

## **Zinc acetate-catalyzed, green and efficient synthesis of xanthene derivatives under ultrasound irradiation: X-ray crystallographic analysis and *in silico* study**

Rayene Sayad<sup>1</sup>, Abdeslem Bouzina<sup>1\*</sup>, Yousra Ouafa Bouone<sup>1</sup>, Dounia Beldjezzia<sup>1</sup>, Abdelhak Djemel<sup>2</sup>, Malika Ibrahim-Ouali<sup>3</sup>, Nour-Eddine Aouf<sup>1</sup>, Zineb Aouf<sup>1\*</sup>

*1. Laboratory of Applied Organic Chemistry, Bioorganic Chemistry Group, Department of Chemistry, Sciences Faculty, Badji Mokhtar Annaba University, Box 12, 23000 Annaba, Algeria.*

*2. Research Unit in Medicinal Plants, URPM, 3000 Laghouat, attached to Research Center of Biotechnology, CRBt, 25000 Constantine, Algeria.*

*3. Aix Marseille Univ, CNRS, Centrale Marseille, iSm2, Marseille F-13397, France.*  
*Provide*

Corresponding author: [aouf.zineb27@gmail.com](mailto:aouf.zineb27@gmail.com).

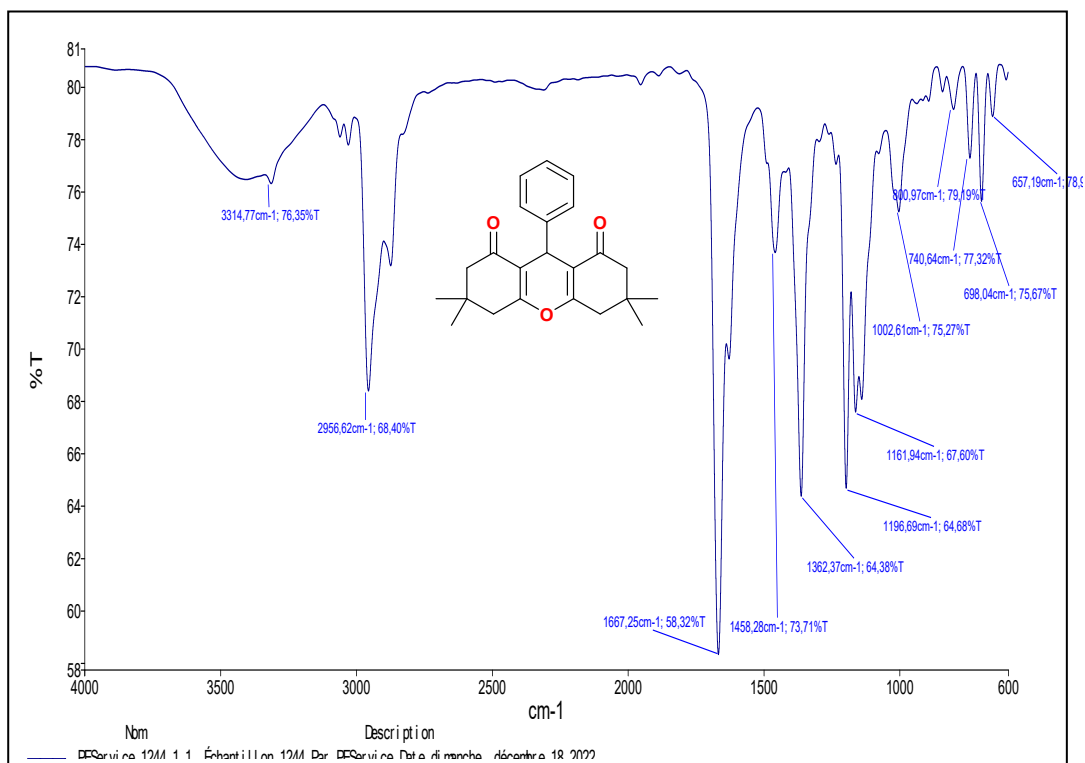
### **Supporting Information**

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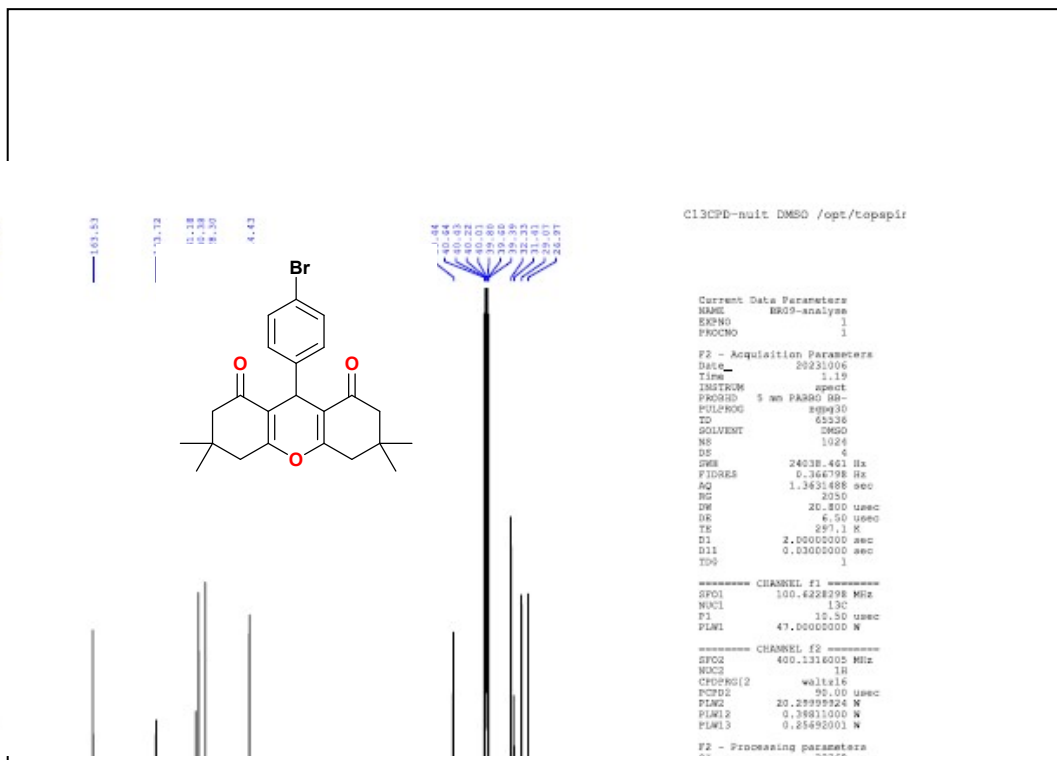
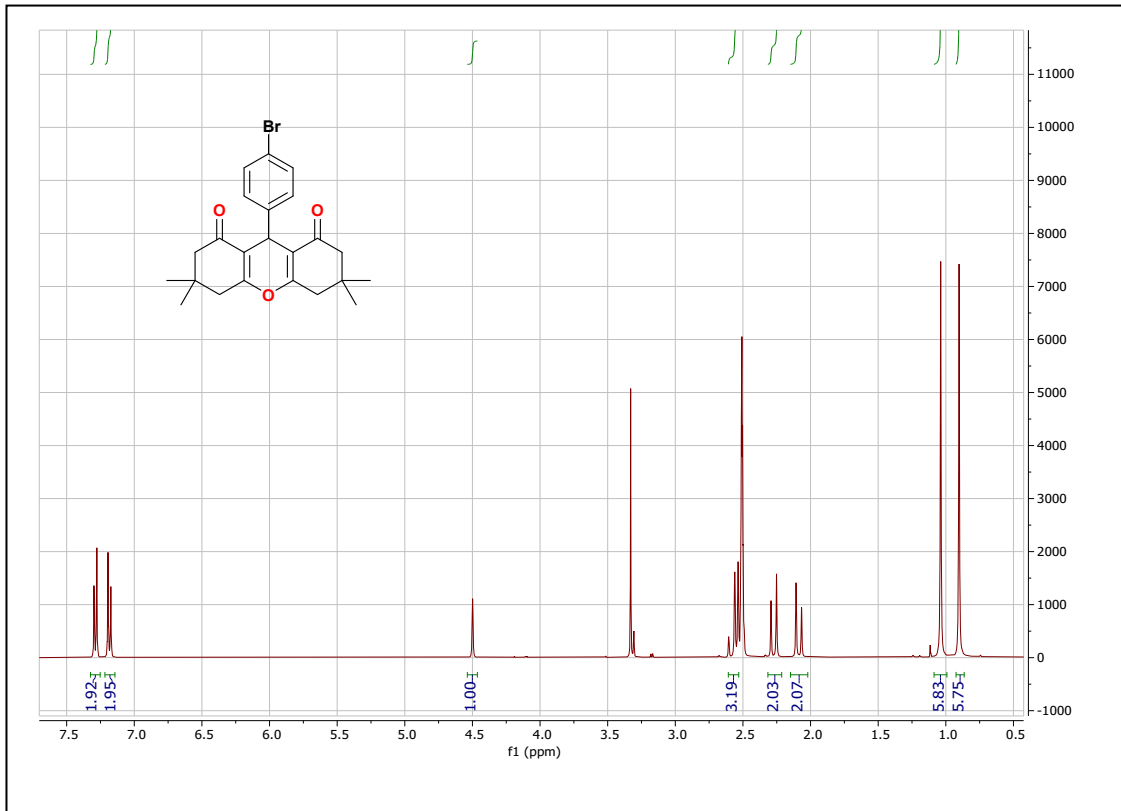
##### **1. Copies of NMR and IR spectra of products**

- <sup>1</sup>H, <sup>13</sup>C NMR and IR spectra of compound 3a
- <sup>1</sup>H, <sup>13</sup>C NMR and IR spectra of compound 3b
- <sup>1</sup>H, <sup>13</sup>C NMR and IR spectra of compound 3c
- <sup>1</sup>H, <sup>13</sup>C, <sup>19</sup>F NMR and IR spectra of compound 3d
- <sup>1</sup>H, <sup>13</sup>C NMR and IR spectra of compound 3e
- <sup>1</sup>H, <sup>13</sup>C NMR and IR spectra of compound 3f
- <sup>1</sup>H, <sup>13</sup>C NMR and IR spectra of compound 3g
- <sup>1</sup>H, <sup>13</sup>C NMR and IR spectra of compound 3h
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- <sup>1</sup>H, <sup>13</sup>C NMR and IR spectra of compound 3n
- <sup>1</sup>H, <sup>13</sup>C NMR and IR spectra of compound 3o
- <sup>1</sup>H, <sup>13</sup>C NMR and IR spectra of compound 3p
- <sup>1</sup>H, <sup>13</sup>C NMR and IR spectra of compound 3r
- <sup>1</sup>H, <sup>13</sup>C NMR and IR spectra of compound 3s



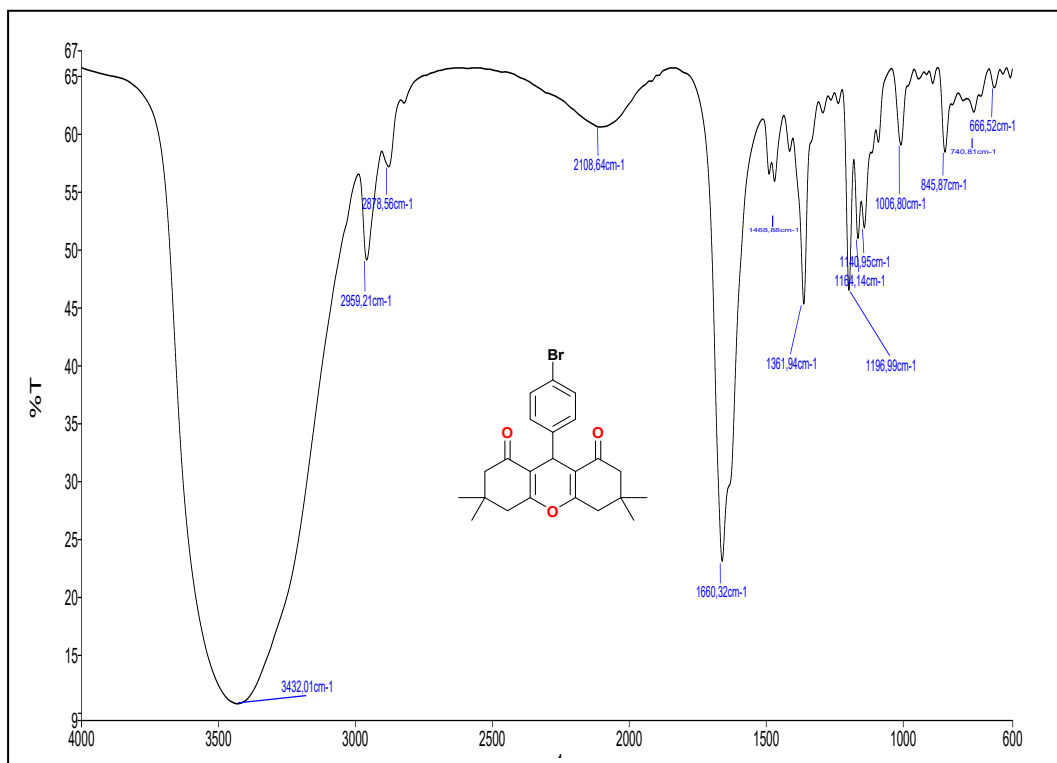


**IR spectrum: 3,3,6,6-tetramethyl-9-phenyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (3a)**

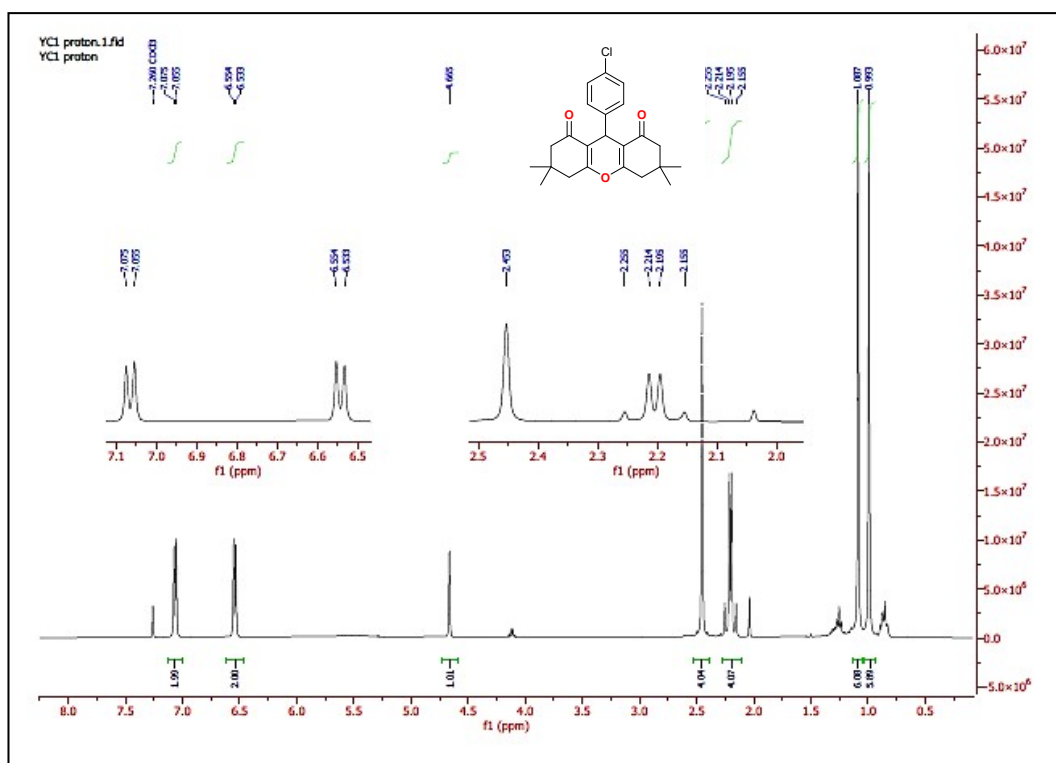


(3b)

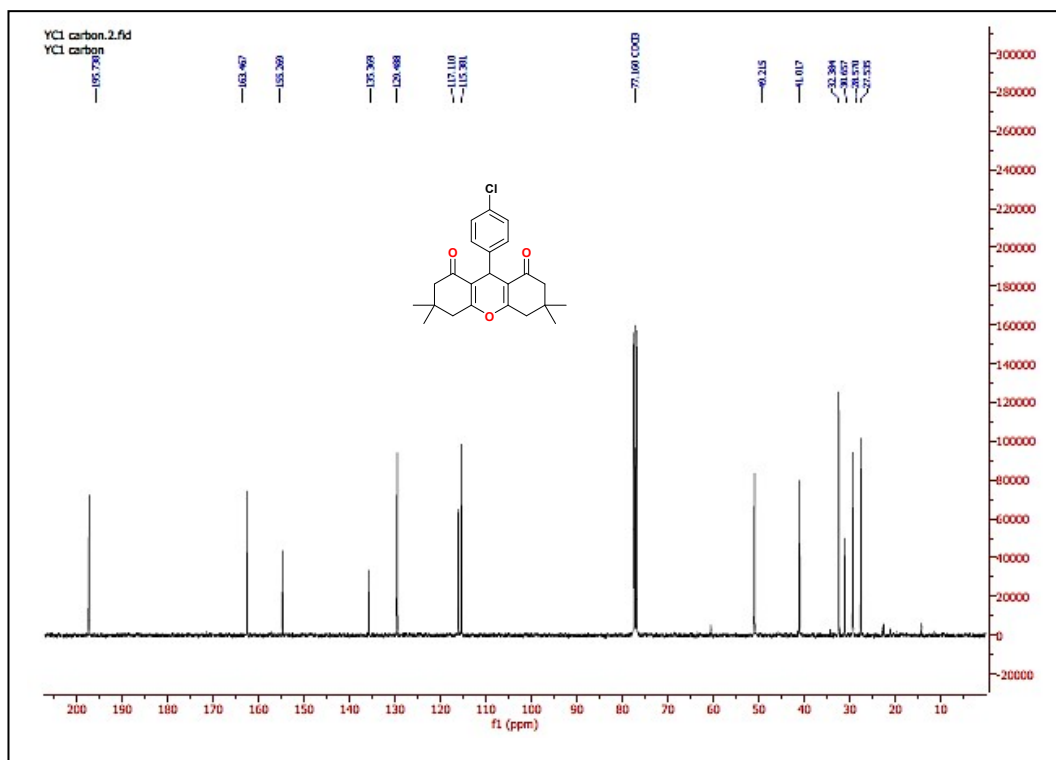
<sup>13</sup>C NMR spectrum (9-(4-bromophenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione  
(3b)



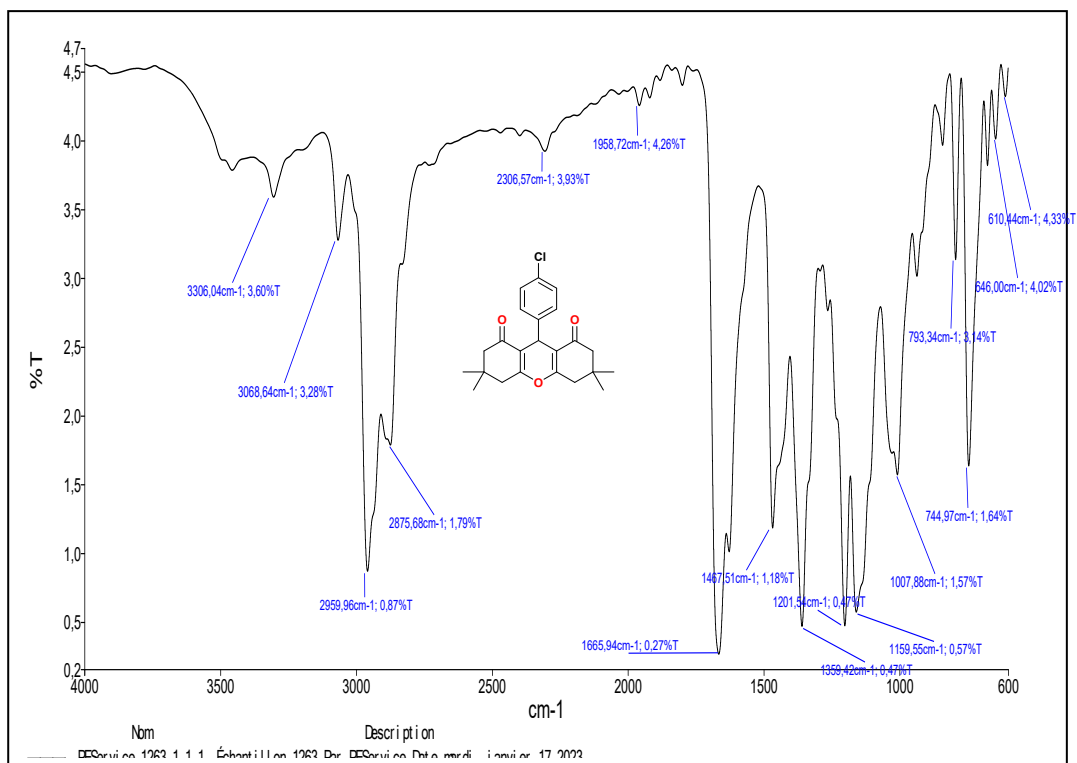
IR spectrum :9-(4-bromophenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (3b)



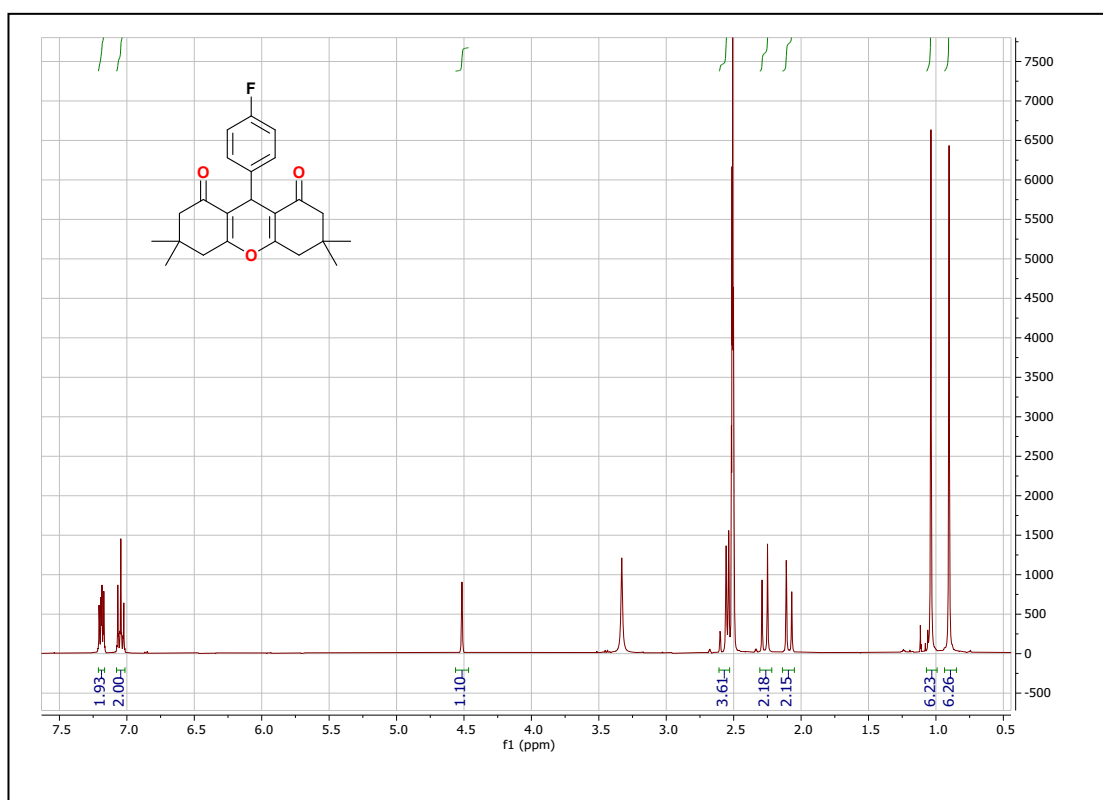
<sup>1</sup>H NMR spectrum: 9-(4-chlorophenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3c**)



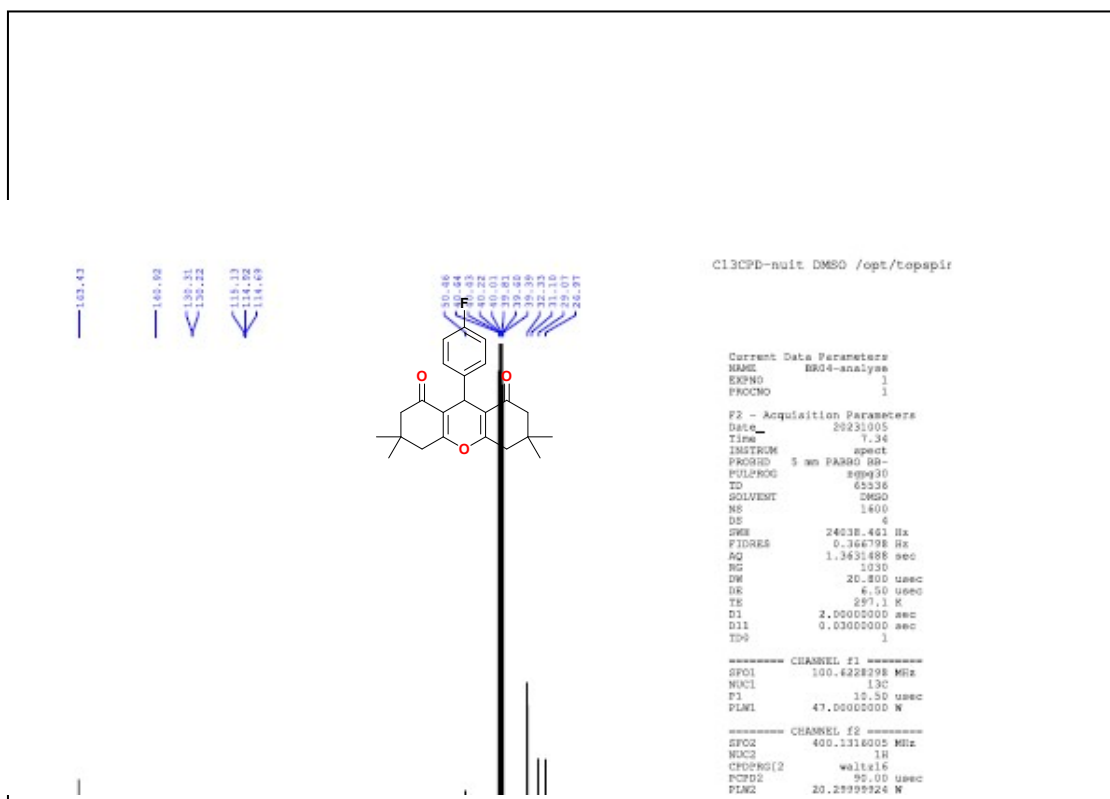
<sup>13</sup>C NMR spectrum: 9-(4-chlorophenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3c**)



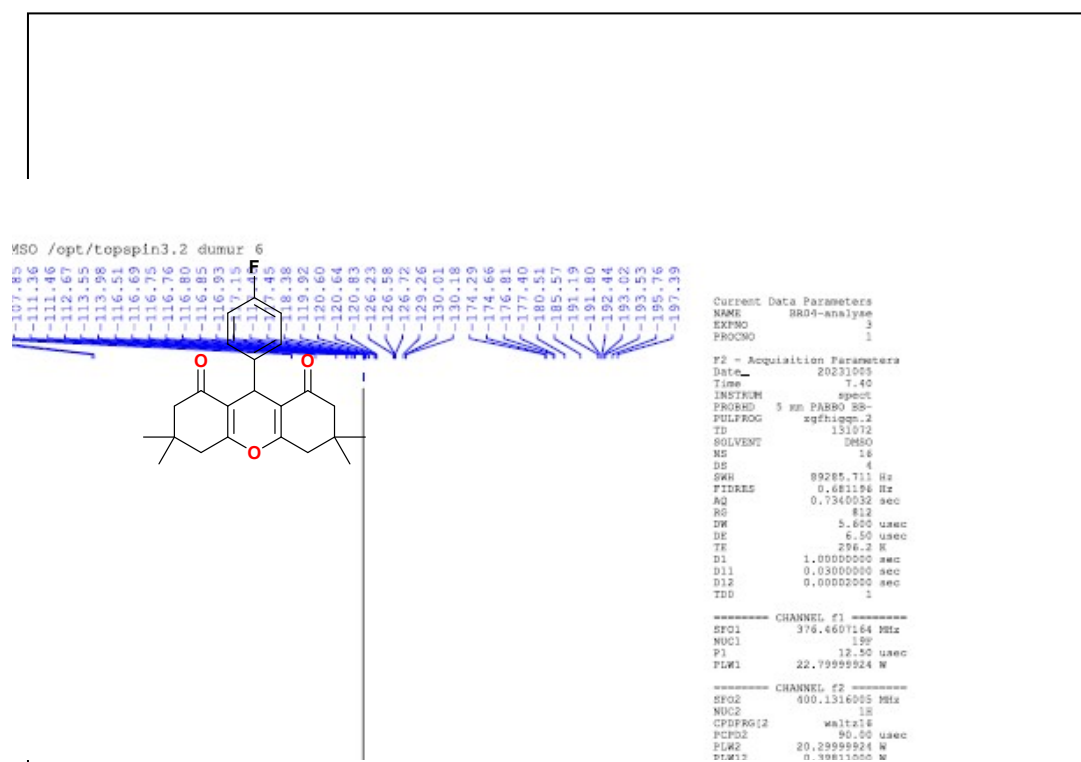
IR spectrum: 9-(4-chlorophenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3c**)



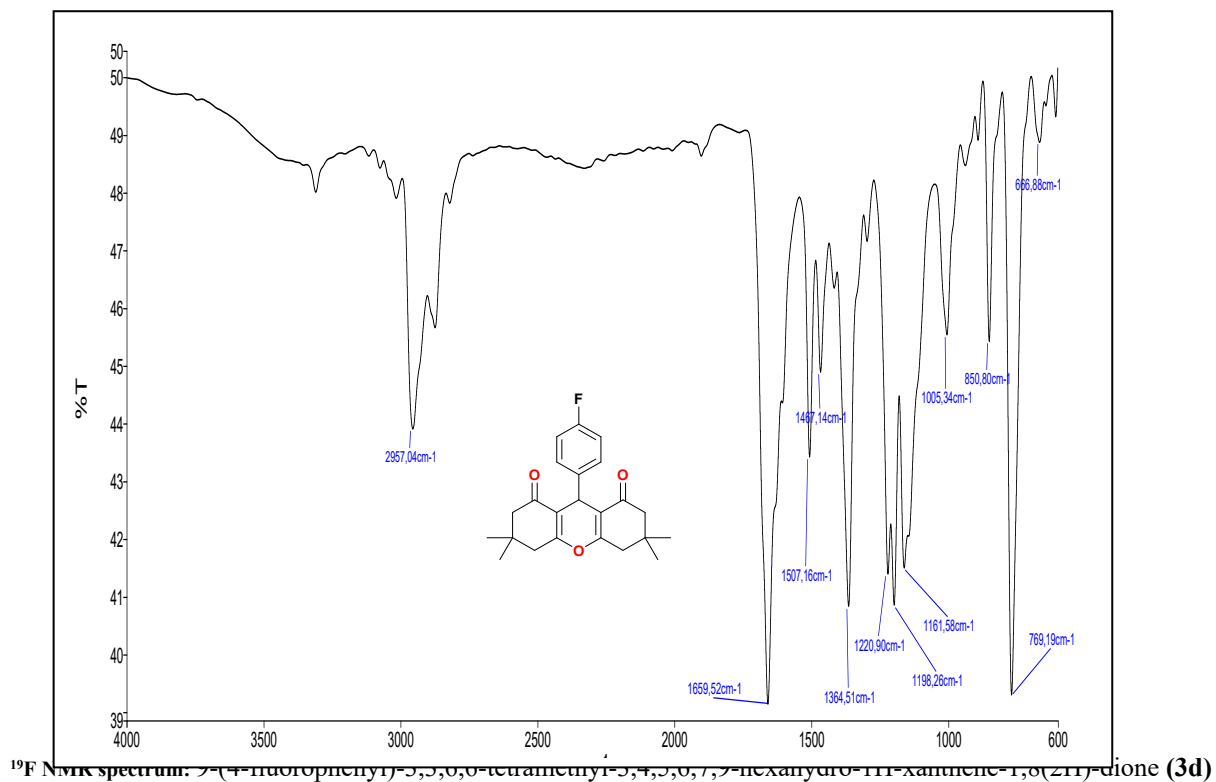
**<sup>1</sup>H NMR spectrum: 9-(4-fluorophenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (3d)**



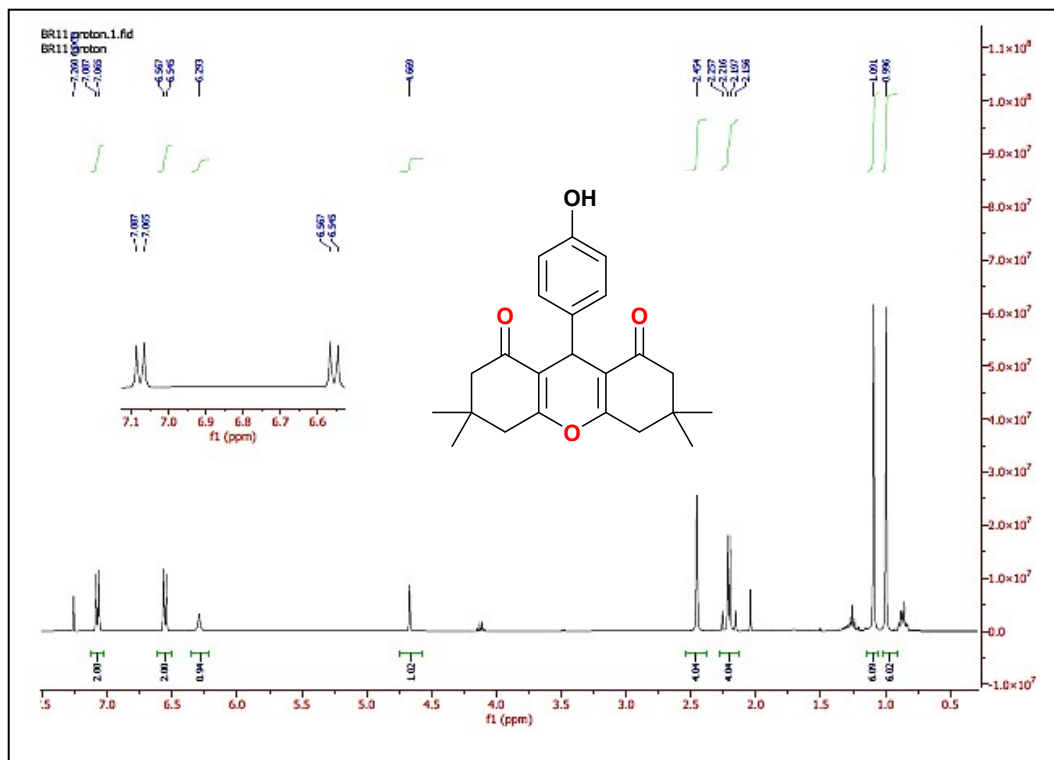
**<sup>13</sup>C NMR spectrum: 9-(4-fluorophenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (3d)**

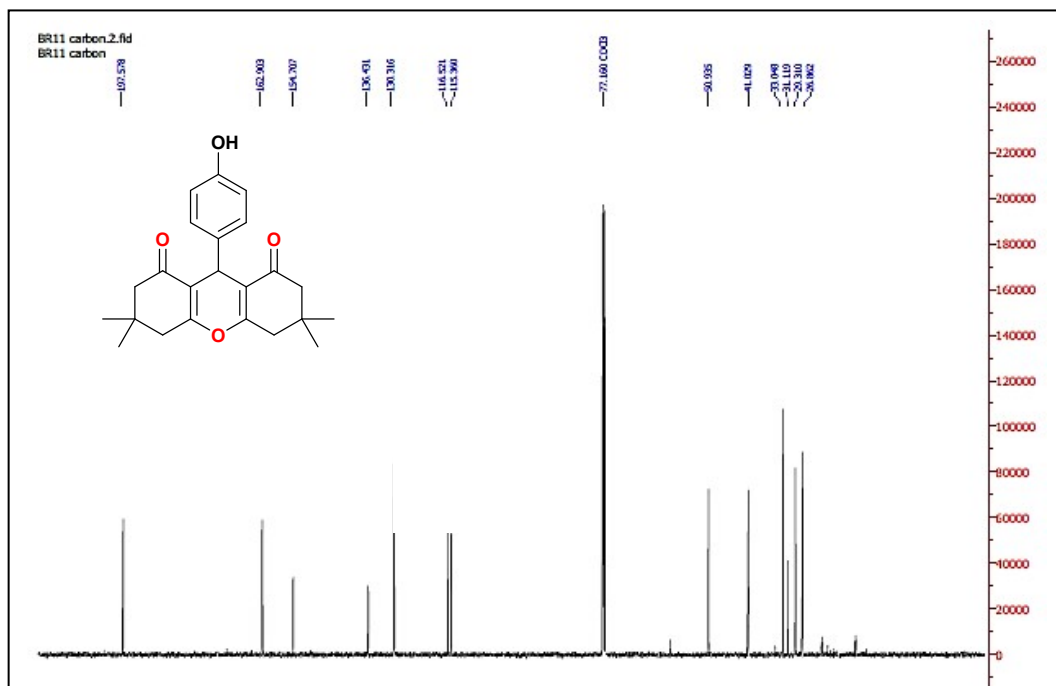




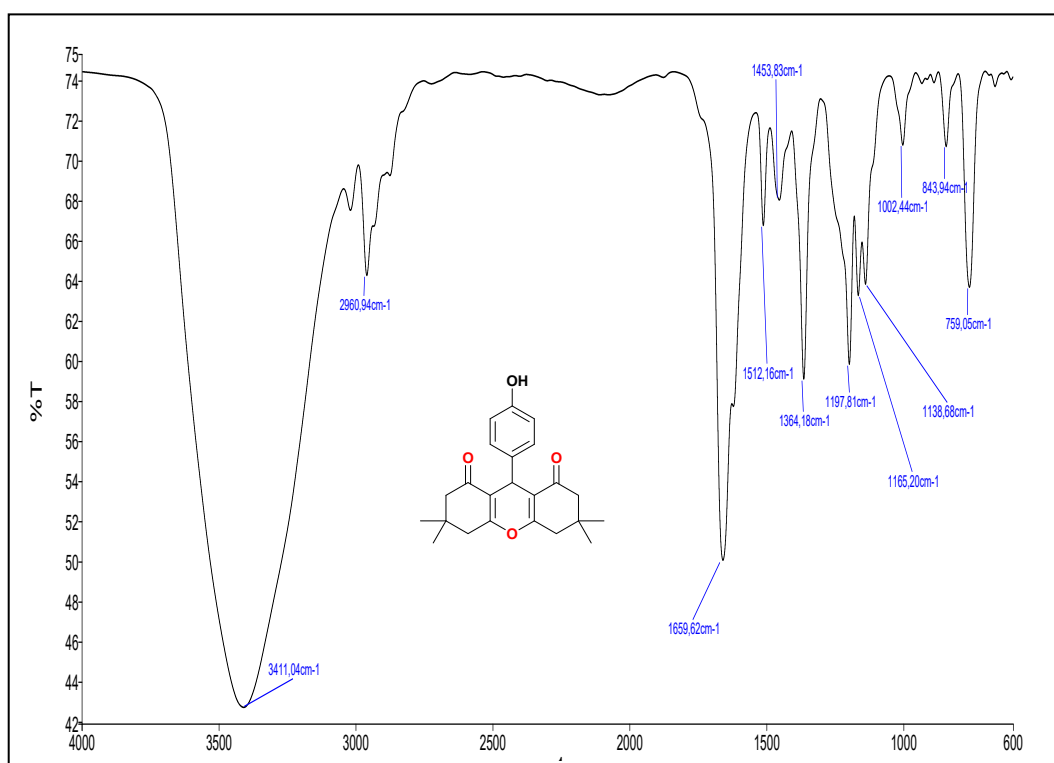


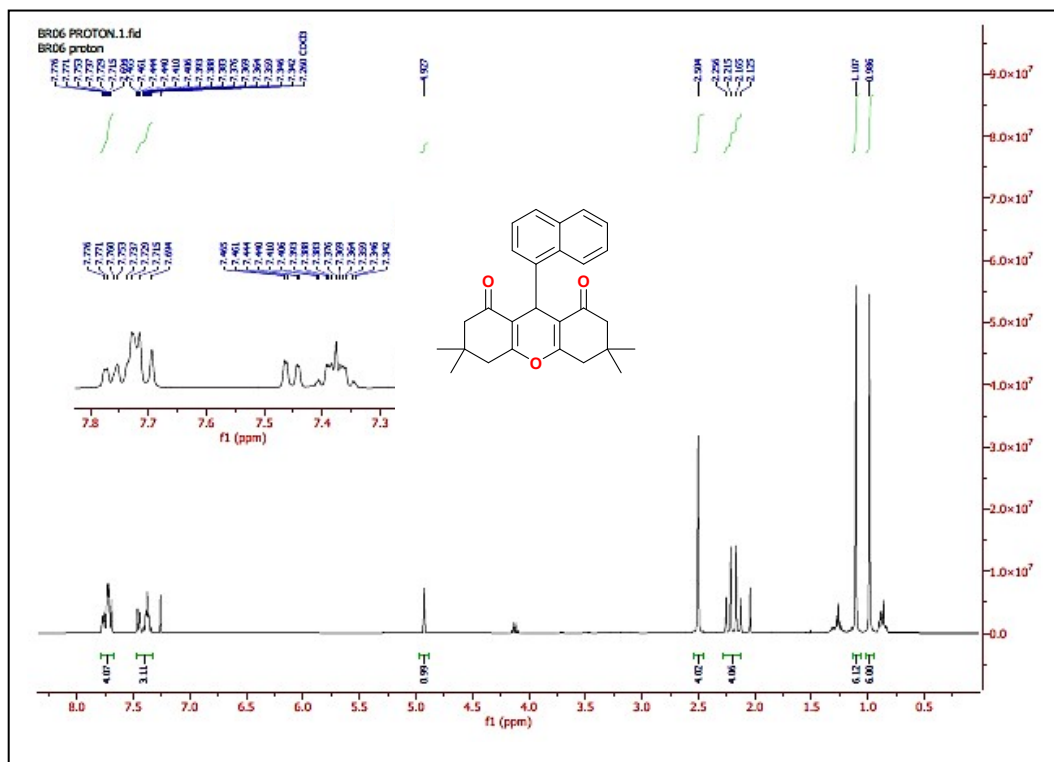
IR NMR spectrum: 9-(4-fluorophenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3d**)



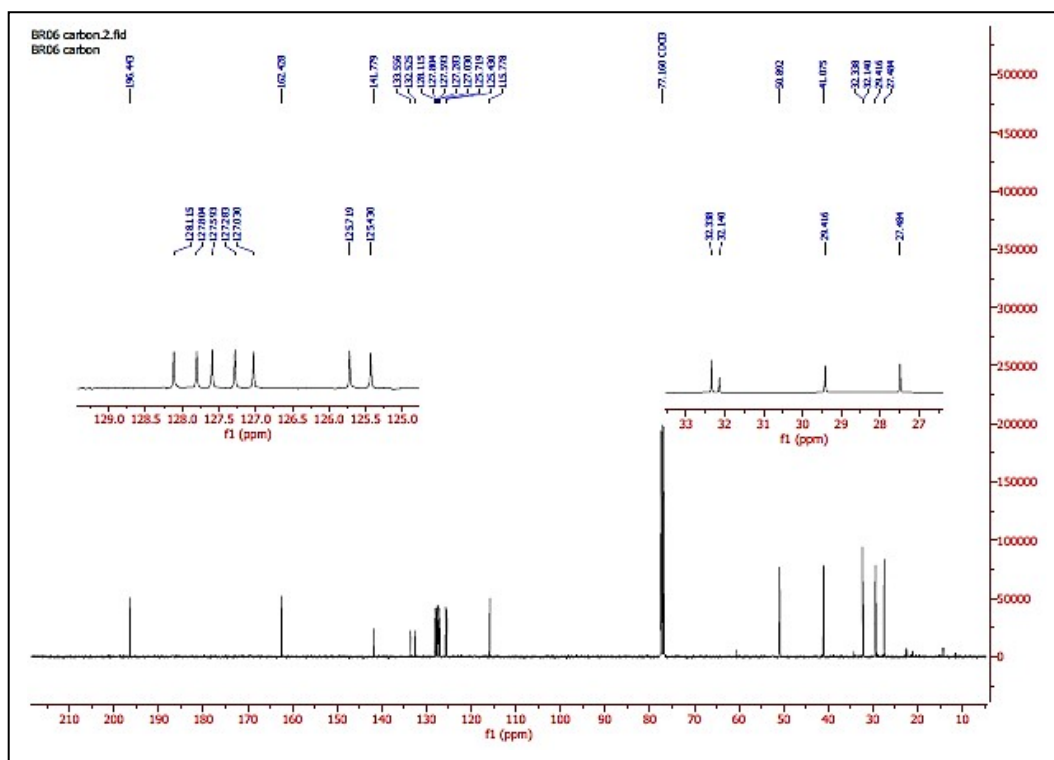


<sup>13</sup>C NMR spectrum: 9-(4-hydroxyphenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3e**)

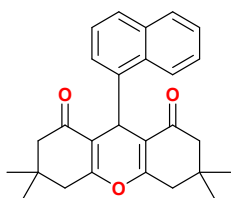


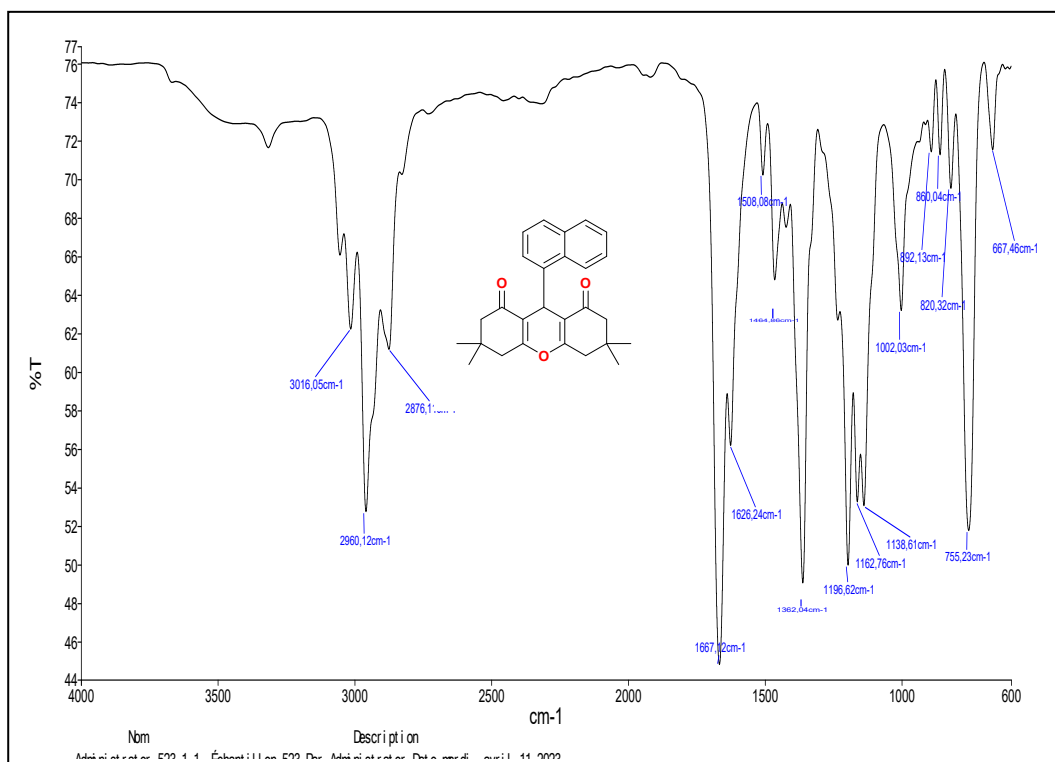


<sup>1</sup>H NMR spectrum :3,3,6,6-tetramethyl-9-(naphthalen-1-yl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3f**)

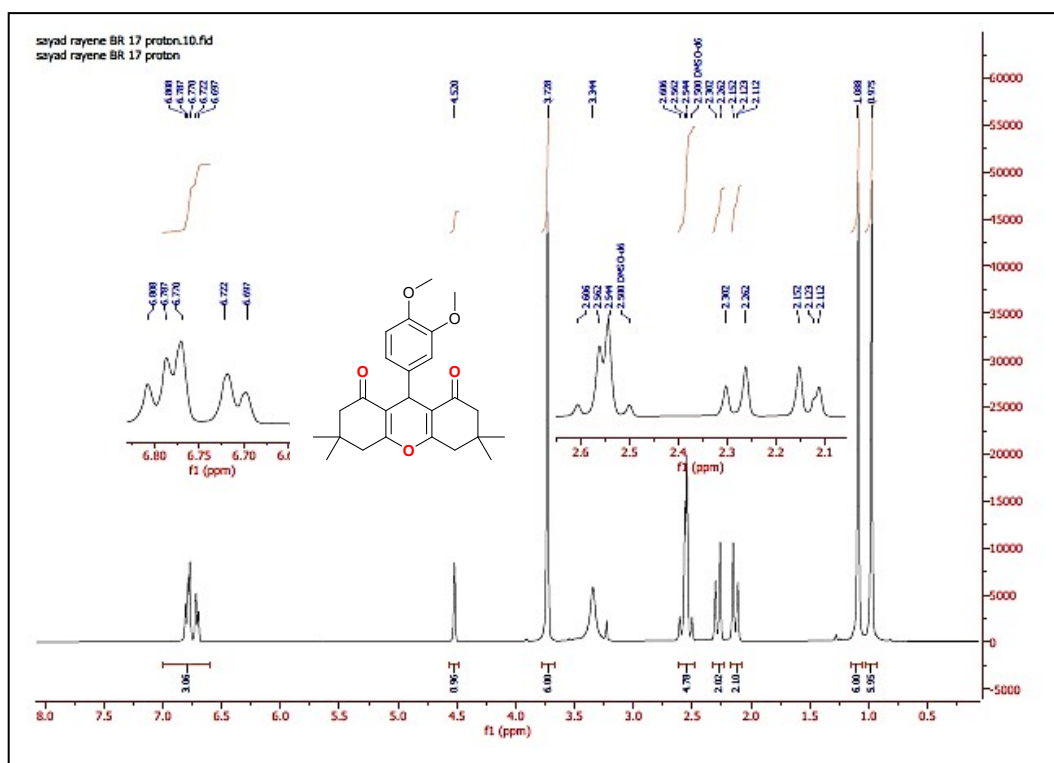


<sup>13</sup>C NMR spectrum :3,3,6,6-tetramethyl-9-(naphthalen-1-yl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3f**)

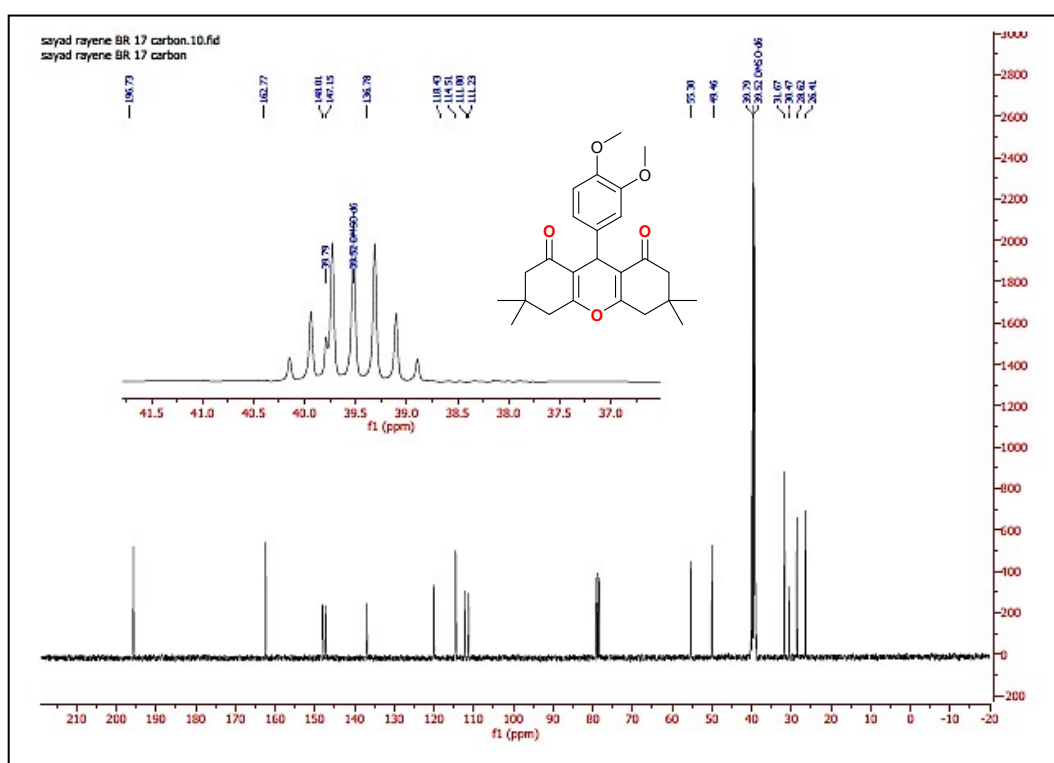




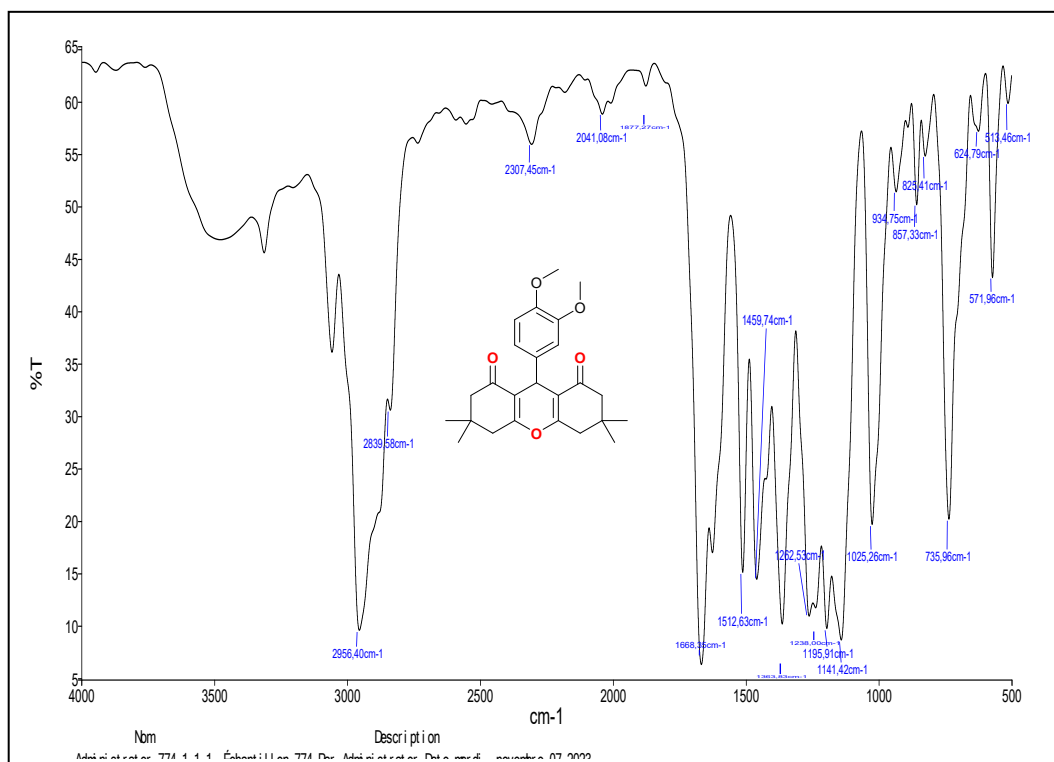
**IR spectrum:** 3,3,6,6-tetramethyl-9-(naphthalen-1-yl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3f**)



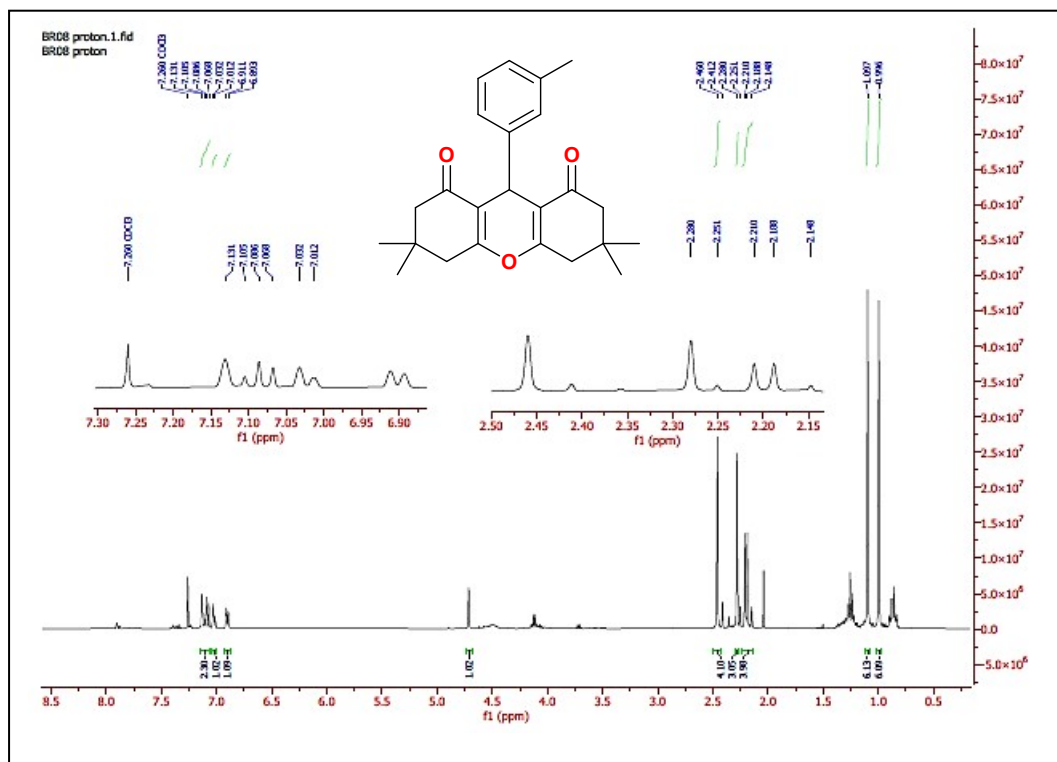
$^1\text{H}$  NMR spectrum: 9-(3,4-dimethoxyphenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3g**)



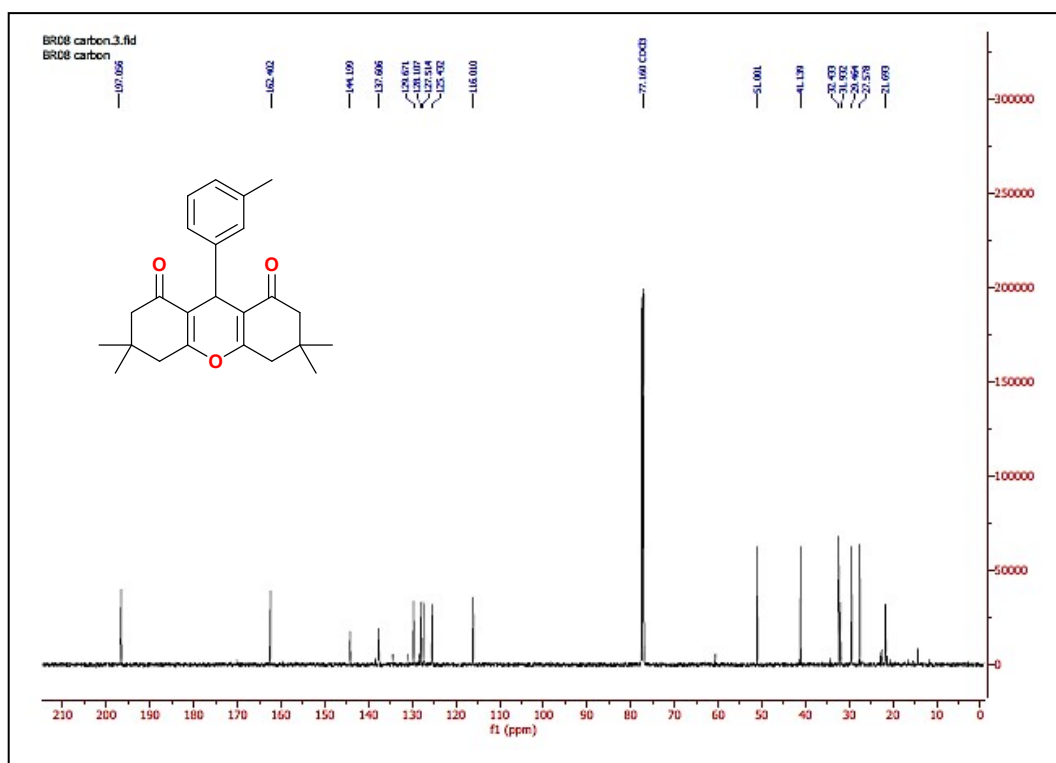
$^{13}\text{C}$  NMR spectrum :9-(3,4-dimethoxyphenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3g**)



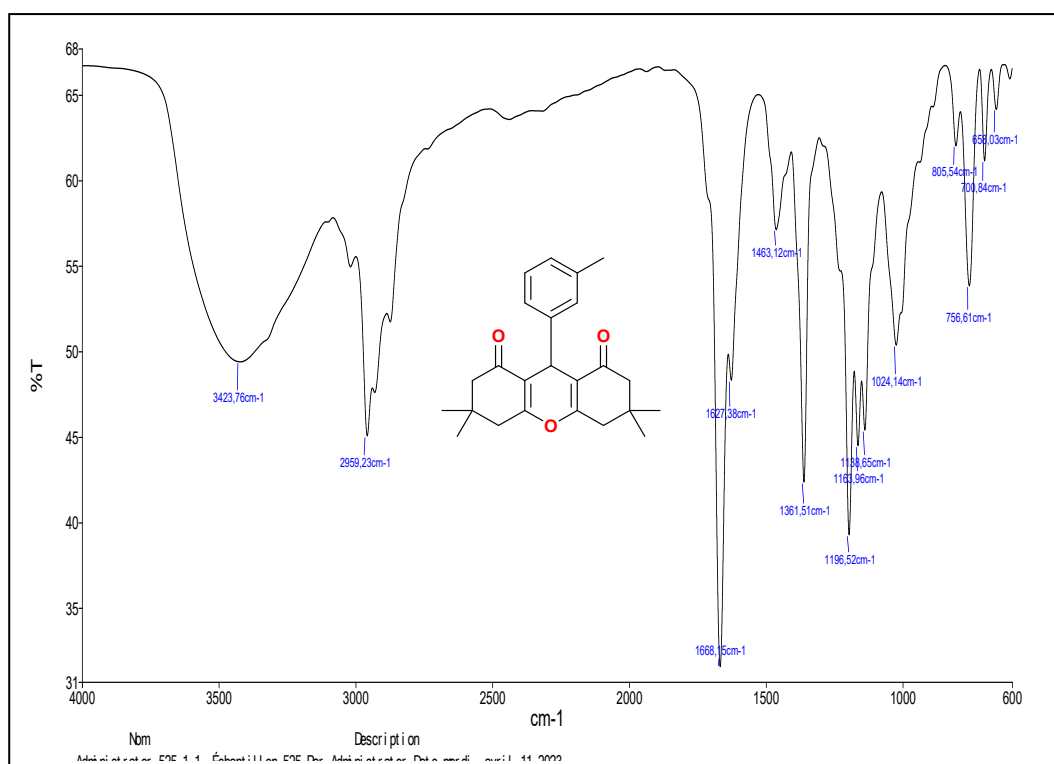
**IR spectrum: 9-(3,4-dimethoxyphenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3g**)**



<sup>1</sup>H NMR spectrum :3,3,6,6-tetramethyl-9-(m-tolyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3h**)

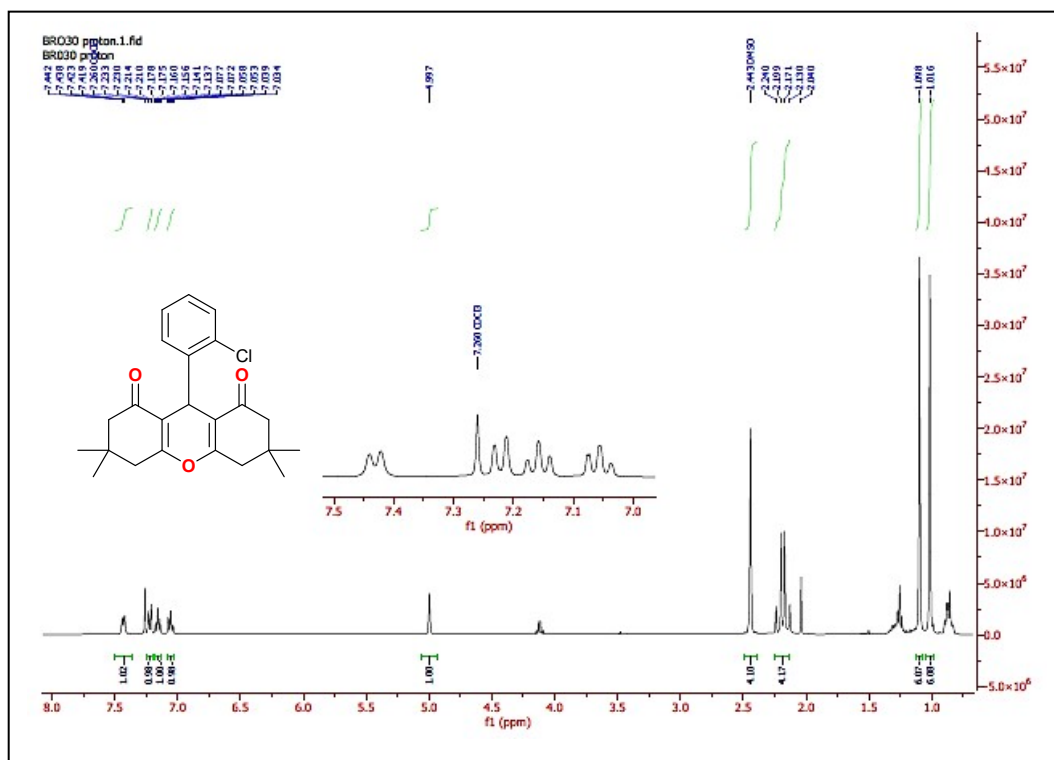


$^{13}\text{C}$  NMR spectrum: 3,3,6,6-tetramethyl-9-(m-tolyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3h**)



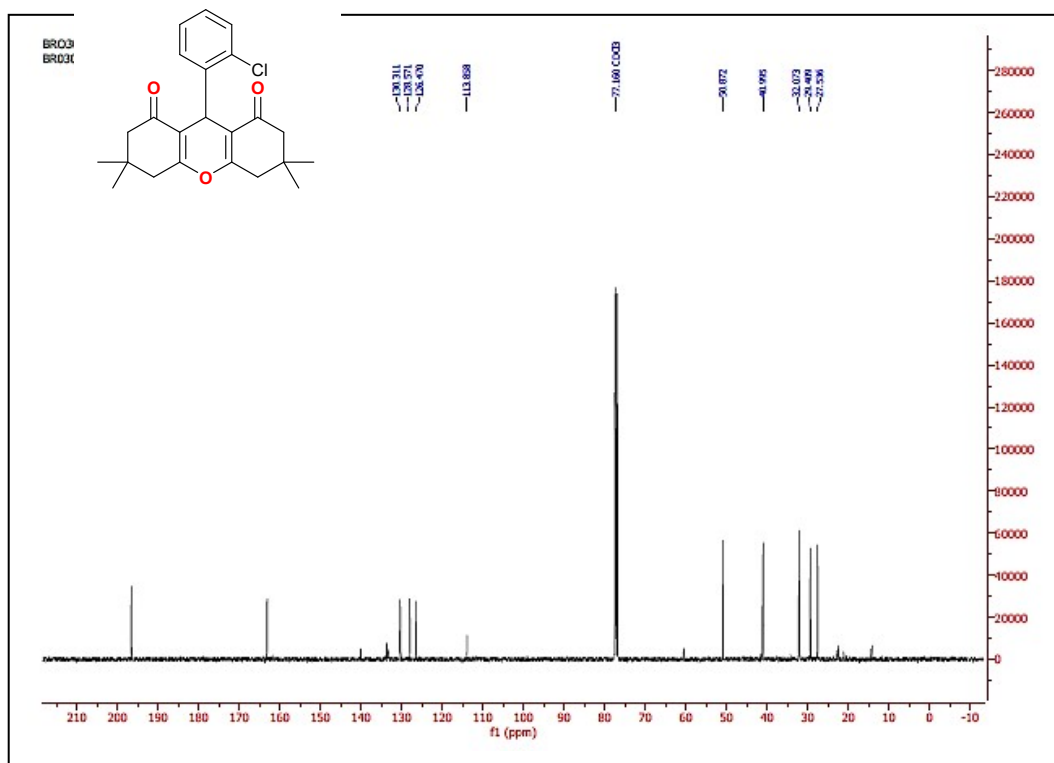
IR spectrum: 3,3,6,6-tetramethyl-9-(m-tolyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3h**)

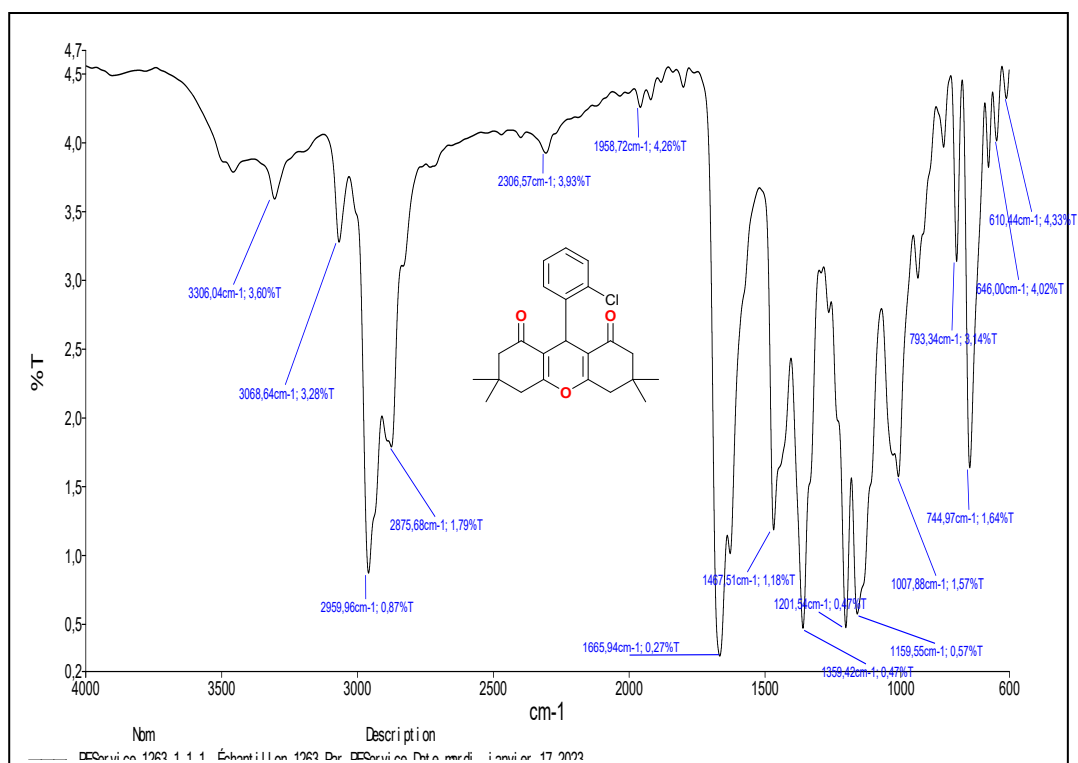




<sup>1</sup>H NMR spectrum :9-(2-chlorophenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3i**)

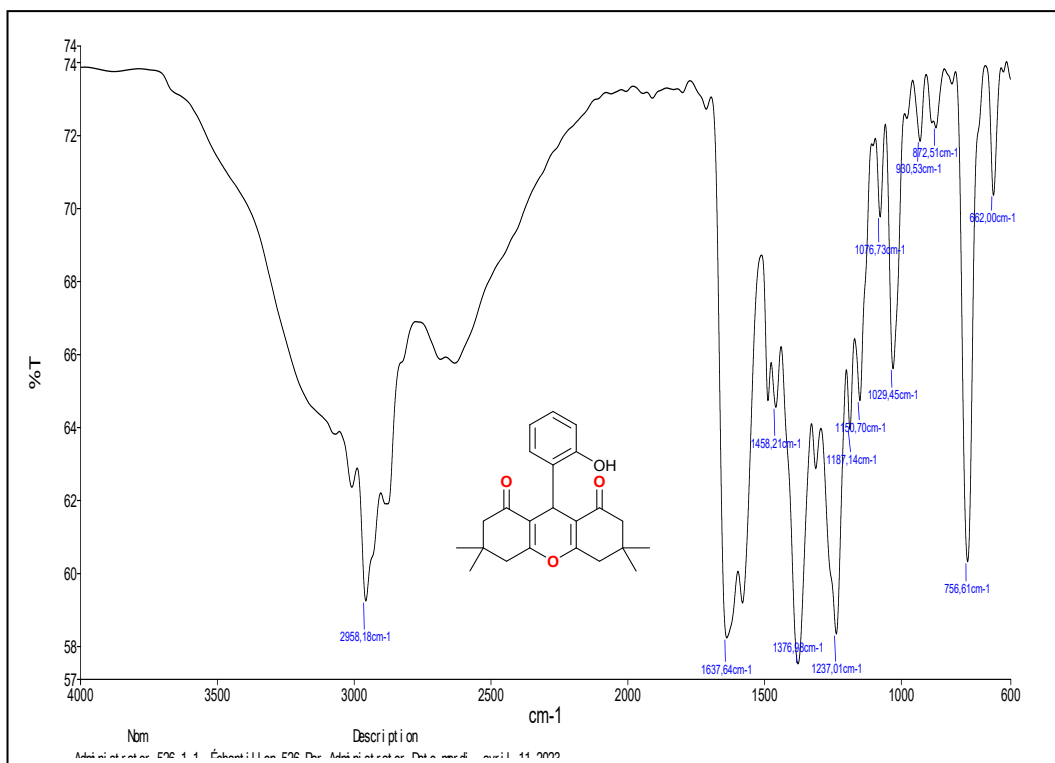
<sup>13</sup>C NMR spectrum :9-(2-chlorophenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3i**)



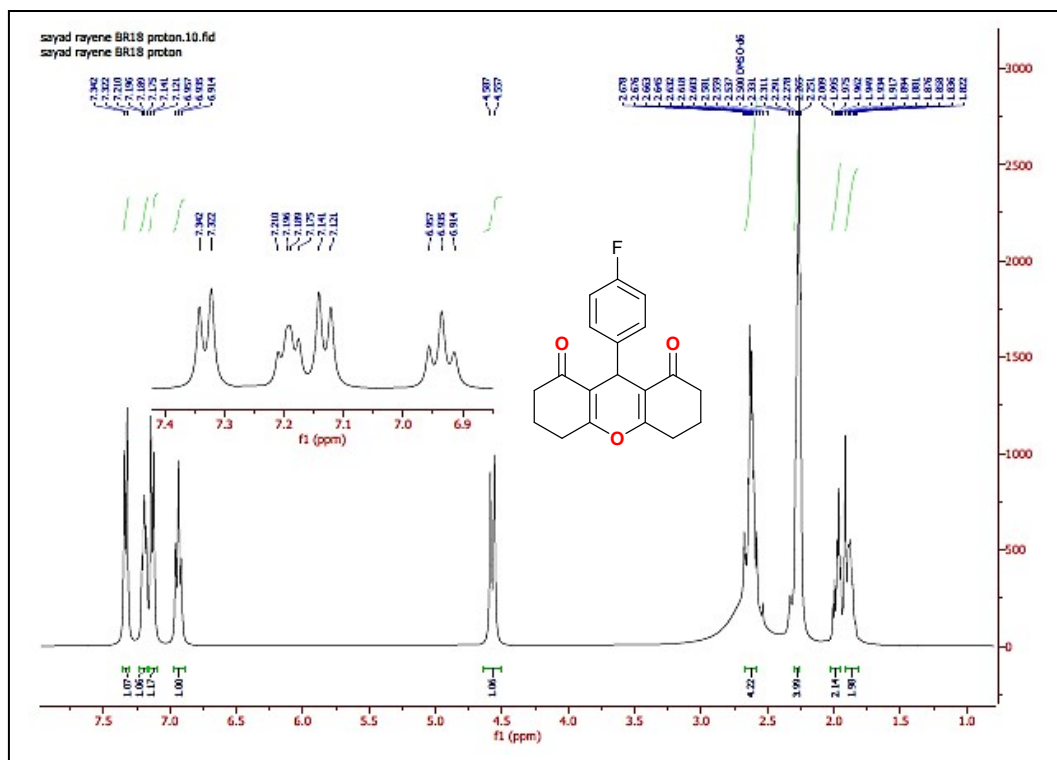


IR spectrum :9-(2-chlorophenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3i**)

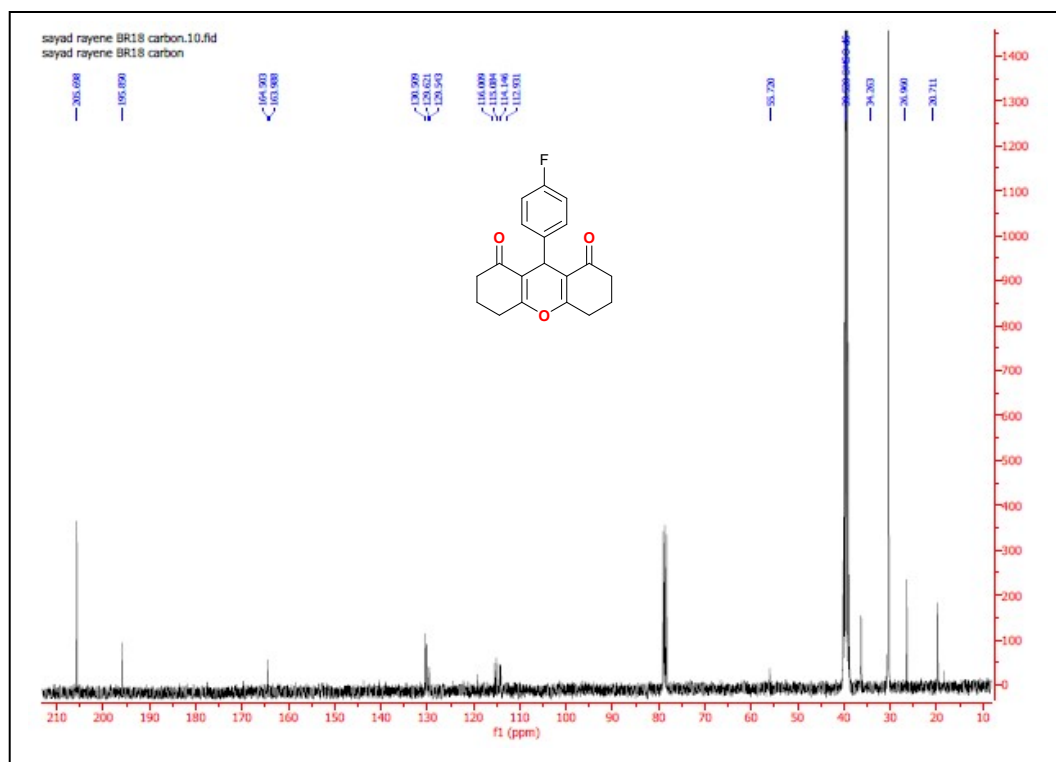




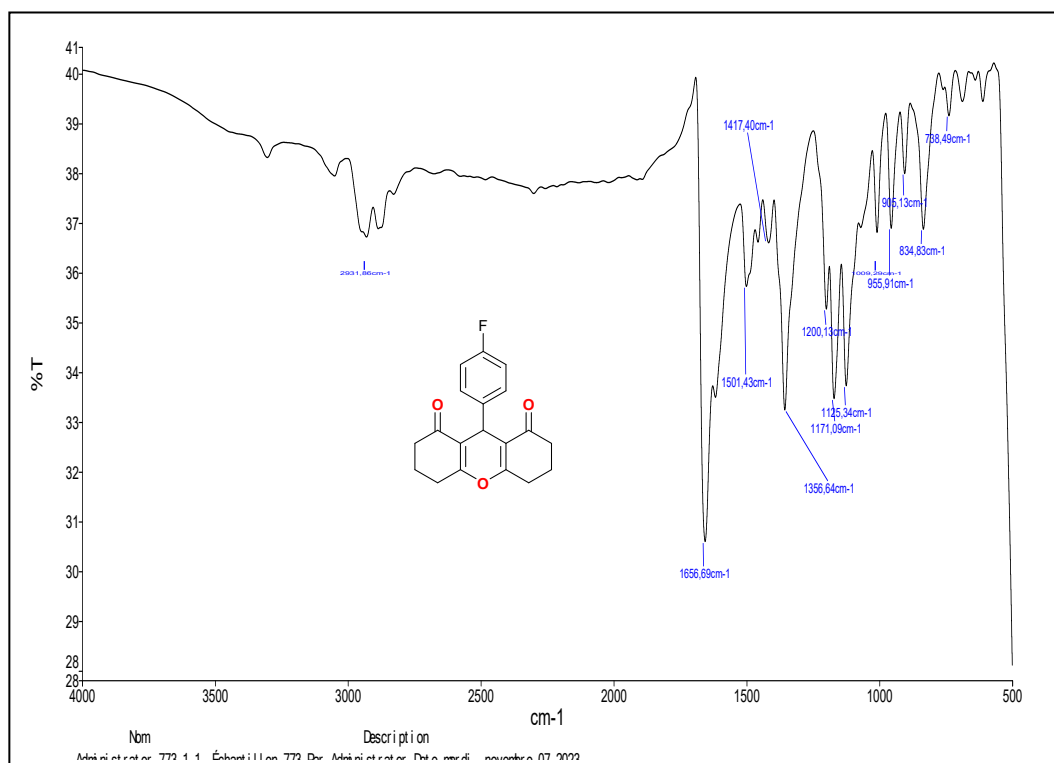
IR spectrum :9-(2-hydroxyphenyl)-3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3j**)



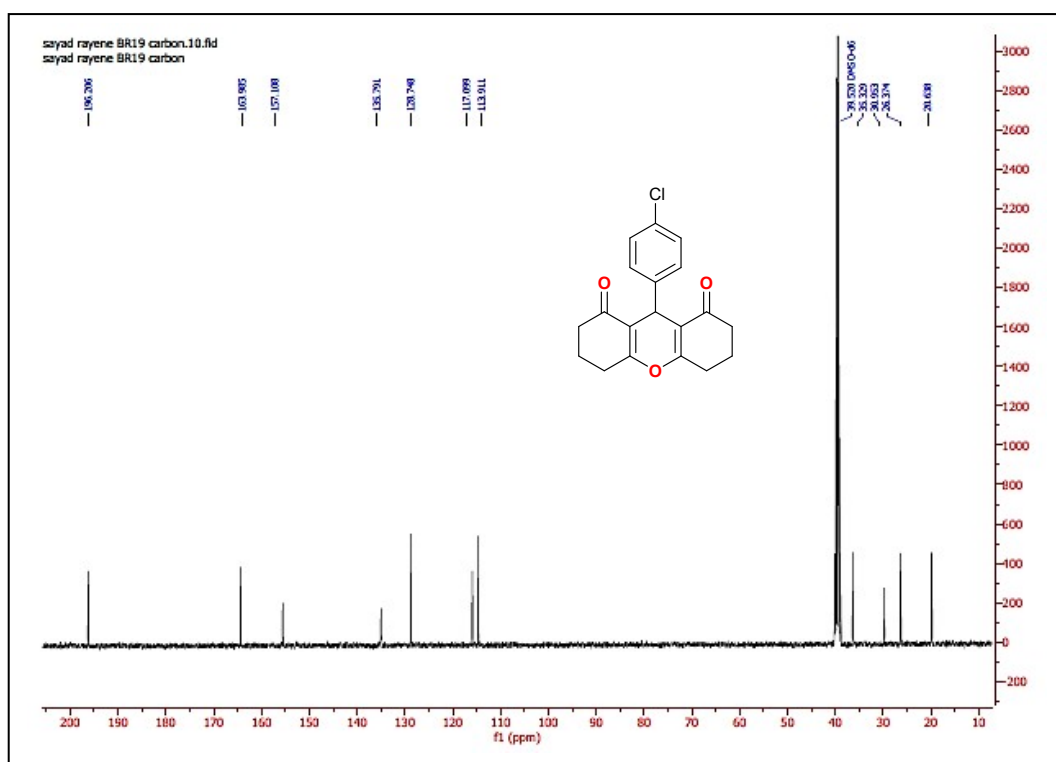
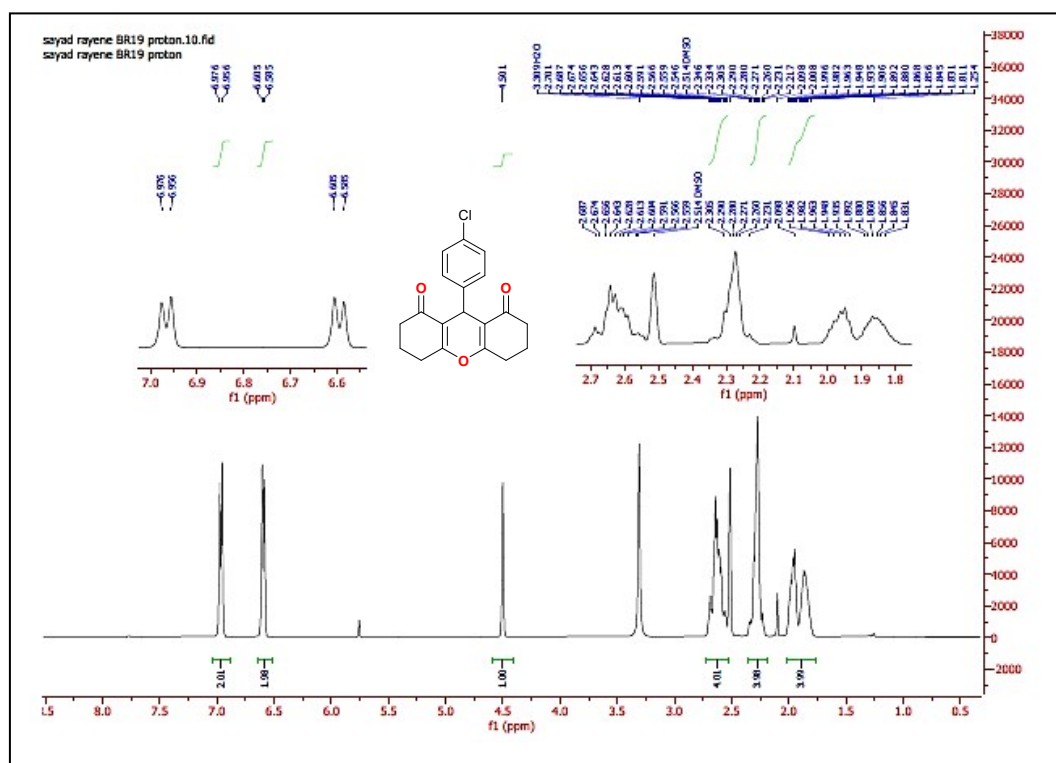
<sup>1</sup>H NMR spectrum :9-(4-fluorophenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3n**)



**<sup>13</sup>C NMR spectrum: 9-(4-fluorophenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (3n)**

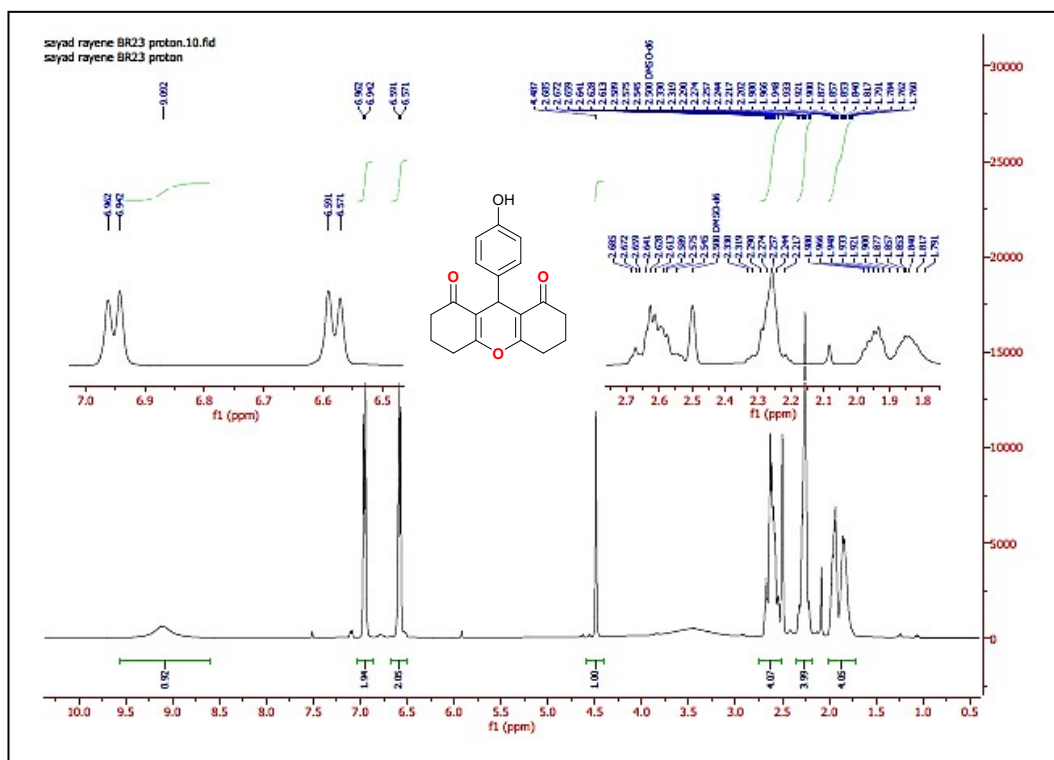
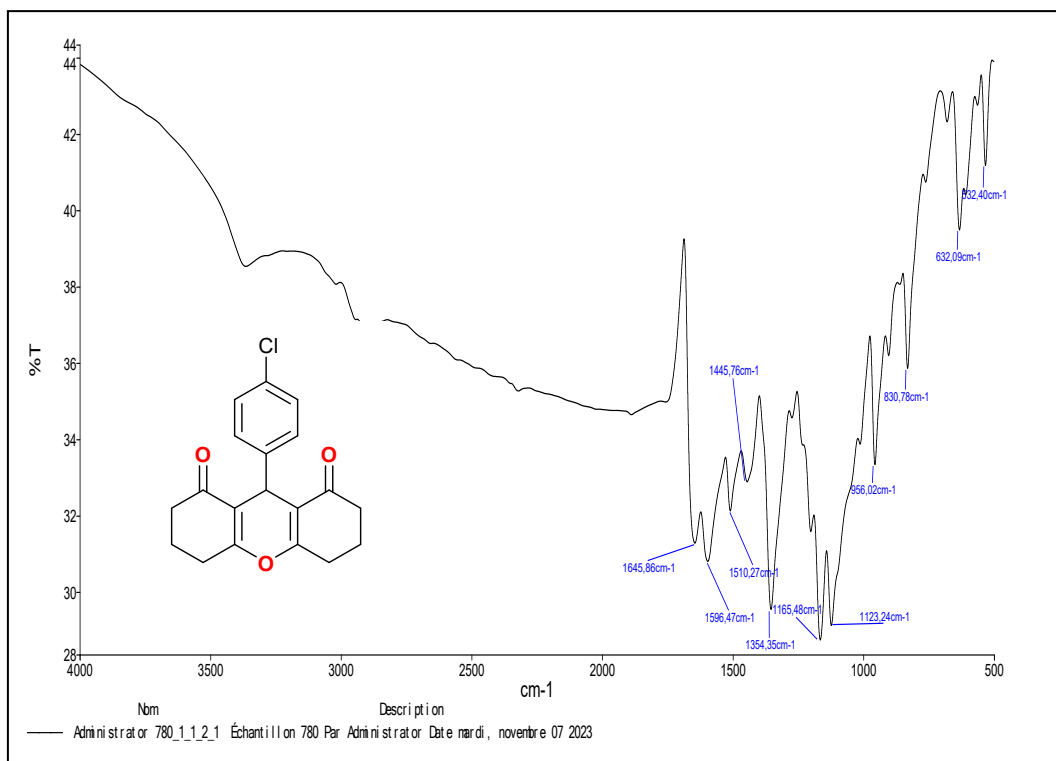


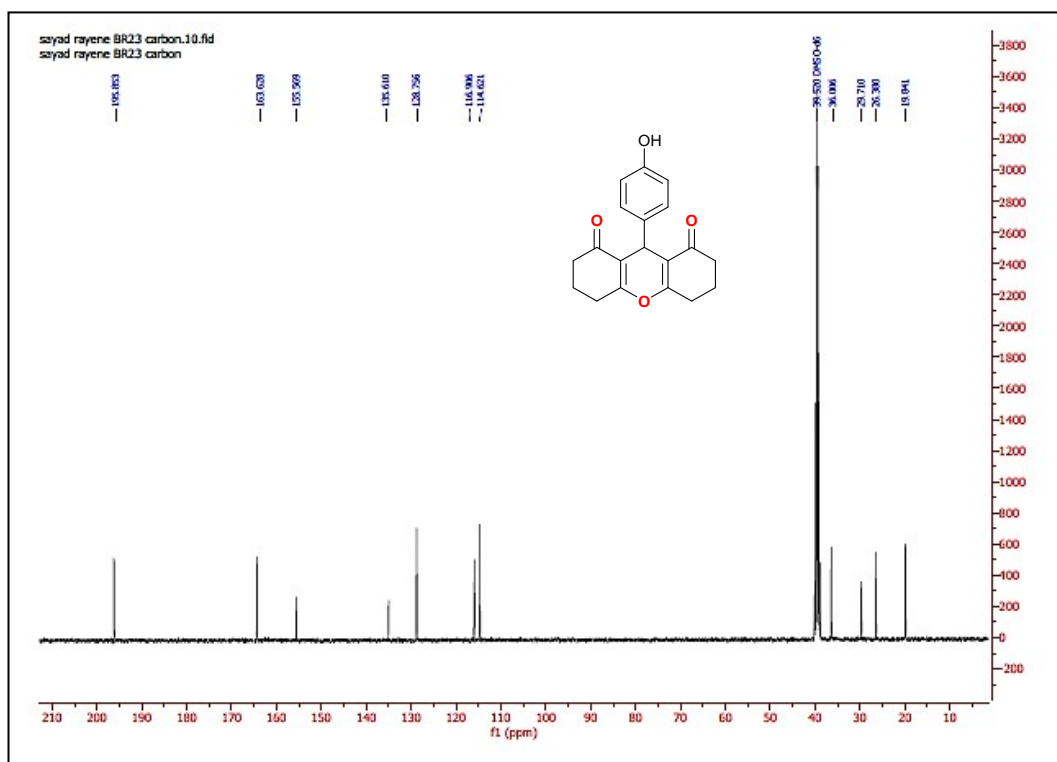
**IR spectrum: 9-(4-fluorophenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (3n)**



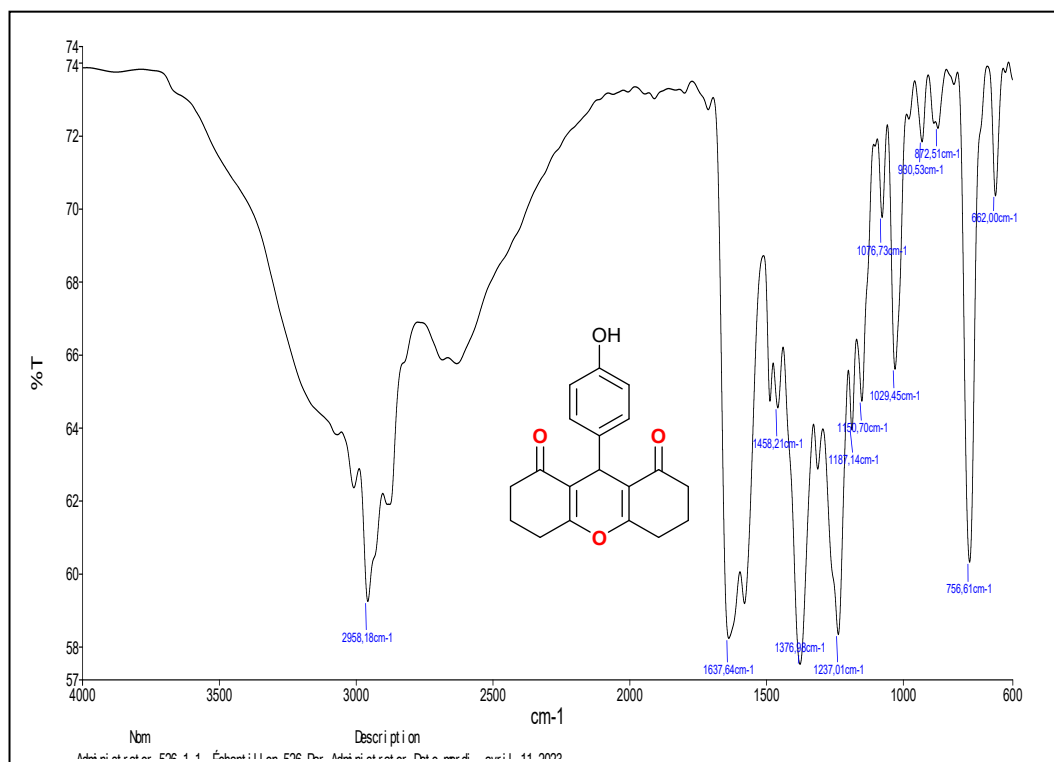
<sup>1</sup>H NMR spectrum: 9-(4-chlorophenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**30**)

<sup>13</sup>C NMR spectrum: 9-(4-chlorophenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**30**)



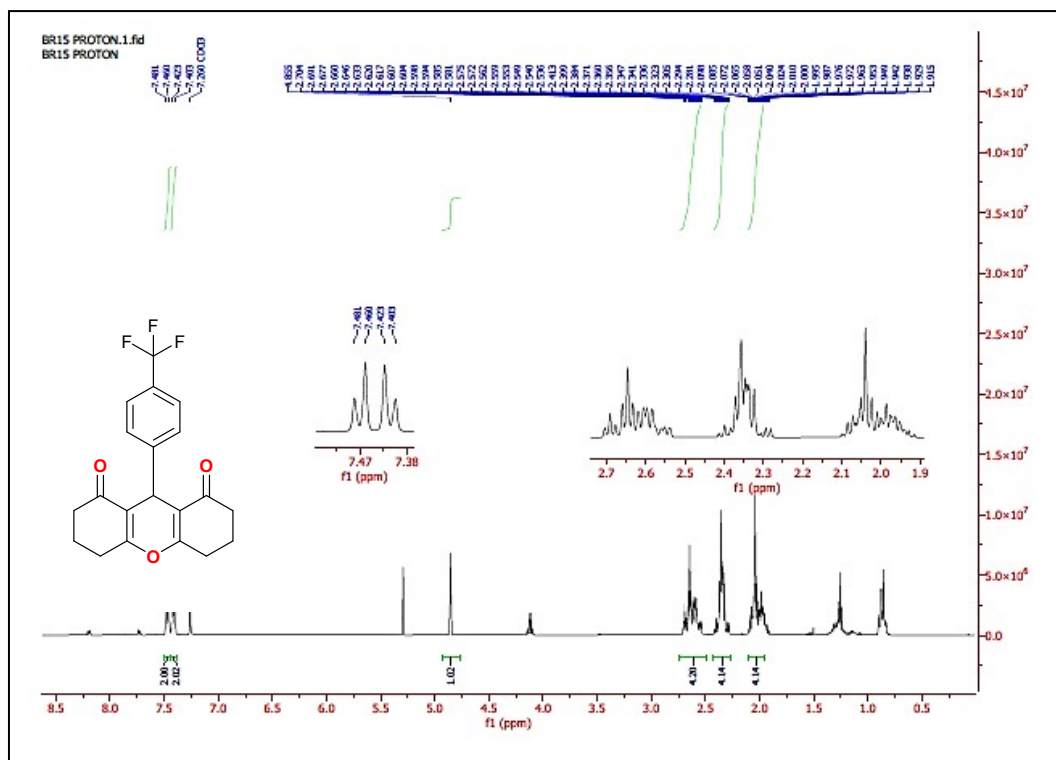


$^{13}\text{C}$  NMR spectrum :9-(4-hydroxyphenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3p**)

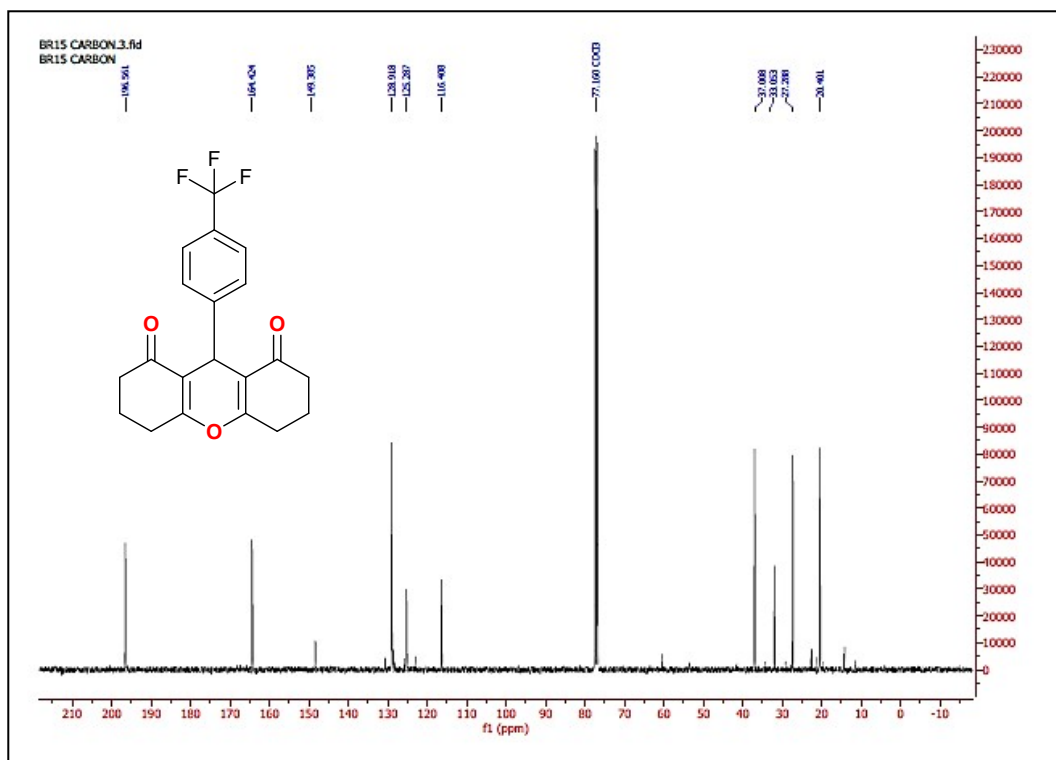


IR spectrum: 9-(4-hydroxyphenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3p**)

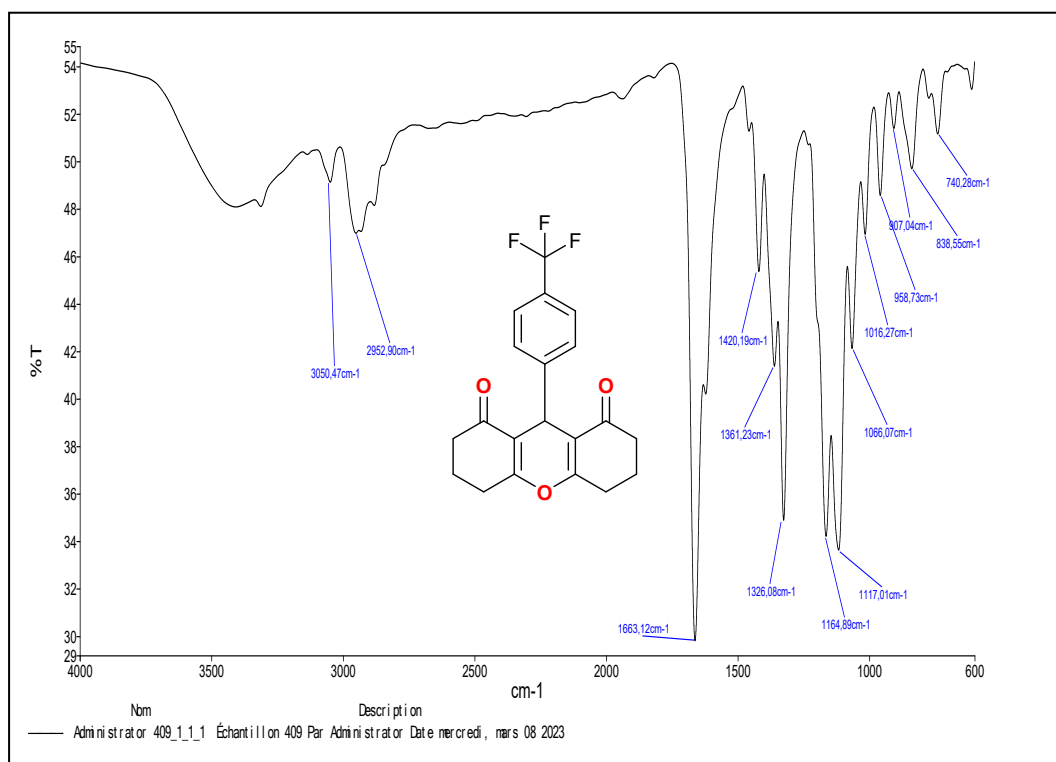




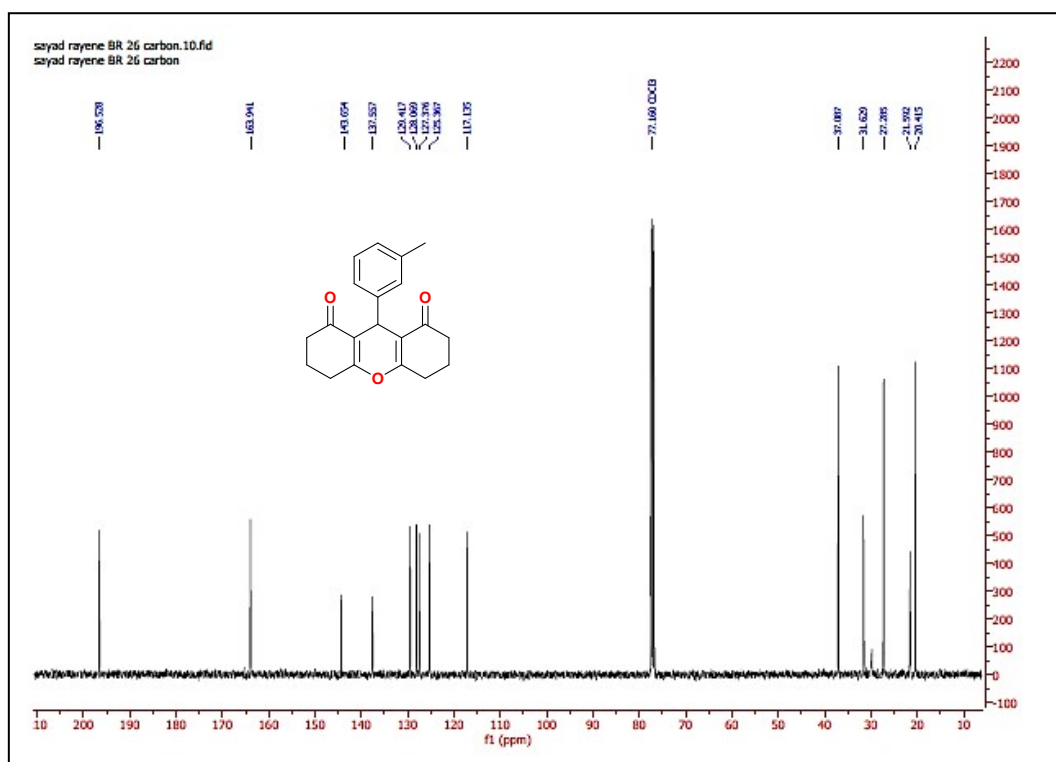
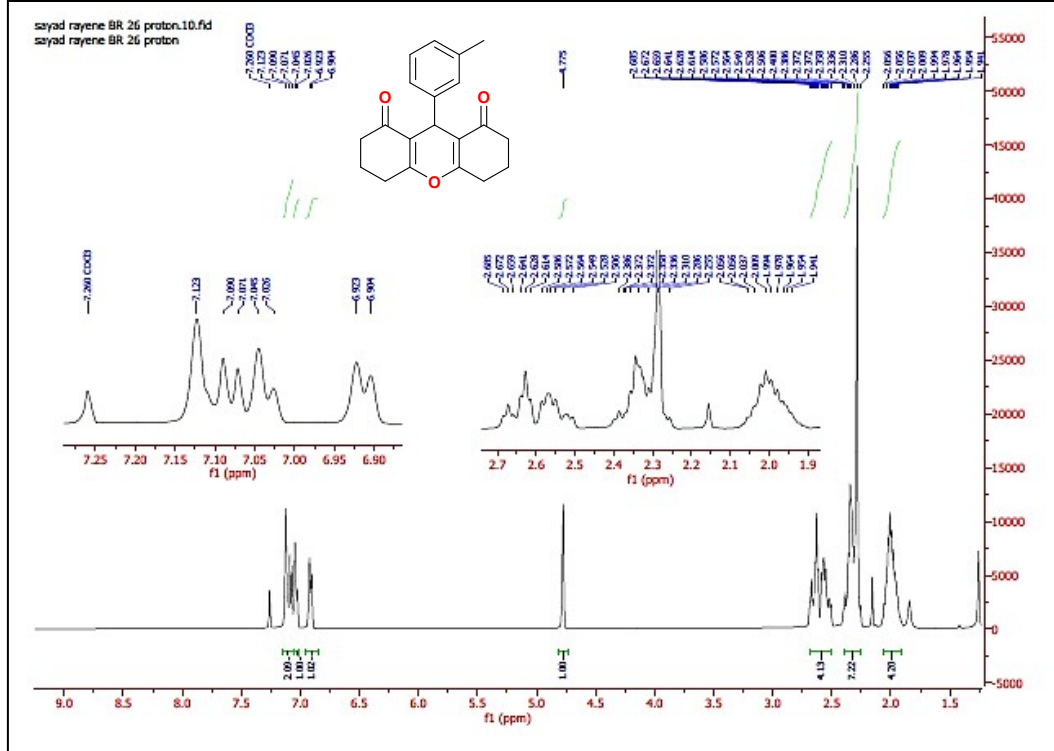
<sup>1</sup>H NMR spectrum :9-(4-(trifluoromethyl)phenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3p**)

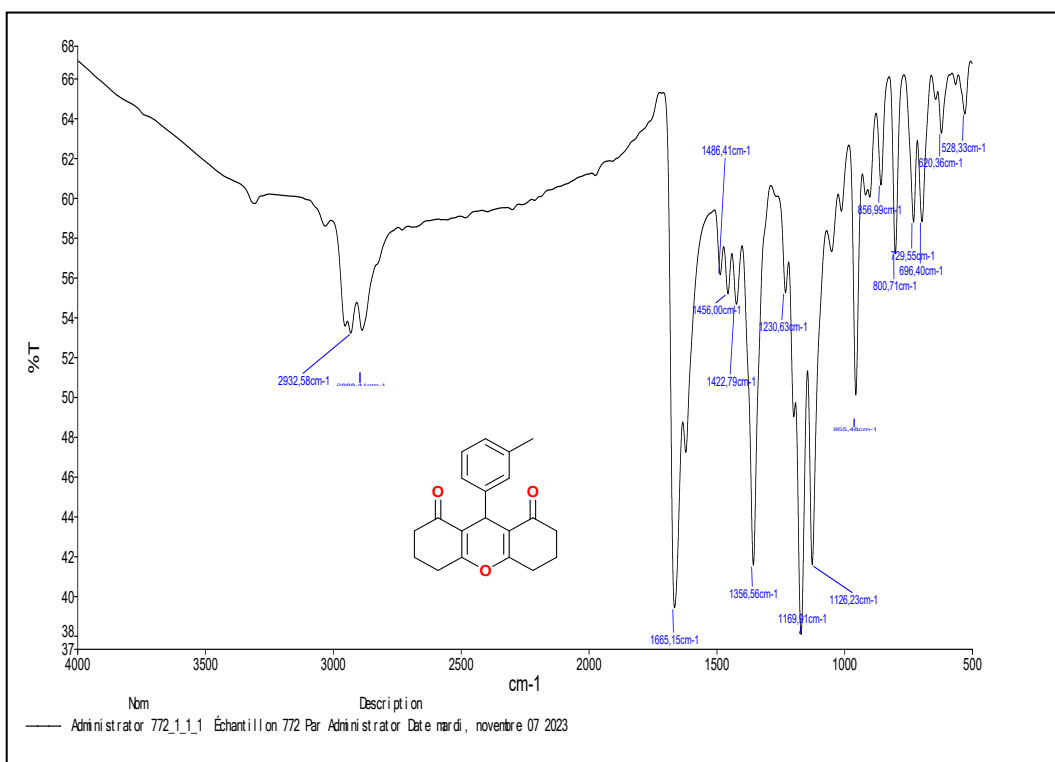


$^{13}\text{C}$  NMR spectrum: 9-(4-(trifluoromethyl)phenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3q**)

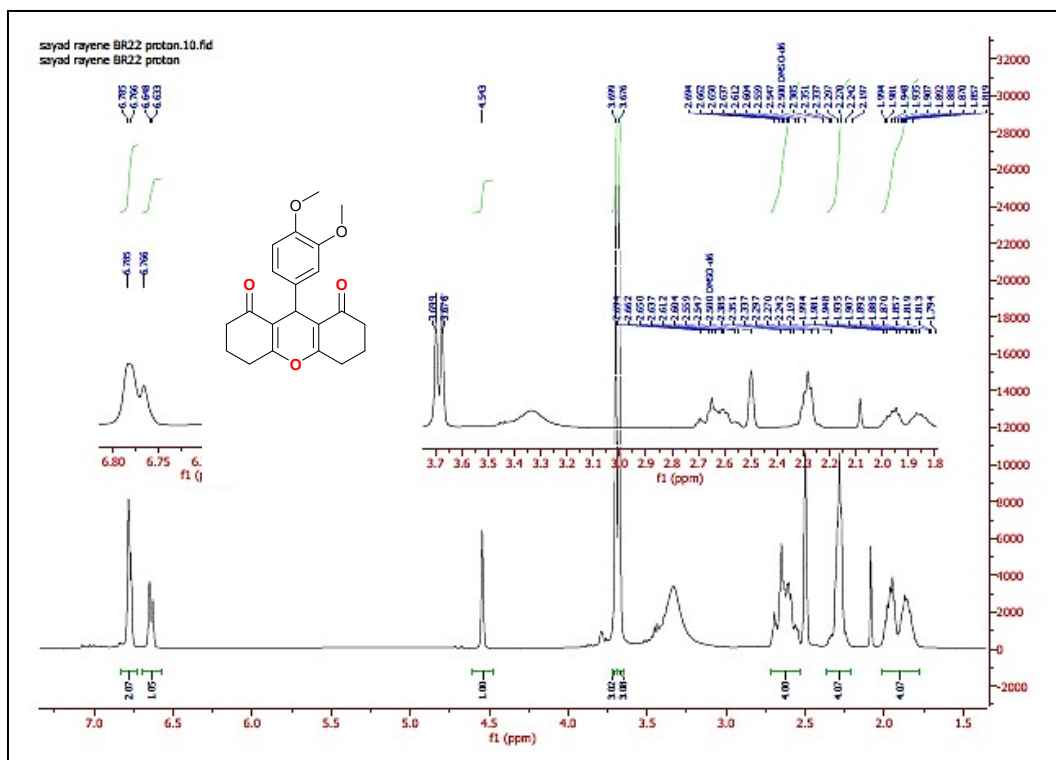


IR spectrum: 9-(4-(trifluoromethyl)phenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3q**)

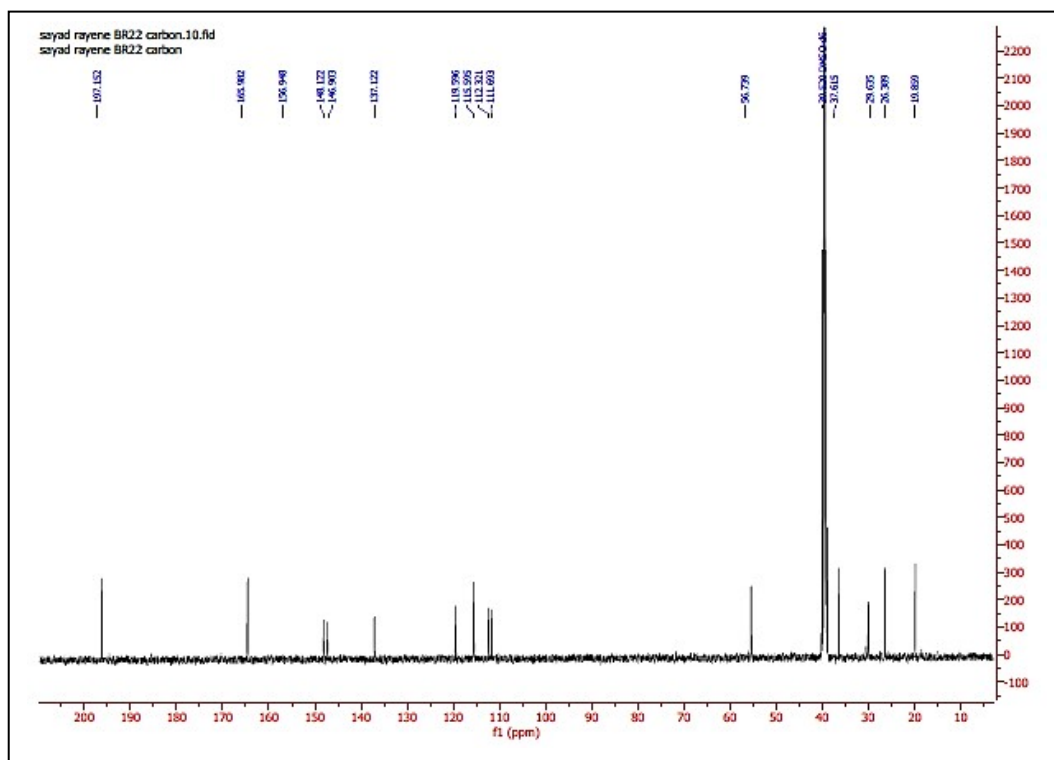




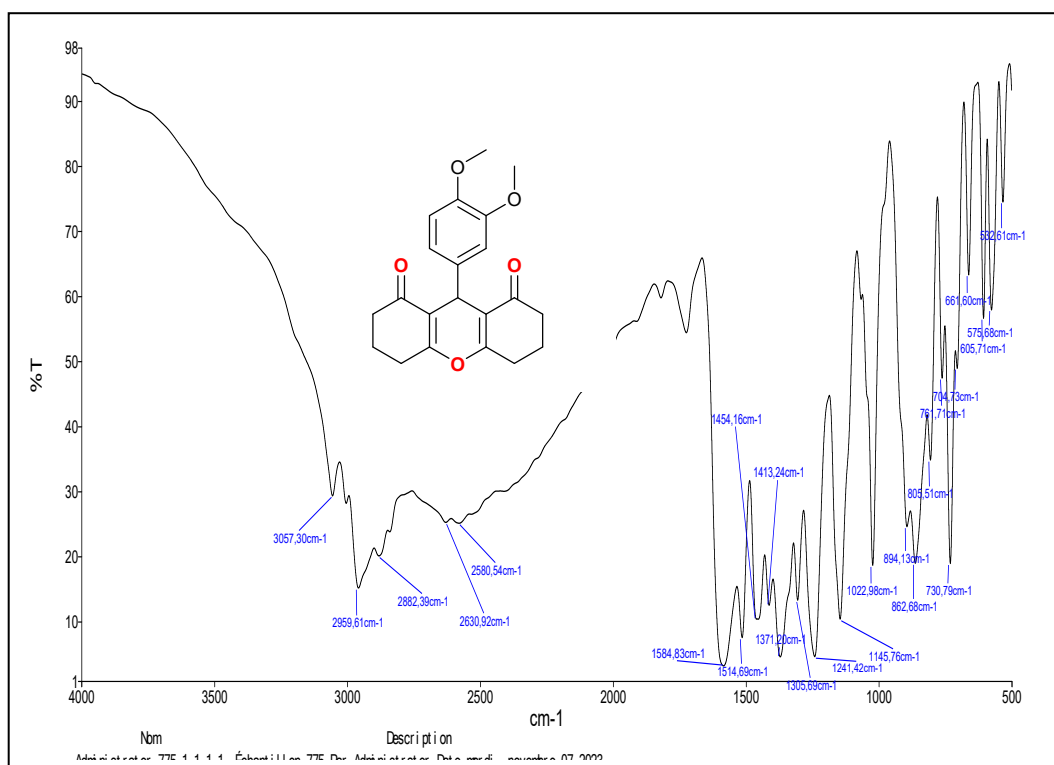
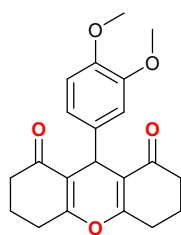
IR spectrum: 9-(m-tolyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (3r)



<sup>1</sup>H  
NMR  
spectrum:  
9-(3,4-dimethoxyphenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione



(3s)

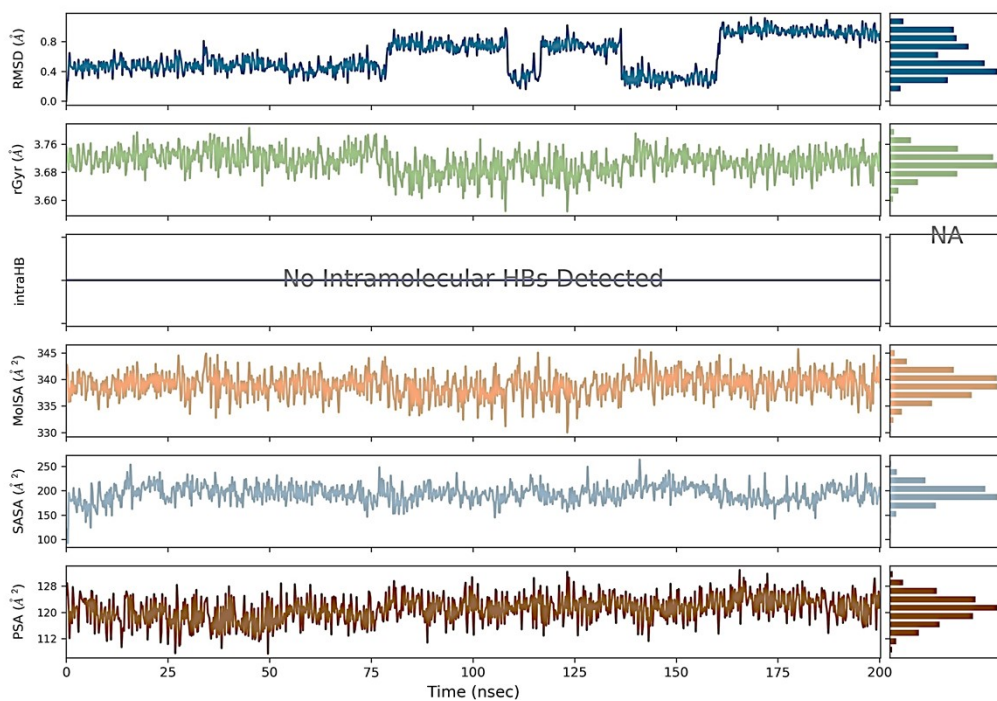


<sup>13</sup>C NMR spectrum: 9-(3,4-dimethoxyphenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3s**)

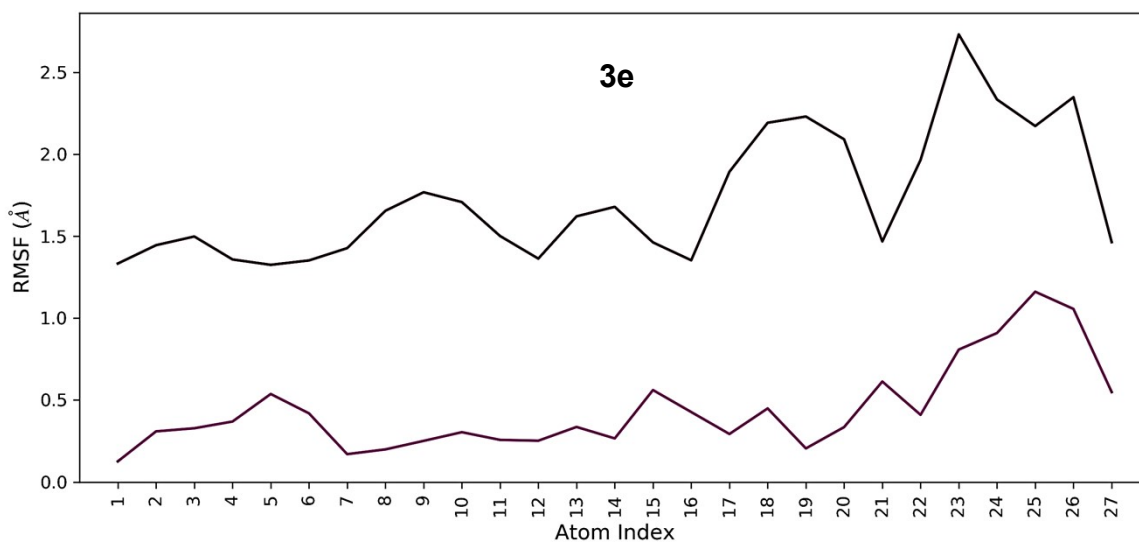
IR spectrum: 9-(3,4-dimethoxyphenyl)-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione (**3s**)



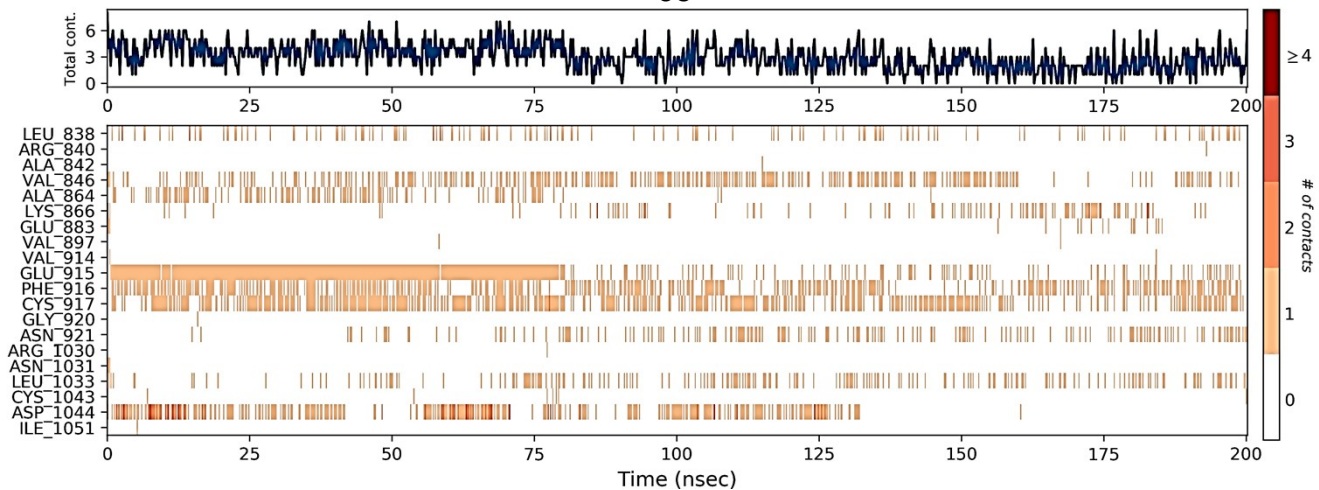
3e



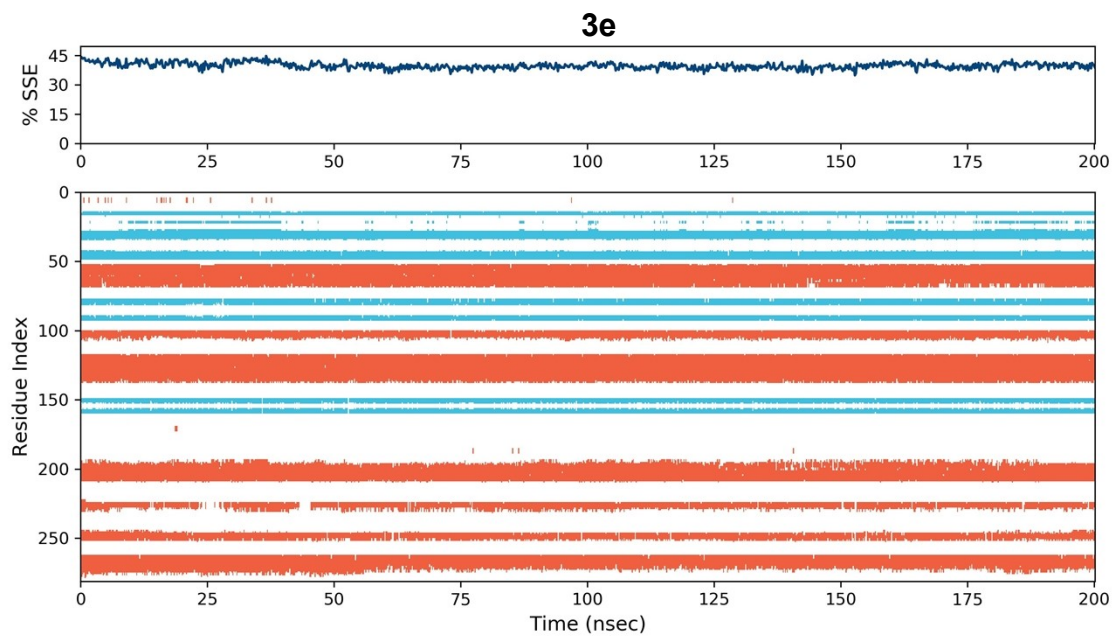
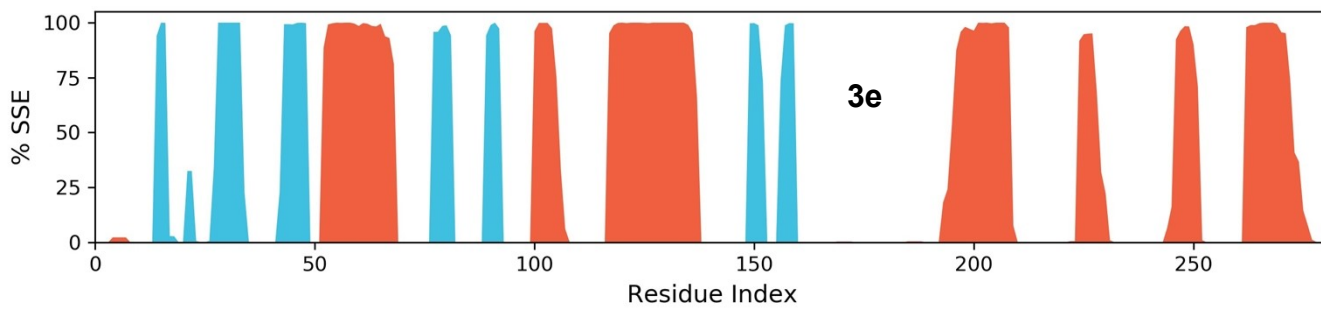
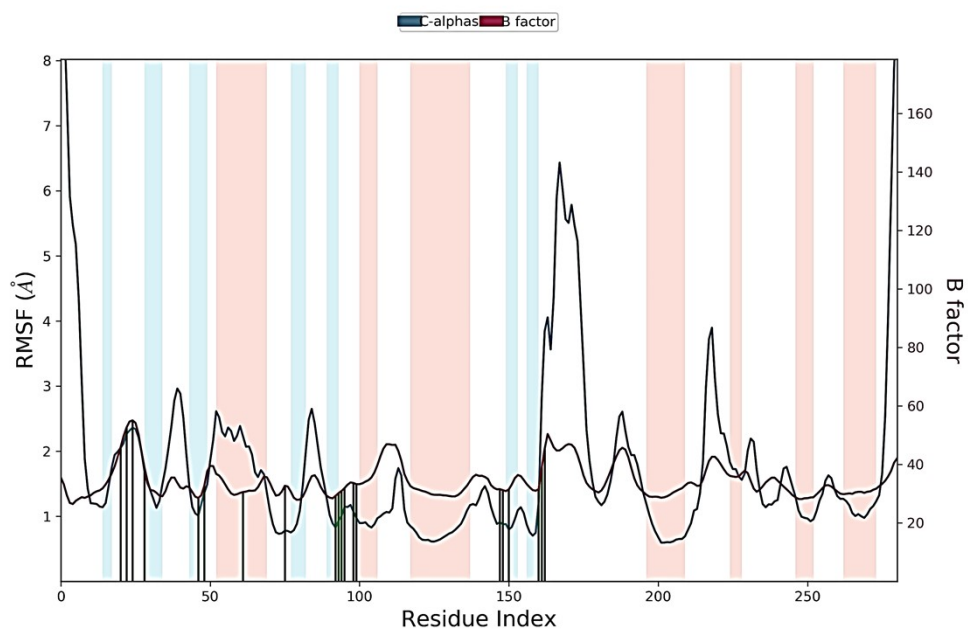
Fit on Protein (black line) Fit on Ligand (purple line)

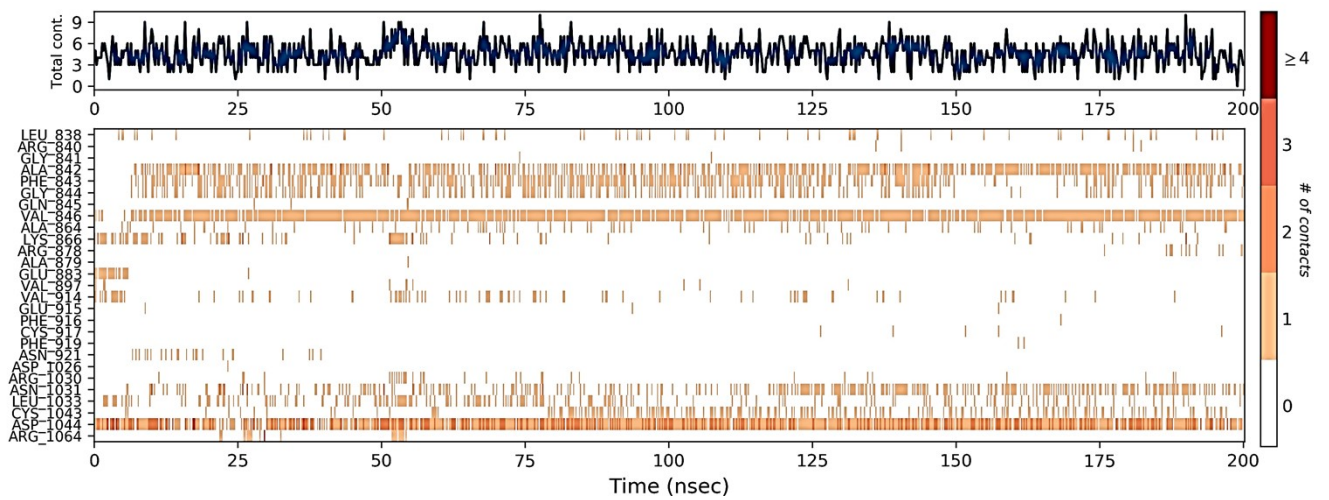
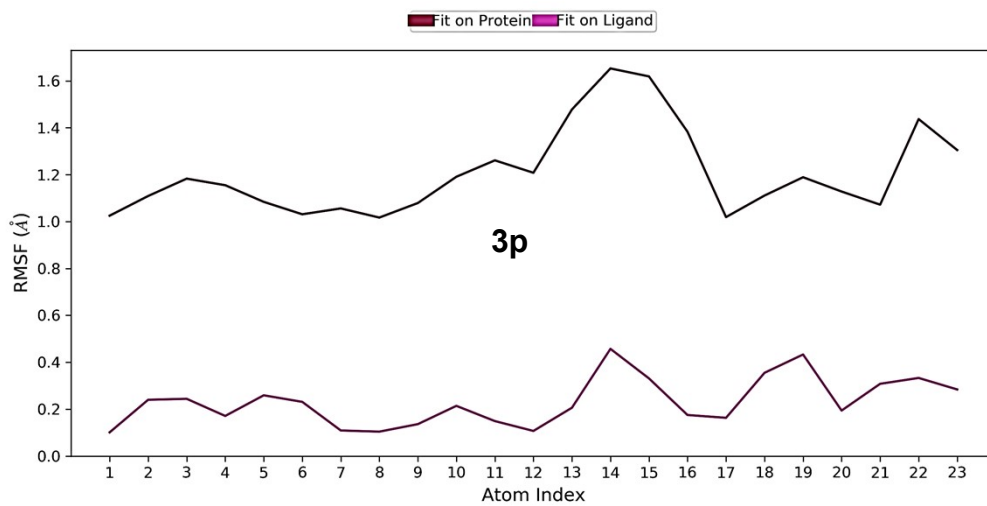
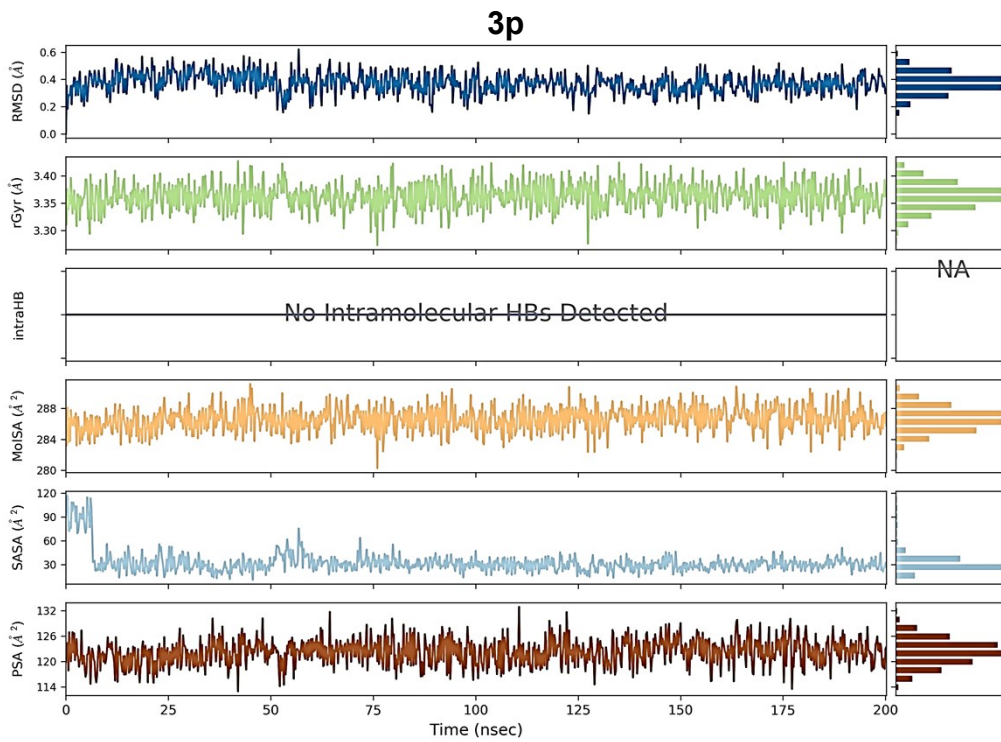


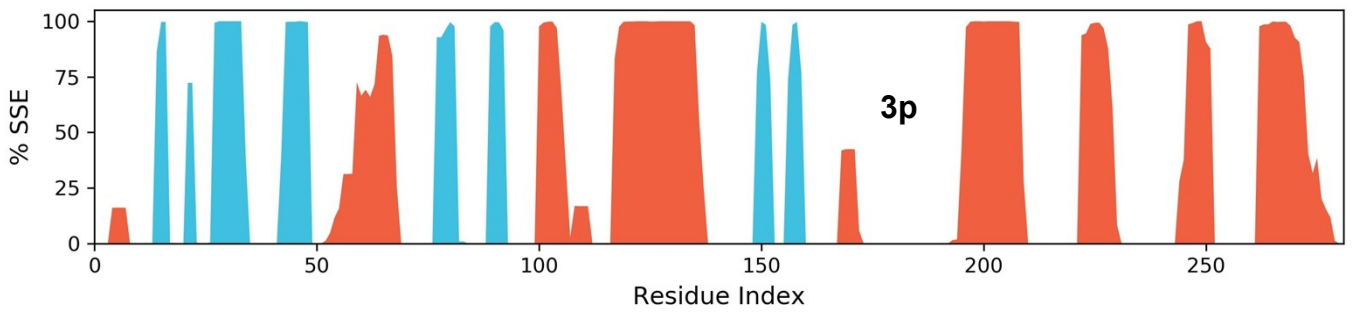
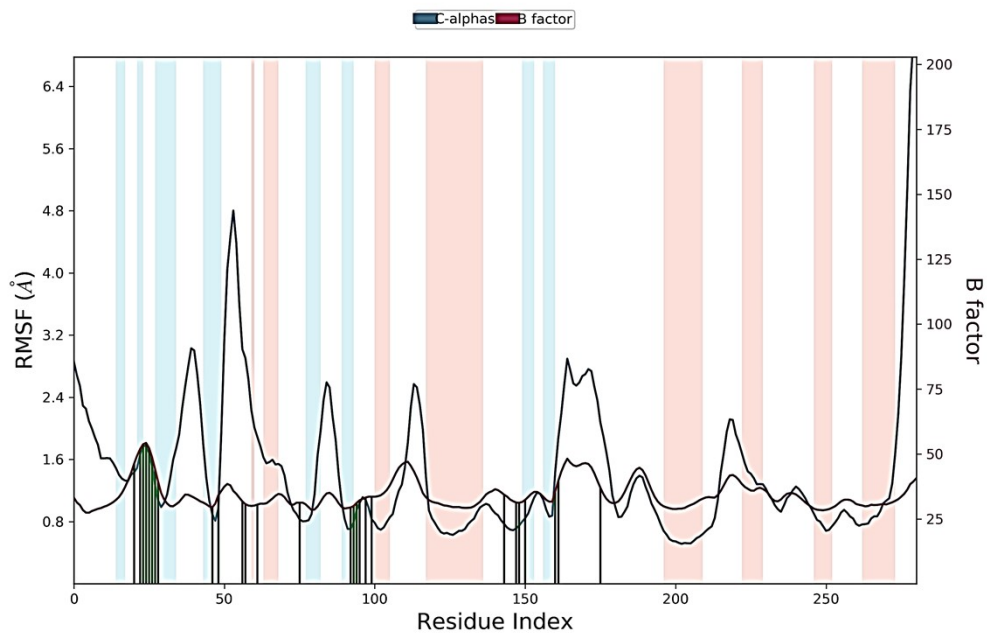
3e











3p

S35

