Probing Catalytic Activity of Highly Efficient Sulfonic Acid Fabricated Cobalt Ferrite Magnetic Nanoparticles for Clean and Scalable Synthesis of Dihydro, Spiro and bis Quinazolinones

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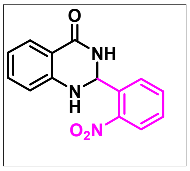
Materials and Methods

Most of the chemicals and reagents used during the experiment were procured from Sigma-Aldrich, Fluka, Merck, Spectrochem, and all of them were of analytical grade and used as such without any further purification. All the reactions were monitored using Thin-layer chromatography (TLC), which were performed on Merck precoated silica gel aluminium plated (60F254) under UV light.

Characterization Techniques. The synthesized nanoparticles acting as nanocatalyst were characterized using aid of different techniques to assure their complete magnetization, functionalization. Bruker diffractometer (D8 Discover) was used to acquire X-ray diffraction (XRD) pattern at room temperature within 2θ range 5−80° (scanning rate = 2°/min, λ = 0.15406 nm, 40 kV, 40 mA). The TEM analysis of synthesized nanoparticles were carried out on FEI TECHNAI (model number G^2 T20) transmission electron microscope (operated at 200 kV). SEM studies were carried out using Carl Zeiss, India (Jeol Japan Mode: JSM 6610LV). N_2 adsorption-desorption isotherm and pore size distribution was measured by Micromeritics Instrument, Gemini Model: 2380. Magnetization measurements M (T, H) of nanoparticles were determined using vibrating sample magnetometer (model number EV-9, Microsense, ADE). The Fourier transform infrared spectra (FT-IR) of the nanoparticles were recorded using a PerkinElmer Spectrum 2000. ^{1}H NMR spectra of the synthesized compounds were recorded on 400 MHz JEOL NMR spectrometer in deuterated dimethylsulfoxide (DMSO) and chloroform ($CDCl_3$). Chemical shifts (δ-values) have been reported in parts per million.

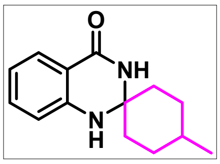
Table S1: Crystal data and structure refinement for compound **3c**.



CCDC Number	2033523
Molecular Formula	C14H11N3O3
Molecular weight	269.08
Temperature	295.4
Radiation	Mo Kα (λ = 0.71073)
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a/Å 20.0038(9) b/Å 10.8076(4) c/Å 12.4320(5) α/° 90 β/° 109.8180(10) γ/° 90
Volume /Å^3	2528.53(18)

Z	50
Density (ρcalcg/cm^3)	1.409
Absorption coefficient (μ/mm^{-1})	0.102
F(000)	1112.6
2θ range for data collection	4.32 to 56.58
Index ranges	$-26 \leq h \leq 26$, $-14 \leq k \leq 14$, $-16 \leq l \leq 16$
Reflections collected	20839
Independent reflections	3136 [R_{int} = 0.0206, R_{sigma} = 0.0188]
Data/restraints/parameters	3136/0/182
Goodness-of-fit on F^2	1.303
Final R indexes [I>=2σ (I)]	R_1 = 0.0850, wR_2 = 0.2335
Final R indexes [all data]	R_1 = 0.1382, wR_2 = 0.2821
Largest diff. peak/hole / e $Å^{-3}$	0.32/-0.80

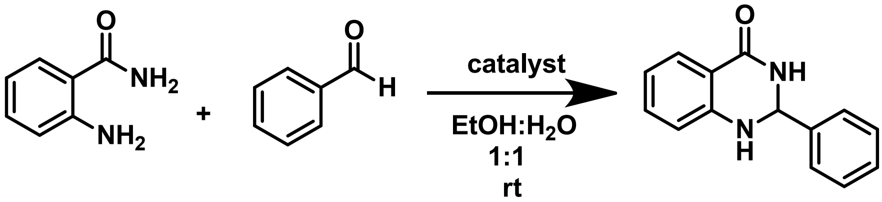
Table S2: Crystal data and structure refinement for compound **5e**.



CCDC Number	2043509
Molecular Formula	C14H18N2O
Molecular weight	230.30
Temperature	293
Radiation	Mo Kα (λ = 0.71073)
Crystal system	orthorhombic
Space group	P1

Unit cell dimensions	a/Å 10.223(8) b/Å 11.333(12) c/Å 21.64(2) α/° 90 β/° 90 γ/° 90
Volume /Å^3	2507(4)
Z	50
Density (ρcalcg/cm^3)	1.222
Absorption coefficient (μ/mm^{-1})	0.078
F(000)	994.4
2θ range for data collection	4.4 to 56.58
Index ranges	$-10 \leq h \leq 11$, $-14 \leq k \leq 15$, $-28 \leq l \leq 17$
Reflections collected	12964
Independent reflections	12500 [R_{int} = 0.2383, R_{sigma} = 0.1422]
Data/restraints/parameters	12500/3/1233
Goodness-of-fit on F^2	1.343
Final R indexes [I>=2σ (I)]	R_1 = 0.1484, wR_2 = 0.3604
Final R indexes [all data]	R_1 = 0.2422, wR_2 = 0.4592
Largest diff. peak/hole / e Å^{-3}	0.49/-0.65

Table S3: Calculation of green chemistry metrics for compound **3l.**



F.W.	136.06	106.04	224.09
mmol	1.0	1.0	0.98
amount	0.136	0.106	0.220

S. No.	**Parameters**	**Formula**	**Characteristics**	**Ideal Value**	**Calculated value for compound 3l**
1.	Environmental (E) factor	[Total mass of raw materials - the total mass of product]/ mass of product	E-factor signifies the total amount of waste generated in a chemical reaction.	0	[(0.136 + 0.106)-0.220]/0.220 = 0.10
2.	Process mass intensity (PMI)	∑ (mass of stoichiometric reactants)/[mass of stoichiometry product]	PMI takes into account reaction efficiency, stoichiometry, amount of solvent and all reagent used in the chemical reaction.	1	(0.136 + 0.106)/ 0.220 = 1.1
3.	Reaction mass efficiency (RME %)	[mass of product/∑ (mass of stoichiometric reactants)] × 100	RME accounts into atom economy, chemical yield and stoichiometry.	100 %	[0.220/ (0.136 + 0.106)] × 100 = 90.90%
4.	Atom economy (AE %)	[MW of product] ÷ ∑(MW of stoichiometric reactants) ×	Atom economy signifies the percentage of atoms wasted in chemical	100 %	[(224.09)/(136.06+106.04)] × 100 = 92.6%

		100	reaction. Higher the value of AE, greener is the reaction. Maximum value of atom economy is 100% which indicates that all the atoms present in reactants lies in the product.		
5.	Carbon efficiency (CE %)	[Amount of carbon in product/ Total carbon present in reactants] x 100	CE signifies the percentage of carbons in the reactants that is left in the product.	100 %	[1 x 14 / (1x 7+ 1 x 7)] x 100 = [14 / (7+7)] x 100 = 100%

^{1}H and ^{13}C NMR chemical shifts (3a-3n, 5a-5f, 7 and 9)

(**3a**)

^{1}H NMR (DMSO-d6, 400 MHz), δ_H (ppm): 8.31 (s, 1H), 7.55 (d, J = 8.4 Hz, 3H), 7.40 (d, J = 8.4 Hz, 2H), 7.21 (t, 1H), 7.12 (s, 1H), 6.70 (d, J = 8.1 Hz, 1H), 6.64 (t, 1H), 5.71 (s, 1H)

^{13}C NMR (DMSO-d6, 101 MHz), δ_c (ppm): 164.01, 148.15, 141.61, 133.94, 131.77, 129.62, 127.89, 122.10, 117.81, 115.45, 114.98, 66.30.

(**3b**)

^{1}H NMR ($CDCl_3$ + DMSO-d6, 400 MHz), δ_H (ppm): 7.92 (d, J = 7.7 Hz, 1H), 7.53 (d, J = 8.2 Hz, 2H), 7.41 (d, J = 8.1 Hz, 2H), 7.34 (t, 1H), 6.90 (t, 1H), 6.67 (d, J = 8.0 Hz, 1H), 6.29 (s, 1H), 5.89 (s, 1H), 4.37 (s, 1H).

^{13}C NMR (DMSO-d6, 101 MHz), δ_c (ppm): 164.00, 148.17, 141.20, 133.92, 133.48, 129.28, 128.83, 127.89, 117.80, 115.46, 114.98, 66.26.

(**3c**)

^{1}H NMR (DMSO-d6, 400 MHz), δ_H (ppm): 8.19 (s, 1H), 8.03 (d, J = 8.1 Hz, 1H), 7.82 (d, J = 7.8 Hz, 1H), 7.75 (t, 1H), 7.60 (q, J = 7.8 Hz, 2H), 7.20-7.24 (m, 1H), 6.97 (s, 1H), 6.66-6.74 (m, 2H), 6.30 (s, 1H).

^{13}C NMR (DMSO-d6, 101 MHz), δ_c (ppm): 163.90, 148.17, 147.65, 136.42, 134.45, 134.09, 130.43, 129.46, 127.84, 125.25, 118.21, 117.09, 115.43, 115.03, 62.68.

(**3d**)

^{1}H NMR (DMSO-d6, 400 MHz), δ_H (ppm): 8.50 (s, 1H), 8.22 (d, J = 8.7 Hz, 2H), 7.71 (d, J = 8.5 Hz, 2H), 7.57 (d, J = 7.8 Hz, 1H), 7.31 (s, 1H), 7.20-7.24 (m, 1H), 6.73 (d, J = 8.1 Hz, 1H), 6.65 (t, 1H), 5.88 (s, 1H)

^{13}C NMR (DMSO-d6, 101 MHz), δ_c (ppm): 163.82, 149.86, 147.92, 147.77, 134.10, 128.56, 127.93, 124.12, 117.99, 115.41, 115.07, 65.77

(**3e**)

^{1}H NMR ($CDCl_3$ + DMSO-d6, 400 MHz), δ_H (ppm): 8.24 (s, 1H), 7.66 (m, 3H), 7.49 (d, J = 8.2 Hz, 1H), 7.26 (t, 1H), 7.04 (s, 1H), 6.70-6.77 (m, 2H), 6.12 (s, 1H)

^{13}C NMR (DMSO-d6, 101 MHz), δ_c (ppm): 169.54, 152.25, 141.46, 139.78, 138.70, 137.98, 134.57, 134.17, 132.72, 132.39, 123.20, 119.70, 68.67.

(**3f**)

^{1}H NMR (DMSO-d6, 400 MHz), δ_H (ppm): 8.22 (s, 1H), 7.61 (d, J = 9.0 Hz, 1H), 7.37 (d, J = 8.0 Hz, 2H), 7.18-7.26 (m, 3H), 7.05 (s, 1H), 6.74 (d, J = 8.0 Hz, 1H), 6.67 (t, 1H), 5.71 (s, 1H), 2.30 (s, 3H).

^{13}C NMR (DMSO-d6, 101 MHz), δ_c (ppm): 164.07, 148.35, 139.13, 138.15, 133.69, 129.25, 127.78, 127.24, 117.50, 115.46, 114.86, 66.82, 21.19

(**3g**)

^{1}H NMR (DMSO-d6, 400 MHz), δ_H (ppm): 8.34 (s, 1H), 7.90 (d, J = 8.2 Hz, 2H), 7.54-7.57 (m, 3H), 7.18-7.22 (m, 2H), 6.70 (d, J = 8.2 Hz, 1H), 6.63 (t, 1H), 5.78 (s, 1H), 3.44 (brs, 1H).

^{13}C NMR (DMSO-d6, 101 MHz), δ_c (ppm): 167.54, 163.96, 148.22, 146.72, 133.96, 129.92, 127.90, 127.28, 117.80, 115.42, 114.98, 66.50.

(**3h**)

^{1}H NMR (DMSO-d6, 400 MHz), δ_H (ppm): 8.36 (s, 1H), 7.91 (s, 1H), 7.86-7.89 (m, 3H), 7.67 (d, J = 8.7, 1H), 7.61 (d, J = 7.8, 1H), 7.48 (m, 2H), 7.19-7.23 (t, 1H), 6.74 (d, J = 7.8 Hz, 1H), 6.64 (t, 1H), 5.90 (s, 1H), 3.86 (brs, 1H)

^{13}C NMR (DMSO-d6, 101 MHz), δ_c (ppm): 164.22, 148.40, 139.39, 133.97, 133.44, 132.98, 128.67, 128.50, 128.11, 127.95, 126.94, 126.35, 125.34, 117.74, 115.43, 114.82, 67.26.

(**3i**)

^{1}H NMR (DMSO-d6, 400 MHz), δ_H (ppm): 8.43 (s, 1H), 7.59 (d, J = 7.7 Hz, 1H), 7.41 (d, J = 4.9 Hz, 1H), 7.23 (t, 1H), 7.10 (d, J = 8.3 Hz, 1H), 6.94 (m, 1H), 6.74 (d, J = 8.1 Hz, 1H), 6.67 (t, 1H), 5.99 (s, 1H).

^{13}C NMR (DMSO-d6, 101 MHz), δ_c (ppm): 163.68, 147.78, 146.98, 133.91, 127.85, 127.00, 126.41, 126.23, 118.06, 115.64, 115.25, 63.10.

(**3j**)

^{1}H NMR (DMSO-d6, 400 MHz), δ_H (ppm): δ 8.10 (d, J = 7.7 Hz, 1H), 8.04 (s, 1H), 7.79 (d, J = 7.6 Hz, 2H), 7.51-7.59 (m, 2H), 7.04-7.10 (m, 2H), 6.35 (s, 1H), 6.13 (s, 1H), 5.12 (s, 1H)

^{13}C NMR ($CDCl_3$ + DMSO-d6, 101 MHz), δ_c (ppm): δ 169.60, 152.35, 147.49, 138.70, 137.05, 135.22, 132.89, 130.86, 127.34, 123.39, 119.85, 119.59, 72.34.

(**3k**)

^{1}H NMR ($CDCl_3$, 400 MHz), δ_H (ppm): δ 7.93 (dd, J = 7.8, 1H), 7.30-7.35 (m, 1H), 7.19 (s, 1H), 7.03 (dd, J = 8.2, 2.0 Hz, 1H), 6.85-6.91 (m, 2H), 6.66 (d, J = 8.0 Hz, 1H), 5.83 (s, 1H), 5.79 (s, 1H), 4.37 (s, 1H), 3.90 (s, 6H)

^{13}C NMR ($CDCl_3$, 101 MHz), δ_c (ppm): δ 164.93, 150.51, 149.66, 147.40, 134.11, 130.93, 128.80, 120.25, 119.77, 115.70, 114.64, 111.10, 109.82, 69.11, 56.10

(**3l**)

^{1}H NMR (DMSO-d6, 400 MHz), δ_H (ppm): δ 8.27 (s, 1H), 7.59 (d, J = 7.7 Hz, 1H), 7.47 (d, J = 6.9 Hz, 2H), 7.31-7.37 (m, 3H), 7.19-7.23 (m, 1H), 6.73 (d, J = 8.1 Hz, 1H), 6.64 (t, 1H), 5.73 (s, 1H)

^{13}C NMR (DMSO-d6, 101 MHz), δ_c (ppm): δ 164.15, 148.41, 142.16, 133.85, 128.98, 128.86, 127.89, 127.40, 117.65, 115.49, 114.94, 67.10.

(**3m**)

^{1}H NMR (DMSO-d6, 400 MHz), δ_H (ppm): δ 8.28 (s, 1H), 7.61 (d, J = 7.8 Hz, 1H), 7.52 (dd, J = 8.5, 5.5 Hz, 2H), 7.23 (dt, J = 20.2, 8.7 Hz, 2H), 6.67-6.76 (m, 2H), 5.77 (d, J = 1.8 Hz, 1H)

^{13}C NMR (DMSO-d6, 101 MHz), δ_c (ppm): δ 164.18, 163.76, 148.14, 135.21, 133.98, 127.84, 117.83, 115.46, 115.25, 114.93, 66.27.

(**3n**)

^{1}H NMR (DMSO-d6, 400 MHz), δ_H (ppm): 8.77 (d, J = 9.3 Hz, 1H), 8.38 (s, 1H), 8.29 (s, 4H), 8.23 (d, J = 9.3 Hz, 1H), 8.19 (d, J = 2.9 Hz, 1H), 8.09 (s, 1H), 7.72 (d, J = 7.7 Hz, 1H), 7.25-7.29 (m, 1H), 7.19 (s, 1H), 6.83 (s, 1H), 6.74-6.78 (m, 2H)

^{13}C NMR (DMSO-d6, 101 MHz), δ_c (ppm): δ 164.66, 149.21, 133.88, 133.57, 131.76, 131.28, 130.69, 128.96, 128.36, 128.13, 128.04, 127.88, 126.94, 126.69, 126.09, 125.97, 125.28, 124.73, 124.44, 124.16, 117.96, 115.71, 115.12, 66.08.

(**5a**)

^{1}H NMR (DMSO-d6, 400 MHz), δ_H (ppm): δ 7.94 (s, 1H), 7.50 (d, J = 7.7 Hz, 1H), 7.15 (t, 1H), 6.69 (d, J = 8.0 Hz, 1H), 6.60 (s, 1H), 6.55 (t, 1H), 1.78-1.89 (m, 4H), 1.46 (s, 10H)

^{13}C NMR (DMSO-d6, 101 MHz), δ_c (ppm): δ 163.54, 147.38, 133.66, 127.58, 116.78, 114.89, 114.79, 71.87, 36.09, 28.21, 24.61, 21.27

(**5b**)

^{1}H NMR ($CDCl_3$, 400 MHz), δ_H (ppm): δ 7.84 (d, J = 7.7, 1H), 7.26 (t, 1H), 6.79 (t, 1H), 6.63 (d, J = 8.0 Hz, 1H), 6.48 (s, 1H), 4.38 (s, 1H), 1.81 (s, 4H), 1.50-1.66 (m, 4H), 1.45 (dd, J = 11.2, 5.4 Hz, 2H)

^{13}C NMR ($CDCl_3$, 101 MHz), δ_c (ppm): δ 164.33, 145.71, 133.97, 128.46, 118.82, 115.32, 114.88, 68.48, 37.88, 24.76, 22.01.

(**5c**)

^{1}H NMR ($CDCl_3$, 400 MHz), δ_H (ppm): δ 7.84 (d, J = 7.7, 1H), 7.23-7.27 (m, 1H), 6.77 (t, 2n), 6.61 (d, J = 8.1 Hz, 1H), 4.44 (s, 1H), 2.00 (m, 4H), 1.48-1.60 (m, 8H)

^{13}C NMR ($CDCl_3$, 101 MHz), δ_c (ppm): δ 164.20, 145.76, 133.88, 128.35, 118.67, 115.30, 114.89, 72.57, 41.58, 29.09, 21.63.

(**5d**)

^{1}H NMR (DMSO-d6, 400 MHz), δ_H (ppm): δ 8.08 (s, 1H), 7.58 (d, J = 9.0 Hz, 1H), 7.19-7.23 (m, 1H), 6.70 (d, J = 8.0 Hz, 1H), 6.63 (t, 1H), 1.79 (s, 4H), 1.67 (s, 4H)

^{13}C NMR (DMSO-d6, 101 MHz), δ_c (ppm): δ 163.90, 147.97, 133.45, 127.70, 117.00, 115.05, 114.81, 77.66, 22.46

(**5e**)

^{1}H NMR (DMSO-d6, 400 MHz), δ_H (ppm): δ 7.83 (s, 1H), 7.52 (d, J = 7.7 Hz, 1H), 7.16 (t, 1H), 6.83 (d, J = 8.1 Hz, 1H), 6.51-6.64 (m, 2H), 1.87 (d, J = 10.3 Hz, 2H), 1.27-1.44 (m, 7H), 0.85 (s, 3H)

^{13}C NMR (DMSO-d6, 101 MHz), δ_c (ppm): δ 163.85, 147.12, 127.54, 116.99, 115.20, 115.02, 114.83, 114.74, 68.12, 37.05, 31.48, 29.84, 29.20, 22.19

(**5f**)

^{1}H NMR (DMSO-d6, 400 MHz), δ_H (ppm): δ 8.11-8.17 (m, 1H), 7.68-7.79 (m, 1H), 7.54 (dd, J = 7.8, 1.8 Hz, 1H), 7.19-7.24 (m, 1H), 6.78 (q, 1H), 6.62 (t, 1H), 3.96 (t, 2H), 3.75-3.85 (m, 2H), 1.80 (dd, J = 13.5, 4.8 Hz, 4H)

^{13}C NMR (DMSO-d6, 101 MHz), δ_c (ppm): δ 169.66, 163.62, 153.69, 146.76, 134.39, 128.22, 117.99, 115.67, 114.78, 67.12, 42.51, 36.57

(**7**)

Proton-NMR (400 MHz, CHLOROFORM-D) δ_H (ppm): δ 7.80 (s, 2n), 7.54 (d, J = 6.3 Hz, 2n), 7.20 (t, J = 8.5 Hz, 2n), 6.75-6.69 (2n), 6.60-6.64 (m, 2n), 6.42 (s, 2n), 1.75-1.90 (m, 8n)

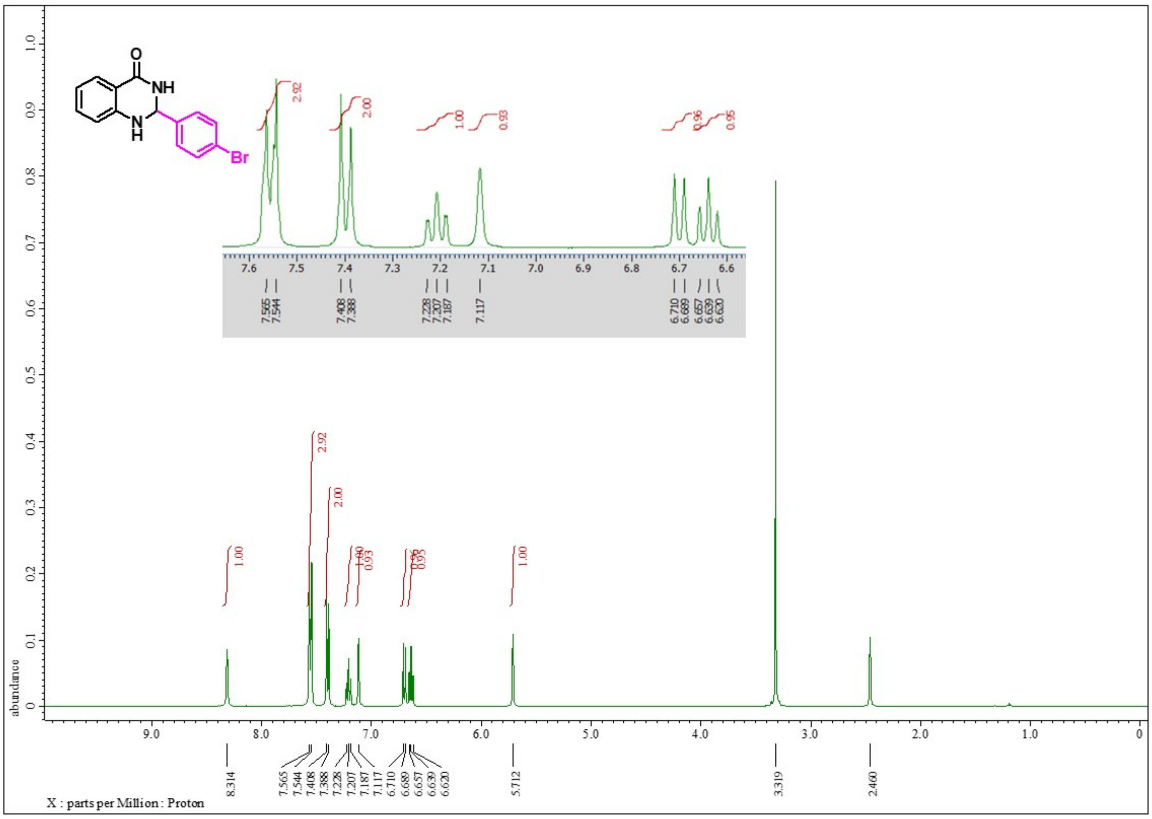
Carbon13-NMR (DMSO-D6, 100 MHz) δ_c (ppm): δ 163.80, 146.97, 133.87, 127.85, 117.56, 115.38, 115.32, 67.26, 32.58.

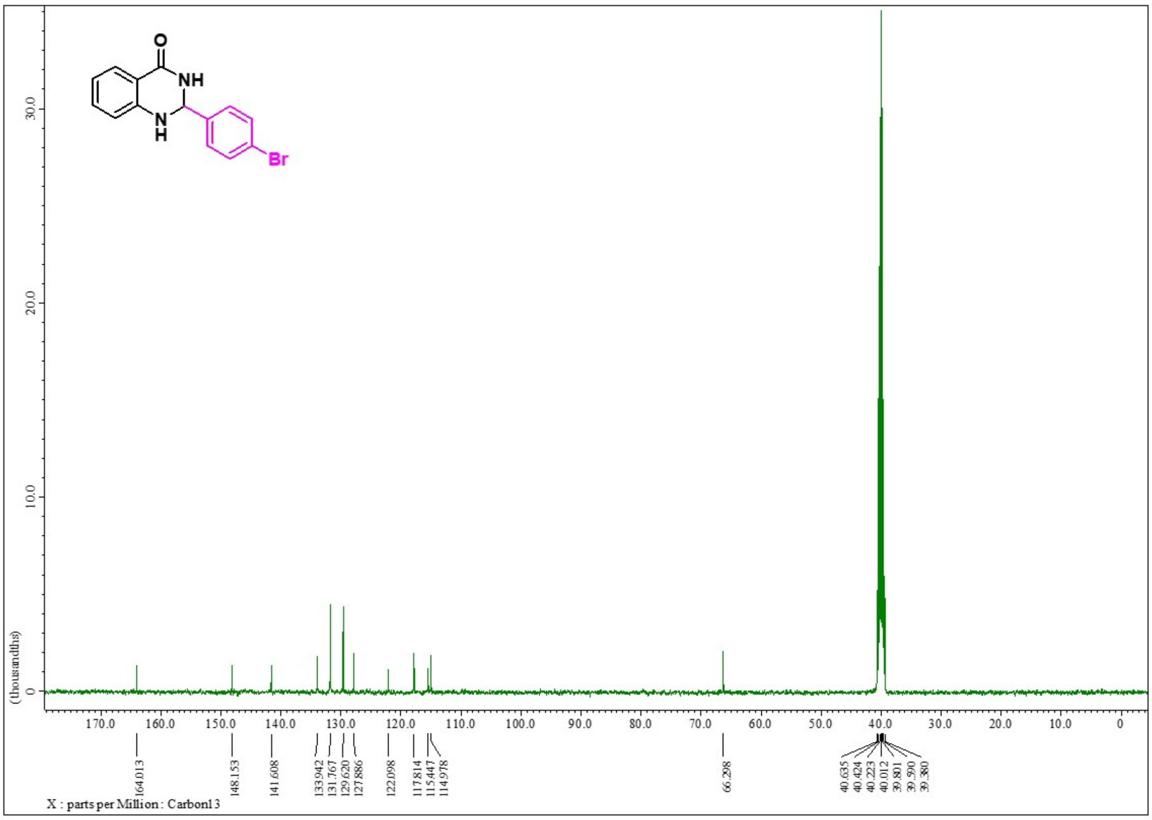
(**9**)

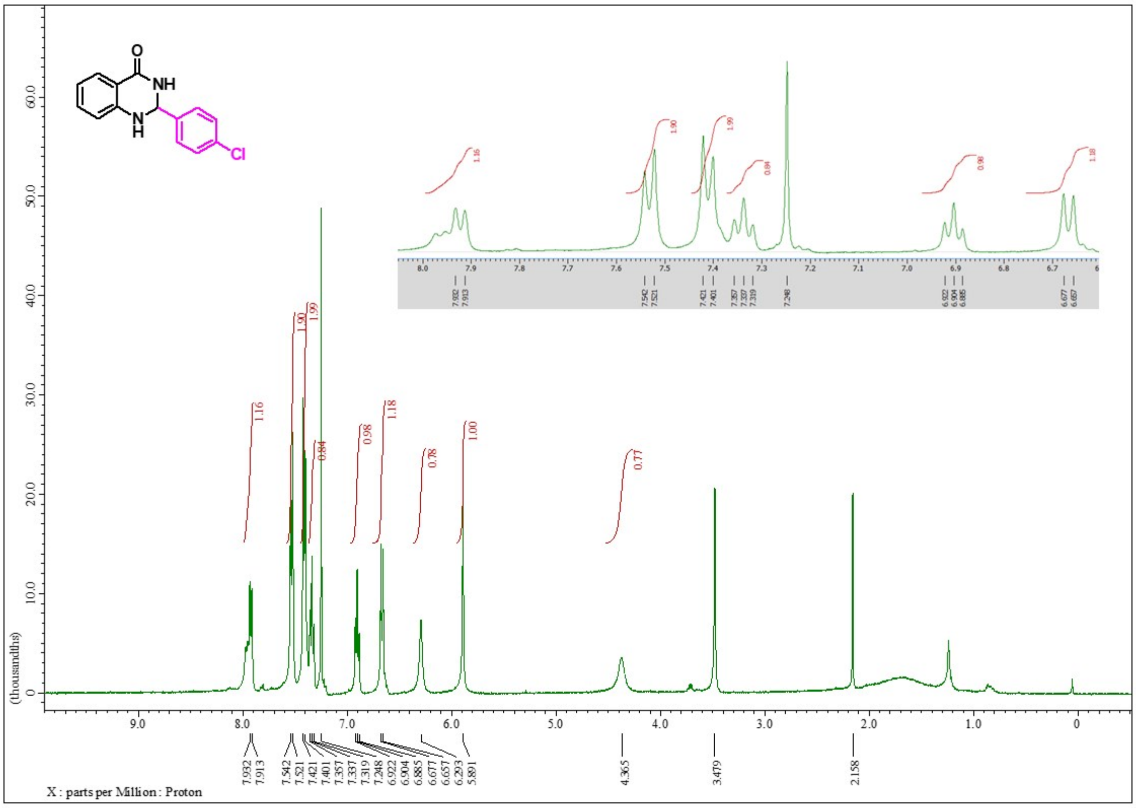
^{1}H NMR (DMSO-d6, 400 MHz),) δ_H (ppm): δ 8.33 (s, 2H), 7.54 (d, J = 6.6 Hz, 2H), 7.43 (s, 4H), 7.19 (t, 2H), 7.12 (s, 2H), 6.68 (d, J = 8.1 Hz, 2H), 6.61 (t, 2H), 5.69 (s, 2H)

^{13}C NMR (DMSO-d6, 100 MHz), δ_c (ppm): δ 164.09, 148.20, 142.49, 133.87, 127.87, 127.19, 117.63, 115.49, 114.96, 66.42.

[1]H and [13]C NMR spectra







X : parts per Million : Proton
(thousandths)
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7.913
7.542
7.521
7.421
7.401
7.357
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7.319
7.248
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6.677
6.657
6.293
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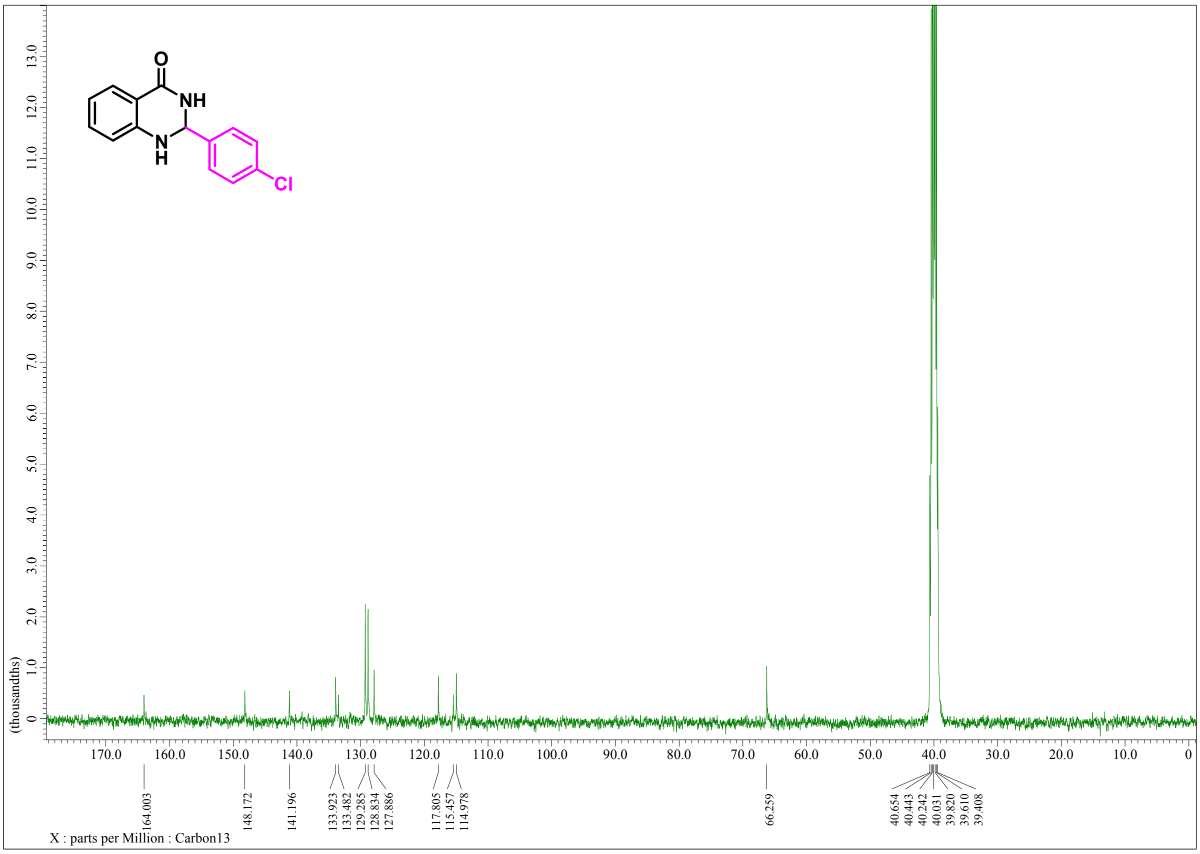
4.365
3.479
2.158



X : parts per Million : Carbon13
(thousandths)
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141.196
133.923
133.482
129.285
128.834
127.886
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39.820
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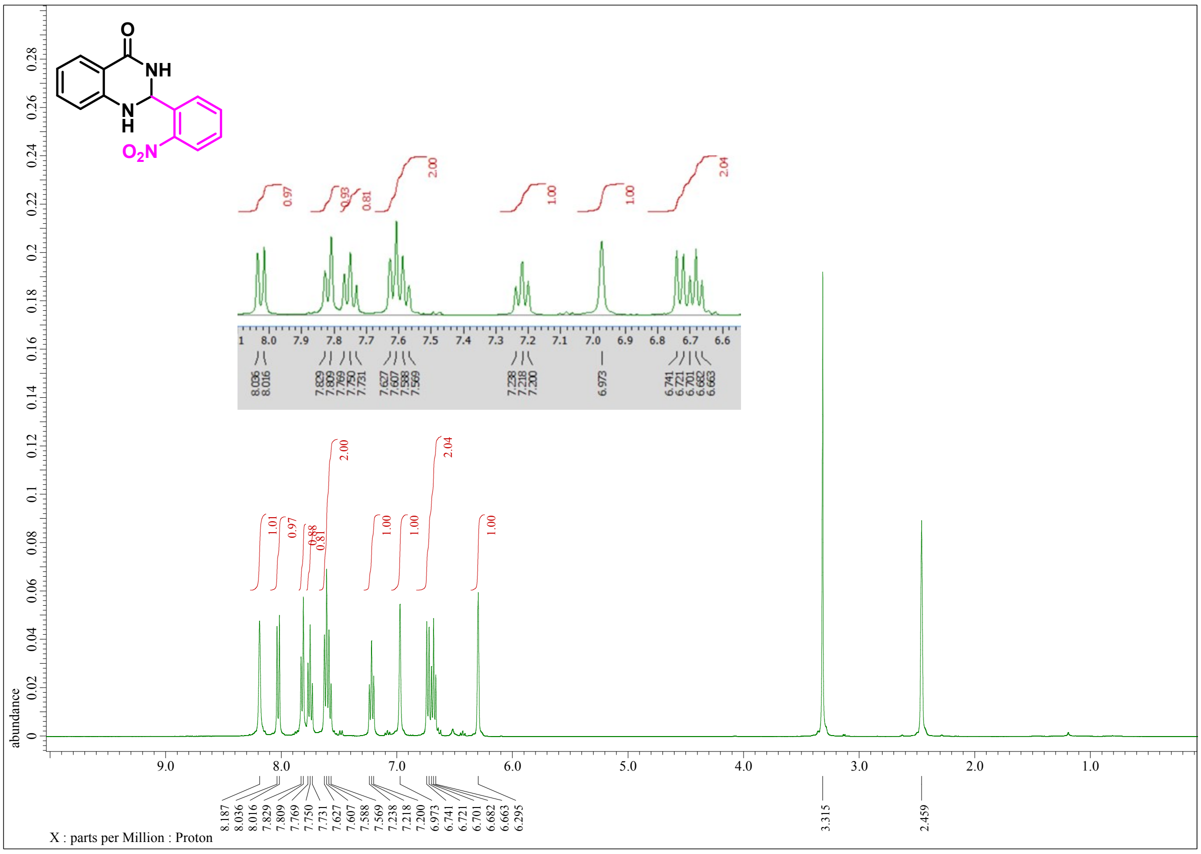
39.408



abundance
X : parts per Million : Proton
8.187
8.036
8.016
7.829
7.809
7.769
7.750
7.731
7.627
7.607
7.588
7.569
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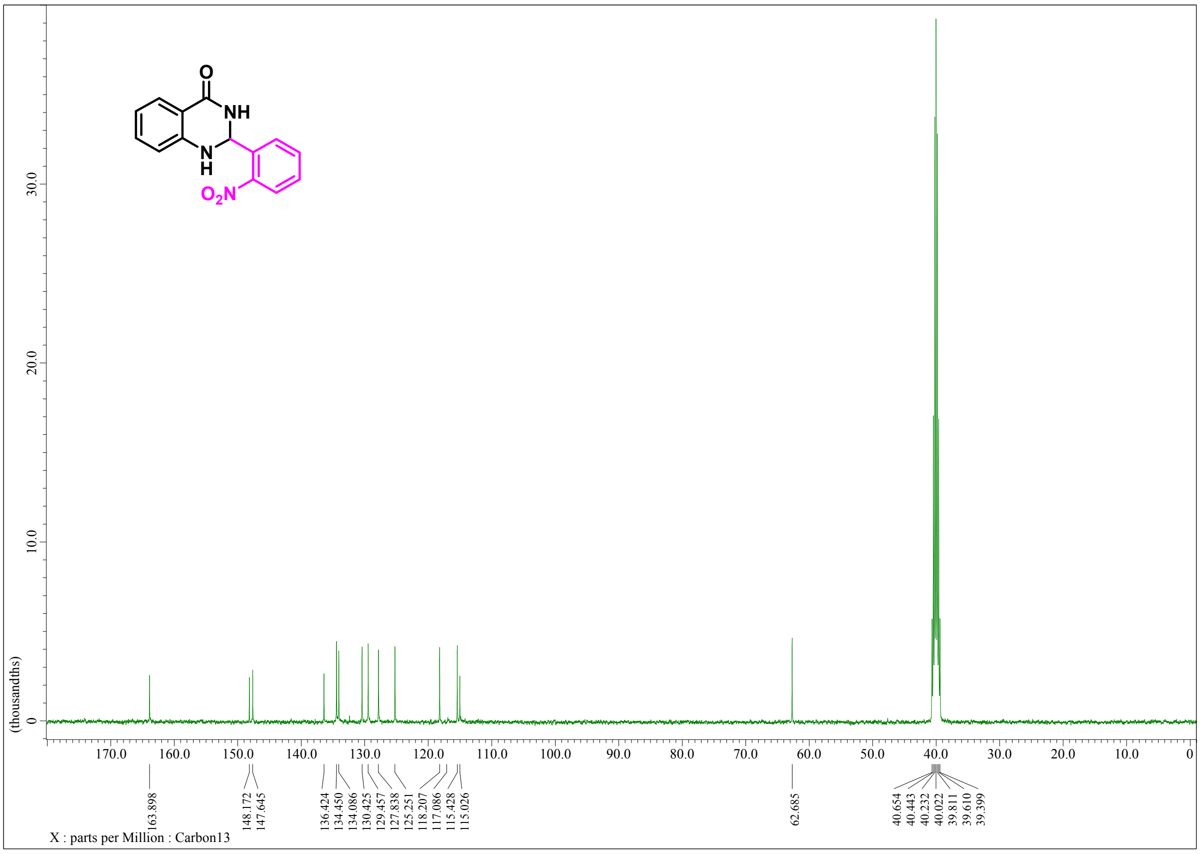
6.295
3.315
2.459



(thousandths)
X : parts per Million : Carbon13
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148.172
147.645
136.424
134.450
134.086
130.425
129.457
127.838
125.251
118.207
117.086
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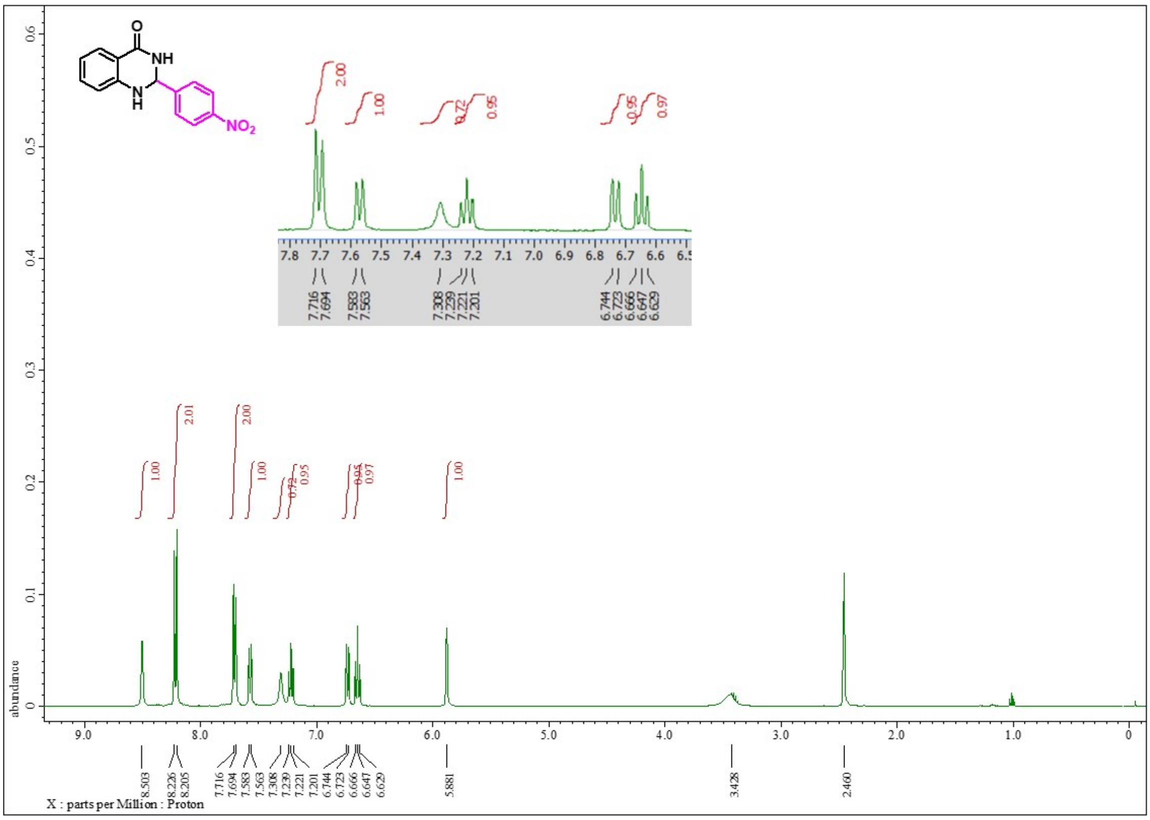
39.811
39.610
39.399



O
NH
N
H
NO2
X : parts per Million : Proton
abundance
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8.226
8.205
5.881
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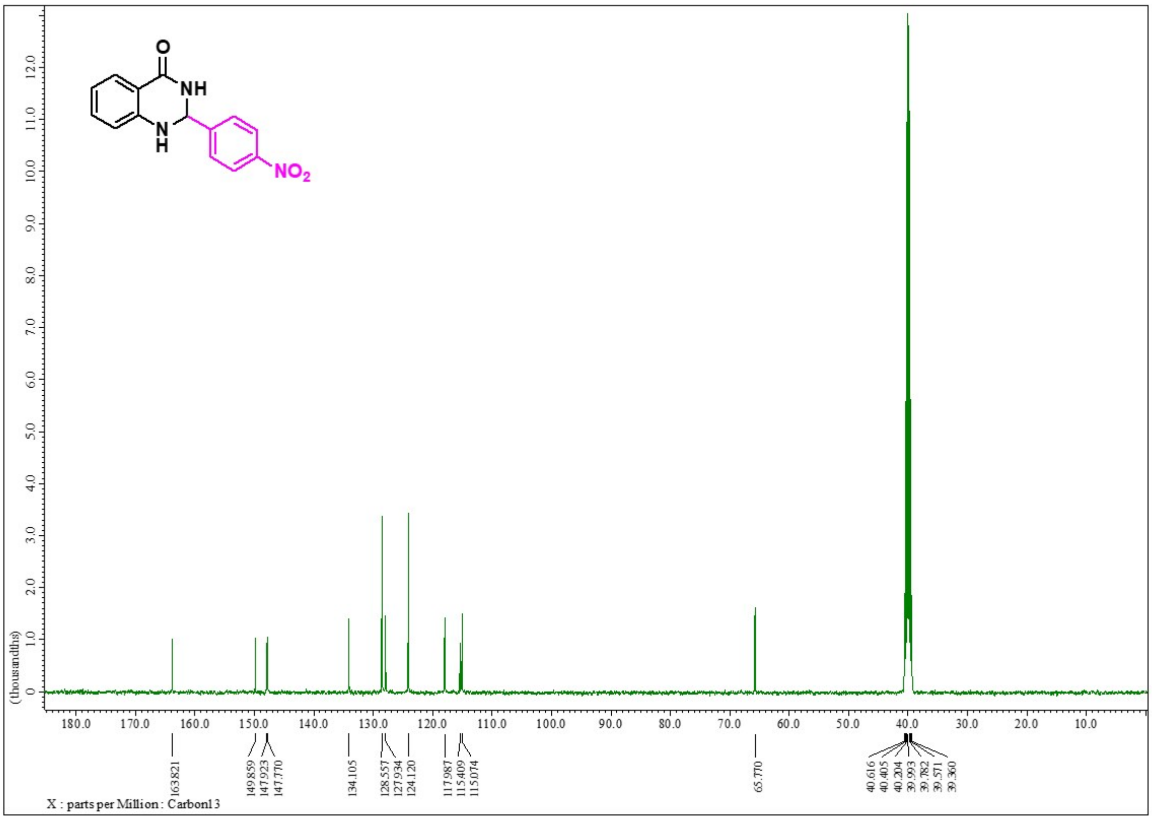
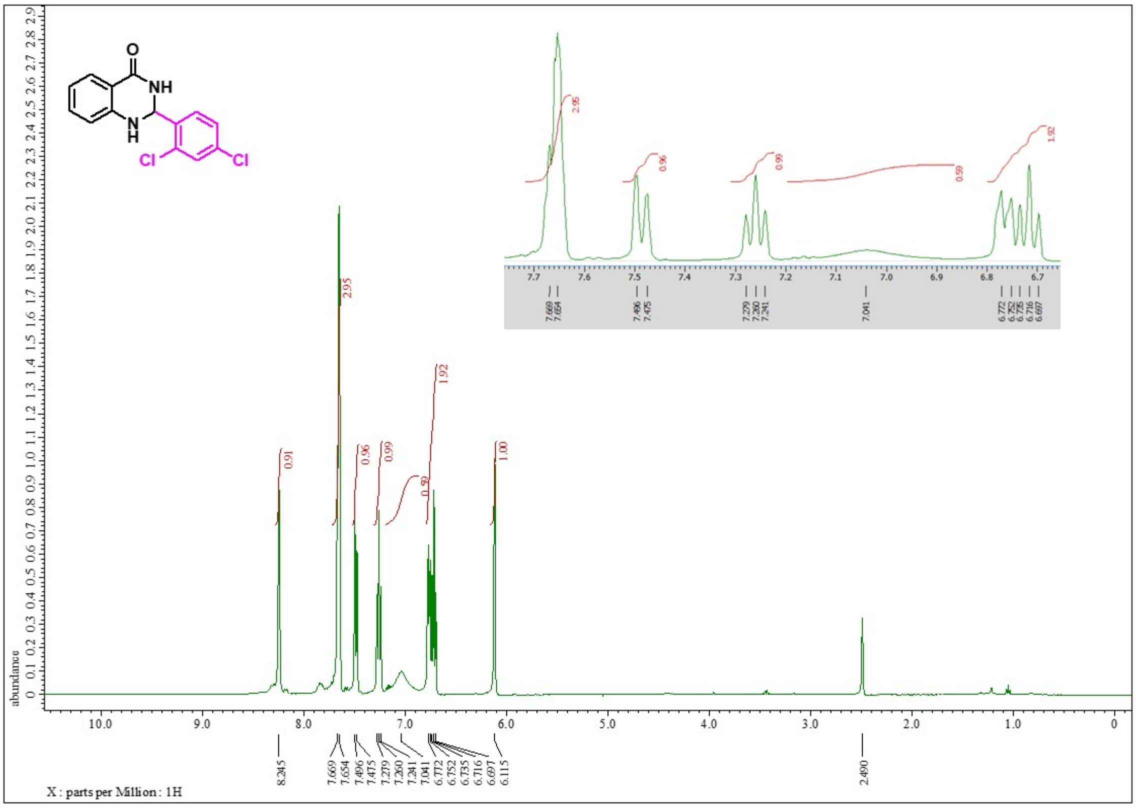
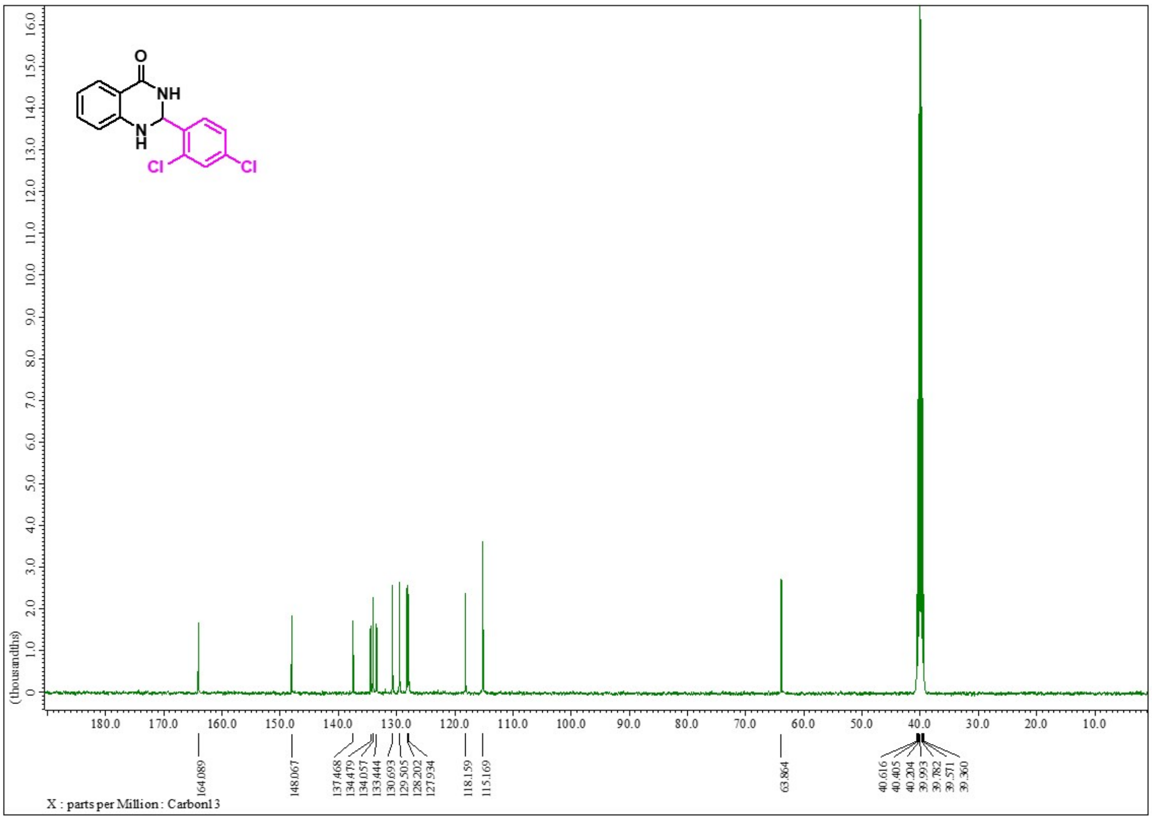
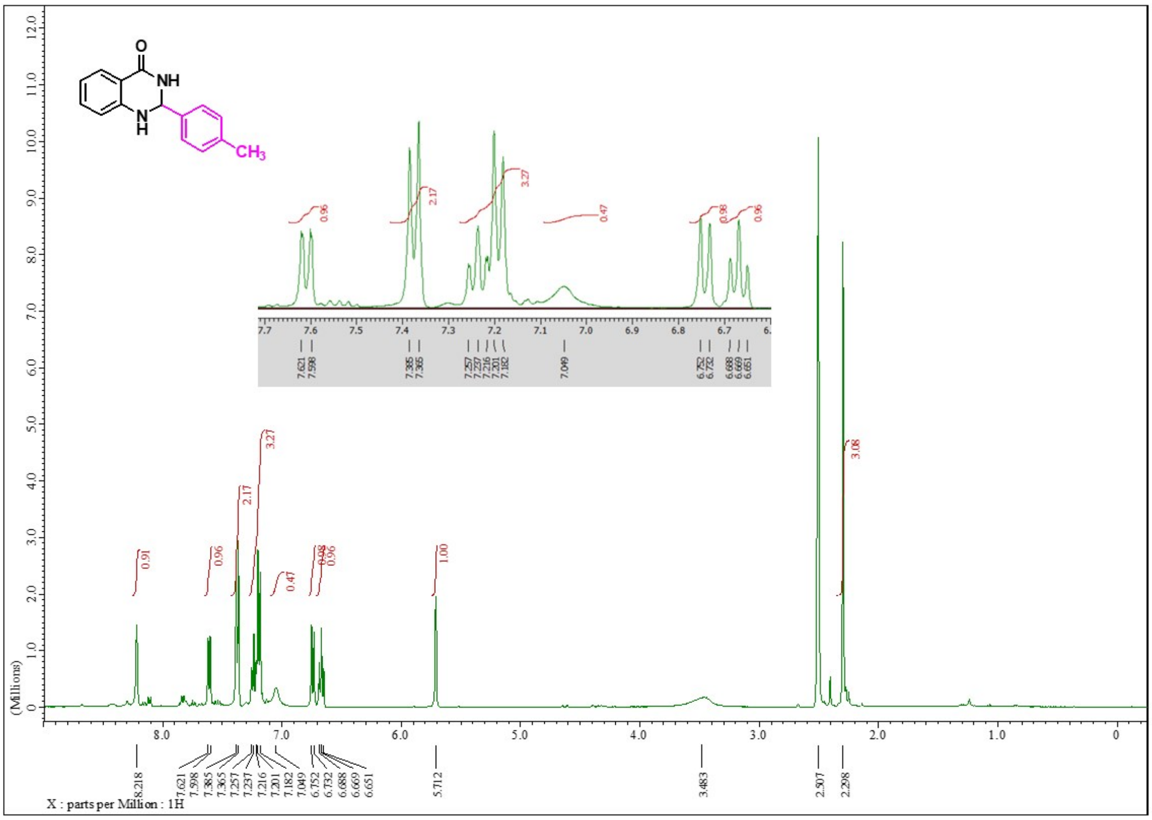
2.460

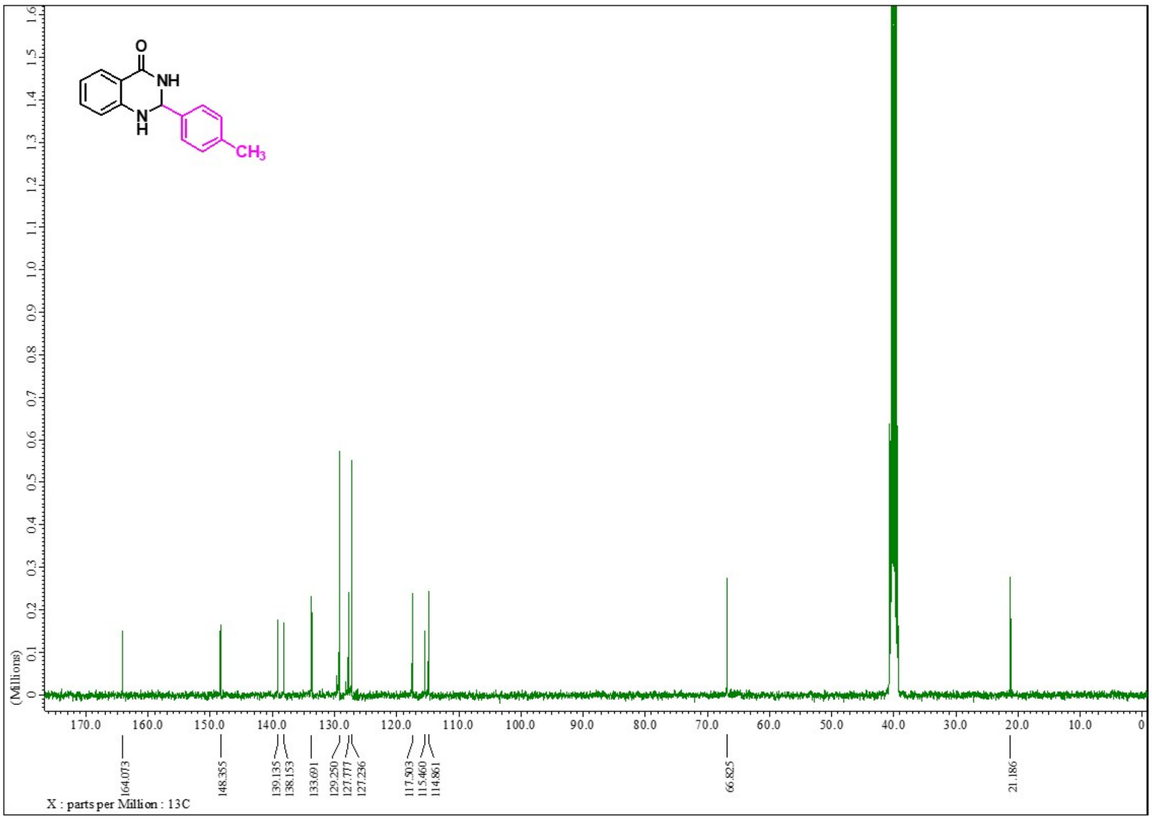


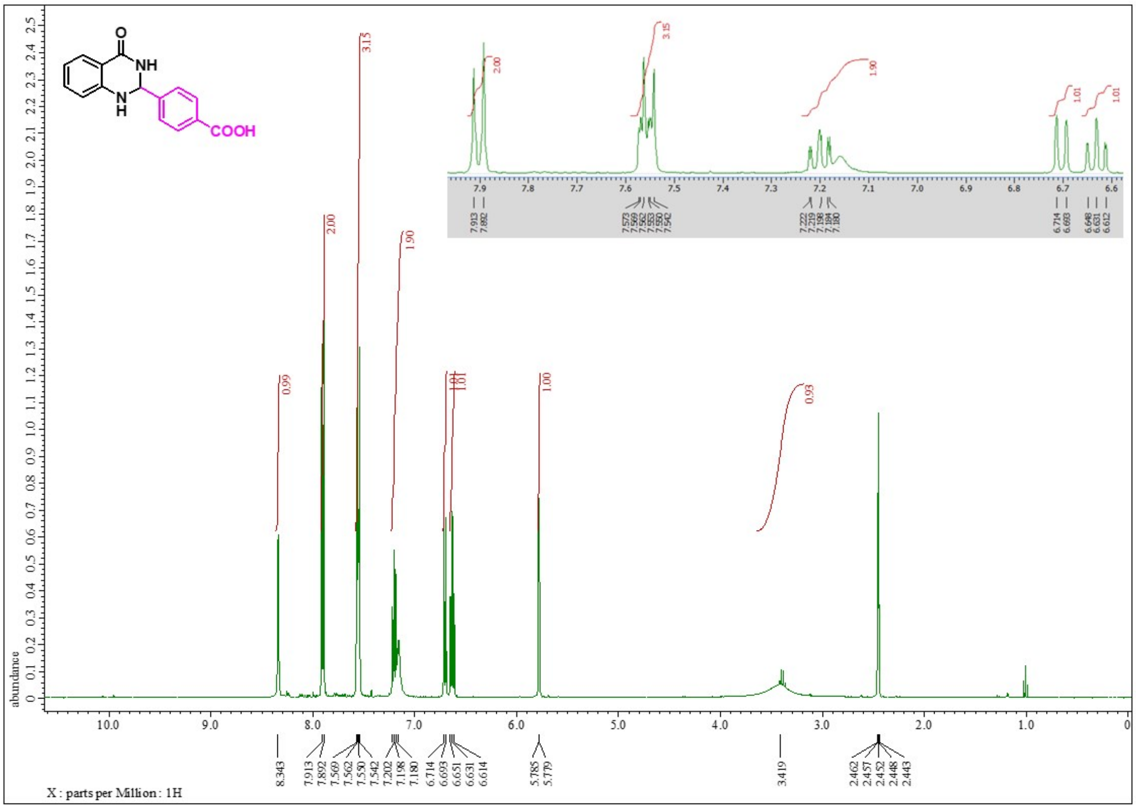
O
NH
N
H
NO2
X : parts per Million : Carbon13
(thousandths)
163.821
149.859
147.923
147.770
134.105
128.557
127.934
124.120
117.987
115.409
115.074
65.770

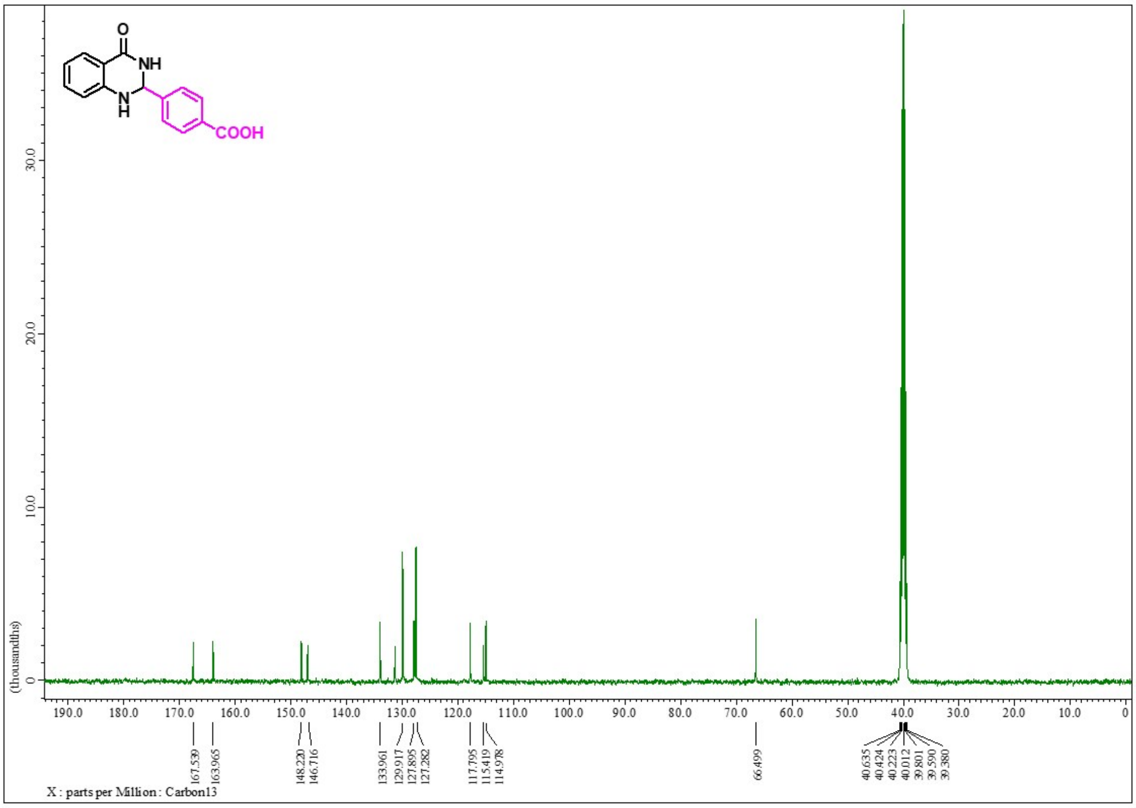

O
NH
N
H
Cl
Cl
abundance
8.245
7.669
7.654
7.496
7.475
7.279
7.260
7.241
7.041
6.772
6.752
6.735
6.716
6.697
6.115
2.490
X : parts per Million : 1H

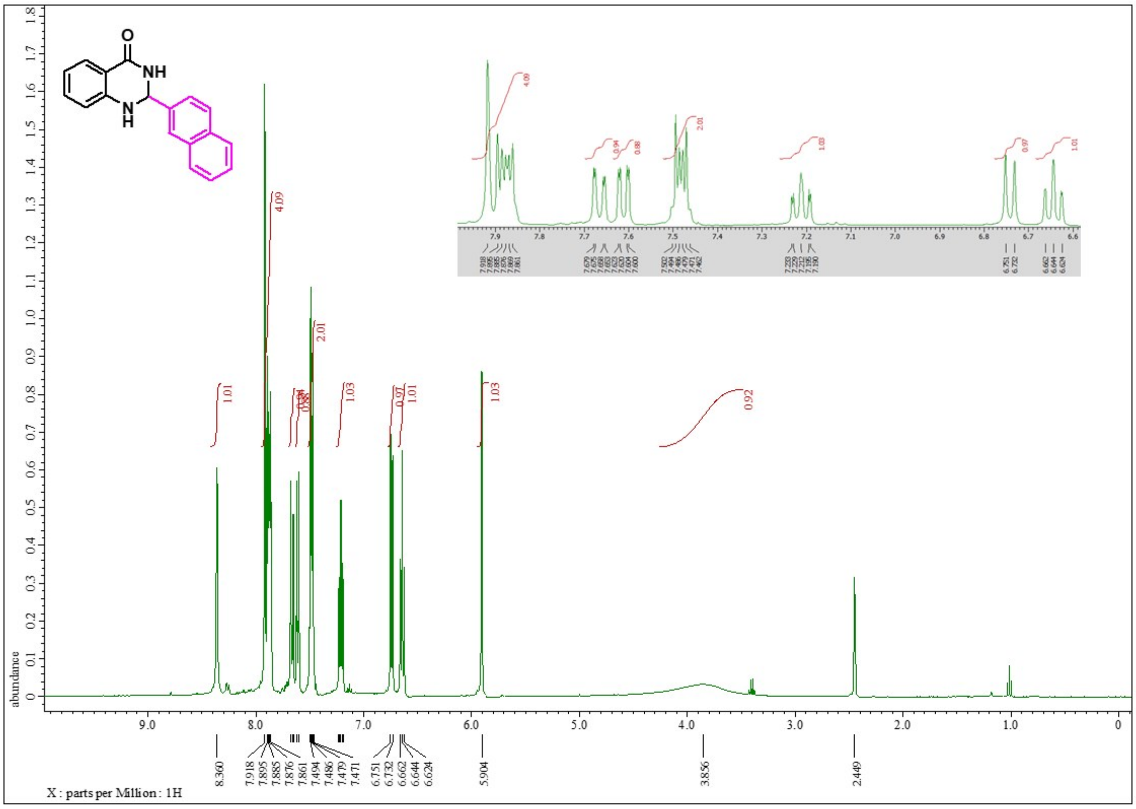

O
NH
N
H
Cl
Cl
(thousandths)
164.089
148.067
137.468
134.479
134.057
133.444
130.693
129.505
128.202
127.934
118.159
115.169
63.864
40.616
40.405
40.204
39.993
39.782
39.571
39.360
X : parts per Million : Carbon13

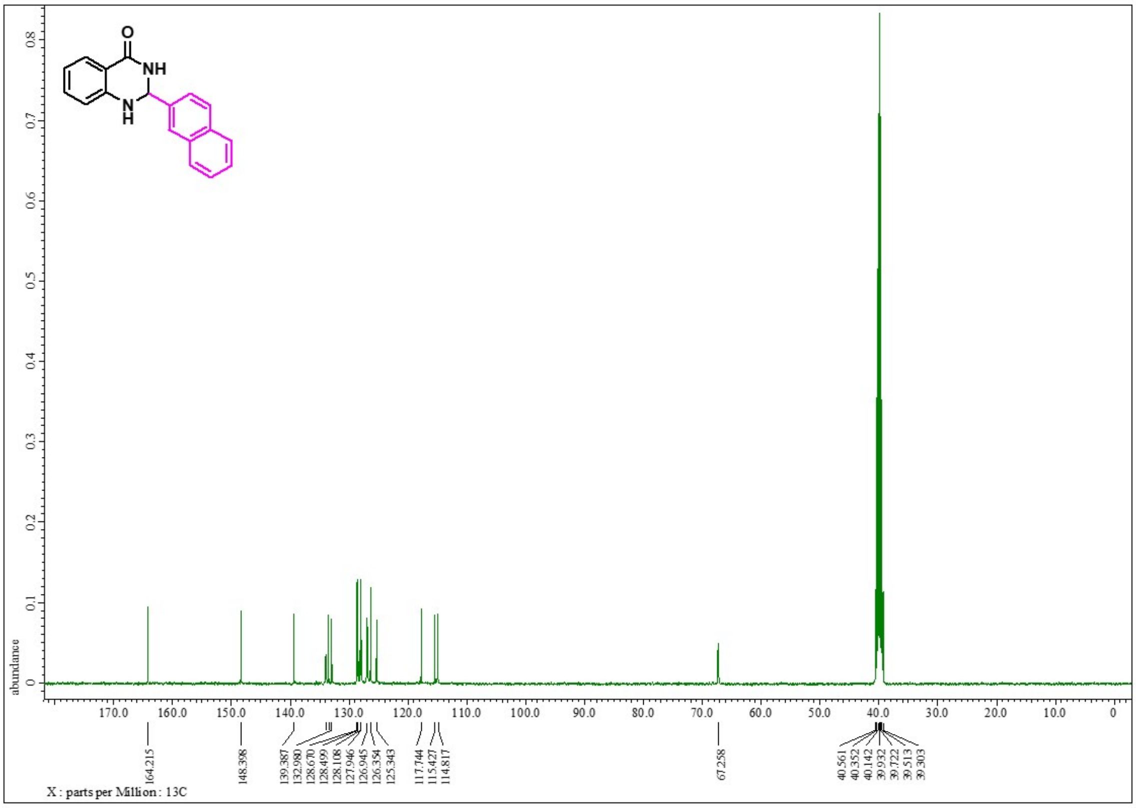


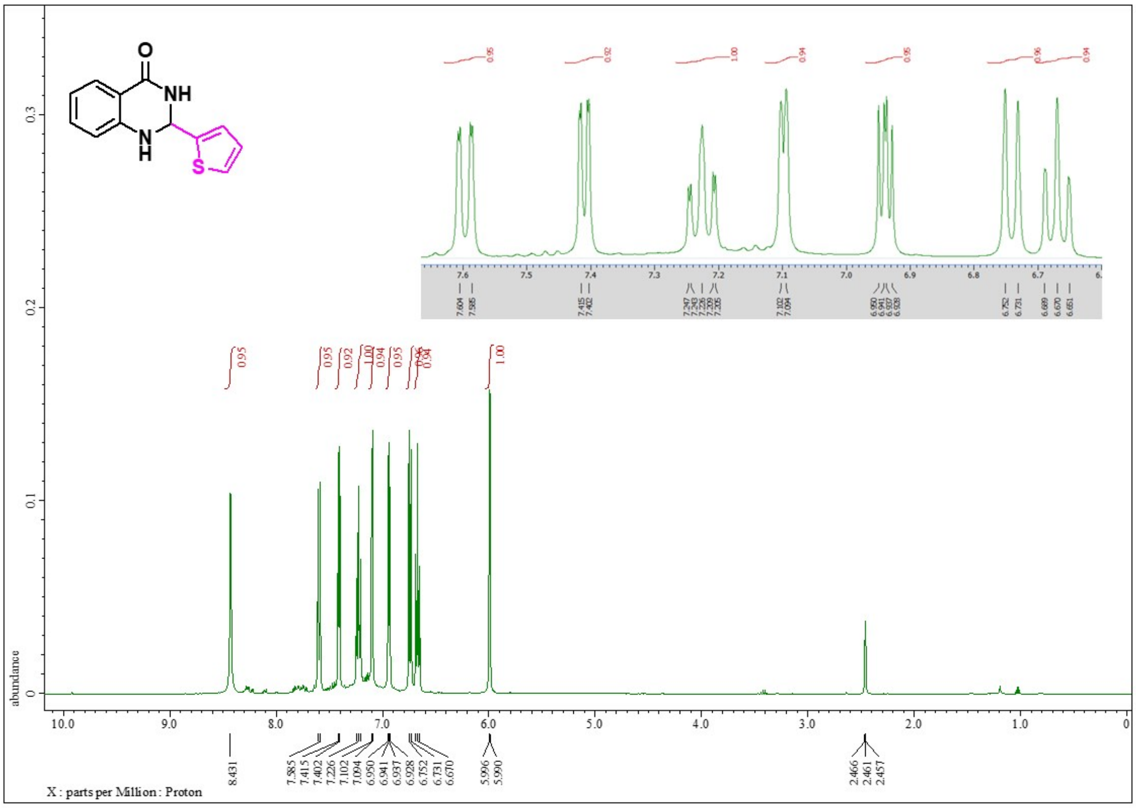




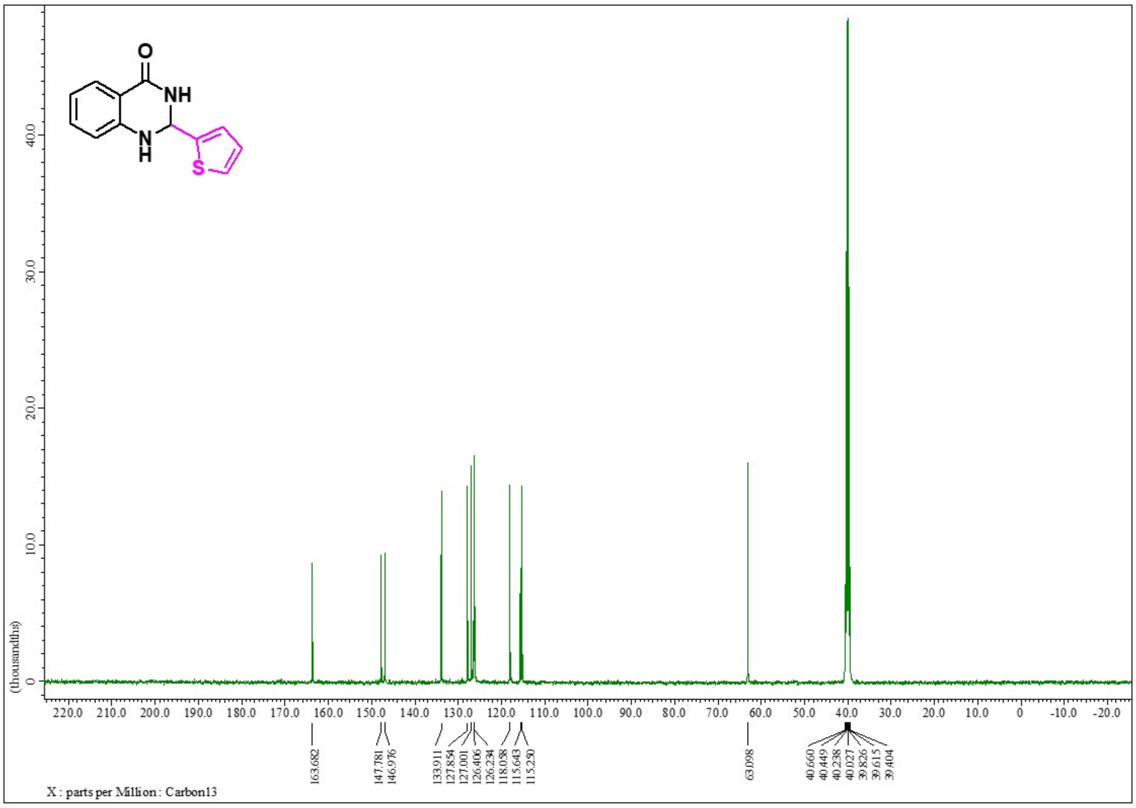



X : parts per Million : 1H
abundance

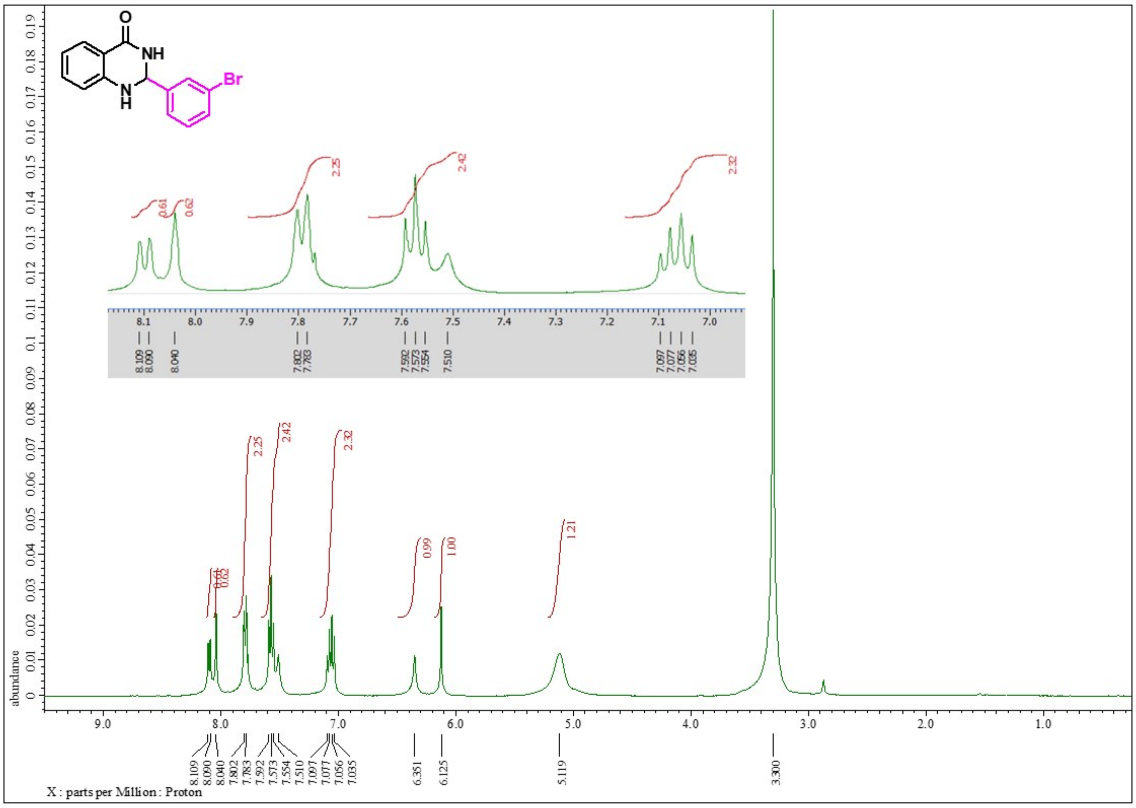

X : parts per Million : 13C
abundance

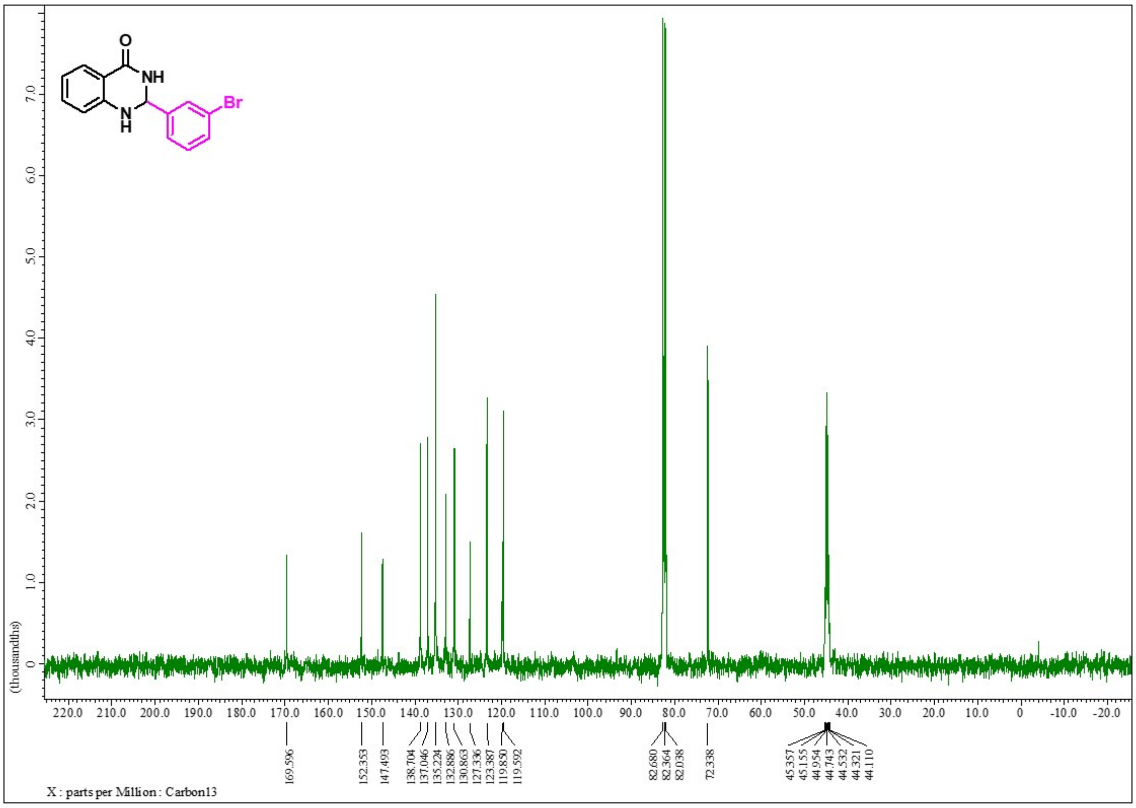


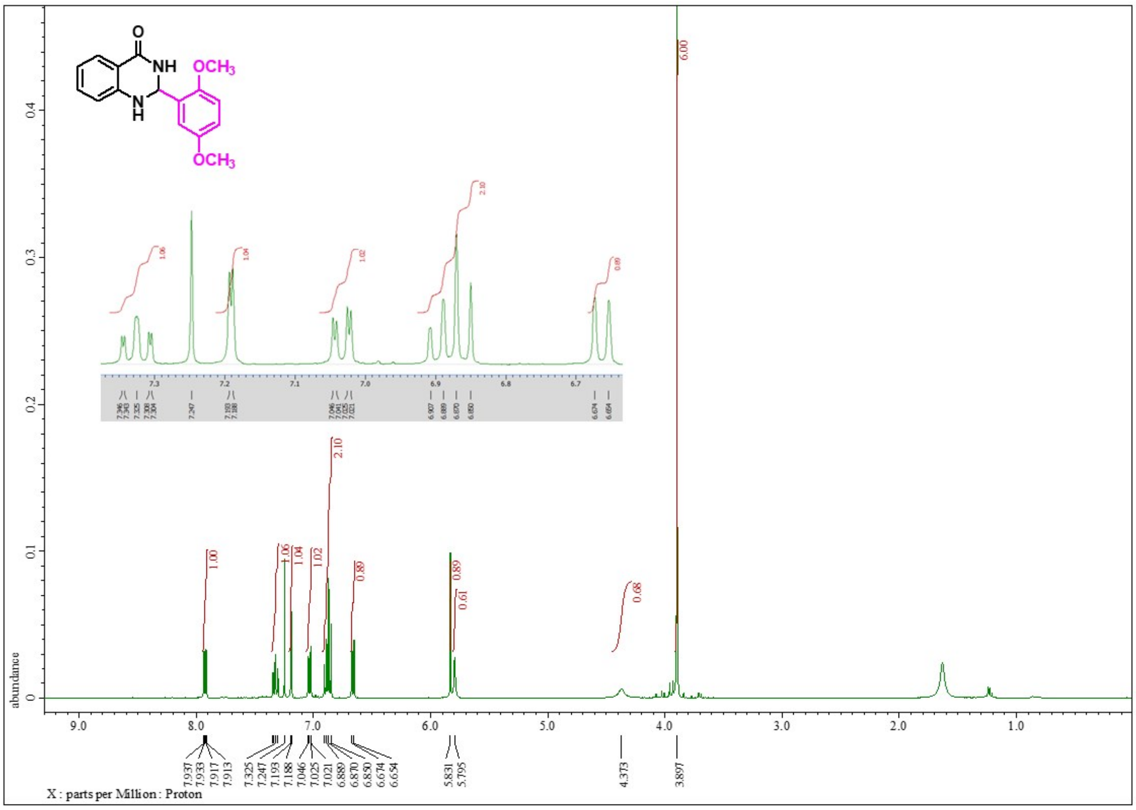
NH
N
H
S
O
abundance
X : parts per Million : Proton
8.431
7.585
7.415
7.402
7.226
7.102
7.094
6.950
6.941
6.937
6.928
6.752
6.731
6.670
5.996
5.990
2.466
2.461
2.457

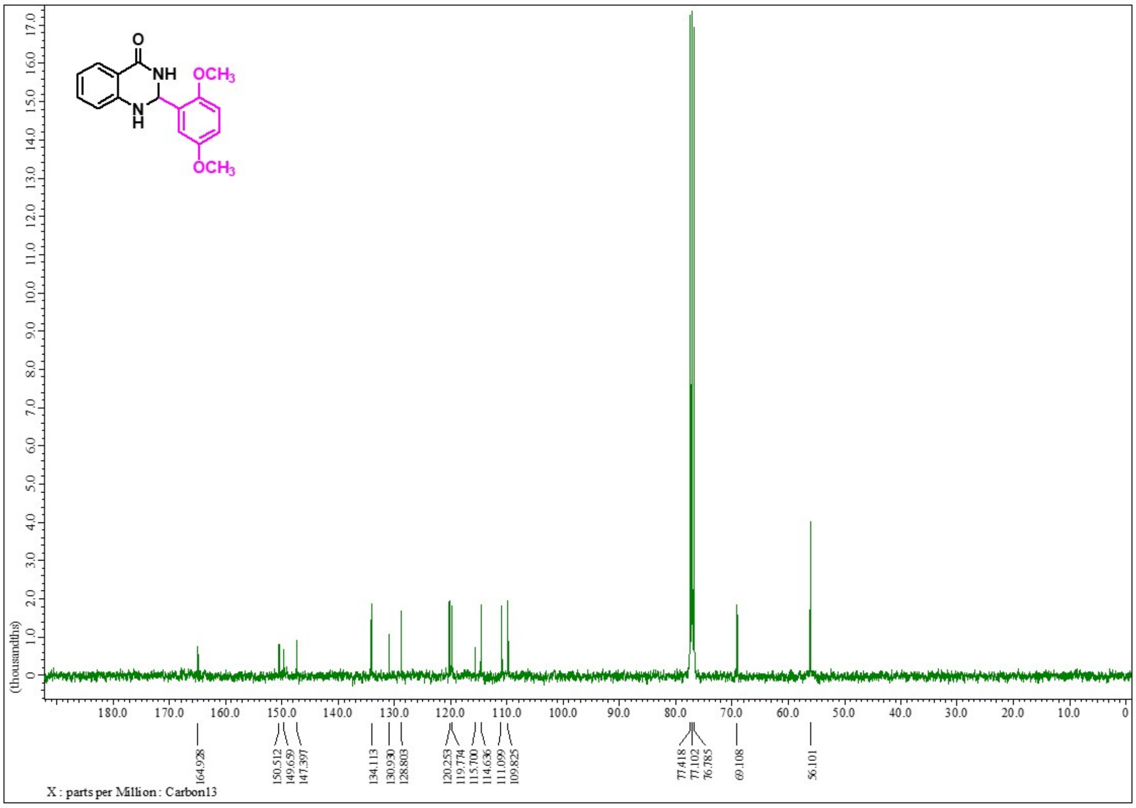


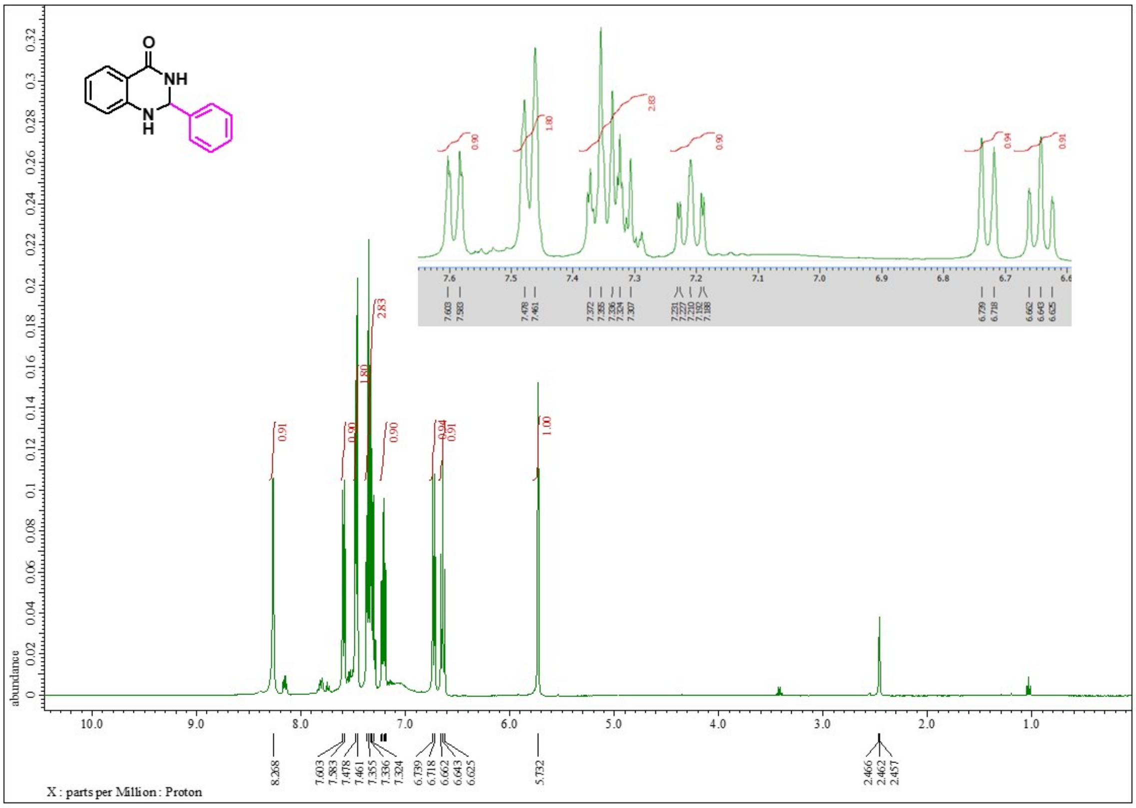
NH
N
H
S
O
(thousandths)
X : parts per Million : Carbon13
163.682
147.781
146.976
133.911
127.854
127.001
126.406
126.234
118.038
115.643
115.290
63.098
40.660
40.449
40.238
40.027
39.826
39.615
39.404

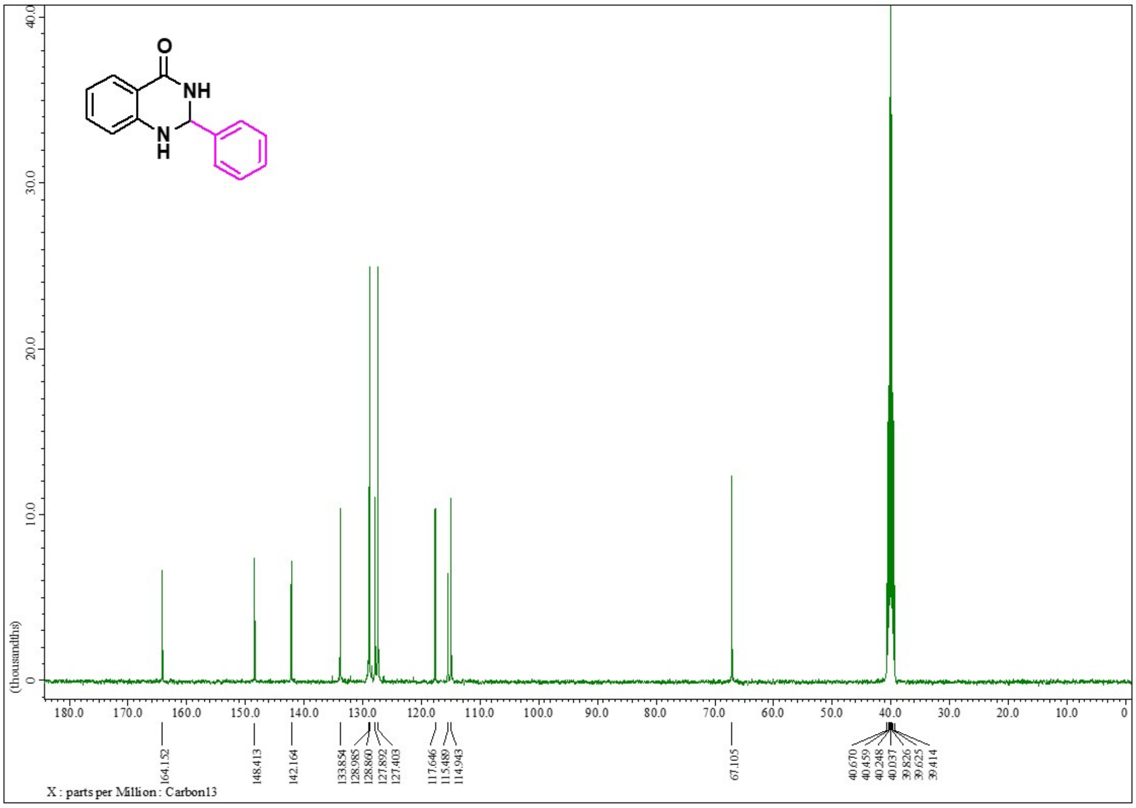


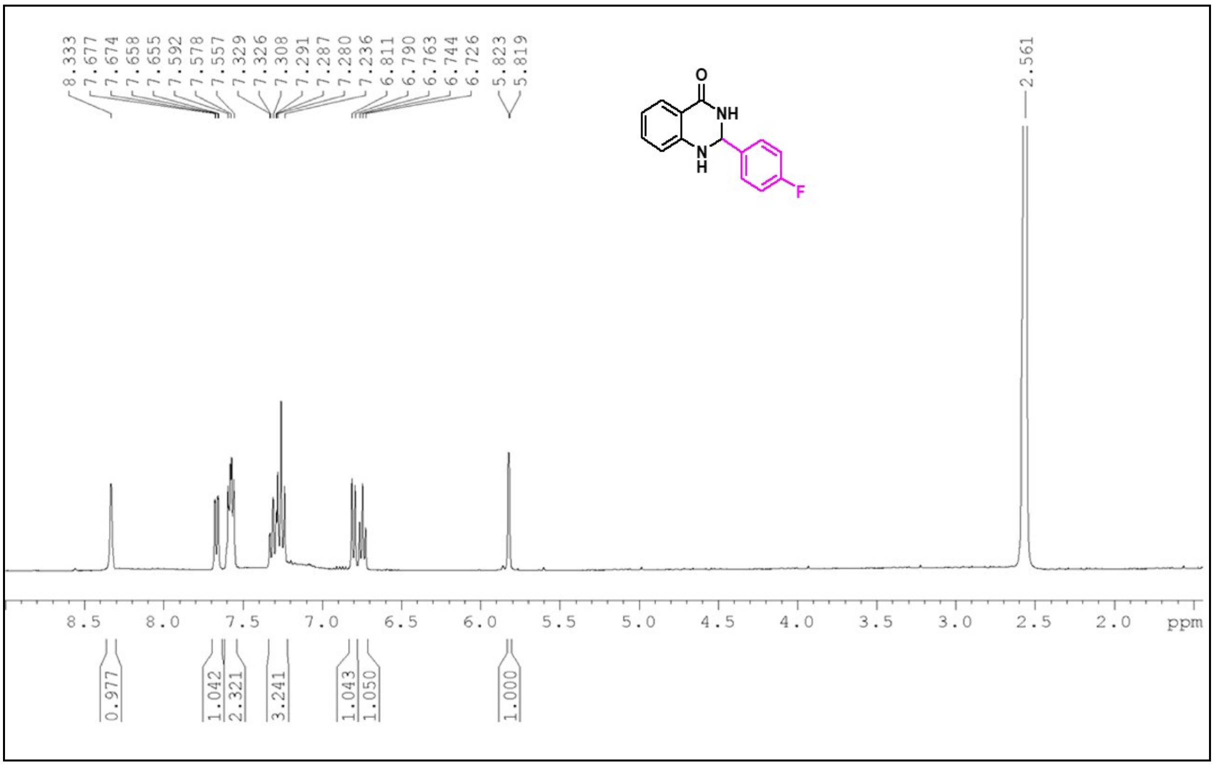


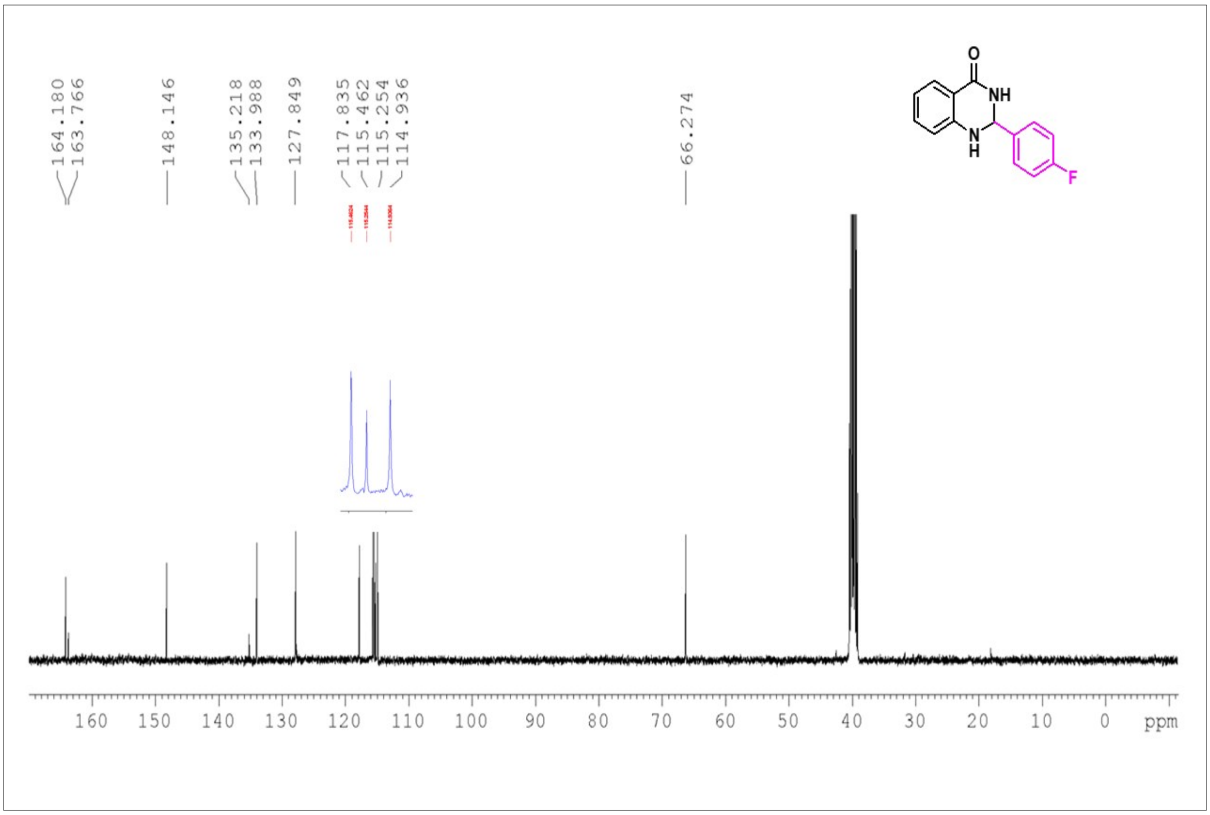

X : parts per Million : Proton
abundance

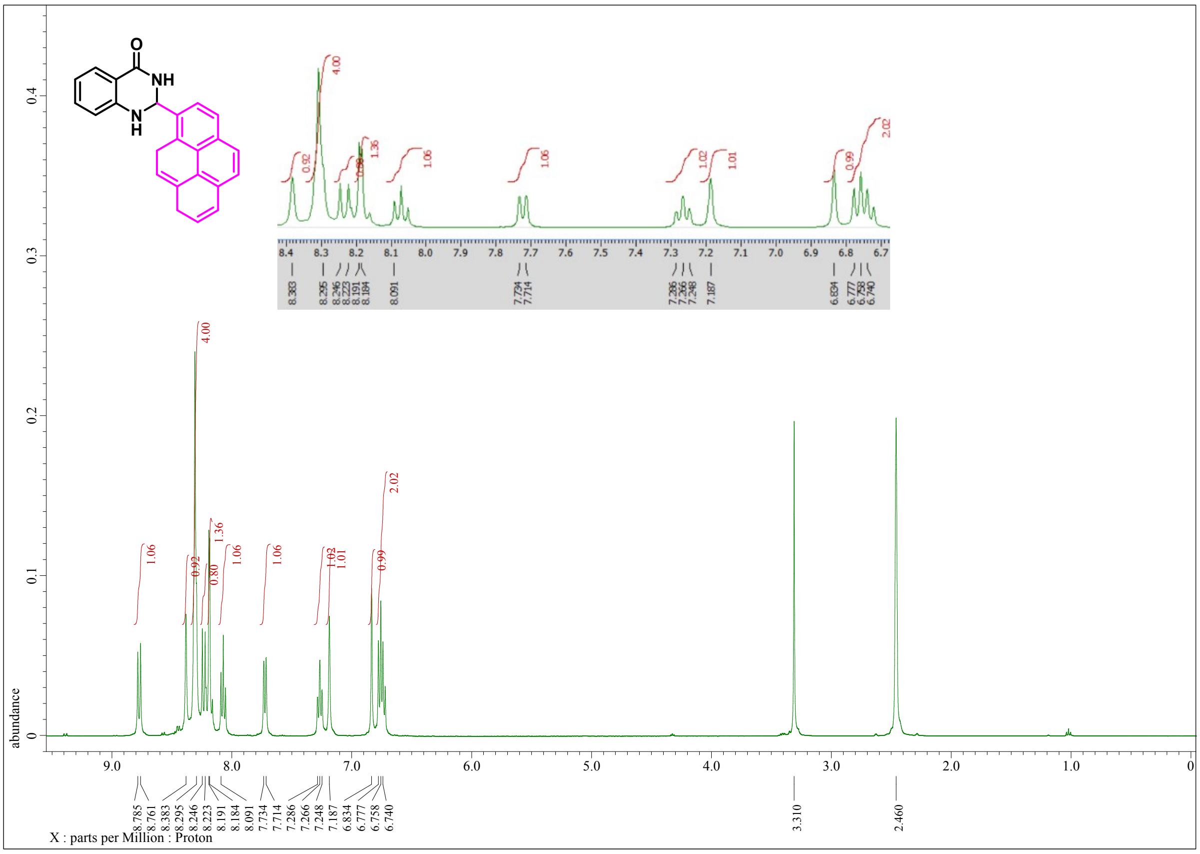

X : parts per Million : Carbon13
(thousandths)

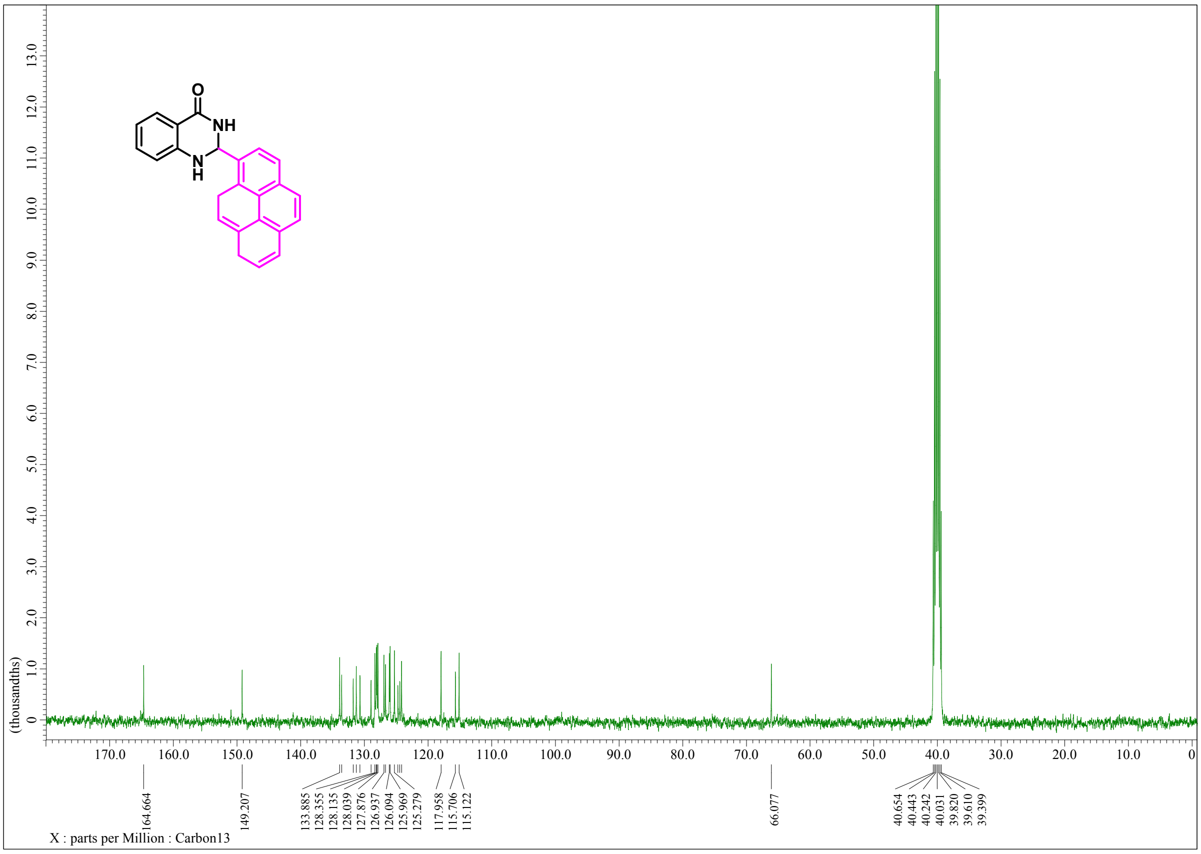

X : parts per Million : Proton
abundance

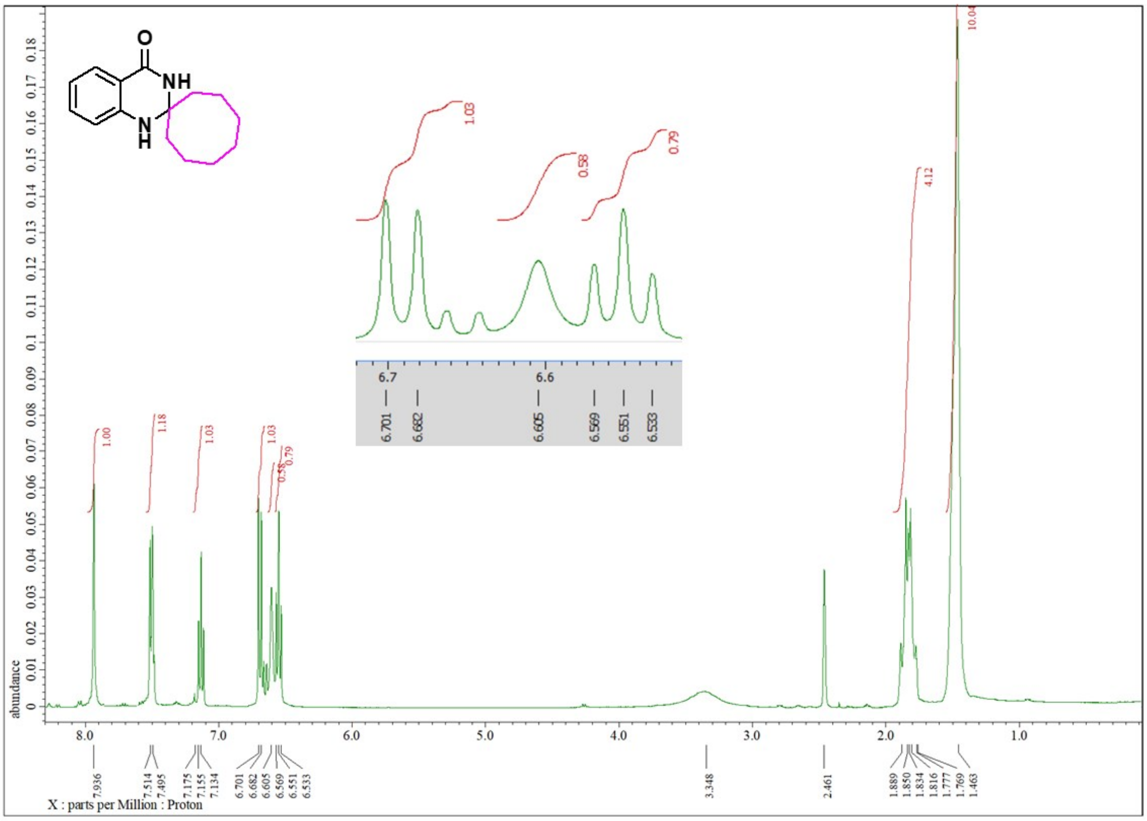

X : parts per Million : Carbon13
(thousandths)


8.333
7.677
7.674
7.658
7.655
7.592
7.578
7.557
7.329
7.326
7.308
7.291
7.287
7.280
7.236
6.811
6.790
6.763
6.744
6.726
5.823
5.819
2.561
O
NH
N
H
F
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 ppm
0.977
1.042
2.321
3.241
1.043
1.050
1.000

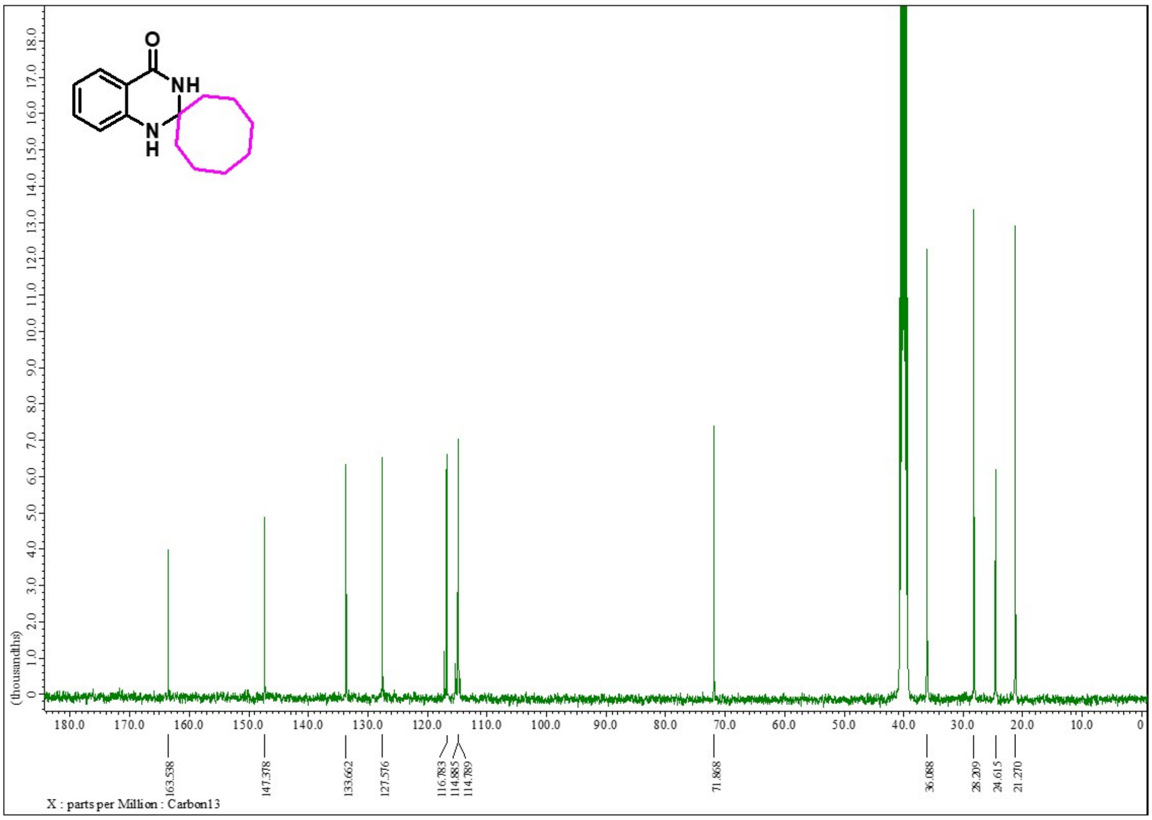

164.180
163.766
148.146
135.218
133.988
127.849
117.835
115.462
115.254
114.936
66.274
O
NH
N
H
F
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



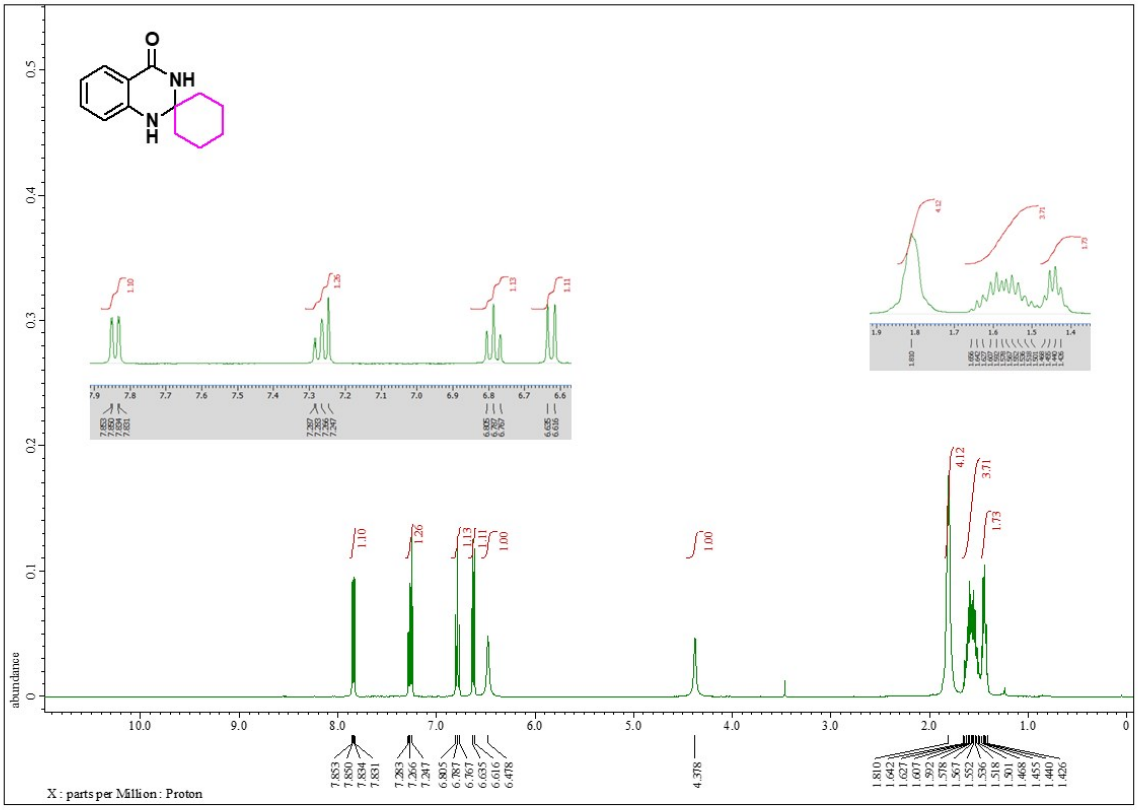


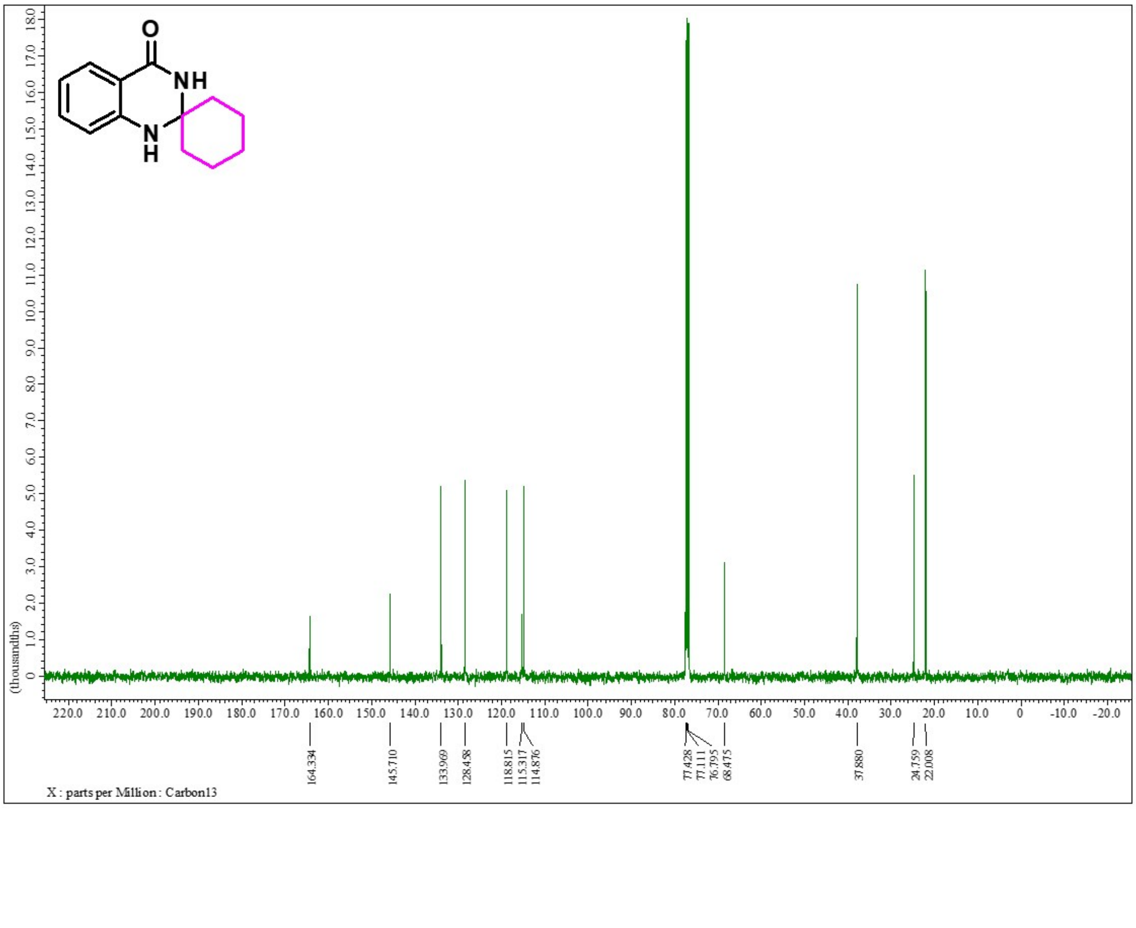


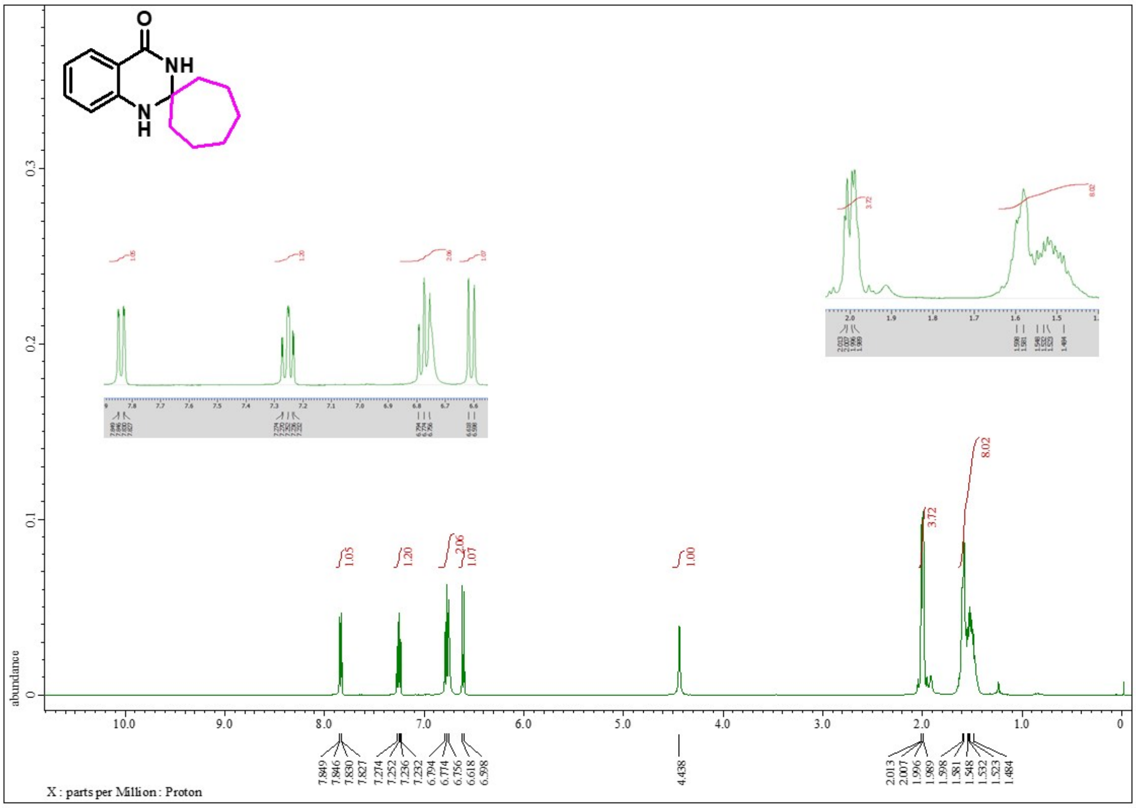
O
NH
N
H
abundance
X : parts per Million : Proton
7.936
7.514
7.495
7.175
7.155
7.134
6.701
6.682
6.605
6.569
6.551
6.533
3.348
2.461
1.889
1.850
1.834
1.816
1.777
1.769
1.463



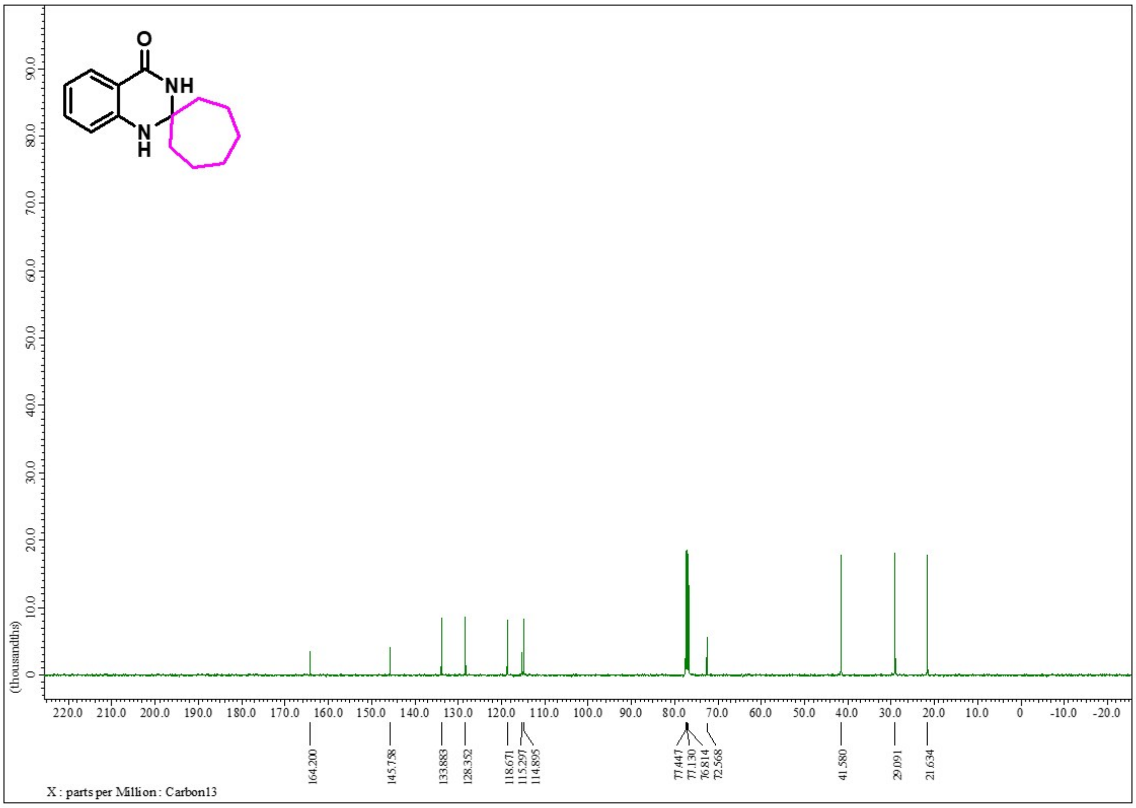
O
NH
N
H
(thousandths)
X : parts per Million : Carbon13
163.538
147.378
133.662
127.576
116.783
114.885
114.789
71.868
36.088
28.209
24.615
21.270


NH
N
H
O
abundance
X : parts per Million : Proton
1.10
1.26
1.13
1.11
1.00
1.00
4.12
3.71
1.73
7.853
7.850
7.834
7.831
7.283
7.266
7.247
6.805
6.787
6.767
6.635
6.616
6.478
4.378
1.810
1.642
1.627
1.607
1.592
1.578
1.567
1.552
1.536
1.518
1.501
1.468
1.455
1.440
1.426

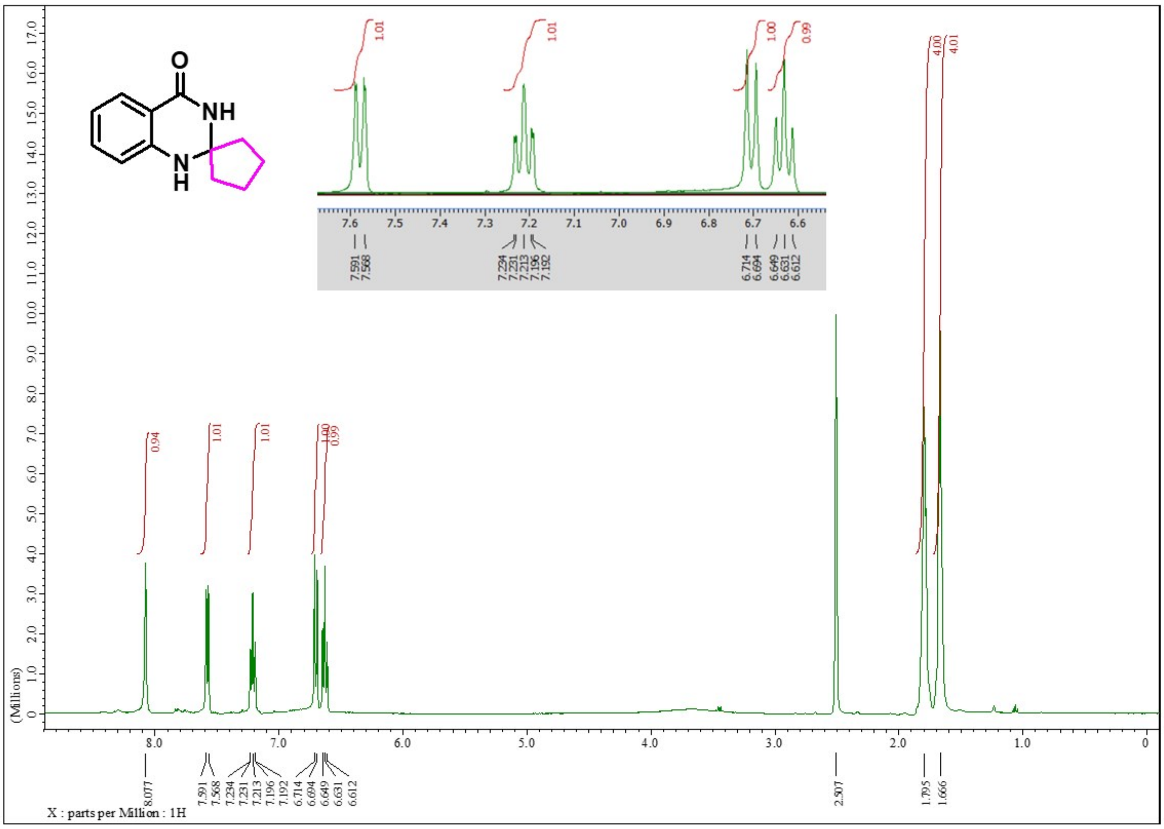

NH
N
H
O
(thousandths)
X : parts per Million : Carbon13
164.334
145.710
133.969
128.458
118.815
115.317
114.876
77.428
77.111
76.795
68.475
37.880
24.159
22.008

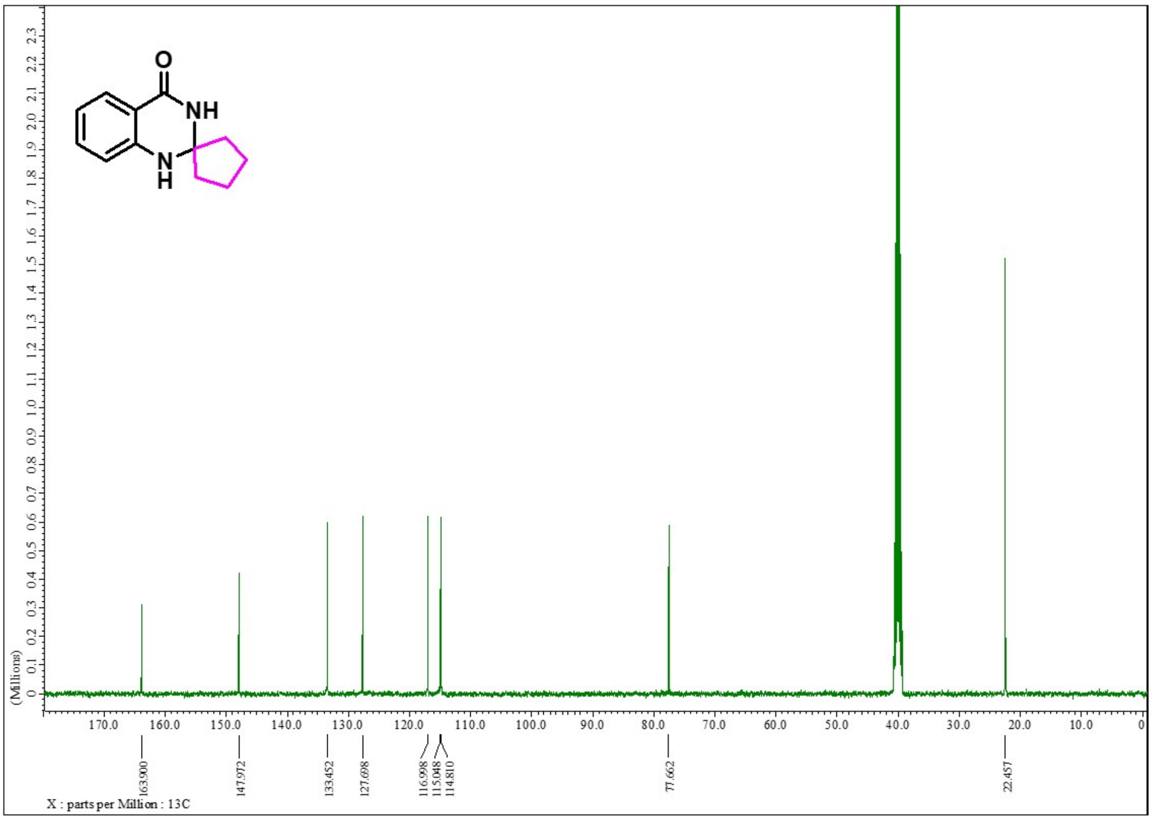


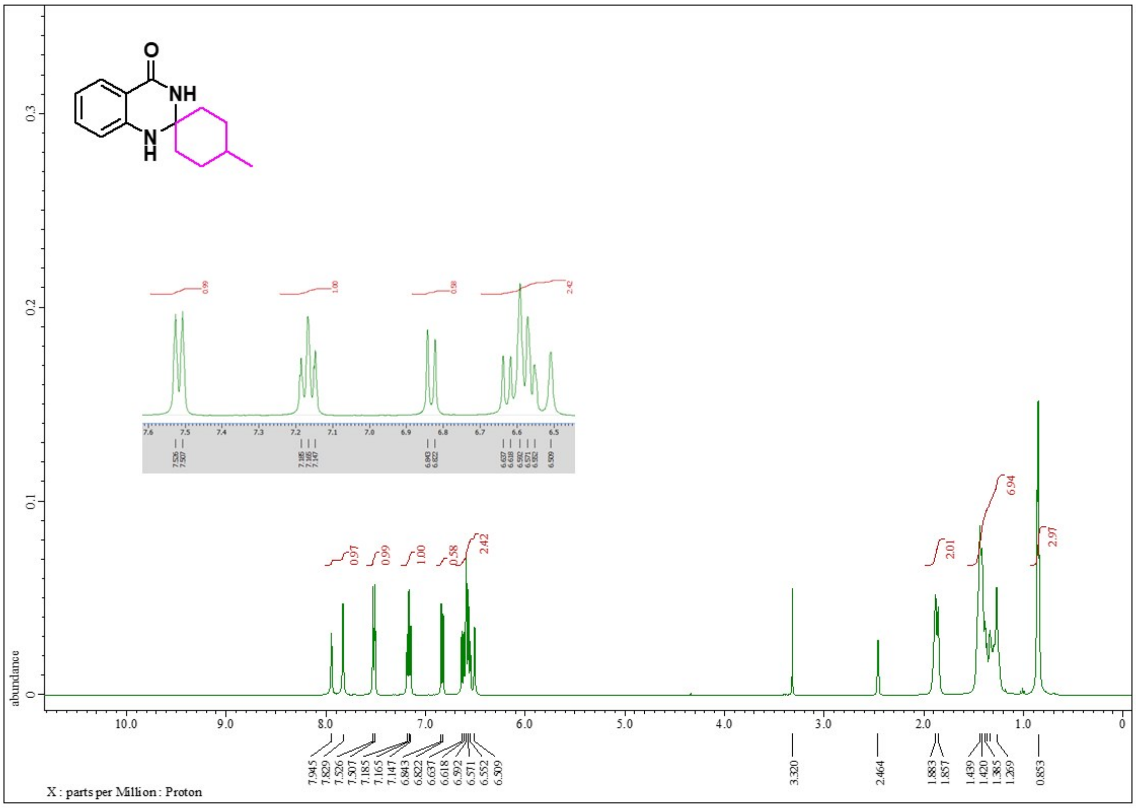
NH
N
H
O
abundance
X : parts per Million : Proton
1.05
1.20
2.06
1.07
1.00
3.72
8.02
7.849
7.846
7.830
7.827
7.274
7.252
7.236
7.232
6.794
6.774
6.756
6.618
6.598
4.438
2.013
2.007
1.996
1.989
1.598
1.581
1.548
1.532
1.523
1.484

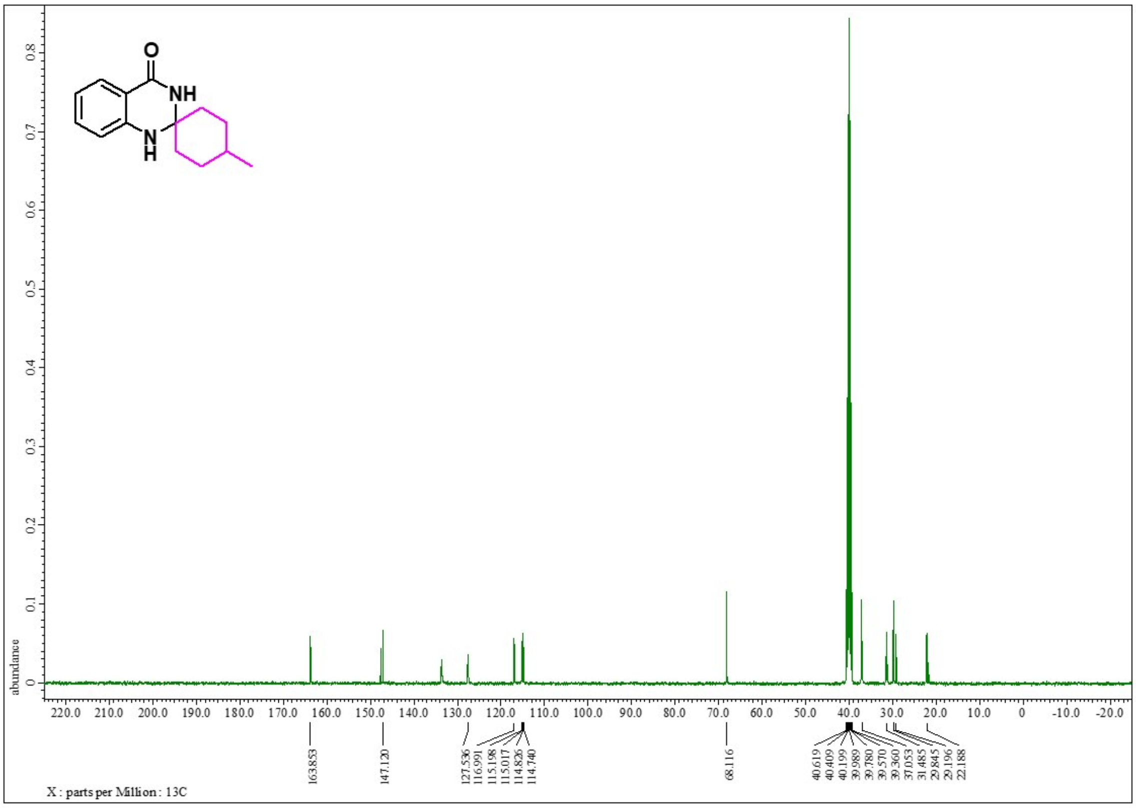


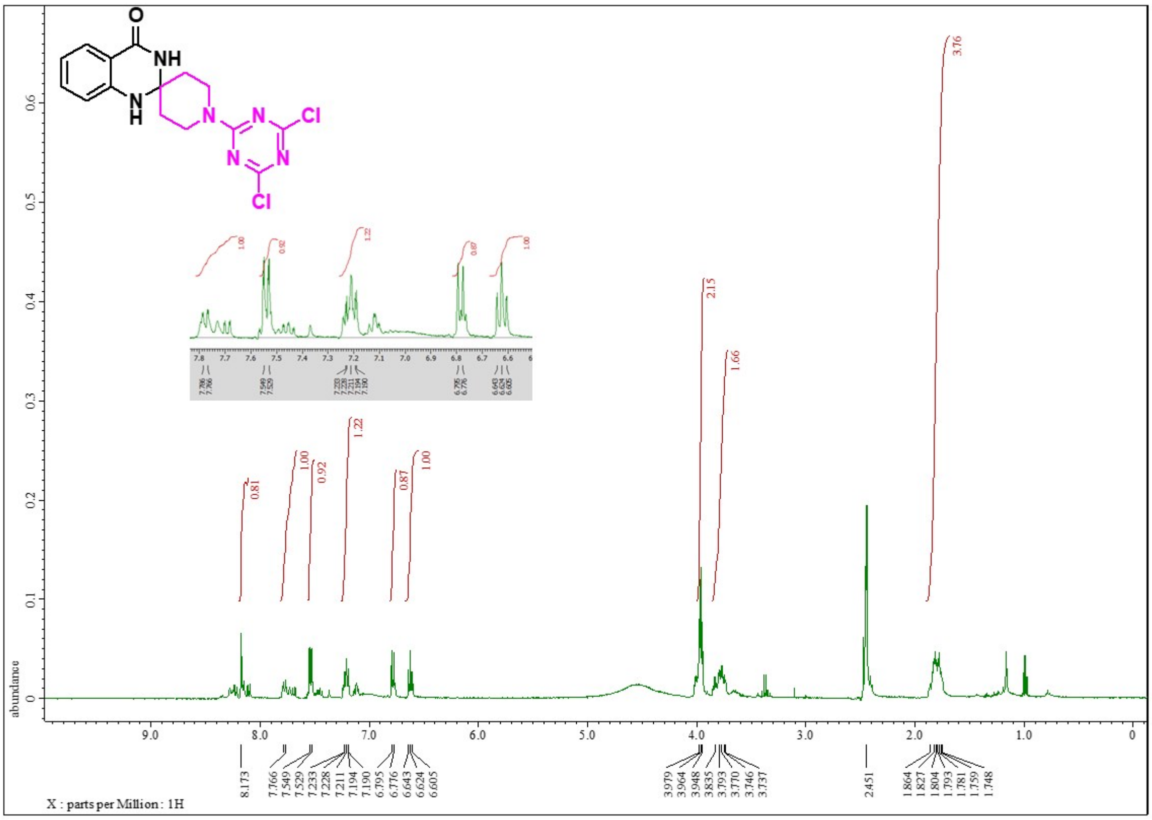
NH
N
H
O
(thousandths)
X : parts per Million : Carbon13
164.200
145.758
133.883
128.352
118.671
115.297
114.895
77.447
77.130
76.814
72.568
41.580
29.091
21.634

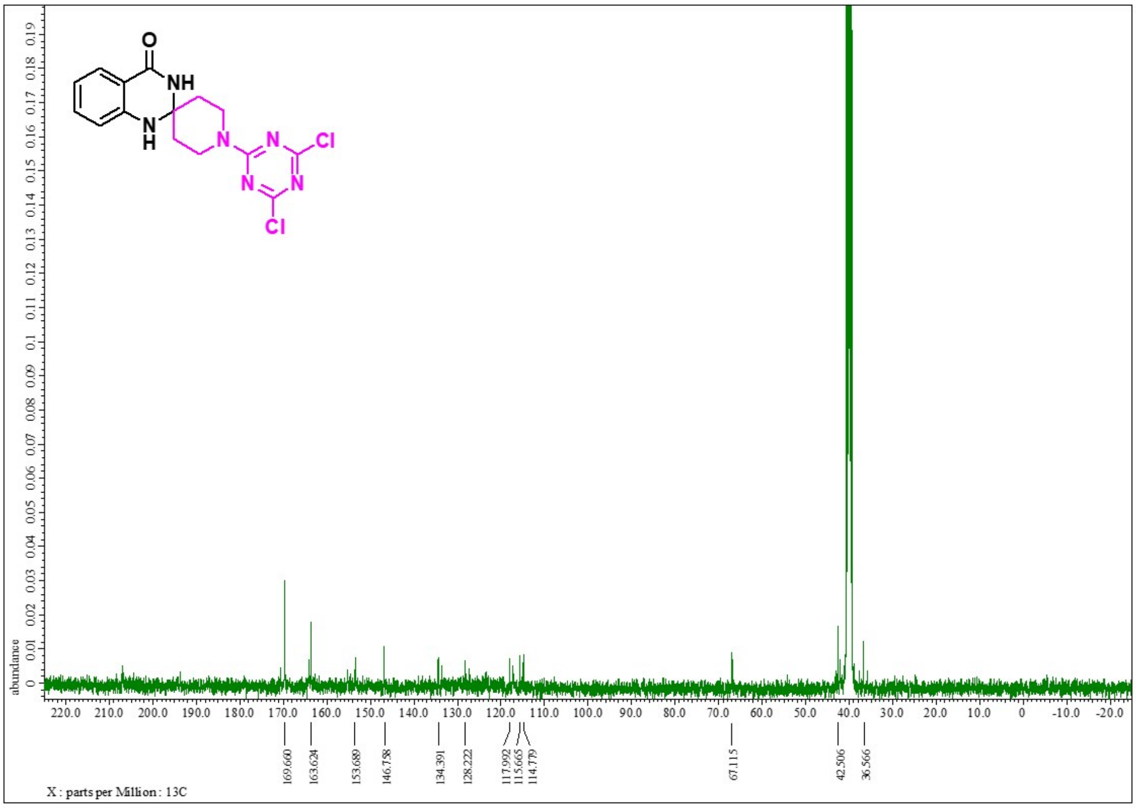

O
NH
N
H
X : parts per Million : 1H
(Millions)
8.077
7.591
7.568
7.234
7.231
7.213
7.196
7.192
6.714
6.694
6.649
6.631
6.612
2.507
1.795
1.666
0.94
1.01
1.01
1.00
0.99
4.00
4.01

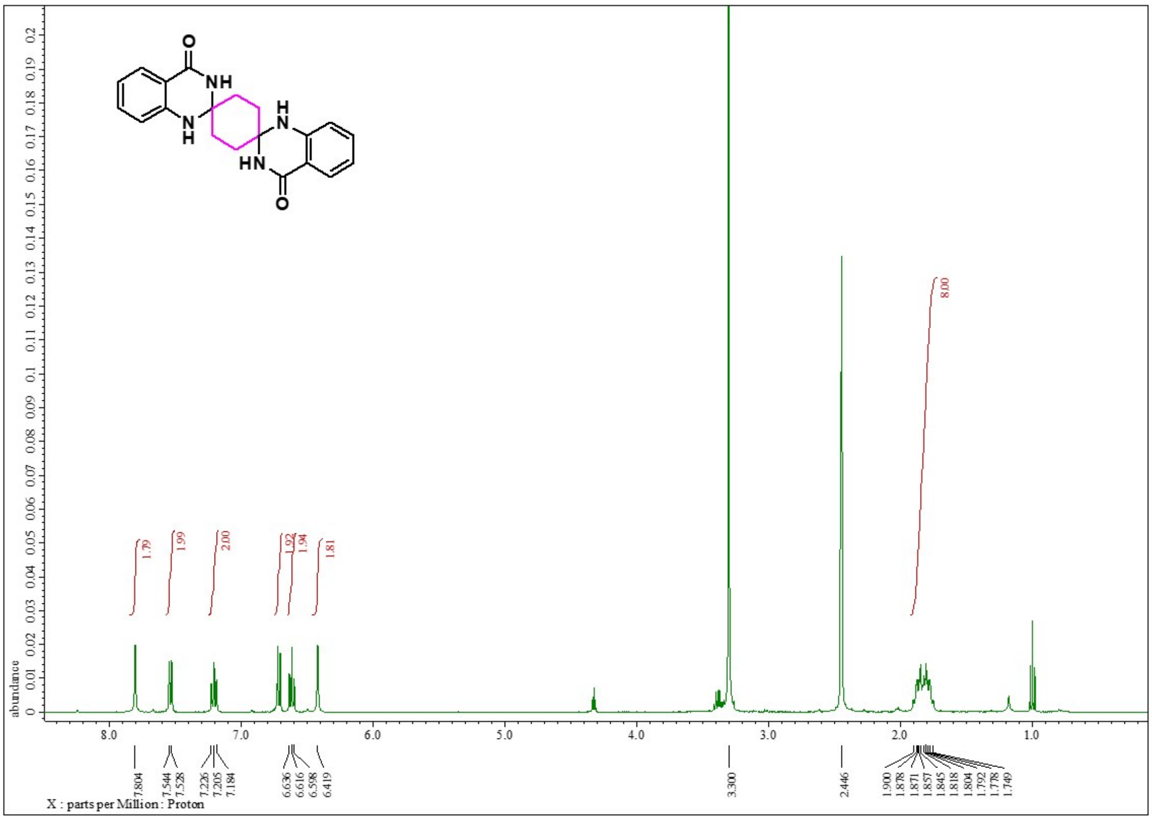

O
NH
N
H
X : parts per Million : 13C
(Millions)
163.900
147.972
133.452
127.698
116.998
115.048
114.810
77.662
22.457

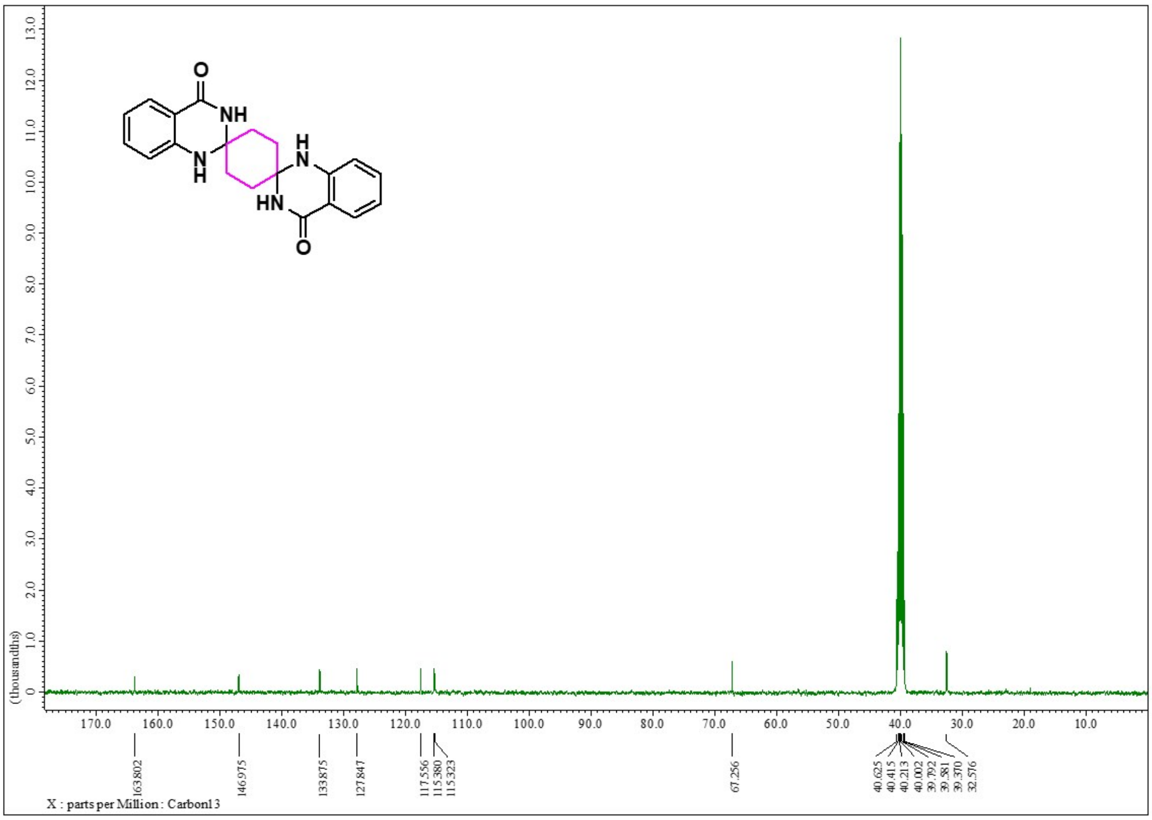


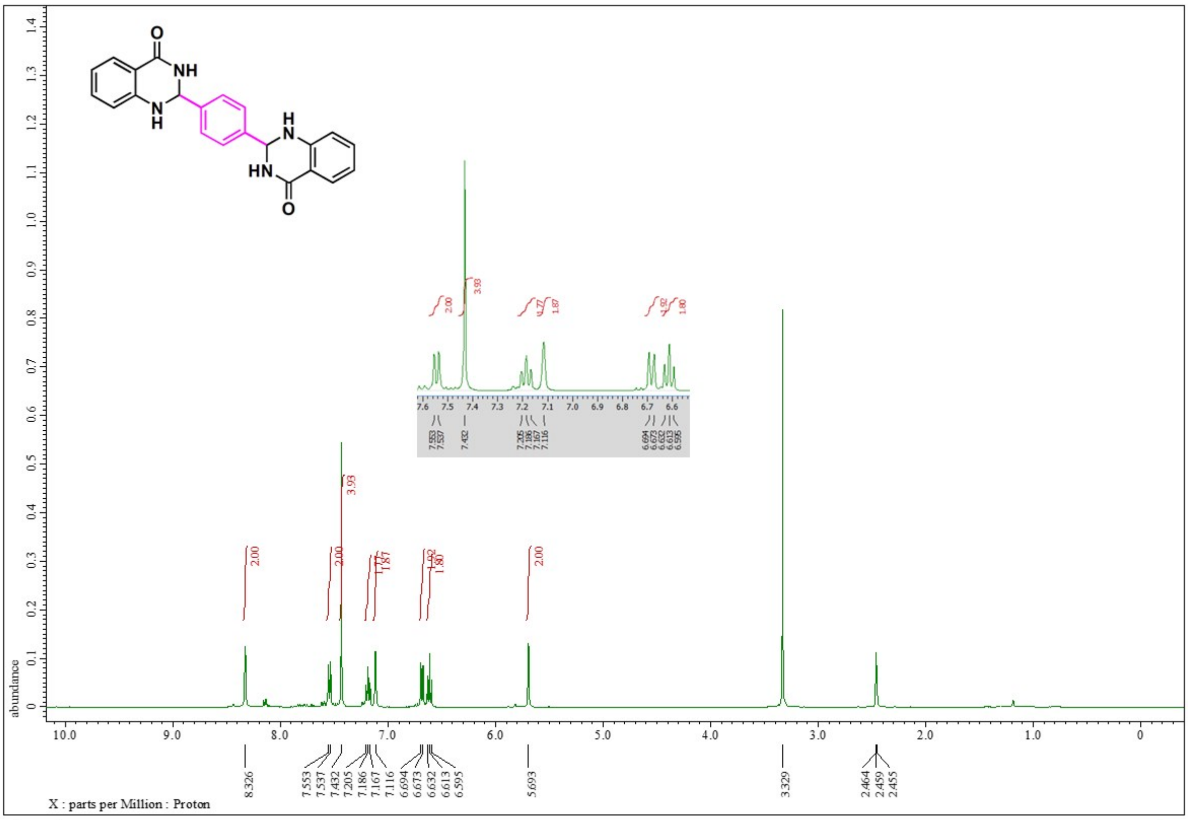


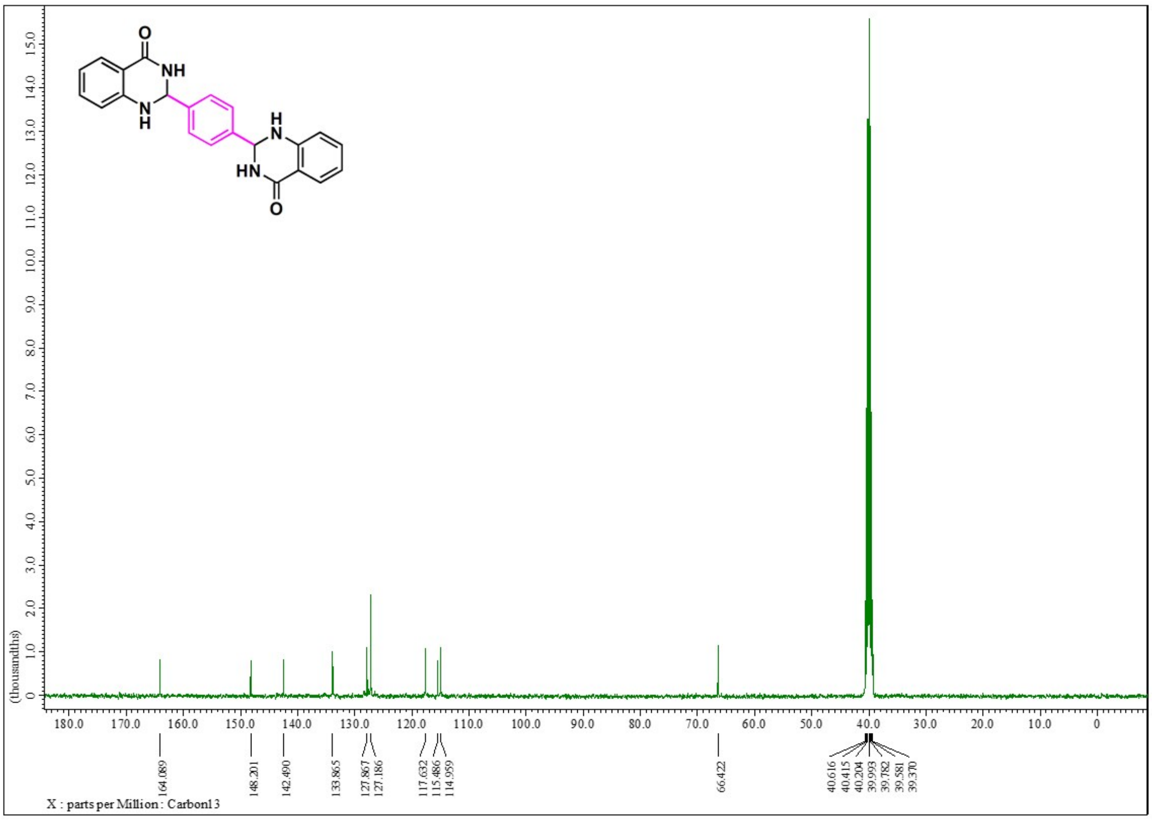

NH
N
H
N
N
N
N
Cl
Cl
X : parts per Million : 1H
abundance


NH
N
H
N
N
N
N
Cl
Cl
X : parts per Million : 13C
abundance


X : parts per Million : Proton
abundance


X : parts per Million : Carbon13
(thousandths)

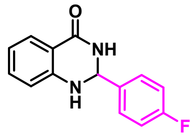

abundance
X : parts per Million : Proton
8.326
7.553
7.537
7.432
7.205
7.186
7.167
7.116
6.694
6.673
6.632
6.613
6.595
5.693
3.329
2.464
2.459
2.455


(thousandths)
X : parts per Million : Carbon13
164.089
148.201
142.490
133.865
127.867
127.186
117.632
115.486
114.959
66.422
40.616
40.415
40.204
39.993
39.782
39.581
39.370

5. Mass spectra of some selected compounds

Qualitative Compound Report

Data File	QC-15.d	**Sample Name**	QC-15
Sample Type	Sample	**Position**	P1-A8
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	05-08-2019 14:03:09
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			



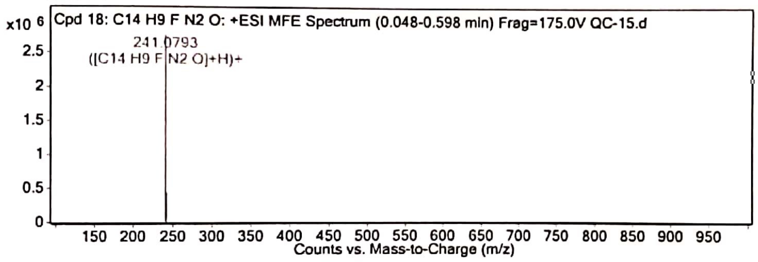
Sample Group		**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)	

Compound Table

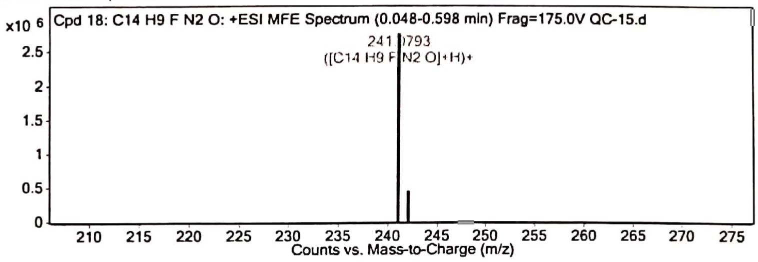
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 18: C14 H9 F N2 O	0.109	240.072	C14 H9 F N2 O	C14 H9 F N2 O	-8.81	C14 H9 F N2 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 18: C14 H9 F N2 O	241.0793	0.109	Find by Molecular Feature	240.072

MFE MS Spectrum



MFE MS Zoomed Spectrum



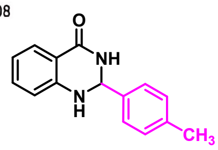
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
241.0793	1	2761729.5	C14 H9 F N2 O	(M+H)+
242.0823	1	438520.15	C14 H9 F N2 O	(M+H)+

--- End Of Report ---

Qualitative Compound Report

Data File	QC-8.d	**Sample Name**	QC-8
Sample Type	Sample	**Position**	P1-B7
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	29-07-2019 12:10:08
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			



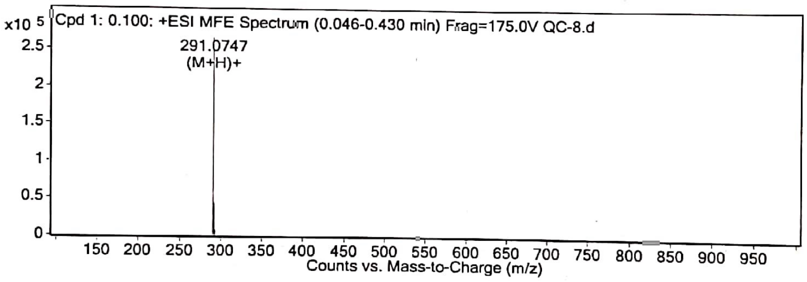
Sample Group		**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)	

Compound Table

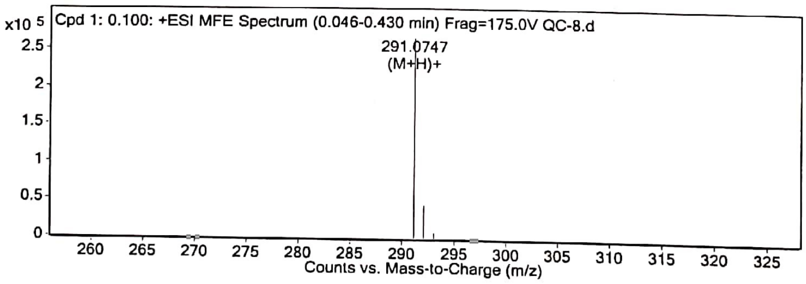
Compound Label	RT	Mass	Formula	MFG Formula	DB Formula
Cpd 1: 0.100	0.1	290.0676	C13 H6 N8 O	C13 H6 N8 O	C13 H6 N8 O

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: 0.100	291.0747	0.1	Find by Molecular Feature	290.0676

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

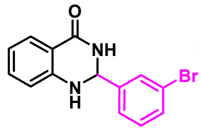
m/z	z	Abund	Ion
291.0747	1	264994.72	(M+H)+
292.0775	1	44133.07	(M+H)+
293.0835	1	8402.72	(M+H)+

--- End Of Report ---

Qualitative Compound Report

Data File	QC-16.d	**Sample Name**	QC-16
Sample Type	Sample	**Position**	P1-D6
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	17-07-2019 17:15:22
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group		**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.1)	

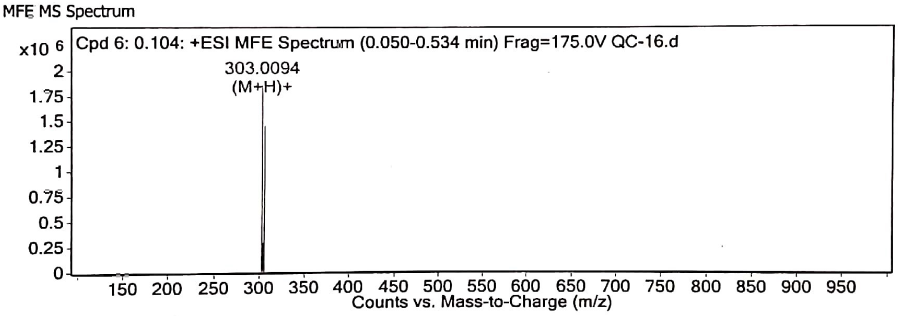


Compound Table

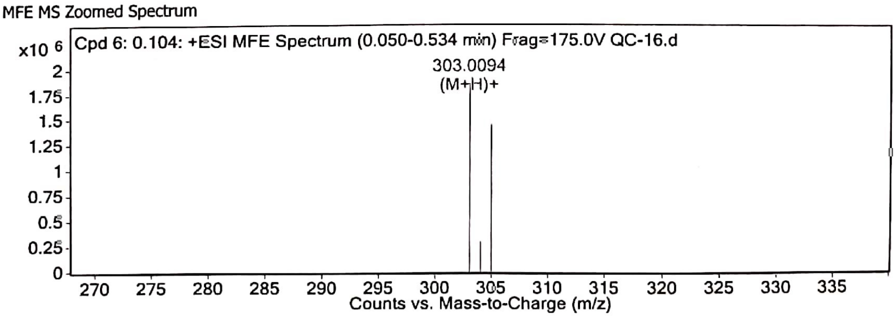
Compound Label	RT	Mass	MFG Formula
Cpd 6: 0.104	0.104	302.0021	<none>

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 6: 0.104	303.0094	0.104	Find by Molecular Feature	302.0021

MFE MS Spectrum



MFE MS Zoomed Spectrum



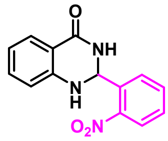
MS Spectrum Peak List

m/z	z	Abund	Ion
303.0094	1	1858237.38	(M+H)+
304.0124	1	289825.91	(M+H)+
305.0109	1	1453844.52	(M+H)+

--- End Of Report ---

Qualitative Compound Report

Data File	QC-3.d	**Sample Name**	QC-3
Sample Type	Sample	**Position**	P1-D1
Instrument Name	Instrument 1	**User Name**	
Acq Method	Damo JK.m	**Acquired Time**	14-06-2019 13:28:58
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			



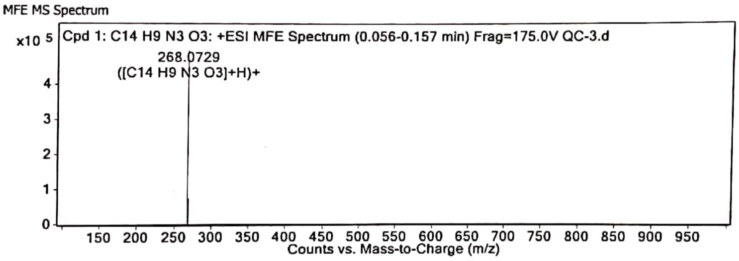
Sample Group		**Info.**
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125.1)	

Compound Table

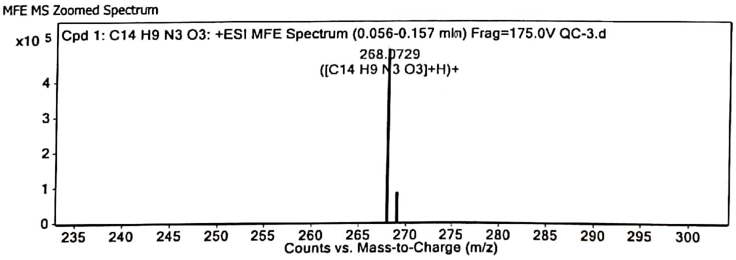
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C14 H9 N3 O3	0.091	267.0656	C14 H9 N3 O3	C14 H9 N3 O3	-4.4	C14 H9 N3 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C14 H9 N3 O3	268.0729	0.091	Find by Molecular Feature	267.0656

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
268.0729	1	497907.19	C14 H9 N3 O3	(M+H)+
269.0757	1	74185.73	C14 H9 N3 O3	(M+H)+

--- End Of Report ---

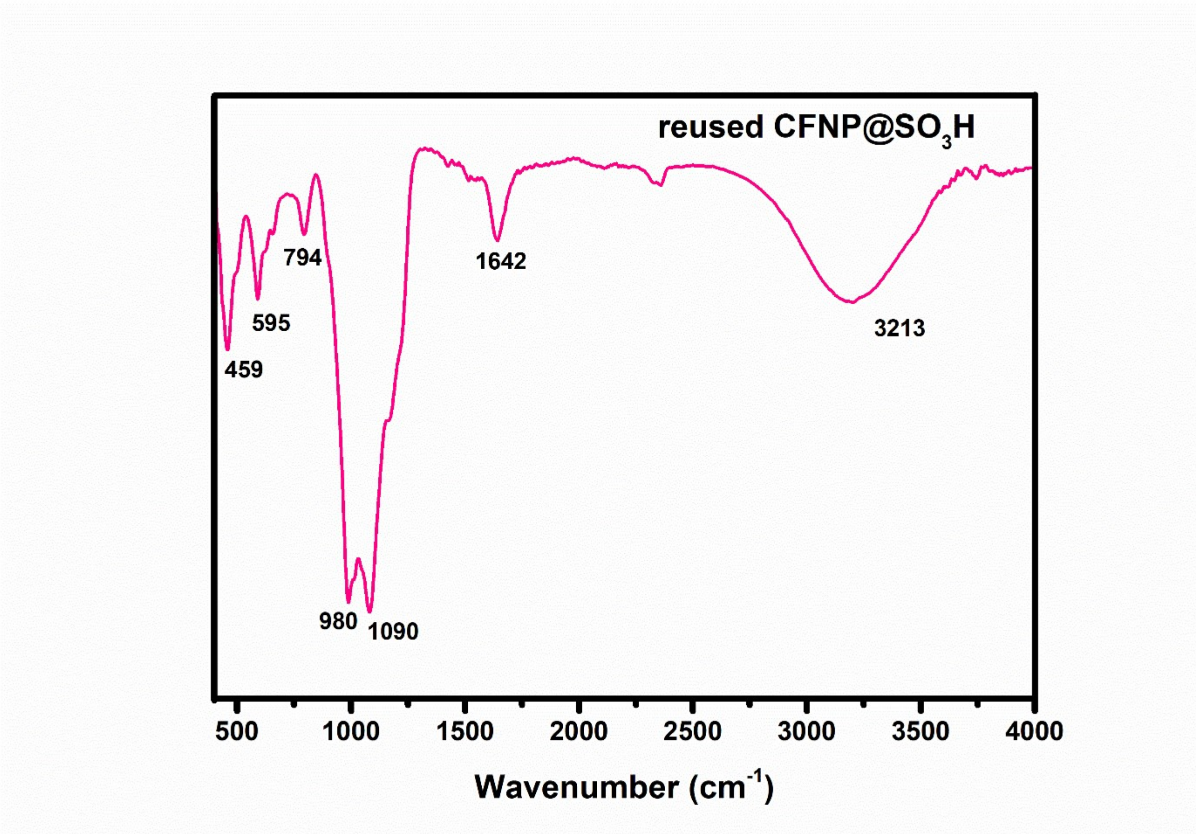


Figure S1: FT-IR spectra of reused catalyst (reused CFNP@SO_3H) after 6 serial runs.

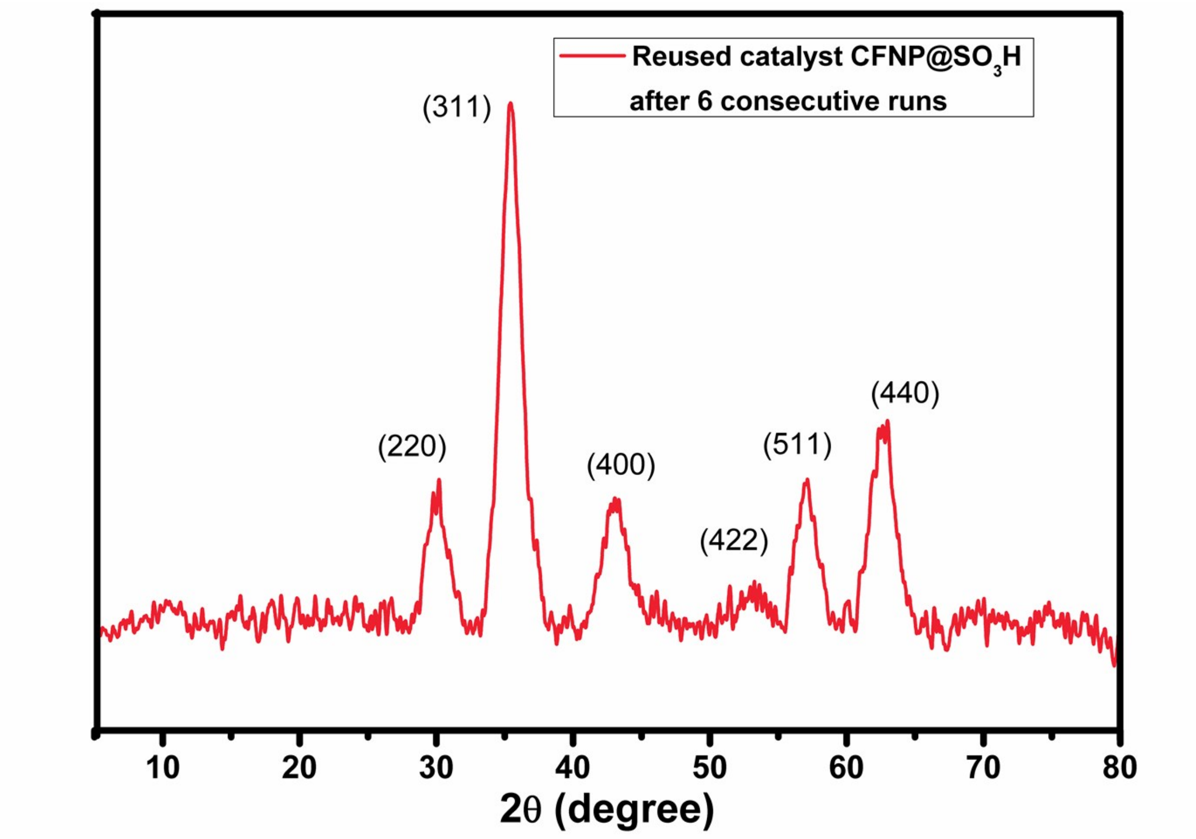


Figure S2: Powder XRD analysis of reused catalyst (reused CFNP@SO_3H) after 6 serial runs.

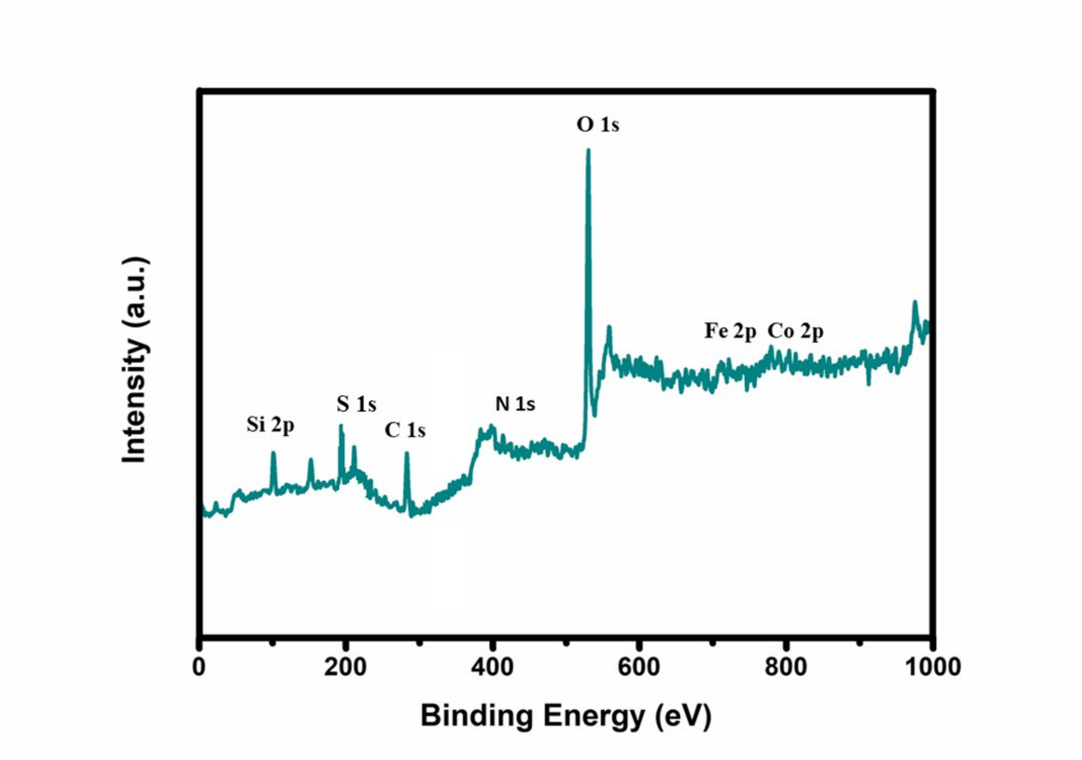


Figure S3: XPS survey spectra of catalyst (CFNP@SO_3H).

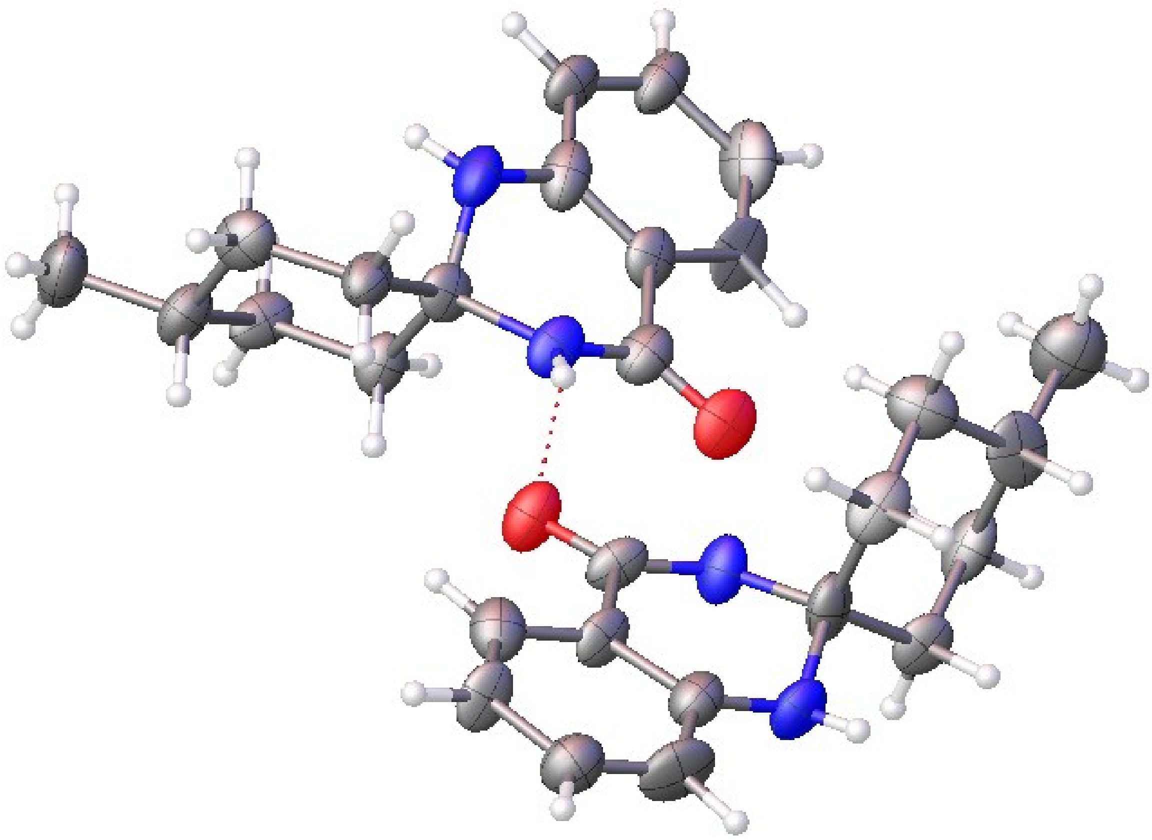


Figure S4: Crystal structure of compound 5e showing H-bonding.

Calculation of the Turn over frequency (TOF) of catalyst

1000 mg (1 g) catalyst (CFNP@SO3H) contains 2.48 mmol free sulfonic acid.

To determine the turn over number of the catalyst we had tested the synthesis of quinazolinone (3l) by taking 1 mmol of anthranilamide and 1 mmol of benzaldehyde in presence of 18 mg of catalyst at room temperature.

As the yield of product formation is 98%,

The turn over number (**TON**) of 3l is = $\frac{mmol\ of\ product}{mmol\ of\ acid\ site\ present\ in\ catalyst}$

1 g catalyst holds 2.48 mmol of acid site, so 18 mg of catalyst holds = 0.04464 mmol acid sites.

The turn over number is = $\frac{0.98}{0.04464}$ = 21.95 (as the yield of product is 98%, mmol of product = 0.98)

And turn over frequency (**TOF**) of 3l is = $\frac{Turn\ over\ number}{reaction\ time} = \frac{21.95}{4/60}$ h^{-1} = 329.25 h^{-1}

Table S4: Calculation of TOF (h^{-1}) for the synthesized products.

Product	**Yield (%)**	**TOF (h^{-1})**
3a	97	325.94
3b	96	322.58
3c	92	247.31
3d	94	252.69
3e	94	252.69
3f	96	322.58
3g	90	201.61
3h	88	197.13
3i	90	403.23
3j	93	312.50
3k	93	249.99
3l	98	329.25
3m	90	201.61
3n	96	258.06

5a	88	197.13
5b	97	315.86
5c	90	302.42
5d	95	255.37
5e	97	325.94
5f	88	295.70