Zip file contains all images, shapes, figures, illustrations, images, photography

Table 1. groups (X) attached to benzaldehyde

4 & 2:	a	b	c	d	e	f	g	h	i	j	k	l
X:	H	2-Cl	4-Cl	2-NO_2	3-NO_2	4-NO_2	2-OH	3-OH	4-OH	3-OCH_3	4-OCH_3	4-CH_3

Table 2. Structure of compounds

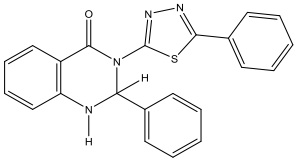
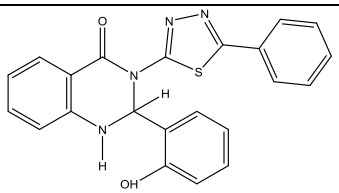
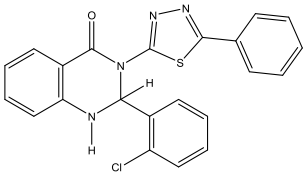
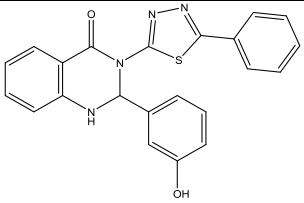
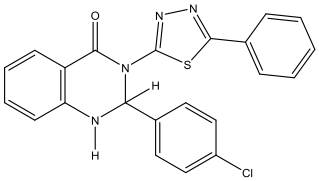
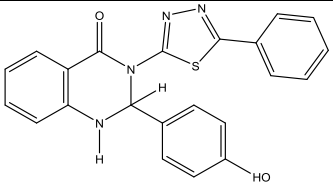
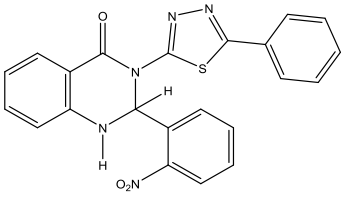
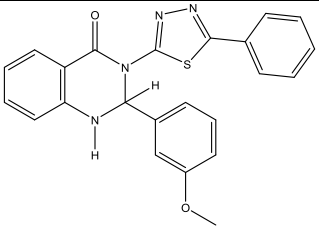
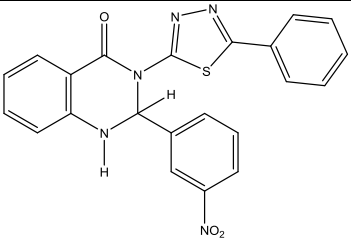
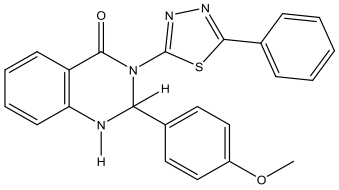
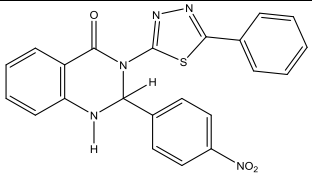
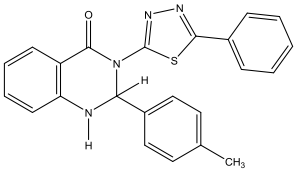
4a		**4g**	
4b		**4h**	
4c		**4i**	
4d		**4j**	
4e		**4k**	
4f		**4l**	

Table 3. Antibacterial activity of compounds 4(a-l)

Concentration of compounds: 1mg/ml

Inhibition Zone (IZ): mm

Minimum Inhibitory Concentration (MIC): 0-1000µg/ml

Minimum Bactericidal Concentration (MBC): 0-1000µg/ml

±: average three times

Cip: Ciprofloxacin

Well diameter: 9mm

	Gr+						**Gr-**					
	S. aureus **PTCC1826**			***S. epidermidis*** **PTCC1856**			***E. coli*** **PTCC1789**			***P. aeruginosa*** **PTCC1950**		
compounds	**IZ**	**MIC**	**MBC**	**IZ**	**MIC**	**MBC**	**IZ**	**MIC**	**MBC**	**IZ**	**MIC**	**MBC**
4a	19±0.22	500	1000	21±0.23	500	1000	17±0.33	1000	1000	21±0.02	500	1000
4b	21±0.21	250	500	22±0.26	250	500	19±0.42	1000	1000	21±0.21	500	1000
4c	17±0.96	500	1000	14±0.75	1000	1000	16±0.78	1000	1000	20±0.48	500	1000
4d	14±0.33	1000	1000	15±0.34	1000	1000	12±0.92	1000	1000	16±0.92	1000	1000
4e	16±0.28	500	1000	19±0.67	500	1000	14±0.28	1000	1000	14±0.35	1000	1000
4f	16±0.66	500	1000	17±0.33	500	1000	19±0.34	1000	1000	19±0.46	1000	1000
4g	16±0.66	500	1000	16±0.33	1000	1000	18±0.39	1000	1000	19±0.44	1000	1000
4h	19±0.56	500	1000	22±0.42	250	500	21±0.37	500	1000	25±0.23	500	1000
4i	18±0.41	500	1000	19±0.22	500	1000	22±0.82	500	1000	**26±0.14**	**250**	**500**
4j	24±0.76	250	500	**28±0.31**	**125**	**250**	24±0.47	500	1000	21±0.29	500	1000
4k	**26±0.52**	**250**	**500**	25±0.57	250	500	26±0.33	500	1000	24±0.68	250	500
4l	24±0.19	250	500	27±0.29	125	250	**31±0.96**	**125**	**250**	24±0.16	250	500
Cip	41±0.35	15.62	31.25	46±0.21	7.81	15.625	37±0.33	31.25	62.50	34±0.66	62.50	125

Table 4. Antifungal activity of compounds 4(a-l).

Concentration of compounds: 1mg/ml

Inhibition Zone (IZ): mm

Minimum Inhibitory Concentration (MIC): 0-1000µg/ml

Minimum Fungicidal Concentration (MFC): 0-1000µg/ml

±: average three times

AB: Amphotericin B

NA: No Activity

Well diameter: 9mm

compounds	*C .albicans* PTCC5027			*A .niger* PTCC5320		
	IZ	**MIC**	**MFC**	**IZ**	**MIC**	**MFC**
4a	21±0.33	500	1000	17±0.66	1000	1000
4b	23±0.33	500	1000	20±0.66	500	1000
4c	20±0.33	500	1000	14±0.66	1000	1000
4d	14±0.33	1000	1000	11±0.66	NA	NA
4e	19±0.33	1000	1000	15±0.66	1000	1000
4f	19±0.33	1000	1000	16±0.66	1000	1000
4g	17±0.33	1000	1000	12±0.66	NA	NA
4h	21±0.33	500	1000	19±0.66	1000	1000
4i	20±0.33	500	1000	14±0.66	1000	1000
4j	**26±0.33**	**250**	**500**	20±0.66	500	1000
4k	25±0.33	500	1000	**21±0.66**	**500**	**1000**
4l	21±0.33	500	1000	19±0.66	1000	1000
AB	36±0.33	62.50	125	34±0.66	62.50	125

Table 5- Molecular docking reports for compounds *4(a-l)* against protein 1hny and 2ze0.

compounds	Total Energy (Kcal/mol)	Alpha-amylase PDB ID: 1hny		Alpha-glucosidase PDB ID: 2ze0	
		Affinity (Kcal/mol)	H-Bond	Affinity (Kcal/mol)	H-Bond
4a	11.3828	-9.6	-	-8.9	Arginine: 407
4b	13.3308	-9.1	-	-9.4	Arginine: 407
4c	11.6324	**-10.0**	**Glutamic acid: 233**	-9.2	Valine: 383
4d	-12.5194	**-10.0**	**Aspartic acid: 197** **Glutamic acid: 233** **Histidine: 299**	-9.1	Arginine: 407
4e	-2.1596	-9.1	-	**-10.6**	**Arginine: 407** **Glutamine: 167**
4f	7.2655	-8.7	-	**-9.5**	**Arginine: 197** **Asparagine: 324**
4g	7.8283	**-10.0**	**Glutamic acid: 233** **Aspartic acid: 300**	-9.0	Arginine: 407
4h	9.9999	-9.1	-	-9.0	Arginine: 407
4i	10.1567	-9.5	-	**-10.1**	**Arginine: 407** **Glutamine: 167**
4j	16.9915	-9.1	-	-9.1	Arginine: 407
4k	17.1349	-9.5	-	-9.0	-
4l	11.1987	-9.8	-	-9.3	-

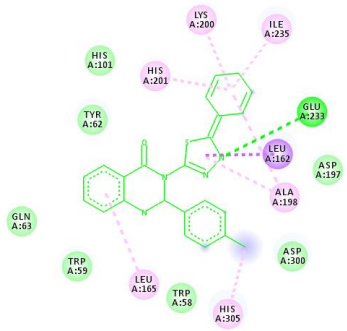
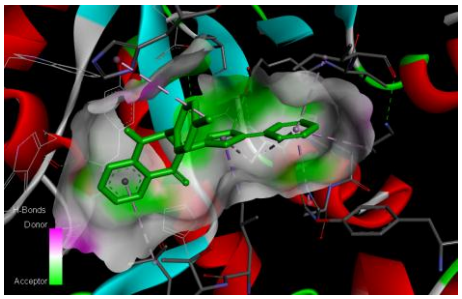
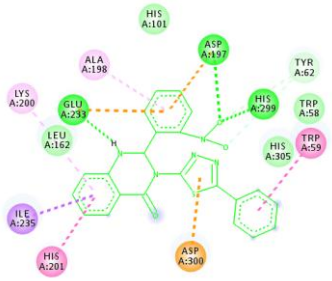
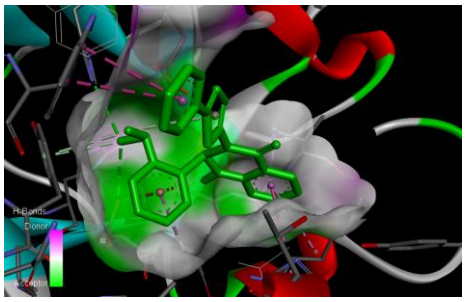
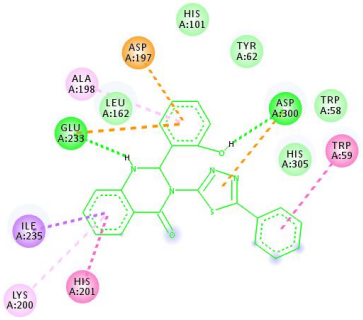
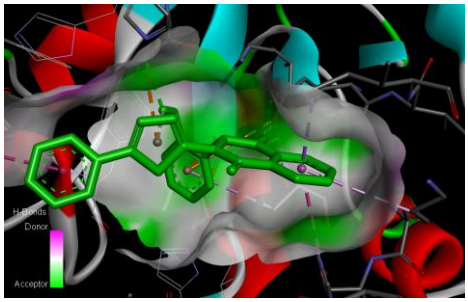
compounds	Alpha-amylase, PDB ID: 1hny	
	2D	3D
4c		
4d		
4g		

Fig 1. Ligand–Protein 2D and 3D interaction on the active site of 1hny.

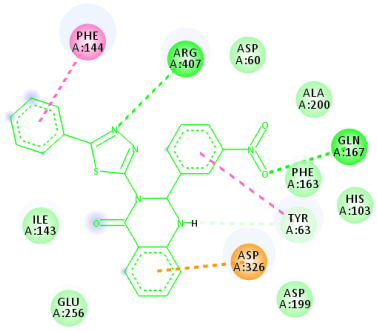
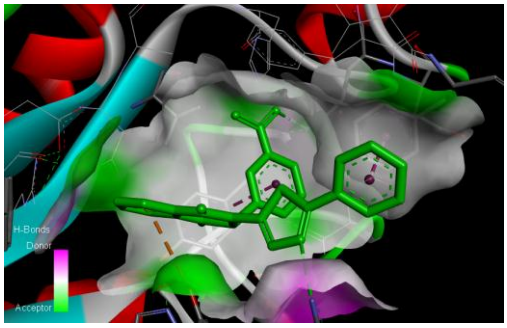
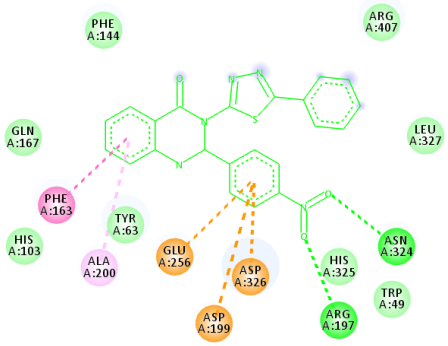
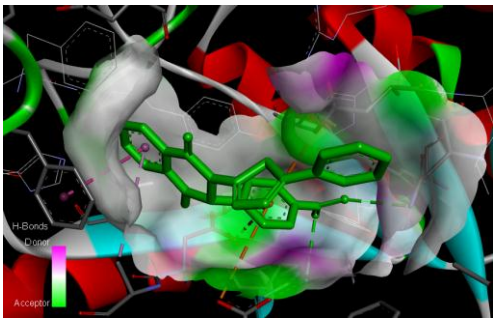
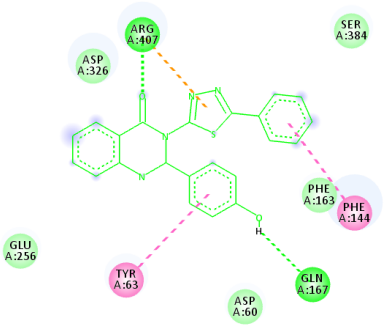
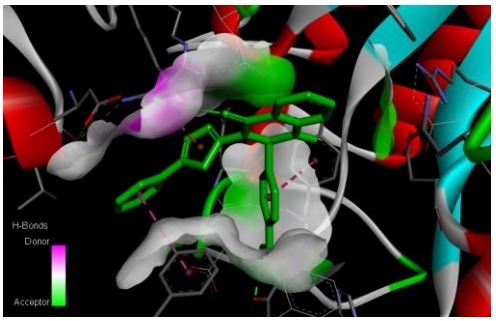
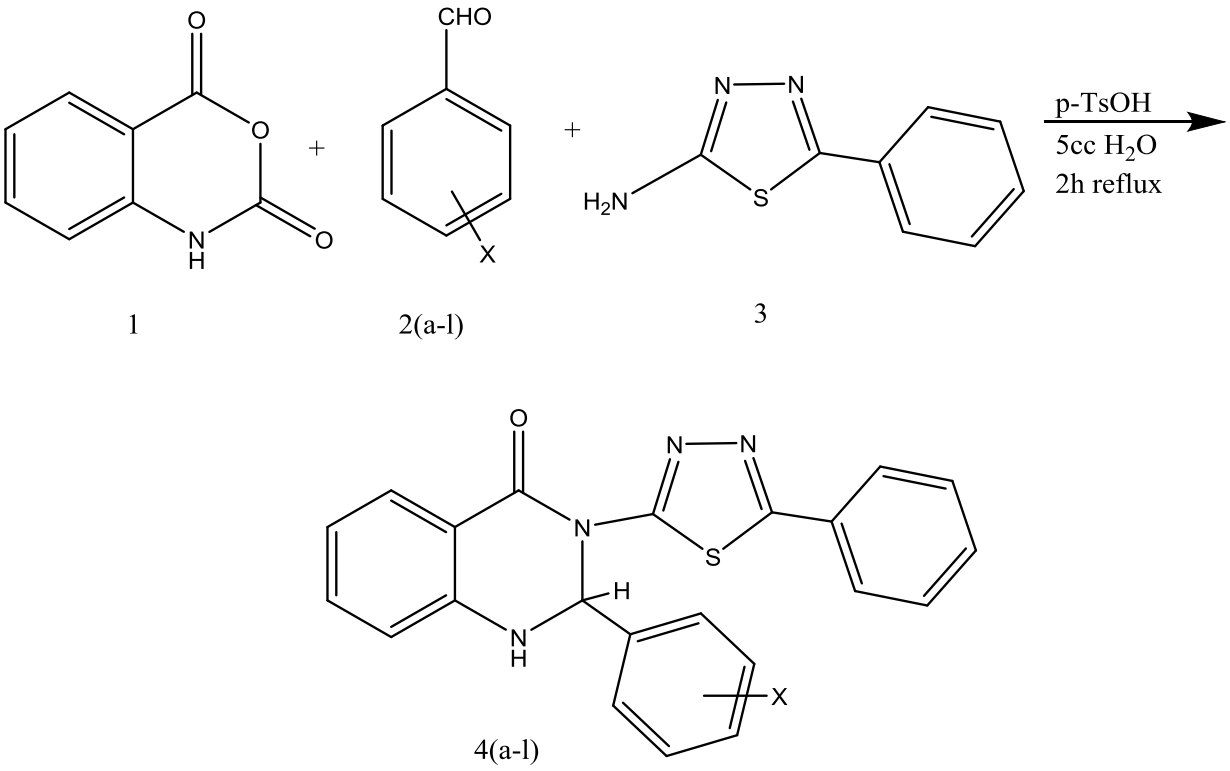
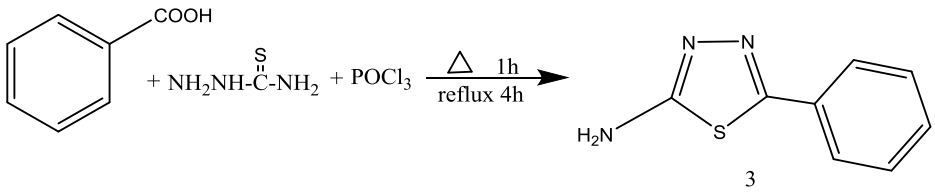
compounds	Alpha-glucosidase, PDB ID: 2ze0	
	2D	3D
4e		
4f		
4i		

Fig 2. Ligand–Protein 2D and 3D interaction on the active site of 2ze0.



X : H, 4-NO_2 , 3-NO_2 , 2-NO_2 , 4-OH, 3-OH, 2-OH , 4-Cl , 2-Cl , 4-OCH_3 , 3-OCH_3 , 4-CH_3

Scheme 1. Synthesis of 2-substituted-2,3-dihydroquinazolin-4(1H)-one derivatives



3

Scheme 2. Synthesis of 5-phenyl-1,3,4-thiadiazol-2-amine

Product representation spectra (^{1}Hnmr, ^{13}Cnmr, IR, mass Respectively)

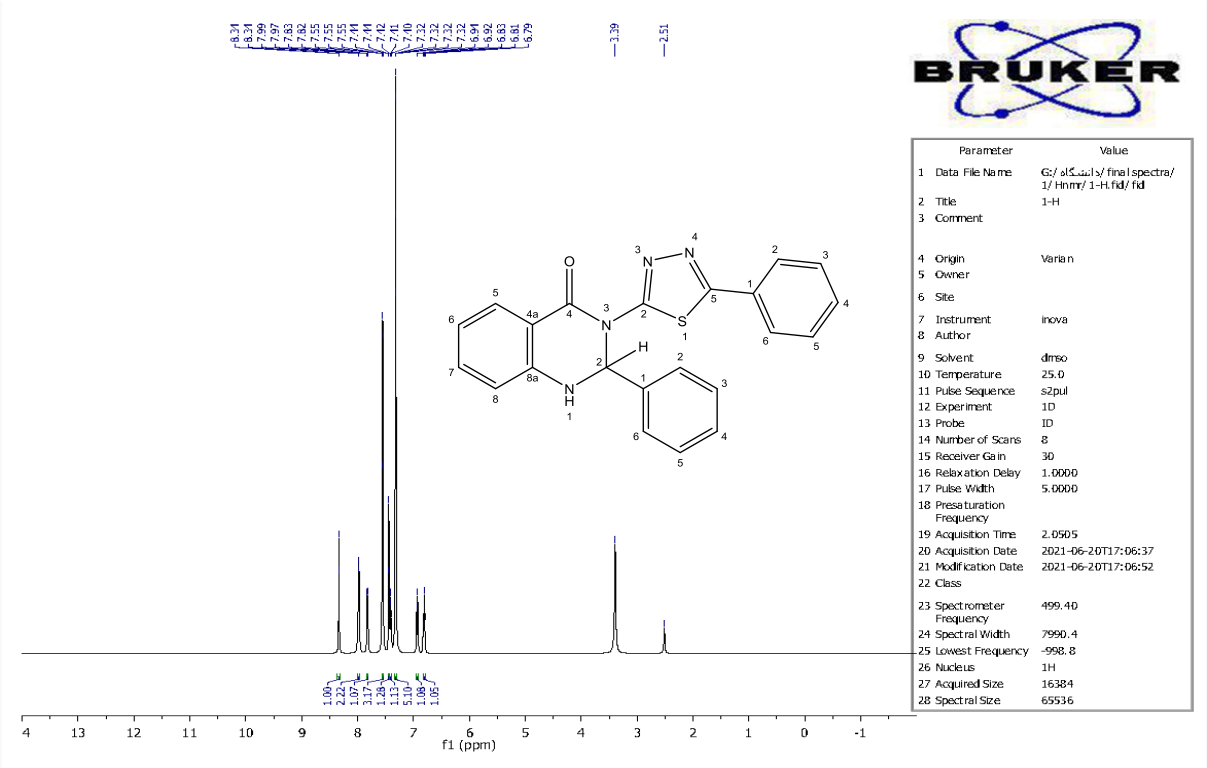


Fig 3. The whole range ^{1}H NMR spectrum of compound (4a)

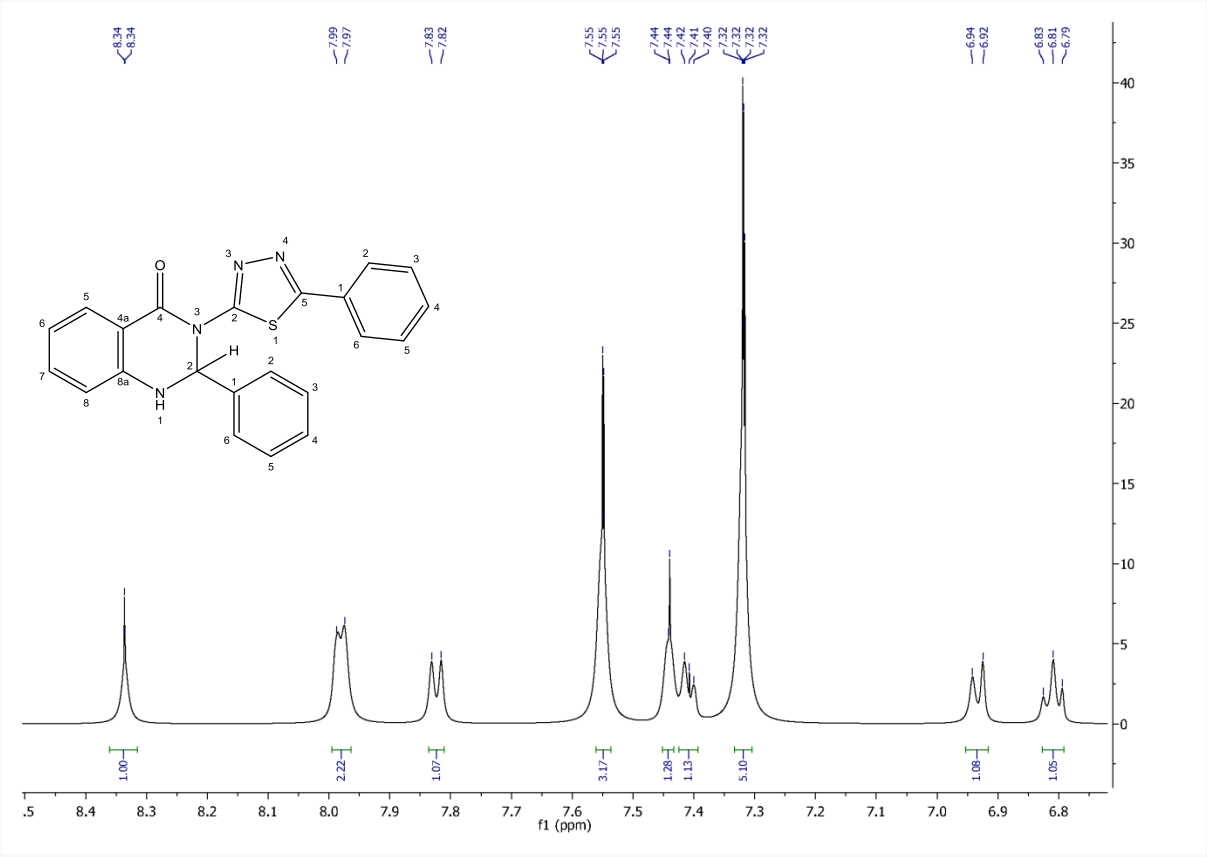


Fig 4. Aromatic range ^{1}H NMR spectrum of compound (4a)

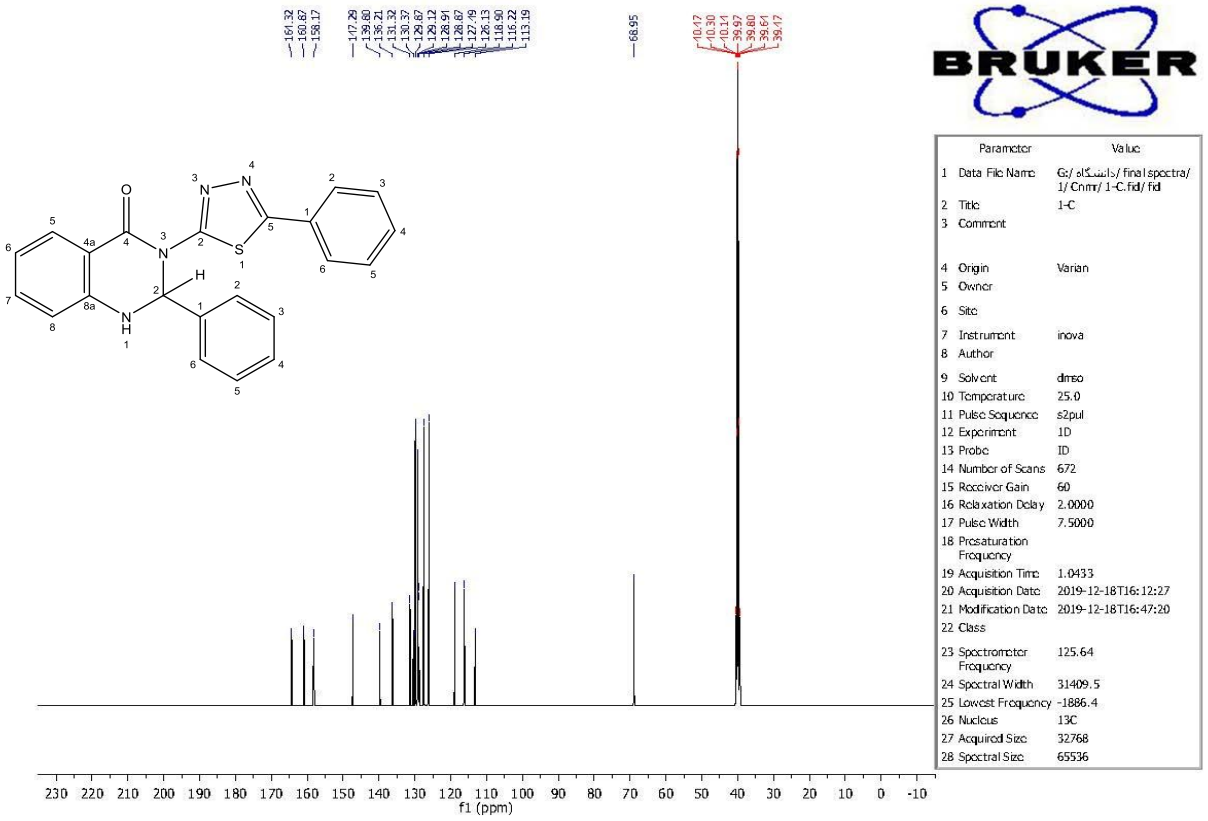


Fig 5. The whole range ^{13}C NMR spectrum of compound (4a)

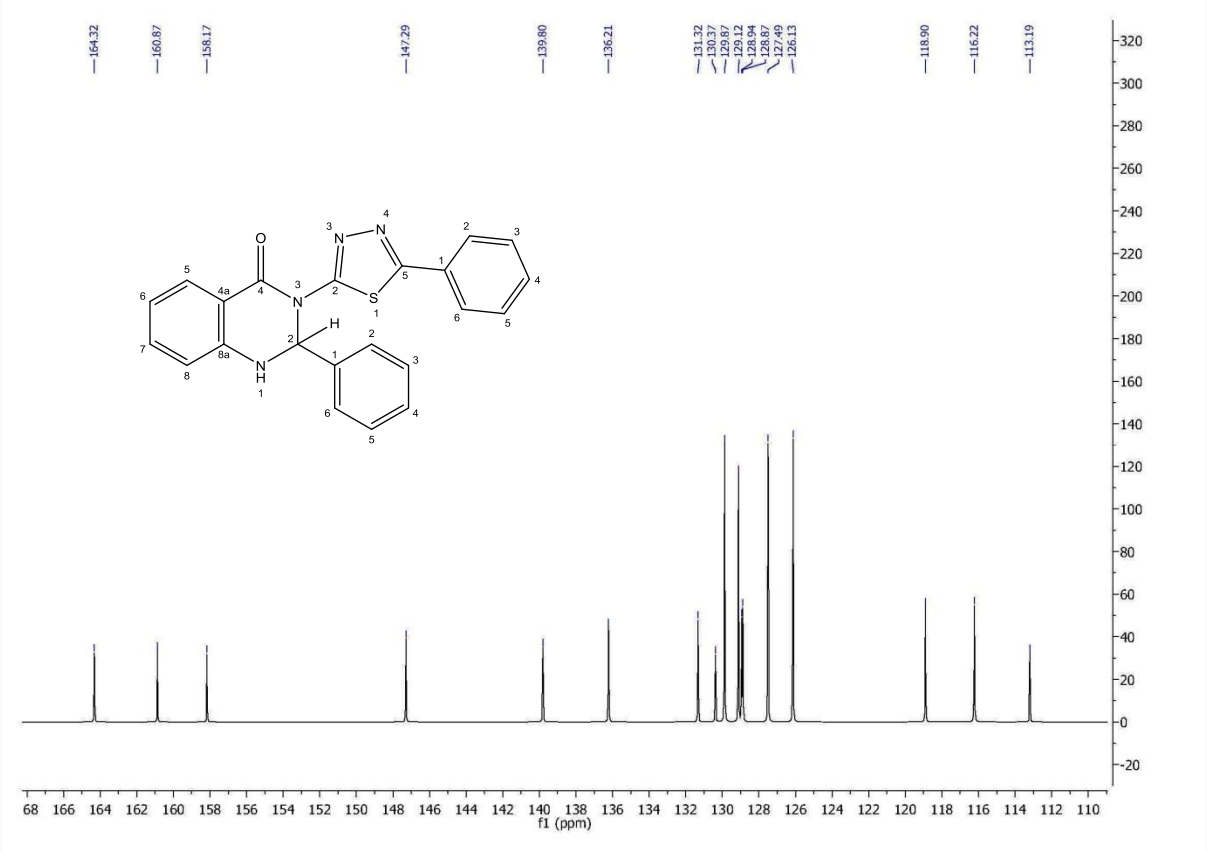


Fig 6. Doubl bond range ^{13}C NMR spectrum of compound (4a)

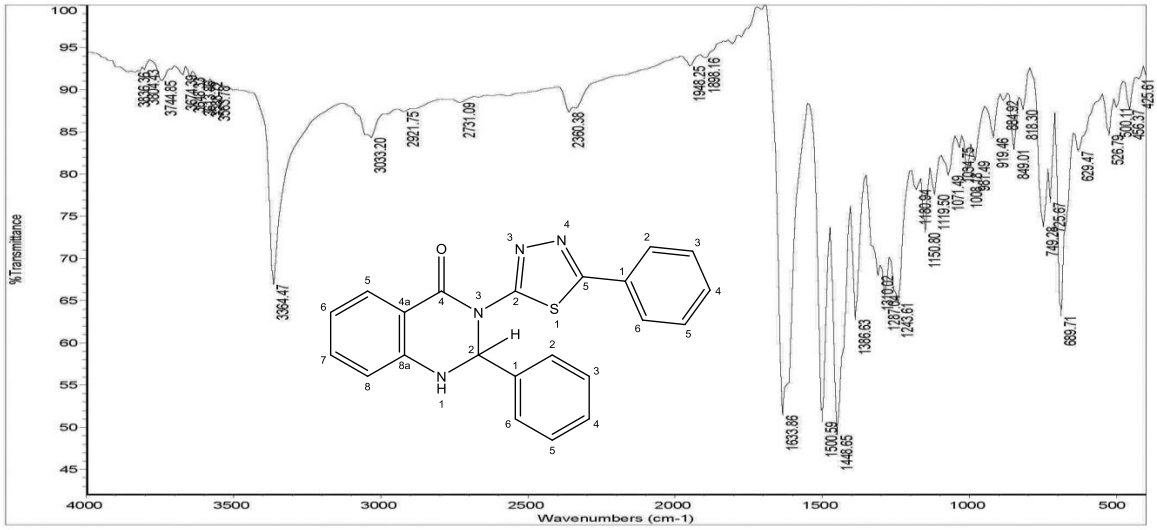


Fig 7. IR spectrum of compound (4a)

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Sample Name: 21
Misc Info :
Vial Number: 1

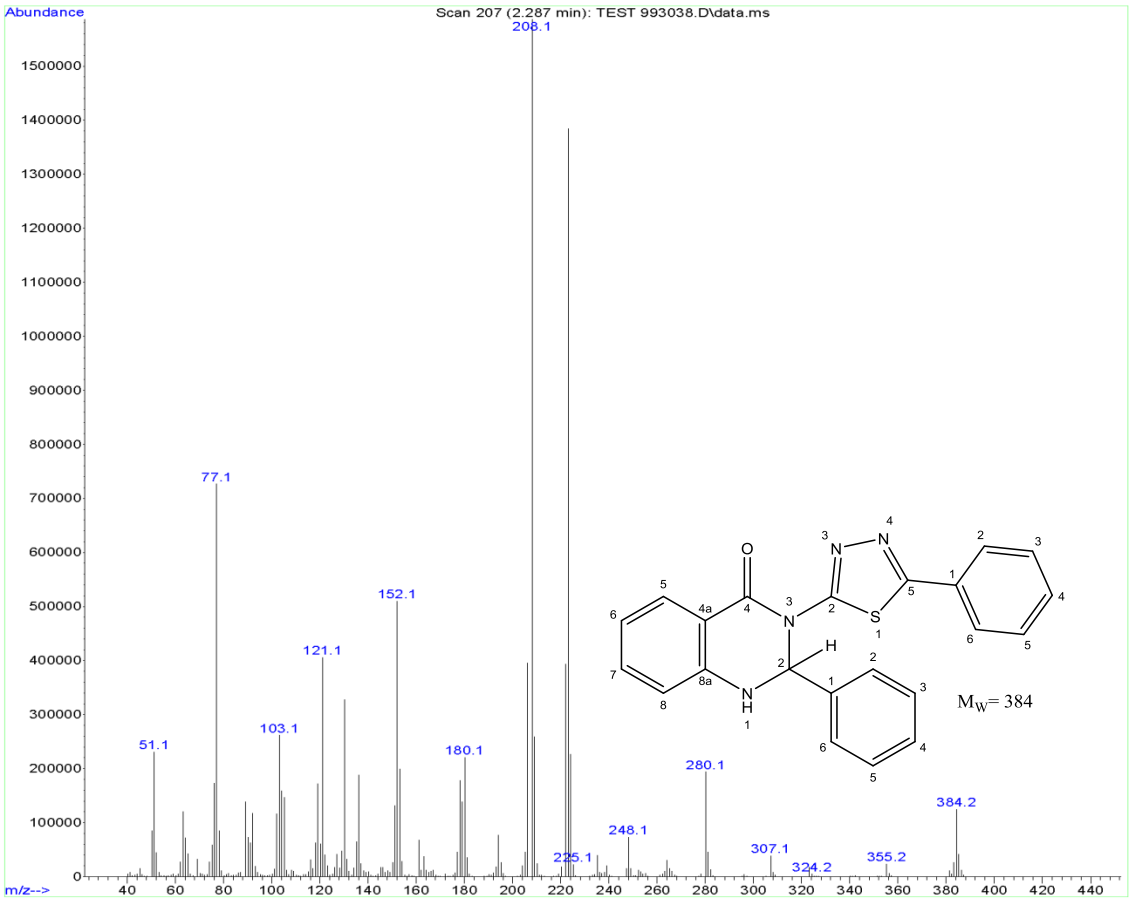

Fig 8. Mass spectrum of compound (4a)

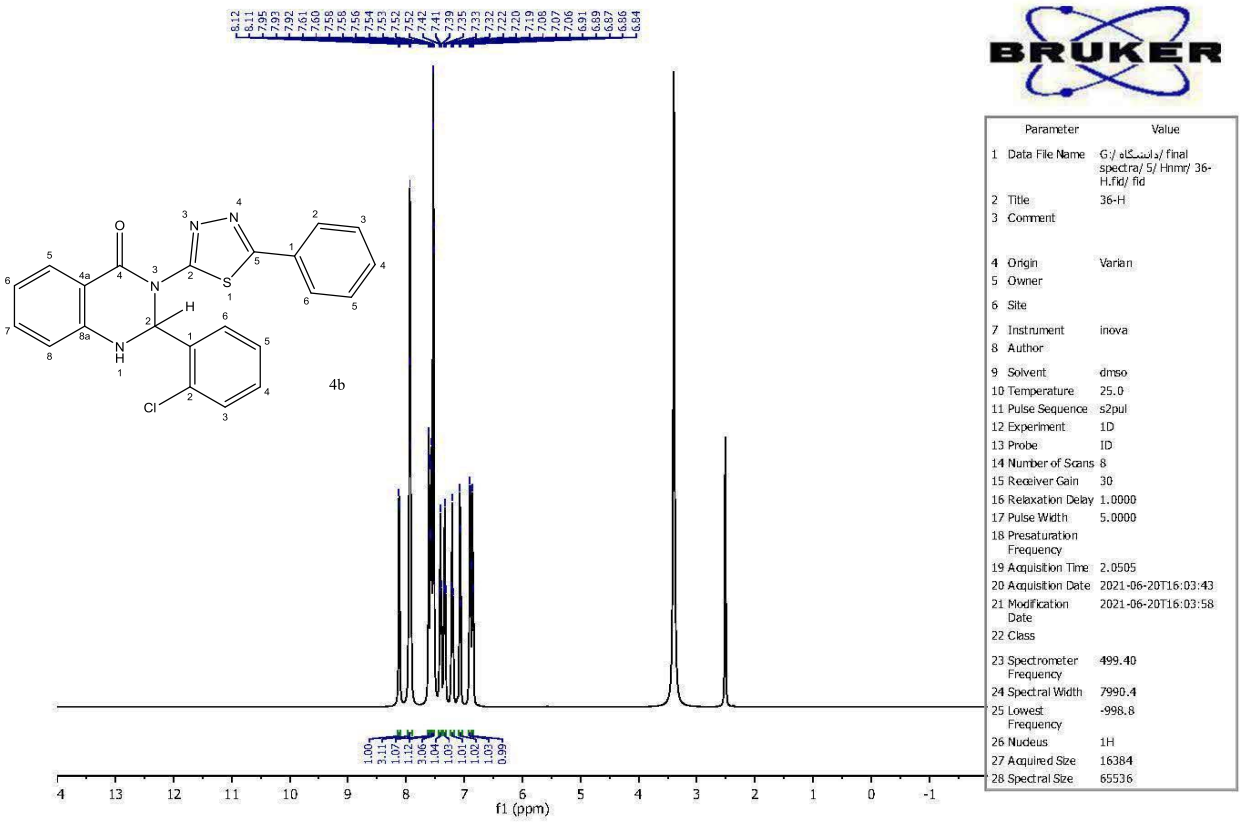

Fig 9. The whole range ^{1}H NMR spectrum of compound (4b)

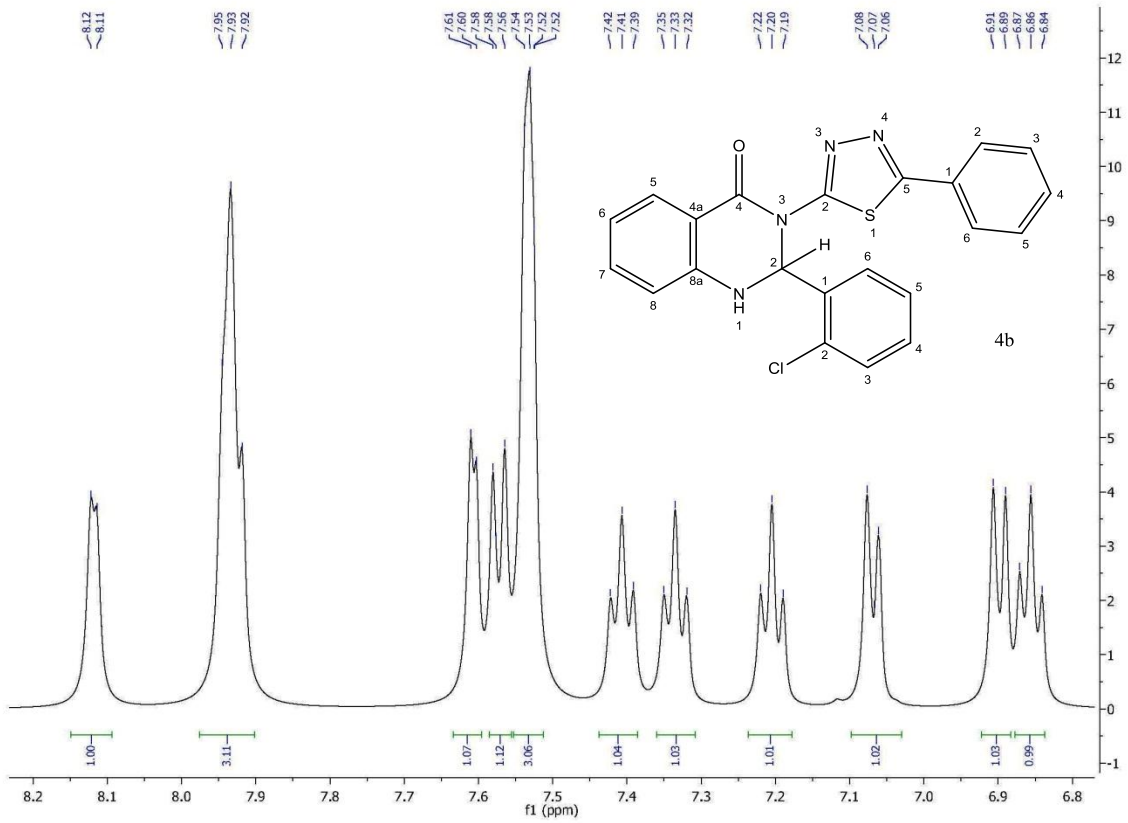

Fig 10. Aromatic range ^{1}H NMR spectrum of compound (4b)

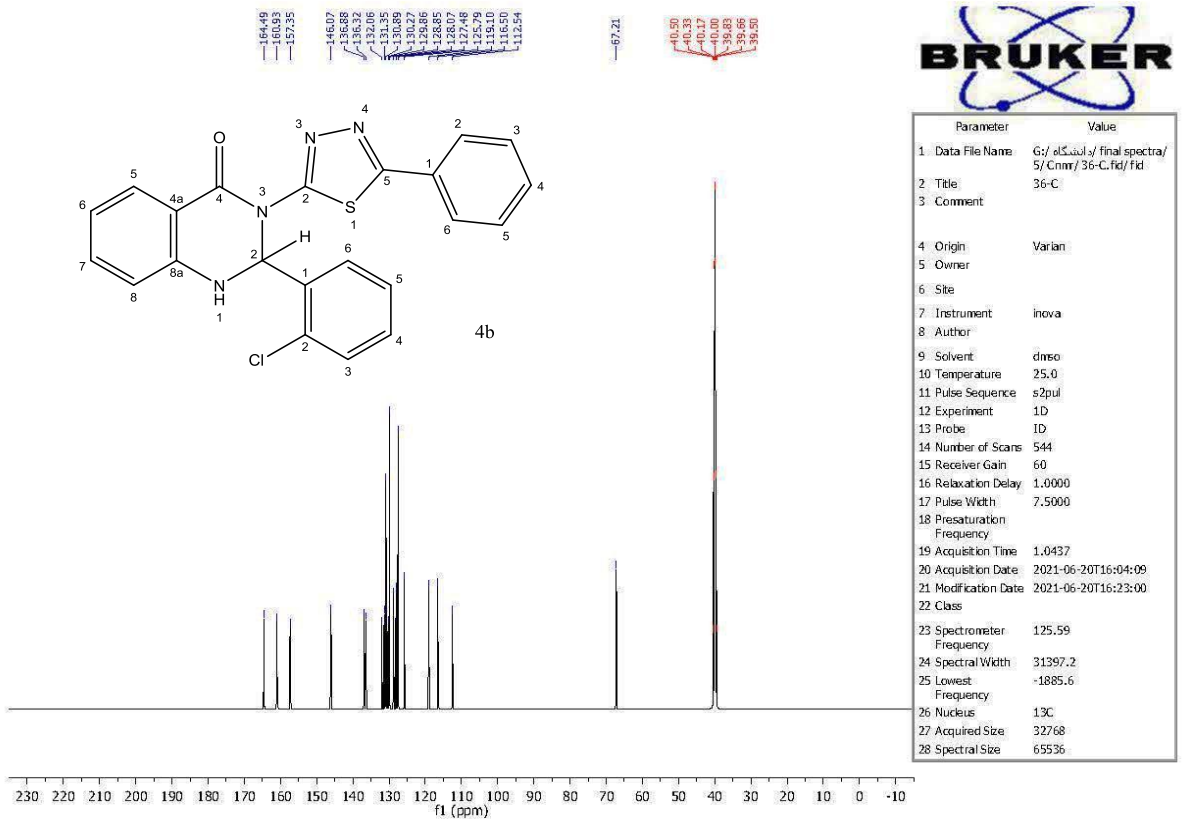

Fig 11. The whole range ^{13}C NMR spectrum of compound (4b)

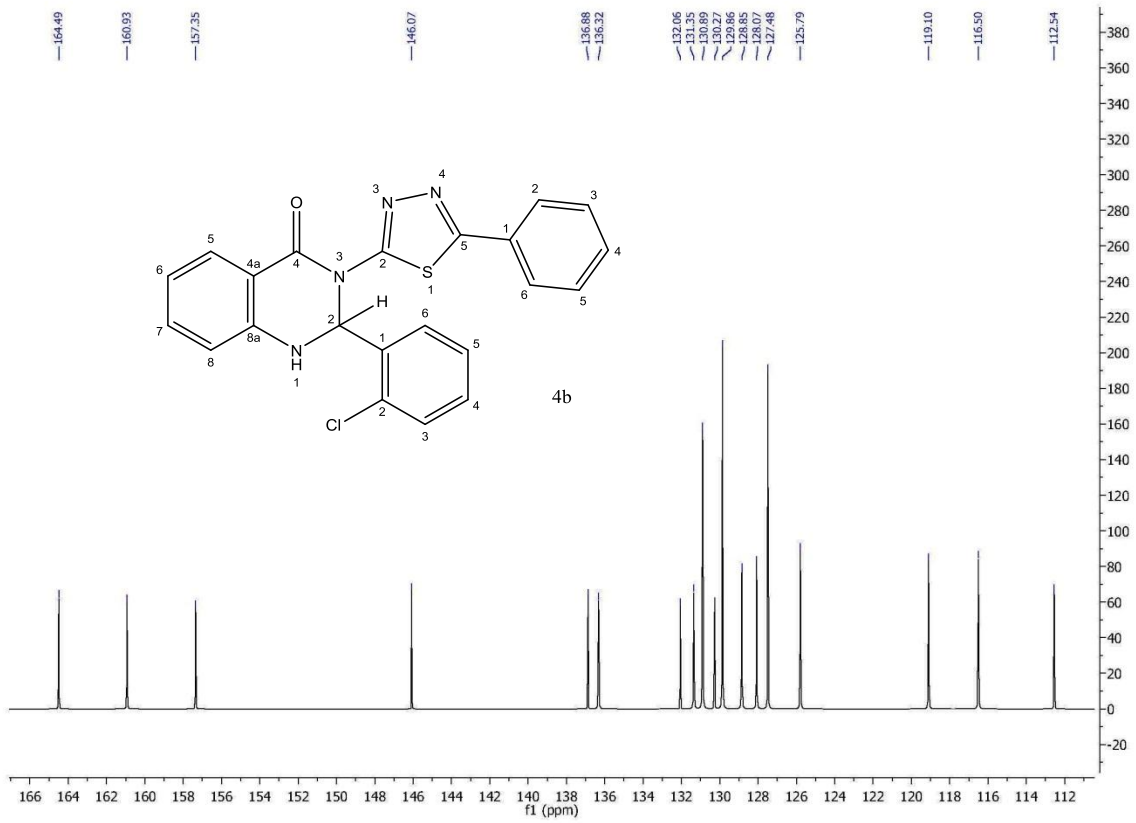

Fig 12. Doubl bond range ^{13}C NMR spectrum of compound (4b)

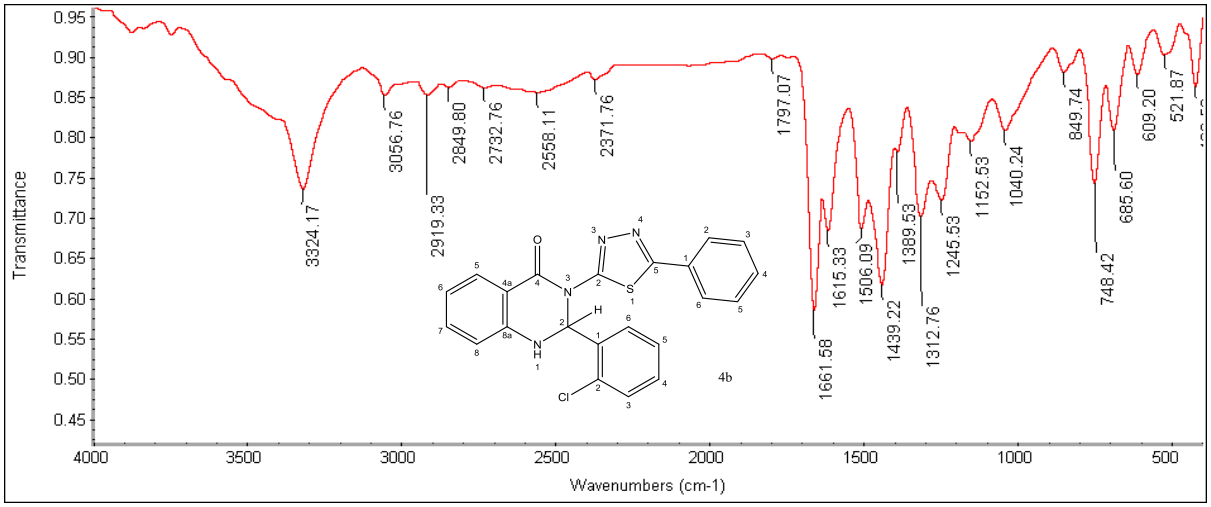

Fig 13. IR spectrum of compound (4b)

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Acquired : 4 Jun 2021 12:13 using AcqMethod test.M
Instrument : MSD
Sample Name: 36
Misc Info :
Vial Number: 1

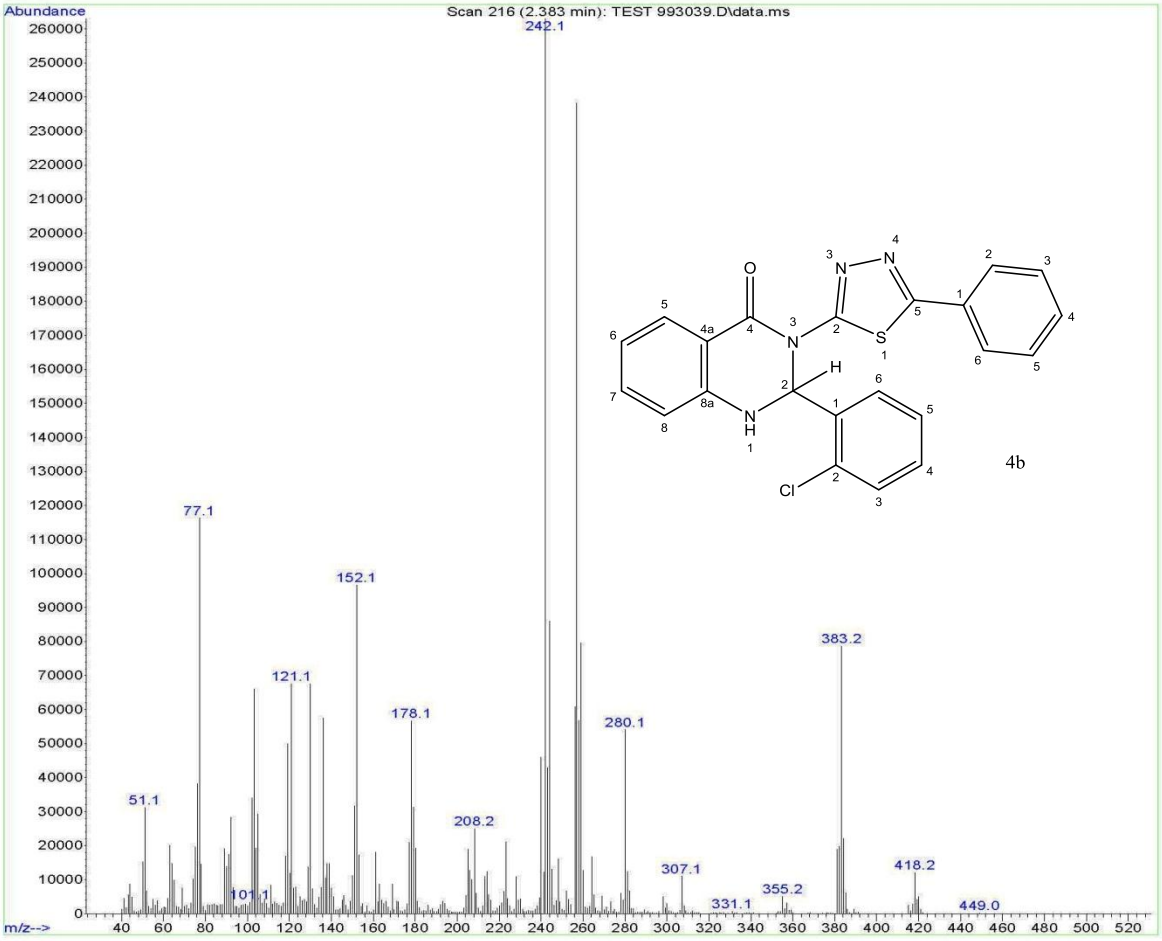
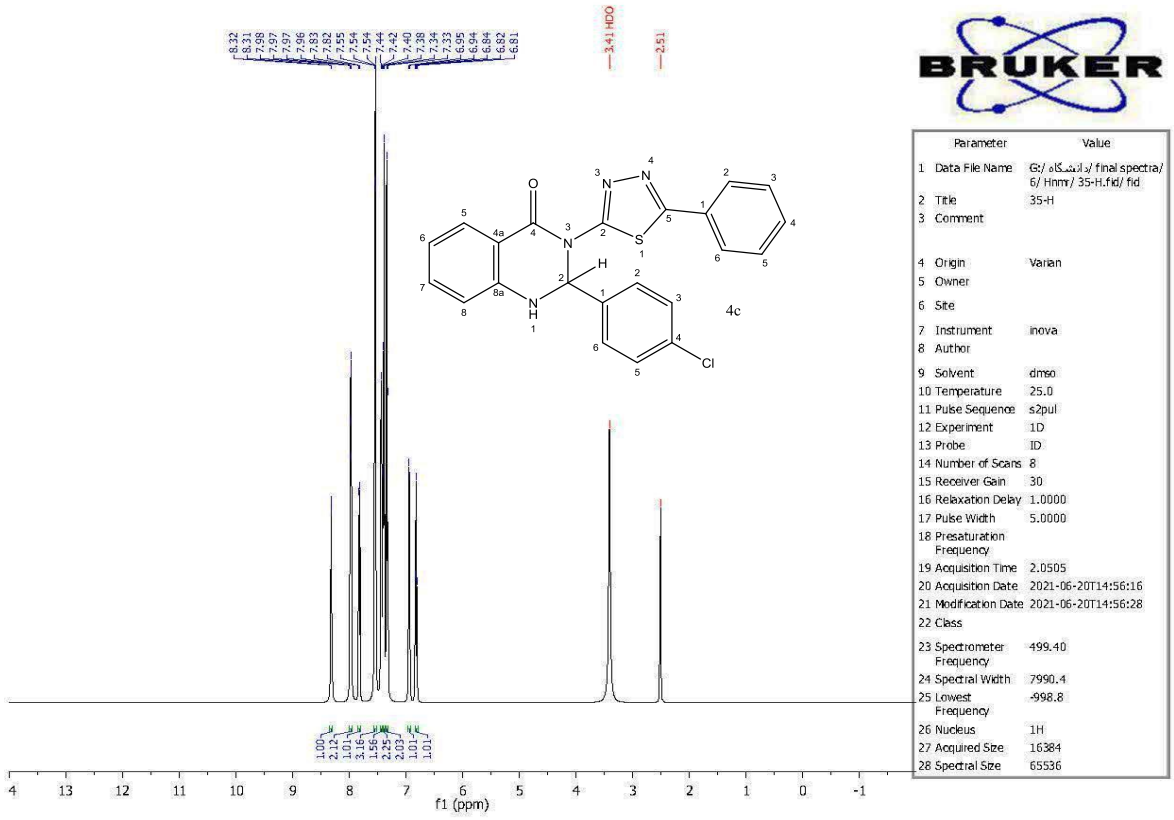


Fig 14. Mass spectrum of compound (4b)



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3	Comment	
4	Origin	Varian
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6	Site	
7	Instrument	inova
8	Author	
9	Solvent	dmso
10	Temperature	25.0
11	Pulse Sequence	s2pul
12	Experiment	1D
13	Probe	ID
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21	Modification Date	2021-06-20T14:56:28
22	Class	
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25	Lowest Frequency	-998.8
26	Nucleus	1H
27	Acquired Size	16384
28	Spectral Size	65536

Fig 15. The whole range ^{1}H NMR spectrum of compound (4c)

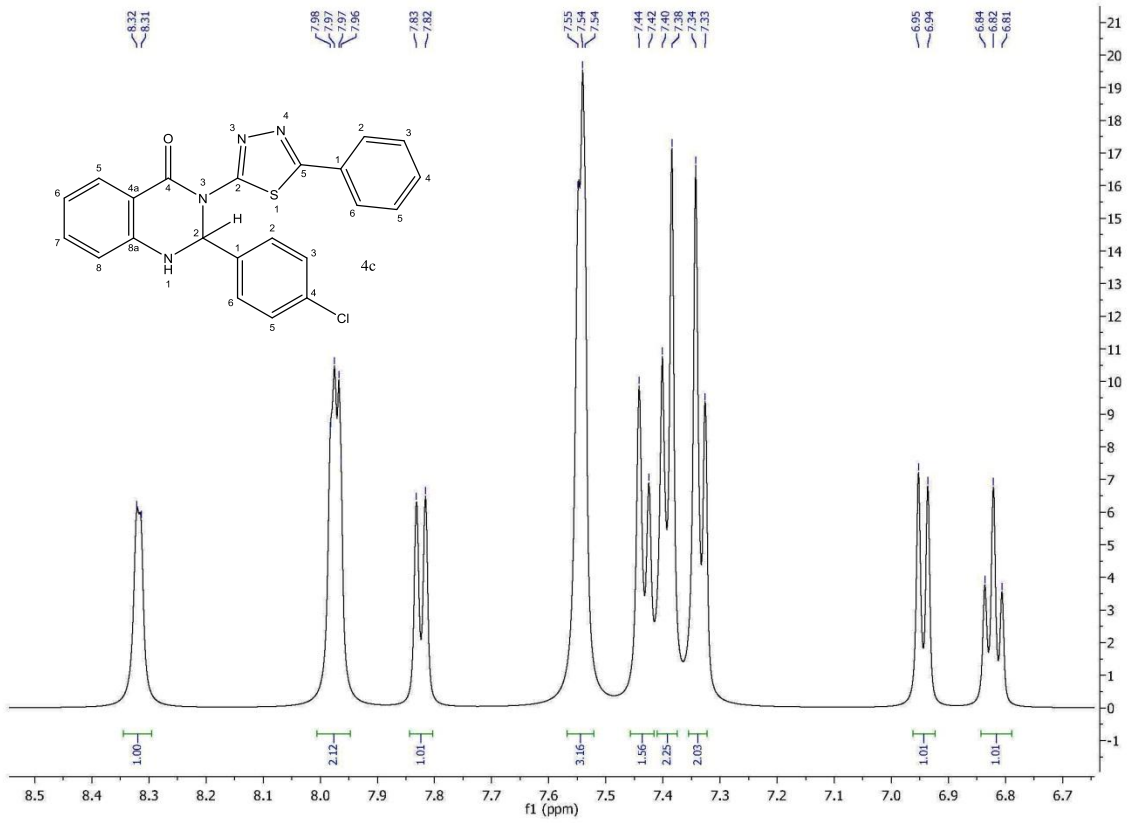

Fig 16. Aromatic range ^{1}H NMR spectrum of compound (4c)

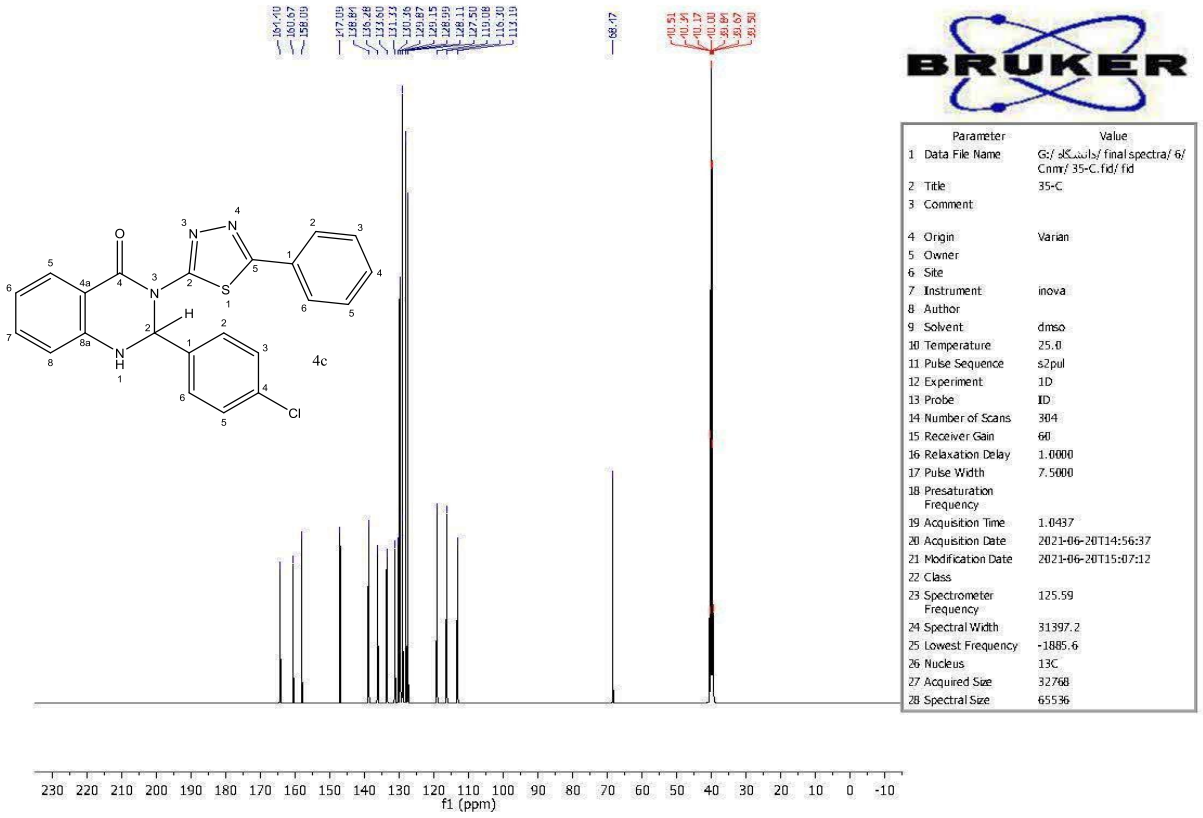

Fig 17. The whole range ^{13}C NMR spectrum of compound (4c)

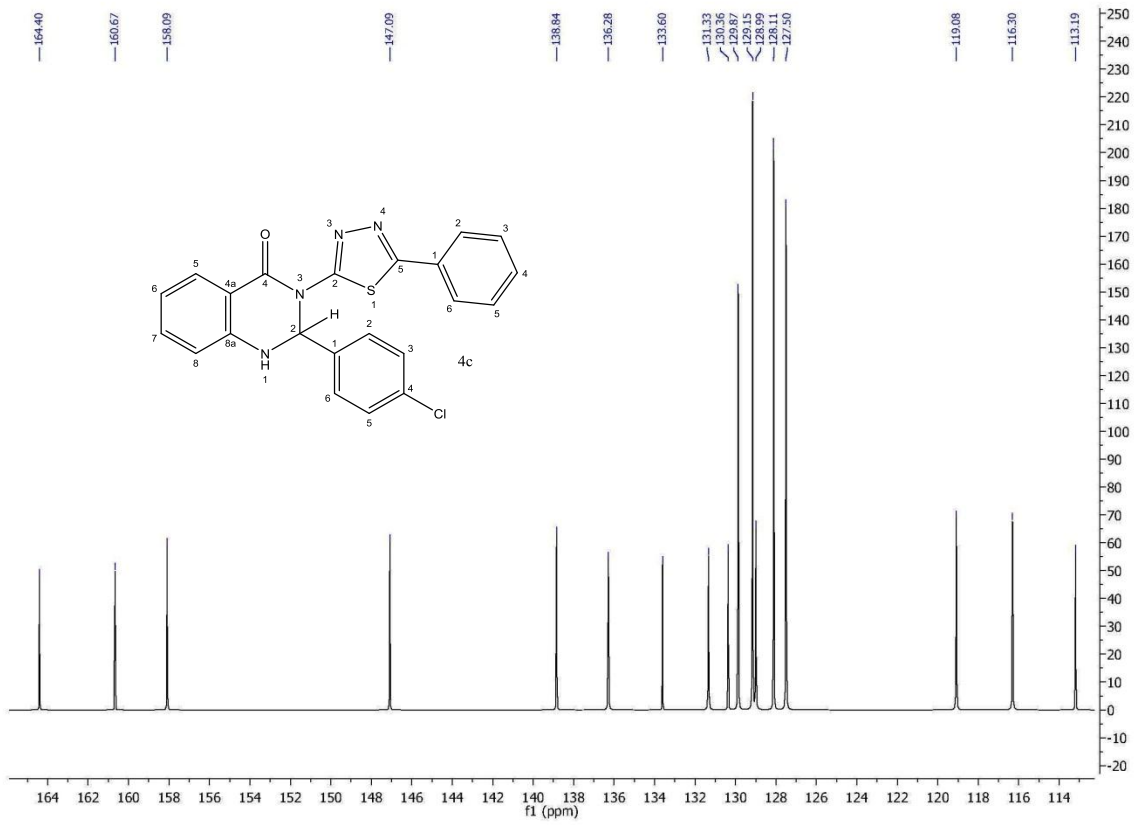

Fig 18. Doubl bond range ^{13}C NMR spectrum of compound (4c)

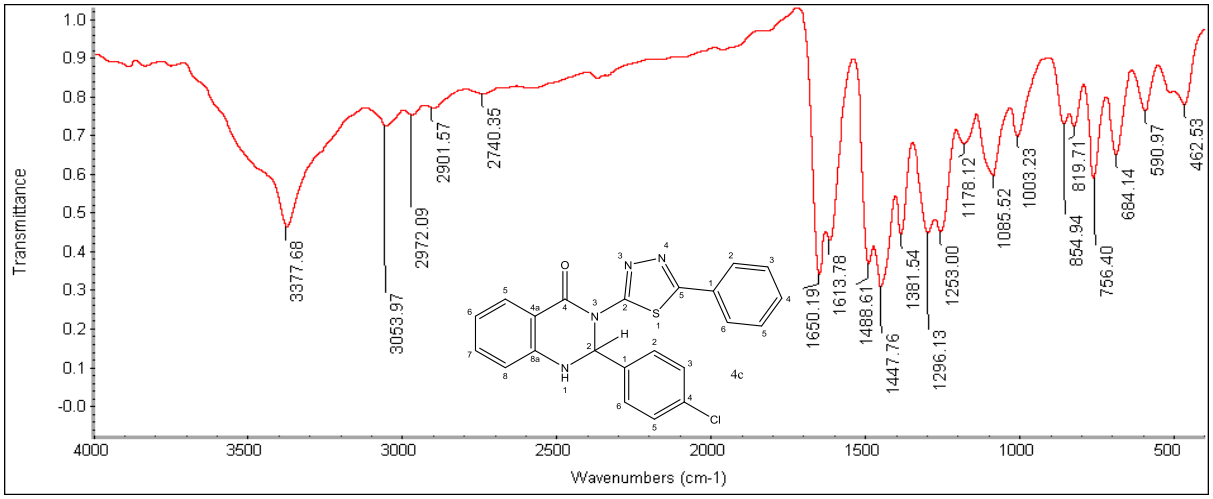

Fig 19. IR spectrum of compound (4c)

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Vial Number: 1

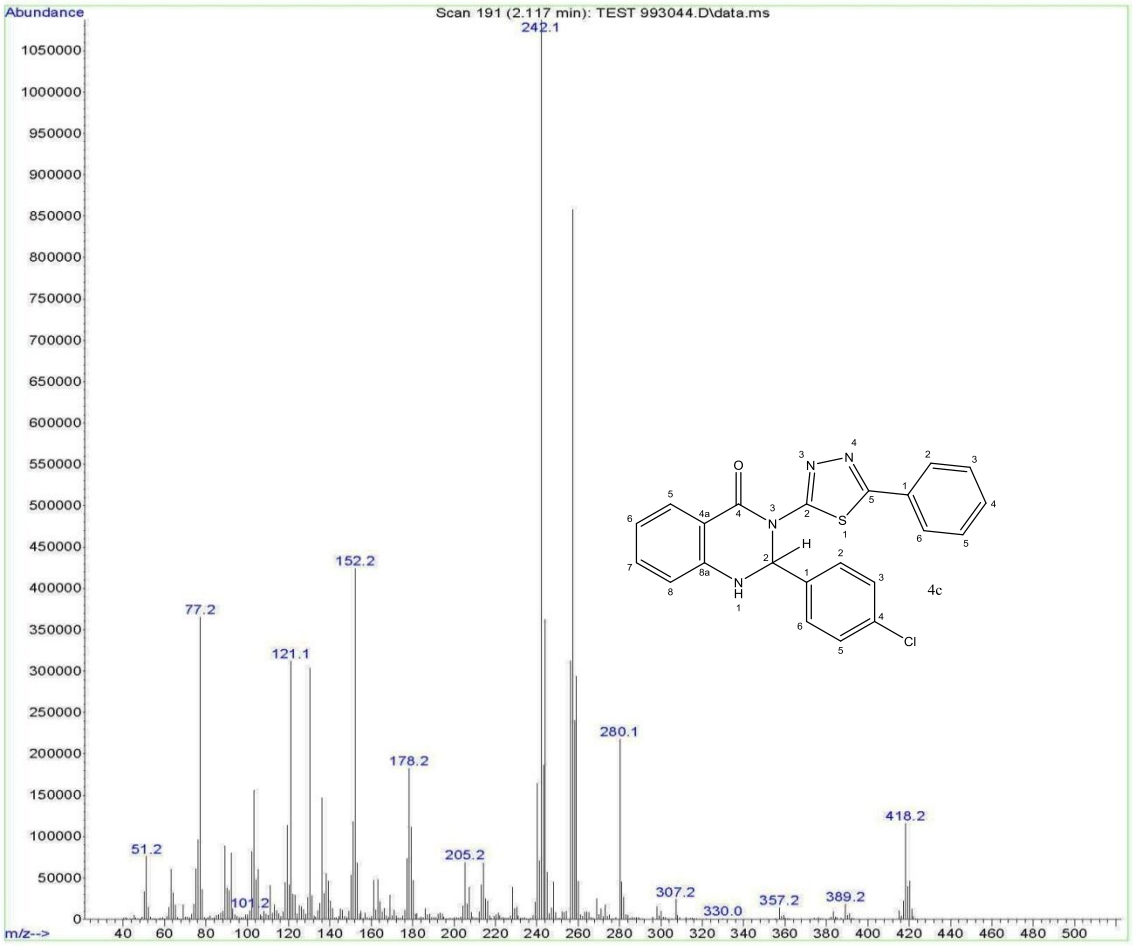

Fig 20. Mass spectrum of compound (4c)

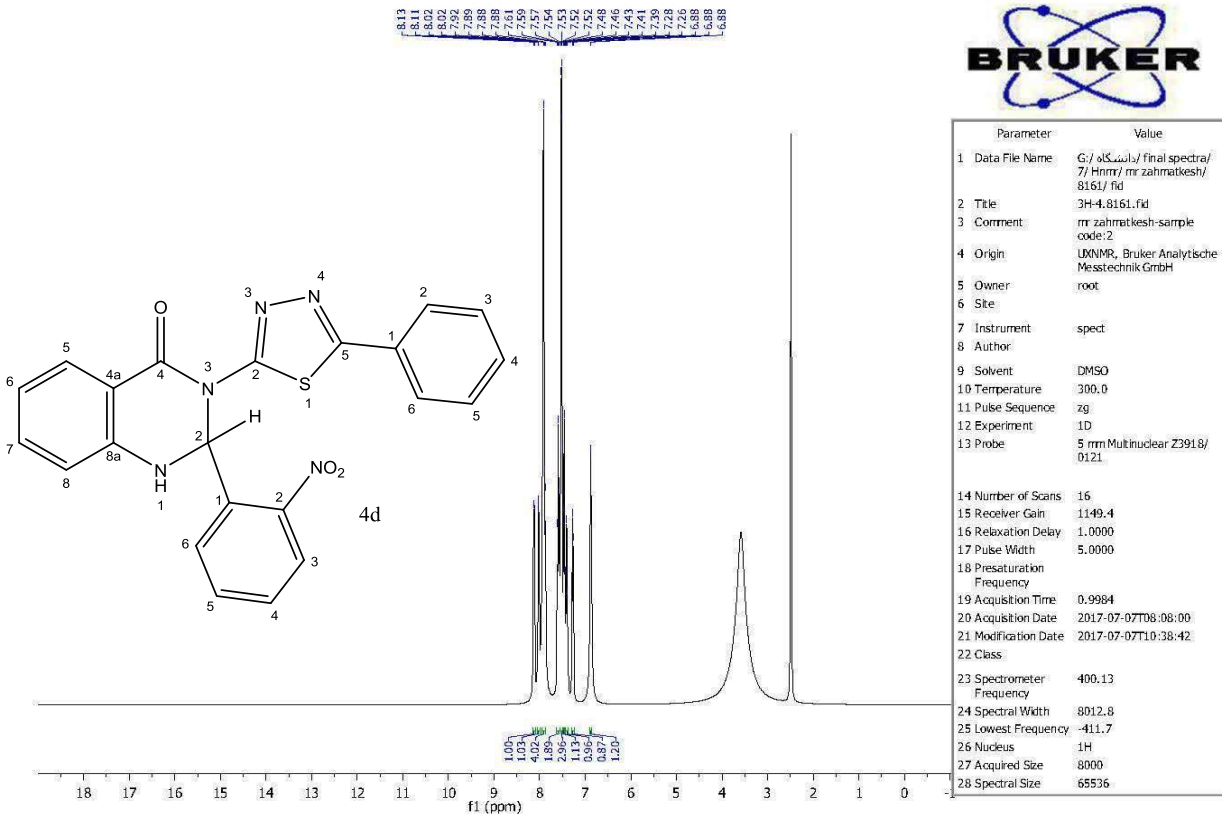

Fig 21. The whole range ^{1}H NMR spectrum of compound (4d)

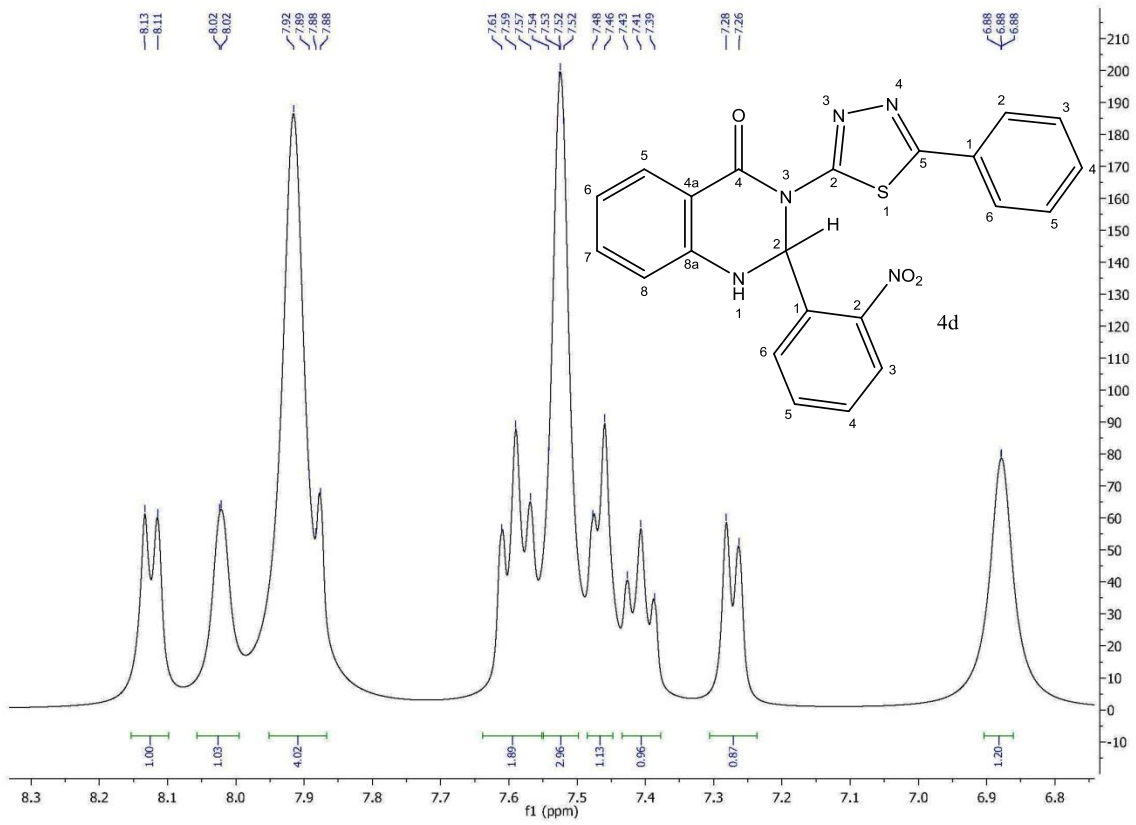

Fig 22. Aromatic range ^{1}H NMR spectrum of compound (4d)

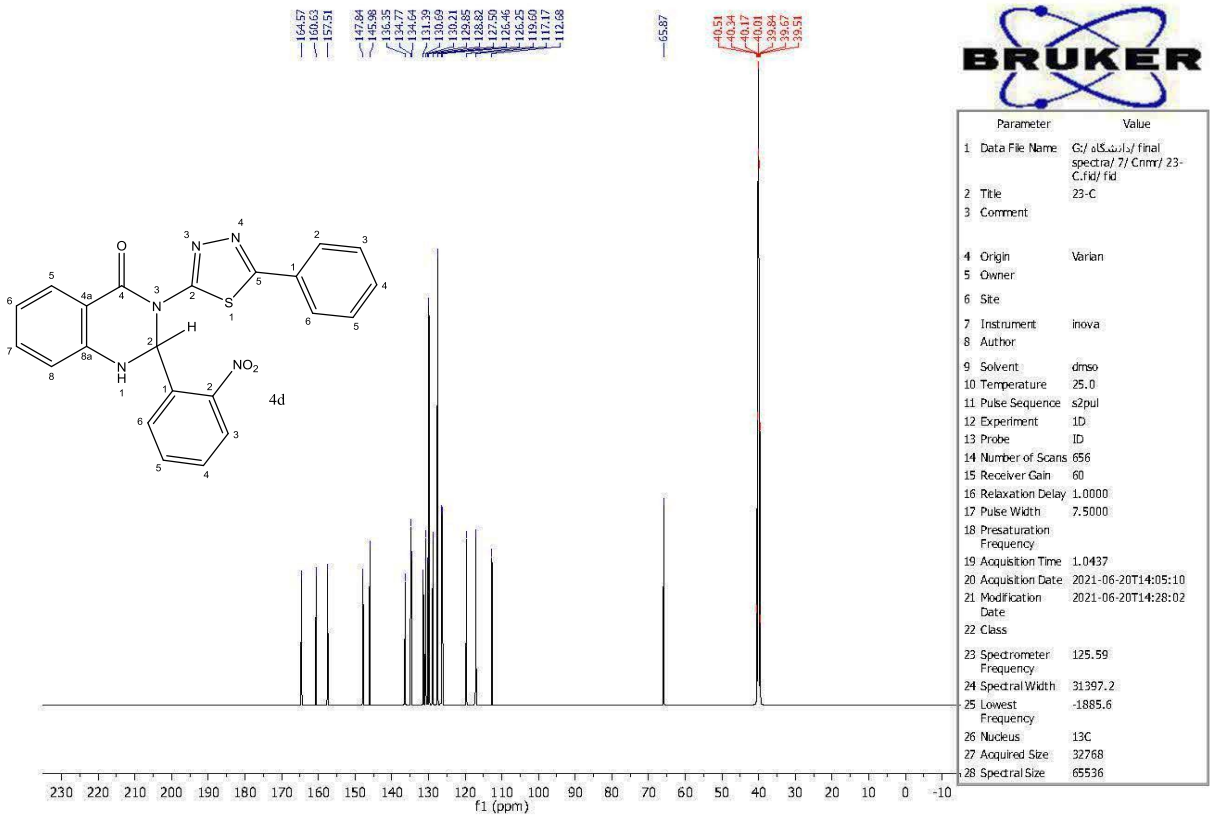

Fig 23. The whole range ^{13}C NMR spectrum of compound (4d)

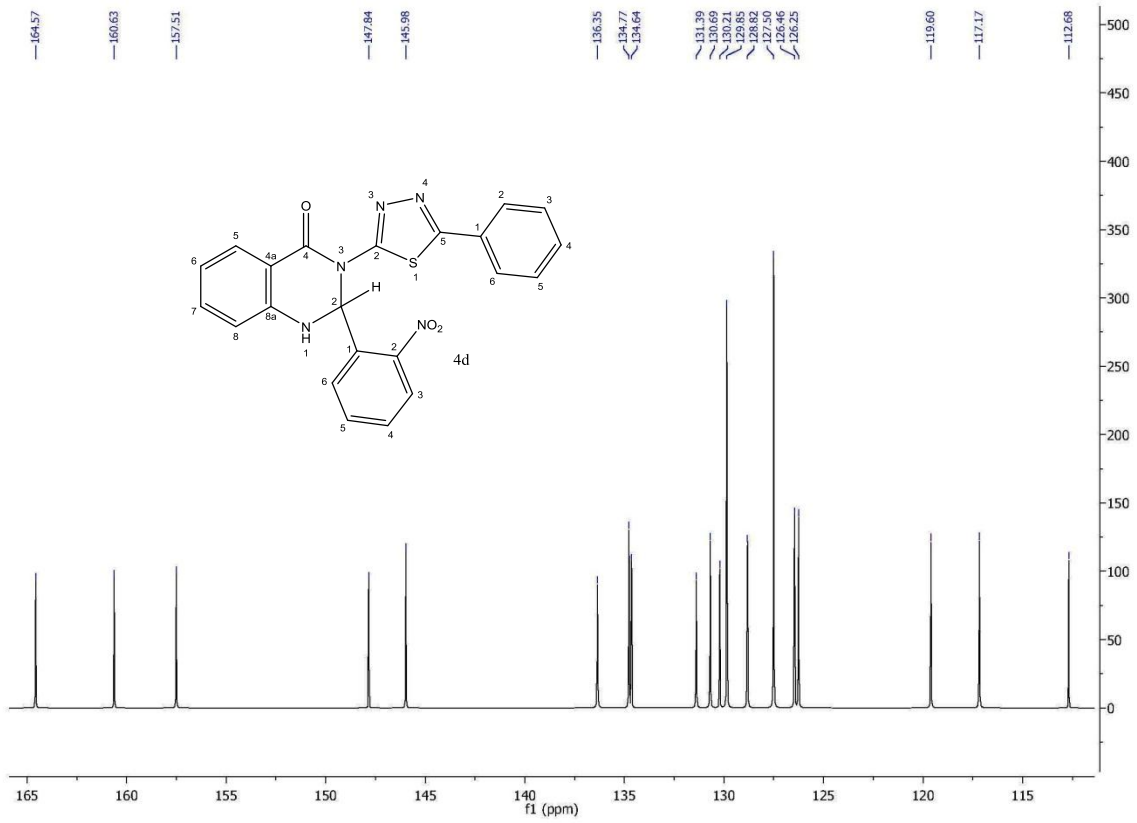

Fig 24. Doubl bond range ^{13}C NMR spectrum of compound (4d)

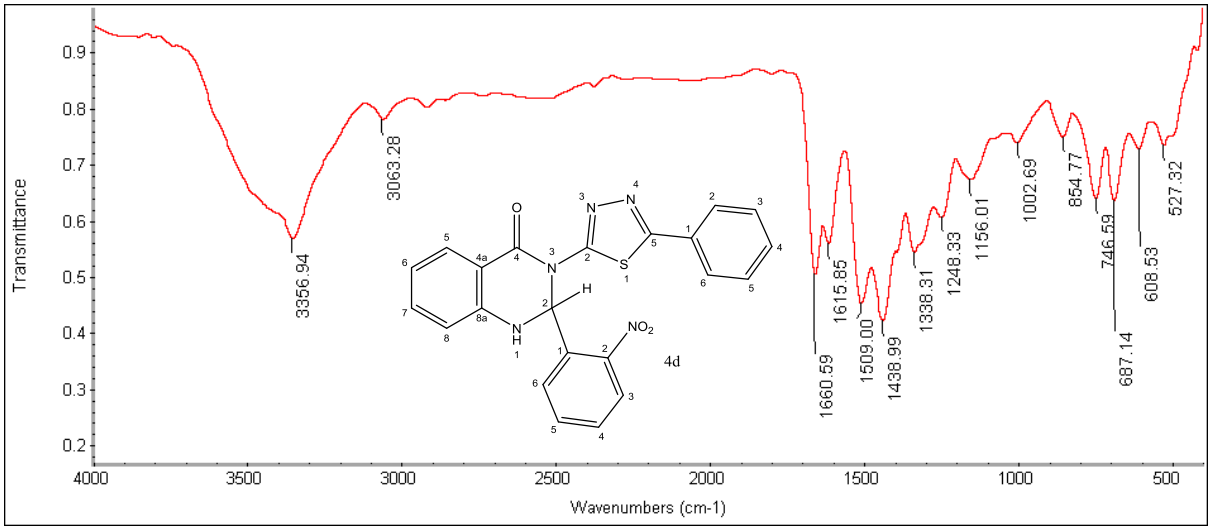

Fig 25. IR spectrum of compound (4d)

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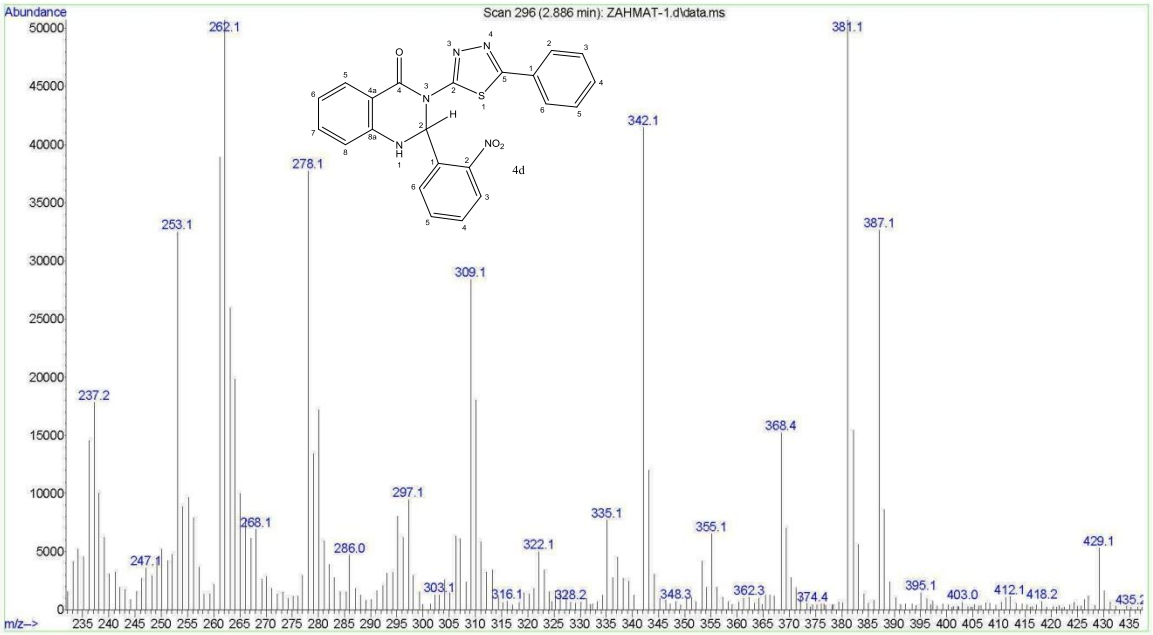

Fig 26. Mass spectrum of compound (4d)

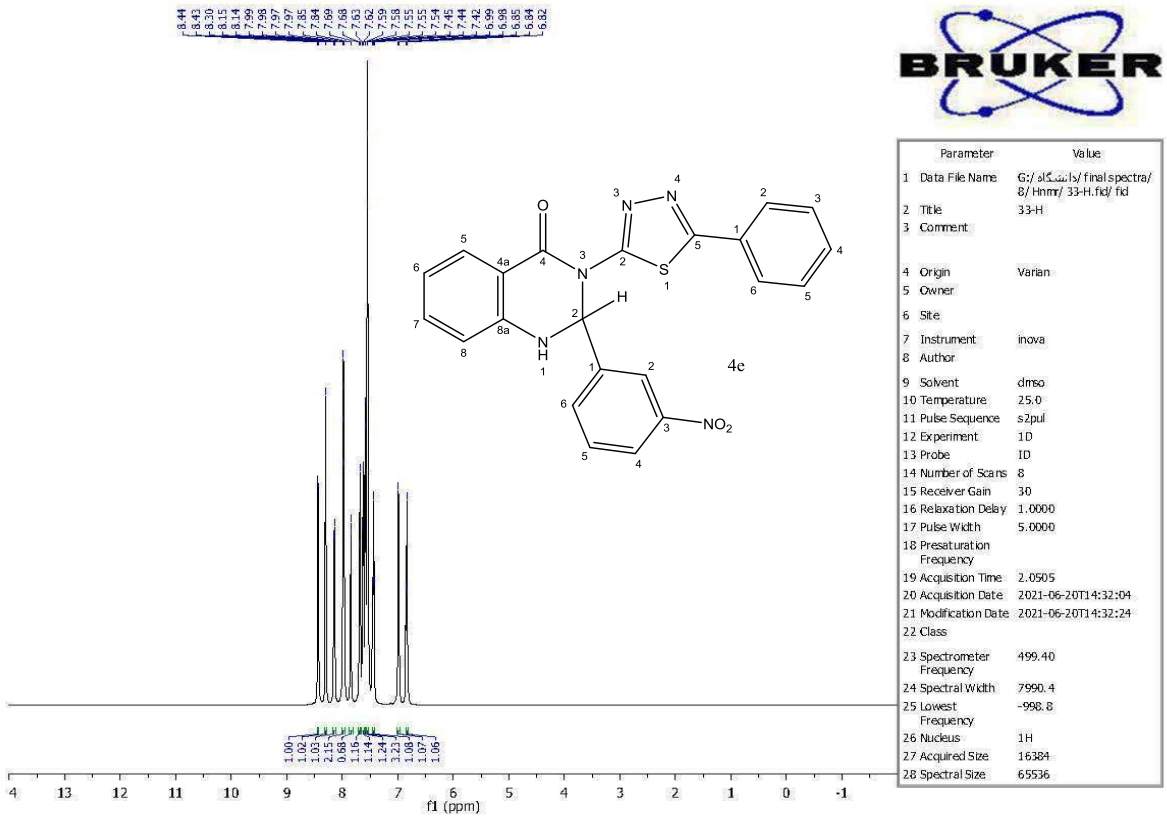

Fig 27. The whole range ^{1}H NMR spectrum of compound (4e)

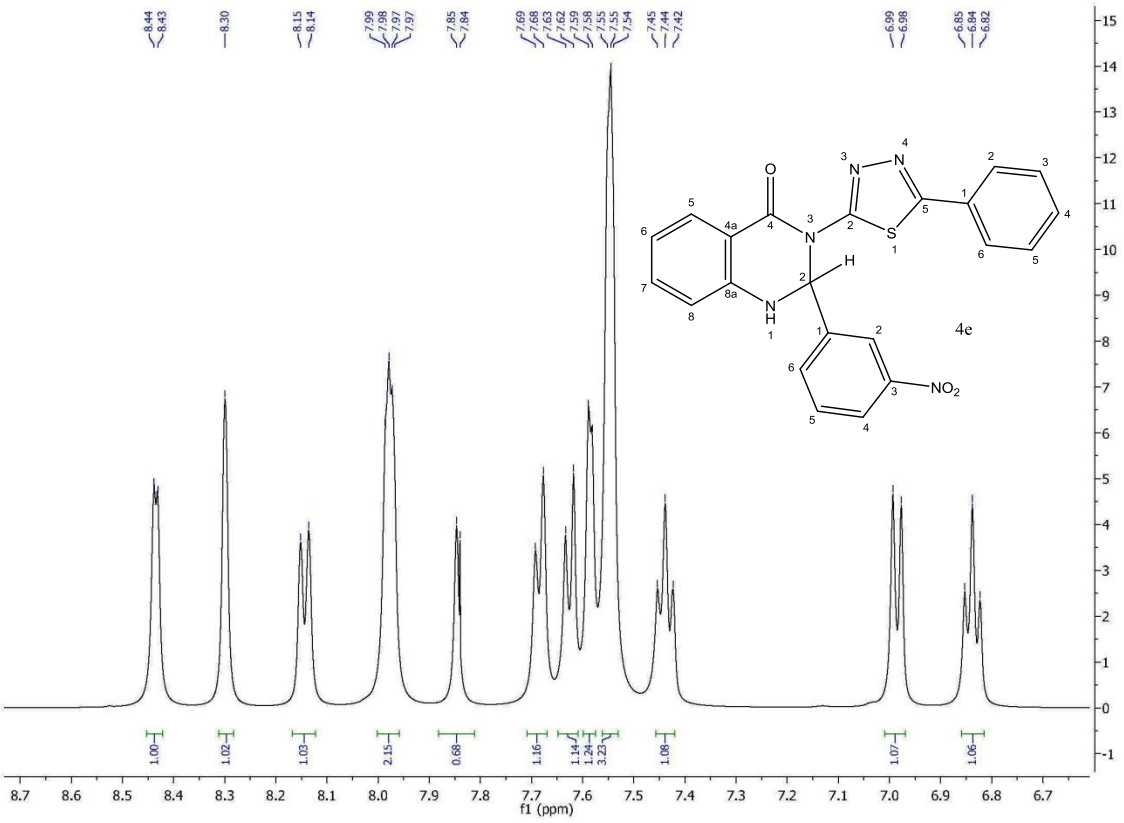

Fig 28. Aromatic range ^{1}H NMR spectrum of compound (4e)

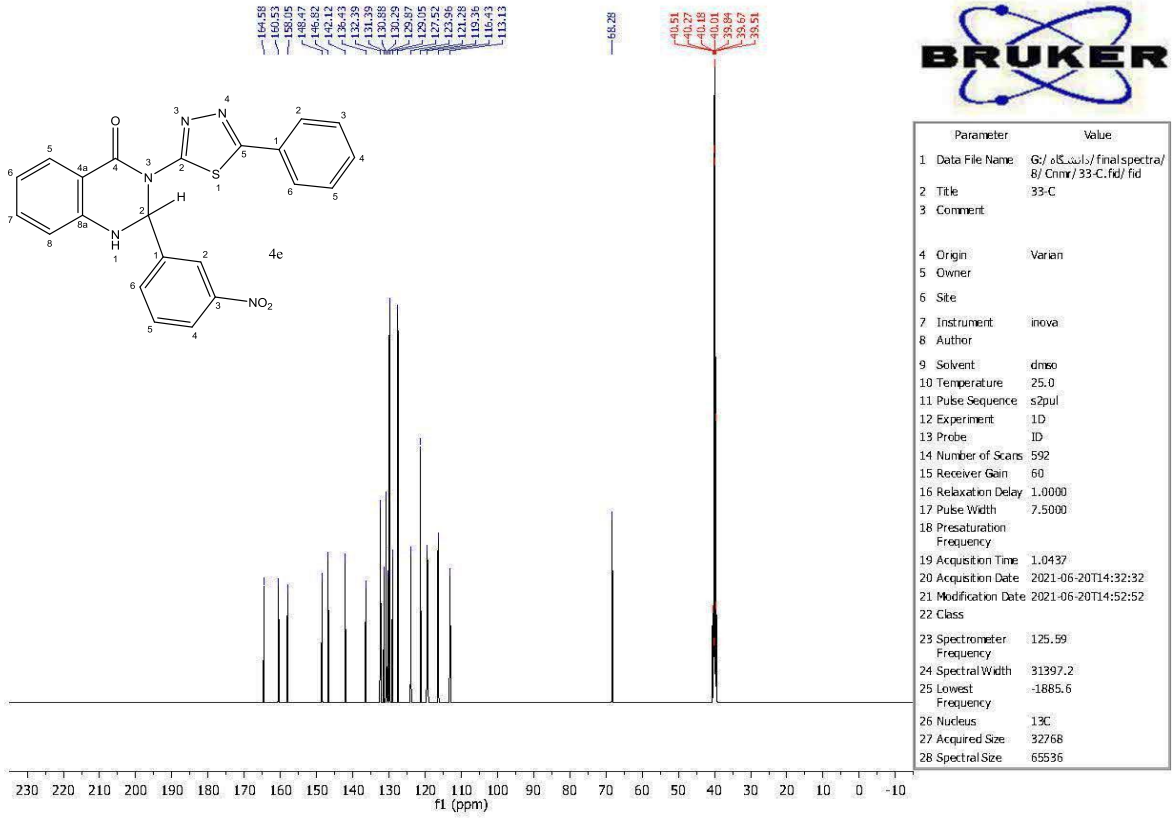

Fig 29. The whole range ^{13}C NMR spectrum of compound (4e)

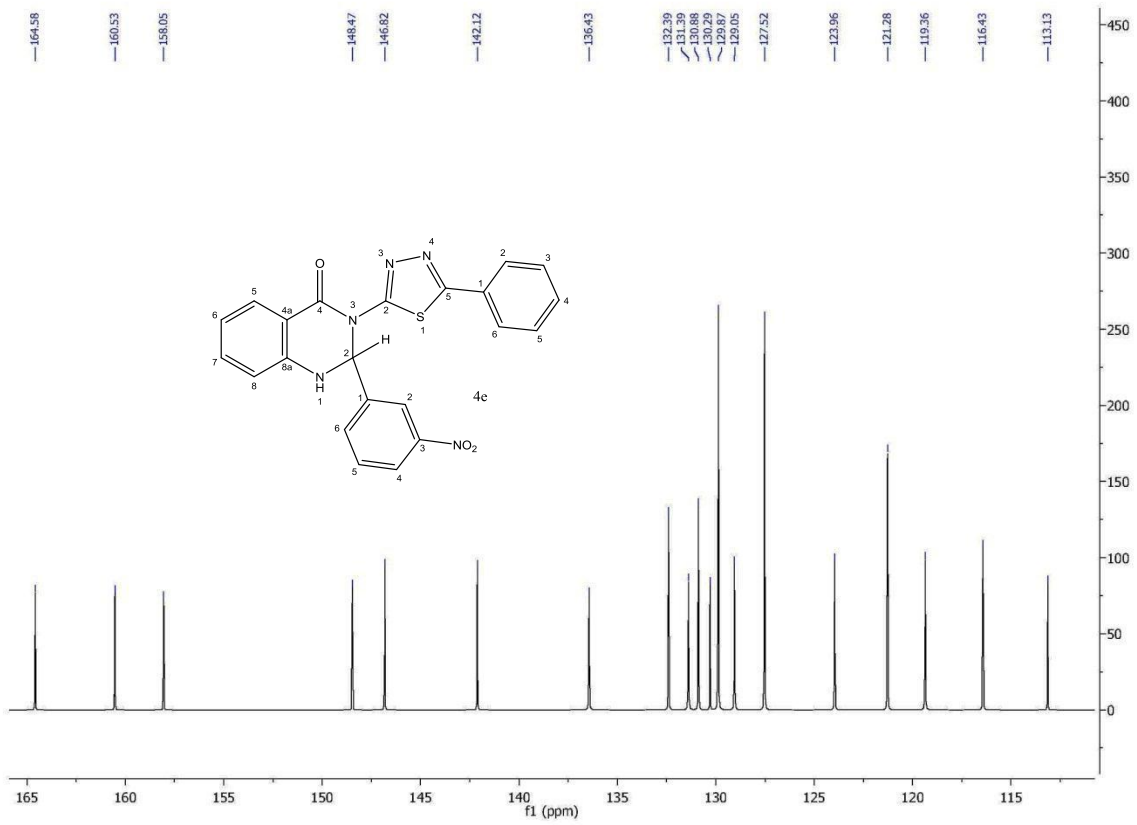

Fig 30. Doubl bond range ^{13}C NMR spectrum of compound (4e)

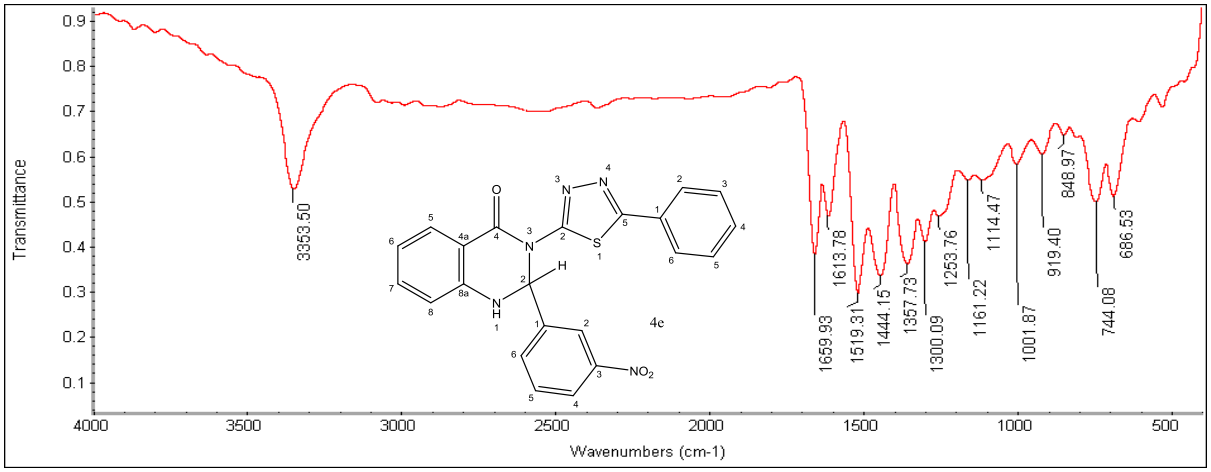

Fig 31. IR spectrum of compound (4e)

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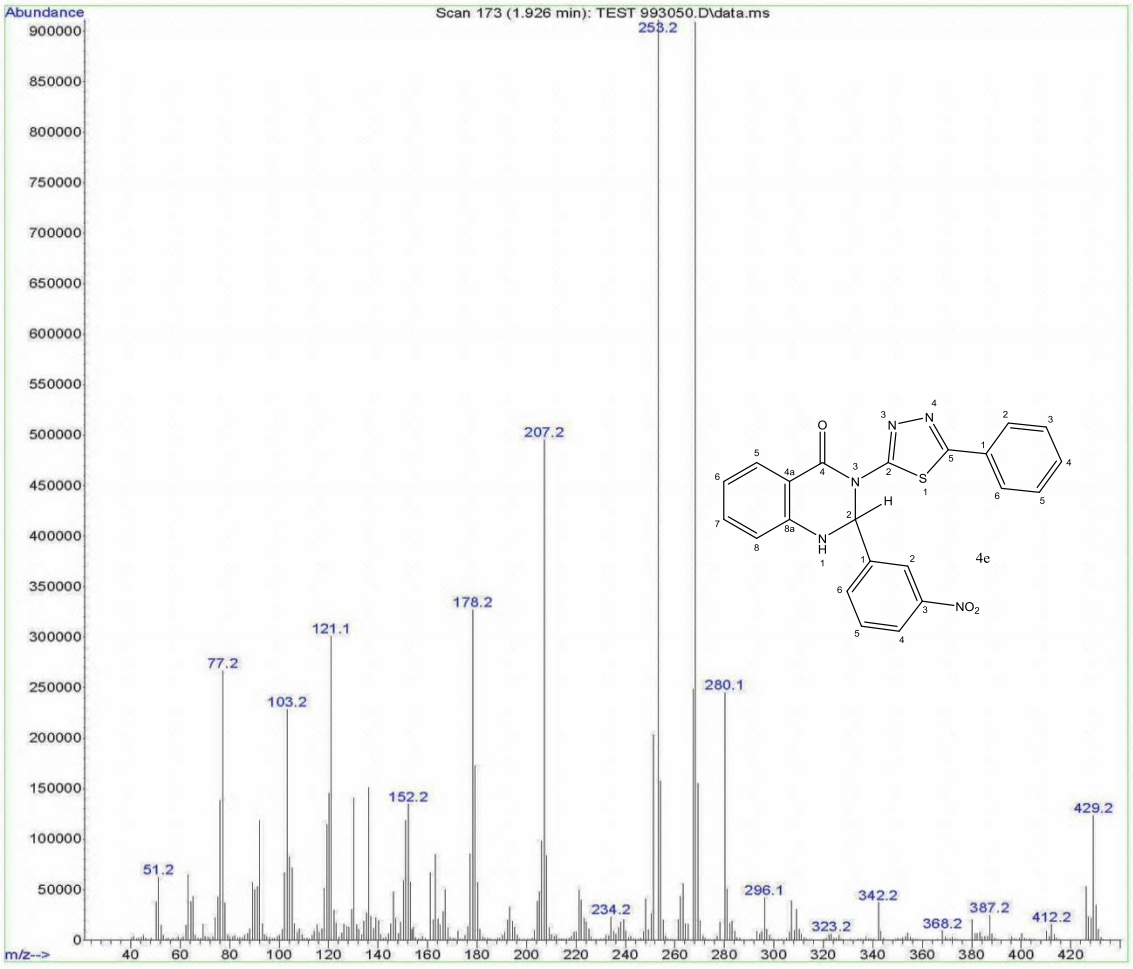

Fig 32. Mass spectrum of compound (4e)

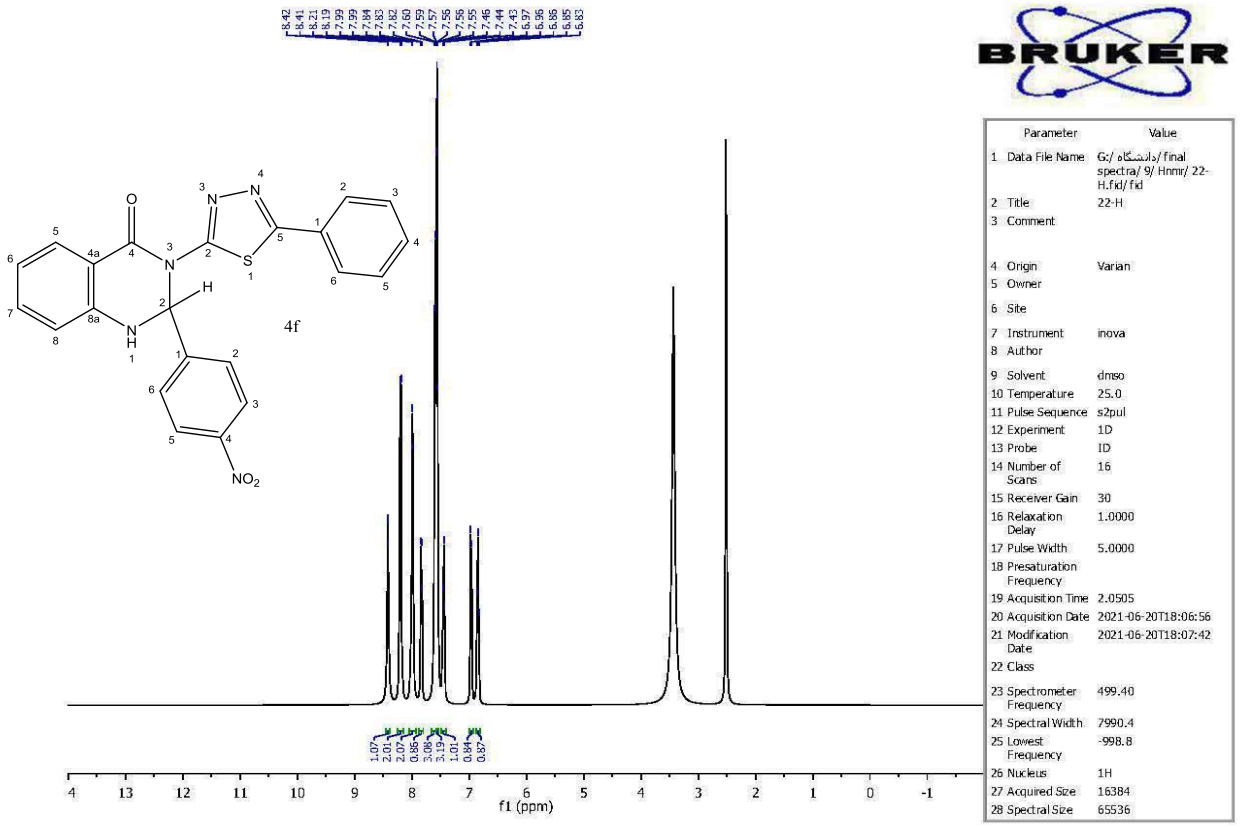

Fig 33. The whole range ^{1}H NMR spectrum of compound (4f)

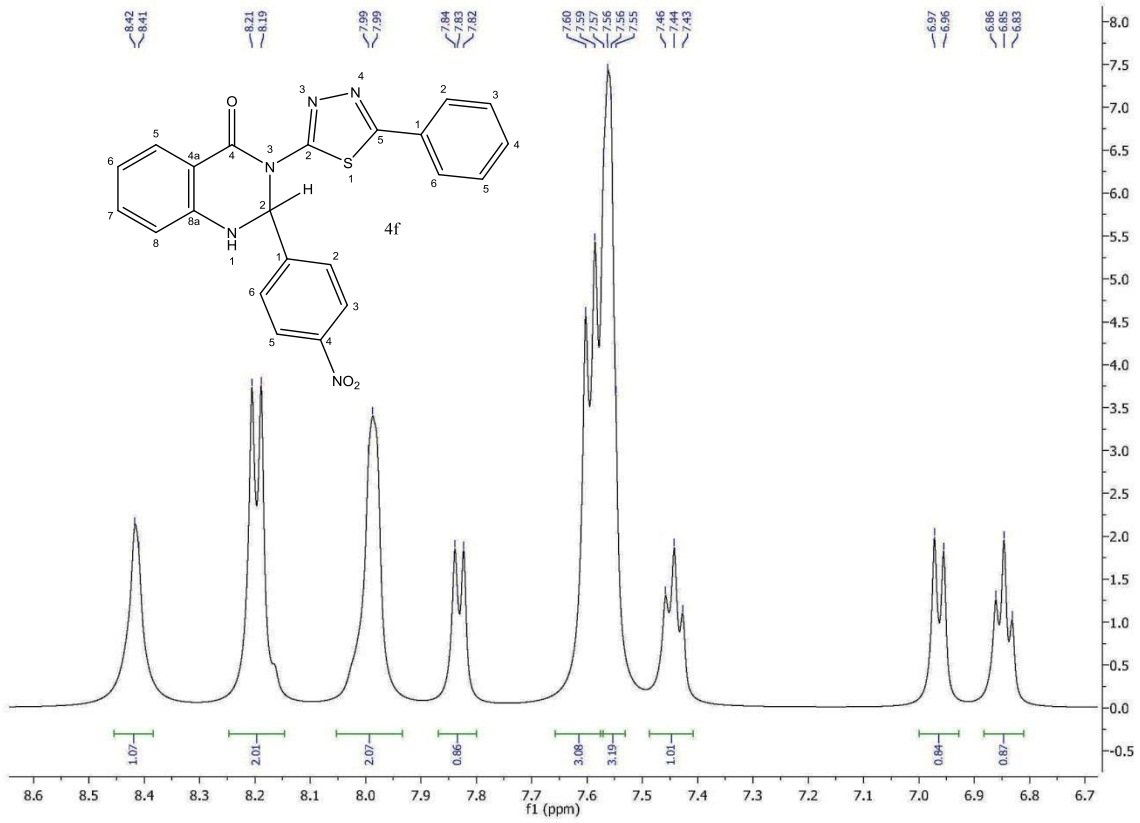

Fig 34. Aromatic range ^{1}H NMR spectrum of compound (4f)

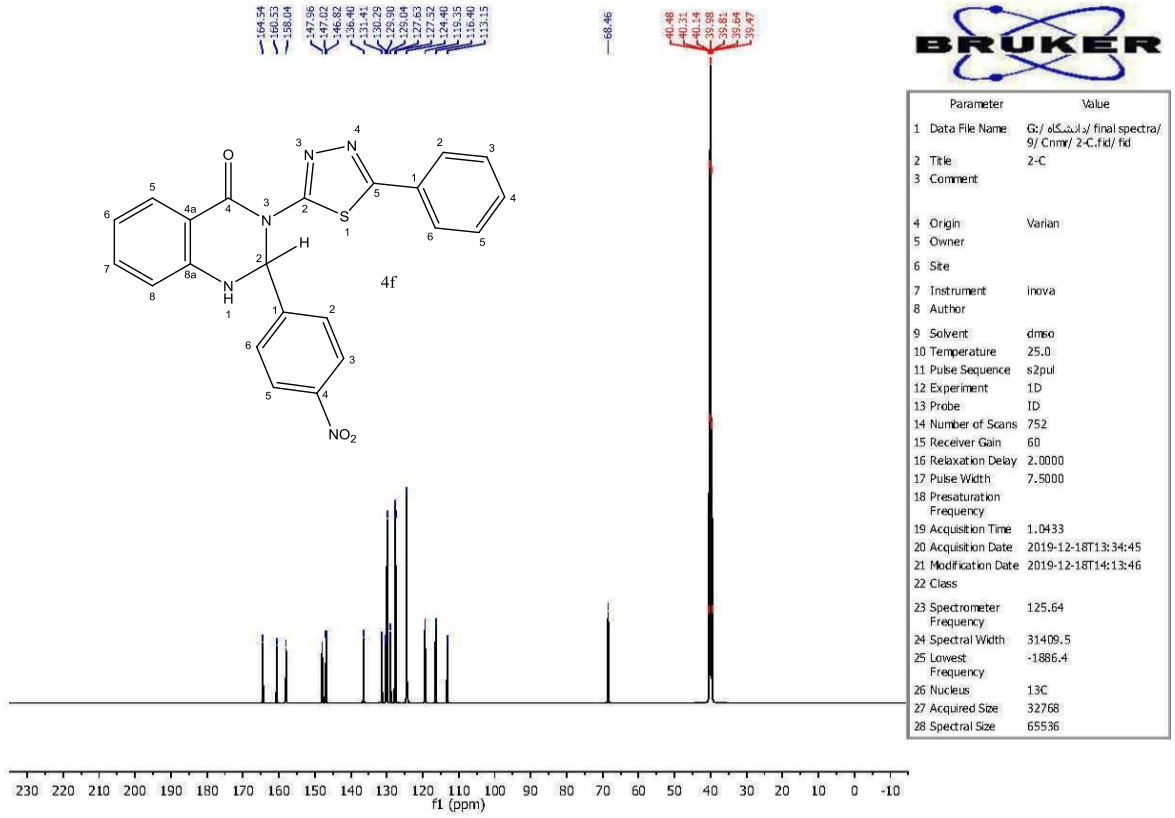

Fig 35. The whole range ^{13}C NMR spectrum of compound (4f)

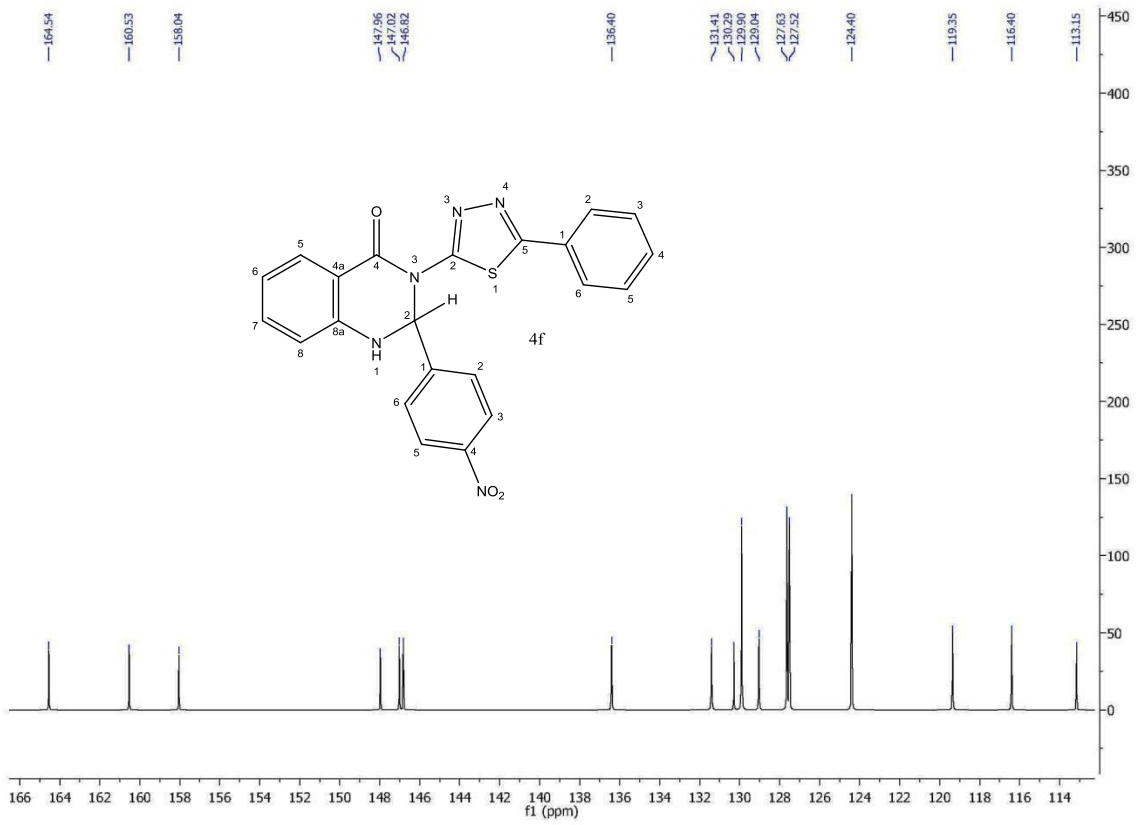

Fig 36. Doubl bond range ^{13}C NMR spectrum of compound (4f)

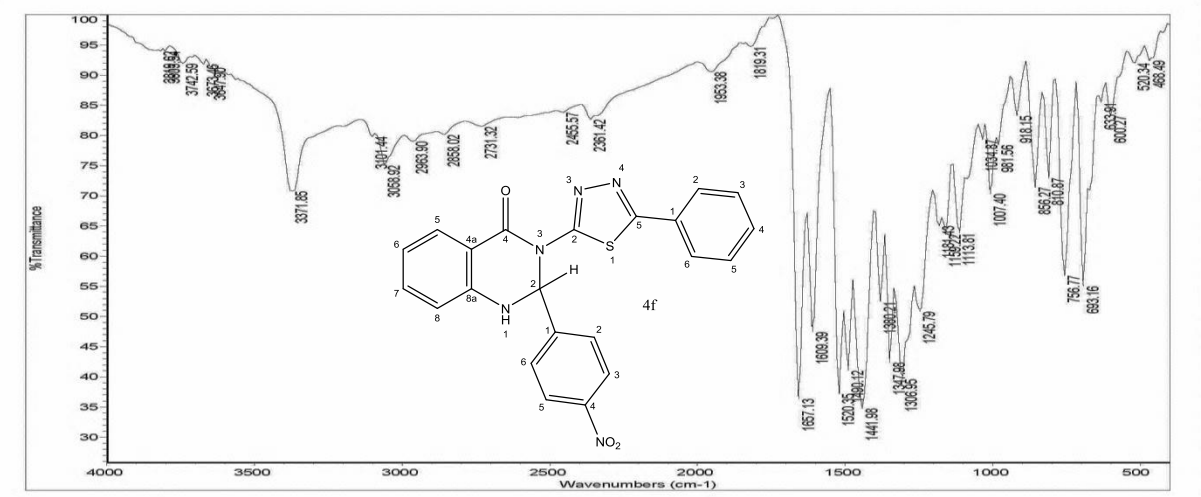

Fig 37. IR spectrum of compound (4f)

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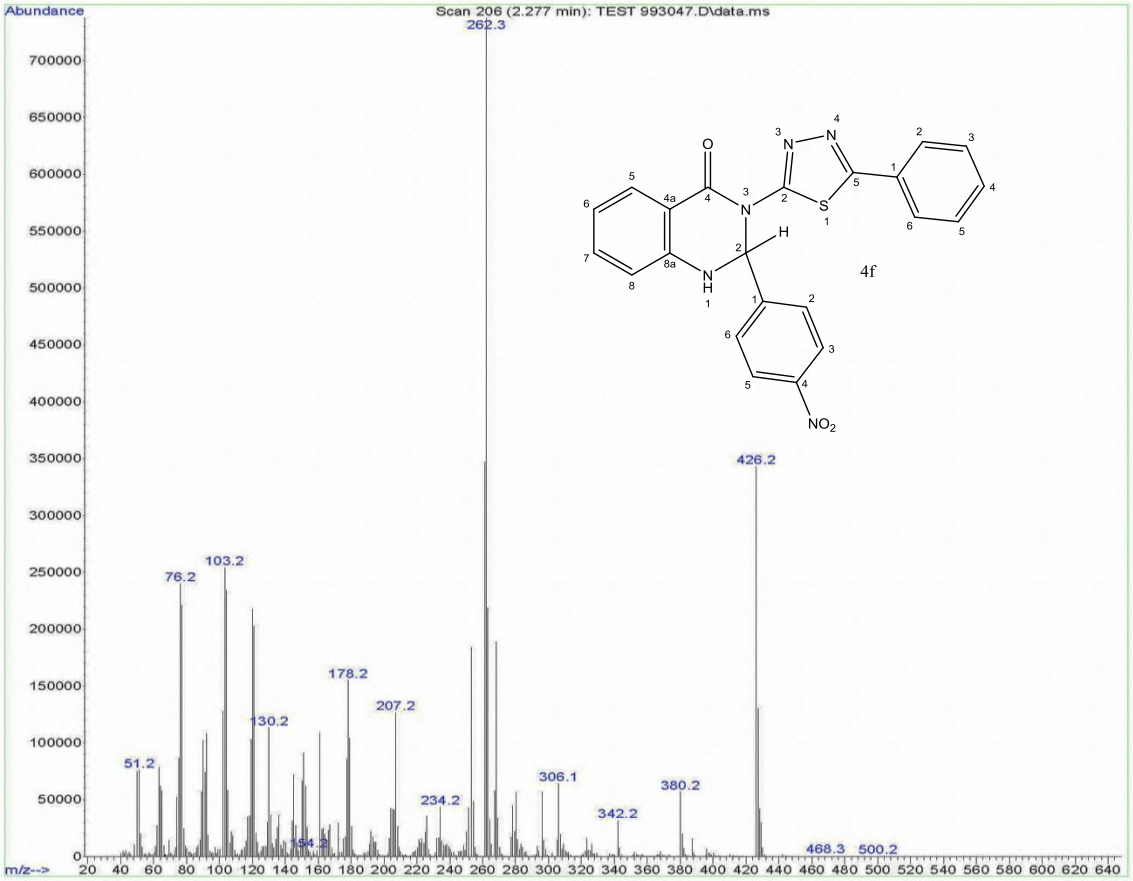

4f

Fig 38. Mass spectrum of compound (4f)

File :C:\msdchem\3\data\Snapshot\TEST 993047.D
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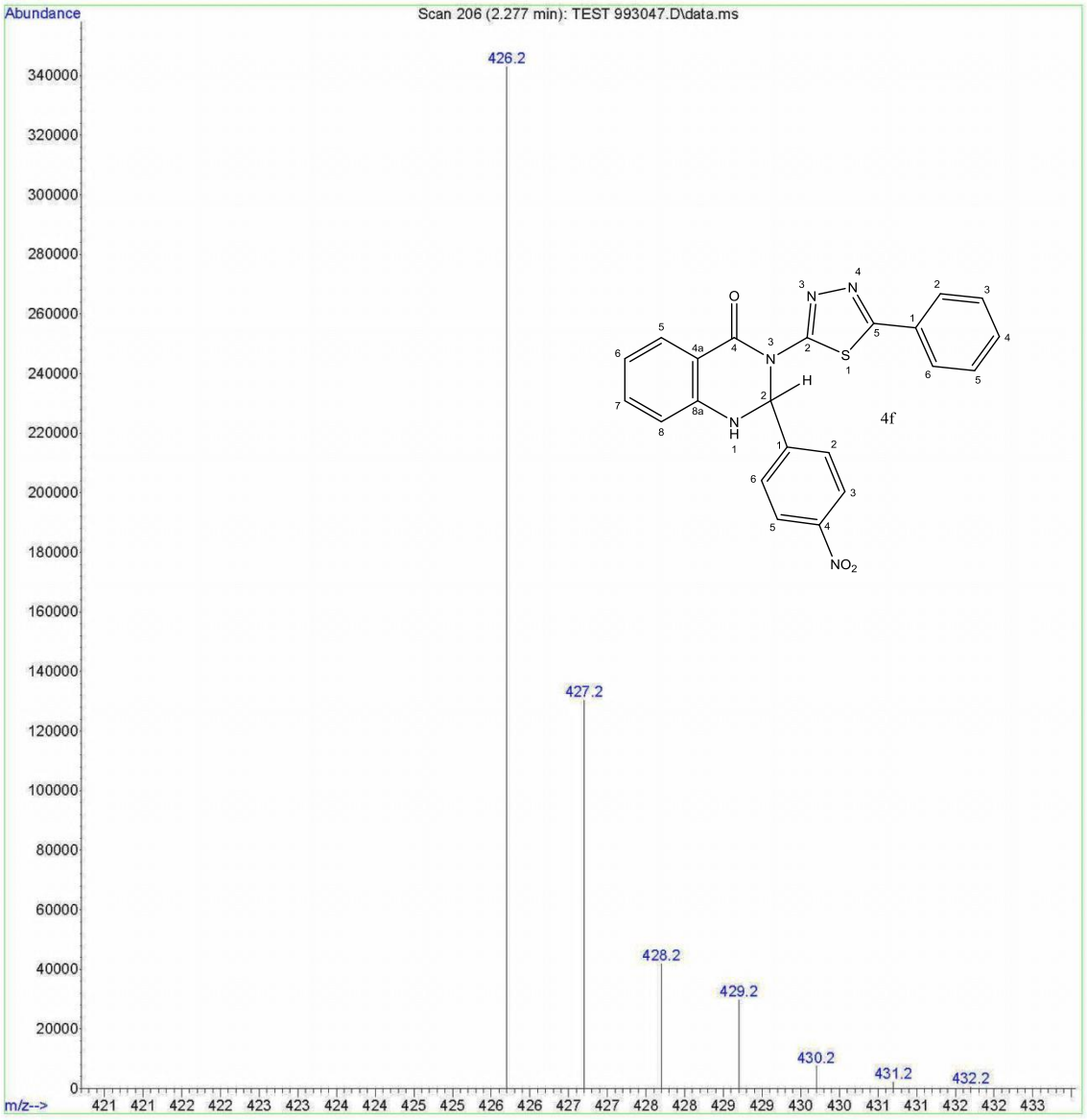

Fig 39. Mass spectrum of compound (4f)**,** From a closer look

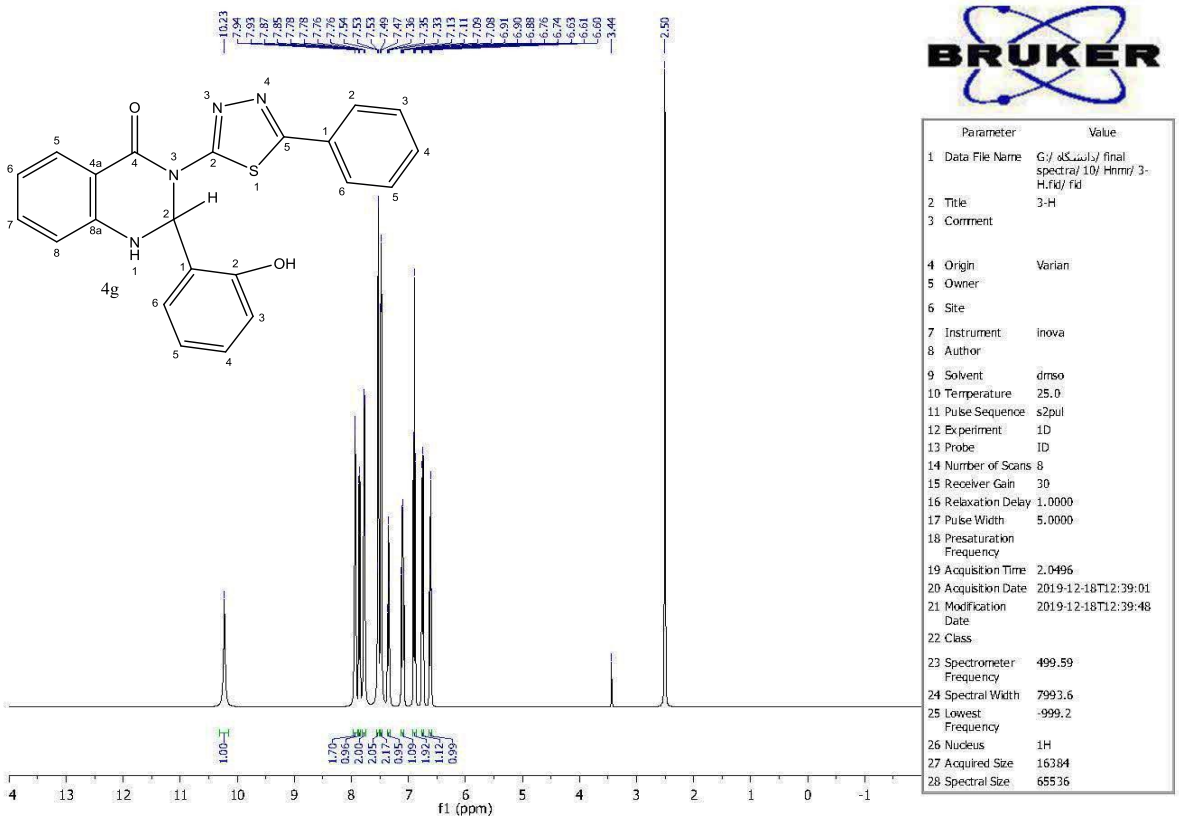

Fig 40. The whole range ^{1}H NMR spectrum of compound (4g)

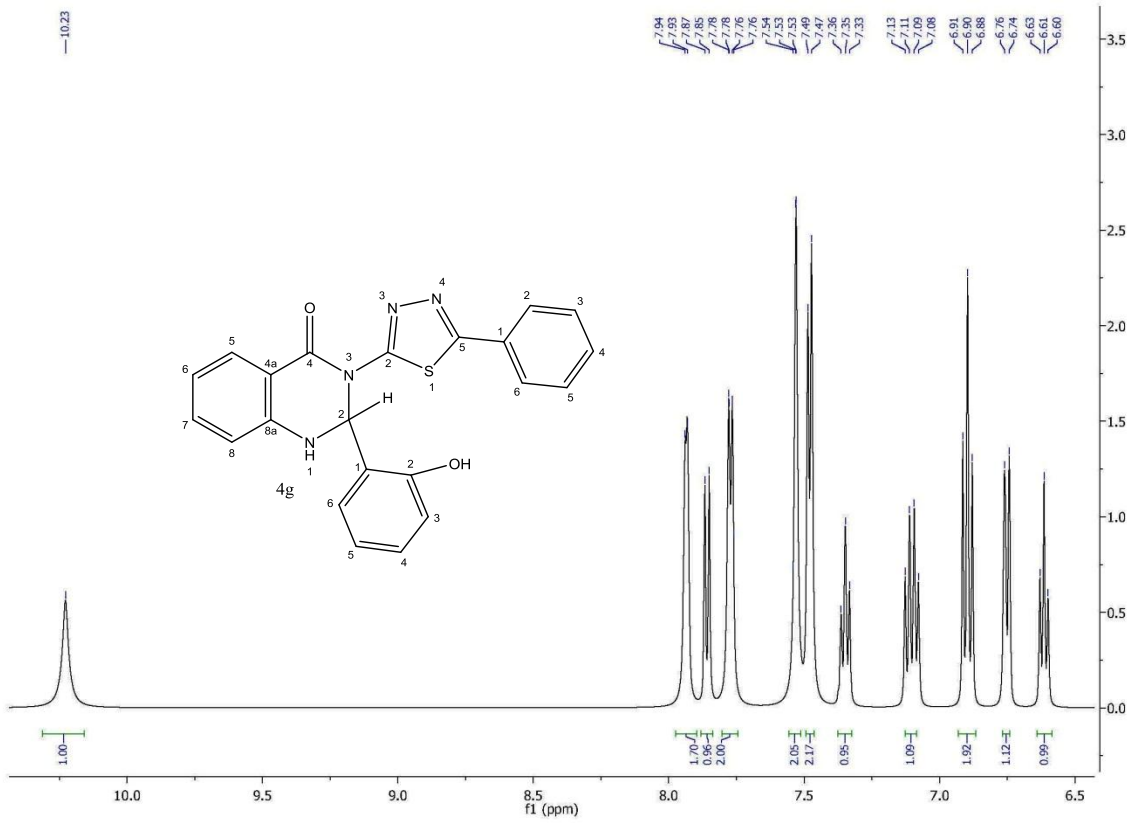

Fig 41. Aromatic range ^{1}H NMR spectrum of compound (4g)

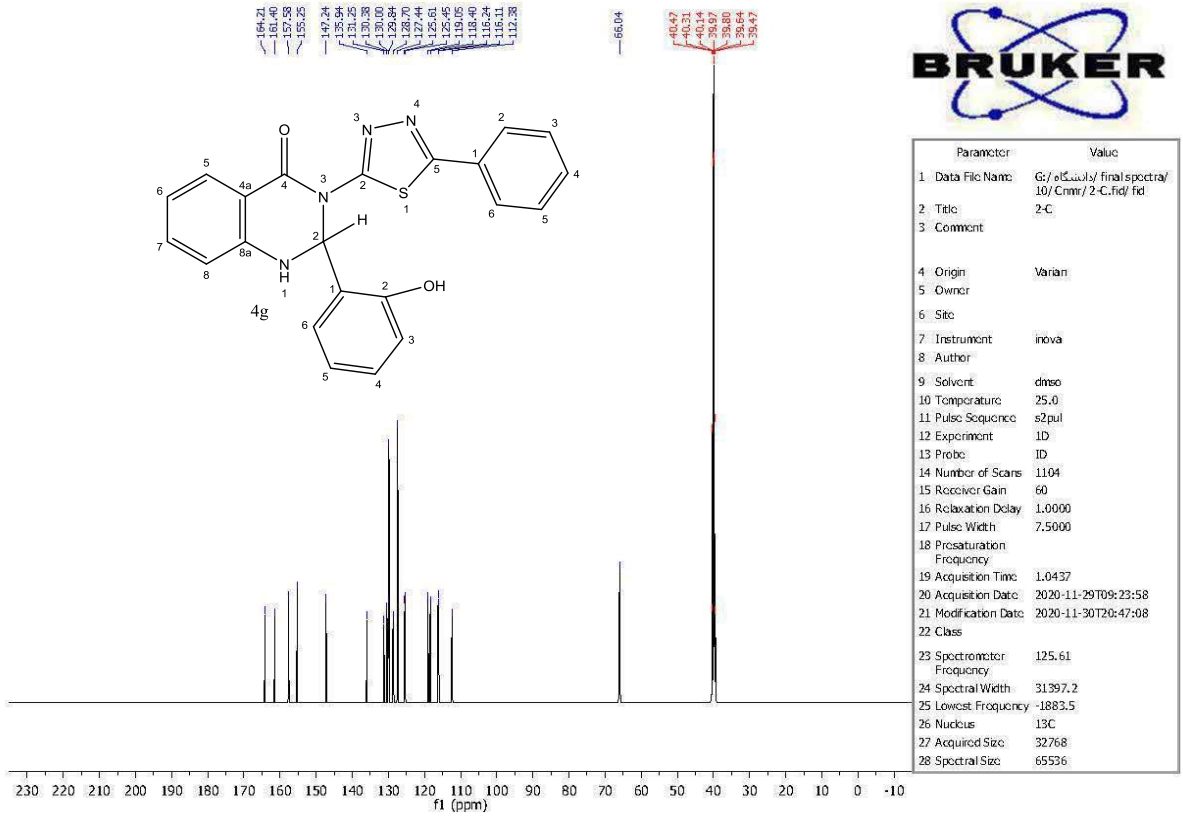

Fig 42. The whole range ^{13}C NMR spectrum of compound (4g)

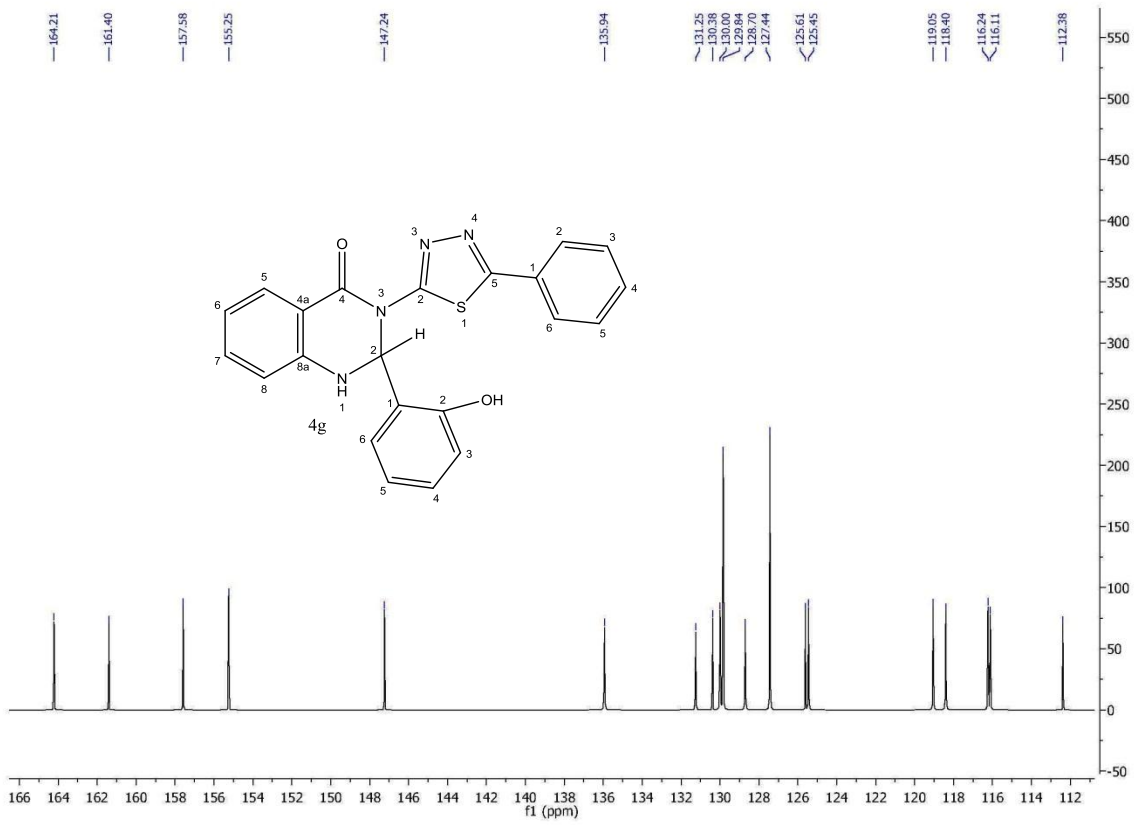

Fig 43. Doubl bond range ^{13}C NMR spectrum of compound (4g)

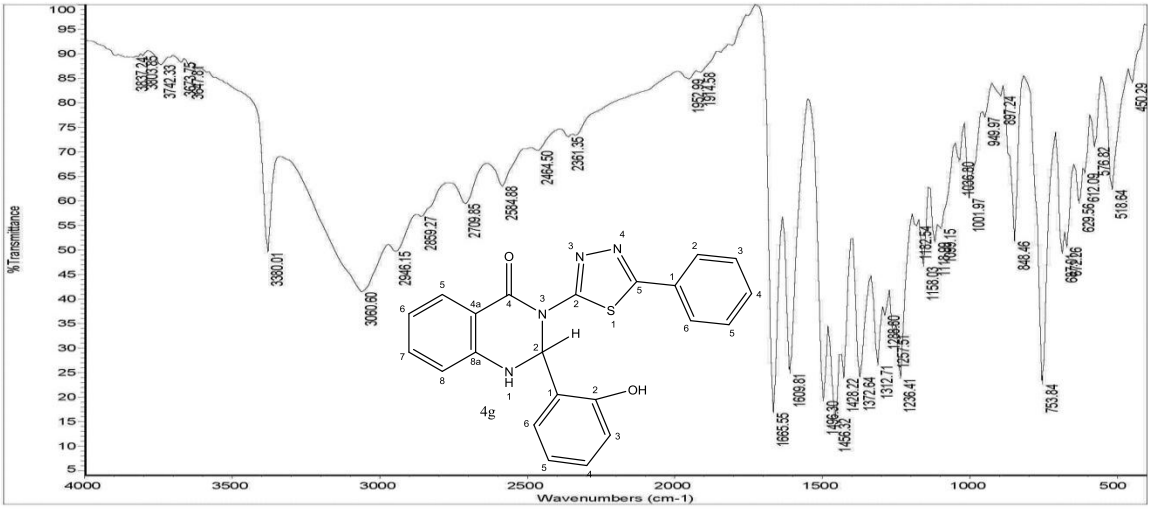

Fig 44. IR spectrum of compound (4g)

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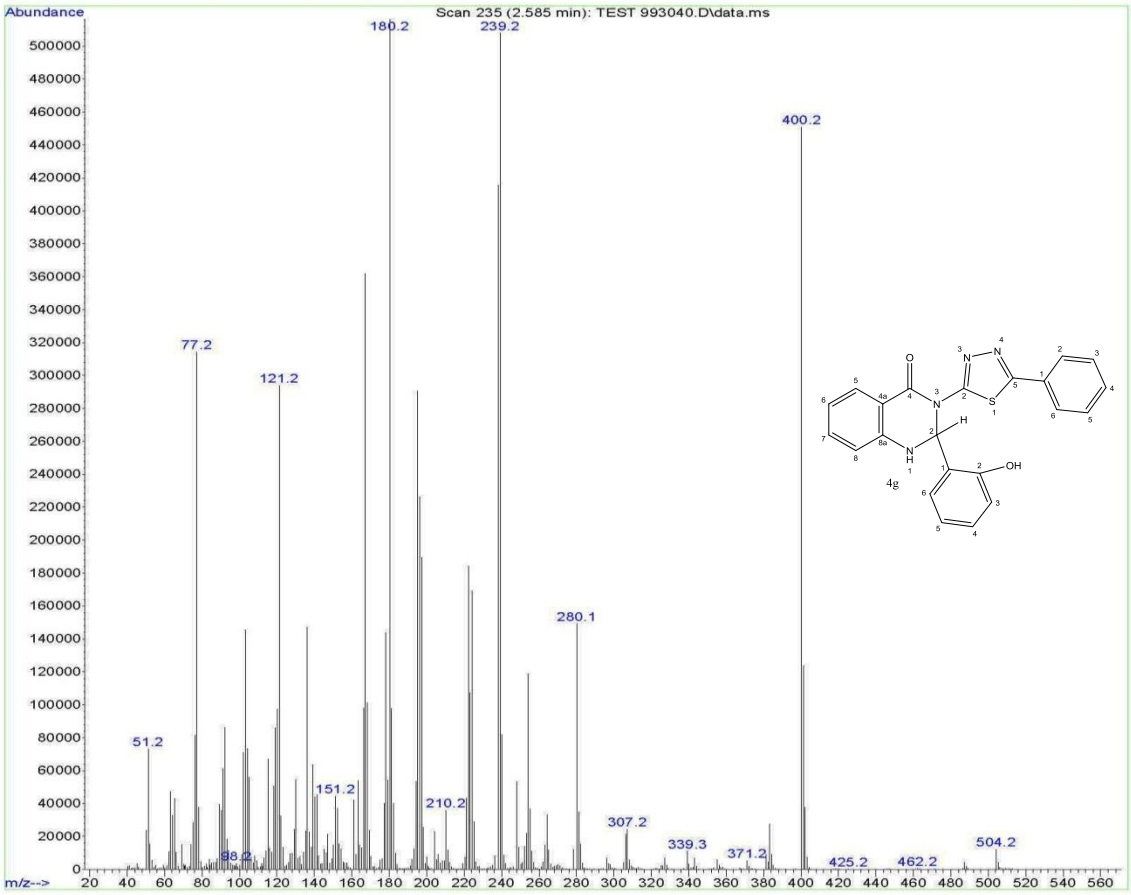


Fig 45. Mass spectrum of compound (4g)

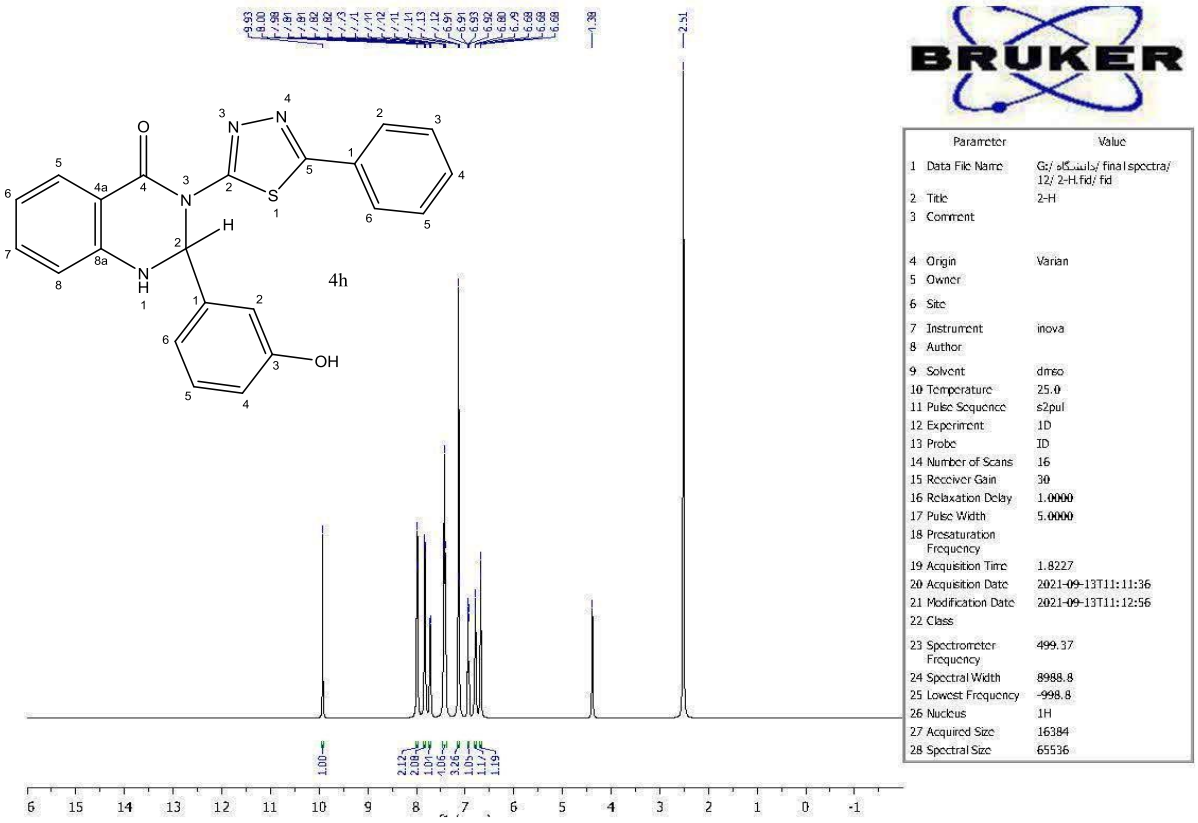


Fig 46. The whole range ^{1}H NMR spectrum of compound (4h)

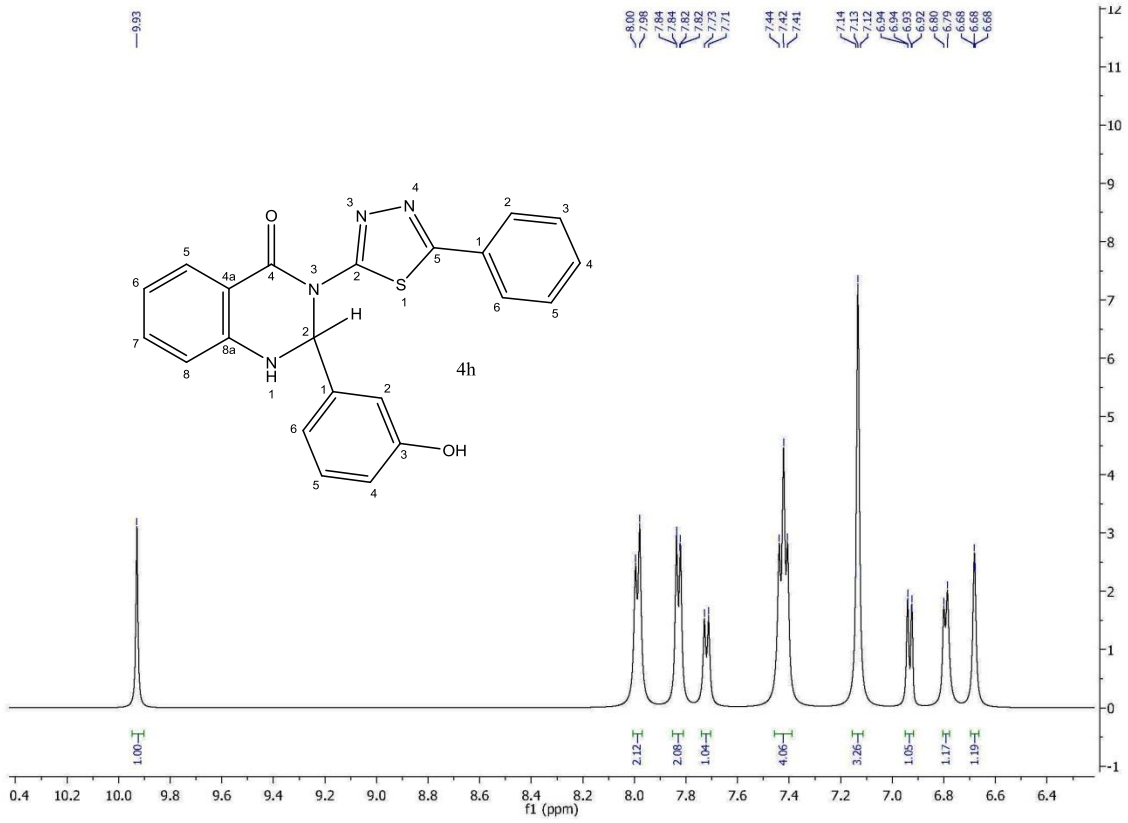


Fig 47. Aromatic range ^{1}H NMR spectrum of compound (4h)

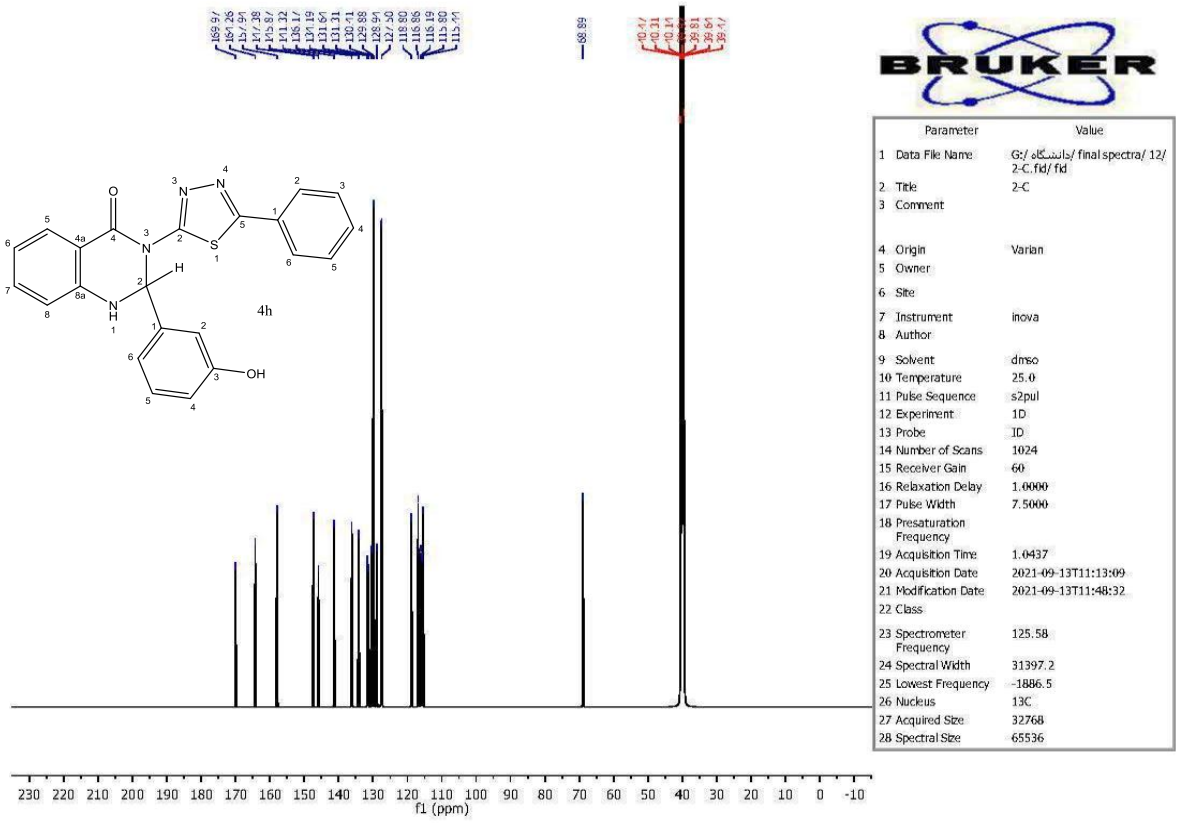


Fig 48. The whole range ^{13}C NMR spectrum of compound (4h)

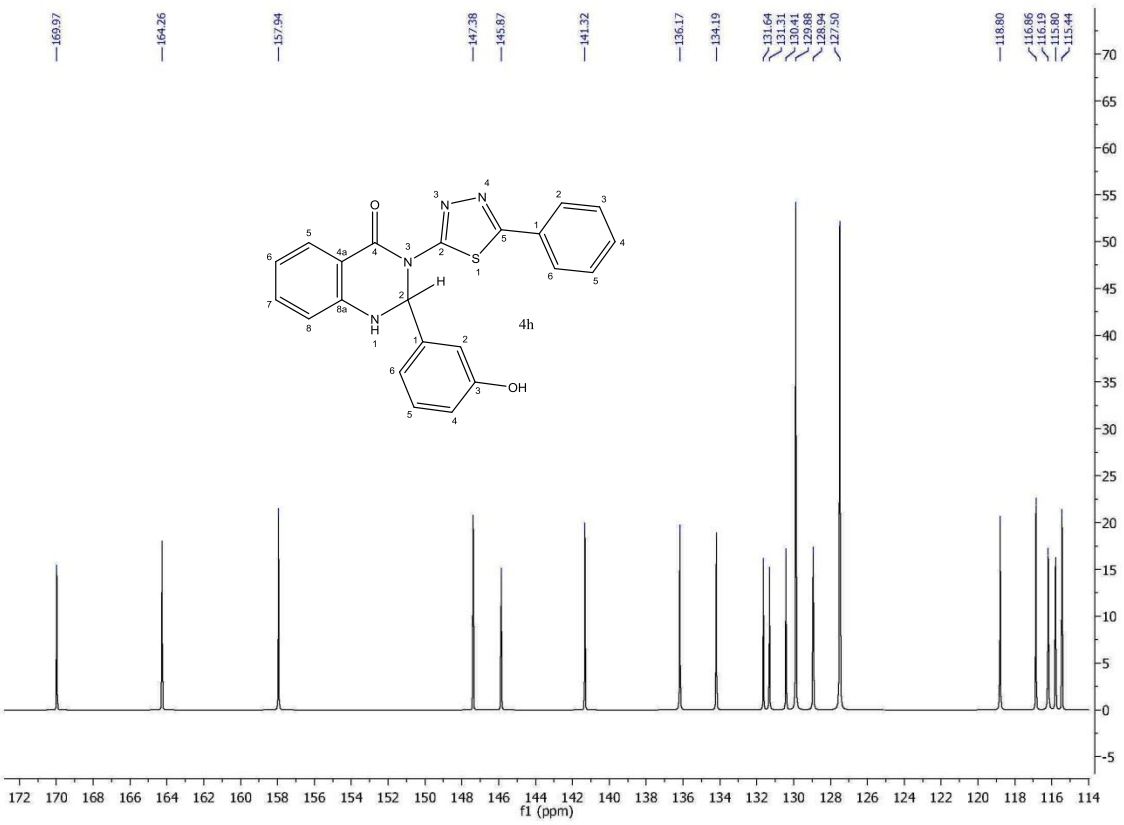
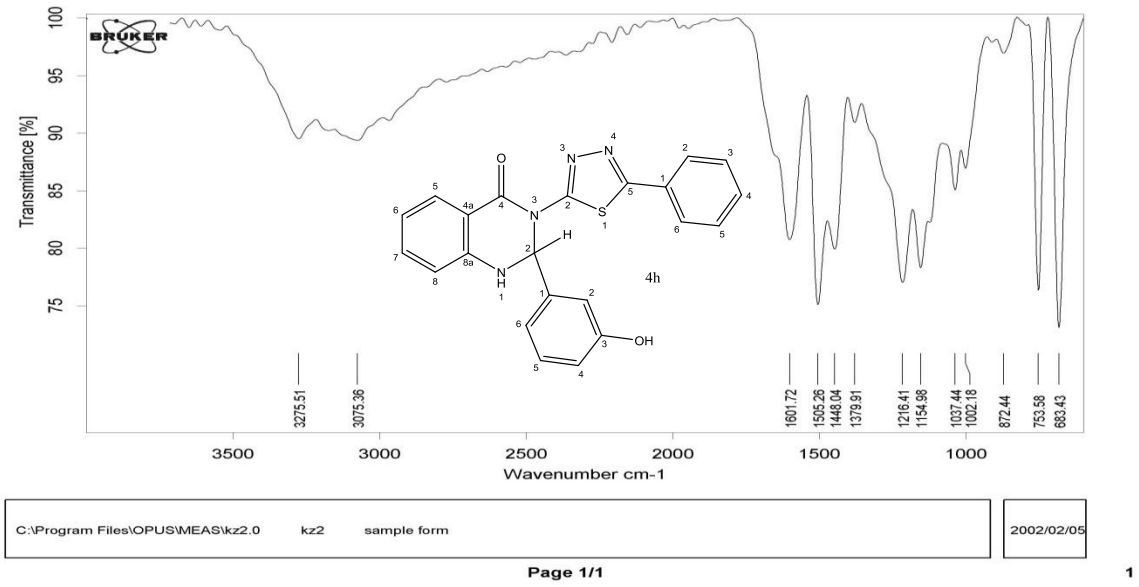


Fig 49. Doubl bond range ^{13}C NMR spectrum of compound (4h)



C:\Program Files\OPUS\MEAS\kz2.0 kz2 sample form 2002/02/05

Page 1/1

Fig 50. IR spectrum of compound (4h)

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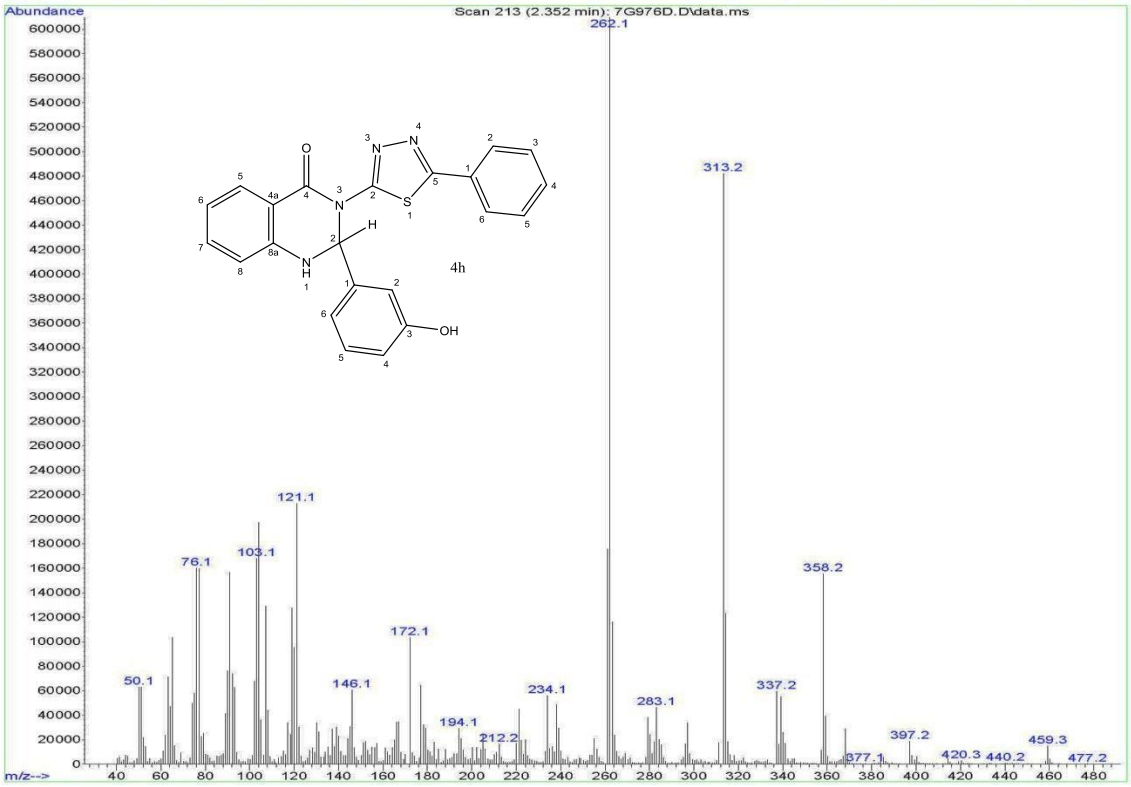

Fig 51. Mass spectrum of compound (4h)

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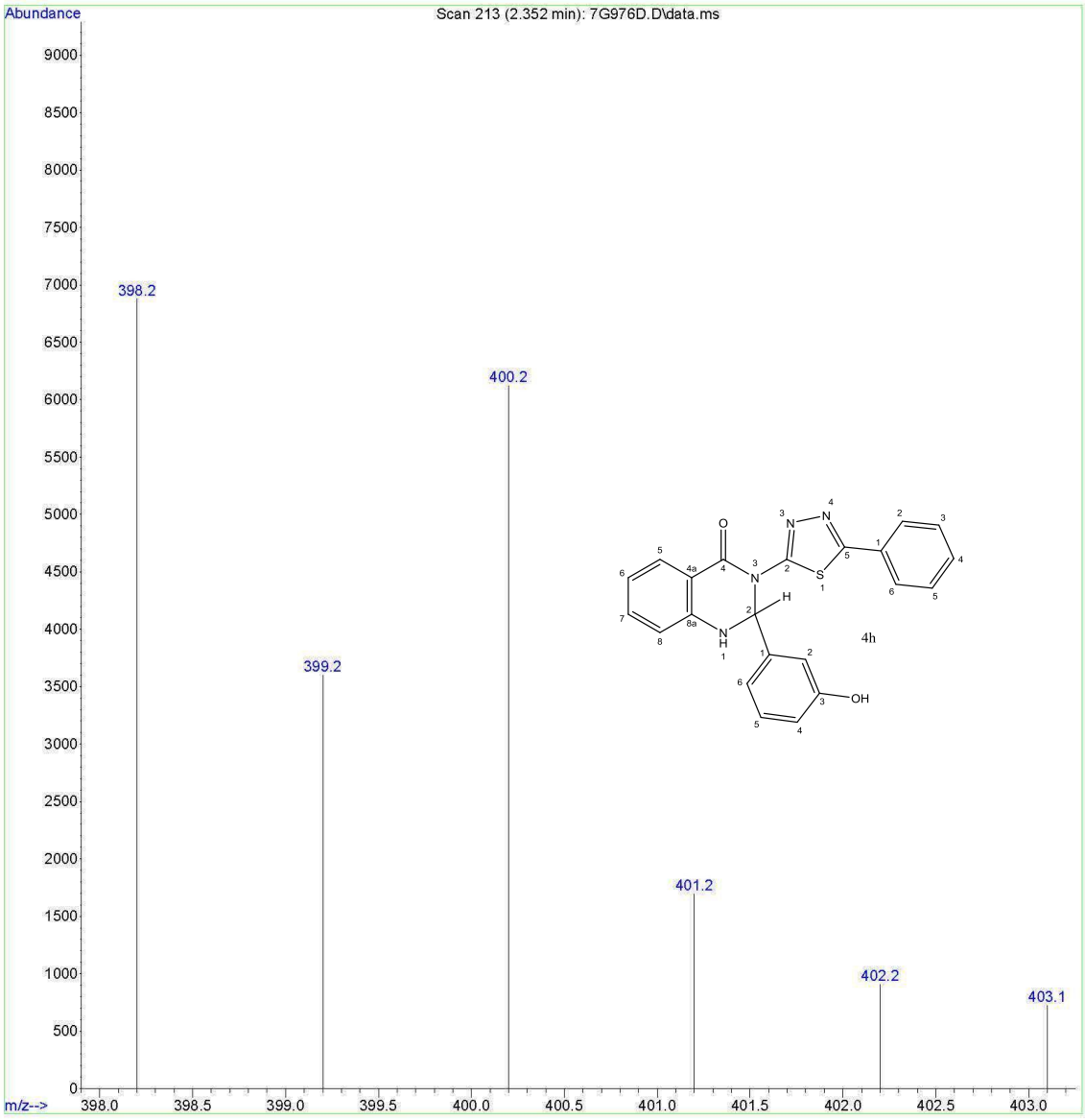

Fig 52. Mass spectrum of compound (4h), from a closer look

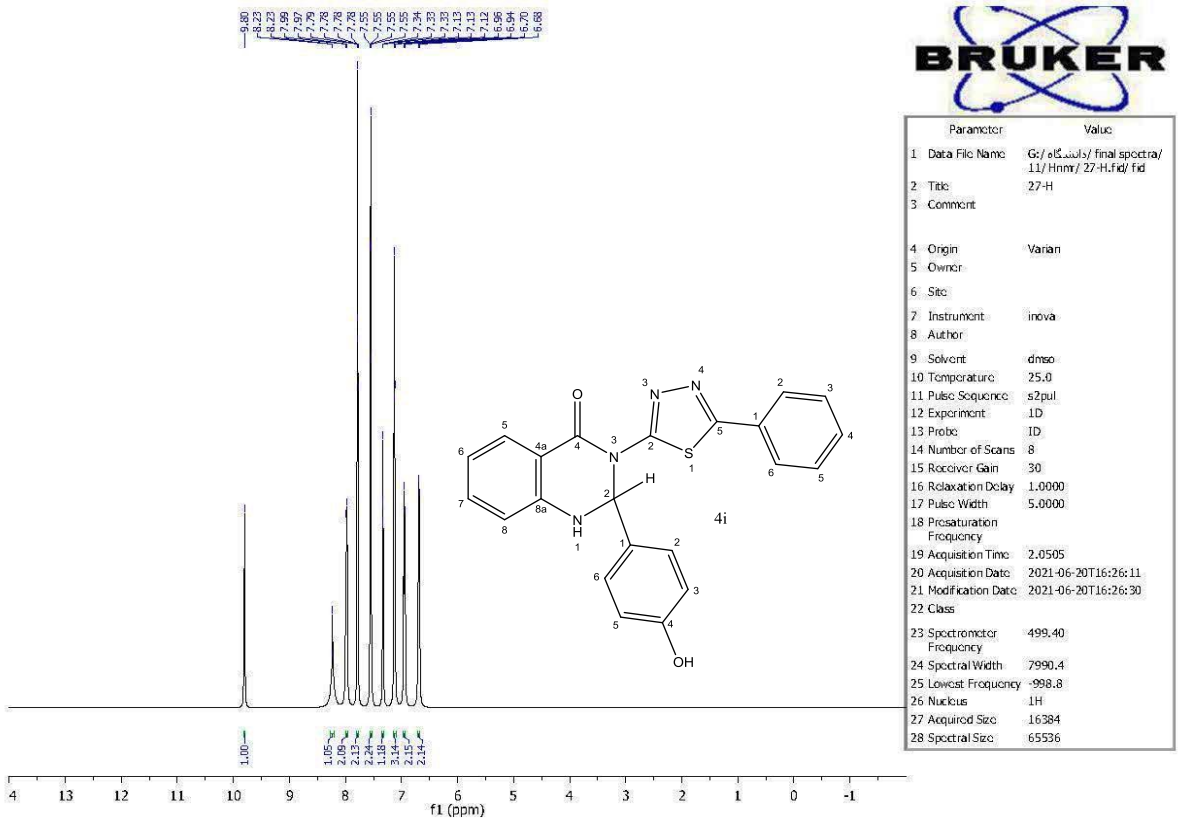

Fig 53. The whole range ^{1}H NMR spectrum of compound (4i)

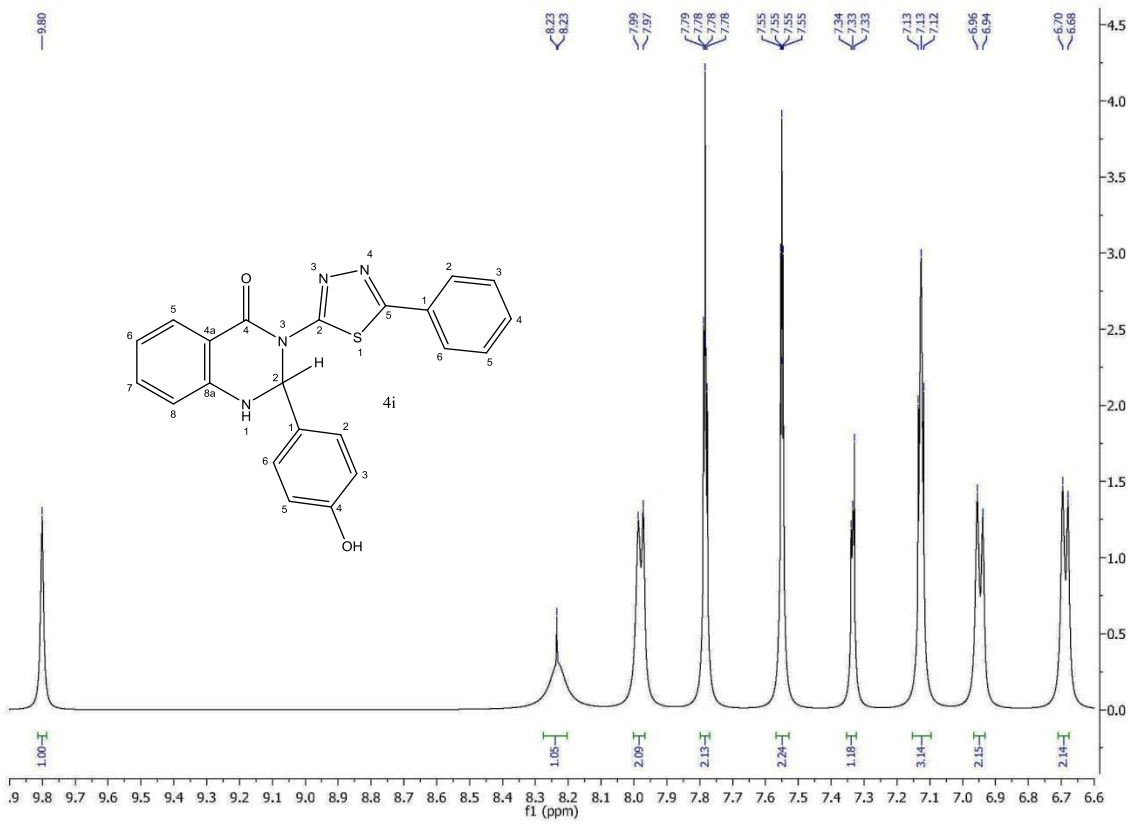

Fig 54. Aromatic range ^{1}H NMR spectrum of compound (4i)

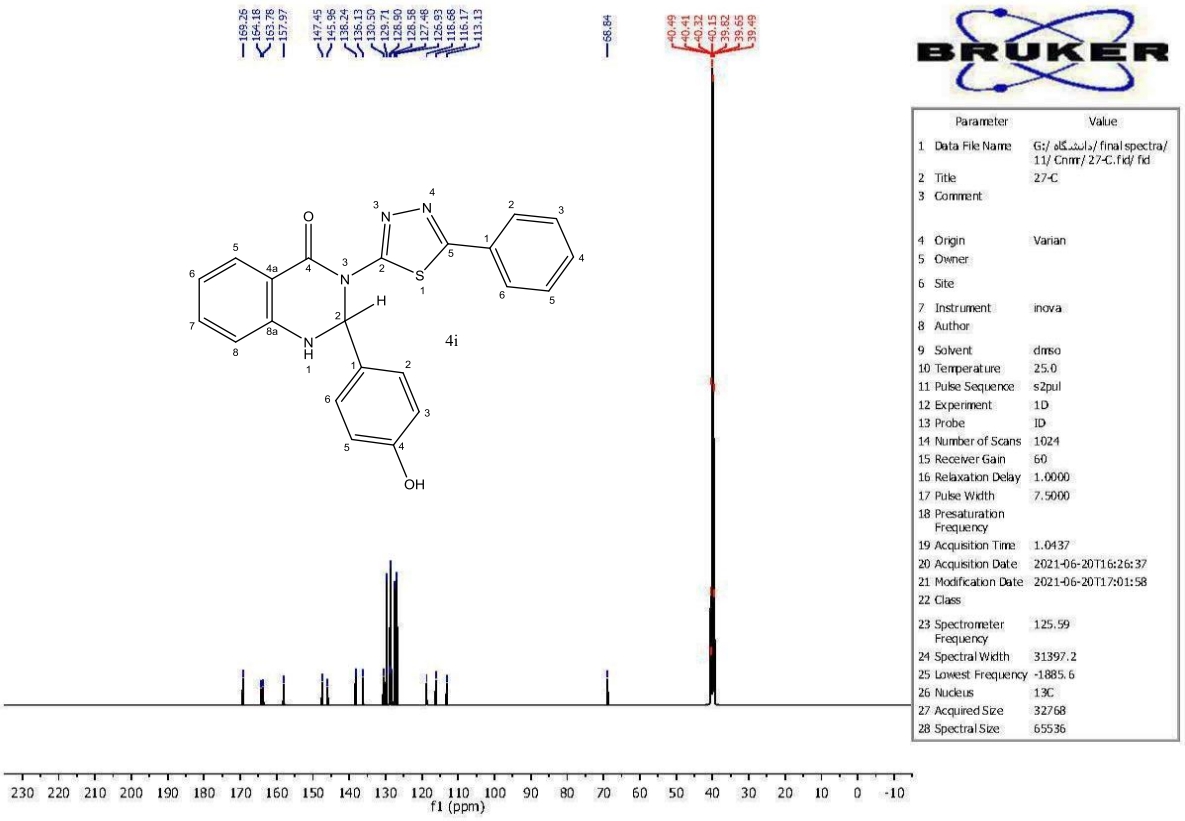

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Fig 55. The whole range ^{13}C NMR spectrum of compound (4i)

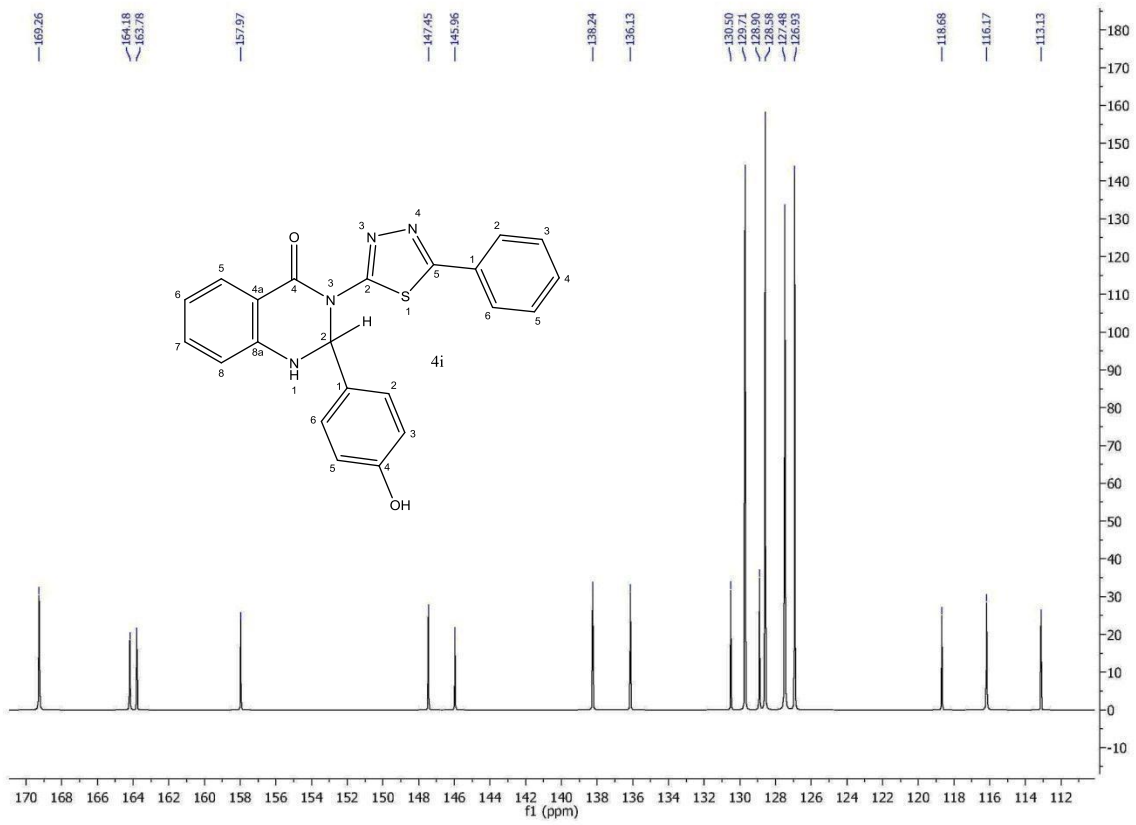

Fig 56. Doubl bond range ^{13}C NMR spectrum of compound (4i)

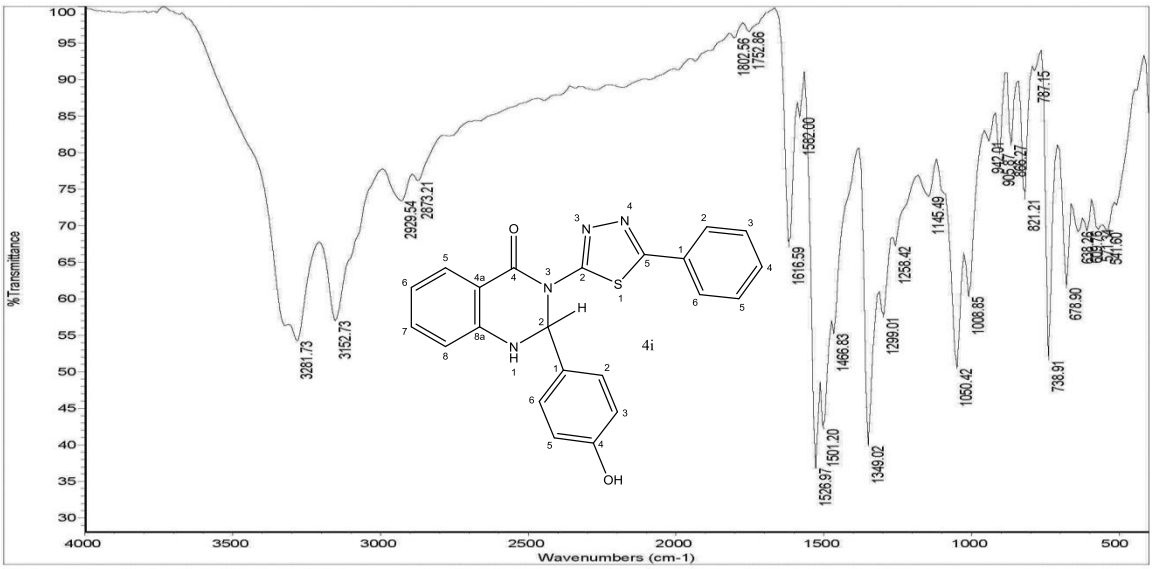

Fig 57. IR spectrum of compound (4i)

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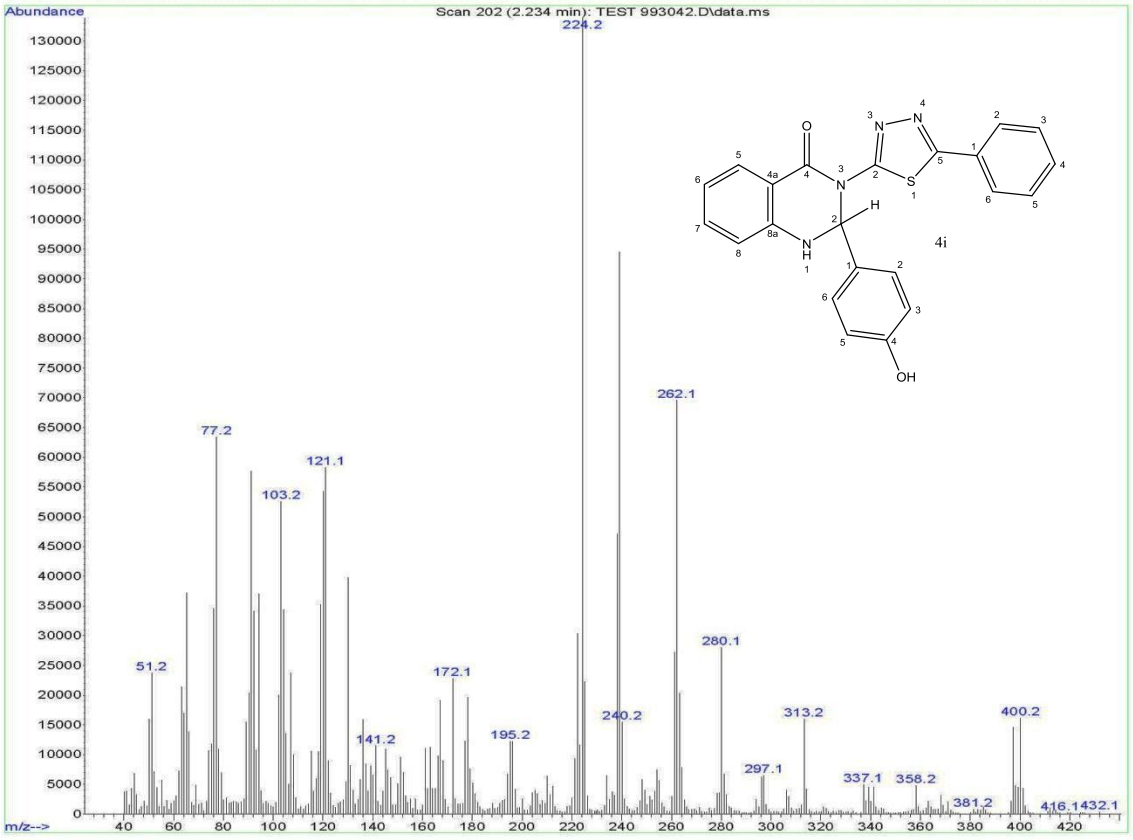

Fig 58. Mass spectrum of compound (4i)

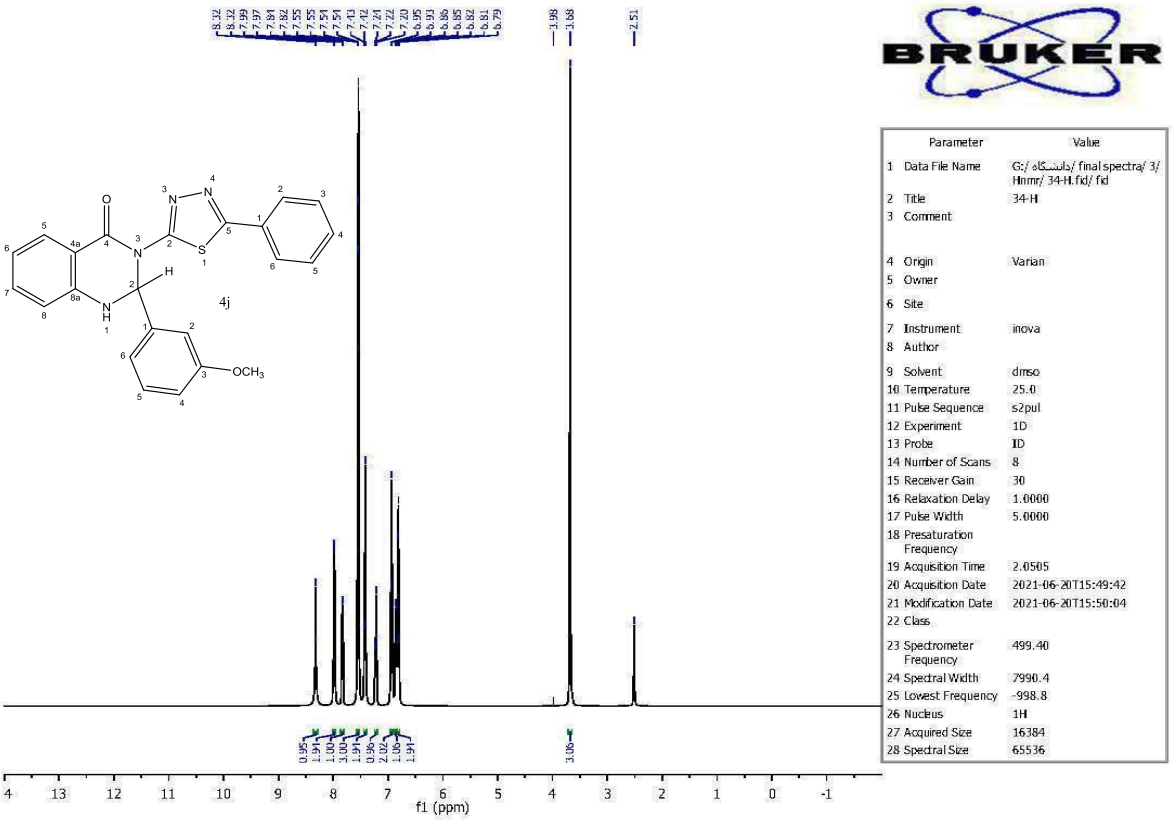

Fig 59. The whole range ^{1}H NMR spectrum of compound (4j)

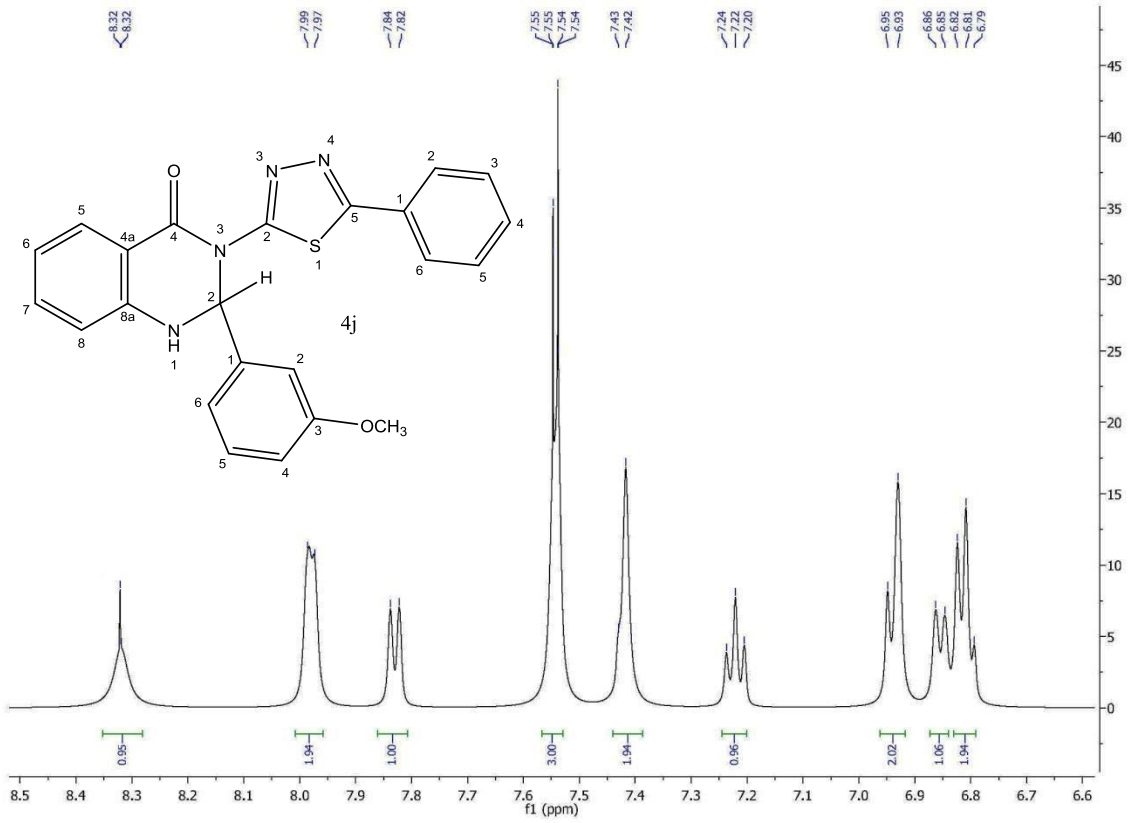

Fig 60. Aromatic range ^{1}H NMR spectrum of compound (4j)

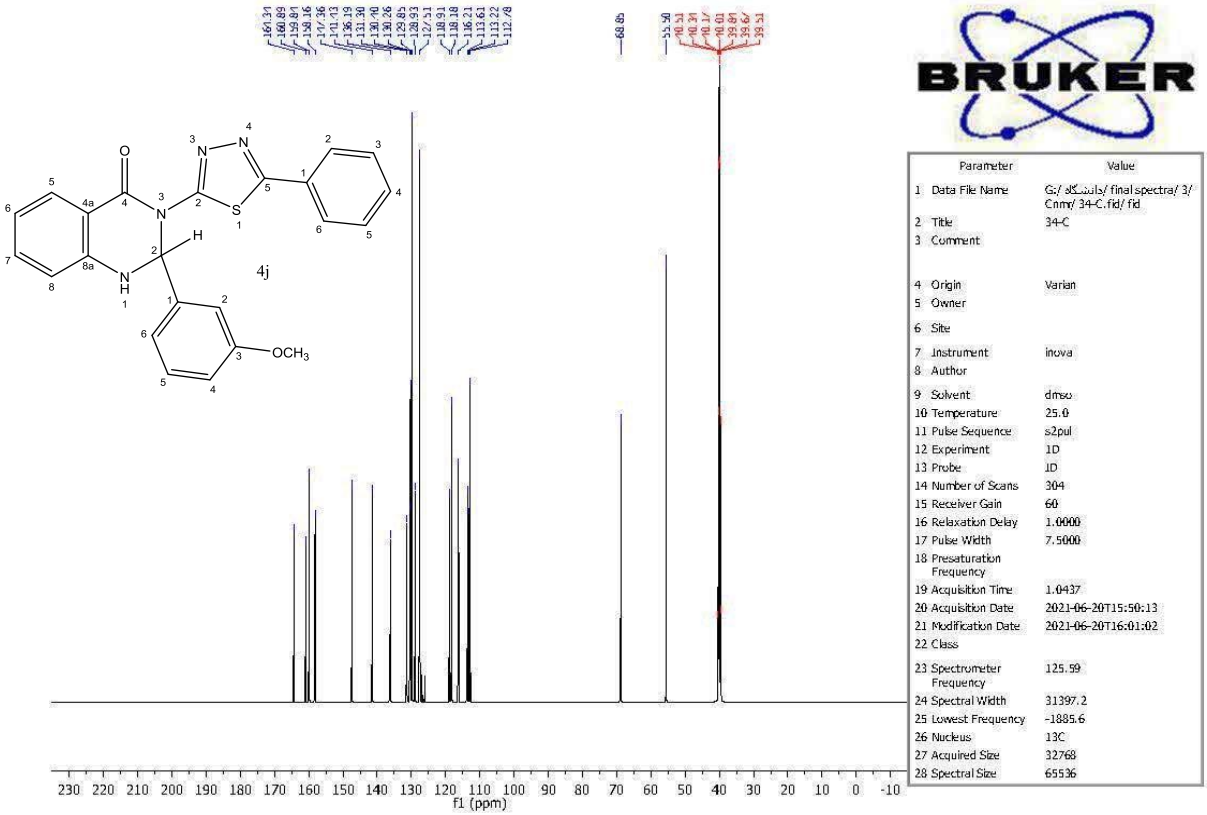

Fig 61. The whole range ^{13}C NMR spectrum of compound (4j)

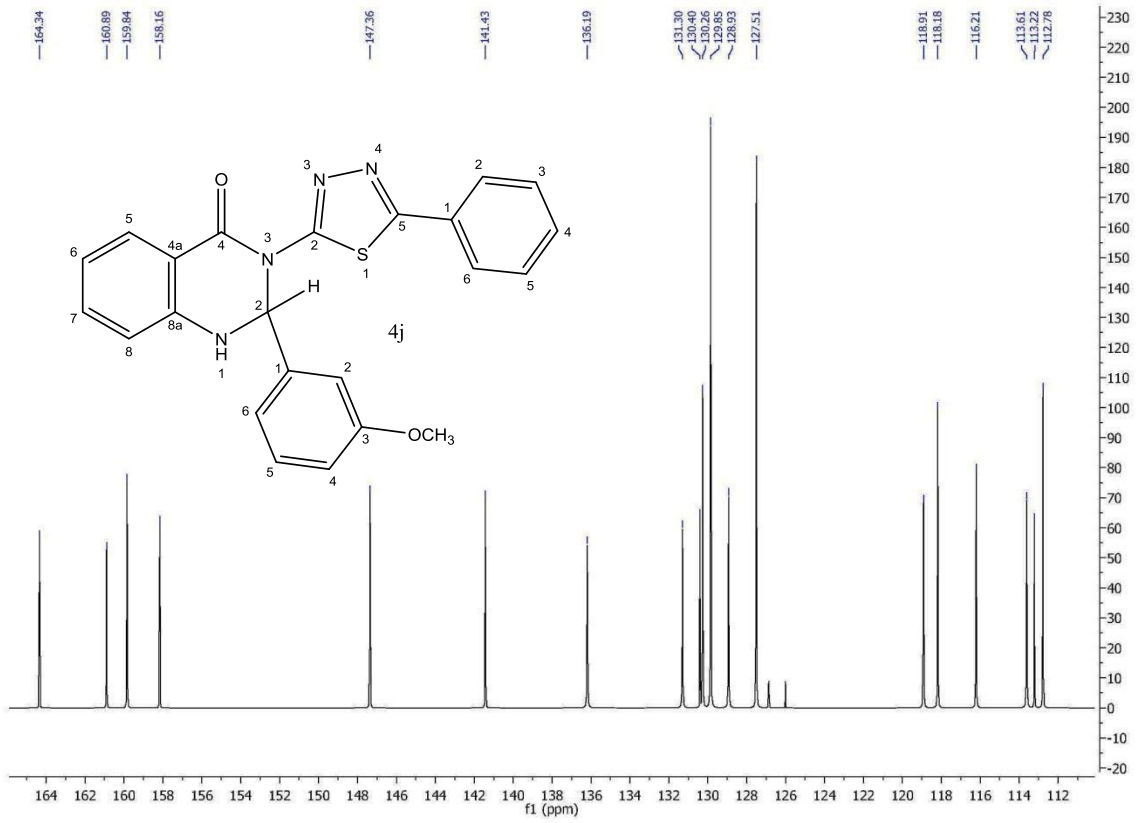

Fig 62. Doubl bond range ^{13}C NMR spectrum of compound (4j)

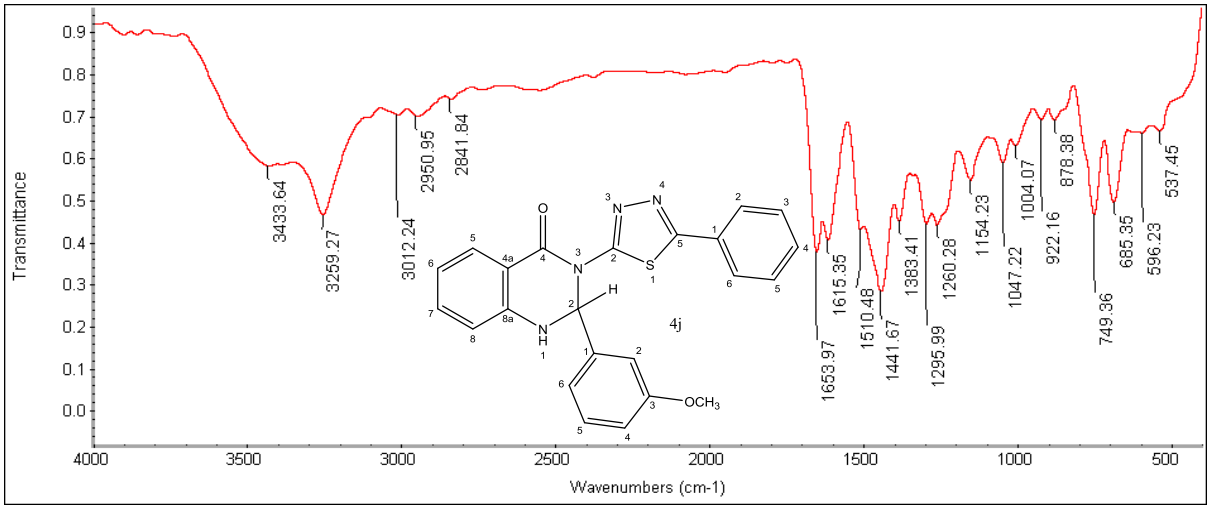

Fig 63. IR spectrum of compound (4j)

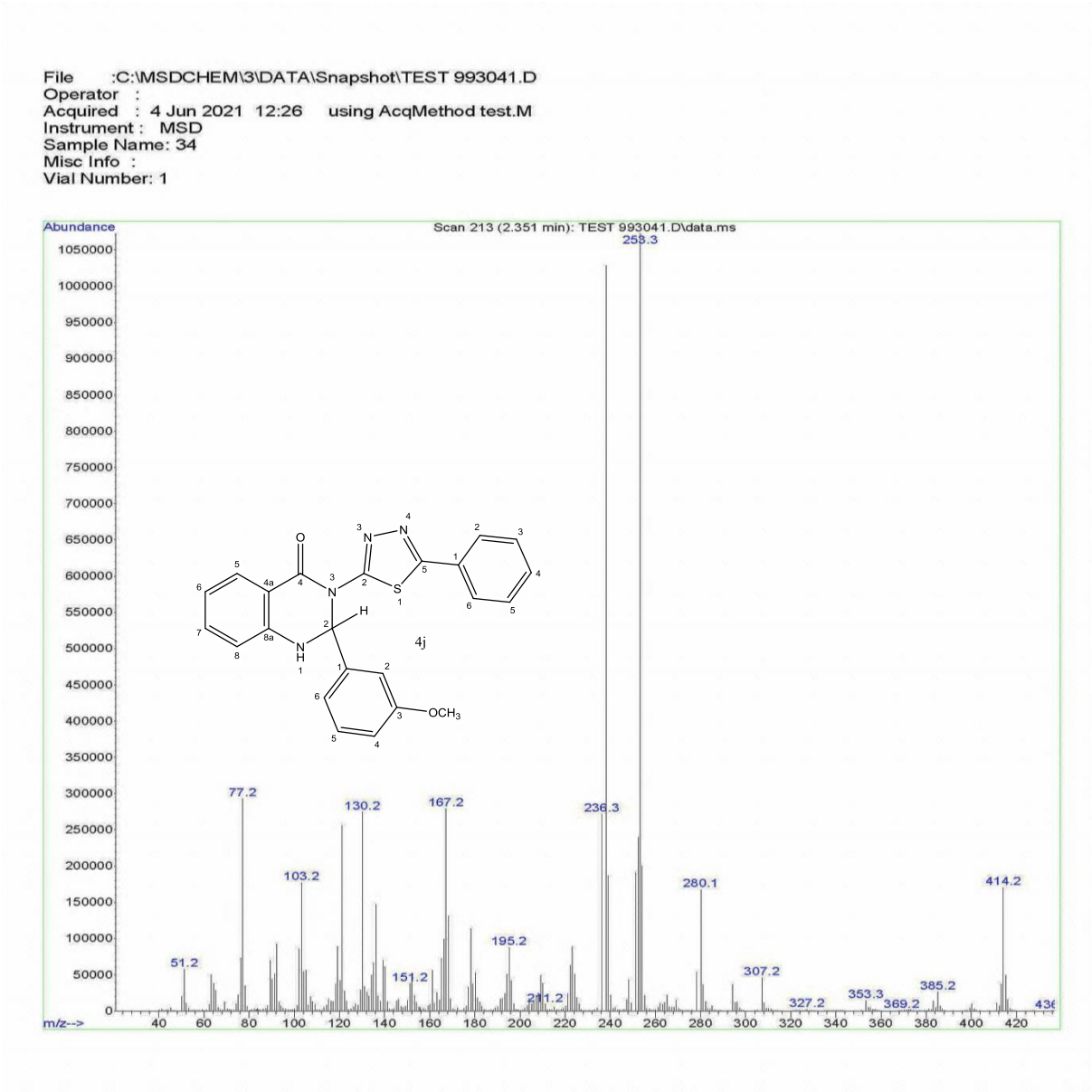

Fig 64. Mass spectrum of compound (4j)

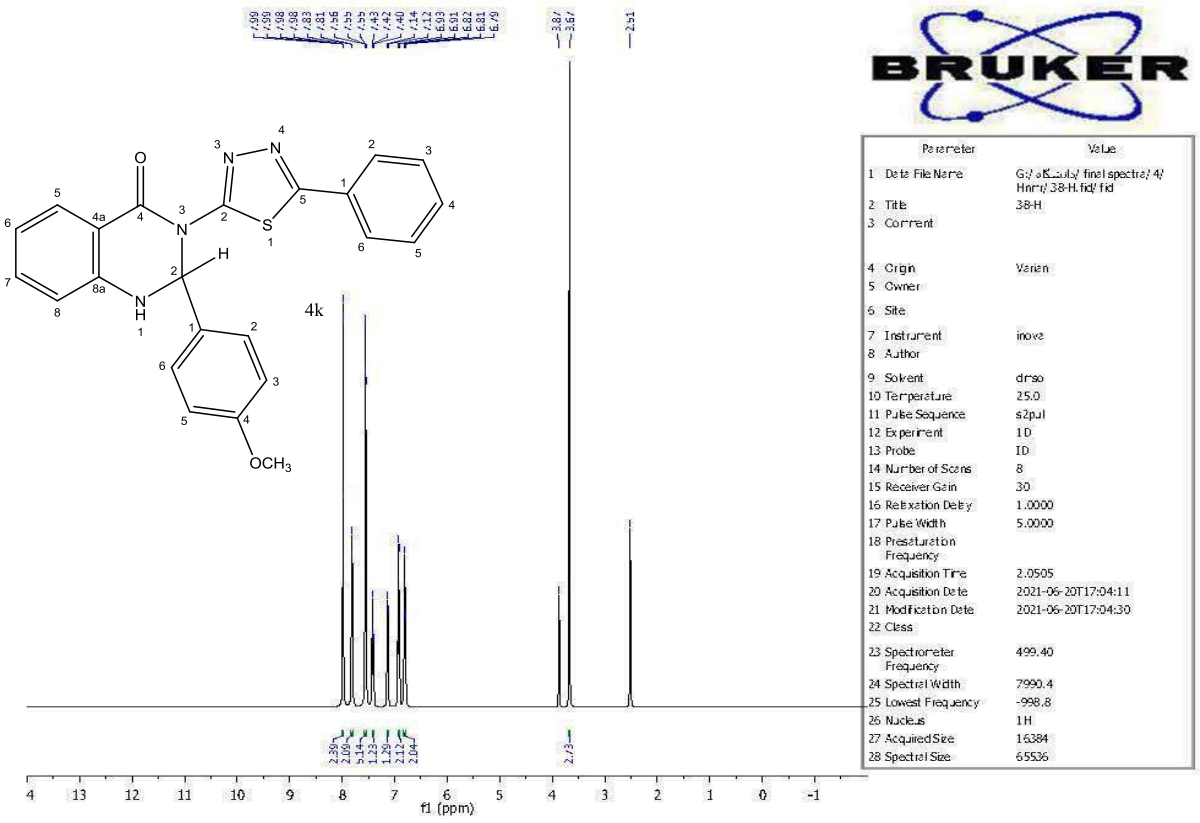

Fig 65. The whole range ^{1}H NMR spectrum of compound (4k)

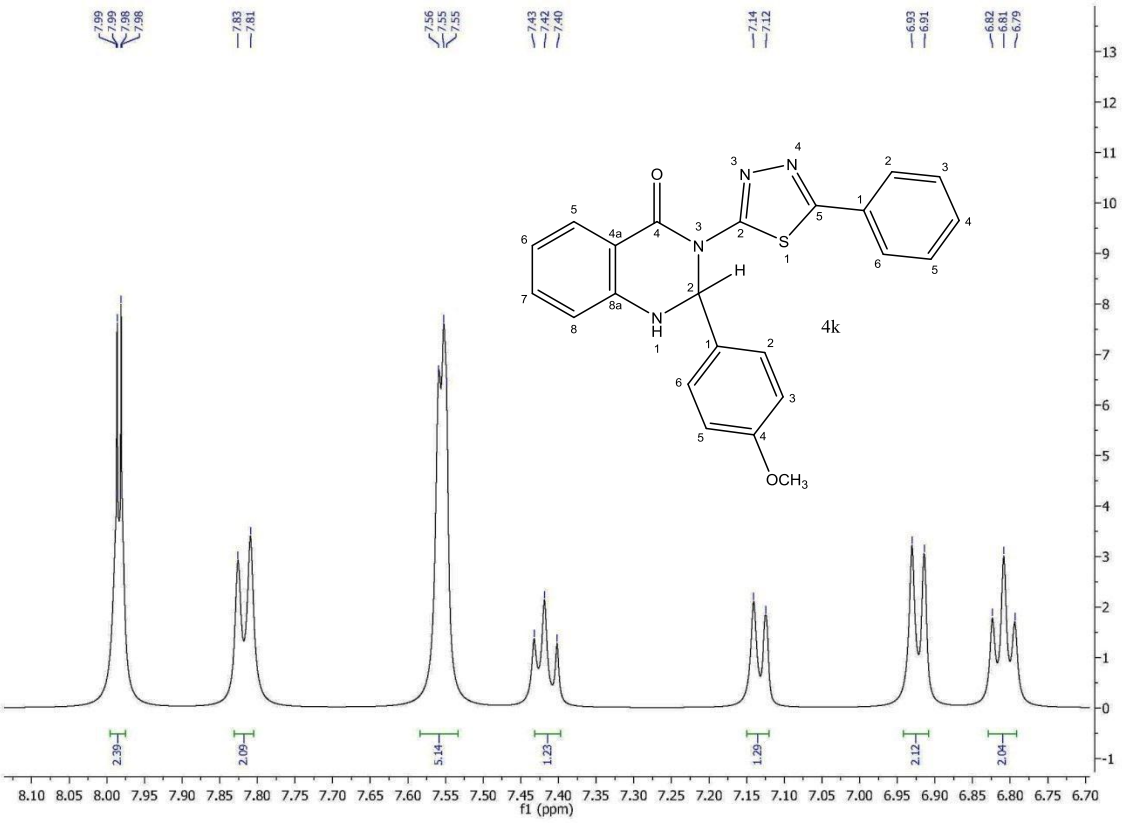

Fig 66. Aromatic range ^{1}H NMR spectrum of compound (4k)

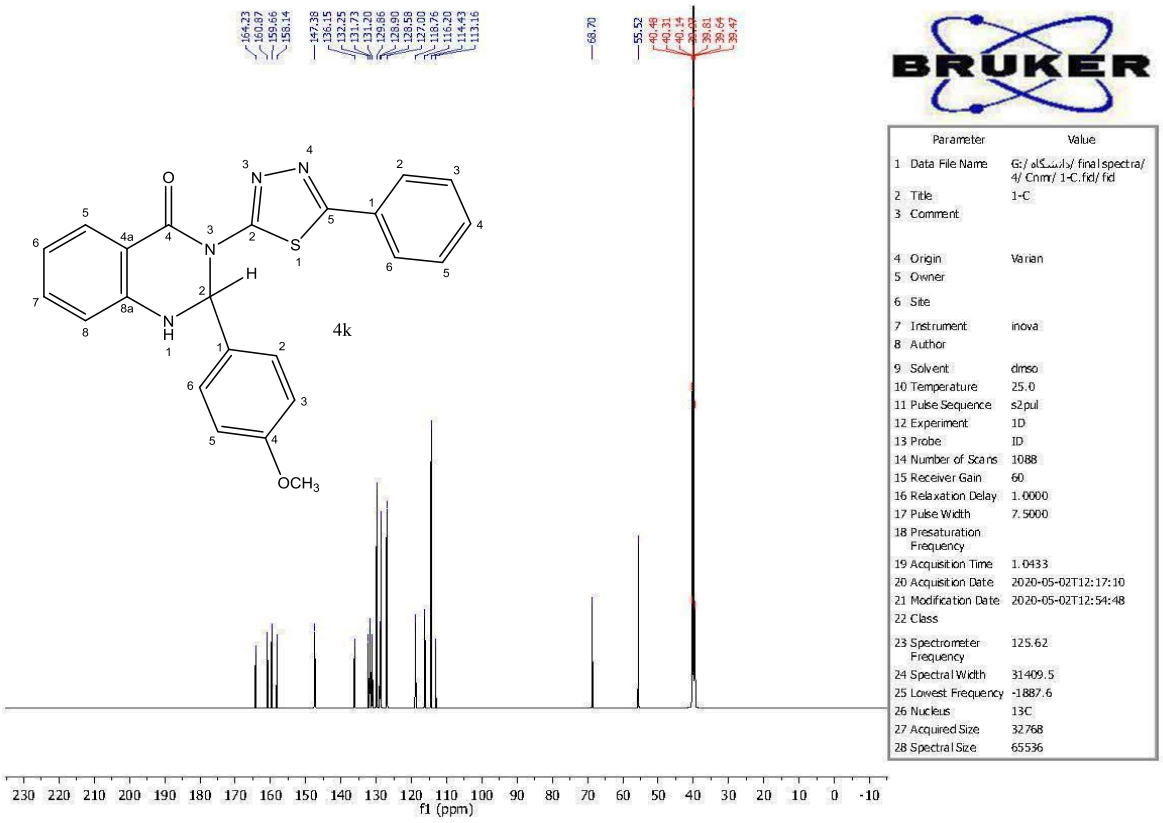

Fig 67. The whole range ^{13}C NMR spectrum of compound (4k)

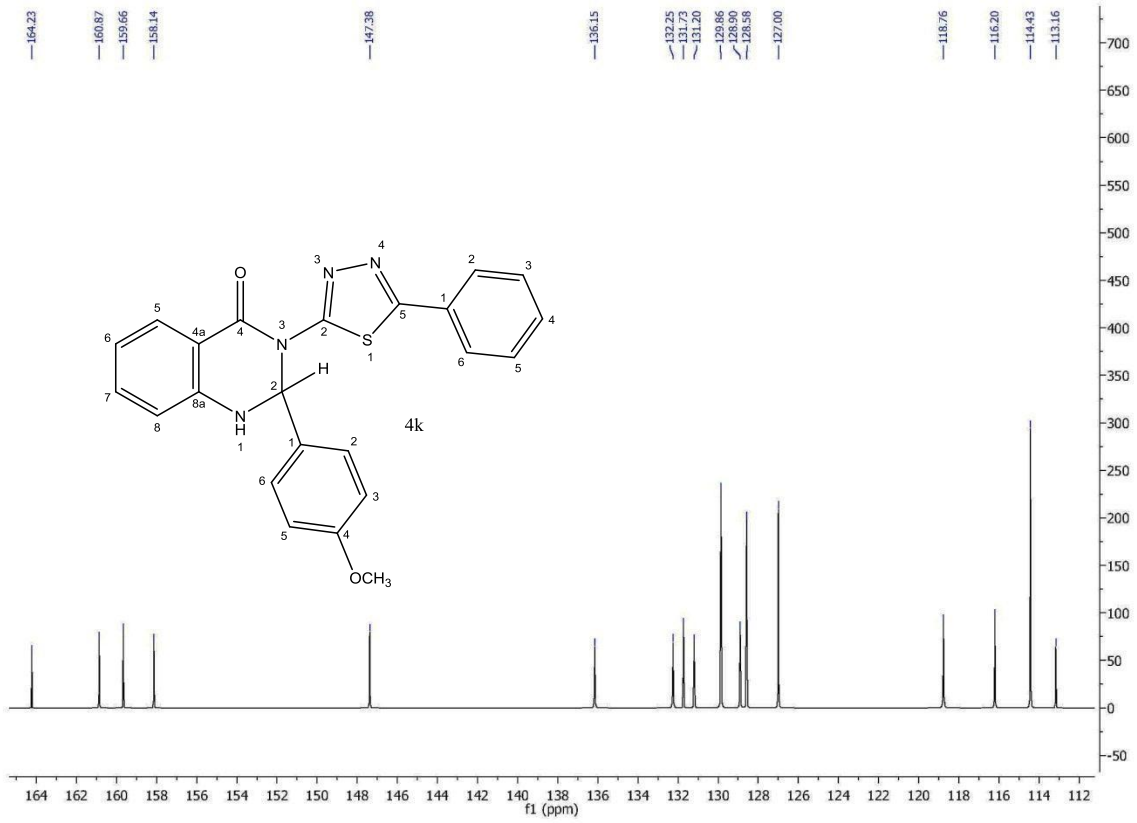

Fig 68. Doubl bond range ^{13}C NMR spectrum of compound (4k)

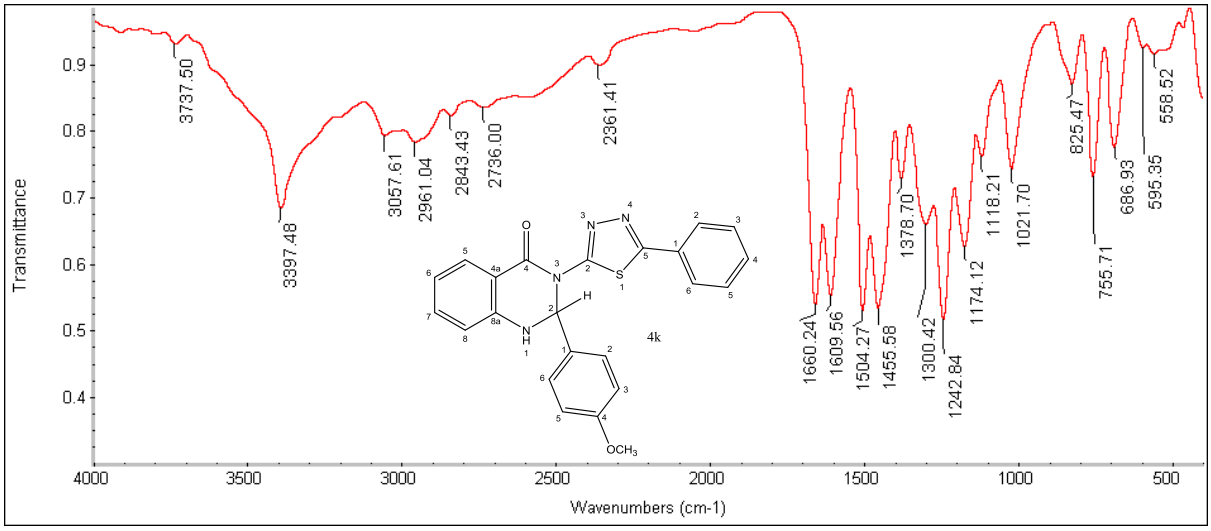

Fig 69. IR spectrum of compound (4k)

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Acquired : 4 Jun 2021 13:00 using AcqMethod test.M
Instrument : MSD
Sample Name: 38
Misc Info :
Vial Number: 1

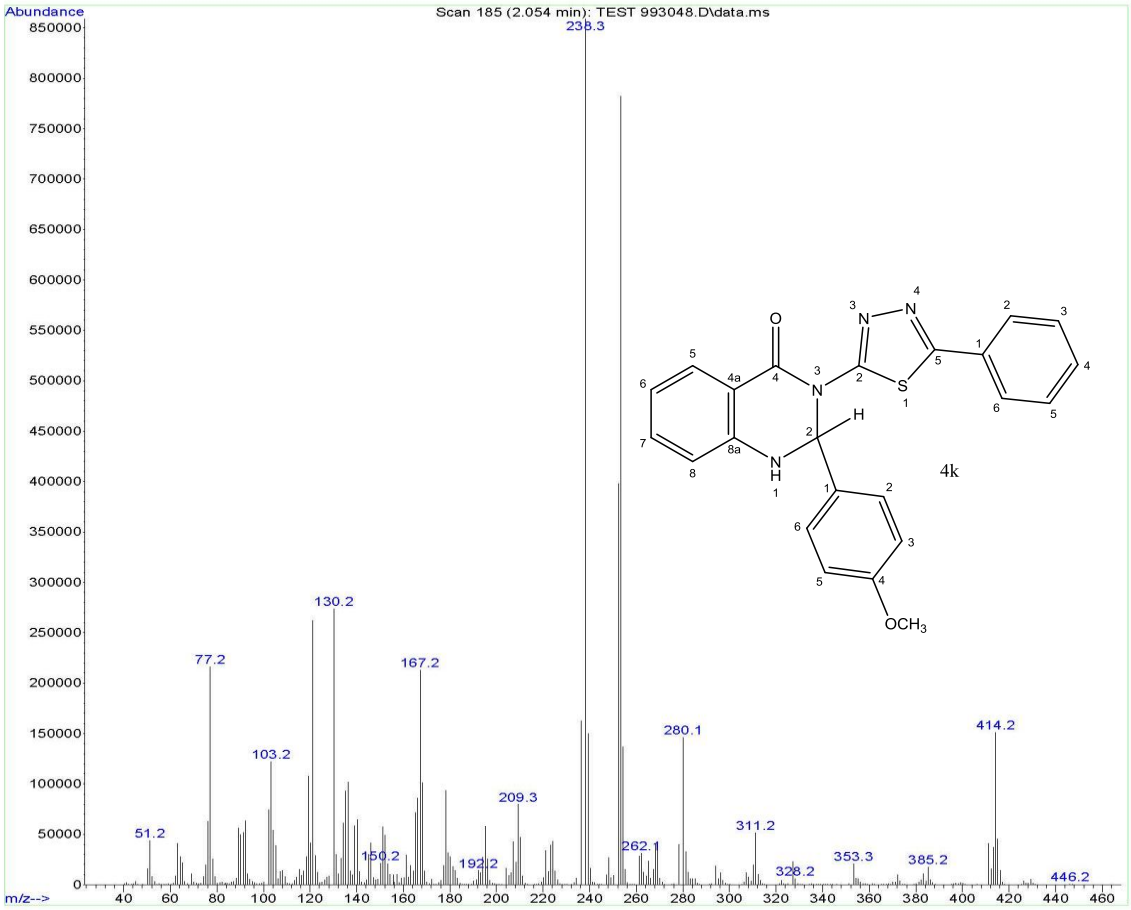


Fig 70. Mass spectrum of compound (4k)

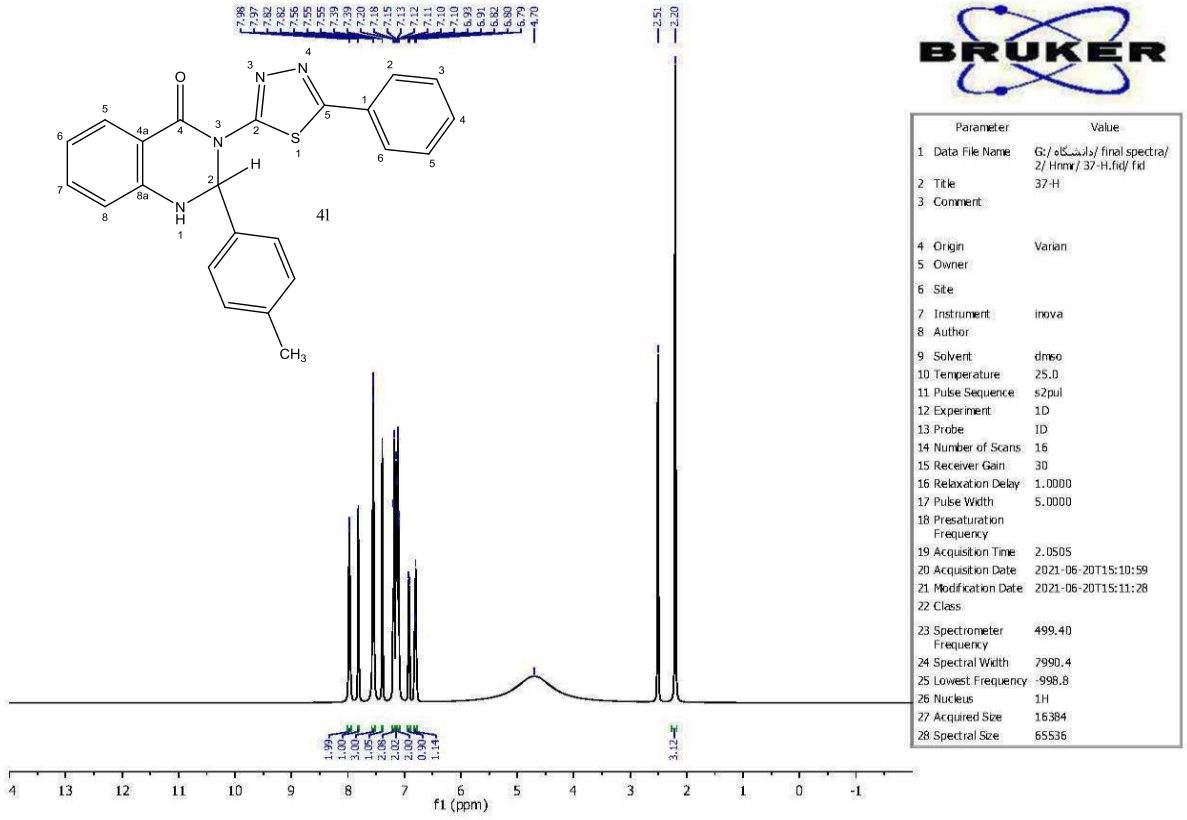


Fig 71. The whole range ^{1}H NMR spectrum of compound (4l)

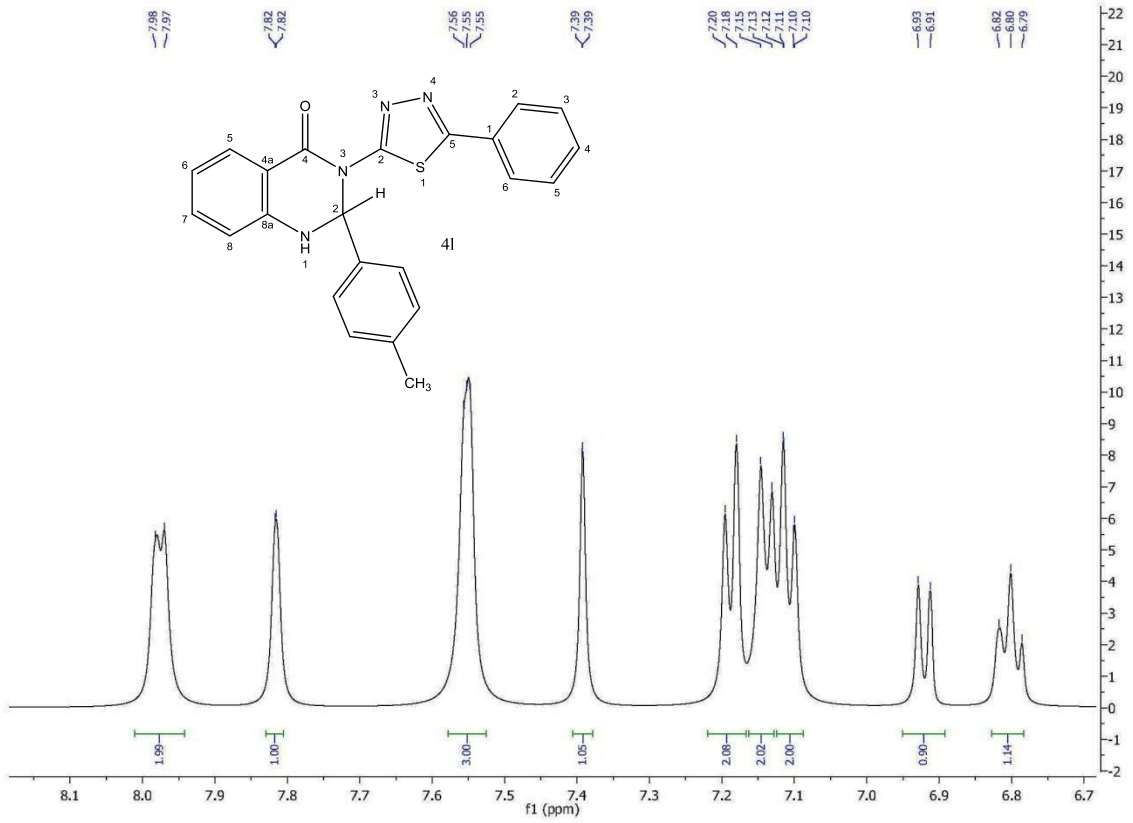
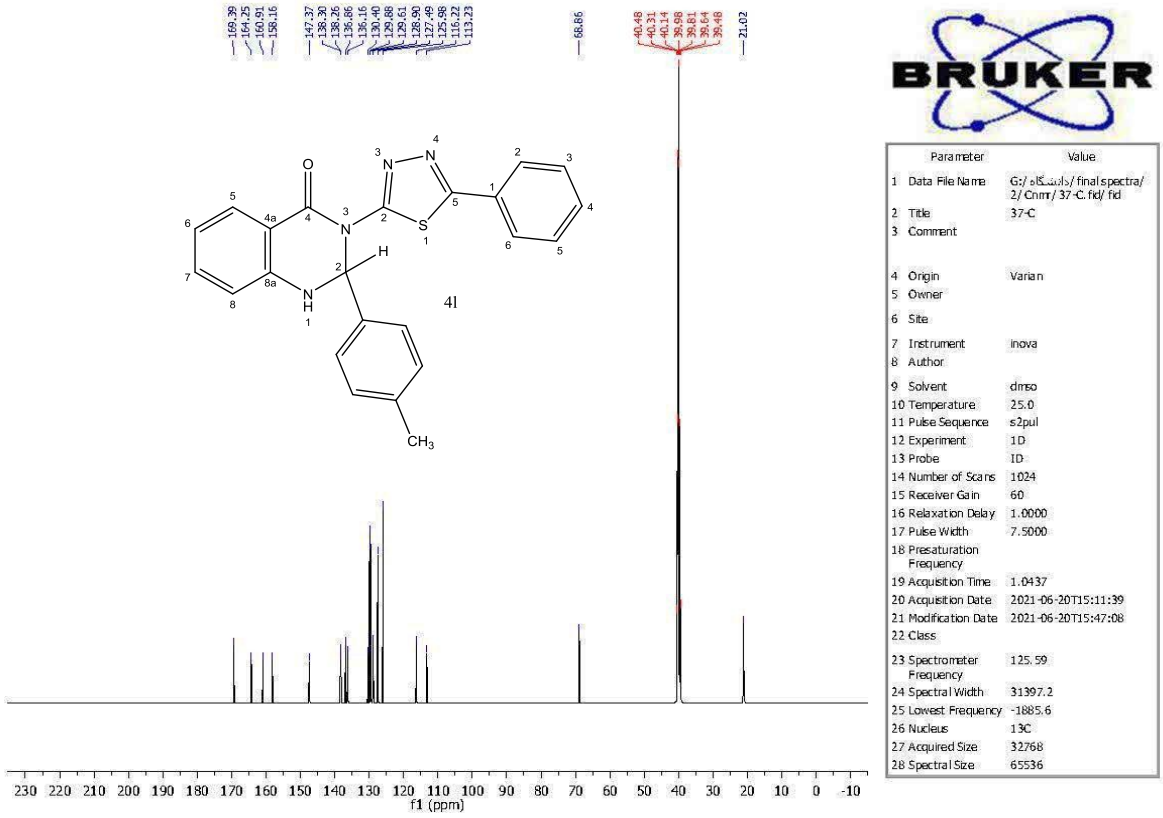


Fig 72. Aromatic range ^{1}H NMR spectrum of compound (4l)



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6	Site	
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8	Author	
9	Solvent	dmso
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12	Experiment	1D
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Fig 73. The whole range ^{13}C NMR spectrum of compound (4l)

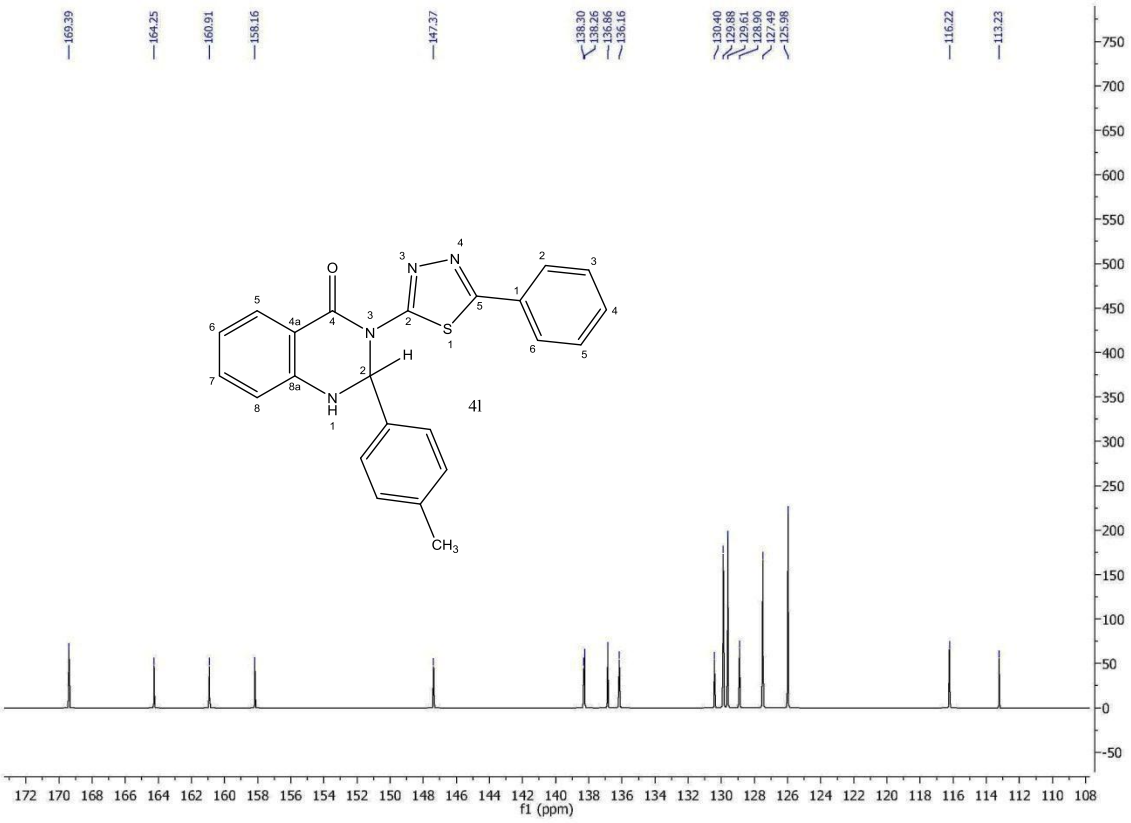

Fig 74. Doubl bond range ^{13}C NMR spectrum of compound (4l)

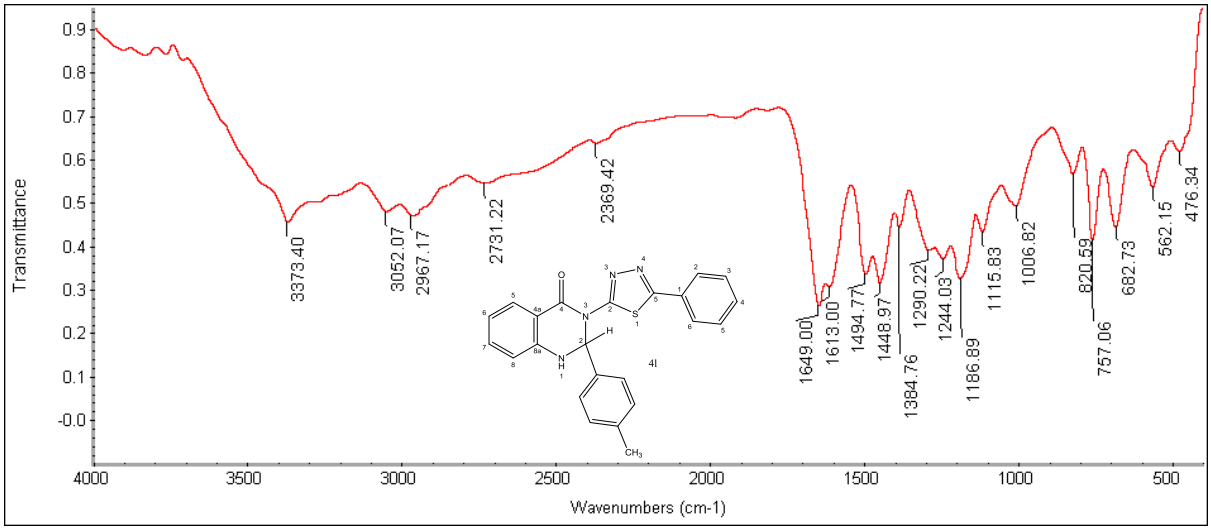

Fig 75. IR spectrum of compound (4l)

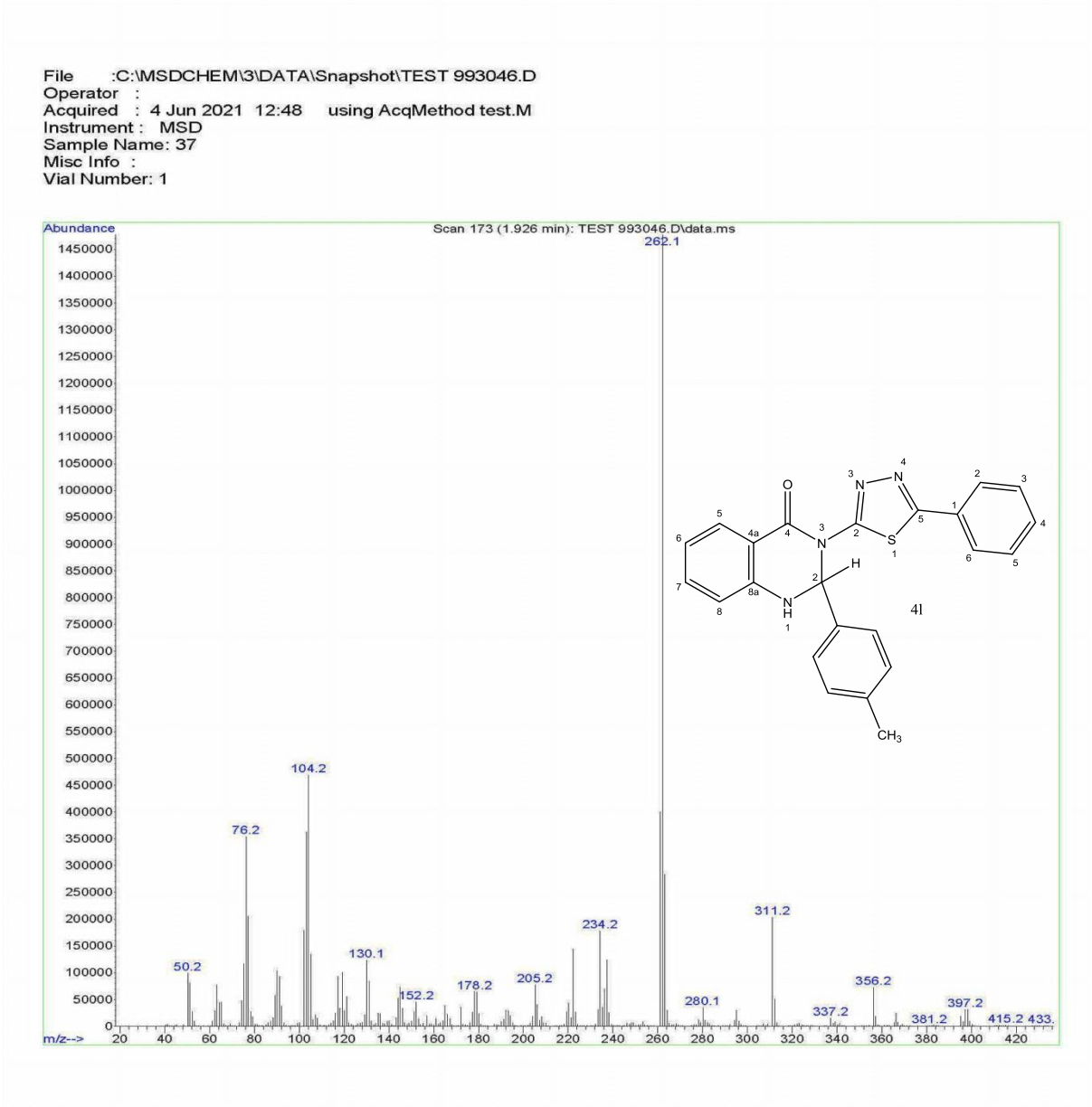

Fig 76. Mass spectrum of compound (4l)