

Supporting Information

A simple and efficient synthesis of a series of N -(thiazol-2-yl)piperidine-2,6-dione
compounds and their interesting NLO properties

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Table 1: Crystal data and CCDC number of compounds 1-5.

	Compound-1	Compound -2	Compound -3	Compound-4	Compound -5
Empirical formula	C ₈ H ₈ N ₂ O ₂ S	C ₉ H ₁₀ N ₂ O ₂ S	C ₉ H ₁₀ N ₂ O ₂ S	C ₁₀ H ₁₂ N ₂ O ₂ S	C ₁₂ H ₁₀ N ₂ O ₂ S
Formula weight	196.22	210.25	210.25	224.28	246.28
Temperature/K	293(2)	293(2)	293(2)	293(2)	293(2)
Crystal system	orthorhombic	orthorhombic	monoclinic	orthorhombic	orthorhombic
Space group	Fdd2	Pna2 ₁	P2 ₁ /c	Pbca	Pbca
a/Å	22.635(4)	17.270(2)	10.4402(13)	11.0048(7)	10.7717(9)
b/Å	18.2458(18)	6.5290(5)	9.0667(12)	9.1927(7)	9.2453(9)
c/Å	8.4549(12)	8.7853(8)	10.6841(15)	21.2407(14)	23.0901(14)
α/°	90	90	90	90	90
β/°	90	90	103.828(12)	90	90
γ/°	90	90	90	90	90
Volume/Å ³	3491.9(8)	990.61(16)	982.0(2)	2148.8(2)	2299.5(3)
Z	16	4	4	8	8
ρ _{calc} /cm ³	1.493	1.410	1.422	1.387	1.423
μ/mm ⁻¹	0.336	0.301	0.304	0.282	0.272
F(000)	1632.0	440.0	440.0	944.0	1024.0
Crystal size/mm ³	0.98 × 0.26 × 0.243	0.94 × 0.79 × 0.6	1.47 × 0.8 × 0.447	1.177 × 0.683 × 0.301	1.26 × 0.693 × 0.346

Radiation	Mo K α ($\lambda = 0.71073$)	Mo K α ($\lambda = 0.71073$)	Mo K α ($\lambda = 0.71073$)	Mo K α ($\lambda = 0.71073$)	Mo K α ($\lambda = 0.71073$)
2 Θ range for data collection/ $^{\circ}$	7.2 to 57.668	6.672 to 57.672	7.704 to 52.74	6.94 to 58.04	6.796 to 52.744
Index ranges	$-26 \leq h \leq 28$, $-16 \leq k \leq 24$, $-11 \leq l \leq 4$	$-23 \leq h \leq 18$, $-7 \leq k \leq 8$, $-6 \leq l \leq 11$	$-13 \leq h \leq 12$, $-11 \leq k \leq 9$, $-13 \leq l \leq 12$	$-13 \leq h \leq 14$, $-12 \leq k \leq 12$, $-25 \leq l \leq 29$	$-13 \leq h \leq 12$, $-11 \leq k \leq 11$, $-28 \leq l \leq 28$
Reflections collected	2347	3049	3834	7976	12129
Independent reflections	1290 [$R_{\text{int}} = 0.0159$, $R_{\text{sigma}} = 0.0232$]	1505 [$R_{\text{int}} = 0.0140$, $R_{\text{sigma}} = 0.0189$]	1982 [$R_{\text{int}} = 0.0148$, $R_{\text{sigma}} = 0.0237$]	2104 [$R_{\text{int}} = 0.0321$, $R_{\text{sigma}} = 0.0459$]	2321 [$R_{\text{int}} = 0.0331$, $R_{\text{sigma}} = 0.0270$]
Data/restraints/parameters	1290/1/118	1505/1/128	1982/0/138	2104/0/139	2321/0/187
Goodness-of-fit on F^2	0.961	1.075	1.060	1.022	0.715
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0347$, $wR_2 = 0.1099$	$R_1 = 0.0412$, $wR_2 = 0.1136$	$R_1 = 0.0367$, $wR_2 = 0.0924$	$R_1 = 0.0460$, $wR_2 = 0.1040$	$R_1 = 0.0525$, $wR_2 = 0.1553$
Final R indexes [all data]	$R_1 = 0.0379$, $wR_2 = 0.1158$	$R_1 = 0.0448$, $wR_2 = 0.1164$	$R_1 = 0.0468$, $wR_2 = 0.0989$	$R_1 = 0.0671$, $wR_2 = 0.1155$	$R_1 = 0.0699$, $wR_2 = 0.1783$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	0.16/-0.16	0.48/-0.41	0.19/-0.22	0.46/-0.15	0.37/-0.21
Flack parameter	0.32(13)	0.18(6)			
CCDC Number	1560120	1561181	2062131	2062127	1561183

Table 2: Geometries of hydrogen bond in Compound-1 to compound-5								
	D	H	A	d(D...H)/Å	d(H...A)/Å	d(D...A)/Å	D-H...A/°	Symmetry operation for A
Compound-1	C7	H7A	O1 ¹	0.97	2.47	3.222 (4)	133.8	¹ -7/4-X,1/4+Y,1/4+Z;
	C5	H5A	O1 ¹	0.97	2.48	3.234 (4)	134.6	
	C3	H3	N1 ²	0.93	2.56	3.224 (4)	129.0	² -7/4-X,-1/4+Y,-1/4+
Compound-2	C2	H2	O2 ¹	0.93	2.62	3.416 (5)	143.7	¹ 3/2-X,-1/2+Y,1/2+Z
	C4	H4B	O2 ¹	0.96	2.57	3.412 (6)	146.0	
Compound-3	C8	H8B	N1 ¹	0.97	2.54	3.399 (2)	147.1	¹ 2-X,1-Y,2-Z;
	C2	H2	O1 ²	0.93	2.56	3.084 (2)	115.7	² 1-X,1/2+Y,3/2-Z;
	C4	H4B	O1 ³	0.96 (4)	2.62 (4)	3.562 (3)	168 (3)	³ +X,1/2-Y,-1/2+Z
Compound-4	C9	H9A	O1 ¹	0.97	2.56	3.433 (3)	150.1	¹ 1/2+X,+Y,3/2-Z;
	C4	H4A	O1 ²	0.96	2.55	3.436 (3)	153.2	² -X,-Y,1-Z
Compound-5	C9	H9B	O2 ¹	0.93 (5)	2.45 (5)	3.281 (4)	148 (4)	¹ 1-X,-1/2+Y,3/2-Z;
	C11	H11C	O1 ²	1.40 (6)	2.65 (6)	3.538 (5)	119 (4)	² 1/2+X,+Y,3/2-Z

Table 3: SHG experimental data of compounds 1-5.

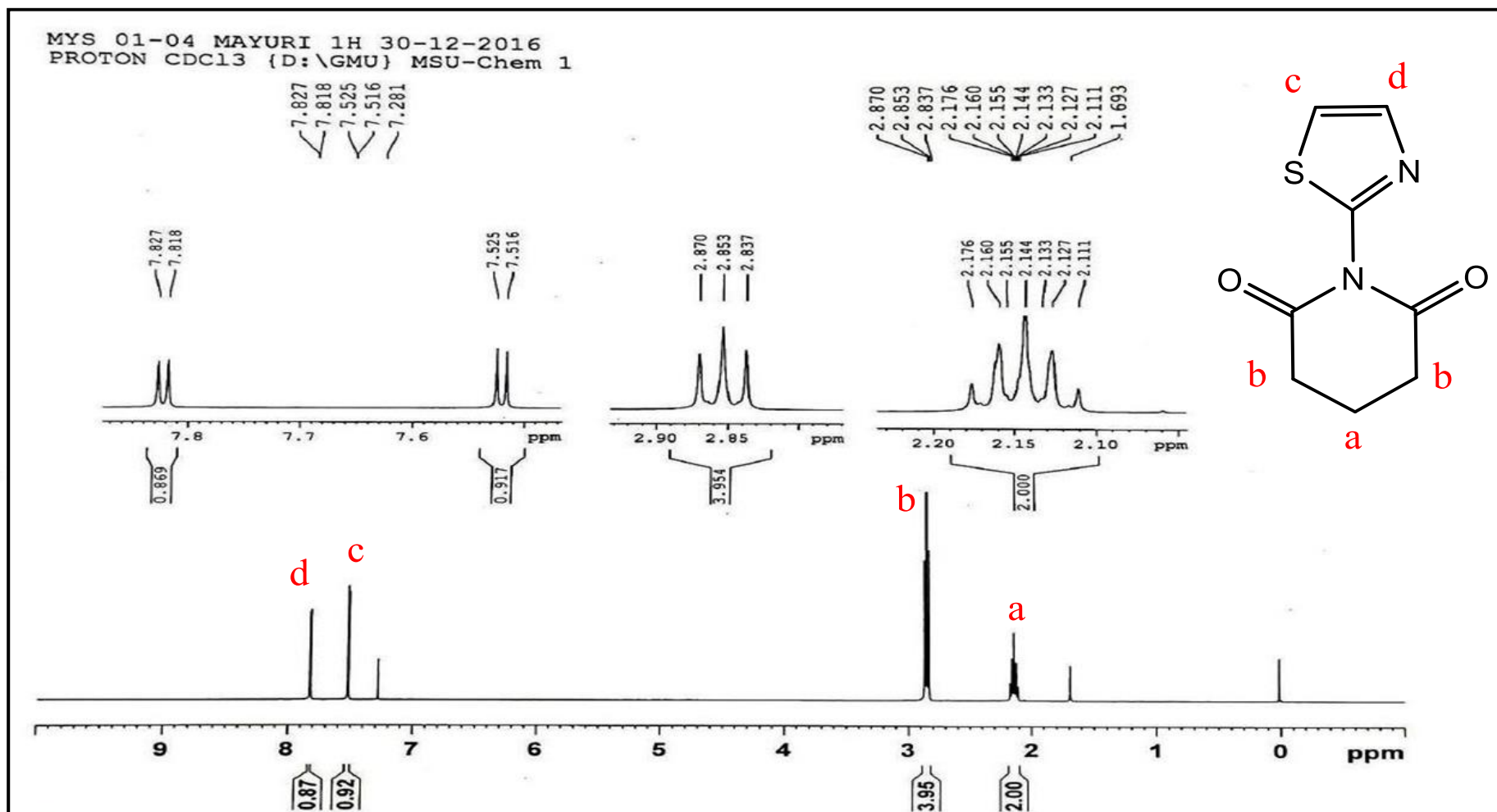
Compound Info.	Compound 1 (2-AT) M.F.:C ₈ H ₈ N ₂ O ₂ S CCDC: 1560120 Fdd ₂	Compound 2 (2-AT-5-Me) M.F.:C ₉ H ₁₀ N ₂ O ₂ S CCDC: 1561181 Pna2 ₁	Compound 3 (2-AT-4-Me) M.F.:C ₉ H ₁₀ N ₂ O ₂ S CCDC: 2062131 P2 ₁ /c	Compound 4 (2-AT-4,5-Dime) M.F.:C ₁₀ H ₁₂ N ₂ O ₂ S CCDC: 2062127 Pbca	Compound 5 (2-AT-Phenyl) M.F.:C ₁₂ H ₁₀ N ₂ O ₂ S CCDC: 1561183 Pbca
NLO-Second Harmonic generation	192 mV 3.05> Urea 6.62> KDP	60mV 0.95> Urea 2.07> KDP	10 mV 0.3 > Urea = KDP	25 mV 0.5> Urea 1.13> KDP	10mV 0.3 > Urea = KDP

Table 4 : % Contribution of various non-covalent interactions in Compound-1to Compound-5 (calculated using Hirshfeld surface analysis)

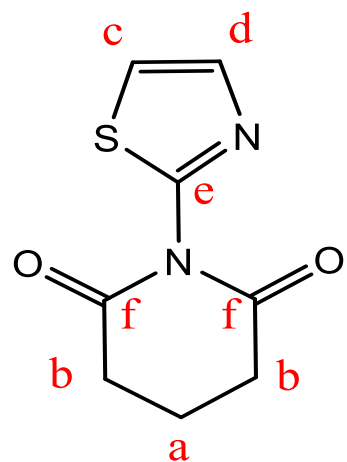
%	C-H	H-C	C-O	O-C	C-N	N-C	C-S	S-C	S-N	N-S	N-O	O-N	C-C	O-O	H-H	O-H	H-O	H-S	S-H	O-S	S-O	H-N	N-H
Compounds																							
2-AT	4.0	3.1	1.0	0.8	0.7	0.7	0.3	0.3	0.2	0.1	0.7	0.7	1.1	0.3	27.6	15.5	13.6	5.2	9.0	1.2	1.6	5.5	6.9
2-A-5-MT	5.1	4.1	0.7	0.7	0.0	0.0	0.0	0.1	0.0	0.0	0.6	0.6	0.0	0.4	36.2	13.8	11.2	3.5	6.7	1.5	2.1	5.4	7.1
2-A-4-MT	5.1	4.2	0.4	0.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.7	1.0	34.0	14.4	11.8	4.5	8.9	1.1	1.7	5.3	6.5
2-A-4,5-DMT	3.6	2.9	0.7	0.6	0.0	0.0	0.7	0.7	0.7	0.6	0.5	0.3	0.3	0.1	42.7	13.8	11.5	3.4	6.1	0.7	1.0	4.0	5.2
2-ABT	9.9	7.9	0.5	0.5	0.0	0.0	1.4	1.4	0.7	0.5	0.4	0.3	4.4	0.5	30.0	12.0	10.0	3.2	5.5	0.8	1.1	3.9	5.1

Physico-Chemical Characterization of Compounds 1-5

Data of Compound -1: Piperidine-2, 6-dione derivative of 2-Aminothiazole



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171.94

155.28

141.13

122.41

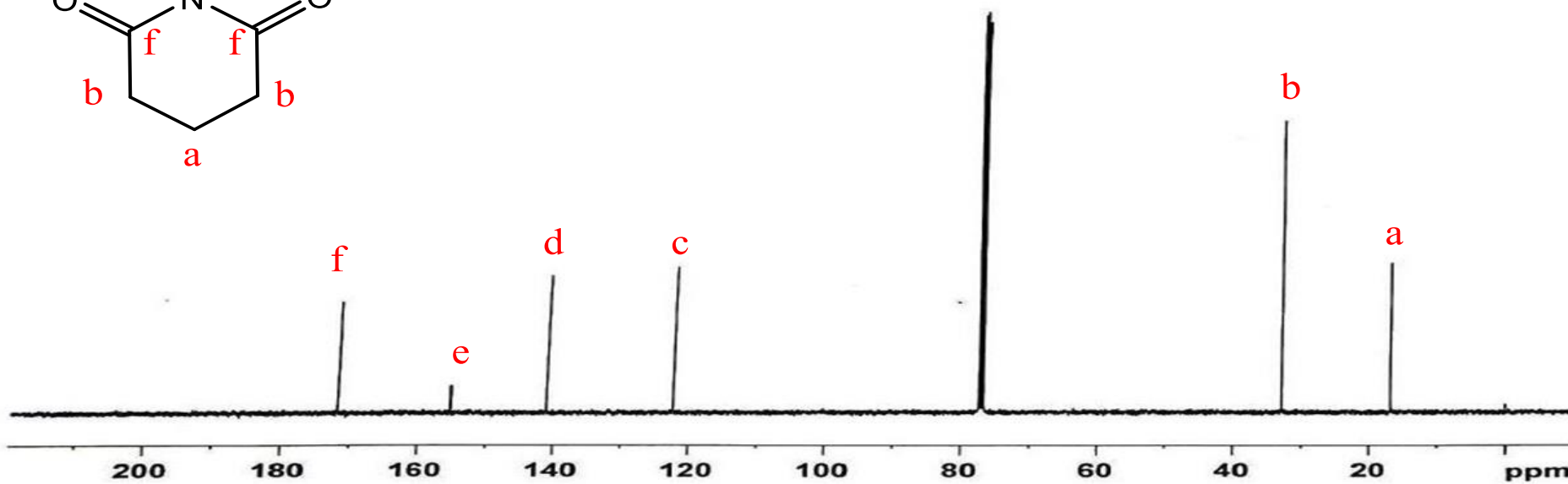
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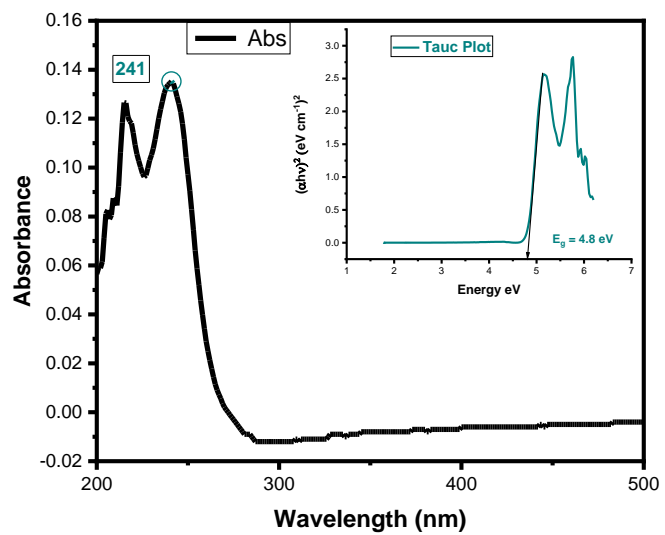
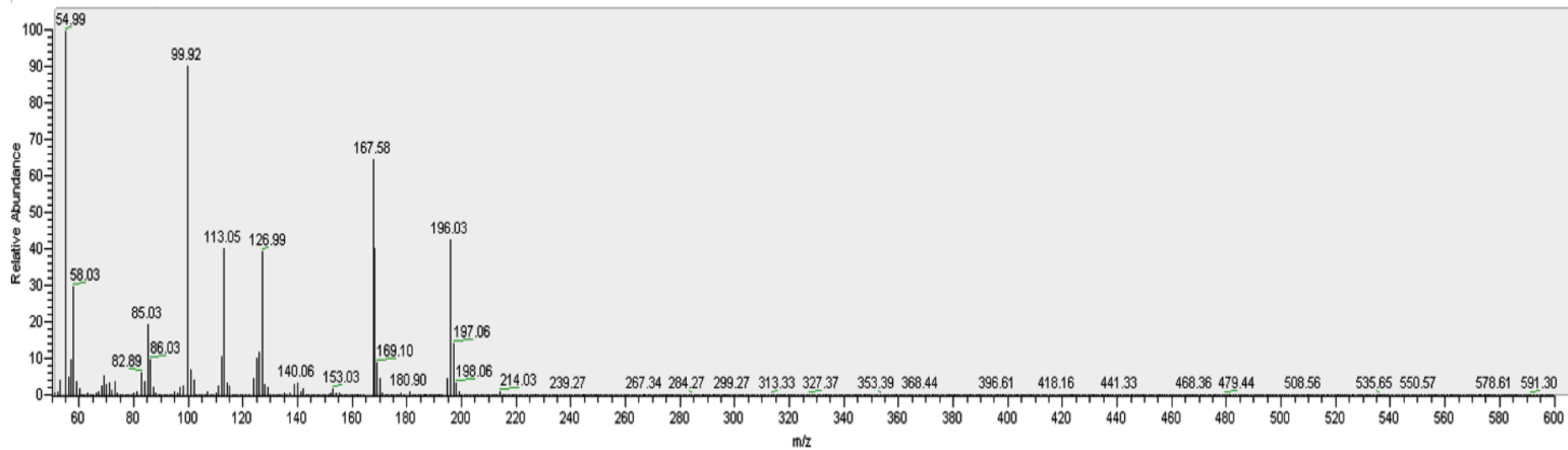
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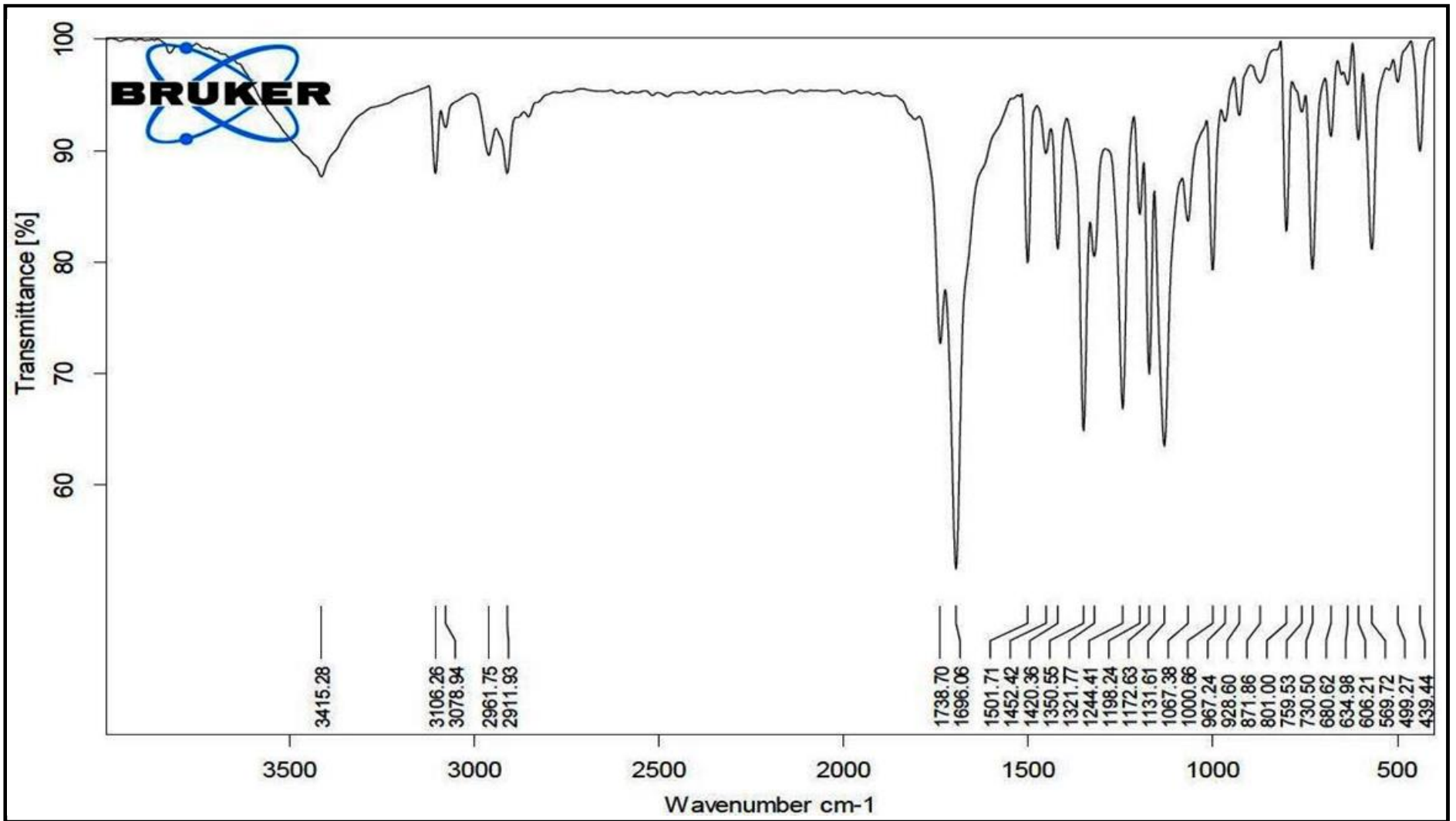
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32.86

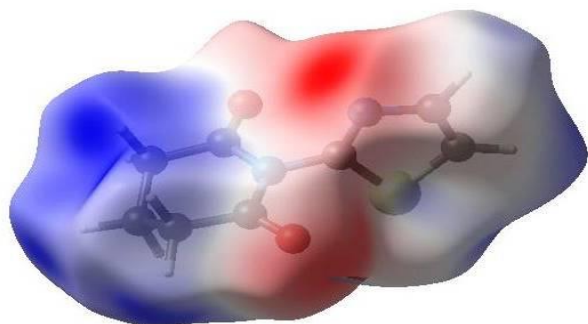
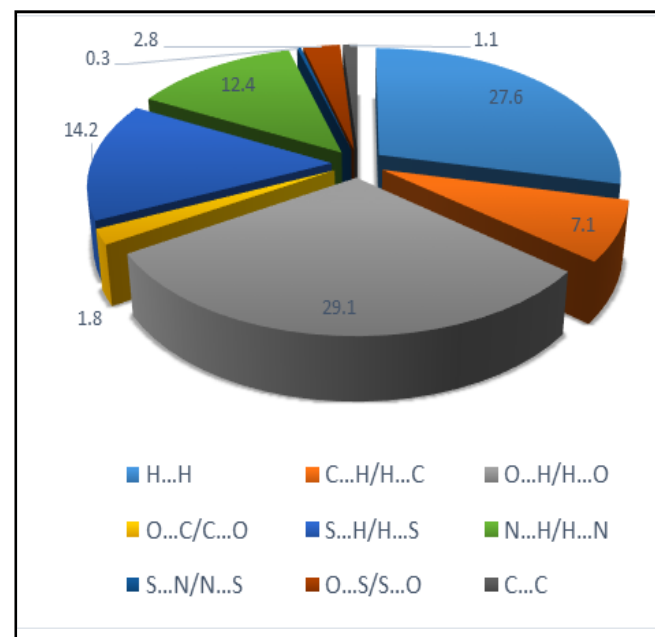
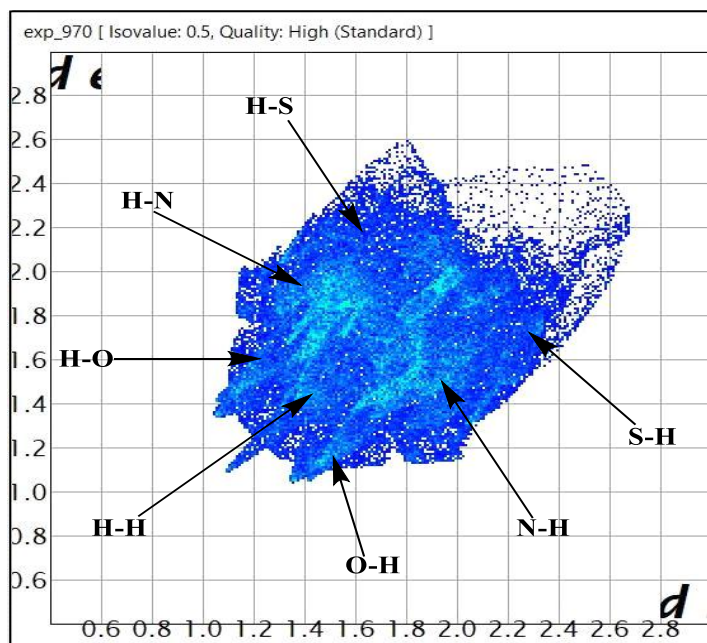
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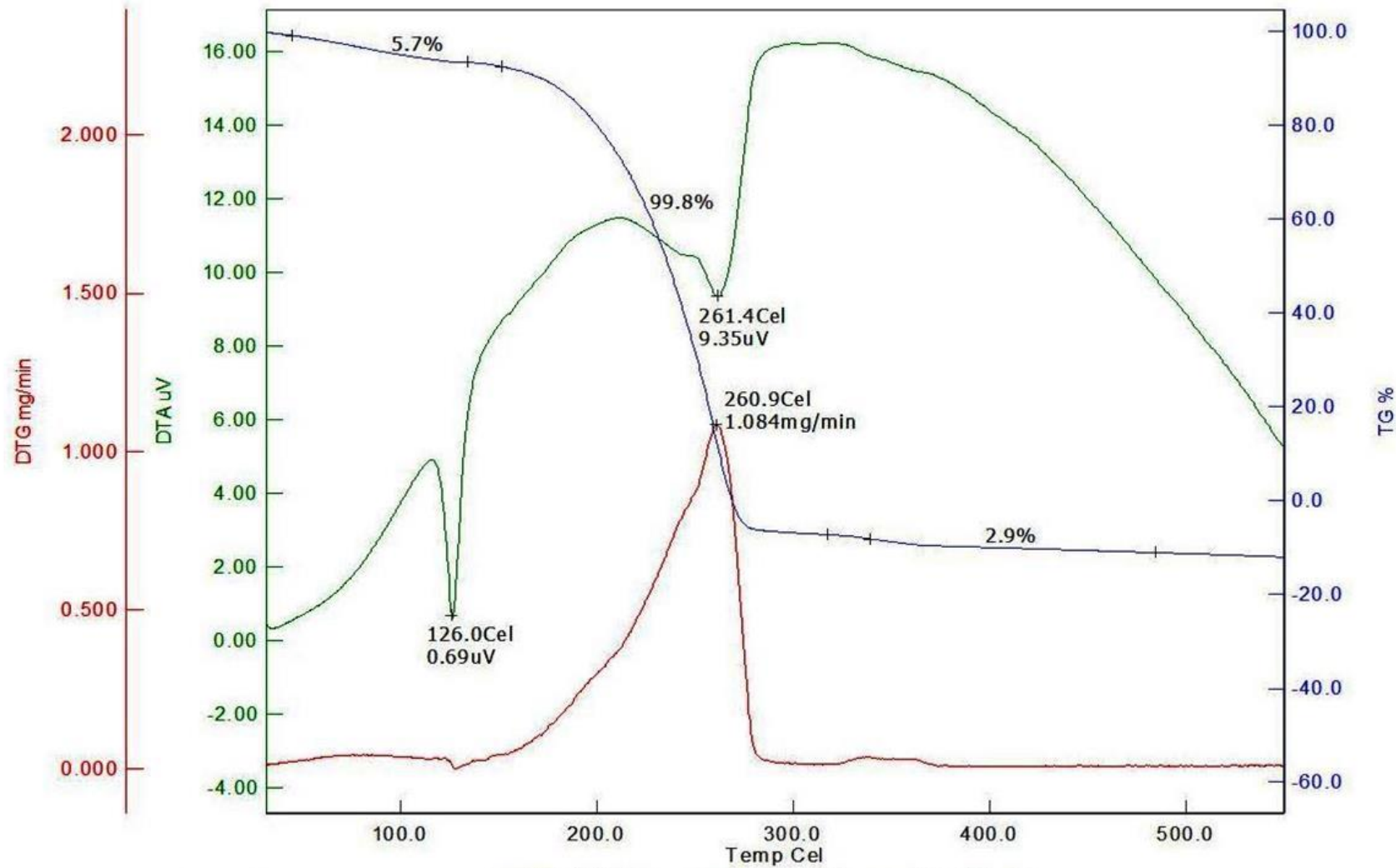




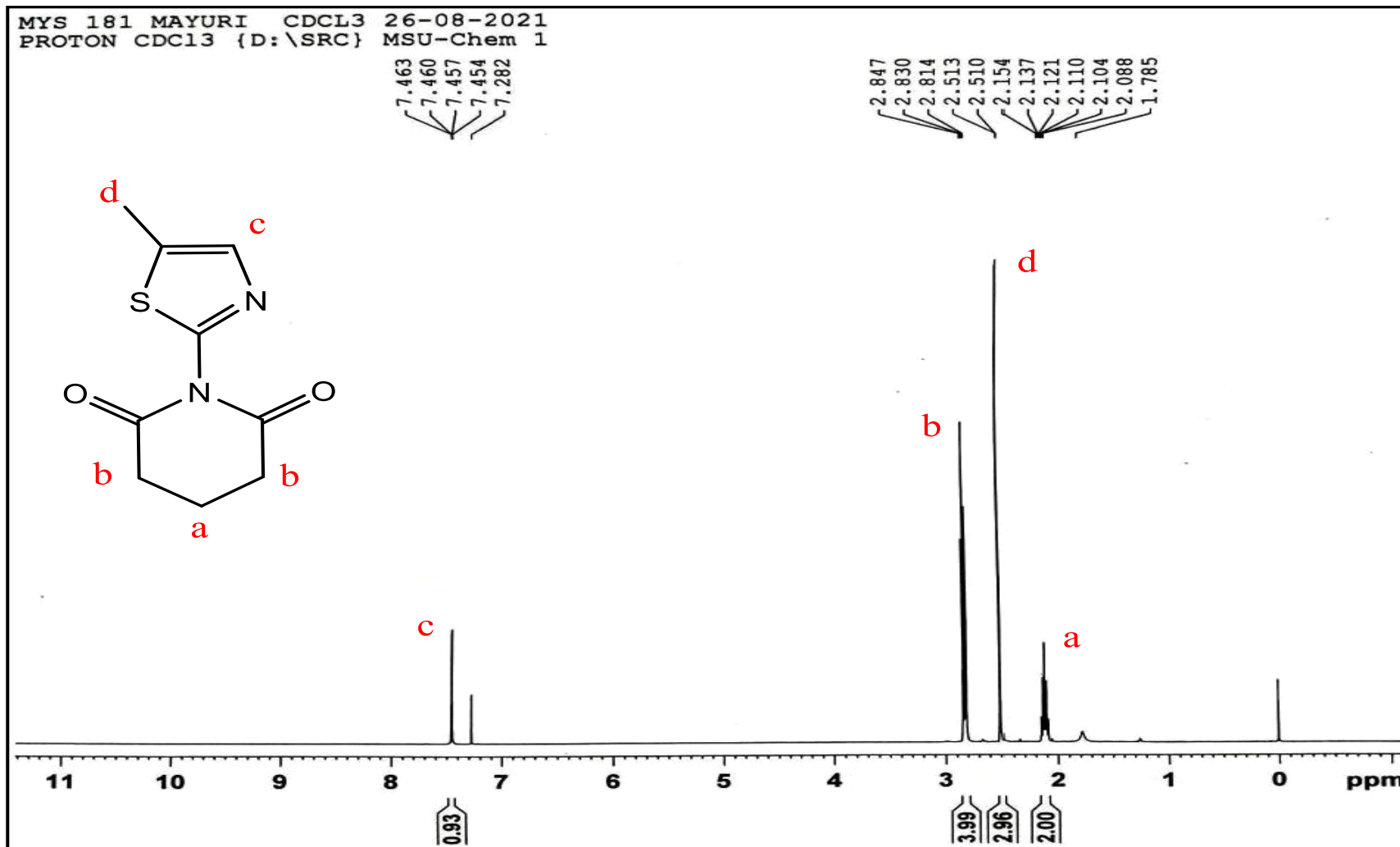


Compound 1: Hirschfeld fingerprint graph and % contribution of weak interactions

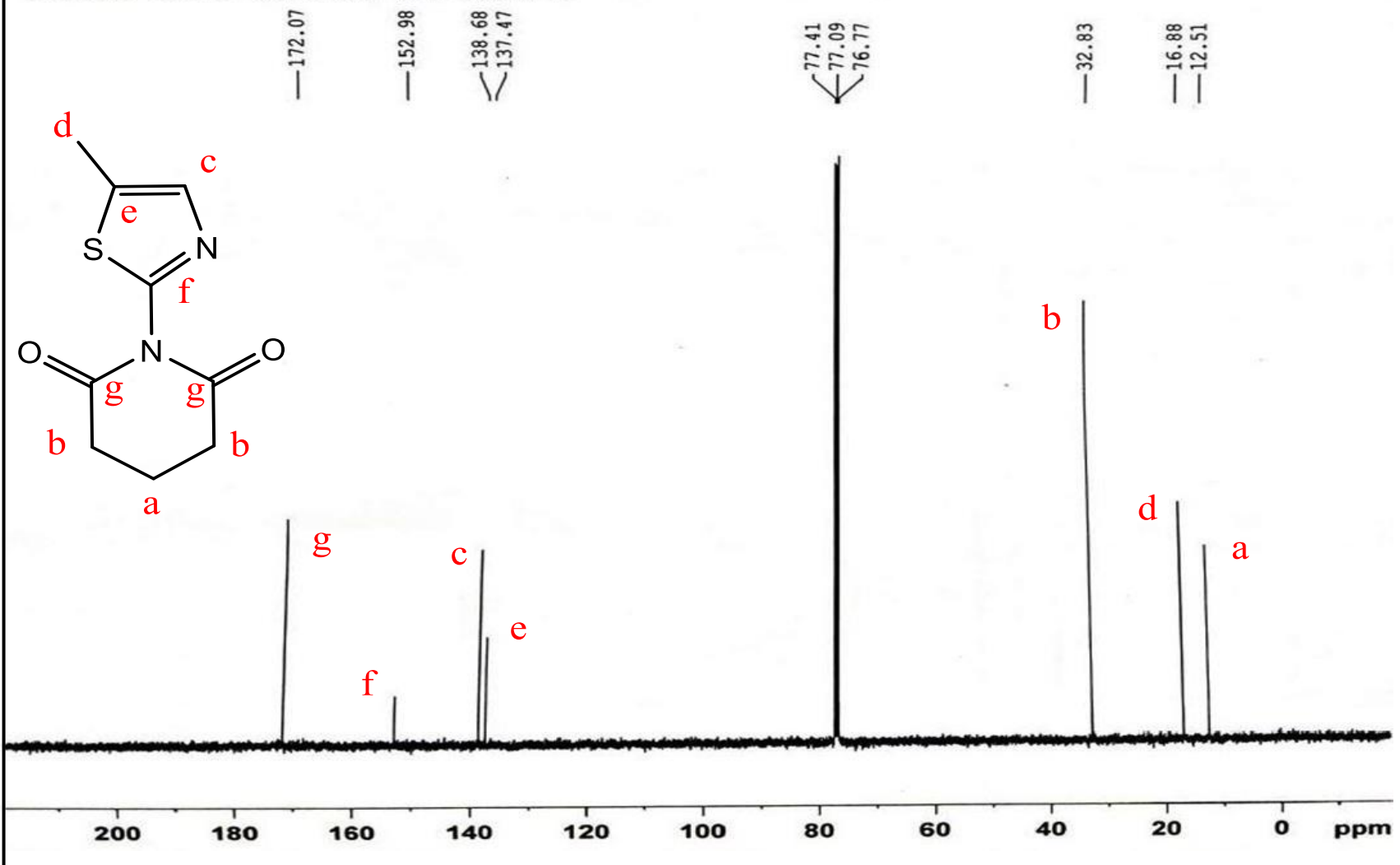


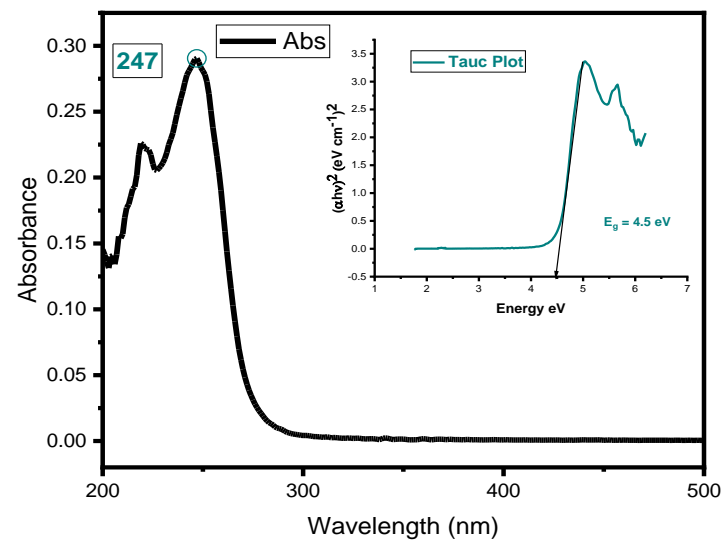
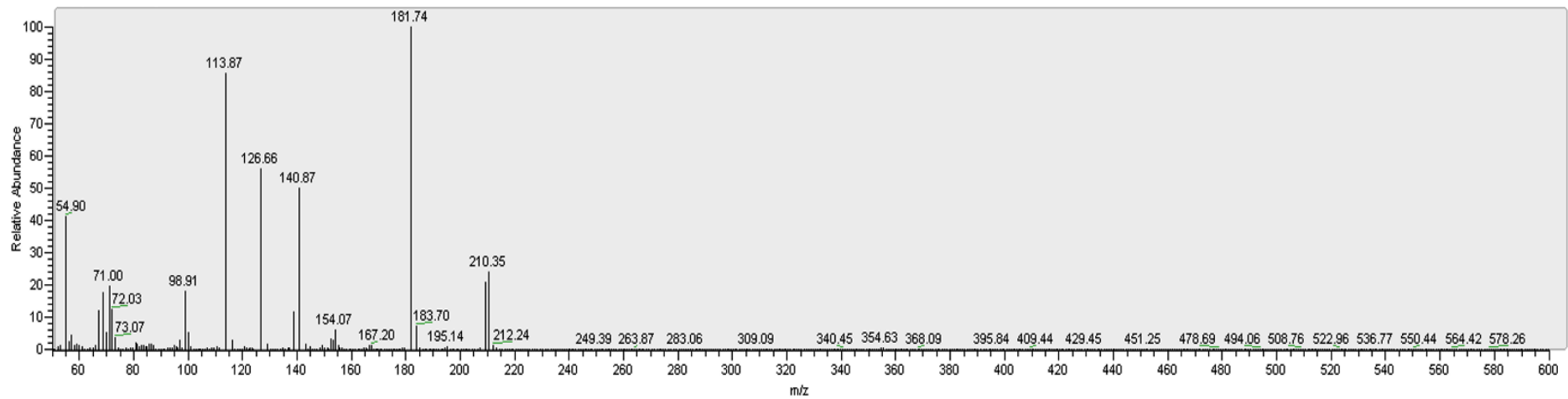


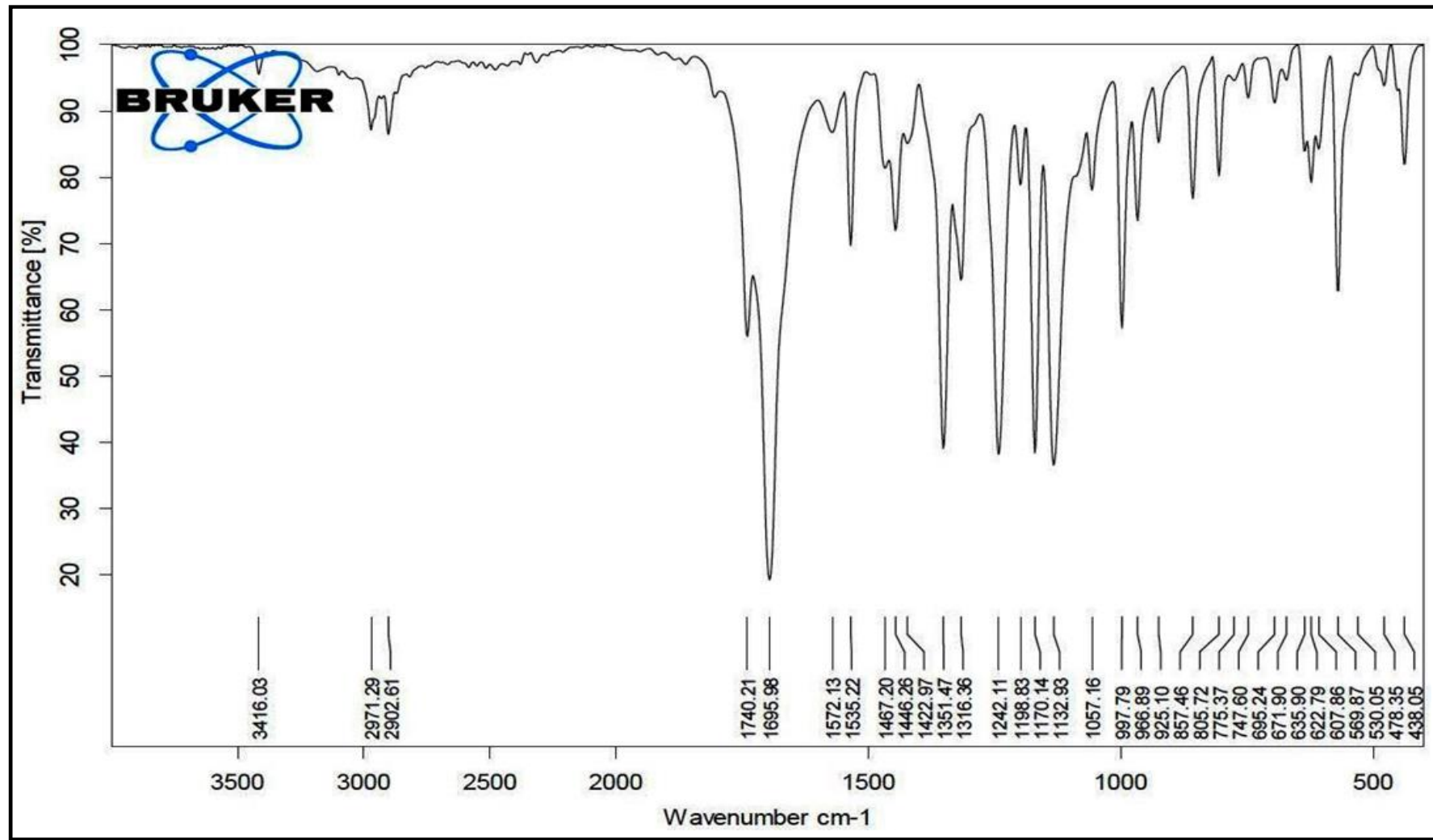
Data of Compound -2: 2-Amino-5-methylthiazole derivative

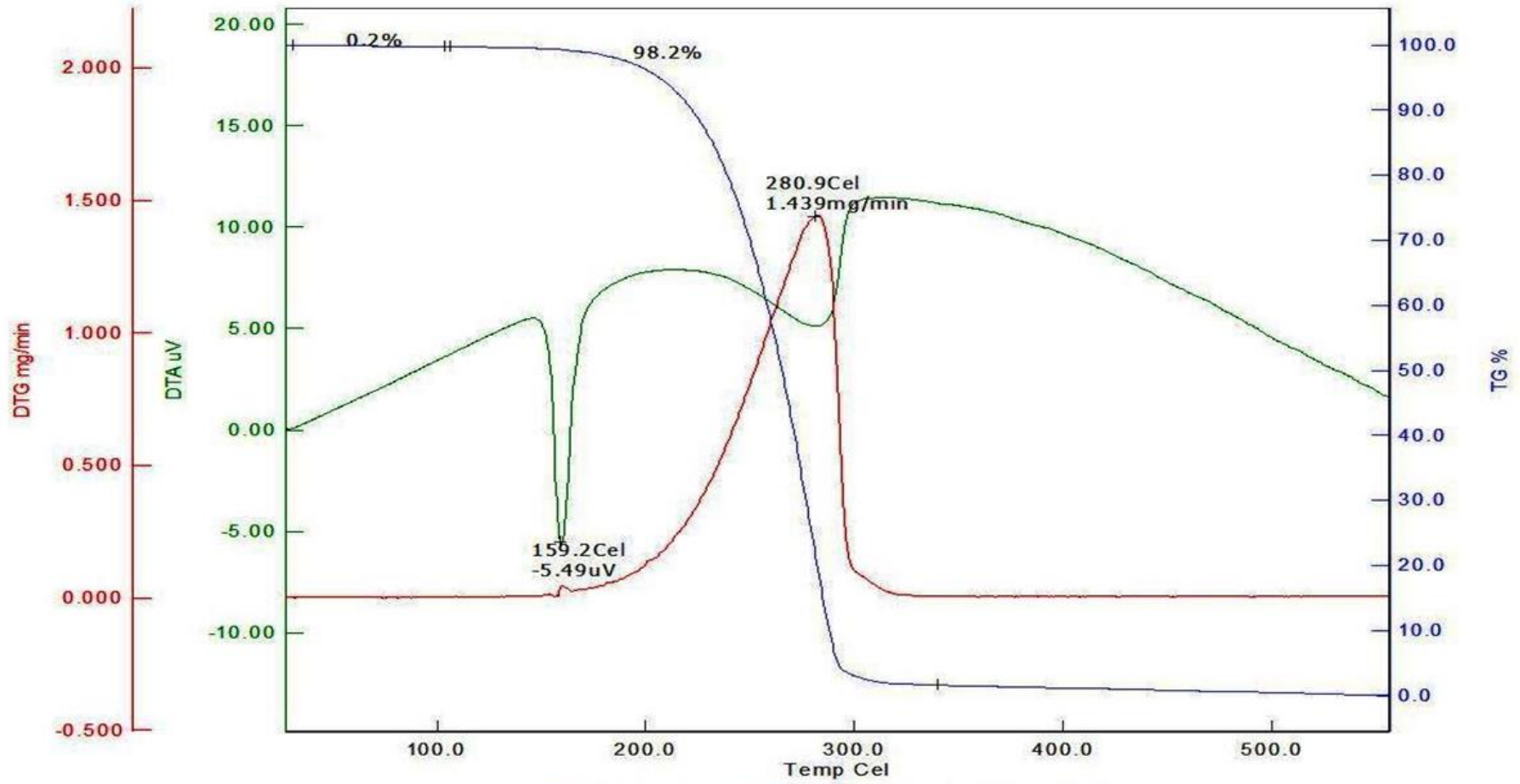


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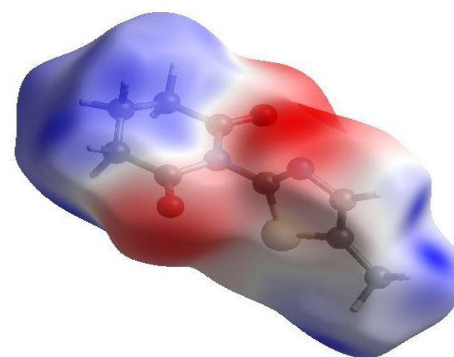
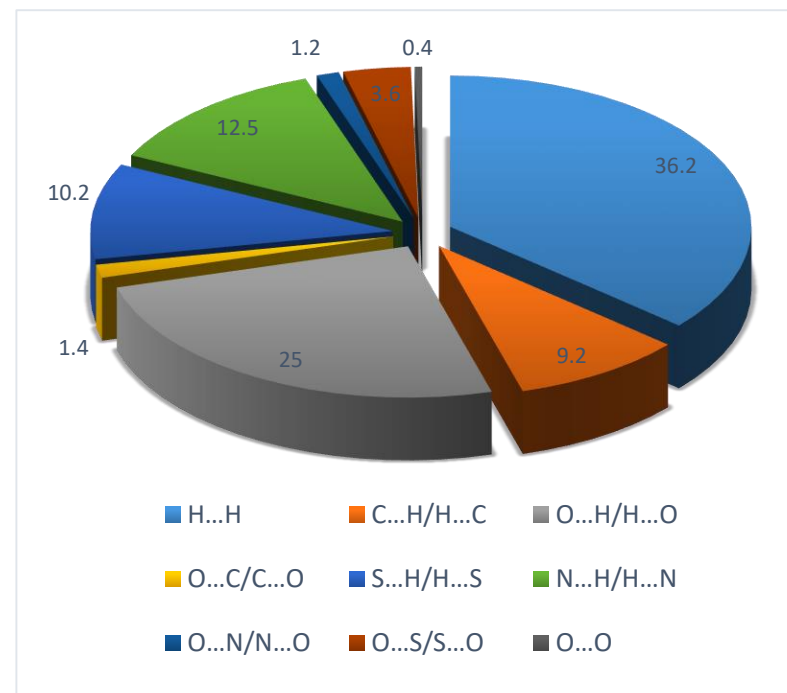
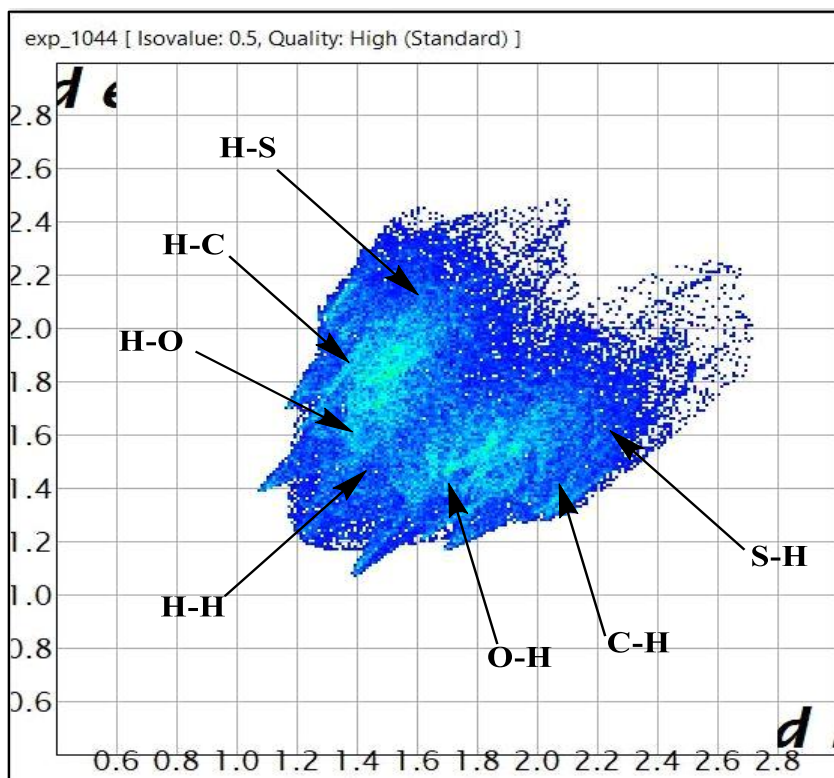




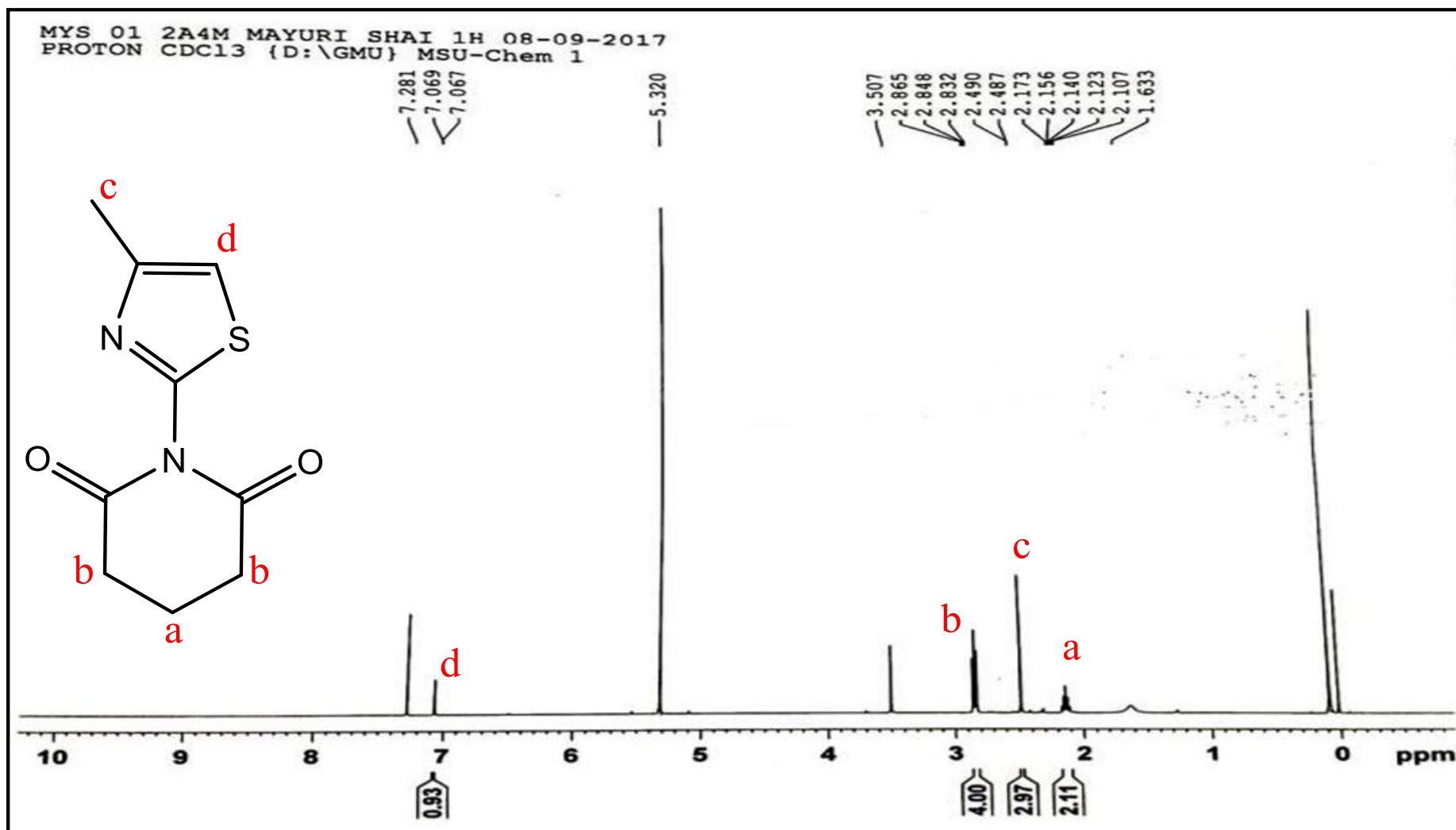
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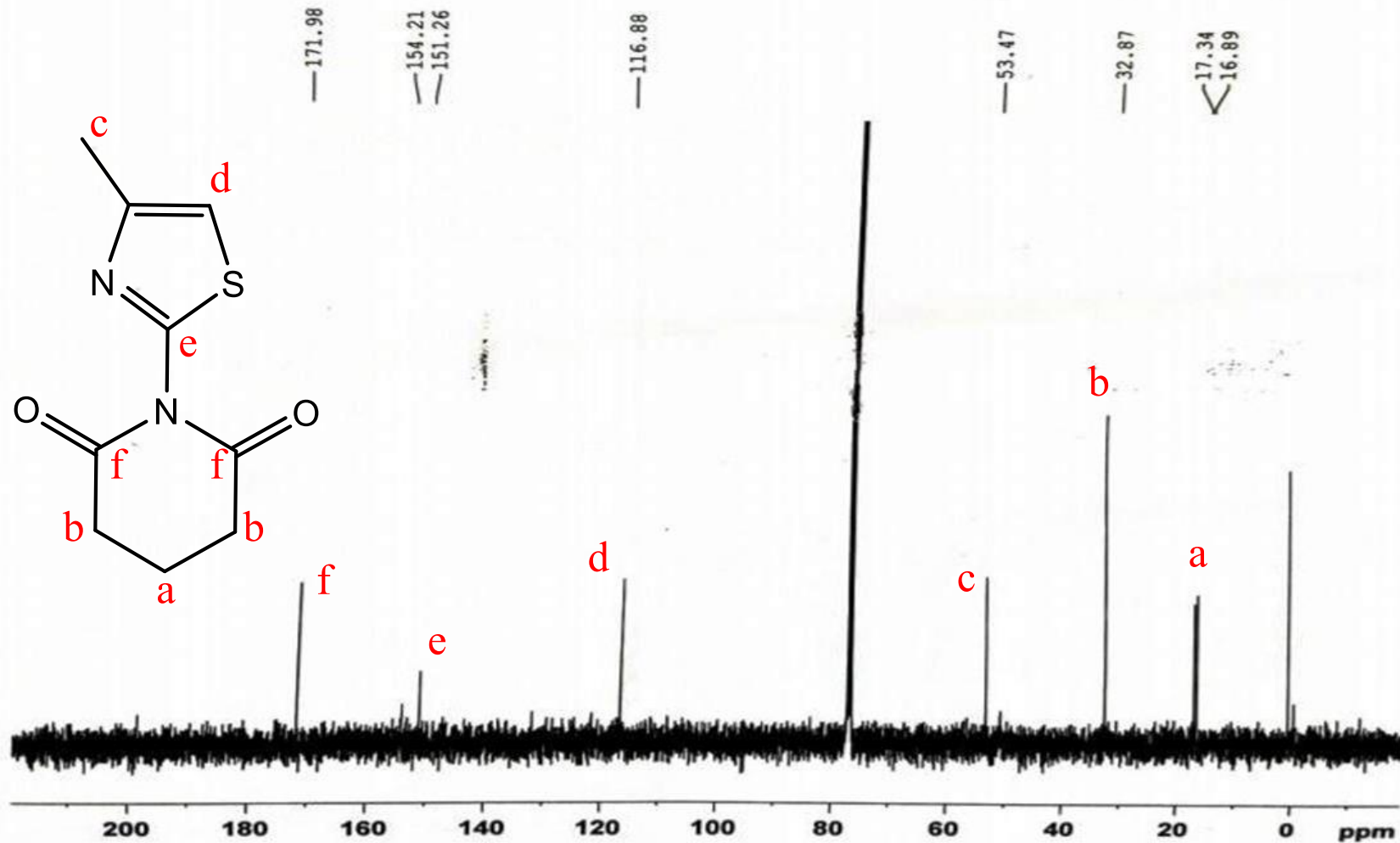
2-A-5MT product: Hirschfeld fingerprint graph and % contribution of weak interactions

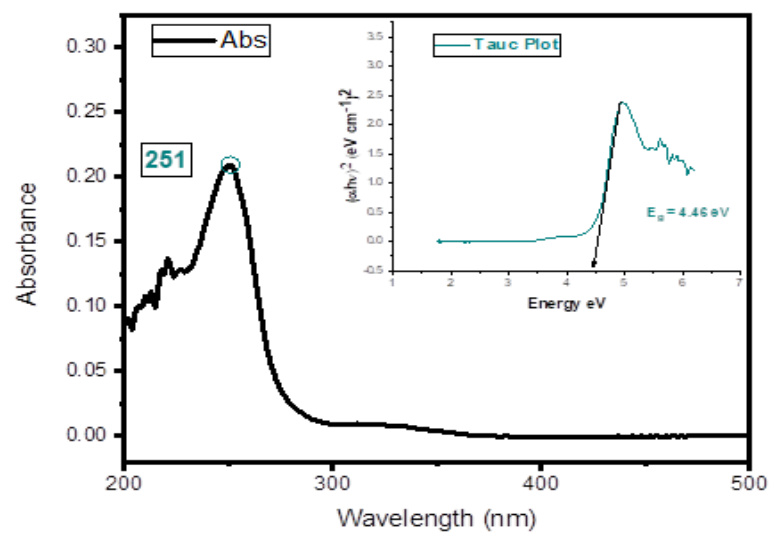
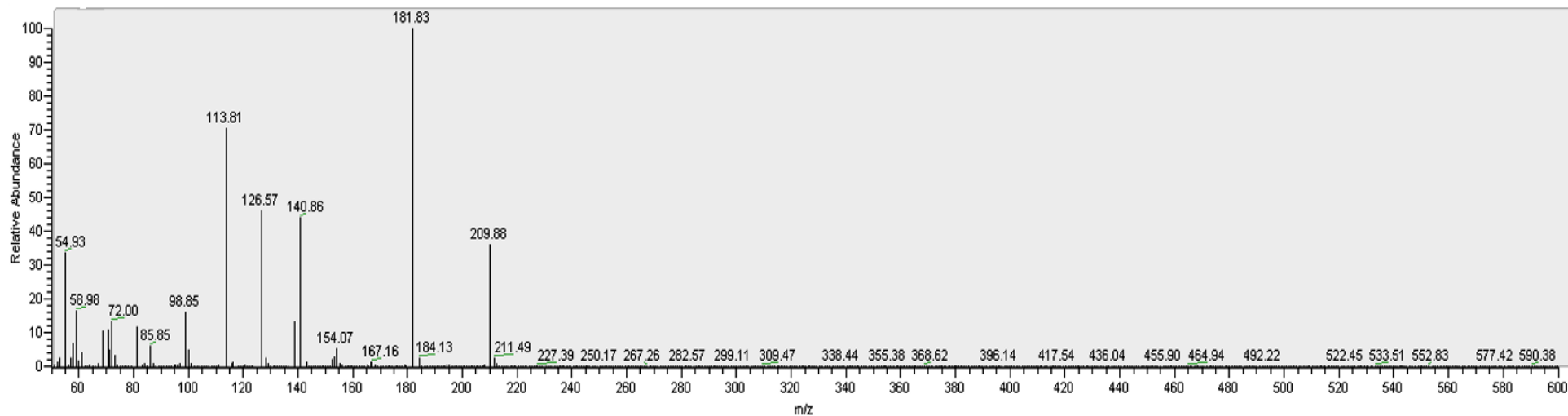


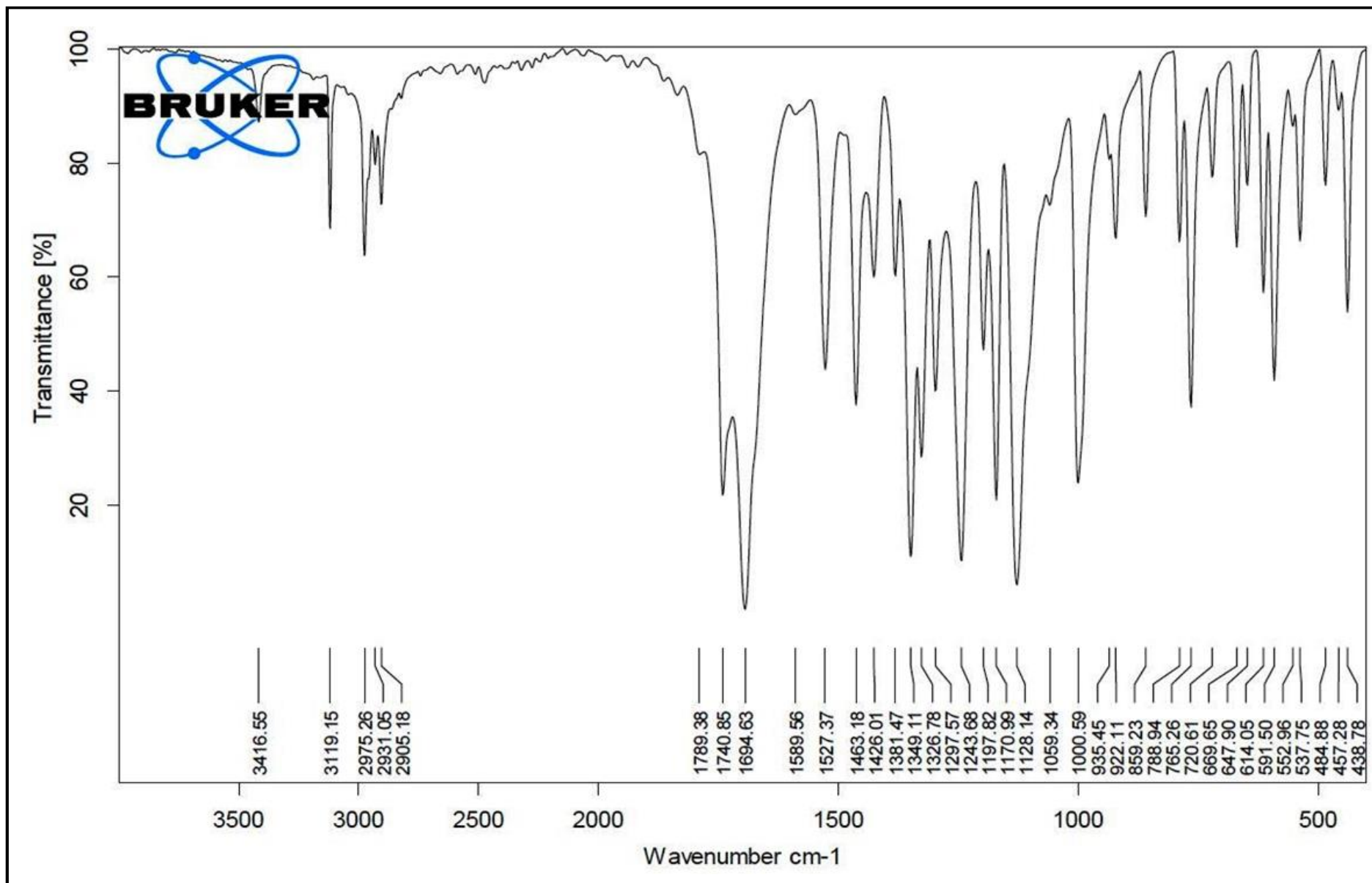
Data of Compound -3: 2-Amino-4-methylthiazole derivative

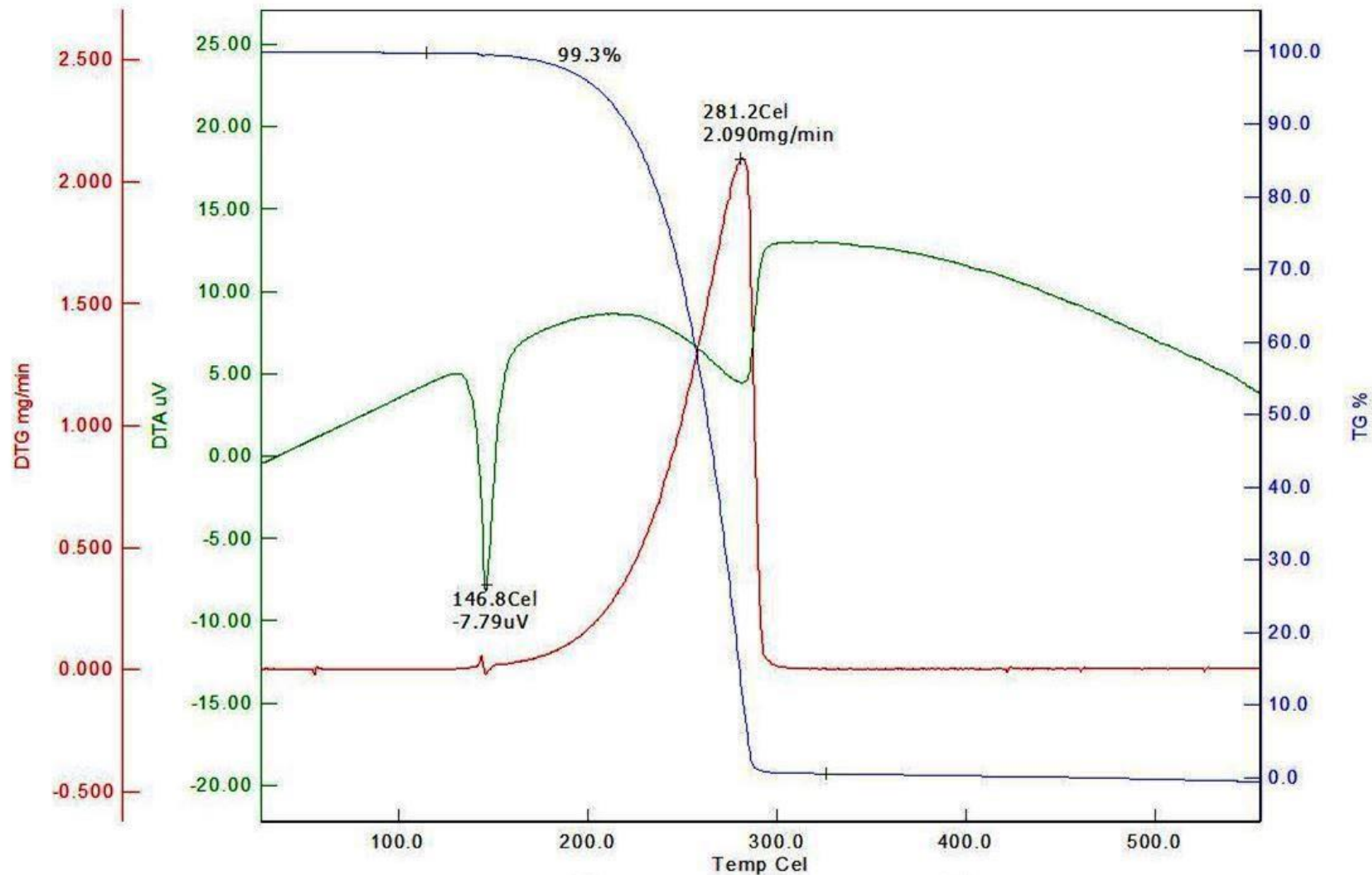


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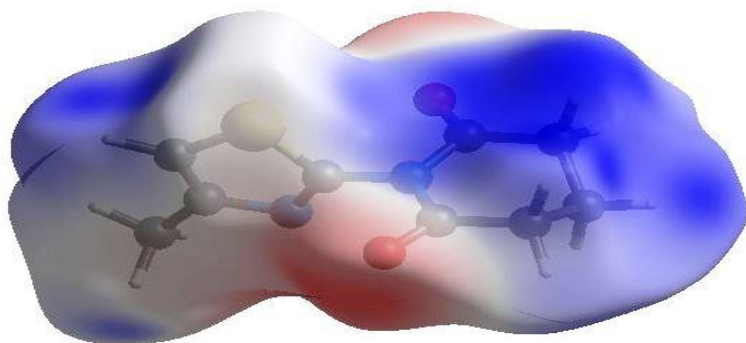
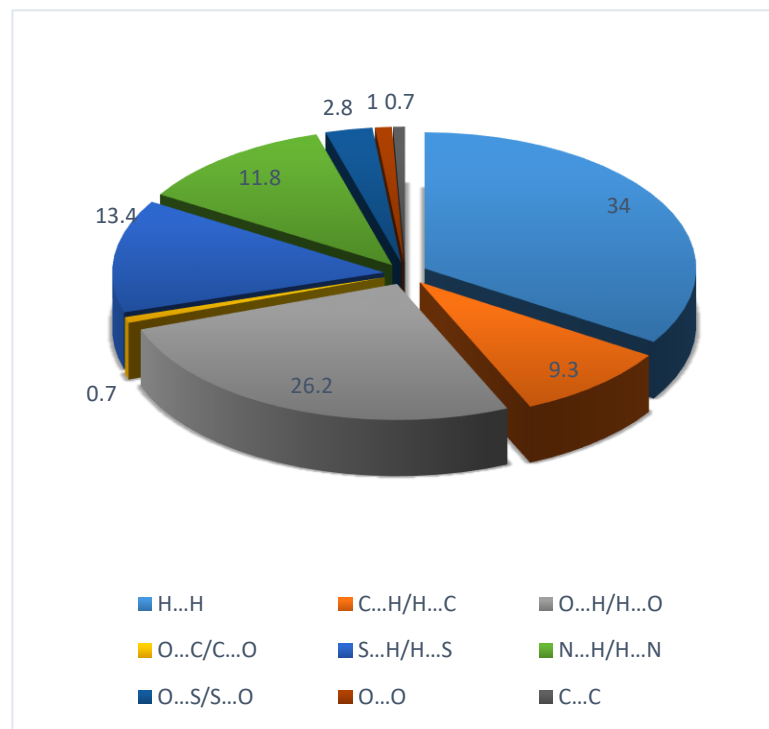
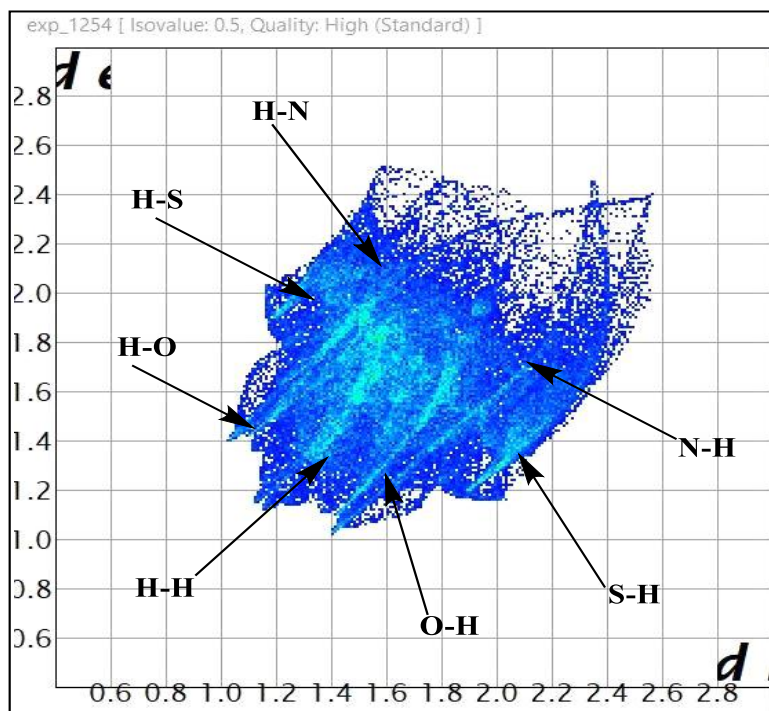




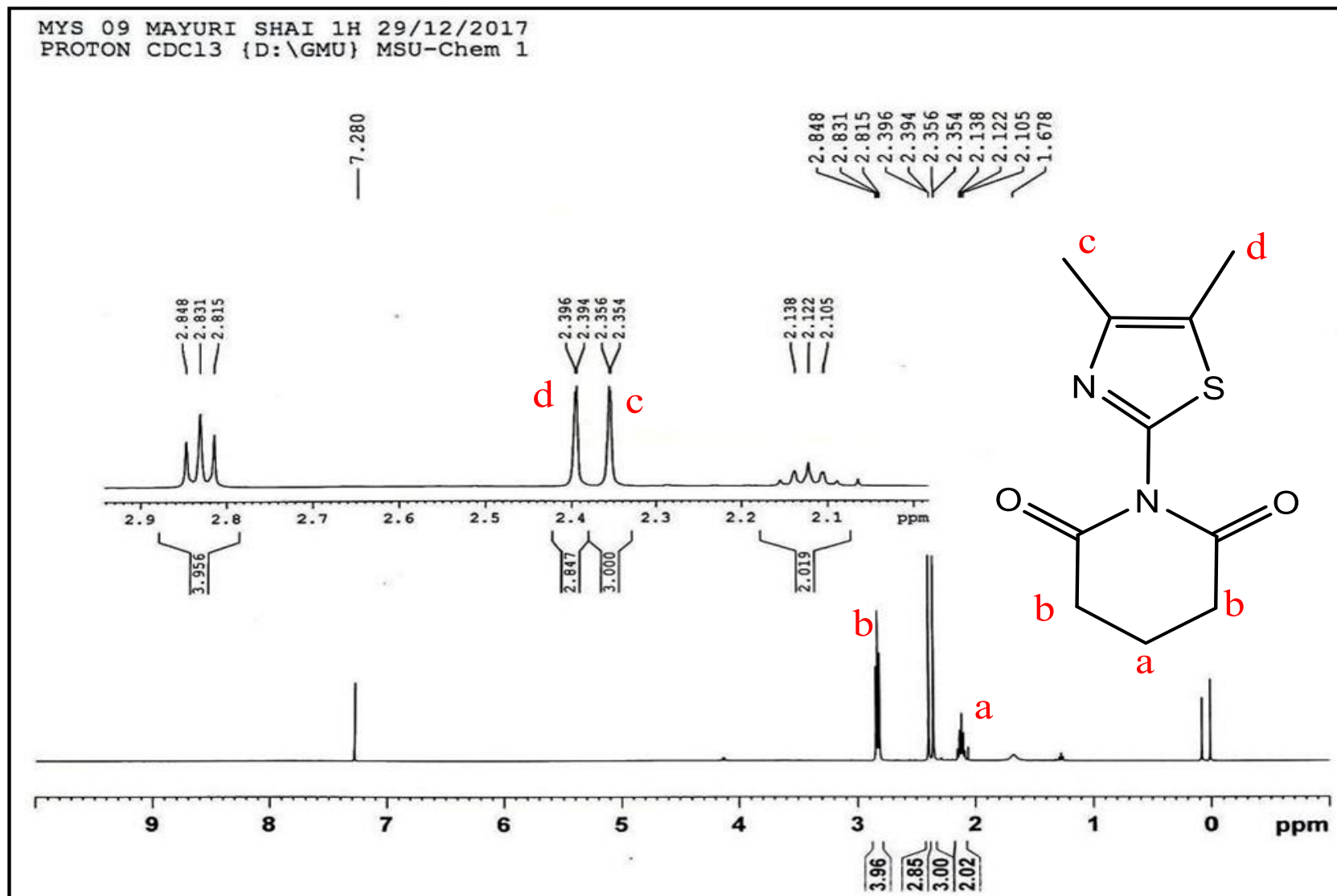
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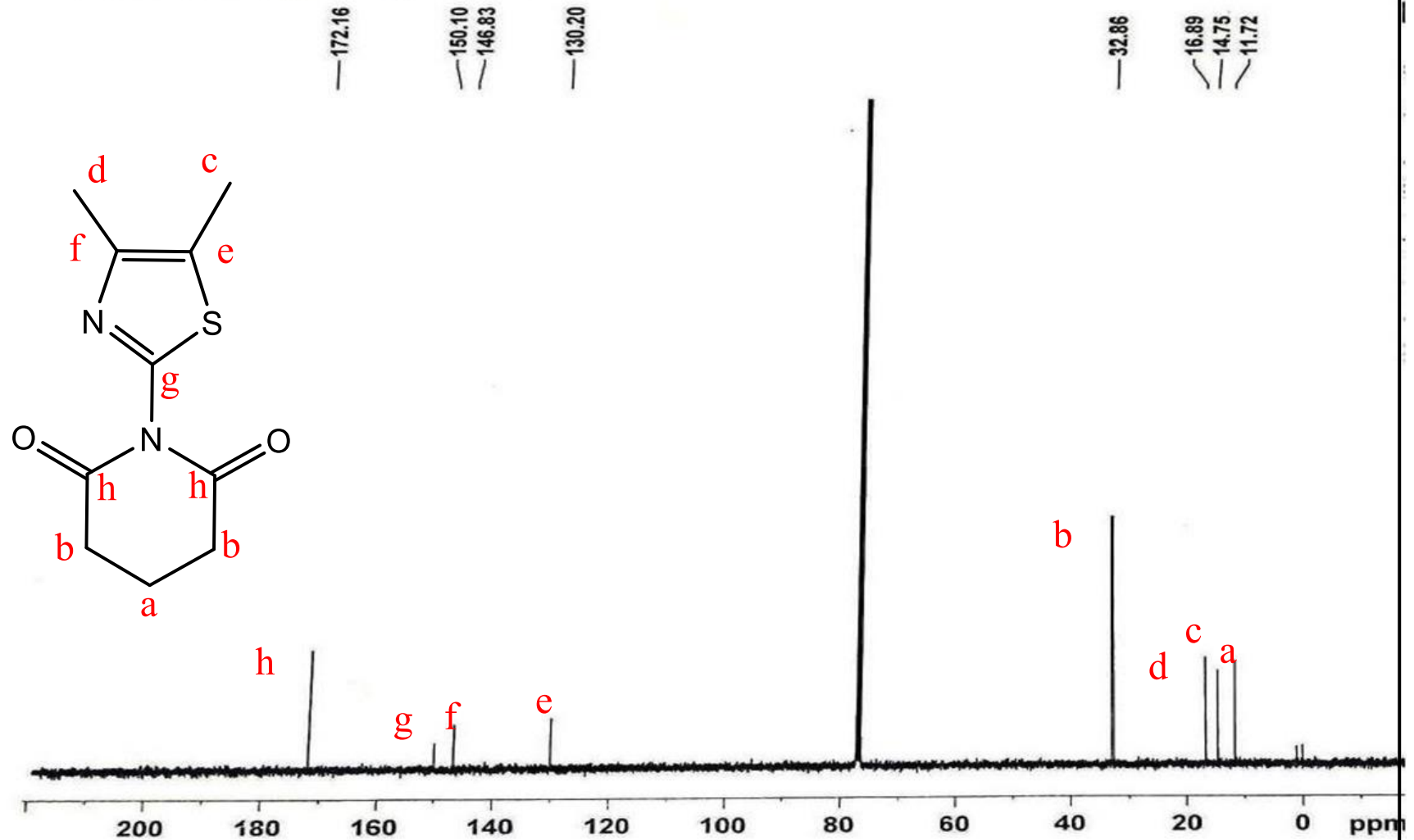
2-A-4-MT product: Hirschfeld fingerprint graph and % contribution of weak interactions

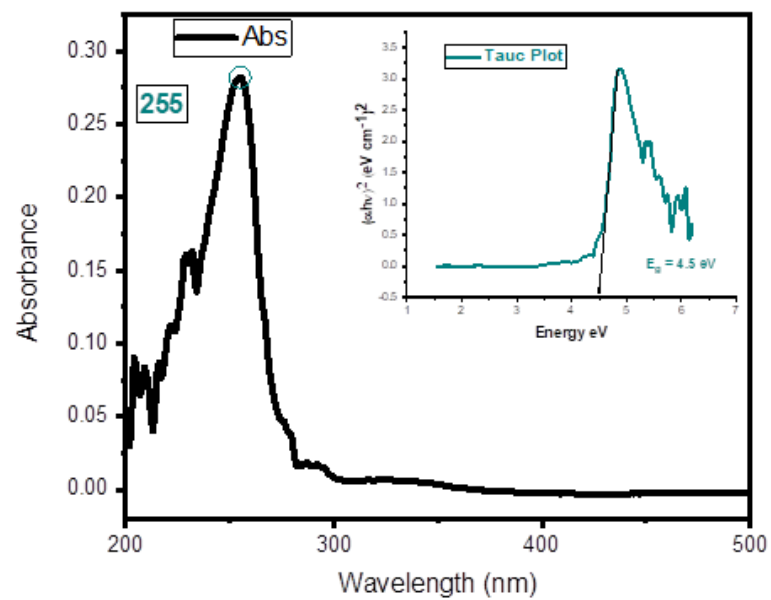
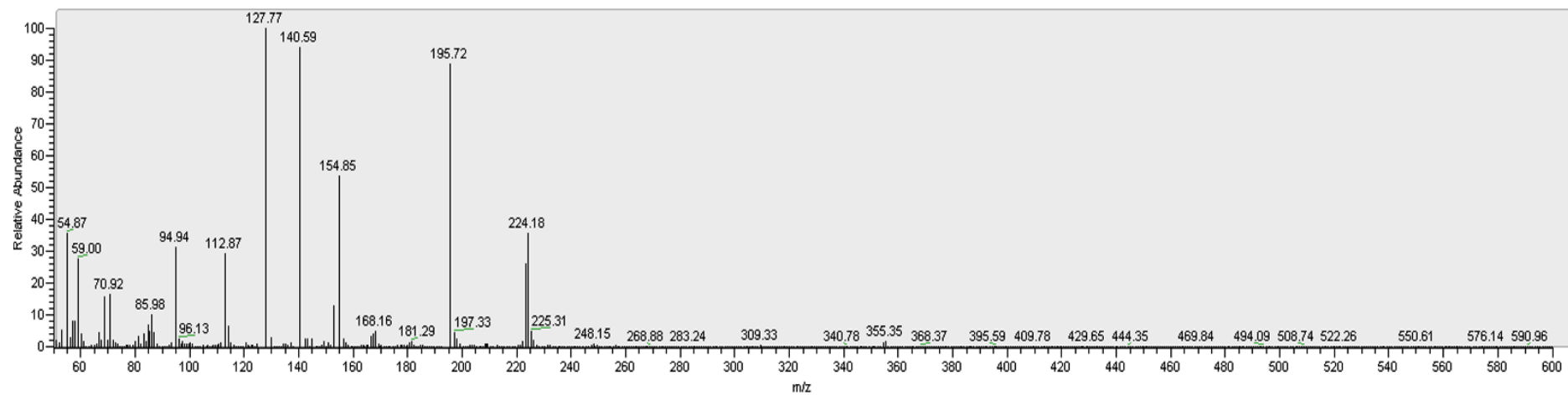


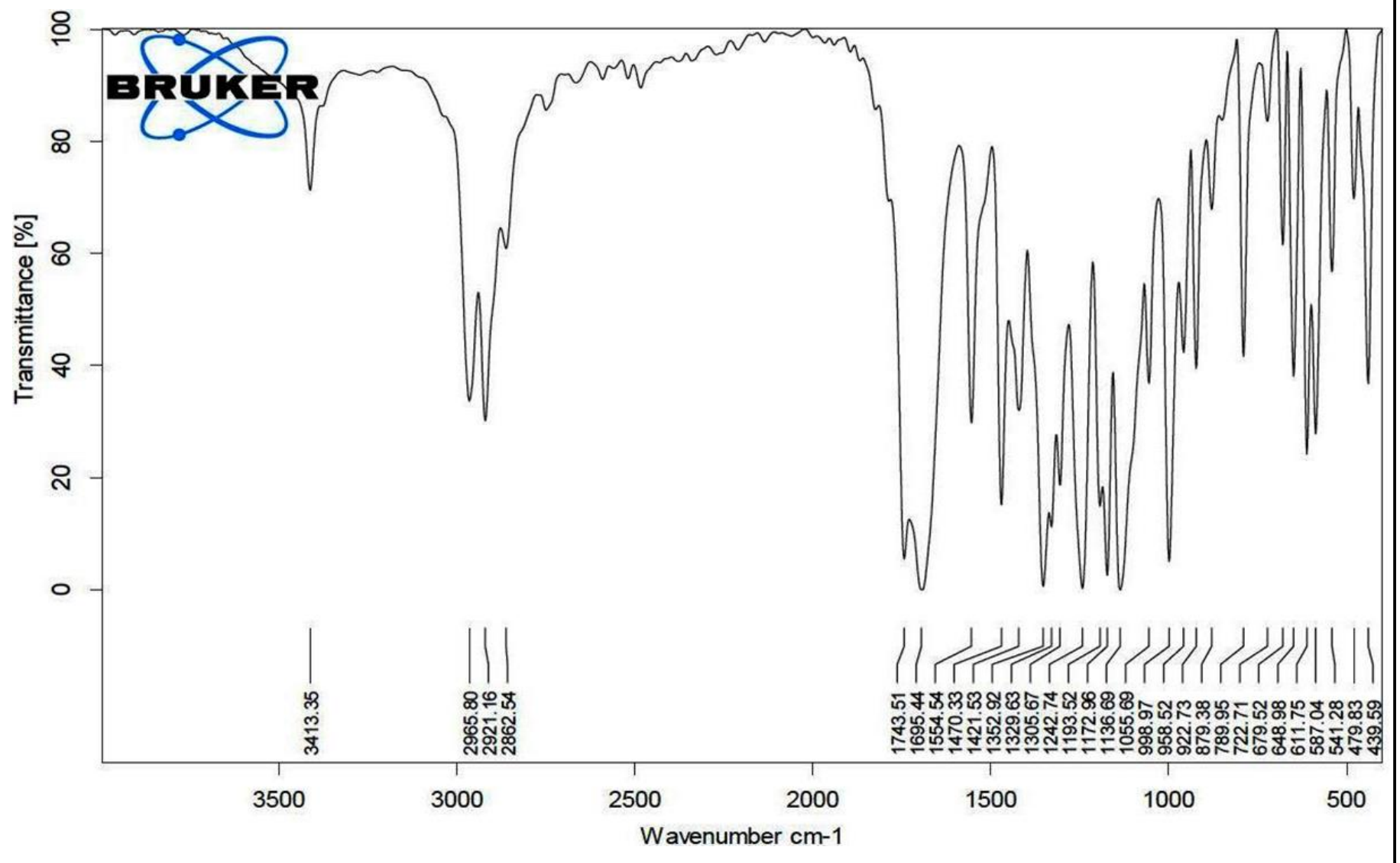
Data of Compound -4: 2-Amino-4,5-dimethylthiazole derivative

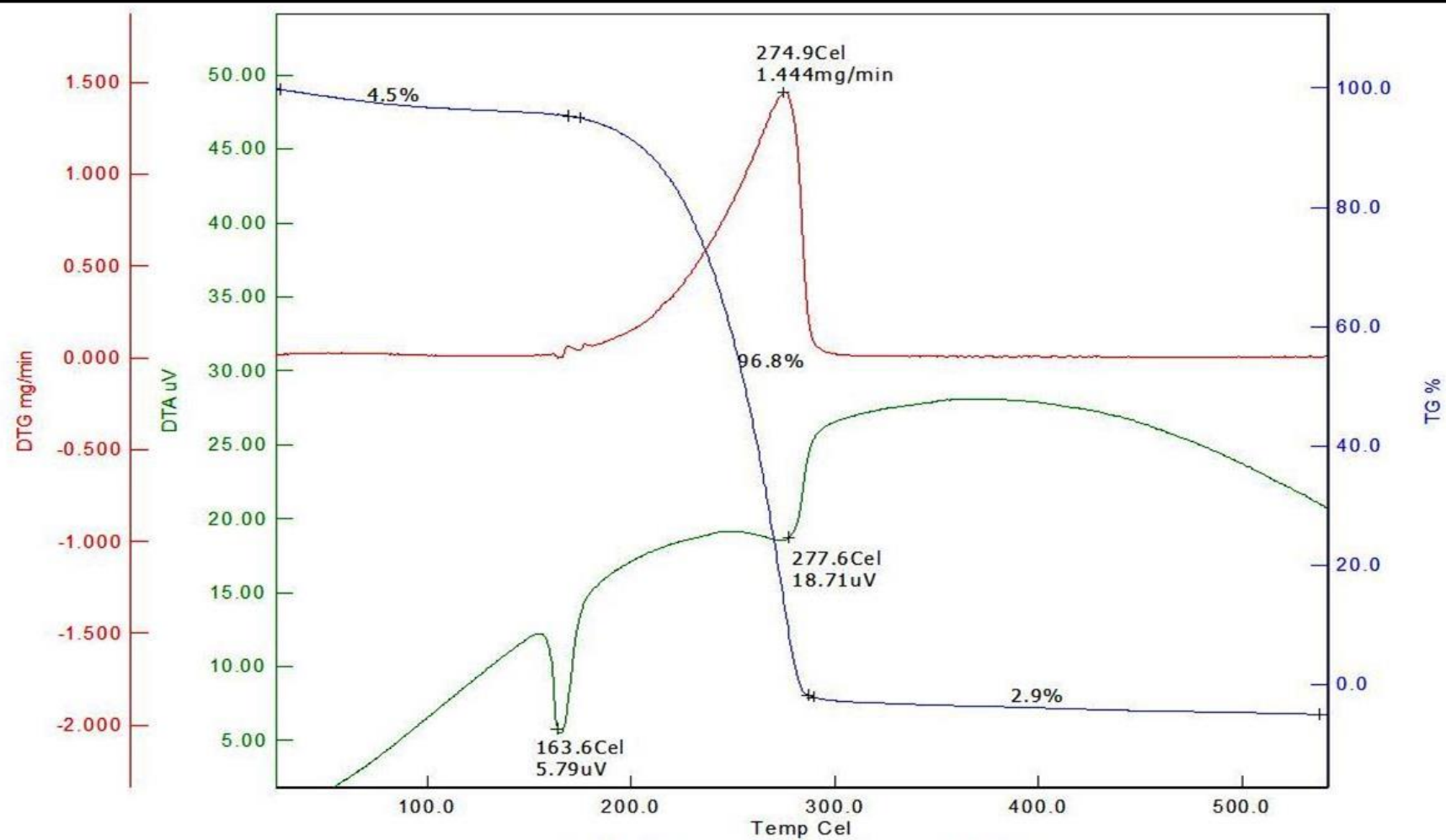


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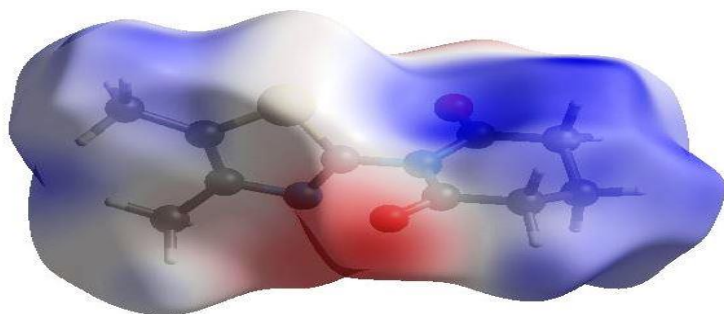
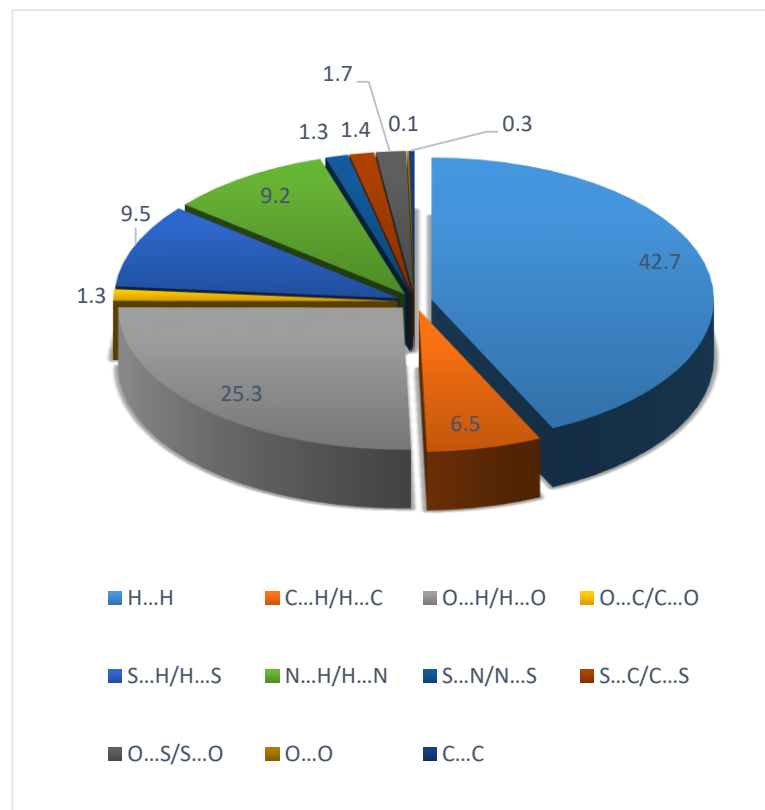
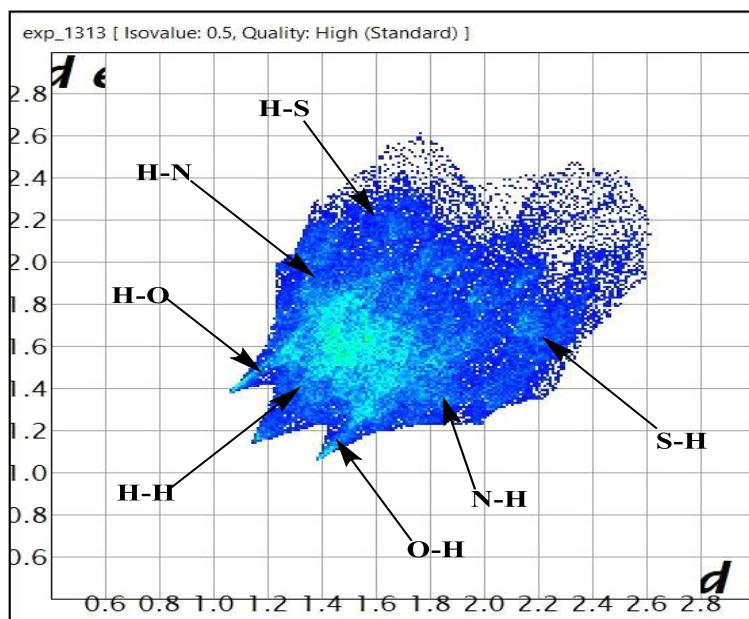




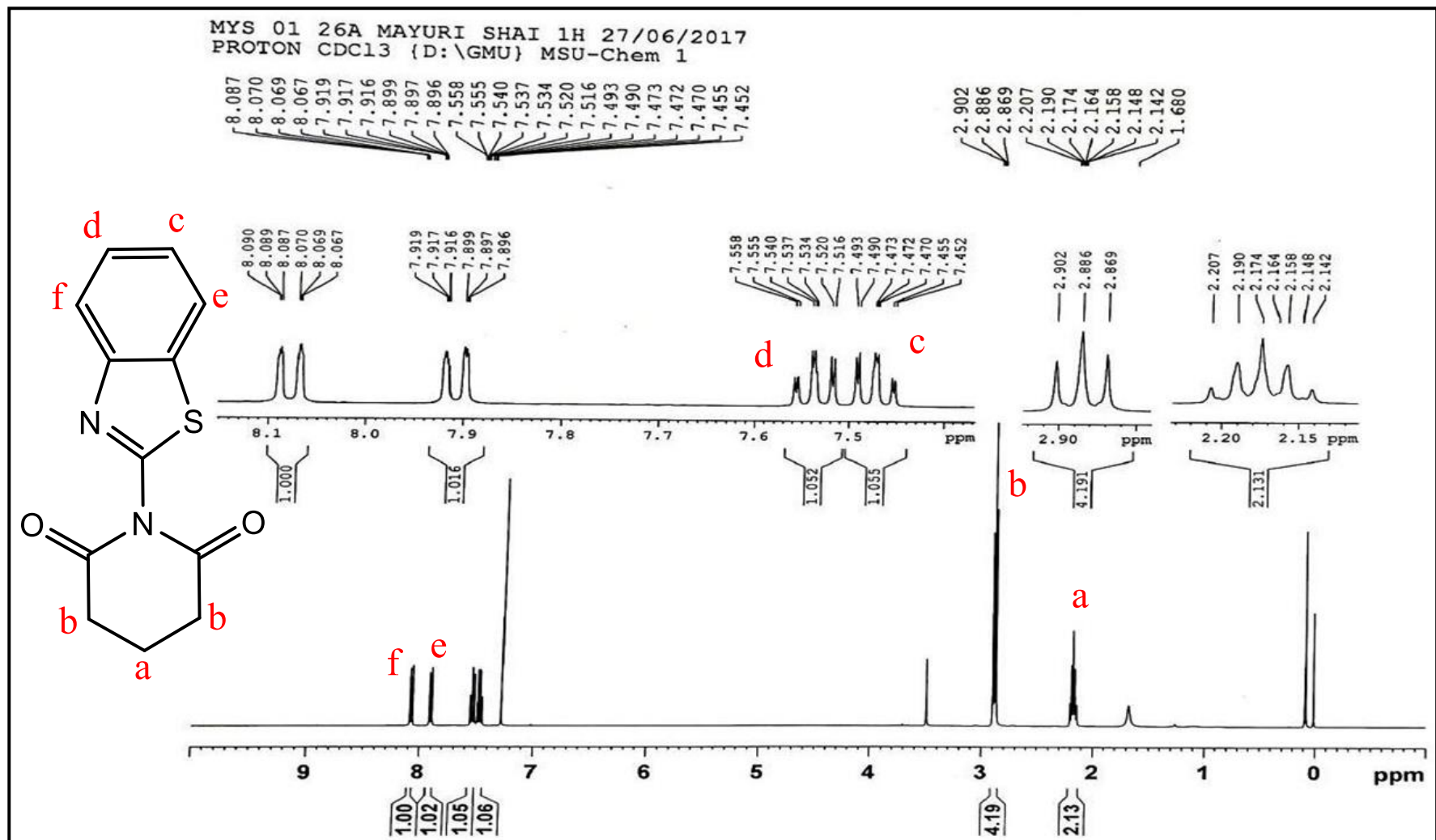
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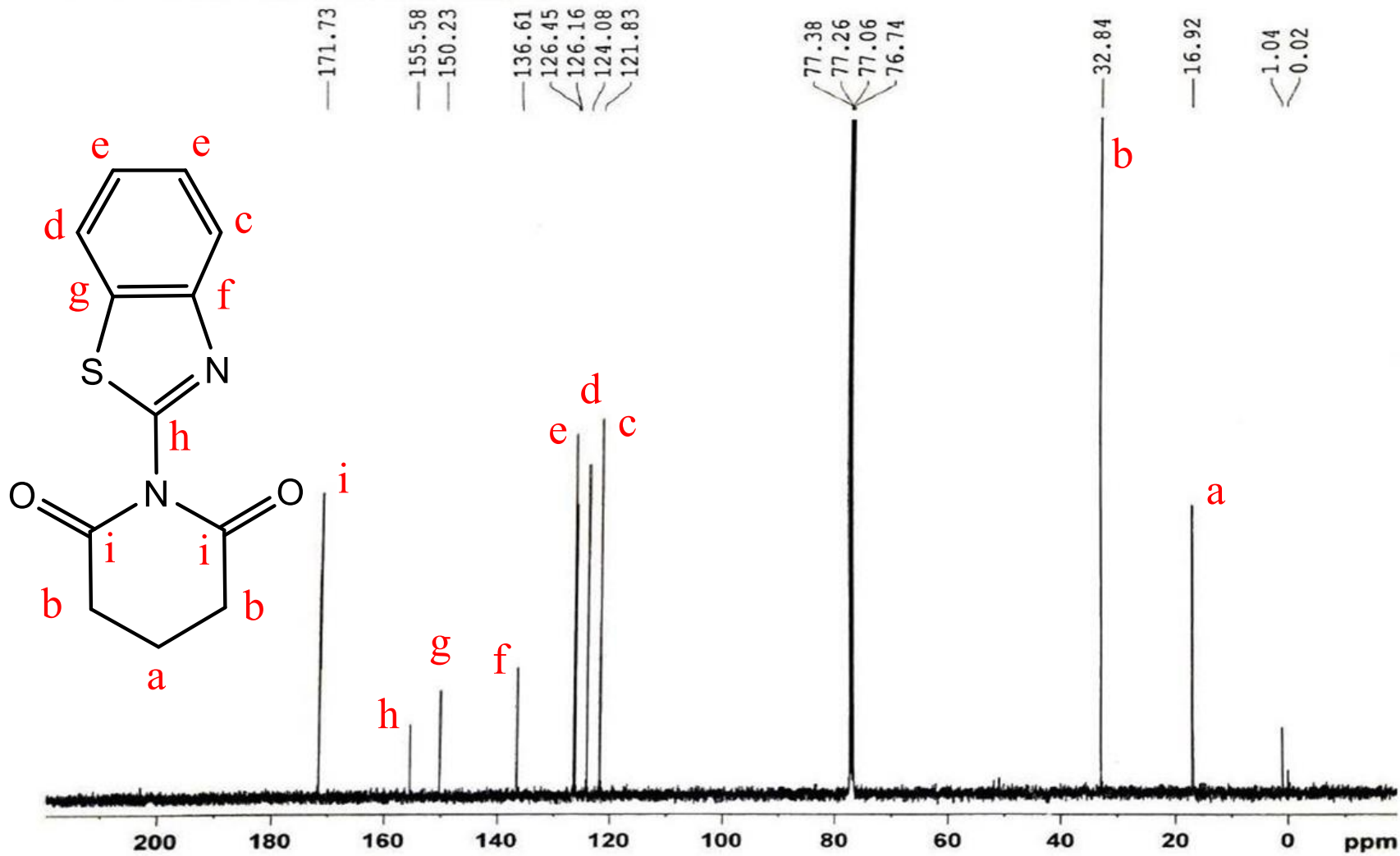
2-A-4,5-DMT product: Hirschfeld fingerprint graph and % contribution of weak interactions

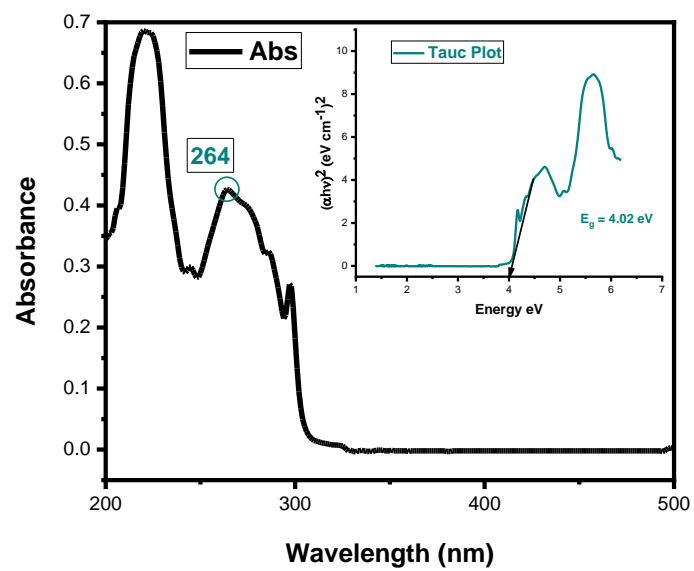
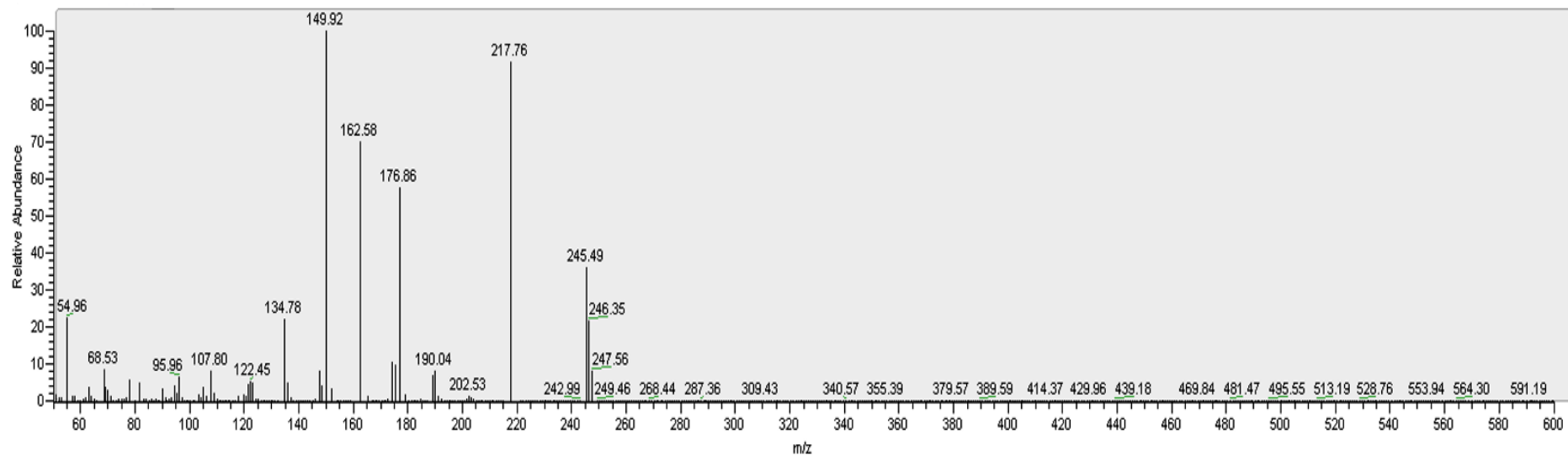


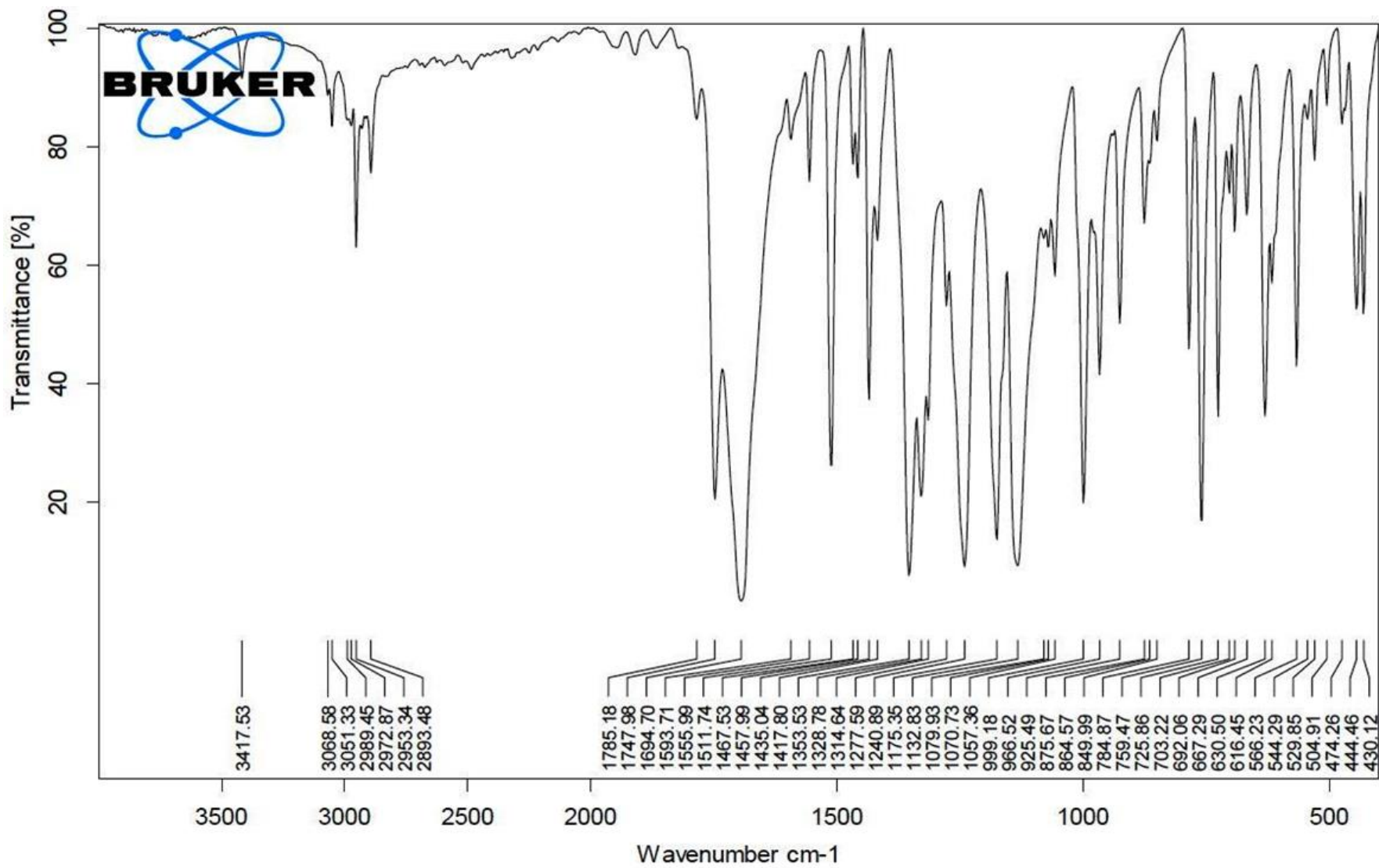
Data of Compound -5: 2-Aminobenzthiazole derivative

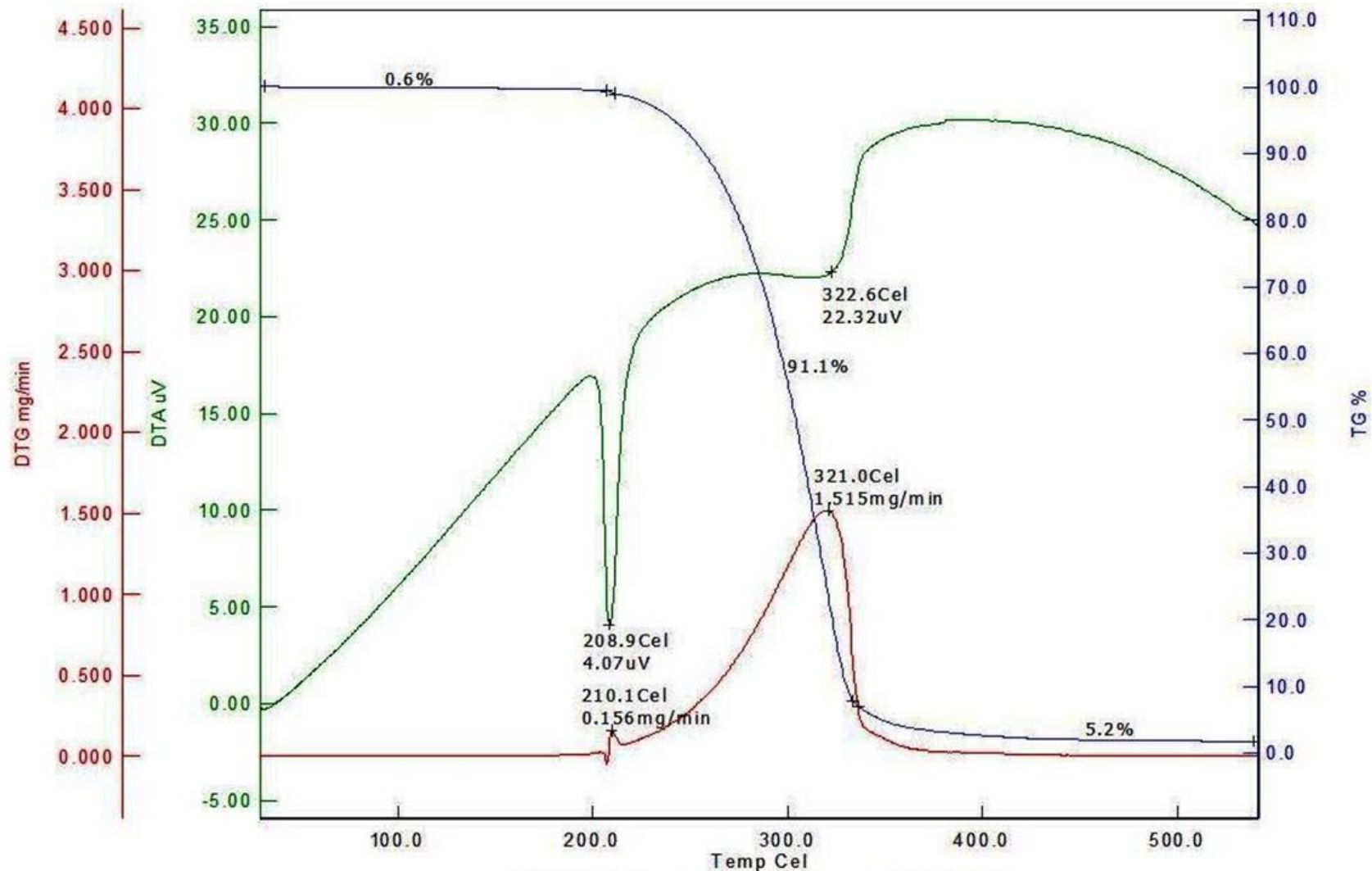


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2-ABT product: Hirschfeld fingerprint graph and % contribution of weak interactions

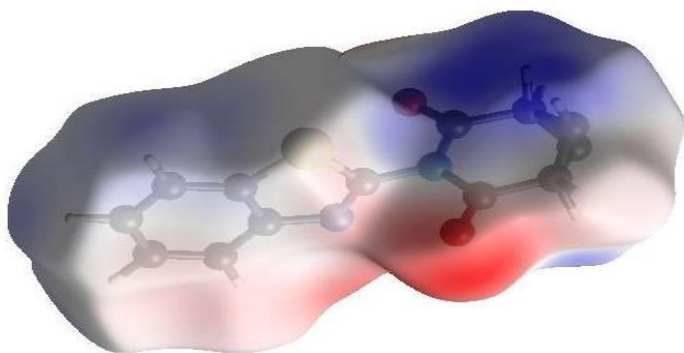
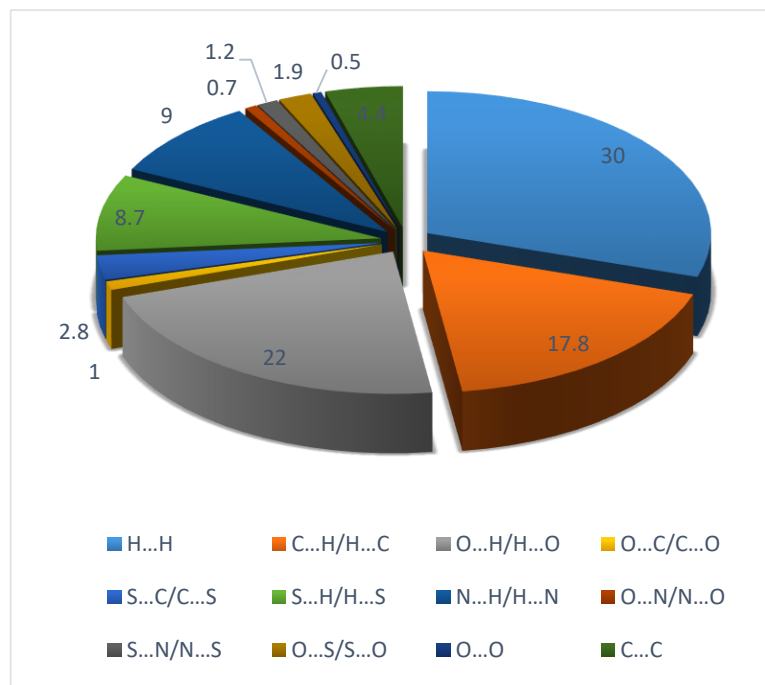
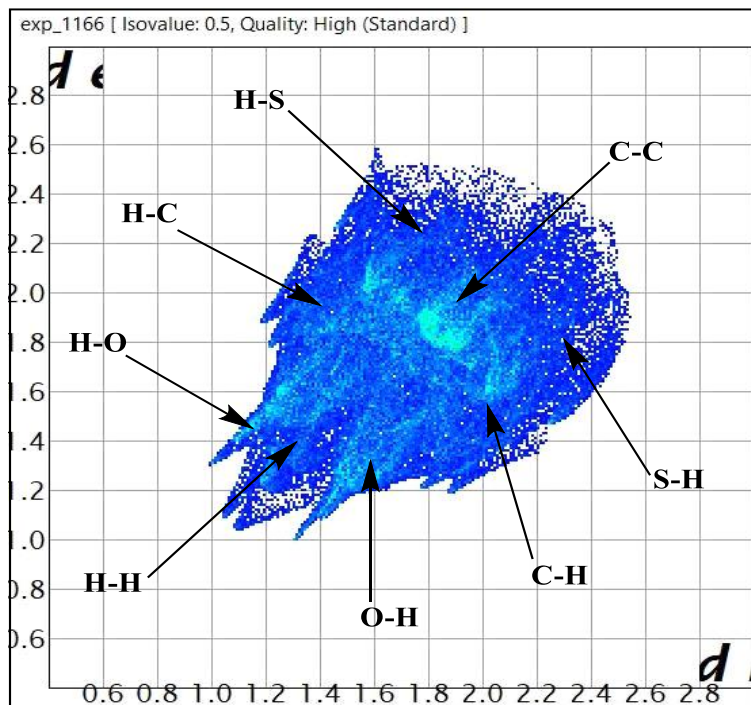


Table 5: The comparative table for band gap obtained from experiments and theoretical calculations

Compounds	Band gap (ev) (UV-Spectra)	Band gap (ev) Tauc plot	Band gap (ev) (Theoretical calculations in gaseous phase)	Band gap (ev) (Theoretical calculations in THF)
1	5.14	4.80	5.87	5.87
2	5.02	4.50	5.65	5.65
3	4.93	4.46	5.58	5.58
4	4.86	4.50	5.36	5.36
5	4.7	4.02	5.30	5.30



Figure S1: A) image of Crystals of compounds (1-5) placed on graph paper (for maximum size); (b) Crystals image in Visible light; C) Crystal image in Short UV light; D) Crystal image in long UV light

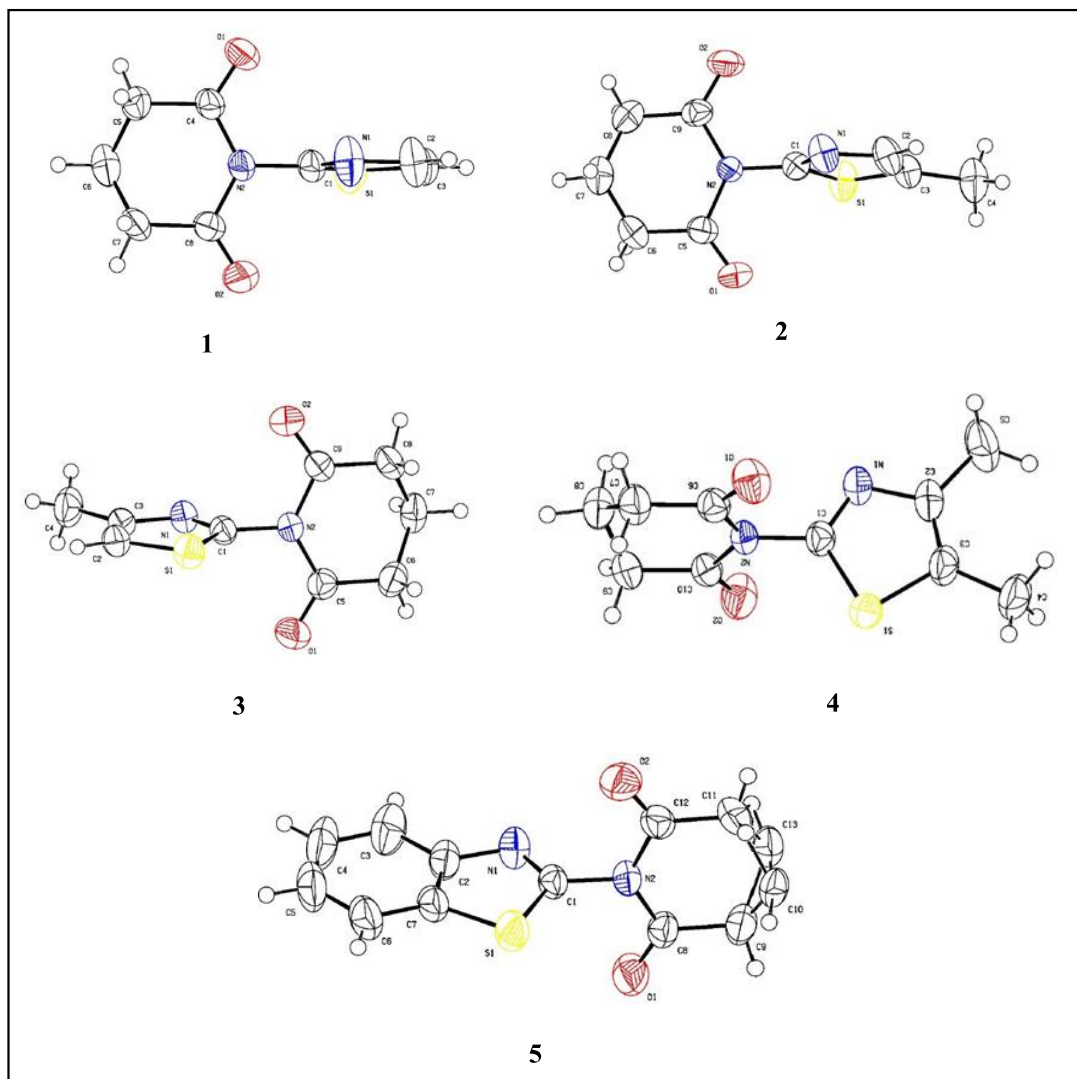


Figure S2: ORTEP (50% probability) diagram of 1–5.

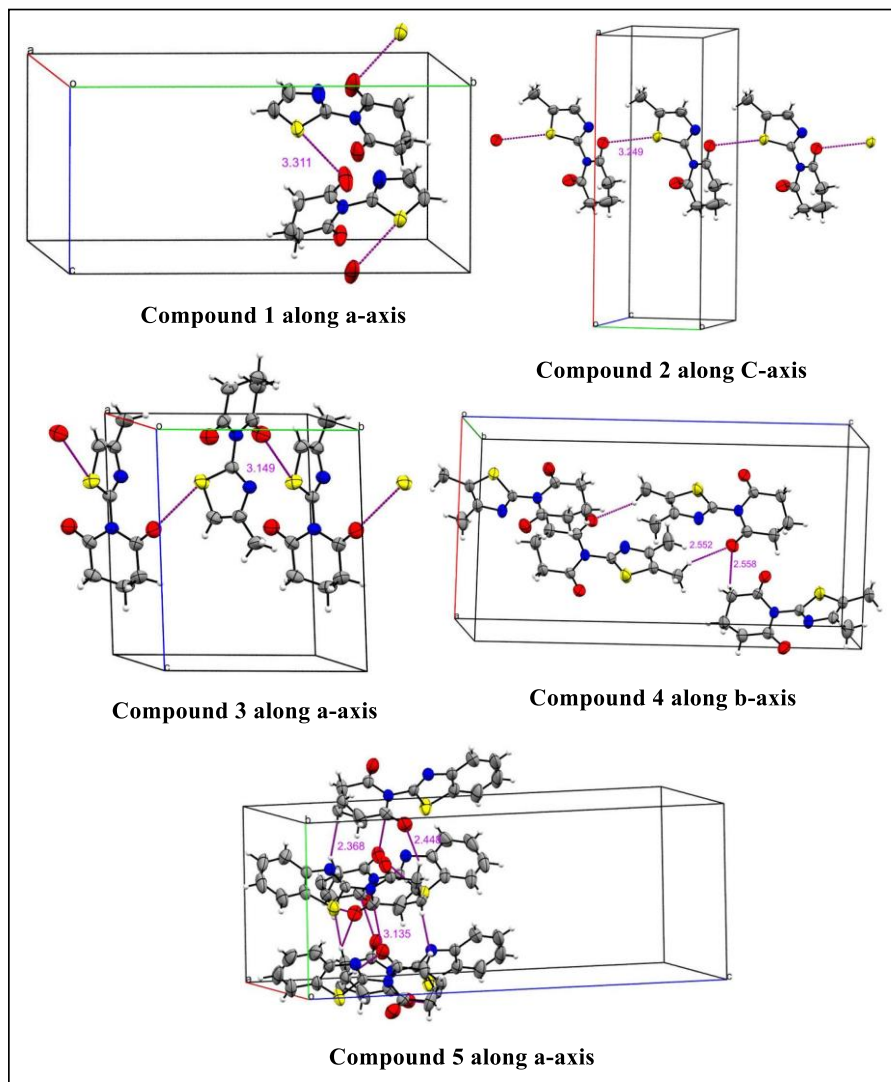


Figure S3: ORTEP diagram of compounds 1-5 with crystallographic axis.

Table 6: The computed global reactivity parameters of all considered systems in the gas phase.

<i>Syste ms/Co mpou nd</i>	<i>ionization potential</i> $(IP = -E_{HOMO})$	<i>electron affinity</i> $((EA = -E_{LUMO})$	<i>electron egativity</i> $(\chi = (IP + EA)/2)$	<i>chemica l potential</i> (μ') $(\mu' = -\chi)$	<i>hardnes s (η), $\eta = (IP - EA)/2)$</i>	<i>softness (S), $S = 1/\eta$</i>	<i>electroph ilicity index</i> (ω) , $(\omega = \mu'^2 / 2\eta)$
1	7.095	1.229	4.162	-4.162	2.933	0.341	2.953
2	6.810	1.156	3.983	-3.983	2.827	0.353	2.805
3	6.764	1.182	3.973	-3.973	2.791	0.358	2.827
4	6.470	1.112	3.791	-3.791	2.679	0.373	2.682
5	6.705	1.407	4.056	-4.056	2.649	0.377	3.105

Table 7: The computed Transition energy (E), maximum wavelength (λ), oscillation strengths (f), and MO contribution of all considered systems in THF solvent.

<i>Compound s</i>	λ (nm)	<i>E</i> (eV)	<i>F</i> (10^{-4})	<i>MO contribution</i>	
1	253.71	4.88	9	H -> L (66.34 %)	H-2->L (28.74 %)
2	257.51	4.82	4	H -> L (68.79%)	H-2->L (14.28%)
3	259.05	4.79	3	H -> L (66.34 %)	H-2->L (20.90 %)
4	270.99	4.58	0	H -> L (77.62 %)	H-2->L (2.86 %)
5	270.40	4.59	488	H -> L (81.09%)	H-2->L+2(10.69 %) H-1->L (4.68%)

Table 8: The computed second-order perturbation energies (E_2), the energy difference between donor and acceptor I and J orbitals ($E(J)-E(I)$), and Fock matrix element ($F(I, J)$) in the gas phase.

<i>Complex</i>	<i>Donor(i)</i>	<i>Type</i>	<i>Acceptor(j)</i>	<i>Type</i>	<i>E(2)</i>	<i>E(J)-E(I)</i>	<i>F(I,J)</i>
<i>C1</i>	π	C12-N13	π^*	C18-C20	17.34	0.34	0.071
	π	C18-H19	π^*	S1-C18	0.51	0.28	0.056
	σ	N13-C20	σ^*	N2-C12	7.42	1.14	0.083
	σ	C18-H19	σ^*	S1-C18	0.51	0.78	0.018
	LP (2)	S1	π^*	C18-C20	20.38	0.26	0.068
	LP(2)	O3/O5	π^*	C12-N13	1.61	0.27	0.02
<i>C2</i>	π	C12-N13	π^*	C18 - C19	15.77	0.35	0.069
	π	S1-C12	π^*	N2 - C4	0.5	0.28	0.057
	σ	N13-C19	σ^*	N 2 - C12	7.5	1.14	0.083
	σ	C 6-C 9	σ^*	C 9 - H11	0.51	1.03	0.021
	LP(1)	N2	π^*	O 3 - C17	43.42	0.29	0.104
	LP(2)	O 3/O5	π^*	C12 - N13	1.58	0.27	0.019
<i>C5</i>	π	C17-N27	π^*	C19 - C22	13.14	0.3	0.084
	π	C19-C22	π^*	C17-N27	1.61	0.28	0.029
	σ	N12-C18	σ^*	N 1 - C11	4.93	1.13	0.095
	σ	C5-C8	σ^*	C 8 - H10	0.25	1.03	0.02
	LP (2)	O2	σ^*	N 1 - C16	14.92	0.65	0.125
	LP*(1)	C 3	σ^*	C 8 - C13	0.44	0.5	0.03
	LP*(1)	C21	π^*	C19 - C22	14.49	0.13	0.085
	LP (2)	O 2	π^*	C11 - N12	0.92	0.28	0.02
	LP (3)	O2	LP*(1)	C16	165.03	0.12	0.186
LP (3)	O4	LP*(1)	C3	165.03	0.12	0.186	
<i>C3</i>	π	C12-N13	π^*	C18 - C19	17.79	0.35	0.074
	π	S1-C12	π^*	N2 - C4	0.58	0.28	0.054
	σ	N13-C19	σ^*	N 2 - C12	7.04	1.14	0.081

	σ	C 6 - C 9	σ^*	C 9 - H11	0.51	1.03	0.021
	LP (1)	O 3	σ^*	N 2 - C17	1.05	1.06	0.03
	LP (1)	N 2	π^*	O 3 - C17	43.38	0.29	0.104
	LP (1)	N 2	π^*	O 3 - C17	43.38	0.29	0.104
	LP (2)	S 1	π^*	C12 - N13	29.83	0.25	0.078
	LP (2)	O 3	π^*	C12 - N13	1.6	0.27	0.02
C4	π	C12-N13	π^*	C18-C19	16.4	0.36	0.072
	π	S1-C12	π^*	N2-C4	0.58	0.28	0.056
	σ	N13-C19	π^*	N2-C12	7	1.14	0.08
	σ	O3-C17	π^*	N2-C17	0.51	1.47	0.025
	LP(1)	N2	π^*	O3-C17	43.59	0.29	0.104
	LP(2)	O3	π^*	C12-N13	1.55	0.27	0.019

Table 9: The computed Transition energy (E), maximum wavelength (λ), oscillation /strengths (f), and MO contribution of all considered systems in the Gas Phase.

<i>Compound in gas phase</i>	<i>Band gap (eV)</i>	μ (D)	a_0 (10^{-24} esu)	$\Delta\alpha$ (10^{-2} esu)	a (10^{-24} esu)	$\Delta\alpha$ (10^{-24} esu)	β_{vec} (10^{-30} esu)	β_{HRS} (10^{-30} esu)	$\beta(-w;w,0)$ (10^{-30} esu)	$\beta(-2w;w,0)$ SHG (10^{-30} esu)	γ_0 (10^{-36} esu)	$\gamma(-\omega;\omega,0,0)$ (10^{-36} esu)	$\gamma(-2\omega;\omega,\omega,0)$ (10^{-36} esu)
1	5.87	2.79	18.52	6.43	18.71	6.53	0.79	0.21	1.27	1.37	14.24	15.02	16.74
2	5.65	2.28	20.67	8.7	20.89	8.87	1.55	0.21	2.02	2.27	16.7	17.68	19.84
3	5.58	2.37	20.56	6.8	20.77	6.9	1.51	0.39	1.98	2.16	16.21	17.13	19.1
4	5.36	1.83	22.57	8.52	22.81	8.67	2.35	0.6	2.75	3.11	18.58	19.72	22.2
5	5.30	2.80	26.13	15.54	26.49	15.97	0.68	0.18	1.19	1.44	22.76	24.75	28.61

Table 10: The computed Transition energy (E), maximum wavelength (λ), oscillation /strengths (f), and MO contribution of all considered systems in THF solvent.

<i>Compound in THF</i>	<i>Band gap (eV)</i>	μ (D)	a_0 (10^{-24} esu)	Δa (10^{-2} esu)	a (-w,w) (10^{-24} esu)	Δa (10^{-24} esu)	b_0 (10^{-30} esu)	b_{HRS} (10^{-30} esu)	$b(-w;w,0)$ (10^{-30} esu)	$b(-2w;w,0)$ SHG (10^{-30} esu)	γ_0 (10^{-36} esu)	$\gamma(-\omega;\omega,0,0)$ (10^{-36} esu)	$\gamma(-2\omega;\omega,\omega,0)$ (10^{-36} esu)
1	5.87	3.77	23.38	6.00	20.8	6.62	0.92	0.39	1.59	1.47	26.39	22.74	23.32
2	5.65	3.24	25.99	8.12	23.18	8.99	2.65	0.12	2.75	2.79	30.39	26.56	27.27
3	5.58	3.18	25.88	6.09	23.06	6.93	2.59	0.59	2.71	2.53	29.86	25.66	26.54
4	5.36	2.6	28.37	7.89	25.32	8.82	4.3	1.03	3.97	3.98	33.59	29.32	30.43
5	5.30	3.47	33.44	17.2	29.68	17.26	0.73	0.43	1.58	1.63	45.76	39.61	42.35