Supplementary Material

Microwave induced synthesis of new class of pyrano isoxazoline and isoxazole annulated chromones - an intramolecular nitrile oxide cycloaddition with tethered olefins and alkynes

Jayaprakash Rao Yerrabellı,* Shyam Prasad Nuligonda,* Sudhakar Mokenapelli* and Prasad Rao Chitneni*

*Natural Products Laboratory, Department of Chemistry, Osmania University, Hyderabad-500007, Telangana, India
Email: yjpr_19@yahoo.com

Table of contents

1. $^1$H, $^{13}$C-NMR and ESI-HRMS spectrums for compound 3a S2
2. $^1$H NMR and ESI-HRMS spectrums for compound 3b S5
3. $^1$H NMR spectra for compound 3c S7
4. $^1$H NMR and ESI-HRMS spectrums for compound 3d S8
5. ESI-HRMS spectrums for compound 3g S10
6. $^1$H, $^{13}$C-NMR and ESI-HRMS spectrums for compound 5a S11
7. $^1$H NMR and ESI-HRMS spectrums for compound 5c S14
$^1$H-NMR of 9,10-dimethyl-3a,4-dihydropyran[2',3':5,6]chromeno[4,3-c]isoxazol-8(3H)-one (3a)
$^{13}$C-NMR of 9,10-dimethyl-3a,4-dihydropyran[2',3':5,6]chromeno[4,3-c]isoxazol-8(3H)-one (3a):
ESI-HRMS of 9,10-dimethyl-3a,4-dihydropyran[2’,3’:5,6]chromeno[4,3-c]isoxazol-8(3H)-one (3a)
$^1$H-NMR spectra of 3,9,10-trimethyl-3a,4-dihydropyano [2',3':5,6] chromeno [4,3-c] isoxazol-8(3H)-one (3b)
ESI-HRMS of 3,9,10-trimethyl-3a,4-dihydropyran-2',3':5,6] chromeno-[4,3-c] isoxazol-8(3H)-one (3b):
$^1$H-NMR Spectra of 3,3,9,10-tetramethyl-3a,4-dihydropyrano[2',3':5,6]chromeno[4,3-c]isoxazol-8(3H)-one (3c):
$^1$H-NMR Spectra of 9,10-dimethyl-3-phenyl-3a,4-dihydropyrano[2',3':5,6]chromeno[4,3-c]isoxazol-8(3H)-one (3d):
ESI-HRMS of 9,10-dimethyl-3-phenyl-3a,4-dihydropyrano[2',3':5,6]chromeno[4,3-c]isoxazol-8(3H)-one (3d)
ESI-HRMS of 6-chloro-3,3,9,10-tetramethyl-3a,4-dihydropyran[2',3':5,6]chromeno[4,3-c]isoxazol-8(3H)-one (3g)

\[ \text{structure image} \]

\[ \text{ESI-HRMS data} \]

\[ \text{Graph showing ESI-HRMS data} \]

\[ \text{NMR spectra image} \]

\[ \text{NMR spectra data} \]

\[ \text{1H-NMR Spectra of 9,10-dimethylpyran[2',3':5,6]chromeno[4,3-c]isoxazol-8(4H)-one (5a)} \]
$^{13}$C-NMR Spectra of 9,10-dimethylpyran[2',3':5,6]chromeno[4,3-c]isoxazol-8(4H)-one (5a):
$^1$H-NMR Spectra of 3-ethyl-9,10-dimethylpyrano[2',3':5,6]chromeno[4,3-c]isoxazol-8(4H)-one (5c)
ESI-HRMS of 3-ethyl-9,10-dimethylpyrano[2',3':5,6]chromeno[4,3-c]isoxazol-8(4H)-one (5c)