Supplementary Material

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


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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).

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\begin{align*}
\text{Wavenumber (cm}^{-1}\text{)} & \quad \text{%Transmittance} \\
4000 & \quad 3271.27 \\
3500 & \quad 1666.5 \\
3000 & \quad 1635.64 \\
2500 & \quad \text{NH} C=O \\
2000 & \quad C=O \\
1500 & \quad \text{NH} \\
1000 & \quad \text{C}=O \\
500 & \quad 0
\end{align*}
\]

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

\[
\begin{align*}
\text{Wavenumber (cm}^{-1}\text{)} & \quad \text{%Transmittance} \\
4000 & \quad 3247.3 \\
3500 & \quad 1654.99 \\
3000 & \quad 1642.46 \\
2500 & \quad \text{NH} \\
2000 & \quad \text{C}=O C=O \\
1500 & \quad \text{NH} \\
1000 & \quad \text{C}=O \\
500 & \quad 0
\end{align*}
\]
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-1\textit{H}-imidazol-2-yl)-6-methyl-4\textit{H}-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)
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).
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).
3.4. Ethyl 1-hydroxy-4-methyl-2-(6-methyl-4-oxo-4H-chromen-3-yl)-1H-imidazole-5-carboxylate (2c).
3.5. Ethyl 1-hydroxy-4-methyl-2-(6-hydroxy-4-oxo-4H-chromen-3-yl)-1H-imidazole-5-carboxylate (2d)
3.6. 3-(5-Acetyl-1-hydroxy-4-methyl-1H-imidazol-2-yl)-6-nitro-4H-chromen-4-one (3a)

Acquisition Info
- Analysis Name: 01Data/Phosphine/2018/Michanov0725009.d
- Method: tenu 30-1620 m
- Sample Name: VMSO P254
- Comment: C15H11N3O6. m/z 330.0720 clc added

Acquisition Parameter
- Source Type: ESI
- Ion Polarity: Positive
- Focus: Not active
- Scan Begin: 50 m/z
- Scan End: 1600 m/z
- SetٷNeill: 4500 V
- Set End Plate Offset: -600 V
- Set Dry Heater: 200 °C
- Set Dry Gas: 4.0 l/min
- Set Divert Valve: Waste

Graphical representation of mass spectrometry data with peaks at m/z 330.027, 330.052, 330.072, 330.340, 335.099, 335.109, 345.109, 352.055.
3.7. 3-(5-Acetyl-1-hydroxy-4-methyl-1H-imidazol-2-yl)-6-methyl-4H-chromen-4-one (3c)
3.8. 3-(5-Acetyl-1-hydroxy-4-methyl-1H-imidazol-2-yl)-6-hydroxy-4H-chromen-4-one (3d).
3.9. 3-(1-Hydroxy-4,5-dimethyl-1H-imidazol-2-yl)-6-methyl-4H-chromen-4-one (4c).
3.10. 3-(1-Hydroxy-4,5-dimethyl-1H-imidazol-2-yl)-6-hydroxy-4H-chromen-4-one (4d).