

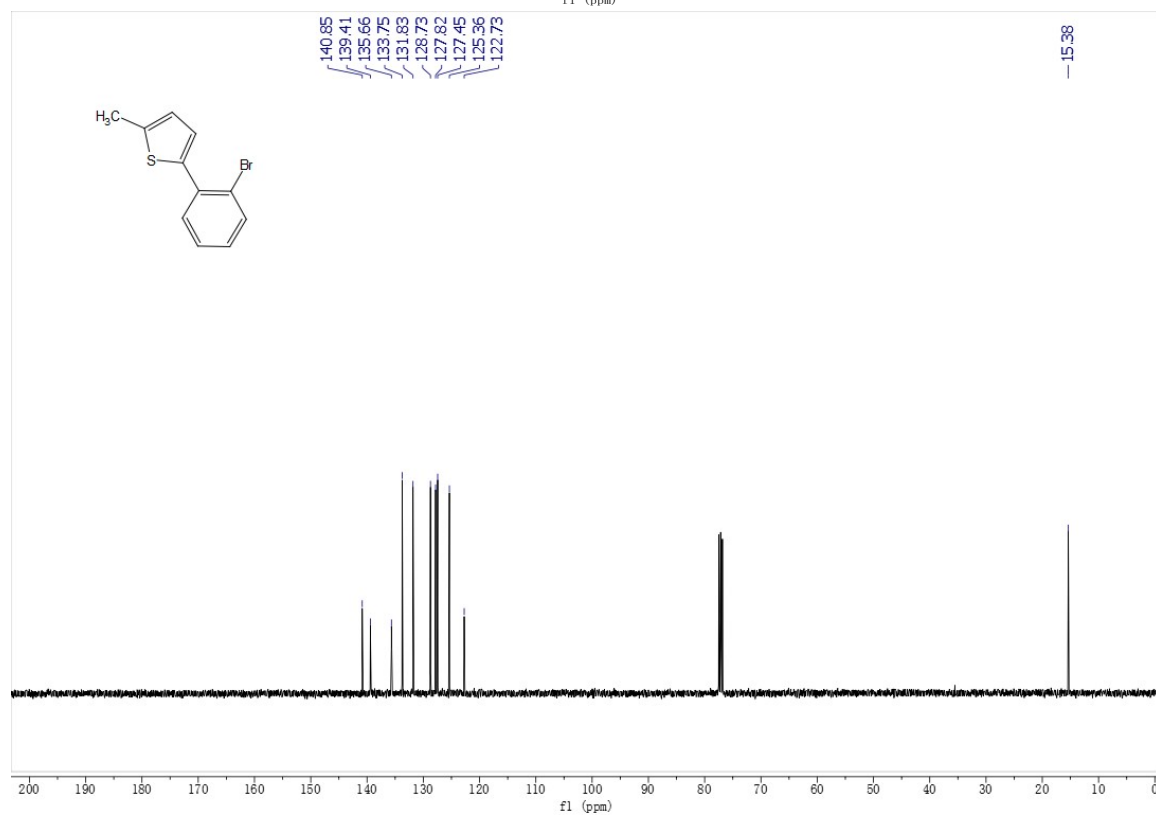
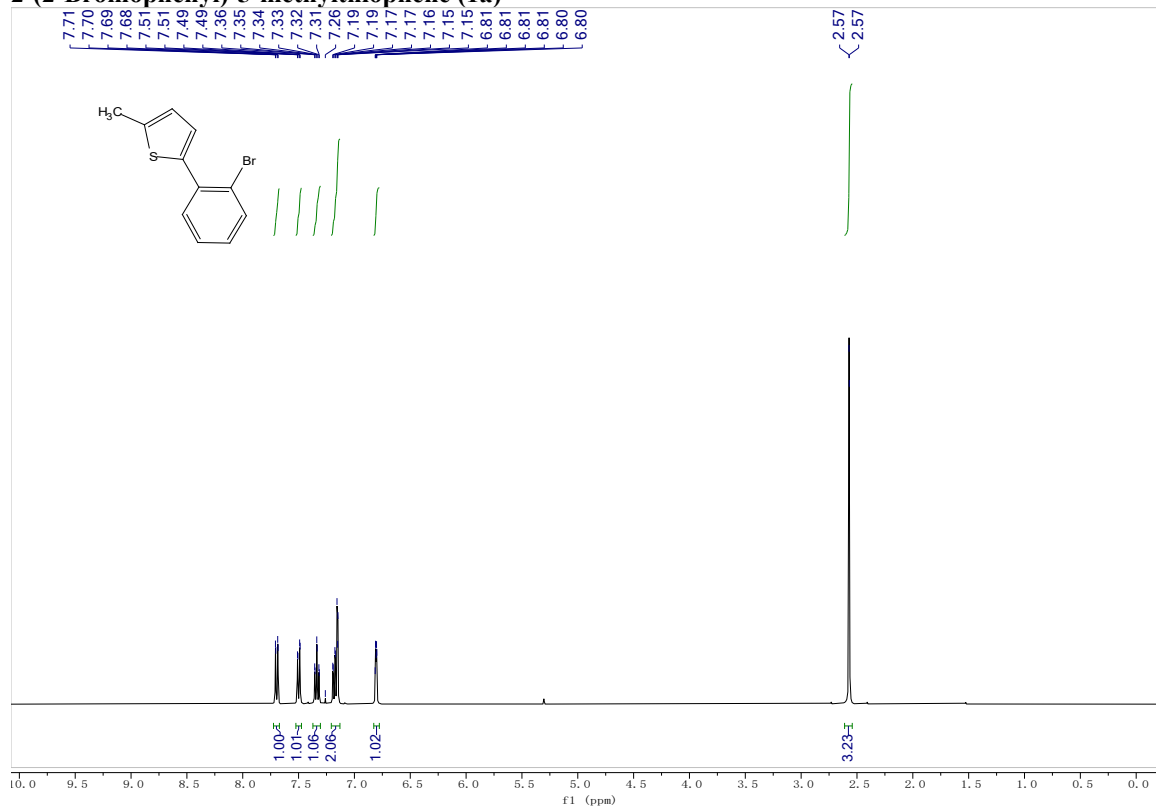
Double C-H Bond Functionalization for C-C Coupling at β -Position of Thiophenes using Palladium-catalyzed 1,4-Migration Associated to Direct Arylation

Linhao Liu, Marie Cordier, Thierry Roisnel, Henri Doucet

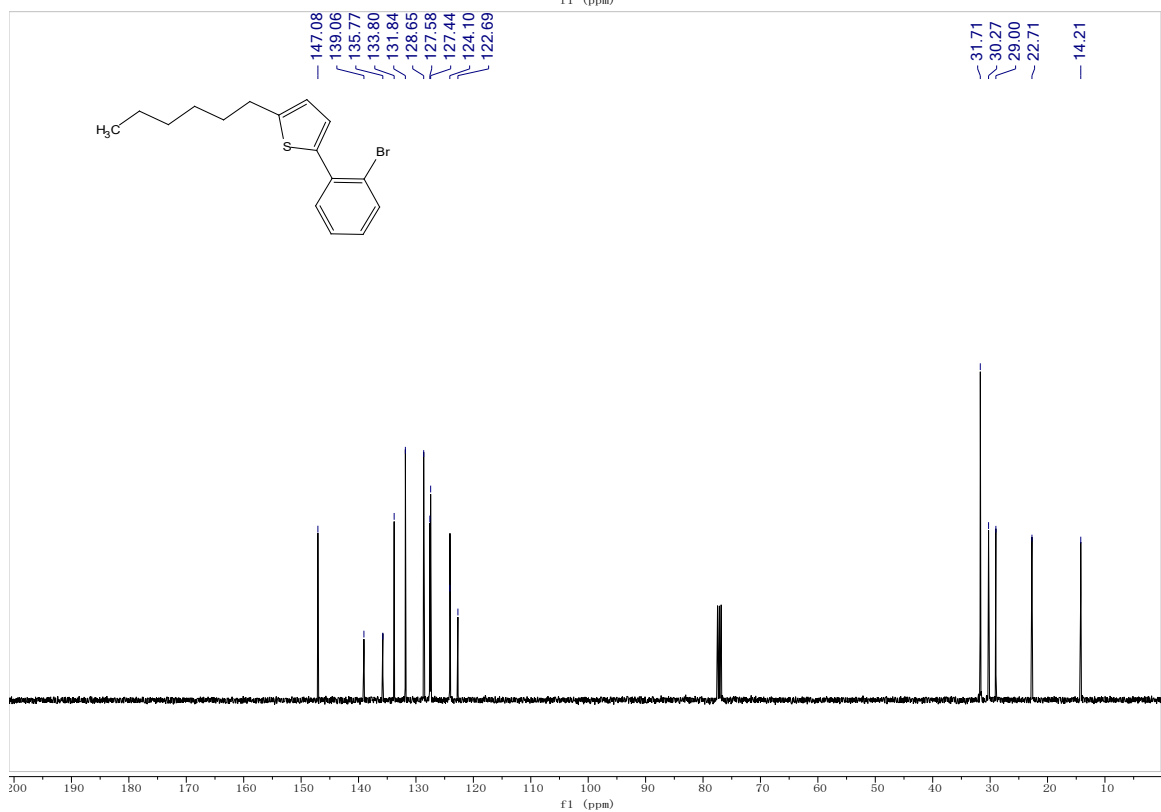
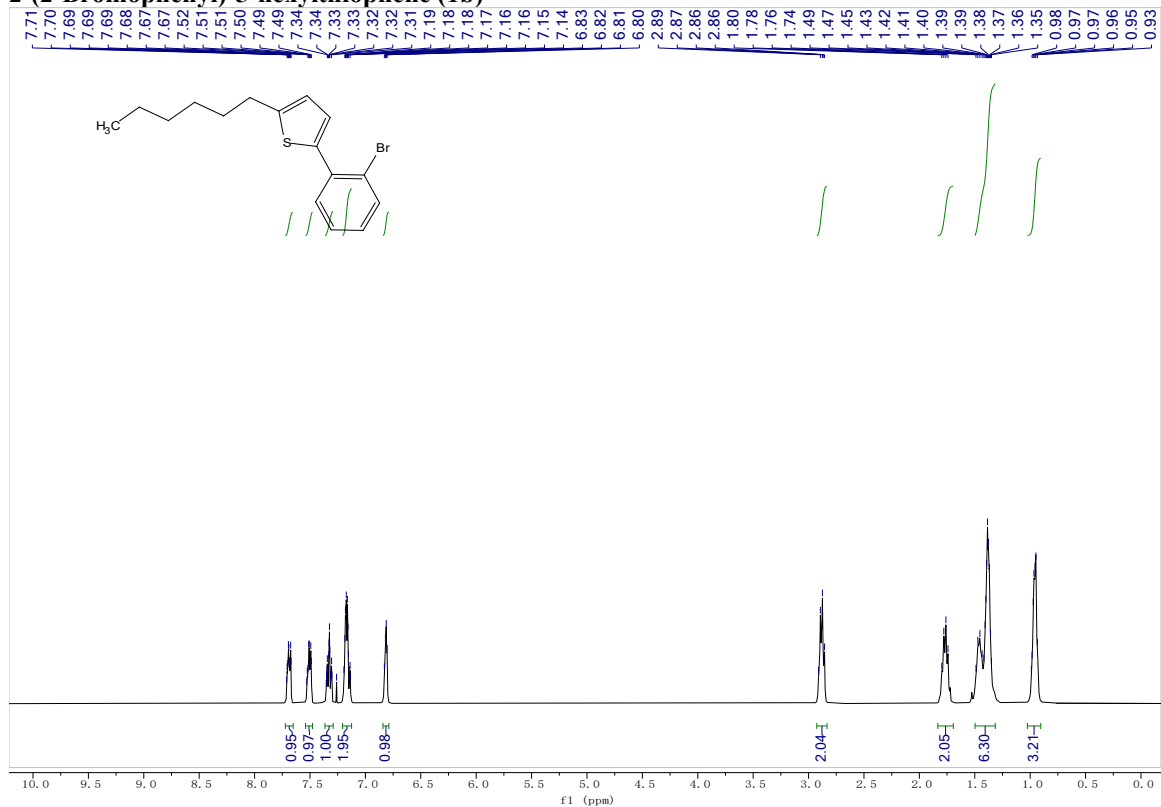
Copies of NMR spectra of all compounds

S2-S49

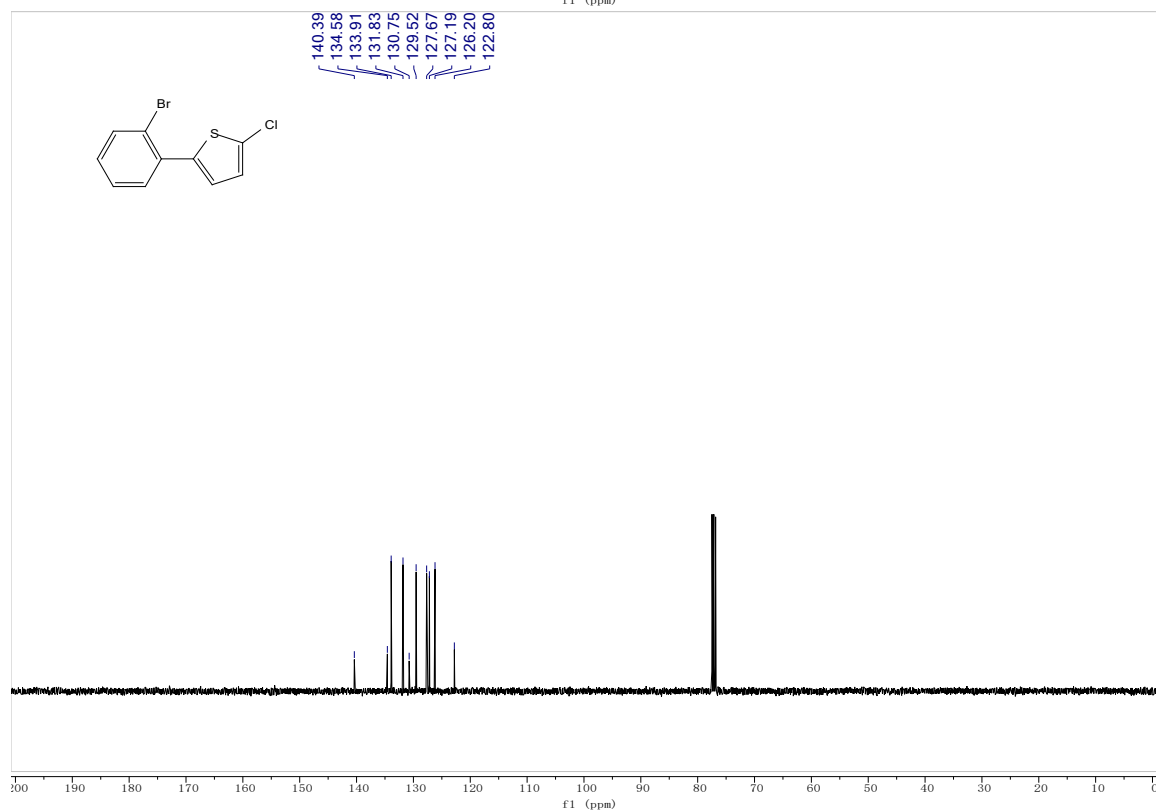
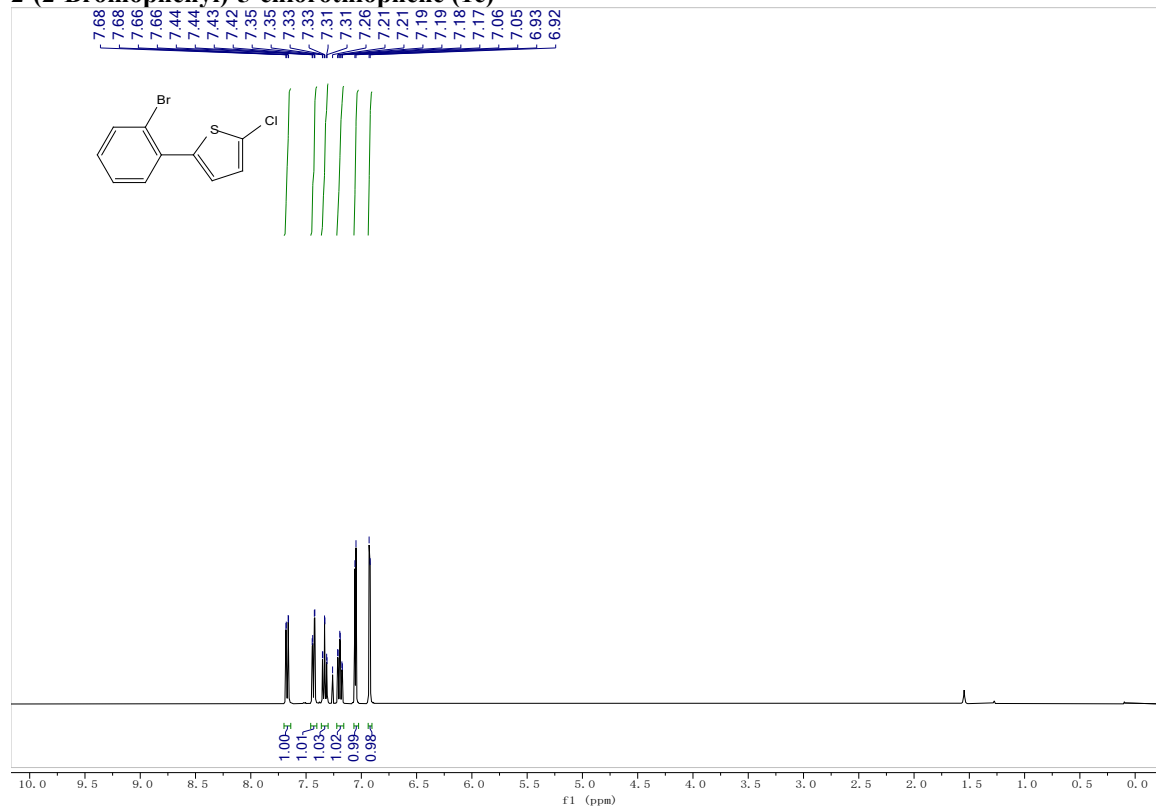
2-(2-Bromophenyl)-5-methylthiophene (1a)



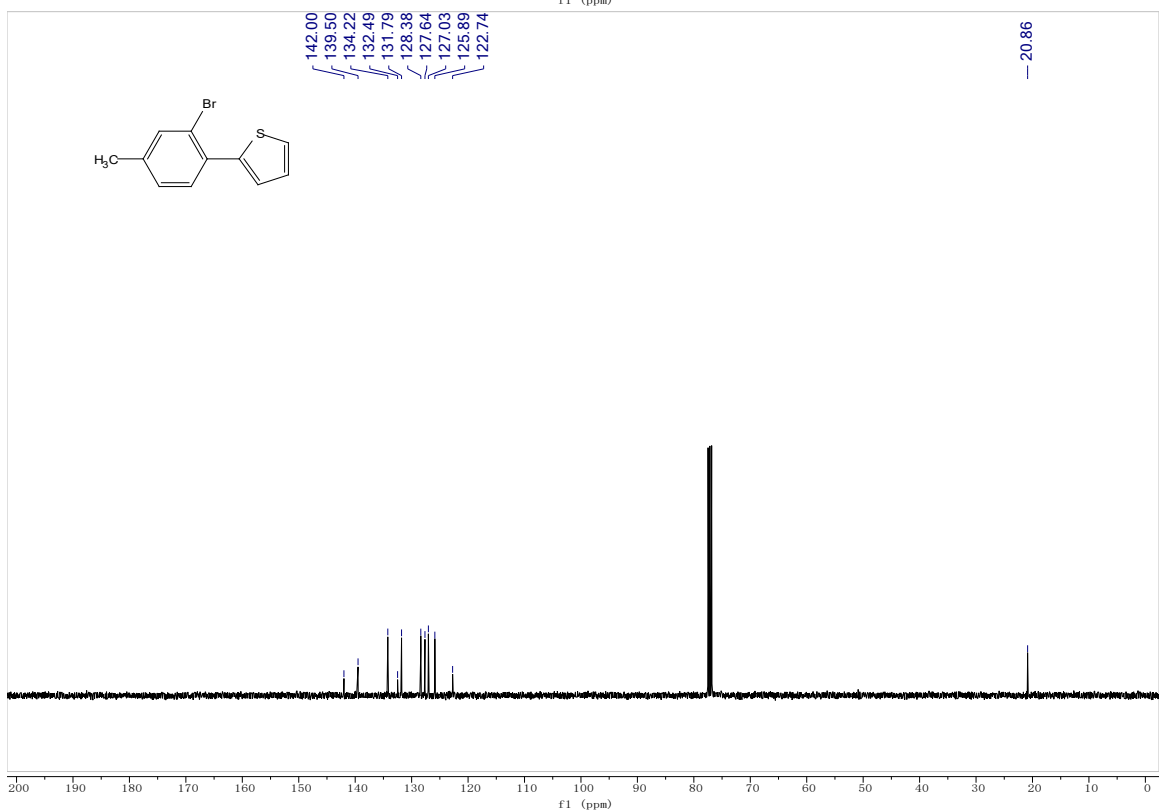
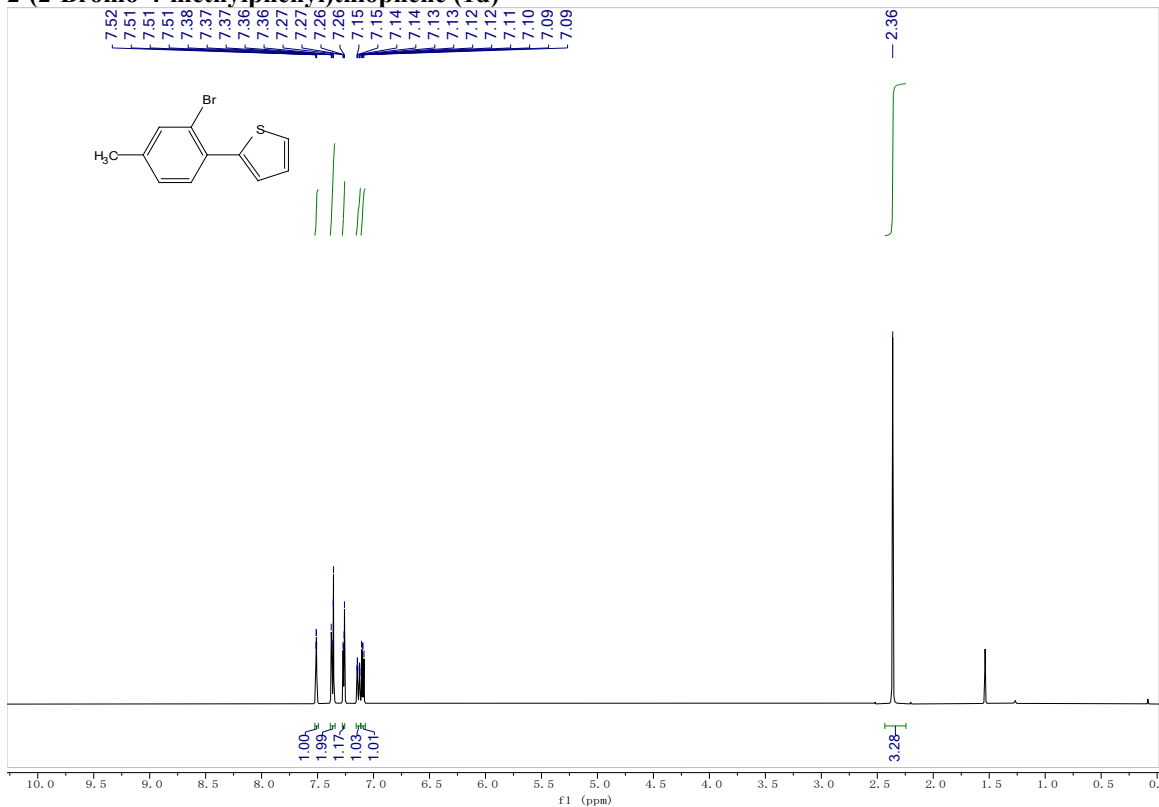
2-(2-Bromophenyl)-5-hexylthiophene (1b)



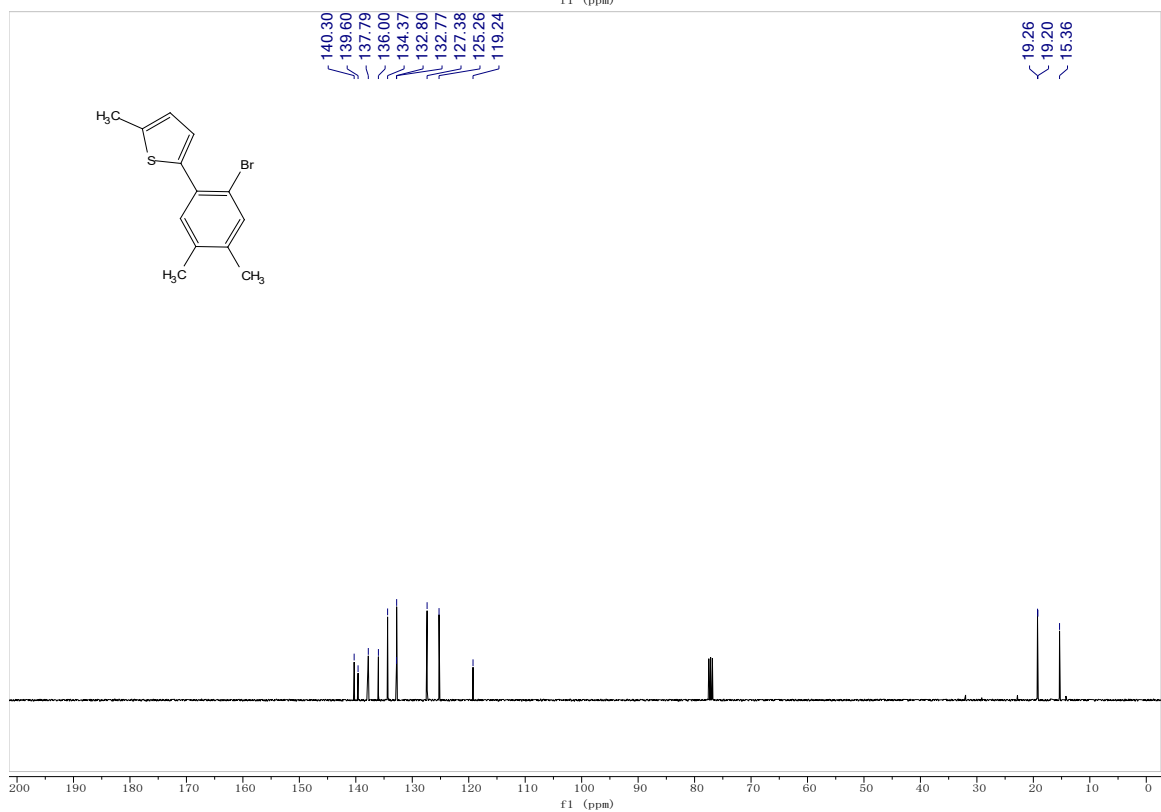
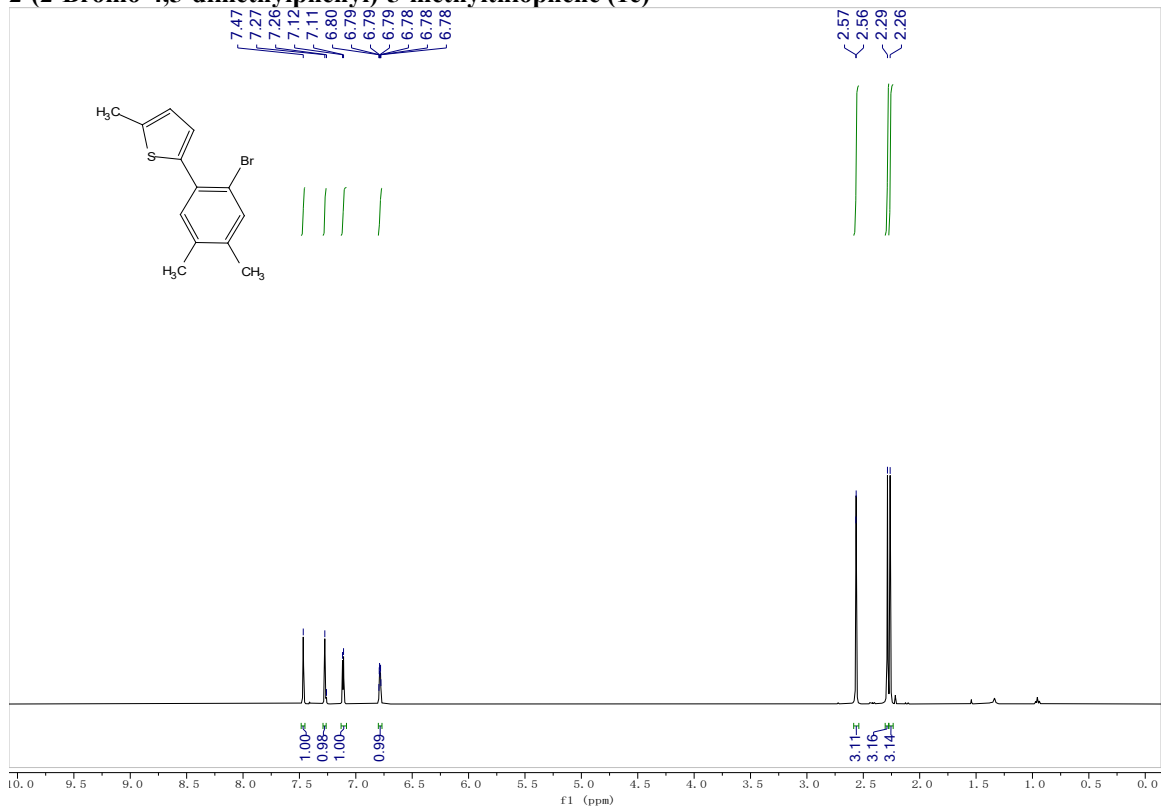
2-(2-Bromophenyl)-5-chlorothiophene (1c)



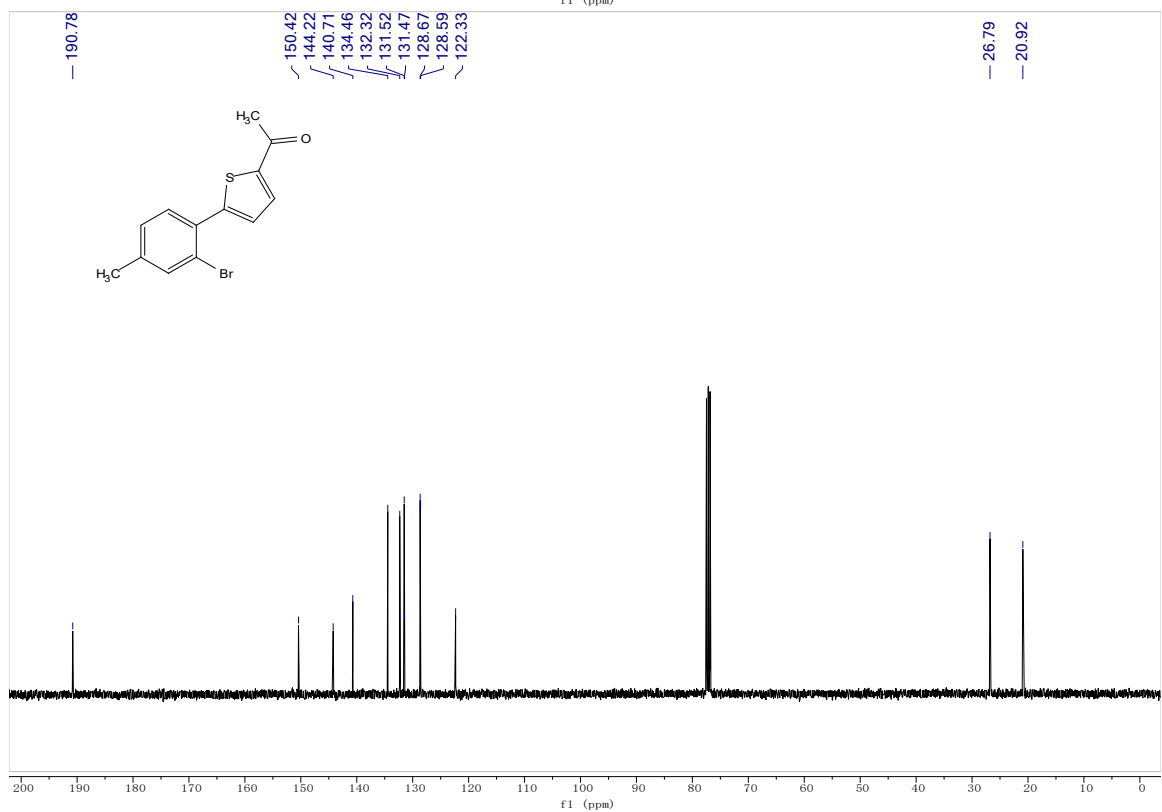
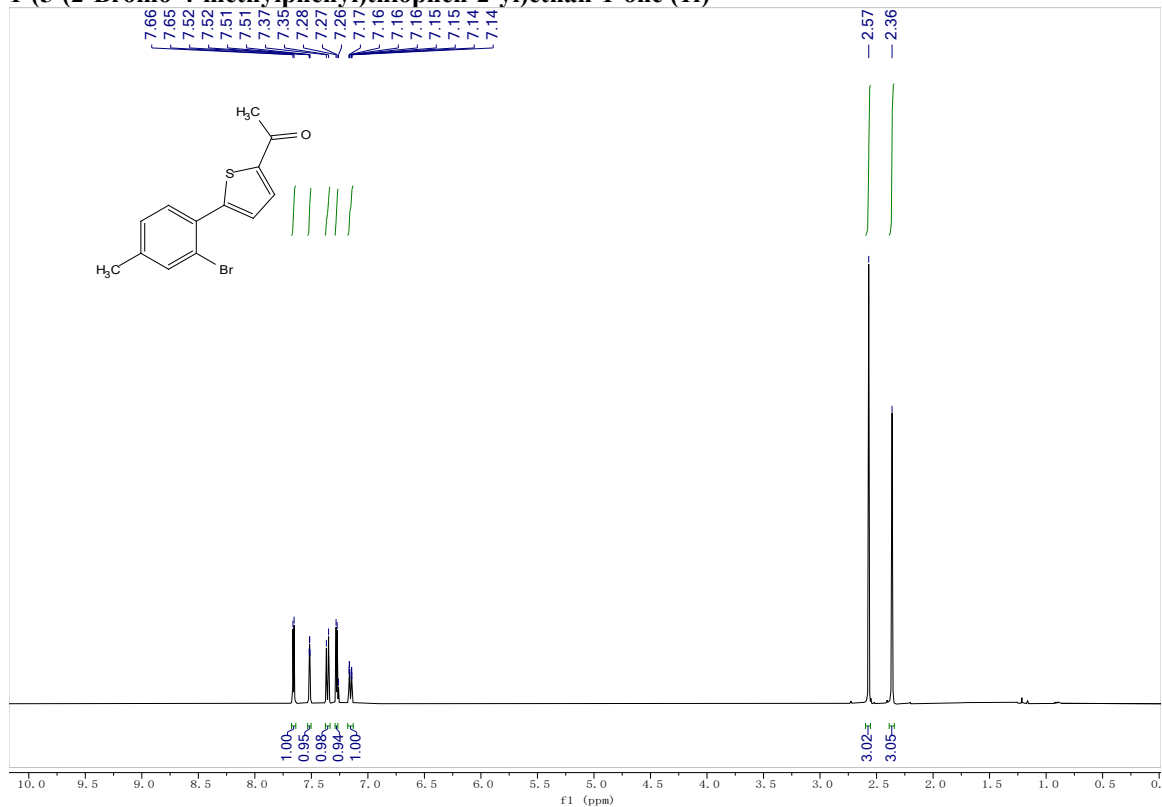
2-(2-Bromo-4-methylphenyl)thiophene (1d)



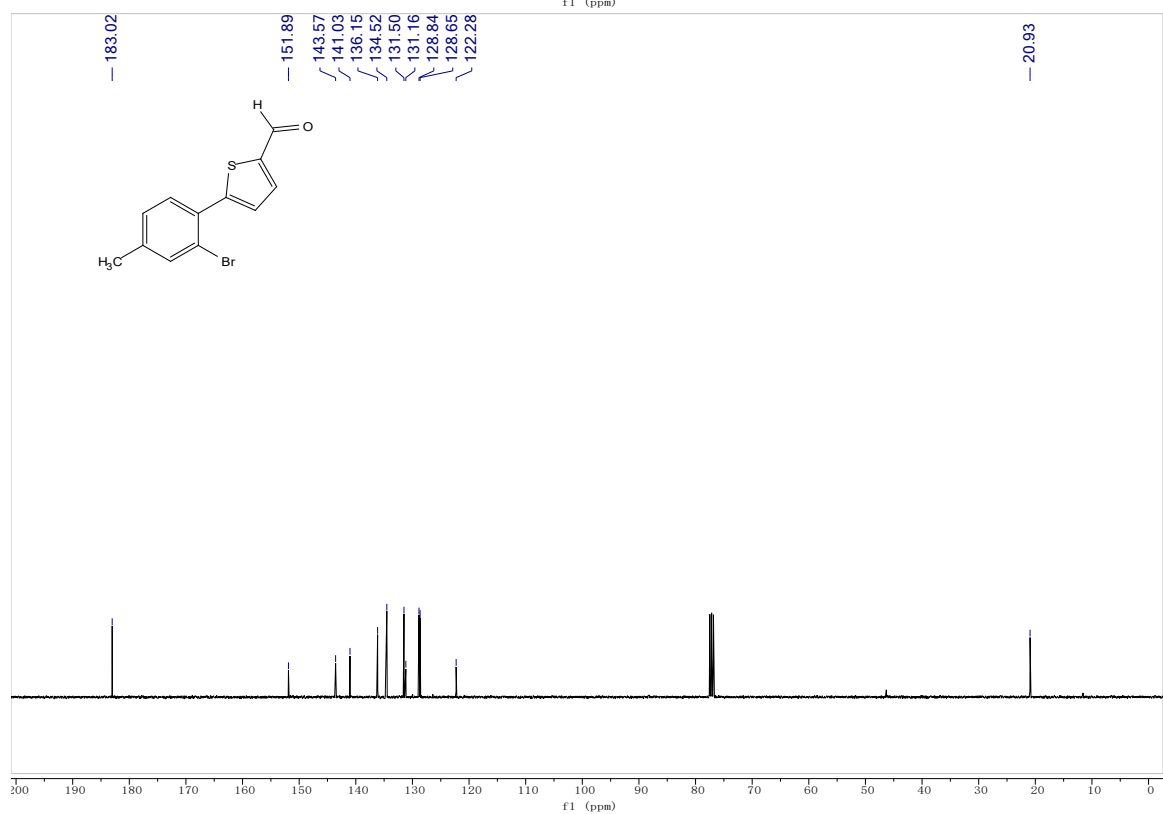
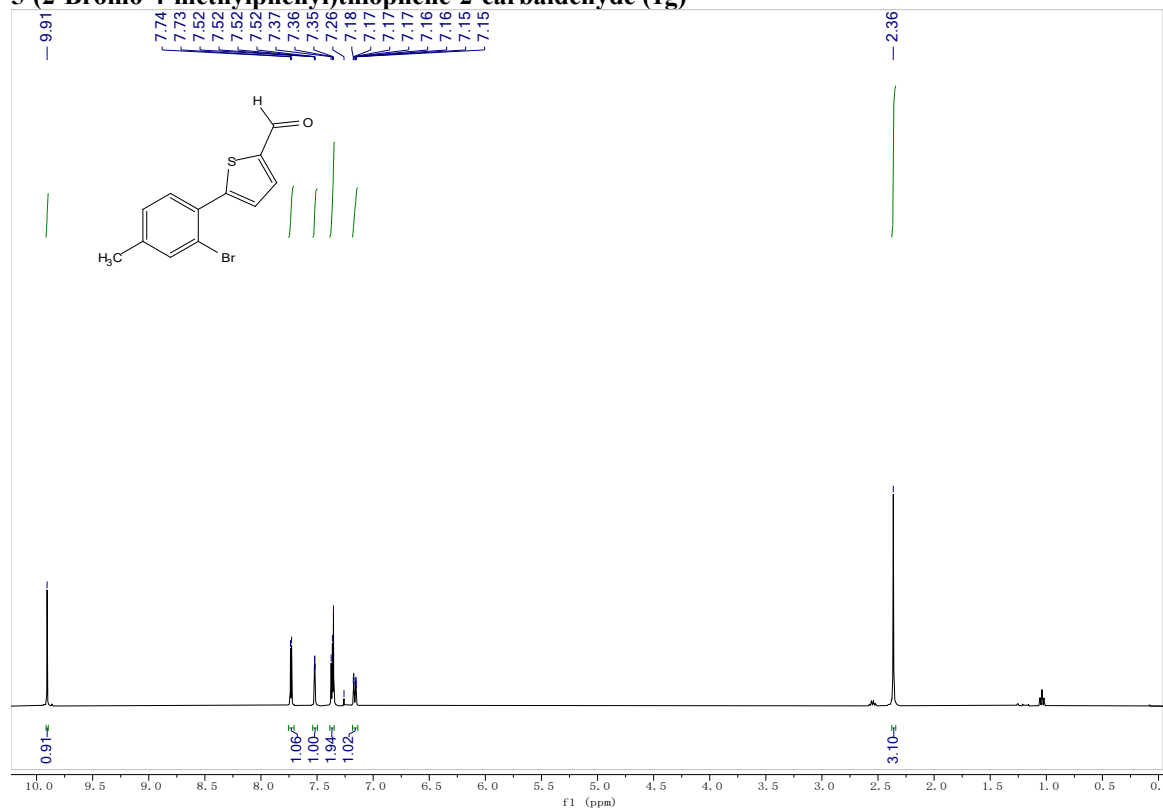
2-(2-Bromo-4,5-dimethylphenyl)-5-methylthiophene (1e)



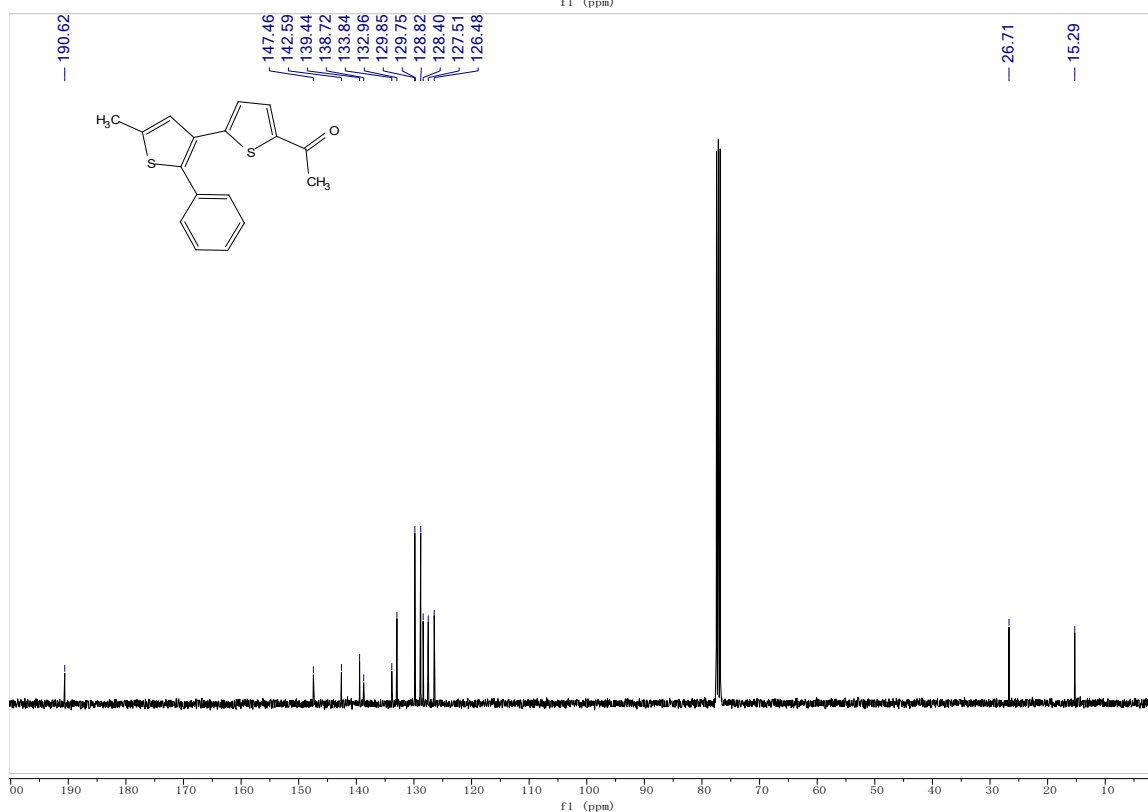
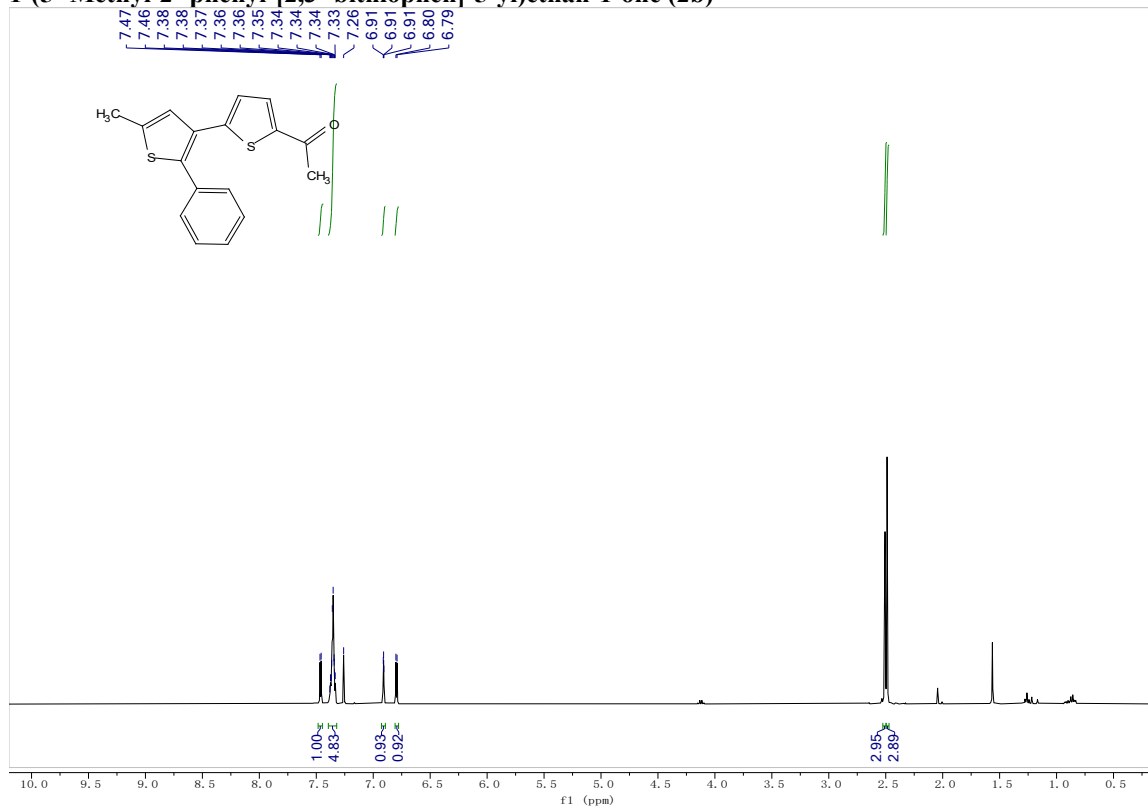
1-(5-(2-Bromo-4-methylphenyl)thiophen-2-yl)ethan-1-one (1f)



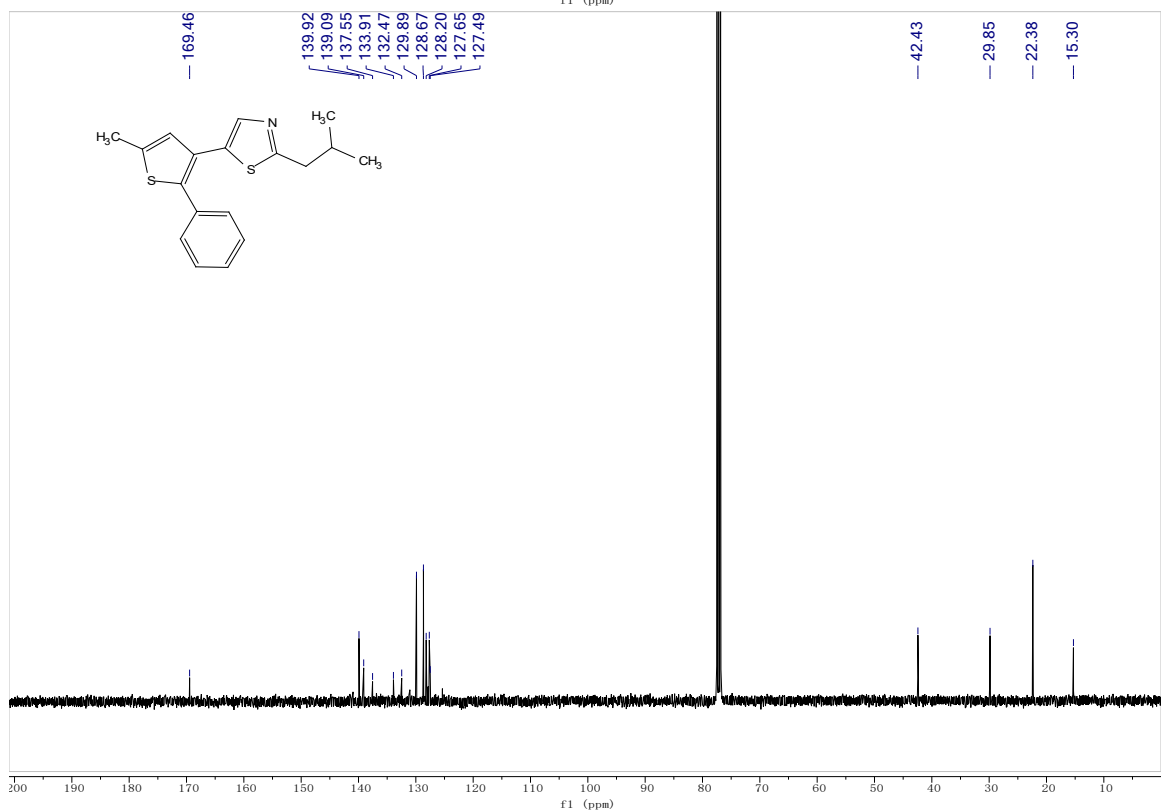
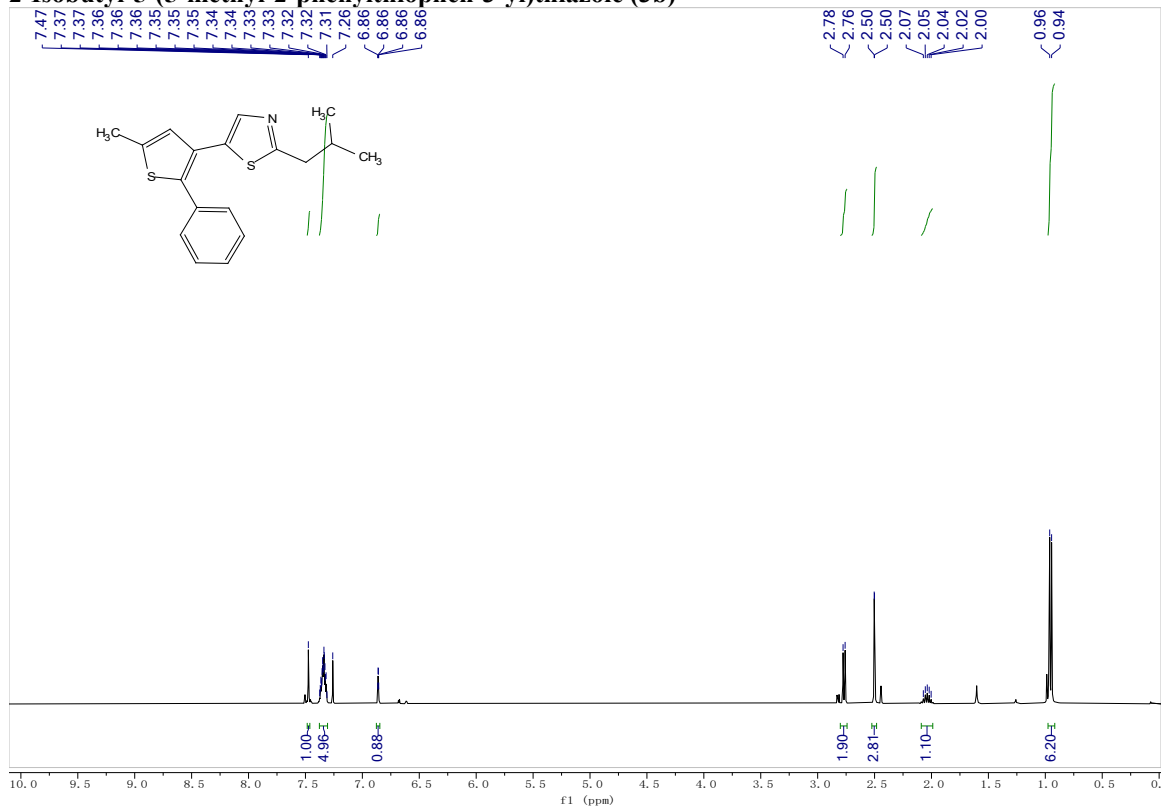
5-(2-Bromo-4-methylphenyl)thiophene-2-carbaldehyde (1g)



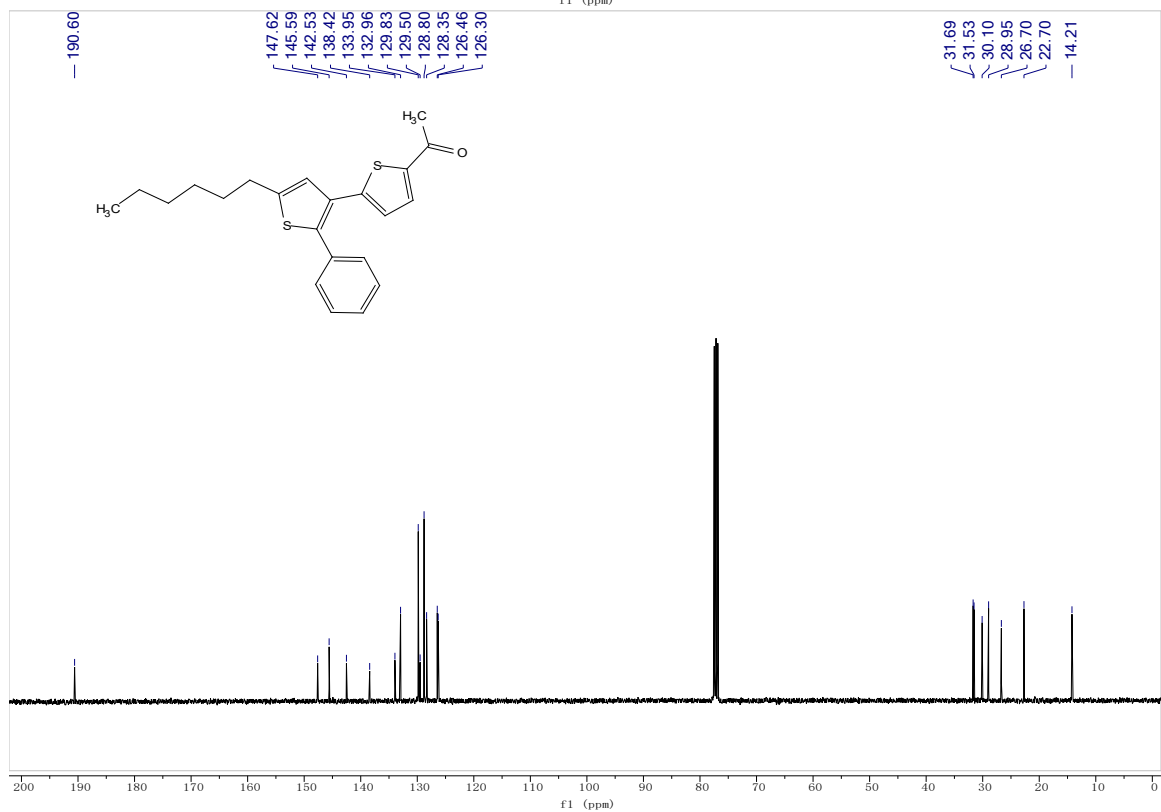
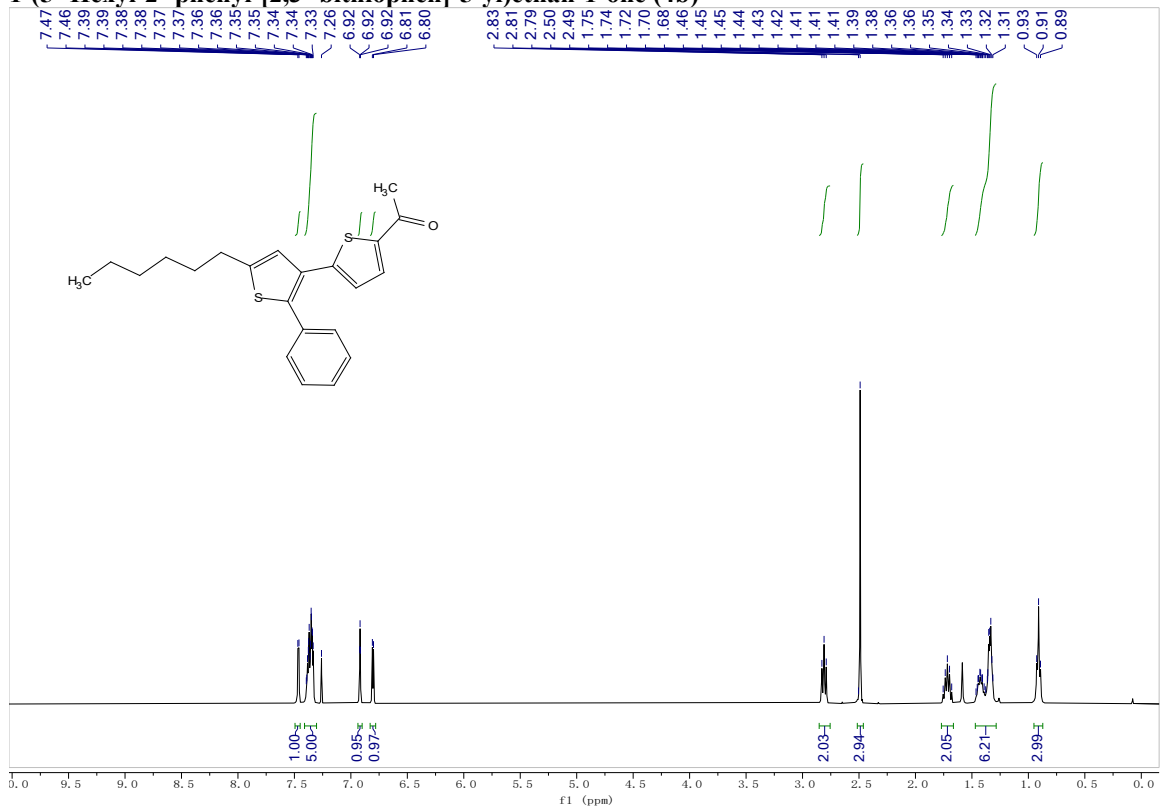
1-(5'-Methyl-2'-phenyl-[2,3'-bithiophen]-5-yl)ethan-1-one (2b)



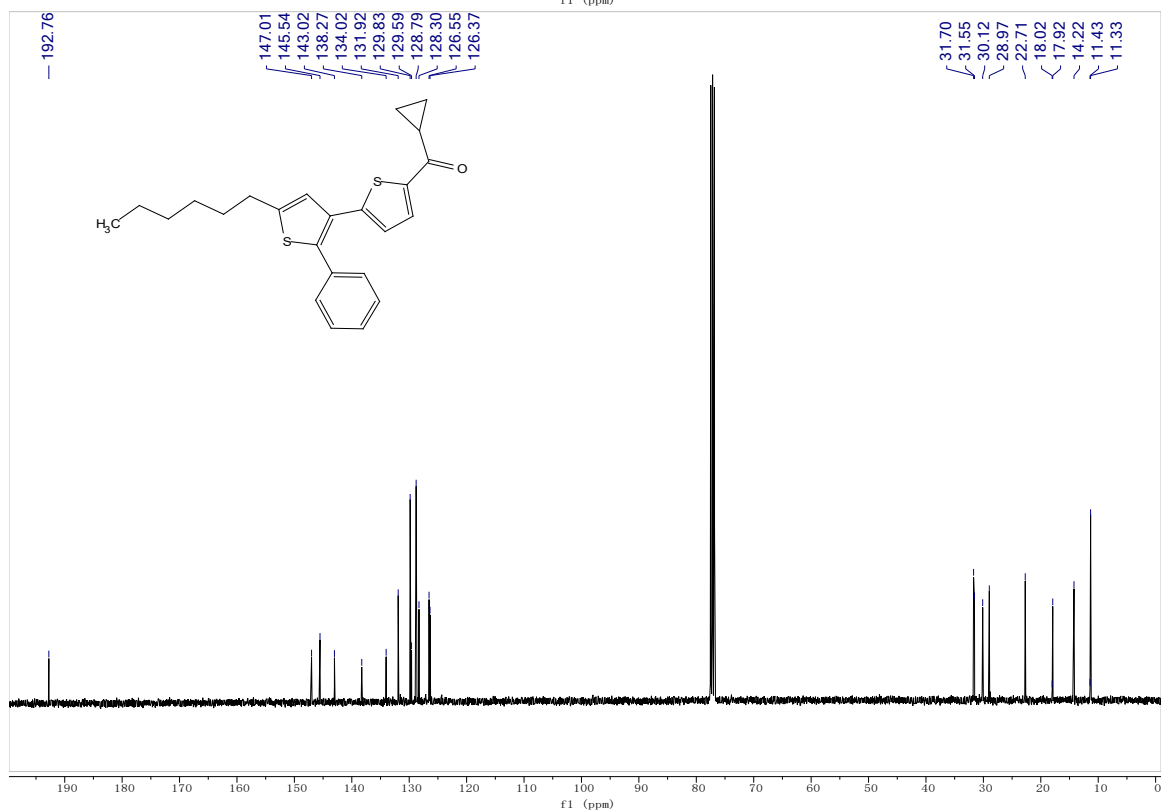
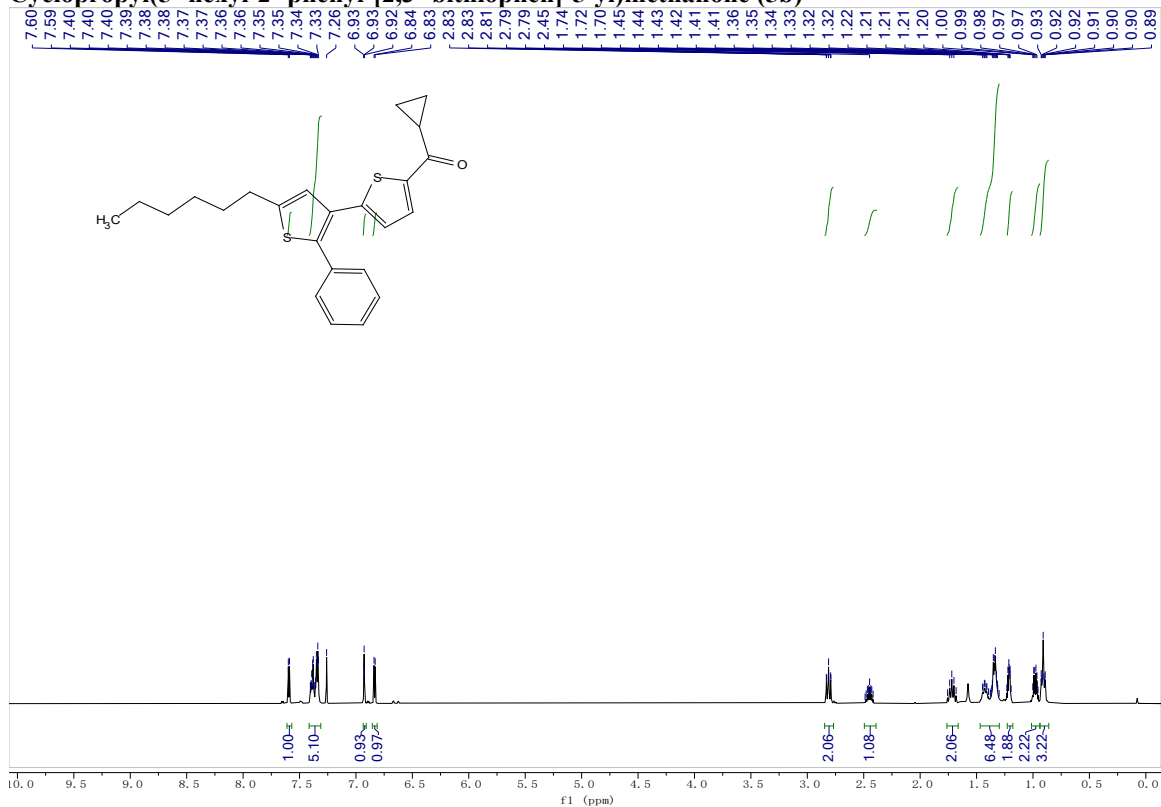
2-Isobutyl-5-(5-methyl-2-phenylthiophen-3-yl)thiazole (3b)



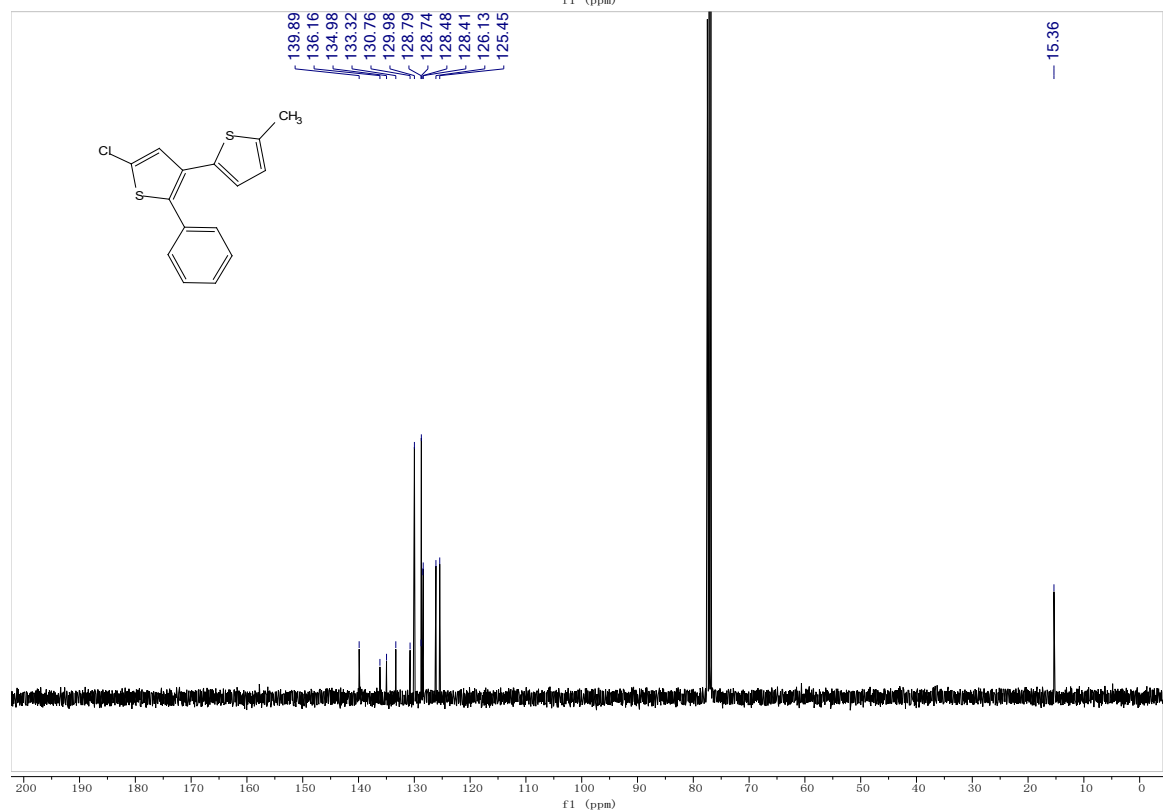
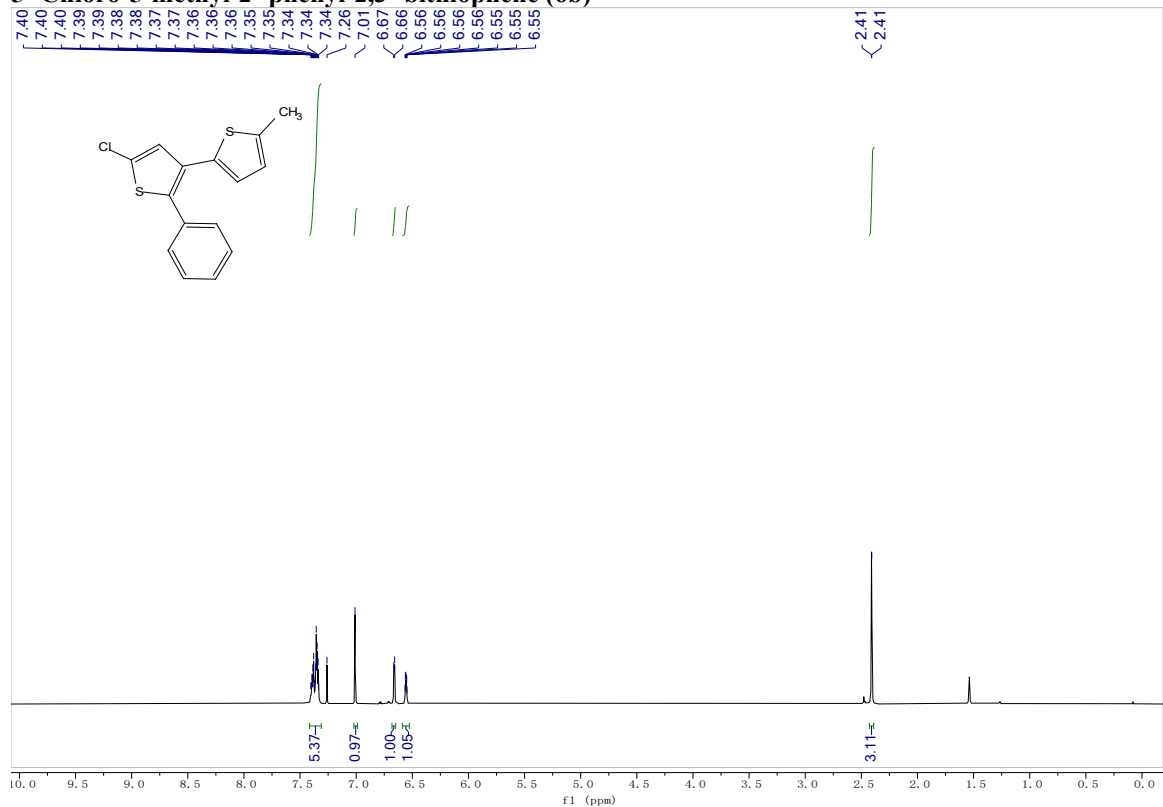
1-(5'-Hexyl-2'-phenyl-[2,3'-bithiophen]-5-yl)ethan-1-one (4b)



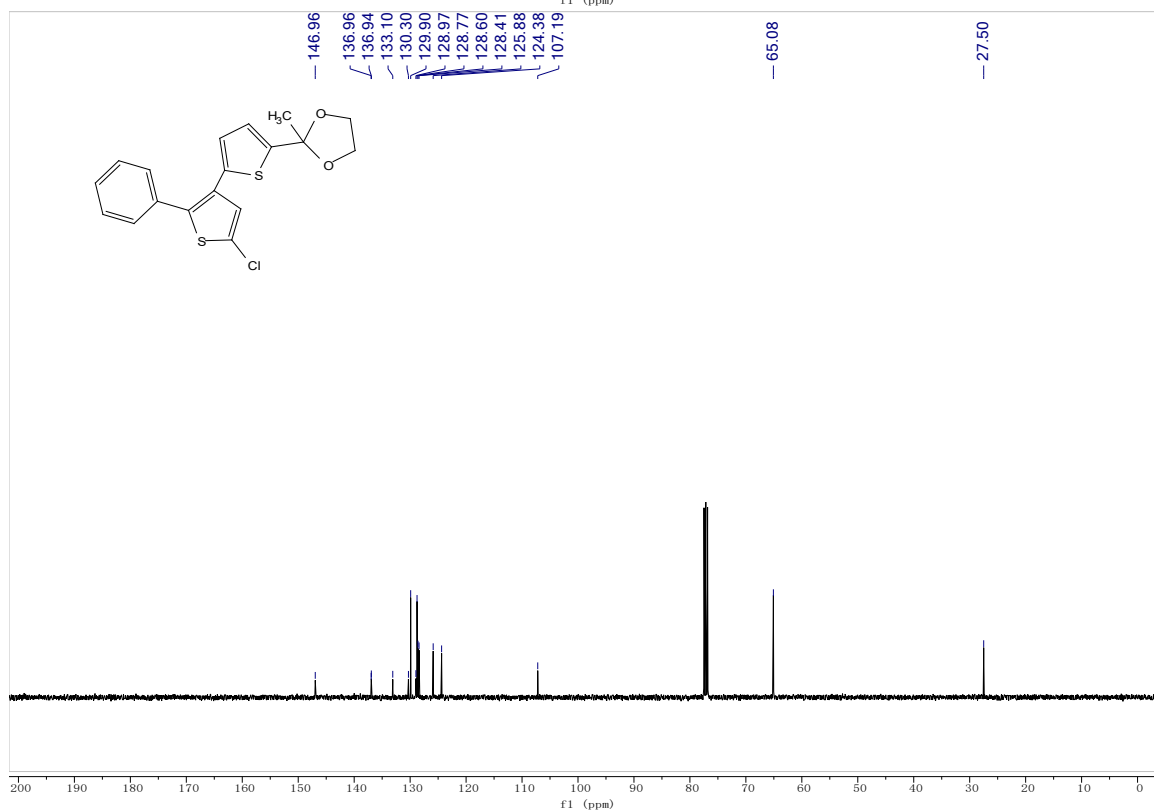
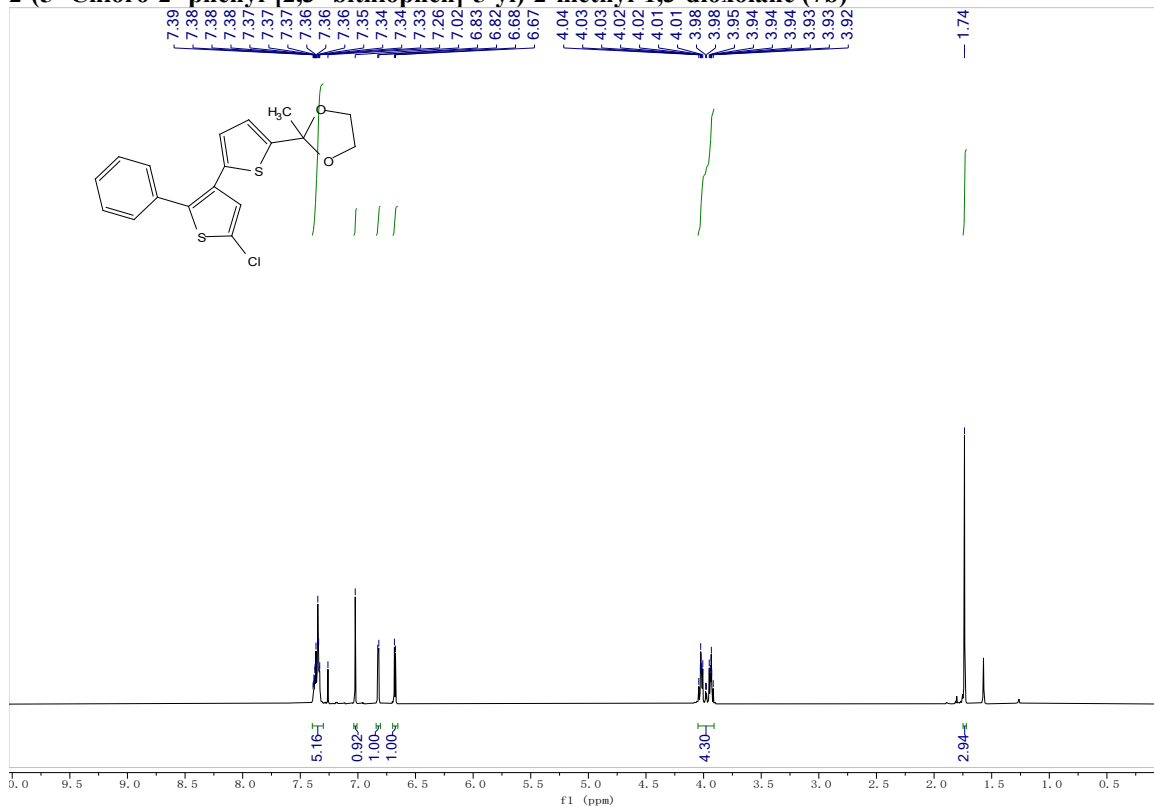
Cyclopropyl(5'-hexyl-2'-phenyl-[2,3'-bithiophen]-5-yl)methanone (5b)



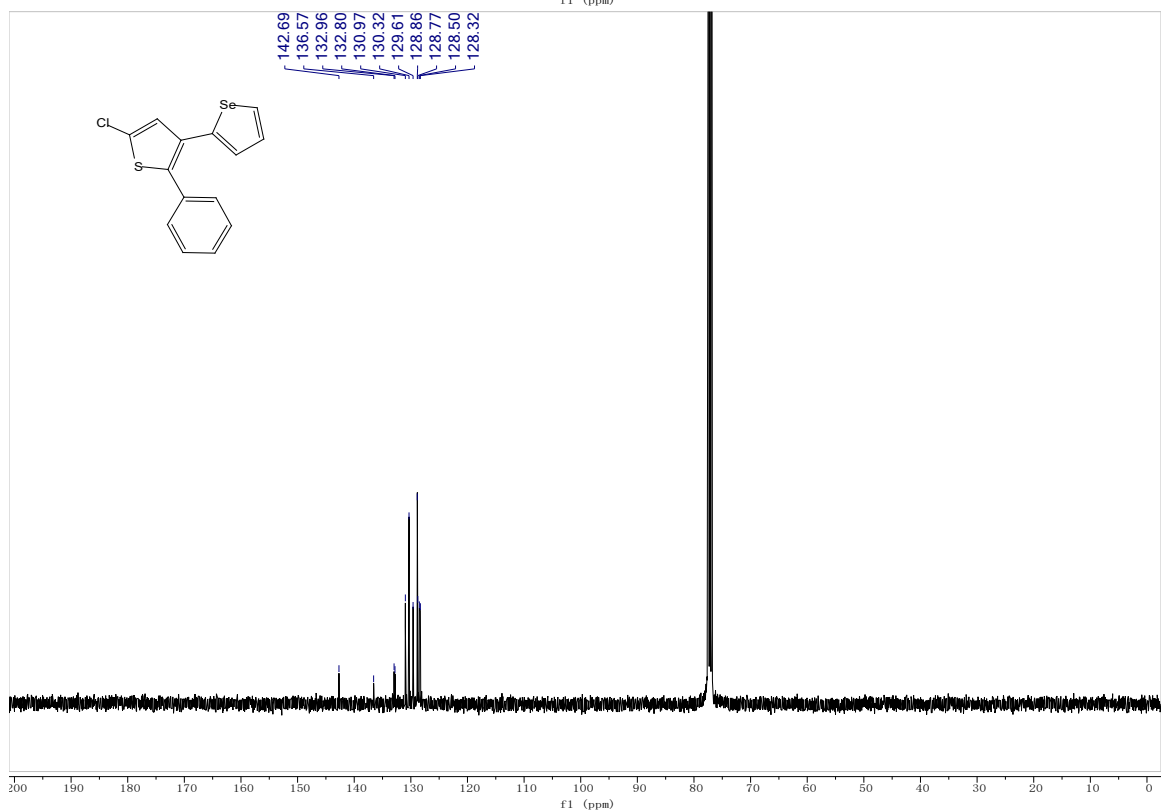
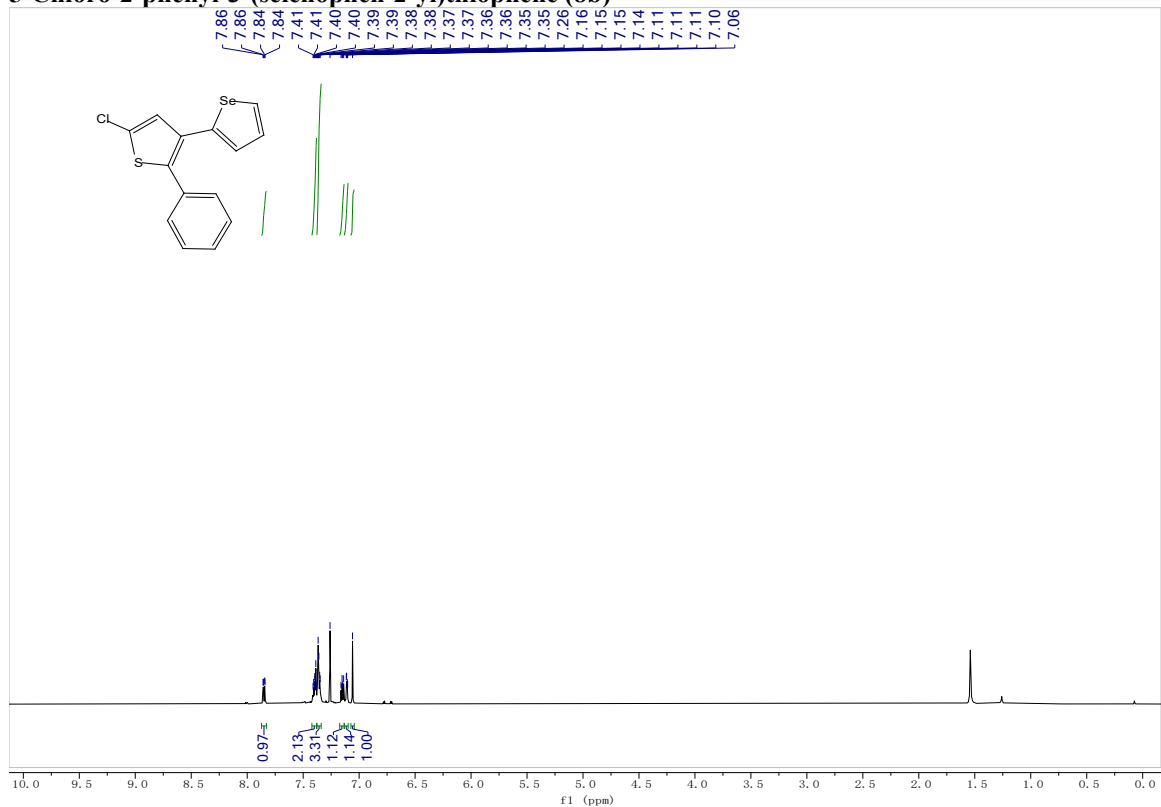
5'-Chloro-5-methyl-2'-phenyl-2,3'-bithiophene (6b)



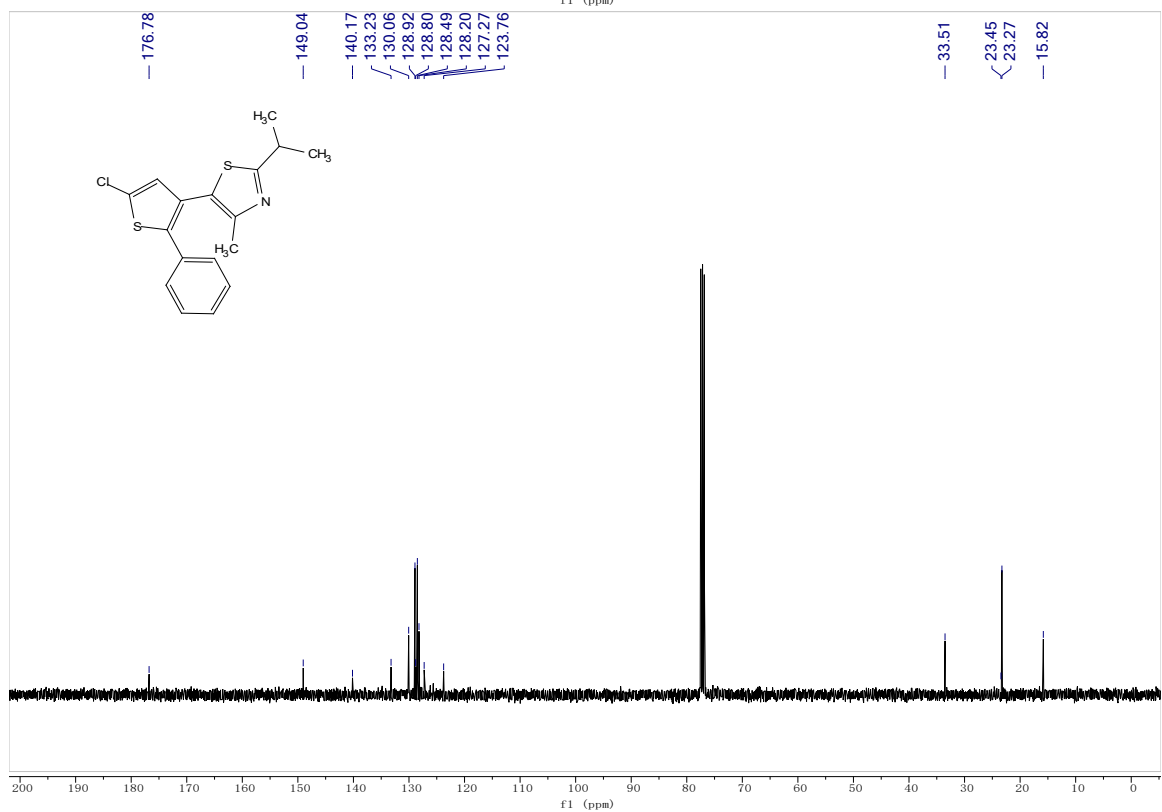
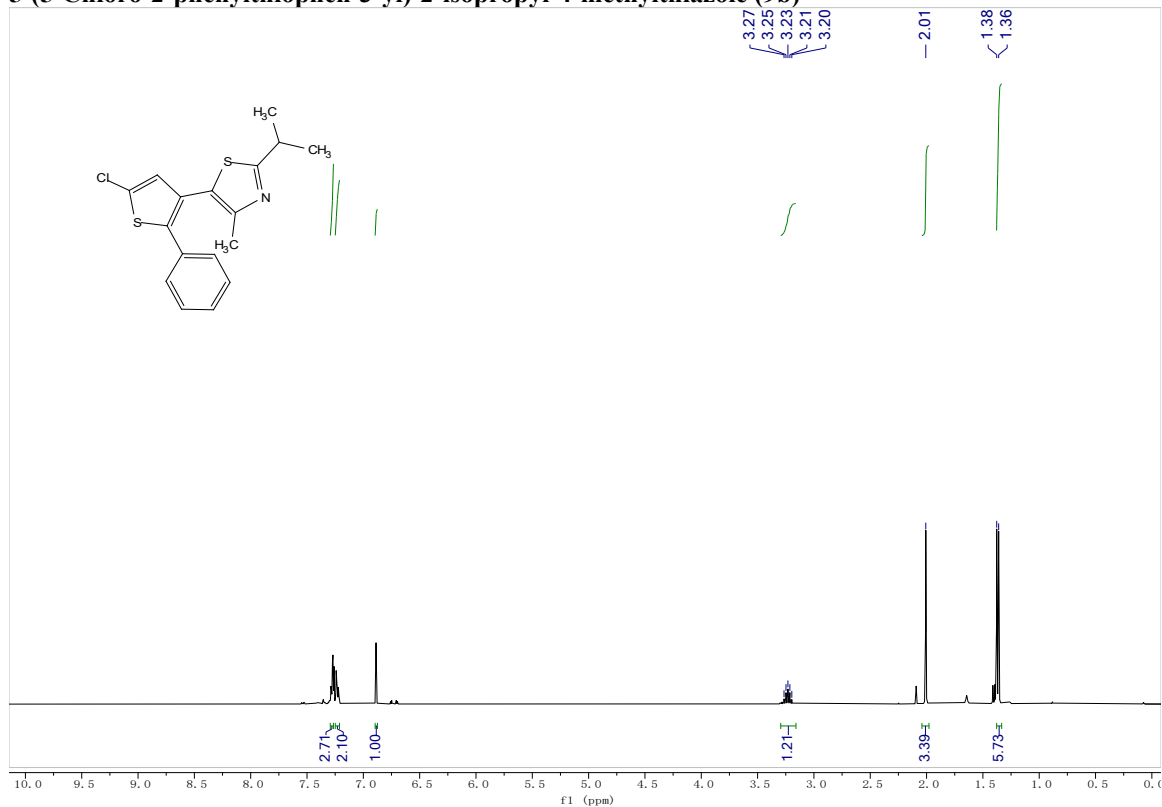
2-(5'-Chloro-2'-phenyl-[2,3'-bithiophen]-5-yl)-2-methyl-1,3-dioxolane (7b)



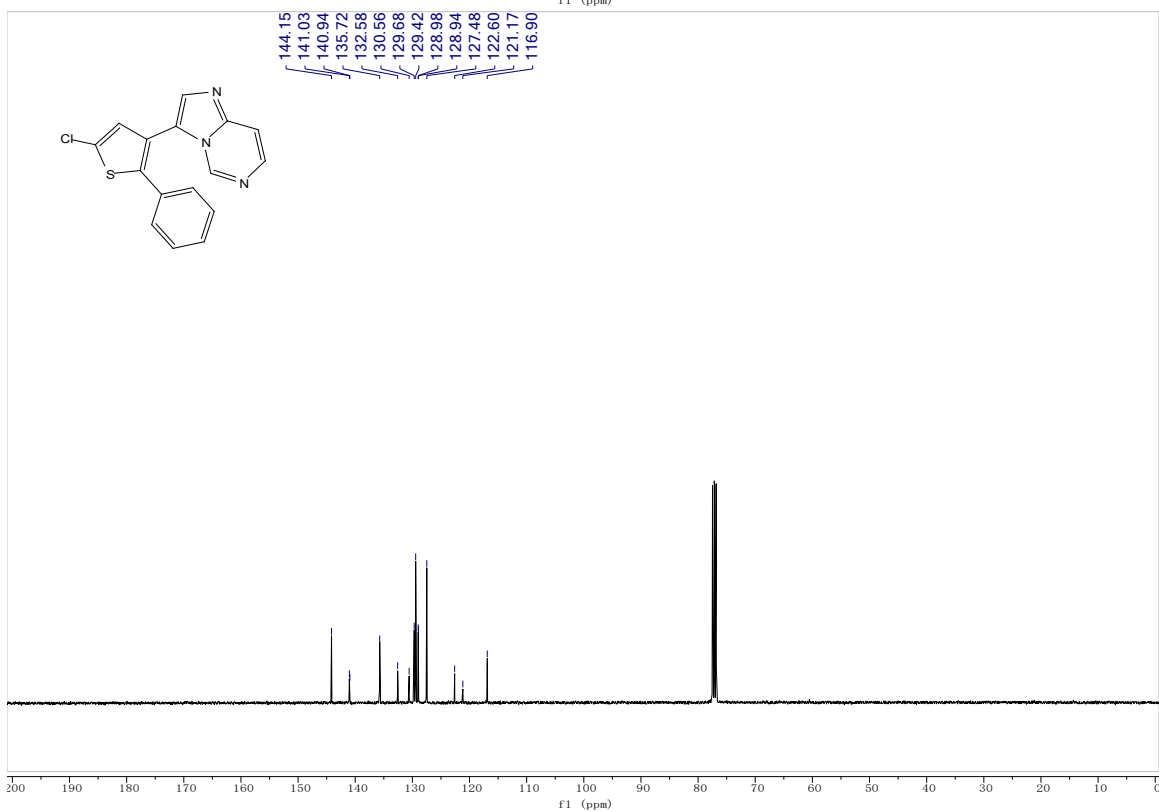
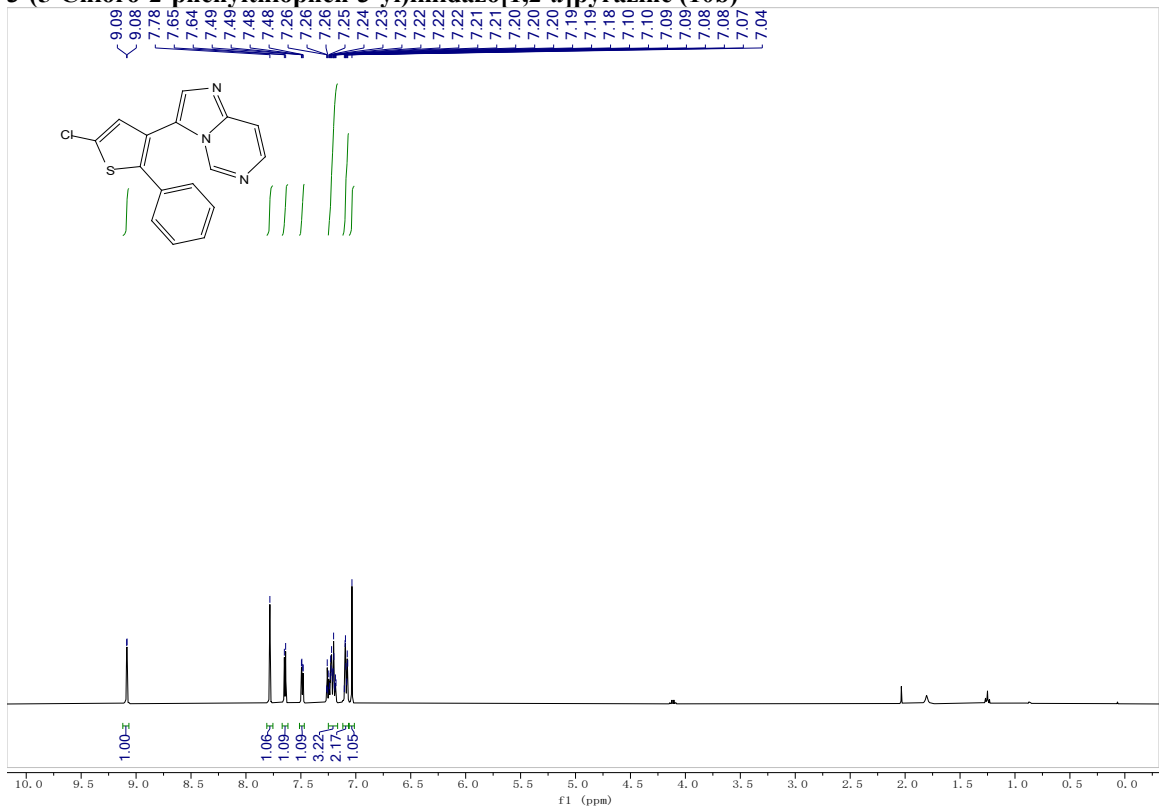
5-Chloro-2-phenyl-3-(selenophen-2-yl)thiophene (8b)



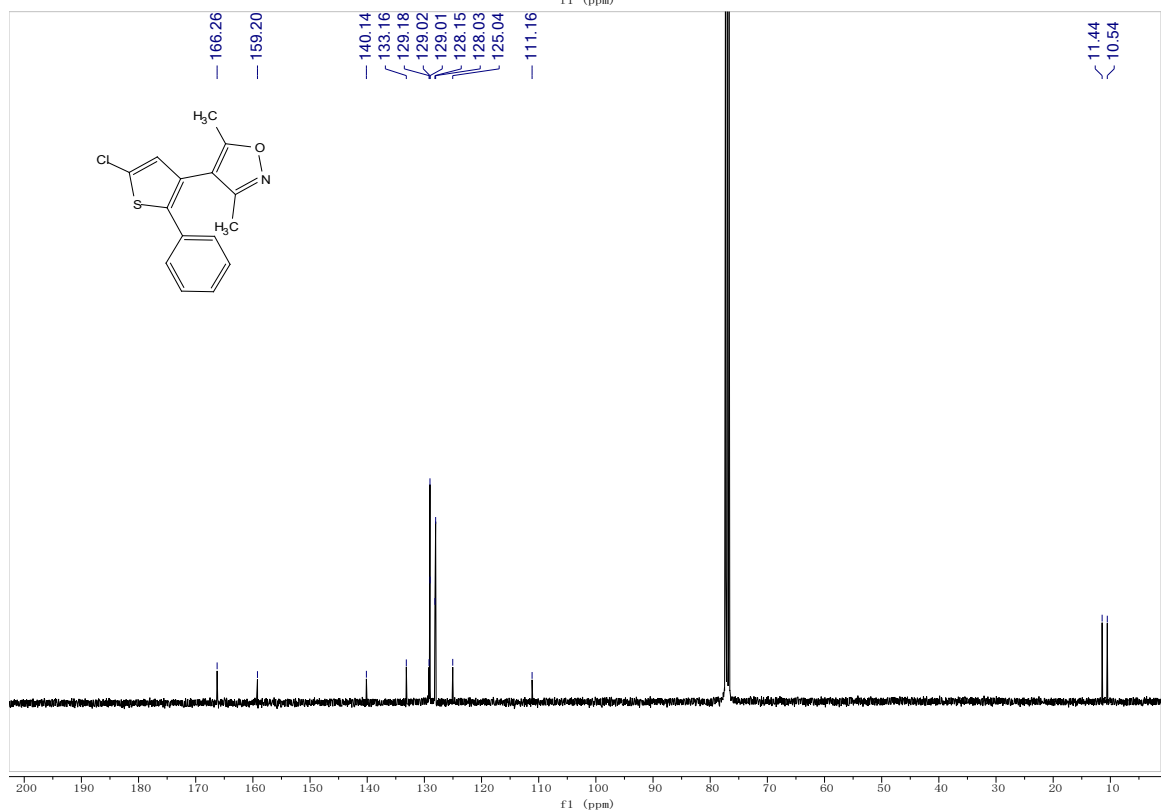
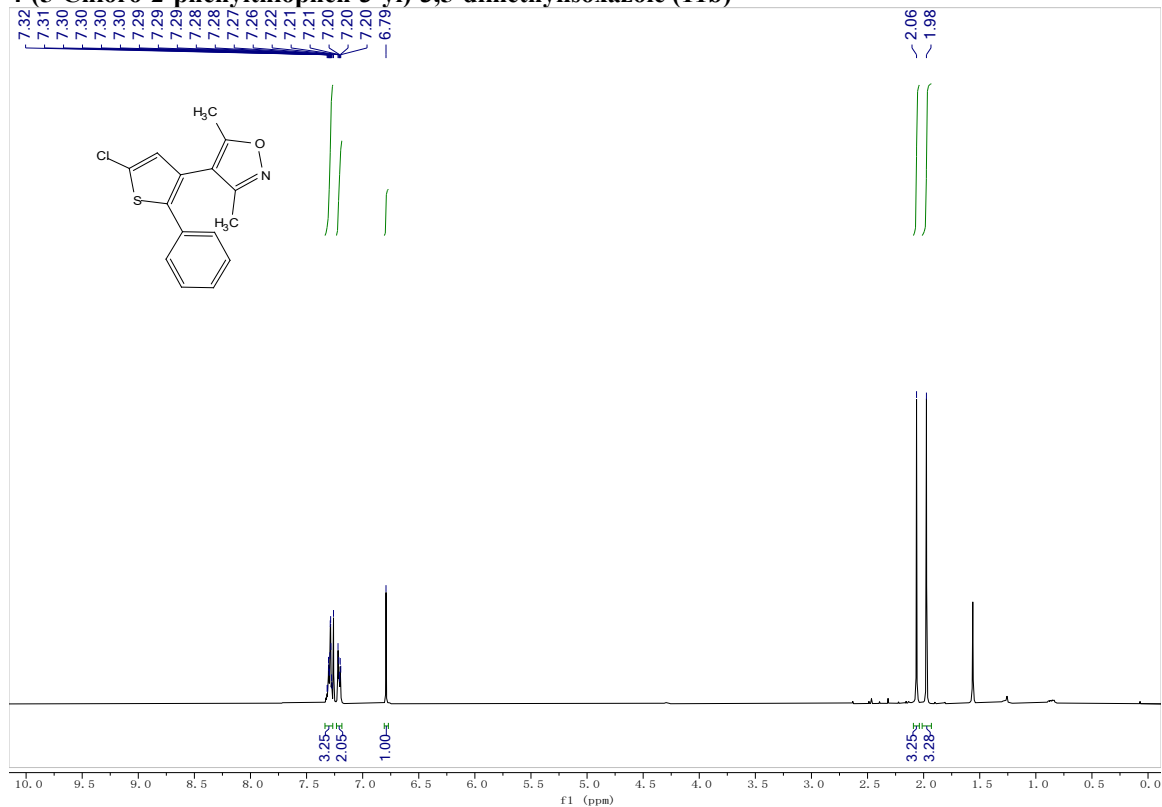
5-(5-Chloro-2-phenylthiophen-3-yl)-2-isopropyl-4-methylthiazole (9b)



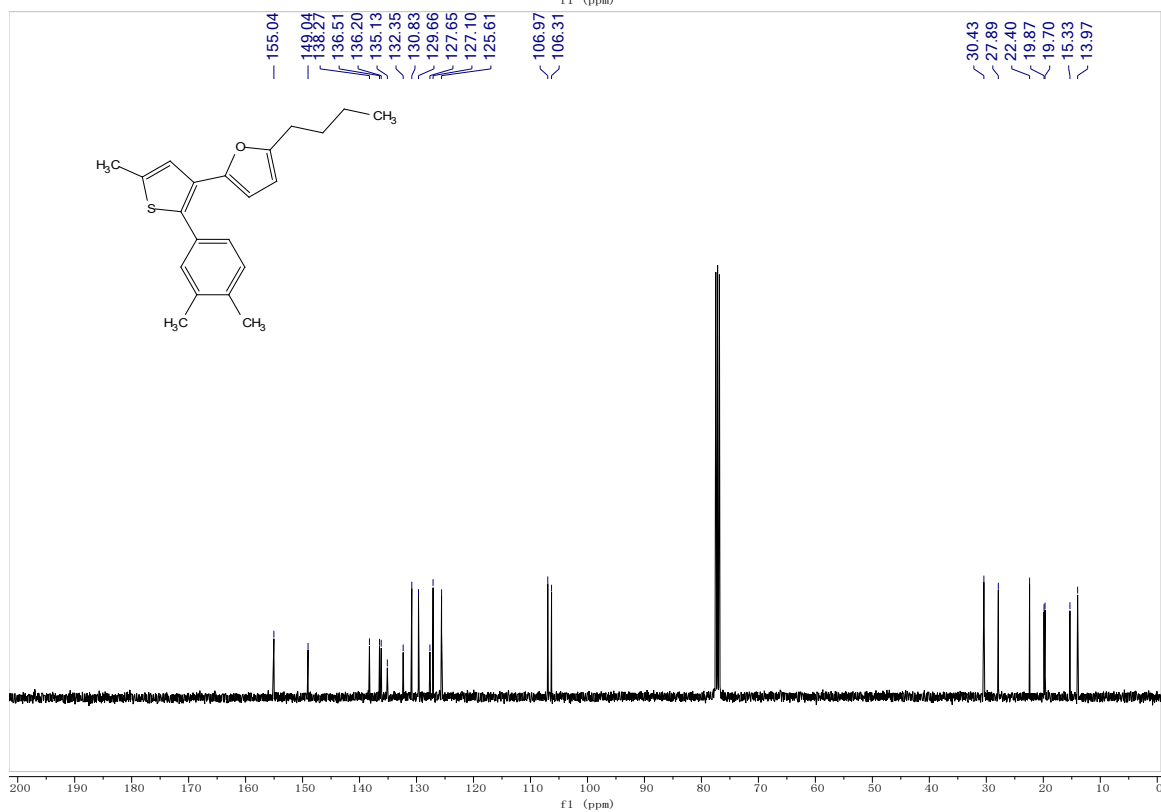
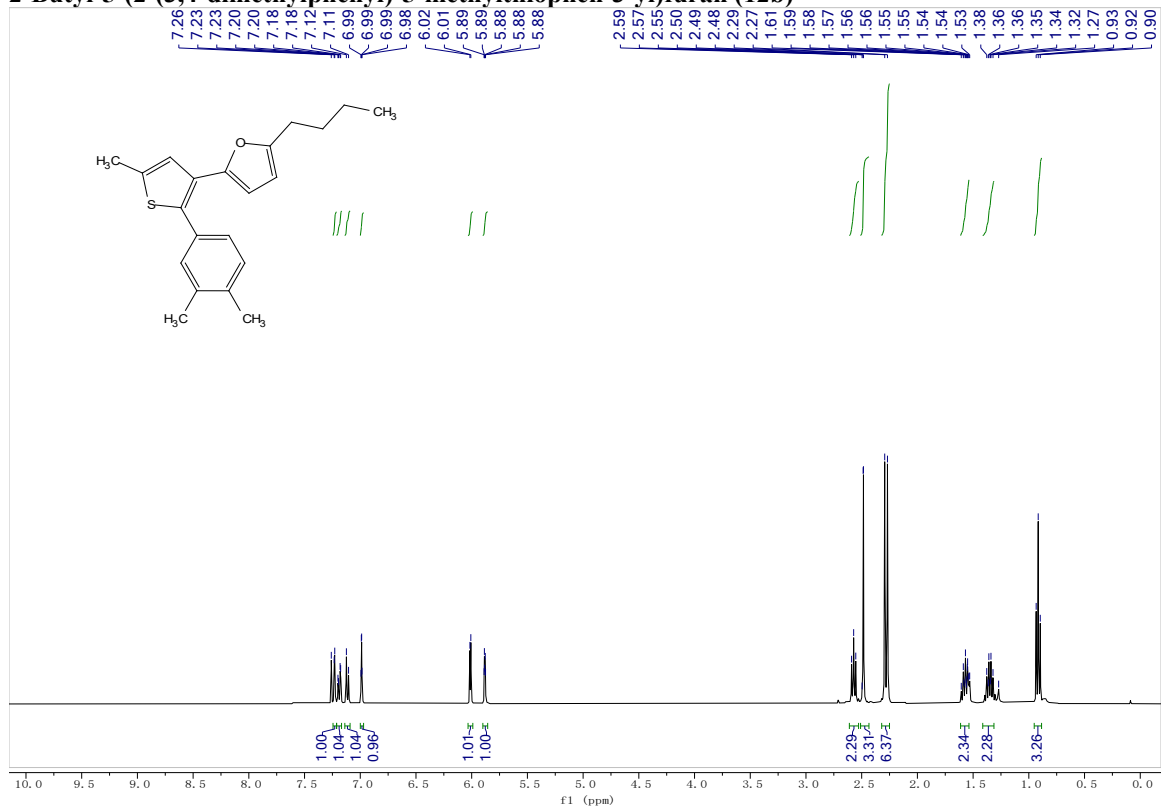
3-(5-Chloro-2-phenylthiophen-3-yl)imidazo[1,2-a]pyrazine (10b)



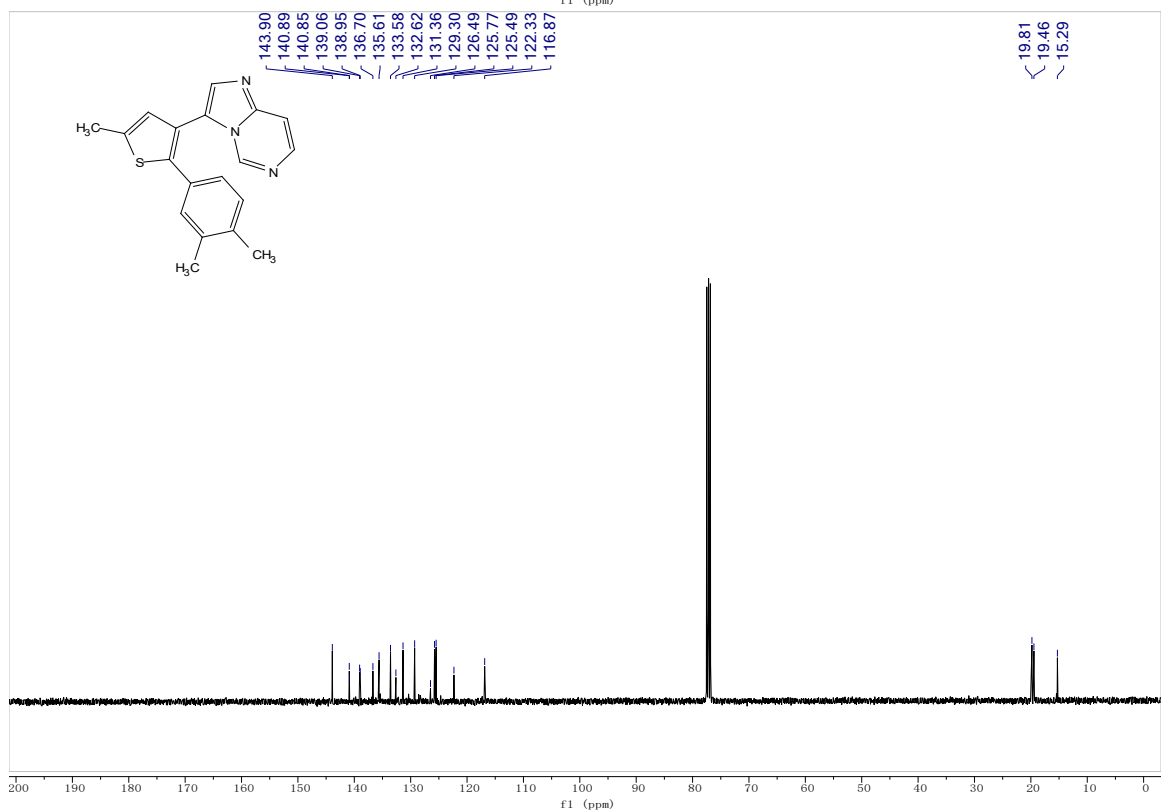
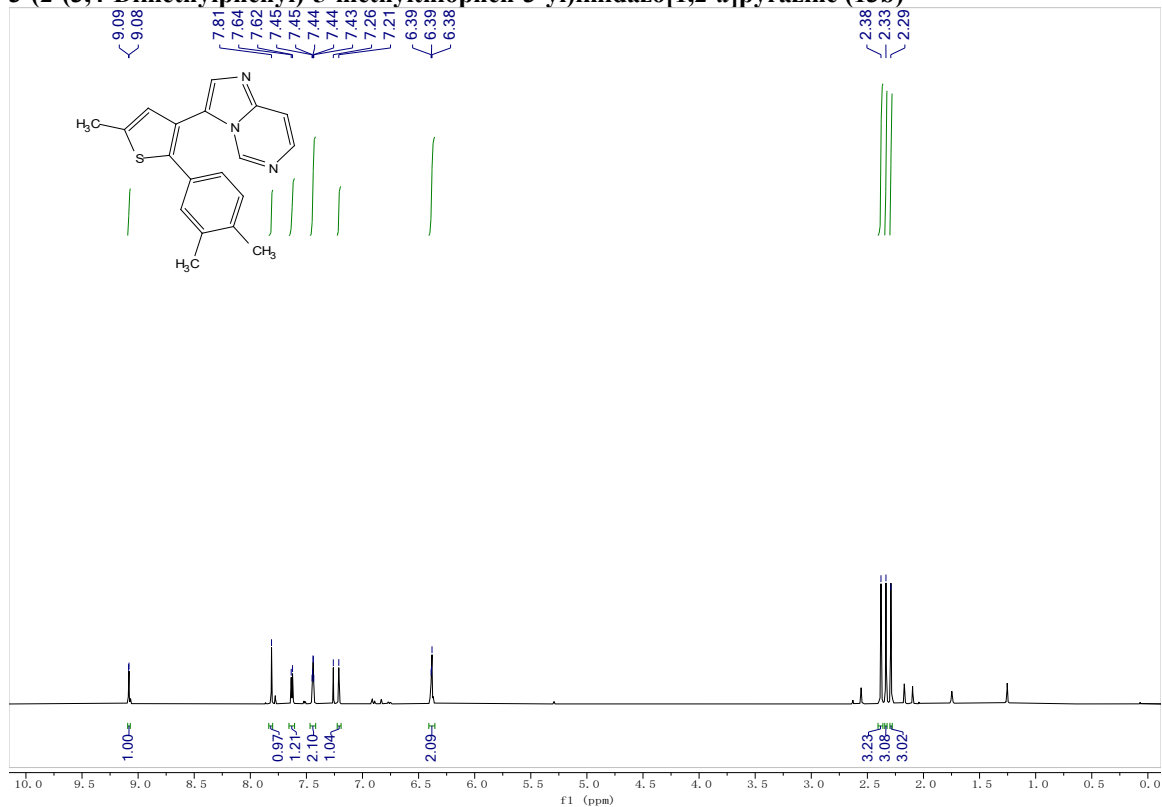
4-(5-Chloro-2-phenylthiophen-3-yl)-3,5-dimethylisoxazole (11b)



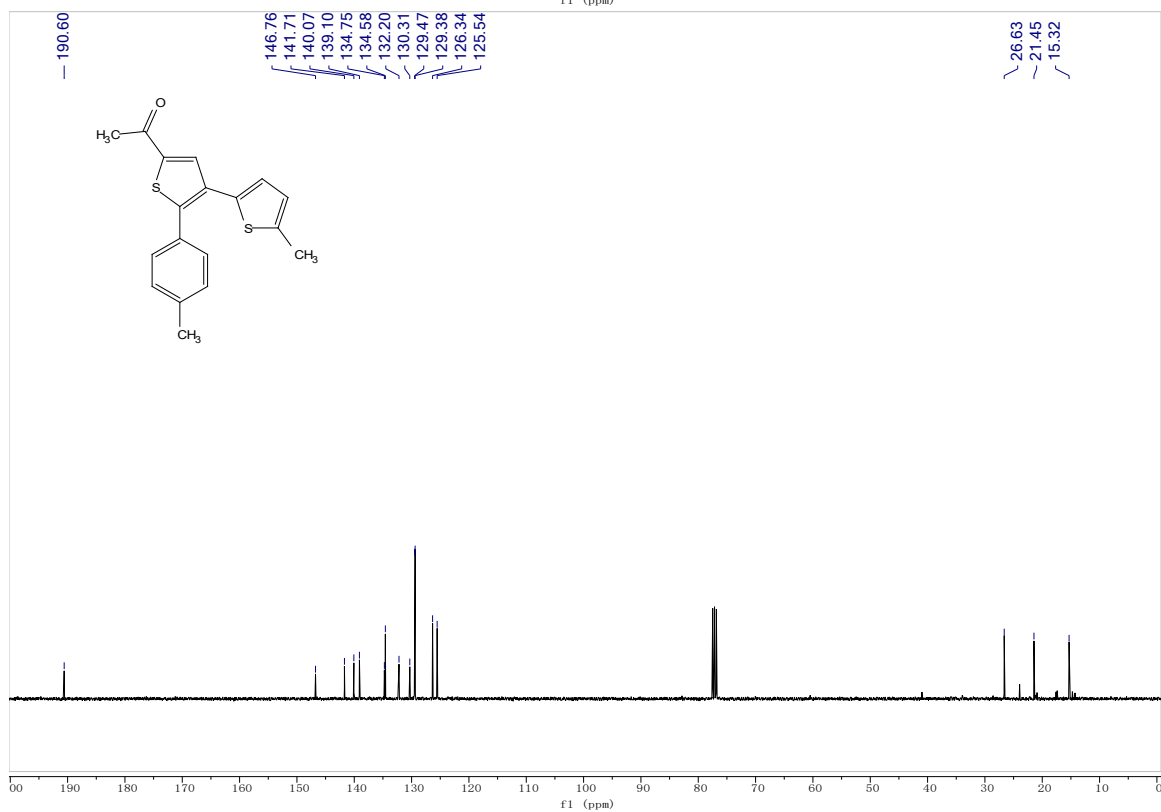
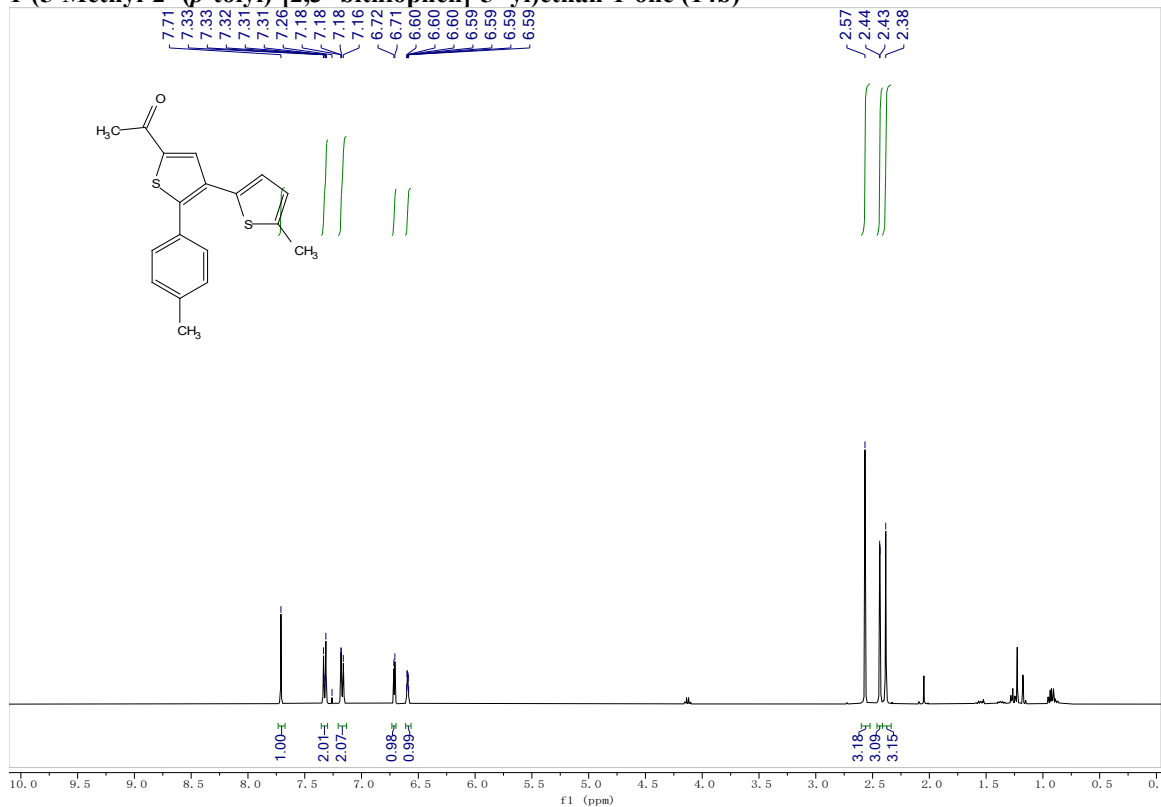
2-Butyl-5-(2-(3,4-dimethylphenyl)-5-methylthiophen-3-yl)furan (12b)



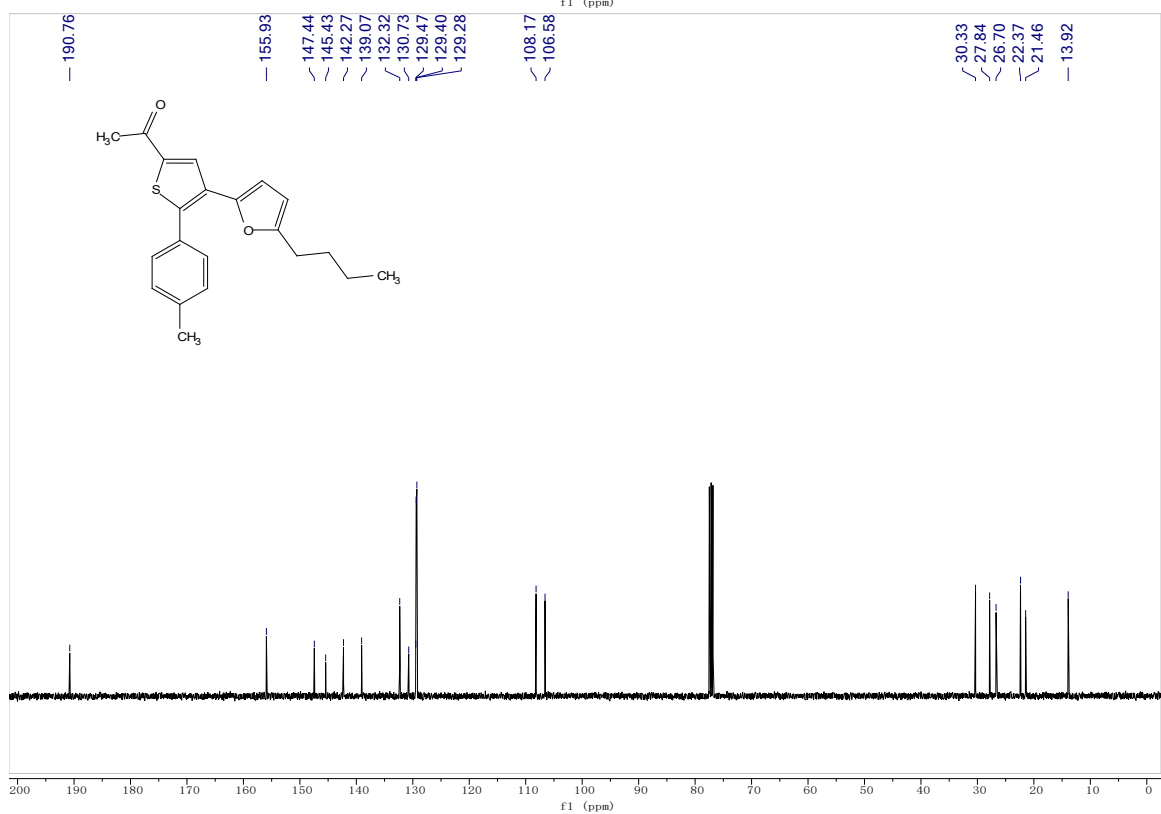
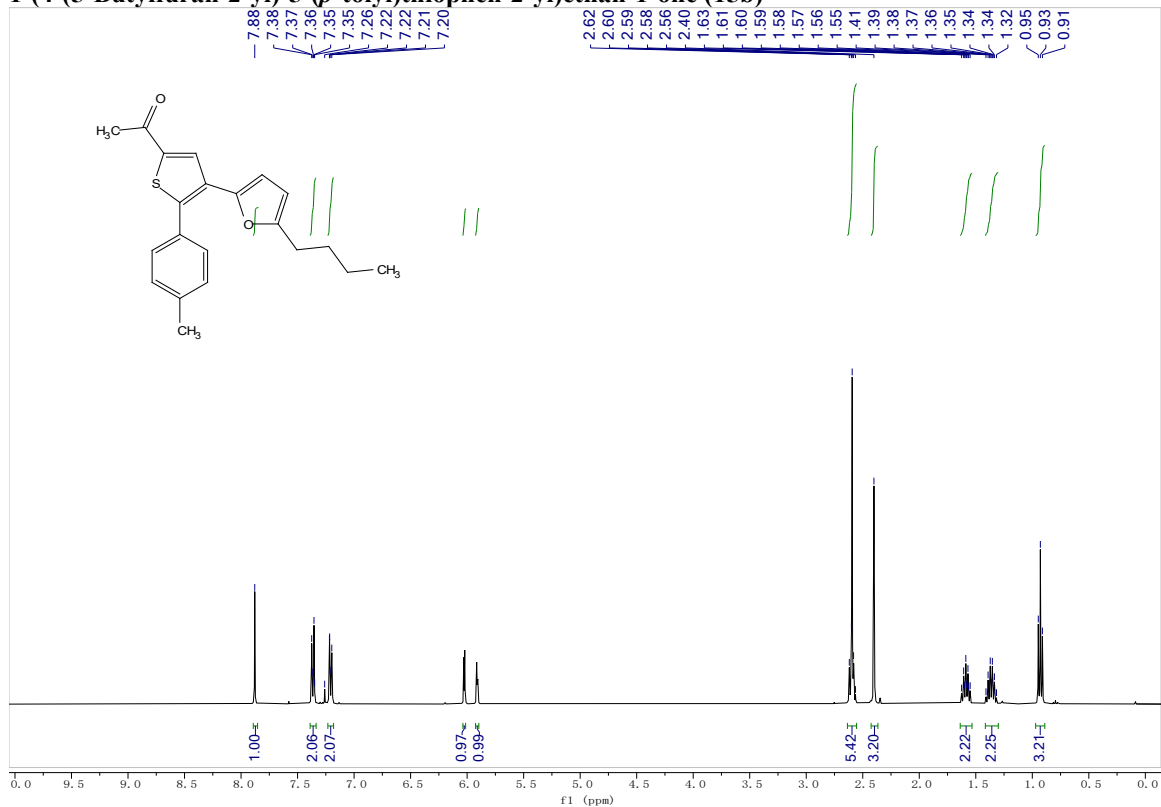
3-(2-(3,4-Dimethylphenyl)-5-methylthiophen-3-yl)imidazo[1,2-a]pyrazine (13b)



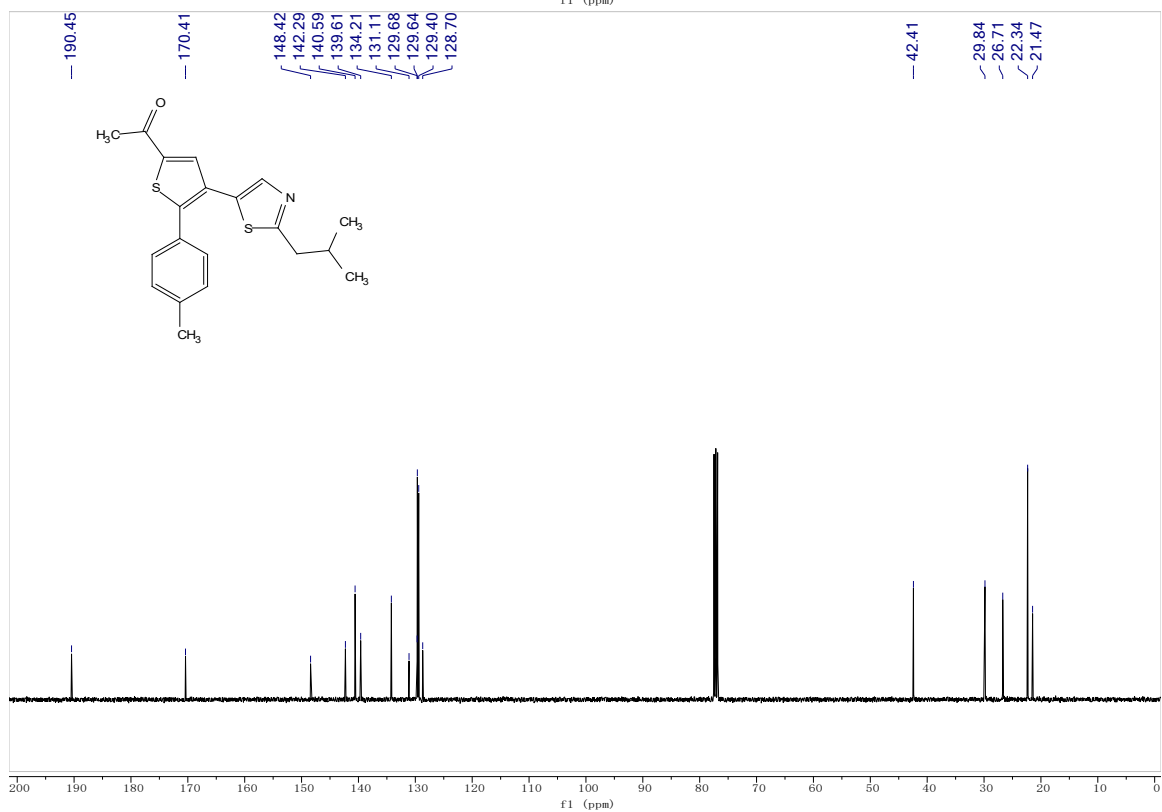
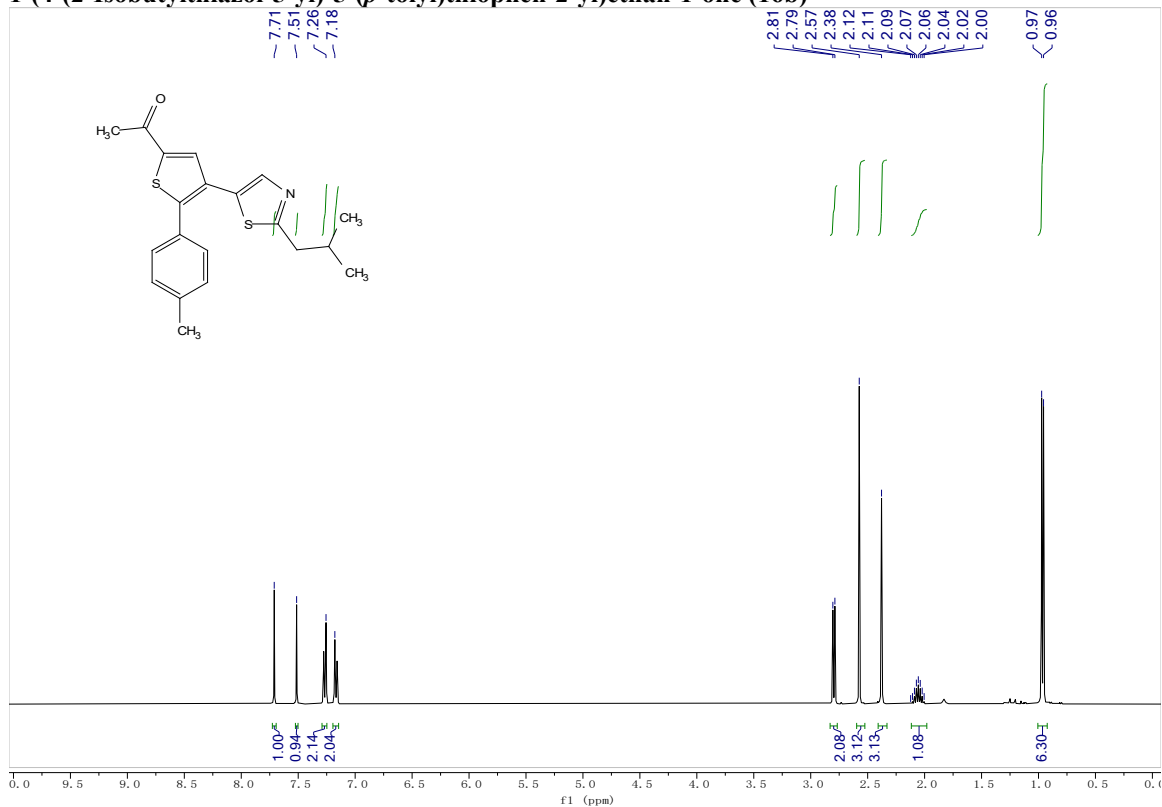
1-(5-Methyl-2'-(*p*-tolyl)-[2,3'-bithiophen]-5'-yl)ethan-1-one (14b)



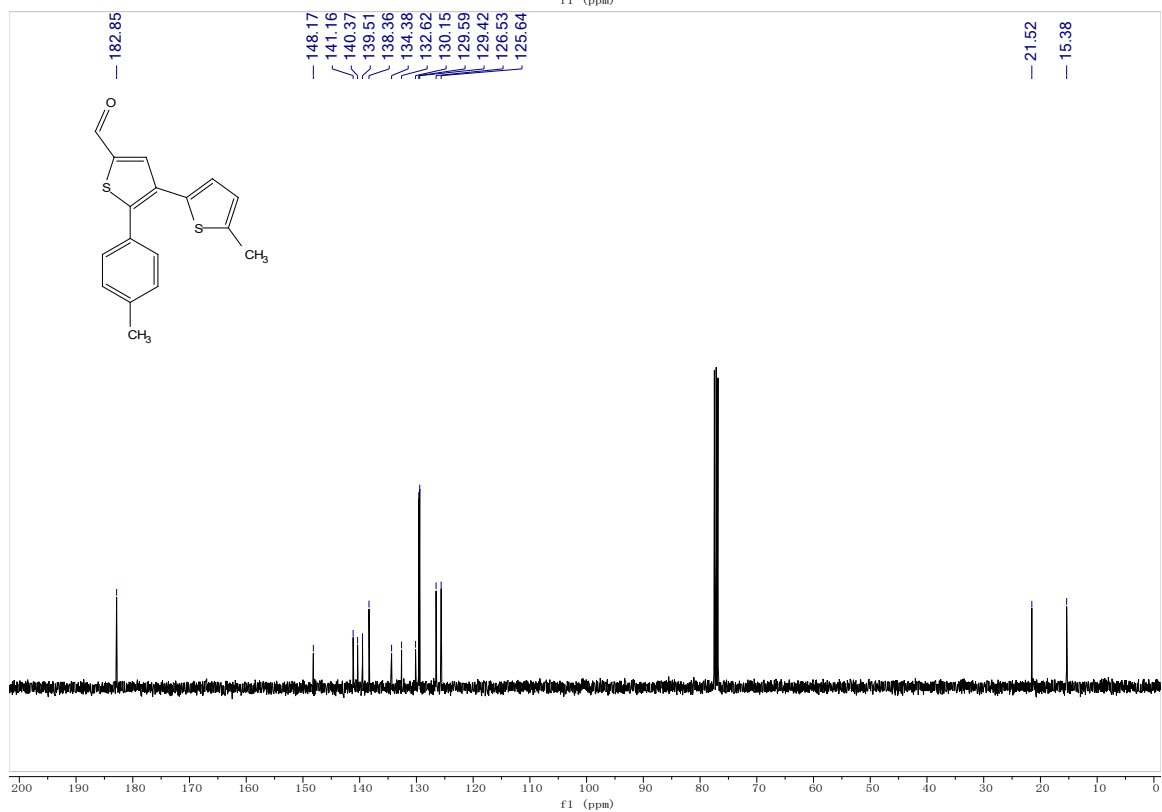
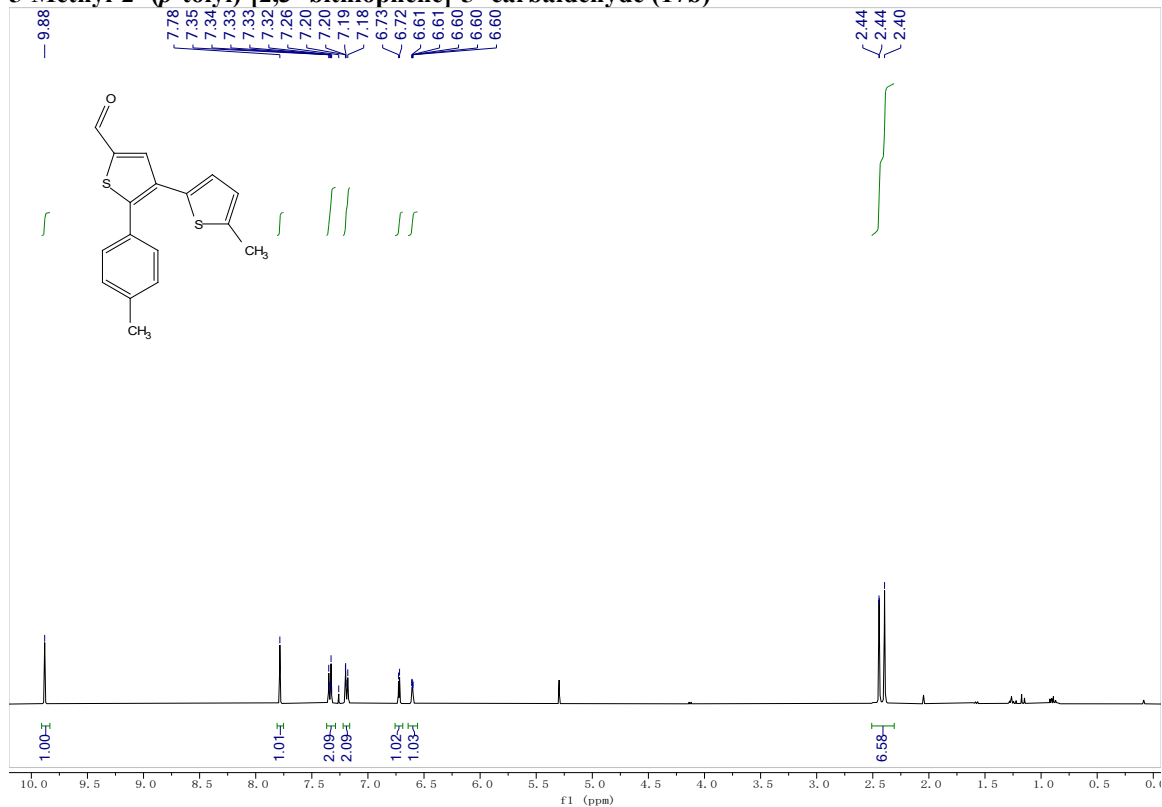
1-(4-(5-Butylfuran-2-yl)-5-(*p*-tolyl)thiophen-2-yl)ethan-1-one (15b)



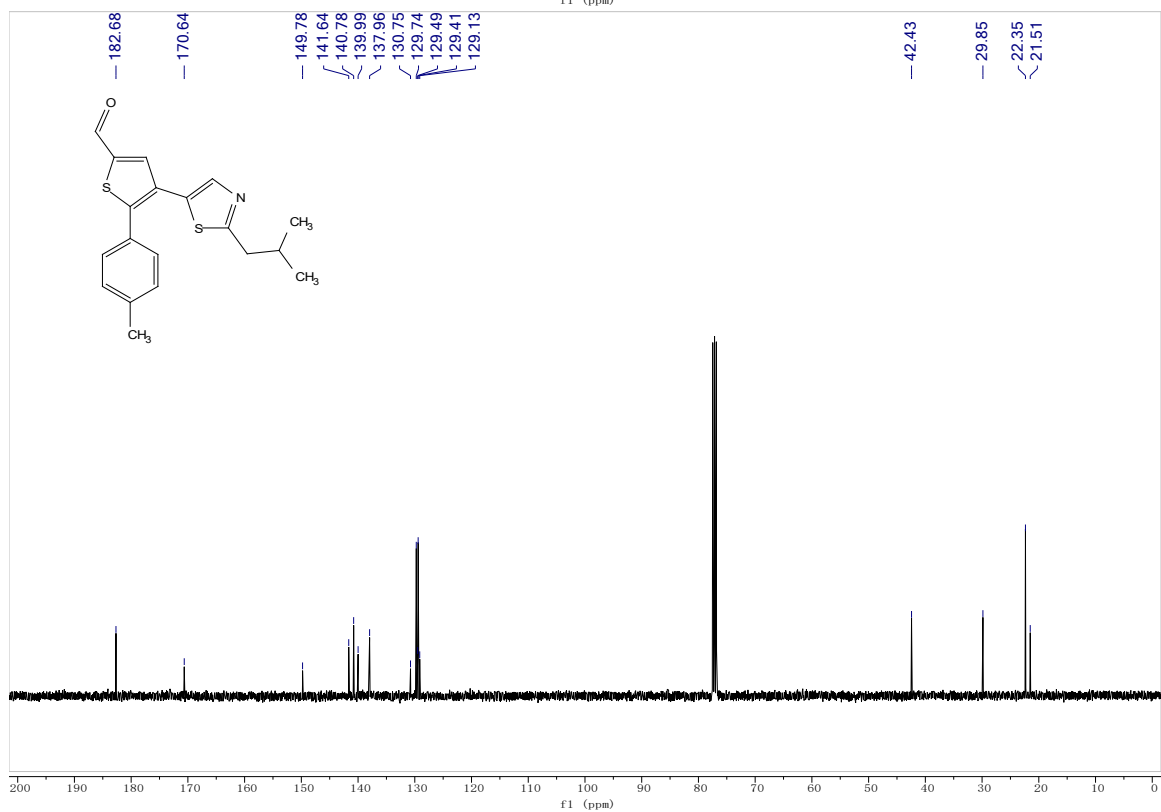
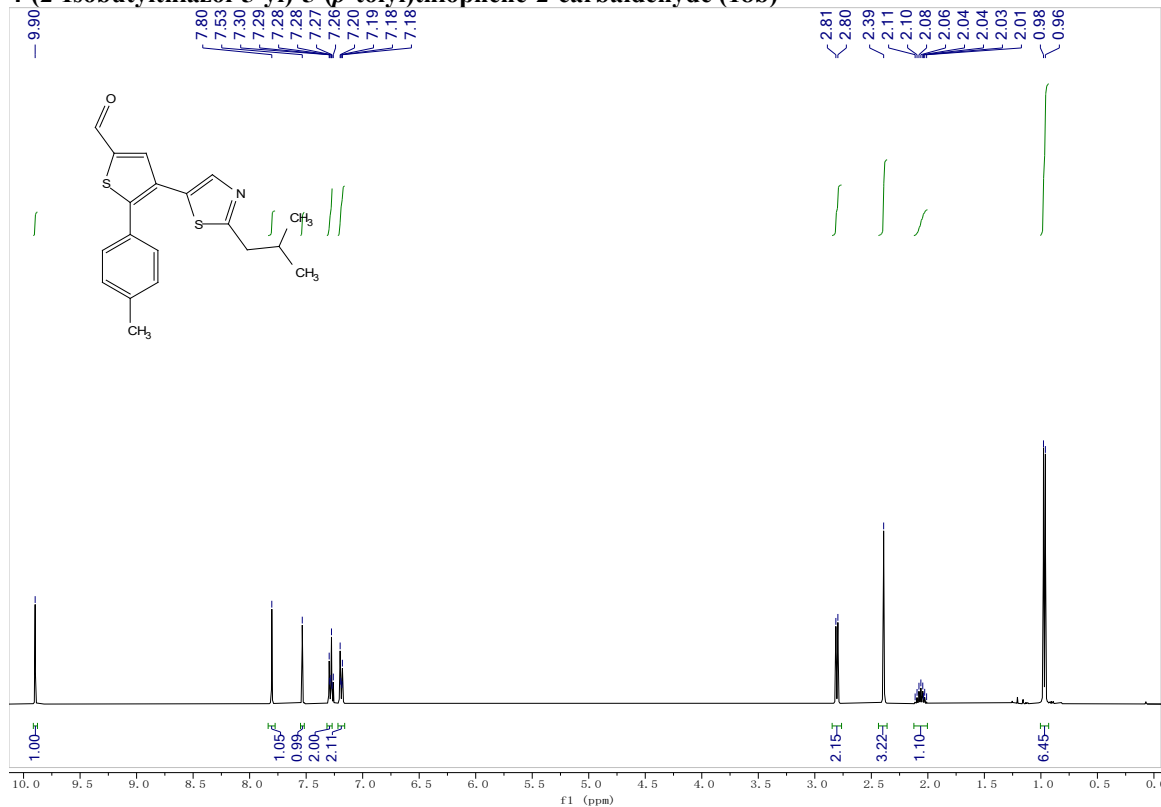
1-(4-(2-Isobutylthiazol-5-yl)-5-(*p*-tolyl)thiophen-2-yl)ethan-1-one (16b)



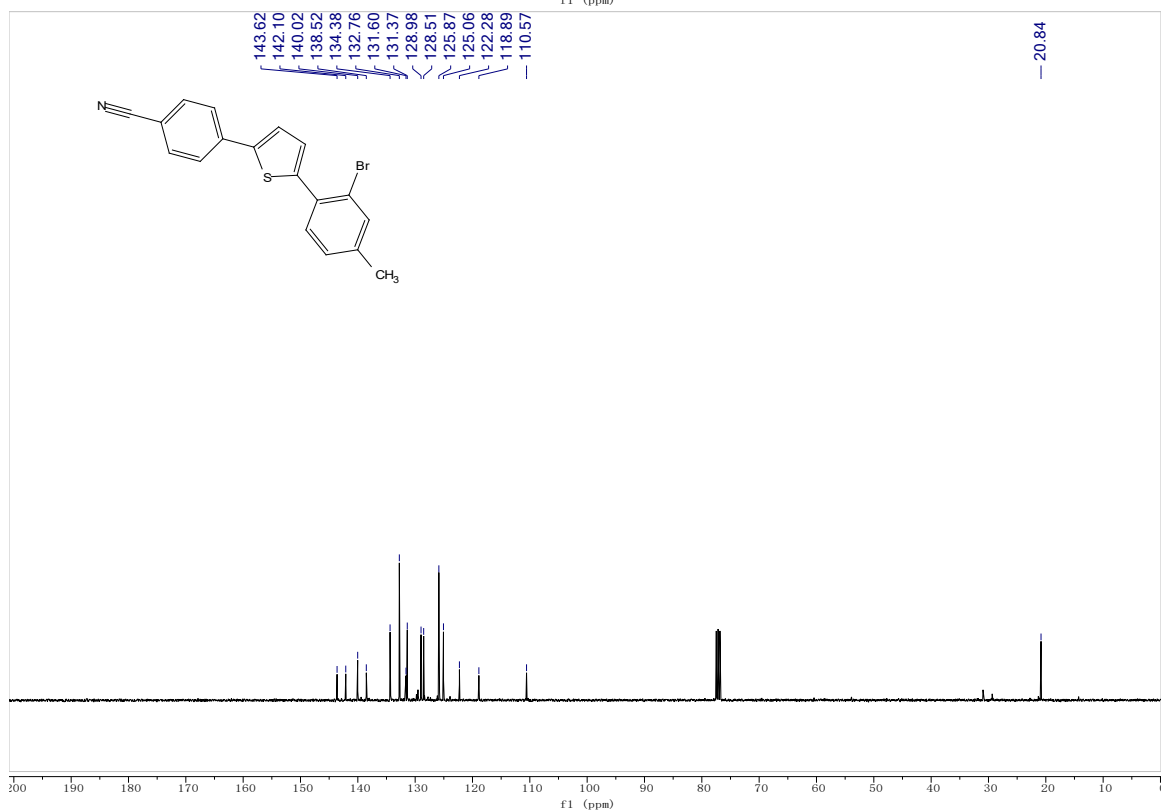
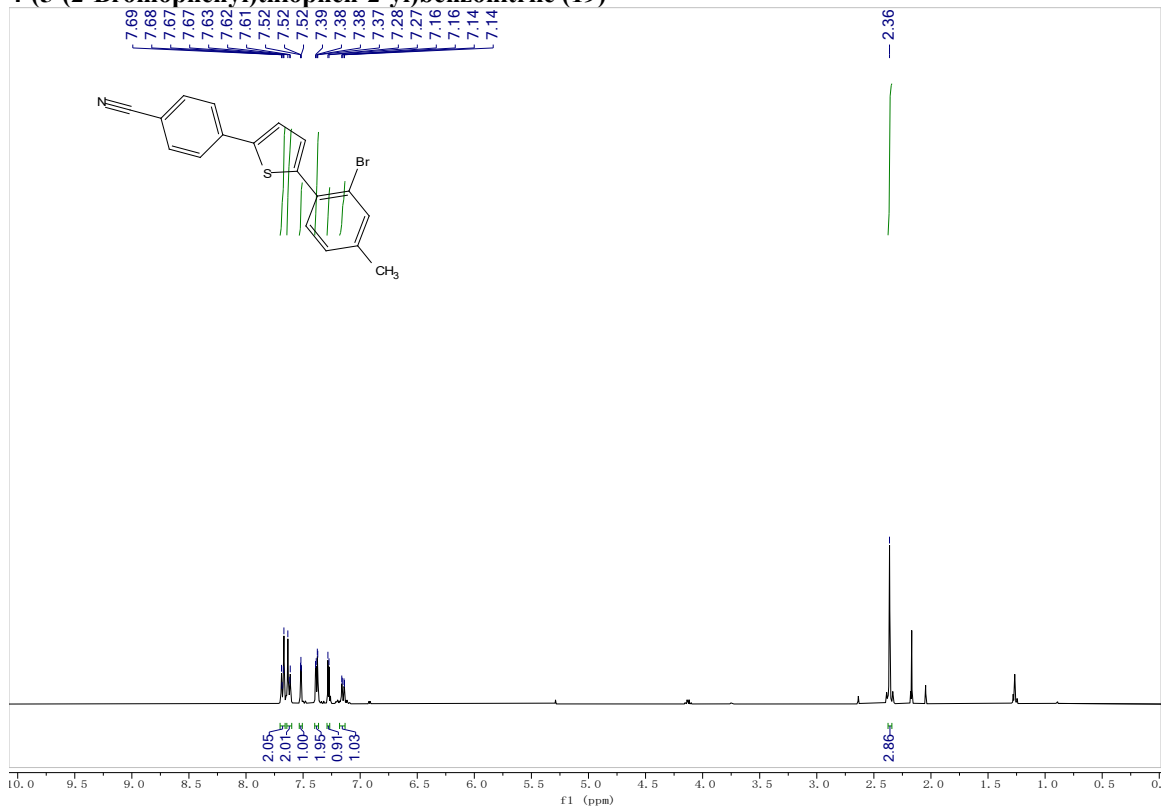
5-Methyl-2'-(*p*-tolyl)-[2,3'-bithiophene]-5'-carbaldehyde (17b)



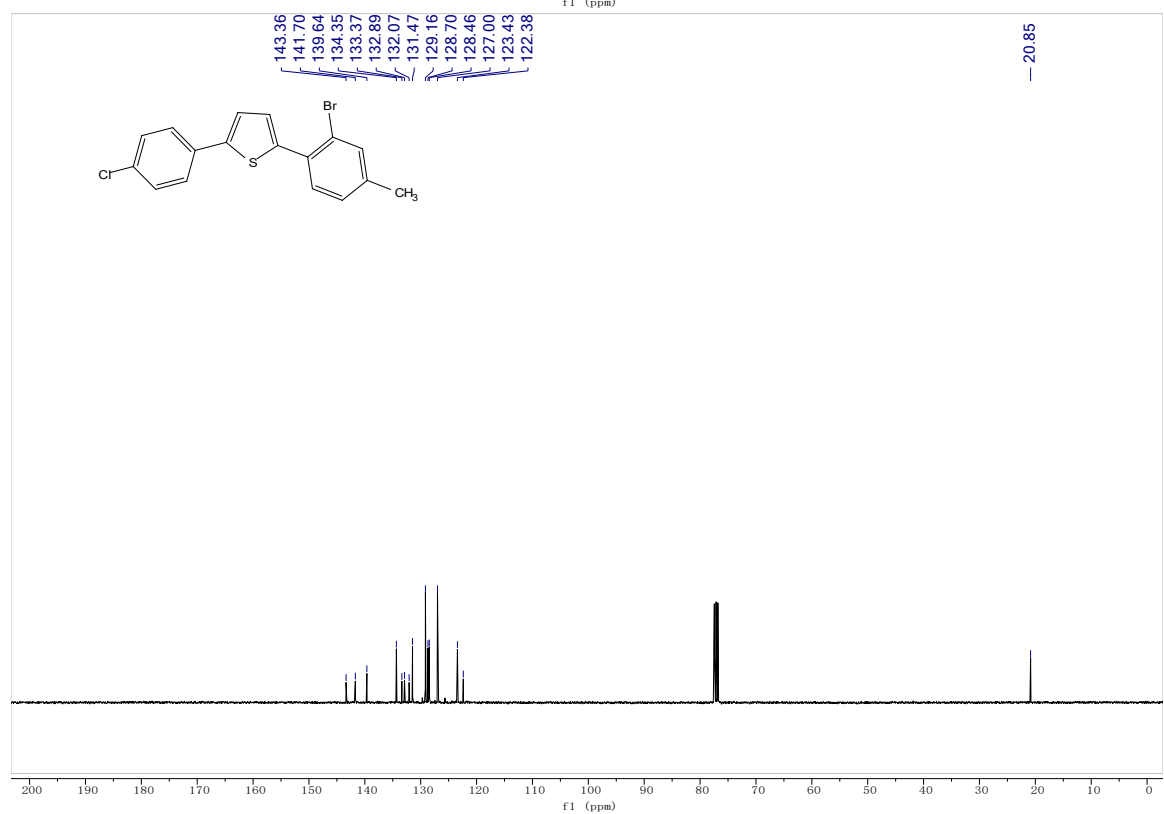
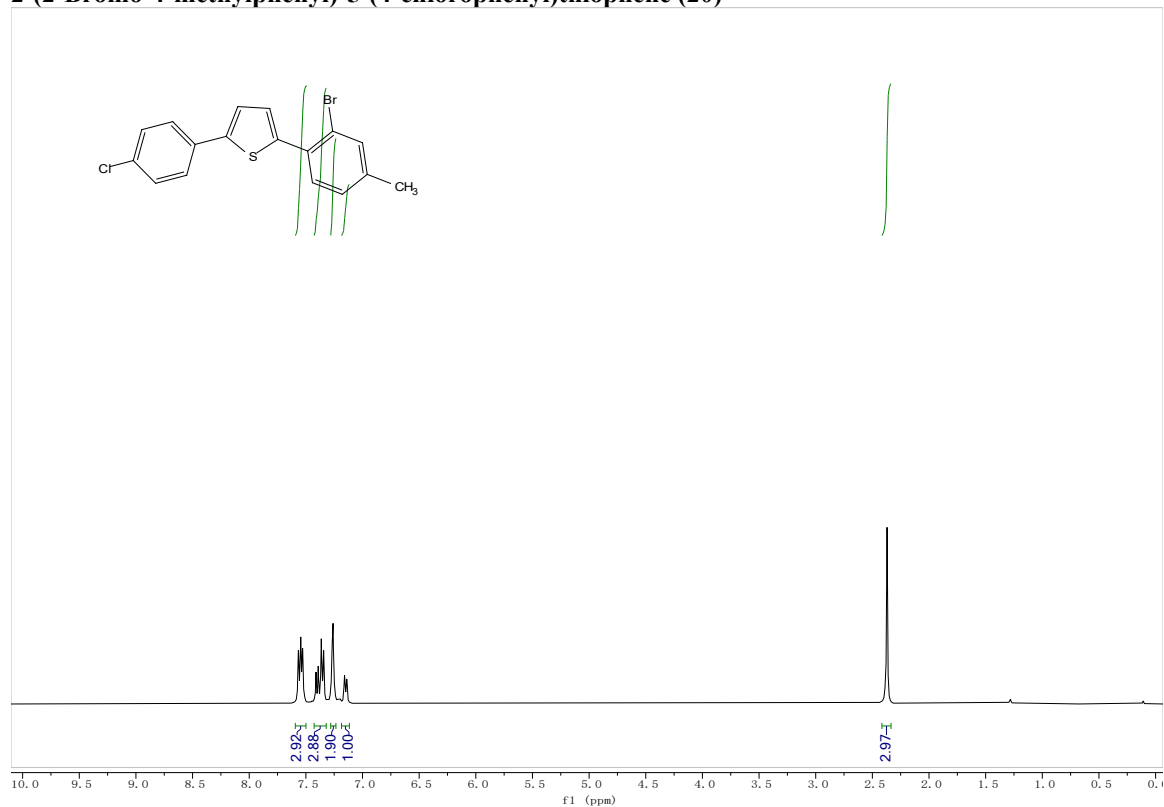
4-(2-Isobutylthiazol-5-yl)-5-(*p*-tolyl)thiophene-2-carbaldehyde (18b)



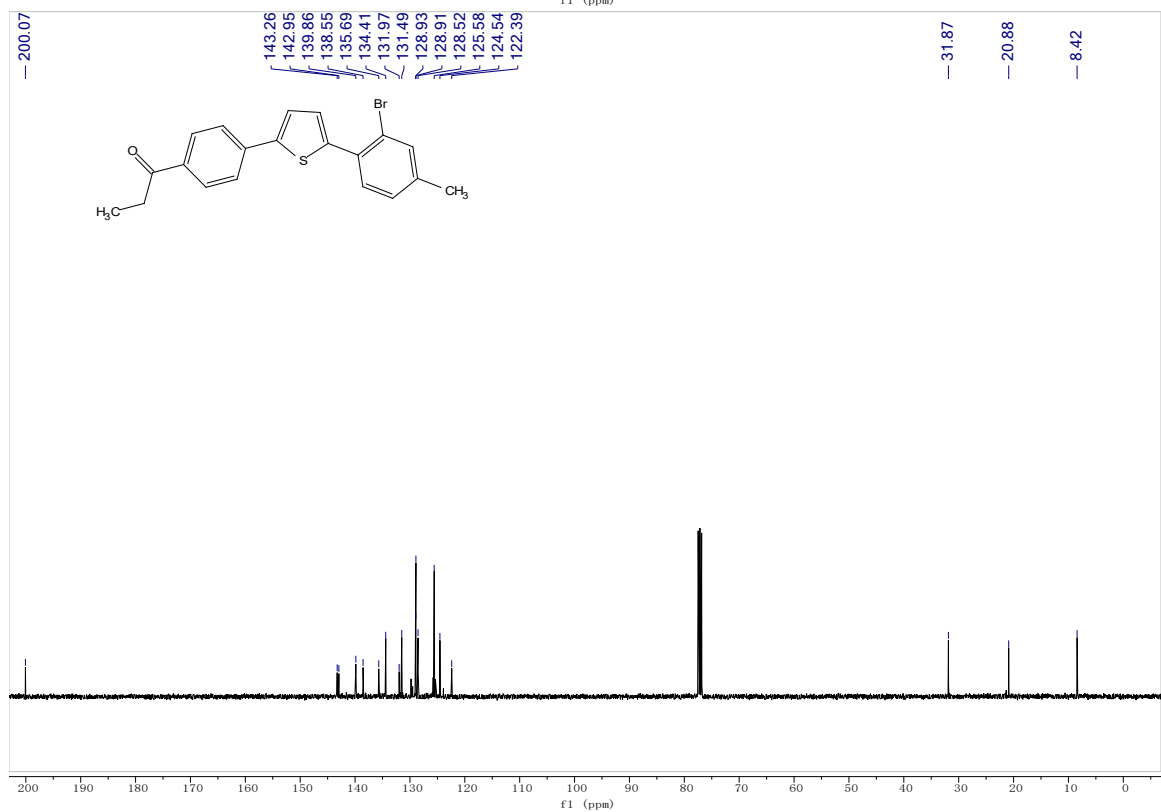
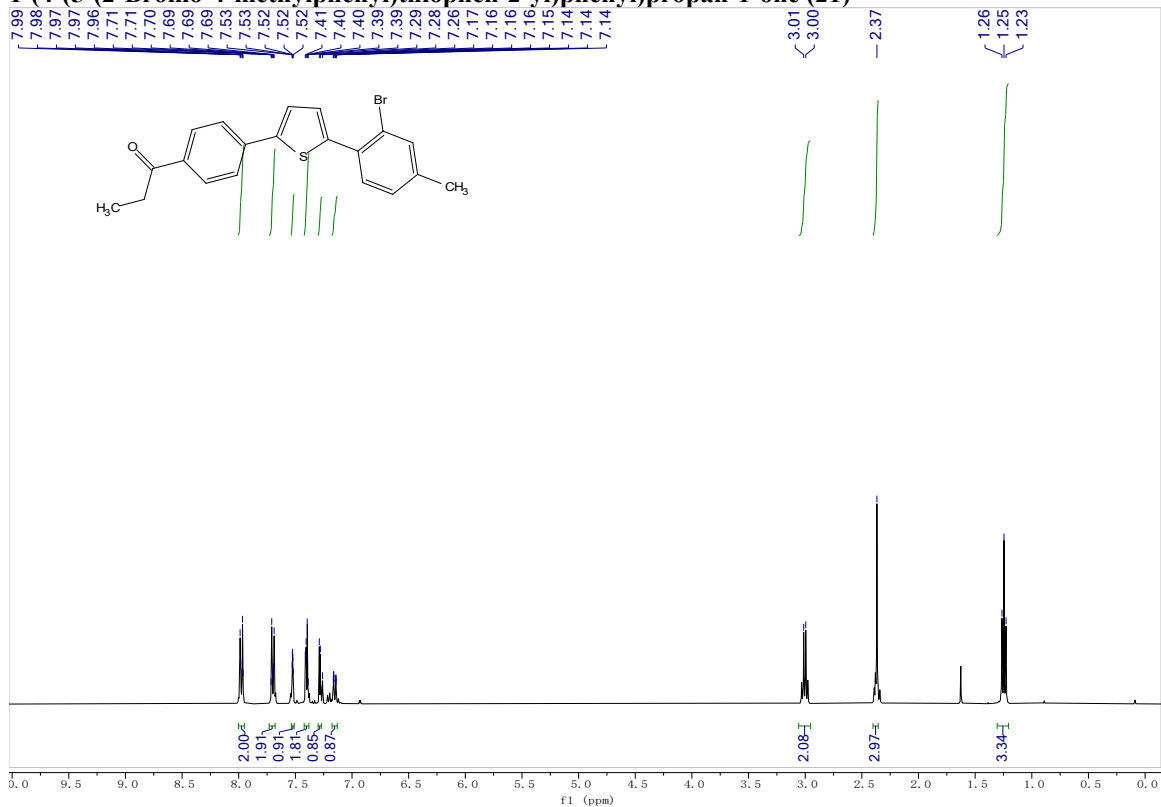
4-(5-(2-Bromophenyl)thiophen-2-yl)benzonitrile (19)



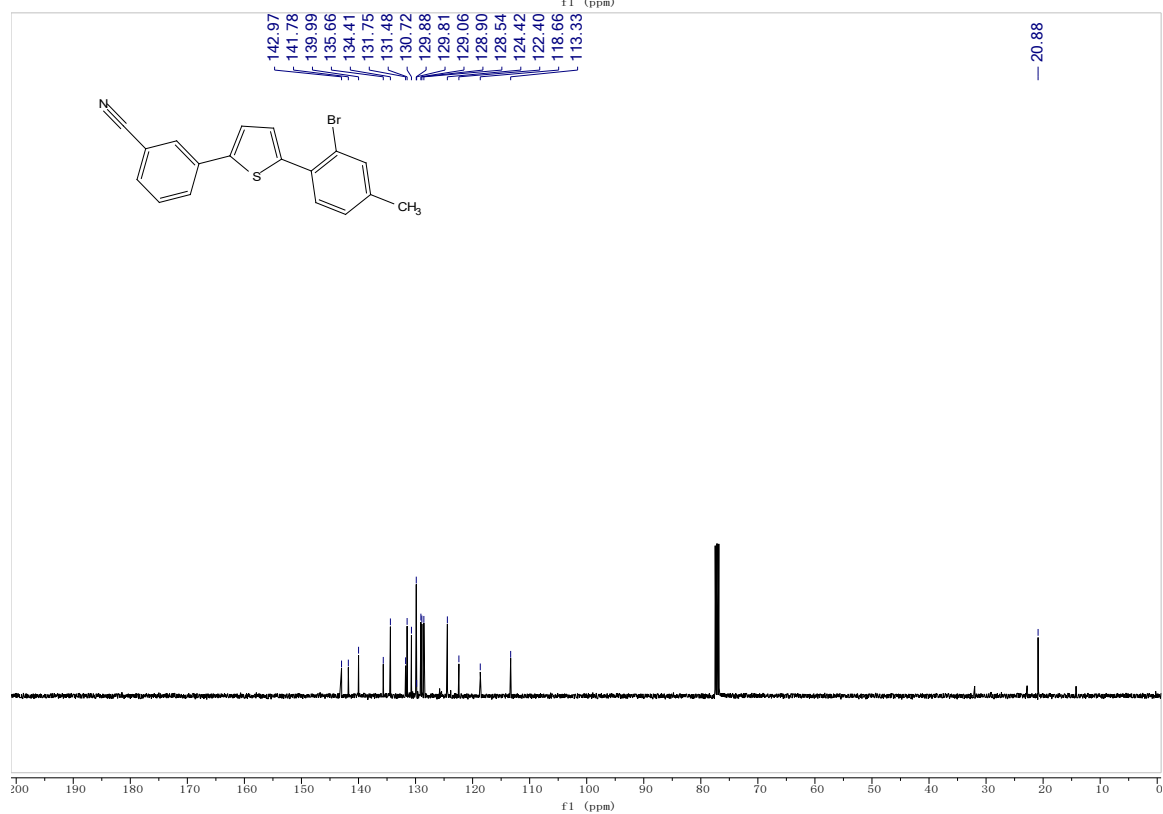
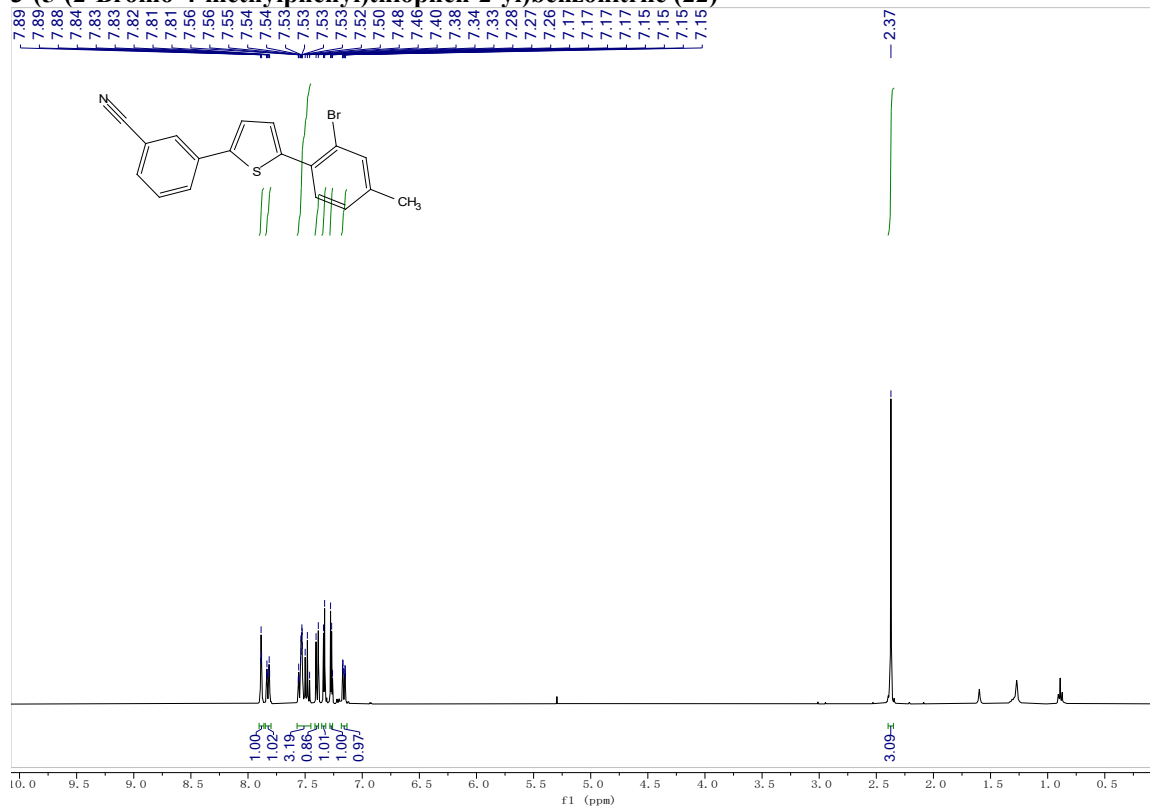
2-(2-Bromo-4-methylphenyl)-5-(4-chlorophenyl)thiophene (20)



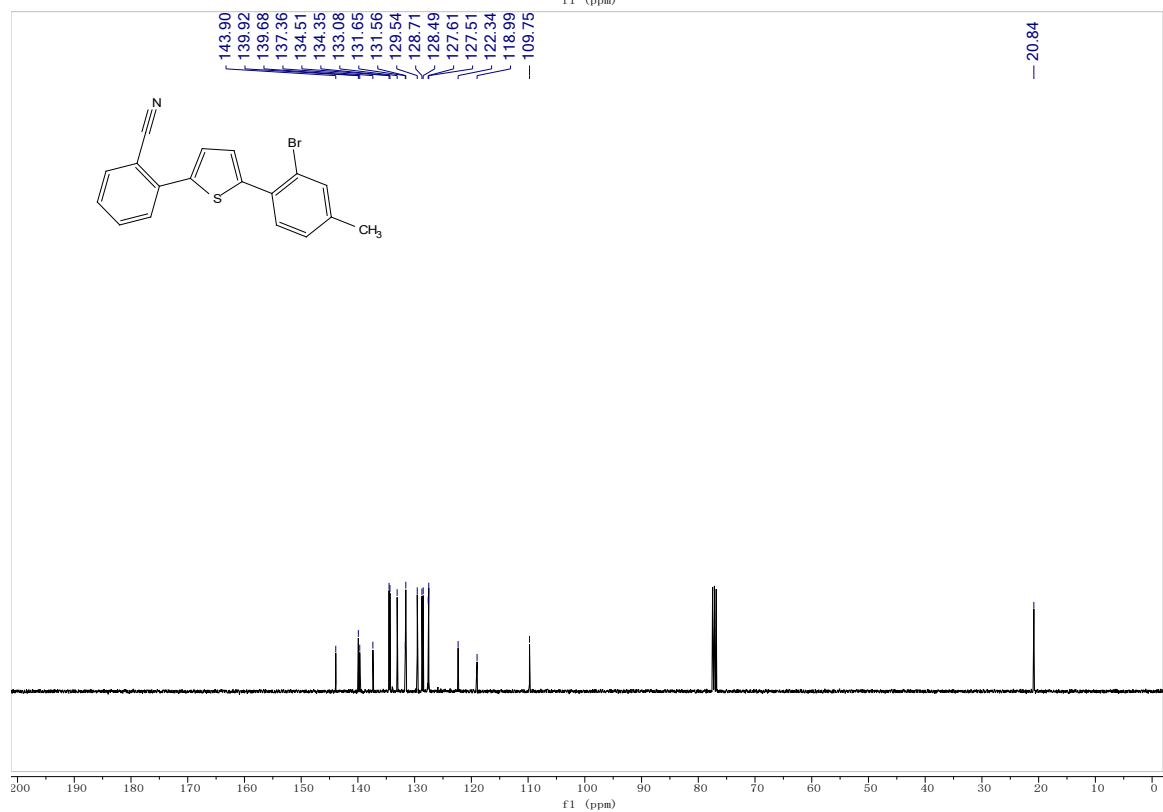
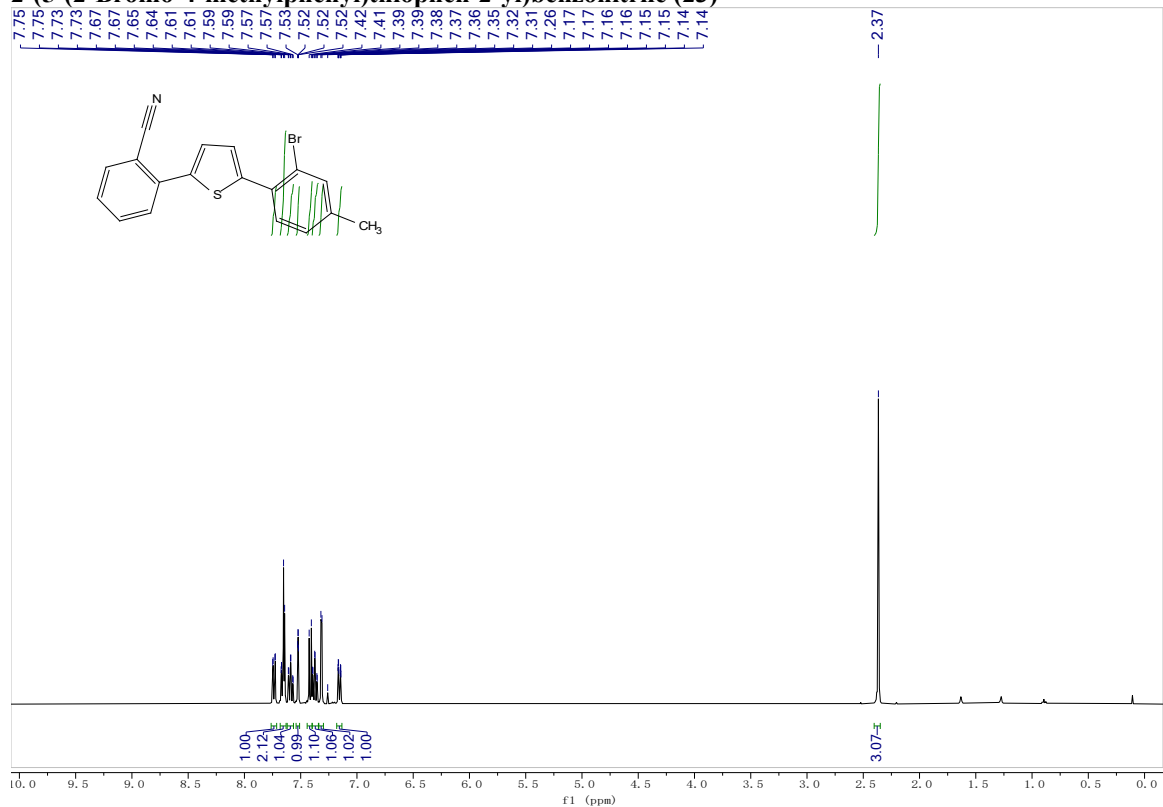
1-(4-(5-(2-Bromo-4-methylphenyl)thiophen-2-yl)phenyl)propan-1-one (21)



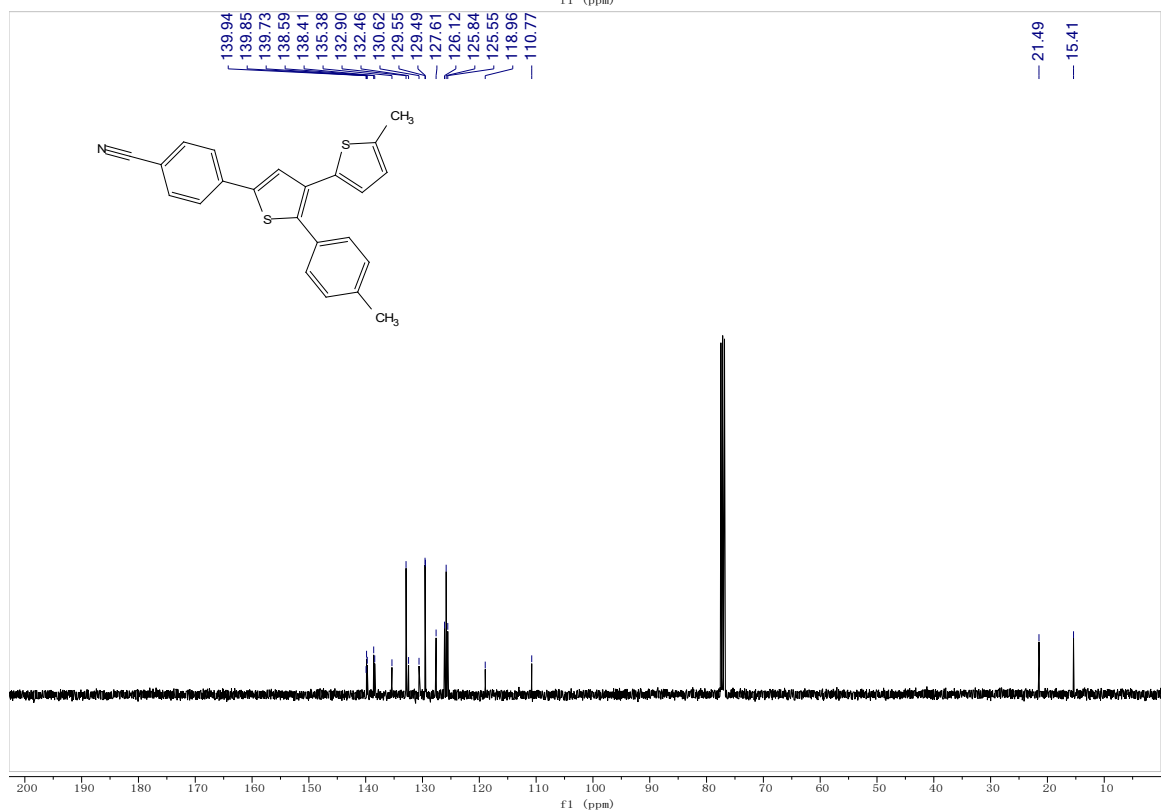
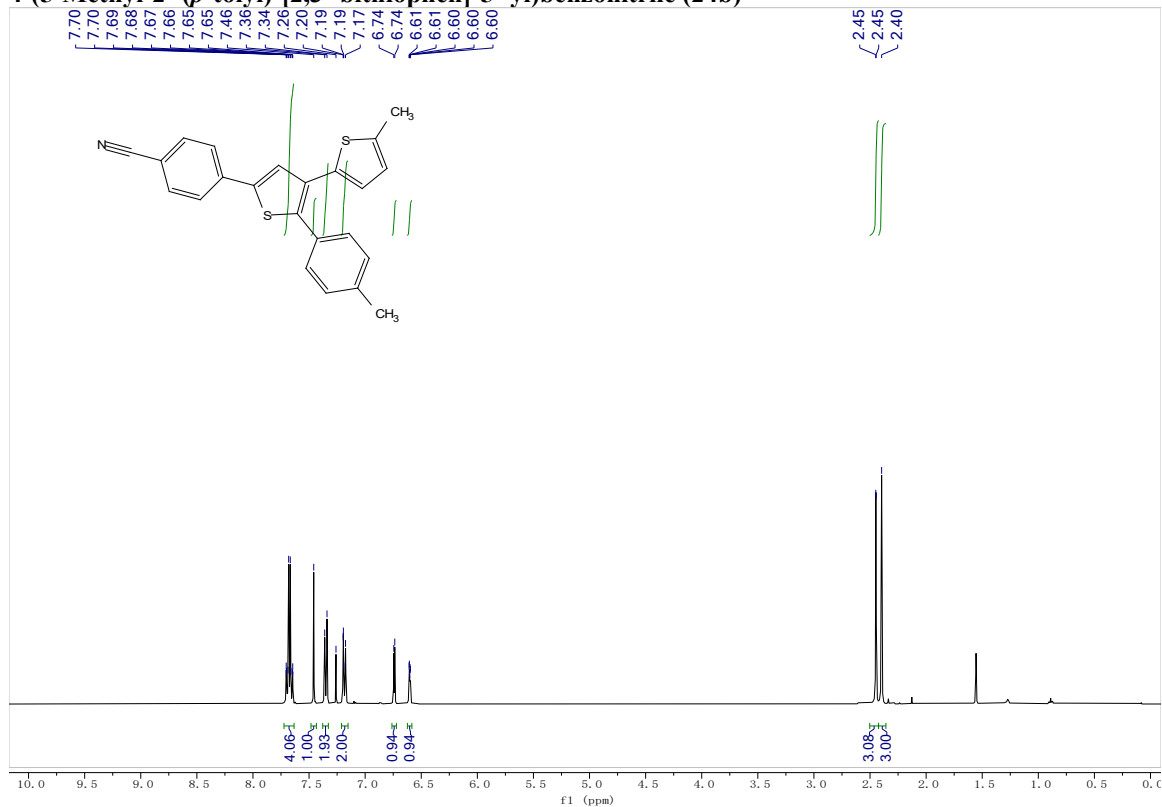
3-(5-(2-Bromo-4-methylphenyl)thiophen-2-yl)benzonitrile (22)



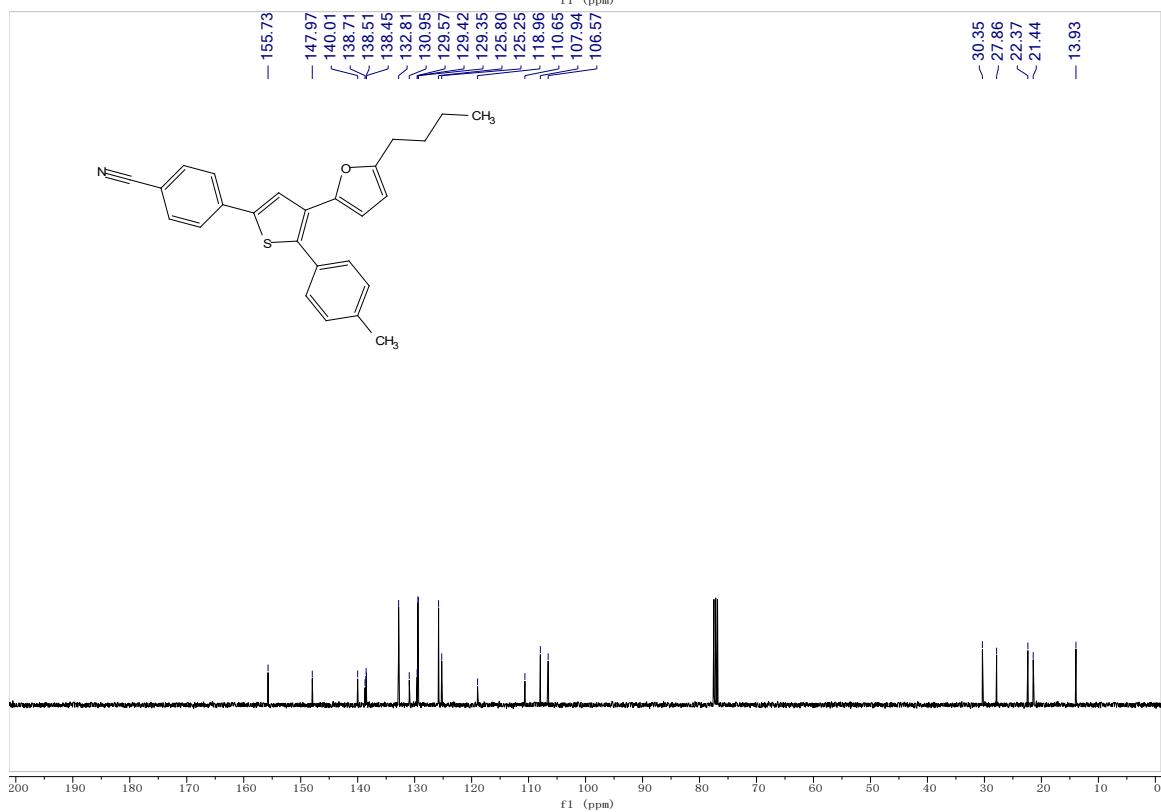
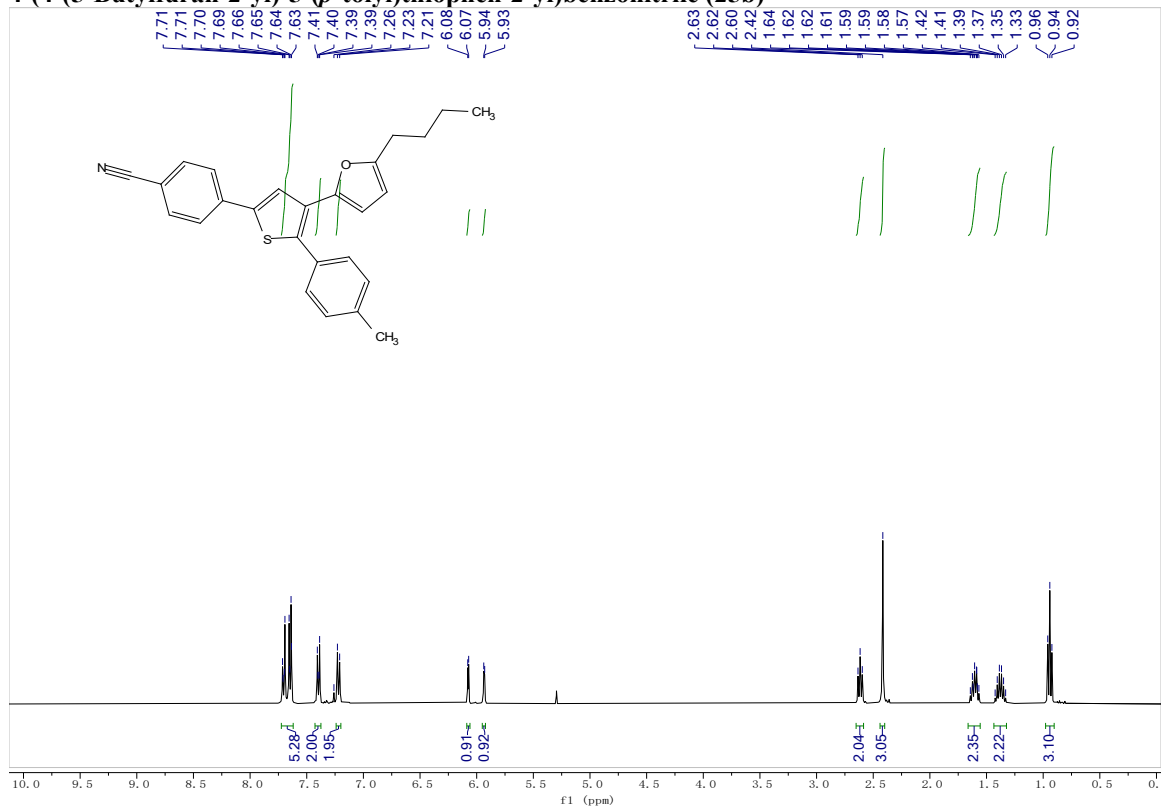
2-(5-(2-Bromo-4-methylphenyl)thiophen-2-yl)benzonitrile (23)



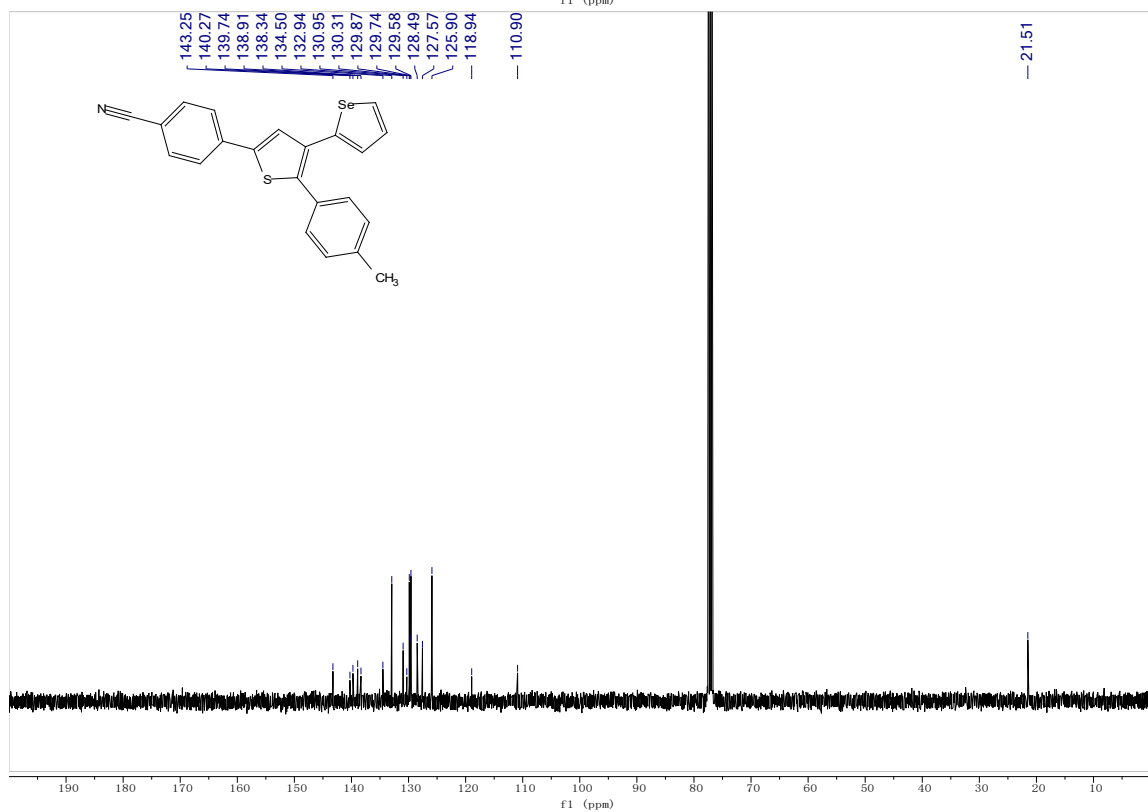
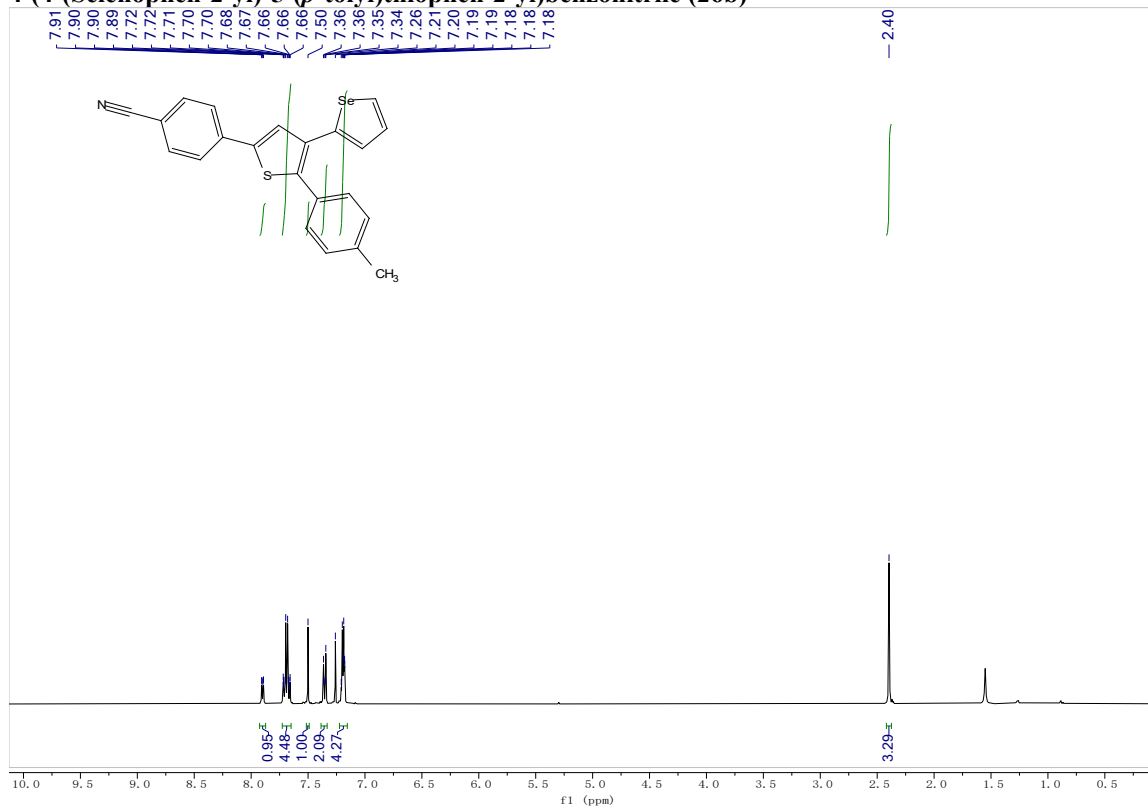
4-(5-Methyl-2'-(*p*-tolyl)-[2,3'-bithiophen]-5'-yl)benzonitrile (24b)



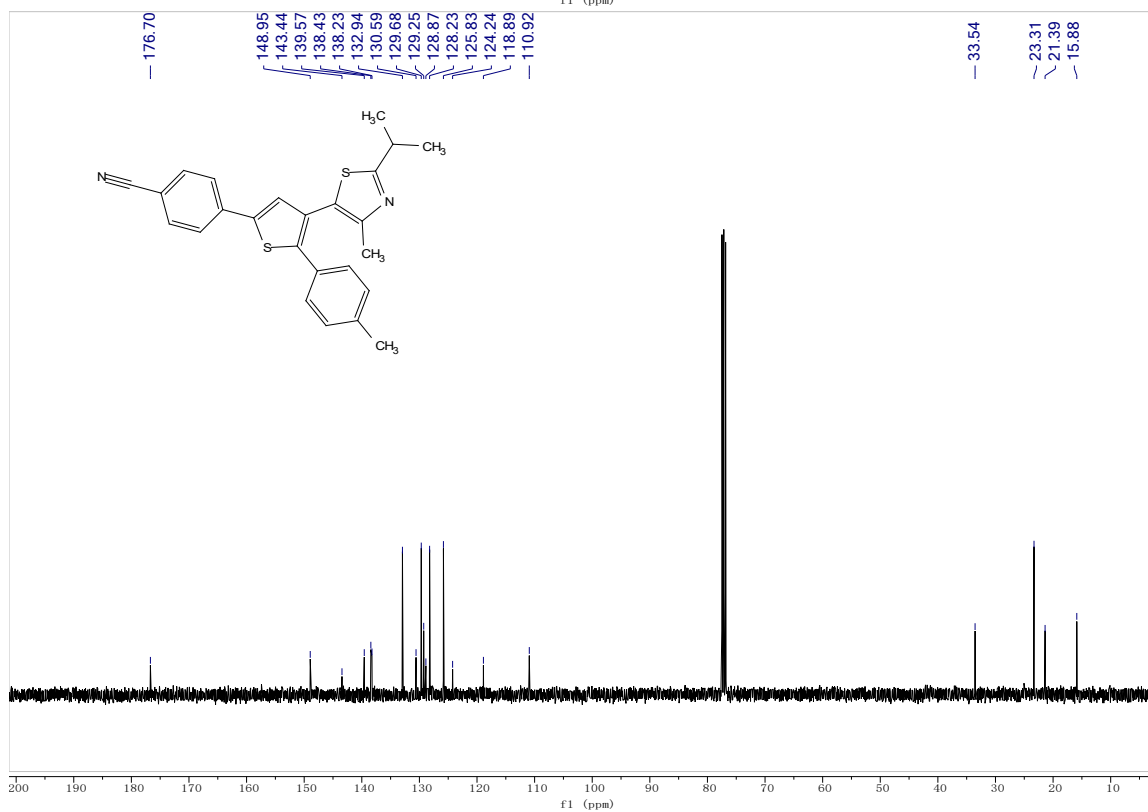
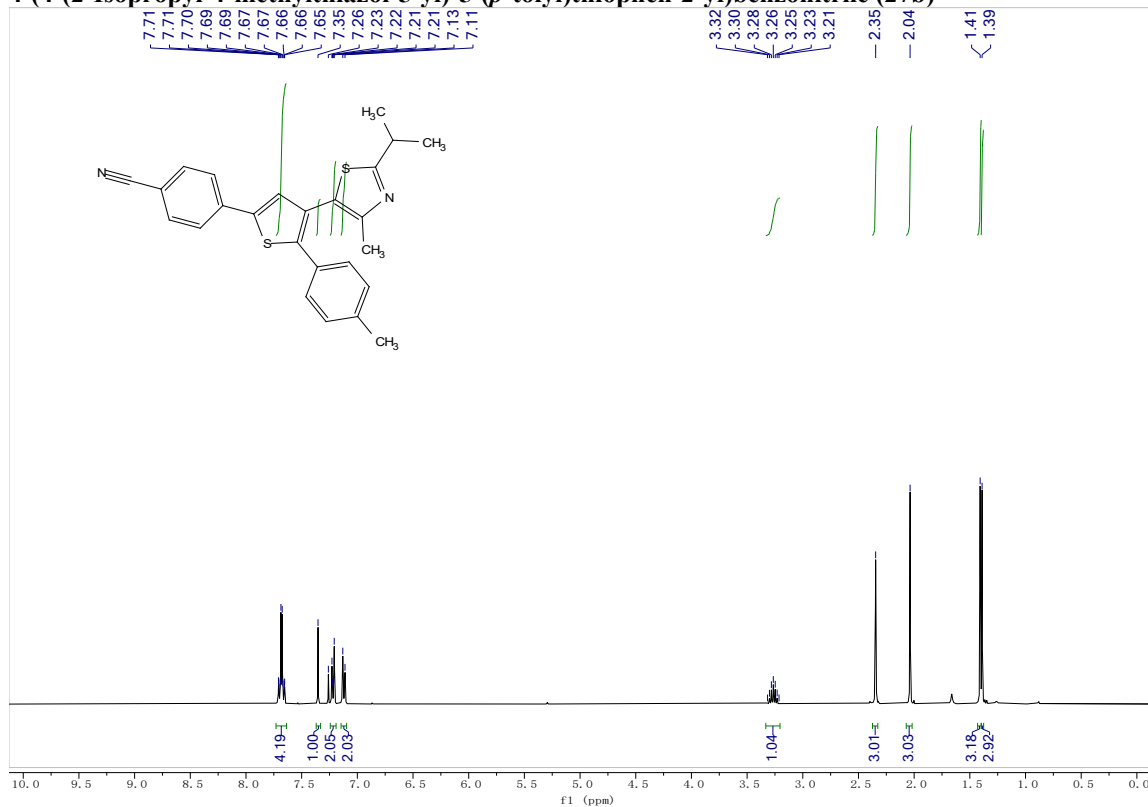
4-(4-(5-Butylfuran-2-yl)-5-(*p*-tolyl)thiophen-2-yl)benzonitrile (25b)



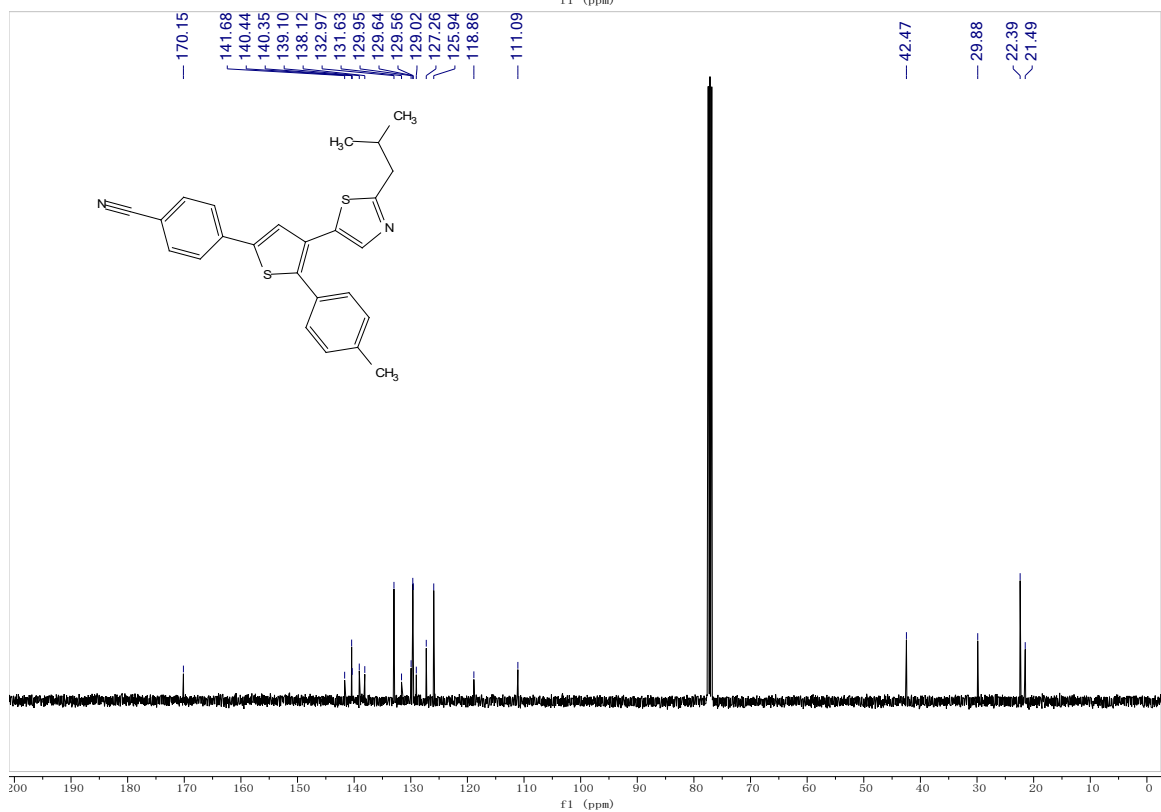
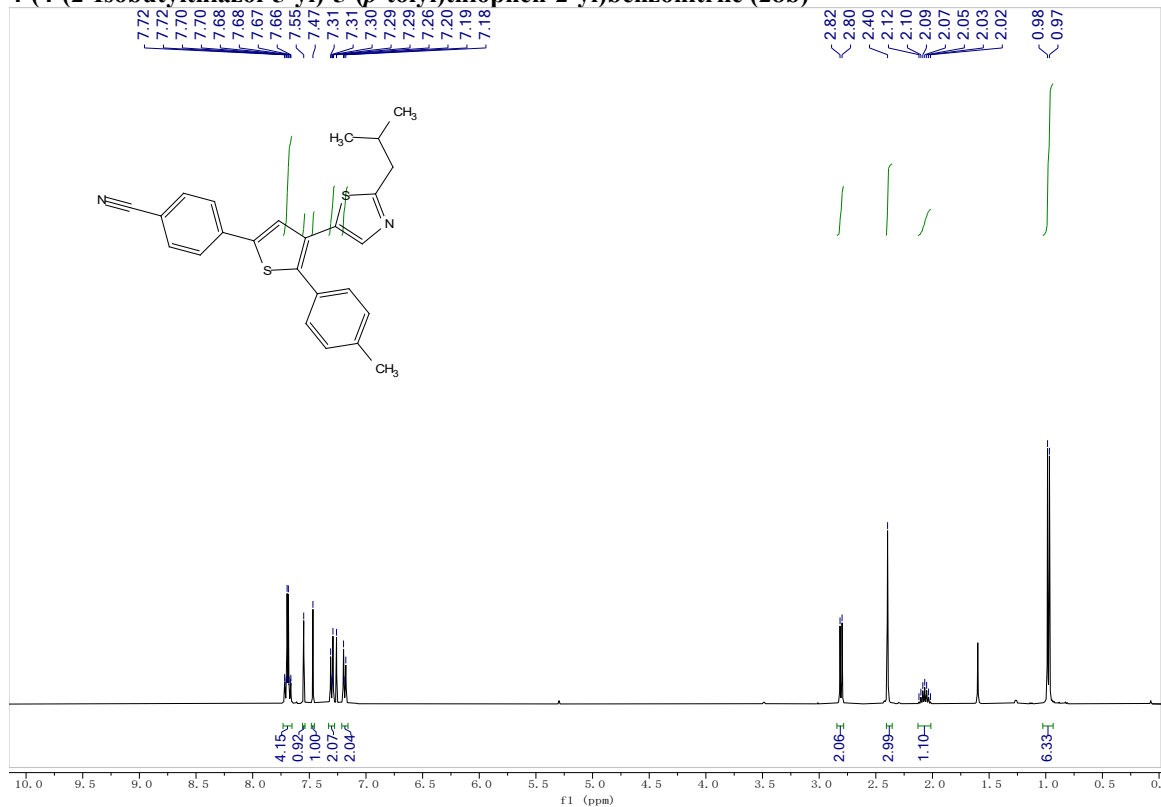
4-(4-(Selenophen-2-yl)-5-(*p*-tolyl)thiophen-2-yl)benzonitrile (26b)



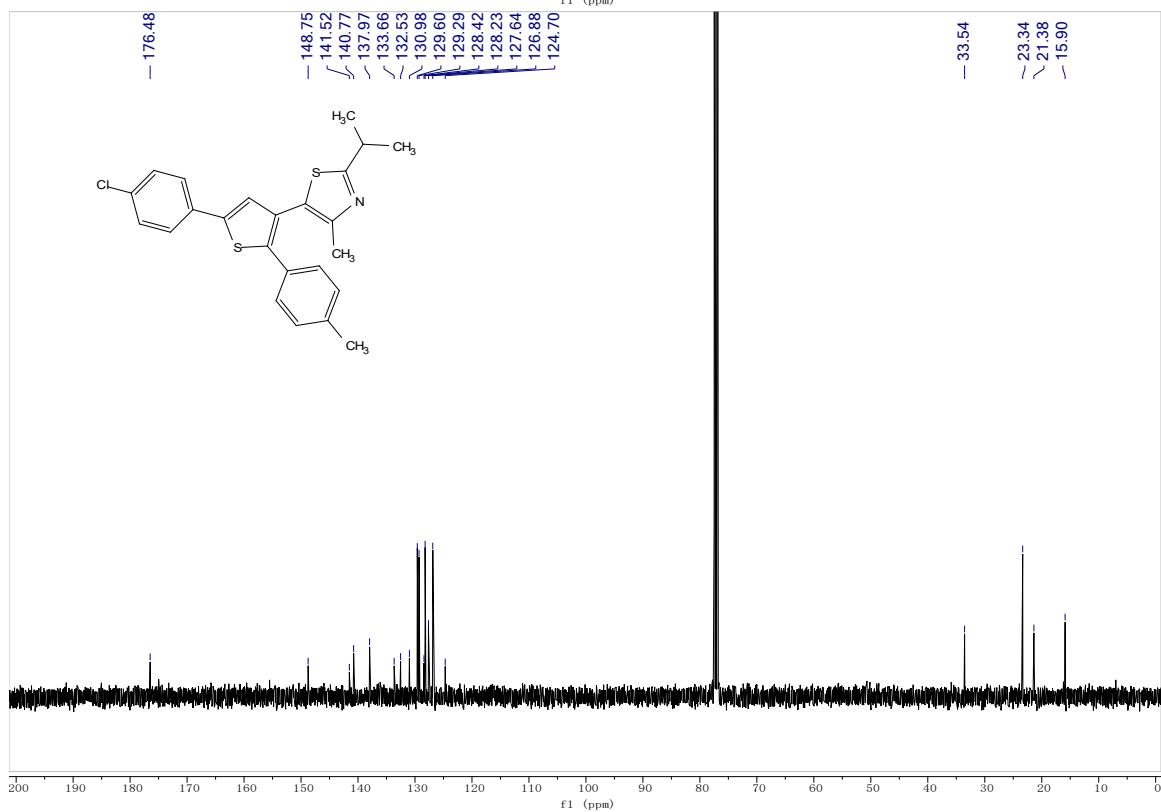
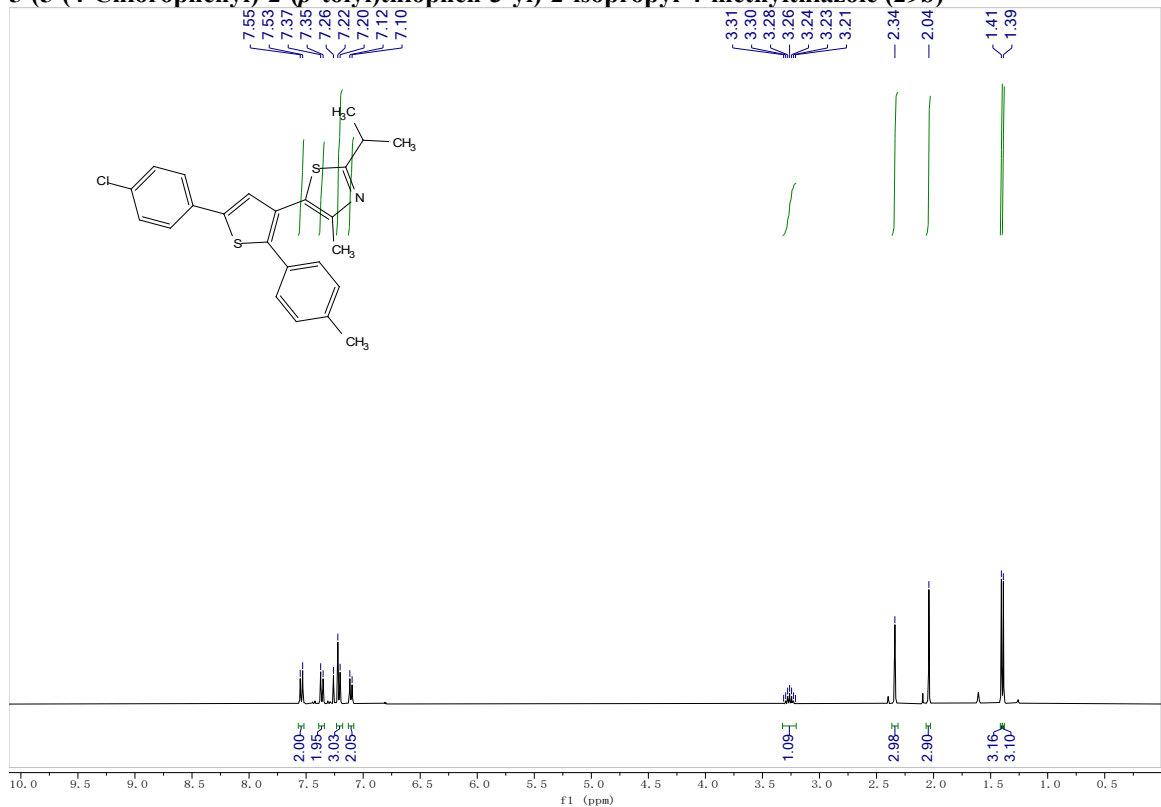
4-(4-(2-Isopropyl-4-methylthiazol-5-yl)-5-(*p*-tolyl)thiophen-2-yl)benzonitrile (27b)



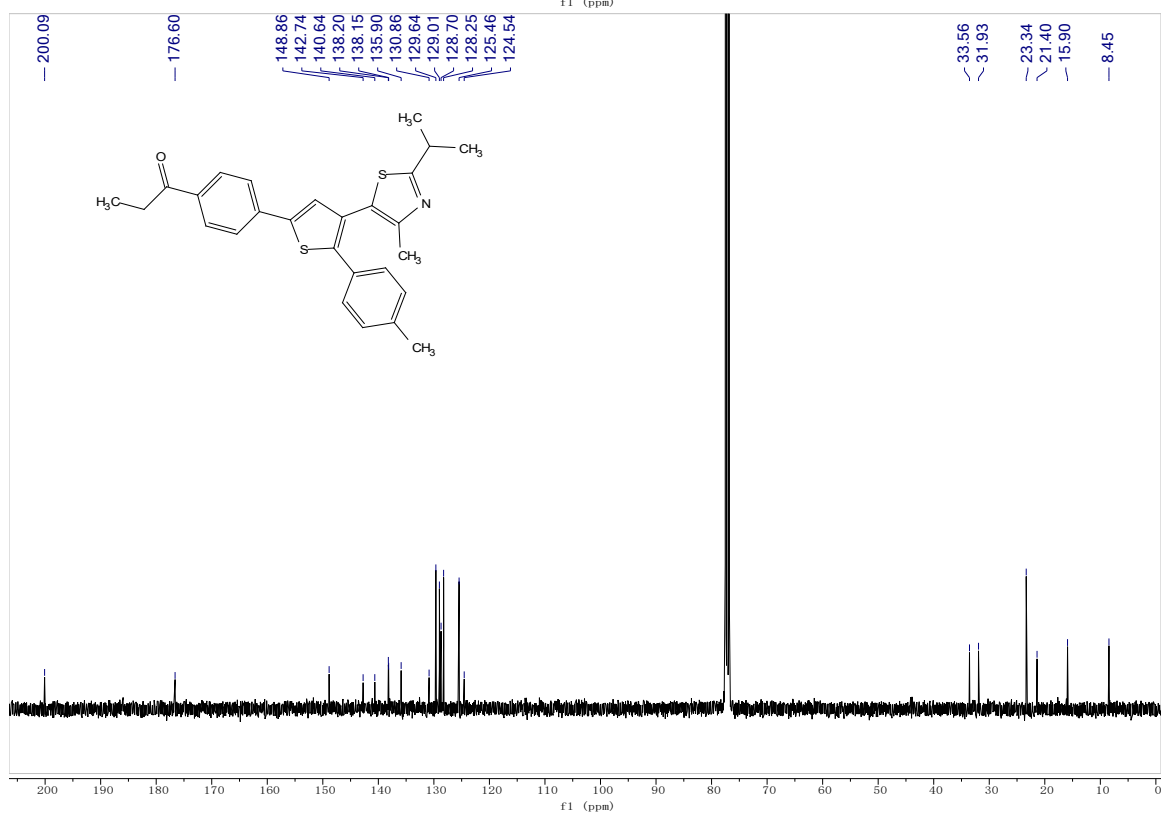
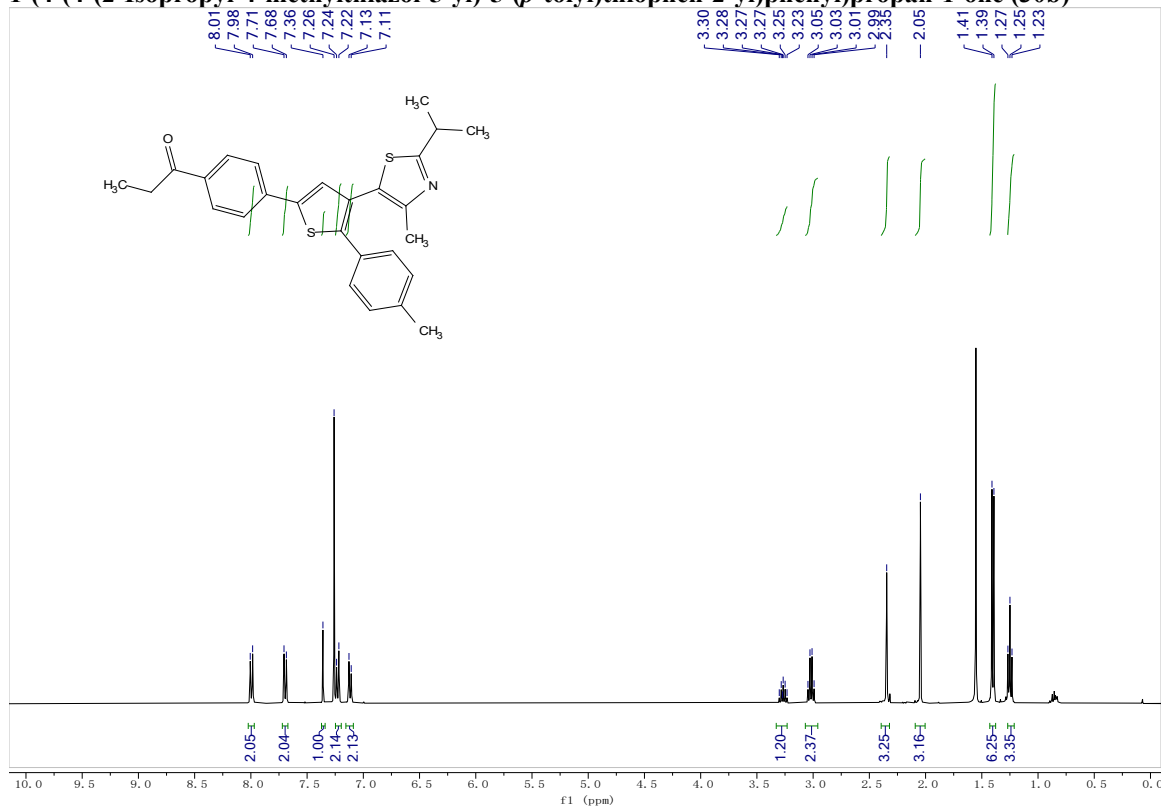
4-(4-(2-Isobutylthiazol-5-yl)-5-(*p*-tolyl)thiophen-2-yl)benzonitrile (28b)



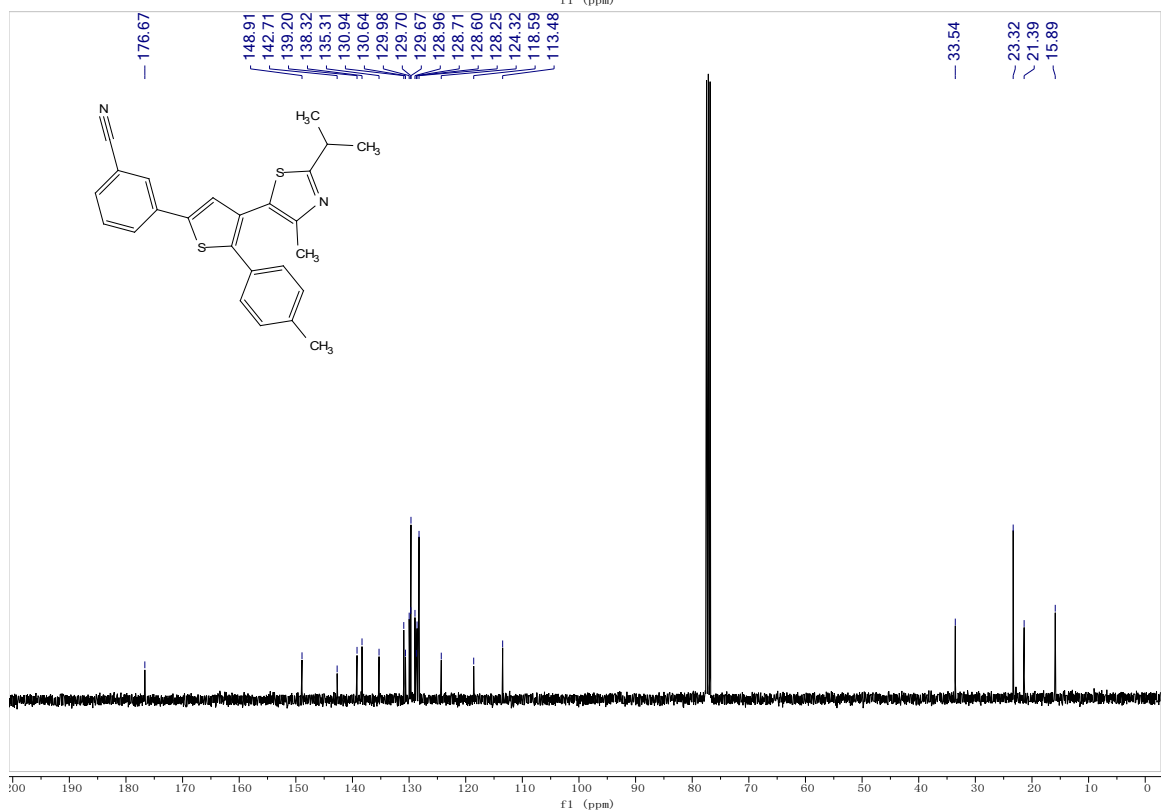
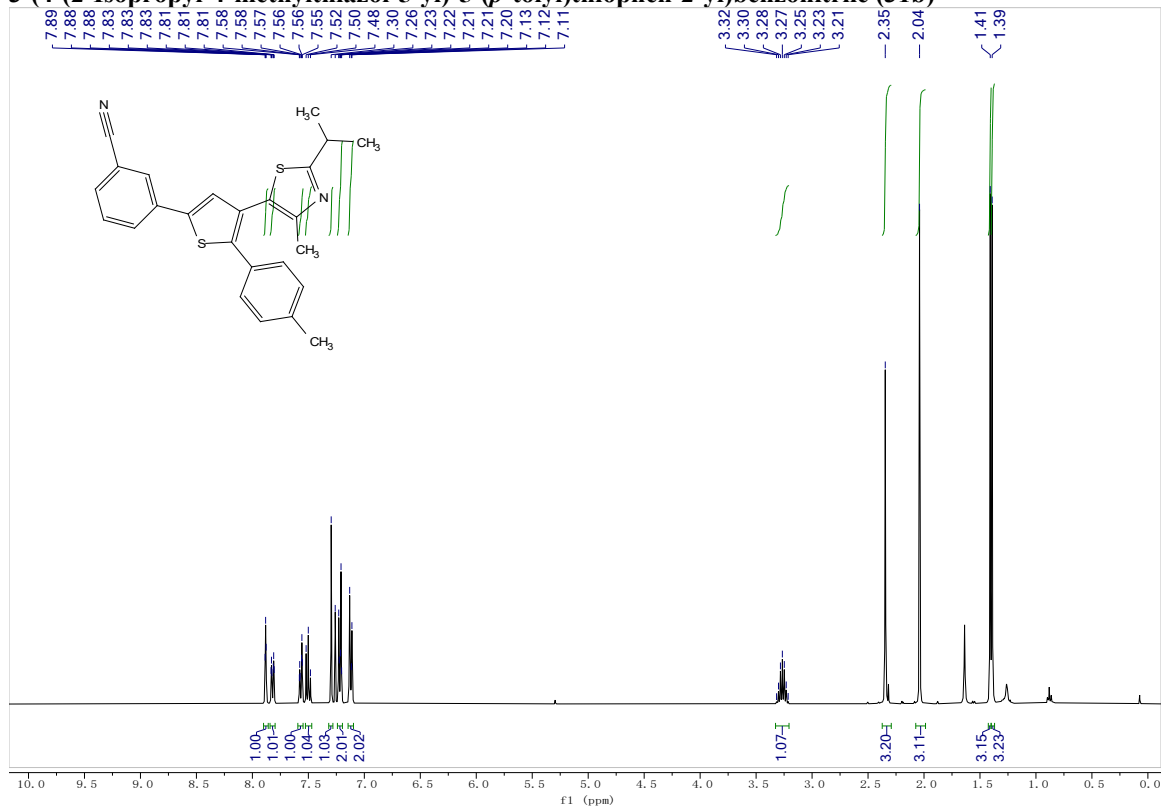
5-(5-(4-Chlorophenyl)-2-(*p*-tolyl)thiophen-3-yl)-2-isopropyl-4-methylthiazole (29b)



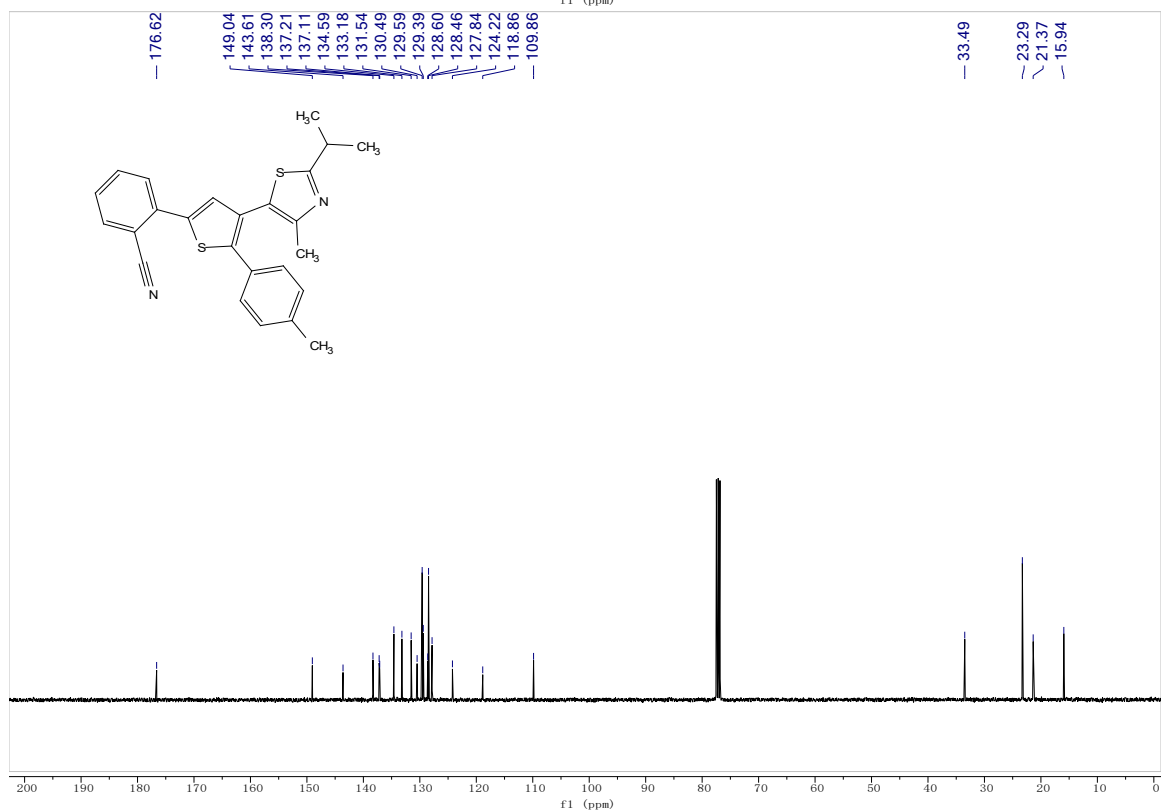
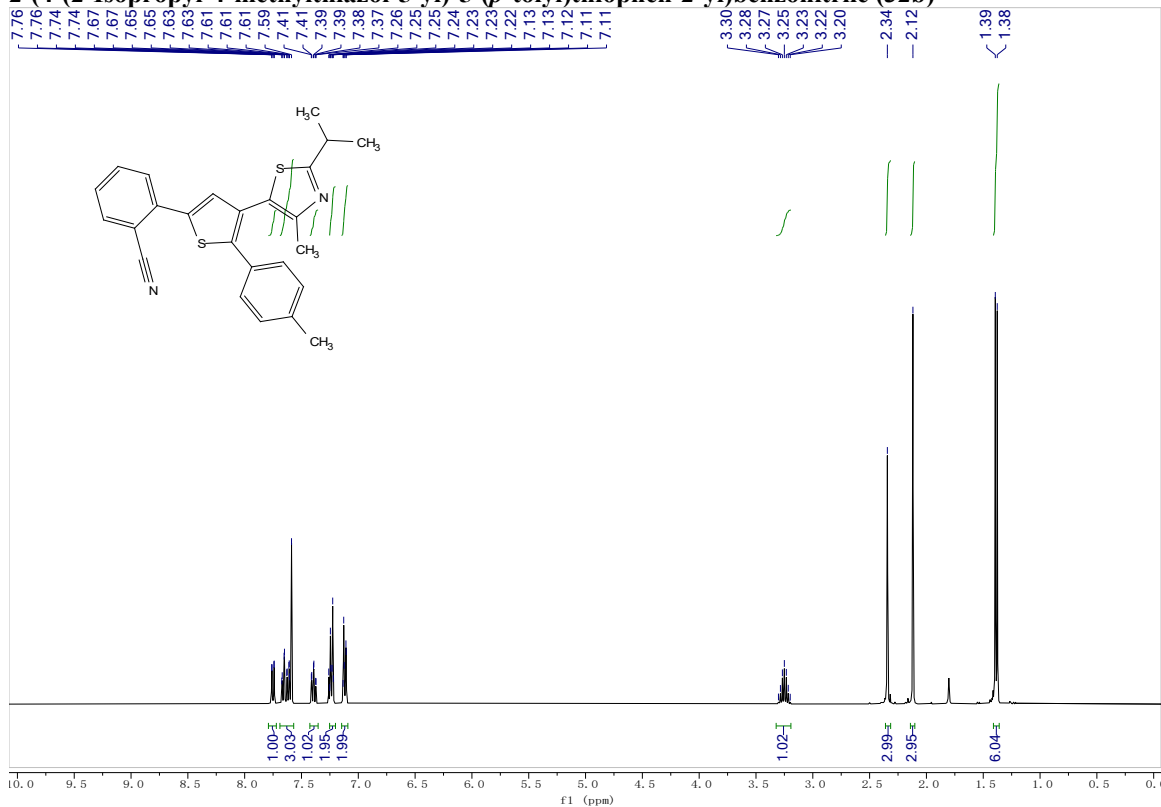
1-(4-(4-(2-Isopropyl-4-methylthiazol-5-yl)-5-(*p*-tolyl)thiophen-2-yl)phenyl)propan-1-one (30b)



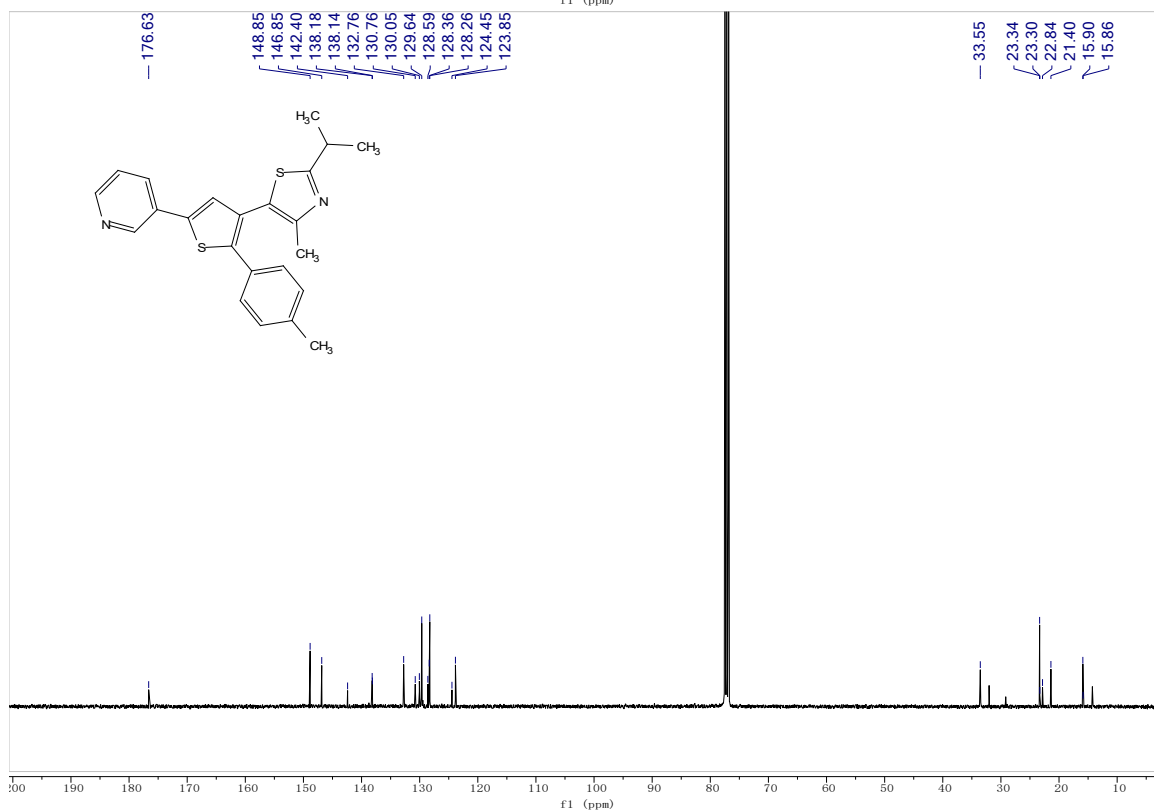
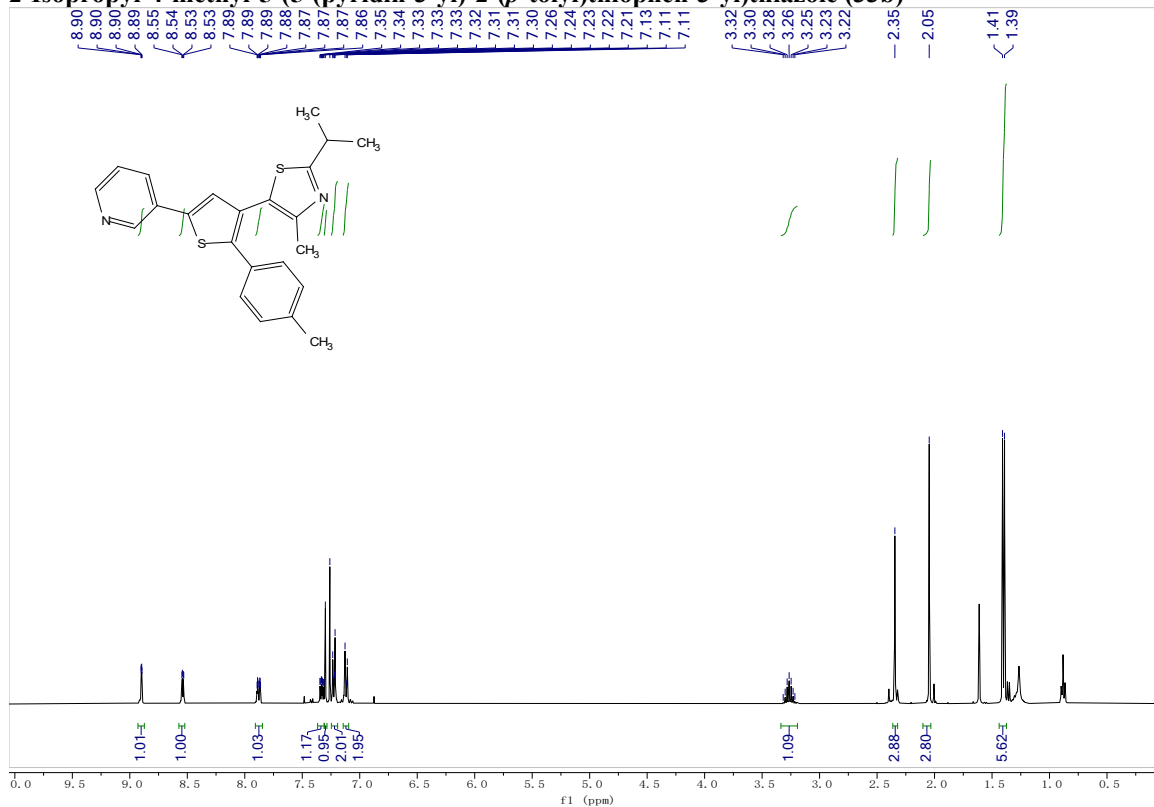
3-(4-(2-Isopropyl-4-methylthiazol-5-yl)-5-(*p*-tolyl)thiophen-2-yl)benzonitrile (31b)



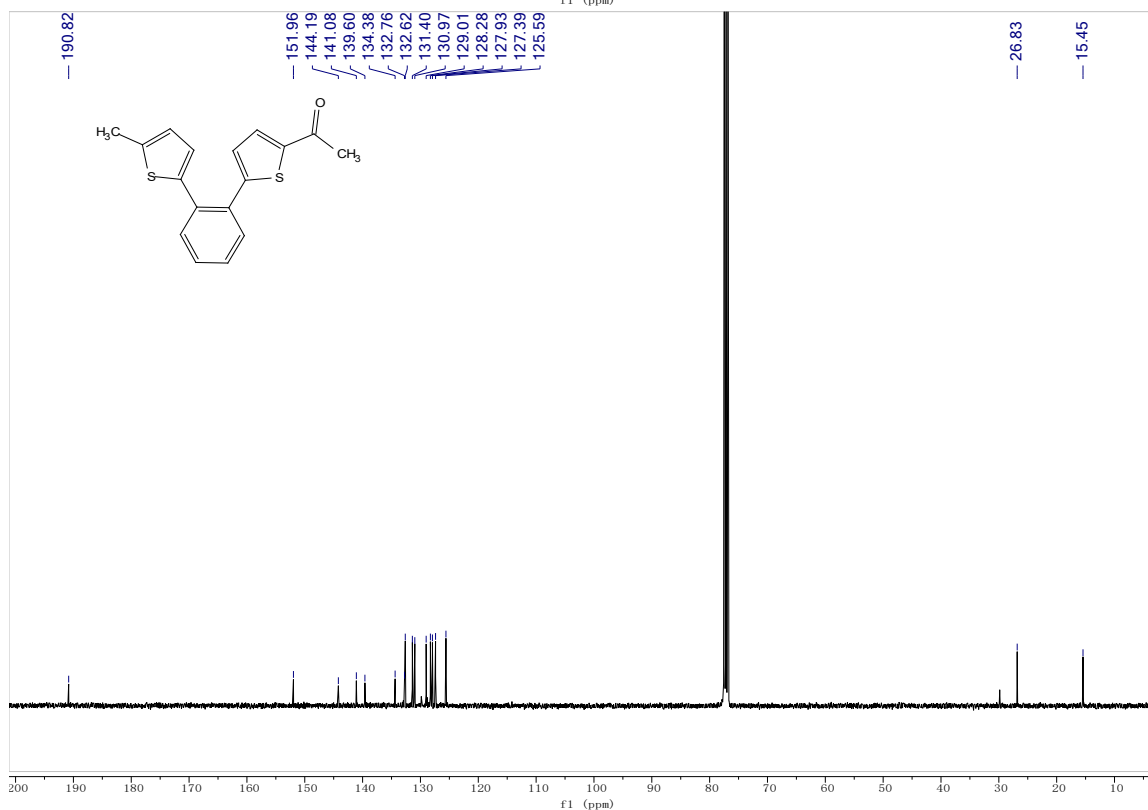
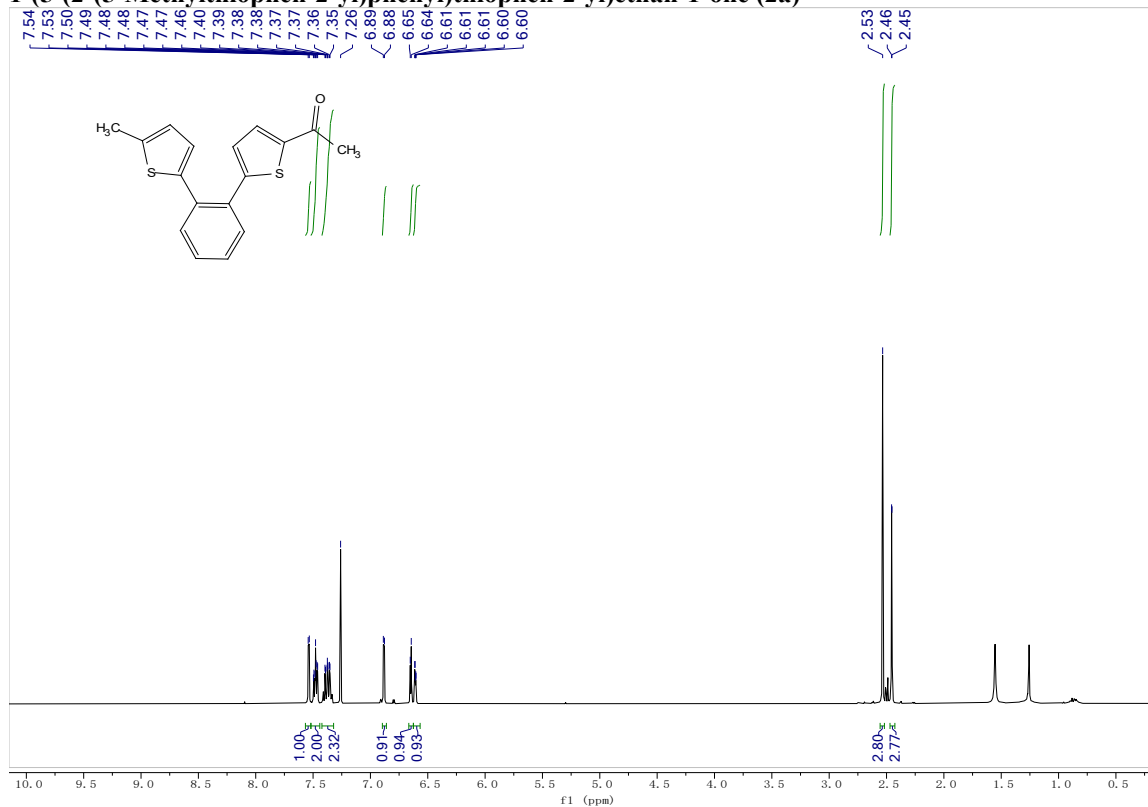
2-(4-(2-Isopropyl-4-methylthiazol-5-yl)-5-(*p*-tolyl)thiophen-2-yl)benzonitrile (32b)



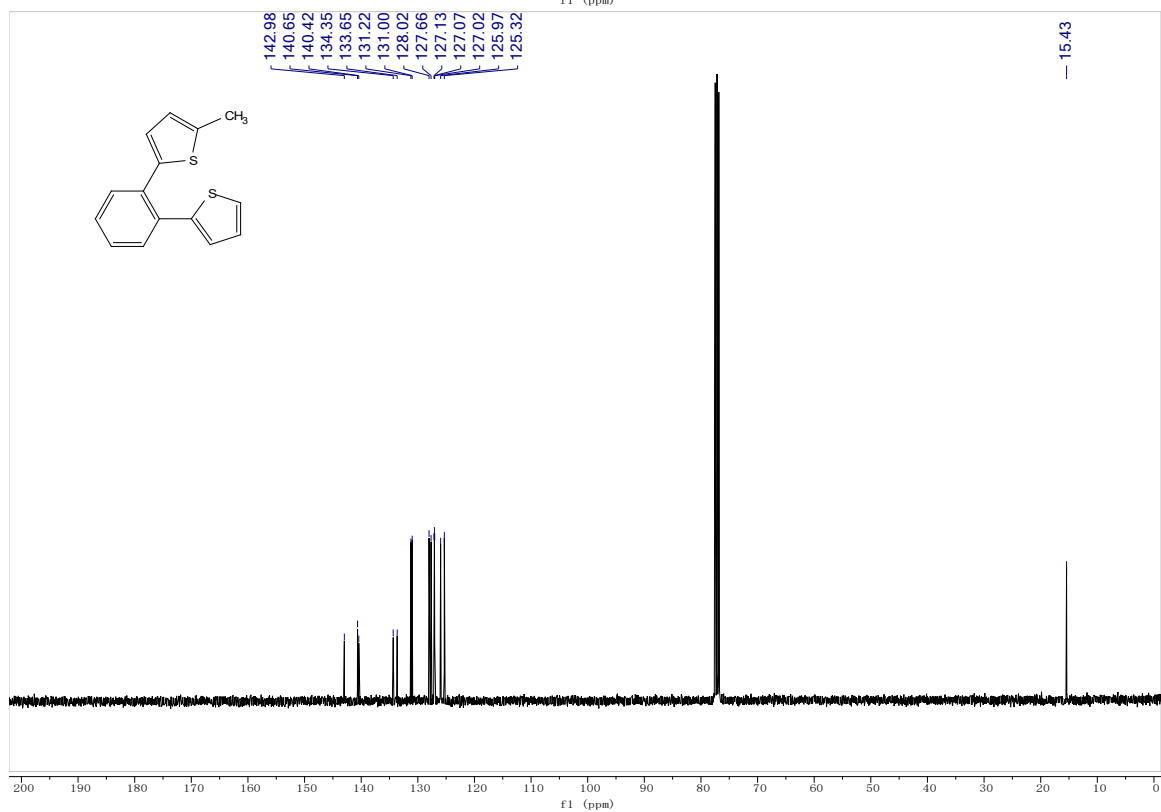
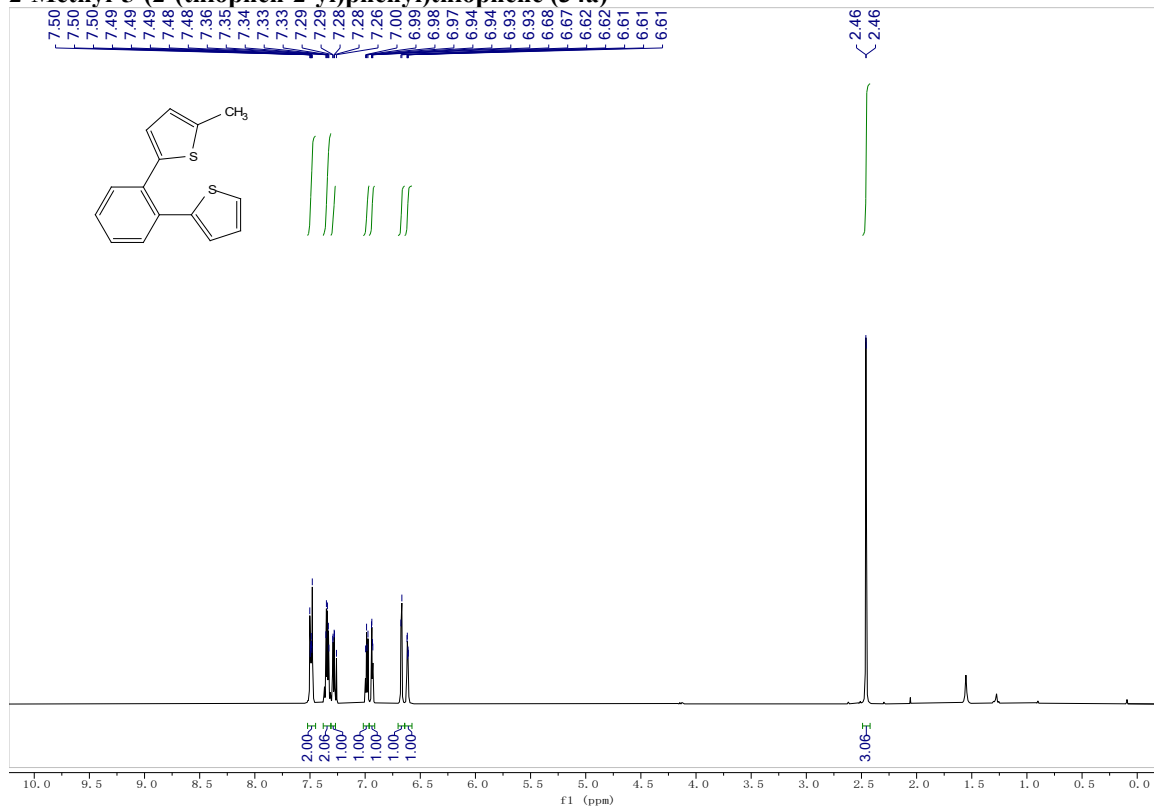
2-Isopropyl-4-methyl-5-(5-(pyridin-3-yl)-2-(*p*-tolyl)thiophen-3-yl)thiazole (33b)



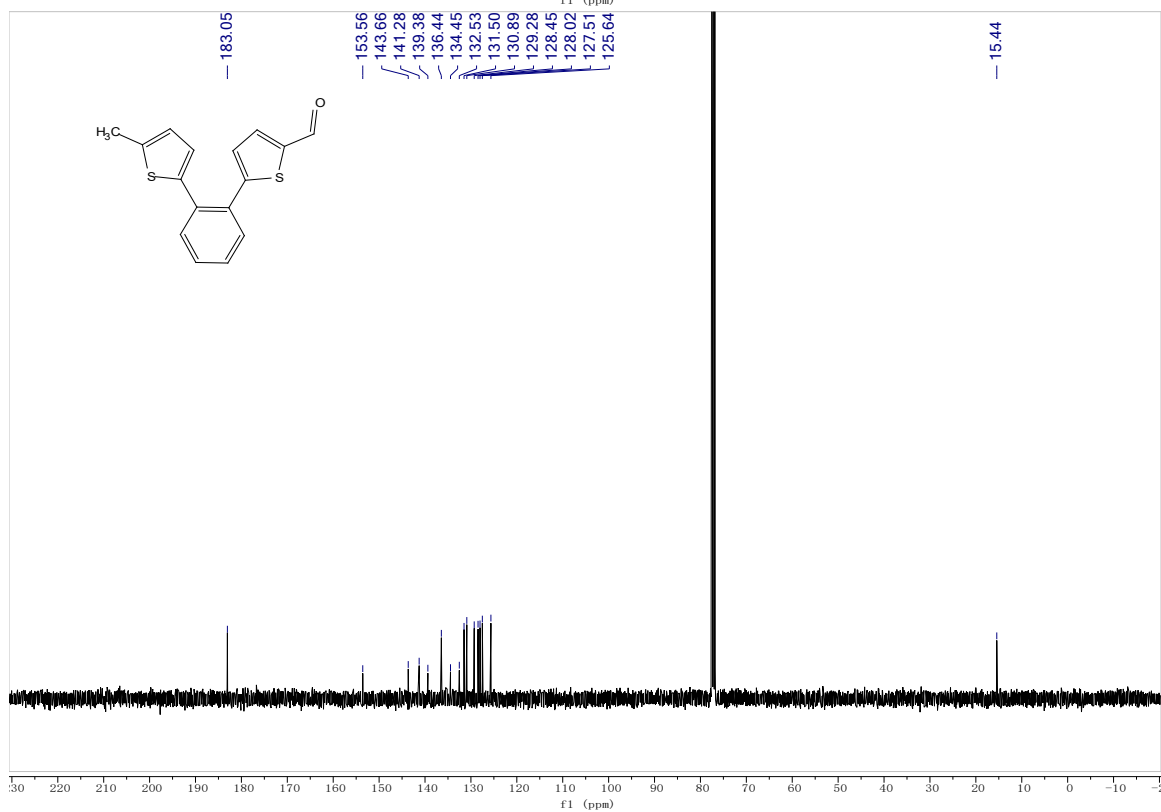
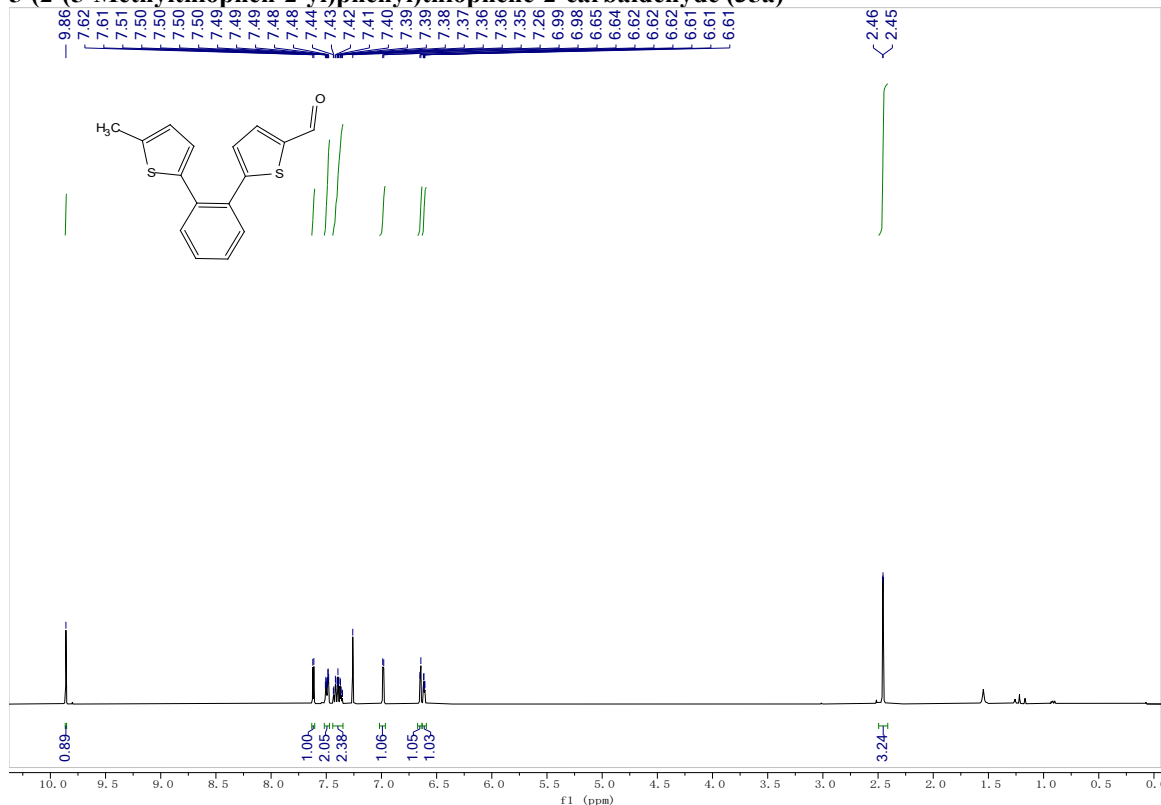
1-(5-(2-(5-Methylthiophen-2-yl)phenyl)thiophen-2-yl)ethan-1-one (2a)



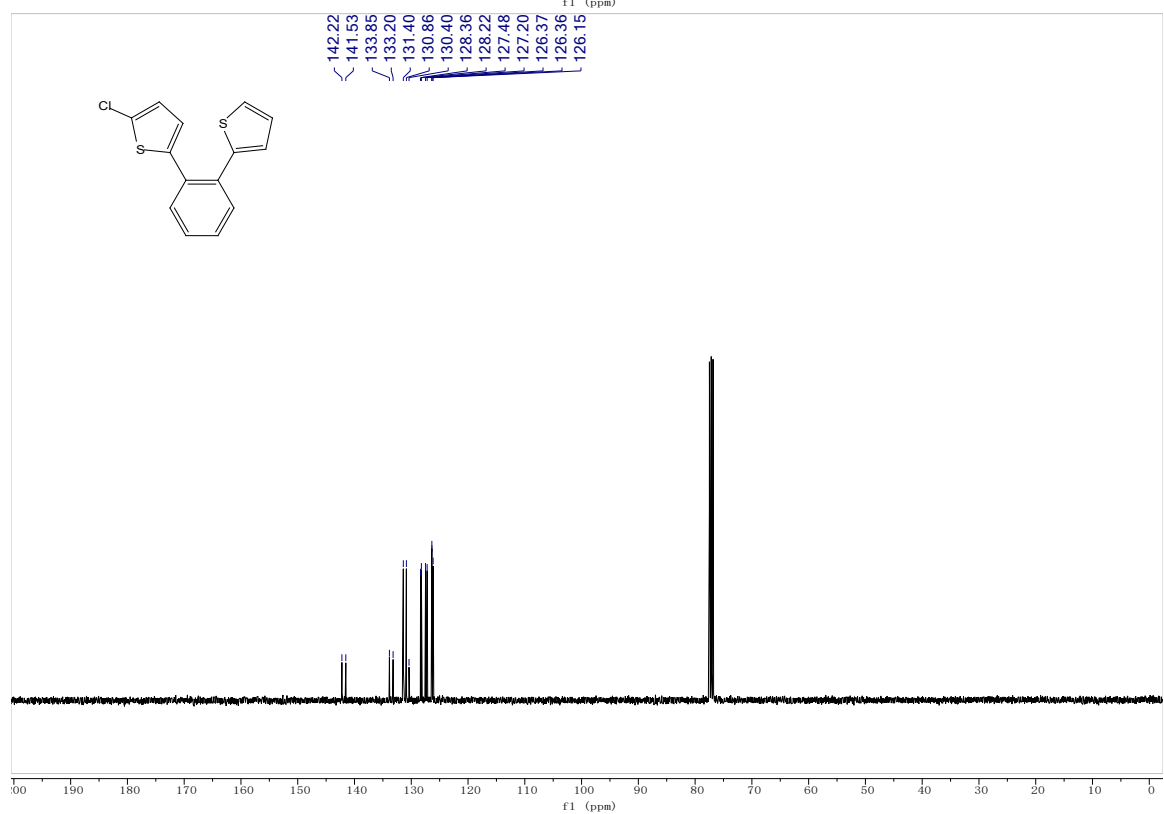
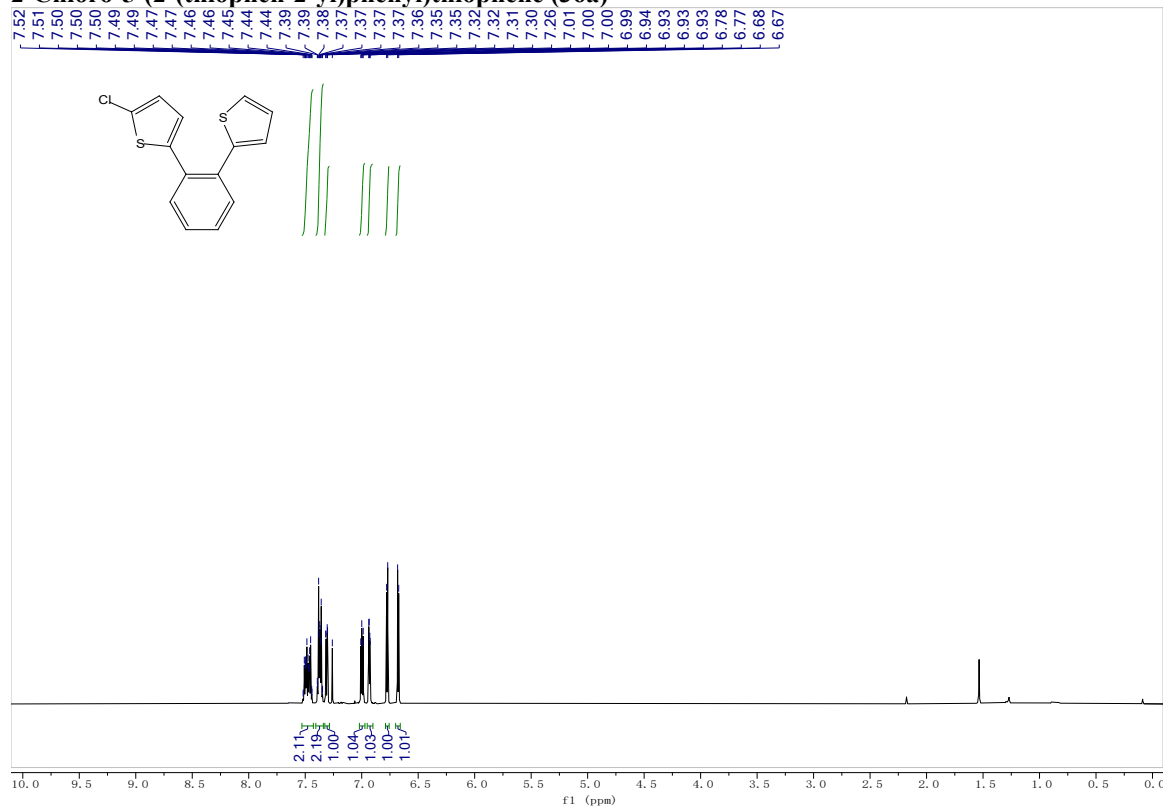
2-Methyl-5-(2-(thiophen-2-yl)phenyl)thiophene (34a)



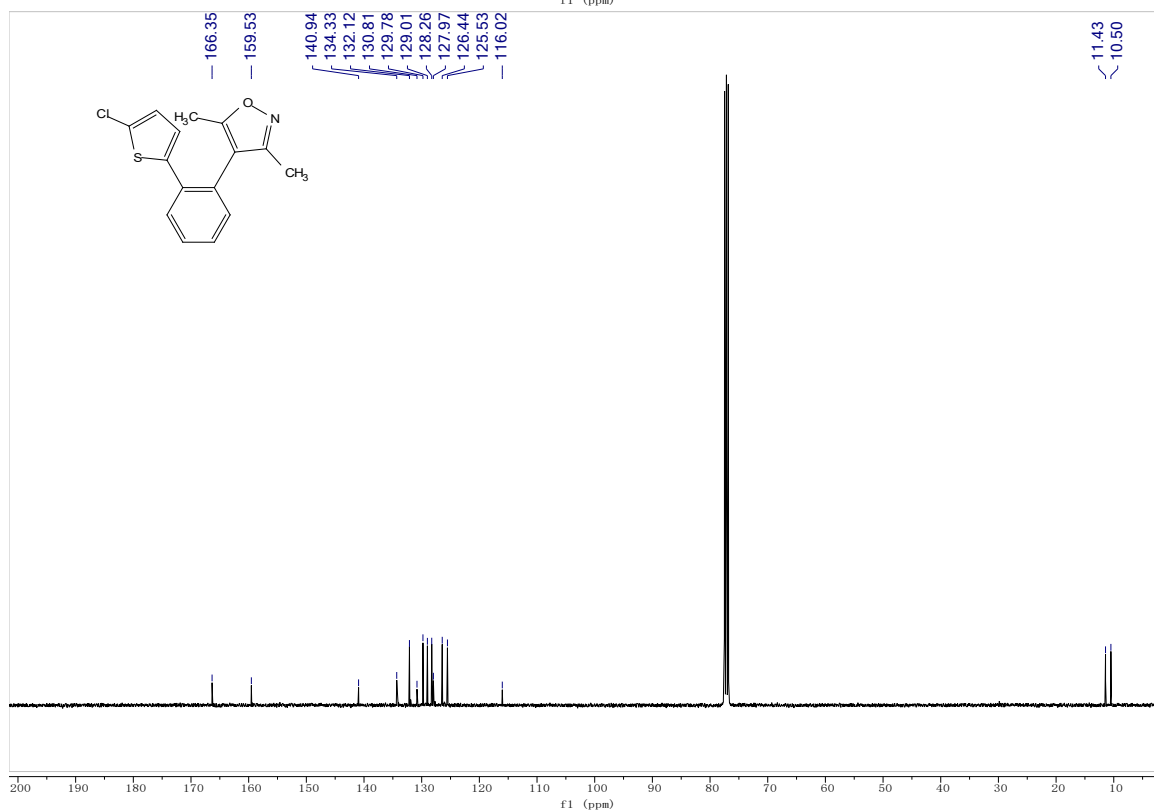
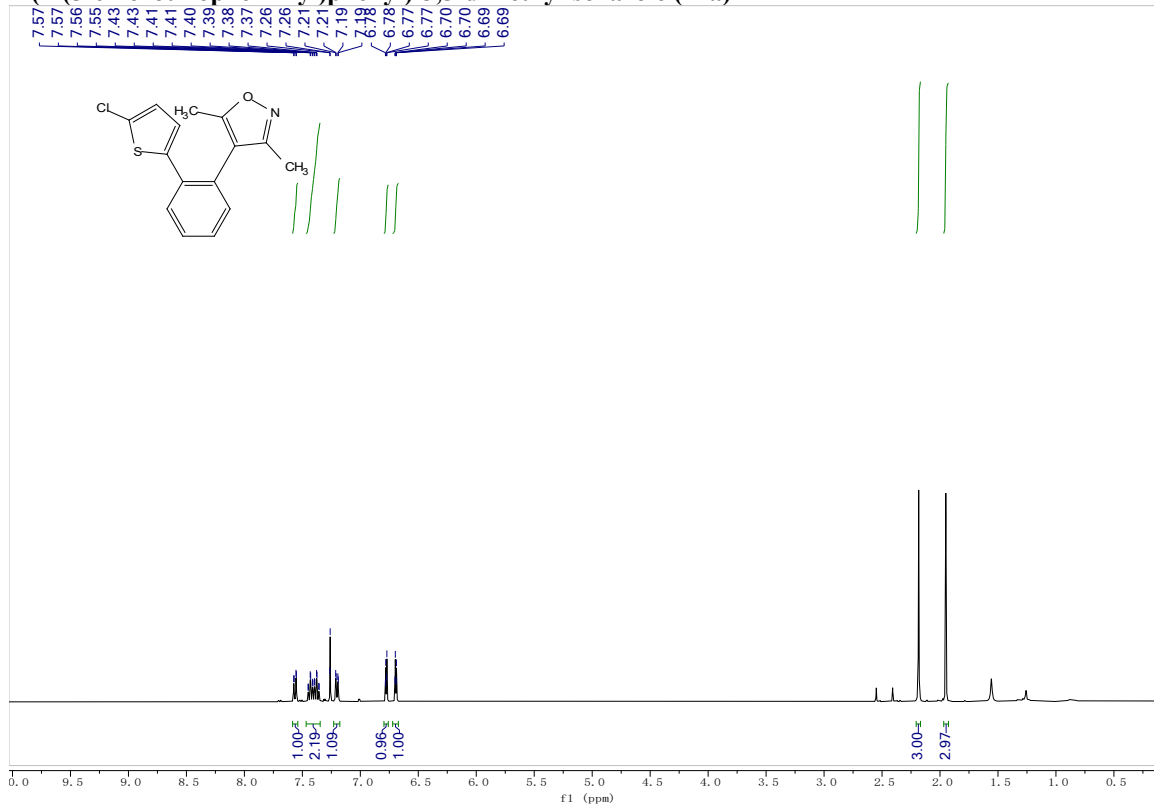
5-(2-(5-Methylthiophen-2-yl)phenyl)thiophene-2-carbaldehyde (35a)



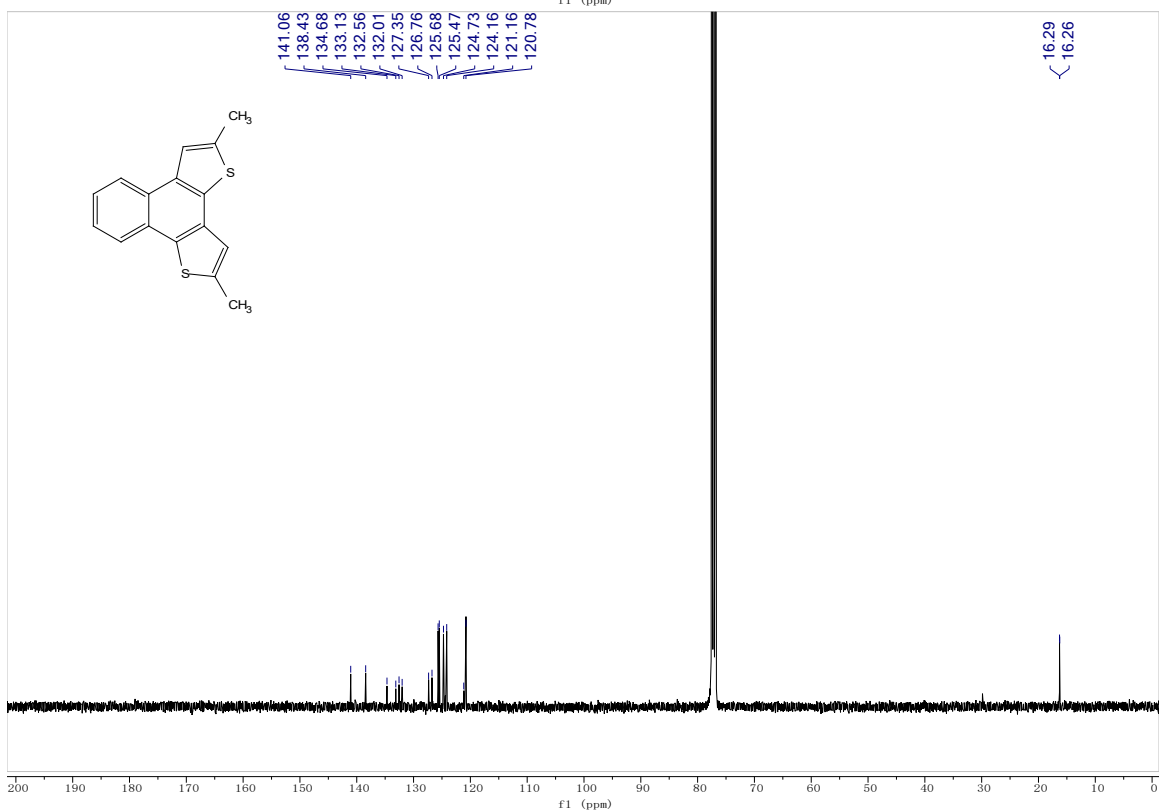
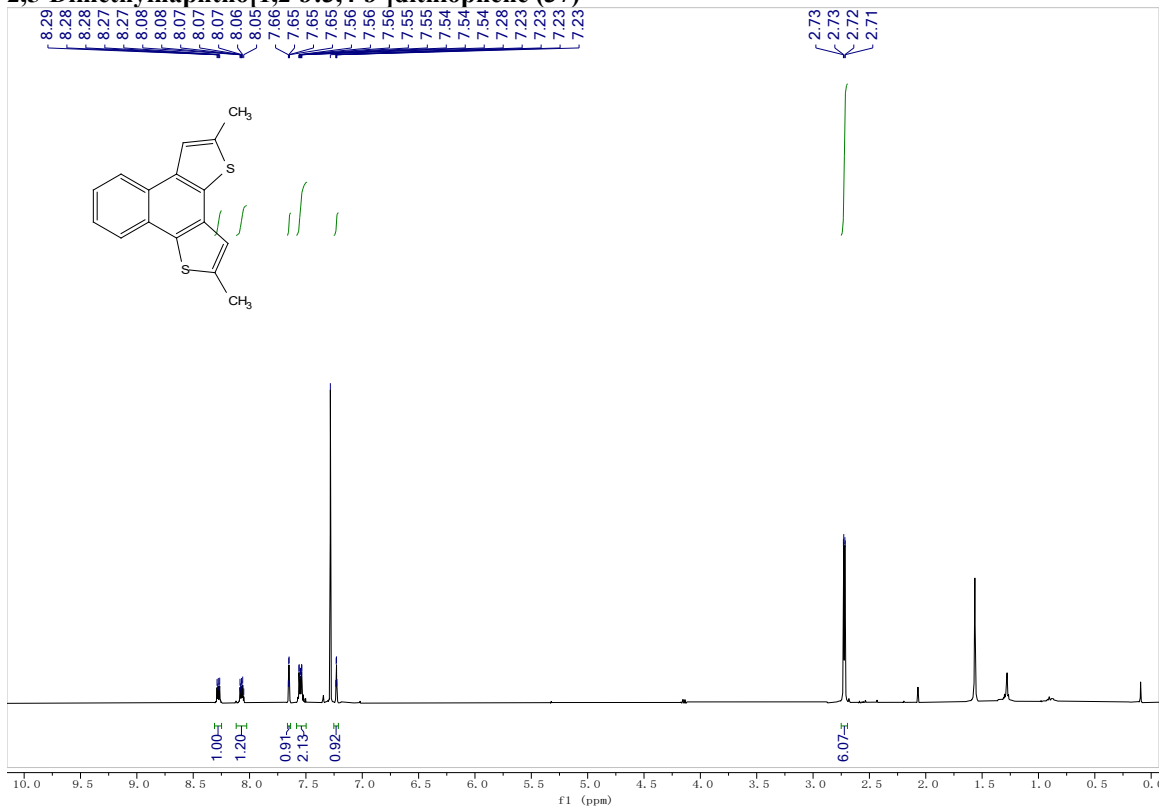
2-Chloro-5-(2-(thiophen-2-yl)phenyl)thiophene (36a)



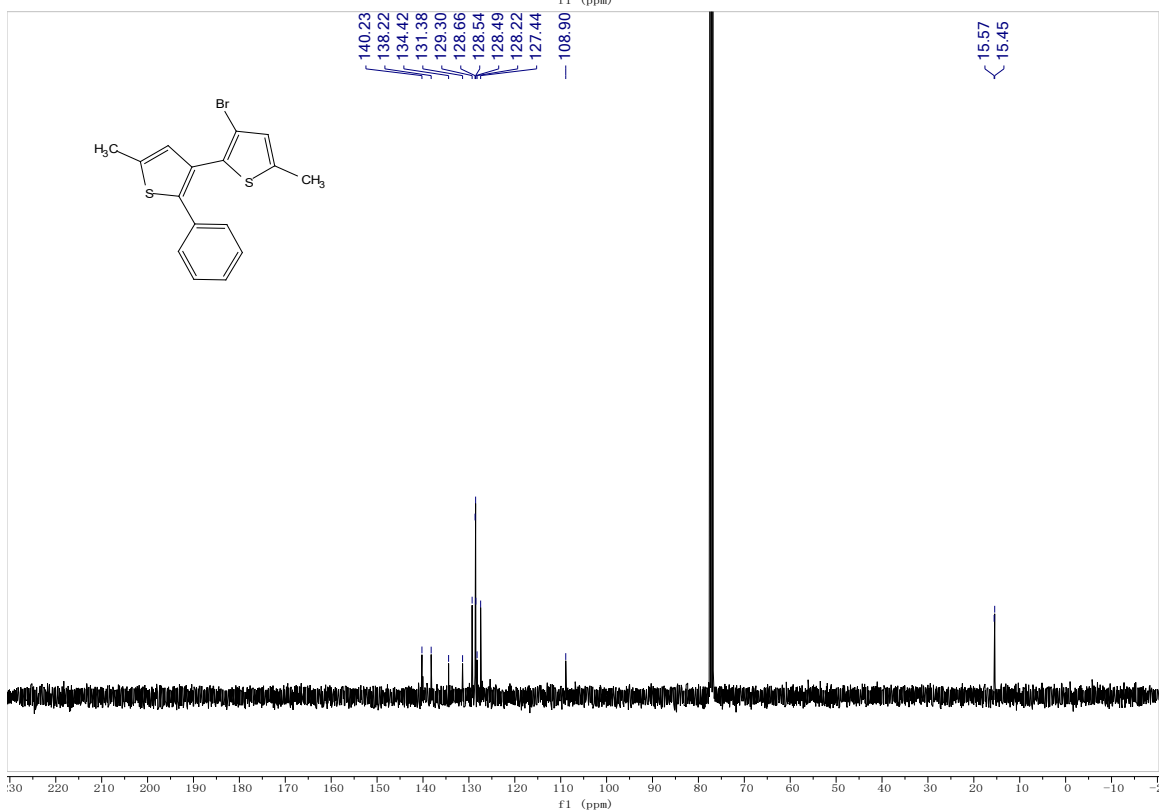
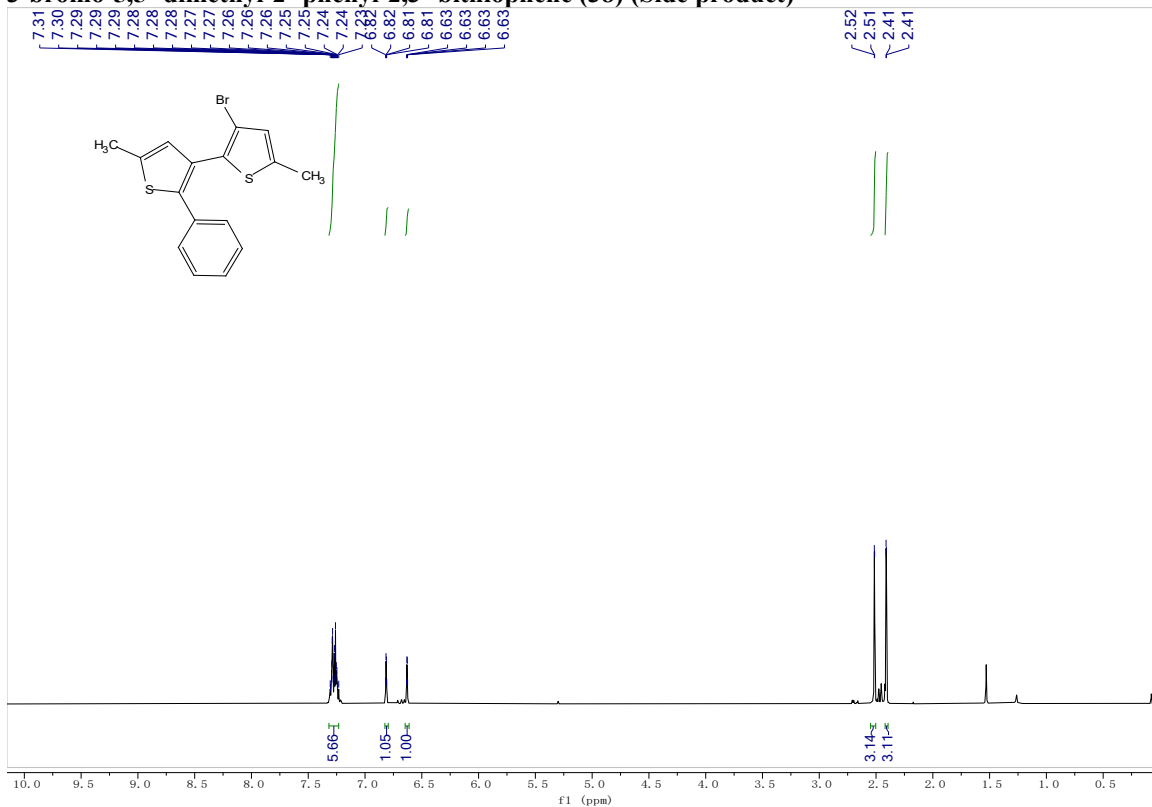
4-(2-(5-chlorothiophen-2-yl)phenyl)-3,5-dimethylisoxazole (11a)



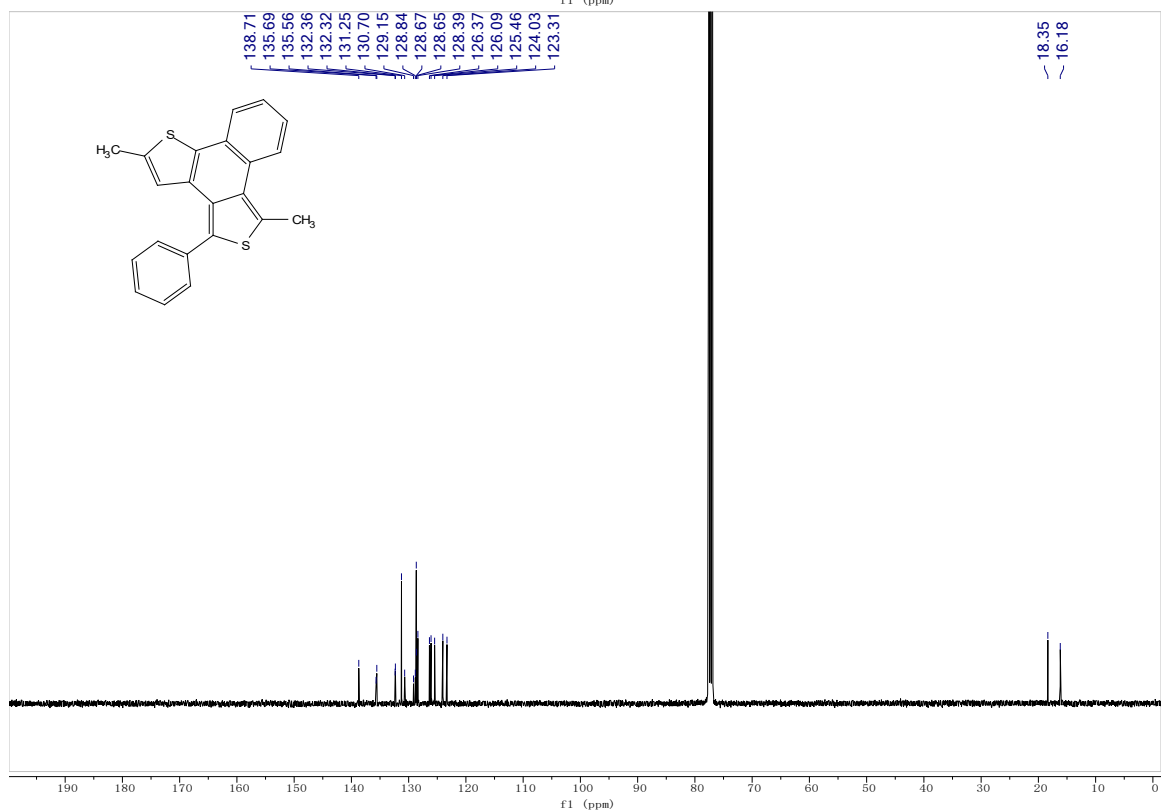
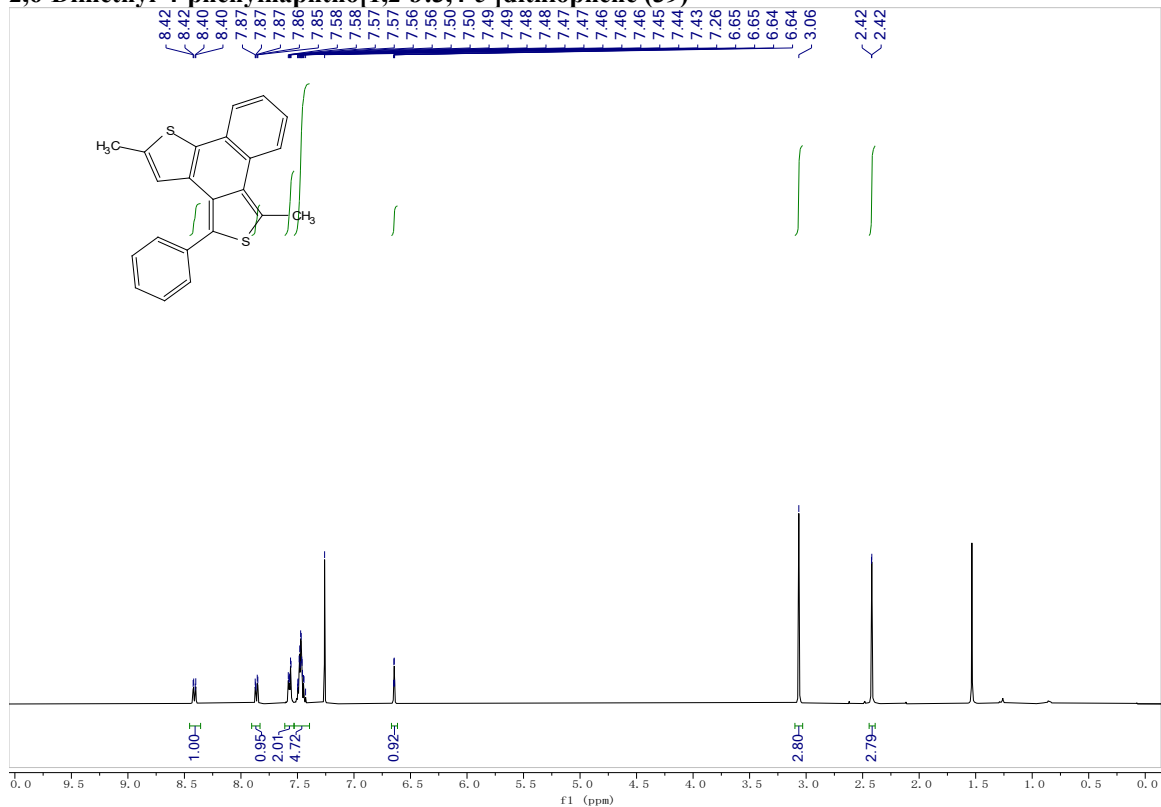
2,5-Dimethylnaphtho[1,2-*b*:3,4-*b'*]dithiophene (37)



3-bromo-5,5'-dimethyl-2'-phenyl-2,3'-bithiophene (38) (Side product)



2,6-Dimethyl-4-phenylnaphtho[1,2-*b*:3,4-*c'*]dithiophene (39)



4-(3,4-Dimethylphenyl)-2,6,8,9-tetramethylnaphtho[1,2-*b*:3,4-*c'*]dithiophene (40)

