


# Fusion of Morpholine and Schiff Base on Novel Benzimidazole Scaffold as Anti-microbial Agents: A Computational Approach and *In-vitro* Evaluation



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## 1. S1: GENERAL INFORMATION

The starting reactants of chemical compounds, reagents and solvent were procured from Sigma Aldrich, Himedia Ltd and Merck Ltd, those were HPLC graded components. The evaluation of melting point for synthesised compounds were performed by digital melting point apparatus by open capillary approach. The chromatogram for synthesised compounds were performed by Silica gel G TLC plates (Merck Ltd) and it was detected by iodine chamber. Further various spectroscopic techniques were utilized for characterisation of synthesised compounds such as  $\lambda$  max (Schimadzu Ultraviolet spectrometer), IR spectrum (Schimadzu FT-IR spectrophotometer) on KBr pellets, elemental analysis (CHNO Analyser), mass spectrum (HRMS mass spectrometer) and <sup>1</sup>H-NMR spectrum (FT-NMR 500 MHz spectrometer) were evaluated from Indian institute of technology, Chennai and VIT university, Vellore.

## 2. S2: SYNTHETIC PROCEDURES

### 2.1. First Step: Synthesis of 4-(1H-Benzimidazol-2-yl)benzamine (1)

The 0.05 M of *o*-phenylenediamine (5.4 gm) dissolved in water (20 ml) with continuous stirring on heating. The

0.05 M of *p*-amino benzoic acid (PABA) (6.9 gm) and concentrated hydrochloric acid (20 ml) were added to the above mixture and refluxed for 2 h in water bath. Cooled it and neutralized with ammonia solution results in precipitation of product, filtered by vacuum suction and recrystallized with ethanol.

### 2.2. Second Step: Synthesis of 4-(1-(morpholinomethyl)-1H-benzimidazol-2-yl)benzamine (2)

The mixture of 0.01 M of 4-(1H-benzimidazol-2-yl)benzamine (2.09 gm), 0.015 M of formaldehyde (0.45 gm) and morpholine (0.87 g; 0.01 mol) in ethanol (25 ml) were stirred by magnetic stirrer for 2 h. The resultant solution was further refluxed for 4 h on water bath, after that poured into crushed ice for cooling and mixed well. The resultant solid was filtered and recrystallized with ethanol.

## 3. S3: CHARACTERISTIC DATA FOR SYNTHETIC COMPOUNDS

### 3.1. Characteristic Data for Compound 1

Yield (%): 74; m.p. (°C): 248-251; IR (cm<sup>-1</sup>): 1632 (C=C), 1657 (C=N), 3021 (Ar-CH), 3374 (NH). <sup>1</sup>H-NMR (6:

ppm): 4.76 (s, 1H, NH), 5.41 (s, 2H, NH<sub>2</sub>), 7.13-8.07 (m, 8H, Ar-H). <sup>13</sup>C-NMR (δ: ppm): 158.52 (C-2), 150.94 (C'-1), 137.27 (C-8 & C-9), 135.76 (C'-3 & C'-5), 123.31 (C-5 & C-6), 121.05 (C'-4), 119.63 (C'-2 & C'-5), 110.41 (C-4 & C-7). MS (EI) *m/z*: 209.310 (M<sup>+</sup>). Anal. Calcd for C<sub>13</sub>H<sub>11</sub>N<sub>3</sub>: C, 74.62; H, 5.30; N, 20.08. Found: C, 74.87; H, 5.28; N, 20.01.

### 3.2. Characteristic Data for Compound 2

Yield (%): 77; m.p. (°C): 274-275; IR (cm<sup>-1</sup>): 1059 (C-O-C), 1616 (C=C), 1671 (C=N), 2938 (CH<sub>2</sub>-CH), 3005 (Ar-CH), 3309 (NH). <sup>1</sup>H-NMR (δ: ppm): 2.71 (t, 4H, CH<sub>2</sub> of morpholine), 3.58 (t, 4H, CH<sub>2</sub> of morpholine), 4.93 (s, 2H, CH<sub>2</sub> linkage), 5.69 (s, 2H, NH<sub>2</sub>), 6.90-7.85 (m, 8H, Ar-H). <sup>13</sup>C-NMR (δ: ppm): 149.74 (C-2), 147.13 (C'-1), 139.06 (C-9), 137.41 (C-8), 131.28 (C'-3 & C'-5), 126.81 (C-5 & C-6), 117.02 (C'-4), 115.63 (C'-2 & C'-5), 112.90 (C-4 & C-7), 61.72 (CH<sub>2</sub> linkage), 62.16 (C-2 & C-6 of morpholine), 45.05 (C-3 & C-5 of morpholine). MS (EI) *m/z*: 308.151 (M<sup>+</sup>). Anal. Calcd for C<sub>18</sub>H<sub>20</sub>N<sub>4</sub>O: C, 70.11; H, 6.54; N, 18.17. Found: C, 70.32; H, 6.52; N, 18.11.

### 3.3. Characteristic Data for Compound 3a-3o

#### 3.3.1. N-(2,4-Dichlorobenzylidene)-4-(1-(morpholinomethyl)-1H-benzimidazol-2-yl) benzenamine (3a)

Yield (%): 72; m.p. (°C): 183-185; IR (cm<sup>-1</sup>): 746 (C-Cl), 1075 (C-O-C), 1607 (C=C), 1642 (C=N), 2874 (CH<sub>2</sub>-CH), 3039 (Ar-CH), 3117 (=CH). <sup>1</sup>H NMR: δ 2.15 (4H, ddd, *J* = 15.3 Hz, CH<sub>2</sub> of morpholine), 3.91 (4H, ddd, *J* = 12.5 Hz, CH<sub>2</sub> of morpholine), 4.67 (s, 2H, CH<sub>2</sub> linkage), 7.03-7.41 [4H, ArH, (7.03 (ddd, *J* = 6.4 Hz), 7.19 (dd, *J* = 8.3 Hz), 7.33 (ddd, *J* = 8.3 Hz), 7.41 (dd, *J* = 1.7 Hz)], 7.46 (2H, ddd, *J* = 8.7 Hz), 7.53-7.92 [4H, ArH, (7.53 (ddd, *J* = 8.7 Hz), 7.83 (ddd, *J* = 5.0 Hz), 7.92 (ddd, *J* = 8.3 Hz)], 8.29 (1H, dd, *J* = 8.3 Hz), 8.42 (s, 1H, N=CH). <sup>13</sup>C-NMR (δ: ppm): 164.93 (N=CH), 155.06 (C-2), 151.72 (C'-1), 144.93 (C-9), 143.52 (C''-4), 138.15 (C''-2), 136.42 (C-8), 133.81 (C''-6), 131.05 (C''-1), 128.92 (C''-3), 128.32 (C'-4), 127.83 (C'-3 & C'-5), 126.06 (C''-5), 120.61 (C-5 & C-6), 118.29 (C'-2 & C'-5), 110.93 (C-4 & C-7), 63.77 (CH<sub>2</sub> linkage), 63.13 (C-2 & C-6 of morpholine), 48.54 (C-3 & C-5 of morpholine). MS (EI) *m/z*: 464.2110 (M<sup>+</sup>); 466.0162 (M<sup>+</sup>). Anal. Calcd for C<sub>25</sub>H<sub>22</sub>Cl<sub>2</sub>N<sub>4</sub>O: C, 64.52; H, 4.76; N, 12.04. Found: C, 64.30; H, 4.75; N, 12.09.

#### 3.3.2. N-(2,4-Difluorobenzylidene)-4-(1-(morpholinomethyl)-1H-benzimidazol-2-yl)benzenamine (3b)

Yield (%): 76; m.p. (°C): 159-161; IR (cm<sup>-1</sup>): 1033.42 (C-O-C), 1141.78(C-F), 1628.51 (C=C), 1681.81 (C=N), 2909.81 (CH<sub>2</sub>-CH), 3034.34 (Ar-CH), 3062.75 (=CH). <sup>1</sup>H NMR: δ 2.97 (4H, ddd, *J* = 15.2 Hz, CH<sub>2</sub> of morpholine), 3.86 (4H, ddd, *J* = 12.6 Hz, CH<sub>2</sub> of morpholine), 5.10 (s, 2H, CH<sub>2</sub> linkage), 7.12-7.31 [6H, ArH, (7.12 (ddd, *J* = 6.3 Hz), 7.18 (dd, *J* = 7.8 Hz), 7.21 (ddd, *J* = 1.6 Hz), 7.24 (dd, *J* = 8.1 Hz), 7.31 (2H, ddd, *J* = 8.7 Hz)], 7.91-8.25 [4H, ArH, (7.91 (ddd, *J* = 8.8 Hz), 7.95 (ddd, *J* = 8.1 Hz), 8.25 (ddd, *J* = 7.8 Hz), 8.26 (1H, dd, *J* = 5.1 Hz), 8.69 (s, 1H, N=CH). <sup>13</sup>C-NMR (δ: ppm): 171.53 (C''-4), 163.26 (C''-2), 161.90 (N=CH), 150.04 (C-2), 149.07 (C'-1), 142.86 (C-9), 138.26 (C-8), 134.66 (C''-6), 129.71 (C'-4), 127.13 (C'-3 & C'-5), 126.90 (C-5 & C-6), 123.04 (C'-2 & C'-5), 112.86 (C-4

& C-7), 110.24 (C''-1), 107.58 (C''-5), 101.90 (C''-3), 64.34 (CH<sub>2</sub> linkage), 64.13 (C-2 & C-6 of morpholine), 50.64 (C-3 & C-5 of morpholine) MS (EI) *m/z*: 432.0271 (M<sup>+</sup>). Anal. Calcd for C<sub>25</sub>H<sub>22</sub>F<sub>2</sub>N<sub>4</sub>O: C, 69.43; H, 5.13; N, 12.96. Found: C, 69.69; H, 5.11; N, 12.92.

#### 3.3.3. 4-((4-(1-(Morpholinomethyl)-1H-benzimidazol-2-yl)phenylimino)methyl)benzene-1,3-diol (3c)

Yield (%): 81; m.p. (°C): 147-149; IR (cm<sup>-1</sup>): 1058 (C-O-C), 1631 (C=C), 1666 (C=N), 2940 (CH<sub>2</sub>-CH), 3005 (Ar-CH), 3082 (=CH), 3387 (OH). <sup>1</sup>H NMR: δ 2.48 (4H, ddd, *J* = 15.3 Hz, CH<sub>2</sub> of morpholine), 3.62 (4H, ddd, *J* = 12.5 Hz, CH<sub>2</sub> of morpholine), 5.10 (s, 2H, CH<sub>2</sub> linkage), 5.63 (s, 1H, OH), 5.87 (s, 1H, OH), 6.75 (1H, ArH, dd, *J* = 2.1 Hz), 6.89 (1H, ArH, dd, *J* = 8.1 Hz), 7.41-7.53 [4H, ArH, 7.41 (ddd, *J* = 5.9 Hz), 7.46 (ddd, *J* = 8.5 Hz), 7.53 (ddd, *J* = 8.0, 5.9, 1.4 Hz)], 7.67-7.83 [4H, ArH, (7.67 (ddd, *J* = 8.5 Hz), 7.78 (dd, *J* = 8.1 Hz)], 7.83 (ddd, *J* = 8.0 Hz)], 7.91 (1H, ddd, *J* = 5.1 Hz), 8.57 (s, 1H, N=CH). <sup>13</sup>C-NMR (δ: ppm): 168.32 (C''-2), 167.64 (C''-4), 162.52 (N=CH), 157.93 (C-2), 155.42 (C'-1), 140.14 (C-9), 136.73 (C-8), 133.52 (C''-6), 130.83 (C'-4), 129.04 (C'-3 & C'-5), 121.63 (C-5 & C-6), 121.13 (C'-2 & C'-5), 119.45 (C-4 & C-7), 105.82 (C''-1), 103.25 (C''-5), 99.04 (C''-3), 61.43 (CH<sub>2</sub> linkage), 60.92 (C-2 & C-6 of morpholine), 47.63 (C-3 & C-5 of morpholine). MS (EI) *m/z*: 428.1214 (M<sup>+</sup>). Anal. Calcd for C<sub>25</sub>H<sub>24</sub>N<sub>4</sub>O<sub>3</sub>: C, 70.08; H, 5.65; N, 13.08. Found: C, 70.30; H, 5.67; N, 13.04.

#### 3.3.4. N-(2,4-Dibromobenzylidene)-4-(1-(morpholinomethyl)-1H-benzimidazol-2-yl)benzenamine (3d)

Yield (%): 75; m.p. (°C): 199-201; IR (cm<sup>-1</sup>): 645 (C-Br), 1071 (C-O-C), 1609 (C=C), 1643 (C=N), 2920 (CH<sub>2</sub>-CH), 3012 (Ar-CH), 3107 (=CH). <sup>1</sup>H NMR: δ 2.63 (4H, ddd, *J* = 15.3 Hz, CH<sub>2</sub> of morpholine), 3.97 (4H, ddd, *J* = 12.5 Hz, CH<sub>2</sub> of morpholine), 4.65 (s, 2H, CH<sub>2</sub> linkage), 6.98-7.02 [2H, 6.98 (ddd, *J* = 6.6 Hz), 7.02 (dd, *J* = 1.7 Hz)], 7.05-7.33 [4H, 7.05 (ddd, *J* = 8.6 Hz), 7.08 (dd, *J* = 8.3 Hz), 7.29 (ddd, *J* = 8.3 Hz)], 7.43-7.82 [4H, 7.43 (ddd, *J* = 8.6 Hz), 7.52 (ddd, *J* = 5.0 Hz), 7.65 (ddd, *J* = 8.3 Hz)], 7.97 (1H, dd, *J* = 8.3 Hz), 8.31 (s, 1H, N=CH). <sup>13</sup>C-NMR (δ: ppm): 157.42 (N=CH), 154.27 (C-2), 152.53 (C'-1), 140.84 (C-9), 137.06 (C''-3), 136.64 (C''-1), 136.23 (C-8), 134.92 (C''-6), 132.14 (C''-5), 127.55 (C'-4), 126.94 (C'-3 & C'-5), 126.37 (C''-4), 122.04 (C''-2), 121.44 (C-5 & C-6), 120.83 (C'-2 & C'-5), 113.15 (C-4 & C-7), 60.92 (CH<sub>2</sub> linkage), 59.73 (C-2 & C-6 of morpholine), 48.25 (C-3 & C-5 of morpholine). MS (EI) *m/z*: 552.1017 (M<sup>+</sup>); 554.2173 (M<sup>+</sup>). Anal. Calcd for C<sub>25</sub>H<sub>22</sub>Br<sub>2</sub>N<sub>4</sub>O: C, 54.17; H, 4.00; N, 10.11. Found: C, 54.35; H, 3.99; N, 10.07.

#### 3.3.5. N-(2,4-Dimethoxybenzylidene)-4-(1-(morpholinomethyl)-1H-benzimidazol-2-yl) benzenamine (3e)

Yield (%): 73; m.p. (°C): 165-167; IR (cm<sup>-1</sup>): 1141.90 (C-O-C), 1620.19 (C=C), 1681.81 (C=N), 2835.16 (CH<sub>2</sub>-CH), 3012.75 (Ar-CH), 3105.10 (=CH). <sup>1</sup>H NMR: δ 2.07 (4H, ddd, *J* = 15.3 Hz, CH<sub>2</sub> of morpholine), 3.76 (4H, ddd, *J* = 12.5 Hz, CH<sub>2</sub> of morpholine), 3.95 (s, 3H, OCH<sub>3</sub>), 4.12 (s, 3H, OCH<sub>3</sub>), 4.95 (s, 2H, CH<sub>2</sub> linkage), 6.95-6.97 [2H, 6.95 (ddd, *J* = 2.1 Hz), 6.97 (dd, *J* = 8.1 Hz)], 7.41-7.78 [4H, 7.46 (ddd, *J* = 5.8 Hz), 7.53 (dd, *J* = 8.5 Hz), 7.67 (ddd, *J* = 7.8 Hz)], 7.81-7.90 [4H, 7.81 (ddd, *J* = 8.5 Hz), 7.83 (ddd, *J*

= 8.1 Hz), 7.90 (ddd,  $J = 7.8$  Hz), 7.93 (1H, dd,  $J = 5.8$  Hz), 8.49 (s, 1H, N=CH).  $^{13}\text{C-NMR}$  ( $\delta$ : ppm): 168.10 (C''-4), 165.02 (C''-2), 162.12 (N=CH), 154.90 (C-2), 153.49 (C'-1), 143.02 (C-9), 138.26 (C-8), 133.61 (C''-6), 130.81 (C'-4), 129.52 (C'-3 & C'-5), 126.10 (C-5 & C-6), 125.75 (C'-2 & C'-5), 113.45 (C-4 & C-7), 108.90 (C''-1), 106.26 (C''-5), 93.52 (C''-3), 64.82 (CH<sub>2</sub> linkage), 64.32 (C-2 & C-6 of morpholine), 53.11 (OCH<sub>3</sub>), 52.75 (OCH<sub>3</sub>), 50.45 (C-3 & C-5 of morpholine). MS (EI)  $m/z$ : 456.5338 (M<sup>+</sup>). Anal. Calcd for C<sub>27</sub>H<sub>28</sub>N<sub>4</sub>O<sub>3</sub>: C, 71.03; H, 6.18; N, 12.27. Found: C, 70.79; H, 6.20; N, 12.32.

### 3.3.6. N-(2,4-Dinitrobenzylidene)-4-(1-(morpholinomethyl)-1H-benzimidazol-2-yl)benzenamine (3f)

Yield (%): 80; m.p. (°C): 153-154; IR (cm<sup>-1</sup>): 1048 (C-O-C), 1352 & 1589 (NO<sub>2</sub>), 1605 (C=C), 1660 (C=N), 2917 (CH<sub>2</sub>-CH), 3039 (Ar-CH), 3081 (=CH).  $^1\text{H NMR}$ :  $\delta$  2.50 (4H, ddd,  $J = 15.3$  Hz, CH<sub>2</sub> of morpholine), 3.59 (4H, ddd,  $J = 12.5$  Hz, CH<sub>2</sub> of morpholine), 4.81 (s, 2H, CH<sub>2</sub> linkage), 6.72 (1H, ArH, ddd,  $J = 7.8$  Hz), 7.41 (1H, ArH, ddd,  $J = 7.8$  Hz), 7.46 (1H, ArH, ddd,  $J = 7.4$  Hz), 7.46-7.81 [(6H, ArH, 7.53 (1H, dd,  $J = 7.3$  Hz), 7.67 (2H, ddd,  $J = 6.9$  Hz), 7.78 (2H, ddd,  $J = 6.9$  Hz), 7.81 (1H, ddd,  $J = 5.0$  Hz)], 7.83 (1H, ArH, dd,  $J = 7.3$  Hz), 7.93 (1H, ArH, dd,  $J = 1.8$  Hz), 8.35 (s, 1H, N=CH).  $^{13}\text{C-NMR}$  ( $\delta$ : ppm): 160.53 (N=CH), 155.74 (C-2), 155.93 (C'-1), 154.22 (C''-4), 150.64 (C''-2), 139.43 (C-9), 133.02 (C-8), 130.87 (C''-1), 130.24 (C''-6), 127.54 (C'-4), 126.93 (C'-3 & C'-5), 126.77 (C''-5), 121.22 (C-5 & C-6), 120.46 (C'-2 & C'-5), 115.04 (C''-3), 114.91 (C-4 & C-7), 62.88 (CH<sub>2</sub> linkage), 62.36 (C-2 & C-6 of morpholine), 54.52 (C-3 & C-5 of morpholine). MS (EI)  $m/z$ : 486.1065 (M<sup>+</sup>). Anal. Calcd for C<sub>25</sub>H<sub>22</sub>N<sub>6</sub>O<sub>5</sub>: C, 61.72; H, 4.56; N, 17.28. Found: C, 61.91; H, 4.54; N, 17.22.

### 3.3.7. N-Benzylidene-4-(1-(morpholinomethyl)-1H-benzimidazol-2-yl)benzenamine (3g)

Yield (%): 78; m.p. (°C): 178-180; IR (cm<sup>-1</sup>): 1036 (C-O-C), 1614 (C=C), 1635 (C=N), 2919 (CH<sub>2</sub>-CH), 3017 (Ar-CH), 3128 (=CH).  $^1\text{H NMR}$ :  $\delta$  2.19 (4H, ddd,  $J = 15.3$  Hz, CH<sub>2</sub> of morpholine), 3.85 (4H, ddd,  $J = 12.5$  Hz, CH<sub>2</sub> of morpholine), 4.63 (s, 2H, CH<sub>2</sub> linkage), 7.20-7.65 [4H, 7.20 (ddd,  $J = 7.5$  Hz), 7.43 (ddd,  $J = 8.1$  Hz), 7.55 (2H), dddd,  $J = 7.8$  Hz], 7.72-8.44 [7H, ArH, 7.82 (tdd,  $J = 7.4$  Hz), 7.98 (ddd,  $J = 5.0$  Hz), 8.09 (2H, ddd,  $J = 8.3$  Hz), 8.44 (2H, ArH, ddd,  $J = 8.3$  Hz), 8.53 (ddd,  $J = 8.1$  Hz)], 8.67 (2H, ArH, dtd,  $J = 7.8$  Hz), 8.86 (s, 1H, N=CH).  $^{13}\text{C-NMR}$  ( $\delta$ : ppm): 165.06 (N=CH), 156.72 (C-2), 155.43 (C'-1), 139.53 (C-9), 136.04 (C-8), 134.83 (C''-1), 130.42 (C''-4), 128.92 (C''-2 & C''-6), 128.33 (C'-4), 128.07 (C''-3 & C''-5), 126.63 (C'-3 & C'-5), 121.82 (C-5 & C-6), 120.54 (C'-2 & C'-5), 114.74 (C-4 & C-7), 63.13 (CH<sub>2</sub> linkage), 62.96 (C-2 & C-6 of morpholine), 44.33 (C-3 & C-5 of morpholine). MS (EI)  $m/z$ : 396.1357 (M<sup>+</sup>). Anal. Calcd for C<sub>25</sub>H<sub>24</sub>N<sub>4</sub>O: C, 75.73; H, 6.10; N, 14.13. Found: C, 75.99; H, 6.08; N, 14.07.

### 3.3.8. 4-(1-(Morpholinomethyl)-1H-benzimidazol-2-yl)-N-(3-phenylallylidene)benzenamine (3h)

Yield (%): 72; m.p. (°C): 189-191; IR (cm<sup>-1</sup>): 1052 (C-O-C), 1617 (C=C), 1639 (C=N), 2874 (CH<sub>2</sub>-CH), 3013 (Ar-CH), 3135 (=CH).  $^1\text{H NMR}$ :  $\delta$  2.82 (4H, ddd,  $J = 15.3$  Hz, CH<sub>2</sub> of morpholine), 3.70 (4H, ddd,  $J = 12.5$  Hz, CH<sub>2</sub> of

morpholine), 5.27 (s, 2H, CH<sub>2</sub> linkage), 5.78 (1H, dd,  $J = 17.7$  Hz, CH=CH), 6.50 (1H, d,  $J = 17.7$  Hz, CH=CH), 7.03-7.20 [3H, ArH, 7.03 (1H, ddd,  $J = 6.4$  Hz), 7.20 (dddd,  $J = 8.0$  Hz)], 7.21-8.36 [10H, ArH, 7.56 (2H, dtd,  $J = 8.0$  Hz), 7.57 (1H, tt,  $J = 6.5$  Hz), 7.60 (1H, ddd,  $J = 8.1$  Hz), 7.79 (2H, ddd,  $J = 8.1$  Hz), 7.83 (2H, ddd,  $J = 8.1$  Hz), 8.12 (1H, ddd,  $J = 5.1$  Hz), 8.22 (1H, ddd,  $J = 8.1$  Hz)], 8.86 (d, 1H,  $J = 8.1$  Hz, N=CH).  $^{13}\text{C-NMR}$  ( $\delta$ : ppm): 155.43 (N=CH), 150.04 (C-2), 148.72 (C'-1), 142.15 (C-9), 139.68 (N=CH-CH=CH-), 138.04 (C''-1), 137.93 (C-8), 133.52 (C'-4), 129.84 (C'-3 & C'-5), 129.42 (C''-3 & C''-5), 128.62 (C''-4), 122.13 (C''-2 & C''-6), 121.81 (C-5 & C-6), 122.12 (C'-2 & C'-5), 117.52 (N=CH-CH=CH-), 111.74 (C-4 & C-7), 66.90 (CH<sub>2</sub> linkage), 66.44 (C-2 & C-6 of morpholine), 50.22 (C-3 & C-5 of morpholine). MS (EI)  $m/z$ : 422.3422 (M<sup>+</sup>). Anal. Calcd for C<sub>27</sub>H<sub>26</sub>N<sub>4</sub>O: C, 76.75; H, 6.20; N, 13.26. Found: C, 76.49; H, 6.22; N, 13.31.

### 3.3.9. 4-(1-(Morpholinomethyl)-1H-benzimidazol-2-yl)-N-(pyridin-4-ylmethylene)benzenamine (3i)

Yield (%): 79; m.p. (°C): 197-198; IR (cm<sup>-1</sup>): 1040 (C-O-C), 1608 (C=C), 1653 (C=N), 2931 (CH<sub>2</sub>-CH), 3006 (Ar-CH), 3059 (=CH).  $^1\text{H NMR}$ :  $\delta$  2.30 (4H, ddd,  $J = 15.3$  Hz, CH<sub>2</sub> of morpholine), 3.63 (4H, ddd,  $J = 12.5$  Hz, CH<sub>2</sub> of morpholine), 4.95 (s, 2H, CH<sub>2</sub> linkage), 6.82-6.91 [4H, ArH, 6.82 (1H, ddd,  $J = 6.0$  Hz), 6.90 (1H, ddd,  $J = 8.1$  Hz), 6.91 (2H, ddd,  $J = 5.1$  Hz)], 7.32-7.98 [6H, ArH, 7.32 (2H, ddd,  $J = 8.3$  Hz), 7.65 (2H, ddd,  $J = 8.3$  Hz), 7.75 (1H, ddd,  $J = 8.1$  Hz), 7.94 (1H, ddd,  $J = 5.0$  Hz)], 8.18 (2H, ddd,  $J = 5.1$  Hz), 8.36 (s, 1H, N=CH).

$^{13}\text{C-NMR}$  ( $\delta$ : ppm): 169.66 (N=CH), 159.22 (C-2), 158.51 (C'-1), 152.02 (C''-2 & C''-6), 149.72 (C''-4), 144.31 (C-9), 139.61 (C-8), 130.43 (C'-4), 129.26 (C'-3 & C'-5), 122.82 (C''-3 & C''-5), 122.53 (C-5 & C-6), 122.02 (C'-2 & C'-5), 112.96 (C-4 & C-7), 69.24 (CH<sub>2</sub> linkage), 68.71 (C-2 & C-6 of morpholine), 57.53 (C-3 & C-5 of morpholine). MS (EI)  $m/z$ : 397.2314 (M<sup>+</sup>). Anal. Calcd for C<sub>24</sub>H<sub>23</sub>N<sub>5</sub>O: C, 72.52; H, 5.83; N, 17.62. Found: C, 72.29; H, 5.85; N, 17.68.

### 3.3.10. N-(4-Chlorobenzylidene)-4-(1-(morpholinomethyl)-1H-benzimidazol-2-yl)benzenamine (3j)

Yield (%): 70; m.p. (°C): 162-163; IR (cm<sup>-1</sup>): 708 (C-Cl), 1035 (C-O-C), 1620 (C=C), 1657 (C=N), 2943 (CH<sub>2</sub>-CH), 3006 (Ar-CH), 3079 (=CH).  $^1\text{H NMR}$ :  $\delta$  2.66 (4H, ddd,  $J = 15.3$  Hz, CH<sub>2</sub> of morpholine), 3.94 (4H, ddd,  $J = 12.5$  Hz, CH<sub>2</sub> of morpholine), 5.06 (s, 2H, CH<sub>2</sub> linkage), 7.29 (1H, ArH, ddd,  $J = 6.5$  Hz), 7.33-7.51 [(5H, ArH, (7.33 (1H, ddd,  $J = 8.3$  Hz), 7.44 (2H, ddd,  $J = 8.0$  Hz), 7.51 (2H, ddd,  $J = 8.0$  Hz)], 7.68 (2H, ArH, ddd,  $J = 8.3$  Hz), 7.75-8.01 [(4H, ArH, (7.75 (2H, ddd,  $J = 8.3$  Hz), 7.81 (1H, ddd,  $J = 8.3$  Hz), 7.94 (1H, ddd,  $J = 5.0$  Hz)], 8.68 (s, 1H, N=CH).  $^{13}\text{C-NMR}$  ( $\delta$ : ppm): 165.34 (N=CH), 159.72 (C-2), 155.01 (C'-1), 142.54 (C-9), 139.13 (C''-4), 135.81 (C-8), 130.43 (C''-1), 129.20 (C''-2 & C''-6), 128.58 (C'-4), 128.14 (C''-3 & C''-5), 126.92 (C'-3 & C'-5), 122.31 (C-5 & C-6), 120.62 (C'-2 & C'-5), 115.94 (C-4 & C-7), 70.24 (CH<sub>2</sub> linkage), 69.07 (C-2 & C-6 of morpholine), 54.82 (C-3 & C-5 of morpholine). MS (EI)  $m/z$ : 430.1464 (M<sup>+</sup>), 432.1311 (M<sup>+</sup>). Anal. Calcd for C<sub>25</sub>H<sub>23</sub>ClN<sub>4</sub>O: C, 69.68; H, 5.38; N, 13.00. Found: C, 69.93; H, 5.36; N, 12.95.

### 3.3.11. N-(4-Fluorobenzylidene)-4-(1-(morpholinomethyl)-1H-benzimidazol-2-yl)benzenamine (3k)

Yield (%): 73; m.p. (°C): 141-142; IR (cm<sup>-1</sup>): 1072 (C-O-C), 1184 (C-F), 1645 (C=C), 1679 (C=N), 2906 (CH<sub>2</sub>-CH), 3024 (Ar-CH), 3114 (=CH). <sup>1</sup>H NMR: δ 2.54 (4H, ddd, *J* = 15.3 Hz, CH<sub>2</sub> of morpholine), 3.47 (4H, ddd, *J* = 12.5 Hz, CH<sub>2</sub> of morpholine), 4.81 (s, 2H, CH<sub>2</sub> linkage), 7.16-7.43 [(4H, ArH, (7.30 (1H, ddd, *J* = 6.5 Hz), 7.33 (2H, ddd, *J* = 8.3 Hz), 7.41 (1H, ddd, *J* = 8.3 Hz)], 7.53-8.14 [(8H, ArH, (7.63 (1H, ddd, *J* = 5.1 Hz), 7.67 (2H, ddd, *J* = 8.7 Hz), 7.78 (2H, ddd, *J* = 8.3 Hz), 7.83 (2H, ddd, *J* = 8.7 Hz), 7.93 (1H, ddd, *J* = 8.3 Hz)], 8.68 (s, 1H, N=CH). <sup>13</sup>C-NMR (δ: ppm): 171.62 (C''-4), 165.91 (N=CH), 159.03 (C-2), 156.24 (C'-1), 140.56 (C-9), 137.14 (C-8), 136.72 (C''-2 & C''-6), 132.81 (C''-1), 129.53 (C'-4), 128.03 (C'-3 & C'-5), 126.64 (C-5 & C-6), 124.37 (C'-2 & C'-5), 110.31 (C''-3 & C''-5), 109.73 (C-4 & C-7), 73.22 (CH<sub>2</sub> linkage), 72.93 (C-2 & C-6 of morpholine), 45.53 (C-3 & C-5 of morpholine). MS (EI) *m/z*: 414.1426 (M<sup>+</sup>). Anal. Calcd for C<sub>25</sub>H<sub>23</sub>FN<sub>4</sub>O: C, 72.45; H, 5.59; N, 13.52. Found: C, 72.20; H, 5.61; N, 13.56.

### 3.3.12. 4-((4-(1-(Morpholinomethyl)-1H-benzimidazol-2-yl)phenylimino)methyl)phenol (3l)

Yield (%): 78; m.p. (°C): 193-194; IR (cm<sup>-1</sup>): 1067 (C-O-C), 1631 (C=C), 1674 (C=N), 2896 (CH<sub>2</sub>-CH), 3028 (Ar-CH), 3123 (=CH), 3360 (OH). <sup>1</sup>H NMR: δ 2.78 (4H, ddd, *J* = 15.3 Hz, CH<sub>2</sub> of morpholine), 3.41 (4H, ddd, *J* = 12.5 Hz, CH<sub>2</sub> of morpholine), 4.76 (s, 2H, CH<sub>2</sub> linkage), 5.43 (s, 1H, OH), 6.86-6.98 [(4H, ArH, (6.88 (2H, ddd, *J* = 8.2 Hz), 6.94 (1H, ddd, *J* = 8.1 Hz), 6.98 (1H, ddd, *J* = 6.2 Hz)], 7.00-7.90 [(8H, ArH, (7.18 (2H, ddd, *J* = 8.6 Hz), 7.27 (2H, ddd, *J* = 8.2 Hz), 7.44 (2H, ddd, *J* = 8.6 Hz), 7.65 (1H, ddd, *J* = 5.1 Hz), 7.88 (1H, ddd, *J* = 8.1 Hz)], 8.57 (s, 1H, N=CH). <sup>13</sup>C-NMR (δ: ppm): 164.51 (C''-4), 163.13 (N=CH), 157.86 (C-2), 156.49 (C'-1), 140.25 (C-9), 138.72 (C-8), 137.04 (C''-2 & C''-6), 133.93 (C'-4), 129.16 (C'-3 & C'-5), 126.83 (C''-1), 125.44 (C-5 & C-6), 121.04 (C'-2 & C'-5), 114.72 (C''-3 & C''-5), 111.24 (C-4 & C-7), 66.31 (CH<sub>2</sub> linkage), 65.96 (C-2 & C-6 of morpholine), 50.61 (C-3 & C-5 of morpholine). MS (EI) *m/z*: 412.2411 (M<sup>+</sup>). Anal. Calcd for C<sub>25</sub>H<sub>24</sub>N<sub>4</sub>O<sub>2</sub>: C, 72.80; H, 5.86; N, 13.58. Found: C, 73.06; H, 5.87; N, 13.53.

### 3.3.13. N-(4-Bromobenzylidene)-4-(1-(morpholinomethyl)-1H-benzimidazol-2-yl)benzenamine (3m)

Yield (%): 75; m.p. (°C): 174-176; IR (cm<sup>-1</sup>): 623 (C-Br), 1069 (C-O-C), 1623 (C=C), 1640 (C=N), 2948 (CH<sub>2</sub>-CH), 3031 (Ar-CH), 3075 (=CH). <sup>1</sup>H NMR: δ 2.76 (4H, ddd, *J* = 15.3 Hz, CH<sub>2</sub> of morpholine), 3.92 (4H, ddd, *J* = 12.5 Hz, CH<sub>2</sub> of morpholine), 5.18 (s, 2H, CH<sub>2</sub> linkage), 6.97 (1H, ArH, ddd, *J* = 6.6 Hz), 7.41-7.53 [(5H, ArH, (7.41 (2H, ddd, *J* = 8.2 Hz), 7.46 (1H, ddd, *J* = 8.3 Hz), 7.53 (2H, ddd, *J* = 8.7 Hz)], 7.67-8.10 [(6H, ArH, (7.78 (2H, ddd, *J* = 8.2 Hz), 7.81 (2H, ddd, *J* = 8.7 Hz), 7.83 (1H, ddd, *J* = 8.3 Hz), 7.92 (1H, ddd, *J* = 5.0 Hz)], 8.34 (s, 1H, N=CH). <sup>13</sup>C-NMR (δ: ppm): 158.94 (N=CH), 156.13 (C-2), 155.54 (C'-1), 142.02 (C-9), 139.84 (C-8), 134.26 (C''-1), 131.61 (C''-3 & C''-5),

131.04 (C''-2 & C''-6), 128.33 (C'-4), 127.94 (C'-3 & C'-5), 124.72 (C''-4), 120.83 (C-5 & C-6), 118.41 (C'-2 & C'-5), 112.94 (C-4 & C-7), 62.53 (CH<sub>2</sub> linkage), 62.13 (C-2 & C-6 of morpholine), 40.25 (C-3 & C-5 of morpholine). MS (EI) *m/z*: 474.1325 (M<sup>+</sup>), 476.0521 (M<sup>+2</sup>). Anal. Calcd for C<sub>25</sub>H<sub>23</sub>BrN<sub>4</sub>O: C, 63.16; H, 4.88; N, 11.79. Found: C, 63.39; H, 4.86; N, 11.75.

### 3.3.14. N-(4-Methoxybenzylidene)-4-(1-(morpholinomethyl)-1H-benzimidazol-2-yl)benzenamine (3n)

Yield (%): 71; m.p. (°C): 156-158; IR (cm<sup>-1</sup>): 1040.24 (C-O-C), 1604.66 (C=C), 1666.13 (C=N), 2921.43 (CH<sub>2</sub>-CH), 3034.13 (Ar-CH), 3094.33 (=CH). <sup>1</sup>H NMR: δ 2.49 (4H, ddd, *J* = 15.3 Hz, CH<sub>2</sub> of morpholine), 3.66 (4H, ddd, *J* = 12.5 Hz, CH<sub>2</sub> of morpholine), 3.83 (s, 3H, OCH<sub>3</sub>), 4.95 (s, 2H, CH<sub>2</sub> linkage), 7.12 (2H, ArH, ddd, *J* = 8.6 Hz), 7.38-7.40 [(2H, ArH, (7.38 (1H, ddd, *J* = 6.2 Hz), 7.40 (1H, ddd, *J* = 8.1 Hz)], 7.41-7.42 [(4H, ArH (7.41 (2H, ddd, *J* = 8.6 Hz), 7.42 (2H, ddd, *J* = 8.6 Hz)], 7.90 (2H, ArH, ddd, *J* = 8.6 Hz), 8.05 (1H, ArH, ddd, *J* = 8.1 Hz), 8.06 (1H, ArH, ddd, *J* = 5.1 Hz), 8.69 (s, 1H, N=CH). <sup>13</sup>C-NMR (δ: ppm): 165.86 (C''-4), 164.66 (N=CH), 157.49 (C-2), 155.95 (C'-1), 144.07 (C-9), 138.26 (C-8), 136.13 (C''-2 & C''-6), 133.24 (C'-4), 129.30 (C'-3 & C'-5), 128.04 (C''-1), 126.53 (C-5 & C-6), 123.24 (C'-2 & C'-5), 115.32 (C-4 & C-7), 113.09 (C''-3 & C''-5), 68.34 (CH<sub>2</sub> linkage), 67.06 (C-2 & C-6 of morpholine), 58.87 (OCH<sub>3</sub>), 53.81 (C-3 & C-5 of morpholine). MS (EI) *m/z*: 426.5338 (M<sup>+</sup>). Anal. Calcd for C<sub>26</sub>H<sub>26</sub>N<sub>4</sub>O<sub>2</sub>: C, 73.22; H, 6.14; N, 13.14. Found: C, 73.01; H, 6.16; N, 13.19.

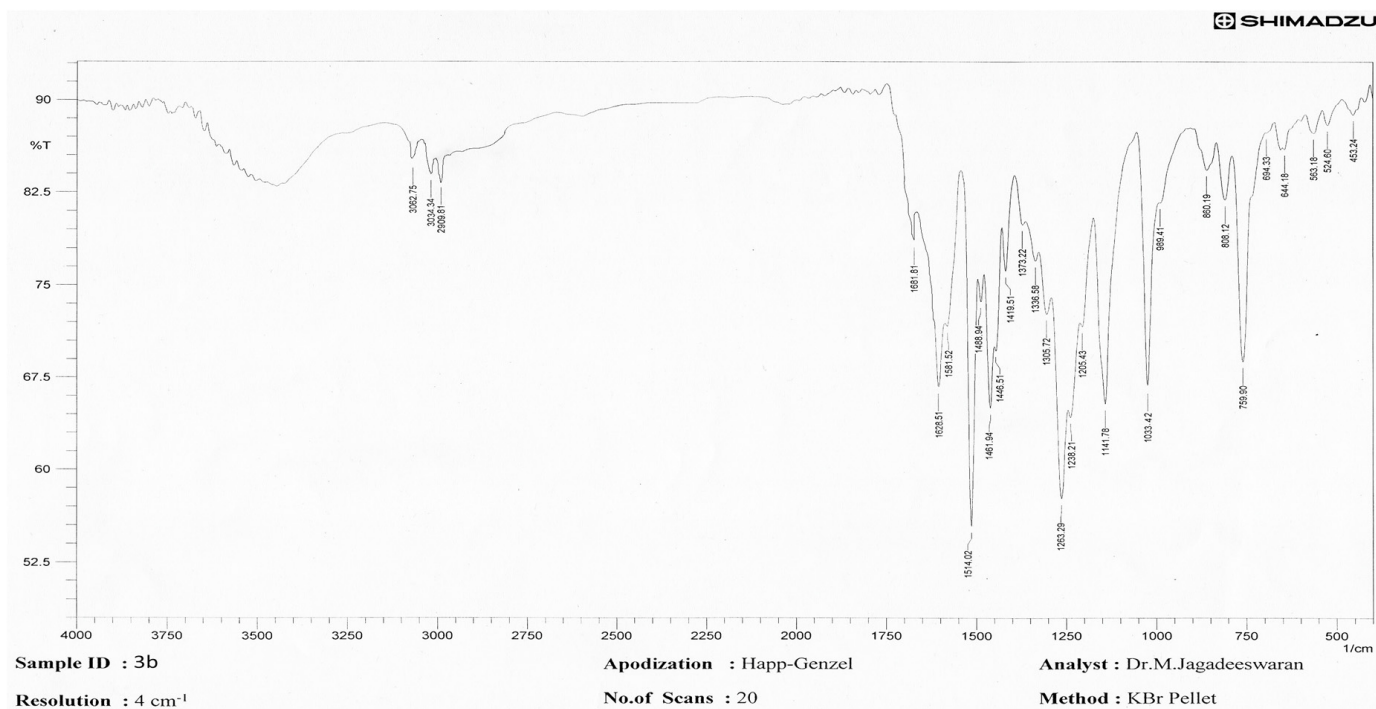
### 3.3.15. N-(2-nitrobenzylidene)-4-(1-(morpholinomethyl)-1H-benzimidazol-2-yl)benzenamine (3o)

Yield (%): 76; m.p. (°C): 186-187; IR (cm<sup>-1</sup>): 1034 (C-O-C), 1375 & 1551 (NO<sub>2</sub>), 1619 (C=C), 1651 (C=N), 2923 (CH<sub>2</sub>-CH), 3015 (Ar-CH), 3096 (=CH). <sup>1</sup>H NMR: δ 2.53 (4H, ddd, *J* = 15.3 Hz, CH<sub>2</sub> of morpholine), 3.39 (4H, ddd, *J* = 12.5 Hz, CH<sub>2</sub> of morpholine), 5.04 (s, 2H, CH<sub>2</sub> linkage), 6.76 (2H, ArH, ddd, *J* = 5.9 Hz), 6.96 (2H, ArH, ddd, *J* = 8.3 Hz), 6.98-7.91 [(10H, ArH, (6.98 (2H, ddd, *J* = 8.0 Hz), 6.99 (2H, ddd, *J* = 8.0 Hz), 7.16 (1H, ddd, *J* = 8.5 Hz), 7.52 (1H, ddd, *J* = 8.3 Hz), 7.54 (1H, ddd, *J* = 7.8 Hz), 7.55 (1H, ddd, *J* = 5.0 Hz), 7.64 (1H, ddd, *J* = 8.5 Hz), 7.91 (1H, ddd, *J* = 7.8 Hz)], 8.50 (s, 1H, N=CH). <sup>13</sup>C-NMR (δ: ppm): 164.61 (N=CH), 155.43 (C-2), 154.85 (C'-1), 153.16 (C''-4), 141.25 (C''-1), 140.52 (C-9), 137.94 (C-8), 134.14 (C''-2 & C''-6), 132.62 (C'-4), 130.36 (C'-3 & C'-5), 128.59 (C-5 & C-6), 120.76 (C'-2 & C'-5), 119.42 (C''-3 & C''-5), 113.13 (C-4 & C-7), 60.87 (CH<sub>2</sub> linkage), 59.24 (C-2 & C-6 of morpholine), 54.76 (C-3 & C-5 of morpholine). MS (EI) *m/z*: 441.0431 (M<sup>+</sup>). Anal. Calcd for C<sub>25</sub>H<sub>23</sub>N<sub>5</sub>O<sub>3</sub>: C, 68.01; H, 5.25; N, 15.86. Found: C, 68.19; H, 5.24; N, 15.80.

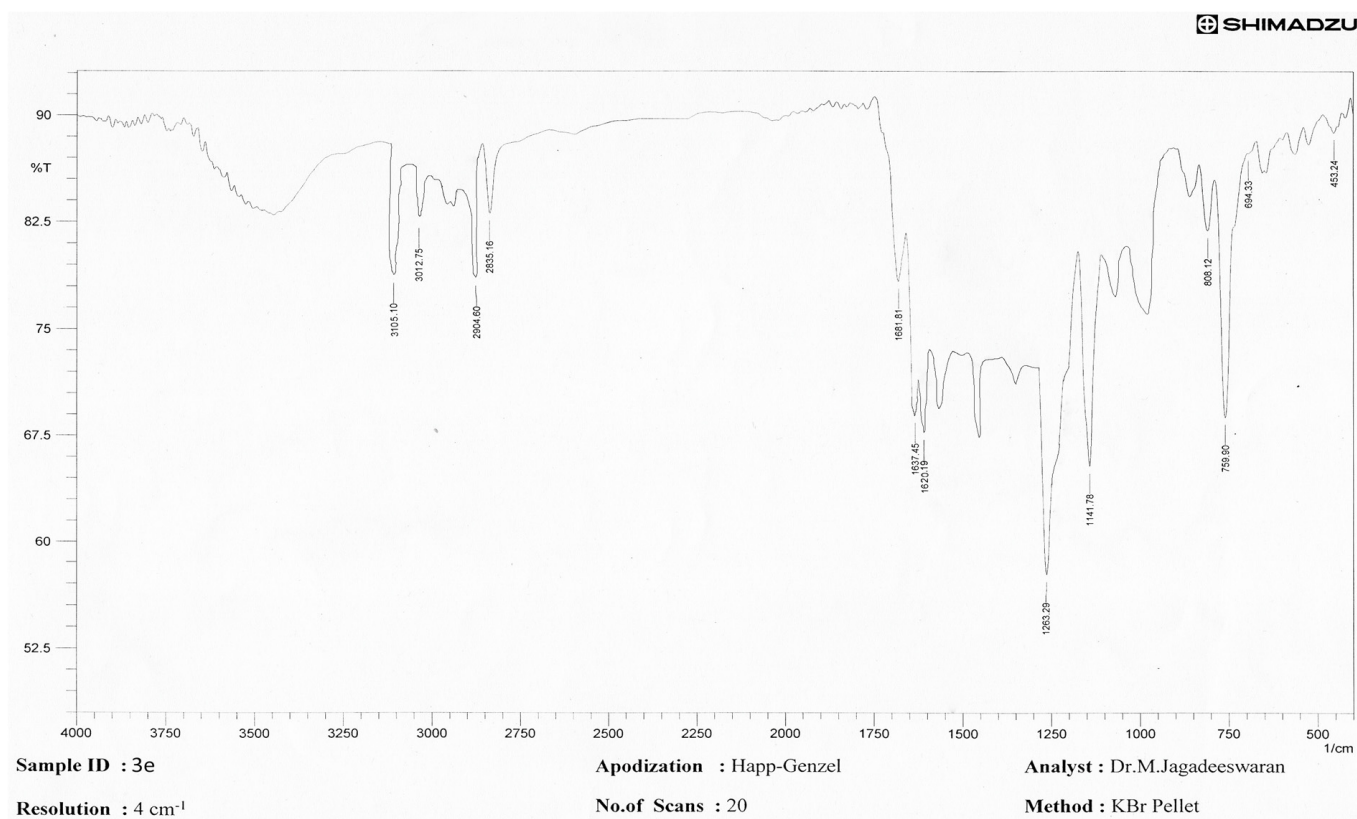
## 4. S4: SPECTRUM DETAILS FOR SYNTHESISED ACTIVE COMPOUNDS

### 4.1. IR SPECTRUM DETAILS

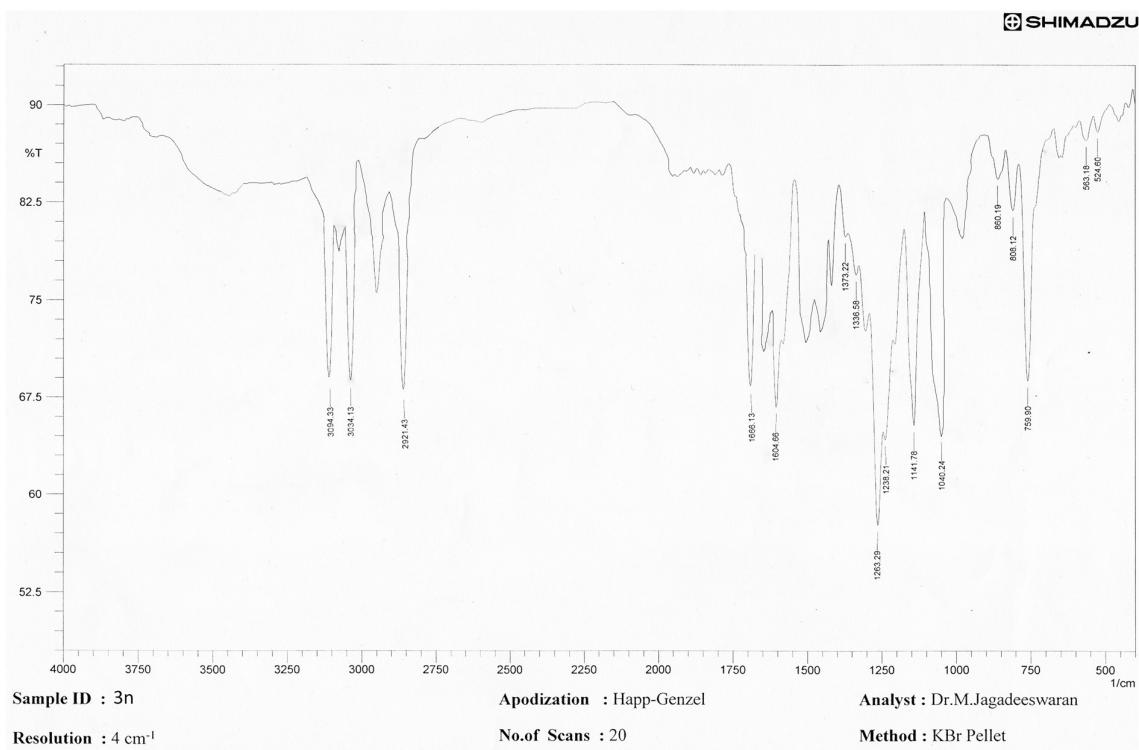
#### 4.1.1. Compound 3b



4.1.2. Compound 3e

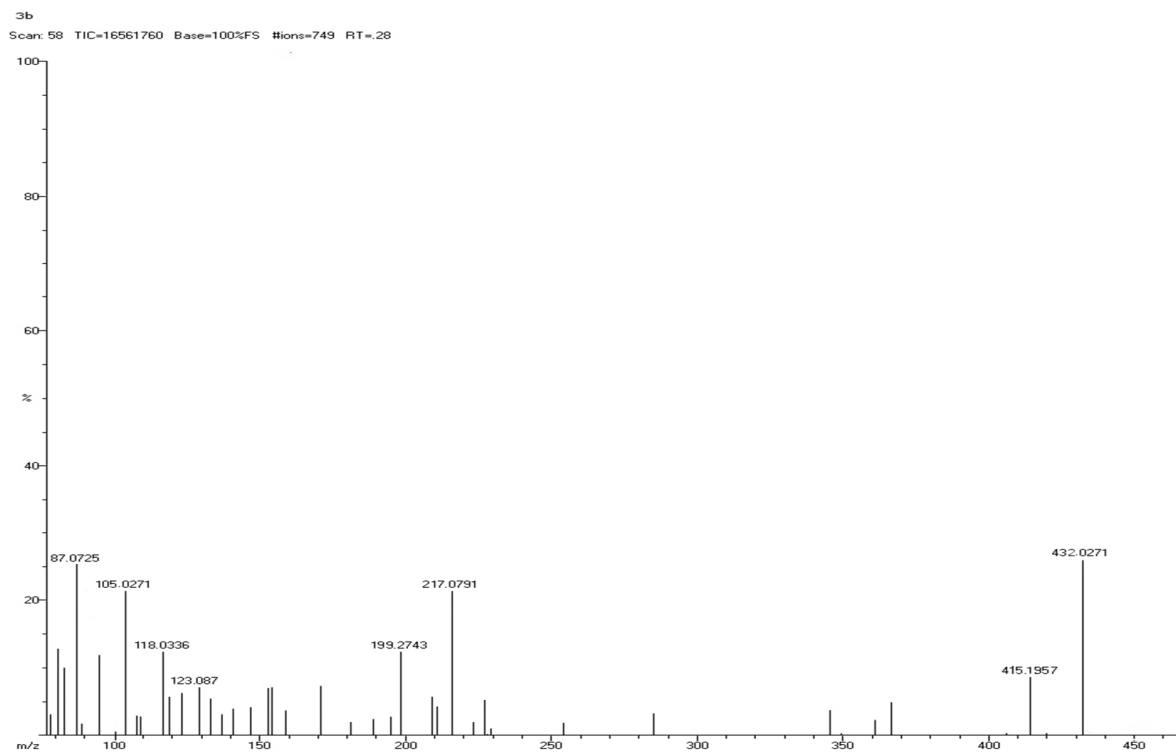


### 4.1.3. Compound 3n

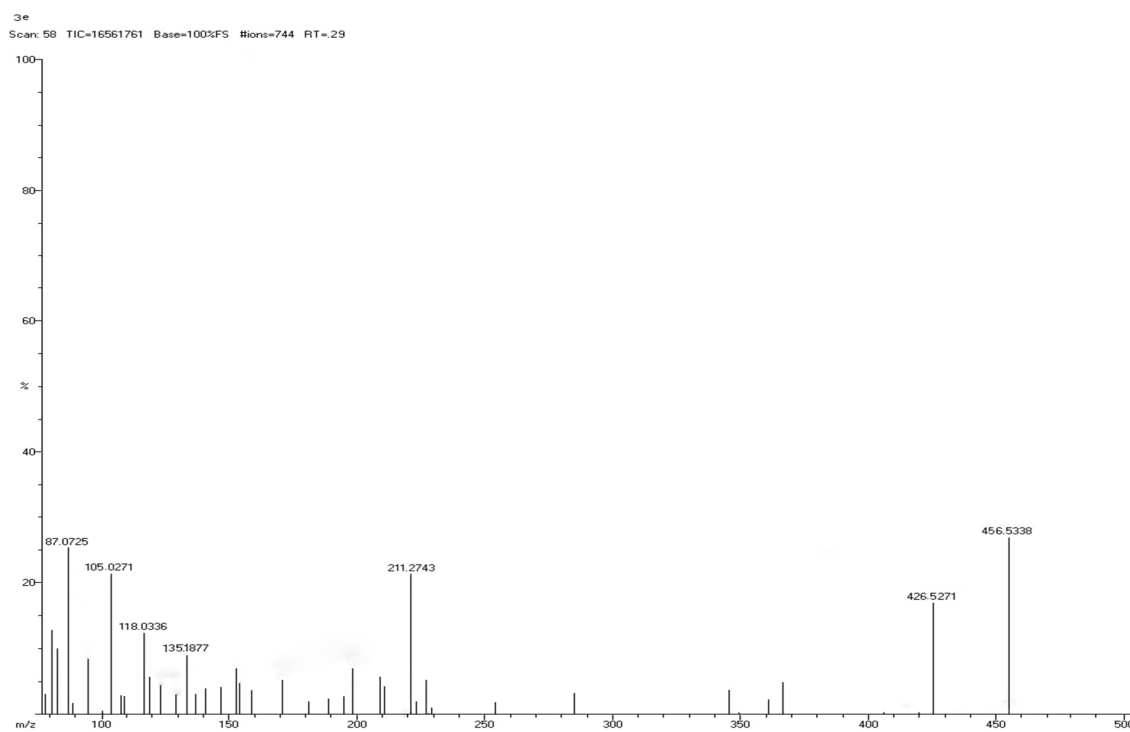


## 4.2. MASS SPECTRUM DETAILS

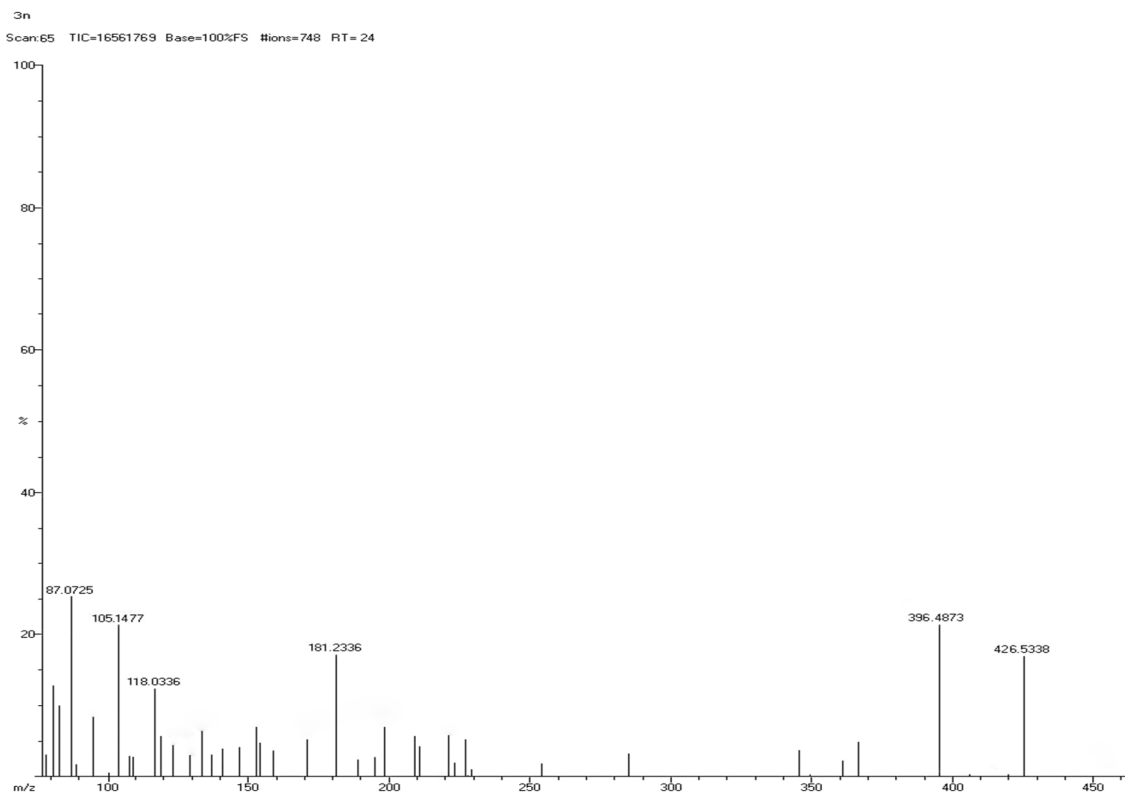
### 4.2.1. Compound 3b



### 4.2.2. Compound 3e



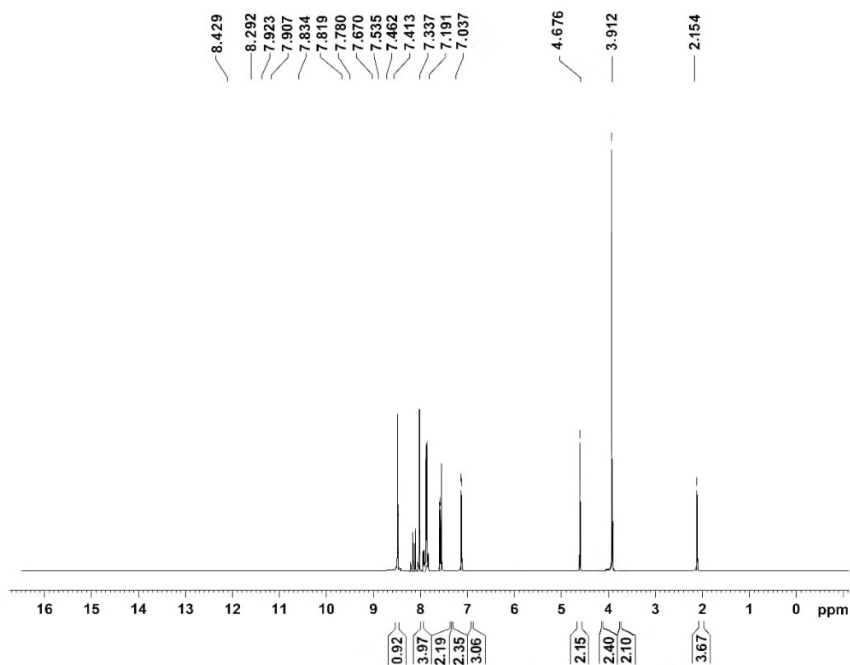
### 4.2.3. Compound 3n



4.3. <sup>1</sup>H NMR SPECTRUM DETAILS

## 4.3.1. Compound 3a

3a



## Current Data Parameters

NAME Jan23-2022  
EXPNO 7  
PROCNO 1

## F2 - Acquisition Parameters

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FIDRES 0.315264 Hz  
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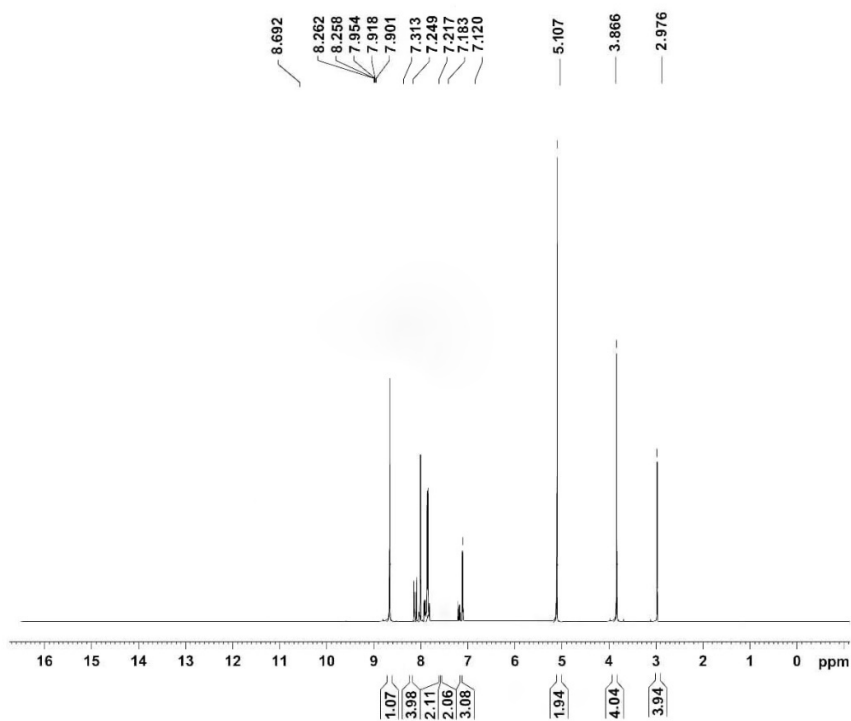
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## F2 - Processing parameters

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## 4.3.2. Compound 3b

3b



## Current Data Parameters

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EXPNO 7  
PROCNO 1

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DE 6.50 usec  
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## CHANNEL f1

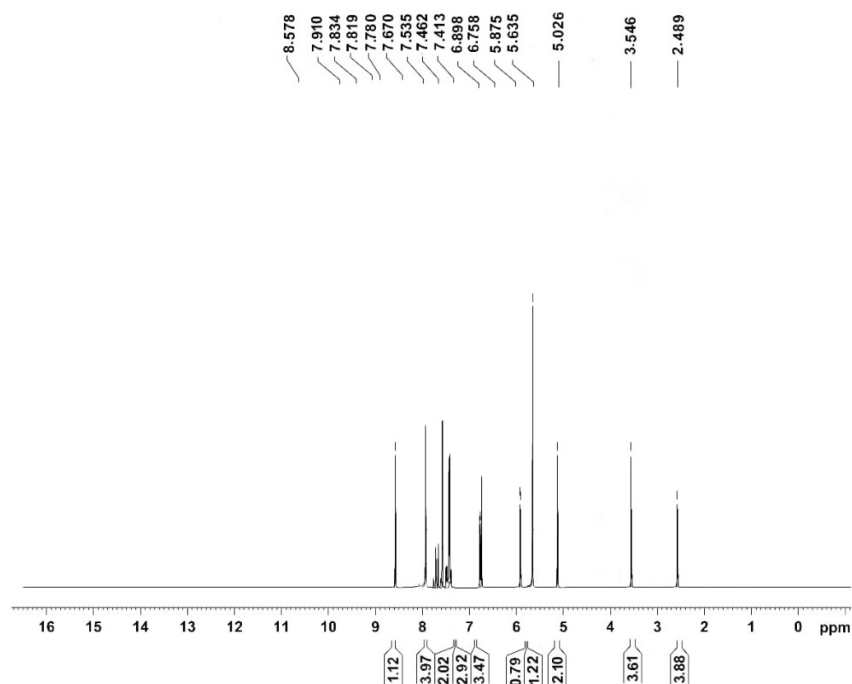
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## F2 - Processing parameters

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### 4.3.3. Compound 3c

3c



Current Data Parameters  
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 PROCNO 1

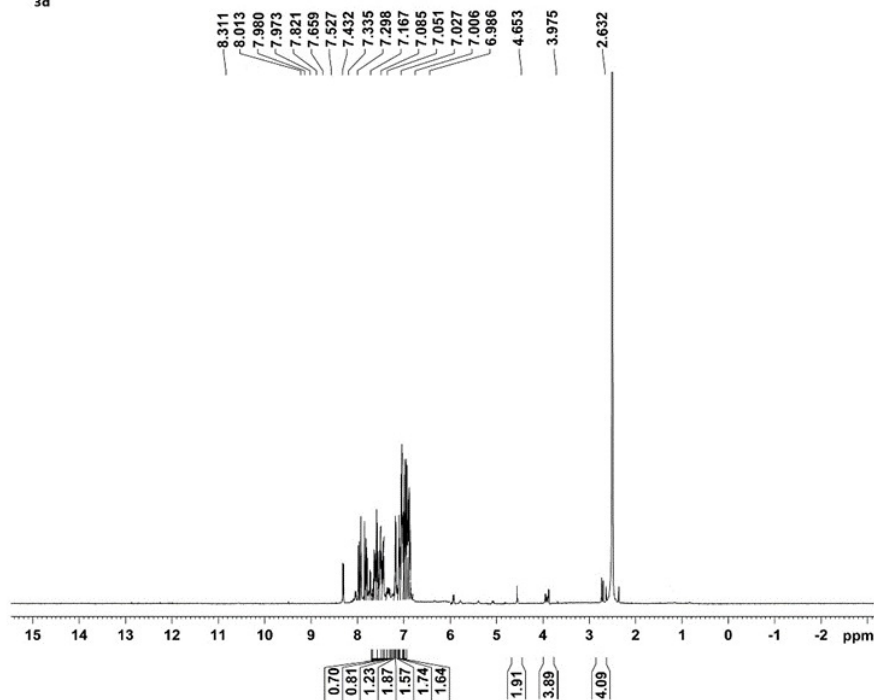
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 FIDRES 0.315264 Hz  
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 DE 6.50 usec  
 TE 296.8 K  
 D1 1.00000000 sec  
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CHANNEL f1  
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F2 - Processing parameters  
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### 4.3.4. Compound 3d

3d



Current Data Parameters  
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 PROCNO 1

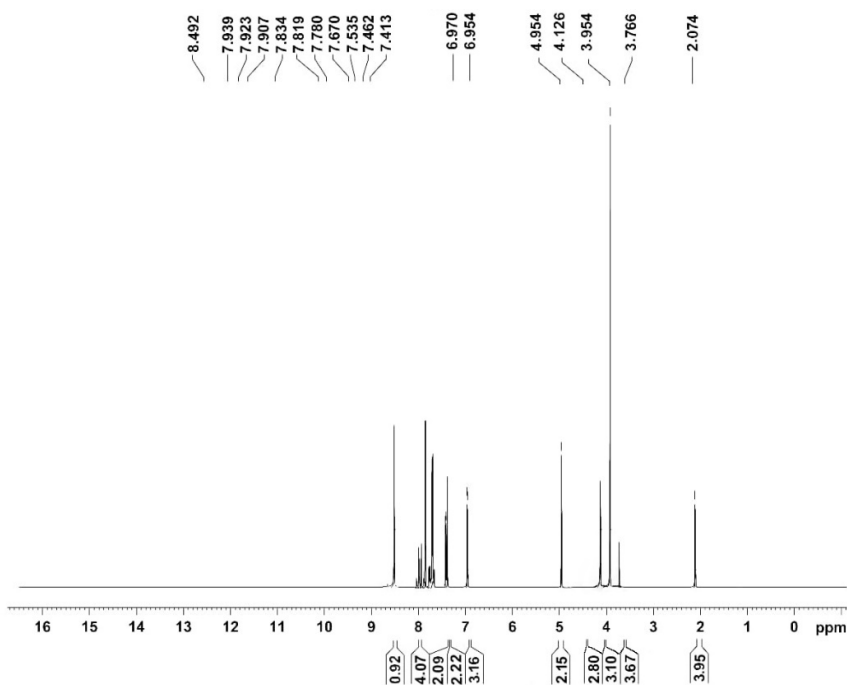
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 SWH 10330.578 Hz  
 FIDRES 0.315264 Hz  
 AQ 1.5859712 sec  
 RG 203  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 296.2 K  
 D1 1.00000000 sec  
 TD0 1

CHANNEL f1  
 NUC1 1H  
 P1 7.95 usec  
 PL1 1.00 dB  
 PL1W 18.69560814 W  
 SFO1 500.1330885 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1300059 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

## 4.3.5. Compound 3e

3e



Current Data Parameters  
 NAME Jan23-2022  
 EXPNO 7  
 PROCNO 1

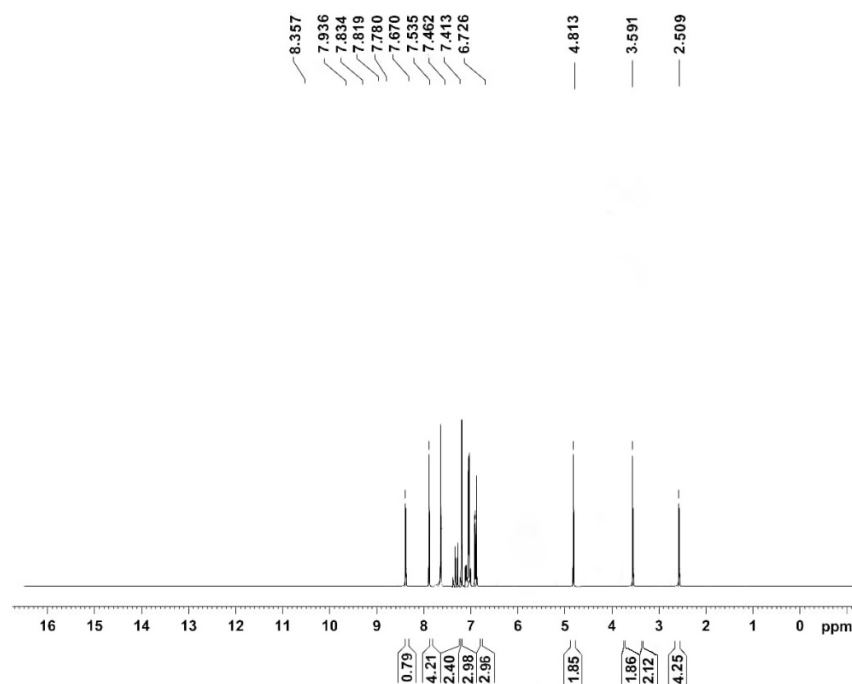
F2 - Acquisition Parameters  
 Date 20220123  
 Time 8.24  
 INSTRUM spect  
 PROBHD 5 mm QXI 1H Z-  
 PULPROG zg30  
 TD 32768  
 SOLVENT DMSO  
 NS 32  
 DS 2  
 SWH 10330.578 Hz  
 FIDRES 0.315264 Hz  
 AQ 1.5859712 sec  
 RG 90.5  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 296.8 K  
 D1 1.00000000 sec  
 TD0 1

CHANNEL f1  
 NUC1 1H  
 P1 7.95 usec  
 PL1 1.00 dB  
 PL1W 18.69560814 W  
 SFO1 500.1330885 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1300059 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

## 4.3.6. Compound 3f

3f



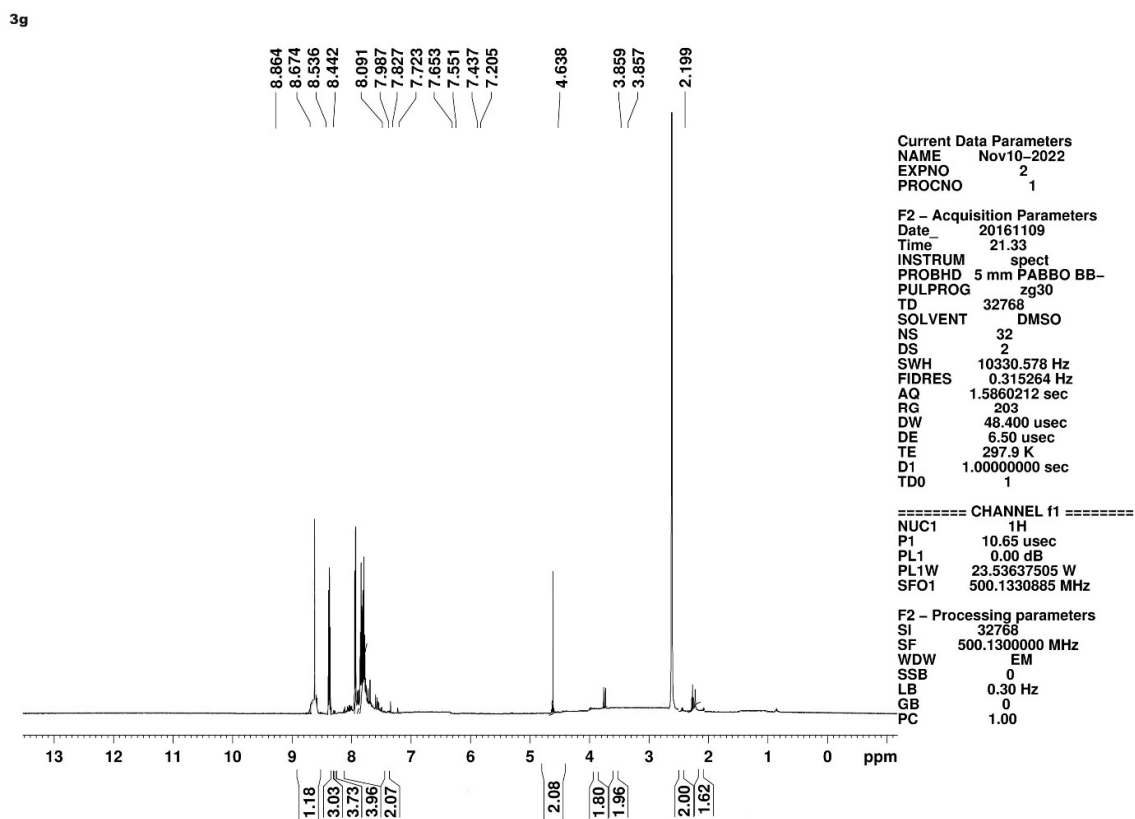
Current Data Parameters  
 NAME Jan23-2022  
 EXPNO 7  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20220123  
 Time 10.27  
 INSTRUM spect  
 PROBHD 5 mm QXI 1H Z-  
 PULPROG zg30  
 TD 32768  
 SOLVENT DMSO  
 NS 32  
 DS 2  
 SWH 10330.578 Hz  
 FIDRES 0.315264 Hz  
 AQ 1.5859712 sec  
 RG 90.5  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 296.8 K  
 D1 1.00000000 sec  
 TD0 1

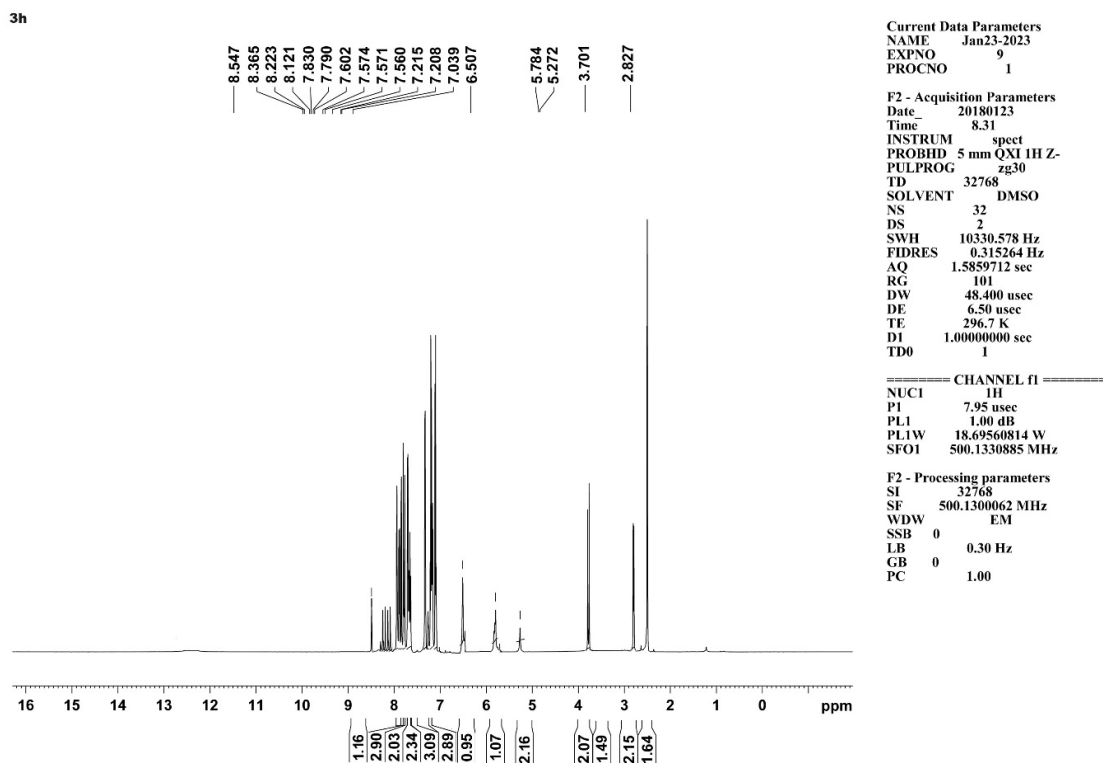
CHANNEL f1  
 NUC1 1H  
 P1 7.95 usec  
 PL1 1.00 dB  
 PL1W 18.69560814 W  
 SFO1 500.1330885 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1300059 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

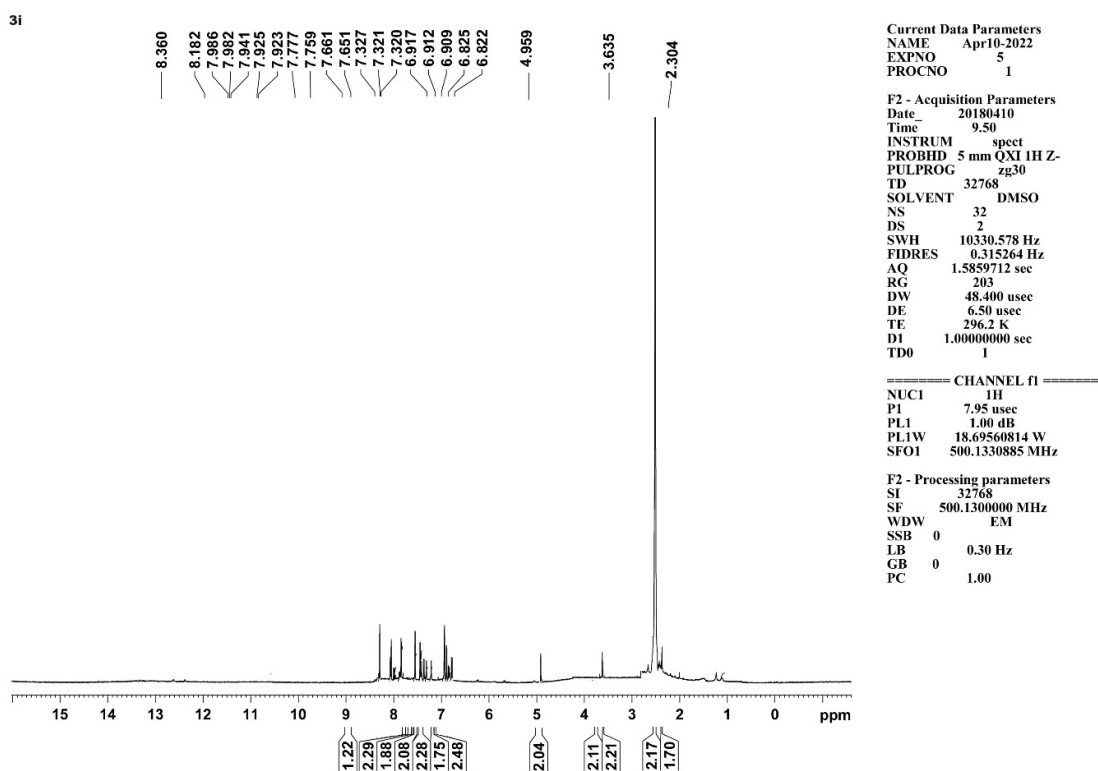
4.3.7. Compound 3g



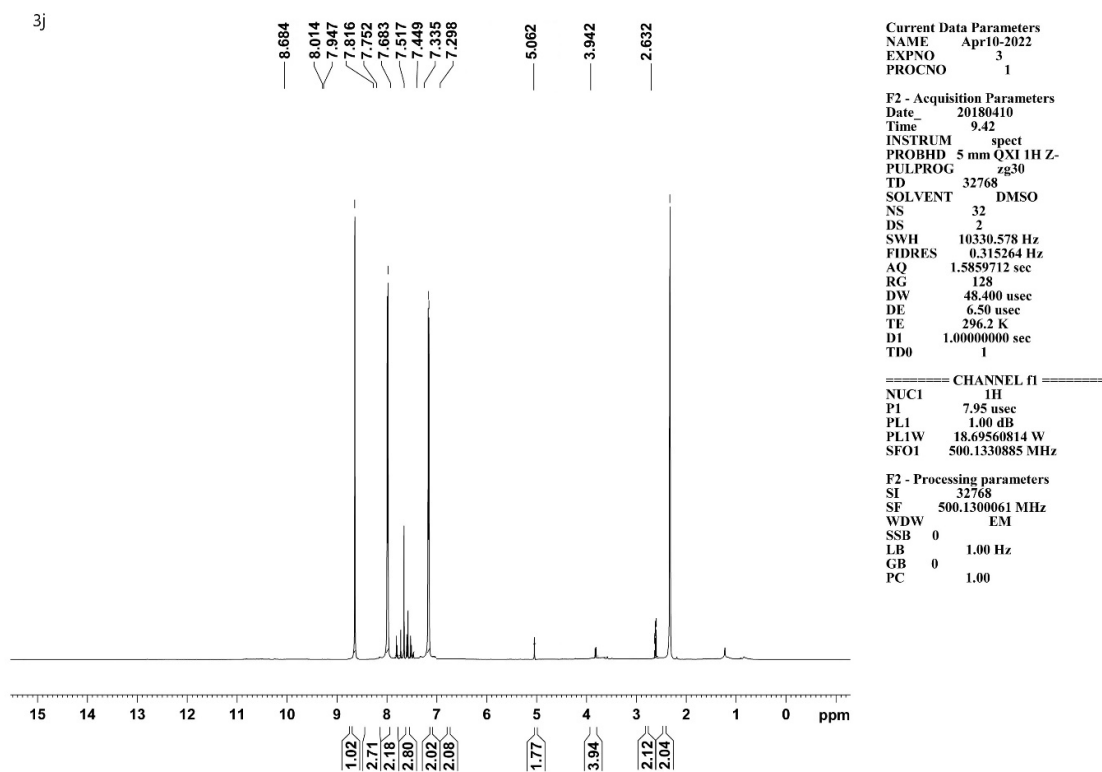
4.3.8. Compound 3h



## 4.3.9. Compound 3i

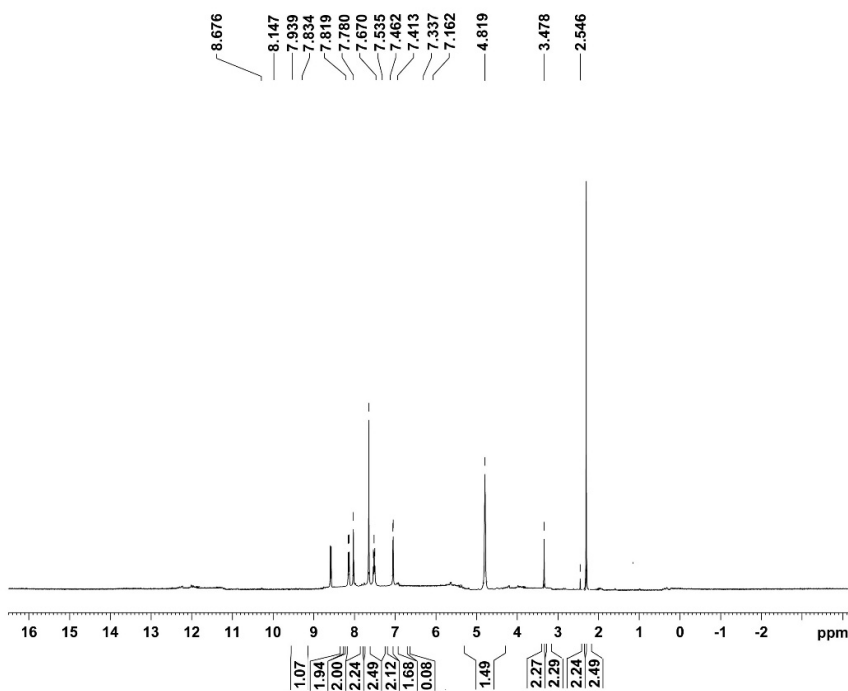


## 4.3.10. Compound 3j



4.3.11. Compound 3k

3k



Current Data Parameters  
 NAME Feb23-2023  
 EXPNO 13  
 PROCNO 1

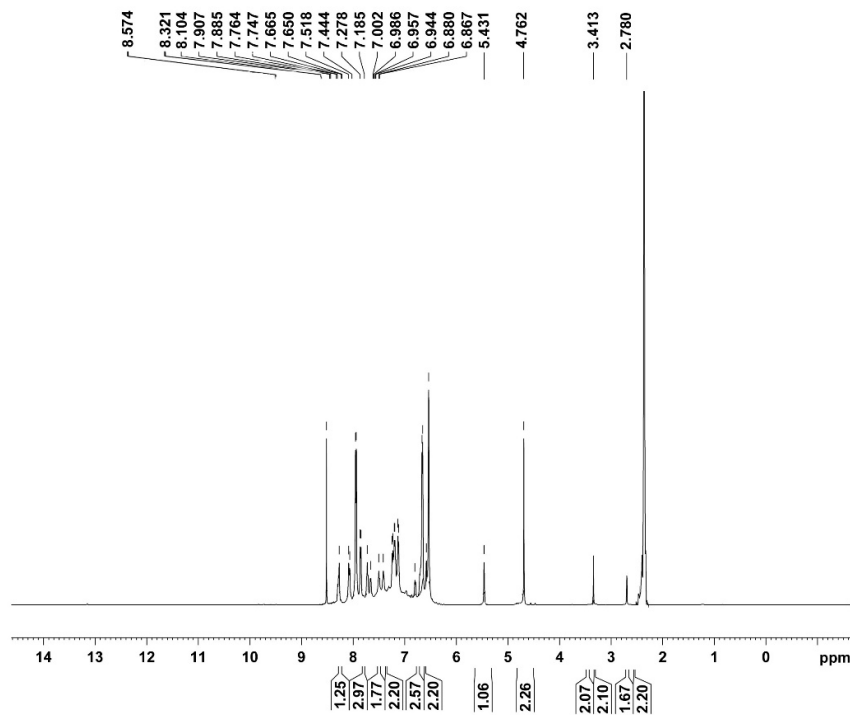
F2 - Acquisition Parameters  
 Date\_ 20230223  
 Time 8.02  
 INSTRUM spect  
 PROBHD 5 mm QXI 1H Z-  
 PULPROG zg30  
 TD 32768  
 SOLVENT DMSO  
 NS 32  
 DS 2  
 SWH 10330.578 Hz  
 FIDRES 0.315264 Hz  
 AQ 1.5859712 sec  
 RG 114  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 296.8 K  
 DI 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.95 usec  
 PL1 1.00 dB  
 PL1W 18.69560814 W  
 SFO1 500.1330885 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1300061 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

4.3.12. Compound 3l

3l



Current Data Parameters  
 NAME Jan23-2023  
 EXPNO 16  
 PROCNO 1

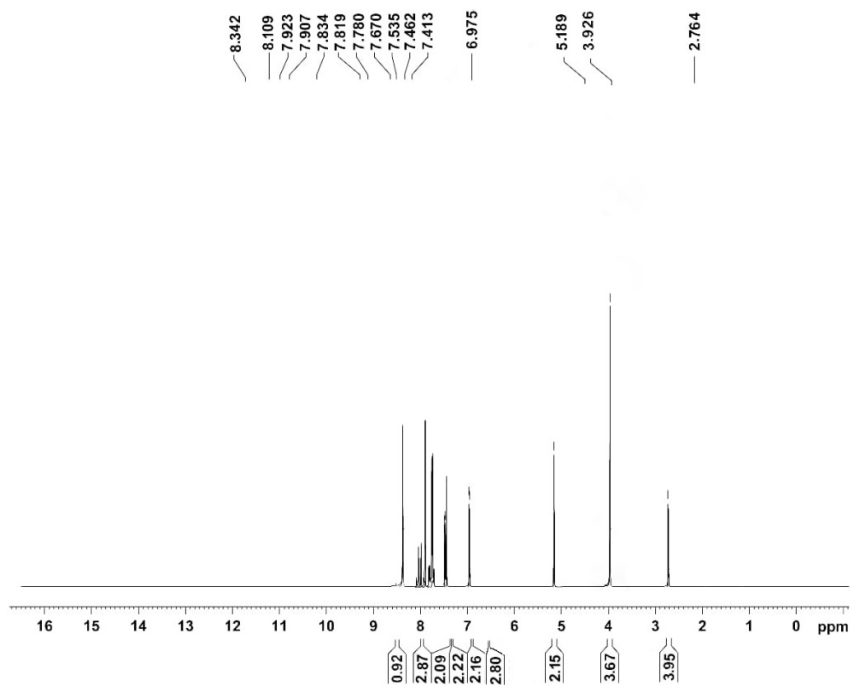
F2 - Acquisition Parameters  
 Date\_ 20230123  
 Time 8.21  
 INSTRUM spect  
 PROBHD 5 mm QXI 1H Z-  
 PULPROG zg30  
 TD 32768  
 SOLVENT DMSO  
 NS 32  
 DS 2  
 SWH 10330.578 Hz  
 FIDRES 0.315264 Hz  
 AQ 1.5859712 sec  
 RG 71.8  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 296.7 K  
 DI 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.95 usec  
 PL1 1.00 dB  
 PL1W 18.69560814 W  
 SFO1 500.1330885 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1300059 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

## 4.3.13. Compound 3m

3m



Current Data Parameters  
 NAME Jan23-2022  
 EXPNO 7  
 PROCNO 1

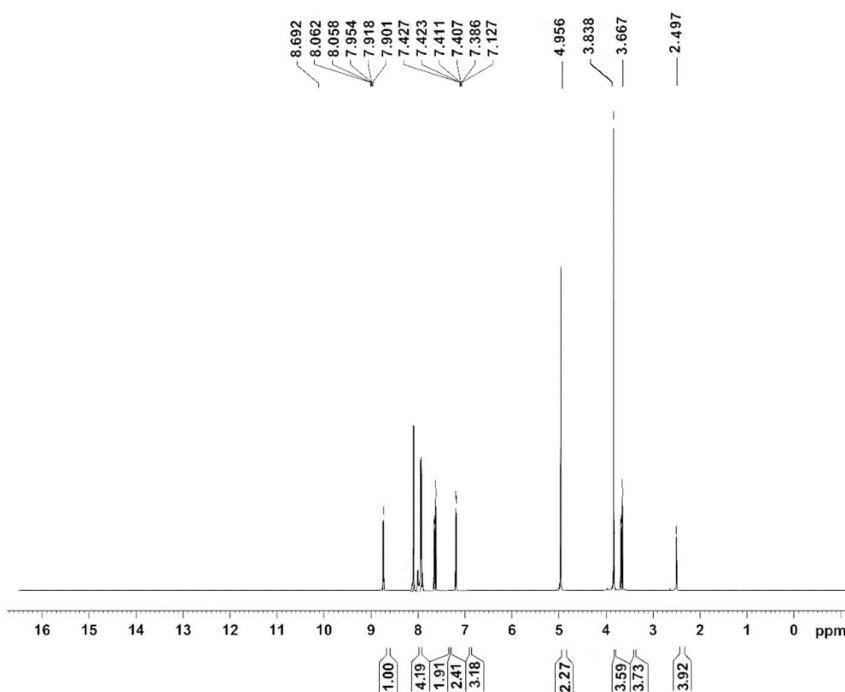
F2 - Acquisition Parameters  
 Date\_ 20220123  
 Time 18.21  
 INSTRUM spect  
 PROBHD 5 mm QXI 1H Z-  
 PULPROG zg30  
 TD 32768  
 SOLVENT DMSO  
 NS 32  
 DS 2  
 SWH 10330.578 Hz  
 FIDRES 0.315264 Hz  
 AQ 1.5859712 sec  
 RG 90.5  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 296.8 K  
 D1 1.00000000 sec  
 TD0 1

CHANNEL f1  
 NUC1 1H  
 P1 7.95 usec  
 PL1 1.00 dB  
 PL1W 18.69560814 W  
 SFO1 500.1330885 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1300059 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

## 4.3.14. Compound 3n

3n



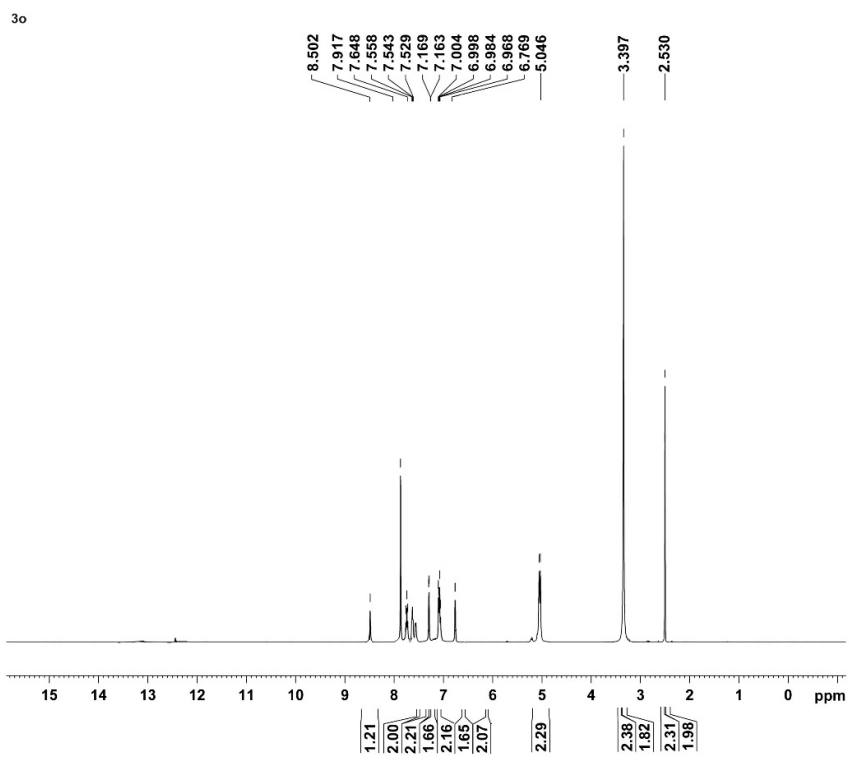
Current Data Parameters  
 NAME Jan23-2022  
 EXPNO 7  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20220123  
 Time 8.24  
 INSTRUM spect  
 PROBHD 5 mm QXI 1H Z-  
 PULPROG zg30  
 TD 32768  
 SOLVENT DMSO  
 NS 32  
 DS 2  
 SWH 10330.578 Hz  
 FIDRES 0.315264 Hz  
 AQ 1.5859712 sec  
 RG 90.5  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 296.8 K  
 D1 1.00000000 sec  
 TD0 1

CHANNEL f1  
 NUC1 1H  
 P1 7.95 usec  
 PL1 1.00 dB  
 PL1W 18.69560814 W  
 SFO1 500.1330885 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1300059 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

4.3.15. Compound 3o



Current Data Parameters  
 NAME Feb06-2023  
 EXPNO 19  
 PROCNO 1

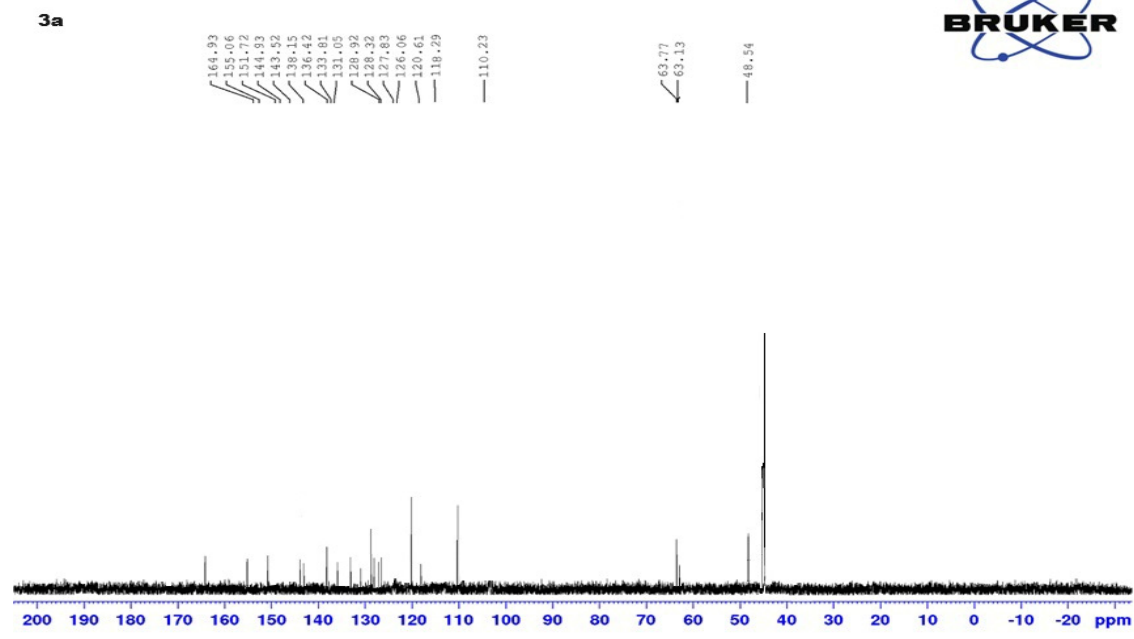
F2 - Acquisition Parameters  
 Date 20230206  
 Time 14.57  
 INSTRUM spect  
 PROBHD 5 mm QXI 1H Z-  
 PULPROG zg30  
 TD 32768  
 SOLVENT DMSO  
 NS 64  
 DS 2  
 SWH 10330.578 Hz  
 FIDRES 0.315264 Hz  
 AQ 1.5859712 sec  
 RG 203  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 295.9 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.95 usec  
 PL1 1.00 dB  
 PL1W 18.69560814 W  
 SFO1 500.1330885 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1300058 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

4.4. <sup>13</sup>CNMR SPECTRUM DETAILS

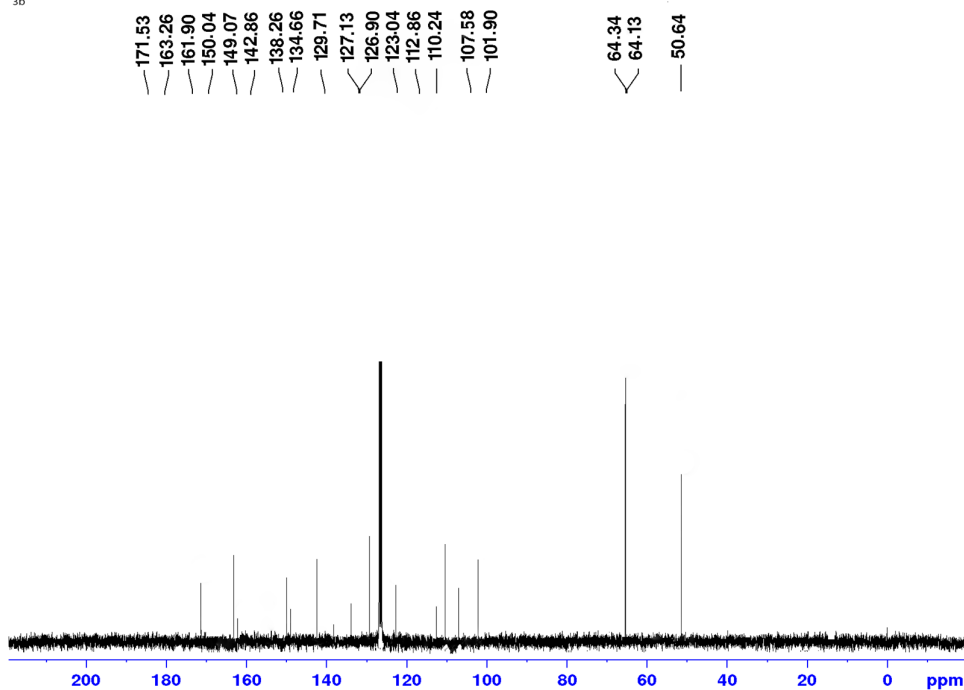
4.4.1. Compound 3a



## 4.4.2. Compound 3b

Signature SIF VIT VELLORE

3b



BRUKER

```

Current Data Parameters
NAME          SBST140819
EXPNO         1
PROCNO       1

F2 - Acquisition Parameters
Date_        20220814
Time         22:09 h
INSTRUM      spect
PROBHD       z108618_0505
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           512
DS           4
SWH          24038.461 Hz
FIDRES       0.733596 Hz
AQ           1.3621888 sec
RG           175.97
DW           20.800 usec
DE           6.50 usec
TE           304.6 K
D1           2.0000000 sec
D11          0.0300000 sec
TD0          1
SFO1         100.6550186 MHz
NUC1         13C
P1           9.80 usec
PLM1         58.0000000 W
SFO2         400.2596010 MHz
NUC2         1H
CPDPRG2      waltz16
PCPD2        90.00 usec
PLW2         16.0000000 W
PLM12        0.38716000 W
PLM13        0.19474000 W

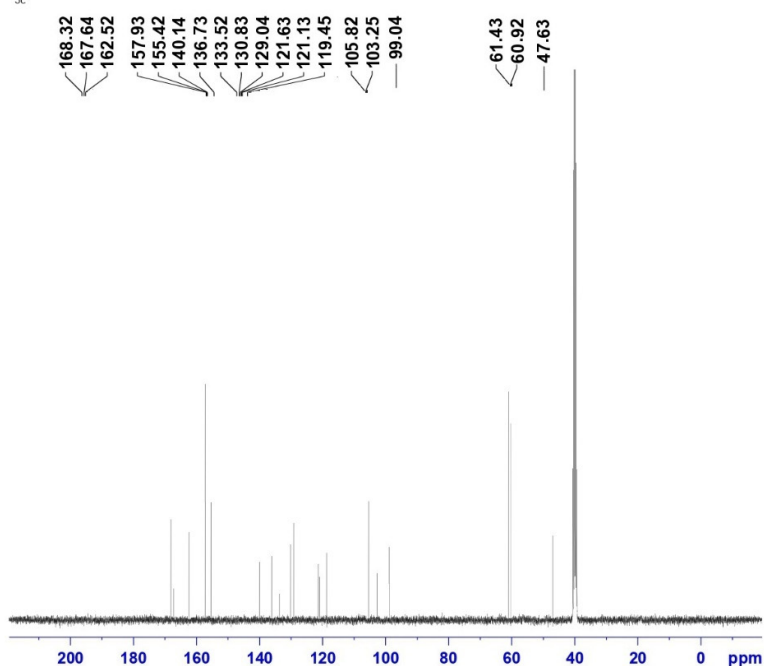
F2 - Processing parameters
SI           32768
SF           100.6449542 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40

```

## 4.4.3. Compound 3c

Signature SIF VIT VELLORE

3c



BRUKER

```

Current Data Parameters
NAME          SBST010719
EXPNO         16
PROCNO       1

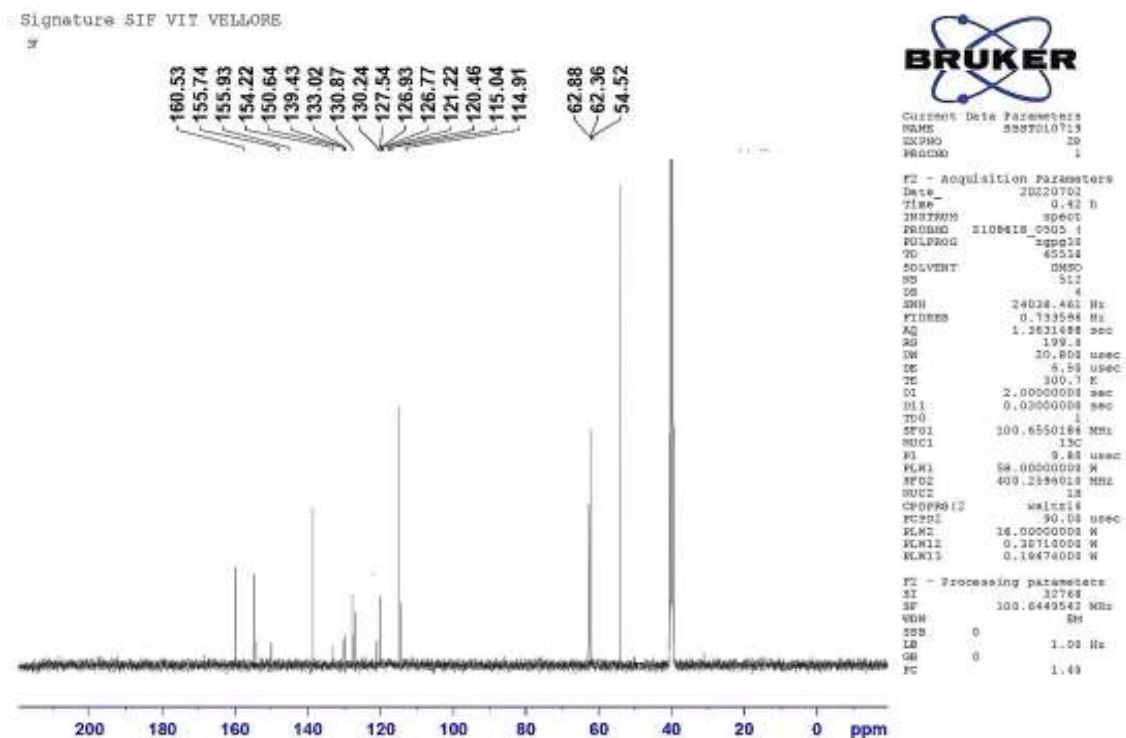
F2 - Acquisition Parameters
Date_        20220701
Time         13:33 h
INSTRUM      spect
PROBHD       z108618_0505
PULPROG      zgpg30
TD           65536
SOLVENT      DMSO
NS           512
DS           4
SWH          24038.461 Hz
FIDRES       0.733596 Hz
AQ           1.3621888 sec
RG           156.91
DW           20.800 usec
DE           6.50 usec
TE           300.8 K
D1           2.0000000 sec
D11          0.0300000 sec
TD0          1
SFO1         100.6550186 MHz
NUC1         13C
P1           9.80 usec
PLM1         58.0000000 W
SFO2         400.2596010 MHz
NUC2         1H
CPDPRG2      waltz16
PCPD2        90.00 usec
PLW2         16.0000000 W
PLM12        0.38716000 W
PLM13        0.19474000 W

F2 - Processing parameters
SI           32768
SF           100.6449542 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40

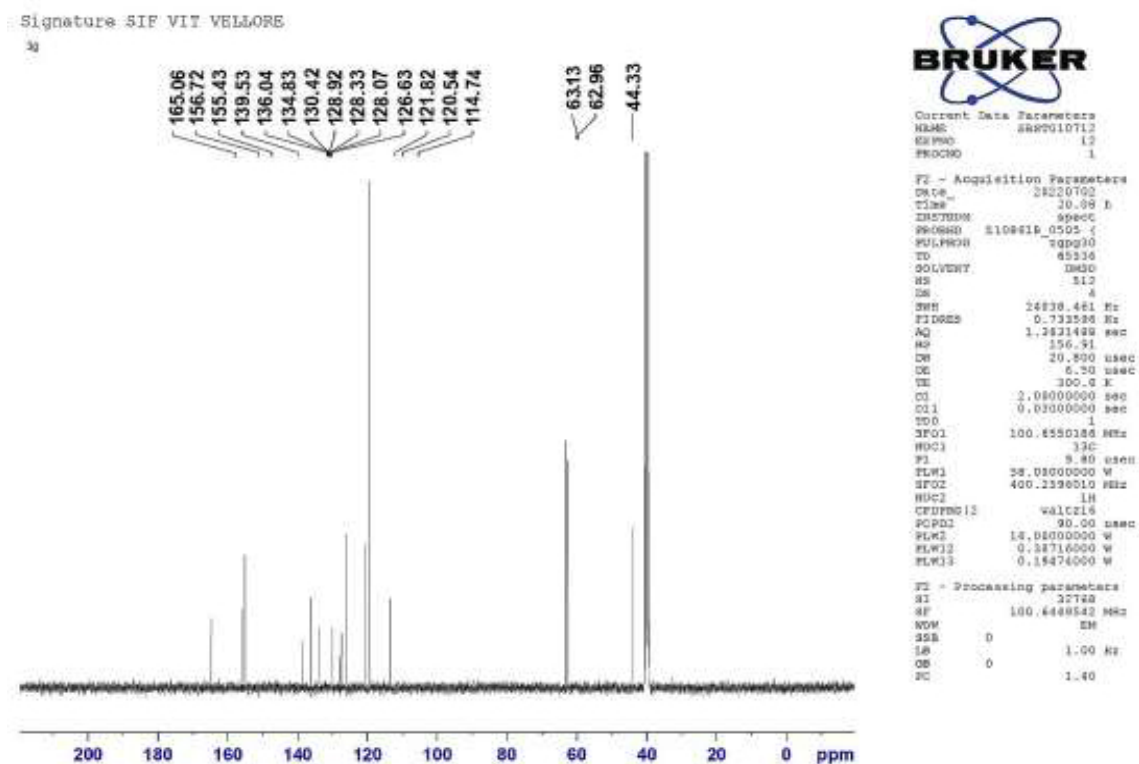
```



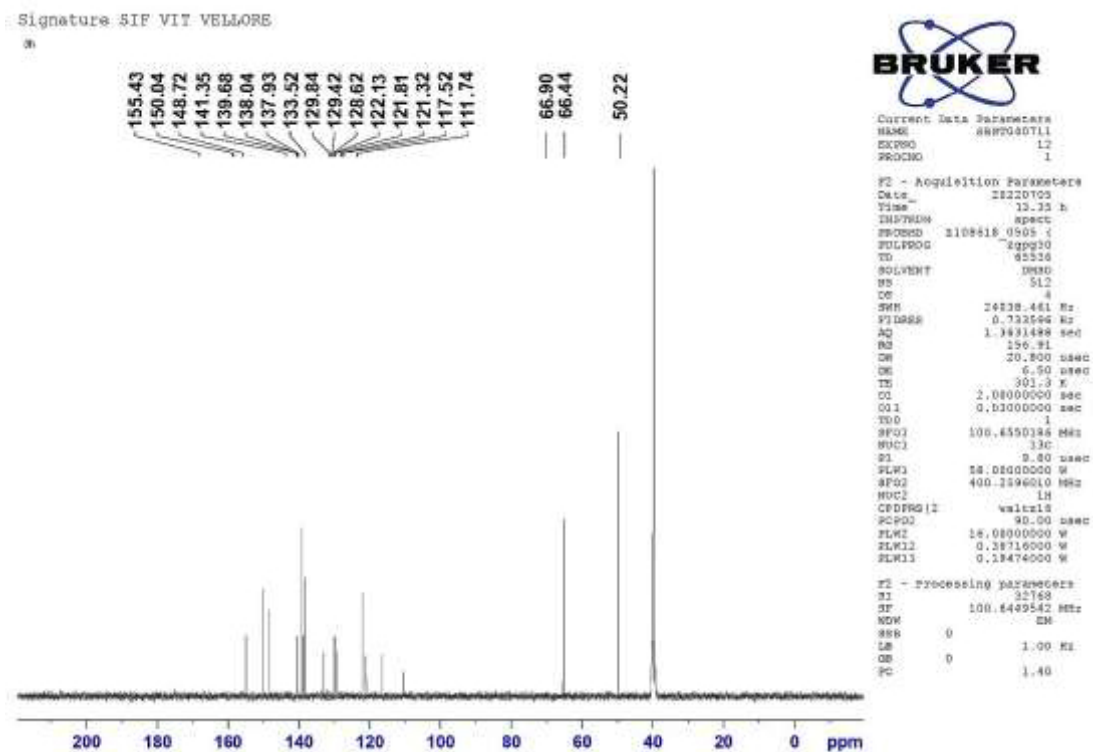
4.4.6. Compound 3f



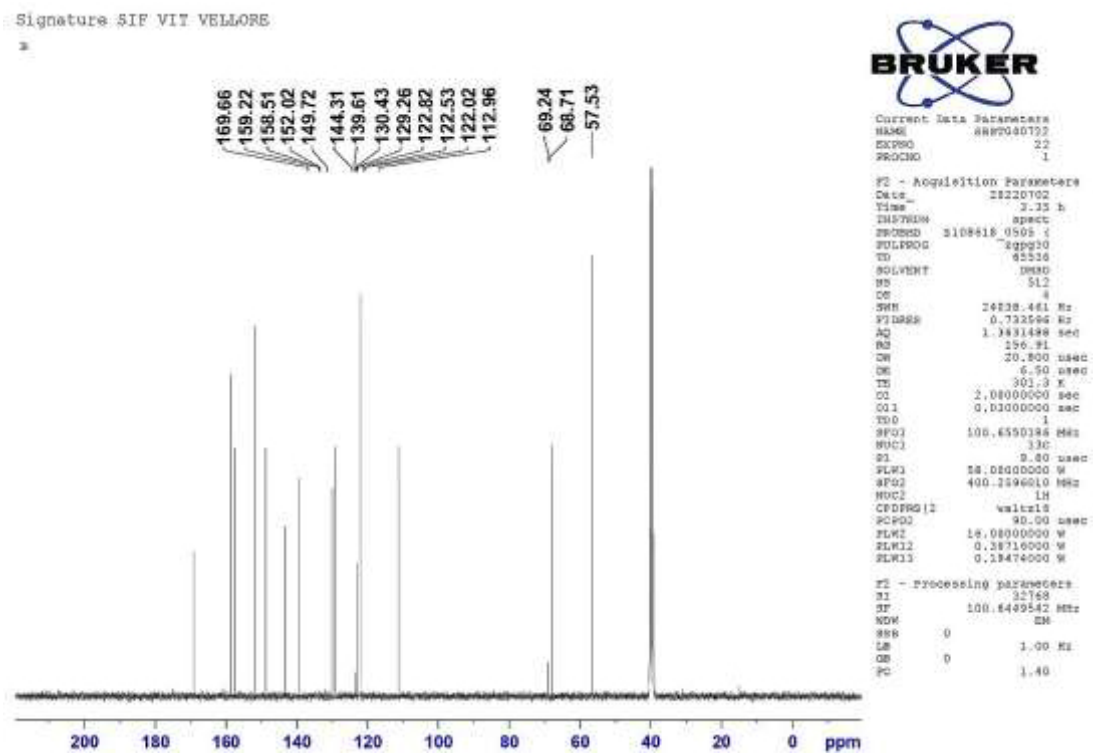
4.4.7. Compound 3g



4.4.8. Compound 3h



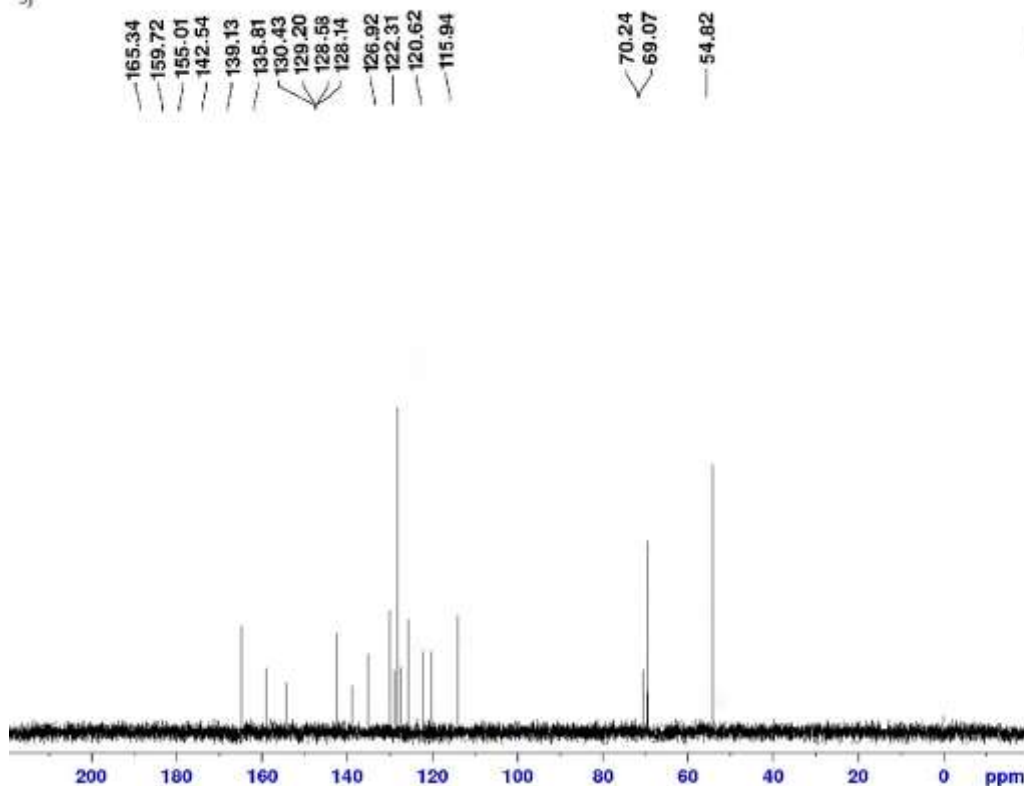
4.4.9. Compound 3i



4.4.10. Compound 3j

Signature SIF VIT VELLORE

3j



**BRUKER**

```

Current Data Parameters
NAME      20220313
EXPNO     1
PROCNO    1

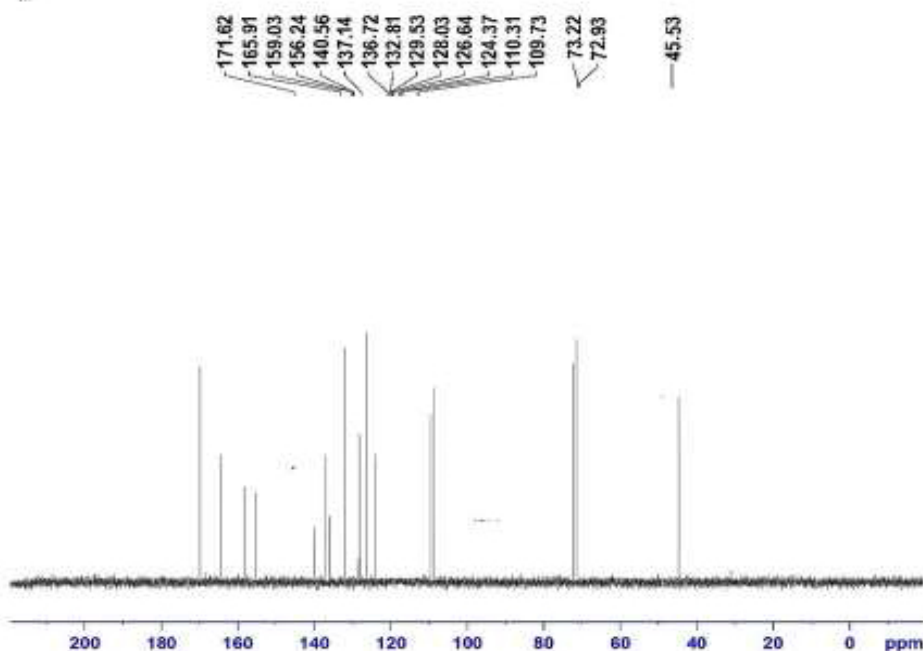
F2 - Acquisition Parameters
Date_     20220313
Time     14.35 h
INSTRUM   spect
PROBHD    E3041L-5531-C
PULPROG   zgpg30
TD        65538
SOLVENT   DMSO
NS        4
DS        4
SWH       24038.461 Hz
FIDRES    0.733588 Hz
AQ        1.3431468 sec
RG        199.4
OR        20.803 usec
SC        4.54 usec
DE        300.7 Hz
DI        2.0000000 sec
D11       0.0200000 sec
ZG0       1
SFO1      100.628168 MHz
NUC1      13C
PI        9.88 usec
PLM1     98.0000000 W
SFO2      400.254018 MHz
NUC2      13
CPDPRG2   waltz16
PCPD2     30.03 usec
PLM2     34.0000000 W
PLM3     0.2871000 W
SFM3     0.1947400 W

F2 - Processing parameters
SI        32768
SF        100.6449542 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.60
    
```

4.4.11. Compound 3k

Signature SIF VIT VELLORE

\*



**BRUKER**

```

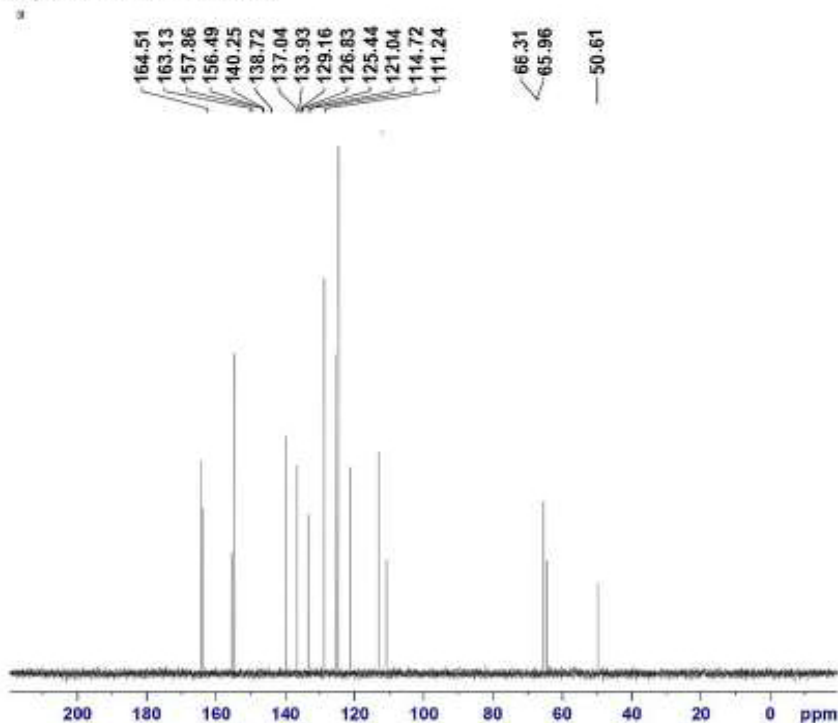
Current Data Parameters
NAME      20220707
EXPNO     21
PROCNO    1

F2 - Acquisition Parameters
Date_     20220707
Time     20.42 h
INSTRUM   spect
PROBHD    E108618-25015-1
PULPROG   zgpg30
TD        65538
SOLVENT   DMSO
NS        4
DS        4
SWH       24038.461 Hz
FIDRES    0.733588 Hz
AQ        1.3431468 sec
RG        199.4
OR        20.803 usec
SC        4.54 usec
DE        300.7 Hz
DI        2.0000000 sec
D11       0.0200000 sec
ZG0       1
SFO1      100.628168 MHz
NUC1      13C
PI        9.88 usec
PLM1     98.0000000 W
SFO2      400.254018 MHz
NUC2      13
CPDPRG2   waltz16
PCPD2     30.03 usec
PLM2     34.0000000 W
PLM3     0.2871000 W
SFM3     0.1947400 W

F2 - Processing parameters
SI        32768
SF        100.6449542 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.60
    
```

4.4.12. Compound 3l

Signature SIF VII VELLORE



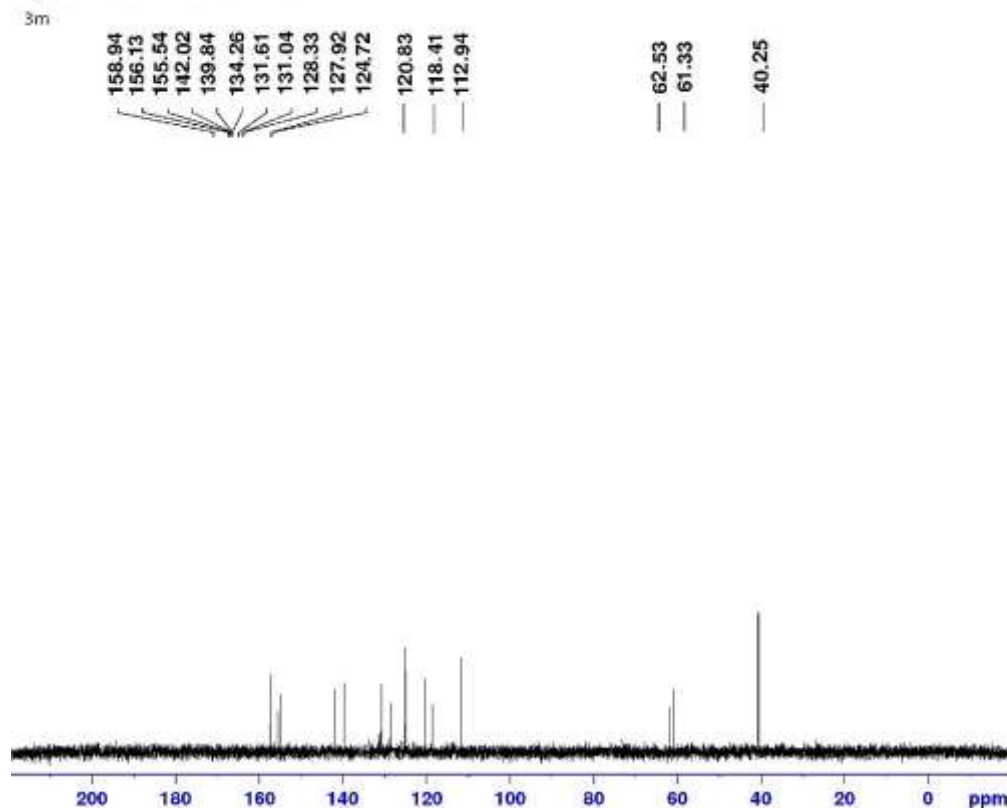
Current Data Parameters  
 NAME: 282010714  
 EXPNO: 14  
 PROCNO: 1

F2 - Acquisition Parameters  
 Date\_ : 28220703  
 Time : 23.33 h  
 INSTRUM : spect  
 PROBR0 : E108E18.0505 ( :  
 PULPROG : zgpg30  
 TD : 65536  
 SOLVENT : DMSO  
 NS : 512  
 DS : 4  
 SWH : 24838.461 Hz  
 FIDRES : 0.733588 Hz  
 AQ : 1.7331488 sec  
 RG : 156.91  
 CW : 20.800 usec  
 CC : 6.50 usec  
 CB : 300.0 K  
 CI : 2.08000000 sec  
 CO1 : 0.03000000 sec  
 TO : 1  
 FFO1 : 100.6250188 MHz  
 HPC1 : 13C  
 W1 : 9.80 usec  
 FLW1 : 38.03000000 W  
 FFO2 : 400.2530010 MHz  
 HPC2 : 1H  
 CPDPRG2 : waltz16  
 PCPD2 : 90.00 usec  
 PLW2 : 18.08000000 W  
 PLW12 : 0.38716000 W  
 PLW13 : 0.15474000 W

F2 - Processing parameters  
 SI : 32768  
 SF : 100.6250188 MHz  
 RG : 328  
 ASB : 0  
 LB : 1.00 Hz  
 GB : 0  
 PC : 1.40

4.4.13. Compound 3m

Signature SIF VII VELLORE



Current Data Parameters  
 NAME: 282140015  
 EXPNO: 14  
 PROCNO: 1

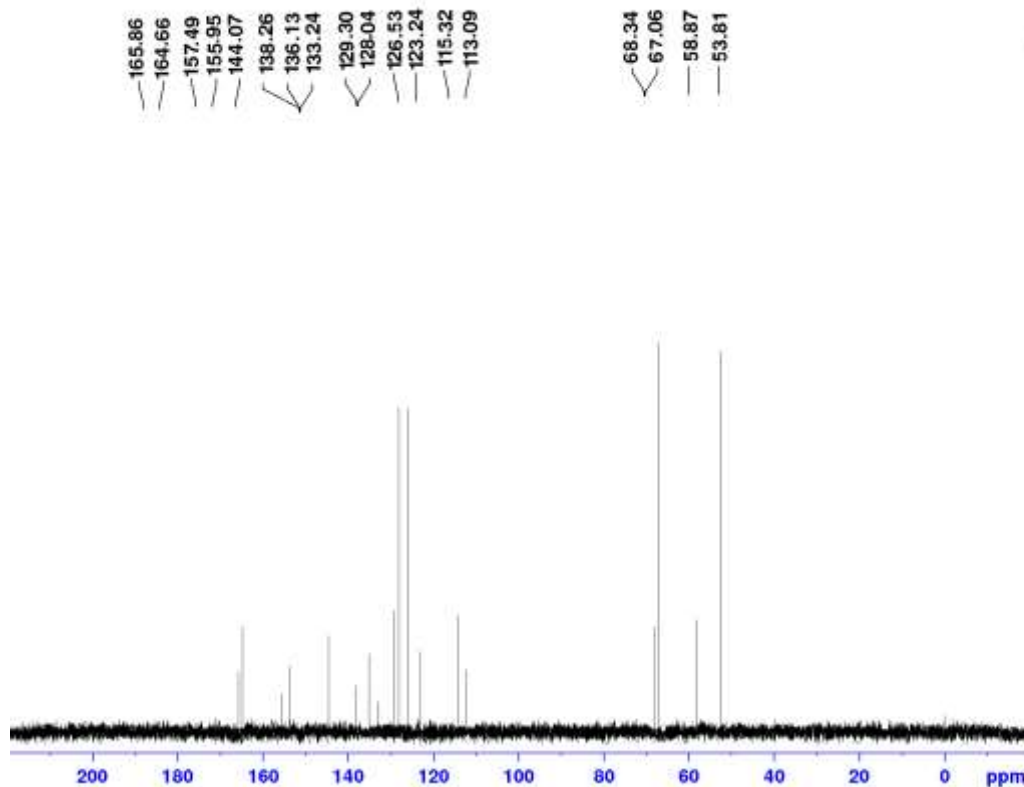
F2 - Acquisition Parameters  
 Date\_ : 28220715  
 Time : 1.13 h  
 INSTRUM : spect  
 PROBR0 : E108E18.0505 ( :  
 PULPROG : zgpg30  
 TD : 65536  
 SOLVENT : DMSO  
 NS : 512  
 DS : 4  
 SWH : 24838.461 Hz  
 FIDRES : 0.733588 Hz  
 AQ : 1.7331488 sec  
 RG : 156.91  
 CW : 20.800 usec  
 CC : 6.50 usec  
 CB : 300.0 K  
 CI : 2.08000000 sec  
 CO1 : 0.03000000 sec  
 TO : 1  
 FFO1 : 100.6250188 MHz  
 HPC1 : 13C  
 W1 : 9.80 usec  
 FLW1 : 38.03000000 W  
 FFO2 : 400.2530010 MHz  
 HPC2 : 1H  
 CPDPRG2 : waltz16  
 PCPD2 : 90.00 usec  
 PLW2 : 18.08000000 W  
 PLW12 : 0.38716000 W  
 PLW13 : 0.15474000 W

F2 - Processing parameters  
 SI : 32768  
 SF : 100.6250188 MHz  
 RG : 328  
 ASB : 0  
 LB : 1.00 Hz  
 GB : 0  
 PC : 1.40

4.4.14. Compound 3n

Signature SIF VIT VELLORE

3n



```

Current Data Parameters
NAME      080714019
EXPNO    1
PROCNO   1

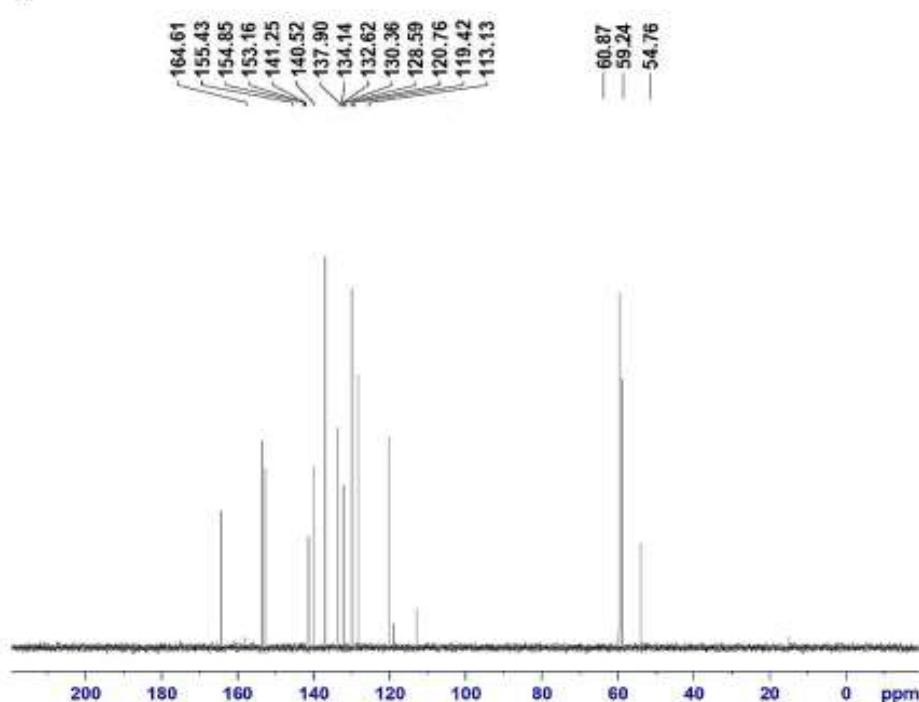
F2 - Acquisition Parameters
Date_    20220719
Time     22:58 h
INSTRUM  spect
PROBHD   E146H1.5AS1
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        512
DS        4
SWH       26970.461 Hz
FIDRES    0.733596 Hz
AQ        1.3812488 sec
RG        172.87
SR        27.870 usec
DE        6.70 usec
TE        301.2 K
O1        3.0000000 sec
O2        0.0300000 sec
TDS       1
SFO1      100.6261286 MHz
NUC1       13C
P1         9.80 usec
PL1       00.0000000 W
SFO2      400.2539910 MHz
NUC2       1H
PCPDPRG12 veltz14
SCPD2     30.00 usec
PLM1      14.0000000 W
PLM2      0.38716000 W
PLM3      0.19474000 W

F2 - Processing parameters
SI        32768
SF        100.6261286 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
    
```

4.4.15. Compound 3o

Signature SIF VIT VELLORE

3o



```

Current Data Parameters
NAME      080700186
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20220709
Time     15:35 h
INSTRUM  spect
PROBHD   E146H1.5AS1
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        512
DS        4
SWH       26970.461 Hz
FIDRES    0.733596 Hz
AQ        1.3812488 sec
RG        172.87
SR        27.870 usec
DE        6.70 usec
TE        301.2 K
O1        3.0000000 sec
O2        0.0300000 sec
TDS       1
SFO1      100.6261286 MHz
NUC1       13C
P1         9.80 usec
PL1       00.0000000 W
SFO2      400.2539910 MHz
NUC2       1H
PCPDPRG12 veltz14
SCPD2     30.00 usec
PLM1      14.0000000 W
PLM2      0.38716000 W
PLM3      0.19474000 W

F2 - Processing parameters
SI        32768
SF        100.6261286 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
    
```

4.5. Selected Images for Anti-microbial Activity

