

Some properties of 1-hydroxy-1*H*-imidazole-2-carboxylic acid esters

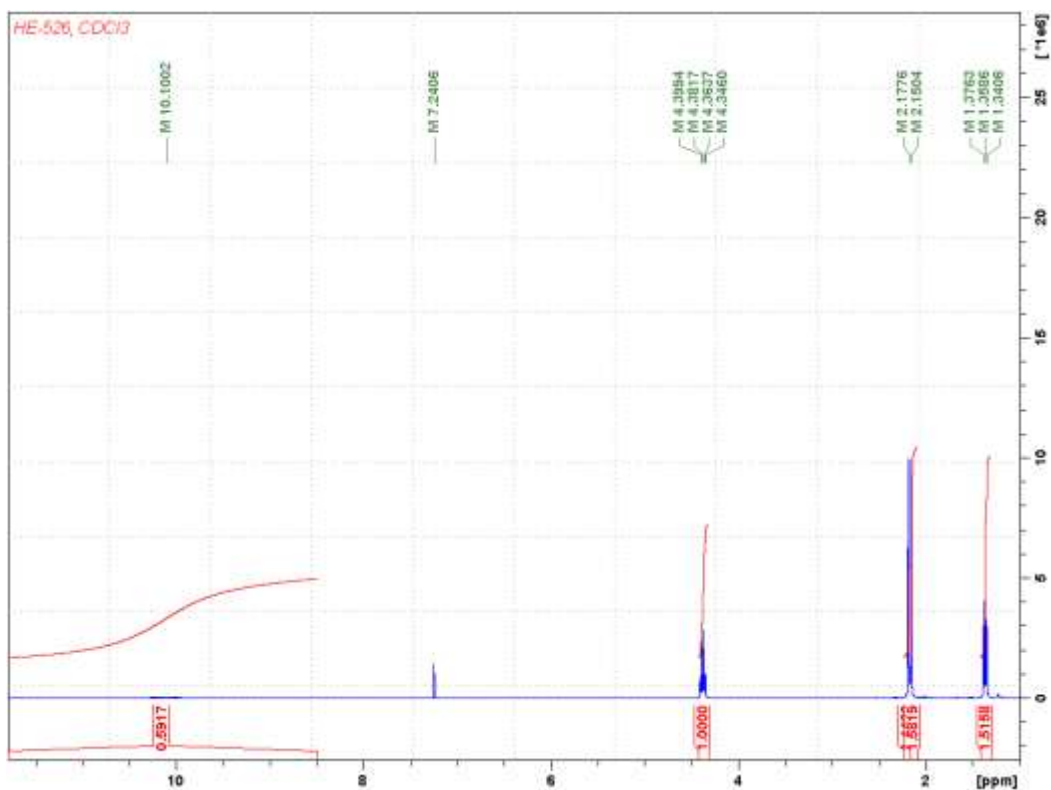
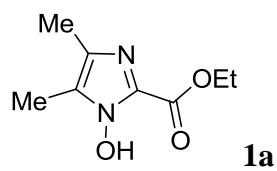
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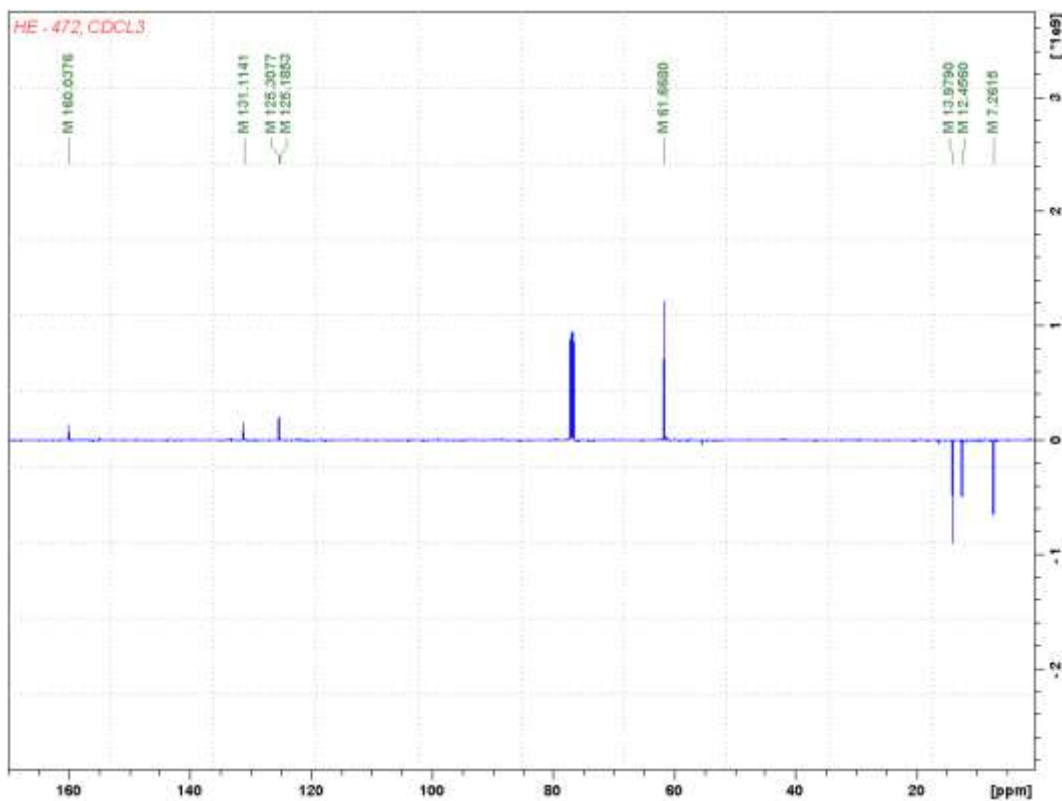
SUPPLEMENTARY INFORMATION

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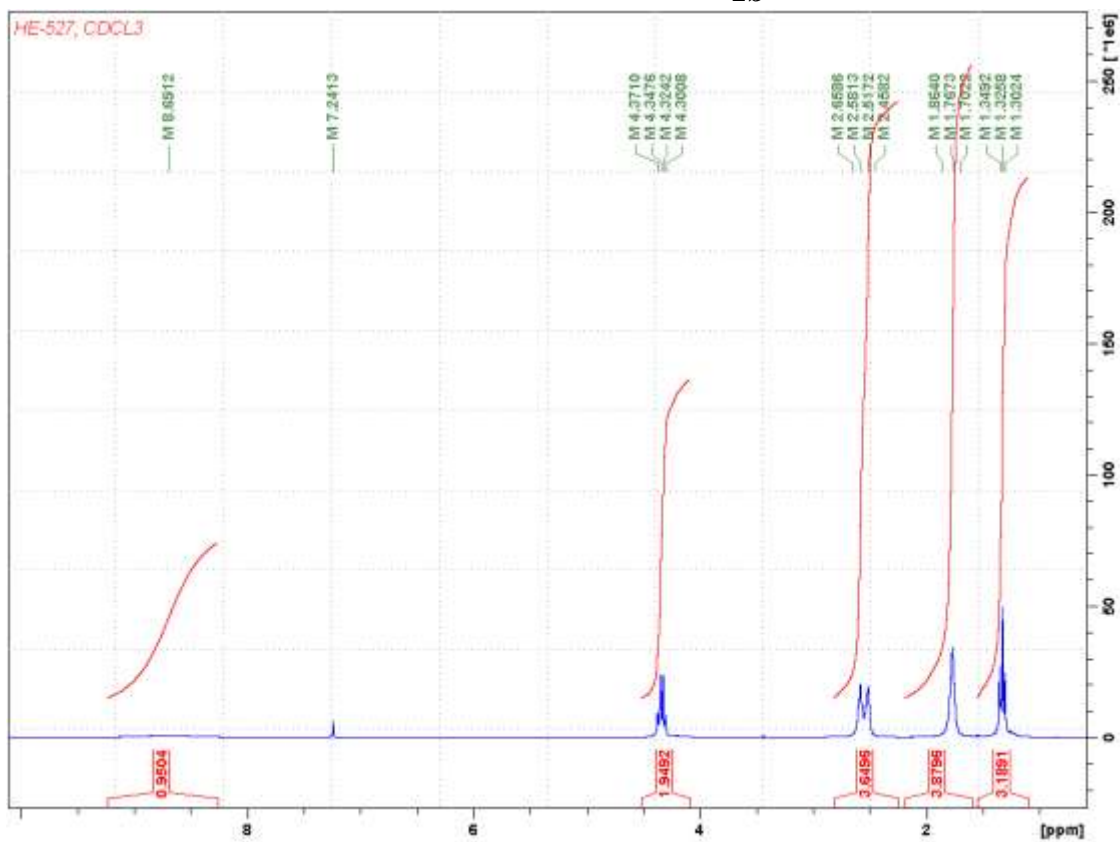
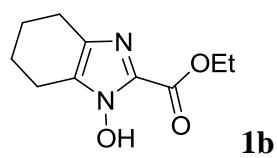
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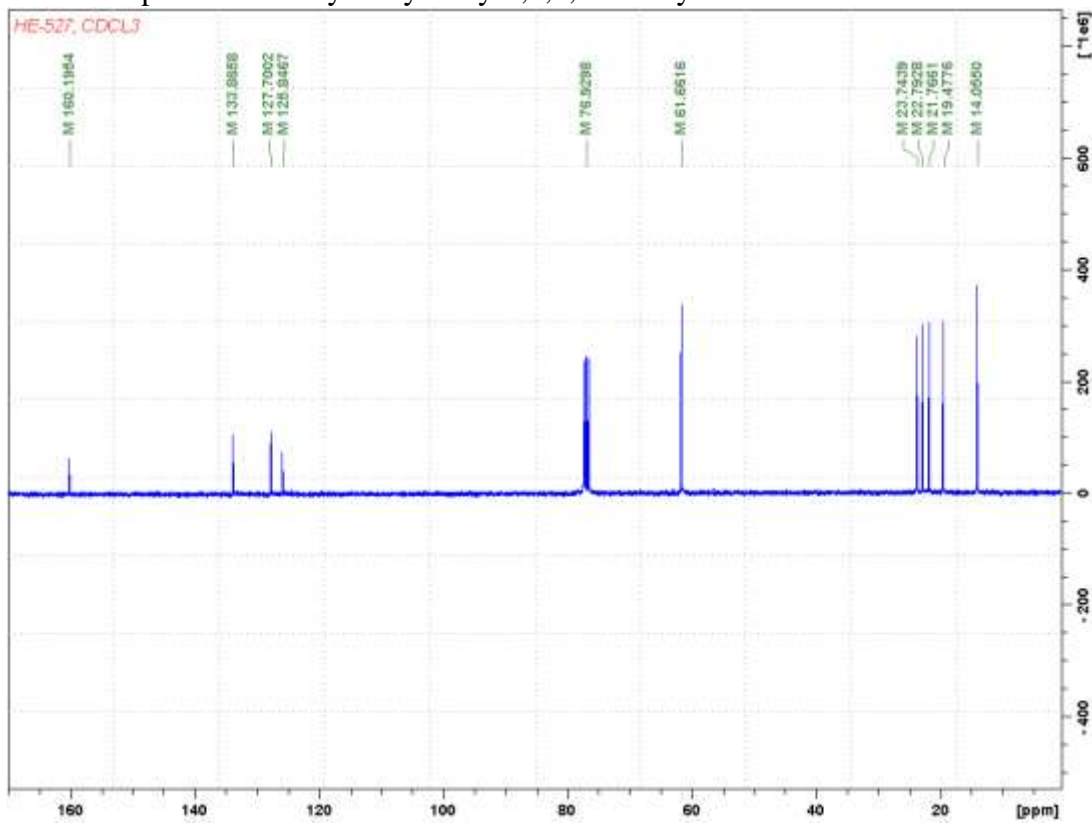
¹H NMR spectrum of ethyl 4,5-dimethyl-1-hydroxy-1*H*-imidazole-2-carboxylate (**1a**).



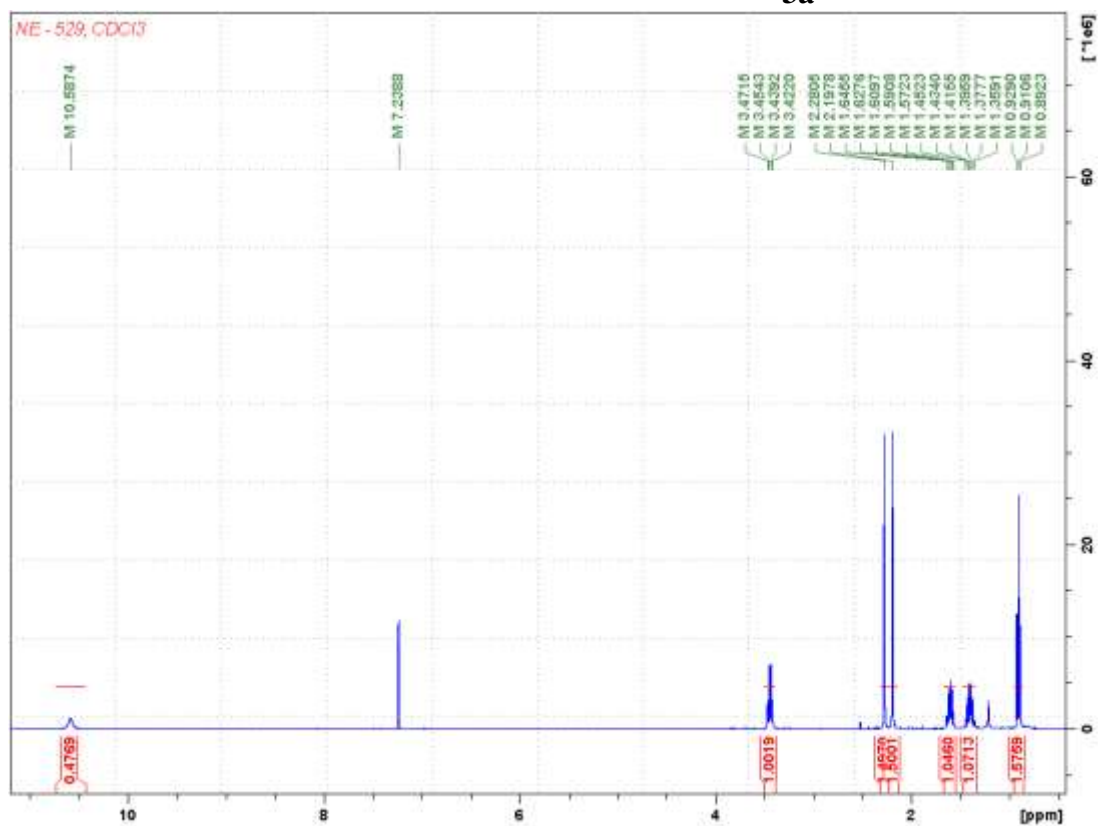
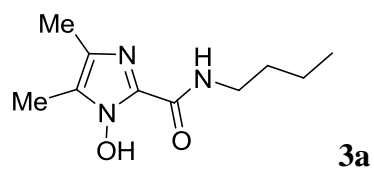
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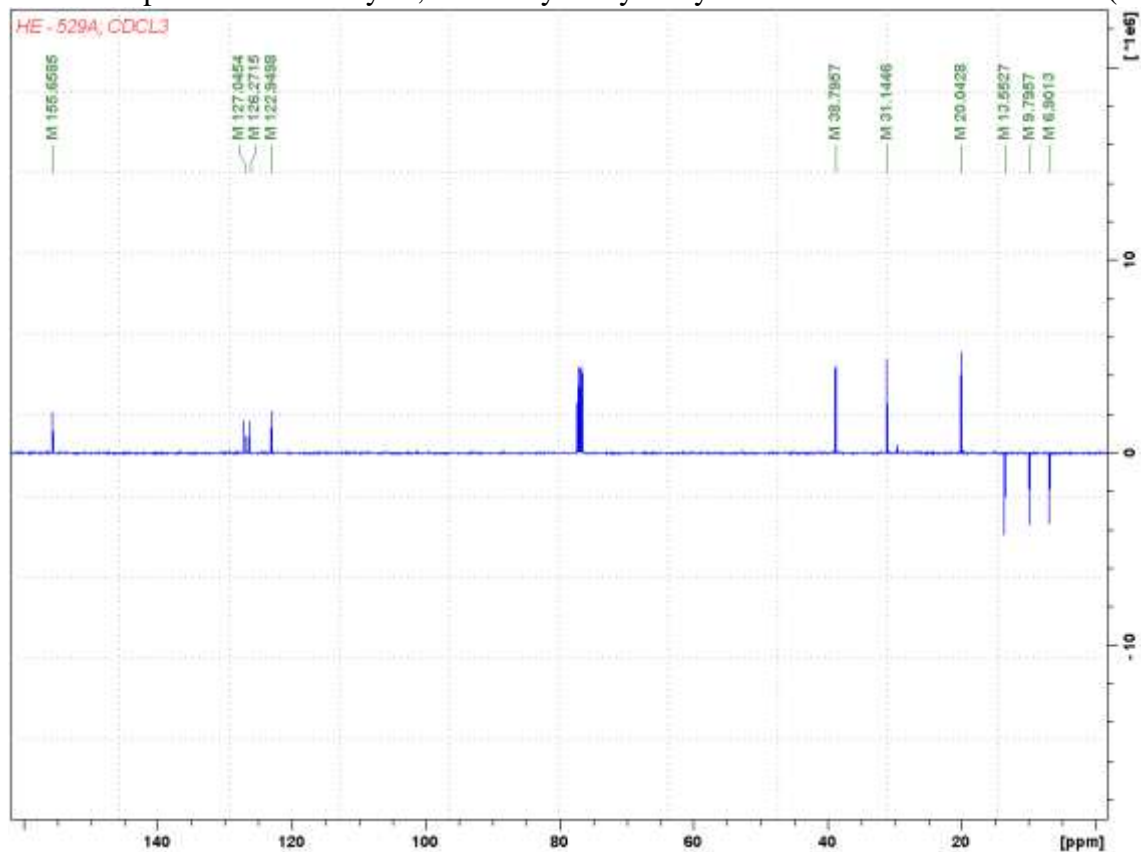
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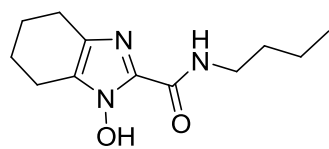
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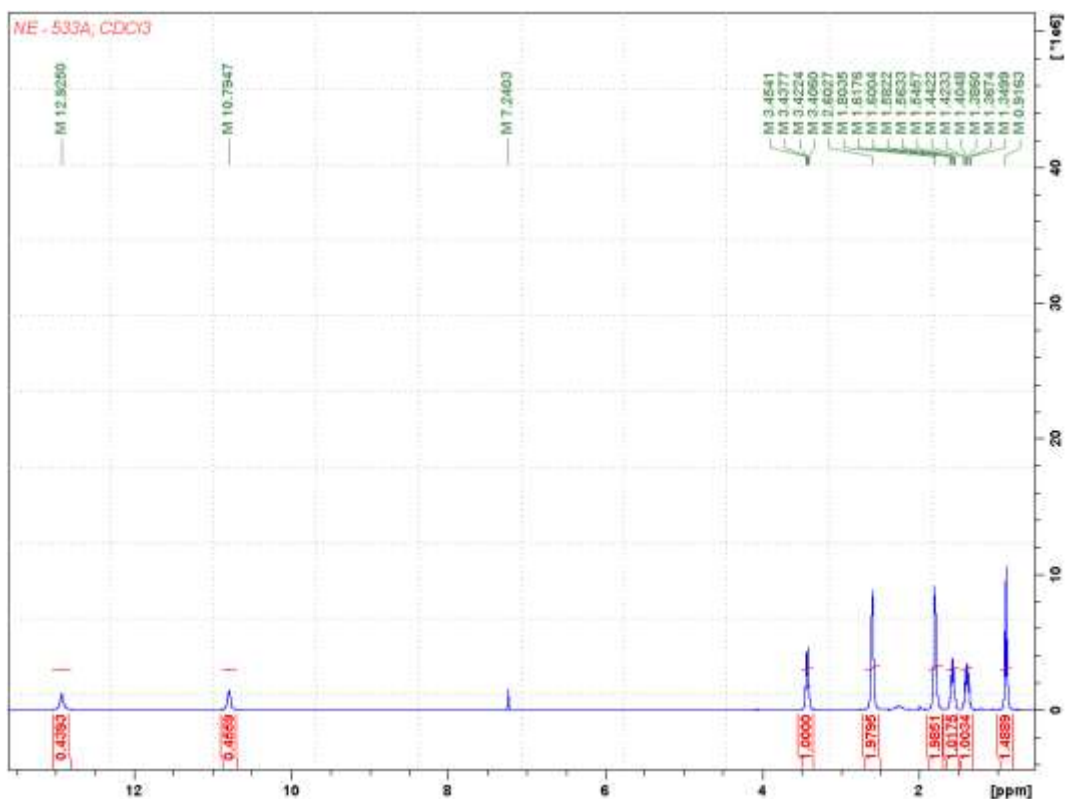
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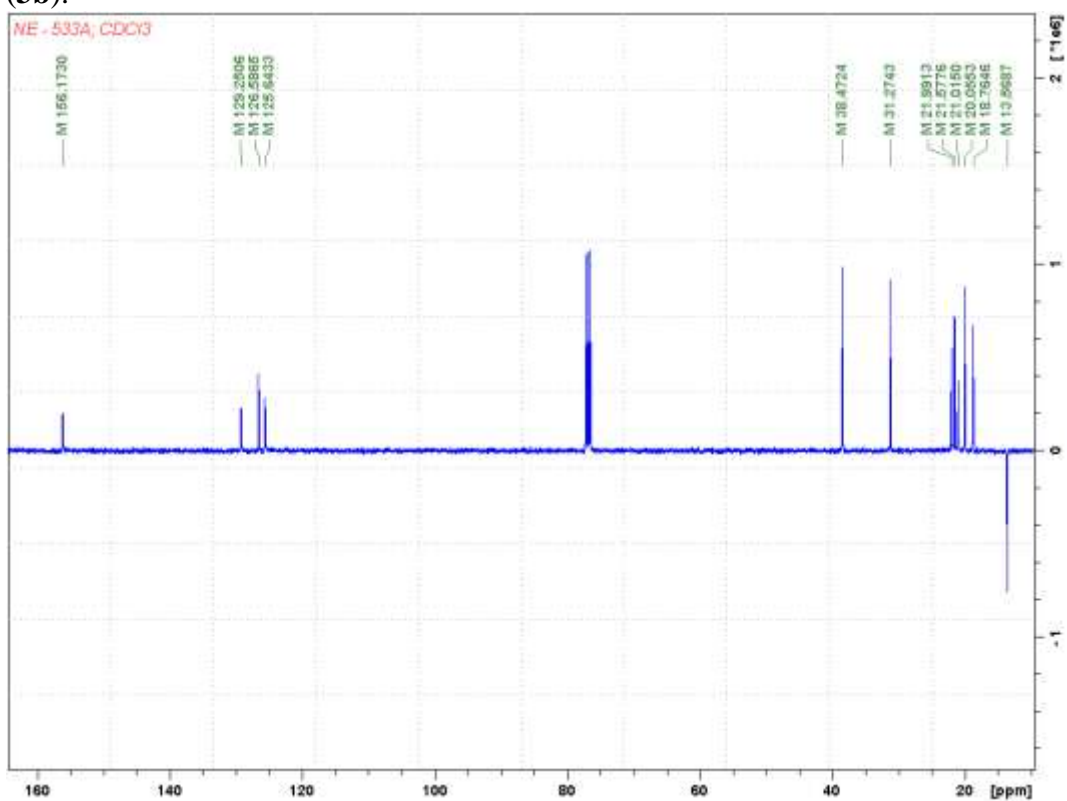
¹³C NMR spectrum of N-butyl-4,5-dimethyl-1-hydroxy-1H-imidazole-2-carboxamide (**3a**).



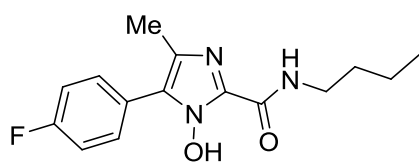
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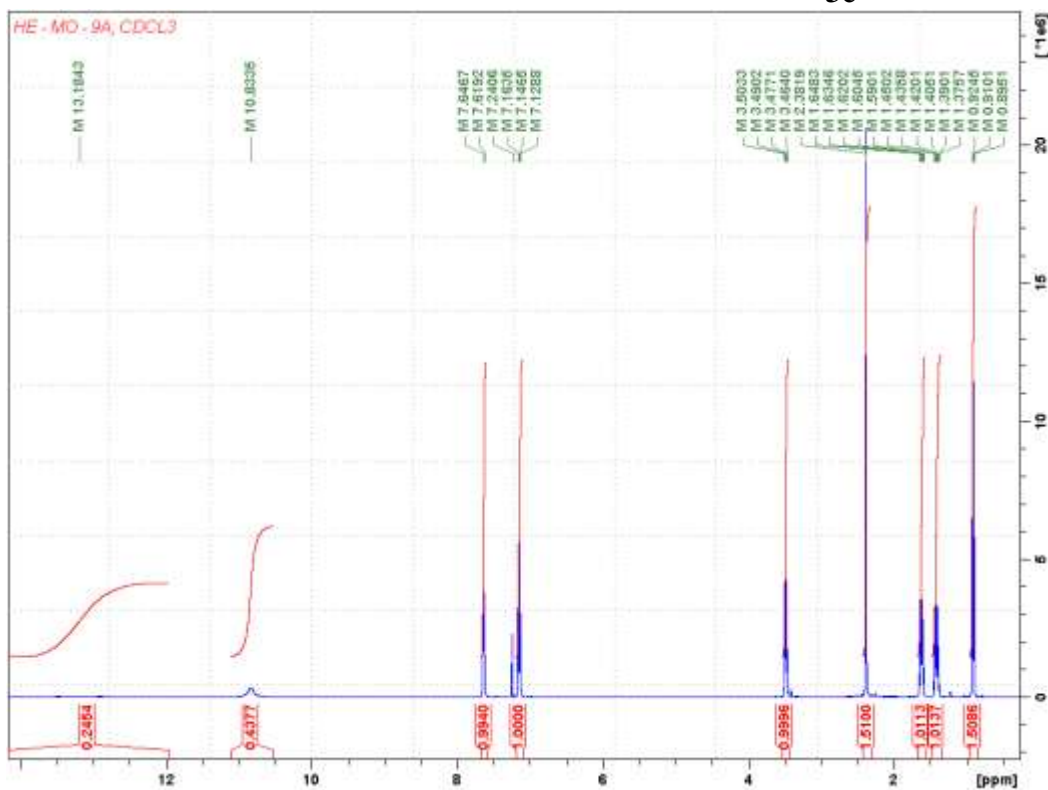
¹H NMR spectrum of N-butyl-1-hydroxy-4,5,6,7-tetrahydro-1H-benzimidazole-2-carboxamide (**3b**).



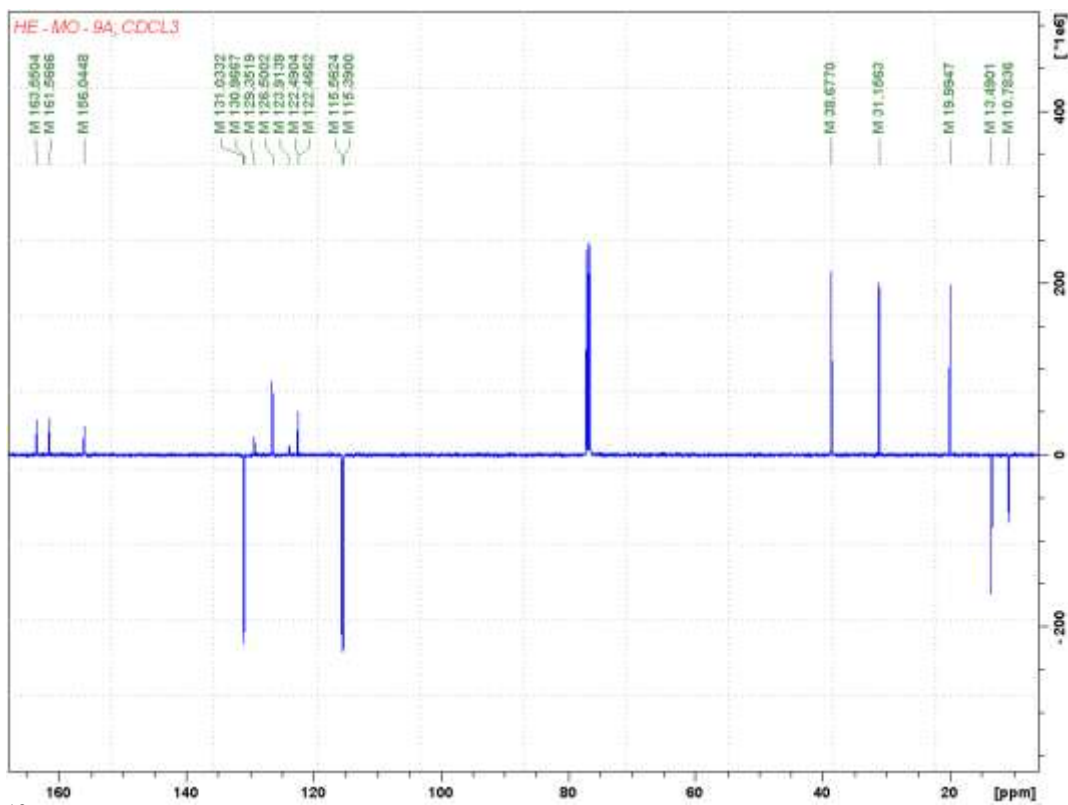
¹³C NMR spectrum of N-butyl-1-hydroxy-4,5,6,7-tetrahydro-1H-benzimidazole-2-carboxamide (**3b**).



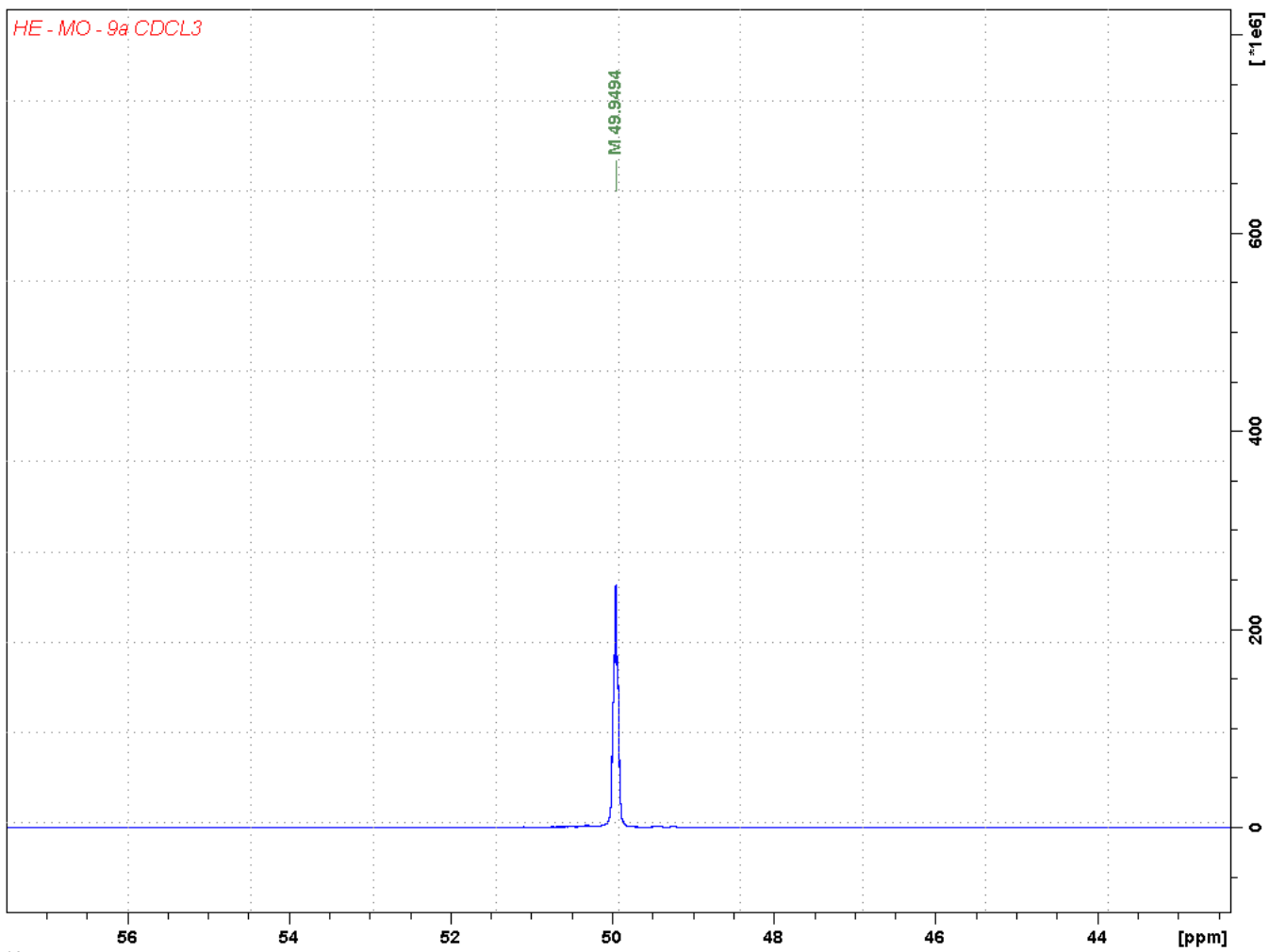
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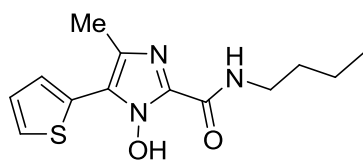
¹H NMR spectrum of N-butyl-5-(4-fluorophenyl)-1-hydroxy-4-methyl-1*H*-imidazole-2-carboxamide (**3c**).



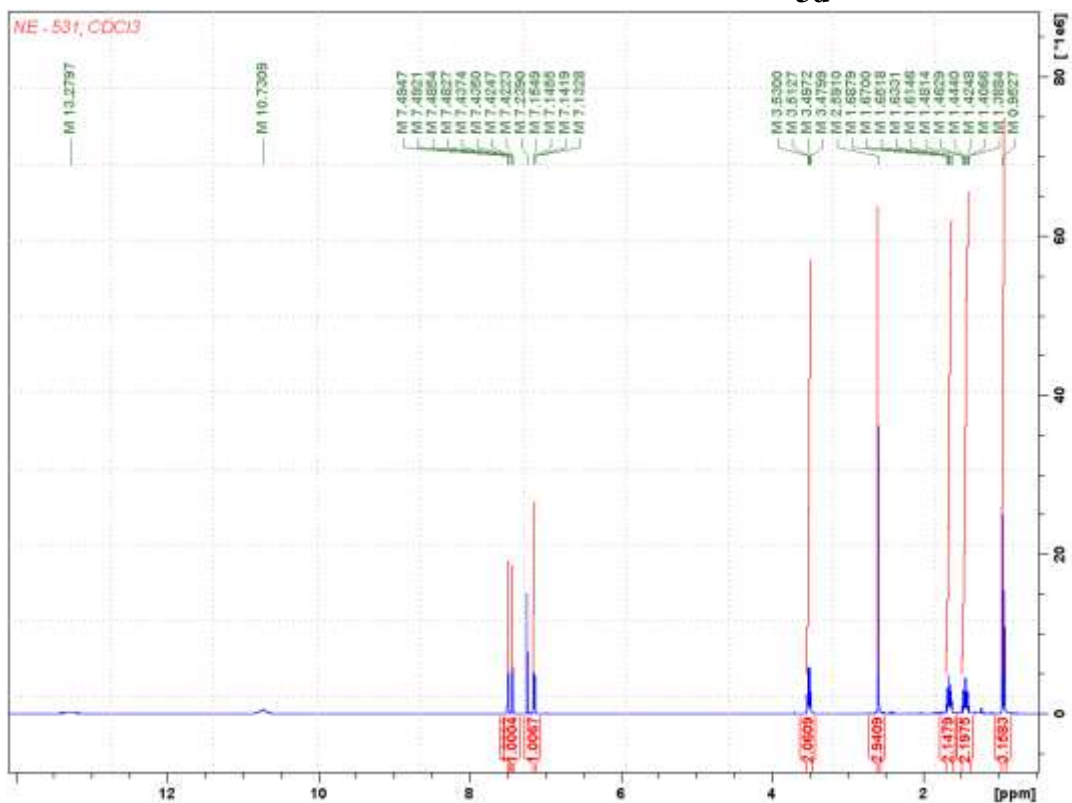
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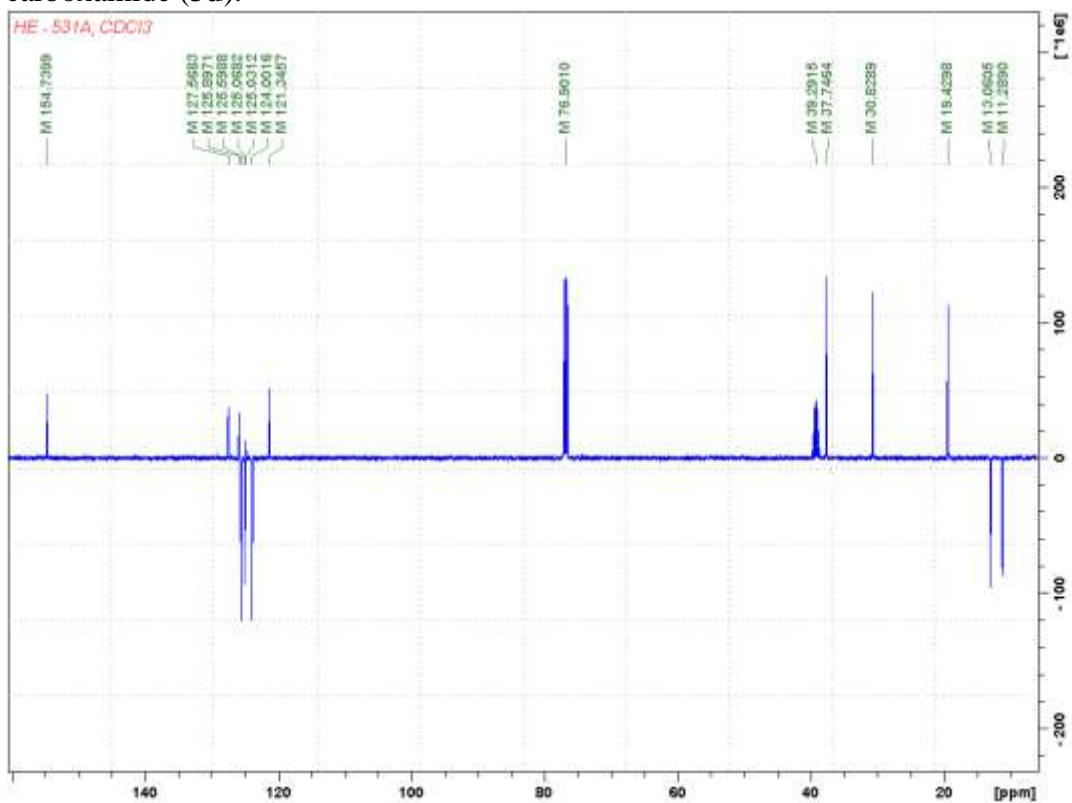
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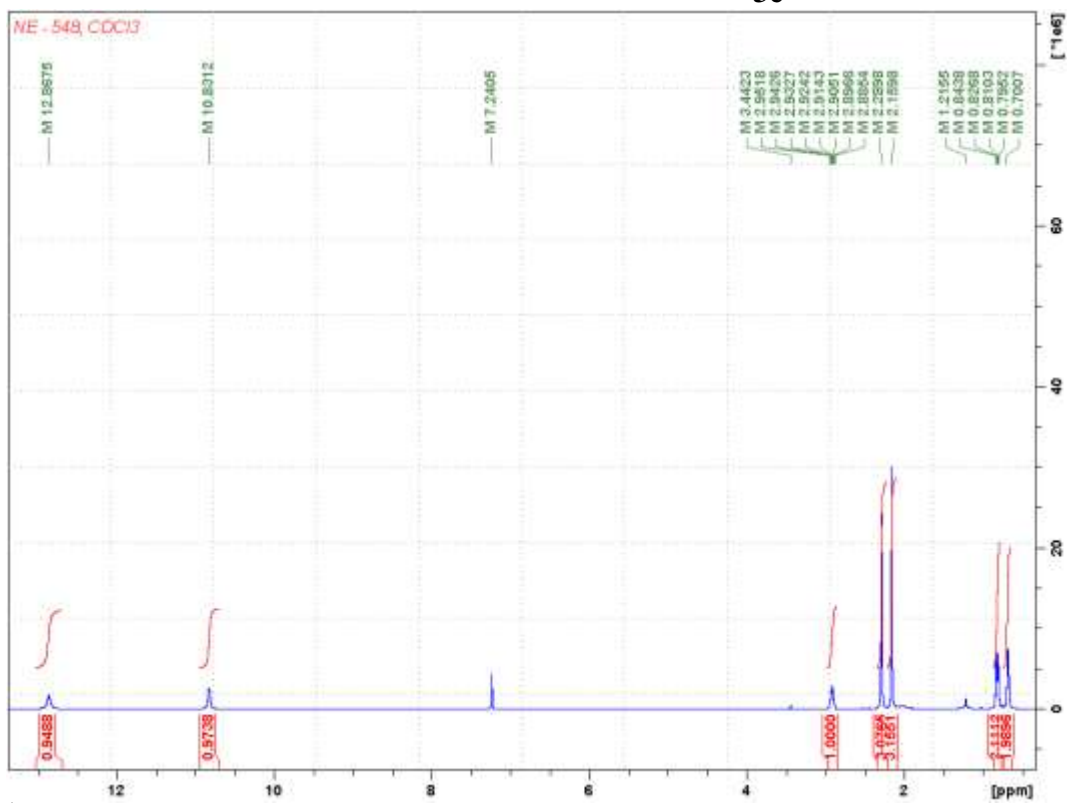
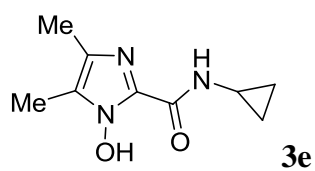
3d



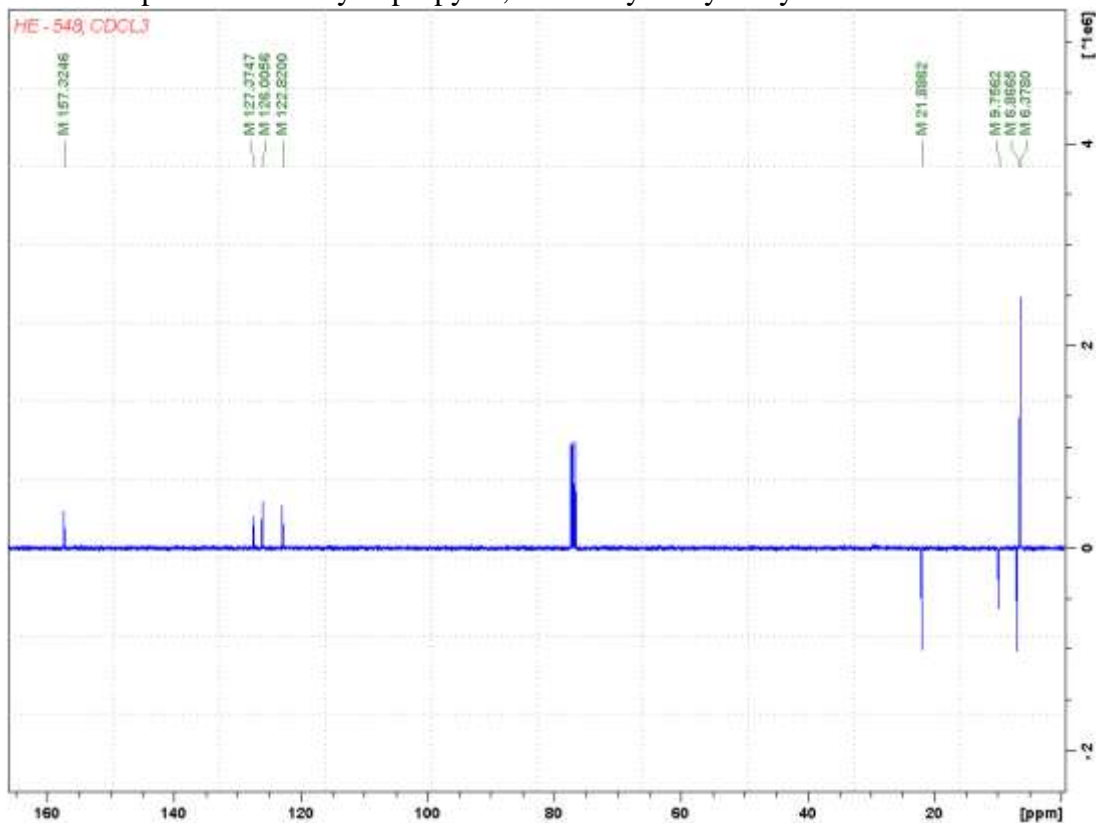
¹H NMR spectrum of N-butyl-1-hydroxy-4-methyl-5-(thiophen-2-yl)-1H-imidazole-2-carboxamide (**3d**).



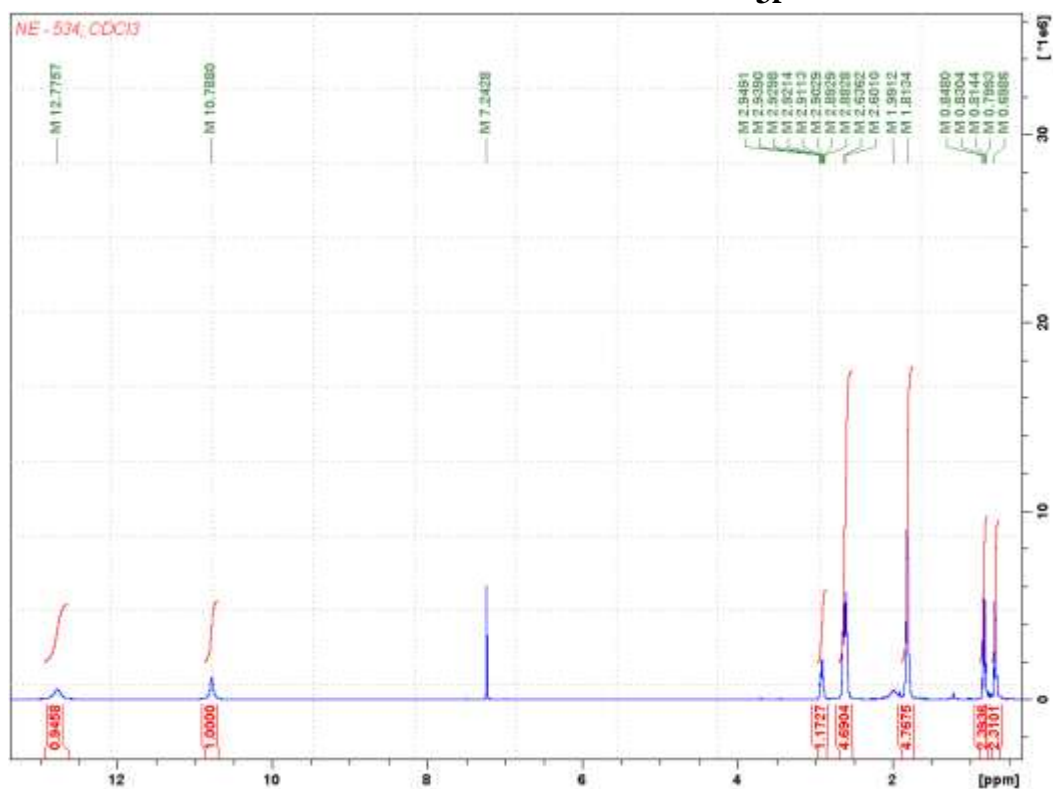
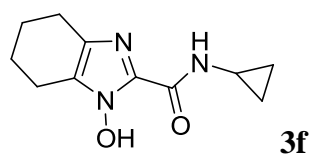
¹³C NMR spectrum of N-butyl-1-hydroxy-4-methyl-5-(thiophen-2-yl)-1H-imidazole-2-carboxamide (**3d**).



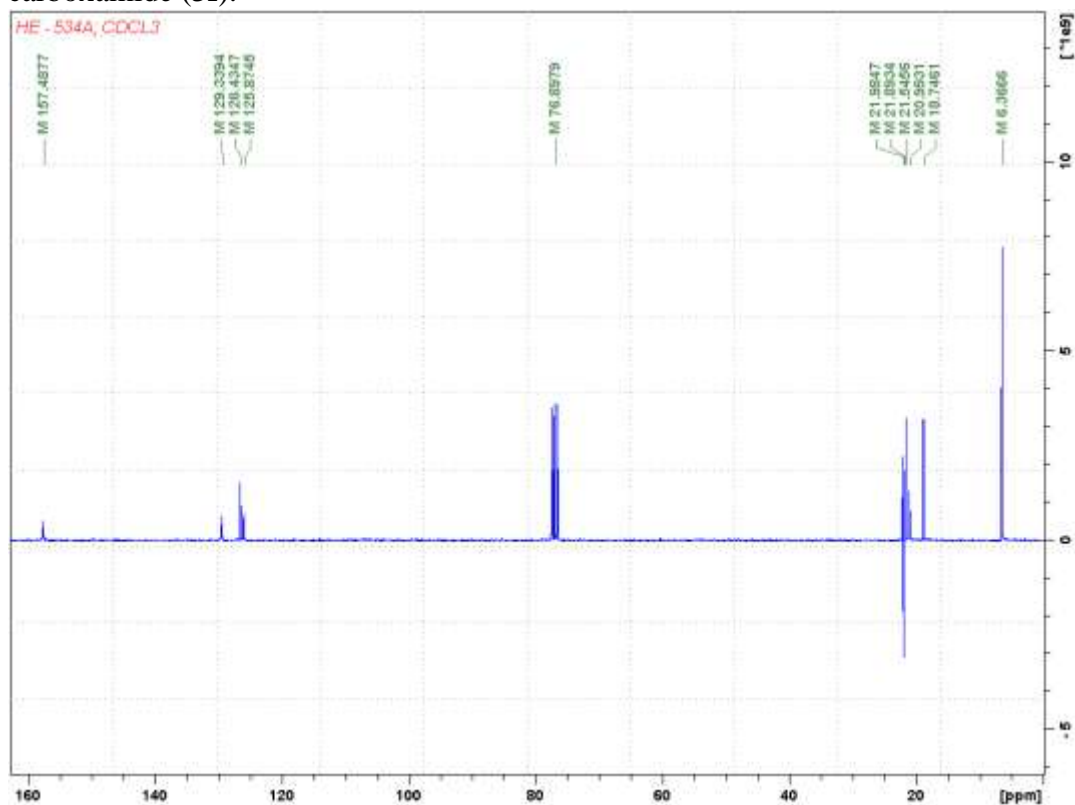
¹H NMR spectrum of N-cyclopropyl-4,5-dimethyl-1-hydroxy-1H-imidazole-2-carboxamide (**3e**).



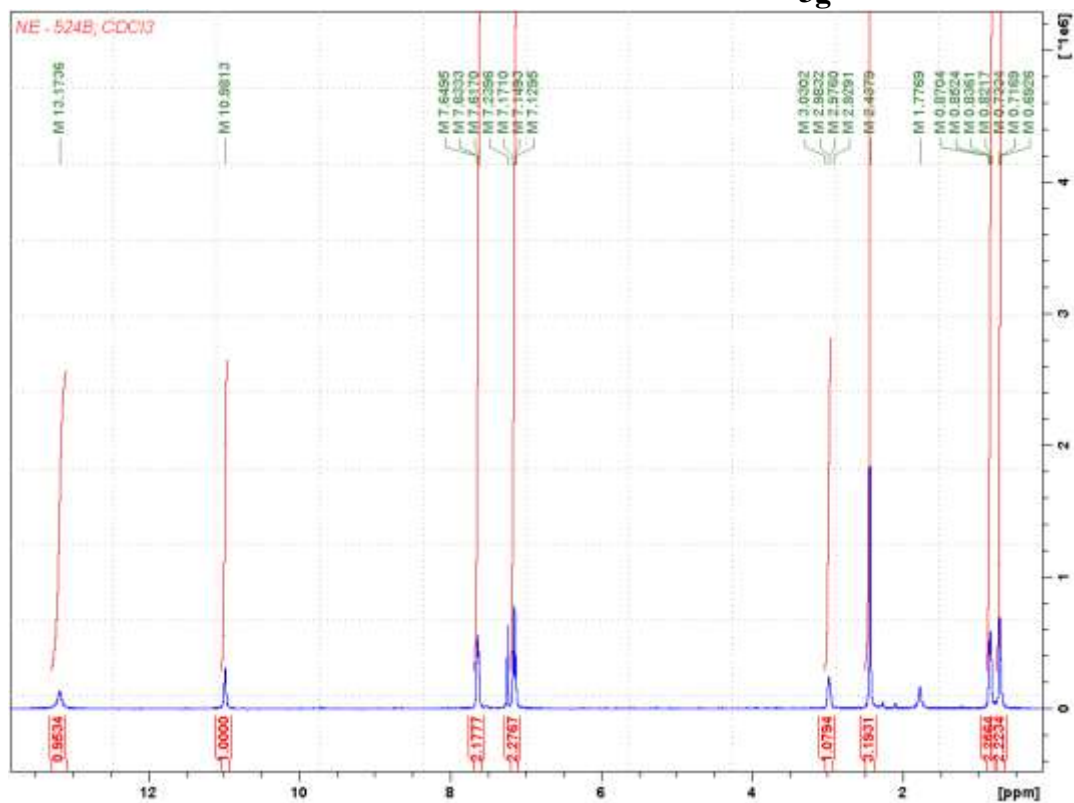
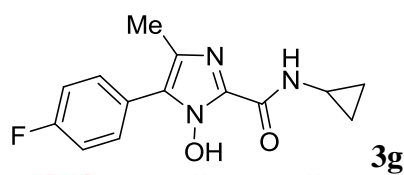
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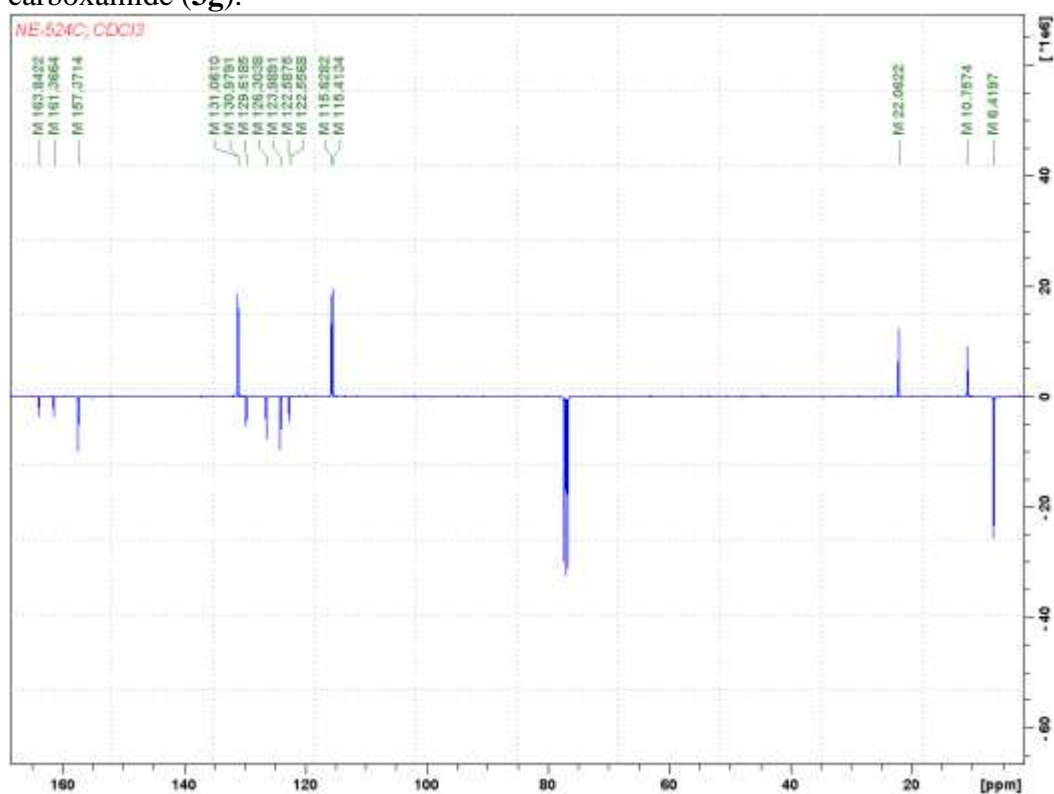
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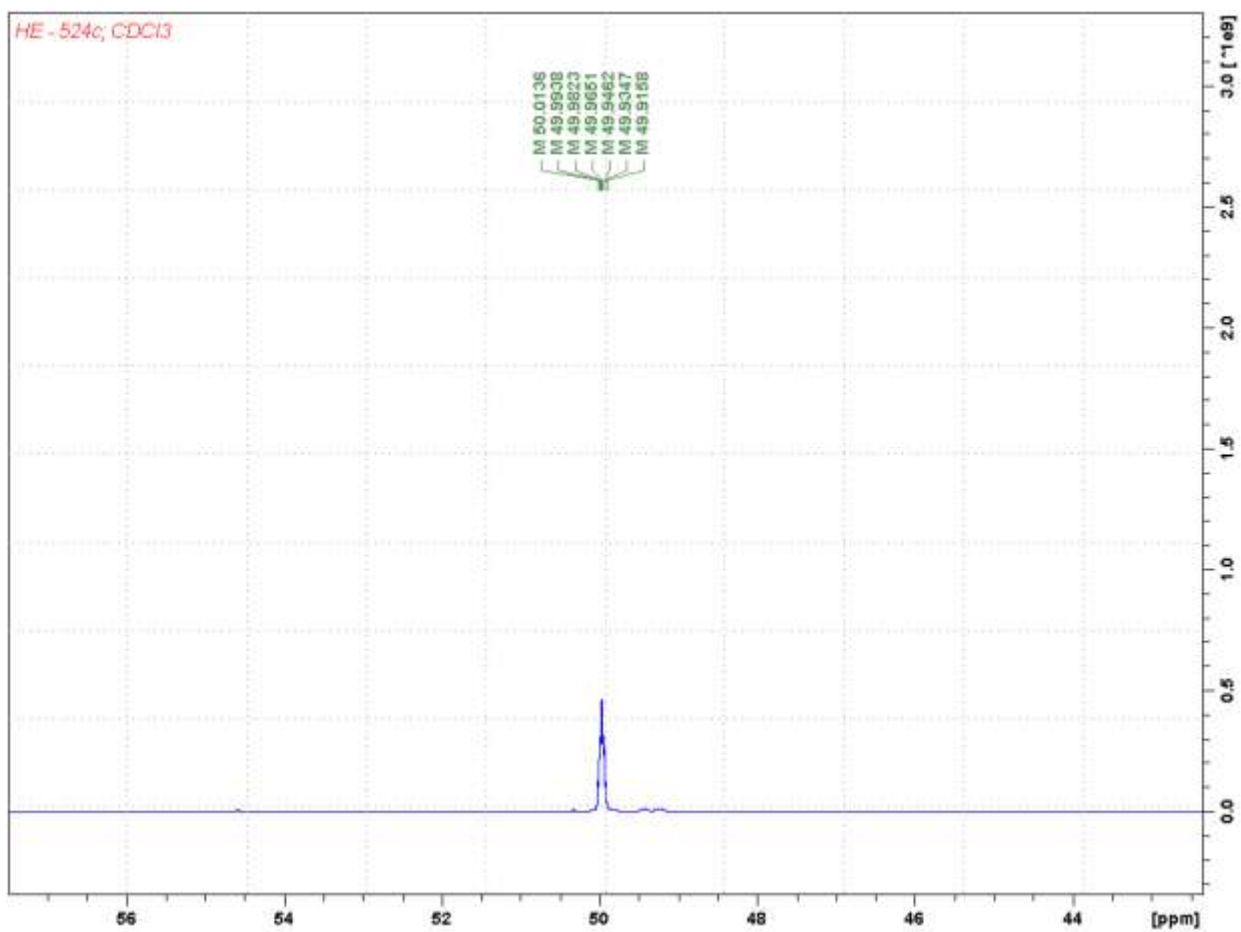
¹³C NMR spectrum of N-cyclopropyl-1-hydroxy-4,5,6,7-tetrahydro-1*H*-benzimidazole-2-carboxamide (**3f**).



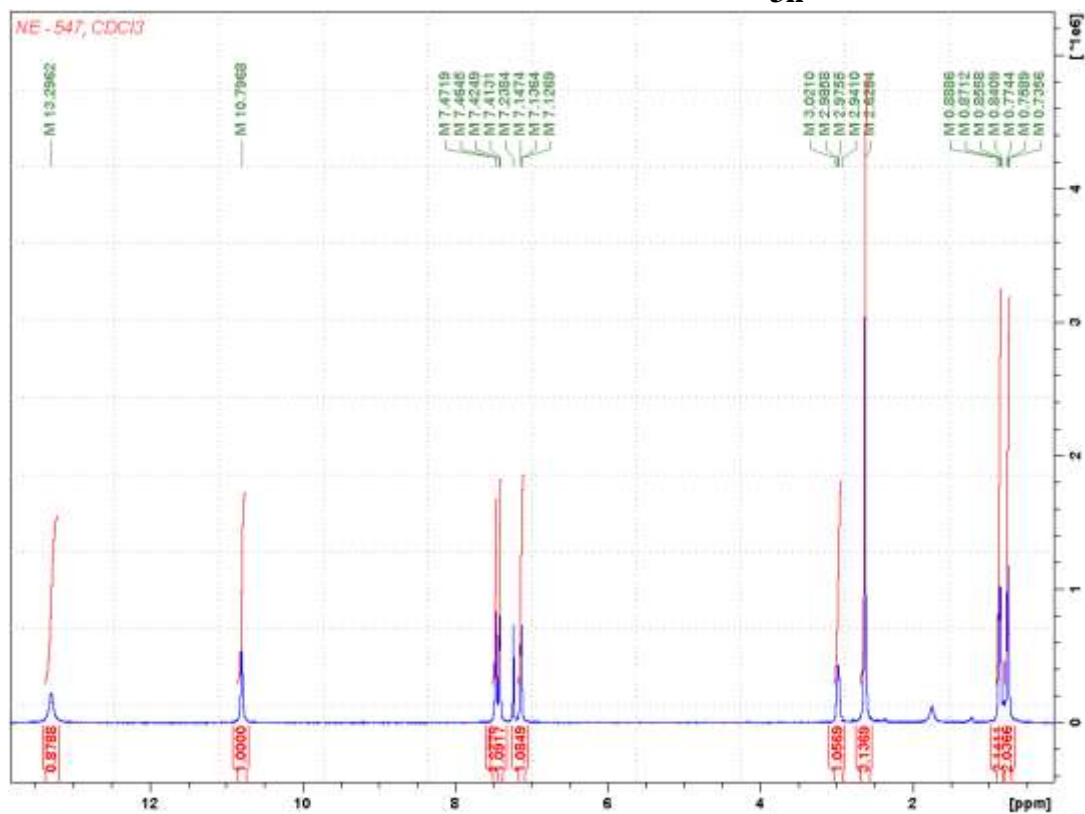
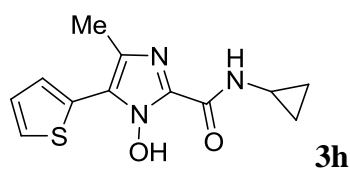
¹H NMR spectrum of N-cyclopropyl-5-(4-fluorophenyl)-1-hydroxy-4-methyl-1H-imidazole-2-carboxamide (**3g**).



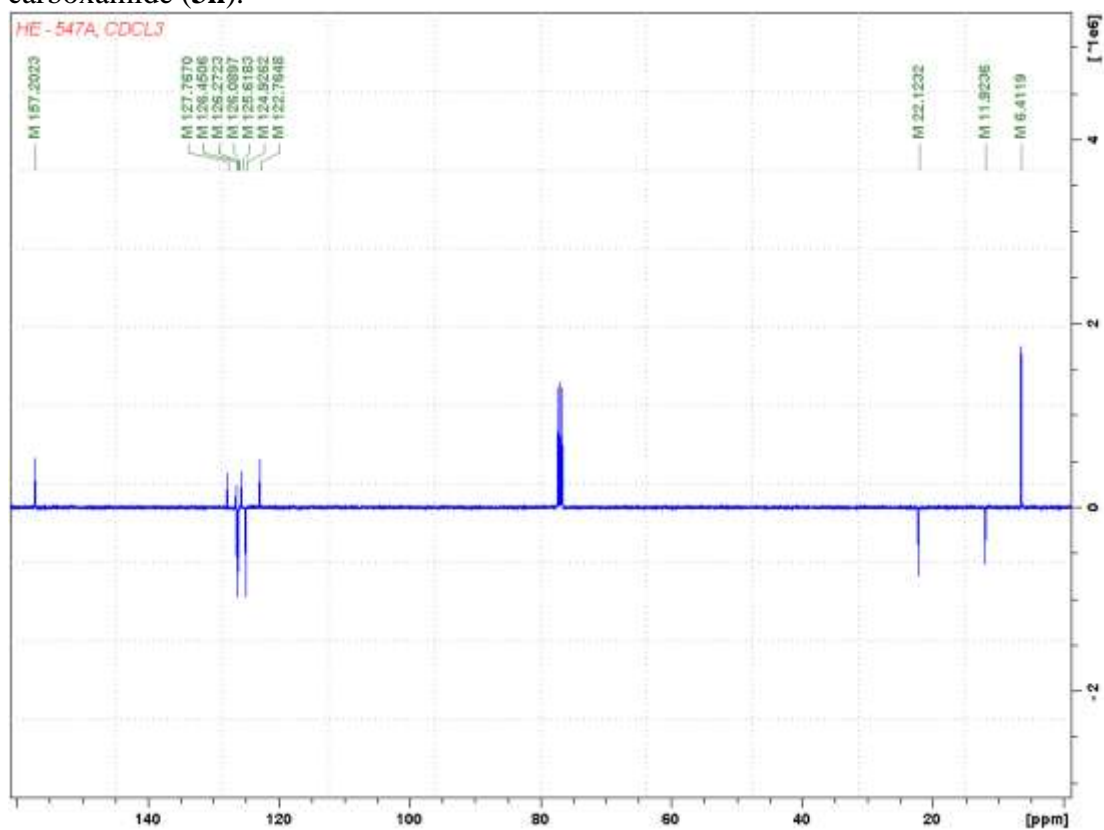
¹³C NMR spectrum of N-cyclopropyl-5-(4-fluorophenyl)-1-hydroxy-4-methyl-1H-imidazole-2-carboxamide (**3g**).



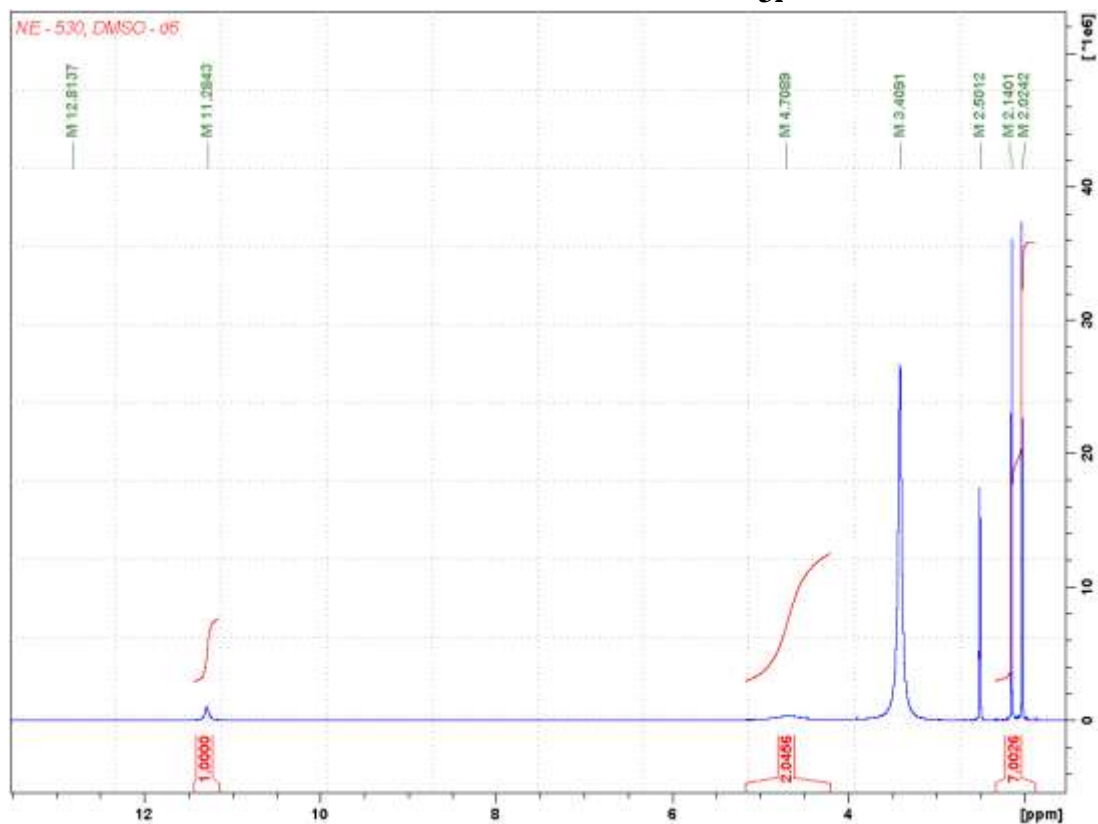
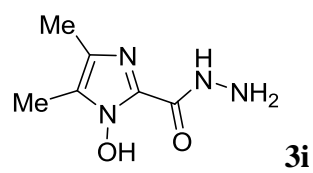
¹⁹F NMR spectrum of N-cyclopropyl-5-(4-fluorophenyl)-1-hydroxy-4-methyl-1*H*-imidazole-2-carboxamide (**3g**).



¹H NMR spectrum of N-cyclopropyl-1-hydroxy-4-methyl-5-(thiophen-2-yl)-1H-imidazole-2-carboxamide (**3h**).



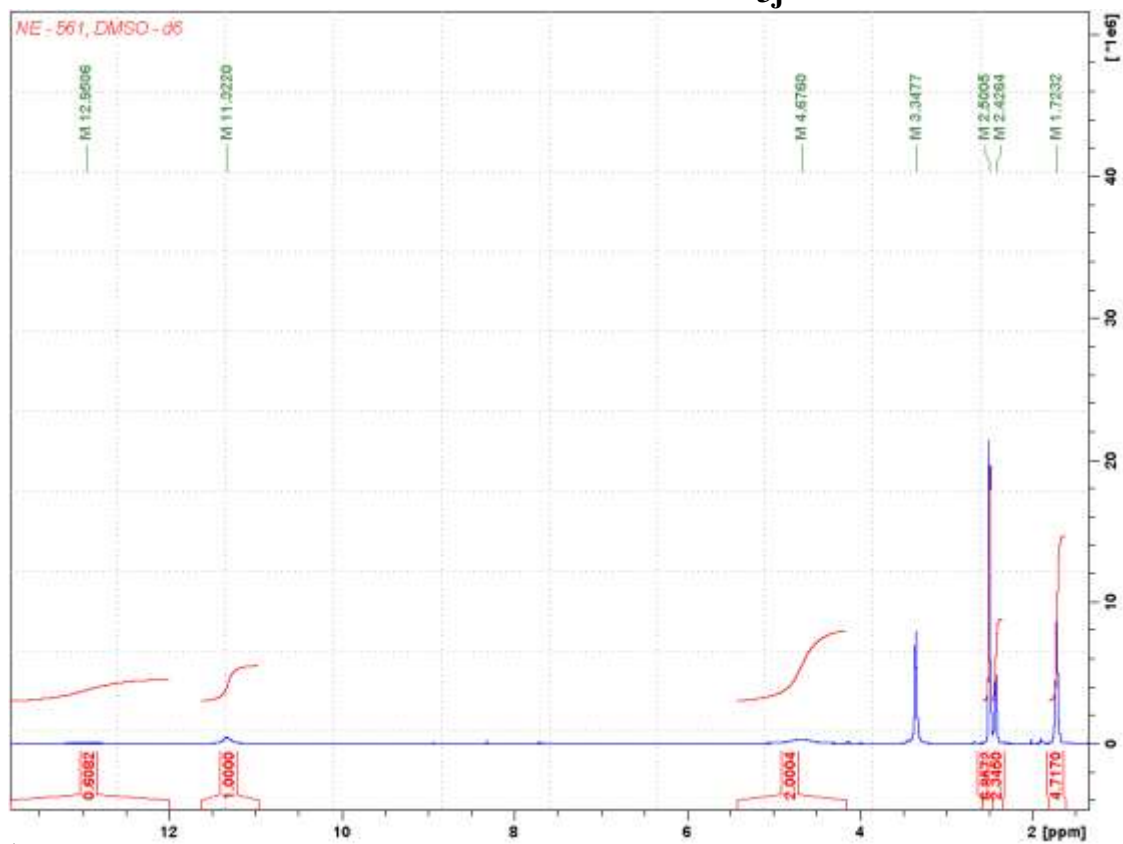
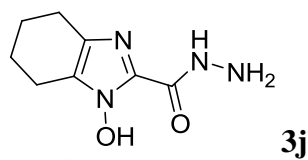
¹³C NMR spectrum of N-cyclopropyl-1-hydroxy-4-methyl-5-(thiophen-2-yl)-1H-imidazole-2-carboxamide (**3h**).



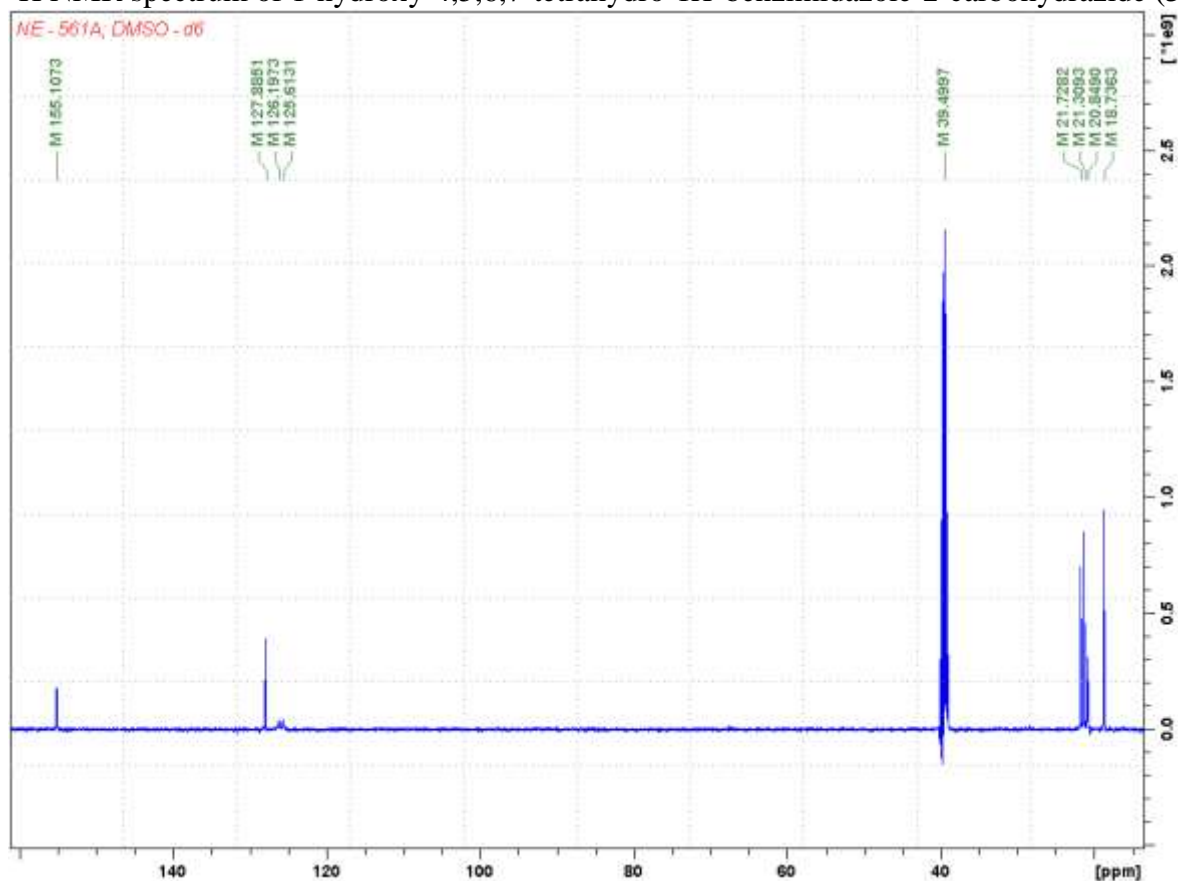
^1H NMR spectrum of 4,5-dimethyl-1-hydroxy-1*H*-imidazole-2-carbohydrazide (**3i**).



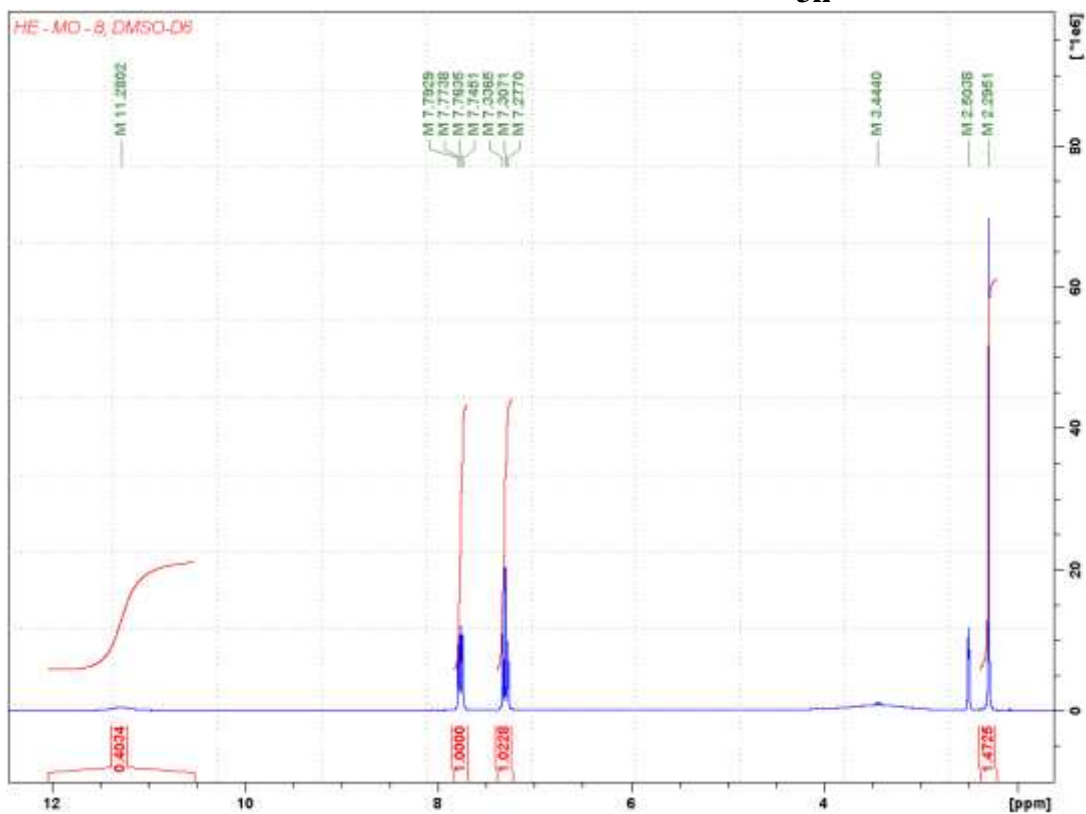
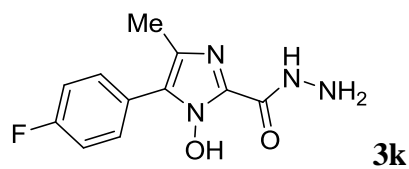
^{13}C NMR spectrum of 4,5-dimethyl-1-hydroxy-1*H*-imidazole-2-carbohydrazide (**3i**).



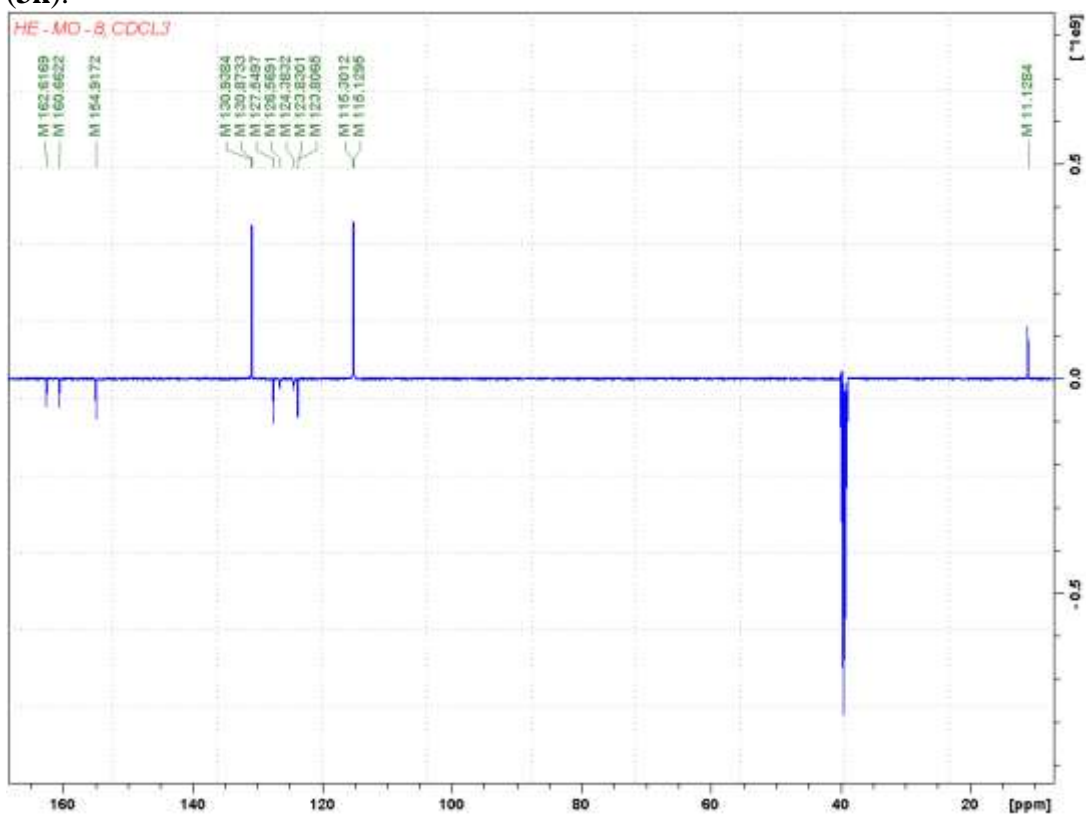
^1H NMR spectrum of 1-hydroxy-4,5,6,7-tetrahydro-1*H*-benzimidazole-2-carbohydrazide (**3j**).



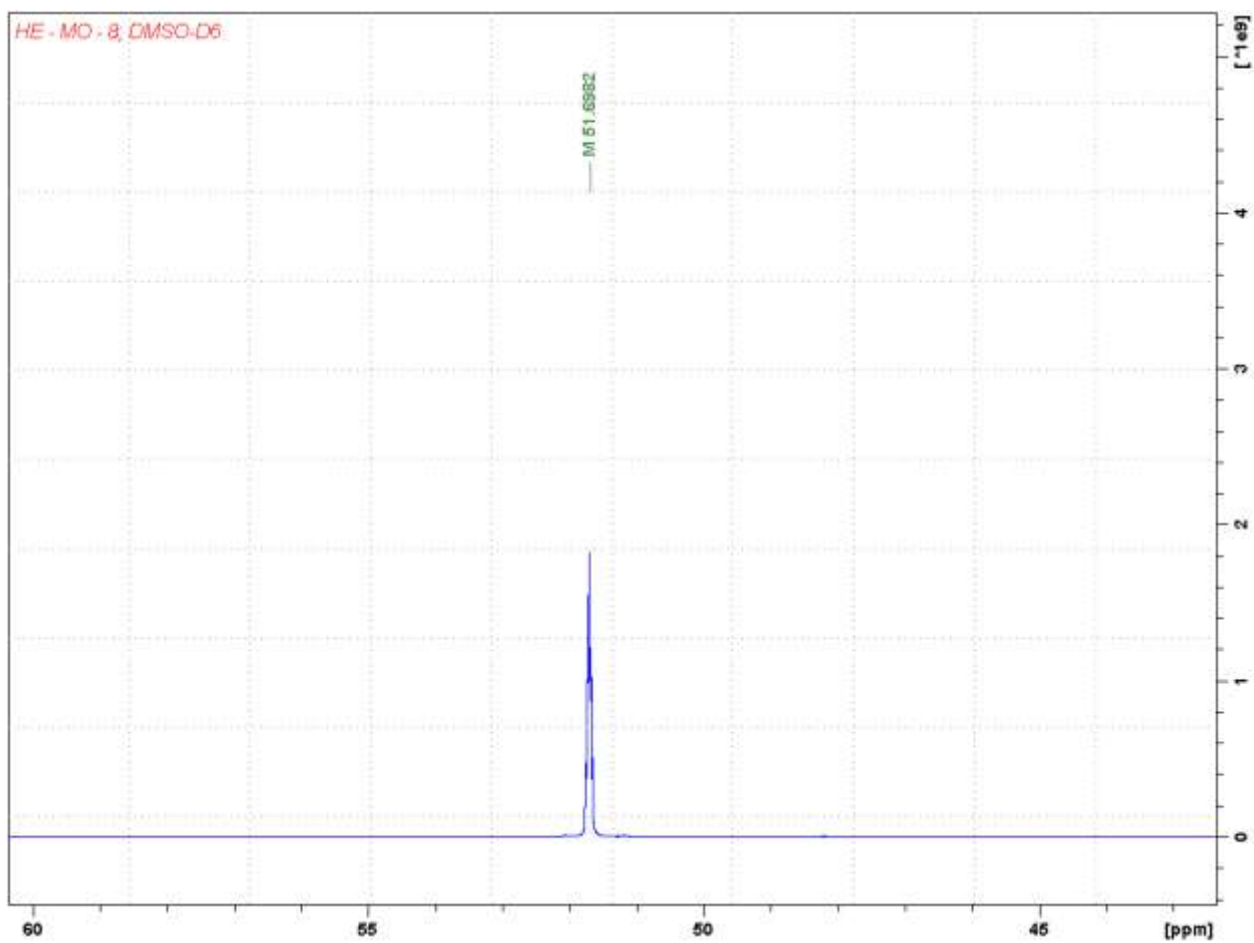
^{13}C NMR spectrum of 1-hydroxy-4,5,6,7-tetrahydro-1*H*-benzimidazole-2-carbohydrazide (**3j**).



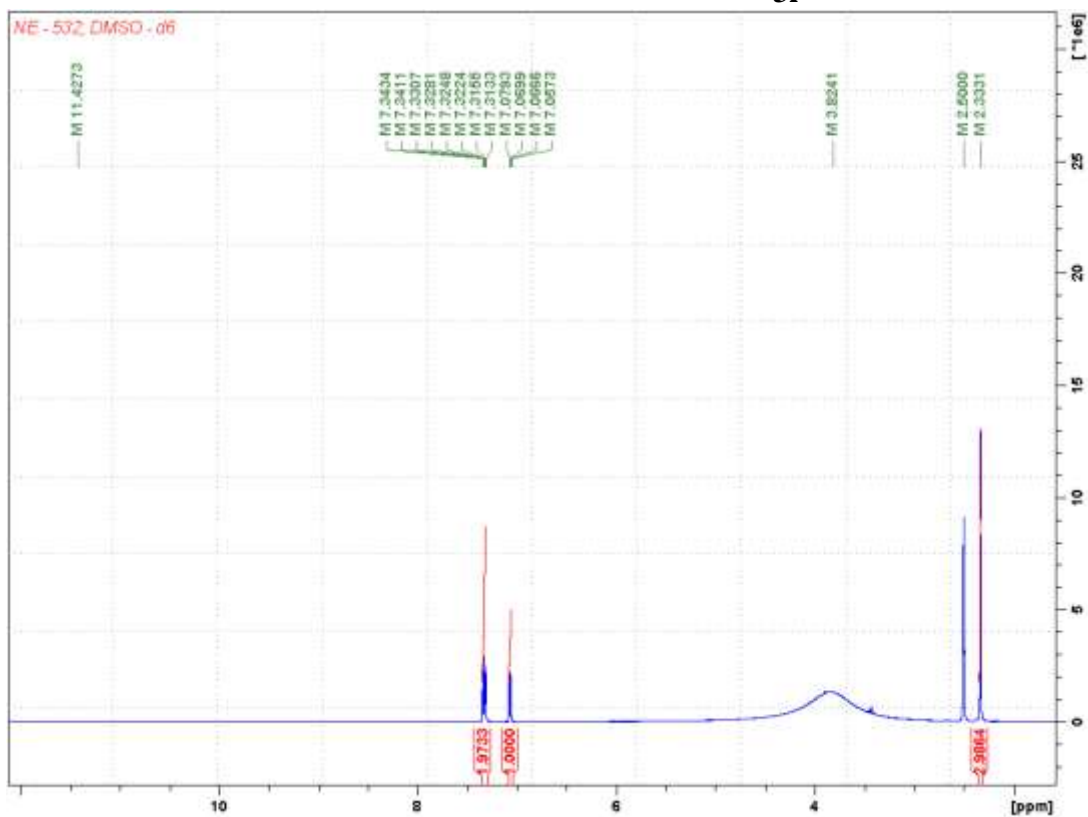
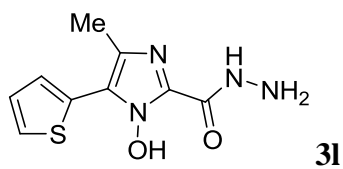
¹H NMR spectrum of 5-(4-fluorophenyl)-1-hydroxy-4-methyl-1*H*-imidazole-2-carbohydrazide (**3k**).



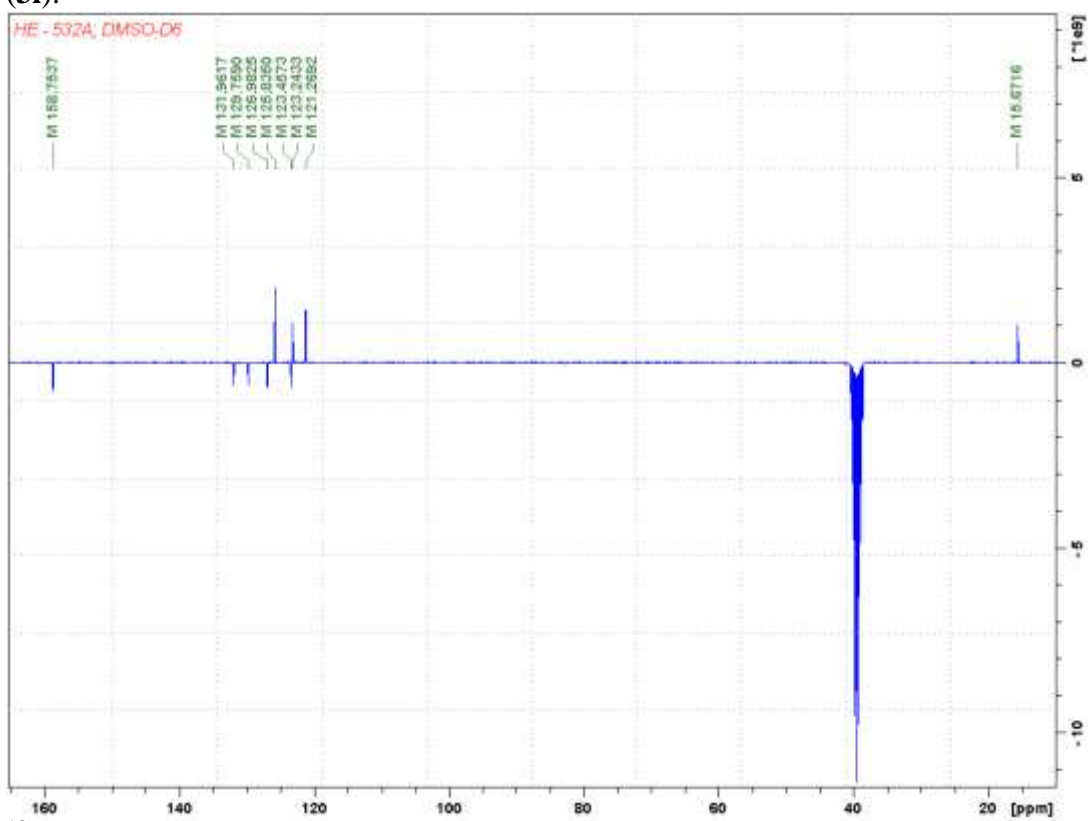
¹³C NMR spectrum of 5-(4-fluorophenyl)-1-hydroxy-4-methyl-1*H*-imidazole-2-carbohydrazide (**3k**).



^{19}F NMR spectrum of 5-(4-fluorophenyl)-1-hydroxy-4-methyl-1*H*-imidazole-2-carbohydrazide (**3k**).

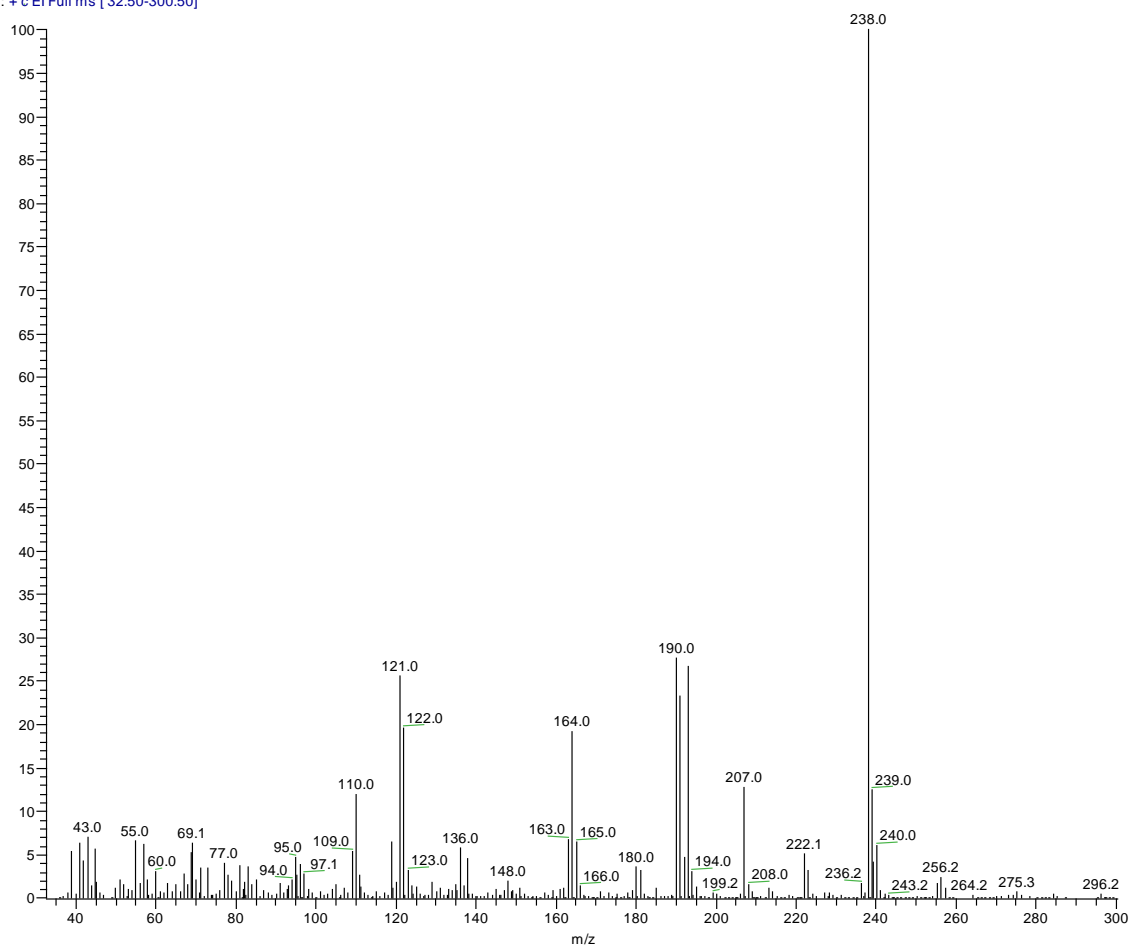


¹H NMR spectrum of 1-hydroxy-4-methyl-5-(thiophen-2-yl)-1*H*-imidazole-2-carbohydrazide (**31**).

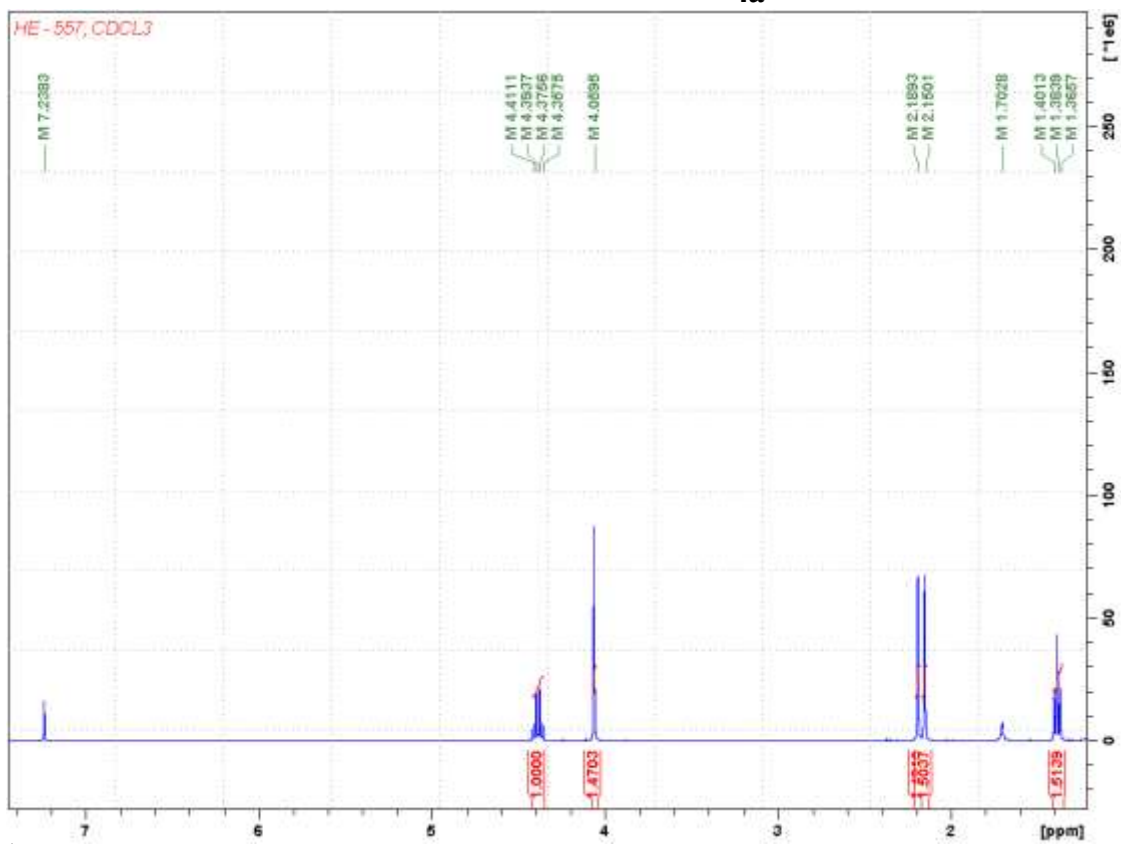
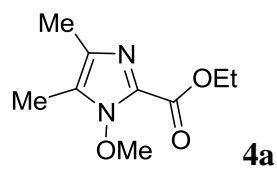


¹³C NMR spectrum of 1-hydroxy-4-methyl-5-(thiophen-2-yl)-1*H*-imidazole-2-carbohydrazide (**31**).

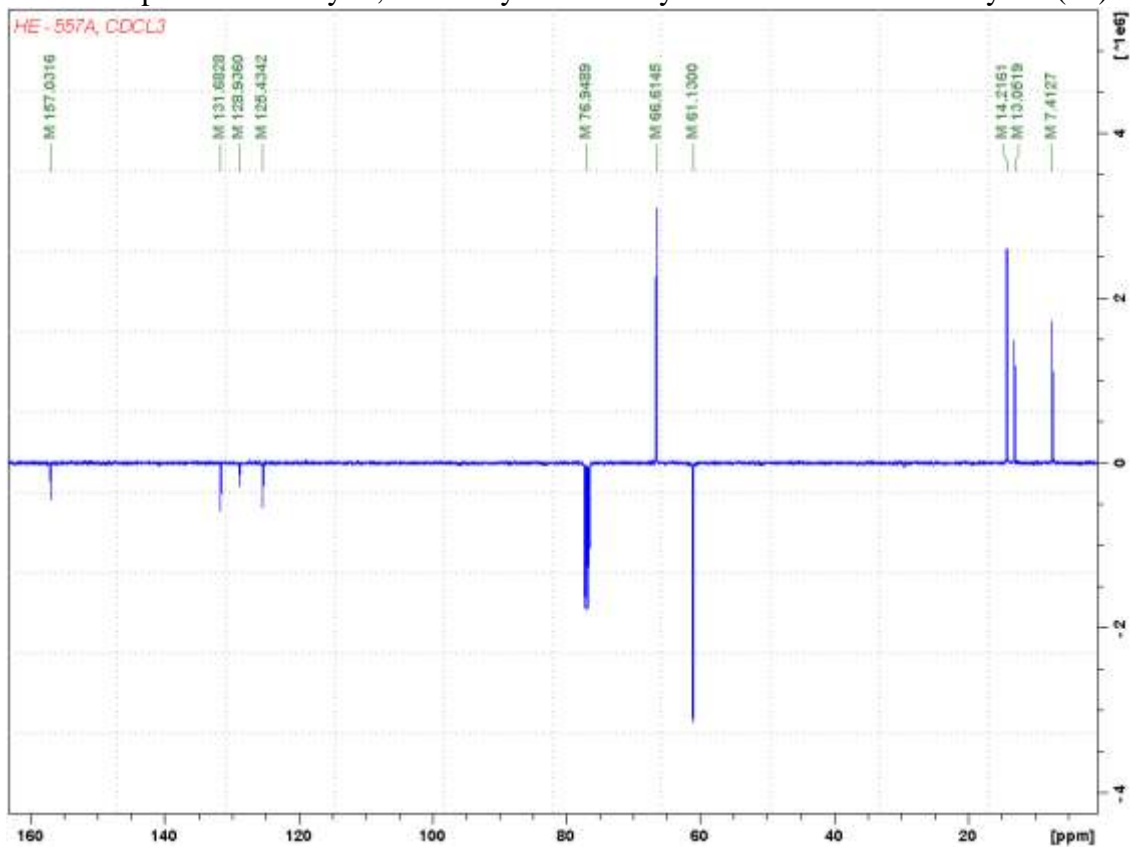
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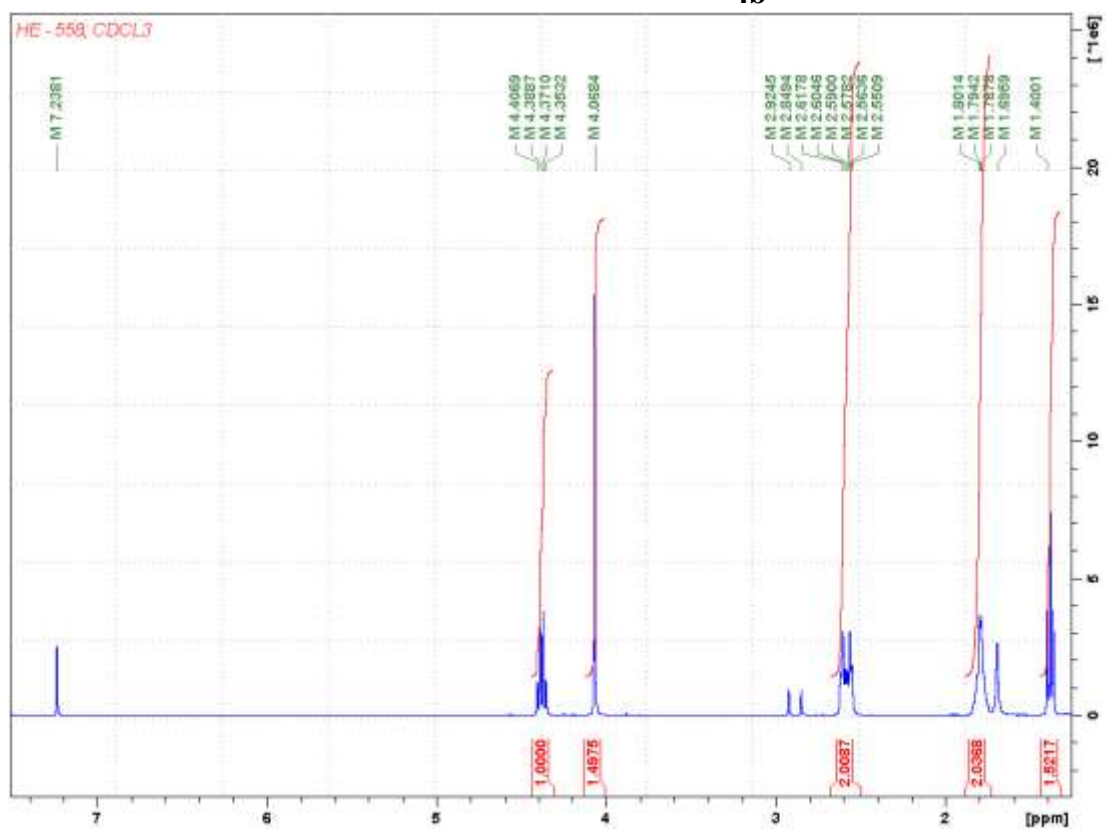
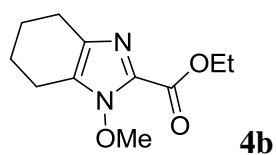
High-resolution mass spectrum of 1-hydroxy-4-methyl-5-(thiophen-2-yl)-1*H*-imidazole-2-carbohydrazide (**31**).



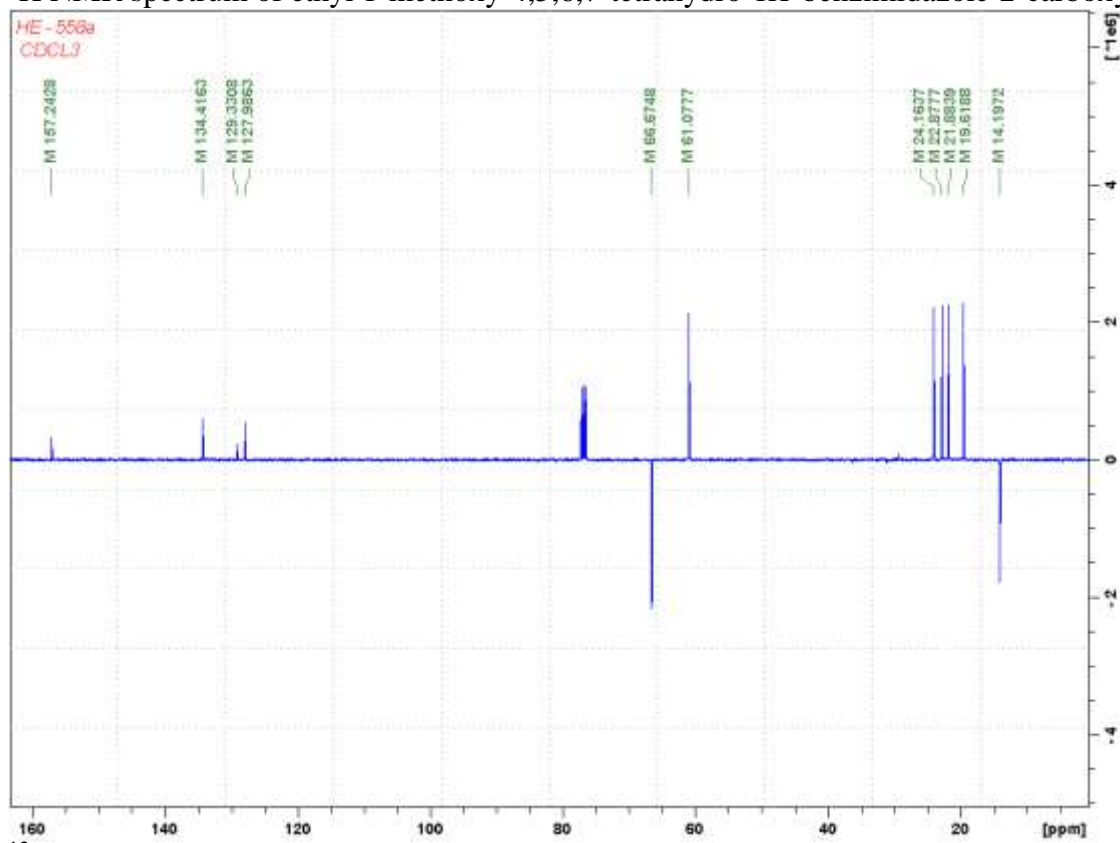
¹H NMR spectrum of ethyl 4,5-dimethyl-1-methoxy-1*H*-imidazole-2-carboxylate (**4a**).



¹³C NMR spectrum of ethyl 4,5-dimethyl-1-methoxy-1*H*-imidazole-2-carboxylate (**4a**).

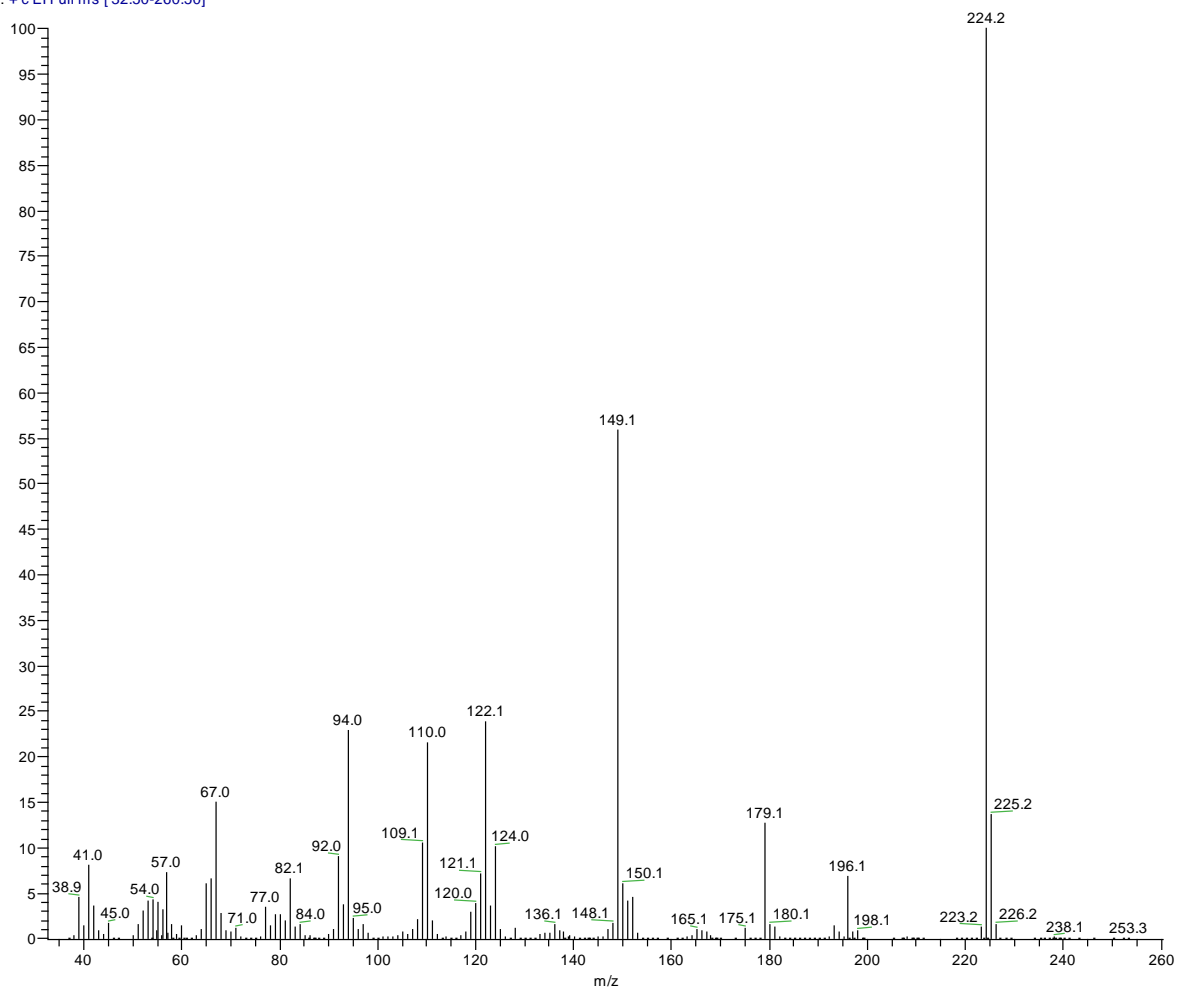


¹H NMR spectrum of ethyl 1-methoxy-4,5,6,7-tetrahydro-1H-benzimidazole-2-carboxylate (**4b**).

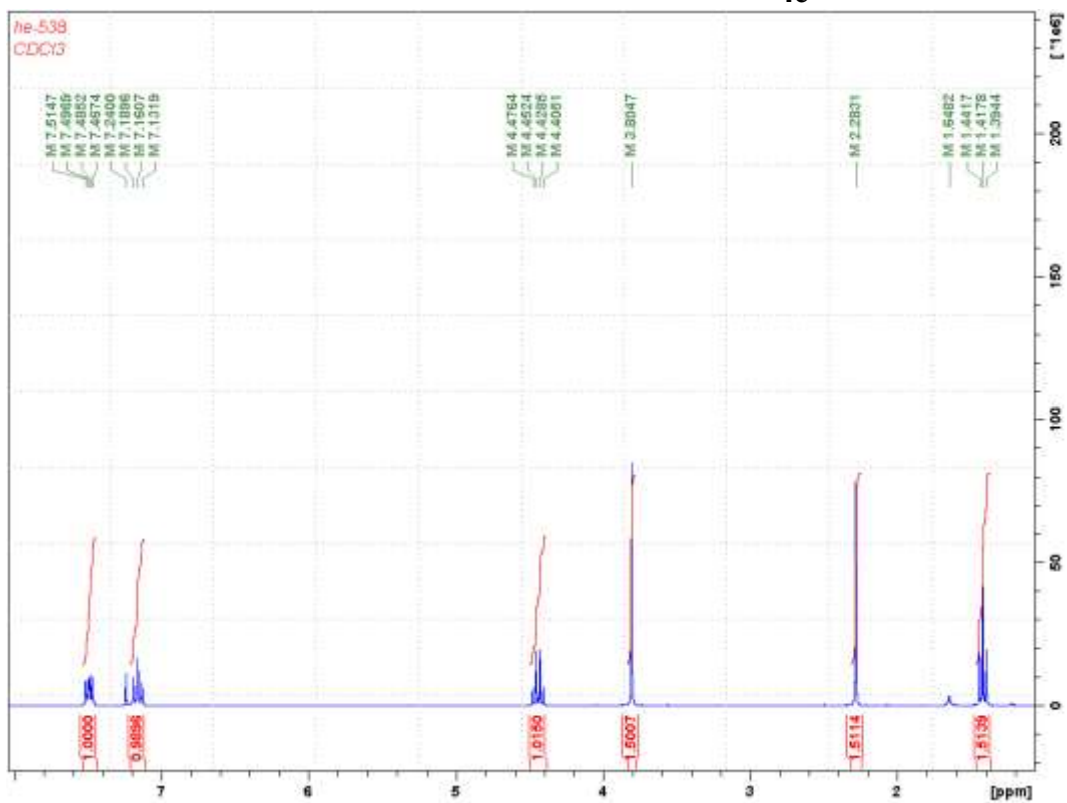
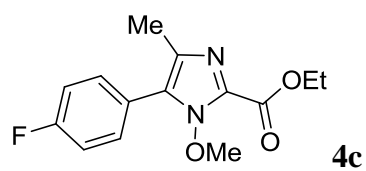


¹³C NMR spectrum of ethyl 1-methoxy-4,5,6,7-tetrahydro-1H-benzimidazole-2-carboxylate (**4b**).

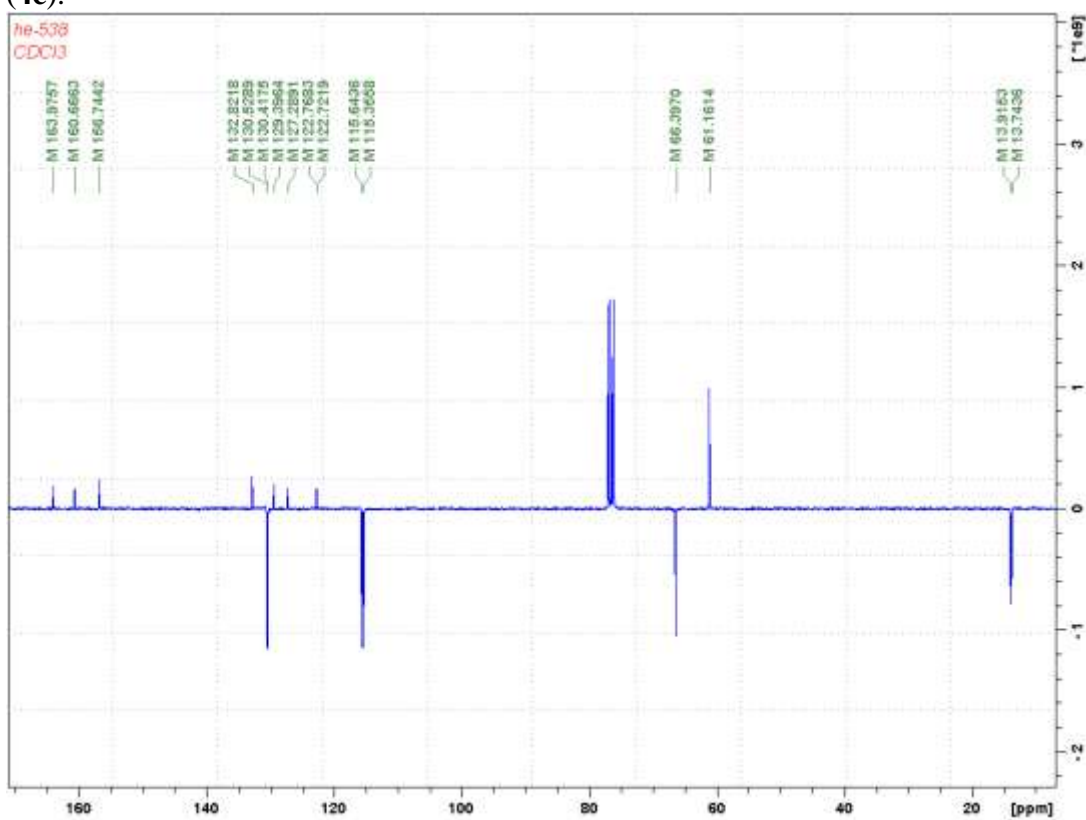
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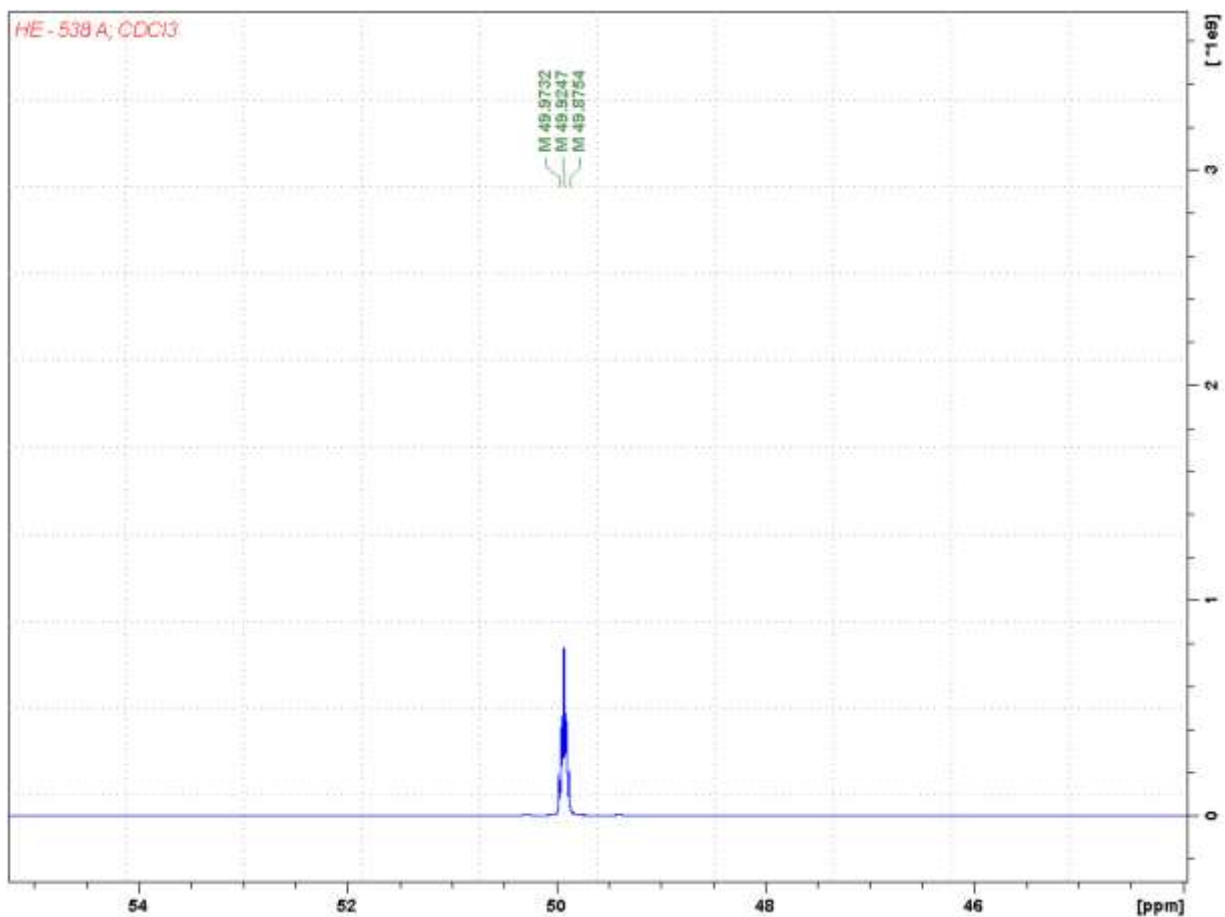
High-resolution mass-spectrum of ethyl 1-methoxy-4,5,6,7-tetrahydro-1*H*-benzimidazole-2-carboxylate (**4b**).



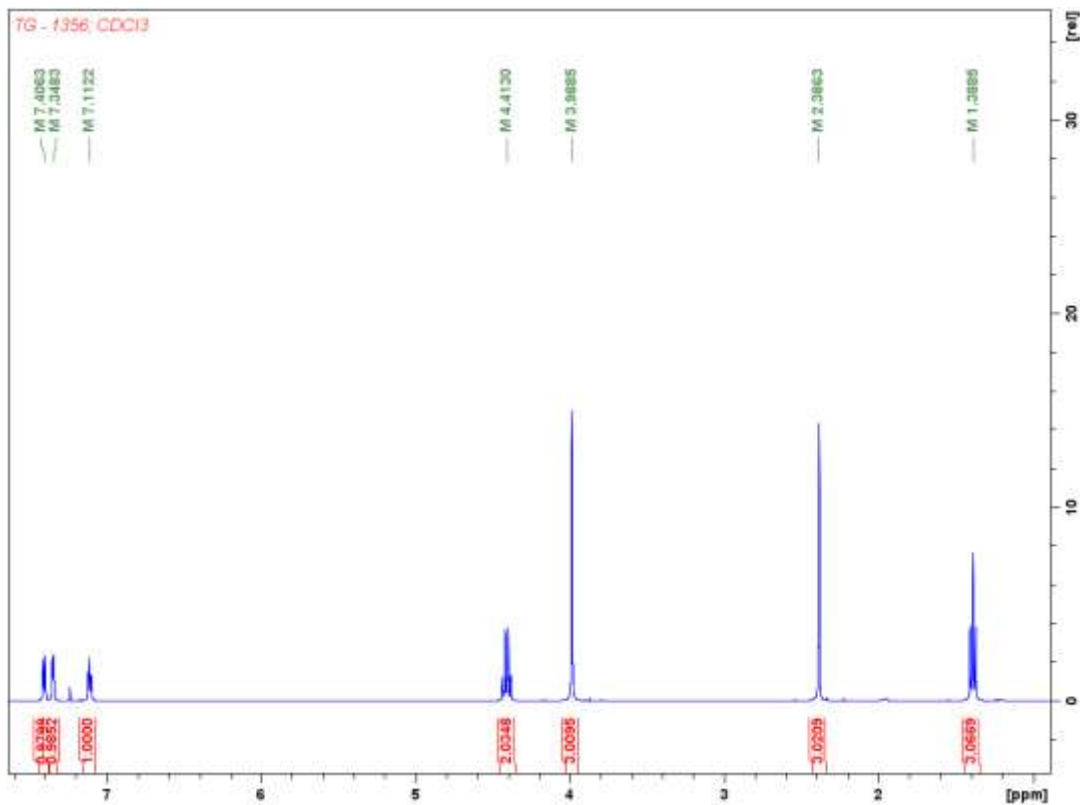
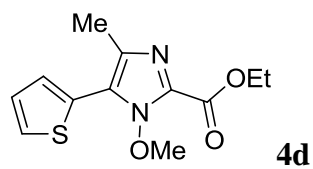
¹H NMR spectrum of ethyl 5-(4-fluorophenyl)-1-methoxy-4-methyl-1*H*-imidazole-2-carboxylate (**4c**).



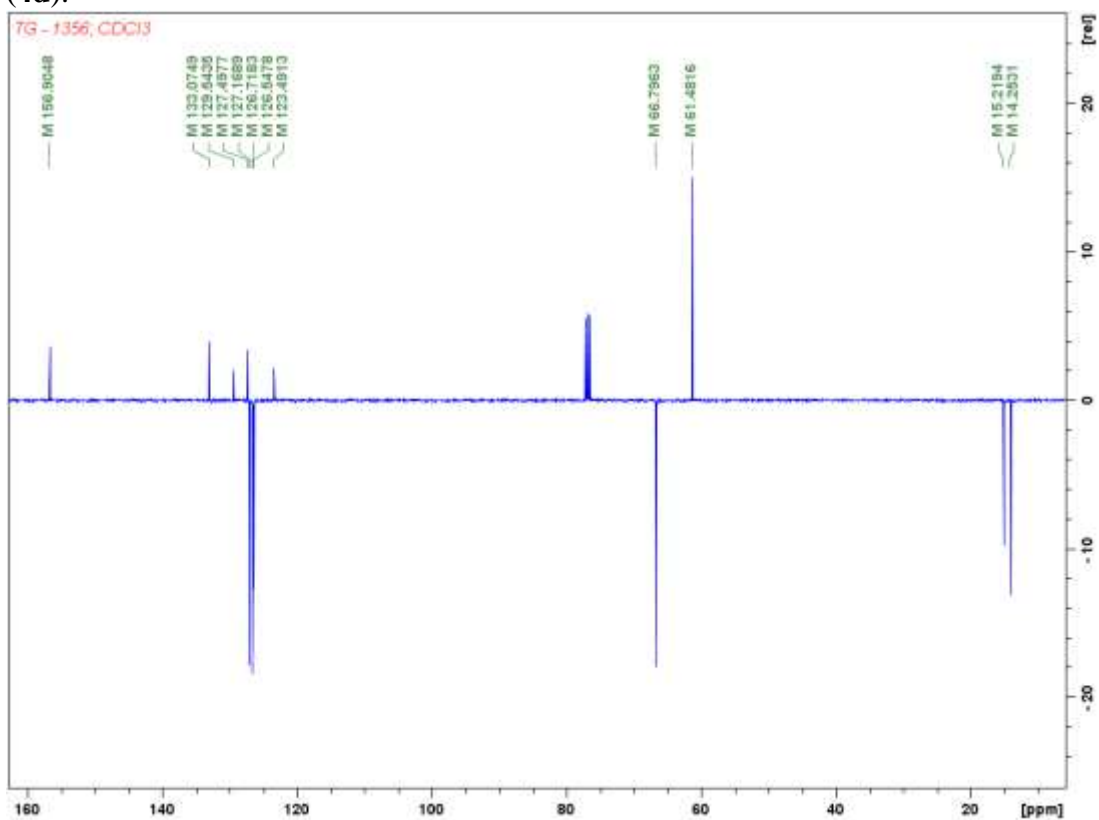
¹³C NMR spectrum of ethyl 5-(4-fluorophenyl)-1-methoxy-4-methyl-1*H*-imidazole-2-carboxylate (**4c**).



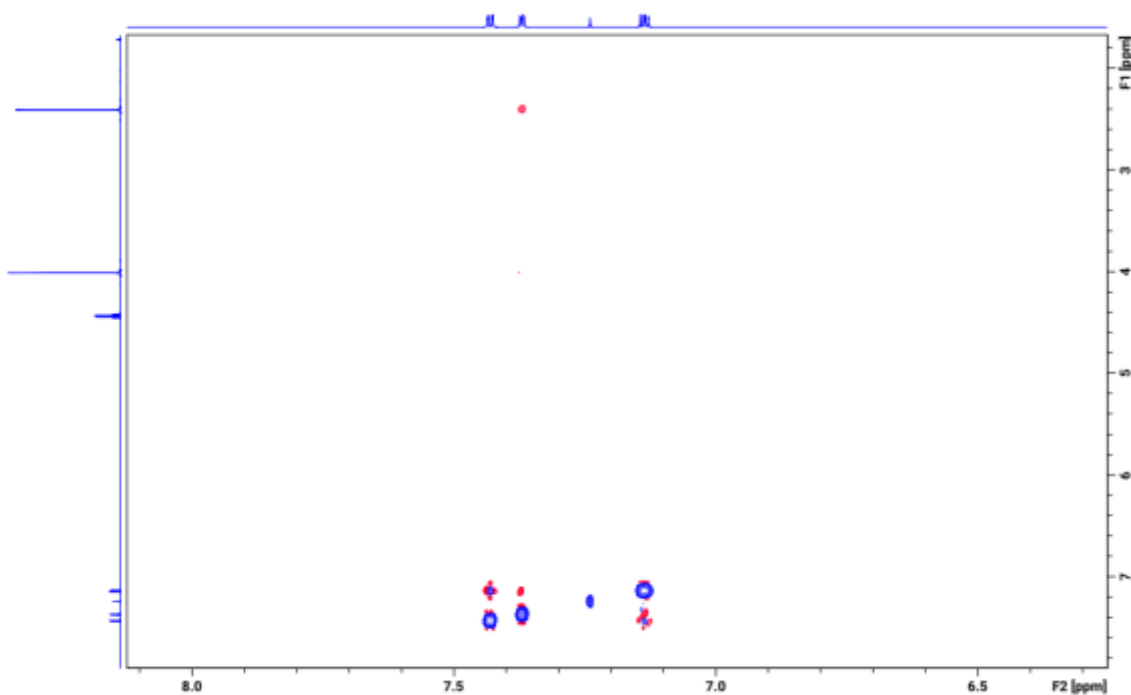
¹⁹F NMR spectrum of ethyl 5-(4-fluorophenyl)-1-methoxy-4-methyl-1*H*-imidazole-2-carboxylate (**4c**).



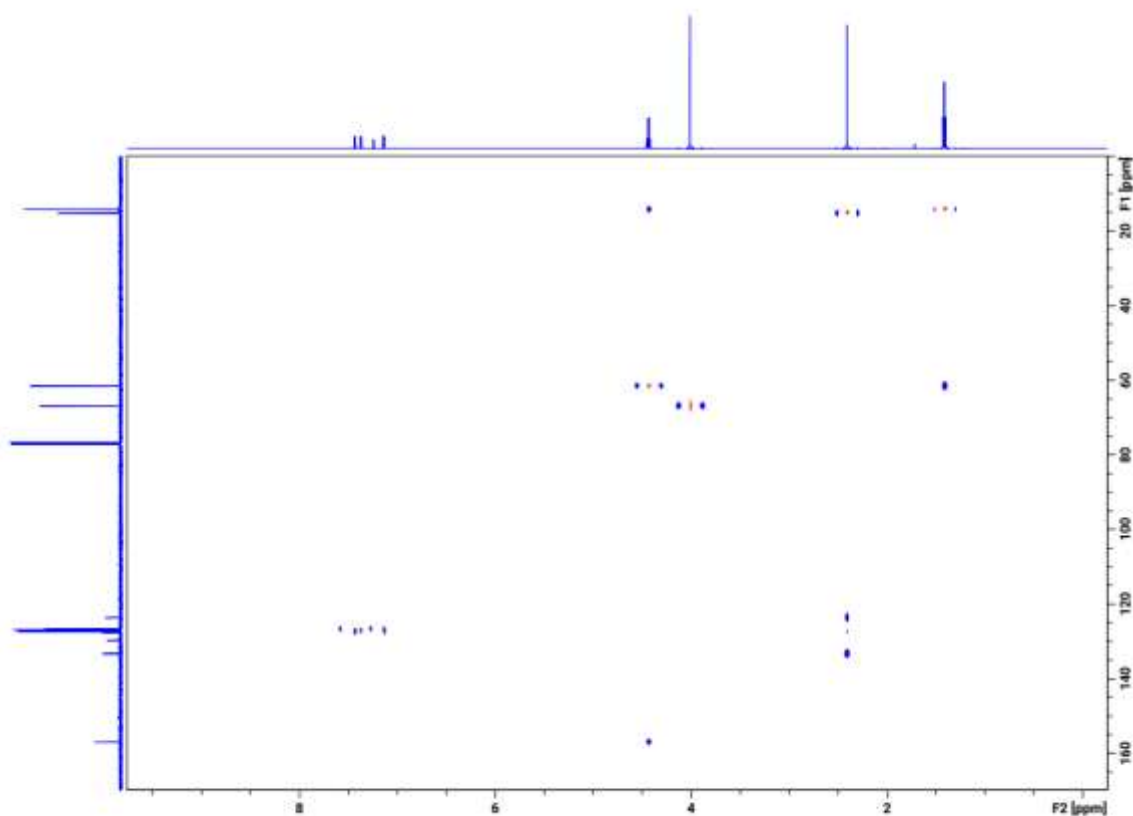
¹H NMR spectrum of ethyl 1-methoxy-4-methyl-5-(thiophen-2-yl)-1*H*-imidazole-2-carboxylate (**4d**).



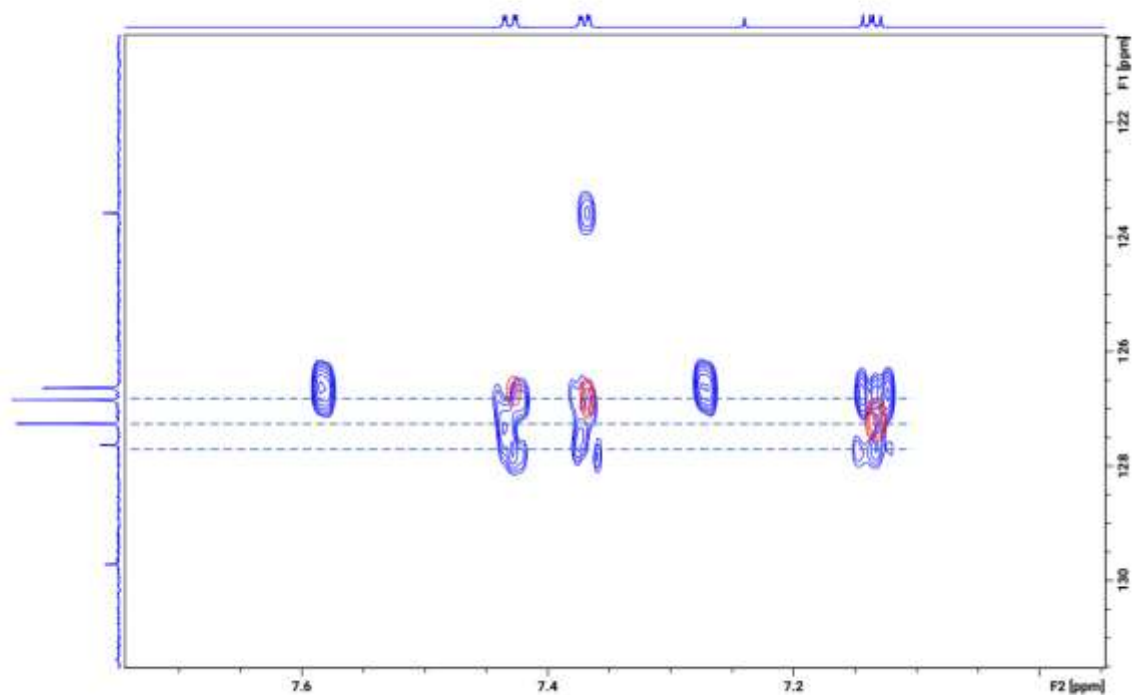
¹³C NMR spectrum of ethyl 1-methoxy-4-methyl-5-(thiophen-2-yl)-1*H*-imidazole-2-carboxylate (**4d**).



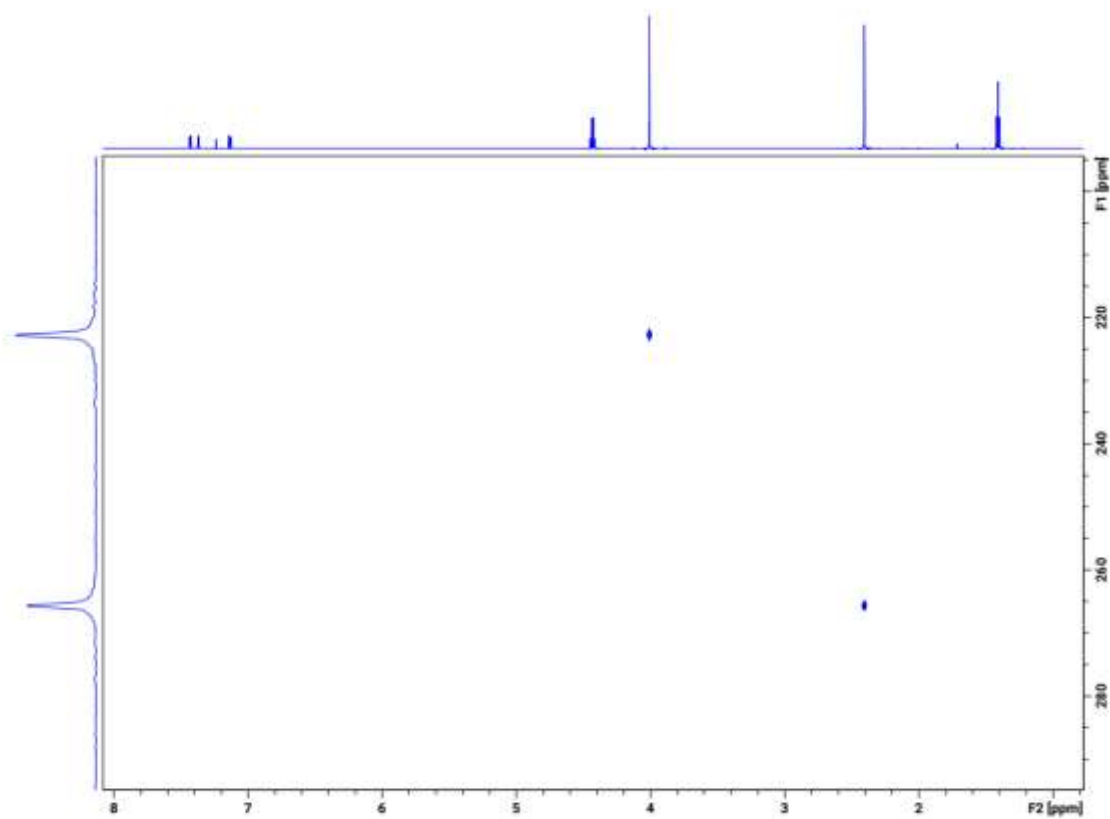
A part of ^1H - ^1H NOESY spectrum of ethyl 1-methoxy-4-methyl-5-(thiophen-2-yl)-1*H*-imidazole-2-carboxylate (**4d**).



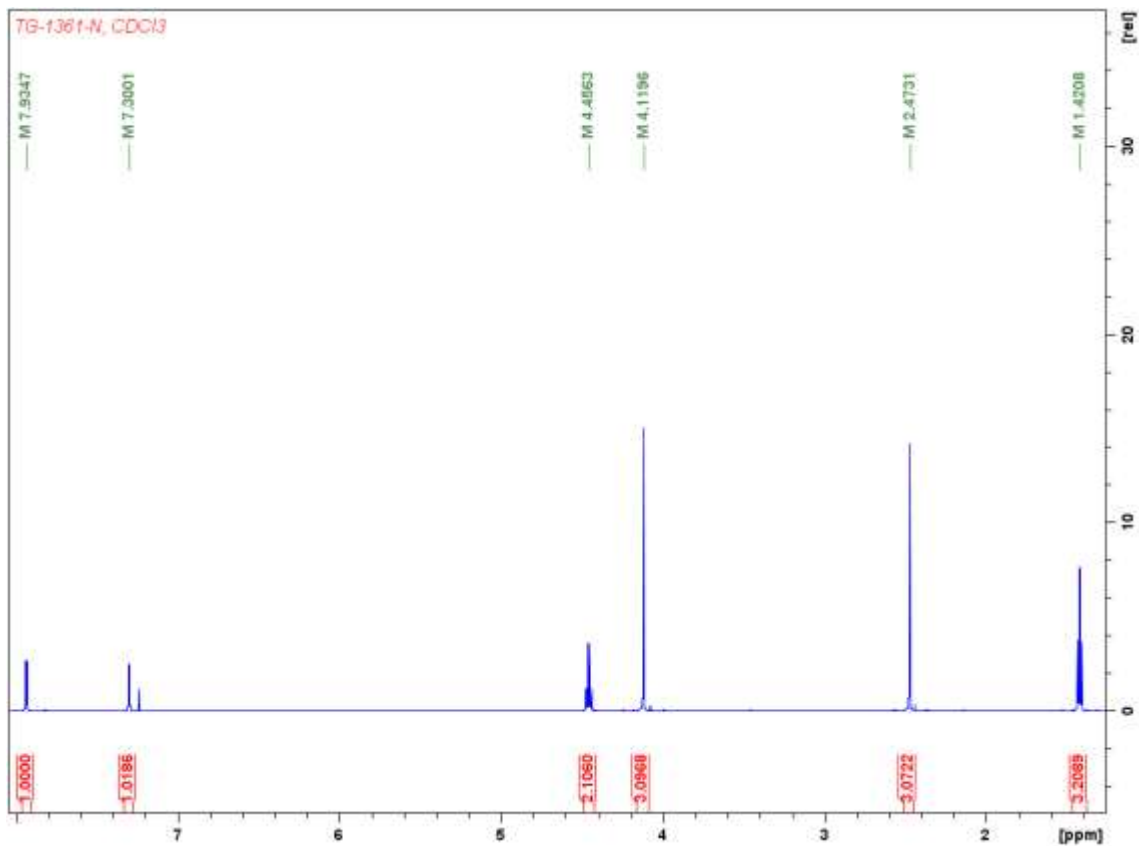
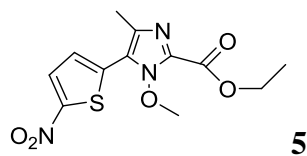
^1H - ^{13}C HSQC (red contour lines) and ^1H - ^{13}C HMBC (blue contour lines) spectra of ethyl 1-methoxy-4-methyl-5-(thiophen-2-yl)-1*H*-imidazole-2-carboxylate (**4d**).



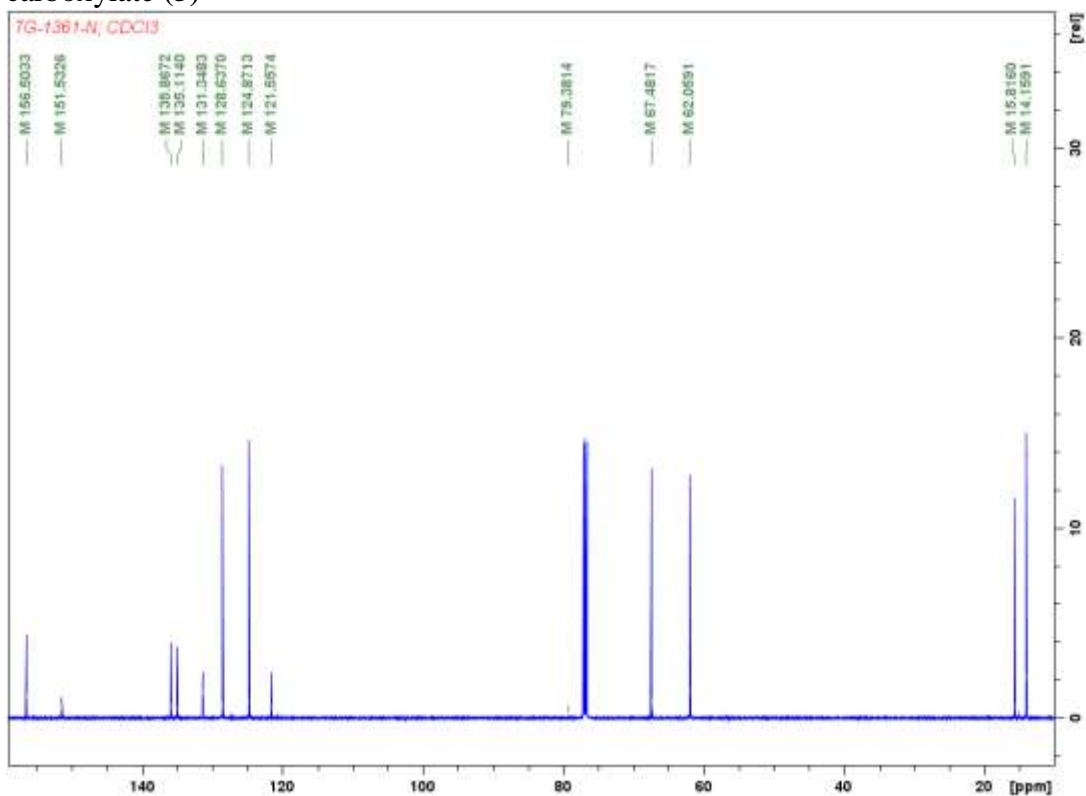
A part of ^1H - ^{13}C HSQC (red contour lines) and ^1H - ^{13}C HMBC (blue contour lines) spectra of ethyl 1-methoxy-4-methyl-5-(thiophen-2-yl)-1*H*-imidazole-2-carboxylate (**4d**).



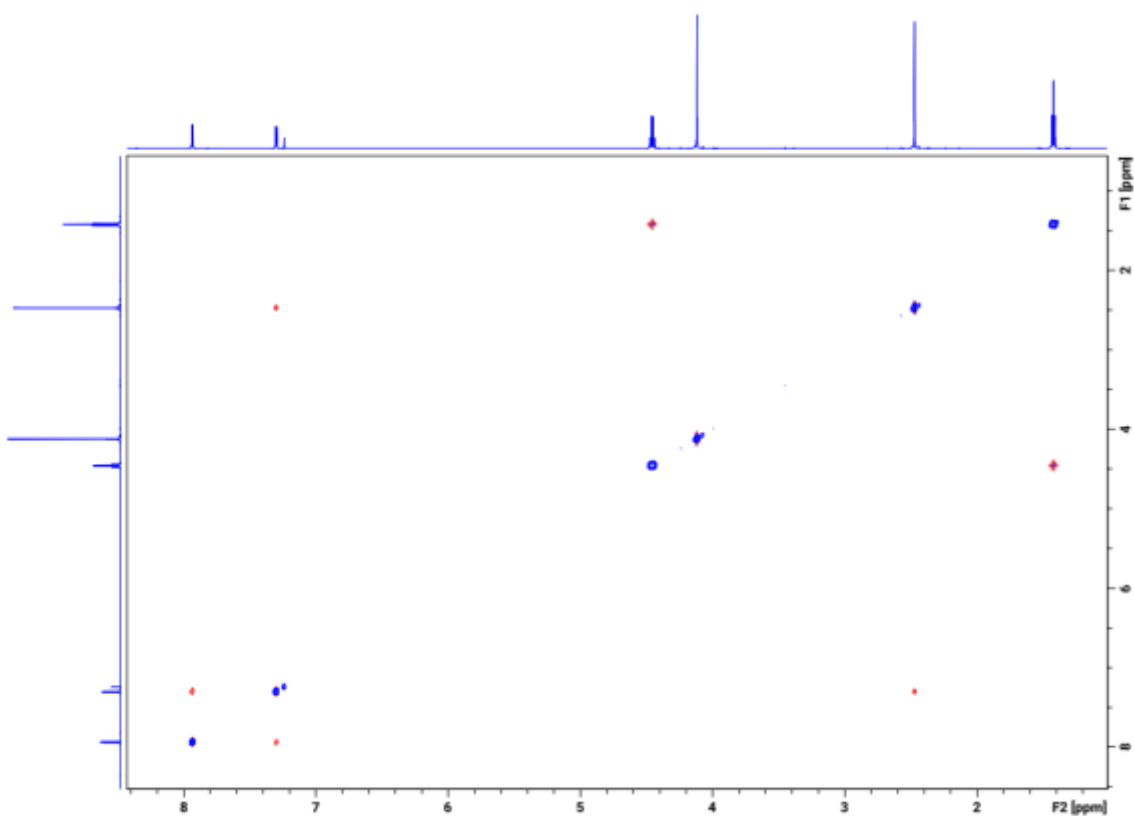
^1H - ^{15}N HMBC spectrum of ethyl 1-methoxy-4-methyl-5-(thiophen-2-yl)-1*H*-imidazole-2-carboxylate (**4d**).



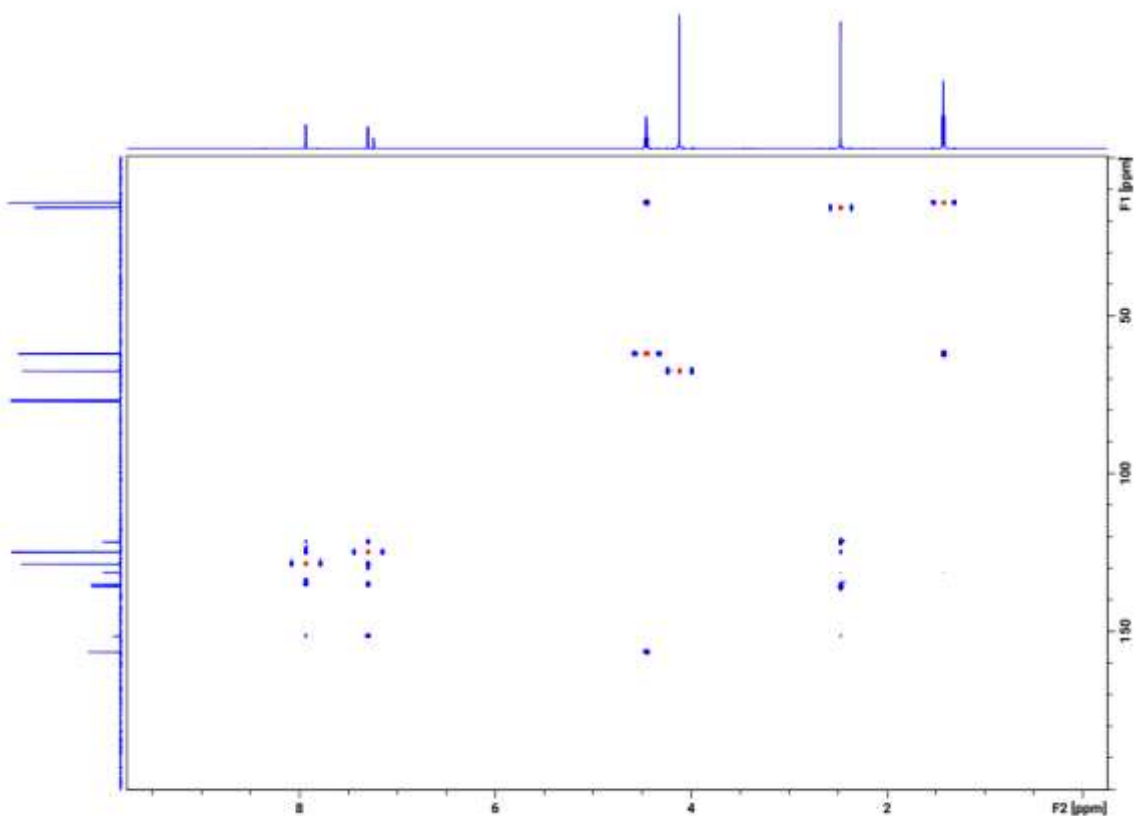
¹H NMR spectrum of ethyl 1-methoxy-4-methyl-5-(5-nitrothiophen-2-yl)-1H-imidazole-2-carboxylate (**5**)



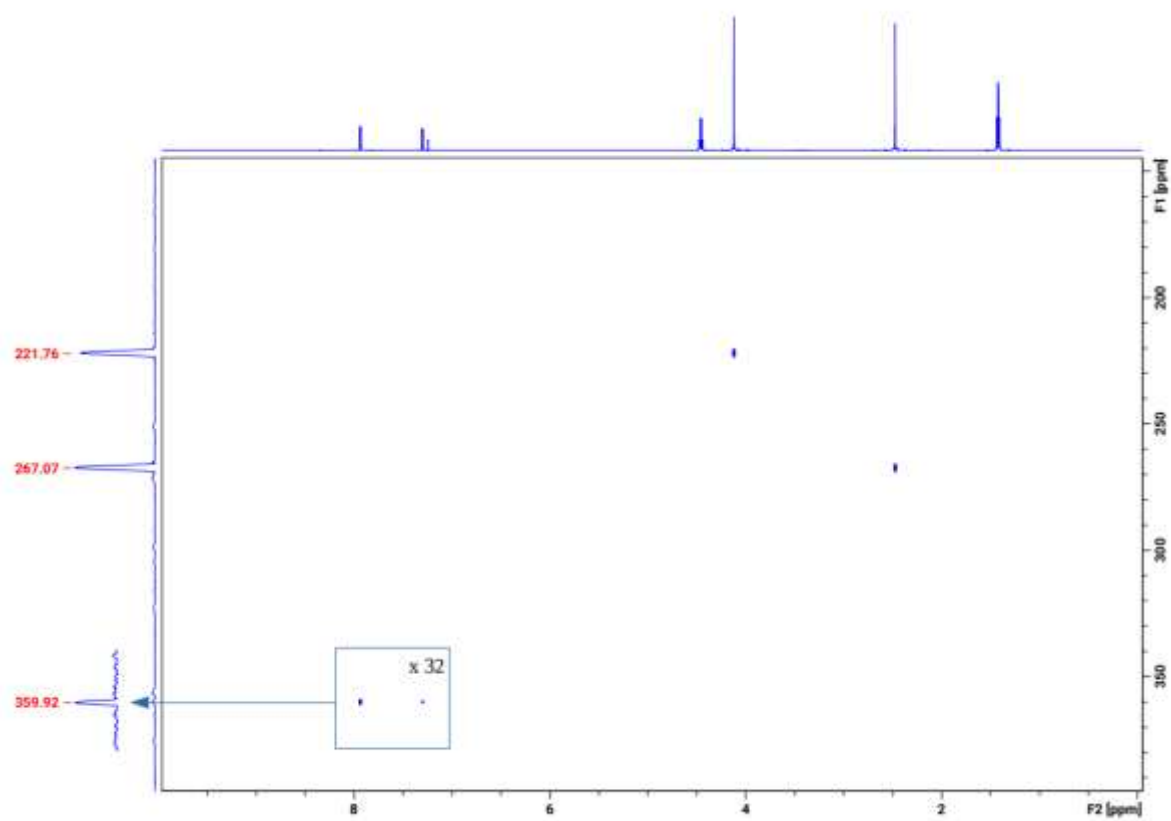
¹³C NMR spectrum of ethyl 1-methoxy-4-methyl-5-(5-nitrothiophen-2-yl)-1H-imidazole-2-carboxylate (**5**)



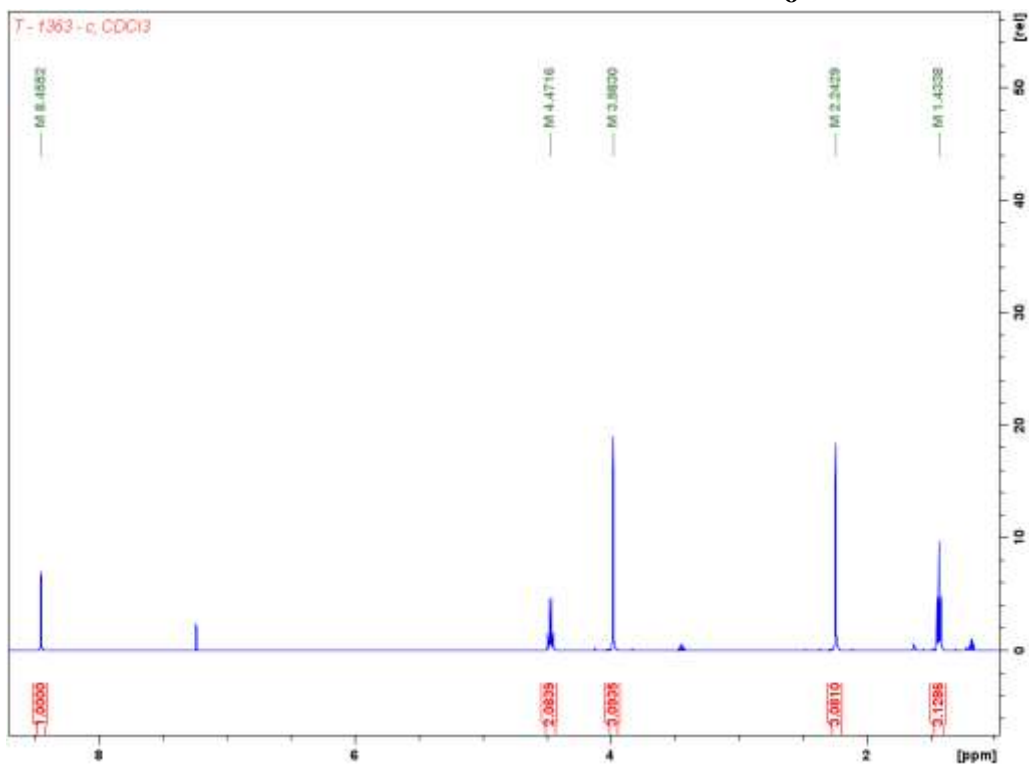
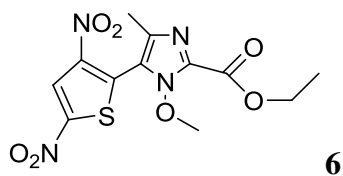
^1H - ^1H NOESY spectrum of ethyl 1-methoxy-4-methyl-5-(5-nitrothiophen-2-yl)-1*H*-imidazole-2-carboxylate (**5**)



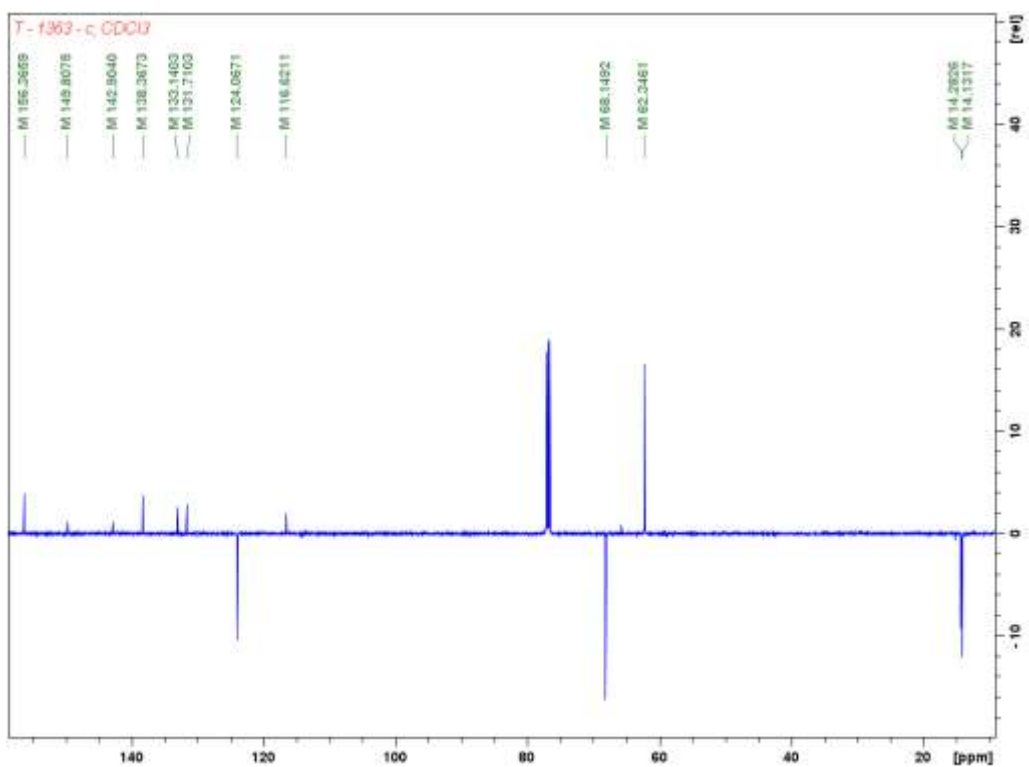
^1H - ^{13}C HSQC (red contour lines) and ^1H - ^{13}C HMBC (blue contour lines) spectra of ethyl 1-methoxy-4-methyl-5-(5-nitrothiophen-2-yl)-1*H*-imidazole-2-carboxylate (**5**)



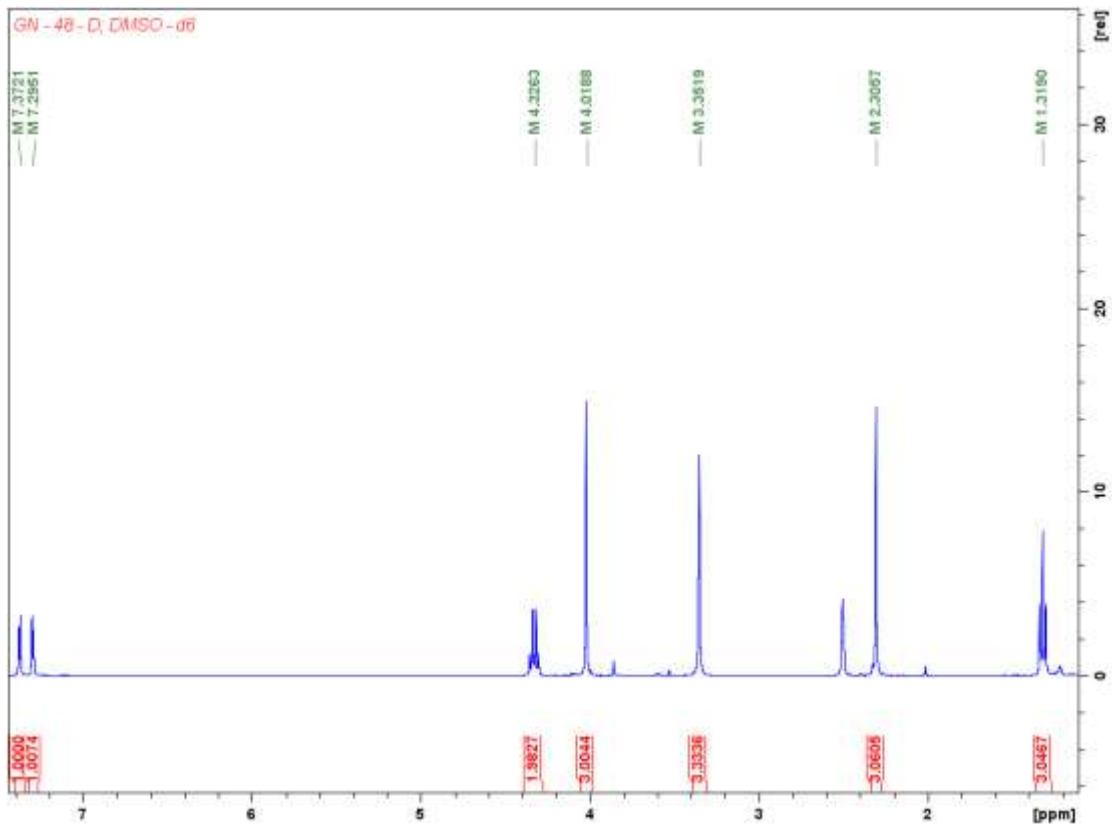
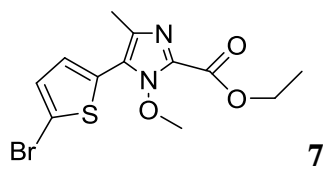
^1H - ^{15}N HMBC spectrum of ethyl 1-methoxy-4-methyl-5-(5-nitrothiophen-2-yl)-1*H*-imidazole-2-carboxylate (**5**)



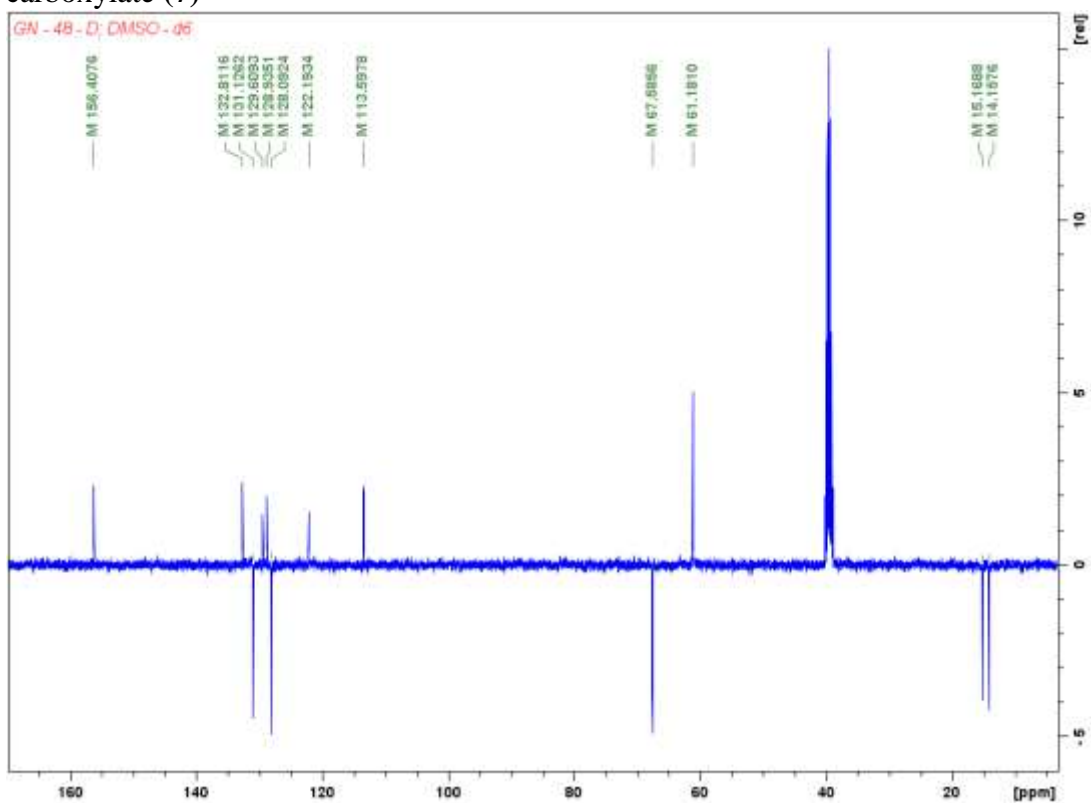
¹H NMR spectrum of ethyl 5-(3,5-dinitrothiophen-2-yl)-1-methoxy-4-methyl-1*H*-imidazole-2-carboxylate (**6**)



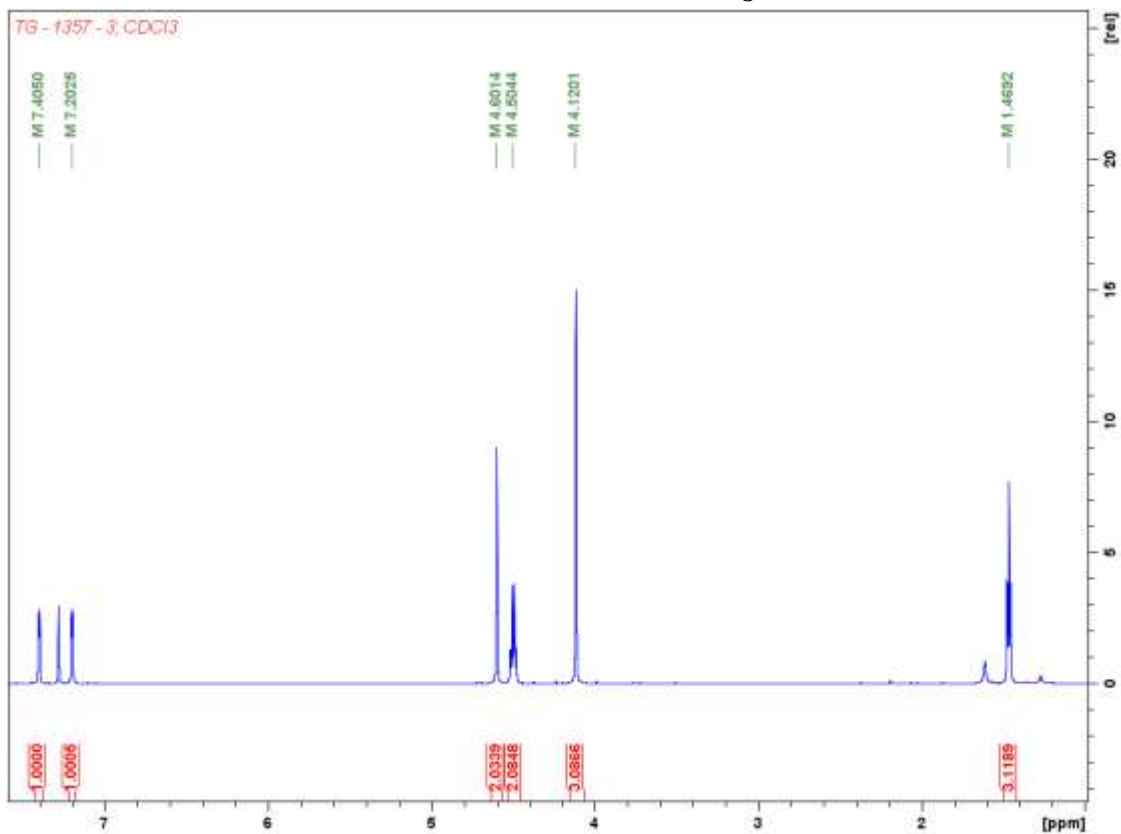
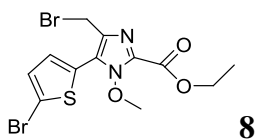
¹³C NMR spectrum of ethyl 5-(3,5-dinitrothiophen-2-yl)-1-methoxy-4-methyl-1*H*-imidazole-2-carboxylate (**6**)



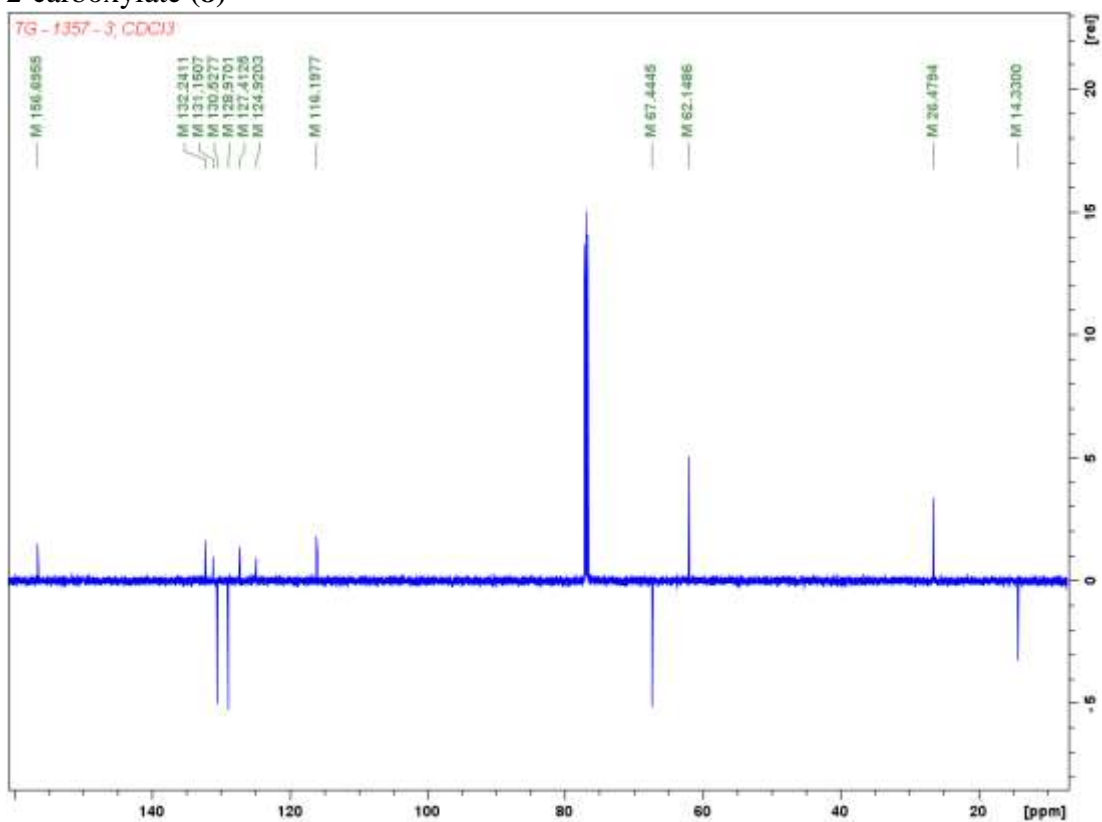
¹H NMR spectrum of ethyl 5-(5-bromothiophen-2-yl)-1-methoxy-4-methyl-1*H*-imidazole-2-carboxylate (**7**)



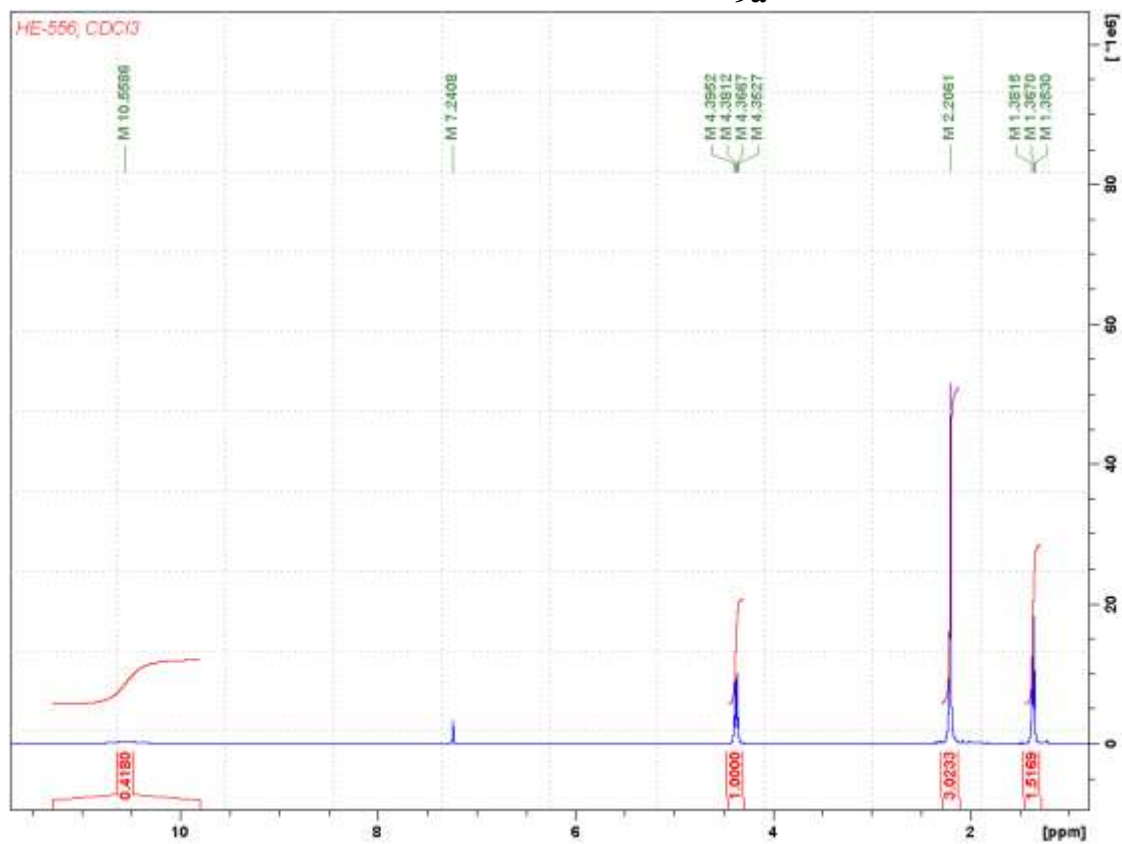
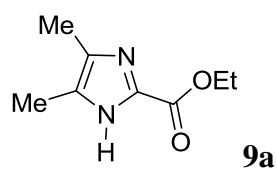
¹³C NMR spectrum of ethyl 5-(5-bromothiophen-2-yl)-1-methoxy-4-methyl-1*H*-imidazole-2-carboxylate (**7**)



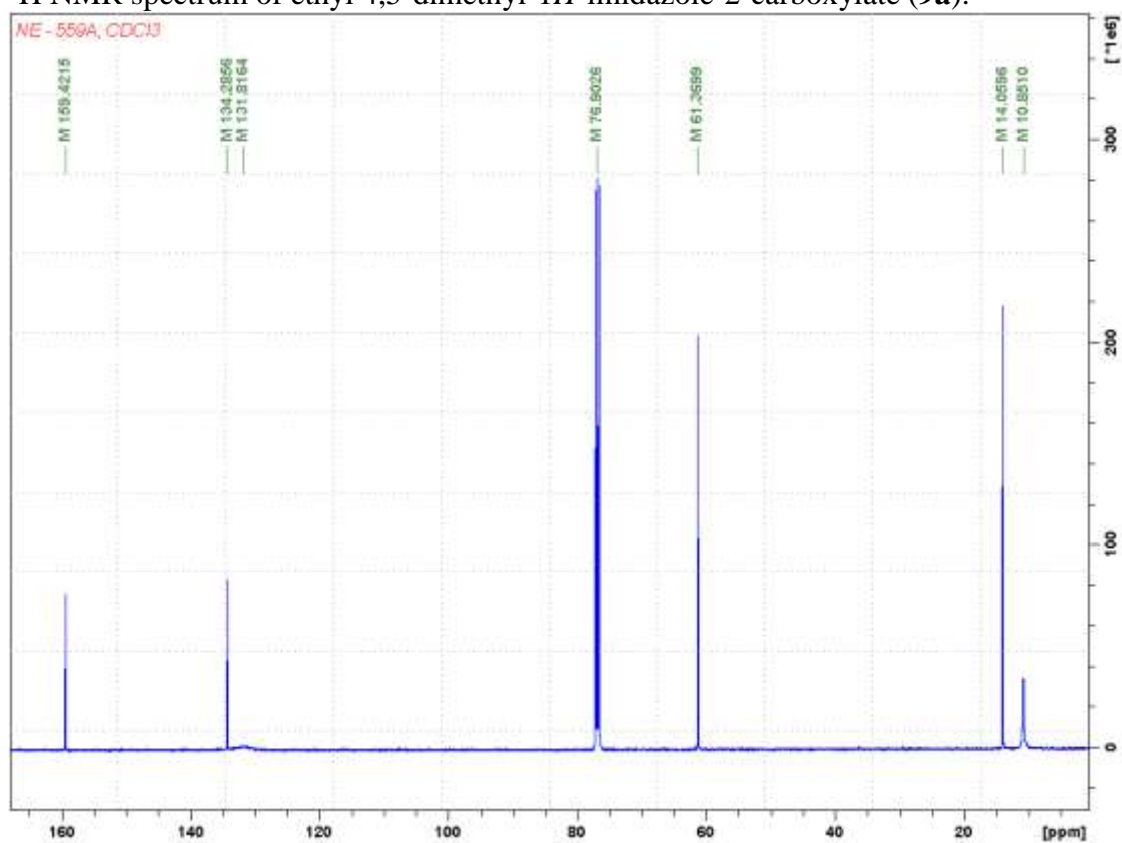
¹H NMR spectrum of ethyl 4-bromomethyl-5-(5-bromothiophen-2-yl)-1-methoxy-1*H*-imidazole-2-carboxylate (**8**)



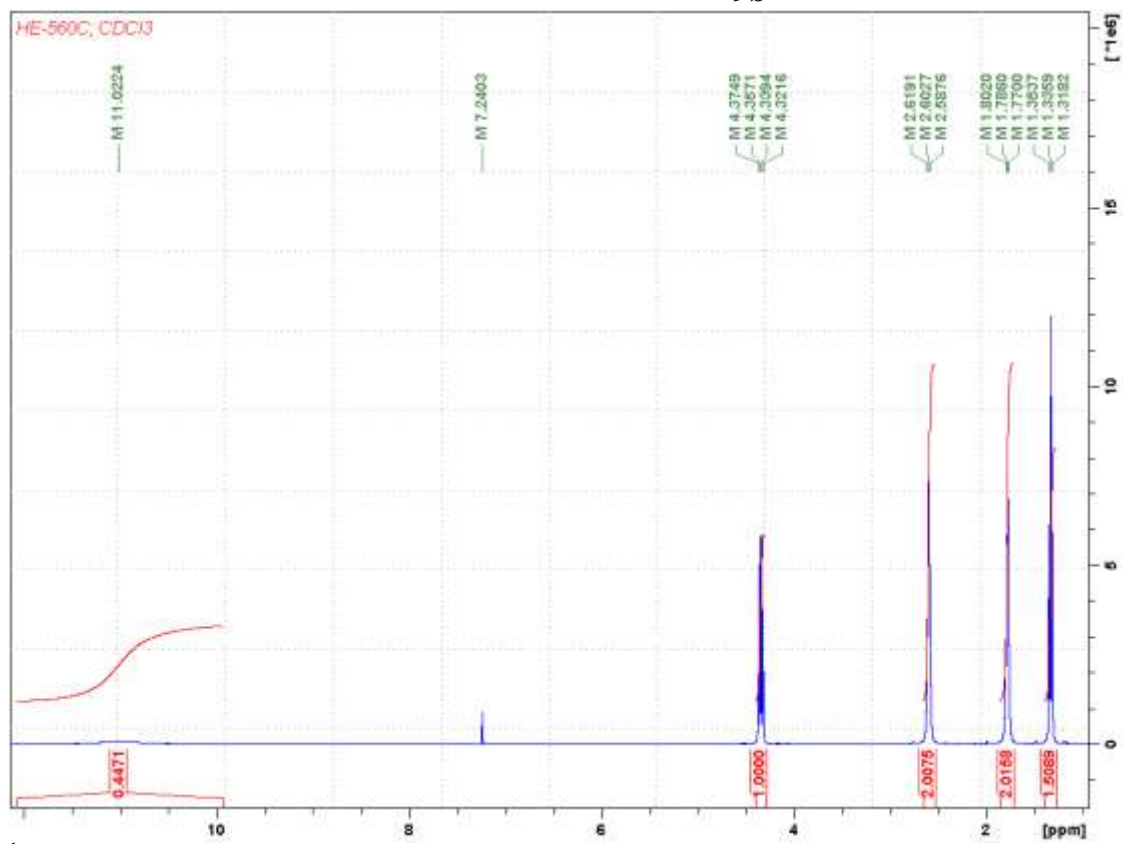
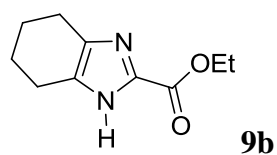
¹³C NMR spectrum of ethyl 4-bromomethyl-5-(5-bromothiophen-2-yl)-1-methoxy-1*H*-imidazole-2-carboxylate (**8**)



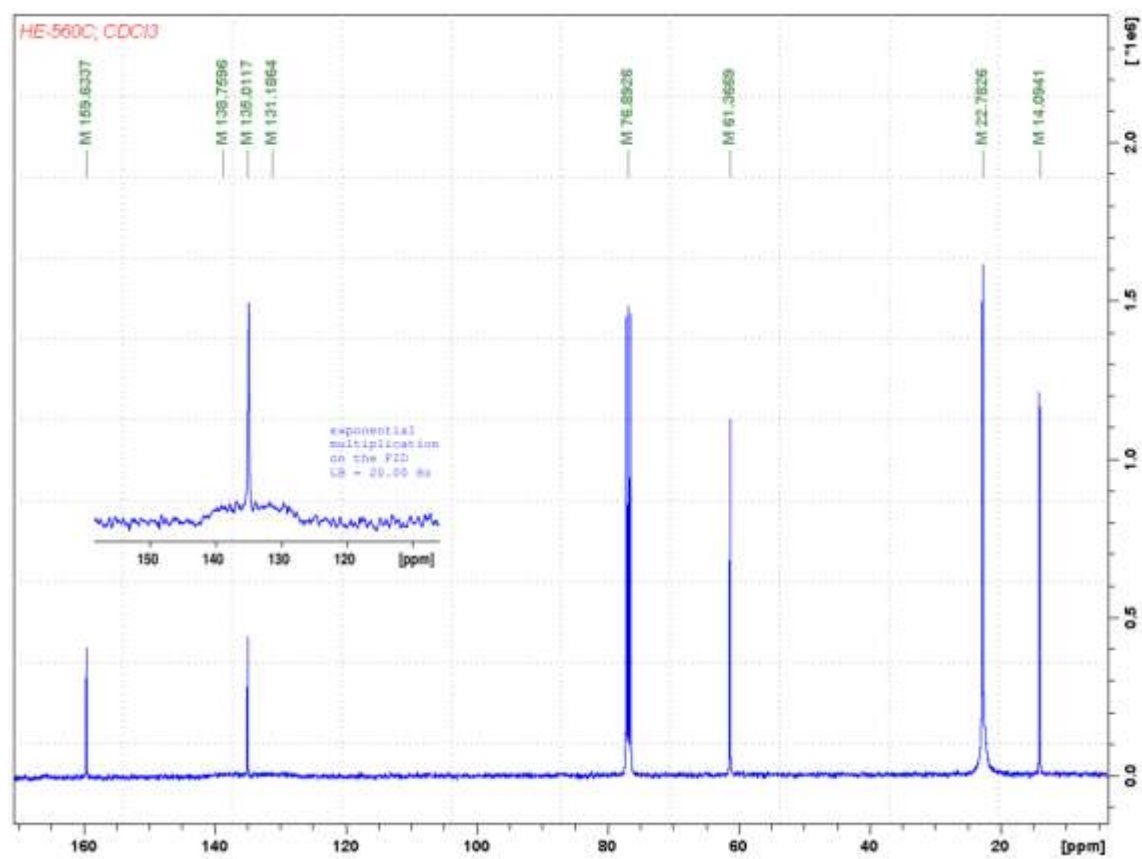
¹H NMR spectrum of ethyl 4,5-dimethyl-1*H*-imidazole-2-carboxylate (**9a**).



¹³C NMR spectrum of ethyl 4,5-dimethyl-1*H*-imidazole-2-carboxylate (**9a**).



¹H NMR spectrum of ethyl 4,5,6,7-tetrahydro-1*H*-benzimidazole-2-carboxylate (**9b**)



¹³C NMR spectrum of ethyl 4,5,6,7-tetrahydro-1*H*-benzimidazole-2-carboxylate (**9b**).