SUPPORTING INFORMATION

Room-Temperature Palladium-Catalysed Suzuki-Miyaura Coupling of Arylboric Acid with Aryl Chlorides†

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1. General Methods

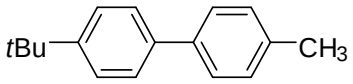
All reactions were conducted under an inert atmosphere of high pure argon. Anhydrous dioxane and benzene (PhH) were purchased from Sigma-Aldrich and used without further purification. Dimethoxyethane (DME), tetrahydrofuran (THF) were dried by Na refluxing with benzophenone as indicator. ^{1}H and ^{13}C NMR spectra were obtained on a Varian Unity INOVA 400/54 spectrometer in $CDCl_3$, CD_3OD or DMSO-d_6 with TMS as the internal standard. Mass spectra were obtained on a VG Auto spec 3000 or on a Finnigan MAT90 instrument. Silica gel H (Qingdao Sea Chemical Factory, Qingdao, China) was used for column chromatography. Spots on TLC (silica gel G) were detected by ultraviolet light. Commercially available reagents and solvents were purchased from Sigma-Aldrich, Aladdin, ChengDu Kelong Chemical Co.,Ltd., Duodian-Chemical and were directly used without further purification.

2. Procedure and characterization of Pd-catalyzed Suzuki reaction

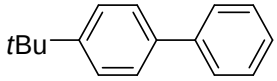
General procedure for the Pd-catalyzed Suzuki cross-coupling of aryl chlorides with arylboronic acids:

An oven-dried 10 mL reaction vial was sealed with plug after been equipped with a stir bar and charged with aryl chloride (0.2 mmol), arylboronic acid (0.24 mmol, 1.2 equiv) and K_2CO_3 (55mg, 0.4mmol, 2equiv) under an inert atmosphere of high pure argon. A stock solution of $Pd(OAc)_2$ (6.28 mg, 0.028 mmol) and NiXantphos (23.19 mg, 0.042 mmol) in 7 mL of dry THF was prepared through 1h stirring under 45℃. For each reaction, a solution of $Pd(OAc)_2$ (0.896 mg, 0.004 mmol) and NiXantphos (3.312 mg, 0.006 mmol) in 1 mL of dry THF was taken up by syringe and added to the reaction vial, followed by the addition of 0.2 mL H_2O. The reaction mixture was then stirred for 6h at room temperature. The

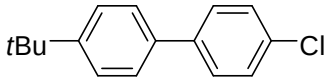
crude material was purified by chromatography on silica gel to give the desired products.



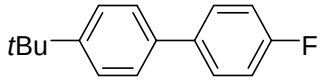
4-*tert*-butyl-4'-methylbiphenyl (3a): This reaction was performed following General Procedure with 4-*tert*-butylphenylboronic acid (**1a**, 42.7 mg, 0.24 mmol, 1.2 equiv) and 1-chloro-4-methylbenzene (**2a**, 25.2 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with petroleum ether) to give the product (42.5 mg, 95% yield) as a white solid. The ^{1}H and $^{13}C\{^{1}H\}$ NMR data for this compound match the literature data.[1]



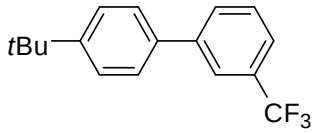
4-tert-butylbiphenyl (3b): This reaction was performed following General Procedure with 4-*tert*-butylphenylboronic acid (**1a**, 42.7 mg, 0.24 mmol, 1.2 equiv) and chlorobenzene (**2b**, 22.5 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with petroleum ether) to give the product (39.5 mg, 94% yield) as a white solid. The ^{1}H and $^{13}C\{^{1}H\}$ NMR data for this compound match the literature data.[1]



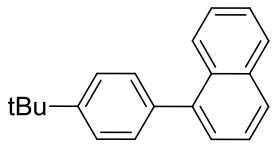
4-tert-butyl-4'-chlorobiphenyl (3c): This reaction was performed following General Procedure with 4-*tert*-butylphenylboronic acid (**1a**, 42.7 mg, 0.24 mmol, 1.2 equiv) and 1,4-dichlorobenzene (**2c**, 29.4 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with petroleum ether) to give the product (46.9 mg, 96% yield) as a white solid. The ^{1}H and $^{13}C\{^{1}H\}$ NMR data for this compound match the literature data.[2]



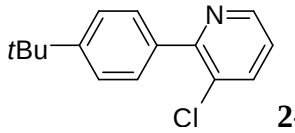
4-tert-butyl-4'-fluorobiphenyl (3d): This reaction was performed following General Procedure with 4-*tert*-butylphenylboronic acid (**1a**, 42.7 mg, 0.24 mmol, 1.2 equiv) and 1-chloro-4-fluorobenzene (**2d**, 26.11 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with petroleum ether) to give the product (44.7 mg, 98% yield) as a white solid. The ^{1}H and $^{13}C\{^{1}H\}$ NMR data for this compound match the literature data.[3]



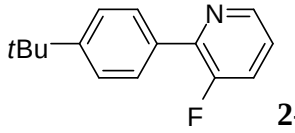
4'-tert-butyl-3-(trifluoromethyl)biphenyl (3e): This reaction was performed following General Procedure with 4-*tert*-butylphenylboronic acid (**1a**, 42.7 mg, 0.24 mmol, 1.2 equiv) and 1-chloro-3-(trifluoromethyl)benzene (**2e**, 36.11 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with petroleum ether) to give the product (51.7 mg, 93% yield) as colorless liquid. The ^{1}H and $^{13}C\{^{1}H\}$ NMR data for this compound match the literature data.[4]



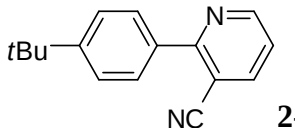
1-(4-(tert-butyl)phenyl)naphthalene (3f): This reaction was performed following General Procedure with 4-*tert*-butylphenylboronic acid (**1a**, 42.7 mg, 0.24 mmol, 1.2 equiv) and 1-chloronaphthalene (**2f**, 32.5 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:5) to give the product (46.5 mg, 90% yield) as a colorless crystal. The ^{1}H and $^{13}C\{^{1}H\}$ NMR data for this compound match the literature data.[5]



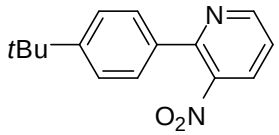
2-(4-(tert-butyl)phenyl)-3-chloropyridine (3g): This reaction was performed following General Procedure with 4-*tert*-butylphenylboronic acid (**1a**, 42.7 mg, 0.24 mmol, 1.2 equiv) and 2,3-dichloropyridine (**2g**, 29.6 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:20) to give the product (44.6 mg, 91% yield) as colourless liquid. ^{1}H-NMR (400 MHz, $CDCl_3$): δ_H 8. 57 (dd, J_1 = 4.8 Hz， J_2 = 1.2 Hz, 1H), 7.78 (dd, J_1 = 8.4 Hz， J_2 = 1.2 Hz, 1H), 7.68 (d, J = 8.4 Hz, 2H), 7.48 (d, J = 8.4 Hz, 2H), 7.20 (dd, J_1 = 8.4 Hz， J_2 = 4.8 Hz, 1H), 1.36 (s, 9H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ_C 156.5, 151.8, 147.5, 138.0, 135.3, 130.0, 129.0, 125.0, 122.8, 34.7, 31.3 ppm. HRMS calculated for $C_{15}H_{17}ClN$, 246.10440, found 246.10440, $[M+H]^+$ and $C_{15}H_{16}ClNNa$, 268.08635 , found 268.08628, $[M+Na]^+$.



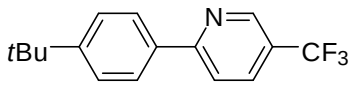
2-(4-(tert-butyl)phenyl)-3-fluoropyridine (3h): This reaction was performed following General Procedure with 4-*tert*-butylphenylboronic acid (**1a**, 42.7 mg, 0.24 mmol, 1.2 equiv) and 2-chloro-3-fluoropyridine (**2h**, 26.3 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:15) to give the product (44.9 mg, 98% yield) as colourless liquid. ^{1}H-NMR (400 MHz, $CDCl_3$): δ_H 8.55 (d, J = 4.8, 1H), 7.97 (d, J = 8.4 Hz, 2H), 7.56 (d, J = 8.4 Hz, 2H), 7.54-7.48 (m, 1H), 7.29 (dd, J_1 = 8.4 Hz J_2 = 4.8 Hz, 1H 1H), 1.41 (s, 9H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ_C 157.5 (d, J = 258.5 Hz), 152.3, 146.3 (d, J = 10.5 Hz), 145.3 (d, J = 5.5 Hz), 132.5 (d, J = 10.5 Hz), 128.4 (d, J = 5.5 Hz), 125.4, 124.0 (d, J = 50.5 Hz), 123.1 (d, J = 3.9 Hz), 34.7, 31.2 ppm. HRMS calculated for $C_{15}H_{16}FNNa$, 268.08635 , found 252.11590, $[M+Na]^+$.



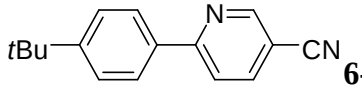
2-(4-(tert-butyl)phenyl)nicotinonitrile (3i): This reaction was performed following General Procedure with 4-*tert*-butylphenylboronic acid (**1a**, 42.7 mg, 0.24 mmol, 1.2 equiv) and 2-Chloro-3-cyano pyridine (**2i**, 27.7 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:5) to give the product (45.81 mg, 97% yield) as a white solid. ^{1}H-NMR (400 MHz, $CDCl_3$): δ_H 8.86 (dd, J_1 = 4.8 Hz， J_2 = 1.6 Hz, 1H), 8.05 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.88 (d, J = 8.0 Hz, 2H), 7.54 (d, J = 8.0 Hz, 2H), 7.35 (dd, J_1 = 8.0 Hz, J_2 = 4.8 Hz, 1H), 1.36 (s, 9H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ_C 160.9, 153.5, 152.6, 141.9, 134.3, 128.6, 125.7, 121.2, 117.9, 107.1, 34.8, 31.2 ppm. HRMS calculated for $C_{16}H_{16}N_2Na$, 259.12057, found 259.12052, $[M+Na]^+$.



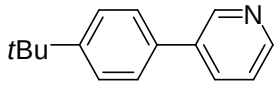
2-(4-(tert-butyl)phenyl)-3-nitropyridine (3j): This reaction was performed following General Procedure with 4-*tert*-butylphenylboronic acid (**1a**, 42.7 mg, 0.24 mmol, 1.2 equiv) and 2-Chloro-3-nitropyridine (**2j**, 31.7 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:5) to give the product (50.19 mg, 98% yield) as a light yellow solid. ^{1}H-NMR (400MHz, $CDCl_3$): δ_H 8.83 (dd, J_1 = 4.8 Hz， J_2 = 1.6 Hz, 1H), 8.11 (dd, J_1 = 8.0 Hz， J_2 = 1.6 Hz, 1H), 7.88 (d, J = 8.0 Hz, 2H), 7.51 (d, J = 8.0 Hz, 2H), 7.40 (dd, J_1 = 8.0 Hz, J_2 = 4.8 Hz, 1H), 1.34 (s, 9H).. ^{13}C-NMR (100MHz, $CDCl_3$): δ_C 160.9, 153.4, 152.6, 141.9, 134.3, 128.6, 125.7, 121.2, 117.9, 107.1, 34.8, 31.2 ppm. HRMS calculated for $C_{15}H_{16}N_2O_2Na$, 279.11040, found 279.11042, $[M+Na]^+$.



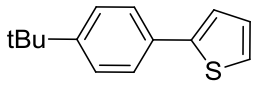
2-(4-(tert-butyl)phenyl)-5-(trifluoromethyl)pyridine (3k): This reaction was performed following General Procedure with 4-*tert*-butylphenylboronic acid (**1a**, 42.7 mg, 0.24 mmol, 1.2 equiv) and 2-chloro-5-(trifluoromethyl) pyridine (**2k**, 36.3 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:40) to give the product (55.23 mg, 99% yield) as a light yellow solid. ^{1}H-NMR (400 MHz, $CDCl_3$): δ_H 8.93 (br.s, 1H), 7.98 (d, J = 8.8 Hz), 7.96 (dd, J_1 = 8.4 Hz，J_2 = 2.4 Hz, 1H), 7.82 (d, J = 8.4 Hz, 1H), 7.54 (d, J = 8.8 Hz, 2H), 1.37 (s, 9H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ_C 160.6 (d, J = 1.3 Hz), 153.4, 146.5 (q, J = 4.0 Hz), 135.1, 133.8 (q, J = 3.5 Hz), 127.0, 125.9, 124.6 (q, J = 280.5 Hz), 119.7, 34.8, 31.2 ppm. HRMS calculated for $C_{16}H_{16}F_3NNa$, 302.11271, found 302.11264, $[M+Na]^+$.



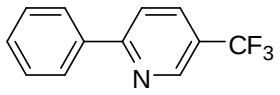
6-(4-(tert-butyl)phenyl)nicotinonitrile (3l): This reaction was performed following General Procedure with 4-*tert*-butylphenylboronic acid (**1a**, 42.7 mg, 0.24 mmol, 1.2 equiv) and 2-Chloro-5-cyanopyridine (**2l**, 27.71 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:15) to give the product (46.75 mg, 95% yield) as a white solid. ^{1}H-NMR (400 MHz, $CDCl_3$): δ_H 8.84 (dd, J_1 = 4.8 Hz，J_2 = 1.2 Hz, 1H), 7.95-7.92 (m, 3H), 7.53 (d, J = 8.4 Hz, 2H), 7.41 (dd, J_1 = 4.8 Hz，J_2 = 1.2 Hz, 1H), 1.36 (s, 9H). ^{13}C-NMR (100MHz, CDCl3): δ_C 158.6, 153.6, 150.6, 134.5, 126.7, 126.7, 126.1, 122.8, 121.8, 121.0, 116.9, 34.8, 31.2 ppm. HRMS calculated for $C_{16}H_{16}N_2Na$, 259.12059, found 259.12057, $[M+Na]^+$.



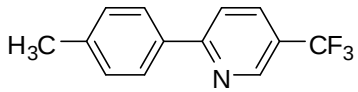
3-(4-(tert-butyl)phenyl)pyridine (3m): This reaction was performed following General Procedure with 4-*tert*-butylphenylboronic acid (**1a**, 42.7 mg, 0.24 mmol, 1.2 equiv) and 3-Chloropyridine (**2m**, 19 μL, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with petroleum ether) to give the product (27.46 mg, 65% yield) as a light yellow solid. The ^{1}H and $^{13}C\{^{1}H\}$ NMR data for this compound match the literature data.[6]



2-(4-(tert-butyl)phenyl)thiophene (3n): This reaction was performed following General Procedure with 4-*tert*-butylphenylboronic acid (**1a**, 42.7 mg, 0.24 mmol, 1.2 equiv) and 2-chlorothiophene (**2n**, 23.7mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:5) to give the product (39.4 mg, 92% yield) as a white crystal. The ^{1}H and $^{13}C\{^{1}H\}$ NMR data for this compound match the literature data.[7]

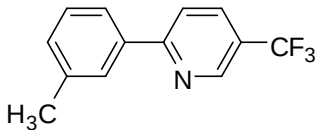


2-phenyl-5-(trifluoromethyl)pyridine (4a): This reaction was performed following General Procedure with phenylboronic acid (**1b**, 29.2 mg, 0.24 mmol, 1.2 equiv) and 2-chloro-5-(trifluoromethyl) pyridine (**2k**, 36.3 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:40) to give the product (42.8 mg, 96% yield) as a white solid. The ^{1}H and $^{13}C\{^{1}H\}$ NMR data for this compound match the literature data.[8]

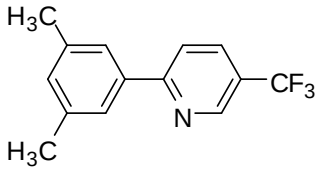


2-(p-tolyl)-5-(trifluoromethyl)pyridine (4b): This reaction was performed following General Procedure with p-tolylboronic acid (**1c**,

32.4 mg, 0.24 mmol, 1.2 equiv) and 2-chloro-5-(trifluoromethyl) pyridine (**2k**, 36.3 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:40) to give the product (44.1 mg, 93% yield) as a white solid. The ^{1}H and ^{13}C{^{1}H} NMR data for this compound match the literature data.[9]

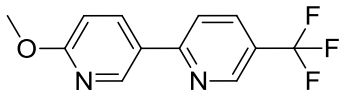


2-(m-tolyl)-5-(trifluoromethyl)pyridine (4c): This reaction was performed following General Procedure with m-tolylboronic acid (**1d**, 32.6 mg, 0.24 mmol, 1.2 equiv) and 2-chloro-5-(trifluoromethyl) pyridine (**2k**, 36.3 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:20) to give the product (44.5 mg, 94% yield) as a yellow crystal. ^{1}H-NMR (400 MHz, $CDCl_3$): δ_H 8.93 (s, 1H), 7.97 (dd, J_1 = 8.4 Hz， J_2 = 2.0 Hz, 1H), 7.86-7.79 (m, 3H), 7.40 (t, J = 8.4 Hz, 1H), 7.30 (d, J = 8.4 Hz, 1H), 2.45 (s, 3H). ^{13}C-NMR (100MHz, $CDCl_3$): δ_C 160.8, 146.5 (q, J = 4.6 Hz), 138.7, 137.9, 133.9 (q, J = 3.5 Hz) 130.8, 128.8, 127.9, 125.13, 124.6 (q, J = 280.5 Hz), 124.3, 120.1, 21.5 ppm.

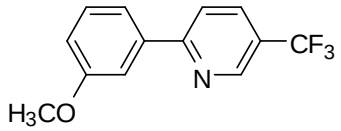


2-(3,5-dimethylphenyl)-5-(trifluoromethyl)pyridine (4d): This reaction was performed following General Procedure with 3,5-dimethylphenylboronic Acid (**1e**, 35.9 mg, 0.24 mmol, 1.2 equiv) and 2-chloro-5-(trifluoromethyl) pyridine (**2k**, 36.3 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:10) to give the product (46.7 mg, 93% yield) as yellow liquid. ^{1}H-NMR (400 MHz, $CDCl_3$): δ_H 8.92 (br. s, 1H), 7.96 (dd, J_1 = 8.4 Hz，J_2 = 2.0 Hz, 1H), 7.82 (d, J = 8.4 Hz, 1H), 7.63 (s, 2H), 7.12 (s, 1H), 2.41 (s, 6H). ^{13}C-NMR

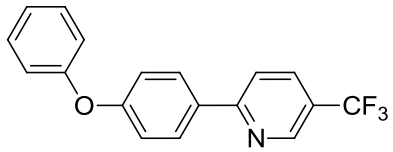
(100MHz, CDCl3): δ_C 161.0, 146.5 (q, J = 4.6 Hz), 138.6, 137.9, 133.8 (q, J = 3.5 Hz), 131.7, 125.1, 124.8 (q, J = 280.5 Hz), 120.1, 21.43 ppm.



6'-methoxy-5-(trifluoromethyl)-2,3'-bipyridine (4e): This reaction was performed following General Procedure with 4-methoxyphenylboronic acid (**1f**, 36.47 mg, 0.24 mmol, 1.2 equiv) and 2-chloro-5-(trifluoromethyl) pyridine (**2k**, 36.3 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:5) to give the product (41.51 mg, 82% yield) as a white crystal. The ^{1}H and ^{13}C{^{1}H} NMR data for this compound match the literature data.[10]

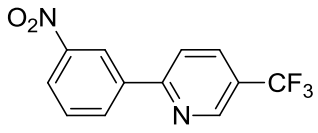


2-(3-methoxyphenyl)-5-(trifluoromethyl)pyridine (4f): This reaction was performed following General Procedure with 3-methoxyphenylboronic acid (**1g**, 36.47 mg, 0.24 mmol, 1.2 equiv) and 2-chloro-5-(trifluoromethyl) pyridine (**2k**, 36.3 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:10) to give the product (40.51 mg, 80% yield) as a brown yellow crystal. The ^{1}H and ^{13}C{^{1}H} NMR data for this compound match the literature data.[11]

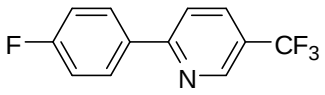


2-(4-phenoxyphenyl)-5-(trifluoromethyl)pyridine (4g): This reaction was performed following General Procedure with (4-phenoxyphenyl)boronic acid (**1h**, 51.4 mg, 0.24 mmol, 1.2 equiv) and 2-chloro-5-(trifluoromethyl) pyridine (**2k**, 36.3 mg, 0.2 mmol, 1.0 equiv). The crude

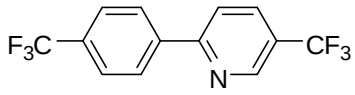
material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:5) to give the product (56.7 mg, 90% yield) as a white crystal. The ^{1}H and $^{13}C\{^{1}H\}$ NMR data for this compound match the literature data.[12]



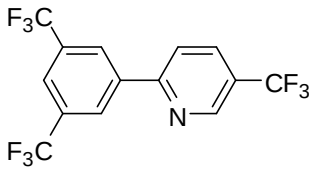
2-(3-nitrophenyl)-5-(trifluoromethyl)pyridine (4h): This reaction was performed following General Procedure with (3-nitrophenyl)boronic acid (**1l**, 40 mg, 0.24 mmol, 1.2 equiv) and 2-chloro-5-(trifluoromethyl) pyridine (**2k**, 36.3 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:5) to give the product (50.4 mg, 94% yield) as a white crystal. ^{1}H-NMR (400 MHz, $CDCl_3$): δ_H 8.98 (s, 1H), 8.90 (t, *J* = 2.0 Hz, 1H), 8.41 (d, *J* = 8.0 Hz, 1H), 8.32 (d, *J* = 8.0 Hz, 1H), 8.07 (d, *J* = 8.0 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.69 (t, J = 8.0 Hz, 1H); ^{13}C-NMR (100MHz, $CDCl_3$): δ_C 157.8, 148.8, 146.9 (q, *J* = 4.6 Hz), 139.5, 134.4 (q, *J* = 3.5 Hz), 132.9, 130.0, 126.0 (q, *J* = 28.5 Hz), 125.6 (q, *J* = 280.5 Hz), 124.5, 122.1, 120.1 ppm. HRMS calculated for $C_{12}H_7F_3N_2O_2Na$, 291.03518 , found 291.03528, $[M+Na]^+$.



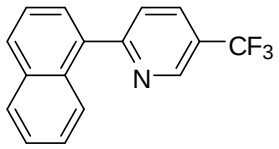
2-(4-fluorophenyl)-5-(trifluoromethyl)pyridine (4i): This reaction was performed following General Procedure with p-Fluorophenylboronic acid (**1j**, 33.58 mg, 0.24 mmol, 1.2 equiv) and 2-chloro-5-(trifluoromethyl) pyridine (**2k**, 36.3 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:30) to give the product (44.8 mg, 93% yield) as a white crystal. The ^{1}H and $^{13}C\{^{1}H\}$ NMR data for this compound match the literature data.[13]



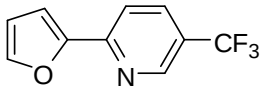
5-(trifluoromethyl)-2-(4-(trifluoromethyl)phenyl)pyridine (4j): This reaction was performed following General Procedure with Trifluoromethylphenyl (**1k**, 45.58 mg, 0.24 mmol, 1.2 equiv) and 2-chloro-5-(trifluoromethyl) pyridine (**2k**, 36.3 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:30) to give the product (51.8 mg, 89% yield) as a white solid. ^{1}H-NMR (400 MHz, $CDCl_3$): δ_H 8.98 (br. s, 1H), 8.15 (d, J = 8.4 Hz, 2H), 8.04 (dd, J_1 = 8.4 Hz，J_2 = 1.6 Hz, 1H), 7.89 (d, J = 8.4 Hz, 1H), 7.76 (d, J = 8.4 Hz, 2H). ^{13}C-NMR (100MHz, $CDCl_3$): δ_C 159.0, 146.8 (q, J = 4.6 Hz), 141.1, 134.2 (q, J = 3.5 Hz), 131.8 (q, J = 324.9 Hz), 127.6, 125.9 (q, J = 28.5 Hz), 125.5 (q, J = 280.5 Hz), 122.6, 122.1, 120.3 ppm.



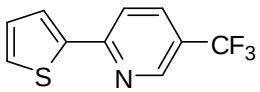
2-(3,5-bis(trifluoromethyl)phenyl)-5-(trifluoromethyl)pyridine (4k): This reaction was performed following General Procedure with 3,5-Bis(trifluoromethyl)phenylboronic acid (**1l**, 61.9 mg, 0.24 mmol, 1.2 equiv) and 2-chloro-5-(trifluoromethyl) pyridine (**2k**, 36.3 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:30) to give the product (63.2 mg, 88% yield) as a light yellow solid. ^{1}H-NMR (400 MHz, $CDCl_3$): δ_H 9.00 (br. s, 1H), 8.52 (s, 2H), 8.09 (dd, J_1 = 8.4 Hz，J_2 = 2.0 Hz, 1H), 7.98 (s, 1H), 7.95 (d, J = 8.4 Hz). ^{13}C-NMR (100 MHz, $CDCl_3$): δ_C 157.2, 147.0 (q, J = 4.0 Hz), 139.7, 134.6 (q, J = 3.4 Hz), 132.4 (q, J = 334.0 Hz), 127.3 (q, J = 30.0 Hz), 126.3 (q, J = 332.2 Hz), 124.6 (d, J = 161.7 Hz), 123.5 (q, J = 35.7 Hz), 121.9 (d, J = 166.0 Hz), 120.2 ppm.



2-(naphthalen-1-yl)-5-(trifluoromethyl)pyridine (4l): This reaction was performed following General Procedure with Naphthalene-1-boronic acid (**1m**, 41.2 mg, 0.24 mmol, 1.2 equiv) and 2-chloro-5-(trifluoromethyl) pyridine (**2k**, 36.3 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:10) to give the product (52.4 mg, 96% yield) as a brown yellow crystal. The ^{1}H and ^{13}C{^{1}H} NMR data for this compound match the literature data.[14]

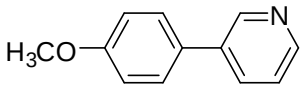


2-(furan-2-yl)-5-(trifluoromethyl)pyridine (4m): This reaction was performed following General Procedure with 2-Furanboronic acid (**1n**, 26.8 mg, 0.24 mmol, 1.2 equiv) and 2-chloro-5-(trifluoromethyl) pyridine (**2k**, 36.3 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:10) to give the product (29.84 mg, 70% yield) as brown yellow liquid. ^{1}H-NMR (400 MHz, $CDCl_3$): δ_H 8.82 (br. s, 1H), 7.93 (dd, J_1 = 8.4 Hz， J_2 = 2.0 Hz, 1H), 7.78 (d, J = 8.4Hz, 1H), 7.58 (br. s, 1H), 7.19 (d, J = 3.6 Hz 1H), 6.57 (dd, J_1 = 3.6 Hz， J_2 = 2.0 Hz, 1H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ_C 152.4, 152.1, 146.5 (q, J = 4.0 Hz), 144.5, 133.9 (q, J = 3.4 Hz), 124.4 (q, J = 280.8 Hz), 122.2, 117.8, 112.5, 111.0 ppm. HRMS calculated for $C_{10}H_7F_3NO$, 214.04742 , found 214.04789, $[M+H]^+$.



2-(thiophen-2-yl)-5-(trifluoromethyl)pyridine (4n): This reaction was performed following General Procedure with 2-thiophenylboric acid (**1o**, 30.7 mg, 0.24 mmol, 1.2 equiv) and 2-chloro-5-(trifluoromethyl) pyridine (**2k**, 36.3 mg, 0.2 mmol, 1.0 equiv). The crude material was purified by chromatography

on silica gel (eluted with EtOAc:petroleum ether = 1:20) to give the product (43.5 mg, 95% yield) as a white solid. The ^{1}H and ^{13}C{^{1}H} NMR data for this compound match the literature data.[15]



3-(4-methoxyphenyl)pyridine (5a): This reaction was performed following General Procedure with 4-Methoxyphenylboronic acid (**1f**, 1.6 g, 10.56 mmol, 1.2 equiv) and 3-Chloropyridine (**2m**, 0.82 mL, 8.8 mmol, 1.0 equiv). The crude material was purified by chromatography on silica gel (eluted with EtOAc:petroleum ether = 1:4) to give the product (0.97 g, 60% yield) as a brown solid. ^{1}H-NMR (400 MHz, $CDCl_3$): δ_H 8.81 (dd, J_1 = 2.4 Hz， J_2 = 0.8 Hz, 1H), 8.54 (dd, J_1 = 4.8 Hz， J_2 = 1.2 Hz, 1H), 7.84 (dq, J_1 = 8.0 Hz， J_2 = 1.2 Hz, 1H), 7.54 (d, J = 8.8 Hz, 2H), 7.33 (ddd, J_1 = 8.0 Hz， J_2 = 4.8 Hz, J_3 = 0.8 Hz, 1H), 7.01 (d, J = 8.8 Hz, 2H), 3.86 (s, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ_C 159.7, 147.9, 147.8, 136.2, 133.9, 130.2, 128.2, 123.5, 114.5, 55.4 ppm. HRMS calculated for $C_{10}H_{12}NO$, 186.09134, found 186.09131, $[M+H]^+$.

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4-tert-butyl-4'-methylbiphenyl (3a)

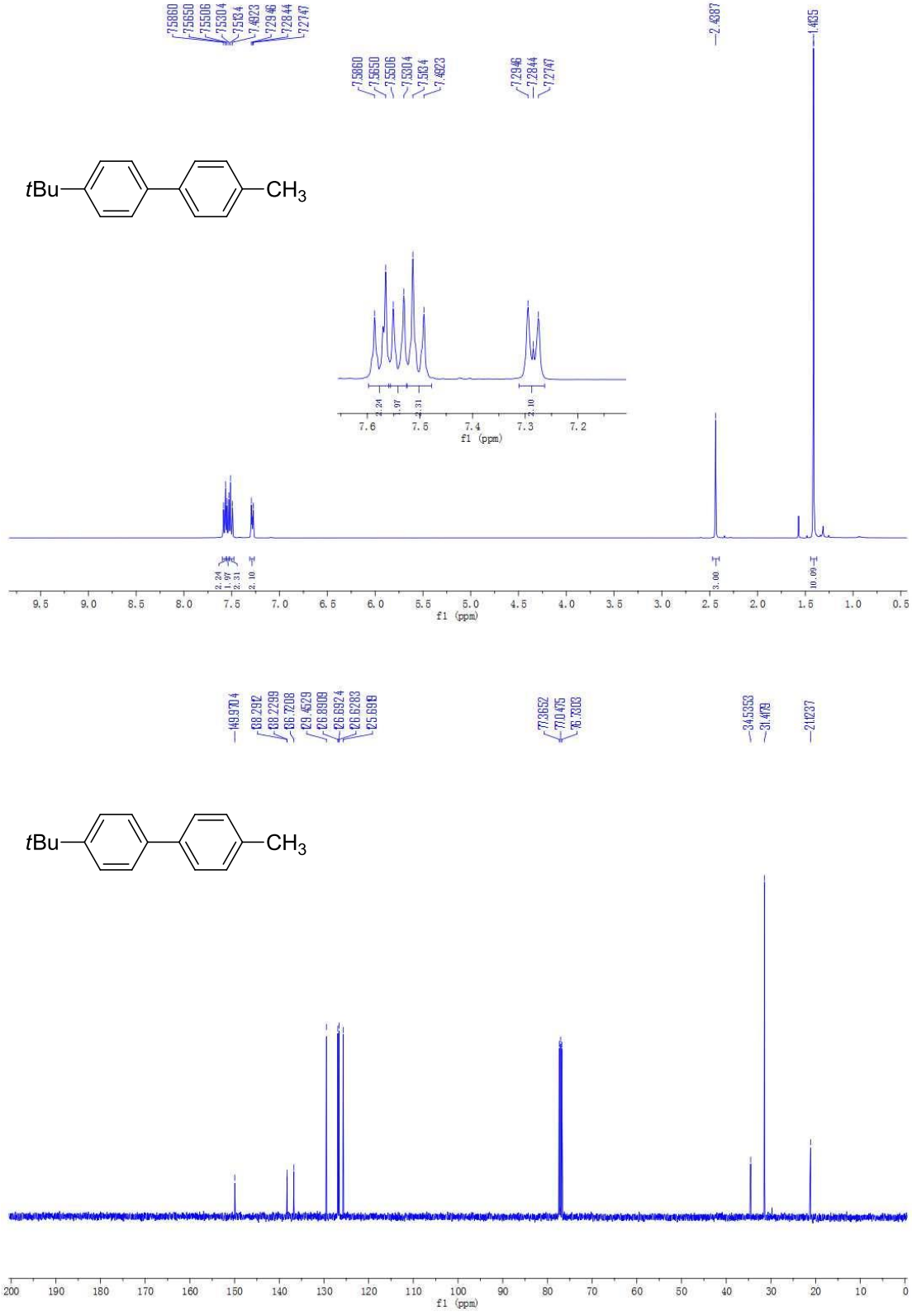

Fig. S1 ^{1}H and ^{13}C NMR spectra of 4-*tert*-butyl-4'-methylbiphenyl (**3a**)

4-tert-butylbiphenyl (3b)

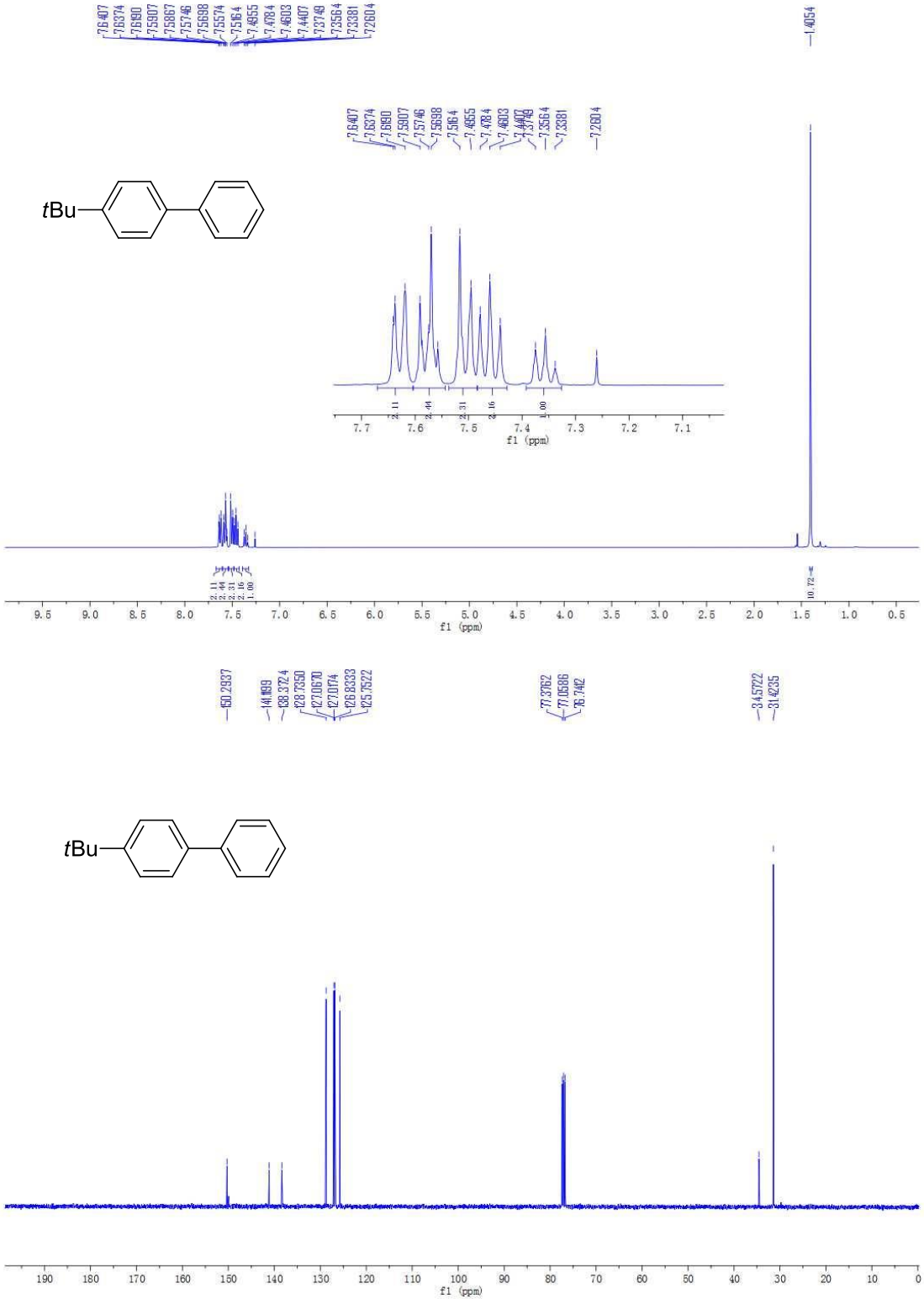

Fig. S2 ^{1}H and ^{13}C NMR spectra of 4-*tert*-butylbiphenyl (**3b**)

4-tert-butyl-4'-chlorobiphenyl (3c)

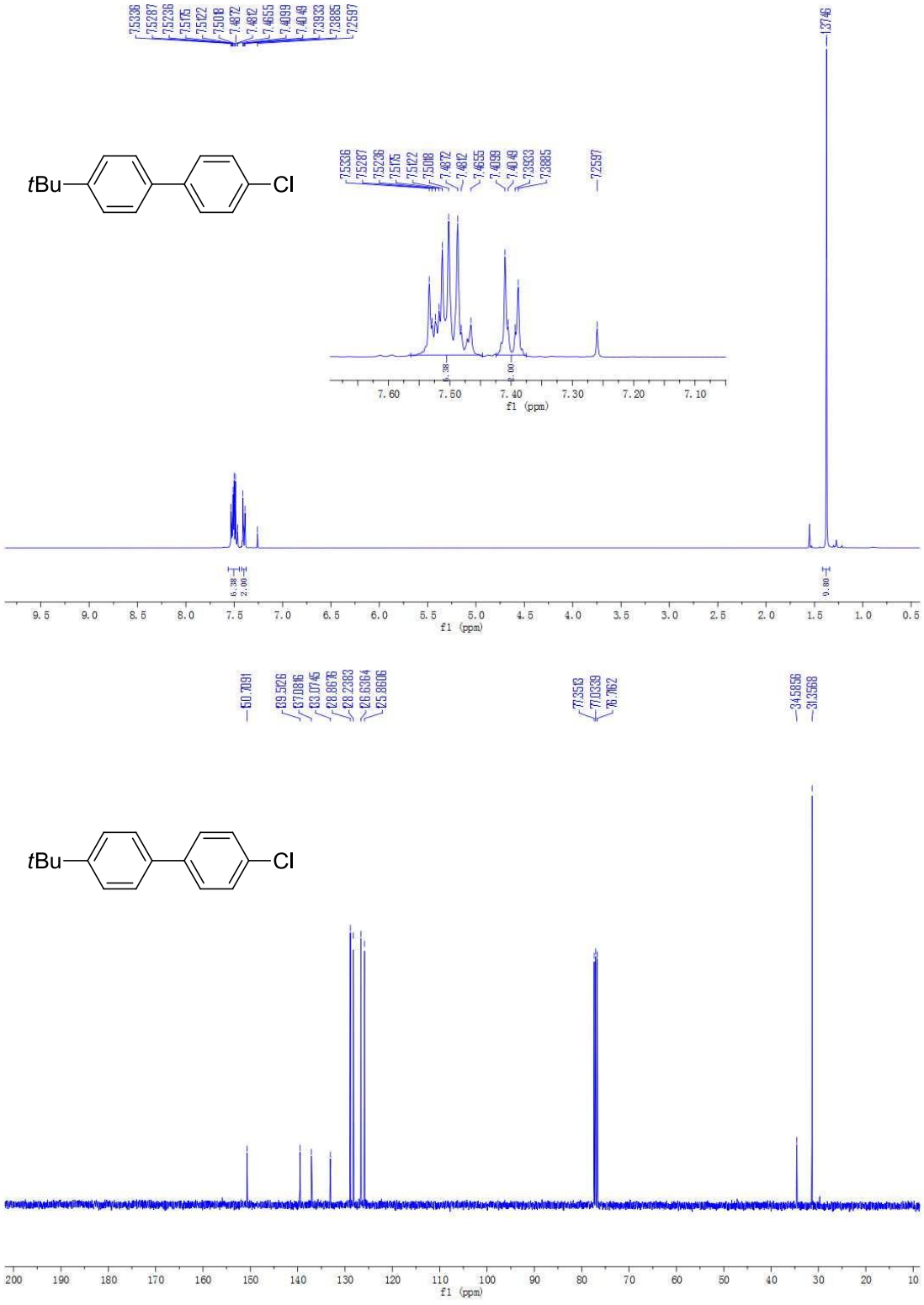

Fig. S3 ^{1}H and ^{13}C NMR spectra of 4-*tert*-butyl-4'-chlorobiphenyl (**3c**)

4-tert-butyl-4'-fluorobiphenyl (3d)

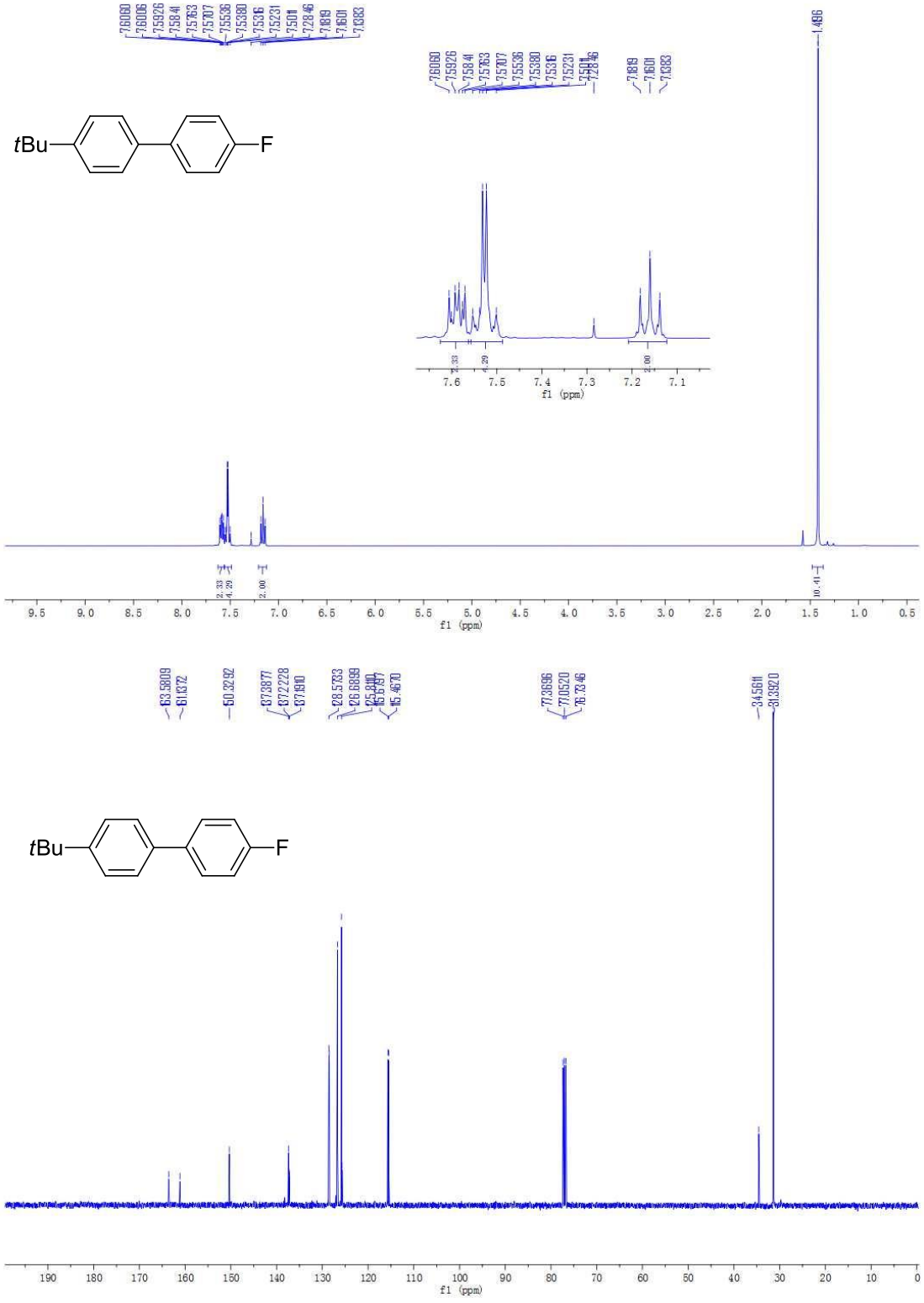

Fig. S4 ^{1}H and ^{13}C NMR spectra of 4-*tert*-butyl-4'-fluorobiphenyl (**3d**)

4'-tert-butyl-3-(trifluoromethyl)biphenyl (3e)

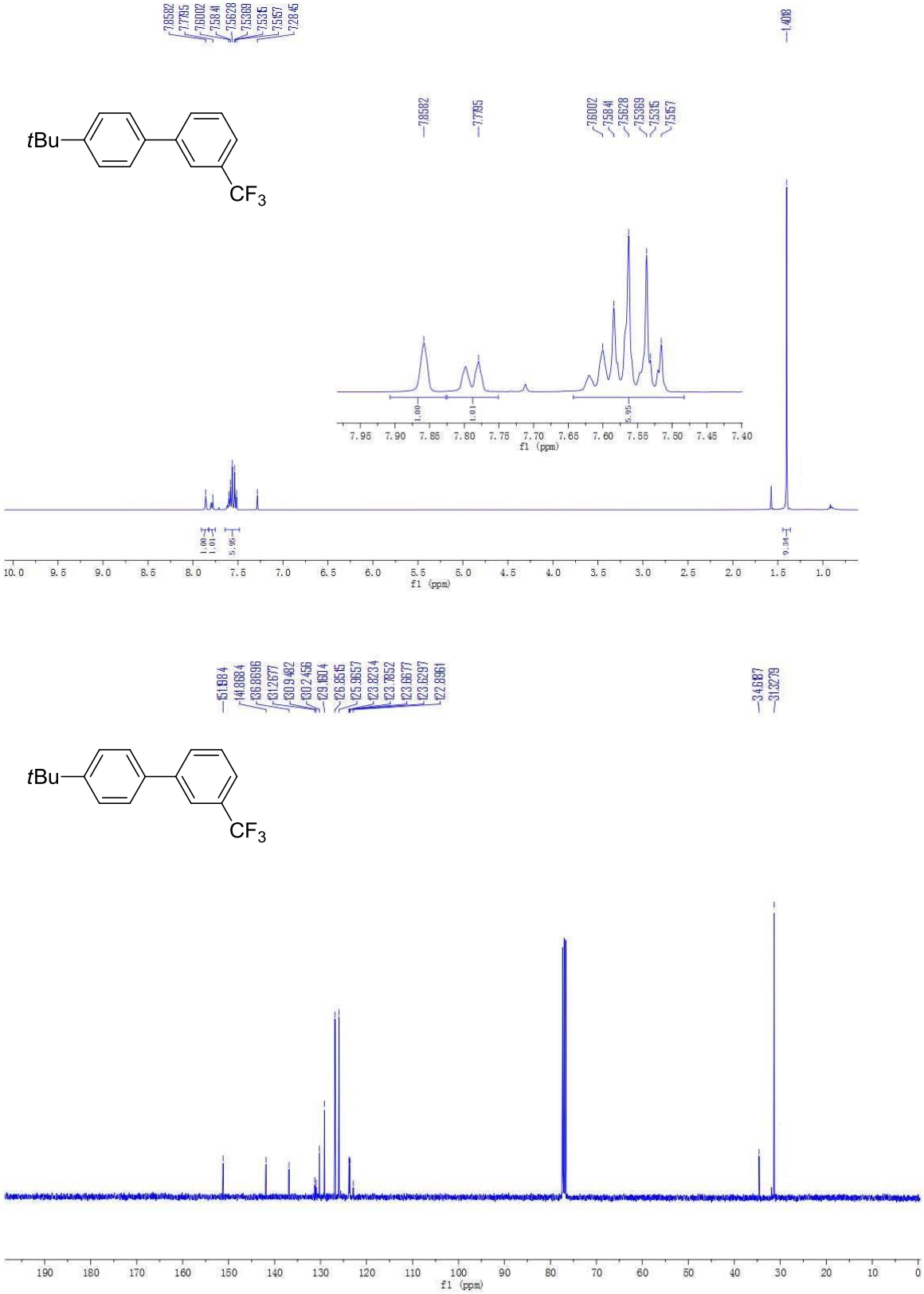

Fig. S5 ^{1}H and ^{13}C NMR spectra of 4'-*tert*-butyl-3-(trifluoromethyl)biphenyl (**3e**)

1-(4-(tert-butyl)phenyl)naphthalene（3f）

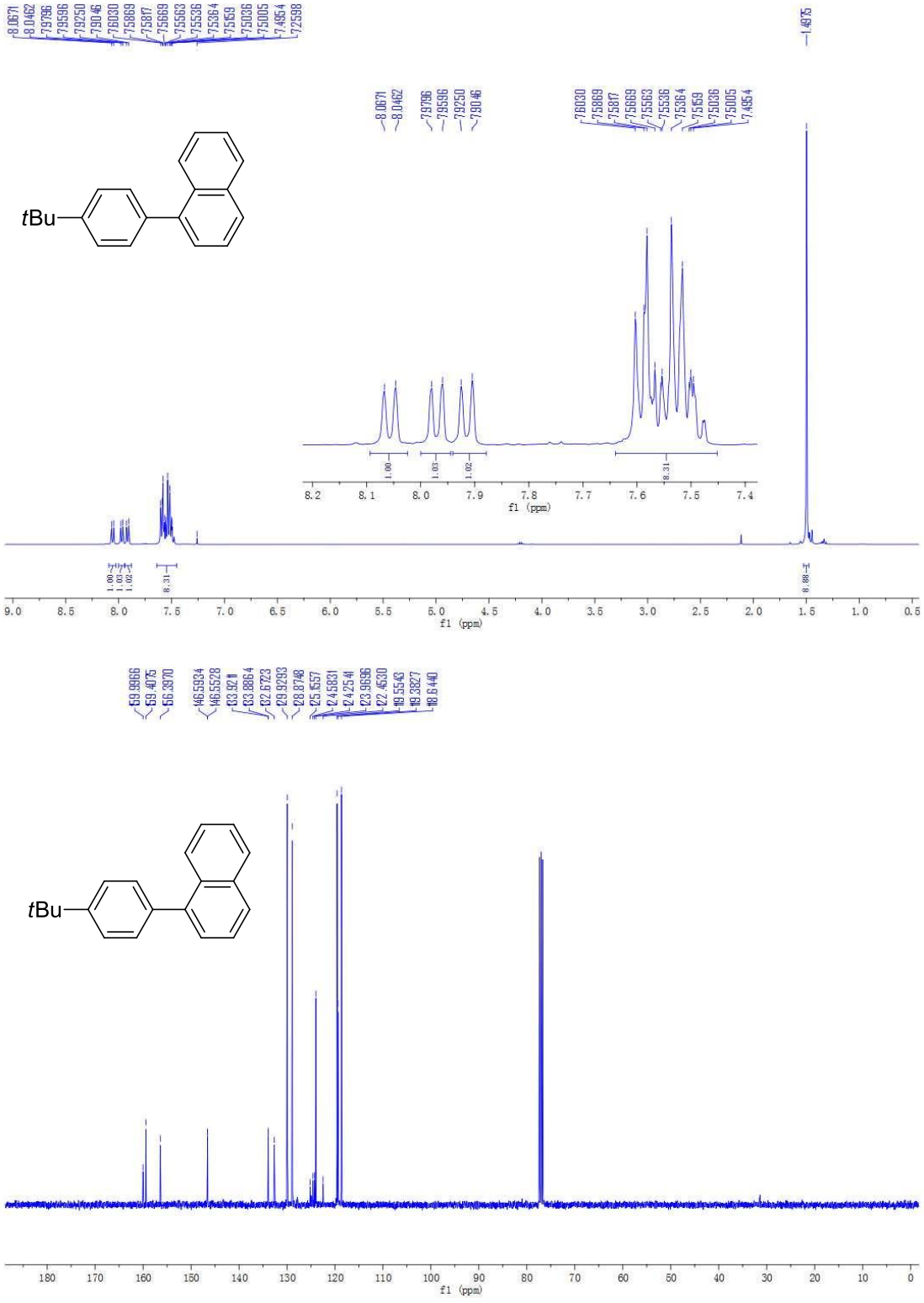

Fig. S6 ^{1}H and ^{13}C NMR spectra of 1-(4-(*tert*-butyl)phenyl)naphthalene（**3f**）

2-(4-tert-butylphenyl)-3-chloropyridine (3g)

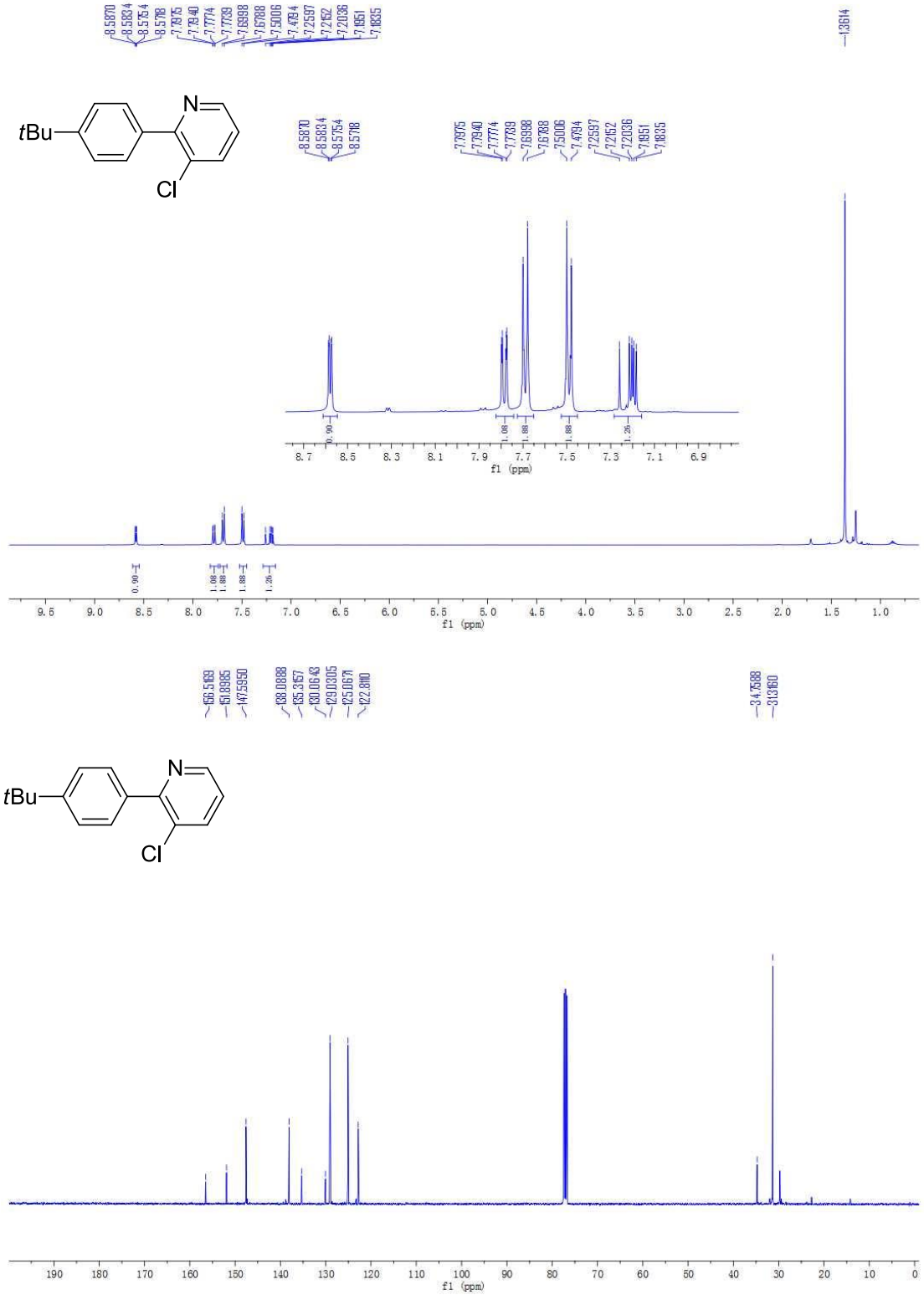

Fig. S7 ^{1}H and ^{13}C NMR spectra of 2-(4-*tert*-butylphenyl)-3-chloropyridine (**3g**)

2-(4-tert-butylphenyl)-3-fluoropyridine (3h)

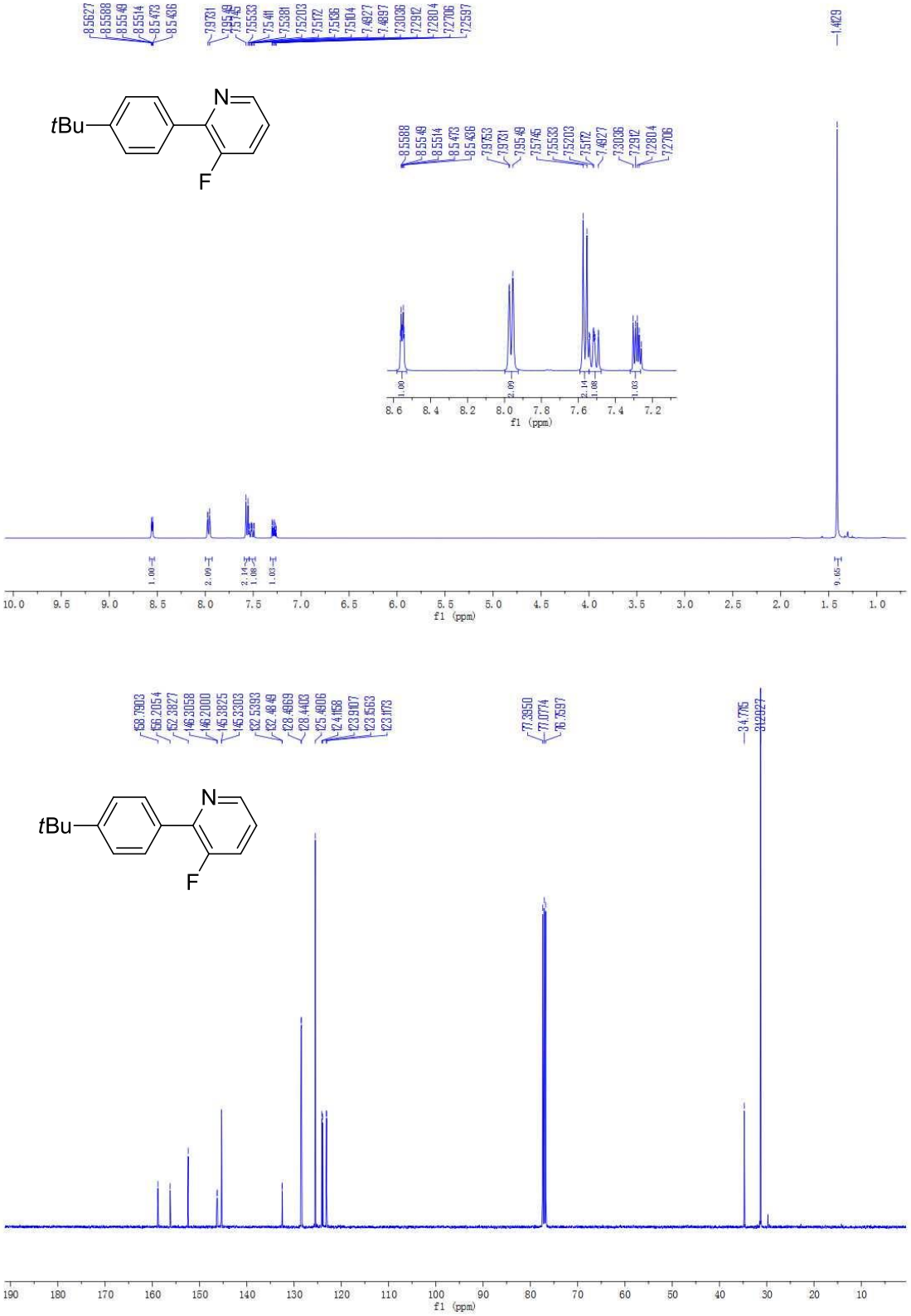

Fig. S8 ^{1}H and ^{13}C NMR spectra of 2-(4-*tert*-butylphenyl)-3-fluoropyridine (**3h**)

2-(4-tert-butylphenyl)nicotinonitrile (3i)

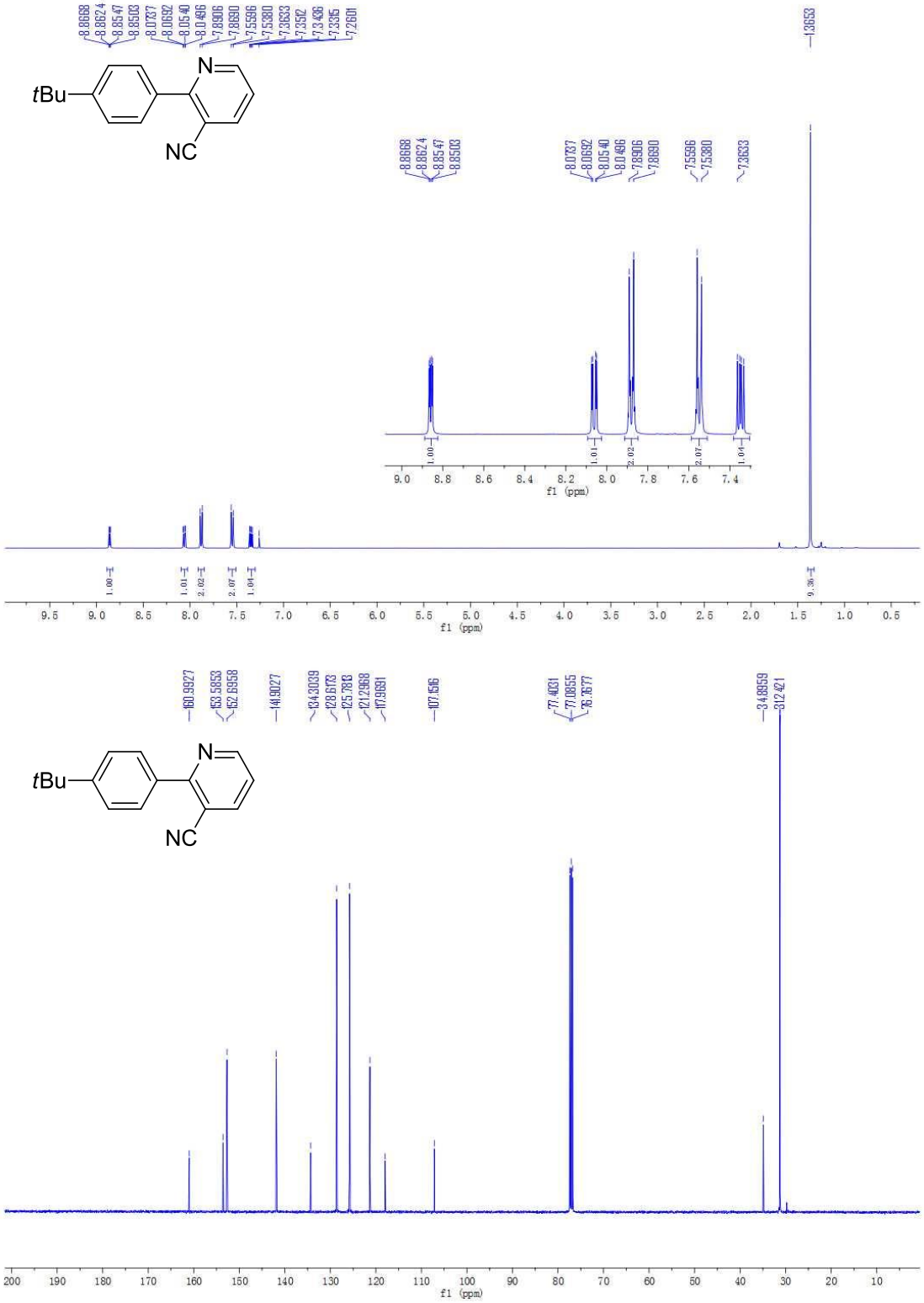

Fig. S9 ^{1}H and ^{13}C NMR spectra of 2-(4-*tert*-butylphenyl)nicotinonitrile (**3i**)

2-(4-tert-butylphenyl)-3-nitropyridine (3j)

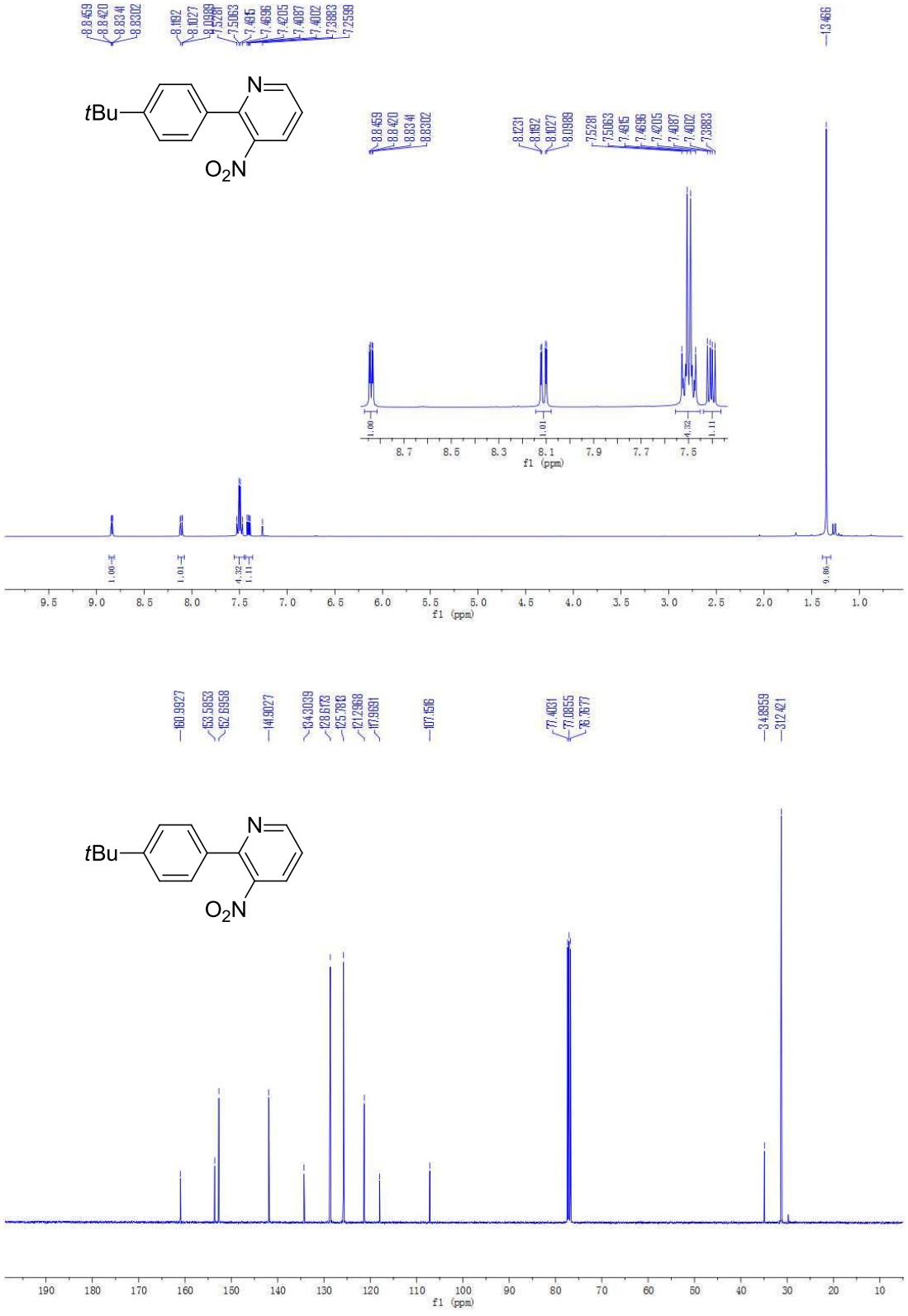

Fig. S10 ^{1}H and ^{13}C NMR spectra of 2-(4-*tert*-butylphenyl)-3-nitropyridine (**3j**)

2-(4-tert-butylphenyl)-5-(trifluoromethyl)pyridine (3k)

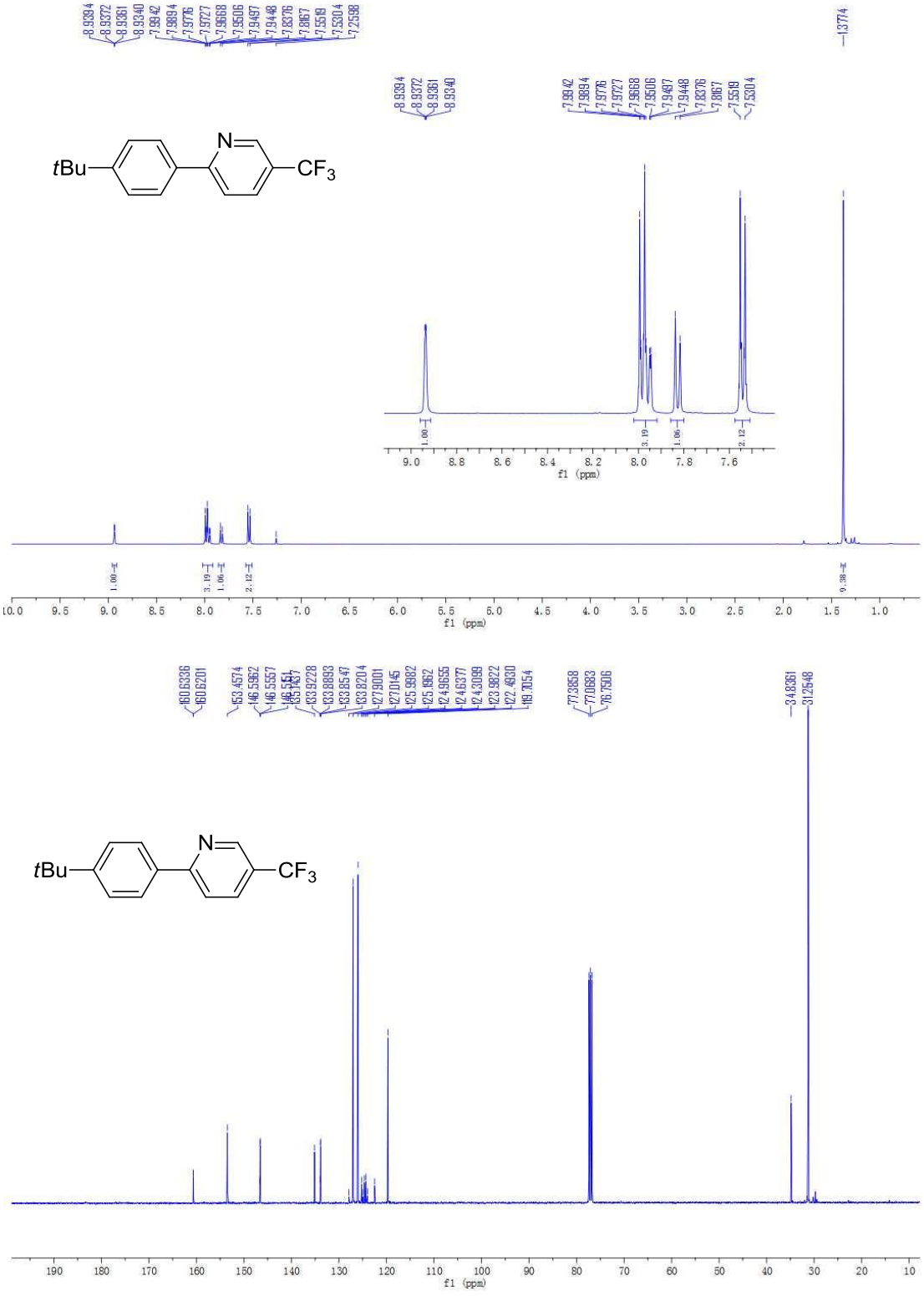

Fig. S11 ^{1}H and ^{13}C NMR spectra of
2-(4-*tert*-butylphenyl)-5-(trifluoromethyl)pyridine (**3k**)

6-(4-tert-butylphenyl)nicotinonitrile (3l)

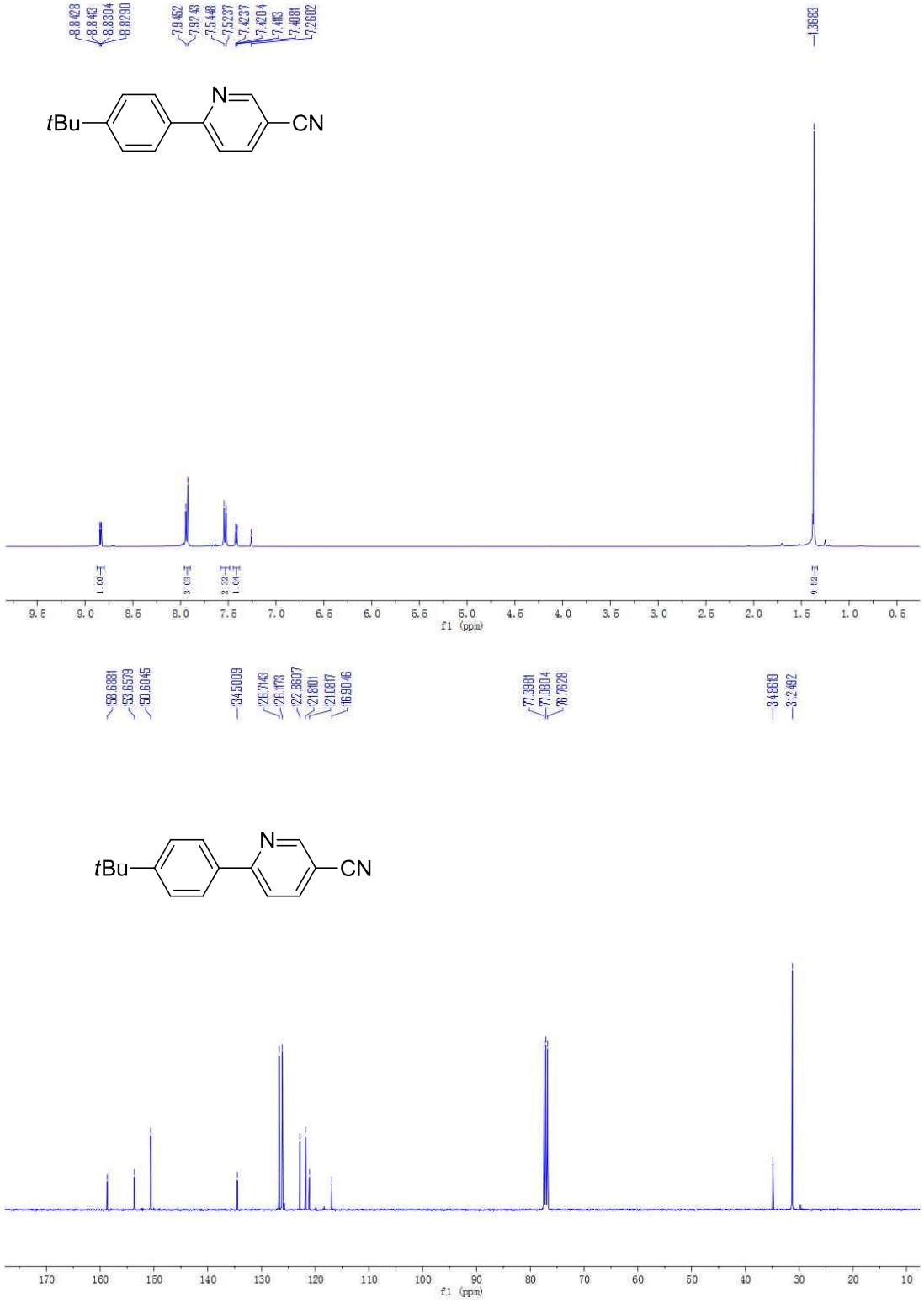

Fig. S12 ^{1}H and ^{13}C NMR spectra of 6-(4-*tert*-butylphenyl)nicotinonitrile (**3l**)

3-(4-tert-butylphenyl)pyridine (3m)

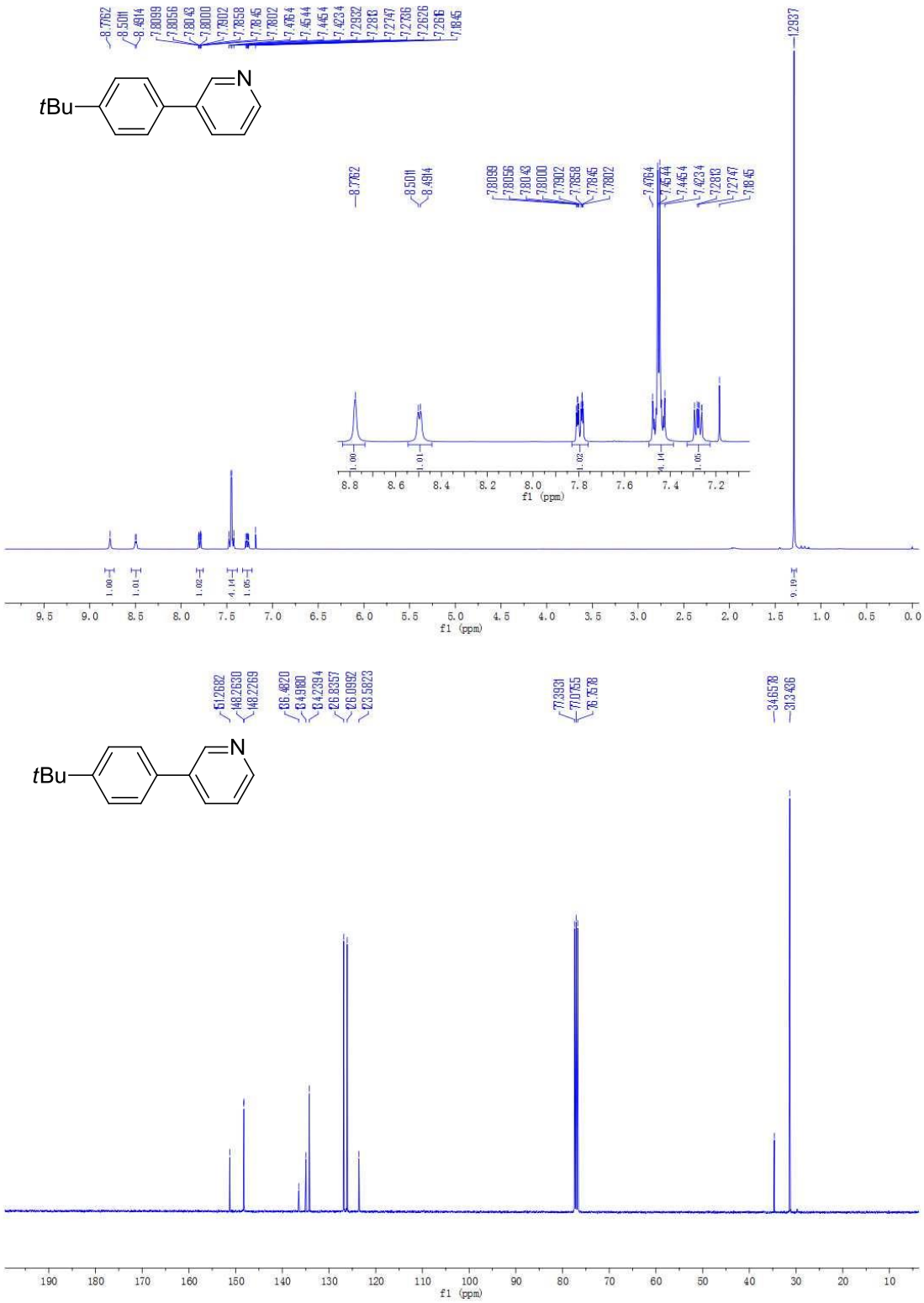

Fig. S13 ^{1}H and ^{13}C NMR spectra of 3-(4-*tert*-butylphenyl)pyridine (**3m**)

2-(4-(tert-butyl)phenyl)thiophene (3n)

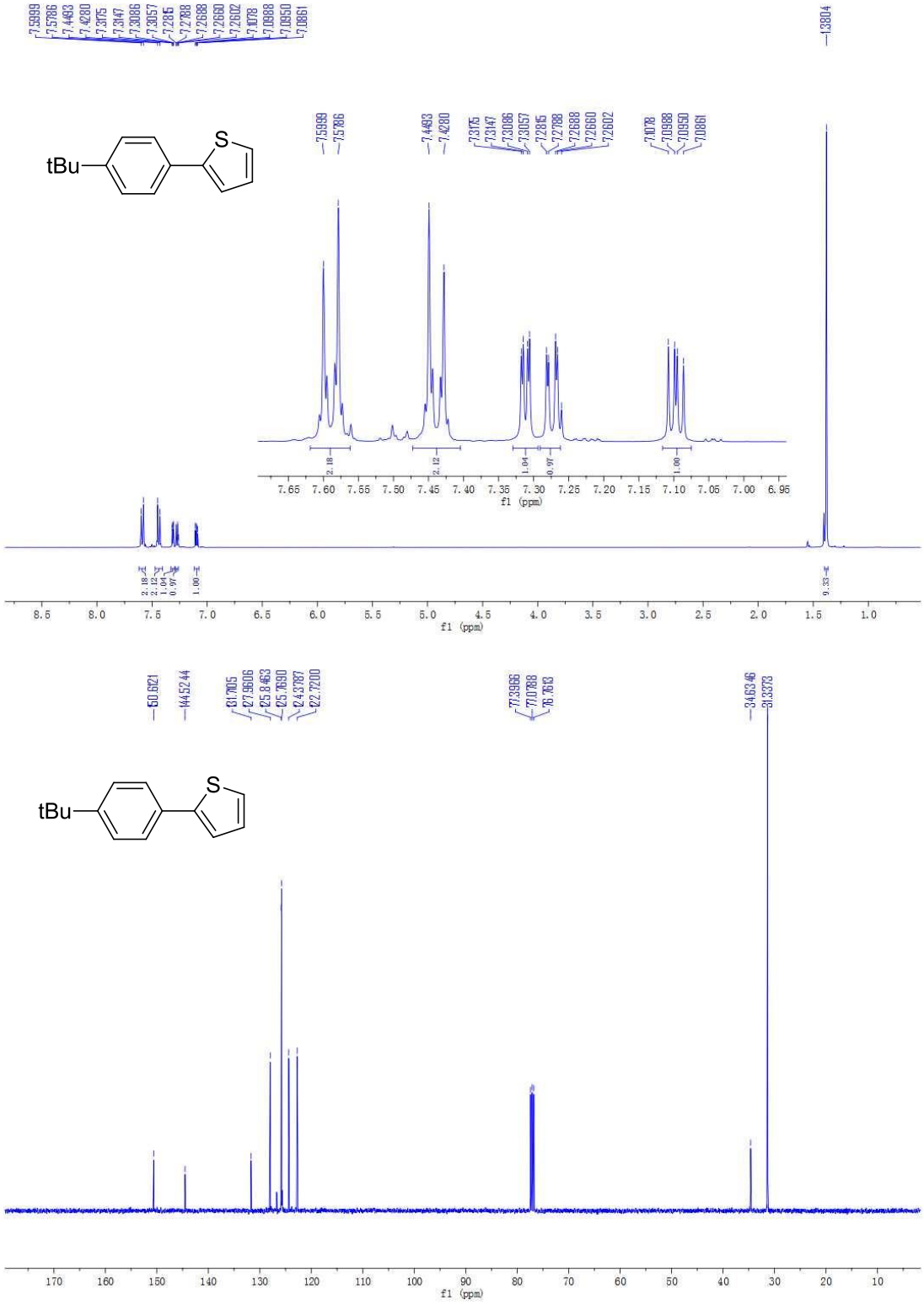

Fig. S14 ^{1}H and ^{13}C NMR spectra of 2-(4-(*tert*-butyl)phenyl)thiophene **(3n)**

2-phenyl-5-(trifluoromethyl)pyridine (4a)

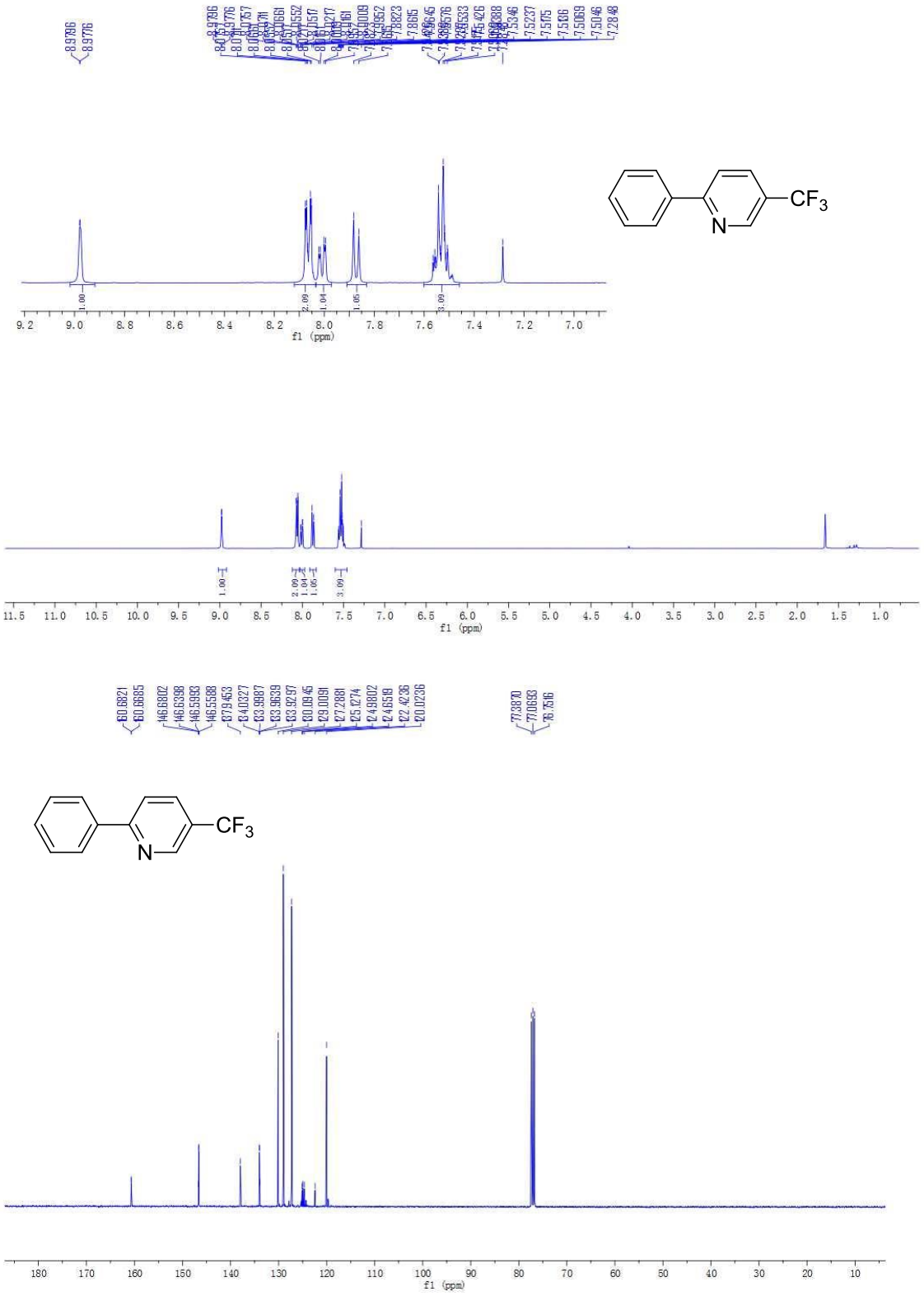

Fig. S15 ^{1}H and ^{13}C NMR spectra of 2-phenyl-5-(trifluoromethyl)pyridine (**4a**)

2-p-tolyl-5-(trifluoromethyl)pyridine (4b)

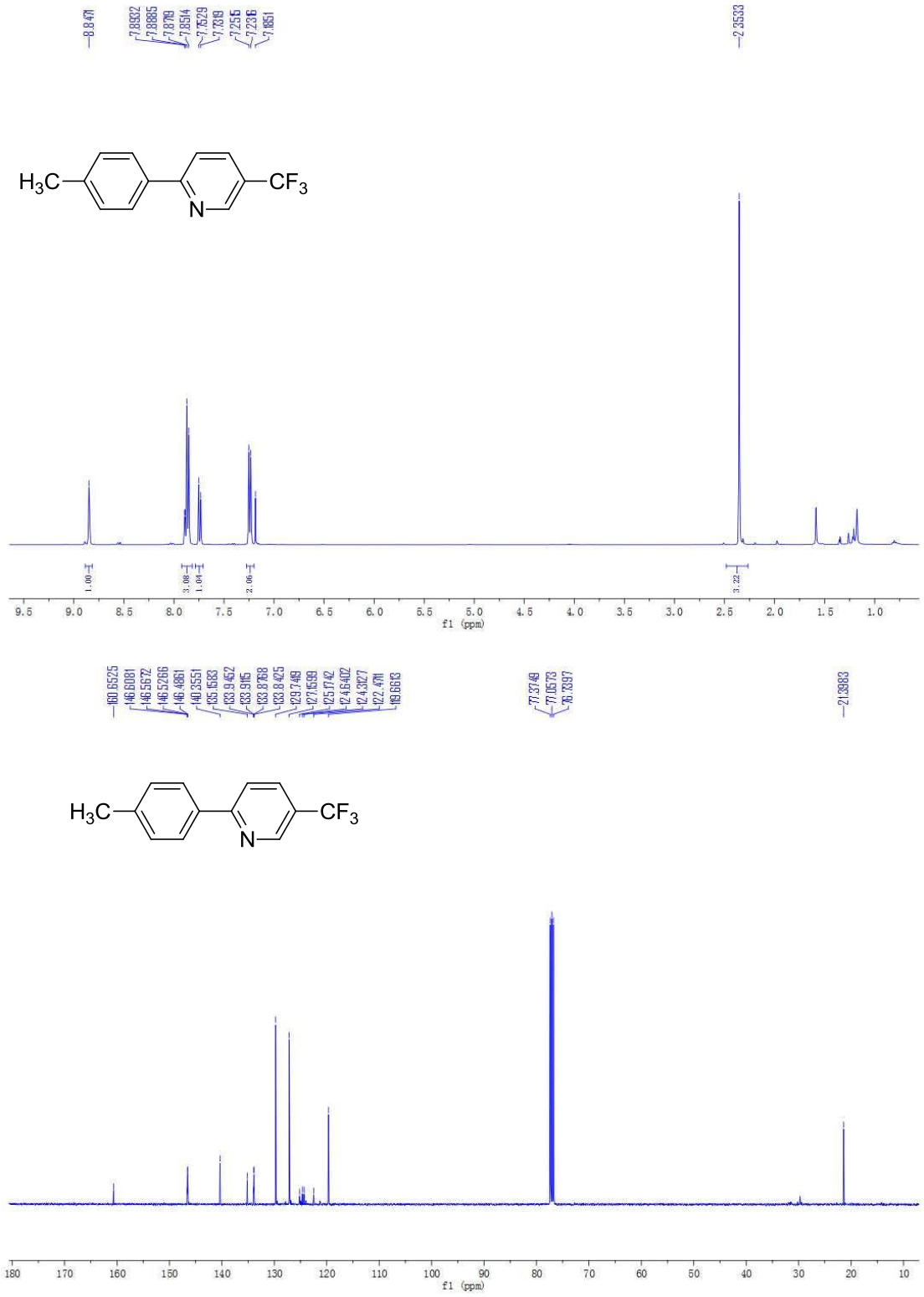

Fig. S16 ^{1}H and ^{13}C NMR spectra of 2-p-tolyl-5-(trifluoromethyl)pyridine (**4b**)

2-m-tolyl-5-(trifluoromethyl)pyridine (4c)

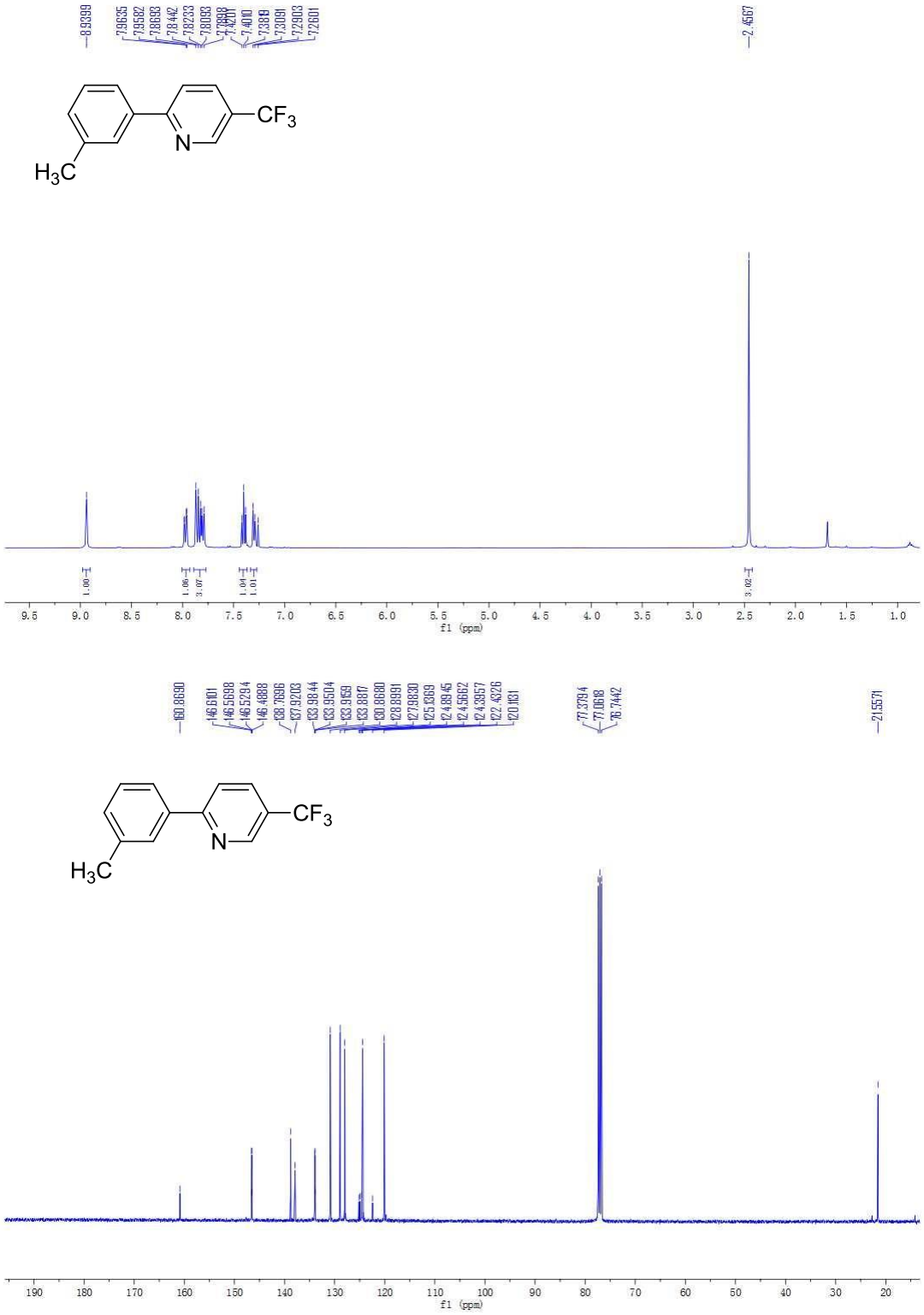

Fig. S17 ^{1}H and ^{13}C NMR spectra of 2-m-tolyl-5-(trifluoromethyl)pyridine (**4c**)

2-(3,5-dimethylphenyl)-5-(trifluoromethyl)pyridine (4d)

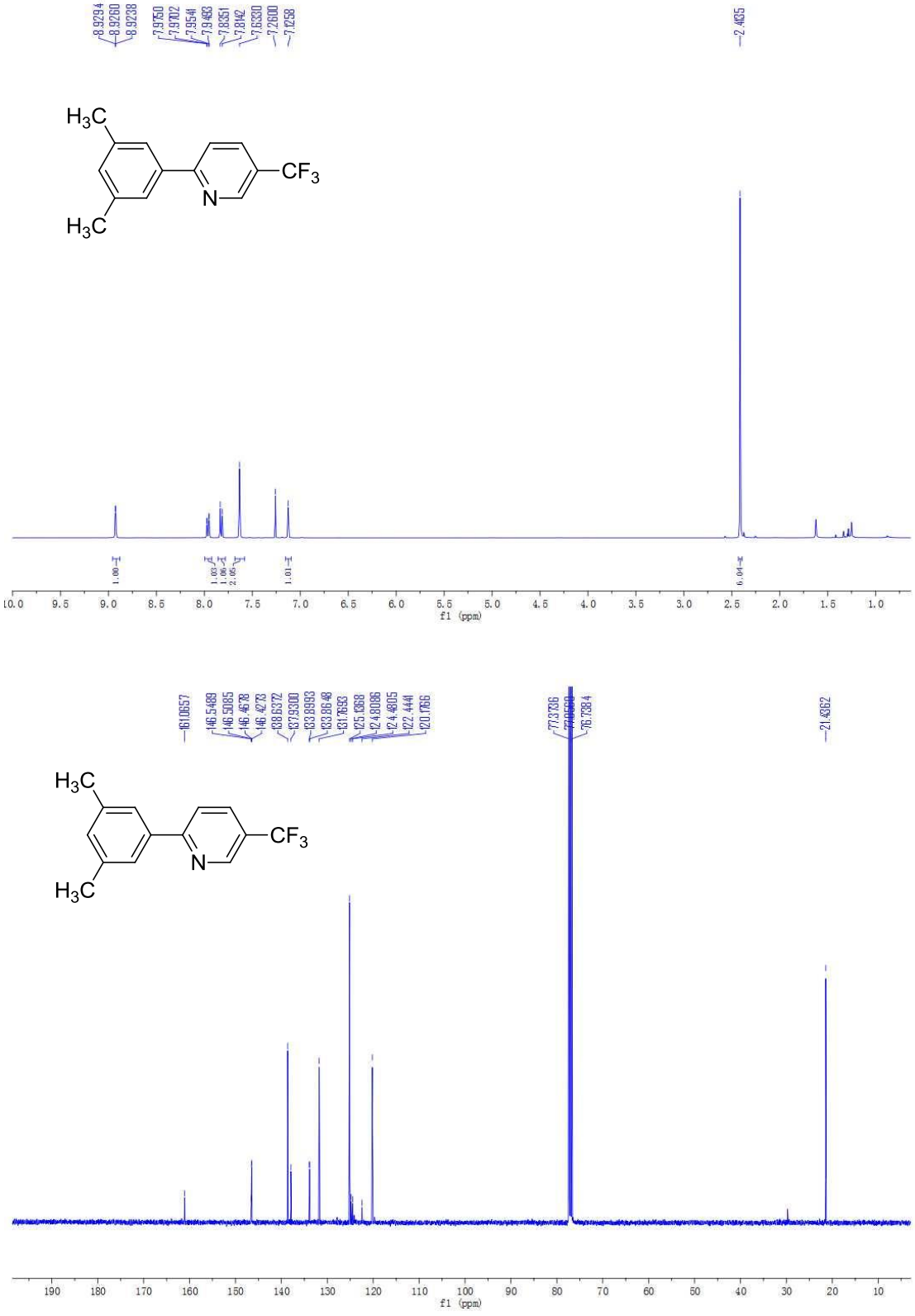

Fig.18 ^{1}H and ^{13}C NMR spectra of 2-(3,5-dimethylphenyl)-5-(trifluoromethyl)pyridine(**4d**)

6'-methoxy-5-(trifluoromethyl)-2,3'-bipyridine (4e)

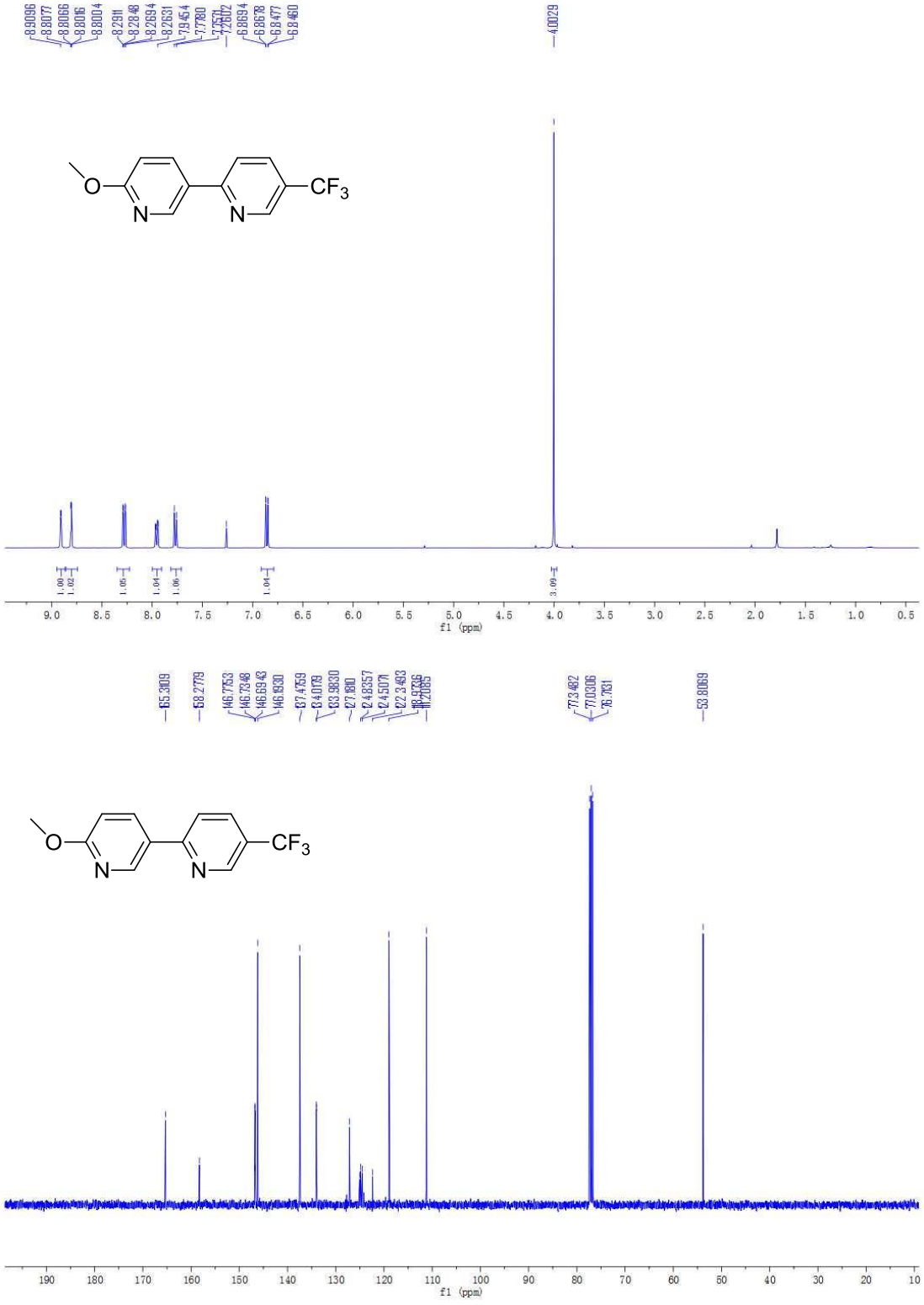

Fig.19 ^{1}H and ^{13}C NMR spectra of 6'-methoxy-5-(trifluoromethyl)-2,3'-bipyridine **(4e)**

2-(3-methoxyphenyl)-5-(trifluoromethyl)pyridine (4f)

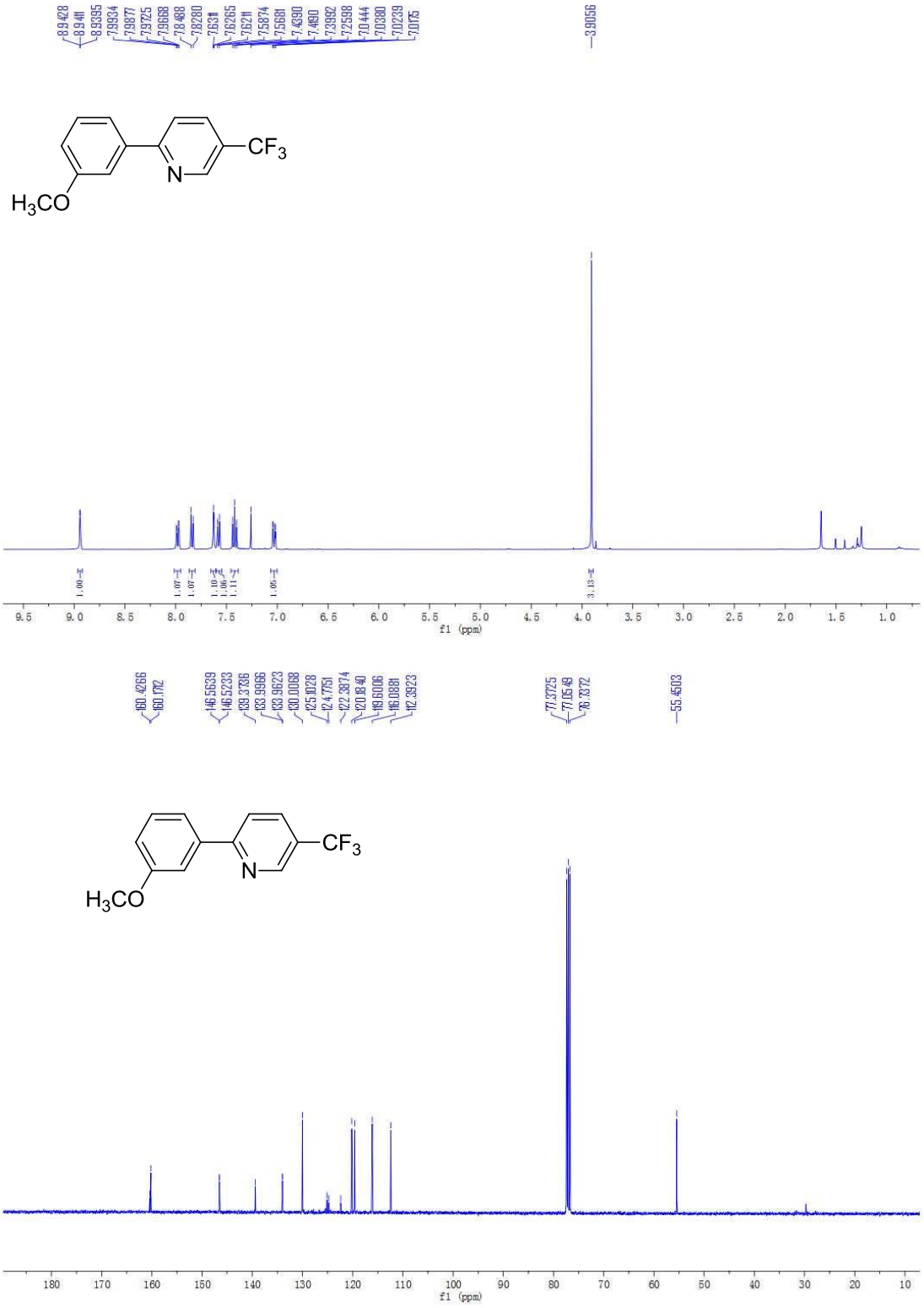

Fig. S20 ^{1}H and ^{13}C NMR spectra of 2-(3-methoxyphenyl)-5-(trifluoromethyl)pyridine (**4f**)

2-(4-phenoxyphenyl)-5-(trifluoromethyl)pyridine (4g)

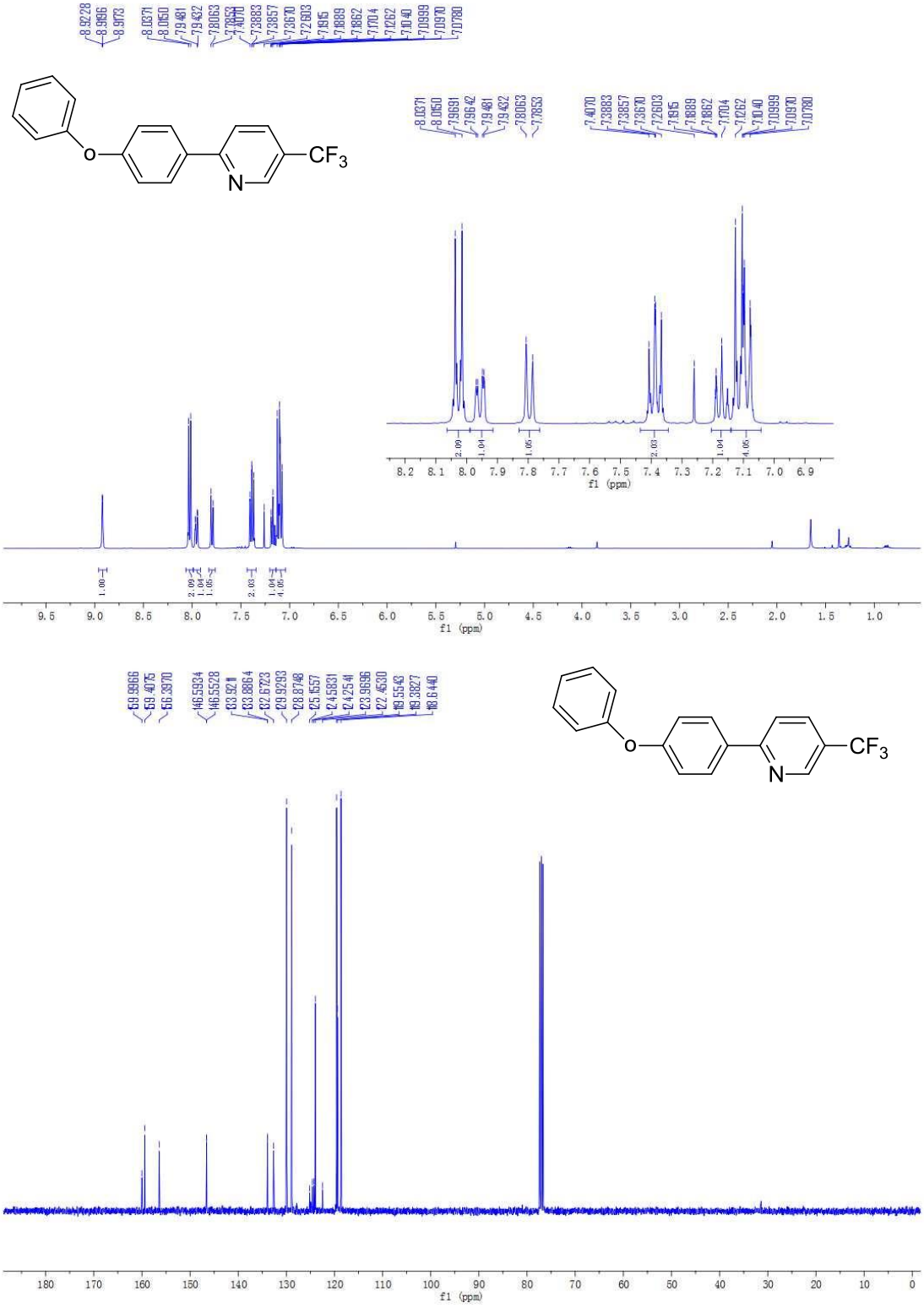

Fig. S21 ^{1}H and ^{13}C NMR spectra of 2-(4-phenoxyphenyl)-5-(trifluoromethyl)pyridine **(4g)**

2-(3-nitrophenyl)-5-(trifluoromethyl)pyridine (4h)

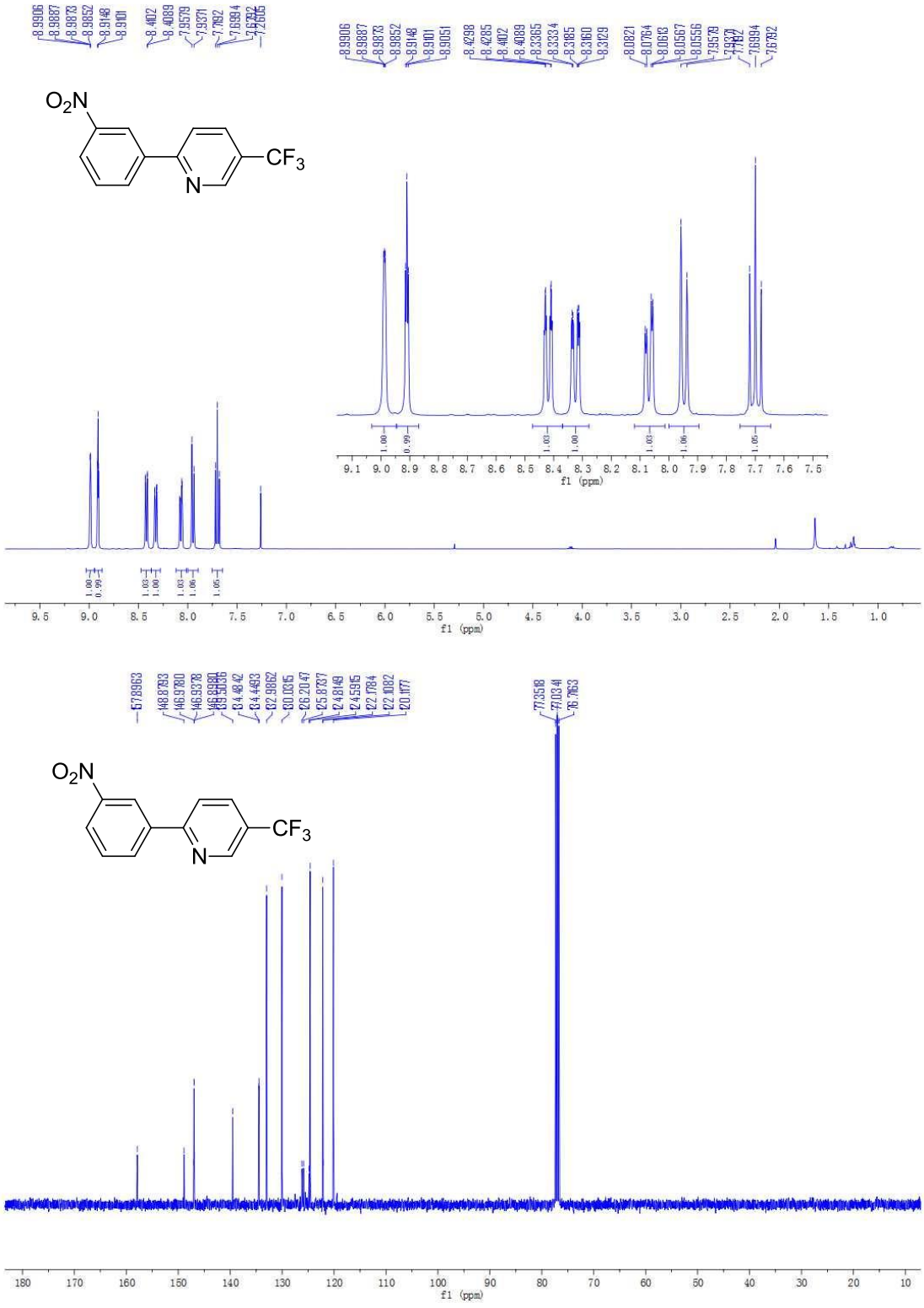

Fig. S22 ^{1}H and ^{13}C NMR spectra of 2-(3-nitrophenyl)-5-(trifluoromethyl)pyridine **(4h)**

2-(4-fluorophenyl)-5-(trifluoromethyl)pyridine (4i)

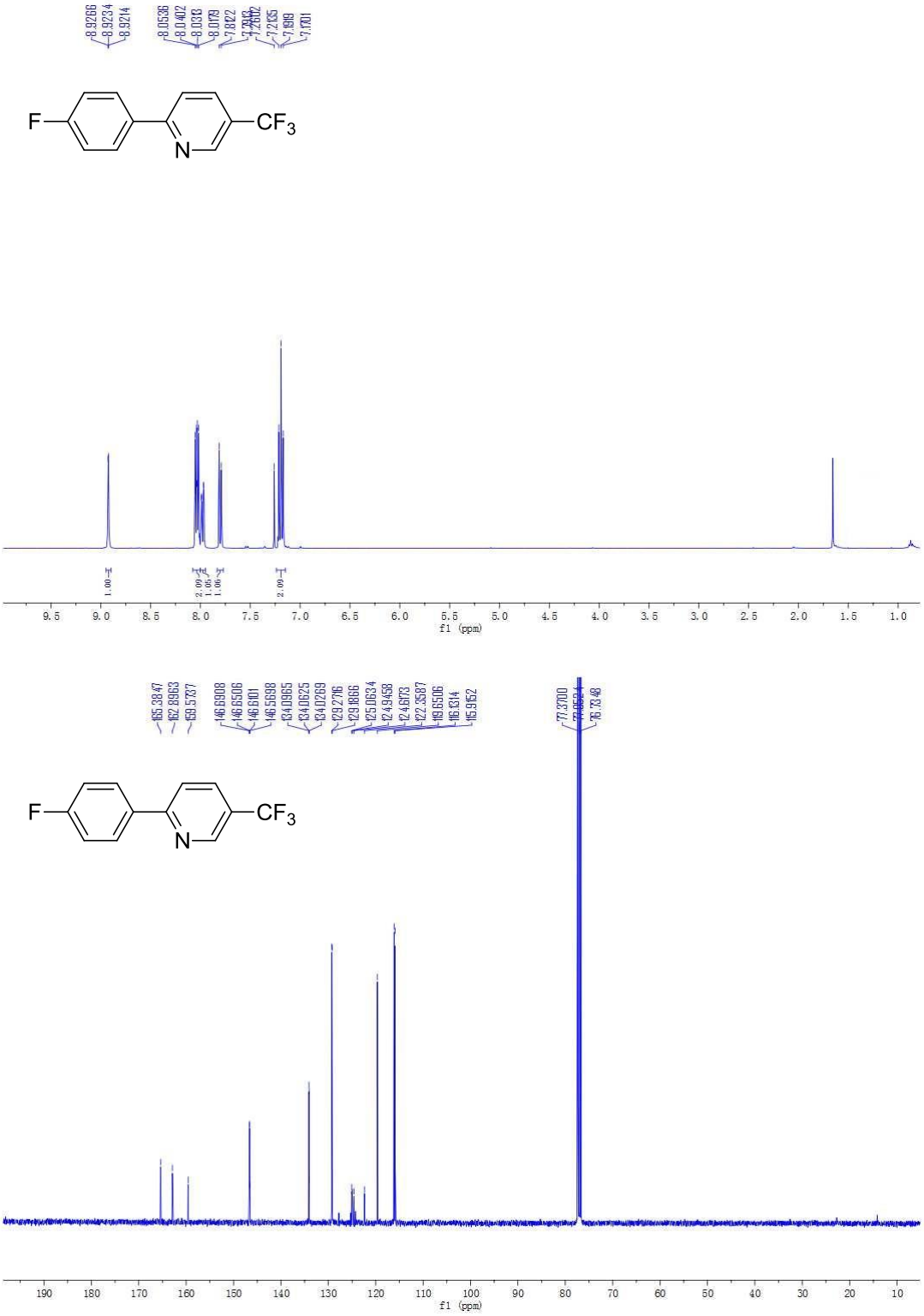

Fig. S23 ^{1}H and ^{13}C NMR spectra of
2-(4-fluorophenyl)-5-(trifluoromethyl)pyridine (**4i**)

5-(trifluoromethyl)-2-(4-(trifluoromethyl)phenyl)pyridine (4j)

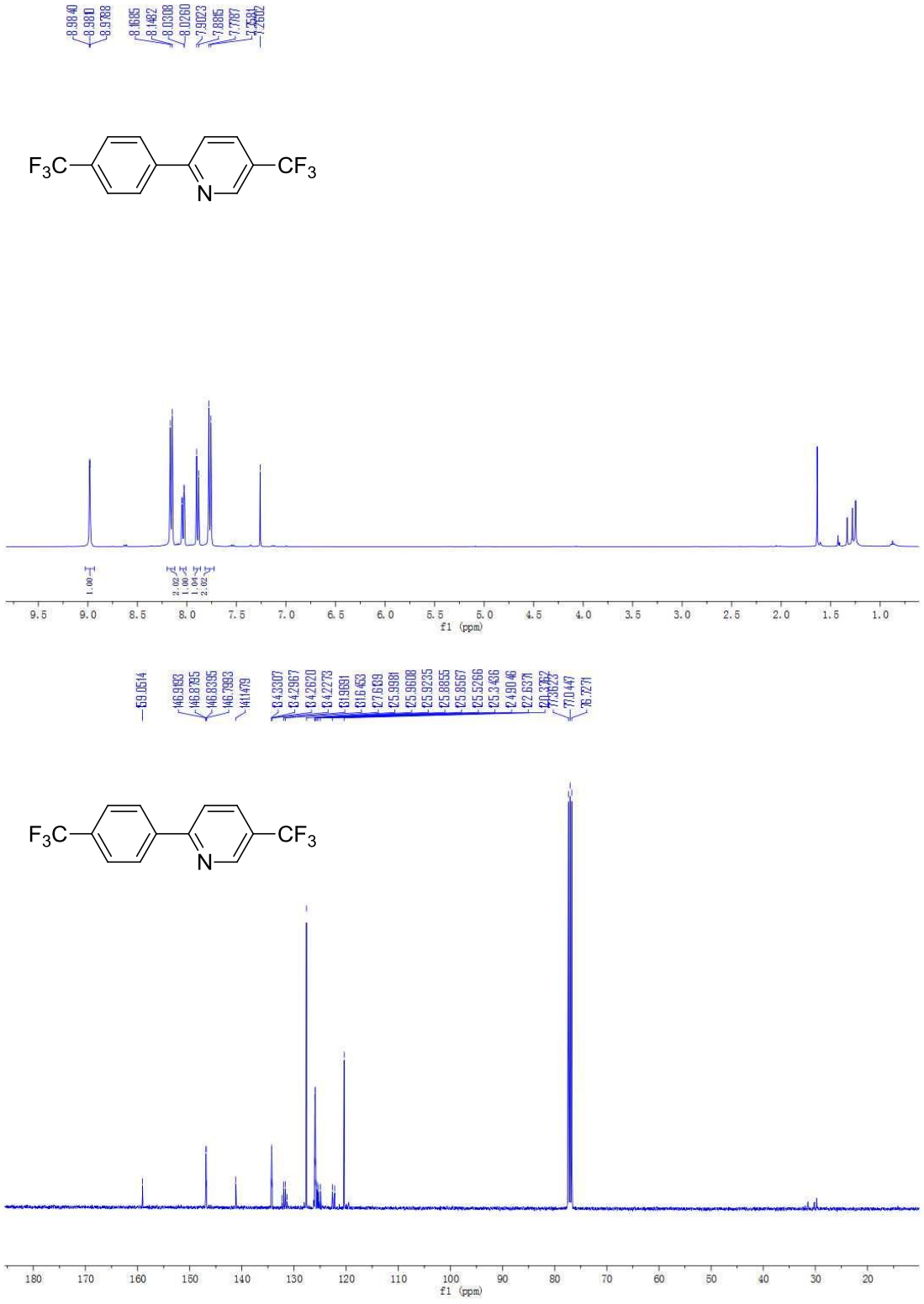

Fig. S24 ^{1}H and ^{13}C NMR spectra of 5-(trifluoromethyl)-2-(4-(trifluoromethyl)phenyl)pyridine (**4j**)

2-(3,5-bis(trifluoromethyl)phenyl)-5-(trifluoromethyl)pyridine (4k)

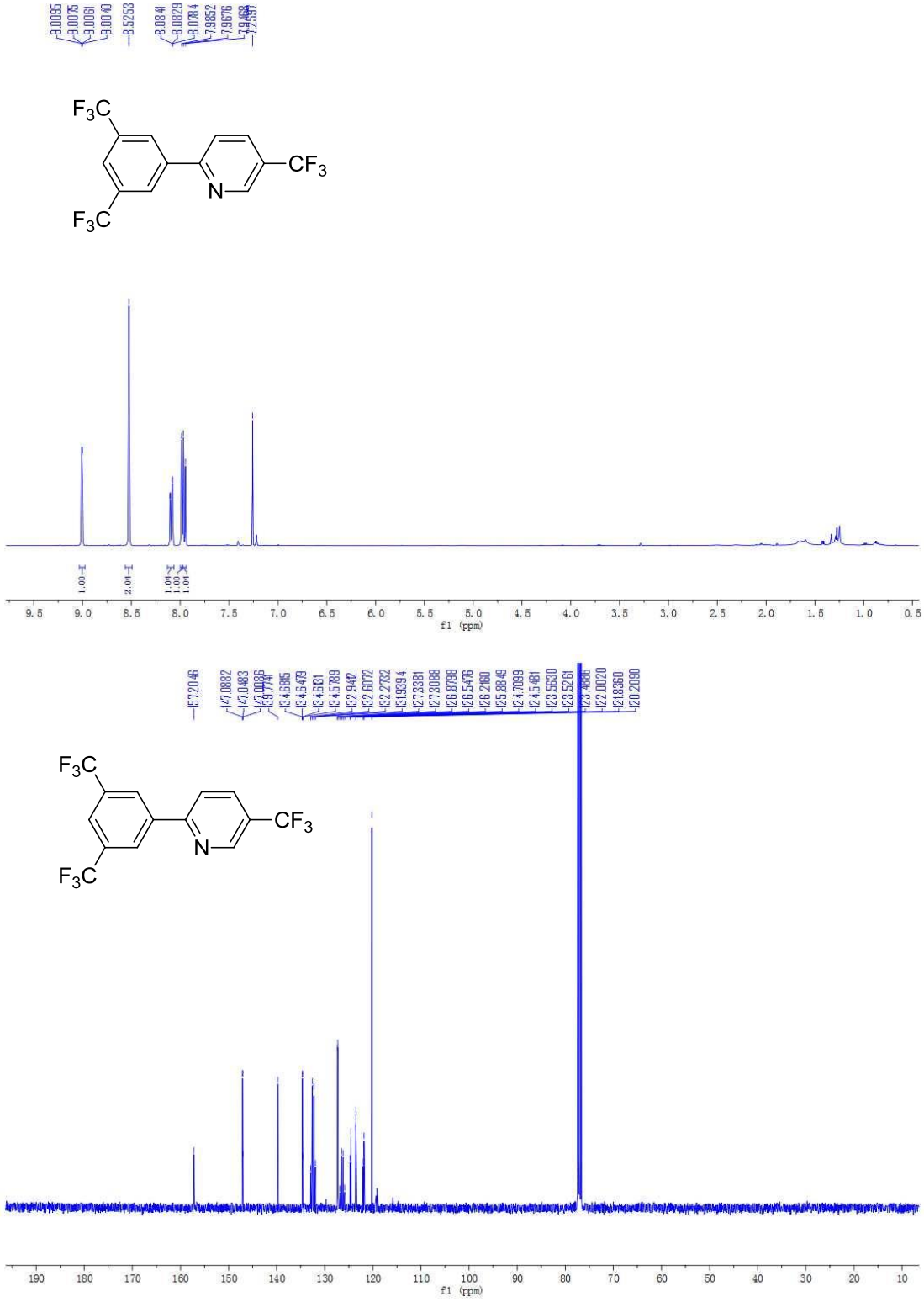

Fig. S25 ^{1}H and ^{13}C NMR spectra of
2-(3,5-bis(trifluoromethyl)phenyl)-5-(trifluoromethyl)pyridine (**4k**)

2-(naphthalen-1-yl)-5-(trifluoromethyl)pyridine (4l)

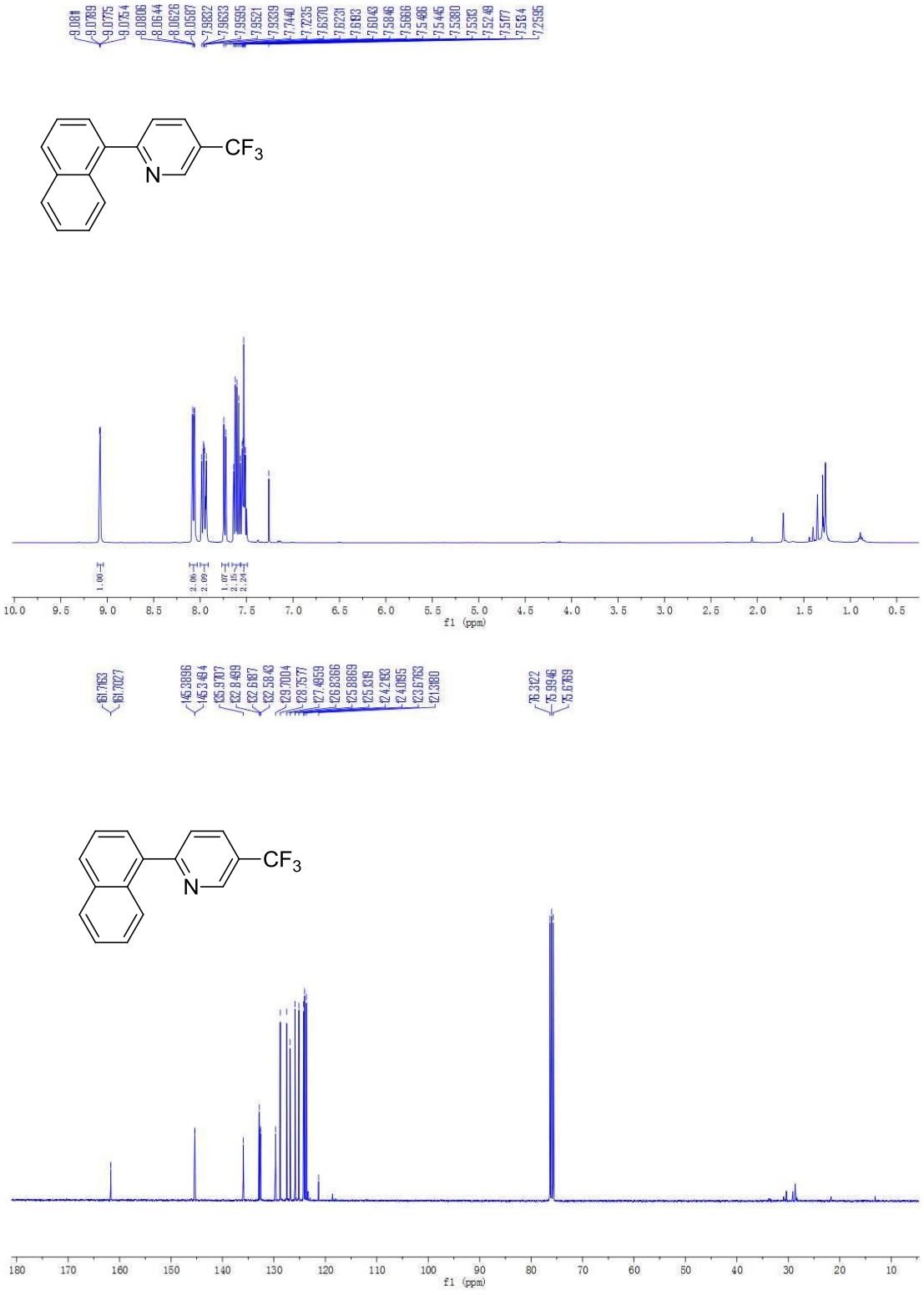

Fig. S26 ^{1}H and ^{13}C NMR spectra of
2-(naphthalen-1-yl)-5-(trifluoromethyl)pyridine (**4l**)

2-(furan-2-yl)-5-(trifluoromethyl)pyridine (4m)

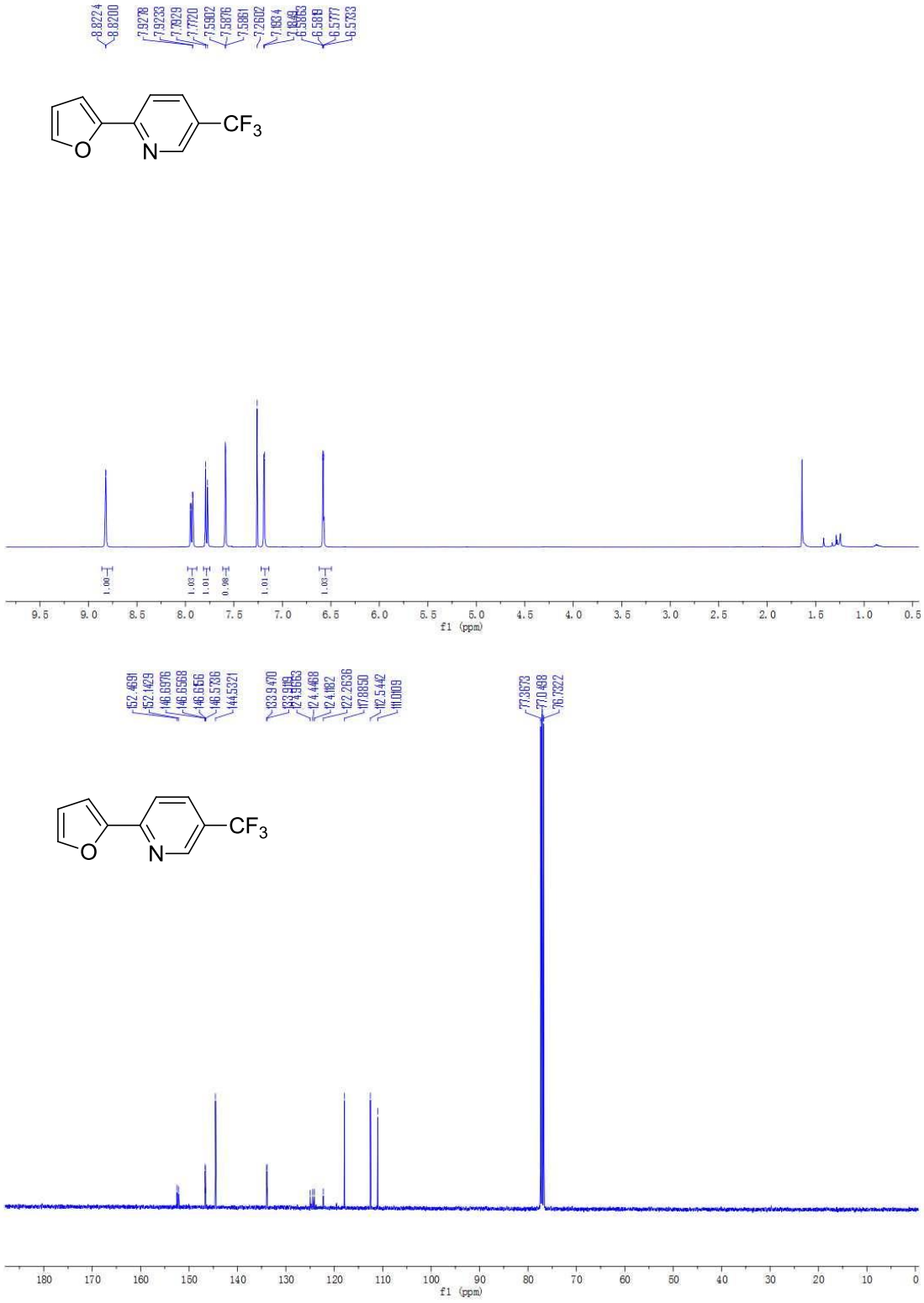

Fig.27 ^{1}H and ^{13}C NMR spectra of 2-(furan-2-yl)-5-(trifluoromethyl)pyridine(**4m**)

2-(thiophen-2-yl)-5-(trifluoromethyl)pyridine (4n)

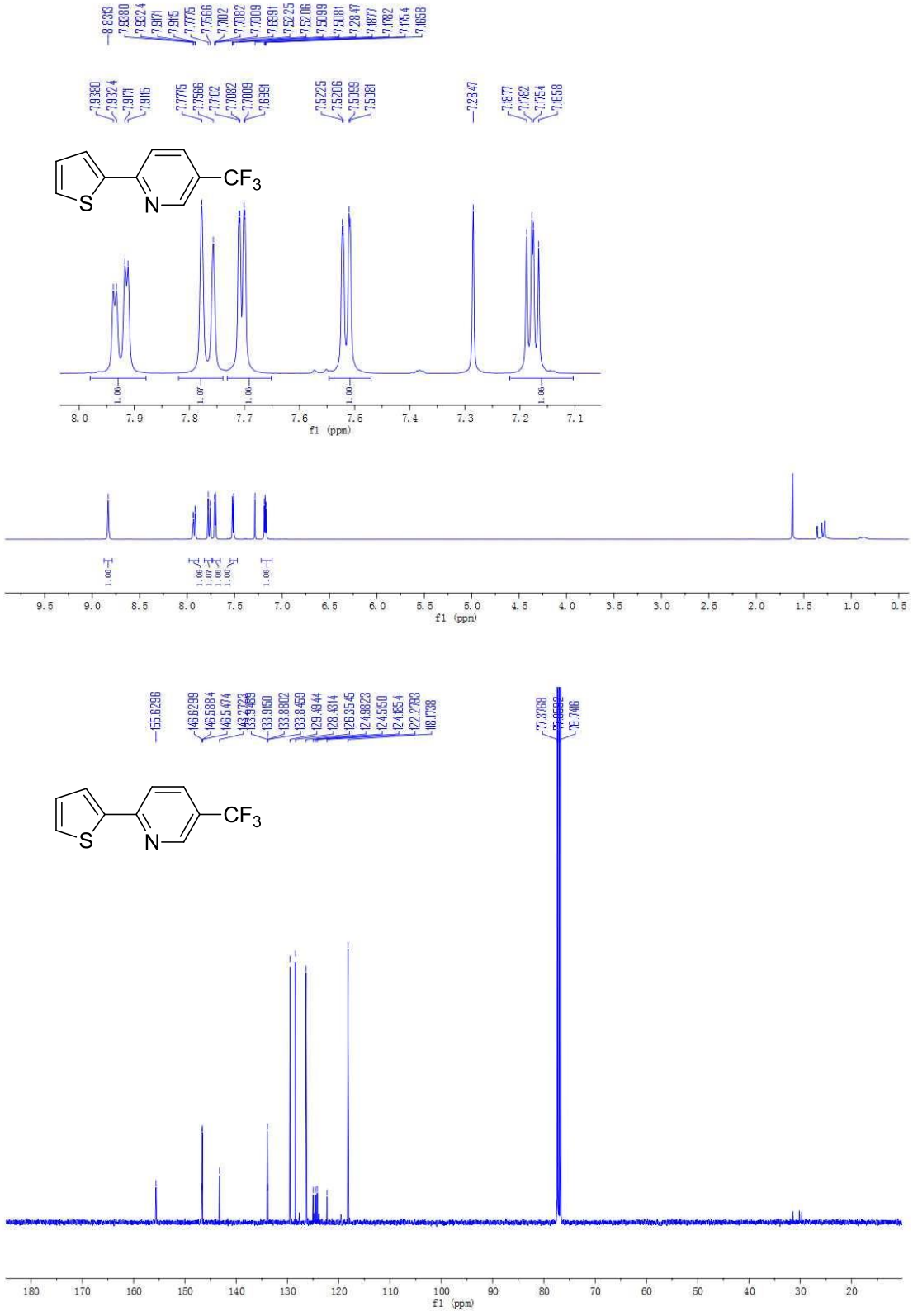

Fig. S28 ^{1}H and ^{13}C NMR spectra of
2-(thiophen-2-yl)-5-(trifluoromethyl)pyridine (**4n**)

3-(4-methoxyphenyl)pyridine (5a)

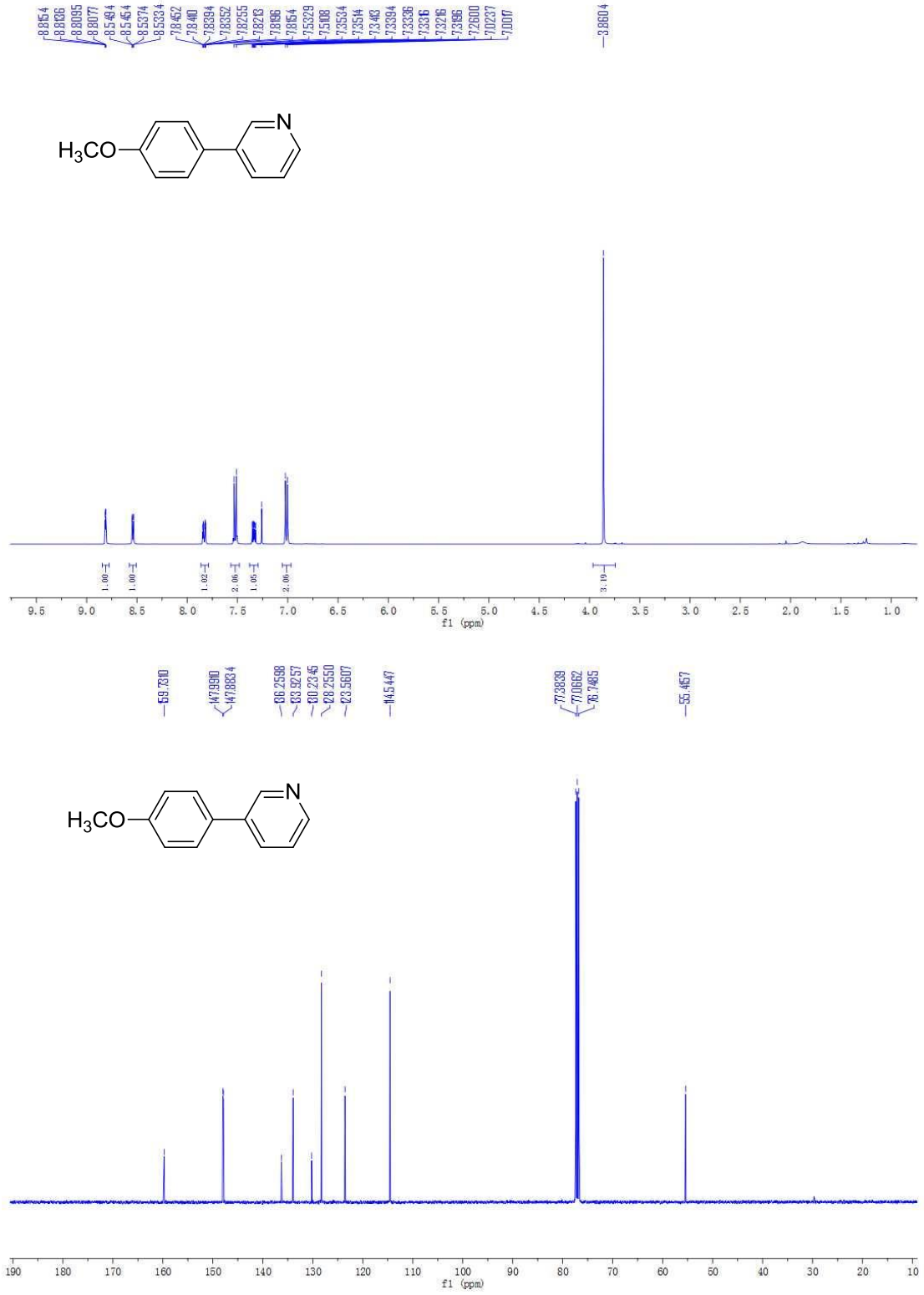

Fig. S29 ^{1}H and ^{13}C NMR spectra of 3-(4-methoxyphenyl)pyridine (**5a**)

Mass Spectrum SmartFormula Report

Analysis Info

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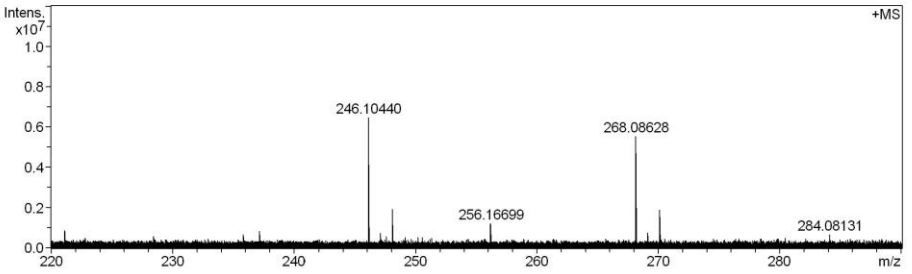
Method	NaFA-original-pos	Operator	
Sample Name	WSQ-3G	Instrument	solariX
Comment			

Acquisition Parameter

Polarity	Positive	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	86.0 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1500.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a		
Pulse Program	basic	n/a	n/a	Calibration Date	Mon Nov 30 11:06:33
Source Accumulation	0.050 sec	n/a	n/a	Data Acquisition Size	2048576
Ion Accumulation Time	0.300 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.001 sec				



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
246.10440	1	C 15 H 17 Cl N	100.00	246.10440	0.00	0.19	33.6	7.5	even	ok
268.08628	1	C 15 H 16 Cl N Na	100.00	268.08635	0.25	0.37	27.8	7.5	even	ok

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Fig. S30 HRMS spectra of **3g**

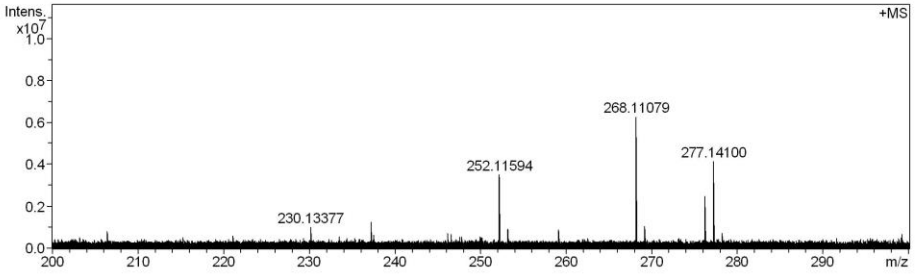
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\201511\WSQ-3H_000001.d	Acquisition Date	11/30/2015 12:17:53 PM
Method	NaFA-original-pos	Operator	
Sample Name	WSQ-3H	Instrument	solariX
Comment			

Acquisition Parameter

Polarity	Positive	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	86.0 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1500.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a		
Pulse Program	basic	n/a	n/a	Calibration Date	Mon Nov 30 11:06:33
Source Accumulation	0.050 sec	n/a	n/a	Data Acquisition Size	2048576
Ion Accumulation Time	0.300 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.001 sec				



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
252.11594	1	C 15 H 16 F N Na	100.00	252.11590	-0.18	-0.19	58.5	7.5	even	ok

Fig. S31 HRMS spectra of **3h**

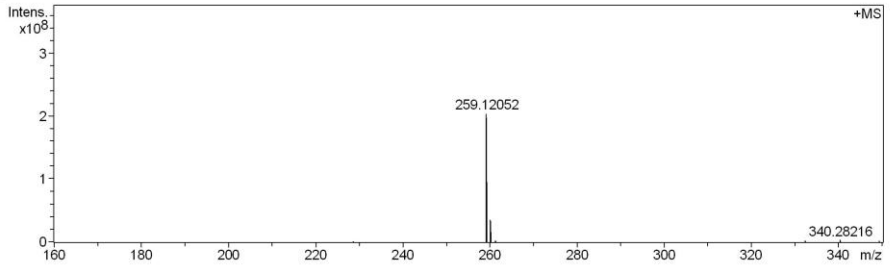
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\201511\WSQ-3I_000001.d	Acquisition Date	11/30/2015 1:25:44 PM
Method	NaFA-original-pos	Operator	
Sample Name	WSQ-3I	Instrument	solariX
Comment			

Acquisition Parameter

Polarity	Positive	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	86.0 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1500.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a		
Pulse Program	basic	n/a	n/a	Calibration Date	Mon Nov 30 11:06:33
Source Accumulation	0.050 sec	n/a	n/a	Data Acquisition Size	2048576
Ion Accumulation Time	0.300 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.001 sec				



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
259.12052	1	C 16 H 16 N 2 Na	100.00	259.12057	0.18	0.15	2.6	9.5	even	ok

Fig. S32 HRMS spectra of **3i**

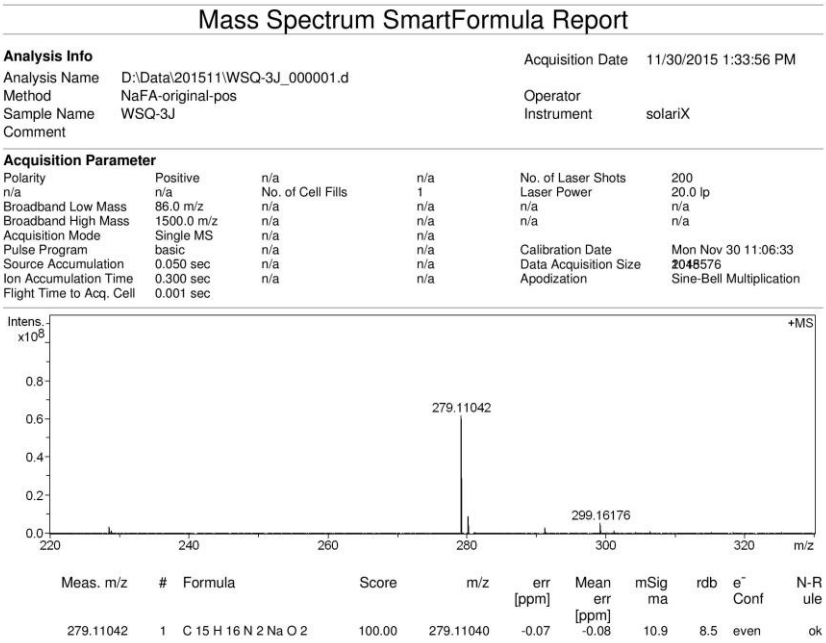


Fig. S33 HRMS spectra of **3j**

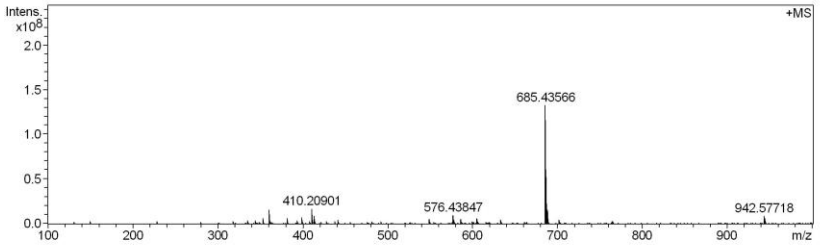
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\201511\WSQ-3K_000001.d	Acquisition Date	11/30/2015 1:43:55 PM
Method	NaFA-original-pos	Operator	
Sample Name	WSQ-3K	Instrument	solariX
Comment			

Acquisition Parameter

Polarity	Positive	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	86.0 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1500.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a		
Pulse Program	basic	n/a	n/a	Calibration Date	Mon Nov 30 11:06:33
Source Accumulation	0.050 sec	n/a	n/a	Data Acquisition Size	2048576
Ion Accumulation Time	0.300 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.001 sec				



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
302.11264	1	C 16 H 16 F 3 N Na	100.00	302.11271	0.23	0.23	102.4	7.5	even	ok

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Fig. S34 HRMS spectra of **3k**

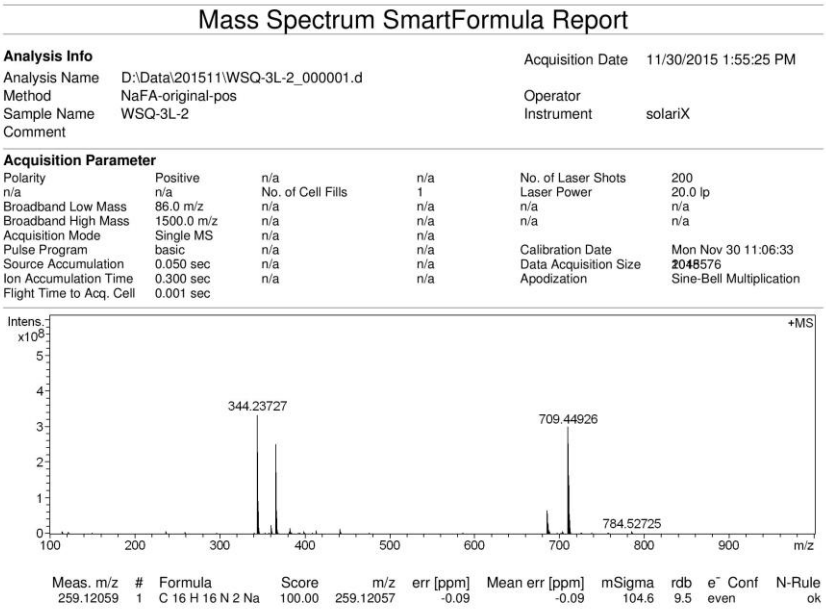


Fig. S35 HRMS spectra of **3l**

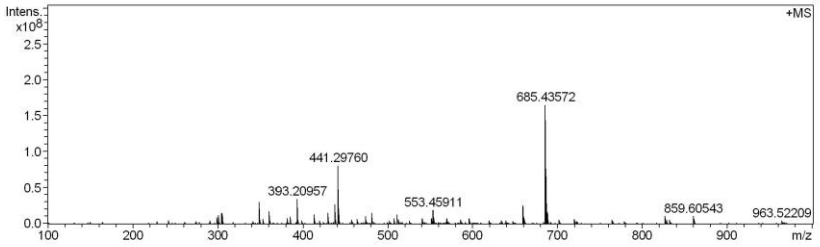
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\201511\WSQ-4H_000001.d	Acquisition Date	11/30/2015 2:31:15 PM
Method	NaFA-original-pos	Operator	
Sample Name	WSQ-4H	Instrument	solariX
Comment			

Acquisition Parameter

Polarity	Positive	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	86.0 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1500.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a		
Pulse Program	basic	n/a	n/a	Calibration Date	Mon Nov 30 11:06:33
Source Accumulation	0.050 sec	n/a	n/a	Data Acquisition Size	2048576
Ion Accumulation Time	0.300 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.001 sec				



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
291.03528	1	C 12 H 7 F 3 N 2 Na O 2	100.00	291.03518	-0.33	-0.28	7.6	8.5	even	ok

Fig. S36 HRMS spectra of **4h**

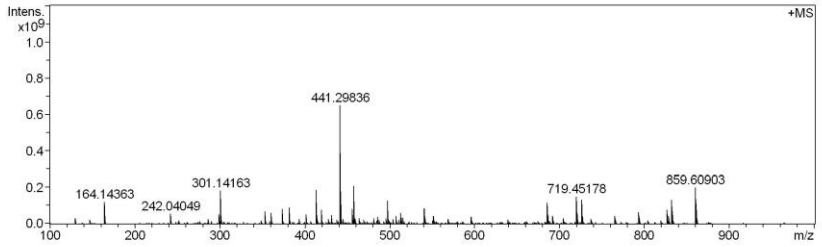
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\201511\WSQ-4M-2_000001.d	Acquisition Date	11/30/2015 3:34:23 PM
Method	NaFA-original-pos	Operator	
Sample Name	WSQ-4M-2	Instrument	solariX
Comment			

Acquisition Parameter

Polarity	Positive	n/a	n/a	No. of Laser Shots	200
n/a	n/a	No. of Cell Fills	1	Laser Power	20.0 lp
Broadband Low Mass	86.0 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1500.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a		
Pulse Program	basic	n/a	n/a	Calibration Date	Mon Nov 30 11:06:33
Source Accumulation	0.050 sec	n/a	n/a	Data Acquisition Size	2048576
Ion Accumulation Time	0.300 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.001 sec				



Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
214.04789	1	C 10 H 7 F 3 N O	100.00	214.04742	-2.16	-2.16	64.7	6.5	even	ok

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Fig. S37 HRMS spectra of **4m**

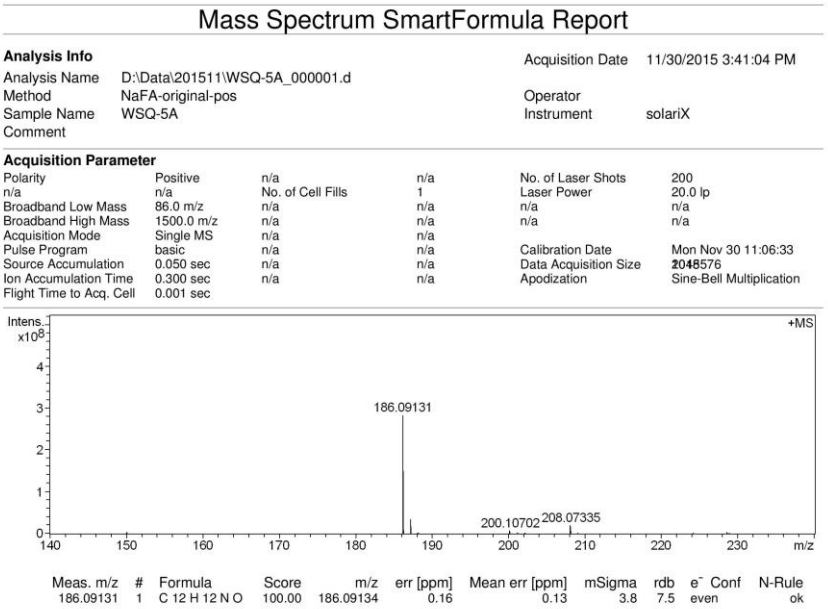

Fig. S38 HRMS spectra of **5a**