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Supporting Information

An efficient and mild oxidative amidation of aldehydes using $B(C_6F_5)_3$ as catalyst and biological evaluation of products as potential antimicrobial agents

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Spectral data

1. 4-((1-phenylethyl)carbomyl)phenyl acetate (**3m**): White solid, mp 140-143 °C; IR (KBr) ν_{max} 3322, 2981, 1758, 1633, 1368, 1195, 1012, 877, 765, 592 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 7.78 (d, J = 8.6 Hz, 2H), 7.39 – 7.32 (m, 4H), 7.28 (dd, J = 5.3, 3.2 Hz, 1H), 7.14 (d, J = 8.6 Hz, 2H), 6.29 (bs, 1H), 5.31 (m, 1H), 2.30 (s, 3H), 1.58 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 169.0, 165.6, 152.9, 142.9, 132.1, 128.7, 128.3, 127.4, 126.2, 121.7, 49.2, 21.6, 21.0; HRMS-ESI: m/z $[M+H]^+$ for calculated $C_{17}H_{17}NO_3^+$ $[M+H]^+$: 284.1281; found: 284.1284
2. *Tert*-butyl (3-(4-phenylpiperazine-1-carbonyl)bicyclo[2.2.1]hept-5-en-2-yl)carbamate (**3n**): White solid, mp 181-184 °C; IR (KBr) ν_{max} 3315, 2973, 1697, 1598, 1338, 1275, 1157, 980, 726, 563 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 7.28 (2H, d, J = 7.8 Hz), 6.98-6.85 (3H, m), 6.26 – 6.20 (2H, m), 4.84 (1H, d, J = 10.5 Hz), 4.03 (1H, t, J = 9.4 Hz), 3.91 – 3.70 (2H, m), 3.67-3.53 (2H, m), 3.25 – 3.16 (2H, m), 3.14 – 3.06 (2H, m), 2.97 (1H, s), 2.77 (1H, d, J = 8.4 Hz), 2.72 (1H, s), 2.01 (1H, d, J = 9.3 Hz), 1.66 (1H, d, J = 9.3 Hz), 1.36 (9H, s); ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.6, 155.2, 139.5, 137.2, 129.2, 116.5, 79.5, 52.4, 49.5, 48.6, 45.6, 45.4, 45.1, 44.7, 41.6, 28.4. HRMS-ESI: m/z $[M+H]^+$ for calculated $C_{23}H_{31}N_3O_3^+$ $[M+H]^+$: 398.2438; found: 398.2440.

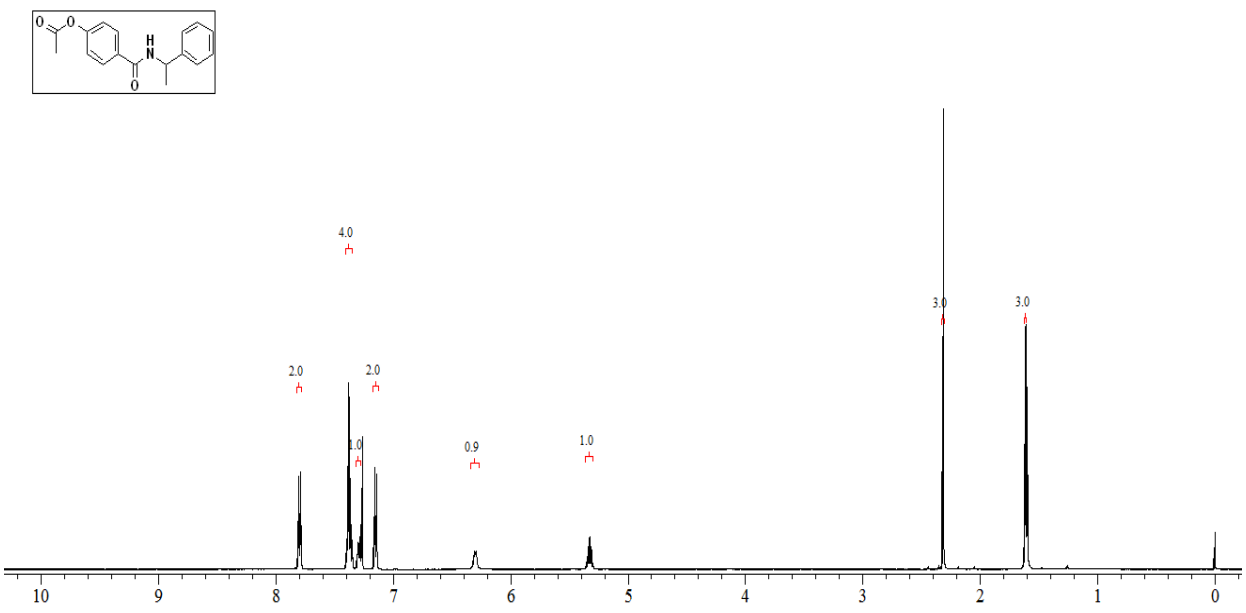
3. *Tert*-butyl (3-(m-tolylcarbamoyl)bicyclo[2.2.1]hept-5-en-2-yl)carbamate (**3o**): White solid, mp 191-194 °C; IR (KBr) ν_{max} 3320, 2973, 1670, 1612, 1455, 1351, 1199,980, 899, 706, 571 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 7.51 (1H, s), 7.38 – 7.34 (1H, m), 7.28 – 7.26 (1H, m), 7.15 (1H, t, J = 7.8 Hz), 6.88 (1H, d, J = 7.4 Hz), 6.25 – 6.17 (2H, m), 4.99 (1H, d, J = 9.1 Hz), 3.98 (1H, t, J = 8.7 Hz), 3.08 (1H, s), 2.71 (1H, s), 2.51 (1H, d, J = 8.1 Hz), 2.30 (3H, s), 2.07 (1H, d, J = 9.2 Hz), 1.66 – 1.63 (1H, m), 1.25 (9H, s); ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.3, 156.2, 139.0, 138.6, 137.8, 137.2, 128.6, 124.8, 120.4, 116.9, 79.7, 53.3, 49.5, 47.9, 45.3, 45.1, 28.2, 21.4; HRMS-ESI: m/z $[M+H]^+$ for calculated $C_{20}H_{26}N_2O_3^+$ $[M+H]^+$: 343.2016; found: 343.2019.

4. (4-(1*H*-imidazol-1-yl)phenyl)(piperidin-1-yl)methanone (**3p**): Creamish white solid, mp 117-120 °C; IR (KBr) ν_{max} 3129, 2942, 2856, 1577,1469, 1105, 1002, 960, 825, 763, 630, 533 cm^{-1}; ^1H NMR (500 MHz, $CDCl_3$) δ 7.97 (1H, bs), 7.52 (2H, d, J = 8.4 Hz), 7.43 (2H, d, J = 8.4 Hz), 7.30 (1H, s), 7.23 (1H, s), 3.71 (2H, bs), 3.36 (2H, m), 1.69 (4H, m),

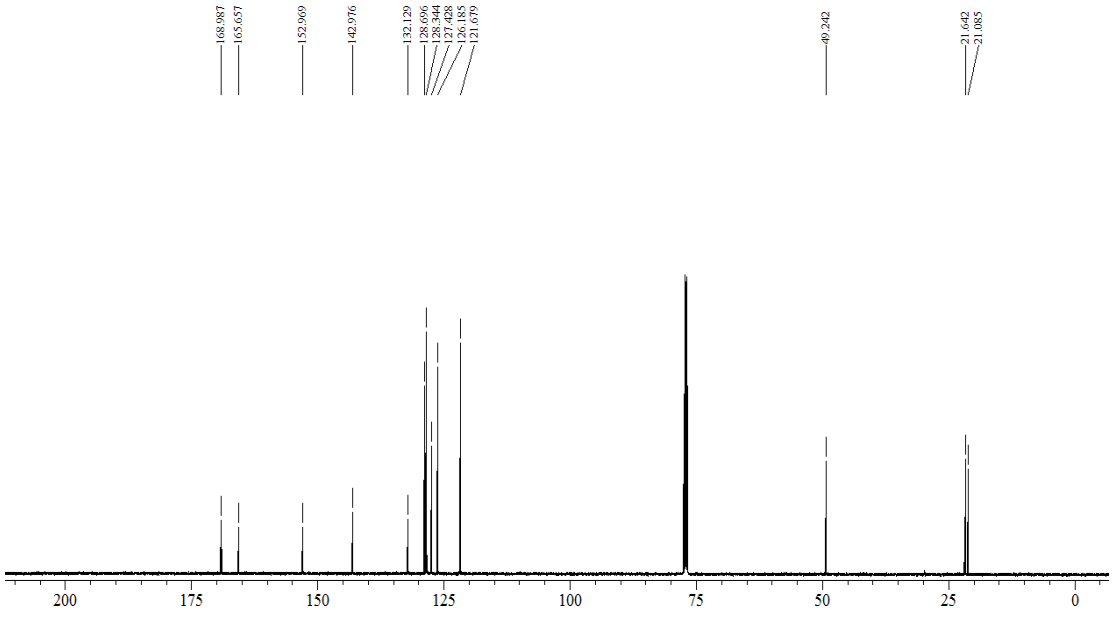
1.54 (2H, m); ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.8, 137.8, 135.5, 135.3, 130.5, 128.6, 121.1, 117.9, 48.7, 43.1, 26.4, 25.4, 24.4; HRMS-ESI: m/z $[M+H]^+$ for calculated $C_{15}H_{17}N_3O^+$ $[M+H]^+$: 256.1444; found: 256.1447.

5. (4-phenylthiophen-2-yl)(piperidi-1-yl)methanone (**3s**): White solid, mp 97-100 °C; IR (KBr) ν_{max} 3071, 2941, 2852, 1602, 1216, 1048, 997, 806, 665, 532 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (1H, bs), 7.54 (1H, s), 7.51 (2H, d, J = 5.5 Hz), 7.40 (2H, t, J = 7.6 Hz), 7.30 (1H, t, J = 7.1 Hz), 3.71 – 3.67 (4H, m), 1.73 – 1.67 (2H, m), 1.66 – 1.62 (4H, m); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.2, 141.7, 138.1, 135.1, 128.8, 127.4, 127.2, 126.2, 122.6, 26.0, 24.5; HRMS-ESI: m/z $[M+H]^+$ for calculated $C_{16}H_{17}NOS^+$ $[M+H]^+$: 272.1104; found: 272.1109.
6. *N*-(4-bromobenzyl)-*N*-phenylbenzamide (**5b**): White solid, mp 110-113 °C; IR (KBr) ν_{max} 3058, 2860, 1640, 1574, 1486, 1446, 1282, 1070, 840, 785 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 –7.29 (m, 3H), 7.29 – 7.27 (m, 5H), 7.24 – 7.21 (m, 2H), 7.19 – 7.12 (m, 2H), 6.76 (d, J = 8.6 Hz, 2H), 5.09 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.4, 142.5, 137.1, 135.5, 132.1, 129.9, 129.2, 128.6, 128.5, 128.3, 127.9, 127.5, 120.2, 53.7; HRMS-ESI: m/z $[M+H]^+$ for calculated $C_{20}H_{16}BrNO^+$ $[M+H]^+$: 366.0488; found: 366.0494.
7. *N*-(4-methylbenzyl)-*N*-phenylbenzamide (**5c**): White solid, mp 105-108 °C; IR (KBr) ν_{max} 3112, 2230, 1615, 1568, 1376, 1296, 1213, 1174, 1021, 960, 834 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 – 7.30 (m, 2H), 7.21 – 7.17 (m, 3H), 7.16 – 7.10 (m, 4H), 7.10 – 7.06 (m, 3H), 6.91 – 6.88 (m, 2H), 5.08 (s, 2H), 2.31 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.4, 143.5, 136.9, 136.0, 134.5, 129.5, 129.1, 128.9, 128.7, 128.3, 127.7, 127.6, 126.5, 53.5, 21.1; HRMS-ESI: m/z $[M+H]^+$ for calculated $C_{21}H_{19}NO^+$ $[M+H]^+$: 302.1539; found: 302.1540.

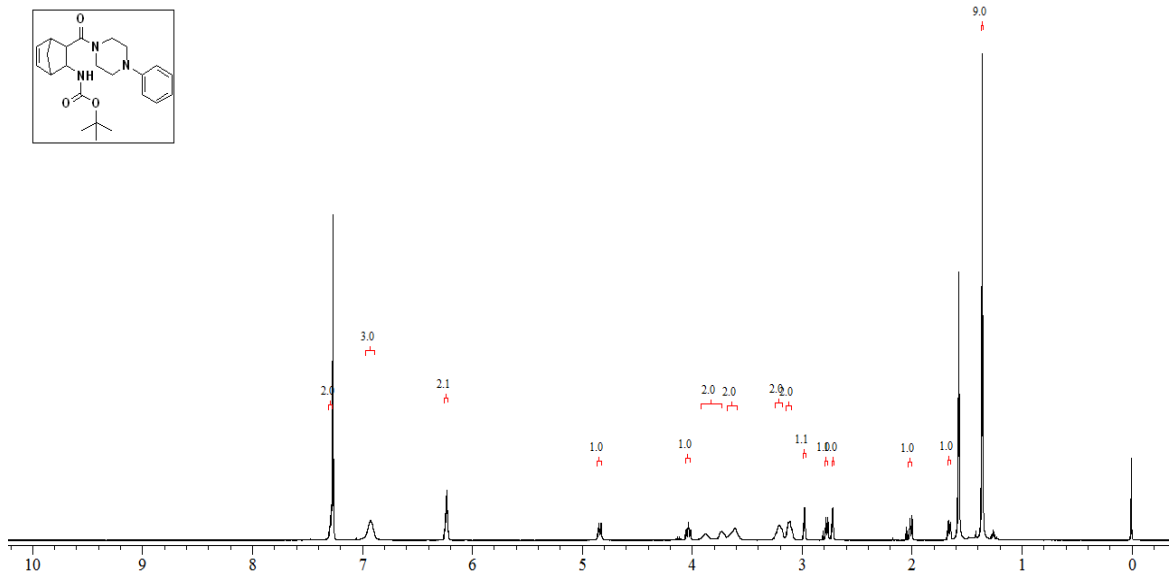
8. *N*-(4-bromophenyl)-*N*-(4-methylbenzyl)benzamide (**5d**): White solid, mp 112-115 °C; IR (KBr) ν_{max} 3432, 2835, 1630, 1532, 1473, 1421, 1258, 1170, 1018, 940, 746 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 – 7.28 (m, 2H), 7.25 – 7.22 (m, 3H), 7.20 – 7.14 (m, 4H), 7.10 – 7.06 (m, 2H), 6.78 – 6.72 (m, 2H), 5.05 (s, 2H), 2.31 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.3, 142.5, 137.1, 135.6, 134.0, 132.1, 129.8, 129.3, 129.2, 128.7, 128.3, 127.9, 120.1, 53.4, 21.1; HRMS-ESI: m/z $[M+H]^+$ for calculated $C_{21}H_{18}BrNO^+$ $[M+H]^+$: 380.0645; found: 380.0650.



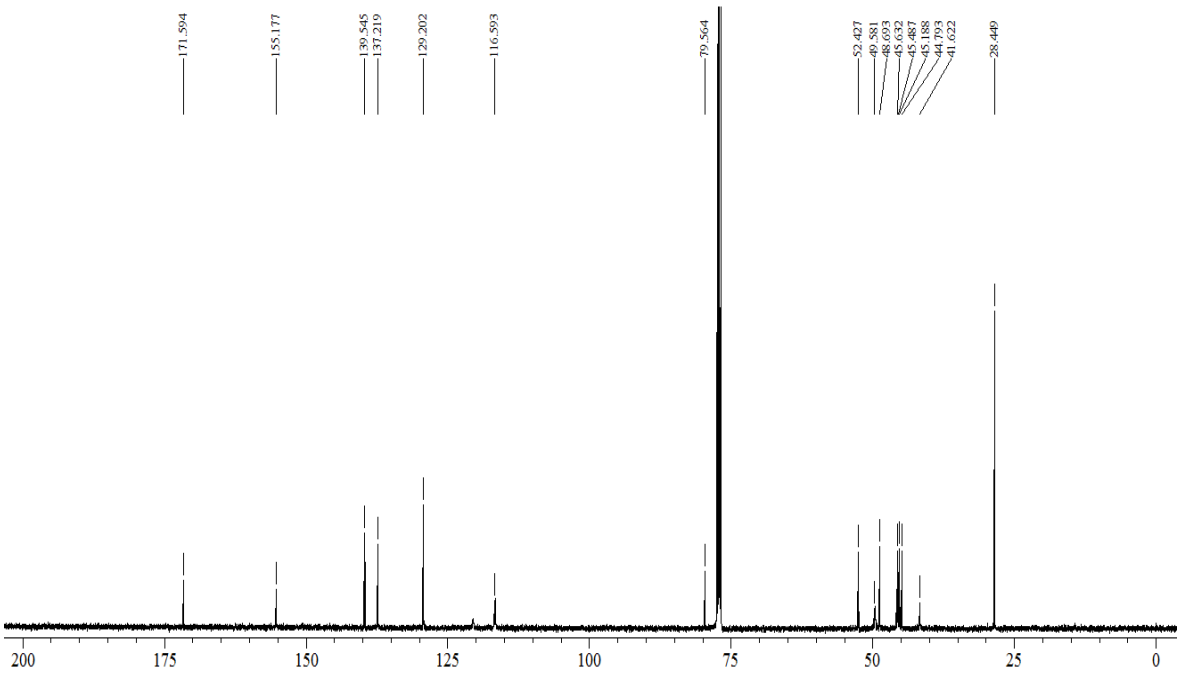
^{1}H NMR Spectrum of methyl 4-((1-phenylethyl)carbomyl)phenyl acetate (3m).



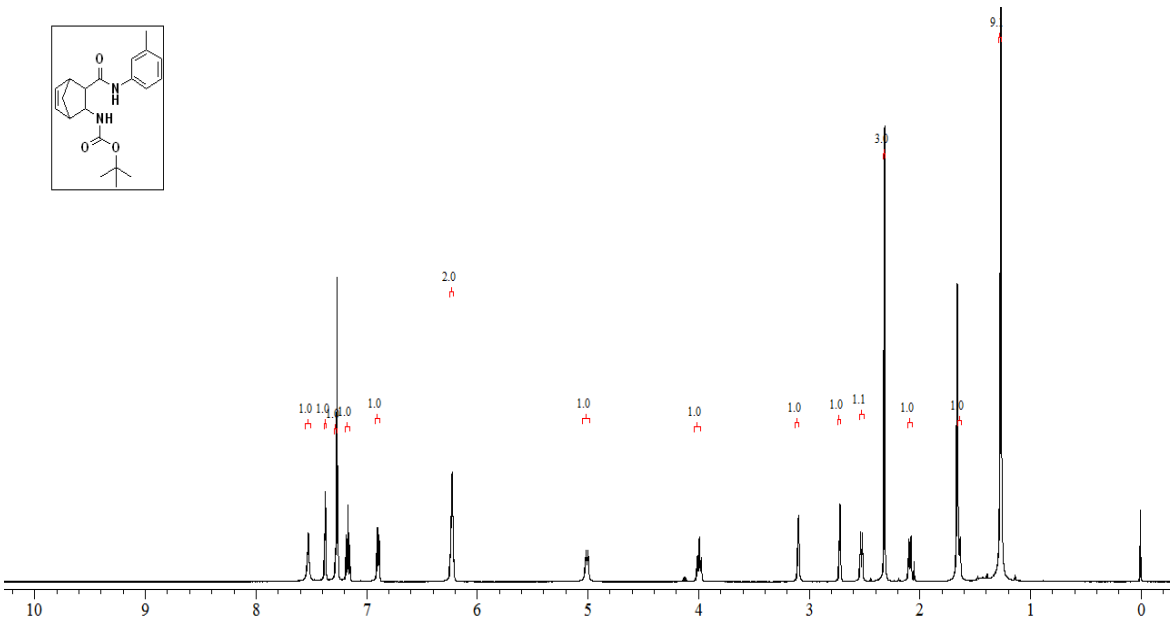
^{13}C NMR Spectrum of methyl 4-((1-phenylethyl)carbomyl)phenyl acetate (3m).



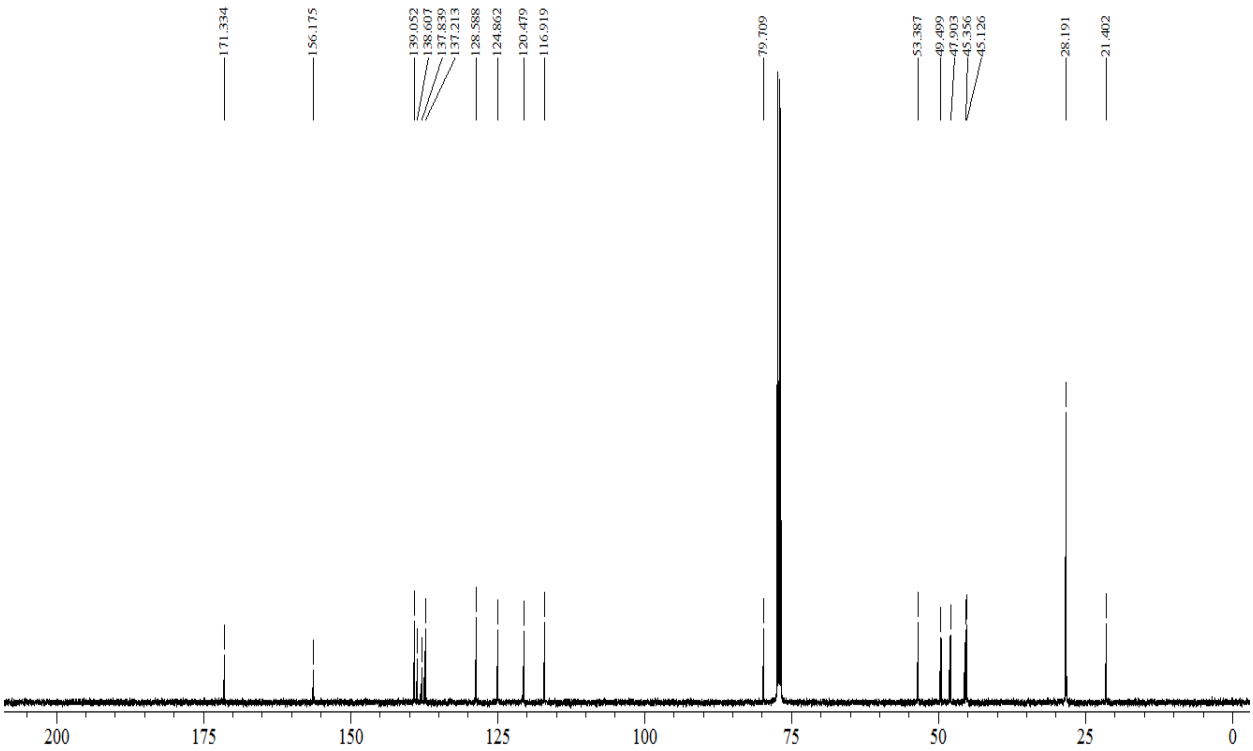
^{1}H NMR Spectrum of *tert*-butyl (3-(4-phenylpiperazine-1-carbonyl)bicyclo[2.2.1]hept-5-en-2-yl)carbamate (3n).



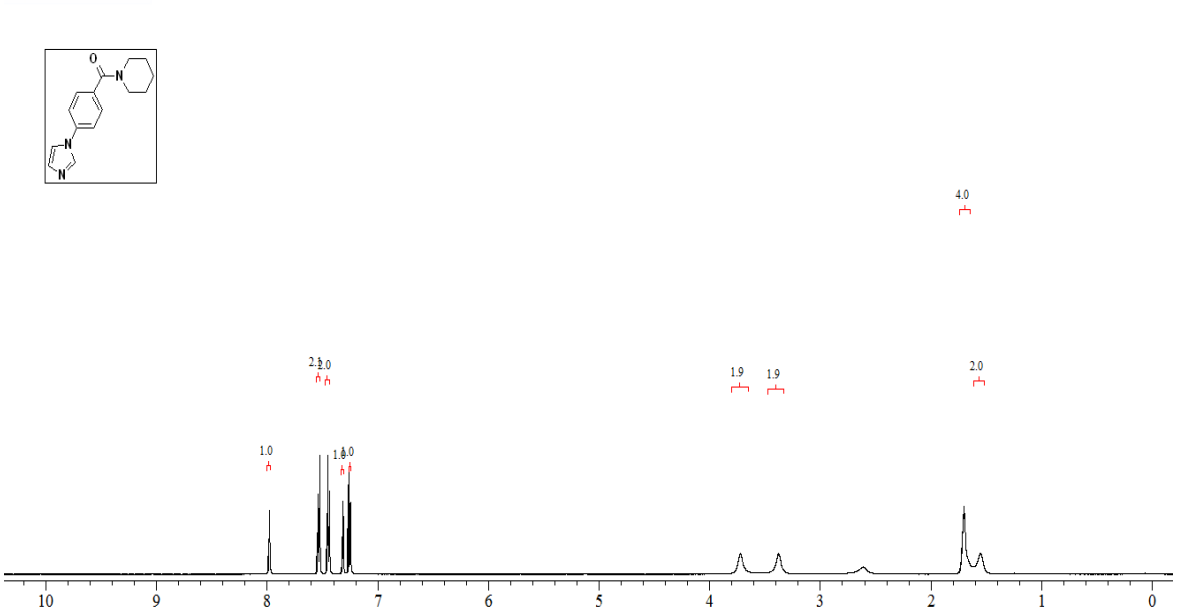
^{13}C NMR Spectrum of *tert*-butyl (3-(4-phenylpiperazine-1-carbonyl)bicyclo[2.2.1]hept-5-en-2-yl)carbamate (3n).



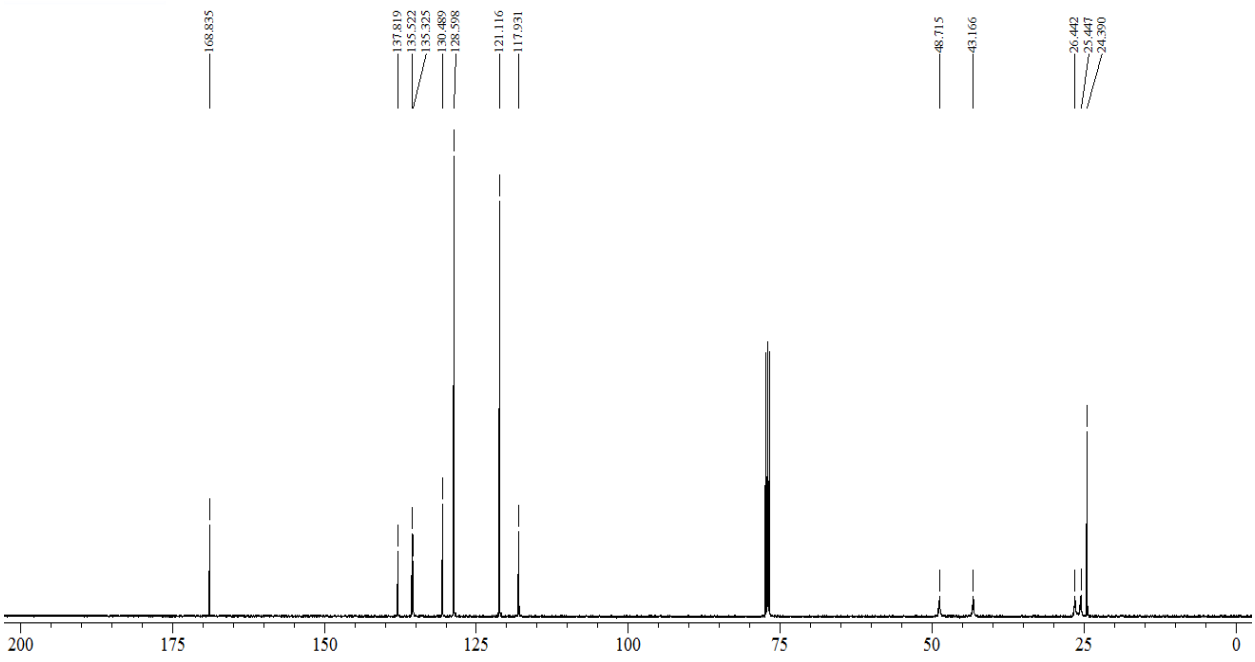
^{1}H NMR Spectrum of *tert*-butyl (3-(m-tolylcarbamoyl)bicyclo[2.2.1]hept-5-en-2-yl)carbamate (3o).



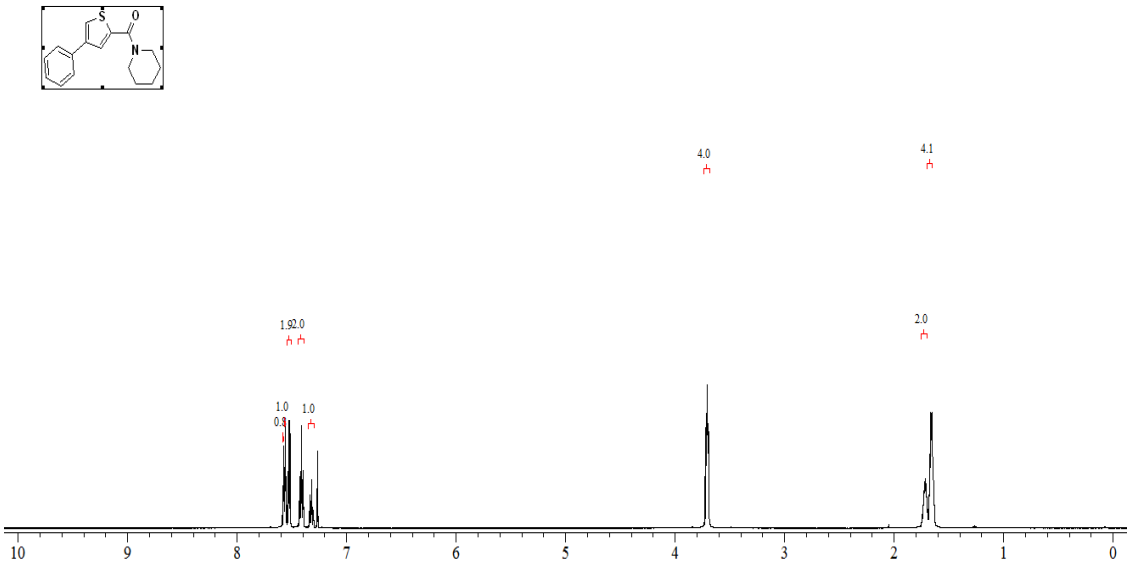
^{13}C NMR Spectrum of *tert*-butyl (3-(m-tolylcarbamoyl)bicyclo[2.2.1]hept-5-en-2-yl)carbamate (3o).



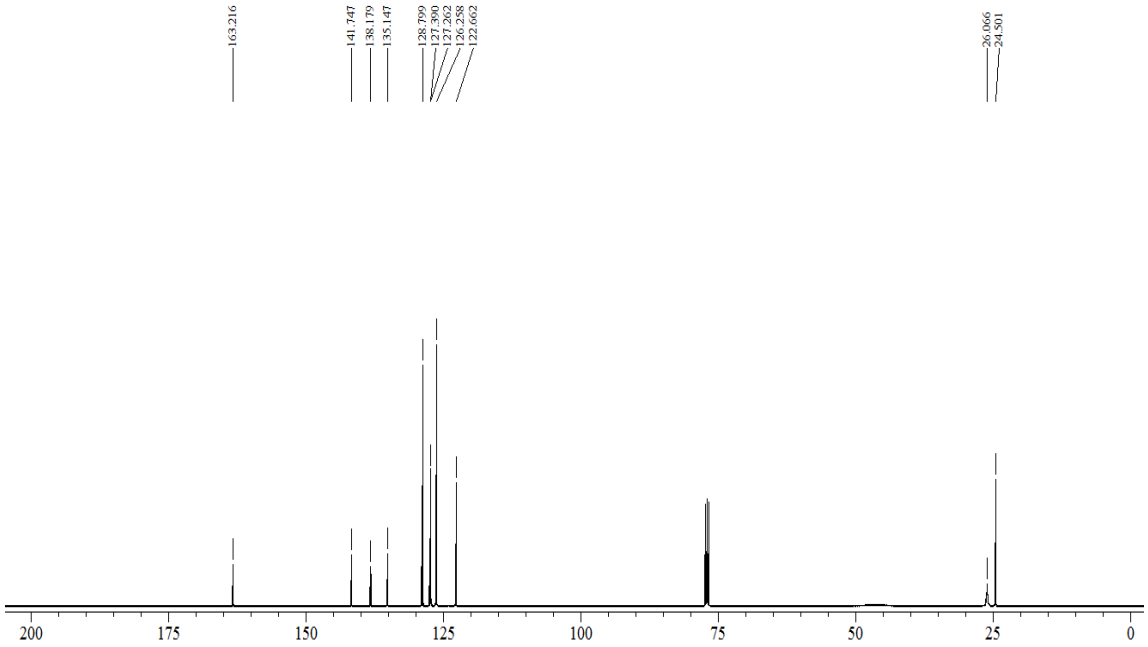
^{1}H NMR Spectrum of (4-(1*H*-imidazol-1-yl)phenyl)(piperidin-1-yl)methanone (3p).



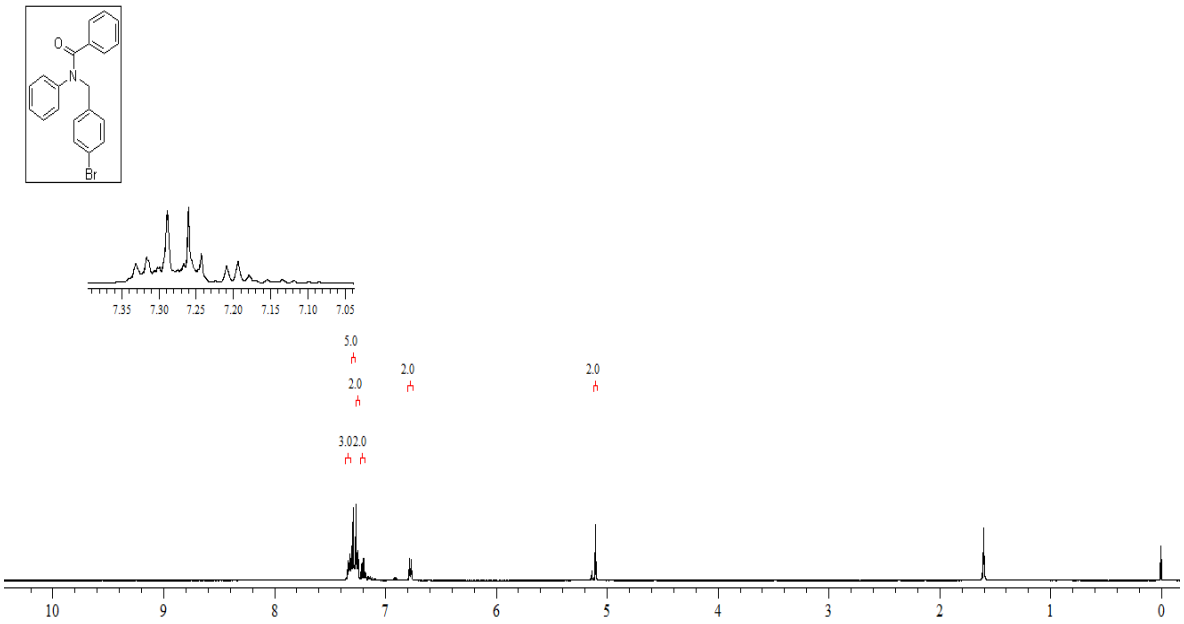
^{13}C NMR Spectrum of (4-(1*H*-imidazol-1-yl)phenyl)(piperidin-1-yl)methanone (3p).



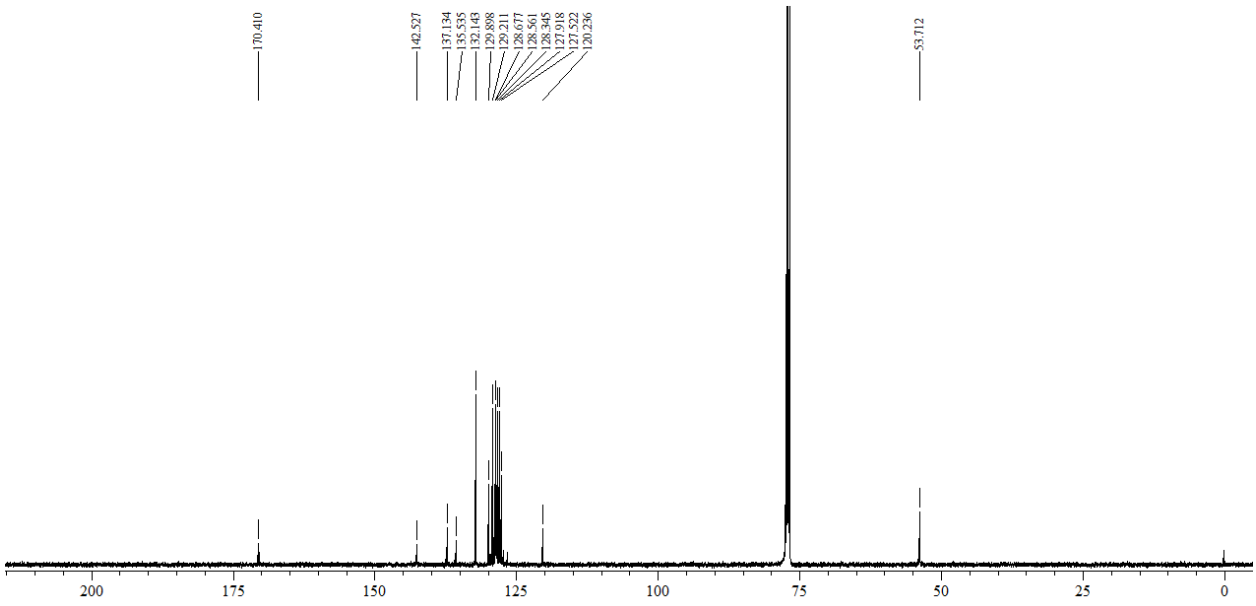
^{1}H NMR Spectrum of (4-phenylthiophen-2-yl)(piperidi-1-yl)methanone (3s).



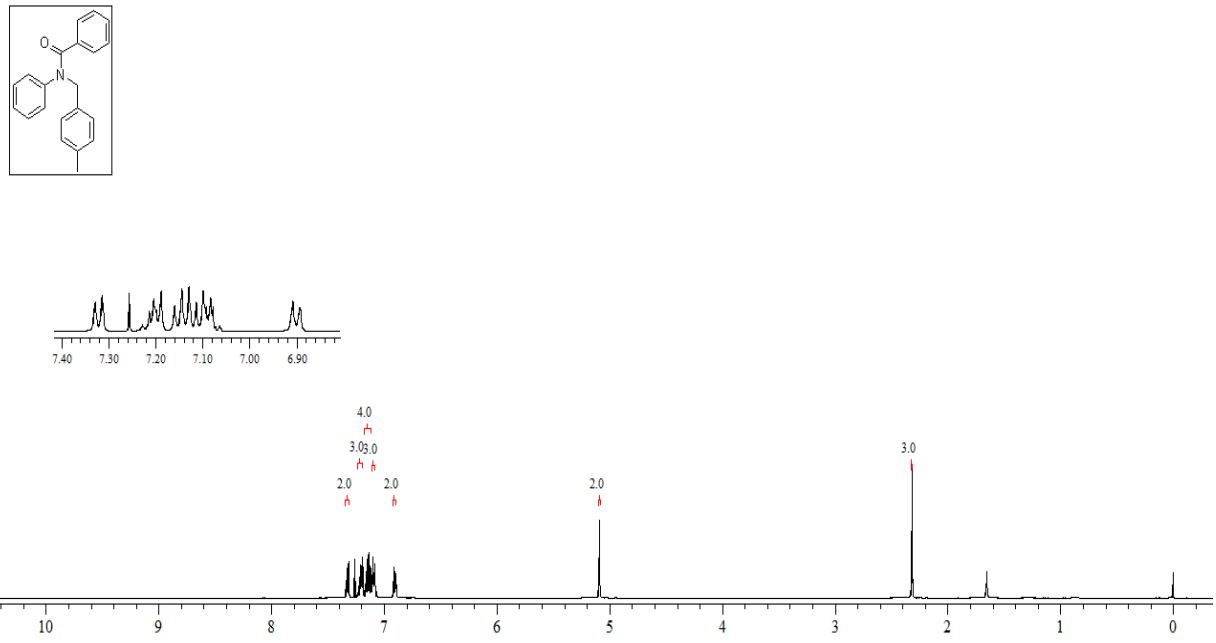
^{13}C NMR Spectrum of (4-phenylthiophen-2-yl)(piperidi-1-yl)methanone (3s).



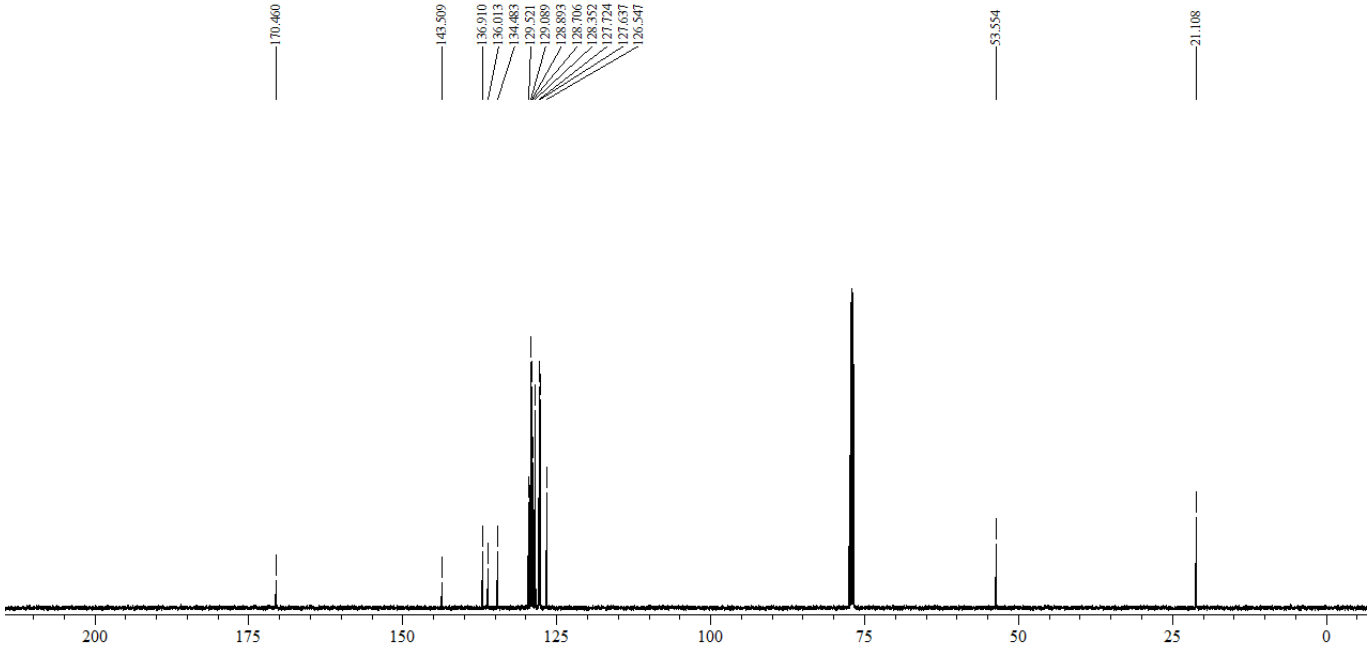
^{1}H NMR Spectrum of *N*-(4-bromobenzyl)-*N*-phenylbenzamide (5b).



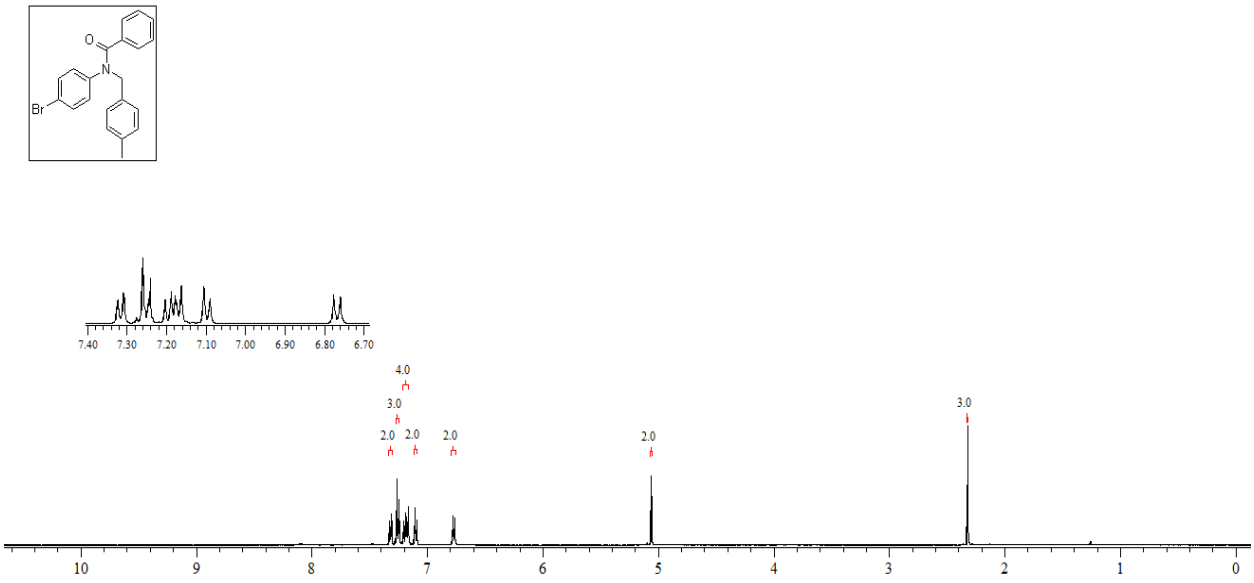
^{13}C NMR Spectrum of *N*-(4-bromobenzyl)-*N*-phenylbenzamide (5b).



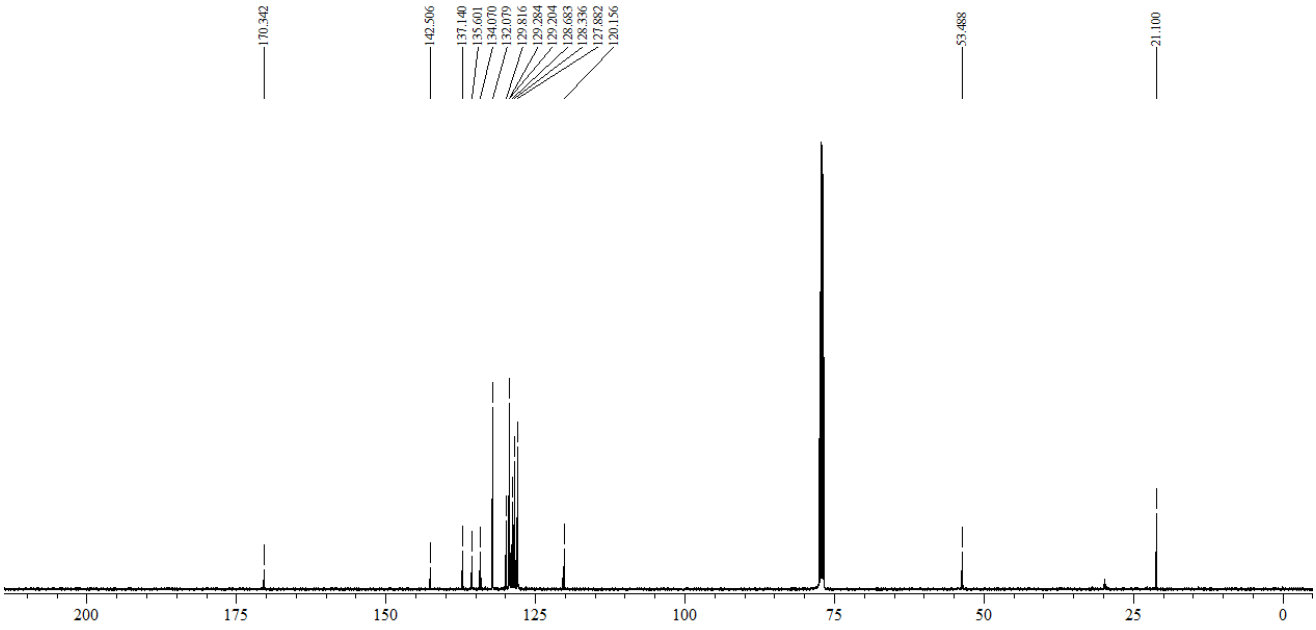
^{1}H NMR Spectrum of *N*-(4-methylbenzyl)-*N*-phenylbenzamide (5c).



^{13}C NMR Spectrum of *N*-(4-methylbenzyl)-*N*-phenylbenzamide (5c).



^{1}H NMR Spectrum of *N*-(4-bromophenyl)-*N*-(4-methylbenzyl)benzamide (5d).



^{13}C NMR Spectrum of *N*-(4-bromophenyl)-*N*-(4-methylbenzyl)benzamide (5d).

Antibacterial Assay

The antimicrobial activities of the synthesized compounds were determined by cup plate diffusion method.[27]The compounds were evaluated for antibacterial activity against *Staphylococcus aureus* MTCC 737, *Bacillus subtilis* MTCC 441, *Escherichia coli* MTCC 118 and *Pseudomonas aeruginosa* MTCC 424. Commercial antibiotic Ciprofloxacin (250 μg/mL) was used as reference drug for antibacterial activity. Dimethyl sulphoxide (1%, DMSO) was used as control (without compound). Culture strains of bacteria were maintained on nutrient agar slant at 37 °C for 24 h. Antibacterial activity was evaluated using nutrient agar plate seeded with 0.1 mL of respective bacterial culture strain suspension prepared in sterile saline (0.85%) of 105 CFU/mL dilutions. Wells of 6 mm diameter were filled with 0.1 mL of compound solution at a fixed concentration 250 μg/mL separately for each bacterial strain. The MIC value, representing the lowest concentration that completely inhibited the formation of visible growth, was evaluated after 18 h of incubation at 37°C. All the experiments were carried out in duplicates and the mean values are represented.