, 2H), 7.05 (d, J = 8 Hz, 4H), 7.19 (t, J = 8 Hz, 4H), 8.12 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 117.3, 120.1, 129.7, 143.9

3,4-Dimethoxy-*N*-phenylamine (**3b**) [2]



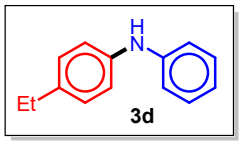
Synthesized as per the general experimental procedure **A**; obtained as a colourless solid, Yield: (154 mg, 90%); mp 98-99 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 3.66 (s, 3H), 3.67 (s, 3H), 6.59 (d, J = 8 Hz, 1H), 6.65-6.69 (m, 2H), 6.81 (d, J = 8 Hz, 1H), 6.91 (d, J = 8 Hz, 2H), 7.12 (t, J = 8 Hz, 2H), 7.81 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 55.8, 56.5, 104.7, 110.4, 113.6, 115.7, 118.9, 129.6, 137.3, 143.7, 145.3, 149.9

Bis-(4-methoxyphenyl)amine (**3c**) [3]



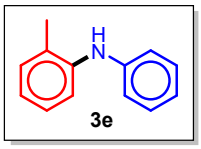
Synthesized as per the general experimental procedure **A**; obtained as a colourless solid, Yield: (146 mg, 85%); mp 100-101 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 3.64 (s, 6H), 6.76 (d, J = 8 Hz, 4H), 6.87 (d, J = 8 Hz, 4H), 7.46 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 55.7, 115.0, 118.5, 138.5, 153.3

4-Ethyl-*N*-phenylamine (**3d**) [4]



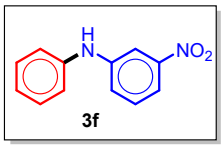
Synthesized as per the general experimental procedure **A**; obtained as a light yellow oil, Yield: (110 mg, 75%); ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 1.11 (t, J = 8 Hz, 3H), 2.48 (q, J = 8 Hz, 2H), 6.70-6.73 (m, 1H), 6.96-6.98 (m, 4H), 7.03 (d, J = 8 Hz, 2H), 7.14 (t, J = 8 Hz, 2H), 7.96 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 16.4, 28.0, 116.4, 118.0, 119.5, 128.8, 129.5, 135.8, 141.4, 144.5

2-Methyl-*N*-phenylamine (**3e**) [5]



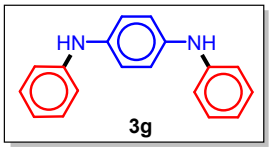
Synthesized as per the general experimental procedure **A**; obtained as a yellow oil, Yield: (50 mg, 40%); ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 2.17 (s, 3H), 6.71-6.73 (m, 1H), 6.86 (d, J = 8 Hz, 3H), 7.06-7.09 (m, 1H), 7.13-7.16 (m, 4H), 7.35 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 18.5, 116.5, 119.2, 120.0, 122.3, 126.9, 129.5, 129.8, 131.3, 141.8, 145.4

3-Nitro-*N*-phenylamine (**3f**) [1]



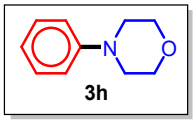
Synthesized as per the general experimental procedure **A**; obtained as a orange solid, Yield: (112 mg, 70%); mp 87-88 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 6.93 (t, J = 8 Hz, 1H), 7.12 (d, J = 8 Hz, 2H), 7.28 (t, J = 8 Hz, 2H), 7.36-7.43 (m, 2H), 7.53 (d, J = 8 Hz, 1H), 7.75 (s, 1H), 8.69 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 109.2, 113.6, 119.2, 121.9, 122.2, 130.0, 130.9, 142.0, 145.8, 149.2

N^1,N^4-diphenylbenzene-1,4-diamine (**3g**) [6]



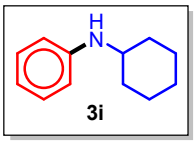
Synthesized as per the general experimental procedure **A**; obtained as a off-white solid, Yield: (98 mg, 50%); mp 147-148 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 6.67 (t, J = 8 Hz, 2H), 6.91 (d, J = 8 Hz, 4H), 6.99 (s, 4H), 7.12 (t, J = 8 Hz, 4H), 7.84 (br s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 115.5 , 118.8, 120.2, 129.5, 136.9, 145.4

4-phenylmorpholine (**3h**) [1]



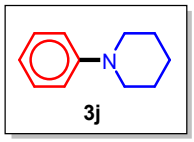
Synthesized as per the general experimental procedure **A**; obtained as a light yellow solid, Yield: (95 mg, 78%); mp 50-51 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 3.03-3.05 (m, 4H), 3.68-3.70 (m, 4H), 6.76 (t, J = 8 Hz, 1H), 6.89 (d, J = 8 Hz, 2H), 7.18 (t, J = 8 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 48.9, 66.6, 115.6, 119.6, 129.5, 151.6

N-cyclohexylamine (**3i**) [7]



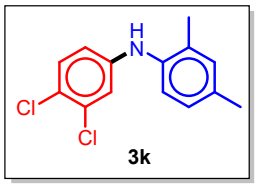
Synthesized as per the general experimental procedure **A**; obtained as a colourless oil, Yield: (117 mg, 89%); ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 1.07-1.19 (m, 3H), 1.25-1.34 (m, 2H), 1.54-1.58 (m, 1H), 1.66-1.71 (m, 2H), 1.88-1.91 (m, 2H), 3.11-3.16 (m, 1H), 5.22 (s, 1H), 6.44 (t, J = 8 Hz, 1H), 6.52 (d, J = 8 Hz, 2H), 7.00 (t, J = 8 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 25.1, 26.2, 33.1, 51.1, 112.8, 115.6, 129.3, 148.5

1-Phenylpiperidine (**3j**) [8]



Synthesized as per the general experimental procedure **A**; obtained as a light yellow oil, Yield: (78 mg, 65%); ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 1.46-1.49 (m, 2H), 1.53-1.59 (m, 4H), 3.05-3.07 (m, 4H), 6.69 (t, J = 8 Hz, 1H), 6.86 (d, J = 8 Hz, 2H), 7.14 (t, J = 8 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 24.4, 25.7, 50.1, 116.3, 118.8, 129.4, 152.2

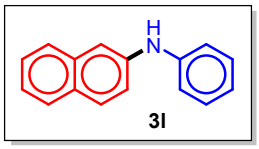
N-(3,4-dichlorophenyl)-2,4-dimethylaniline (**3k**)



3k

Synthesized as per the general experimental procedure **A**; obtained as a colourless solid, Yield: (126 mg, 63%); mp 187-188 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 2.07 (s, 3H), 2.19 (s, 3H), 6.61 (d, J = 8 Hz, 1H), 6.77 (d, J = 8 Hz, 1H), 6.92 (d, J = 8 Hz, 1H), 7.00 (d, J = 8 Hz, 2H), 7.24 (d, J = 8 Hz, 1H), 7.76 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 18.1, 20.9, 114.6, 115.2, 123.9, 127.8, 131.2, 131.8, 132.2, 132.50, 133.8, 137.2, 147.2

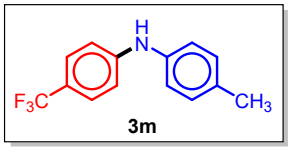
N-phenylnapthalen-2-amine (**3l**) [9]



3l

Synthesized as per the general experimental procedure **A**; obtained as a colourless solid, Yield: (131 mg, 80%); mp 109-110 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 7.18 (d, J = 8 Hz, 2H), 7.20-7.27 (m, 4H), 7.31-7.34 (m, 1H), 7.44 (s, 1H), 7.63 (d, J = 8 Hz, 1H), 7.70 (d, J = 8 Hz, 1H), 7.73 (d, J = 8 Hz, 1H), 8.40 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 109.5, 117.8, 120.4, 120.7, 123.2, 126.7, 127.9, 128.2, 128.6, 129.3, 129.7, 134.9, 141.9, 143.6

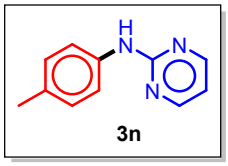
N-methyl-*N*-(4-trifluoromethyl)phenyl)aniline (**3m**) [10]



3m

Synthesized as per the general experimental procedure **A**; obtained as a yellow solid, Yield: (139 mg, 74%); mp 78-79 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 2.26 (s, 3H), 7.08 (d, J = 8 Hz, 4H), 7.13 (d, J = 8 Hz, 2H), 7.48 (d, J = 8 Hz, 2H), 8.56 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 20.8, 114.5, 120.3, 124.1, 127.0, 130.2, 131.5, 139.2, 148.6

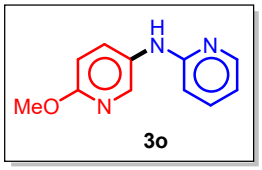
N-(*p*-tolyl)pyrimidin-2-amine (**3n**) [11]



3n

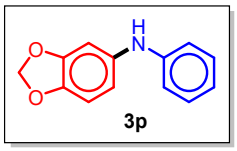
Synthesized as per the general experimental procedure **A**; obtained as a colourless solid, Yield: (70 mg, 50%); mp 122-124 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 2.25 (s, 3H), 6.78-6.81 (m, 1H), 7.08 (d, J = 8 Hz, 2H), 7.63 (d, J = 8 Hz, 2H), 8.45 (d, J = 8 Hz, 2H), 9.47 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 20.8, 112.5, 119.4, 129.3, 130.6, 138.3, 158.4, 160.5

N-(6-methoxypyridin-3-yl)pyridine-2-amine (**3o**)



Synthesized as per the general experimental procedure **A**; obtained as a yellow oil, Yield: (82 mg, 55%); ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 3.76 (s, 3H), 6.64-6.67 (m, 1H), 6.71 (t, J = 8 Hz, 2H), 7.49 (t, J = 8 Hz, 1H), 7.97 (d, J = 8 Hz, 1H), 8.04 (d, J = 8 Hz, 1H), 8.35 (s, 1H), 8.87 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 53.4, 110.1, 110.5, 110.9, 114.4, 127.7, 131.4, 132.8, 133.0, 137.1, 137.7, 147.6, 149.0, 156.4, 157.3, 158.6

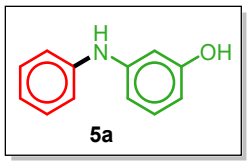
N-phenylbenzo[*d*][1,3]dioxol-5-amine (**3p**) [9]



Synthesized as per the general experimental procedure **A**; obtained as a colourless solid, Yield: (117 mg, 73%); mp 150-152 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 5.90 (s, 2H), 6.51 (dd, J = 8 Hz, 2 Hz, 1H), 6.65 (d, J = 8 Hz, 1H), 6.68-6.71 (m, 1H), 6.76 (d, J = 8 Hz, 1H), 6.90 (d, J = 8 Hz, 2H), 7.13 (t, J = 8 Hz, 2H), 7.85 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 101.3, 109.0, 111.3, 115.9, 119.2, 129.6, 138.3, 141.7, 145.1, 148.2

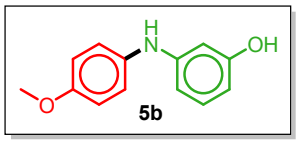
*^{1}H and ^{13}C NMR spectral analysis of 3-arylaminophenols (**5**)*

3-(Phenylamino)phenol (**5a**) [12]



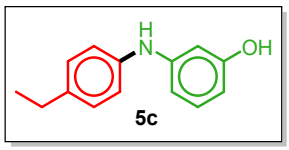
Synthesized as per the general experimental procedure **B**; obtained as a brown solid, Yield: (108 mg, 78%); mp 77-78 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 6.21 (d, J = 8 Hz, 1H), 6.47 (t, J = 8 Hz, 2H), 6.76 (t, J = 8 Hz, 1H), 6.96 (t, J = 8 Hz, 1H), 7.02 (d, J = 8 Hz, 2H), 7.17 (t, J = 8 Hz, 2H), 7.98 (br s, 1H), 9.14 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 104.0, 107.4, 108.2, 117.5, 120.0, 129.6, 130.3, 143.9, 145.1, 158.7

3-((4-Methoxyphenyl)amino)phenol (**5b**) [13]



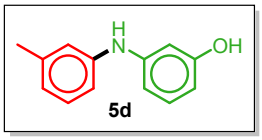
Synthesized as per the general experimental procedure **B**; obtained as a brown solid, Yield: (132 mg, 82%); mp 69-70 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 3.66 (s, 3H), 6.08 (d, J = 8 Hz, 1H), 6.30 (d, J = 8 Hz, 2H), 6.81 (d, J = 8 Hz, 2H), 6.88 (t, J = 8 Hz, 1H), 6.97 (d, J = 8 Hz, 2H), 7.68 (br s, 1H), 9.04 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 55.6, 102.0, 106.2, 114.9, 121.2, 130.2, 136.6, 146.9, 154.2, 158.7

3-((4-Ethylphenyl)amino)phenol (**5c**)



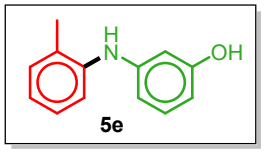
Synthesized as per the general experimental procedure **B**; obtained as a brown solid, Yield: (120 mg, 75%); mp 84-85 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 1.10 (t, J = 8 Hz, 3H), 2.47 (q, J = 8 Hz, 2H), 6.15 (dd, J = 8 Hz, 1.2 Hz, 1H), 6.41 (t, J = 8 Hz, 2H), 6.90-6.95 (m, 3H), 7.02 (d, J = 8 Hz, 2H), 7.86 (br s, 1H), 9.10 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 16.4, 19.4, 103.0, 106.8, 107.5, 118.3, 128.8, 130.2, 135.7, 141.4, 145.7, 158.6

3-(*m*-tolylamino)phenol (**5d**)



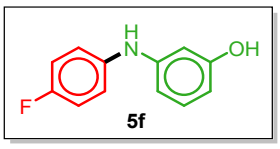
Synthesized as per the general experimental procedure **B**; obtained as a yellow solid, Yield: (108 mg, 73%); mp 79-80 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 2.20 (s, 3H), 6.22 (d, J = 8 Hz, 1H), 6.48 (t, J = 8 Hz, 2H), 6.59 (d, J = 8 Hz, 1H), 6.84 (d, J = 8 Hz, 2H), 6.96 (t, J = 8 Hz, 1H), 7.06 (t, J = 8 Hz, 1H), 7.92 (br s, 1H), 9.16 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 21.7, 103.9, 107.4, 108.3, 114.7, 118.2, 120.9, 129.4, 130.3, 138.7, 143.9, 145.2, 158.7

3-(*o*-tolylamino)phenol (**5e**) [12]



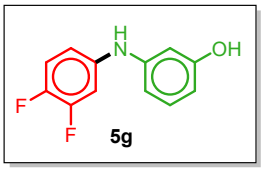
Synthesized as per the general experimental procedure **B**; obtained as a yellow oil, Yield: (94 mg, 63%); ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 2.13 (s, 3H), 6.12 (dd, J = 8 Hz, 2 Hz, 1H), 6.24-6.28 (m, 2H), 6.84 (d, J = 8 Hz, 1H), 6.89 (t, J = 8 Hz, 1H), 7.05 (t, J = 8 Hz, 1H), 7.12 (t, J = 8 Hz, 2H), 7.21 (br s, 1H), 9.03 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 18.5, 103.1, 106.5, 107.6, 120.8, 122.4, 126.9, 130.2, 131.31, 141.8, 146.8, 158.6

3-((4-Fluorophenyl)amino)phenol (**5f**) [11]



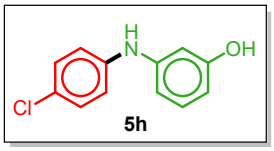
Synthesized as per the general experimental procedure **B**; obtained as a yellow oil, Yield: (119 mg, 78%); ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 6.17 (d, J = 8 Hz, 1H), 6.37-6.41 (m, 2H), 6.93 (t, J = 8 Hz, 1H), 7.02 (d, J = 8 Hz, 4H), 7.93 (br s, 1H), 9.13 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 103.3, 107.2, 107.6, 116.1, 119.6, 130.3, 140.3, 145.7, 156.8 (d, $J_{C\text{-}F}$ = 240 Hz), 158.7

3-((3,4-Difluorophenyl)amino)phenol (**5g**)[13]



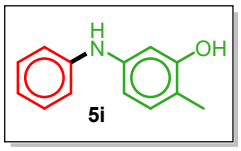
Synthesized as per the general experimental procedure **B**; obtained as a orange solid, Yield: (132 mg, 80%); mp 101-103 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 6.31 (d, J = 8 Hz, 1H), 6.50 (d, J = 8 Hz, 2H), 6.83 (d, J = 8 Hz, 1H), 6.96-6.99 (m, 1H), 7.02-7.05 (m, 1H), 7.22-7.29 (m, 1H), 8.20 (br s, 1H), 9.27 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 104.4, 105.3, 105.5, 108.3, 108.6, 113.1, 118.0, 118.2, 130.4, 141.5, 143.5 (d, $J_{C\text{-}F}$ = 240 Hz), 144.3, 150.1 (d, $J_{C\text{-}F}$ = 250 Hz), 158.7

3-((4-Chlorophenyl)amino)phenol (**5h**) [13]



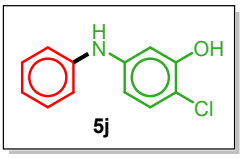
Synthesized as per the general experimental procedure **B**; obtained as a brown solid, Yield: (125 mg, 76%); mp 109-110 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 6.23 (d, J = 8 Hz, 1H), 6.45 (d, J = 8 Hz, 2H), 6.95-7.01 (m, 3H), 7.19 (d, J = 8 Hz, 2H), 8.15 (br s, 1H), 9.23 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 104.4, 108.1, 108.7, 117.4, 118.5, 123.0, 129.3, 130.5, 143.1, 144.4, 158.7

2-Methyl-5-(phenylamino)phenol (**5i**) [14]



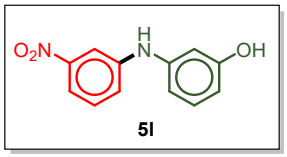
Synthesized as per the general experimental procedure **B**; obtained as a brown solid, Yield: (119 mg, 80%); mp 93-94 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 1.98 (s, 3H), 6.38 (d, J = 8 Hz, 1H), 6.55 (s, 1H), 6.70 (t, J = 8 Hz, 1H), 6.84 (d, J = 8 Hz, 1H), 6.95 (d, J = 8 Hz, 2H), 7.13 (t, J = 8 Hz, 2H), 7.84 (br s, 1H), 9.05 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 15.9, 104.6, 108.8, 115.9, 116.6, 119.3, 129.5, 131.3, 142.4, 144.6, 156.3

2-Chloro-5-(phenylamino)phenol (**5j**) [13]



Synthesized as per the general experimental procedure **B**; obtained as a brown solid, Yield: (132 mg, 80%); mp 91-92 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 6.50 (d, J = 8 Hz, 1H), 6.75 (s, 1H), 6.85 (t, J = 8 Hz, 1H), 7.06 (d, J = 8 Hz, 2H), 7.12 (d, J = 8 Hz, 1H), 7.23-7.26 (m, 2H), 8.17 (br s, 1H), 9.92 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 104.5, 109.0, 110.1, 117.9, 120.5, 129.6, 130.4, 143.4, 143.9, 153.9

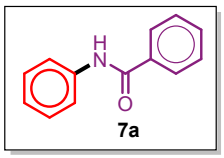
3-((3-Nitrophenyl)amino)phenol (**5l**) [12]



Synthesized as per the general experimental procedure **B**; obtained as a yellow liquid, Yield: (120 mg, 70%); ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 6.41 (d, J = 8 Hz, 1H), 6.59-6.61 (m, 2H), 7.11 (t, J = 8 Hz, 1H), 7.42 (d, J = 8 Hz, 1H), 7.46 (t, J = 8 Hz, 1H), 7.58 (d, J = 8 Hz, 1H), 7.81 (s, 1H), 8.62 (br s, 1H), 9.40 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 105.9, 109.4, 109.5, 109.8, 113.5, 122.1, 130.5, 130.8, 143.2, 145.8, 149.1, 158.8

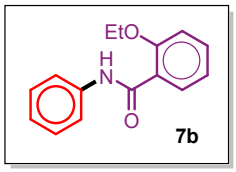
*^{1}H and ^{13}C NMR spectral analysis of N-arylamides (**7**)*

N-phenylbenzamide (**7a**) [15]



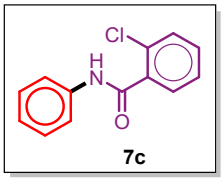
Synthesized as per the general experimental procedure **C**; obtained as a colourless solid, Yield: (94 mg, 64%); mp 162-163 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 7.06 (t, J = 8 Hz, 1H), 7.31 (t, J = 8 Hz, 2H), 7.49 (t, J = 8 Hz, 2H), 7.55 (t, J = 8 Hz, 1H), 7.74 (d, J = 8 Hz, 2H), 7.92 (t, J = 8 Hz, 2H), 10.20 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 120.9, 124.2, 128.1, 128.8, 129.1, 132.0, 135.5, 139.7, 166.1

2-Ethoxy-*N*-phenylbenzamide (**7b**) [16]



Synthesized as per the general experimental procedure **C**; obtained as a colourless solid, Yield: (115 mg, 64%); mp 71-72 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 1.36 (t, J = 8 Hz, 3H), 4.13 (q, J = 8 Hz, 2H), 7.03 (q, J = 8 Hz, 2H), 7.12 (d, J = 8 Hz, 1H), 7.30 (t, J = 8 Hz, 2H), 7.45 (t, J = 8 Hz, 1H), 7.66-7.70 (m, 3H), 10.10 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 15.0, 64.8, 113.4, 119.9, 121.0, 123.9, 124.8, 129.3, 130.5, 132.8, 139.5, 156.4, 164.6

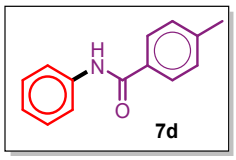
2-Chloro-*N*-phenylbenzamide (**7c**) [17]



Synthesized as per the general experimental procedure **C**; obtained as a white solid, Yield: (111 mg, 64%); mp 113-115 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 7.05-7.08 (m, 1H), 7.31 (t, J = 8 Hz, 2H), 7.41 (t, J = 8 Hz, 1H), 7.45-7.48 (m, 1H), 7.53 (t, J = 8 Hz, 2H), 7.68 (d, J = 8 Hz, 2H), 10.47 (br s, 1H); ^{13}C NMR (100 MHz,

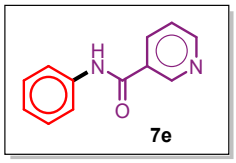
DMSO-d_6): δ_C (ppm) 120.0, 124.3, 127.8, 129.3, 130.2, 130.4, 131.5, 137.5, 139.4, 165.4

4-Methyl-*N*-phenylbenzamide (**7d**) [1]



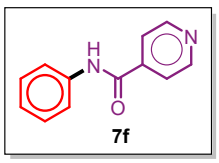
Synthesized as per the general experimental procedure **C**; obtained as a white solid, Yield: (101 mg, 64%); mp 156-157 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 2.42 (s, 3H), 7.13 (t, J = 8 Hz, 1H), 7.36-7.40 (m, 4H), 7.82 (d, J = 8 Hz, 2H), 7.92 (d, J = 8 Hz, 2H), 10.20 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 21.4, 120.8, 124.0, 128.1, 129.0, 129.37, 132.5, 139.7, 142.0, 165.8

N-phenylnicotinamide (**7e**) [18]



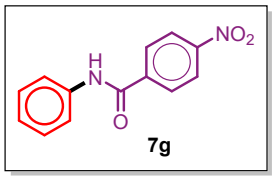
Synthesized as per the general experimental procedure **C**; obtained as a brown solid, Yield: (119 mg, 80%); mp 117-118 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 7.16 (t, J = 8 Hz, 1H), 7.40 (t, J = 8 Hz, 2H), 7.60 (t, J = 8 Hz, 1H), 7.82 (d, J = 8 Hz, 2H), 8.33 (d, J = 8 Hz, 1H), 8.80 (s, 1H), 9.15 (s, 1H), 10.48 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 120.8, 123.9, 124.4, 129.1, 131.1, 135.9, 139.3, 149.1, 152.5, 164.5

N-phenylisonicotinamide (**7f**) [19]



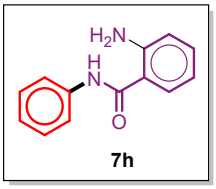
Synthesized as per the general experimental procedure **C**; obtained as a light brown solid, Yield: (110 mg, 74%); mp 169-170 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 7.15 (t, J = 8 Hz, 1H), 7.39 (t, J = 8 Hz, 2H), 7.79 (d, J = 8 Hz, 2H), 7.88 (d, J = 8 Hz, 2H), 8.80 (d, J = 8 Hz, 2H), 10.51 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 120.9, 122.0, 124.6, 129.1, 139.0, 142.4, 150.7, 164.4

4-Nitro-*N*-phenylbenzamide (**7g**) [15]



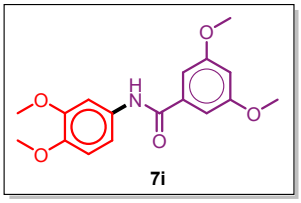
Synthesized as per the general experimental procedure **C**; obtained as a Off-white solid, Yield: (116 mg, 64%); mp 199-200 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 7.15 (t, J = 8 Hz, 1H), 7.39 (t, J = 8 Hz, 2H), 7.79 (d, J = 8 Hz, 2H), 8.19 (d, J = 8 Hz, 2H), 8.38 (d, J = 8 Hz, 2H), 10.57 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 120.9, 124.0, 124.6, 129.1, 129.6, 139.1, 141.1, 149.6, 164.3

2-Amino-*N*-phenylbenzamide (**7h**) [20]



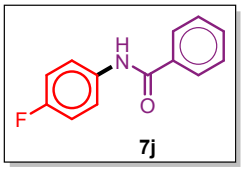
Synthesized as per the general experimental procedure **C**; obtained as a colourless solid, Yield: (116 mg, 73%); mp 131-132 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 6.31 (s, 2H), 6.60 (t, J = 8 Hz, 1H), 6.76 (d, J = 8 Hz, 1H), 7.08 (t, J = 8 Hz, 1H), 7.19-7.22 (m, 1H), 7.33 (t, J = 8 Hz, 2H), 7.63 (d, J = 8 Hz, 1H), 7.72 (d, J = 8 Hz, 2H), 9.98 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 115.1, 115.7, 116.8, 121.0, 123.8, 128.9, 129.1, 132.5, 139.7, 150.1, 168.3

N-(3,4-dimethoxyphenyl)-3,5-dimethoxybenzamide (**7i**) [21]



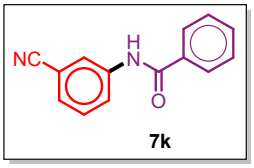
Synthesized as per the general experimental procedure **C**; obtained as a light purple solid, Yield: (142 mg, 60%); mp 188-189 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 3.75 (s, 3H), 3.76 (s, 3H), 3.83 (s, 6H), 6.71 (s, 1H), 6.94 (d, J = 8 Hz, 1H), 7.11 (s, 2H), 7.32 (dd, J = 8 Hz, 2.4 Hz, 1H), 7.47 (s, 1H), 10.02 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 55.8, 55.9, 56.2, 103.6, 106.0, 106.1, 112.3, 112.9, 133.0, 137.5, 145.7, 148.9, 160.8, 165.0

N-(4-fluorophenyl)benzamide (**7j**) [22]



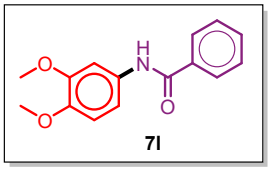
Synthesized as per the general experimental procedure **C**; obtained as a colourless solid, Yield: (129 mg, 80%); mp 183-184 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 7.20 (t, J = 8 Hz, 2H), 7.54 (t, J = 8 Hz, 2H), 7.60 (t, J = 8 Hz, 1H), 7.80-7.83 (m, 2H), 7.97 (d, J = 8 Hz, 2H), 10.31 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 115.5, 115.7, 122.6, 122.7, 128.0, 128.8, 132.0, 135.3, 136.0, 158.7 (d, $J_{C\text{-}F}$ = 240 Hz), 165.9

N-(3-cyanophenyl)benzamide (**7k**) [23]



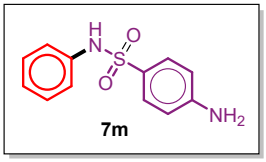
Synthesized as per the general experimental procedure **C**; obtained as a colourless solid, Yield: (113 mg, 68%); mp 135-136 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 7.55 (d, J = 8 Hz, 2H), 7.59 (d, J = 8 Hz, 2H), 7.63 (t, J = 8 Hz, 1H), 7.98 (d, J = 4 Hz, 2H), 8.06 (d, J = 8 Hz, 1H), 8.27 (s, 1H), 10.56 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 111.9, 119.2, 123.4, 125.3, 127.6, 128.2, 128.9, 129.3, 130.6, 132.4, 134.8, 140.4, 166.4

N-(3,4-dimethoxyphenyl)benzamide (**7l**) [22]



Synthesized as per the general experimental procedure **C**; obtained as a colourless solid, Yield: (158 mg, 82%); mp 179-180 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 3.75 (s, 3H), 3.77 (s, 3H), 6.94 (d, *J* = 8 Hz, 1H), 7.36 (d, *J* = 8 Hz, 1H), 7.53 (t, *J* = 8 Hz, 3H), 7.58 (d, *J* = 8 Hz, 1H), 7.97 (d, *J* = 8 Hz, 2H), 10.11 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 55.8, 56.2, 106.0, 112.4, 112.8, 127.9, 128.8, 131.8, 133.2, 135.5, 145.6, 148.9, 165.5

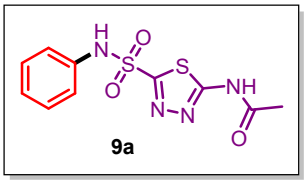
4-Amino-*N*-phenylbenzenesulfonamide (**7m**) [24]



Synthesized as per the general experimental procedure **C**; obtained as a dark-red solid, Yield: (149 mg, 80%); mp 197-198 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 5.94 (br s, 2H), 6.54 (d, *J* = 8 Hz, 2H), 6.97 (t, *J* = 8 Hz, 1H), 7.07 (d, *J* = 8 Hz, 2H), 7.20 (t, *J* = 8 Hz, 2H), 7.40 (d, *J* = 8 Hz, 2H), 9.83 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 113.0, 119.9, 123.7, 124.9, 129.1, 129.4, 129.8, 138.9, 153.2

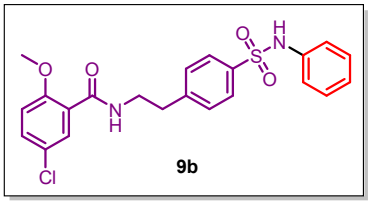
*^{1}H and ^{13}C NMR spectral analysis of **9a** and **9b***

N-(5-(*N*-phenylsulfamoyl)-1,3,4-thiadiazol-2-yl)acetamide (**9a**)



Synthesized as per the general experimental procedure **C**; obtained as a colourless solid, Yield: (157 mg, 70%); mp 288-289 °C; ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 2.21 (s, 3H), 7.15 (d, *J* = 8 Hz, 1H), 7.20 (d, *J* = 8 Hz, 2H), 7.31 (d, *J* = 8 Hz, 2H), 11.17 (s, 1H), 13.07 (br s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 22.7, 121.5, 125.6, 129.8, 136.7, 161.0, 162.1, 170.0; HRMS-ESI *m/z*: $[M+H]^+$ calcd for $C_{10}H_{10}N_4O_3S_2$, 298.0194; found, 299.0275

5-Chloro-2-methoxy-*N*-(4-(*N*-phenylsulfamoyl)phenethyl)benzamide (**9b**)



Synthesized as per the general experimental procedure **C**; obtained as a light orange oil, Yield: (166 mg, 50%); ^{1}H NMR (400 MHz, $CDCl_3$): δ_H (ppm); 2.93-2.96 (m , 2H), 3.66 (s, 3H), 3.69-3.74 (m, 2H), 6.83 (t, *J* = 8 Hz, 1H), 7.09 (t, *J* = 8 Hz, 3H), 7.20-7.24 (m, 3H), 7.30 (d, *J* = 8 Hz, 2H), 7.36 (dd, *J* = 8 Hz, 2.8 Hz, 1H), 7.73 (d, *J* = 8 Hz, 2H), 7.78 (br s, 1H), 8.14 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ_C (ppm) 35.4, 40.5, 56.1, 112.9, 121.5, 122.6, 125.3, 126.7, 127.5, 129.3, 129.5, 131.9, 132.4, 136.5, 137.5, 144.9, 155.9, 164.1; HRMS-ESI *m/z*: $[M+H]^+$ calcd for $C_{22}H_{21}ClN_2O_4S$, 444.0911; found, 445.1014

3. References

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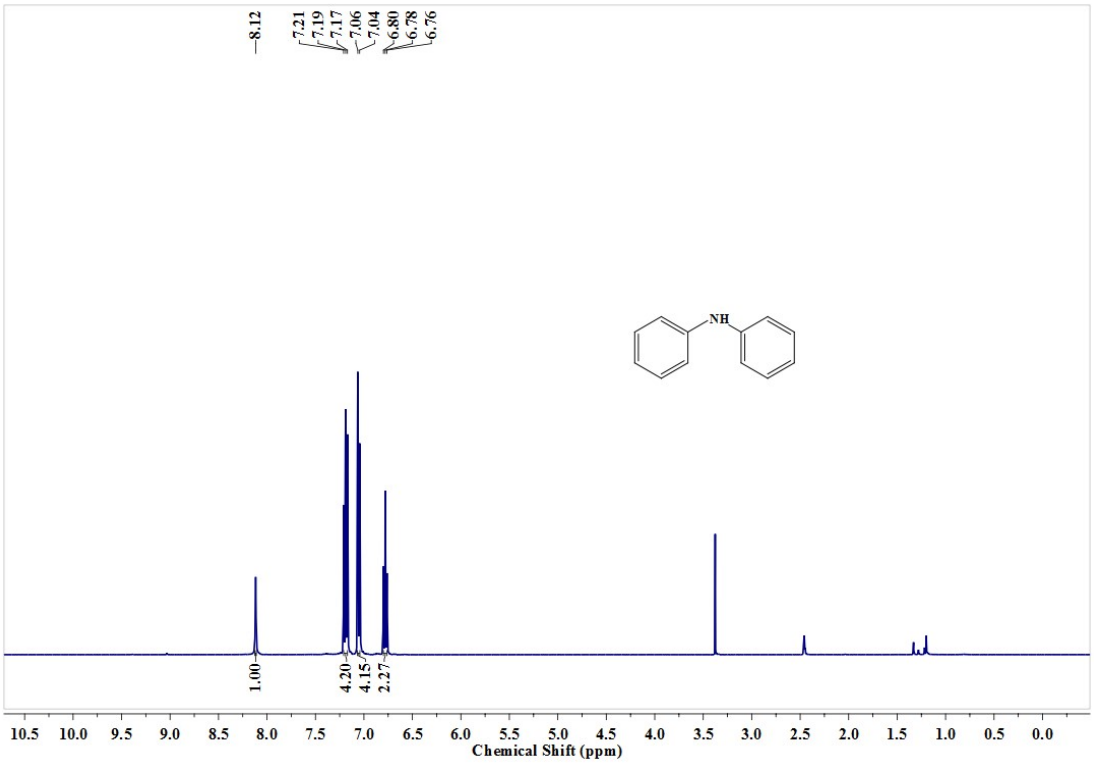
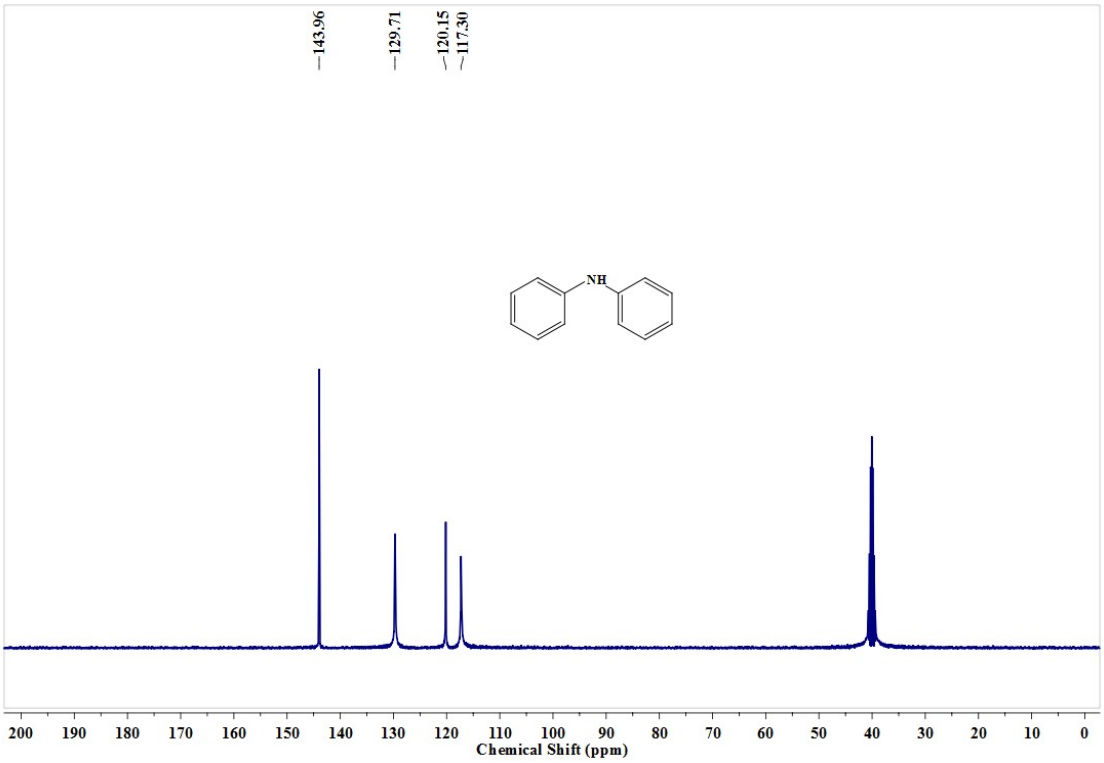
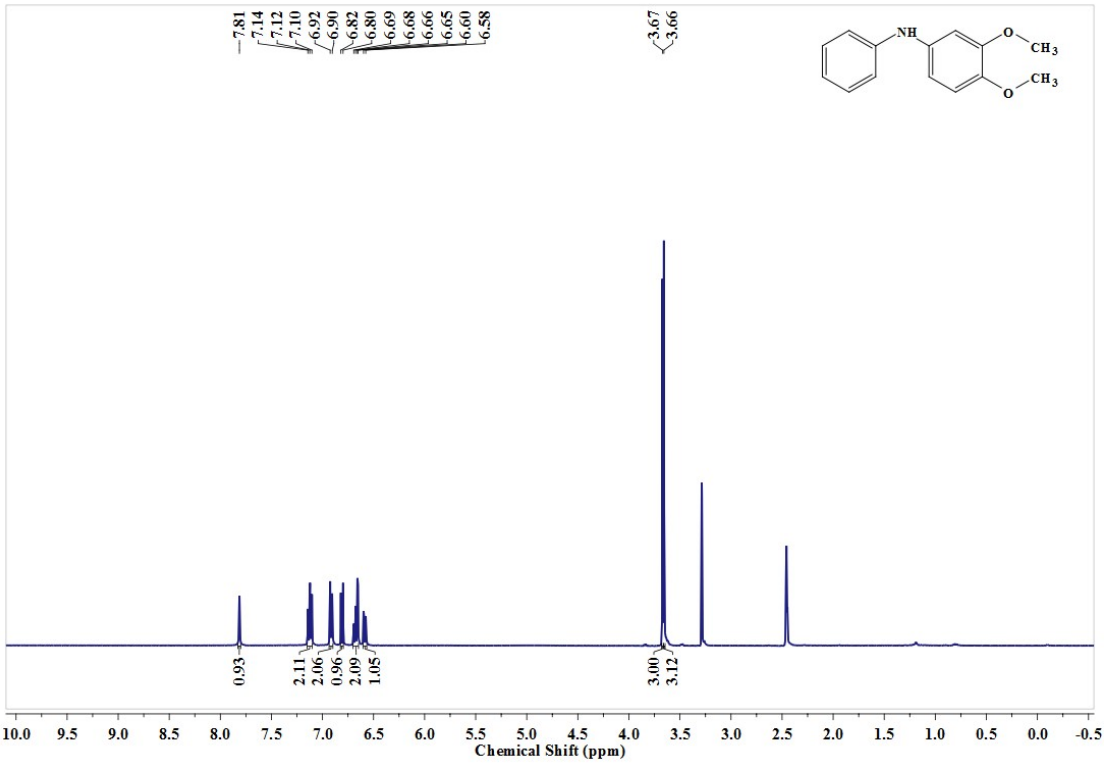
4. ^{1}H and ^{13}C NMR spectra of *N*-aryl derivatives:

4.1 *^{1}H and ^{13}C NMR spectra of N-arylamines (**3**)*



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6.80
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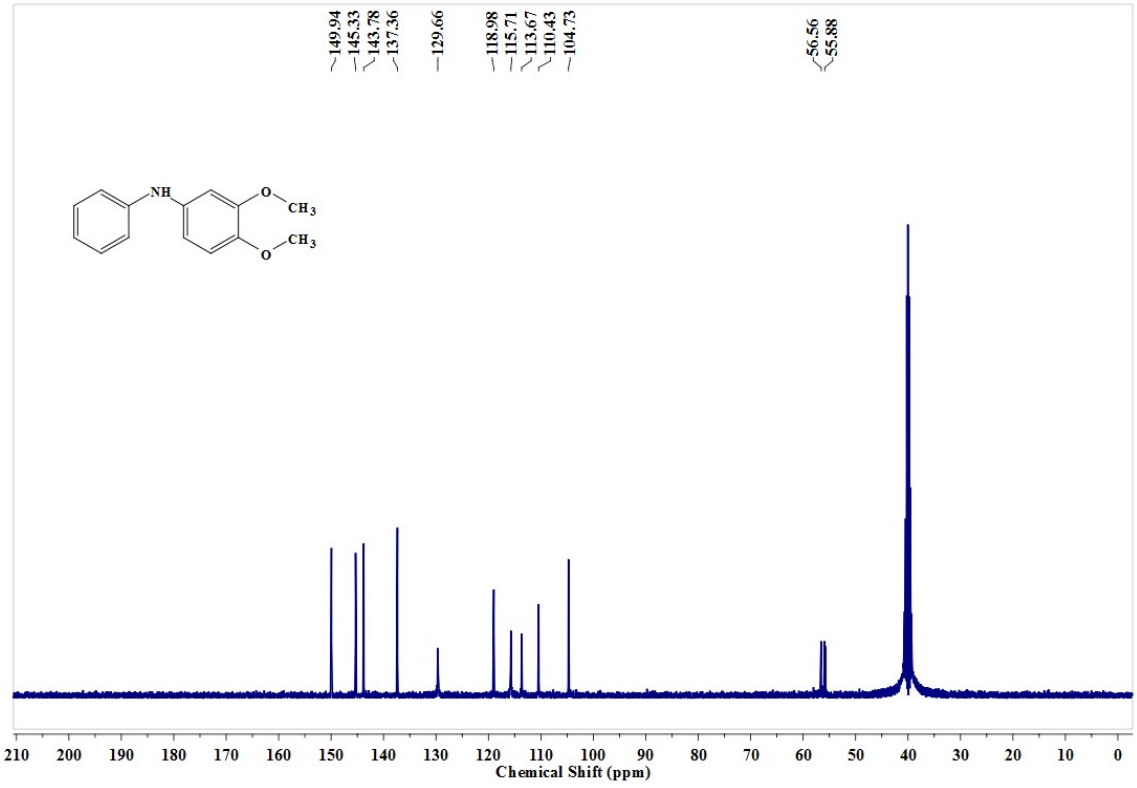
6.68
6.66
6.65
6.60
6.58
3.67
3.66
NH
O
CH3
CH3
O
0.93
2.11
2.06
0.96
2.09
1.05
3.00
3.12
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
Chemical Shift (ppm)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115.71
113.67
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CH3
O
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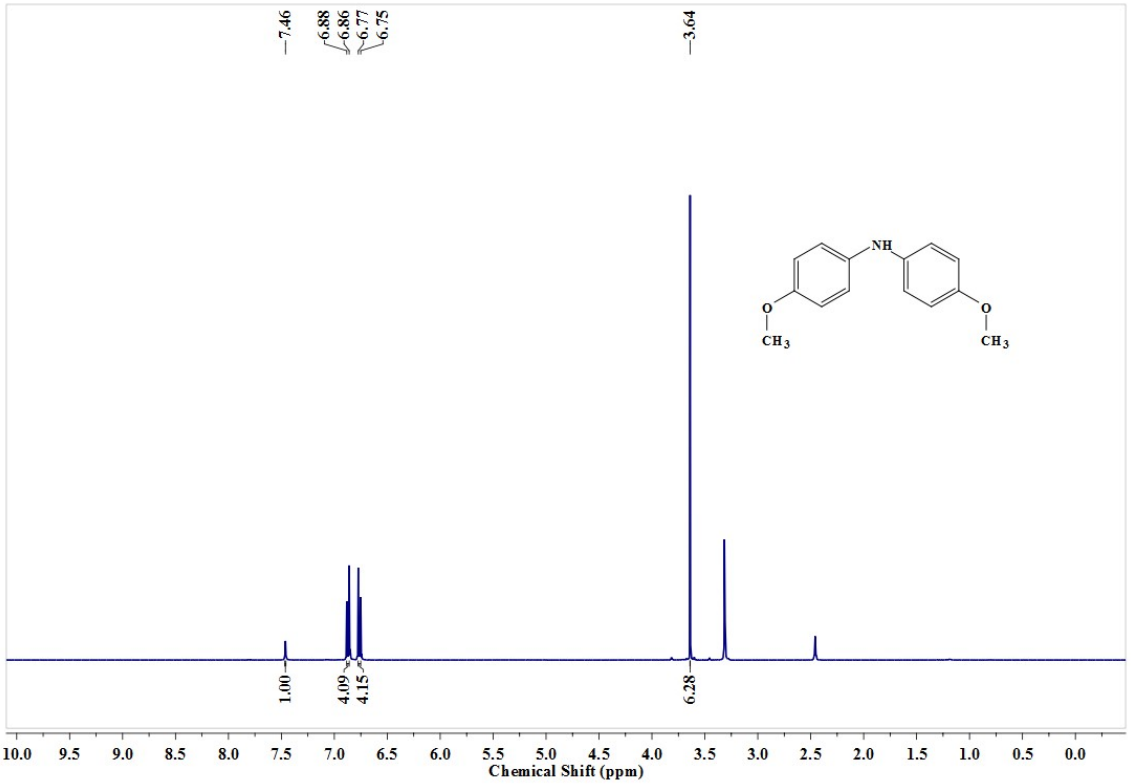
Chemical Shift (ppm)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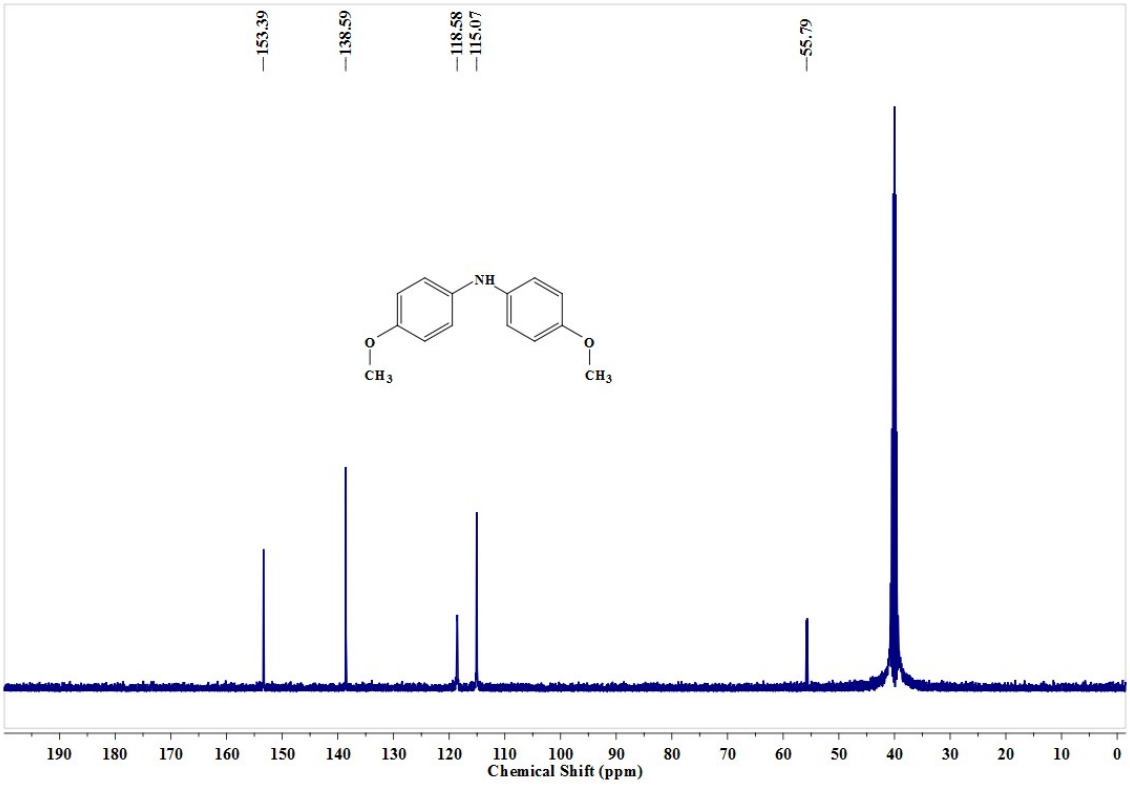
6.28
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical Shift (ppm)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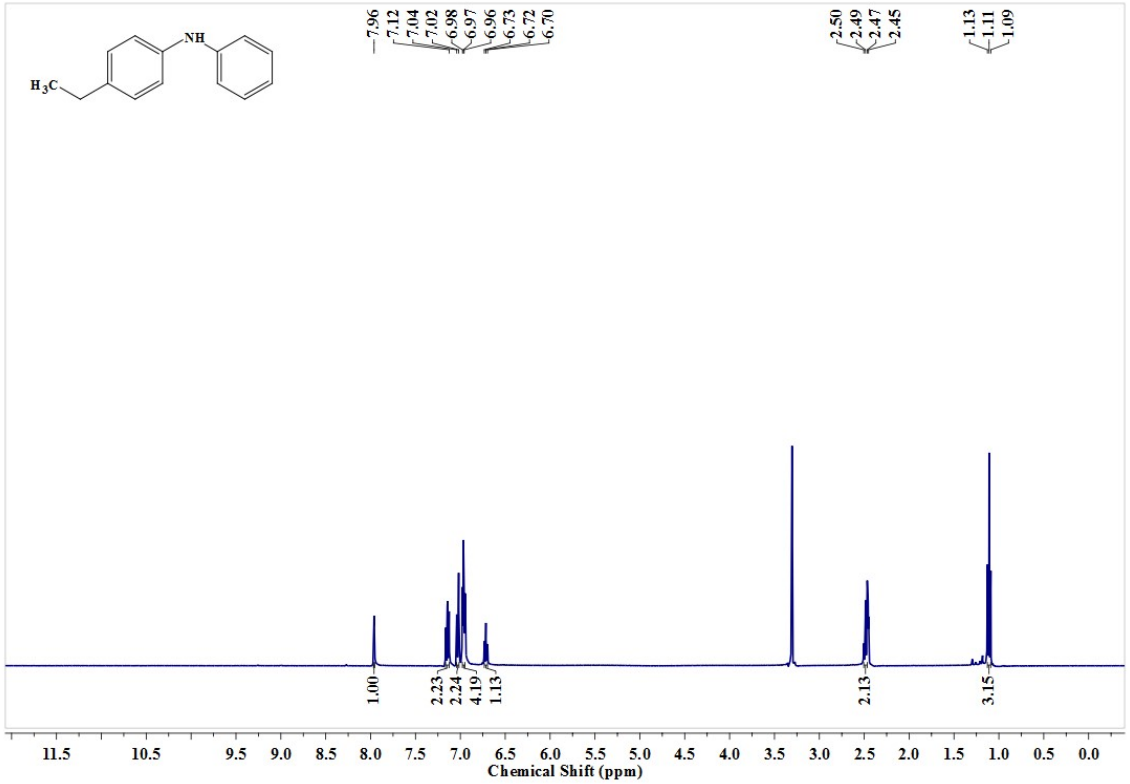
Chemical Shift (ppm)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7.12
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6.72
6.70
2.50
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2.47
2.45
1.13
1.11
1.09
NH
H3C
1.00
2.23
2.24
4.19
1.13
2.13
3.15
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
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1.0
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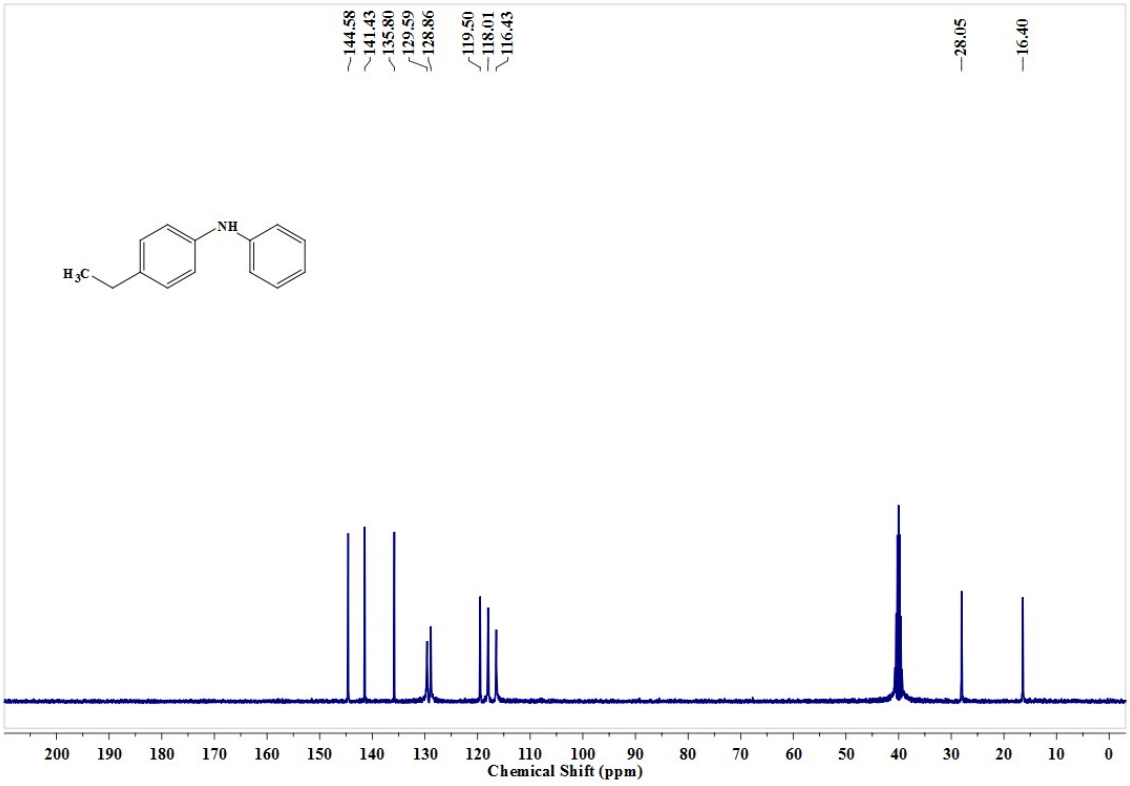
0.0
Chemical Shift (ppm)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16.40
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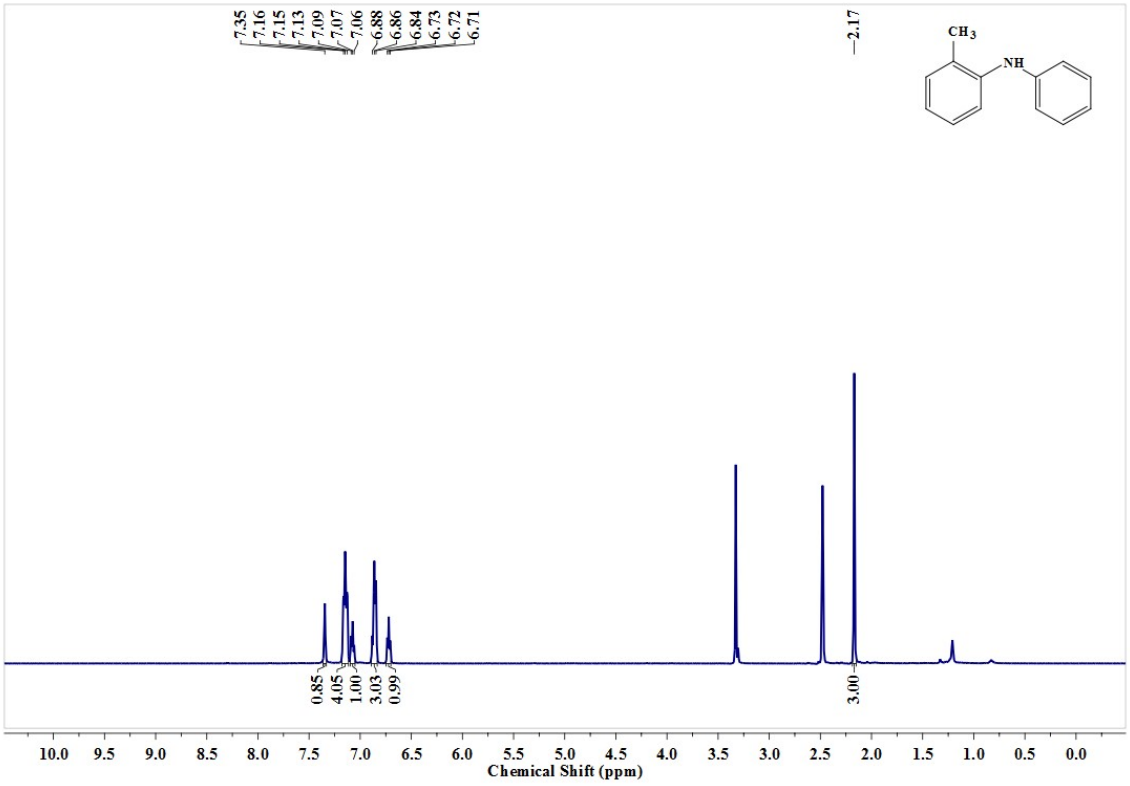
H3C
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)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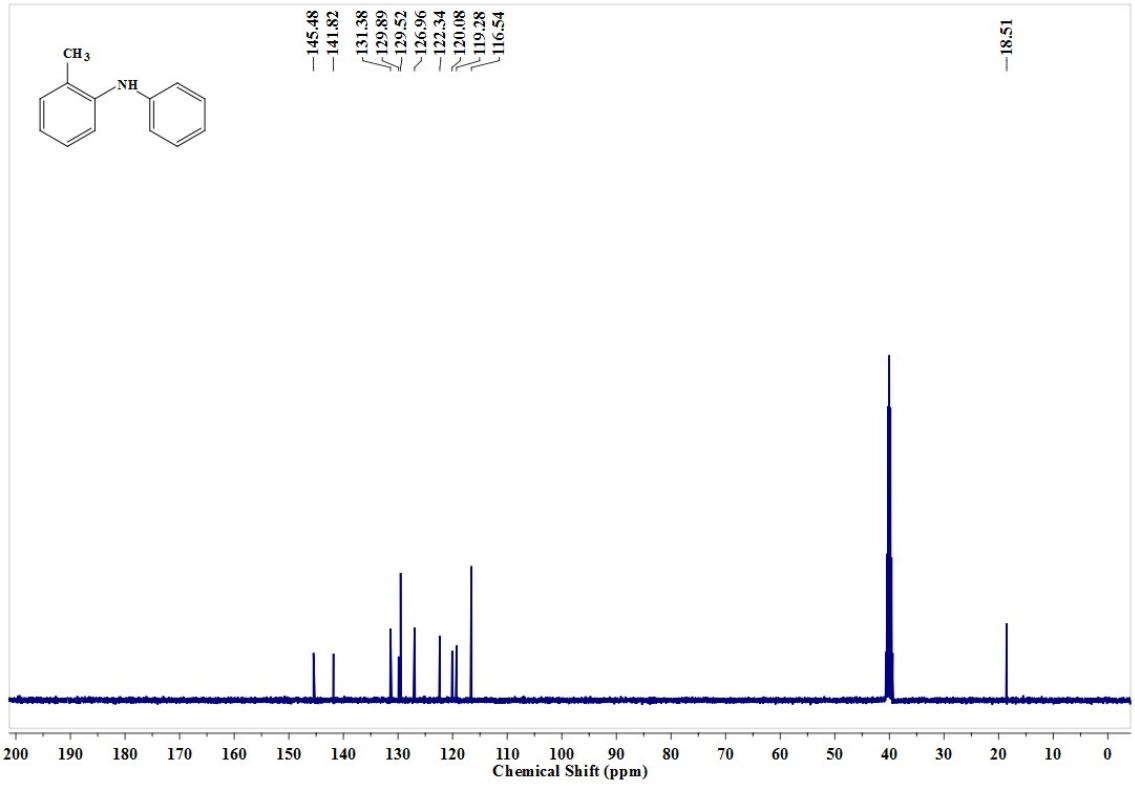
6.71
2.17
CH3
NH
0.85
4.05
1.00
3.03
0.99
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical Shift (ppm)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119.28
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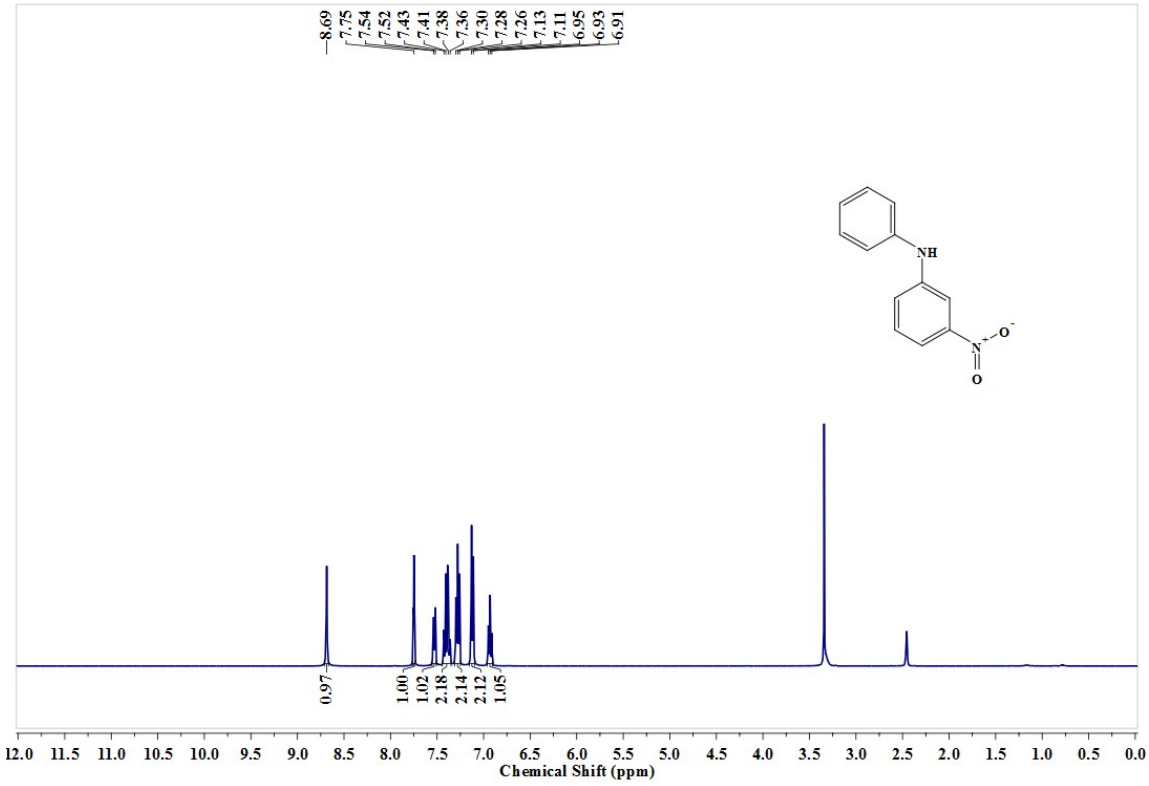
Chemical Shift (ppm)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7.11
6.95
6.93
6.91
NH
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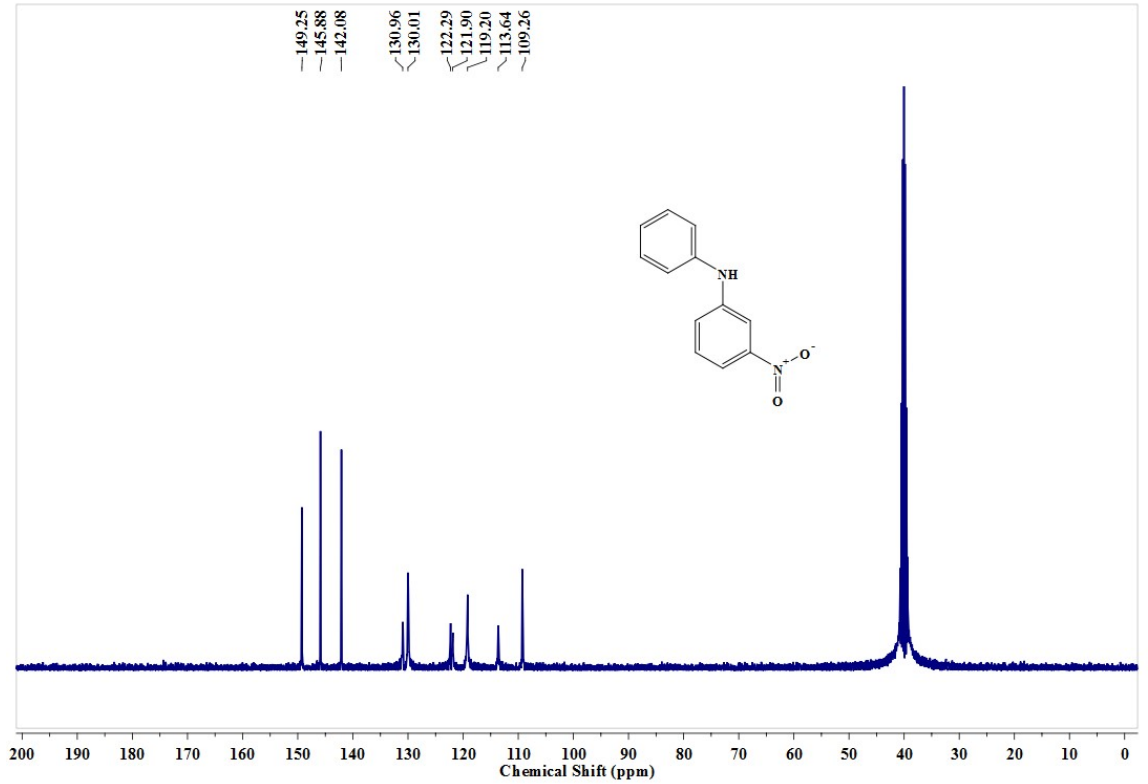
1.00
1.02
2.18
2.14
2.12
1.05
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical Shift (ppm)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O
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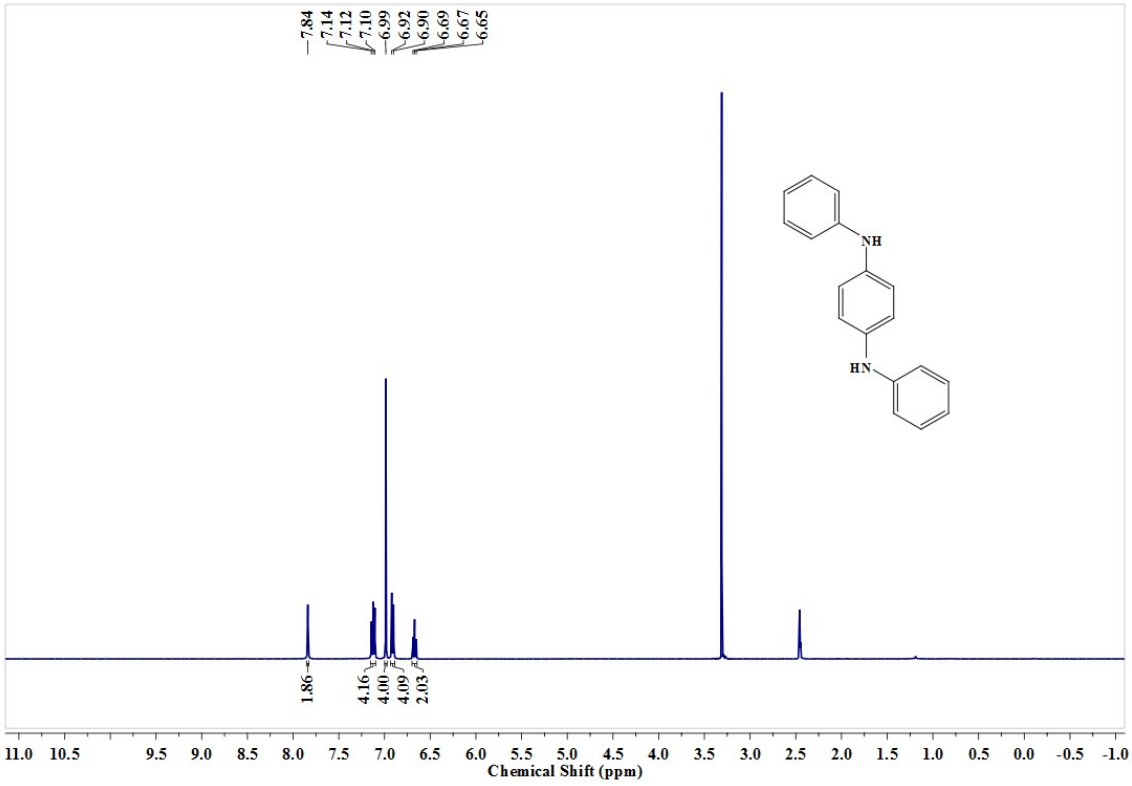
Chemical Shift (ppm)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6.65
NH
HN
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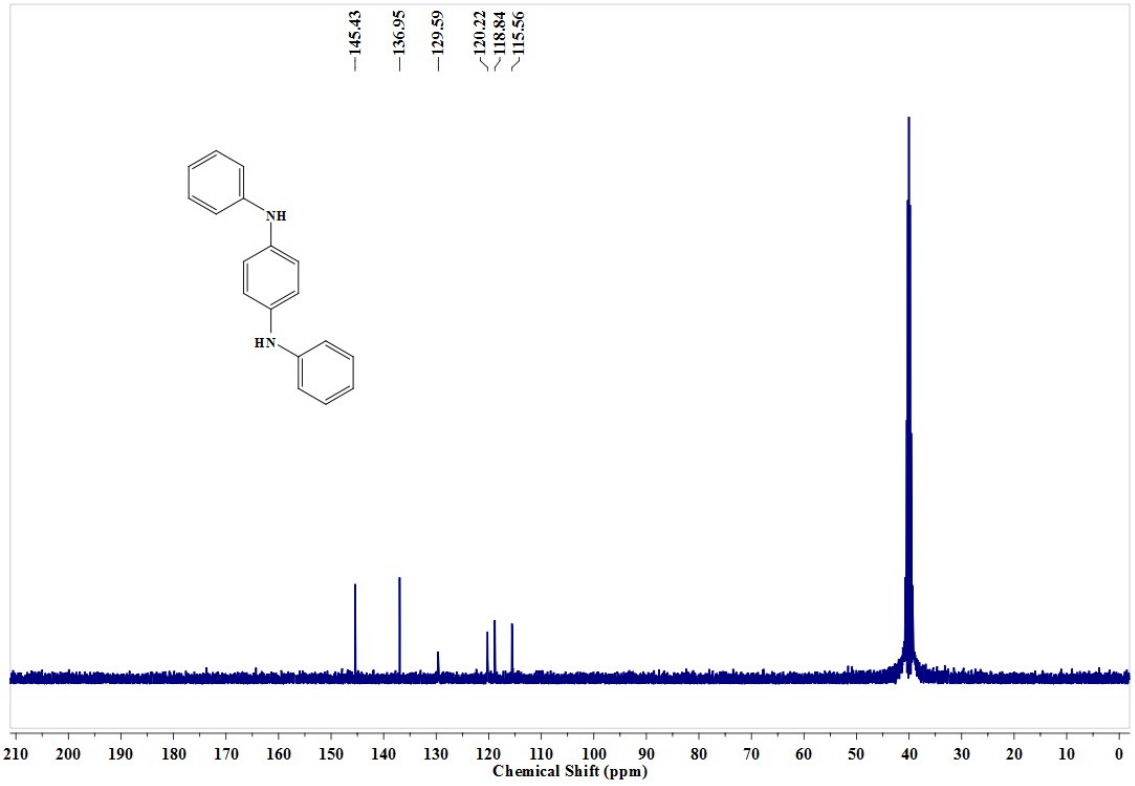
4.16
4.00
4.09
2.03
11.0 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
Chemical Shift (ppm)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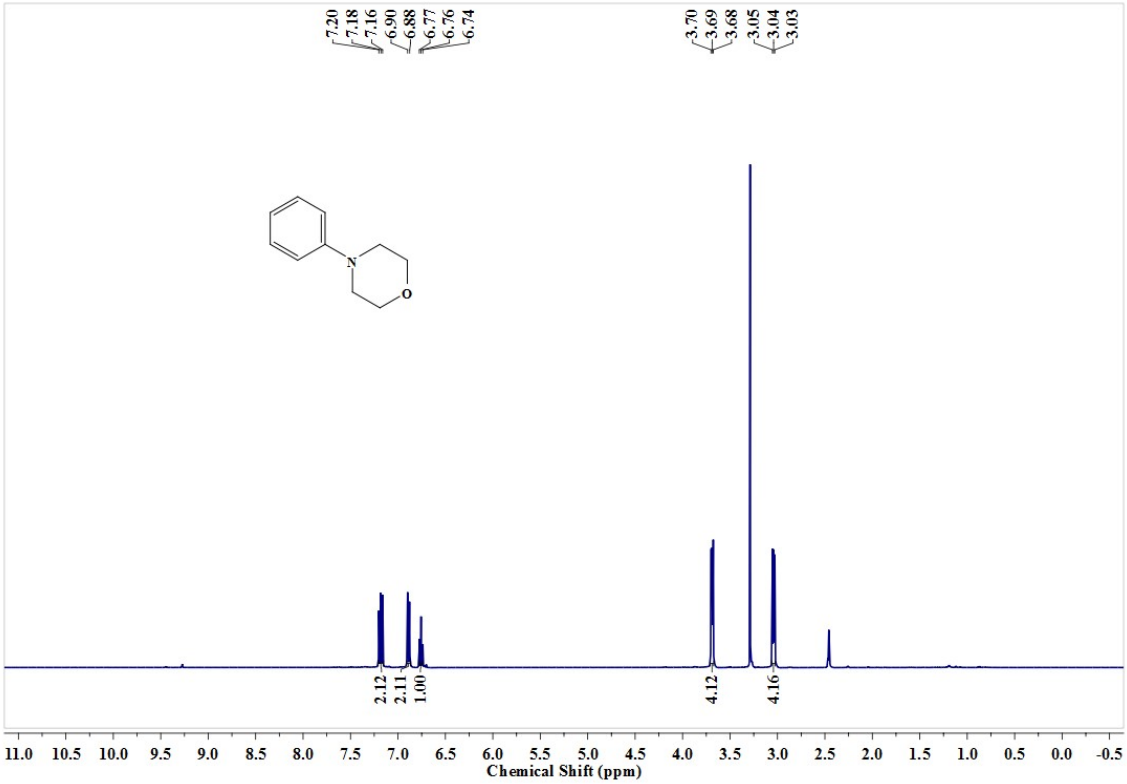
Chemical Shift (ppm)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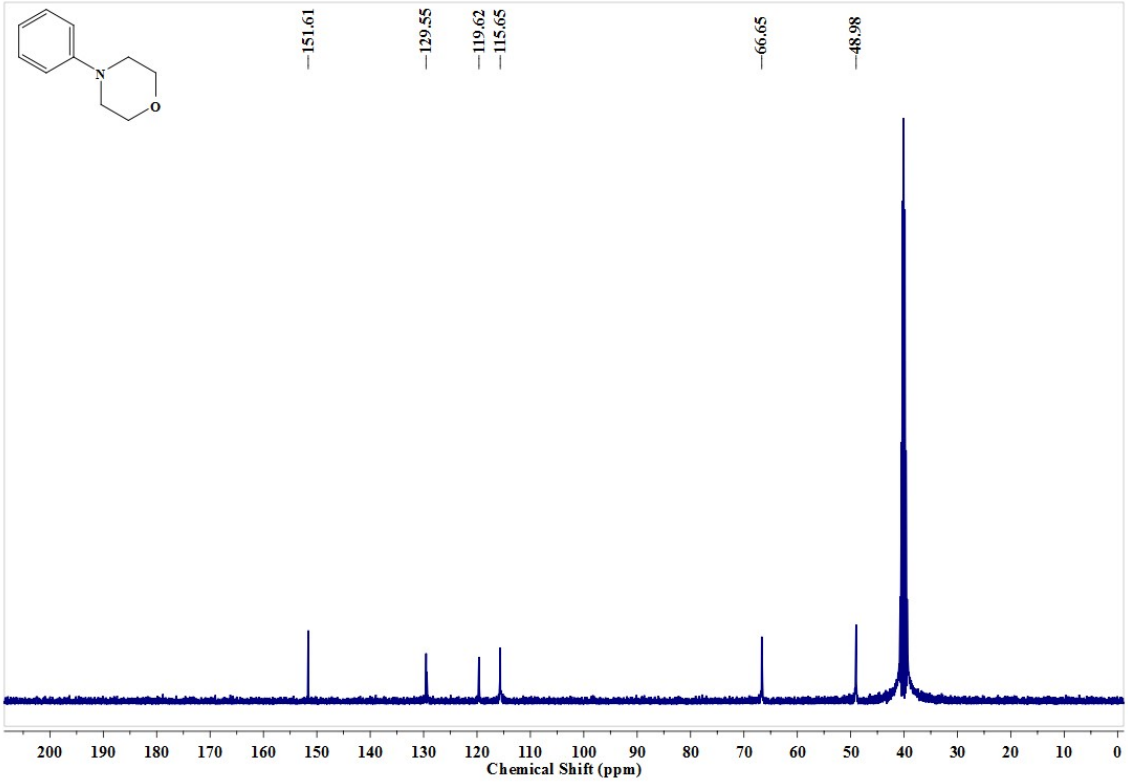
3.04
3.03
2.12
2.11
1.00
4.12
4.16
Chemical Shift (ppm)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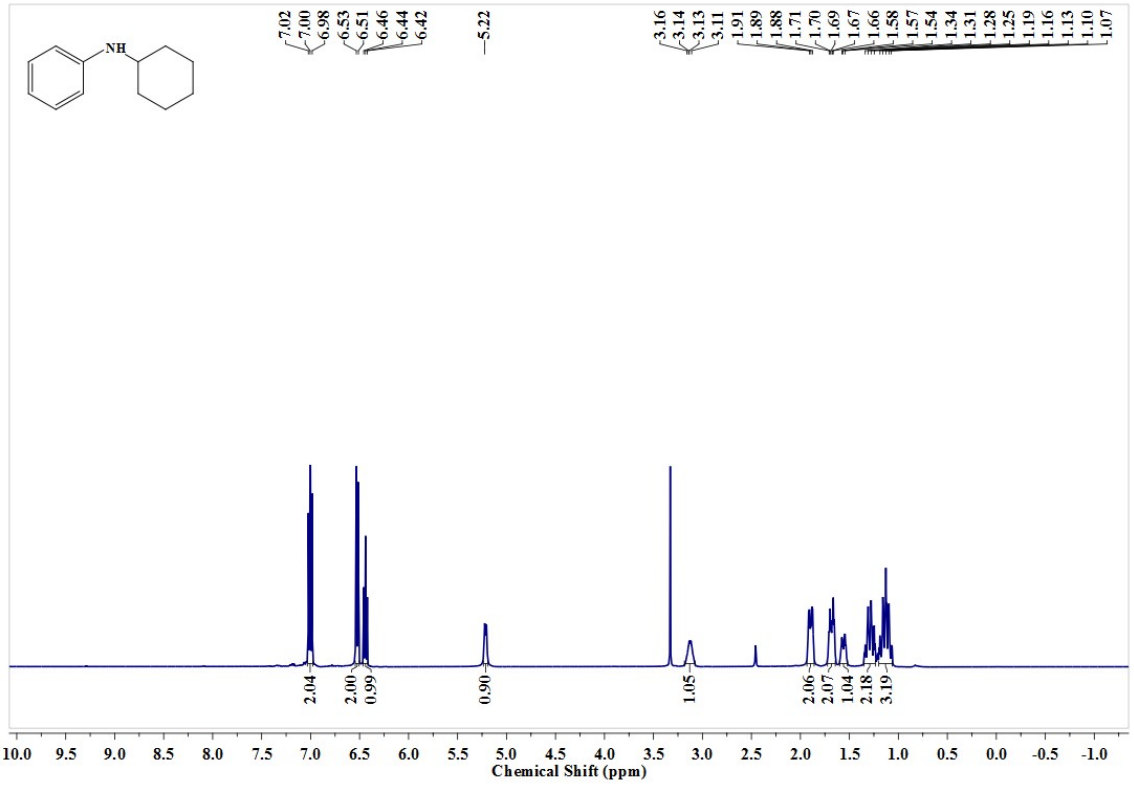
Chemical Shift (ppm)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6.42
5.22
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1.67
1.66
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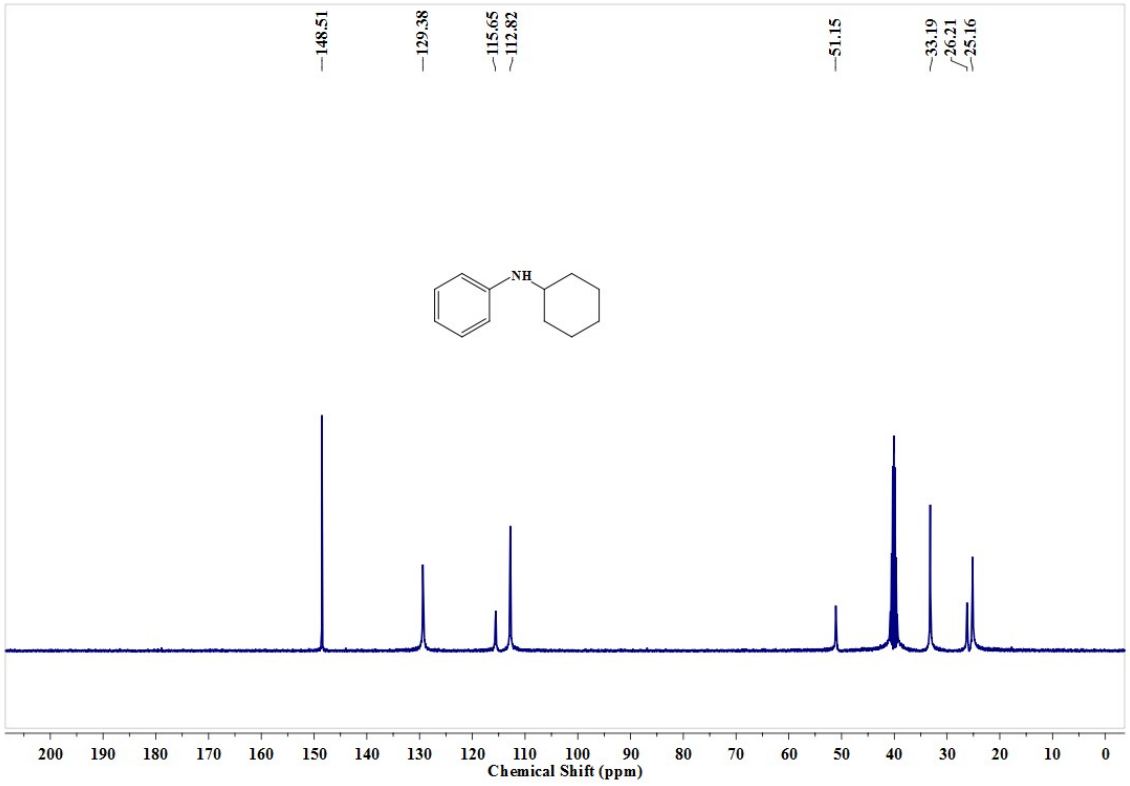
1.57
1.54
1.34
1.31
1.28
1.25
1.19
1.16
1.13
1.10
1.07
2.04
2.00
0.99
0.90
1.05
2.06
2.07
1.04
2.18
3.19
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
Chemical Shift (ppm)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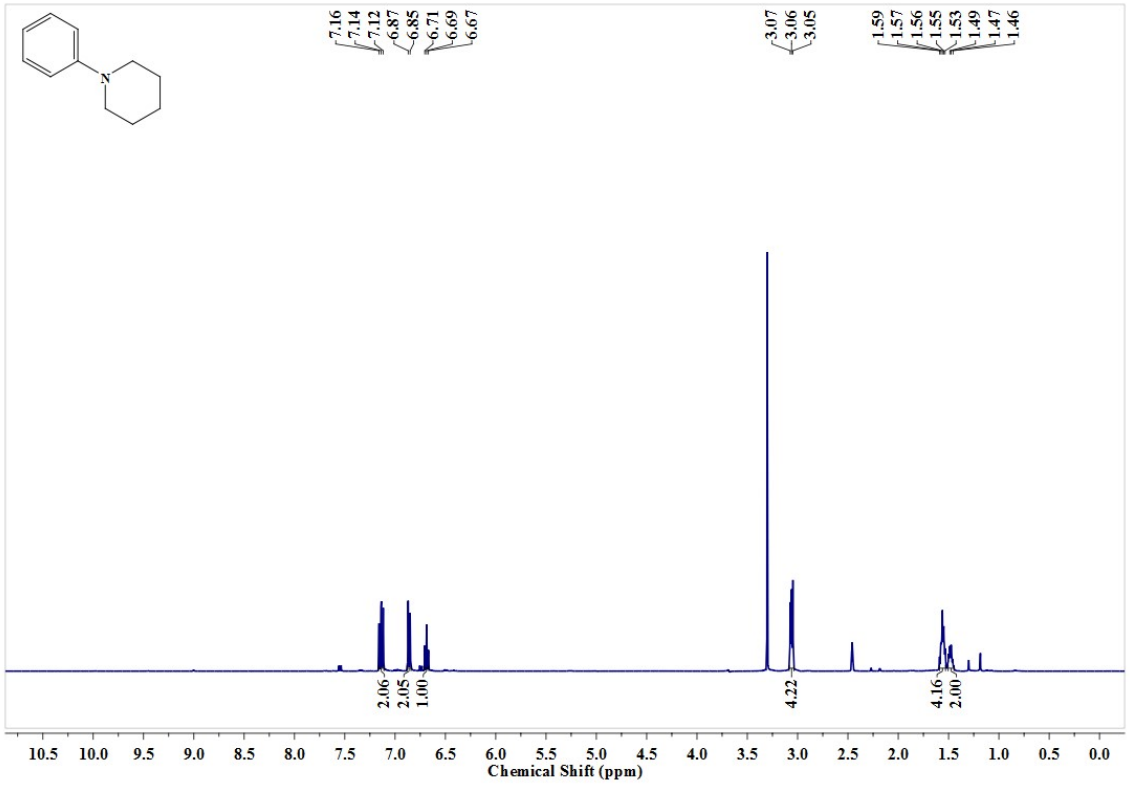
Chemical Shift (ppm)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6.69
6.67
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3.06
3.05
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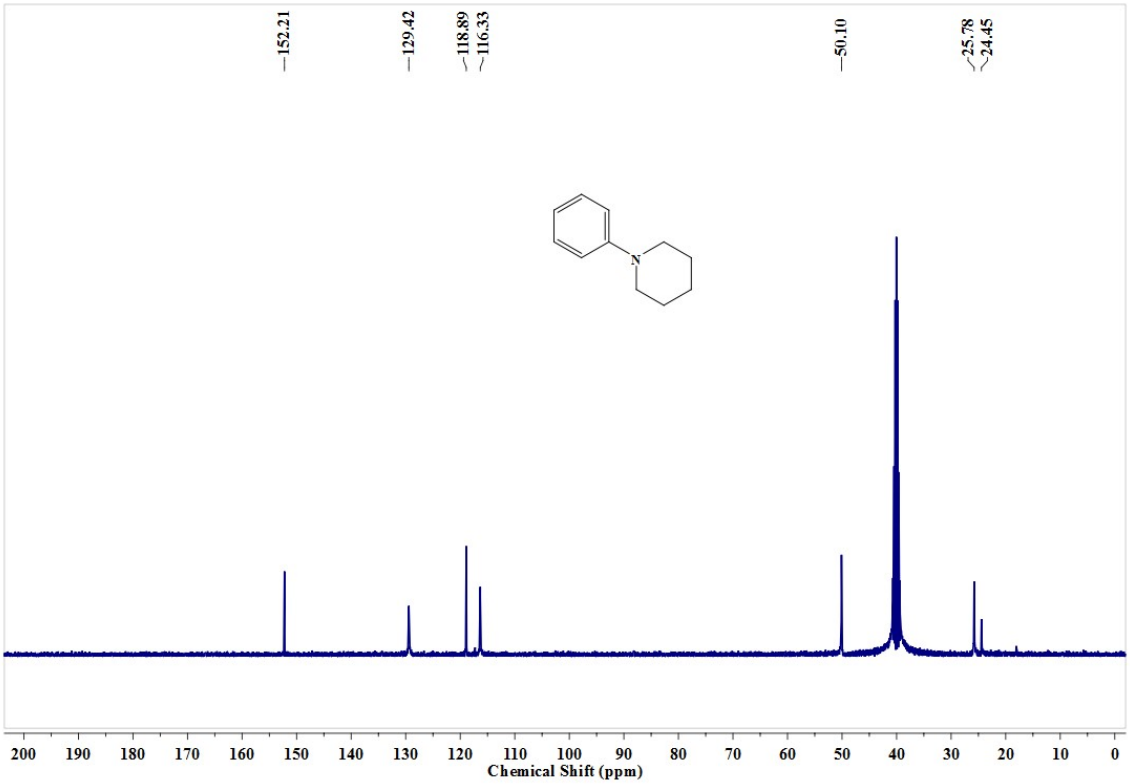
1.57
1.56
1.55
1.53
1.49
1.47
1.46
2.06
2.05
1.00
4.22
4.16
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical Shift (ppm)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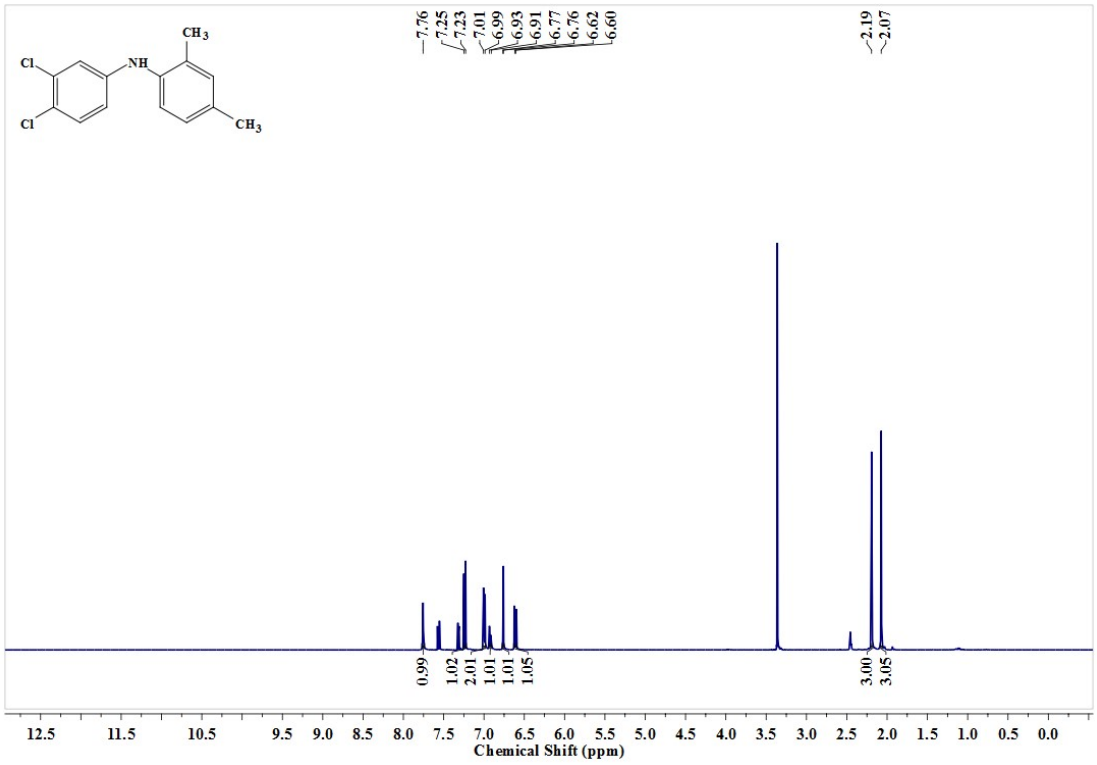
Chemical Shift (ppm)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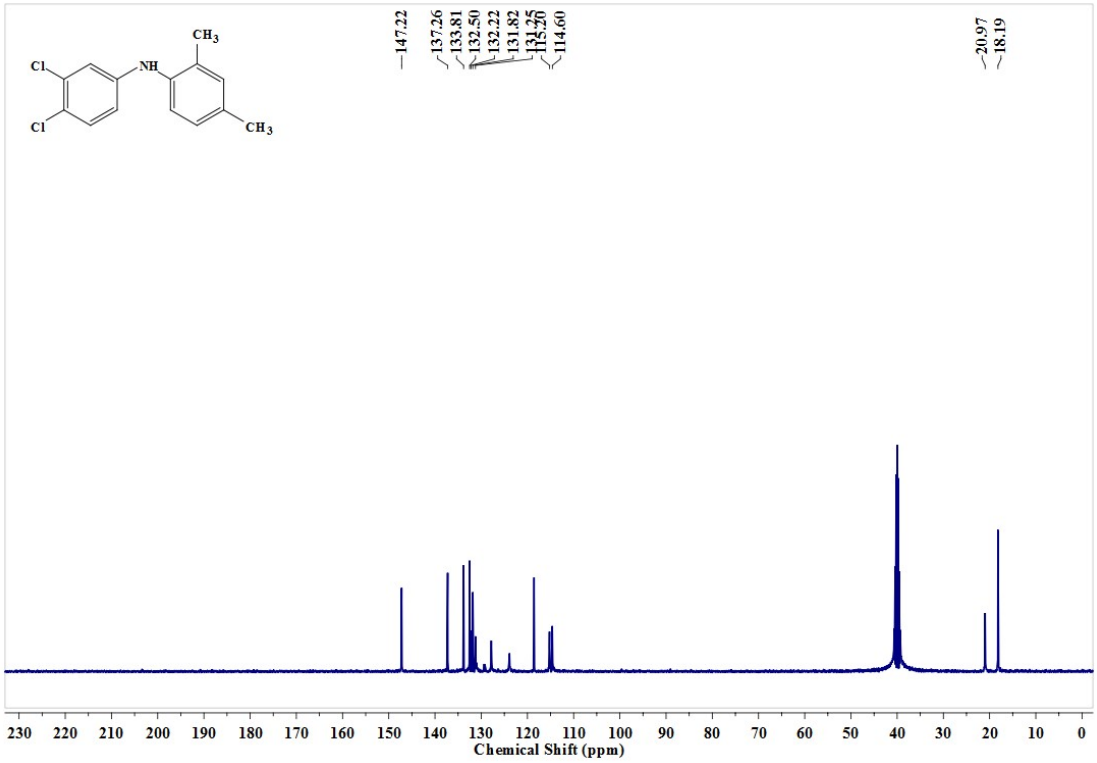
6.76
6.62
6.60
2.19
2.07
0.99
1.02
2.01
1.01
1.01
1.05
3.00
3.05
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical Shift (ppm)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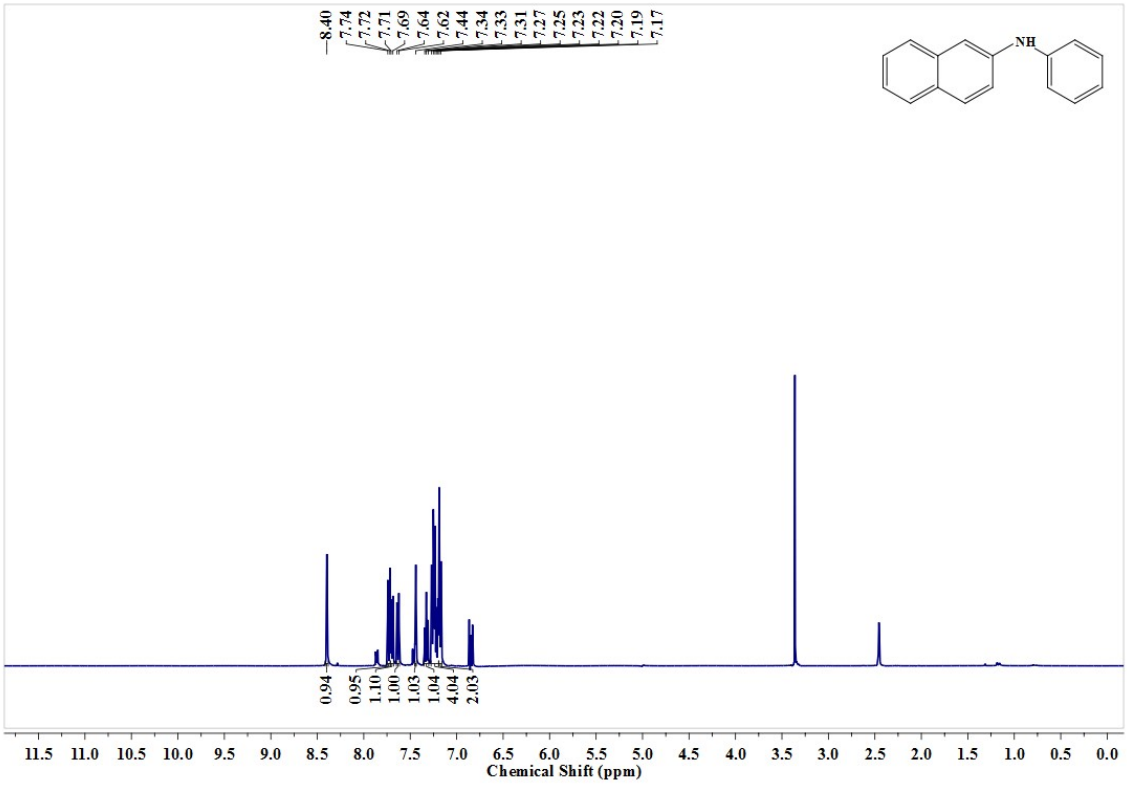
114.60
20.97
18.19
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)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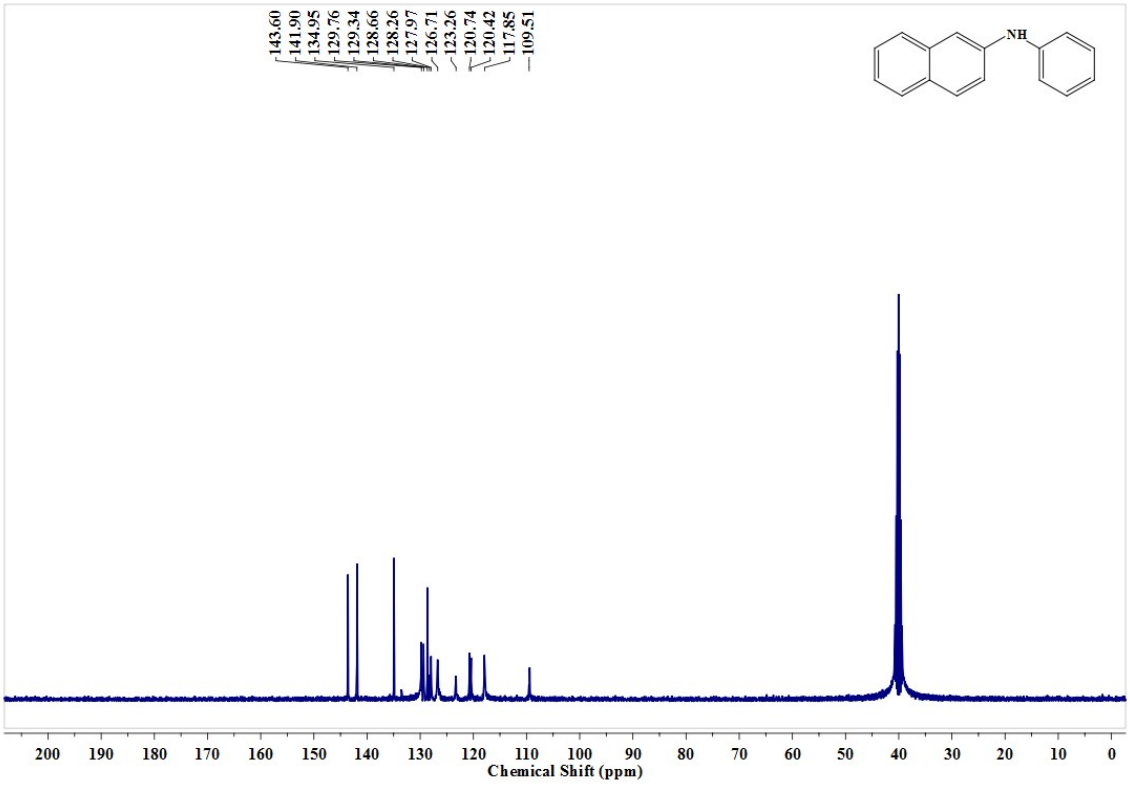
7.33
7.31
7.27
7.25
7.23
7.22
7.20
7.19
7.17
NH
0.94
0.95
1.10
1.00
1.03
1.04
4.04
2.03
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical Shift (ppm)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128.66
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127.97
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120.42
117.85
109.51
NH
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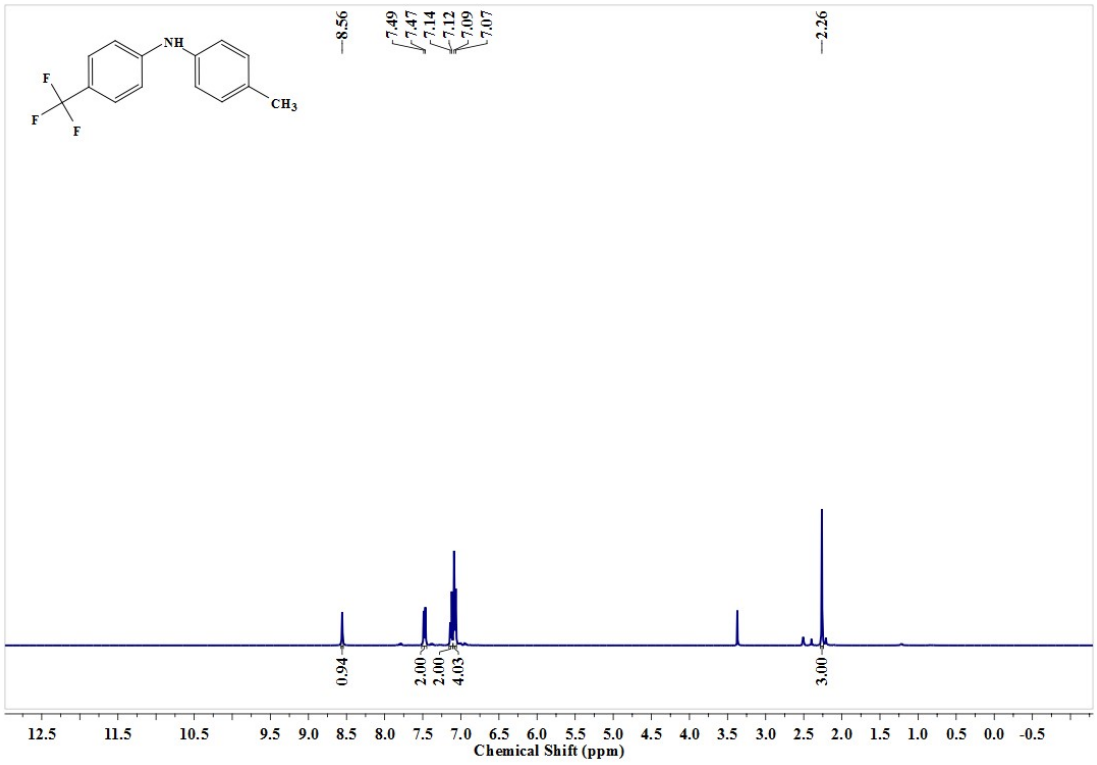
Chemical Shift (ppm)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2.26
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F
F
CH3
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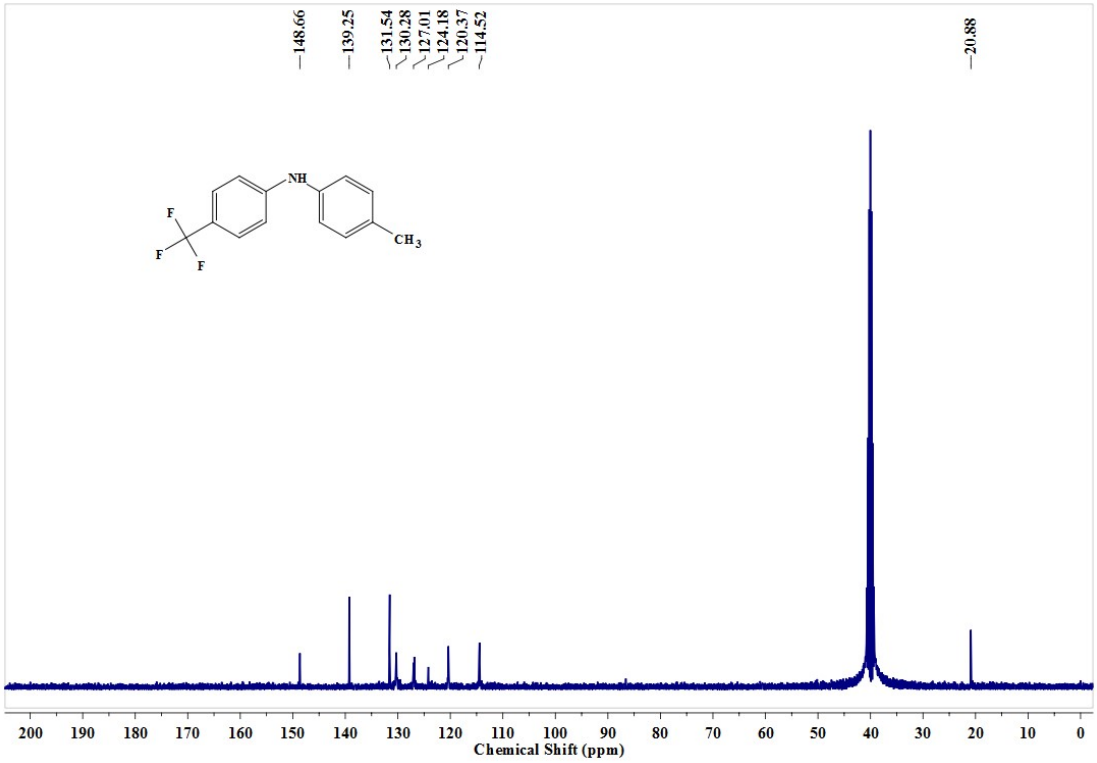
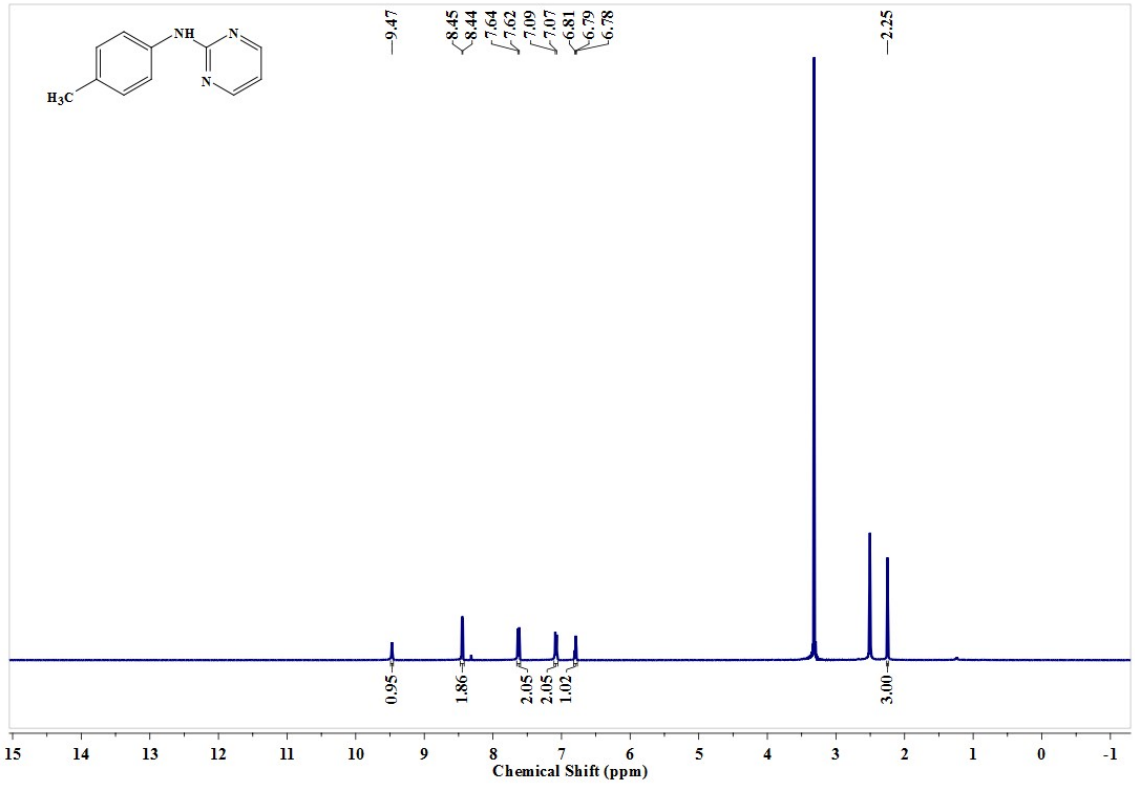
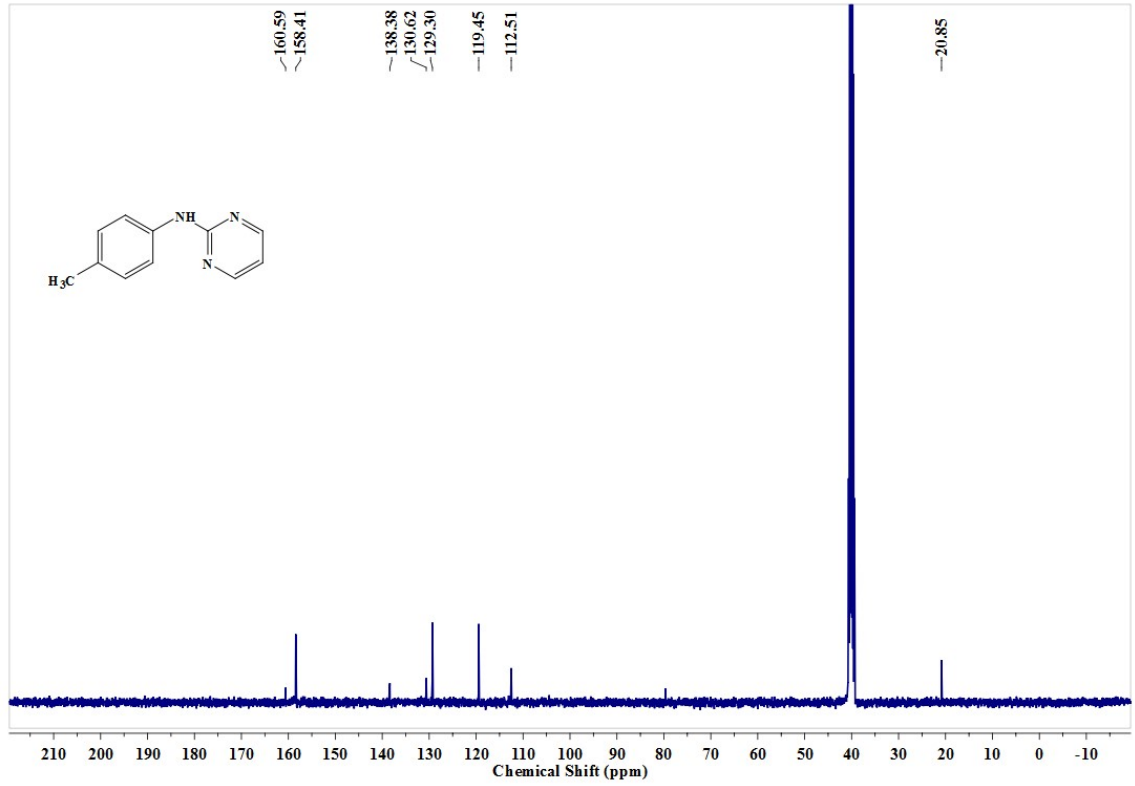
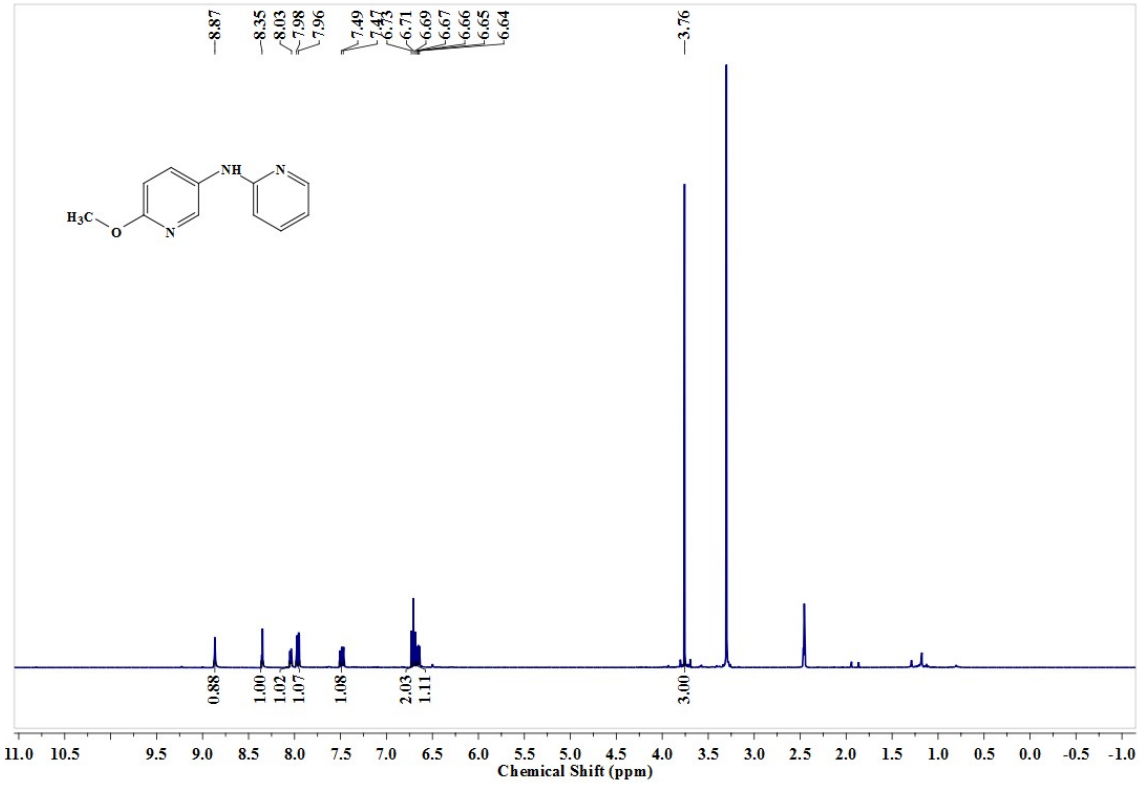
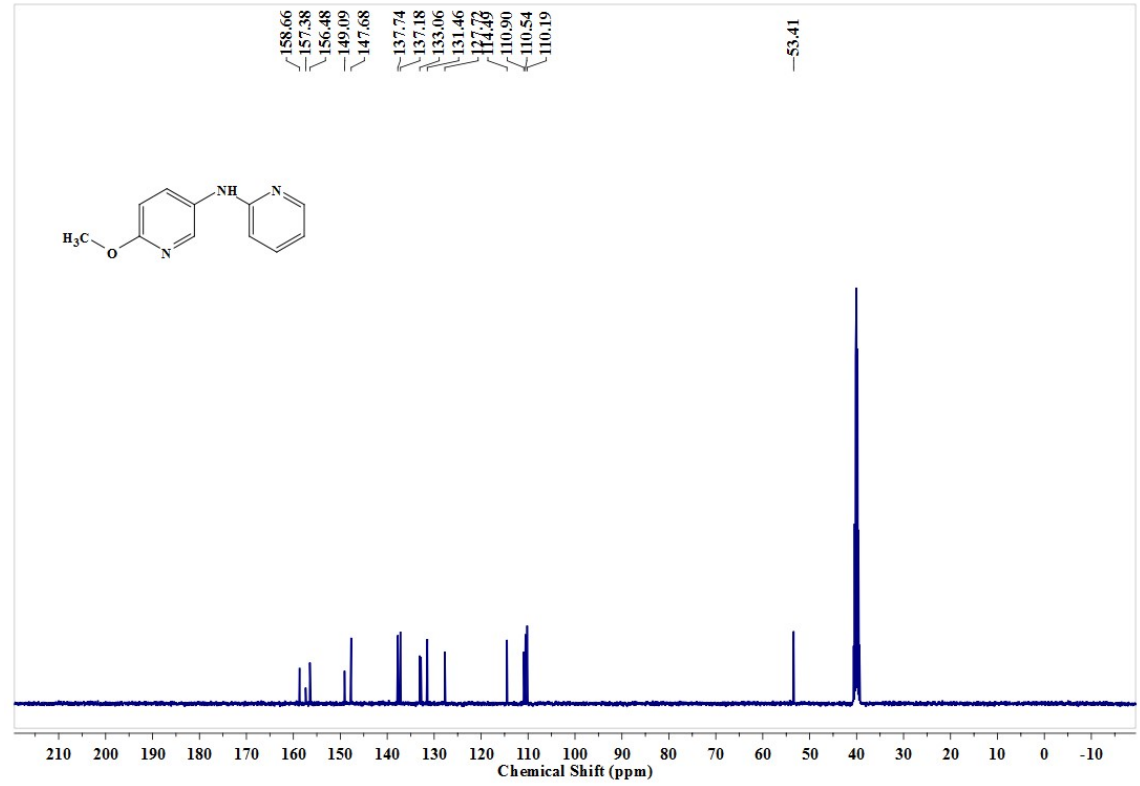
2.00
2.00
4.03
3.00
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
Chemical Shift (ppm)

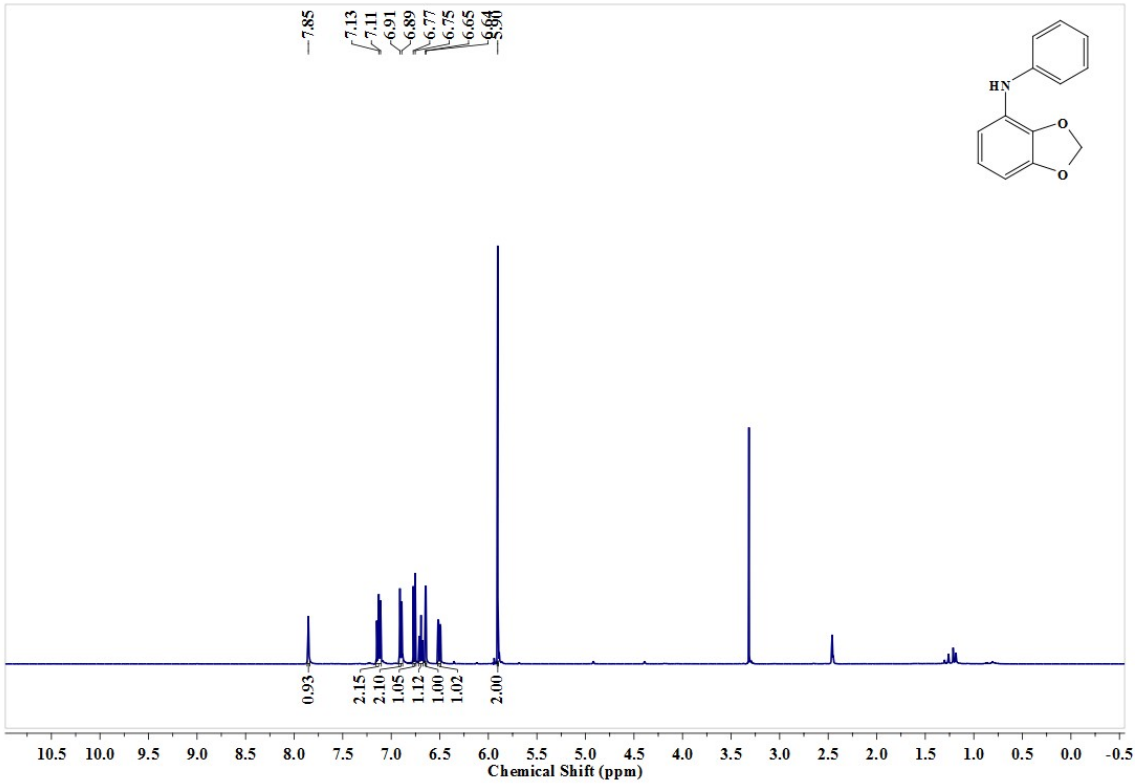

148.66
139.25
131.54
130.28
127.01
124.18
120.37
114.52
20.88
NH
F
F
F
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)

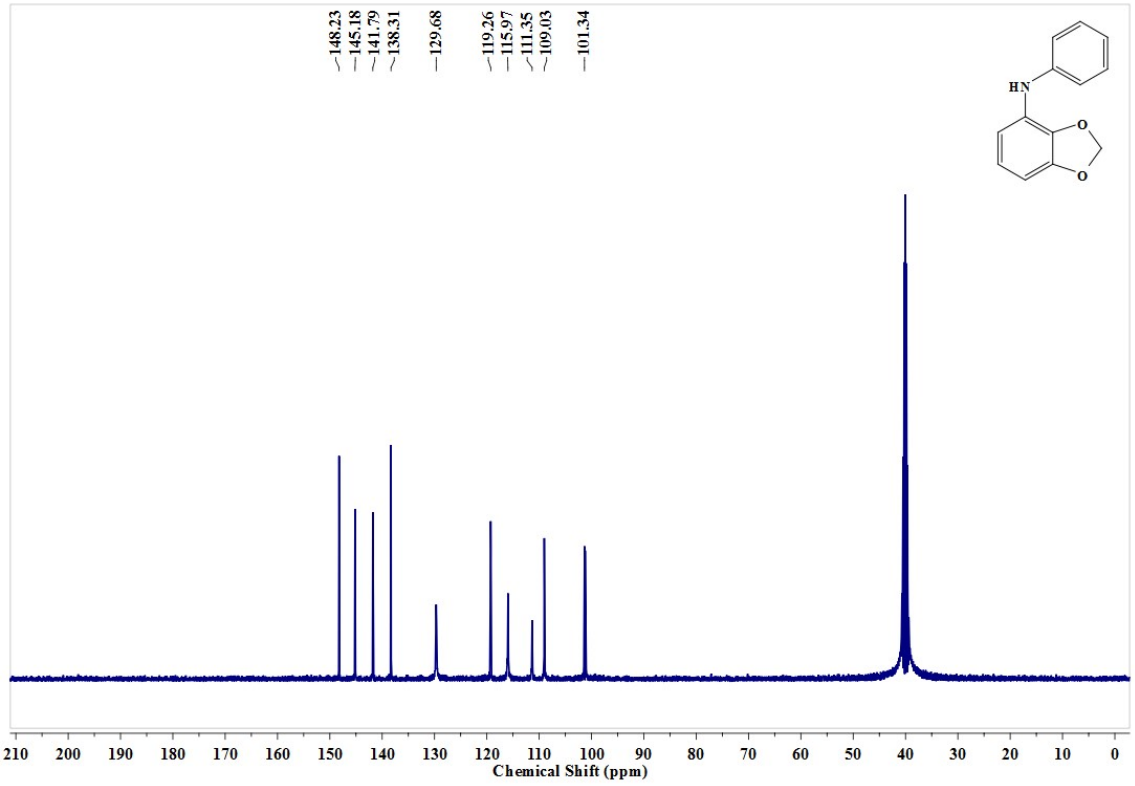

9.47
8.45
8.44
7.64
7.62
7.09
7.07
6.81
6.79
6.78
2.25
0.95
1.86
2.05
2.05
1.02
3.00
Chemical Shift (ppm)


160.59
158.41
138.38
130.62
129.30
119.45
112.51
20.85
Chemical Shift (ppm)

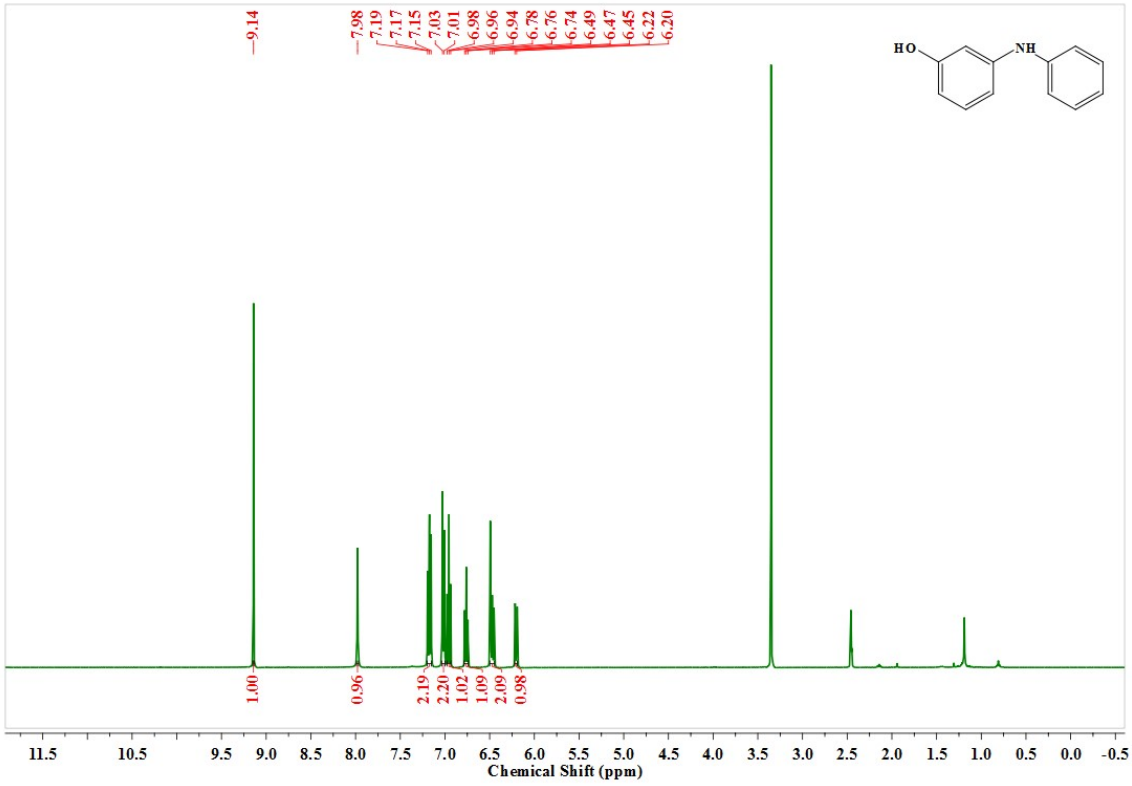

8.87
8.35
8.03
7.98
7.96
7.49
7.47
6.71
6.69
6.67
6.66
6.65
6.64
3.76
NH
N
H3C
O
N
0.88
1.00
1.02
1.07
1.08
2.03
1.11
3.00
11.0 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
Chemical Shift (ppm)

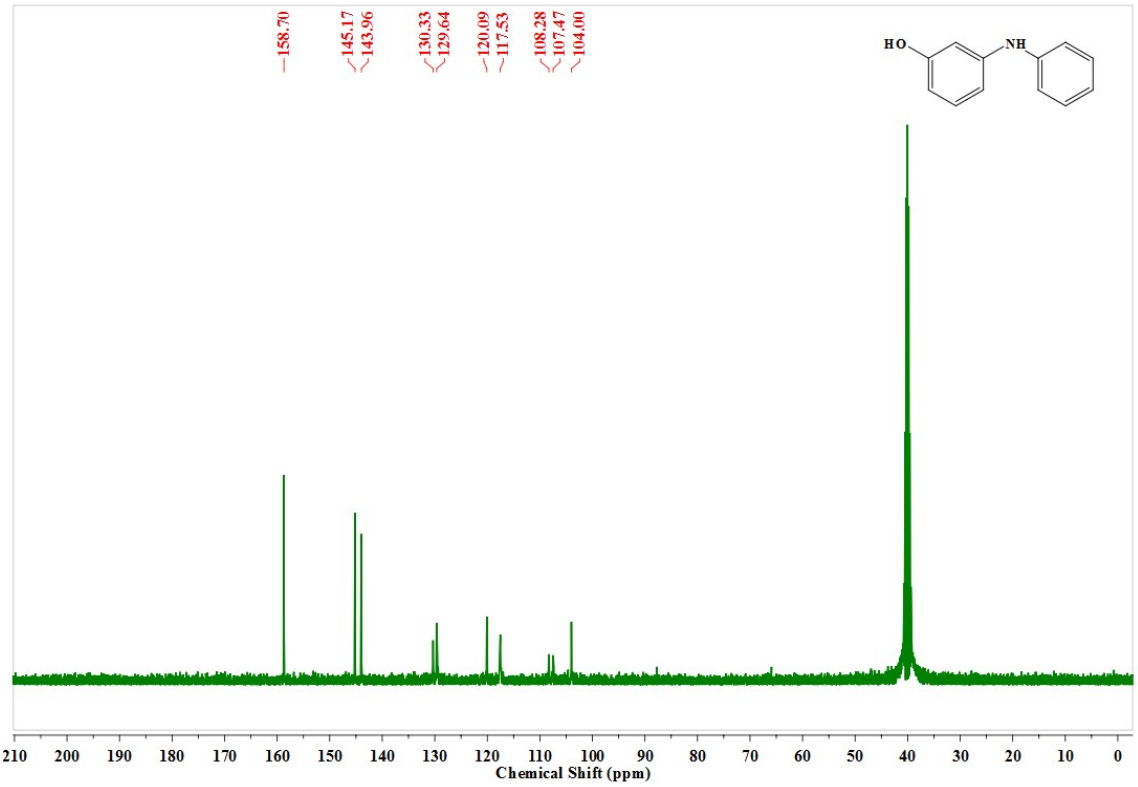

158.66
157.38
156.48
149.09
147.68
137.74
137.18
133.06
131.46
110.90
110.54
110.19
53.41
NH
N
H3C
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
Chemical Shift (ppm)

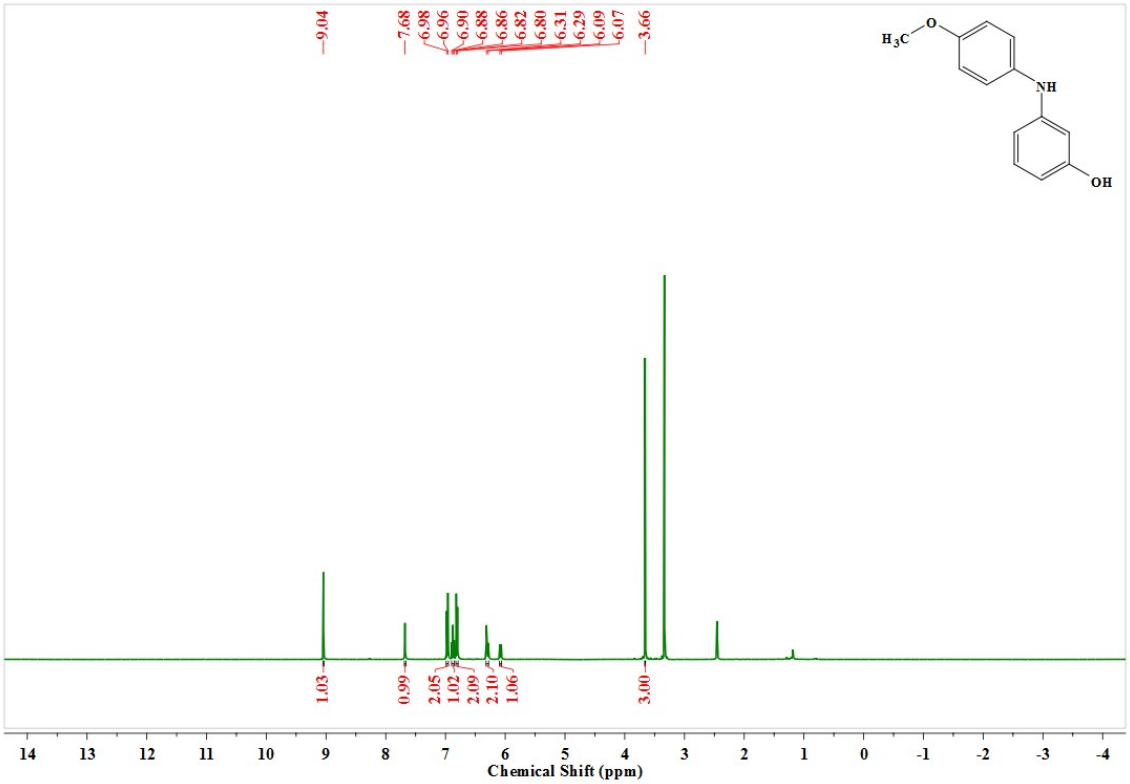

7.85
7.13
7.11
6.91
6.89
6.77
6.75
6.65
6.64
5.90
HN
O
O
0.93
2.15
2.10
1.05
1.12
1.00
1.02
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
Chemical Shift (ppm)

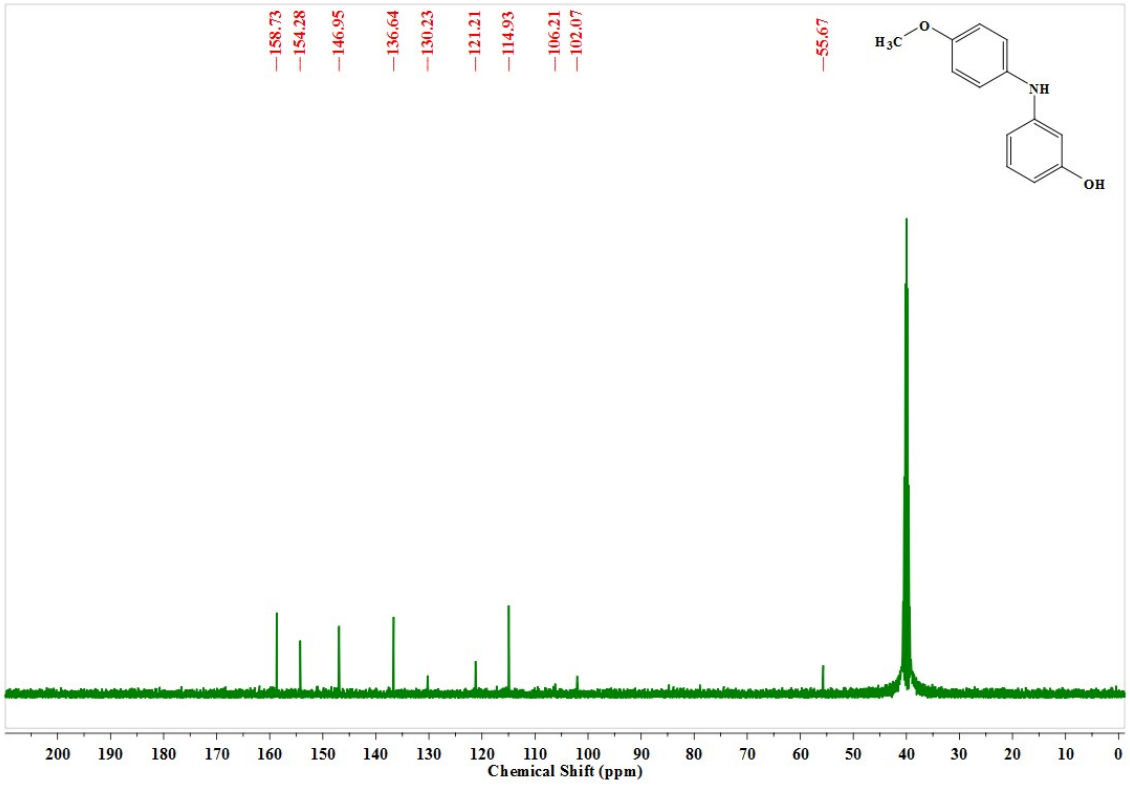

148.23
145.18
141.79
138.31
129.68
119.26
115.97
111.35
109.03
101.34
HN
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)

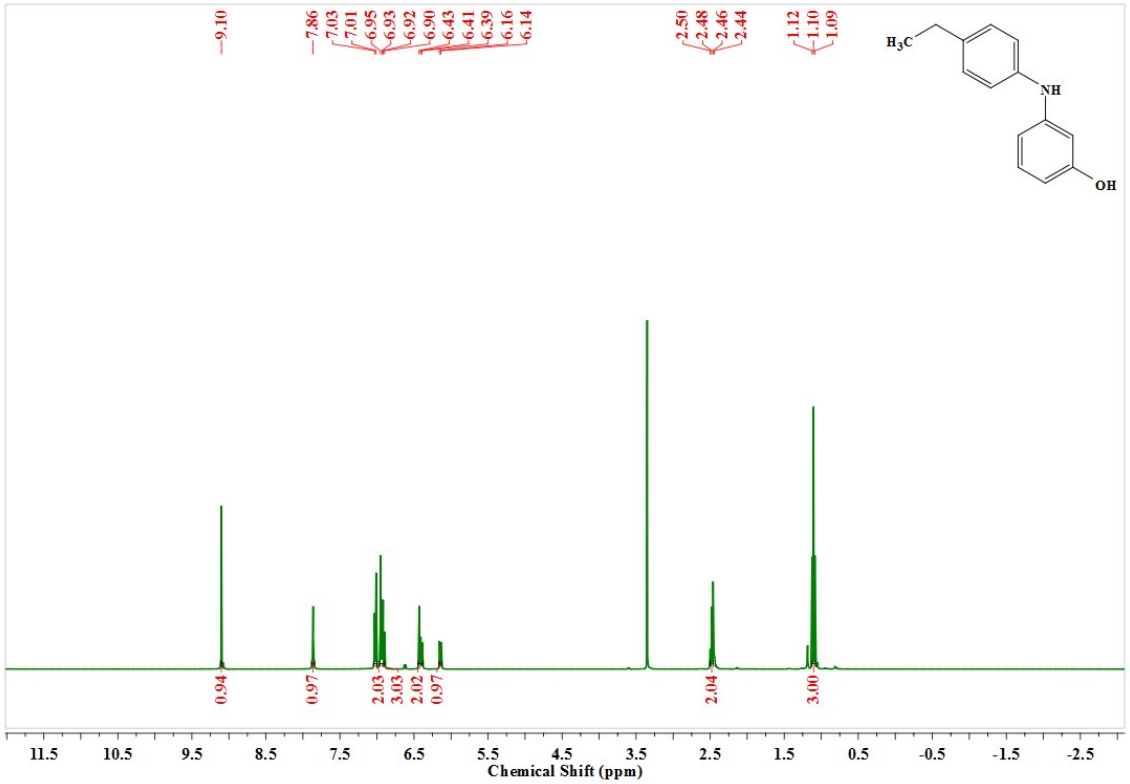
4.2 *^{1}H and ^{13}C NMR spectra of 3-arylaminophenols (**5**)*

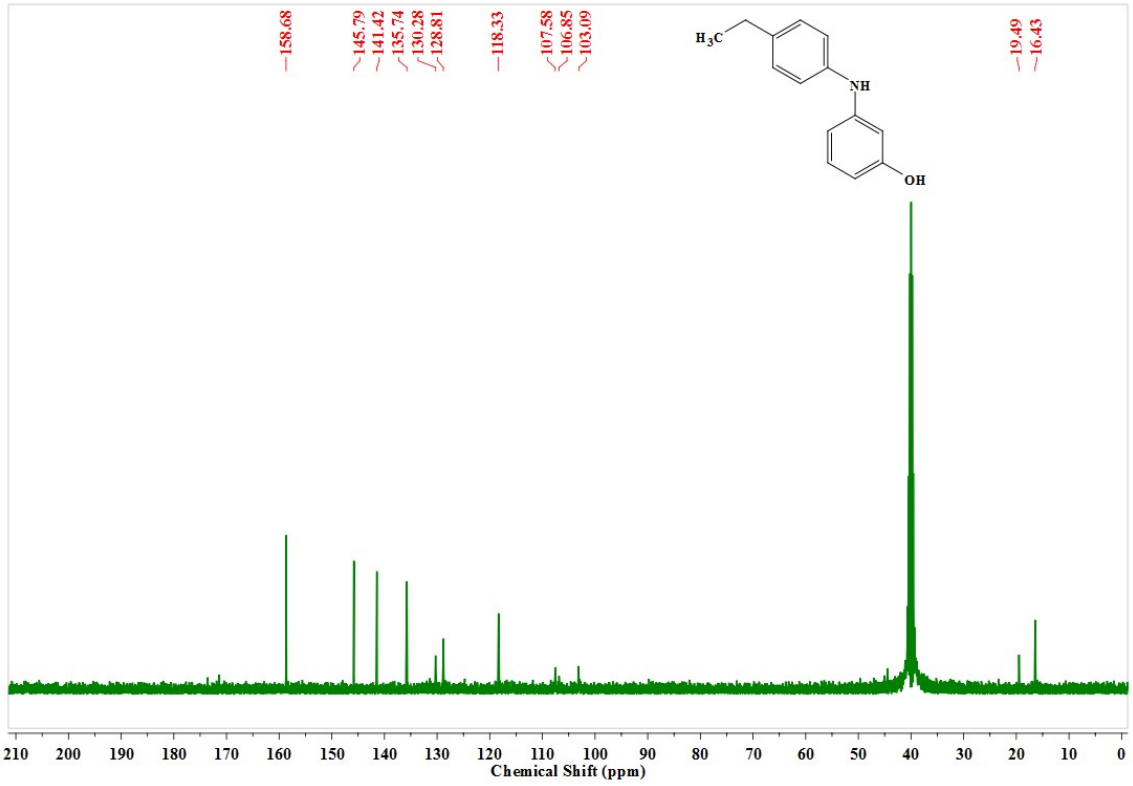


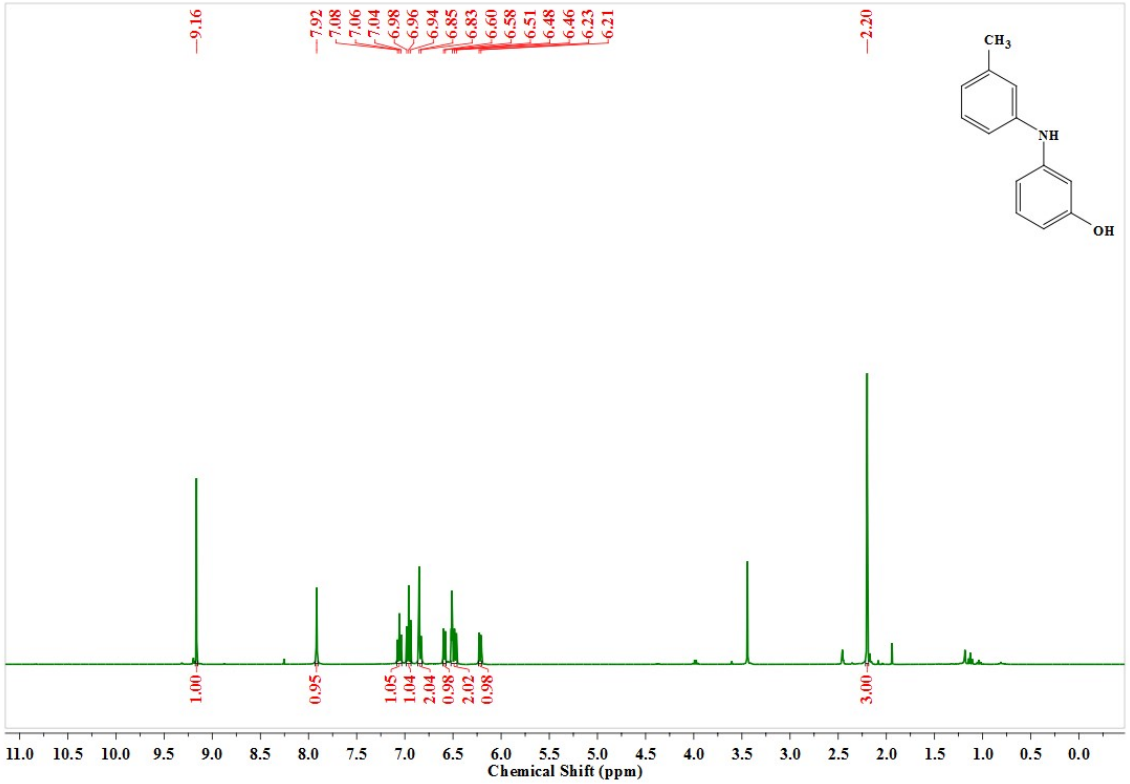


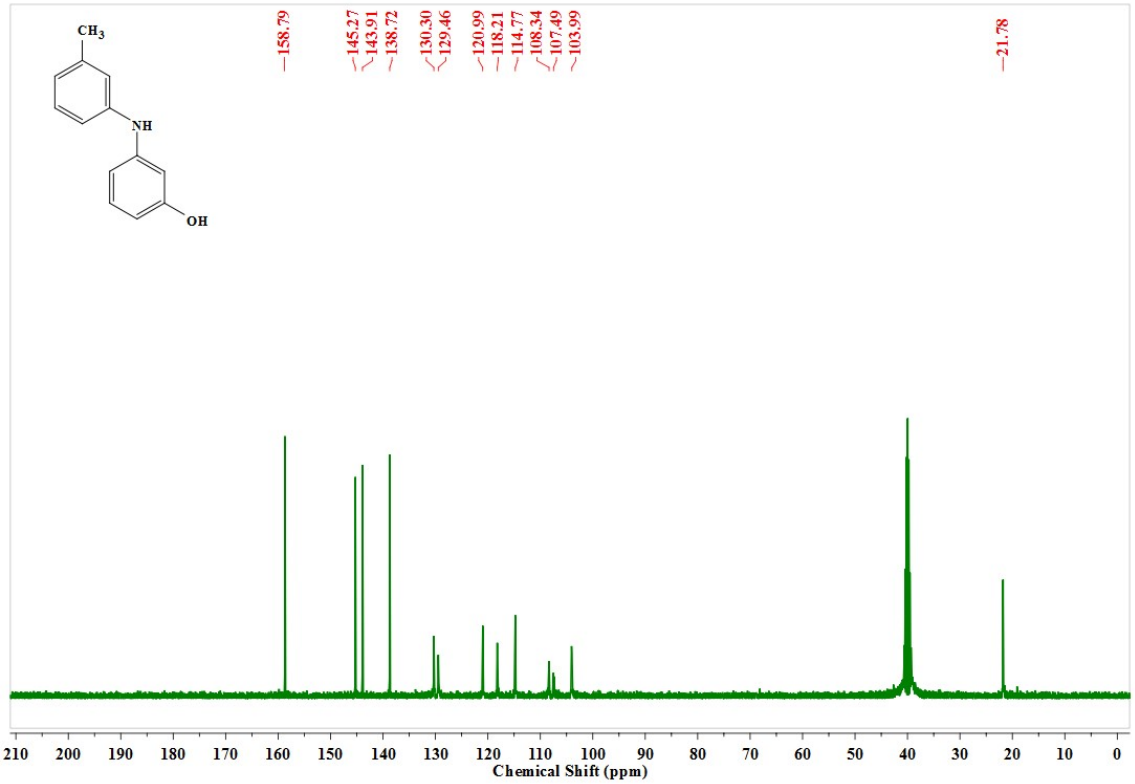

9.04
7.68
6.98
6.96
6.90
6.88
6.86
6.82
6.80
6.31
6.29
6.09
6.07
3.66
H3C
O
NH
OH
1.03
0.99
2.05
1.02
2.09
2.10
1.06
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
Chemical Shift (ppm)

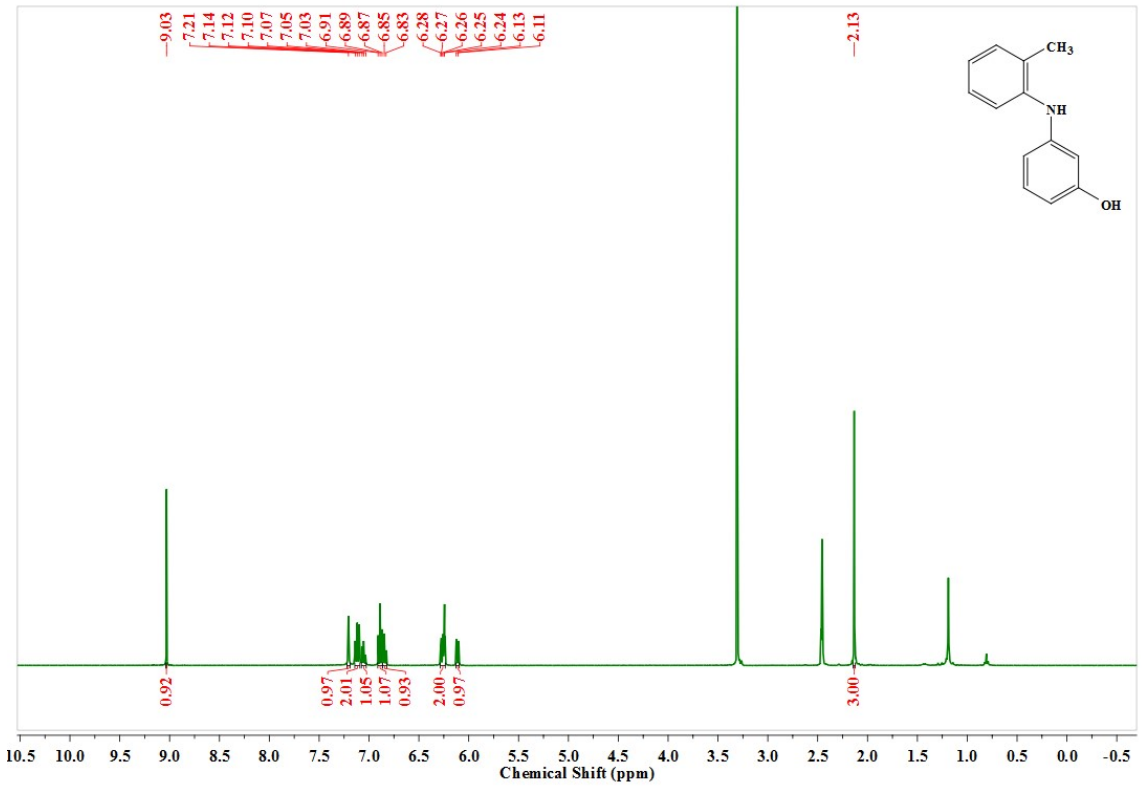

158.73
154.28
146.95
136.64
130.23
121.21
114.93
106.21
102.07
55.67
H3C
O
NH
OH
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)

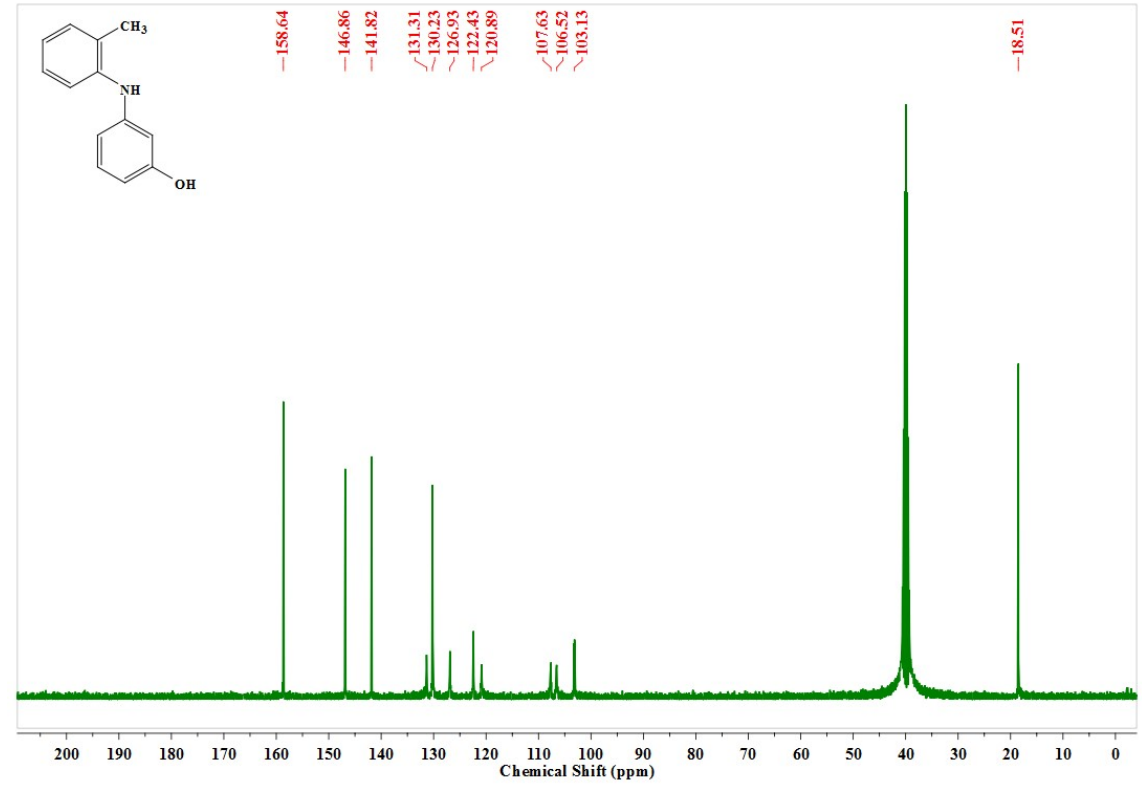

9.10
7.86
7.03
7.01
6.95
6.93
6.92
6.90
6.43
6.41
6.39
6.16
6.14
2.50
2.48
2.46
2.44
1.12
1.10
1.09
H3C
NH
OH
0.94
0.97
2.03
3.03
2.02
0.97
2.04
3.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
-2.5
Chemical Shift (ppm)

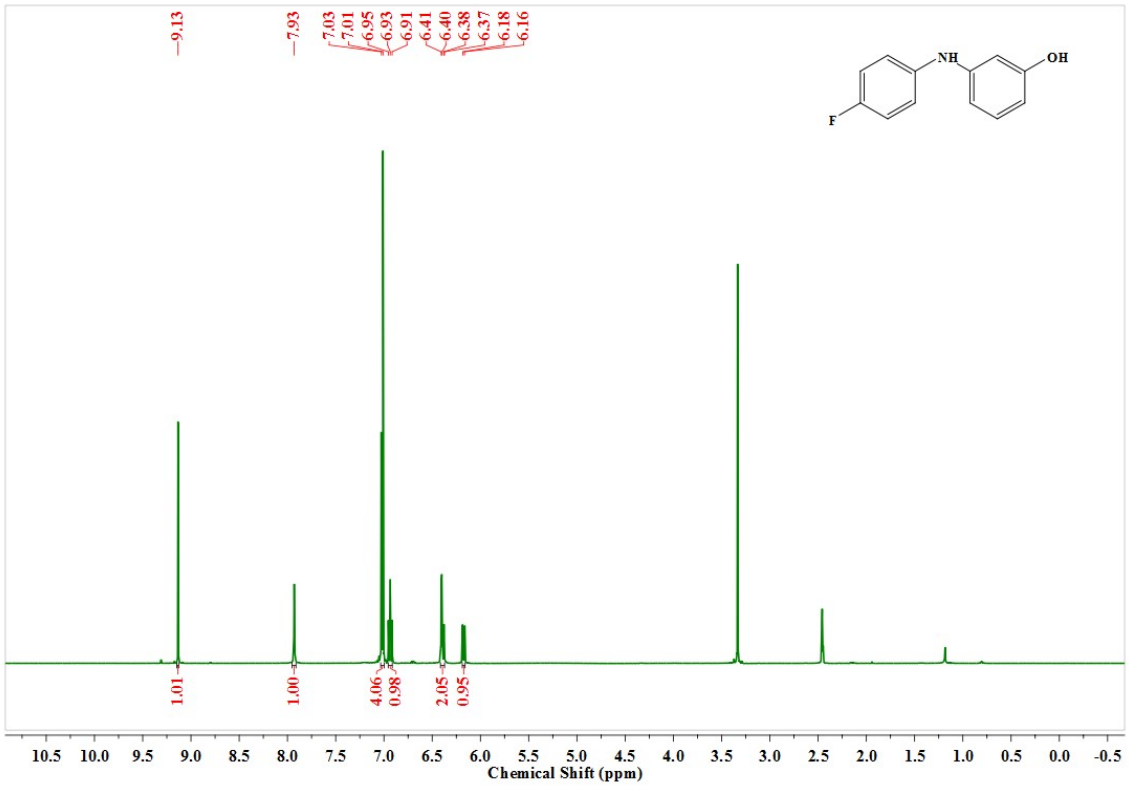

158.68
145.79
141.42
135.74
130.28
128.81
118.33
107.58
106.85
103.09
19.49
16.43
H3C
NH
OH
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

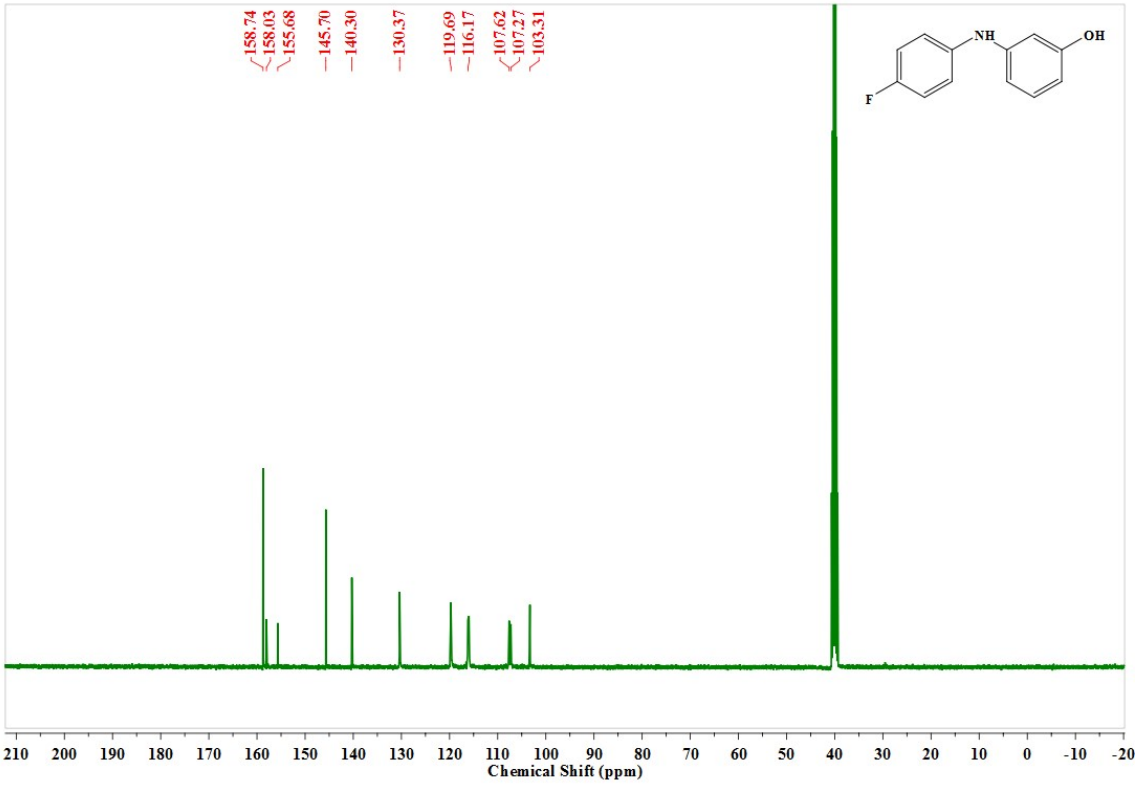

9.16
7.92
7.08
7.06
7.04
6.98
6.96
6.94
6.85
6.83
6.60
6.58
6.51
6.48
6.46
6.23
6.21
2.20
CH3
NH
OH
1.00
0.95
1.05
1.04
2.04
0.98
2.02
0.98
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical Shift (ppm)

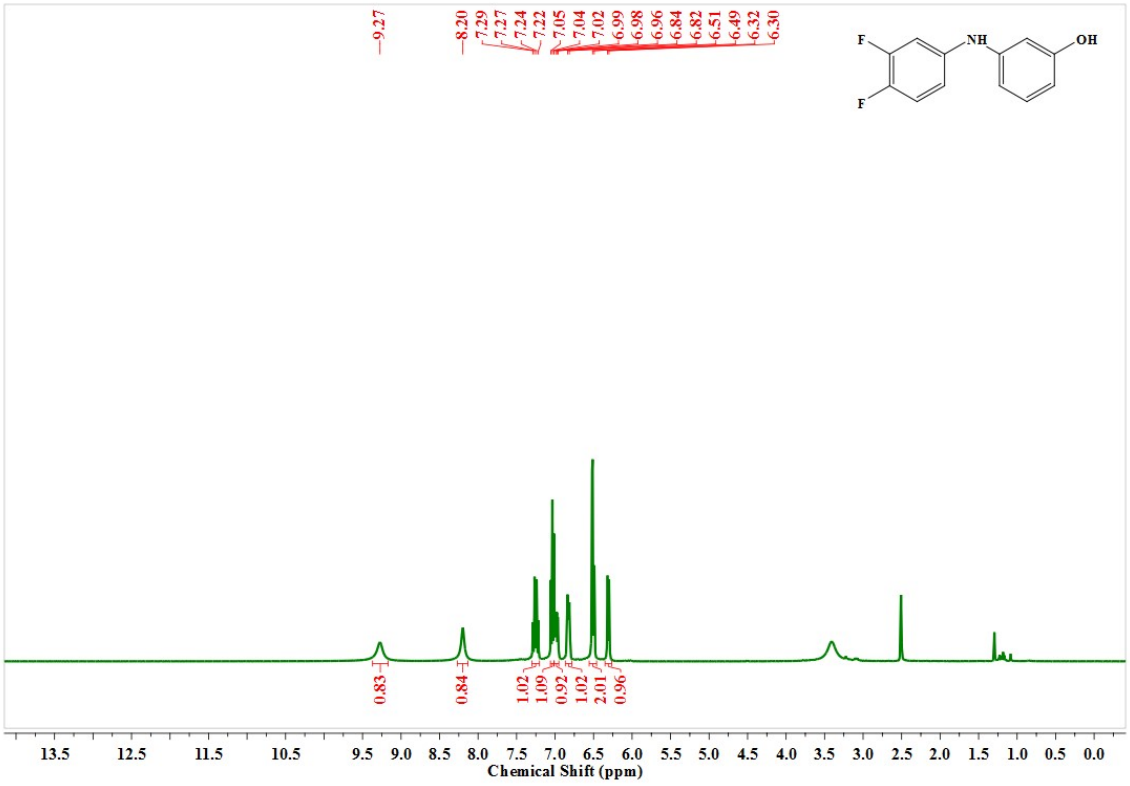

158.79
145.27
143.91
138.72
130.30
129.46
120.99
118.21
114.77
108.34
107.49
103.99
21.78
CH3
NH
OH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)

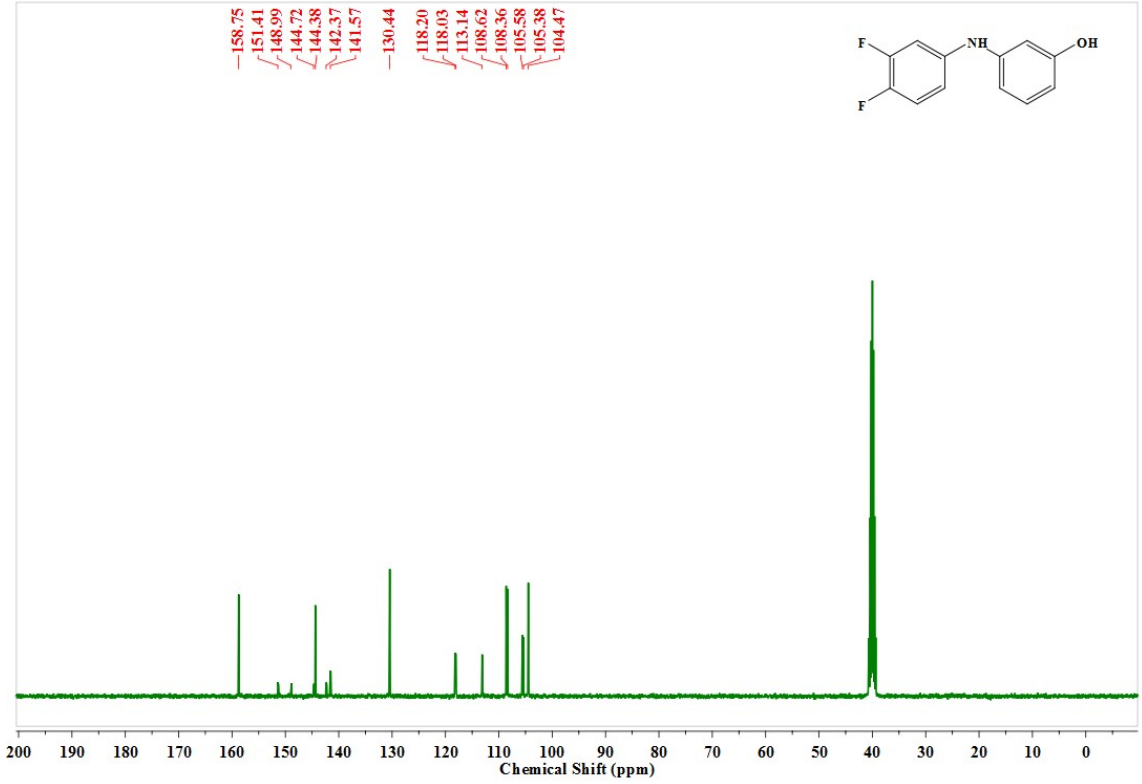

9.03
7.21
7.14
7.12
7.10
7.07
7.05
7.03
6.91
6.89
6.87
6.85
6.83
6.28
6.27
6.26
6.25
6.24
6.13
6.11
2.13
CH3
NH
OH
0.92
0.97
2.01
1.05
1.07
0.93
2.00
0.97
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
Chemical Shift (ppm)

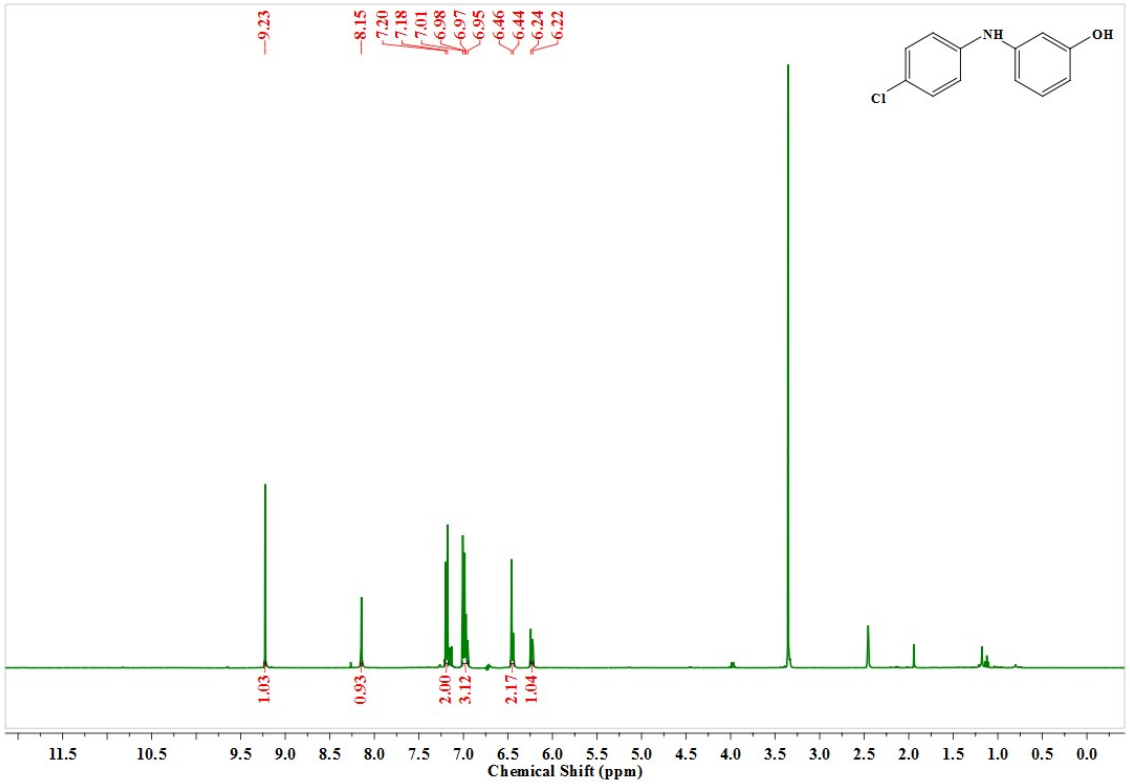

CH3
NH
OH
158.64
146.86
141.82
131.31
130.23
126.93
122.43
120.89
107.63
106.52
103.13
18.51
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)

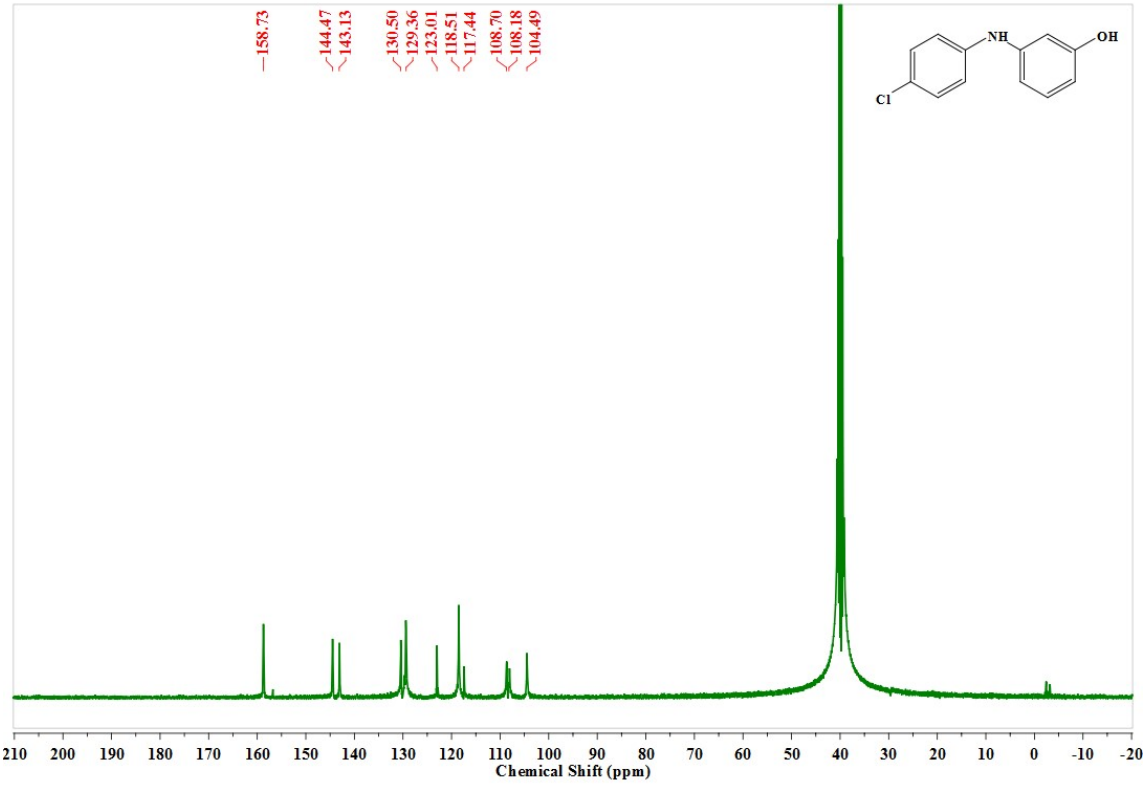

9.13
7.93
7.03
7.01
6.95
6.93
6.91
6.41
6.40
6.38
6.37
6.18
6.16
NH
OH
F
1.01
1.00
4.06
0.98
2.05
0.95
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
Chemical Shift (ppm)

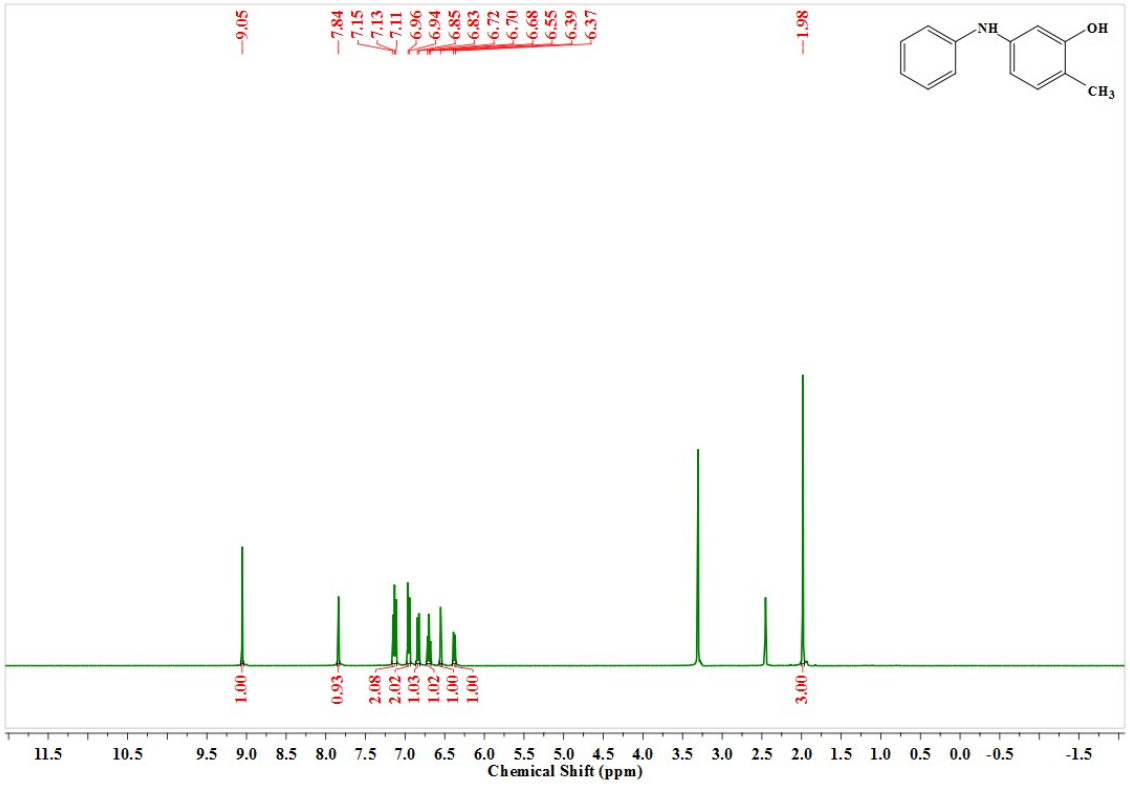

158.74
158.03
155.68
145.70
140.30
130.37
119.69
116.17
107.62
107.27
103.31
NH
OH
F
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
Chemical Shift (ppm)

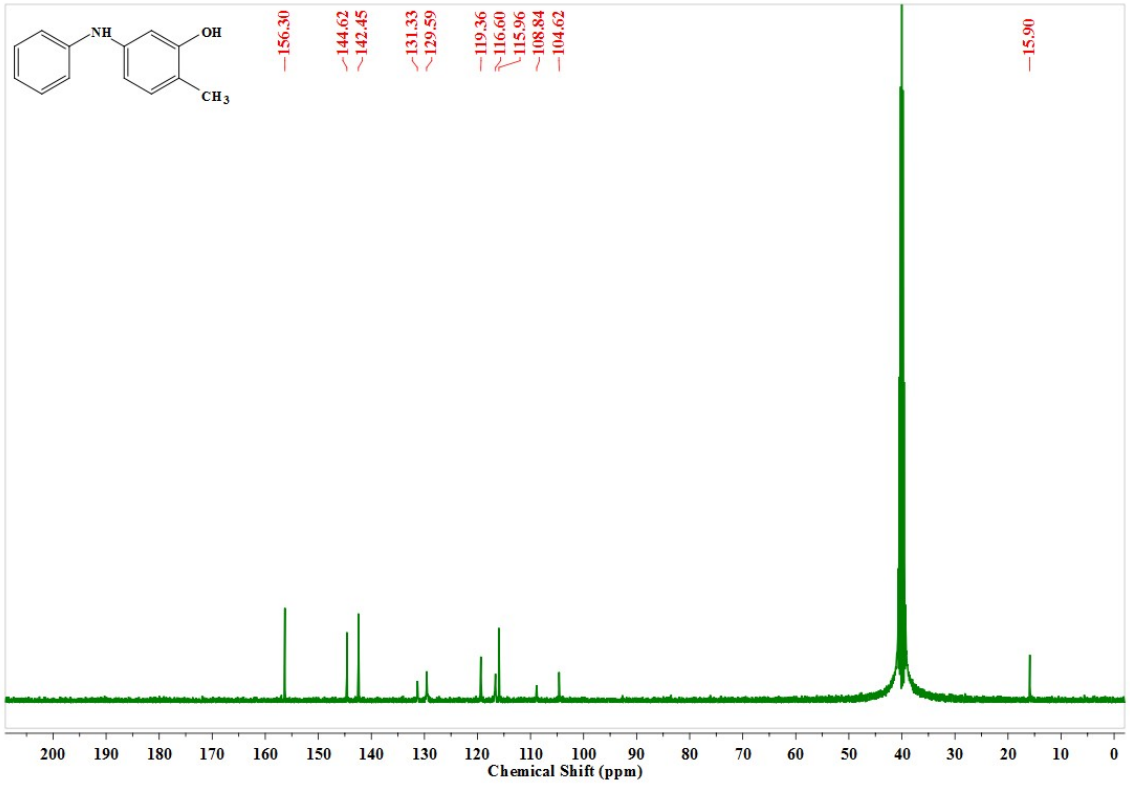

9.27
8.20
7.29
7.27
7.24
7.22
7.05
7.04
7.02
6.99
6.98
6.96
6.84
6.82
6.51
6.49
6.32
6.30
F
NH
OH
F
0.83
0.84
1.02
1.09
0.92
1.02
2.01
0.96
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical Shift (ppm)

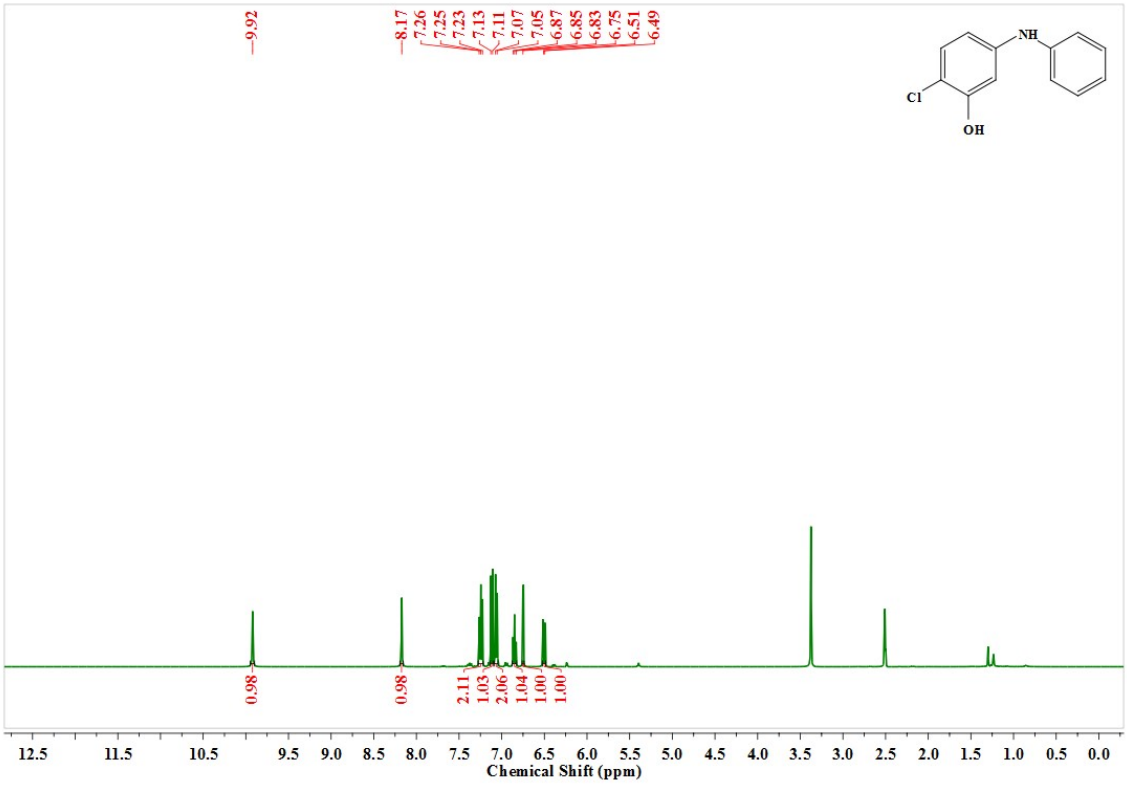

158.75
151.41
148.99
144.72
144.38
142.37
141.57
130.44
118.20
118.03
113.14
108.62
108.36
105.58
105.38
104.47
F
NH
OH
F
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)

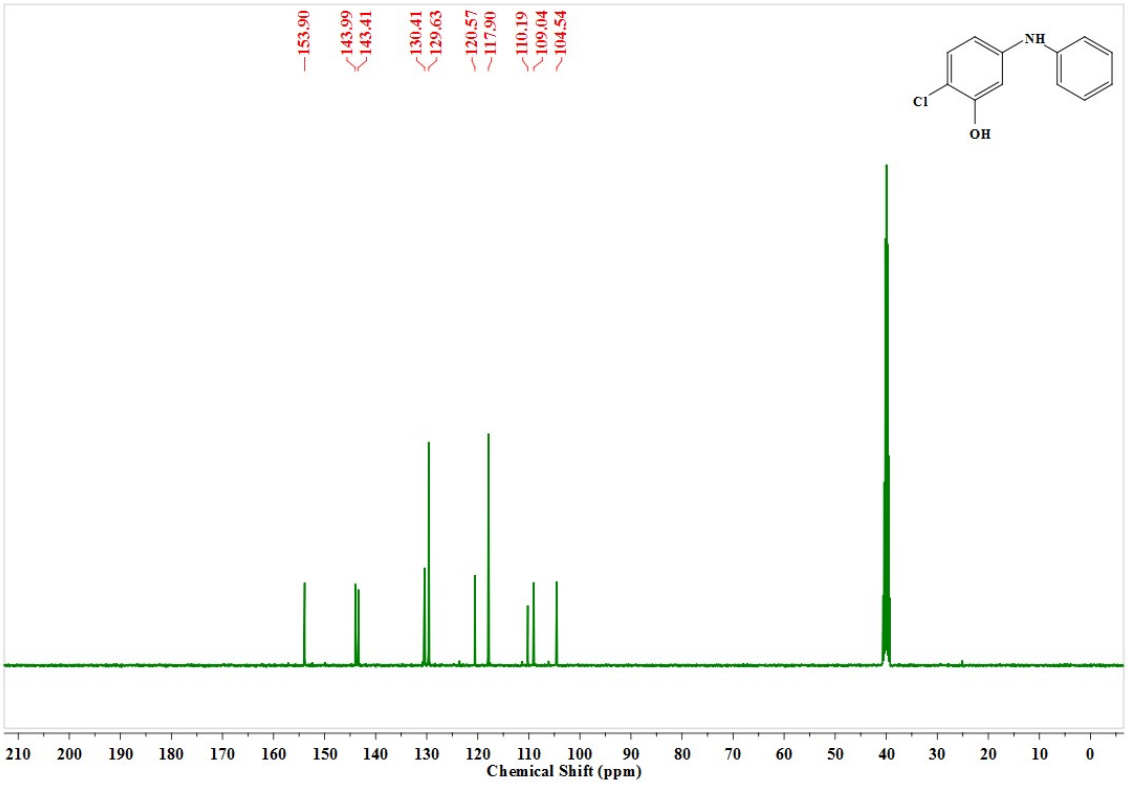

9.23
8.15
7.20
7.18
7.01
6.98
6.97
6.95
6.46
6.44
6.24
6.22
NH
OH
Cl
1.03
0.93
2.00
3.12
2.17
1.04
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical Shift (ppm)

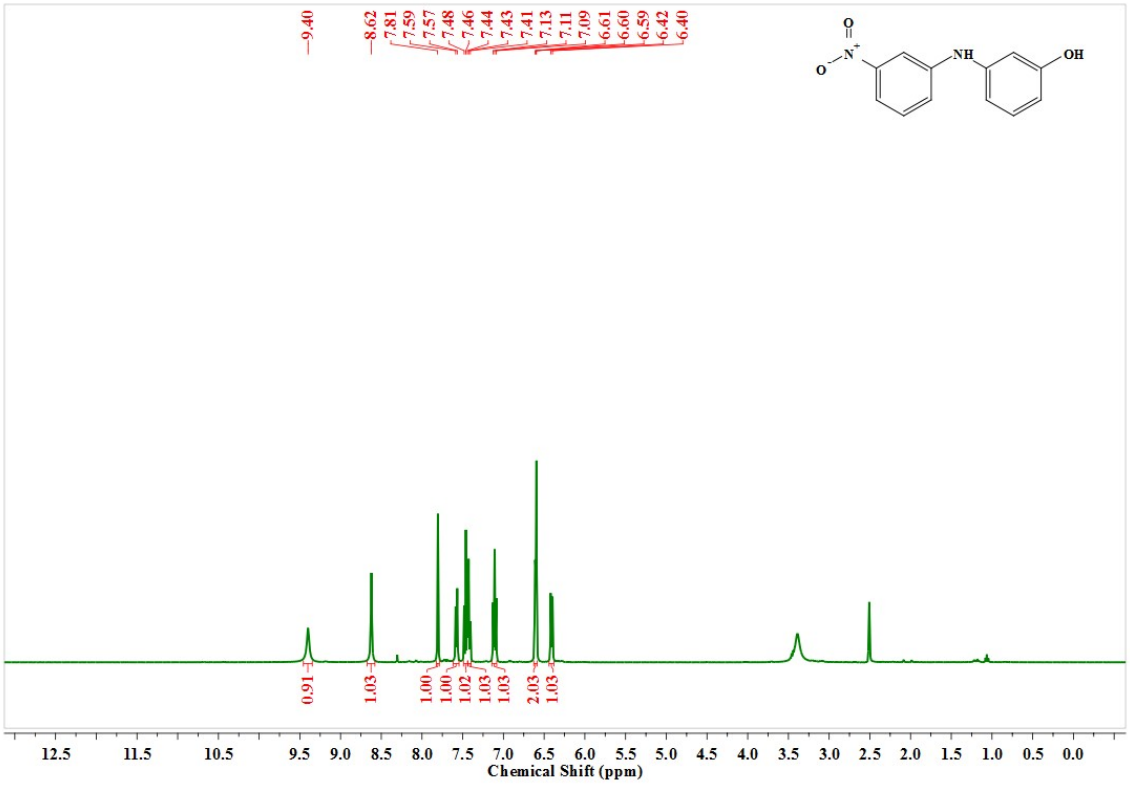

158.73
144.47
143.13
130.50
129.36
123.01
118.51
117.44
108.70
108.18
104.49
NH
OH
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
Chemical Shift (ppm)

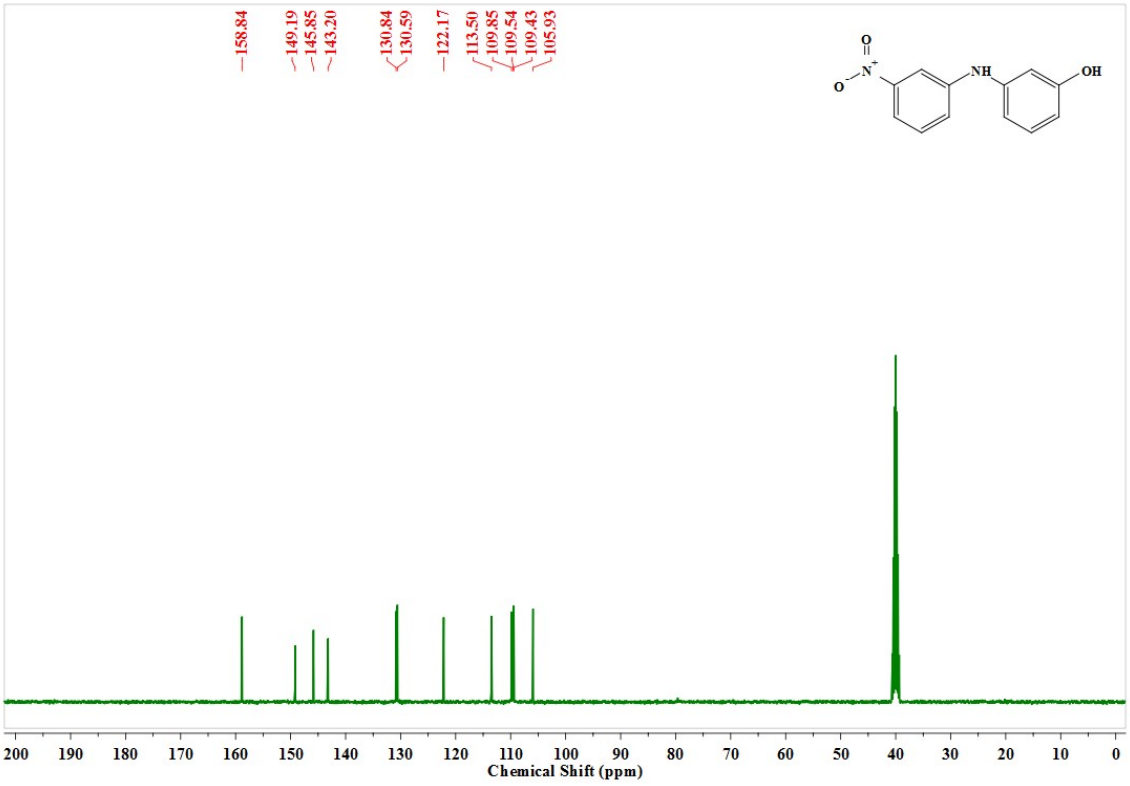

9.05
7.84
7.15
7.13
7.11
6.96
6.94
6.85
6.83
6.72
6.70
6.68
6.55
6.39
6.37
1.98
NH
OH
CH3
1.00
0.93
2.08
2.02
1.03
1.02
1.00
1.00
3.00
Chemical Shift (ppm)


NH
OH
CH3
156.30
144.62
142.45
131.33
129.59
119.36
116.60
115.96
108.84
104.62
15.90
Chemical Shift (ppm)

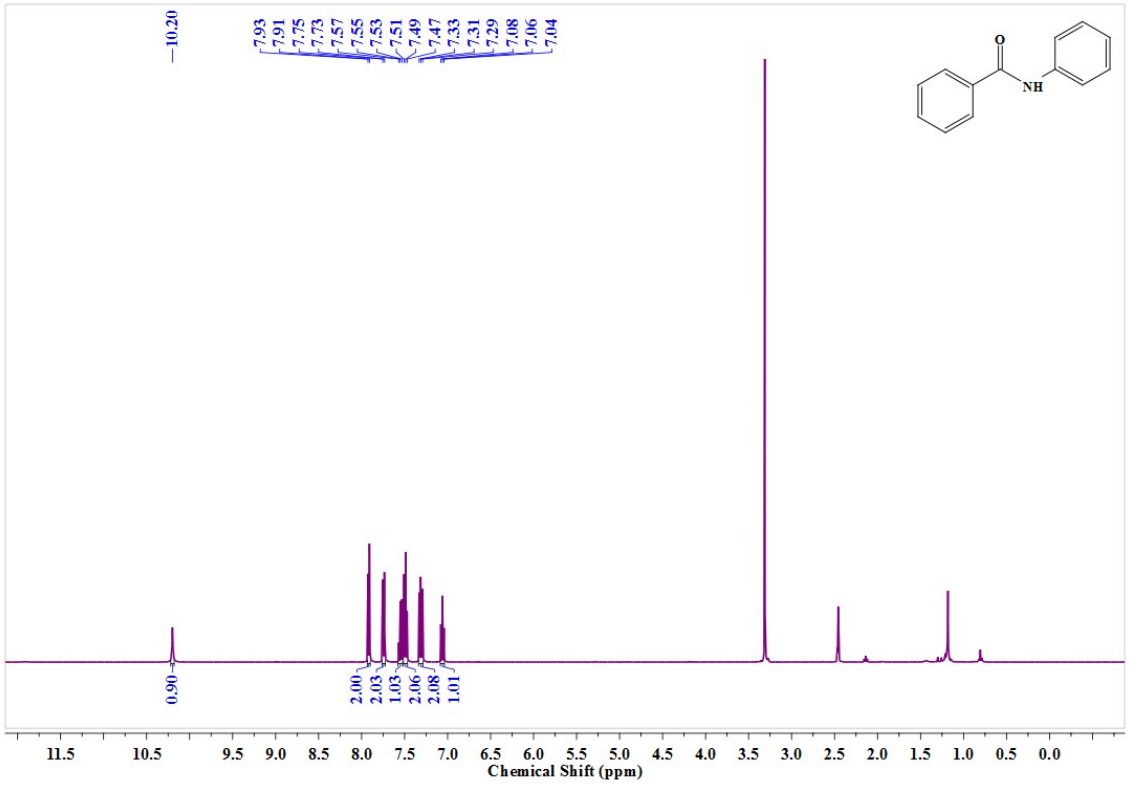

9.92
8.17
7.26
7.25
7.23
7.13
7.11
7.07
7.05
6.87
6.85
6.83
6.75
6.51
6.49
NH
Cl
OH
0.98
0.98
2.11
1.03
2.06
1.04
1.00
1.00
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical Shift (ppm)

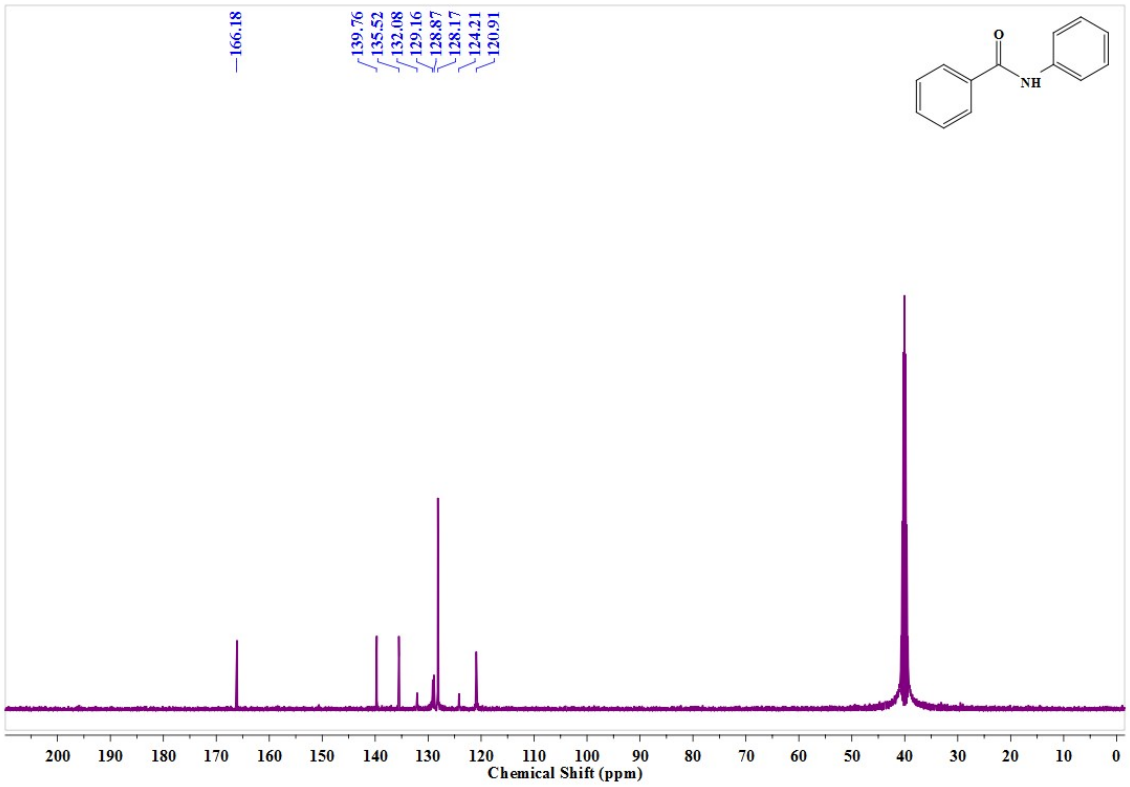

153.90
143.99
143.41
130.41
129.63
120.57
117.90
110.19
109.04
104.54
NH
Cl
OH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)

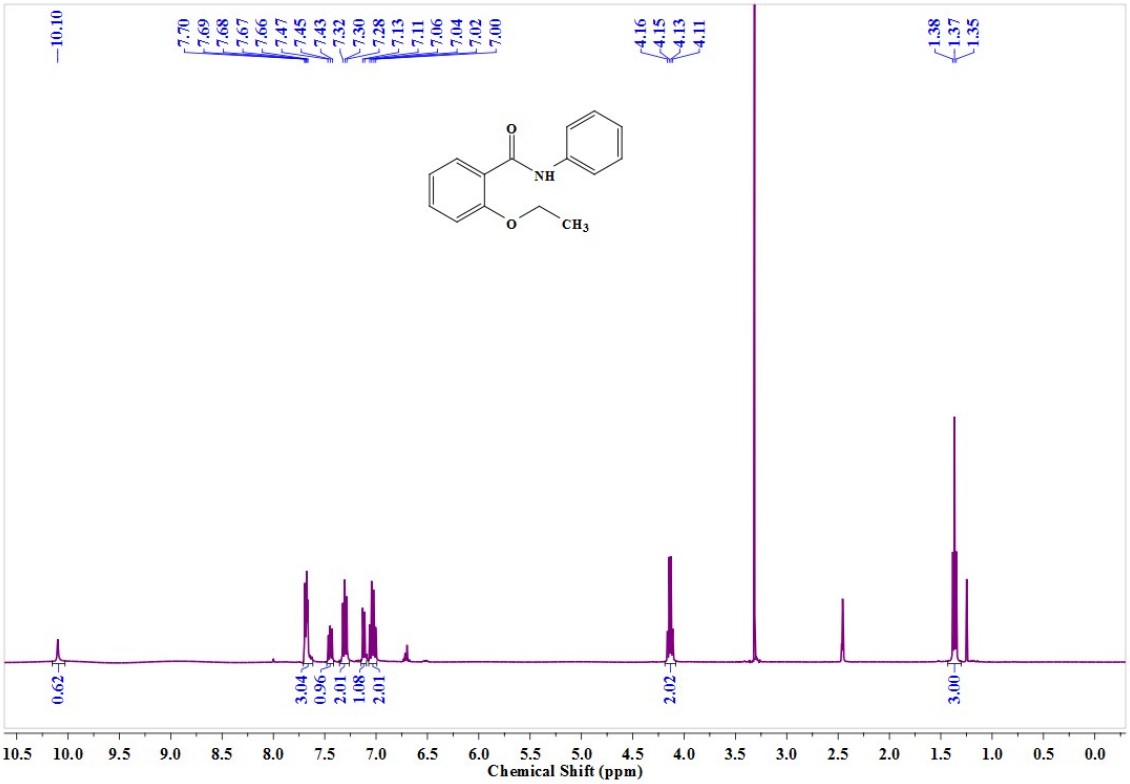

9.40
8.62
7.81
7.59
7.57
7.48
7.46
7.44
7.43
7.41
7.13
7.11
7.09
6.61
6.60
6.59
6.42
6.40
NH
OH
0.91
1.03
1.00
1.00
1.02
1.03
1.03
2.03
1.03
Chemical Shift (ppm)

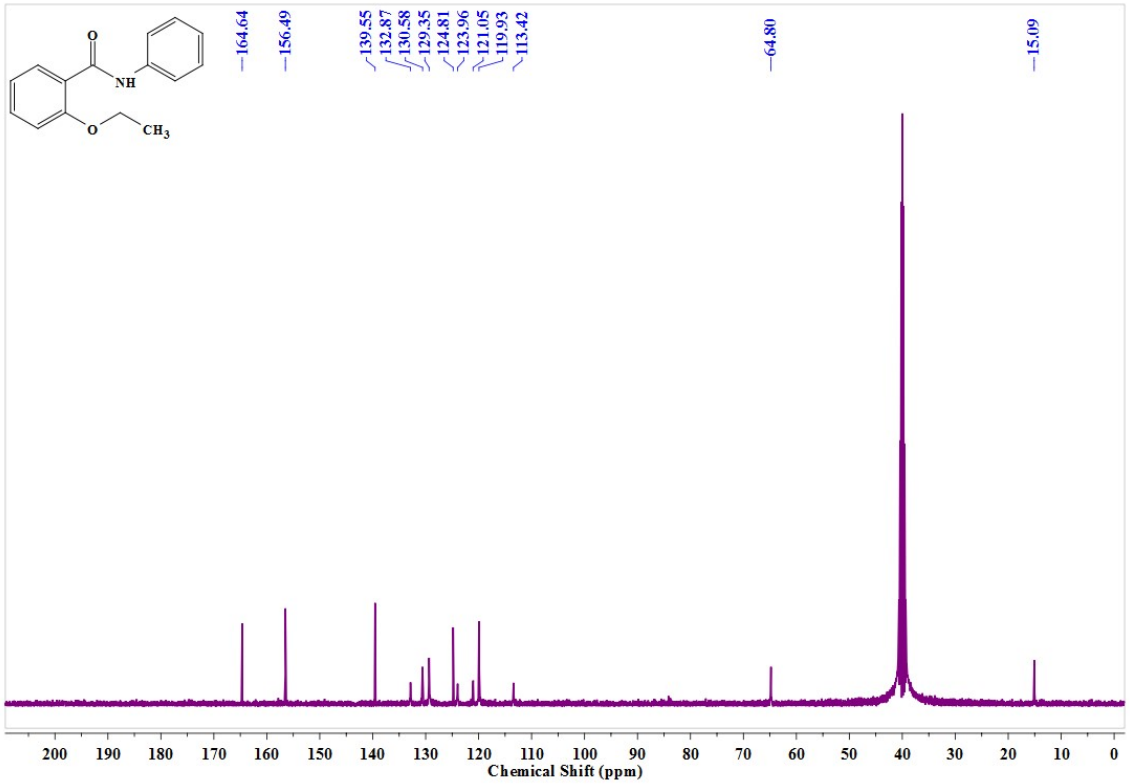

158.84
149.19
145.85
143.20
130.84
130.59
122.17
113.50
109.85
109.54
109.43
105.93
NH
OH
Chemical Shift (ppm)

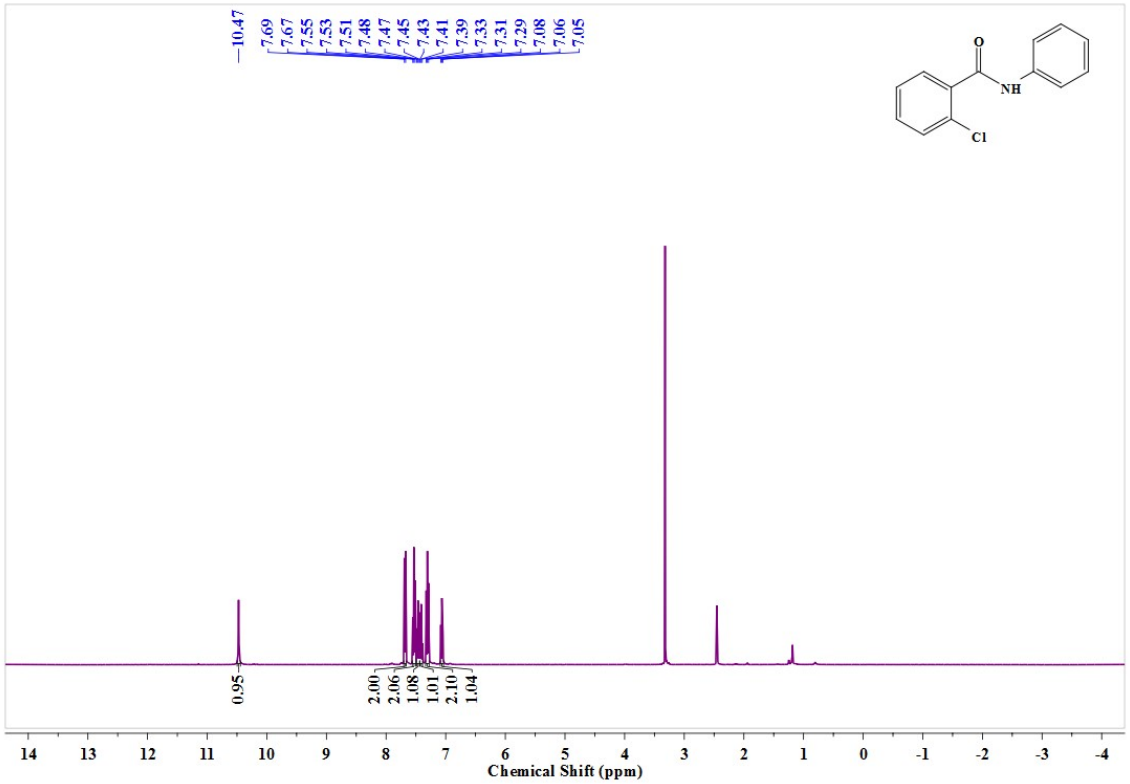
4.3 *^{1}H and ^{13}C NMR spectra of 3-arylamides (**7**)*

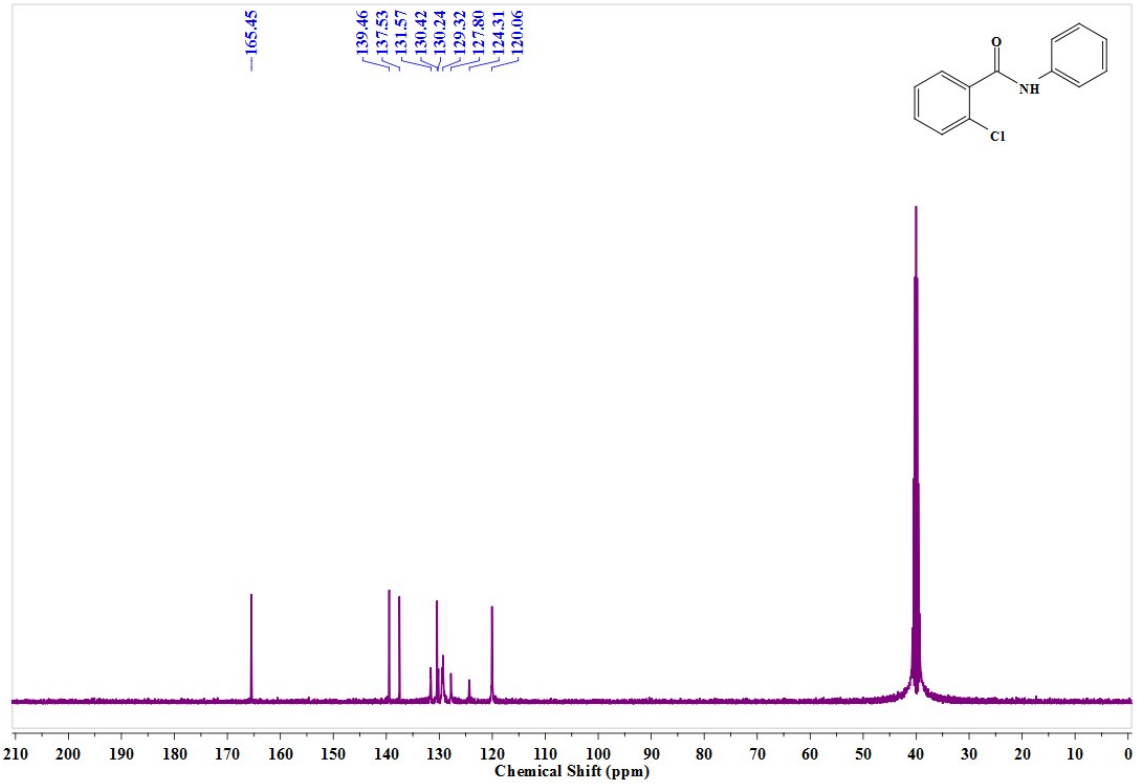


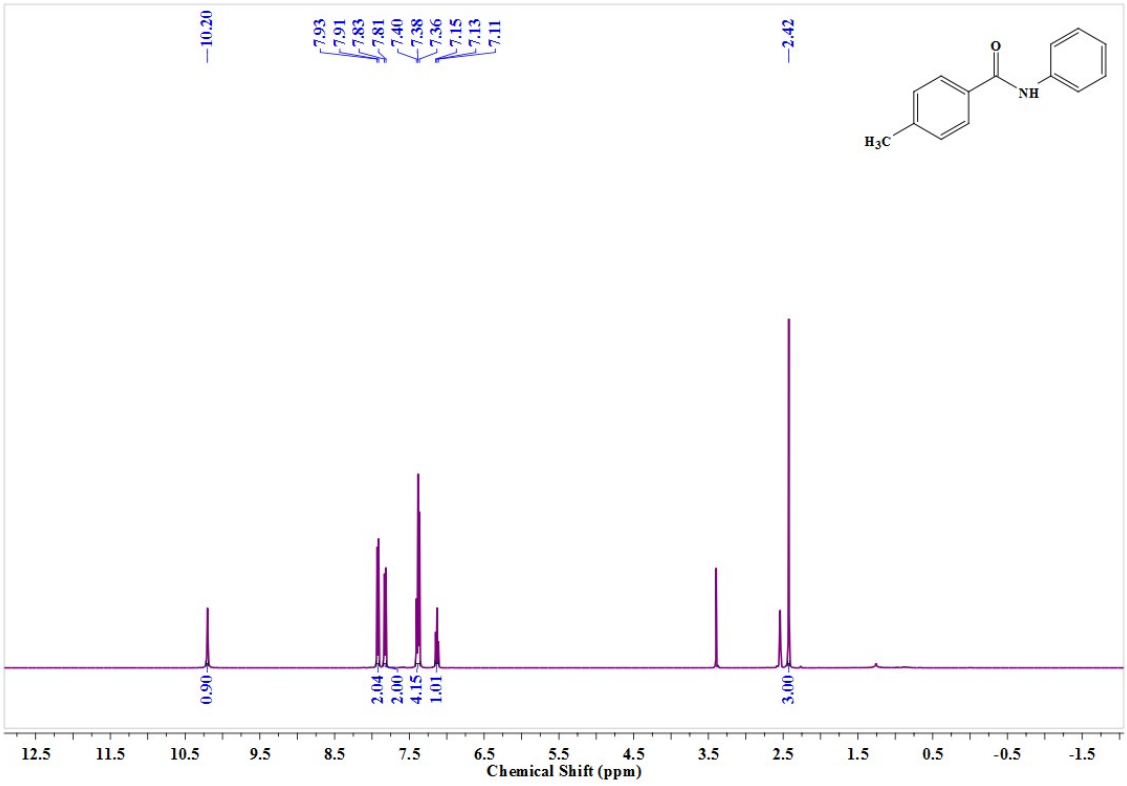


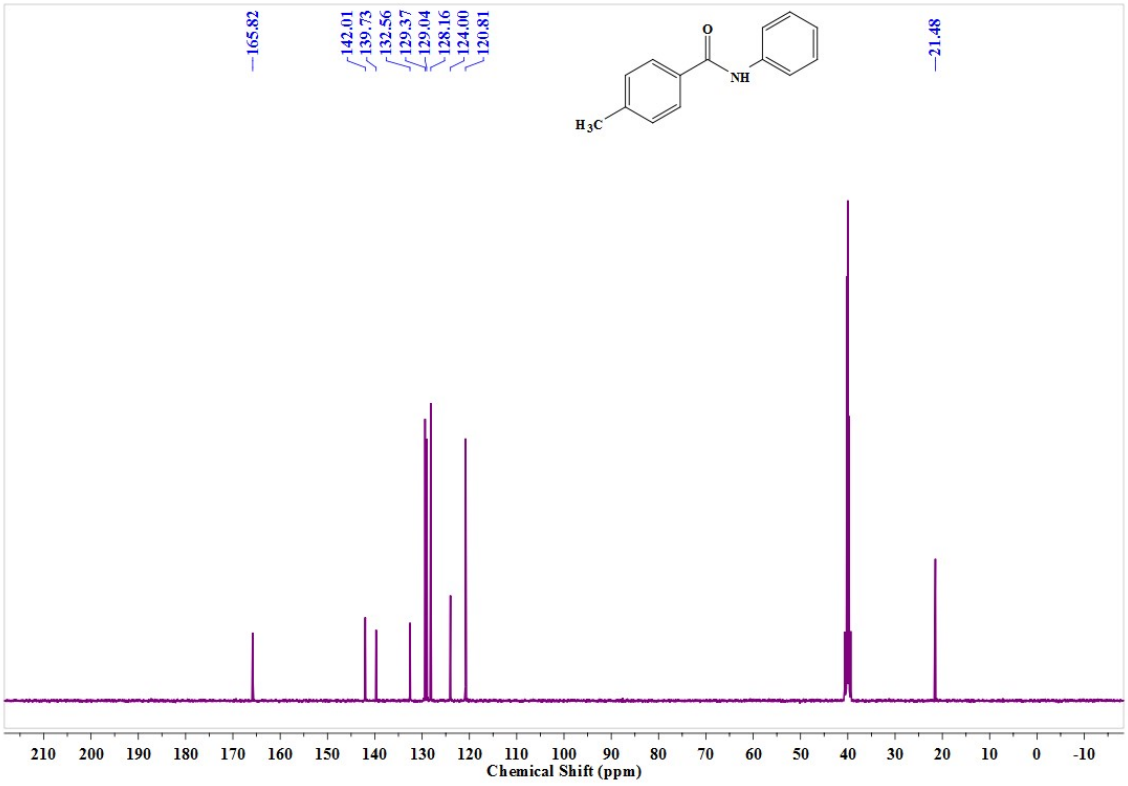

10.10
7.70
7.69
7.68
7.67
7.66
7.47
7.45
7.43
7.32
7.30
7.28
7.13
7.11
7.06
7.04
7.02
7.00
4.16
4.15
4.13
4.11
1.38
1.37
1.35
O
NH
O
CH3
0.62
3.04
0.96
2.01
1.08
2.01
2.02
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical Shift (ppm)

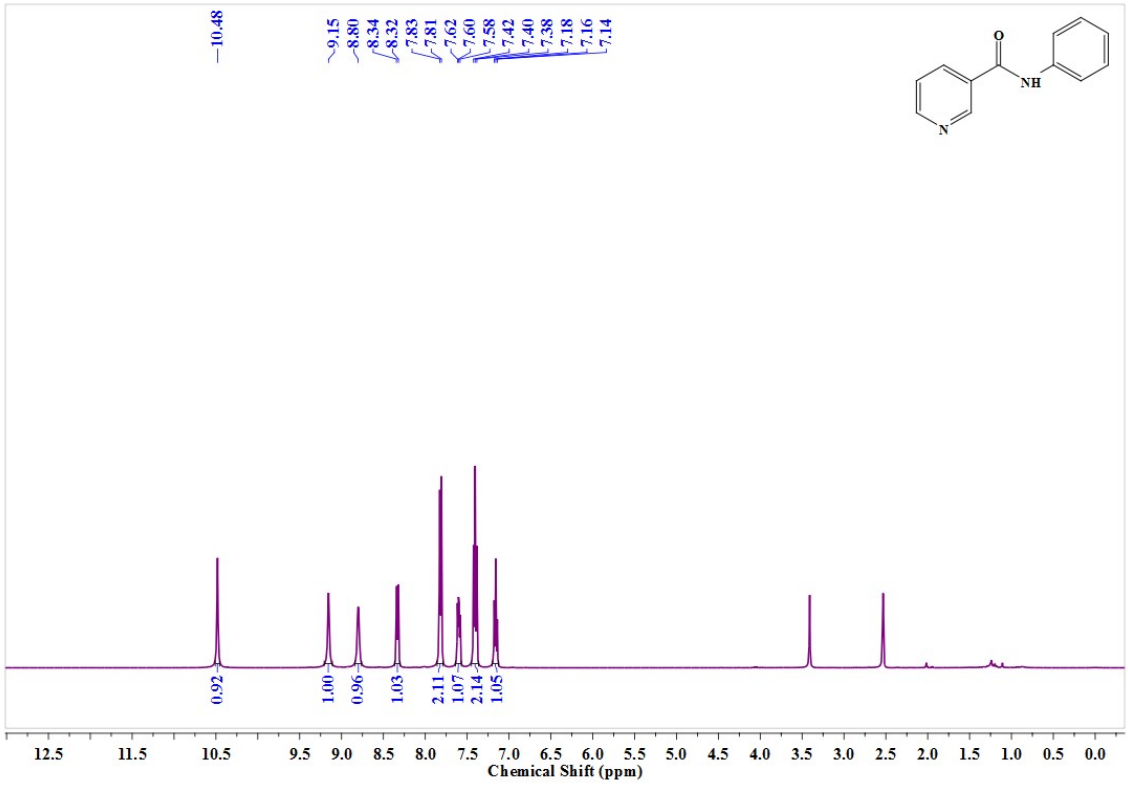

O
NH
O
CH3
164.64
156.49
139.55
132.87
130.58
129.35
124.81
123.96
121.05
119.93
113.42
64.80
15.09
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)

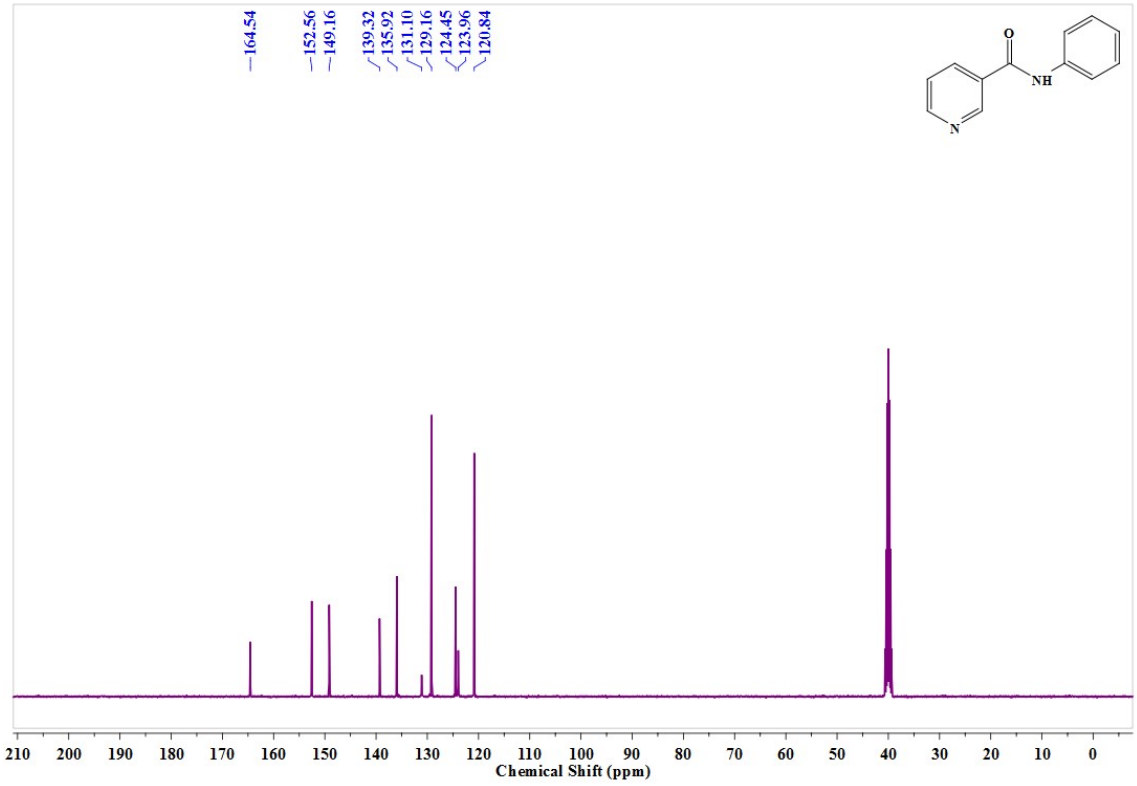

10.47
7.69
7.67
7.55
7.53
7.51
7.48
7.47
7.45
7.43
7.41
7.39
7.33
7.31
7.29
7.08
7.06
7.05
O
NH
Cl
0.95
2.00
2.06
1.08
1.01
2.10
1.04
Chemical Shift (ppm)

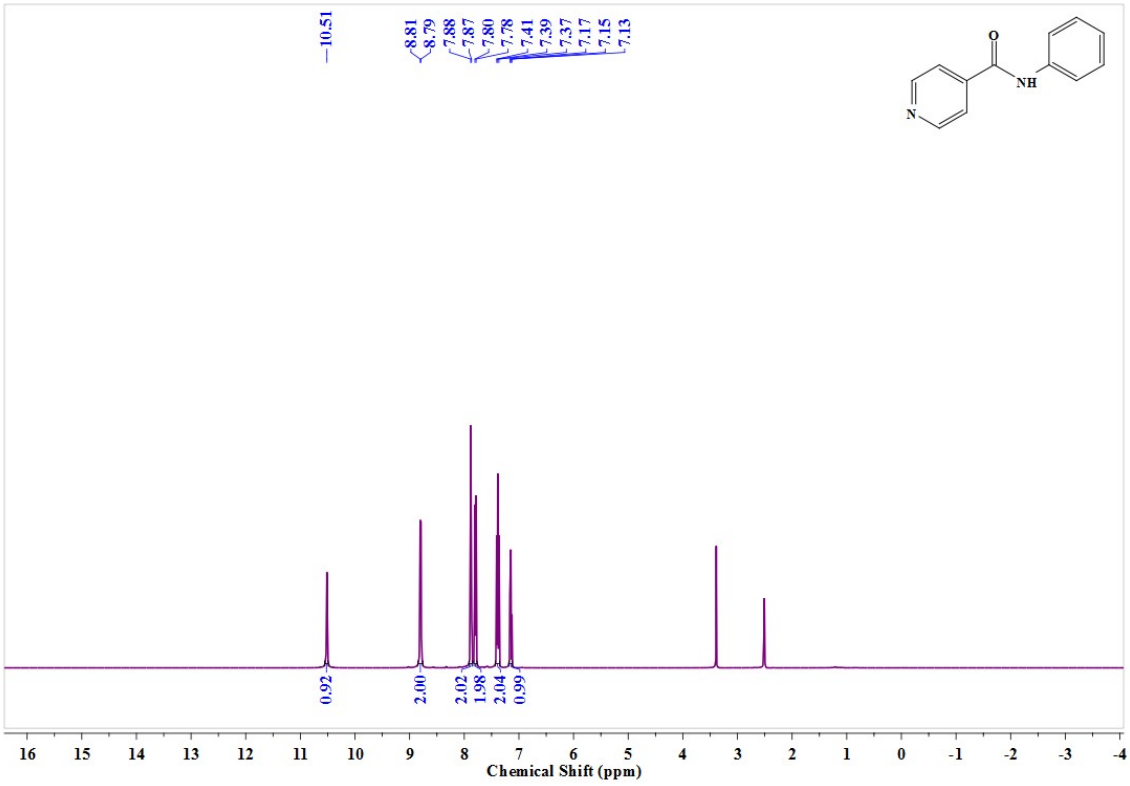

165.45
139.46
137.53
131.57
130.42
130.24
129.32
127.80
124.31
120.06
O
NH
Cl
Chemical Shift (ppm)

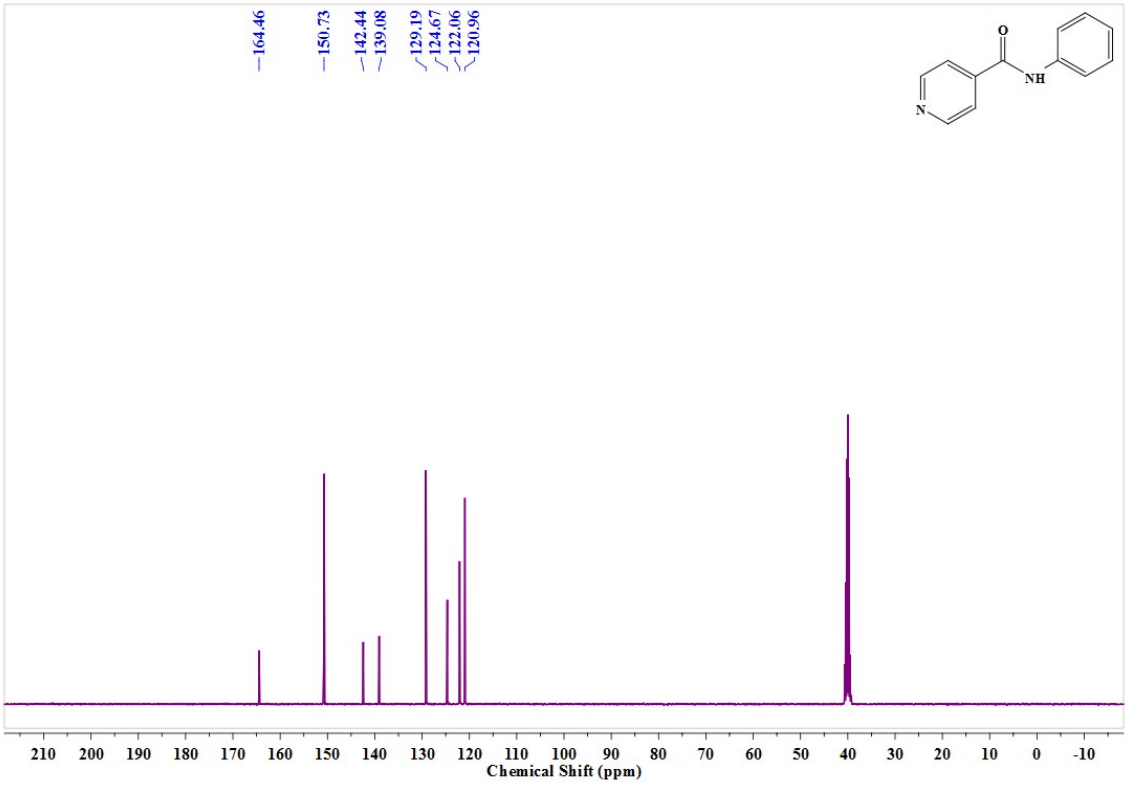

10.20
7.93
7.91
7.83
7.81
7.40
7.38
7.36
7.15
7.13
7.11
2.42
O
NH
H3C
0.90
2.04
2.00
4.15
1.01
3.00
12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5 -1.5
Chemical Shift (ppm)

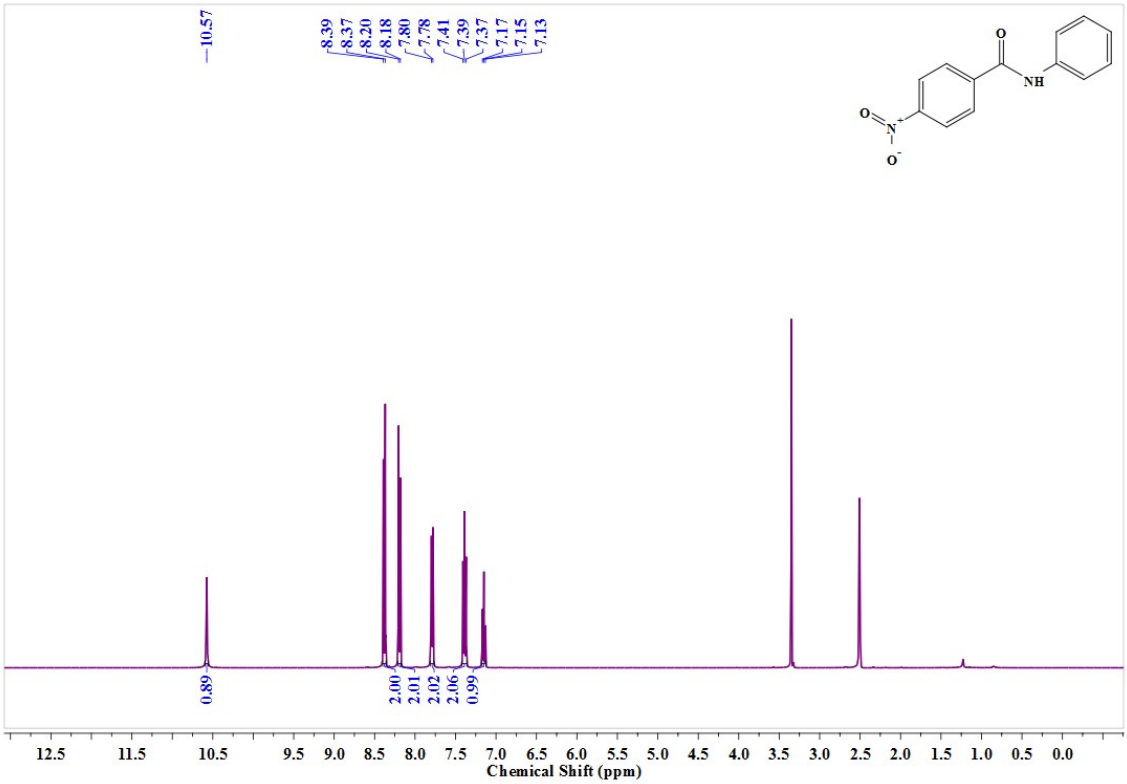

165.82
142.01
139.73
132.56
129.37
129.04
128.16
124.00
120.81
21.48
O
NH
H3C
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
Chemical Shift (ppm)

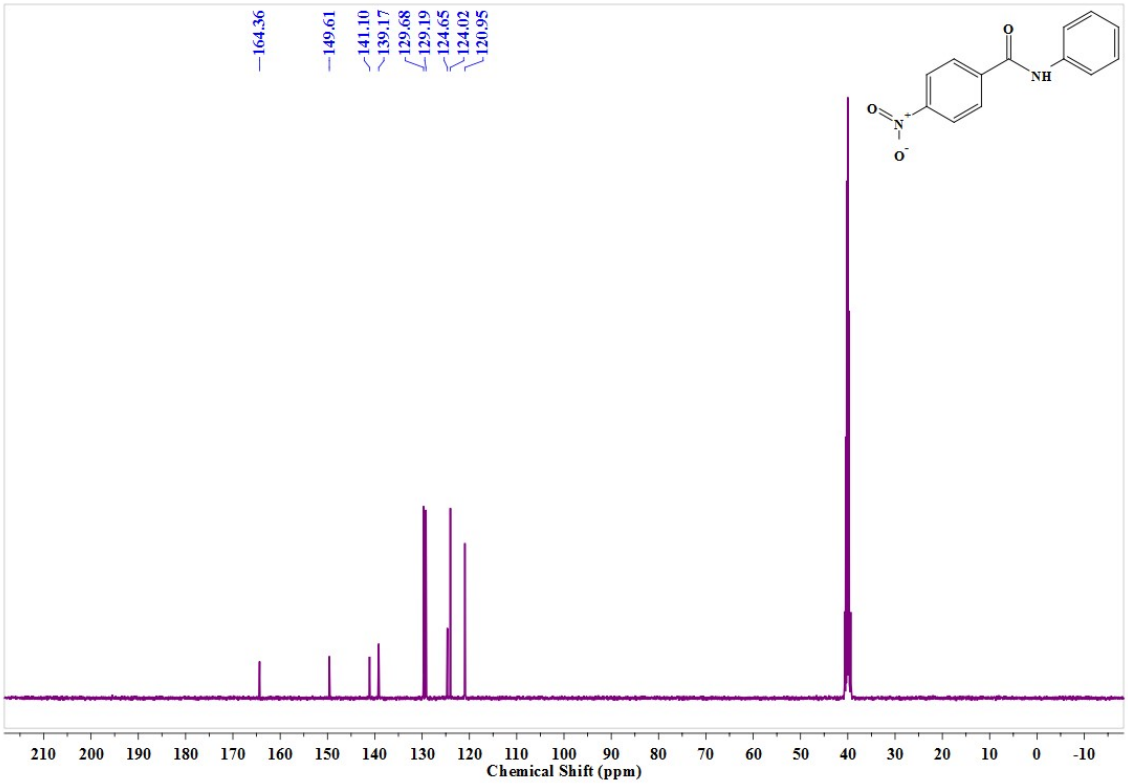

10.48
9.15
8.80
8.34
8.32
7.83
7.81
7.62
7.60
7.58
7.42
7.40
7.38
7.18
7.16
7.14
O
NH
N
0.92
1.00
0.96
1.03
2.11
1.07
2.14
1.05
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical Shift (ppm)

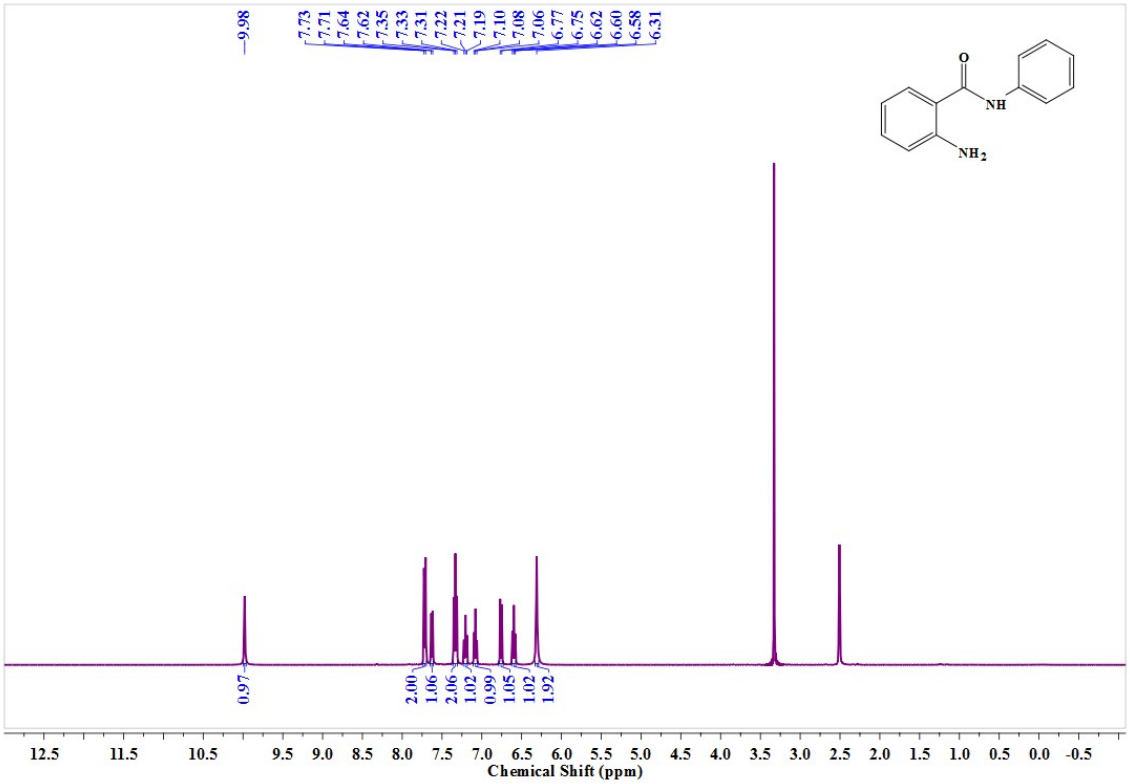

164.54
152.56
149.16
139.32
135.92
131.10
129.16
124.45
123.96
120.84
O
NH
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)

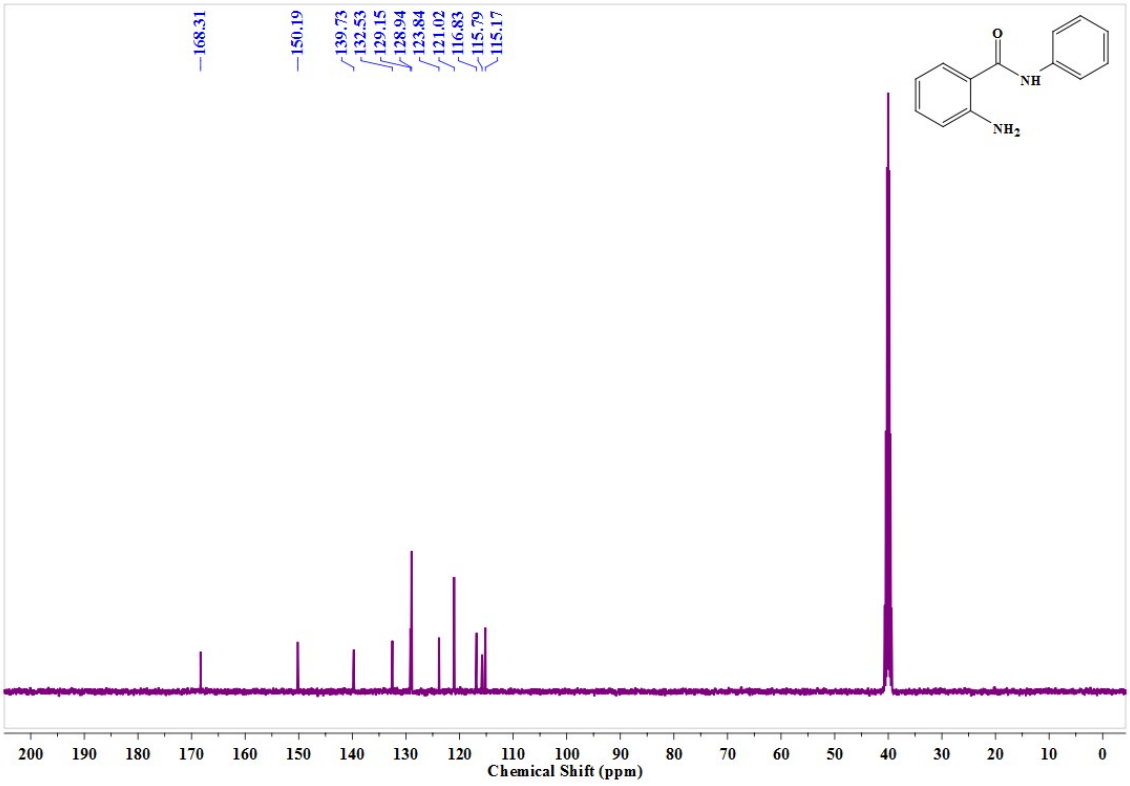

10.51
8.81
8.79
7.88
7.87
7.80
7.78
7.41
7.39
7.37
7.17
7.15
7.13
O
NH
N
0.92
2.00
2.02
1.98
2.04
0.99
Chemical Shift (ppm)

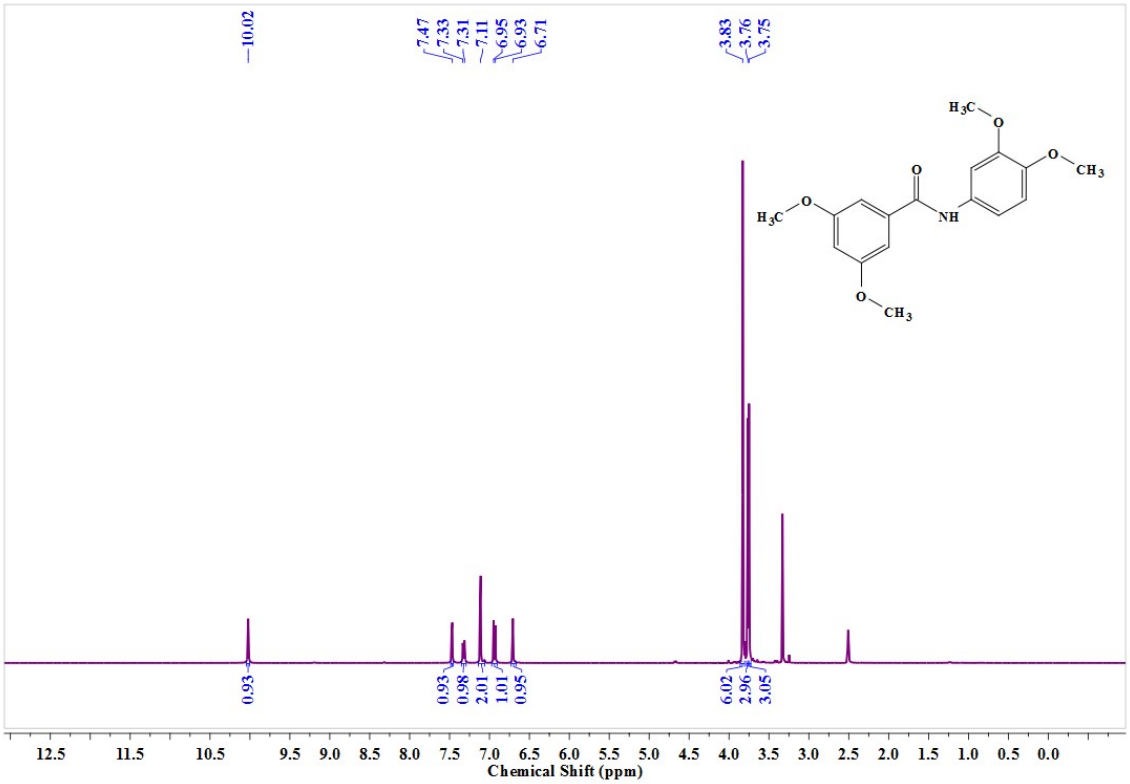

164.46
150.73
142.44
139.08
129.19
124.67
122.06
120.96
O
NH
N
Chemical Shift (ppm)

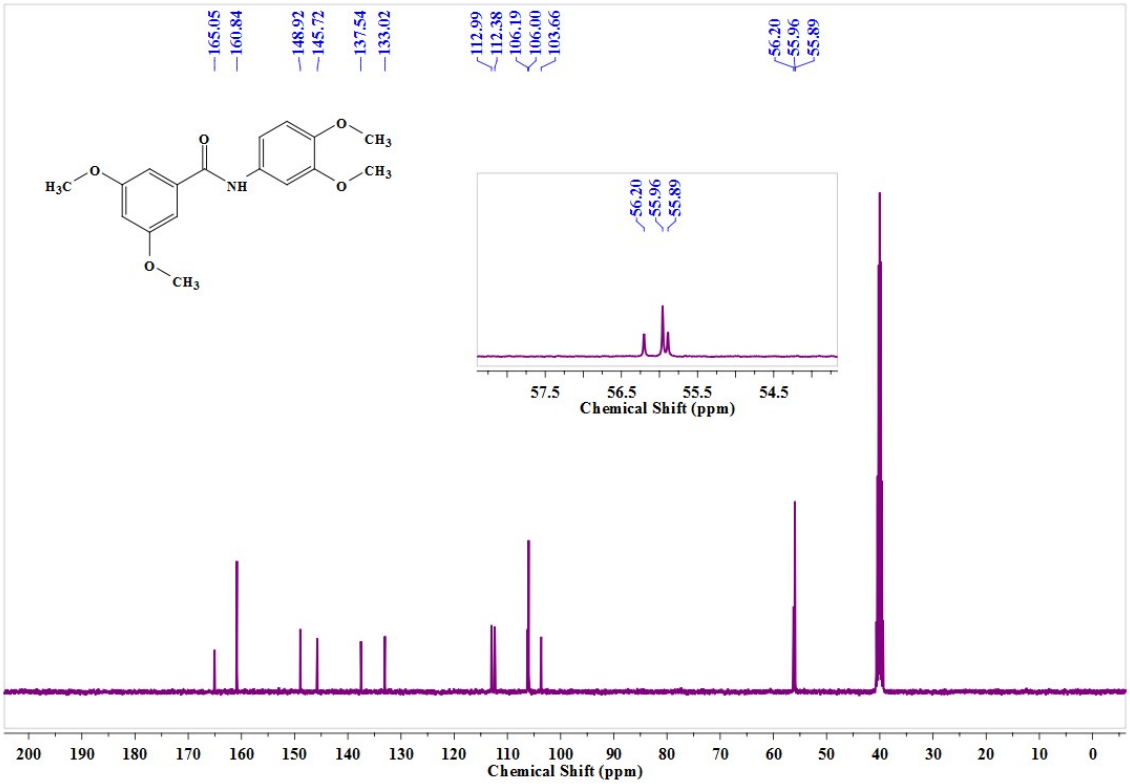

10.57
8.39
8.37
8.20
8.18
7.80
7.78
7.41
7.39
7.37
7.17
7.15
7.13
O
NH
O
N+
O-
0.89
2.00
2.01
2.02
2.06
0.99
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical Shift (ppm)

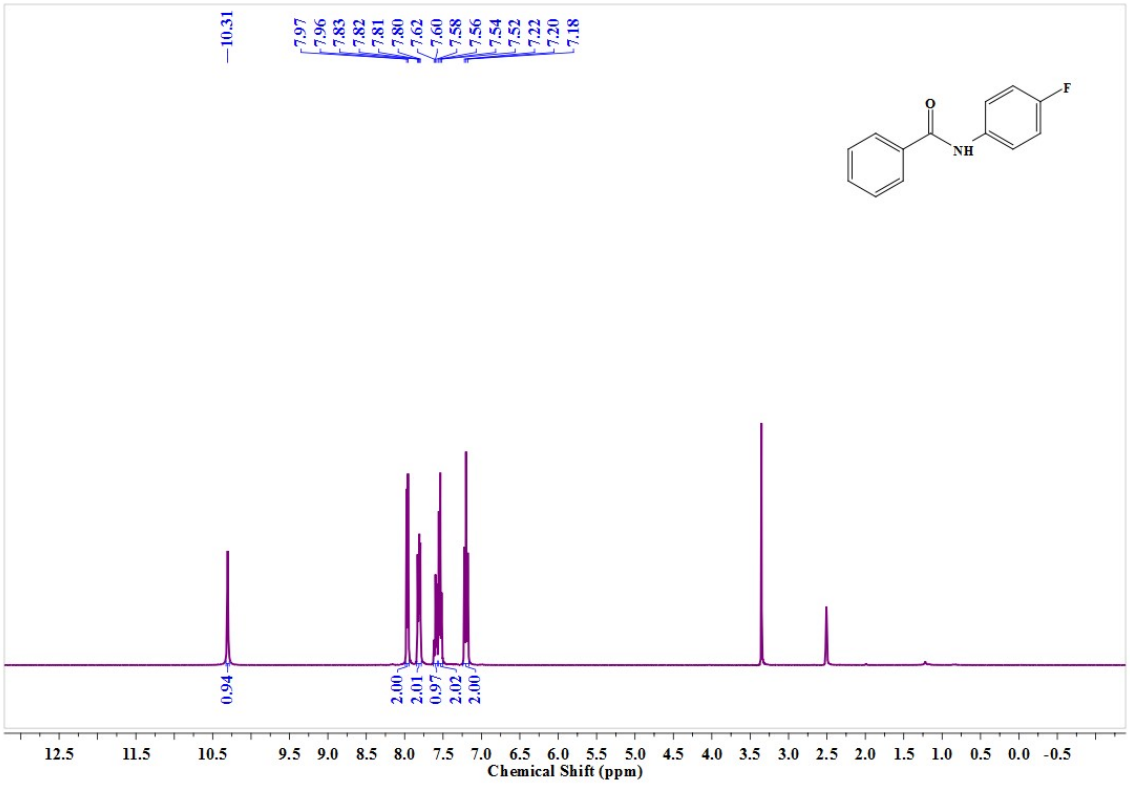

164.36
149.61
141.10
139.17
129.68
129.19
124.65
124.02
120.95
O
NH
O
N+
O-
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
Chemical Shift (ppm)

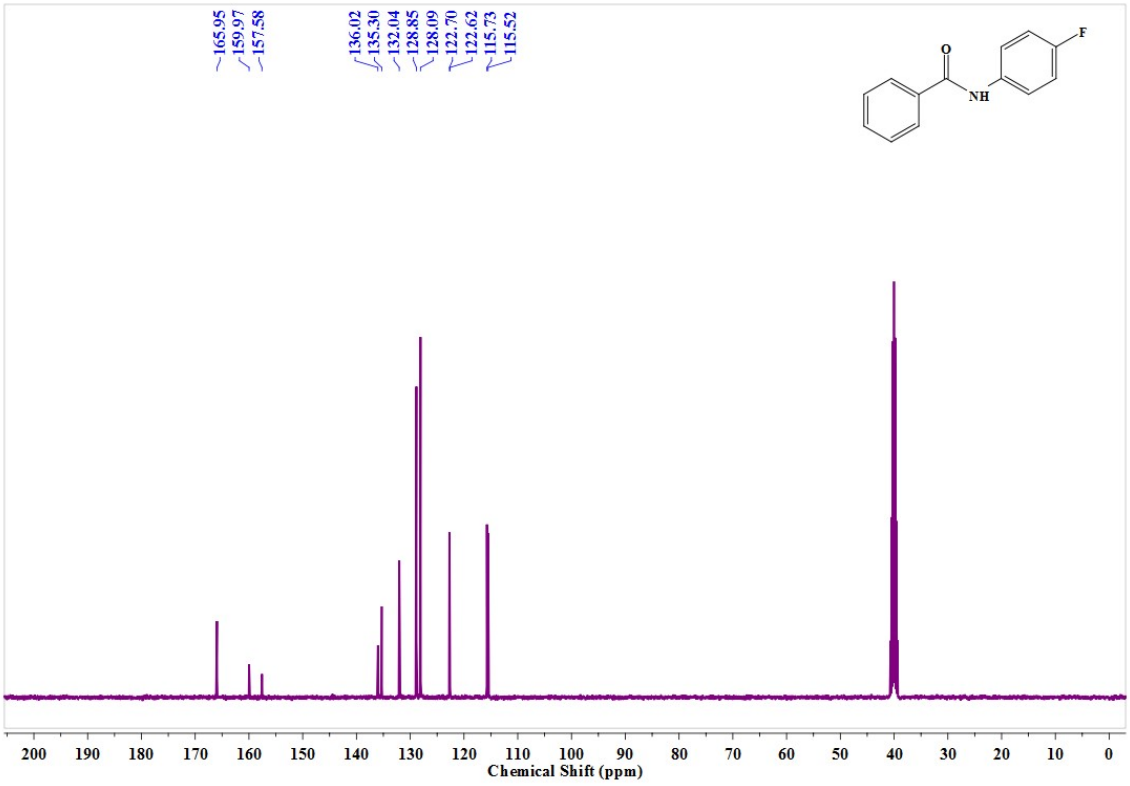

9.98
7.73
7.71
7.64
7.62
7.35
7.33
7.31
7.22
7.21
7.19
7.10
7.08
7.06
6.77
6.75
6.62
6.60
6.58
6.31
O
NH
NH2
0.97
2.00
1.06
2.06
1.02
0.99
1.05
1.02
1.92
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
Chemical Shift (ppm)

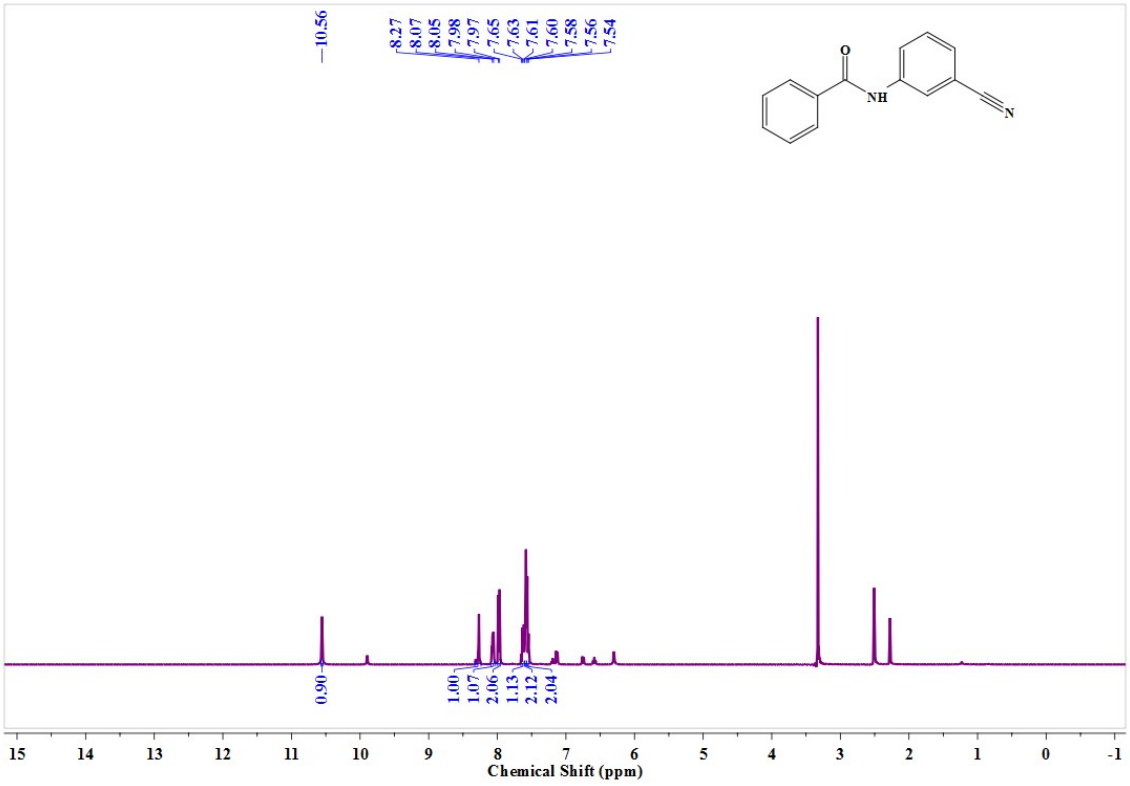

168.31
150.19
139.73
132.53
129.15
128.94
123.84
121.02
116.83
115.79
115.17
O
NH
NH2
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)

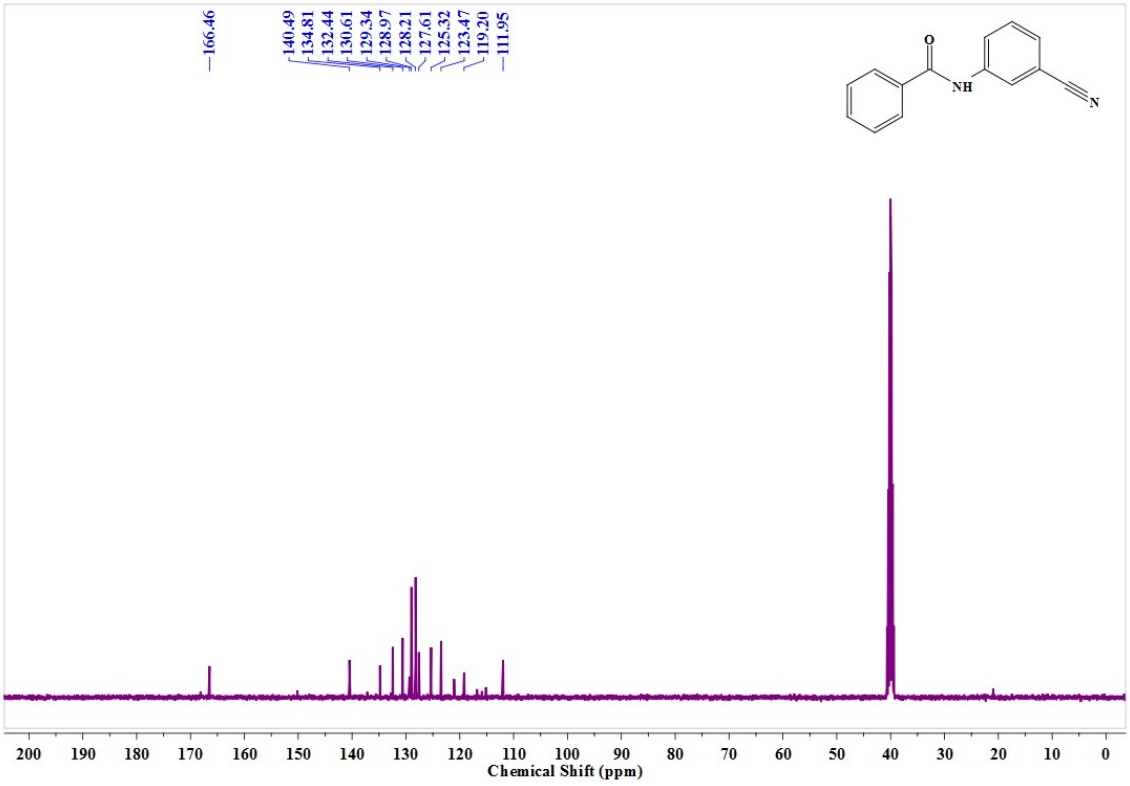

10.02
7.47
7.33
7.31
7.11
6.95
6.93
6.71
3.83
3.76
3.75
0.93
0.93
0.98
2.01
1.01
0.95
6.02
2.96
3.05
Chemical Shift (ppm)

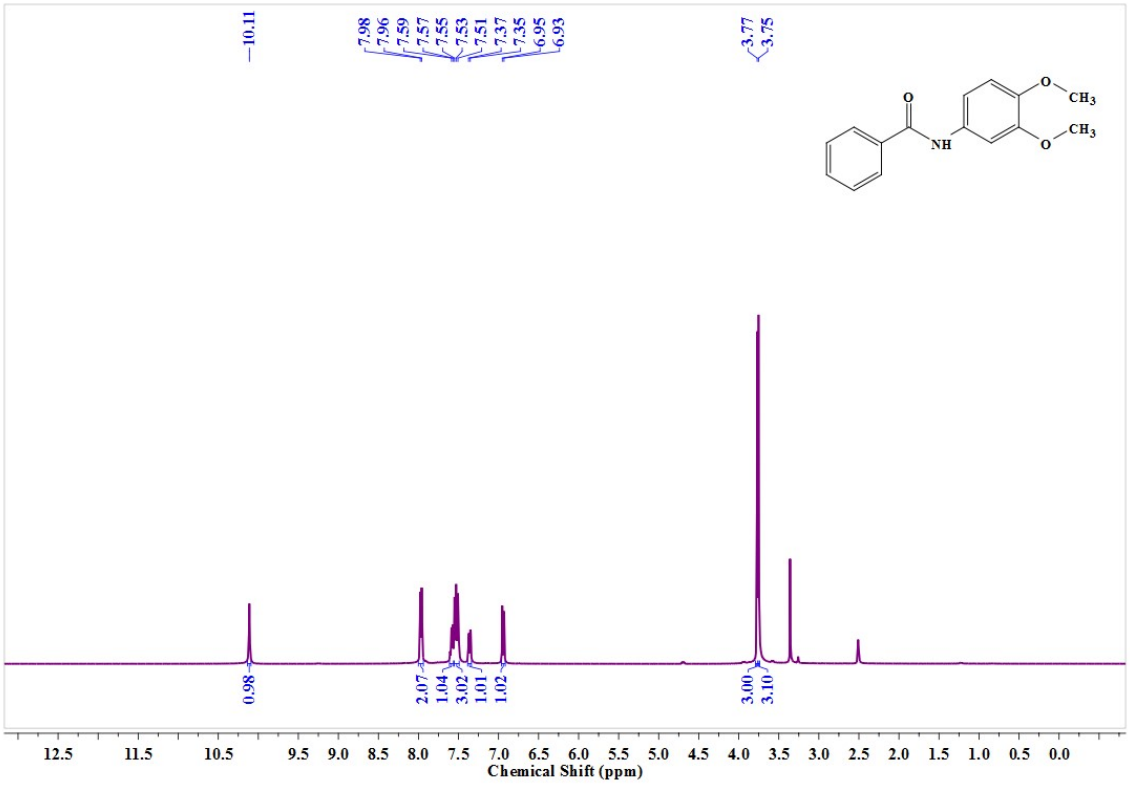

165.05
160.84
148.92
145.72
137.54
133.02
112.99
112.38
106.19
106.00
103.66
56.20
55.96
55.89
Chemical Shift (ppm)
Chemical Shift (ppm)

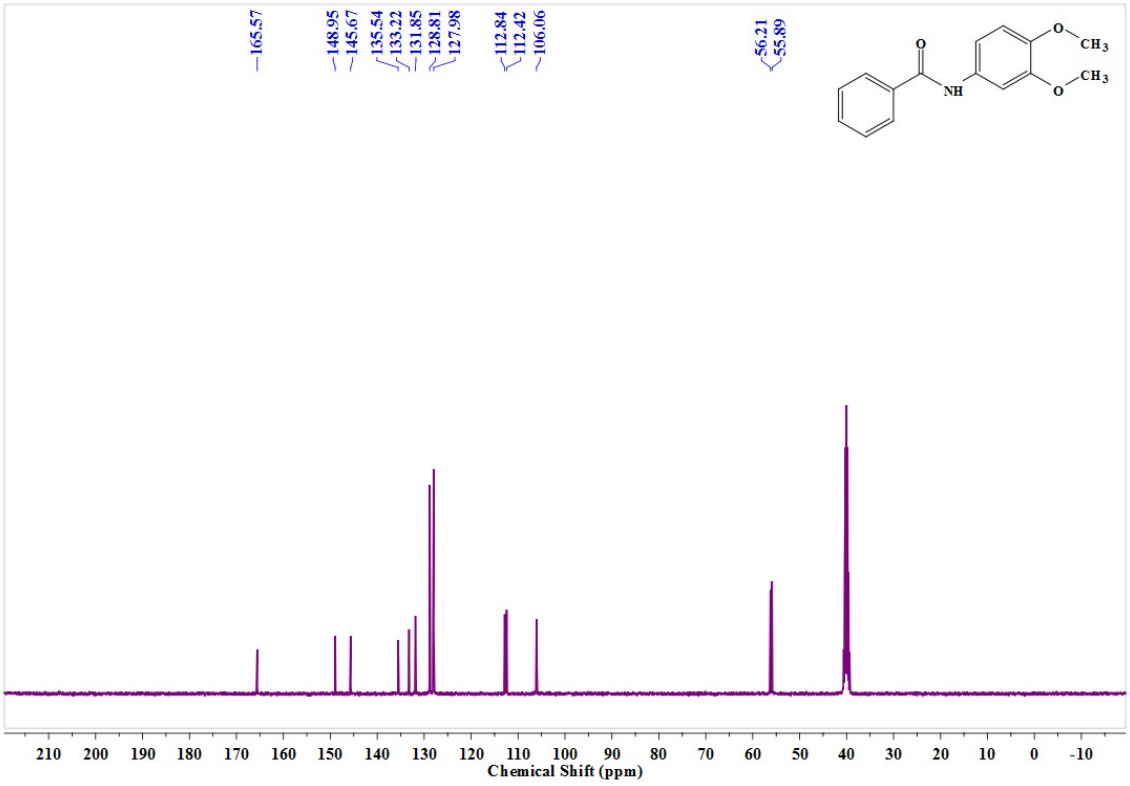

10.31
7.97
7.96
7.83
7.82
7.81
7.80
7.62
7.60
7.58
7.56
7.54
7.52
7.22
7.20
7.18
O
NH
F
0.94
2.00
2.01
0.97
2.02
2.00
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
Chemical Shift (ppm)

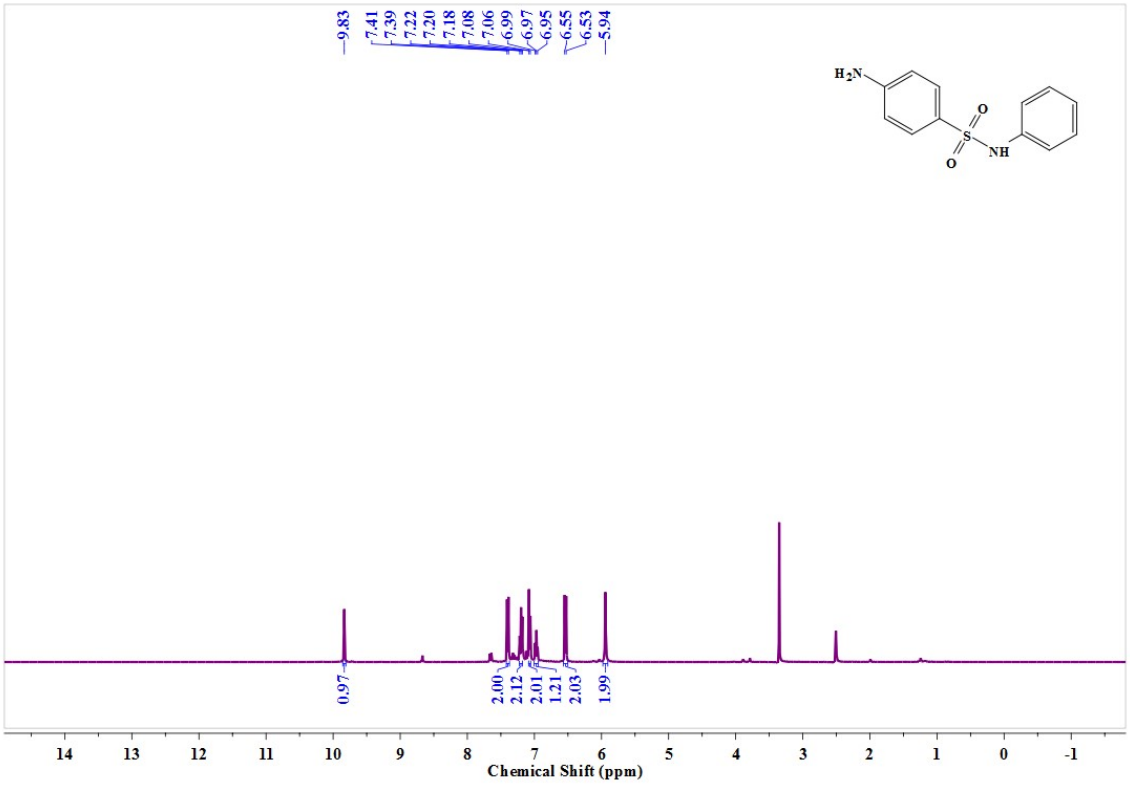

165.95
159.97
157.58
136.02
135.30
132.04
128.85
128.09
122.70
122.62
115.73
115.52
O
NH
F
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)

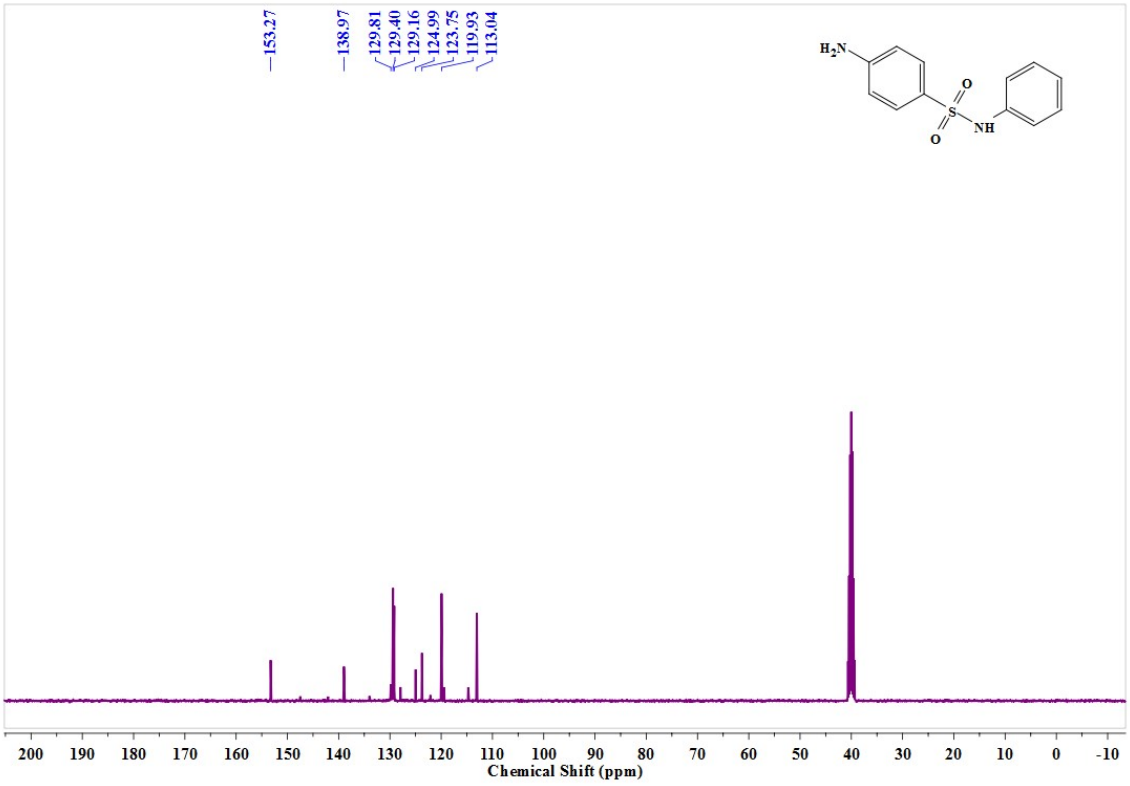

10.56
8.27
8.07
8.05
7.98
7.97
7.65
7.63
7.61
7.60
7.58
7.56
7.54
O
NH
N
0.90
1.00
1.07
2.06
1.13
2.12
2.04
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
Chemical Shift (ppm)


166.46
140.49
134.81
132.44
130.61
129.34
128.97
128.21
127.61
125.32
123.47
119.20
111.95
O
NH
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
Chemical Shift (ppm)

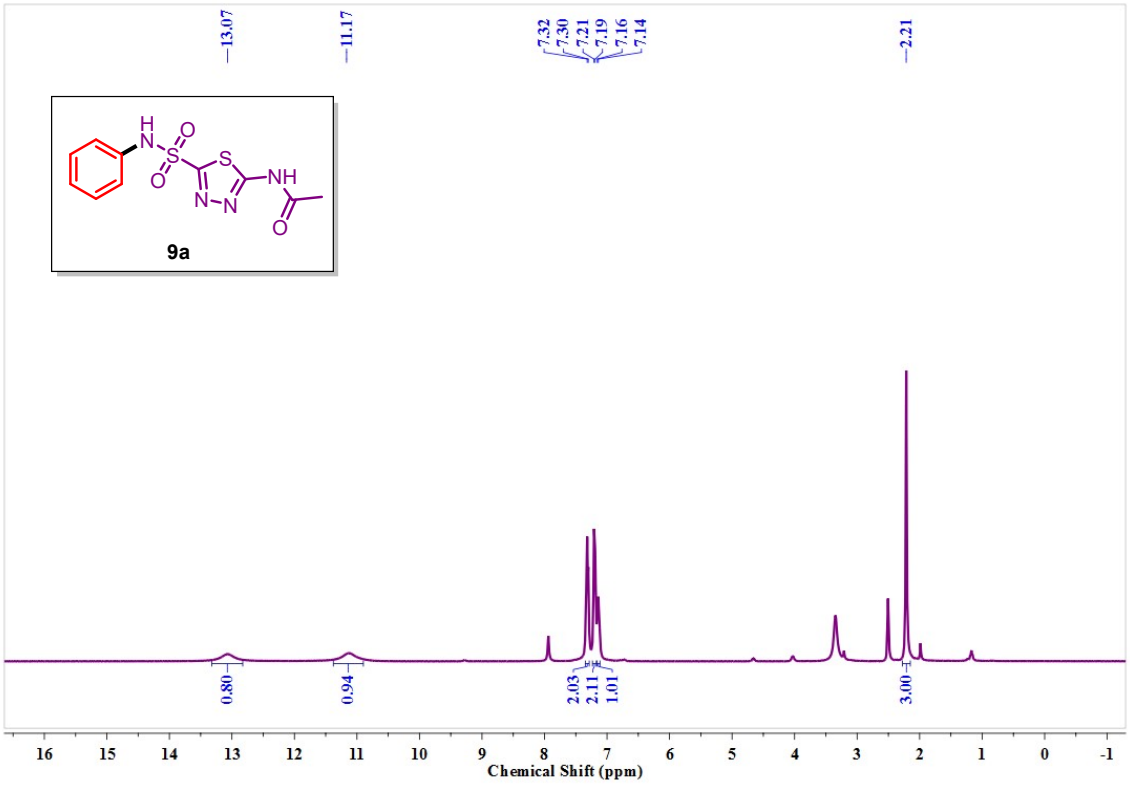

10.11
7.98
7.96
7.59
7.57
7.55
7.53
7.51
7.37
7.35
6.95
6.93
3.77
3.75
O
NH
O
CH3
O
CH3
0.98
2.07
1.04
3.02
1.01
1.02
3.00
3.10
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
Chemical Shift (ppm)

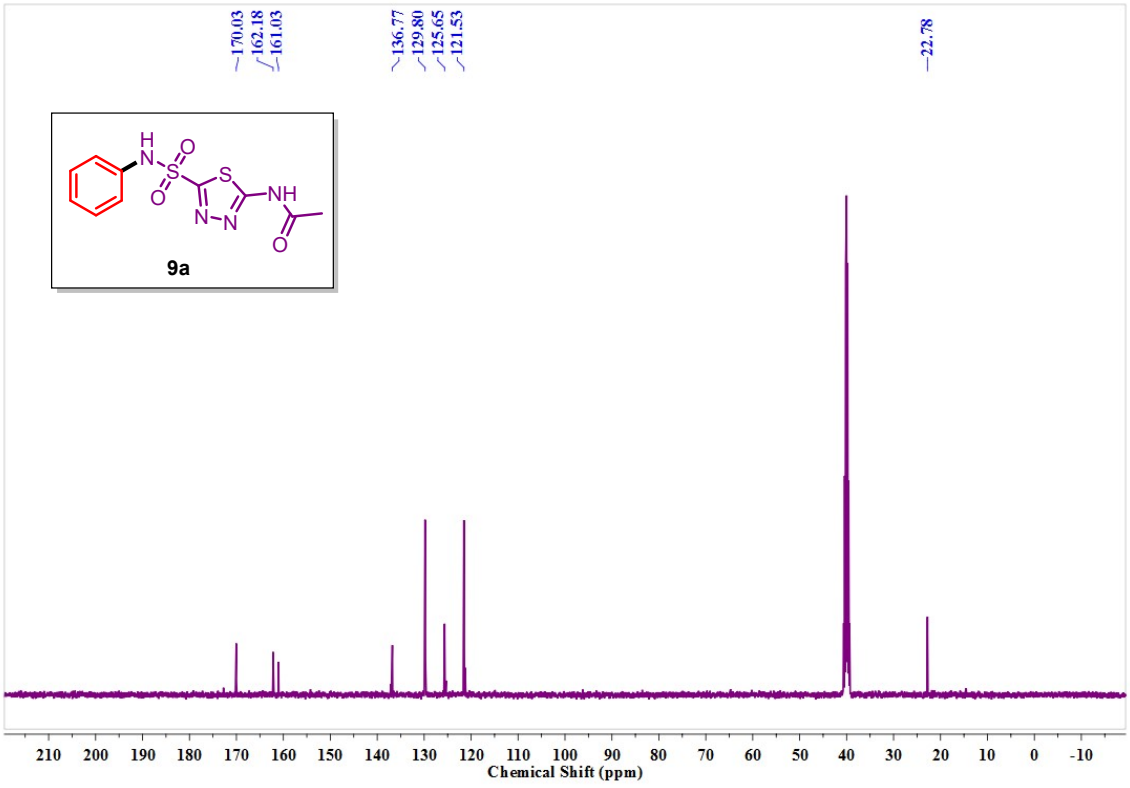

165.57
148.95
145.67
135.54
133.22
131.85
128.81
127.98
112.84
112.42
106.06
56.21
55.89
O
NH
O
CH3
O
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
Chemical Shift (ppm)

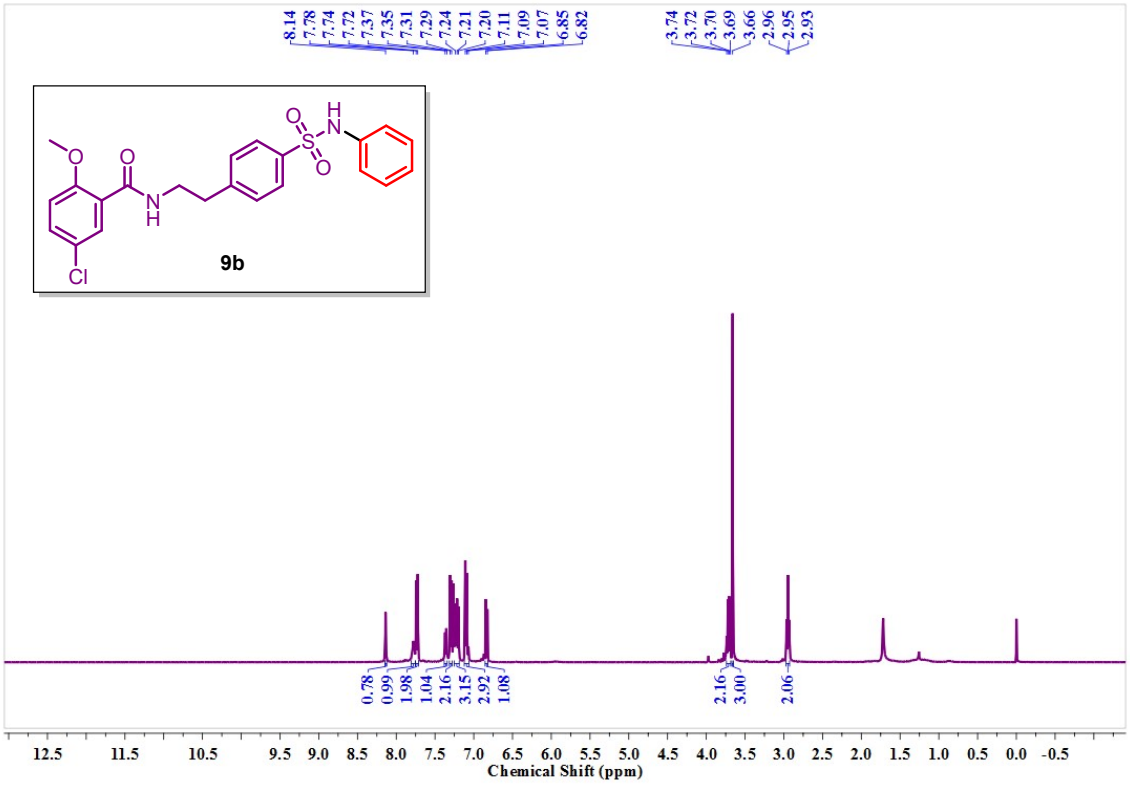

9.83
7.41
7.39
7.22
7.20
7.18
7.08
7.06
6.99
6.97
6.95
6.55
6.53
5.94
H2N
O
S
O
NH
0.97
2.00
2.12
2.01
1.21
2.03
1.99
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
Chemical Shift (ppm)

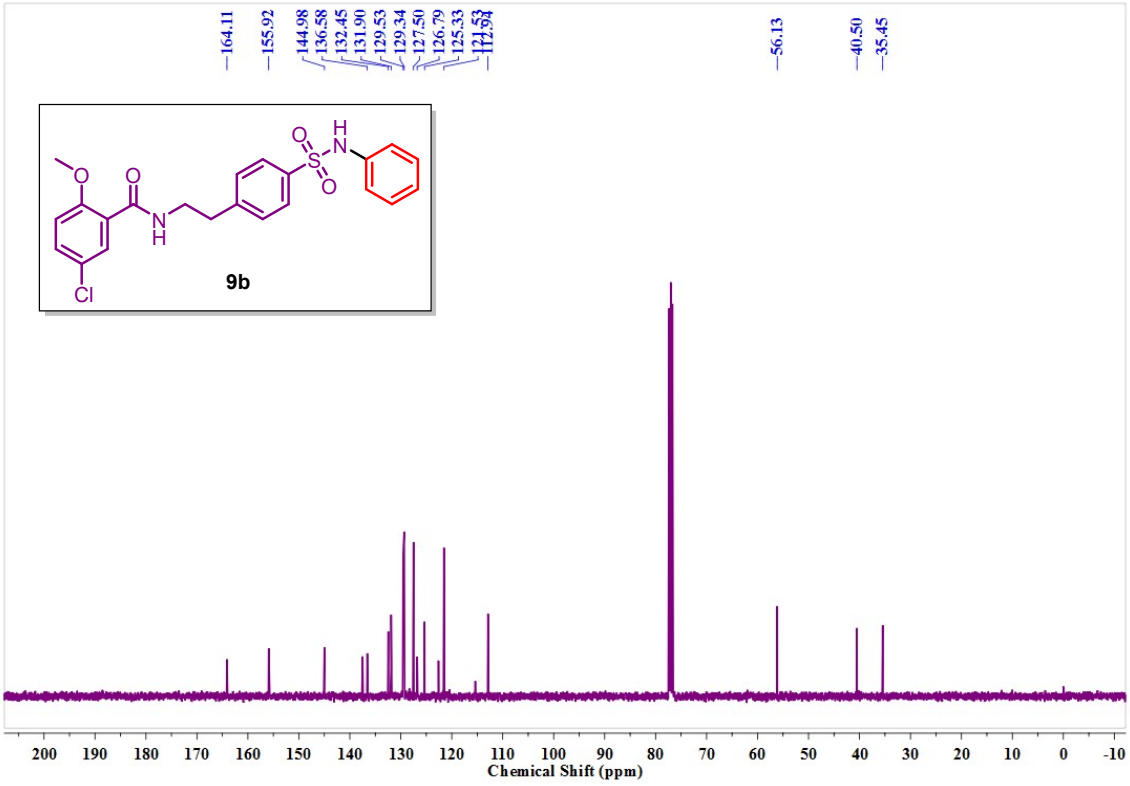

153.27
138.97
129.81
129.40
129.16
124.99
123.75
119.93
113.04
H2N
O
S
O
NH
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
Chemical Shift (ppm)

4.4 *[1]H and [13]C NMR spectra of **9a** and **9b***






8.14
7.78
7.74
7.72
7.37
7.35
7.31
7.29
7.24
7.21
7.20
7.11
7.09
7.07
6.85
6.82
3.74
3.72
3.70
3.69
3.66
2.96
2.95
2.93
9b
0.78
0.99
1.98
1.04
2.16
3.15
2.92
1.08
2.16
3.00
2.06
Chemical Shift (ppm)


164.11
155.92
144.98
136.58
132.45
131.90
129.53
129.34
127.50
126.79
125.33
56.13
40.50
35.45
9b
Chemical Shift (ppm)