This SI replaces the original version published on 24 Jun 2025, which contained an error in the spelling of B.A.'s name.

Supplementary Information

γ-Fe_2O_3@Zn-LDH-EAE-SO_3H for multi-component synthesis of chromeno[4,3-*b*]quinoline-6,8-dione derivatives

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General information

The purity determinations of the products and the progress of the reactions were accomplished by TLC on silica gel polygram STL G/UV 254 plates. The melting points of the products were determined with an Electrothermal Type 9100 melting point apparatusThe FT-IR spectra were recorded on pressed KBr pellets using an AVATAR 370 FT-IR spectrometer (Therma Nicolet spectrometer, USA) at room temperature in the range between 4000 and 400 cm^{-1} with a resolution of 4 cm^{-1}. The NMR spectra were obtained in Brucker Avance 300 MHz instruments in DMSO-d_6 as solvent. Mass spectra were determined at 70 eV on a CH7A Varianmat Bremem instrument elemental analyses were performed using a Thermo Finnigan Flash EA 1112 Series instrument. All yields refer to isolated products after purification by column chromatography.

Spectral and physical data of 2(a-p)

7-phenyl-7,10,11,12-tetrahydro-*6H*-chromeno[4,3-*b*]quinoline-6,8(*9H*)-dione (2a)[1]

Light yellow solid; (0.325g, 95%); Mp=324-325 °C (Lit. 324-326 °C); IR (KBr) (υ_{max}/cm^{-1}): 3338 (NH), 3092, 3047 (C-H aromatic), 2953, 2876 (C-H aliphatic), 1703(C=O), 1632, 1605 (C=C); ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ (ppm): 9.78 (s, 1H, NH), 8.34 (d, *J* = 8.1 Hz, 1H, ArH, H_1), 7.66 (t, *J* = 7.8 Hz, 1H, ArH, H_3), 7.46 (t, *J* = 7.6 Hz, 1H, ArH, H_2), 7.40 (d, *J* = 8.3 Hz, 1H, ArH, H_4), 7.28-7.19 (m, 4H, ArH, H_{14}, H_{15}, H_{17}, H_{18}), 7.12 (t, *J* = 5.9 Hz, 1H, ArH, H_{16}), 5.02 (s, 1H, CH, H_7), 2.91-2.83 (m, 1H, CH_2, H_9), 2.78-2.66 (m, 1H, CH_2, H_9), 2.36-2.25 (m, 2H, CH_2, H_{11}), 2.07-1.97 (m, 1H, CH_2, H_{10}), 1.95-1.85 (m, 1H, CH_2, H_{10}); ^{13}C NMR (75 MHz, DMSO-*d*$_6$): δ (ppm): 195.45 (C_8), 160.84 (C_6), 152.52 (C_{4a}), 152.17 (C_{11a}), 146.41 (C_{12a}), 142.55 (C_{13}), 132.44 (C_3), 128.53 (C_{17},C_{15}), 128.17 (C_{18},C_{14}), 126.69 (C_{16}), 124.49 (C_1), 123.45 (C_2), 117.36 (C_4), 113.52 (C_{12b}), 112.36 (C_{7a}), 102.28 (C_{6a}), 37.16 (C_9), 34.63 (C_7), 26.87 (C_{11}), 21.22 (C_{10}); MS: (m/z, %): 343 (M^+, 10), 341 (M^+-2, 70), 266 (68), 210 (10), 76 (10), 28 (100); Anal. Calcd. for $C_{22}H_{17}NO_3$ (343): C: 76.95, H: 4.99, N: 4.08%. Found: C: 76.88, H: 4.91, N: 3.99%.

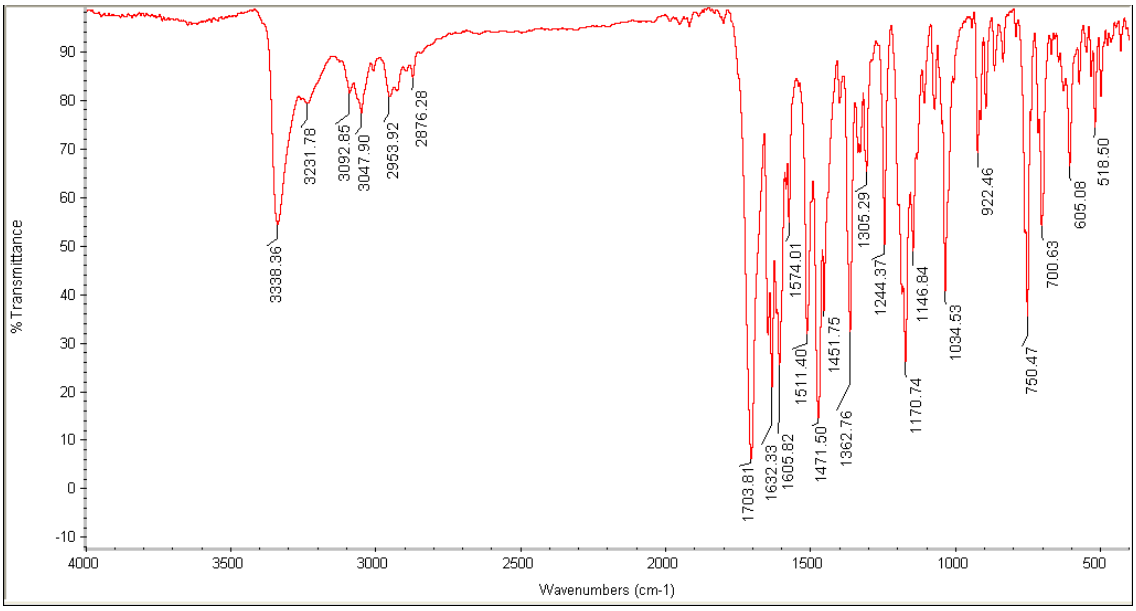


Figure 1. IR spectrum of compound **2a**

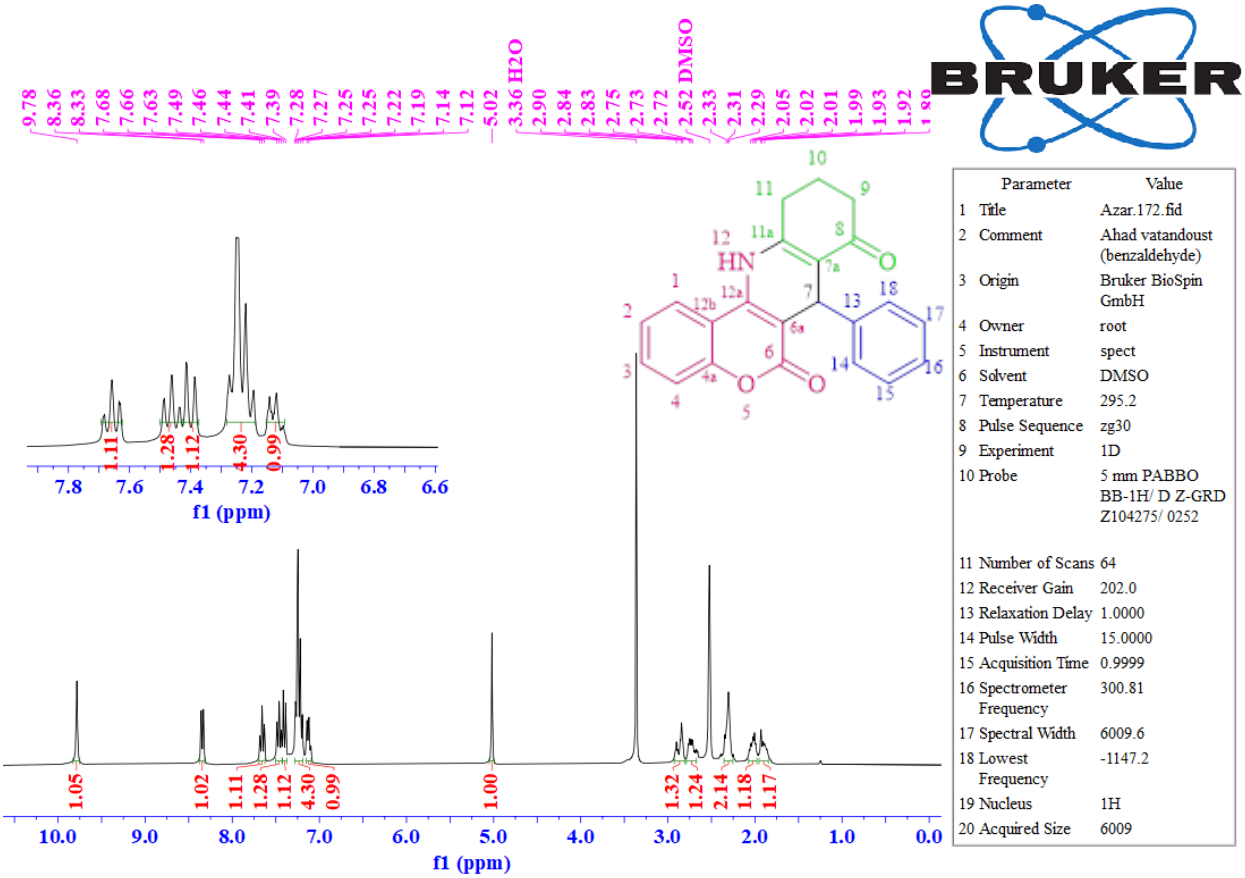


Figure 2. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of compound **2a**

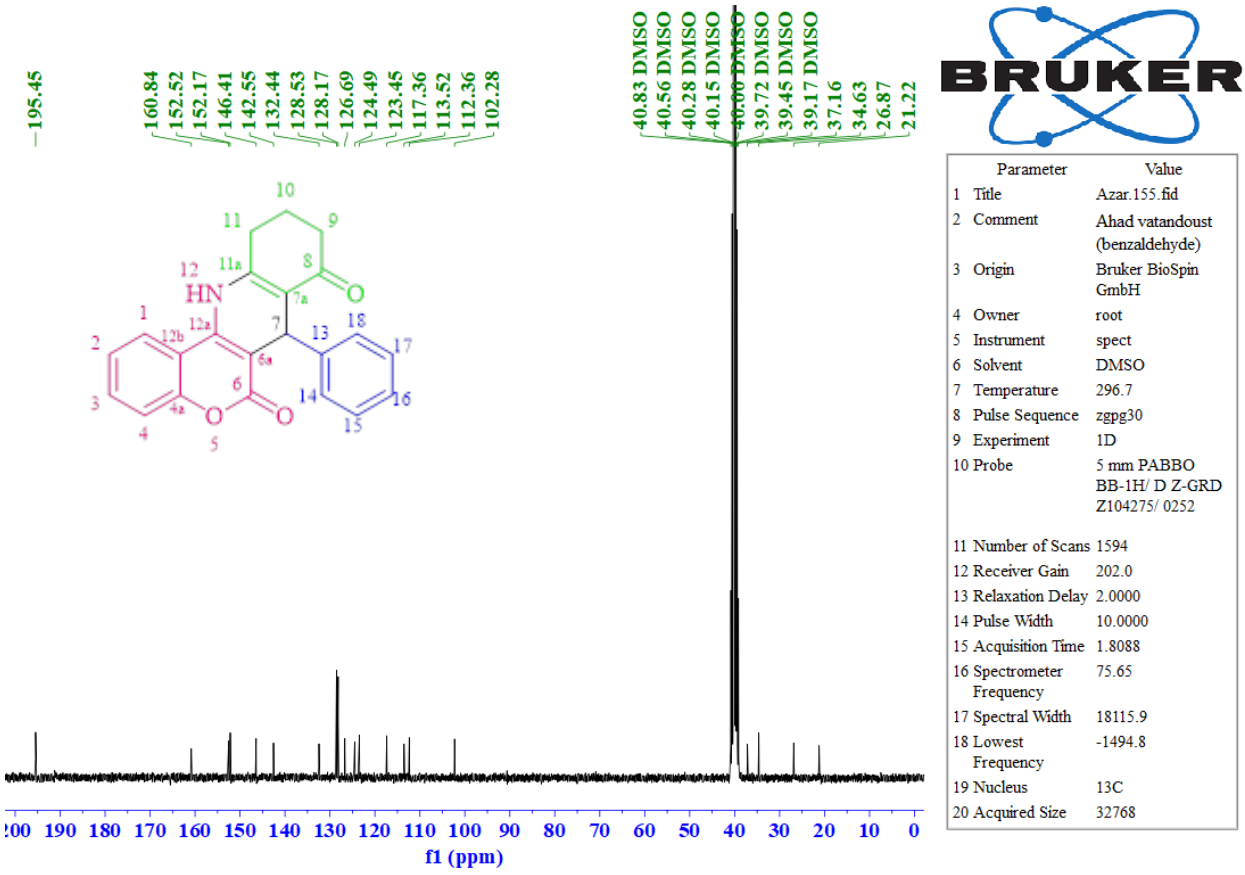


Figure 3. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of compound **2a**

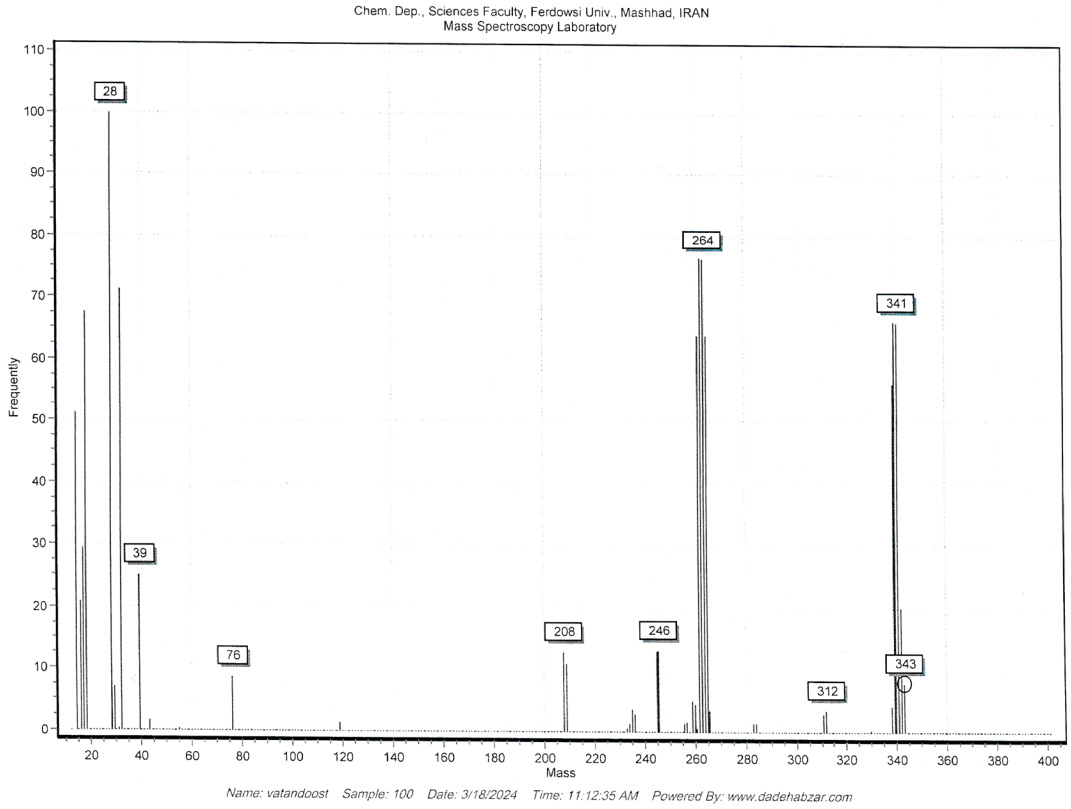


Figure 4. Mass spectrum of compound **2a**

Eager 300 Summarize Results

Date: 24/04/2024 at 13:07:30

Method Name: NCHS

Method Filename: Copy of N C H S-bkp.mth

Filename		As Method				Vial
Vatandoust-187						
# Group Sample Name		Tayp Weig. Prof. F			---	-----
187-1	100	UNK	0.622	6.25	---	-----
Component Name	Element%					
Nitrogen%	3.995759434					
Carbon%	76.88702856					
Hydrogen%	4.917127304					
Sulphur%	0					

1 Sample (s) in Group No:1

Component Name	Average
Nitrogen%	3.995759434
Carbon%	76.88702856
Hydrogen%	4.917127304
Sulphur%	0

Figure 5. CHNS spectrum of compound **2a**

Anal. Calcd. for $C_{22}H_{17}NO_3$ (343)		
C: 76.95 %	H: 4.99 %	N: 4.08 %

7-(4-nitrophenyl)-7,10,11,12-tetrahydro-6H-chromeno[4,3-b]quinoline-6,8(9H)-dione (2b)[2]

Light yellow solid; (0.368g, 95%); Mp=259-261 °C (Lit. 260-262 °C) ; IR (KBr) (υ_{max}/cm^{-1}): 3321 (NH), 3092 (C-H aromatic), 2942, 2884 (C-H aliphatic), 1671 (C=O), 1645, 1609 (C=C); ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ (ppm): 9.88 (s, 1H, NH), 8.35 (d, *J* = 8.1 Hz, 1H, ArH, H$_1$), 8.10 (d, *J* = 8.6 Hz, 2H, ArH, H$_{15}$, H$_{17}$), 7.66 (t, *J* = 7.8 Hz, 1H, ArH, H$_3$), 7.54 (d, *J* = 8.5 Hz, 2H, ArH, H$_{14}$, H$_{18}$), 7.46 (t, *J* = 7.7 Hz, 1H, ArH, H$_2$), 7.38 (d, *J* = 8.3 Hz, 1H, ArH, H$_4$), 5.11 (s, 1H, CH, H$_7$), 2.89-2.85 (m, 1H, CH$_2$, H$_9$), 2.78-2.67 (m, 1H, CH$_2$, H$_9$), 2.34-2.26 (m, 2H, CH$_2$, H$_{11}$), 2.07-1.99 (m, 1H, CH$_2$, H$_{10}$), 1.93-1.85 (m, 1H, CH$_2$, H$_{10}$); ^{13}C NMR (75 MHz, DMSO-*d*$_6$): δ (ppm): 195.41 (C$_8$), 160.71 (C$_6$), 153.66 (C$_{4a}$), 152.80 (C$_{11a}$), 152.63 (C$_{13}$), 146.44 (C$_{12a}$), 143.07 (C$_{16}$), 132.71 (C$_3$), 129.64 (C$_{14}$,C$_{18}$), 124.56 (C$_1$), 123.78 (C$_{15}$,C$_{17}$), 123.62 (C$_2$), 117.41 (C$_4$), 113.32 (C$_{12b}$), 111.48 (C$_{7a}$), 101.15 (C$_{6a}$), 37.02 (C$_9$), 35.50 (C$_7$), 26.89 (C$_{11}$), 21.13 (C$_{10}$); MS: (m/z, %): 388 (M$^+$,10), 386 (M$^+$-2, 28), 266 (35), 28 (100); Anal. Calcd. for C$_{22}$H$_{17}$NO$_3$(388): C: 68.04, H: 4.15, N: 7.21%. Found: C: 67.91, H: 4.08, N: 7.12%.

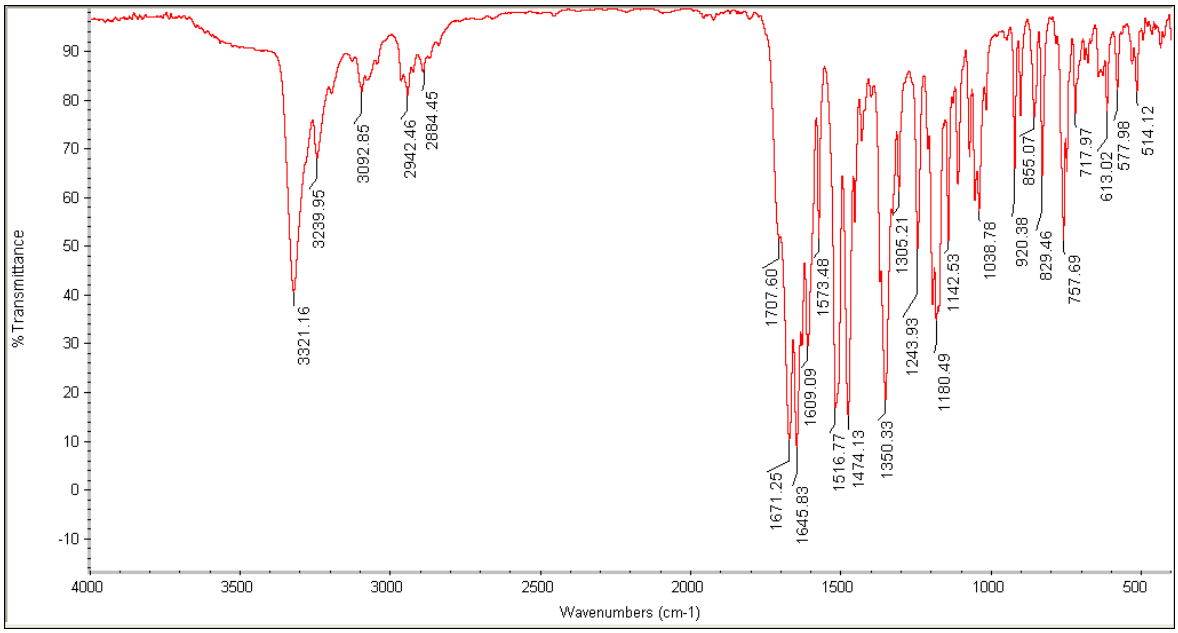


Figure 6. IR spectrum of compound **2b**

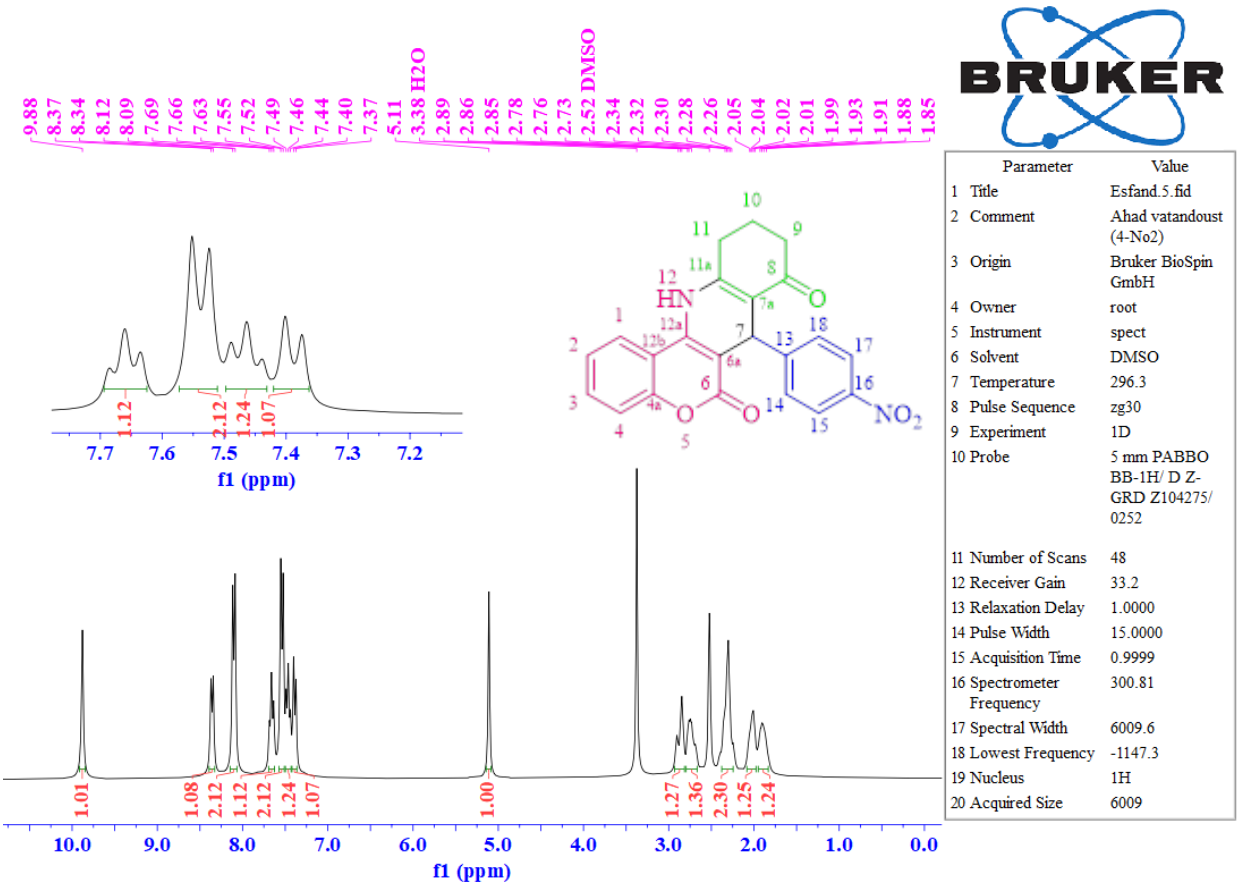


Figure 7. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of compound **2b**

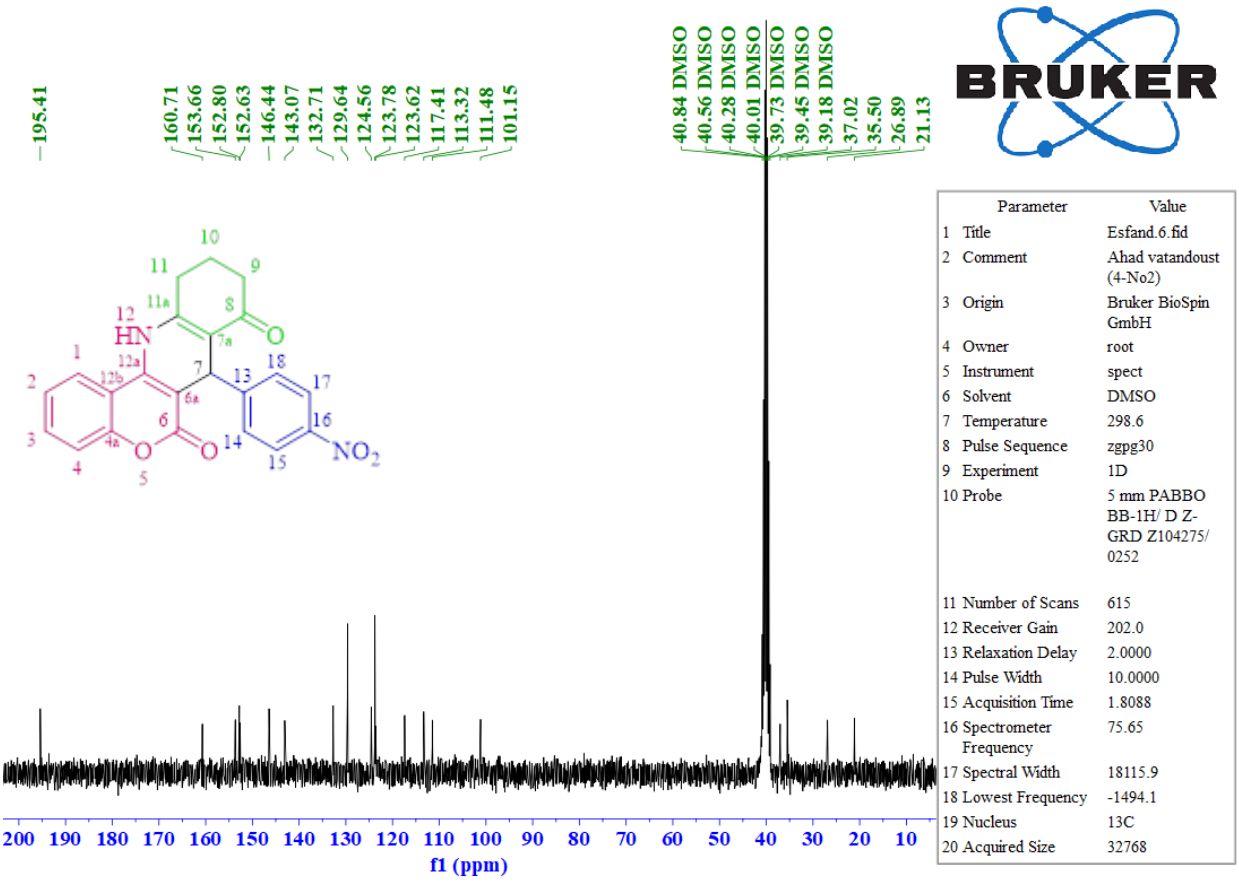


Figure 8. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of compound **2b**

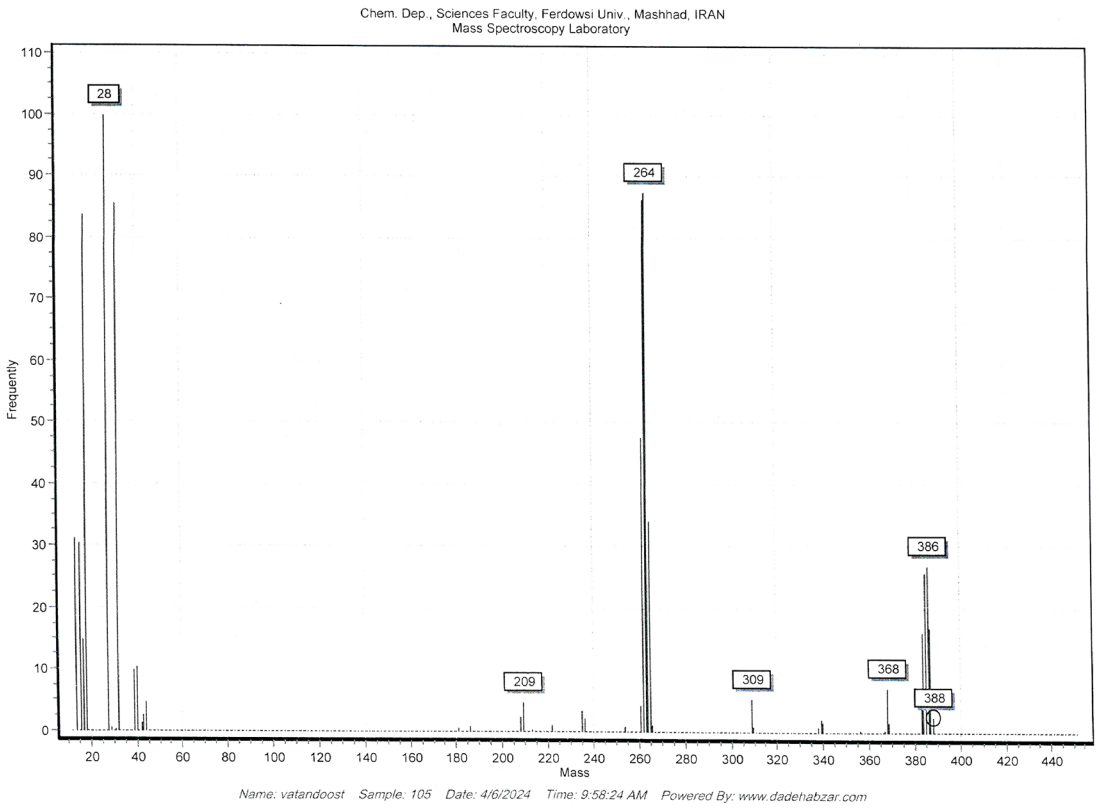


Figure 9. Mass spectrum of compound **2b**

Eager 300 Summarize Results

Date: 24/04/2024 at 13:05:03

Method Name: NCHS

Method Filename: Copy of N C H S-bkp.mth

Filename		As Method				Vial
Vatandoust-174						
# Group Sample Name		Tayp Weig. Prof. F			---	-----
174-1	105	UNK	0.643	6.25	---	-----

Component Name	Element%
Nitrogen%	7.121024971
Carbon%	67.91162109
Hydrogen%	4.087371998
Sulphur%	0

1 Sample (s) in Group No:1

Component Name	Average
Nitrogen%	7.121024971
Carbon%	67.91162109
Hydrogen%	4.087371998
Sulphur%	0

Figure 10. CHNS spectrum of compound **2b**

Anal. Calcd. for $C_{22}H_{17}NO_3$(388)		
C: 68.04 %	H: 4.15 %	N: 7.21 %

7-(4-cyanophenyl)-7,10,11,12-tetrahydro-6H-chromeno[4,3-b]quinoline-6,8(9H)-dione (2c)

Light yellow solid; (0.349g, 95%); Mp=336-338 °C; IR (KBr) (υ_{max}/cm^{-1}): 3341 (NH), 3096, 3051 (C-H aromatic), 2937, 2880 (C-H aliphatic), 2224 (CN), 1684 (C=O), 1640,1605 (C=C); ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ (ppm): 9.85 (s, 1H, NH), 8.35 (d, *J* = 8.0 Hz, 1H, ArH, H_1), 7.71-7.63 (m, 3H, ArH, H_2, H_3, H_4), 7.48-7.37 (m, 4H, ArH, H_{14}, H_{15}, H_{17}, H_{18}), 5.06 (s, 1H, CH, H_7), 2.90-2.84 (m, 1H, CH_2, H_9), 2.75-2.67 (m, 1H, CH_2, H_9), 2.33-2.28 (m, 2H, CH_2, H_{11}), 2.02-1.98(m, 1H, CH_2, H_{10}), 1.93-1.85 (m, 1H, CH_2, H_{10}); ^{13}C NMR (75 MHz, DMSO-*d*$_6$): δ (ppm): 195.42 (C_8), 160.74 (C_6), 152.74 (C_{4a}), 152.60 (C_{11a}), 151.64 (C_{12a}), 143.01 (C_{13}), 132.66 (C_3), 132.54 (C_{15},C_{17}), 129.40 (C_{14},C_{18}), 124.54 (C_1), 123.59 (C_2), 119.37 (CN), 117.39 (C_4), 113.33 (C_{12b}), 111.51 (C_{7a}), 109.52 (C_{16}), 101.23 (C_{6a}), 37.02 (C_9), 35.54 (C_7), 26.86 (C_{11}), 21.14 (C_{10}); MS: (m/z, %): 368 (M^+, 10), 366 (M^+-2, 70), 266 (80), 28 (75); Anal. Calcd. for $C_{23}H_{16}N_2O_3$(368): C: 74.99, H: 4.38, N: 7.60%. Found: C: 74.82, H: 4.30, N: 7.55%.

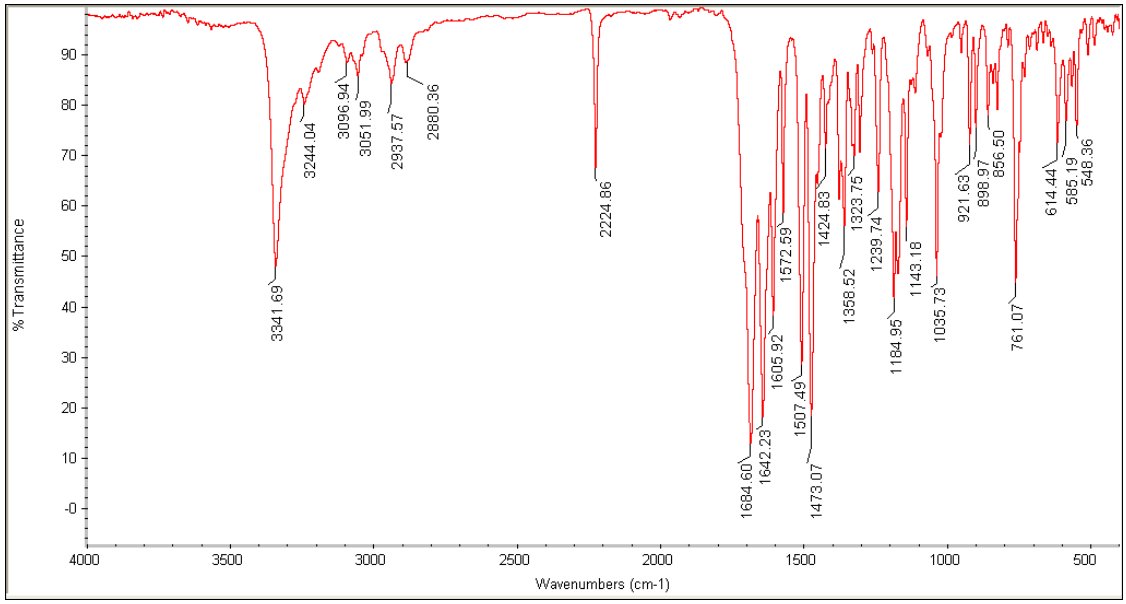


Figure 11. IR spectrum of compound **2c**

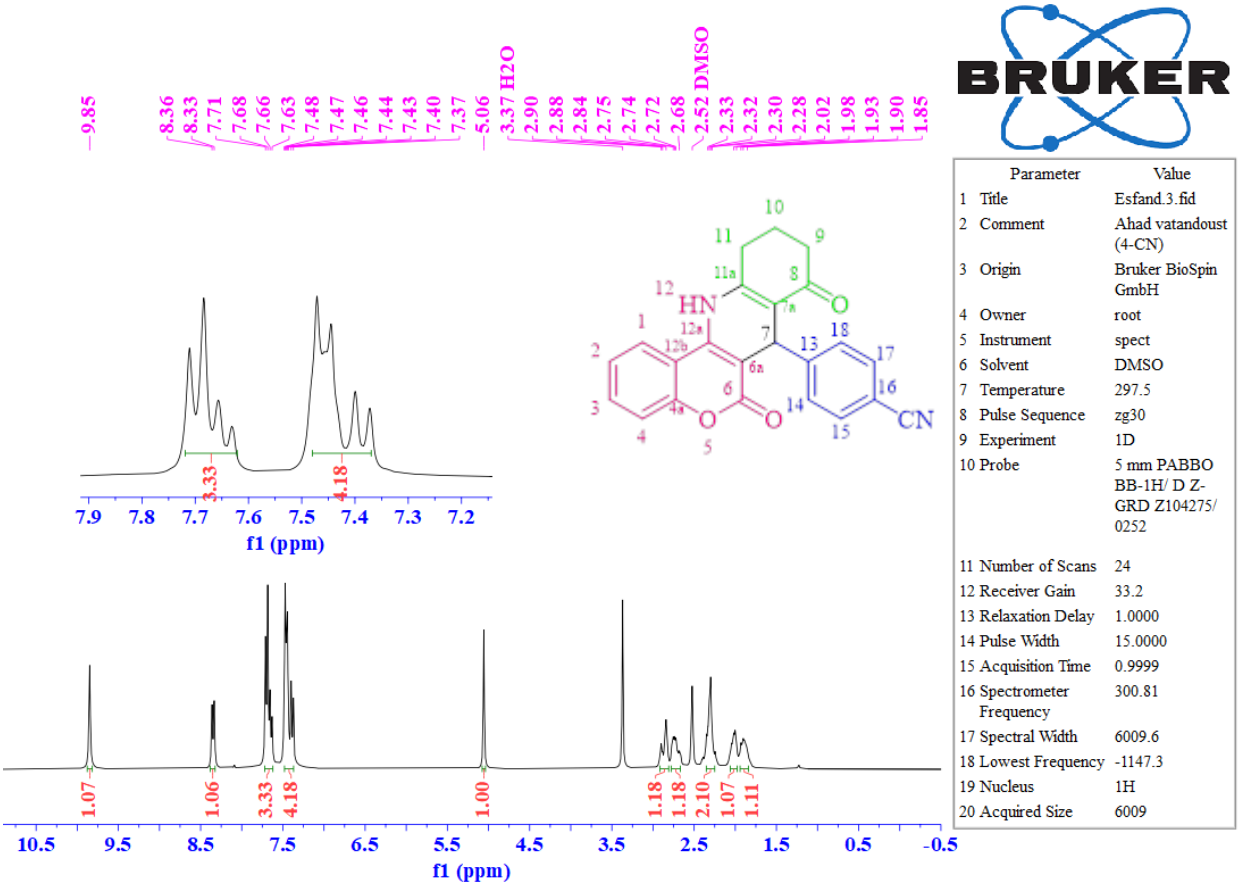


Figure 12. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of compound **2c**

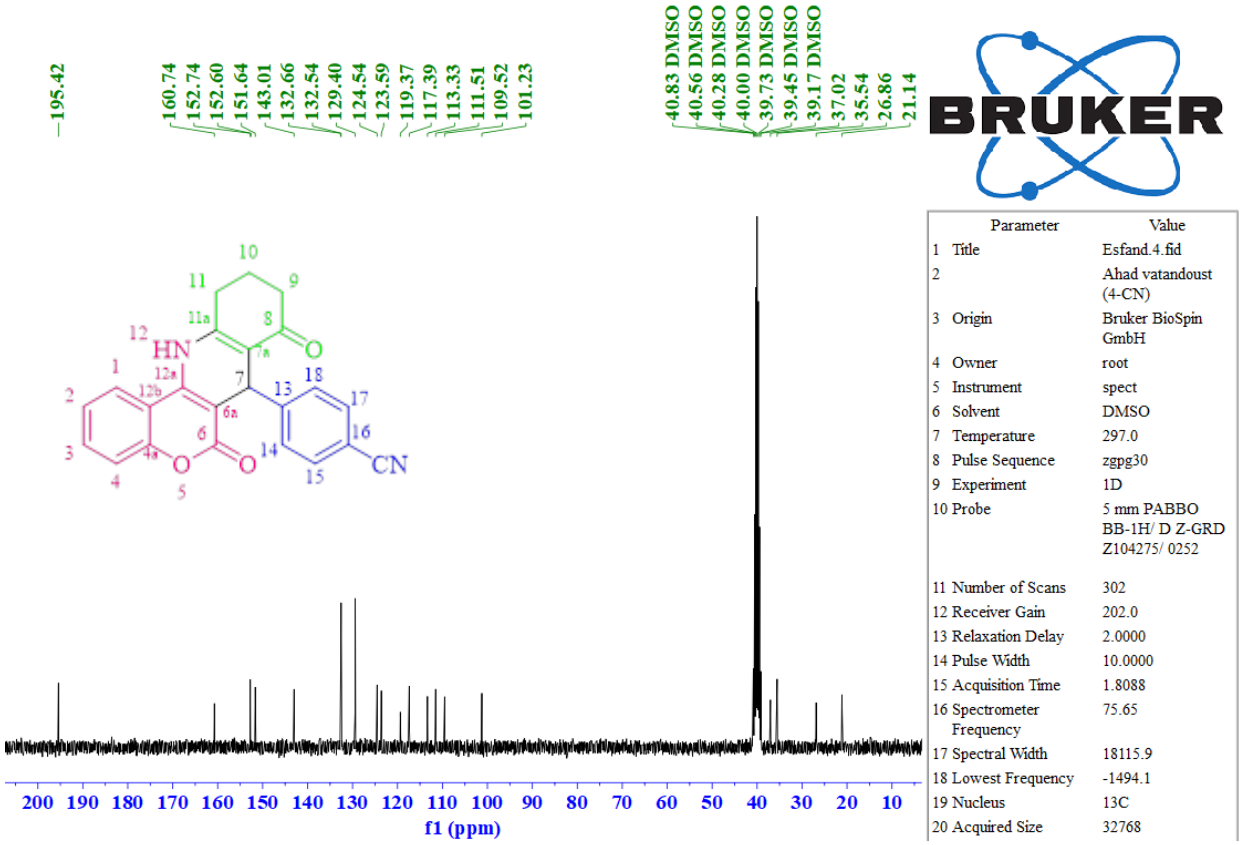


Figure 13. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of compound **2c**

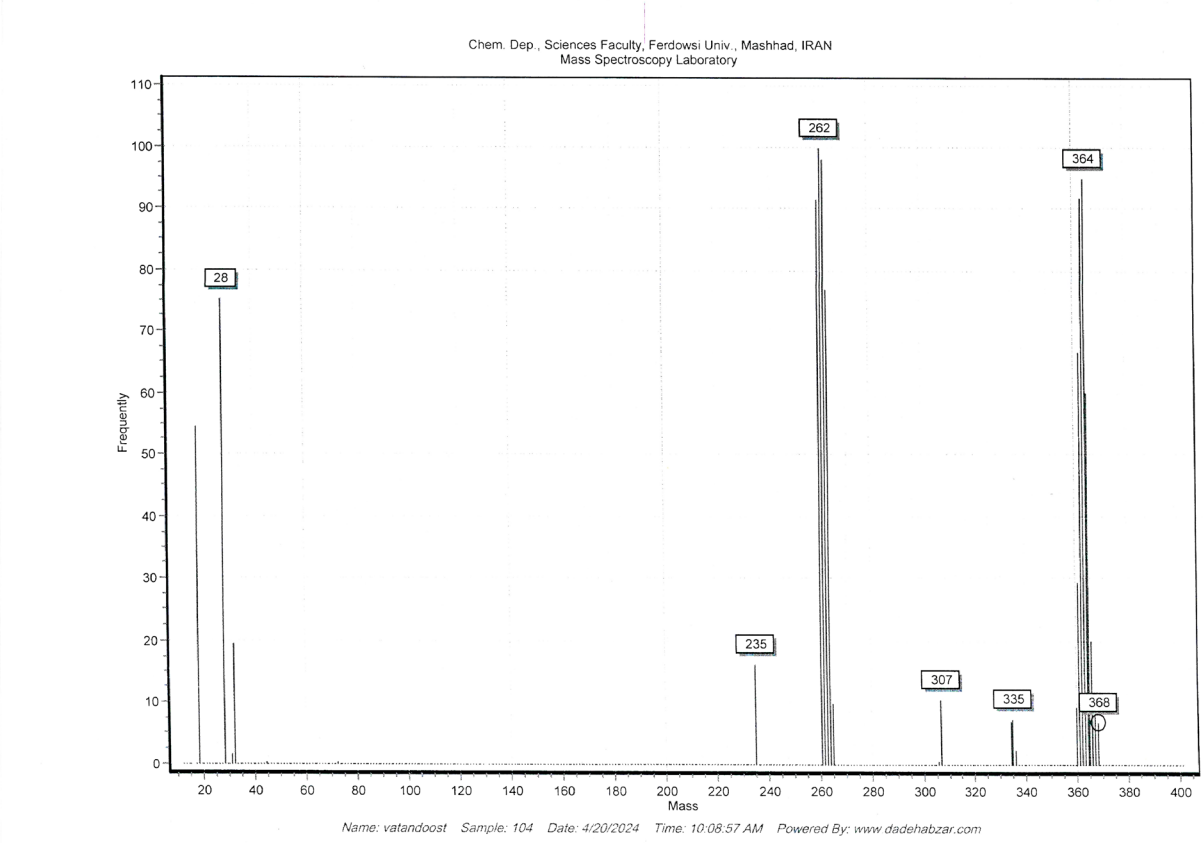


Figure 14. Mass spectrum of compound **2c**

Eager 300 Summarize Results

Date: 24/04/2024 at 13:05:18

Method Name: NCHS

Method Filename: Copy of N C H S-bkp.mth

Filename	As Method	Vial
Vatandoust-175		
# Group Sample Name	Tayp Weig. Prof. F ---	-----
175-1 104	UNK 0.645 6.25 ---	-----
Component Name Element%		
Nitrogen% 7.558488731		
Carbon% 74.82396332		
Hydrogen% 4.304181957		
Sulphur% 0		

1 Sample (s) in Group No:1

Component Name	Average
Nitrogen%	7.558488731
Carbon%	74.82396332
Hydrogen%	4.304181957
Sulphur%	0

Figure 15. CHNS spectrum of compound **2c**

Anal. Calcd. for $C_{23}H_{16}N_2O_3$(368)		
C: 74.99 %	H: 4.38 %	N: 7.60 %

7-(4-chlorophenyl)-7,10,11,12-tetrahydro-6H-chromeno[4,3-b]quinoline-6,8(9H)-dione (2d)[3]

Light yellow solid; (0.32g, 85%) Mp=215-216 °C (Lit. 214-216 °C); IR (KBr) (υ_{max}/cm^{-1}): 3334 (NH), 3051 (C-H aromatic), 2941, 2884 (C-H aliphatic), 1673 (C=O), 1643, 1607 (C=C); ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ (ppm): 9.80 (s, 1H, NH), 8.35 (d, *J* = 8.0 Hz, 1H, ArH, H_1), 7.65 (t, *J* = 7.7 Hz, 1H, ArH, H_3), 7.45 (t, *J* = 7.6 Hz, 1H, ArH, H_2), 7.40 (d, *J* = 8.3 Hz, 1H, ArH, H_4), 7.27 (s, 4H, ArH, H_{14}, H_{15}, H_{17}, H_{18}), 4.99 (s, 1H, CH, H_7), 2.89-2.83 (m, 1H, CH_2, H_9), 2.76-2.71 (m, 1H, CH_2, H_9), 2.33-2.28 (m, 2H, CH_2, H_{11}), 2.04-2.00 (m, 1H, CH_2, H_{10}), 1.93-1.88 (m, 1H, CH_2, H_{10}); ^{13}C NMR (75 MHz, DMSO-*d*$_6$): δ (ppm): 195.44 (C_8), 160.78 (C_6), 152.55 (C_{4a}), 152.32 (C_{11a}), 145.33 (C_{12a}), 142.69 (C_{13}), 132.52 (C_3), 131.26 (C_{16}), 130.10 (C_{15},C_{17}), 128.45 (C_{14},C_{18}), 124.50 (C_1), 123.51 (C_2), 117.37 (C_4), 113.42 (C_{12b}), 112.03 (C_{7a}), 101.82 (C_{6a}), 37.10 (C_9), 34.44 (C_7), 26.85 (C_{11}), 21.18 (C_{10}); MS: (m/z, %): 377 (M^+, 20), 375 (M^+-2, 65), 266 (50), 28(100); Anal. Calcd. for $C_{22}H_{16}ClNO_3$(377): C: 69.94, H: 4.27, N: 3.71%. Found: C: 69.88, H: 4.17, N: 3.64%.

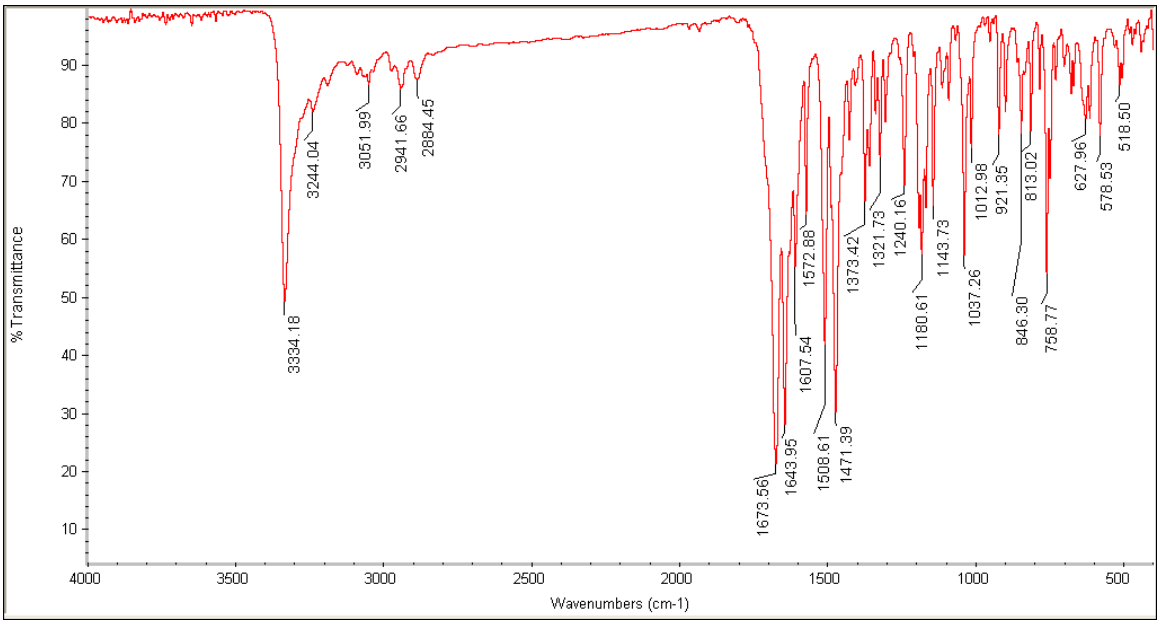


Figure 16. IR spectrum of compound **2d**

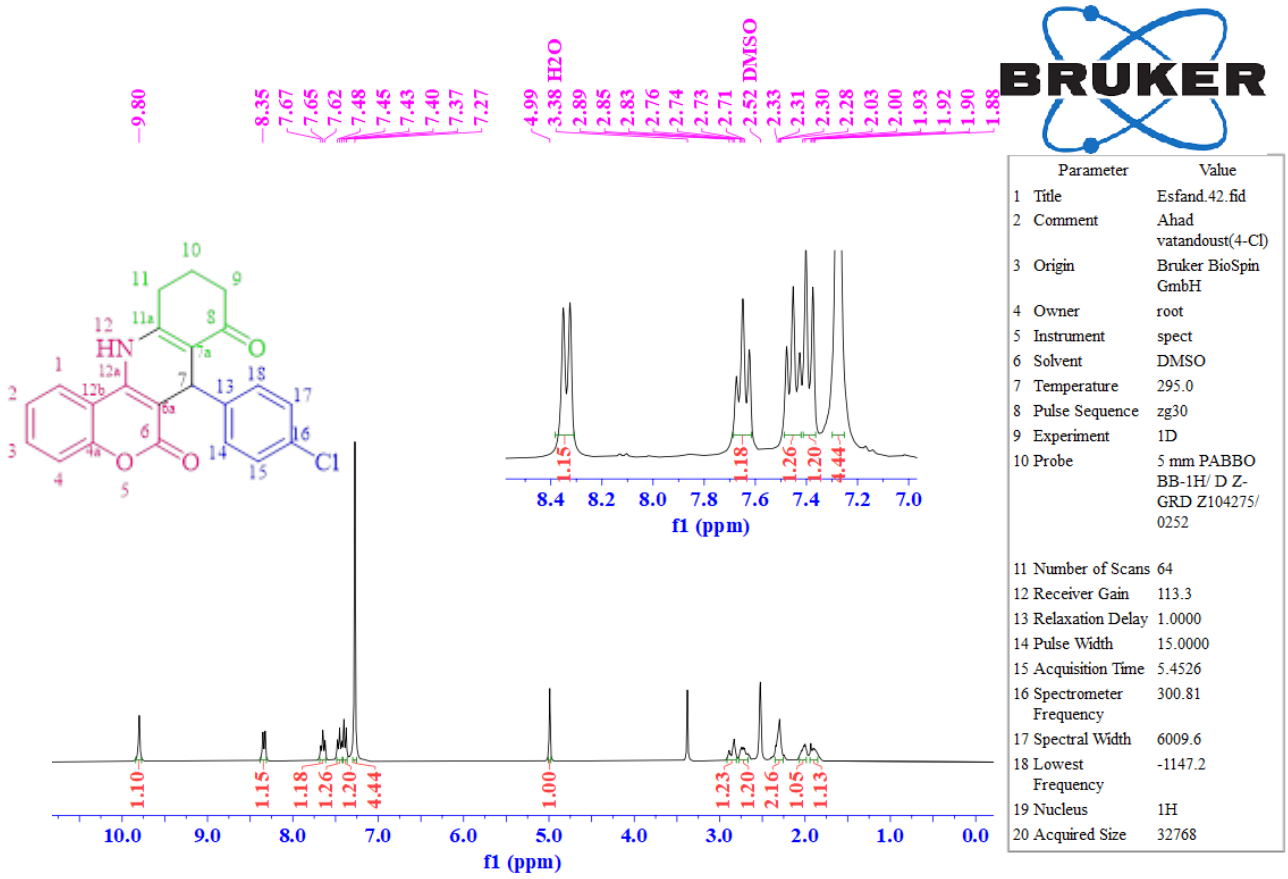


Figure 17. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of compound **2d**

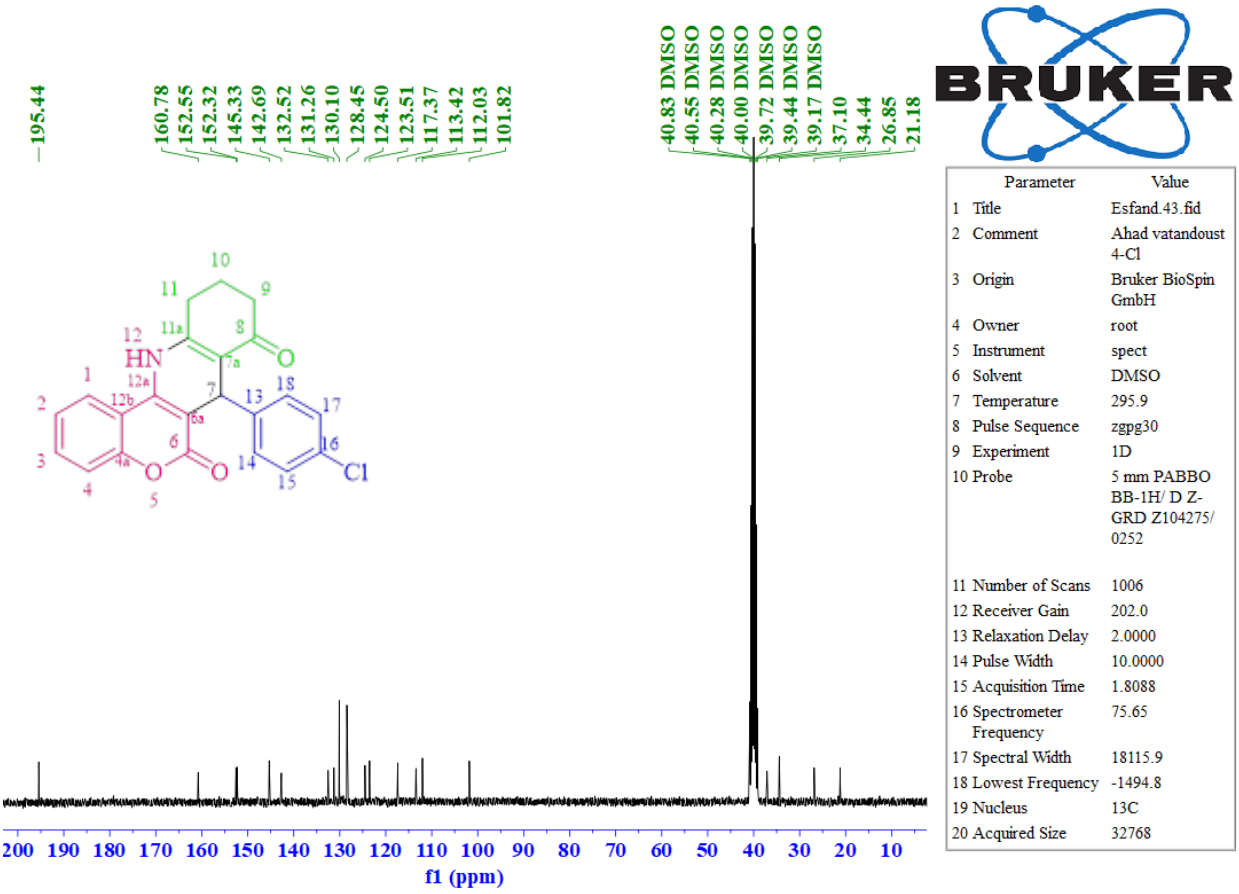


Figure 18. ^{13}C NMR (75MHz, DMSO-d_6) spectrum of compound **2d**

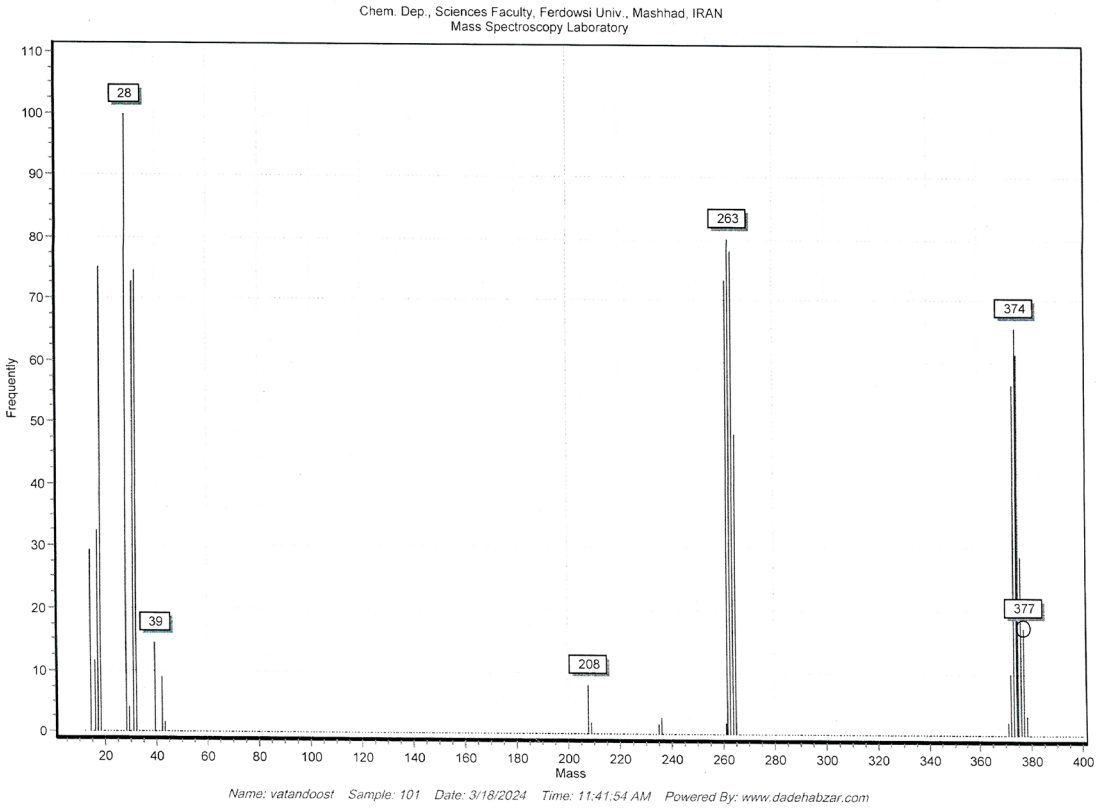


Figure 19. Mass spectrum of compound **2d**

Eager 300 Summarize Results

Date: 24/04/2024 at 13:07:15

Method Name: NCHS

Method Filename: Copy of N C H S-bkp.mth

Filename	As Method	Vial
Vatandoust-186		
# Group Sample Name	Tayp Weig. Prof. F ---	-----
186-1 101	UNK 0.673 6.25 ---	-----
Component Name Element%		
Nitrogen% 3.649792671		
Carbon% 69.88464691		
Hydrogen% 4.171821172		
Sulphur% 0		

1 Sample (s) in Group No:1

Component Name	Average
Nitrogen%	3.649792671
Carbon%	69.88464691
Hydrogen%	4.171821172
Sulphur%	0

Anal. Calcd. for $C_{22}H_{16}ClNO_3$(377)		
C: 69.94 %	H: 4.27 %	N: 3.71 %

Figure 20. CHNS spectrum of compound **2d**

7-(4-bromophenyl)-7,10,11,12-tetrahydro-6H-chromeno[4,3-b]quinoline-6,8(9H)-dione (2e)[3]

Light yellow solid; (0.336g, 80%); Mp=295-296°C (Lit. 294-296 °C); IR (KBr) (υ_{max}/cm^{-1}): 3331(NH), 3043 (C-H aromatic), 2941, 2884 (C-H aliphatic), 1670 (C=O); MS: (m/z, %): 421 (M^+, 48), 419 (M^+-2,60), 266 (28), 28 (100); Anal. Calcd. for $C_{22}H_{16}BrNO_3$(421): C: 62.58, H: 3.82, N: 3.32 %. Found: C: 62.38, H: 3.67, N: 3.18%.

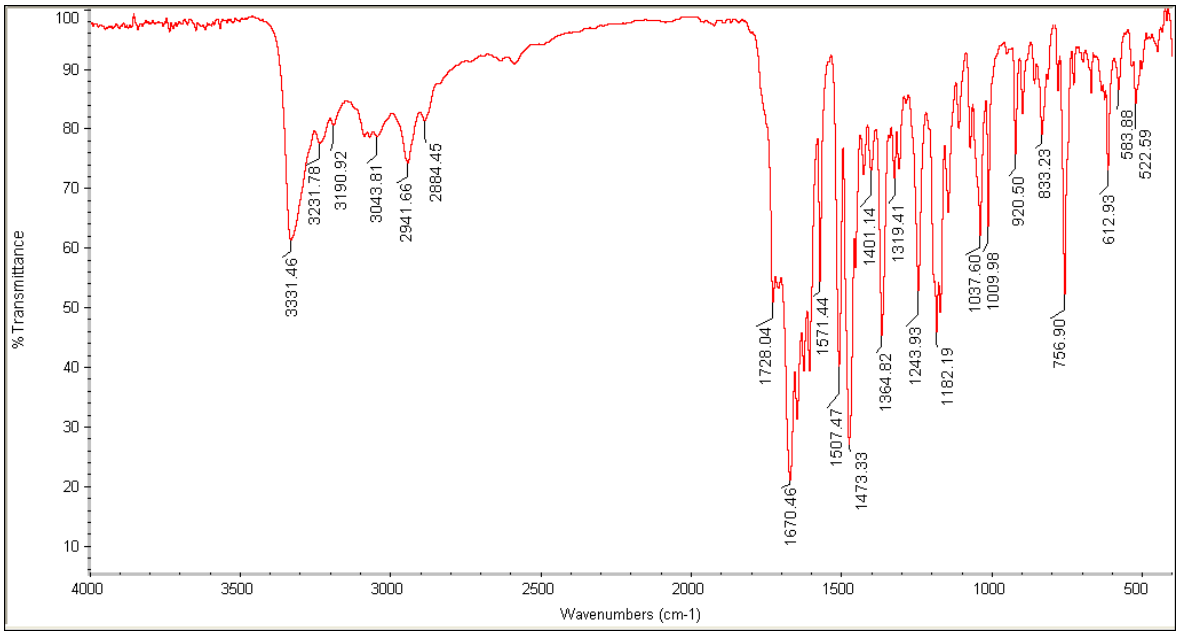


Figure 21. IR spectrum of compound **2e**

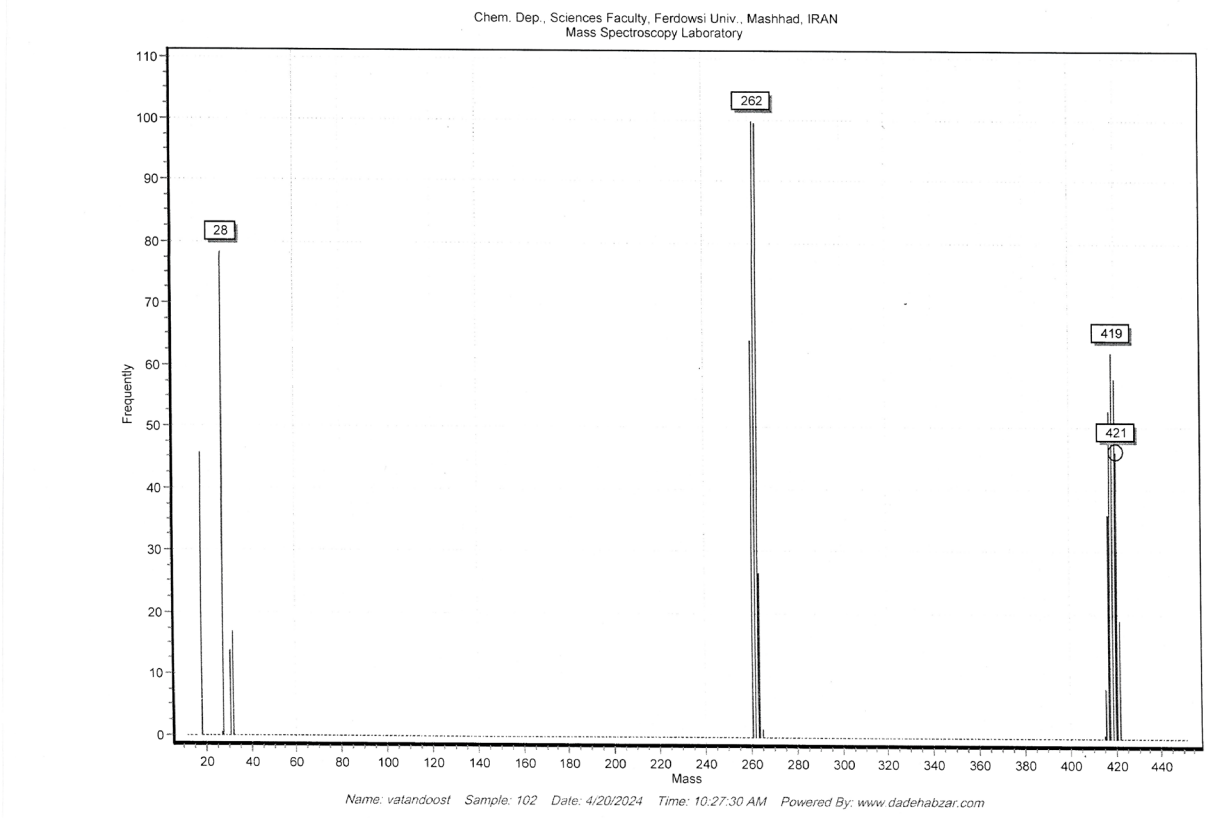


Figure 22. Mass spectrum of compound **2e**

Eager 300 Summarize Results

Date: 24/04/2024 at 13:07:05

Method Name: NCHS

Method Filename: Copy of N C H S-bkp.mth

Filename	As Method	Vial
Vatandoust-184		
# Group Sample Name	Tayp Weig. Prof. F ---	-----
184-1 102	UNK 0.618 6.25 ---	-----

Component Name	Element%
Nitrogen%	3.185758247
Carbon%	62.3849939
Hydrogen%	3.670049191
Sulphur%	0

1 Sample (s) in Group No:1

Component Name	Average
Nitrogen%	3.185758247
Carbon%	62.3849939
Hydrogen%	3.670049191
Sulphur%	0

Figure 23. CHNS spectrum of compound **2e**

Anal. Calcd. for $C_{22}H_{16}BrNO_3$(421)		
C: 62.58 %	H: 3.82 %	N: 3.32 %

7-(3-bromophenyl)-7,10,11,12-tetrahydro-6H-chromeno[4,3-b]quinoline-6,8(9H)-dione (2f)[3]

Light yellow solid; (0.33g, 80%) Mp=265-266 °C (Lit. 267-269 °C); IR (KBr) (υ_{max}/cm^{-1}): 3324(NH), 3092(C-H aromatic), 2942, 2892 (C-H aliphatic), 1668 (C=O), 1633,1606 (C=C); ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ (ppm): 9.85 (s, 1H, NH), 8.35 (d, *J* = 8.1 Hz, 1H, ArH, H_1), 7.68 (t, *J* = 7.8 Hz, 1H, ArH, H_3), 7.48 (t, *J* = 7.2 Hz, 1H, ArH, H_2), 7.43-7.41 (m, 2H, ArH, H_{14}, H_{16}), 7.34 (d, *J* = 7.0 Hz, 1H, ArH, H_4), 7.25-7.20 (m, 2H, ArH, H_{17},H_{18}), 4.99 (s, 1H, CH, H_7), 2.89-2.84 (m, 1H, CH_2, H_9), 2.77-2.72 (m, 1H,CH_2, H_9), 2.36-2.30 (m, 2H, CH_2, H_{11}), 2.07-1.99 (m, 1H, CH_2, H_{10}), 1.93-1.88 (m, 1H, CH_2, H_{10}); ^{13}C NMR (75 MHz, DMSO-*d*$_6$): δ (ppm): 195.49 (C_8), 160.80 (C_6), 152.57 (C_{4a}), 148.95 (C_{11a}), 142.85 (C_{12a}), 132.64 (C_{13}), 130.99 (C_3), 130.94 (C_{14},C_{16}), 129.65 (C_{17}), 127.26 (C_{18}), 124.57 (C_1), 123.58 (C_{15}), 121.76 (C_2), 117.44 (C_4), 113.40 (C_{12b}), 111.80 (C_{7a}), 101.60 (C_{6a}), 37.08 (C_9), 34.88 (C_7), 26.86 (C_{11}), 21.19 (C_{10}); MS: (m/z, %): 421 (M^+, 78), 419 (M^+-2, 85), 266 (68), 28 (100); Anal. Calcd. for $C_{22}H_{16}BrNO_3$(421): C: 62.58, H: 3.82, N: 3.32%. Found: C: 62.45, H: 3.69, N: 3.28%.

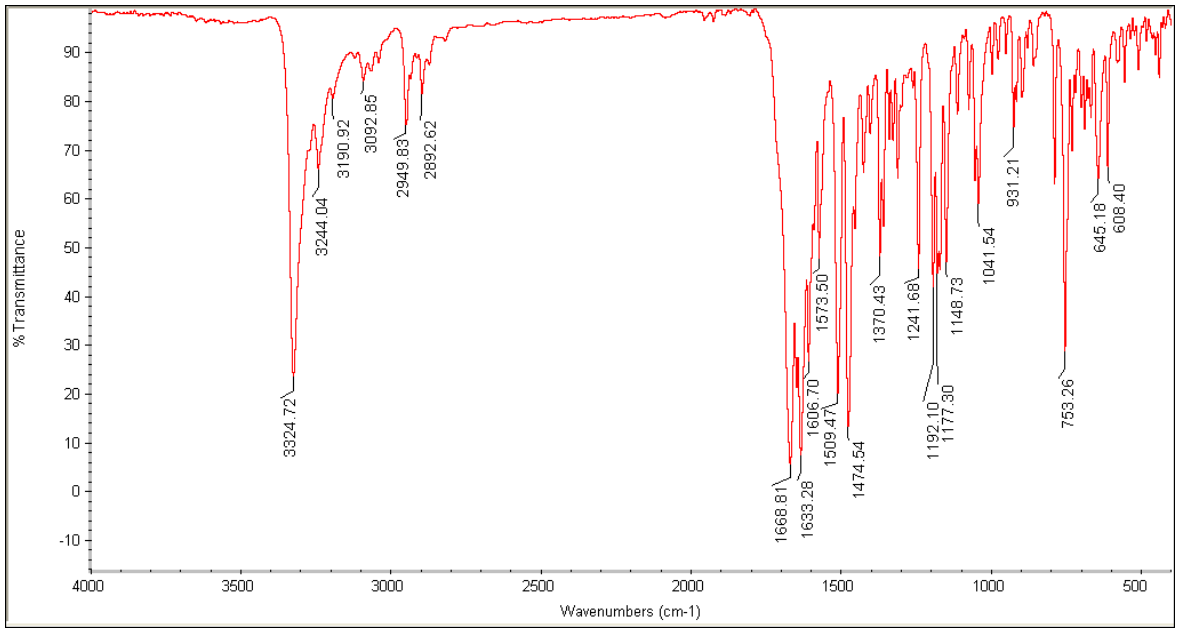


Figure 24. IR spectrum of compound **2f**

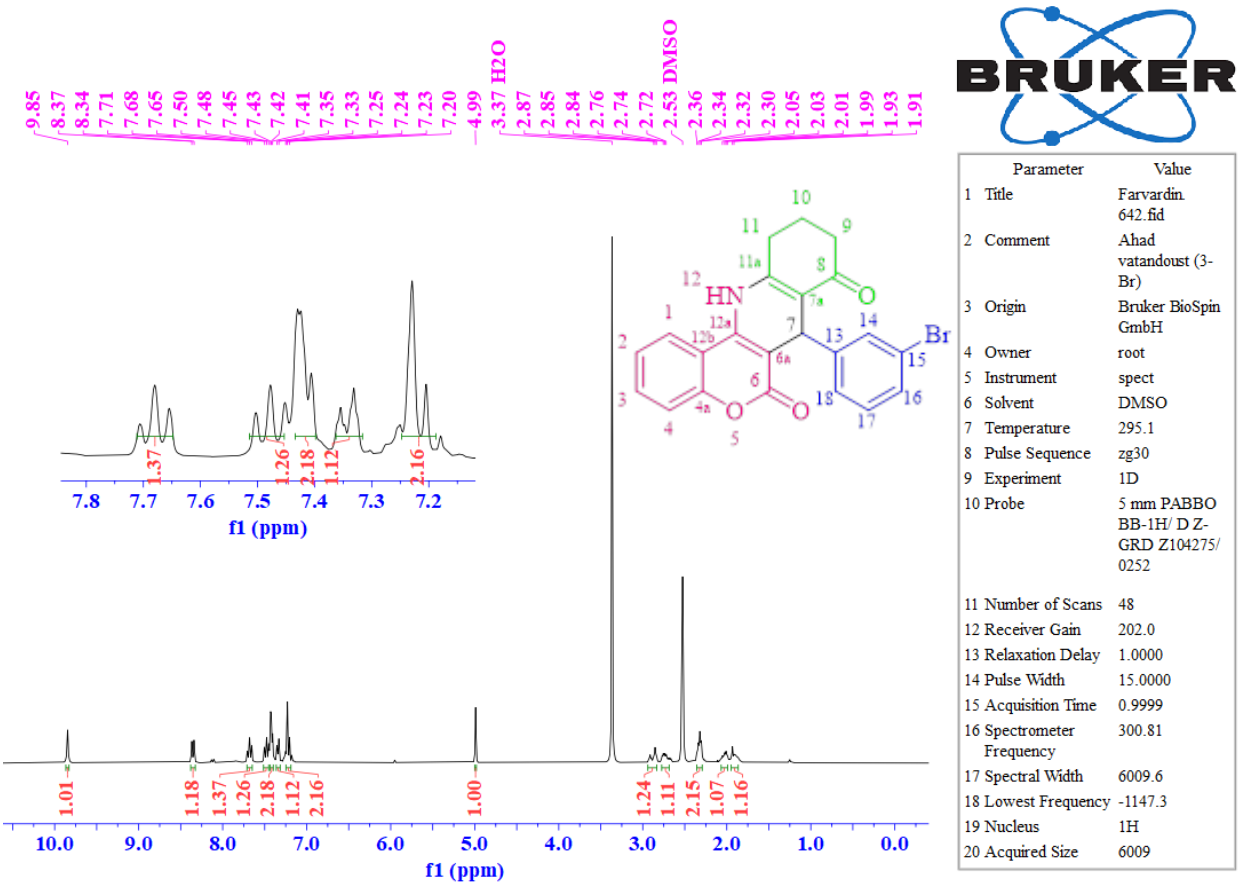


Figure 25. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of compound **2f**

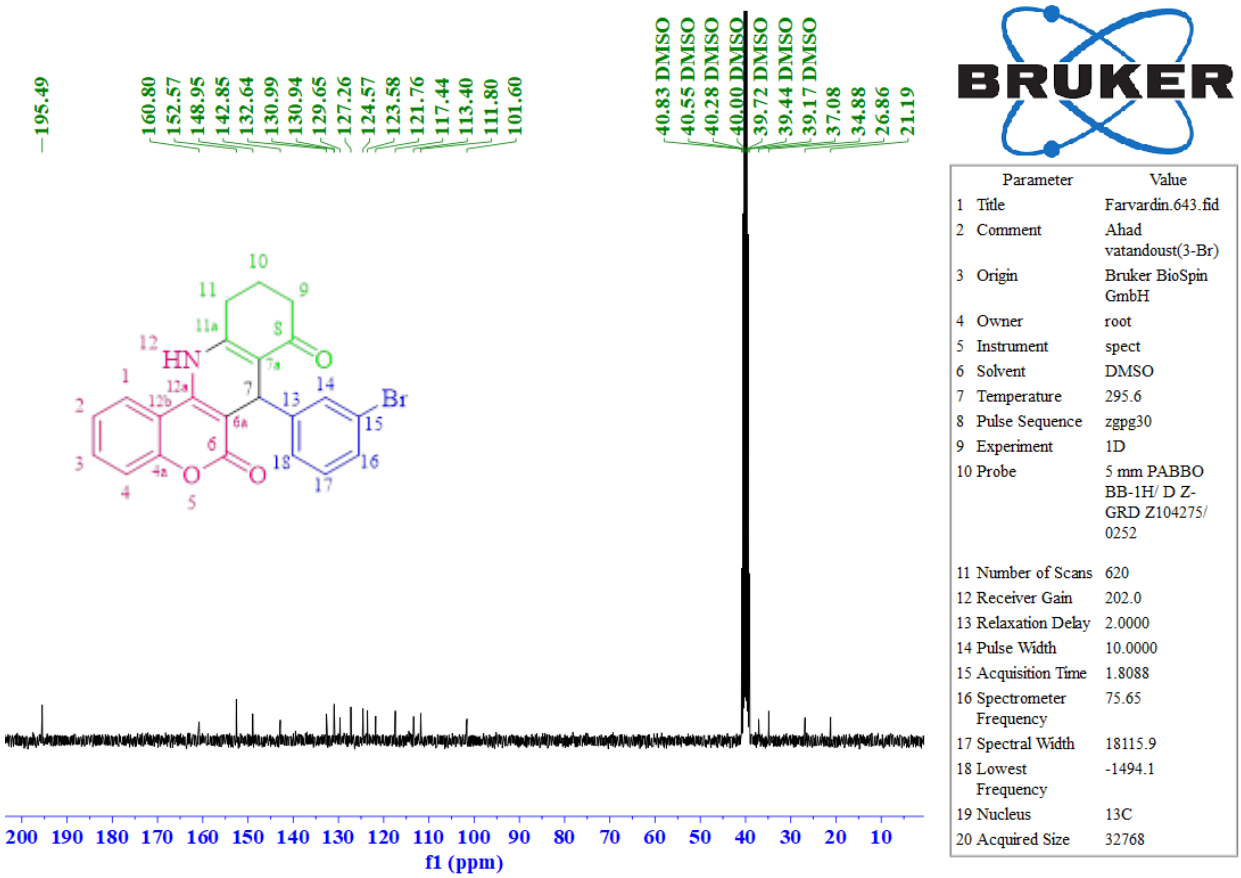


Figure 26. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of compound **2f**

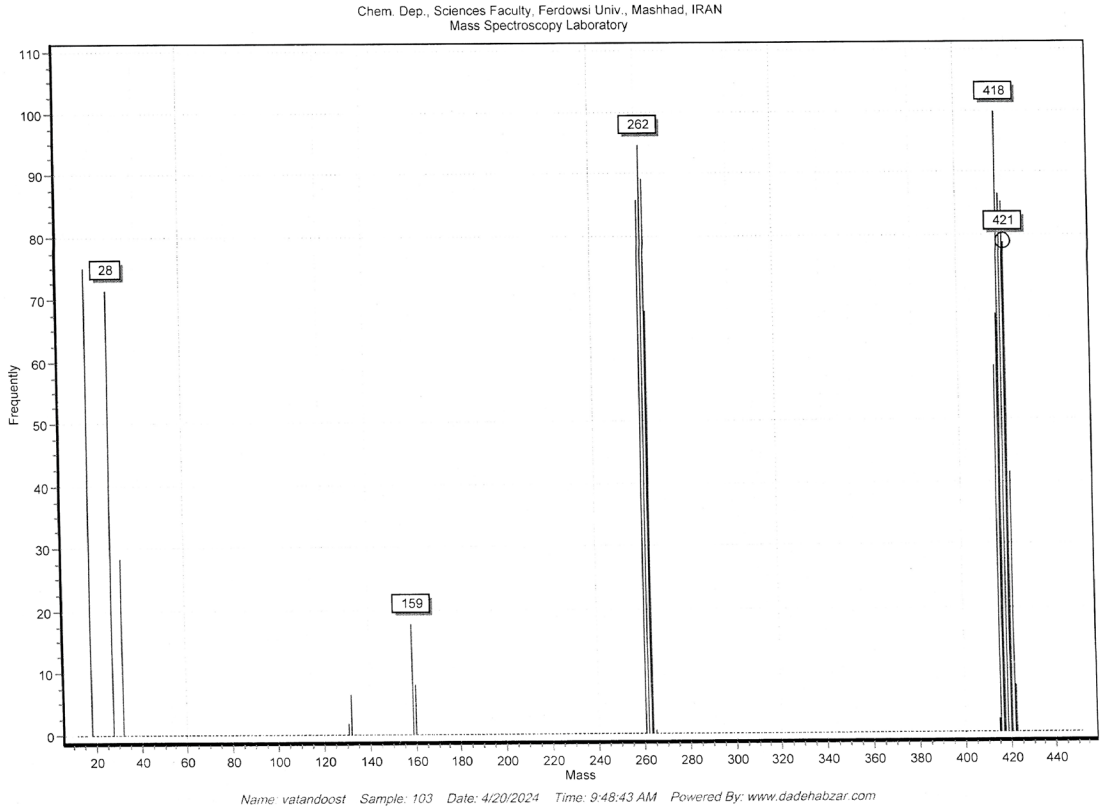


Figure 27. Mass spectrum of compound **2f**

Eager 300 Summarize Results

Date: 24/04/2024 at 13:06:50

Method Name: NCHS

Method Filename: Copy of N C H S-bkp.mth

Filename	As Method	Vial
Vatandoust-183		
# Group Sample Name	Tayp Weig. Prof. F ---	-----
183-1 103	UNK 0.604 6.25 ---	-----

Component Name	Element%
Nitrogen%	3.281792812
Carbon%	62.45877167
Hydrogen%	3.691780491
Sulphur%	0

1 Sample (s) in Group No:1

Component Name	Average
Nitrogen%	3.281792812
Carbon%	62.45877167
Hydrogen%	3.691780491
Sulphur%	0

Figure 28. CHNS spectrum of compound **2b**

Anal. Calcd. for $C_{22}H_{16}BrNO_3$(421)		
C: 62.58 %	H: 3.82 %	N: 3.32 %

7-(4-hydroxyphenyl)-7,10,11,12-tetrahydro-6H-chromeno[4,3-b]quinoline-6,8(9H)-dione (2g)[1]

White solid; (0.287g, 80%); Mp=337-339 °C (Lit. 338-340 °C); IR (KBr) (υ_{max}/cm^{-1}): 3344(NH), 3288(OH), 3088 (C-H aromatic), 2925, 2876 (C-H aliphatic), 1672 (C=O), 1634,1607 (C=C); ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ (ppm): 9.70 (s, 1H, NH), 9.17 (s, 1H, OH), 8.31 (d, *J* = 8.1 Hz, 1H, ArH, H_1), 7.62 (t, *J* = 7.8 Hz, 1H, ArH, H_3), 7.43 (t, *J* = 7.6 Hz, 1H, ArH, H_2), 7.37 (d, *J* = 8.3 Hz, 1H, ArH, H_4), 7.04 (d, *J* = 8.1 Hz, 2H, ArH, H_{14}, H_{18}), 6.61 (d, *J* = 8.0 Hz, 2H, ArH, H_{15}, H_{17}), 4.91 (s, 1H, CH, H_7), 2.88-2.82 (m, 1H, CH_2, H_9), 2.74-2.67 (m, 1H, CH_2, H_9), 2.32-2.28 (m, 2H, CH_2, H_{11}), 2.04-2.00 (m, 1H, CH_2, H_{10}), 1.94-1.89 (m, 1H, CH_2, H_{10}); ^{13}C NMR (75 MHz, DMSO-*d*$_6$): δ (ppm): 195.47 (C_8), 160.87 (C_6), 156.24 (C_{16}), 152.44 (C_{4a}), 151.72 (C_{11a}), 142.10 (C_{12a}), 137.12 (C_{13}), 132.22 (C_3), 129.09 (C_{14},C_{18}), 124.39 (C_1), 123.33 (C_2), 117.27 (C_4), 115.21 (C_{15},C_{17}), 113.60 (C_{12b}), 112.72(C_{7a}), 102.76 (C_{6a}), 37.23 (C_9), 33.55 (C_7), 26.85 (C_{11}), 21.26 (C_{10}); MS: (m/z, %):359 (M^+, 10), 357 (M^+-2, 85), 266 (68), 93 (68), 28 (100); Anal. Calcd. for $C_{22}H_{17}NO_4$ (359): C: 73.53, H: 4.77, N: 3.90%. Found: C: 73.48, H: 4.72, N: 3.87%.

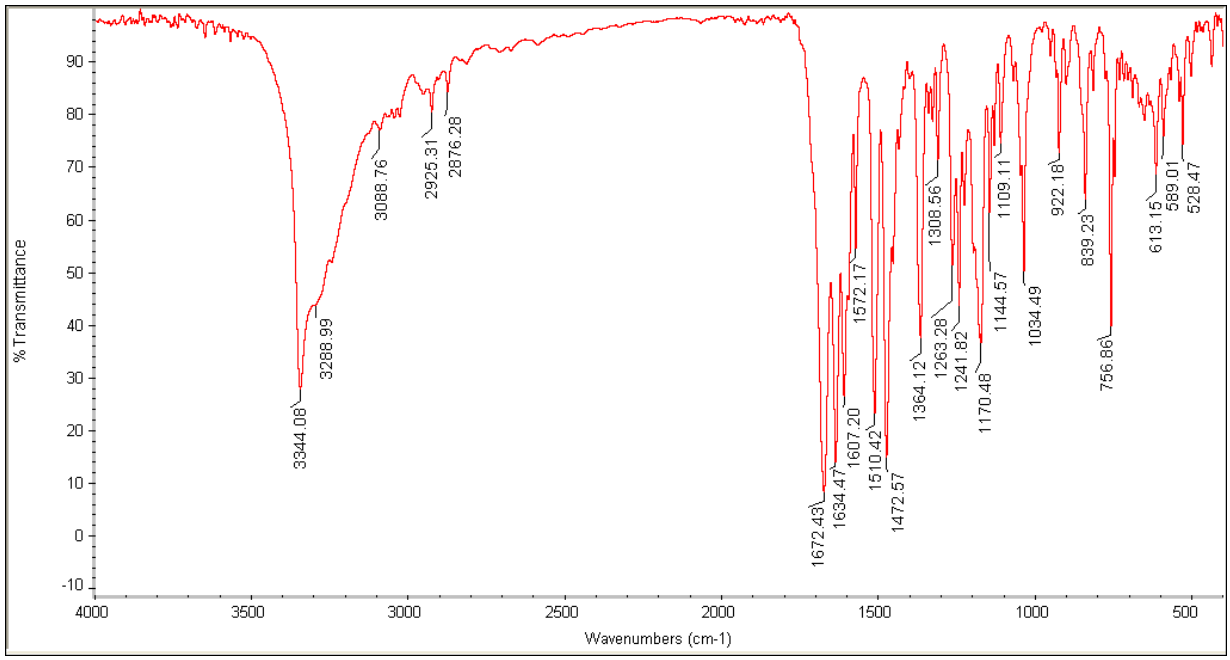


Figure 29. IR spectrum of compound **2g**

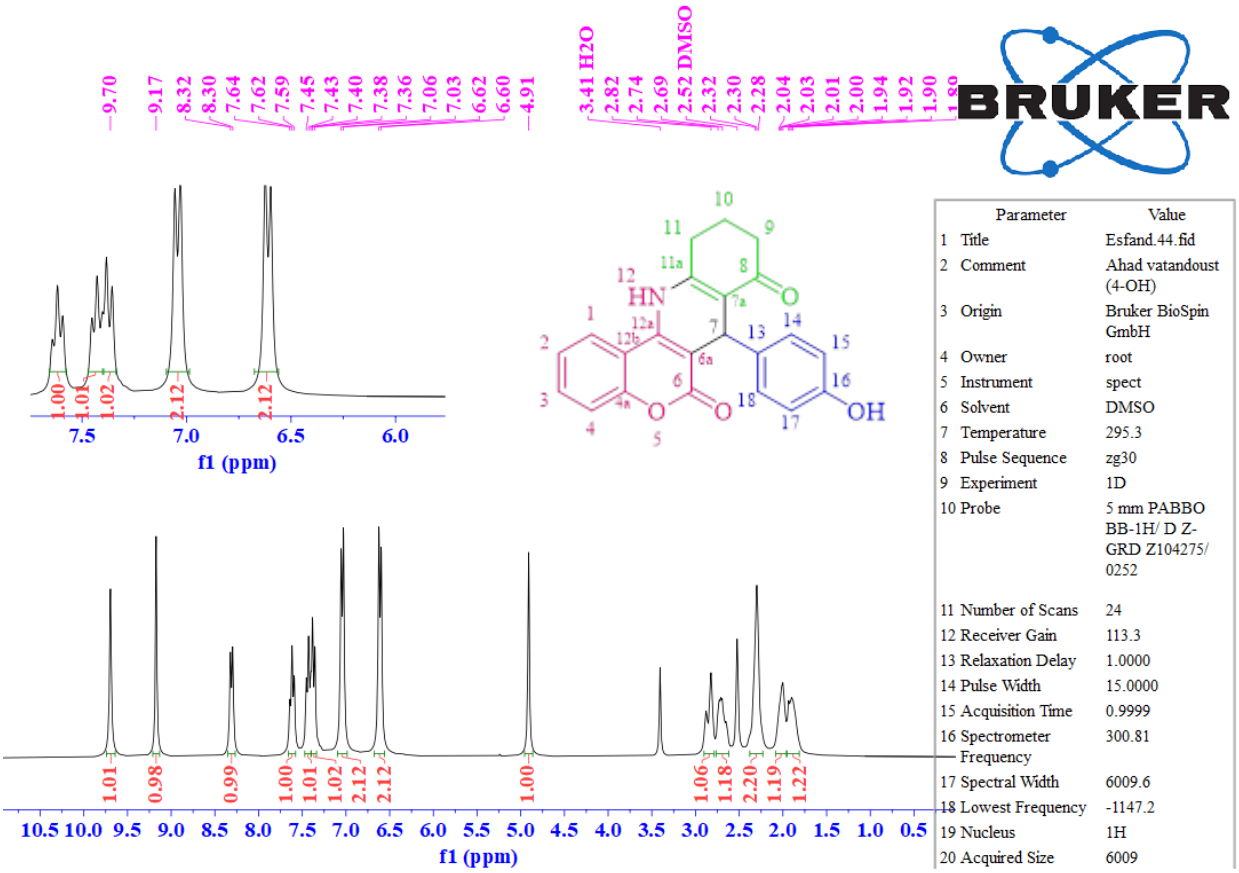


Figure 30. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of compound **2g**

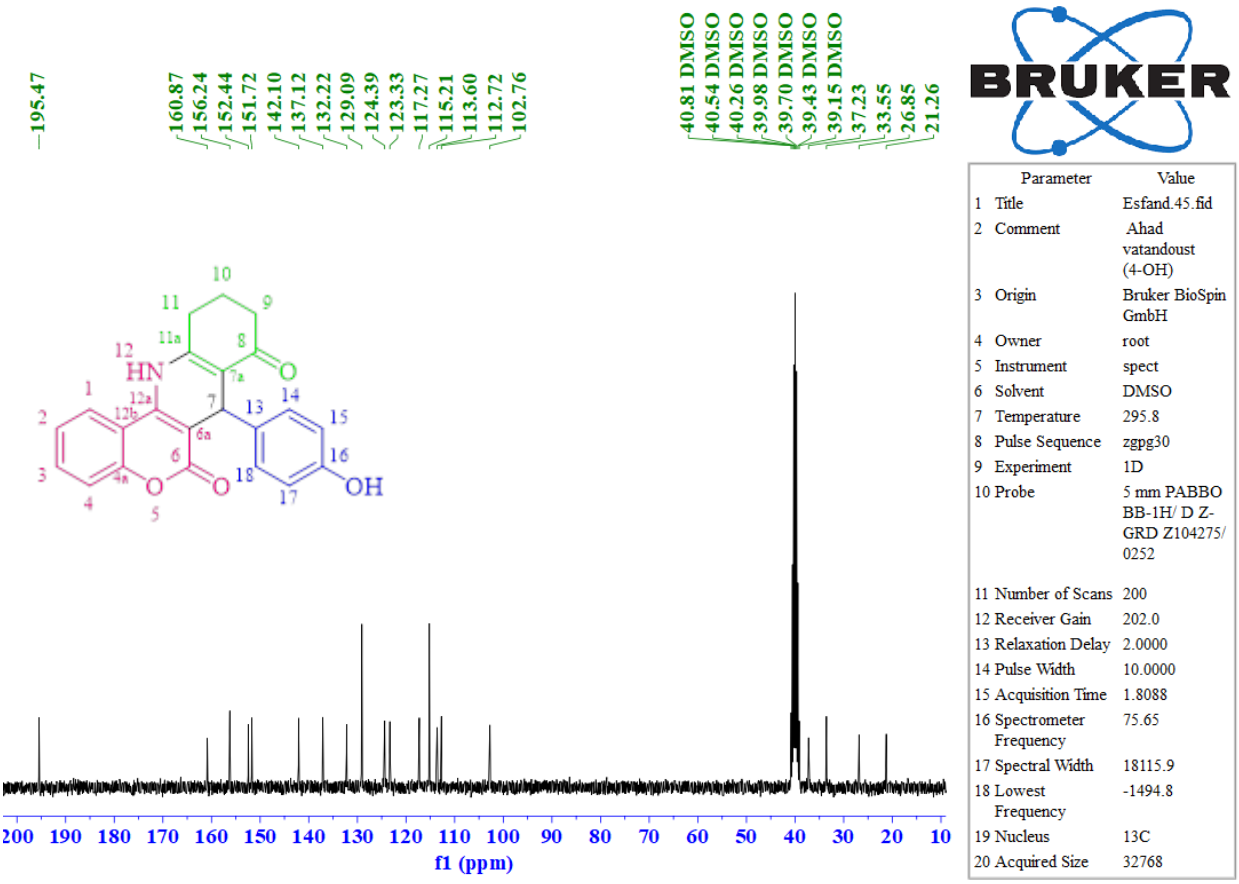


Figure 31. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of compound **2g**

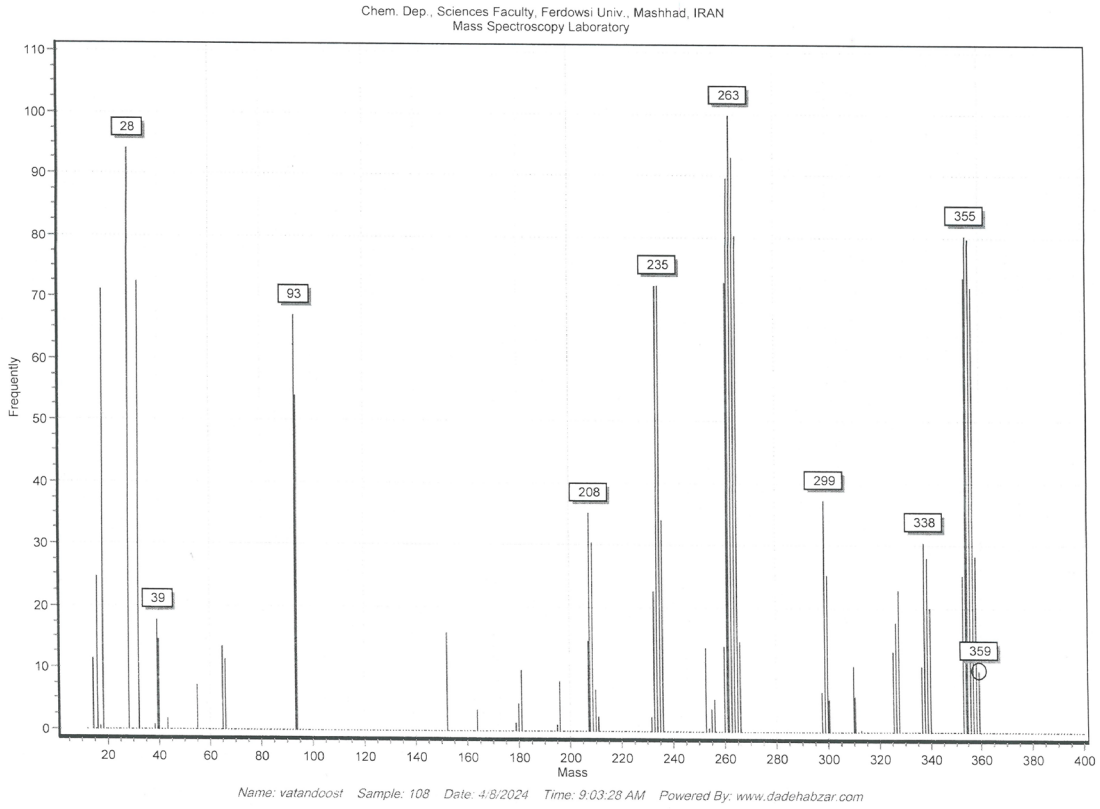


Figure 32. Mass spectrum of compound **2g**

Eager 300 Summarize Results

Date: 24/04/2024 at 13:10:23

Method Name: NCHS

Method Filename: Copy of N C H S-bkp.mth

Filename	As Method	Vial
Vatandoust-171		
# Group Sample Name	Tayp Weig. Prof. F ---	-----
171-1 108	UNK 0.643 6.25 ---	-----

Component Name	Element%
Nitrogen%	3.727560558
Carbon%	73.43045807
Hydrogen%	4.725502014
Sulphur%	0

1 Sample (s) in Group No:1

Component Name	Average
Nitrogen%	3.727560558
Carbon%	73.43045807
Hydrogen%	4.725502014
Sulphur%	0

Figure 33. CHNS spectrum of compound **2g**

Anal. Calcd. for $C_{22}H_{17}NO_4$ (359)		
C: 73.53 %	H: 4.77 %	N: 3.90 %

7-(2-hydroxyphenyl)-7,10,11,12-tetrahydro-6H-chromeno[4,3-b]quinoline-6,8(9H)-dione (2h)[4]

White solid; (0.28g, 80%); Mp=337-338 °C (Lit. 338-340 °C); IR (KBr) (υ_{max}/cm^{-1}): 3350(NH), 3199(OH), 3092, 3047(C-H aromatic), 2937, 2896 (C-H aliphatic), 1674 (C=O), 1648,1596 (C=C); ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ (ppm): 9.91 (s, 1H, NH), 9.33 (s, 1H, OH), 8.37 (d, *J* = 8.2 Hz, 1H, ArH, H_1), 7.66 (t, *J* = 7.9 Hz, 1H, ArH, H_3), 7.48 (t, *J* = 7.7 Hz, 1H, ArH, H_2), 7.42 (d, *J* = 7.6 Hz, 1H, ArH, H_4), 7.02-6.95 (m, 2H, ArH, H_{16}, H_{18}), 6.70 (d, *J* = 7.7 Hz, 2H ArH, H_{15}, H_{17}), 5.05 (s, 1H, CH, H_7), 2.86-2.80 (m, 1H, CH_2, H_9), 2.73-2.67 (m, 1H, CH_2, H_9), 2.37-2.27 (m, 2H, CH_2, H_{11}), 2.03-1.93 (m, 1H, CH_2, H_{10}), 1.88-1.79 (s, 1H, CH_2, H_{10}); ^{13}C NMR (75 MHz, DMSO-*d*$_6$): δ (ppm): 195.62 (C_8), 160.82 (C_6), 154.92 (C_{14}), 153.60 (C_{4a}), 152.47 (C_{11a}), 140.21 (C_{12a}), 132.59 (C_3), 132.55 (C_{13}), 129.99 (C_{18}), 127.89 (C_{16}), 124.53 (C_1), 123.02 (C_2), 119.83 (C_{17}), 117.57 (C_4), 117.17(C_{15}), 113.31 (C_{12b}), 111.75(C_{7a}), 101.58 (C_{6a}), 36.58 (C_9), 31.09 (C_7), 27.14 (C_{11}), 21.19 (C_{10}); MS: (m/z, %): 359 (M^+, 78), 357 (M^+-2, 38), 266 (42), 93 (56), 28 (100); Anal. Calcd. for $C_{22}H_{17}NO_4$ (359): C: 73.53, H: 4.77, N: 3.90%. Found: C: 73.51, H: 4.74, N: 3.88%.

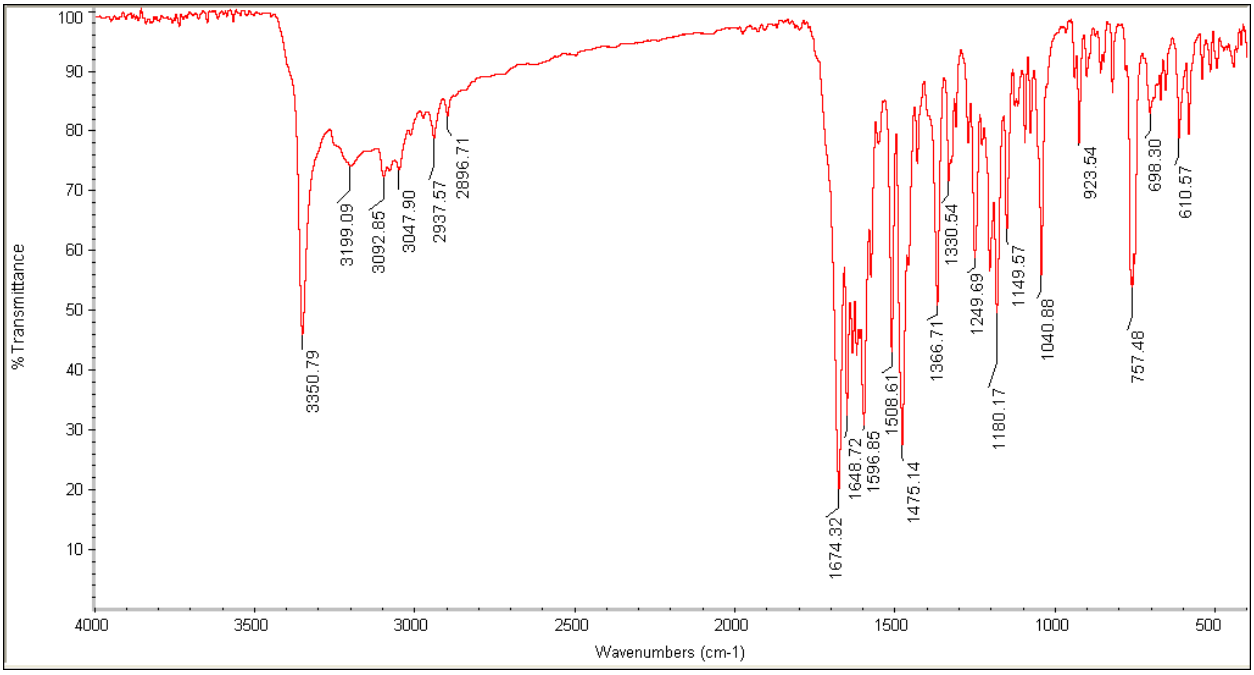


Figure 34. IR spectrum of compound **2h**

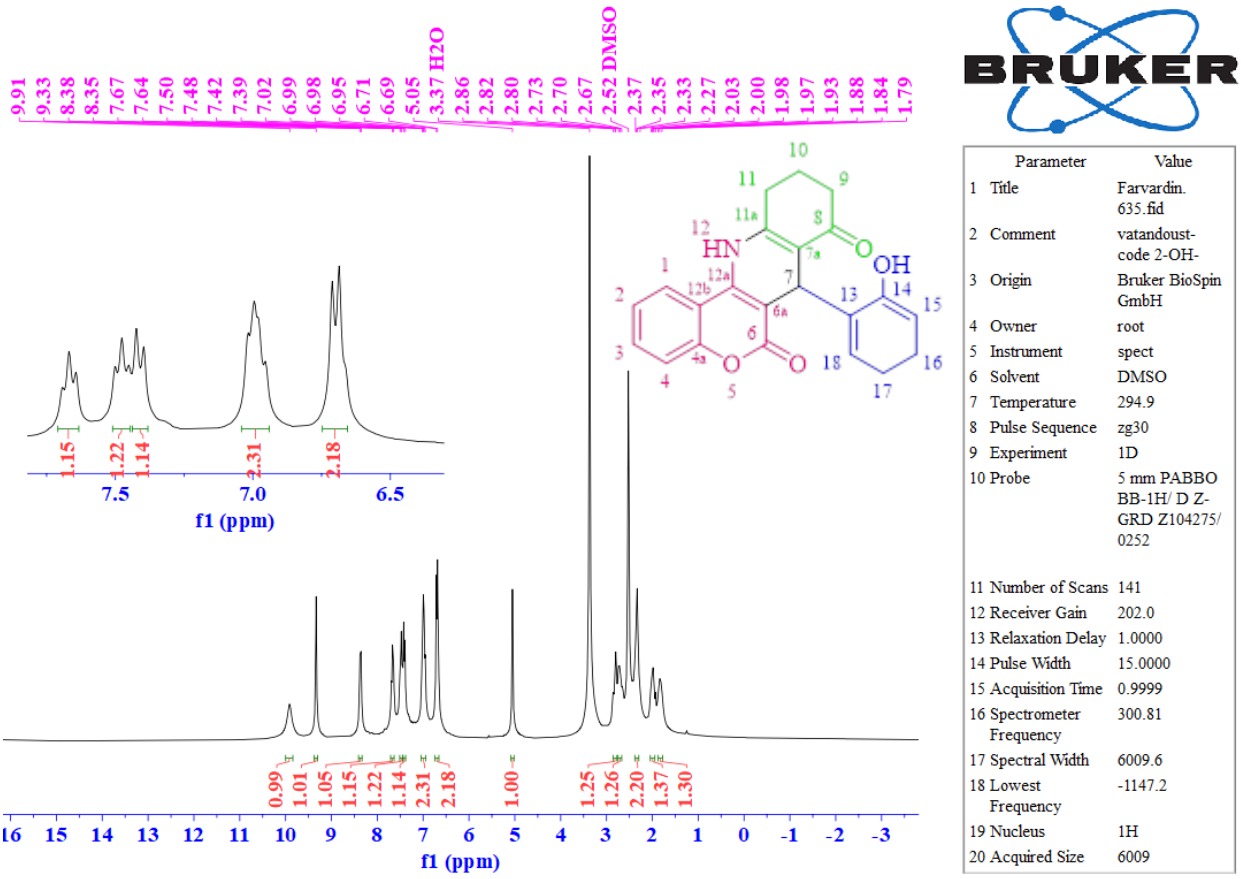


Figure 35. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of compound **2h**

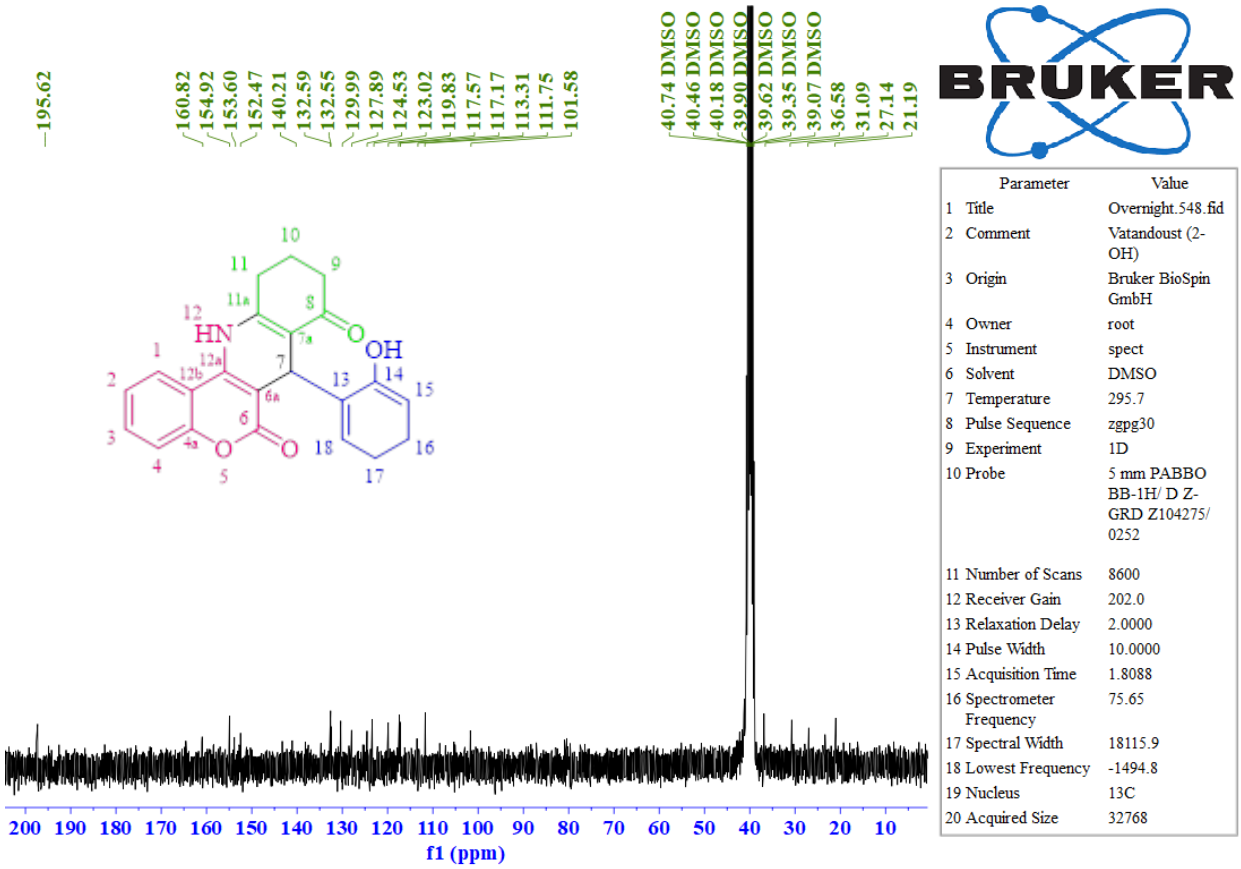


Figure 36. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of compound **2h**

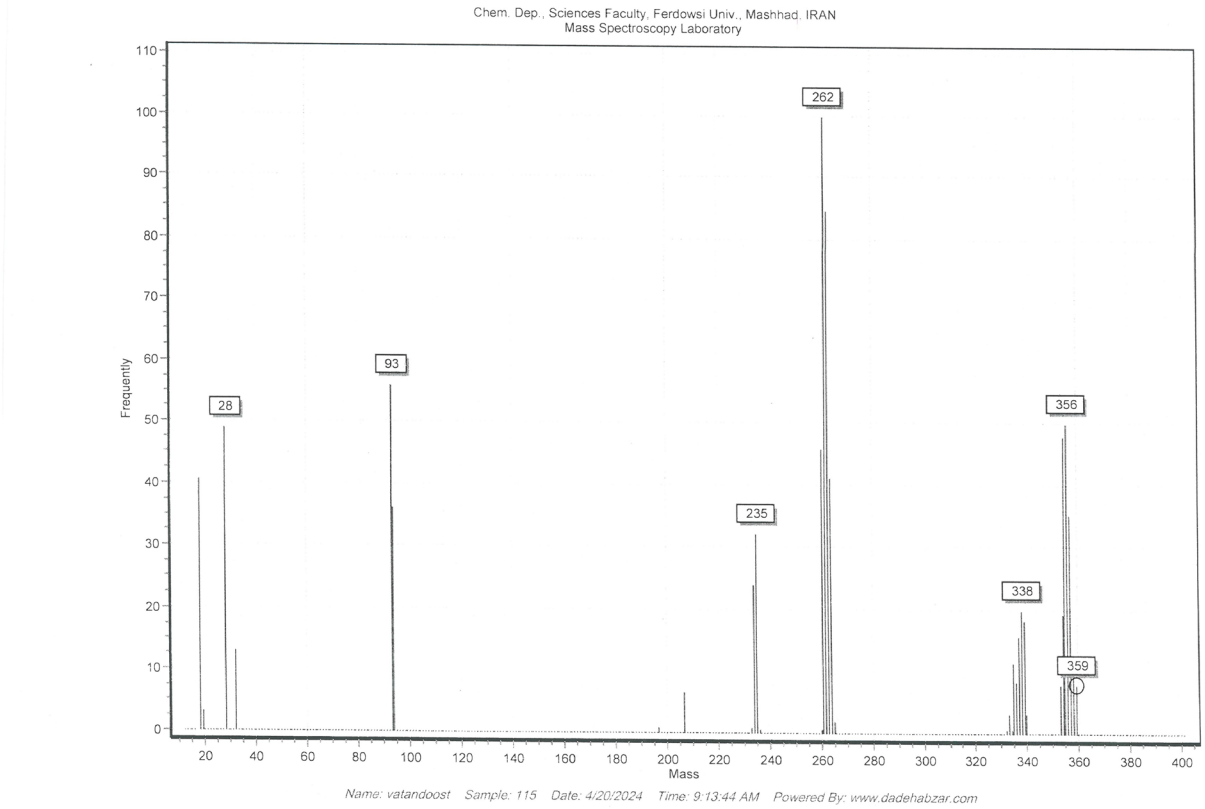


Figure 37. Mass spectrum of compound **2h**

Eager 300 Summarize Results

Date: 24/04/2024 at 13:02:47

Method Name: NCHS

Method Filename: Copy of N C H S-bkp.mth

Filename	As Method	Vial
Vatandoust-163		
# Group Sample Name	Tayp Weig. Prof. F ---	-----
163-1 115	UNK 0.591 6.25 ---	-----
Component Name Element%		
Nitrogen% 3.889078617		
Carbon% 73.51745331		
Hydrogen% 4.744987651		
Sulphur% 0		

1 Sample (s) in Group No:1

Component Name	Average
Nitrogen%	3.889078617
Carbon%	73.51745331
Hydrogen%	4.744987651
Sulphur%	0

Figure 38. CHNS spectrum of compound **2h**

Anal. Calcd. for $C_{22}H_{17}NO_4$ (359)		
C: 73.53 %	H: 4.77 %	N: 3.90 %

7-(4-methoxyphenyl)-7,10,11,12-tetrahydro-6H-chromeno[4,3-b]quinoline-6,8(9H)-dione (2i)[2]

Light yellow solid; (0.298g, 80%); Mp=274-275 °C (Lit 276-278 °C); IR (KBr) (υ_{max}/cm^{-1}): 3325(NH), 3087, 3039(C-H aromatic), 2947, 2839 (C-H aliphatic),1669 (C=O), 1605 (C=C); MS: (m/z, %): 373 (M^+, 22), 371 (M^+-2, 100), 343 (5) 266 (56), 28 (100).

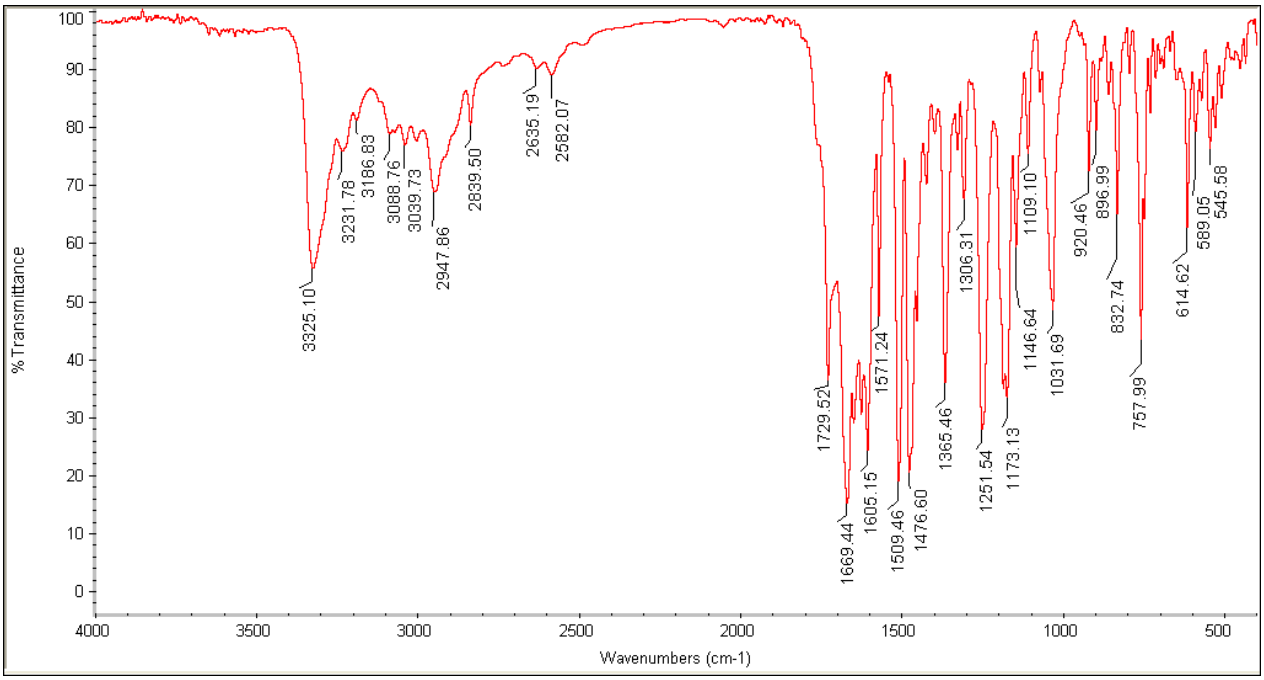


Figure 39. IR spectrum of compound **2i**

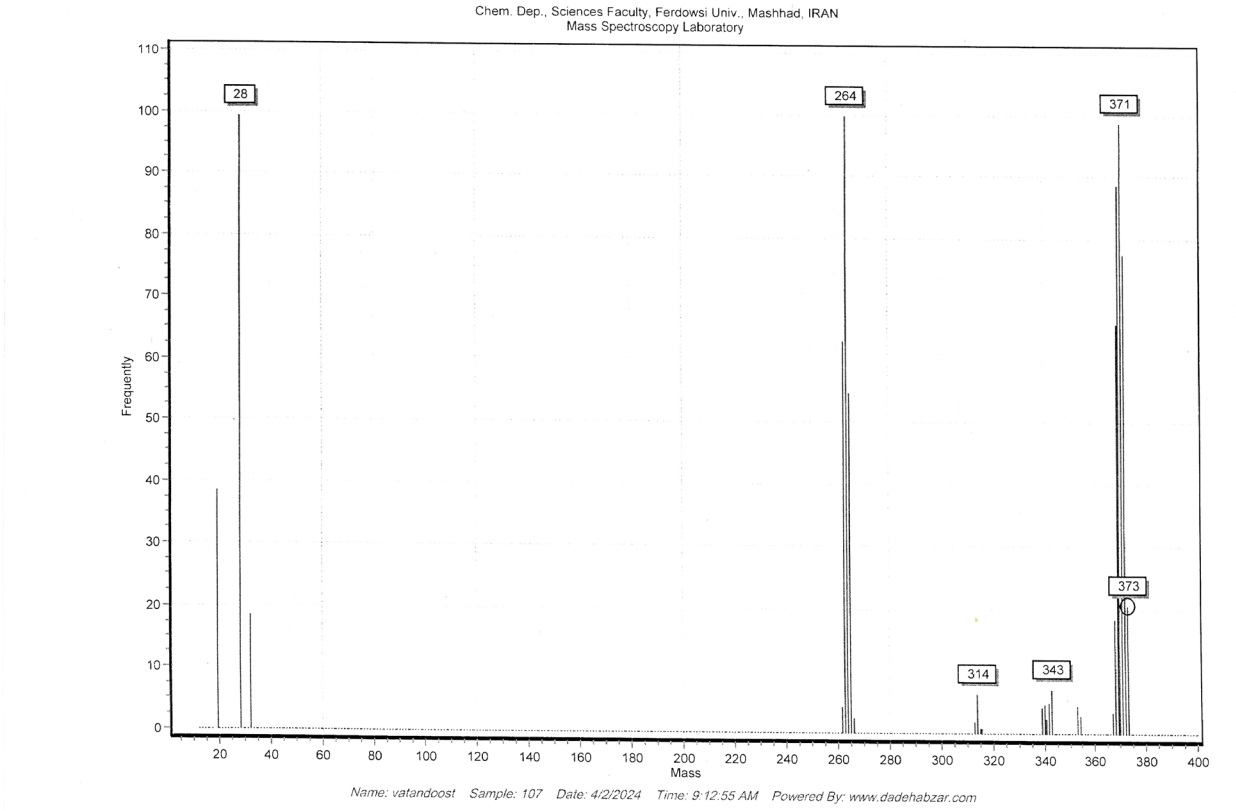


Figure 40. Mass spectrum of compound **2i**

7-(p-tolyl)-7,10,11,12-tetrahydro-6H-chromeno[4,3-b]quinoline-6,8(9H)-dione (2j)[2]

Light yellow solid; (0.285g, 80%); Mp=302-303 °C (Lit. 304-305 °C); IR (KBr) (υ_{max}/cm^{-1}): 3308(NH), 3088 (C-H aromatic), 2953, 2896 (C-H aliphatic), 1665 (C=O), 1634,1605 (C=C); ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ (ppm): 9.71 (s,1H, NH), 8.31 (d, *J* = 7.9 Hz, 1H, ArH, H$_1$), 7.65 (t, *J* = 7.7 Hz, 1H, ArH, H$_3$), 7.43 (m, 2H, ArH, H$_2$, H$_4$), 7.13 (d, *J* = 8.2 Hz, 2H, ArH, H$_{14}$, H$_{18}$), 7.02 (d, *J* = 8.2 Hz, 2H, ArH, H$_{15}$, H$_{17}$), 4.97 (s, 1H, CH, H$_7$), 2.87-2.78 (m, 1H, CH$_2$, H$_9$) 2.75-2.65 (m, 1H, CH$_2$, H$_9$), 2.35-2.24 (m, 2H, CH$_2$, H$_{11}$), 2.20 (s, 3H, CH$_3$), 2.06-1.92 (m, 1H, CH$_2$, H$_{10}$), 1.89-1.83 (m, 1H, CH$_2$, H$_{10}$); ^{13}C NMR (75 MHz, DMSO-*d*$_6$): δ (ppm): 195.41 (C$_8$), 160.81 (C$_6$), 152.49 (C$_{4a}$), 151.94 (C$_{11a}$), 143.55 (C$_{12a}$), 142.38 (C$_{13}$), 135.68 (C$_{16}$), 132.35(C$_3$), 129.05 (C$_{15}$,C$_{17}$), 128.03 (C$_{14}$,C$_{18}$), 124.44 (C$_1$), 123.39 (C$_2$), 117.31(C$_4$), 113.76 (C$_{12b}$), 112.50 (C$_{7a}$), 102.42 (C$_{6a}$), 37.16(C$_9$), 34.17 (C$_7$), 26.83 (C$_{11}$), 21.22 (C$_{10}$), 21.05 (CH$_3$); MS: (m/z, %): 357 (M$^+$, 10), 355 (M$^+$-2, 40), 266 (60), 152 (88), 91 (28), 28 (100); Anal. Calcd. for C$_{23}$H$_{19}$NO$_3$ (357): C: 77.29, H: 5.36, N: 3.92%. Found: C: 77.12, H: 5.22, N: 3.78%.

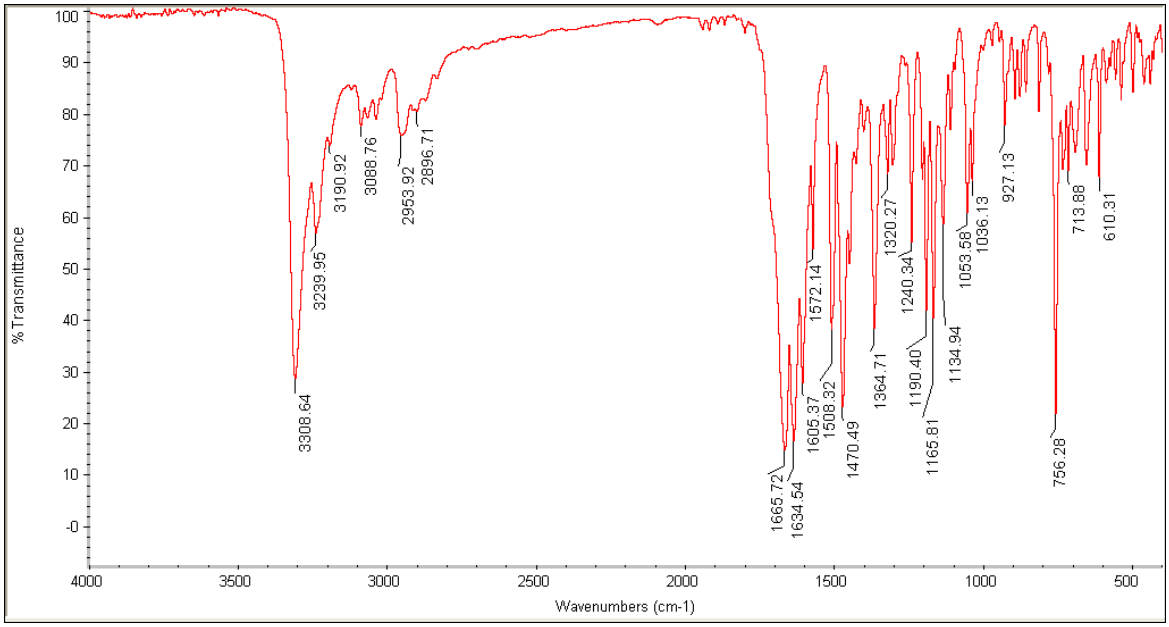


Figure 41. IR spectrum of compound **2j**

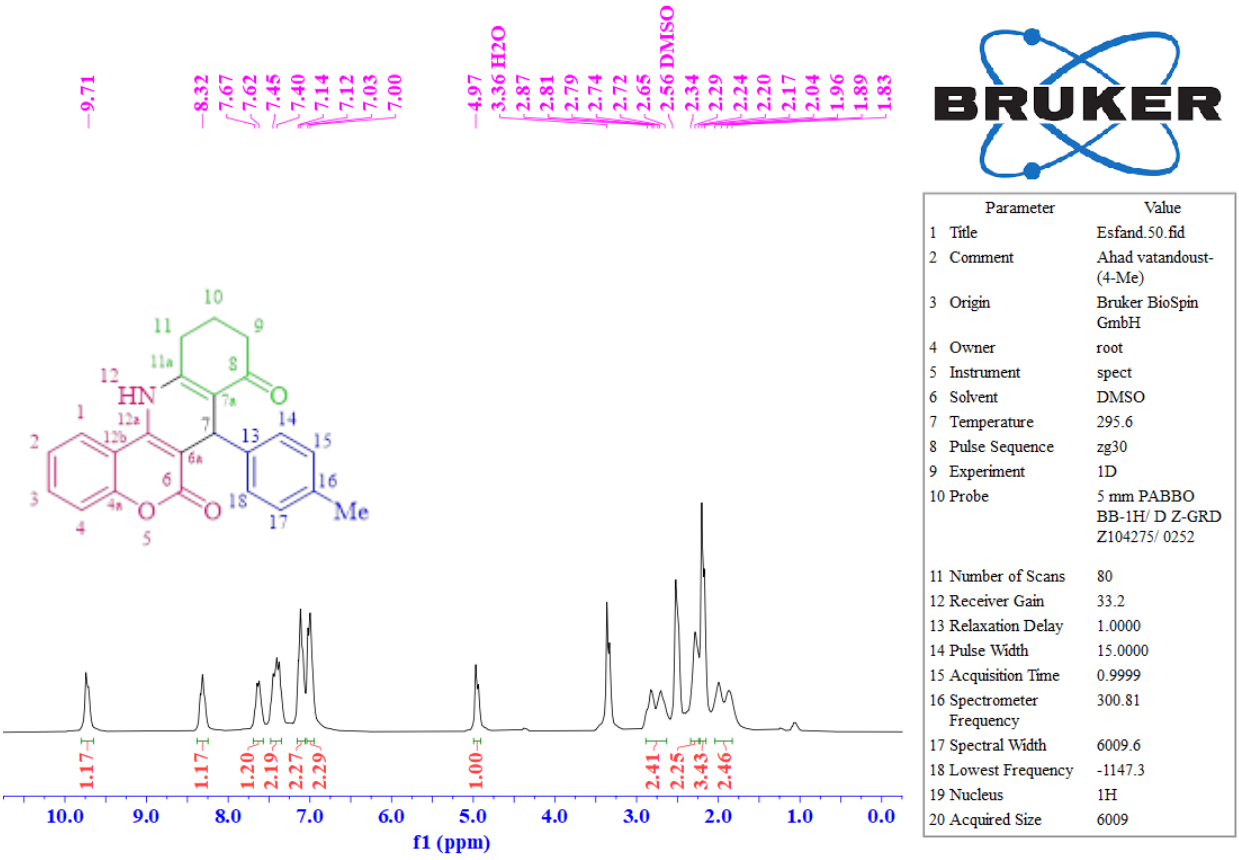


Figure 42. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of compound **2j**

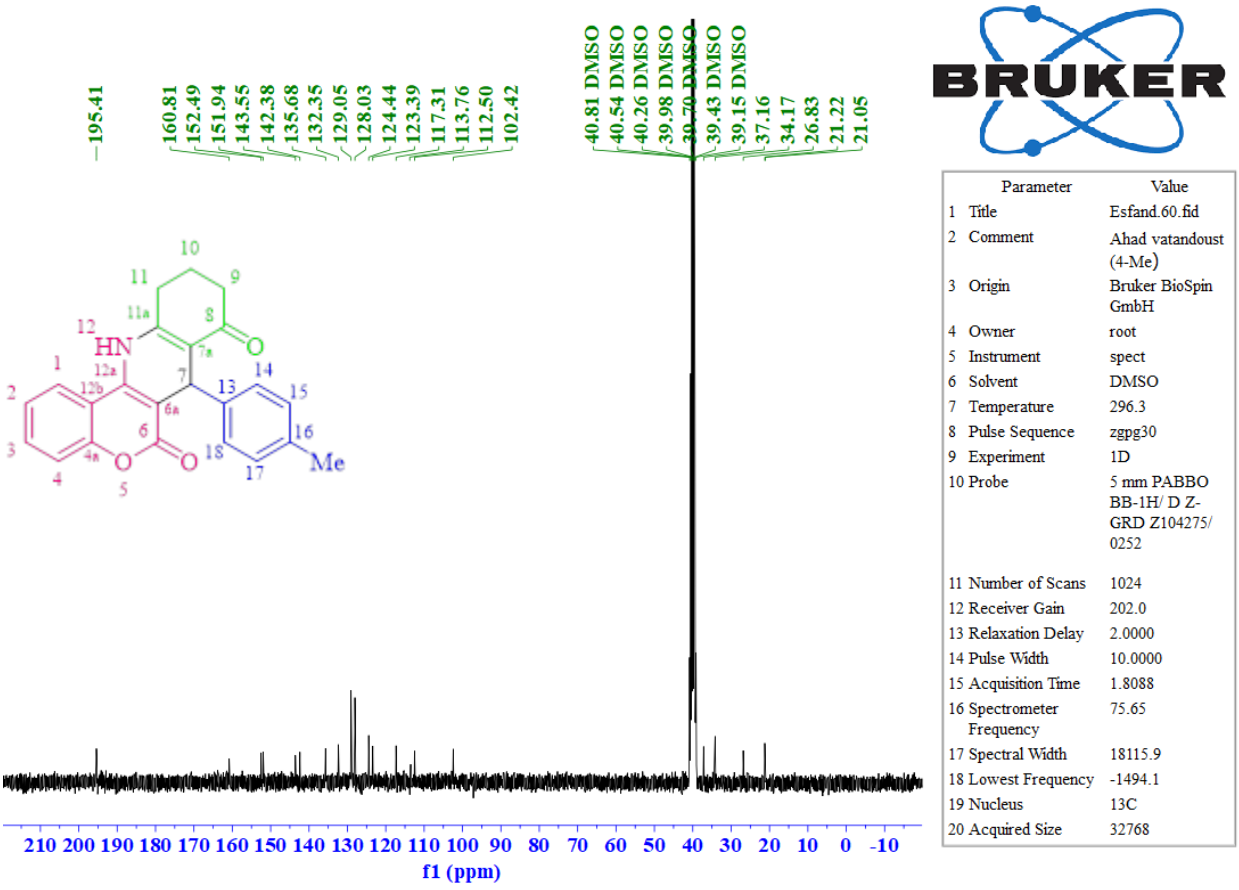


Figure 43. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of compound **2j**

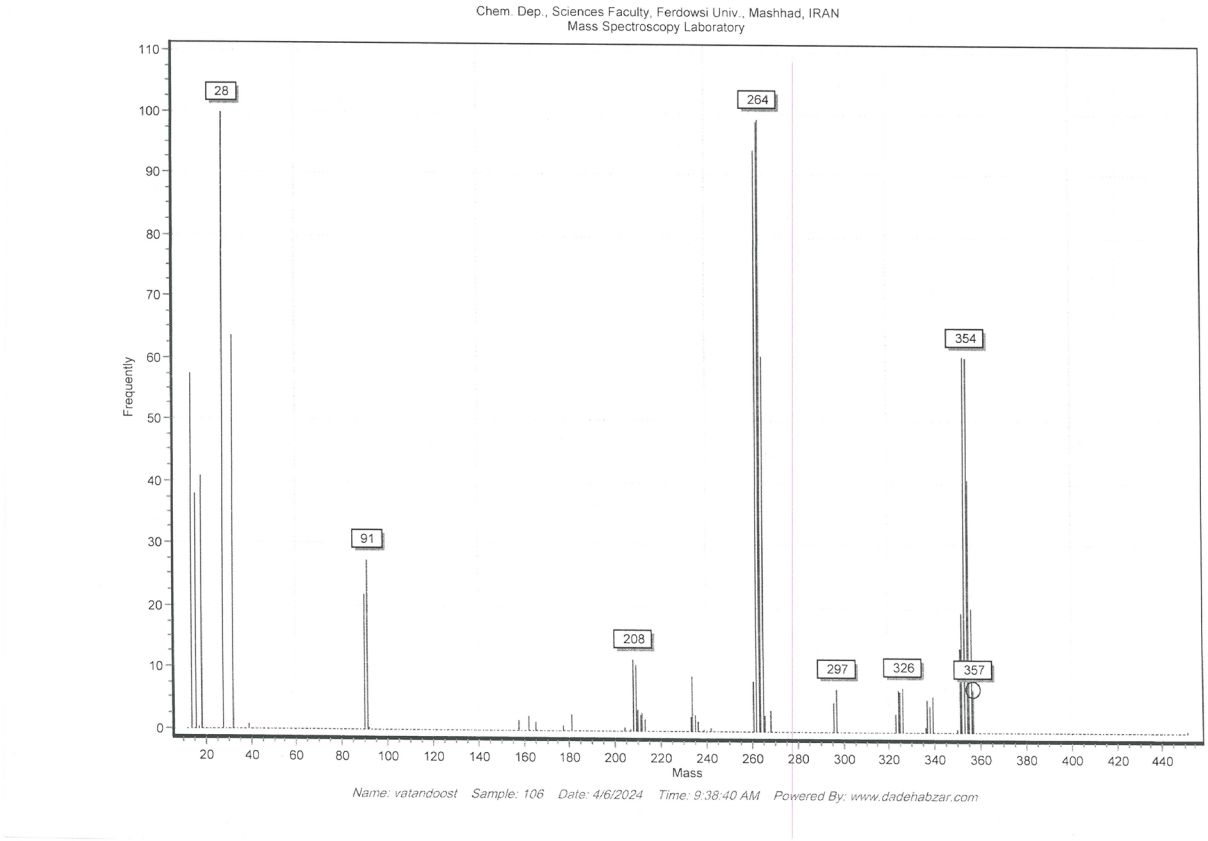


Figure 44. Mass spectrum of compound **2j**

Eager 300 Summarize Results

Date: 24/04/2024 at 13:04:57

Method Name: NCHS

Method Filename: Copy of N C H S-bkp.mth

Filename	As Method	Vial
Vatandoust-173		
# Group Sample Name	Tayp Weig. Prof. F ---	-----
173-1 106	UNK 0.651 6.25 ---	-----

Component Name	Element%
Nitrogen%	3.782251453
Carbon%	77.1215451
Hydrogen%	5.224343908
Sulphur%	0

1 Sample (s) in Group No:1

Component Name	Average
Nitrogen%	3.782251453
Carbon%	77.1215451
Hydrogen%	5.224343908
Sulphur%	0

Figure 45. CHNS spectrum of compound **2j**

Anal. Calcd. for $C_{23}H_{19}NO_3$ (357)		
C: 77.29 %	H: 5.36 %	N: 3.92 %

7-(m-tolyl)-7,10,11,12-tetrahydro-6H-chromeno[4,3-b]quinoline-6,8(9H)-dione (2k)[5]

Light yellow solid; (0.267g, 75%); Mp=309-311 °C (Lit. 310 °C); IR (KBr) (υ_{max}/cm^{-1}): 3308(NH), 3084,3035 (C-H aromatic), 2945 (C-H aliphatic), 1665 (C=O), 1634,1605 (C=C); ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ (ppm): 9.76 (s, 1H, D_2O exchangeable, NH), 8.33 (d, *J* = 7.9 Hz, 1H, ArH, H_1), 7.65 (t, *J* = 8.0 Hz, 1H, ArH, H_3), 7.45 (t, *J* = 7.7 Hz, 1H, ArH, H_2), 7.39 (d, *J* = 8.3 Hz, 1H, ArH, H_4), 7.12-7.01 (m, 3H, ArH, H_{14}, H_{17}, H_{18}), 6.93 (s, 1H, ArH, H_{16}), 4.98 (s, 1H, CH, H_7), 2.90-2.82 (m, 1H, CH_2, H_9), 2.74-2.70 (m, 1H, CH_2, H_9), 2.32-2.28 (m, 2H, CH_2, H_{11}), 2.23 (s, 3H, CH_3), 2.06-2.00 (m, 1H, CH_2, H_{10}), 1.93-1.90 (m, 1H, CH_2, H_{10}); ^{13}C NMR (75 MHz, DMSO-*d*$_6$): δ (ppm): 195.43 (C_8), 160.82 (C_6), 152.49 (C_{4a}), 152.08(C_{11a}), 146.39(C_{12a}), 142.48(C_{13}), 137.34(C_{15}), 132.39 (C_3), 128.80 (C_{17}), 128.49(C_{16}), 127.40 (C_{14}), 125.29 (C_1), 124.47 (C_{18}), 123.43 (C_2), 117.34 (C_4), 113.53 (C_{12b}), 112.40 (C_{7a}), 102.33 (C_{6a}), 37.18 (C_9), 34.53 (C_7), 26.88 (C_{11}), 21.62 (C_{10}), 21.22 (CH_3). MS: (m/z, %): 357 (M^+, 10), 355 (M^+-2, 70), 266(50), 28 (100); Anal. Calcd. for $C_{23}H_{19}NO_3$(357): C: 77.29, H: 5.36, N: 3.92%. Found: C: 77.14, H: 5.28, N: 3.80%.

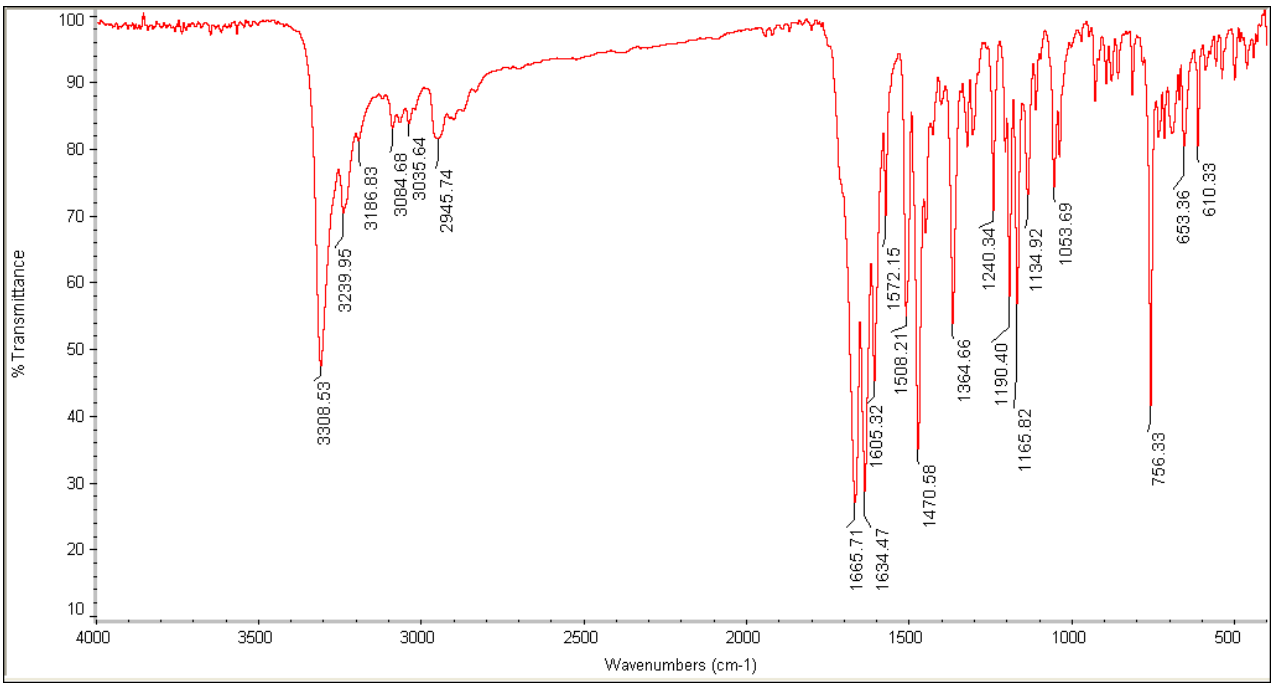


Figure 46. IR spectrum of compound **2k**

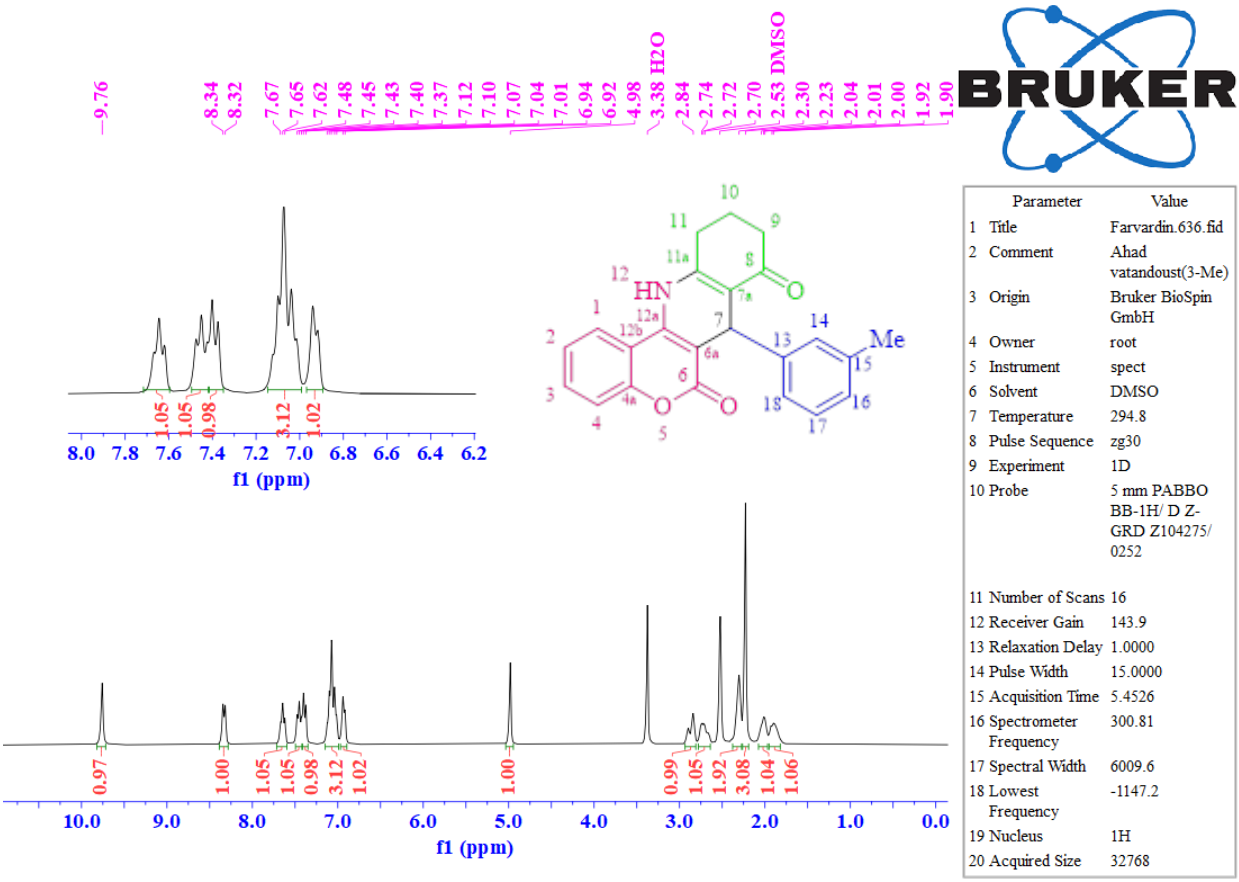


Figure 47. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of compound **2k**

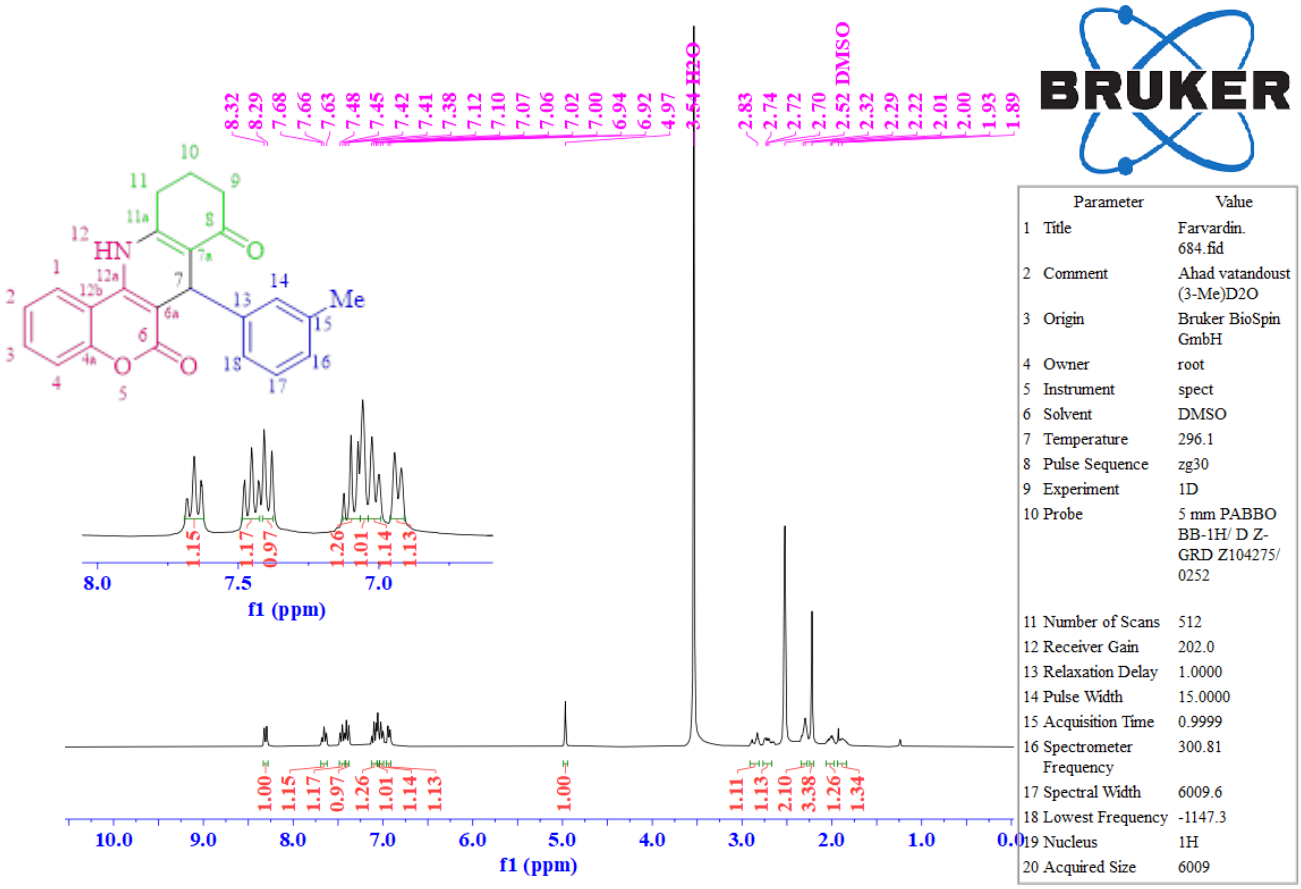


Figure 48. ^{1}H NMR (300 MHz, DMSO-d_6) (D_2O) spectrum of compound **2k**

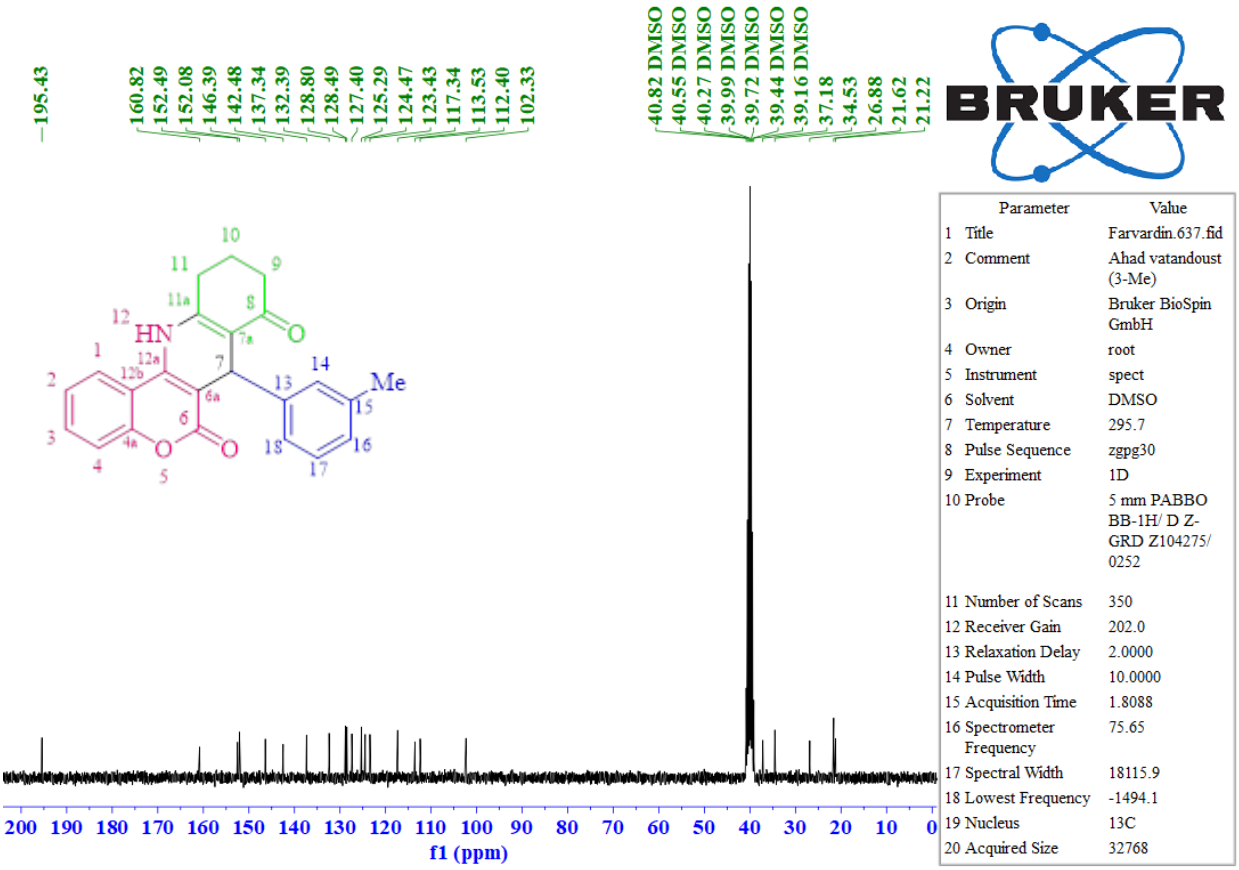


Figure 49. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of compound **2k**

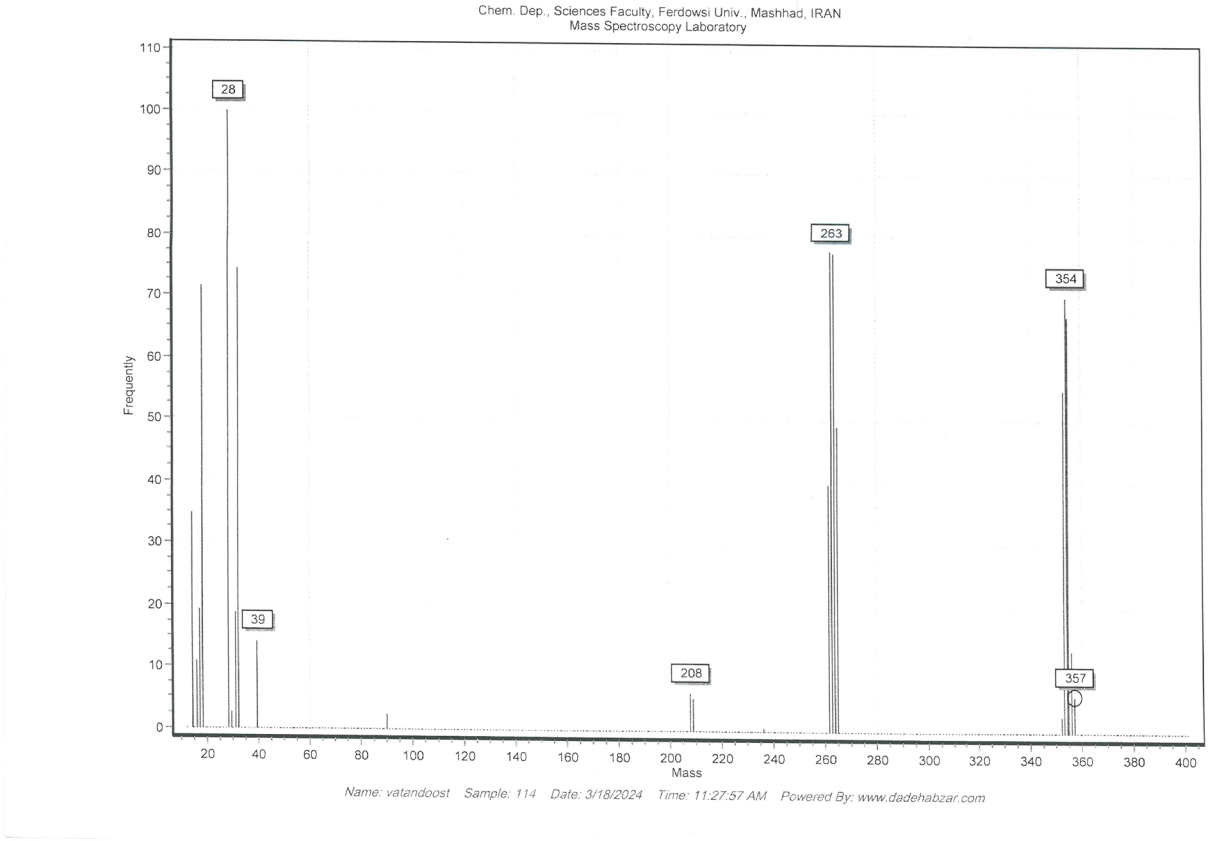


Figure 50. Mass spectrum of compound **2k**

Eager 300 Summarize Results

Date: 24/04/2024 at 13:03:23

Method Name: NCHS

Method Filename: Copy of N C H S-bkp.mth

Filename	As Method	Vial
Vatandoust-166		
# Group Sample Name	Tayp Weig. Prof. F ---	-----
166-1 114	UNK 0.607 6.25 ---	-----
Component Name Element%		
Nitrogen% 3.80542572		
Carbon% 77.14088562		
Hydrogen% 5.288564281		
Sulphur% 0		

1 Sample (s) in Group No:1

Component Name	Average
Nitrogen%	3.80542572
Carbon%	77.14088562
Hydrogen%	5.288564281
Sulphur%	0

Figure 51. CHNS spectrum of compound **2k**

Anal. Calcd. for $C_{23}H_{19}NO_3$(357)		
C: 77.29 %	H: 5.36 %	N: 3.92 %

7-(2-hydroxy-5-nitrophenyl)-7,10,11,12-tetrahydro-6H-chromeno[4,3-b]quinoline-6,8(9H)-dione (2l)

Light yellow solid; (0.343g, 85%); Mp=323-324 °C; IR (KBr) (υ_{max}/cm^{-1}): 3348 (NH), 3252 (OH) 3050 (C-H aromatic), 2941 (C-H aliphatic), 1676 (C=O), 1649, 1599 (C=C); ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ (ppm): 10.90 (s, 1H, OH), 9.82 (s, 1H, NH), 8.33 (d, *J* = 8.1 Hz, 1H, ArH, H_1), 8.05 (s, 1H, ArH, H_{18}), 7.92 (d, *J* = 9.4 Hz, 1H, ArH, H_{16}), 7.64 (t, *J* = 7.9 Hz, 1H, ArH, H_3), 7.45 (t, *J* = 7.7 Hz, 1H, ArH, H_2), 7.37 (d, *J* = 8.3 Hz, 1H, ArH, H_4), 6.83 (d, *J* = 9.0 Hz, 1H, ArH, H_{15}), 5.11 (s, 1H, CH, H_7), 2.83-2.64(m, 1H, CH_2, H_9), 2.74-2.70(m, 1H, CH_2, H_9), 2.37-2.25 (m, 2H, CH_2, H_{11}), 2.00-1.93 (m, 1H, CH_2, H_{10}), 1.88-1.78 (m, 1H, CH_2, H_{10}); ^{13}C NMR (75 MHz, DMSO-*d*$_6$): δ (ppm): 195.89 (C_8), 162.70 (C_6), 160.64 (C_{14}), 153.35 (C_{4a}), 152.59 (C_{11a}), 143.50 (C_{12a}), 139.55 (C_{17}), 132.45 (C_3), 131.95 (C_{13}), 127.56 (C_1), 124.45 (C_{18}), 124.30 (C_{16}), 123.36 (C_2), 117.35 (C_{15}), 116.87 (C_4), 113.29 (C_{12b}), 110.28 (C_{7a}), 100.16 (C_{6a}), 37.02 (C_9), 33.49 (C_7), 26.88 (C_{11}), 21.18 (C_{10}); MS: (m/z, %):404 (M^+, 8), 402 (M^+-2, 10), 387(10), 266(10),138(35) 28(68); Anal. Calcd. for $C_{22}H_{16}N_2O_4$ (404): C: 65.35, H: 3.99, N: 6.92%. Found: C: 65.30, H: 3.92, N: 6.88%.

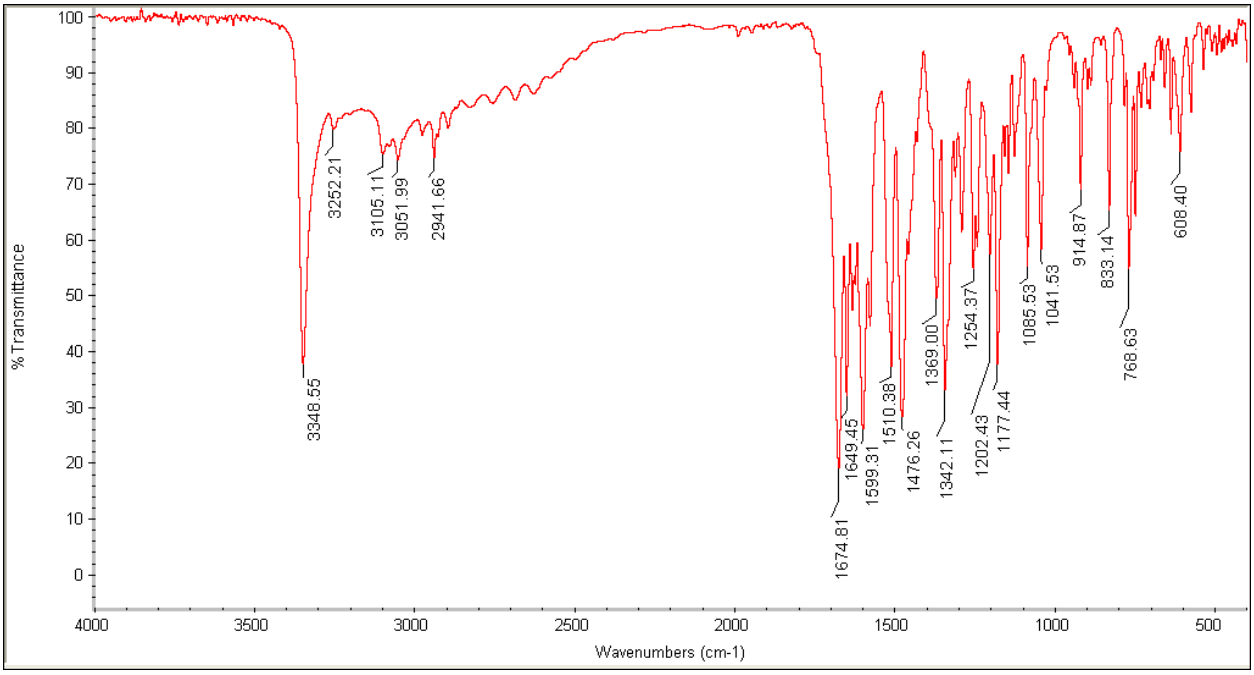


Figure 52. IR spectrum of compound **2l**

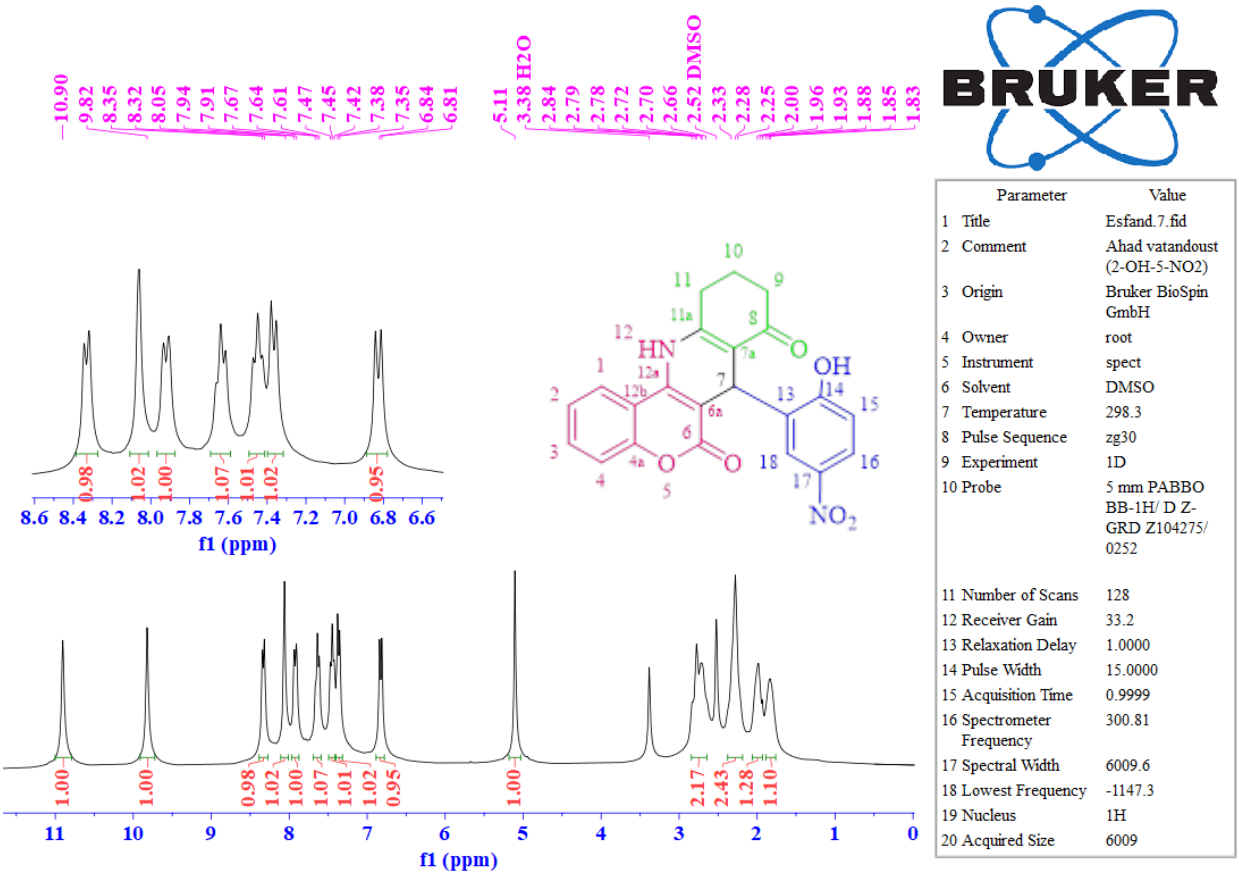


Figure 53. ^{1}H NMR (300 MHz, DMSO-d_6) spectra of compound **2l**

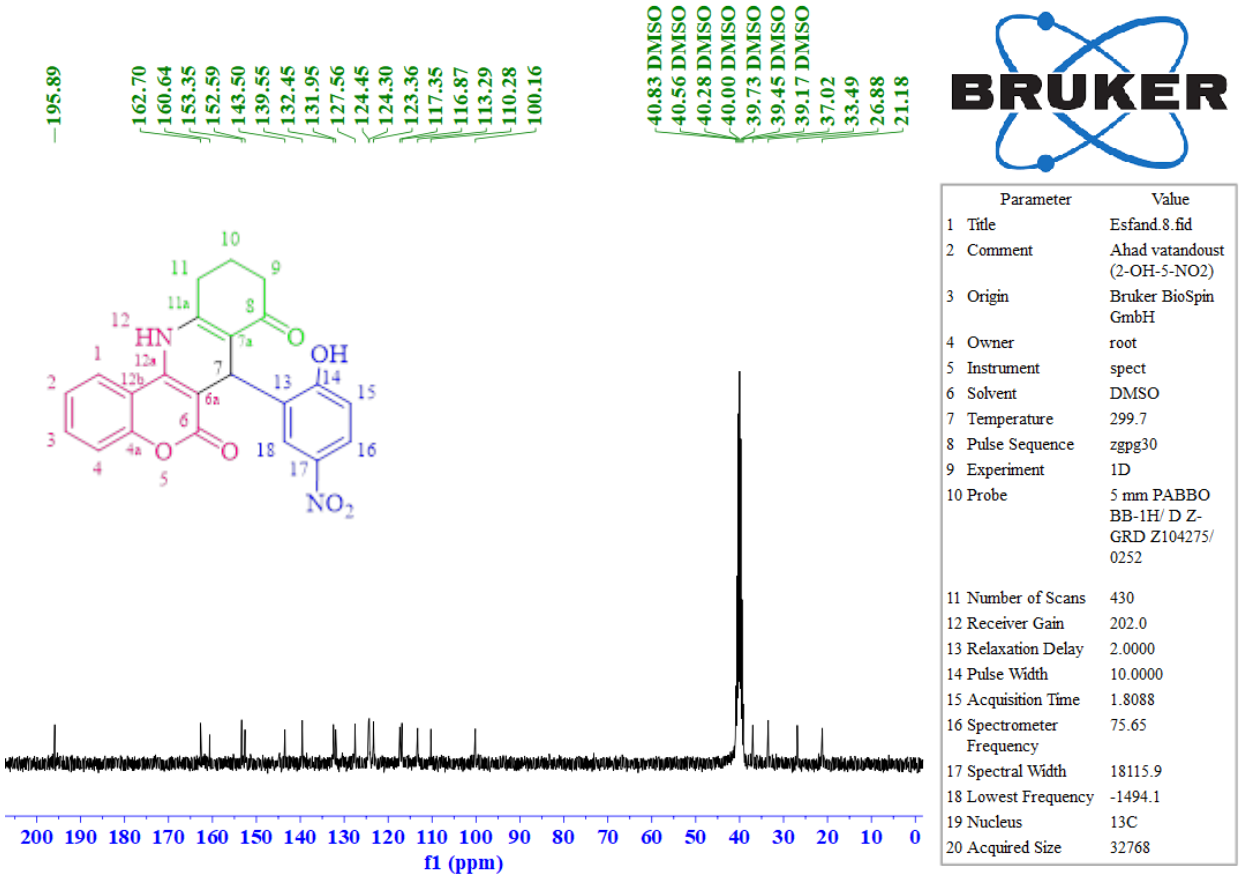


Figure 54. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of compound **2l**

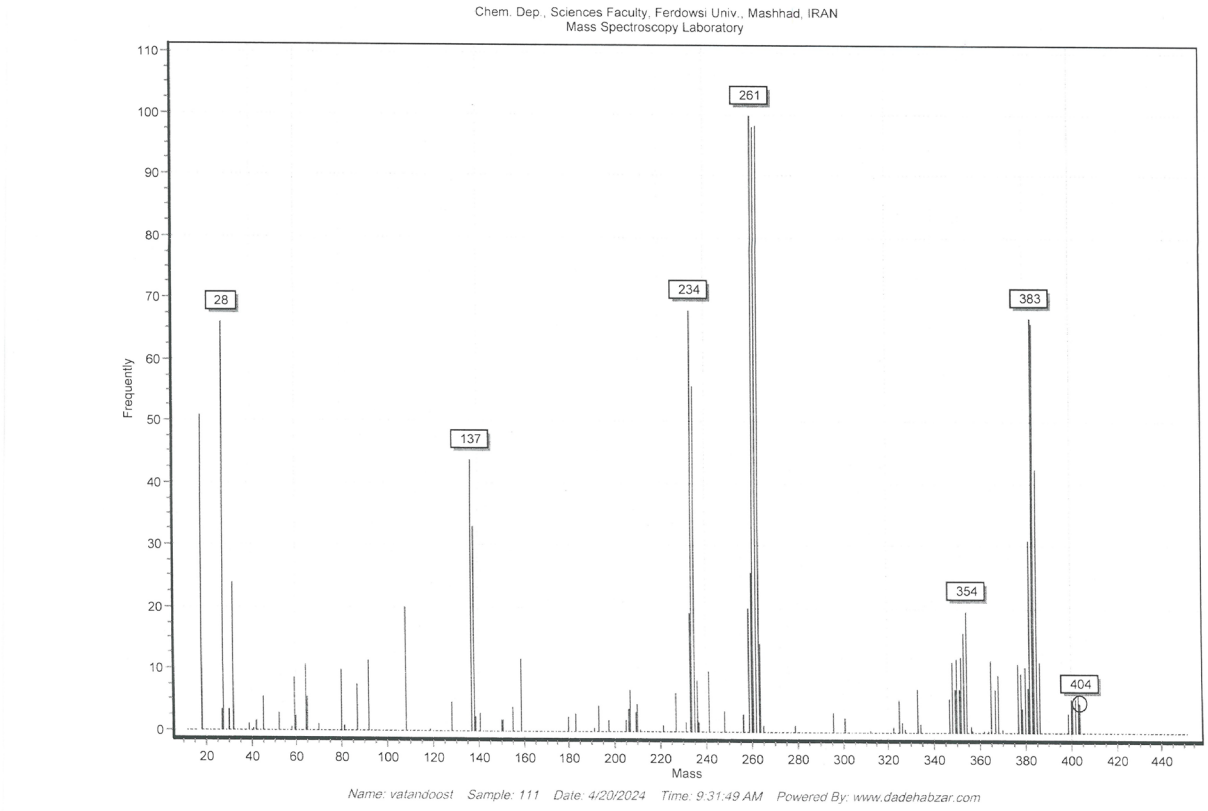


Figure 55. Mass spectrum of compound **2l**

Eager 300 Summarize Results

Date: 24/04/2024 at 13:03:43

Method Name: NCHS

Method Filename: Copy of N C H S-bkp.mth

Filename		As Method				Vial
Vatandoust-167						
# Group Sample Name		Tayp Weig. Prof. F			---	-----
167-1	111	UNK	0.699	6.25	---	-----
Component Name	Element%					
Nitrogen%	6.884370518					
Carbon%	65.30261581					
Hydrogen%	3.920376778					
Sulphur%	0					

1 Sample (s) in Group No:1

Component Name	Average
Nitrogen%	6.884370518
Carbon%	65.30261581
Hydrogen%	3.920376778
Sulphur%	0

Figure 56. CHNS spectrum of compound **2l**

Anal. Calcd. for $C_{22}H_{16}N_2O_4$ (404)		
C: 65.35 %	H: 3.99 %	N: 6.92 %

7-(5-bromo-2-hydroxyphenyl)-7,10,11,12-tetrahydro-6H-chromeno[4,3-b]quinoline-6,8(9H)-dione (2m)

Light yellow solid; (0.35g, 80%); Mp=308-310 °C; IR (KBr) (υ_{max}/cm^{-1}): 3348 (NH), 3101 (OH) 3050 (C-H aromatic), 2941 (C-H aliphatic), 1675 (C=O), 1608 (C=C); ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ (ppm): 9.83 (s, 1H, NH), 9.59 (s, 1H, OH), 8.35 (s, 1H, ArH, H_1), 7.65 (s, 1H, ArH, H_{18}), 7.43 (m, 2H, ArH, H_3,H_2), 7.19 (m, 2H, ArH, H_4,H_{16}), 6.71 (s, 1H, ArH, H_{15}), 4.97 (s, 1H, CH, H_7), 2.84-2.65 (m, 2H, CH_2, H_9), 2.31 (s, 2H, CH_2, H_{11}), 2.03-1.83 (m, 2H, CH_2, H_{10}); ^{13}C NMR (75 MHz, DMSO-*d*$_6$): δ (ppm): 196.46 (C_8), 160.75 (C_6), 155.24 (C_{14}), 153.47(C_{4a}), 152.55(C_{11a}), 143.34 (C_{12a}), 134.20 (C_3), 133.41(C_{16}), 132.41(C_{13}), 130.44 (C_{18}), 124.46 (C_1), 123.39 (C_2), 119.08 (C_{15}), 117.35 (C_4), 113.38 (C_{17}), 110.68 (C_{12b}), 110.52 (C_{7a}), 100.62 (C_{6a}), 36.98 (C_9), 32.52 (C_7), 26.93 (C_{11}), 21.09 (C_{10}); MS: (m/z, %):438 (M^+, 48), 436 (M^+-2, 38),420 (68),358 (5),266 (45),170 (35) 28 (100); Anal. Calcd. for $C_{22}H_{16}BrNO_4$ (438): C: 60.29, H: 3.68, N: 3.20%. Found: C: 60.18, H: 3.62, N: 3.11%.

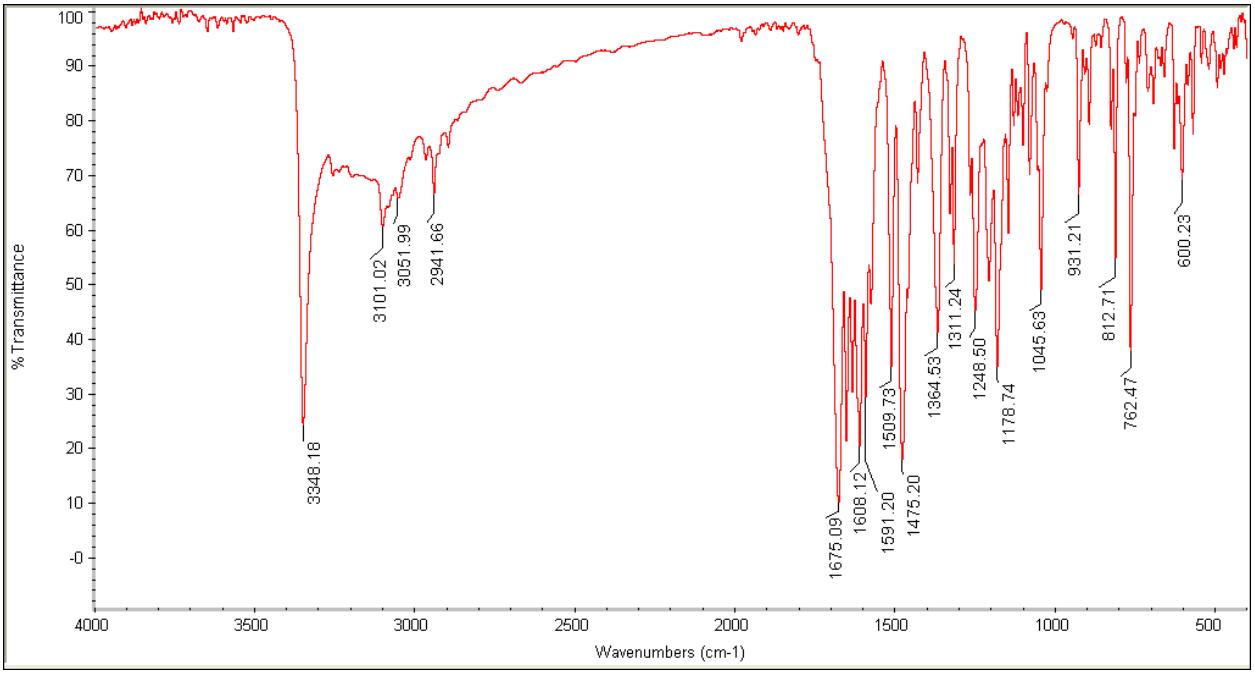
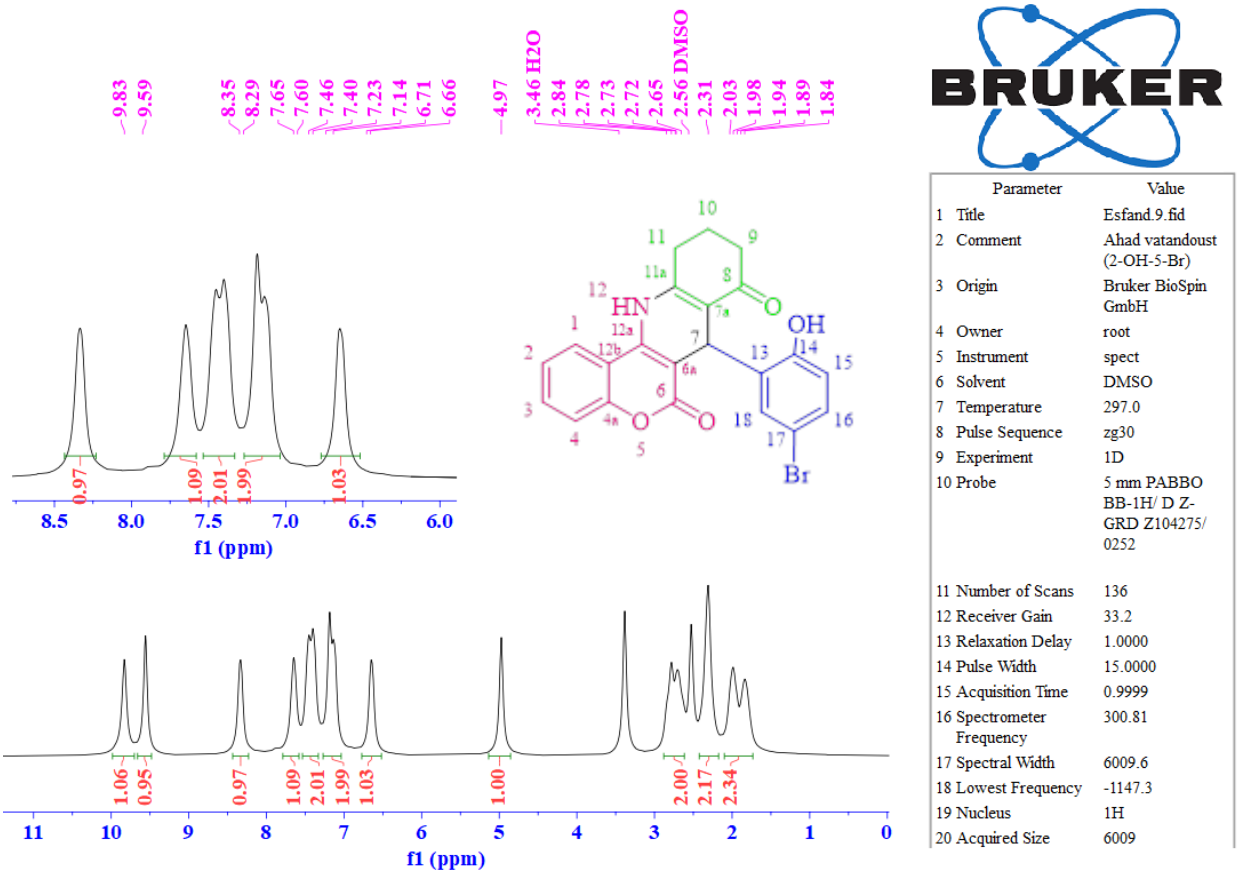


Figure 57. IR spectrum of compound **2m**



BRUKER

	Parameter	Value
1	Title	Esfand.9.fid
2	Comment	Ahad vatandoust (2-OH-5-Br)
3	Origin	Bruker BioSpin GmbH
4	Owner	root
5	Instrument	spect
6	Solvent	DMSO
7	Temperature	297.0
8	Pulse Sequence	zg30
9	Experiment	1D
10	Probe	5 mm PABBO BB-1H/ D Z-GRD Z104275/ 0252
11	Number of Scans	136
12	Receiver Gain	33.2
13	Relaxation Delay	1.0000
14	Pulse Width	15.0000
15	Acquisition Time	0.9999
16	Spectrometer Frequency	300.81
17	Spectral Width	6009.6
18	Lowest Frequency	-1147.3
19	Nucleus	1H
20	Acquired Size	6009

Figure 58. [1]H NMR (300 MHz, DMSO-d_6) spectrum of compound **2m**

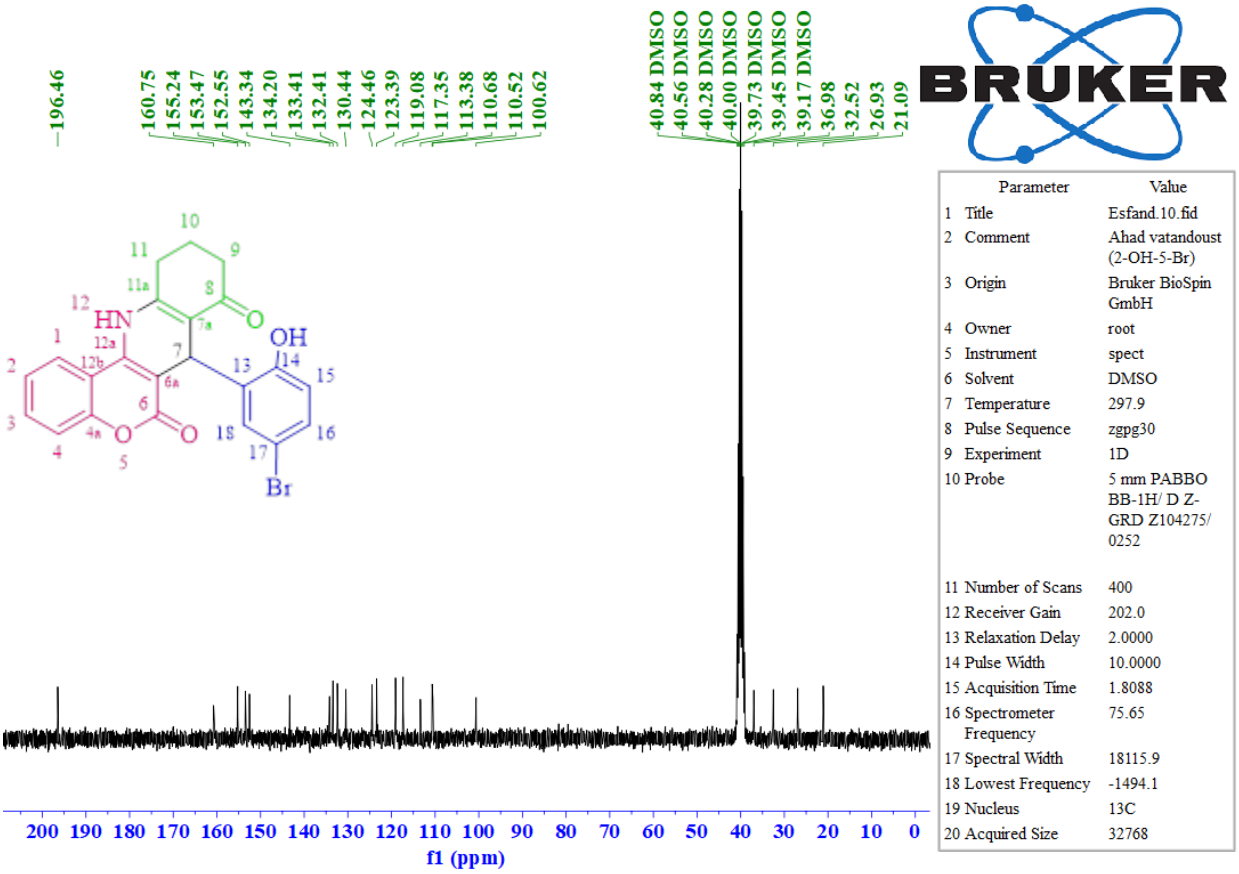


Figure 59. [13]C NMR (75 MHz, DMSO-d_6) spectrum of compound **2m**

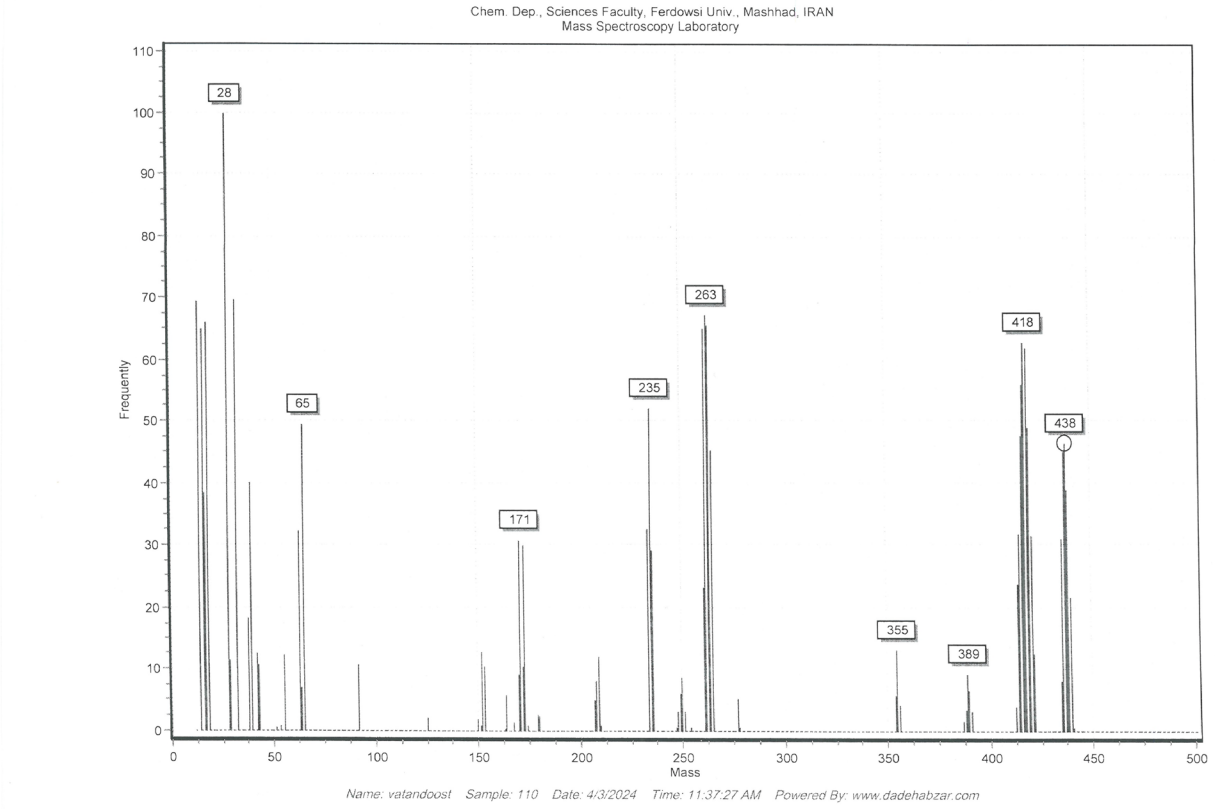


Figure 60. IR spectrum of compound **2m**

Eager 300 Summarize Results

Date: 24/04/2024 at 13:03:58

Method Name: NCHS

Method Filename: Copy of N C H S-bkp.mth

Filename	As Method	Vial
Vatandoust-168		
# Group Sample Name	Tayp Weig. Prof. F ---	-----
168-1 110	UNK 0.781 6.25 ---	-----

Component Name	Element%
Nitrogen%	3.117592270
Carbon%	60.18610611
Hydrogen%	3.628347397
Sulphur%	0

1 Sample (s) in Group No:1

Component Name	Average
Nitrogen%	3.117592270
Carbon%	60.18610611
Hydrogen%	3.628347397
Sulphur%	0

Figure 61. CHNS spectrum of compound **2m**

Anal. Calcd. for $C_{22}H_{16}BrNO_4$ (438)		
C: 60.29 %	H: 3.68 %	N: 3.20 %

7-(3,4-dihydroxyphenyl)-7,10,11,12-tetrahydro-6H-chromeno[4,3-b]quinoline-6,8(9H)-dione (2n)

White solid; (0.281g, 75%); Mp=310-311 °C; IR (KBr) (υ_{max}/cm^{-1}): 3460 (OH), 3320 (NH) 3084 (C-H aromatic), 2966, 2872 (C-H aliphatic), 1672 (C=O), 1633, 1604 (C=C); ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ (ppm): 9.69 (s, 1H, NH), 8.74 (s, 1H, OH), 8.59 (s, 1H, OH), 8.31 (d, *J* = 8.1 Hz, 1H, ArH, H$_1$), 7.63 (t, *J* = 7.8 Hz, 1H, ArH, H$_3$), 7.46-7.37 (m, 2H, ArH, H$_2$, H$_4$), 6.68 (s, 1H, ArH, H$_{14}$), 6.56 (d, *J* = 8.2 Hz, 1H, ArH, H$_{17}$), 6.49 (d, *J* = 8.3 Hz, 1H, ArH, H$_{18}$), 4.87 (s, 1H, CH, H$_7$), 2.87-2.80 (m, 1H, CH$_2$, H$_9$), 2.74-2.71 (m, 1H, CH$_2$, H$_9$), 2.38-2.25 (m, 2H, CH$_2$, H$_{11}$), 2.06-1.99 (m, 1H, CH$_2$, H$_{10}$), 1.94-1.87 (m, 1H, CH$_2$, H$_{10}$); ^{13}C NMR (75 MHz, DMSO-*d*$_6$): δ (ppm): 195.46 (C$_8$), 160.90 (C$_6$), 152.43 (C$_{4a}$), 151.55 (C$_{11a}$), 145.07(C$_{12a}$), 144.20 (C$_{16}$), 142.08 (C$_{15}$), 137.62 (C$_{13}$), 132.21 (C$_3$), 124.40 (C$_1$), 123.26 (C$_2$), 118.81 (C$_{18}$), 117.29 (C$_4$), 115.74 (C$_{17}$), 115.61 (C$_{14}$), 113.64 (C$_{12b}$), 112.78 (C$_{7a}$), 102.71(C$_{6a}$), 37.27 (C$_9$), 33.44 (C$_7$), 26.86 (C$_{11}$), 21.24 (C$_{10}$); MS: (m/z, %):(m/z, %):375 (M^+, 8), 373 (M^+-2, 35),266(64), 109(72) 28(100); Anal. Calcd. for $C_{22}H_{17}NO_5$ (375): C: 70.39, H: 4.56, N: 3.73%. Found: C: 70.22, H: 4.46, N: 3.60%.

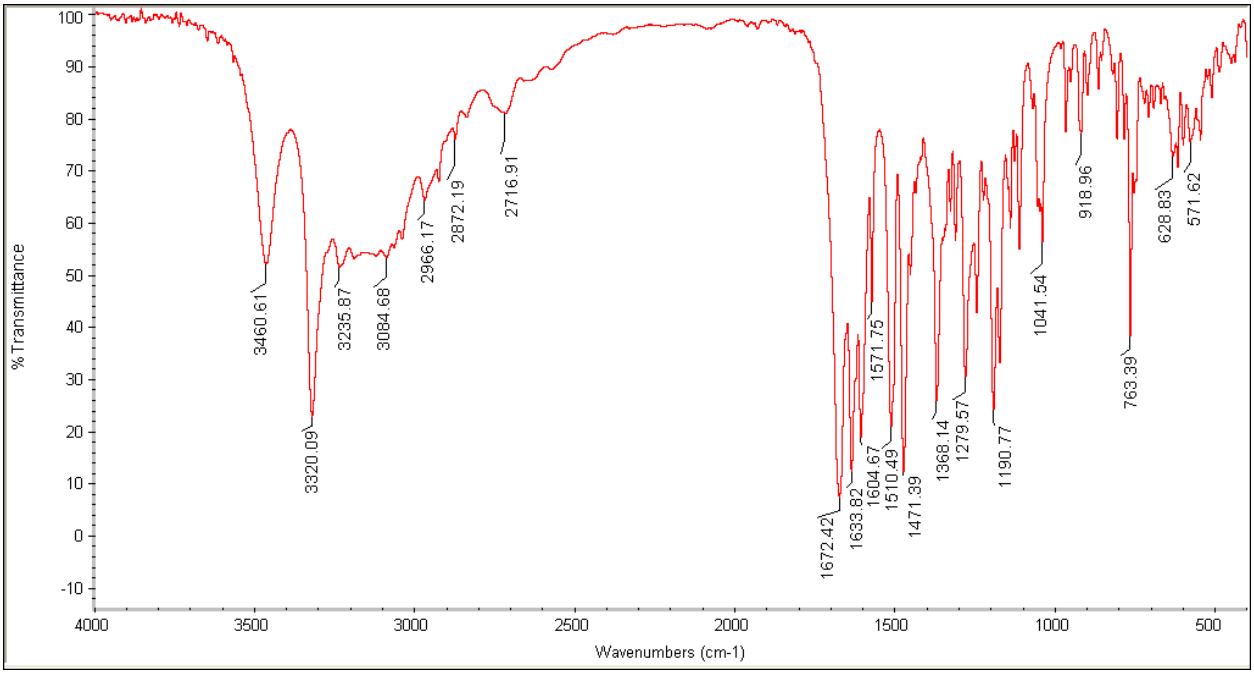


Figure 62. IR spectrum of compound **2n**

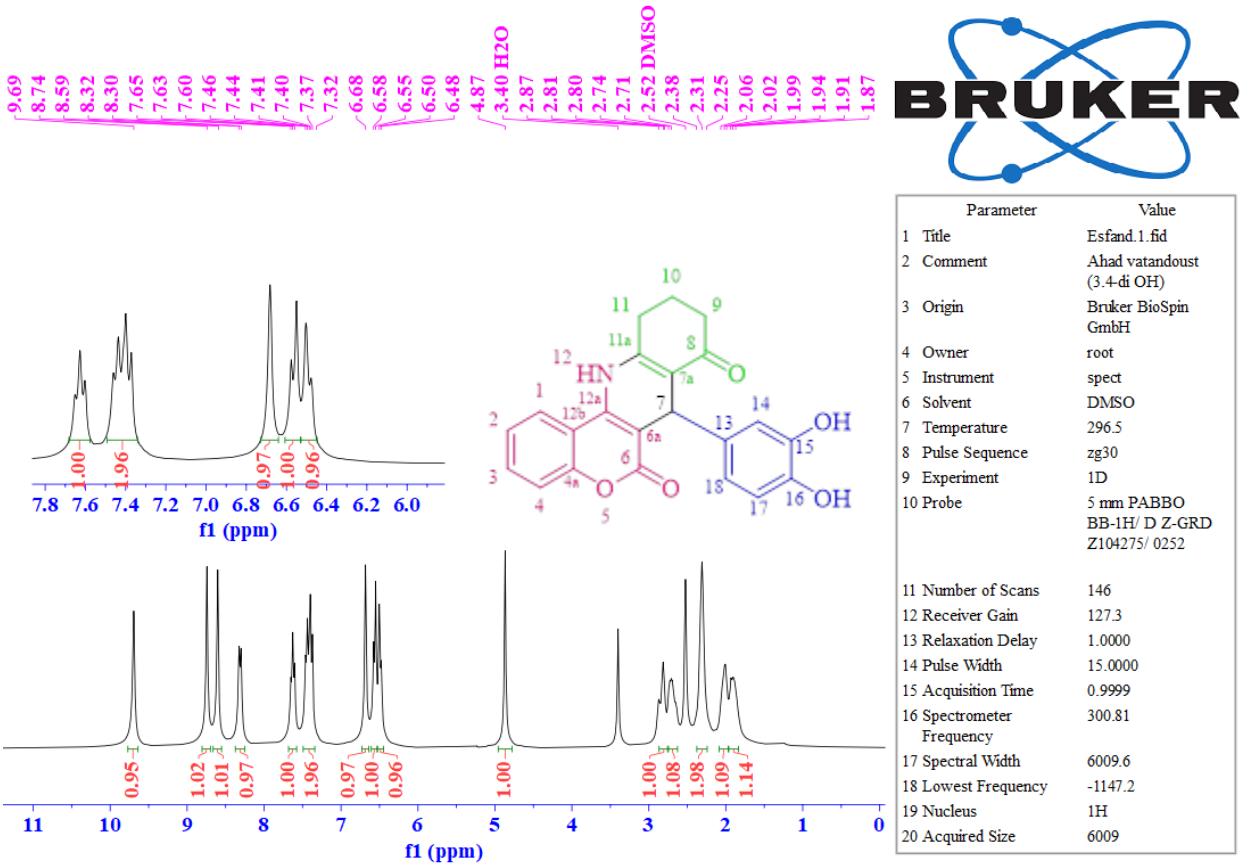


Figure 63. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of compound **2n**

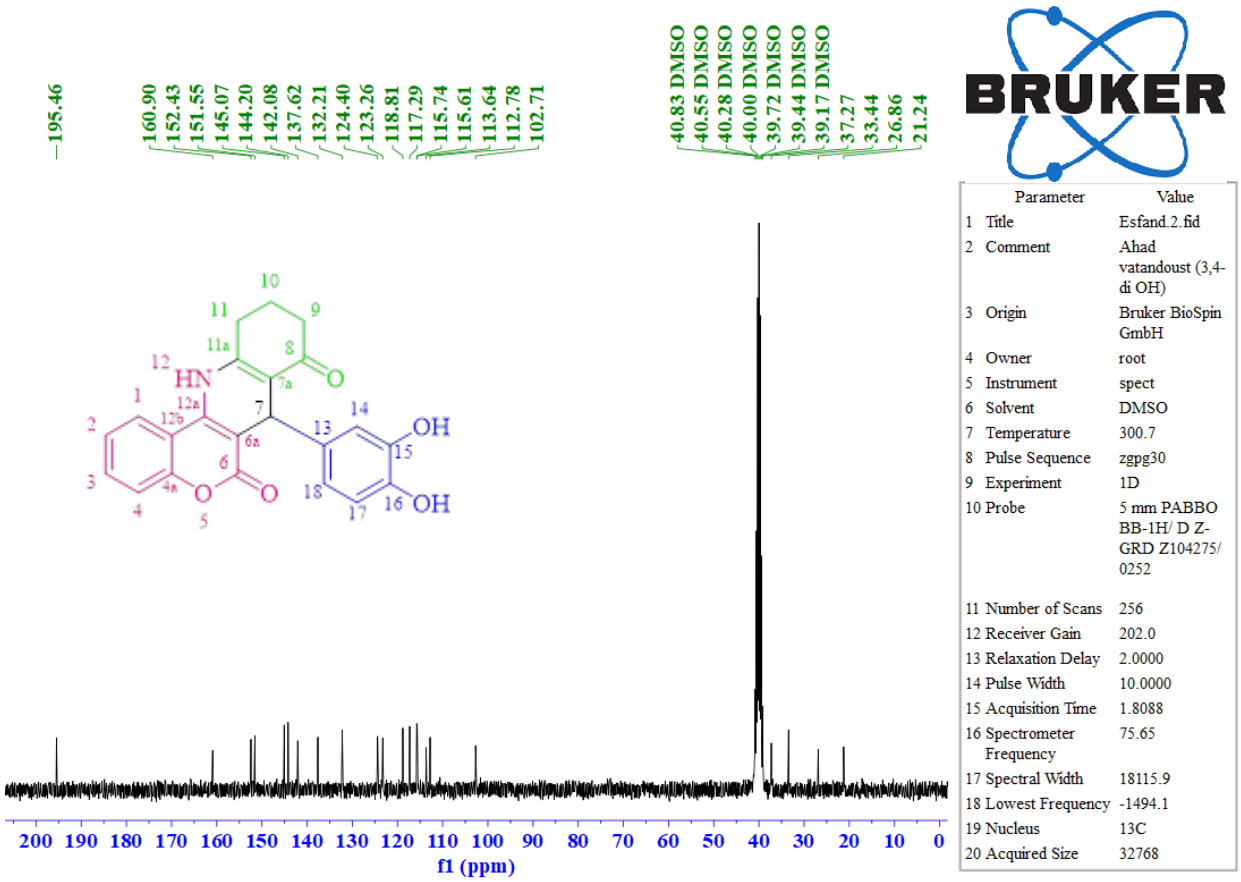


Figure 64. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of compound **2n**

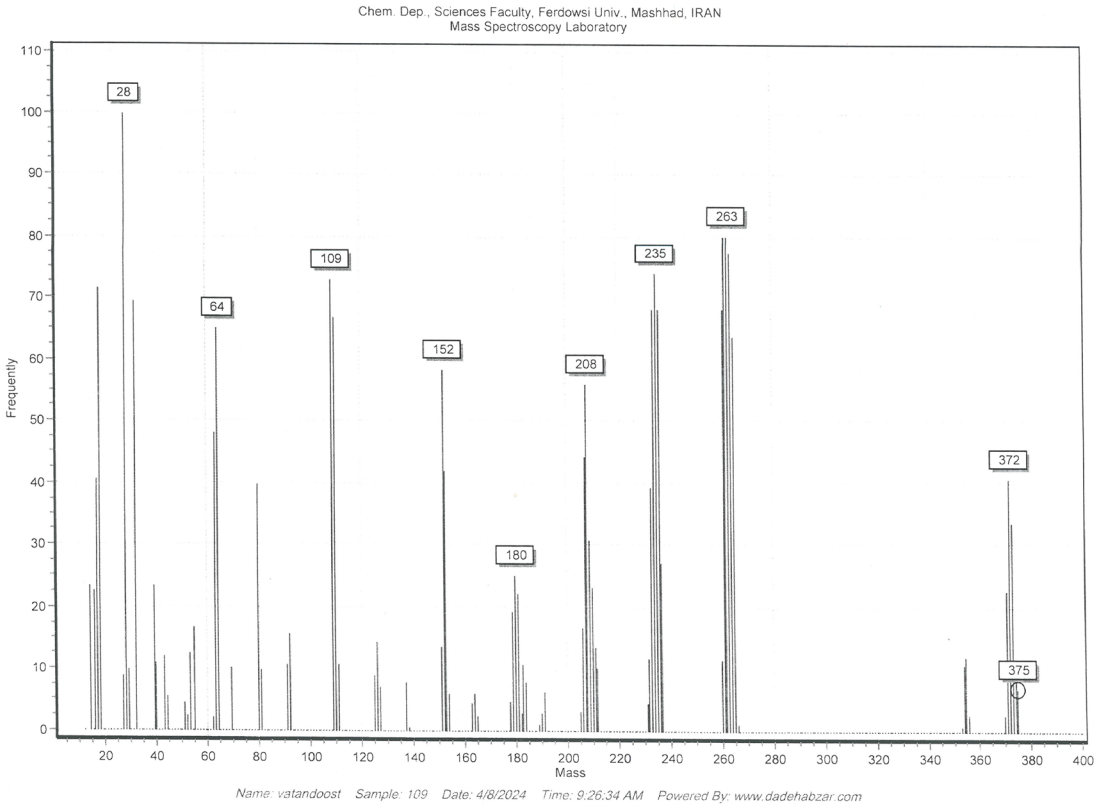


Figure 65. Mass spectrum of compound **2n**

Eager 300 Summarize Results

Date: 24/04/2024 at 13:04:08

Method Name: NCHS

Method Filename: Copy of N C H S-bkp.mth

Filename	As Method	Vial
Vatandoust-169		
# Group Sample Name	Tayp Weig. Prof. F ---	-----
169-1 109	UNK 0.653 6.25 ---	-----

Component Name	Element%
Nitrogen%	3.607834187
Carbon%	70.22381805
Hydrogen%	4.465614891
Sulphur%	0

1 Sample (s) in Group No:1

Component Name	Average
Nitrogen%	3.607834187
Carbon%	70.22381805
Hydrogen%	4.465614891
Sulphur%	0

Figure 66. CHNS spectrum of compound **2n**

Anal. Calcd. for $C_{22}H_{17}NO_5$ (375)		
C: 70.39 %	H: 4.56 %	N: 3.73 %

7-(thiophen-2-yl)-7,10,11,12-tetrahydro-6H-chromeno[4,3-b]quinoline-6,8(9H)-dione (2o)[1]

Dark brown solid; (0.279g, 80%); Mp=335-337 °C (Lit. 336-338 °C); IR (KBr) (υ_{max}/cm^{-1}): 3307 (NH) 3096 (C-H aromatic), 2958, 2880 (C-H aliphatic), 1701 (C=O), 1647, 1602 (C=C); ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ (ppm):9.91 (s, 1H, NH), 8.31 (d, *J* = 8.1 Hz, 1H, ArH, H$_1$), 7.67 (t, *J* = 7.8 Hz, 1H, ArH, H$_3$), 7.47-7.37 (m, 2H, ArH, H$_2$, H$_4$), 7.22 (s, 1H, ArH, H$_{15}$), 6.88-6.76 (m, 2H, ArH, H$_{16}$, H$_{17}$), 5.32 (s, 1H, CH, H$_7$), 2.90-2.82 (m, 1H, CH$_2$, H$_9$), 2.76-2.68 (m, 1H, CH$_2$, H$_9$), 2.40-2.34 (m, 2H, CH$_2$, H$_{11}$), 2.10-2.02 (m, 1H, CH$_2$, H$_{10}$), 1.98-1.93(m, 1H, CH$_2$, H$_{10}$); ^{13}C NMR (75 MHz, DMSO-*d*$_6$): δ (ppm): 195.33 (C$_8$), 160.87 (C$_6$), 152.48 (C$_{4a}$), 152.36 (C$_{11a}$), 149.93 (C$_{12a}$), 142.47 (C$_{13}$), 132.56 (C$_3$), 127.18 (C$_{17}$), 124.55 (C$_1$,C$_{15}$), 124.05 (C$_{16}$), 123.42 (C$_2$), 117.43 (C$_4$), 113.45 (C$_{12b}$), 111.85 (C$_{7a}$), 101.63 (C$_{6a}$), 37.12 (C$_9$), 29.32 (C$_7$), 26.83 (C$_{11}$), 21.24 (C$_{10}$); MS: (m/z, %): 349 (M$^+$, 38), 347 (M$^+$-2, 100), 266(98), 28(88); Anal. Calcd. for $C_{20}H_{15}NO_3S$ (349): C: 68.75, H: 4.33, N: 4.01, S: 9.18%. Found: C: 68.70, H: 4.29, N: 3.97, S: 9.12%.

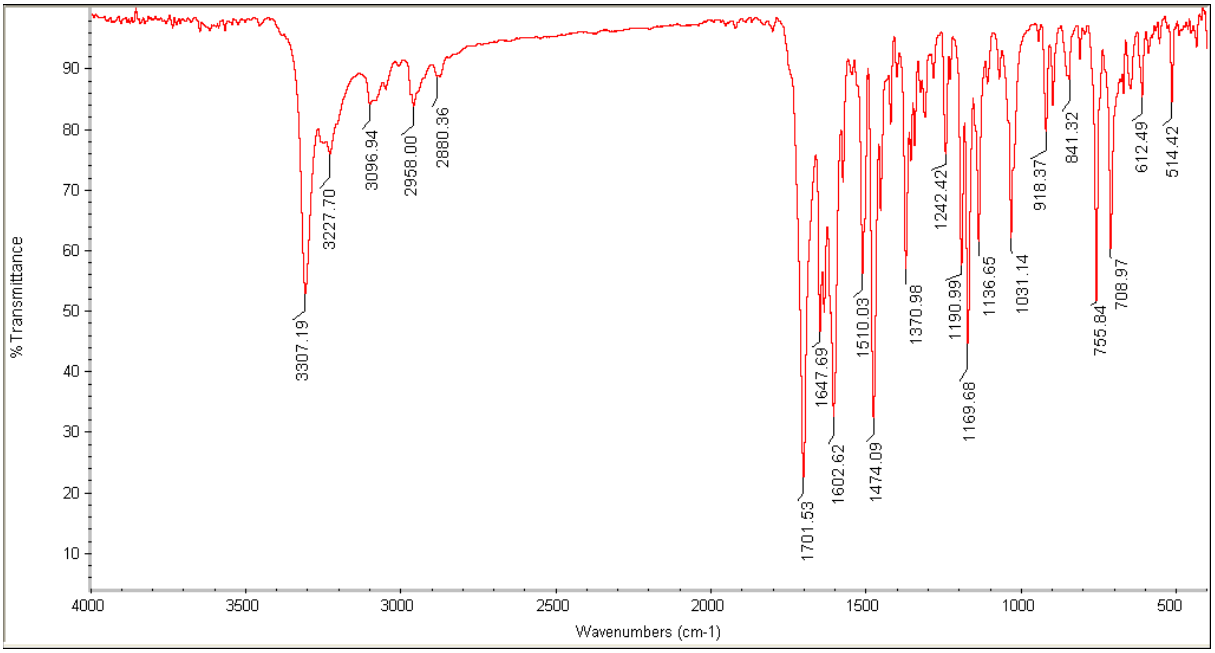


Figure 67. IR spectrum of compound **2o**

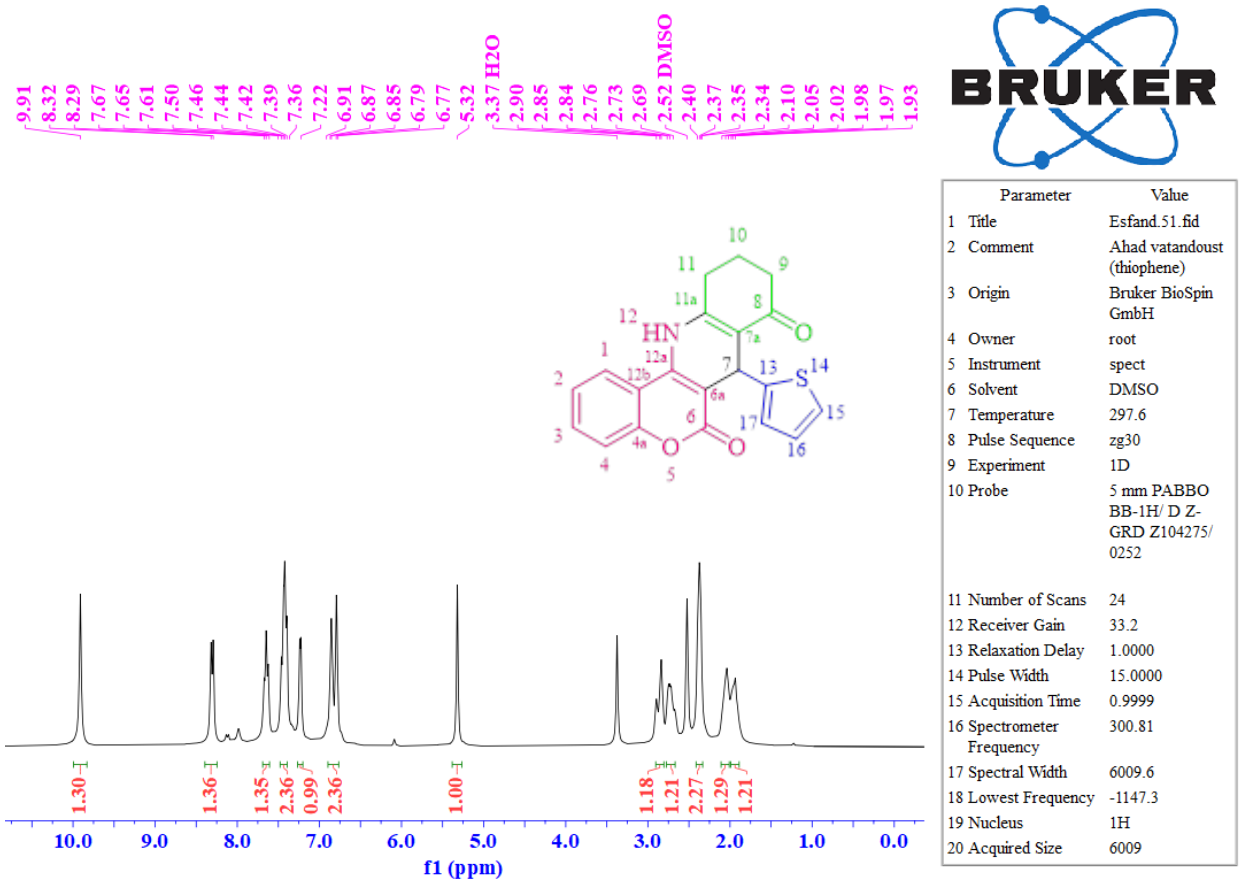


Figure 68. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of compound **2o**

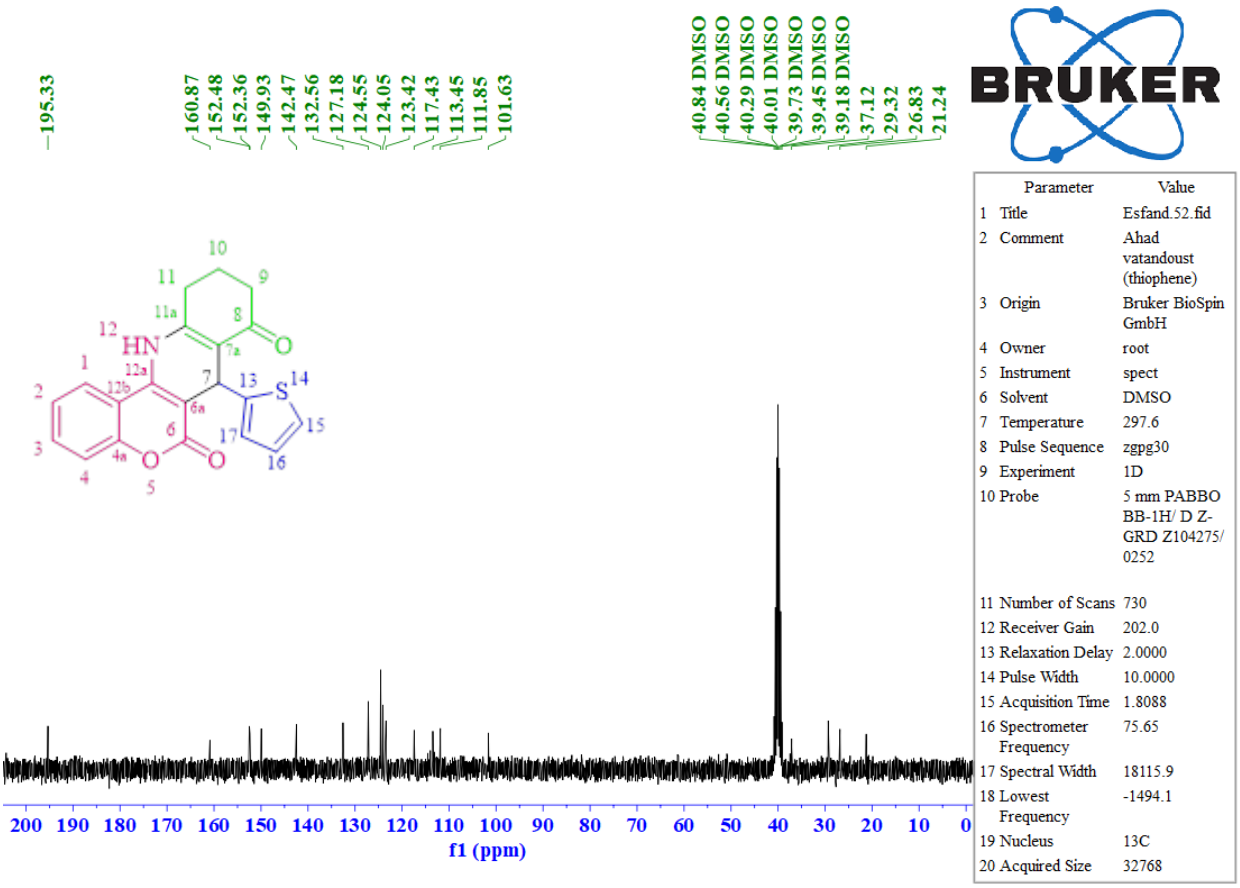


Figure 69. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of compound **2o**

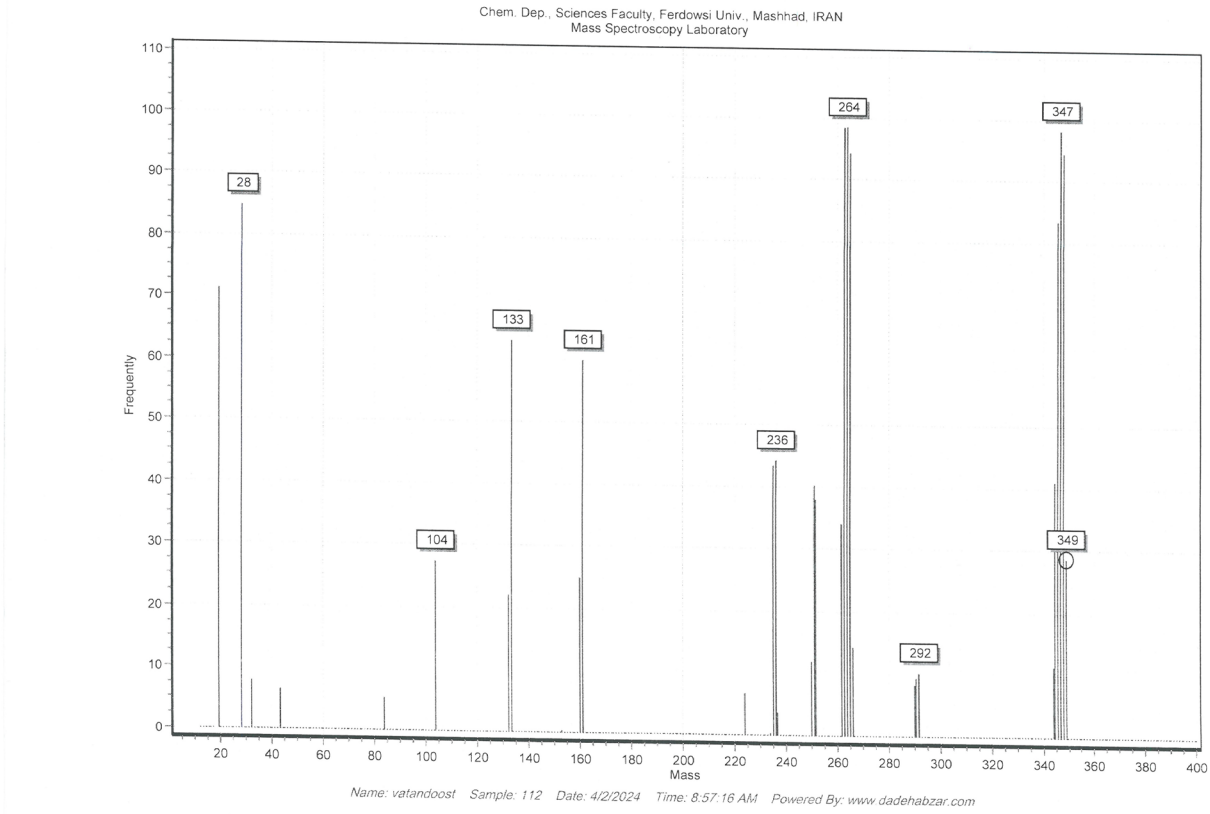


Figure 70. Mass spectrum of compound **2o**

Eager 300 Summarize Results

Date: 24/04/2024 at 13:02:16

Method Name: NCHS

Method Filename: Copy of N C H S-bkp.mth

Filename	As Method	Vial
Vatandoust-162		
# Group Sample Name	Tayp Weig. Prof. F ---	-----
162-1 112	UNK 0.651 6.25 ---	-----
Component Name Element%		
Nitrogen% 3.979906257		
Carbon% 68.70428131		
Hydrogen% 4.291711521		
Sulphur% 9.12617751		

1 Sample (s) in Group No:1

Component Name	Average
Nitrogen%	3.979906257
Carbon%	68.70428131
Hydrogen%	4.291711521
Sulphur%	9.12617751

Figure 71. CHNS spectrum of compound **2o**

Anal. Calcd. for $C_{20}H_{15}NO_3S$ (349)			
C: 68.75%	H: 4.33 %	N: 4.01 %	S: 9.18 %

7-(furan-2-yl)-7,10,11,12-tetrahydro-6H-chromeno[4,3-b]quinoline-6,8(9H)-dione (2p)[1]

Gray solid; (0.266g, 80%); Mp=302-304 ºC (Lit. 303-305 ºC); IR (KBr) (υ_{max}/cm^{-1}): 3324 (NH) 3096 (C-H aromatic), 2944, 2872 (C-H aliphatic), 1676 (C=O), 1643, 1607 (C=C); ^{1}H NMR (300 MHz, DMSO-*d*$_6$): δ (ppm): 9.86 (s, 1H, NH), 8.31 (d, *J* = 8.0 Hz, 1H, ArH, H$_1$), 7.67 (t, *J* = 7.8 Hz, 1H, ArH, H$_3$), 7.48-7.41 (m, 3H, H$_2$, H$_4$, H$_{15}$), 6.29 (s, 1H, ArH, H$_{17}$), 6.02 (s, 1H, ArH, H$_{16}$), 5.18 (s, 1H, CH, H$_7$), 2.89-2.80 (m, 1H, CH$_2$, H$_9$), 2.75-2.65 (m, 1H, CH$_2$, H$_9$), 2.38-2.36 (m, 2H, CH$_2$, H$_{11}$), 2.08-2.00 (m, 1H, CH$_2$, H$_{10}$), 1.99-1.90 (m, 1H, CH$_2$, H$_{10}$); ^{13}C NMR (75 MHz, DMSO-*d*$_6$): δ (ppm): 195.36 (C$_8$), 160.74 (C$_6$), 156.97 (C$_{13}$), 152.93 (C$_{4a}$), 152.49 (C$_{11a}$), 143.13 (C$_{12a}$), 141.90 (C$_{15}$), 132.62 (C$_3$), 124.57 (C$_1$), 123.32 (C$_2$), 117.44 (C$_4$), 113.46 (C$_{12b}$), 110.89 (C$_{7a}$), 109.42 (C$_{16}$), 105.78 (C$_{17}$), 99.14 (C$_{6a}$), 37.04 (C$_9$), 28.41 (C$_7$), 26.85 (C$_{11}$), 21.18 (C$_{10}$); MS: (m/z, %): 333 (M$^+$, 38), 331 (M$^+$-2, 86), 225(22), 28(10); Anal. Calcd. for $C_{20}H_{15}NO_4$ (333): C: 72.06, H: 4.54, N: 4.20 %. Found: C: 71.96, H: 4.46, N: 4.16%.

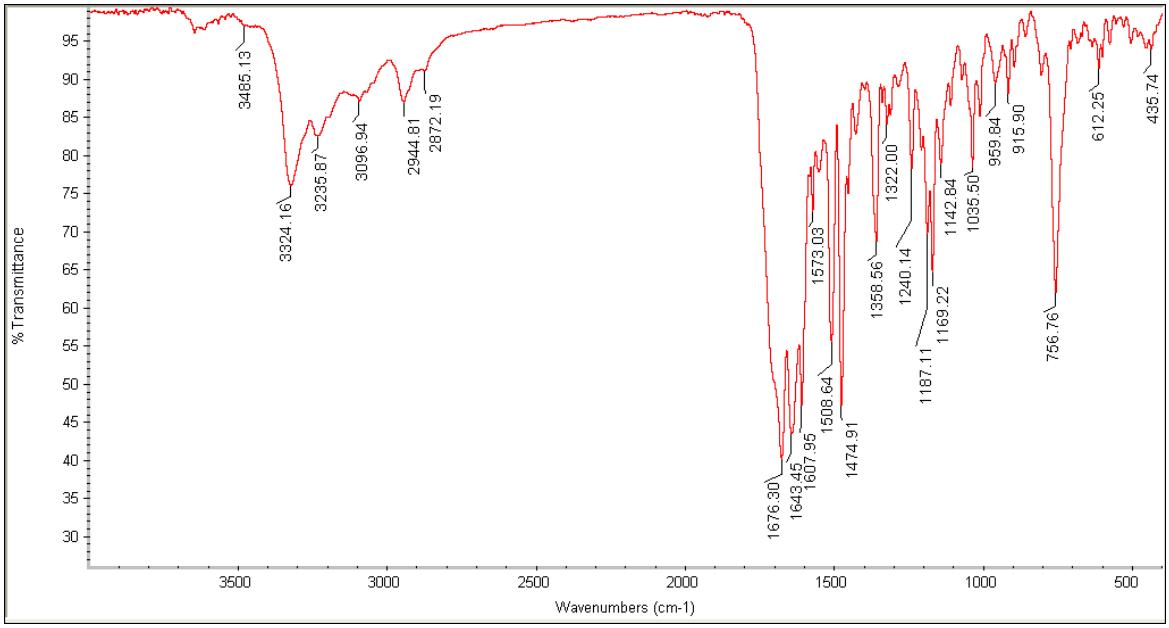


Figure 72. IR spectrum of compound **2p**

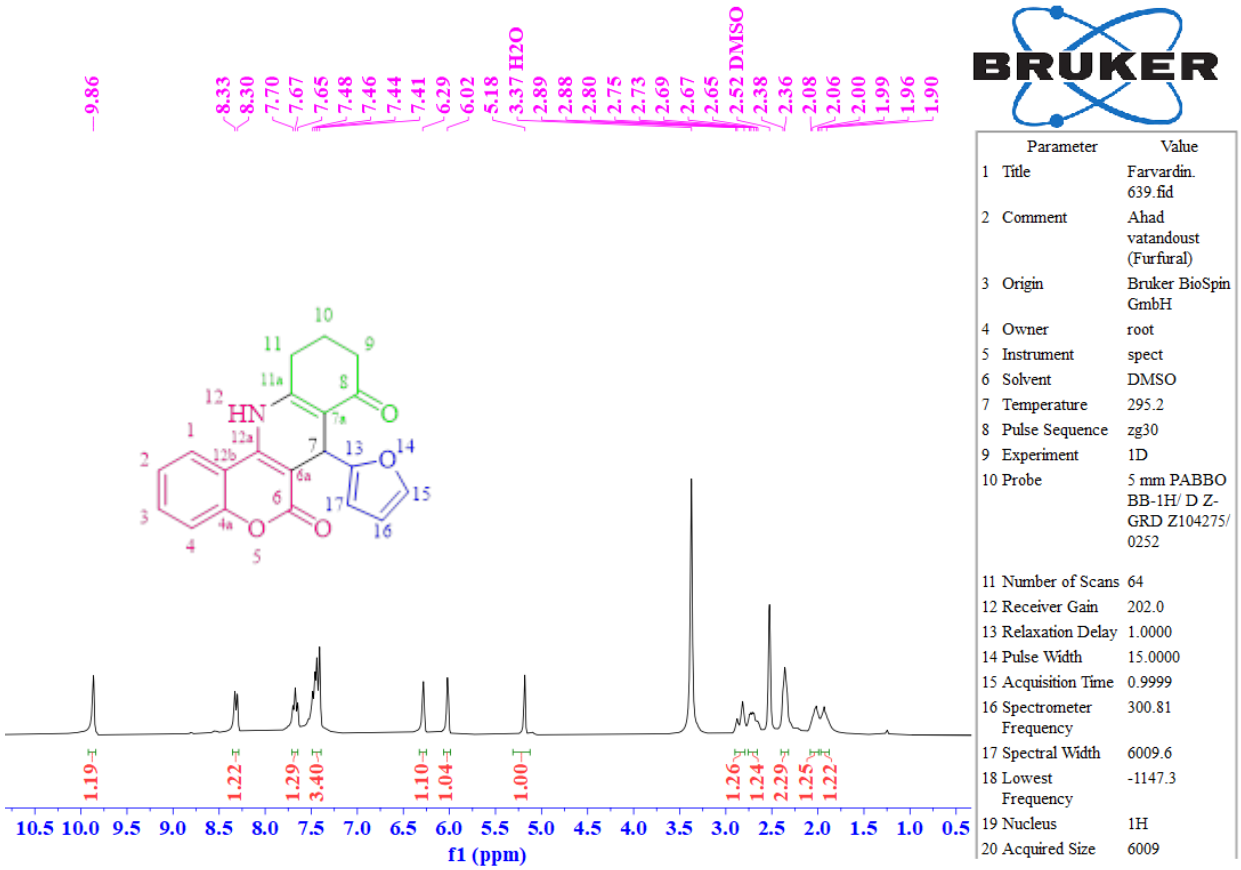


Figure 73. ^{1}H NMR (300 MHz, DMSO-d_6) spectrum of compound **2p**

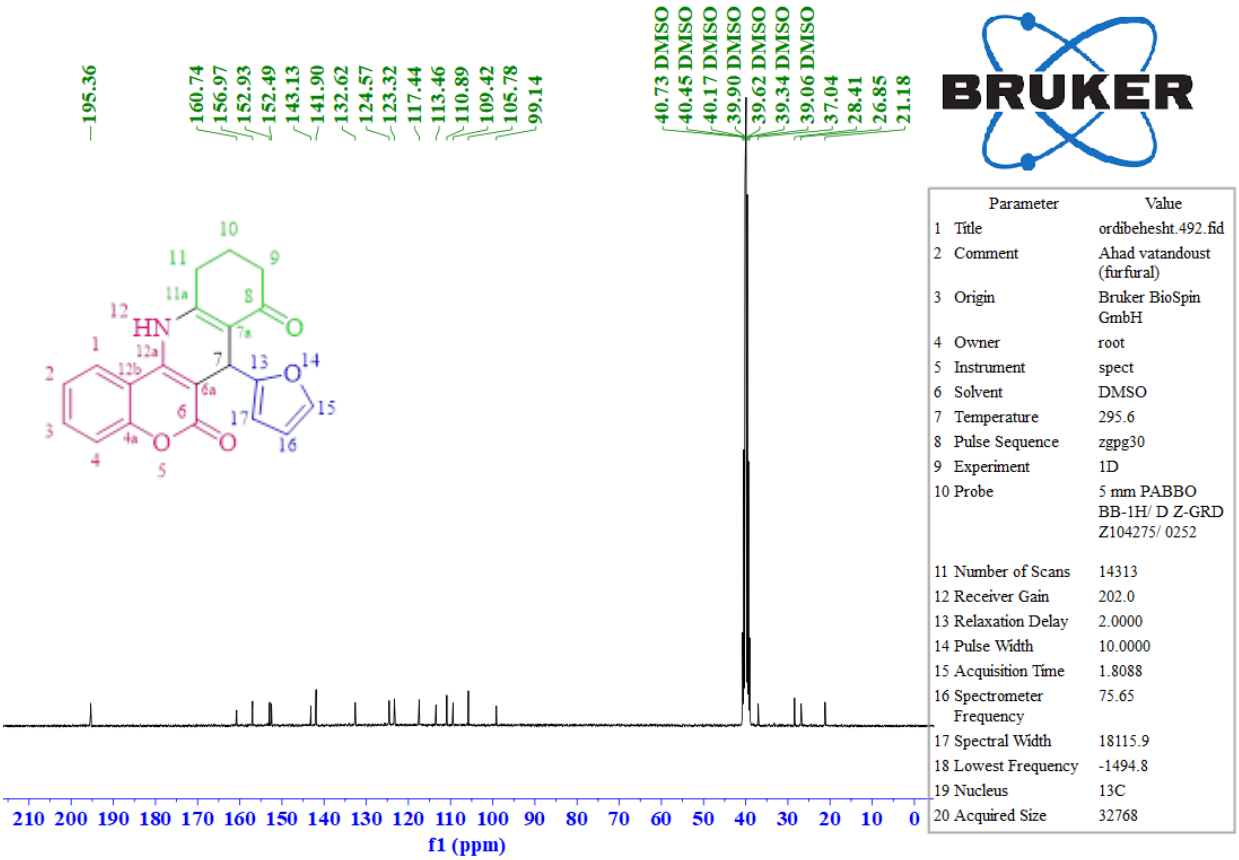


Figure 74. ^{13}C NMR (75 MHz, DMSO-d_6) spectrum of compound **2p**

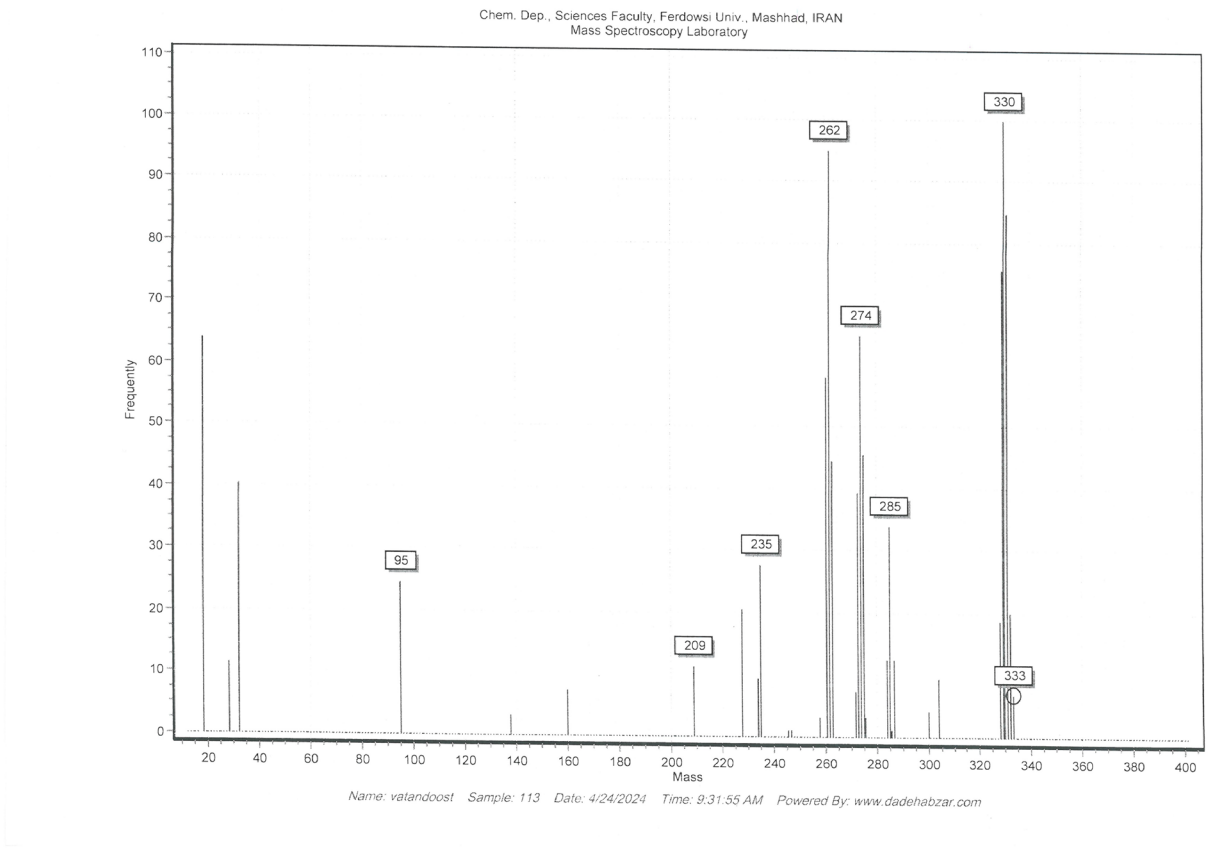


Figure 75. Mass spectrum of compound **2p**

Eager 300 Summarize Results

Date: 24/04/2024 at 13:04:39

Method Name: NCHS

Method Filename: Copy of N C H S-bkp.mth

Filename	As Method	Vial
Vatandoust-172		
# Group Sample Name	Tayp Weig. Prof. F ---	-----
172-1 113	UNK 0.602 6.25 ---	-----
Component Name Element%		
Nitrogen% 4.160822124		
Carbon% 71.96075546		
Hydrogen% 4.46627367		
Sulphur% 0		

1 Sample (s) in Group No:1

Component Name	Average
Nitrogen%	4.160822124
Carbon%	71.96075546
Hydrogen%	4.46627367
Sulphur%	0

Figure 76. CHNS spectrum of compound **2p**

Anal. Calcd. for $C_{20}H_{15}NO_4$ (333)		
C: 72.06 %	H: 4.54 %	N: 4.20 %

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[2] C. J. Hua, K. Zhang, M. Xin, T. Ying, J. R. Gao, J. h. Jia and Y. j. Li, *RSC adv.,* 2016, ***6***, 49221-49227.

[3] R. Motamedi, G. R. Bardajee and S. Shakeri, *Heterocycl. Commun.*, 2014, **20**, 181-184.

[4] C. J. Hua, H. Zheng, K. Zhang, M. Xin, J. R. Gao and Y. J. Li, *Tetrahedron*, 2016, **72**, 8365-8372.

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