

Supplementary Material

Synthesis and Study of Prototropic Tautomerism of 2-(2-Furyl)-1-hydroxyimidazoles

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^ADepartment of Fine Organic Synthesis and Chemistry of Dyes, D. I. Mendeleev University of Chemical Technology of Russia, Miusskaya Square, 9, Moscow, 125047, Russia.

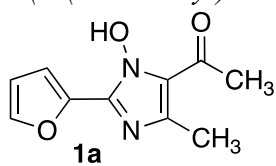
^BA. N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Vavilova Street, 28, Moscow, 119991, Russia.

^CCorresponding author. Email: polinandrevna@yandex.ru

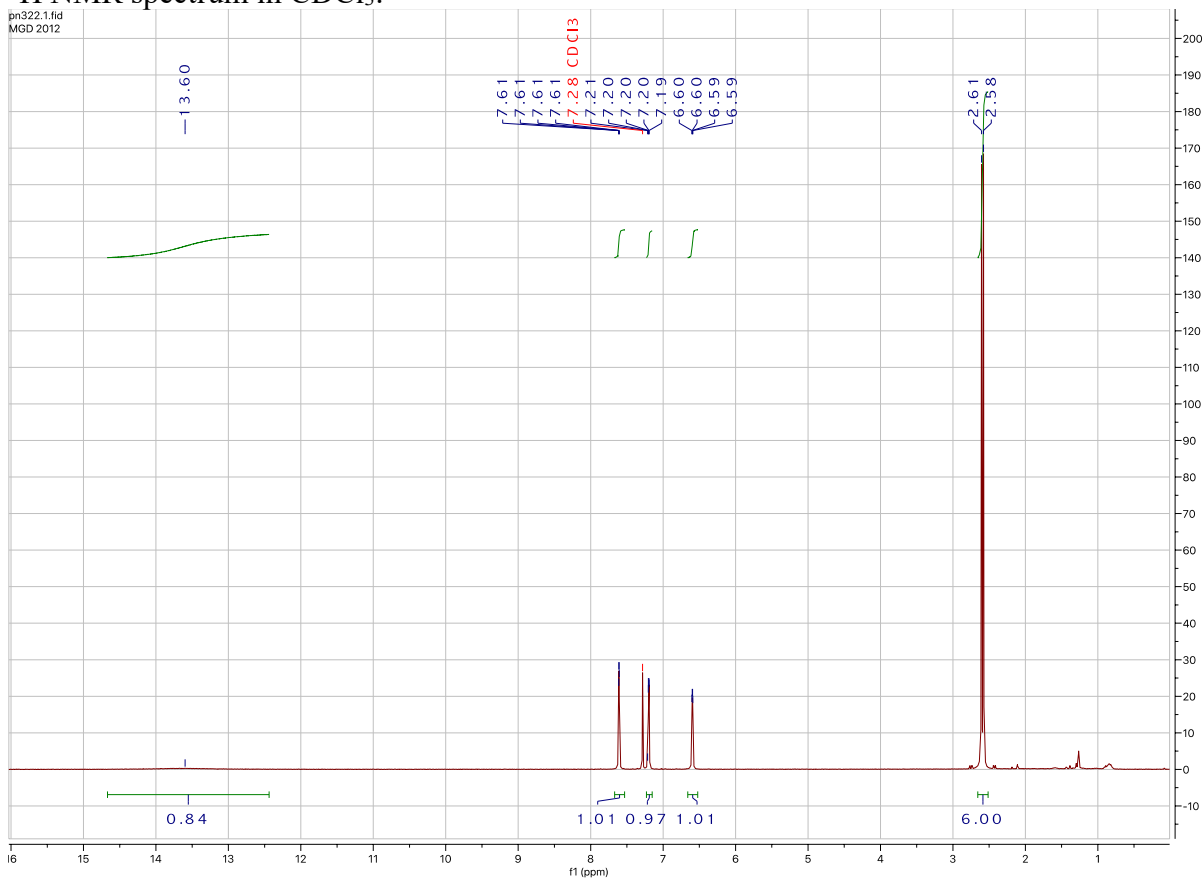
- 1. Copies of ¹H and ¹³C NMR spectra of compounds under consideration**
- 2. Copies of 2D NMR spectra of compounds 1a, 2a, 3a.**
- 3. Copies of IR spectra of compounds under consideration**
- 4. Copies of HRMS spectra of compounds under consideration**

1. Copies of ^1H and ^{13}C NMR spectra of compounds under consideration

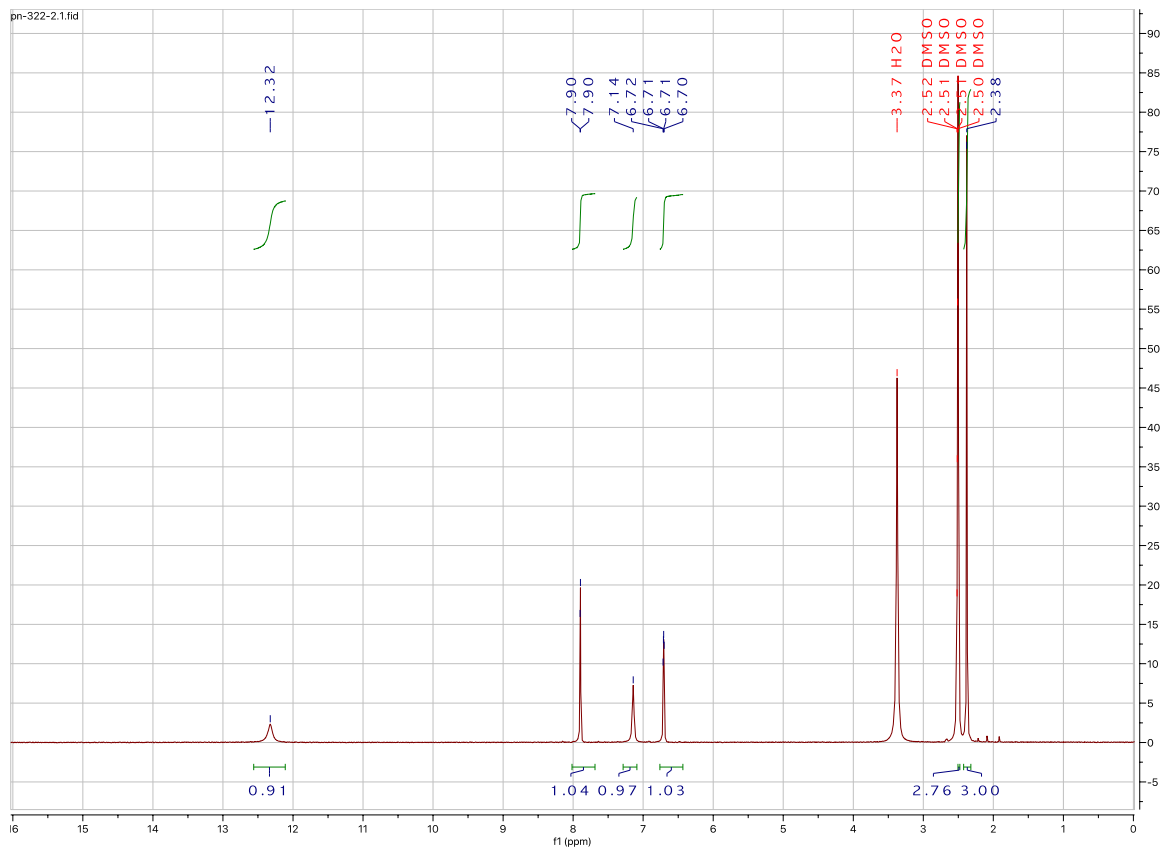
1-(2-(Furan-2-yl)-1-hydroxy-4-methyl-1H-imidazol-5-yl)ethanone (1a)



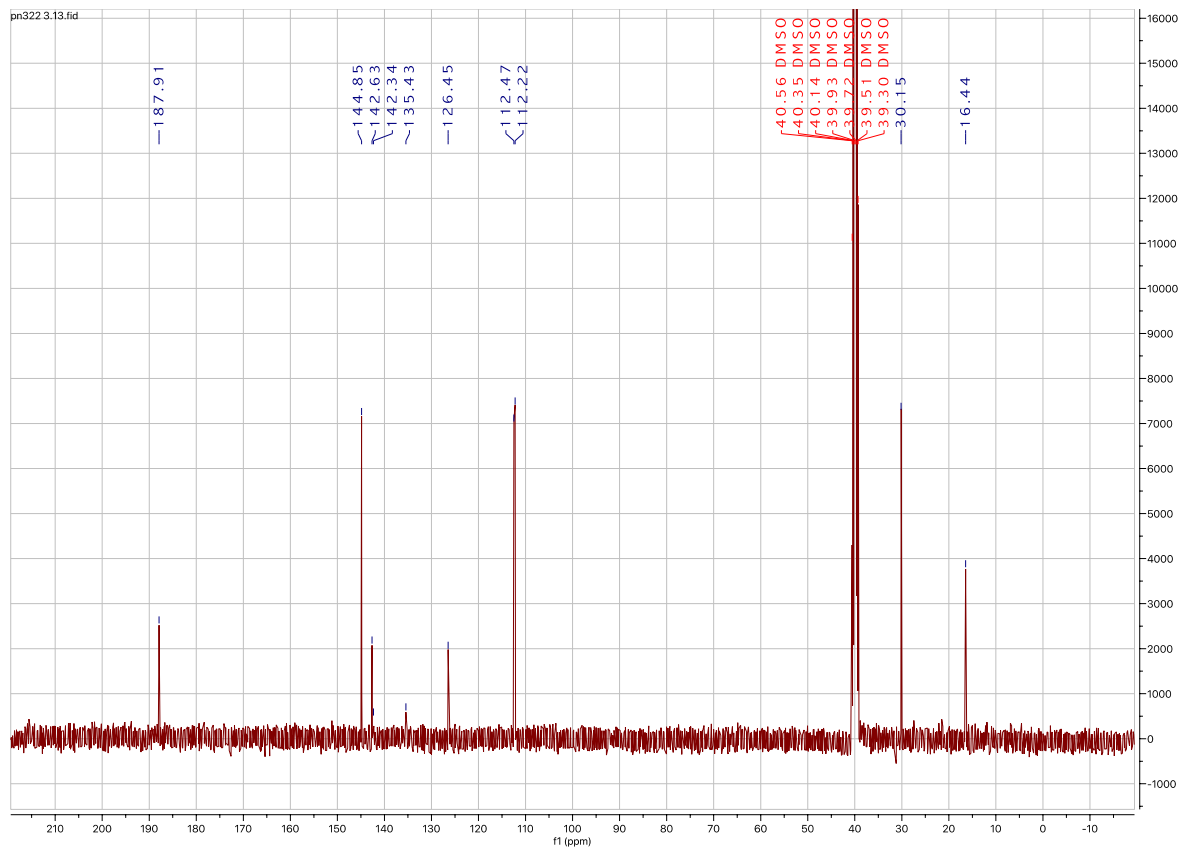
^1H NMR spectrum in CDCl_3 :



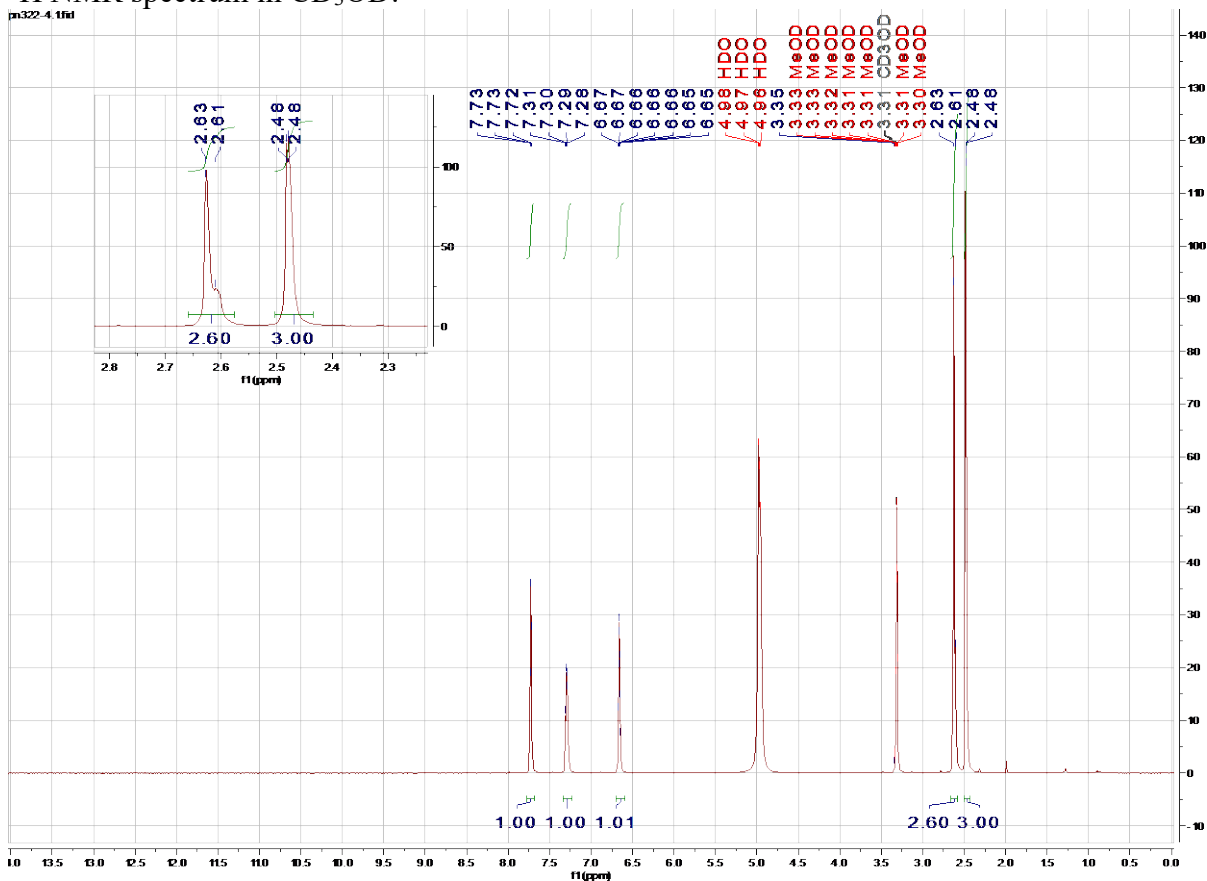
¹H NMR spectrum in DMSO-d₆:



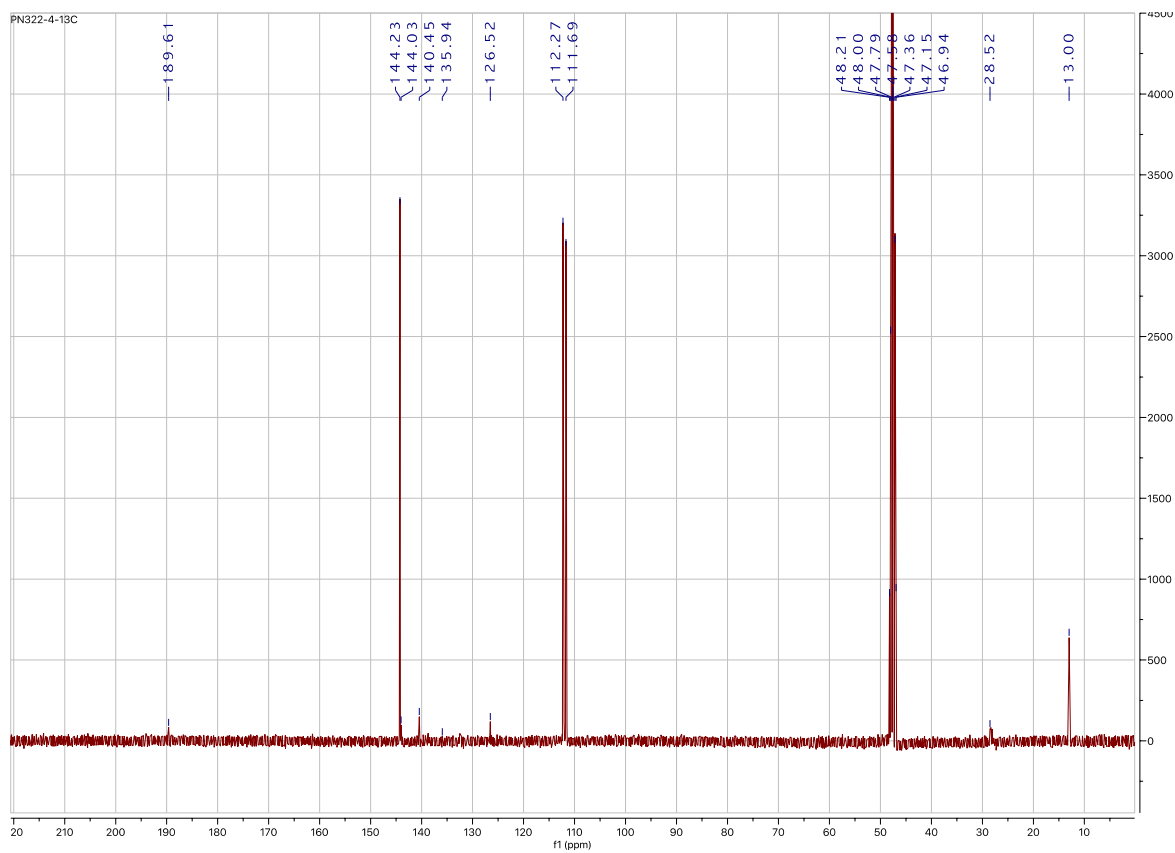
¹³C NMR spectrum in DMSO-d₆:



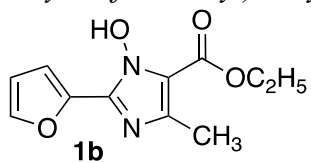
¹H NMR spectrum in CD₃OD:



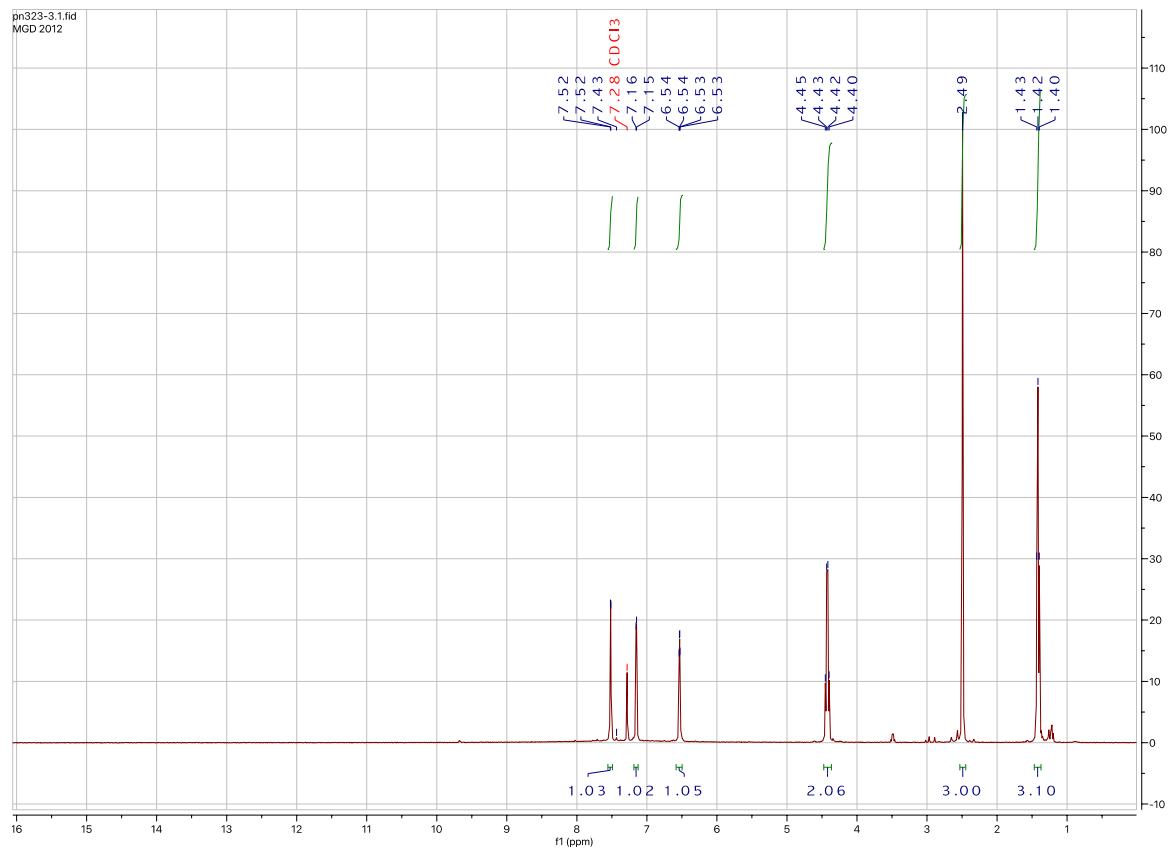
¹³C NMR spectrum in CD₃OD:



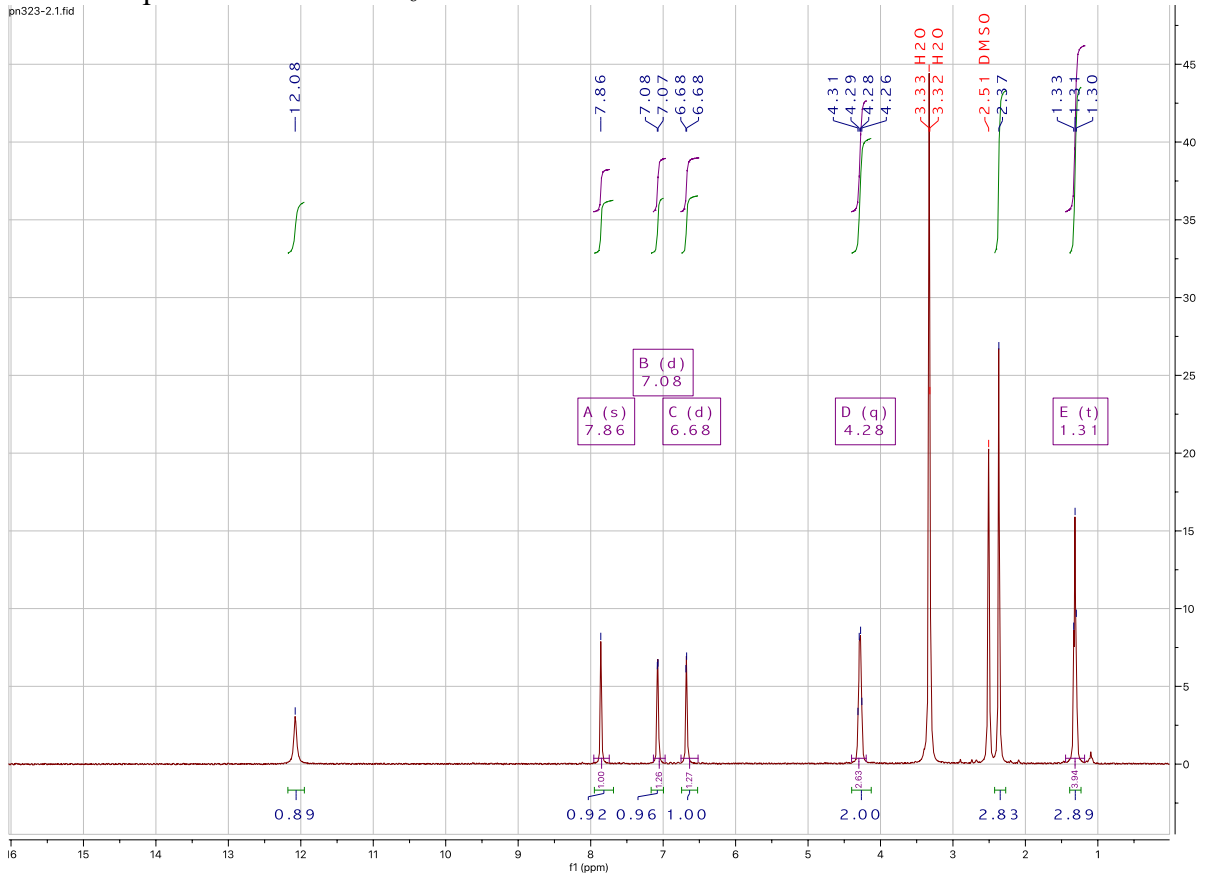
Ethyl 2-(furan-2-yl)-1-hydroxy-4-methyl-1H-imidazole-5-carboxylate (1b)



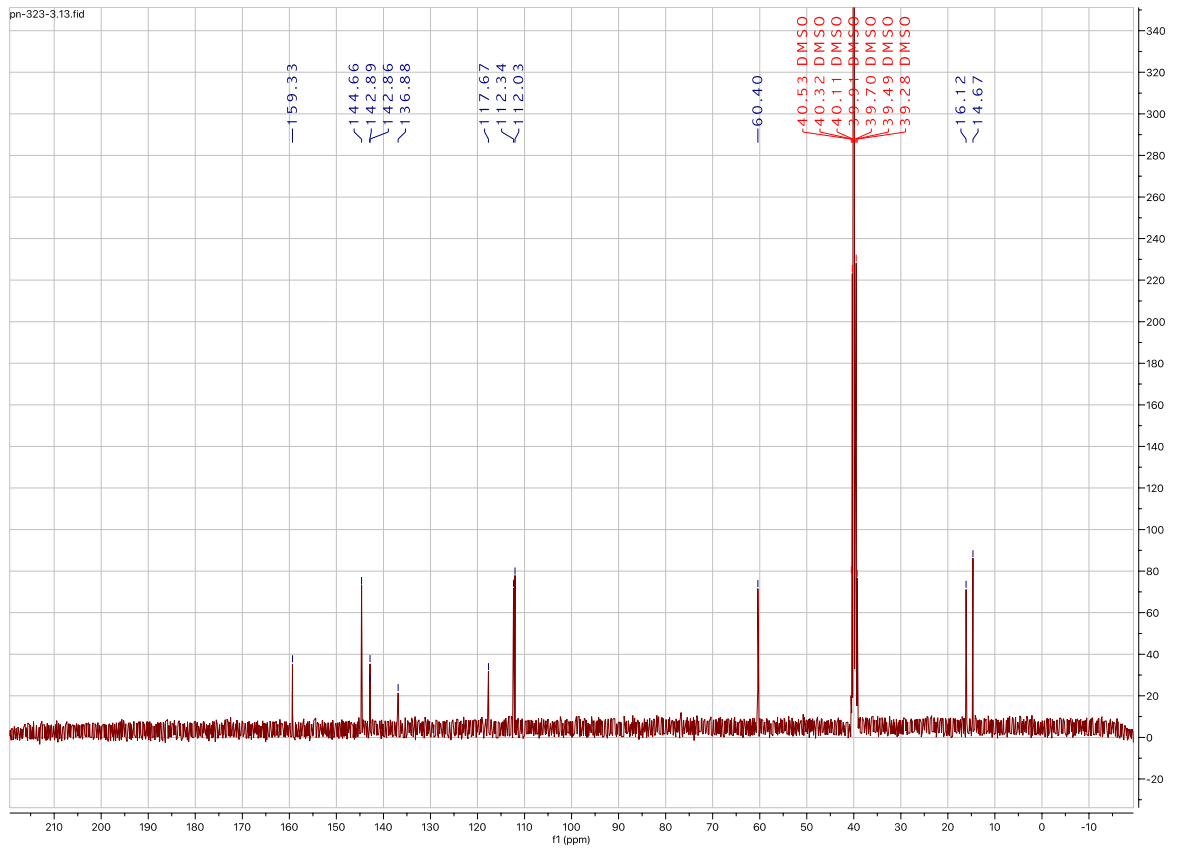
¹H NMR spectrum in CDCl₃:



¹H NMR spectrum in DMSO-d₆:



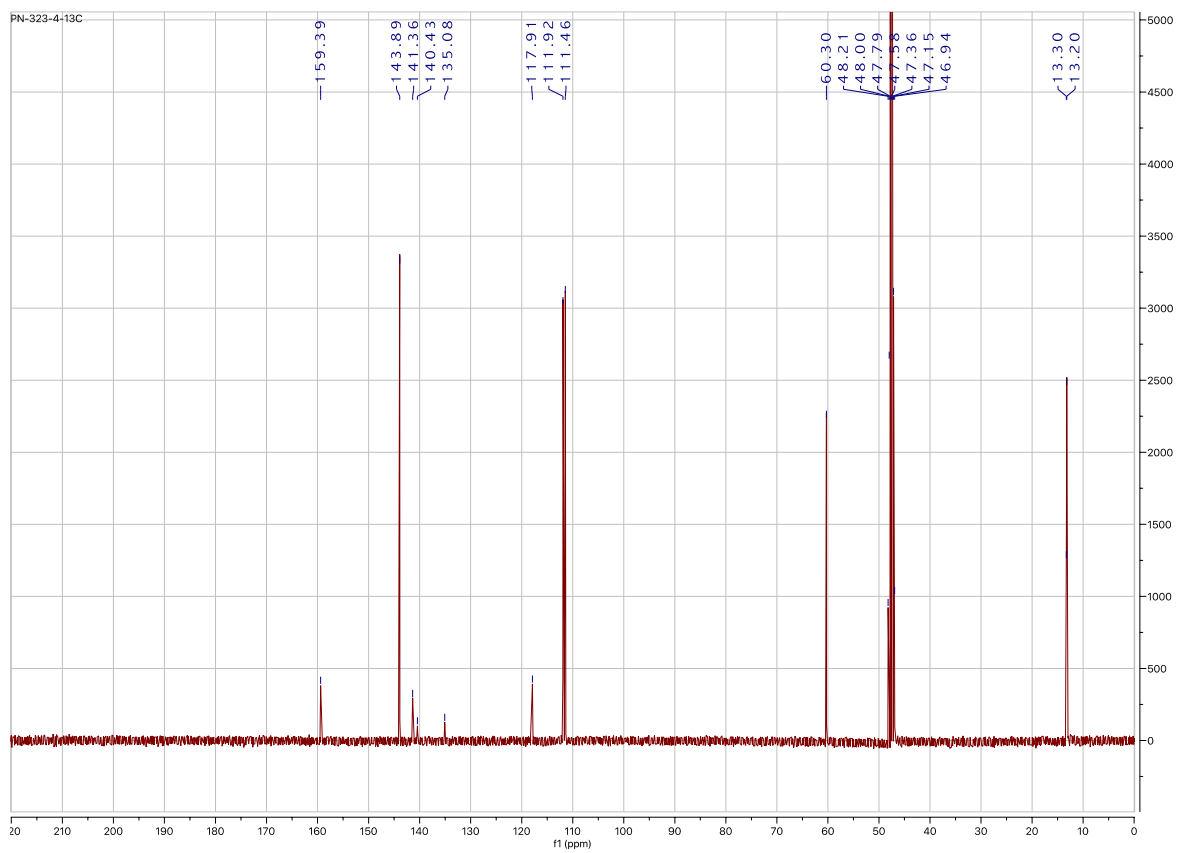
¹³C NMR spectrum in DMSO-d₆:



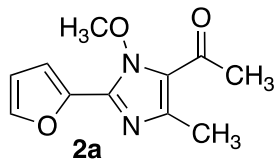
^1H NMR spectrum in CD_3OD :



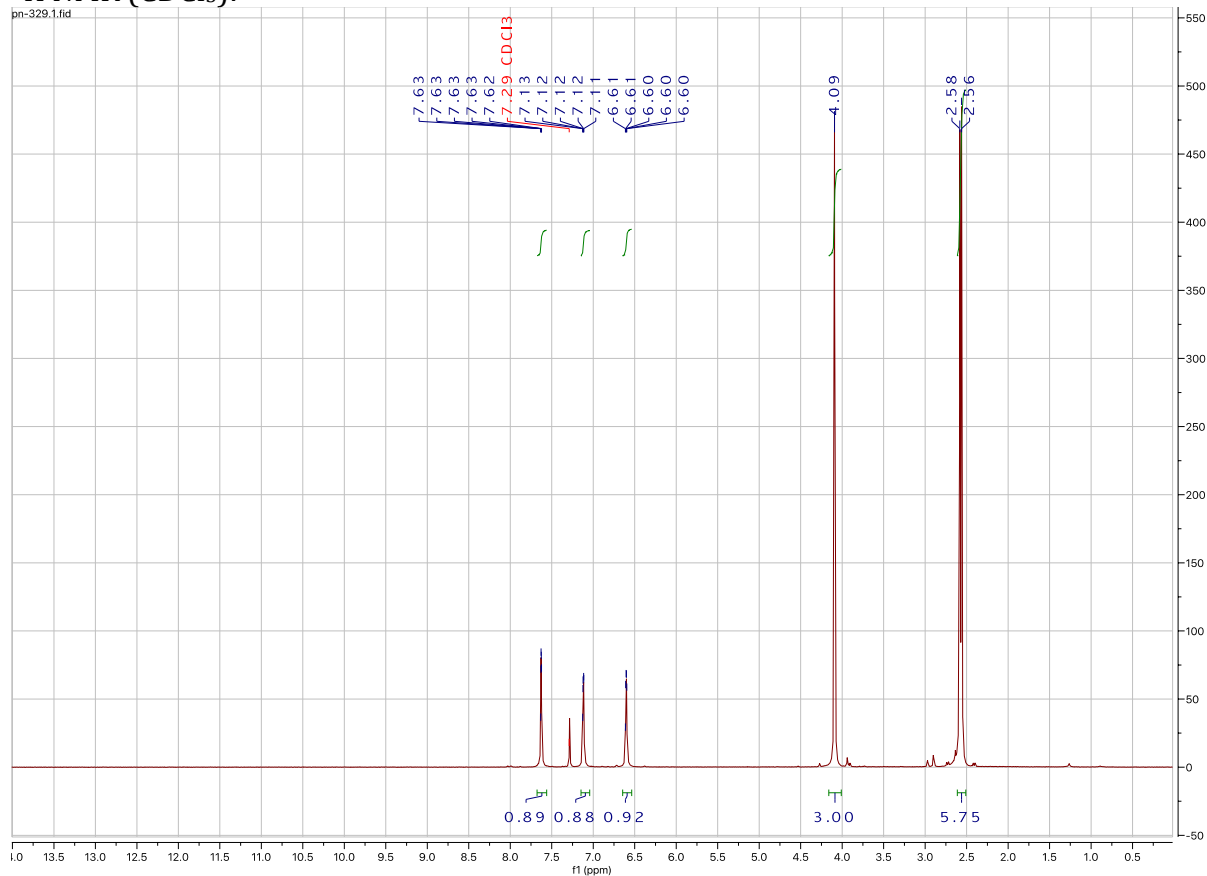
^{13}C NMR spectrum in CD_3OD :



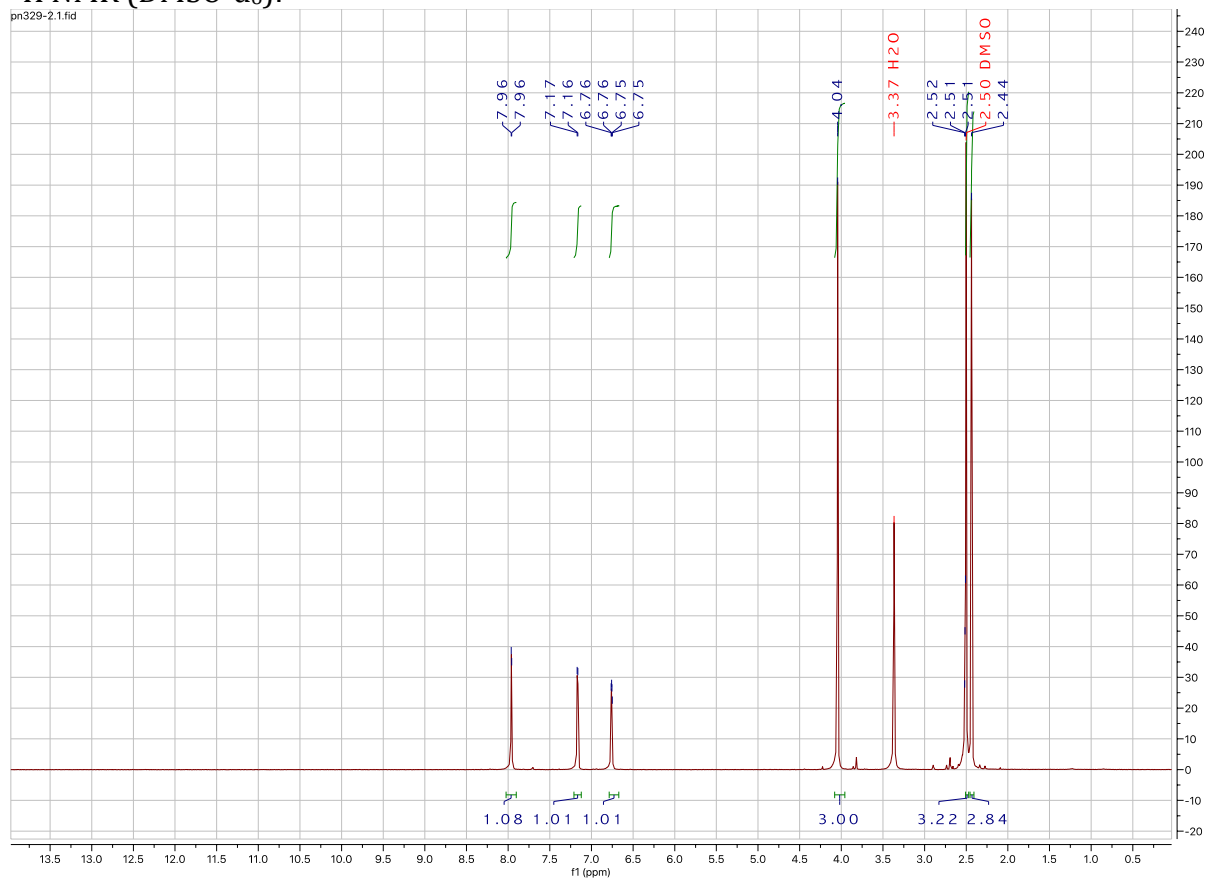
1-(2-(Furan-2-yl)-1-methoxy-4-methyl-1H-imidazol-5-yl)ethanone (**2a**)



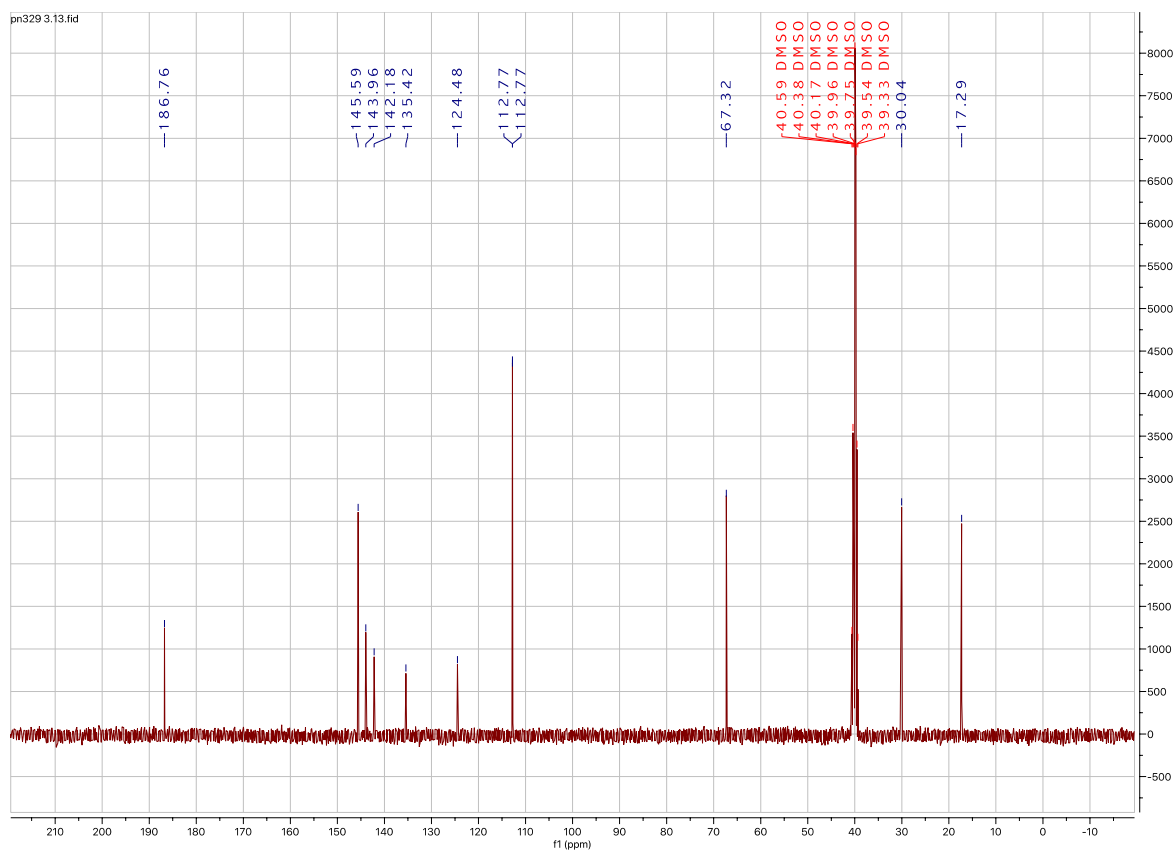
¹H NMR (CDCl₃):



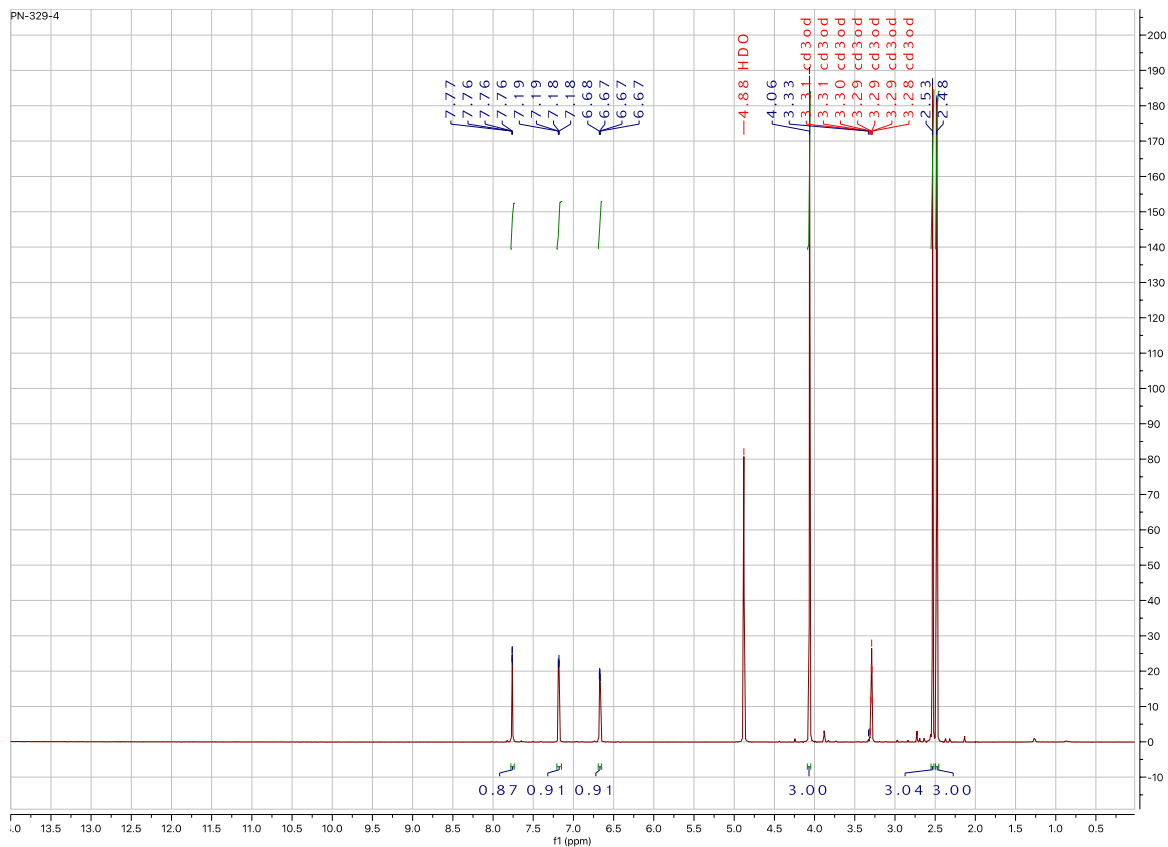
¹H NMR (DMSO-d₆):



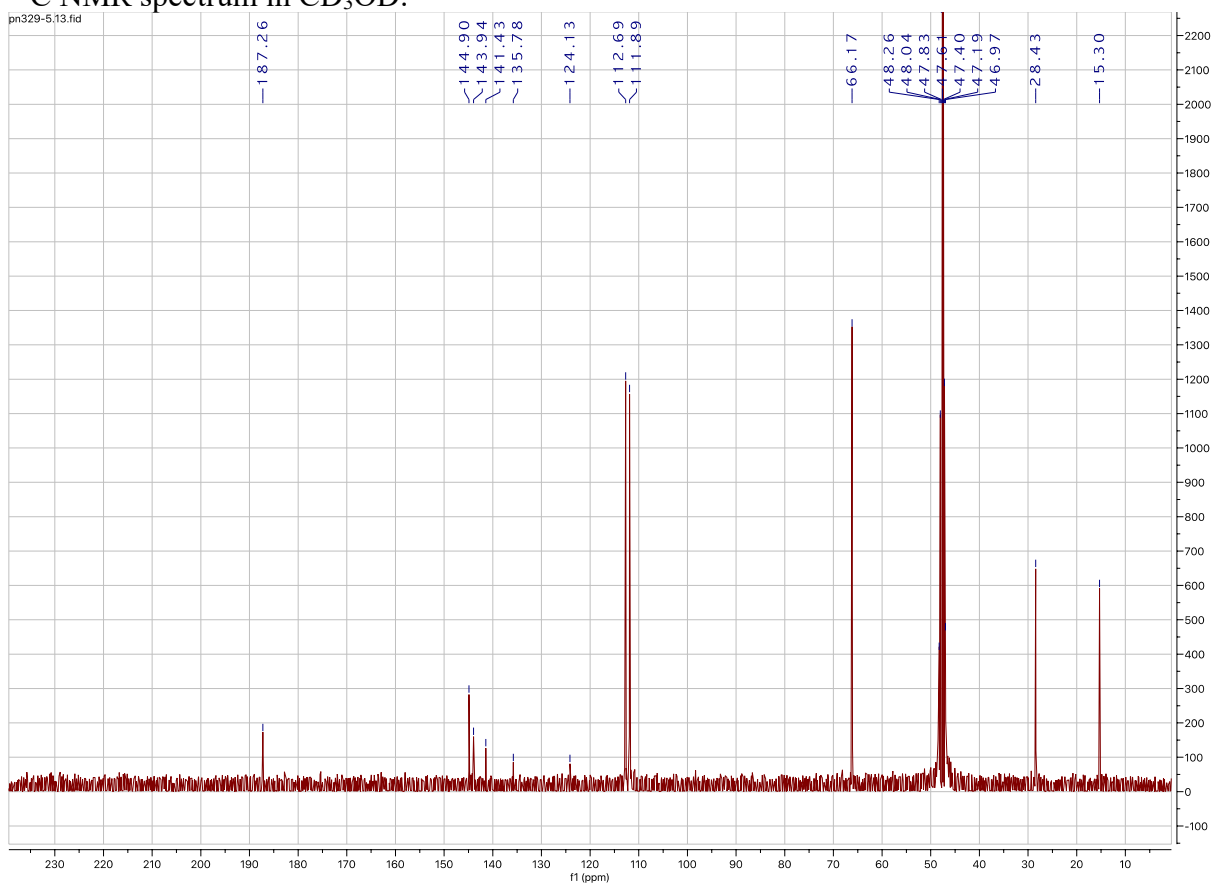
¹³C NMR (DMSO-d₆):



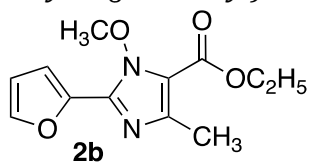
^1H NMR spectrum in CD_3OD :



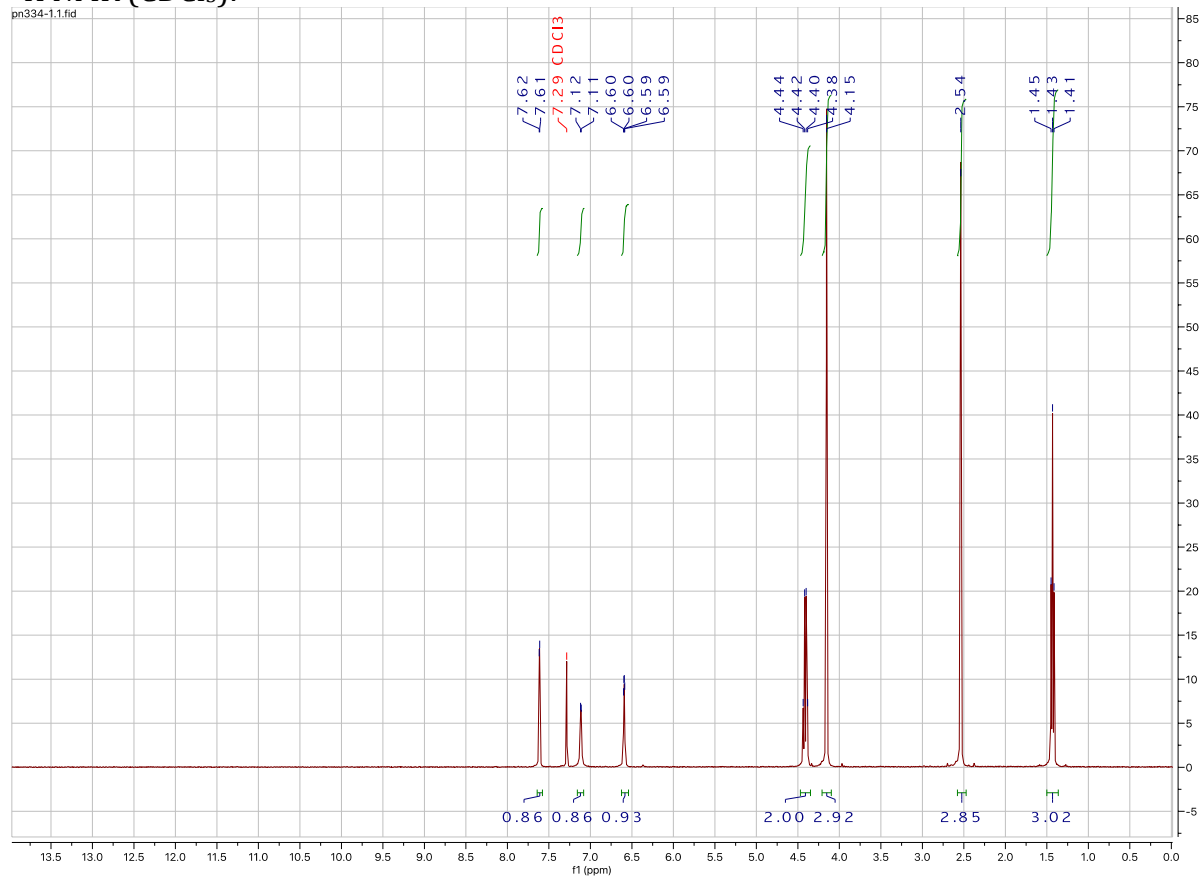
^{13}C NMR spectrum in CD_3OD :



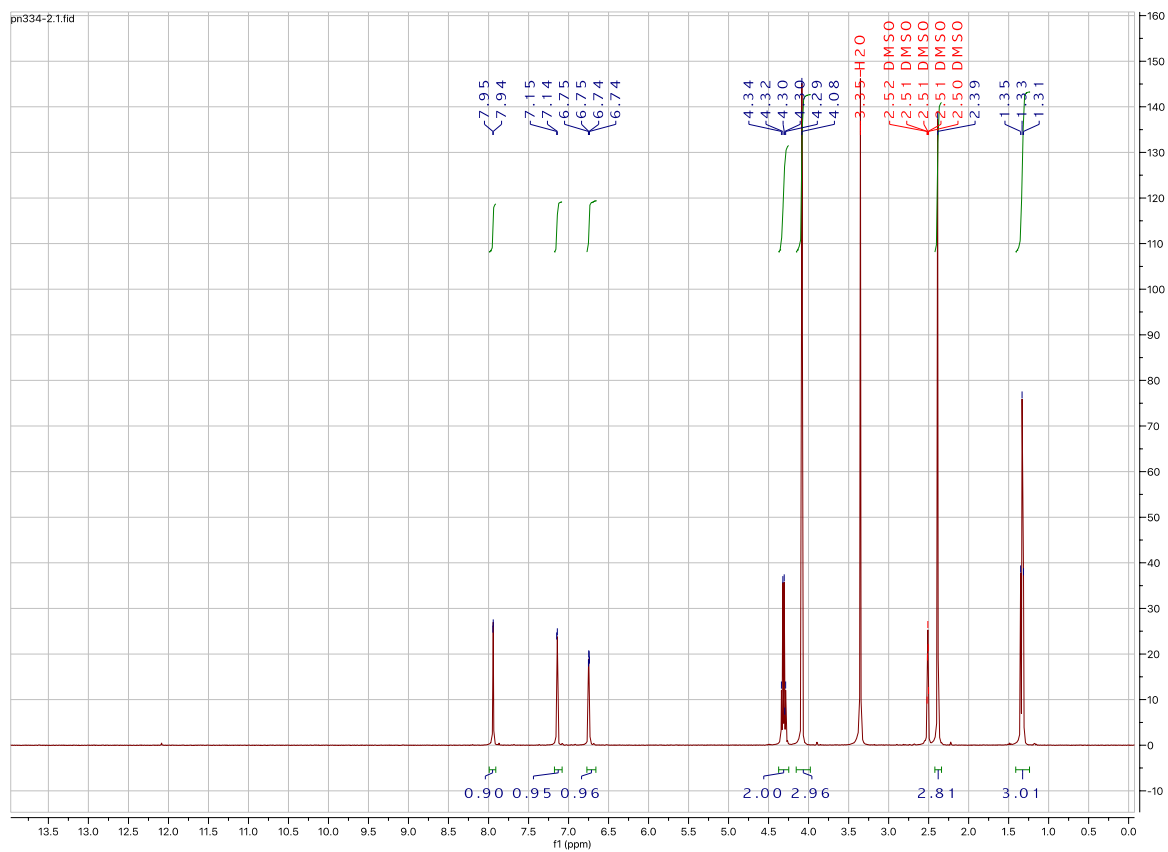
Ethyl 2-(furan-2-yl)-1-methoxy-4-methyl-1H-imidazole-5-carboxylate (**2b**)



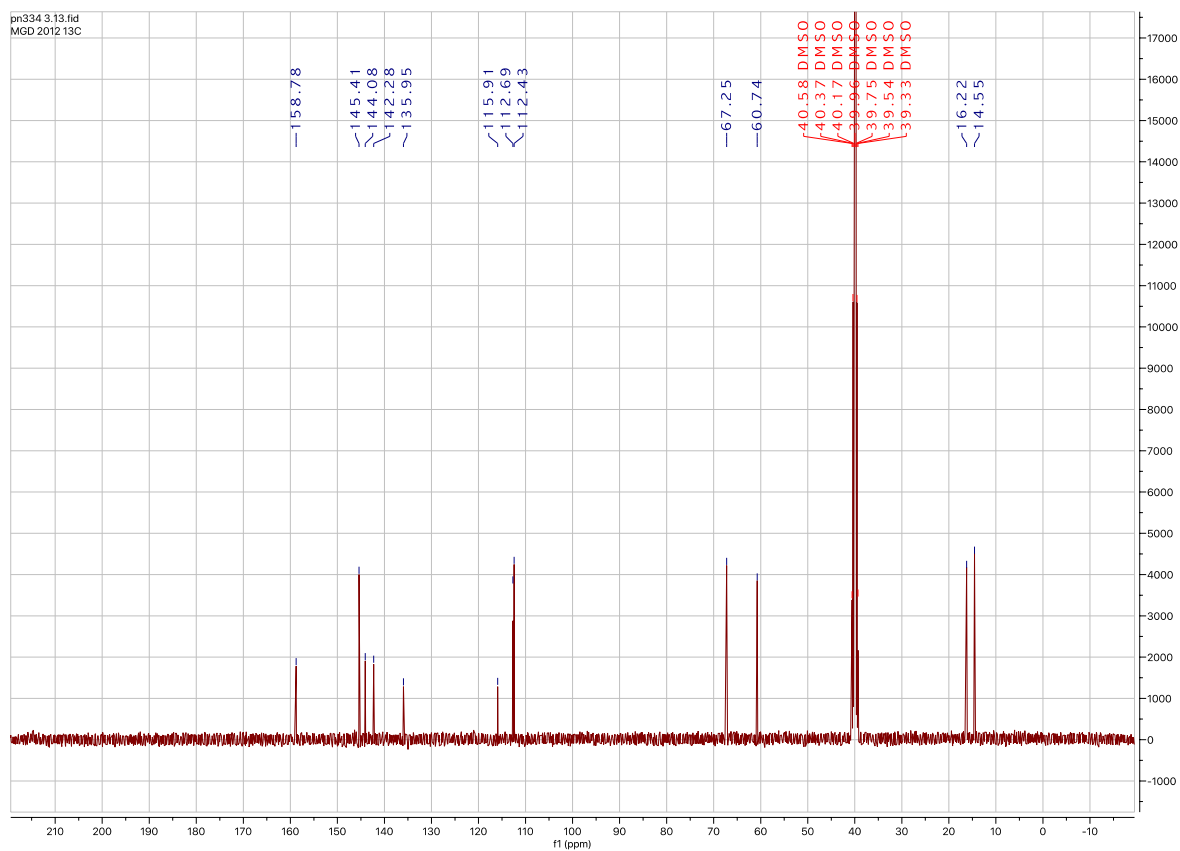
¹H NMR (CDCl₃):



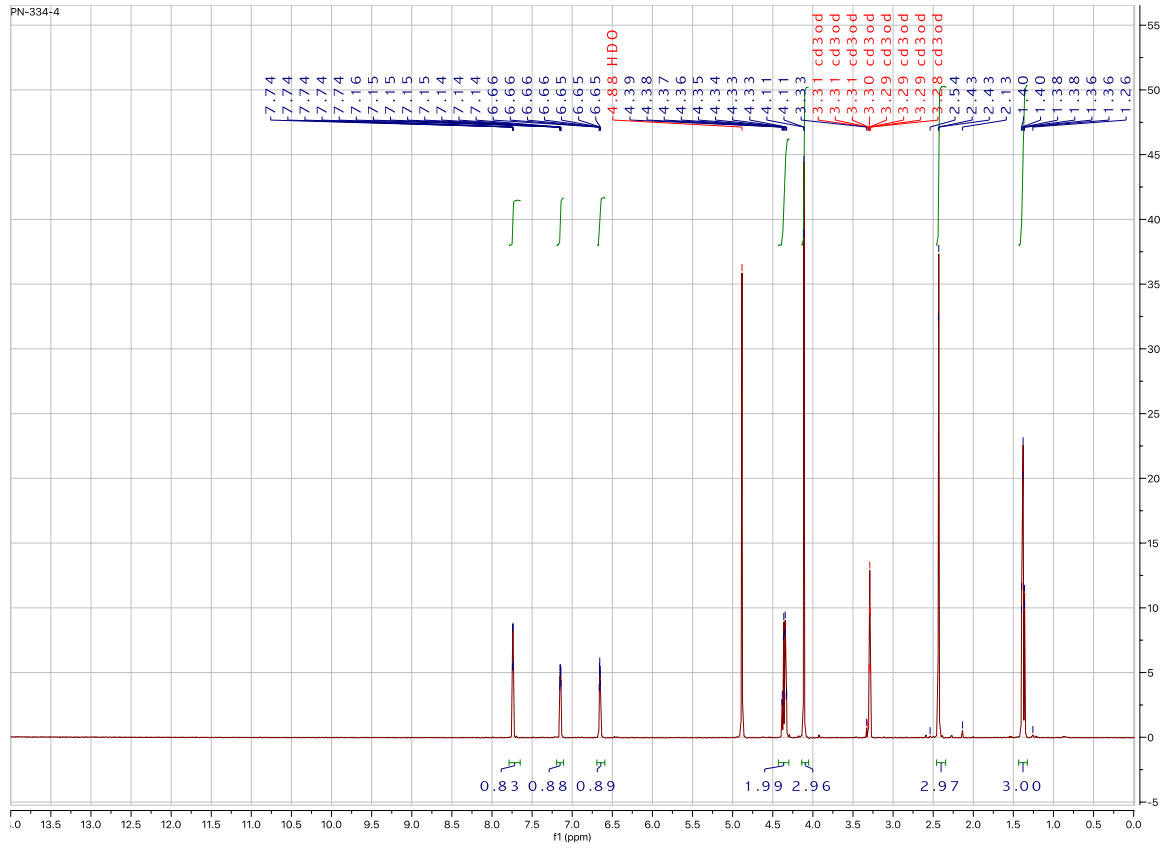
¹H NMR (DMSO-d₆):



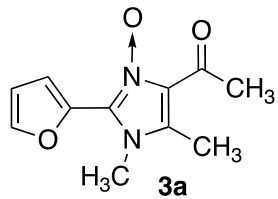
¹³C NMR (DMSO-d₆):



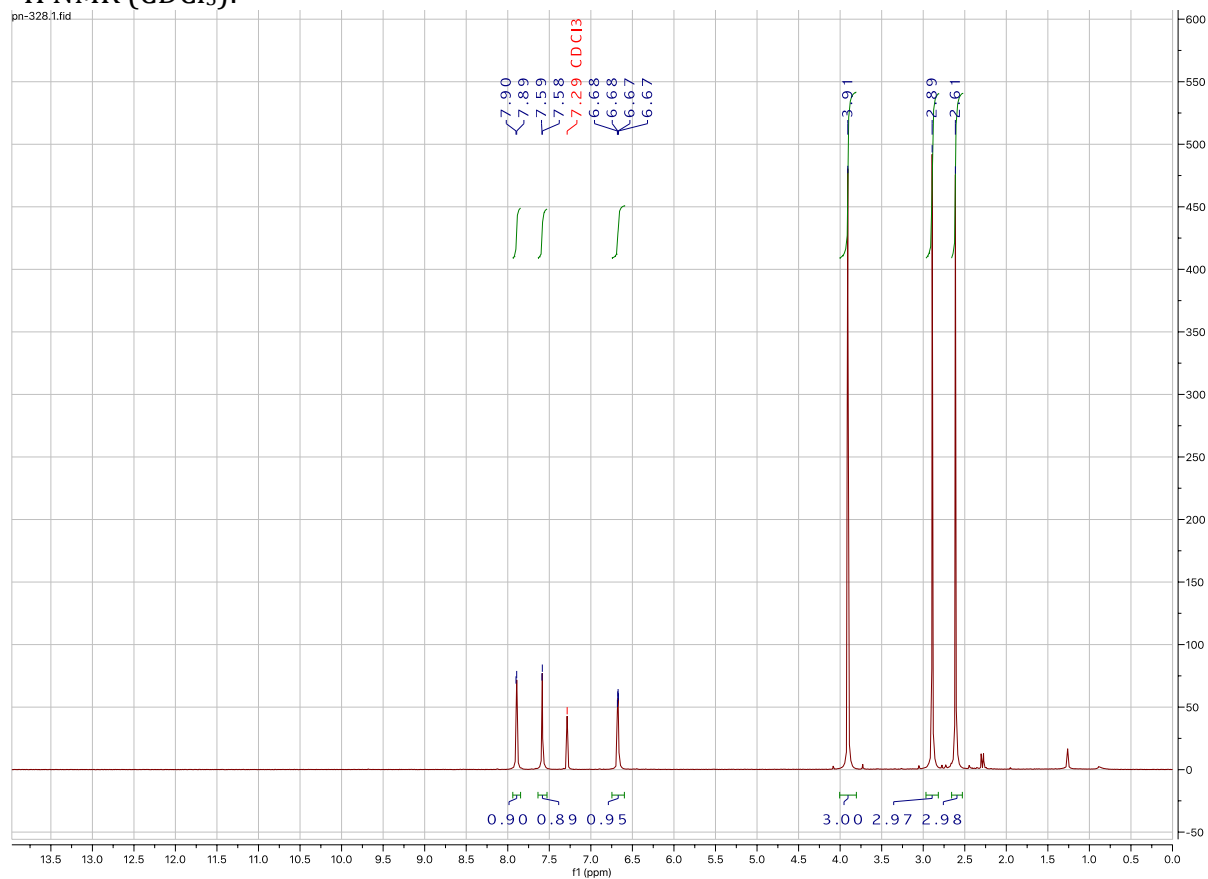
¹H NMR spectrum in CD₃OD:



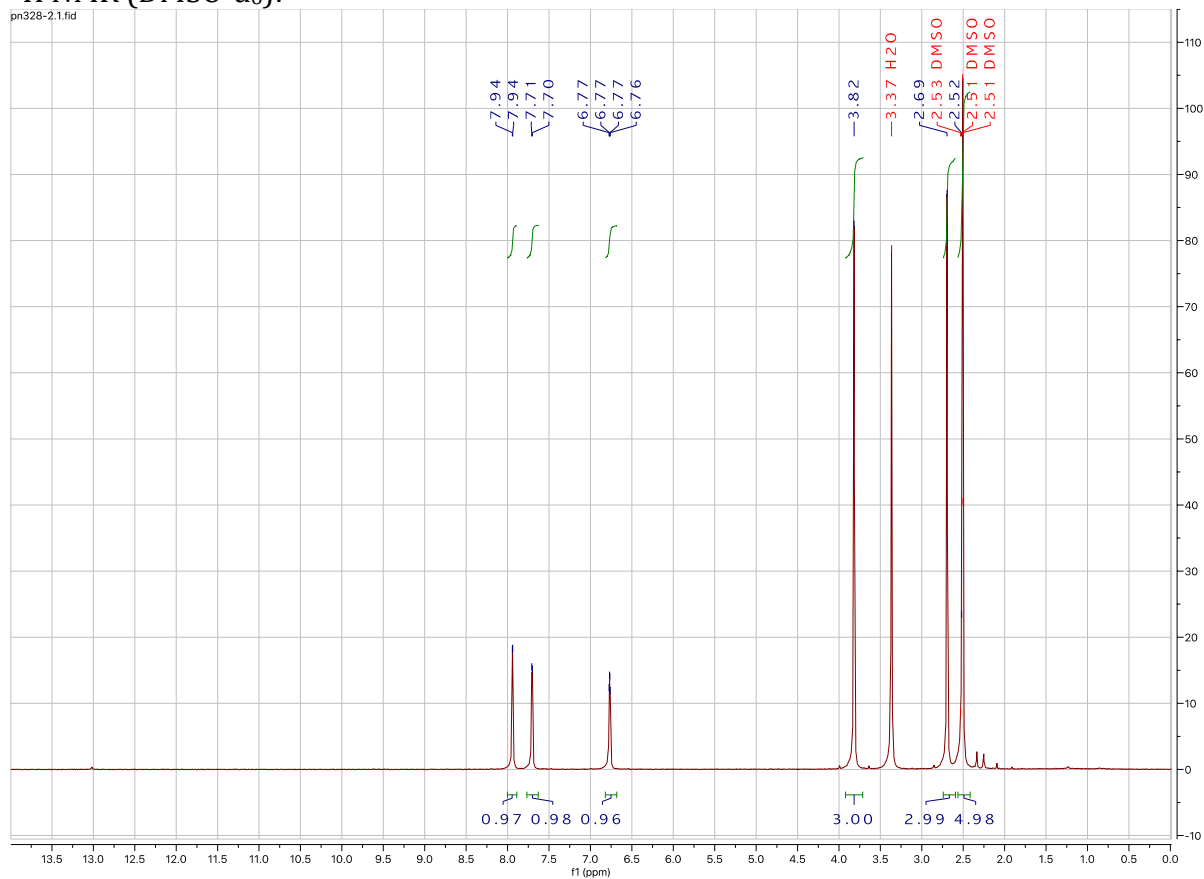
4-Acetyl-2-(furan-2-yl)-1,5-dimethyl-1H-imidazole 3-oxide (**3a**).



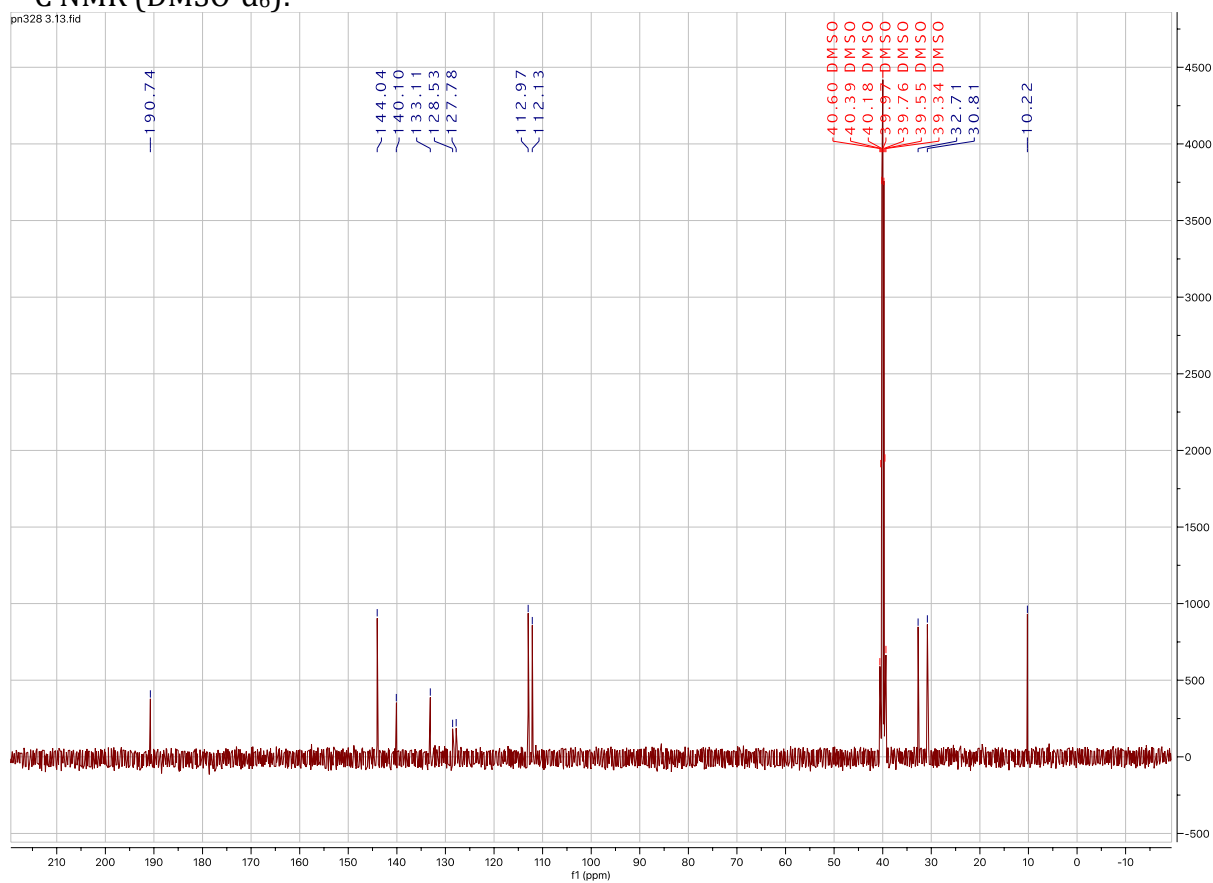
^1H NMR (CDCl_3):



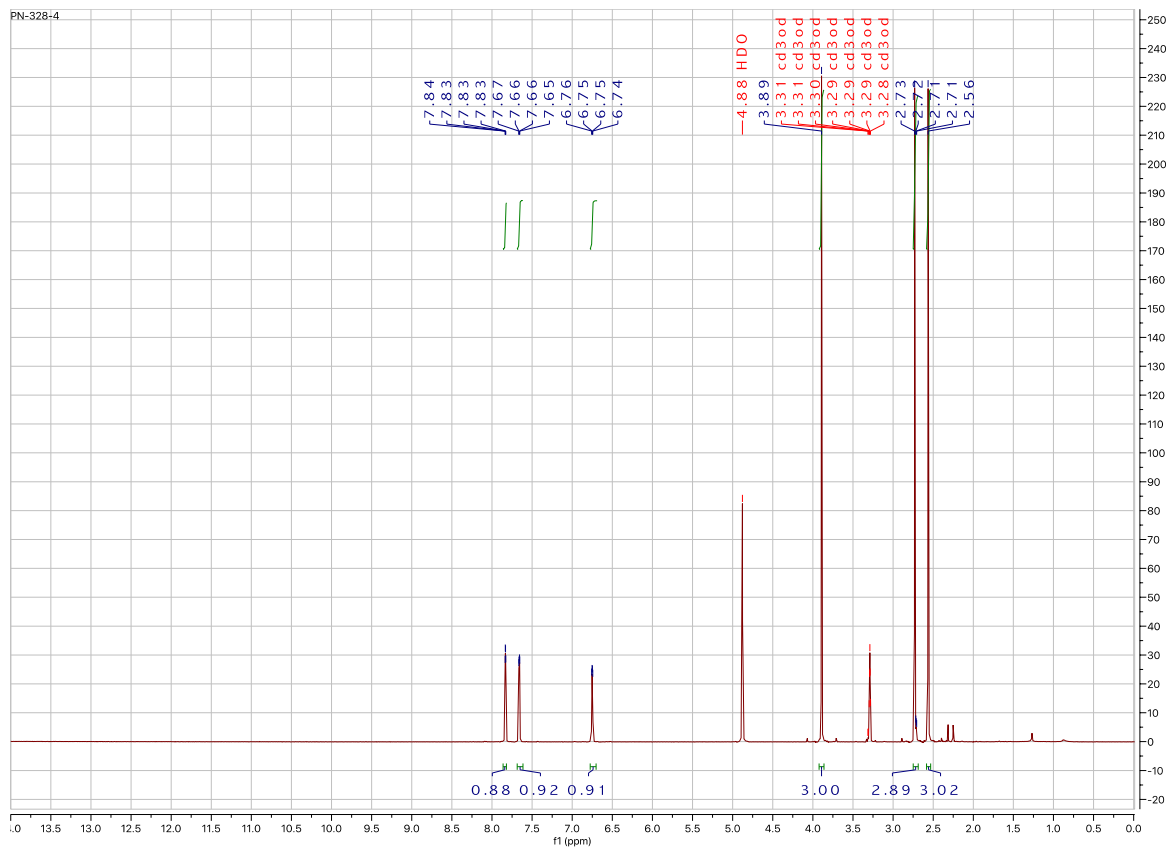
¹H NMR (DMSO-d₆):



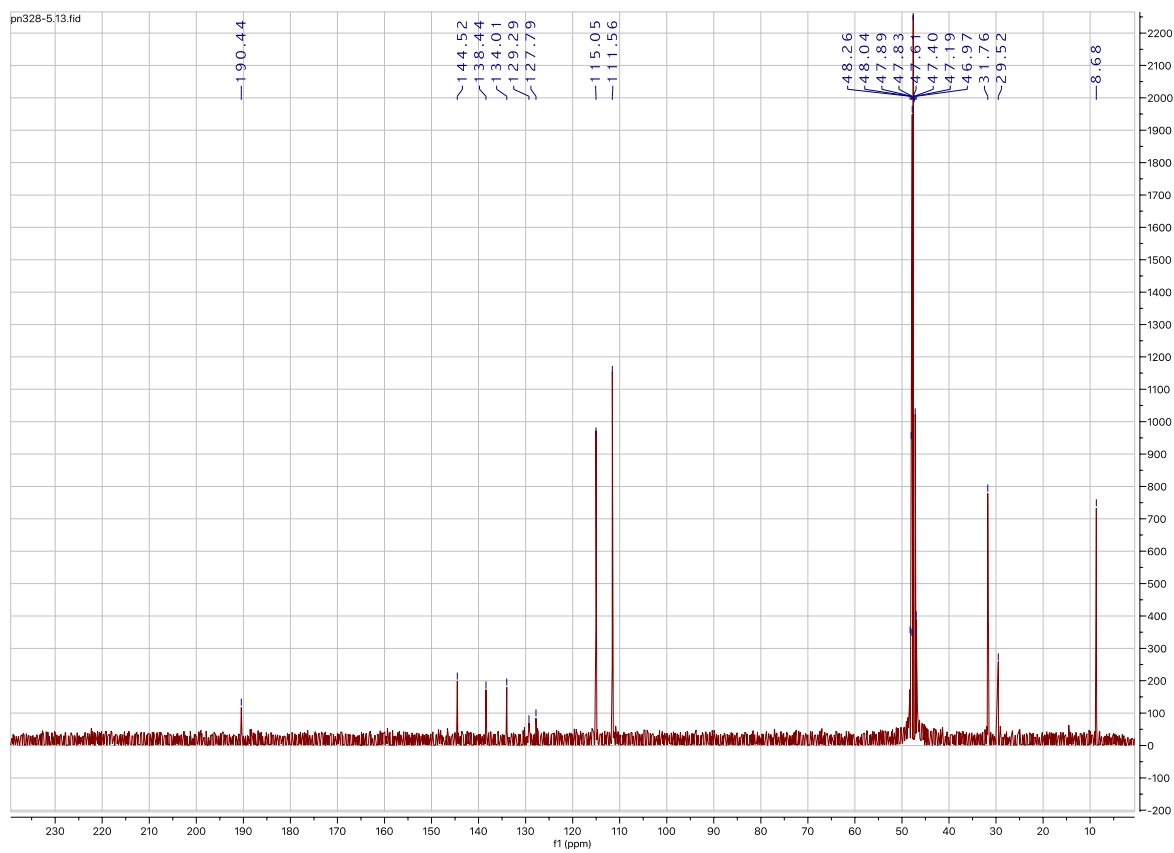
¹³C NMR (DMSO-d₆):



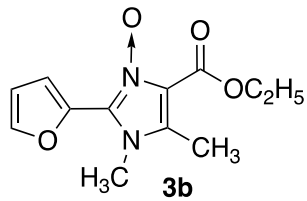
^1H NMR spectrum in CD_3OD :



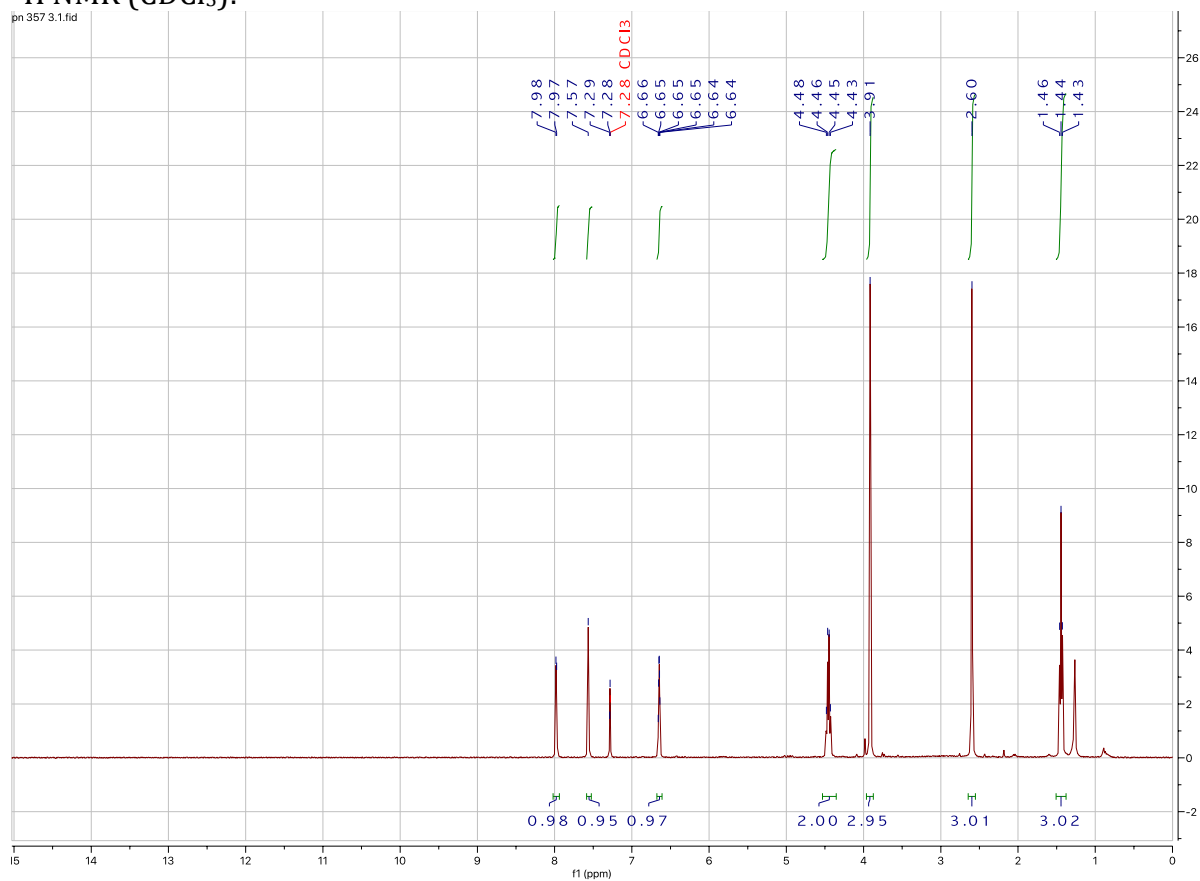
^{13}C NMR spectrum in CD_3OD :



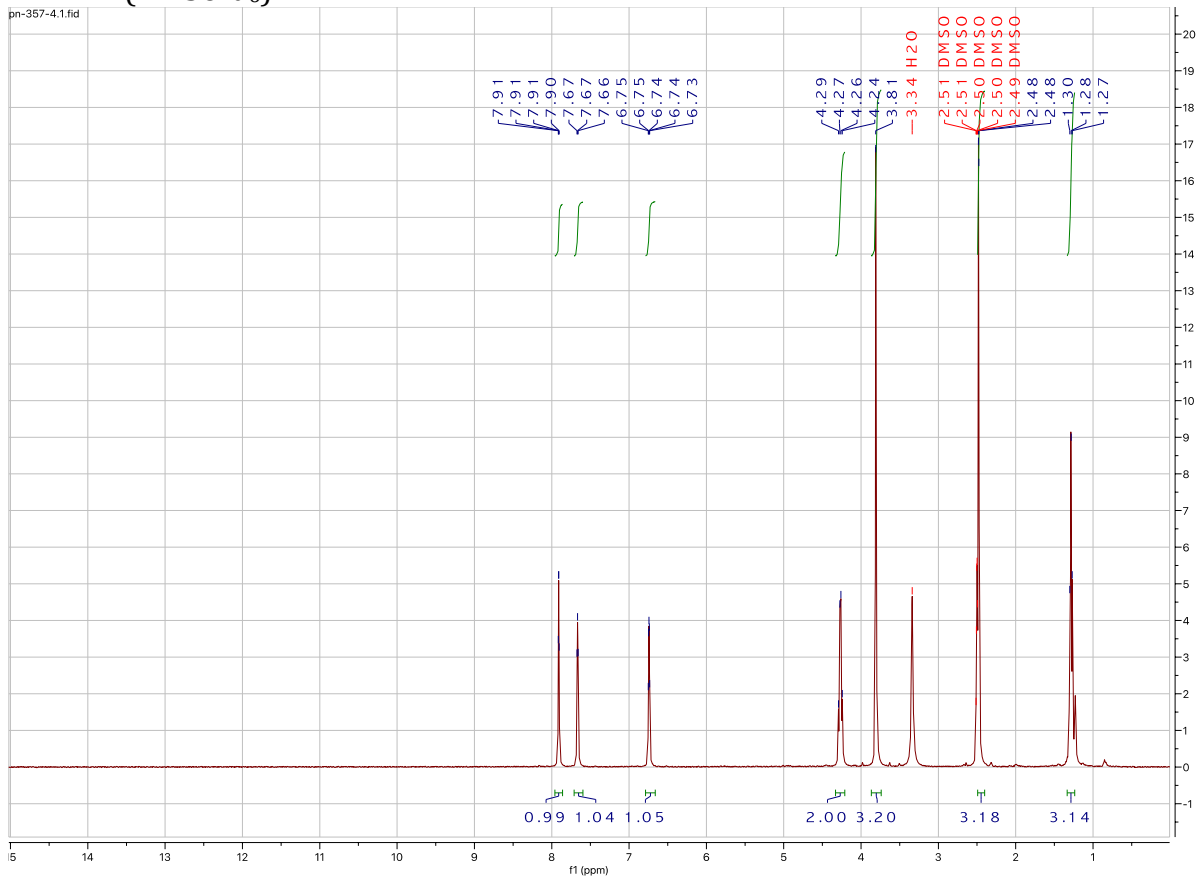
4-(Ethoxycarbonyl)-2-(furan-2-yl)-1,5-dimethyl-1H-imidazole 3-oxide (**3b**).



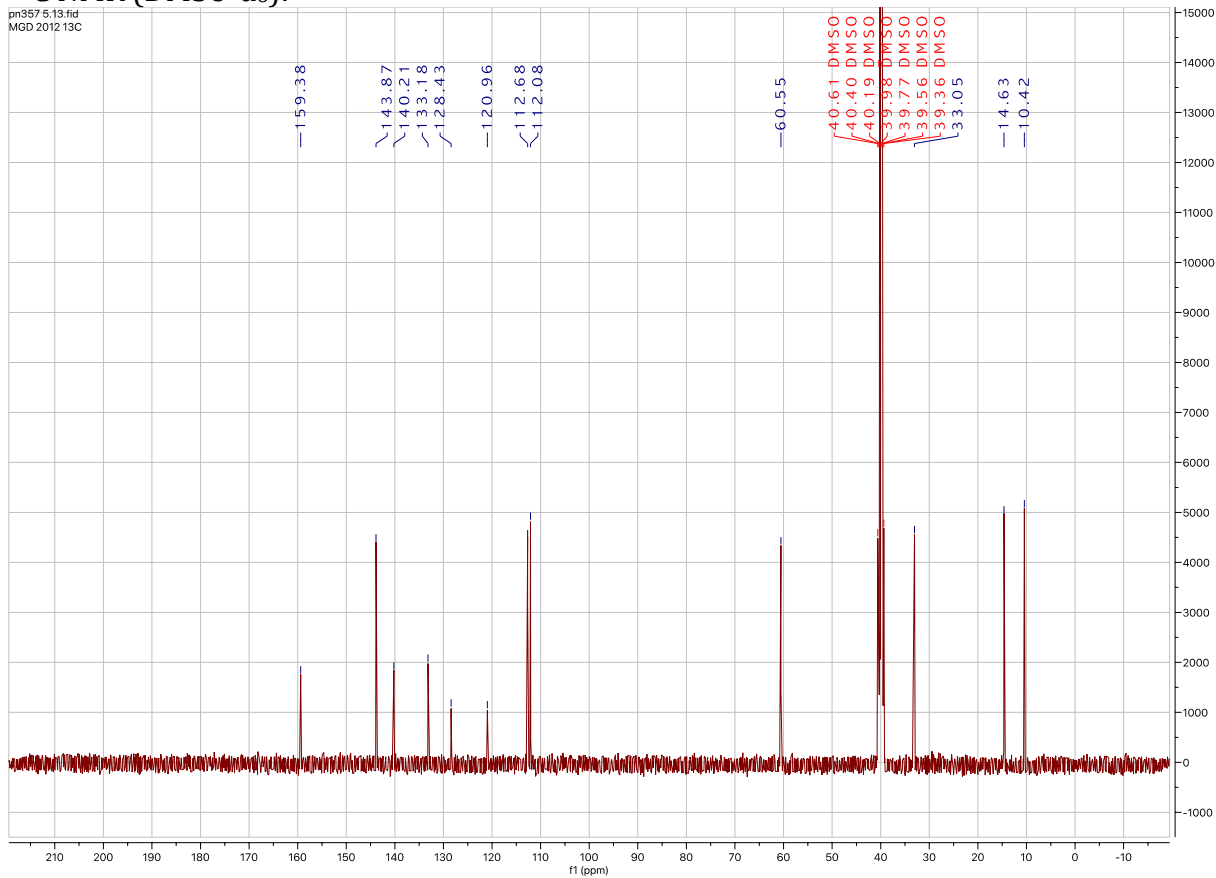
^1H NMR (CDCl_3):



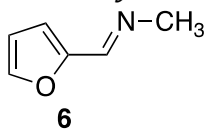
¹H NMR (DMSO-d₆):



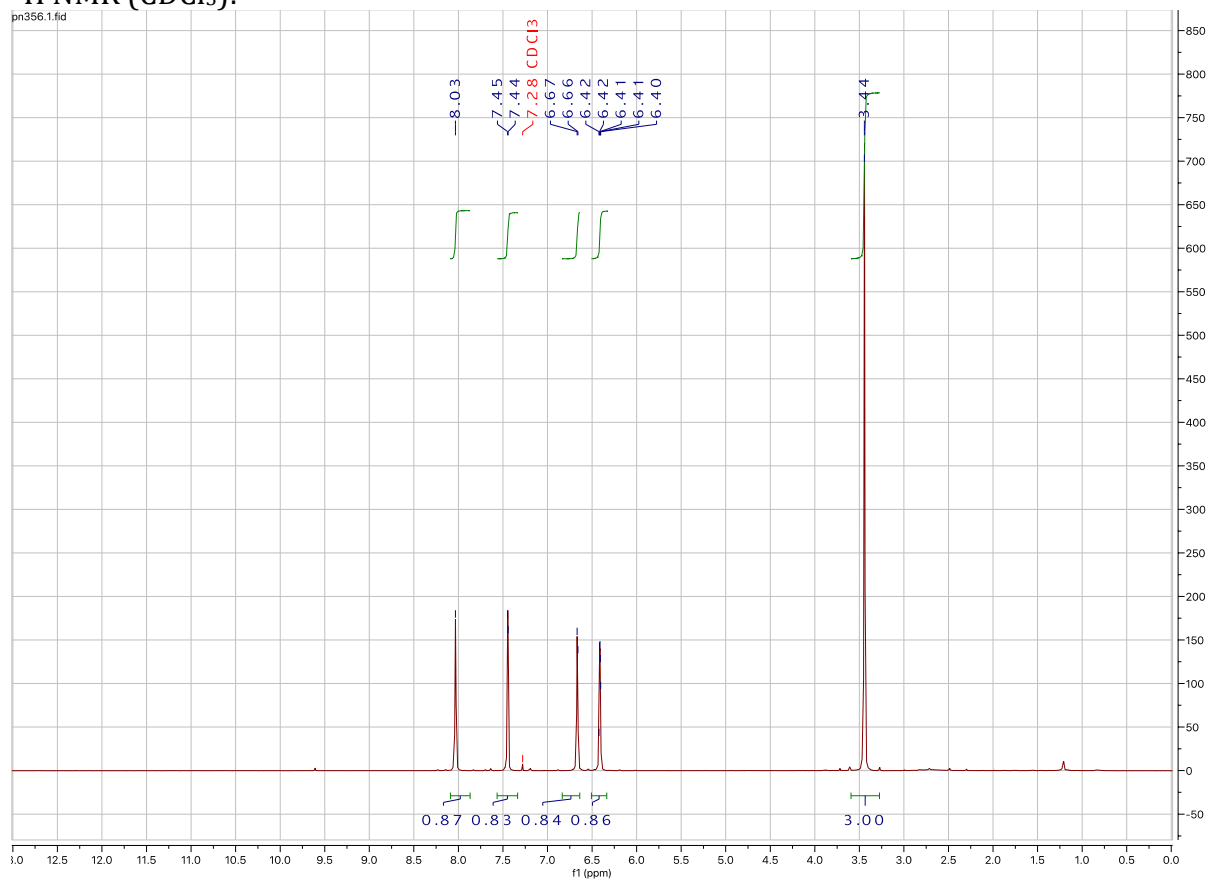
¹³C NMR (DMSO-d₆):



Furan-2-yl-N-methylmethanimine (**6**)

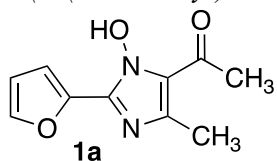


¹H NMR (CDCl₃):



2. Copies of 2D NMR spectra of compounds 1a, 2a, 3a.

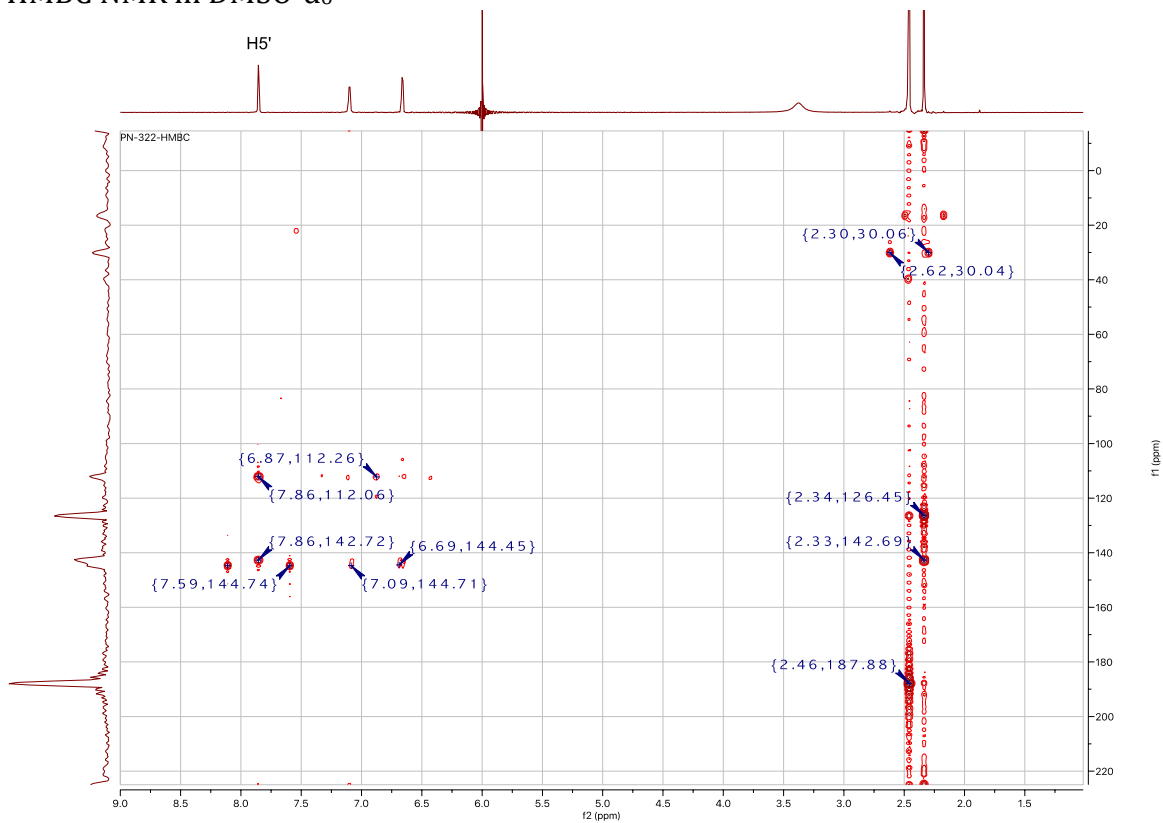
1-(2-(Furan-2-yl)-1-hydroxy-4-methyl-1H-imidazol-5-yl)ethanone (1a)



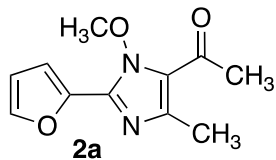
2D HSQC NMR in DMSO-d₆



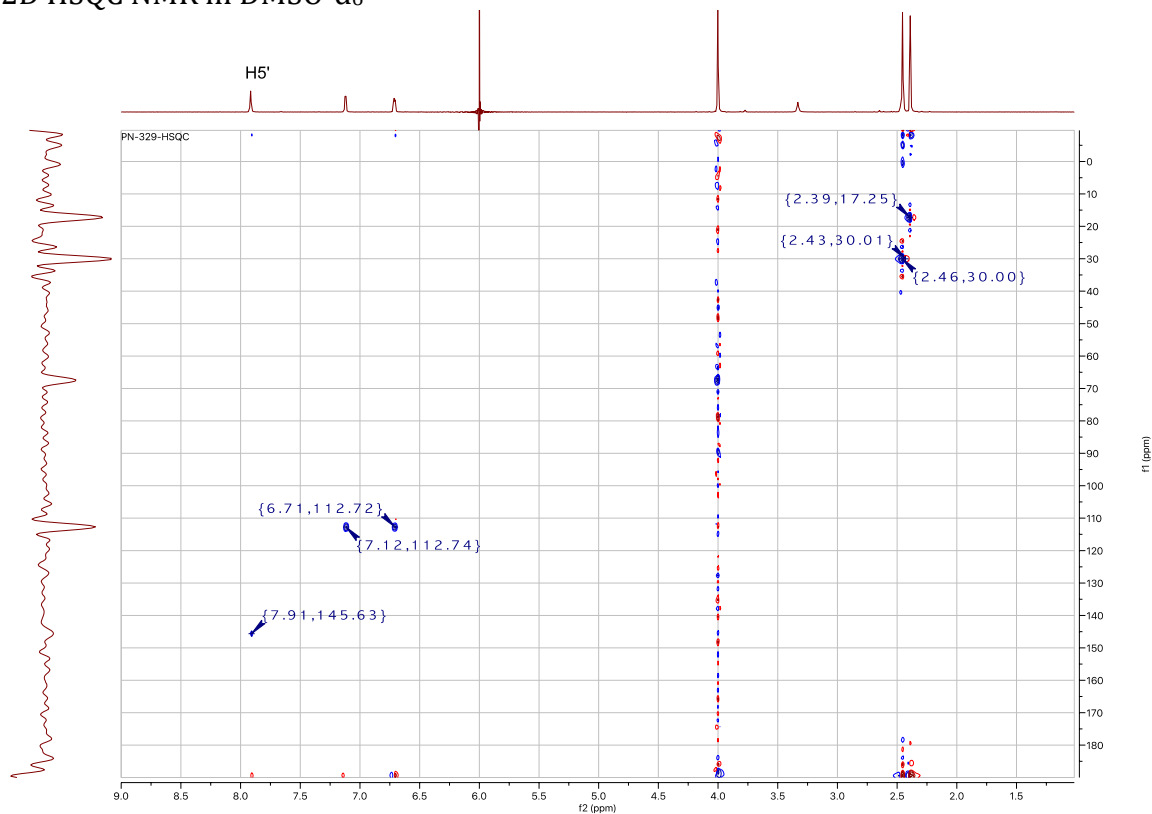
2D HMBC NMR in DMSO-d₆



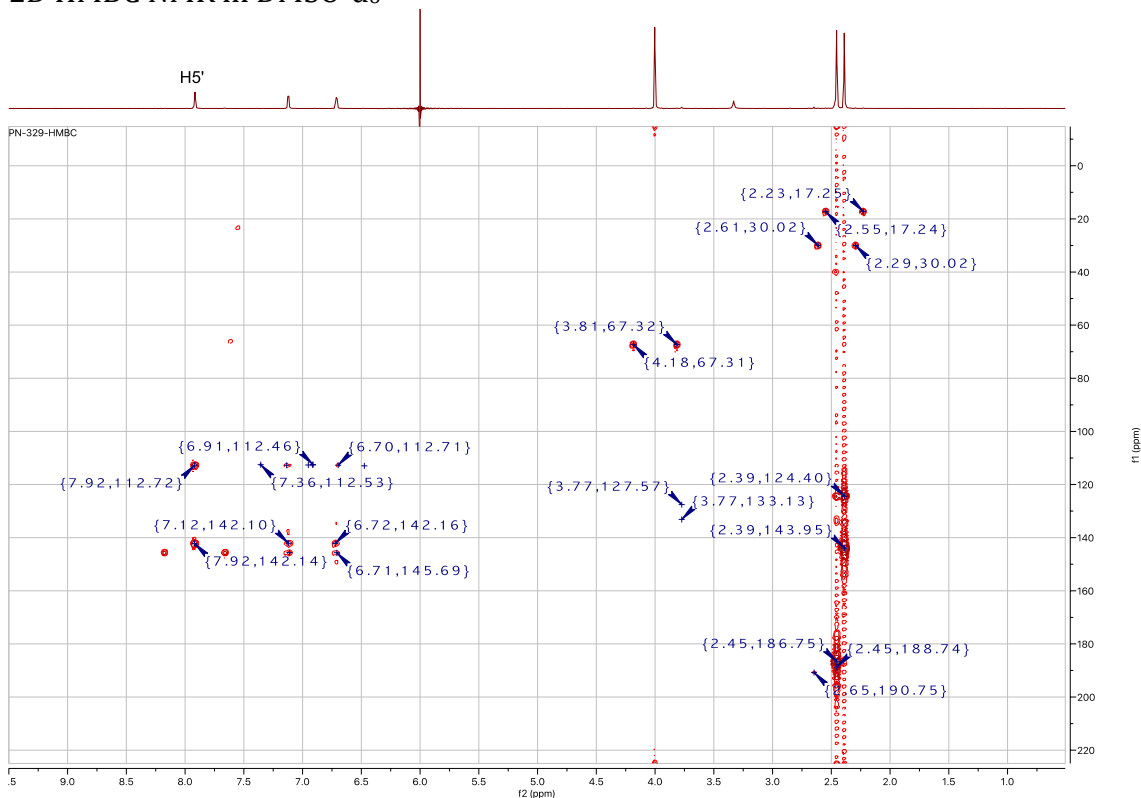
1-(2-(Furan-2-yl)-1-methoxy-4-methyl-1H-imidazol-5-yl)ethanone (2a)



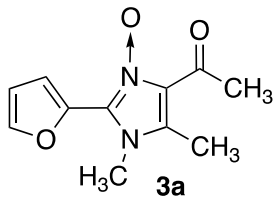
2D HSQC NMR in DMSO-d₆



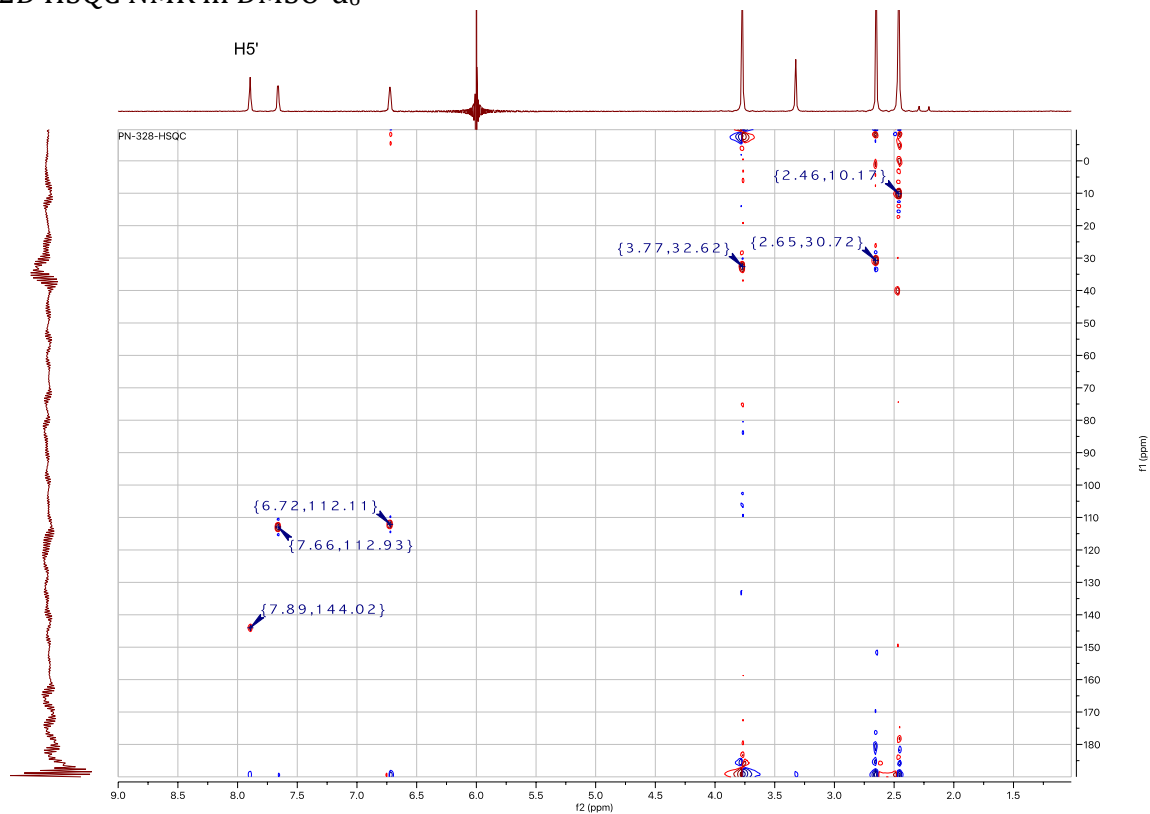
2D HMBC NMR in DMSO-d₆



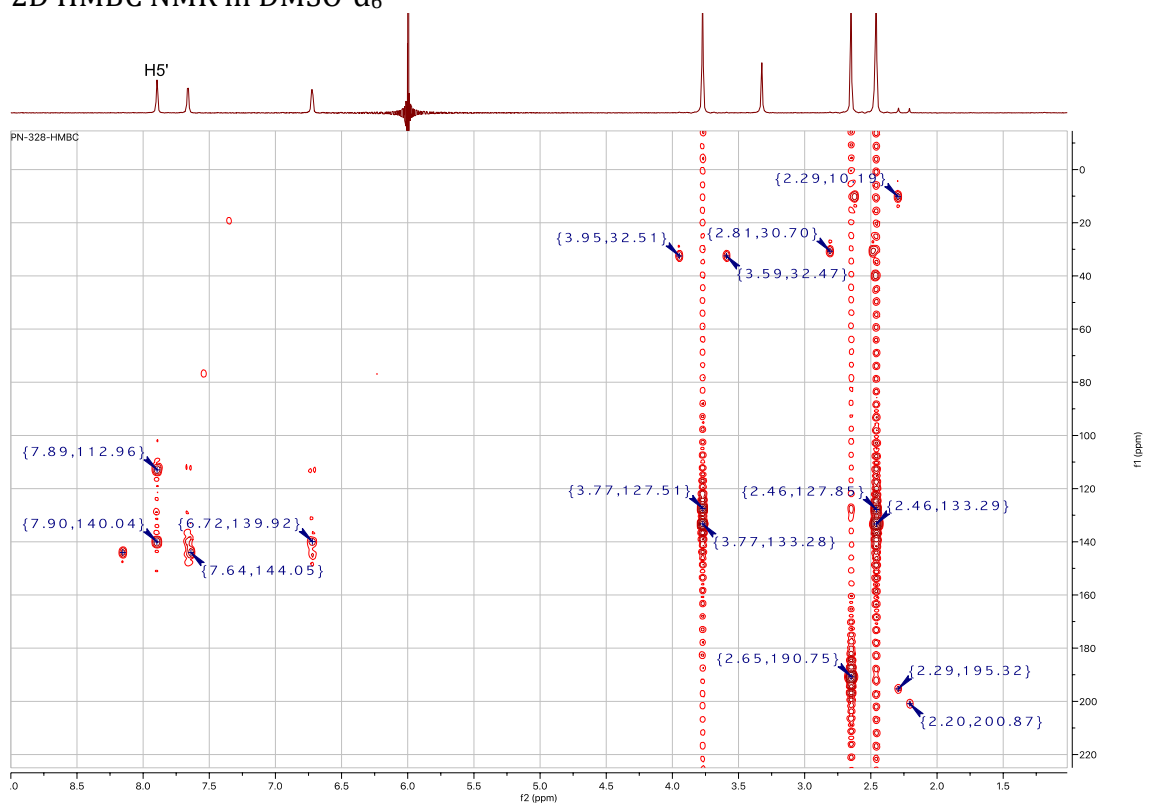
4-Acetyl-2-(furan-2-yl)-1,5-dimethyl-1H-imidazole 3-oxide (**3a**).



2D HSQC NMR in DMSO-d₆

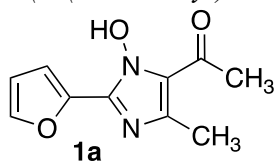


2D HMBC NMR in DMSO-d₆

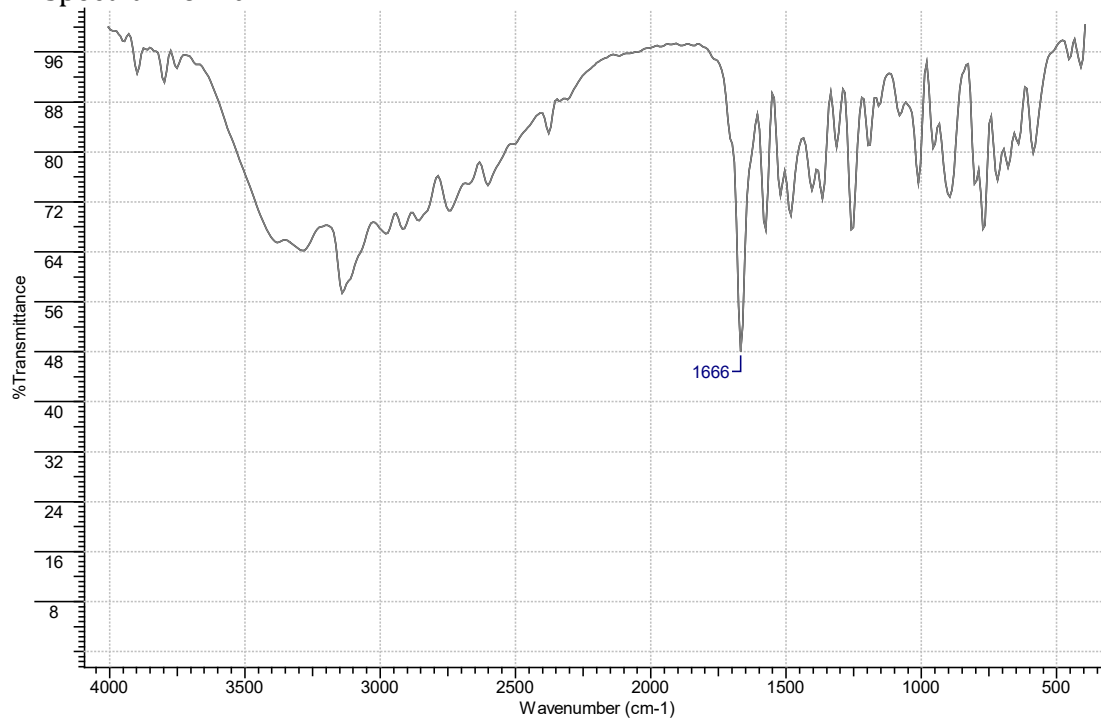


3. Copies of IR spectra of compounds under consideration

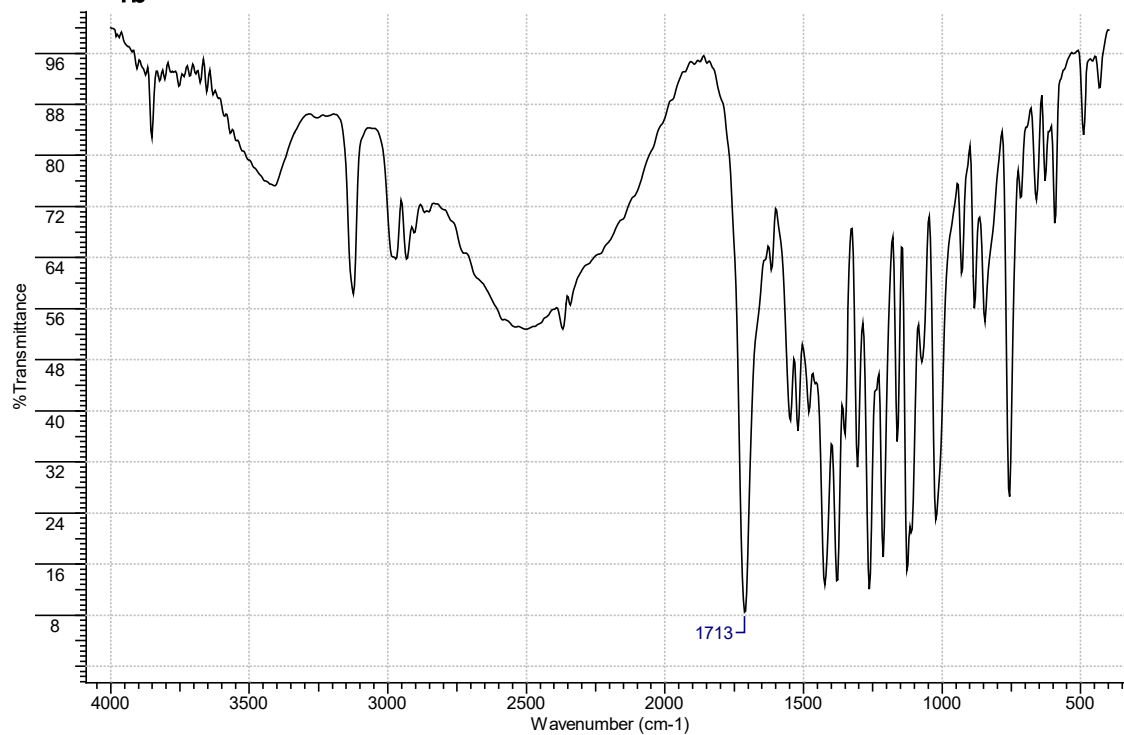
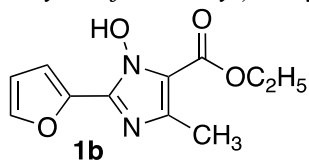
1-(2-(Furan-2-yl)-1-hydroxy-4-methyl-1H-imidazol-5-yl)ethanone (1a)



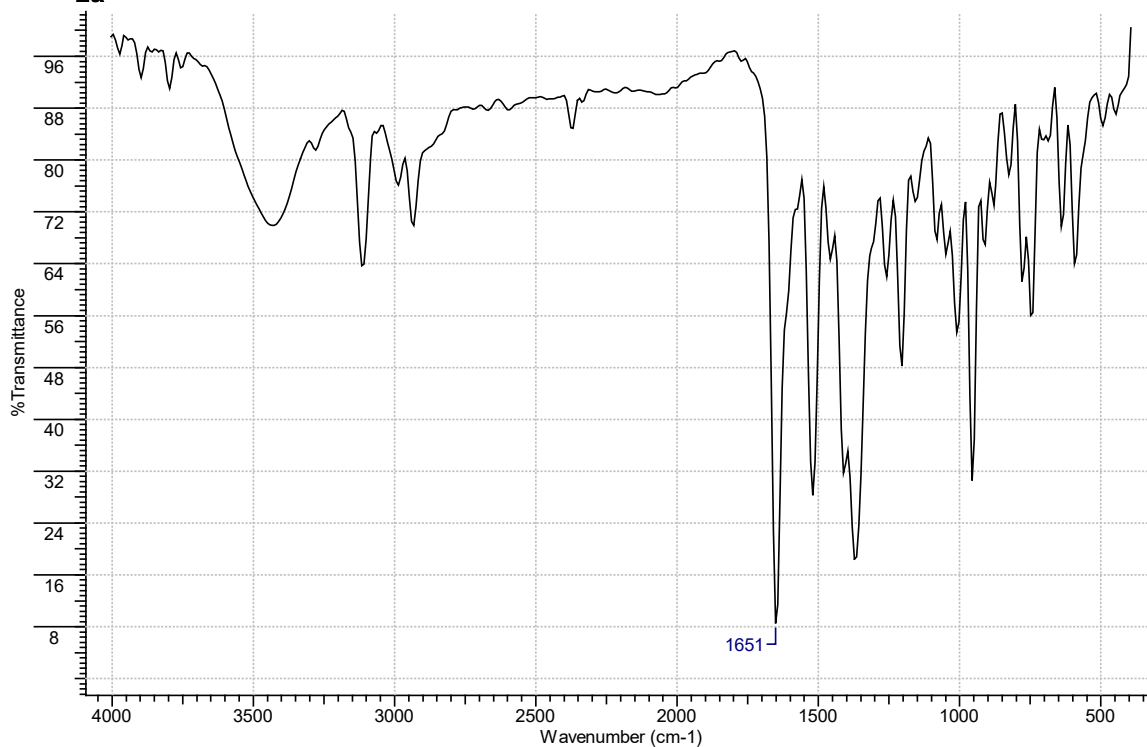
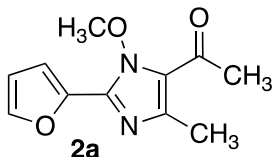
IR spectrum of **1a** in KBr:



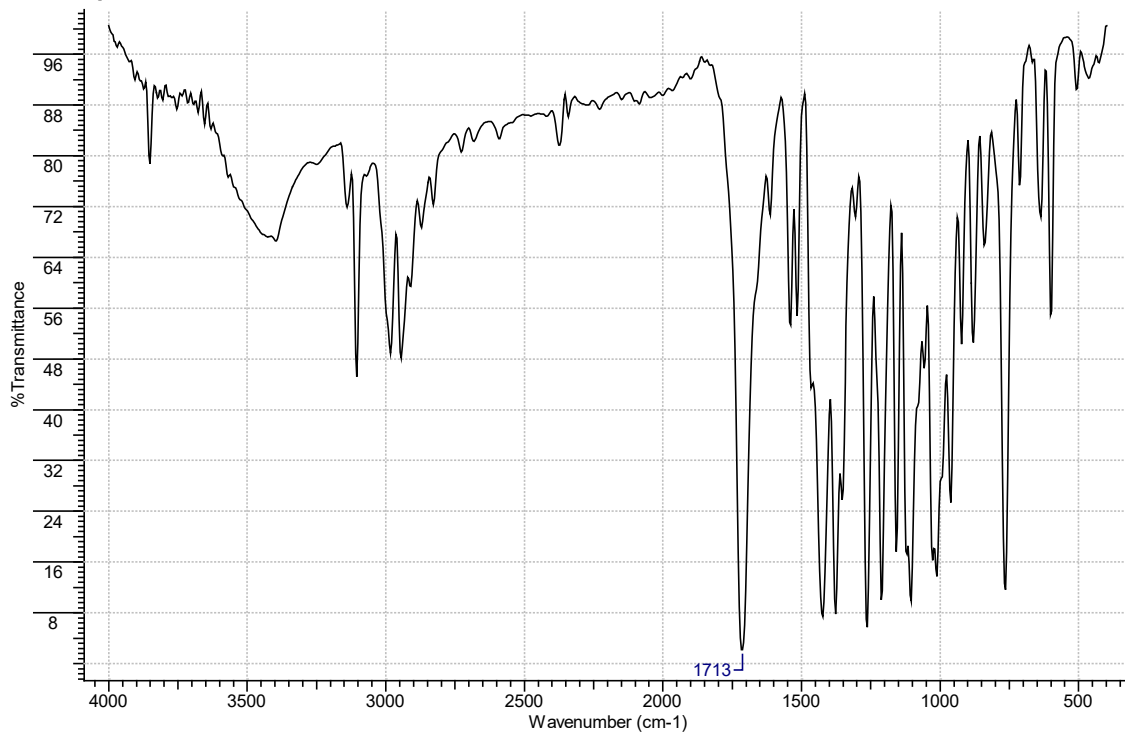
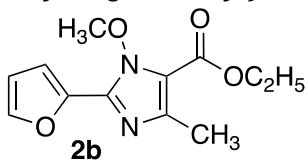
Ethyl 2-(furan-2-yl)-1-hydroxy-4-methyl-1H-imidazole-5-carboxylate (1b)



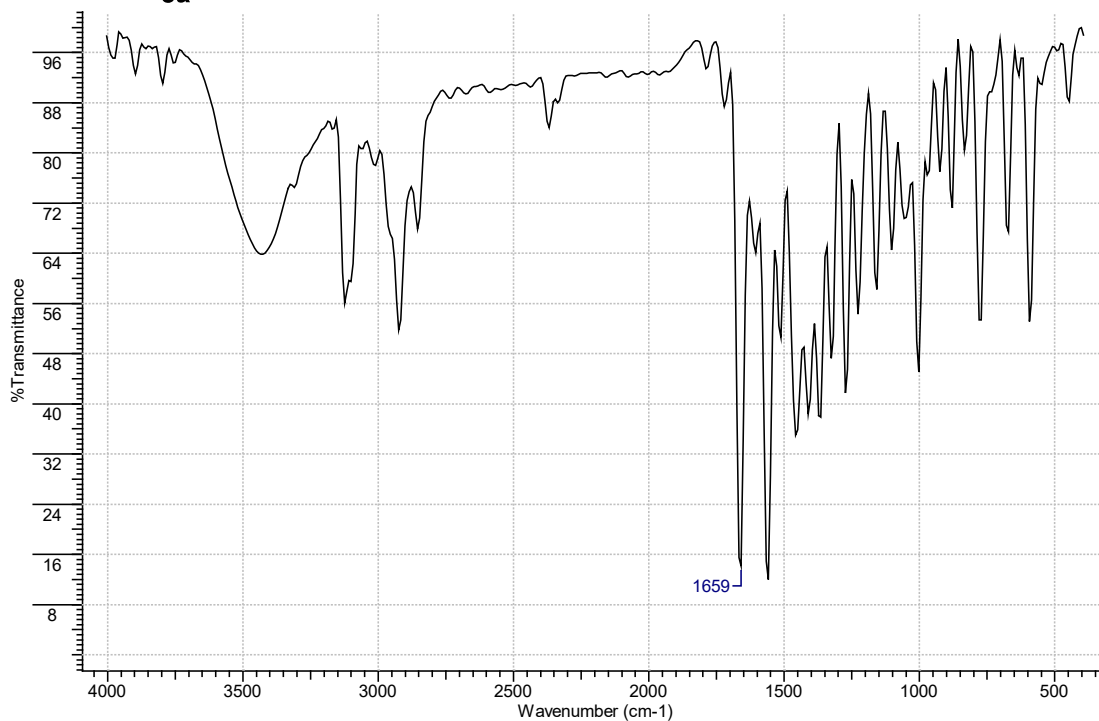
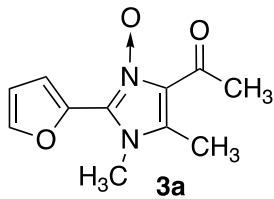
1-(2-(Furan-2-yl)-1-methoxy-4-methyl-1H-imidazol-5-yl)ethanone (2a)



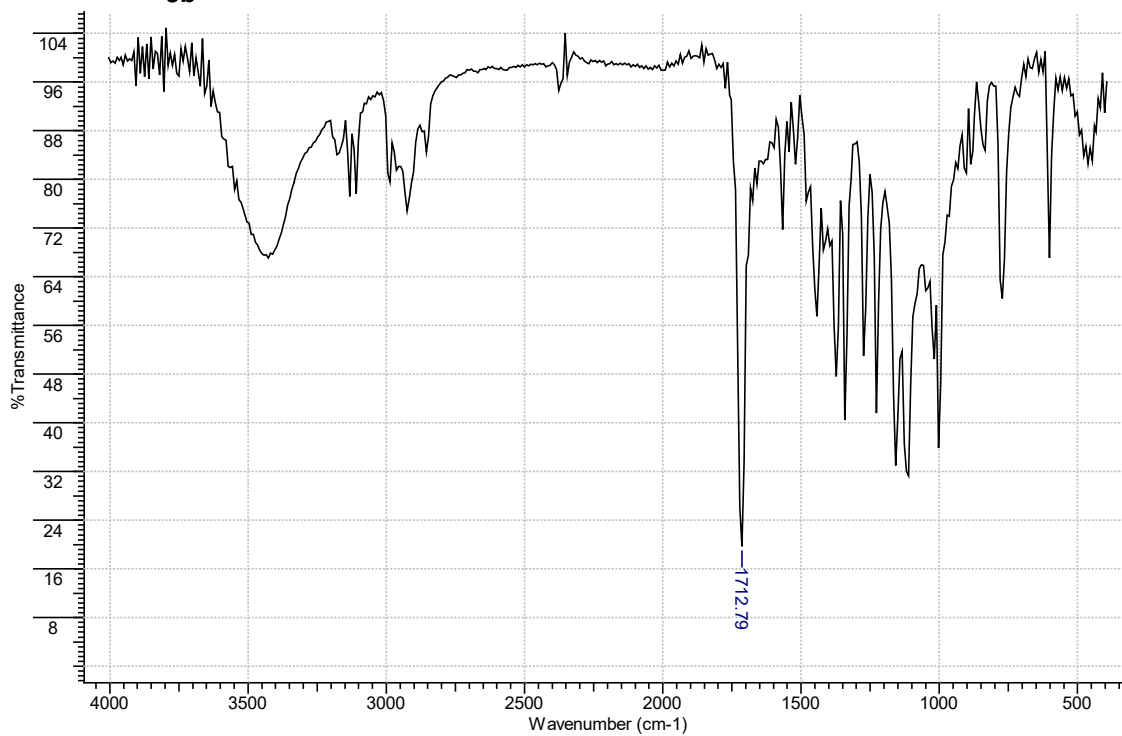
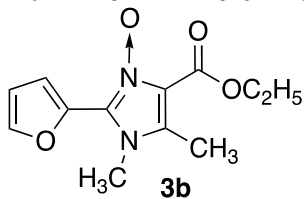
Ethyl 2-(furan-2-yl)-1-methoxy-4-methyl-1H-imidazole-5-carboxylate (2b)



4-Acetyl-2-(furan-2-yl)-1,5-dimethyl-1H-imidazole 3-oxide (**3a**).

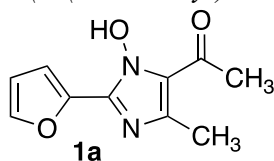


4-(Ethoxycarbonyl)-2-(furan-2-yl)-1,5-dimethyl-1H-imidazole 3-oxide (**3b**).



4. Copies of HRMS spectra of compounds under consideration

1-(2-(Furan-2-yl)-1-hydroxy-4-methyl-1H-imidazol-5-yl)ethanone (1a)



Display Report

Analysis Info

Analysis Name D:\Data\Kolotyrkina\2020\Mityanov\0122007.d
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Sample Name /MBCI PN-322
Comment C10H10N2O3 mH 207.0764 calibrant added CH3CN

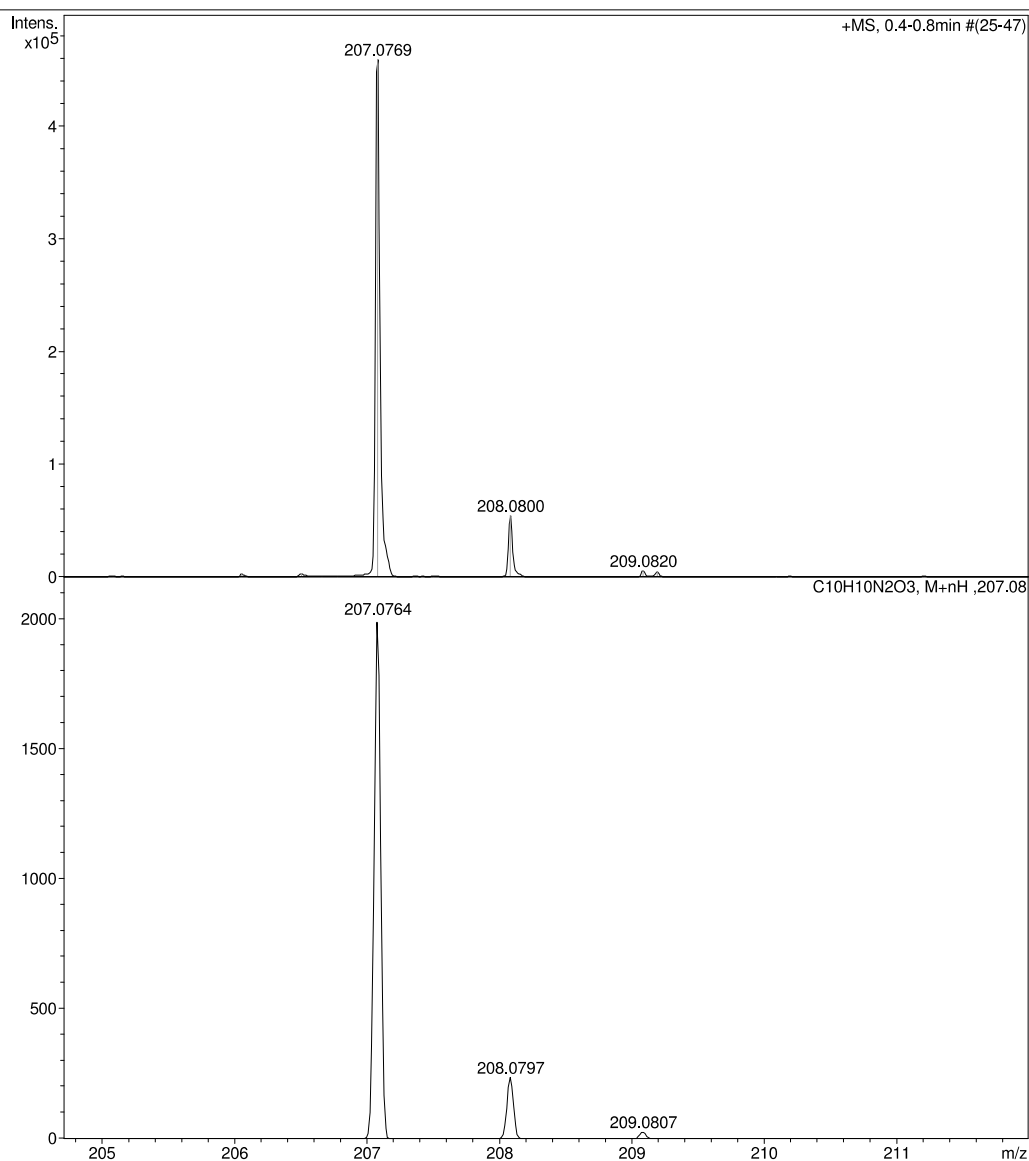
Acquisition Date 22.01.2020 13:24:57

Operator BDAL@DE

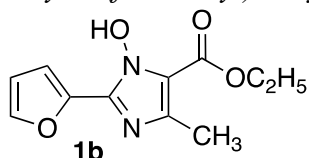
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

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Ethyl 2-(furan-2-yl)-1-hydroxy-4-methyl-1H-imidazole-5-carboxylate (1b)



Display Report

Analysis Info

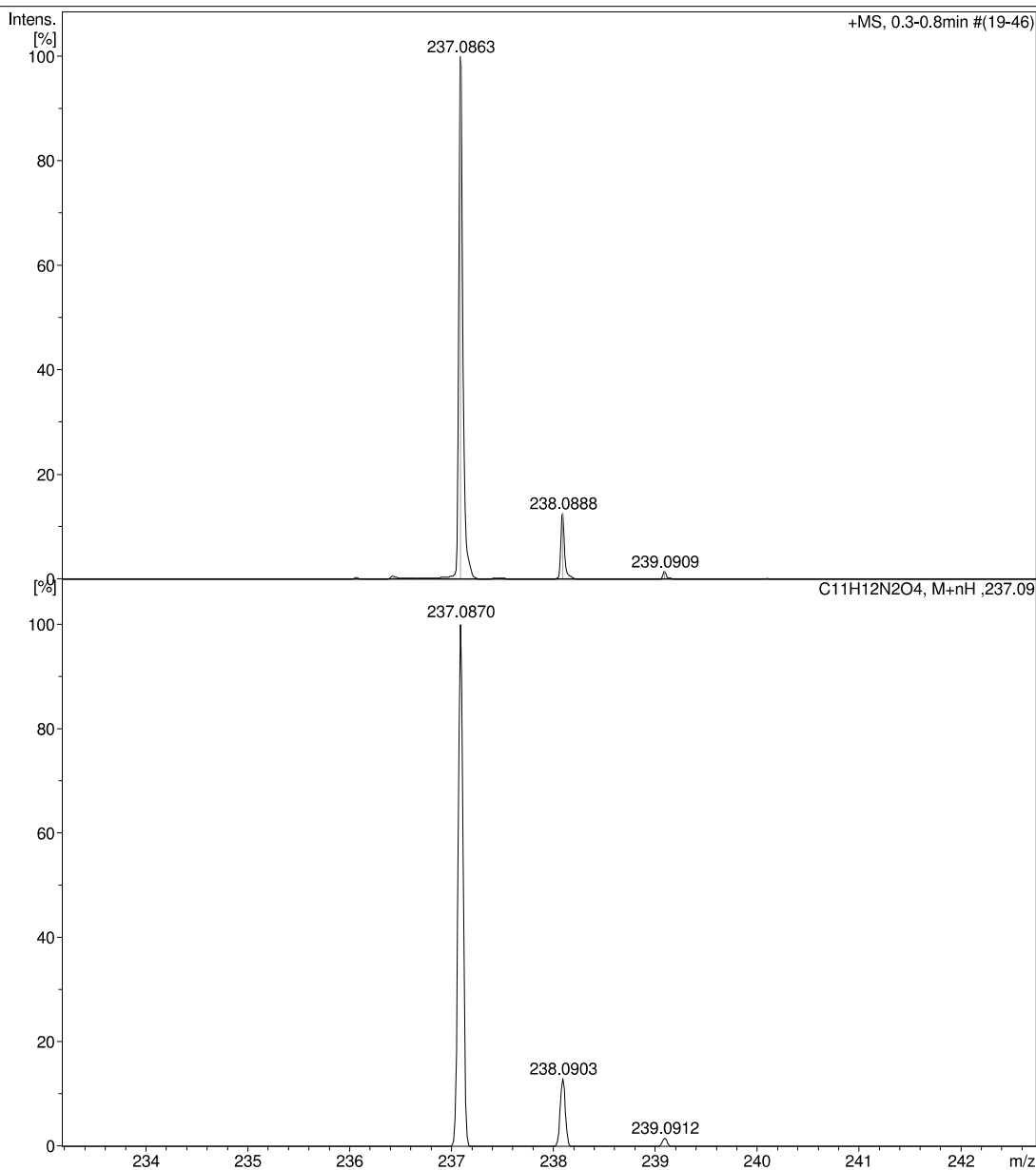
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Acquisition Date 22.01.2020 15:00:21

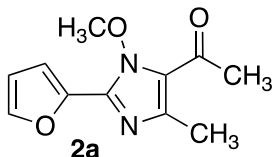
Operator BDAL@DE
Instrument / Ser# microTOF 10248

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Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



1-(2-(Furan-2-yl)-1-methoxy-4-methyl-1H-imidazol-5-yl)ethanone (2a)



Display Report

Analysis Info

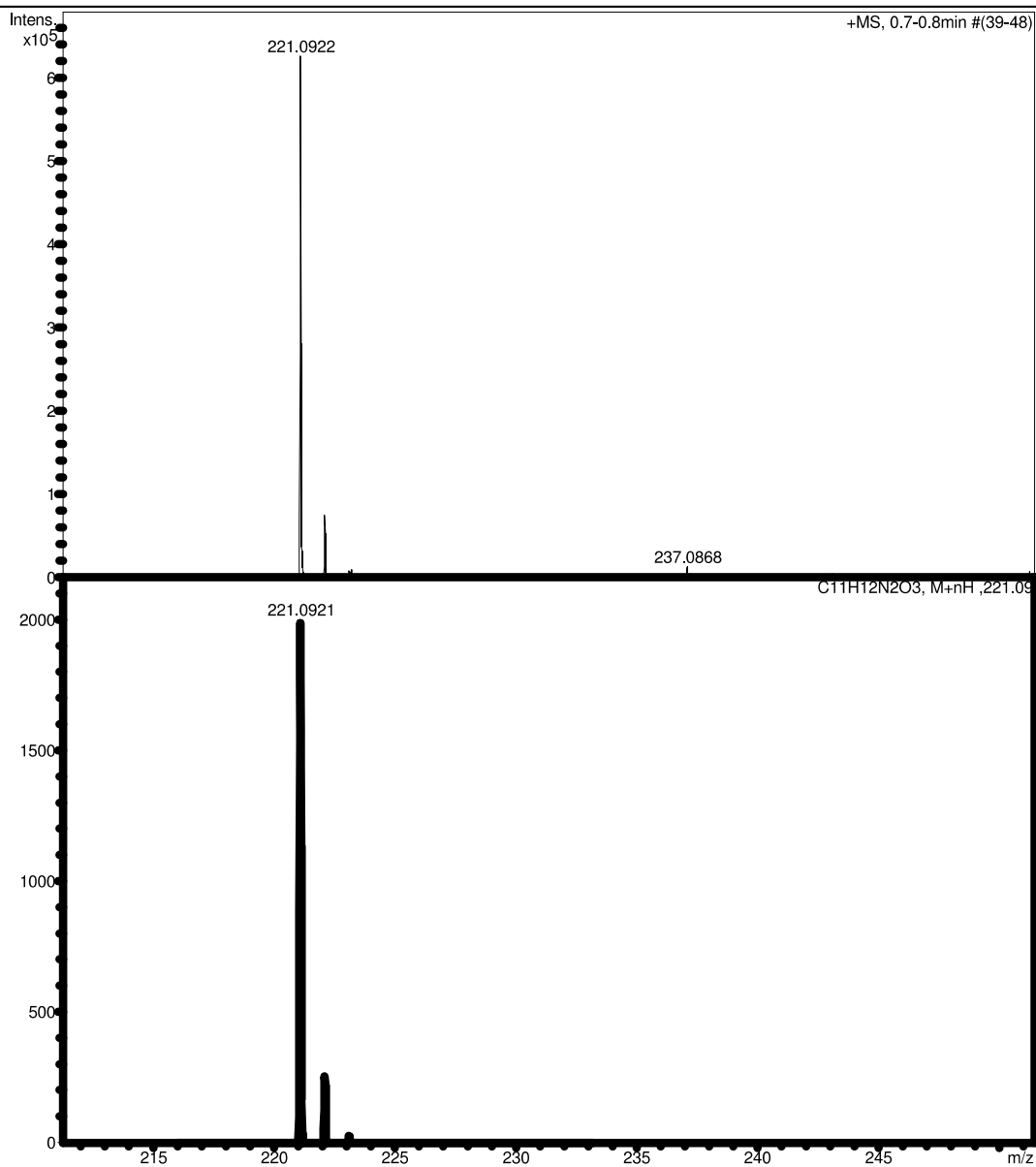
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Acquisition Date 22.01.2020 13:52:00

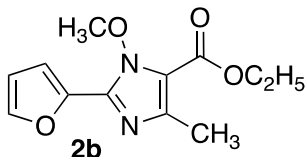
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

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Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Ethyl 2-(furan-2-yl)-1-methoxy-4-methyl-1H-imidazole-5-carboxylate (**2b**)



Display Report

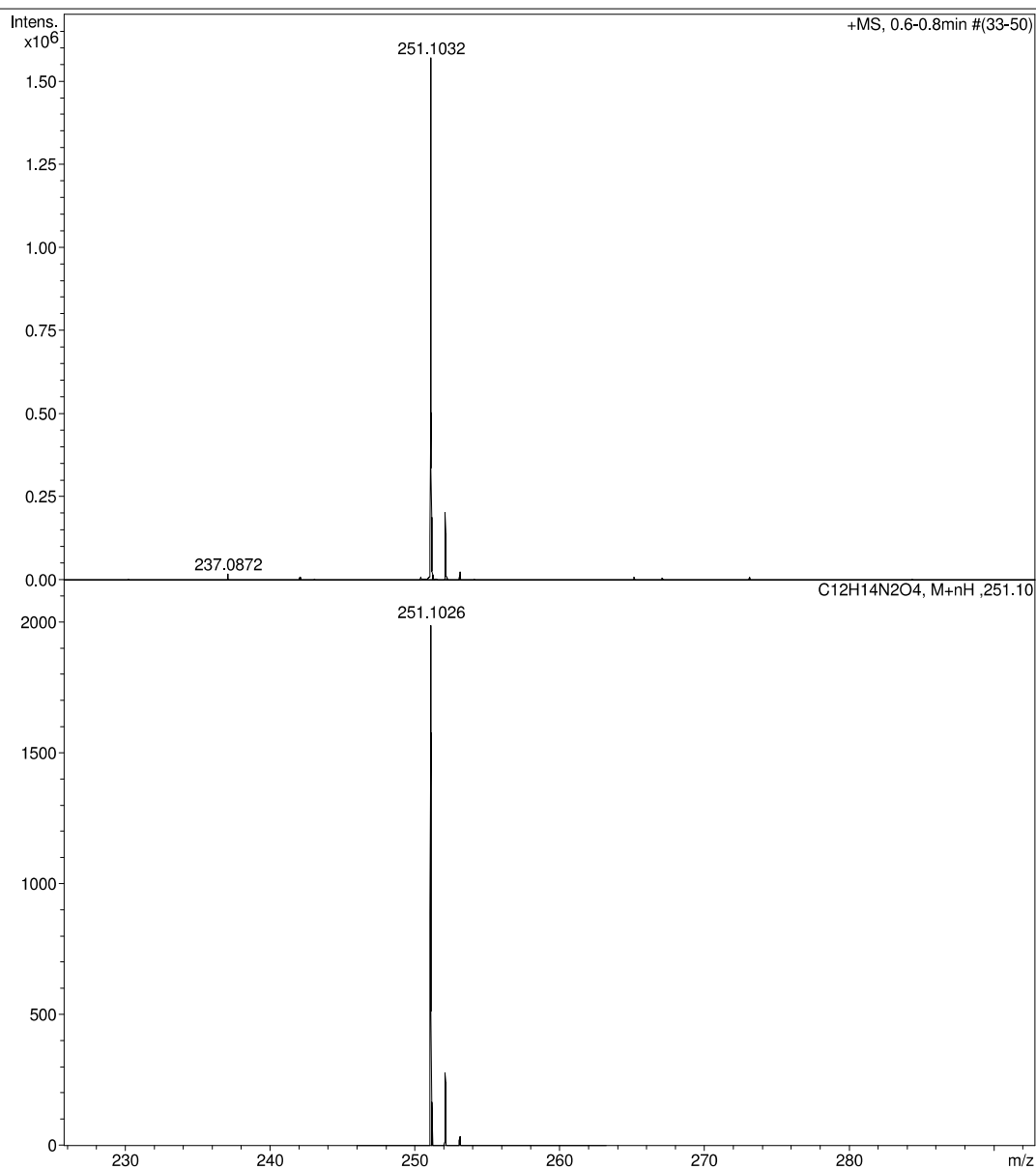
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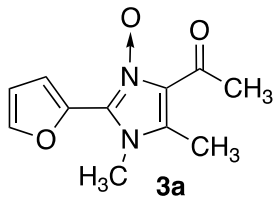
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Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

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Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



4-Acetyl-2-(furan-2-yl)-1,5-dimethyl-1H-imidazole 3-oxide (**3a**).



Display Report

Analysis Info

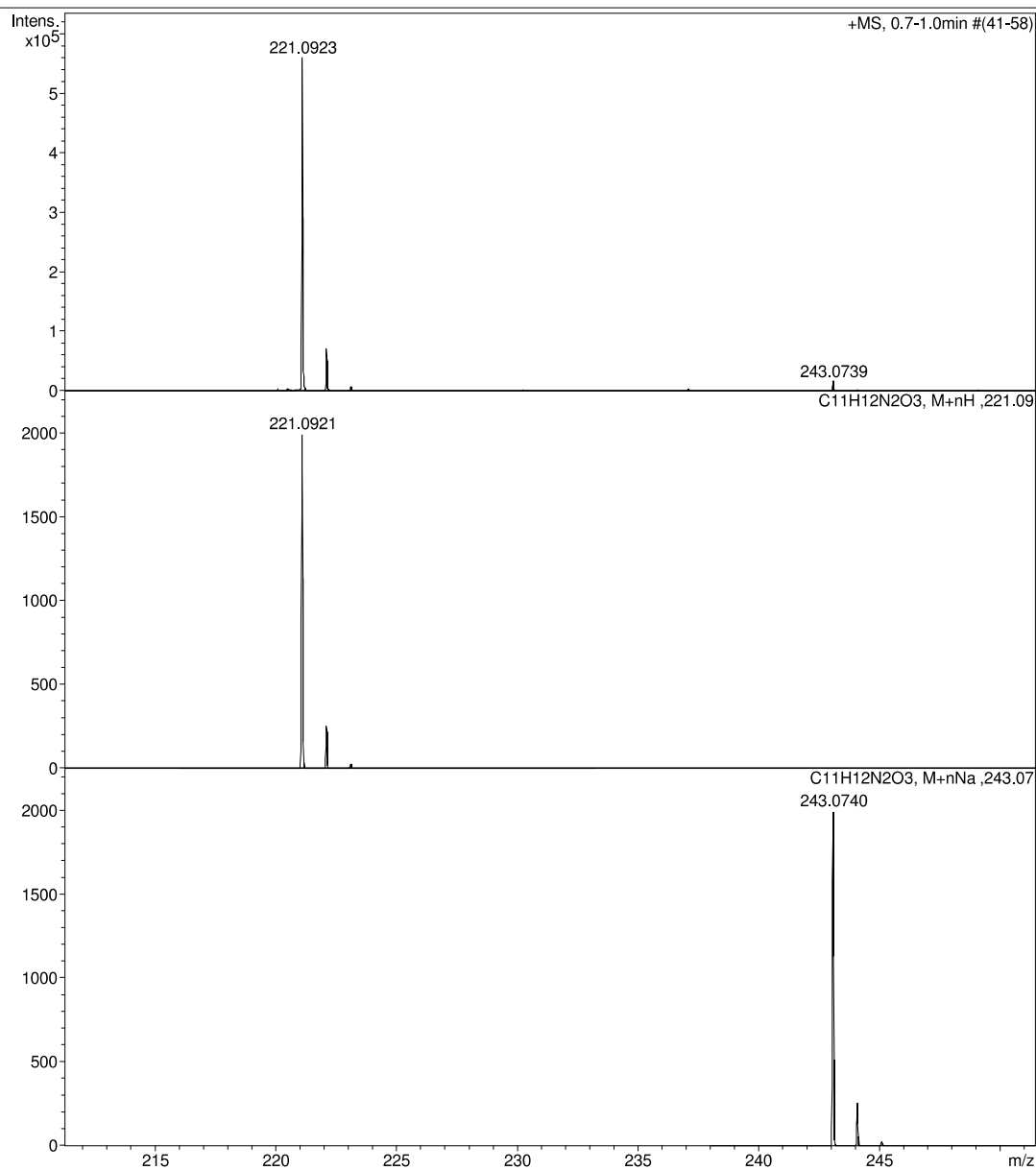
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Acquisition Date 22.01.2020 13:47:19

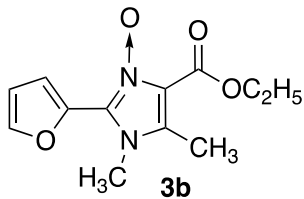
Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



4-(Ethoxycarbonyl)-2-(furan-2-yl)-1,5-dimethyl-1H-imidazole 3-oxide (**3b**).



Display Report

Analysis Info

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Acquisition Date 22.01.2020 14:02:16

Operator BDAL@DE
Instrument / Ser# micrOTOF 10248

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1600 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste

