

## Supporting Information

### Halogen bonding assisted site-selective C-3 triaryl methylation of indoles and *N*-triaryl methylation of imidazoles

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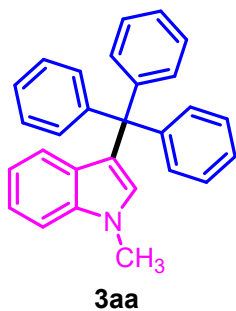
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E-mail: [utbora@yahoo.co.in](mailto:utbora@yahoo.co.in), [ubora@tezu.ernet.in](mailto:ubora@tezu.ernet.in)

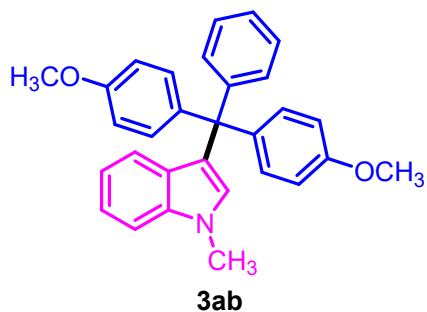
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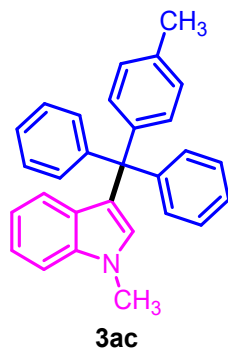
$^1\text{H}$  and  $^{13}\text{C}$  NMR analytical data:



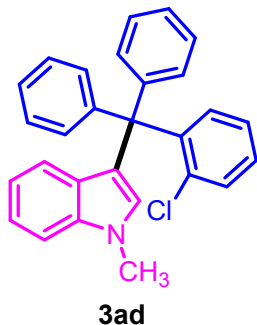
**1-methyl-3-trityl-1*H*-indole (3aa):** White solid (188 mg, 100% yield)<sup>1,2</sup>, mp 192-194 °C, purified by recrystallization.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 7.31–7.08 (m, 18H), 6.77 (t,  $J = 7.5$  Hz, 1H), 6.65 (d,  $J = 8.8$  Hz, 2H), 3.70 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 146.7, 137.7, 130.8, 130.2, 128.3, 127.4, 126.0, 122.9, 122.3, 121.3, 118.7, 109.0, 59.5, 32.8.



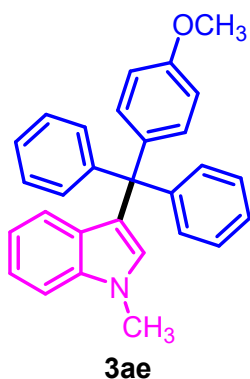
**3-(bis(4-methoxyphenyl)(phenyl)methyl)-1-methyl-1*H*-indole (3ab):** White solid (195 mg, 90% yield)<sup>3</sup>, mp 124-126 °C, purified by chromatography.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 7.32–7.13 (m, 12H), 6.86–6.76 (m, 5H), 6.72–6.65 (m, 2H), 3.81 (s, 6H), 3.74 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 157.5, 147.2, 139.2, 137.7, 131.7, 130.6, 130.0, 128.3, 127.3, 125.9, 123.0, 122.8, 121.2, 118.7, 112.6, 109.0, 58.0, 55.2, 32.7.



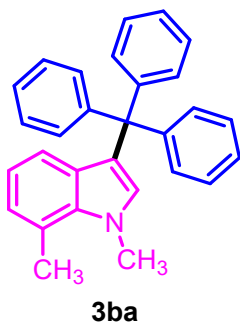
**3-(diphenyl(*p*-tolyl)methyl)-1-methyl-1*H*-indole (3ac):** White solid (195 mg, 100% yield)<sup>3</sup>, mp 261-263 °C, purified by re-crystallization.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 7.22–7.00 (m, 15H), 6.95 (d,  $J = 7.5$  Hz, 2H), 6.70 (t,  $J = 7.5$  Hz, 1H), 6.61–6.56 (m, 2H), 3.62 (s, 3H), 2.23 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 146.8, 143.7, 137.7, 135.4, 130.8, 130.7, 130.2, 128.3, 128.1, 127.4, 125.9, 123.0, 122.4, 121.2, 118.6, 109.0, 59.1, 32.8, 21.0.



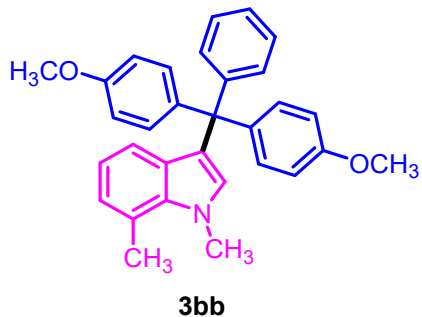
**3-((2-chlorophenyl)diphenylmethyl)-1-methyl-1H-indole (3ad):** White solid (167 mg, 82% yield)<sup>3</sup>, mp 124–126 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.43–7.11 (m, 17H), 6.79 (t, *J* = 7.6 Hz, 1H), 6.69–6.57 (m, 2H), 3.74 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 144.3, 144.0, 137.6, 136.4, 132.4, 131.9, 130.8, 128.2, 128.1, 127.3, 126.2, 126.0, 122.2, 121.2, 121.0, 118.8, 109.0, 59.8, 32.8.



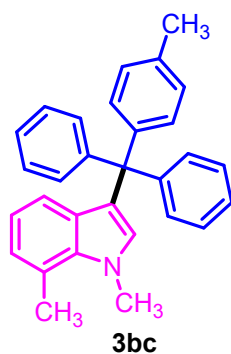
**3-((4-methoxyphenyl)diphenylmethyl)-1-methyl-1H-indole (3ae):** White solid (178 mg, 88% yield)<sup>3</sup>, mp 176–178 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.32–7.22 (m, 12H), 7.20–7.14 (m, 3H), 6.85–6.79 (m, 3H), 6.71 (d, *J* = 9.7 Hz, 2H), 3.82 (s, 3H), 3.75 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 157.6, 146.9, 138.9, 137.7, 131.8, 130.7, 130.1, 128.3, 127.4, 125.9, 123.0, 122.5, 121.2, 118.7, 112.6, 109.0, 58.7, 55.2, 32.8.



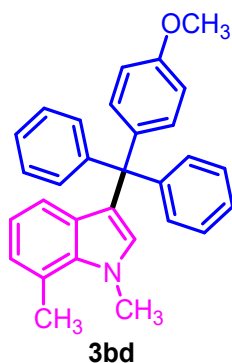
**1,7-dimethyl-3-trityl-1H-indole (3ba):** White solid (190 mg, 98% yield), mp 284–287 °C, purified by recrystallization. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.31–7.27 (m, 5H), 7.21 (s, 11H), 6.79 (d, *J* = 6.9 Hz, 1H), 6.61 (t, *J* = 7.6 Hz, 1H), 6.55–6.47 (m, 2H), 3.96 (s, 3H), 2.74 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 146.6, 132.1, 130.8, 129.3, 128.0, 127.3, 125.9, 124.0, 121.8, 121.2, 120.8, 118.8, 59.4, 36.9, 19.9. HRMS (ESI) *m/z*: [M+H]<sup>+</sup> for C<sub>29</sub>H<sub>25</sub>N, calcd 388.2065; found 388.2027.



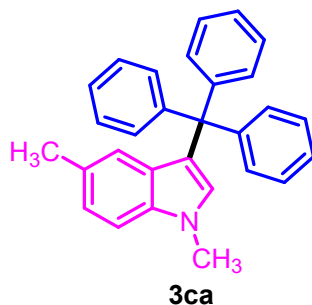
**3-(bis(4-methoxyphenyl)(phenyl)methyl)-1,7-dimethyl-1H-indole (3bb):** White solid (195 mg, 87% yield), mp 298-300 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.14–7.09 (m, 5H), 7.08–7.00 (m, 4H), 6.73–6.65 (m, 5H), 6.58–6.53 (m, 1H), 6.43 (d, *J* = 8.7 Hz, 2H), 3.88 (d, *J* = 4.6 Hz, 3H), 3.69 (s, 6H), 2.67 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 157.5, 147.1, 139.1, 136.5, 131.9, 131.7, 130.6, 129.3, 127.3, 125.8, 123.9, 122.3, 121.3, 120.8, 118.8, 112.6, 58.0, 55.2, 36.9, 19.9. HRMS (ESI) *m/z*: [M+H]<sup>+</sup> for C<sub>31</sub>H<sub>29</sub>NO<sub>2</sub>, calcd 448.2277; found 448.2234.



**3-(diphenyl(*p*-tolyl)methyl)-1,7-dimethyl-1H-indole (3bc):** White solid (153 mg, 76% yield), mp 146-148 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.17–7.08 (m, 10H), 7.01 (d, *J* = 8.3 Hz, 2H), 6.94 (d, *J* = 8.2 Hz, 2H), 6.71 (d, *J* = 7.0 Hz, 1H), 6.57–6.51 (m, 1H), 6.47–6.40 (m, 2H), 3.88 (s, 3H), 2.67 (s, 3H), 2.23 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 146.7, 143.6, 136.5, 135.4, 132.0, 130.8, 130.7, 129.3, 128.1, 127.3, 125.9, 124.0, 121.9, 121.3, 120.8, 118.8, 59.0, 36.9, 21.0, 19.9. HRMS (ESI) *m/z*: [M+H]<sup>+</sup> for C<sub>30</sub>H<sub>27</sub>N, calcd 402.2222; found 402.2186.

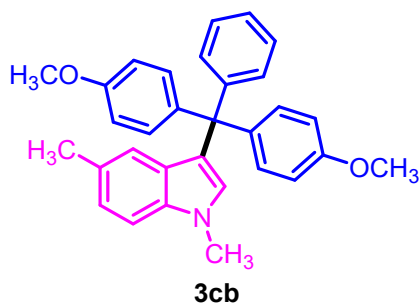


**3-((4-methoxyphenyl)diphenylmethyl)-1,7-dimethyl-1H-indole (3bd):** White solid (155 mg, 74% yield), mp 162-164 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.17–7.07 (m, 10H), 7.06–7.01 (m, 2H), 6.75–6.64 (m, 3H), 6.58–6.51 (m, 1H), 6.42 (d, *J* = 8.9 Hz, 2H), 3.88 (s, 3H), 3.70 (d, *J* = 7.8 Hz, 3H), 2.67 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 157.6, 146.9, 138.8, 136.5, 132.0, 131.8, 130.7, 129.3, 127.3, 125.9, 124.0, 122.0, 121.3, 120.8, 118.8, 112.6, 58.7,

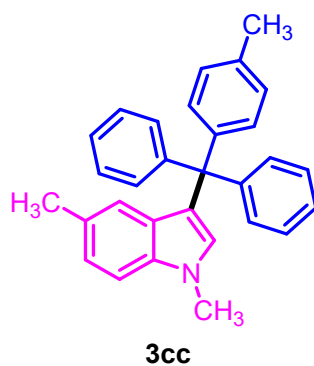


55.2, 36.9, 19.9. HRMS (ESI)  $m/z$ :  $[M+H]^+$  for  $C_{30}H_{27}NO$ , calcd 418.2171; found 418.2141.

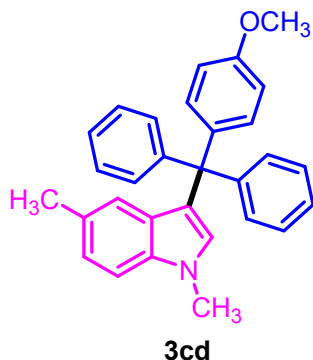
**1,5-dimethyl-3-trityl-1H-indole (3ca):** White solid (192 mg, 99% yield), mp 307-309 °C, purified by recrystallization.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  (ppm) 7.32–7.26 (m, 5H), 7.21 (dd,  $J = 7.4, 2.6$  Hz, 10H), 7.14 (d,  $J = 8.3$  Hz, 1H), 6.97–6.92 (m, 1H), 6.60 (s, 1H), 6.40 (s, 1H), 3.67 (s, 3H), 2.14 (s, 3H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  (ppm) 146.6, 136.2, 130.8, 130.4, 128.6, 127.9, 127.3, 125.9, 122.9, 122.5, 121.6, 108.6, 59.4, 32.8, 21.5. Anal. for  $C_{29}H_{25}N$ , calcd C, 89.88; H, 6.50; N, 3.61; found C, 89.58; H, 6.37; N, 3.30.



**3-(bis(4-methoxyphenyl)(phenyl)methyl)-1,5-dimethyl-1H-indole (3cb):** White solid (194 mg, 87% yield), mp 108-110 °C, purified by chromatography.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  (ppm) 7.29–7.22 (m, 5H), 7.17 (t,  $J = 8.1$  Hz, 5H), 6.99 (t,  $J = 8.3$  Hz, 1H), 6.80 (d,  $J = 8.9$  Hz, 4H), 6.61 (s, 1H), 6.48 (s, 1H), 3.82 (s, 6H), 3.71 (s, 3H), 2.20 (s, 3H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  (ppm) 157.5, 147.3, 139.2, 136.2, 131.7, 130.7, 130.2, 128.5, 127.6, 127.3, 125.8, 122.9, 122.6, 122.2, 112.6, 108.6, 58.0, 55.2, 32.8, 21.5. HRMS (ESI)  $m/z$ :  $[M+H]^+$  for  $C_{31}H_{29}NO_2$ , calcd 448.2277; found 448.2231.



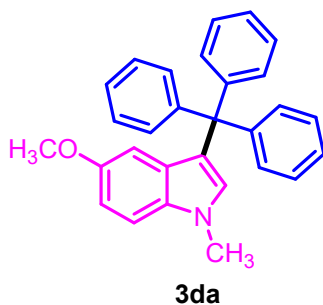
**3-(diphenyl(*p*-tolyl)methyl)-1,5-dimethyl-1H-indole (3cc):** White solid (155 mg, 77% yield), mp 106-108 °C, purified by chromatography.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  (ppm) 7.17–7.00 (m, 13H), 6.95 (d,  $J = 8.3$  Hz, 2H), 6.88–6.84 (m, 1H), 6.52 (s, 1H), 6.34 (s, 1H), 3.59 (s, 3H), 2.24 (s, 3H), 2.07 (s, 3H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  (ppm) 146.8, 143.8, 136.2, 135.3, 130.8, 130.7, 130.3, 128.5, 128.1, 127.6, 127.3, 125.8, 122.9, 122.6,



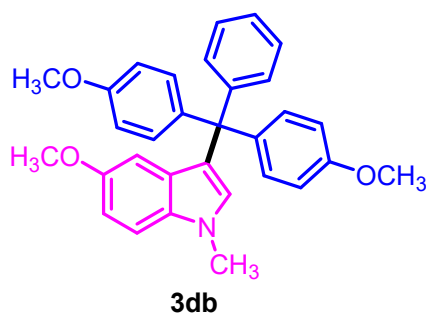
121.8, 108.6, 59.1, 32.8, 21.5, 21.0. HRMS (ESI)  $m/z$ :  $[M+H]^+$  for  $C_{30}H_{27}N$ , calcd 402.2222; found 402.2186.

**3-((4-methoxyphenyl)diphenylmethyl)-1,5-dimethyl-**

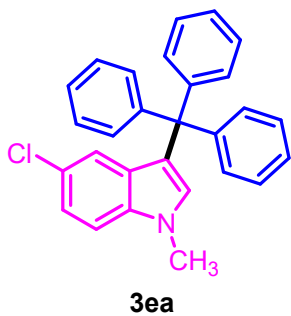
**1H-indole (3cd):** White solid (149 mg, 71% yield), mp 251-254 °C, purified by chromatography.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  (ppm) 7.29–7.13 (m, 14H), 6.97 (d,  $J = 8.3$  Hz, 1H), 6.80 (t,  $J = 6.0$  Hz, 2H), 6.62 (s, 1H), 6.45 (s, 1H), 3.81 (s, 3H), 3.71 (s, 3H), 2.18 (s, 3H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  (ppm) 157.5, 147.0, 138.9, 136.2, 131.8, 130.7, 130.2, 128.5, 127.6, 127.3, 125.8, 122.9, 122.6, 121.9, 112.6, 108.6, 58.7, 55.2, 32.8, 21.5. Anal. for  $C_{30}H_{27}NO$ , calcd C, 86.30; H, 6.52; N, 3.35; found C, 86.35; H, 7.03; N, 2.81.



**5-methoxy-1-methyl-3-trityl-1H-indole (3da):** White solid (200 mg, 99% yield), mp 378-380 °C, purified by recrystallization.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  (ppm) 7.31–7.27 (m, 2H), 7.24–7.18 (m, 14H), 7.12 (d,  $J = 8.8$  Hz, 1H), 6.76 (dd,  $J = 8.8, 2.5$  Hz, 1H), 6.64 (s, 1H), 6.03 (d,  $J = 2.4$  Hz, 1H), 3.67 (s, 3H), 3.37 (s, 3H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  (ppm) 153.1, 146.6, 133.1, 130.8, 128.6, 127.9, 127.4, 125.9, 121.7, 111.6, 109.5, 104.4, 59.4, 55.5, 32.9. HRMS (ESI)  $m/z$ :  $[M+H]^+$  for  $C_{29}H_{25}N$ , calcd 404.2014; found 404.1987.

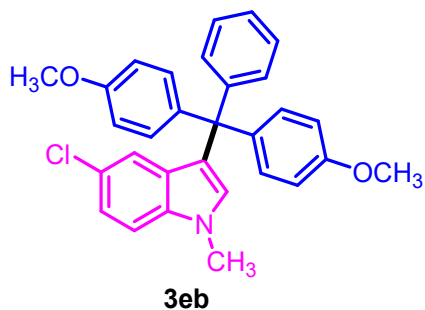


**3-(bis(4-methoxyphenyl)(phenyl)methyl)-5-methoxy-1-methyl-1H-indole (3db):** White solid (202 mg, 87% yield)<sup>3</sup>, mp 134-136 °C, purified by chromatography.  $^1H$  NMR (400 MHz,  $CDCl_3$ ):  $\delta$  (ppm) 7.31–7.15 (m, 10H), 6.83 (t,  $J = 5.8$  Hz, 5H), 6.68 (s, 1H), 6.13 (d,  $J = 1.8$  Hz, 1H), 3.82 (s, 6H), 3.71 (s, 3H), 3.46 (s, 3H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ ):  $\delta$  (ppm) 157.6, 153.0, 147.2, 139.2, 133.1, 131.7, 130.7, 130.5, 128.6, 127.4, 125.9, 122.4,

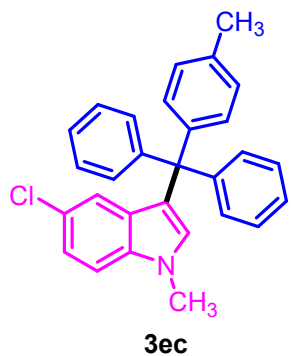


112.6, 111.6, 109.7, 104.5, 58.0, 55.2, 32.9.

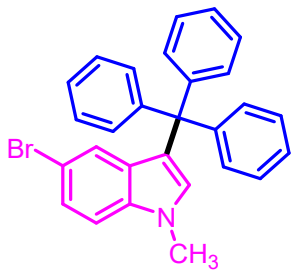
**5-chloro-1-methyl-3-trityl-1H-indole (3ea):** White solid (194 mg, 95% yield), mp 354-356 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.34–7.16 (m, 16H), 7.09 (dd, *J* = 8.7, 2.0 Hz, 1H), 6.74 (s, 1H), 6.62 (d, *J* = 1.9 Hz, 1H), 3.72 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 146.2, 136.1, 131.3, 130.7, 129.2, 128.0, 127.5, 126.2, 124.5, 122.0, 121.7, 110.1, 59.3, 33.0. Anal. for C<sub>28</sub>H<sub>22</sub>ClN calcd C, 82.44; H, 5.44; N, 3.43; found C, 81.89; H, 5.31; N, 3.10.



**3-(bis(4-methoxyphenyl)(phenyl)methyl)-5-chloro-1-methyl-1H-indole (3eb):** White solid (197 mg, 84% yield)<sup>3</sup>, mp 216-218 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.17–6.95 (m, 12H), 6.68 (d, *J* = 8.9 Hz, 4H), 6.59–6.53 (m, 2H), 3.70 (s, 6H), 3.59 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 157.7, 146.8, 138.7, 136.1, 131.6, 131.2, 130.5, 129.2, 127.5, 126.0, 124.5, 122.6, 122.0, 121.7, 112.7, 110.1, 57.9, 55.2, 32.9.

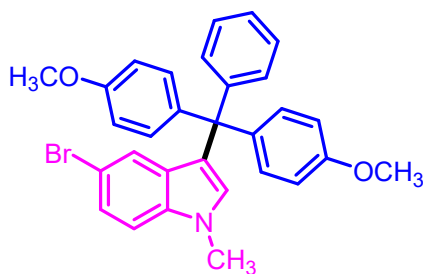


**5-chloro-3-(diphenyl(*p*-tolyl)methyl)-1-methyl-1H-indole (3ec):** White solid (184 mg, 87% yield), mp 114-116 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.19–6.94 (m, 16H), 6.62 (s, 1H), 6.52 (s, 1H), 3.61 (s, 3H), 2.25 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 146.4, 143.3, 136.1, 135.6, 131.3, 130.7, 130.5, 129.2, 128.2, 127.5, 126.1, 124.5, 122.2, 122.0, 121.7, 110.1, 58.9, 32.9, 21.0. HRMS (ESI) *m/z*: [M+H]<sup>+</sup> for C<sub>29</sub>H<sub>24</sub>ClN, calcd 421.1676; 421.1561.



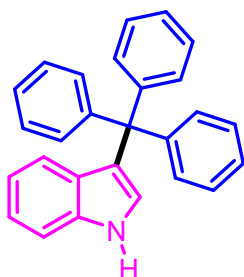
**3fa**

**5-bromo-1-methyl-3-trityl-1H-indole (3fa):** White solid (82 mg, 36% yield), mp 351-354 °C, purified by chromatography.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 7.19–7.10 (m, 16H), 7.04 (d,  $J = 8.7$  Hz, 1H), 6.64 (d,  $J = 1.8$  Hz, 1H), 6.60 (d,  $J = 3.6$  Hz, 1H), 3.61 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 146.2, 136.4, 131.2, 130.7, 129.8, 127.5, 126.1, 125.0, 124.3, 122.0, 112.2, 110.6, 59.3, 32.9. Anal. for  $\text{C}_{28}\text{H}_{22}\text{BrN}$  calcd C, 74.34; H, 4.90; N, 3.10; found C, 74.01; H, 4.71; N, 2.83.



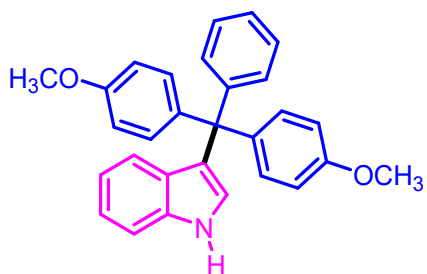
**3fb**

**3-(bis(4-methoxyphenyl)(phenyl)methyl)-5-bromo-1-methyl-1H-indole (3fb):** White solid (162 mg, 63% yield)<sup>3</sup>, mp 171-173 °C, purified by chromatography.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 7.30–7.10 (m, 12H), 6.85–6.77 (m, 5H), 6.68 (s, 1H), 3.82 (s, 6H), 3.71 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 157.7, 146.8, 138.7, 136.4, 131.6, 131.0, 130.5, 129.8, 127.5, 126.0, 125.1, 124.2, 122.6, 112.7, 112.2, 110.6, 57.9, 55.2, 32.9.



**3ga**

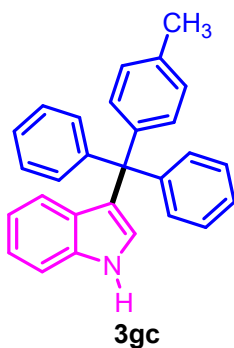
**3-trityl-1H-indole (3ga):** White solid (177 mg, 98% yield)<sup>4</sup>, mp 319-322 °C, purified by re-crystallization.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 7.90 (s, 1H), 7.33–7.16 (m, 17H), 7.08 (t,  $J = 7.6$  Hz, 1H), 6.78 (dd,  $J = 11.0, 4.3$  Hz, 2H), 6.67 (d,  $J = 8.1$  Hz, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 146.5, 137.0, 130.8, 128.0, 127.8, 127.4, 126.0, 125.5, 124.0, 122.8, 121.7, 119.2, 111.0, 59.5.



**3gb**

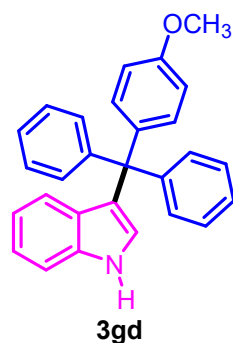
**3-(bis(4-methoxyphenyl)(phenyl)methyl)-1H-indole (3gb):** White solid (187 mg, 89% yield)<sup>3</sup>, mp 162-164 °C, purified by chromatography.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 7.96 (s, 1H), 7.36–7.10 (m, 13H), 6.88–6.71 (m, 8H), 3.81 (s, 6H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 157.6, 147.1, 139.0, 137.0, 131.7, 130.6, 127.8, 127.4, 125.9, 125.3, 124.5, 122.9, 121.7, 119.2, 112.6,



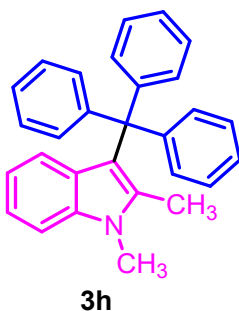


110.9, 58.0, 55.2.

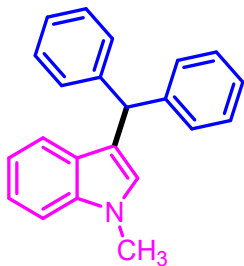
**3-(diphenyl(*p*-tolyl)methyl)-1*H*-indole (3gc):** White solid (159 mg, 85% yield), mp 133-135 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.68 (s, 1H), 7.20–6.95 (m, 19H), 6.91 (d, *J* = 8.1 Hz, 2H), 6.67 (m, 2H), 6.59 (d, *J* = 8.1 Hz, 1H), 2.20 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 146.7, 143.5, 137.0, 135.5, 130.8, 130.7, 128.7, 128.1, 127.9, 127.4, 127.2, 126.0, 125.5, 124.1, 122.9, 121.7, 119.2, 110.9, 59.1, 21.0. HRMS (ESI) *m/z*: [M+H]<sup>+</sup> for C<sub>28</sub>H<sub>23</sub>N, calcd 374.1909; found 374.1879.



**3-((4-methoxyphenyl)diphenylmethyl)-1*H*-indole (3gd):** White solid (177 mg, 91% yield)<sup>5</sup>, 140-142 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.83 (s, 1H), 7.25–7.18 (m, 2H), 7.17–7.07 (m, 10H), 7.06–6.98 (m, 3H), 6.77–6.58 (m, 5H), 3.68 (d, *J* = 4.3 Hz, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 157.6, 146.8, 138.7, 137.0, 131.8, 137.0, 131.8, 130.7, 127.9, 127.8, 127.4, 126.0, 125.4, 124.2, 122.9, 121.7, 119.2, 112.6, 111.0, 58.7, 55.2.

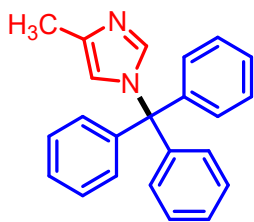


**1,2-dimethyl-3-trityl-1*H*-indole (3h):** White solid (121 mg, 62% yield), mp 323-325 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.43 (m, 6H), 7.24–7.11 (m, 10H), 7.03 (m, 1H), 6.73 (m, 1H), 6.40 (d, *J* = 8.2 Hz, 1H), 3.60 (s, 3H), 1.82 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 147.1, 136.8, 134.9, 130.6, 127.4, 125.5, 122.0, 120.0, 118.3, 117.7, 108.3, 60.3, 29.5, 13.8. Anal. for C<sub>29</sub>H<sub>25</sub>N calcd C, 89.88; H, 6.50; N, 3.61; found C, 89.71; H, 6.35; N, 3.38.



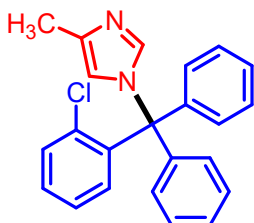
**3i**

**3-benzhydryl-1-methyl-1H-indole (3i):** White solid (86 mg, 58% yield)<sup>3</sup>, mp 104-107 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.21–7.05 (m, 15H), 6.90–6.83 (m, 1H), 6.30 (s, 1H), 5.57 (s, 1H), 3.53 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 144.2, 142.3, 137.6, 129.1, 128.8, 128.5, 128.4, 127.4, 126.3, 121.7, 120.1, 118.9, 109.2, 48.9, 32.7.



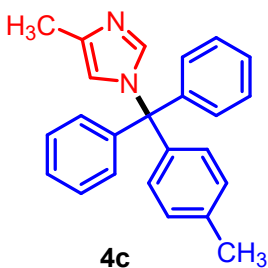
**4a**

**4-methyl-1-trityl-1H-imidazole (4a):** White solid (131 mg, 81% yield)<sup>6</sup>, mp 341-344 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.38–7.32 (m, 10H), 7.17 (dd, *J* = 6.2, 3.5 Hz, 6H), 6.54 (s, 1H), 2.22 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 142.6, 138.2, 137.1, 129.8, 128.0, 127.9, 118.2, 75.0, 13.9.



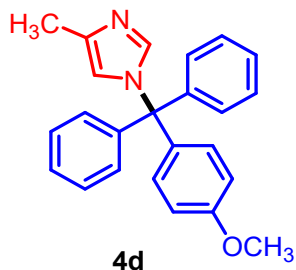
**4b**

**1-((2-chlorophenyl)diphenylmethyl)-4-methyl-1H-imidazole (4b):** White solid (126 mg, 70% yield)<sup>7</sup>, mp 189-191 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.32–7.19 (m, 9H), 7.18–7.07 (m, 5H), 6.85 (dd, *J* = 8.0, 1.6 Hz, 1H), 6.34 (s, 1H), 2.09 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 141.0, 140.3, 138.2, 137.0, 135.5, 132.2, 130.4, 130.2, 129.8, 128.1, 128.0, 127.0, 118.0, 75.0, 13.7.

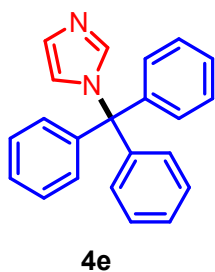


**4c**

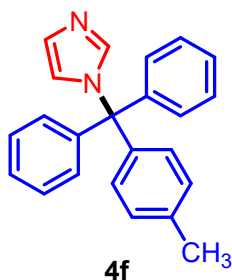
**1-(diphenyl(*p*-tolyl)methyl)-4-methyl-1H-imidazole (4c):** White solid (95 mg, 56% yield), mp 239-241 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.39–7.27 (m, 7H), 7.16 (m, 6H), 7.04 (d, *J* = 8.3 Hz, 2H), 6.54 (s, 1H), 2.38 (s, 3H), 2.22 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 142.8, 139.7, 138.2, 137.7, 137.1, 129.8, 128.7, 127.9, 118.1, 74.8, 21.0, 13.9. HRMS (ESI) *m/z*: [M+H]<sup>+</sup> for C<sub>24</sub>H<sub>22</sub>N<sub>2</sub>, calcd 339.1861; found 339.1835.



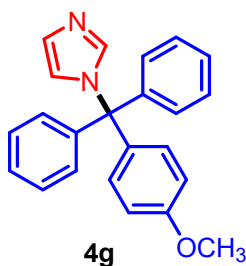
**1-((4-methoxyphenyl)diphenylmethyl)-4-methyl-1H-imidazole (4d):** White solid (36 mg, 20% yield), mp 219–221 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.37–7.30 (m, 7H), 7.18–7.12 (m, 4H), 7.09–7.05 (m, 2H), 6.88–6.83 (m, 2H), 6.53 (s, 1H), 3.83 (s, 3H), 2.22 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 159.0, 142.9, 138.1, 137.0, 134.7, 131.2, 129.7, 127.9, 118.1, 113.2, 74.6, 55.3, 13.9. HRMS (ESI) m/z: [M+H]<sup>+</sup> for C<sub>24</sub>H<sub>22</sub>N<sub>2</sub>O, calcd 355.1810; found 355.1783.



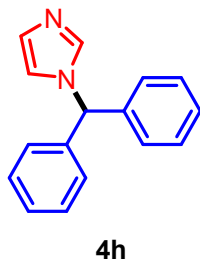
**1-trityl-1H-imidazole (4e):** White solid (59 mg, 38% yield)<sup>8,9</sup>, mp 337–339 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.39 (s, 1H), 7.29–7.21 (m, 9H), 7.10–7.02 (m, 6H), 6.99 (s, 1H), 6.75 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 142.5, 139.0, 129.8, 128.3, 128.1, 121.7, 75.2.



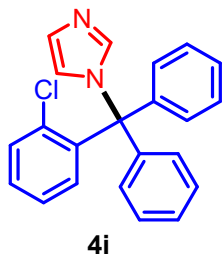
**1-(diphenyl(*p*-tolyl)methyl)-1H-imidazole (4f):** White solid (107 mg, 66% yield)<sup>9</sup>, mp 220–222 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.49 (s, 1H), 7.39–7.28 (m, 6H), 7.16 (m, 6H), 7.10–7.02 (m, 3H), 6.85 (s, 1H), 2.38 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 142.7, 139.6, 139.0, 137.9, 129.8, 128.7, 128.2, 128.0, 127.8, 121.7, 75.1, 21.0.



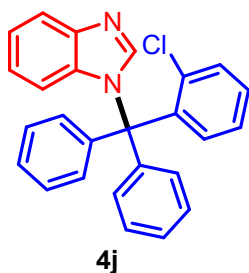
**1-((4-methoxyphenyl)diphenylmethyl)-1H-imidazole (4g):** White solid (68 mg, 40% yield)<sup>10</sup>, mp 223–225 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ (ppm) 7.37 (s, 1H), 7.27–7.18 (m, 6H), 7.12–7.01 (m, 4H), 7.00–6.95 (m, 3H), 6.79–6.70 (m, 3H), 3.72 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ (ppm) 159.1, 142.8, 139.0, 134.6, 131.2, 129.7, 128.2, 128.0, 121.7, 113.3, 74.9, 55.3.



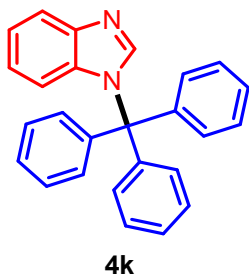
**1-benzhydryl-1H-imidazole (4h):** Colourless liquid (33 mg, 28% yield), purified by chromatography.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 7.33 (d,  $J = 8.5$  Hz, 1H), 7.32–7.23 (m, 6H), 7.03 (dd,  $J = 4.9, 2.7$  Hz, 5H), 6.77 (s, 1H), 6.44 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 139.1, 137.4, 129.2, 128.9, 128.4, 128.1, 65.1. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  for  $\text{C}_{16}\text{H}_{14}\text{N}_2$ , calcd 235.1235; found 235.1215.



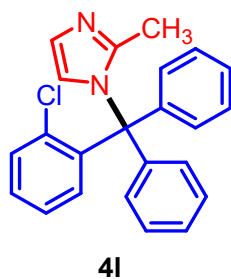
**1-((2-chlorophenyl)diphenylmethyl)-1H-imidazole (4i):** White solid (116 mg, 67% yield)<sup>3</sup>, mp 125-128 °C, purified by chromatography.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 7.38 (s, 1H), 7.32 (dd,  $J = 7.8, 1.4$  Hz, 1H), 7.26–7.20 (m, 7H), 7.18–7.07 (m, 5H), 6.96 (s, 1H), 6.84 (dd,  $J = 8.0, 1.6$  Hz, 1H), 6.66 (s, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 140.9, 140.4, 139.1, 135.6, 132.2, 130.4, 130.2, 129.9, 128.4, 128.2, 128.0, 127.0, 121.6, 75.1.



**1-((2-chlorophenyl)diphenylmethyl)-1H-benzo[d]imidazole (4j):** White solid (121 mg, 61% yield), mp 255-258 °C, purified by chromatography.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 8.02 (s, 1H), 7.80 (d,  $J = 8.1$  Hz, 1H), 7.44–7.14 (m, 15H), 6.95–6.86 (m, 1H), 6.45 (d,  $J = 8.3$  Hz, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 144.8, 144.5, 135.9, 134.6, 132.5, 131.4, 130.5, 129.9, 128.2, 128.1, 126.8, 122.5, 122.1, 120.3, 114.8, 75.6. HRMS (ESI)  $m/z$ :  $[\text{M}+\text{H}]^+$  for  $\text{C}_{26}\text{H}_{19}\text{ClN}_2$ , calcd 395.1315; found 395.1280.



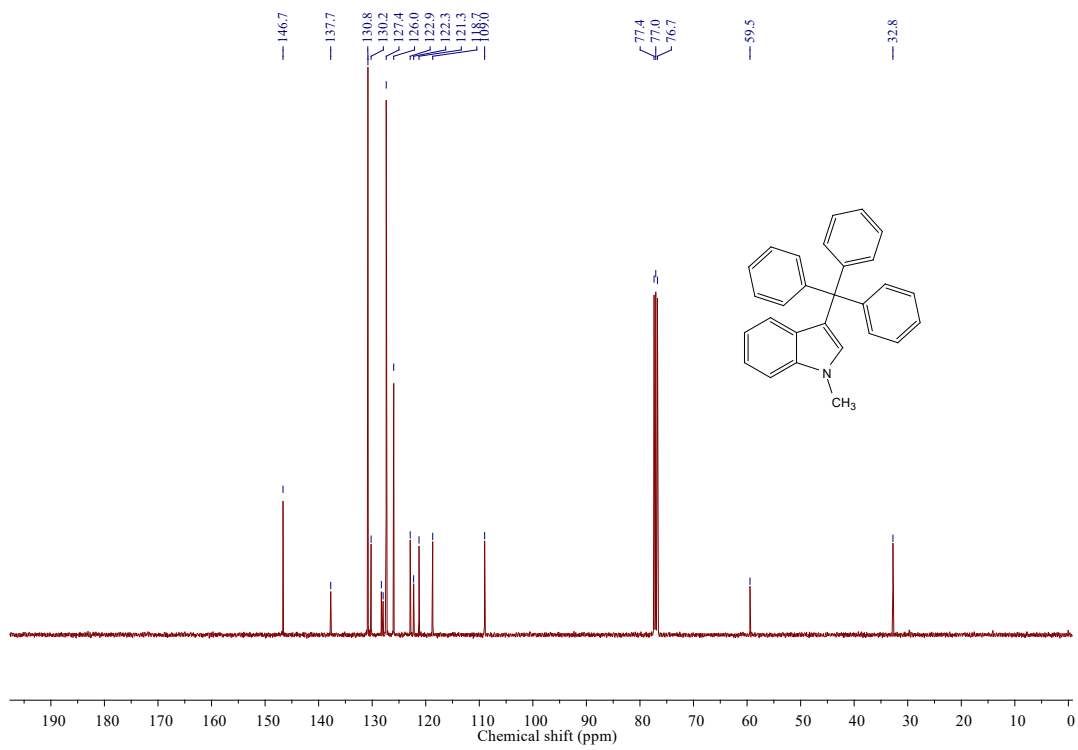
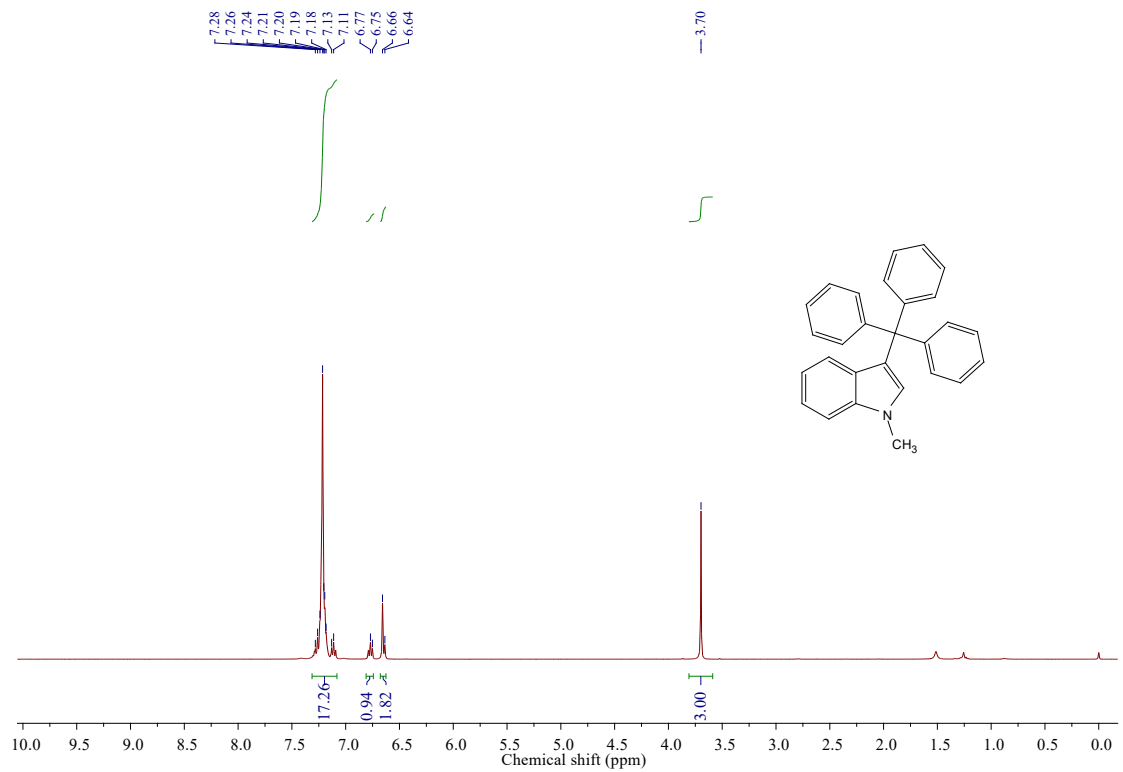
**1-trityl-1H-benzo[d]imidazole (4k):** White solid (44 mg, 24% yield)<sup>10,11</sup>, mp 228-230 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) 7.92 (s, 1H), 7.81 (d,  $J$  = 8.1 Hz, 1H), 7.37–7.30 (m, 9H), 7.24–7.16 (m, 7H), 6.92 (t,  $J$  = 7.7 Hz, 1H), 6.50 (d,  $J$  = 8.3 Hz, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) 144.5, 144.1, 141.3, 134.7, 130.0, 128.2, 128.0, 122.4, 122.1, 120.2, 115.4, 75.5.



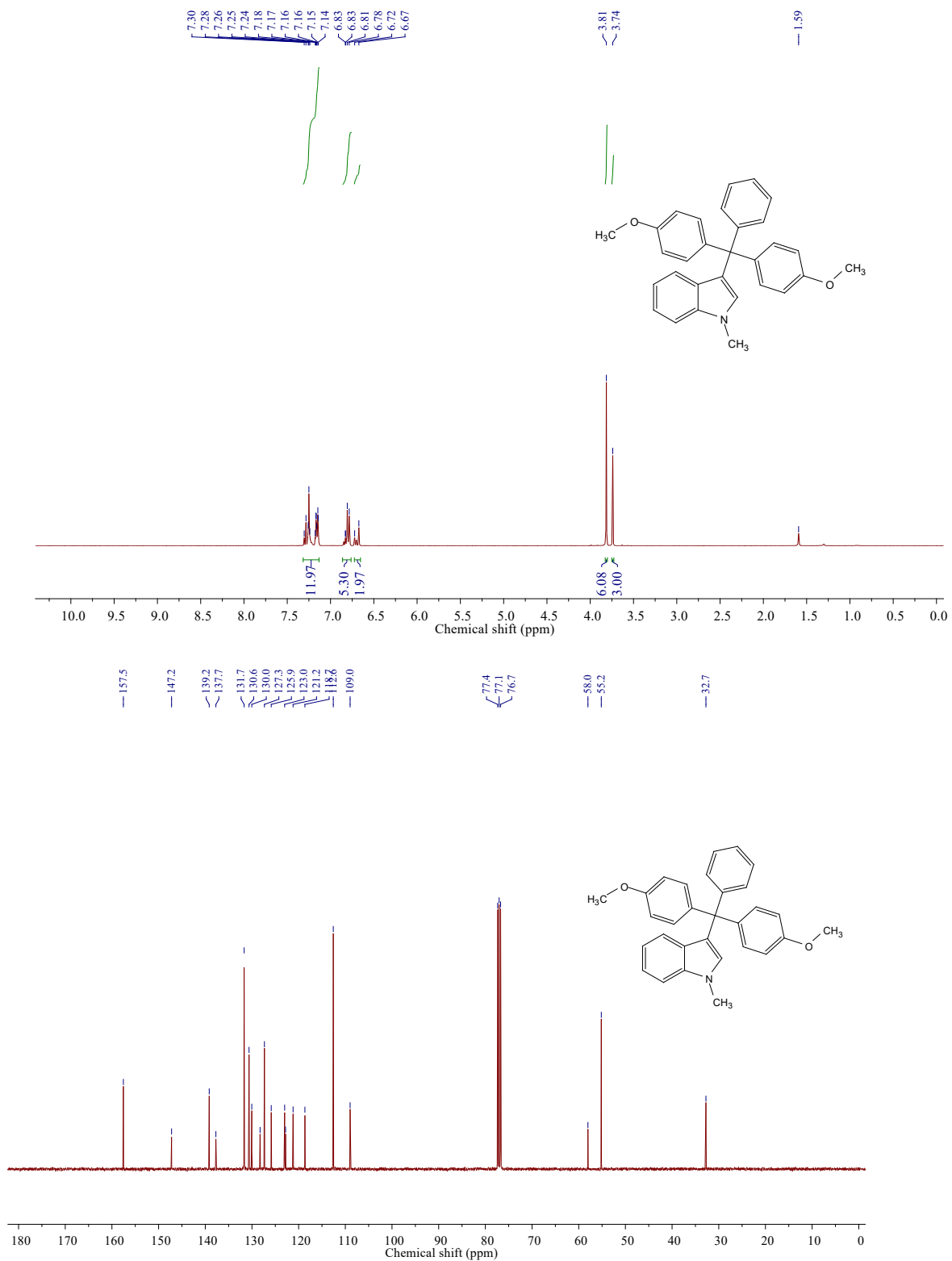
**1-((2-chlorophenyl)diphenylmethyl)-2-methyl-1H-imidazole (4l):** White solid (95 mg, 53% yield), mp 276-278 °C, purified by chromatography. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) 7.35 (dd,  $J$  = 7.8, 1.5 Hz, 1H), 7.29–7.17 (m, 8H), 7.06 (dd,  $J$  = 18.4, 5.6 Hz, 5H), 6.81 (d,  $J$  = 1.5 Hz, 1H), 6.74 (s, 1H), 1.49 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) 146.8, 139.8, 135.8, 132.6, 130.8, 130.7, 129.8, 128.0, 127.8, 126.8, 124.9, 122.1, 75.2, 17.1. Anal. for C<sub>23</sub>H<sub>19</sub>ClN<sub>2</sub> calcd C, 76.98; H, 5.34; N, 7.81; found C, 76.78; H, 5.30; N, 7.68.

# NMR spectra

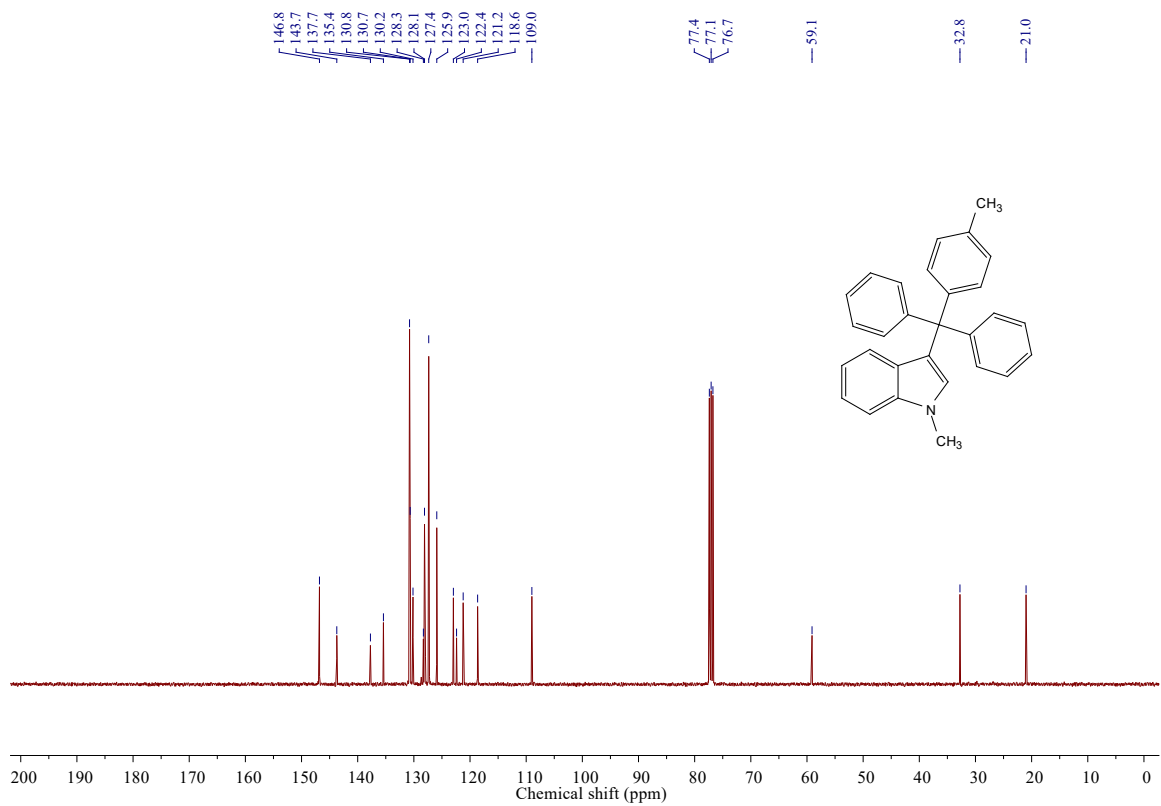
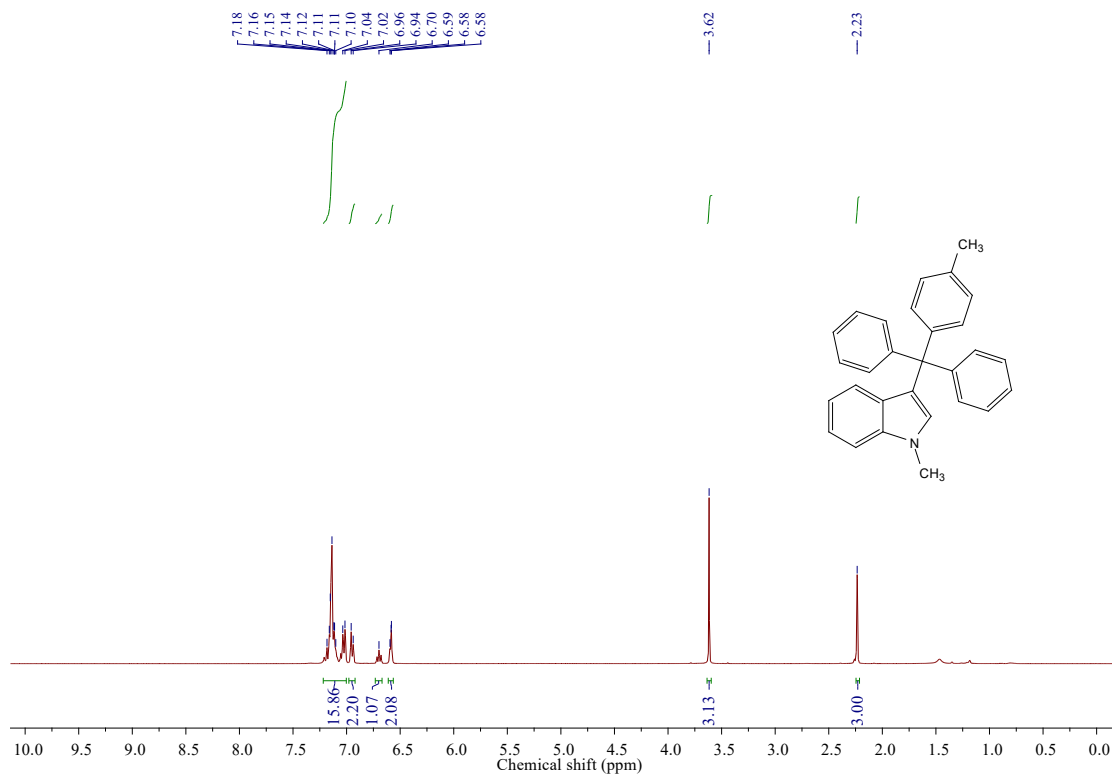
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3ab.

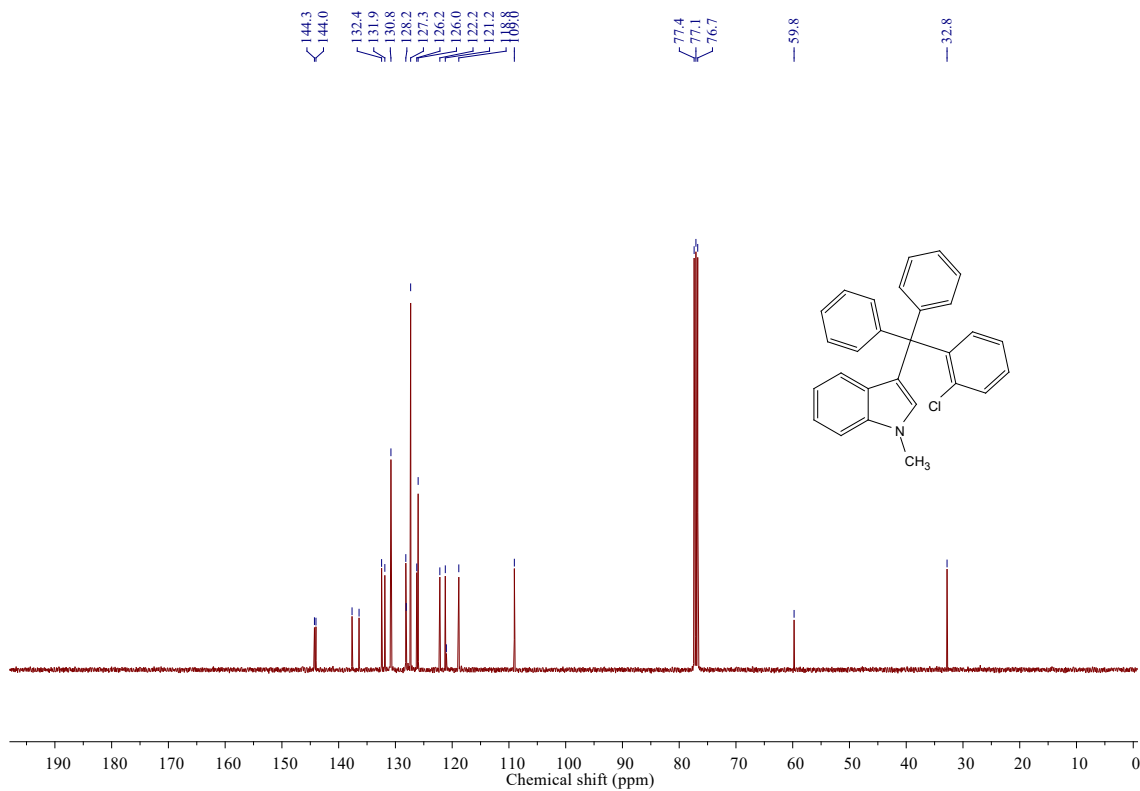
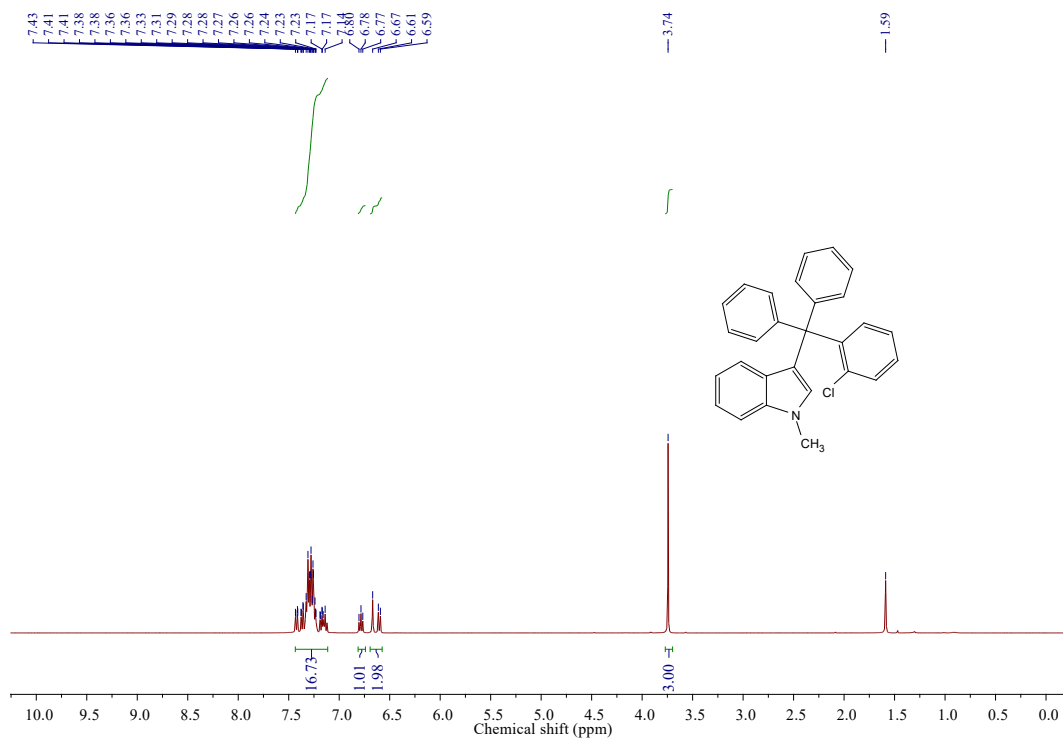


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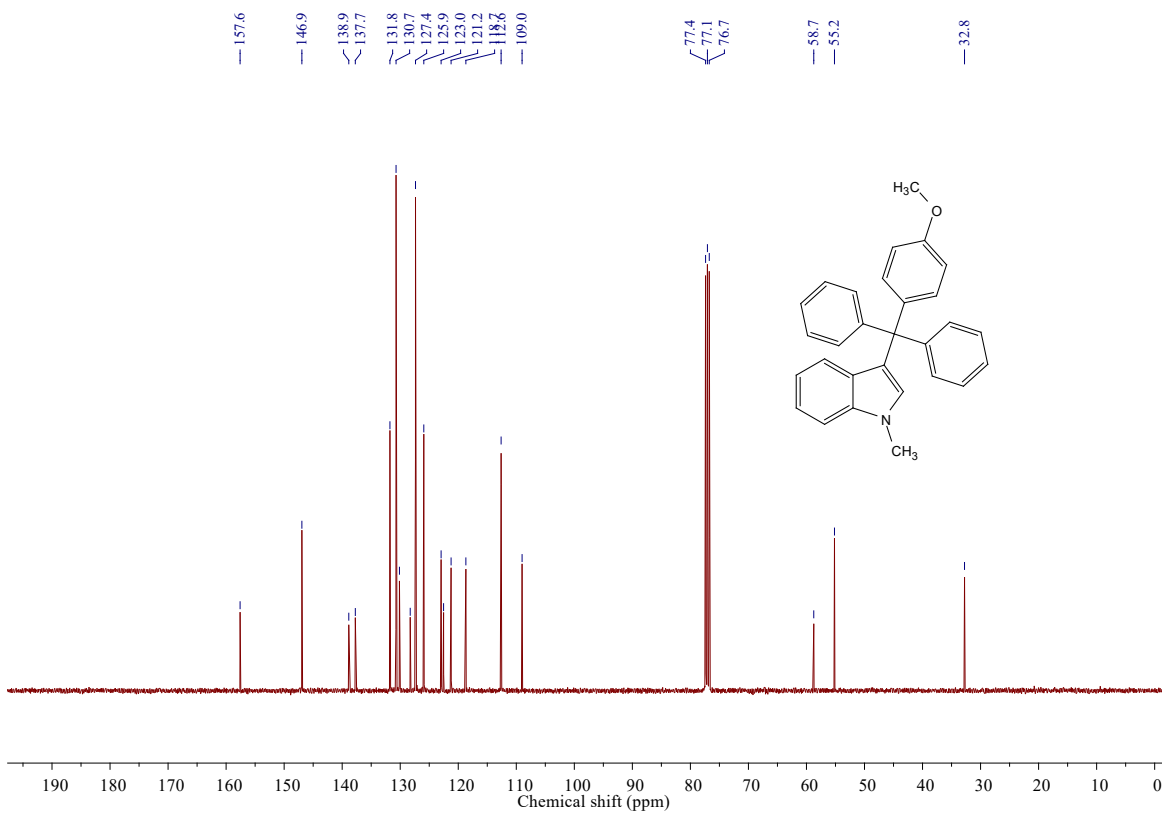
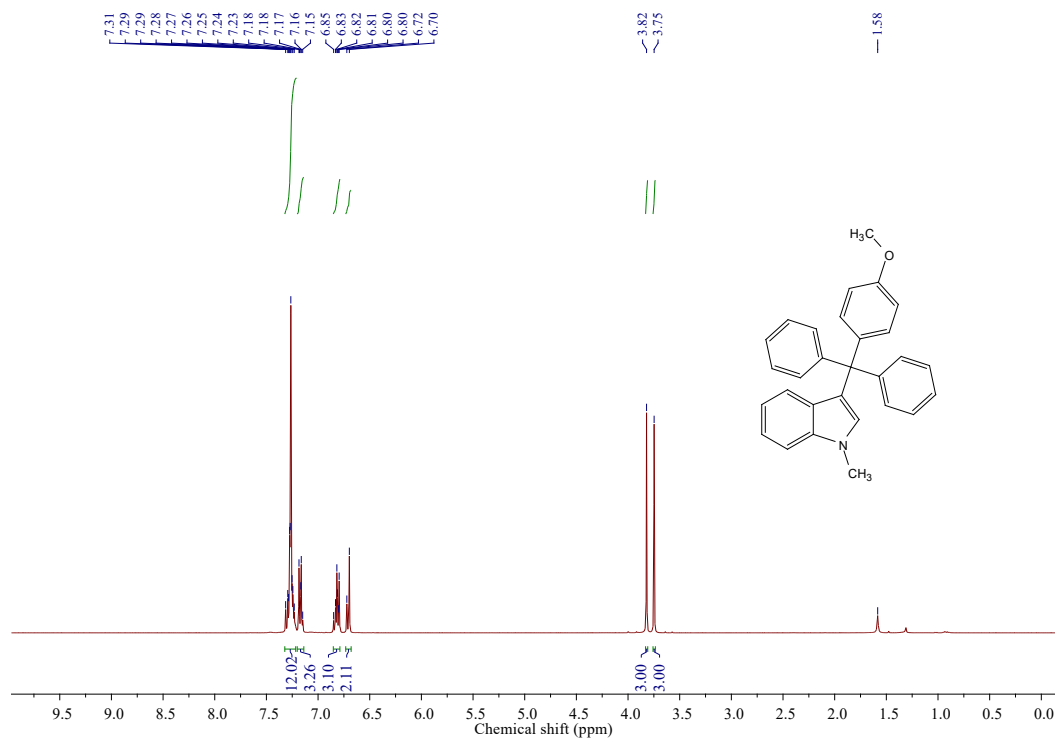




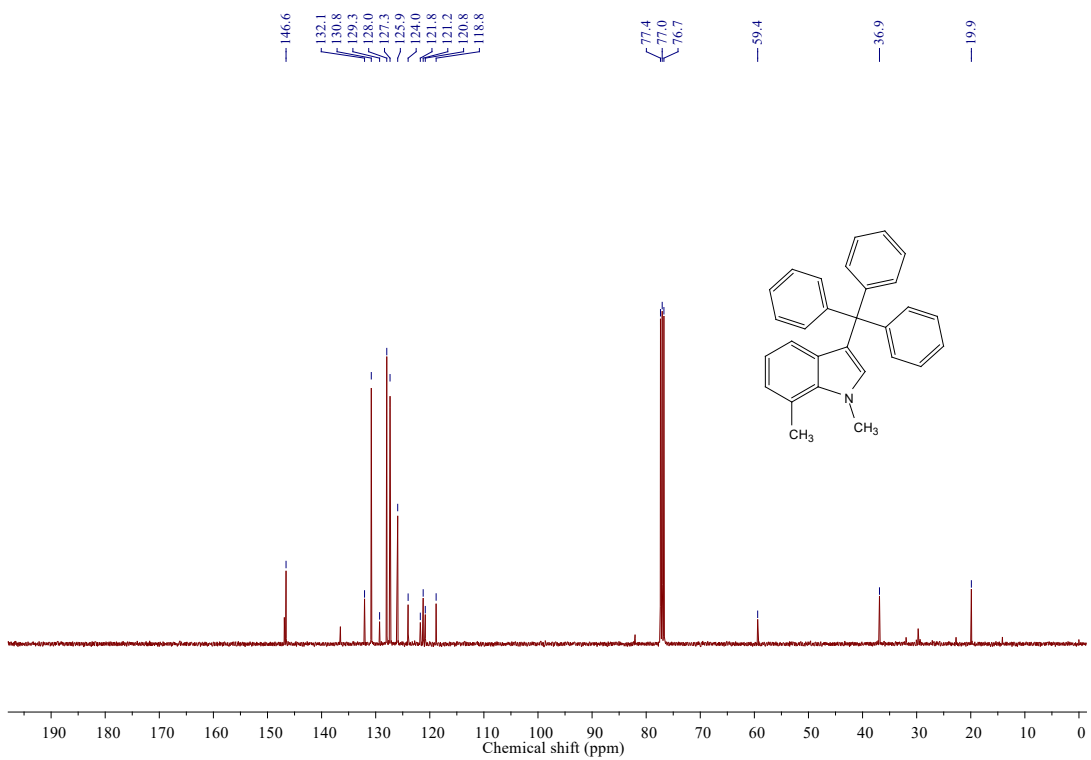
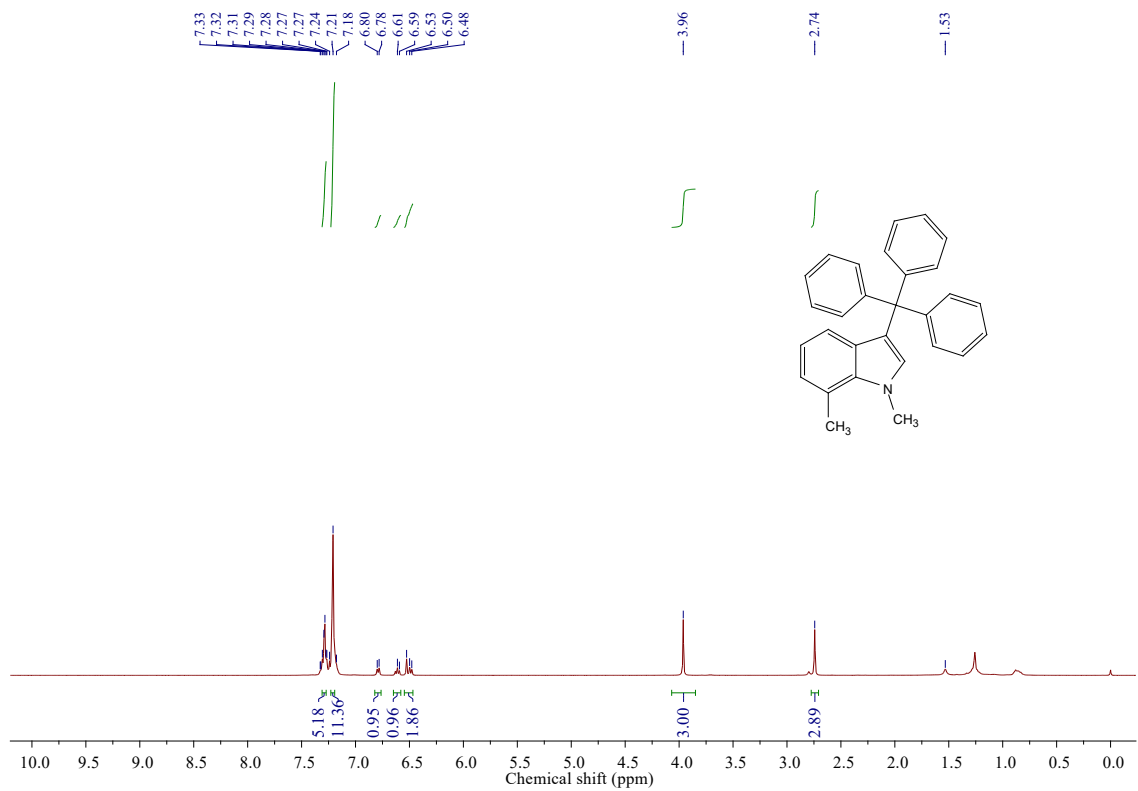
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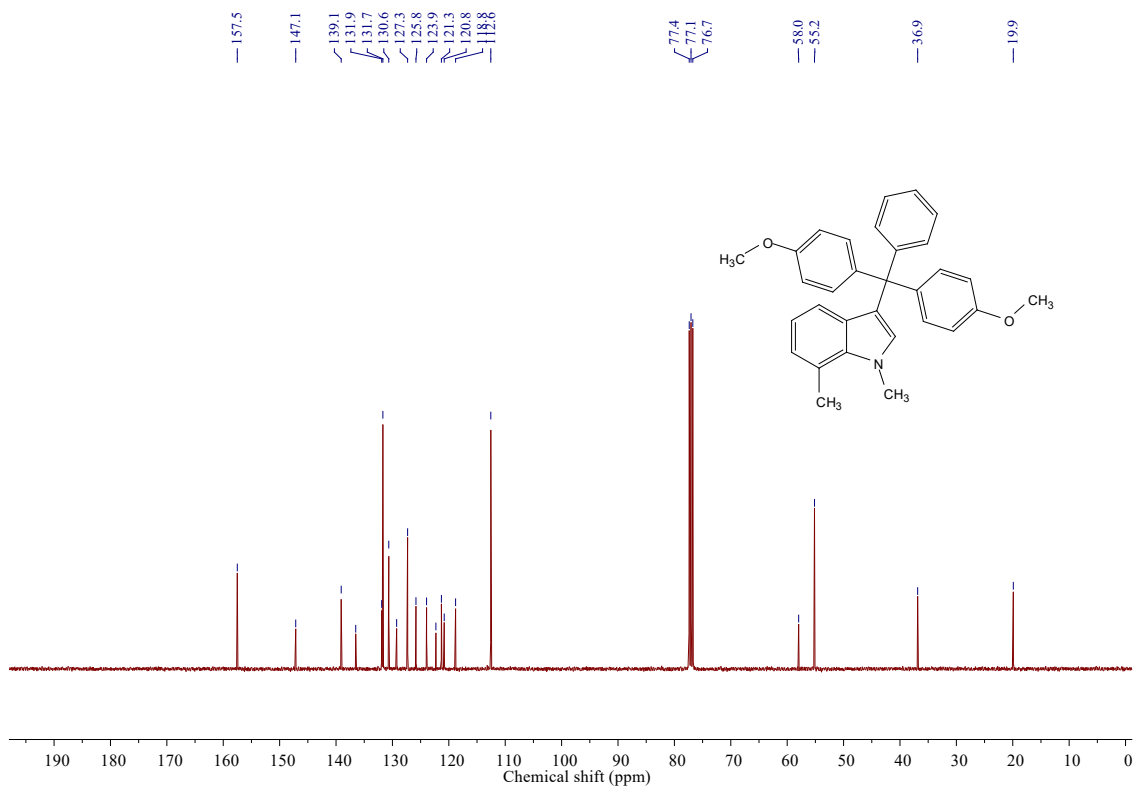
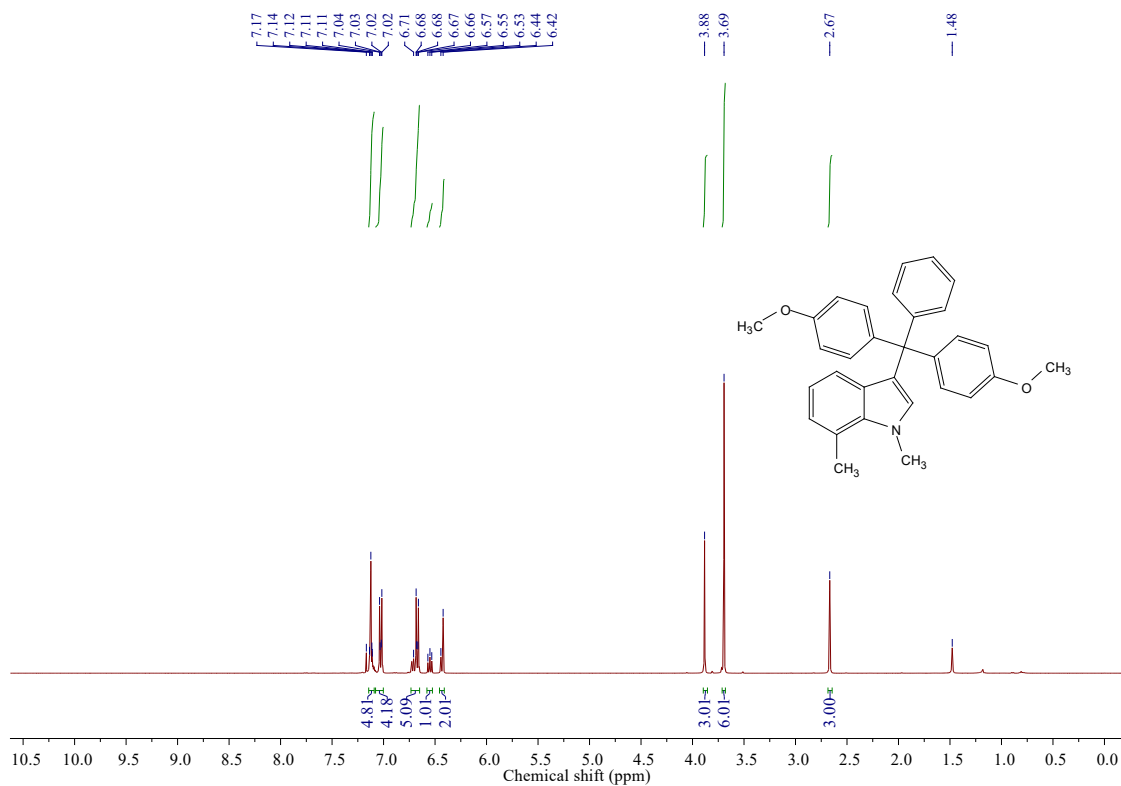
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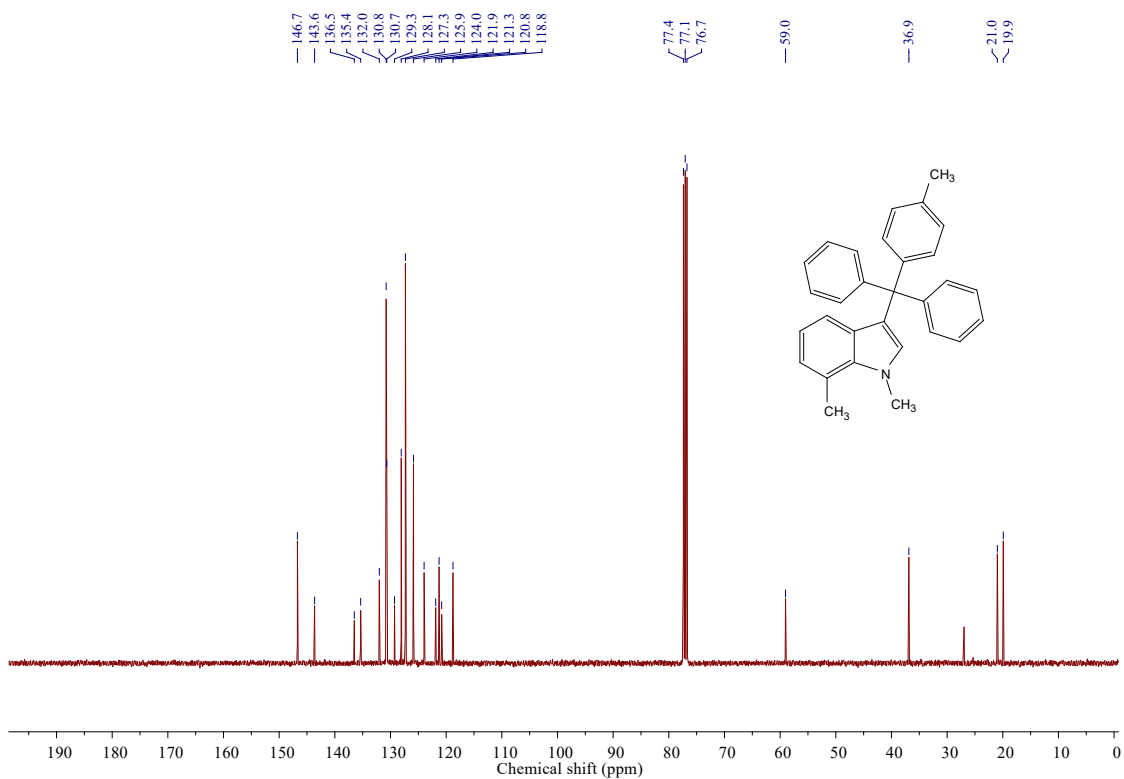
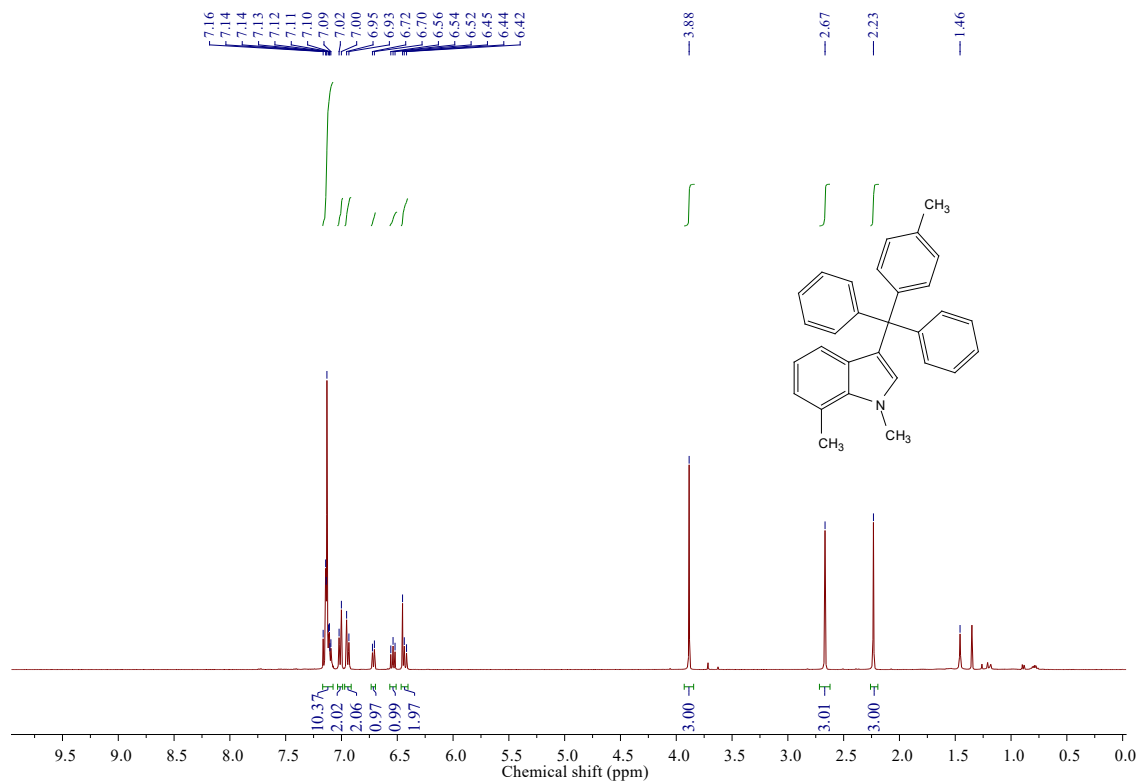
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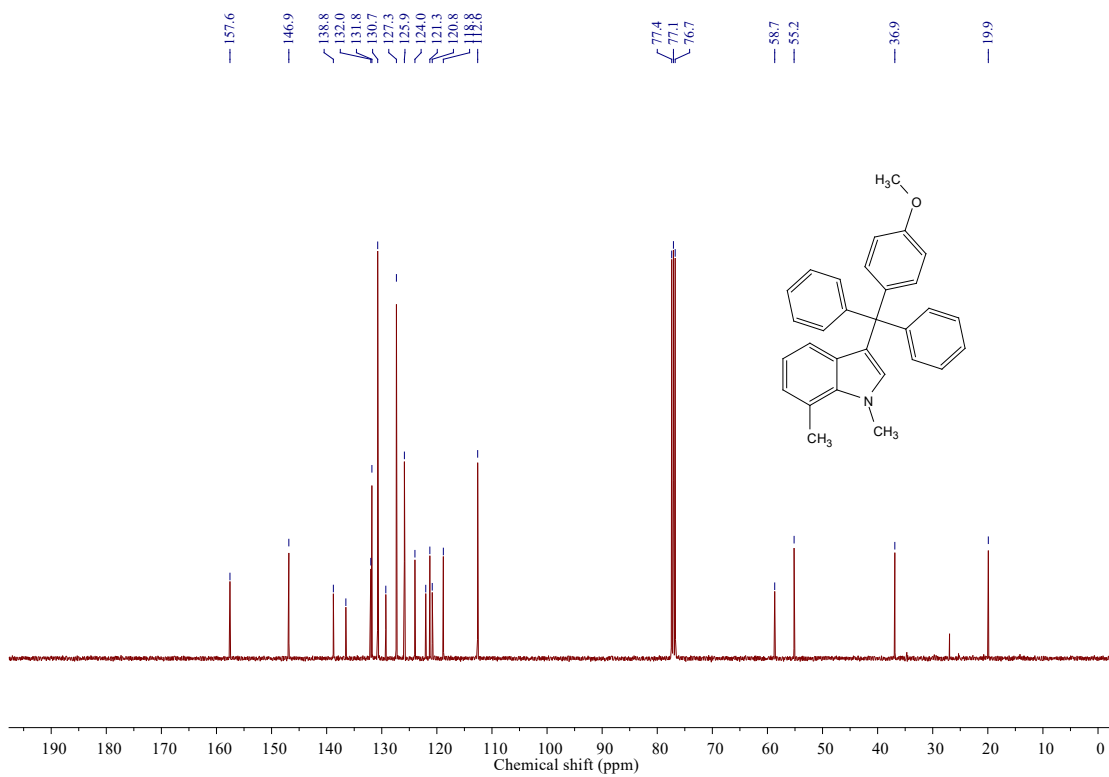
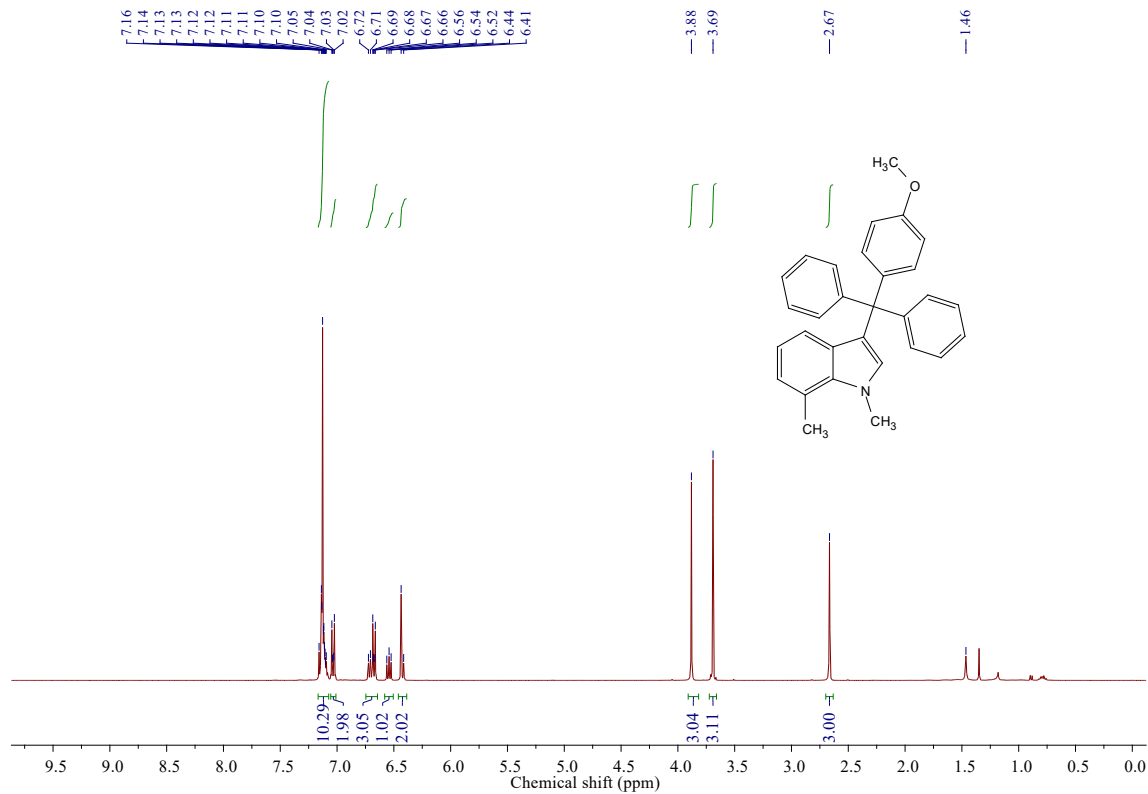
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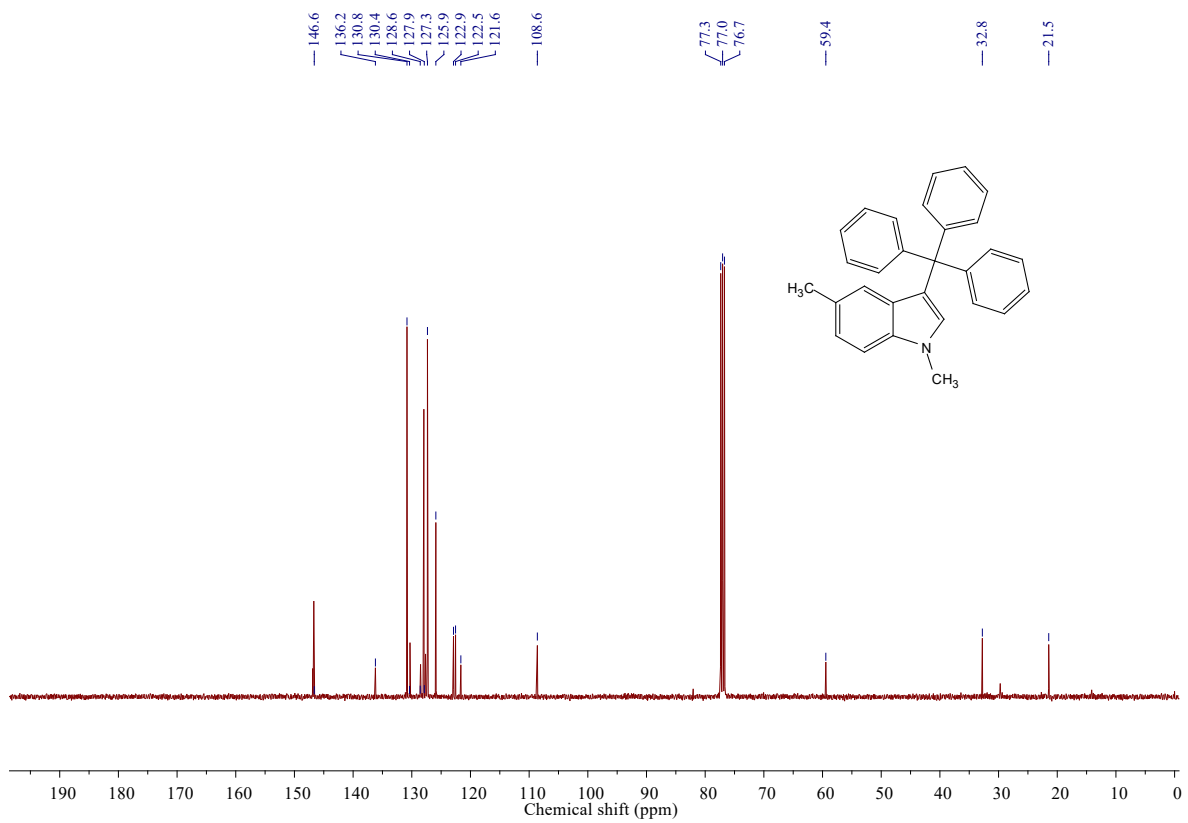
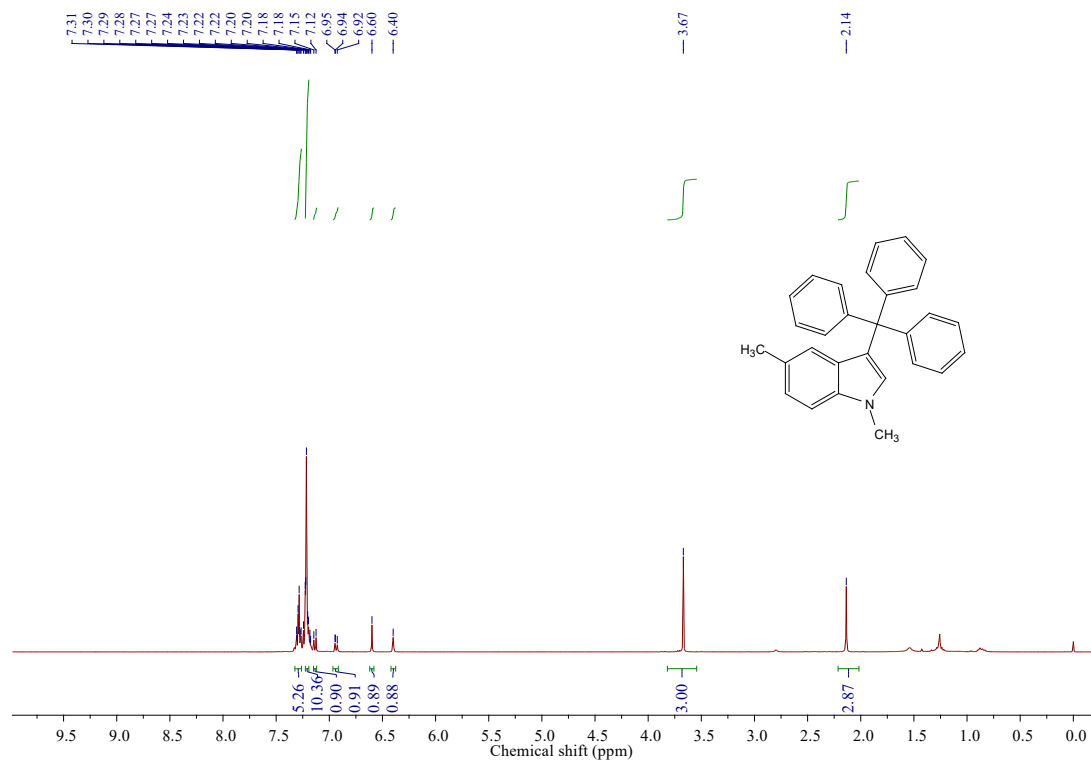
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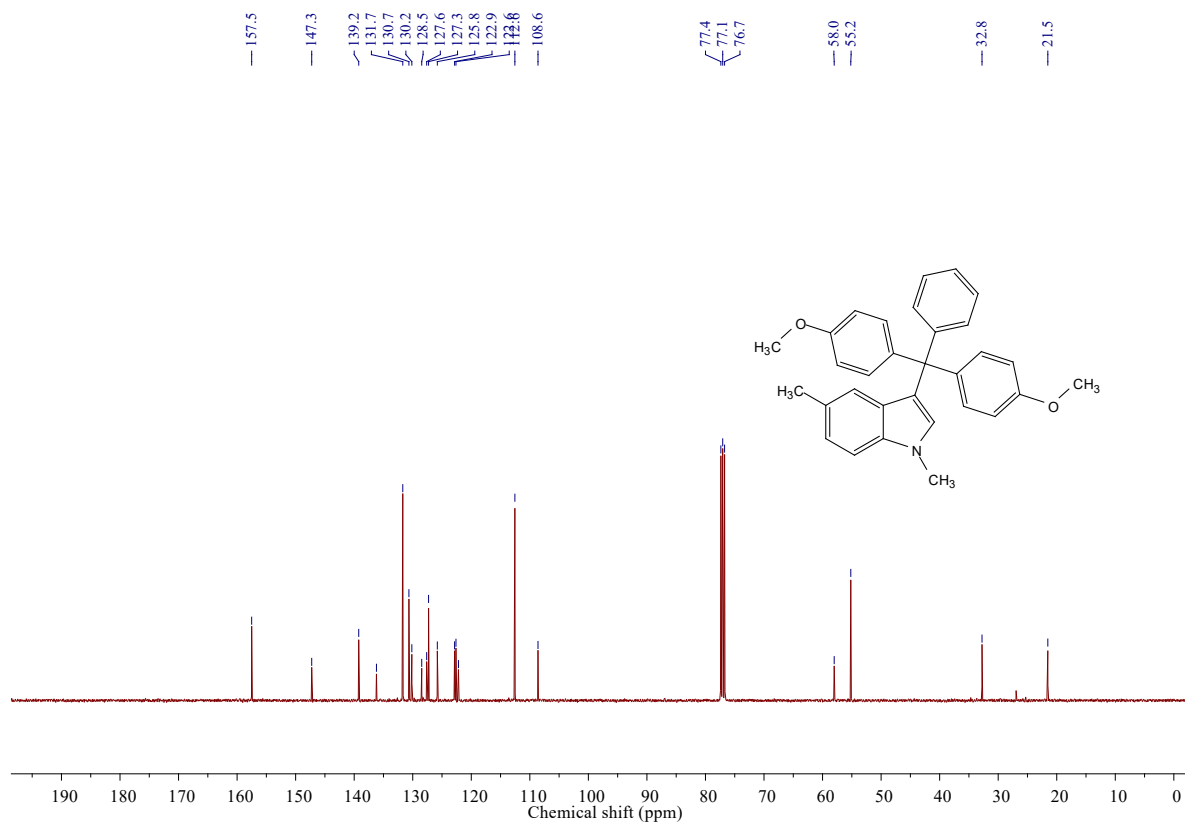
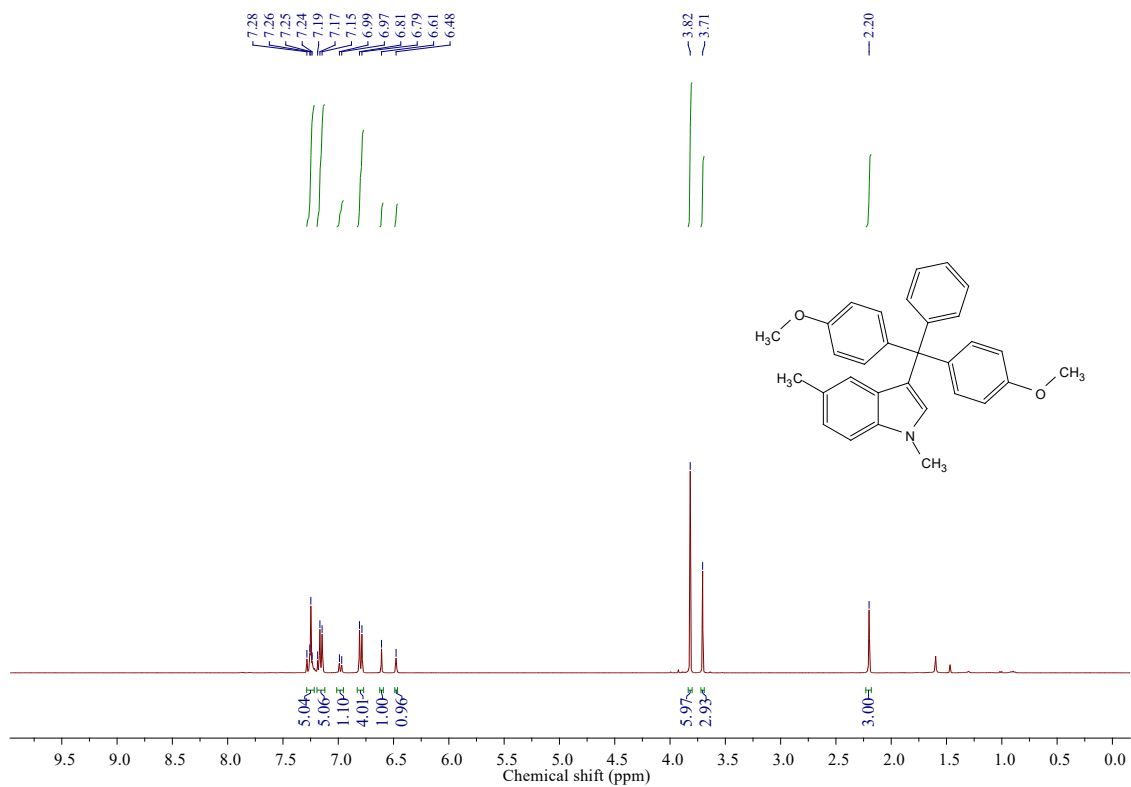
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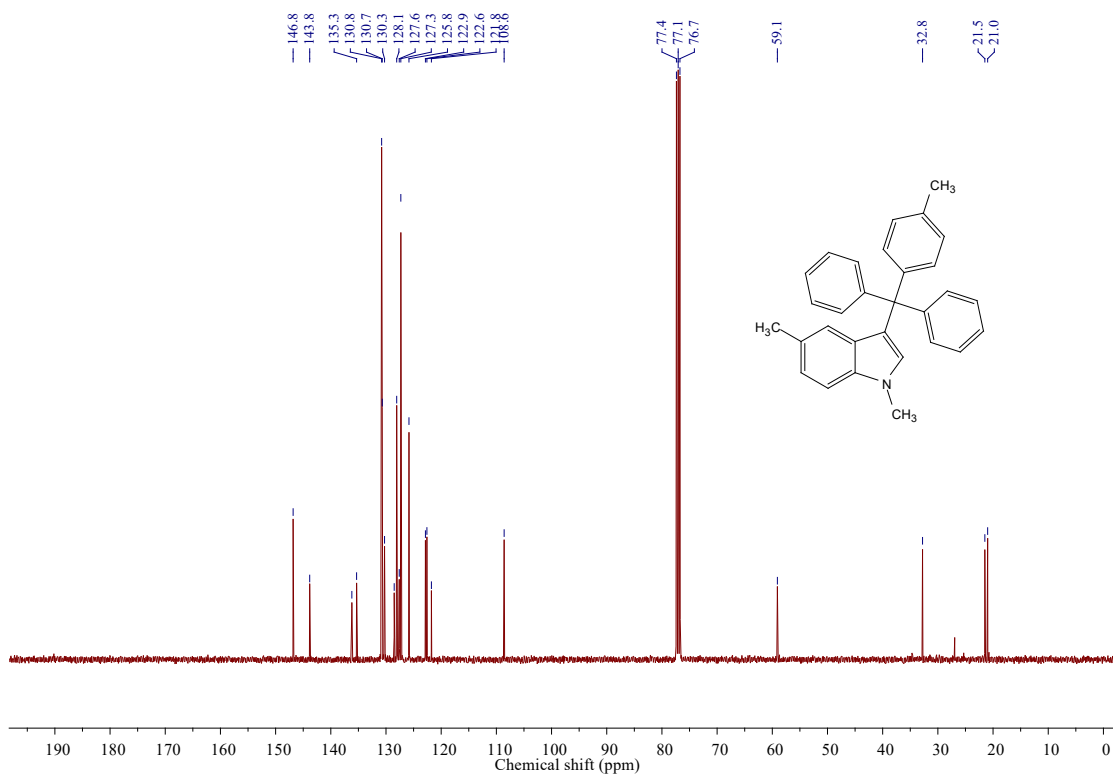
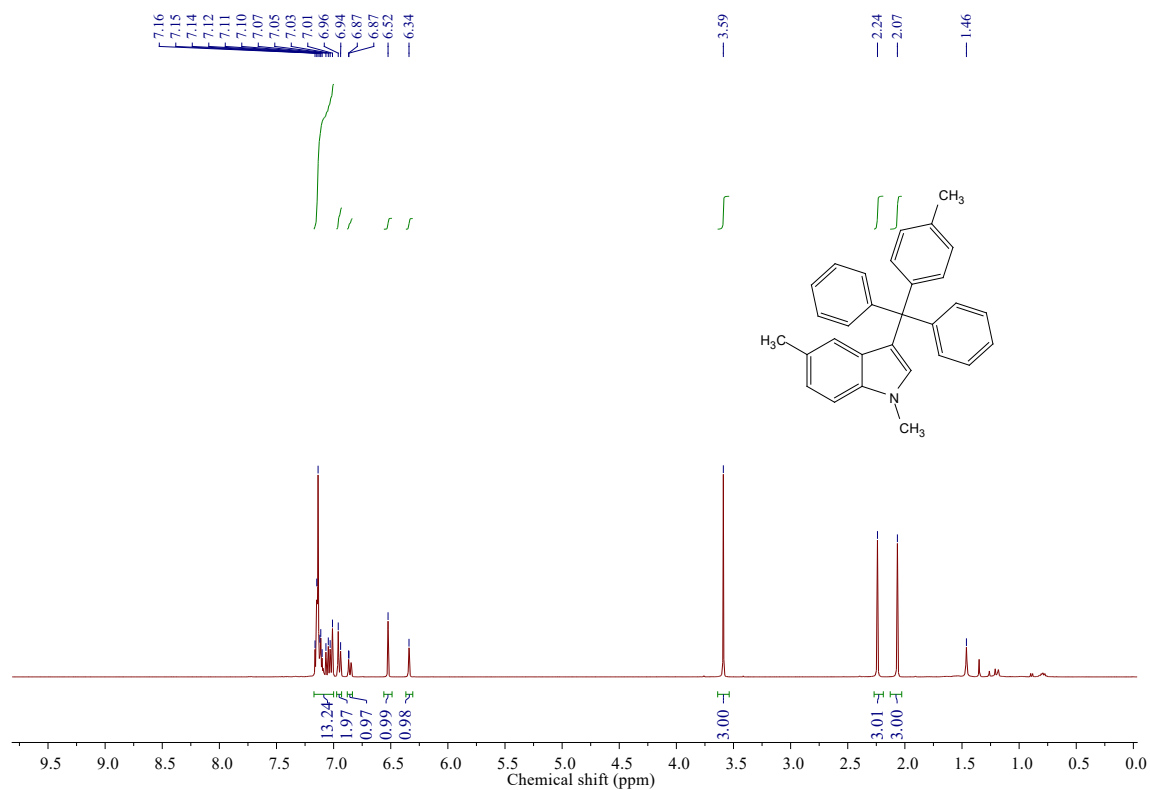


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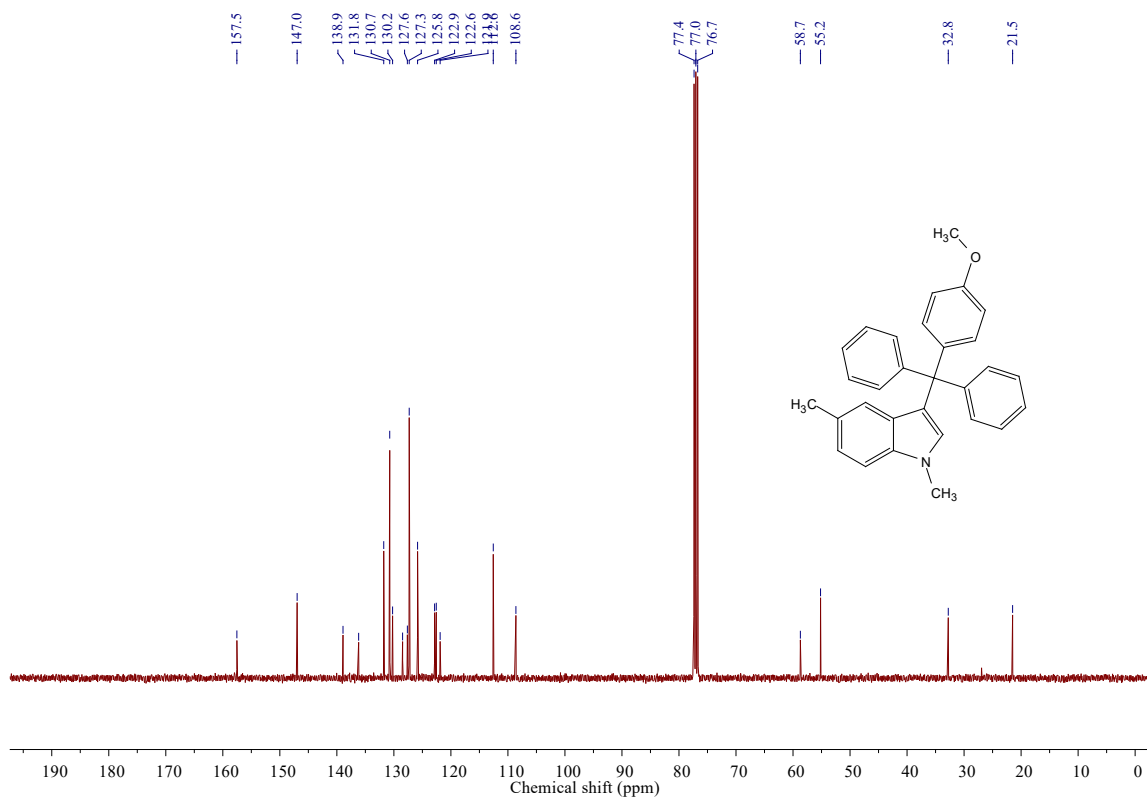
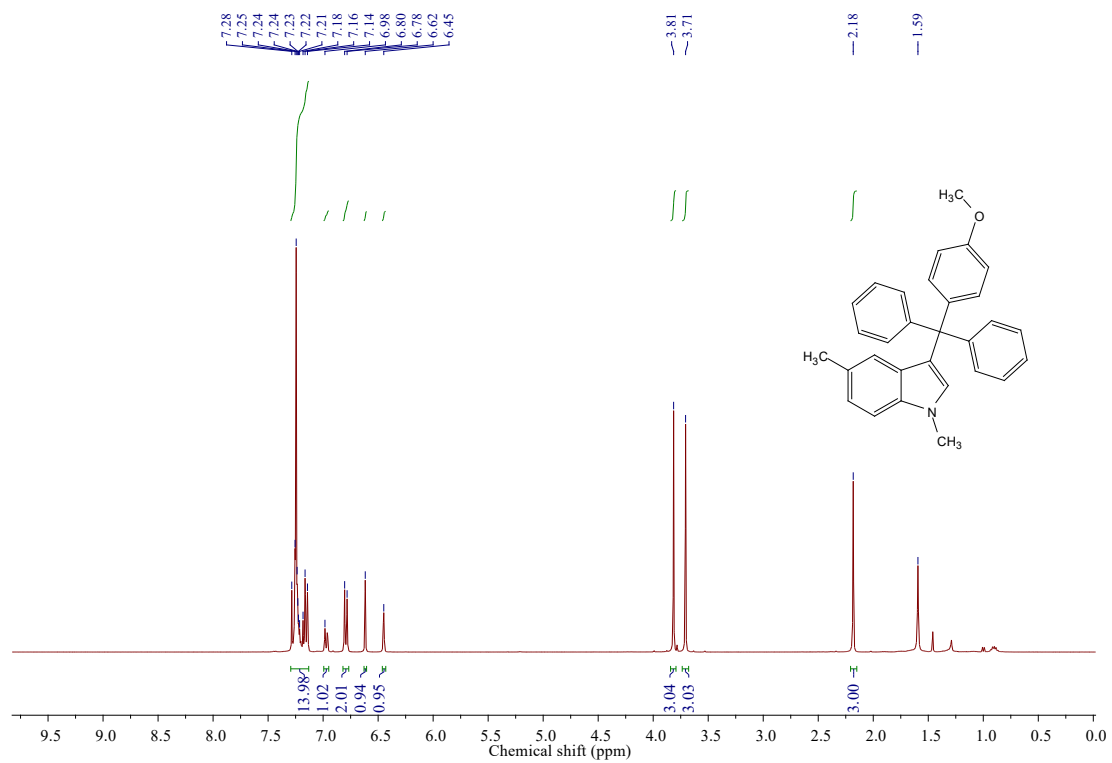




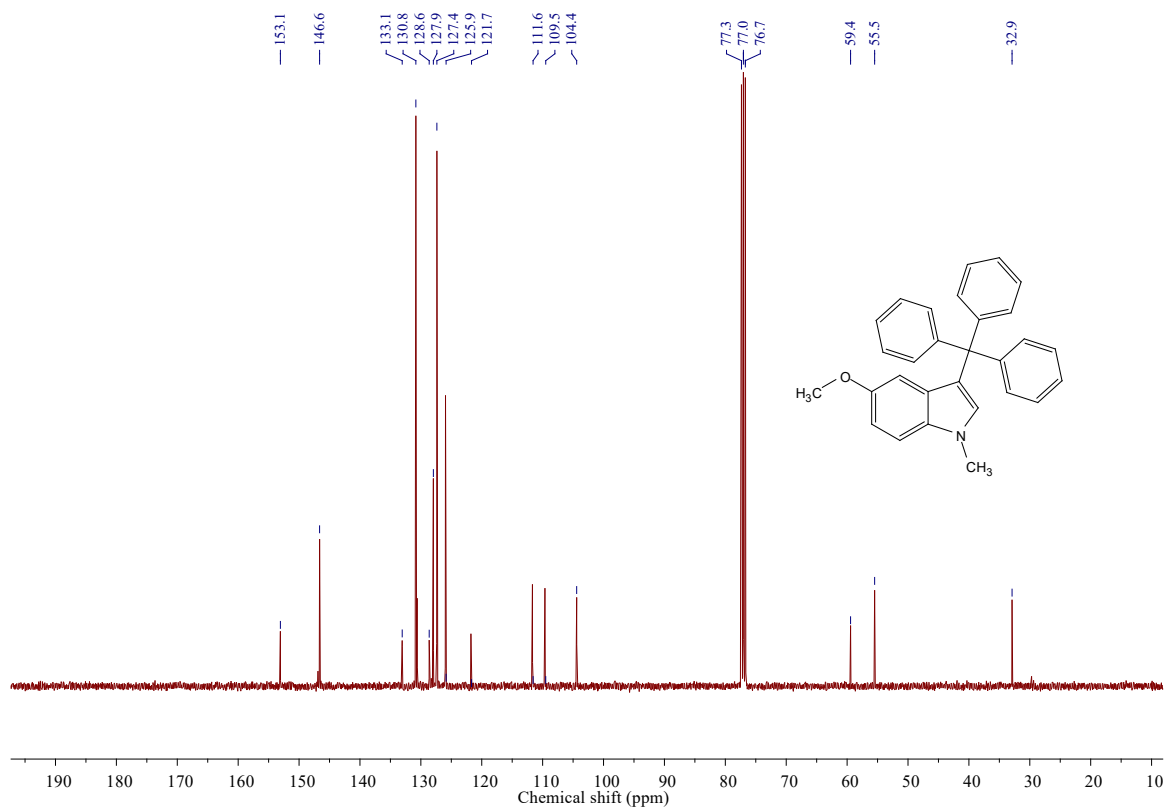
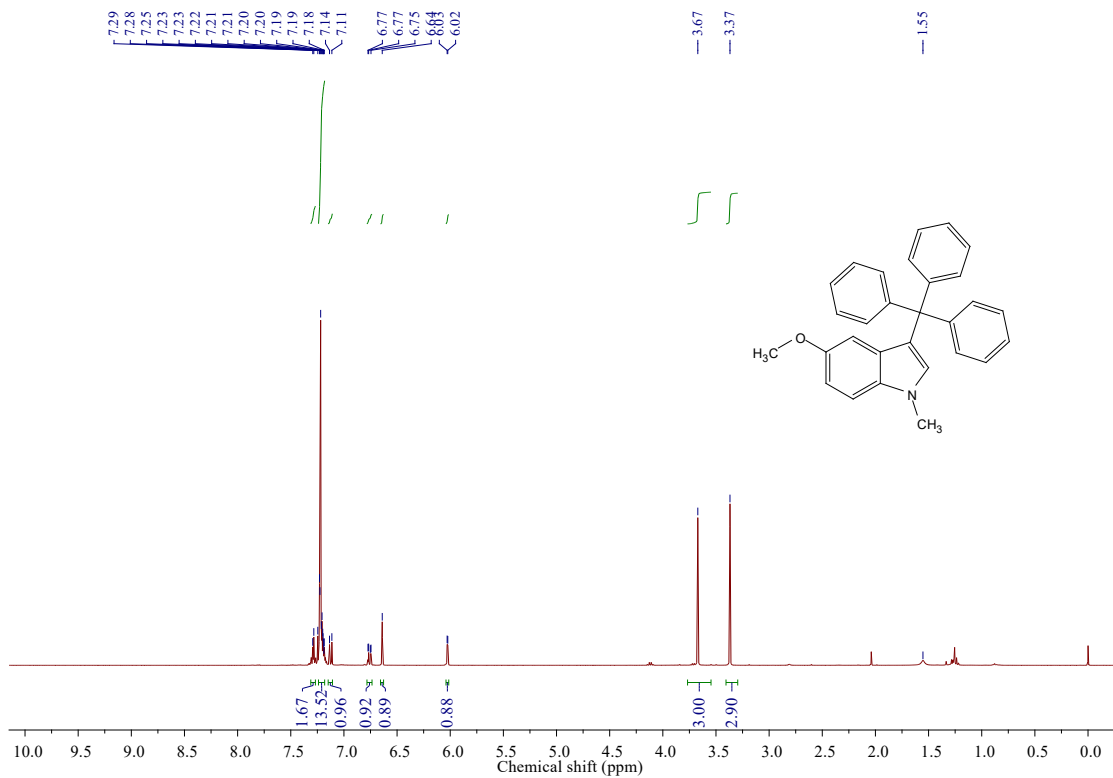
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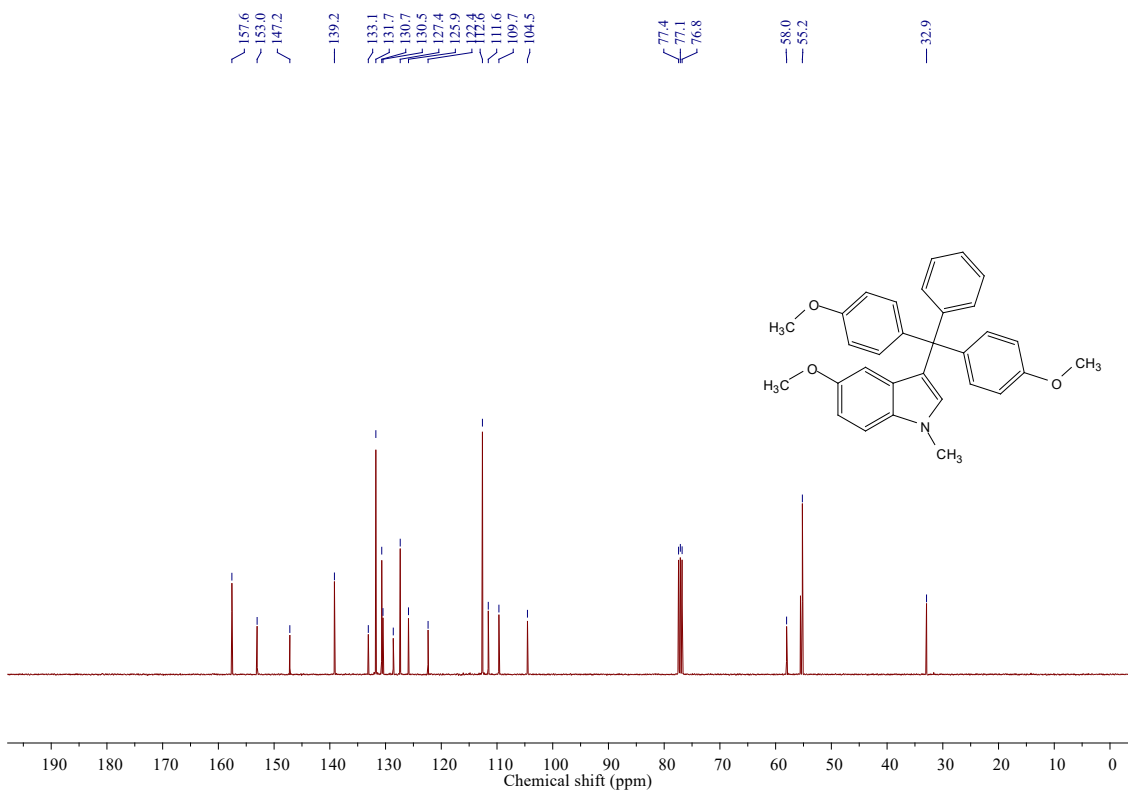
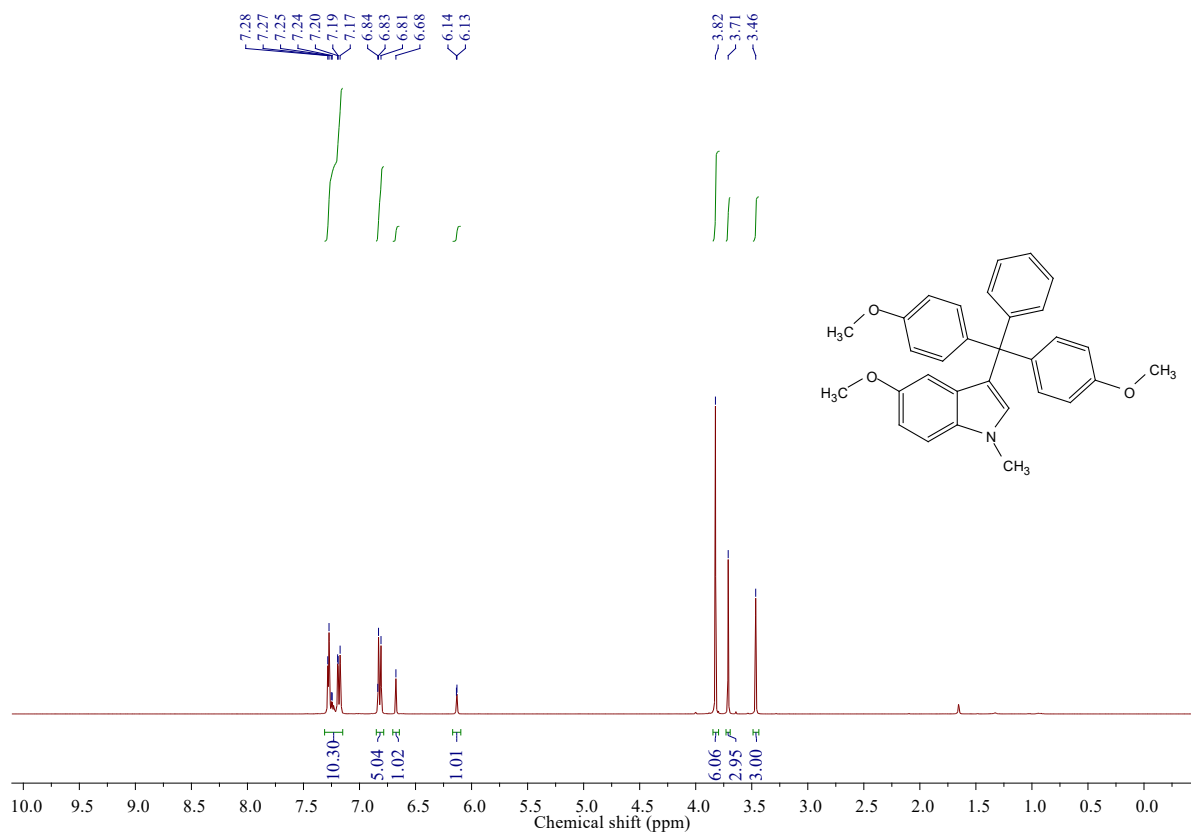
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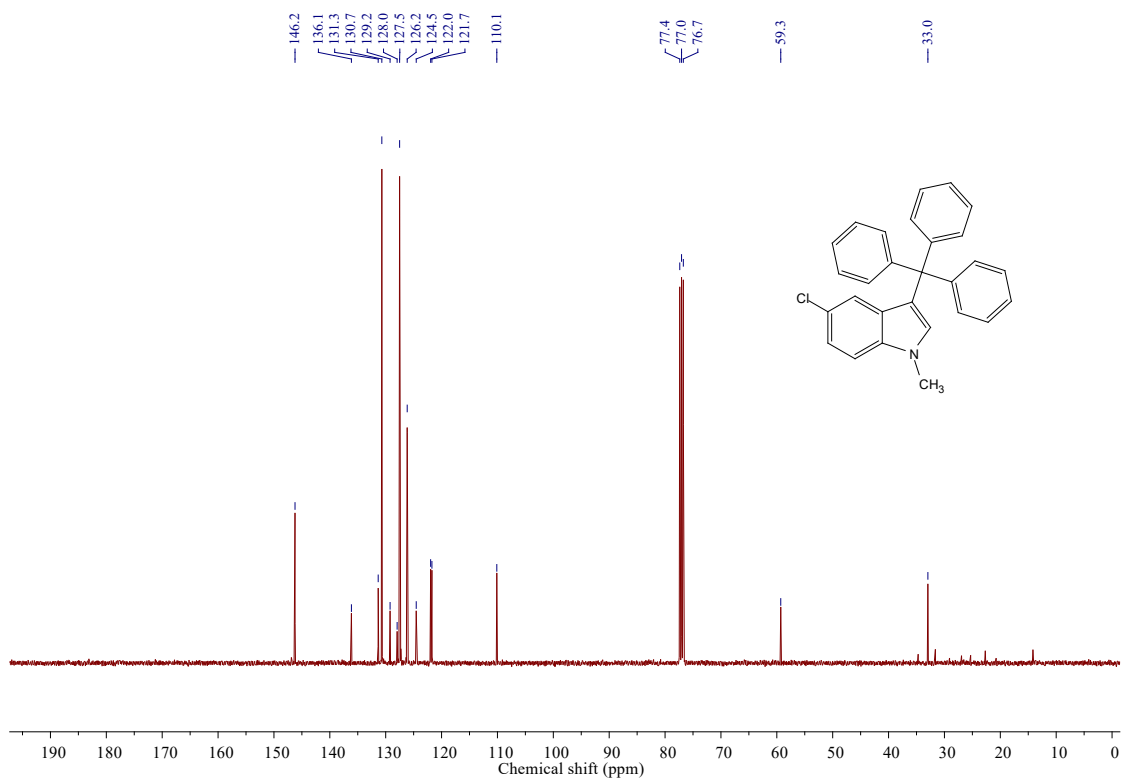
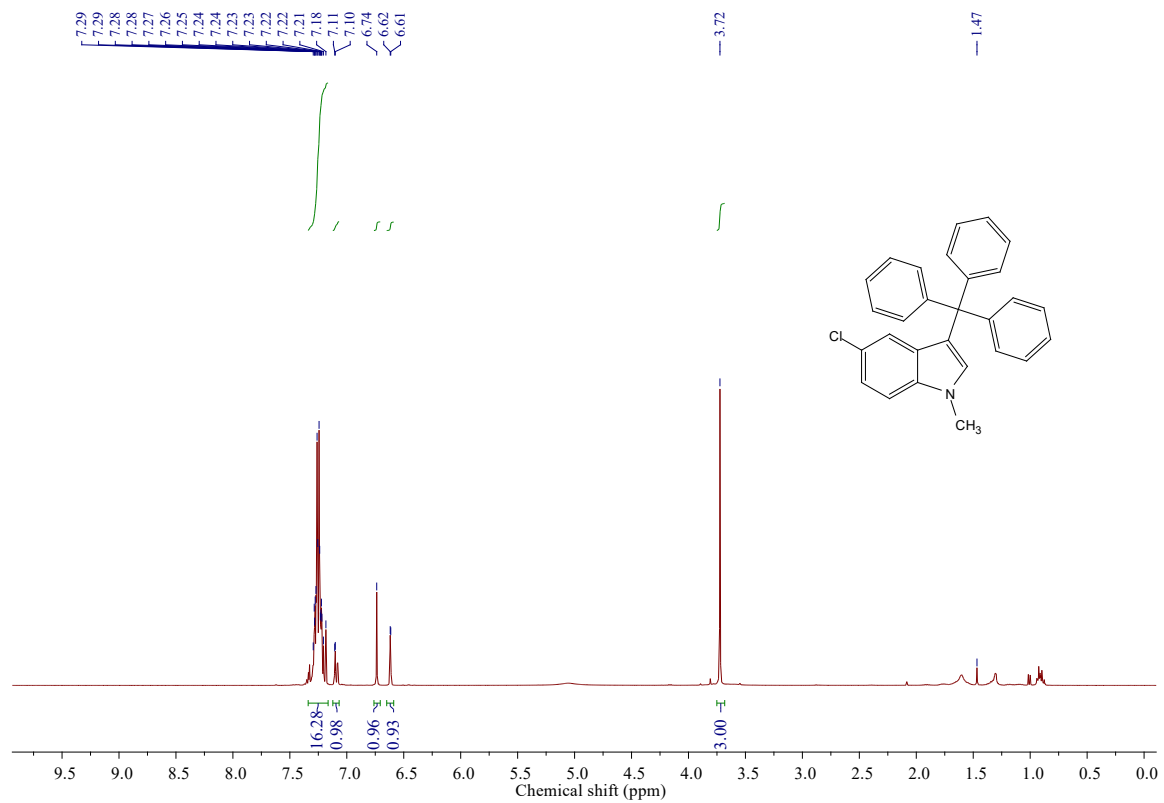
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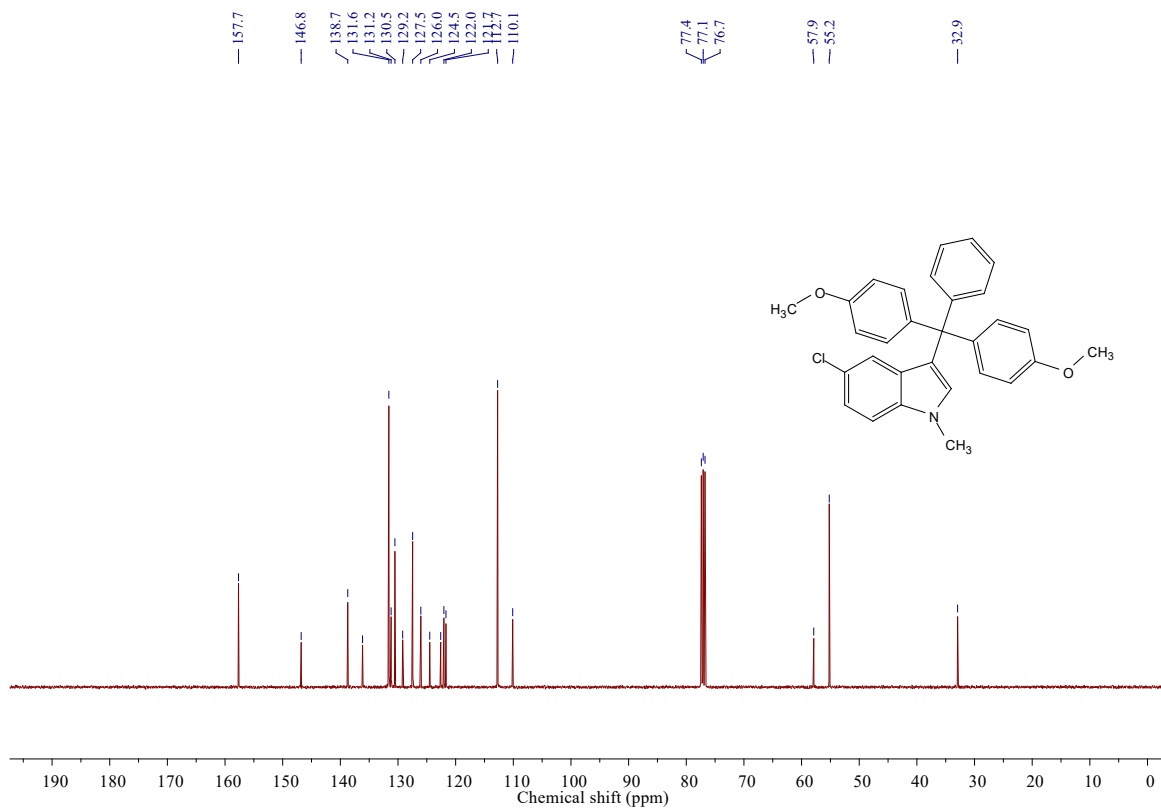
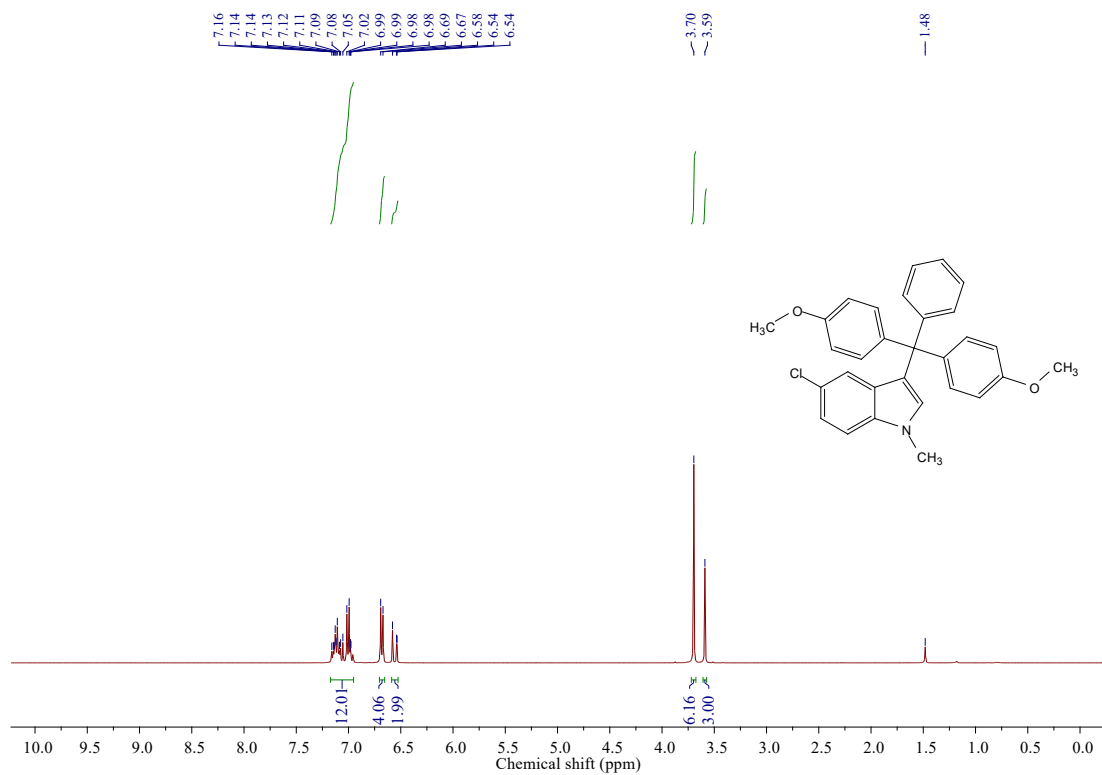
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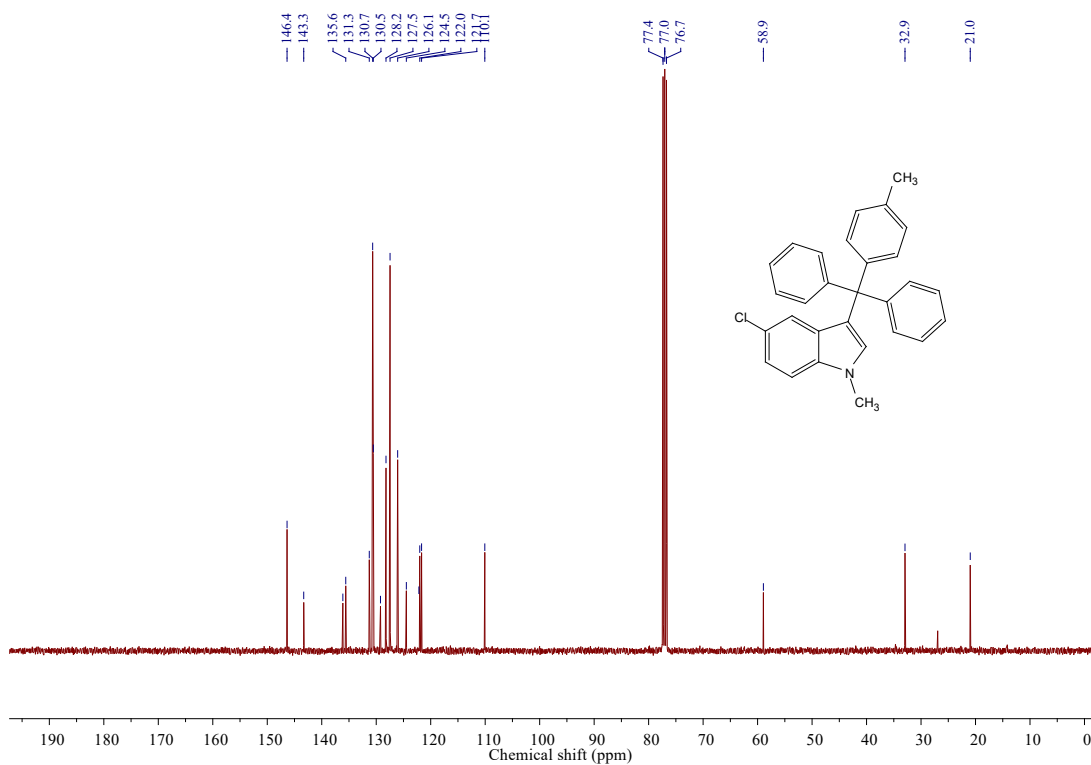
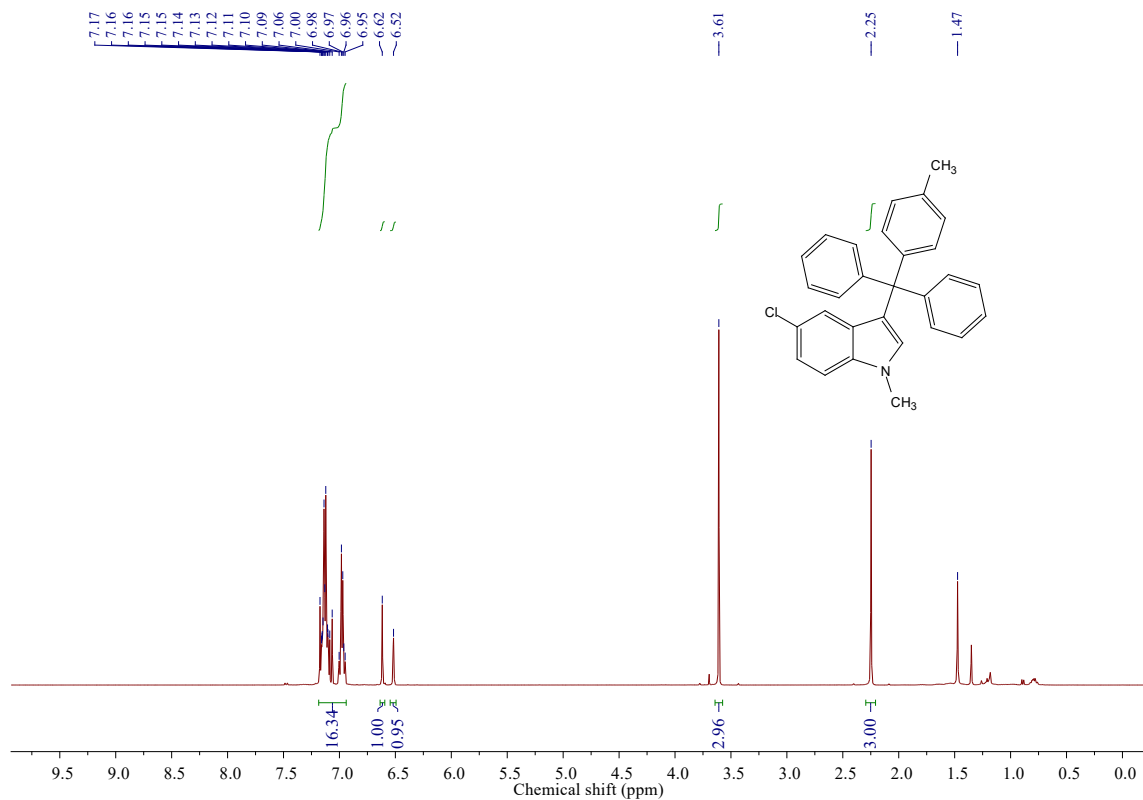
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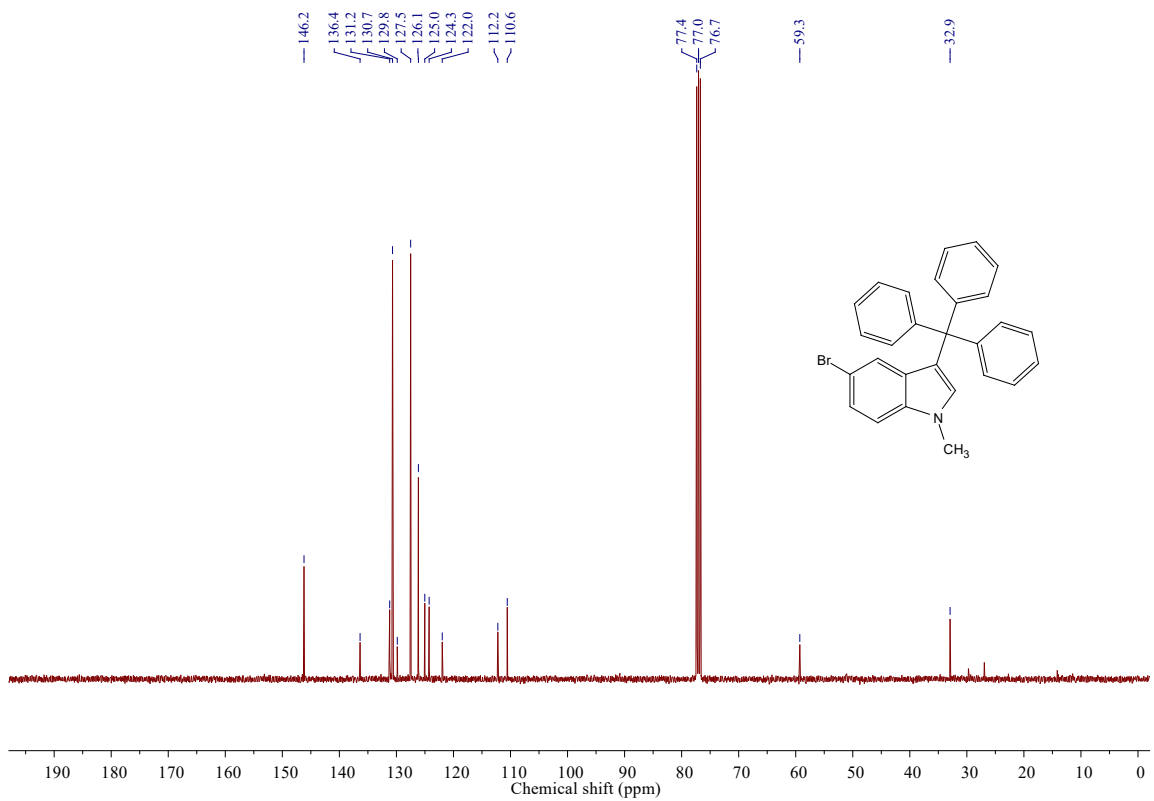
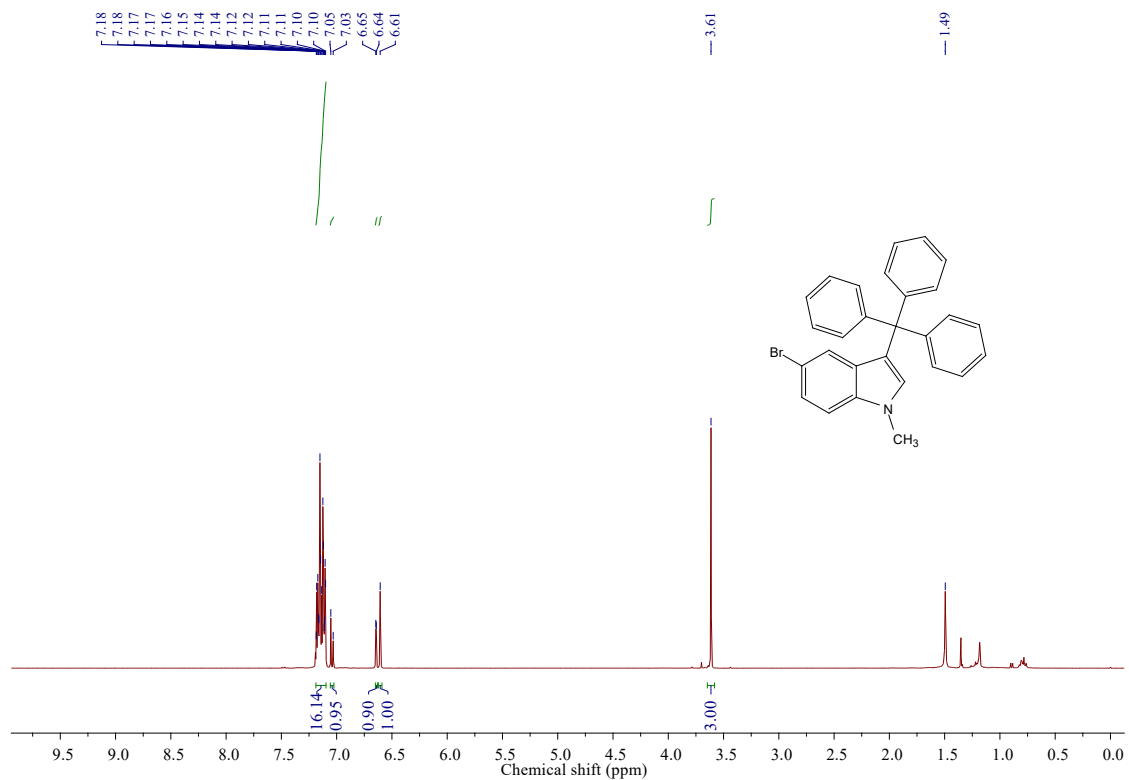
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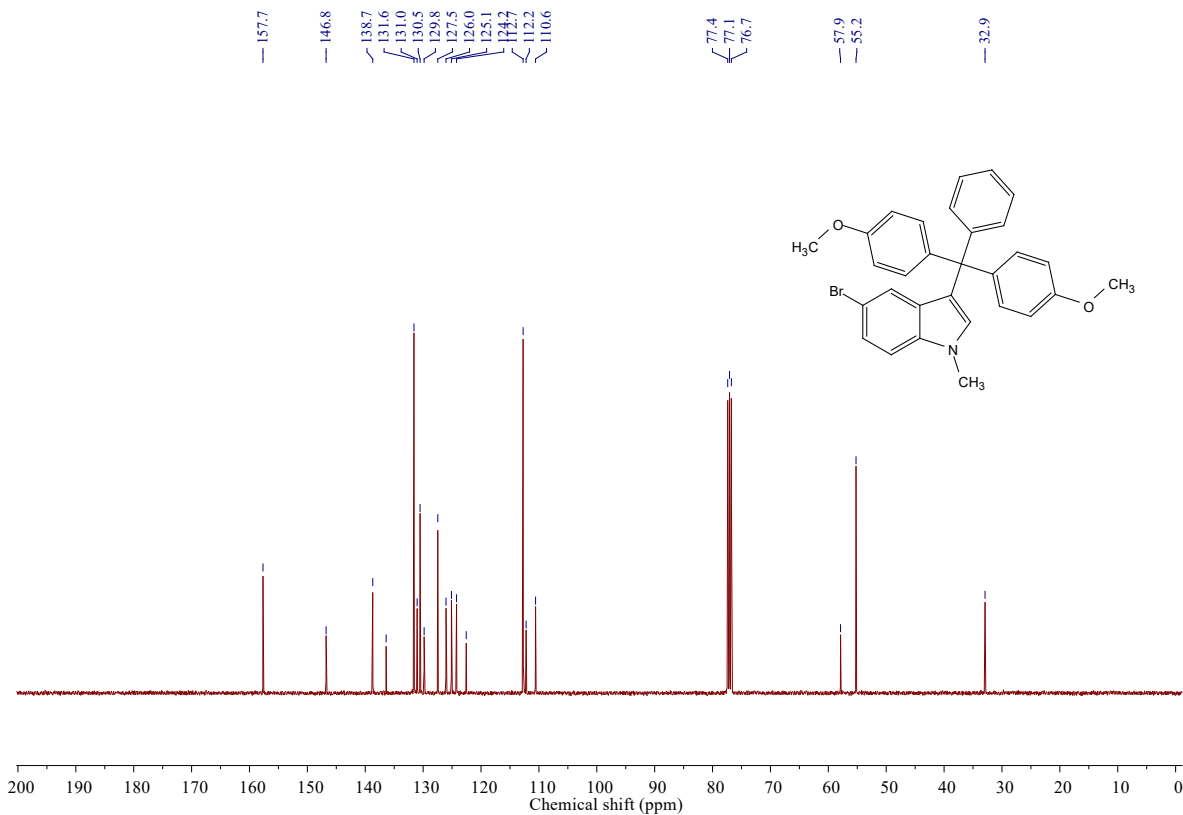
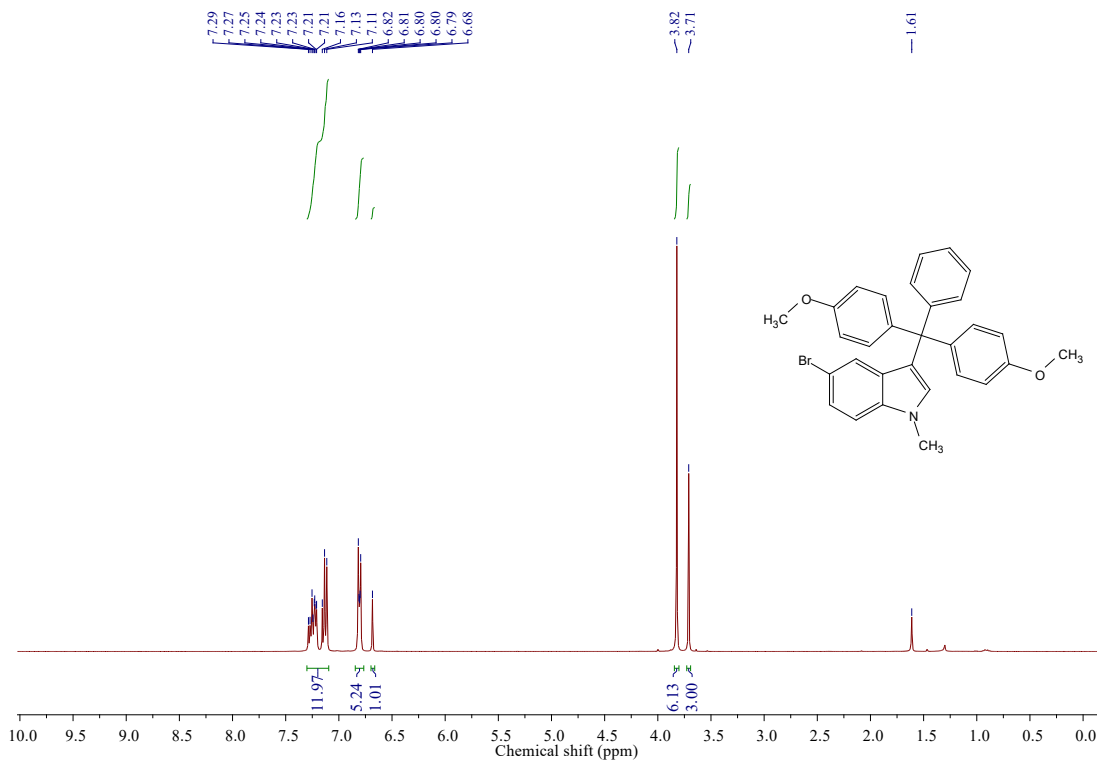


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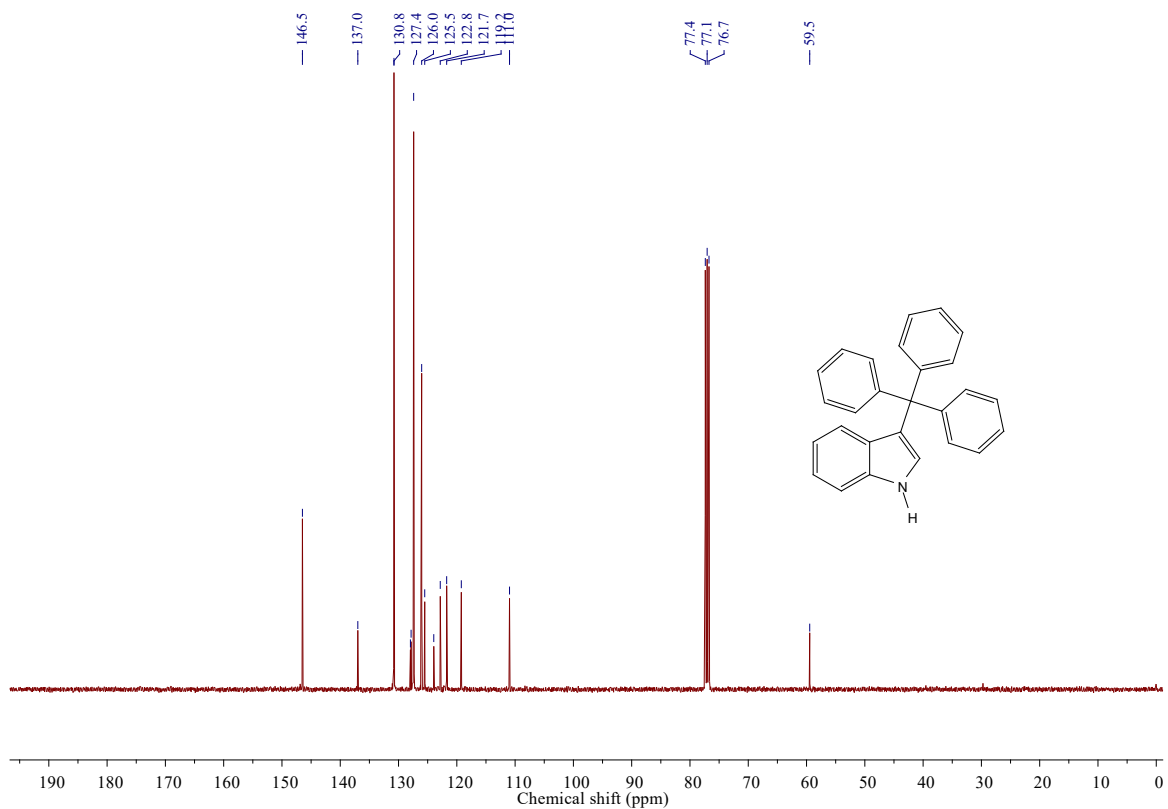
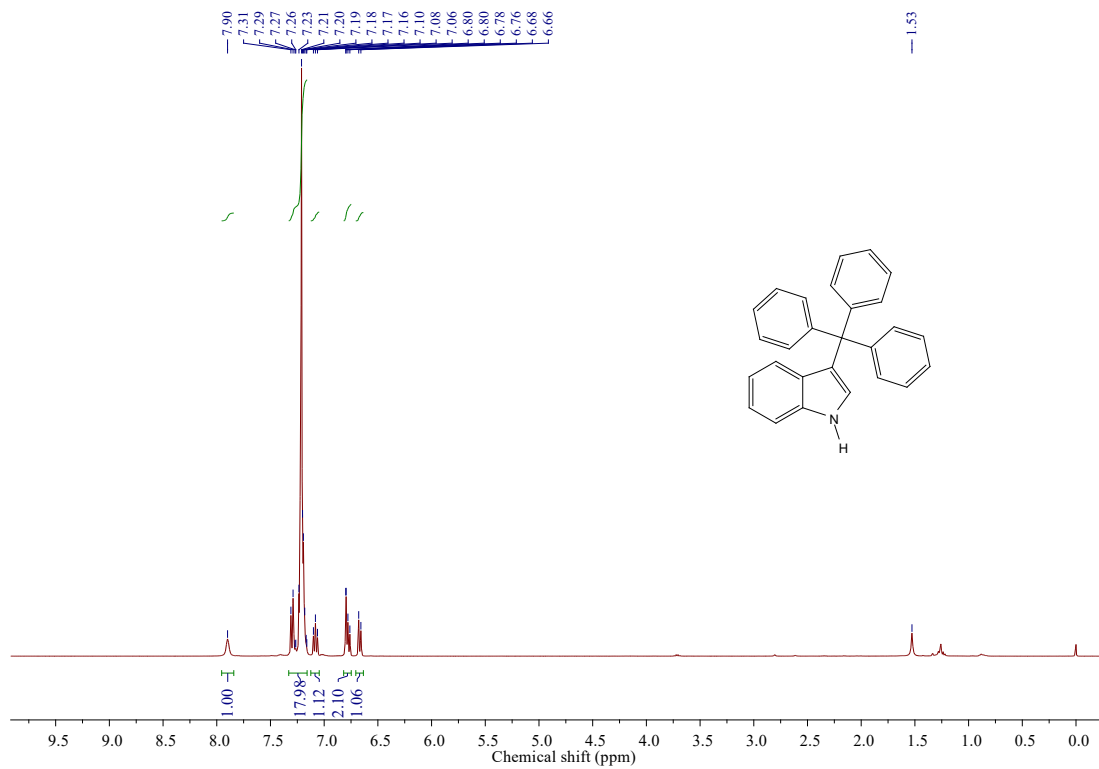




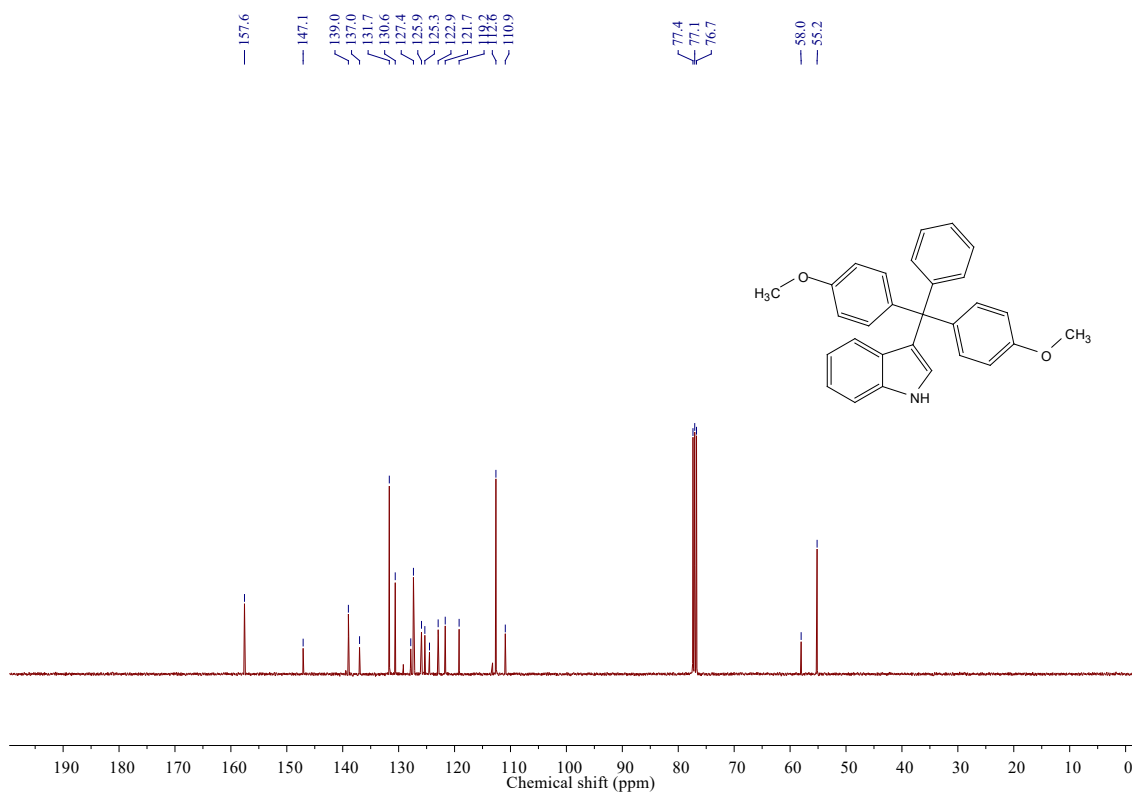
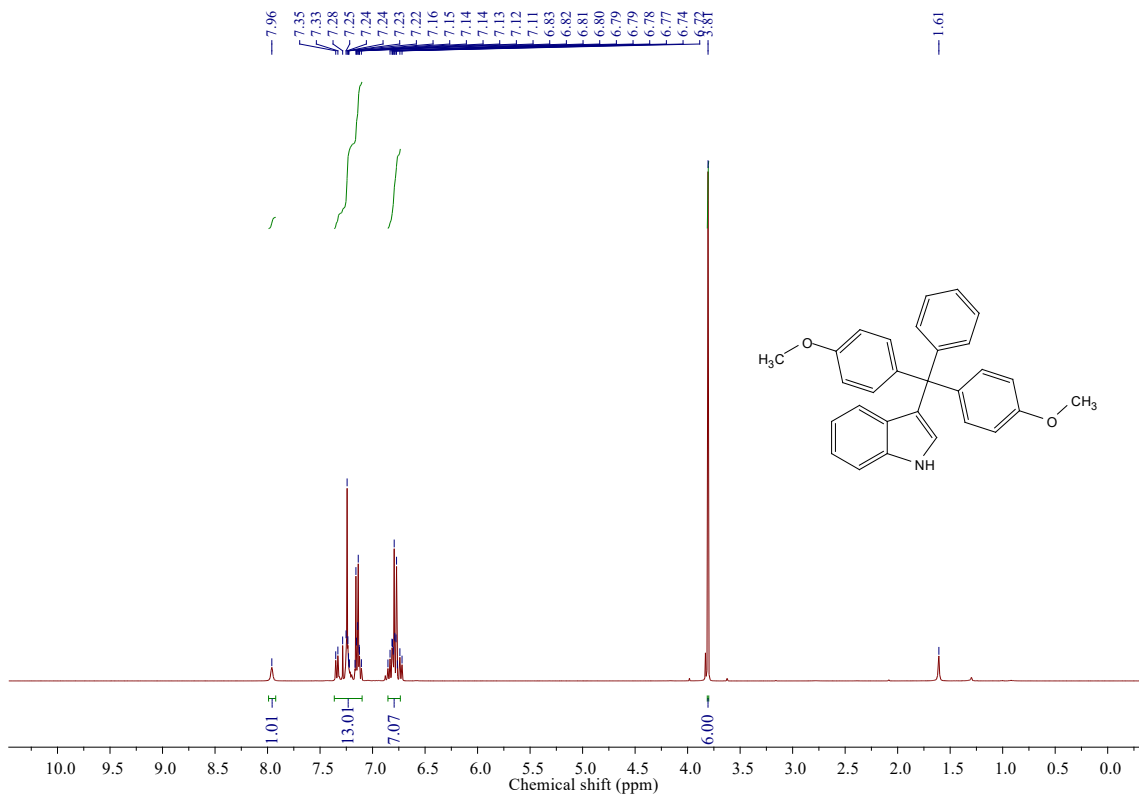
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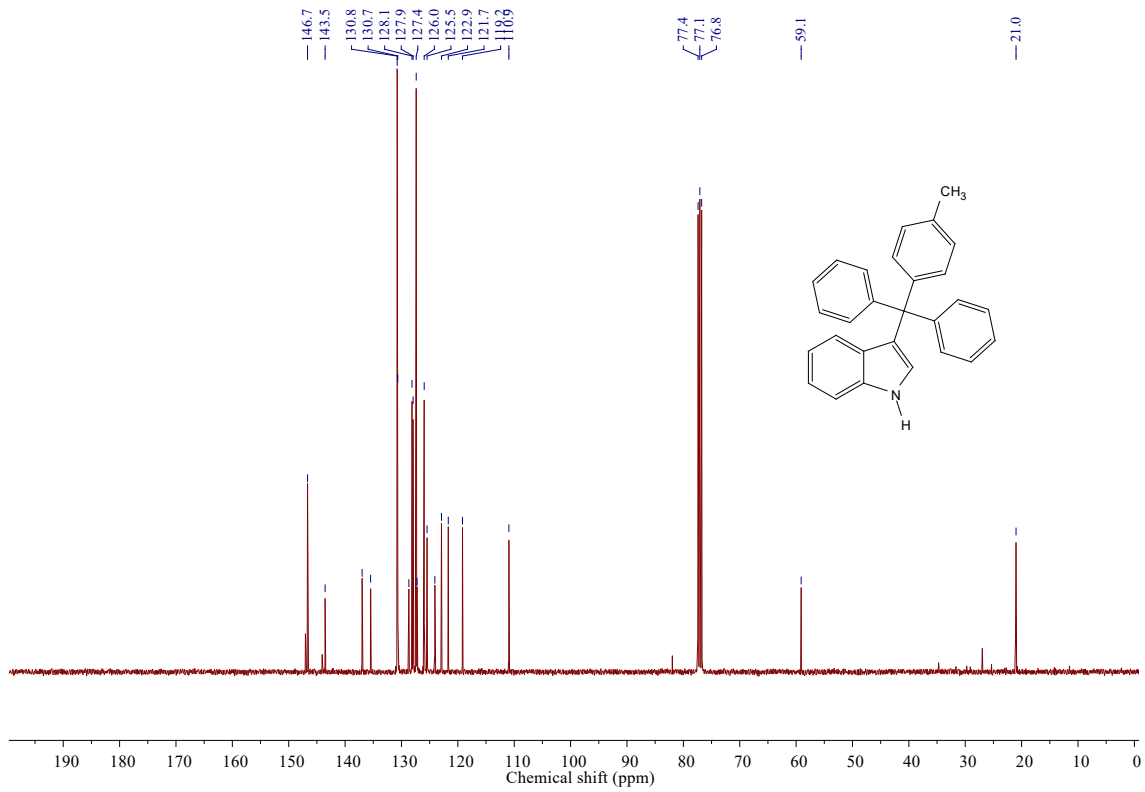
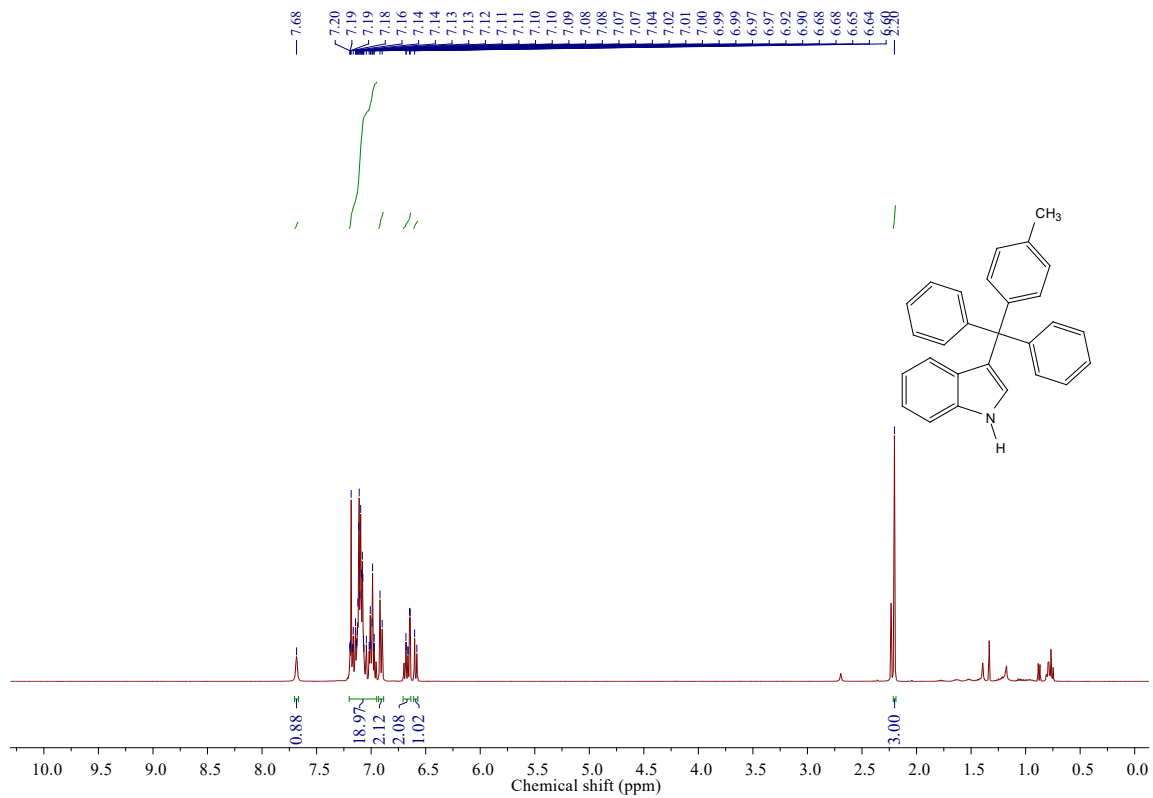
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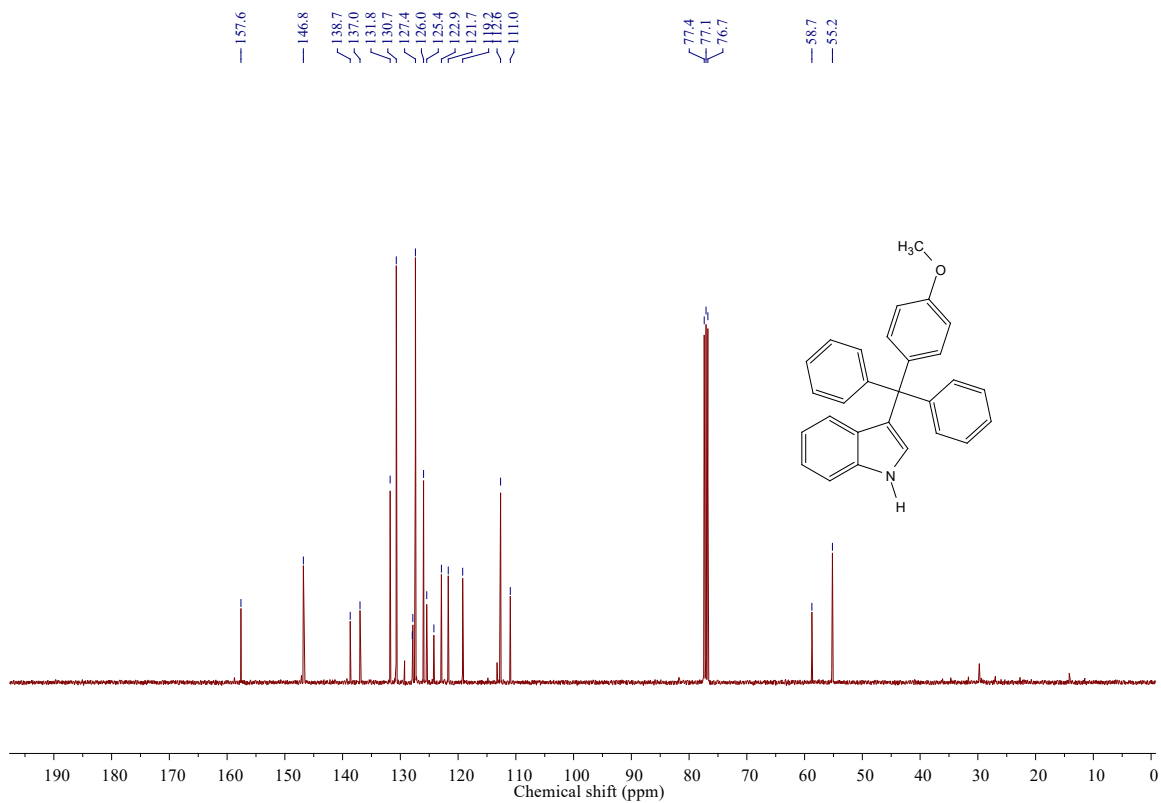
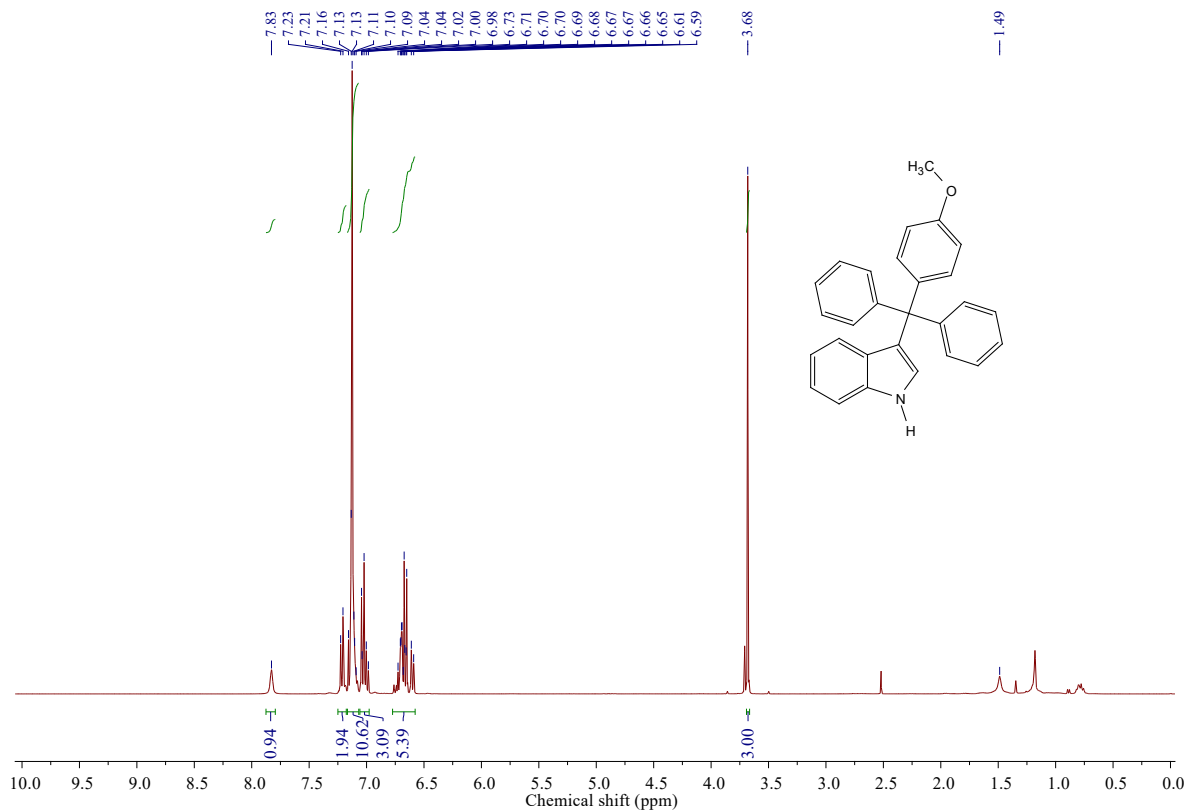
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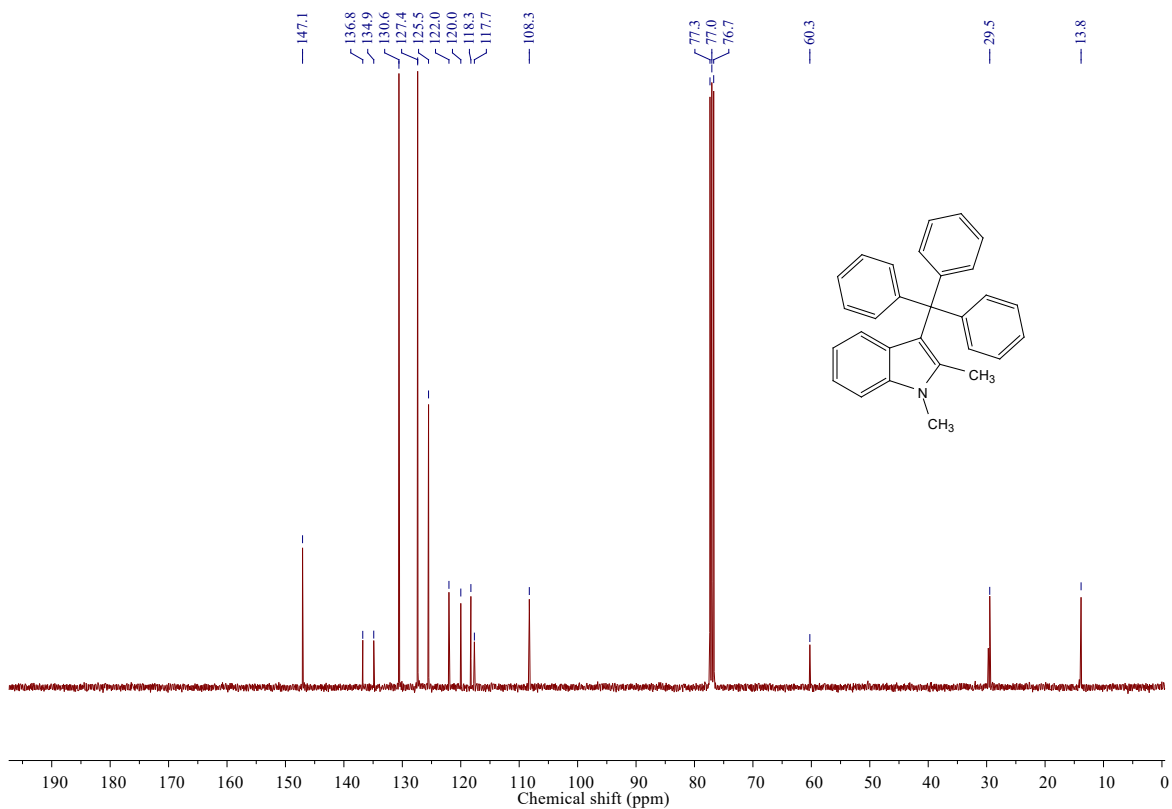
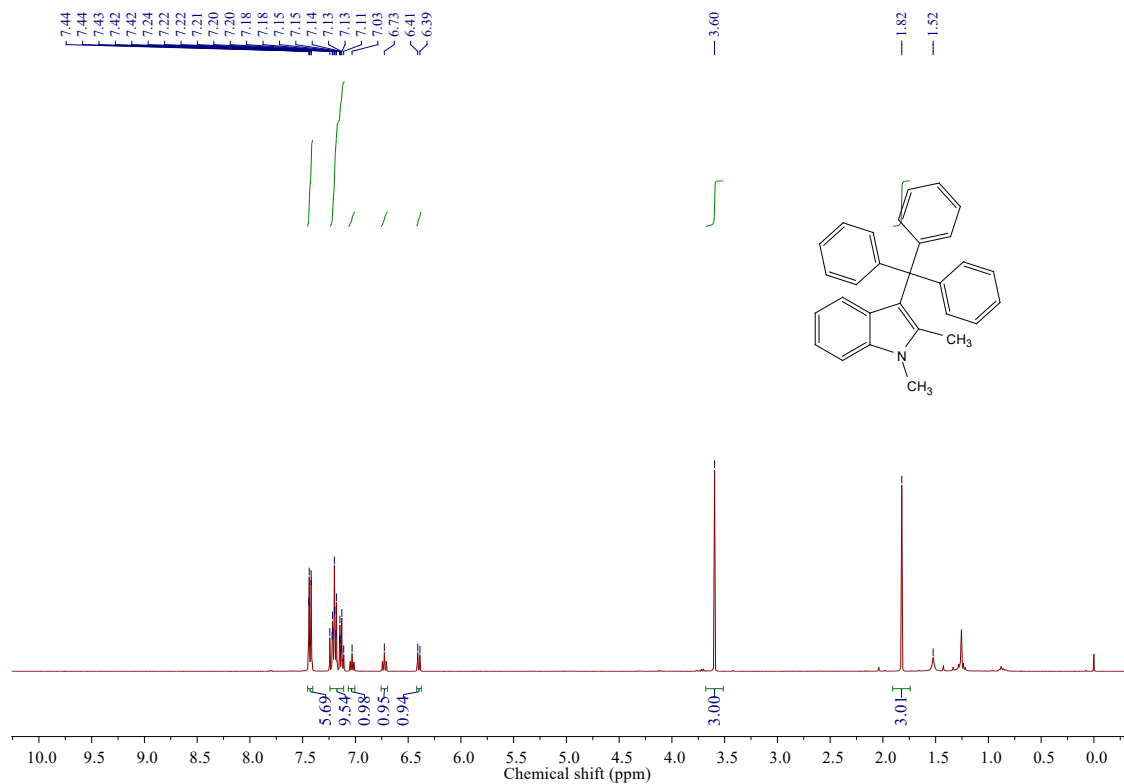
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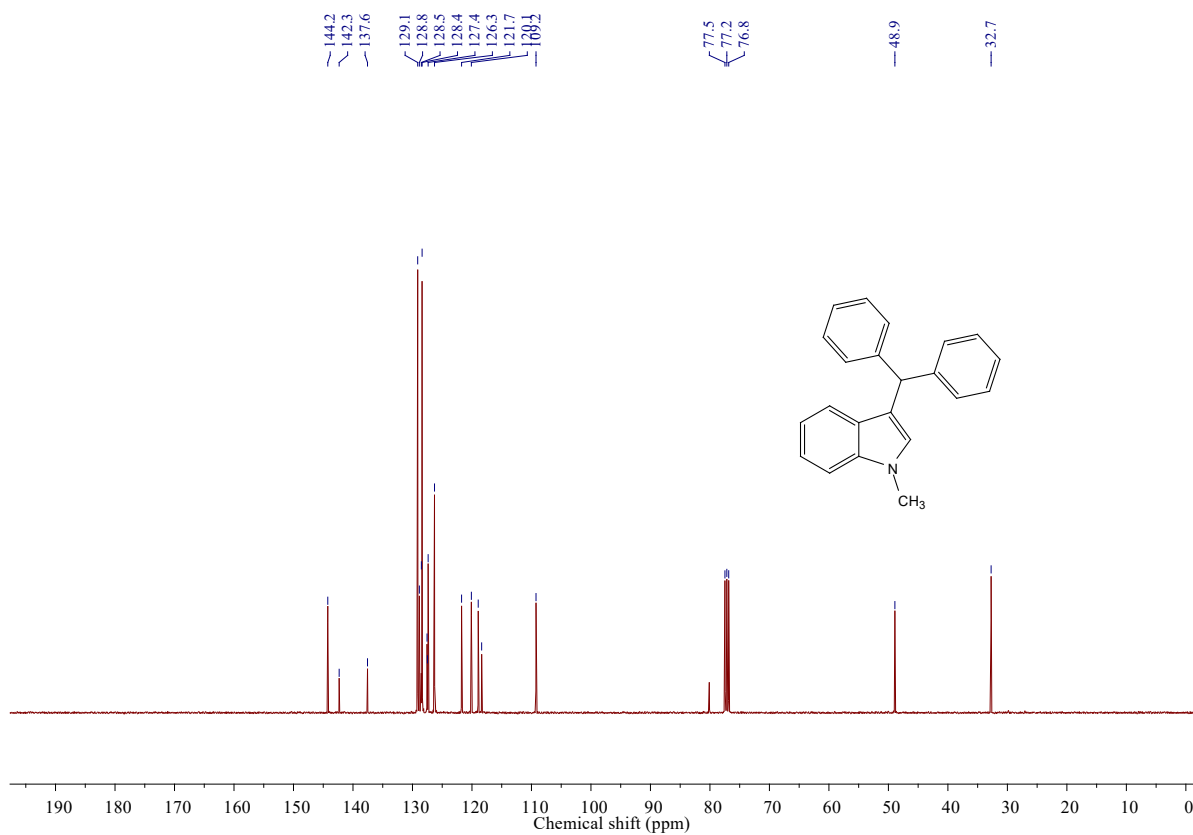
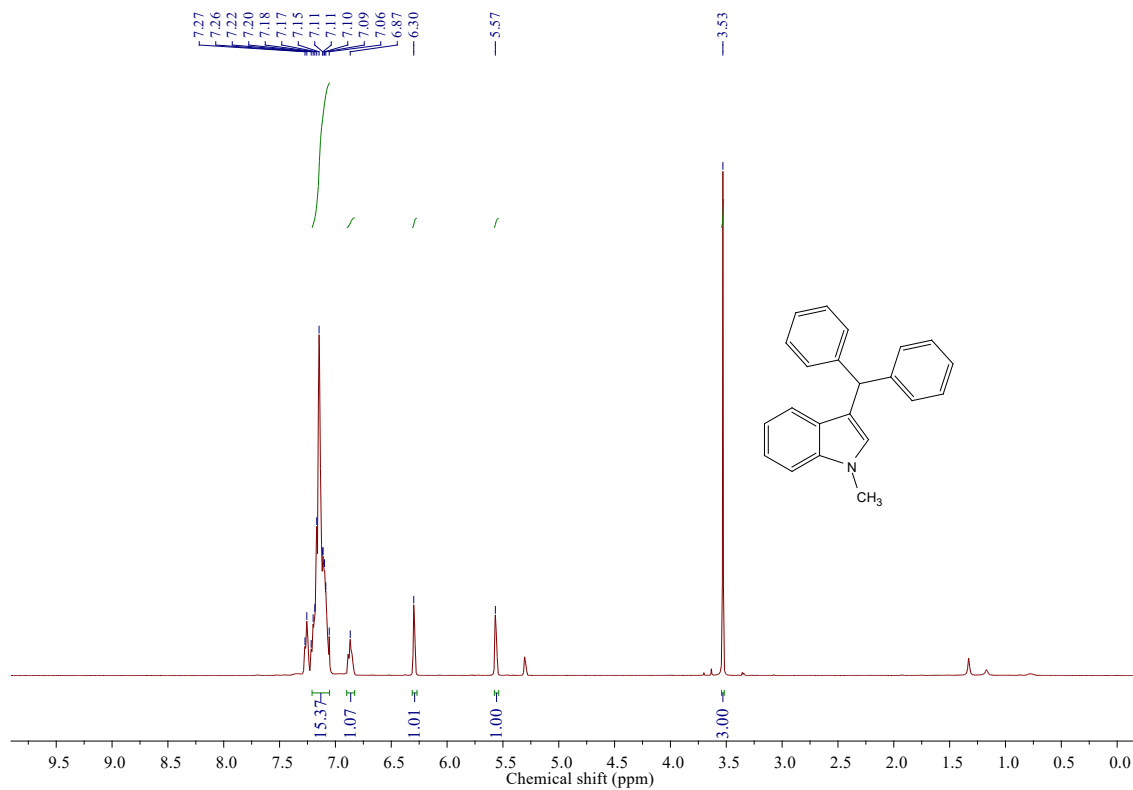
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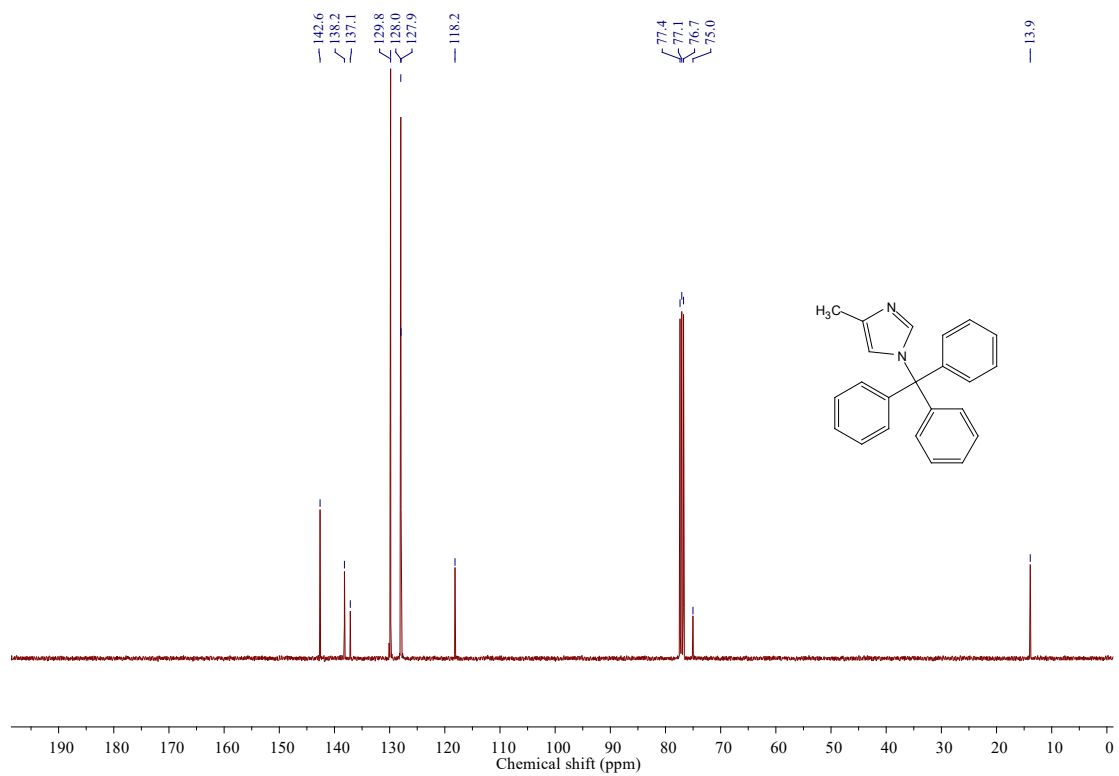
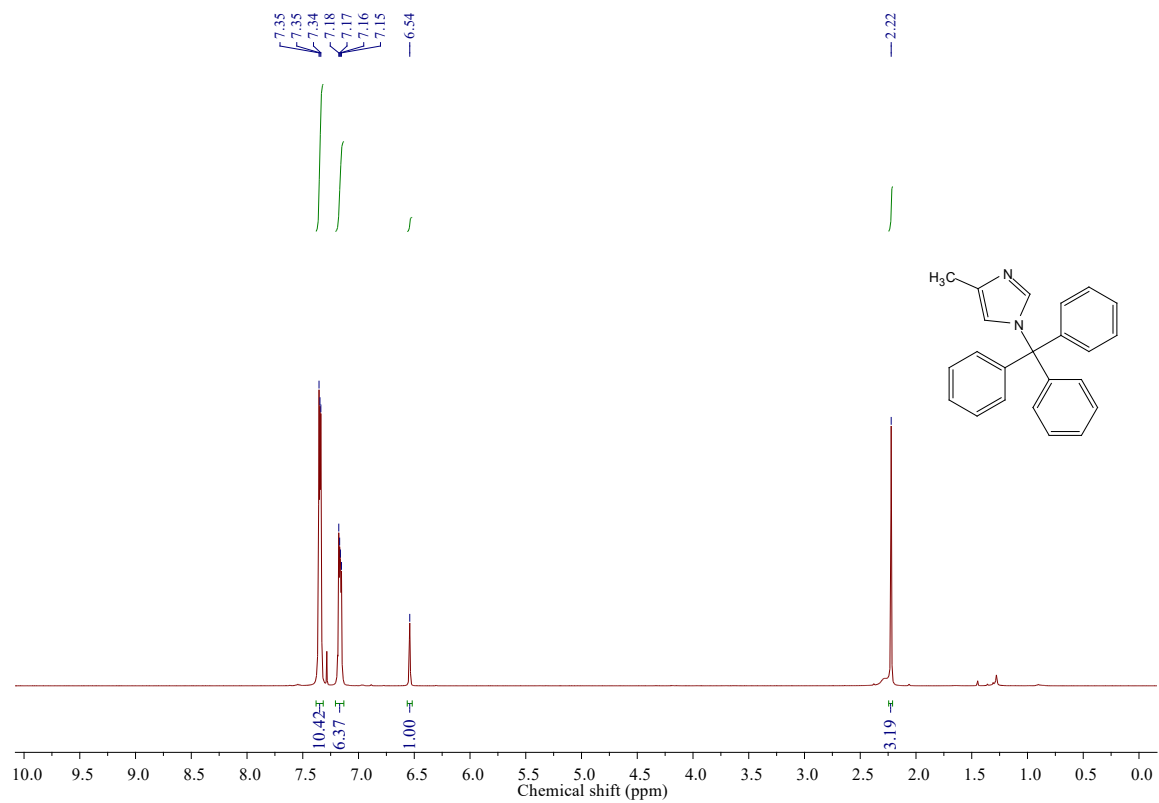
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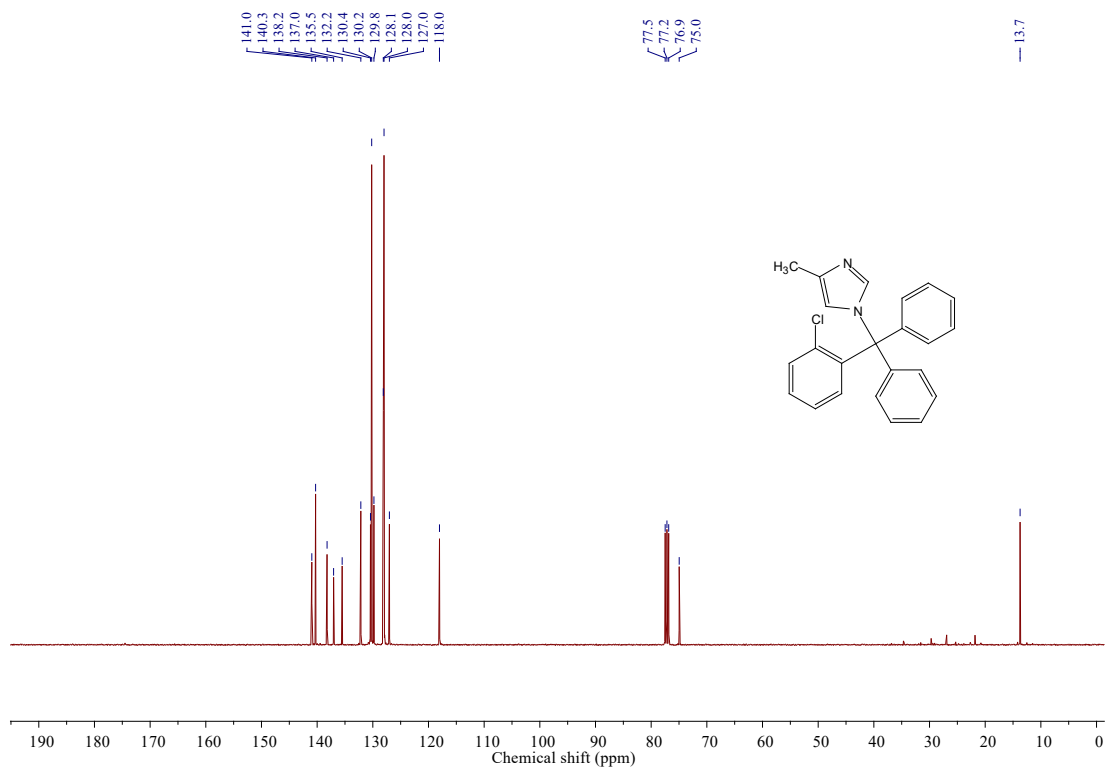
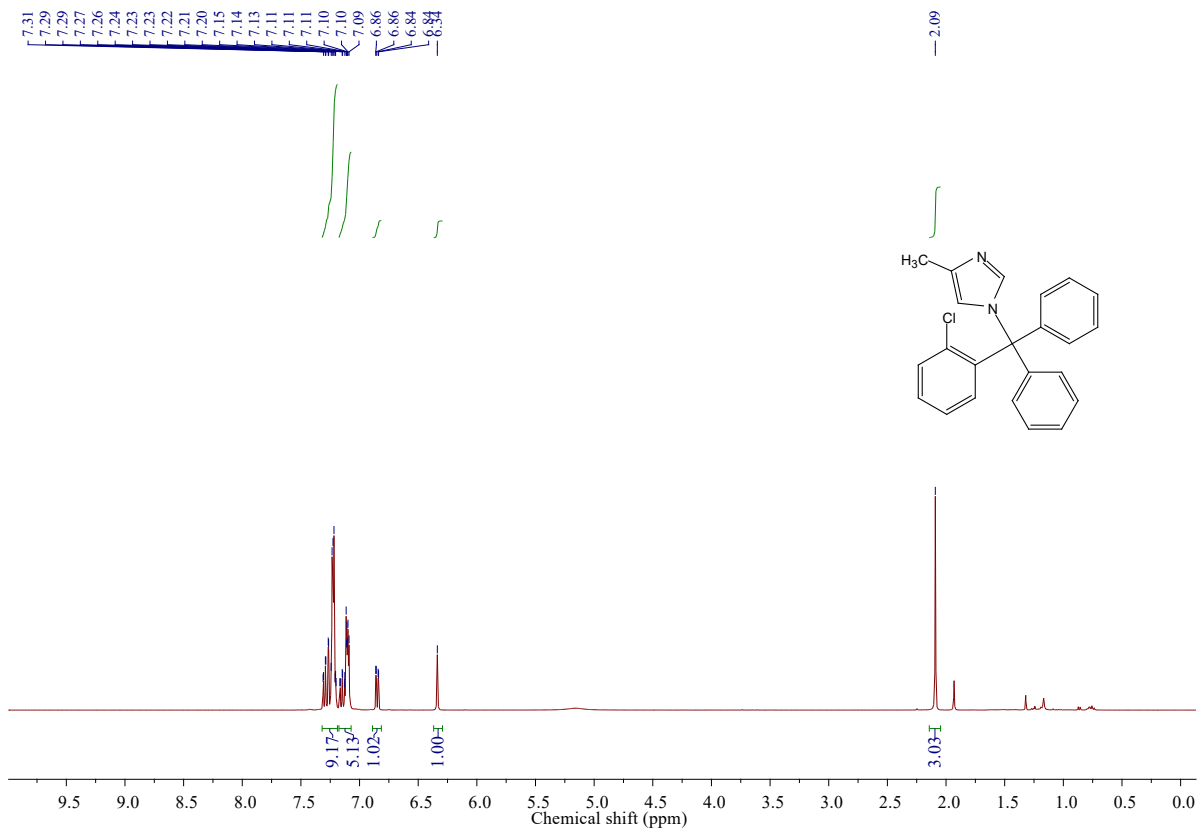


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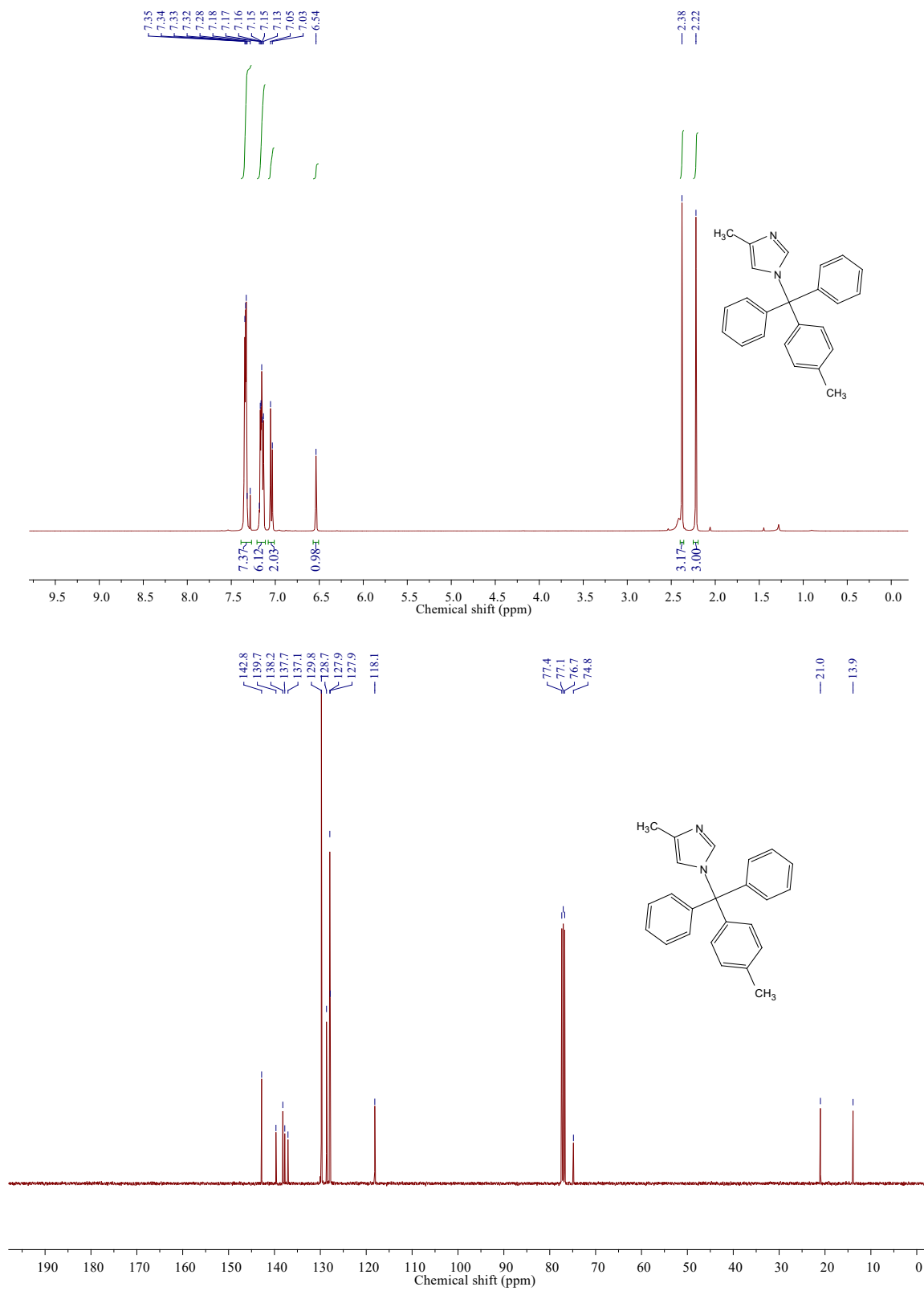




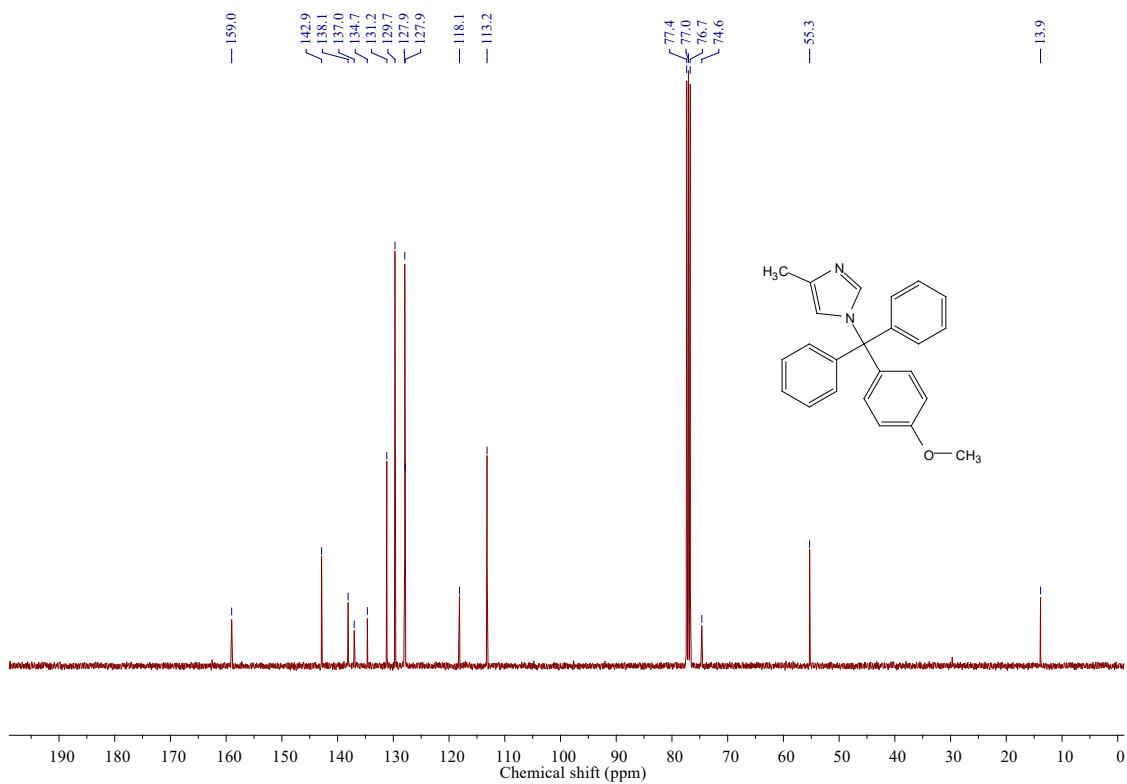
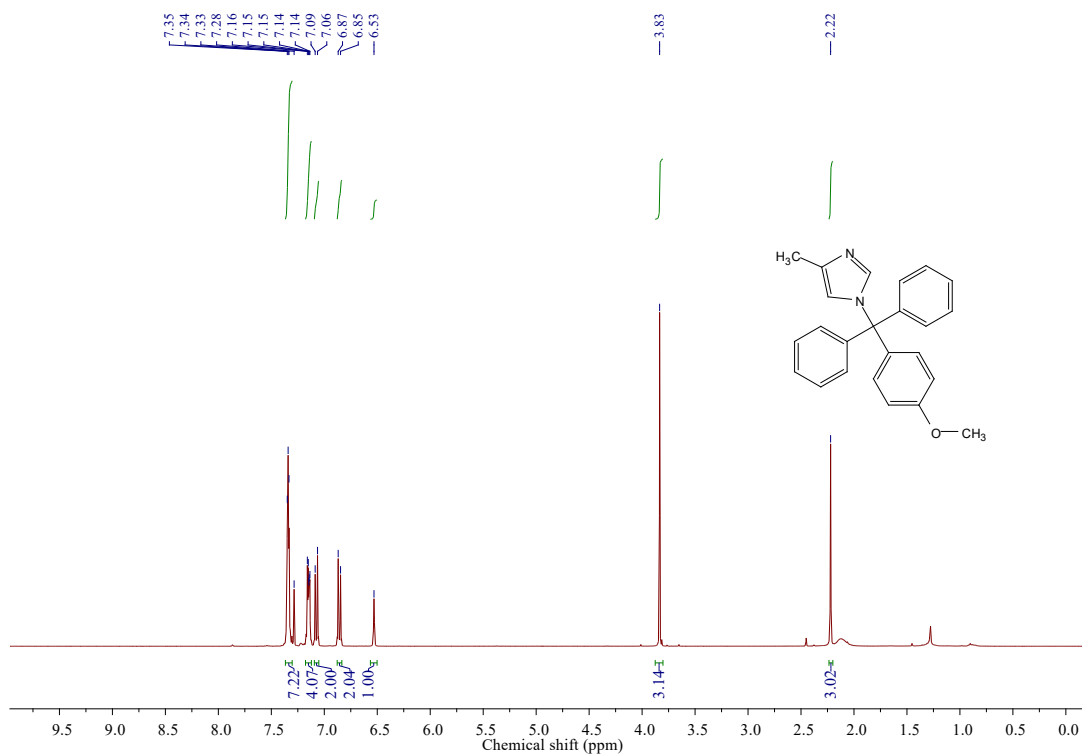
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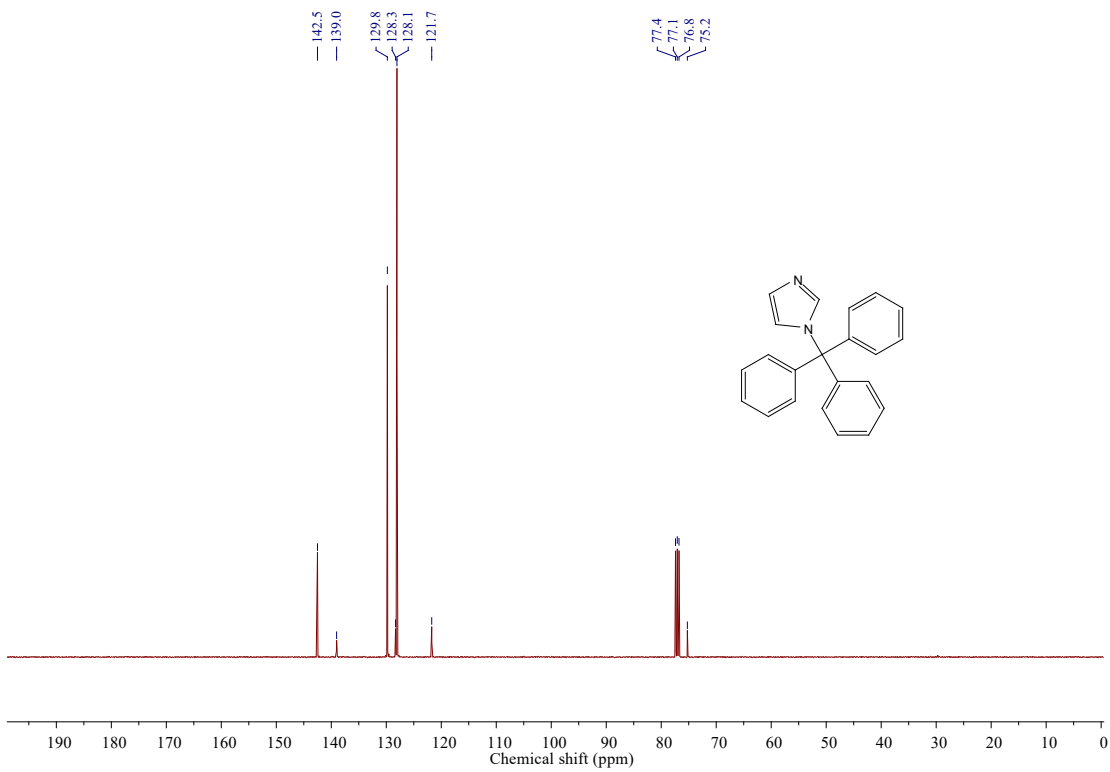
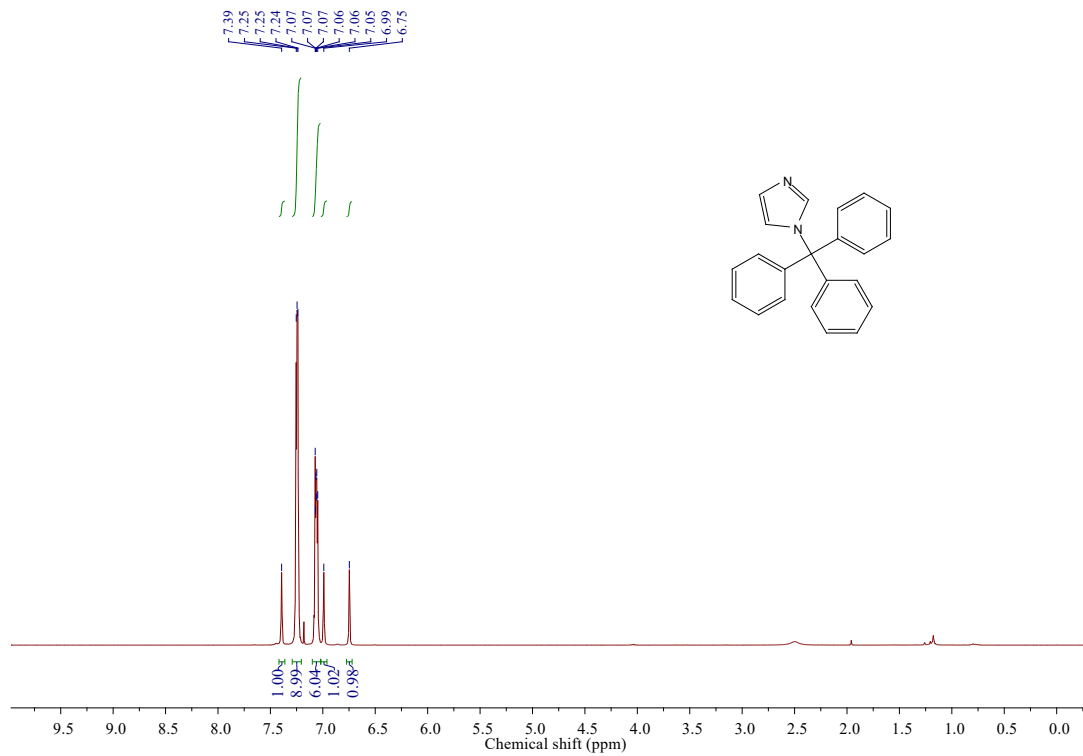
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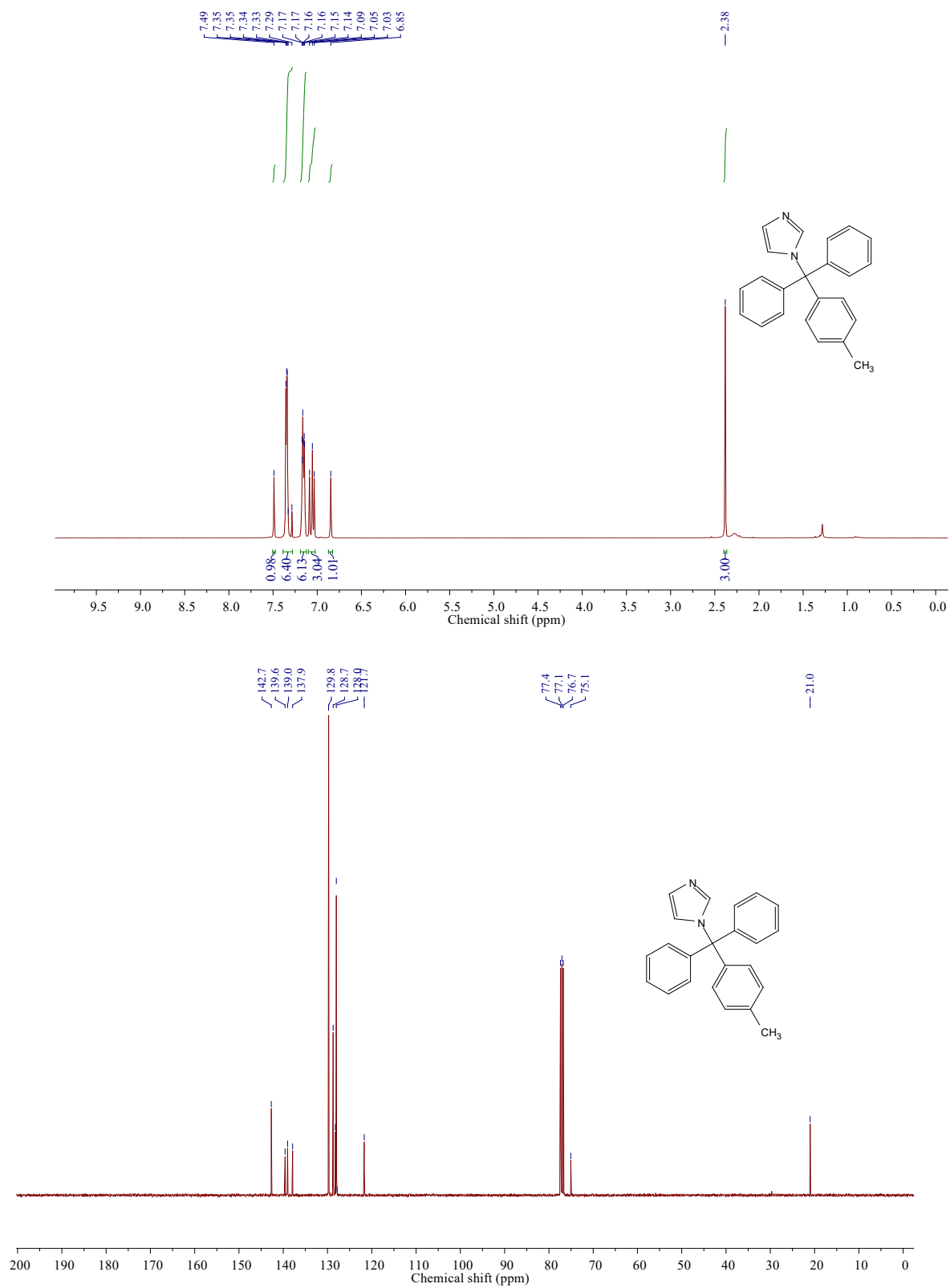
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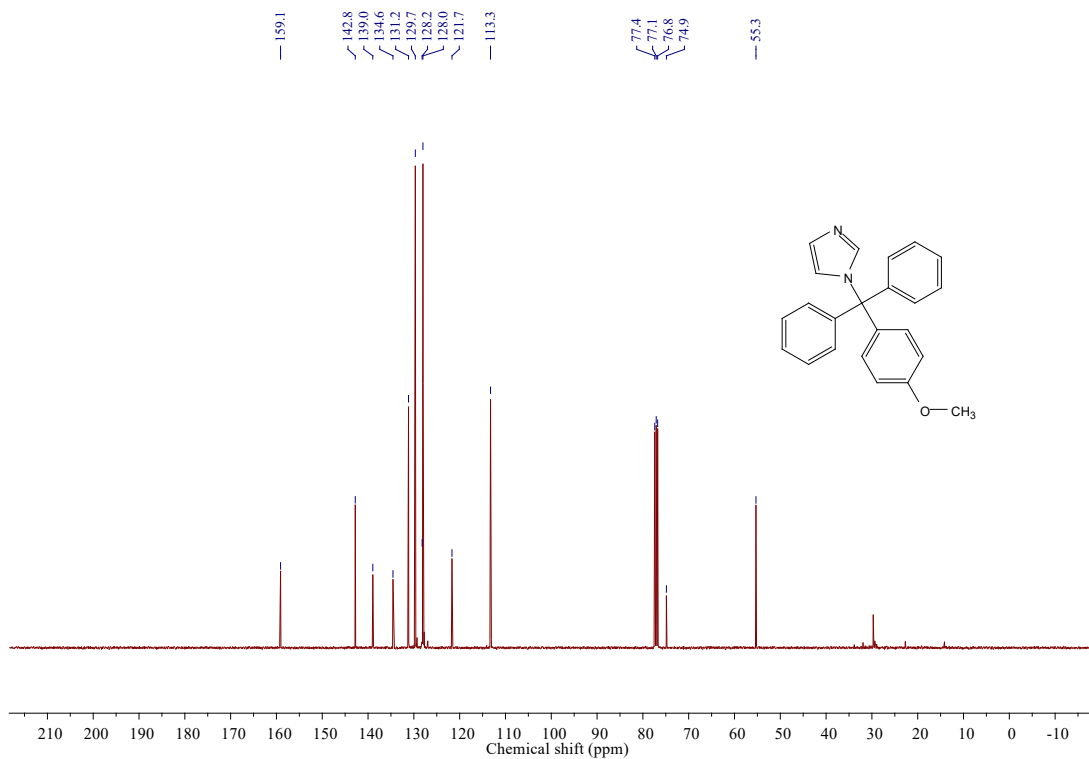
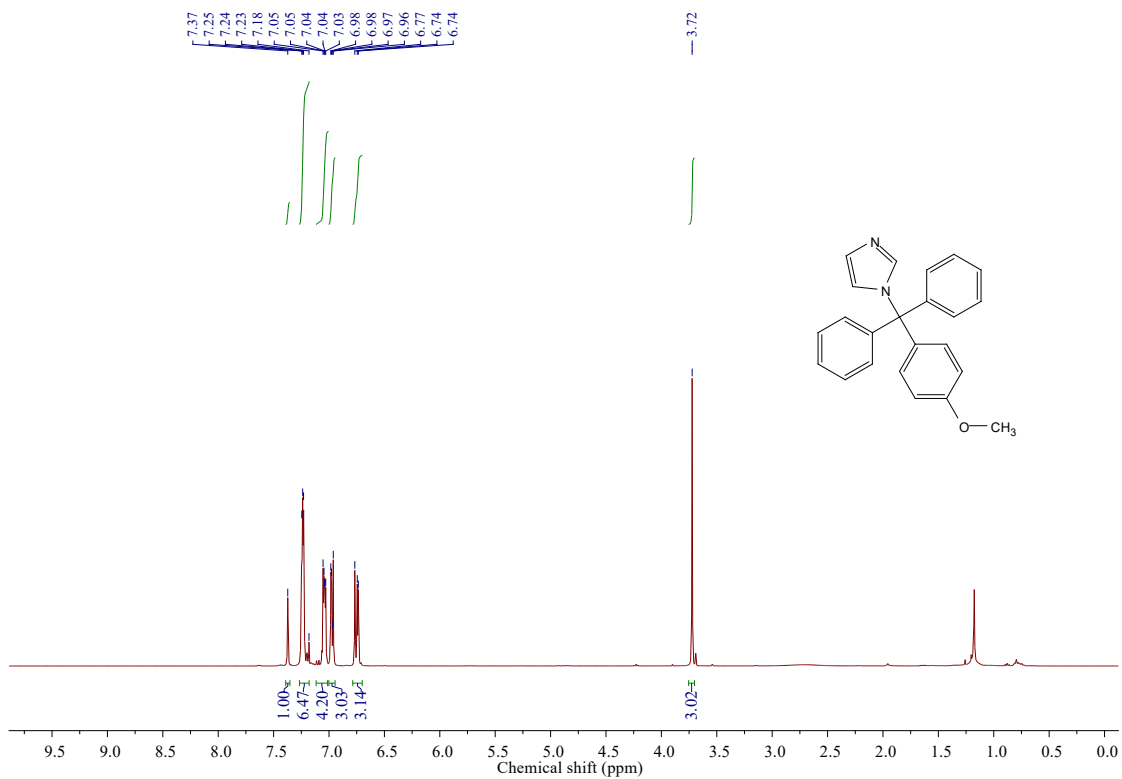
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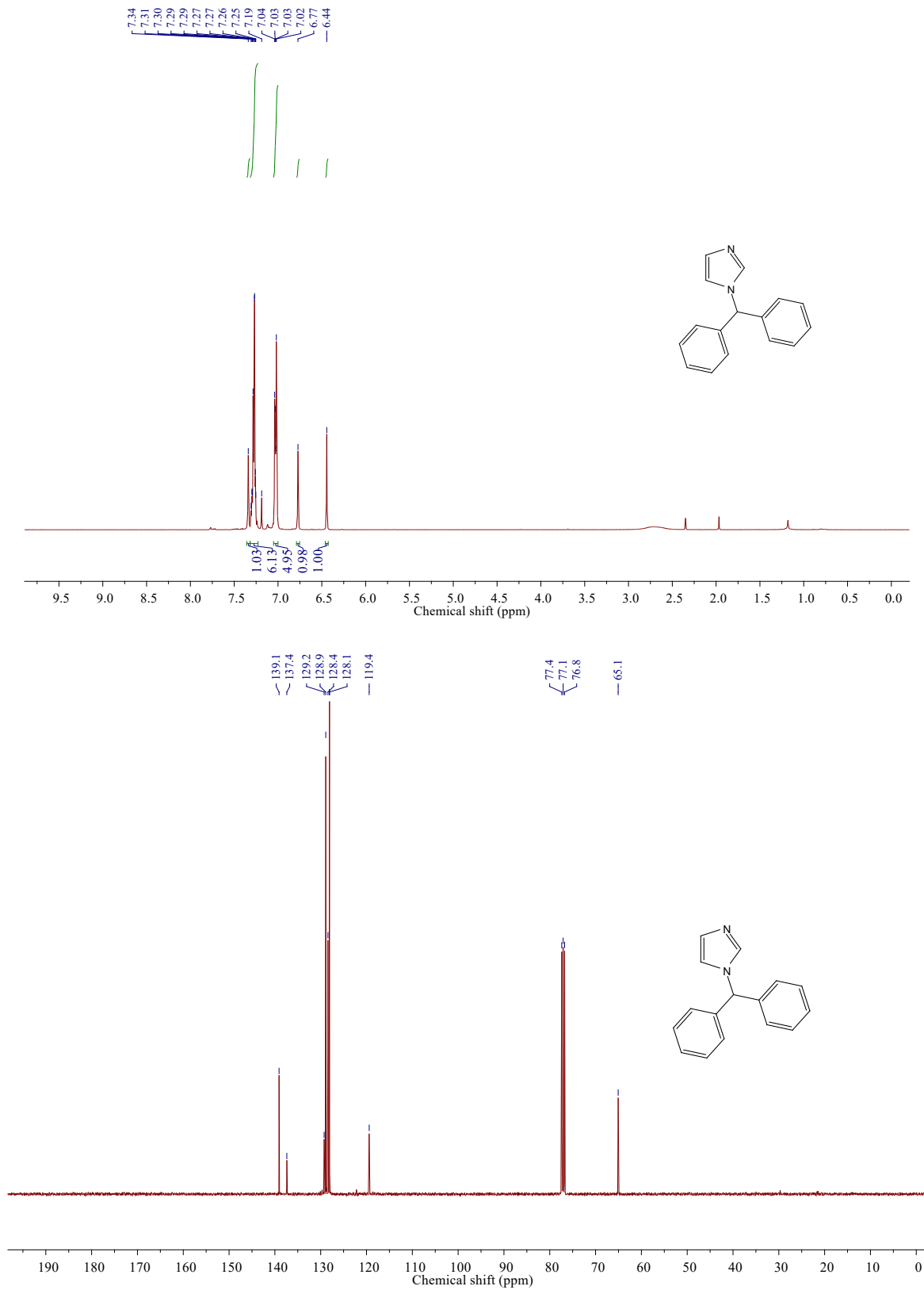
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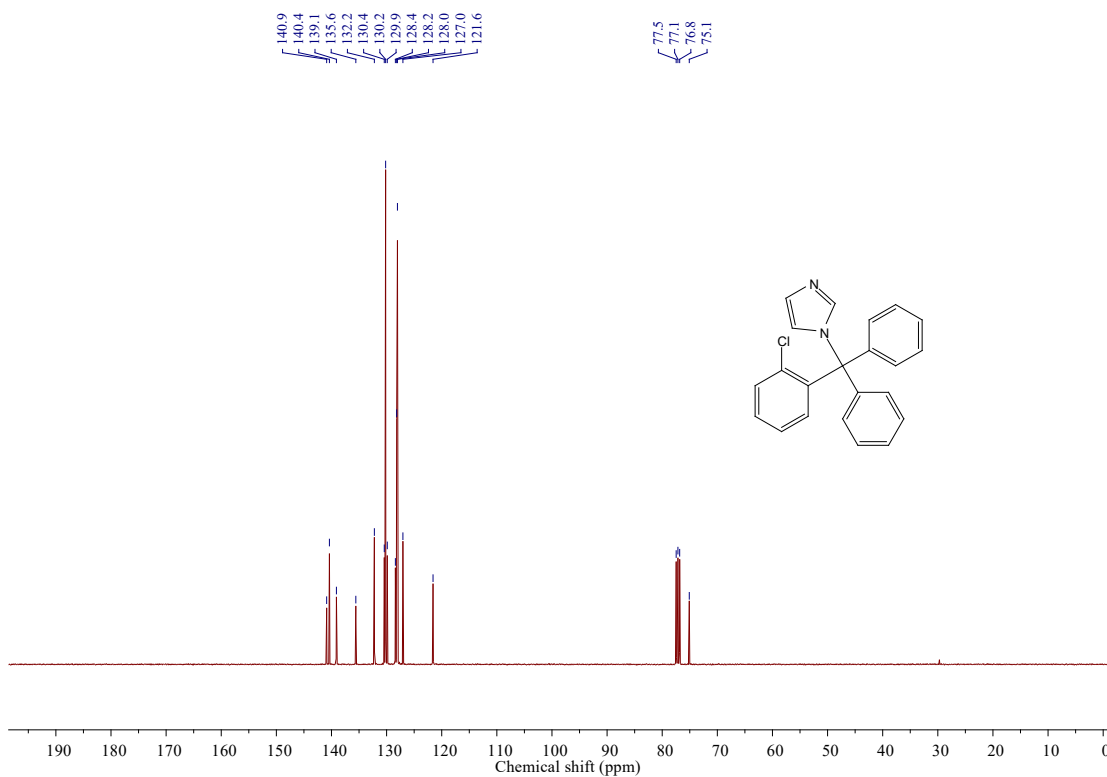
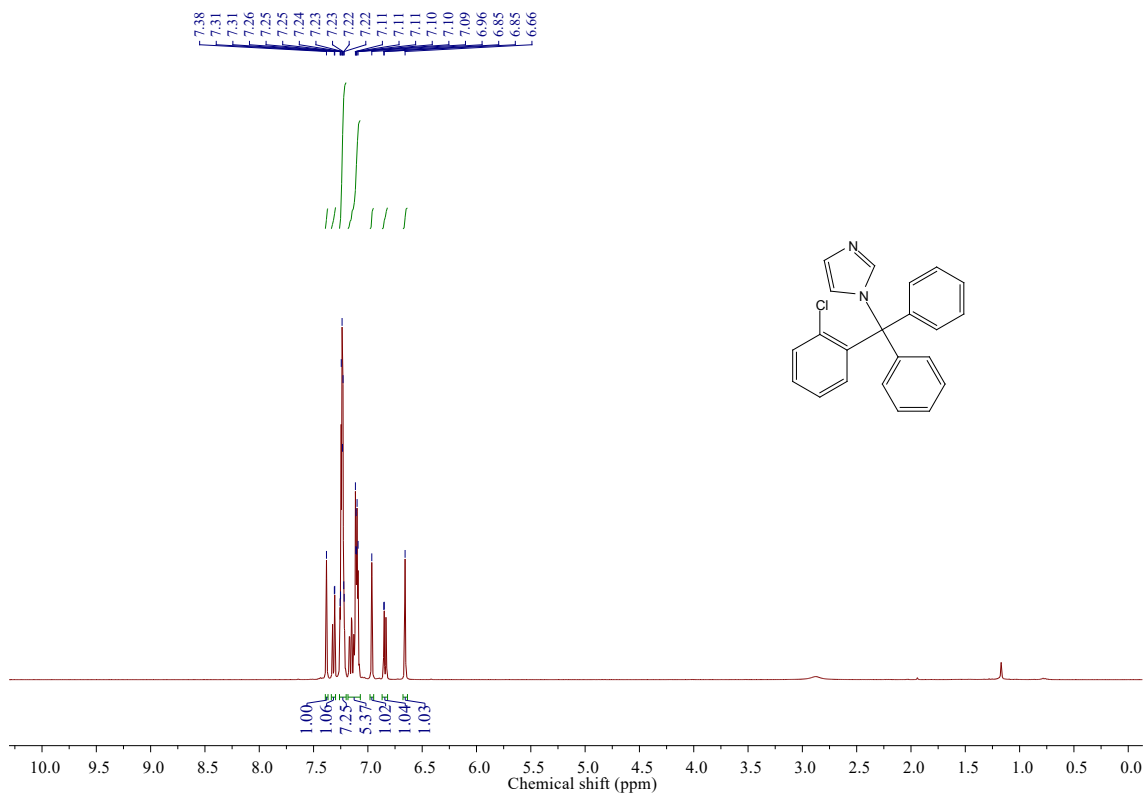
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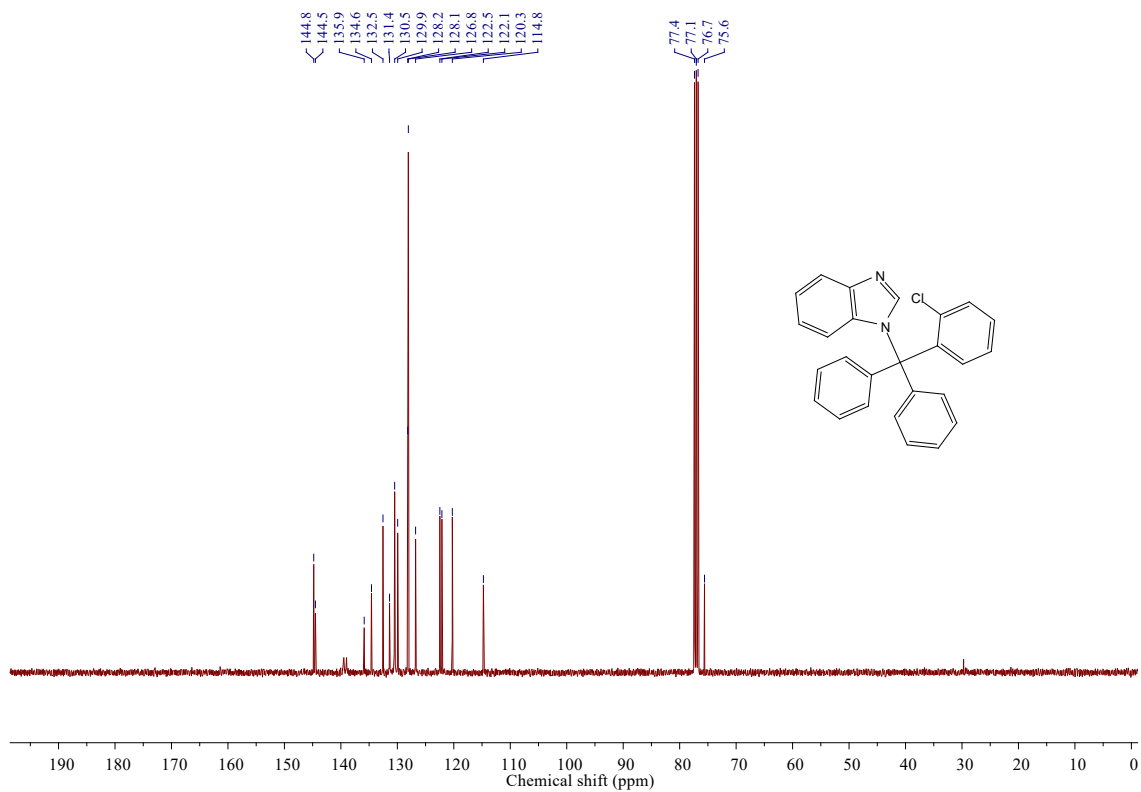
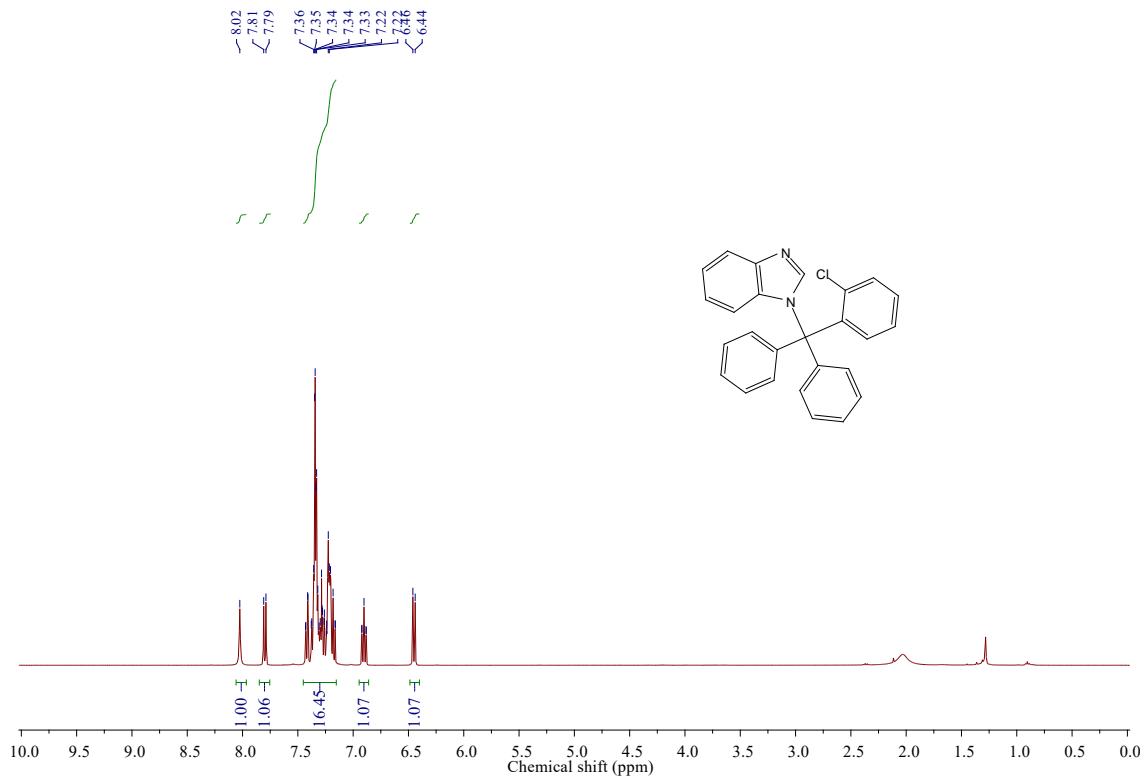


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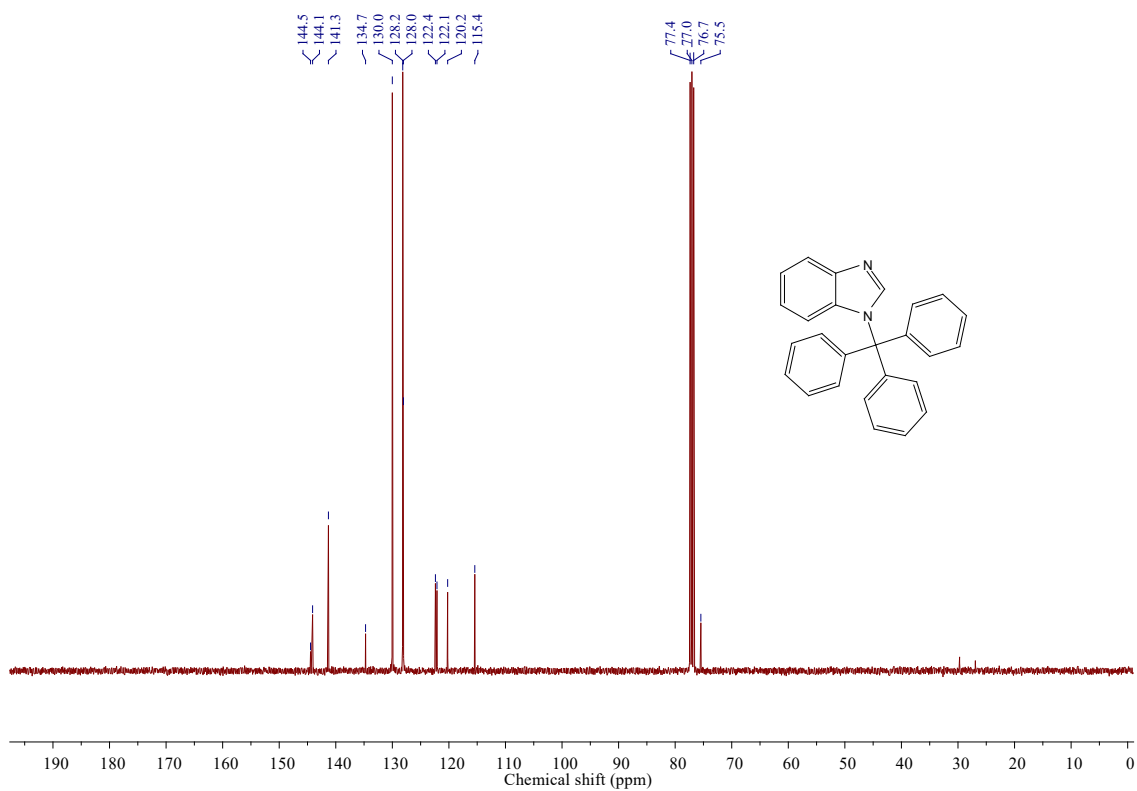
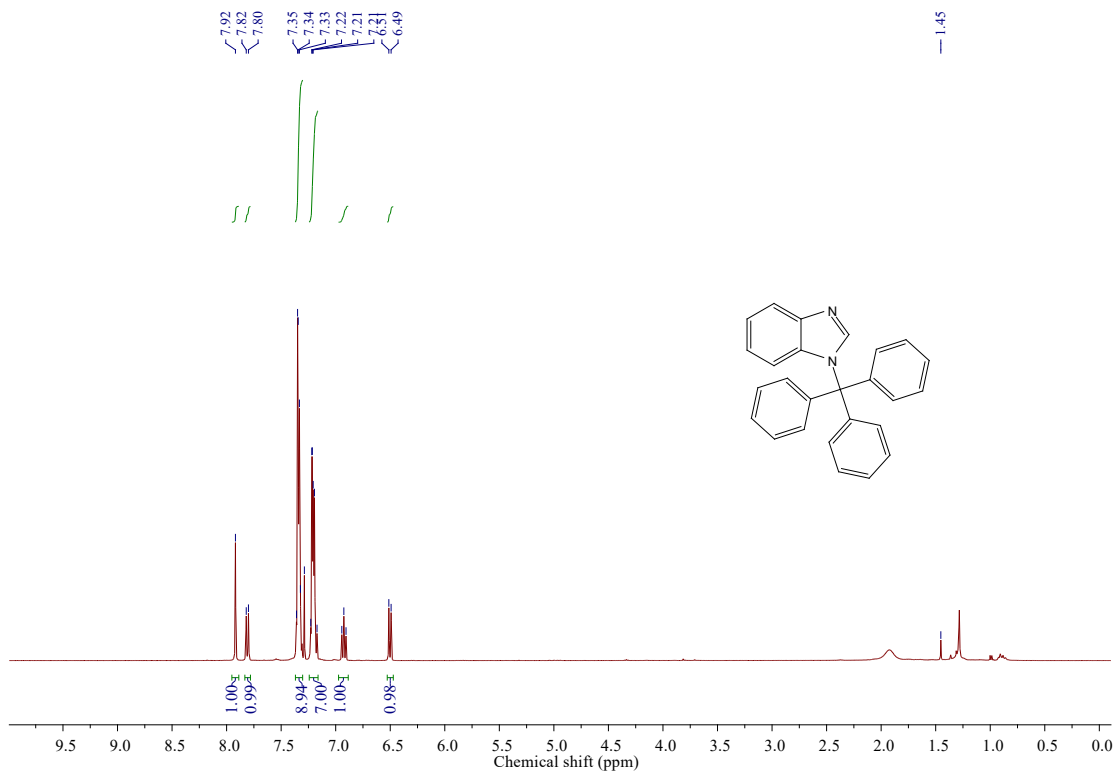




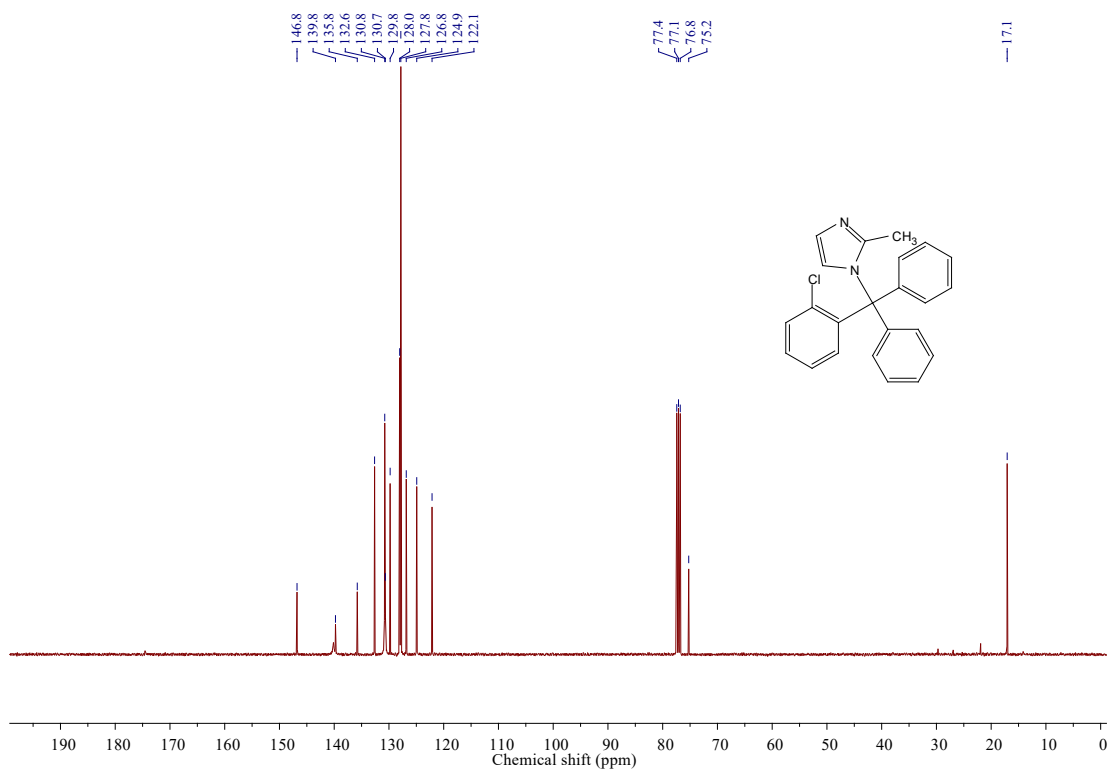
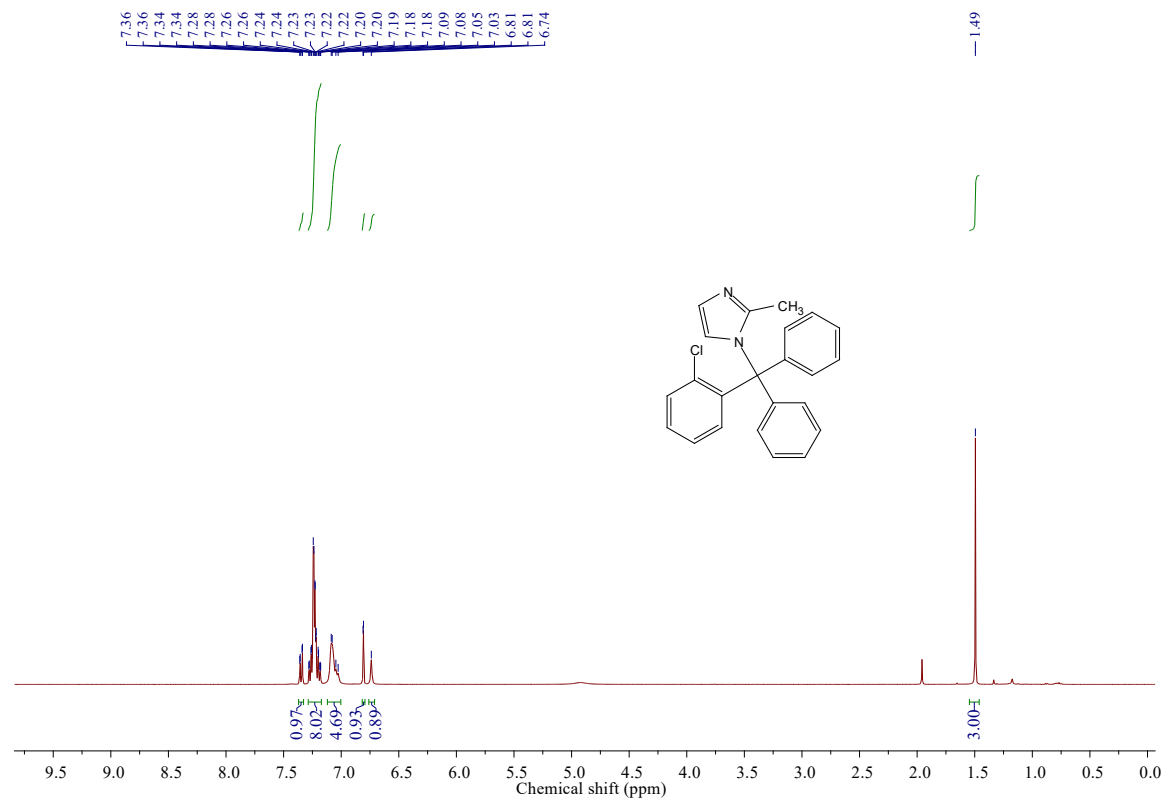
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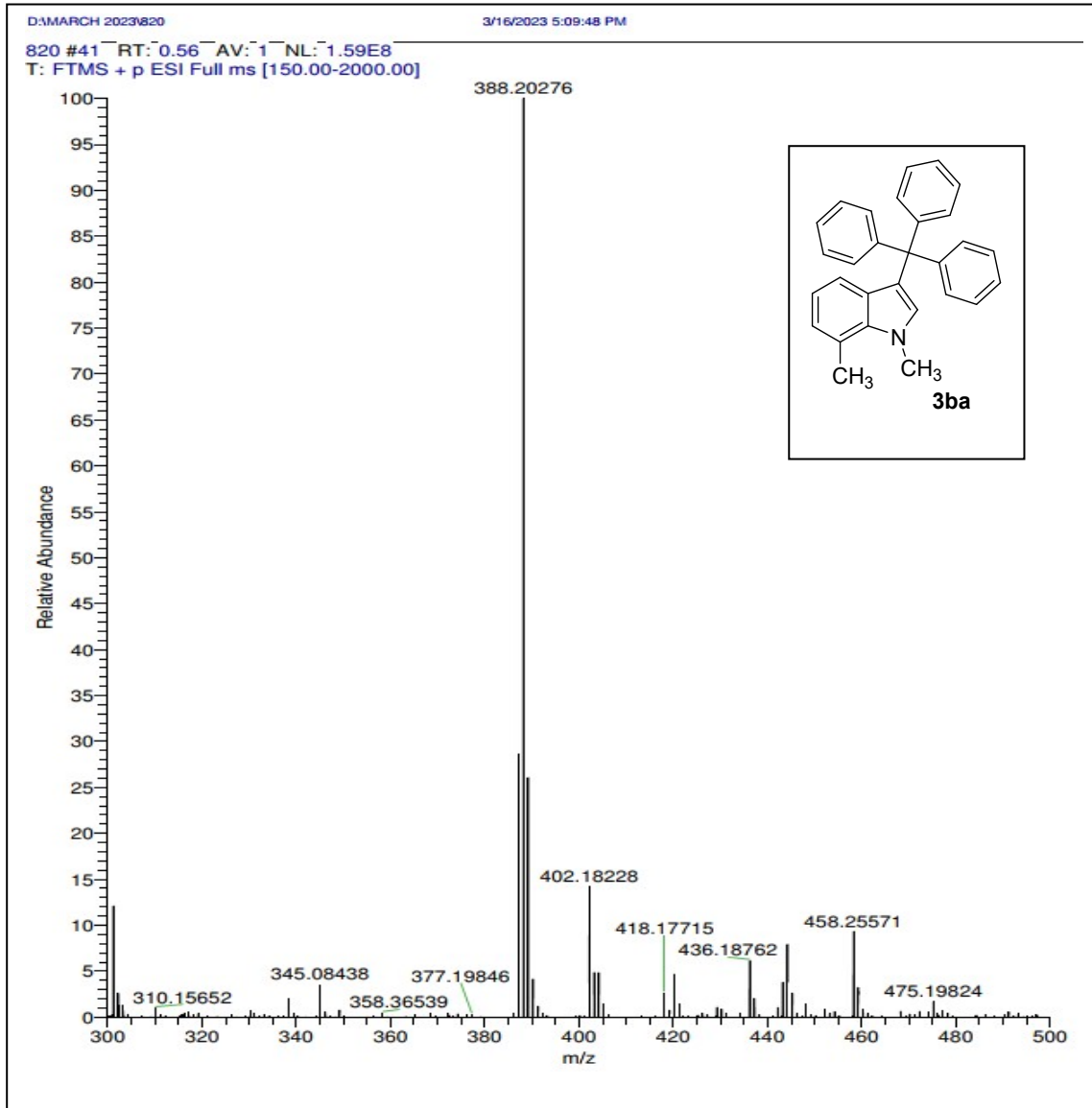
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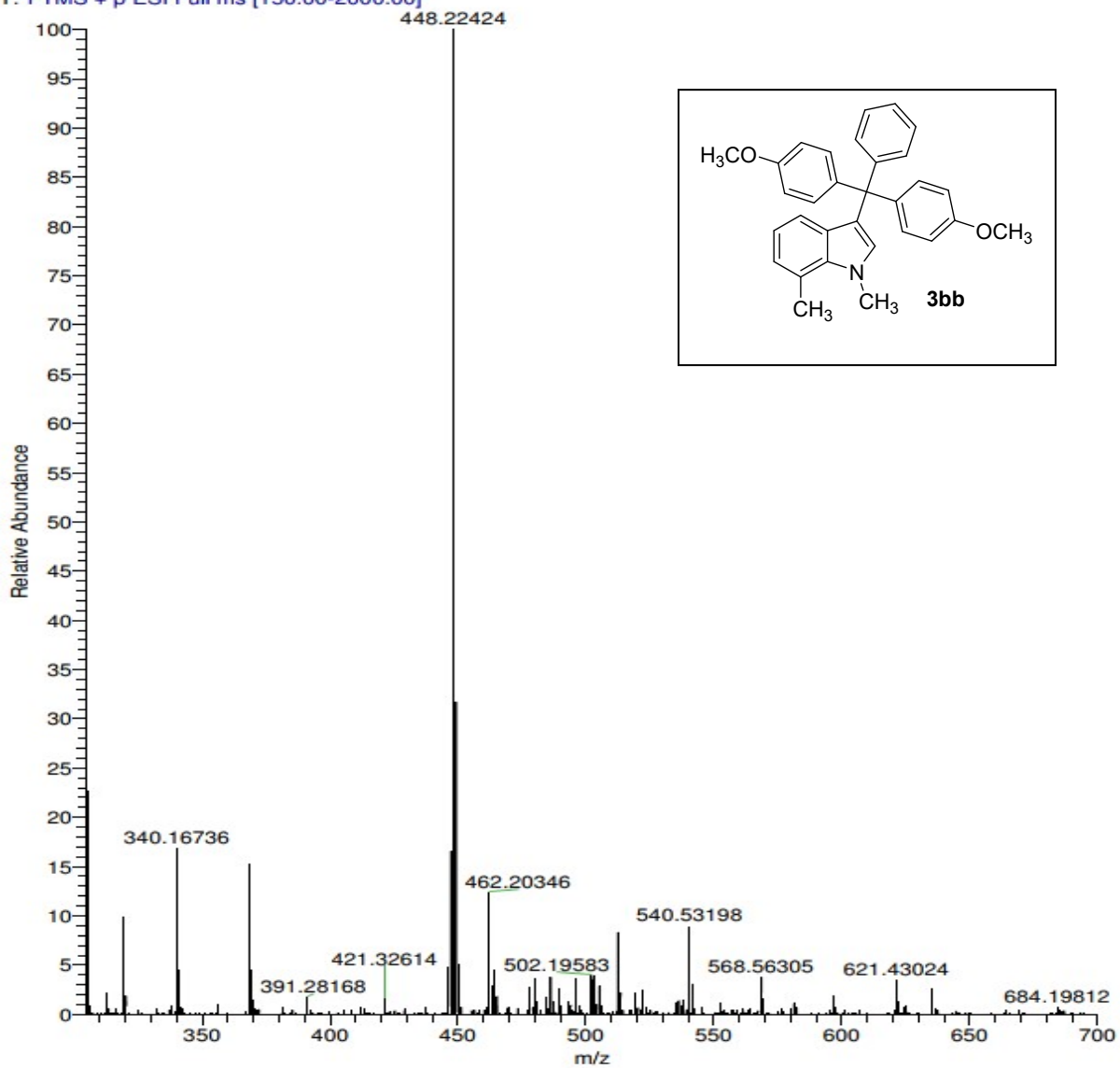


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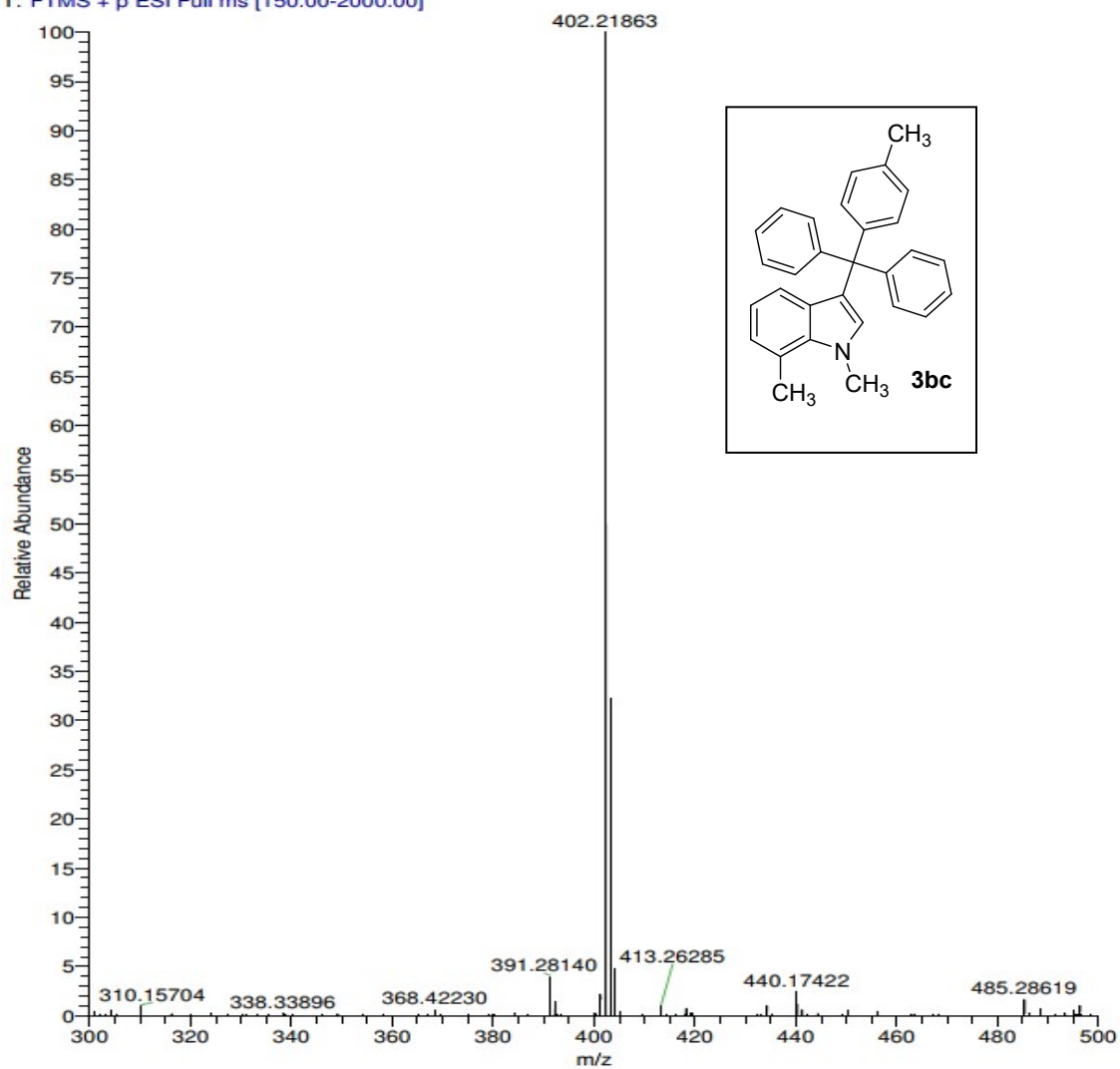


# Mass spectra

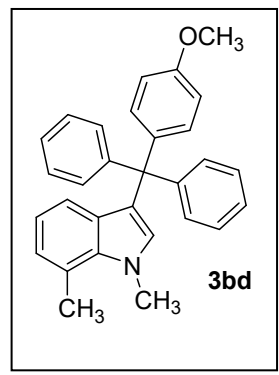
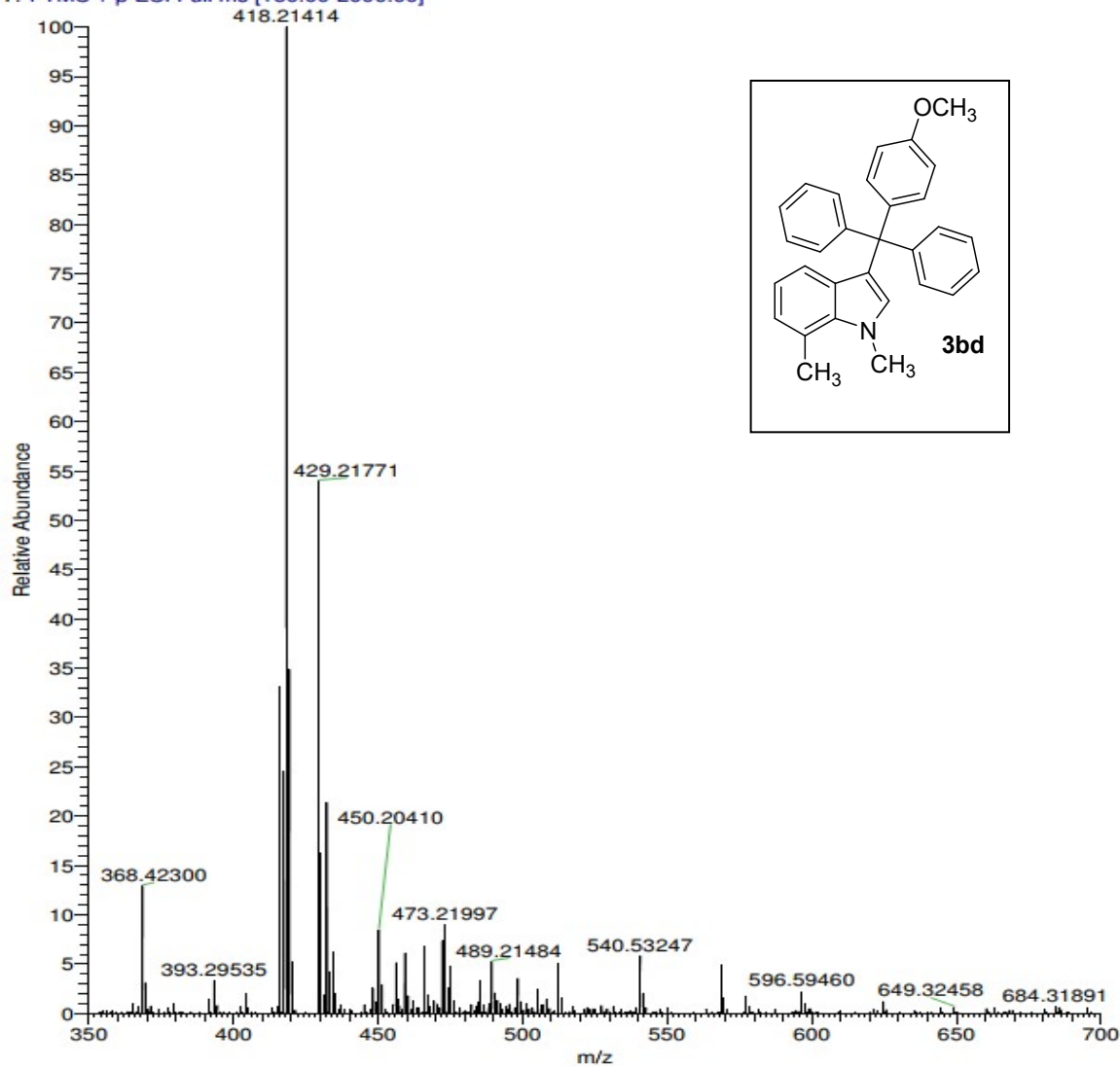


846 #73 RT: 1.01 AV: 1 NL: 4.95E7  
T: FTMS + p ESI Full ms [150.00-2000.00]

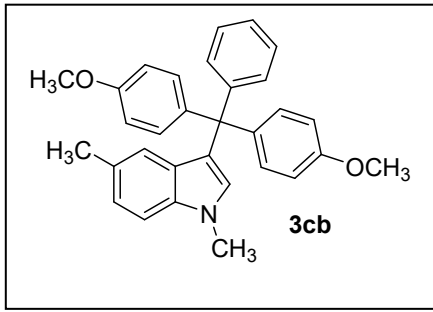
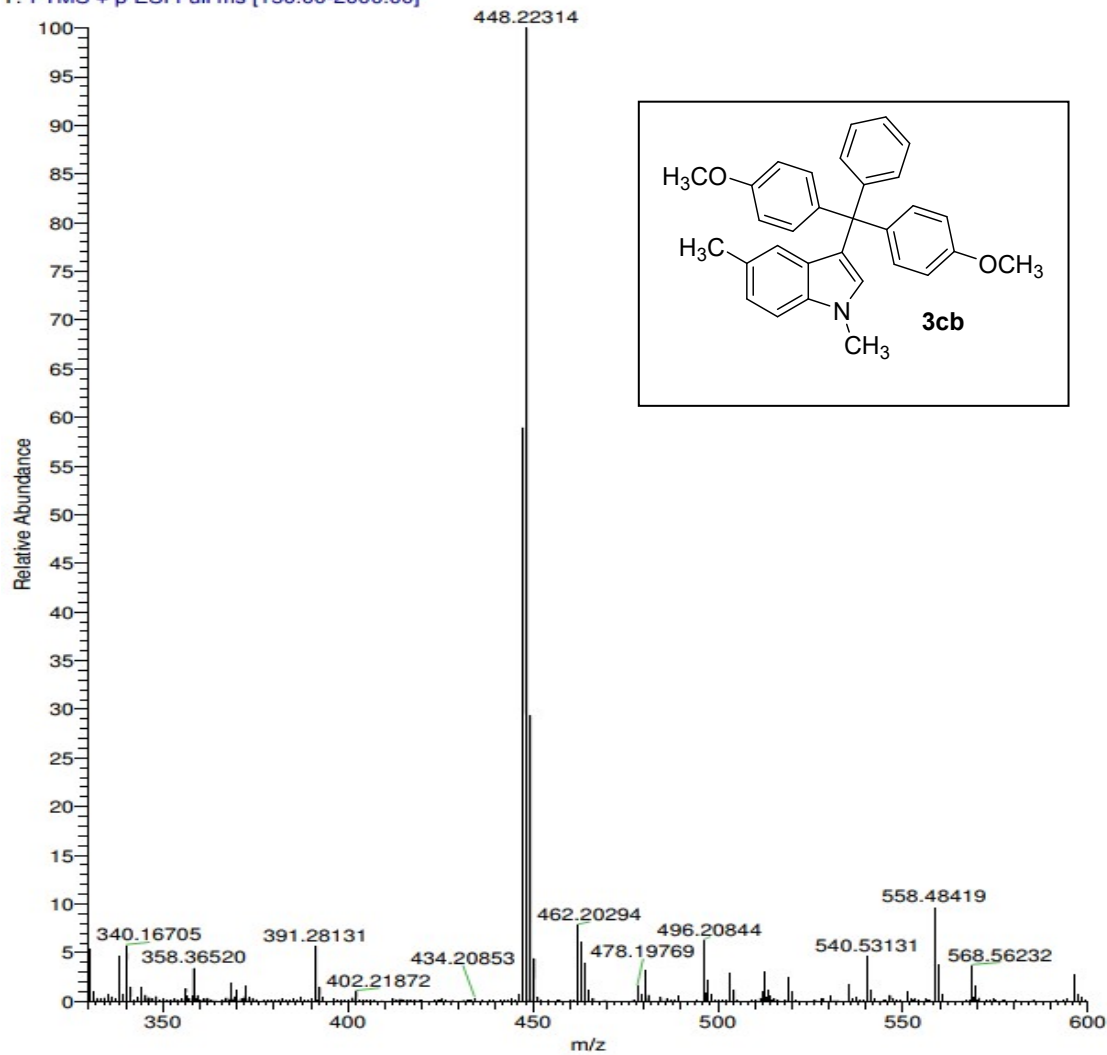
865 #23 RT: 0.31 AV: 1 NL: 2.99E8  
T: FTMS + p ESI Full ms [150.00-2000.00]



867\_230406130909 #75 RT: 1.04 AV: 1 NL: 7.61E7  
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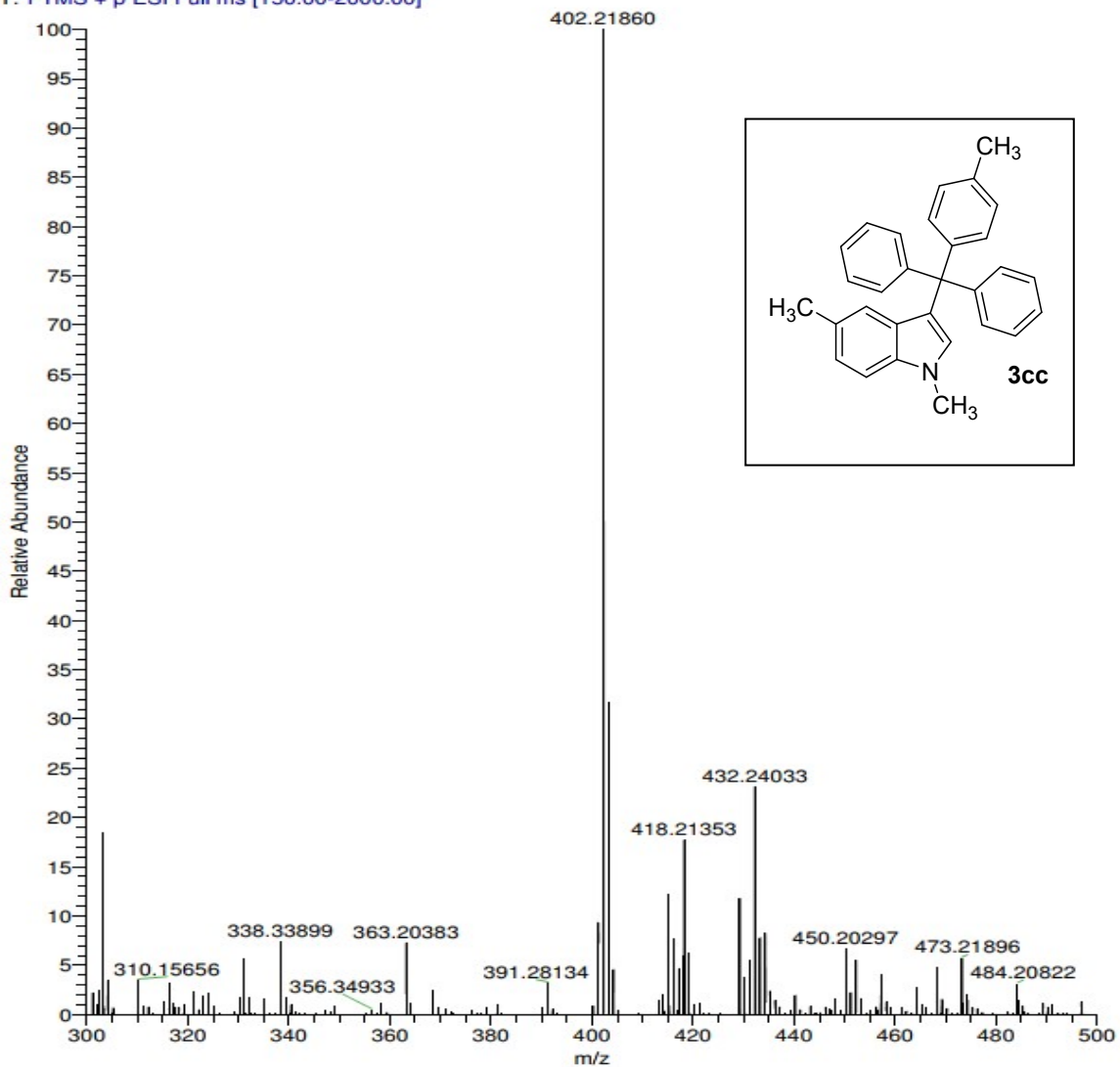
850 #43 RT: 0.59 AV: 1 NL: 2.78E7  
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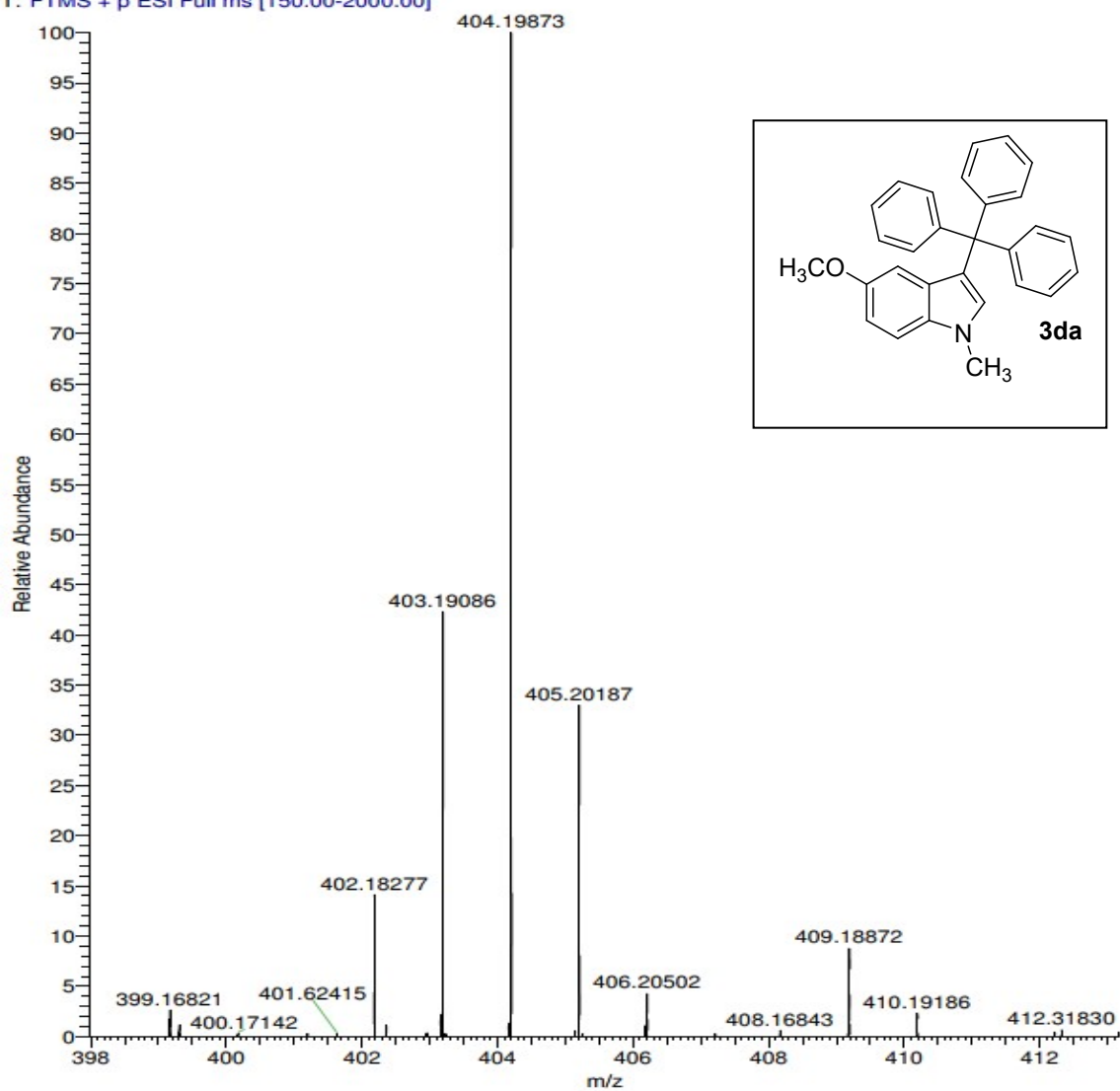
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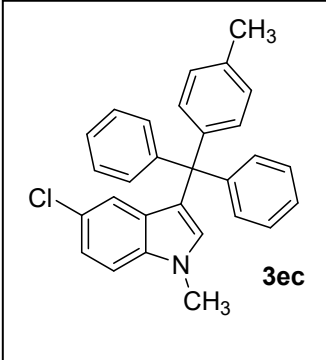
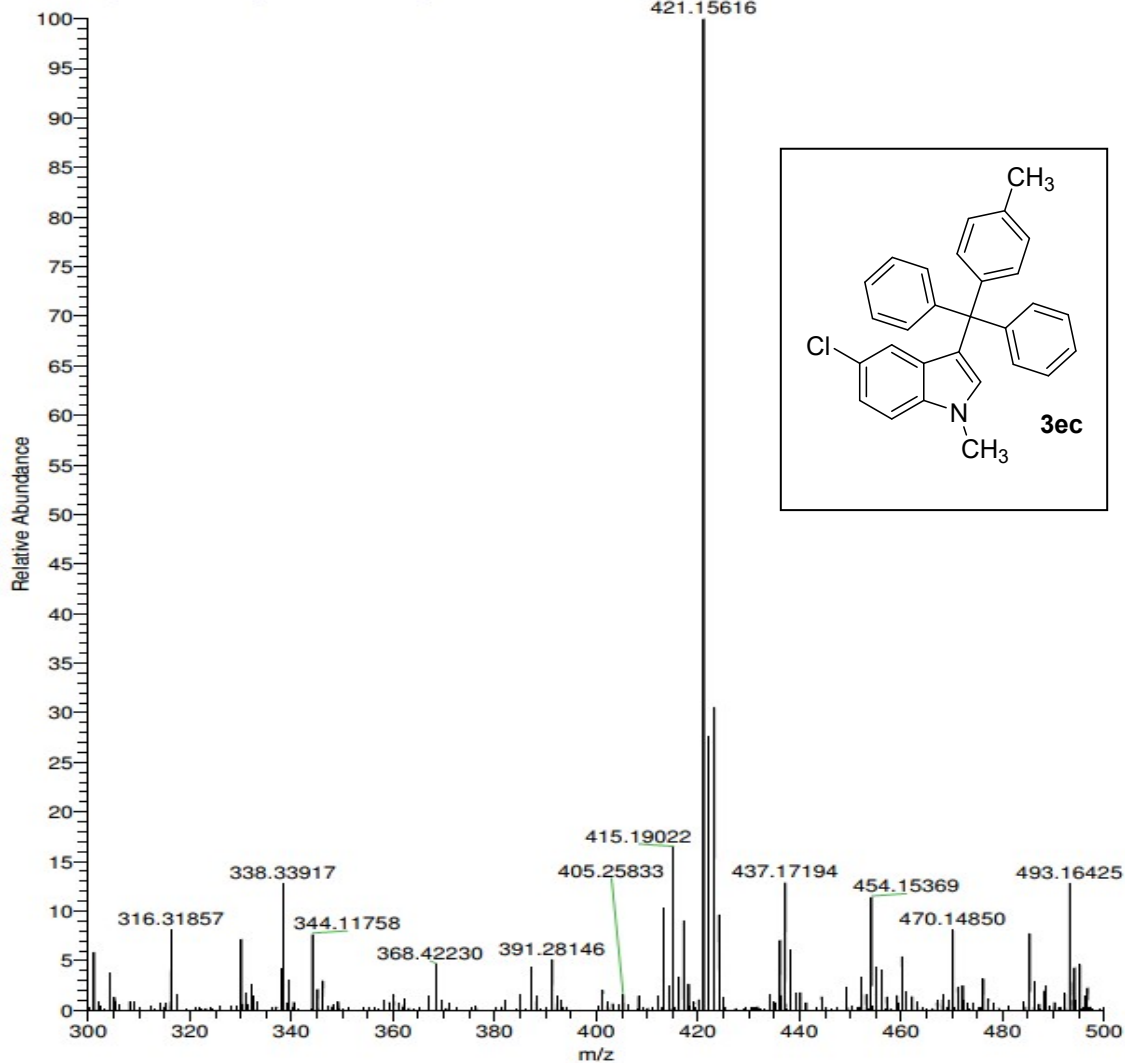


827 #73 RT: 1.01 AV: 1 NL: 5.24E7

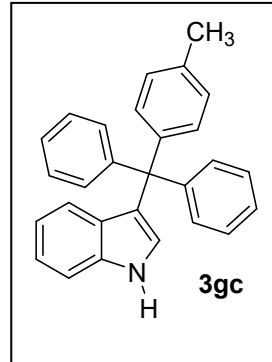
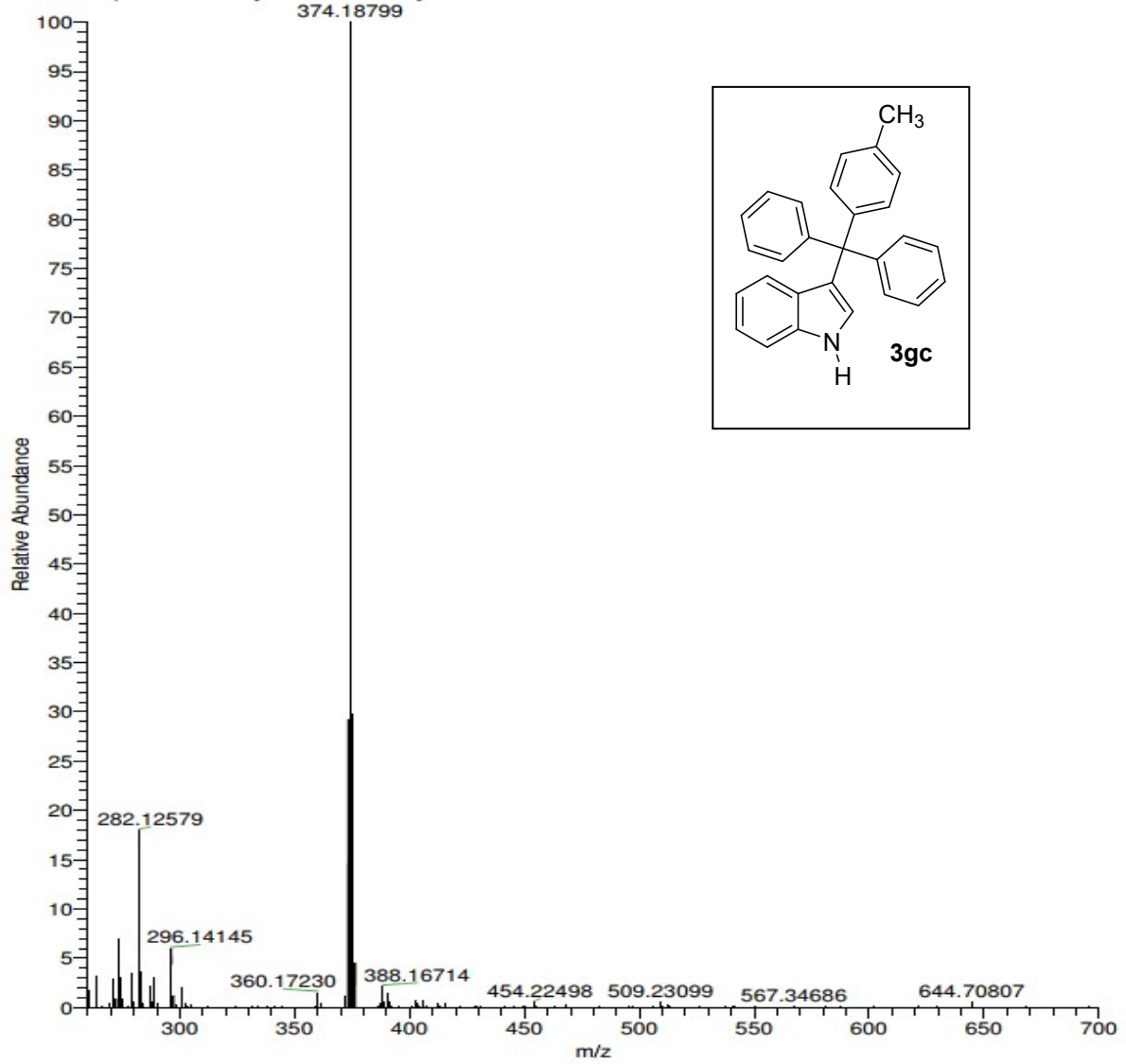
T: FTMS + p ESI Full ms [150.00-2000.00]



868 #31 RT: 0.42 AV: 1 NL: 4.25E7  
T: FTMS + p ESI Full ms [150.00-2000.00]



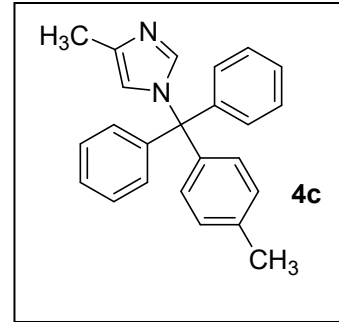
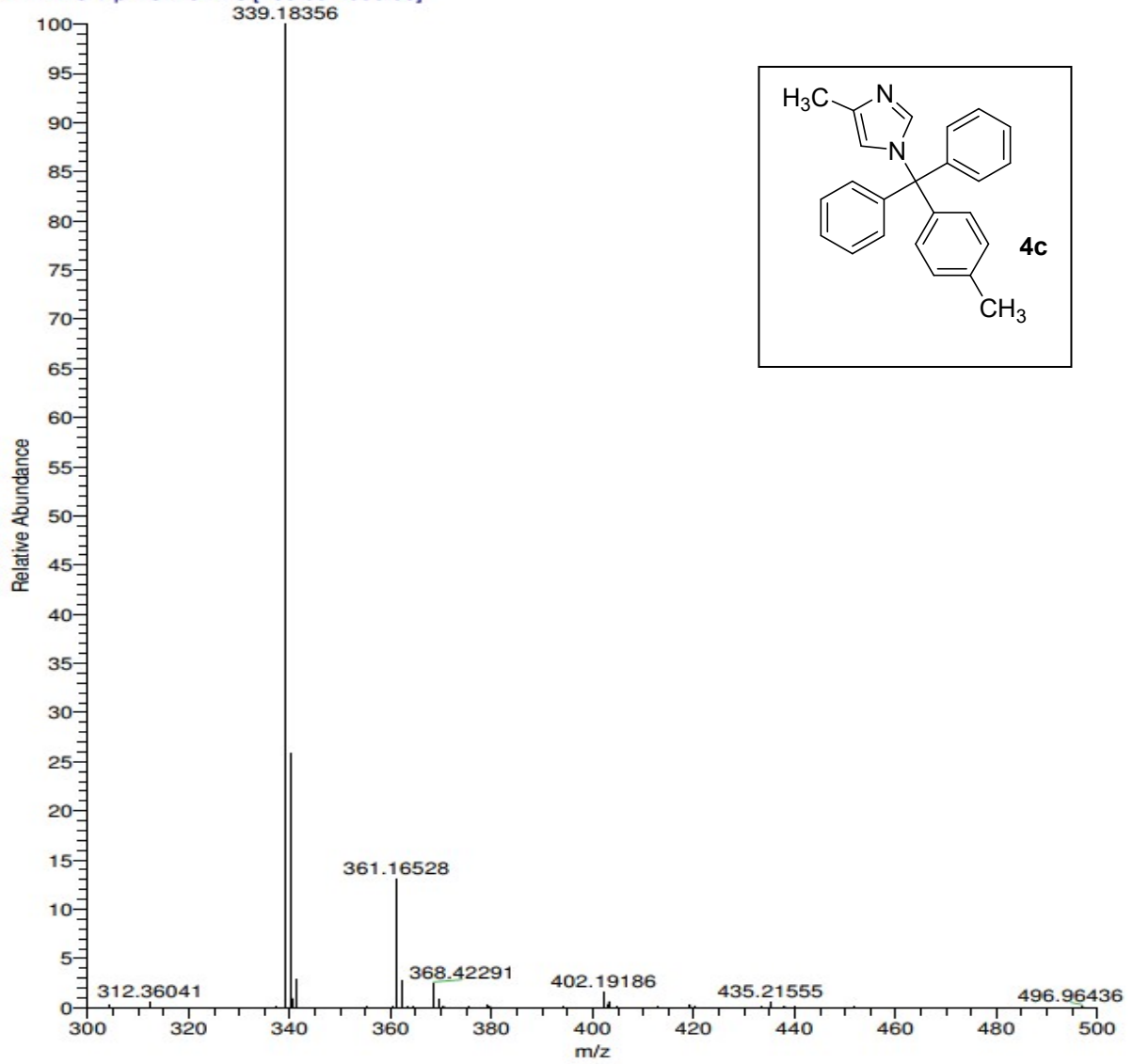
869 #65 RT: 0.90 AV: 1 NL: 1.89E8  
T: FTMS + p ESI Full ms [150.00-2000.00]



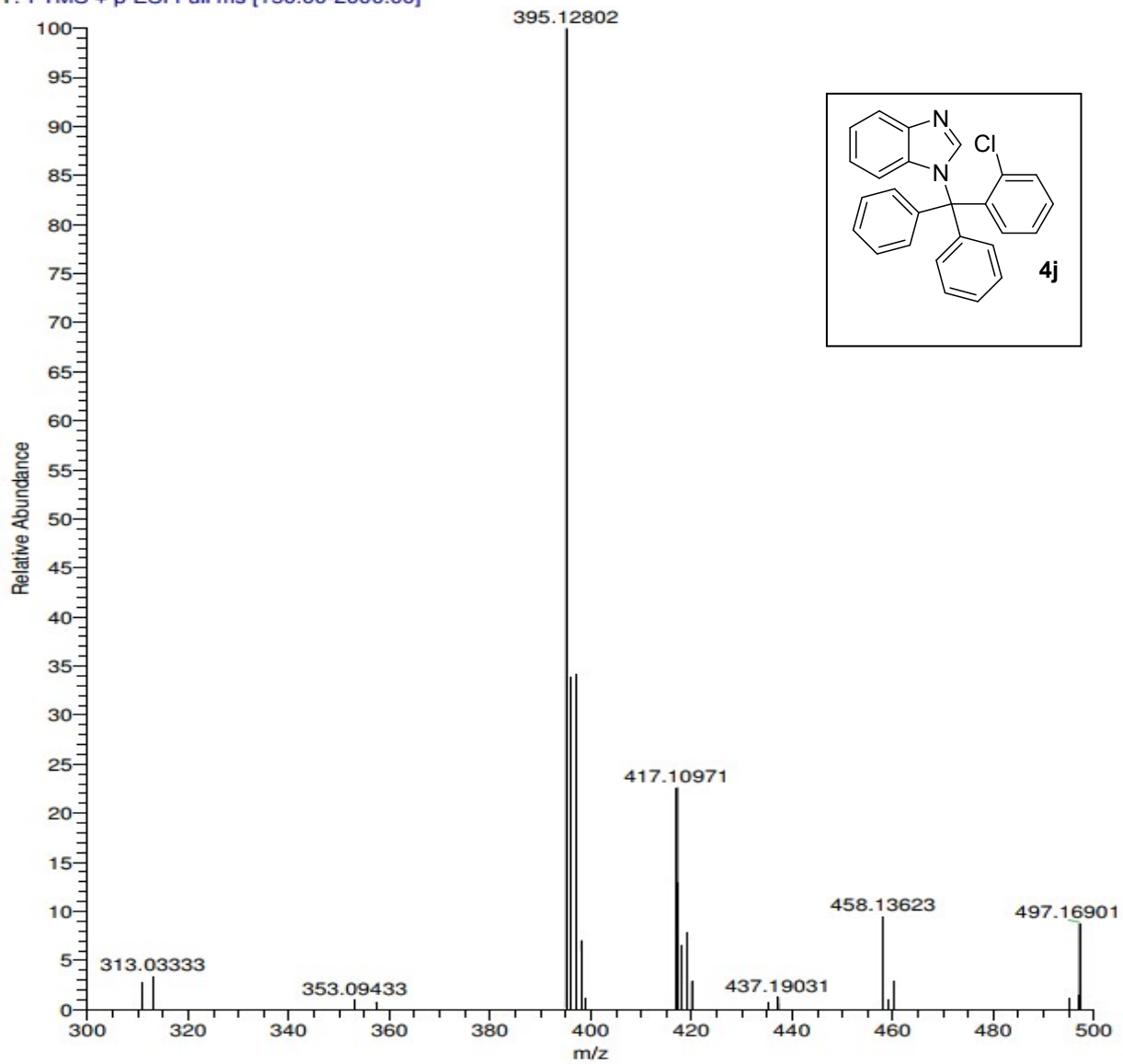
D:\MARCH 2023\A

4/6/2023 1:18:57 PM

A #73 RT: 1.01 AV: 1 NL: 6.52E8  
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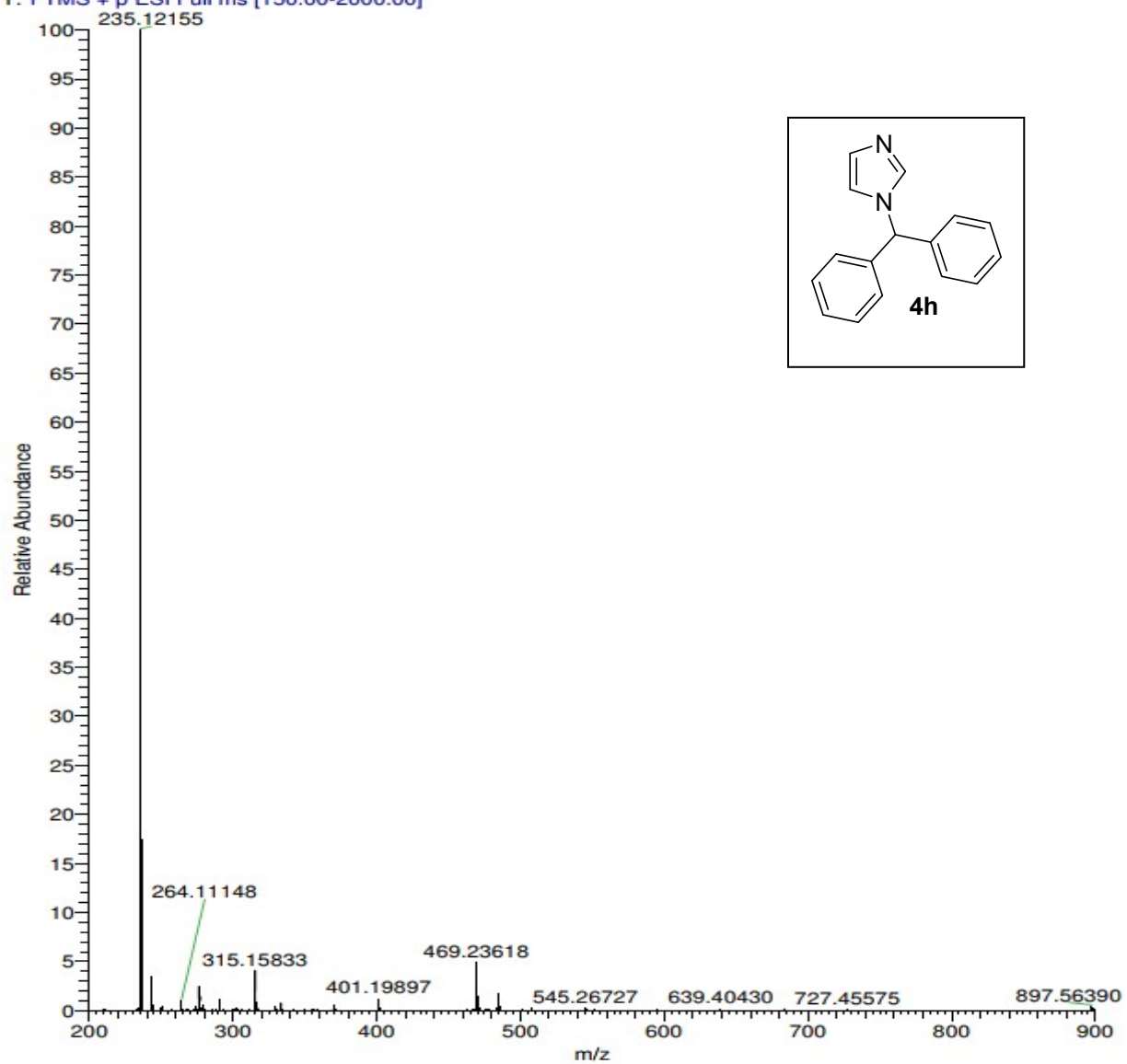
888 #21 RT: 0.28 AV: 1 NL: 1.24E8  
T: FTMS + p ESI Full ms [150.00-2000.00]



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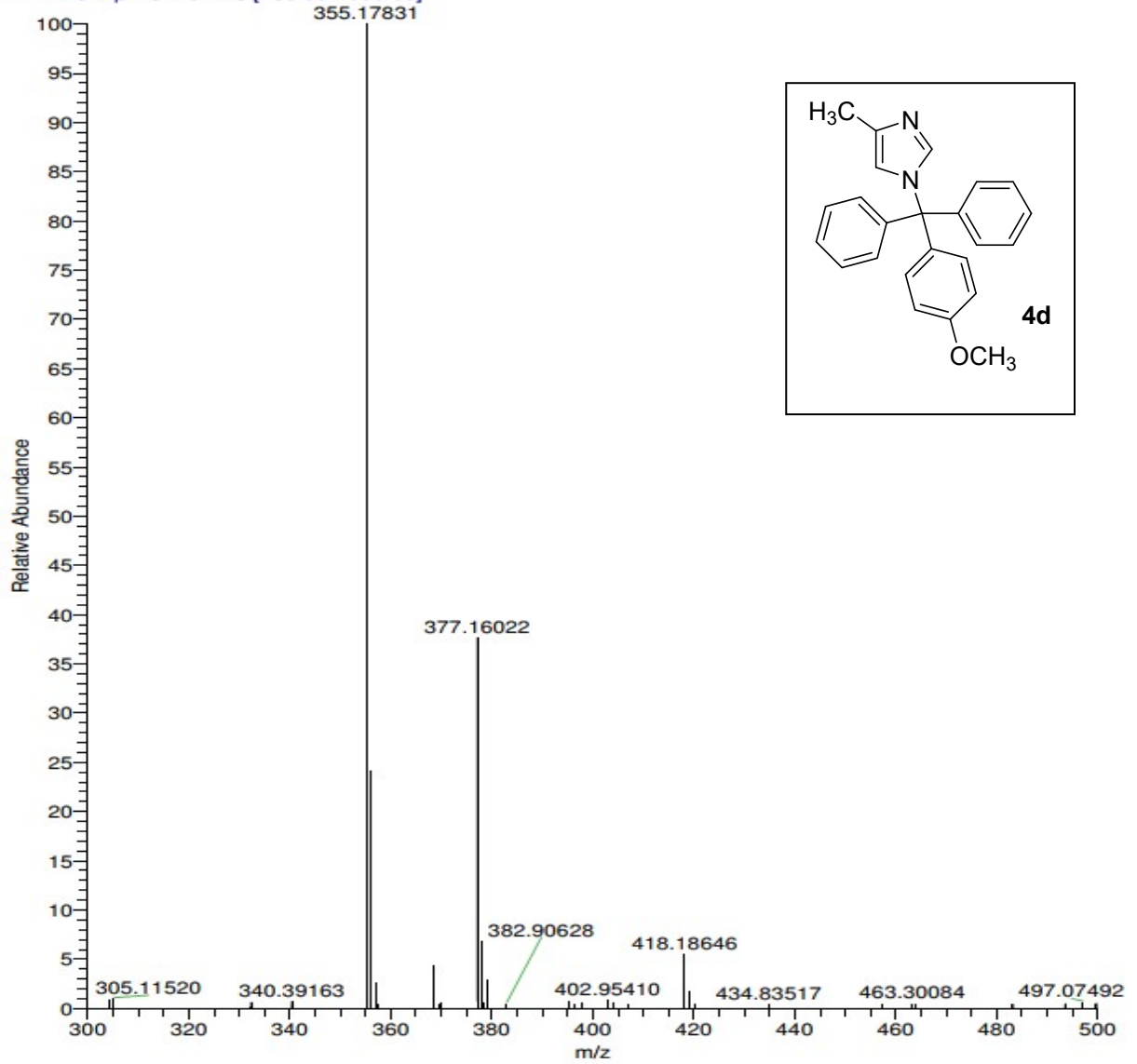
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B #65 RT: 0.91 AV: 1 NL: 2.53E9  
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892 #73 RT: 1.01 AV: 1 NL: 1.77E8

T: FTMS + p ESI Full ms [150.00-2000.00]





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