Electronic Supplementary Information

Direct reductive amination of 5-hydroxymethylfurfural with primary/secondary amines via Ru-complex catalyzed hydrogenation

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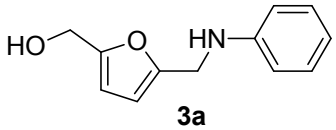
1. General Methods

NMR spectra were obtained in $CDCl_3$ on a 400 MHz instrument and recorded at the following frequencies: proton (^1H, 400 MHz), carbon (^{13}C, 100 MHz). ^1H NMR chemical shifts were reported in ppm using tetramethylsilane (TMS, δ (ppm) = 0.00 ppm) as the internal standard. ^{13}C NMR spectra were reported in ppm using $CDCl_3$ as the internal standard. Column chromatography was performed using silica gel and analytical thin-layer chromatography (TLC) was performed on silica gel plates. All the reagents used were of analytical grade, purchased locally and used without any purification unless otherwise specified.

2. Experimental Procedures

To a solution of 5-HMF (63.0 mg, 0.5 mmol) in solvent (1.0 mL) at room temperature was added a catalyst (0.5 mol% to 5-HMF) and amine (0.55 mmol, 1.1 equiv to 5-HMF). A high throughput reactor (Freeslate, USA) was used which was purged with H_2 (173 psi) three times at ambient temperature before heated to the set temperature. The reactors were shaking at a rate of 700 rpm/min until completion of reaction. After removing solvent, the residual in each vial was purified on silica gel column (petroleum ether: ethyl acetate, 5:2) to afford product.

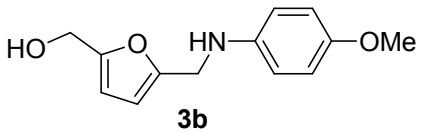
3. Analytical data



3a

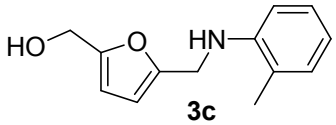
(5-((phenylamino)methyl)furan-2-yl)methanol (**3a**) colorless oil, 94.4 mg, 93% yield. ^1H NMR ($CDCl_3$, 400 MHz) δ 3.13 (br s, 2H, NH and OH), 4.30 (s, 2H, C*H*$_2$NH), 4.54 (s, 2H, C*H*$_2$OH), 6.18 (d, *J* = 3.1 Hz, 1H, furanH), 6.21 (d, *J* = 3.1 Hz, 1H, furanH), 6.67−6.78 (m, 3H, ArH), 7.18−7.22 (m, 2H, ArH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 41.6, 57.4, 107.8, 108.6, 113.3, 118.2, 129.3,

147.6, 152.9, 153.5. IR ν_{max}/cm^{-1} 3388, 3052, 2926, 2864, 1602, 1506, 1317, 1011, 795, 750, 692. HRMS (ESI) Calc. for $C_{12}H_{14}NO_2$ $[M+H]^+$: 204.1019, found: 204.1029.



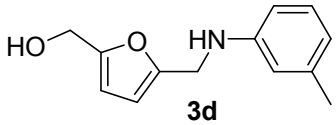
3b

(5-(((4-methoxyphenyl)amino)methyl)furan-2-yl)methanol (**3b**) yellow oil, 103.8 mg, 89% yield. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.27 (br s, 2H, NH and OH), 3.73 (s, 3H, OMe), 4.21 (s, 2H, C*H*$_2$NH), 4.51 (s, 2H, C*H*$_2$OH), 6.14 (d, *J* = 3.1 Hz, 1H, furanH), 6.17 (d, *J* = 3.1 Hz, 1H, furanH), 6.61−6.79 (m, 4H, ArH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 42.6, 55.8, 57.3, 107.8, 108.5, 114.85, 114.86, 141.7, 152.6, 153.0, 153.5. IR ν_{max}/cm^{-1} 3370, 2929, 1513, 1459, 1234, 1026, 821, 777. HRMS (ESI) Calc. for $C_{13}H_{16}NO_3$ $[M+H]^+$: 234.1125, found: 234.1122.



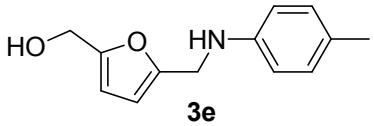
3c

(5-((o-tolylamino)methyl)furan-2-yl)methanol (**3c**) colorless oil, 85.8 mg, 79% yield. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.76 (br s, 1H, OH), 2.16, (s, 3H, Me), 3.86 (br s, 1H, NH), 4.35 (s, 2H, C*H*$_2$NH), 4.58 (s, 2H, C*H*$_2$OH), 6.19 (d, *J* = 3.1 Hz, 1H, furanH), 6.22 (d, *J* = 3.1 Hz, 1H, furanH), 6.67−7.13 (m, 4H, ArH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 17.5, 41.6, 57.6, 107.8, 108.7, 110.2, 117.7, 122.4, 127.1, 130.2, 145.6, 153.0, 153.5. IR ν_{max}/cm^{-1} 3402, 3016, 2925, 2857, 1606, 1512, 1011, 793, 748. HRMS (ESI) Calc. for $C_{13}H_{15}NNaO_2$ $[M+Na]^+$: 240.0995, found: 240.0998.



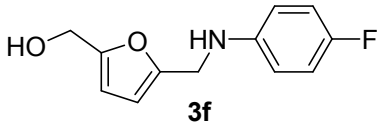
3d

(5-((m-tolylamino)methyl)furan-2-yl)methanol (**3d**) colorless oil, 98.0 mg, 90% yield. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.92 (br s, 1H, OH), 2.27 (s, 3H, Me), 3.95 (br s, 1H, NH), 4.28 (s, 2H, C*H*$_2$NH), 4.55 (s, 2H, C*H*$_2$OH), 6.17 (d, *J* = 3.1 Hz, 1H, furanH), 6.20 (d, *J* = 3.1 Hz, 1H, furanH), 6.47−6.49 (m, 2H, ArH), 6.57 (d, *J* = 7.3 Hz, 1H, ArH), 7.05−7.09 (m, 1H, ArH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.6, 41.6, 57.5, 107.8, 108.7, 110.3, 114.1, 119.1, 129.1, 139.1, 147.6, 153.0, 153.4. IR ν_{max}/cm^{-1} 3380, 3024, 2920, 2862, 1606, 1591, 1491, 1177, 1011, 771, 692. HRMS (ESI) Calc. for $C_{13}H_{16}NO_2$ $[M+H]^+$: 218.1176, found: 218.1173.



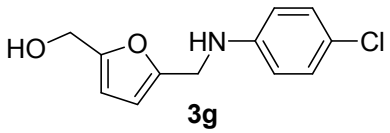
3e

(5-((p-tolylamino)methyl)furan-2-yl)methanol (**3e**) yellow solid, mp 53 °C, 99.2 mg, 91% yield. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.23 (s, 3H, Me), 4.26 (s, 2H, C*H*$_2$NH), 4.54 (s, 2H, C*H*$_2$OH), 6.15 (d, *J* = 3.0 Hz, 1H, furanH), 6.19 (d, *J* = 3.0 Hz, 1H, furanH), 6.59 (d, *J* = 8.4 Hz, 2H, ArH), 6.99 (d, *J* = 8.4 Hz, 2H, ArH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 20.4, 41.9, 57.5, 107.8, 108.7, 113.5, 127.4, 129.8, 145.3, 153.1, 153.4. IR ν_{max}/cm^{-1} 3369, 3019, 2920, 2864, 1617, 1520, 1252, 1011, 806. HRMS (ESI) Calc. for $C_{13}H_{16}NO_2$ $[M+H]^+$: 218.1176, found: 218.1168.



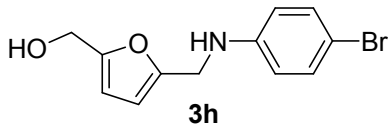
3f

(5-(((4-fluorophenyl)amino)methyl)furan-2-yl)methanol (**3f**) colorless oil, 104.0 mg, 94% yield. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.11 (br s, 2H, OH and NH), 4.23 (s, 2H, C*H*$_2$NH), 4.53 (s, 2H, C*H*$_2$OH), 6.16 (d, *J* = 3.1 Hz, 1H, furanH), 6.19 (d, *J* = 3.1 Hz, 1H, furanH), 6.57−6.62 (m, 2H, ArH), 6.85−6.92 (m, 2H, ArH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 42.2, 57.4, 107.9, 108.6, 114.2 (d, *J* = 7.4 Hz), 115.7 (d, *J* = 22.2 Hz), 143.9 (d, *J* = 1.9 Hz), 152.6, 153.5, 156.2 (d, *J* = 234.2 Hz). IR ν_{max}/cm^{-1} 3353, 2929, 2866, 1511, 1220, 1011, 822, 797. HRMS (ESI) Calc. for $C_{12}H_{12}FNNaO_2$ $[M+Na]^+$: 244.0744, found: 244.0750.



3g

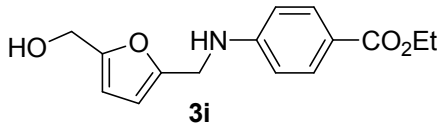
(5-(((4-chlorophenyl)amino)methyl)furan-2-yl)methanol (**3g**) colorless oil, 113.0 mg, 95% yield. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.11 (br s, 2H, OH and NH), 4.26 (s, 2H, C*H*$_2$NH), 4.55 (s, 2H, C*H*$_2$OH), 6.16 (d, *J* = 3.1 Hz, 1H, furanH), 6.21 (d, *J* = 3.1 Hz, 1H, furanH), 6.56−6.61 (m, 2H, ArH), 7.08−7.14 (m, 2H, ArH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 41.6, 57.5, 108.0, 108.7, 114.3, 122.7, 129.1, 146.1, 152.4, 153.6. IR ν_{max}/cm^{-1} 3351, 2928, 2865, 1600, 1499, 1009, 816, 795. HRMS (ESI) Calc. for $C_{12}H_{12}ClNNaO_2$ $[M+Na]^+$: 260.0449, found: 260.0453.



3h

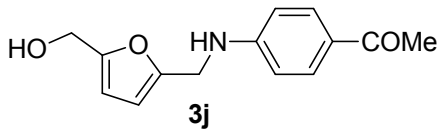
(5-(((4-bromophenyl)amino)methyl)furan-2-

yl)methanol (**3h**) yellow solid, mp 83 °C, 133.7 mg, 95% yield. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.85 (br s, 1H, OH), 4.07 (br s, 1H, NH), 4.26 (s, 2H, C*H*$_2$NH), 4.56 (s, 2H, C*H*$_2$OH), 6.16 (d, *J* = 3.0 Hz, 1H, furanH), 6.20 (d, *J* = 3.0 Hz, 1H, furanH), 6.15−7.26 (m, 4H, ArH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 41.5, 57.5, 108.0, 108.7, 109.7, 114.8, 132.0, 146.5, 152.3, 153.6. IR ν_{max}/cm^{-1} 3399, 2927, 2865, 1594, 1497, 1316, 1010, 813. HRMS (ESI) Calc. for $C_{12}H_{12}BrNNaO_2$ $[M+Na]^+$: 303.9944, found: 303.9953.



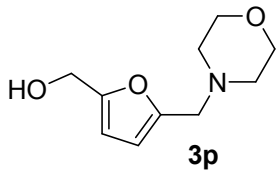
3i

ethyl 4-(((5-(hydroxymethyl)furan-2-yl)methyl)amino)benzoate (**3i**) light yellow solid, mp 133 °C, 95.0 mg, 69% yield. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.37 (t, *J* = 7.1 Hz, 3H, OCH$_2$C*H*$_3$), 4.30−4.35 (m, 4H), 4.58 (s, 2H, C*H*$_2$OH), 6.19 (d, *J* = 3.0 Hz, 1H, furanH), 6.22 (d, *J* = 3.0 Hz, 1H, furanH), 6.63 (d, *J* = 8.8 Hz, 2H, ArH), 7.88 (d, *J* = 8.8 Hz, 2H, ArH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 14.4, 40.9, 57.4, 60.3, 108.2, 108.6, 111.9, 131.5, 151.2, 151.8, 153.8, 168.9. IR ν_{max}/cm^{-1} 3405, 2927, 2865, 1680, 1595, 1495, 1314, 1010, 815. HRMS (ESI) Calc. for $C_{15}H_{17}NNaO_4$ $[M+Na]^+$: 298.1055, found: 298.1061.



3j

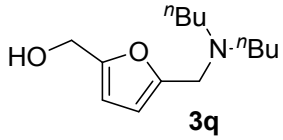
1-(4-(((5-(hydroxymethyl)furan-2-yl)methyl)amino)phenyl)ethanone (**3j**) yellow solid, mp 154 °C, 80.8 mg, 66% yield. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.39 (s, 3H, COC*H*$_3$), 4.30−4.35 (m, 4H), 4.30−4.35 (m, 1H), 6.19 (d, *J* = 3.0 Hz, 1H, furanH), 6.23 (d, *J* = 3.0 Hz, 1H, furanH), 6.67 (d, *J* = 8.8 Hz, 2H, ArH), 6.99−7.02 (m, 1H), 7.71 (d, *J* = 8.8 Hz, 2H, ArH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 26.4, 56.2, 108.0, 108.3, 111.6, 125.8, 130.8, 152.0, 152.9, 155.2, 195.5. IR ν_{max}/cm^{-1} 3410, 2927, 2864, 1710, 1598, 1494, 1319, 1010, 813. HRMS (ESI) Calc. for $C_{14}H_{16}NO_3$ $[M+H]^+$: 246.1130, found: 246.1135.



3p

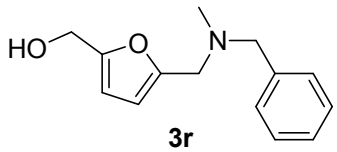
(5-(morpholinomethyl)furan-2-yl)methanol (**3j**) white solid, mp

78 °C, 81.7 mg, 83% yield. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.47 (t, *J* = 4.5 Hz, 4H, CH_2OCH_2), 2.65 (br s, 1H, OH), 3.51 (s, 2H, $CH_2N(CH_2CH_2)_2$), 3.71 (t, *J* = 4.5 Hz, 4H, $CH_2N(CH_2CH_2)_2$), 4.57 (s, 2H, CH_2OH), 6.17 (d, *J* = 3.0 Hz, 1H, furanH), 6.21 (d, *J* = 3.0 Hz, 1H, furanH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 53.3, 55.4, 57.4, 66.7, 108.2, 110.0, 151.0, 154.2. IR ν_{max}/cm^{-1} 3397, 2922, 2858, 2816, 1453, 1115, 1006, 791. HRMS (ESI) Calc. for $C_{10}H_{16}NO_3$ $[M+H]^+$: 198.1125, found: 198.1127.



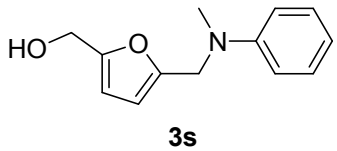
3q

(5-((dibutylamino)methyl)furan-2-yl)methanol (**3k**) colorless oil, 80.5 mg, 67% yield. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 0.90 (t, *J* = 7.3 Hz, 6H, Me), 1.24−1.49 (m, 8H, CH_2CH_2), 2.41−2.45 (m, 4H, NCH_2CH_2), 2.49 (br s, 1H, OH), 3.61 (s, 2H, CH_2N), 4.55 (s, 2H, CH_2OH), 6.10 (d, *J* = 3.1 Hz, 1H, furanH), 6.20 (d, *J* = 3.1 Hz, 1H, furanH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 14.0, 20.7, 29.0, 50.2, 53.6, 57.5, 108.1, 109.1, 152.8, 153.5. IR ν_{max}/cm^{-1} 3367, 2957, 2932, 2871, 1459, 1377, 1015, 791. HRMS (ESI) Calc. for $C_{16}H_{26}NO_2$ $[M+H]^+$: 240.1958, found: 240.1972.



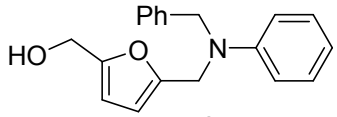
3r

(5-((benzyl(methyl)amino)methyl)furan-2-yl)methanol (**3l**) colorless oil, 100.6 mg, 87% yield. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.23 (s, 3H, Me), 3.53 (s, 2H, CH_2N), 3.55 (s, 2H, CH_2N), 4.57 (s, 2H, CH_2OH), 6.15 (d, *J* = 3.1 Hz, 1H, furanH), 6.21 (d, *J* = 3.1 Hz, 1H, furanH), 7.23−7.32 (m, 5H, ArH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 42.1, 53.5, 57.6, 61.3, 108.3, 109.4, 127.1, 128.3, 129.2, 138.5, 152.4, 153.7. IR ν_{max}/cm^{-1} 3370, 2925, 2840, 2793, 1453, 1014, 794, 739, 699. HRMS (ESI) Calc. for $C_{14}H_{18}NO_2$ $[M+H]^+$: 232.1332, found: 232.1347.



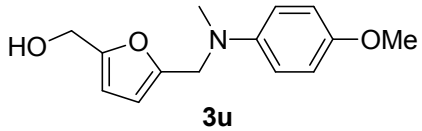
3s

(5-((methyl(phenyl)amino)methyl)furan-2-yl)methanol (**3m**) colorless oil, 85.8 mg, 79% yield. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.76 (br s, 1H, OH), 2.98 (s, 3H, Me), 4.43 (s, 2H, CH_2N), 4.54 (s, 2H, CH_2OH), 6.06 (d, *J* = 3.1 Hz, 1H, furanH), 6.18 (d, *J* = 3.1 Hz, 1H, furanH), 6.71−7.25 (m, 5H, ArH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 38.4, 50.1, 57.6, 108.0, 108.6, 113.1, 117.2, 129.1, 149.3, 152.5, 153.4. IR ν_{max}/cm^{-1} 3369, 2928, 1599, 1506, 1011, 748, 794, 692. HRMS (ESI) Calc. for $C_{13}H_{15}NNaO_2$ $[M+Na]^+$: 240.0995, found: 240.0984.



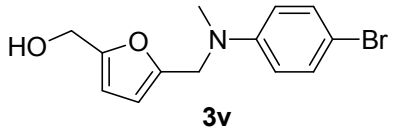
3t

(5-((benzyl(phenyl)amino)methyl)furan-2-yl)methanol (**3n**) colorless oil, 108.6 mg, 74% yield. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.74 (br s, 1H, OH), 4.51 (s, 4H, N(CH_2)$_2$), 4.60 (s, 2H, CH_2OH), 6.10 (d, J = 3.1 Hz, 1H, furanH), 6.17 (d, J = 3.1 Hz, 1H, furanH), 6.70−7.32 (m, 10H, ArH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 47.8, 54.4, 57.6, 108.3, 108.6, 113.0, 117.3, 126.7, 126.9, 128.6, 129.2, 138.7, 148.8, 152.4, 153.5. IR ν_{max}/cm^{-1} 3368, 3060, 2925, 1598, 1505, 1011, 793, 748, 730, 693. HRMS (ESI) Calc. for $C_{19}H_{20}NO_2$ $[M+H]^+$: 294.1489, found: 294.1493.



3u

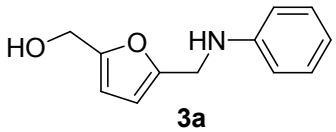
(5-(((4-methoxyphenyl)(methyl)amino)methyl)furan-2-yl)methanol (**3o**) colorless oil, 89.1 mg, 72% yield. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.28 (br s, 1H, OH), 2.87 (s, 3H, NMe), 3.74 (s, 3H, OMe), 4.31 (s, 2H, CH_2N), 4.52 (s, CH_2OH), 6.04 (d, J = 3.1 Hz, 1H, furanH), 6.16 (d, J = 3.1 Hz, 1H, furanH), 6.79−6.82 (m, 4H, ArH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 39.2, 51.5, 55.7, 57.5, 108.38, 108.43, 114.7, 115.8, 144.1, 152.3, 152.5, 153.5. IR ν_{max}/cm^{-1} 3393, 2933, 1513, 1244, 1036, 816. HRMS (ESI) Calc. for $C_{14}H_{18}NO_3$ $[M+H]^+$: 248.1281, found: 248.1287.



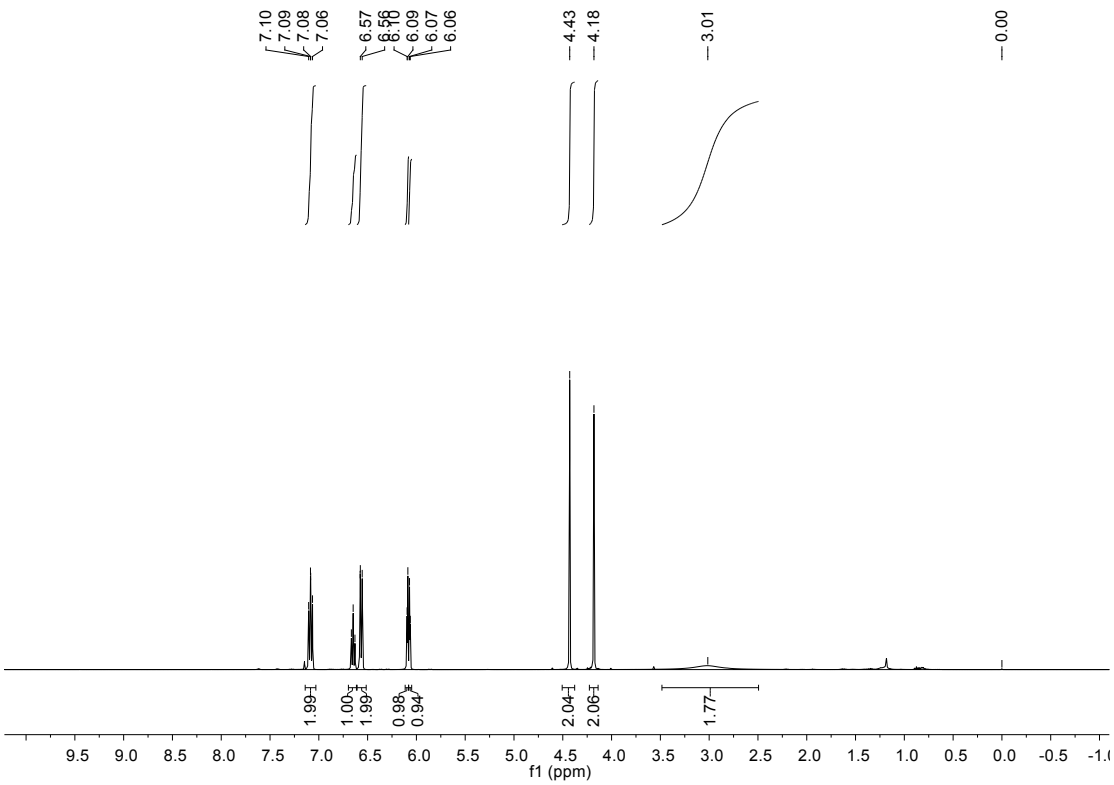
3v

(5-(((4-bromophenyl)(methyl)amino)methyl)furan-2-yl)methanol (**3p**) colorless oil, 99.3 mg, 67% yield. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.84 (br s, 1H, OH), 2.96 (s, 3H, NMe), 4.40 (s, 2H, NCH_2), 4.53 (s, 2H, CH_2OH), 6.04 (d, J = 3.1 Hz, 1H, furanH), 6.17 (d, J = 3.1 Hz, 1H, furanH), 6.65−7.29 (m, 4H, ArH); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 38.5, 50.0, 57.5, 108.1, 108.6, 109.1, 114.6, 131.8, 148.2, 151.9, 153.5. IR ν_{max}/cm^{-1} 3399, 2927, 2865, 1594, 1497, 1316, 1010, 813. HRMS (ESI) Calc. for $C_{13}H_{15}BrNO_2$ $[M+H]^+$: 296.0281, found: 296.0272.

4. ^{1}H- and ^{13}C-NMR spectra



3a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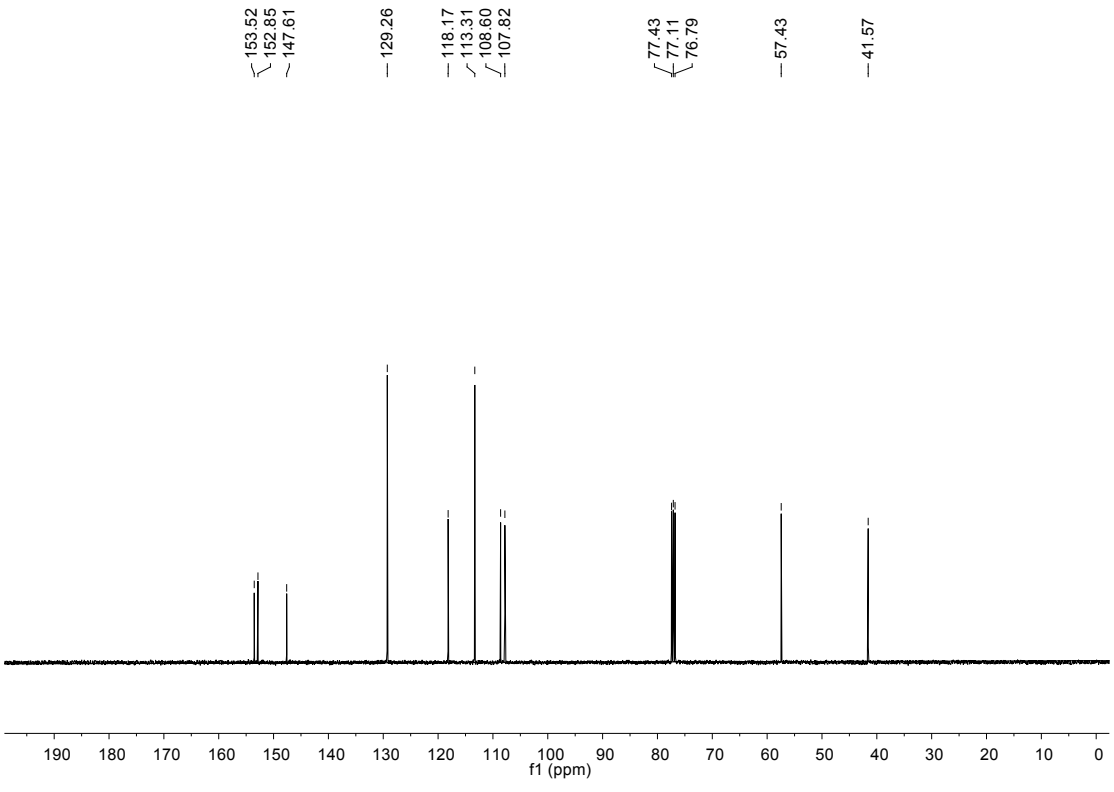
7.09
7.08
7.06
6.57
6.56
6.10
6.09
6.07
6.06
4.43
4.18
3.01
0.00
1.99
1.00
1.99
0.98
0.94
2.04
2.06
1.77
f1 (ppm)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113.31
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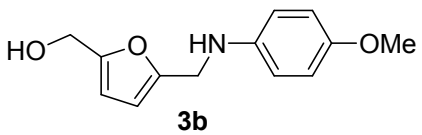
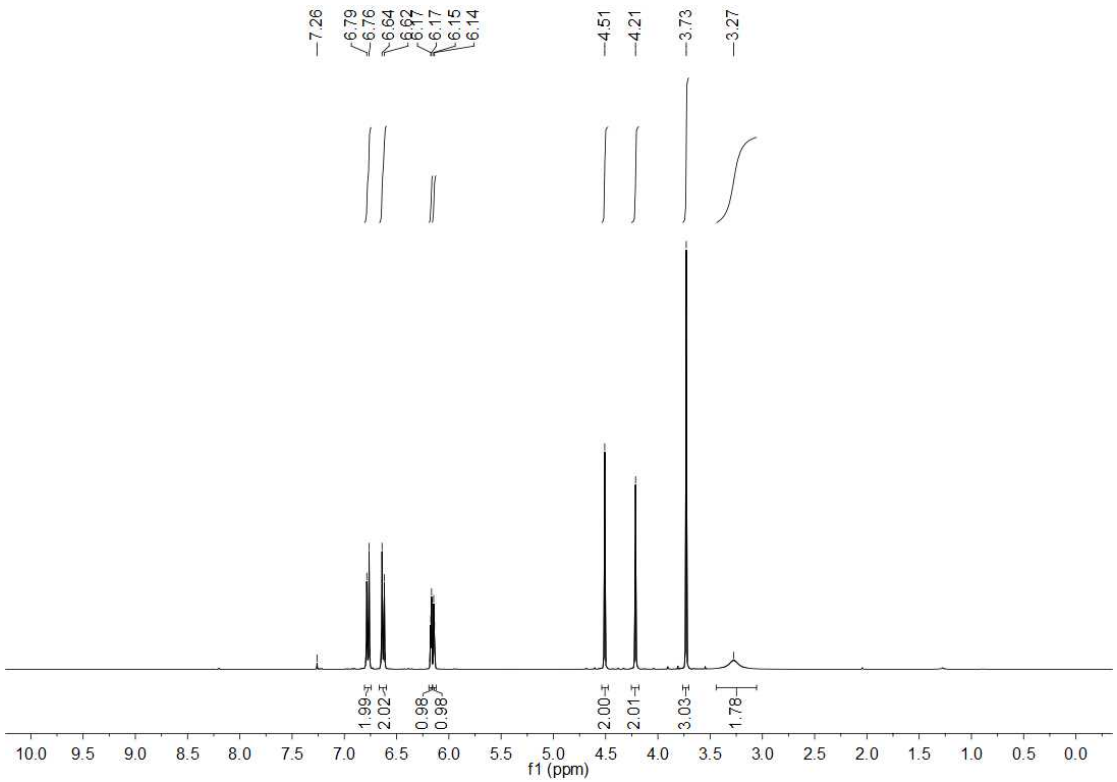
107.82
77.43
77.11
76.79
57.43
41.57
f1 (ppm)


HO
O
HN
OMe

3b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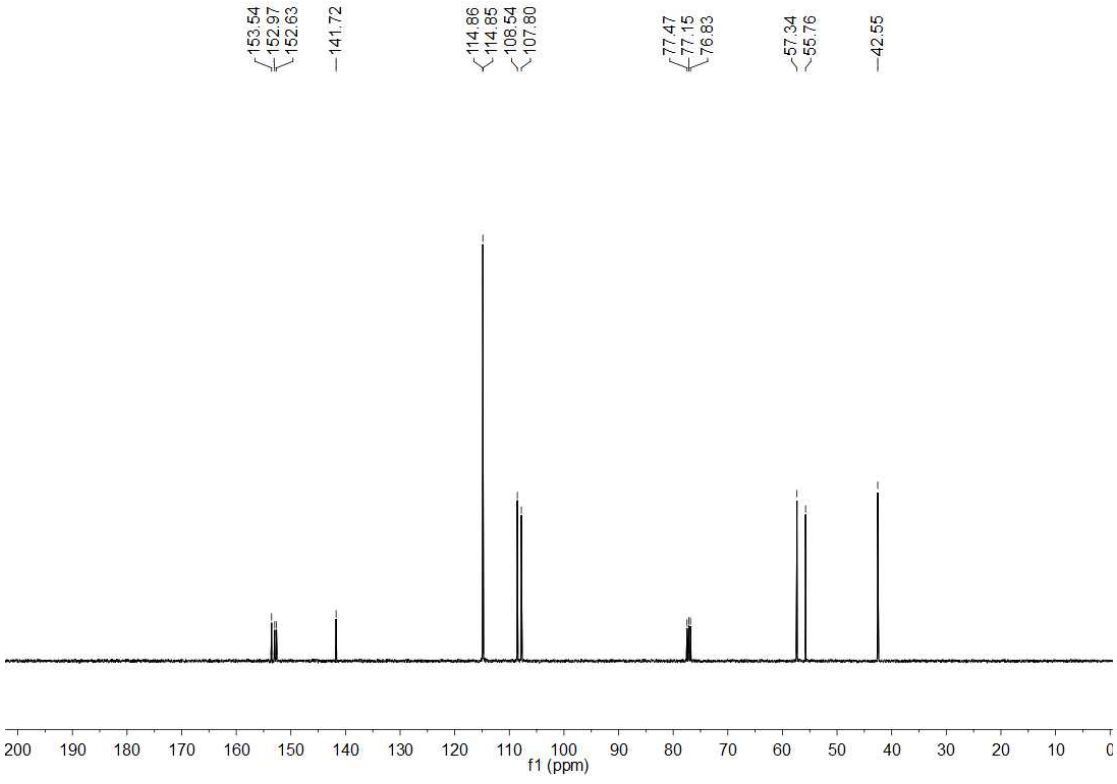
6.79
6.76
6.64
6.62
6.17
6.15
6.14
4.51
4.21
3.73
3.27
1.99
2.02
0.98
0.98
2.00
2.01
3.03
1.78
f1 (ppm)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152.63
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114.85
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107.80
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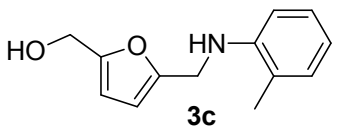
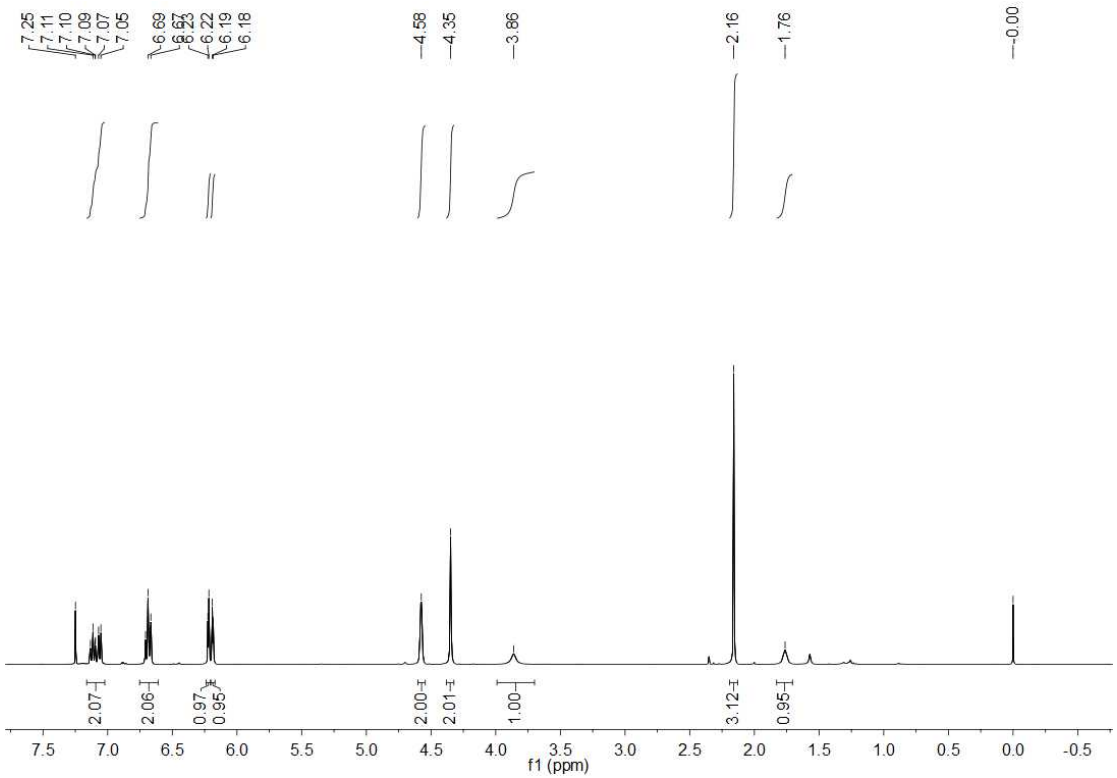
77.15
76.83
57.34
55.76
42.55
f1 (ppm)


HO
O
HN

3c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6.67
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6.22
6.19
6.18
4.58
4.35
3.86
2.16
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0.95
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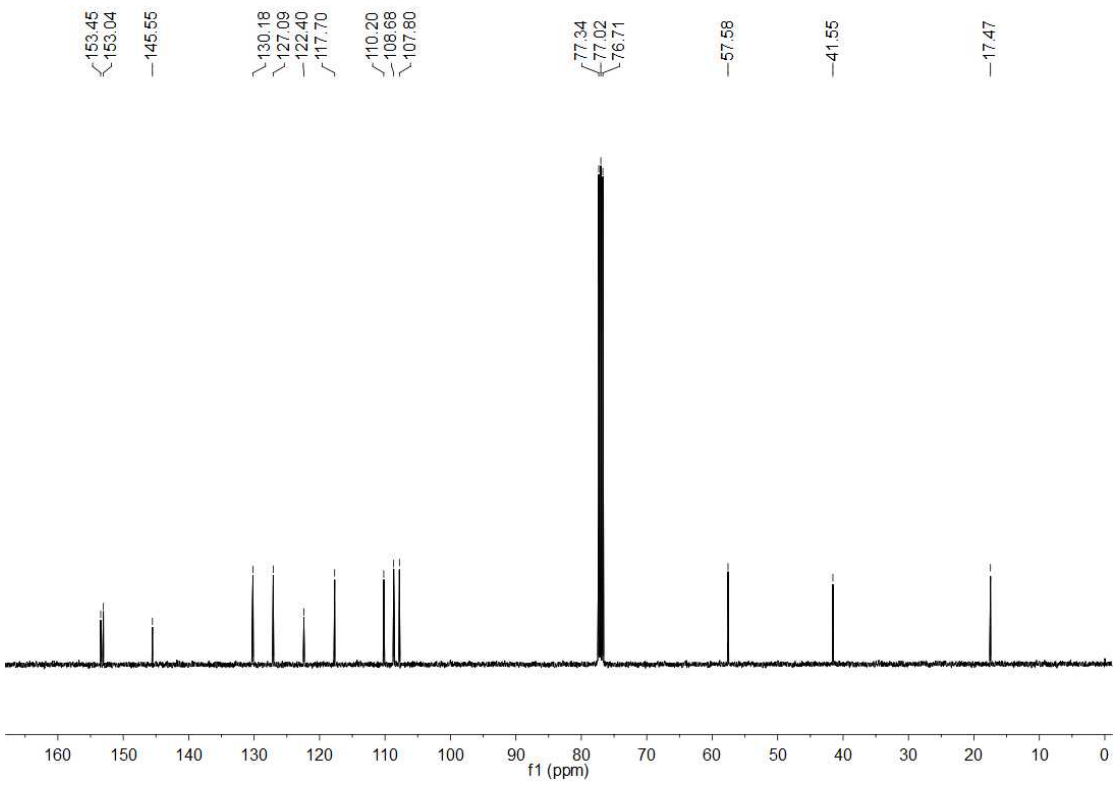
f1 (ppm)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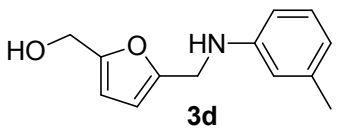
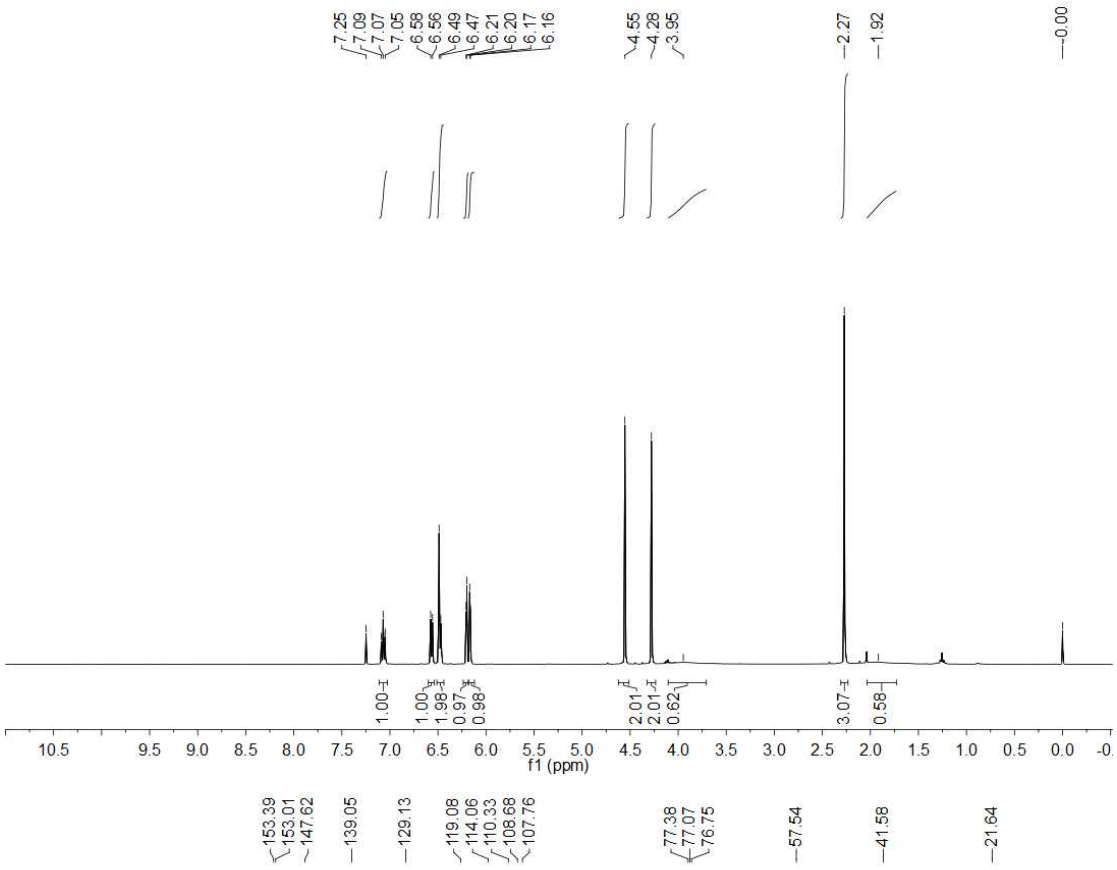
107.80
77.34
77.02
76.71
57.58
41.55
17.47
f1 (ppm)


HO
O
HN

3d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6.17
6.16
4.55
4.28
3.95
2.27
1.92
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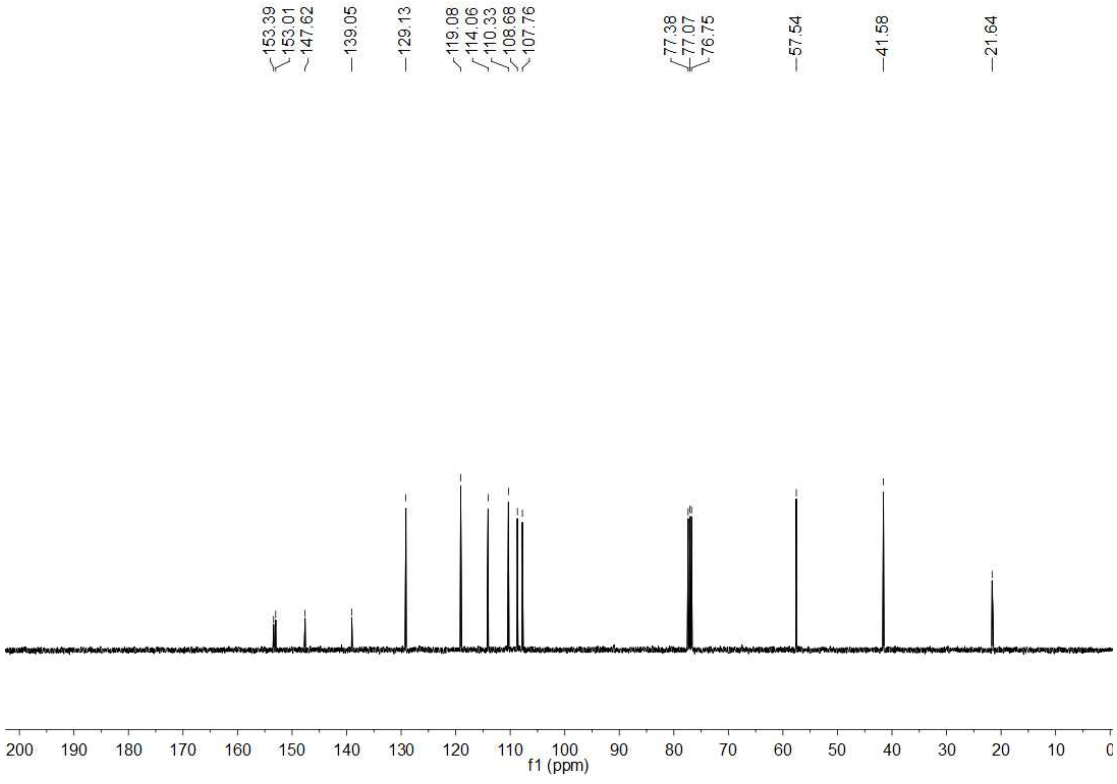
1.98
0.97
0.98
2.01
2.01
0.62
3.07
0.58
f1 (ppm)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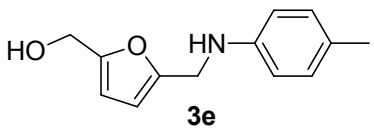
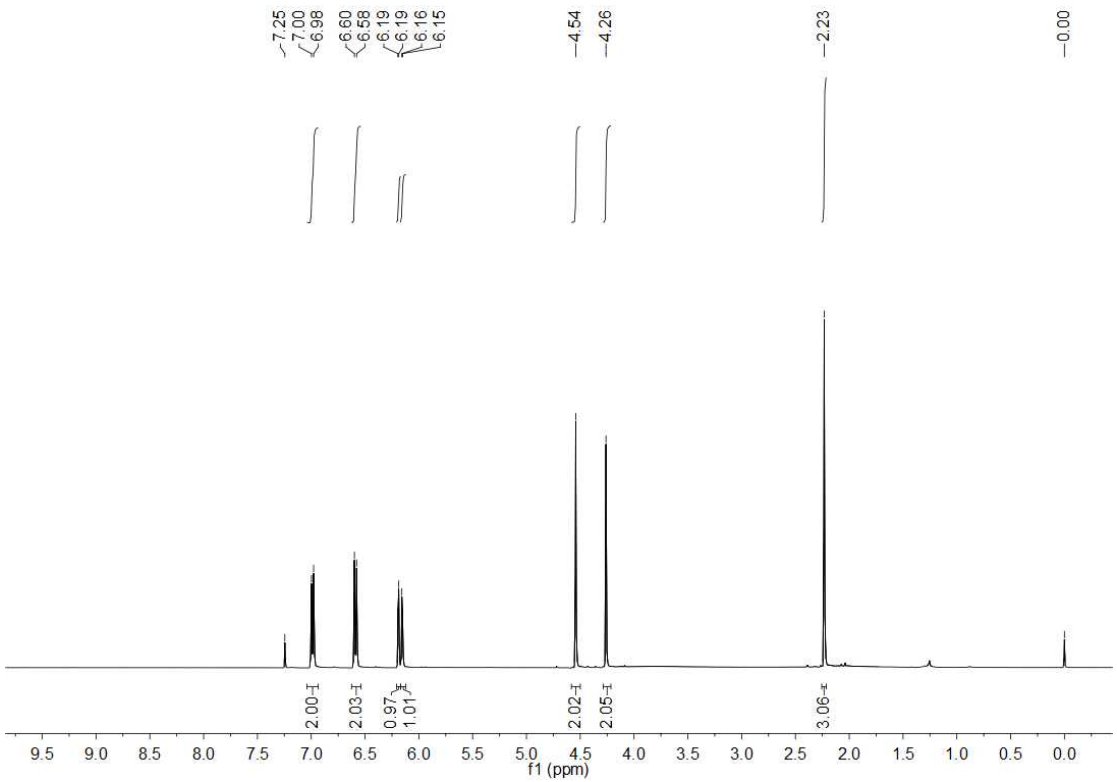
107.76
77.38
77.07
76.75
57.54
41.58
21.64
f1 (ppm)


HO
O
HN

3e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6.19
6.19
6.16
6.15
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4.26
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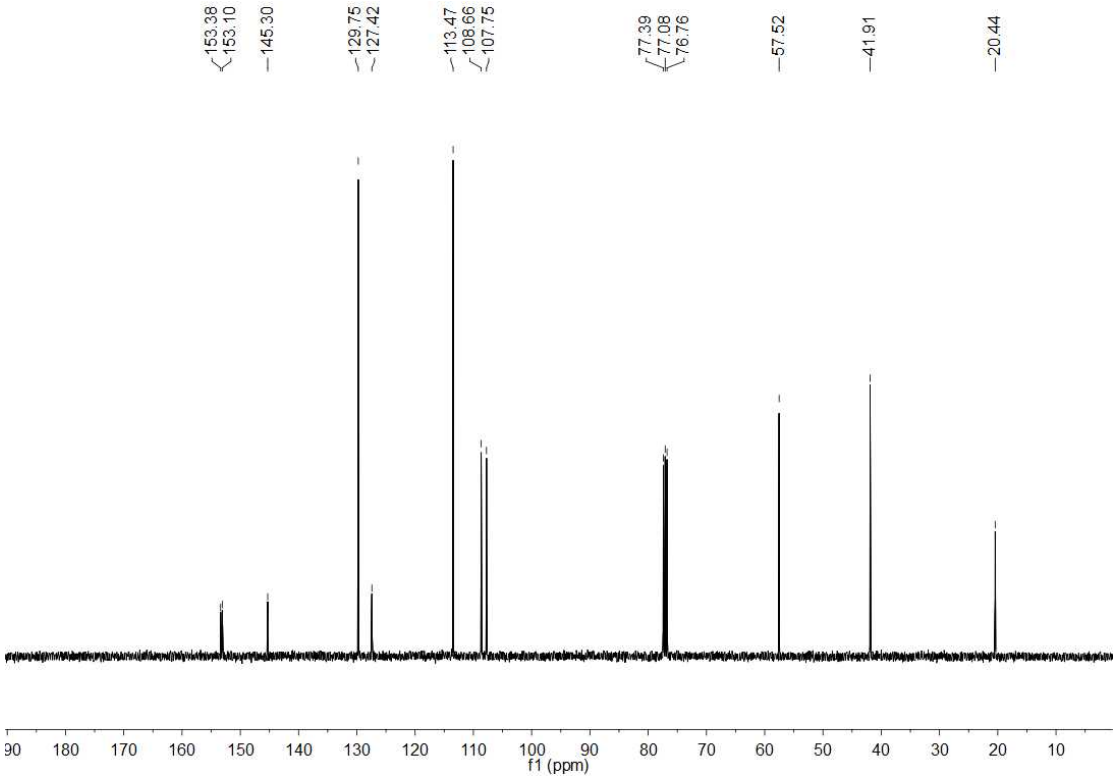
2.00
2.03
0.97
1.01
2.02
2.05
3.06
f1 (ppm)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107.75
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77.08
76.76
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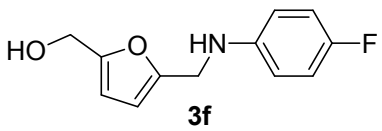
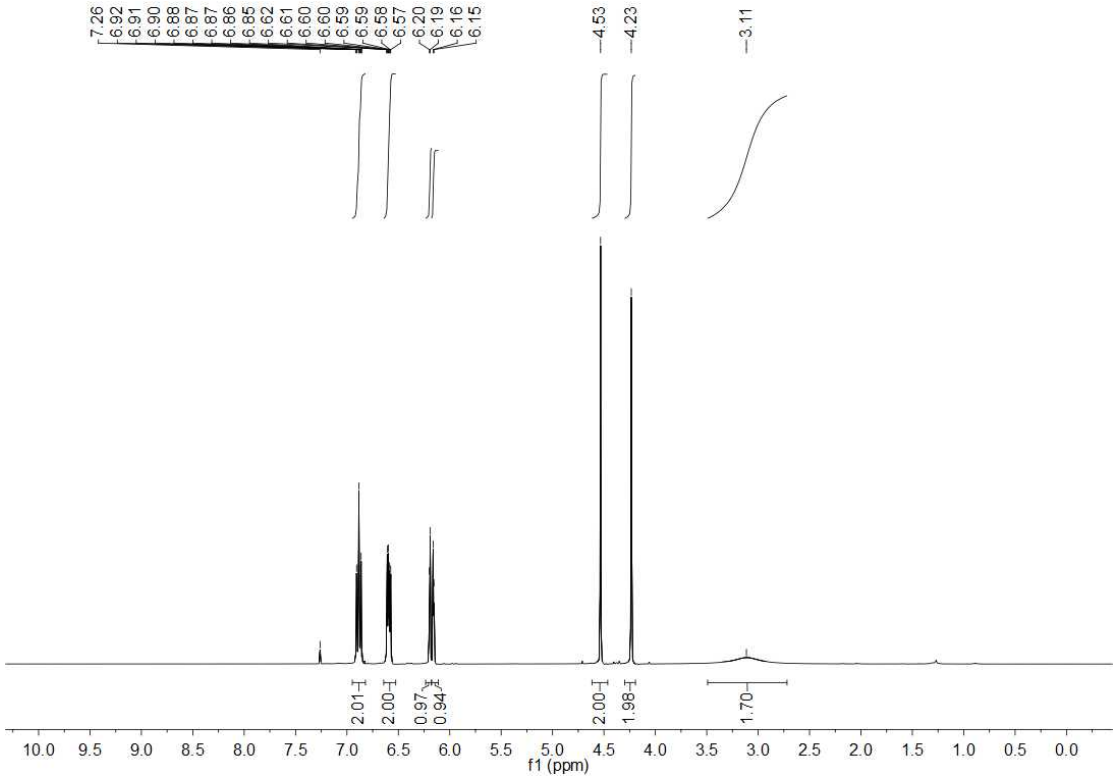
20.44
f1 (ppm)


HO
O
HN
F

3f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6.87
6.87
6.86
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6.62
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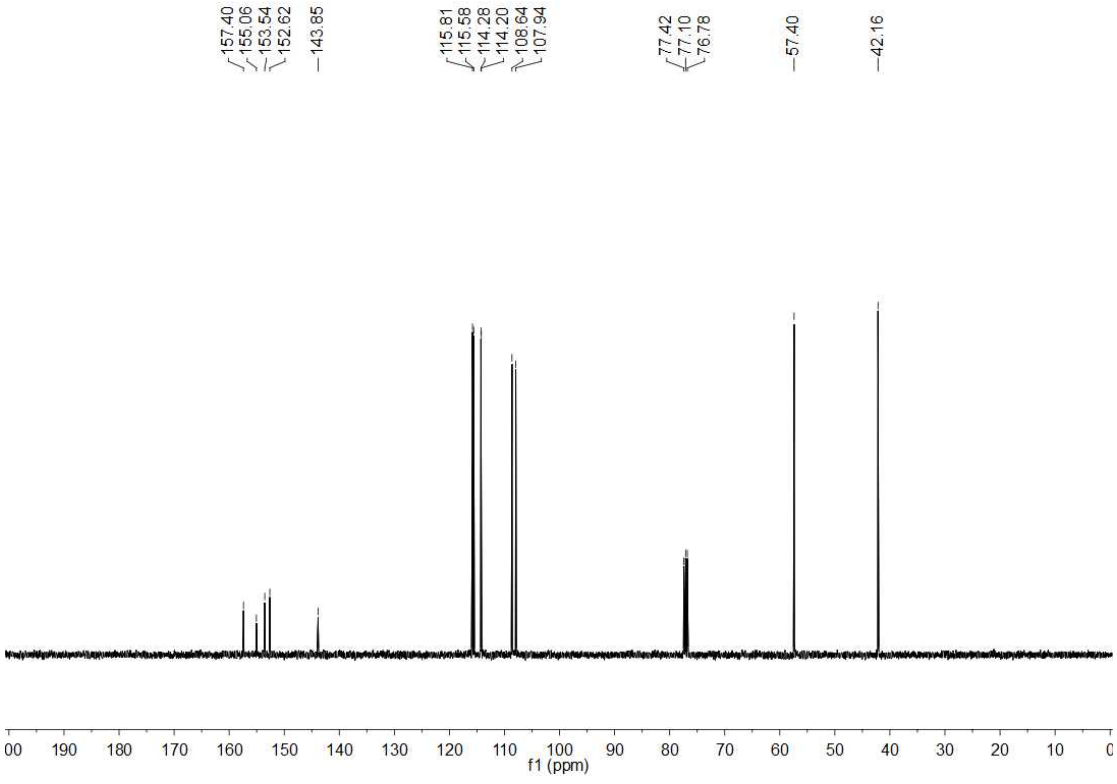
6.60
6.60
6.59
6.59
6.58
6.57
6.20
6.19
6.16
6.15
4.53
4.23
3.11
2.01
2.00
0.97
0.94
2.00
1.98
1.70
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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114.28
114.20
108.64
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77.10
76.78
57.40
42.16
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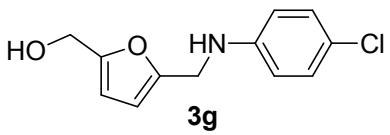
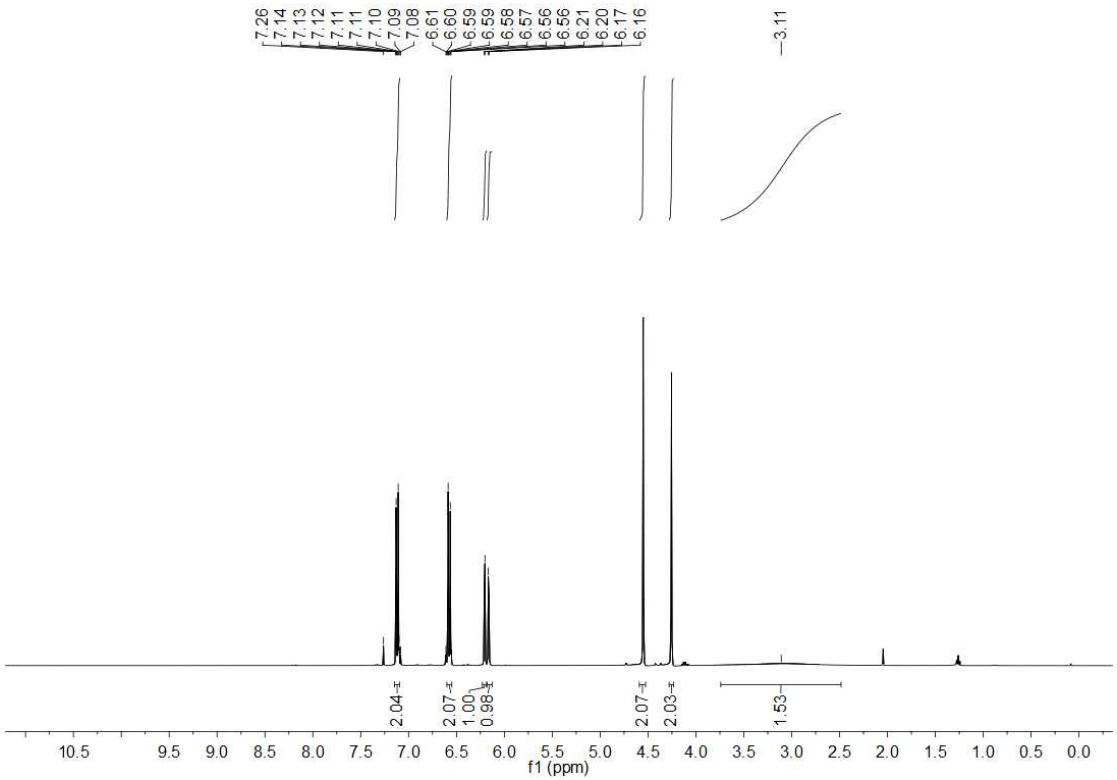
f1 (ppm)


HO
O
HN
Cl

3g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7.13
7.12
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7.11
7.10
7.09
7.08
6.61
6.60
6.59
6.59
6.58
6.57
6.56
6.56
6.21
6.20
6.17
6.16
3.11
2.04
2.07
1.00
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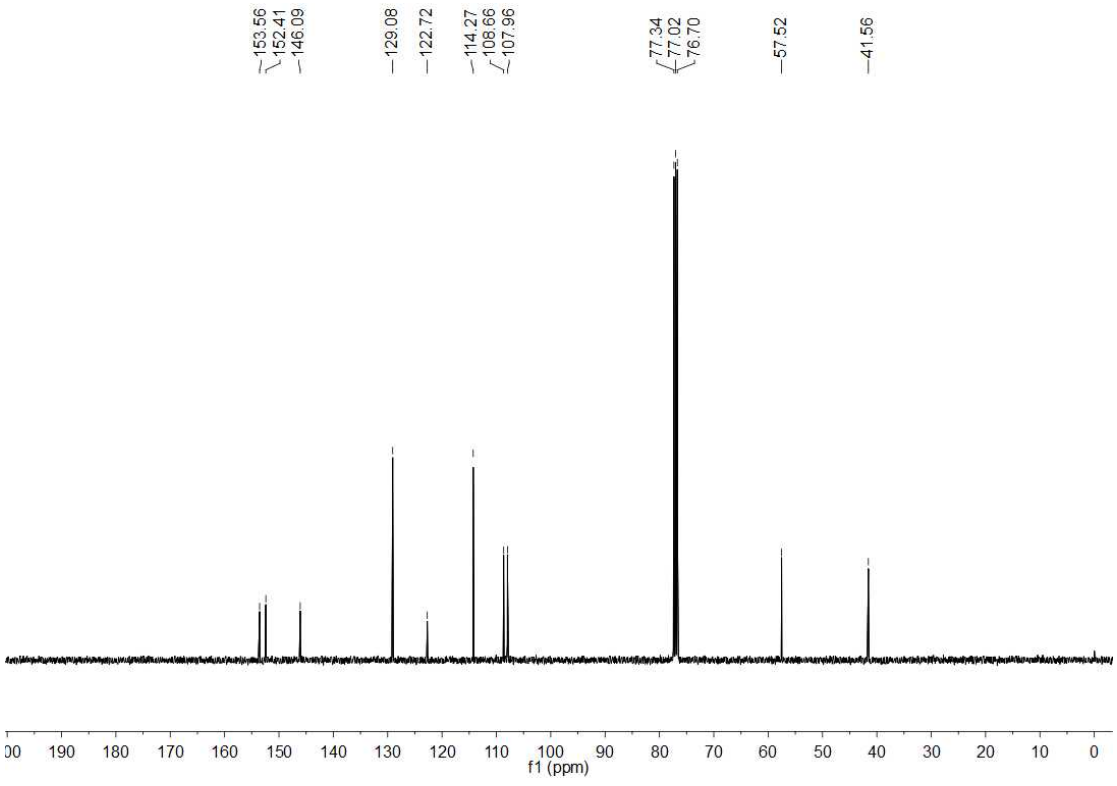
2.07
2.03
1.53
f1 (ppm)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76.70
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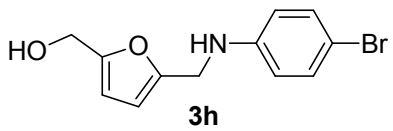
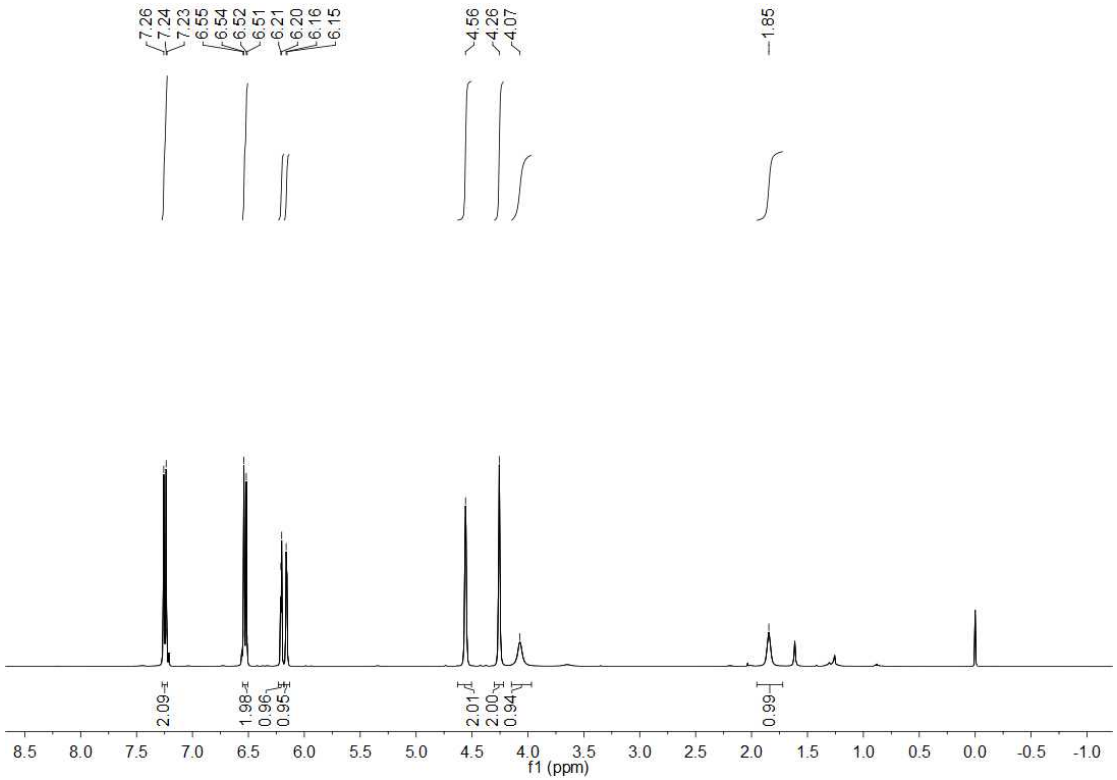
41.56
f1 (ppm)


HO
O
HN
Br

3h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6.15
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2.01
2.00
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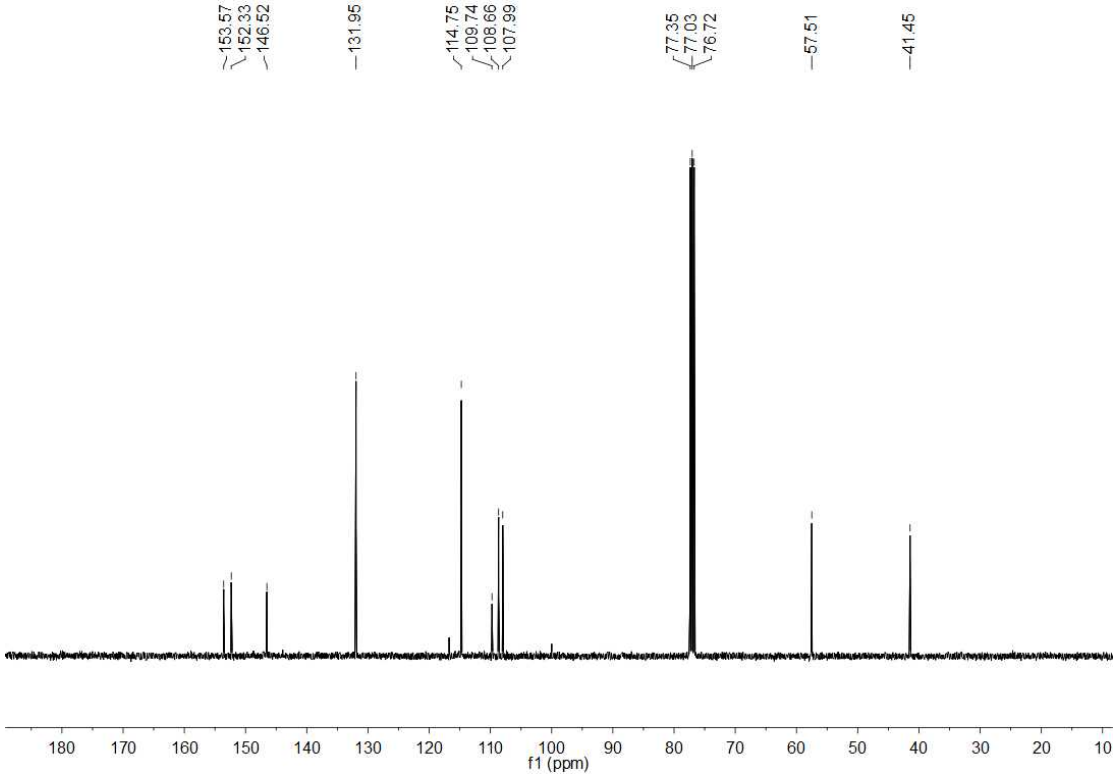
0.99
f1 (ppm)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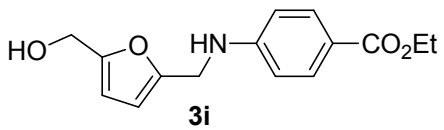
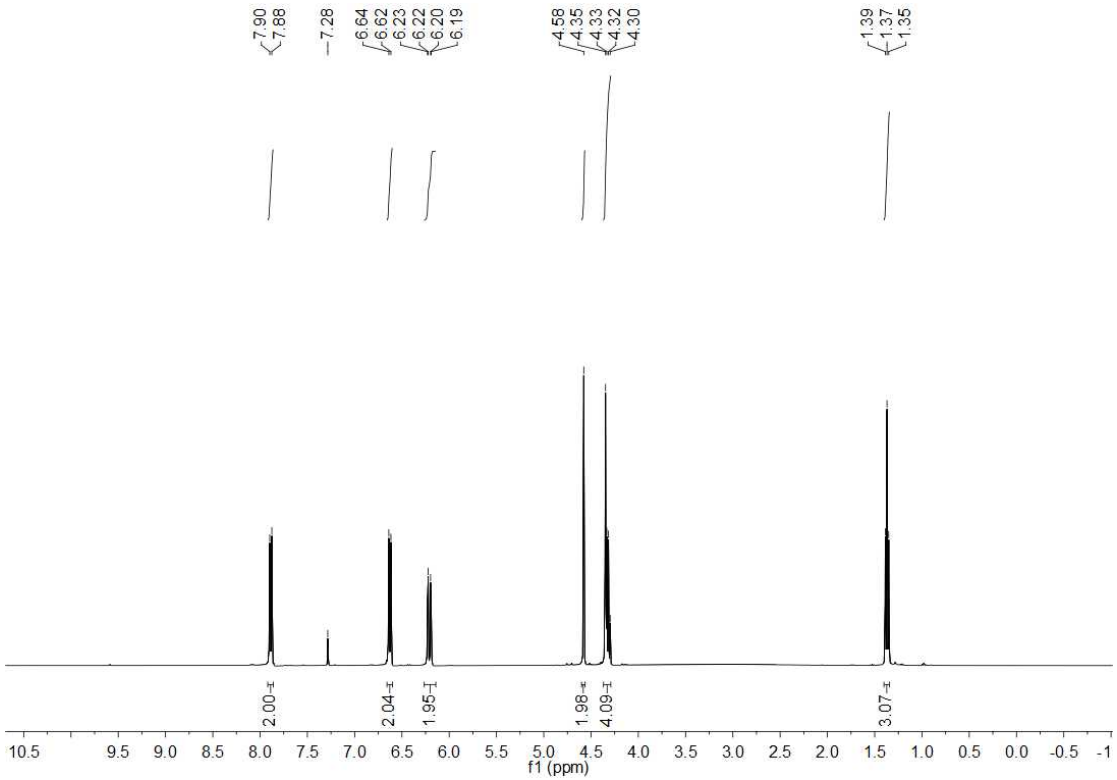
76.72
57.51
41.45
f1 (ppm)


HO
O
HN
CO2Et

3i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2.00
2.04
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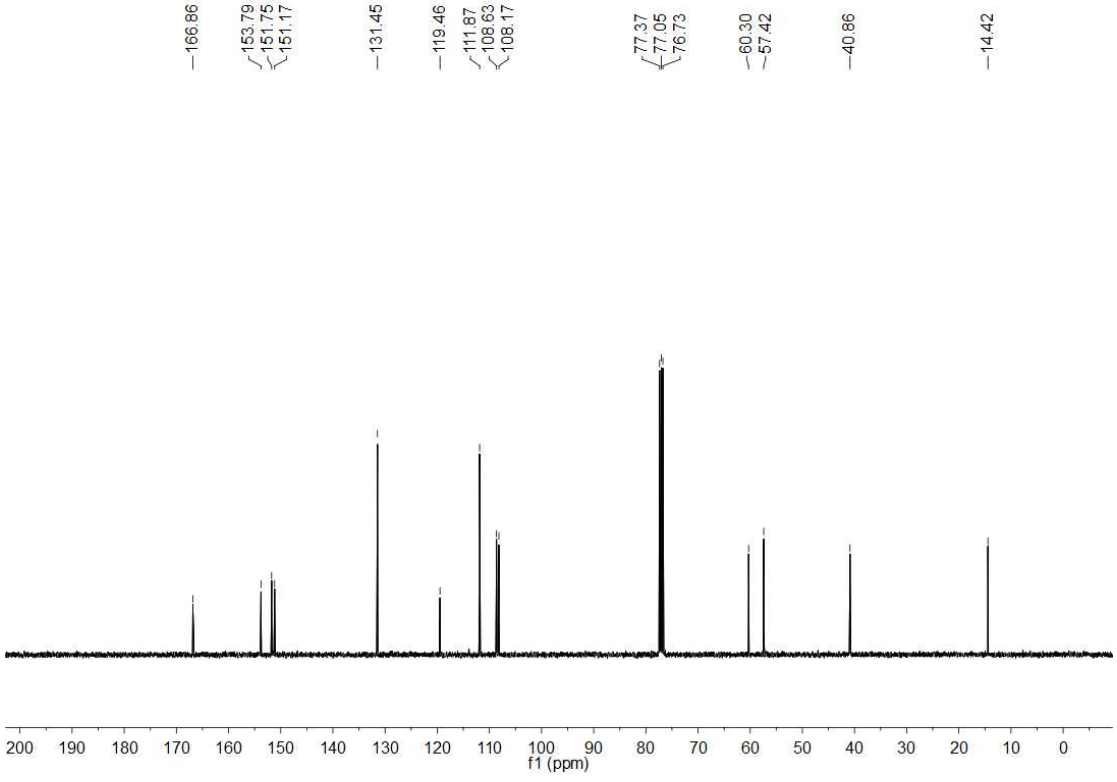
3.07
f1 (ppm)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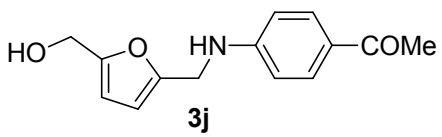
f1 (ppm)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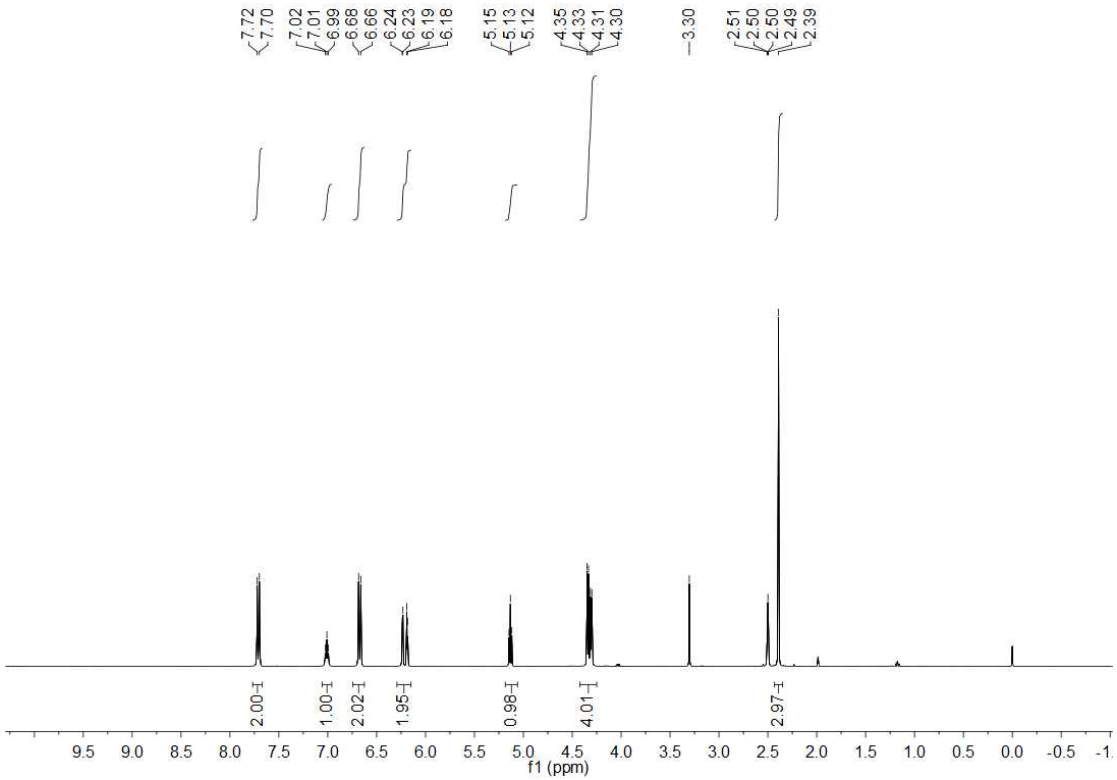
O
HN
COMe

3j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4.33
4.31
4.30
3.30
2.51
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2.39
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1.00
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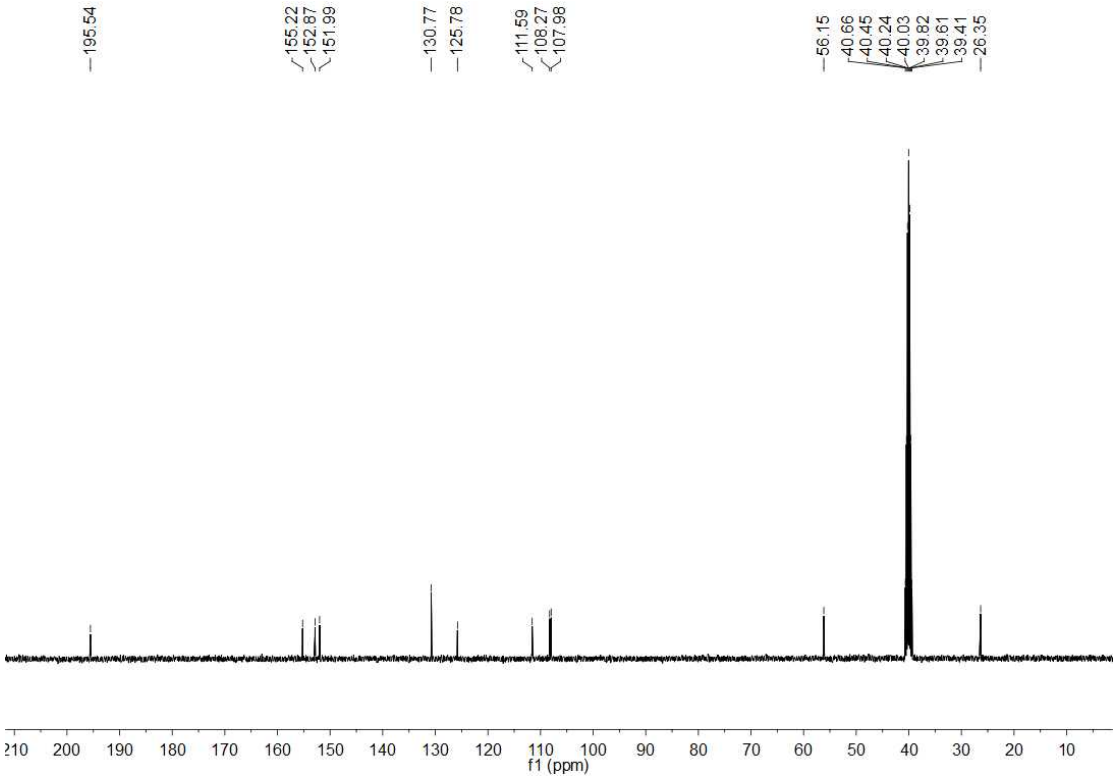
0.98
4.01
2.97
f1 (ppm)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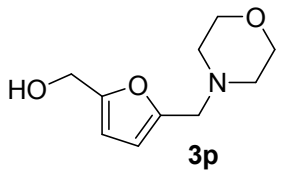
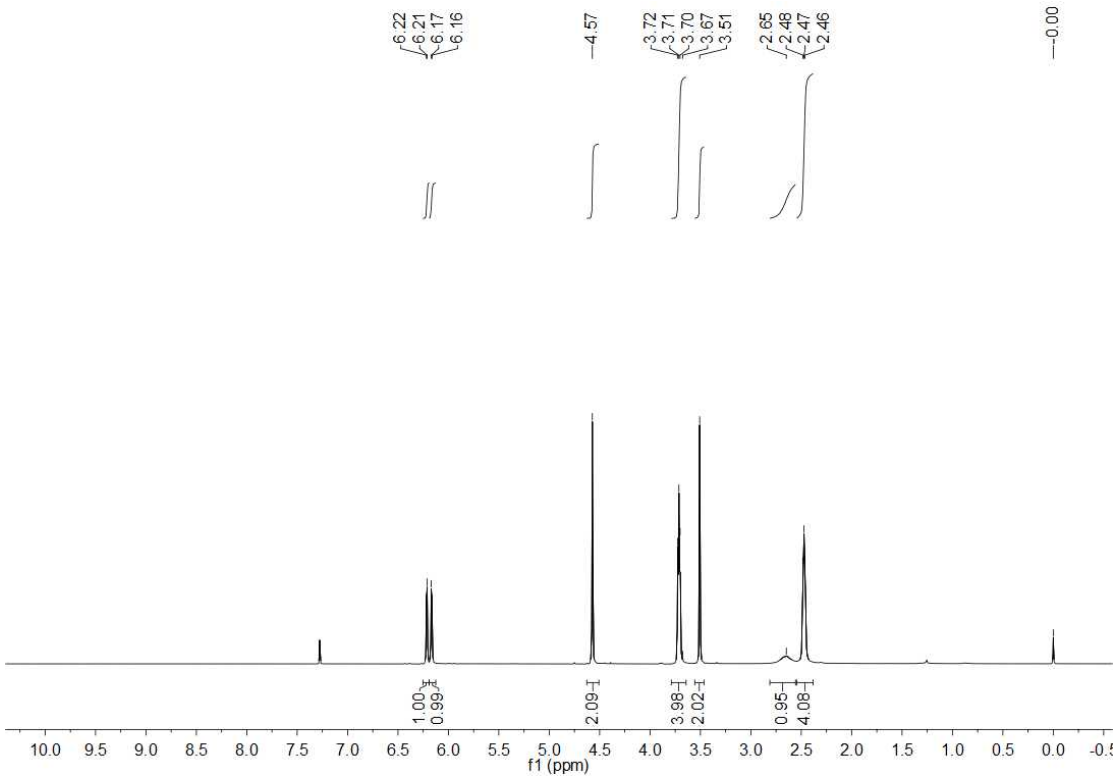
39.61
39.41
26.35
f1 (ppm)


HO
O
N
O

3p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2.02
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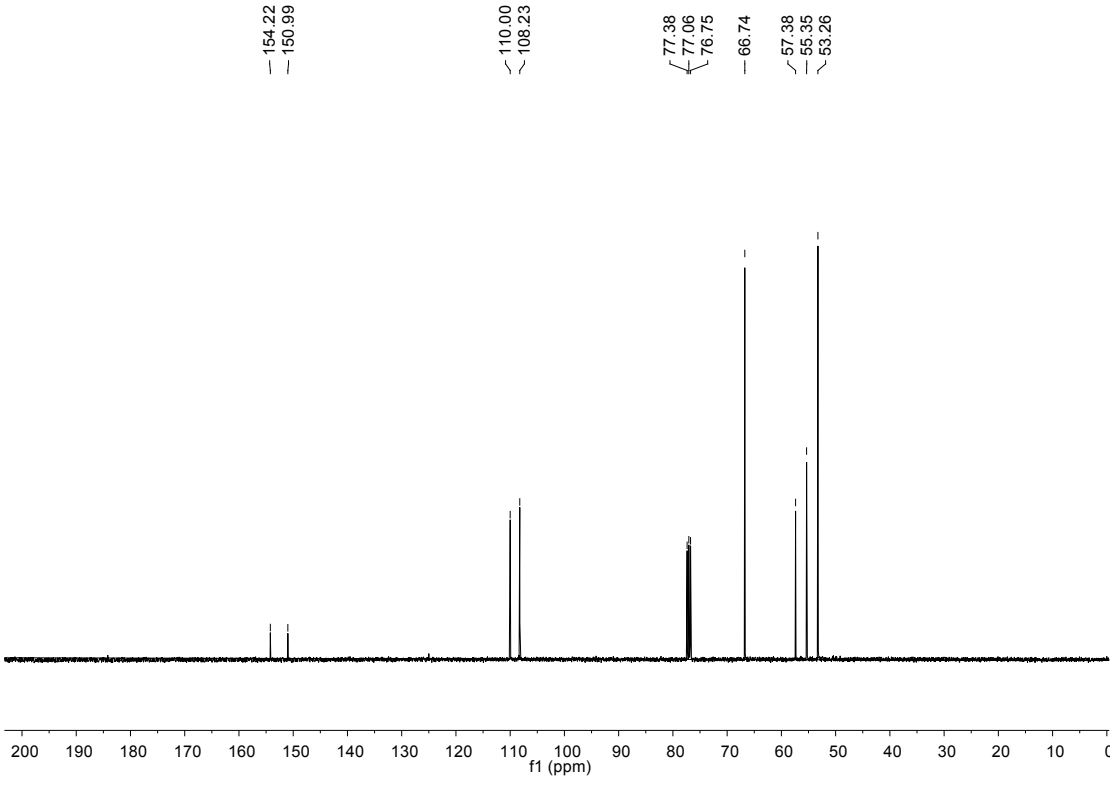
4.08
f1 (ppm)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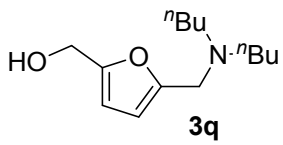
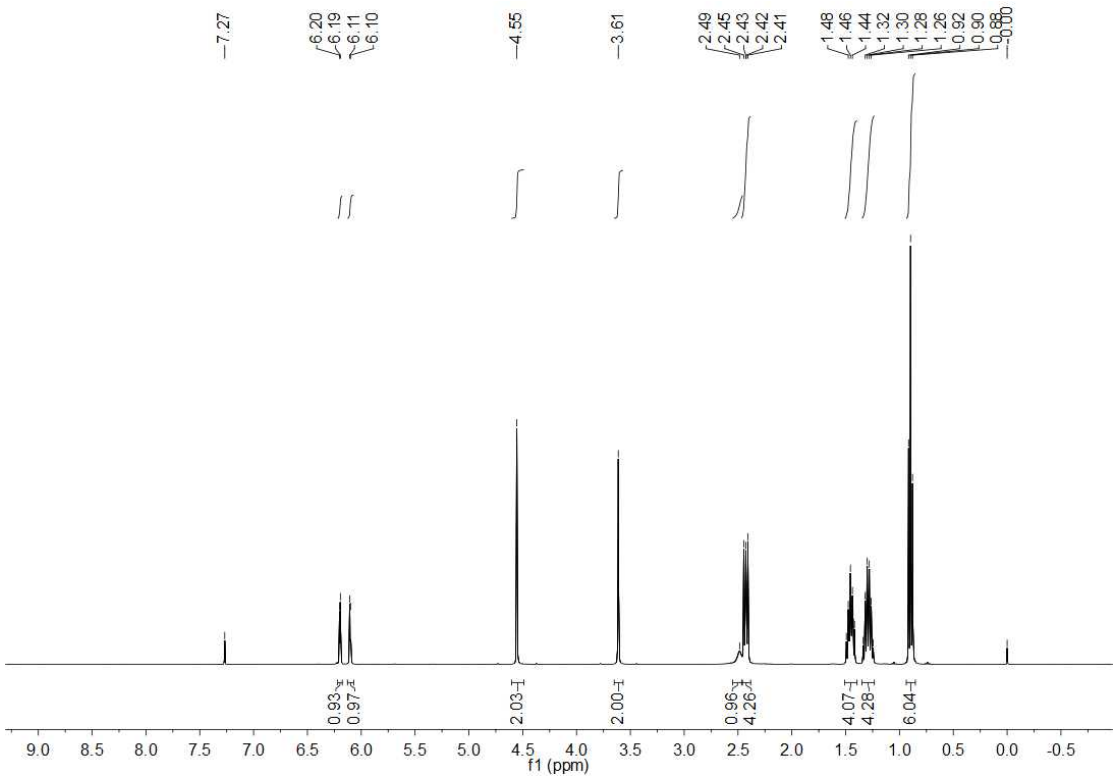

HO
O
N
nBu
nBu

3q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3.61
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2.43
2.42
2.41
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1.46
1.44
1.32
1.30
1.28
1.26
0.92
0.90
0.88
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0.97
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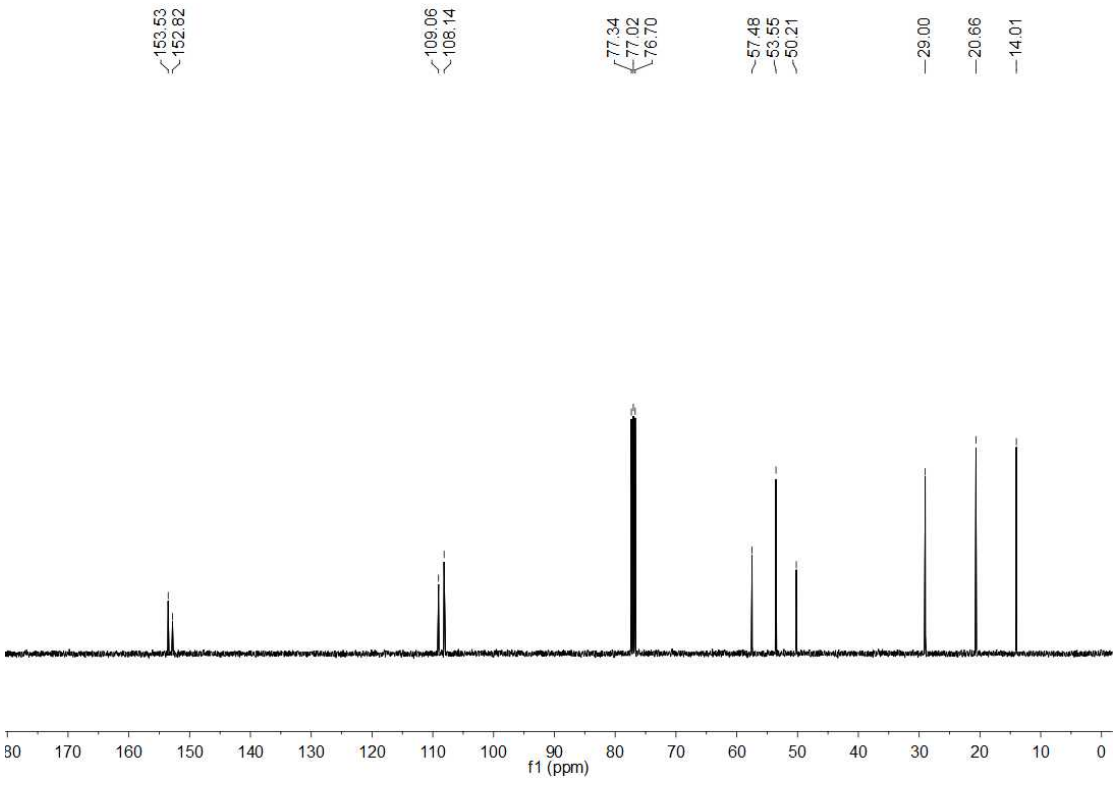
2.00
0.96
4.26
4.07
4.28
6.04
f1 (ppm)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57.48
53.55
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29.00
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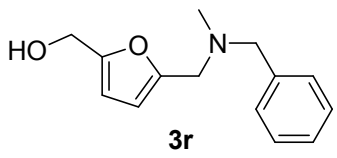
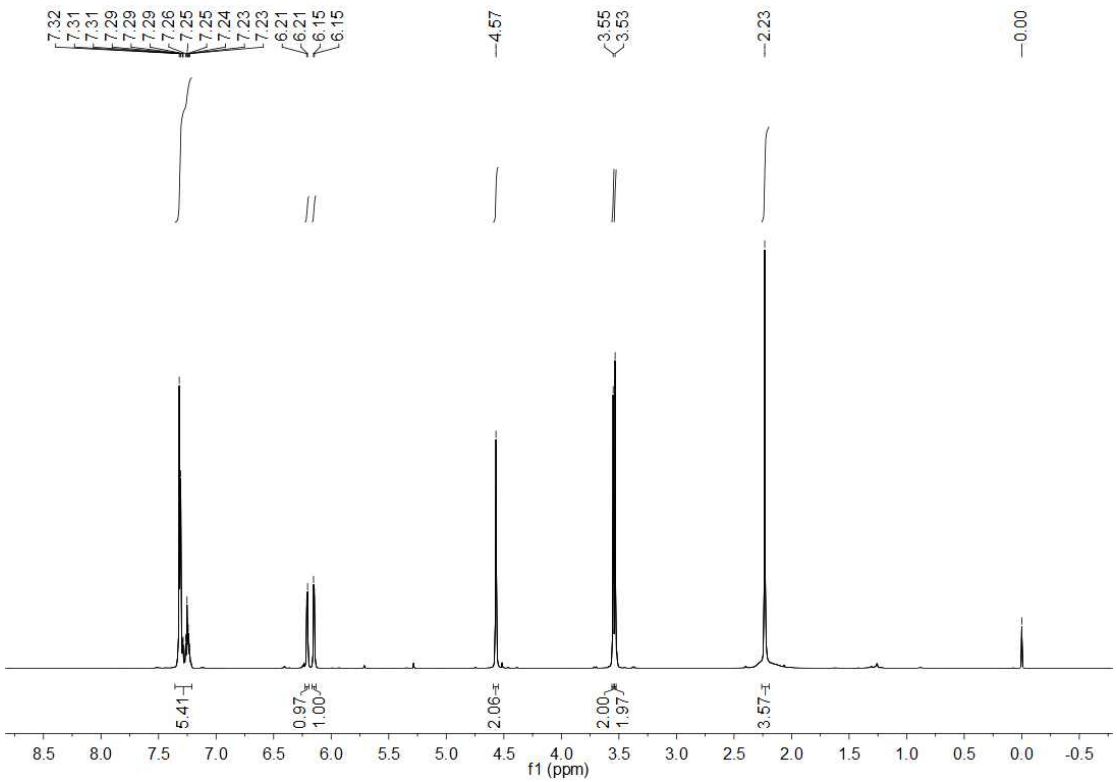
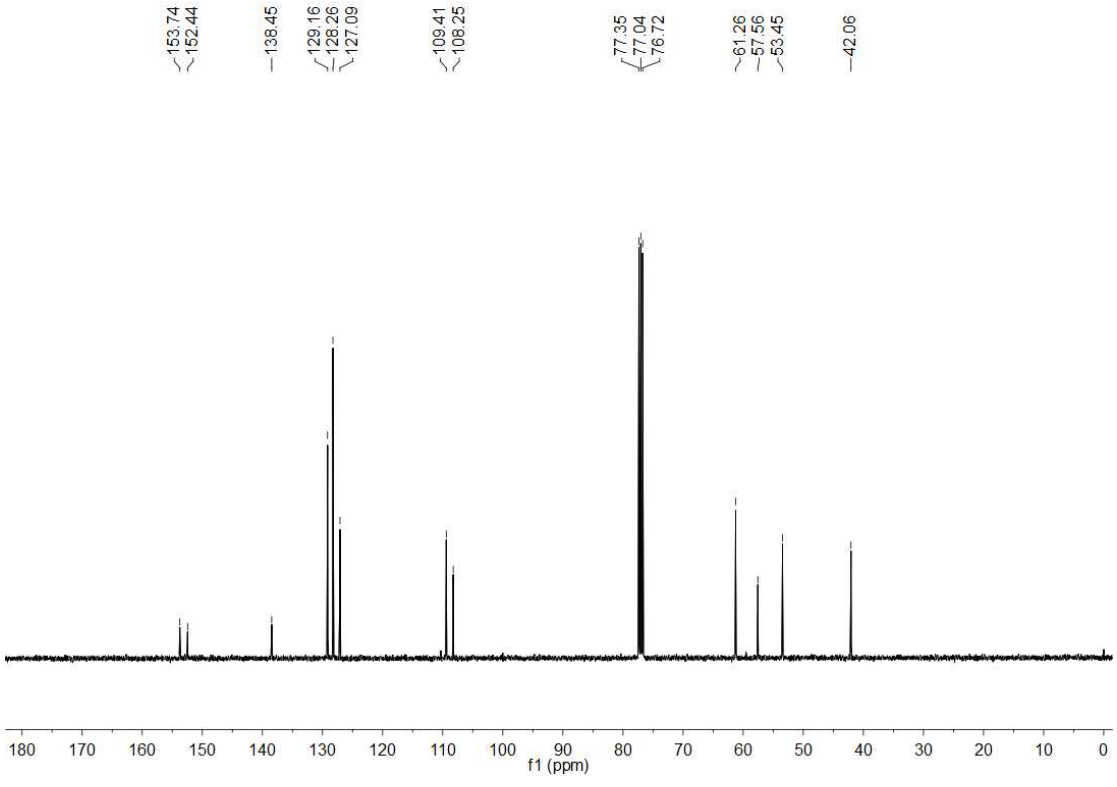
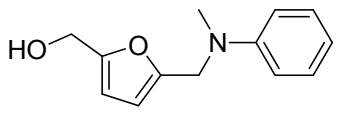
14.01
f1 (ppm)


HO
O
N

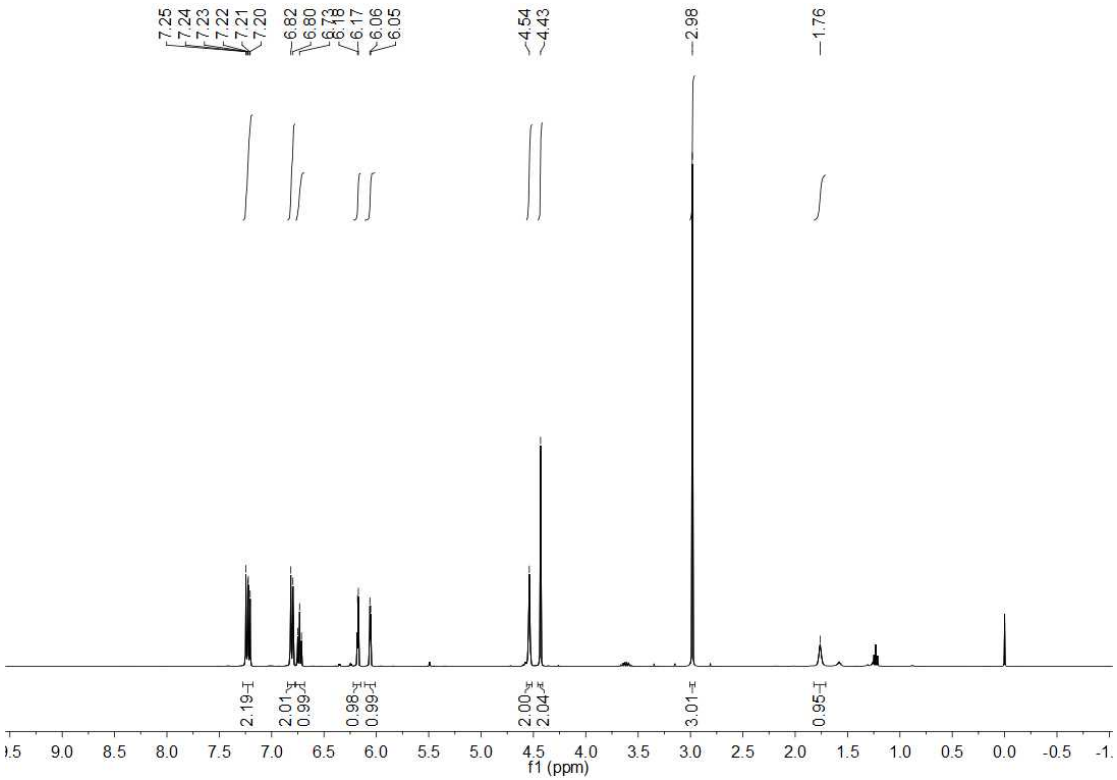
3r

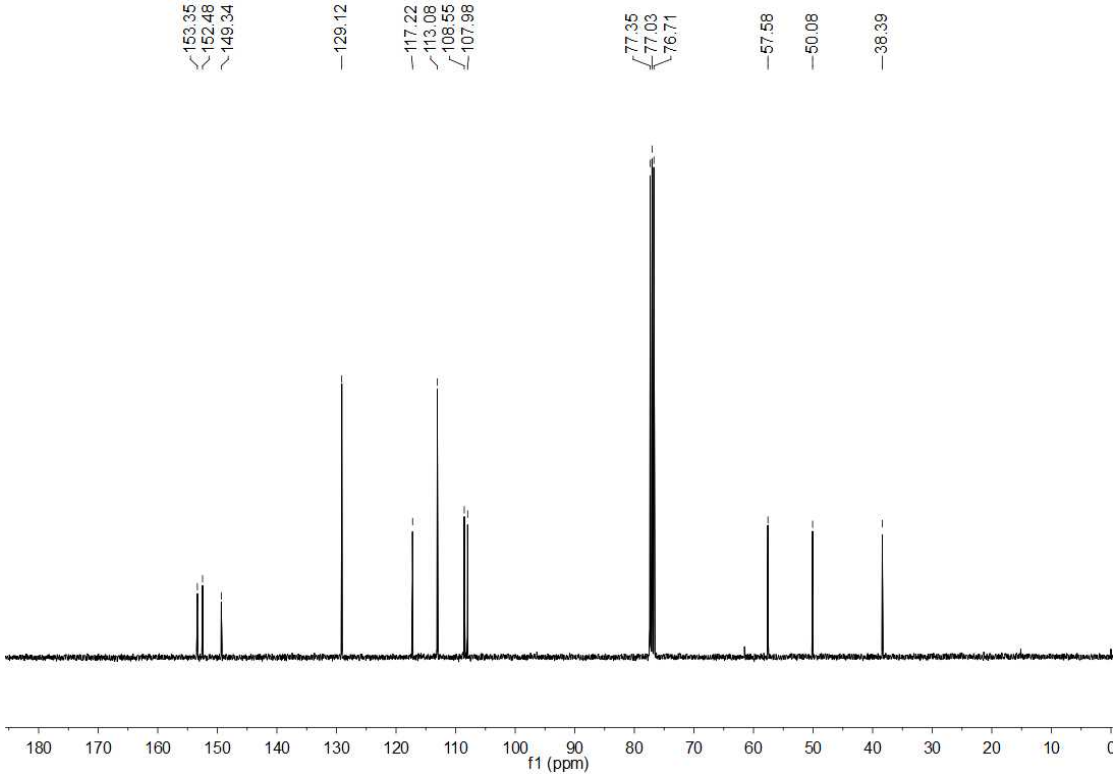

7.32
7.31
7.31
7.29
7.29
7.29
7.26
7.25
7.25
7.24
7.23
7.23
6.21
6.21
6.15
6.15
4.57
3.55
3.53
2.23
0.00
5.41
0.97
1.00
2.06
2.00
1.97
3.57
f1 (ppm)

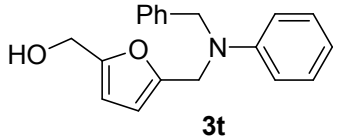

153.74
152.44
138.45
129.16
128.26
127.09
109.41
108.25
77.35
77.04
76.72
61.26
57.56
53.45
42.06
f1 (ppm)


HO
O
N

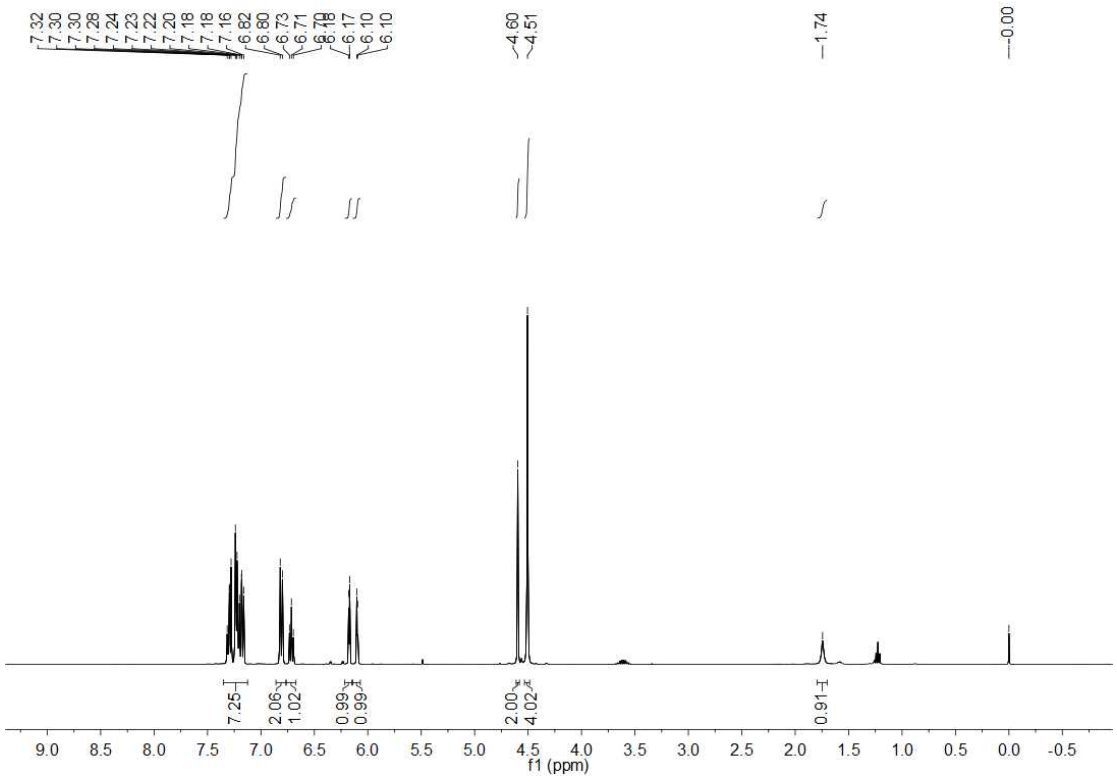
3s


7.25
7.24
7.23
7.22
7.21
7.20
6.82
6.80
6.18
6.17
6.06
6.05
4.54
4.43
2.98
1.76
2.19
2.01
0.99
0.98
0.99
2.00
2.04
3.01
0.95
f1 (ppm)


153.35
152.48
149.34
129.12
117.22
113.08
108.55
107.98
77.35
77.03
76.71
57.58
50.08
38.39
f1 (ppm)


Ph
HO
O
N

3t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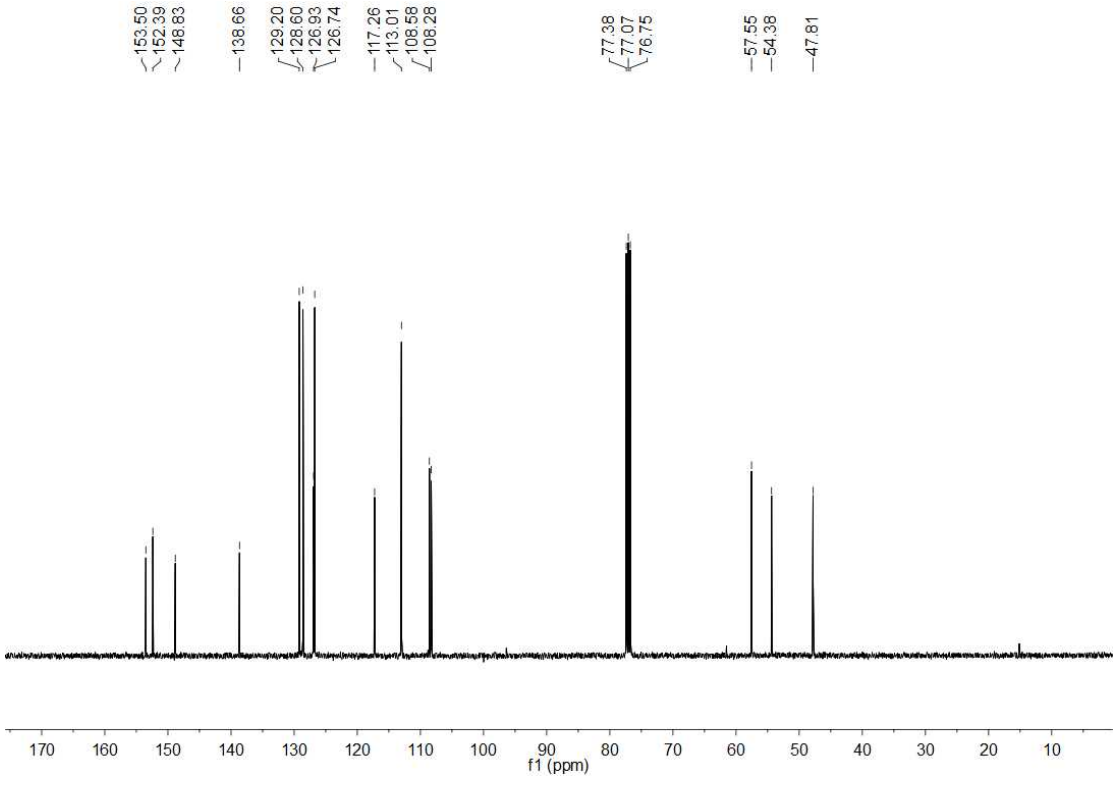
7.30
7.30
7.28
7.24
7.23
7.22
7.20
7.18
7.18
7.16
6.82
6.80
6.73
6.71
6.70
6.18
6.17
6.10
6.10
4.60
4.51
1.74
0.00
7.25
2.06
1.02
0.99
0.99
2.00
4.02
0.91
f1 (ppm)


153.50
152.39
148.83
138.66
129.20
128.60
126.93
126.74
117.26
113.01
108.58
108.28
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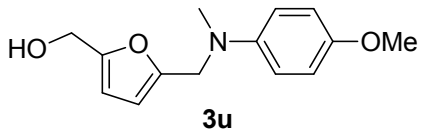
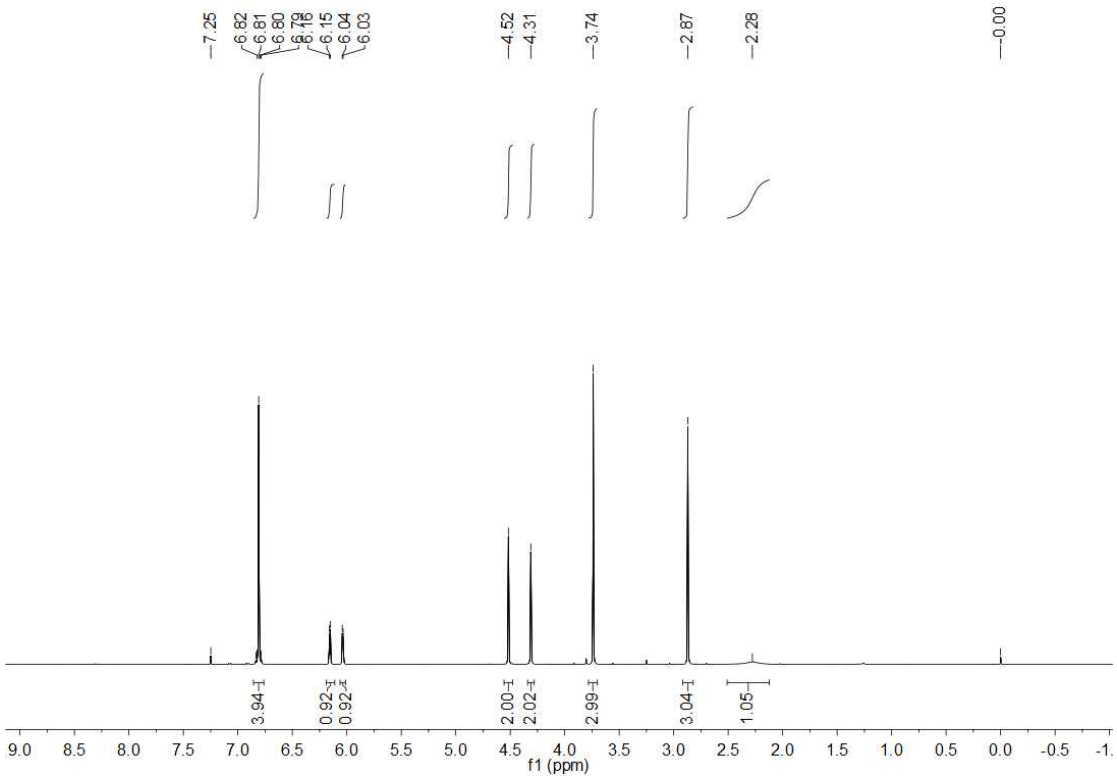
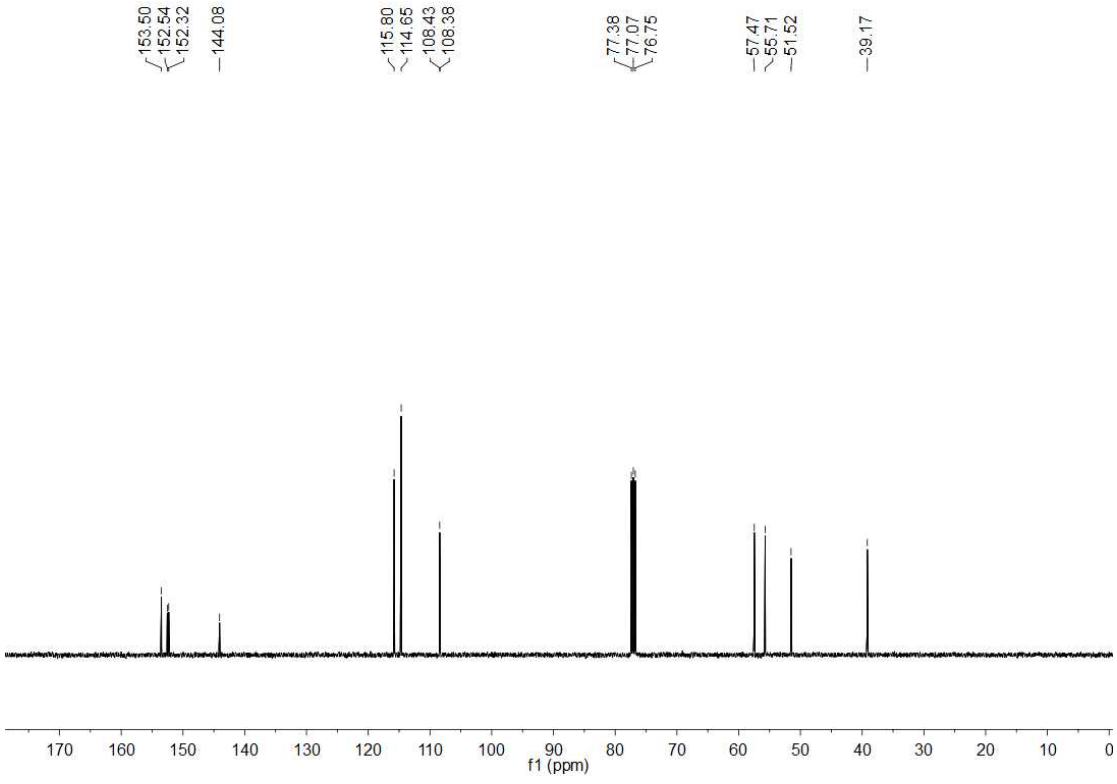
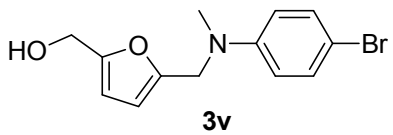
77.07
76.75
57.55
54.38
47.81
f1 (ppm)


HO
O
N
OMe

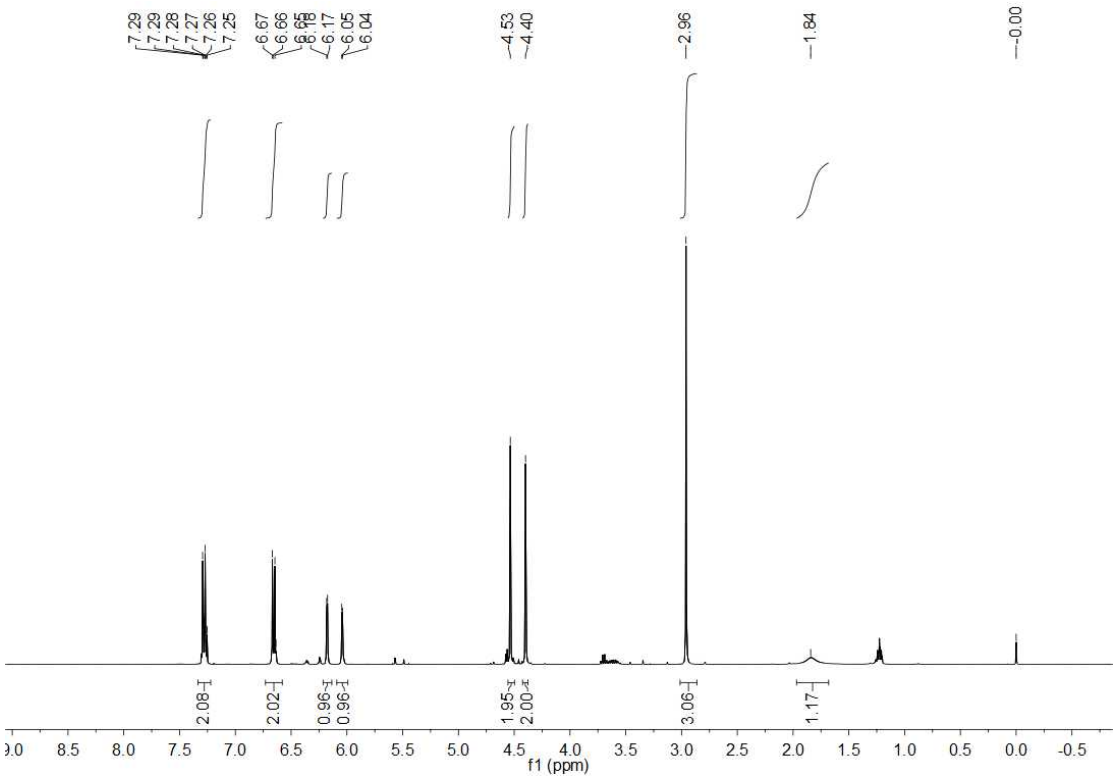
3u

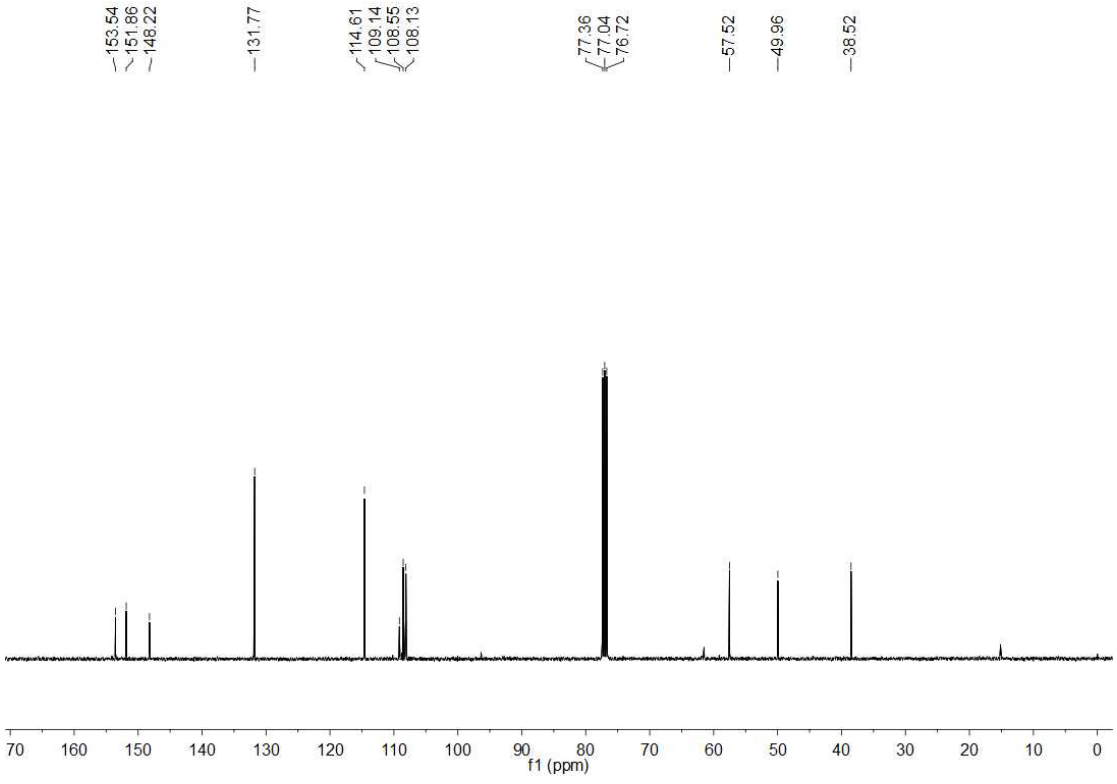

7.25
6.82
6.81
6.80
6.16
6.15
6.04
6.03
4.52
4.31
3.74
2.87
2.28
0.00
3.94
0.92
0.92
2.00
2.02
2.99
3.04
1.05
f1 (ppm)


153.50
152.54
152.32
144.08
115.80
114.65
108.43
108.38
77.38
77.07
76.75
57.47
55.71
51.52
39.17
f1 (ppm)


HO
O
N
Br

3v


7.29
7.29
7.28
7.27
7.26
7.25
6.67
6.66
6.65
6.18
6.17
6.05
6.04
4.53
4.40
2.96
1.84
0.00
2.08
2.02
0.96
0.96
1.95
2.00
3.06
1.17
f1 (ppm)


153.54
151.86
148.22
131.77
114.61
109.14
108.55
108.13
77.36
77.04
76.72
57.52
49.96
38.52
f1 (ppm)