Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

for

Gold-Catalyzed formation of Indole Derivatives from 2-Alkynyl Arylazides and Oxygen-Containing Heterocycles

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General Considerations

Analytical thin layer chromatography (TLC) was performed using Merck 60 F254 pre-coated silica gel plate. Visualization was achieved by UV light (254 nm). Flash chromatography was performed using Merck silica gel 60 with freshly distilled solvents. Unless otherwise stated, ^{1}H and ^{13}C NMR spectra were measured on Bruker AVANCE III 600 MHz spectrometer. Unless otherwise stated, chemical shifts (ppm) were recorded with respect to TMS in $CDCl_3$. Multiplicities were given as: s (singlet), bs (broad singlet), d (doublet), t (triplet), dd (doublet, doublet) or m (multiplets). The number of protons (n) for a given resonance is indicated by nH. Coupling constants are reported as a J value in Hz. Infrared spectra were recorded on NICOLET 6700 FTIR Spectrometer. High Resolution Mass (HRMS) spectra were obtained using LTQ Orbitrap. Mass spectral data were reported in units of mass to charge (m/z).

General procedure for gold-catalyzed formation of indole derivatives from 2-alkynyl arylazides and oxygen-containing heterocycles:

To a solution of 2-alkynyl arylazides **1**(0.1 mmol), oxygen-containing heterocycles **2** (0.5 mL) and MsOH (0.3mmol) was added *t*BuXPhosAuNTf$_2$ (2 mol%). The mixture was stirred at room temperature or 60 ℃ and monitored by TLC analysis. On completion, the reaction mixture was directly subjected to purification by flash column chromatography on silica gel (eluent: petrol ether: ethyl acetate = 8:1 to 4:1) to give the desired product **3**.

2-(2-((2-phenyl-1*H*-indol-3-yl)oxy)ethoxy)ethyl methanesulfonate (3a):

yield: 35.6 mg (95%); brown oil; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 2.99 (s, 3H), 3.70-3.71 (m, 2H), 3.77-3.78 (m, 2H), 4.25-4.26 (m, 2H), 4.33-4.34 (m, 2H), 7.11-7.13 (m, 1H), 7.18-7.21 (m, 1H), 7.29-7.31 (m, 1H), 7.33 (d, J = 8.1 Hz, 1H), 7.44-7.47 (m, 2H), 7.65 (d, J = 7.8 Hz, 1H), 7.84 (d, J = 7.8 Hz, 2H), 7.97 (br, 1H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 37.6, 68.9, 69.2, 70.4, 72.8, 111.4, 117.9, 119.8, 122.6, 122.8, 124.8, 125.7, 127.2, 128.8, 131.3, 133.7, 135.9; IR (neat): 2924, 1541, 1173, 785 cm^{-1}; HRMS (ESI) calcd. For $C_{19}H_{21}NO_5SNa$ $[M+Na]^+$ 398.1038, found: 398.1015.

2-(2-((2-(4-methoxyphenyl)-1*H*-indol-3yl)oxy) ethoxy)ethyl methanesulfonate (3b): yield: 34.4 mg (85%); brown oil; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 3.00 (s, 3H), 3.71-3.73 (m, 2H), 3.77-3.78 (m, 2H), 3.85 (s, 3H), 4.23-4.24 (m, 2H), 4.34-4.36 (m, 2H), 7.00 (d, J = 8.8 Hz, 2H), 7.09-7.16 (m, 2H), 7.31 (d, J = 8.1 Hz, 1H), 7.61 (d, J = 7.4 Hz, 1H), 7.77 (d, J = 8.7 Hz, 2H), 7.89 (br, 1H); 13C NMR ($CDCl_3$, 150 MHz) δ: 37.6, 55.3, 68.9, 69.2, 70.5, 72.7, 111.2, 114.3, 117.6, 119.7, 122.4, 124.0, 124.9, 127.1, 133.5, 158.8; IR (neat): 2915, 1182, 744 cm^{-1}; HRMS (ESI) calcd. For $C_{20}H_{23}NO_6SNa$ $[M+Na]^+$ 428.1144, found: 428.1118.

2-(2-((2-(4-ethylphenyl)-1*H*-indol-3-yl)oxy)ethoxy)ethyl methanesulfonate (3c):

yield: 37.5 mg (93%); brown oil; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 1.28 (t, J = 7.7 Hz, 3H), 2.67-2.71 (q, J = 7.7 Hz, 3H), 3.00 (s, 3H), 3.71-3.72 (m, 2H), 3.77-3.79 (m, 2H), 4.24-4.26 (m, 2H), 4.34-4.36 (m, 2H), 7.10-7.12 (m, 1H), 7.16-7.19 (m, 1H), 7.28 (d, J = 8.3 Hz, 2H), 7.31 (d, J = 8.2 Hz, 1H), 7.63 (d, J = 7.9 Hz, 1H), 7.75 (d, J = 8.2 Hz, 2H), 7.97

(br, 1H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 15.4, 28.6, 37.6, 68.9, 69.2, 70.4, 72.7, 111.3, 117.7, 119.7, 122.6, 122.7, 125.0, 125.7, 128.3, 128.7, 133.6, 135.4, 143.4; IR (neat): 2931, 1176, 771 cm^{-1}; HRMS (ESI) calcd. For $C_{21}H_{25}NO_5SNa$ $[M+Na]^+$ 426.1351, found: 426.1324.

2-(2-((2-(*p*-tolyl)-1*H*-indol-3-yl)oxy)ethoxy)ethyl methanesulfonate (3d):

yield: 34.2 mg (88%); brown oil; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 2.39 (s, 3H), 3.00 (s, 3H), 3.71-3.73 (m, 2H), 3.77-3.79 (m, 2H), 4.24-4.25 (m, 2H), 4.34-4.36 (m, 2H), 7.10-7.12 (m, 1H), 7.16-7.19 (m, 1H), 7.25 (d, J = 7.9 Hz, 2H), 7.31 (d, J = 8.1 Hz, 1H), 7.63 (d, J = 7.8 Hz, 1H), 7.73 (d, J = 8.2 Hz, 2H), 7.93 (br, 1H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 21.2, 37.6, 68.9, 69.2, 70.5, 72.7, 111.3, 117.7, 119.7, 122.6, 122.7, 125.0, 125.6, 128.5, 129.6, 133.6, 135.4, 137.1; IR (neat): 2923, 1175, 770 cm^{-1}; HRMS (ESI) calcd. For $C_{20}H_{23}NO_5SNa$ $[M+Na]^+$ 412.1195, found: 412.1170.

2-(2-((2-(4-chlorophenyl)-1*H*-indol-3-yl)oxy)ethoxy)ethyl methanesulfonate(3e):

yield: 27.0 mg (66%); brown oil; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 3.00 (s, 3H), 3.72-3.73 (m, 2H), 3.77-3.79 (m, 2H), 4.26 (br, 2H), 4.34-4.36 (m, 2H), 7.10-7.20 (m, 2H), 7.31 (d, J = 8.2 Hz, 1H), 7.40 (d, J = 8.6 Hz, 2H), 7.64 (d, J = 7.1 Hz, 1H), 7.77 (d, J = 8.5 Hz, 2H), 7.92 (br, 1H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 37.6, 69.0, 69.1, 70.4, 72.7, 111.5, 118.0, 120.0, 123.2, 123.6, 126.8, 129.0, 129.8, 132.7, 133.9; IR (neat): 2923, 1174, 746 cm^{-1}; HRMS (ESI) calcd. For $C_{19}H_{20}NO_5SClNa$ $[M+Na]^+$ 432.0648, found: 432.0622.

2-(2-((2-(thiophen-3-yl)-1*H*-indol-3-yl)oxy)ethoxy)ethyl methanesulfonate(3f):

yield: 29.0 mg (76%); brown oil; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 3.02 (s, 3H), 3.75-3.76 (m, 2H), 3.81-3.82 (m, 2H), 4.29-4.30 (m, 2H), 4.37-4.39 (m, 2H), 7.10-7.12 (m, 1H), 7.17-7.19 (m, 1H), 7.31 (d, J = 8.1 Hz, 1H), 7.42-7.43 (m, 1H), 7.62-7.66 (m, 3H), 7.91 (br, 1H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 37.6, 69.0, 69.1, 70.4, 72.7, 111.5, 118.0, 120.0, 123.2, 123.6, 126.8, 129.0, 129.8, 132.7, 133.9; IR (neat): 2923, 1075, 769 cm^{-1}; HRMS (ESI) calcd. For $C_{17}H_{19}NO_5S_2Na$ $[M+Na]^+$ 404.0602, found: 404.0580.

2-(2-((2-pentyl-1*H*-indol-3-yl)oxy)ethoxy)ethyl methanesulfonate(3g):

yield: 18.7 mg (63%); brown oil; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 0.90 (t, J = 7.1 Hz, 3H), 1.34-1.37 (m, 4H), 1.64-1.69 (m, 2H), 2.74 (t, J = 7.6 Hz, 2H), 3.00 (s, 3H), 3.81-3.83 (m, 2H), 3.84-3.86 (m, 2H), 4.19-4.20 (m, 2H), 4.42-4.44 (m, 2H), 7.06-7.08 (m, 1H), 7.10-7.12 (m, 1H), 7.23 (d, J = 8.0 Hz, 1H), 7.55 (d, J = 8.1 Hz, 1H), 7.54 (br, 1H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 14.0, 22.4, 24.6, 28.9, 31.5, 37.6, 69.1, 69.3, 70.6, 73.4, 110.8, 116.9, 119.2, 121.3, 121.8, 127.5, 132.8, 134.5; IR (neat): 2925, 1075, 746 cm^{-1}; HRMS (ESI) calcd. For $C_{18}H_{27}NO_5SNa$ $[M+Na]^+$ 392.1508, found: 392.1490.

2-(2-((2-(*tert*-butyl)-1*H*-indol-3-yl)oxy)ethoxy)ethyl methanesulfonate(3h):

yield: 10.0 mg (28%); brown oil; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 1.45 (s, 9H), 3.08 (s, 3H), 3.89-3.90 (m, 4H), 4.22-4.23 (m, 2H), 4.45-4.46 (m, 2H), 7.05-7.07 (m, 1H), 7.10-7.12 (m, 1H), 7.51 (br, 1H), 7.55 (d, J = 8.0 Hz, 2H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 29.7, 32.0, 37.7, 69.2, 69.3, 70.9, 73.2, 110.9, 117.2, 119.2, 121.3, 122.4, 131.9, 133.6,

133.8; IR (neat): 2924, 1174, 748 cm^{-1}; HRMS (ESI) calcd. For $C_{17}H_{25}NO_5SNa$ $[M+Na]^+$ 378.1351, found: 378.1330.

2-(2-((2-butyl-1*H*-indol-3-yl)oxy)ethoxy)ethyl methanesulfonate(3i):

yield: 17.9 mg (60%); brown oil; ^1H NMR ($CDCl_3$, 600 MHz) δ: 0.94 (t, J = 7.4 Hz, 3H), 1.38-1.43 (m, 2H), 1.62-1.67 (m, 4H), 2.75 (t, J = 7.6 Hz, 2H), 3.06 (s, 1H), 3.81-3.83 (m, 2H), 3.84-3.86 (m, 2H), 4.19-4.20 (m, 2H), 4.42-4.44 (m, 2H), 7.05-7.08 (m, 1H), 7.09-7.12 (m, 1H), 7.23 (d, J = 8.0 Hz, 1H), 7.54-7.55 (m, 2H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 13.8, 22.5, 24.4, 31.4, 37.7, 69.1, 69.3, 70.6, 73.4, 110.8, 116.9, 119.2, 121.3, 121.8, 127.5, 132.8, 134.5; IR (neat): 2925, 1175, 755 cm^{-1}; HRMS (ESI) calcd. For $C_{17}H_{25}NO_5SNa$ $[M+Na]^+$ 378.1351, found: 378.1326.

2-(2-((6-chloro-2-phenyl-1*H*-indol-3-yl)oxy)ethoxy)ethyl methanesulfonate(3l):

yield: 36.8 mg (90%); brown oil; ^1H NMR ($CDCl_3$, 600 MHz) δ: 3.00 (s, 3H), 3.70-3.71 (m, 2H), 3.76-3.77 (m, 2H), 4.21-4.22 (m, 2H), 4.33-4.34 (m, 2H), 7.06-7.08 (m, 1H), 7.29-7.32 (m, 2H), 7.43-7.46 (m, 2H), 7.54 (d, J = 8.5 Hz, 1H), 7.80-7.82 (m, 2H), 8.04 (br, 1H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 37.6, 69.0, 69.1, 70.4, 72.9, 111.3, 118.8, 120.5, 121.2, 125.5, 125.7, 127.4, 128.6, 128.9, 130.9, 133.9, 135.7; IR (neat): 2924, 1074, 770 cm^{-1}; HRMS (ESI) calcd. For $C_{19}H_{21}NO_5SClNa$ $[M+Na]^+$ 432.0648, found: 432.0622.

2-(2-((5,7-dichloro-2-phenyl-1*H*-indol-3-yl)oxy)ethoxy)ethyl methanesulfonate(3m):

yield: 24.8 mg (56%); brown oil; ^1H NMR ($CDCl_3$, 600 MHz) δ: 3.02 (s, 3H), 3.72-3.73 (m, 2H), 3.76-3.78 (m, 2H), 4.19-4.21 (m, 2H), 4.35-4.36 (m, 2H), 7.19 (s, 1H), 7.35-

7.37 (m, 1H), 7.47-7.50 (m, 2H), 7.54 (s, 1H), 7.84-7.86 (m, 2H), 8.07 (br, 1H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 37.6, 69.0, 69.0, 70.3, 73.1, 116.2, 117.3, 122.1, 124.5, 125.5, 126.0, 127.4, 128.1, 129.0, 129.1, 130.3, 135.7; IR (neat): 2924, 1174, 772 cm^{-1}; HRMS (ESI) calcd. For $C_{19}H_{19}NO_5SCl_2Na$ $[M+Na]^+$ 466.0259, found: 466.0233.

5,7-dichloro-2-phenyl-1*H*-indol-3-yl methanesulfonate(4b):

yield: 10.3 mg (29%); brown oil; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 2.80 (s, 3H), 7.15-7.16 (m, 1H), 7.33-7.36 (m, 1H), 7.41-7.44 (m, 2H), 7.55 (s, 1H), 7.65-7.67 (m, 2H), 8.24 (br, 1H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 37.3, 117.1, 117.4, 123.1, 124.1, 125.1, 127.1, 128.6, 128.8, 128.9, 129.5, 130.2, 134.3; IR (neat): 2923, 1075, 775 cm^{-1}; HRMS (ESI) calcd. For $C_{15}H_{11}NO_3SCl_2Na$ $[M+Na]^+$ 377.9734, found: 3377.9738.

2-(2-((5,7-dimethyl-2-phenyl-1*H*-indol-3-yl)oxy)ethoxy)ethyl methanesulfonate(3n):

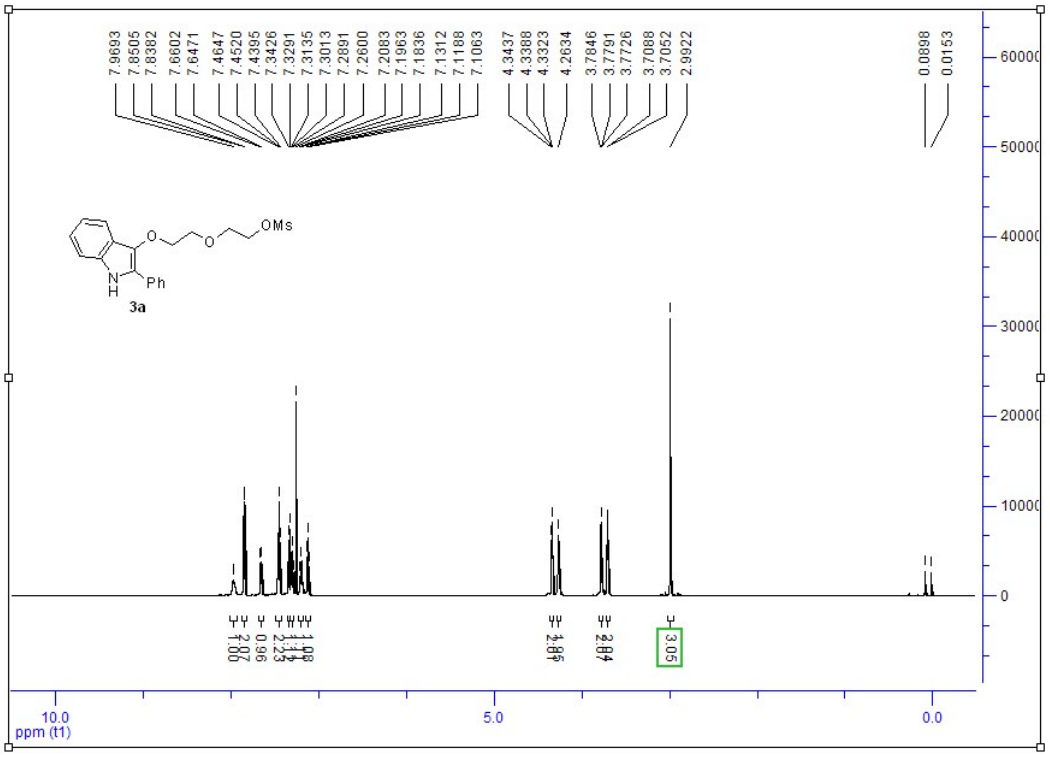
yield: 17.7 mg (44%); brown oil; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 2.43 (s, 3H), 2.47 (s, 3H), 3.00 (s, 3H), 3.71-3.72 (m, 2H), 3.77-3.79 (m, 2H), 4.25-4.26 (m, 2H), 4.34-4.36 (m, 2H), 6.85 (s, 1H), 7.28-7.31 (m, 2H), 7.44-7.47 (m, 2H), 7.59 (br, 1H), 7.85 (d, J = 7.3 Hz, 2H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 16.1, 21.4, 37.6, 69.0, 69.3, 70.5, 72.7, 115.2, 120.2, 122.4, 124.8, 125.3, 125.7, 127.1, 127.6, 128.8, 129.4, 131.7, 136.1; IR (neat): 2923, 1174, 768 cm^{-1}; HRMS (ESI) calcd. For $C_{21}H_{25}NO_5SNa$ $[M+Na]^+$ 426.1351, found: 426.1324.

5-((2-phenyl-1*H*-indol-3-yl)oxy)pentyl methanesulfonate (3o):

yield: 27.2 mg (73%); brown oil; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 1.61-1.67 (m, 2H), 1.77-1.86 (m, 4H), 4.13-4.15 (m, 2H), 4.23 (t, J = 6.5 Hz, 2H), 7.13-7.15 (m, 1H), 7.21-7.23 (m, 1H), 7.31-7.36 (m, 2H), 7.46-7.49 (m, 2H), 7.65 (d, J = 7.7 Hz, 1H), 7.83 (d, J = 7.4 Hz, 2H), 7.91 (br, 1H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 22.2, 28.9, 29.6, 37.3, 69.8, 73.4, 111.4, 118.0, 119.7, 122.8, 124.6, 125.7, 127.1, 128.8, 131.5, 133.8; IR (neat): 2922, 1071,768 cm^{-1}; HRMS (ESI) calcd. For $C_{20}H_{23}NO_4SNa$ $[M+Na]^+$ 396.1245, found: 396.1267.

2-(2-((2-phenyl-1*H*-indol-3-yl)oxy)ethoxy)ethyl 4-methylbenzenesulfonate (5):

yield: 27.6 mg (61%); yellow oil; ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 2.38 (s, 3H), 3.63-3.65 (m, 2H), 3.67-3.69 (m, 2H), 4.11-4.13 (m, 2H), 4.15-4.16 (m, 2H), 7.09-7.11 (m, 1H), 7.16-7.21 (m, 1H), 7.27 (d, J = 7.8 Hz, 3H), 7.33 (d, J = 8.4 Hz, 1H),7.40-7.42 (m, 2H), 7.63-7.65 (m, 1H), 7.78 (d, J = 8.4 Hz, 2H), 7.82 (d, J = 7.8 Hz, 2H), 7.94 (br, 1H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 21.5, 68.6, 69.2, 70.3, 72.8, 111.3, 118.0, 118.1, 119.7, 119.8, 122.7, 122.8, 124.8, 125.7, 127.1, 127.9, 128.8, 129.8, 133.0, 144.7; IR (neat): 2924, 1075, 776 cm^{-1}; HRMS (ESI) calcd. For $C_{25}H_{25}NO_5SNa$ $[M+Na]^+$ 474.1351, found: 474.1360.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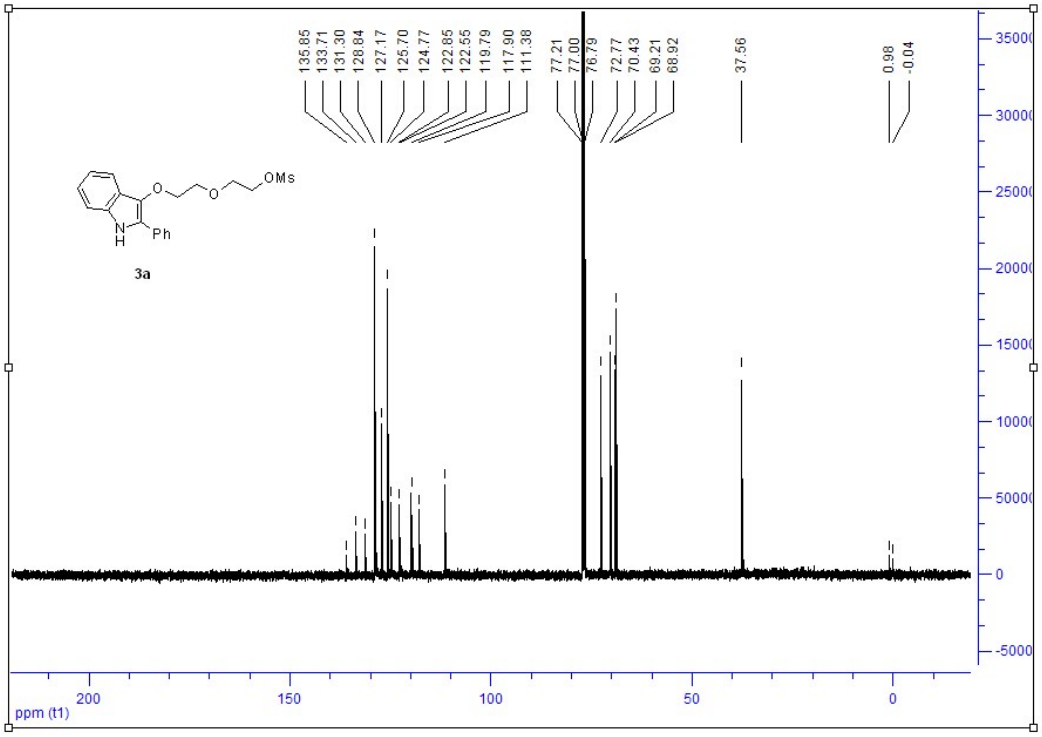
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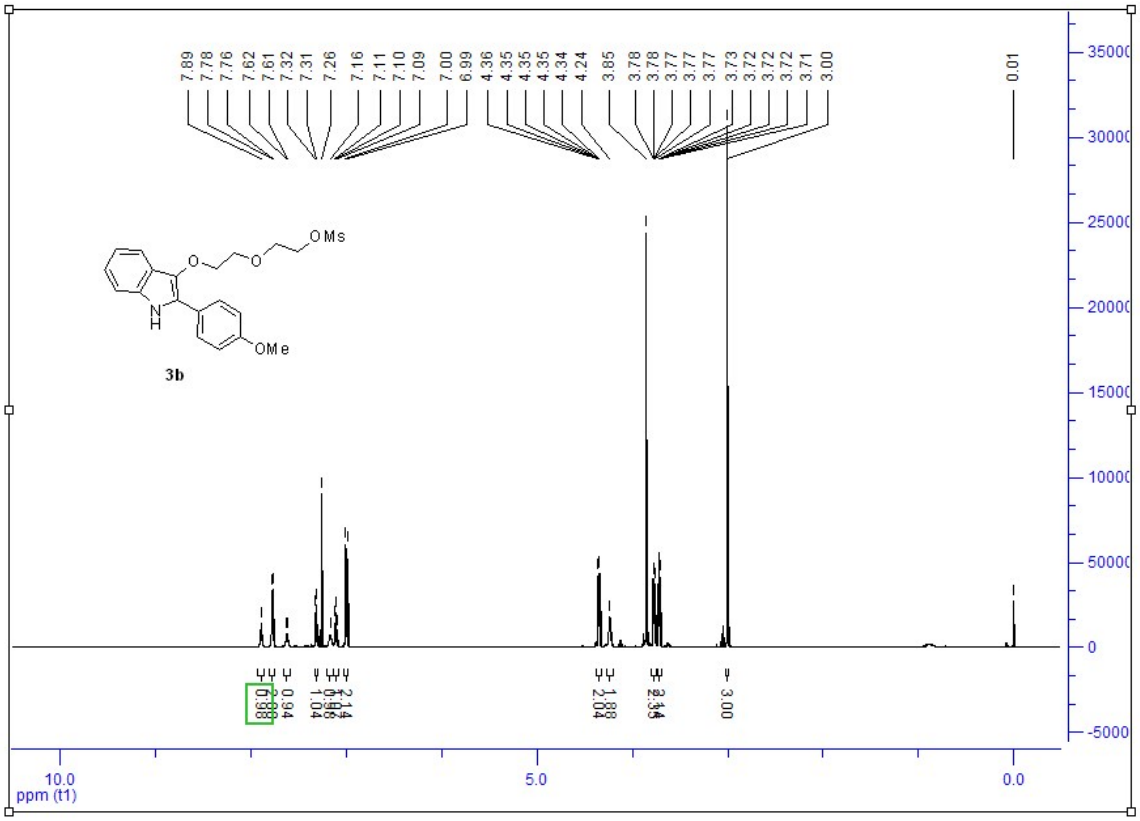
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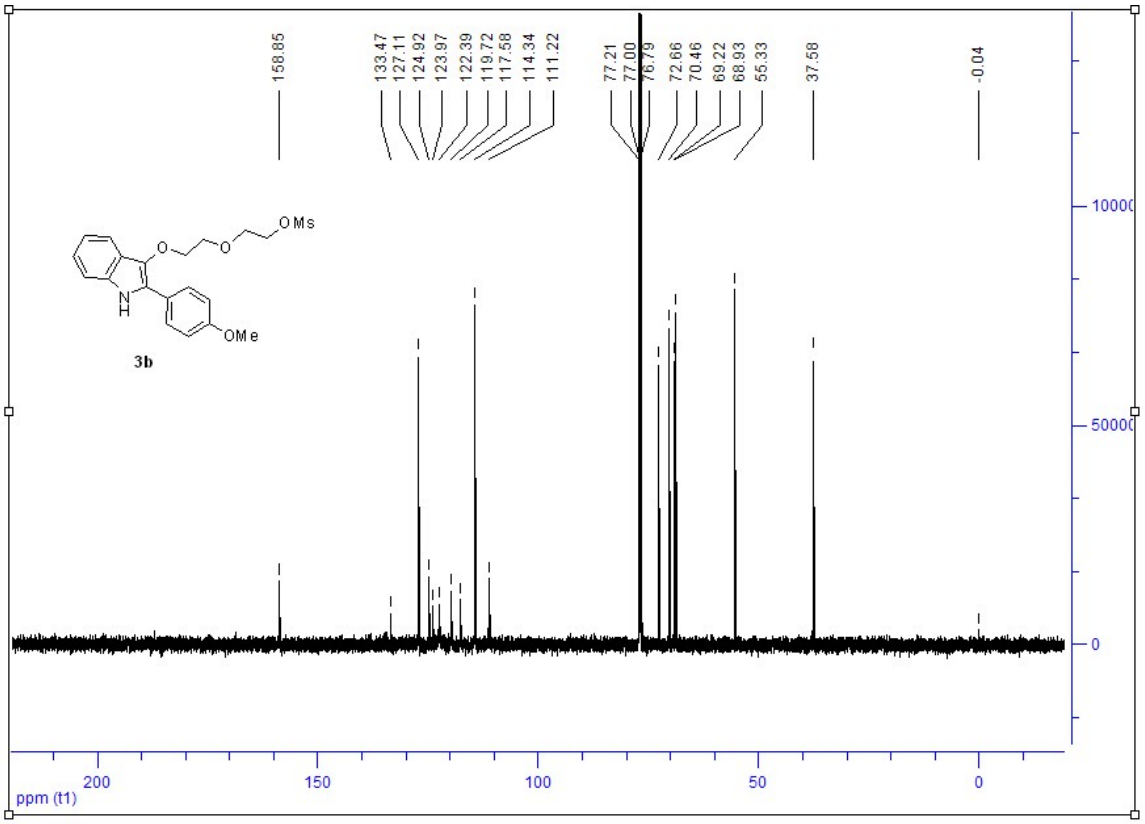
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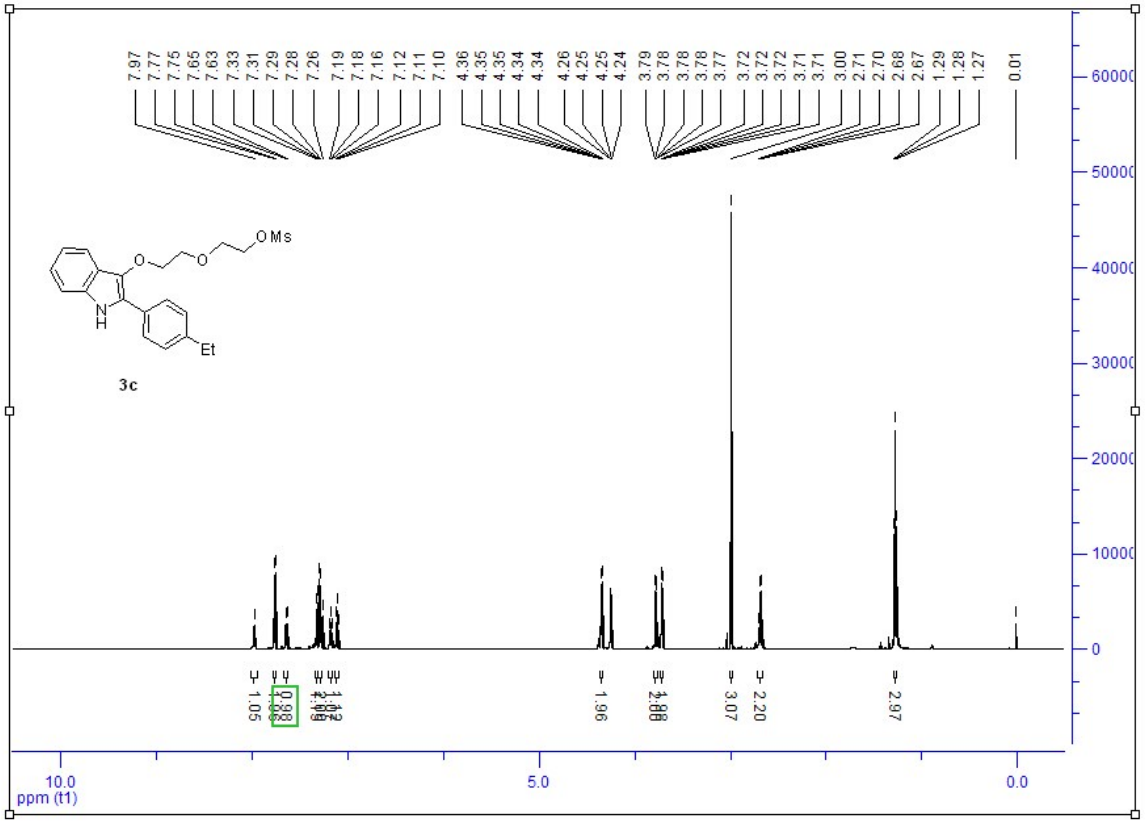
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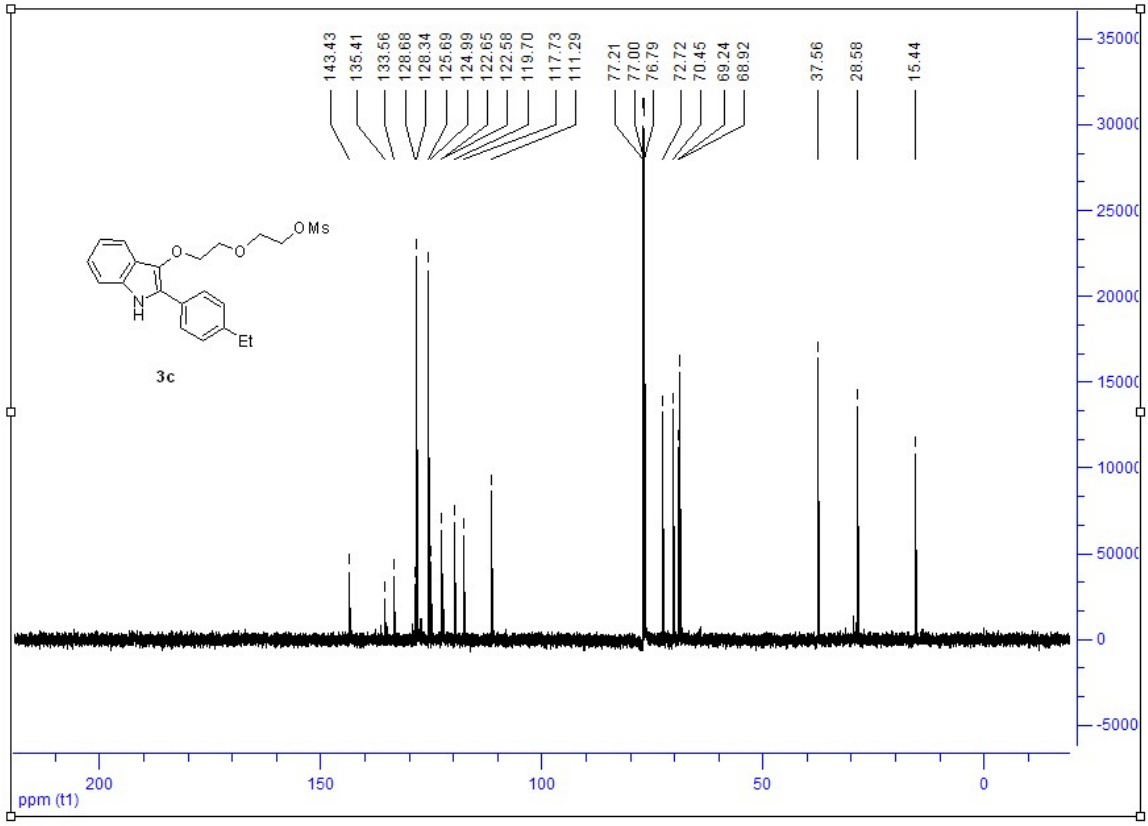
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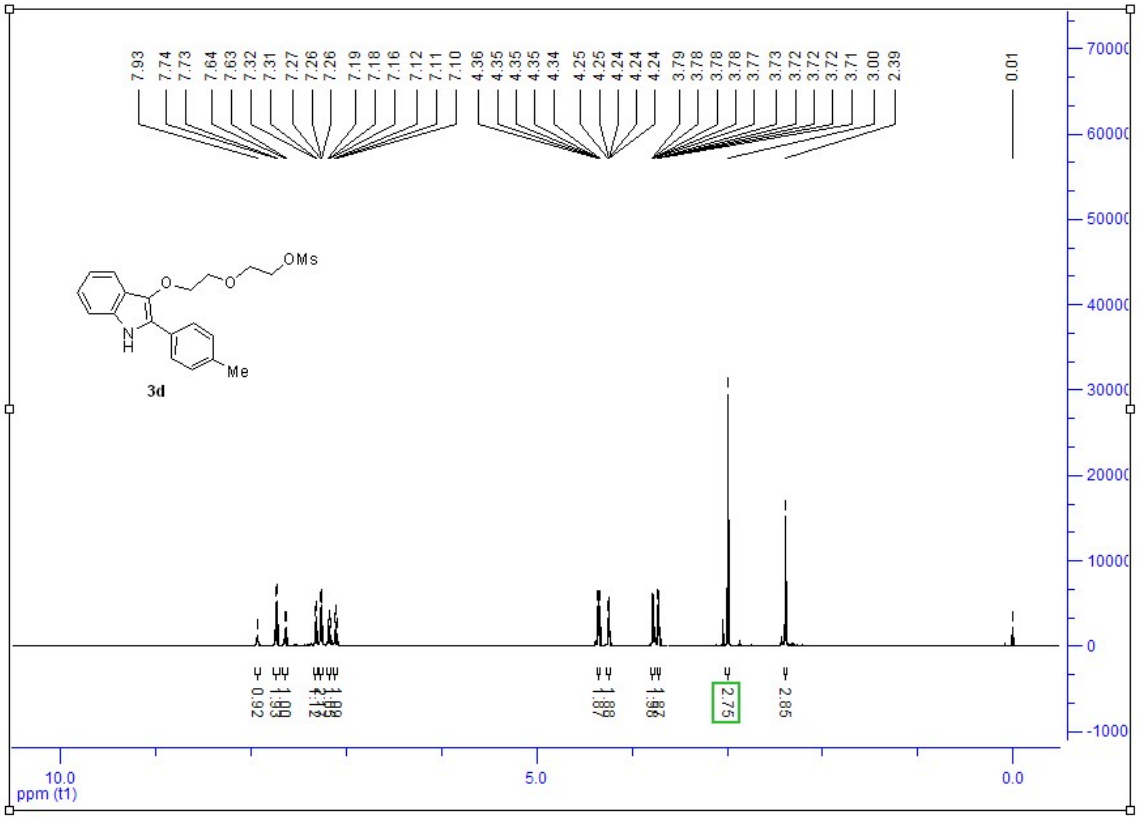
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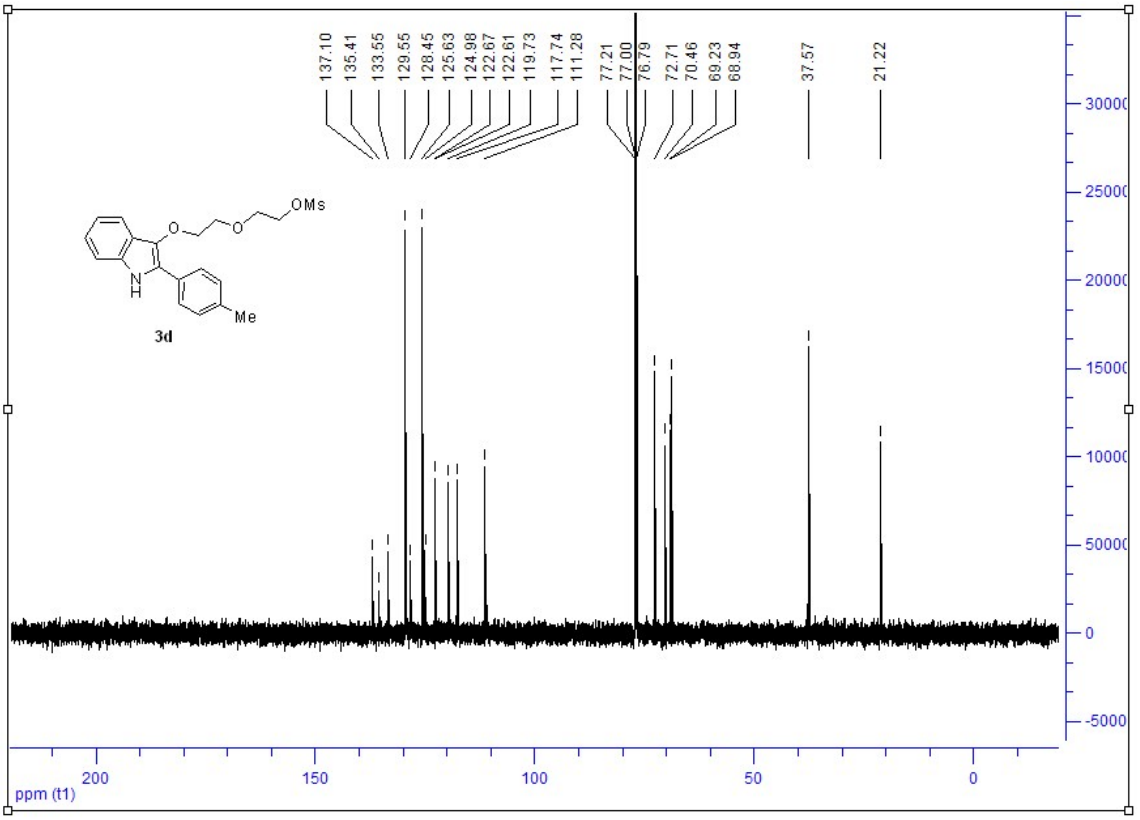
4.25
4.25
4.24
4.24
4.24
3.79
3.78
3.78
3.78
3.77
3.73
3.72
3.72
3.71
3.00
2.39
0.01
OMs
O
O
N
H
Me
3d
0.92
1.99
2.12
1.88
1.89
1.98
2.76
2.85
70000
60000
50000
40000
30000
20000
10000
0
-10000
10.0
5.0
0.0
ppm (t1)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135.41
133.55
129.55
128.45
125.63
124.98
122.67
122.61
119.73
117.74
111.28
77.21
77.00
76.79
72.71
70.46
69.23
68.94
37.57
21.22
OMs
O
O
N
H
Me
3d
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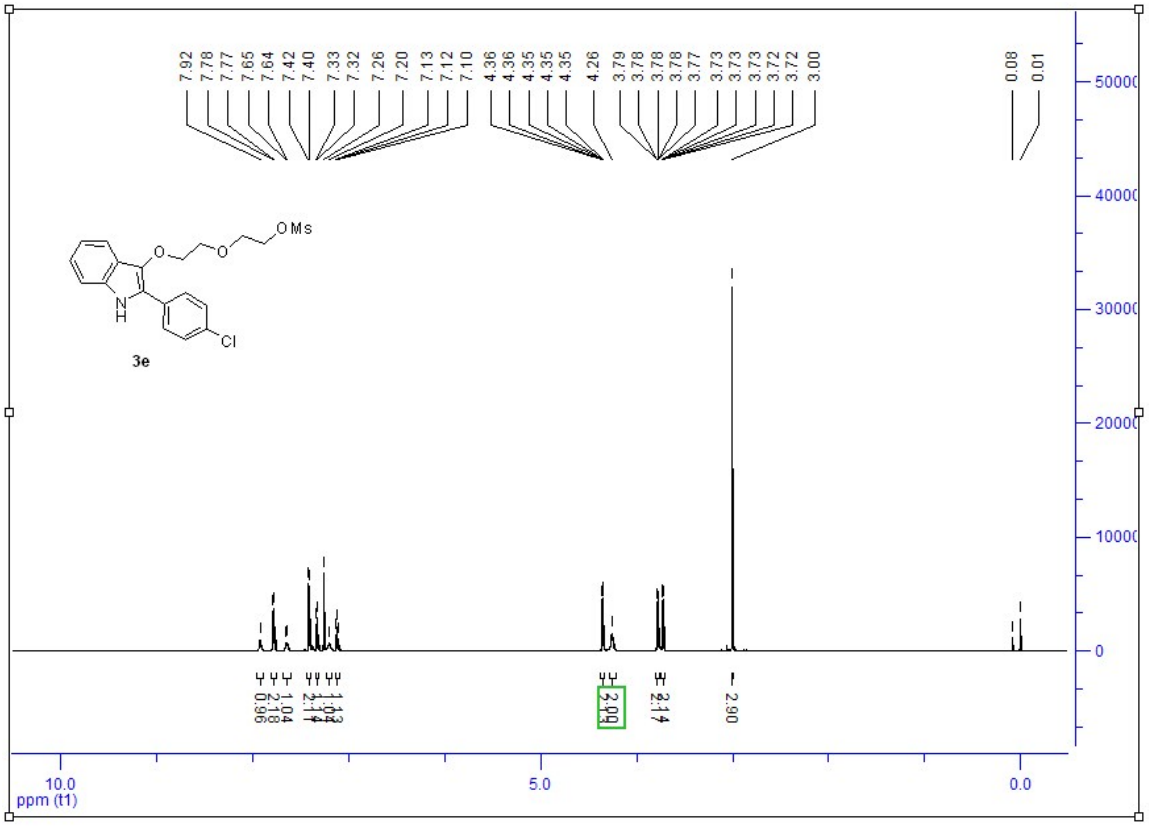
25000
20000
15000
10000
50000
0
-5000
200
150
100
50
0
ppm (t1)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7.78
7.77
7.65
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7.42
7.40
7.33
7.32
7.26
7.20
7.13
7.12
7.10
4.36
4.36
4.35
4.35
4.35
4.26
3.79
3.78
3.78
3.77
3.73
3.73
3.73
3.72
3.72
3.00
0.08
0.01
OMs
O
O
N
H
Cl
3e
0.96
2.18
1.04
2.14
2.09
2.17
2.90
10.0
ppm (t1)
5.0
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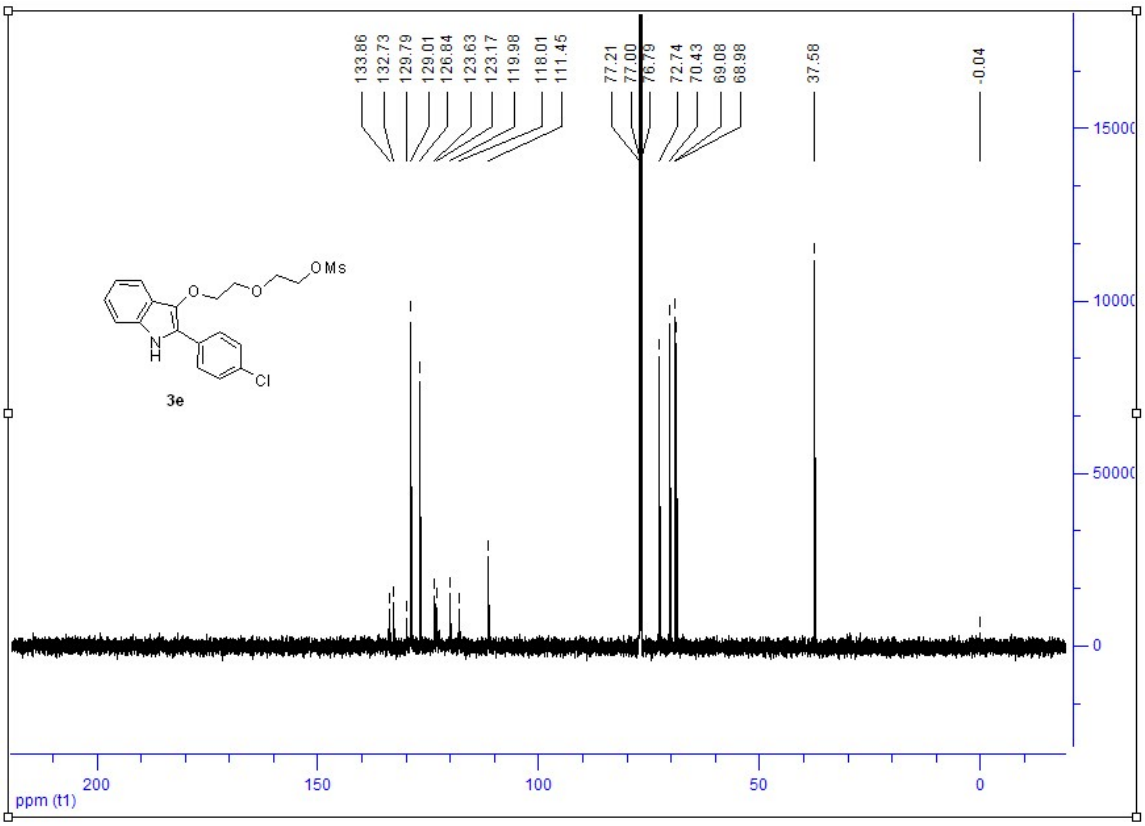
50000
40000
30000
20000
10000
0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129.79
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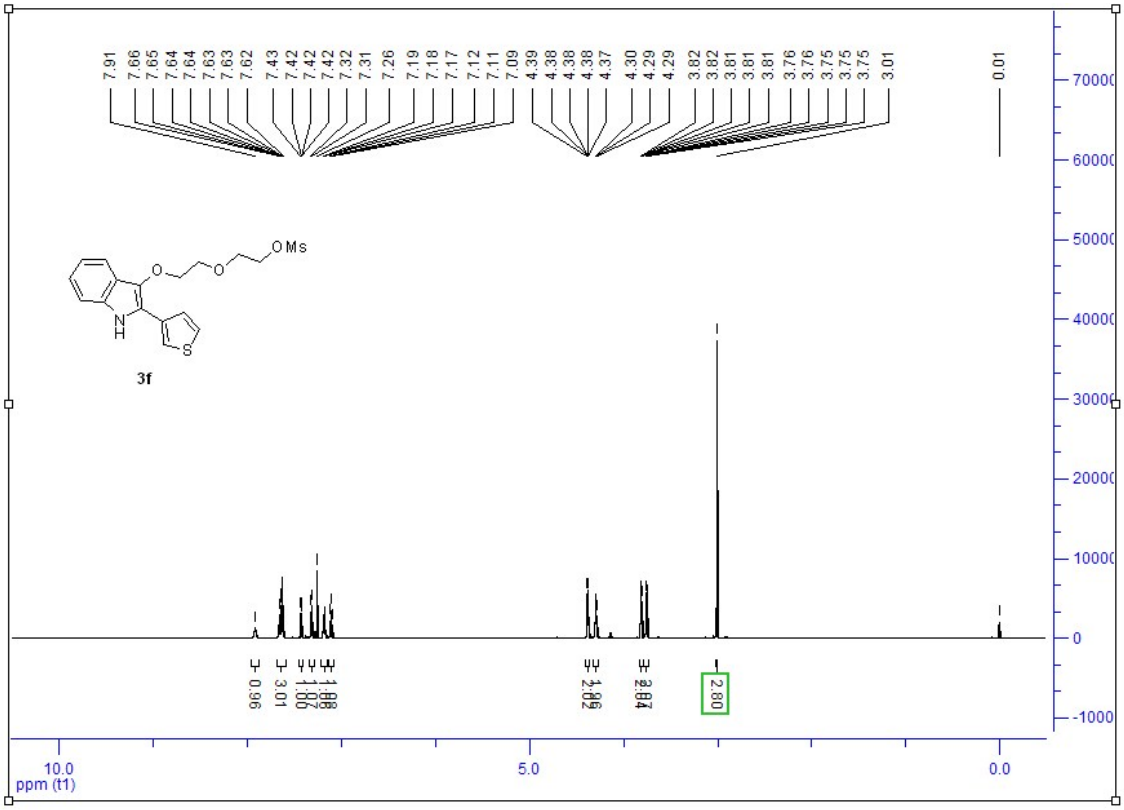
126.84
123.63
123.17
119.98
118.01
111.45
77.21
77.00
76.79
72.74
70.43
69.08
68.98
37.58
-0.04
OMs
O
O
N
H
Cl
3e
200
150
100
50
0
ppm (t1)
15000
10000
50000
0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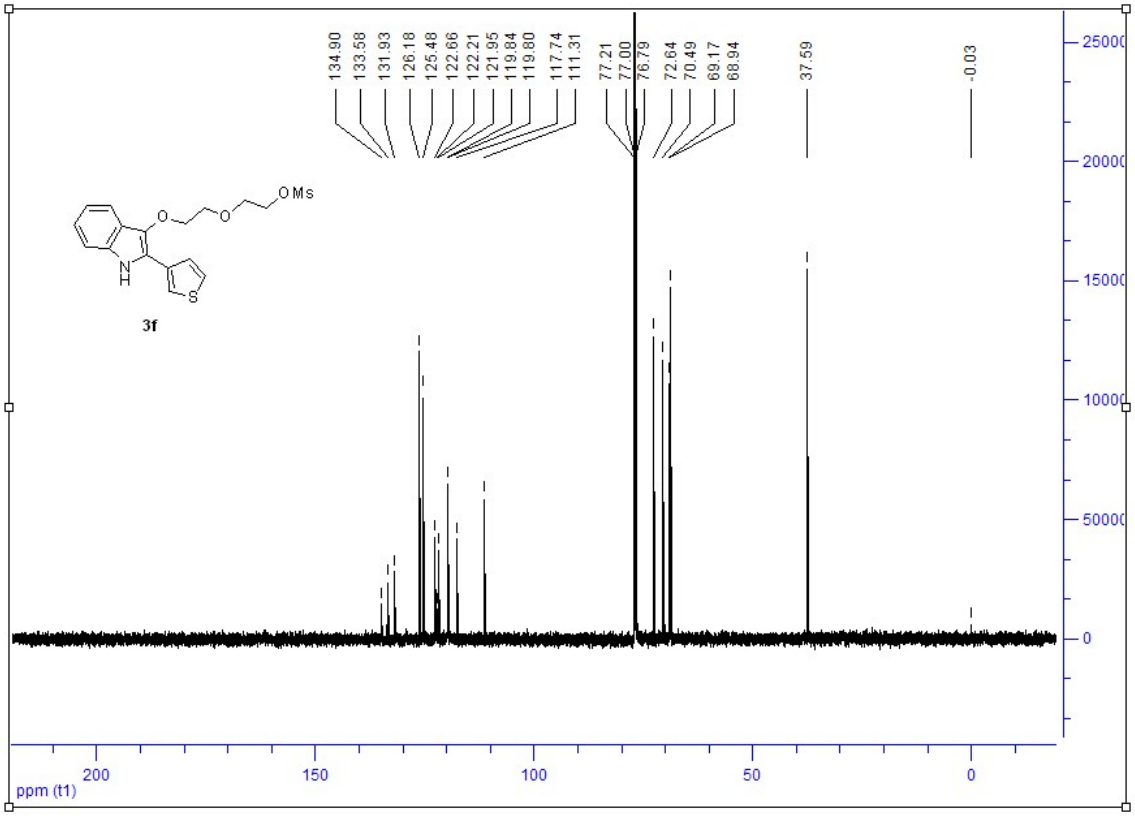
7.65
7.64
7.64
7.63
7.63
7.62
7.43
7.42
7.42
7.42
7.32
7.31
7.26
7.19
7.18
7.17
7.12
7.11
7.09
4.39
4.38
4.38
4.38
4.37
4.30
4.29
4.29
3.82
3.82
3.81
3.81
3.81
3.76
3.76
3.75
3.75
3.75
3.01
0.01
OMs
O
O
N
H
S
3f
0.996
3.301
2.280
10.0
ppm (t1)
5.0
0.0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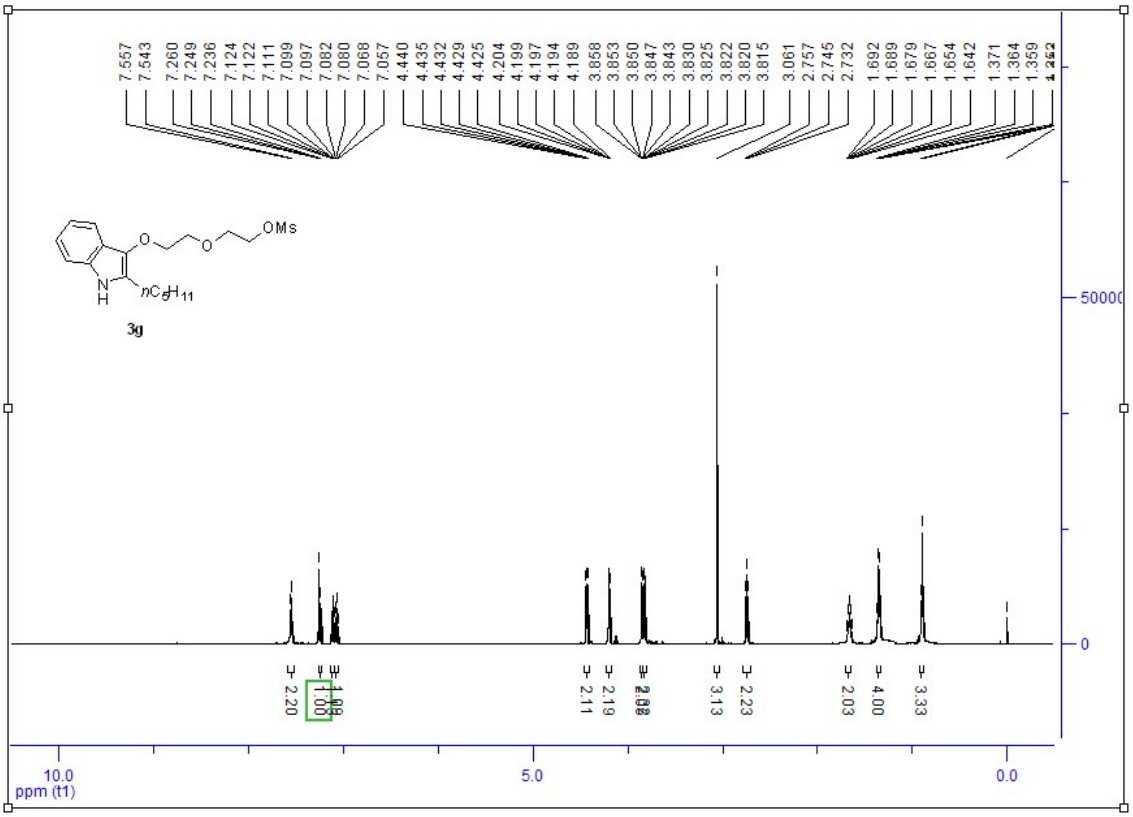
133.58
131.93
126.18
125.48
122.66
122.21
121.95
119.84
119.80
117.74
111.31
77.21
77.00
76.79
72.64
70.49
69.17
68.94
37.59
-0.03
OMs
O
O
N
H
S
3f
200
ppm (t1)
150
100
50
0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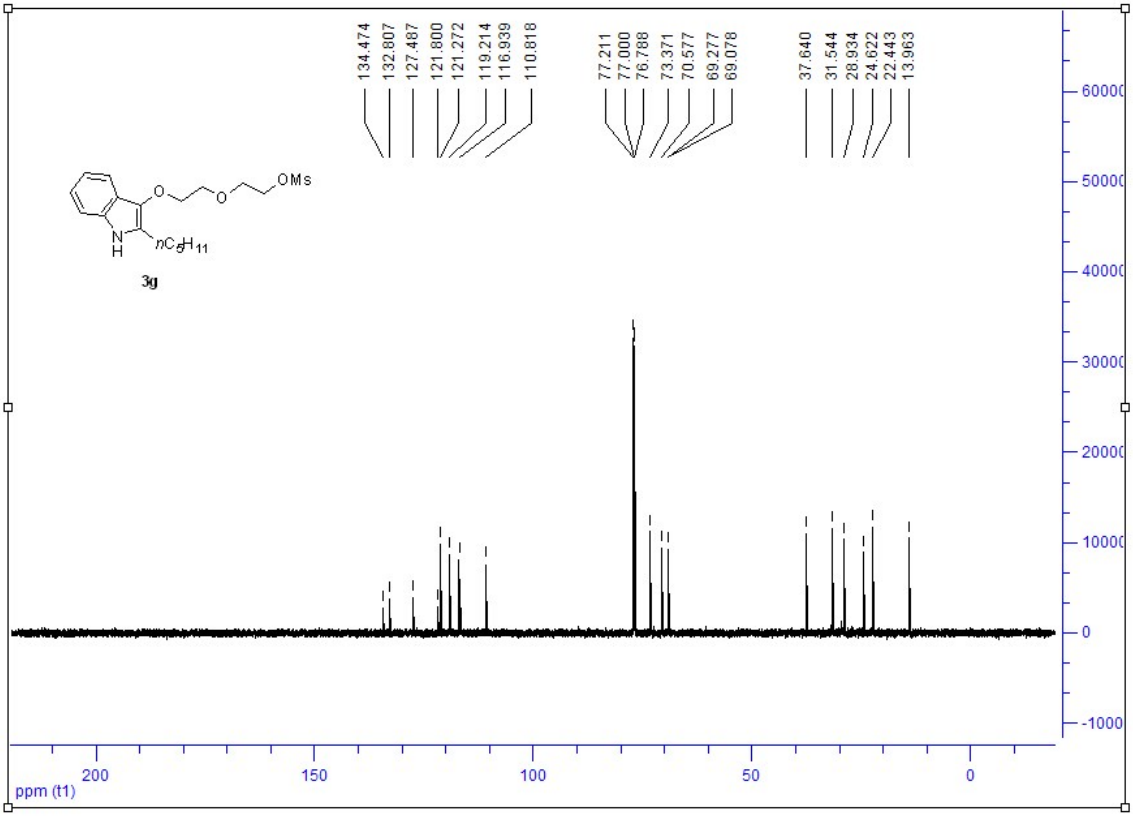
7.543
7.260
7.249
7.236
7.124
7.122
7.111
7.099
7.097
7.082
7.080
7.068
7.057
4.440
4.435
4.432
4.429
4.425
4.204
4.199
4.197
4.194
4.189
3.858
3.853
3.850
3.847
3.843
3.830
3.825
3.822
3.820
3.815
3.061
2.757
2.745
2.732
1.692
1.689
1.679
1.667
1.654
1.642
1.371
1.364
1.359
OMs
nC5H11
3g
50000
0
2.20
1.00
2.11
2.19
3.13
2.23
2.03
4.00
3.33
10.0
5.0
0.0
ppm (t1)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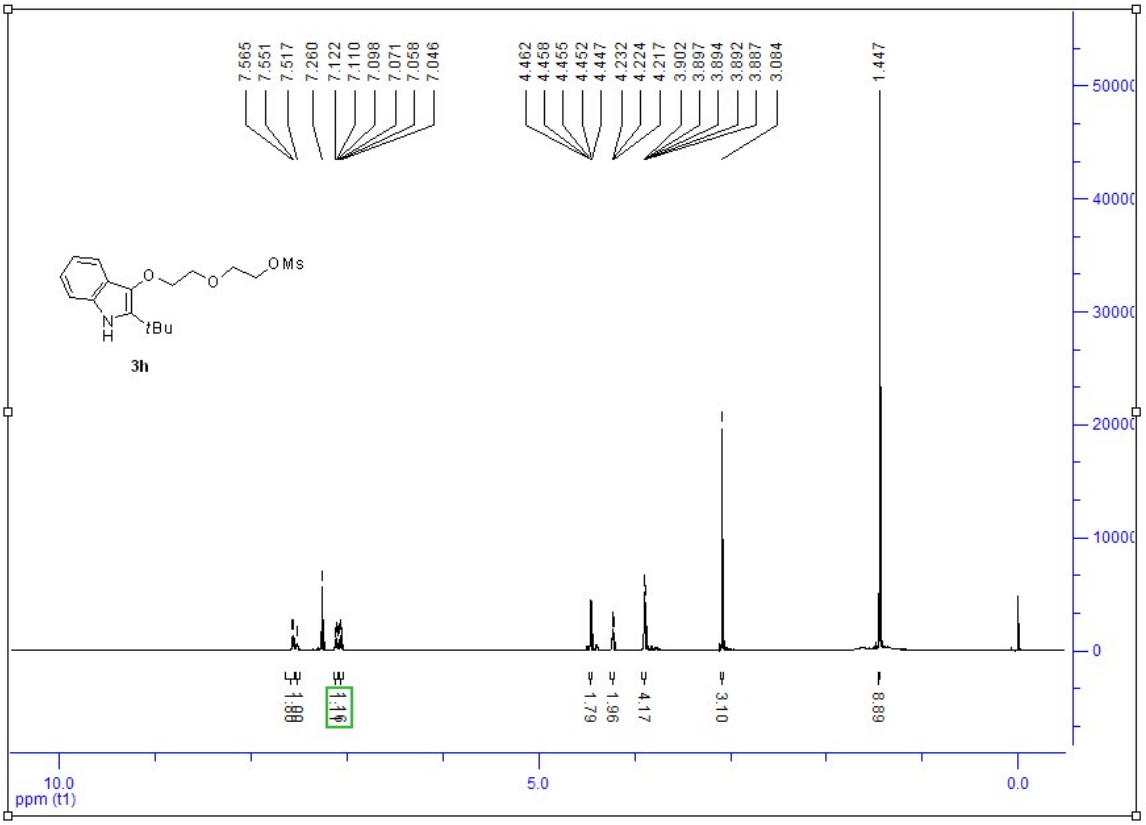
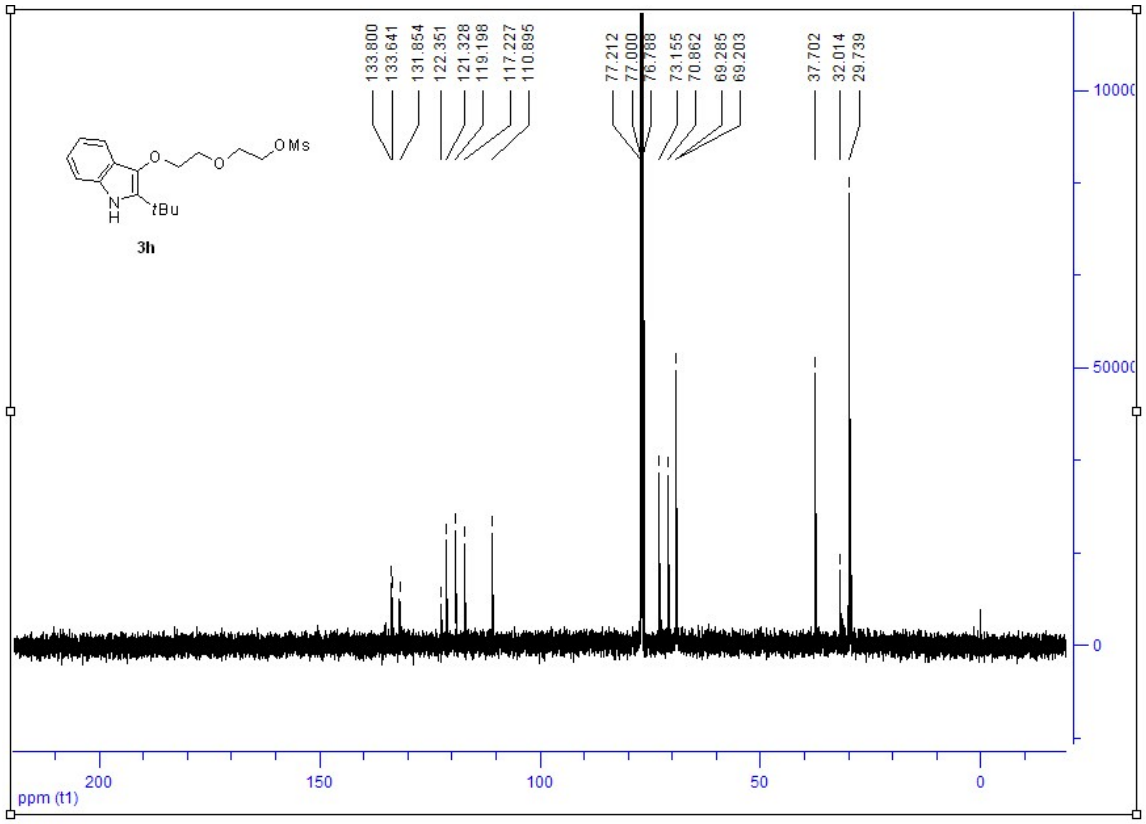
132.807
127.487
121.800
121.272
119.214
116.939
110.818
77.211
77.000
76.788
73.371
70.577
69.277
69.078
37.640
31.544
28.934
24.622
22.443
13.963
OMs
nC5H11
3g
60000
50000
40000
30000
20000
10000
0
-10000
200
150
100
50
0
ppm (t1)


7.565
7.551
7.517
7.260
7.122
7.110
7.098
7.071
7.058
7.046
4.462
4.458
4.455
4.452
4.447
4.232
4.224
4.217
3.902
3.897
3.894
3.892
3.887
3.084
1.447
OMs
tBu
3h
1.88
1.16
1.79
1.96
4.17
3.10
8.89
10.0
ppm (t1)
5.0
0.0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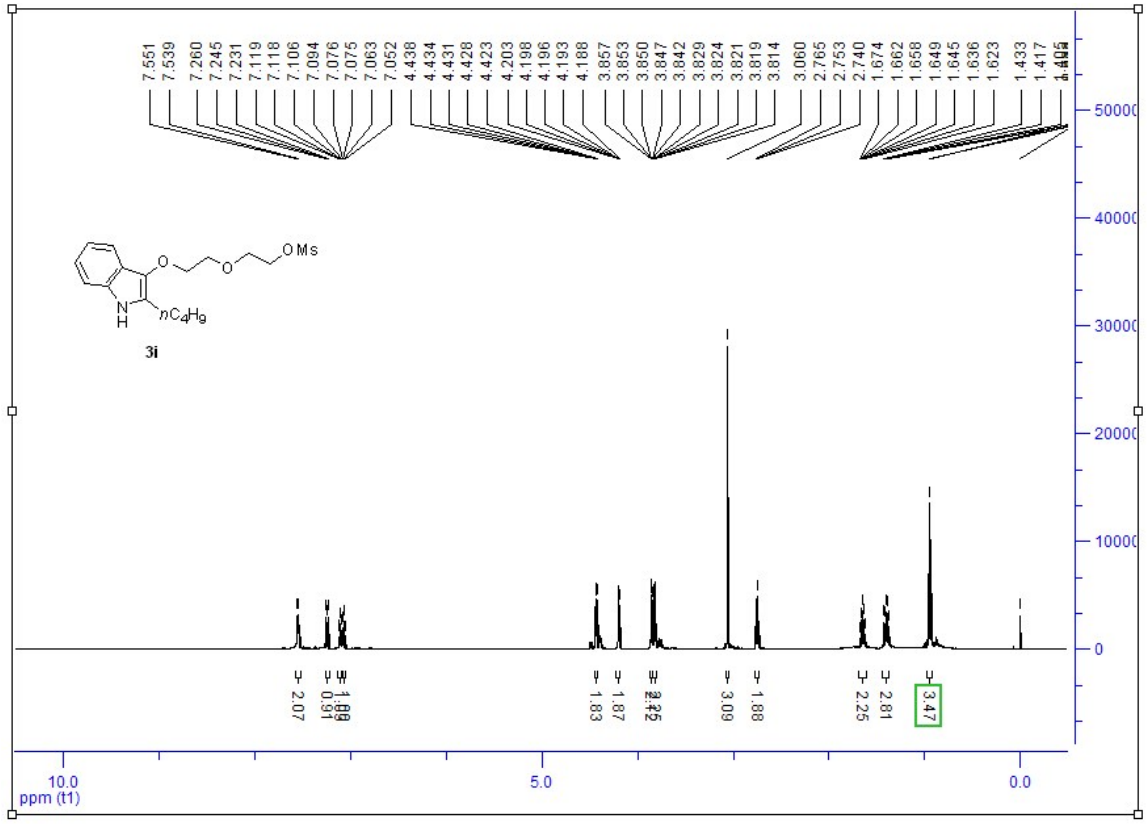
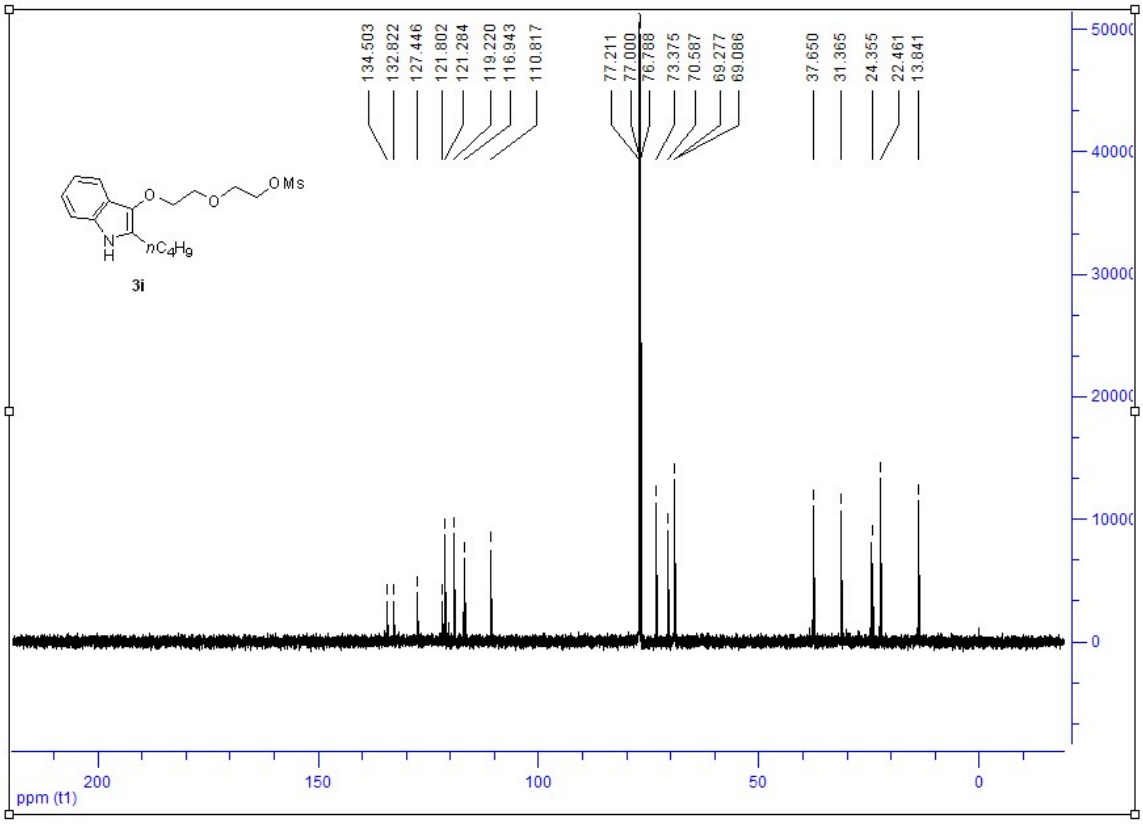
133.641
131.854
122.351
121.328
119.198
117.227
110.895
77.212
77.000
76.788
73.155
70.862
69.285
69.203
37.702
32.014
29.739
OMs
tBu
3h
200
150
100
50
0
ppm (t1)


7.551
7.539
7.260
7.245
7.231
7.119
7.118
7.106
7.094
7.076
7.075
7.063
7.052
4.438
4.434
4.431
4.428
4.423
4.203
4.198
4.196
4.193
4.188
3.857
3.853
3.850
3.847
3.842
3.829
3.824
3.821
3.819
3.814
3.060
2.765
2.753
2.740
1.674
1.662
1.658
1.649
1.645
1.636
1.623
1.433
1.417
OMs
nC4H9
3i
2.07
0.91
1.83
1.87
3.09
1.88
2.25
2.81
3.47
10.0
5.0
0.0
ppm (t1)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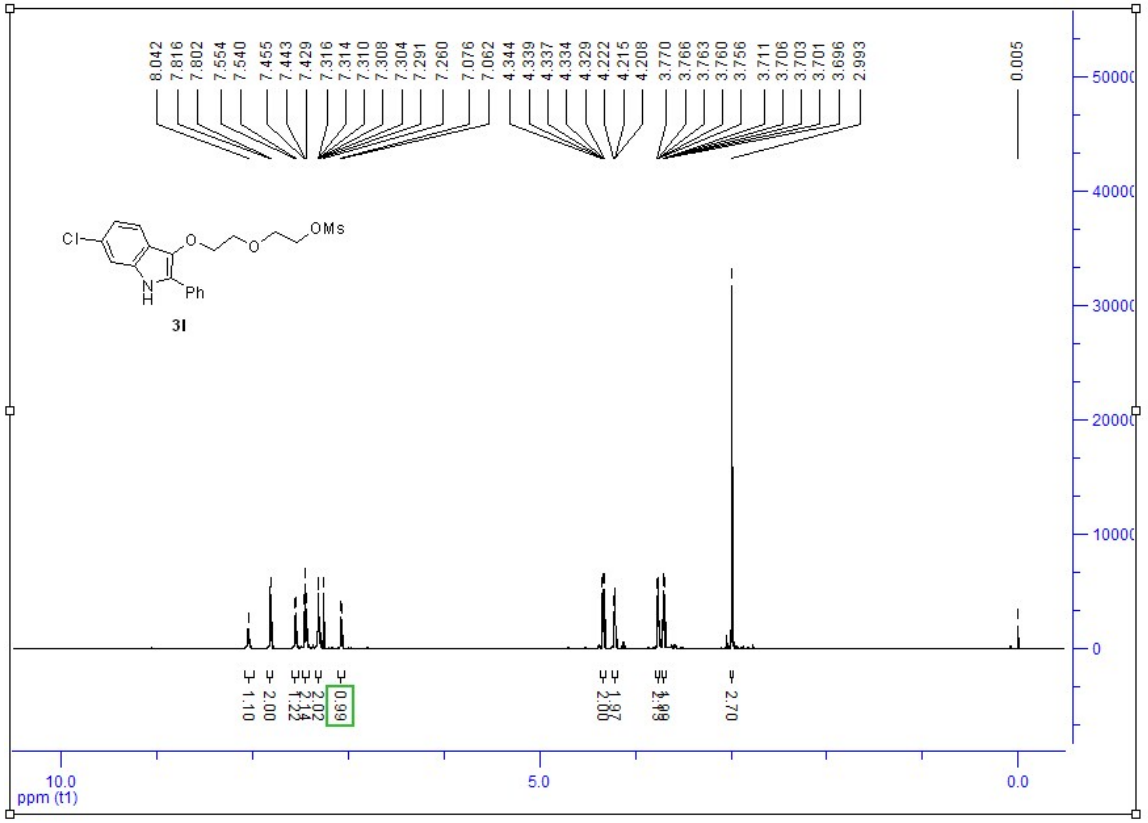
127.446
121.802
121.284
119.220
116.943
110.817
77.211
77.000
76.788
73.375
70.587
69.277
69.086
37.650
31.365
24.355
22.461
13.841
OMs
nC4H9
3i
200
150
100
50
0
ppm (t1)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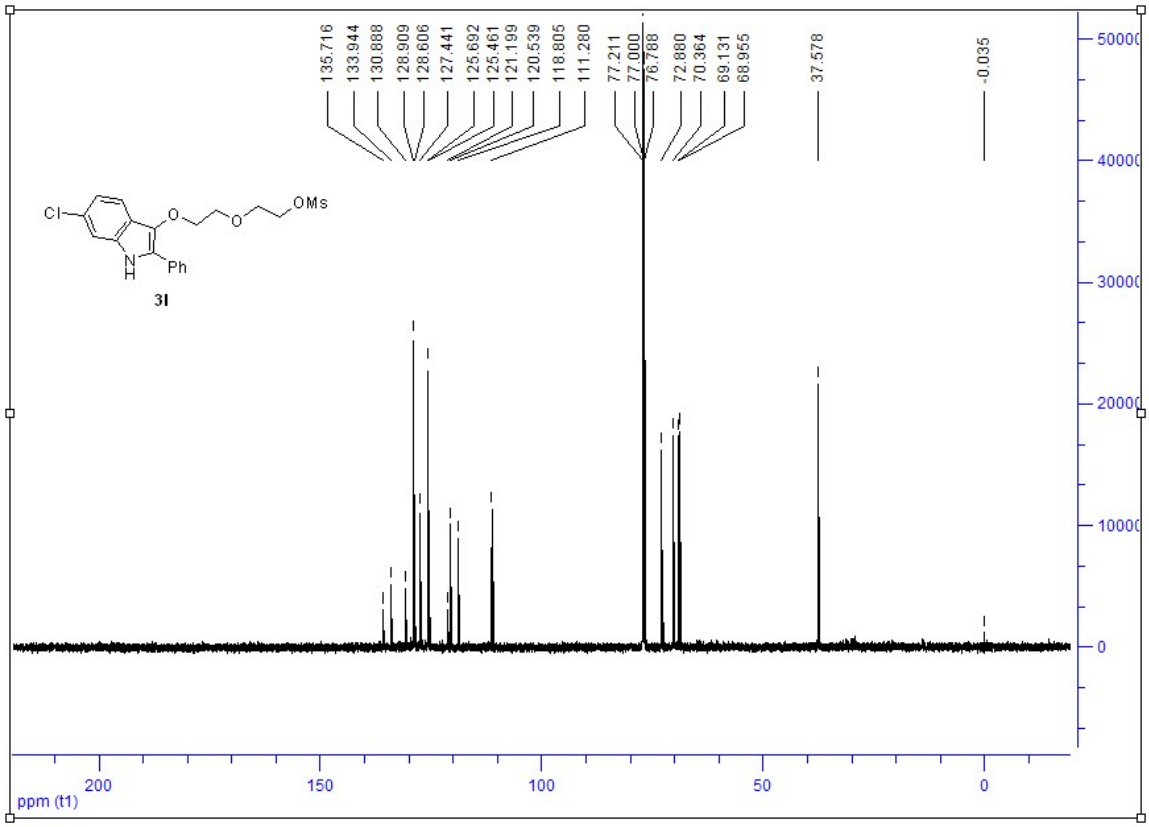
7.816
7.802
7.554
7.540
7.455
7.443
7.429
7.316
7.314
7.310
7.308
7.304
7.291
7.260
7.076
7.062
4.344
4.339
4.337
4.334
4.329
4.222
4.215
4.208
3.770
3.766
3.763
3.760
3.756
3.711
3.706
3.703
3.701
3.696
2.993
0.005
Cl
O
O
OMs
N
H
Ph
3l
1.10
2.00
2.02
2.14
2.22
0.99
2.00
1.97
4.09
2.70
10.0
5.0
0.0
ppm (t1)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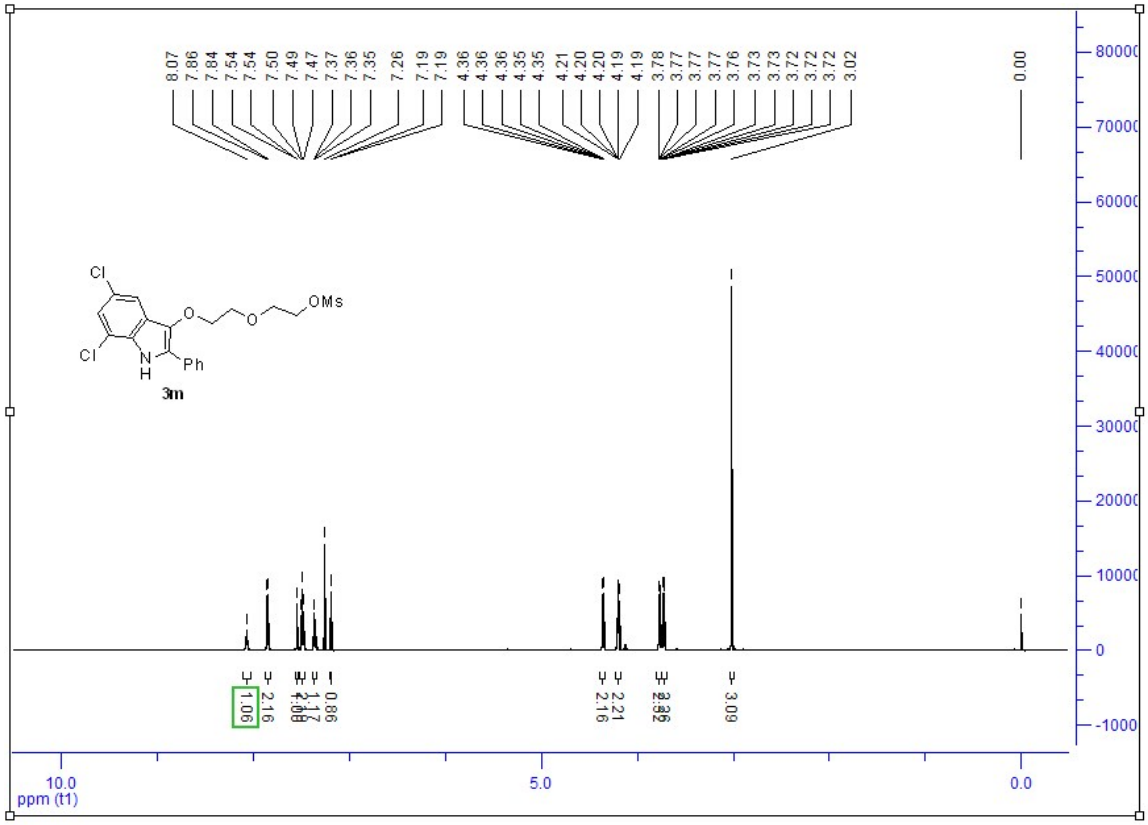
133.944
130.888
128.909
128.606
127.441
125.692
125.461
121.199
120.539
118.805
111.280
77.211
77.000
76.788
72.880
70.364
69.131
68.955
37.578
-0.035
Cl
O
O
OMs
N
H
Ph
3l
200
150
100
50
0
ppm (t1)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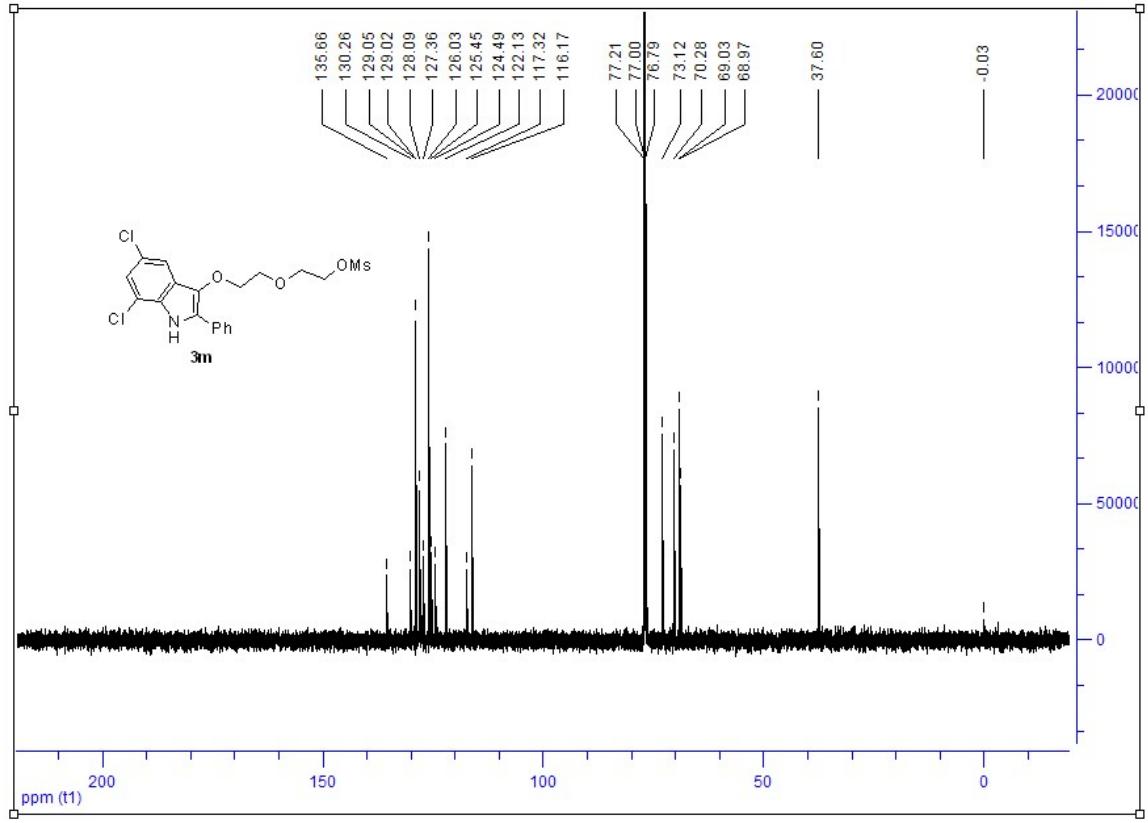
7.86
7.84
7.54
7.54
7.50
7.49
7.47
7.37
7.36
7.35
7.26
7.19
7.19
4.36
4.36
4.36
4.35
4.35
4.21
4.20
4.20
4.19
3.78
3.77
3.77
3.77
3.76
3.73
3.73
3.72
3.72
3.72
3.02
0.00
Cl
Cl
N
H
O
O
OMs
Ph
3m
1.00
2.16
2.08
2.17
0.86
2.16
2.21
2.92
3.09
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
10.0
5.0
0.0
ppm (t1)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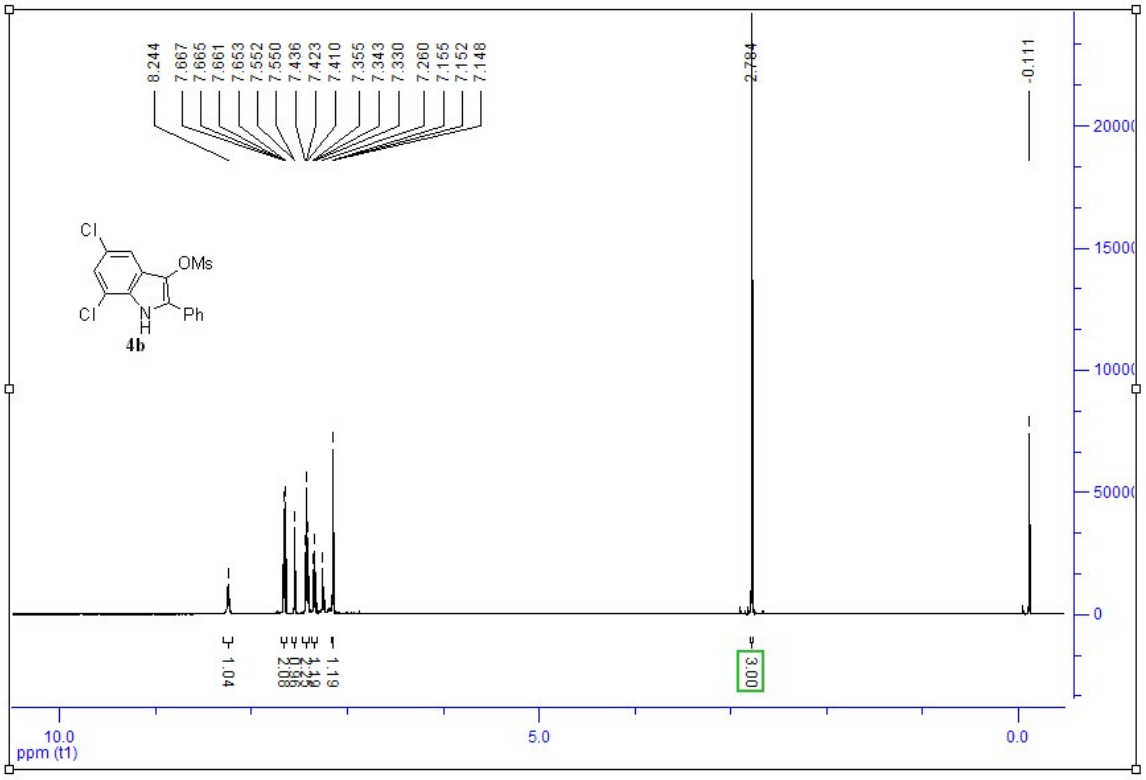
130.26
129.05
129.02
128.09
127.36
126.03
125.45
124.49
122.13
117.32
116.17
77.21
77.00
76.79
73.12
70.28
69.03
68.97
37.60
-0.03
Cl
Cl
N
H
O
O
OMs
Ph
3m
20000
15000
10000
5000
0
200
150
100
50
0
ppm (t1)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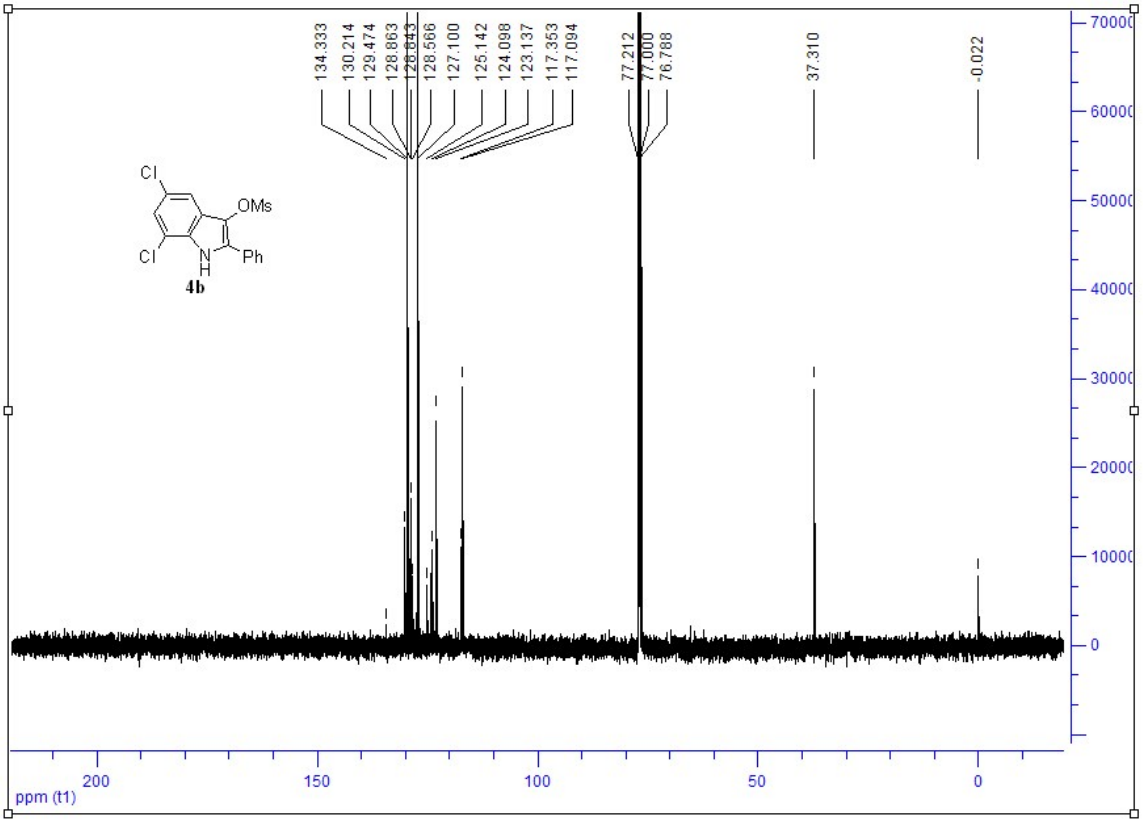
7.665
7.661
7.653
7.552
7.550
7.436
7.423
7.410
7.355
7.343
7.330
7.260
7.155
7.152
7.148
2.784
-0.111
Cl
OMs
Cl
N
H
Ph
4b
1.04
2.08
2.08
2.08
2.08
2.08
1.19
3.00
10.0
ppm (t1)
5.0
0.0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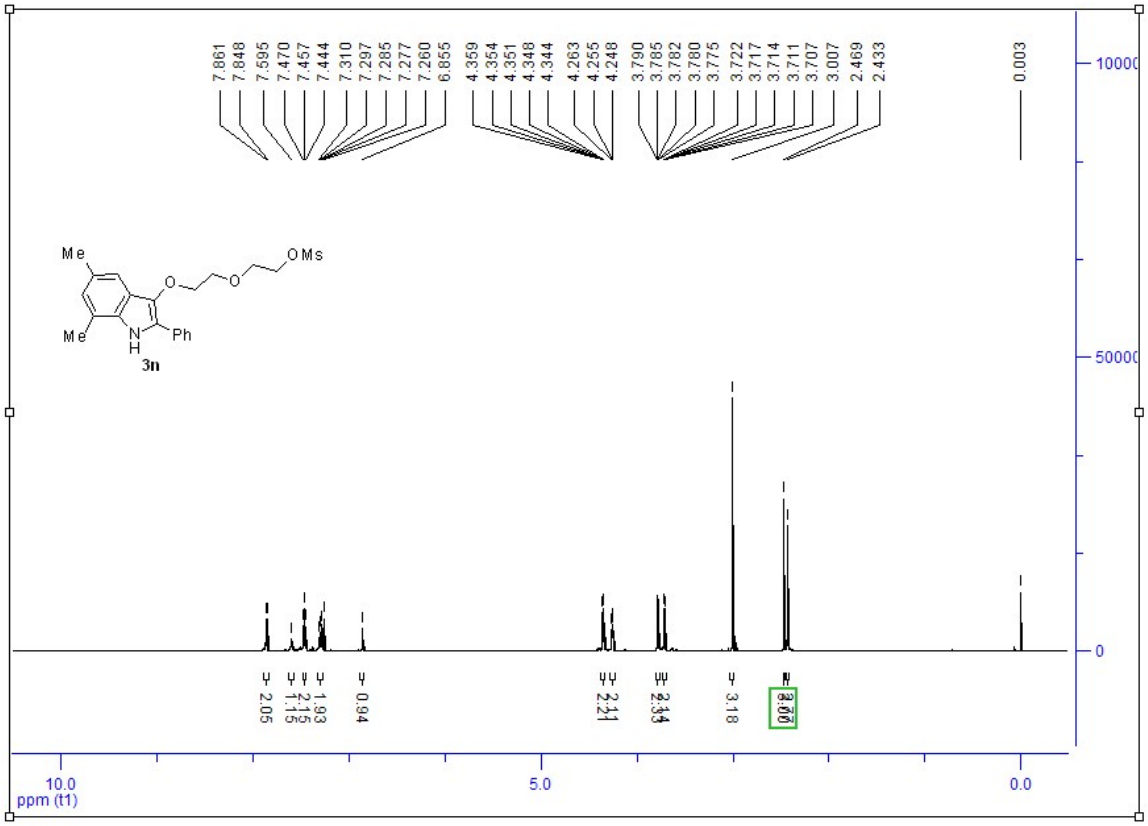
130.214
129.474
128.863
128.643
128.566
127.100
125.142
124.098
123.137
117.353
117.094
77.212
77.000
76.788
37.310
-0.022
Cl
OMs
Cl
N
H
Ph
4b
200
ppm (t1)
150
100
50
0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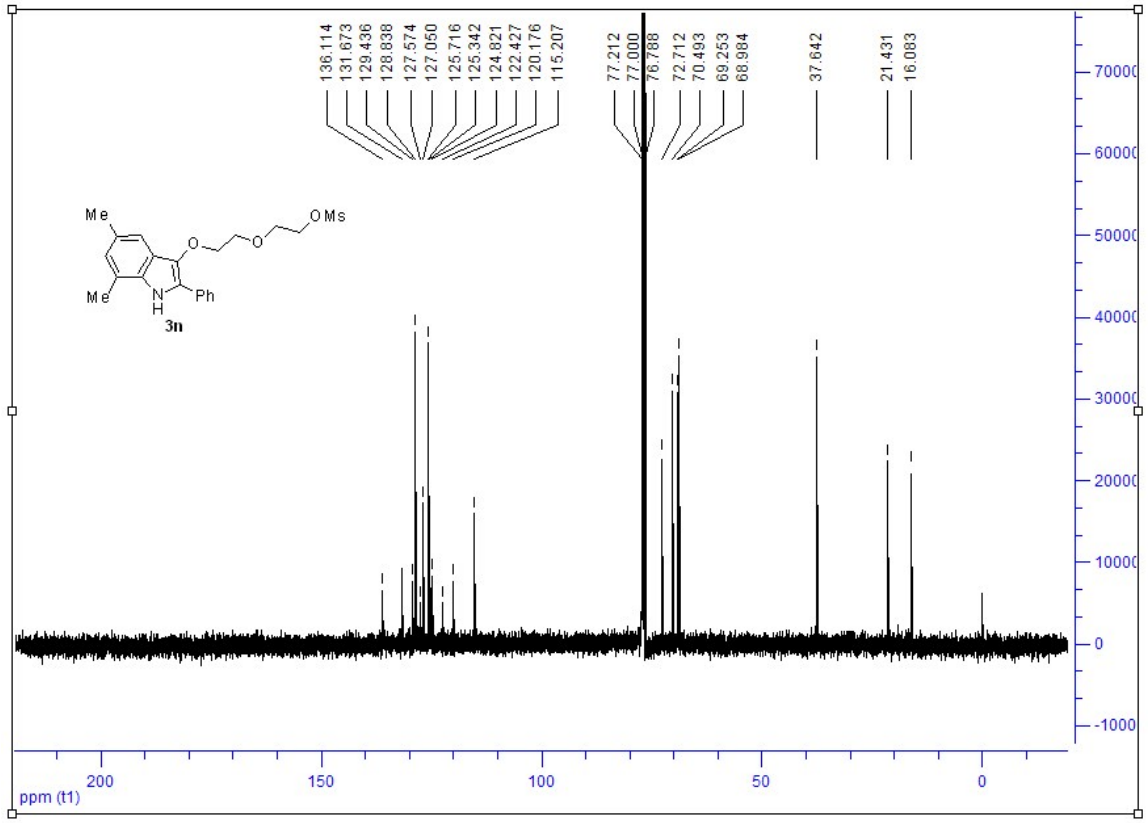
7.848
7.595
7.470
7.457
7.444
7.310
7.297
7.285
7.277
7.260
6.855
4.359
4.354
4.351
4.348
4.344
4.263
4.255
4.248
3.790
3.785
3.782
3.780
3.775
3.722
3.717
3.714
3.711
3.707
3.007
2.469
2.433
0.003
Me
OMs
O
O
Me
N
H
Ph
3n
2.05
1.15
2.15
1.93
0.94
2.11
2.33
3.18
3.00
10.0
5.0
0.0
ppm (t1)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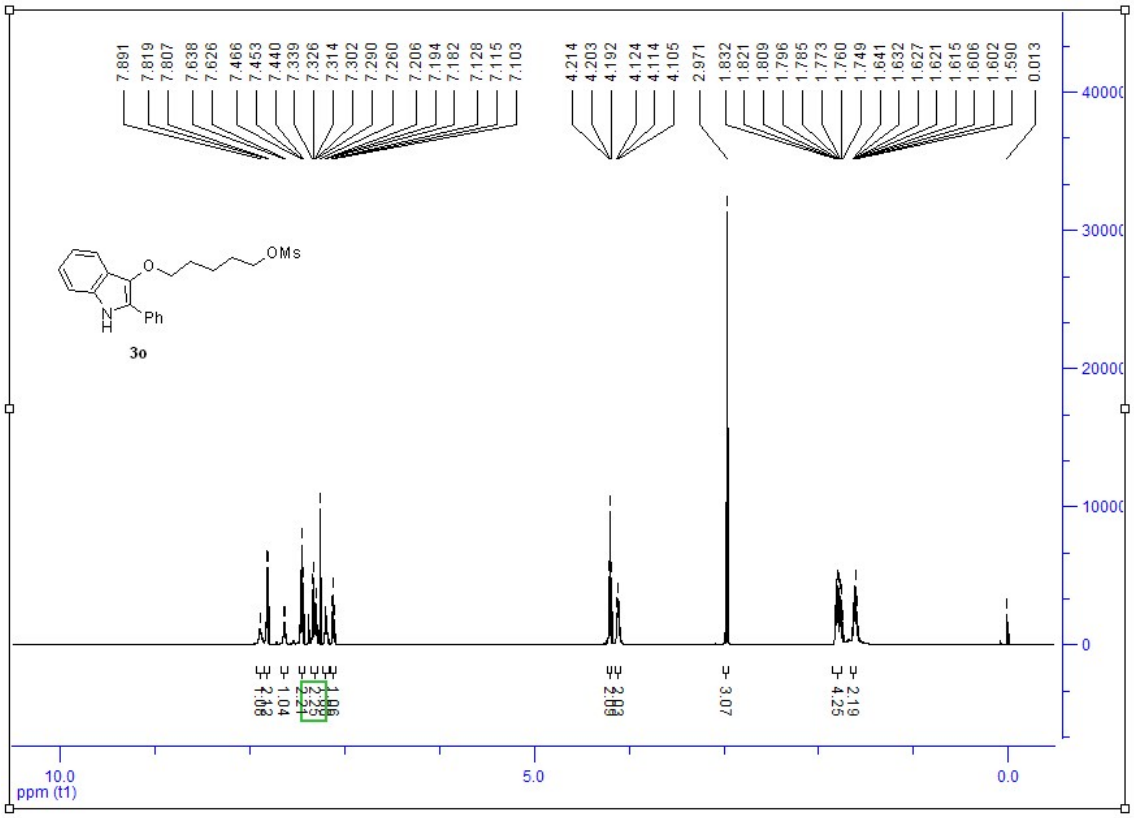
131.673
129.436
128.838
127.574
127.050
125.716
125.342
124.821
122.427
120.176
115.207
77.212
77.000
76.788
72.712
70.493
69.253
68.984
37.642
21.431
16.083
Me
OMs
O
O
Me
N
H
Ph
3n
200
150
100
50
0
ppm (t1)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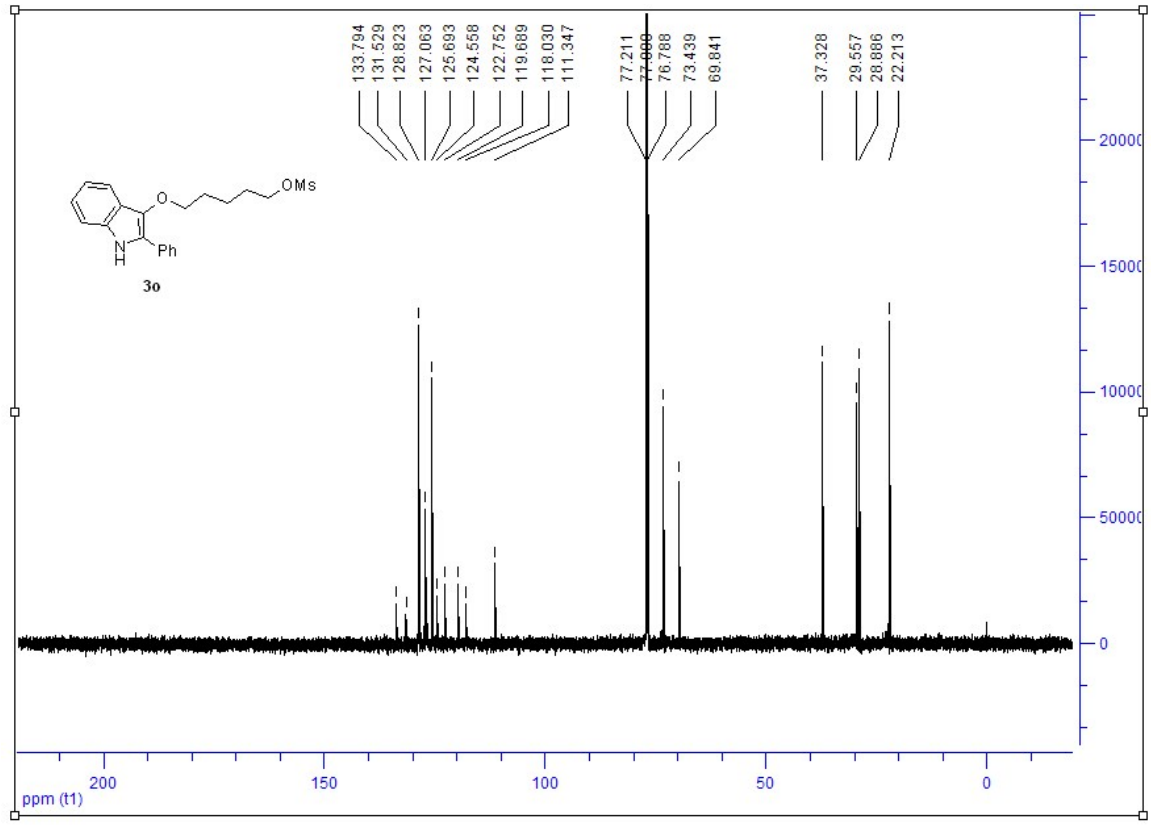
7.638
7.626
7.466
7.453
7.440
7.339
7.326
7.314
7.302
7.290
7.260
7.206
7.194
7.182
7.128
7.115
7.103
4.214
4.203
4.192
4.124
4.114
4.105
2.971
1.832
1.821
1.809
1.796
1.785
1.773
1.760
1.749
1.641
1.632
1.627
1.621
1.615
1.606
1.602
1.590
0.013
OMs
O
N
H
Ph
3o
2.08
1.04
2.25
2.21
1.06
2.08
3.07
2.19
4.25
40000
30000
20000
10000
0
10.0
5.0
0.0
ppm (t1)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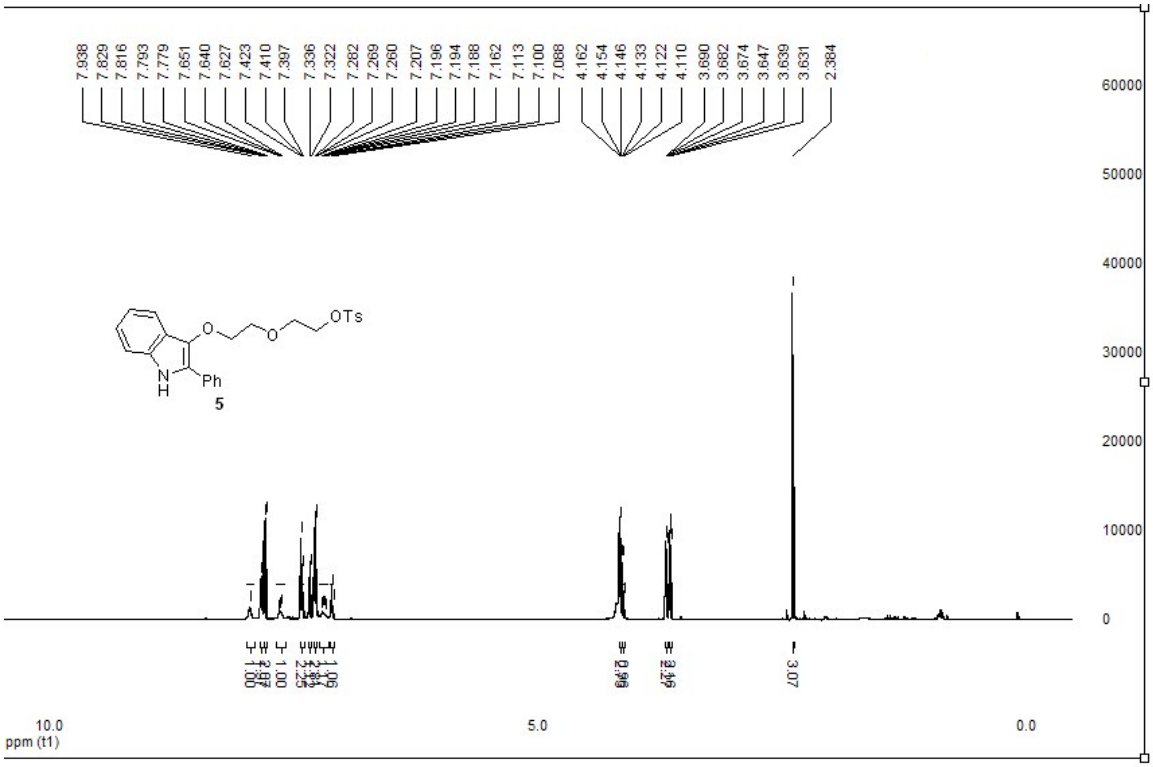
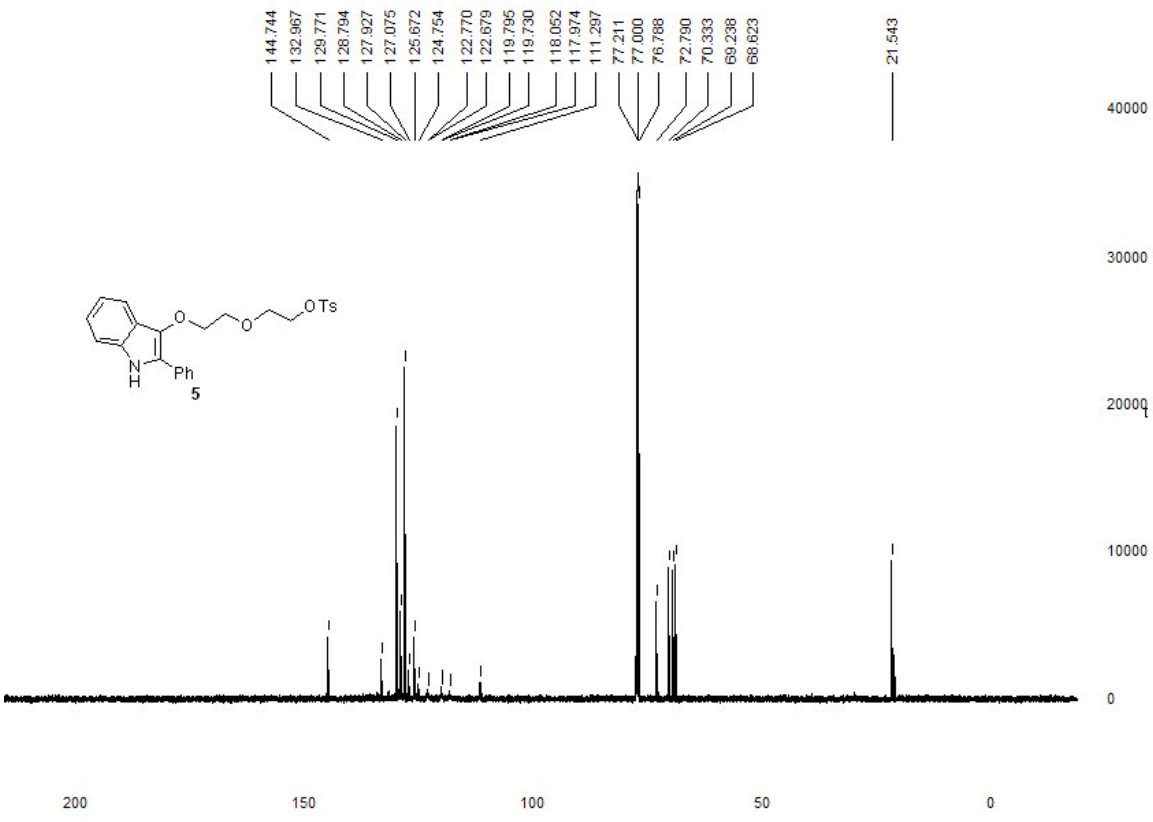
131.529
128.823
127.063
125.693
124.558
122.752
119.689
118.030
111.347
77.211
77.000
76.788
73.439
69.841
37.328
29.557
28.886
22.213
OMs
O
N
H
Ph
3o
20000
15000
10000
5000
0
200
150
100
50
0
ppm (t1)


7.938
7.829
7.816
7.793
7.779
7.651
7.640
7.627
7.423
7.410
7.397
7.336
7.322
7.282
7.269
7.260
7.207
7.196
7.194
7.188
7.162
7.113
7.100
7.088
4.162
4.154
4.146
4.133
4.122
4.110
3.690
3.682
3.674
3.647
3.639
3.631
2.384
OTs
O
O
N
H
Ph
5
60000
50000
40000
30000
20000
10000
0
10.0
ppm (t1)
5.0
0.0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128.794
127.927
127.075
125.672
124.754
122.770
122.679
119.795
119.730
118.052
117.974
111.297
77.211
77.000
76.788
72.790
70.333
69.238
68.623
21.543
OTs
O
O
N
H
Ph
5
40000
30000
20000
10000
0
200
150
100
50
0