

Supplementary Material

A simple route for synthesis of 5-(furan-3-yl)barbiturate/thiobarbiturate derivatives *via* a multi-component reaction between arylglyoxals, acetylacetone and barbituric/thiobarbituric acid

Fatemeh Dehghanzadeh, Fereshteh Shahrokhbadi, and Mohammad Anary-Abbasinejad*

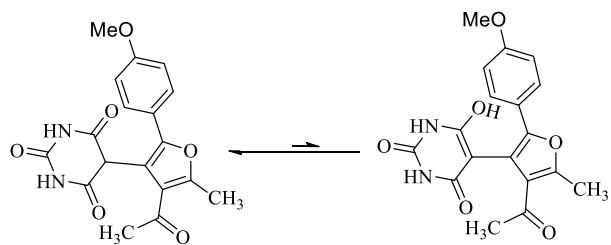
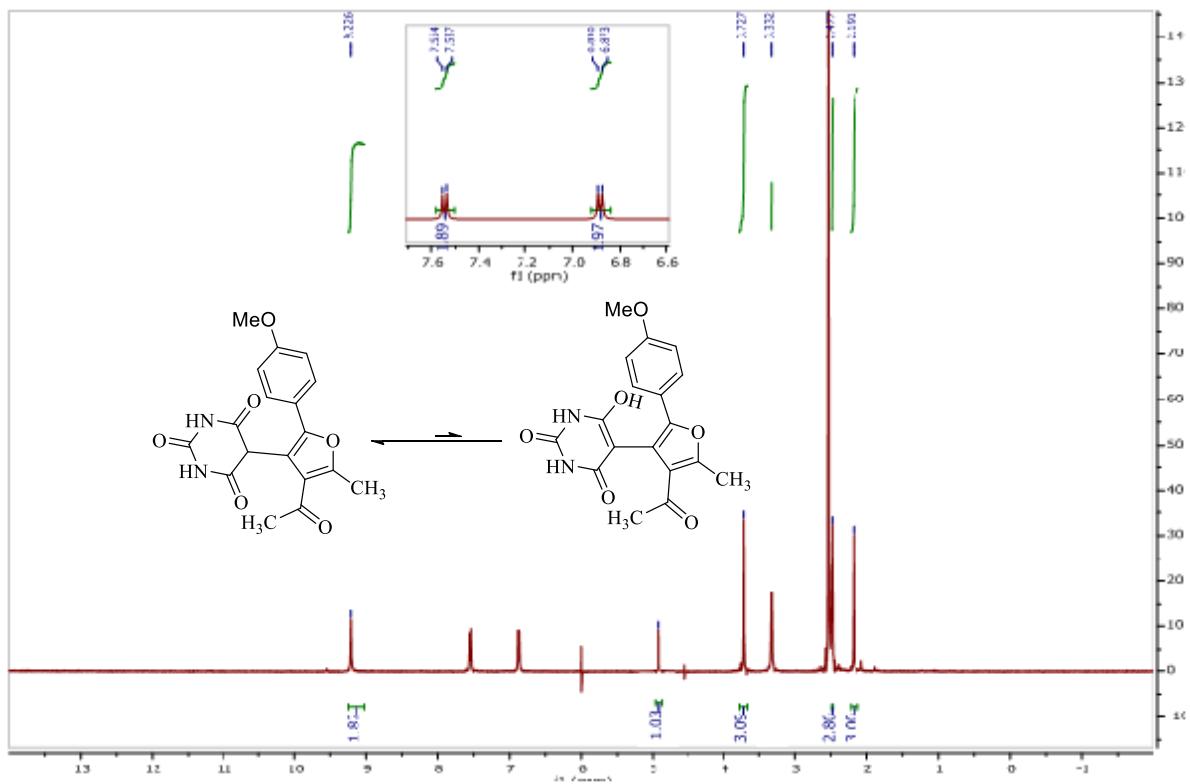
^a*Department of Chemistry, Faculty of Science, Vali-e-Asr University of Rafsanjan, Rafsanjan 77176, Iran*

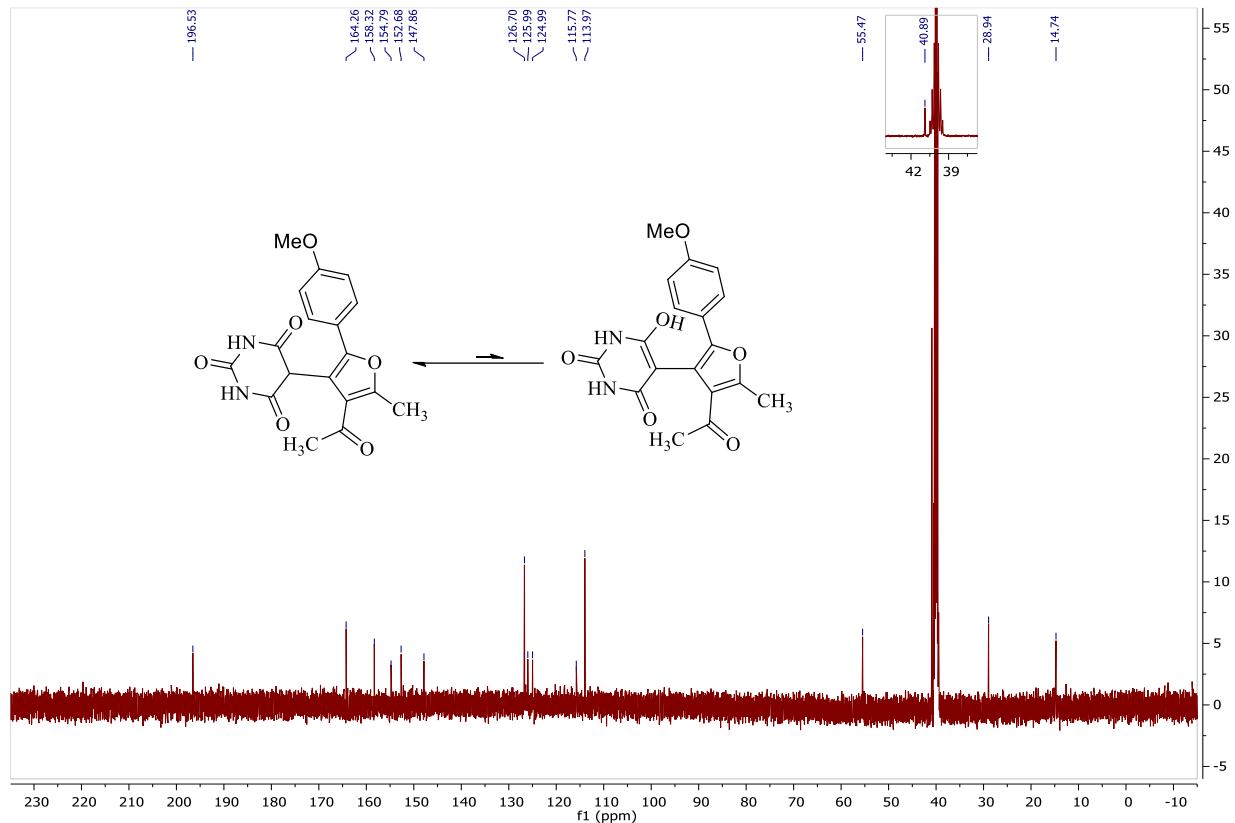
E-mail: m.anary@vru.ac.ir

Table of Contents

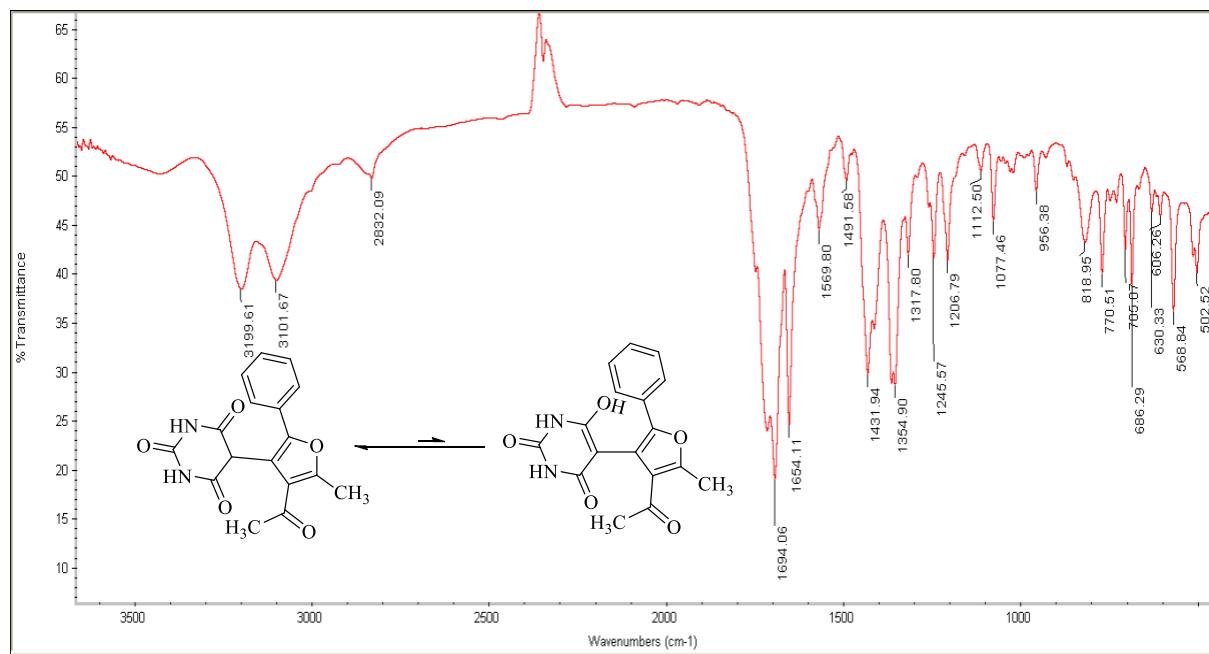
1. IR Spectrum (IR (KBr) $\nu_{\max}/\text{cm}^{-1}$) of compound 4a	S3
2. ^1H NMR Spectrum (500 MHz, d_6 -DMSO) of compound 4a	S3
3. ^{13}C NMR (125 MHz, d_6 -DMSO) spectrum of compound 4a	S4
4. IR Spectrum (IR (KBr) $\nu_{\max}/\text{cm}^{-1}$) of compound 4b	S4
5. ^1H NMR Spectrum (500 MHz, d_6 -DMSO) of compound 4b	S5
6. ^{13}C NMR (125 MHz, d_6 -DMSO) spectrum of compound 4b	S5
7. IR Spectrum (IR (KBr) $\nu_{\max}/\text{cm}^{-1}$) of compound 4c	S6
8. ^1H NMR Spectrum (500 MHz, d_6 -DMSO) of compound 4c	S6
9. ^{13}C NMR (125 MHz, d_6 -DMSO) spectrum of compound 4c	S7
10. IR Spectrum (IR (KBr) $\nu_{\max}/\text{cm}^{-1}$) of compound 4d	S7
11. ^1H NMR Spectrum (500 MHz, d_6 -DMSO) of compound 4d	S8
12. ^{13}C NMR (125 MHz, d_6 -DMSO) spectrum of compound 4d	S8
13. IR Spectrum (IR (KBr) $\nu_{\max}/\text{cm}^{-1}$) of compound 4e	S9
14. ^1H NMR Spectrum (500 MHz, d_6 -DMSO) of compound 4e	S9
15. ^{13}C NMR (125 MHz, d_6 -DMSO) spectrum of compound 4e	S10
16. IR Spectrum (IR (KBr) $\nu_{\max}/\text{cm}^{-1}$) of compound 4f	S10
17. ^1H NMR Spectrum (500 MHz, d_6 -DMSO) of compound 4f	S11
18. ^{13}C NMR (125 MHz, d_6 -DMSO) spectrum of compound 4f	S11
19. IR Spectrum (IR (KBr) $\nu_{\max}/\text{cm}^{-1}$) of compound 4g	S12
20. ^1H NMR Spectrum (500 MHz, d_6 -DMSO) of compound 4g	S12
21. ^{13}C NMR (125 MHz, d_6 -DMSO) spectrum of compound 4g	S12
22. ^{13}C NMR (125 MHz, d_6 -DMSO) spectrum of compound 4i	S13
23. IR Spectrum (IR (KBr) $\nu_{\max}/\text{cm}^{-1}$) of compound 4h	S13
24. ^1H NMR Spectrum (500 MHz, d_6 -DMSO) of compound 4h	S14
25. ^{13}C NMR (125 MHz, d_6 -DMSO) spectrum of compound 4h	S14
26. IR Spectrum (IR (KBr) $\nu_{\max}/\text{cm}^{-1}$) of compound 4i	S15
27. ^1H NMR Spectrum (500 MHz, d_6 -DMSO) of compound 4i	S15
28. ^{13}C NMR (125 MHz, d_6 -DMSO) spectrum of compound 4i	S16

29. IR Spectrum (IR (KBr) ν_{max} /cm $^{-1}$) of compound 4j	S16
30. ^1H NMR Spectrum (500 MHz, d ₆ -DMSO) of compound 4j	S17
31. ^{13}C NMR (125 MHz, d ₆ -DMSO) spectrum of compound 4j	S17
32. IR Spectrum (IR (KBr) ν_{max} /cm $^{-1}$) of compound 4k	S18
33. ^1H NMR Spectrum (500 MHz, d ₆ -DMSO) of compound 4k	S18
34. ^{13}C NMR (125 MHz, d ₆ -DMSO) spectrum of compound 4k	S19
35. IR Spectrum (IR (KBr) ν_{max} /cm $^{-1}$) of compound 4l	S19
36. ^1H NMR Spectrum (500 MHz, d ₆ -DMSO) of compound 4l	S20
37. ^{13}C NMR (125 MHz, d ₆ -DMSO) spectrum of compound 4l	S20
38. IR Spectrum (IR (KBr) ν_{max} /cm $^{-1}$) of compound 4m	S21
39. ^1H NMR Spectrum (500 MHz, d ₆ -DMSO) of compound 4m	S21
40. ^{13}C NMR (125 MHz, d ₆ -DMSO) spectrum of compound 4m	S22

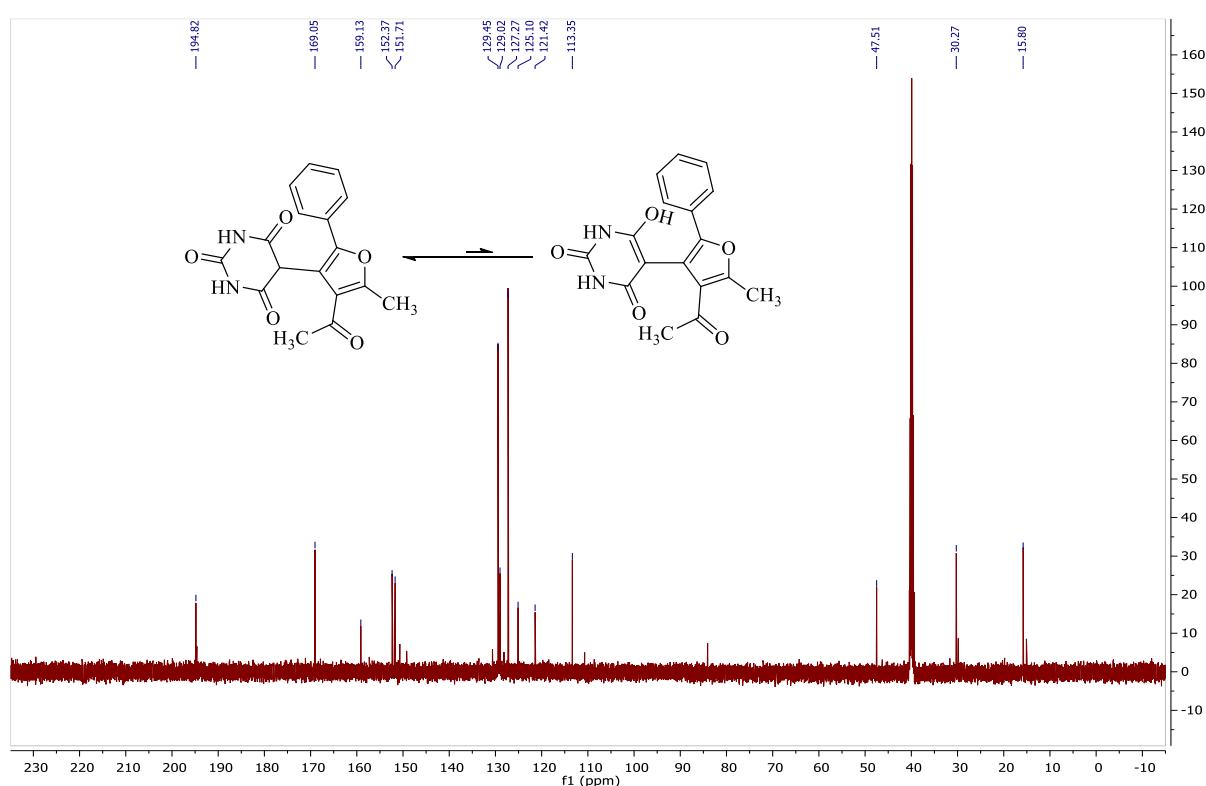
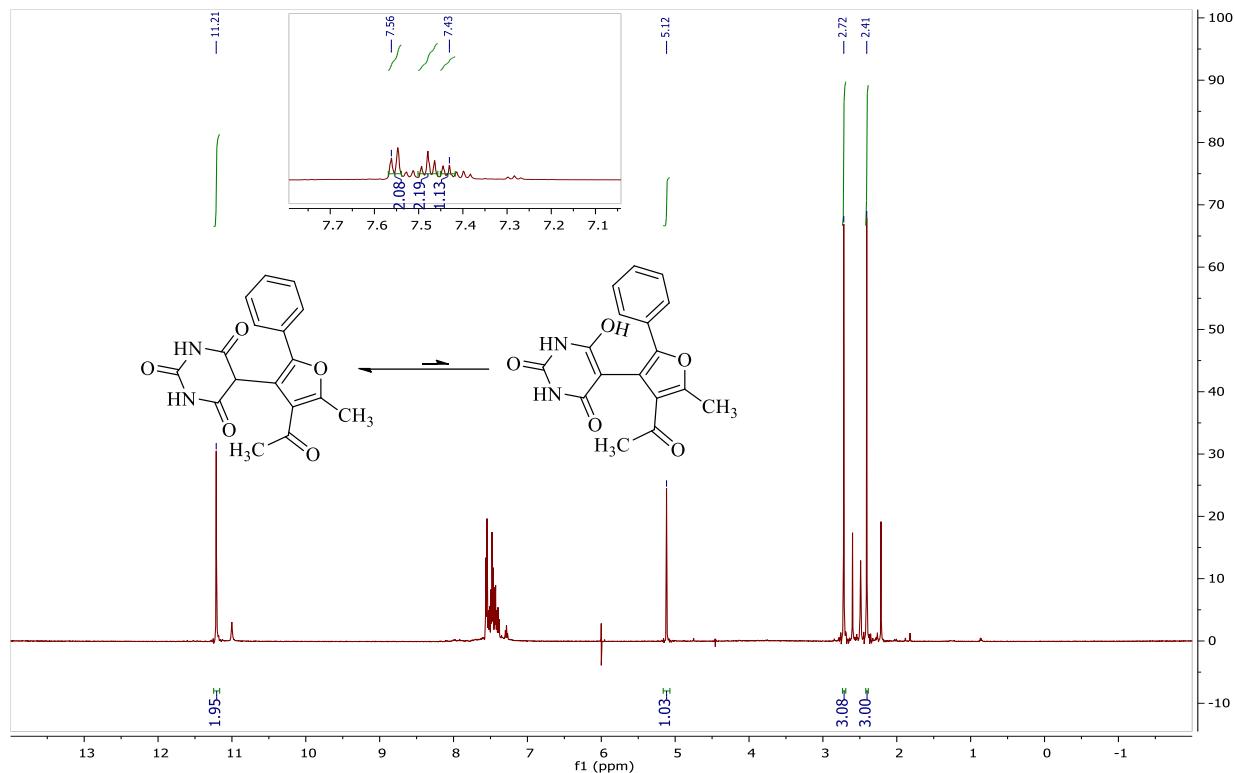
IR Spectrum (IR (KBr) $\bar{\nu}_{\text{max}}/\text{cm}^{-1}$) of compound 4a

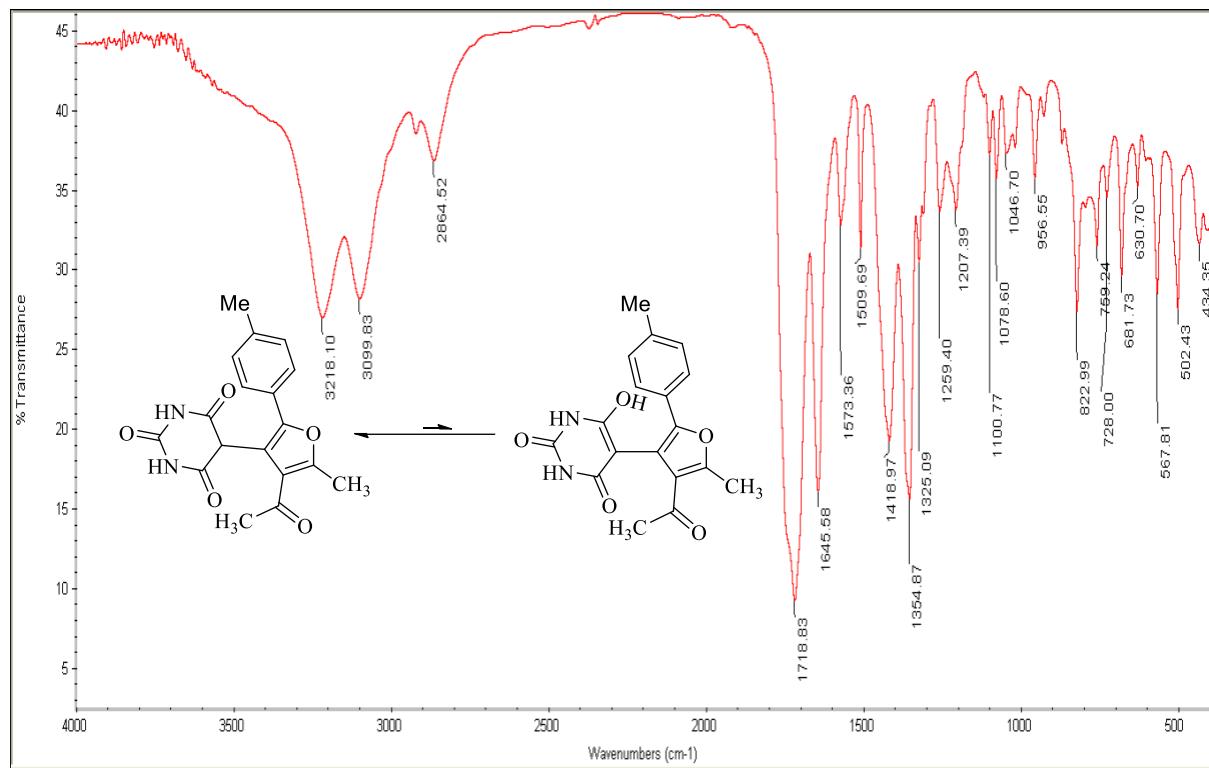
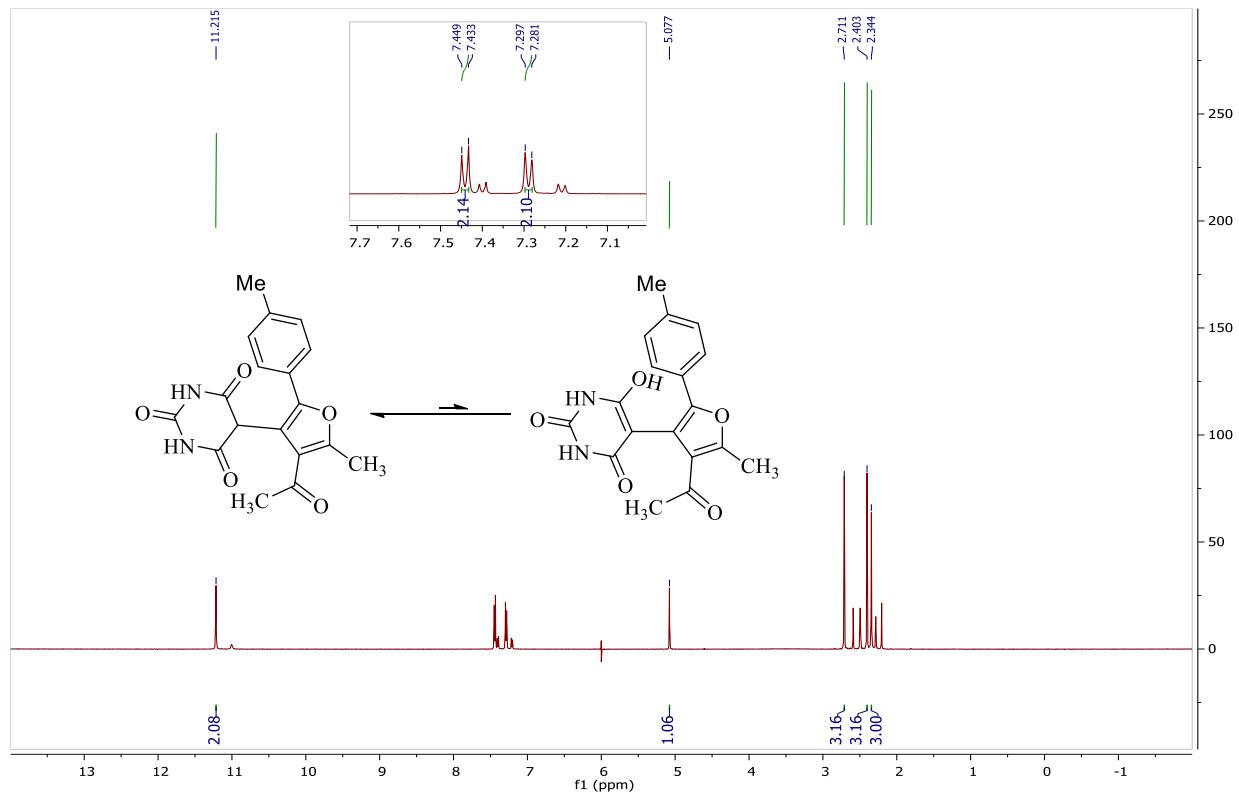


^{13}C NMR (125 MHz, $d_6\text{-DMSO}$) spectrum of compound **4a**

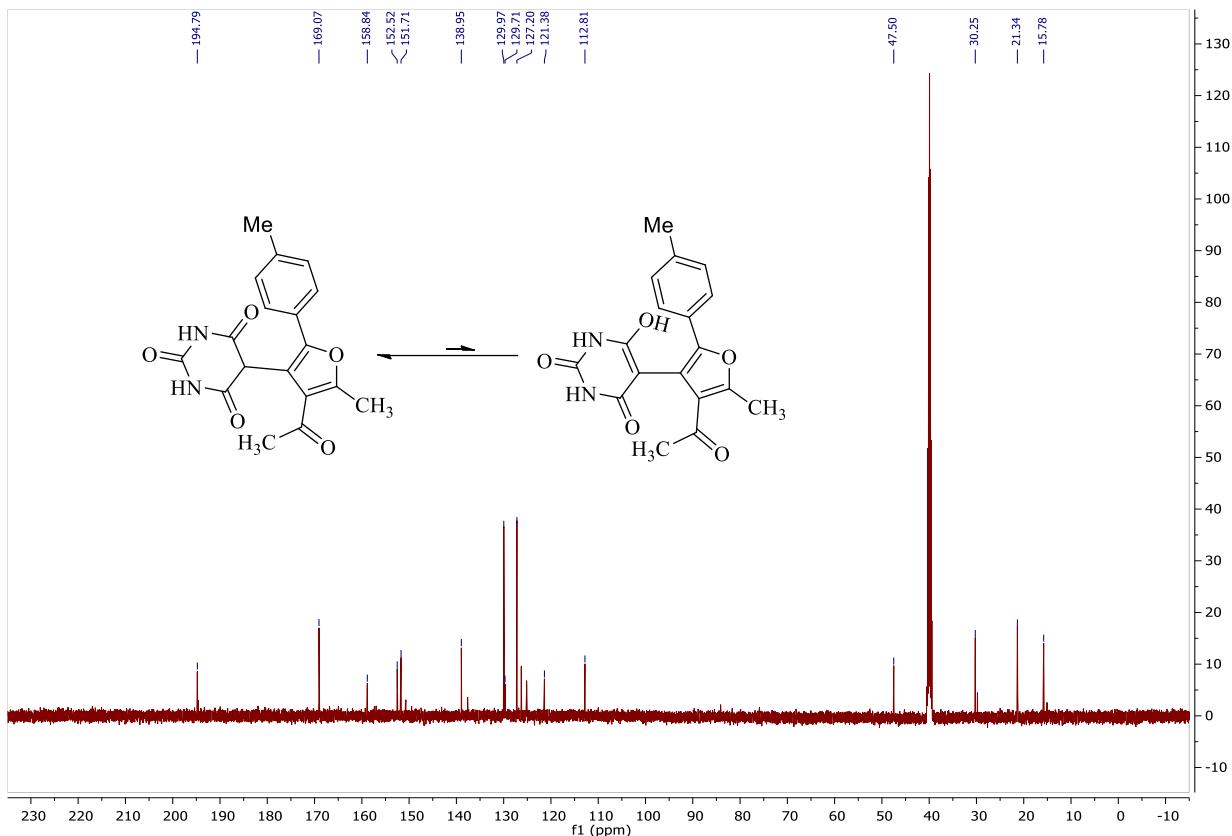


IR Spectrum (IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$) of compound **4b**

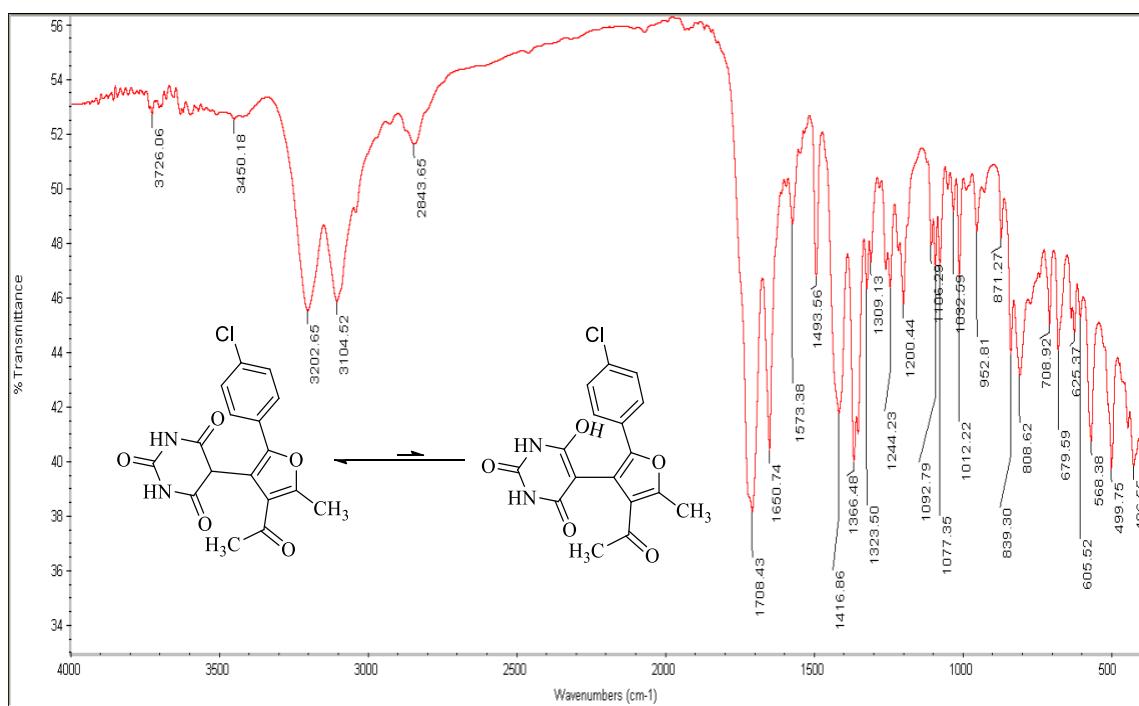


IR Spectrum (IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$) of compound 4c¹H NMR Spectrum (500 MHz, d₆-DMSO) of compound 4c

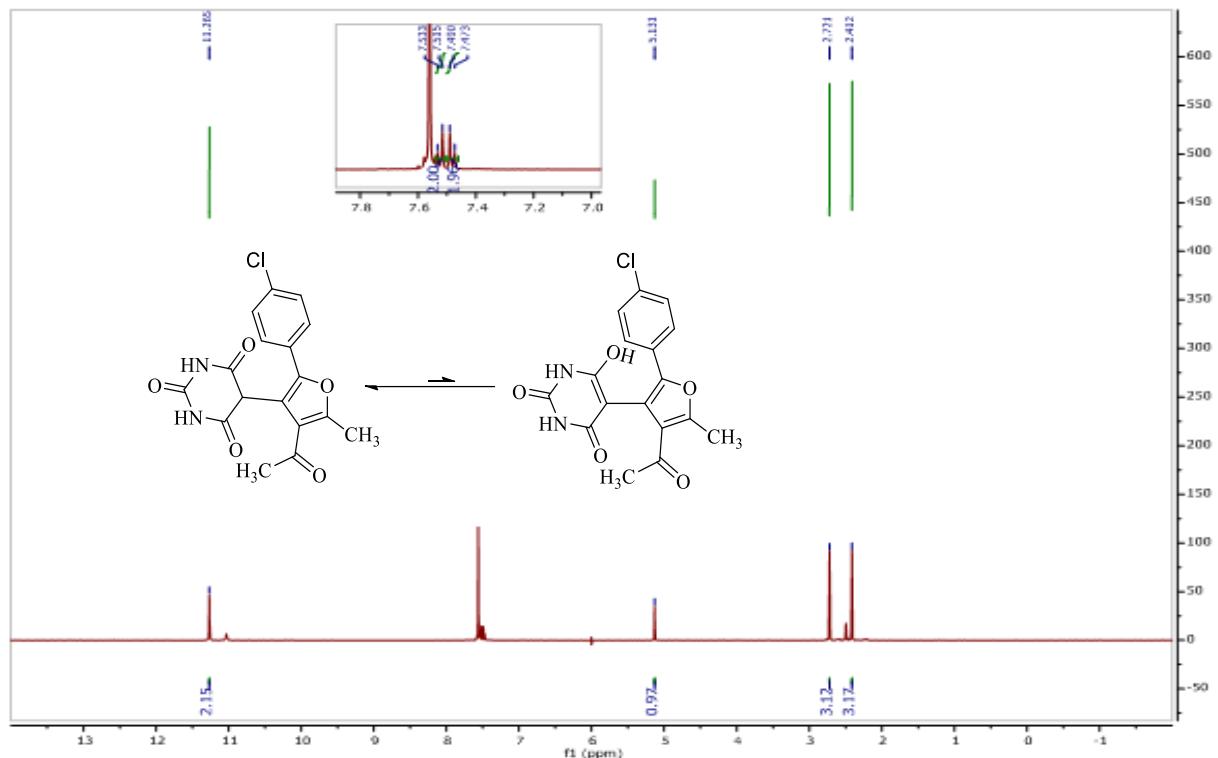
:



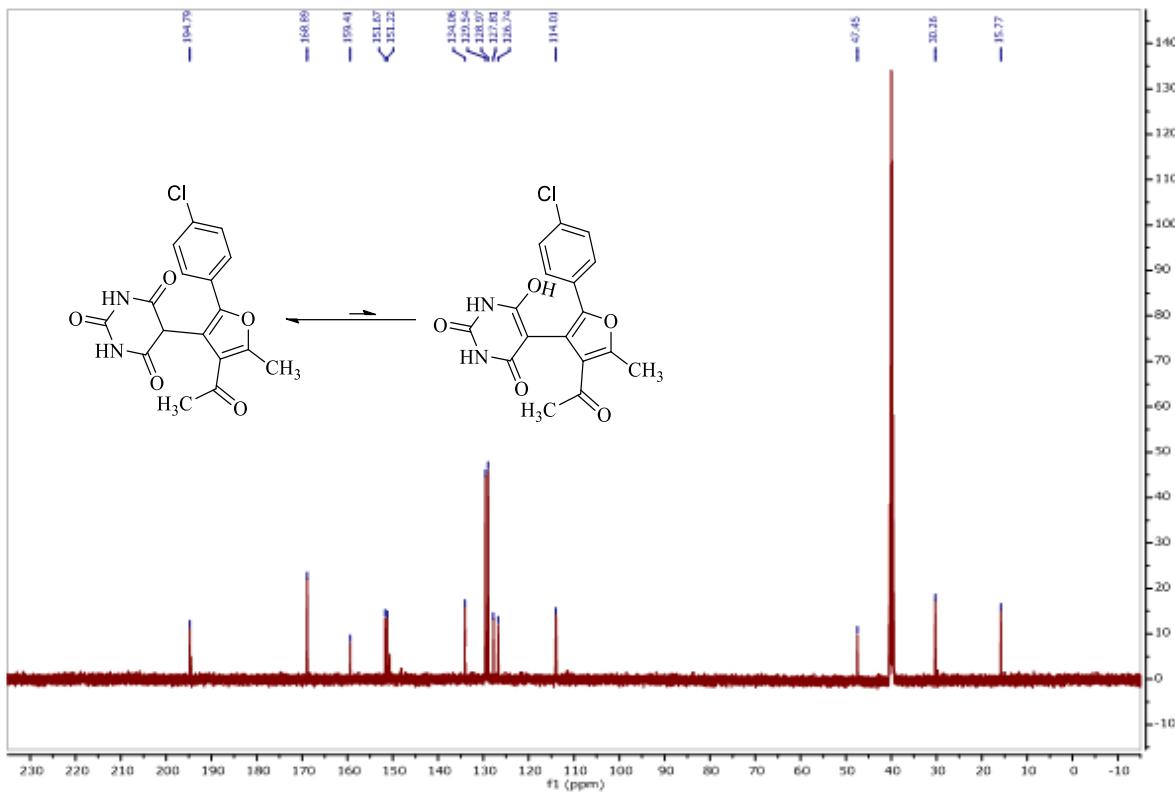
^{13}C NMR (125 MHz, d₆-DMSO) spectrum of compound **4c**



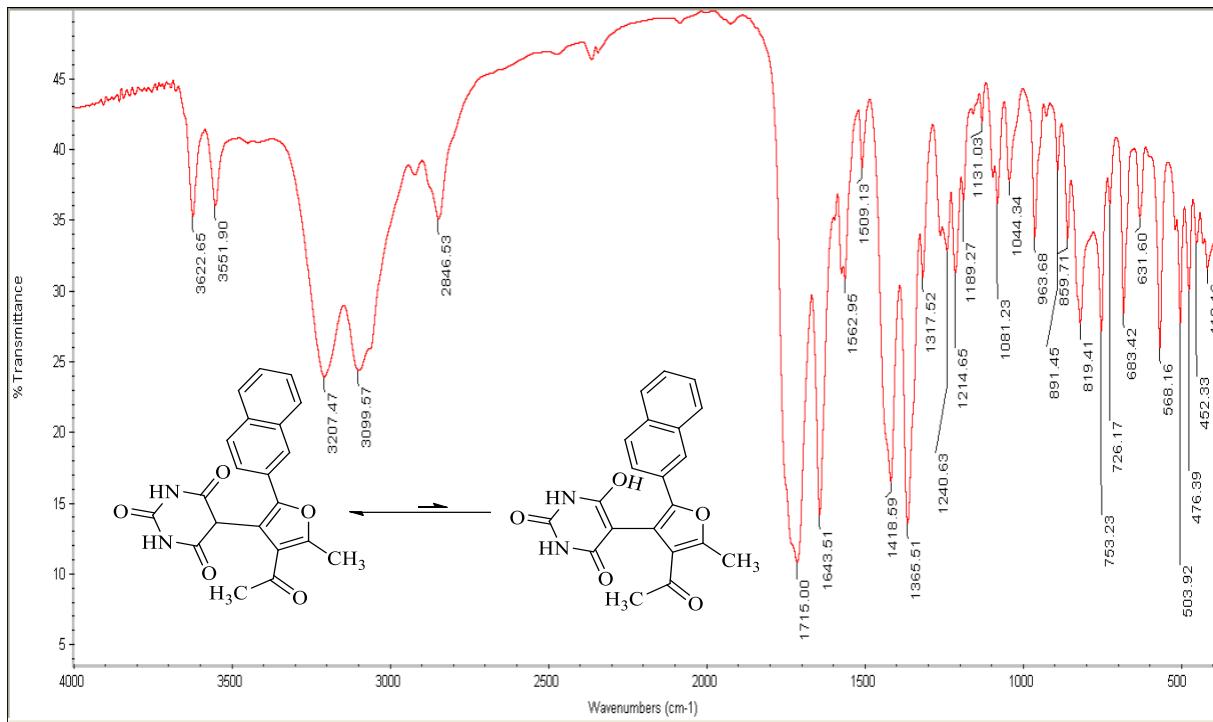
IR Spectrum (IR (KBr) ν_{max} /cm⁻¹) of compound **4d**



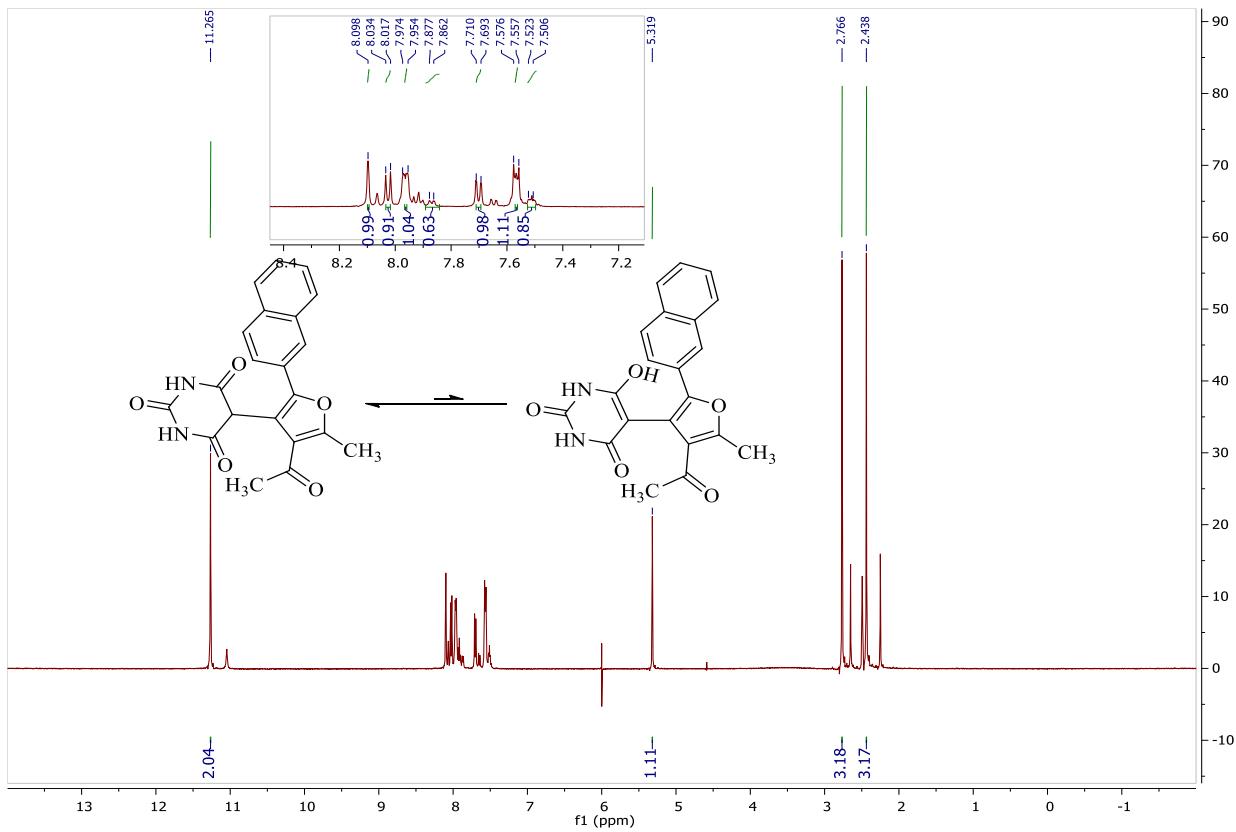
¹H NMR Spectrum (500 MHz, d₆-DMSO) of compound 4d



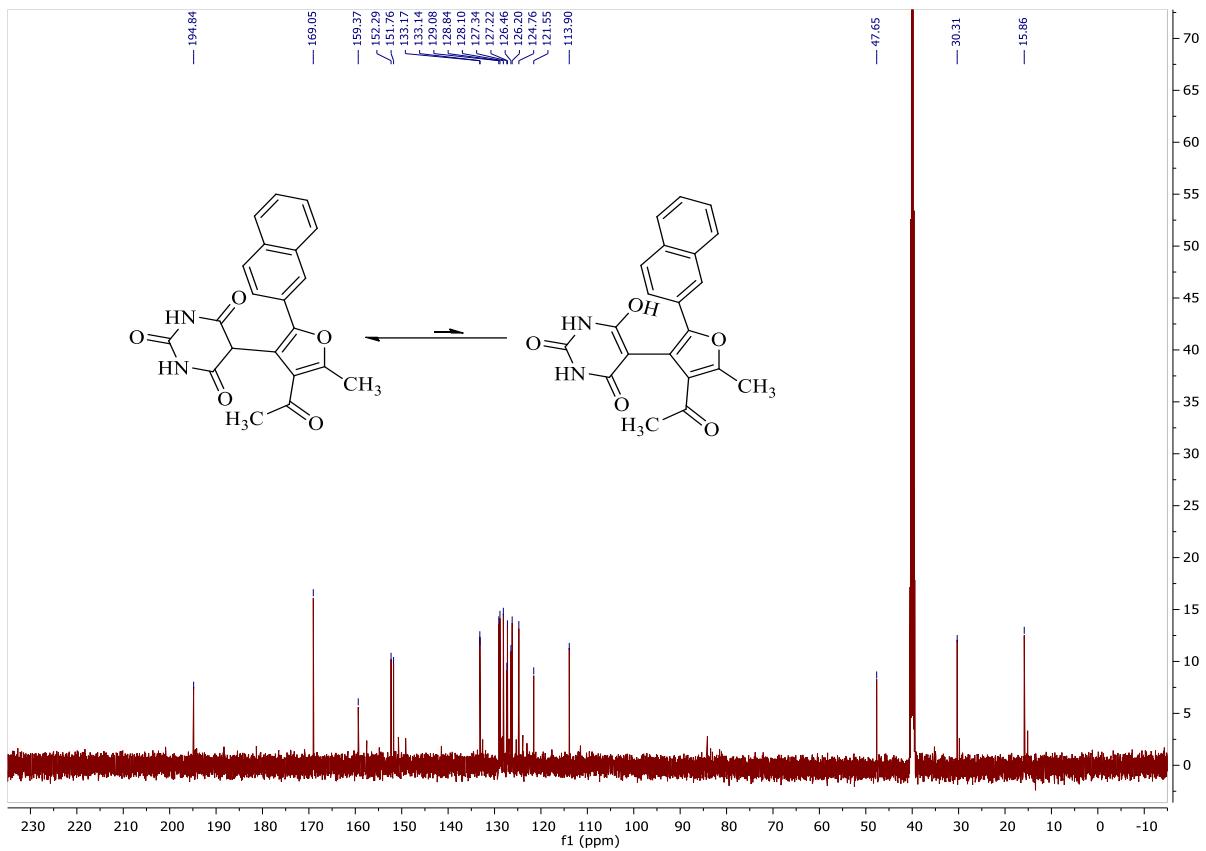
¹³C NMR (125 MHz, d₆-DMSO) spectrum of compound 4d



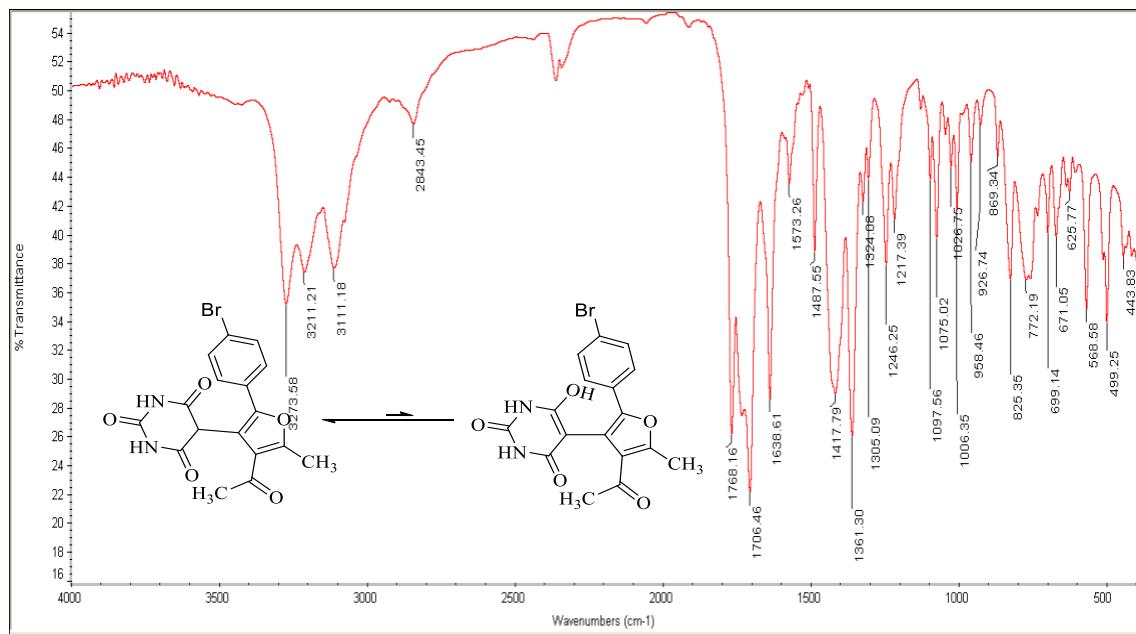
IR Spectrum (IR (KBr) ν_{max} /cm⁻¹) of compound **4e**



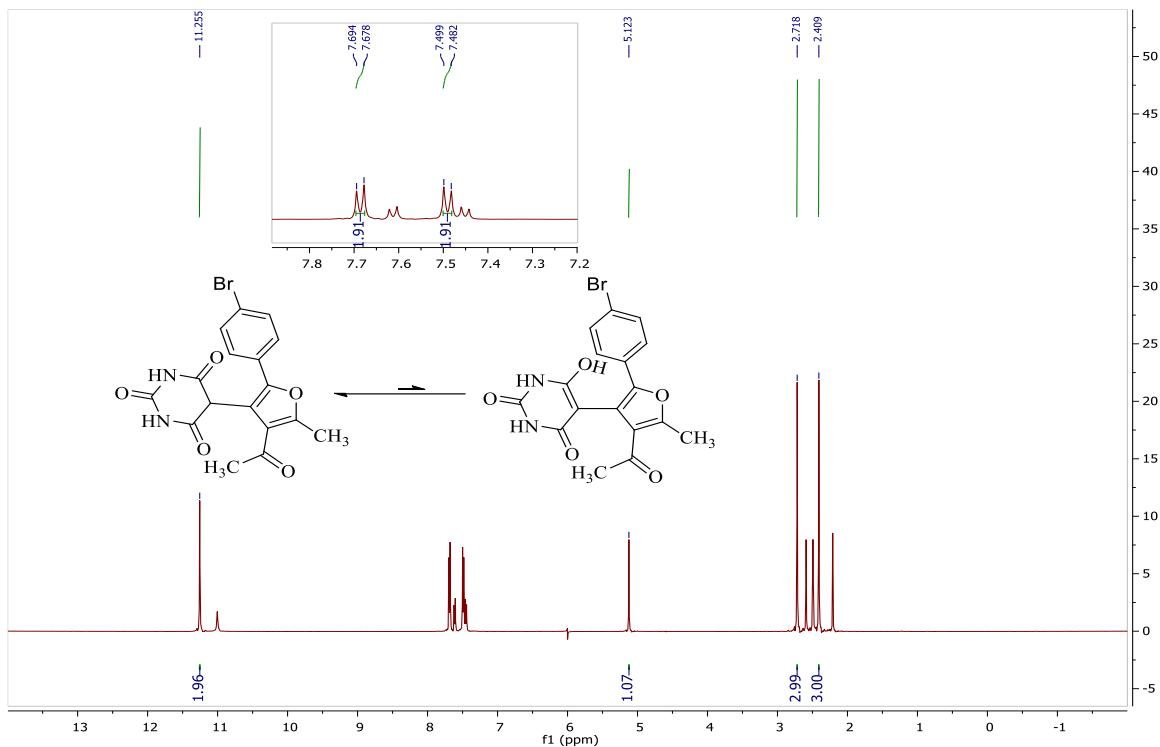
¹H NMR Spectrum (500 MHz, d₆-DMSO) of compound 4e



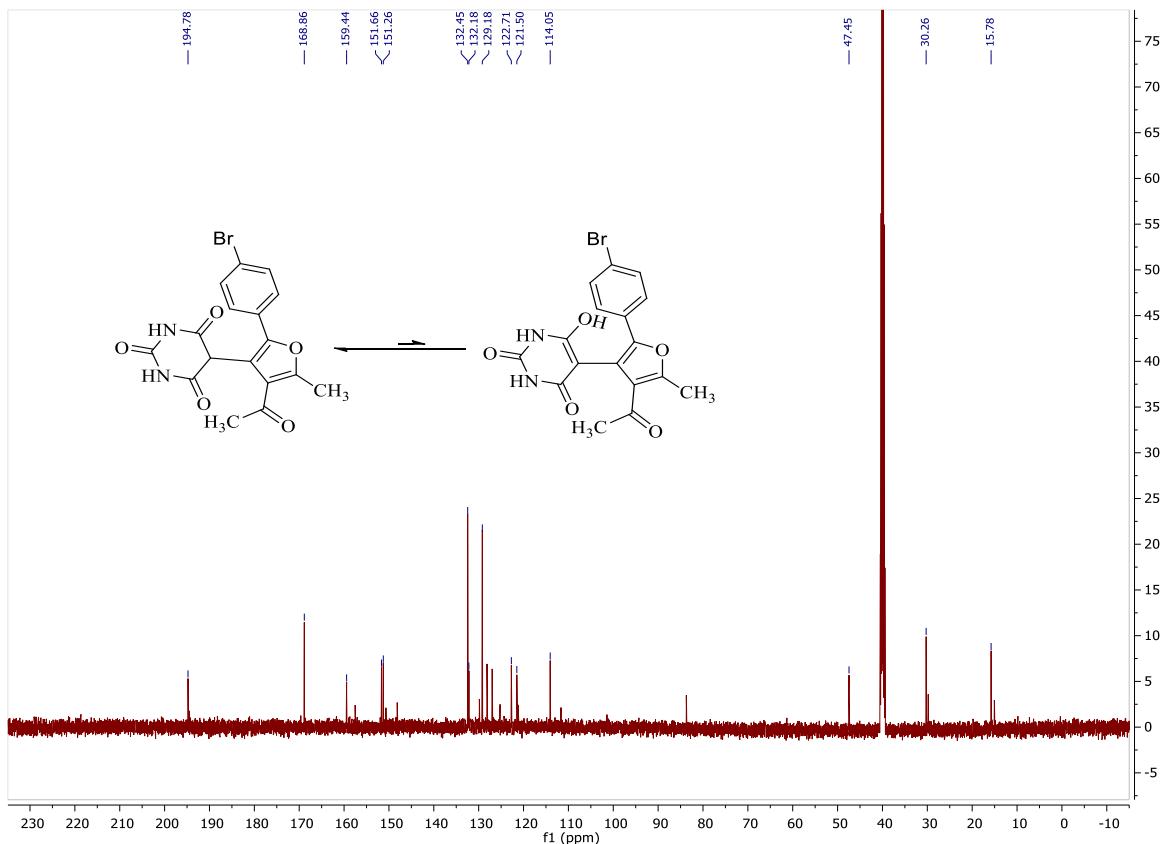
^{13}C NMR (125 MHz, d₆-DMSO) spectrum of compound **4e**



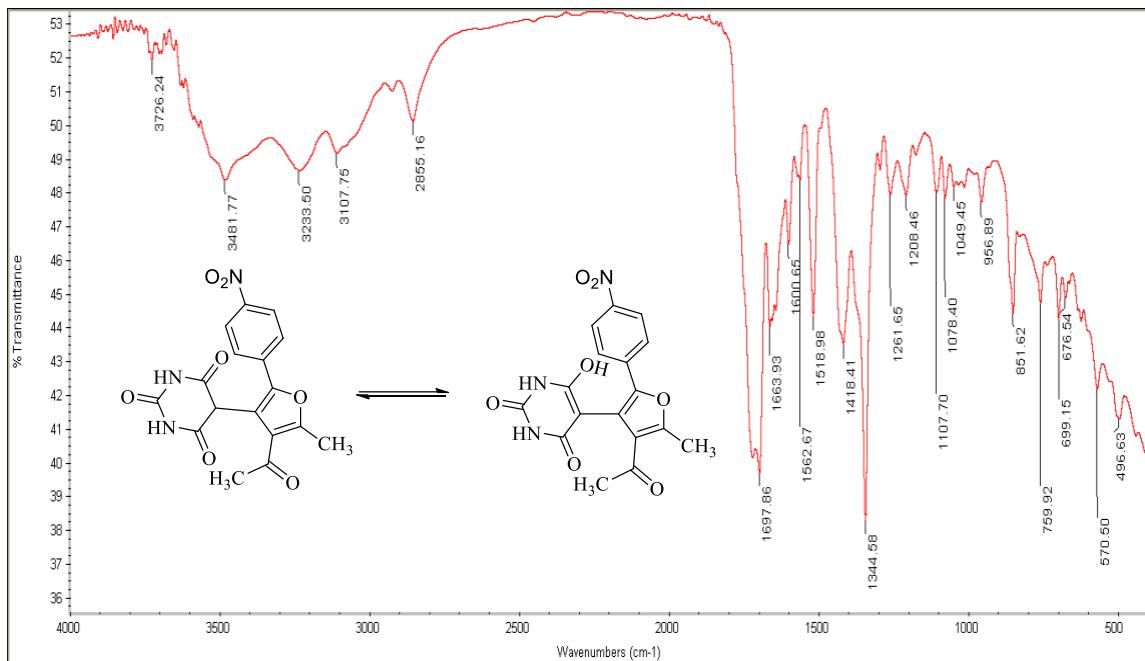
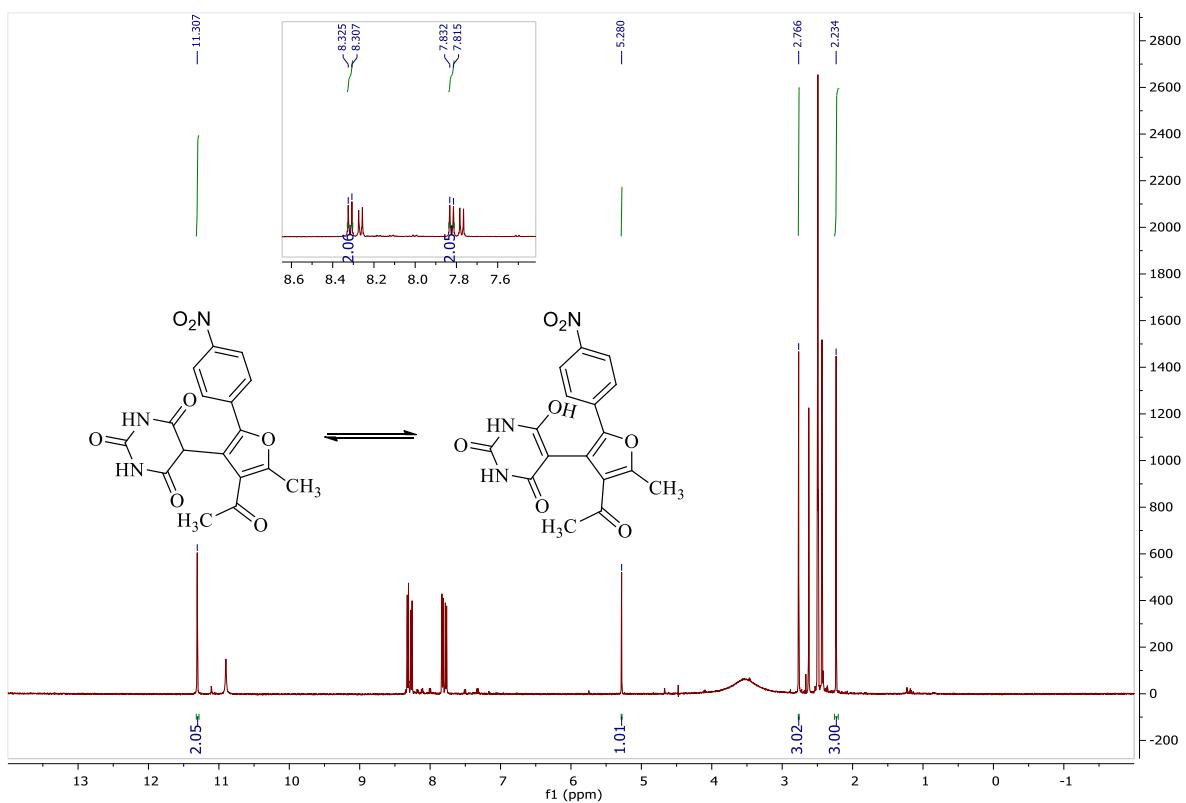
IR Spectrum (IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$) of compound **4f**

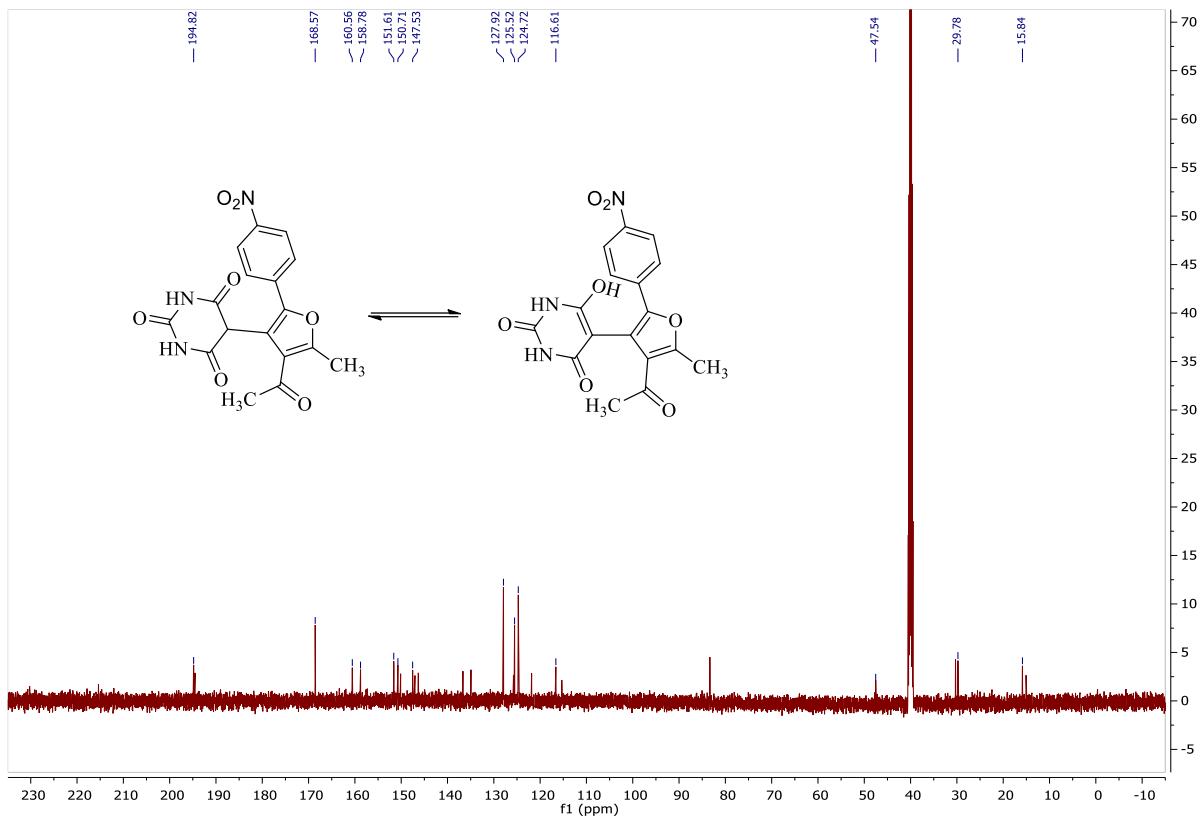
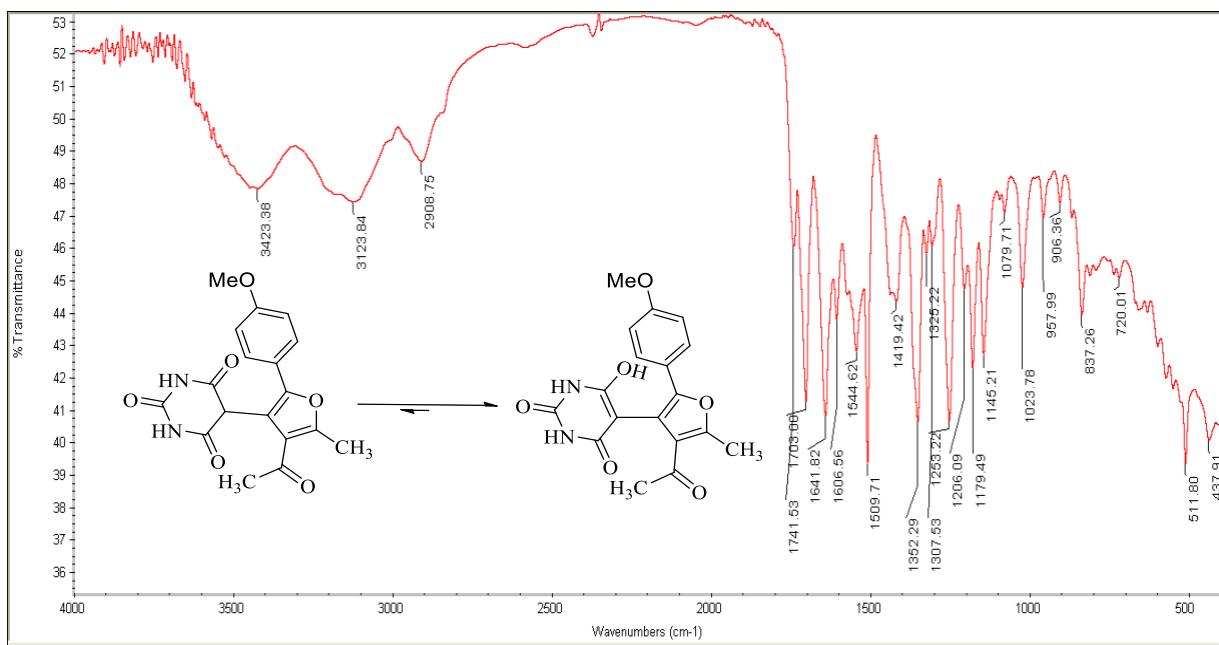


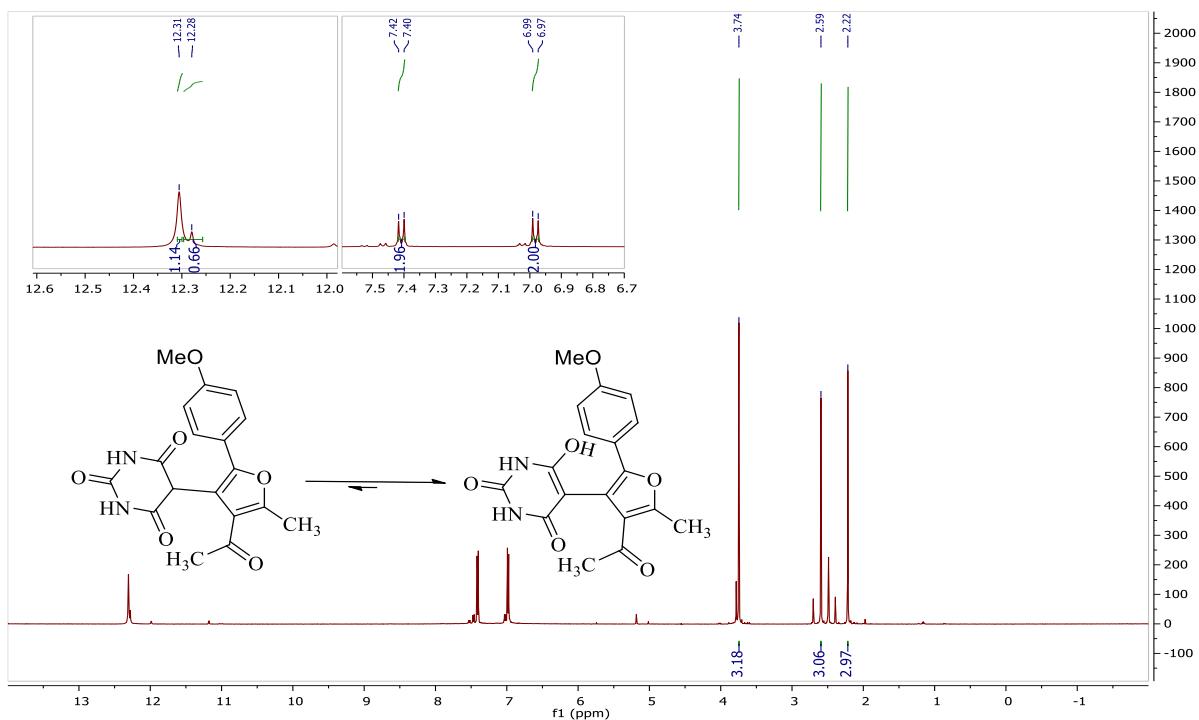
¹H NMR Spectrum (500 MHz, d₆-DMSO) of compound 4f



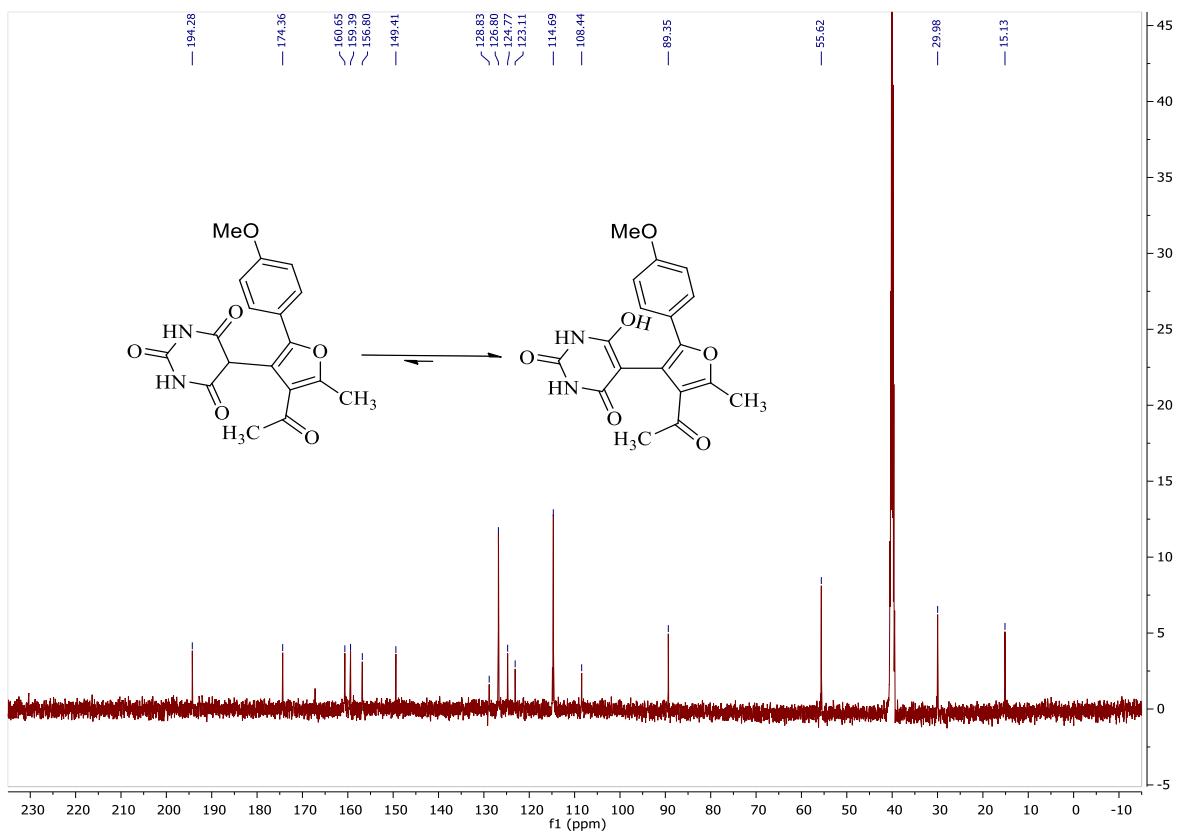
¹³C NMR (125 MHz, d₆-DMSO) spectrum of compound 4f

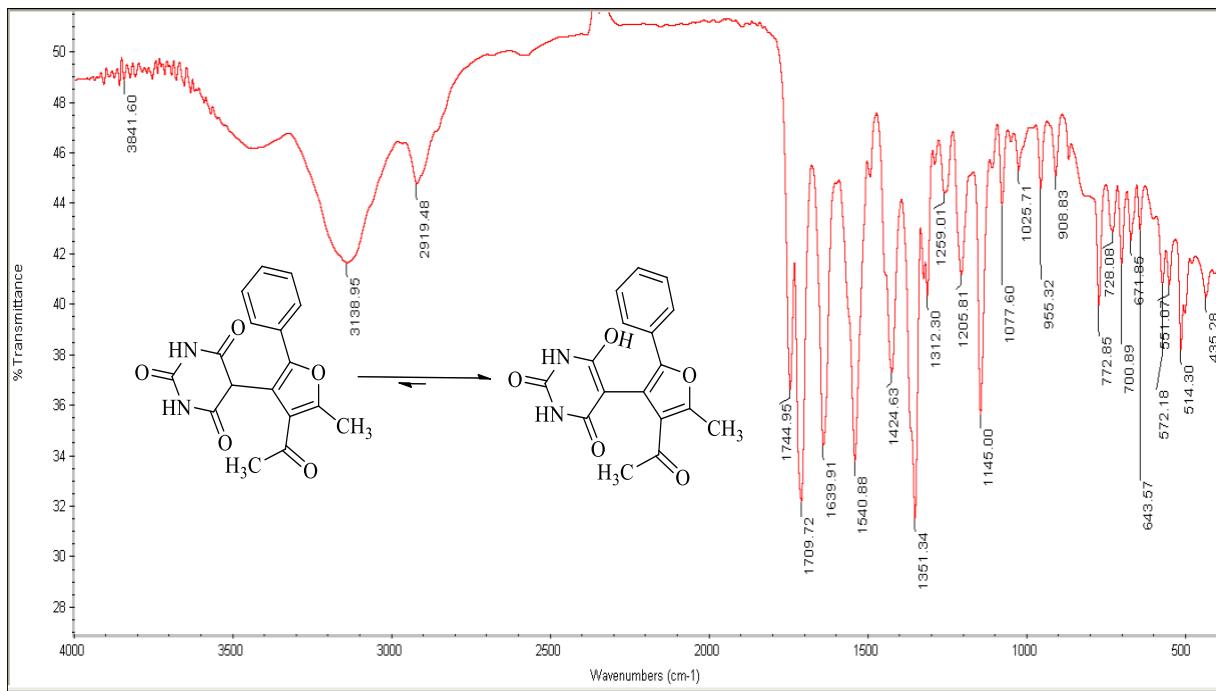
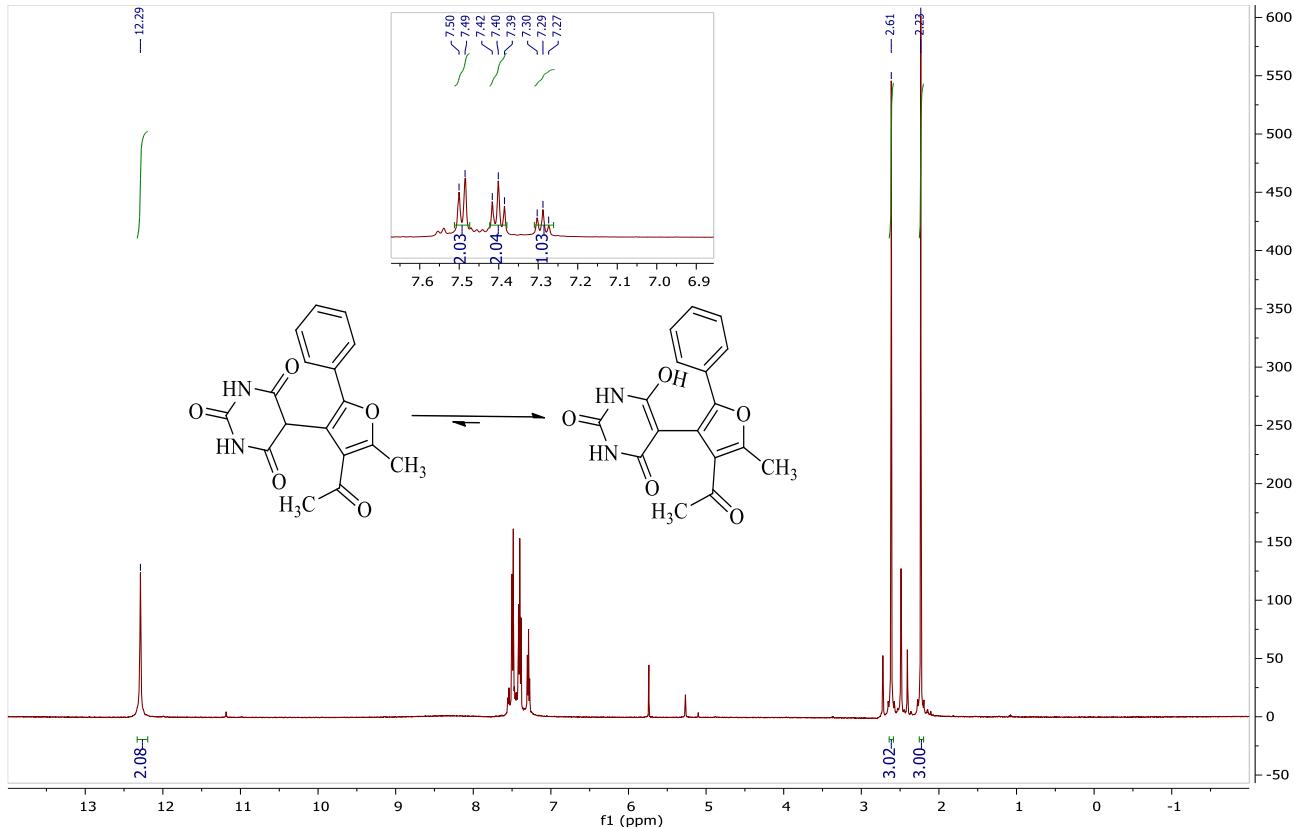
IR Spectrum (IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$) of compound 4g¹H NMR Spectrum (500 MHz, d₆-DMSO) of compound 4g

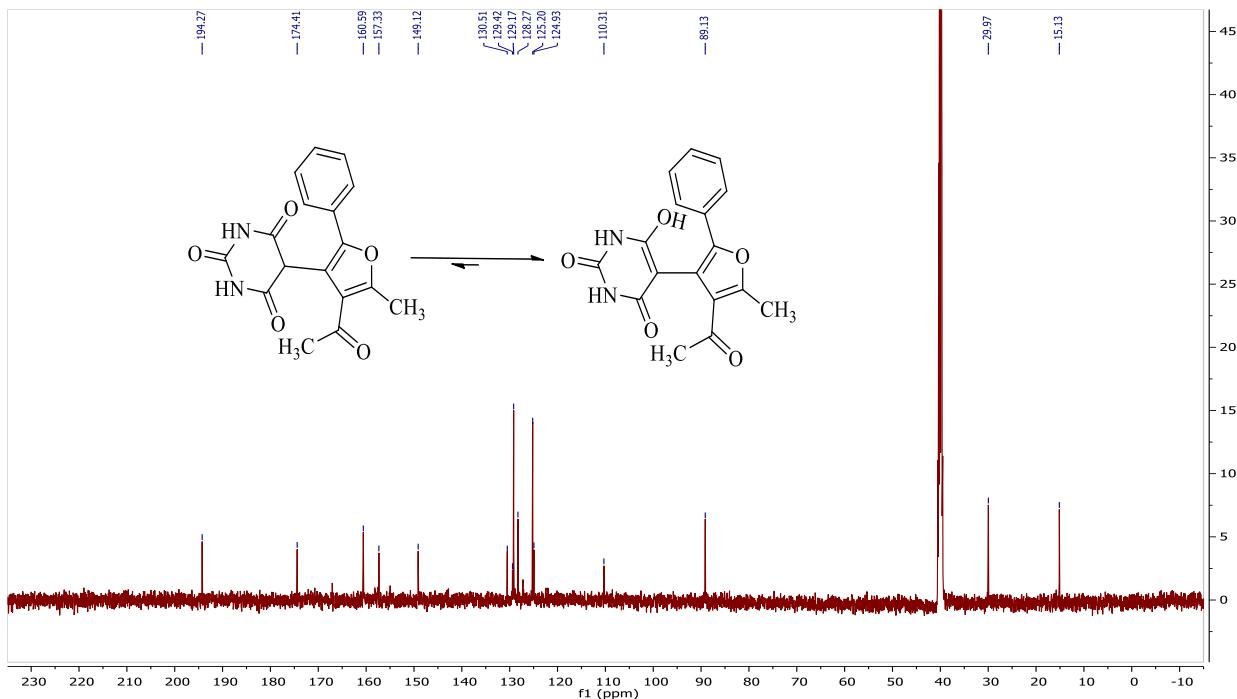
 ^{13}C NMR (125 MHz, d₆-DMSO) spectrum of compound **4g**IR Spectrum (IR (KBr) ν_{max} /cm⁻¹) of compound **4h**



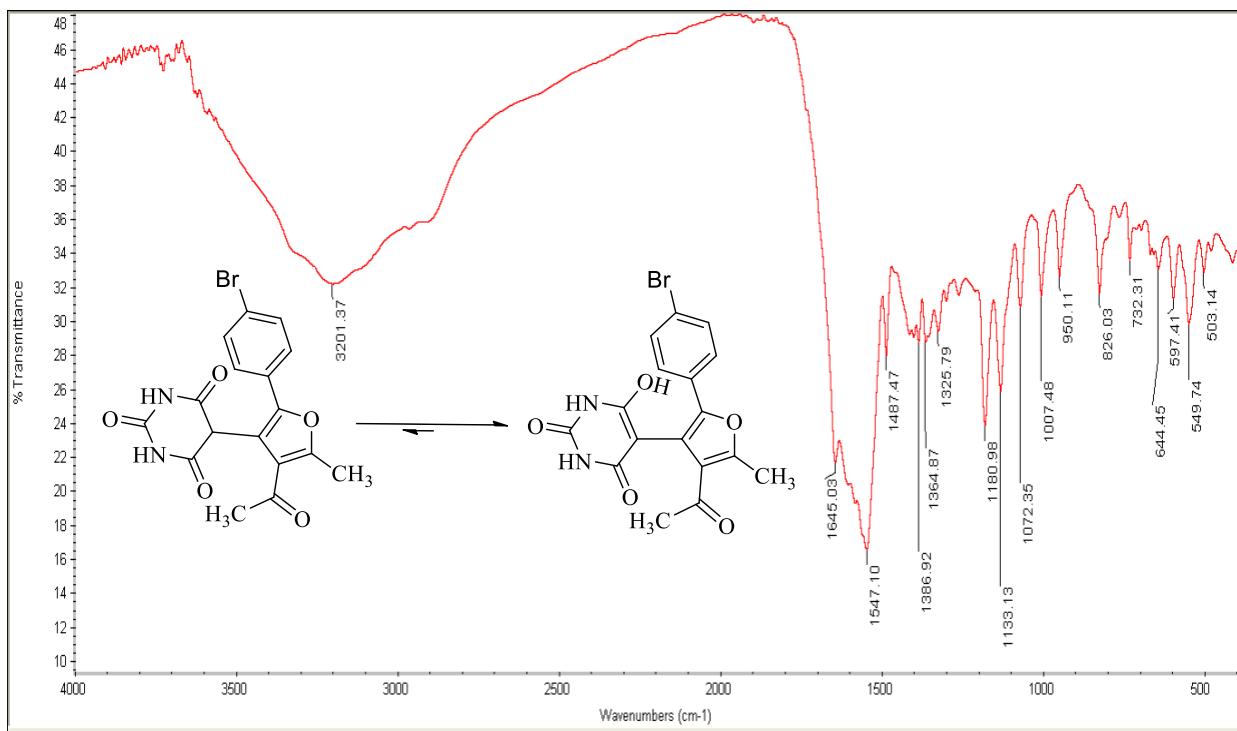
¹H NMR Spectrum (500 MHz, d₆-DMSO) of compound **4h**



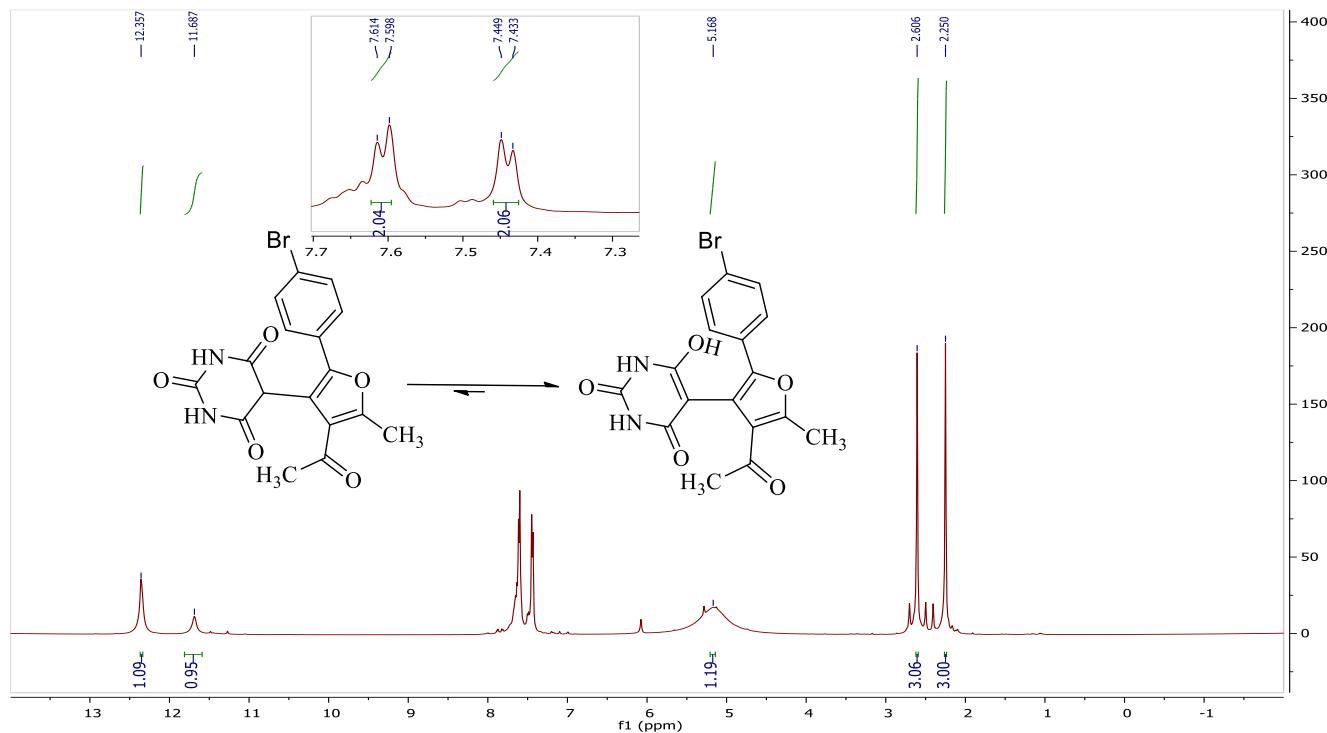
IR Spectrum (IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$) of compound 4i¹H NMR Spectrum (500 MHz, d₆-DMSO) of compound 4i



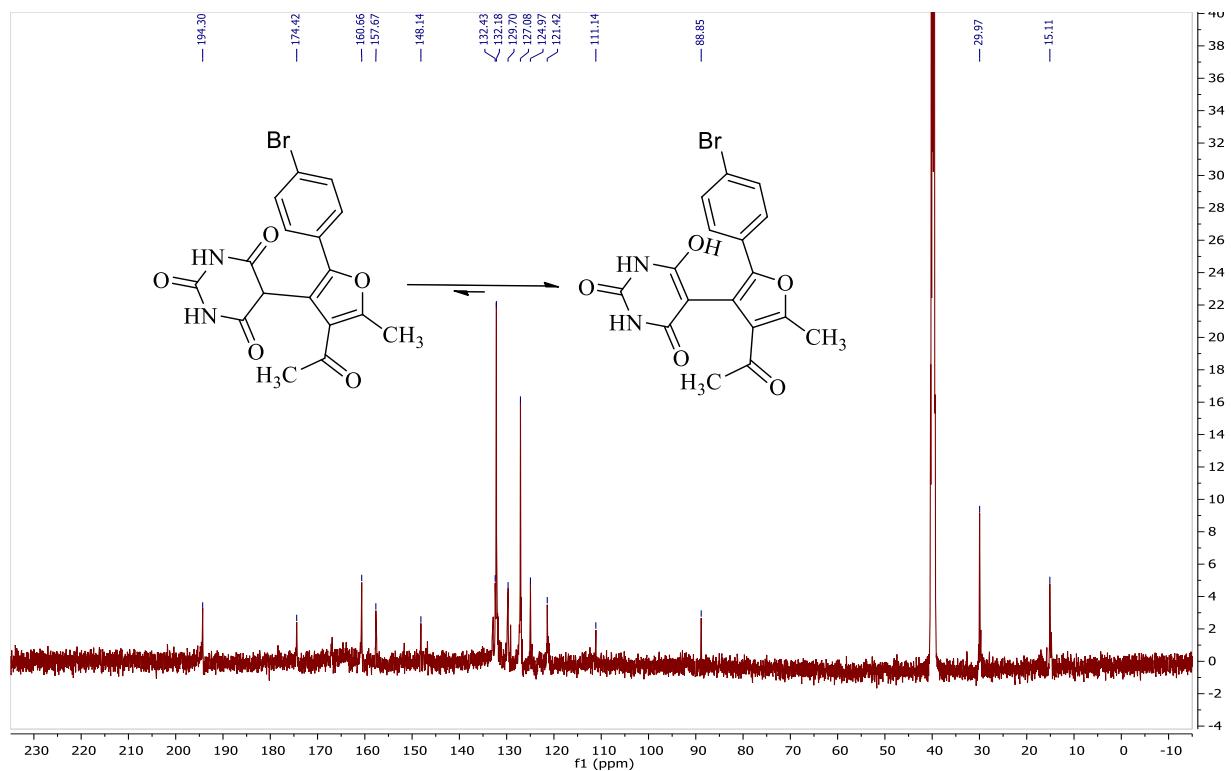
^{13}C NMR (125 MHz, d₆-DMSO) spectrum of compound **4i**



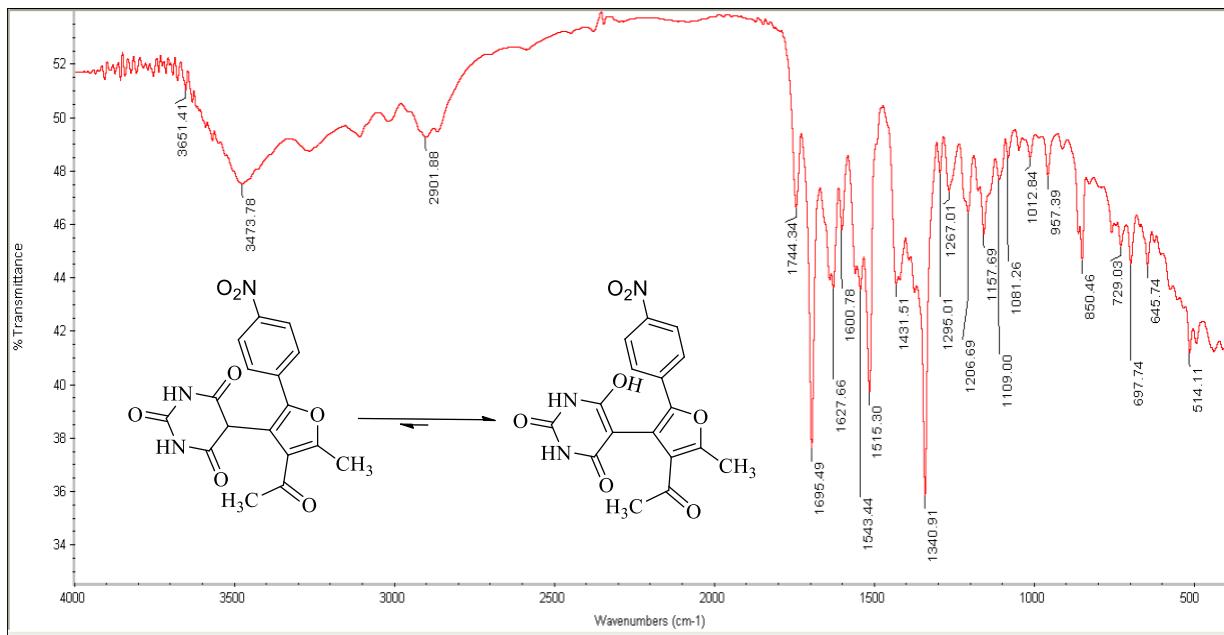
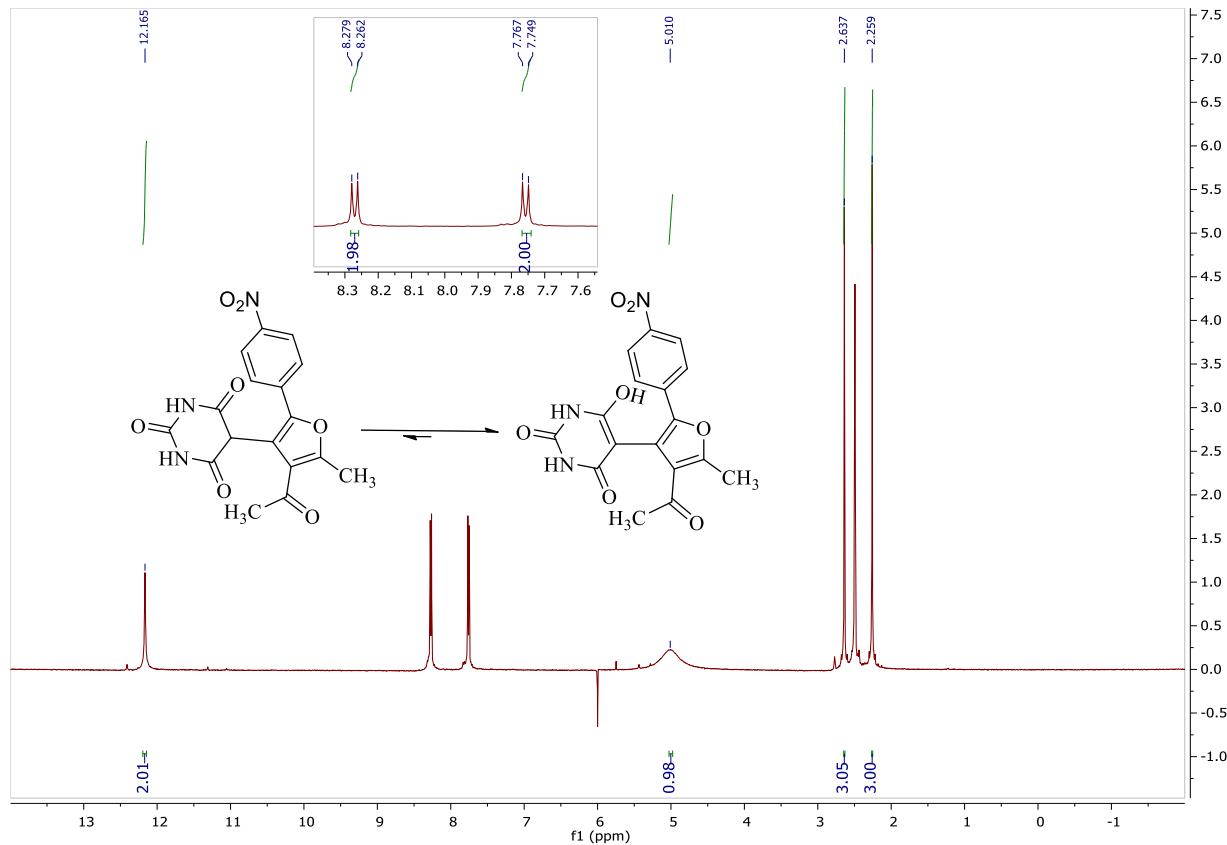
IR Spectrum (IR (KBr) ν_{max} /cm⁻¹) of compound **4j**

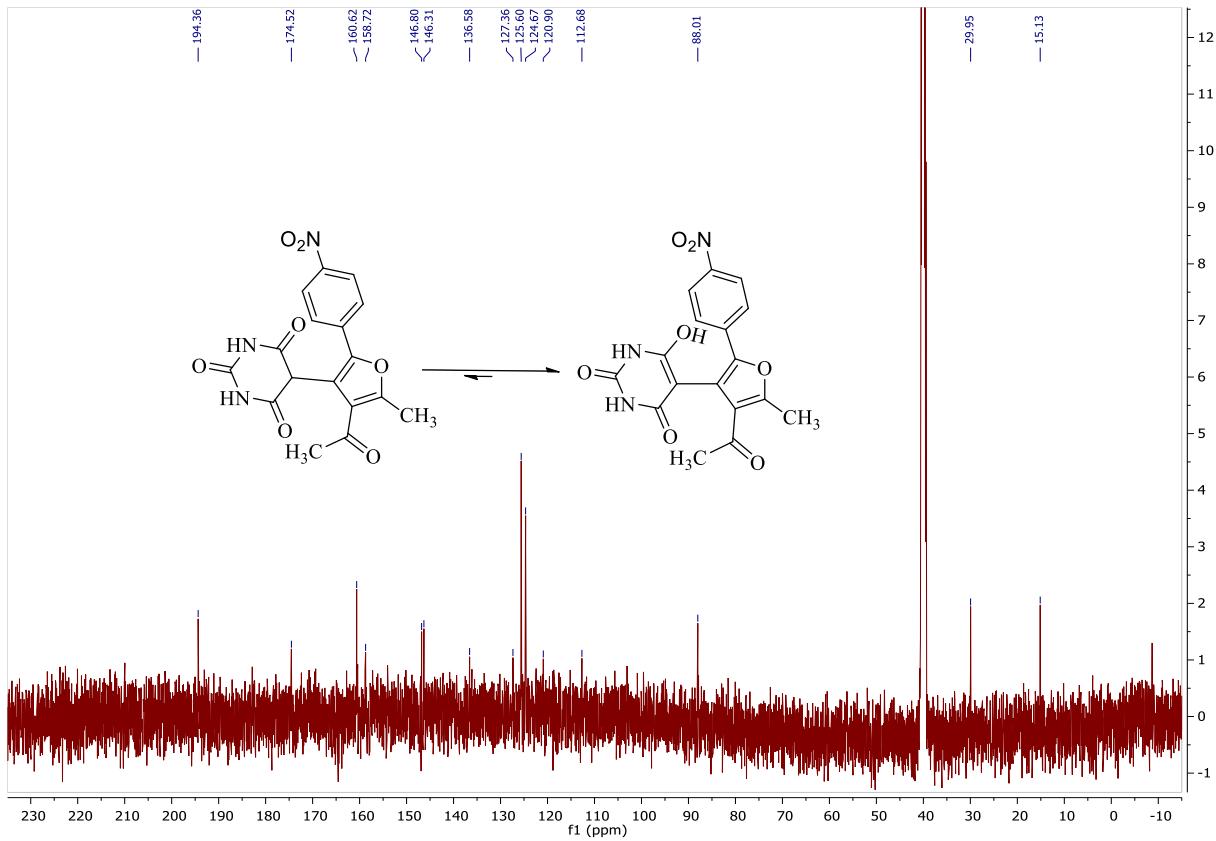


¹H NMR Spectrum (500 MHz, d₆-DMSO) of compound 4j

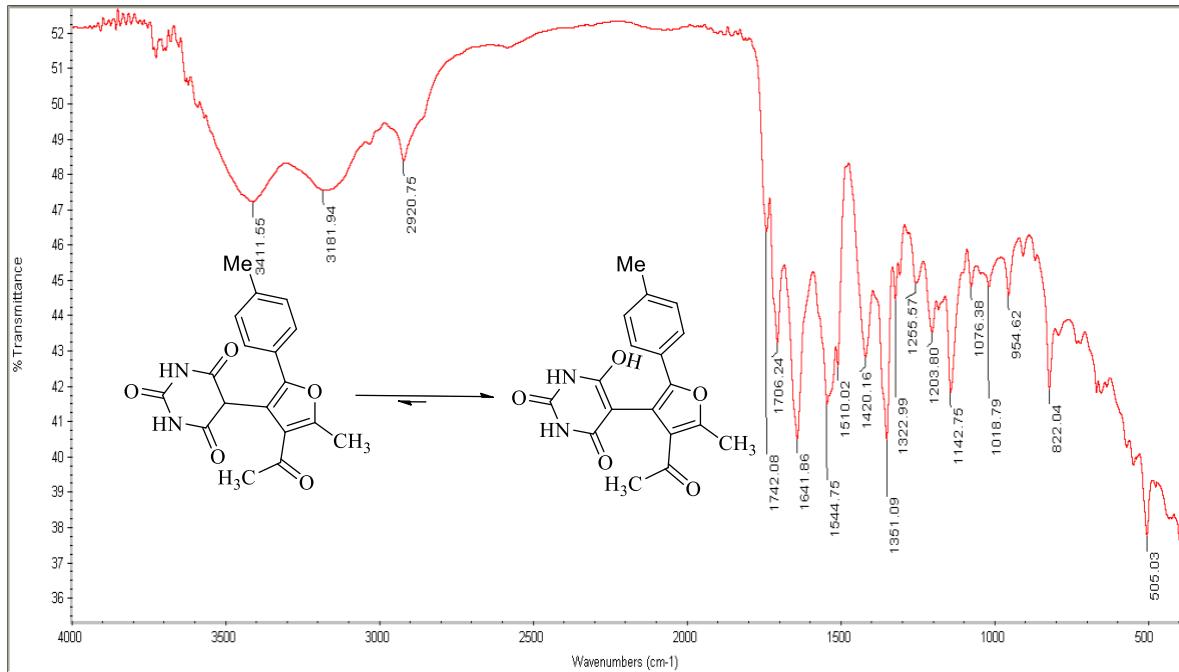


¹³C NMR (125 MHz, d₆-DMSO) spectrum of compound 4j

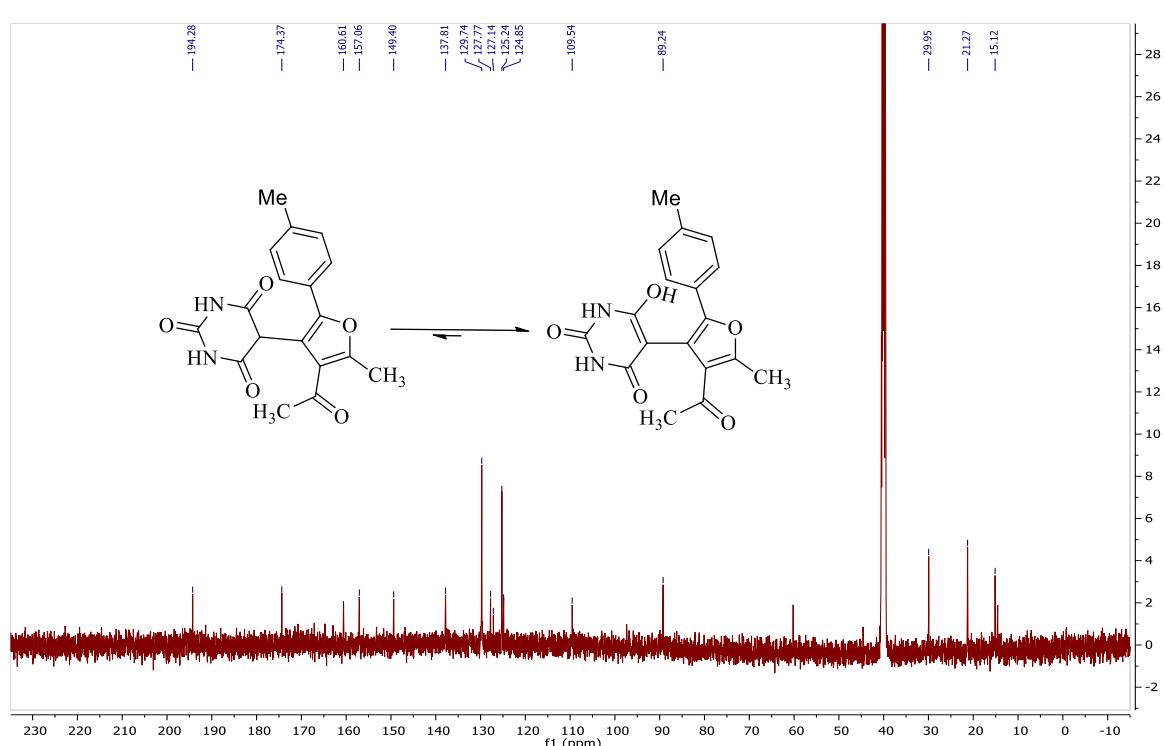
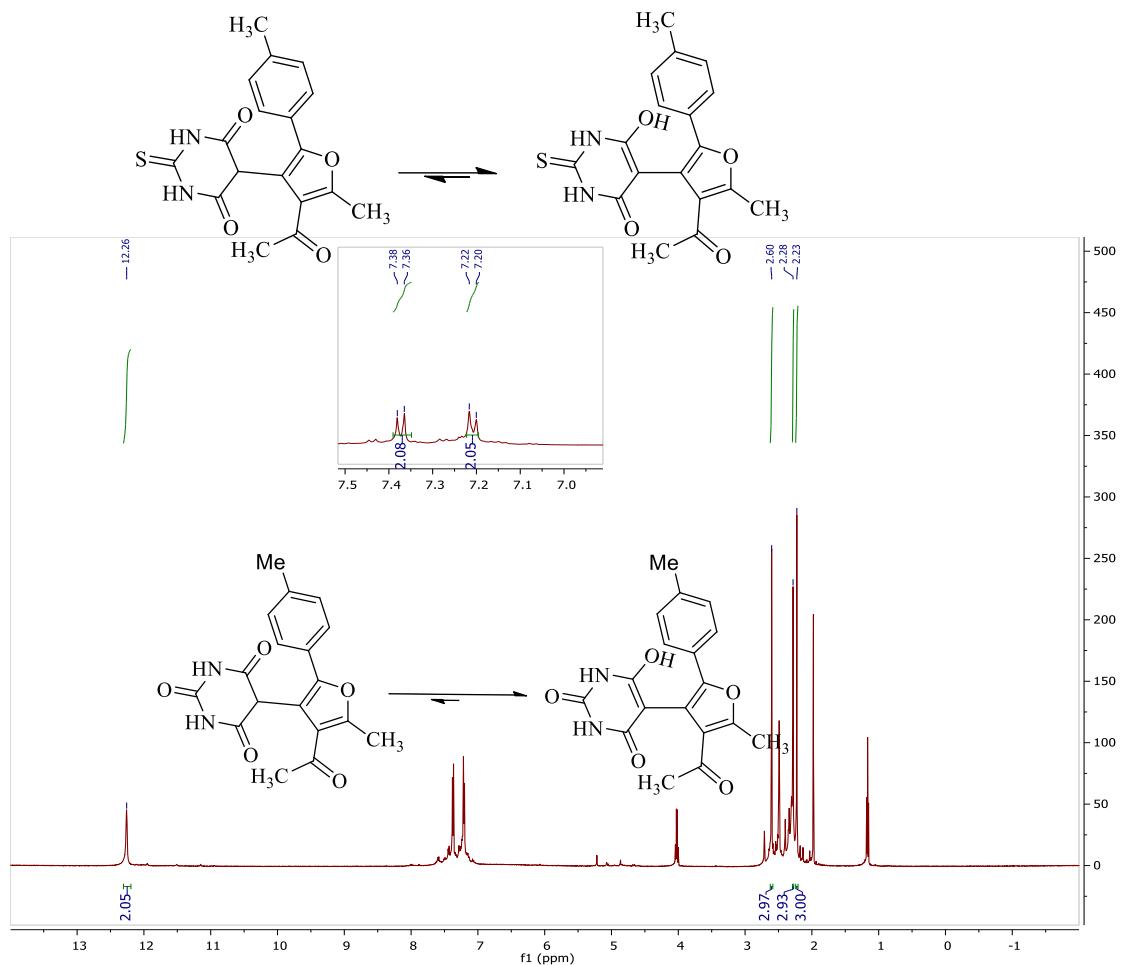
IR Spectrum (IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$) of compound **4k**¹H NMR Spectrum (500 MHz, d₆-DMSO) of compound **4k**



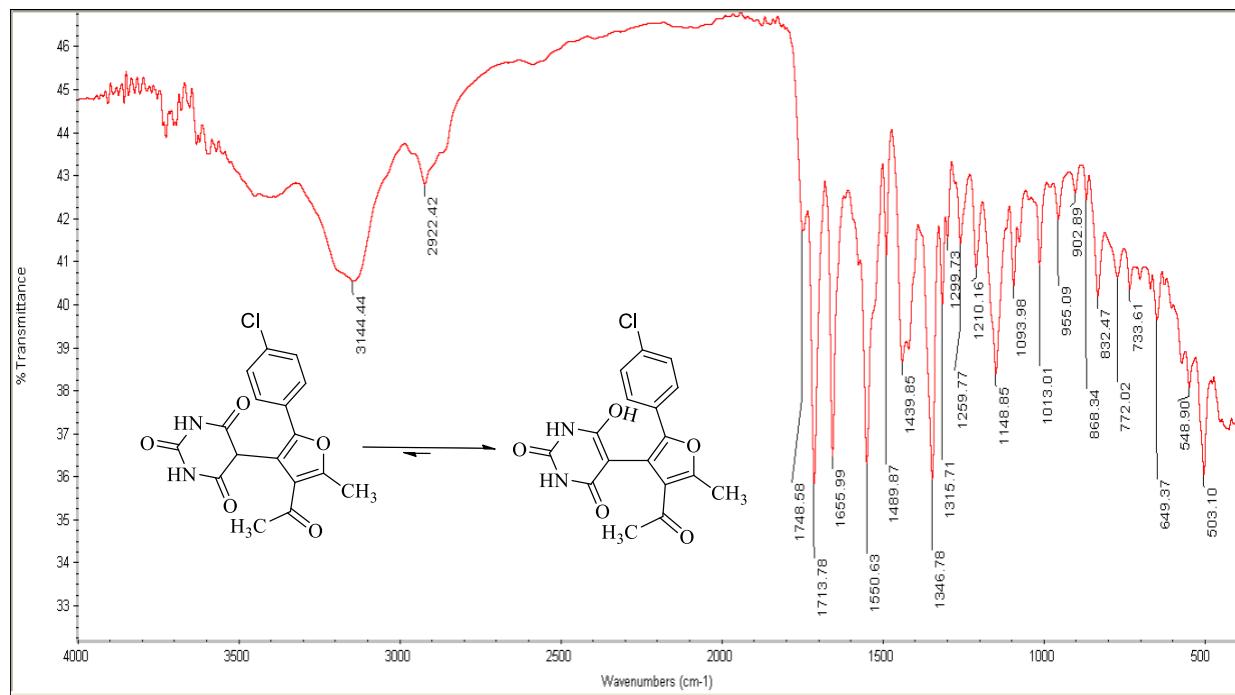
^{13}C NMR (125 MHz, d6-DMSO) spectrum of compound **4k**



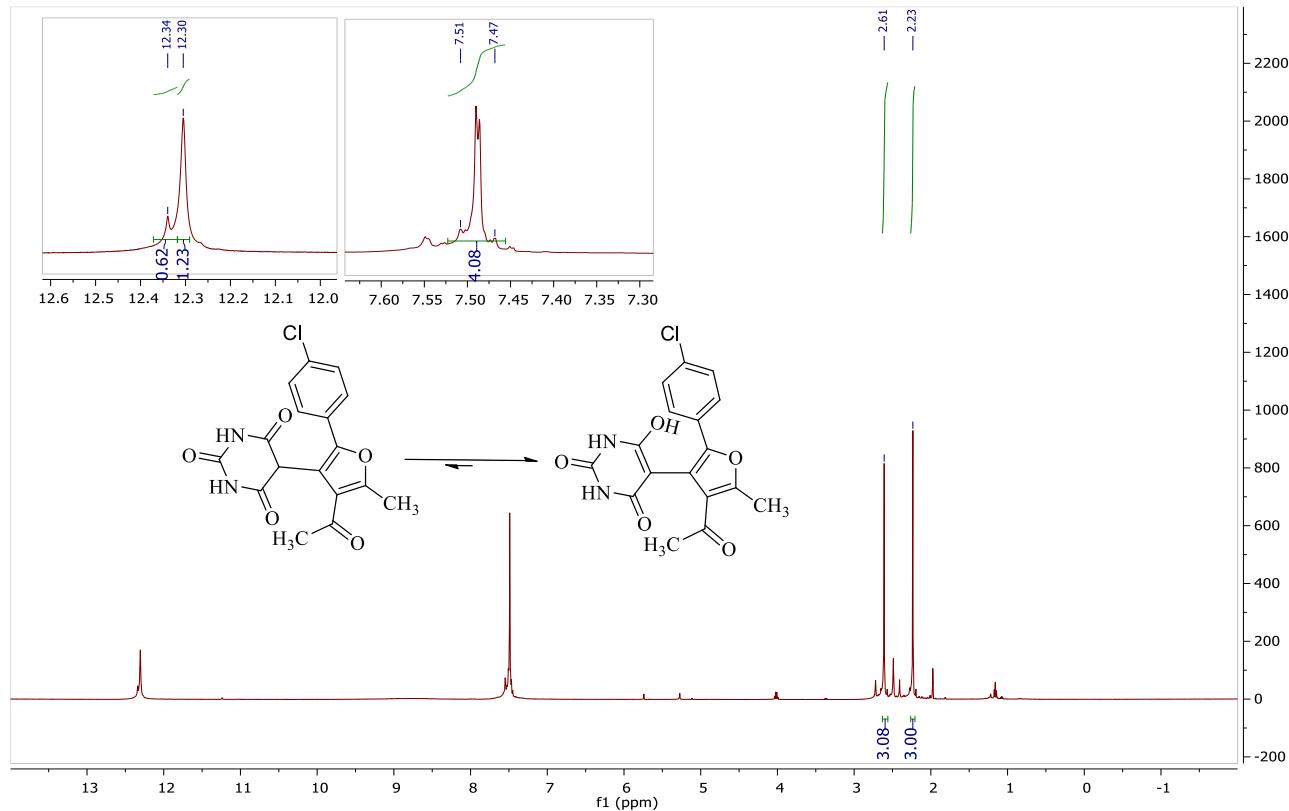
IR Spectrum (IR (KBr) ν_{max} /cm⁻¹) of compound **4l**

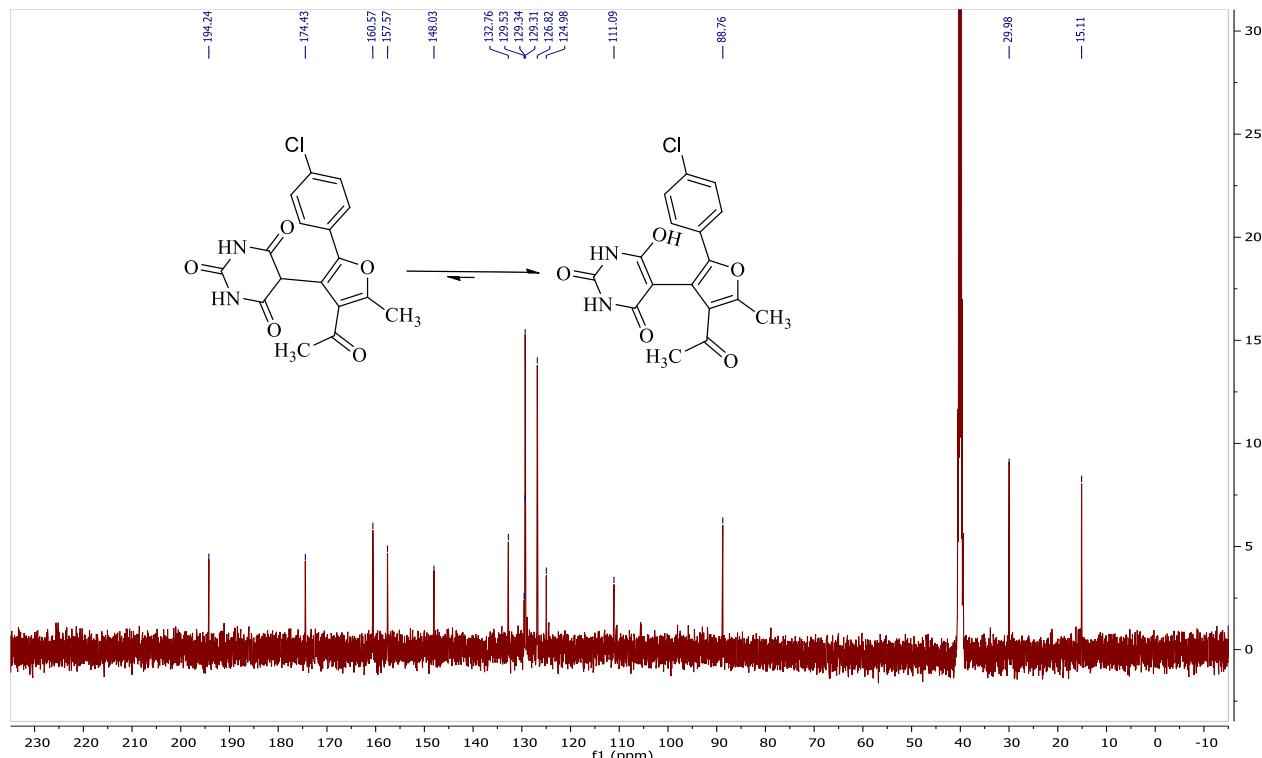


^{13}C NMR (125 MHz, d6-DMSO) spectrum of compound **4l**



IR Spectrum (IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$) of compound **4m**



¹H NMR Spectrum (500 MHz, d₆-DMSO) of compound **4m**¹³C NMR (125 MHz, d₆-DMSO) spectrum of compound **4m**