

Supplementary Materials

Crystal structures, computational studies, and Hirshfeld surface analysis on 7-hydroxy-4-methyl-2H-chromen-2-one and 7-hydroxy-4-methyl-8-nitro-2H-chromen-2-one

Felix Odame ^{1,*}, Nathaniel Owusu Boadi ², Salifu Nanga ¹, Albert Aniagyei ¹ and Eric Hosten ³

¹ Department of Basic Sciences, School of Basics and Biomedical Sciences University of Health and Allied Sciences, PMB 31, Ho, Ghana.

² Department of Chemistry, Kwame Nkrumah University of Science and Technology, Kumasi, Ghana.

³ Department of Chemistry, Nelson Mandela University, PO Box 77000, Gqeberha 6031, South Africa.

* Corresponding author at: Department of Basic Sciences, School of Basics and Biomedical Sciences University of Health and Allied Sciences, PMB 31, Ho, Ghana. e-mail: felixessah15@gmail.com (F. Odame).

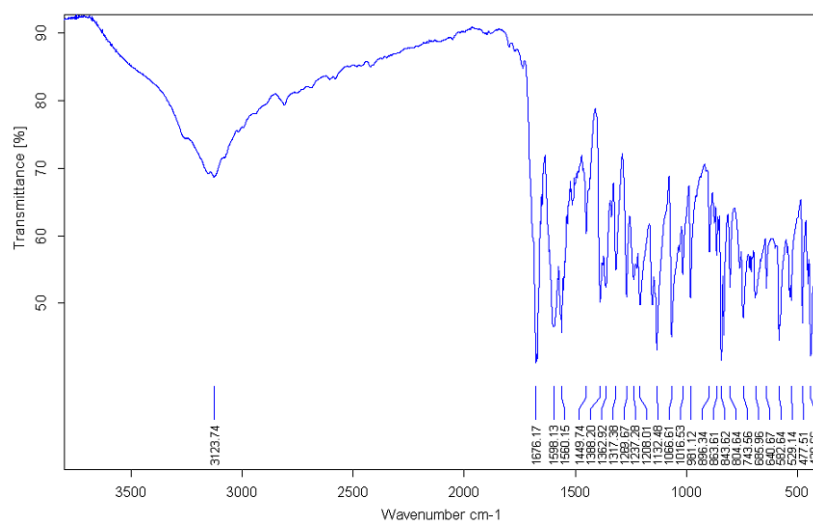


Figure S1. IR spectrum of 7-hydroxy-4-methyl-2H-chromen-2-one (1).

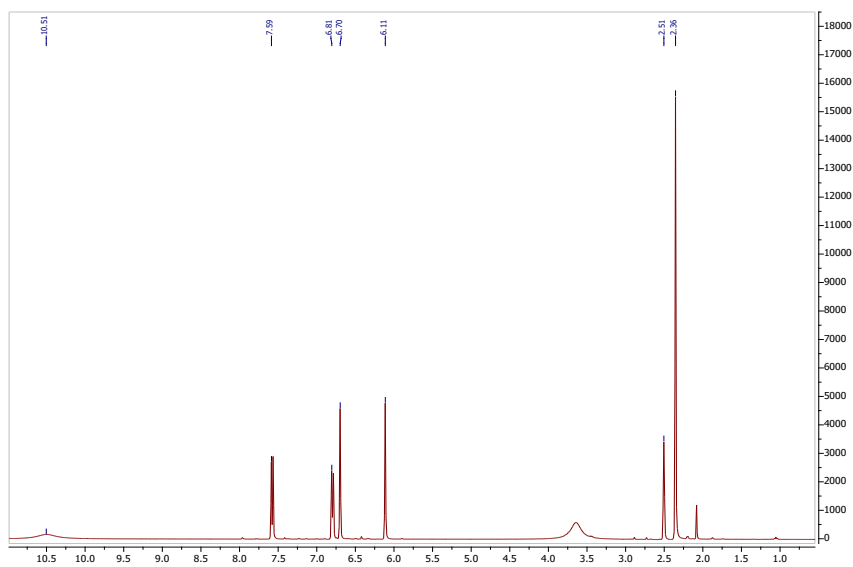


Figure S2. ¹H NMR spectrum of 7-hydroxy-4-methyl-2H-chromen-2-one (1).

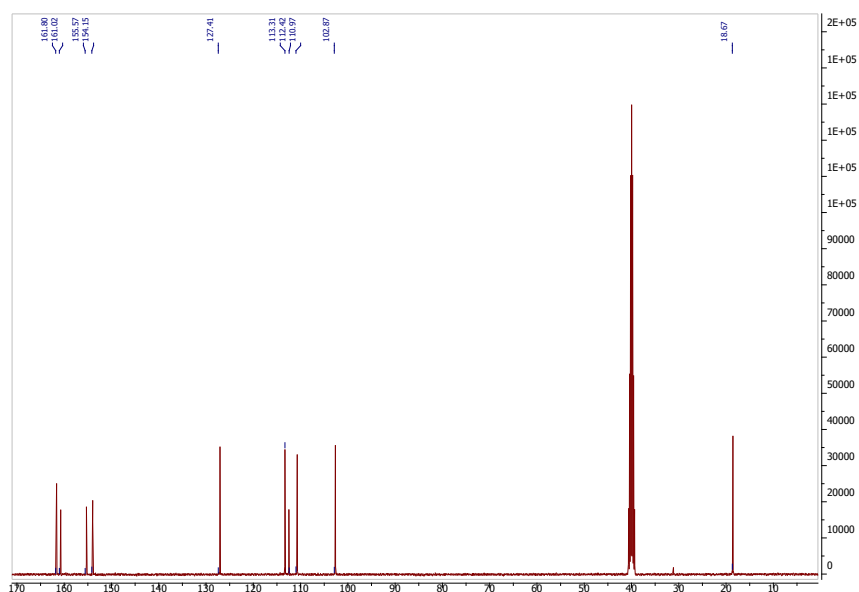


Figure S3. ¹³C NMR spectrum of 7-hydroxy-4-methyl-2H-chromen-2-one (1).

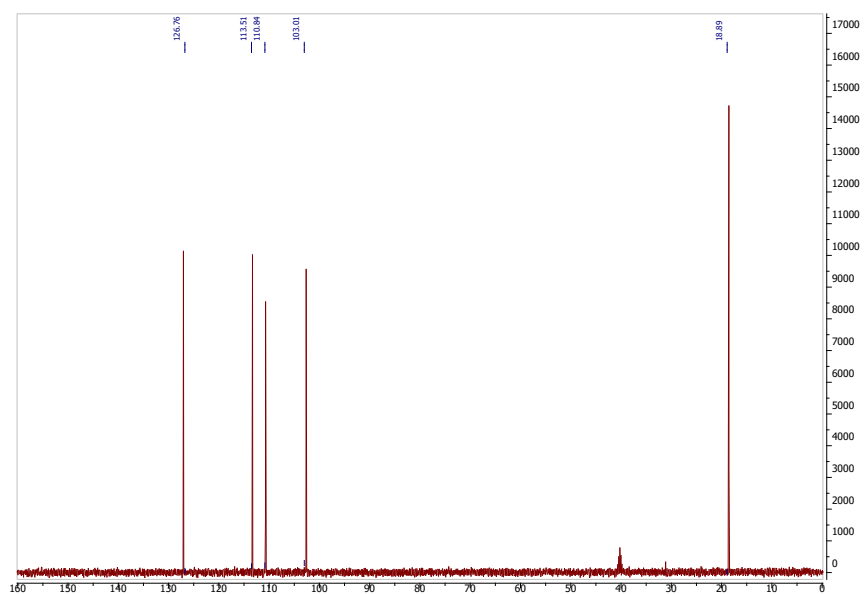


Figure S4. DEPT spectrum of 7-hydroxy-4-methyl-2H-chromen-2-one (1).

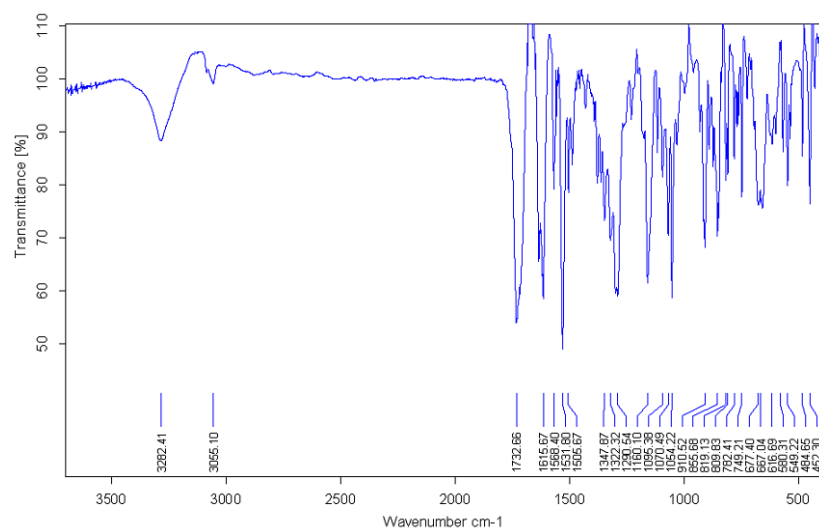


Figure S5. IR spectrum of 7-hydroxy-4-methyl-8-nitro-2H-chromen-2-one (2).

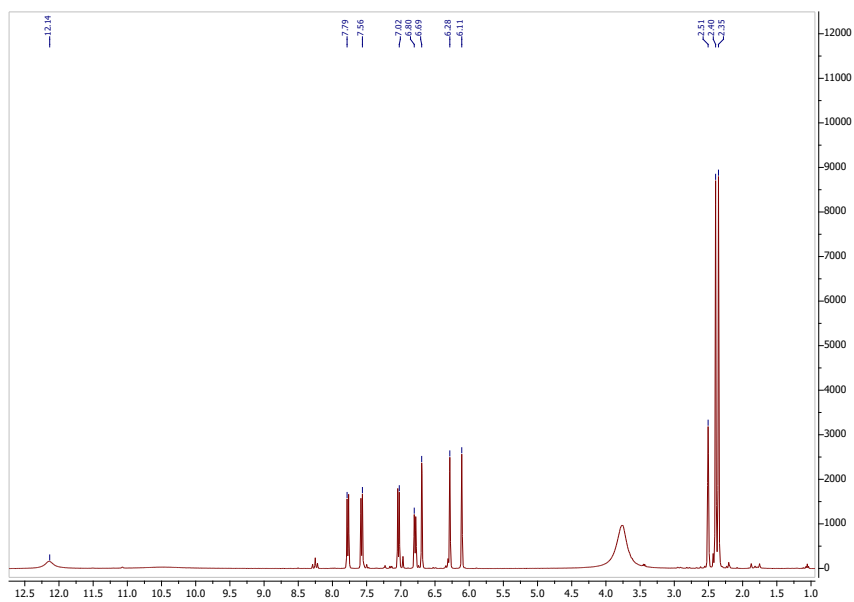


Figure S6. ^1H NMR spectrum of 7-hydroxy-4-methyl-8-nitro-2H-chromen-2-one (2).

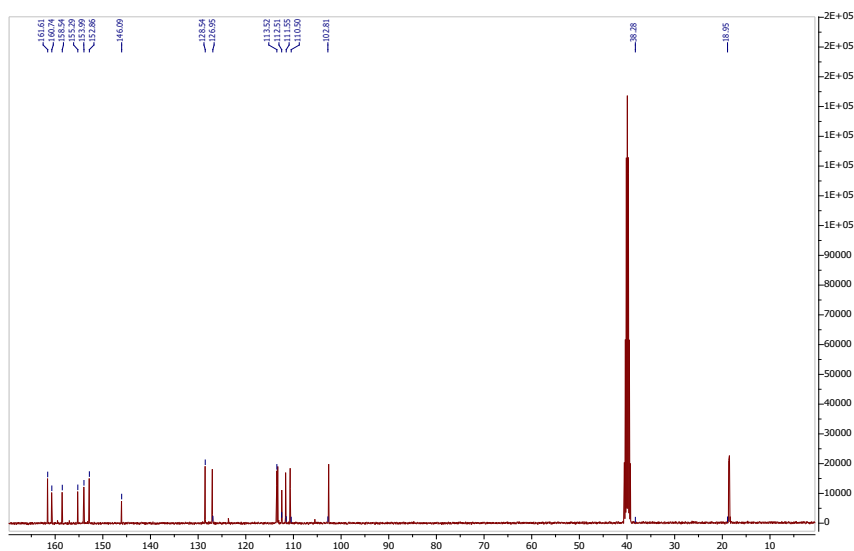


Figure S7. ^{13}C NMR spectrum of 7-hydroxy-4-methyl-8-nitro-2H-chromen-2-one (2).

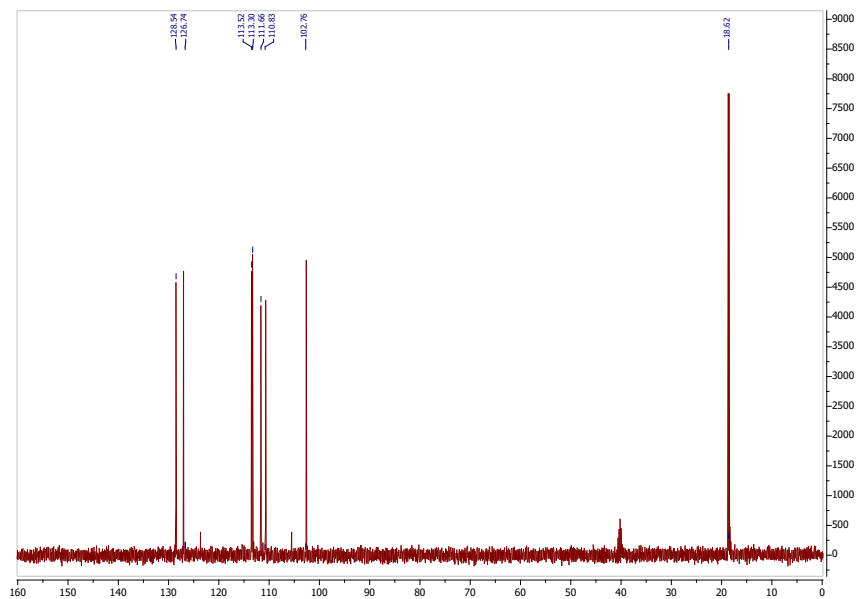


Figure S8. DEPT spectrum of 7-hydroxy-4-methyl-8-nitro-2H-chromen-2-one (2).

Table 1. HOMO-LUMO (Structures-compound 1).

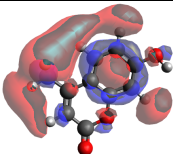
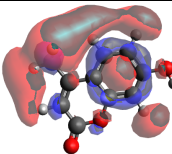
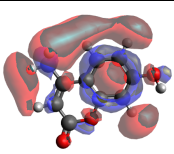
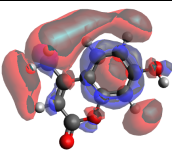
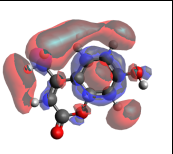
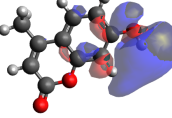
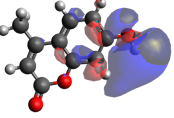
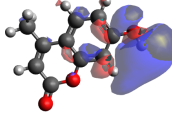
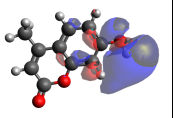
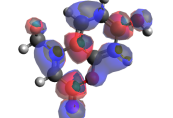
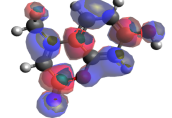
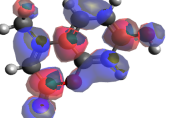
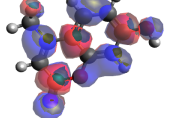
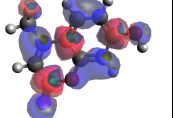
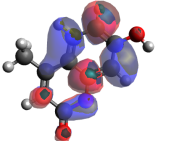
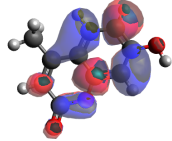
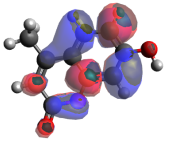
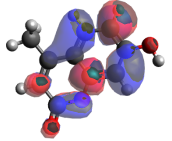
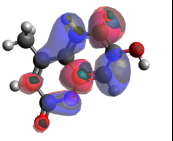
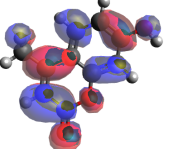
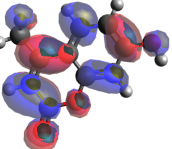
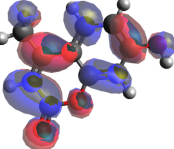
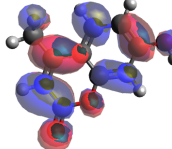
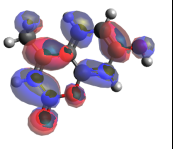
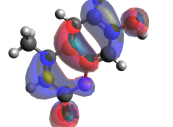
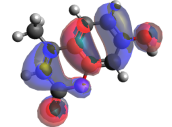
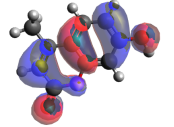
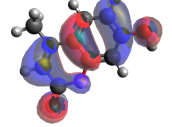
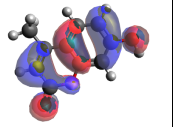
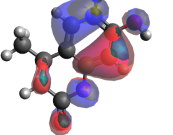
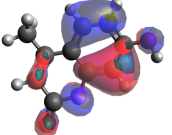
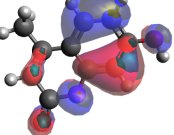
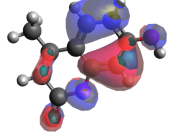
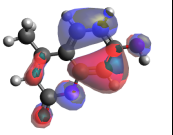
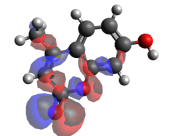
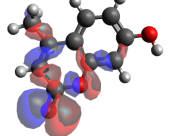
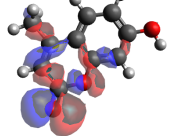
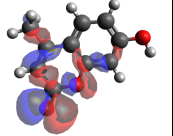
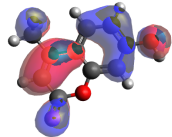
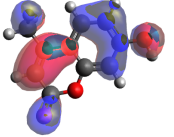
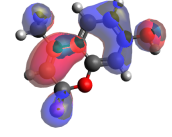
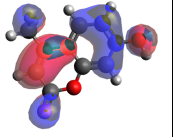
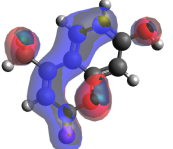
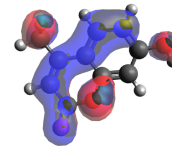
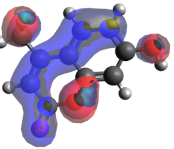
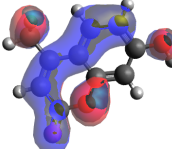
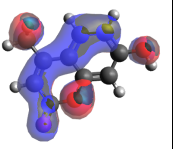
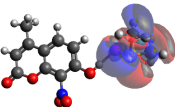
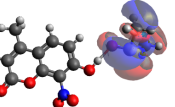
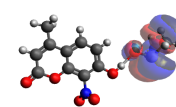
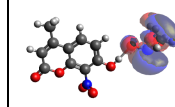
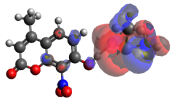
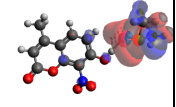
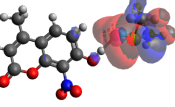
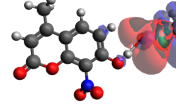
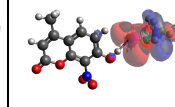
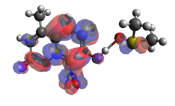
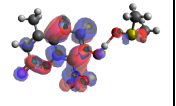
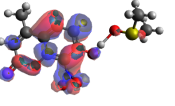
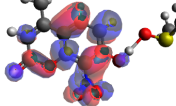
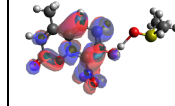
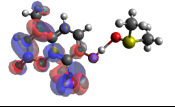
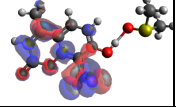
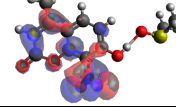
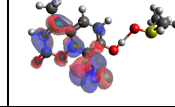
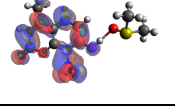
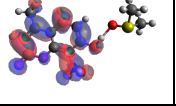
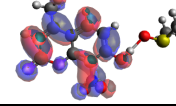
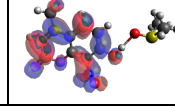
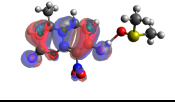
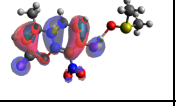
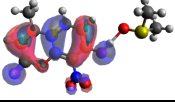
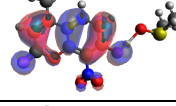
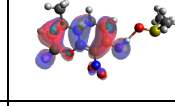
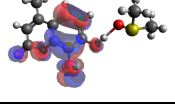
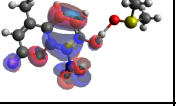
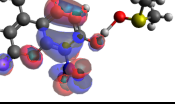
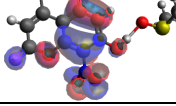
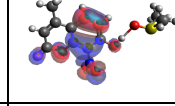
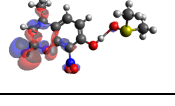
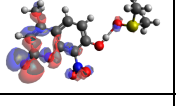
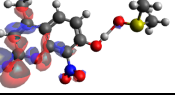
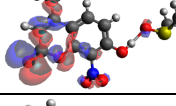
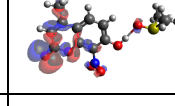
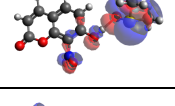
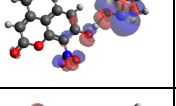
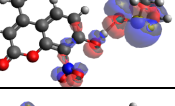
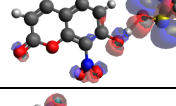
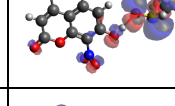
	B3LYP	CAM-B3LYP	B3PW91	WB97XD	M06
LUMO+4					
LUMO+3					
LUMO+2					
LUMO+1					
LUMO					
HOMO					
HOMO-1					
HOMO-2					
HOMO-3					
HOMO-4					

Table 2. HOMO-LUMO (Structures compound 2).

	B3LYP	CAM-B3LYP	B3PW91	WB97XD	M06
LUMO+4					
LUMO+3					
LUMO+2					
LUMO+1					
LUMO					
HOMO					
HOMO-1					
HOMO-2					
HOMO-3					
HOMO-4	