

Regioselective Electrophilic Fluorination of Rationally Designed Imidazole Derivatives

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United States

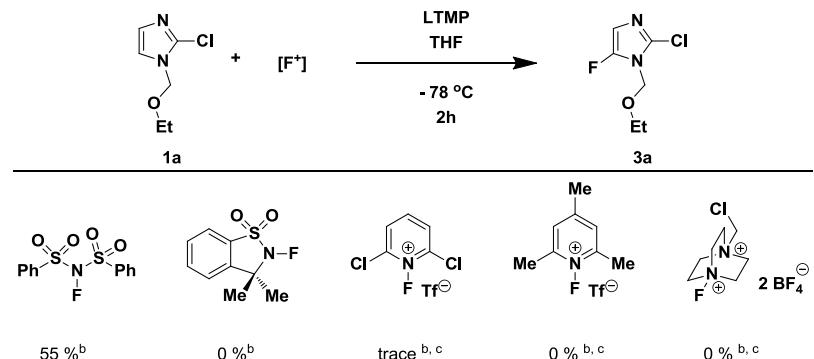
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Supporting Information

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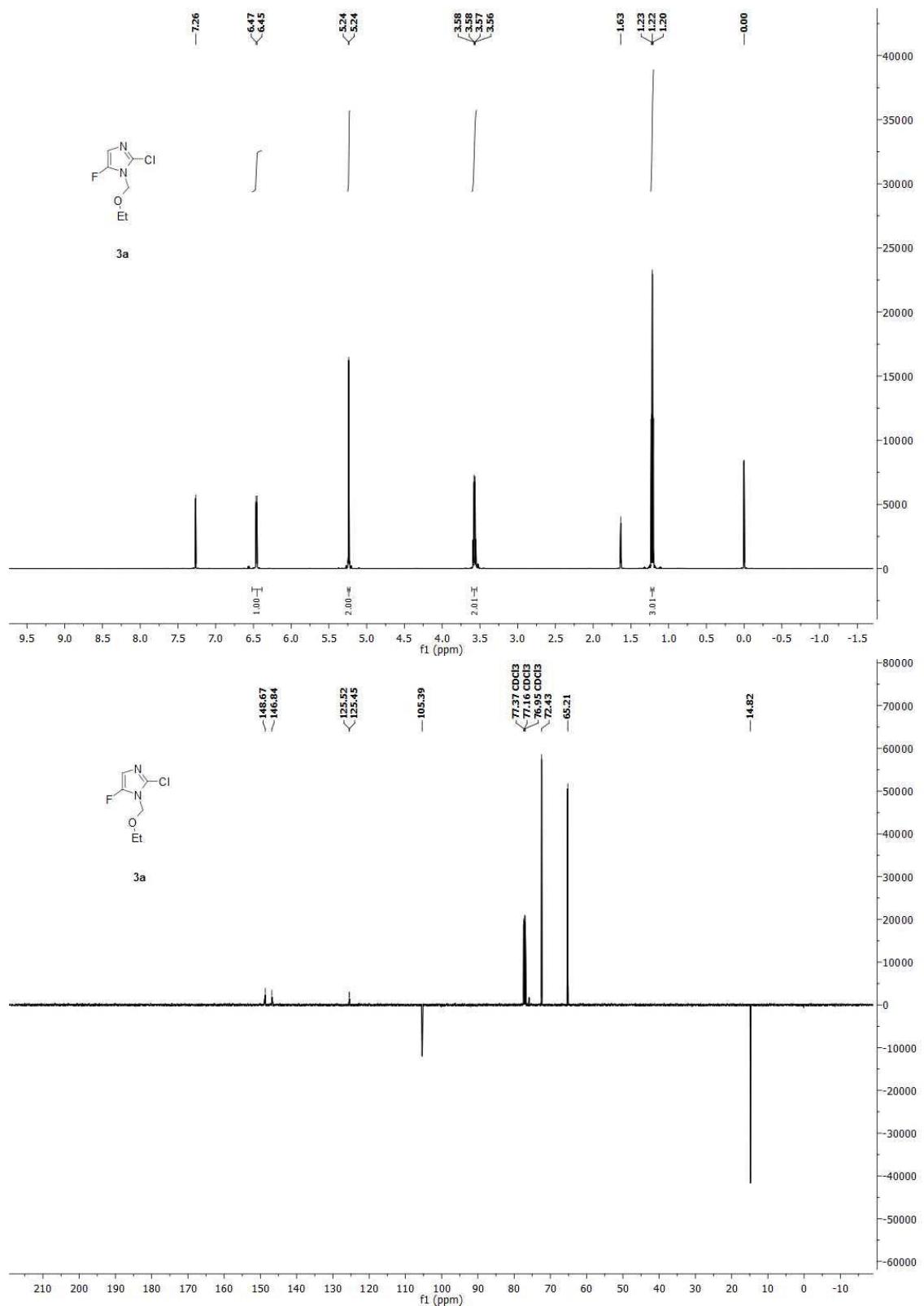
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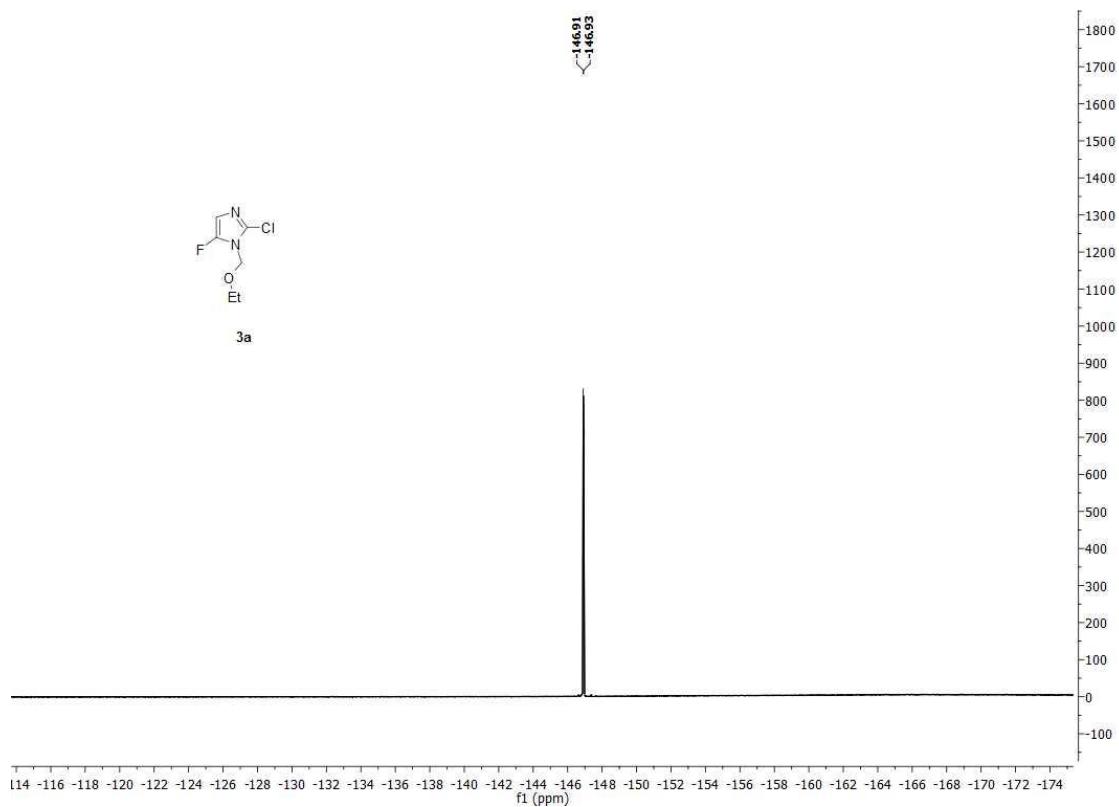
1. Screen of Fluorinating Reagents



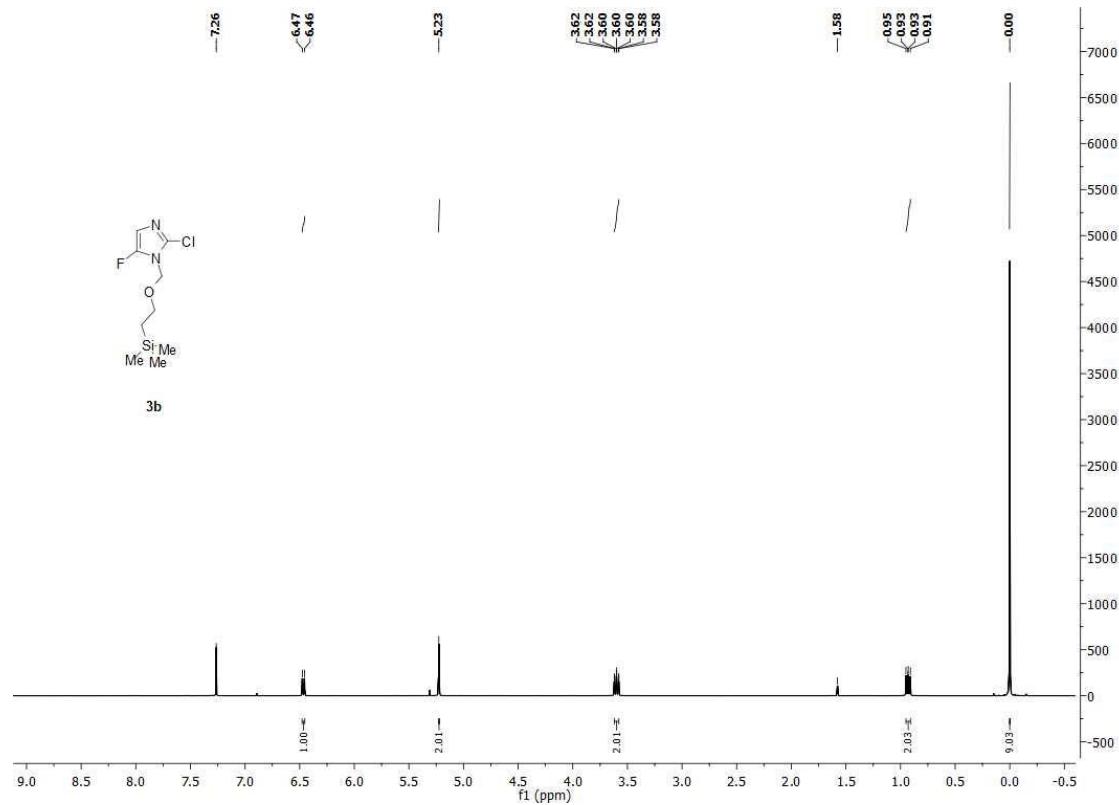
^a Reaction conditions: **1a** (2.49mmol, 1 equiv.), fluorinating reagent (F^+) (2.74 mmol, 1.6 equiv.), LTMP (4.98 mmol, 2 equiv.), THF (22 ml). ^b Percent conversion determined by ^1H NMR of the crude reaction mixture. ^c (F^+) (2.74 mmol 1.1 equiv.).

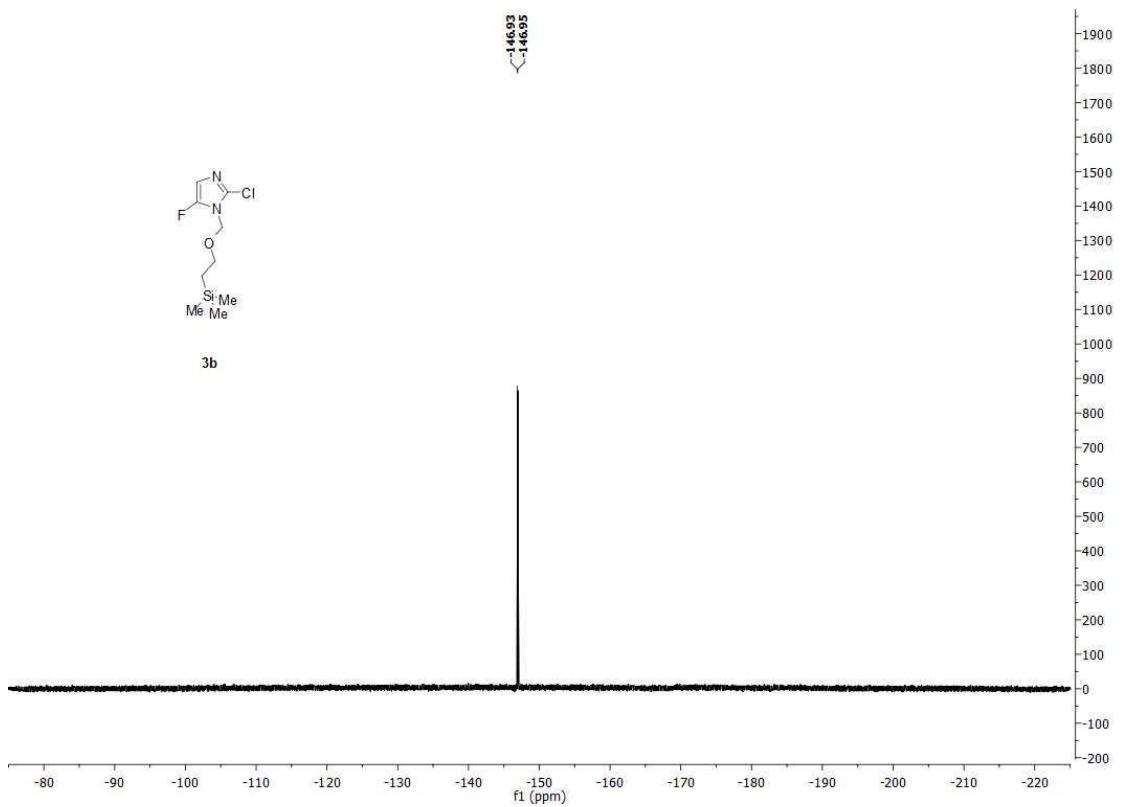
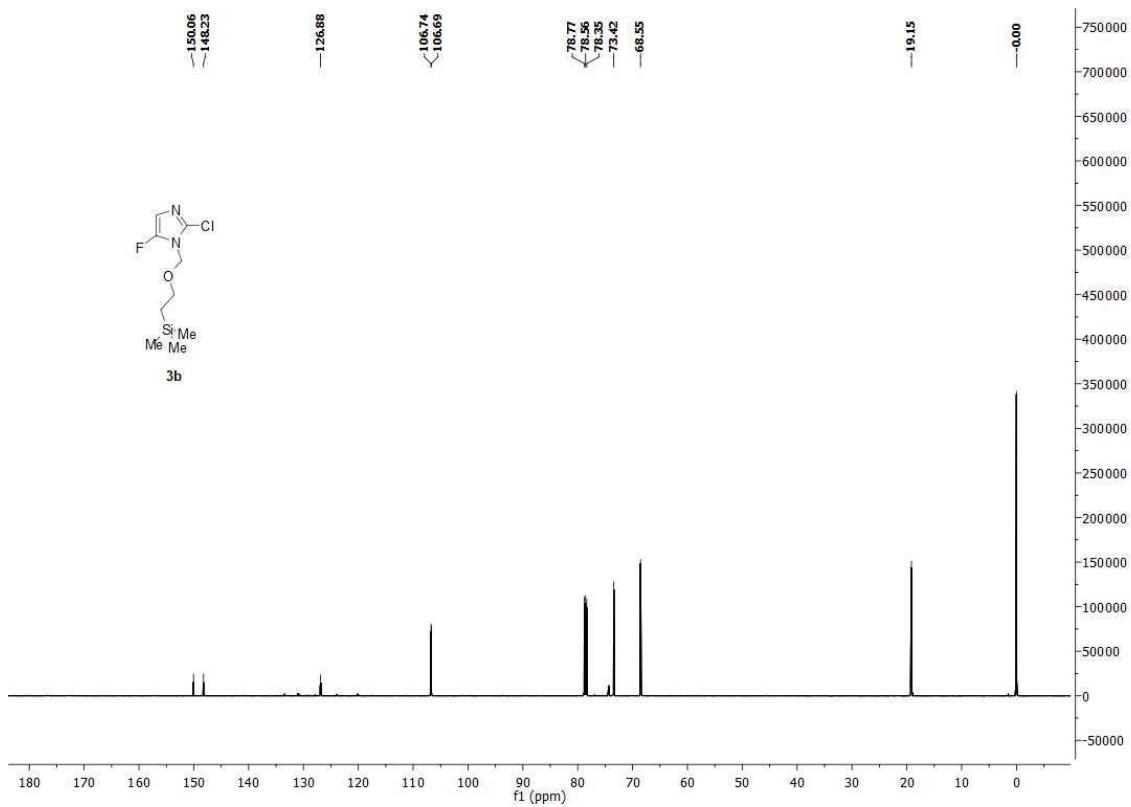
2-chloro-1-(ethoxymethyl)-5-fluoro-1*H*-imidazole (3a**).**



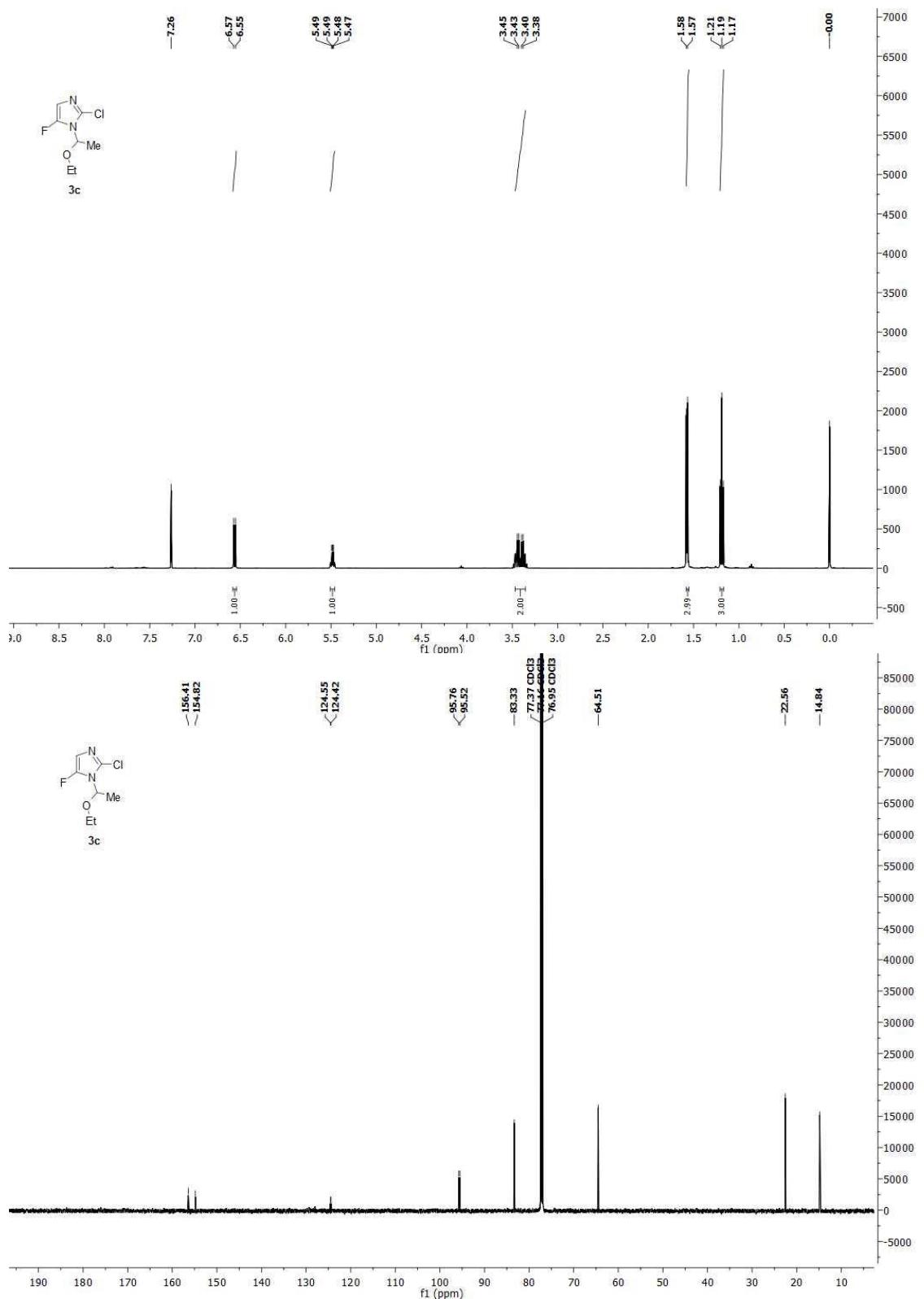


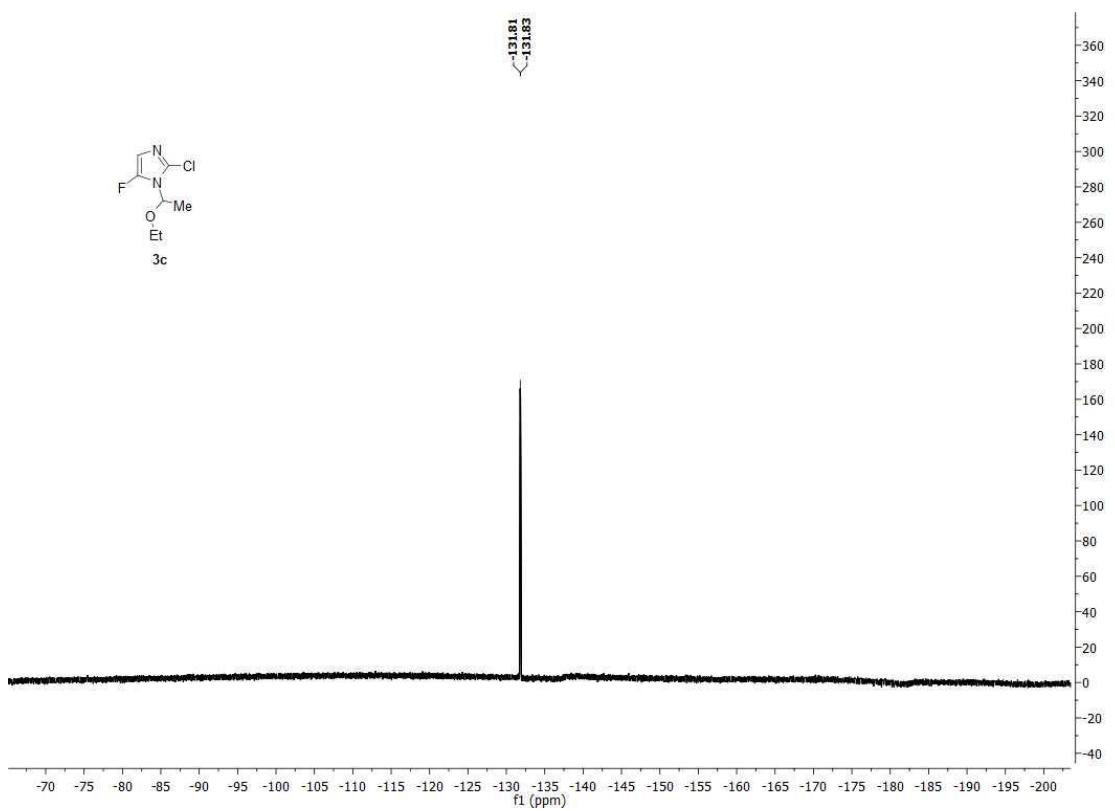
2-chloro-5-fluoro-1-((2-(trimethylsilyl)ethoxy)methyl)-1*H*-imidazole (3b**).**



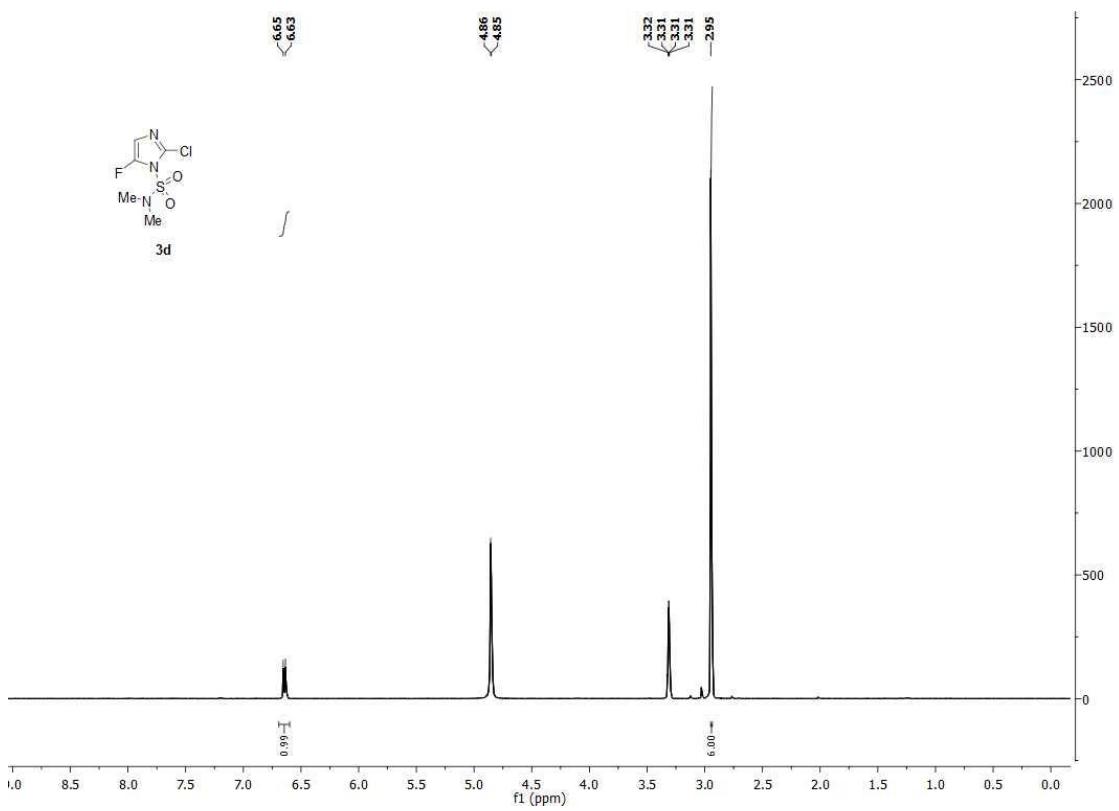


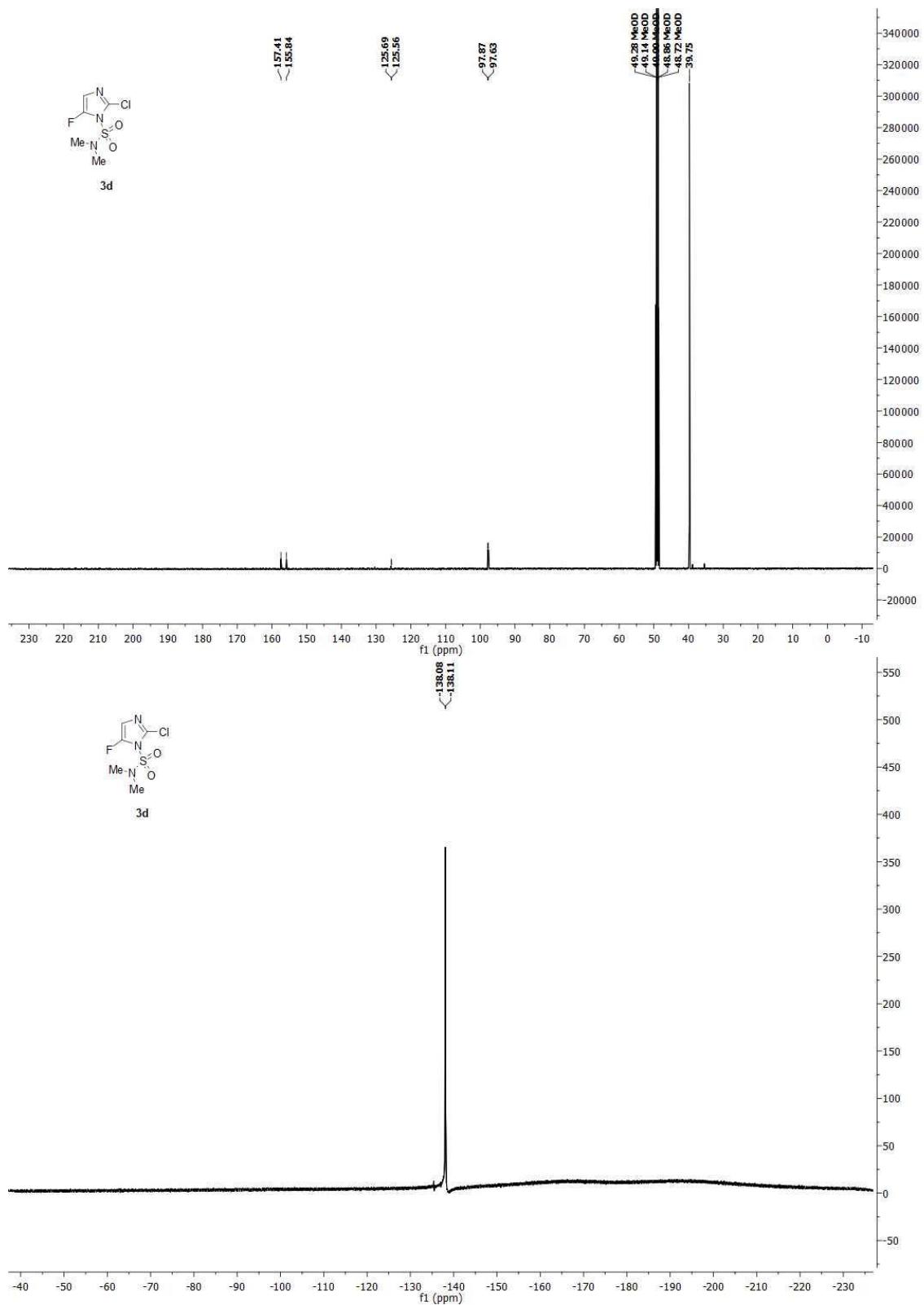
2-chloro-1-(1-ethoxyethyl)-5-fluoro-1*H*-imidazole (3c**).**



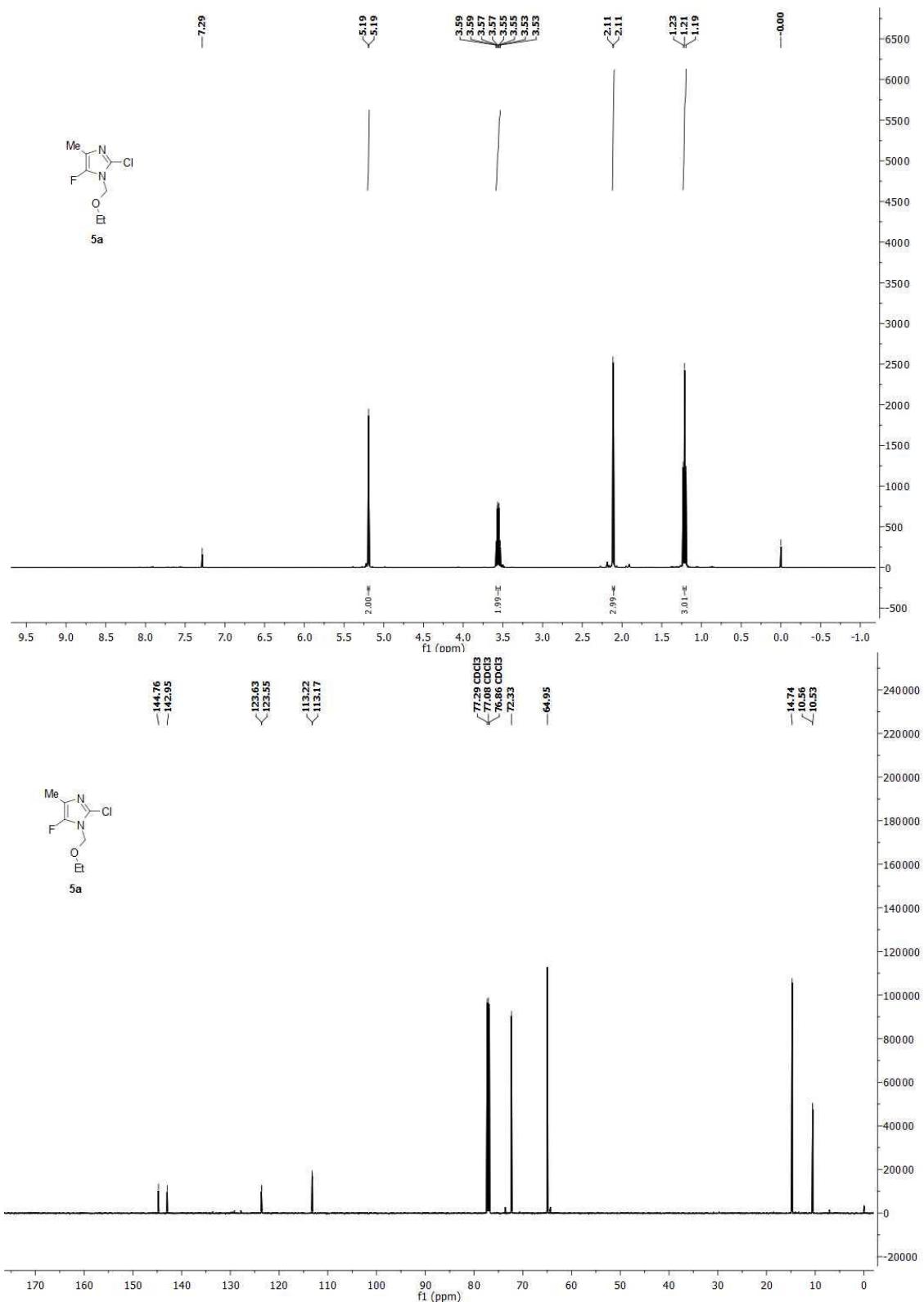


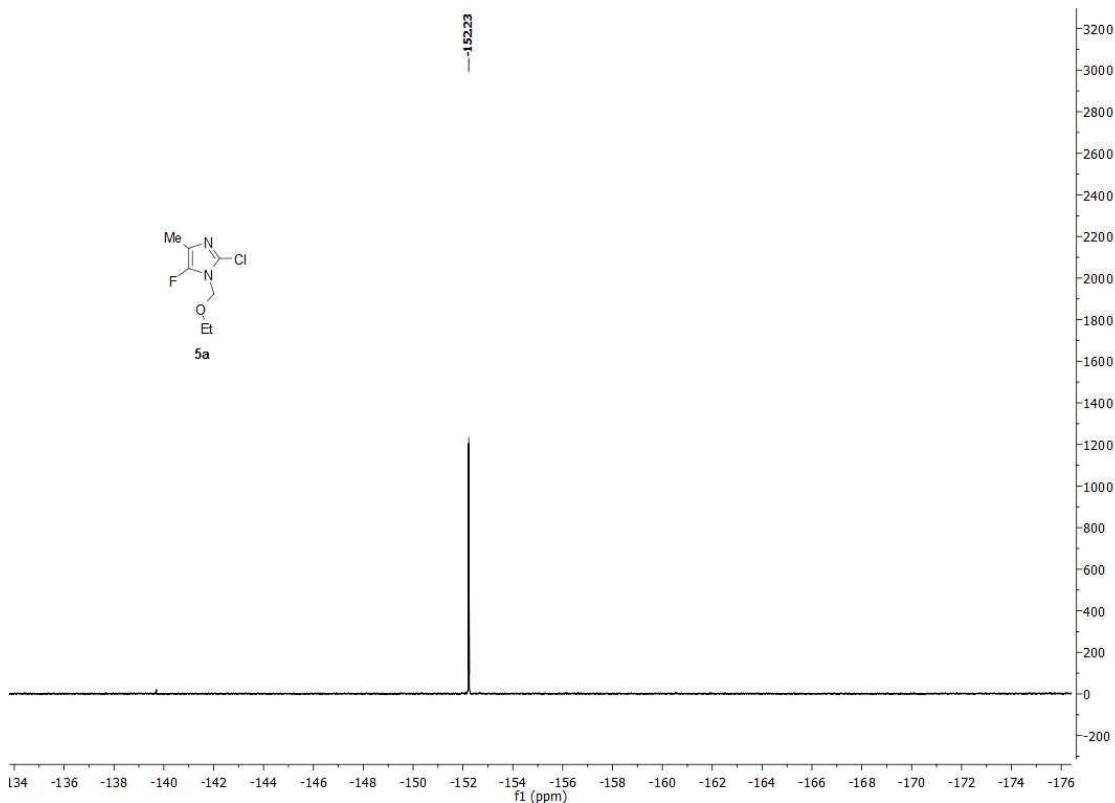
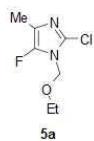
2-chloro-5-fluoro-N,N-dimethyl-1*H*-imidazole-1-sulfonamide (3d**).**



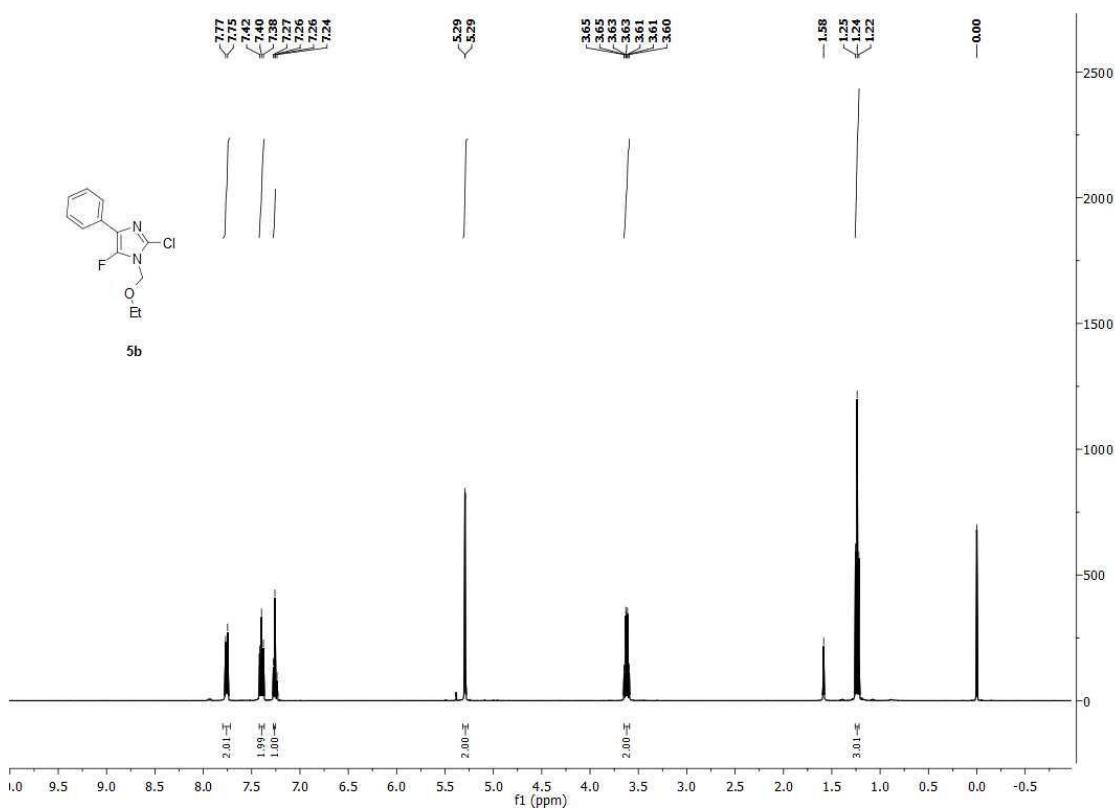
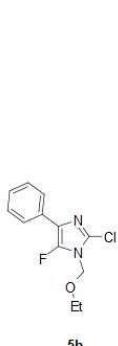


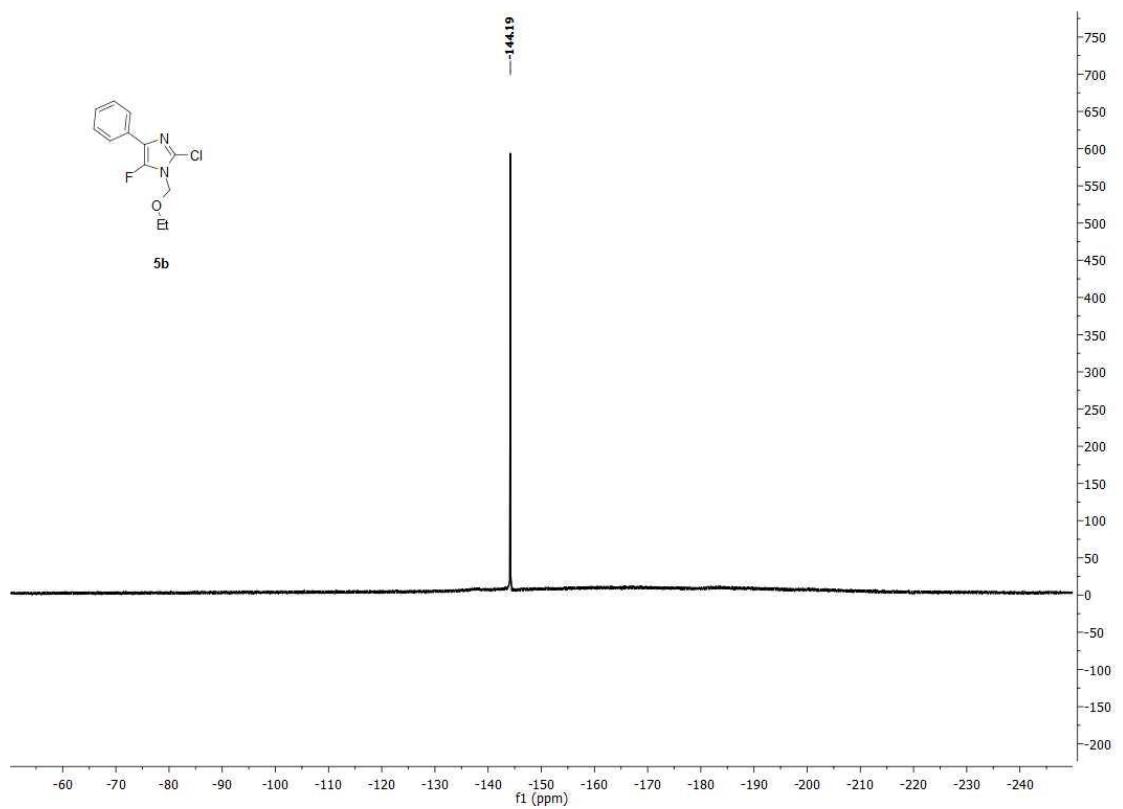
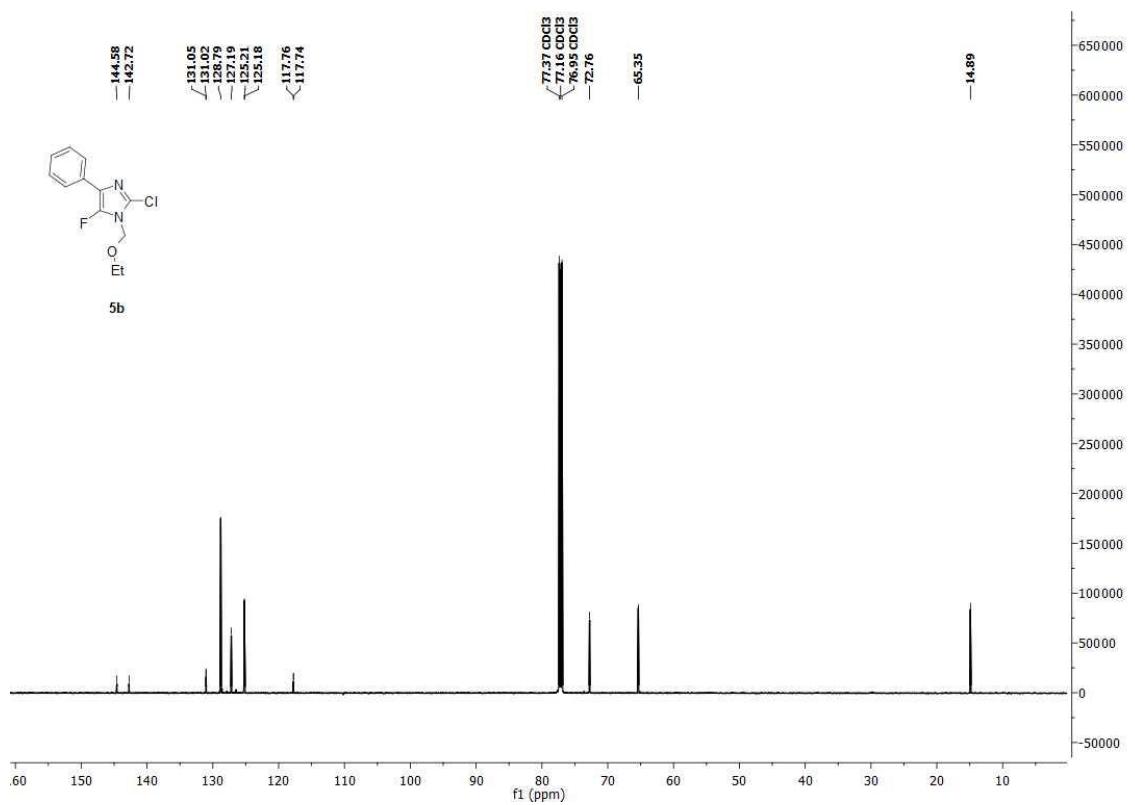
2-chloro-1-(ethoxymethyl)-5-fluoro-4-methyl-1*H*-imidazole (**5a**).



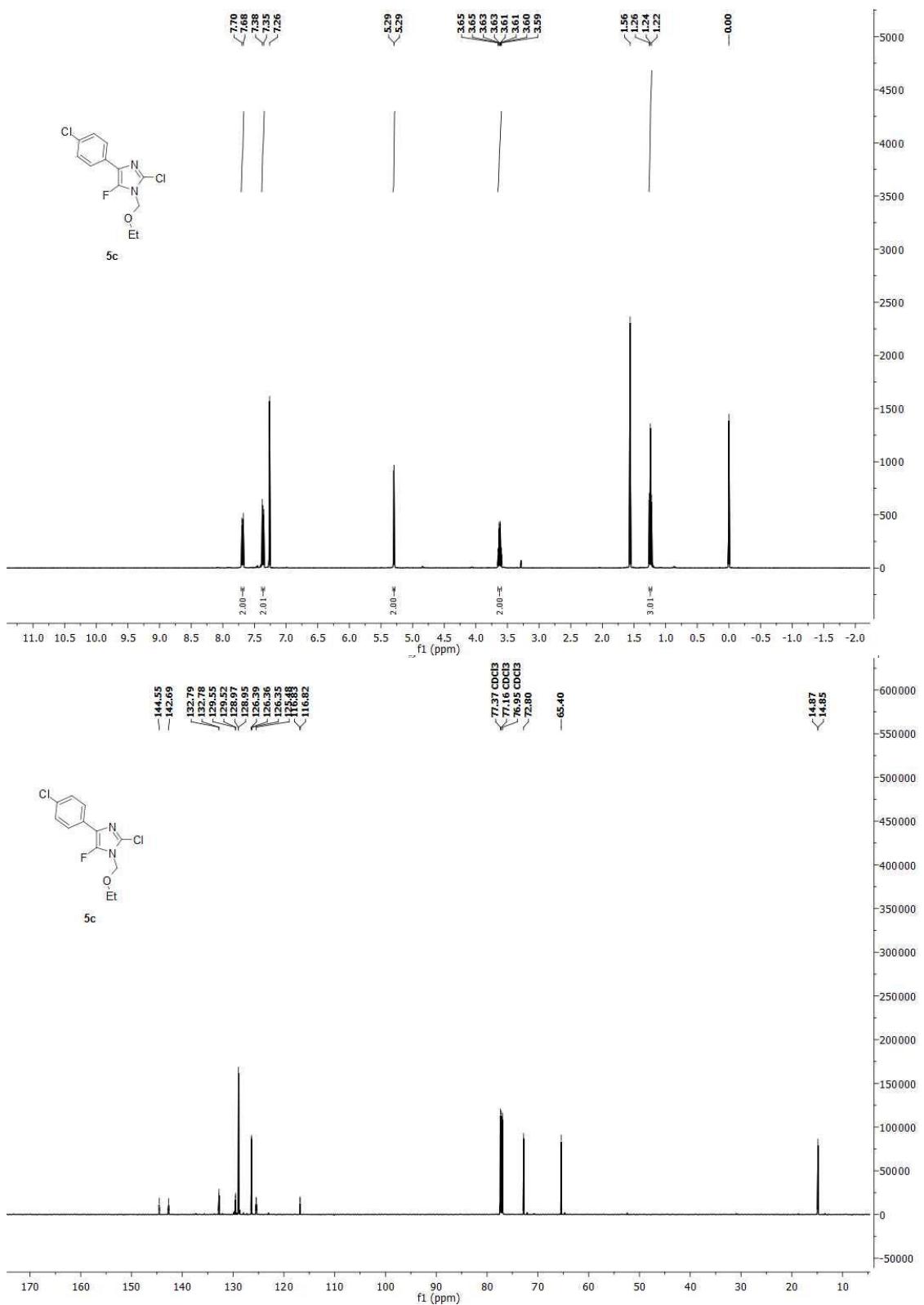


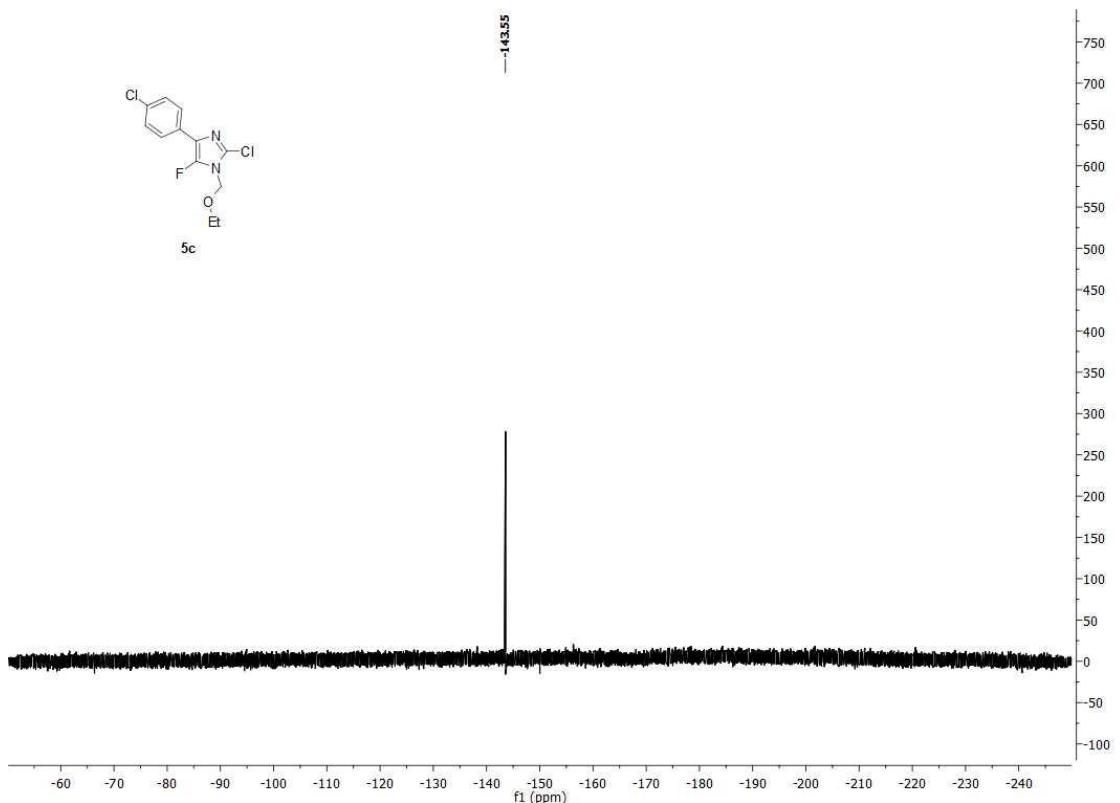
2-chloro-1-(ethoxymethyl)-5-fluoro-4-phenyl-1*H*-imidazole (**5b**)



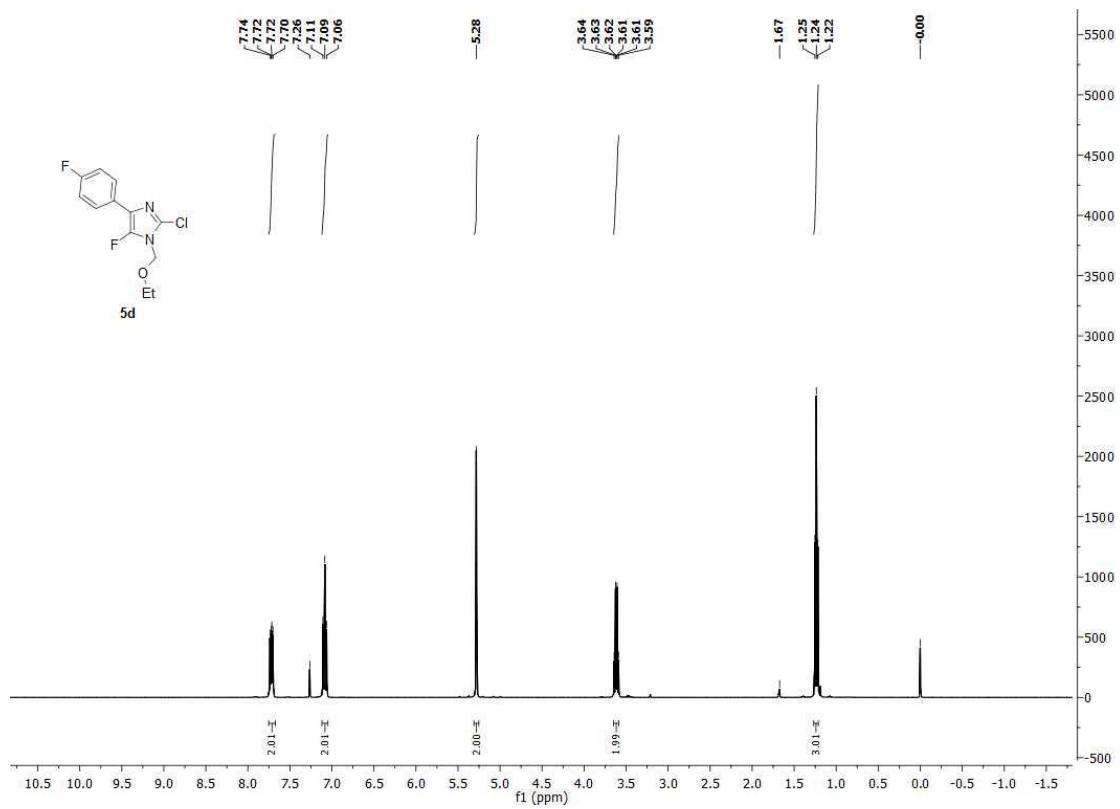


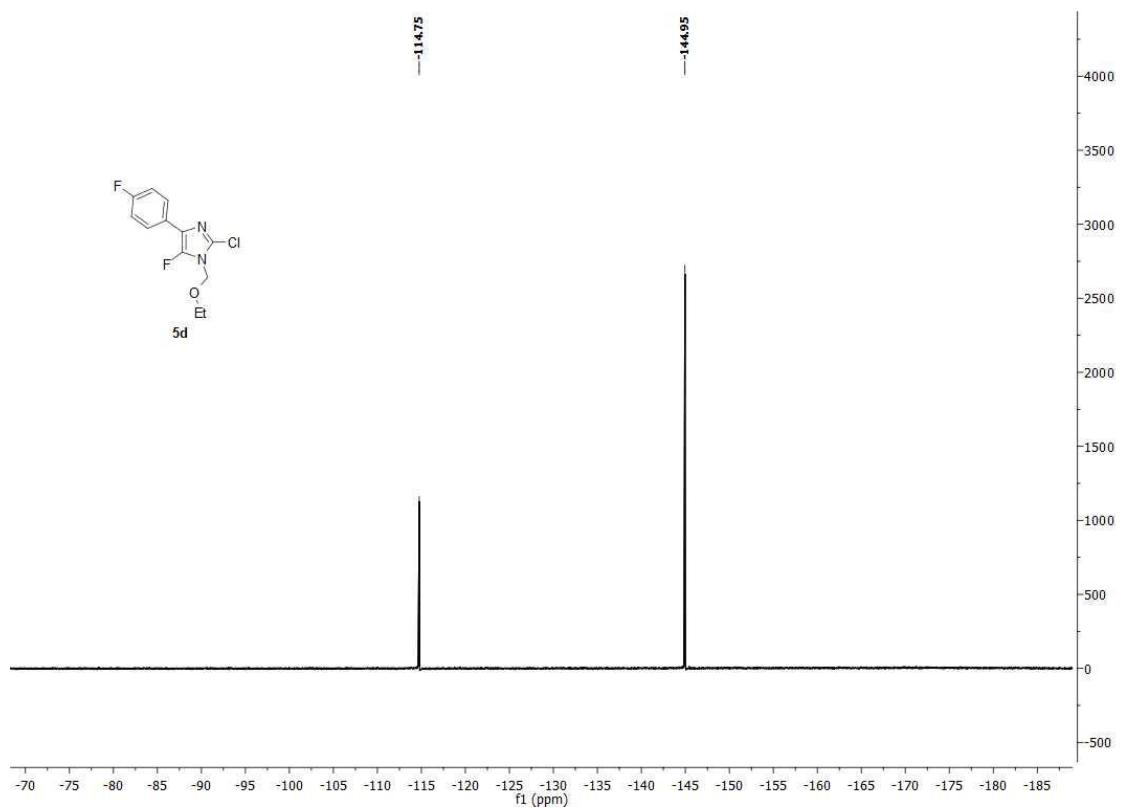
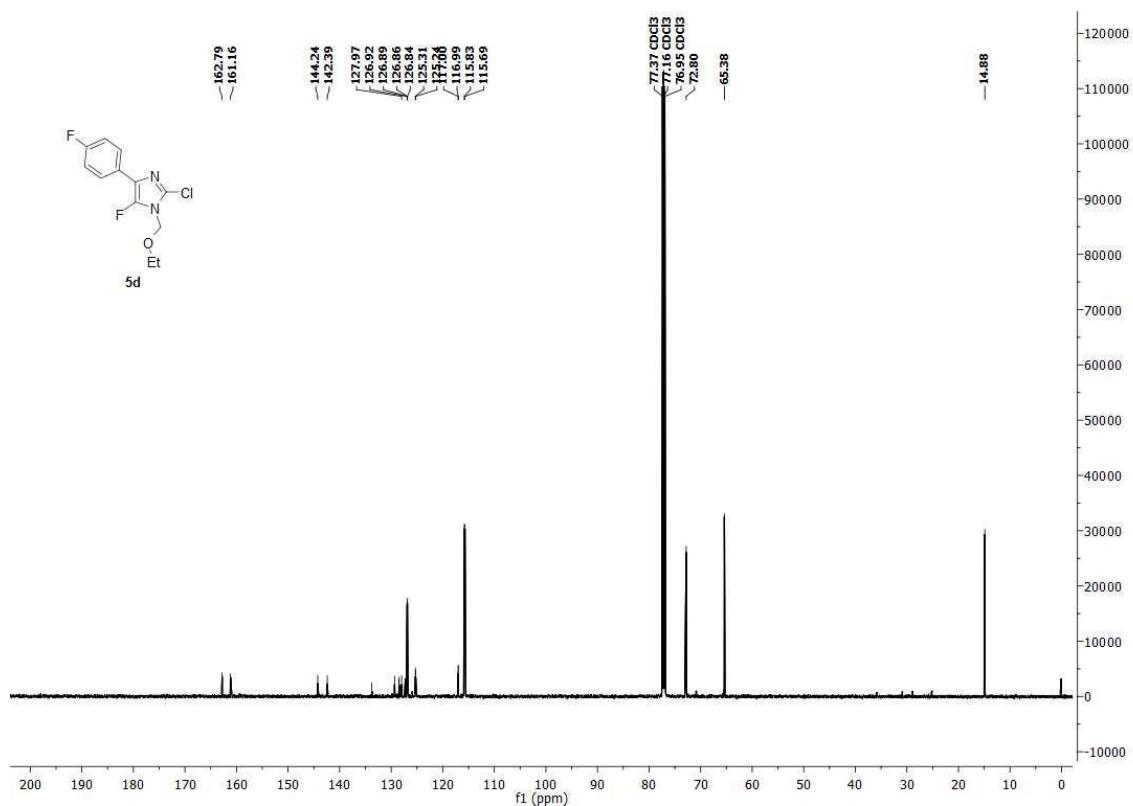
2-chloro-4-(4-chlorophenyl)-1-(ethoxymethyl)-5-fluoro-1*H*-imidazole (**5c**).



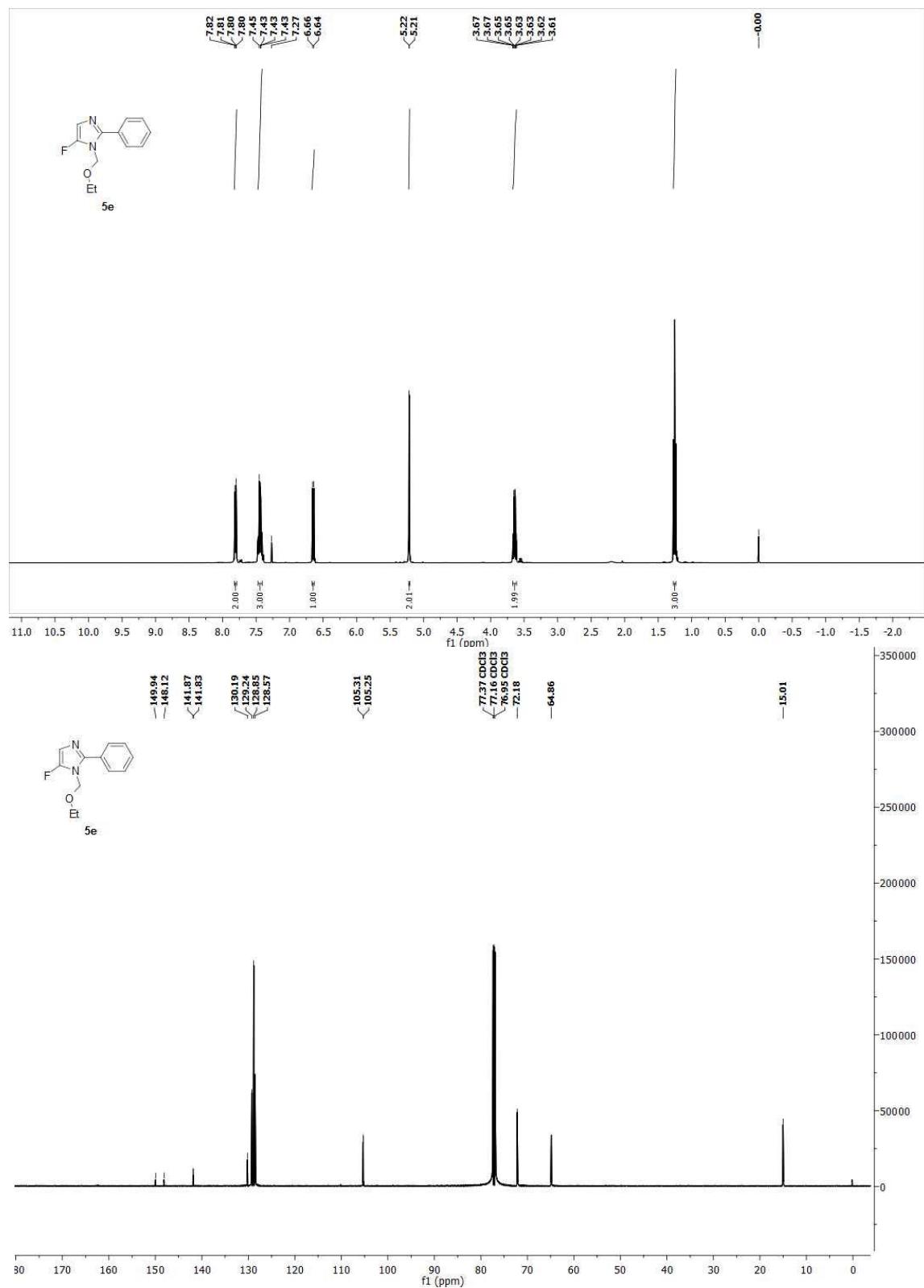


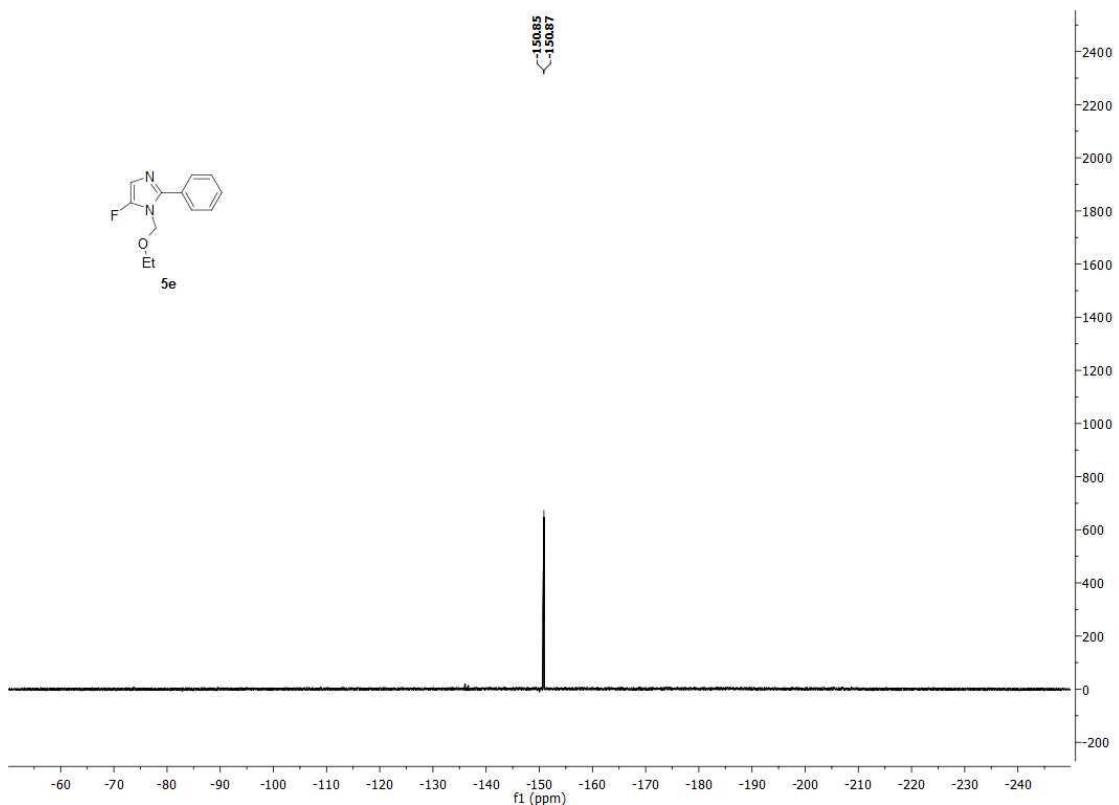
2-chloro-1-(ethoxymethyl)-5-fluoro-4-(4-fluorophenyl)-1*H*-imidazole (**5d**)



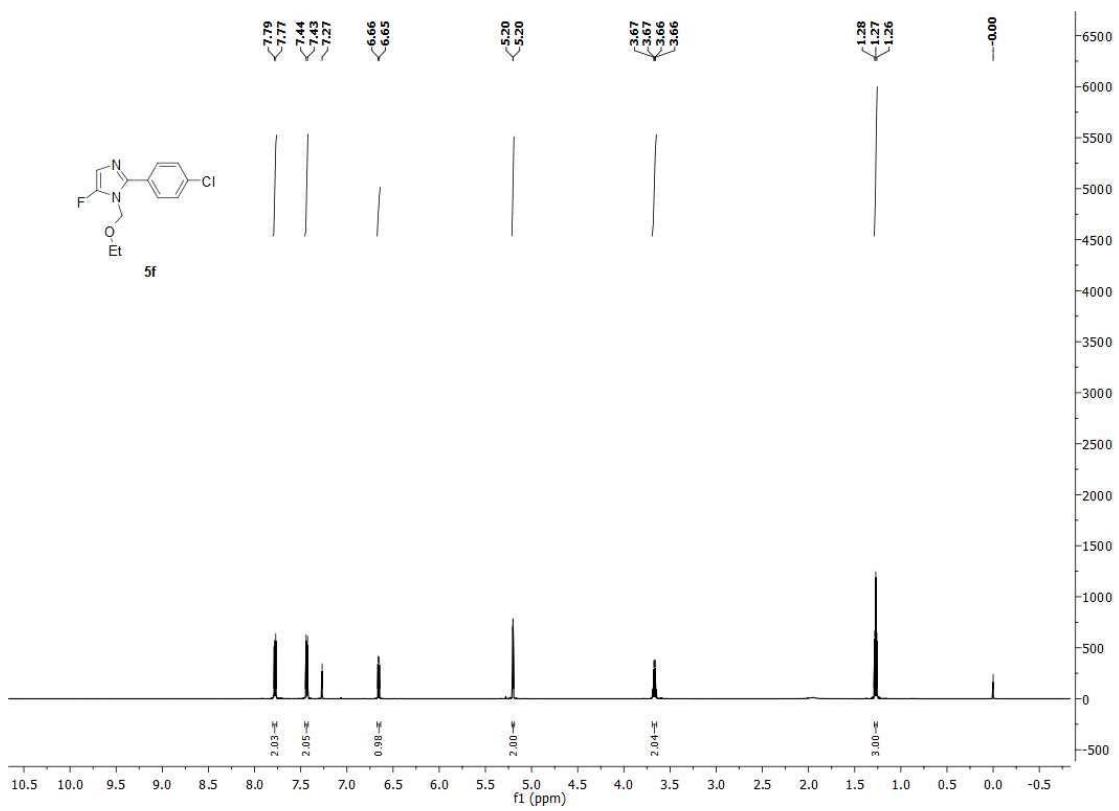


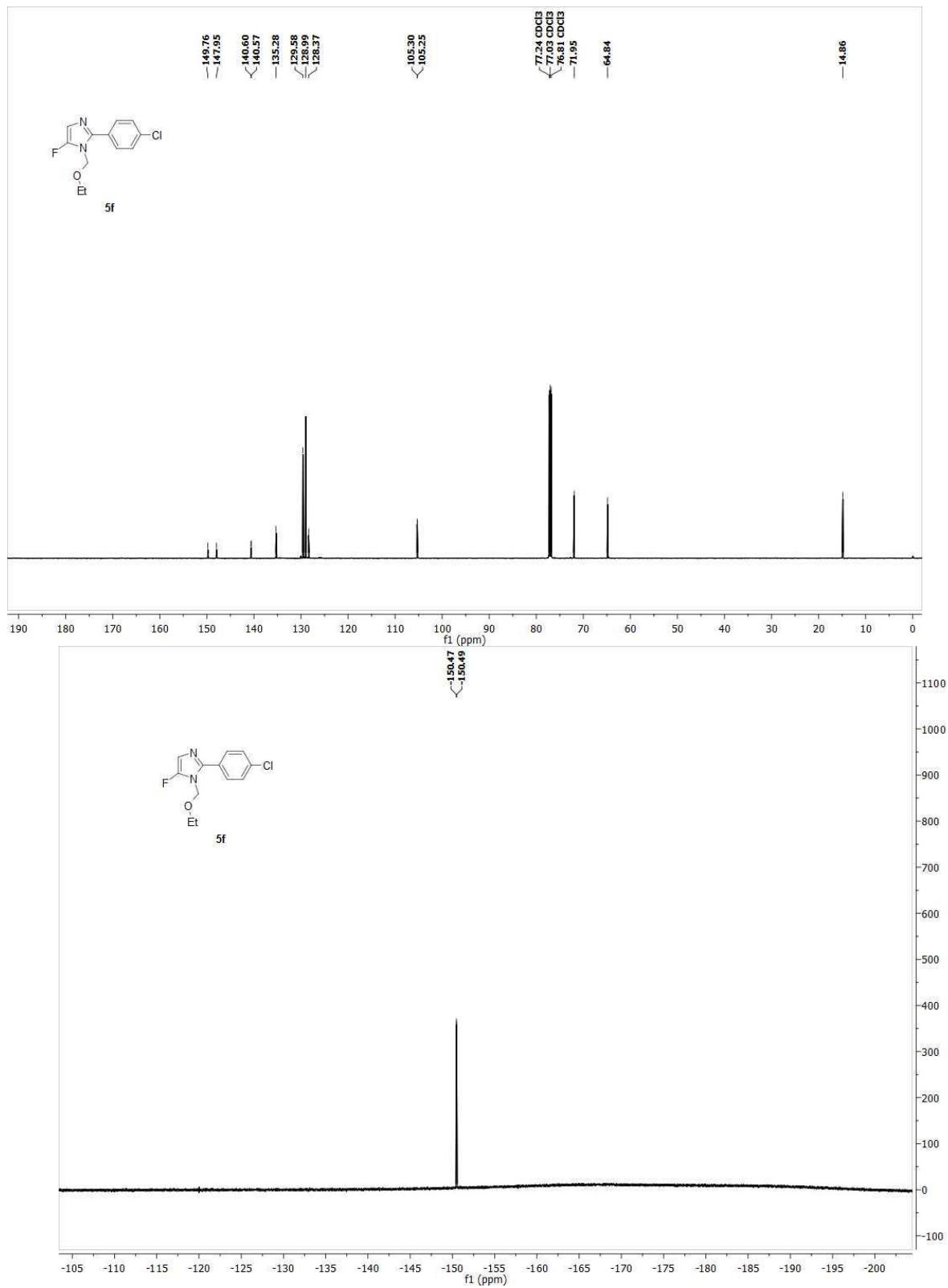
1-(ethoxymethyl)-5-fluoro-2-phenyl-1*H*-imidazole (5e**).**



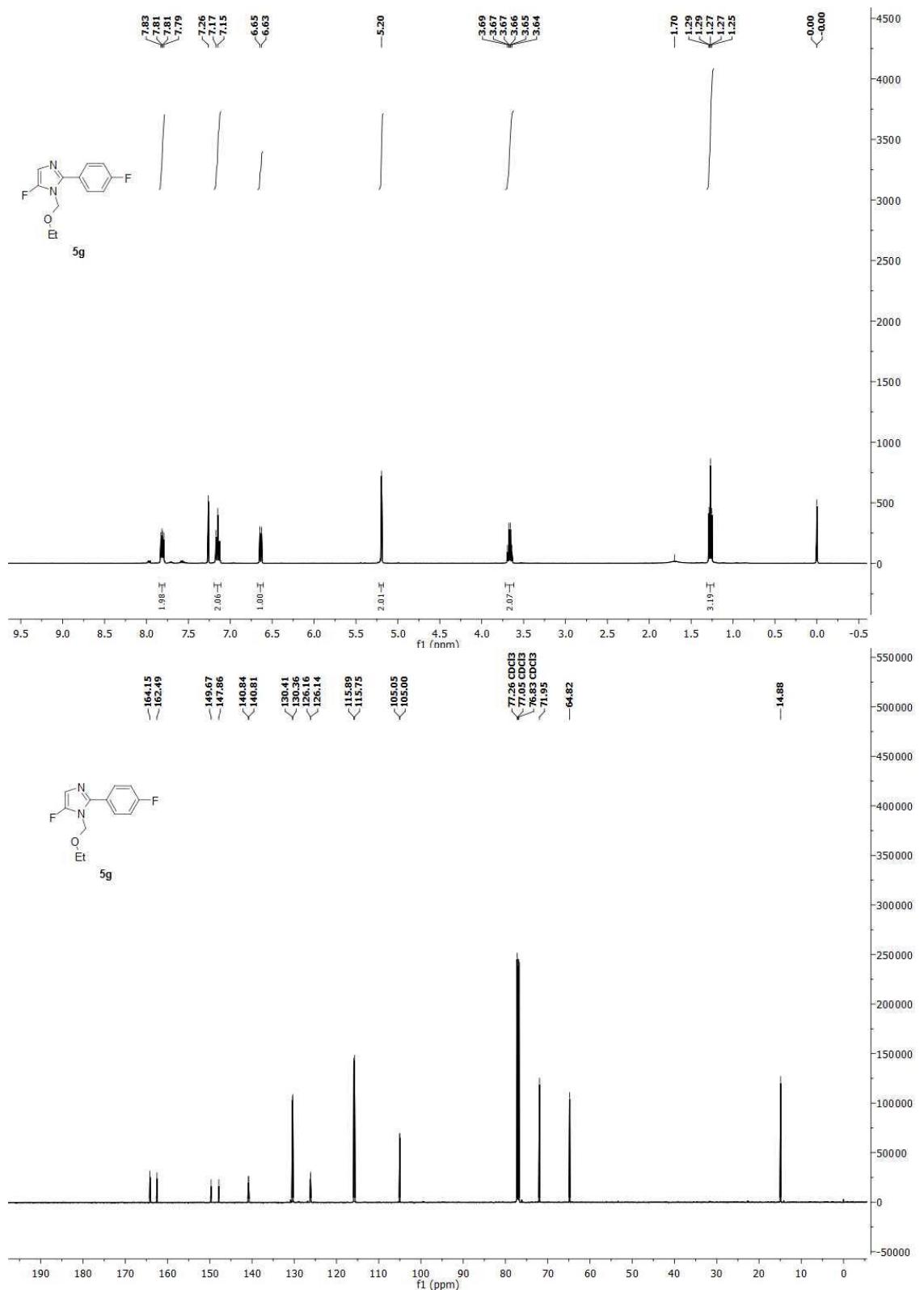


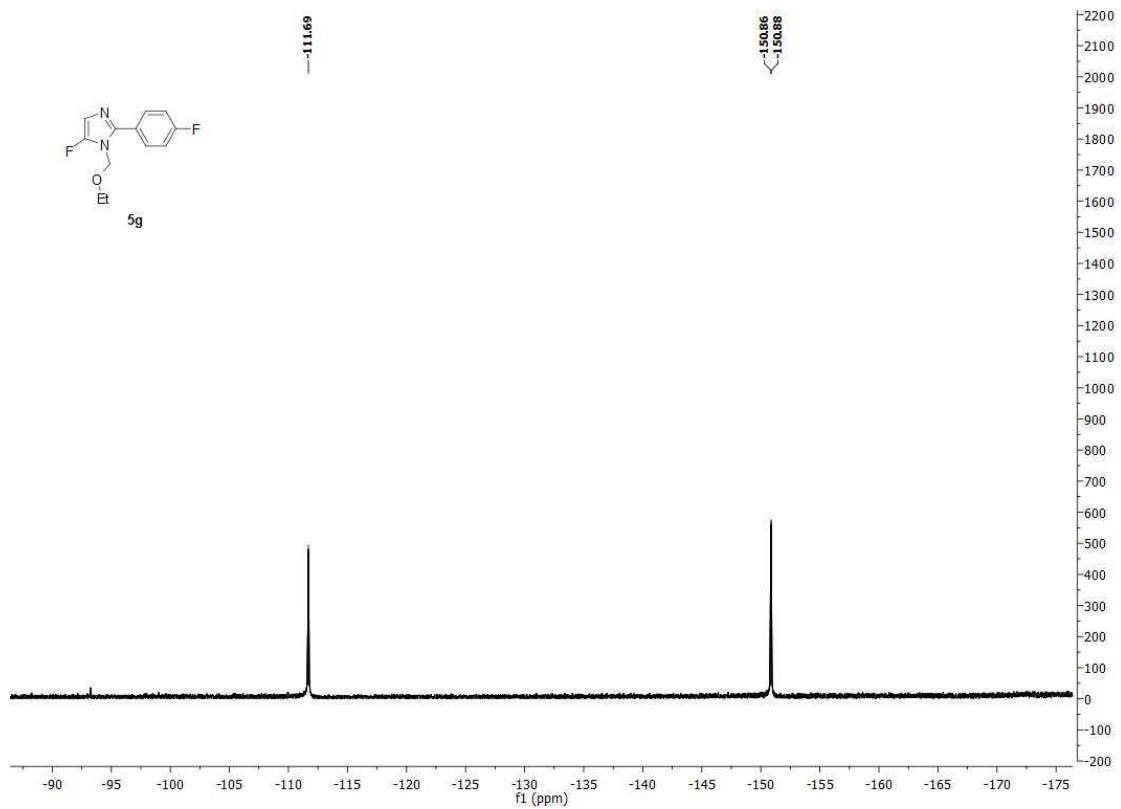
2-(4-chlorophenyl)-1-(ethoxymethyl)-5-fluoro-1*H*-imidazole (**5f**)



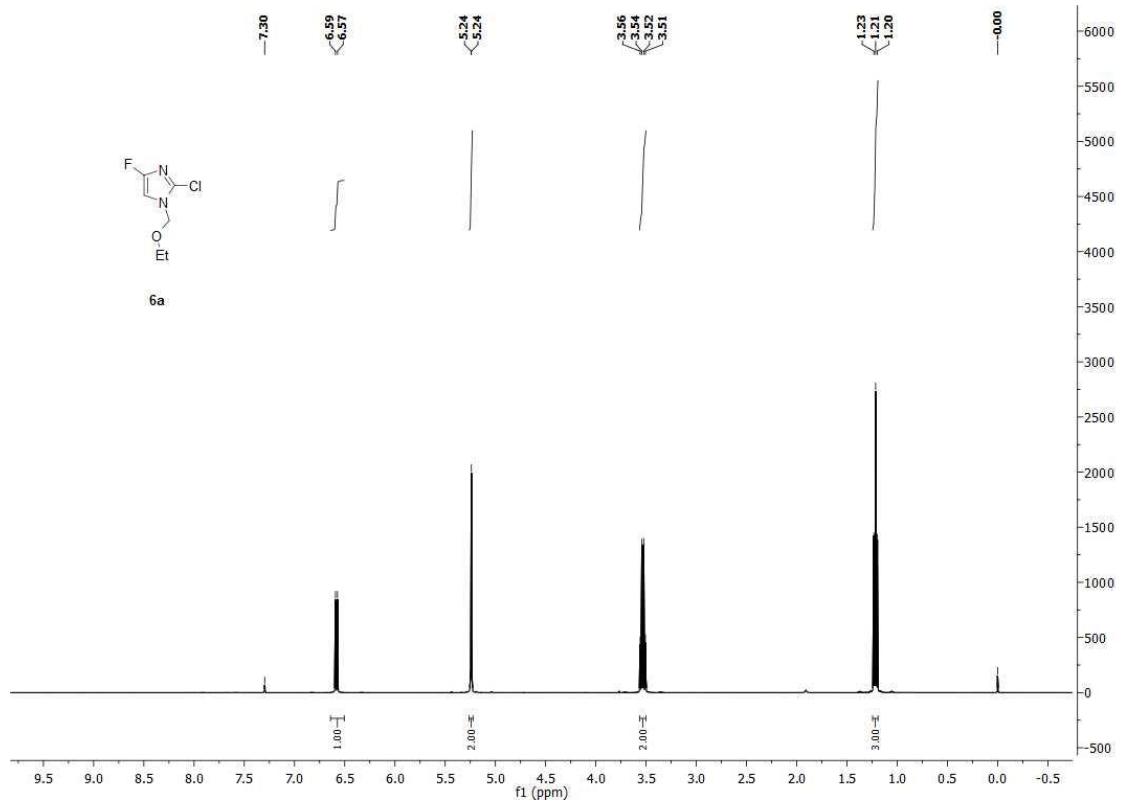


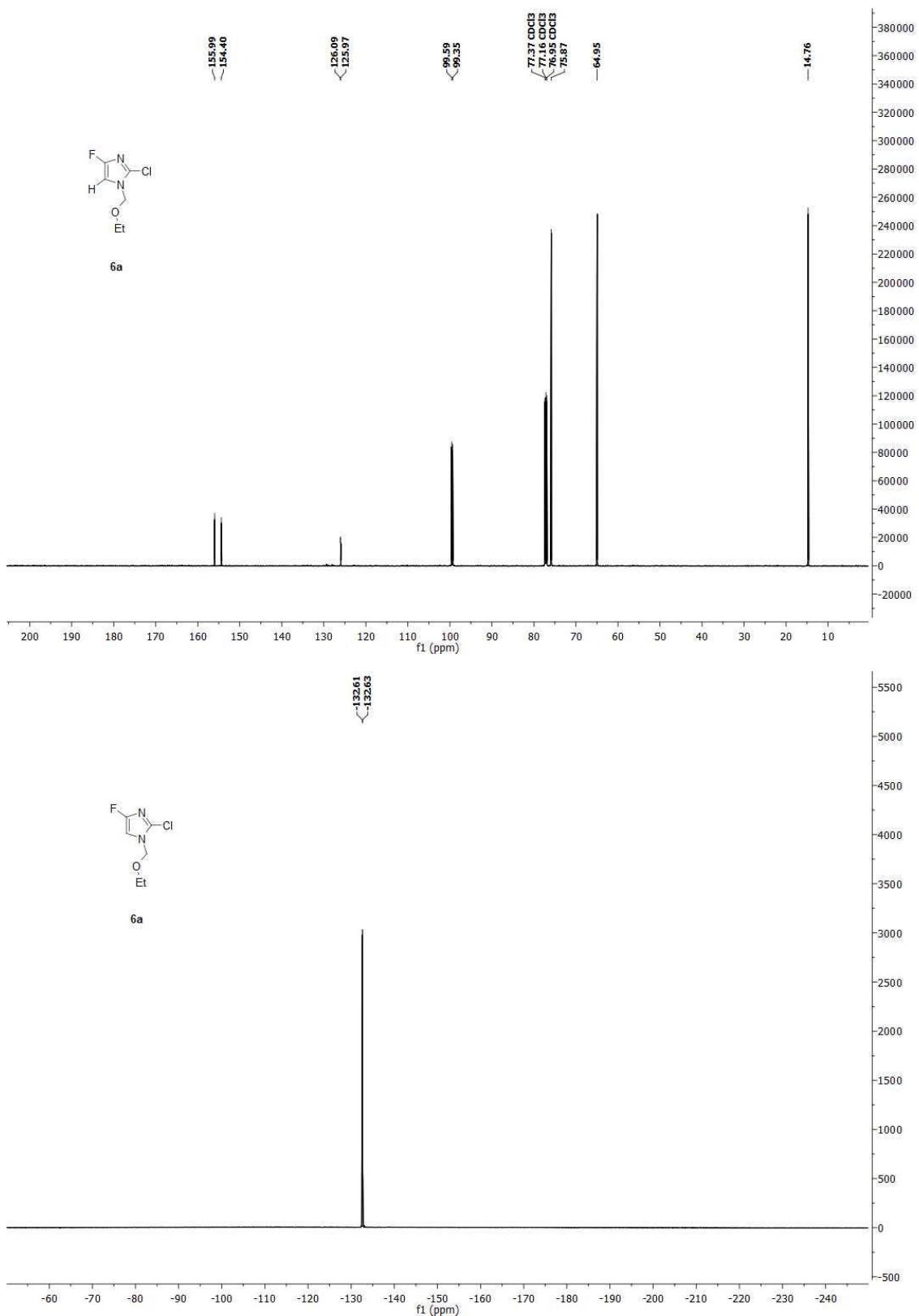
1-(ethoxymethyl)-5-fluoro-2-(4-fluorophenyl)-1*H*-imidazole (5g**).**



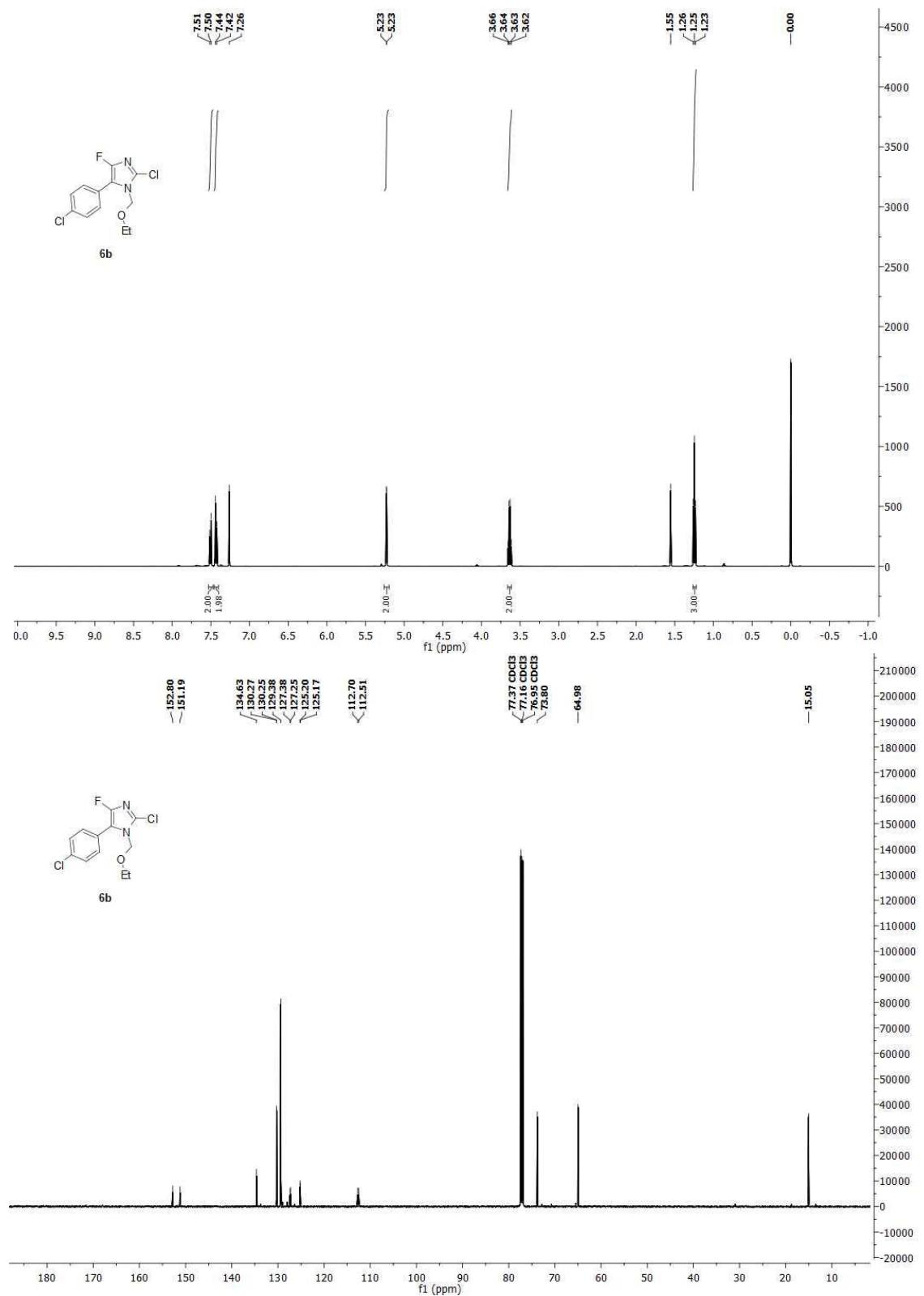


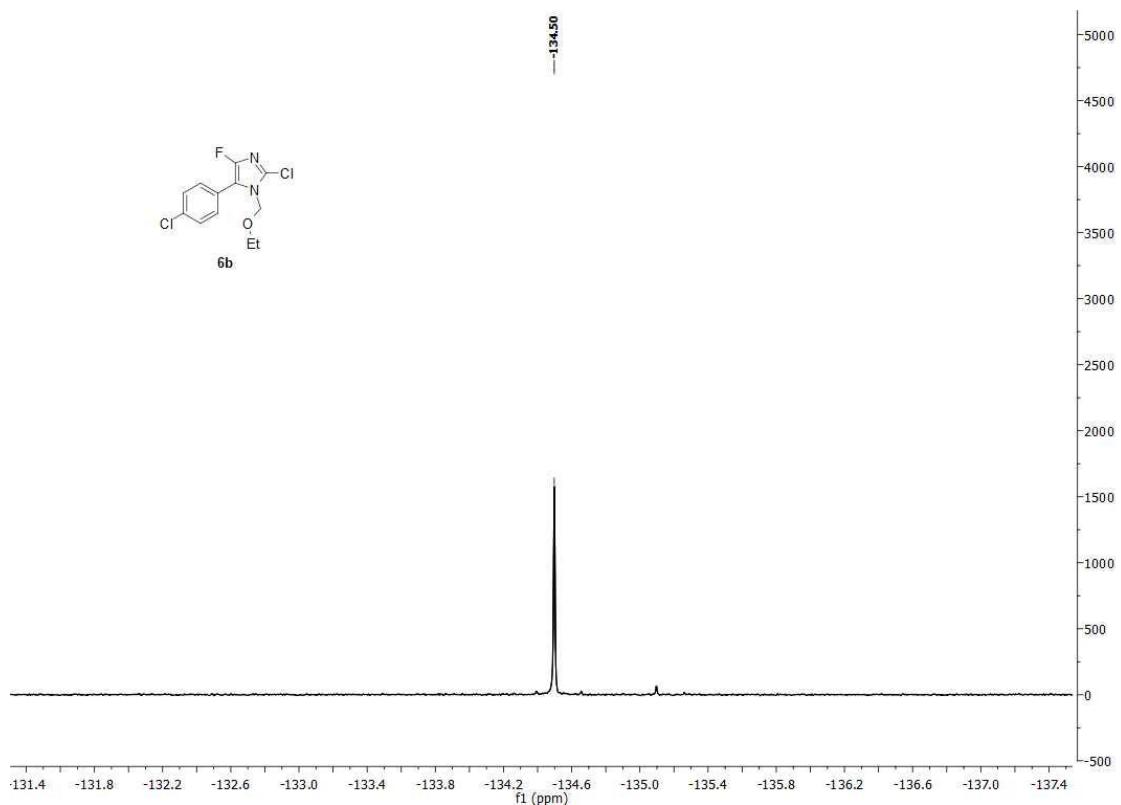
2-chloro-1-(ethoxymethyl)-4-fluoro-1*H*-imidazole (**6a**).



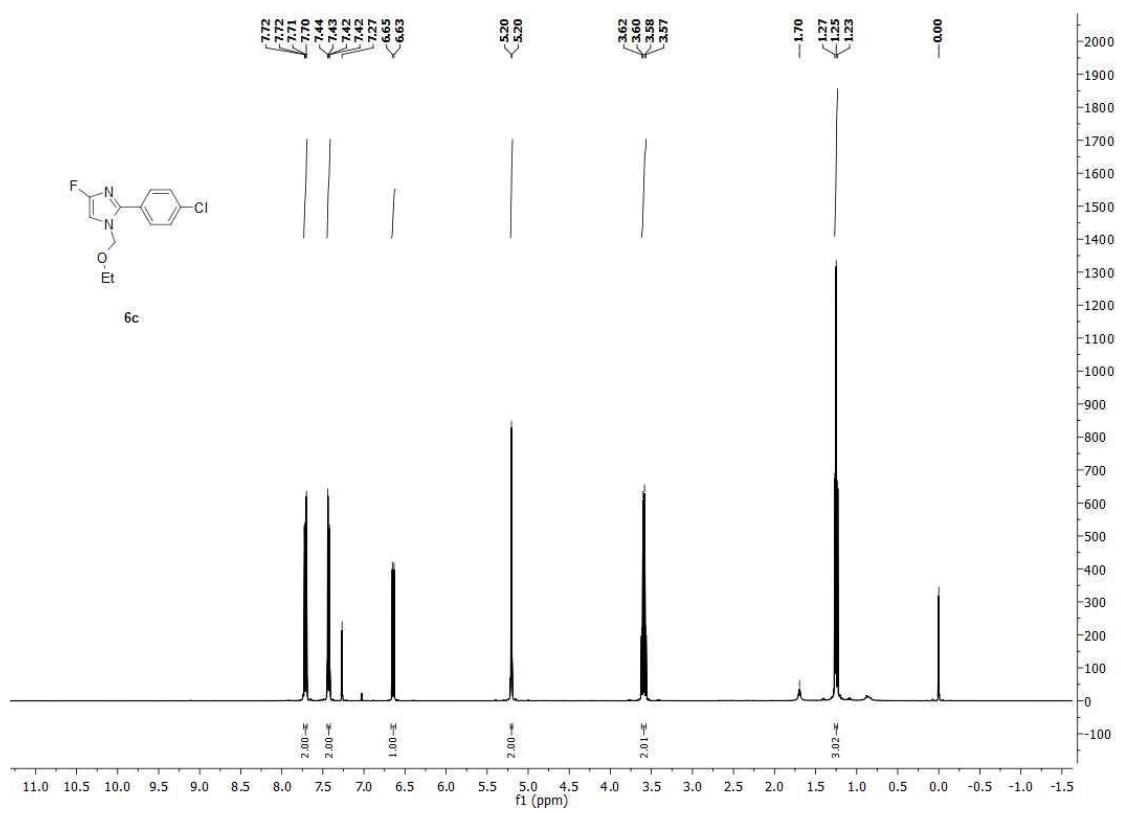


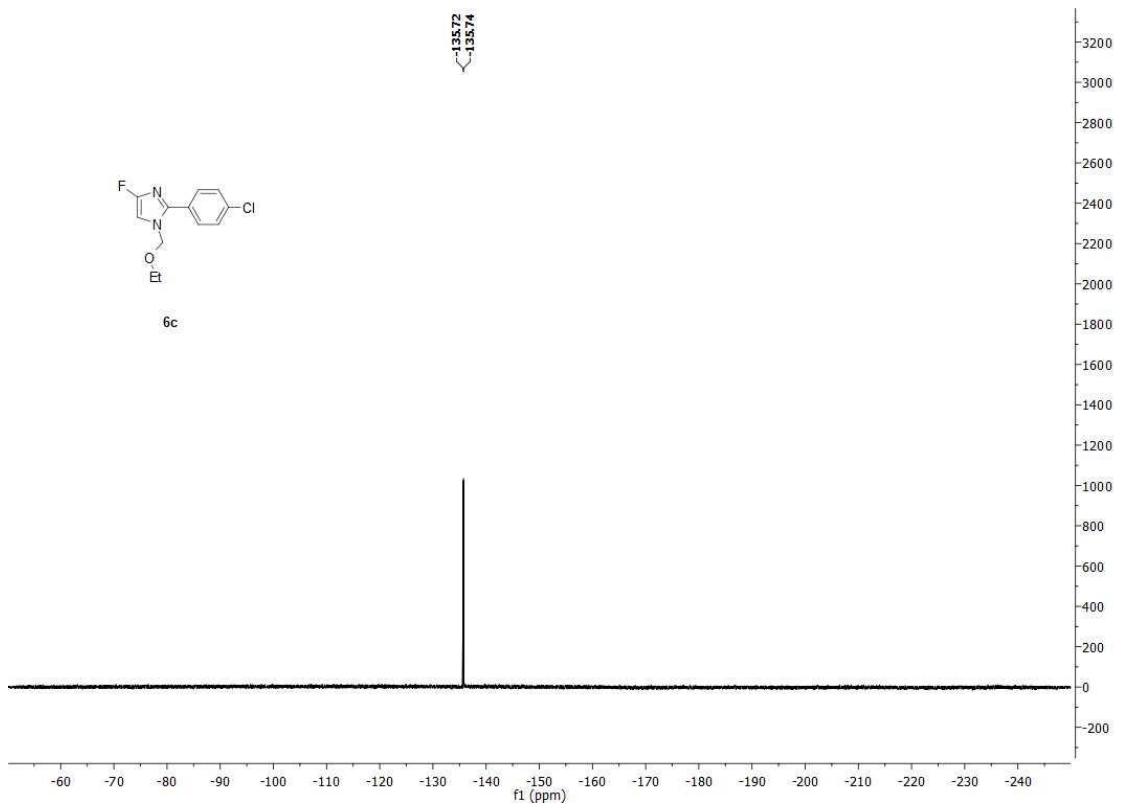
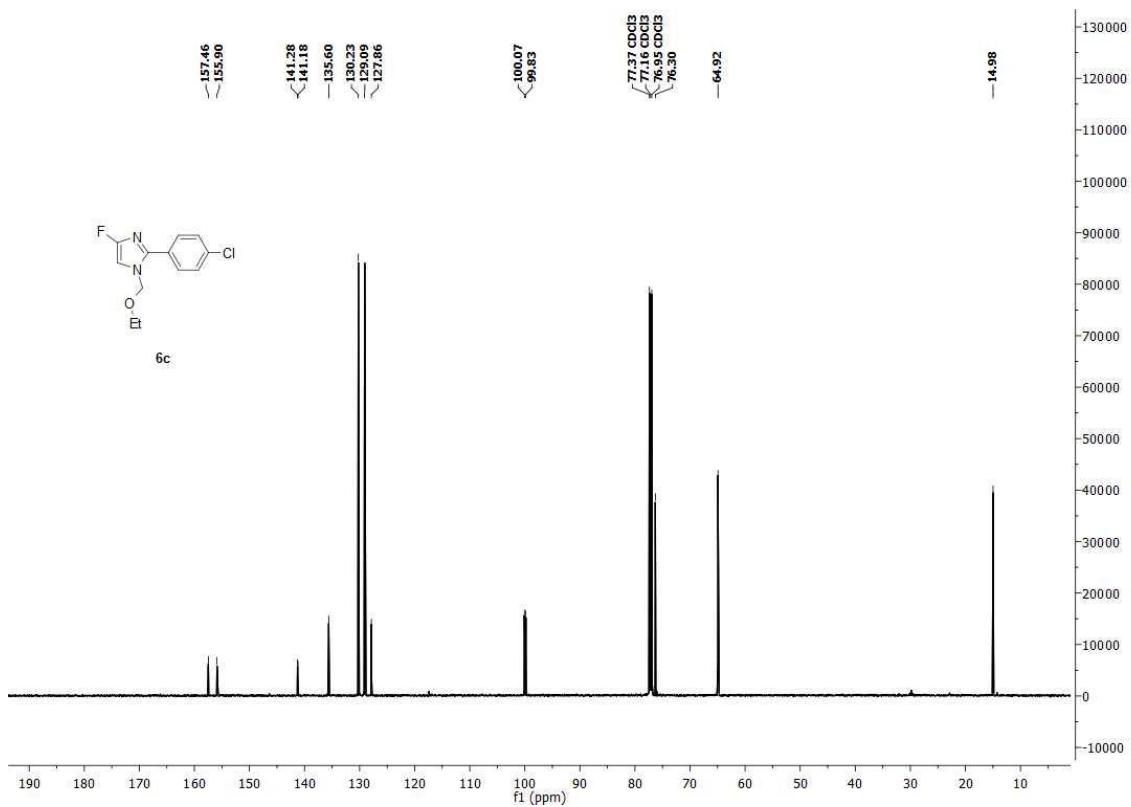
2-chloro-5-(4-chlorophenyl)-1-(ethoxymethyl)-4-fluoro-1*H*-imidazole (**6b**).



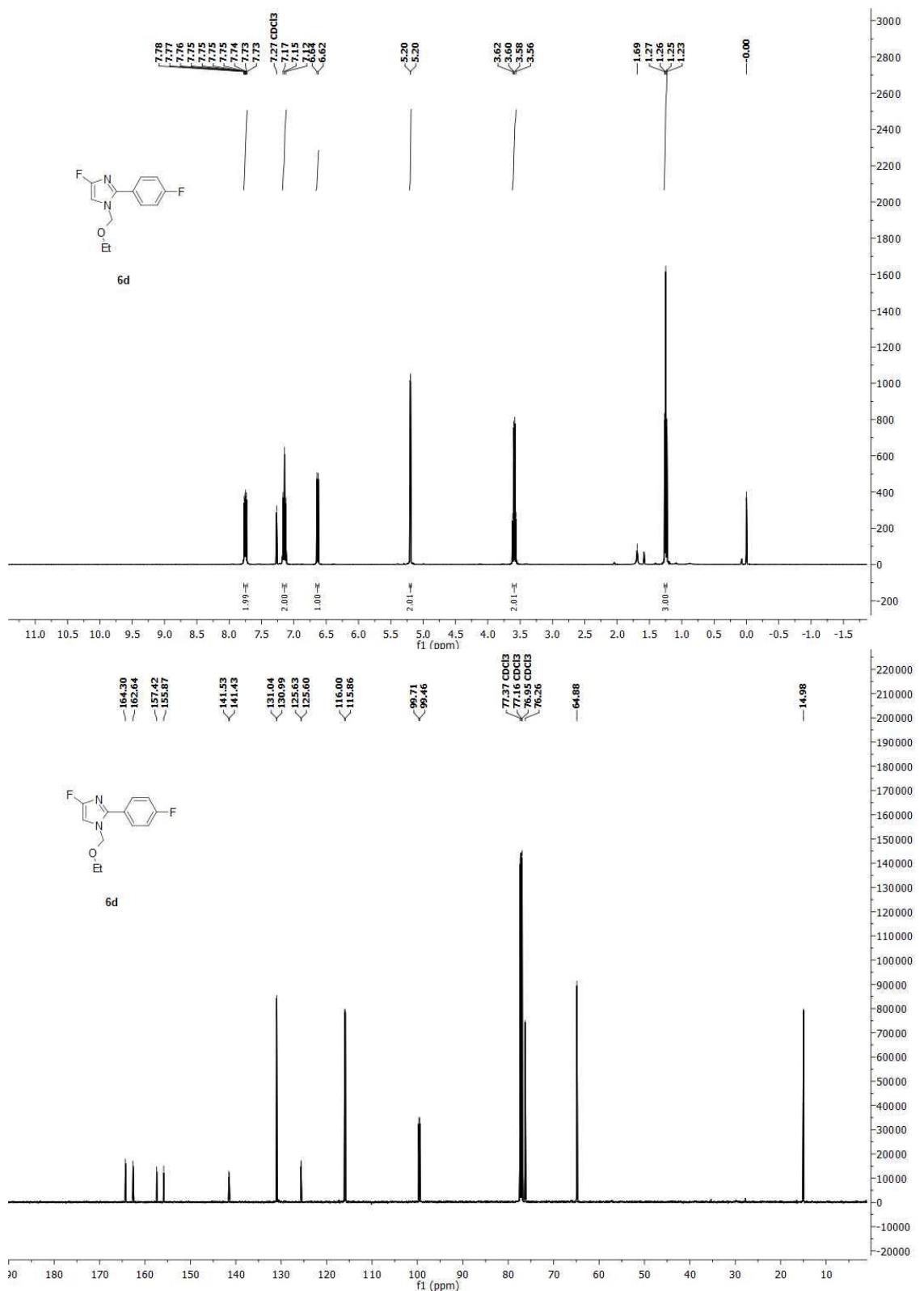


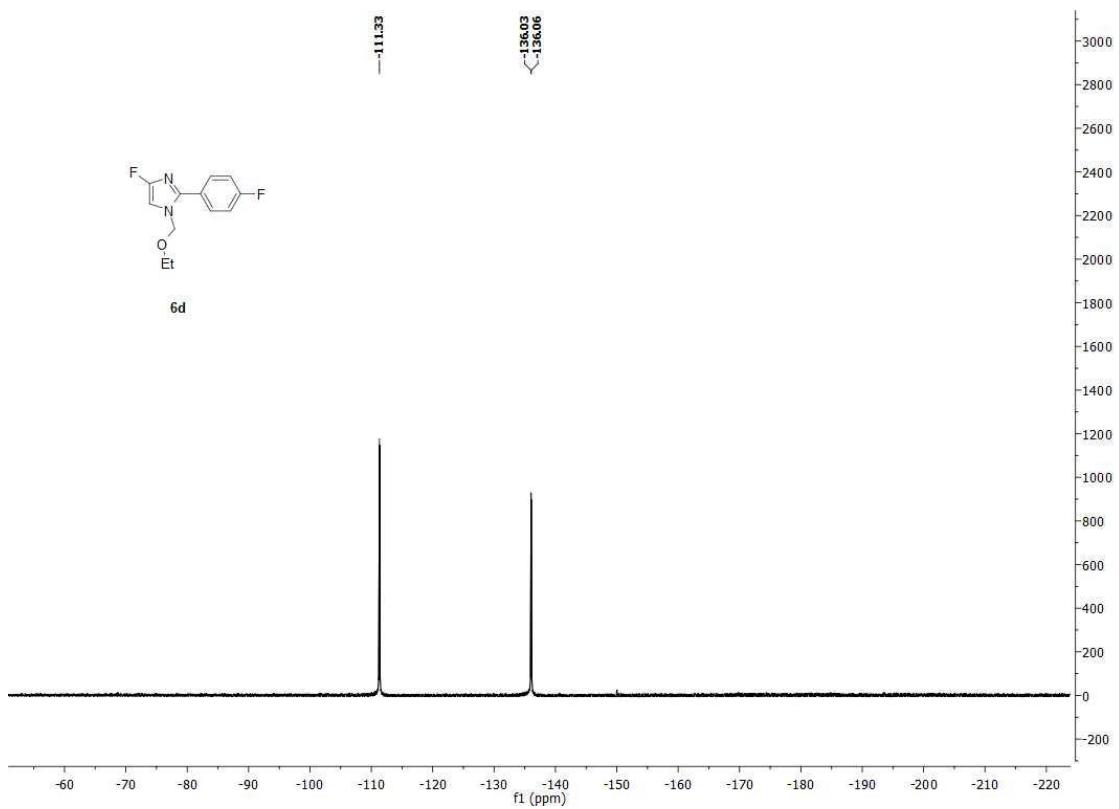
2-(4-chlorophenyl)-1-(ethoxymethyl)-4-fluoro-1*H*-imidazole (**6c**).



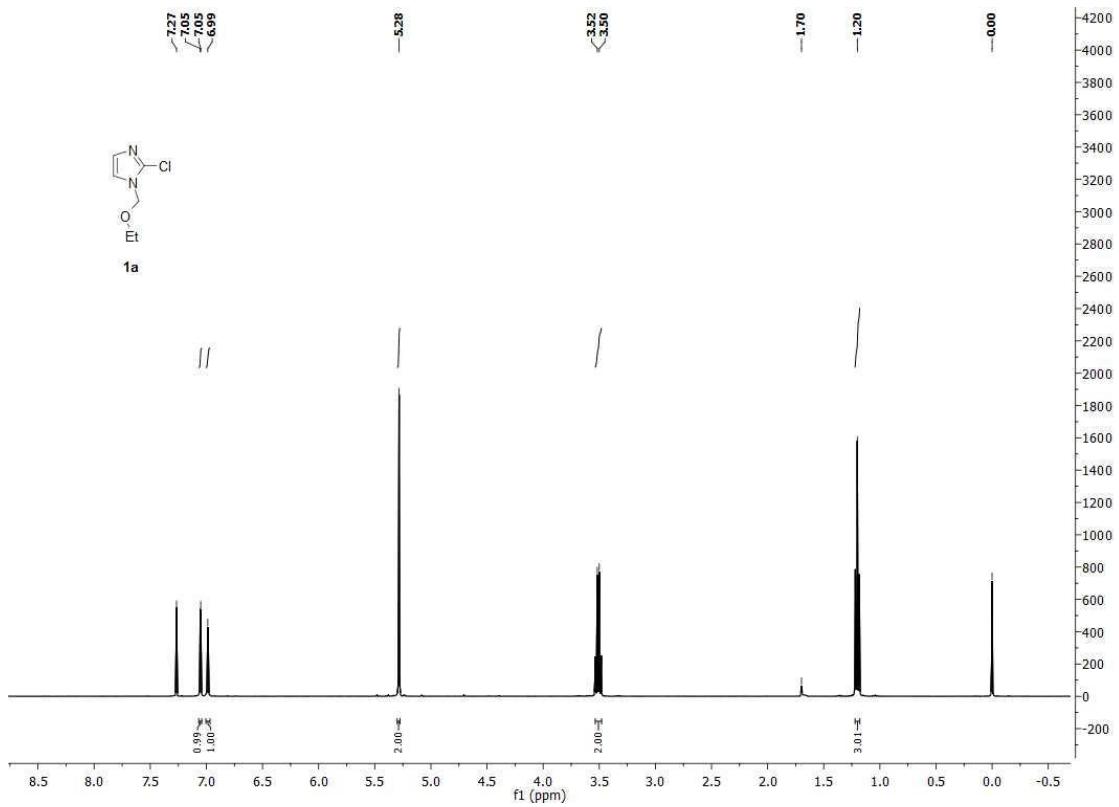


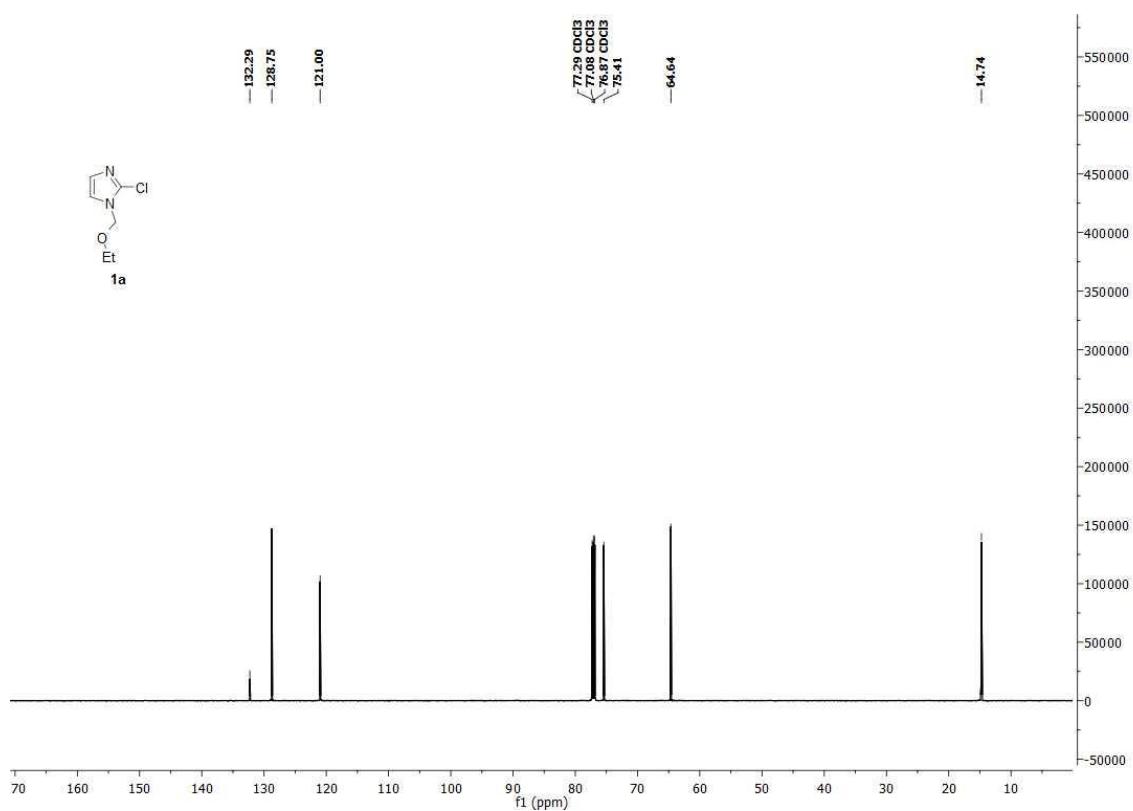
1-(ethoxymethyl)-4-fluoro-2-(4-fluorophenyl)-1*H*-imidazole (**6d**).



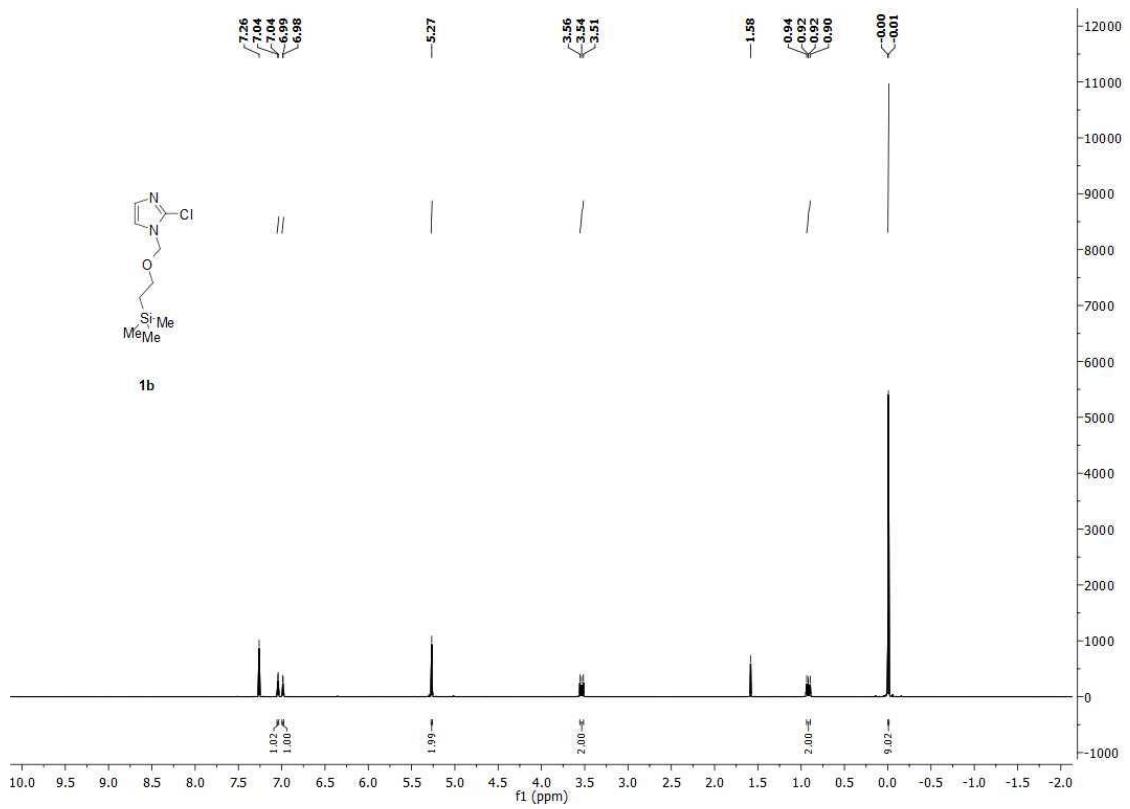


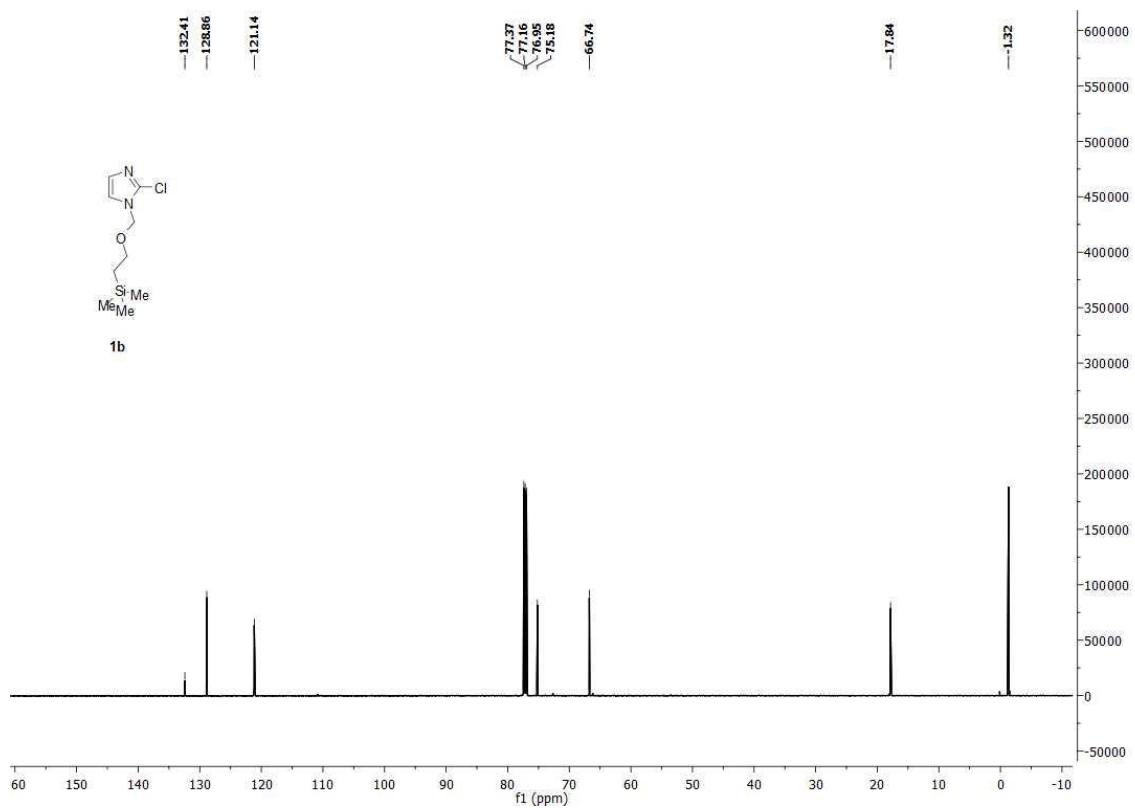
2-chloro-1-(ethoxymethyl)-1*H*-imidazole (1a**).**



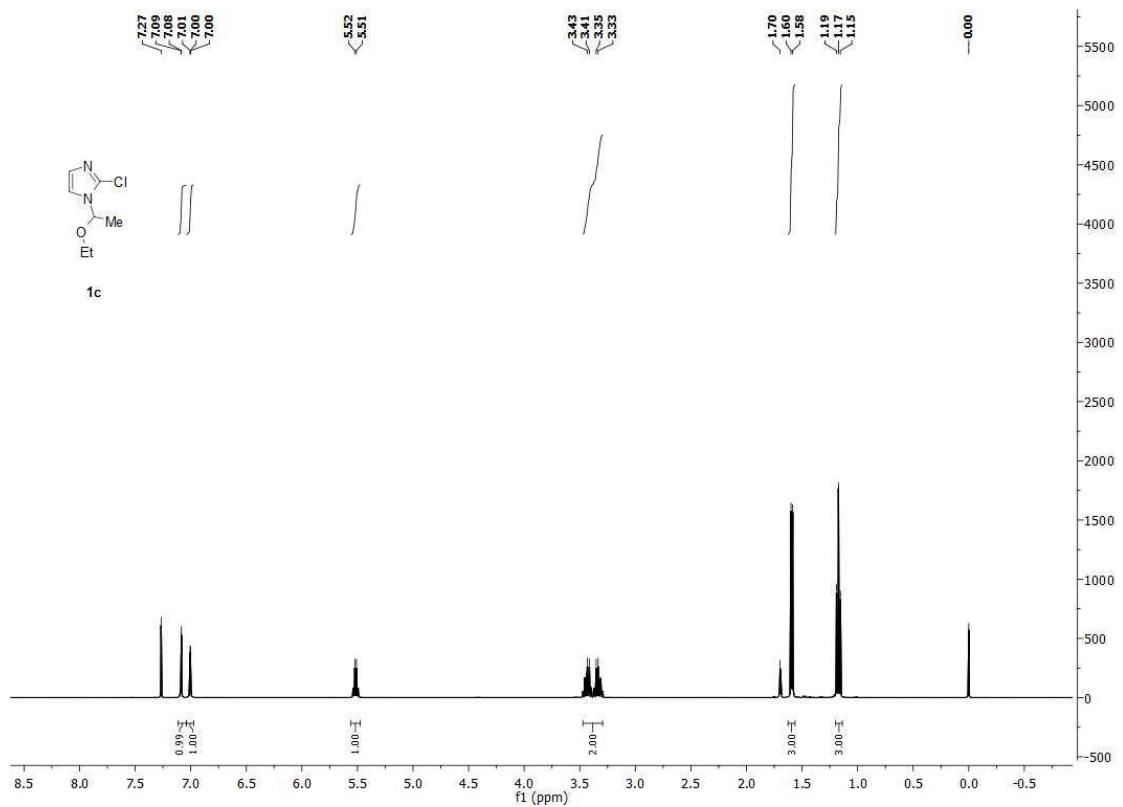


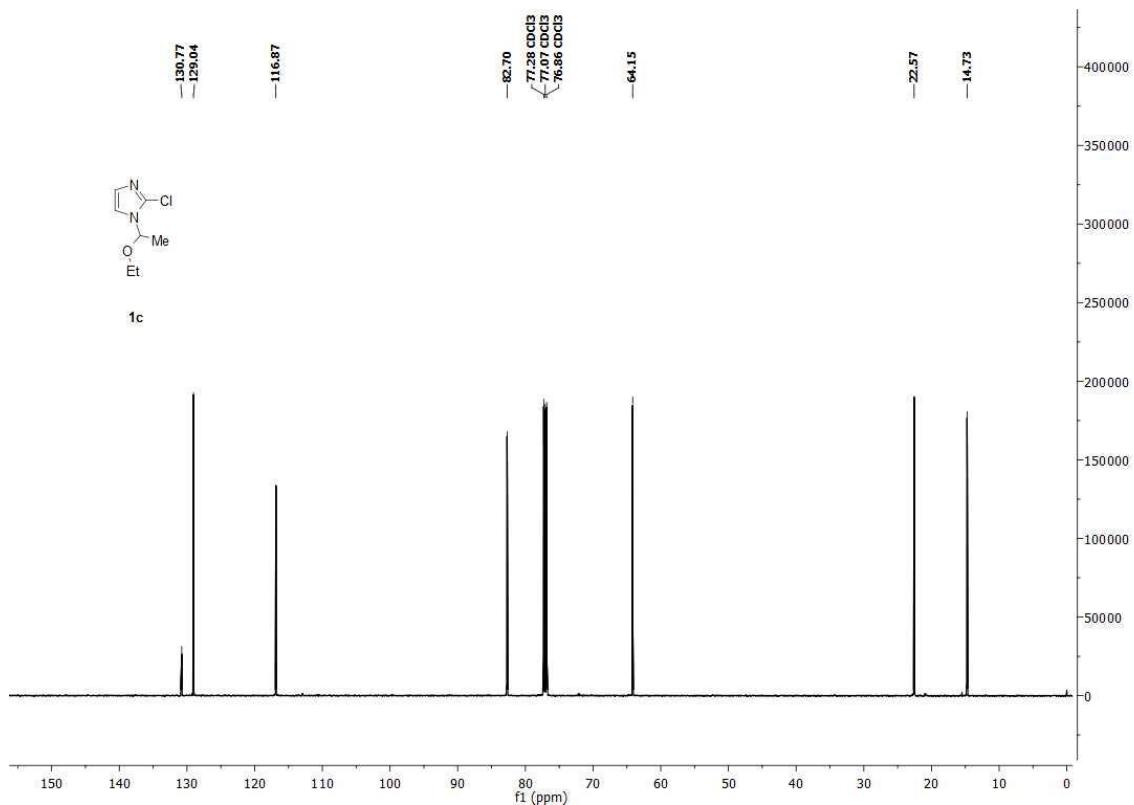
2-chloro-1-((2-(trimethylsilyl)ethoxy)methyl)-1*H*-imidazole (**1b**).



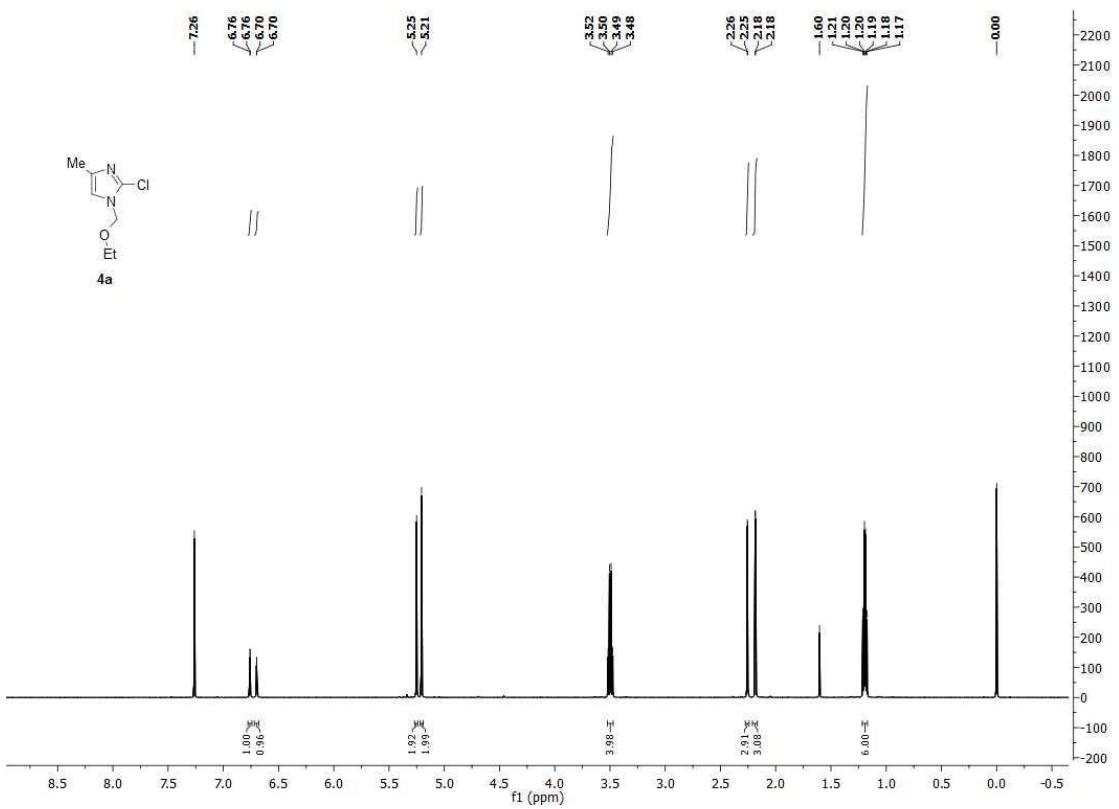


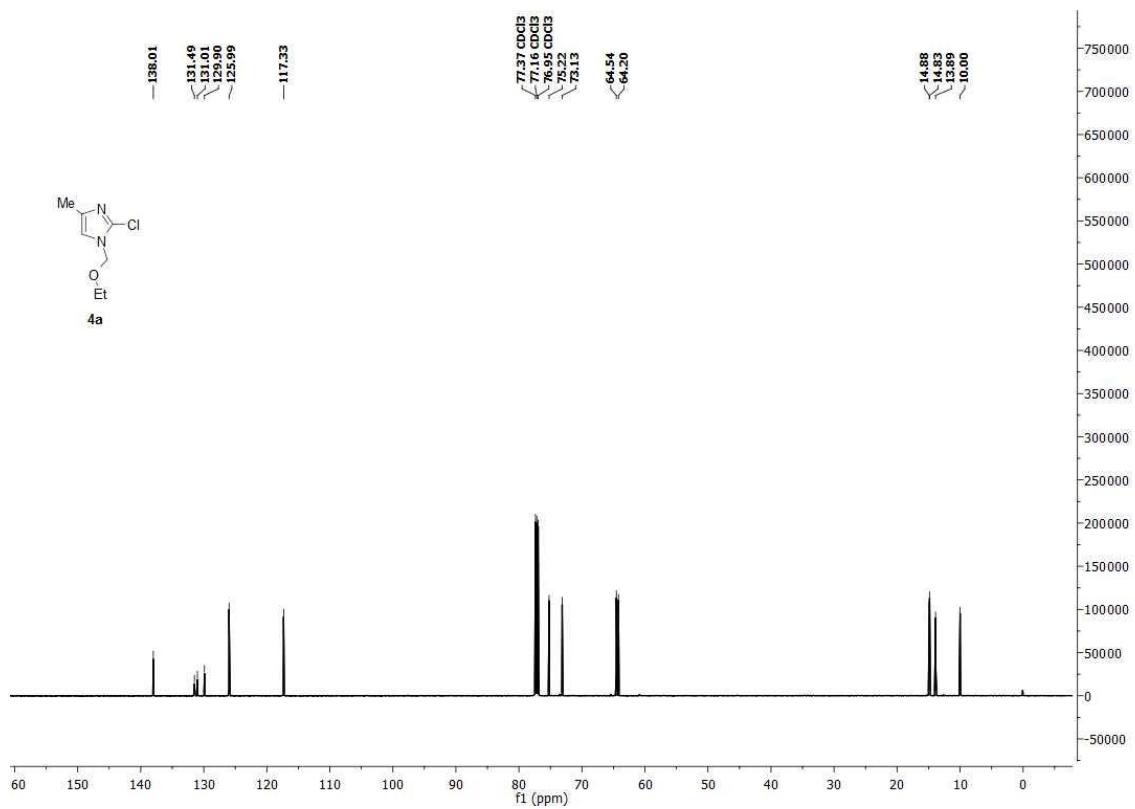
2-chloro-1-(1-ethoxyethyl)-1*H*-imidazole (**1c**).



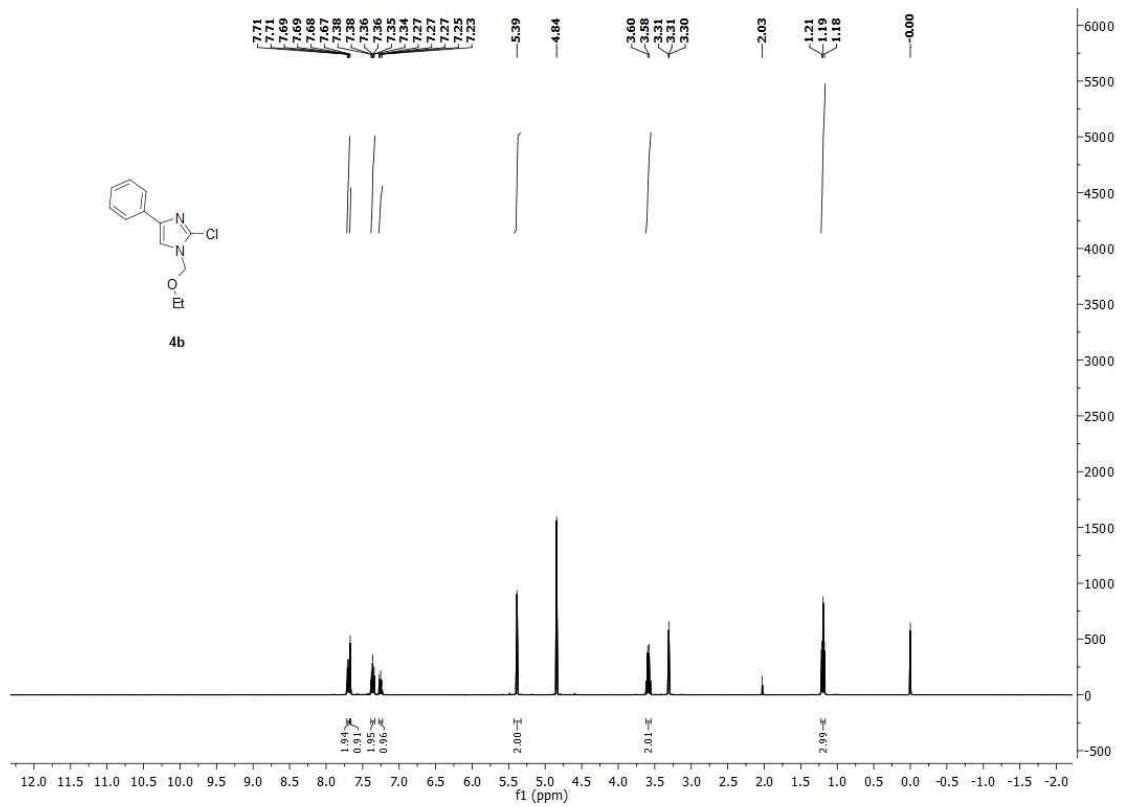


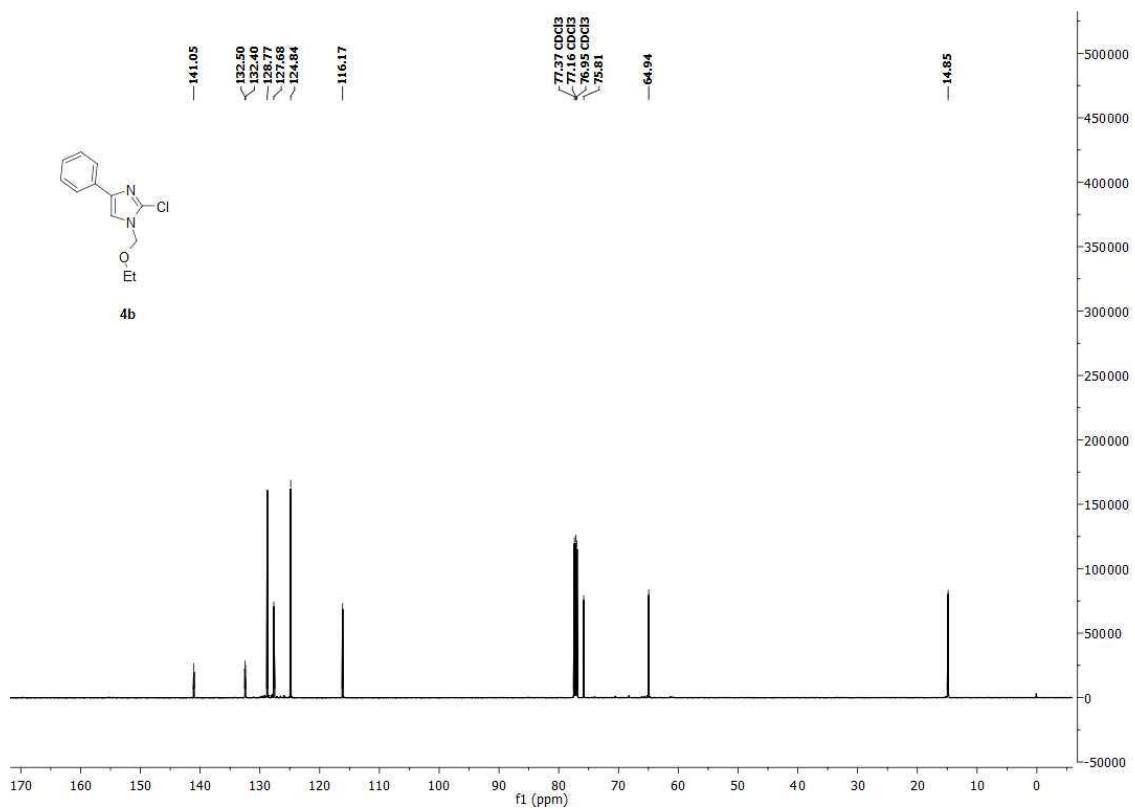
2-chloro-1-(ethoxymethyl)-4/5-methyl-1*H*-imidazole (**4a**) (1:1 regioisomeric mixture).



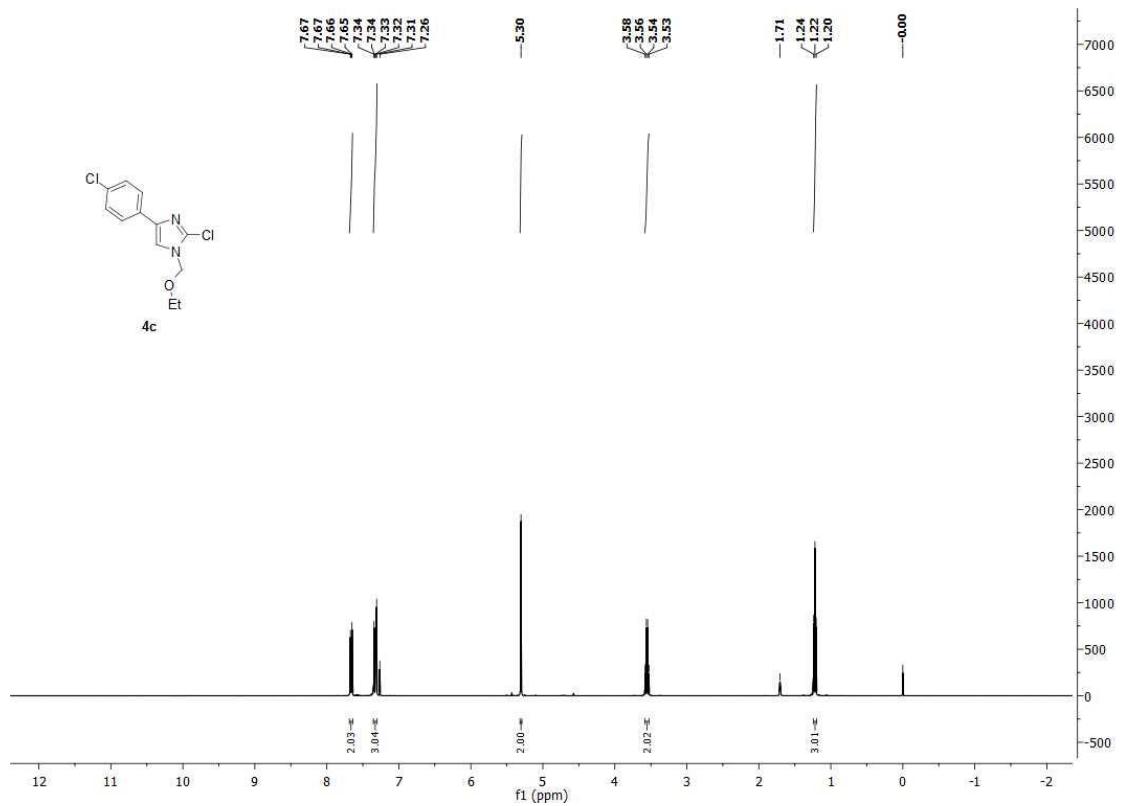


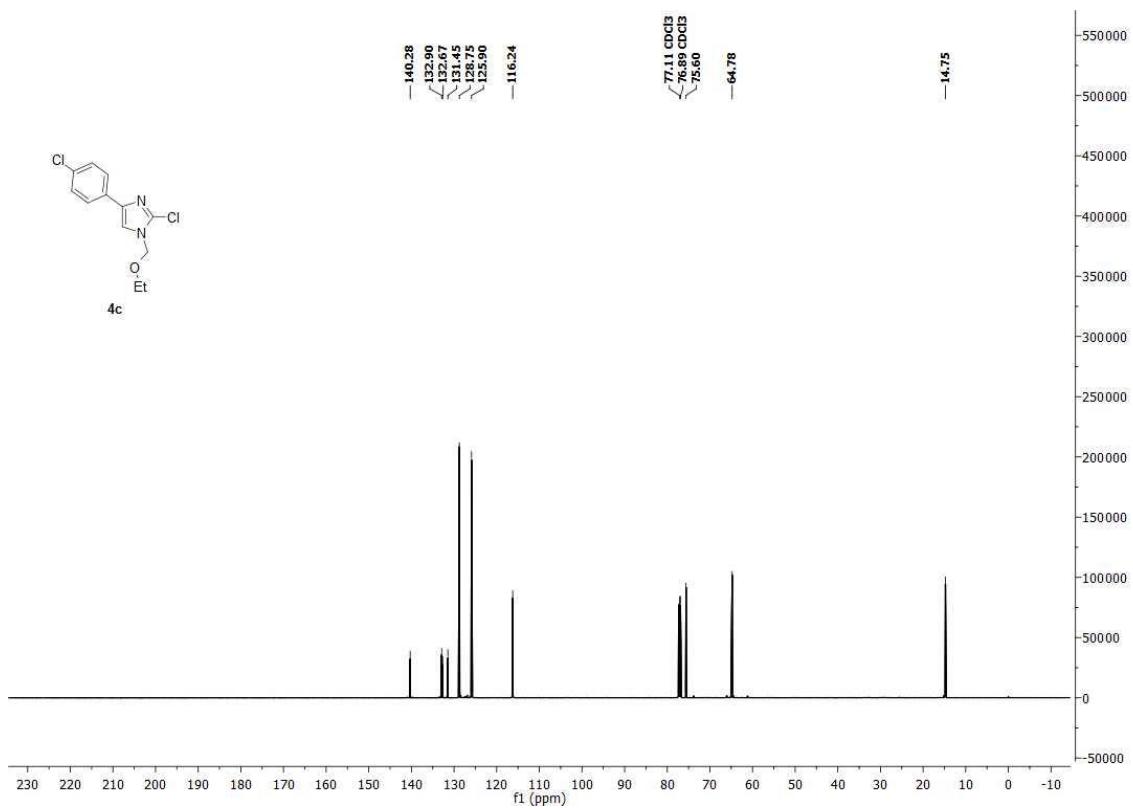
2-chloro-1-(ethoxymethyl)-4-phenyl-1*H*-imidazole (**4b**).



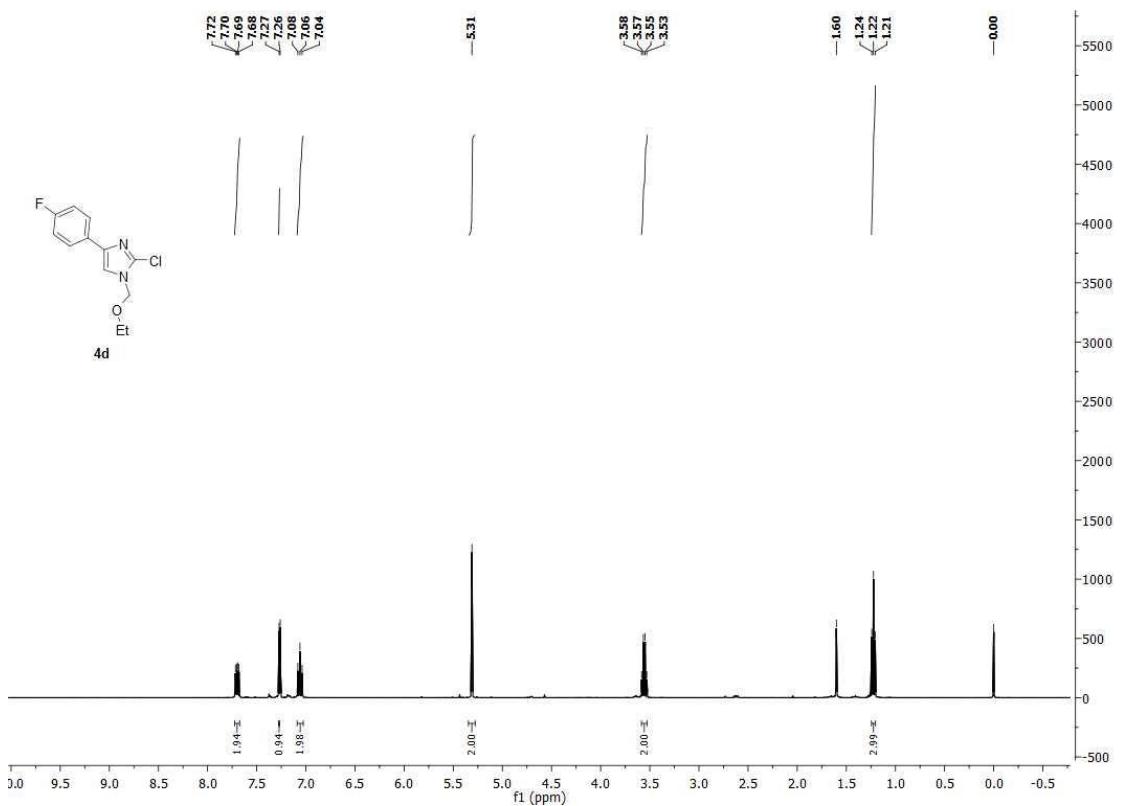


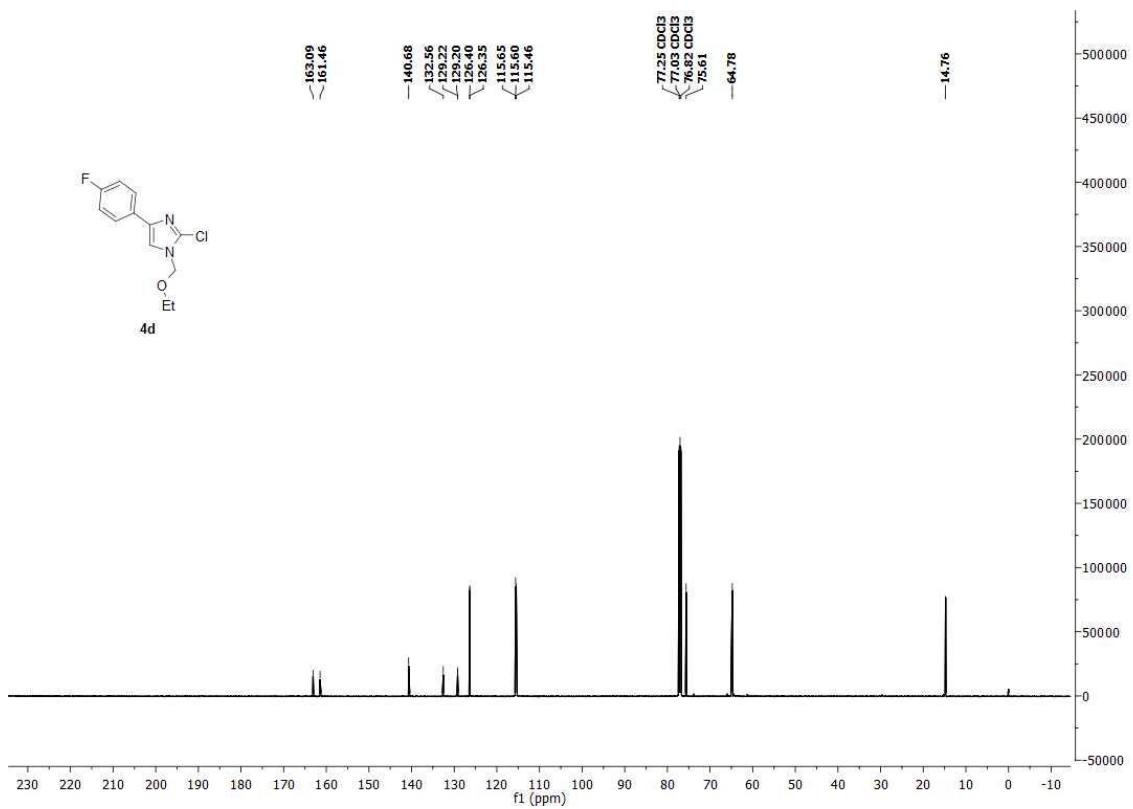
2-chloro-4-(4-chlorophenyl)-1-(ethoxymethyl)-1*H*-imidazole (**4c**).



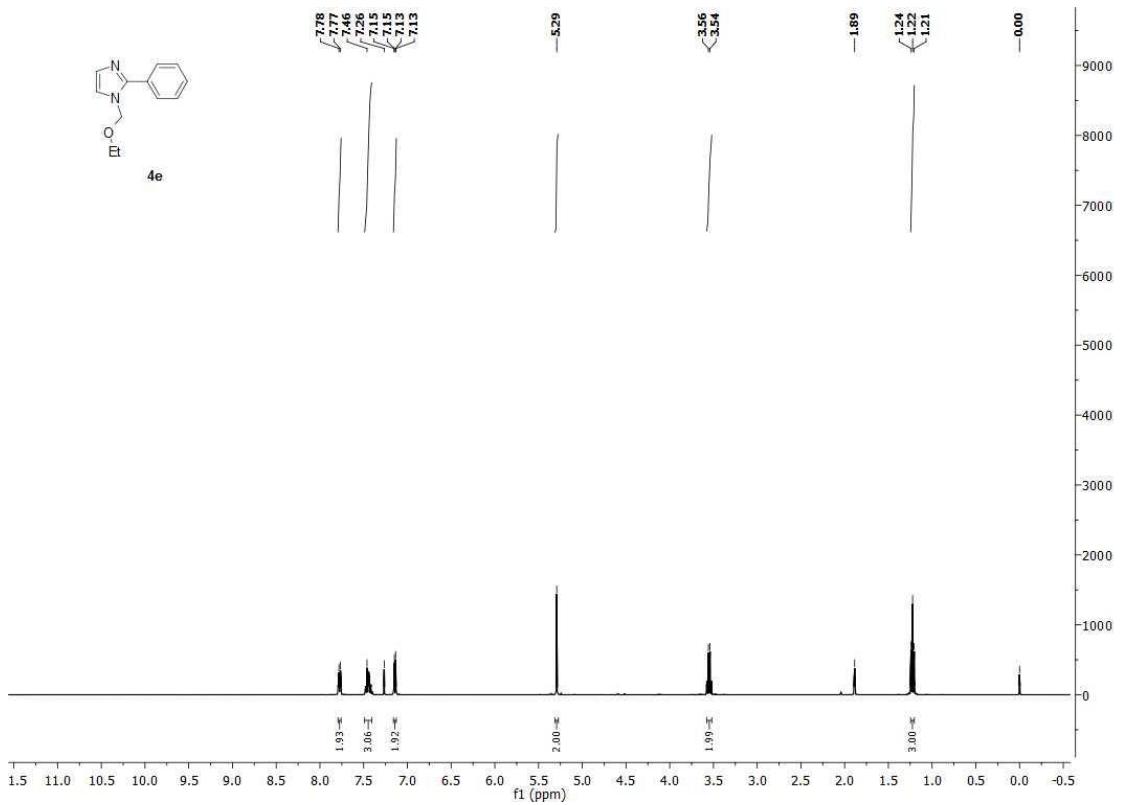


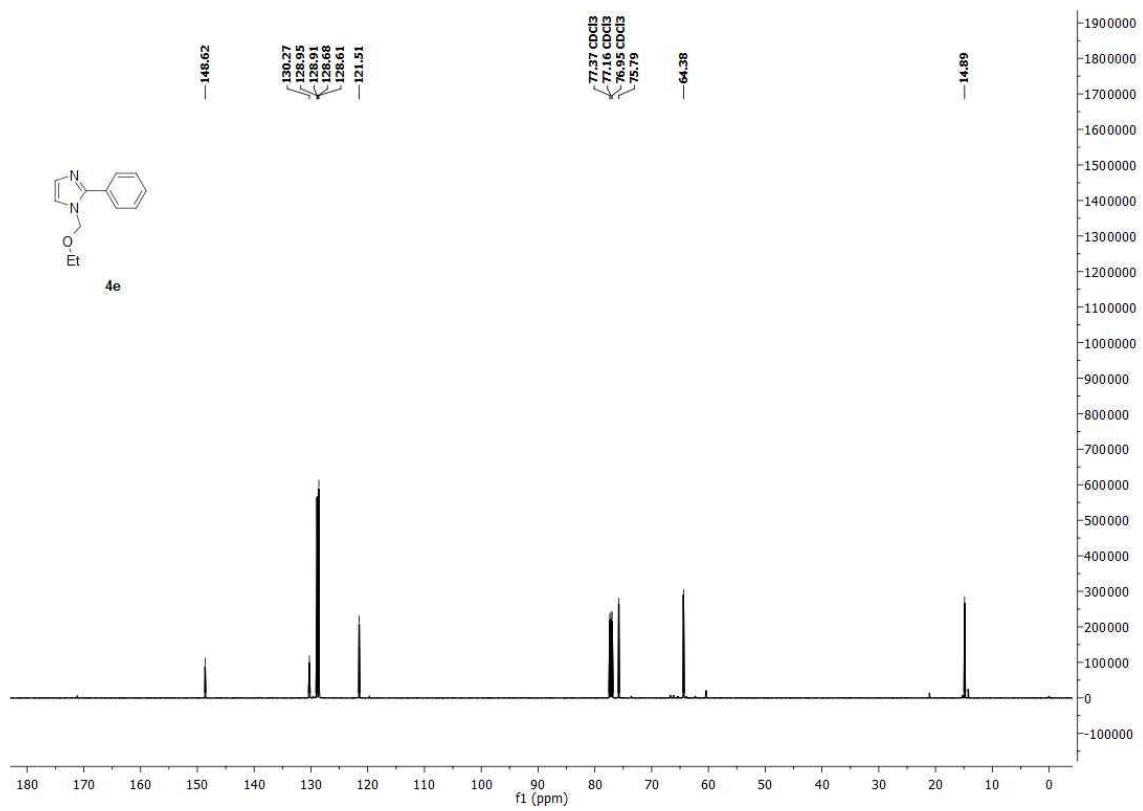
2-chloro-1-(ethoxymethyl)-4-(4-fluorophenyl)-1*H*-imidazole (**4d**).



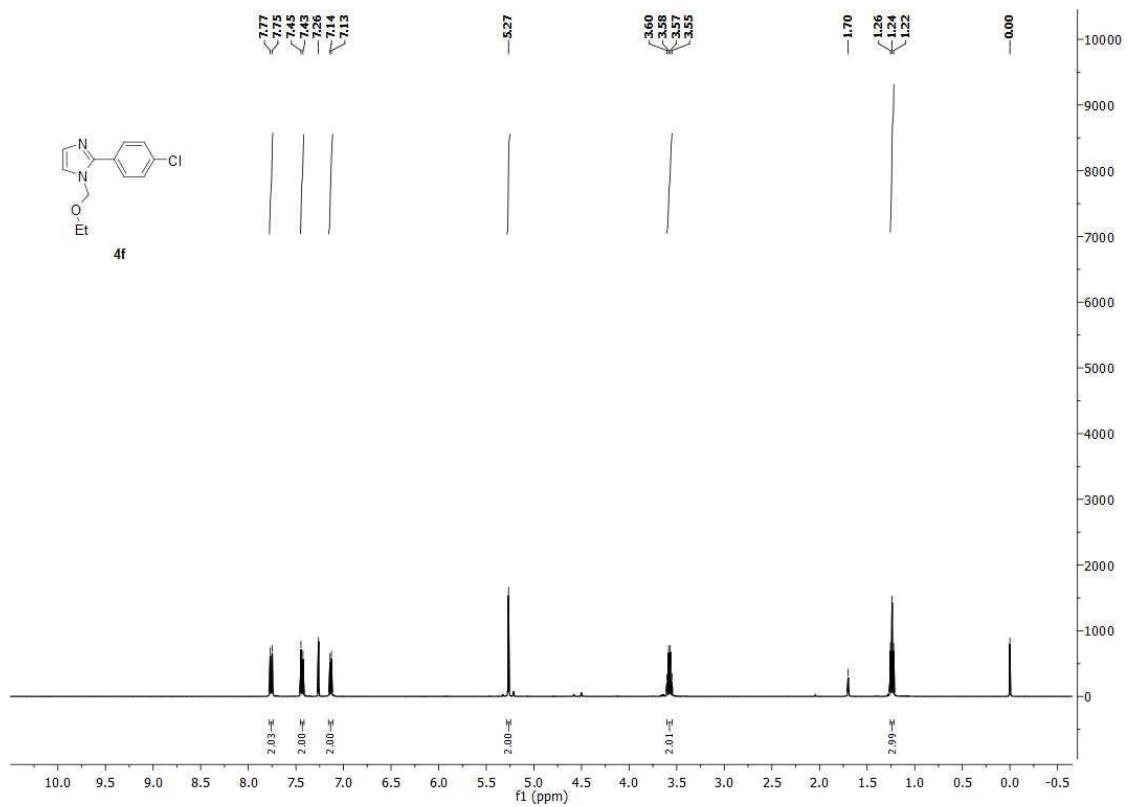


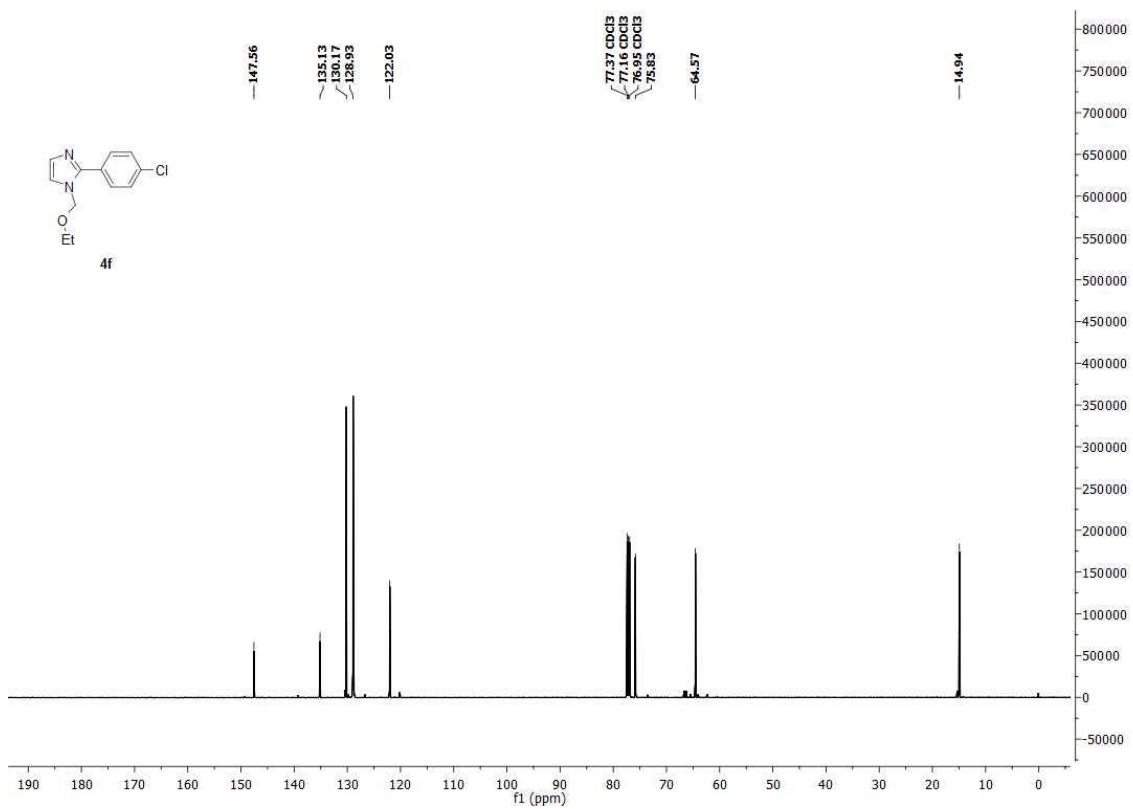
1-(ethoxymethyl)-2-phenyl-1*H*-imidazole (**4e**).





2-(4-chlorophenyl)-1-(ethoxymethyl)-1*H*-imidazole (**4f**).





1-(ethoxymethyl)-2-(4-fluorophenyl)-1H-imidazole (**4g**).

