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Supporting Information

Photophysical, Electrochemical Properties and Temperature Dependent Geometrical Isomerism in Alkyl Quinacridonediimines

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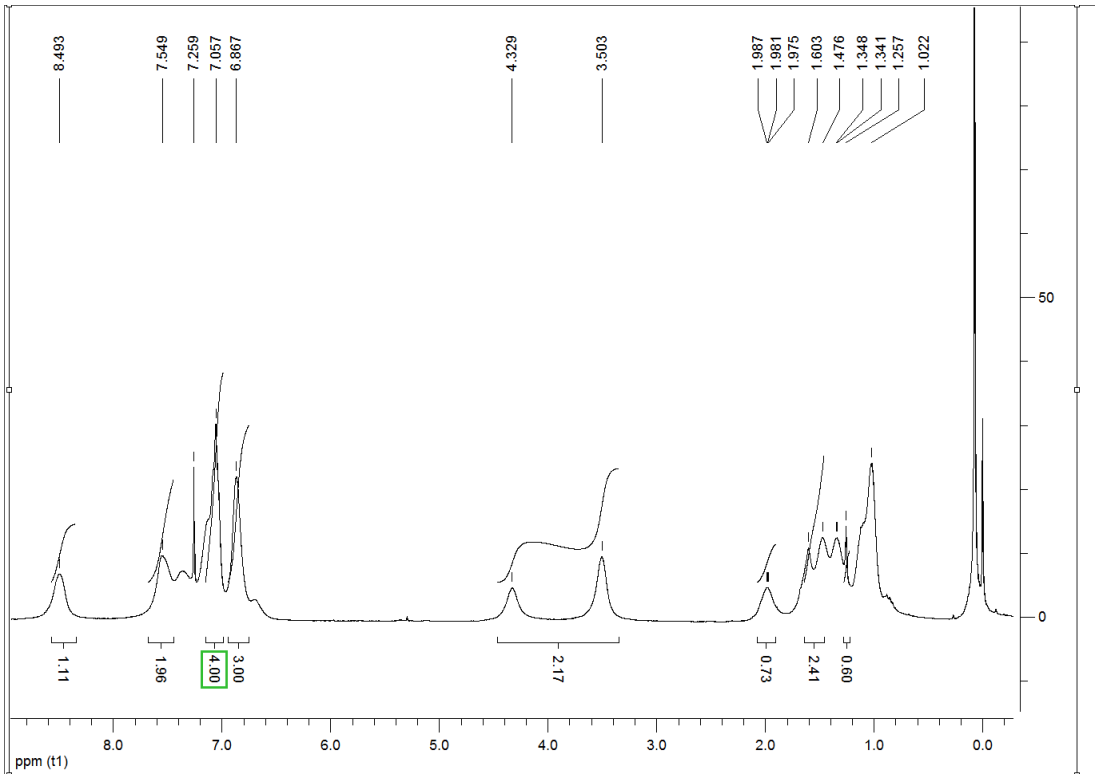
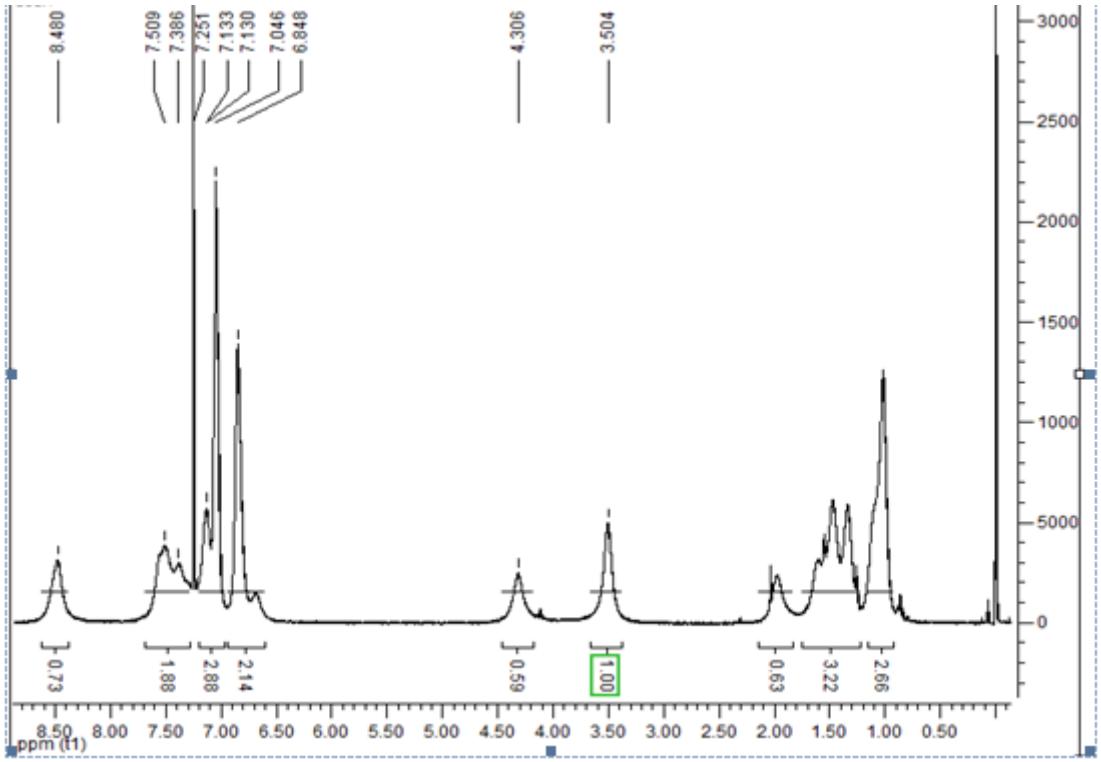
Contents

^{1}H NMR spectrum of Compound **1**



^{1}H NMR spectrum of Compound **2**



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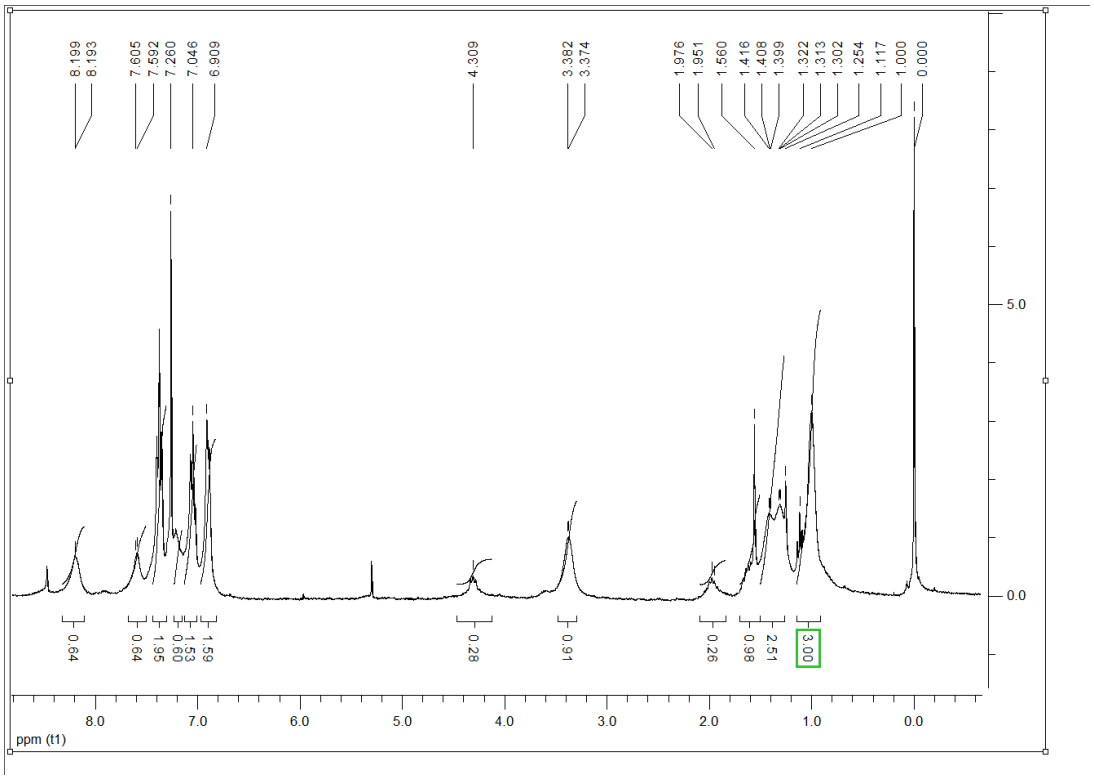

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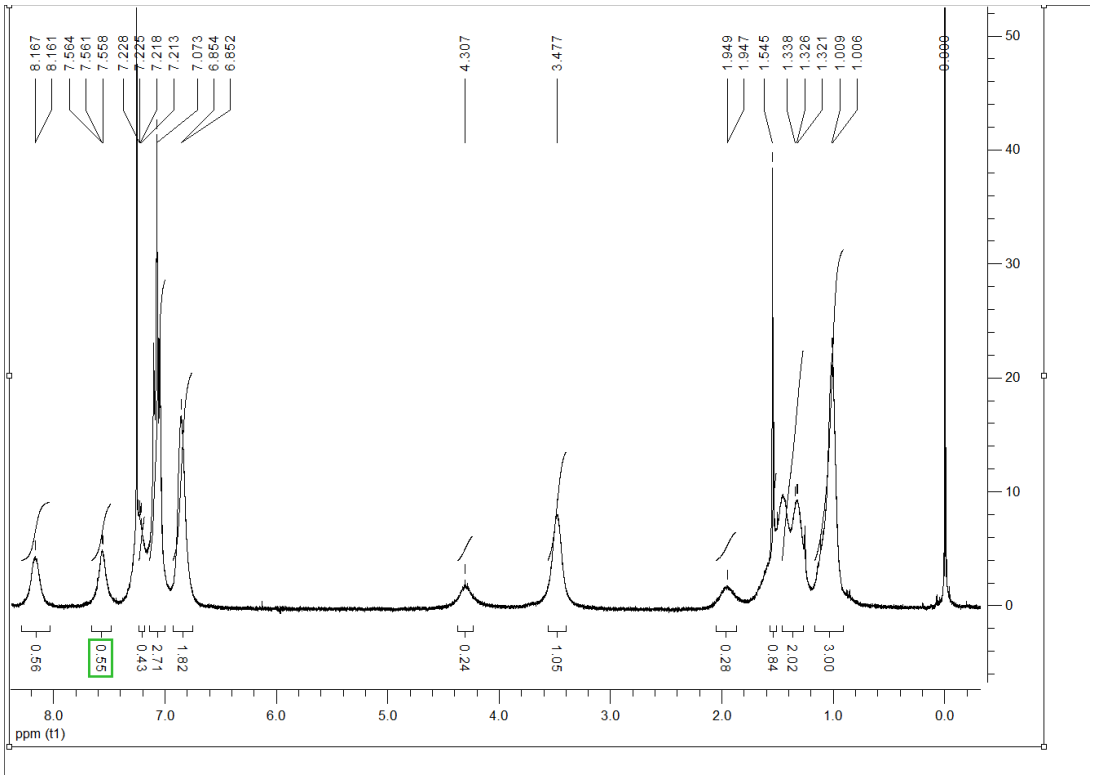
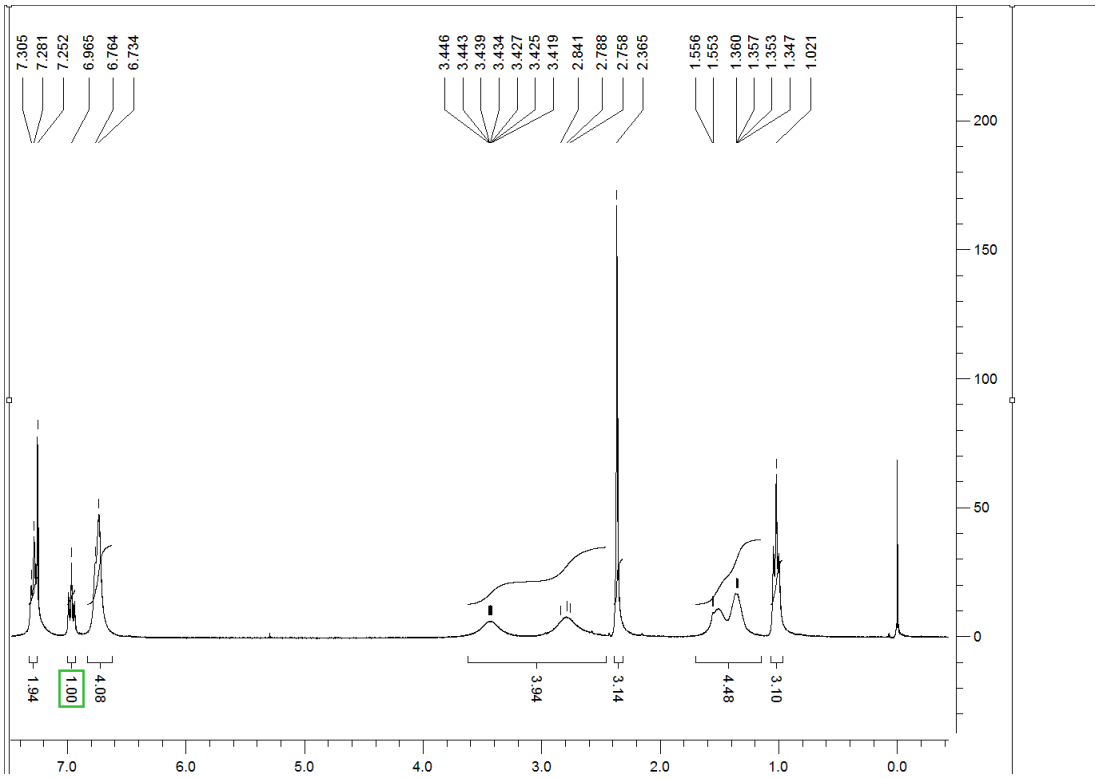


^{1}H NMR spectrum of Compound **5**



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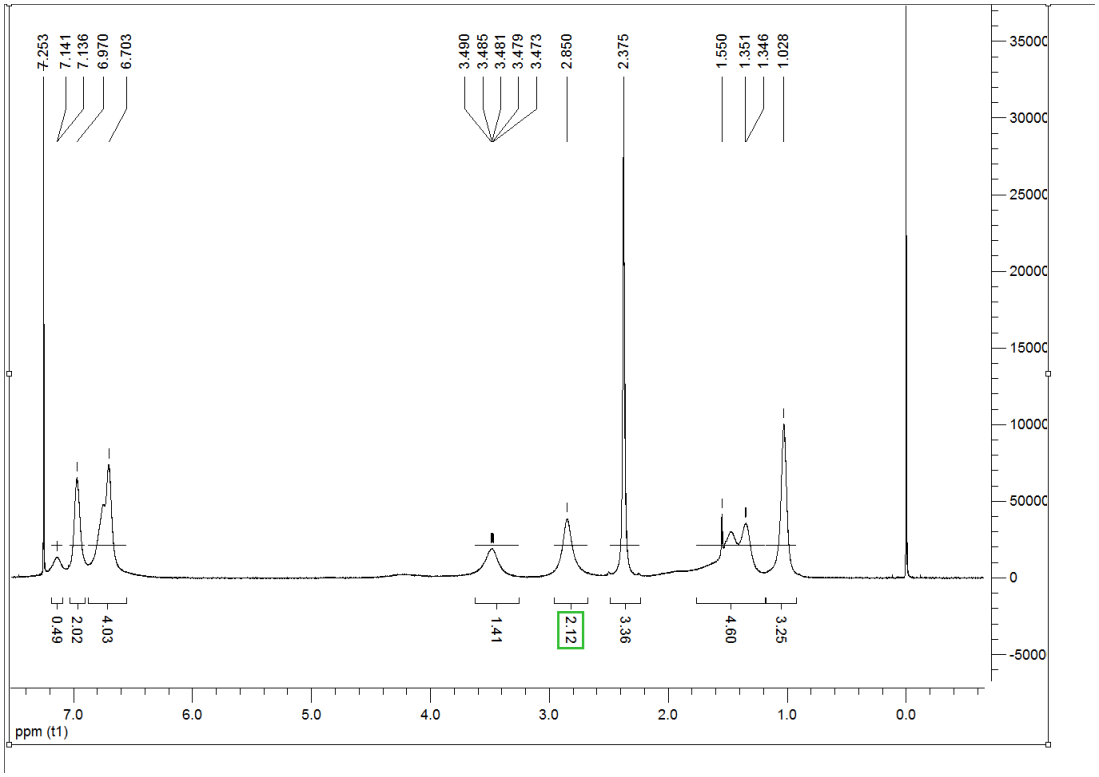

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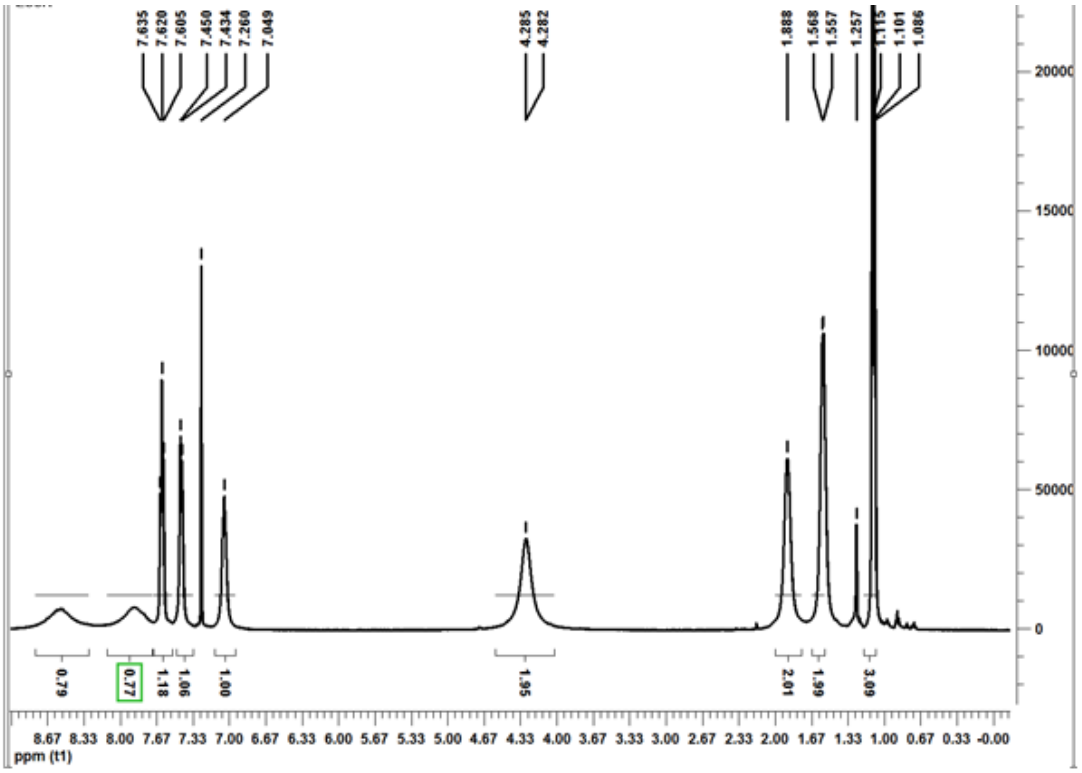

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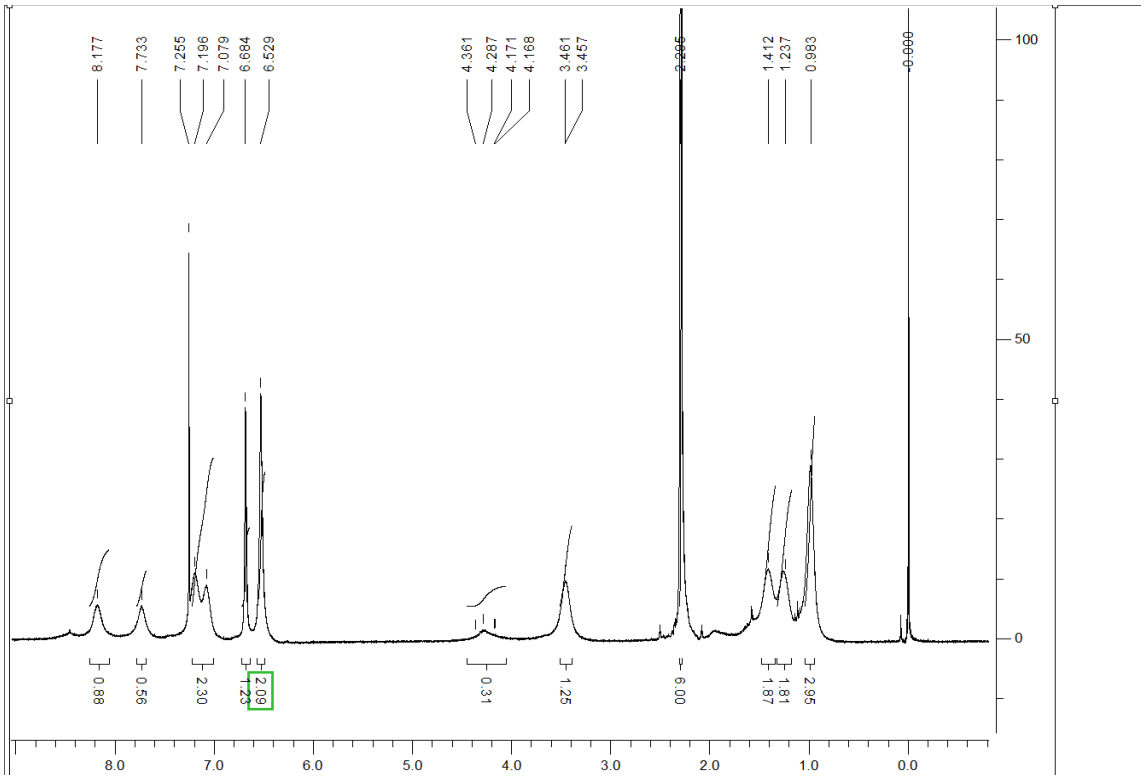

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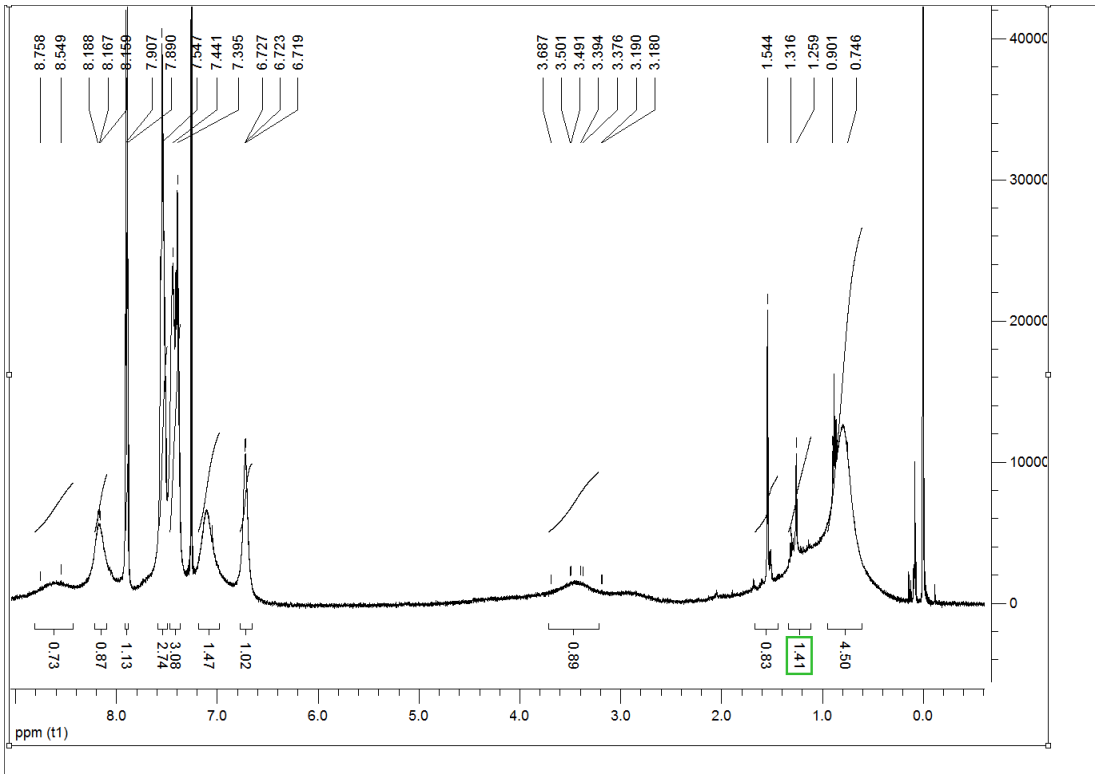

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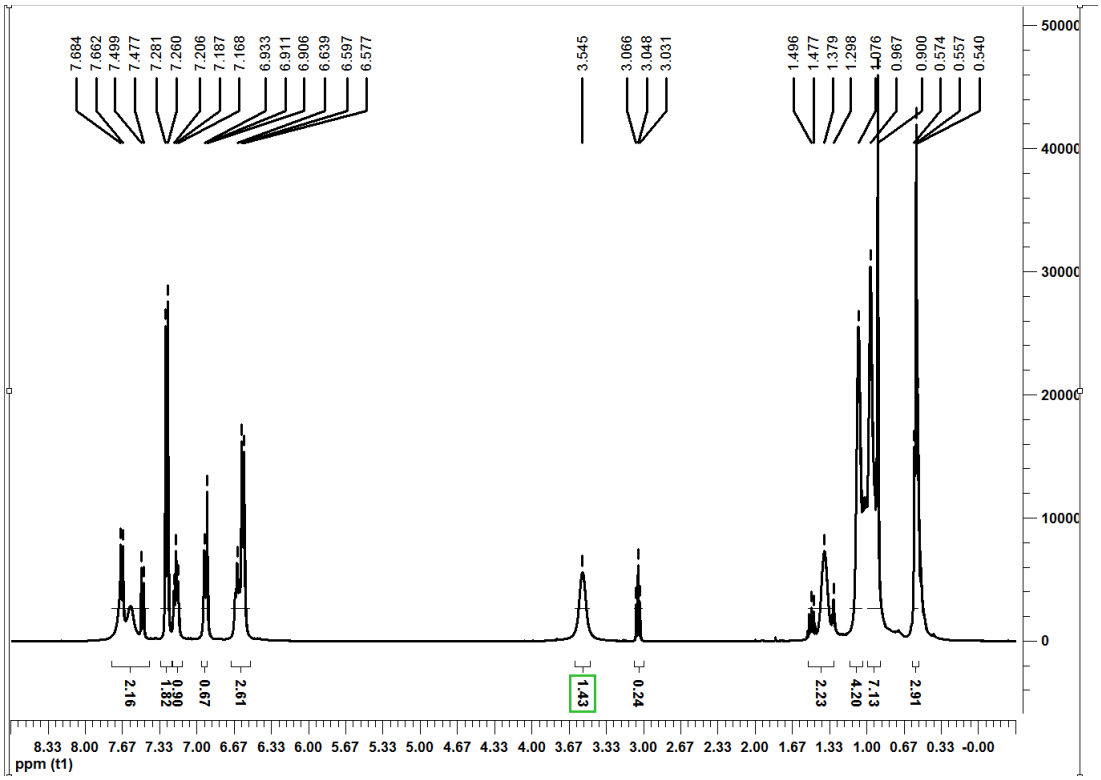
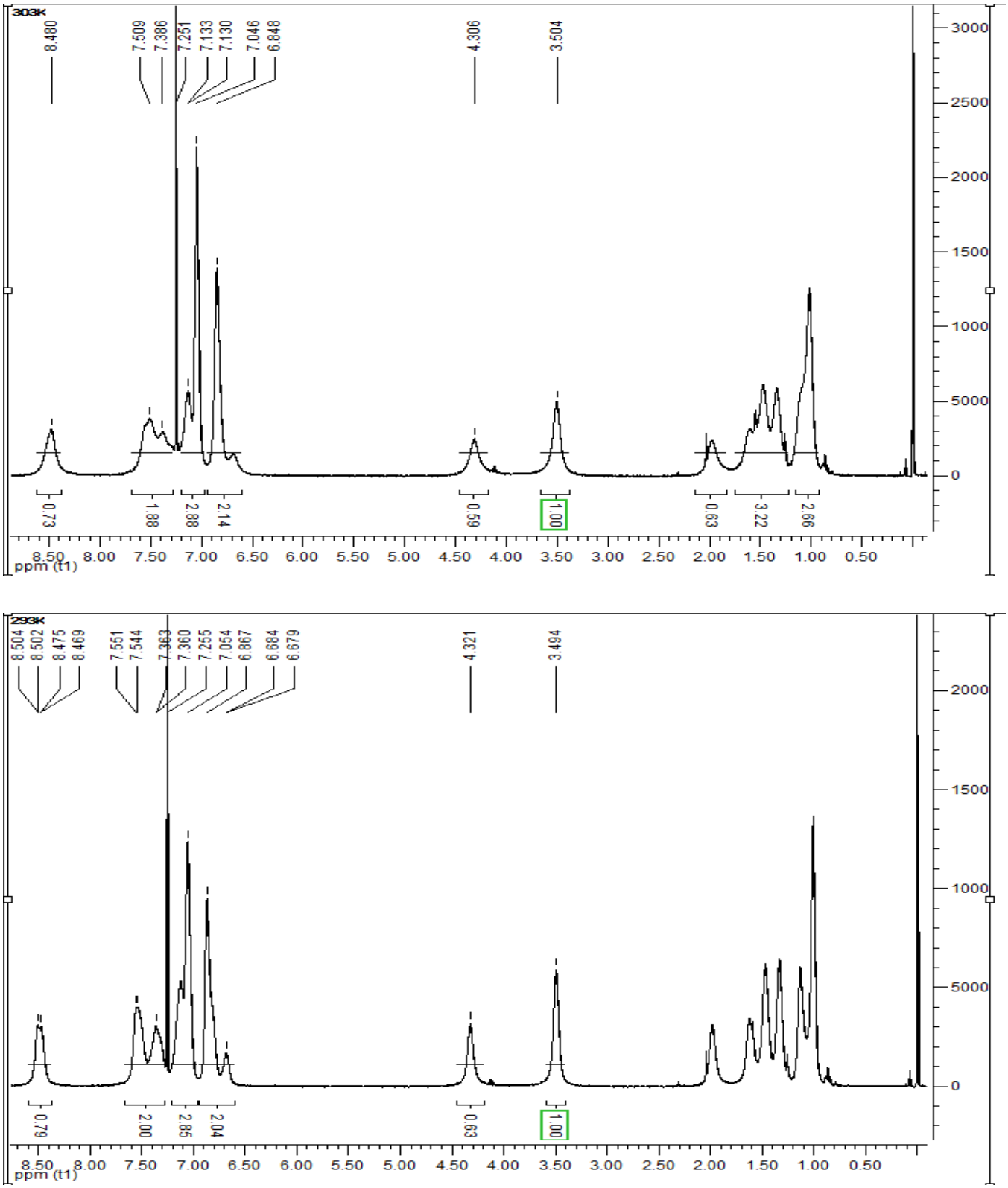
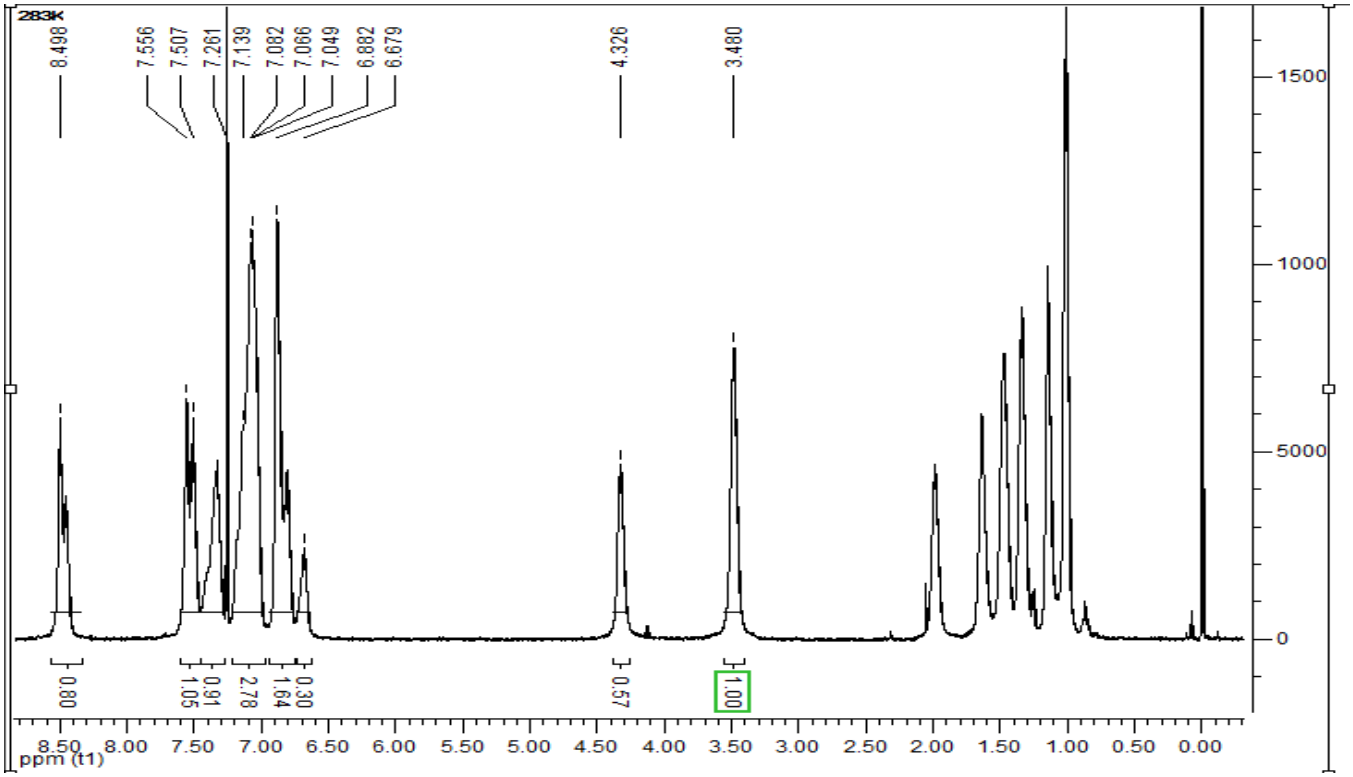
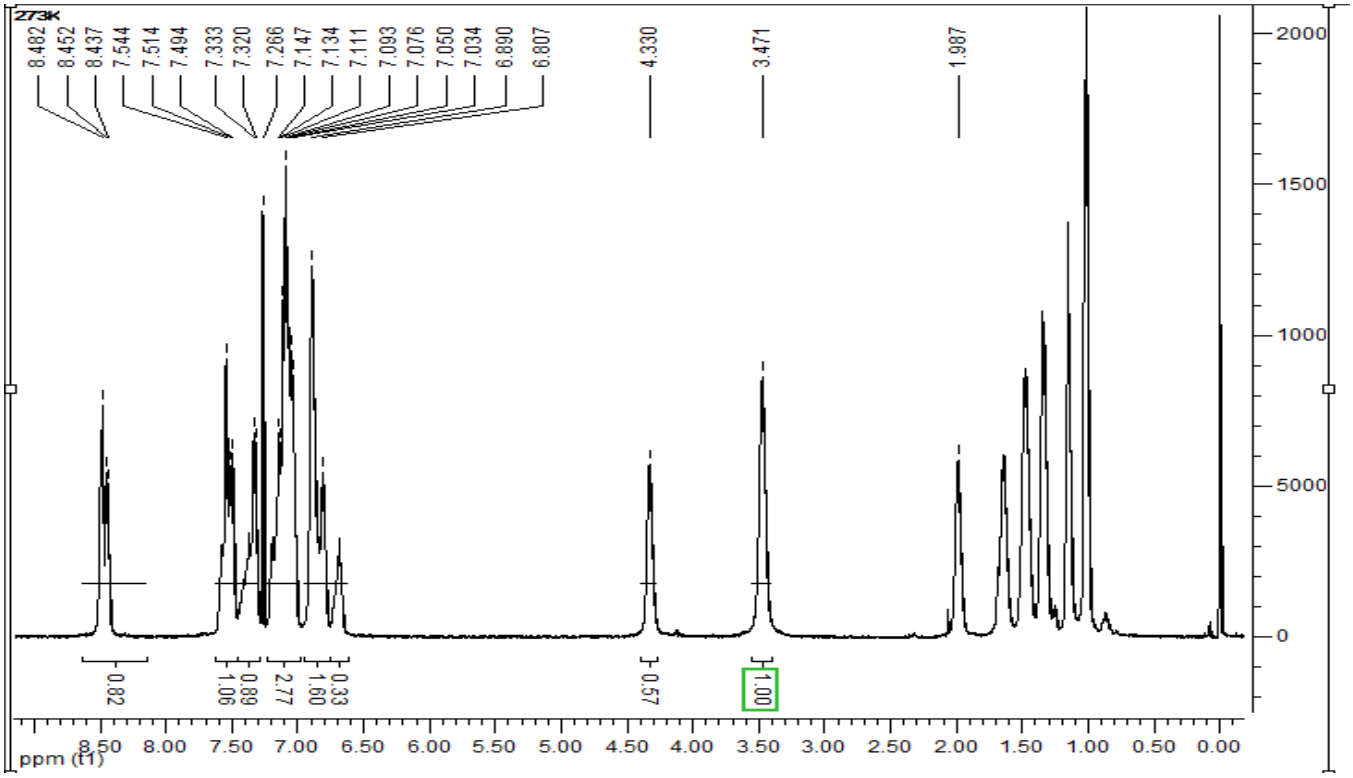
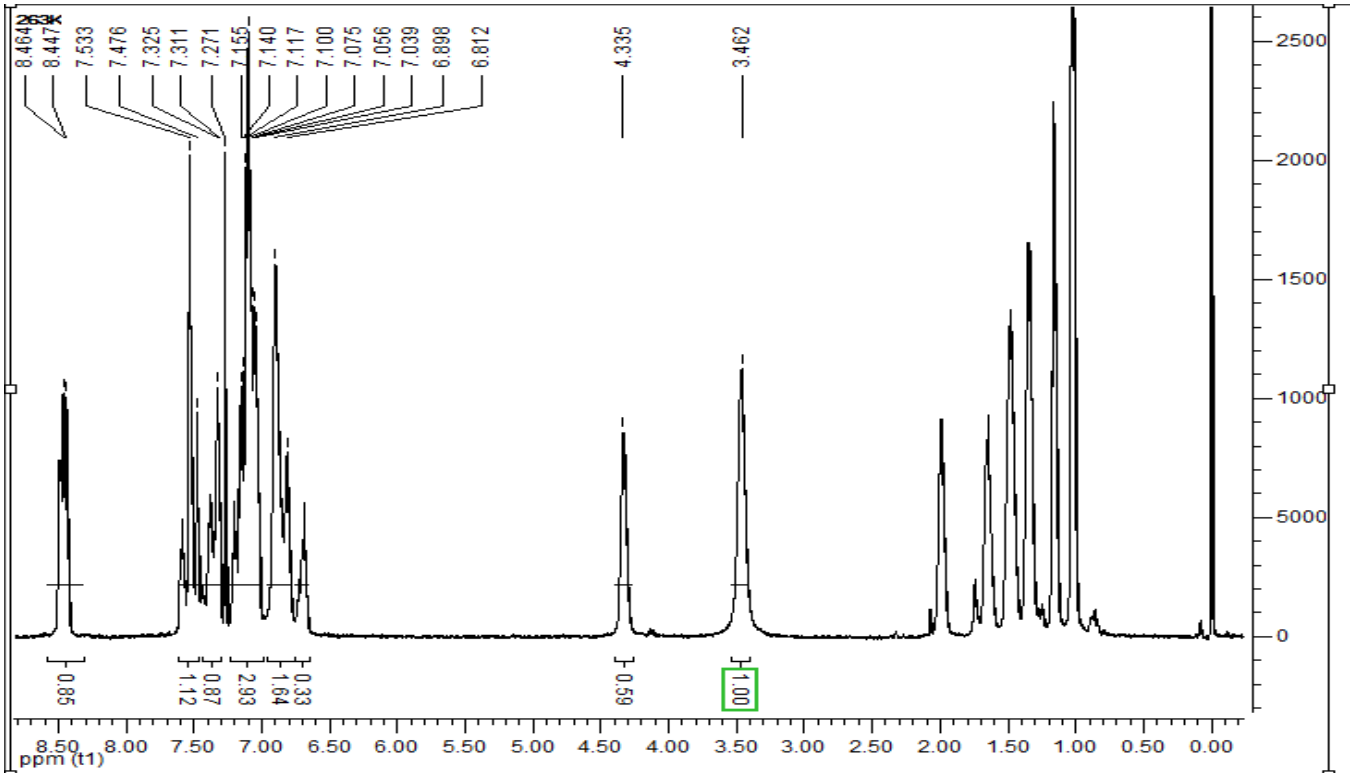


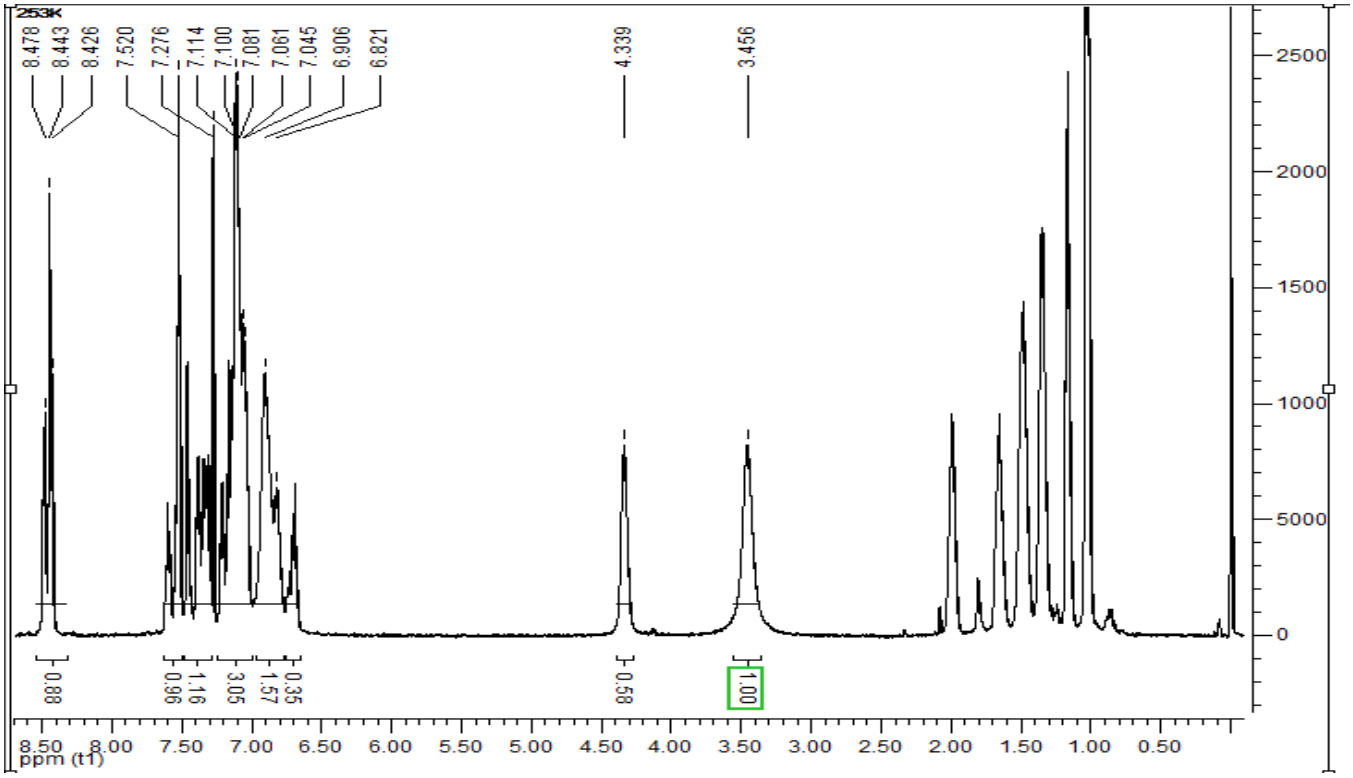
Variable temperature ^{1}HNMR (213K-303K) of **2**

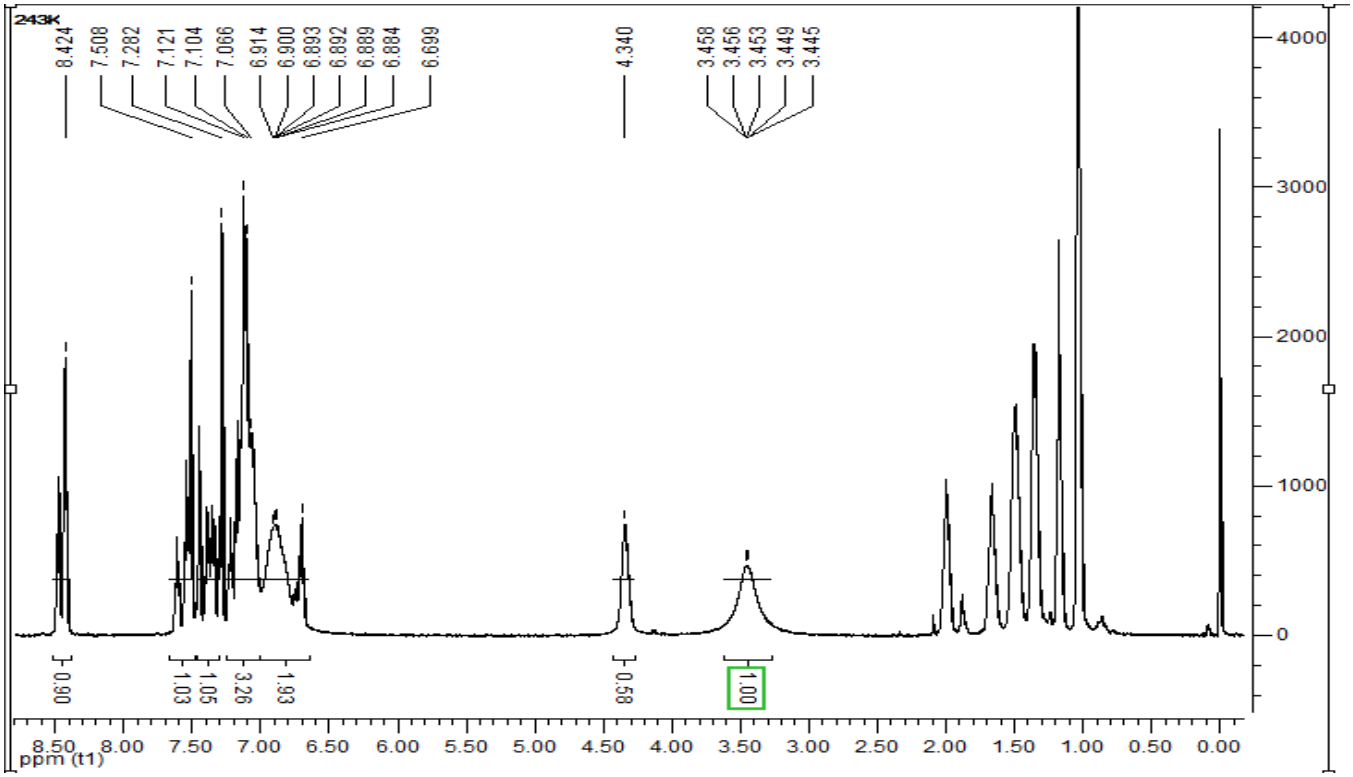


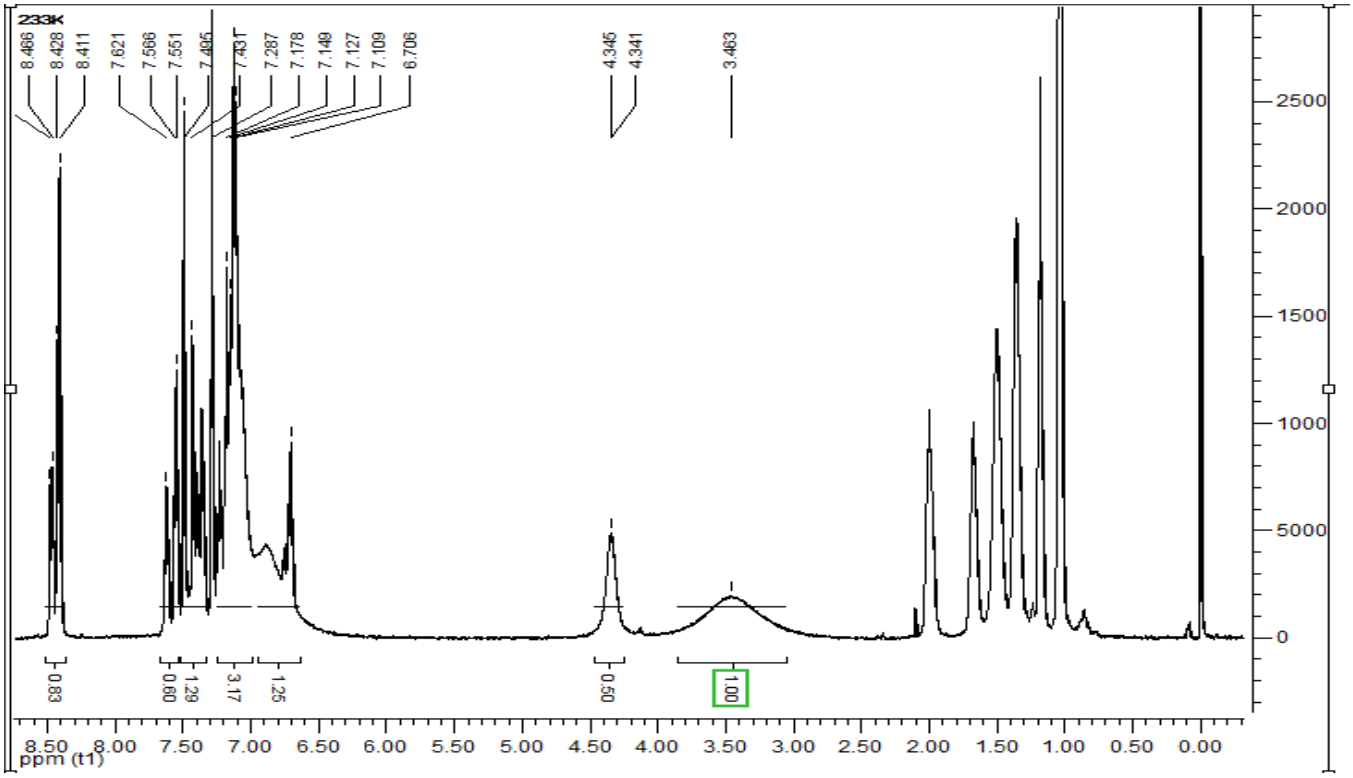


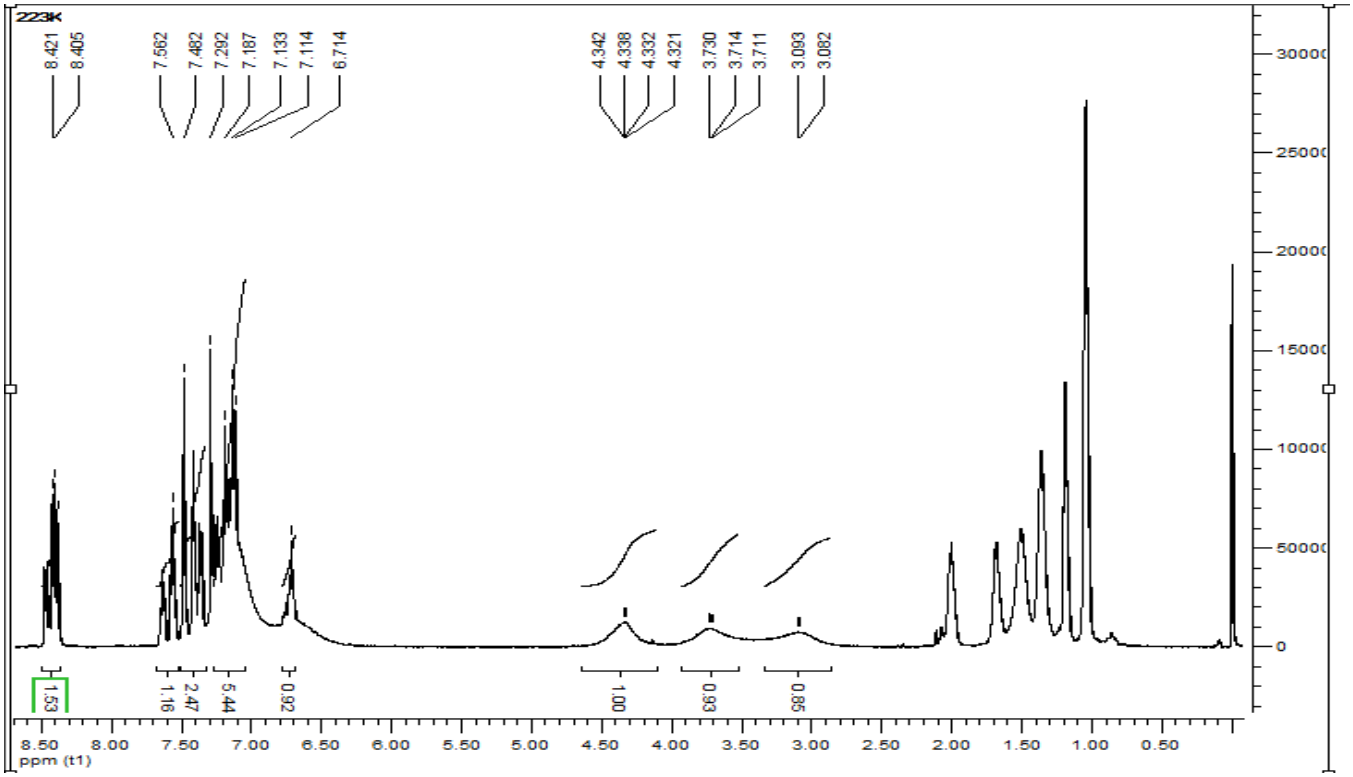


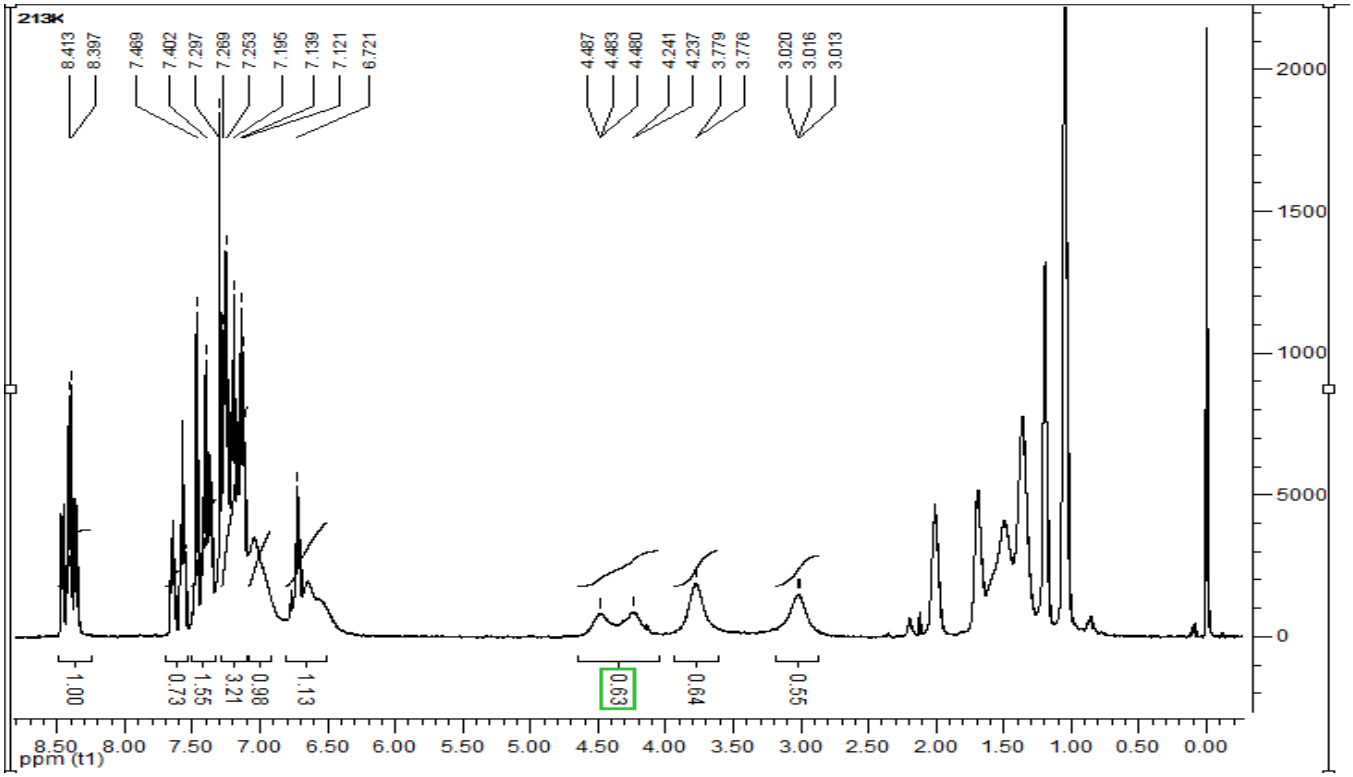




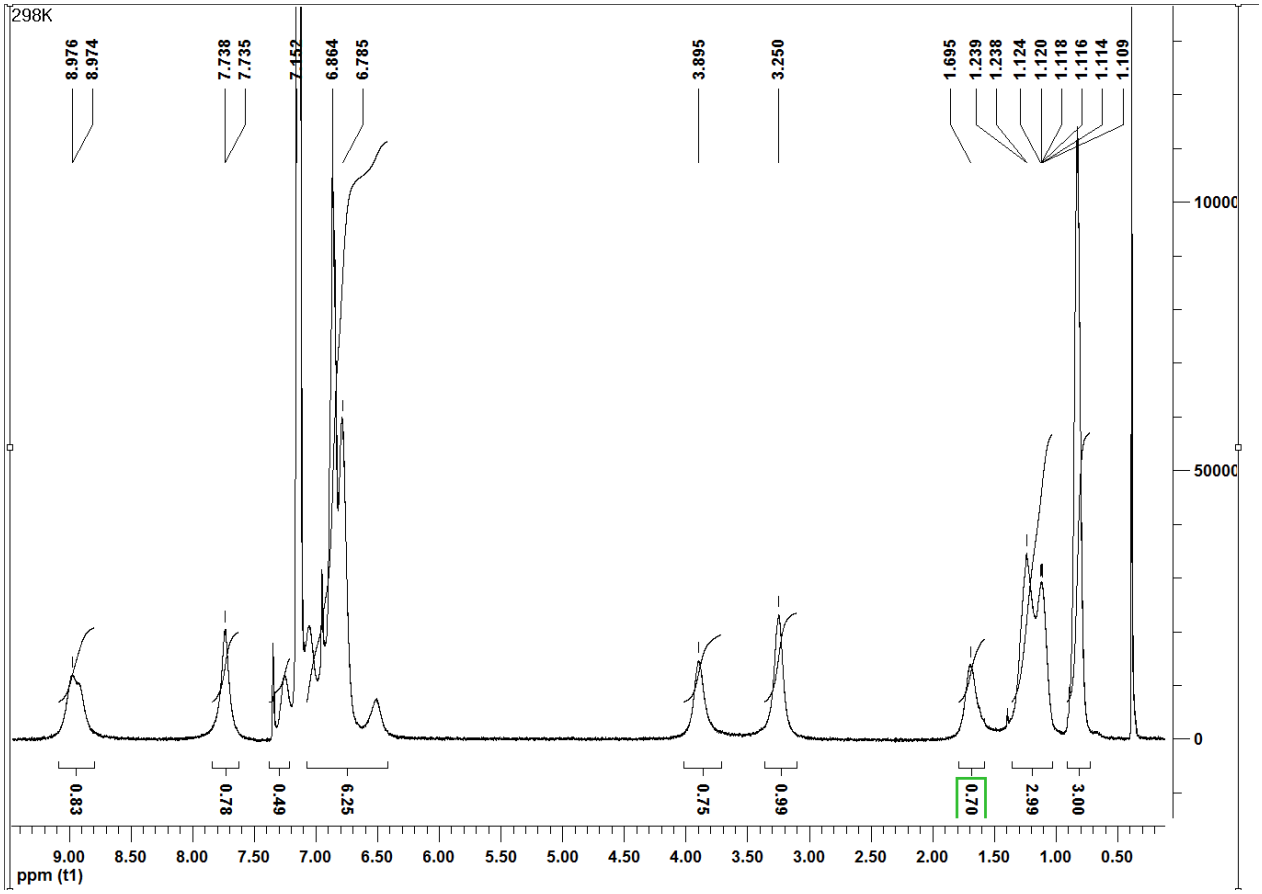


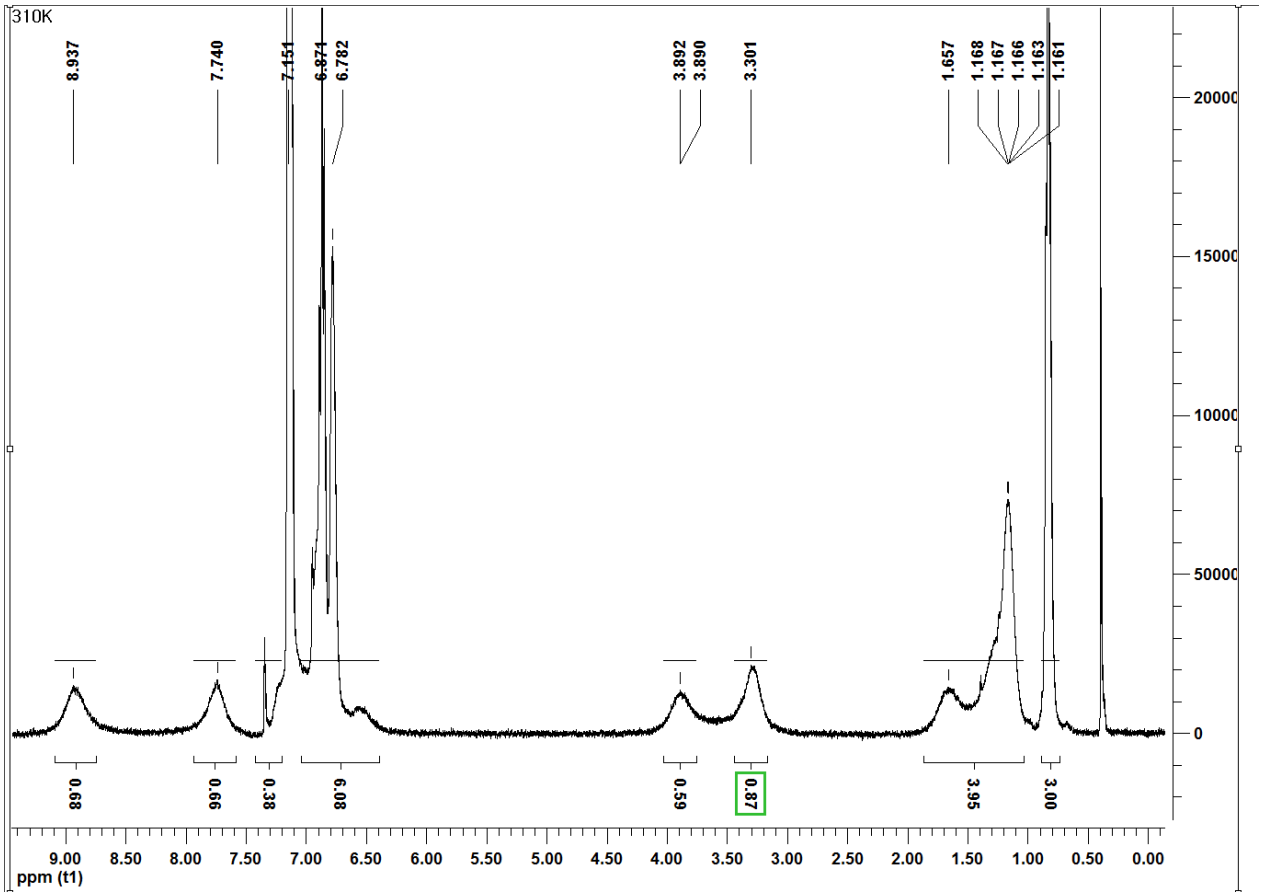


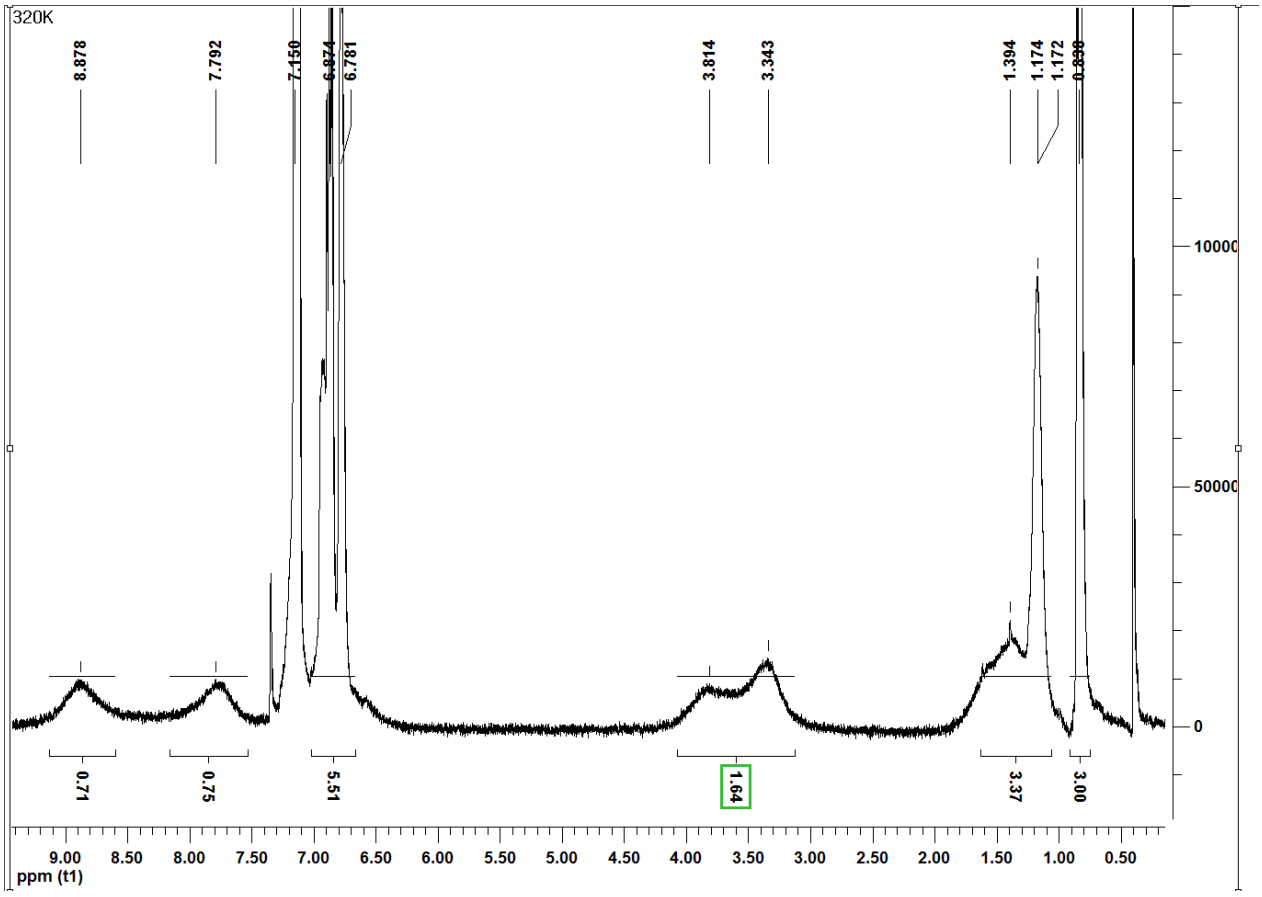


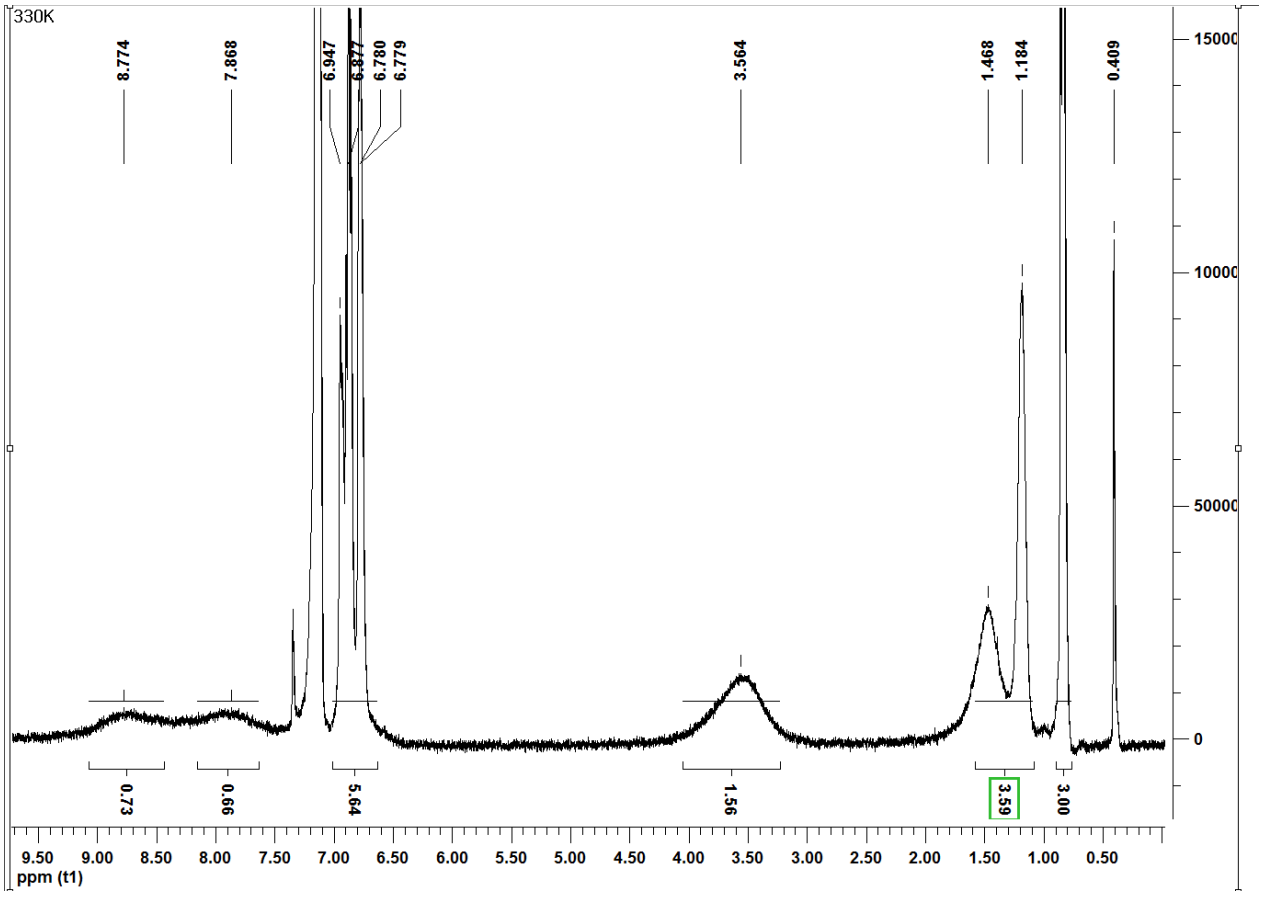


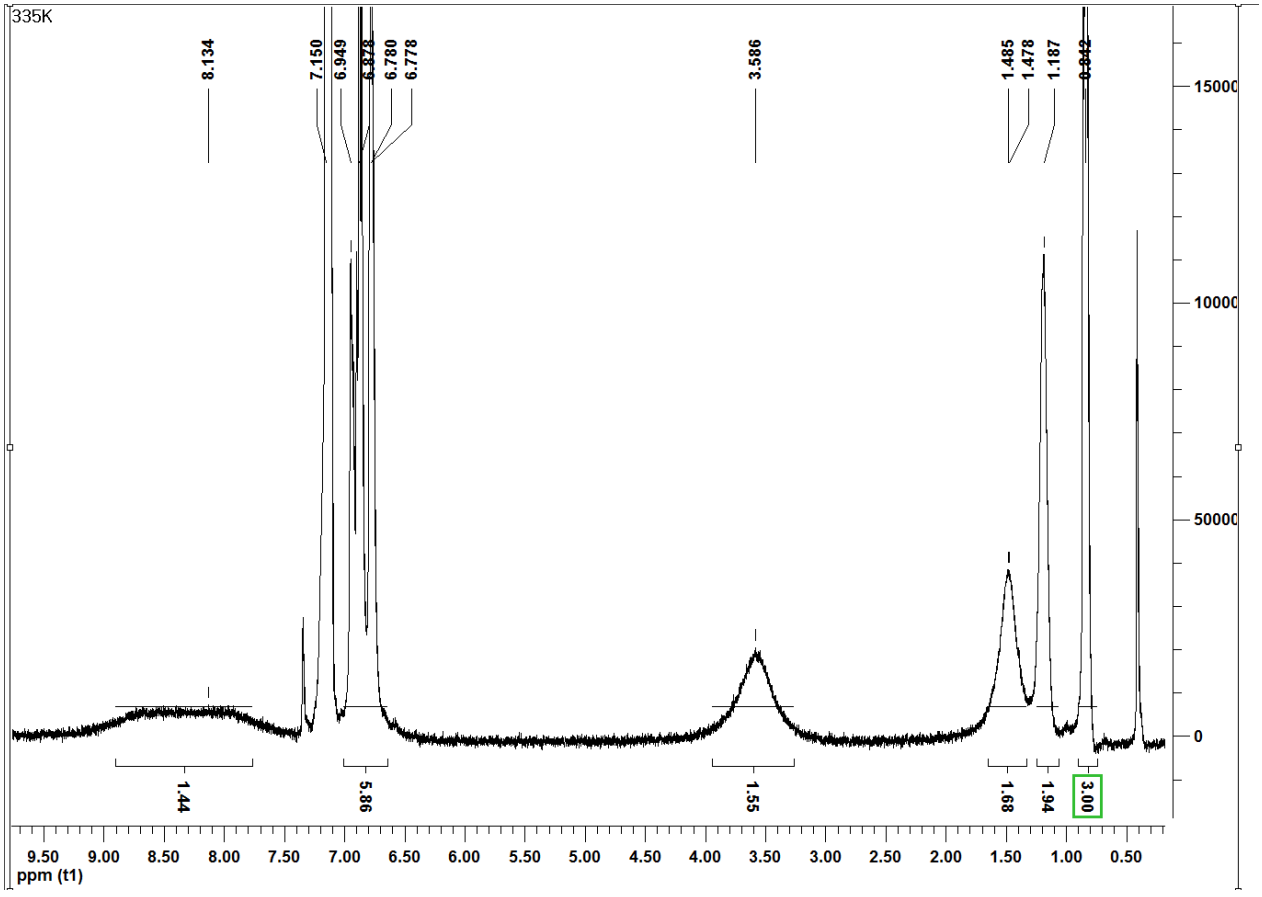
Variable temperature ^{1}HNMR (298-335K) of **2**



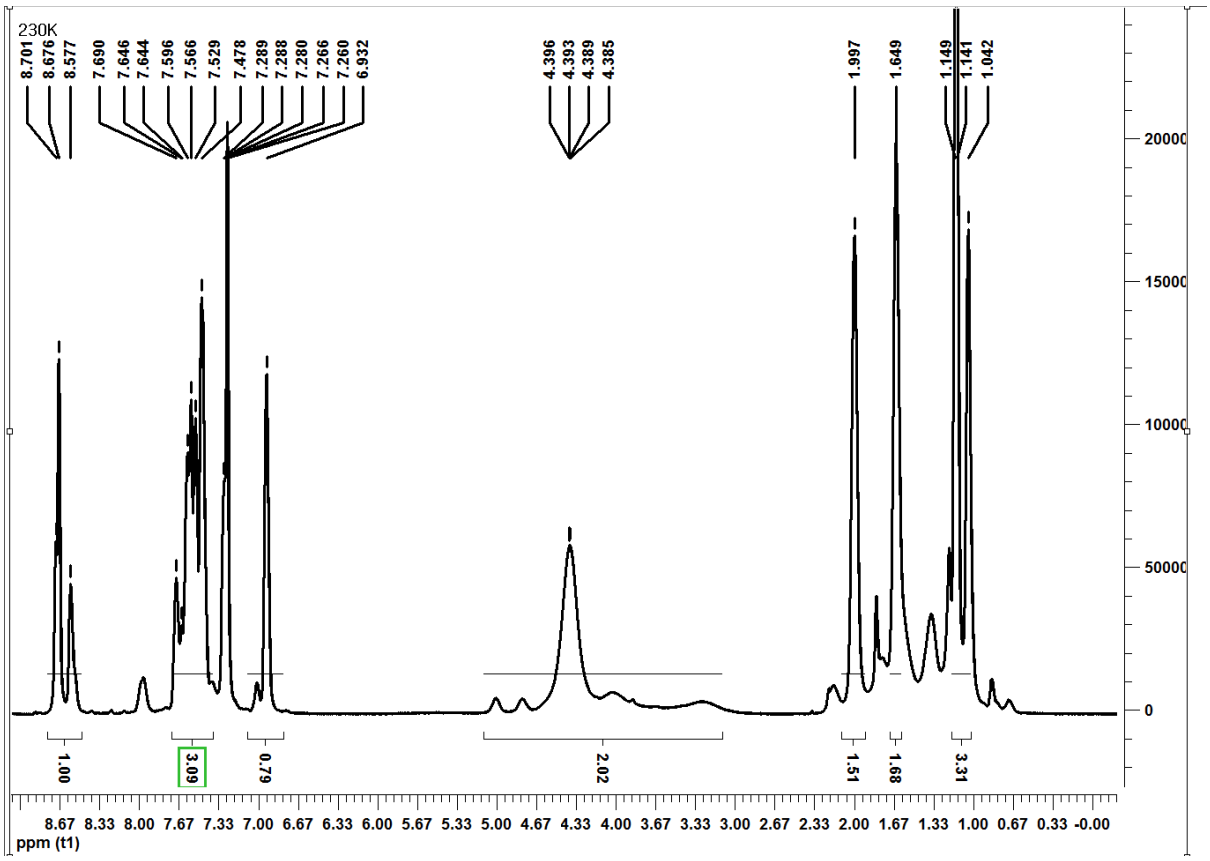


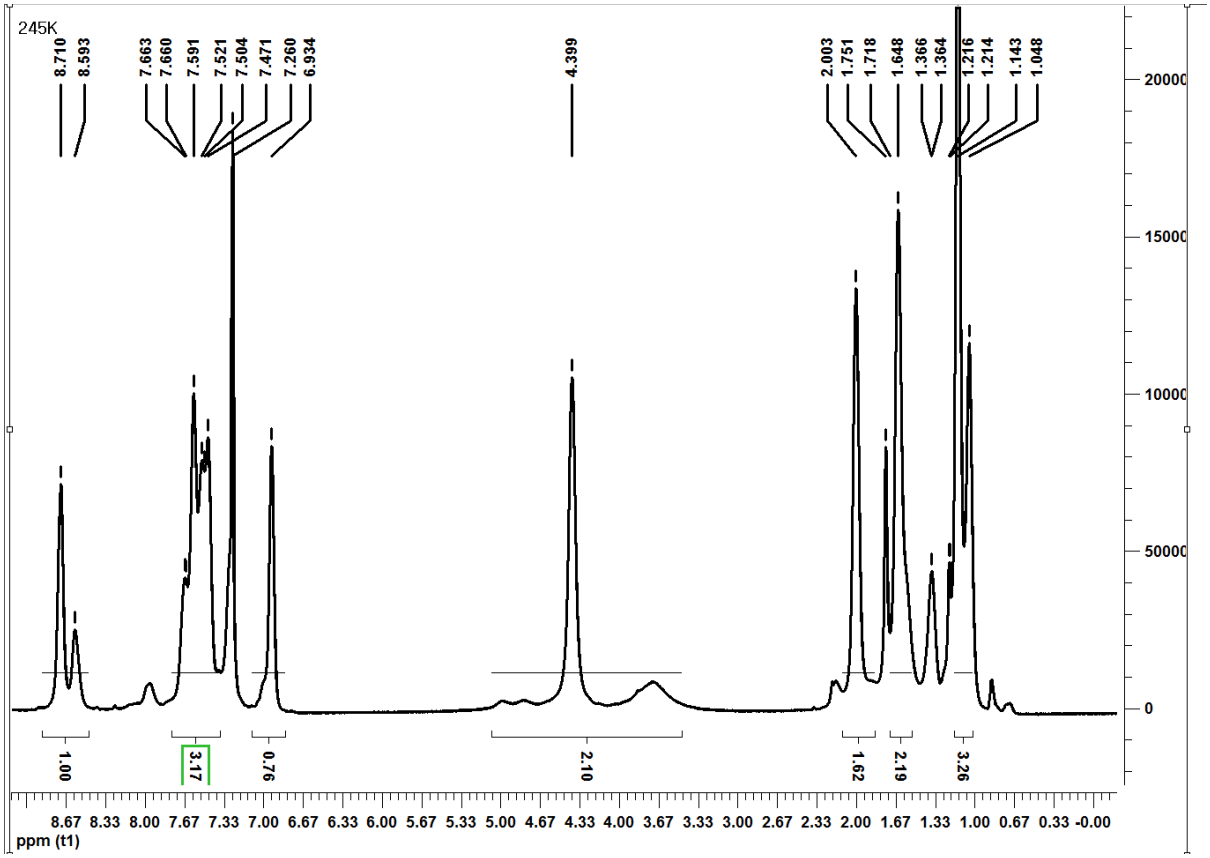


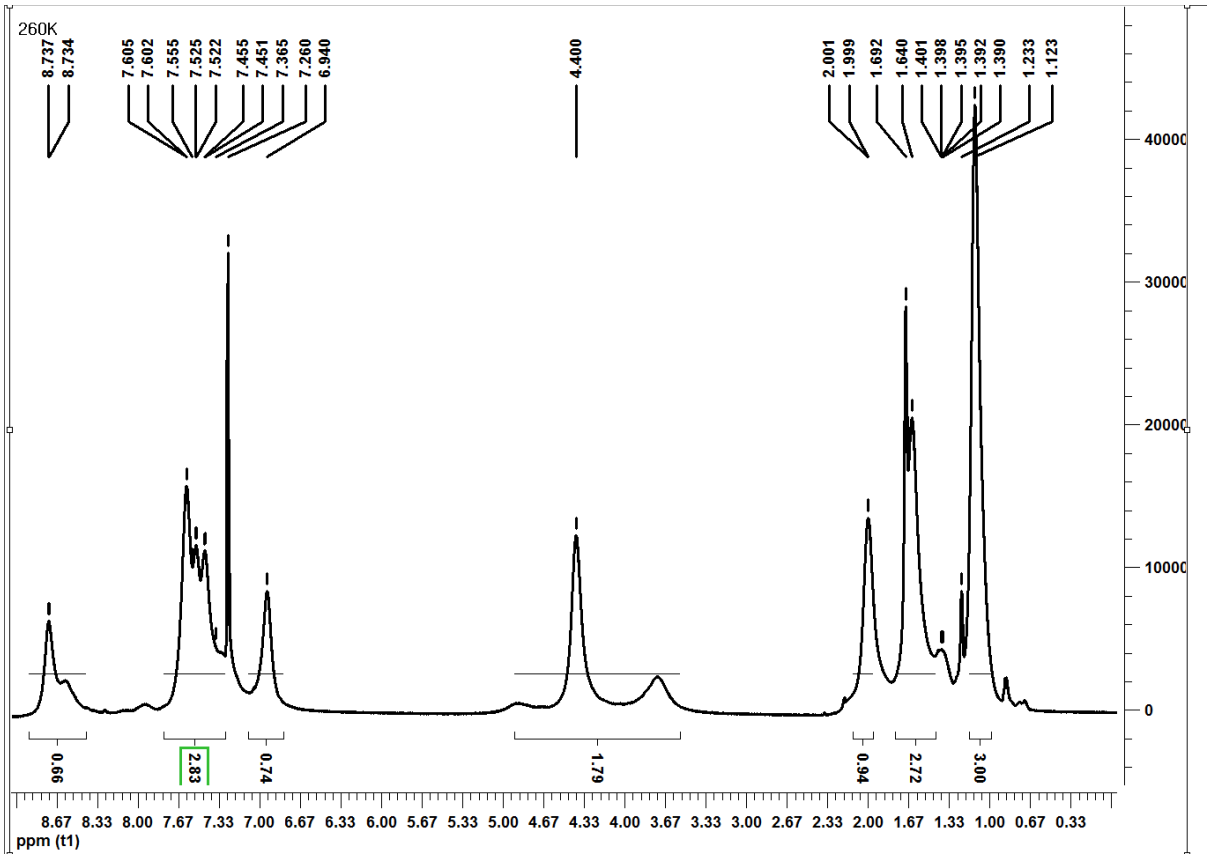


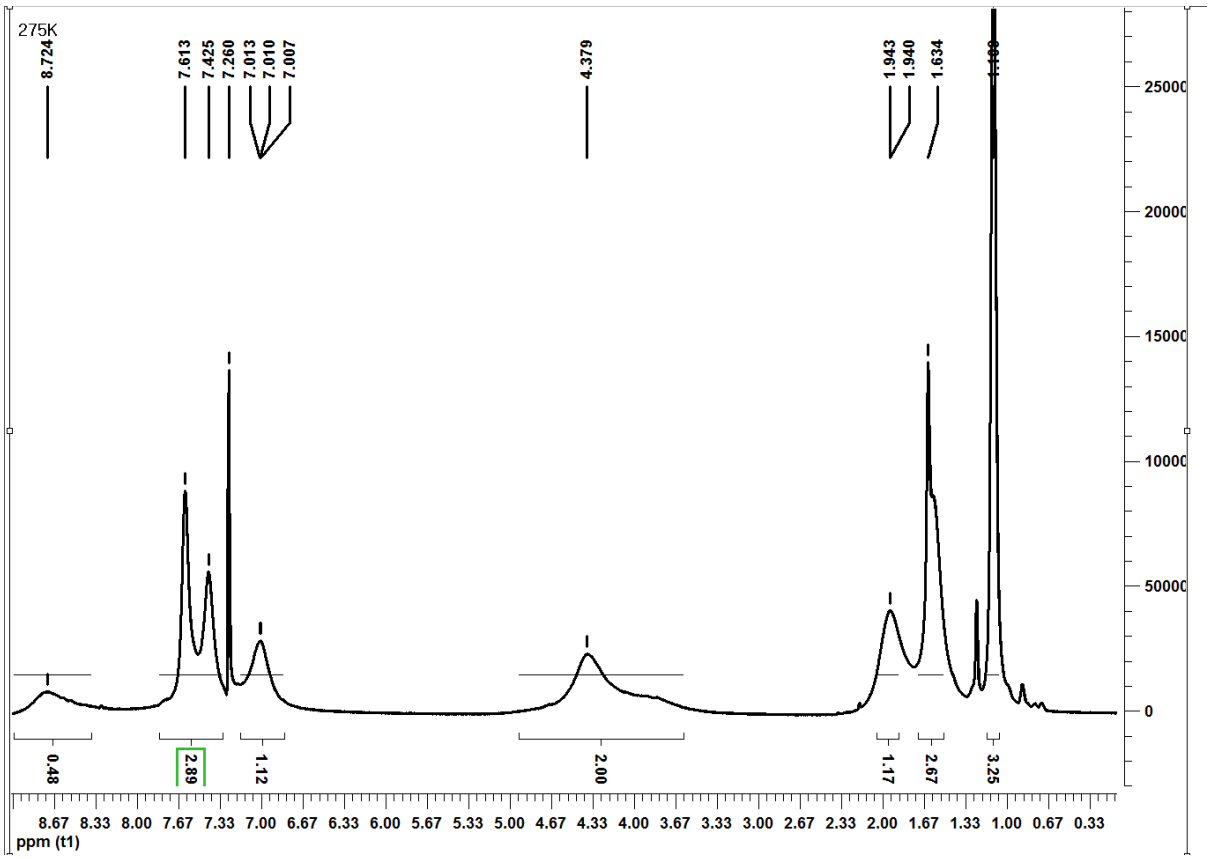


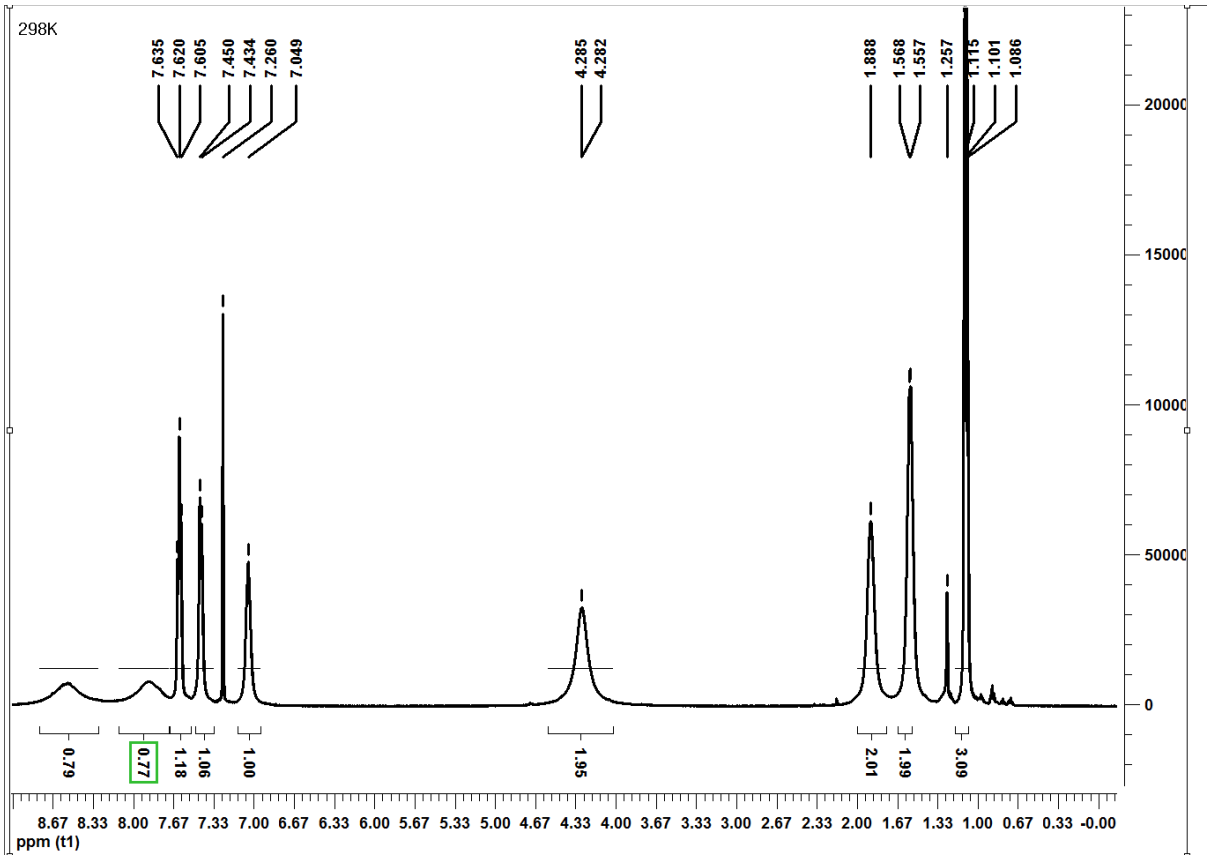
Variable temperature ^{1}HNMR (230K-298K) of **7**



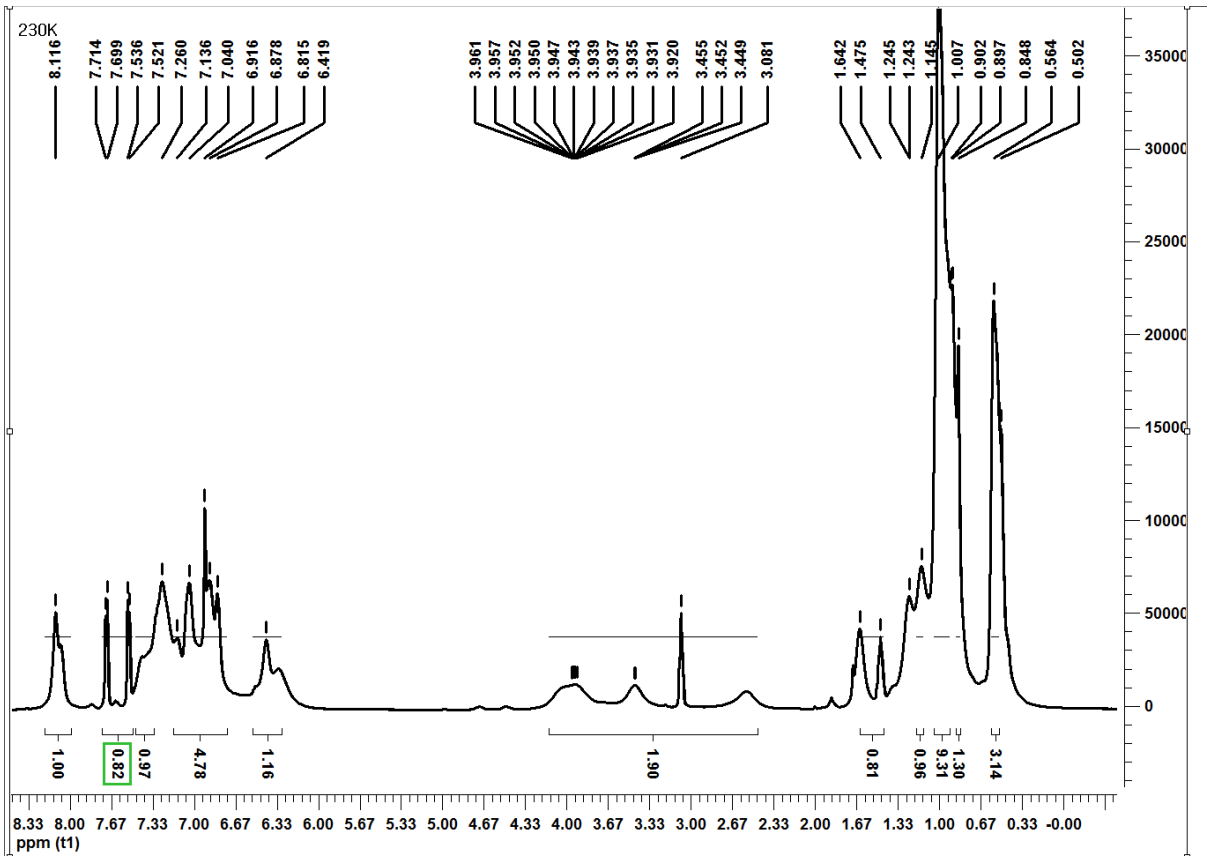


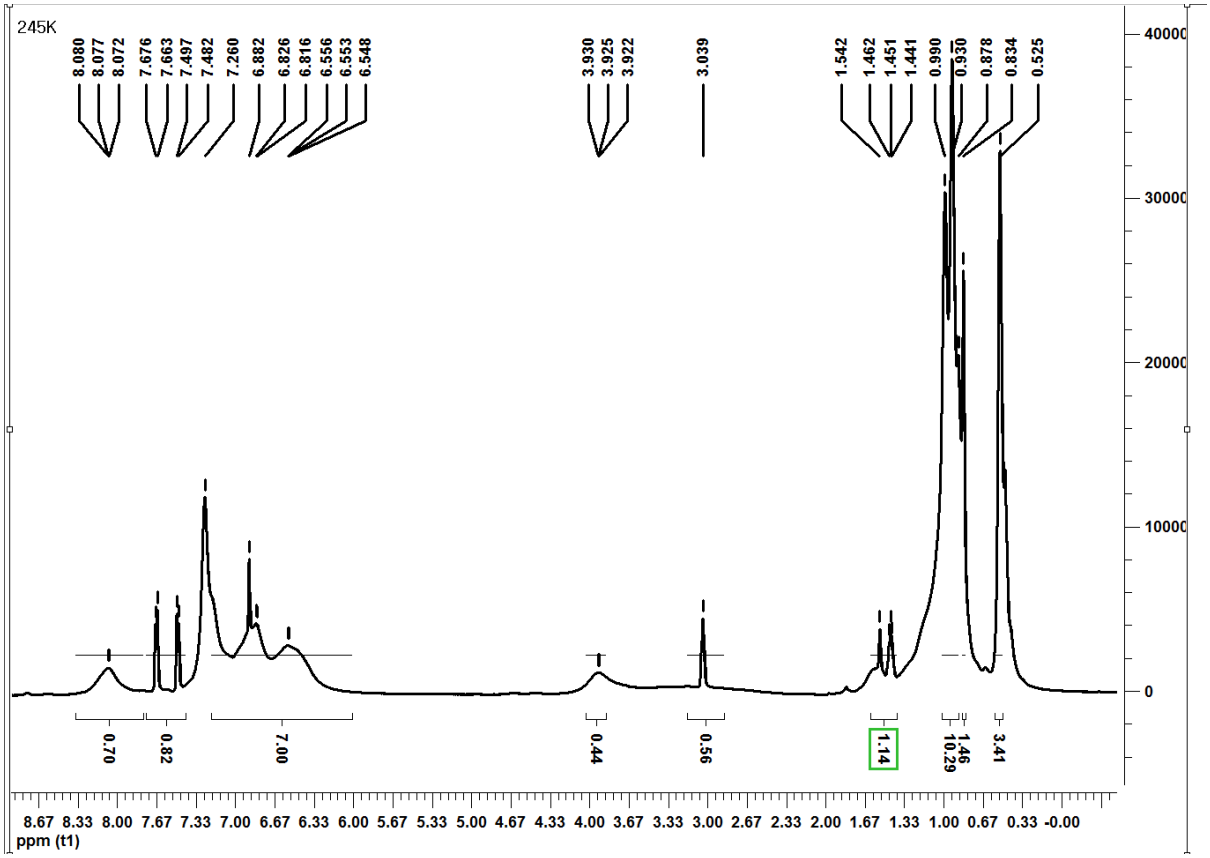


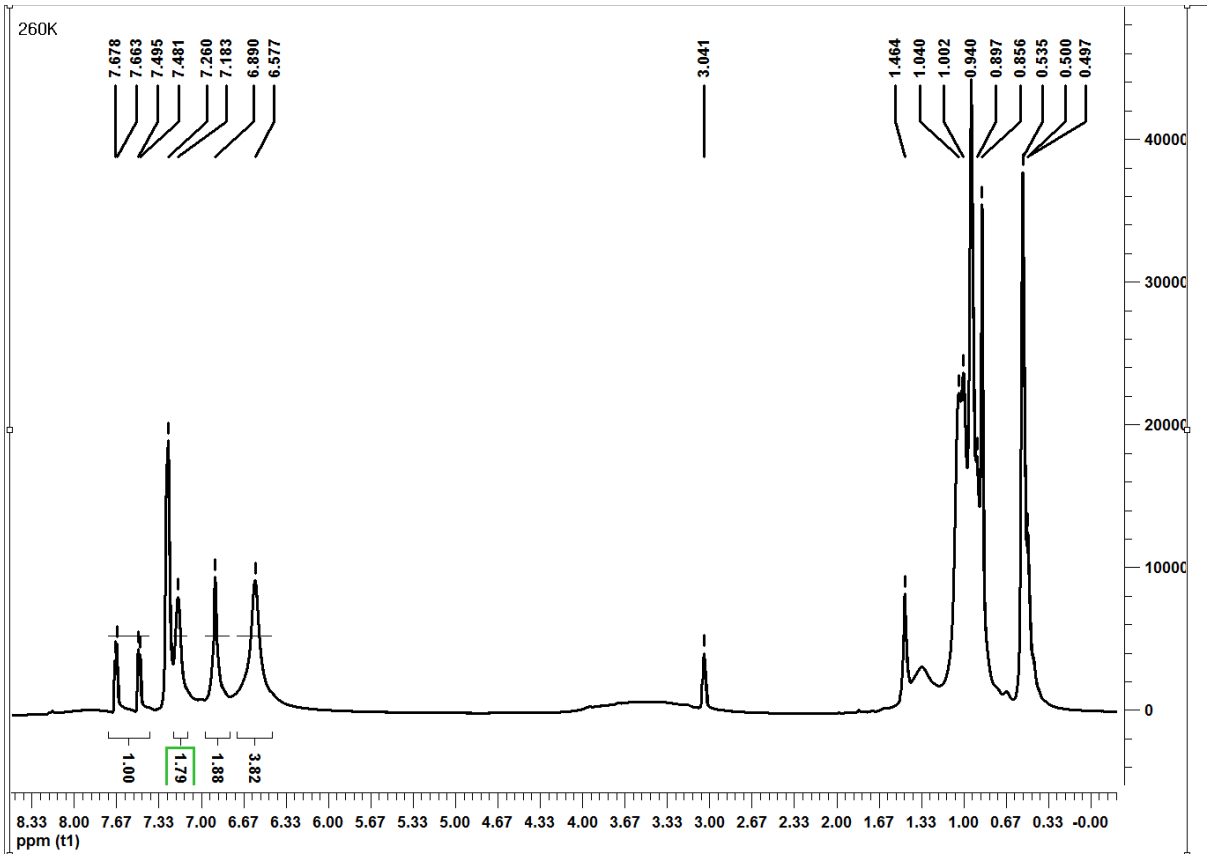


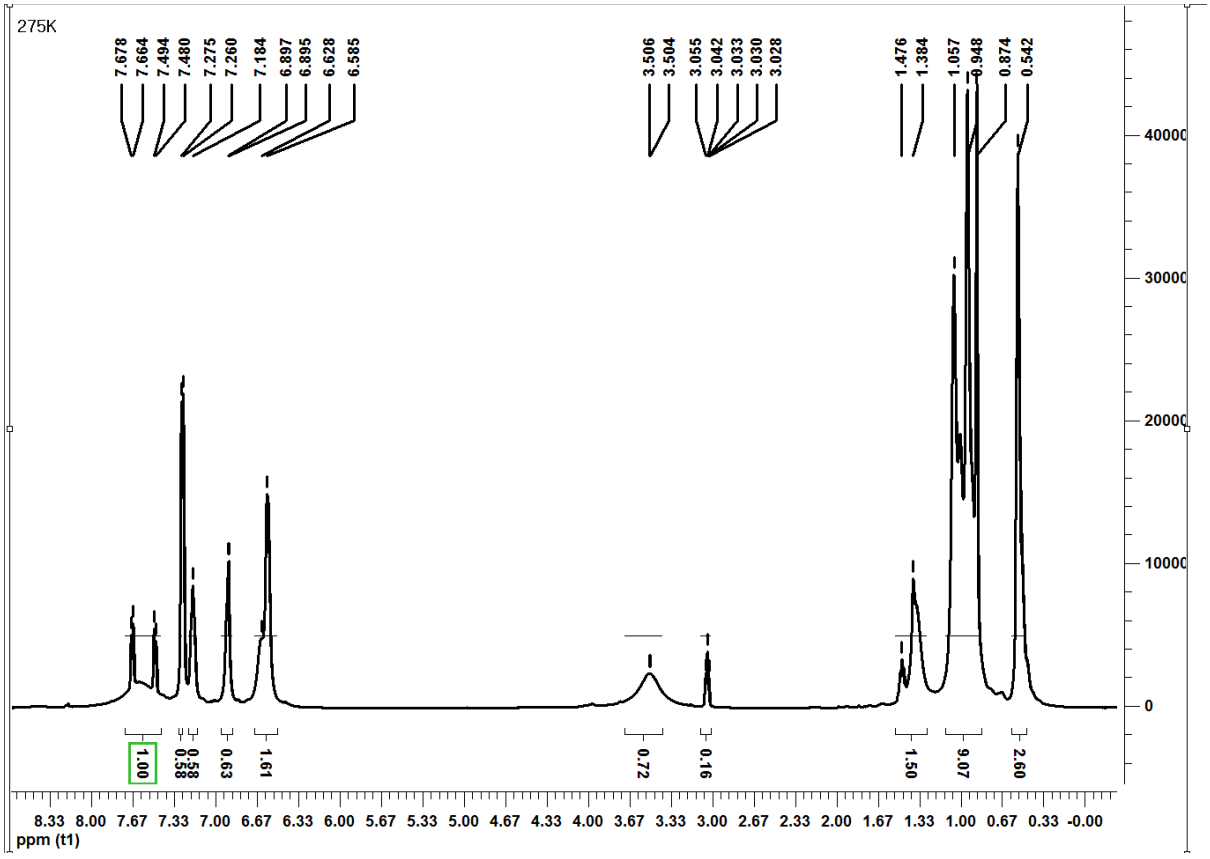


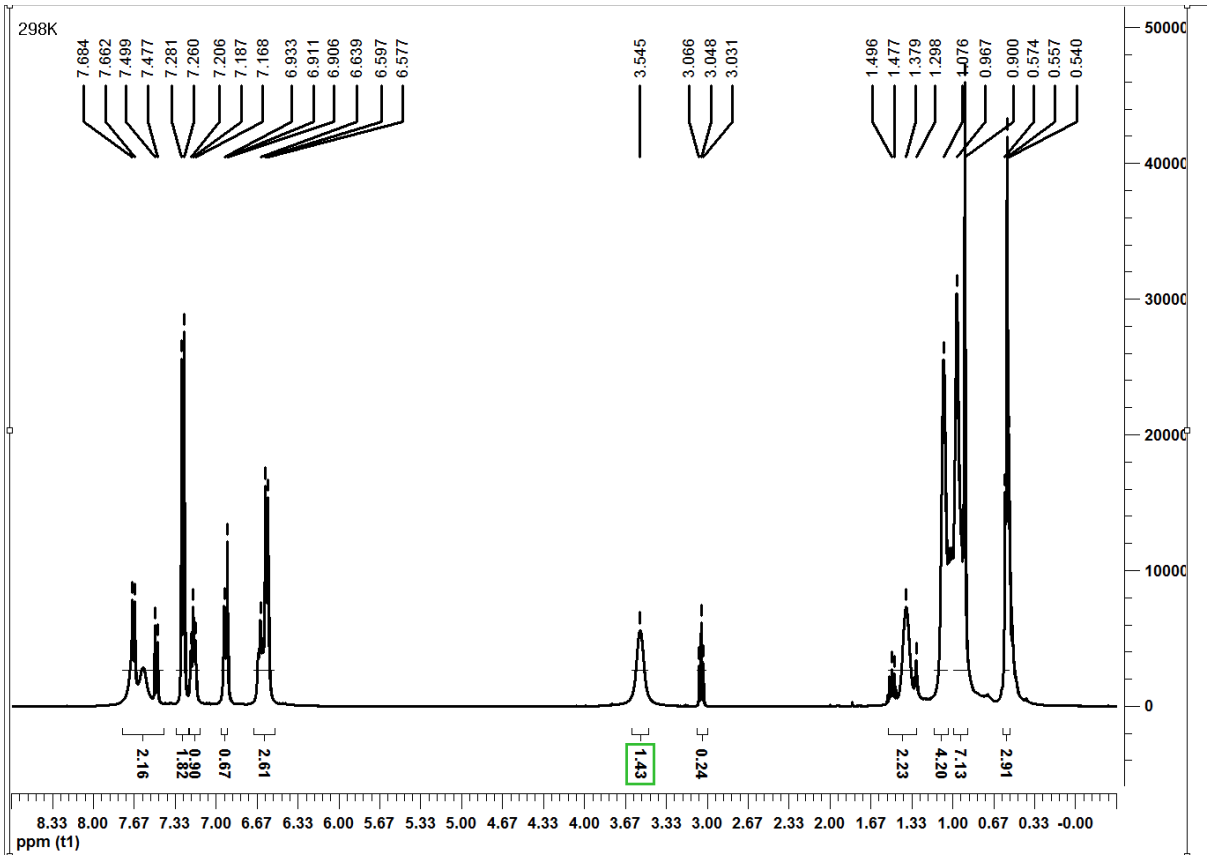
Variable temperature ^{1}HNMR (230K-298K) of **10**



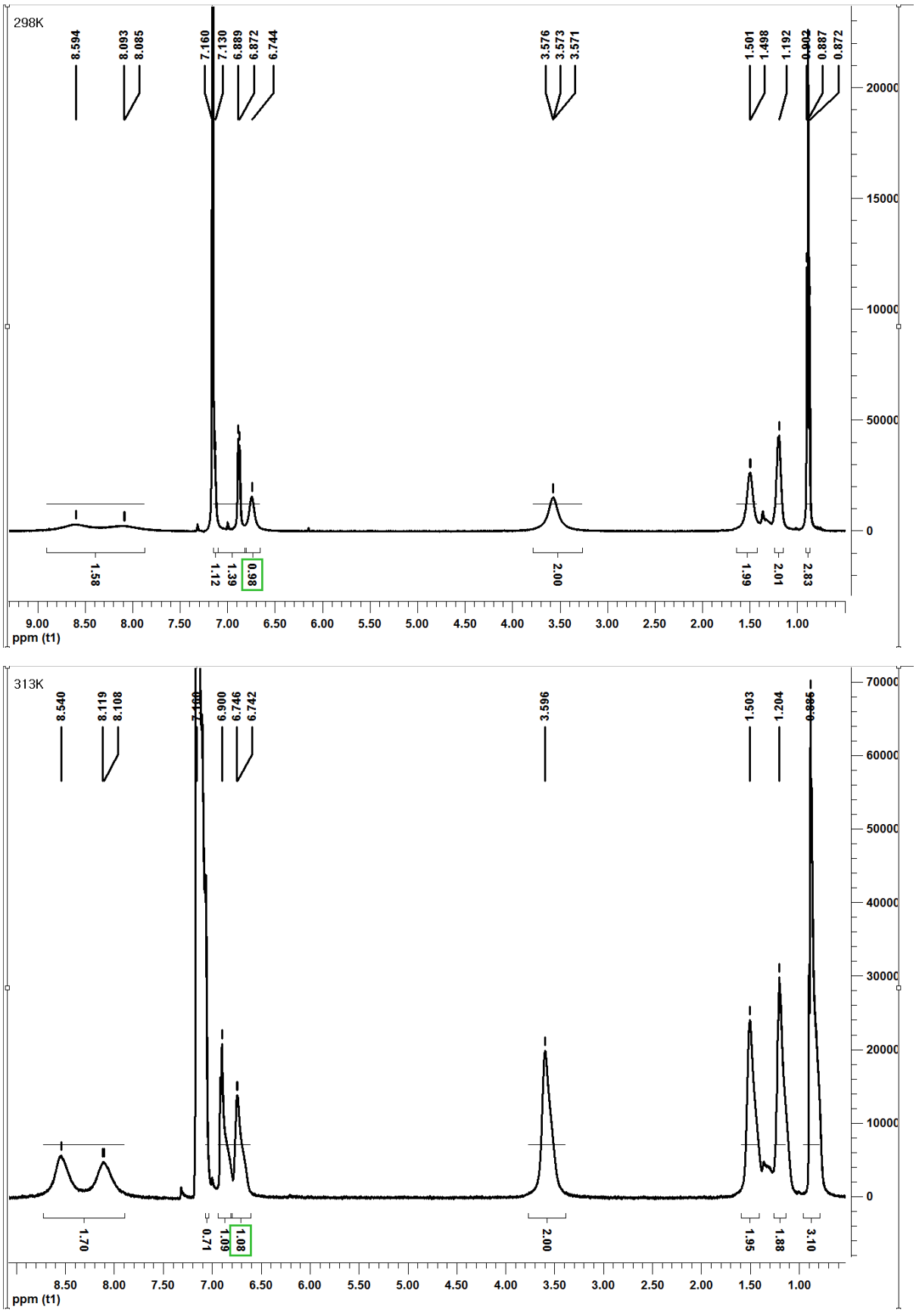


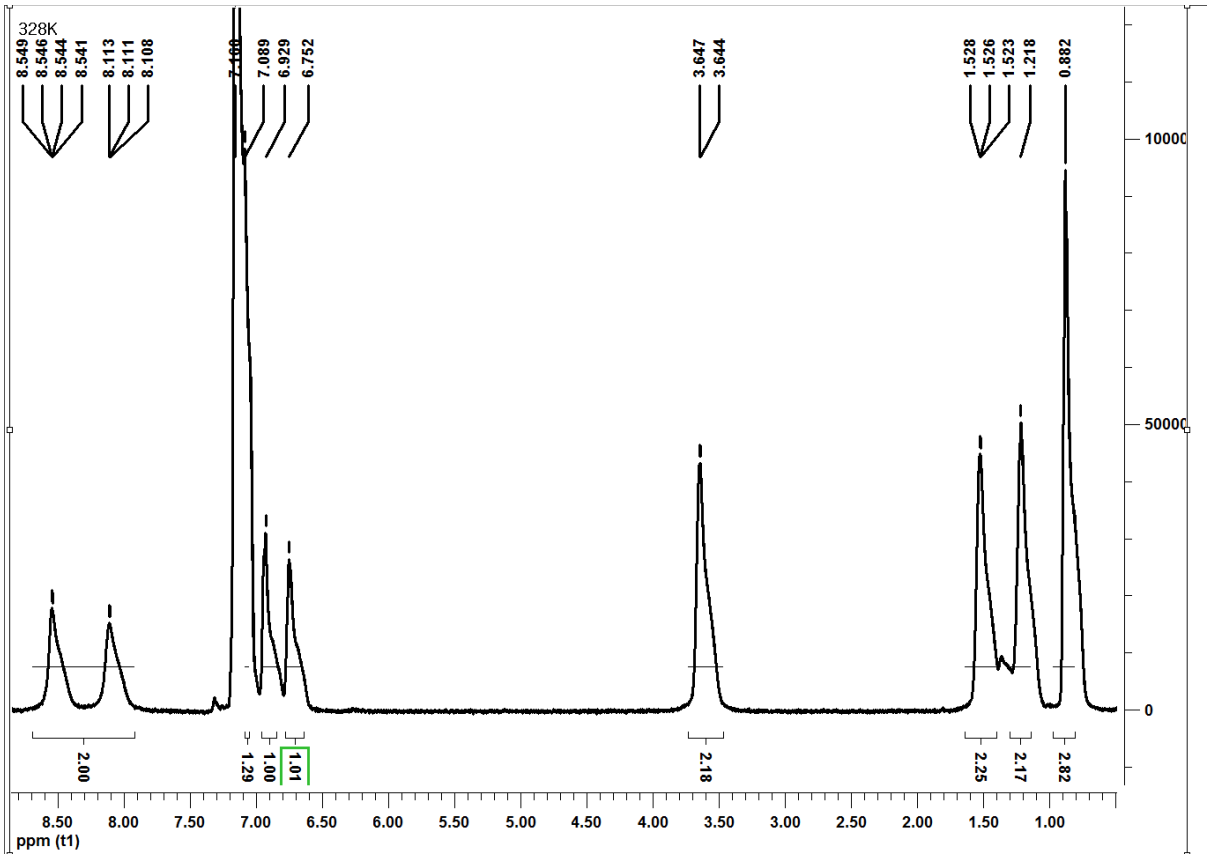


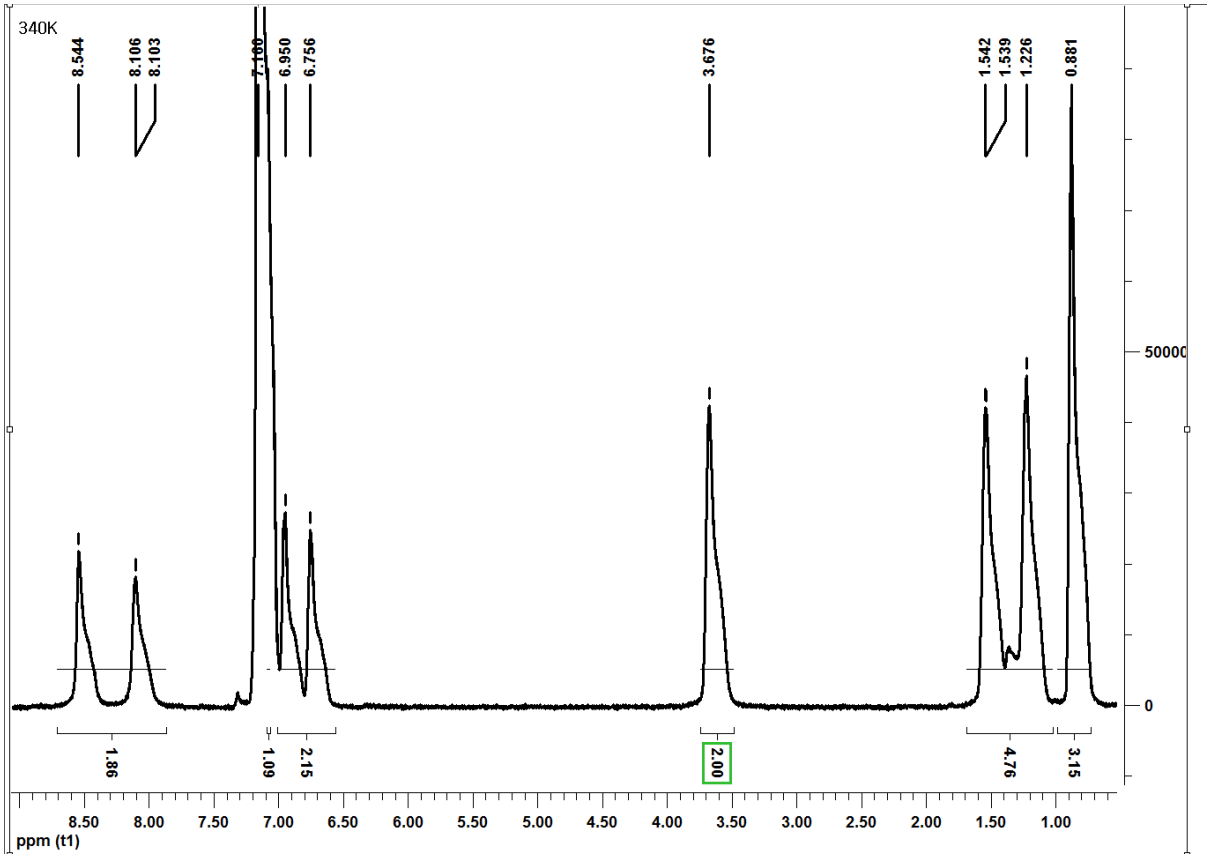




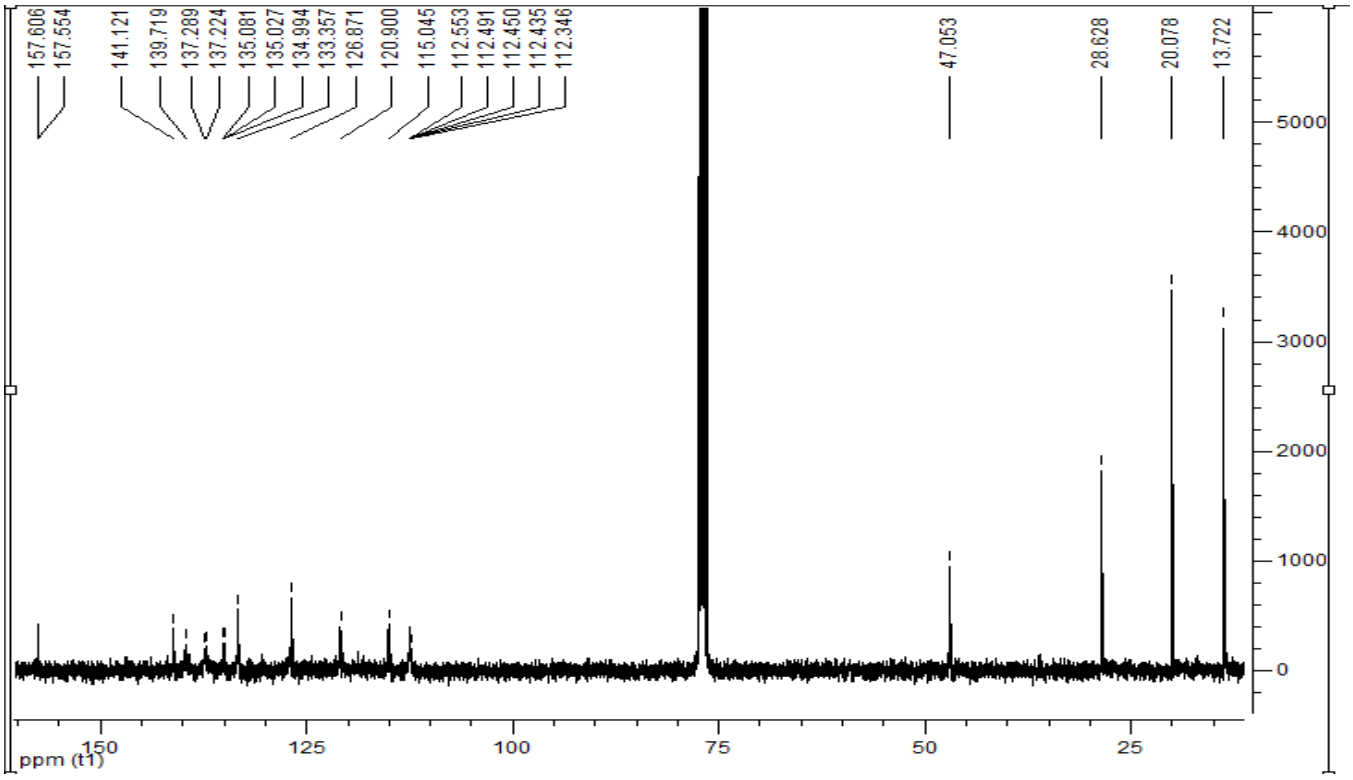
Variable high temperature ^{1}HNMR (298K-338K) of **7**







^{13}CNMR compound **7**



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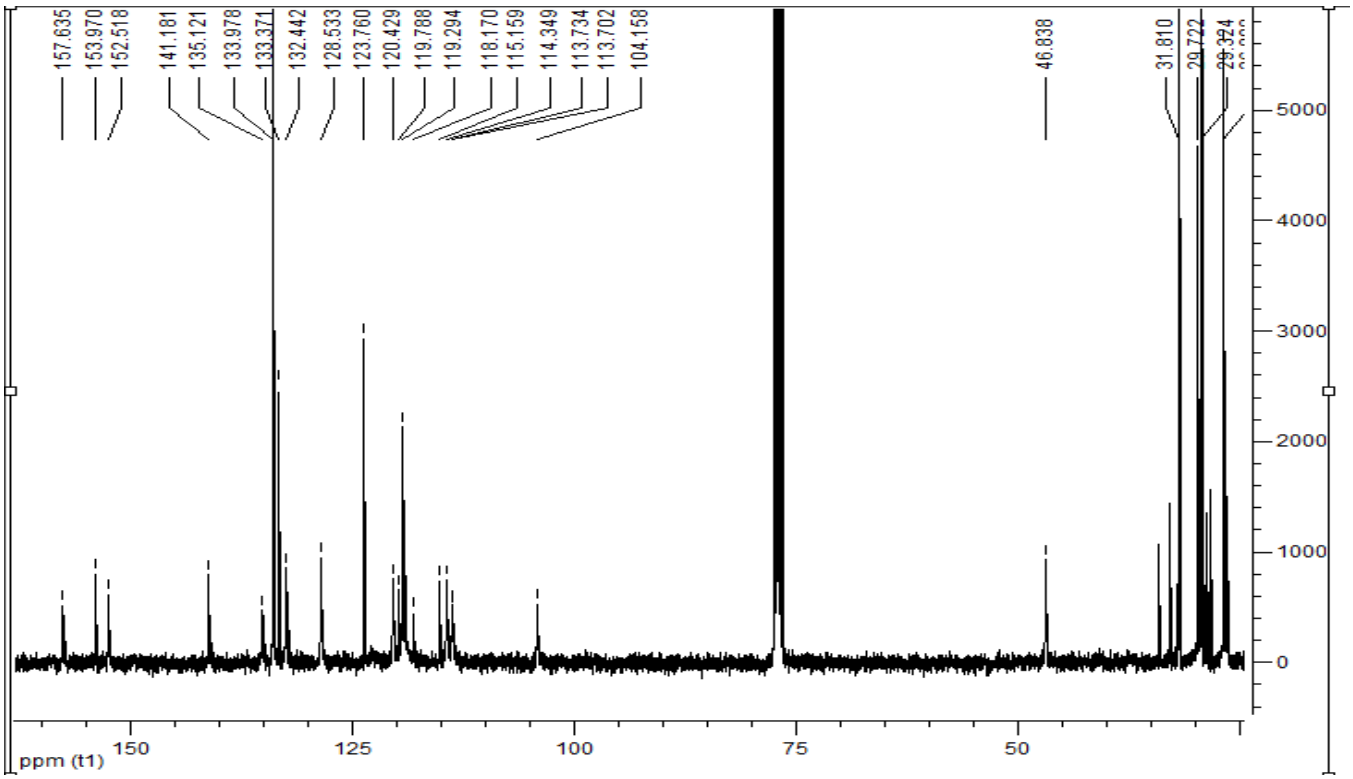

S1: Crystal Data of Compounds 2, 3, 6, 7, 8 and 10

Crystal data: 2, $C_{40}H_{36}N_4F_2$, M = 610.73 g.mol^{-1}, red needles, 0.15, 0.13, 0.10 mm^3, Triclinic, space group *P -1*, a = 7.1105(14), b = 9.868(2), c = 12.576(3) Å, α = 73.23(3)°, β = 78.56(3)°, γ = 70.79(3) V = 792.76(3) Å^3, Z = 1, Dc = 1.28 g.cm^{-3}, $F000$ = 322, MoKα radiation, λ = 0.71073 Å, T = 263 (2) K, $2\theta max$ = 55.0°, 7761 reflection collected, 3580 unique (R_{int} = 0.022), Final $GooF$ = 1.084, R1 = 0.046, wR_2 = 0.130, R indices based on 2728 reflections with I>2δ(I) (refinement on F^2) 209 parameters, μ = 0.084 mm^{-1}.

Crystal data: 3, $C_{40}H_{36}N_4F_2.CH_2Cl_2$, M = 695.65 g.mol^{-1}, red needles, 0.14, 0.12, 0.12 mm^3, Triclinic, space group *P -1*, a = 8.602(5), b = 13.889(8), c = 15.854(1) Å, α = 70.40(2)°, β = 79.41(2)°, γ = 88.92(2) V = 1752.1(2) Å^3, Z = 2, Dc = 1.32 g.cm^{-3}, $F000$ = 728, MoKα radiation, λ = 0.71073 Å, T = 263 (2) K, $2\theta max$ = 50.0°, 13676 reflection collected, 6111 unique (R_{int} = 0.026), Final $GooF$ = 0.963, R1 = 0.063, wR_2 = 0.221, R indices based on 3853 reflections with I>2σ(I) (refinement on F^2) 460 parameters, μ = 0.232 mm^{-1}.

Crystal data: 6, $C_{44}H_{44}N_4F_2$, M = 666.83 g.mol^{-1}, red needles, 0.12, 0.11, 0.10 mm^3, Triclinic, space group *P -1*, a = 8.778(5), b = 9.171(6), c = 13.365(8) Å, α = 71.67(3)°, β = 72.14(2)°, γ = 62.81(3) V = 891.3(1) Å^3, Z = 1, Dc = 1.24 g.cm^{-3}, $F000$ = 354, MoKα radiation, λ = 0.71073 Å, T = 263 (2) K, $2\theta max$ = 55.0°, 8855 reflection collected, 4050 unique (R_{int} = 0.027), Final $GooF$ = 1.06, R1 = 0.055, wR_2 = 0.160, R indices based on 2788 reflections with I>2σ(I) (refinement on F^2) 237 parameters, μ = 0.080 mm^{-1}.

Crystal data: 7, $C_{40}H_{28}N_4F_{10}$, M = 754.66 g.mol^{-1}, red needles, 0.15, 0.13, 0.10 mm^3, Triclinic, space group *P -1*, a = 7.3925(2), b = 9.2554(2), c = 12.899(3) Å, α = 88.42(3)°, β = 75.51(3)°, γ = 87.38(3)° V = 853.5(3) Å^3, Z = 1, Dc = 1.47 g.cm^{-3}, $F000$ = 386, MoKα radiation, λ = 0.71073 Å, T = 263 (2) K, $2\theta max$ = 50°, 6758 reflection collected, 2979 unique (R_{int} = 0.023), Final $GooF$ = 1.05,

R1 = 0.059, wR_2 = 0.183, *R* indices based on 2039 reflections with I>2σ(I) (refinement on F^2) 245 parameters, μ = 0.125 mm^{-1}.

Crystal data: 8, $C_{44}H_{44}N_4F_2$, *M* = 666.83 $g.mol^{-1}$, red needles, 0.12, 0.11, 0.10 mm^3, Monoclinic, space group *C 2/c*, *a* = 16.453(3), *b* = 7.222(14), *c* = 31.554(1) Å, *ß* = 110.38(3)°, *V* = 3514.7(15) $Å^3$, Z = 4, *Dc* = 1.26 $g.cm^{-3}$, *F000* = 1416, MoKα radiation, λ = 0.71073 Å, *T* = 173 (2) K, 2*θmax* = 50.0°, 13280 reflection collected, 3092 unique (R_{int} = 0.084), Final *GooF* = 1.028, R1 = 0.064, wR_2 = 0.162, *R* indices based on 1789 reflections with I>2σ(I) (refinement on F^2) 229 parameters, μ = 0.081 mm^{-1}.

Crystal data: 10, $C_{50}H_{52}N$, *M* = 736.98 $g.mol^{-1}$, red needles, 0.15, 0.13, 0.10 mm^3, Triclinic, space group *P -1*, *a* = 8.8472(2), *b* = 9.2195(2), *c* = 14.044(3) Å, α = 84.46(3)°, *ß* = 76.26(3)°, γ = 64.35(3)° *V* = 1003.1(3) $Å^3$, Z = 1, *Dc* = 1.22 $g.cm^{-3}$, *F000* = 394, MoKα radiation, λ = 0.71073 Å, *T* = 263 (2) K, 2*θmax* = 55.0°, 9921 reflection collected, 4544 unique (R_{int} = 0.070), Final *GooF* = 0.988, R1 = 0.066, wR_2 = 0.158, *R* indices based on 2000 reflections with I>2σ(I) (refinement on F^2) 254 parameters, μ = 0.072 mm^{-1}.

Table.1. Reaction conditions for compounds **2**–**10**

Product	Reactant A (mmoles)	Reactant B (mmoles)	TEA (mmoles)	$TiCl_4$ (mmoles)	Yield (%)
Compound **2**	DBQA (1)	P-Fluoroaniline (4)	8.5	5.4	85
Compound **3**	DFDBQA (1)	Aniline (4)	8.5	5.4	70
Compound **4**	DFDBQA (1)	P-Fluoroaniline (4)	8.5	5.4	66
Compound **5**	TMDBQA (1)	Aniline (4)	8.5	5.4	63
Compound **6**	TMDBQA (1)	P-Fluoroaniline (4)	8.5	5.4	51
Compound **7**	DBQA (1)	2,3,4,5,6-pentafluoroaniline (4)	8.5	5.4	55
Compound **8**	DFDBQA (1)	dimethylaniline (4)	8.5	5.4	45
Compound **9**	DBQA (1)	Naphthylamine (4)	8.5	5.4	40
Compound **10**	8CQA (1)	p-Cyanoaniline (4)	8.5	5.4	60

Table.2. Photophysical properties of compounds **1**–**10**

Compound	Chloroform λ_{max}(nm)	Toluene λ_{max} (nm)	Acetone λ_{max}(nm)	Thin film λ_{max}(nm)
1	519	518	514	527
2	520	518	515	528
3	535	532	529	541
4	536	534	530	545
5	498	497	492	503
6	500	499	494	512
7	540	542	540	554
8	534	532	531	538
9	525	524	521	535
10	532	529	526	538

Table.3. A comparison of eigenvalues of HOMOs and LUMOs of quinacridones **1-10** (**A** and **B**) at three different levels of theory.

Structure	HOMO	LUMO	Gap B3PW91	HOMO	LUMO	Gap B3LYP	HOMO	LUMO	Gap PBEPBE	Exp.
1a	-4.98	-1.99	2.99	-5.15	-2.21	2.94	-4.27	-2.47	1.80	2.26
2a	-5.06	-2.11	2.95	-5.25	-2.35	2.90	-4.31	-2.55	1.76	2.27
3a	-5.06	-2.17	2.89	-5.26	-2.41	2.85	-4.33	-2.61	1.72	2.22
4a	-5.14	-2.28	2.86	-5.36	-2.54	2.82	-4.37	-2.69	1.68	2.20
5a	-4.81	-1.83	2.98	-4.97	-2.04	2.93	-4.10	-2.30	1.80	2.32
6a	-4.88	-1.92	2.96	-5.07	-2.15	2.92	-4.14	-2.36	1.78	2.38
7a	-5.39	-2.52	2.87	-5.63	-2.81	2.82	-4.60	-2.89	1.71	2.07
8a	-5.00	-2.09	2.91	-5.19	-2.33	2.86	-4.25	-2.53	1.72	2.21
9a	-5.07	-2.05	3.02	-5.24	-2.26	2.98	-4.31	-2.54	1.77	1.99
10a	-5.48	-2.58	2.90	-5.64	-2.78	2.86	-4.78	-3.03	1.75	1.81
1b	-5.00	-2.12	2.88	-5.17	-2.34	2.83	-4.28	-2.58	1.70	2.26
2b	-5.08	-2.22	2.86	-5.28	-2.45	2.83	-4.32	-2.65	1.67	2.27
3b	-5.09	-2.30	2.79	-5.29	-2.54	2.75	-4.34	-2.72	1.62	2.22
4b	-5.17	-2.40	2.77	-5.39	-2.65	2.74	-4.39	-2.79	1.60	2.20
5b	-4.89	-1.89	3.00	-5.05	-2.09	2.96	-4.16	-2.36	1.80	2.32
6b	-4.97	-1.99	2.98	-5.15	-2.21	2.94	-4.21	-2.44	1.77	2.38
7b	-5.44	-2.61	2.83	-5.69	-2.90	2.79	-4.64	-2.98	1.66	2.07
8b	-5.02	-2.34	2.68	-5.21	-2.47	2.74	-4.26	-2.65	1.61	2.21
9b	-5.04	-2.13	2.91	-5.21	-2.34	2.87	-4.29	-2.61	1.68	1.99
10b	-5.49	-2.71	2.78	-5.65	-2.91	2.74	-4.78	-3.14	1.64	1.81

Table .4. A comparison of eigenvalues of HOMOs and LUMOs of quinacridones **1-10** (A and B), theoretical and experimental

	1A			1B			Exp.		
Structure	HOMO	LUMO	Gap	$HOMO_{Th}$	$LUMO_{Th}$	Gap	HOMO	LUMO	Gap
1	-4.98	-1.99	2.99	-5.00	-2.12	2.88	-5.05	-2.78	2.26
2	-5.06	-2.11	2.95	-5.08	-2.22	2.86	-5.19	-2.92	2.27
3	-5.06	-2.17	2.89	-5.09	-2.30	2.79	-5.21	-2.99	2.22
4	-5.14	-2.28	2.86	-5.17	-2.40	2.77	-5.23	-3.03	2.20
5	-4.81	-1.83	2.98	-4.89	-1.89	3.00	-5.05	-2.73	2.32
6	-4.88	-1.92	2.96	-4.97	-1.99	2.98	-5.12	-2.74	2.38
7	-5.39	-2.52	2.87	-5.44	-2.61	2.83	-5.34	-3.27	2.07
8	-5.00	-2.09	2.91	-5.02	-2.34	2.68	-5.08	-2.86	2.21
9	-5.07	-2.05	3.02	-5.04	-2.13	2.91	-4.94	-2.95	1.99
10	-5.48	-2.58	2.90	-5.49	-2.71	2.78	-5.30	-3.48	1.81

S2. Cyclic votammograms of compound **1-10** recorded in CH_2Cl_2 with scan rate of $100mVs^{-1}$

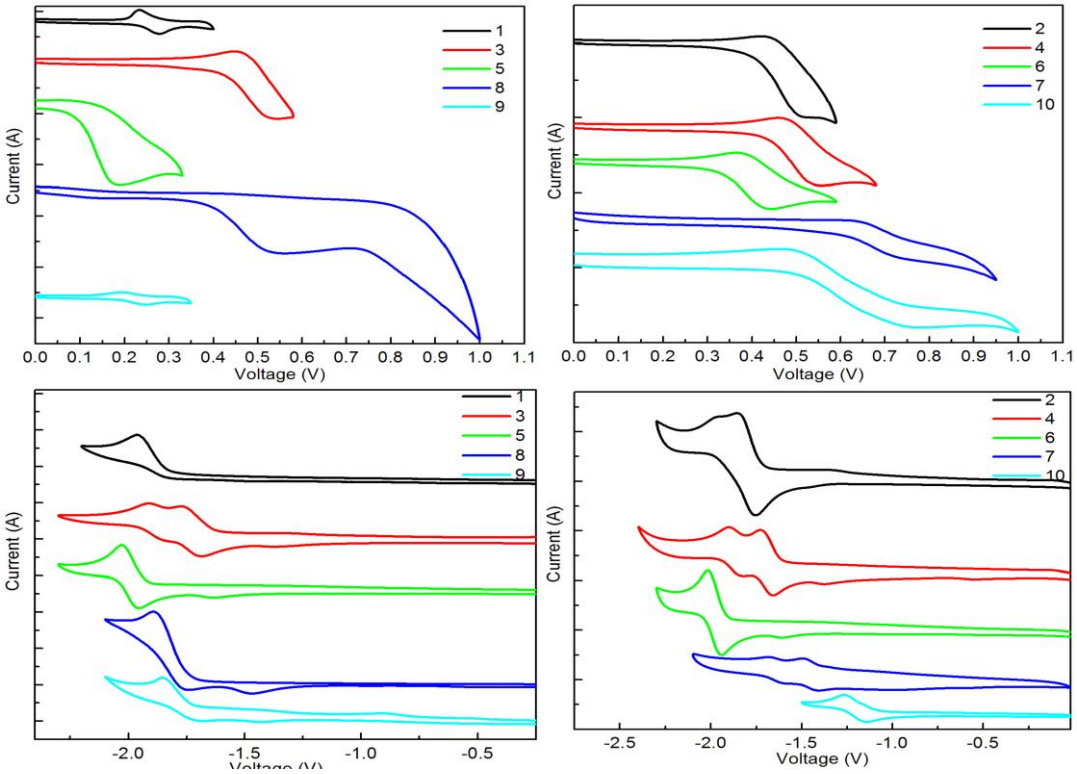

Table.5. Electrochemical data and HOMO, LUMO energy level of compounds **1**-**10**

Compound	$E_{ox}^{1/2}$(V)	$E_{red}^{1/2}$(V)	LUMO	HOMO	E_g
1	+0.25	−1.95	−2.78	−5.05	2.26
2	+0.47	−1.80	−2.92	−5.19	2.27
3	+0.49	−1.72	−2.99	−5.21	2.22
4	+0.50	−1.69	−3.03	−5.23	2.20
5	+0.40	−1.99	−2.73	−5.05	2.32
6	+0.41	−1.98	−2.74	−5.12	2.38
7	+0.68	−1.45	−3.27	−5.34	2.07
8	+0.54	−1.82	−2.86	−5.08	2.21
9	+0.22	−1.78	−2.95	−4.94	−1.99
10	+0.62	−1.20	−3.48	−5.30	1.81

Table.6. Absoulte and relative energies (parenthesis) of **EE**, **EZ** and **ZZ** isomers of Quinacridonediimines **7** and **10**

Compound	**EE**	**EZ**	**ZZ**
7	-2757.4270159 (0.0)	-2757.4230023(2.5)	-2757.4176056 (5.9)
10	-1949.9373194 (0.0)	-1949.9348575 (1.54)	-1949.9288255 (5.33)

Table.7. Calculated energies of EE, EZ and ZZ isomers of Quinacridonediimines **7** and **10**

7EE

Total energy -2757.4270159

C	0.22265900	-3.67189500	-0.76631000
N	-0.74561500	-2.70235800	-0.25221300
C	-0.36945000	-1.36874700	-0.12207600
C	0.95542800	-0.95836900	-0.28274600
C	1.33653200	0.37729700	-0.17002000
C	0.36944900	1.36874500	0.12206100
C	-0.95542800	0.95836700	0.28273100
H	-1.75916500	1.65900400	0.46887600
C	-1.33653300	-0.37729800	0.17000400
C	-2.75716100	-0.73650800	0.28197000
C	-3.01491300	-2.16604500	0.47277800
C	-2.00019100	-3.11490300	0.16756900
C	-2.29643400	-4.48761400	0.31311700
C	-3.52506700	-4.90494500	0.79120600
C	-4.50232200	-3.97417500	1.15846900
C	-4.23697400	-2.62859500	0.99525000
H	-4.98356400	-1.90133100	1.29123500

H	-5.45235100	-4.30086200	1.57006800
H	-3.71407600	-5.96939600	0.90327000
H	-1.54671100	-5.23562900	0.08754700
N	-3.60132400	0.24660700	0.24175600
C	-4.97145600	0.17536700	0.10237900
C	-5.60557500	-0.45780800	-0.98203900
C	-6.97396300	-0.35717100	-1.19852200
C	-7.76225100	0.40260500	-0.33918500
C	-7.16553100	1.05163300	0.73741200
C	-5.79345900	0.95436400	0.93467600
F	-5.24843000	1.60070800	1.97054800
F	-7.91233700	1.78003900	1.57048900
F	-9.07806000	0.49859600	-0.53946600
F	-7.53587400	-0.98116400	-2.23644000
F	-4.87663800	-1.18811700	-1.83300900
N	0.74561500	2.70235500	0.25220200
C	2.00019200	3.11490100	-0.16757800
C	3.01491300	2.16604300	-0.47278700
C	4.23696900	2.62859000	-0.99527100
C	4.50231800	3.97416900	-1.15849400
C	3.52506600	4.90494100	-0.79122800
C	2.29643400	4.48761200	-0.31313200
H	1.54671200	5.23562700	-0.08756500
H	3.71407300	5.96939100	-0.90329900
H	5.45234500	4.30085400	-1.57010000
H	4.98355600	1.90132300	-1.29126200
C	2.75716100	0.73650700	-0.28198300
N	3.60132700	-0.24660400	-0.24176900

C	4.97145500	-0.17536200	-0.10237500
C	5.79346900	-0.95435000	-0.93467400
C	7.16553900	-1.05162000	-0.73739700
C	7.76224700	-0.40260700	0.33921600
C	6.97394800	0.35715600	1.19855500
C	5.60556300	0.45779600	0.98205900
F	4.87661600	1.18809100	1.83303200
F	7.53584800	0.98113400	2.23648800
F	9.07805300	-0.49859800	0.53950900
F	7.91235300	-1.78001400	-1.57047600
F	5.24845000	-1.60068000	-1.97056000
C	-0.22266000	3.67189200	0.76629900
H	-0.83026700	3.15965300	1.51851500
H	0.33223500	4.44032000	1.31300100
C	-1.12023400	4.30657600	-0.29944100
H	-1.64821500	3.51683400	-0.84889900
H	-0.50024600	4.82827400	-1.04035800
C	-2.13377600	5.27756000	0.30855800
H	-2.75251100	4.74358600	1.04327100
H	-1.60224600	6.06018100	0.86915400
C	-3.03504400	5.92483900	-0.74027200
H	-3.75381800	6.60967700	-0.27749100
H	-2.44933400	6.49803300	-1.46895400
H	-3.60408900	5.16832300	-1.29329700
H	1.75916500	-1.65900600	-0.46888900
H	-0.33223800	-4.44032800	-1.31300500
H	0.83026100	-3.15965900	-1.51853200
C	1.12024100	-4.30657200	0.29942900

H	1.64821800	-3.51682400	0.84888300
H	0.50025900	-4.82827200	1.04034900
C	2.13378700	-5.27755000	-0.30857200
H	1.60226100	-6.06017500	-0.86916600
H	2.75251700	-4.74357300	-1.04328700
C	3.03506200	-5.92482300	0.74025700
H	2.44935600	-6.49802000	1.46893900
H	3.75383900	-6.60965600	0.27747400
H	3.60410200	-5.16830300	1.29328000

7EZ

Total energy -2757.4230023

N	0.49666700	3.36201400	0.06494700
C	1.70283300	4.02141100	-0.13450900
C	1.75335400	5.42082100	-0.31357400
C	2.96320100	6.06847900	-0.49426100
C	4.16655800	5.35373000	-0.50363700
C	4.13060200	3.98444400	-0.32579600
C	2.91834900	3.29770100	-0.14472100
C	2.93048100	1.85102700	0.09460300
N	4.07218000	1.30354100	0.35826300
C	4.35612900	0.05279200	0.85256800
C	3.81998700	-0.41498900	2.07399900
H	3.08743500	0.19415700	2.59502700
C	4.23404000	-1.61999800	2.61612700
C	5.19516000	-2.40703000	1.95770100
C	5.74406700	-1.94369800	0.74944600

C	5.33965400	-0.73188600	0.21407000
H	5.78126200	-0.36168800	-0.70640200
H	6.50144600	-2.53645700	0.24467200
H	3.81855100	-1.96269000	3.55947100
H	5.03944900	3.39149400	-0.31519400
H	5.11253100	5.86647400	-0.65032200
H	2.96657000	7.14571200	-0.63970900
H	0.84272000	6.00643100	-0.33773500
C	-0.73476500	4.12774600	0.26441100
H	-1.38250700	3.54987600	0.93069600
H	-0.47316100	5.02985200	0.82263300
C	-1.47270100	4.46981300	-1.03401700
H	-0.82533100	5.08984900	-1.66830200
H	-1.64479100	3.54263700	-1.59382300
C	-2.81087400	5.18057300	-0.80423400
H	-3.45205500	4.55292700	-0.16905100
H	-3.32710100	5.25639700	-1.76964800
C	-2.69347600	6.57691200	-0.19295600
H	-2.05735100	7.22599900	-0.80771600
H	-3.67655000	7.05438100	-0.11900600
H	-2.27059000	6.55441100	0.81796700
C	5.61137400	-3.65540200	2.51078300
N	5.94395600	-4.67889900	2.95609000
C	-0.78731000	1.30458900	-0.07965900
C	-0.87759700	-0.07561500	-0.23108200
C	0.29776800	-0.85391700	-0.34291700
C	1.52461900	-0.19082700	-0.23953300
H	2.44801600	-0.74331400	-0.33133700

N	0.21483100	-2.23027100	-0.53361900
C	-1.00092500	-2.81947000	-0.85311500
C	-2.21985600	-2.09357000	-0.74323100
C	-3.41597200	-2.71076800	-1.15606100
C	-3.44833800	-4.01417600	-1.61281900
C	-2.25524500	-4.74057500	-1.66680500
C	-1.05516400	-4.15689100	-1.30262400
H	-0.14842500	-4.73952000	-1.40214300
H	-2.25575300	-5.76909700	-2.01819700
H	-4.38581900	-4.46156300	-1.92835900
H	-4.33490900	-2.13914400	-1.12240300
C	-2.20481200	-0.71313000	-0.24619300
N	-3.20043100	0.01716900	0.13620700
C	-4.49653500	-0.36053700	0.42063300
C	-5.56683600	0.26509500	-0.24903400
C	-6.87988600	-0.01489800	0.09323100
C	-7.16675200	-0.90856500	1.13807300
C	-6.10480200	-1.51494700	1.83011100
C	-4.79289300	-1.24746800	1.47737500
H	-3.97538200	-1.71346900	2.01939900
H	-6.31992300	-2.19822100	2.64647900
H	-7.69594800	0.46368500	-0.44014300
H	-5.34388100	0.96828100	-1.04612500
C	1.43124700	-3.04444000	-0.48547500
H	2.09951200	-2.60640400	0.26126600
H	1.15970300	-4.02544900	-0.08483700
C	2.14454100	-3.18908100	-1.83276600
H	2.47555700	-2.20064100	-2.17794300

H	1.43155700	-3.54827500	-2.58649600
C	3.34048100	-4.13898200	-1.75621500
H	4.03885900	-3.78399700	-0.98688000
H	2.99963800	-5.12954800	-1.42254300
C	4.07262000	-4.27570900	-3.08910200
H	4.91925700	-4.96579900	-3.00700600
H	3.40631600	-4.65732300	-3.87213100
H	4.46213300	-3.30853500	-3.42887100
H	-1.73366700	1.82727200	-0.03185700
C	-8.51969700	-1.19100200	1.49682000
N	-9.62343600	-1.42261400	1.78695700
C	0.43649300	1.97520700	-0.01557500
C	1.62192100	1.18968400	-0.04260000

7 ZZ

Total Energy -2757.4176056

C	-2.67524300	2.37816700	-1.20928500
H	-2.62748100	1.56614900	-1.94206900
H	-2.71801300	3.30086300	-1.79503600
C	-3.92136300	2.22759100	-0.33112300
H	-3.91590900	2.99796800	0.45050900
H	-3.86959300	1.26805900	0.19597100
C	-5.23199800	2.30557200	-1.12330700
H	-5.21584600	1.56659700	-1.93682400
H	-6.05053000	1.99846500	-0.46110700
C	-5.54806800	3.68880200	-1.69293700
H	-5.58930400	4.44311000	-0.89721500

H	-6.52071300	3.68929000	-2.19667400
H	-4.80505200	4.01835400	-2.42865100
N	-1.40472600	2.39296700	-0.48095900
C	-0.90586400	3.59347800	0.00972400
C	-1.70266400	4.75757200	0.04798000
C	-1.19567300	5.94478100	0.54760900
C	0.11967400	6.02377700	1.02041000
C	0.91862000	4.89868000	0.96300300
C	0.43031400	3.67924900	0.46459000
C	1.33149200	2.53610900	0.31284300
C	0.65477400	1.23920700	0.14886000
C	-0.70648800	1.21115200	-0.25731900
C	-1.31477200	-0.03800400	-0.41469900
H	-2.34697900	-0.09555900	-0.72987500
C	-0.65473100	-1.23907600	-0.14892600
C	0.70653900	-1.21102400	0.25723600
C	1.31482100	0.03813600	0.41462400
H	2.34702500	0.09569700	0.72980700
N	1.40476500	-2.39284800	0.48087900
C	0.90589100	-3.59335100	-0.00980400
C	1.70270000	-4.75743800	-0.04810100
C	1.19570700	-5.94464000	-0.54774400
C	-0.11965000	-6.02363400	-1.02052200
C	-0.91859800	-4.89854100	-0.96308500
C	-0.43028800	-3.67911600	-0.46466200
C	-1.33146100	-2.53597800	-0.31289100
N	-2.60120200	-2.77961500	-0.37294700
C	-3.63894200	-1.96610700	0.02241300

C	-3.77420900	-1.51008000	1.34743300
C	-4.93221200	-0.89001700	1.80120100
C	-6.00471700	-0.70081500	0.93421200
C	-5.90374100	-1.13959200	-0.38216300
C	-4.74845700	-1.77568800	-0.81887500
F	-4.68471800	-2.19205800	-2.08739300
F	-6.91764200	-0.93669300	-1.22705500
F	-7.10627800	-0.06935700	1.34912900
F	-5.02117400	-0.47844100	3.06757400
F	-2.76763600	-1.69381900	2.20847200
H	-1.95290700	-4.92175800	-1.29069000
H	-0.50788700	-6.95613800	-1.41919100
H	1.83975500	-6.81977300	-0.57802500
H	2.73164800	-4.73180600	0.28830500
C	2.67527900	-2.37809100	1.20921200
H	2.62761400	-1.56598300	1.94190400
H	2.71792700	-3.30072400	1.79507000
C	3.92143000	-2.22782800	0.33104200
H	3.91584300	-2.99830100	-0.45049600
H	3.86983900	-1.26835000	-0.19616900
C	5.23204300	-2.30596400	1.12324600
H	5.21603600	-1.56686800	1.93665700
H	6.05064500	-1.99912300	0.46101000
C	5.54782200	-3.68917700	1.69307700
H	5.58890400	-4.44360800	0.89746500
H	6.52046500	-3.68979400	2.19681800
H	4.80473400	-4.01846700	2.42883600
N	2.60123300	2.77973500	0.37291100

C	3.63895600	1.96617400	-0.02237700
C	3.77416500	1.50996900	-1.34734100
C	4.93214400	0.88983100	-1.80106900
C	6.00468200	0.70073800	-0.93409700
C	5.90376000	1.13968800	0.38222300
C	4.74849600	1.77584500	0.81889800
F	4.68480300	2.19237000	2.08736800
F	6.91768600	0.93687900	1.22710700
F	7.10621700	0.06920600	-1.34897000
F	5.02105000	0.47807900	-3.06738900
F	2.76755500	1.69359300	-2.20836100
H	1.95292500	4.92190000	1.29061900
H	0.50791000	6.95628600	1.41906800
H	-1.83971500	6.81992000	0.57785800
H	-2.73160100	4.73194700	-0.28845700

10 EE

Total energy -1949.9373194

C	0.13676500	3.62716100	0.97038400
N	-0.81860200	2.65955900	0.43056400
C	-0.40731300	1.34795300	0.20998100
C	0.93056900	0.96496400	0.33058500
C	1.34900900	-0.34932600	0.13313000
C	0.40730600	-1.34793600	-0.21000500
C	-0.93057600	-0.96494700	-0.33061000
H	-1.71739000	-1.67493600	-0.55123800
C	-1.34901600	0.34934300	-0.13315600

C	-2.78293500	0.67095200	-0.21667300
C	-3.09156200	2.10524500	-0.27921400
C	-2.09752500	3.06049400	0.07332900
C	-2.43960500	4.42986300	0.04205400
C	-3.69645500	4.84302000	-0.36192100
C	-4.65807000	3.91224000	-0.76577500
C	-4.34613400	2.56694400	-0.72039100
H	-5.08331600	1.84227900	-1.04266900
H	-5.63320200	4.23723500	-1.11521400
H	-3.92021900	5.90641900	-0.38462000
H	-1.70665600	5.18387300	0.30028100
N	-3.60106600	-0.32926300	-0.26538700
C	-4.97340900	-0.33558300	-0.12883300
C	-5.60044600	0.08532500	1.06352400
C	-6.96818000	-0.04967300	1.23031600
C	-7.75919500	-0.60675300	0.21121700
C	-7.14150300	-1.03892900	-0.97390200
C	-5.77063600	-0.91846900	-1.13419900
H	-5.29022400	-1.26704600	-2.04371600
H	-7.74569300	-1.47790100	-1.76242800
H	-7.43832600	0.27624000	2.15358300
H	-4.99270900	0.51045900	1.85678200
N	0.81859400	-2.65954300	-0.43058800
C	2.09751800	-3.06047800	-0.07335600
C	3.09155500	-2.10522800	0.27918500
C	4.34613200	-2.56692400	0.72035000
C	4.65807100	-3.91222000	0.76573100
C	3.69645400	-4.84300100	0.36188400

C	2.43960100	-4.42984600	-0.04208400
H	1.70665200	-5.18385700	-0.30030700
H	3.92022100	-5.90640000	0.38458000
H	5.63320700	-4.23721300	1.11516100
H	5.08331600	-1.84225700	1.04262000
C	2.78292800	-0.67093600	0.21664700
N	3.60106200	0.32927500	0.26537200
C	4.97340800	0.33558300	0.12884700
C	5.77061900	0.91848600	1.13421600
C	7.14149100	1.03892900	0.97394500
C	7.75920500	0.60671500	-0.21114900
C	6.96820600	0.04961400	-1.23025000
C	5.60046700	-0.08536500	-1.06348500
H	4.99274300	-0.51051600	-1.85674400
H	7.43836900	-0.27632900	-2.15349700
H	7.74566800	1.47791600	1.76247200
H	5.29019100	1.26709100	2.04371300
C	-0.13677400	-3.62714500	-0.97040700
H	-0.78667800	-3.09242800	-1.66962400
H	0.42023200	-4.34333600	-1.58189000
C	-0.97303500	-4.35248800	0.08690400
H	-1.51912900	-3.61484300	0.68852200
H	-0.30671500	-4.87787900	0.78356800
C	-1.95899400	-5.34220400	-0.53619200
H	-2.62252600	-4.80686700	-1.22984900
H	-1.40880100	-6.07408100	-1.14515900
C	-2.79932500	-6.07514300	0.50692400
H	-3.49689500	-6.77503400	0.03442400

H	-2.16653100	-6.64816600	1.19519200
H	-3.38835900	-5.37073700	1.10576000
H	1.71738300	1.67495300	0.55121300
H	-0.42024300	4.34335900	1.58185800
H	0.78666200	3.09244700	1.66961000
C	0.97303600	4.35249600	-0.08692600
H	1.51913400	3.61484600	-0.68853300
H	0.30672300	4.87788300	-0.78359800
C	1.95899200	5.34221400	0.53617200
H	1.40879500	6.07409700	1.14512900
H	2.62251700	4.80688100	1.22983900
C	2.79933200	6.07514400	-0.50694300
H	2.16654500	6.64816300	-1.19522000
H	3.49690000	6.77503800	-0.03444200
H	3.38837000	5.37073300	-1.10576900
C	9.17069000	0.73891100	-0.38113100
C	-9.17067600	-0.73896700	0.38122600
N	10.32217900	0.84522000	-0.51879700
N	-10.32216100	-0.84529100	0.51891400

10 EZ

Total energy -1949.9348575

C	1.60449100	1.37885500	-0.23008300
C	0.39927000	2.06281100	0.08731300
N	0.37552200	3.44665700	0.21014200
C	1.44091400	4.20270000	-0.25964200
C	1.33829700	5.60205400	-0.41139700

C	2.41151400	6.34311200	-0.87501200
C	3.62515900	5.72589700	-1.20124200
C	3.74358600	4.35889100	-1.04274200
C	2.67021600	3.57956300	-0.57953200
C	2.85377800	2.14564000	-0.34699700
N	4.07191600	1.70683500	-0.30874700
C	4.50612900	0.48589600	0.15741400
C	4.27164600	0.05026400	1.47544200
C	4.89068900	-1.07664100	2.00305400
C	5.77661000	-1.81336300	1.22183500
C	6.03380000	-1.40786300	-0.08389900
C	5.42236500	-0.26955600	-0.59433700
F	5.69304600	0.09476900	-1.85170000
F	6.86283000	-2.12385700	-0.84799400
F	6.34997800	-2.91764400	1.70763800
F	4.64299200	-1.45233200	3.25961800
F	3.43834400	0.74561000	2.25664100
H	4.67166600	3.84184300	-1.26420300
H	4.46092900	6.31272900	-1.57054200
H	2.29690600	7.41761500	-0.99317200
H	0.40867100	6.11262500	-0.19132600
C	-0.80549500	4.10479800	0.76936100
H	-1.21177300	3.44844000	1.54503000
H	-0.46364900	5.00219600	1.29453200
C	-1.89234000	4.46096500	-0.24880000
H	-1.47553900	5.12742900	-1.01519900
H	-2.21256500	3.55465500	-0.77791700
C	-3.09941000	5.12315300	0.41767400

H	-2.77125200	6.02273100	0.95836200
H	-3.51137300	4.44477800	1.17788600
C	-4.19530900	5.49757200	-0.57736200
H	-4.56852200	4.61268500	-1.10614700
H	-5.04643900	5.96695400	-0.07224100
H	-3.82429400	6.20258100	-1.33100500
C	1.49110100	-2.74988100	-1.31113600
N	0.36196400	-2.11535600	-0.62723000
C	0.39707300	-0.75156500	-0.34765200
C	-0.77896500	-0.07702000	0.05627500
C	-2.05286700	-0.80258700	0.17649600
C	-1.92714100	-2.26060200	0.21698400
C	-0.72665500	-2.87759400	-0.23017300
C	-0.66367200	-4.28788500	-0.25096000
C	-1.71789300	-5.05549700	0.20934500
C	-2.87103000	-4.45240600	0.72180600
C	-2.96072800	-3.07435200	0.71703900
H	-3.84641900	-2.59865000	1.12090600
H	-3.68193300	-5.05464700	1.11974800
H	-1.62865100	-6.13855500	0.19215300
H	0.23163000	-4.79130500	-0.59280500
N	-3.11962900	-0.07236600	0.26779500
C	-4.43391800	-0.48080600	0.17507000
C	-4.95855500	-1.14893700	-0.94577800
C	-6.31948500	-1.38464400	-1.09410300
C	-7.21421500	-0.93929800	-0.12538900
C	-6.72983500	-0.26419600	0.99086200
C	-5.36753100	-0.02276400	1.12036300

H	1.08318500	-3.54168600	-1.94473800
H	1.91463400	-2.01315200	-2.00141900
C	2.57986200	-3.29187900	-0.38018800
H	2.98763400	-2.46068000	0.20675600
H	2.13217700	-3.98105700	0.34768600
C	3.71877700	-3.99574500	-1.12747300
H	4.12712500	-3.32201900	-1.89394900
H	4.53774700	-4.16810300	-0.41859400
C	3.33043300	-5.32729100	-1.77070600
H	2.57285400	-5.20938400	-2.55468600
H	4.20085900	-5.80274700	-2.23560300
H	2.93407600	-6.02624900	-1.02363300
C	-0.75778200	1.30054600	0.25455700
C	1.56899200	0.00214900	-0.46829300
H	-1.71232700	1.74901800	0.49759400
H	2.49575200	-0.47970600	-0.74549800
F	-4.93412200	0.63985700	2.19735500
F	-7.57845900	0.16398700	1.92800100
F	-8.52184700	-1.16744100	-0.26046300
F	-6.77446300	-2.03049000	-2.17016800
F	-4.12727400	-1.58175600	-1.90000200

10ZZ

Total energy -1949.9288255

C	3.04454600	-1.88179900	-1.21524200
H	2.84994000	-1.08413300	-1.93935900
H	3.22163600	-2.78254800	-1.81018600
C	4.27305100	-1.53711900	-0.36814100

H	4.39782500	-2.28584900	0.42475000
H	4.10259200	-0.58344800	0.14426100
C	5.55894200	-1.44640300	-1.19882400
H	5.41066900	-0.73167500	-2.02070900
H	6.34389800	-1.01626300	-0.56612300
C	6.05382700	-2.78036500	-1.75891600
H	6.23309200	-3.50400200	-0.95401000
H	6.99968800	-2.64890600	-2.29560700
H	5.34503500	-3.23126600	-2.46368000
N	1.80715700	-2.10982600	-0.46366500
C	1.52644500	-3.38129100	0.02120000
C	2.51382000	-4.38955500	0.04669100
C	2.22313500	-5.65152000	0.53555100
C	0.94336800	-5.96200200	1.01041800
C	-0.03795700	-4.99102400	0.96790400
C	0.22773200	-3.70093300	0.47923300
C	-0.86190000	-2.73082400	0.34383700
C	-0.42562300	-1.33421900	0.16305700
C	0.91129300	-1.06920400	-0.24323100
C	1.29144500	0.26669400	-0.40952300
H	2.30269200	0.50385800	-0.70957800
C	0.42562500	1.33423700	-0.16306800
C	-0.91129100	1.06922100	0.24321600
C	-1.29144300	-0.26667600	0.40951300
H	-2.30268700	-0.50383700	0.70957800
N	-1.80715400	2.10984100	0.46366000
C	-1.52644300	3.38131000	-0.02119500
C	-2.51381800	4.38957300	-0.04668900

C	-2.22313200	5.65154000	-0.53554100
C	-0.94336300	5.96202600	-1.01040000
C	0.03796200	4.99104800	-0.96788800
C	-0.22772800	3.70095500	-0.47922500
C	0.86190300	2.73084300	-0.34383400
N	2.06808500	3.18454800	-0.43416200
C	3.26489500	2.62914800	-0.05662500
C	3.49240600	2.17697800	1.26357200
H	2.66344300	2.16105900	1.96487600
C	4.75851700	1.79673000	1.67532900
C	5.84274500	1.84051600	0.78169000
C	5.62560200	2.28562300	-0.53380800
C	4.36317800	2.68141700	-0.94156100
H	4.20161200	3.05582300	-1.94807600
H	6.46069000	2.33172700	-1.22662700
H	4.92080000	1.46470400	2.69675600
H	1.05088100	5.19602300	-1.29905400
H	-0.72406800	6.95156200	-1.40024800
H	-3.00966700	6.40150700	-0.55568600
H	-3.52113700	4.18207700	0.29131100
C	-3.04454400	1.88179800	1.21523200
H	-2.84994000	1.08410300	1.93931800
H	-3.22162600	2.78252500	1.81021100
C	-4.27305400	1.53716100	0.36812100
H	-4.39784100	2.28594300	-0.42471900
H	-4.10259200	0.58352600	-0.14434500
C	-5.55893800	1.44637600	1.19880900
H	-5.41064900	0.73159900	2.02064900

H	-6.34389100	1.01626400	0.56608700
C	-6.05384000	2.78029600	1.75898500
H	-6.23312100	3.50397900	0.95412500
H	-6.99969600	2.64878900	2.29567500
H	-5.34505100	3.23116500	2.46377400
N	-2.06808100	-3.18452800	0.43417900
C	-3.26489400	-2.62914500	0.05662300
C	-3.49242000	-2.17705500	-1.26359900
H	-2.66346900	-2.16118700	-1.96491700
C	-4.75853500	-1.79682400	-1.67536100
C	-5.84275000	-1.84054100	-0.78170200
C	-5.62558900	-2.28556600	0.53382100
C	-4.36316300	-2.68134900	0.94157900
H	-4.20158500	-3.05569200	1.94811400
H	-6.46066700	-2.33161800	1.22665600
H	-4.92083100	-1.46486100	-2.69680700
H	-1.05087500	-5.19599700	1.29907500
H	0.72407300	-6.95153600	1.40027000
H	3.00967000	-6.40148800	0.55569300
H	3.52113600	-4.18206100	-0.29131900
C	7.14466800	1.43310600	1.20140100
C	-7.14467400	-1.43314400	-1.20141800
N	-8.20522800	-1.08743400	-1.53698300
N	8.20521900	1.08738500	1.53696100