10.1071/CH19222_AC

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Supplementary Material

Prototropic Tautomerism and Some Features of IR Spectra of 2-(3-Chromenyl)-1-hydroxyimidazoles

Polina A. Nikitina,[A,B,D] Tatiana Yu. Koldaeva,[A] Vitaly S. Mityanov,[A,C] Vladimir S. Miroshnikov,[A] Elizaveta I. Basanova,[A] and Valery P. Perevalov[A]

[A]Department of Fine Organic Synthesis and Chemistry of Dyes, D. I. Mendeleev University of Chemical Technology of Russia, Miusskaya sq., 9, Moscow, 125047, Russia.
[B]A. N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Vavilova str., 28, Moscow, 119991, Russia.
[C]N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Leninsky av., 47, Moscow, 119991, Russia.
[D]Corresponding author. Email: polinandrevna@yandex.ru

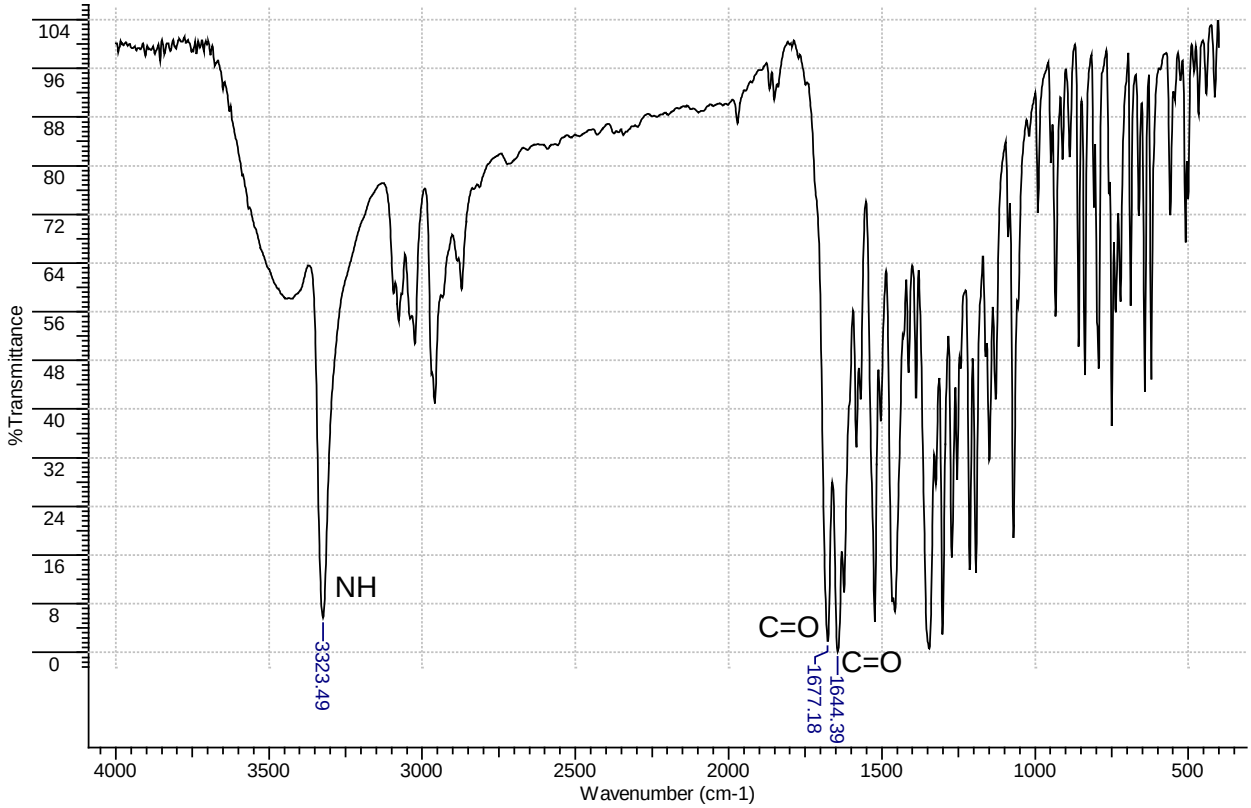
1. Copies of IR spectra of the compounds under consideration

2. Copies of ^{1}H and ^{13}C spectra of new compounds

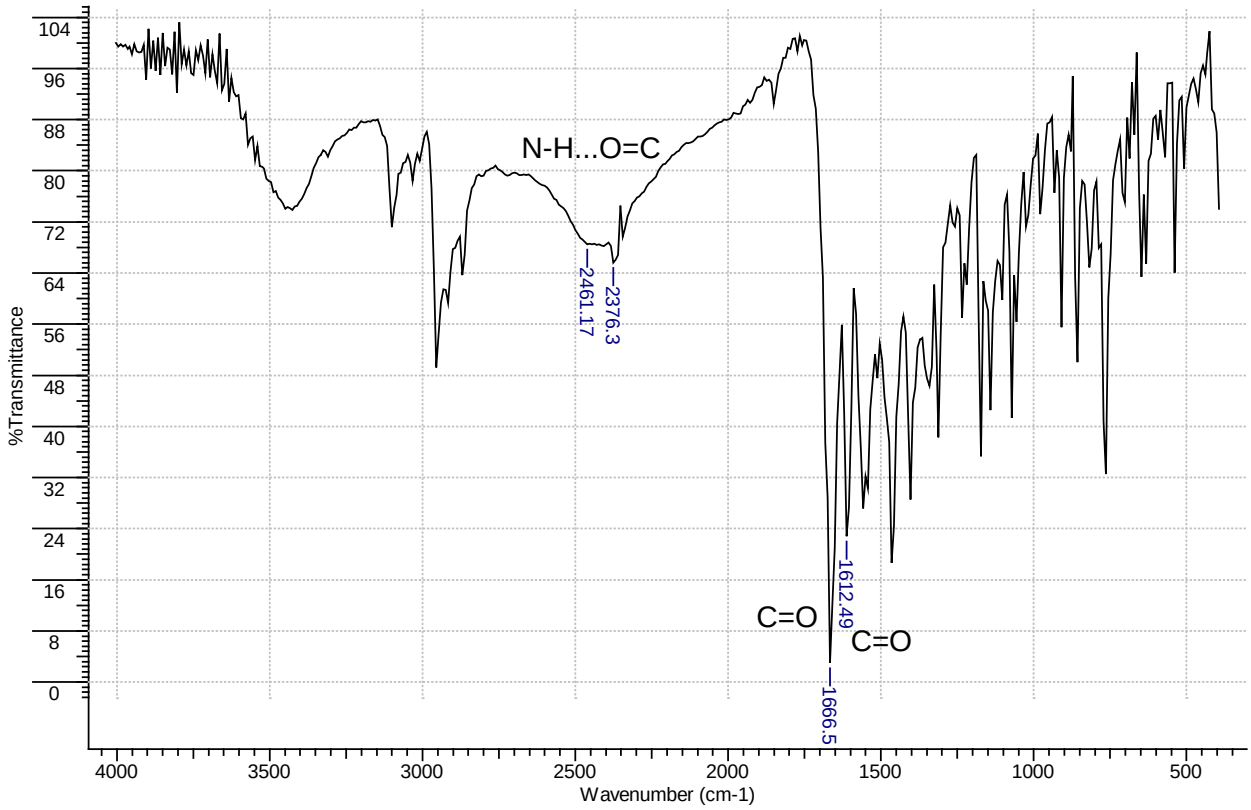
3. Copies of HRMS spectra of new compounds

1. Copies of IR spectra of compounds (KBr)

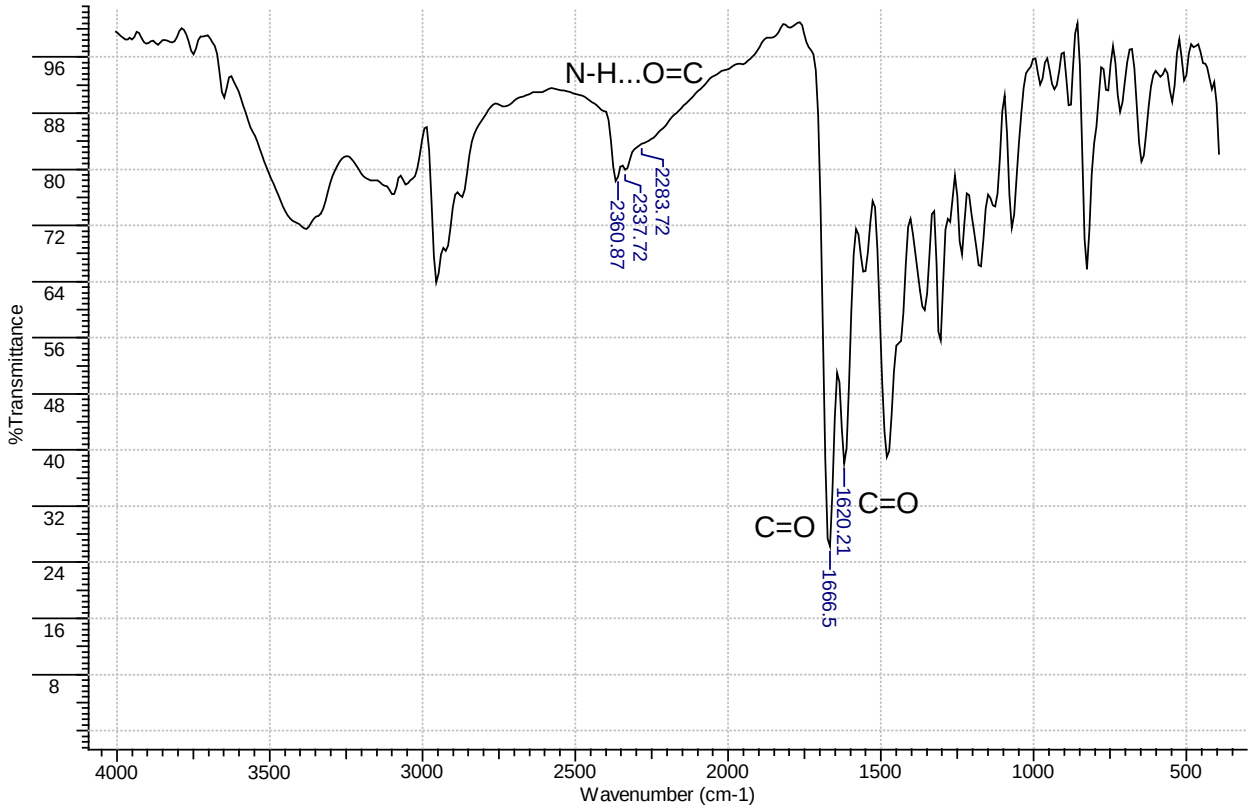
1.1. 1-Hydroxy-5,5-dimethyl-2-(6-nitro-4-oxo-4H-chromen-3-yl)-4,5,6,7-tetrahydro-4H-benzimidazol-7-one (1a)



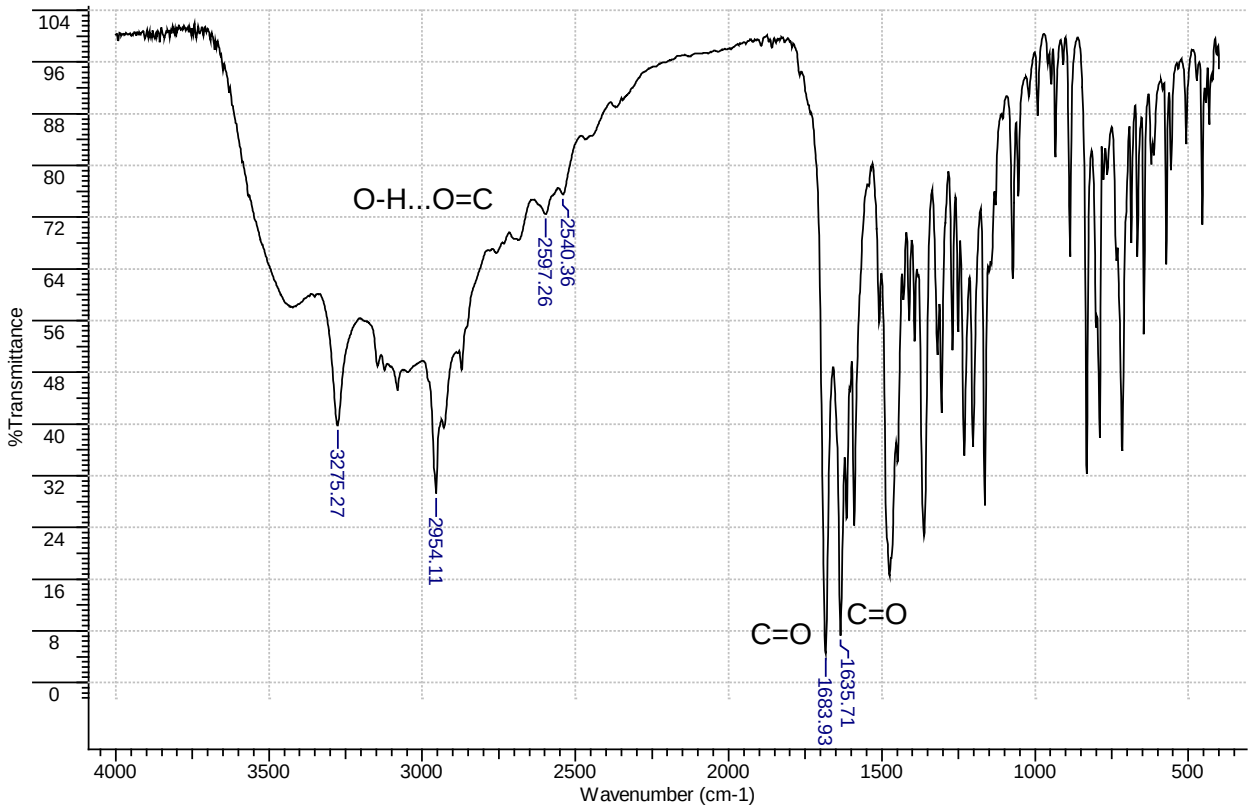
1.2. 1-Hydroxy-5,5-dimethyl-2-(4-oxo-4H-chromen-3-yl)-4,5,6,7-tetrahydro-4H-benzimidazol-7-one (1b)



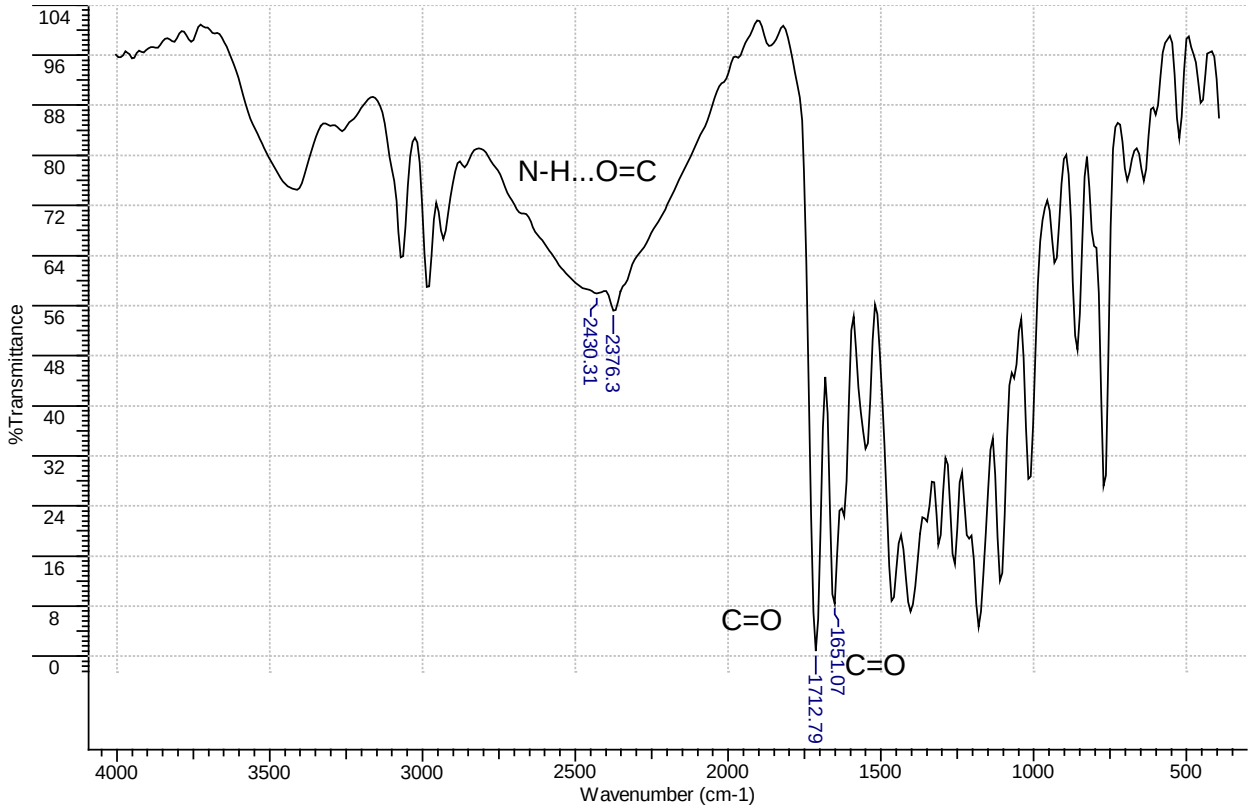
1.3. 1-Hydroxy-5,5-dimethyl-2-(6-methyl-4-oxo-4H-chromen-3-yl)-4,5,6,7-tetrahydro-4H-benzimidazol-7-one (1c).



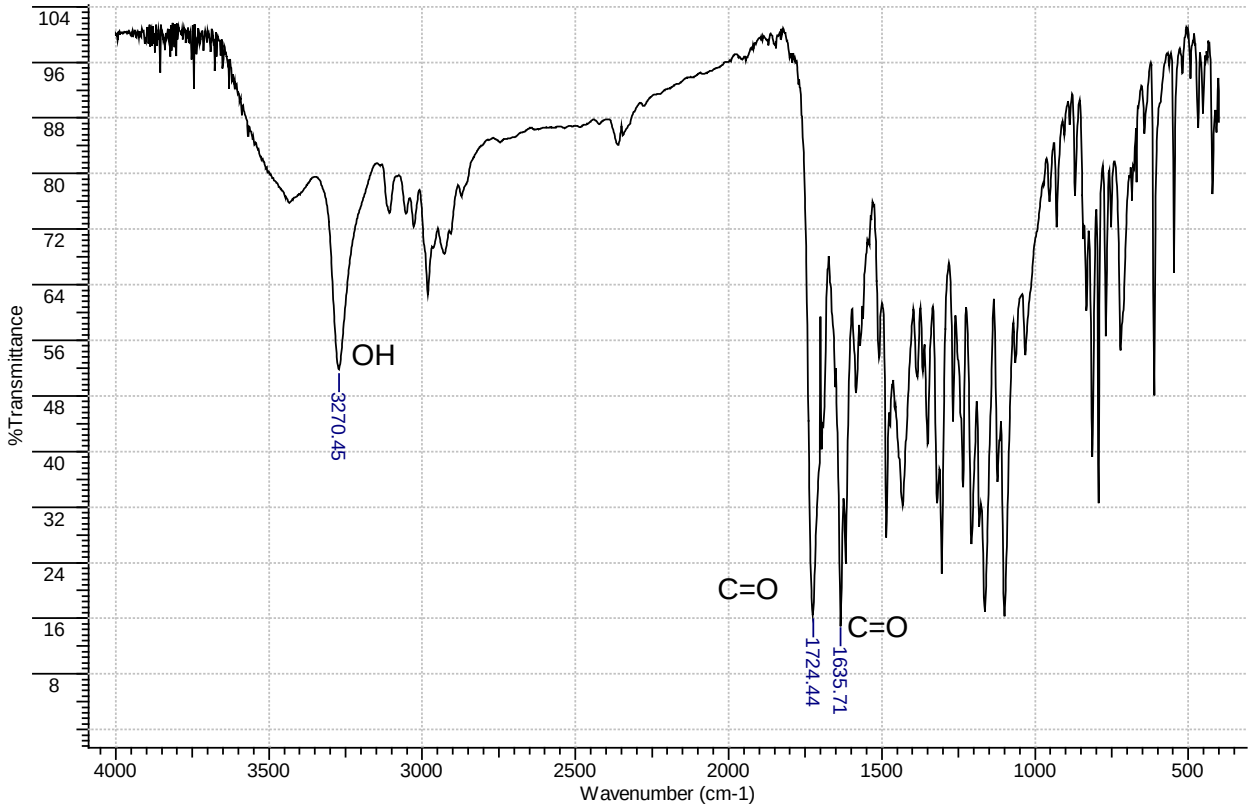
1.4. 1-Hydroxy-5,5-dimethyl-2-(6-hydroxy-4-oxo-4H-chromen-3-yl)-4,5,6,7-tetrahydro-4H-benzimidazol-7-one (1d).



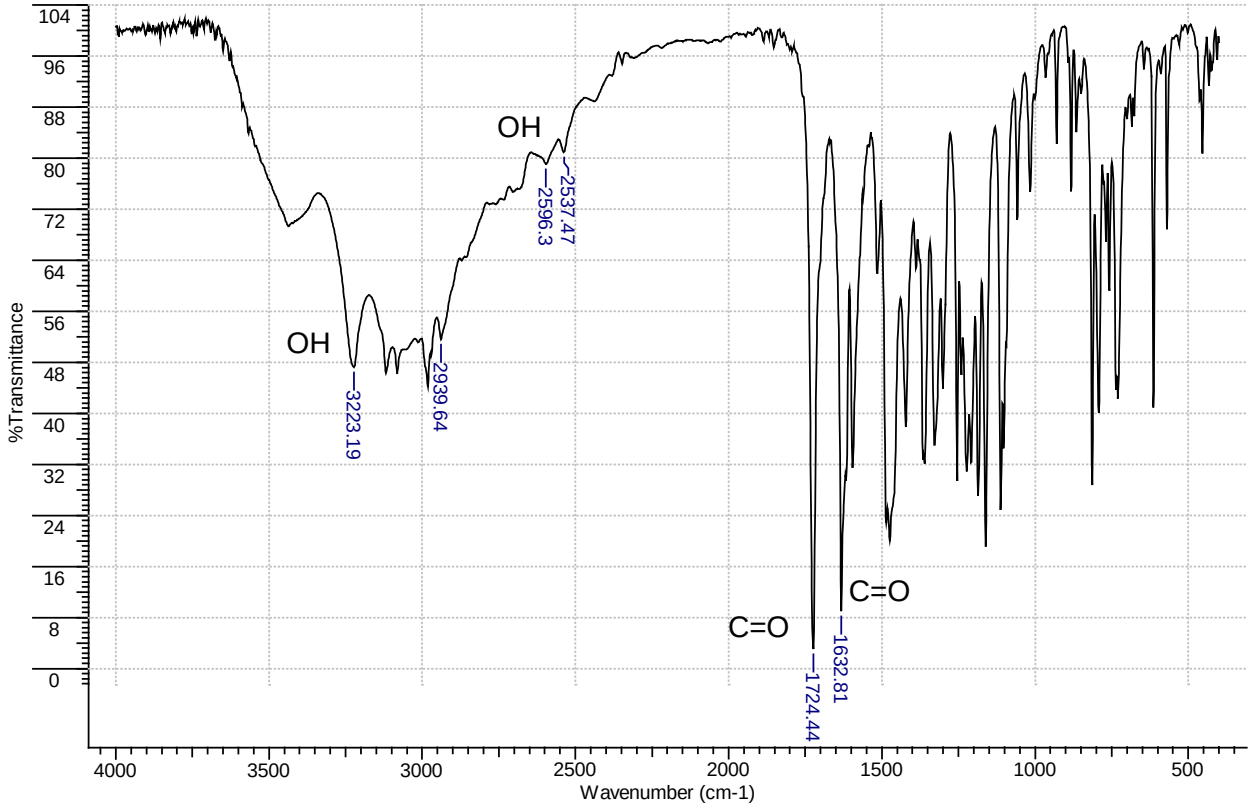
1.5. Ethyl 1-hydroxy-4-methyl-2-(4-oxo-4H-chromen-3-yl)-1H-imidazole-5-carboxylate (2b).



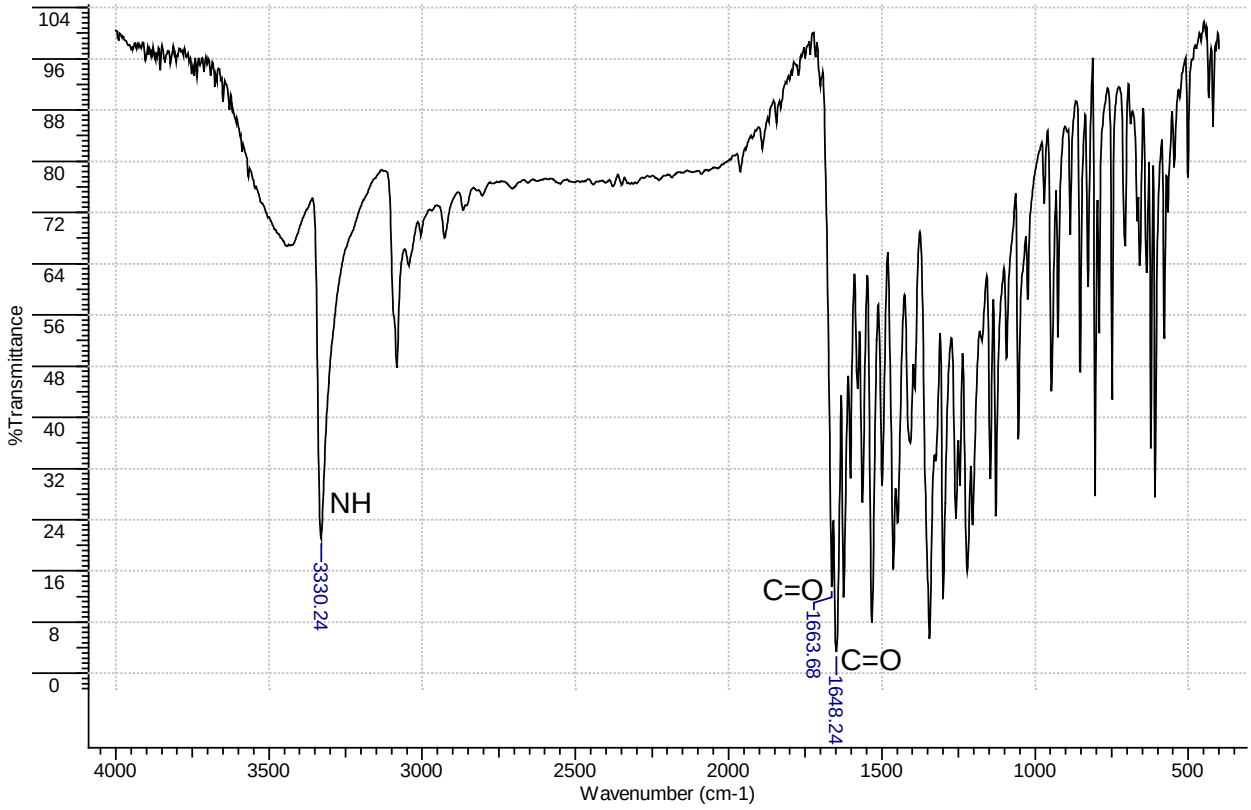
1.6. Ethyl 1-hydroxy-4-methyl-2-(6-methyl-4-oxo-4H-chromen-3-yl)-1H-imidazole-5-carboxylate (2c).



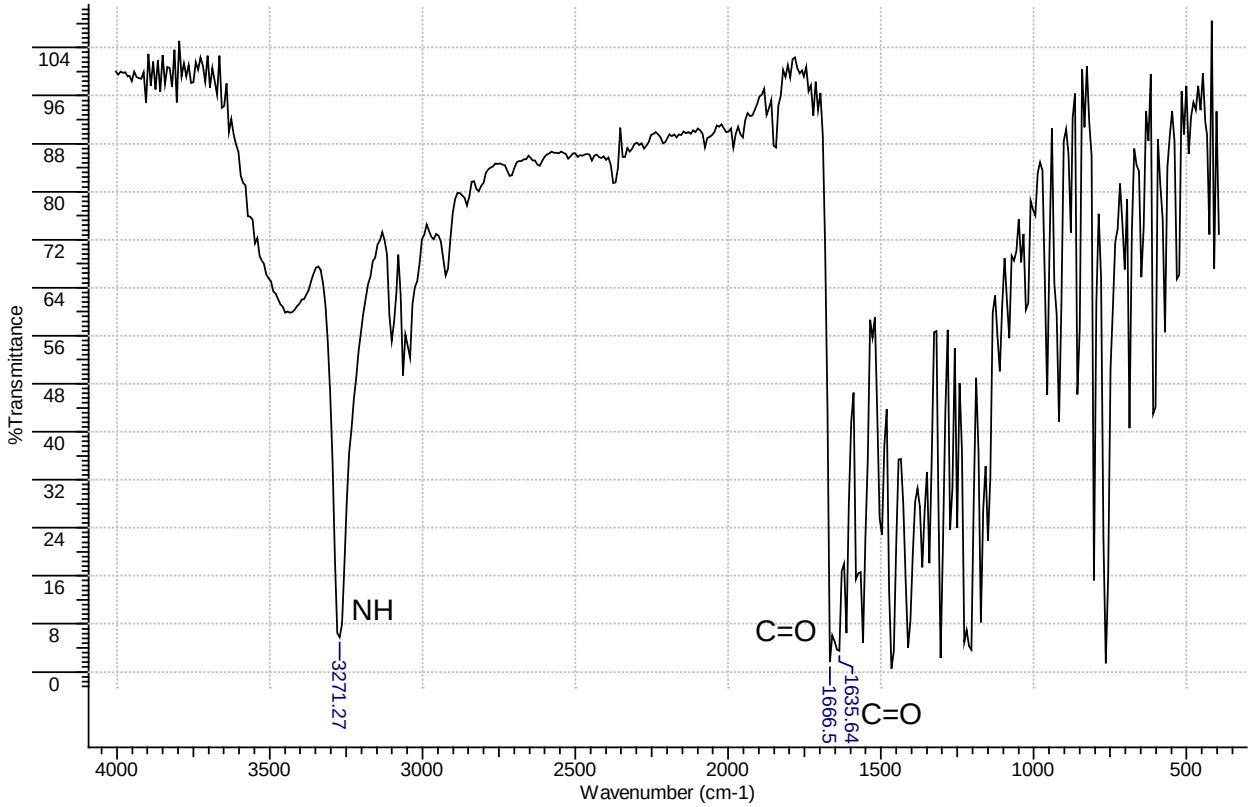
1.7. Ethyl 1-hydroxy-4-methyl-2-(6-hydroxy-4-oxo-4H-chromen-3-yl)-1H-imidazole-5-carboxylate (2d)



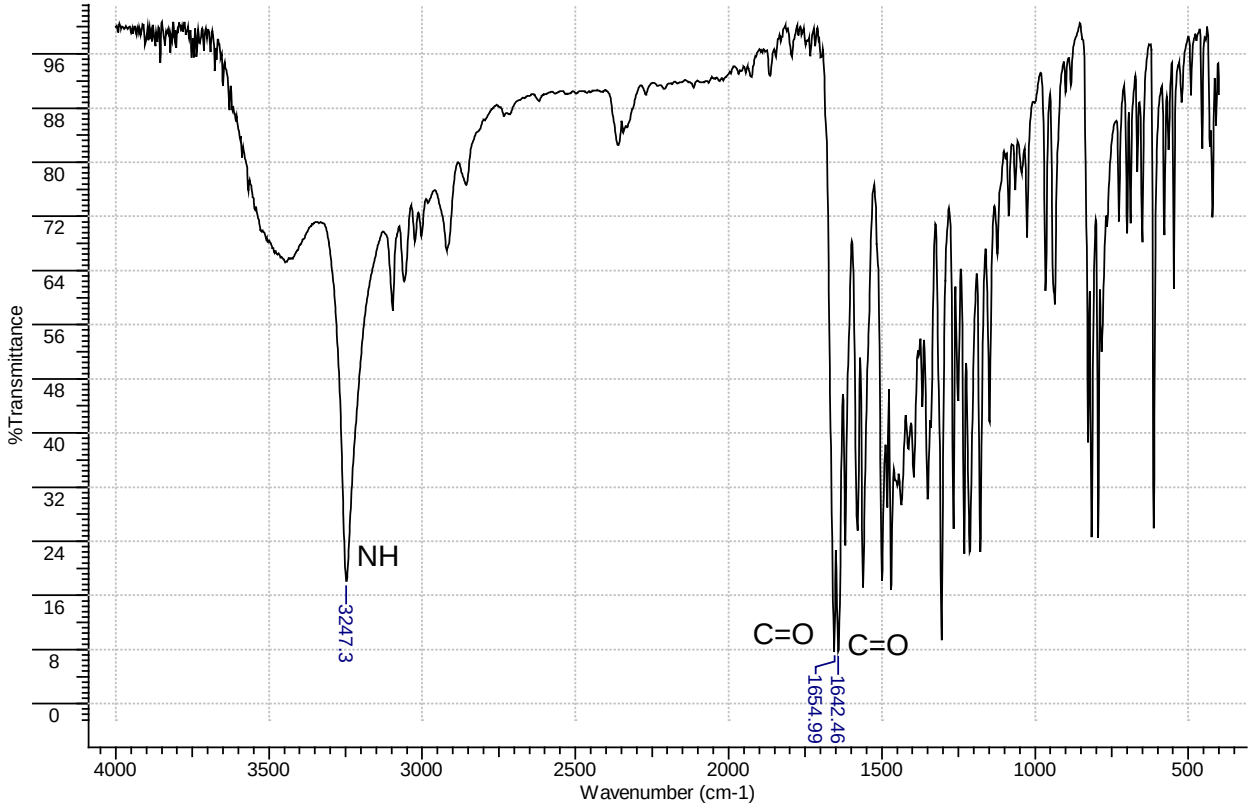
1.8. 3-(5-Acetyl-1-hydroxy-4-methyl-1H-imidazol-2-yl)-6-nitro-4H-chromen-4-one (3a).



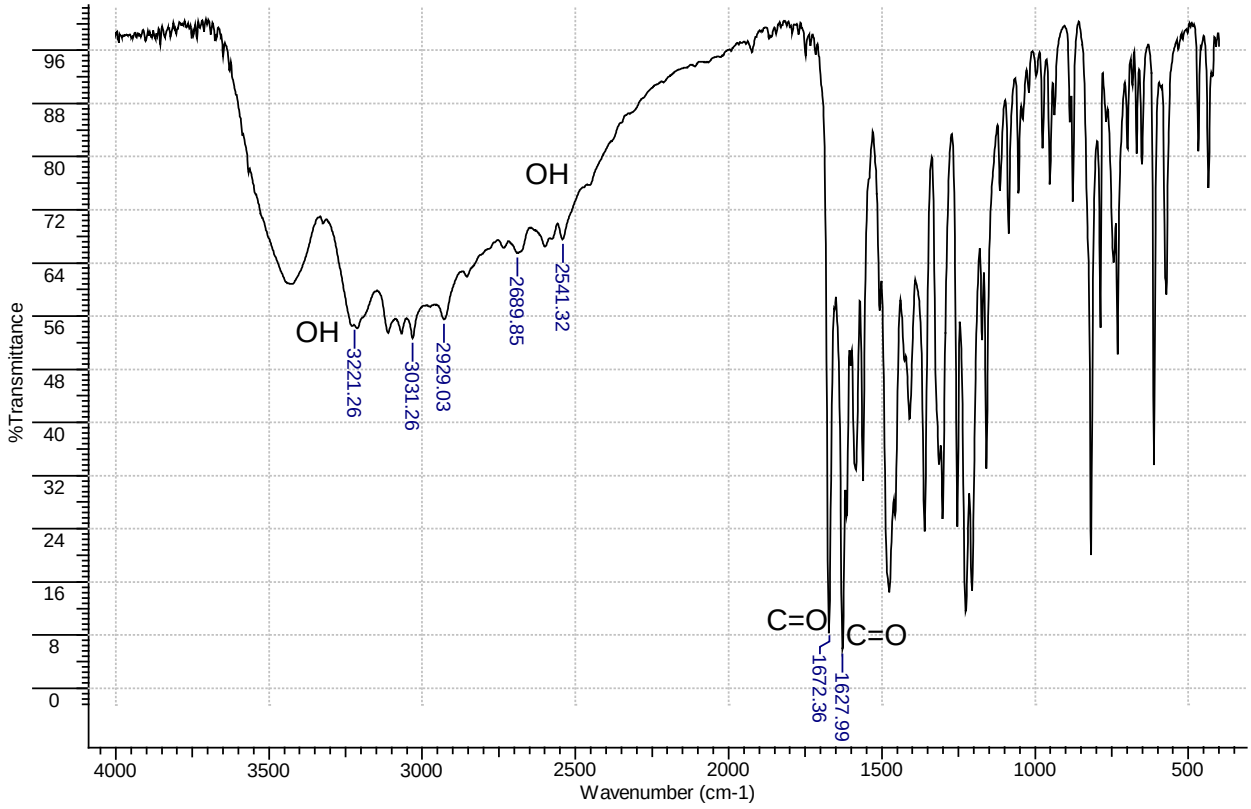
1.9. 3-(5-Acetyl-1-hydroxy-4-methyl-1H-imidazol-2-yl)-4H-chromen-4-one (3b).



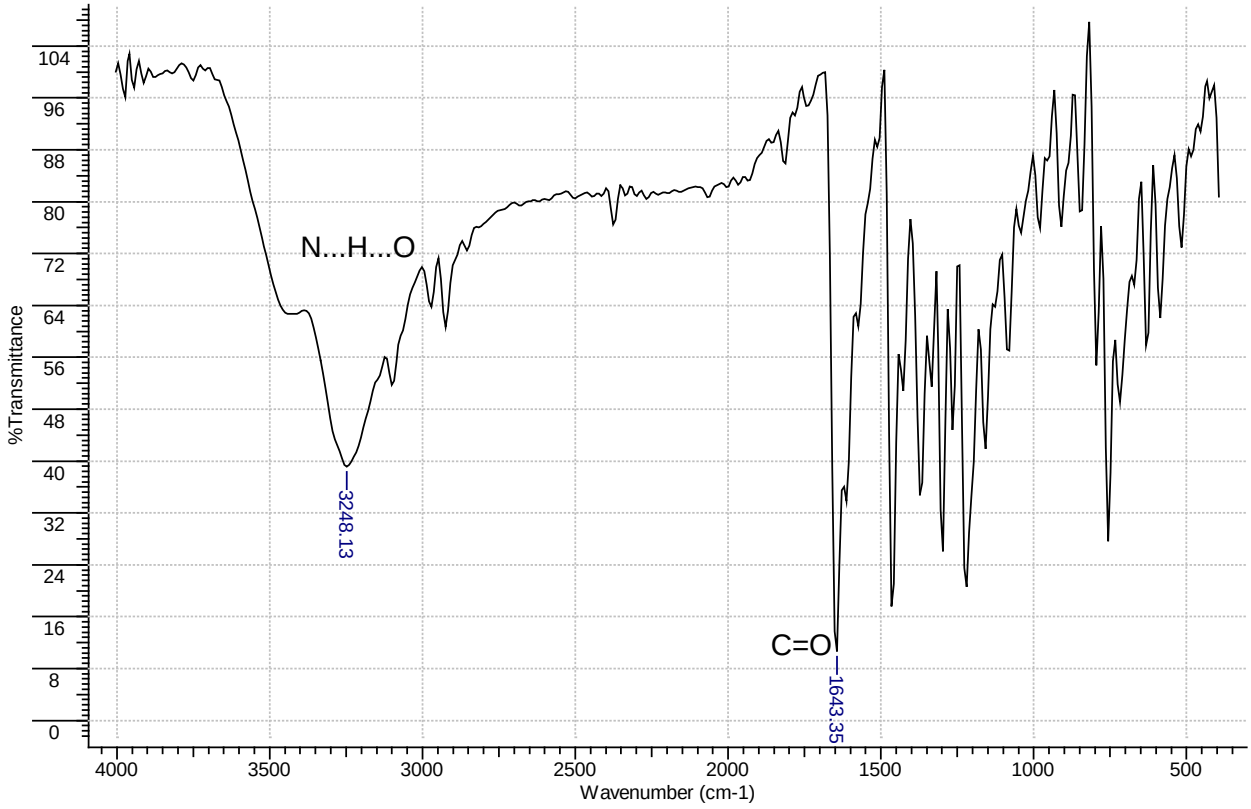
1.10. 3-(5-Acetyl-1-hydroxy-4-methyl-1H-imidazol-2-yl)-6-methyl-4H-chromen-4-one (3c).



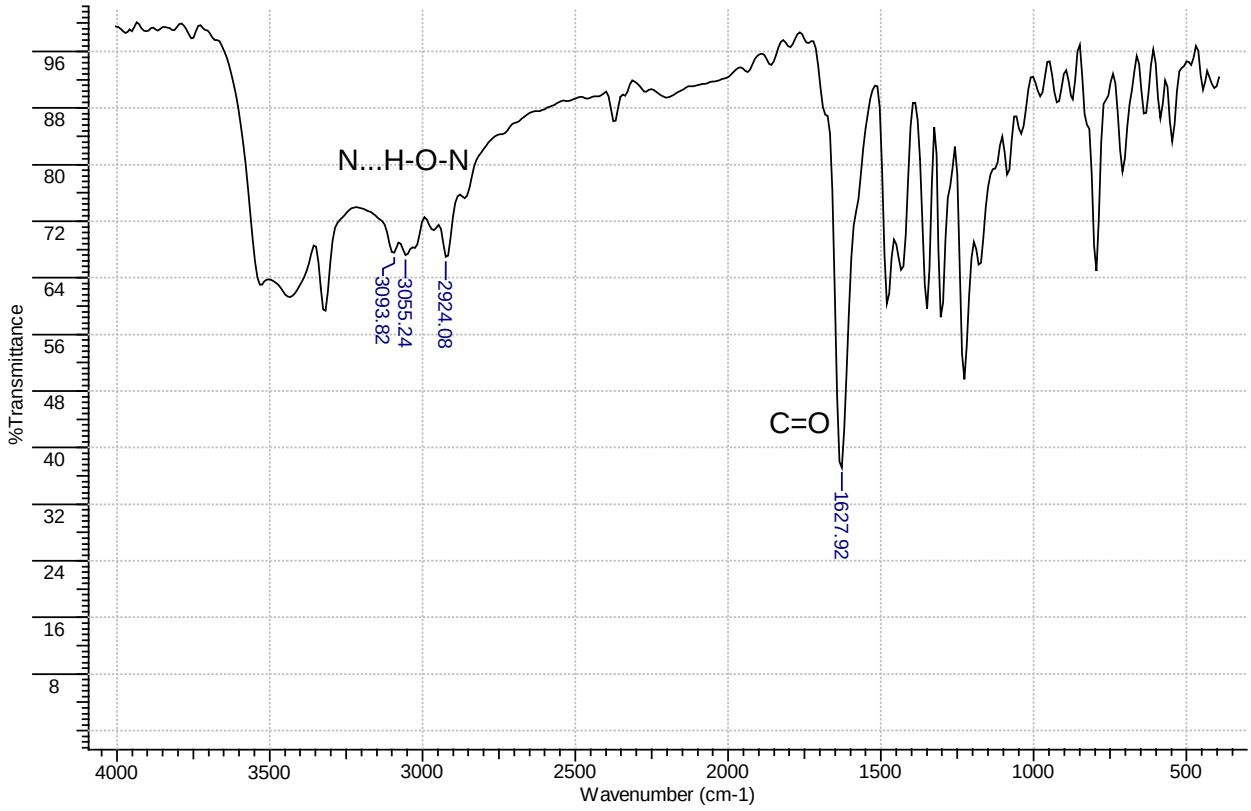
1.11. 3-(5-Acetyl-1-hydroxy-4-methyl-1H-imidazol-2-yl)-6-hydroxy-4H-chromen-4-one (3d).



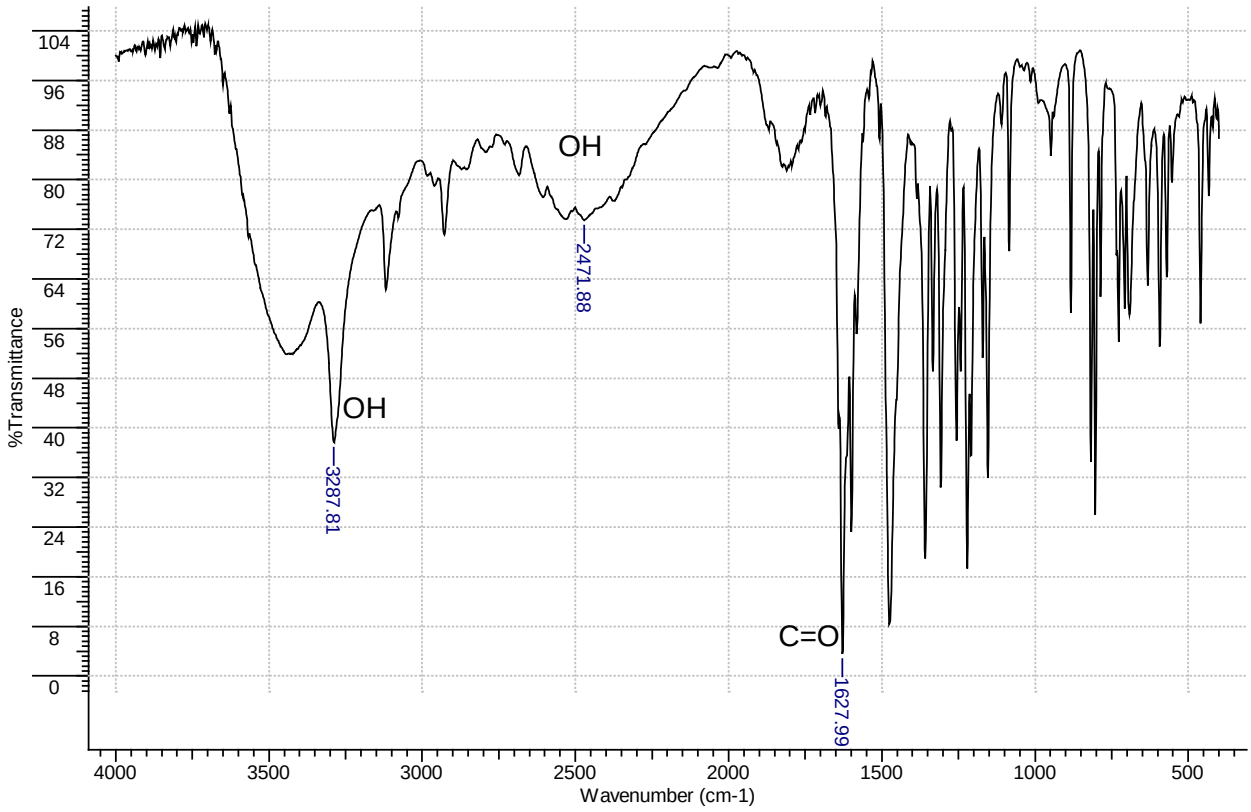
1.12. 3-(1-Hydroxy-4,5-dimethyl-*1H*-imidazol-2-yl)-*4H*-chromen-4-one (4b).



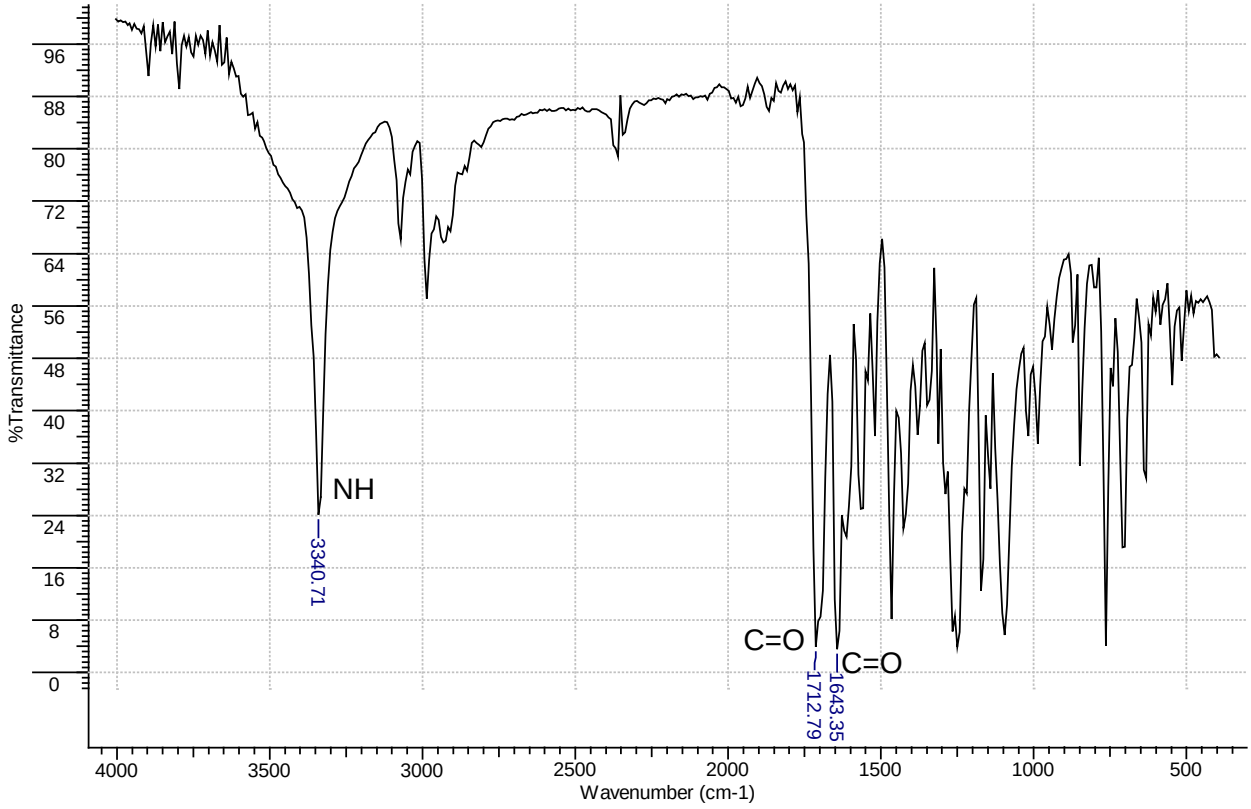
1.13. 3-(1-Hydroxy-4,5-dimethyl-*1H*-imidazol-2-yl)-6-methyl-*4H*-chromen-4-one (4c).



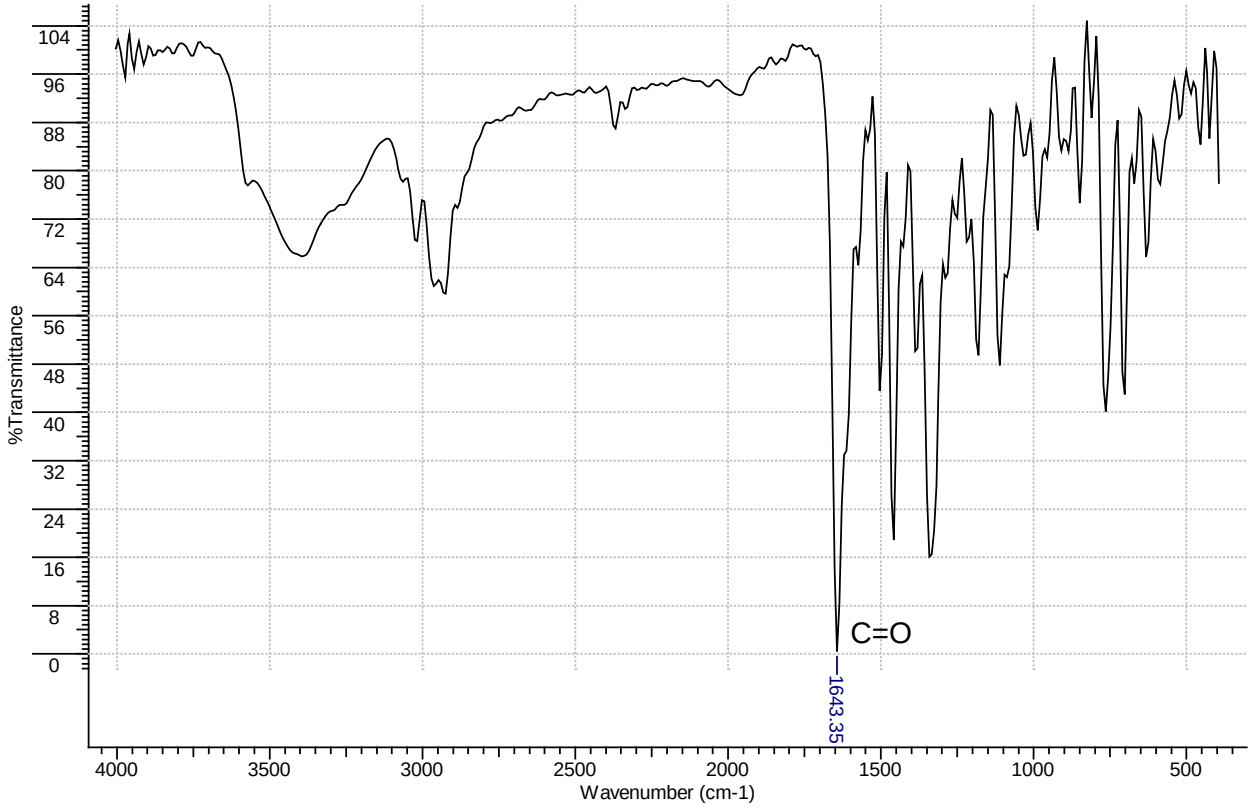
1.14. 3-(1-Hydroxy-4,5-dimethyl-1H-imidazol-2-yl)-6-hydroxy-4H-chromen-4-one (4d).



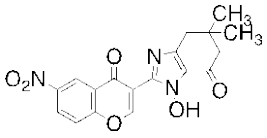
1.15. Ethyl 5-methyl-2-(4-oxo-4H-chromen-3-yl)-1H-imidazole-4-carboxylate (10).



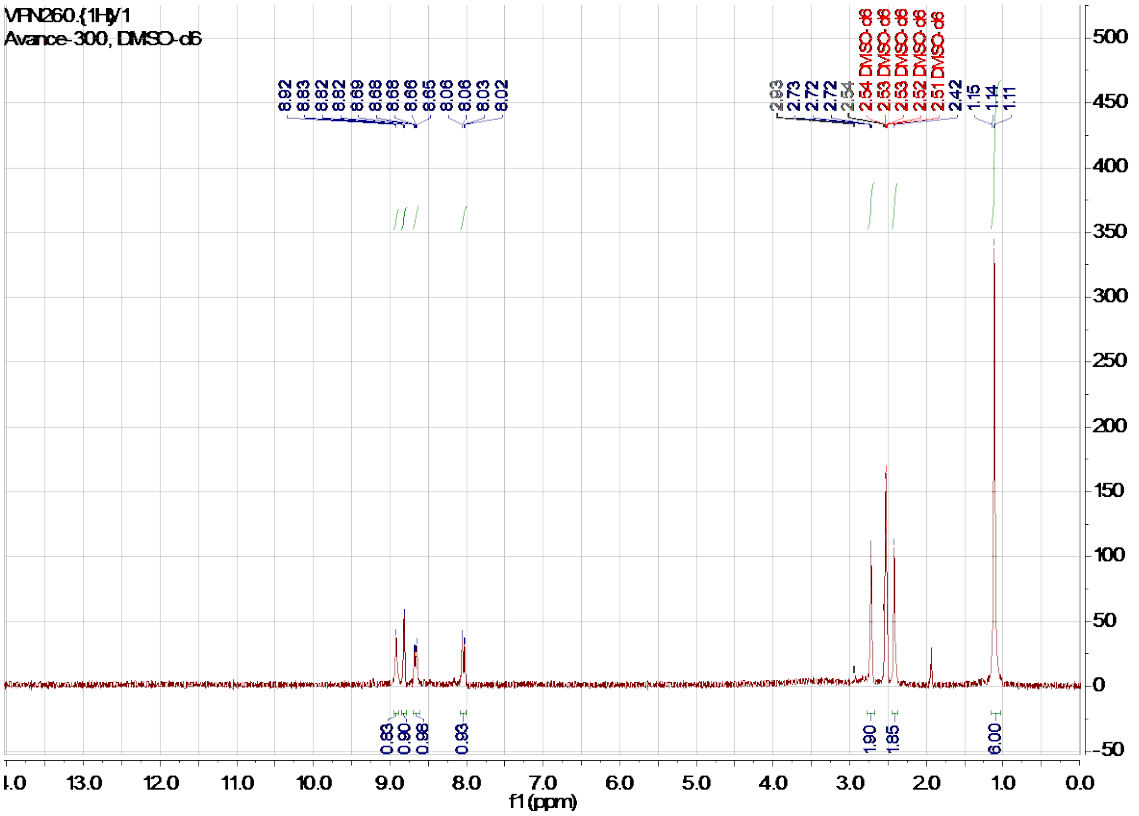
1.16. 1-Benzyl-4,5-dimethyl-2-(4-oxo-4H-chromen-3-yl)-1H-imidazole 3-oxide (11).

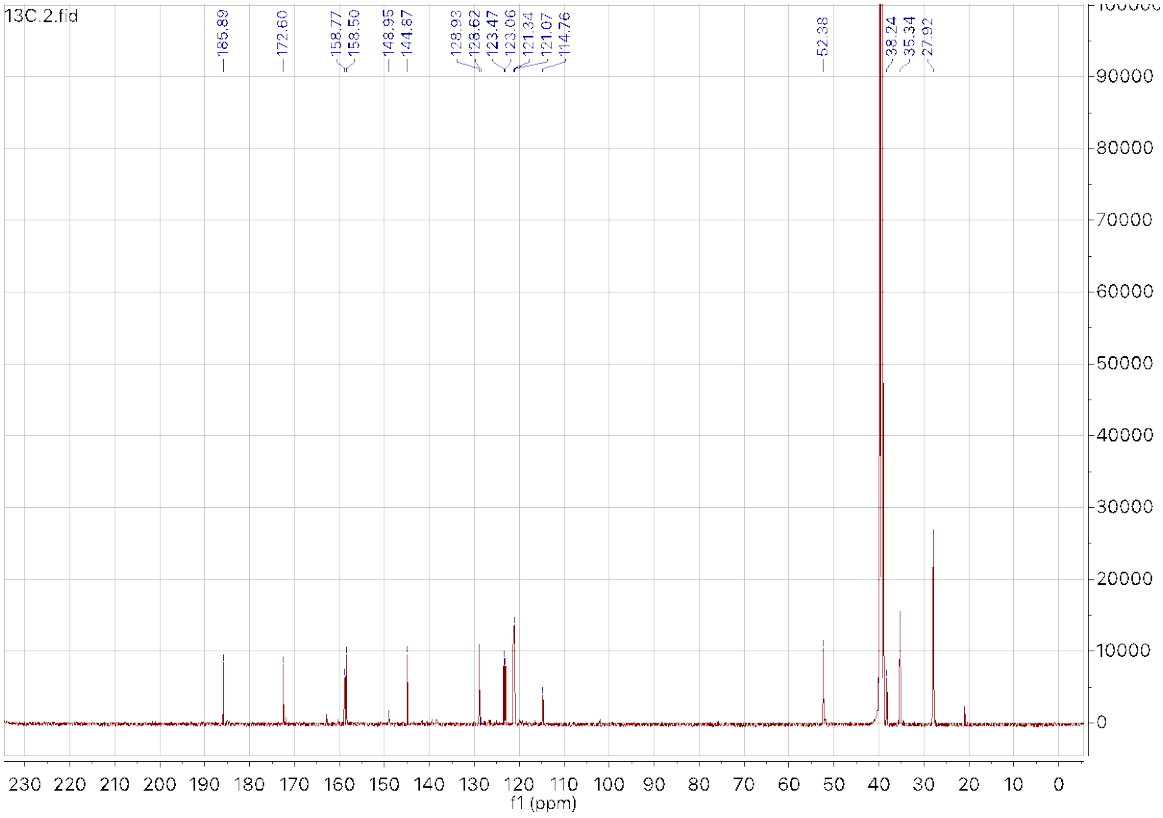


2. Copies of ^{1}H and ^{13}C spectra of new compounds (DMSO-d_6).

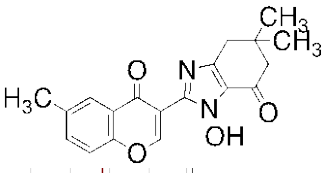


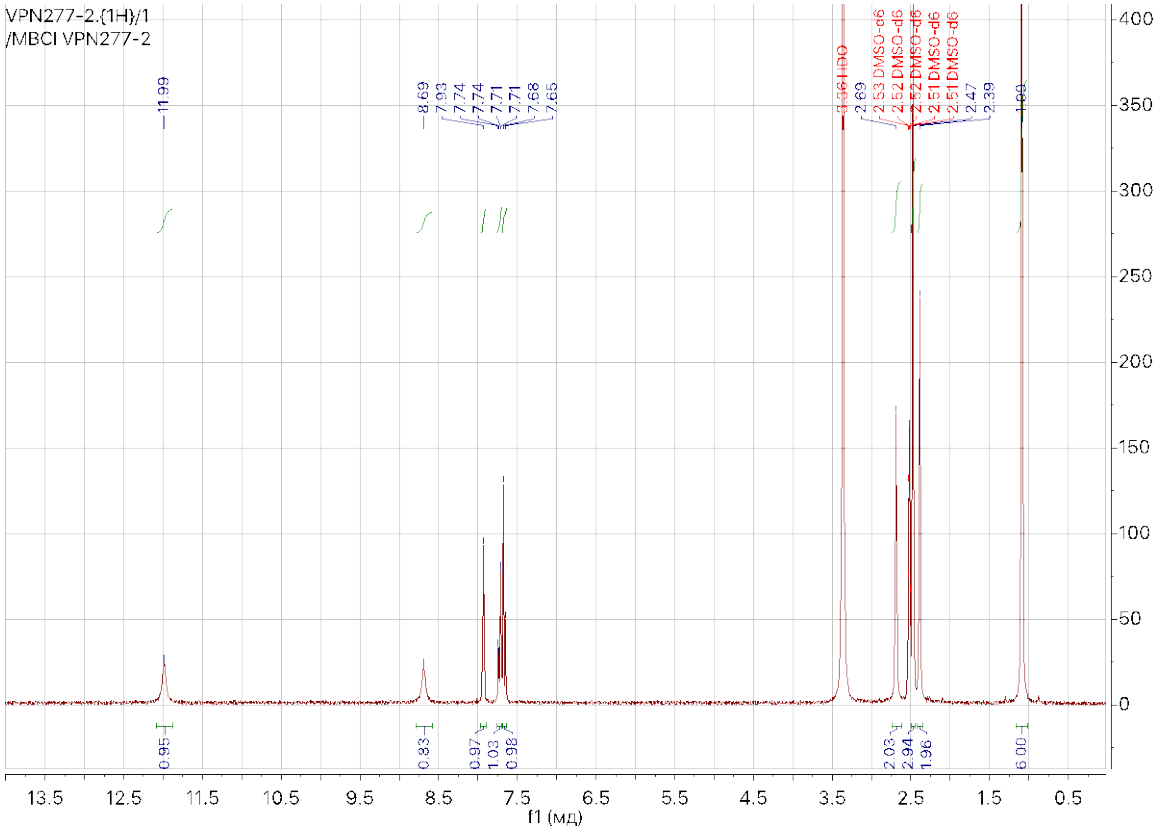
2.1. 1-Hydroxy-5,5-dimethyl-2-(6-nitro-4-oxo-4H-chromen-3-yl)-4,5,6,7-tetrahydro-4H-benzimidazol-7-one (1a)

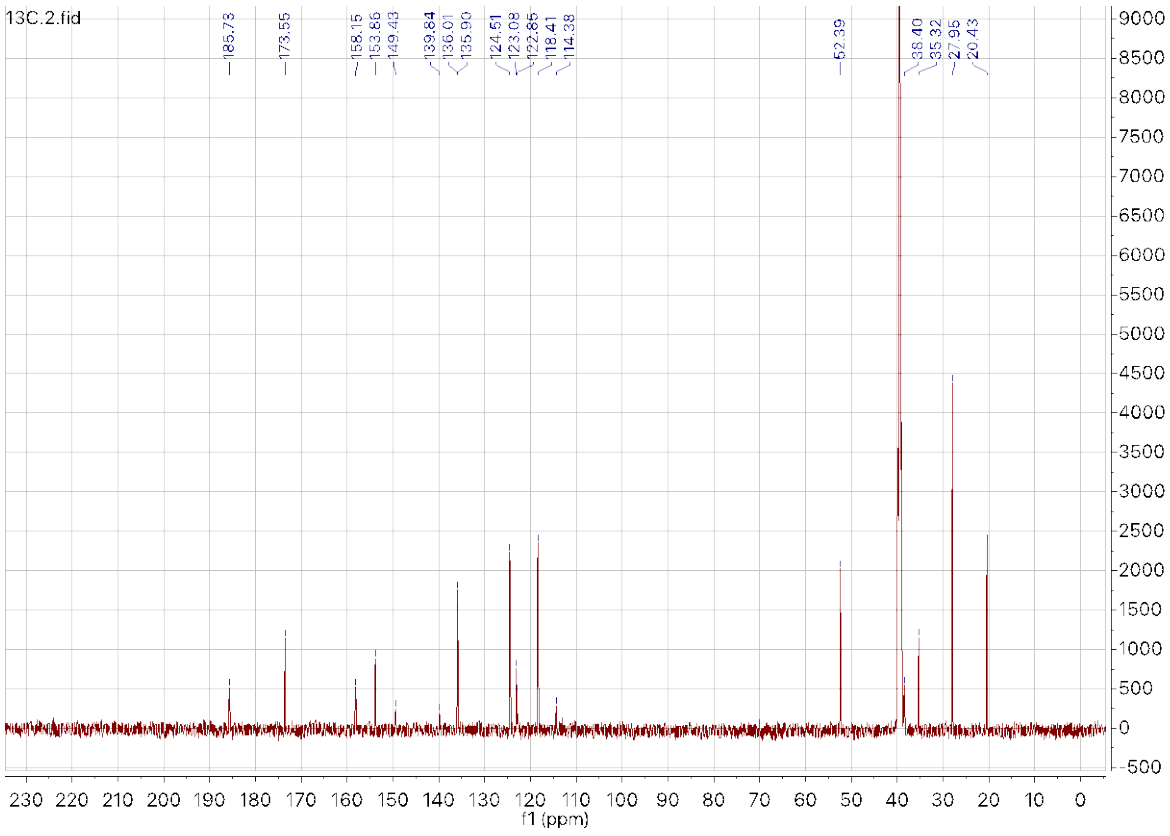




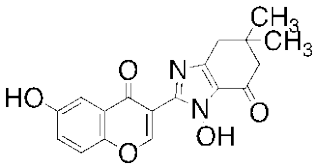
2.2. 1-Hydroxy-5,5-dimethyl-2-(6-methyl-4-oxo-4H-chromen-3-yl)-4,5,6,7-tetrahydro-4H-benzimidazol-7-one (1c).

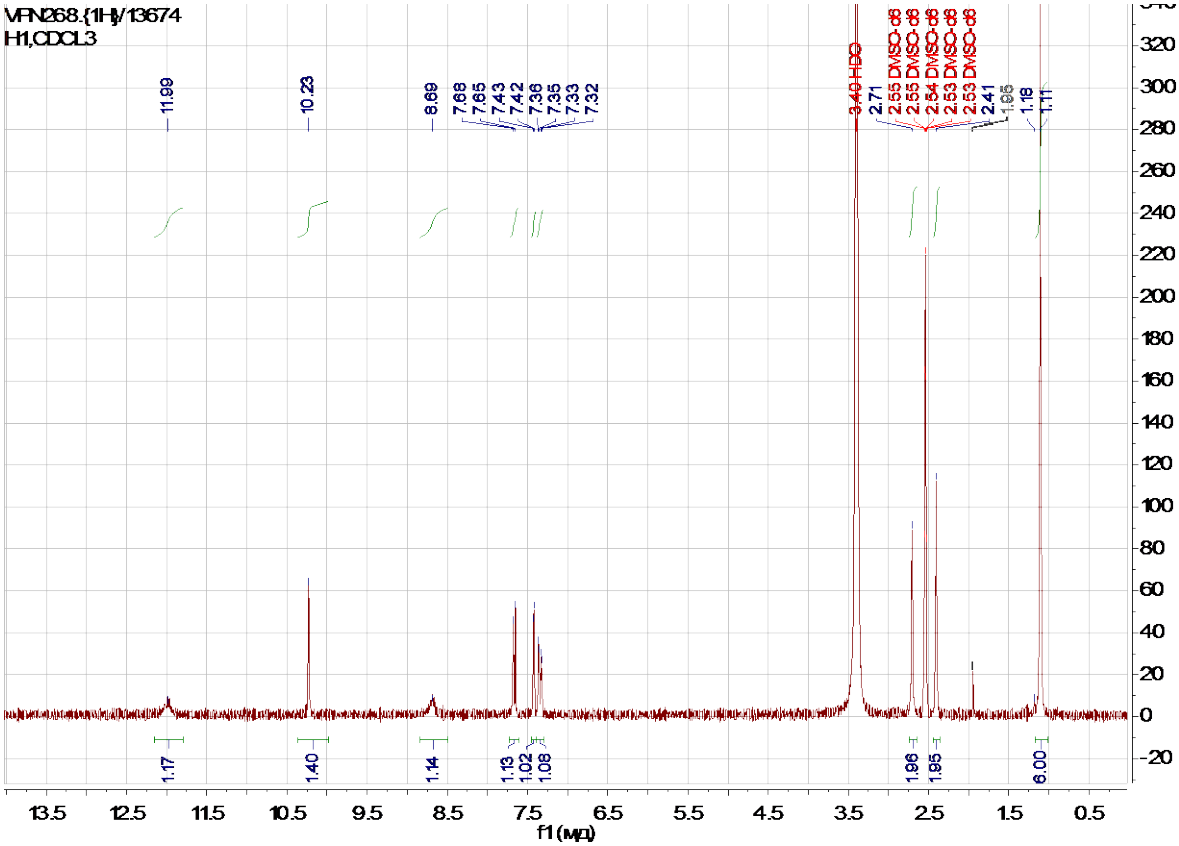


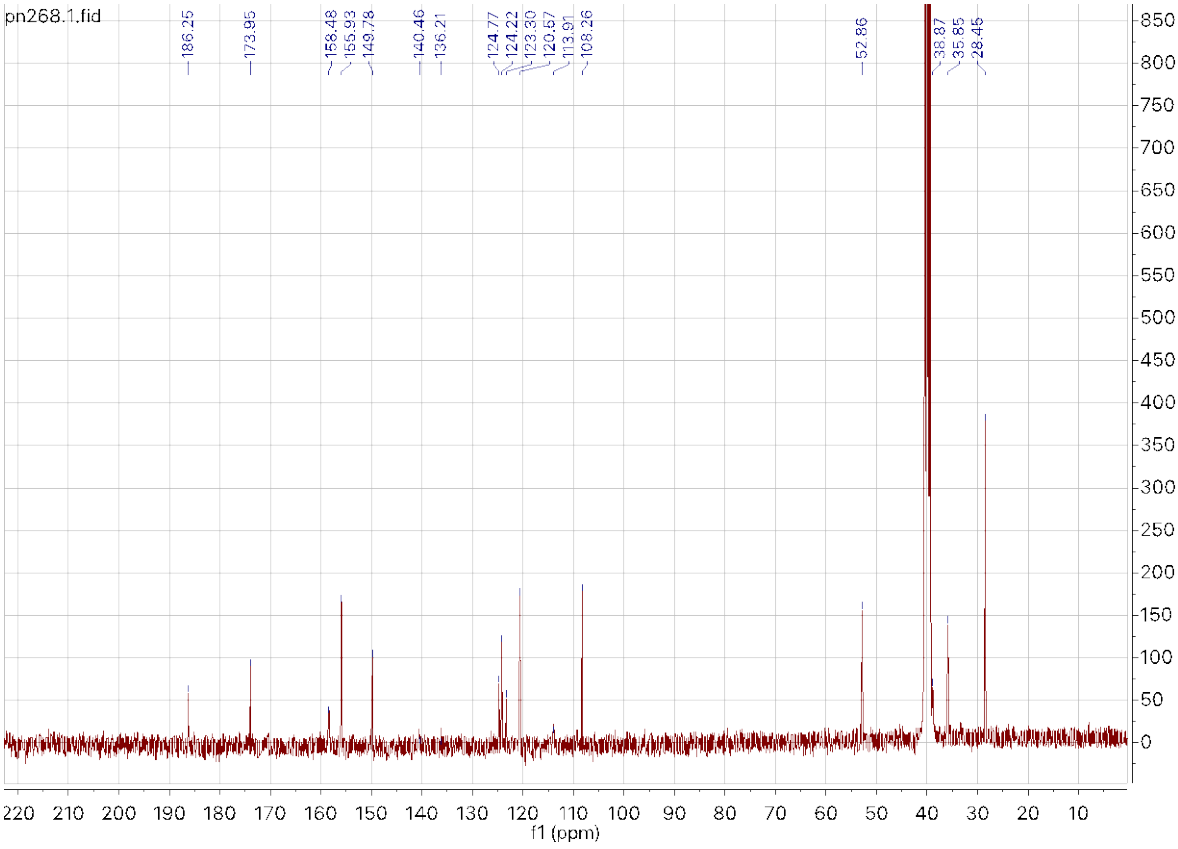




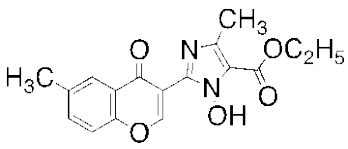
2.3. 1-Hydroxy-5,5-dimethyl-2-(6-hydroxy-4-oxo-4H-chromen-3-yl)-4,5,6,7-tetrahydro-4H-benzimidazol-7-one (1d).

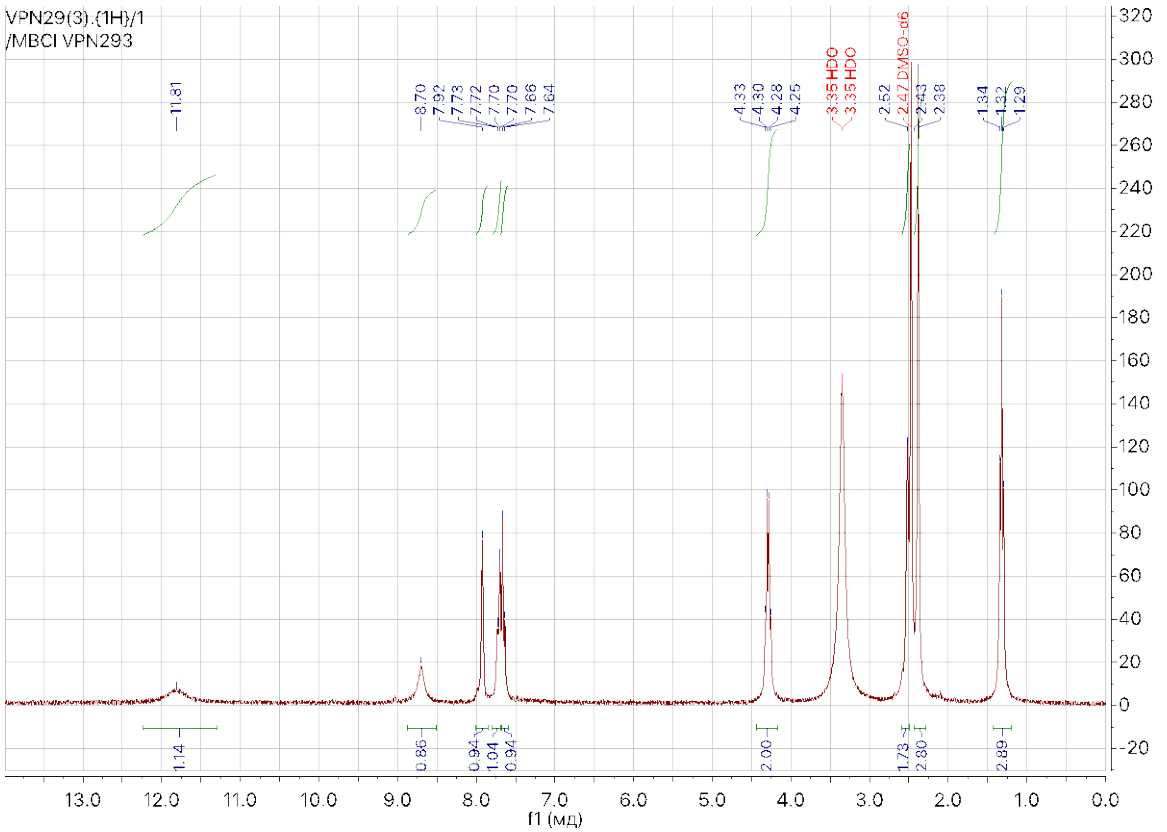


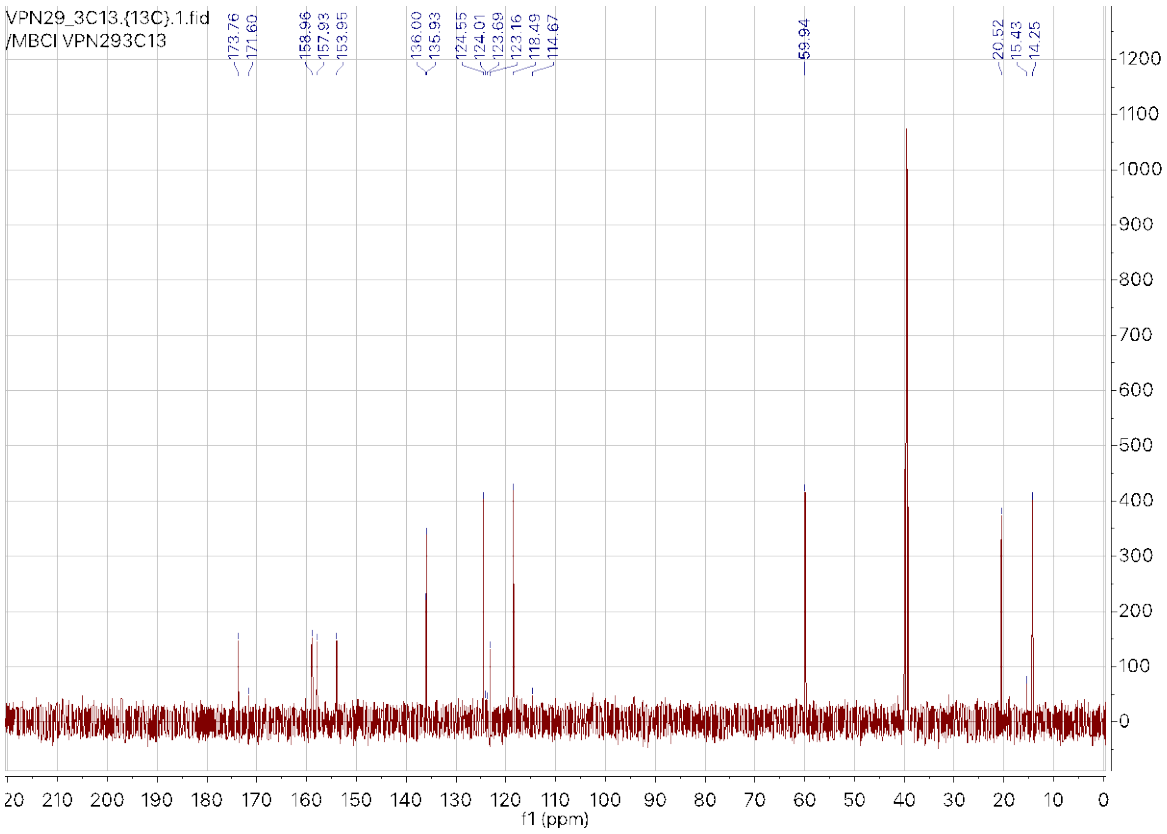




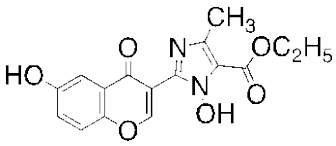
2.4. Ethyl 1-hydroxy-4-methyl-2-(6-methyl-4-oxo-4H-chromen-3-yl)-1H-imidazole-5-carboxylate (2c).

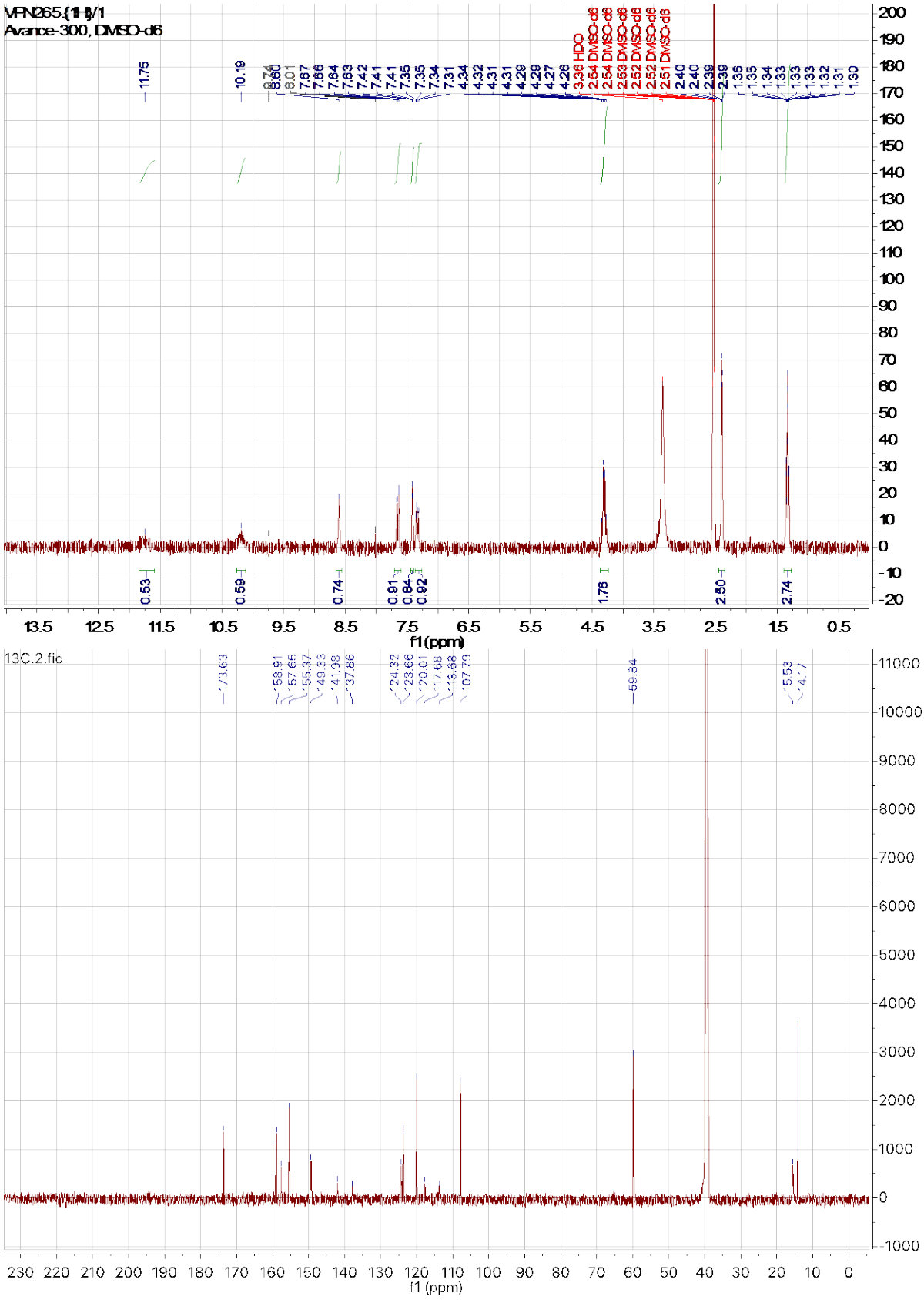




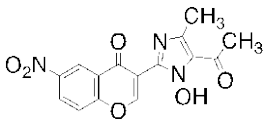


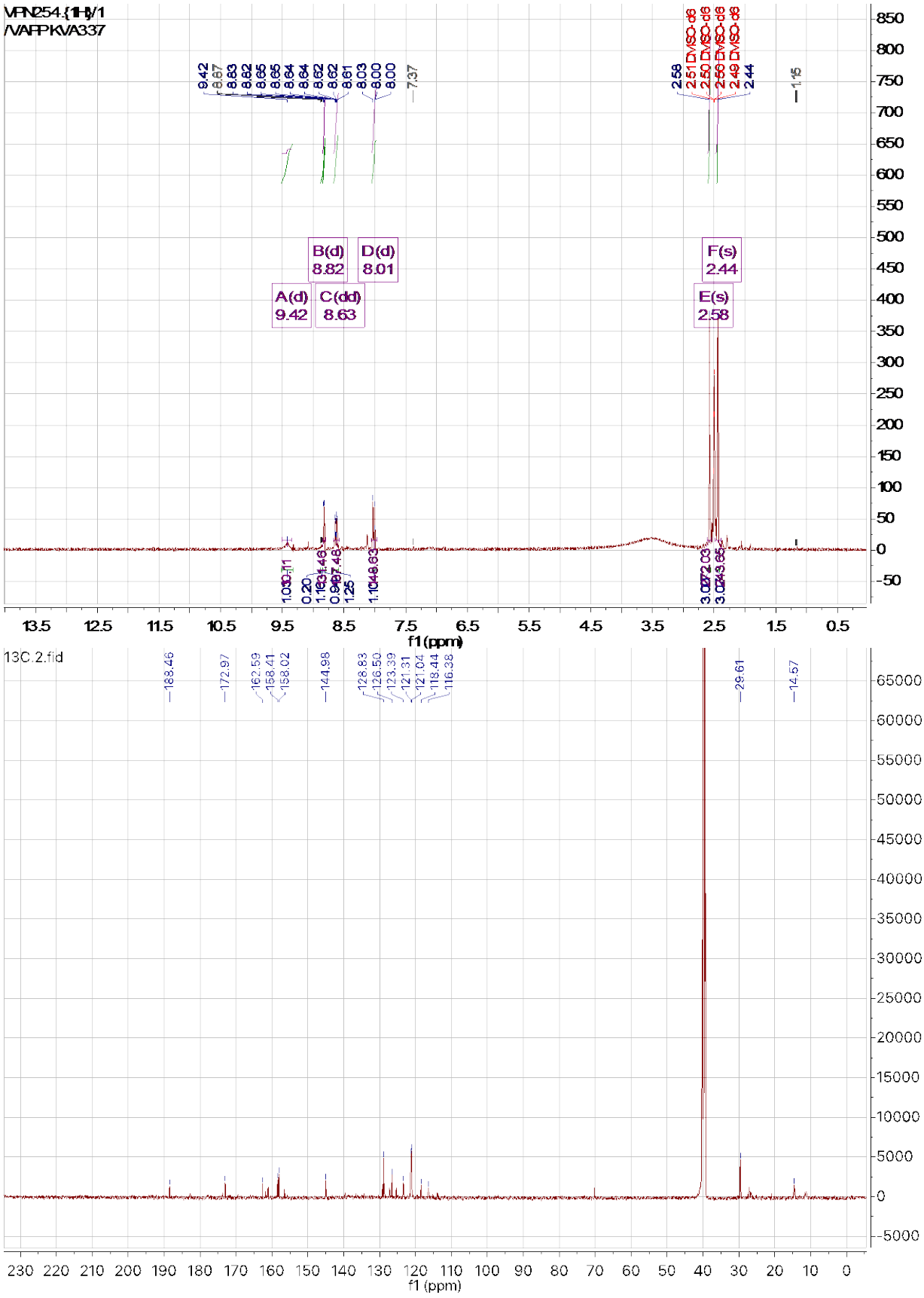
2.5. Ethyl 1-hydroxy-4-methyl-2-(6-hydroxy-4-oxo-4H-chromen-3-yl)-1H-imidazole-5-carboxylate (2d).



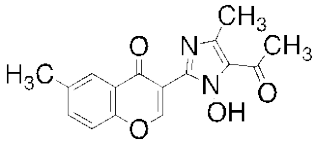


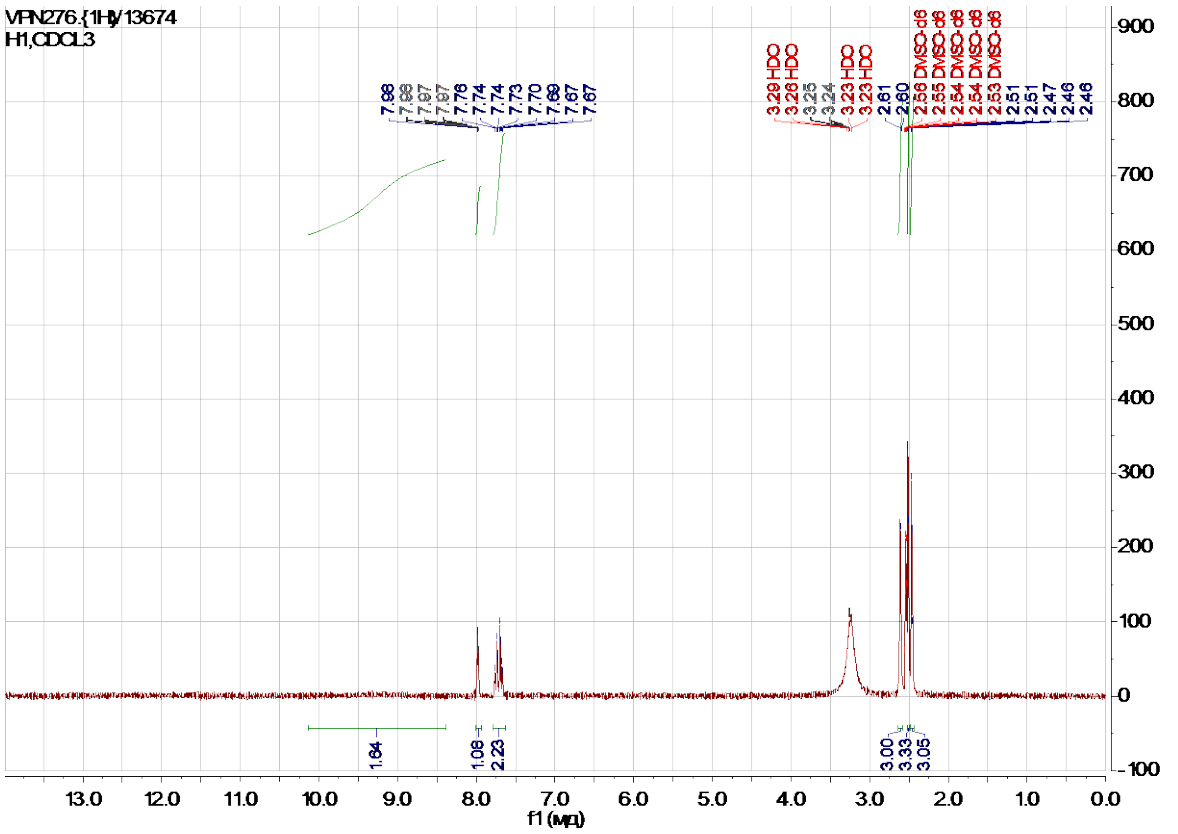
2.6. 3-(5-Acetyl-1-hydroxy-4-methyl-1H-imidazol-2-yl)-6-nitro-4H-chromen-4-one (3a).

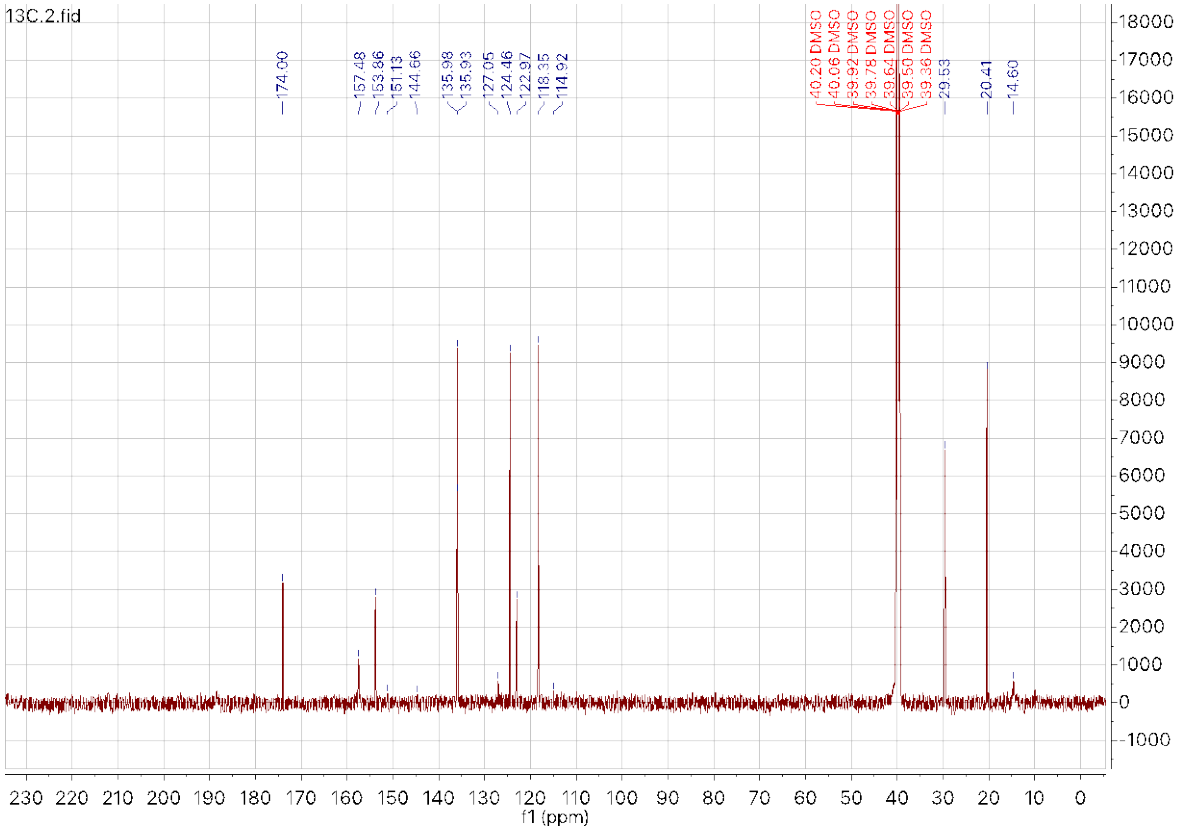




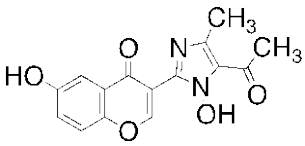
2.7. 3-(5-Acetyl-1-hydroxy-4-methyl-1H-imidazol-2-yl)-6-methyl-4H-chromen-4-one (3c).

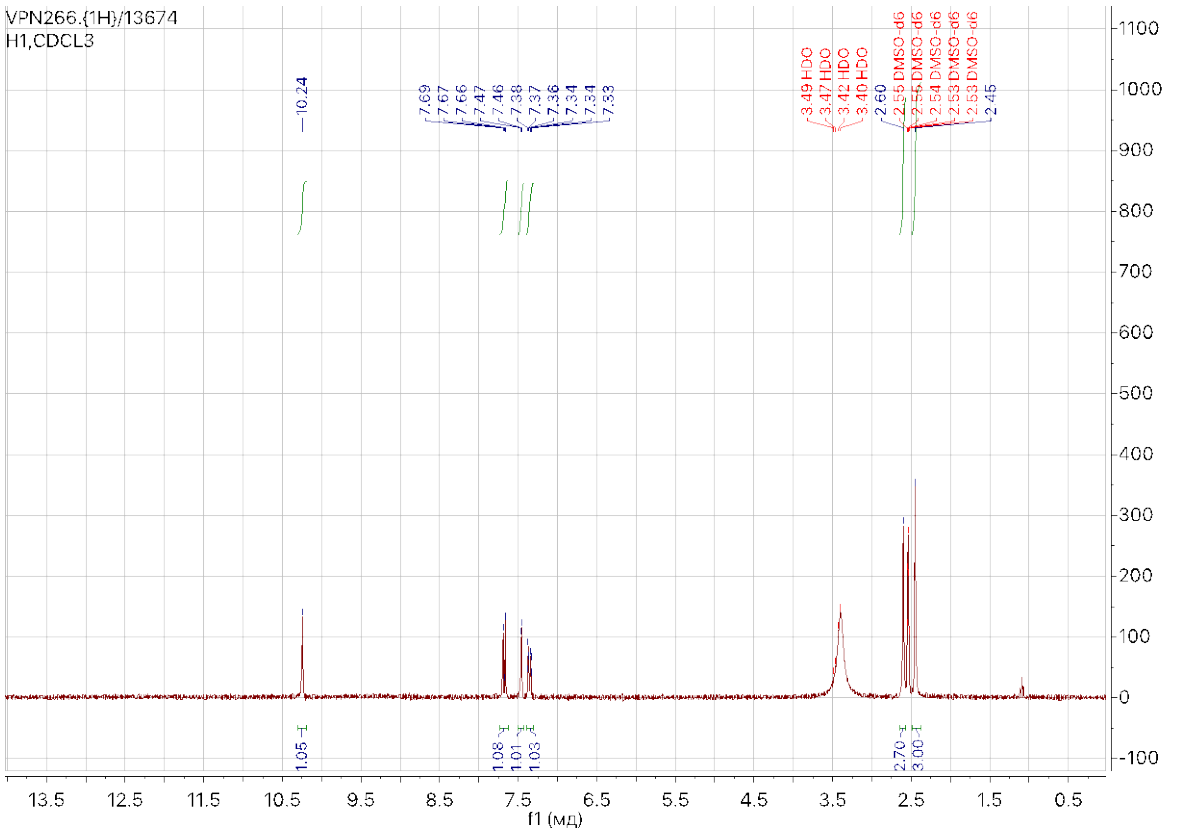


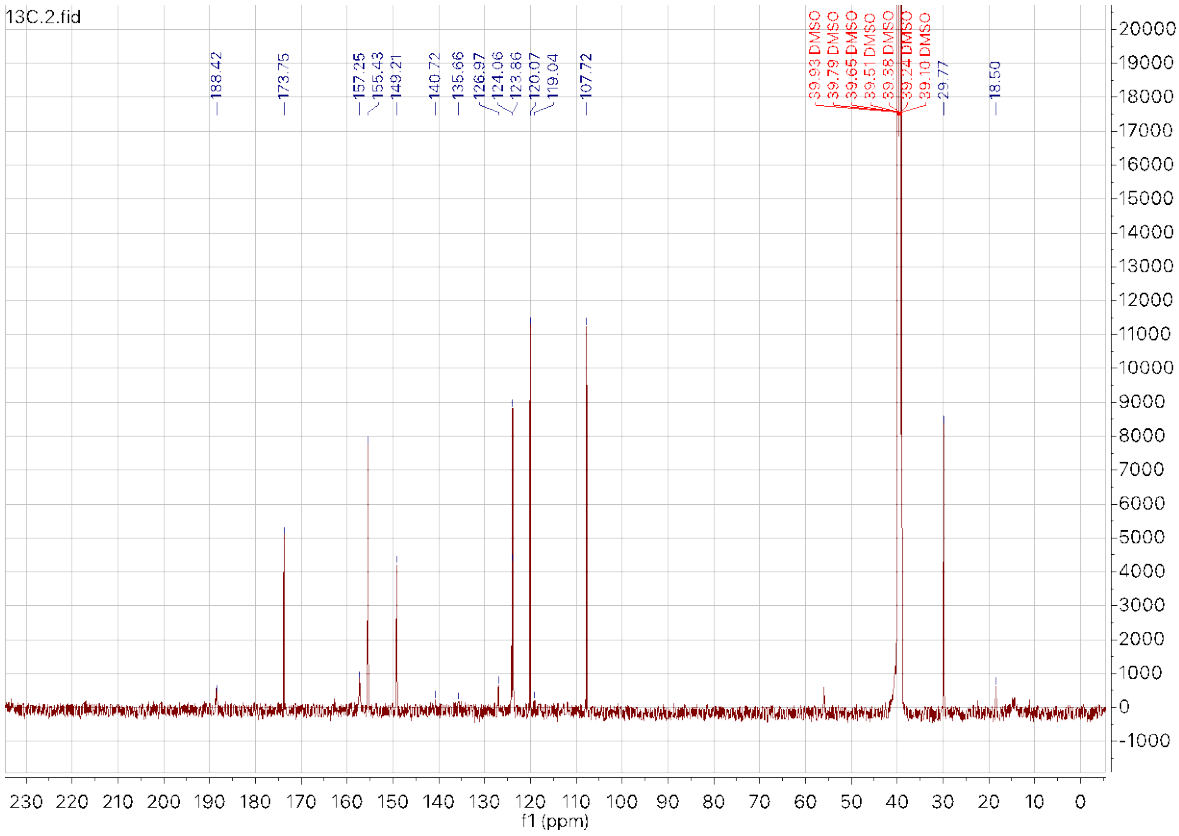




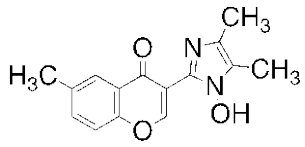
2.8. 3-(5-Acetyl-1-hydroxy-4-methyl-1H-imidazol-2-yl)-6-hydroxy-4H-chromen-4-one (3d).

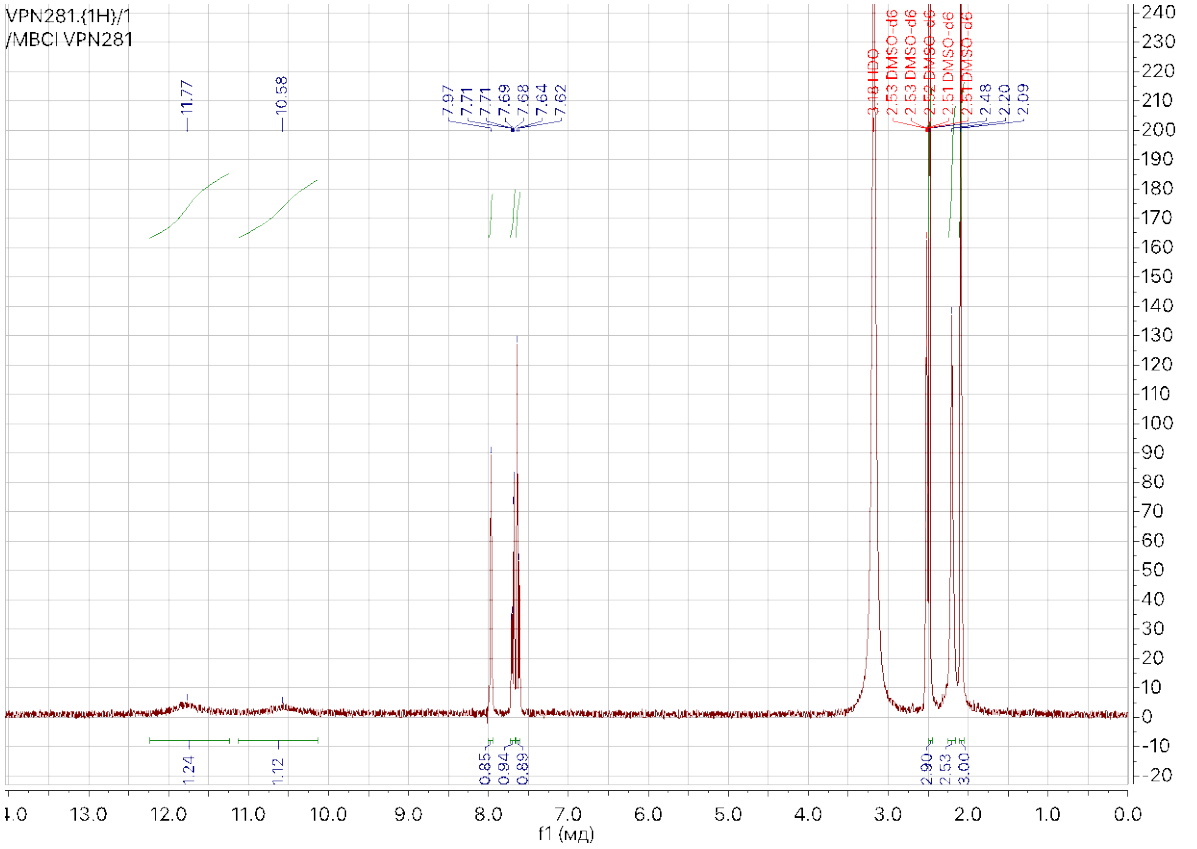


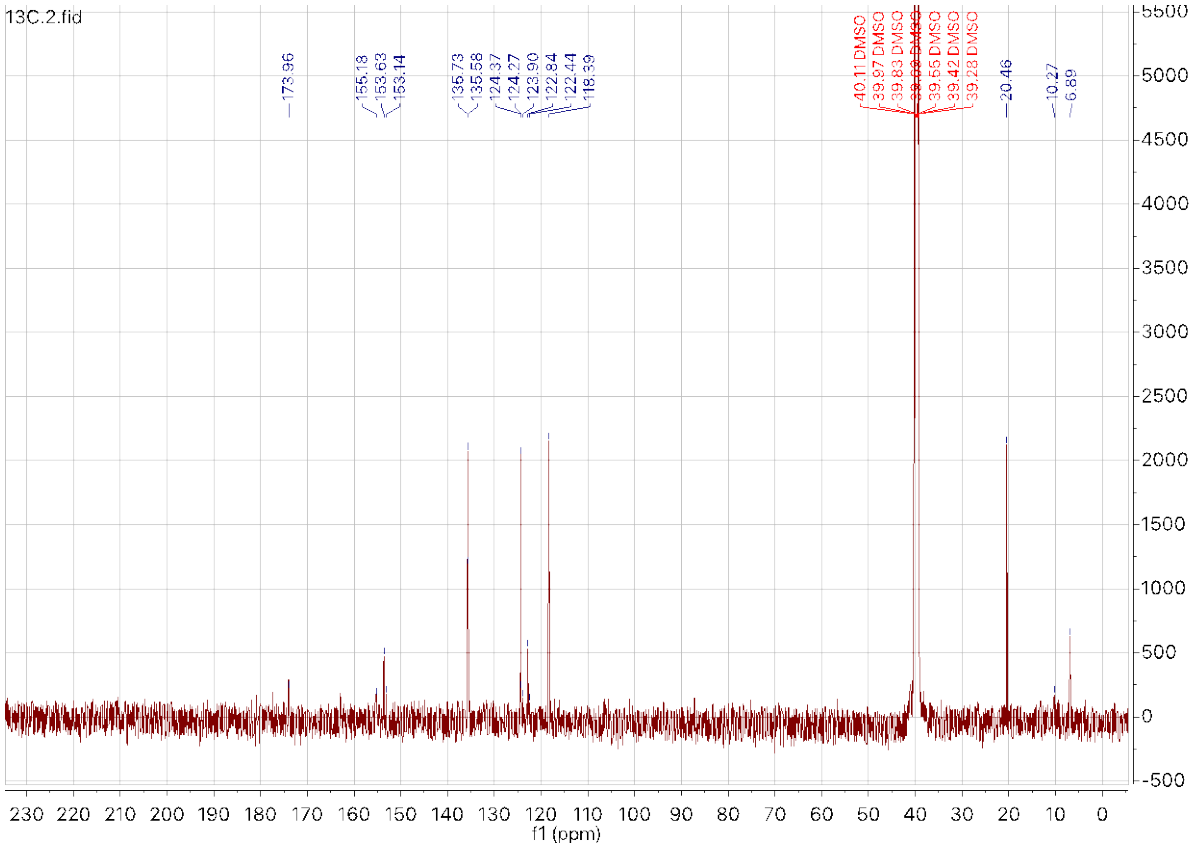




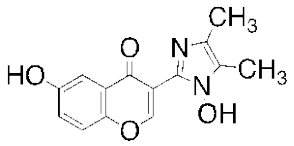
2.9. 3-(1-Hydroxy-4,5-dimethyl-*1H*-imidazol-2-yl)-6-methyl-*4H*-chromen-4-one (4c).

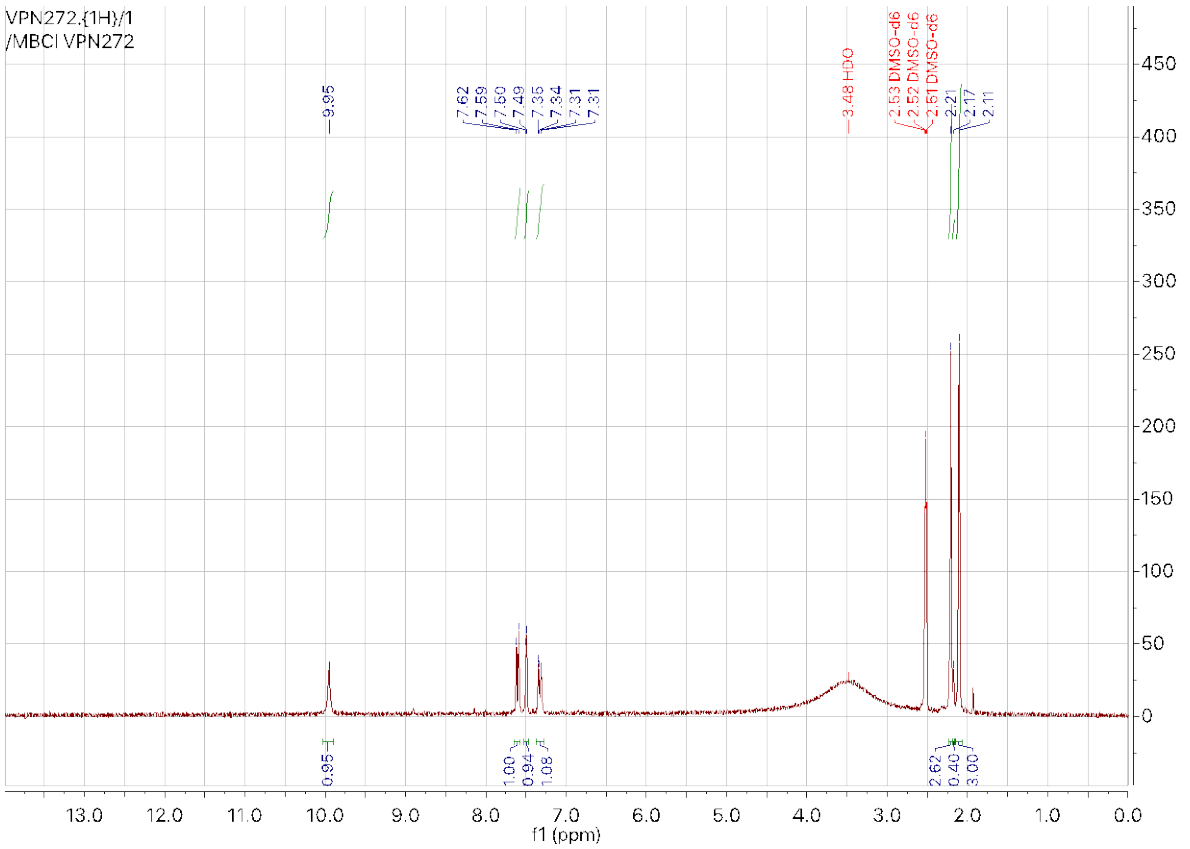


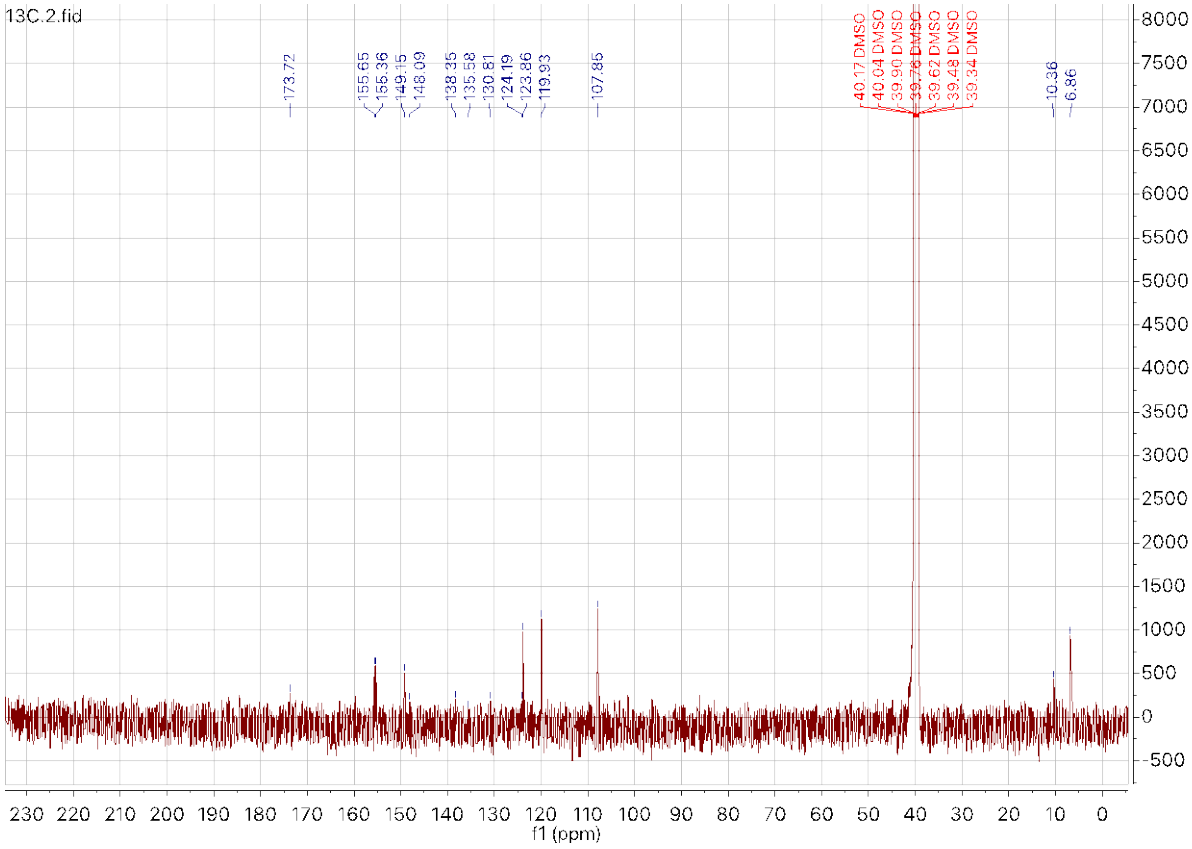




2.10. 3-(1-Hydroxy-4,5-dimethyl-1H-imidazol-2-yl)-6-hydroxy-4H-chromen-4-one (4d).







3. Copies of HRMS spectra of new compounds

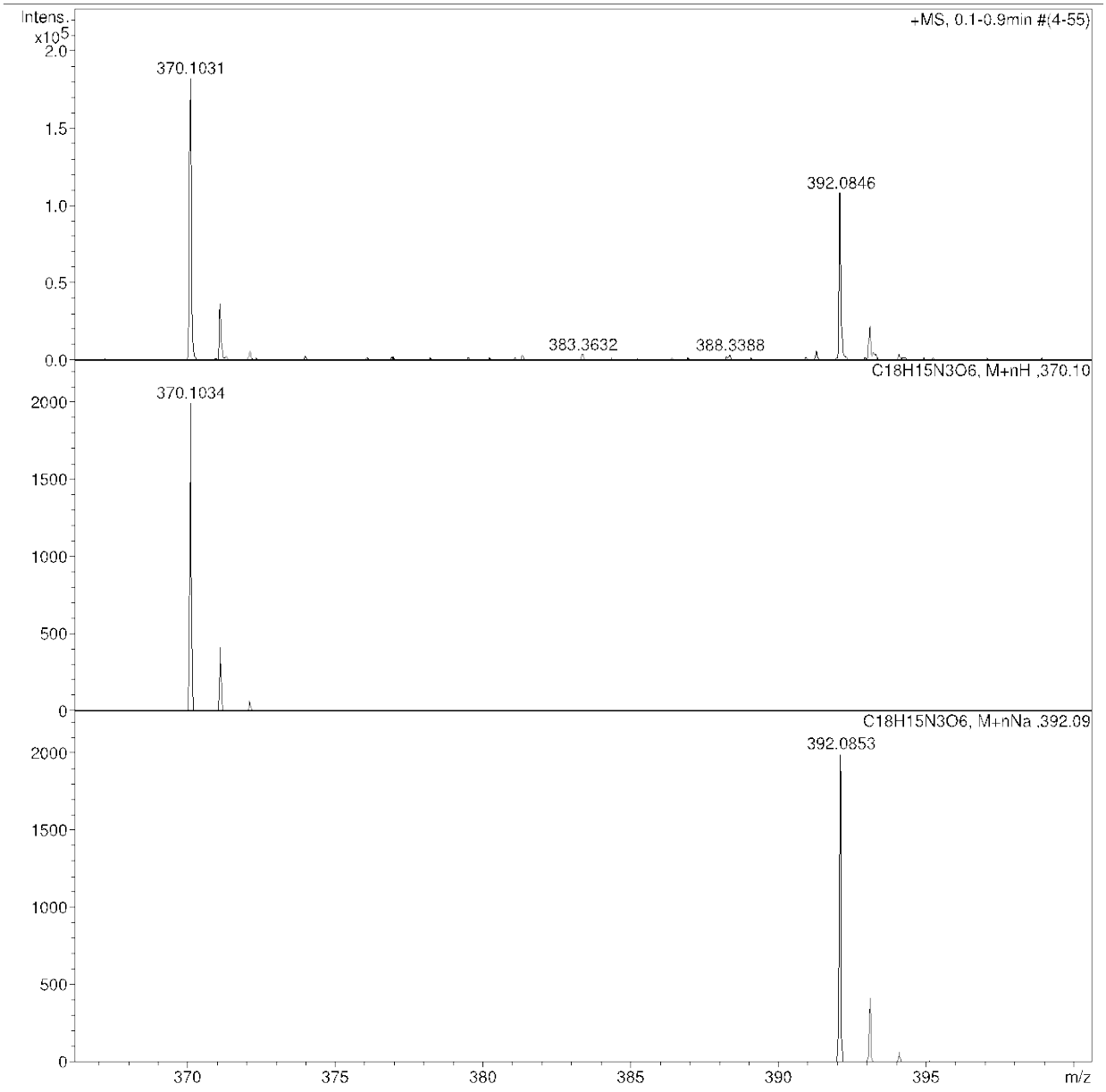
3.1. 1-Hydroxy-5,5-dimethyl-2-(6-nitro-4-oxo-4H-chromen-3-yl)-4,5,6,7-tetrahydro-4H-benzimidazol-7-one (1a)

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2018\Mityanov\0730002.d	Acquisition Date	30.07.2018 15:07:16
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/MBCI PN260	Instrument / Ser#	micrOTOF 10248
Comment	C18H15N3O6 mH 370.1033 clb added		

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



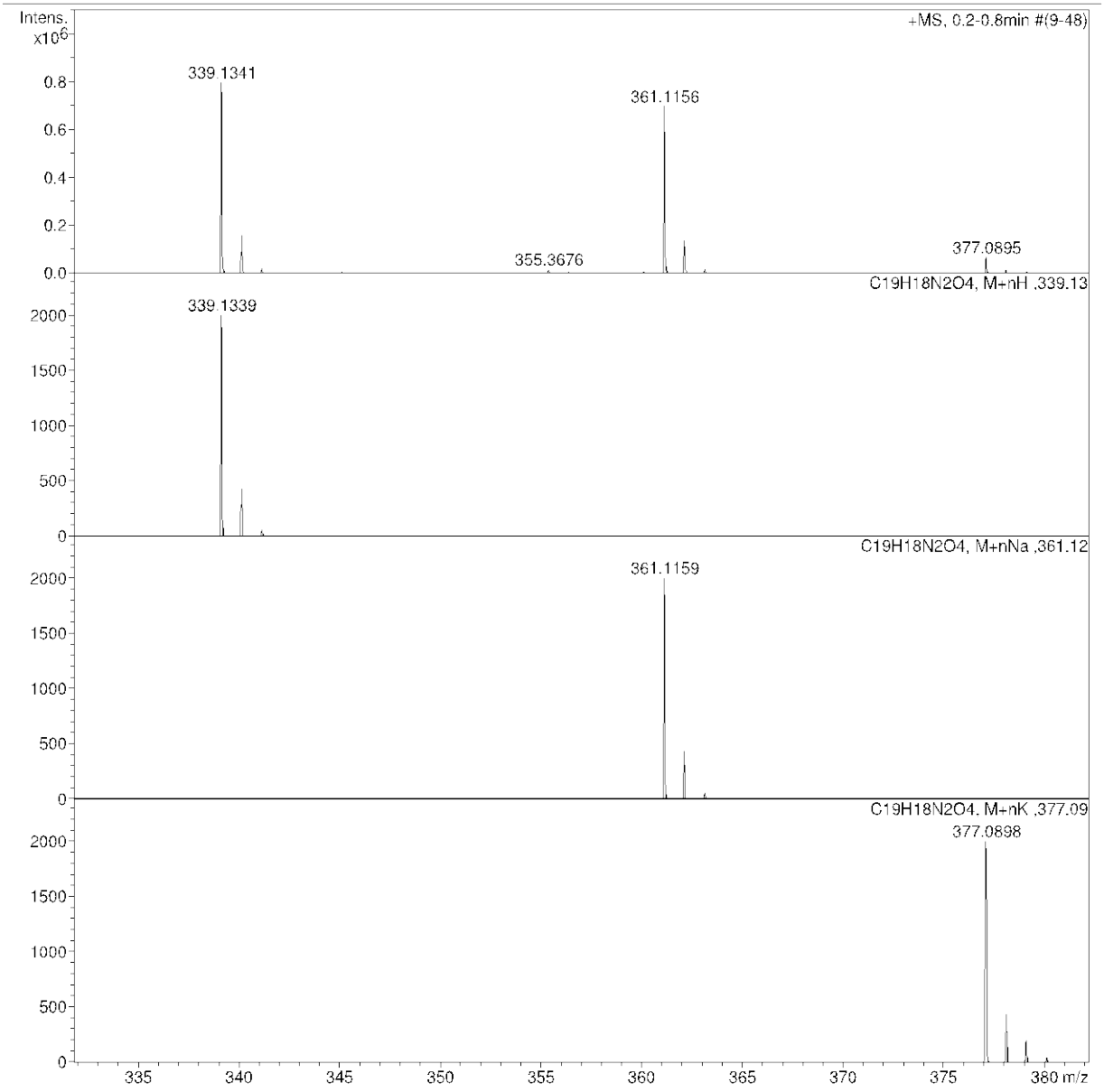
3.2. 1-Hydroxy-5,5-dimethyl-2-(6-methyl-4-oxo-4H-chromen-3-yl)-4,5,6,7-tetrahydro-4H-benzimidazol-7-one (1c).

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2018\Mityanov\0724009.d	Acquisition Date	24.07.2018 14:47:28
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/MBCI PN277	Instrument / Ser#	micrOTOF 10248
Comment	C19H18N2O4 mH 339.1339 clb added		

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



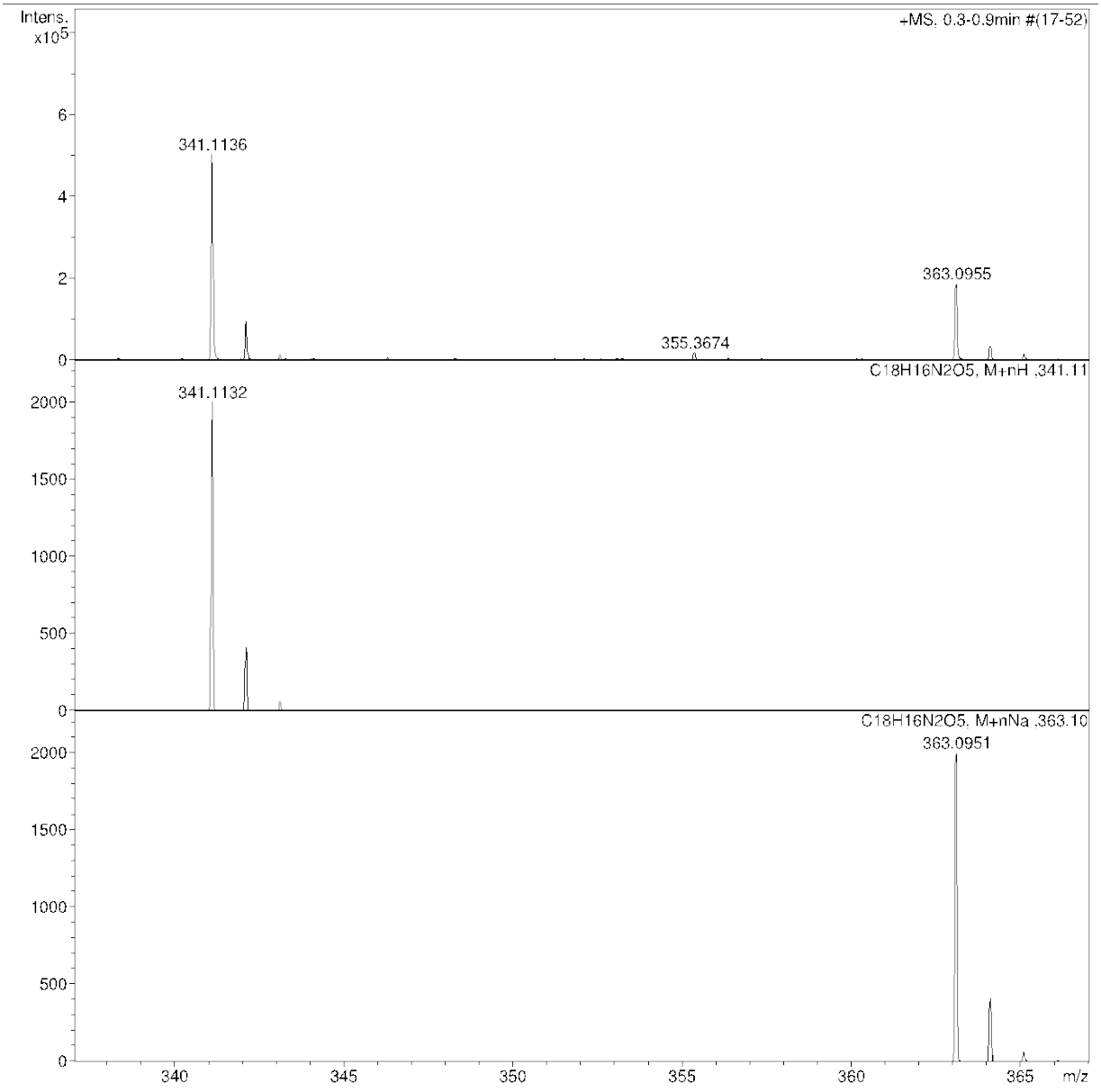
3.3. 1-Hydroxy-5,5-dimethyl-2-(6-hydroxy-4-oxo-4H-chromen-3-yl)-4,5,6,7-tetrahydro-4H-benzimidazol-7-one (1d).

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2018\Mityanov\0726016.d	Acquisition Date	26.07.2018 14:17:07
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/MBCI PN268	Instrument / Ser#	micrOTOF 10248
Comment	C18H16N2O5 mH 341.1131 clb added		

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



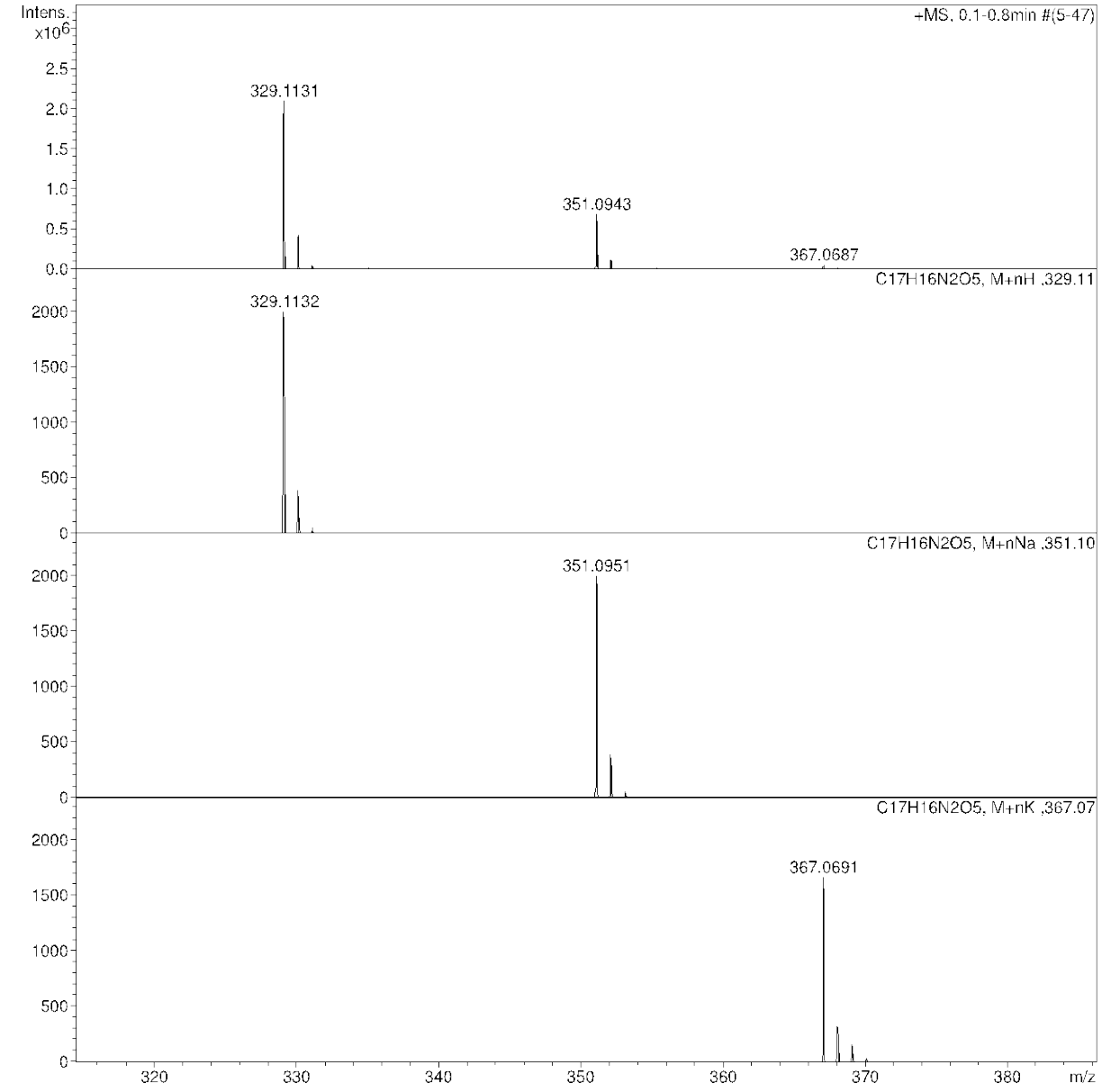
3.4. Ethyl 1-hydroxy-4-methyl-2-(6-methyl-4-oxo-4H-chromen-3-yl)-1H-imidazole-5-carboxylate (2c).

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2018\Mityanov\0724007.d	Acquisition Date	24.07.2018 14:26:51
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/MBCI PN29	Instrument / Ser#	micrOTOF 10248
Comment	C17H16N2O5 mH 329.1131 clb added		

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



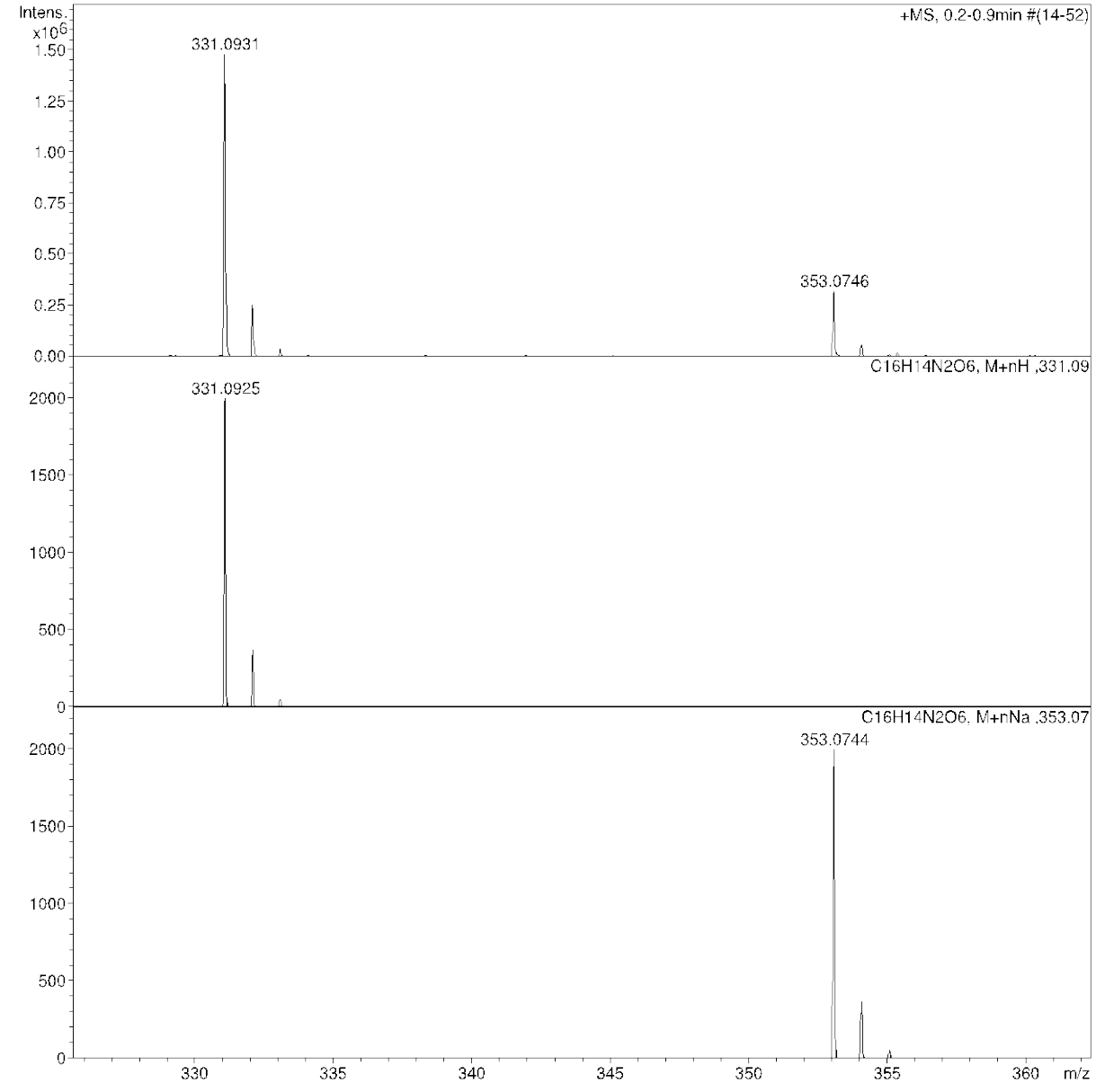
3.5. Ethyl 1-hydroxy-4-methyl-2-(6-hydroxy-4-oxo-4H-chromen-3-yl)-1H-imidazole-5-carboxylate (2d)

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2018\Mityanov\0726015.d	Acquisition Date	26.07.2018 14:11:13
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/MBCI PN265	Instrument / Ser#	micrOTOF 10248
Comment	C16H14N2O6 mH 331.0934 clb added		

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



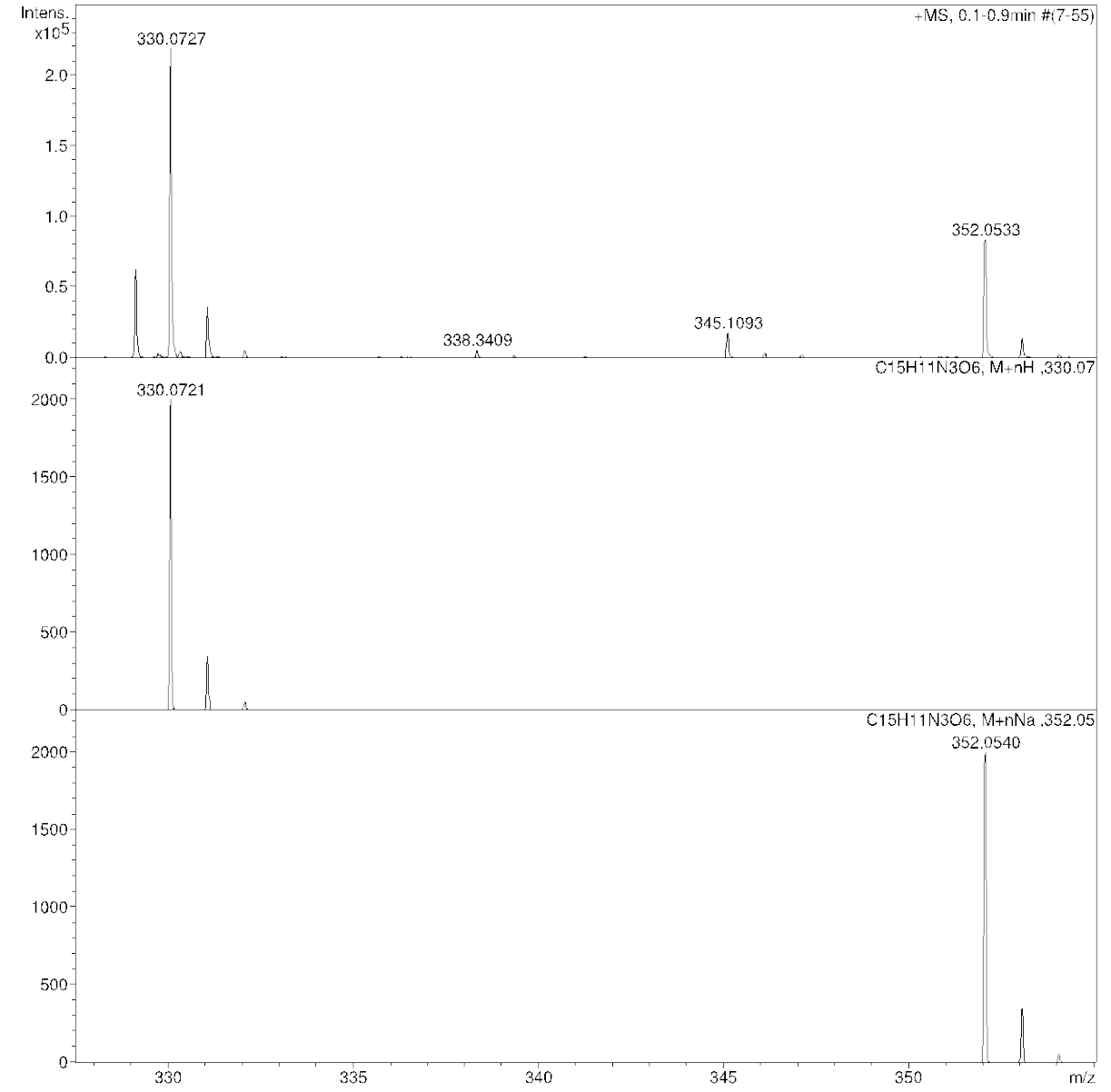
3.6. 3-(5-Acetyl-1-hydroxy-4-methyl-1H-imidazol-2-yl)-6-nitro-4H-chromen-4-one (3a)

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2018\Mityanov\0725009.d	Acquisition Date	25.07.2018 16:17:09
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/MBCI PN254	Instrument / Ser#	micrOTOF 10248
Comment	C15H11N3O6 mH 330.0720 clb added		

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



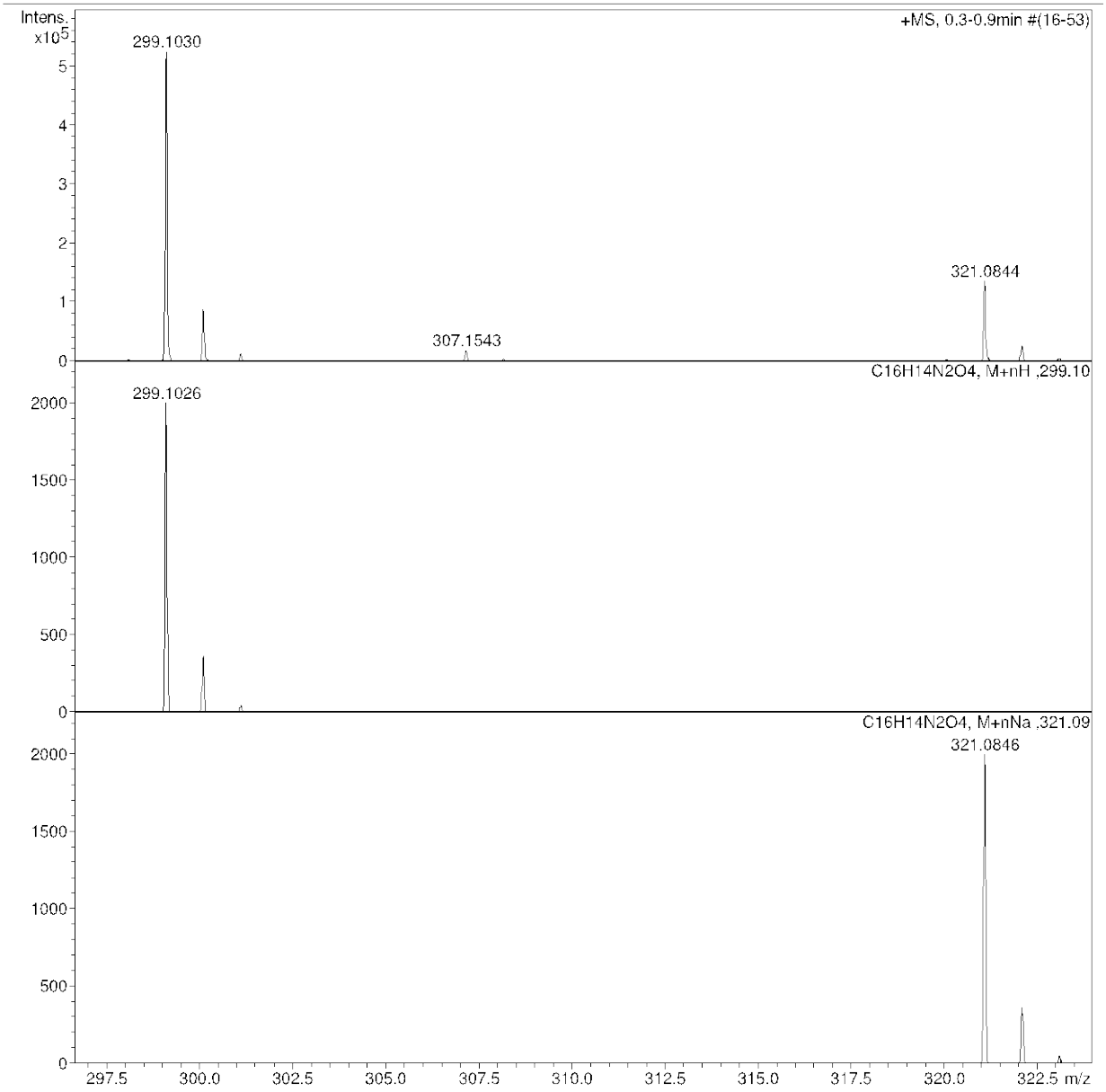
3.7. 3-(5-Acetyl-1-hydroxy-4-methyl-1H-imidazol-2-yl)-6-methyl-4H-chromen-4-one (3c)

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2018\Mityanov\0725011.d	Acquisition Date	25.07.2018 16:31:19
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/MBCI PN276	Instrument / Ser#	micrOTOF 10248
Comment	C16H14N2O4 mH 299.1026 clb added		

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



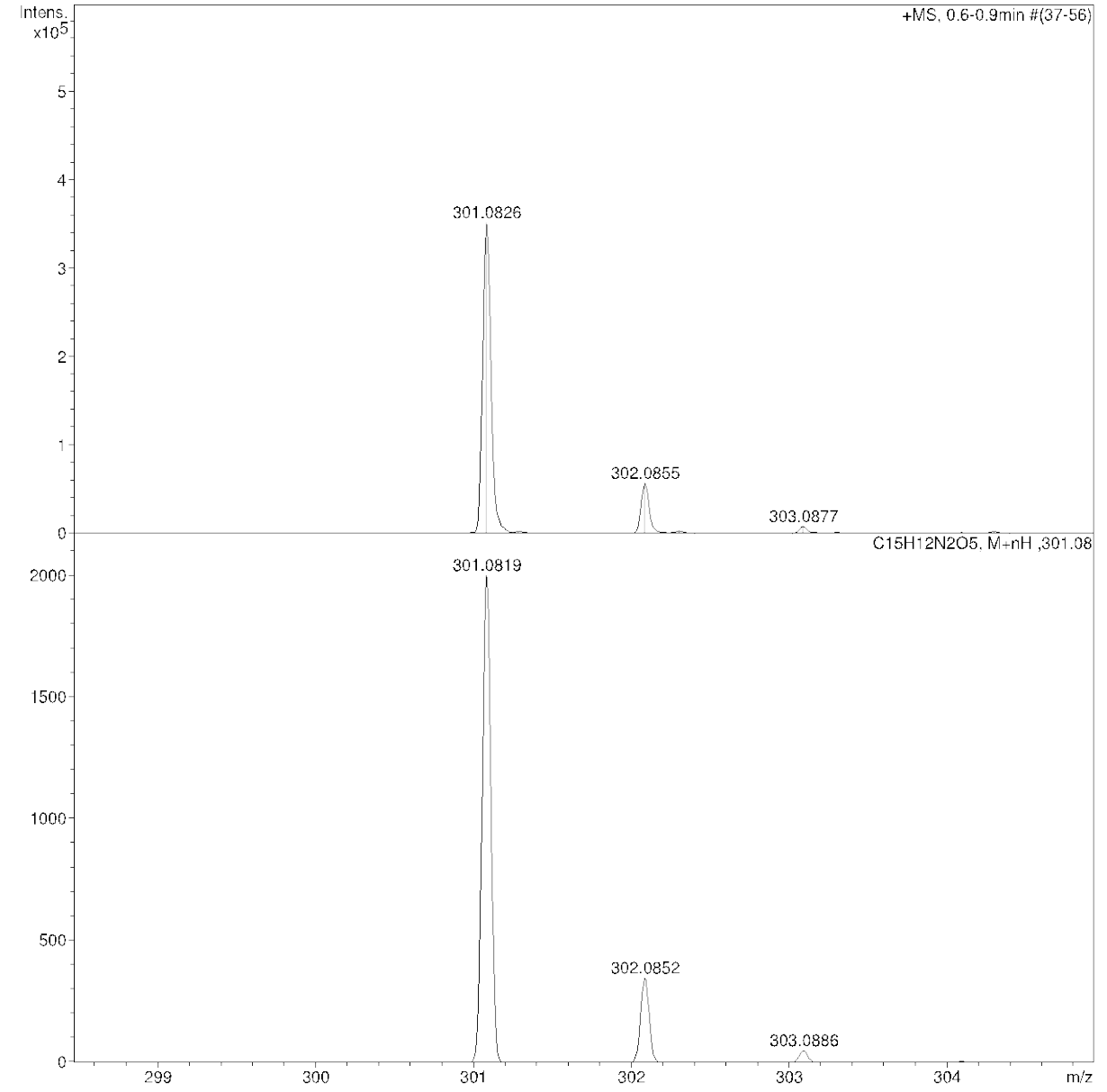
3.8. 3-(5-Acetyl-1-hydroxy-4-methyl-1H-imidazol-2-yl)-6-hydroxy-4H-chromen-4-one (3d).

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2018\Mityanov\0725010.d	Acquisition Date	25.07.2018 16:25:49
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/MBCI PN266	Instrument / Ser#	micrOTOF 10248
Comment	C15H12N2O5 mH 301.0818 clb added		

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



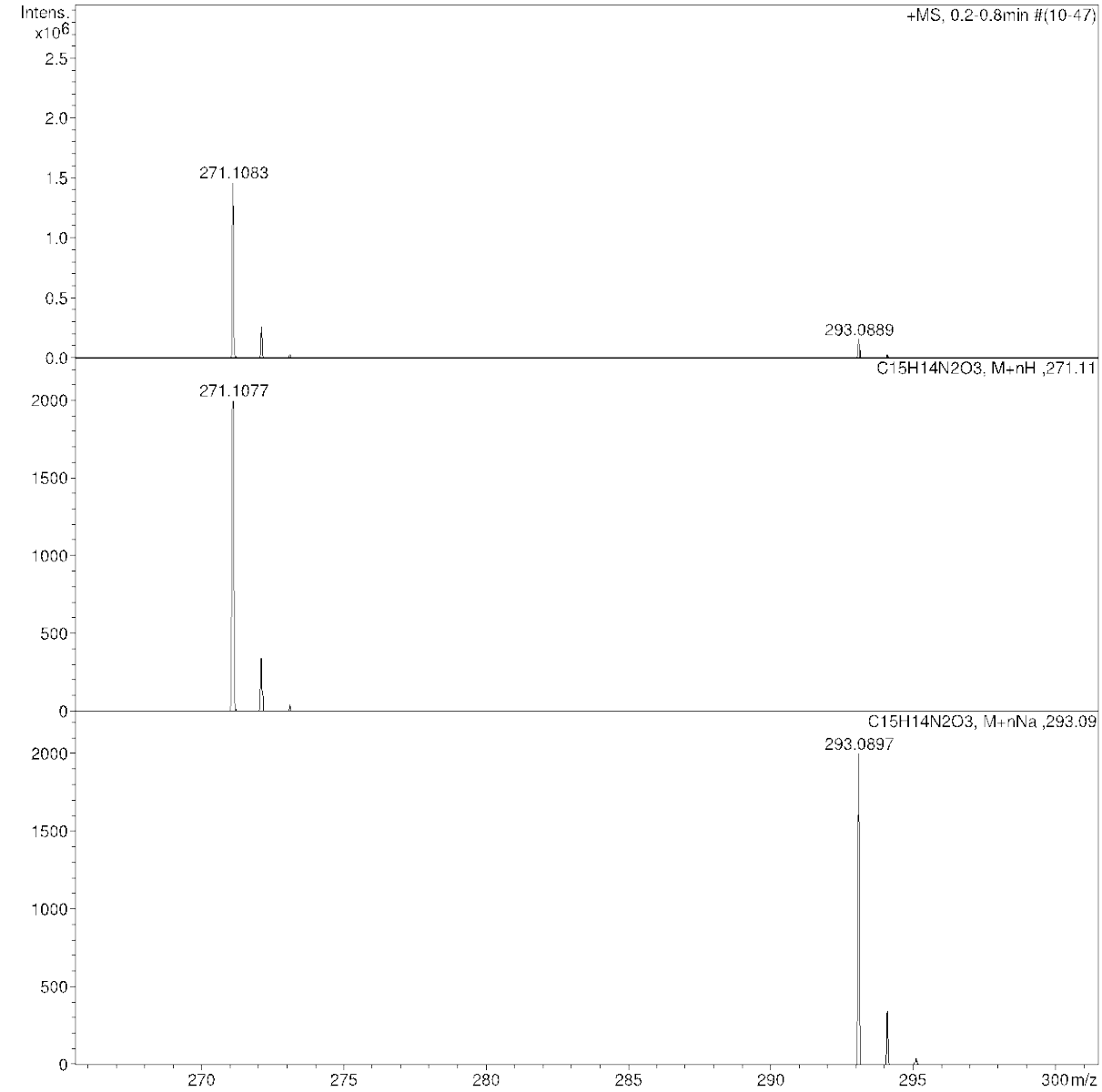
3.9. 3-(1-Hydroxy-4,5-dimethyl-*1H*-imidazol-2-yl)-6-methyl-*4H*-chromen-4-one (4c).

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2018\Mityanov\0724010.d	Acquisition Date	24.07.2018 14:53:57
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/MBCI PN281	Instrument / Ser#	micrOTOF 10248
Comment	C15H14N2O3 mH 271.1077 clb added		

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



3.10. 3-(1-Hydroxy-4,5-dimethyl-1H-imidazol-2-yl)-6-hydroxy-4H-chromen-4-one (4d).

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2018\Mityanov\0724008.d	Acquisition Date	24.07.2018 14:42:12
Method	tune_50-1600.m	Operator	BDAL@DE
Sample Name	/MBCI PN272	Instrument / Ser#	micrOTOF 10248
Comment	C14H12N2O4 mH 273.0869 clb added		

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