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Supporting Information

Copper-Catalyzed C−N Bond Formation with Imidazo[1,2-*a*]pyridines

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I. General Remarks:

All reagents were purchased from commercial sources and used without further purification. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker Ascend™ 400 spectrometer in deuterated solvents containing TMS as an internal reference standard. High-resolution mass spectrometry (HRMS) analyses were conducted on a Waters LCT Premier/XE. IR spectra (KBr) were recorded on a Magna-560 FTIR spectrophotometer in the range of 400~4000 cm^{-1}. Melting points were measured on a melting point apparatus equipped with a thermometer and were uncorrected. All the reactions were monitored by thin-layer chromatography (TLC) using GF254 silica gel-coated TLC plates. Purification by flash column chromatography was performed over SiO_2 (silica gel 200−300 mesh).

II. General procedure for the preparation of 3 (3a as an example):

2-Phenylimidazo[1,2-*a*]pyridine **1a** (58.2 mg, 0.3 mmol), saccharin **2** (54.9 mg, 0.3 mmol), $Cu(OAc)_2$ (5.4 mg, 0.03 mmol), Selectfluor (212.4 mg, 0.6 mmol) and Na_2CO_3 (74.4 mg, 0.6 mmol) mixed in 3 mL DCE. The mixture was stirred at 120 °C for 12 h in a Schlenk tube. The reaction was monitored by TLC before being quenched with water (10 mL) and extracted with dichloromethane (5 × 3 mL). The extracted organics were dried over anhydrous sodium sulfate, and the solvent was removed under reduced pressure. The residue was purified by flash silica gel column chromatography using ethyl acetate/petroleum ether (1:5) as an eluent to give compound **3a** as a white solid (95.6 mg, 83%).

III. Analytical data of products obtained in this study

2-(2-phenylimidazo[1,2-*a*]pyridin-3-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide (3a). White solid, mp 208-209 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 6.87 (t, J = 6.4, 1H), 7.32-7.38 (m, 4H), 7.71 (d, J = 9.2, 1H), 7.91-7.97 (m, 7H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 103.7, 113.3, 118.1, 121.7, 123.2, 126.2, 126.3, 127.5, 128.6, 128.8, 132.1, 134.8, 135.9, 138.0, 145.2, 146.4, 158.1. HRMS (ESI-TOF) Calcd for $C_{20}H_{14}N_3O_3S$, $[M+H]^+$ 376.0574; Found 376.0578. IR (KBr, cm-1): 3032, 1747, 1355,

1185, 669.

2-(2-(*m*-tolyl)imidazo[1,2-*a*]pyridin-3-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide (3b). White solid, mp 116-117 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 2.34 (s, 3H), 6.93 (t, *J* = 6.8, 1H), 7.16 (d, *J* =6.8, 1H), 7.22 (d, *J* = 7.6, 1H), 7.40 (t, *J* = 8.0, 1H), 7.65 (t, *J* = 7.6, 1H), 7.87-7.96 (m, 3H), 8.01-8.06 (m, 3H), 8.12 (d, *J* =6.4, 1H),. ^{13}C NMR (100 MHz; $CDCl_3$): δ = 21.4, 113.6, 117.9, 121.7, 123.3, 124.4, 126.2, 127.3, 128.5, 128.7, 129.9, 131.2, 133.9, 134.8, 135.9, 138.1, 138.4, 144.9, 146.2, 158.1. HRMS (ESI-TOF) Calcd for $C_{21}H_{16}N_3O_3S$, $[M+H]^+$ 390.0913; Found 390.0906. IR (KBr, cm-1): 3046, 1766, 1345, 1130, 733.

2-(2-(*p*-tolyl)imidazo[1,2-*a*]pyridin-3-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide (3c). White solid, mp 223-224 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 6.86 (t, *J* = 6.4, 1H), 7.18 (d, *J* = 8.0, 2H), 7.34 (t, *J* = 7.2, 1H), 7.71 (d, *J* = 9.2, 1H), 7.83 (d, *J* = 8.0, 2H), 7.95-8.10 (m, 4H), 8.20 (d, *J* = 7.2, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 21.3, 103.3, 113.2, 118.1, 121.7, 123.2, 126.2, 126.3, 126.7, 127.3, 129.2, 129.4, 134.8, 135.8, 138.1, 138.8, 145.2, 146.5, 158.1. HRMS (ESI-TOF) Calcd for $C_{21}H_{16}N_3O_3S$, $[M+H]^+$ 390.0913; Found 390.0908. IR (KBr, cm-1): 3039, 2855, 1758, 1353, 1183, 732.

2-(2-(4-cyclohexylphenyl)imidazo[1,2-*a*]pyridin-3-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide (3d). White solid, mp 236-237 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 1.34-1.43 (m, 4H), 1.71-1.85 (m, 6H), 2.48 (t, *J* = 7.6, 1H), 6.85 (t, *J* = 6.8, 1H), 7.20-7.35 (m, 3H), 7.71 (d, *J* = 8.8, 1H), 7.88-8.20 (m, 7H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 26.1, 26.8, 34.2, 44.3, 113.2, 118.0, 121.7, 123.2, 126.2, 126.7, 126.7, 127.3, 129.4, 134.8, 135.8, 138.1, 145.2, 146.4, 148.8, 158.1. HRMS (ESI-TOF) Calcd for $C_{26}H_{14}N_3O_3S$, $[M+H]^+$ 458.1538; Found 458.1532. IR (KBr, cm-1): 3079, 1746, 1386, 1184, 591.

2-(2-(4-methoxyphenyl)imidazo[1,2-*a*]pyridin-3-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide (3e). White solid, mp 221-222 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 3.80

(s, 3H), 6.89 (q, *J* = 7.2, 3H), 7.34 (q, *J* = 6.8, 1H), 7.05 (d, *J* = 8.8, 1H), 7.89-7.97 (m, 7H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 55.1, 113.1, 114.1, 118.0, 121.7, 123.1, 124.6, 126.2, 126.4, 126.6, 128.8, 134.8, 135.8, 138.1, 145.2, 146.3, 158.1, 160.1. HRMS (ESI-TOF) Calcd for $C_{21}H_{16}N_3O_4S$, $[M+H]^+$ 406.0863; Found 406.0865. IR (KBr, cm-1): 3093, 1756, 1337, 733.

2-(2-(3,4-dimethylphenyl)imidazo[1,2-*a*]pyridin-3-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide (3f). White solid, mp 114-115 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 2.24-2.26 (d, 6H), 6.89 (d, *J* = 6.8, 1H), 7.10 (d, *J* = 7.6, 1H), 7.34 (t, *J* = 8.0, 1H), 7.58 (d, *J* = 8.0, 1H), 7.72 (d, *J* = 8.8, 1H), 7.82 (s, 1H), 7.97-8.05 (m, 4H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 19.6, 19.7, 113.2, 118.0, 121.7, 123.2, 124.4, 126.2, 126.4, 126.6, 128.9, 129.5, 129.8, 134.8, 135.8, 136.9, 137.5, 138.1, 145.2, 146.6, 158.1. HRMS (ESI-TOF) Calcd for $C_{22}H_{18}N_3O_3S$, $[M+H]^+$ 404.1065; Found 404.1069. IR (KBr, cm-1): 3092, 1749, 1495, 1343, 582.

2-(2-(2-chlorophenyl)imidazo[1,2-*a*]pyridin-3-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide (3g). White solid, mp 214-216 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 6.91 (t, *J* = 6.8, 1H), 7.29-7.45 (m, 4H), 7.63 (d, *J* = 6.8, 1H), 7.74 (d, *J* = 9.2, 1H), 7.90-8.02 (m, 5H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 106.0, 113.6, 118.5, 121.6, 123.1, 126.0, 126.3, 126.4, 126.8, 130.0, 131.5, 132.1, 133.9, 134.7, 135.6, 137.9, 144.6, 145.0, 157.9. HRMS (ESI-TOF) Calcd for $C_{20}H_{13}ClN_3O_3S$, $[M+H]^+$ 410.0367; Found 410.0374. IR (KBr, cm-1): 3049, 1747, 1339, 581.

2-(2-(3-chlorophenyl)imidazo[1,2-*a*]pyridin-3-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide (3h). White solid, mp 218-219 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 6.88 (d, *J* = 6.8, 1H), 7.29-7.37 (m, 3H), 7.71 (d, *J* = 9.2, 1H), 7.79 (d, *J* = 5.2, 1H), 7.92-7.98 (m, 6H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 113.6, 118.2, 121.8, 123.3, 125.4, 126.3, 127.1, 127.9, 128.9, 129.8, 130.8, 133.8, 134.6, 134.9, 136.0, 145.2, 158.1, 167.6. HRMS (ESI-TOF) Calcd for $C_{20}H_{13}ClN_3O_3S$, $[M+H]^+$ 410.0367; Found 410.0371. IR (KBr, cm-1): 3091, 1742, 1349, 1185, 571.

2-(2-(4-fluorophenyl)imidazo[1,2-*a*]pyridin-3-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide (3i). White solid, mp 172-173 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 6.88 (t, J = 6.8, 1H), 7.07 (t, J = 8.4, 2H), 7.37 (t, J = 8.0, 1H), 7.74 (d, J = 8.8, 1H), 7.91-7.99 (m, 7H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 104.1, 113.6, 118.2, 121.8, 123.3, 125.3, 126.3, 127.8, 128.8, 128.9, 129.9, 130.9, 132.3, 133.8, 134.6, 135.0, 136.0 (d, J = 190 Hz), 137.9, 144.9, 145.2, 158.1, 167.7. HRMS (ESI-TOF) Calcd for $C_{20}H_{13}FN_3O_3S$, $[M+H]^+$ 394.0664; Found 394.0669. IR (KBr, cm-1): 3033, 1741, 1186, 731, 501.

2-(2-(4-bromophenyl)imidazo[1,2-*a*]pyridin-3-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide (3j). White solid, mp 226-227 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 6.89 (t, J = 6.8, 1H), 7.35 (d, J = 7.6, 1H), 7.39 (t, J = 7.2, 2H), 7.50 (d, J = 8.4, 1H), 7.81 (d, J = 8.4, 2H), 7.97-8.09 (m, 5H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 113.5, 118.2, 121.8, 123.3, 126.2, 126.3, 127.0, 129.0, 131.0, 131.8, 134.9, 136.0, 138.0, 145.3, 158.0. HRMS (ESI-TOF) Calcd for $C_{20}H_{13}BrN_3O_3S$, $[M+H]^+$ 453.9864; Found 453.9861. IR (KBr, cm-1): 3091, 1748, 1341, 1011, 510.

2-(2-(4-(trifluoromethyl)phenyl)imidazo[1,2-*a*]pyridin-3-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide (3k). White solid, mp 223-224 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 6.90 (t, J = 6.8, 1H), 7.36 (d, J = 7.6, 1H), 7.73 (d, J = 8.0, 2H), 7.96-8.08 (m, 8H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 104.5, 113.7, 118.3, 121.8, 122.7, 125.4, 125.5 (q, $J_{C\text{-}F}$ = 12 Hz), 125.6, 126.1, 126.3, 127.2, 127.7, 130.4, 130.7, 135.0, 135.6, 136.0, 138.0, 144.4, 145.4, 158.0. HRMS (ESI-TOF) Calcd for $C_{21}H_{13}F_3N_3O_3S$, $[M+H]^+$ 444.0633; Found 444.0636. IR (KBr, cm-1): 3037, 1760, 1321, 1068, 772.

2-(2-(2,3,4-trichlorophenyl)imidazo[1,2-*a*]pyridin-3-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide (3l). White solid, mp 224-225 °C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 6.96 (t, J = 6.8, 1H), 7.41 (t, J = 9.6, 2H), 7.48 (d, J = 8.4, 1H), 7.75 (t, J = 8.4, 1H), 7.75-7.97 (m, 4H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 106.1, 113.9, 118.6, 121.7, 123.2, 126.2, 127.1, 127.9, 128.8, 130.1, 132.0, 134.3, 134.7, 134.8, 135.8, 137.8, 143.7, 145.1, 157.8. HRMS (ESI-TOF) Calcd for $C_{20}H_{11}Cl_3N_3O_3S$, $[M+H]^+$ 477.9586;

Found 477.9594. IR (KBr, cm-1): 3083, 1740, 1339, 749, 502.

2-(2-(3,5-bis(trifluoromethyl)phenyl)imidazo[1,2-*a*]pyridin-3-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide (3m). White solid, mp 198-199 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 6.97 (d, J = 6.8, 1H), 7.43 (s, 1H), 7.77 (d, J = 9.2, 2H), 8.00-8.16 (m, 5H), 8.23 (d, J = 13.2, 2H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 105.0, 114.1, 118.4, 121.8, 122.3, 123.4, 124.5, 125.9, 126.3, 127.5, 127.6, 131.4 (q, $J_{C\text{-}F}$ = 34 Hz), 131.8, 132.1, 132.4, 134.2, 135.1, 136.3, 137.9, 143.1, 145.4, 158.1. HRMS (ESI-TOF) Calcd for $C_{22}H_{12}F_6N_3O_3S$, $[M+H]^+$ 512.0504; Found 512.0509. IR (KBr, cm-1): 3046, 1757, 1278, 738, 585.

2-(2-(thiophen-2-yl)imidazo[1,2-*a*]pyridin-3-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide (3n). White solid, mp 231-233 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 6.88 (t, J = 6.8, 1H), 7.32 (dd, J_1 = 3.2, J_2 = 4.8, 2H), 7.60 (d, J = 4.2, 1H), 7.69 (d, J = 9.2, 1H), 7.92-8.08 (m, 6H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 103.0, 113.3, 117.9, 121.8, 123.2, 126.0, 126.3, 126.6, 126.9, 133.1, 134.9, 136.0, 138.0, 142.6, 145.3, 157.9. HRMS (ESI-TOF) Calcd for $C_{18}H_{12}N_3O_3S_2$, $[M+H]^+$ 382.0320; Found 382.0316. IR (KBr, cm-1): 3030, 1745, 1341, 1058, 585.

2-(2-(5-chlorothiophen-2-yl)imidazo[1,2-*a*]pyridin-3-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide (3o). White solid, mp 241-242 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 6.82 (d, J =3.6, 1H), 6.88 (t, J = 6.8, 1H), 7.34 (t, J = 9.2, 2H), 7.67 (d, J = 9.2, 1H), 7.98-8.08 (m, 5H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 103.0, 113.3, 117.9, 121.8, 123.2, 126.0, 126.3, 126.6, 126.9, 133.1, 134.9, 136.0, 138.0, 142.6, 145.3, 157.9. HRMS (ESI-TOF) Calcd for $C_{18}H_{11}ClN_3O_3S_2$, $[M+H]^+$ 415.9931; Found 415.9938. IR (KBr, cm-1): 3077, 1741, 1448, 735, 496.

2-(6-fluoro-2-phenylimidazo[1,2-*a*]pyridin-3-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide (3p). White solid, mp 220-221 ^{o}C; ^{1}H NMR (400 MHz; $CDCl_3$): δ = 7.26 (d, J =7.6, 1H), 7.36 (d, J = 7.2, 3H), 7.68 (q, J =4.8, 1H), 7.92-8.00 (m, 7H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 110.3, 110.7, 118.7, 118.8, 119.0, 121.8, 126.2, 126.3, 127.4,

128.6, 129.0, 131.8, 134.9, 136.0, 138.0, 142.8, 147.6, 154.9 (d, J = 238 Hz), 157.9. HRMS (ESI-TOF) Calcd for $C_{20}H_{13}FN_3O_3S$, $[M+H]^+$ 394.0664; Found 394.0668. IR (KBr, cm-1): 3092, 1746, 1339, 1185, 1177, 503.

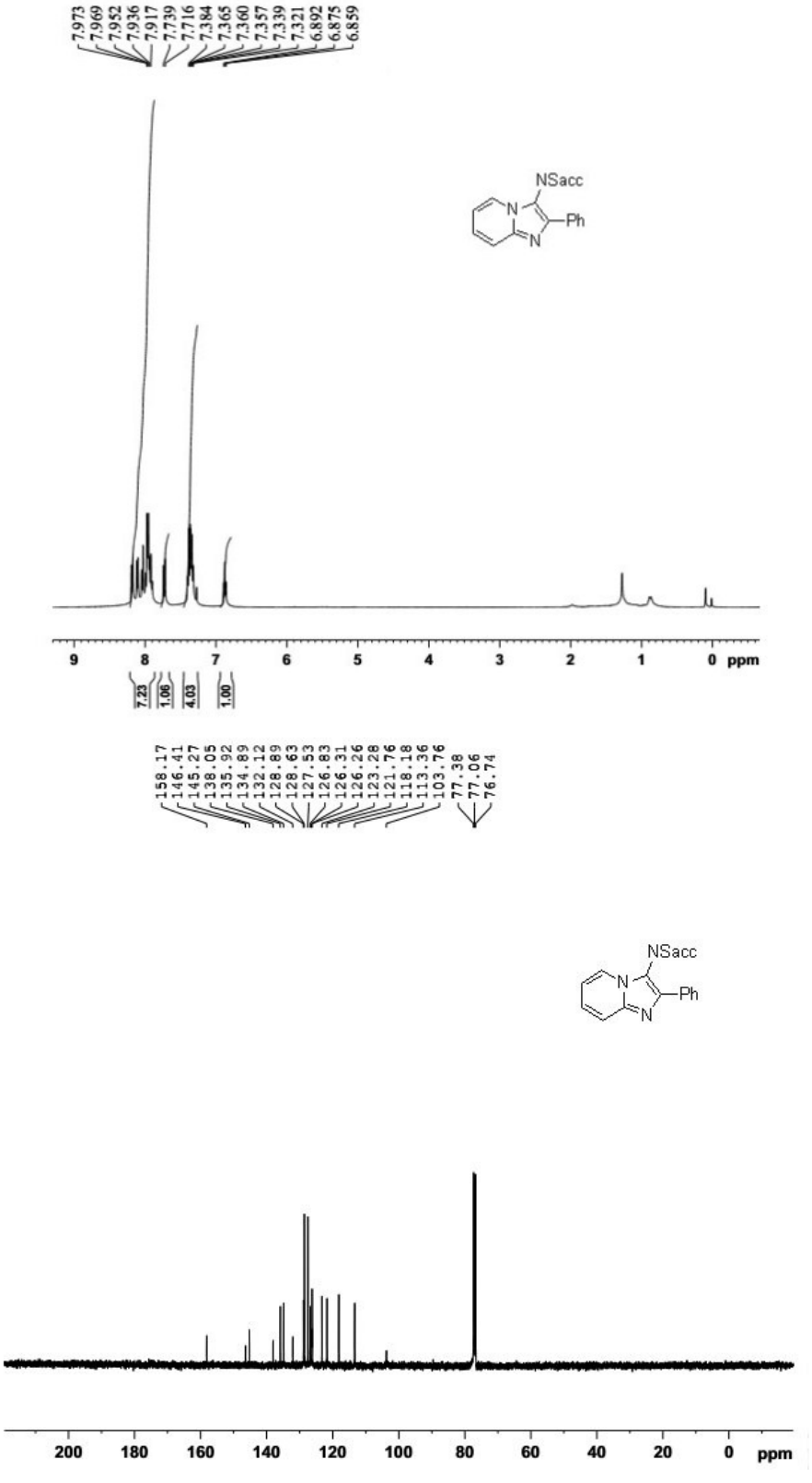
2-(7-methyl-2-phenylimidazo[1,2-*a*]pyridin-3-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide (3q). White solid, mp 242-243 ^oC; ^1H NMR (400 MHz; $CDCl_3$): δ = 2.45 (s, 3H), 6.71 (d, J = 6.8, 1H), 7.33 (q, J =7.6, 3H), 7.49 (s, 1H), 7.92-7.97 (m, 6H), 8.01 (d, J = 7.2, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 21.4, 115.9, 116.6, 121.7, 122.4, 126.3, 127.4, 128.5, 128.7, 132.2, 134.8, 135.8, 138.0, 145.6, 158.2. HRMS (ESI-TOF) Calcd for Calcd for $C_{21}H_{16}N_3O_3S$, $[M+H]^+$ 390.0913; Found 390.0906. IR (KBr, cm-1): 3087, 1758, 1339, 1185, 586.

2-(8-methyl-2-phenylimidazo[1,2-*a*]pyridin-3-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide (3r). White solid, mp 52-53 ^oC; ^1H NMR (400 MHz; $CDCl_3$): δ = 2.72 (s, 3H), 6.80 (s, 1H), 7.13 (q, J=7.2, 1H), 7.35 (q, J=7.6, 3H), 7.94-8.04 (m, 6H), 8.19 (d, J = 7.6, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 22.6, 103.9, 113.3, 121.0, 121.7, 125.4, 126.2, 126.4, 127.7, 128.2, 128.5, 128.6, 132.3, 134.8, 135.8, 138.1, 145.5, 146.1, 158.2. HRMS (ESI-TOF) Calcd for $C_{21}H_{16}N_3O_3S$, $[M+H]^+$ 390.0913; Found 390.0909. IR (KBr, cm-1): 3055, 1741, 1342, 743, 582.

2-(7-chloroimidazo[1,2-*a*]pyridin-3-yl)benzo[*d*]isothiazol-3(2*H*)-one 1,1-dioxide (3t). White solid, mp 164-165 ^oC; ^1H NMR (400 MHz; $CDCl_3$): δ = 6.89 (dd, J_1 =1.6, J_2=7.6, 1H), 7.72 (d, J =1.2, 1H), 7.89 (s, 1H), 7.96-7.98 (s, 4H), 8.02 (d, J = 7.26, 1H). ^{13}C NMR (100 MHz; $CDCl_3$): δ = 115.3, 117.5, 121.8, 123.3, 126.1, 126.3, 133.2, 134.9, 135.5, 135.9, 137.9, 158.0. HRMS (ESI-TOF) Calcd for $C_{14}H_9ClN_3O_3S$, $[M+H]^+$ 334.0057; Found 334.0053. IR (KBr, cm-1): 3078, 17504, 13446, 1175, 578.

V. ^{1}H NMR and ^{13}C NMR spectra copies of compounds 3

Compound **3a**



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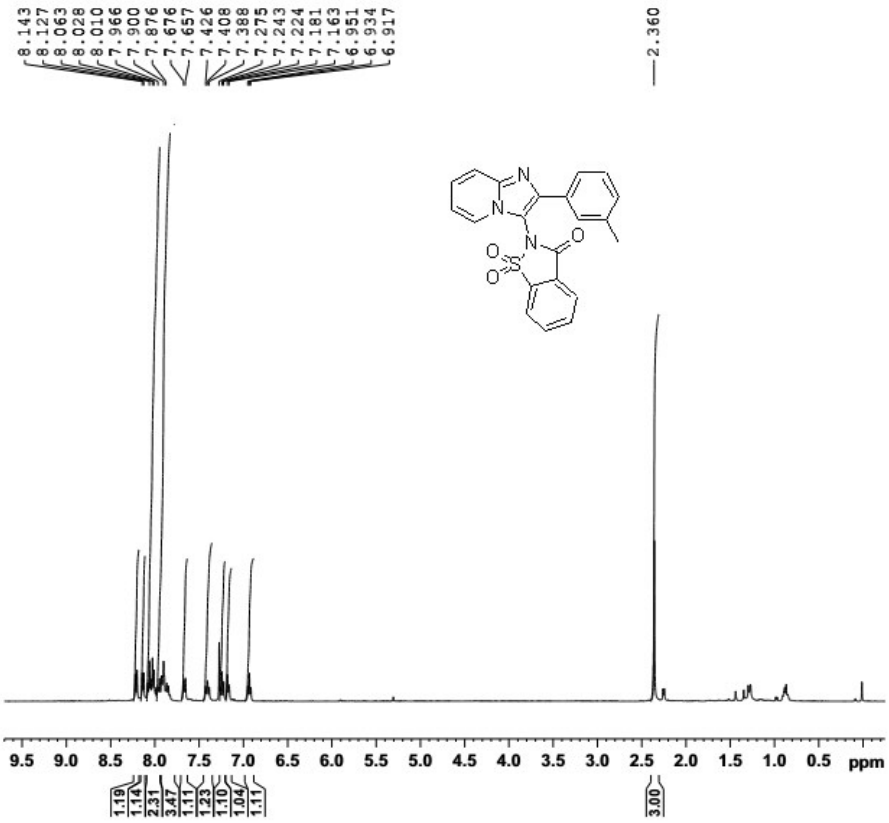
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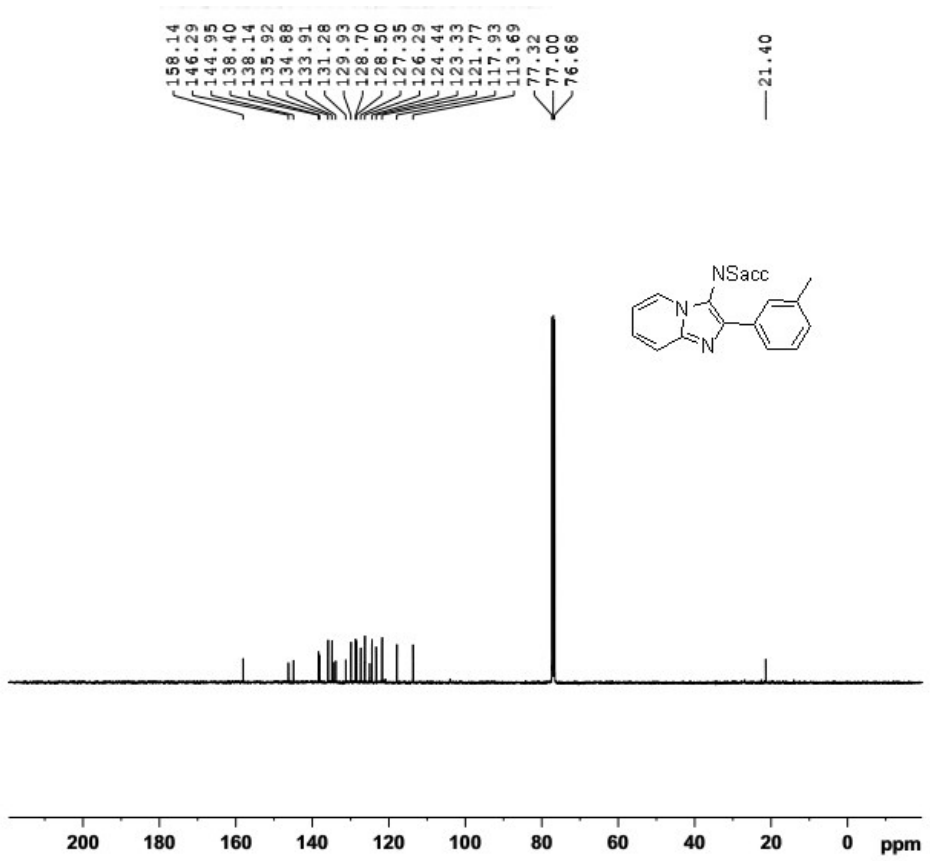
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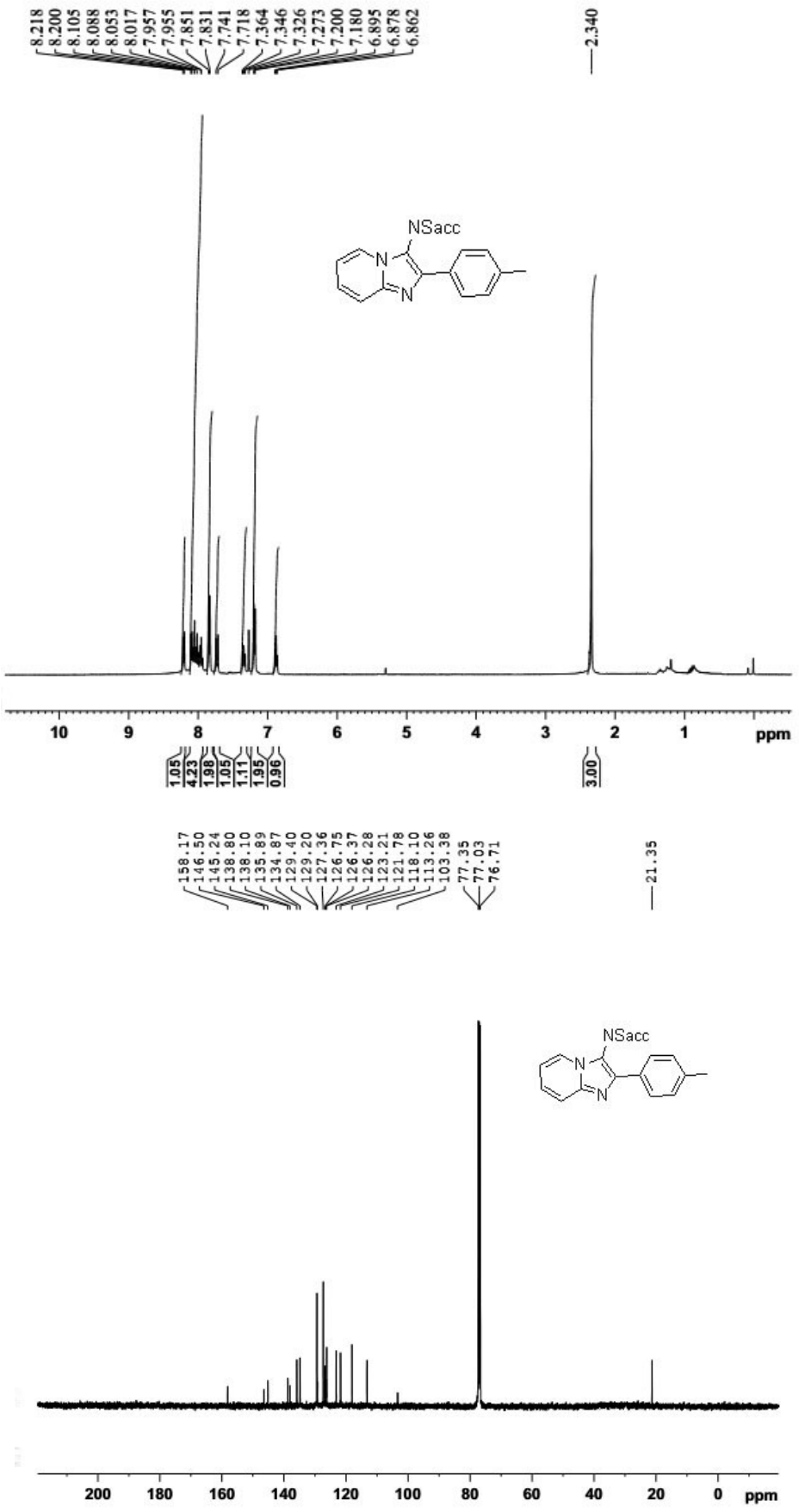
Compound **3c**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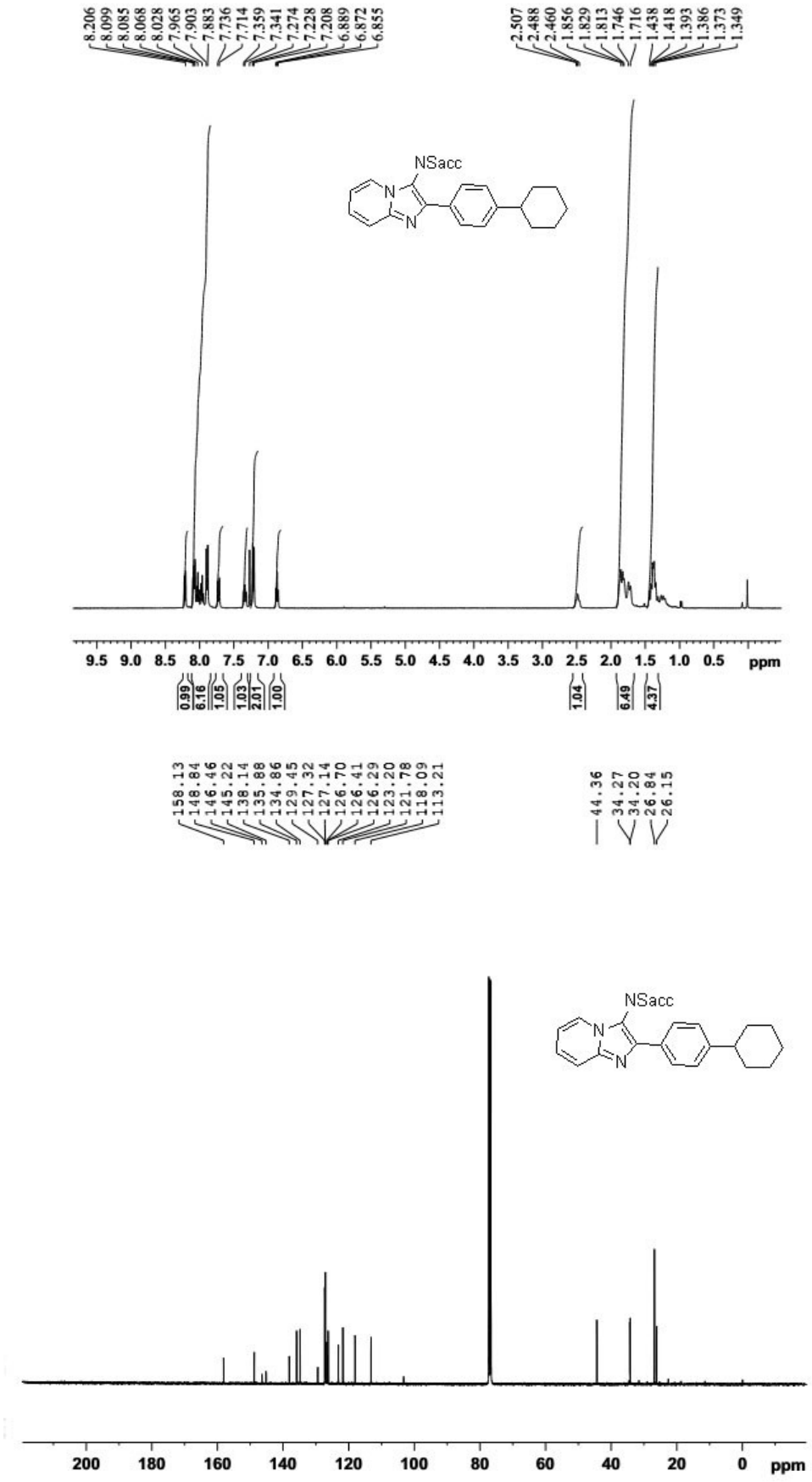
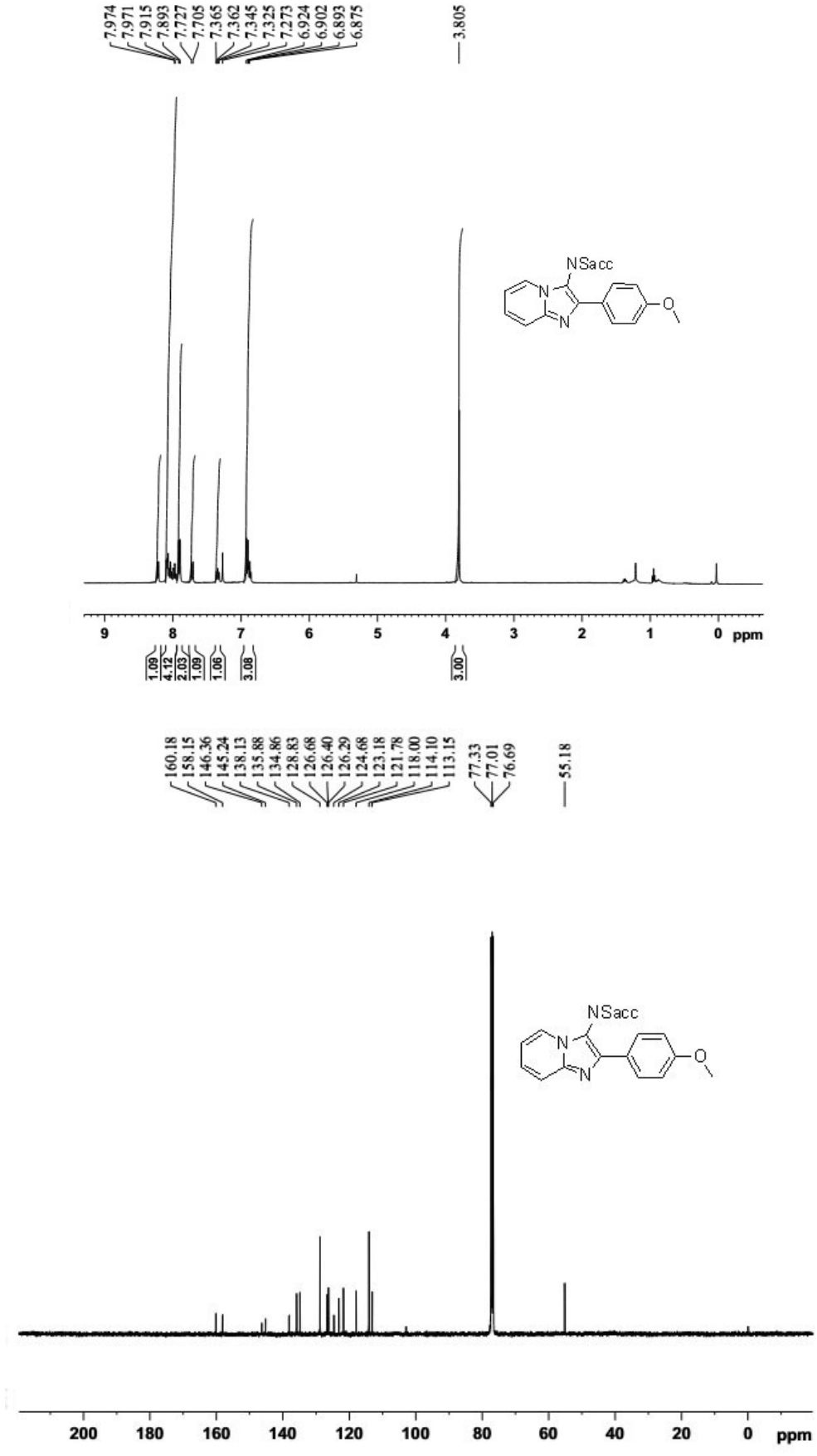
77.35
77.03
76.71
21.35
NSacc
200
180
160
140
120
100
80
60
40
20
0
ppm

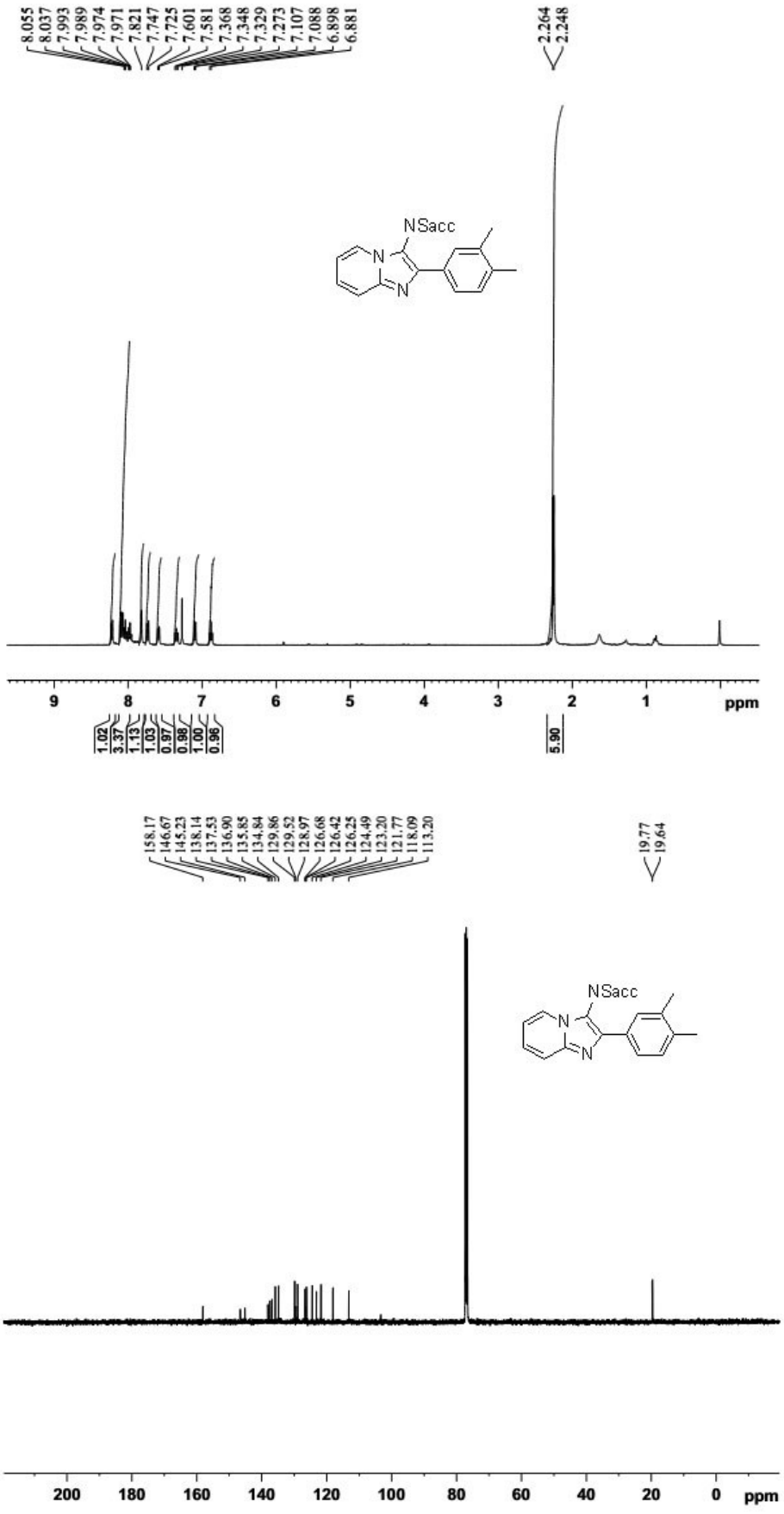
Compound **3d**


8.206
8.099
8.085
8.068
8.028
7.965
7.903
7.883
7.736
7.714
7.359
7.341
7.274
7.228
7.208
6.889
6.872
6.855
2.507
2.488
2.460
1.856
1.829
1.813
1.746
1.716
1.438
1.418
1.393
1.386
1.373
1.349
NSacc
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 ppm
0.99
6.16
1.05
1.03
2.01
1.00
1.04
6.49
4.37
158.13
148.84
146.46
145.22
138.14
135.88
134.86
129.45
127.32
127.14
126.70
126.41
126.29
123.20
121.78
118.09
113.21
44.36
34.27
34.20
26.84
26.15
NSacc
200 180 160 140 120 100 80 60 40 20 0 ppm

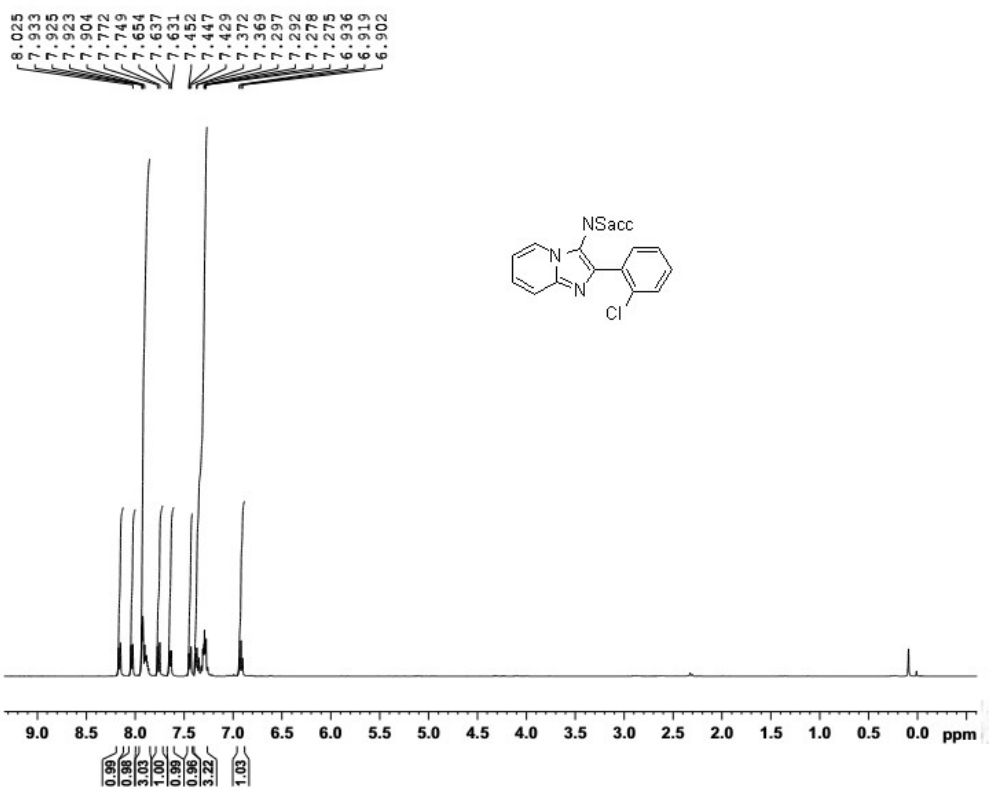
Compound **3e**

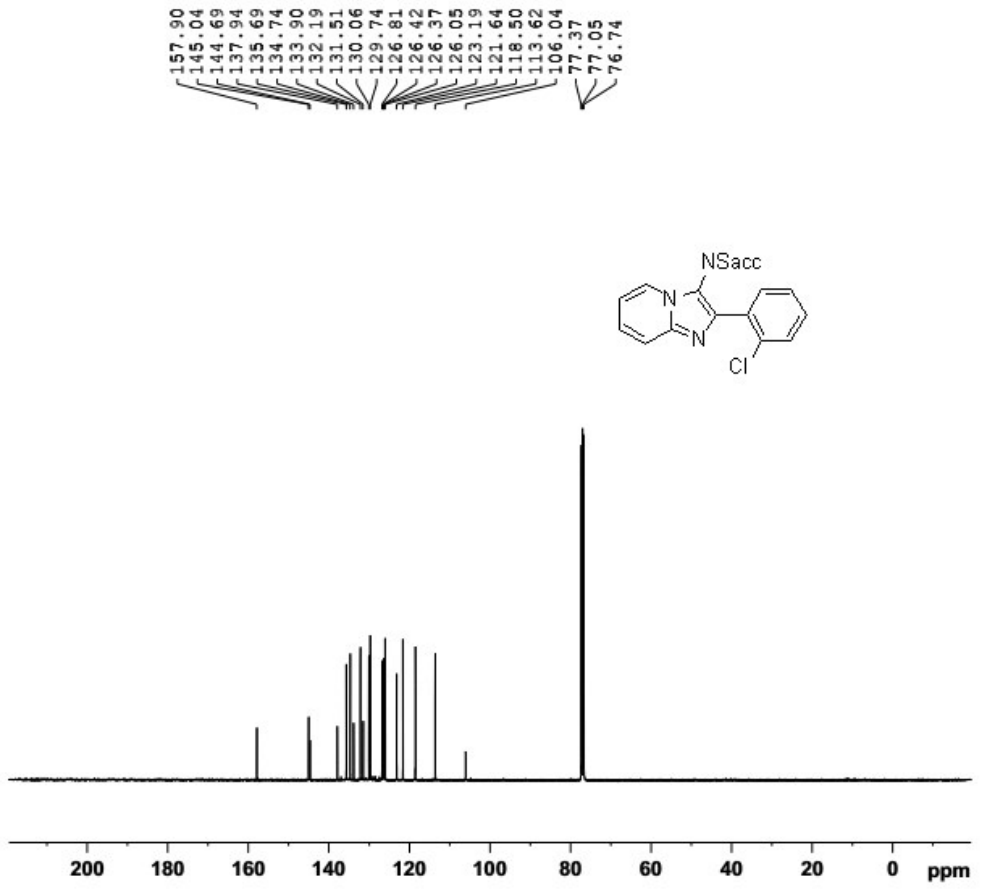

7.974
7.971
7.915
7.893
7.727
7.705
7.365
7.362
7.345
7.325
7.273
6.924
6.902
6.893
6.875
3.805
NSacc
O
9
8
7
6
5
4
3
2
1
0
ppm
1.09
4.12
2.03
1.09
1.06
3.08
3.00
160.18
158.15
146.36
145.24
138.13
135.88
134.86
128.83
126.68
126.40
126.29
124.68
123.18
121.78
118.00
114.10
113.15
77.33
77.01
76.69
55.18
NSacc
O
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound **3f**

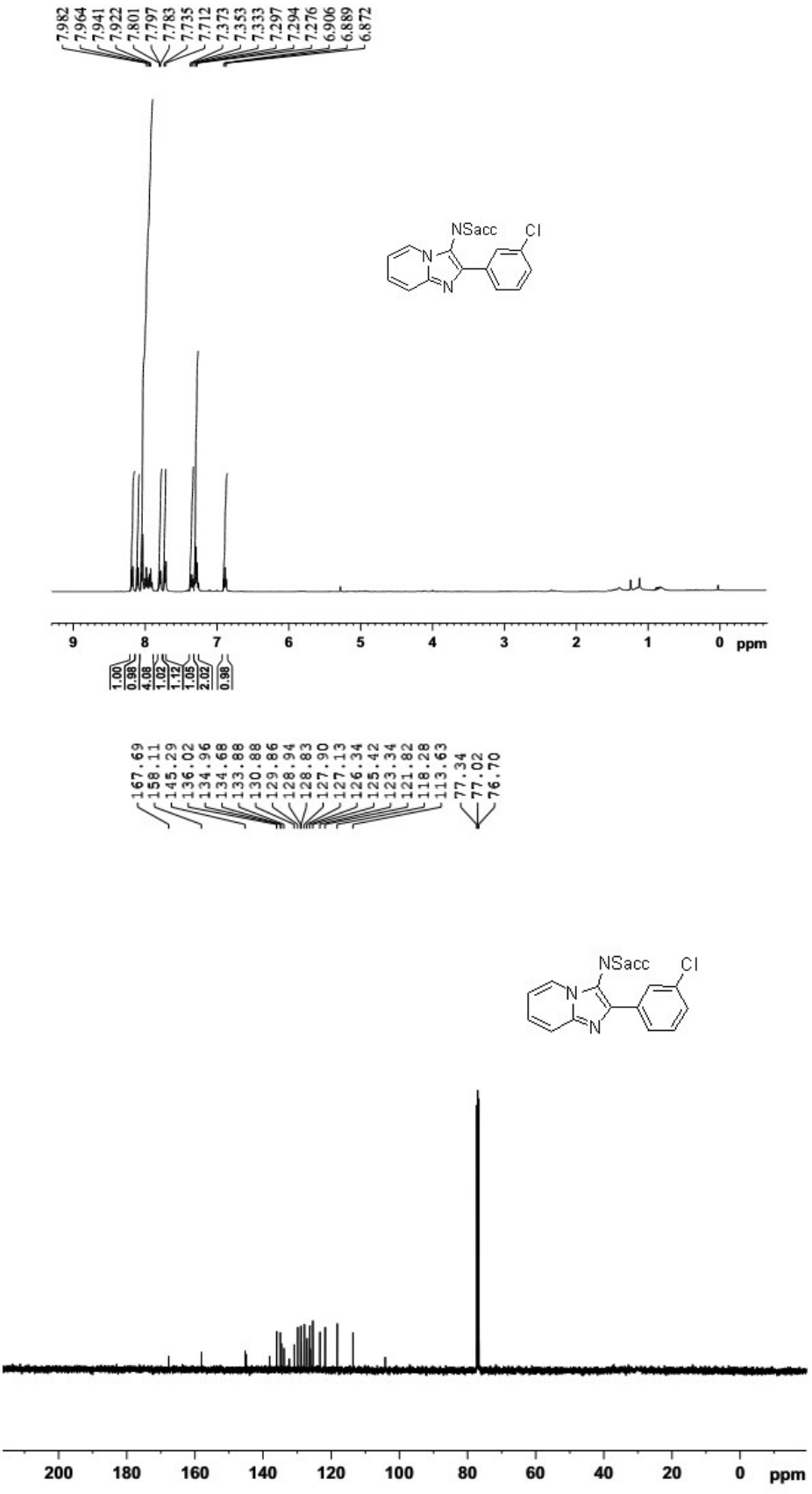

8.055
8.037
7.993
7.989
7.974
7.971
7.821
7.747
7.725
7.601
7.581
7.368
7.348
7.329
7.273
7.107
7.088
6.898
6.881
2.264
2.248
NSacc
N
N
9
8
7
6
5
4
3
2
1
ppm
1.02
3.37
1.13
1.03
0.97
0.88
1.00
0.96
5.90
158.17
146.67
145.23
138.14
137.53
136.90
135.85
134.84
129.86
129.52
128.97
126.68
126.42
126.25
124.49
123.20
121.77
118.09
113.20
19.77
19.64
NSacc
N
N
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound **3g**

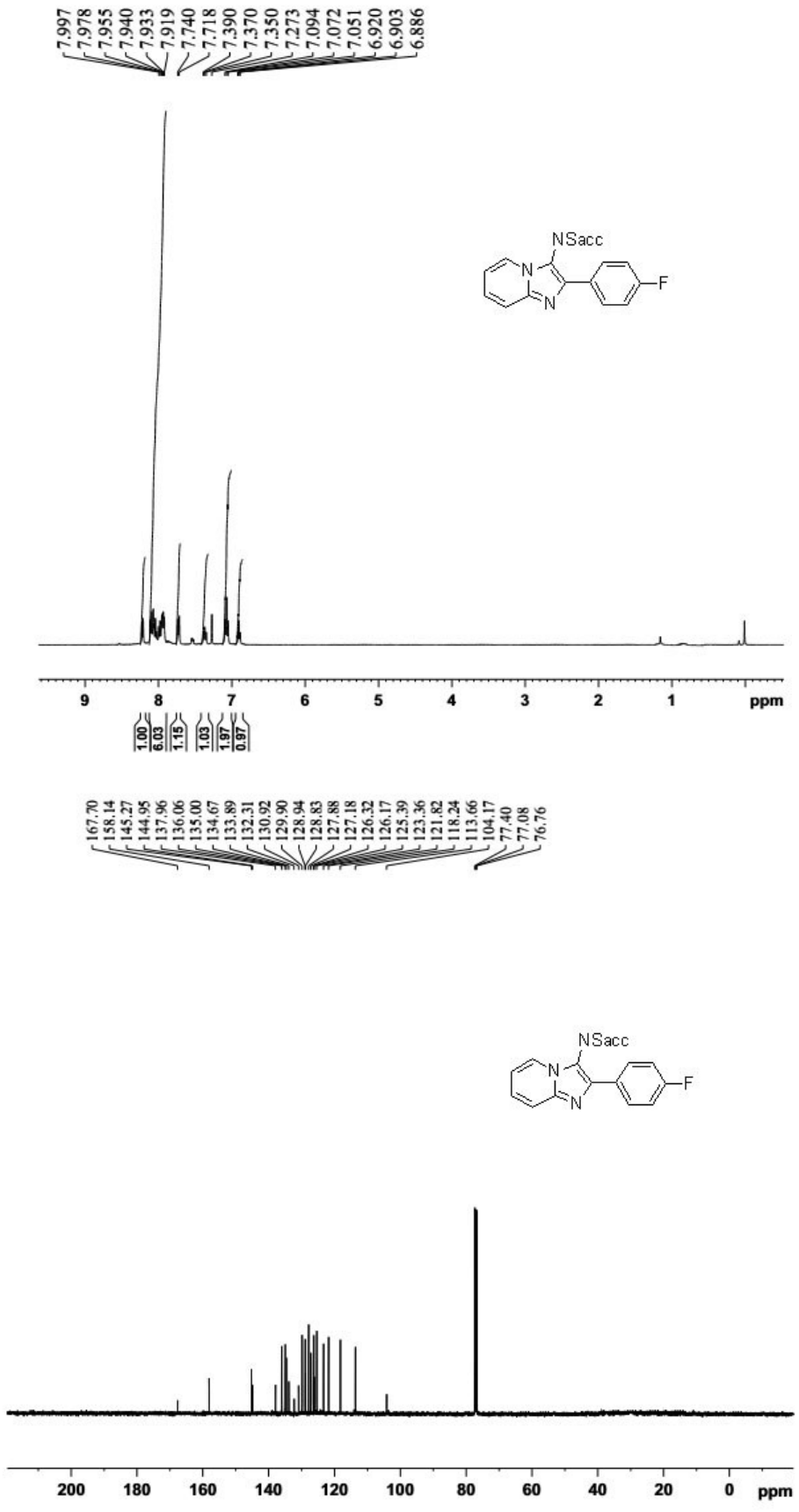

8.025
7.933
7.925
7.923
7.904
7.772
7.749
7.654
7.637
7.631
7.452
7.447
7.429
7.372
7.369
7.297
7.292
7.278
7.275
6.936
6.919
6.902
NSacc
Cl
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.99
0.98
3.03
1.00
0.99
0.96
3.22
1.03


157.90
145.04
144.69
137.94
135.69
134.74
133.90
132.19
131.51
130.06
129.74
126.81
126.42
126.37
126.05
123.19
121.64
118.50
113.62
106.04
77.37
77.05
76.74
NSacc
Cl
200 180 160 140 120 100 80 60 40 20 0 ppm

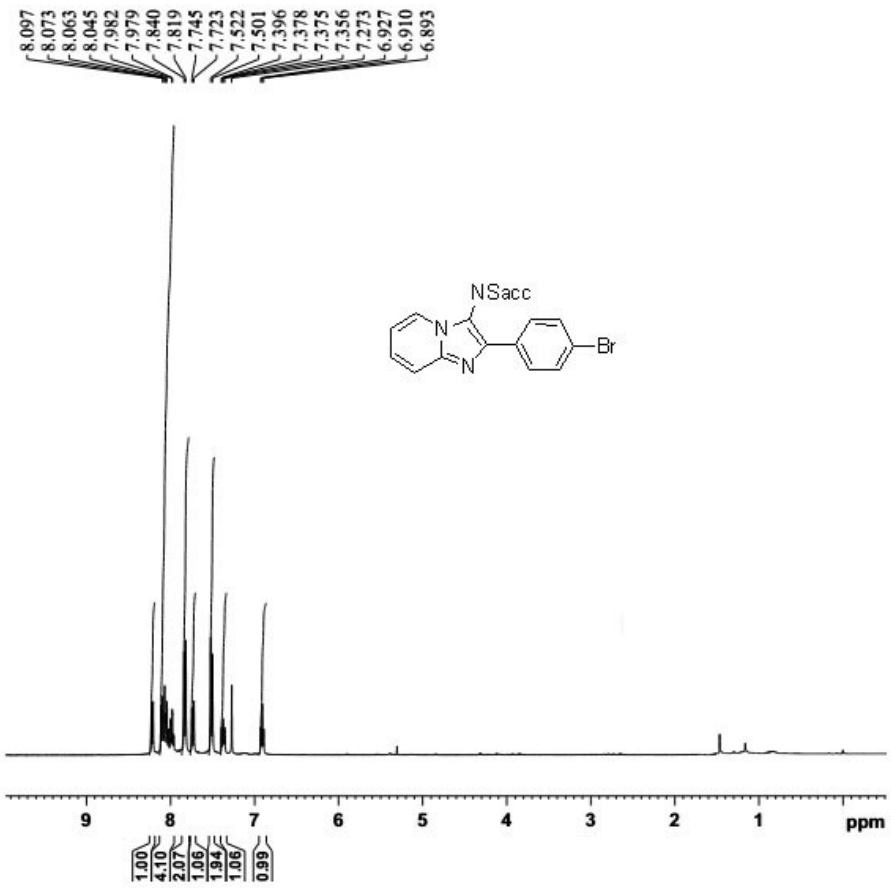
Compound **3h**

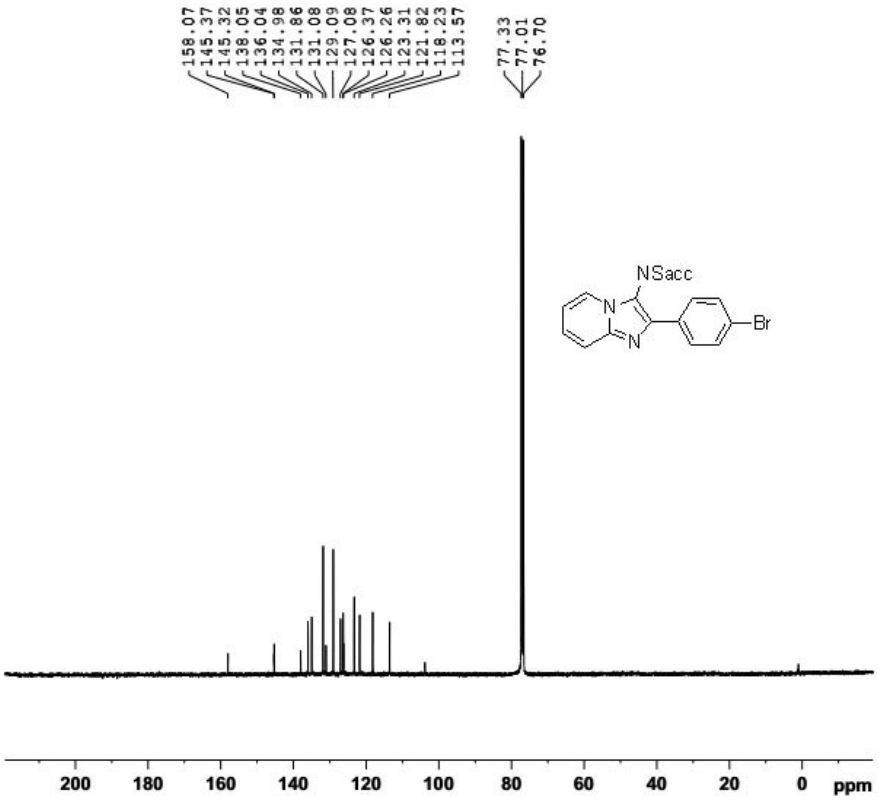

7.982
7.964
7.941
7.922
7.801
7.797
7.783
7.735
7.712
7.373
7.353
7.333
7.297
7.294
7.276
6.906
6.889
6.872
NSacc
Cl
N
N
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.98
4.08
1.02
1.12
1.05
2.02
0.98
167.69
158.11
145.29
136.02
134.96
134.68
133.88
130.88
129.86
128.94
128.83
127.90
127.13
126.34
125.42
123.34
121.82
118.28
113.63
77.34
77.02
76.70
NSacc
Cl
N
N
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound **3i**

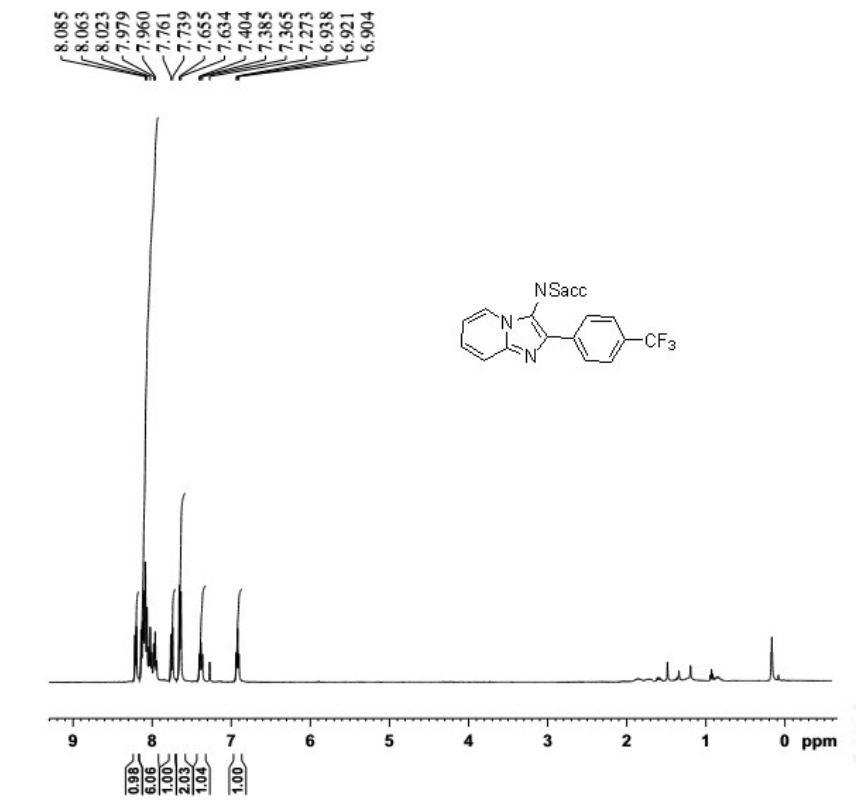

7.997
7.978
7.955
7.940
7.933
7.919
7.740
7.718
7.390
7.370
7.350
7.273
7.094
7.072
7.051
6.920
6.903
6.886
NSacc
N
N
F
9
8
7
6
5
4
3
2
1
ppm
1.00
6.03
1.15
1.03
1.97
0.97
167.70
158.14
145.27
144.95
137.96
136.06
135.00
134.67
133.89
132.31
130.92
129.90
128.94
128.83
127.88
127.18
126.32
126.17
125.39
123.36
121.82
118.24
113.66
104.17
77.40
77.08
76.76
NSacc
N
N
F
200
180
160
140
120
100
80
60
40
20
0
ppm

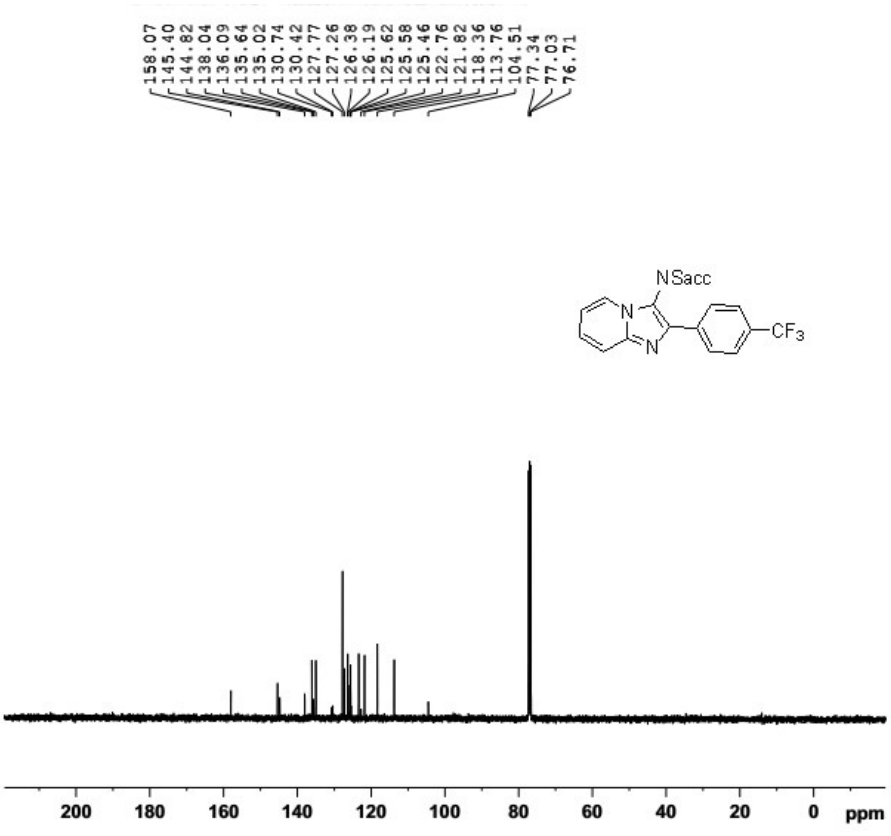
Compound **3j**


8.097
8.073
8.063
8.045
7.982
7.979
7.840
7.819
7.745
7.723
7.522
7.501
7.396
7.378
7.375
7.356
7.273
6.927
6.910
6.893
NSacc
N
N
Br
9
8
7
6
5
4
3
2
1
ppm
1.00
4.10
2.07
1.06
1.94
1.06
0.99

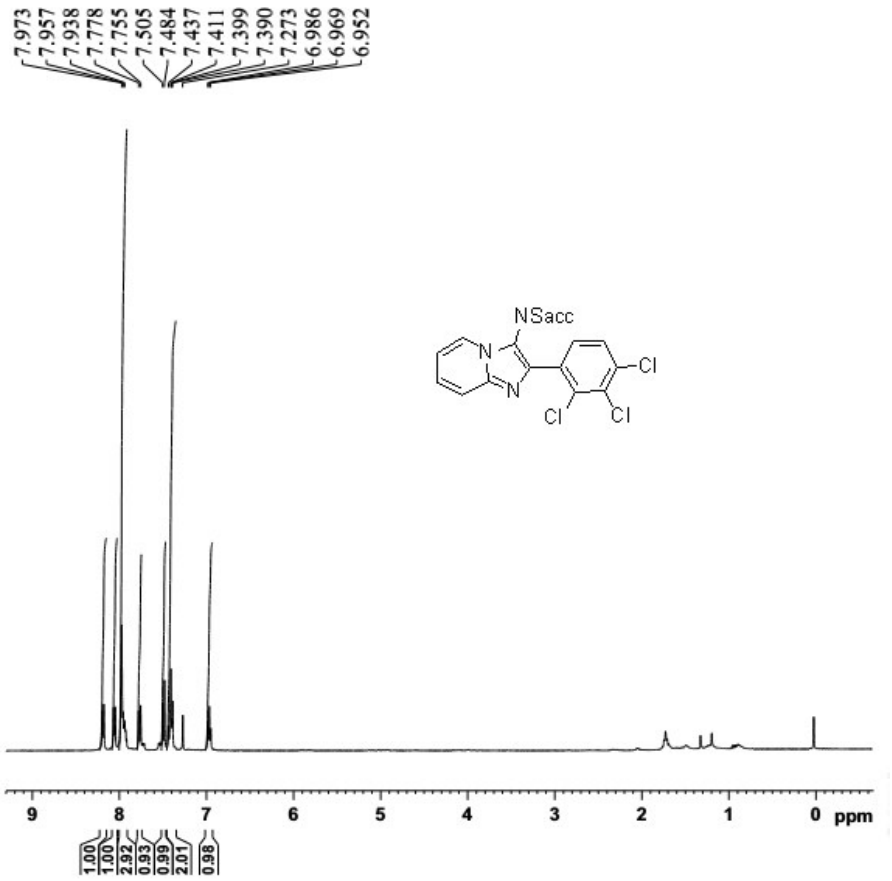

158.07
145.37
145.32
138.05
136.04
134.98
131.86
131.08
129.09
127.08
126.37
126.26
123.31
121.82
118.23
113.57
77.33
77.01
76.70
NSacc
N
N
Br
200
180
160
140
120
100
80
60
40
20
0
ppm

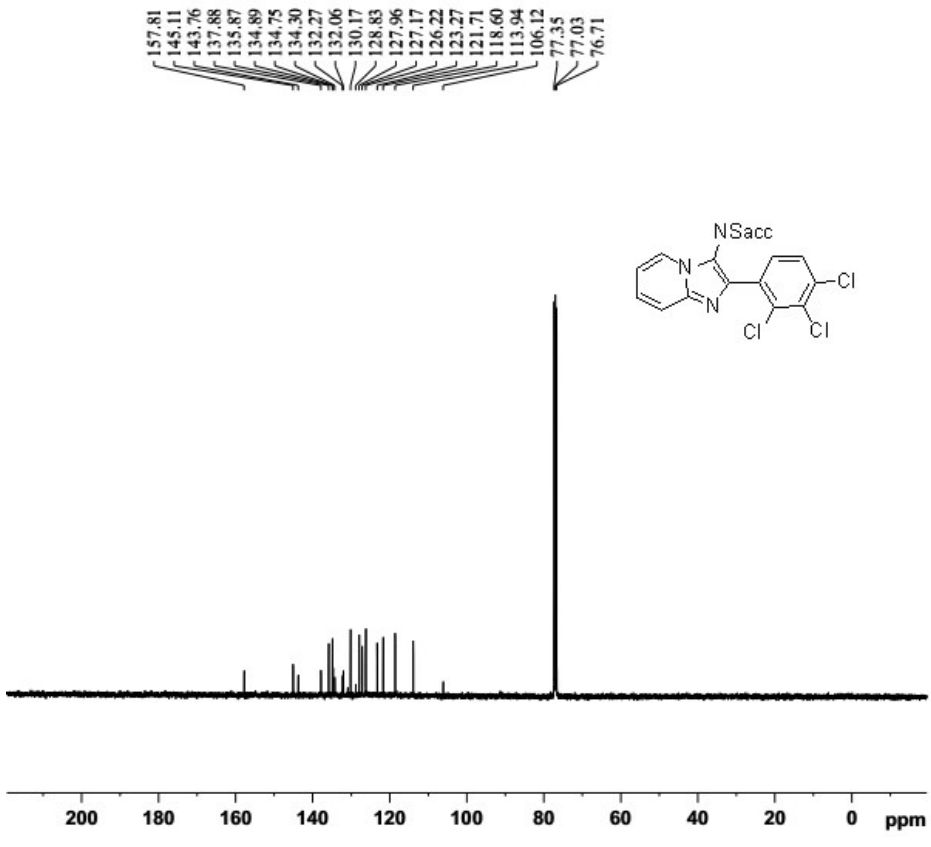
Compound **3k**


8.085
8.063
8.023
7.979
7.960
7.761
7.739
7.655
7.634
7.404
7.385
7.365
7.273
6.938
6.921
6.904
NSacc
N
N
CF3
9
8
7
6
5
4
3
2
1
0 ppm
0.98
6.06
1.00
2.03
1.04
1.00

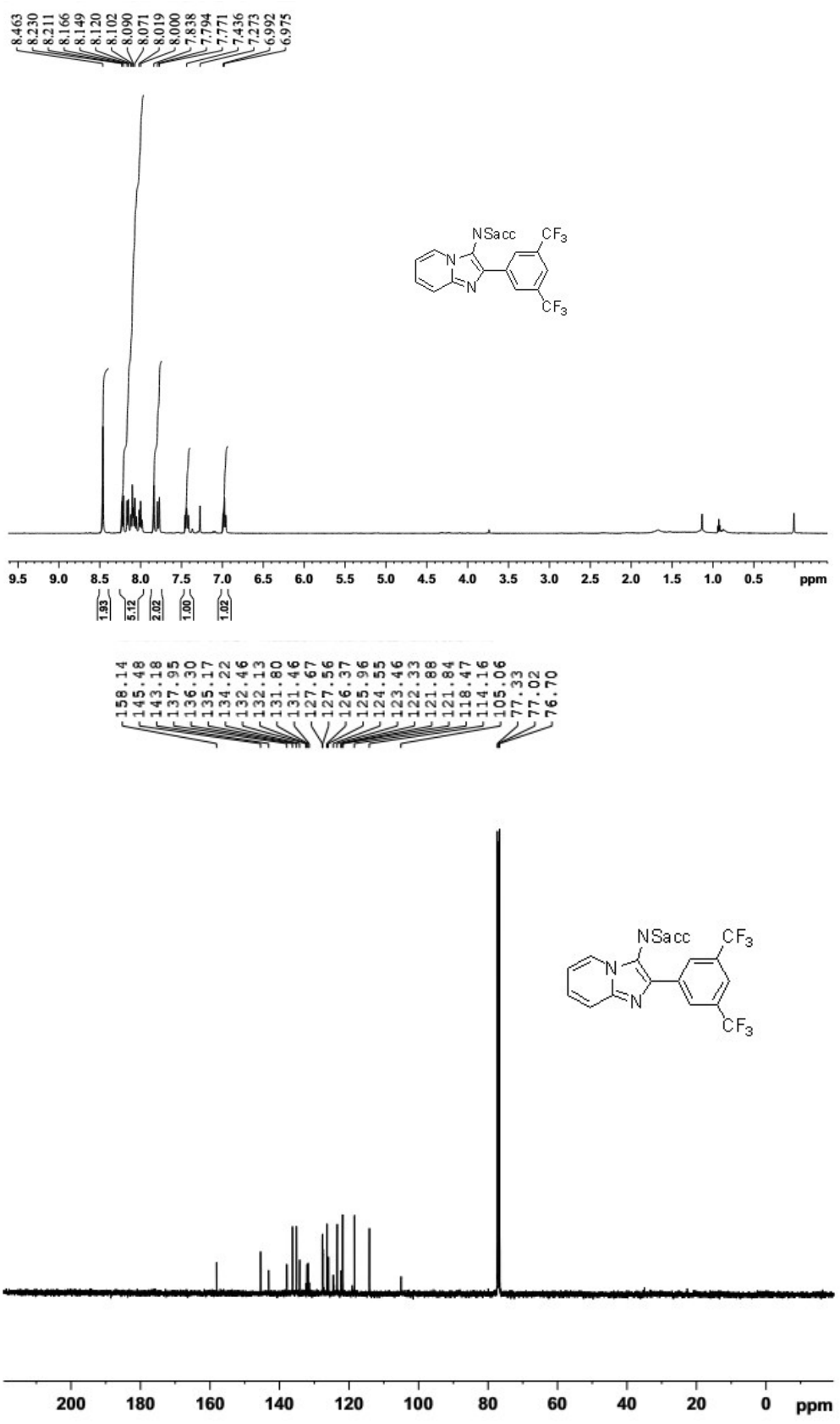

158.07
145.40
144.82
138.04
136.09
135.64
135.02
130.74
130.42
127.77
127.26
126.38
126.19
125.62
125.58
125.46
122.76
121.82
118.36
113.76
104.51
77.34
77.03
76.71
NSacc
N
N
CF3
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound **3l**

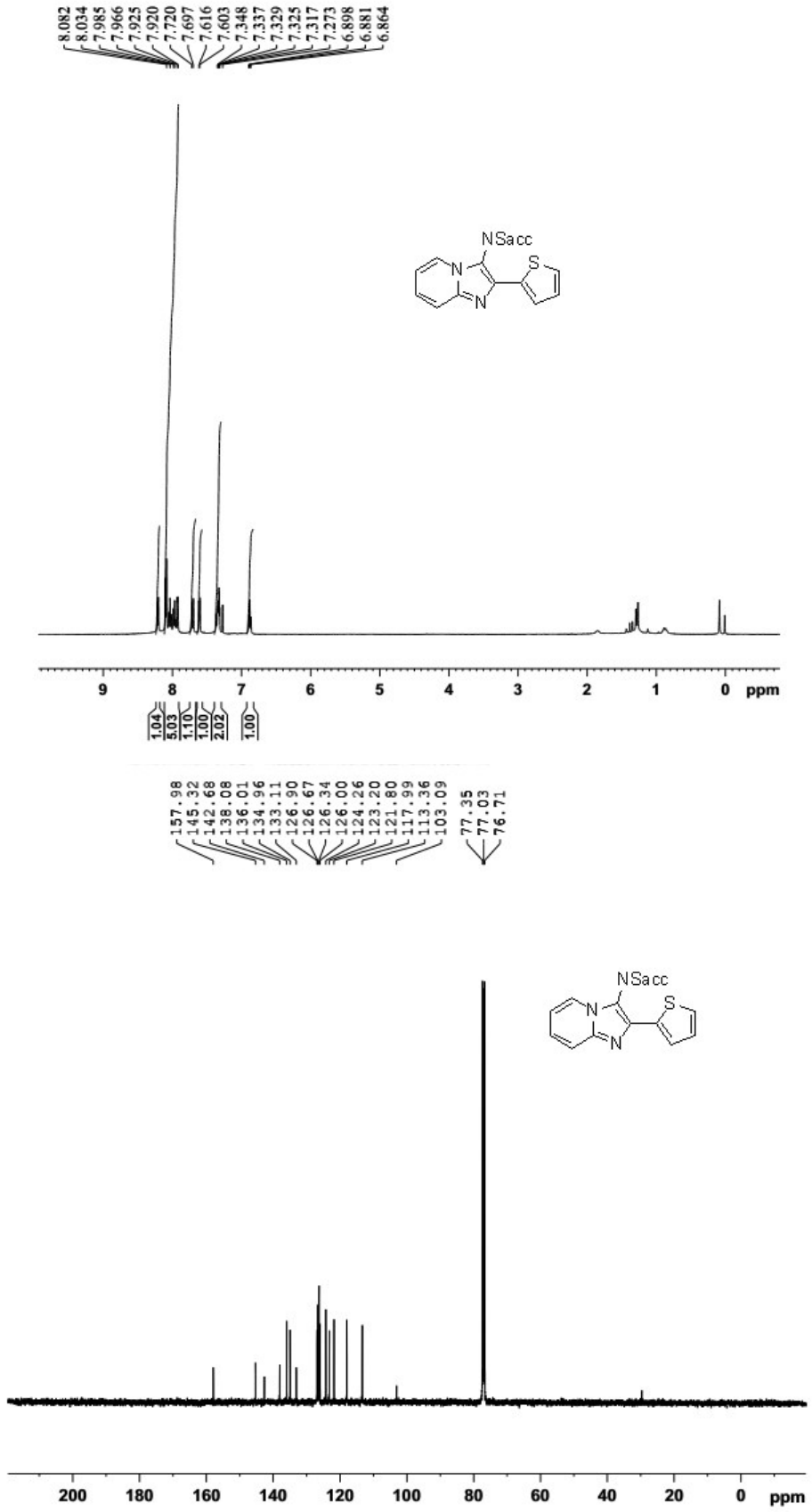

7.973
7.957
7.938
7.778
7.755
7.505
7.484
7.437
7.411
7.399
7.390
7.273
6.986
6.969
6.952
NSacc
Cl
Cl
Cl
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.00
2.92
0.93
0.99
2.01
0.98


157.81
145.11
143.76
137.88
135.87
134.89
134.75
134.30
132.27
132.06
130.17
128.83
127.96
127.17
126.22
123.27
121.71
118.60
113.94
106.12
77.35
77.03
76.71
NSacc
Cl
Cl
Cl
200
180
160
140
120
100
80
60
40
20
0
ppm

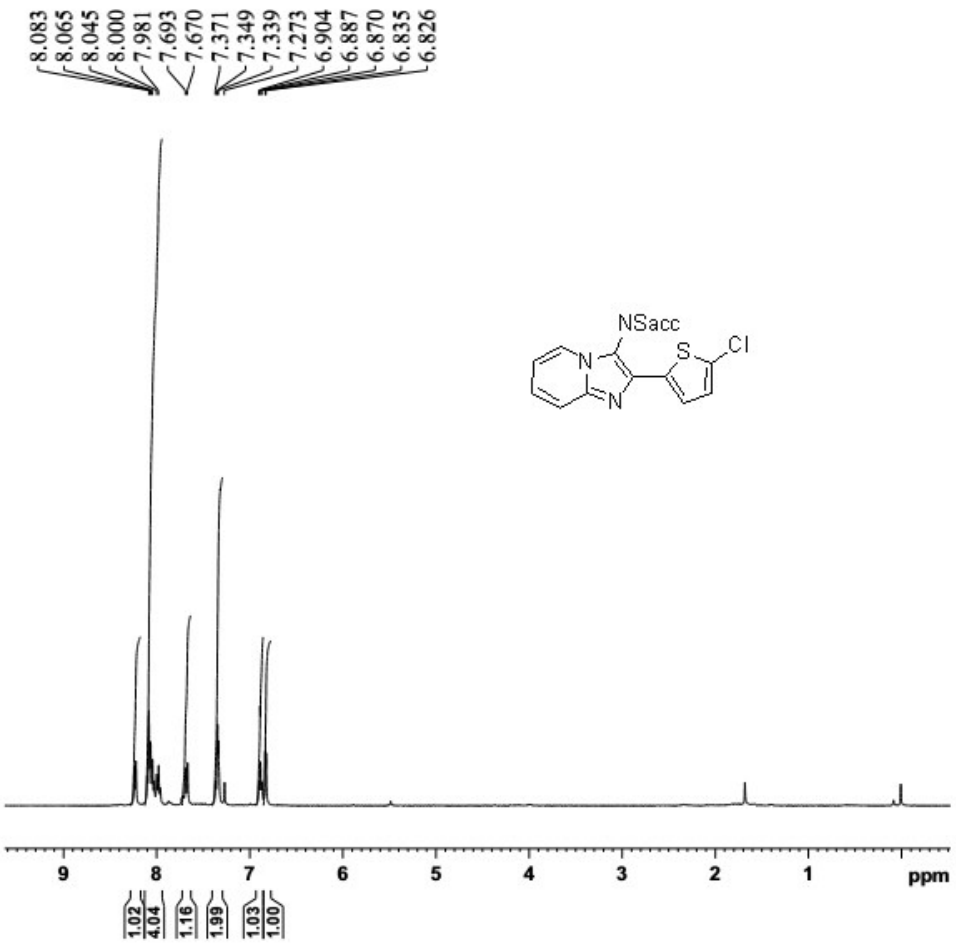
Compound **3m**

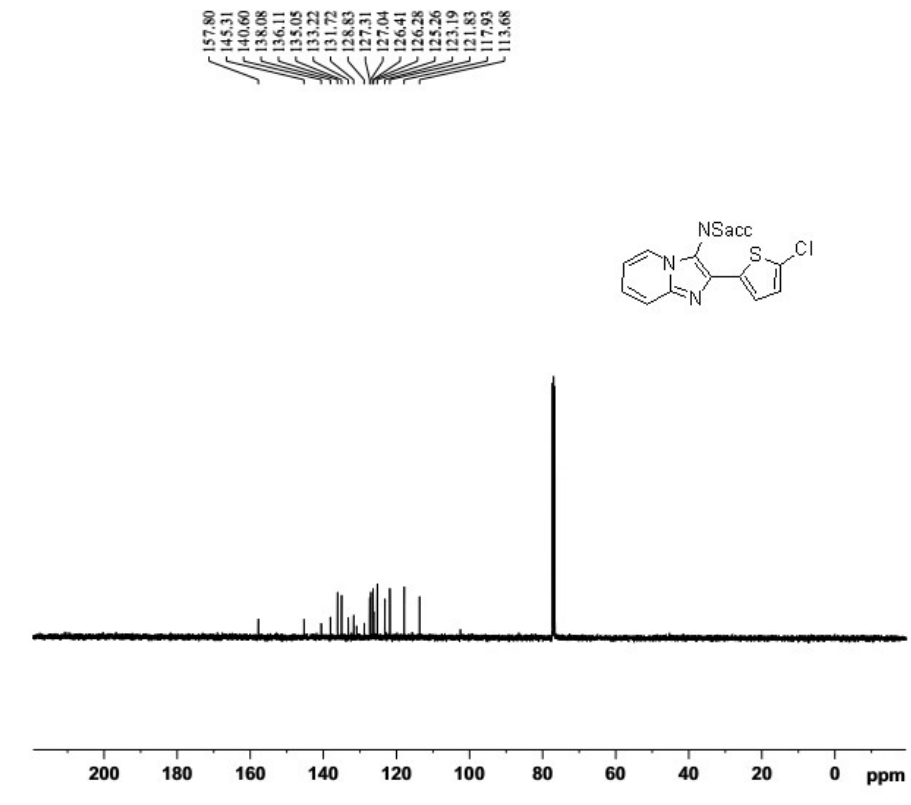

8.463
8.230
8.211
8.166
8.149
8.120
8.102
8.090
8.071
8.019
8.000
7.838
7.794
7.771
7.436
7.273
6.992
6.975
NSacc
CF3
CF3
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.93
5.12
2.02
1.00
1.02
158.14
145.48
143.18
137.95
136.30
135.17
134.22
132.46
132.13
131.80
131.46
127.67
127.56
126.37
125.96
124.55
123.46
122.33
121.88
121.84
118.47
114.16
105.06
77.33
77.02
76.70
NSacc
CF3
CF3
200 180 160 140 120 100 80 60 40 20 0 ppm

Compound **3n**

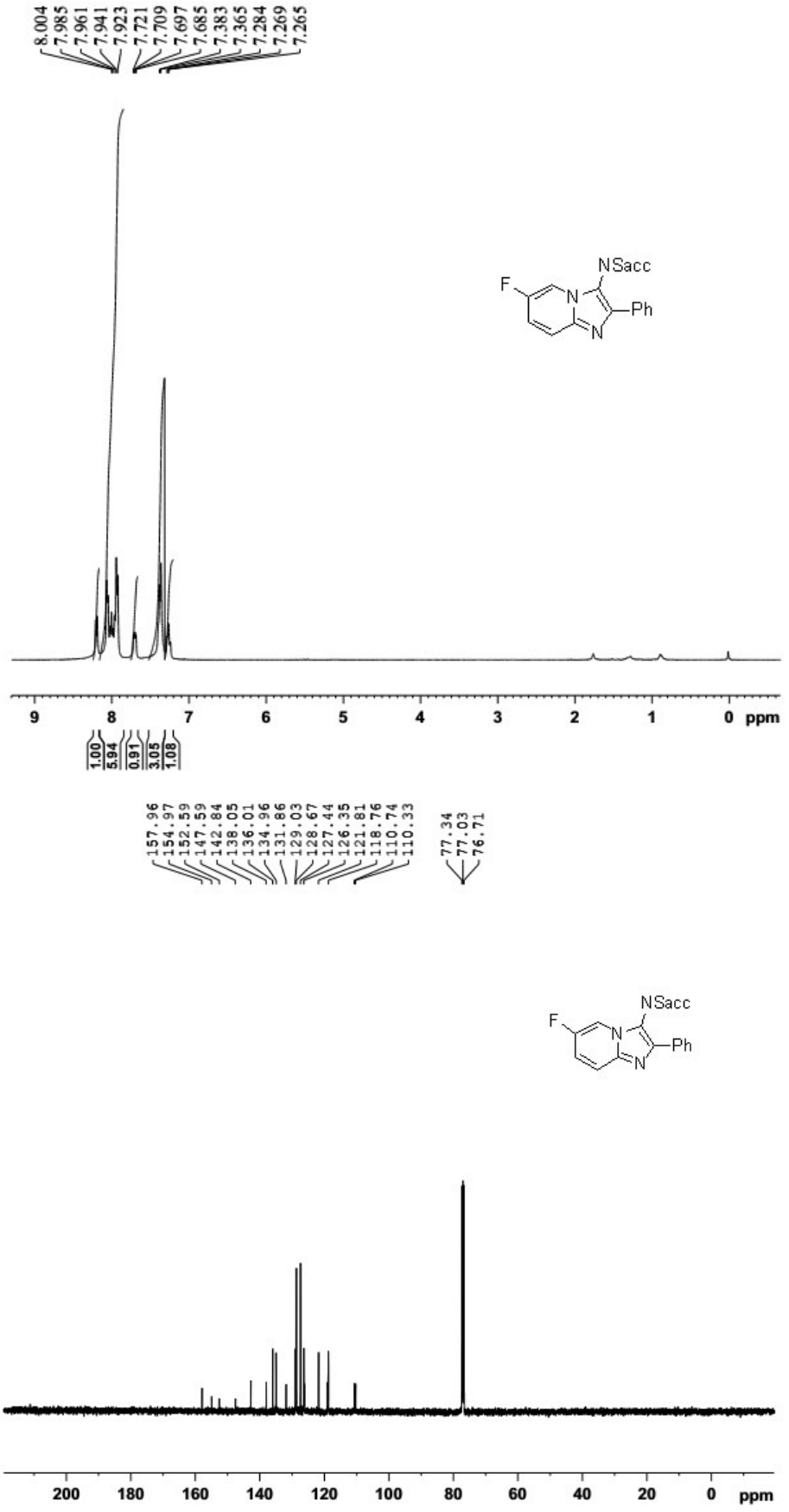


Compound **3o**

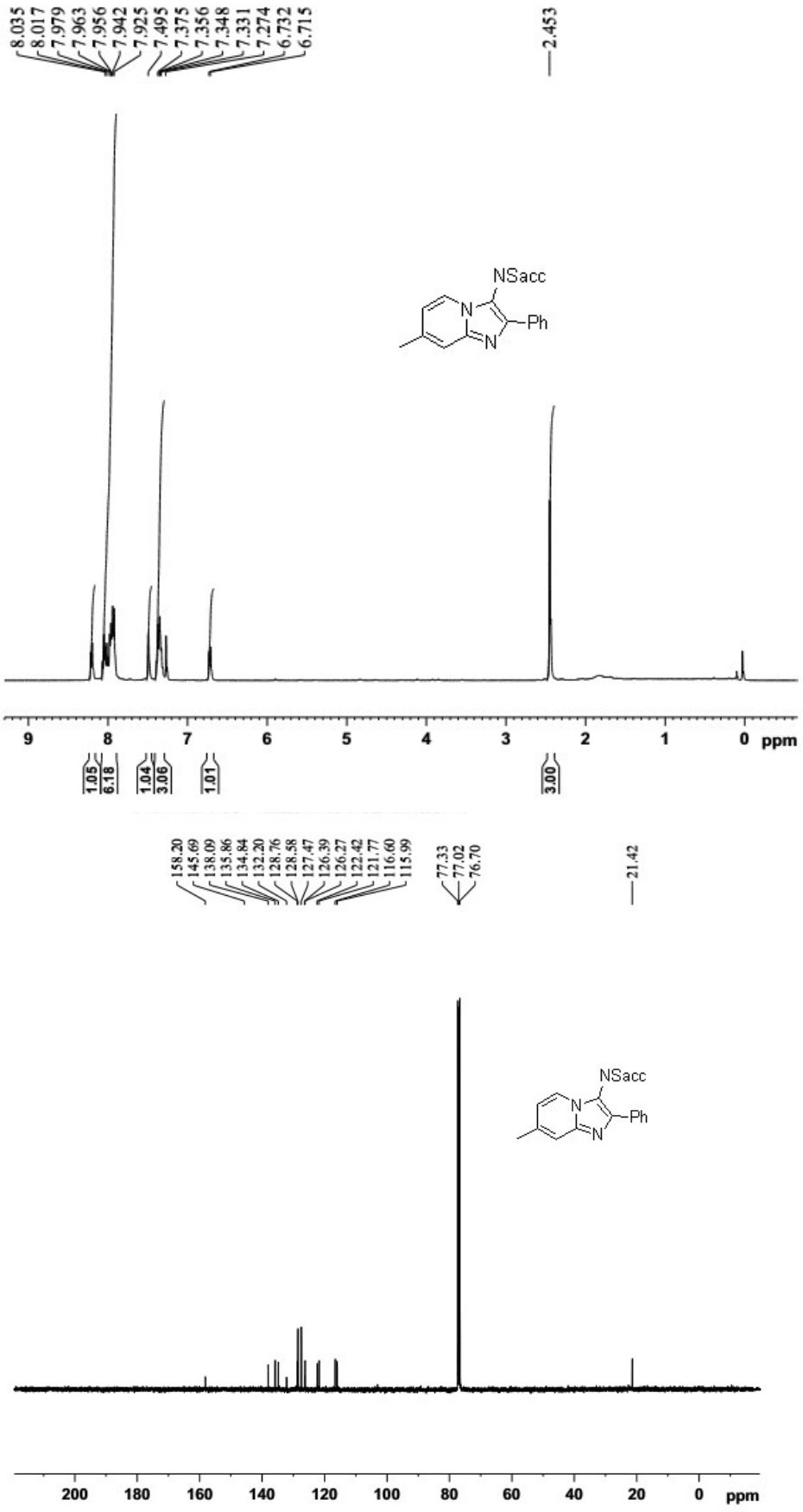

8.083
8.065
8.045
8.000
7.981
7.693
7.670
7.371
7.349
7.339
7.273
6.904
6.887
6.870
6.835
6.826
NSacc
N
S
Cl
N
9
8
7
6
5
4
3
2
1
ppm
1.02
4.04
1.16
1.99
1.03
1.00


157.80
145.31
140.60
138.08
136.11
135.05
133.22
131.72
128.83
127.31
127.04
126.41
126.28
125.26
123.19
121.83
117.93
113.68
NSacc
N
S
Cl
N
200
180
160
140
120
100
80
60
40
20
0
ppm

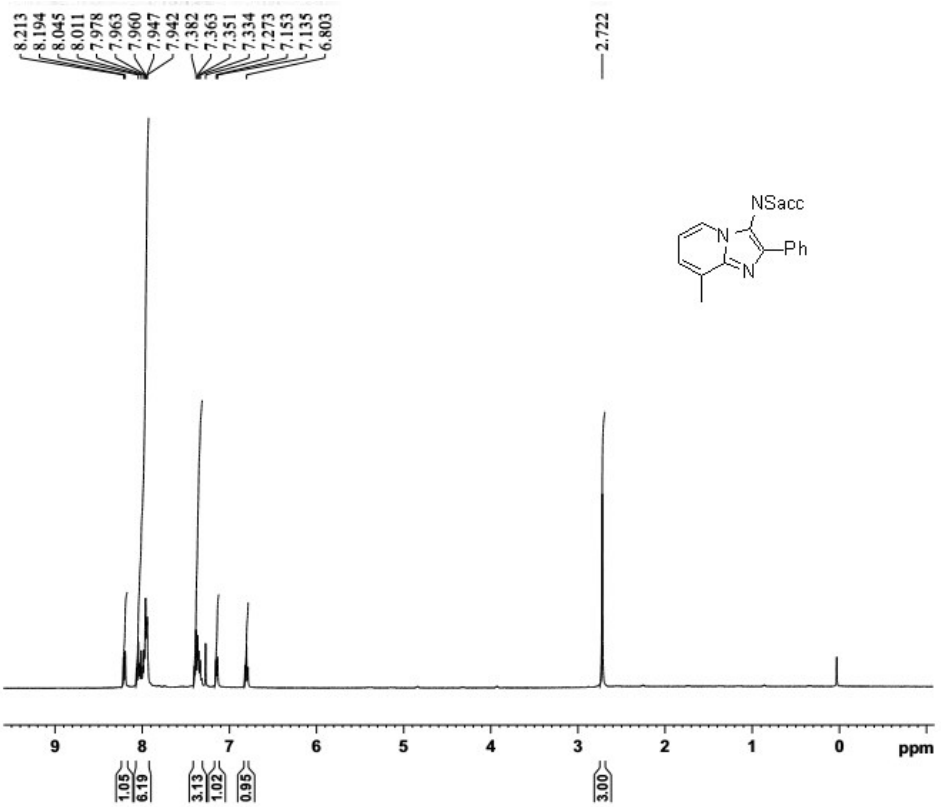
Compound **3p**

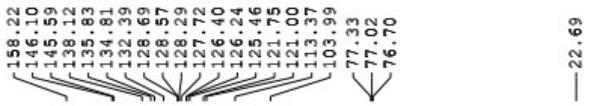

8.004
7.985
7.961
7.941
7.923
7.721
7.709
7.697
7.685
7.383
7.365
7.284
7.269
7.265
NSacc
F
N
Ph
N
9
8
7
6
5
4
3
2
1
0 ppm
1.00
5.94
0.91
3.05
1.08
157.96
154.97
152.59
147.59
142.84
138.05
136.01
134.96
131.86
129.03
128.67
127.44
126.35
121.81
118.76
110.74
110.33
77.34
77.03
76.71
NSacc
F
N
Ph
N
200
180
160
140
120
100
80
60
40
20
0 ppm

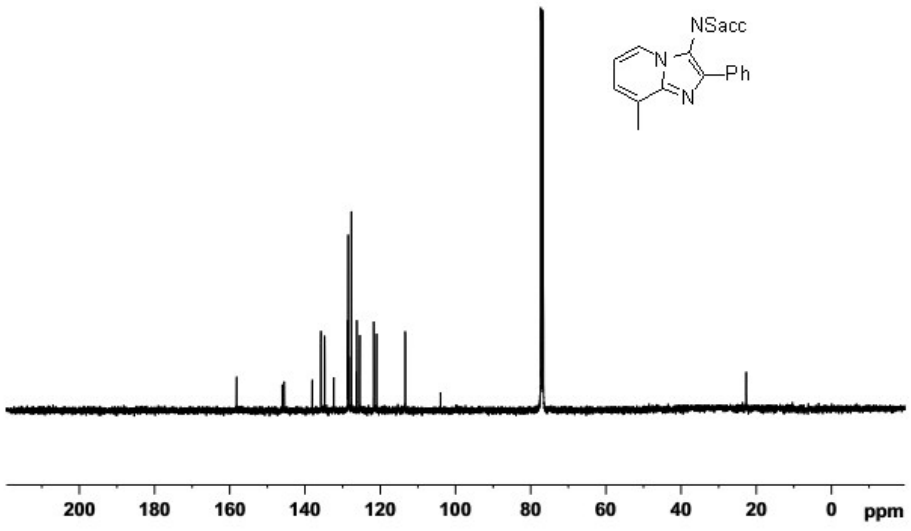
Compound **3q**


8.035
8.017
7.979
7.963
7.956
7.942
7.925
7.495
7.375
7.356
7.348
7.331
7.274
6.732
6.715
2.453
NSacc
Ph
N
N
9
8
7
6
5
4
3
2
1
0
ppm
1.05
6.18
1.04
3.06
1.01
3.00
158.20
145.69
138.09
135.86
134.84
132.20
128.76
128.58
127.47
126.39
126.27
122.42
121.77
116.60
115.99
77.33
77.02
76.70
21.42
NSacc
Ph
N
N
200
180
160
140
120
100
80
60
40
20
0
ppm

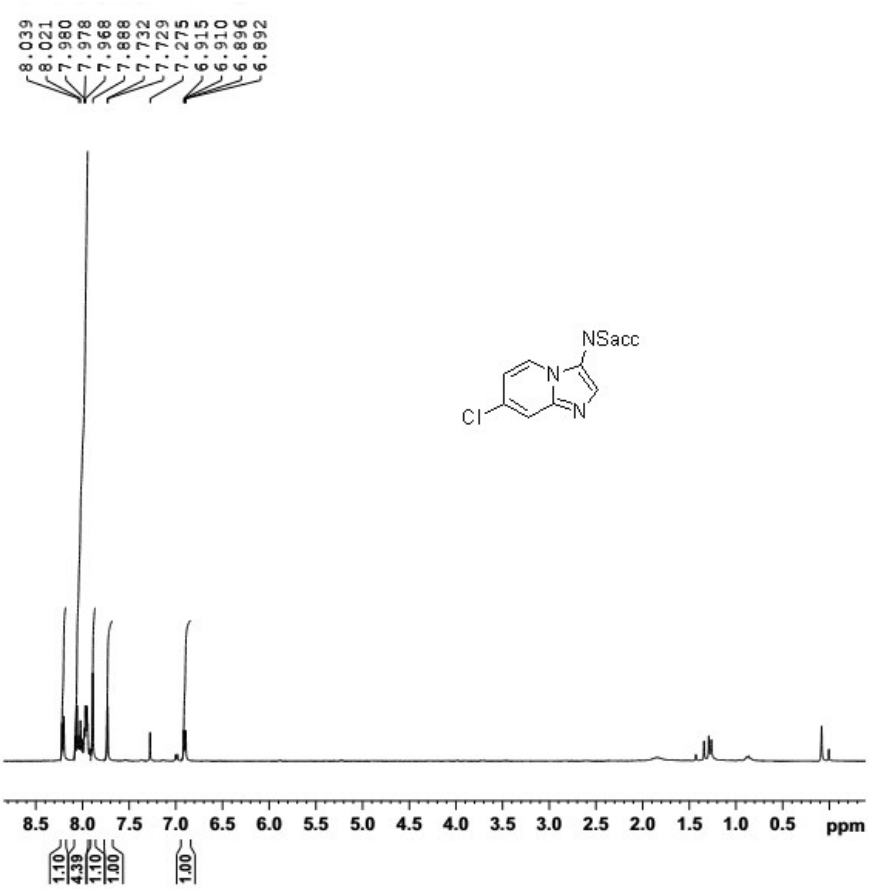
Compound **3r**

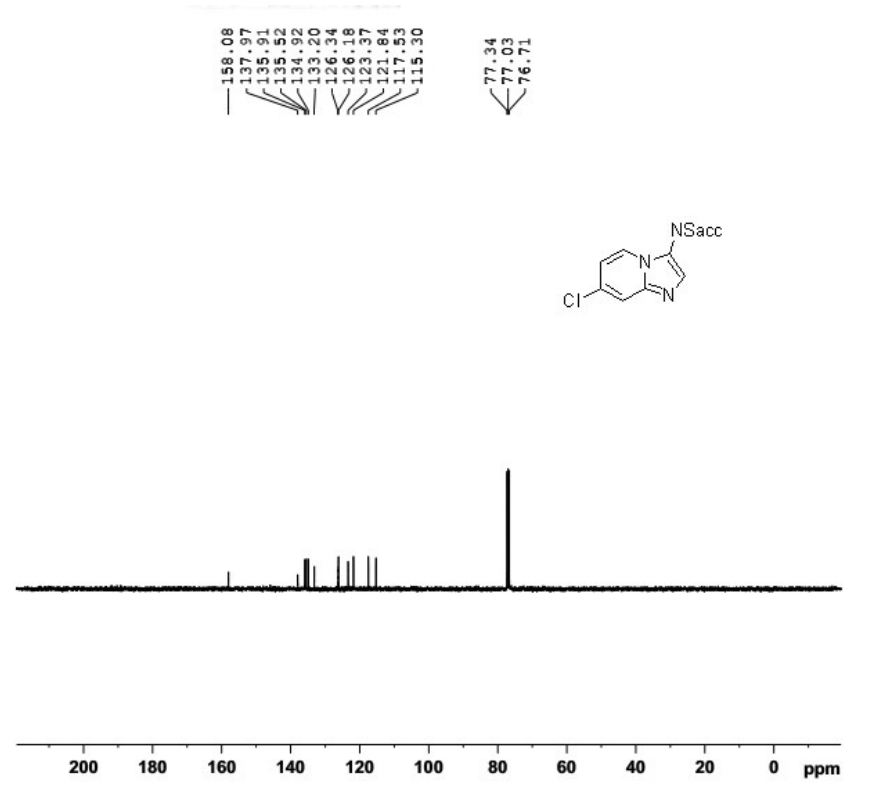

8.213
8.194
8.045
8.011
7.978
7.963
7.960
7.947
7.942
7.382
7.363
7.351
7.334
7.273
7.153
7.135
6.803
2.722
NSacc
Ph
N
N
9
8
7
6
5
4
3
2
1
0
ppm
1.05
6.19
3.13
1.02
0.95
3.00


158.22
146.10
145.59
138.12
135.83
134.81
132.39
128.69
128.57
128.29
127.72
126.40
126.24
125.46
121.75
121.00
113.37
103.99
77.33
77.02
76.70
22.69


NSacc
Ph
N
N
200
180
160
140
120
100
80
60
40
20
0
ppm

Compound **3t**


8.039
8.021
7.980
7.978
7.968
7.888
7.732
7.729
7.275
6.915
6.910
6.896
6.892
NSacc
N
Cl
N
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 ppm
1.10
4.39
1.10
1.00
1.00


158.08
137.97
135.91
135.52
134.92
133.20
126.34
126.18
123.37
121.84
117.53
115.30
77.34
77.03
76.71
NSacc
N
Cl
N
200 180 160 140 120 100 80 60 40 20 0 ppm