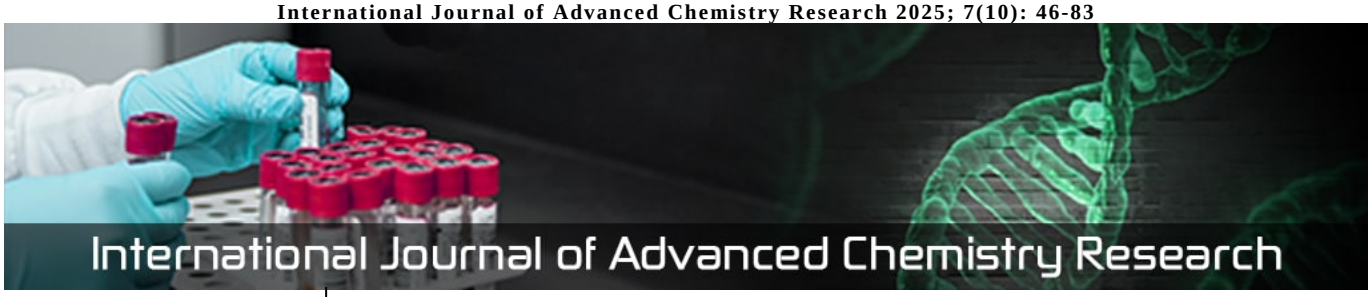

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Synthesis and spectral characterization of novel 1,3,5 triazines derivative with substituted amines

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Abstract
The 1,3,5-triazine scaffold is a versatile heterocyclic platform with wide applications in medicinal and materials chemistry. In this work we report the design, synthesis, and comprehensive spectral characterization of a novel library of 1,3,5-triazine derivatives functionalized with a range of substituted amines. Target compounds were prepared via controlled nucleophilic substitution on a tris-activated triazine precursor under mild conditions, enabling systematic variation of electronic and steric properties at the three substitution sites. Purification was achieved by recrystallization and/or column chromatography. Structural confirmation was obtained from FT-IR (diagnostic triazine ring and amine vibrations), and multinuclear NMR (^{1}H and ^{13}C) showing expected chemical shifts, coupling patterns, and integration for each derivative. Elemental analysis further supported composition.

Keywords: 1,3,5-Triazine, substituted amines, nucleophilic substitution, FT-IR, ^{1}H NMR, ^{13}C NMR, mass spectrometry

Introduction
The chemistry of heterocyclic compounds has always been a central area of research owing to their diverse structural features and broad spectrum of biological and industrial applications. Among these, 1,3,5-triazines represent an important class of nitrogen-containing heterocycles characterized by a symmetrical six-membered ring with alternating carbon and nitrogen atoms. Their unique electronic configuration imparts exceptional chemical stability and versatile reactivity, making them valuable scaffolds in pharmaceutical, agrochemical, polymer, and material sciences [1-5].

Triazine derivatives have been widely employed as anticancer, antimicrobial, antifungal, antiviral, and anti-inflammatory agents, while industrially they are key intermediates in resins, dyes, herbicides, UV stabilizers, and functional polymers. The presence of multiple substitution sites in the triazine ring provides opportunities for structural diversification through nucleophilic substitution reactions, enabling the systematic introduction of electron-donating, electron-withdrawing, or sterically demanding substituents. This versatility allows researchers to modulate physicochemical, thermal, and biological properties in a predictable manner [5-10].

In recent years, amine-substituted 1,3,5-triazines have attracted considerable attention due to their ability to form stable conjugates, hydrogen-bonding interactions, and biologically active frameworks. The incorporation of substituted amines often enhances lipophilicity, bioavailability, and receptor binding, thereby improving biological efficacy [11]. Moreover, the straightforward synthetic accessibility of these derivatives from cyanuric chloride (a readily available precursor) under mild conditions makes them excellent candidates for both structural exploration and activity optimization [12].

Comprehensive spectral characterization plays a crucial role in confirming the structures and substitution patterns of these compounds. Techniques such as FT-IR, UV–Vis, ^{1}H NMR, ^{13}C NMR, mass spectrometry, and elemental analysis provide detailed insights into functional groups, electronic transitions, molecular frameworks, and overall composition. Furthermore, thermogravimetric analysis (TGA) is employed to assess the thermal stability and potential material applications of triazine derivative s [13-20].

The present work focuses on the synthesis and detailed spectral characterization of novel 1,3,5-triazine derivatives substituted with various amines. By correlating structural modifications with spectral characterization, this study aims to expand the chemical diversity of triazines and identify new leads**.** And Techniques such as FT-IR, ^{1}H NMR, ^{13}C NMR, mass spectrometry was tested for newly synthesised compounds.

Material and Methods

All the chemicals used were of analytical grade (AR) and used as received. Distilled water was used for the preparation of the solutions during analysis.

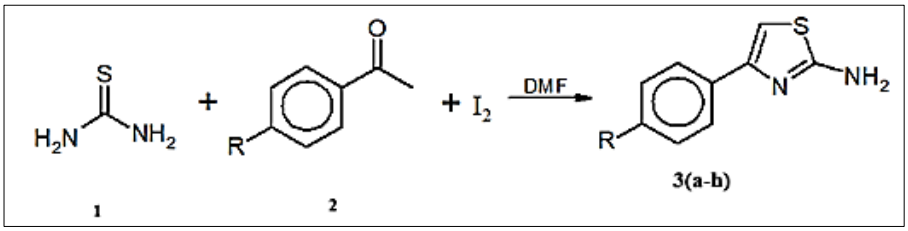
The methodology constitutes the backbone of any scientific investigation, as it provides a systematic framework for conducting research and ensures the reliability, reproducibility, and validity of the results obtained. In the present study, the methodology was carefully designed to accomplish the primary objective of synthesizing, characterizing, and evaluating a large library of 1,3,5-triazine derivatives. The approach combined both traditional organic synthesis techniques and modern analytical tools in order to obtain novel compounds with potential biological significance.

- **General procedure for synthesis of 1,3,5 triazine derivatives with substituted acetophenone and cyclohexane methyl amines for Scheme-I**

Step 1-Synthesis of 2-aminothiazole from substituted acetophenone

In this step reaction of 1 molar thiourea and 1 molar substituted acetophenone in presence of Iodine and DMF was reflux about 3 hours to give 2-aminothiodiazole via a Hantzsch thiazole synthesis-like pathway. The iodine acts as an oxidant and cyclizing agent to facilitate the condensation and ring formation.

The progress of the reaction was monitored by TLC. After completion of reaction, the precipitate formed was filtered and washed with distilled water, dried and the crude product was recrystallized from ethanol to obtained product **(3)** (5.39 g, yield 94%) as Light-yellow crystals; Melting point, 86 to 89 °C; Solubility in water

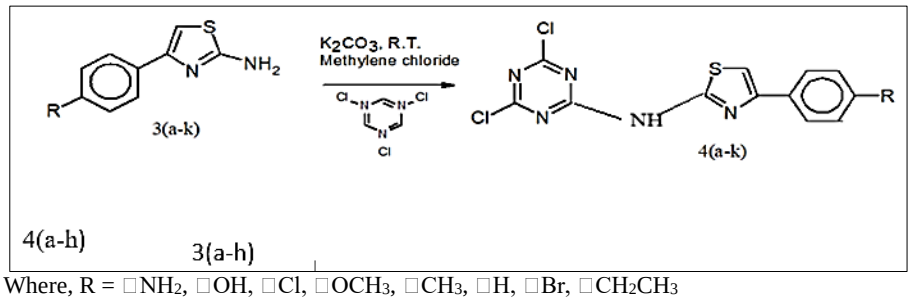


Where, R = □NH_2, □OH, □Cl, □OCH_3, □CH_3, □H, □Br, □CH_2CH_3.

Scheme 1: Synthesis of 2-aminothiazole from substituted acetophenone

Step 2: Reaction of substituted 2-aminothiazole with Cyanuric chloride

In this step reaction 4(a-h) was synthesised by the reaction of Cyanuric chloride (0.02 mol) with substituted 2-aminothiodiazole (0.02 mol) in 25 cm^3 acetone methylene chloride and K_2CO_3 at R.T with constant stirring for Four hours. The progress of the reaction was monitored by TLC. After completion of reaction, the reaction was neutralised by crushed ice poured into the reaction mixture The precipitate formed was filtered and washed with distilled water, dried and the crude product was recrystallized from ethanol to obtained product (6.39 g, yield 95%) as pale-yellow powder M.P. 220°C.

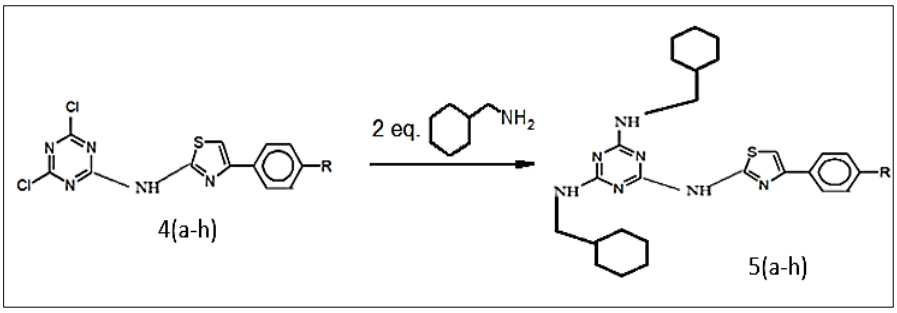


Where, R = □NH_2, □OH, □Cl, □OCH_3, □CH_3, □H, □Br, □CH_2CH_3

Scheme 2: Reaction of substituted 2-aminothiazole with Cyanuric chlorid

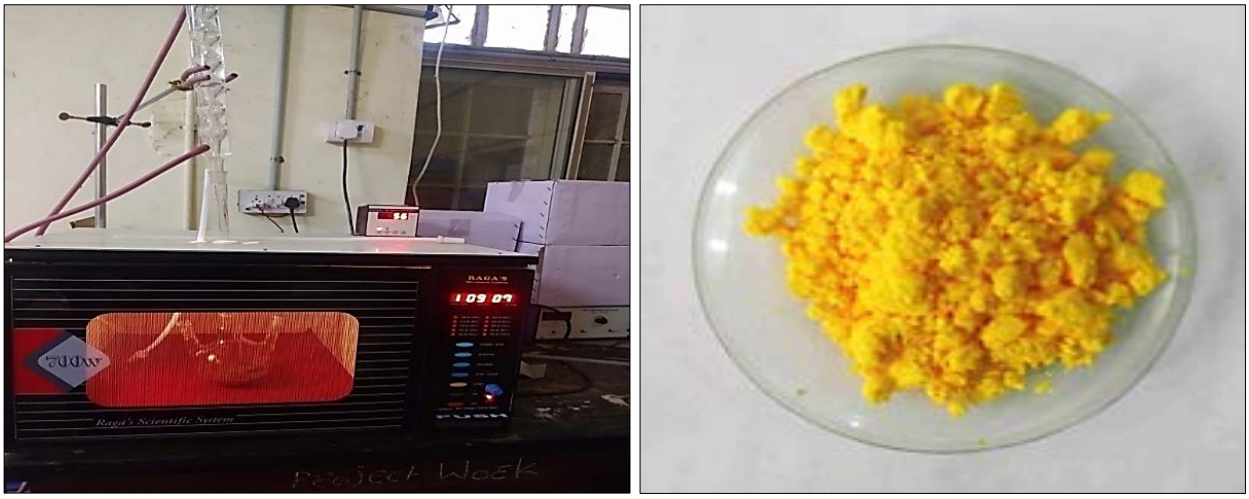
Step 3: Synthesis of 1,3,5-triazine derivative from cyclohexane methyl amines

In this step **(5a-h)** was synthesised by using cyclohexane methyl amine (0.005 mol) and *4 (a-k)* 0.005 mol) in methylene chloride 25 cm^3. The reaction mixture was exposed under microwave irradiation at 140 watts for Ten min. The progress of the reaction was monitored by TLC. After completion of reaction, the reaction was neutralised by 10% potassium carbonate solution and crushed ice poured into the reaction mixture The precipitate formed was filtered and washed with distilled water, dried and the crude product was recrystallized from ethanol to obtain 5 (a-h) (3.55 g, yield 92 %) as yellow powder M.P. 185°C. and same reaction will be carried out for different substituted benzophenone.



Where, R = □NH_2, □OH, □Cl, □OCH_3, □CH_3, □H, □Br, □CH_2CH_3.

Scheme 3: Synthesis of 1,3,5-triazine derivatives from cyclohexane methyl amine.

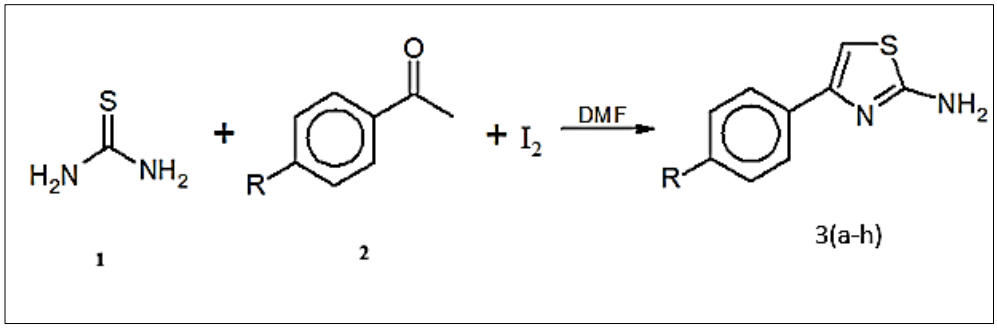


General procedure for synthesis of 1, 3, 5-triazine derivatives for Scheme-II:

Step 1: Synthesis of 2-aminothiazole from substituted acetophenone

In this step reaction of 1 molar thiourea and 1 molar substituted acetophenone in presence of Iodine and DMF was reflux about 3 hours to give 2-aminothiodiazole via a Hantzsch thiazole synthesis-like pathway. The iodine acts as an oxidant and cyclizing agent to facilitate the condensation and ring formation.

The progress of the reaction was monitored by TLC. After completion of reaction, the precipitate formed was filtered and washed with distilled water, dried and the crude product was recrystallized from ethanol to obtained product **(3)** (5.39 g, yield 94%) as Light-yellow crystals; Melting point, 86 to 89 °C; Solubility in water

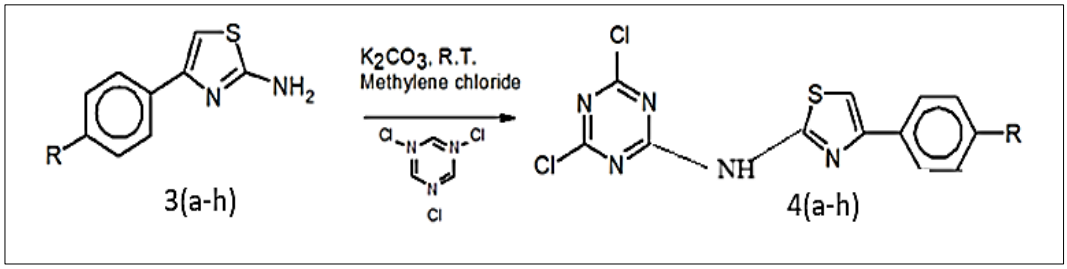


Where, R = □NH_2, □OH, □Cl, □OCH_3, □CH_3, □H, □Br, □CH_2CH_3.

Scheme 1: Synthesis of 2-aminothiazole from substituted acetophenone

Step 2: Reaction of substituted 2-aminothiazole with Cyanuric chloride

In this step reaction 4(a-h) was synthesised by the reaction of Cyanuric chloride (0.02 mol) with substituted 2-aminothiodiazole (0.02 mol) in 25 cm^3 acetone methylene chloride and K_2CO_3 at R.T with constant stirring for Four hours. The progress of the reaction was monitored by TLC. After completion of reaction, the reaction was neutralised by crushed ice poured into the reaction mixture The precipitate formed was filtered and washed with distilled water, dried and the crude product was recrystallized from ethanol to obtained product (6.39 g, yield 95%) as pale-yellow powder M.P. 220°C.

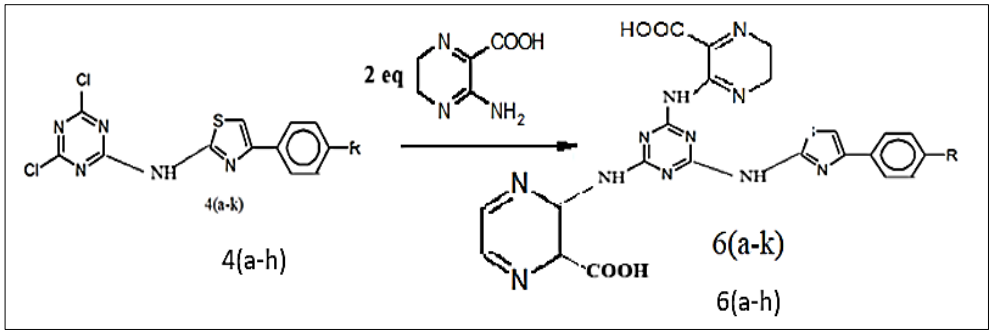


Where, R = □NH_2, □OH, □Cl, □OCH_3, □CH_3, □H, □Br, □CH_2CH_3.

Scheme 2: Reaction of substituted 2-aminothiazole with Cyanuric chloride

Step 3: Synthesis of 1,3,5-triazine derivative from 2-amino-2-pyrazine carboxylic acid.

In this step **6(a-h)** was synthesised by using 2-amino-2-pyrazine carboxylic acid (0.005 mol) and *4 (a-k)* 0.005 mol). The reaction mixture was exposed under microwave irradiation at 140 watts for Ten min. The progress of the reaction was monitored by TLC. After completion of reaction, the reaction was neutralised by 10% potassium carbonate solution and crushed ice poured into the reaction mixture The precipitate formed was filtered and washed with distilled water, dried and the crude product was recrystallized from ethanol to obtain (6 a-h) (3.78 g, yield 93 %) as yellow powder M.P. 197°C. and same reaction will be carried out for different substituted benzophenone.



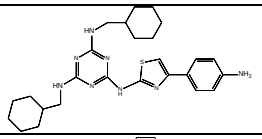
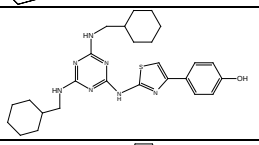
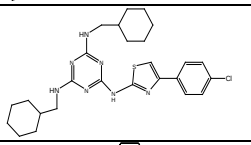
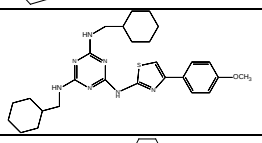
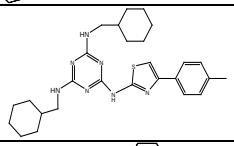
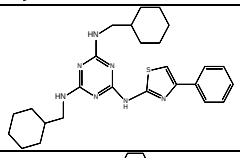
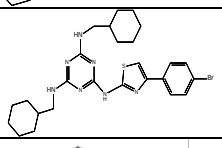
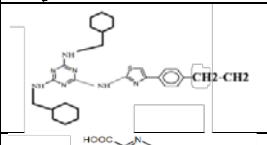
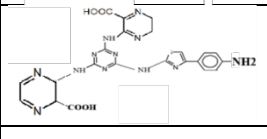
Where, R = □NH_2, □OH, □Cl, □OCH_3, □CH_3, □H, □Br, □CH_2CH_3

Scheme 4: Synthesis of 1,3,5-triazine derivative from 2-amino-2-pyrazine carboxylic acid

Physical Data of Synthesized Compounds: The designed compounds synthesized by the various substituted ketones react with the cyanuric chloride to formed Novel *s*-triazine derivatives. The molecular formula, IUPAC name, physical appearance, percentage yield, melting point, and solubility of the compound are determined. These details are given as following data in Table No: 2 and 3. The data is good agreement with literature values. [21-23]

Table 3.1: Physical Data of Newly synthesized 1,3,5-Triazine derivatives

The molecular formula, IUPAC name, and calculated elemental analysis of newly synthesised 1,3,5-triazine derivatives as shown in table in 3.2.

Sr. No.	Name of Compounds	Structure of Compound	Molecular Weight (g/mole)	Colour	Solubility	% Yield	Melting Point (°C)
1.	Compound – 5a		492	Light Yellow	DMSO	94.40	228
2.	Compound – 5b		494	Light Yellow	DMSO	83.98	217
3.	Compound – 5c		511	Pale Yellow	DMSO	76.53	272
4.	Compound – 5d		508	Light Yellow	DMSO	84.33	238
5.	Compound – 5e		492	Light Yellow	DMSO	89.40	276
6.	Compound – 5f		478	Light Yellow	DMSO	88.62	235
7.	Compound – 5g		557	Brown	DMSO	89.03	264
8.	Compound – 5h		506	Lemon	DMSO	87.40	301
9.	Compound – 6a		548	Light Yellow	DMSO	86.44	269
10.	Compound – 6b		549	Light	DMSO	87.39	263

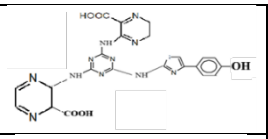
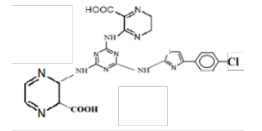
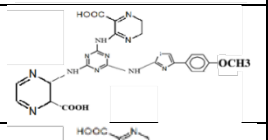
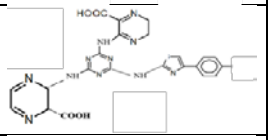
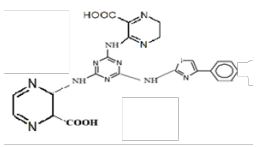
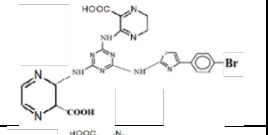
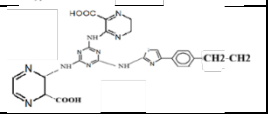
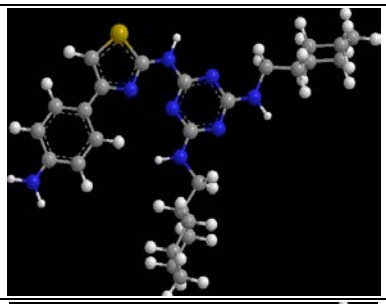
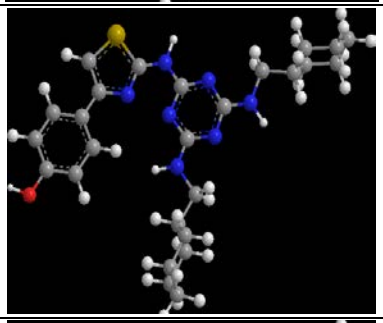
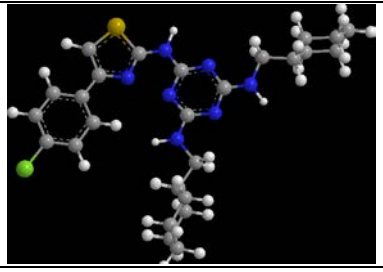
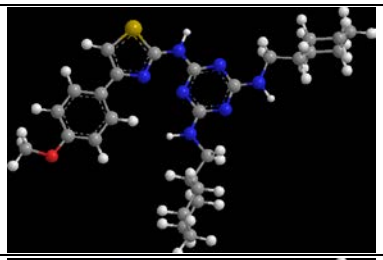
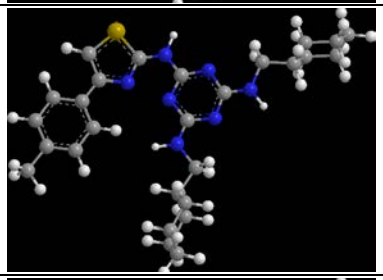
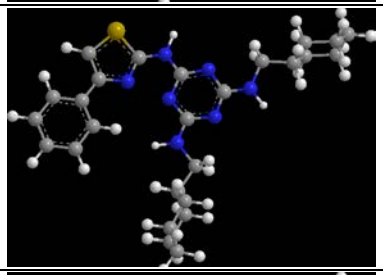
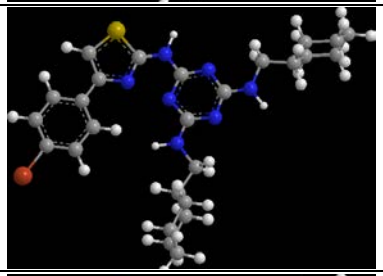
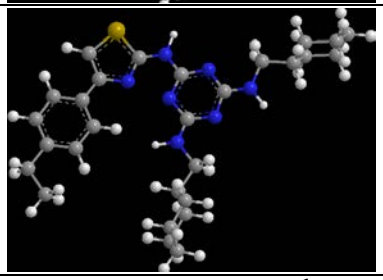
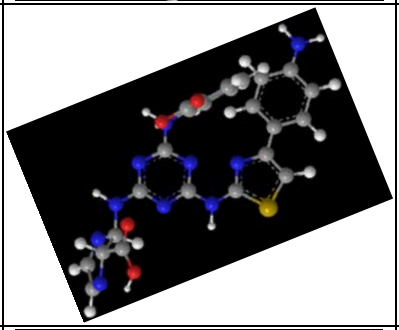
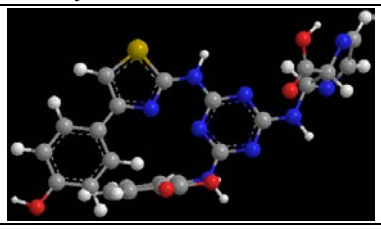
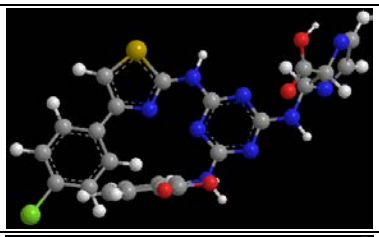
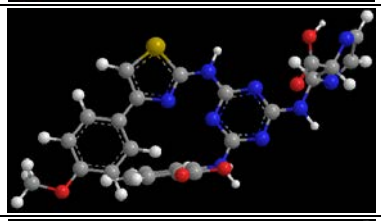
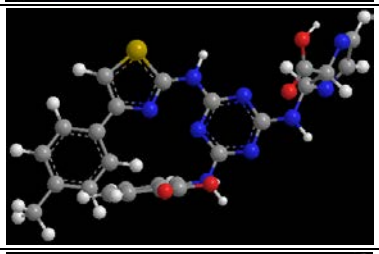
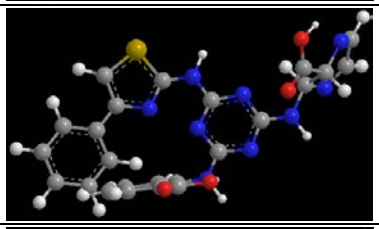
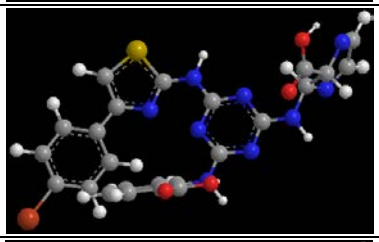
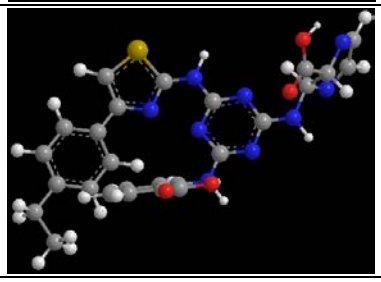
				Yellow			
11.	Compound – 6c		568	Yellow	DMSO	84.33	256
12	Compound – 6d		564	Yellow	DMSO	89.40	298
13	Compound – 6e		547	Colorless	DMSO	88.62	265
14	Compound – 6f		533	Light Yellow	DMSO	89.03	238
15	Compound – 6g		612	Brown	DMSO	87.40	278
16	Compound – 6h		561	Pale Yellow	DMSO	90.00	287

Table 1.2: IUPAC Names of Newly synthesised 1,3,5-Triazine derivatives

Compound Name	3D Structure	IUPAC Name	Elemental Analysis Calculated
Compound – 5a		N2-(4-(4-aminophenyl) thiazol-2-yl)-N4, N6-bis(cyclohexylmethyl)-1,3,5-triazine-2,4,6-triamine	C-64.33, H-8.10, N-21.43, S-6.13
Compound – 5b		4-(2-((4,6-bis((cyclohexylmethyl)amino)-1,3,5-triazin-2-yl) amino) thiazol-4-yl) phenol	C-63.26, H-7.15, N-19.86, O-3.24, S-6.49
Compound – 5c		N2-(4-(4-chlorophenyl) thiazol-2-yl)-N4, N6-bis(cyclohexylmethyl)-1,3,5-triazine-2,4,6-triamine	C-60.98, H-6.69, Cl-6.92, N-19.15, S-6.26.

Compound – 5d		N2, N4-bis(cyclohexylmethyl)-N6-(4-(4-methoxyphenyl) thiazol-2-yl)-1,3,5-triazine-2,4,6-triamine	C-63.88, H-7.35, N-19.31, O-3.15, S-6.32.
Compound – 5e		N2, N4-bis(cyclohexylmethyl)-N6-(4-(p-tolyl) thiazol-2-yl)-1,3,5-triazine-2,4,6-triamine	C-65.95, H-7.58, N-19.94, S-6.52
Compound – 5f		N2, N4-bis(cyclohexylmethyl)-N6-(4-phenylthiazol-2-yl)-1,3,5-triazine-2,4,6-triamine	C-65.38, H-7.39, N-20.53, S-6.71
Compound – 5g		N2-(4-(4-bromophenyl) thiazol-2-yl)-N4, N6-bis(cyclohexylmethyl)-1,3,5-triazine-2,4,6-triamine	C-56.11, H-6.16, Br-14.36, N-17.62, S-5.76
Compound – 5h		N2, N4-bis(cyclohexylmethyl)-N6-(4-(4-ethylphenyl) thiazol-2-yl)-1,3,5-triazine-2,4,6-triamine	C-66.50, H-7.77, N-19.39, S-6.34
Compound – 6a		3-((4-((4-(4-aminophenyl) thiazol-2-yl) amino) --((2-carboxyphenyl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2-carboxylic acid	C-52.94%, H-3.70%, N-25.72 %, O-11.75%, S-5.89%
Compound – 6b		3-((4-((2-carboxyphenyl) amino)-6-((4-(4-hydroxyphenyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2-carboxylic acid	C-52.84%, H-3.51%,N-23.11% O-14.66 %, S-5.88%

Compound – 6c		3-((4-((2-carboxyphenyl) amino)-6-((4-(4-chlorophenyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2-carboxylic acid	C-51.11%, H-3.22%,N-22.35 % O-11.35 %, S-5.69%, Cl-6.29 %.
Compound – 6d		3-((4-((2-carboxyphenyl) amino)-6-((4-(4-methoxyphenyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2-carboxylic acid	C-53.66 %, H-3.78%, N-22.53%, O-14.30%, S-5.73%
Compound – 6e		3-((4-((2 carboxyphenyl) amino)-6-((4-(p-tolyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2-carboxylic acid	C-56.53, H-4.74, N-21.98, O-11.16, S-5.59
Compound – 6f		3-((4-((2-carboxyphenyl) amino)-6-((4-phenylthiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2-carboxylic acid	C-55.80, H-4.50, N-22.53, O-11.44, S-5.73
Compound – 6g		3-((4-((4-(4-bromophenyl) thiazol-2-yl) amino)-6-((2-carboxyphenyl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2-carboxylic acid	C-47.38, H2.98, Br-13.13, N-20.72, O-10.52, S-5.27
Compound – 6h		3-((4-((2-carboxyphenyl) amino)-6-((4-(4-ethylphenyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2-carboxylic acid	C-57.23, H-4.97, N-21.45, O-10.89, S-5.46

Results and Discussion

Thin Layer Chromatography

The purity of compound was checked by the TLC by using solvent system ethyl acetate and Hexane ether ratio (1:4). All the synthesized compounds were characterized by recording the R*f* values in TLC. The R*f* values from the TLC, of all the synthesized compounds are mentioned in Table No: 4 below [24-26].

Table 3.3: R*f* values of newly synthesized derivatives in TLC

Sr. No.	Compound Name	R*f* - value
1	Compound – 5a	0.744
2	Compound – 5b	0.390
3	Compound – 5c	0.383
4	Compound – 5d	0.368
5	Compound – 5e	0.355
6	Compound – 5f	0.337
7	Compound – 5g	0.395
8	Compound – 5h	0.457
9	Compound – 6a	0.586
10	Compound – 6b	0.259
11	Compound – 6c	0.229

12	Compound – 6d	0.447
13	Compound – 6e	0.269
14	Compound – 6f	0.456
15	Compound – 6g	0.897
16	Compound – 6h	0.892

Spectral Characterization: The spectral characterization of newly synthesized derivatives carried out by using FTIR, and ^{1}H NMR, ^{13}C NMR and Mass spectrometry.

Fourier Transform Infrared Spectroscopy (FTIR):
Infrared spectra of compound 1 to 16 provide valuable information regarding the nature of the functional groups present in ligand and its metal complexes. IR spectral technique has proved to be the most suitable one to arrive information related to nature of bonding of the ligand to the metal ion. The FTIR spectra for newly synthesised compounds are shown in Table No: 3.4 and Figure No: 3.1 to 3.16. The FTIR data of compounds shows the information about the functional group present and substituents attached.

Table 3.4: FTIR Data of newly synthesised 1,3,5-Triazine Derivatives

Sr. No.	Compound Name	Observed Value in Wave Number in cm^{-1}	Figure No.
1	Compound – 5a	3509 (NH_2, amine), 3462, and 3483 (NH amine attach to triazine ring), 3173 (C-H thiazole), 3094, 3096 3065 (C-H phenyl),3046, 3041 (C-H ethylene) 1584 (N-H), 1525 (N-H triazine), 856 (para subs) 1615-1423, 2850 and 2910 (C-H cyclohexane) 1560 (C-C Strach)	3.1
2	Compound – 5b	3517 (OH starch), 3467, and 3463 (NH amine attach to triazine ring), 3174 (C-H thiazole), 3094, 3096 3065 (C-H phenyl),3046, 3041 (C-H ethylene) 1584 (N-H), 1525 (N-H triazine), 856 (para subs) 1615-1423, 2850 and 2910 (C-H cyclohexane) 1567 (C-C Strach)	3.2
3	Compound – 5c	849 (Cl starch), 3481, and 3480 (NH amine attach to triazine ring), 3174 (C-H thiazole), 3094, 3096 3065 (C-H phenyl),3046, 3041 (C-H ethylene) 1584 (N-H), 1525 (N-H triazine), 856 (para subs) 1615-1423, 2850 and 2910 (C-H cyclohexane), 1562 (C-C Strach)	3.3
4	Compound – 5d	2930 (OCH_3 starch), 3480, and 3479 (NH amine attach to triazine ring), 3174 (C-H thiazole), 3095, 3096 3065 (C-H phenyl),3046, 3041 (C-H ethylene) 1584 (N-H), 1525 (N-H triazine), 856 (para subs) 1615-1423, 2850 and 2910 (C-H cyclohexane), 1560 (C-C Strach)	3.4
5	Compound – 5e	2990 (CH_3 starch), 3480, and 3479 (NH amine attach to triazine), 3174 (C-H thiazole), 3173, 3111 3065 (C-H phenyl),3046, 3045 (C-H ethylene) 1584 (N-H), 1525 (N-H triazine), 856 (para subs) 1615-1423, 2850 and 2910 (C-H cyclohexane), 1560 (C-C Strach) 1493(C-H)	3.5
6	Compound – 5f	3065-3082(C-H aromatic), 3420, and 3460 (NH amine attach to triazine ring), 3174 (C-H thiazole), 3173, 3111 3065 (C-H phenyl),3046, 3045 (C-H ethylene) 1584 (N-H), 1525 (N-H triazine), 1615-1423, 2850 and 2910 (C-H cyclohexane), 1560 (C-C Strach) 1493(C-H)	3.6
7	Compound – 5g	864 (Br starch), 3481, and 3480 (NH amine attach to triazine), 3174 (C-H thiazole), 3094, 3096 3065 (C-H phenyl),3046, 3041 (C-H ethylene) 1584 (N-H), 1525 (N-H triazine), 856 (para subs) 1615-1423, 2850 and 2910 (C-H cyclohexane), 1562 (C-C Strach) 856 (para subs)	3.7
8	Compound – 5h	1274, 1799, 3201, (CH2-CH3 starch), 3481, and 3480 (NH amine attach to triazine), 3174 (C-H thiazole), 3094, 3096 3065 (C-H phenyl),3046, 3041 (C-H ethylene) 1584 (N-H), 1525 (N-H triazine), 856 (para subs) 1615-1423, 2850	3.8
9	Compound – 6a	3290 (OH Starch), 3390 (N-H attached to pyridine ring), 1671 (C=O in carboxylic acid) 3012 at (C-H in pyridine ring) 3509 (NH_2, amine), 3462, and 3483 (NH amine attach to triazine ring), 3173(C-H thiazole), 3094, 3096 3065 (C-H phenyl), 1584 (N-H), 1525 (N-H triazine), 856 (para subs) 1560 (C-C Strach)	3.9
10	Compound – 6b	3517 (OH starch), 3467, and 3463 (NH amine attach to triazine ring), 3174 (C-H thiazole), 3094, 3096 3065 (C-H phenyl), 1584 (N-H), 1525 (N-H triazine), 856 (para subs) 3290 (OH Starch), 3390 (N-H attached to pyridine ring), 1671 (C=O in carboxylic acid) 3012 at (C-H in pyridine ring)	3.10
11	Compound – 6c	849 (Cl starch), 3481, and 3480 (NH amine attach to triazine ring), 3174 (C-H thiazole), 3094, 3096 3065 (C-H phenyl), 1584 (N-H), 1525 (N-H triazine), 856 (para subs), 1562 (C-C Strach) 3290 (OH Starch), 3390 (N-H attached to pyridine ring), 1671 (C=O in carboxylic acid) 3012 at (C-H in pyridine ring)	3.11
12	Compound – 6d	2930 (OCH_3 starch), 3480, and 3479 (NH amine attach to triazine ring), 3174 (C-H thiazole), 3095, 3096 3065 (C-H phenyl),3046, 3041 (C-H ethylene) 1584 (N-H), 1525 (N-H triazine), 856 (para subs), 1560 (C-C Strach), 3290 (OH Starch), 3390 (N-H attached to pyridine ring), 1671 (C=O in carboxylic acid) 3012 at (C-H in pyridine ring)	3.12
13	Compound – 6e	2990 (CH_3 starch), 3480, and 3479 (NH amine attach to triazine ring), 3174 (C-H thiazole), 3173, 3111 3065 (C-H phenyl),3046, 3045 (C-H ethylene) 1584 (N-H), 1525 (N-H triazine), 856 (para subs), 1560 (C-C Strach) 1493(C-H), 3290 (OH Starch), 3390 (N-H attached to pyridine ring), 1671 (C=O in carboxylic acid) 3012 at (C-H in pyridine ring)	3.13
14	Compound – 6f	3065-3082(C-H aromatic), 3420, and 3460 (NH amine attach to triazine ring), 3174 (C-H thiazole), 3173, 3111 3065 (C-H phenyl),3046, 3045 (C-H ethylene) 1584 (N-H), 1525 (N-H triazine),, 1560 (C-C Strach) 1493(C-H), 3290 (OH Starch), 3390 (N-H attached to pyridine ring), 1671 (C=O in carboxylic acid) 3012 at (C-H in pyridine ring)	3.14
15	Compound – 6g	864 (Br starch), 3481, and 3480 (NH amine attach to triazine), 3174 (C-H thiazole), 3094, 3096 3065 (C-H phenyl),3046, 3041 (C-H ethylene) 1584 (N-H), 1525 (N-H triazine), 856 (para subs), 1562 (C-C Strach) 856 (para subs), 3290 (OH Starch), 3390 (N-H attached to pyridine ring), 1671 (C=O in carboxylic acid) 3012 at (C-H in pyridine ring)	3.15
16	Compound – 6h	1274, 1799, 3201, (CH2-CH3 starch), 3481, and 3480 (NH amine attach to triazine), 3174 (C-H thiazole), 3094, 3096 3065 (C-H phenyl), 1584 (N-H), 1525 (N-H triazine), 856 (para subs) 1615-1423, 2850, 3290 (OH Starch), 3390 (N-H attached to pyridine ring), 1671 (C=O in carboxylic acid) 3012 at (C-H in pyridine ring).	3.16

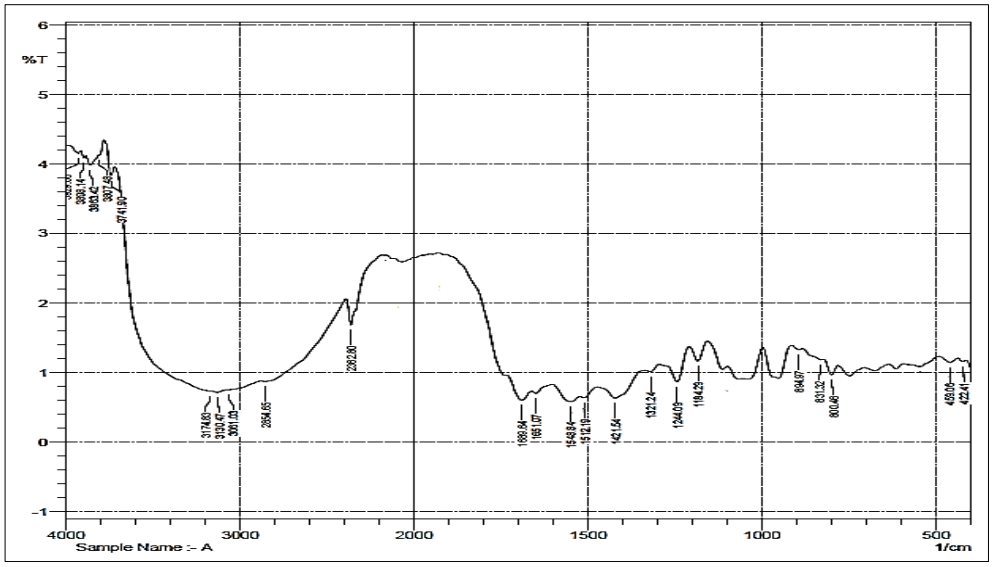


Fig 3.1: FTIR of 5a

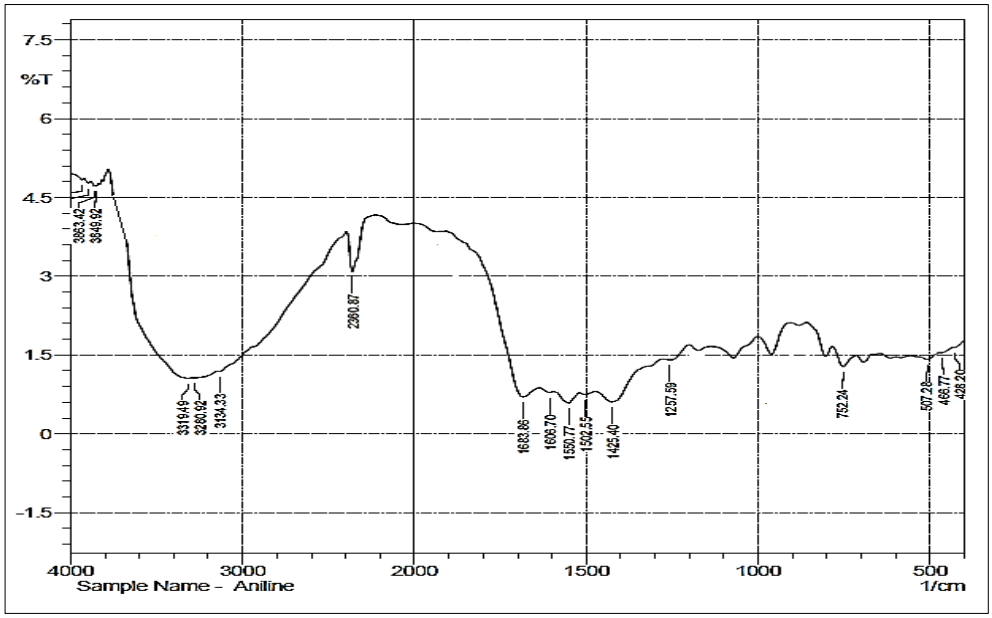
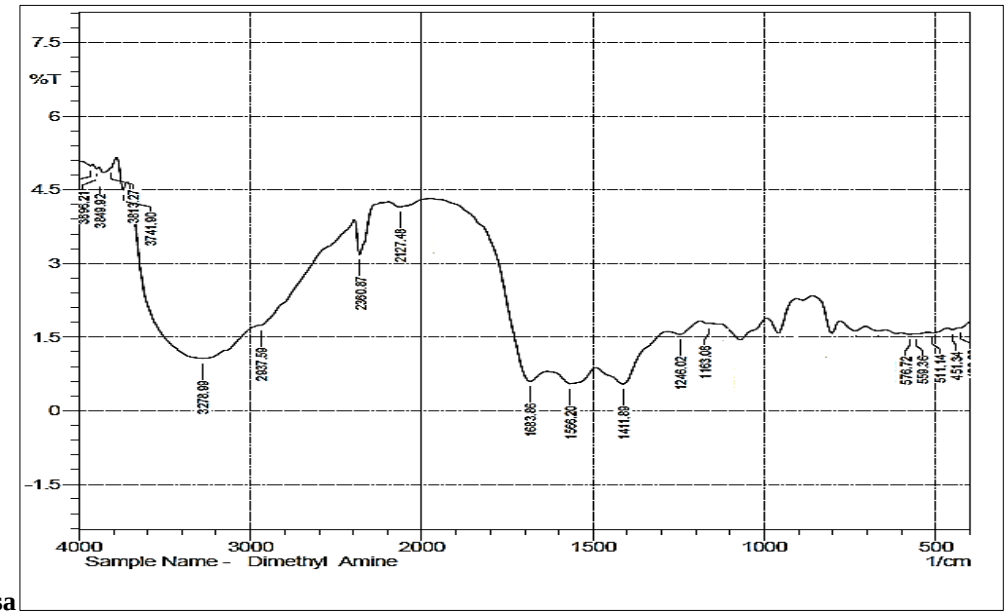


Fig 3.2: FTIR of 5b



sa

Fig 3.3: FTIR of 5c

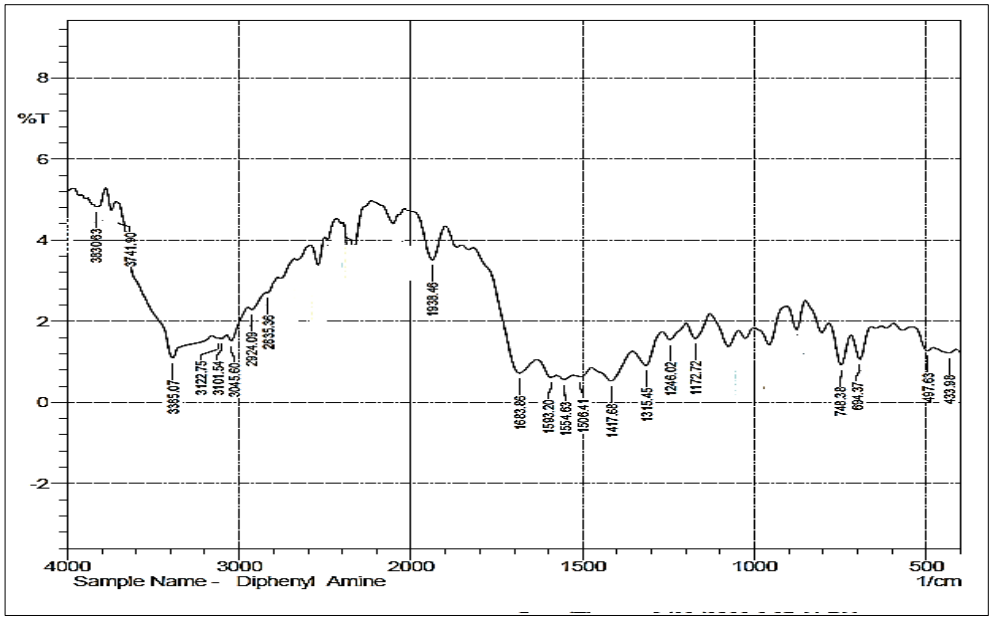


Fig 3.4: FTIR of 5d

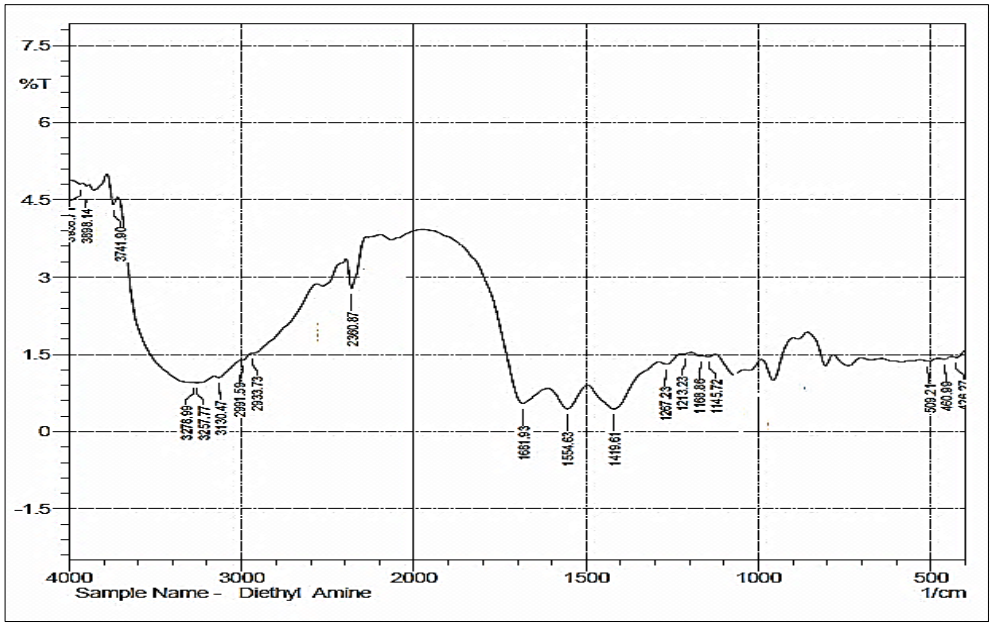


Fig 3.5: FTIR of 5e

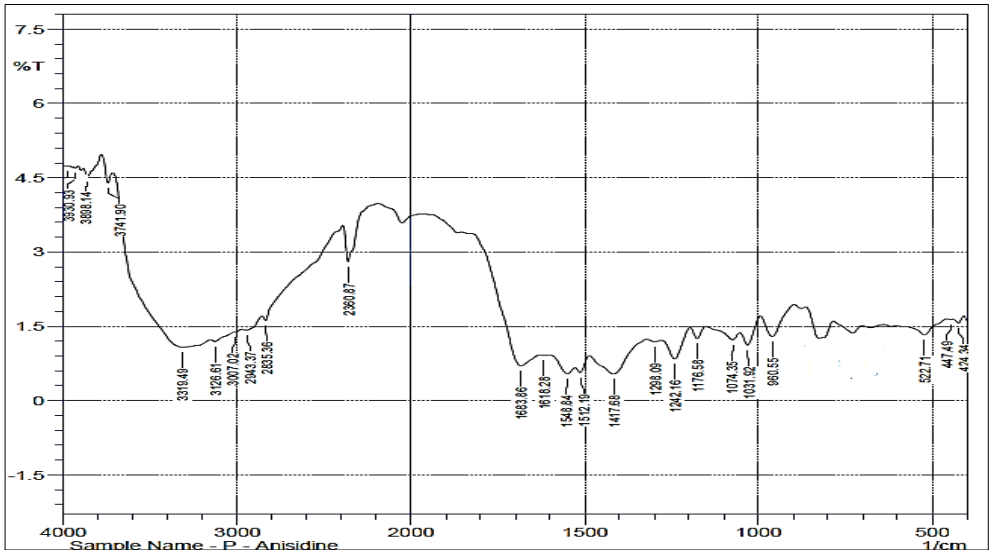


Fig 3.6: FTIR of 5f

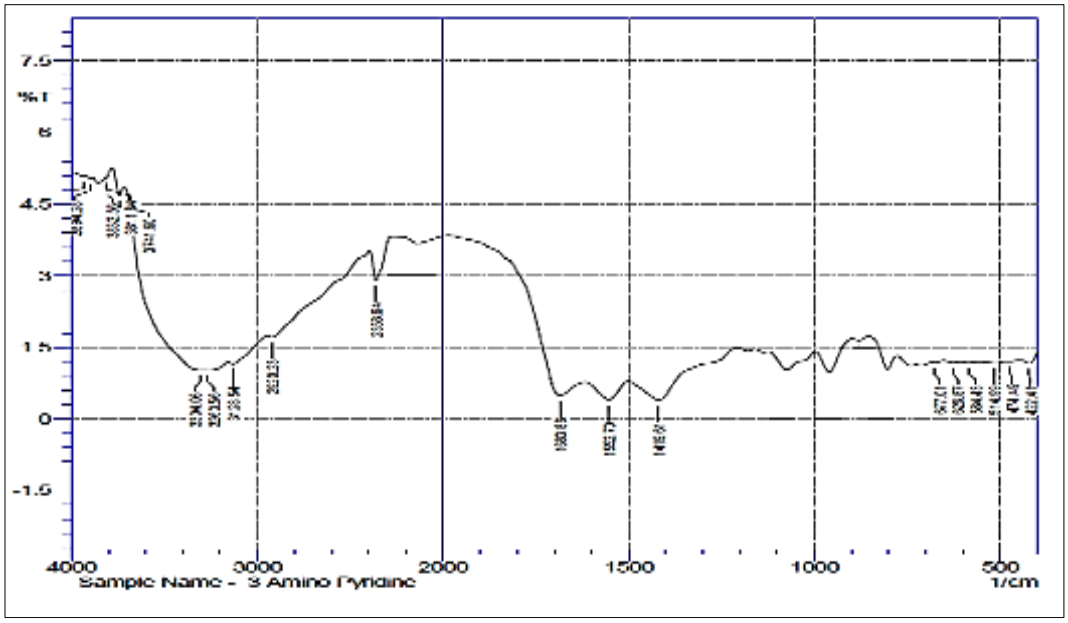


Fig 3.7: FTIR of 5g

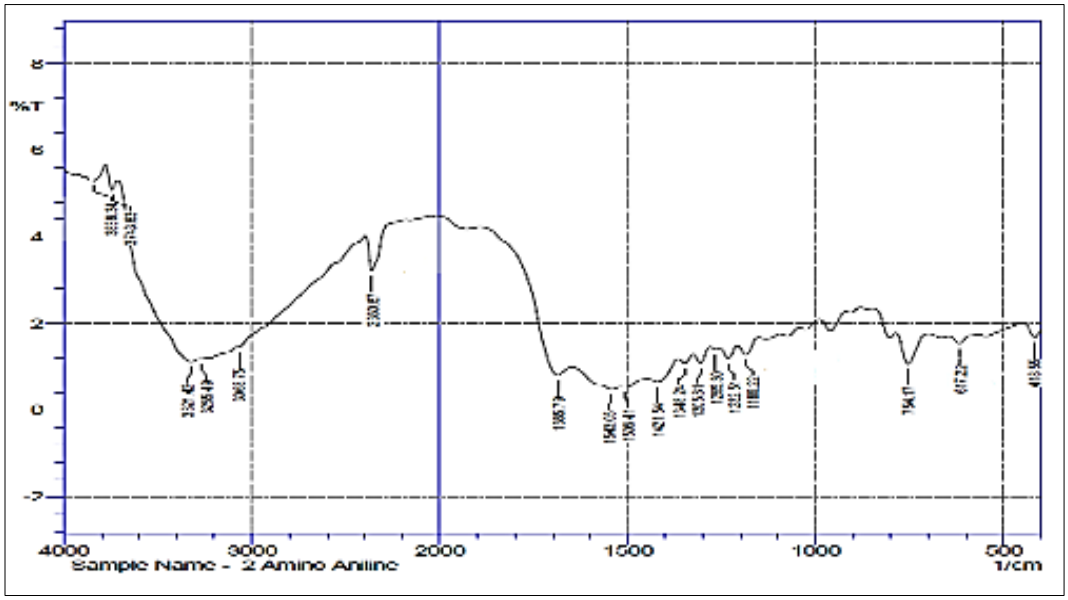


Fig 3.8: FTIR 5h

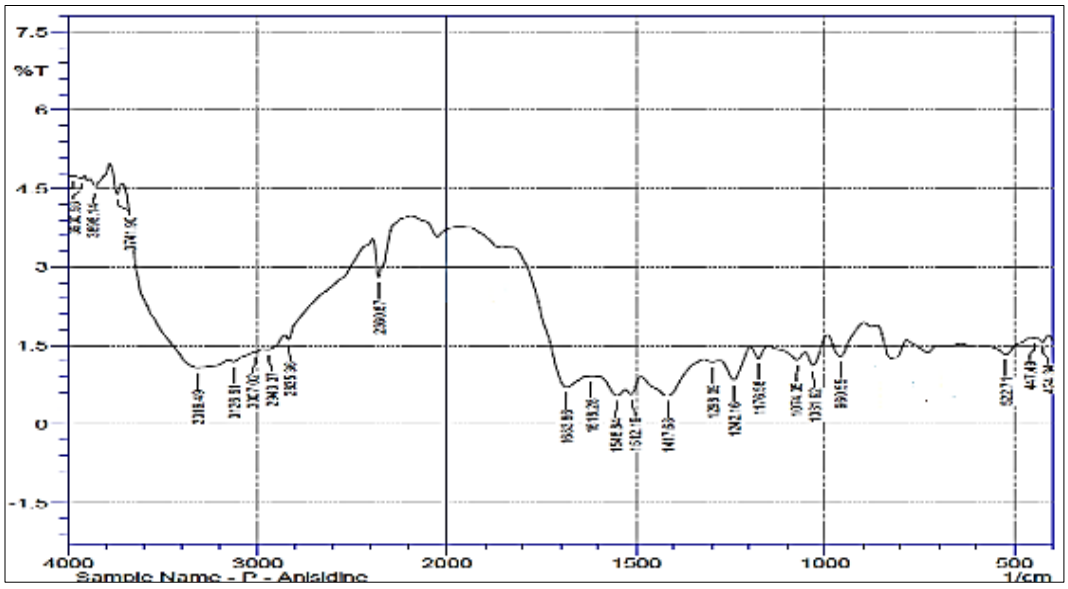


Fig 3.9: FTIR 6a

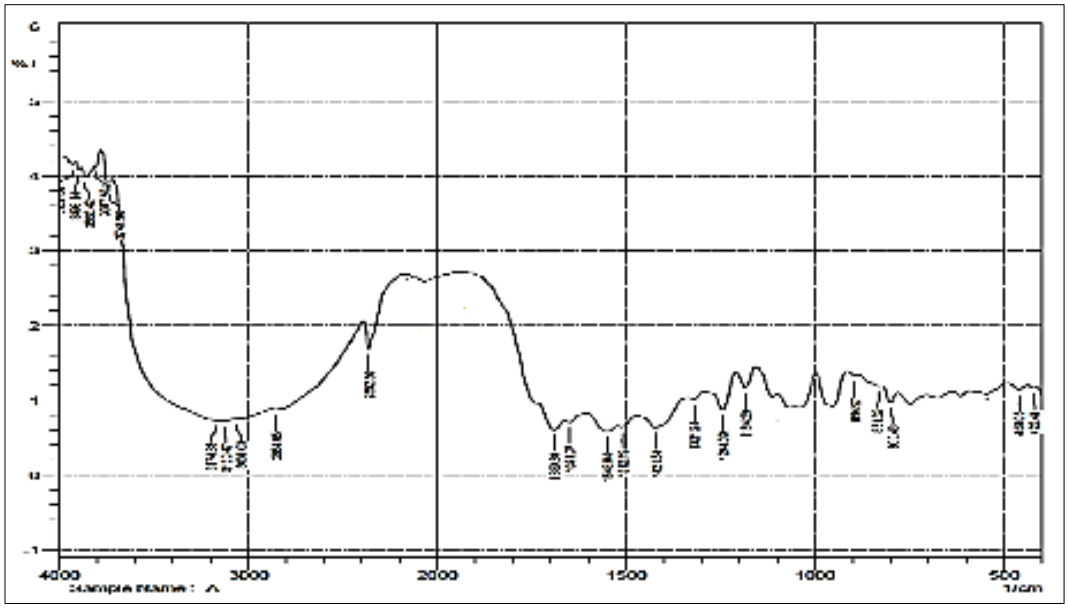


Fig 3.10: FTIR of 6b

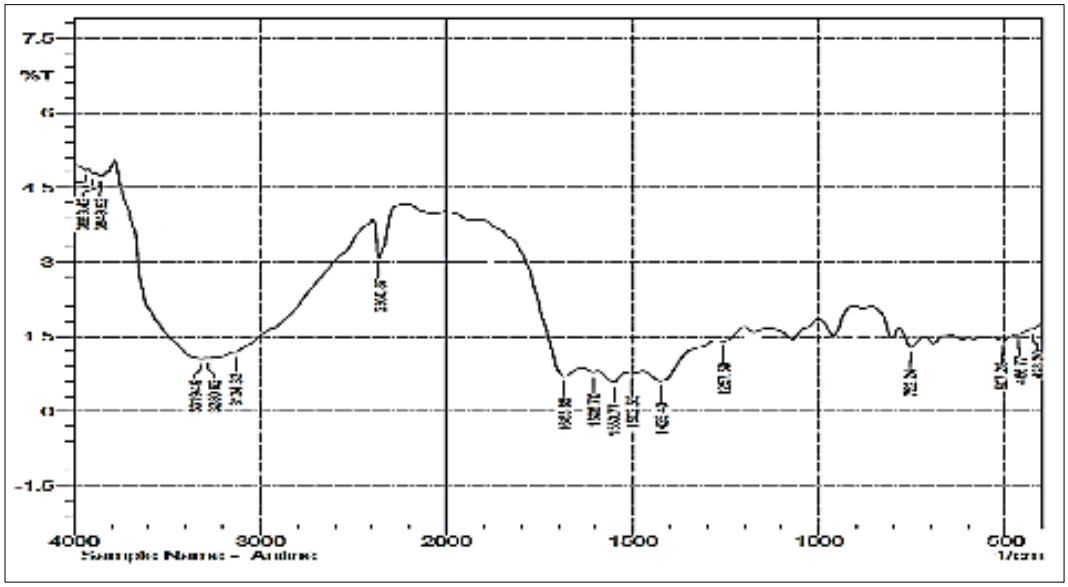


Fig 3.11: FTIR of 6c

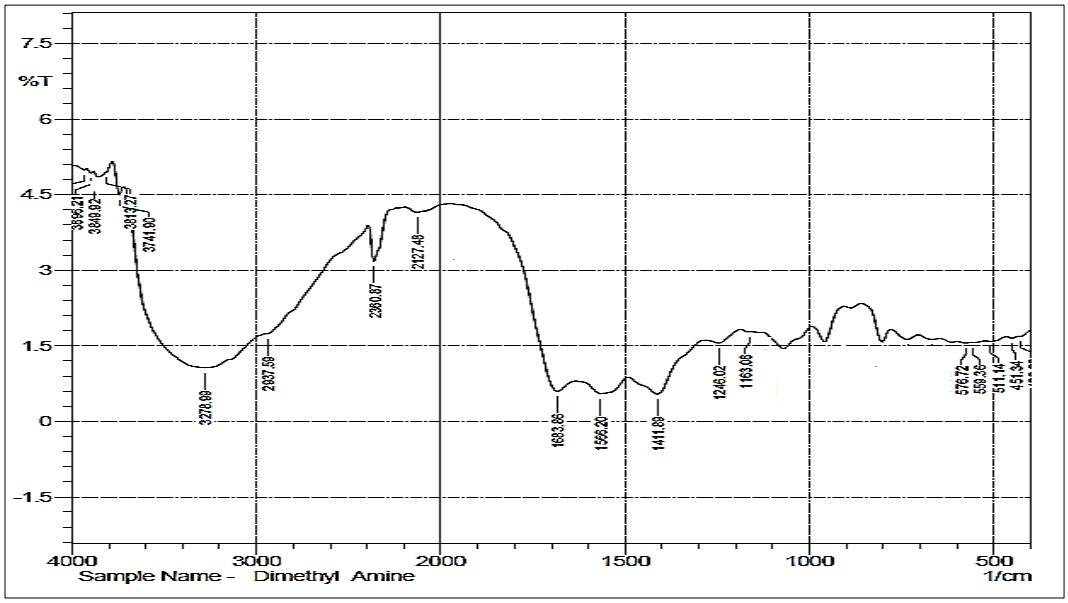


Fig 3.12: FTIR of 6d

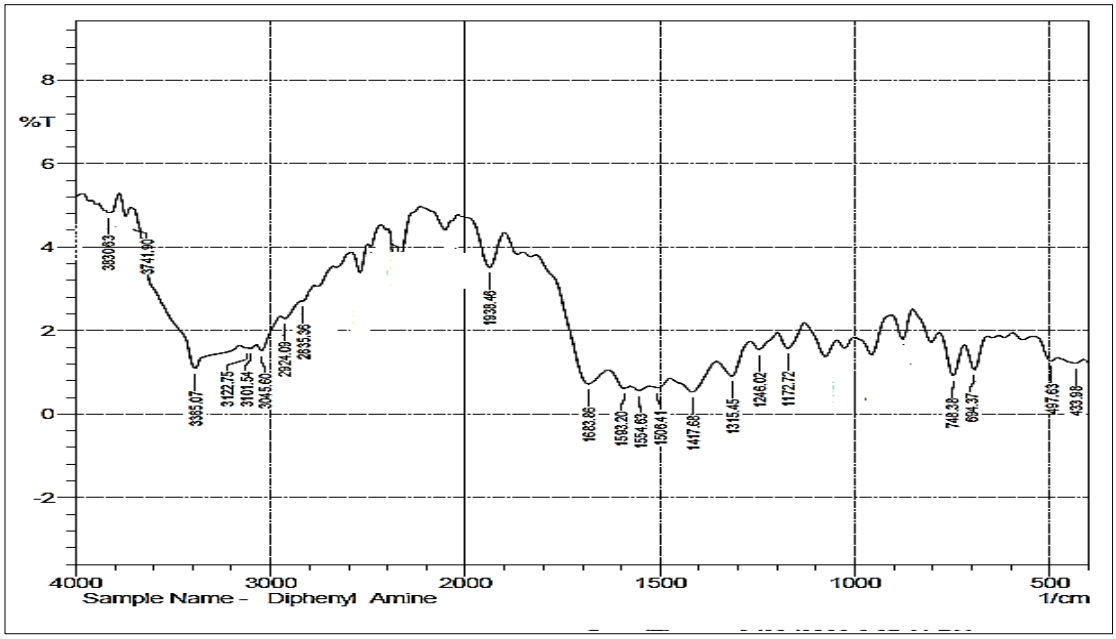


Fig 3.13: FTIR of 6e

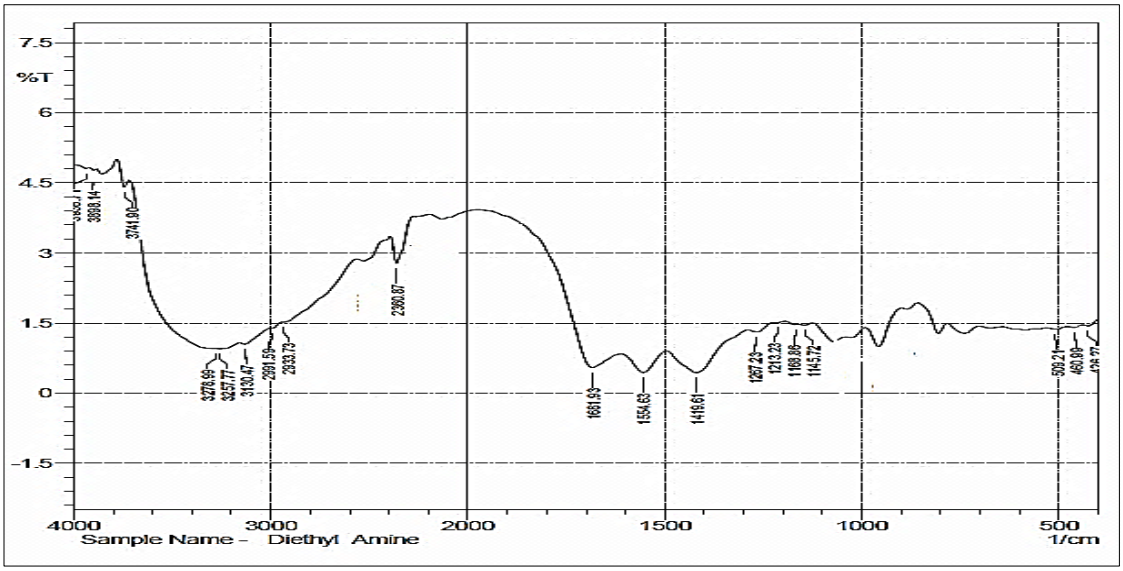


Fig 3.14: FTIR of 6f

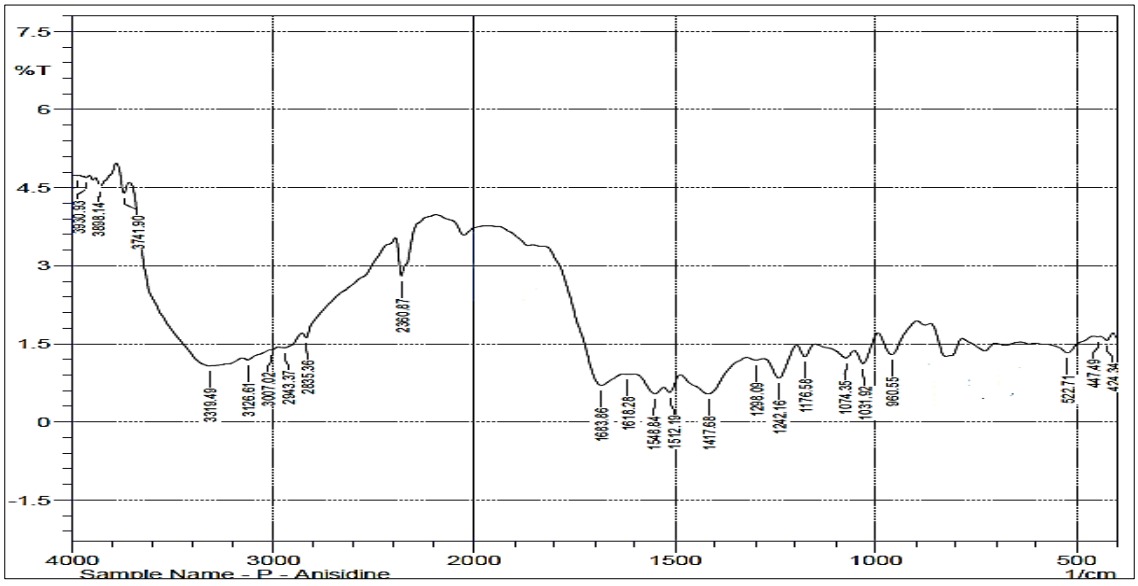


Fig 3.15: FTIR spectra of 6g

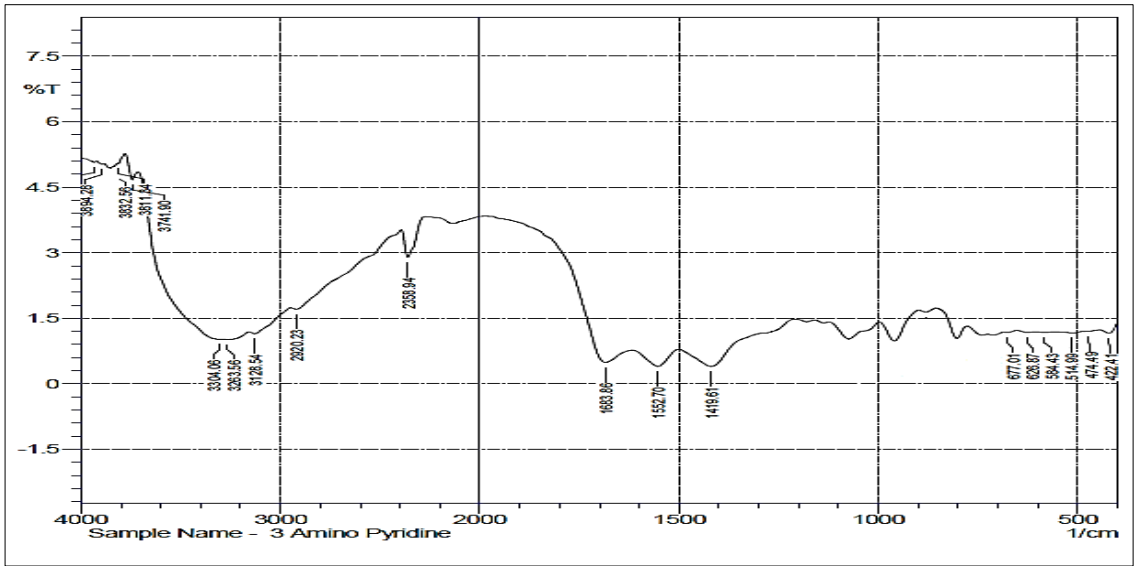


Fig 3.16: FTIR spectra of 6h

The FTIR spectra for newly synthesised compounds are shown in Table No: 3.4 and Figure 3.1 to 3.16 The FTIR data of compounds shows the information about the functional group present and substituents attached. Compound-5a to 5h gives characteristic peak at 3509 due to NH_2 stretch, peak at 3517 due to OH starch, also peak due to Cl at 849 cm.$^{-1}$, A peak at 2930 due to OCH_3 starch obtained broad band. A peak obtained due to CH_3 at 2990 cm^{-1}, also gives peak at 3065-3082 due to C-H aromatic stretch, and a broad band obtained at 864 due to Br substitution starch, a Bendle of peak obtained at 1274, 1799, 3201 due to CH_2-CH_3 starch. The obtained FTIR data of newly synthesised 1,3,5 triazines derivatives with substituted amines was compare with literature values and these values are good accord with literature survey [27].

The FTIR spectra for newly synthesised compounds are shown in Table No: 3.4 and Figure 3.1 to 3.16. The FTIR data of compounds shows the information about the functional group present and substituents attached. Compound-6a to 6h gives characteristic peak at 3509 due to NH_2 stretch, peak at 3517 cm.$^{-1}$ due to OH starch, also peak due to Cl at 849 cm.$^{-1}$, A peak at 2930 cm.$^{-1}$ due to OCH_3 starch obtained broad band. A peak obtained due to CH_3 at 2990 cm^{-1}, also gives peak at 3065-3082 cm.$^{-1}$ due to C-H aromatic stretch, and a broad band obtained at 864 due to Br substitution starch, a Bendle of peak obtained at 1274, 1799, 3201 cm.$^{-1}$ due to CH_2-CH_3 starch. The obtained FTIR data of newly synthesised 1,3,5 triazines derivatives with substituted amines was compare with literature values and these values are good accord with literature survey [28].

The FTIR spectral analysis of the synthesized 1,3,5-triazine derivatives confirmed the presence of characteristic functional groups and supported the proposed structures. The spectra exhibited strong absorption bands corresponding to C=N stretching vibrations of the triazine ring, along with signals arising from C–N stretching and aromatic ring vibrations. The appearance of additional bands due to the substituent groups (such as –NH, –OH, –Cl, –OCH_3, or alkyl moieties) further verified their successful incorporation into the triazine framework. The absence of unexpected peaks indicated good purity of the synthesized compounds.

Thus, FTIR characterization provided clear evidence for the formation of the triazine nucleus and its derivatives, serving as a reliable tool to establish structural confirmation at the preliminary stage.

^{1}H NMR Spectral Study

Proton NMR Spectroscopy gives information about the type of protons; to study the number of equivalent protons and their environment thereby we can ascertain the structure of the molecule. The ^{1}NMR spectrum was recorded on Bruker Avance Neo 500MHz NMR Spectrometer, DMSO used as a solvent. The ^{1}H NMR spectra of all newly synthesized 1,3,5-Triazine derivatives are shown below in Table No: 3.5 and [Figure No: 3.17 to 3.32].

Table 3.5: ^{1}H NMR data of synthesised 1,3,5-Triazine Derivatives

Sr. No.	Compound Name	Chemical Shift (PPM)	Figure No.
1.	Compound – 5a	δ 1.46-1.66 (t, 22H, cy - H), δ 2.98 (m, 2H, methylene proton,) and δ 5.24 (s, 2H, NH_2), δ 12.12 (s 1H, NH)	3.17
2.	Compound – 5b	δ 1.46-1.66 (t, 22H, cy - H), δ 2.98 (m, 2H, methylene proton,) and δ 9.67 (s, 1H, OH), δ 12.12 (s 1H, NH)	3.18
3.	Compound – 5c	δ 1.46-1.66 (t, 22H, cy - H), δ 2.98 (m, 2H, methylene proton,) and δ 12.12 (s 1H, NH)	3.19
4.	Compound – 5d	δ 1.46-1.66 (t, 22H, cy - H), δ 2.98 (m, 2H, methylene proton,) and δ 12.12 (s 1H, NH), δ 3.98 (s 3H, OCH_3).	3.20
5.	Compound – 5e	δ 1.46-1.66 (t, 22H, cy - H), δ 2.98 (m, 2H, methylene proton,) and δ 12.12 (s 1H, NH), δ 2.34 (s 3H, CH_3).	3.21
6.	Compound – 5f	δ 1.46-1.66 (t, 22H, cy - H), δ 2.98 (m, 2H, methylene proton,) and δ 10.12 (s 1H, NH), δ 7.39,7.49, 7.83 (s 5H, benzene).	3.22
7.	Compound – 5g	δ 1.46-1.66 (t, 22H, cy - H), δ 2.98 (m, 2H, methylene proton,) and δ 10.12 (s 1H, NH), δ 7.55,7.76, (s 4H, benzene).	3.23
8.	Compound – 5h	δ 1.46-1.66 (t, 22H, cy - H), δ 2.98 (m, 2H, methylene proton,) and δ 10.12 (s 1H, NH), δ 2.73 (m 2H, CH_2). δ 1.18 (t 3H, CH_3).	3.24

9.	Compound – 6a	δ 7.84, 8.40 (s 4H, pyrazine), δ 8.89 (s, 1H, amine proton,) and δ 12.12 (s 1H, NH), δ 7.68 (s 1H, thiazole). δ 5.42 (s 2H, NH_2).	3.25
10.	Compound –6b	δ 7.84, 8.40 (s 4H, pyrazine), δ 8.89 (s, 1H, amine proton,) and δ 12.12 (s 1H, NH), δ 7.68 (s 1H, thiazole). δ 9.67 (s H, OH), δ 6.86-7.38 (m 4H, phenyl)	3.26
11.	Compound-6c	δ 7.84, 8.40 (s 4H, pyrazine), δ 8.89 (s, 1H, amine proton,) and δ 12.12 (s 1H, NH), δ 7.68 (s 1H, thiazole). δ 6.86-7.38 (m 4H, phenyl)	3.27
12.	Compound-6d	δ 7.84, 8.40 (s 4H, pyrazine), δ 8.89 (s, 1H, amine proton,) and δ 12.12 (s 1H, NH), δ 7.68 (s 1H, thiazole). δ 13.11 (s 2H, OH), δ 1.03, 7.55 (m 4H, phenyl), δ 3.81 (s 3H, OCH_3)	3.28
13.	Compound-6e	δ 7.84, 8.40 (s 4H, pyrazine), δ 8.89 (s, 1H, amine proton,) and δ 12.12 (s 1H, NH), δ 7.68 (s 1H, thiazole). δ 13.11 (s 2H, OH), δ 1.03, 7.55 (m 4H, phenyl), δ 2.34 (s 3H, CH_3)	3.29
14.	Compound-6f	δ 7.84, 8.40 (s 4H, pyrazine), δ 8.89 (s, 1H, amine proton,) and δ 12.12 (s 1H, NH), δ 7.68 (s 1H, thiazole). δ 13.11 (s 2H, OH), δ 1.03, 7.55 (m 4H, phenyl), δ 7.83,7.39, 7.49 (s 5H, Benzene)	3.30
15	Compound-6g	δ 7.84, 8.40 (s 4H, pyrazine), δ 8.89 (s, 1H, amine proton,) and δ 12.12 (s 1H, NH), δ 7.68 (s 1H, thiazole). δ 13.11 (s 2H, OH), δ 1.03, 7.55 (m 4H, phenyl), δ 7.76,7.55 (s 5H, Benzene)	3.31
16	Compound-6h	δ 7.84, 8.40 (s 4H, pyrazine), δ 8.89 (s, 1H, amine proton,) and δ 12.12 (s 1H, NH), δ 7.68 (s 1H, thiazole). δ 13.11 (s 2H, OH), δ 1.03, 7.55 (m 4H, phenyl), δ 2.72 (q, 2H), δ 1.18 (t, 3H)	3.32

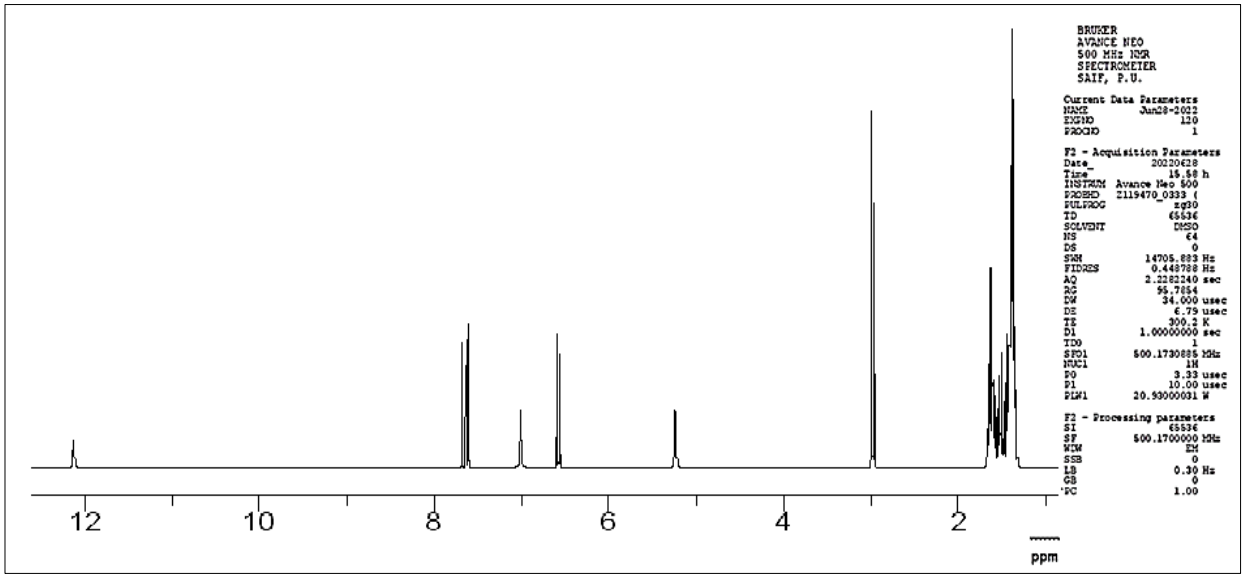


Fig 3.17: ^{1}H NMR spectrum of N2-(4-(4-aminophenyl) thiazol-2-yl)-N4, N6-bis(cyclohexylmethyl)-1,3,5-triazine-2,4,6-triamine (Compound-5a)

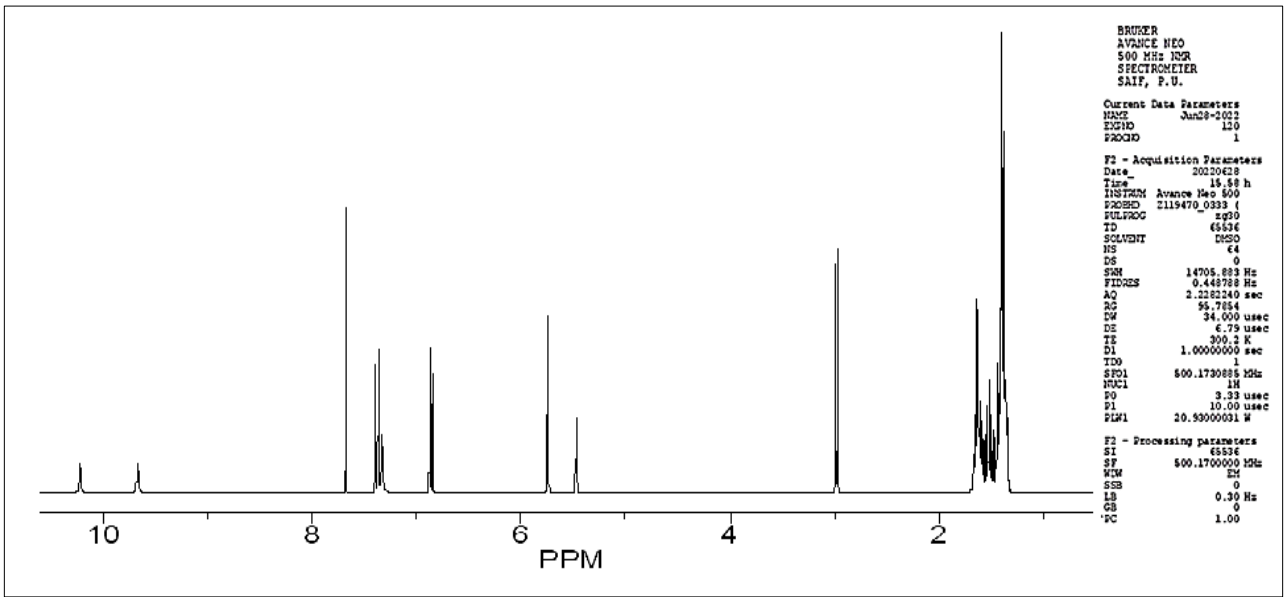


Fig 3.18: ^{1}H NMR spectra of of 4-(2-((4,6-bis ((cyclohexyl methyl) amino)-1,3,5-triazin-2-yl) amino) thiazol-4-yl) phenol (5b)

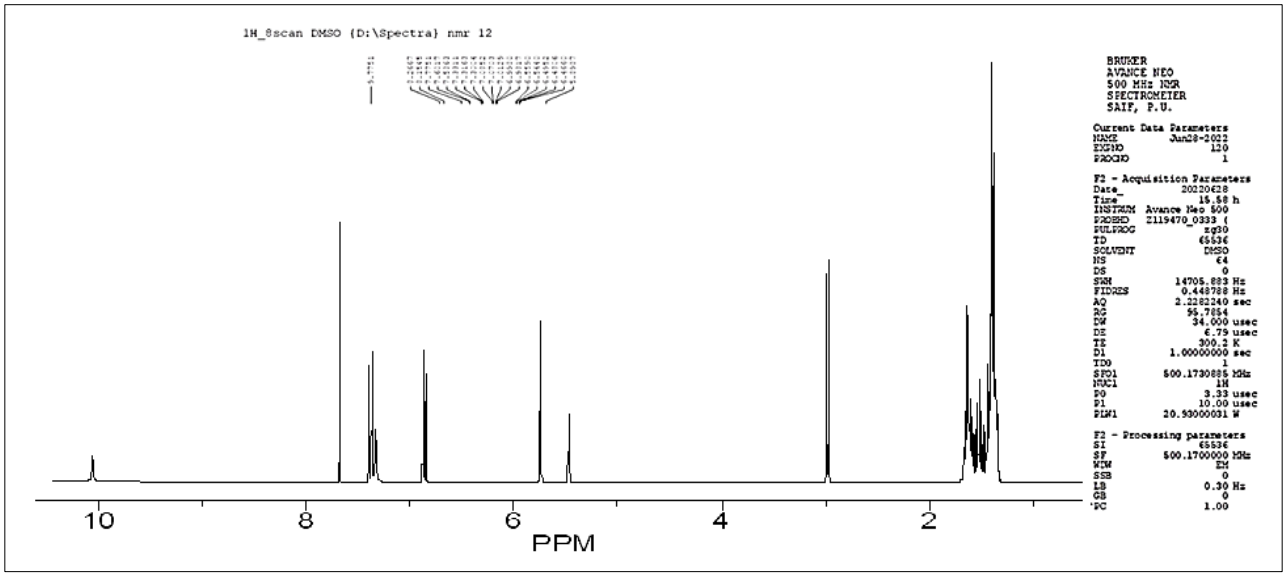


Fig 3.19: [1]H NMR spectra of N2-(4-(4-chlorophenyl) thiazol-2-yl)-N4, N6 bis (cyclohexyl methyl)-1,3,5-triazine-2,4,6-triamine (5c)

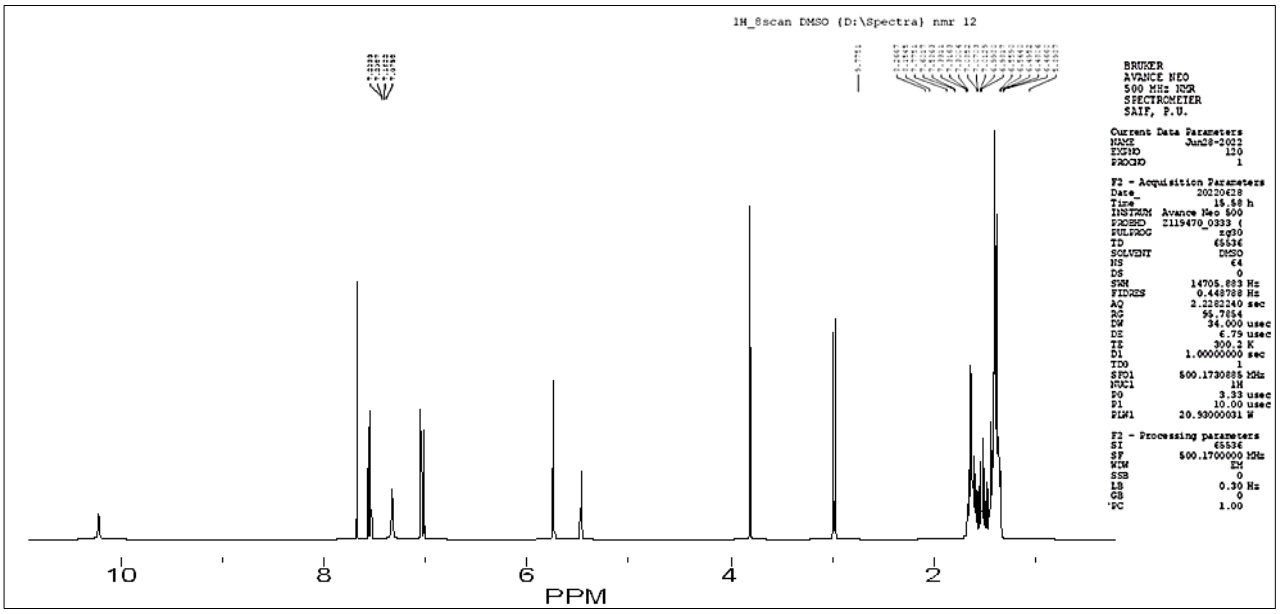


Fig 3.20: [1]H NMR spectra of N2, N4-bis(cyclohexyl methyl)-N6-(4-(4-methoxy phenyl)thiazol-2-yl)-1,3,5-triazine-2,4,6-triamine (5d)

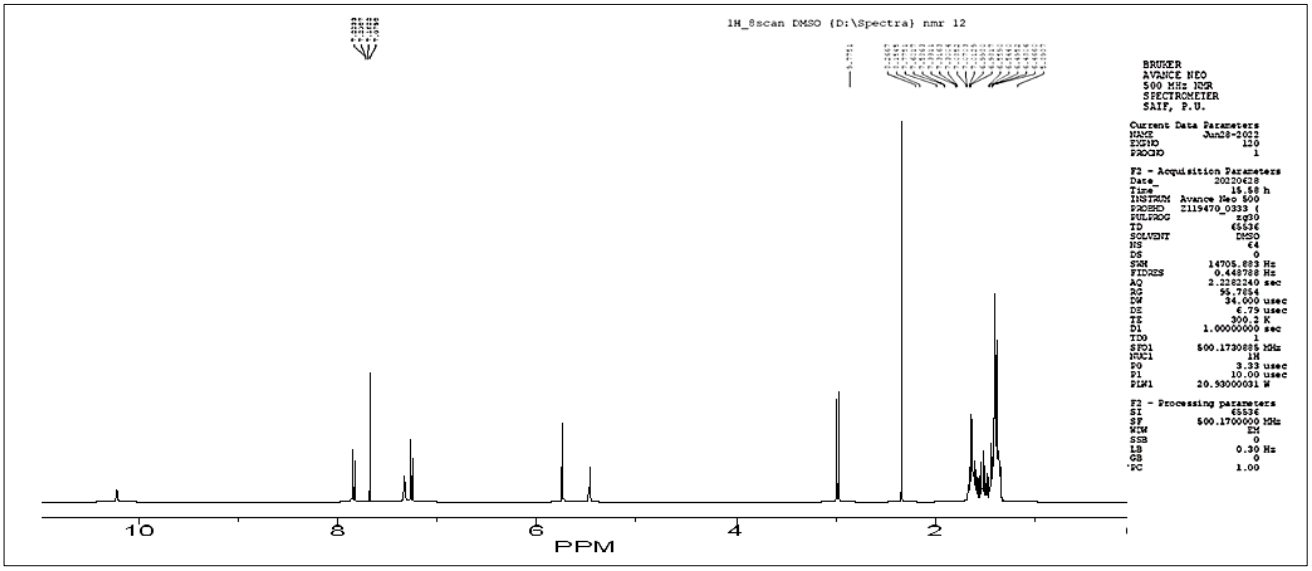


Fig 3.21: [1]H NMR spectra of N2, N4-bis (cyclohexyl methyl)-N6-(4-(p-tolyl) thiazol-2-yl)-1,3,5-triazine-2,4,6-triamine (Compound-5e)

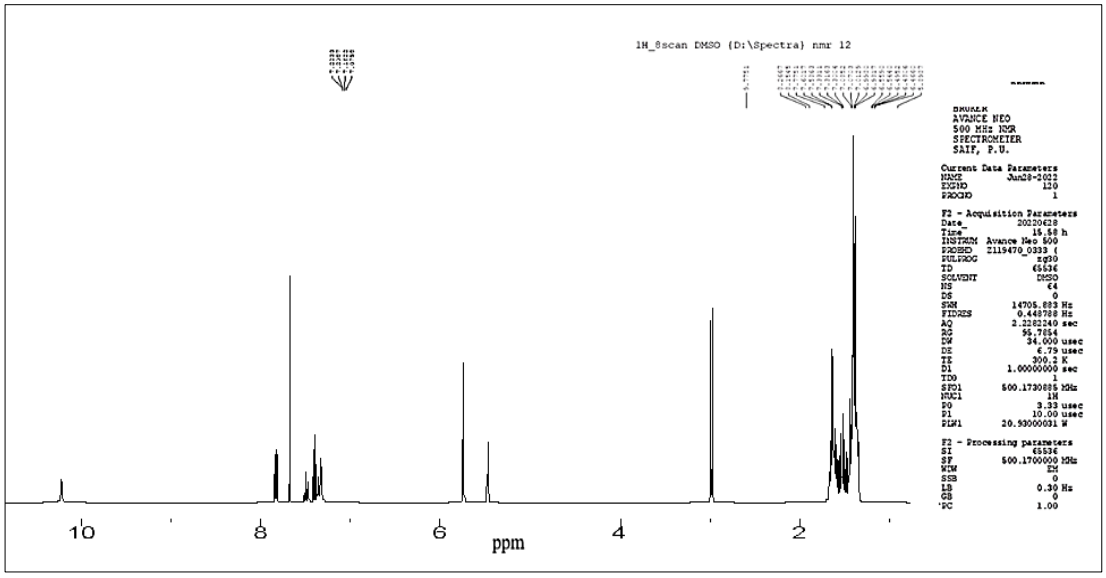


Fig 3.23: [1]H NMR spectra of N2, N4-bis(cyclohexylmethyl)-N6-(4-phenylthiazol-2-yl)-1,3,5-triazine-2,4,6-triamine (Compound-5f)

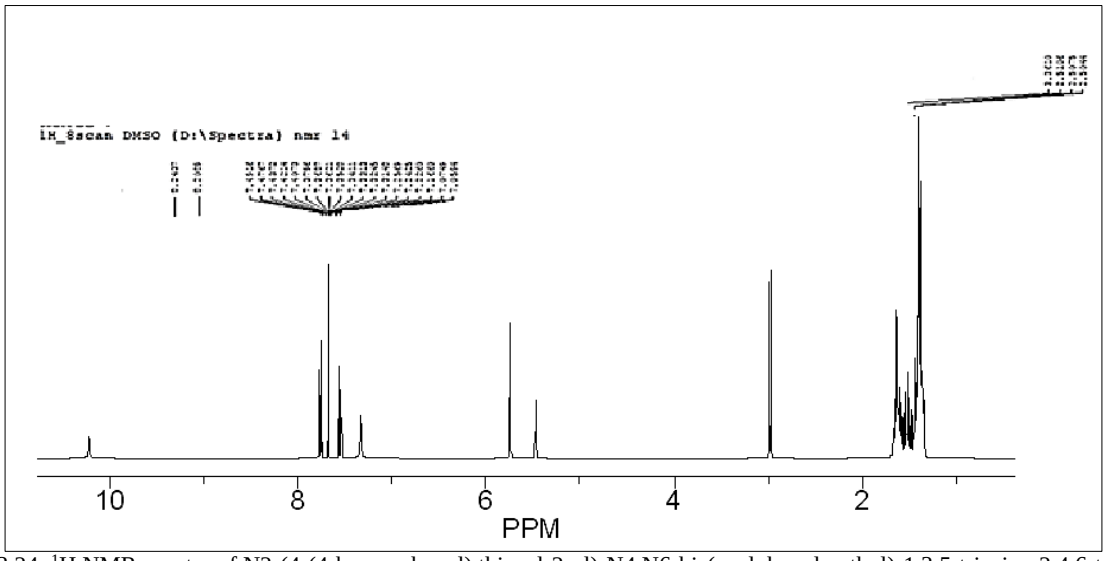


Figure 3.24: [1]H NMR spectra of N2-(4-(4-bromophenyl) thiazol-2-yl)-N4,N6-bis(cyclohexylmethyl)-1,3,5-triazine-2,4,6-triamine (Compound-5g)

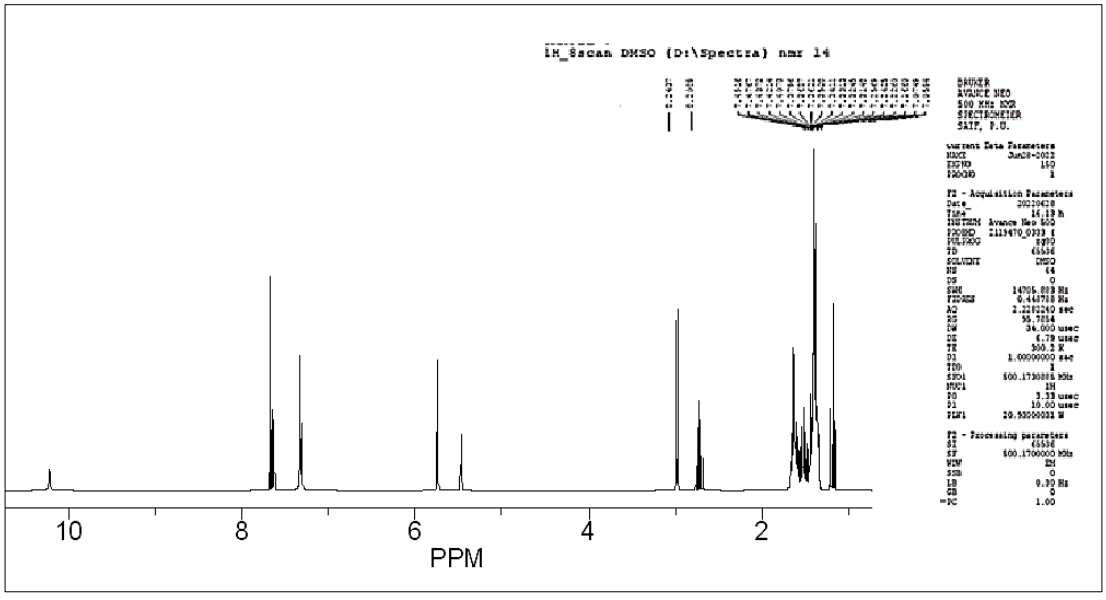


Fig 3.25: [1]H NMR spectra of N2,N4-bis(cyclohexylmethyl)-N6-(4-(4 ethylphenyl)thiazol-2-yl)-1,3,5-triazine-2,4,6-triamine (Compound-5h)

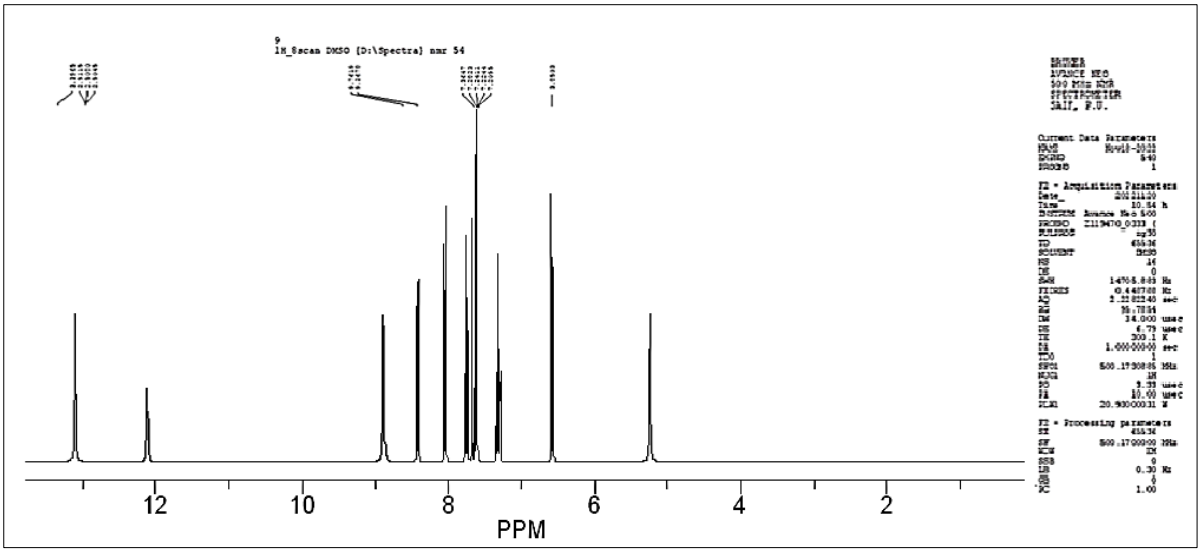


Fig 3.26: [1]HNMR spectrum of 3-((4-((4-(4-aminophenyl) thiazol-2-yl) amino) --((2-carboxyphenyl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2- carboxylic acid (Compound 6a)

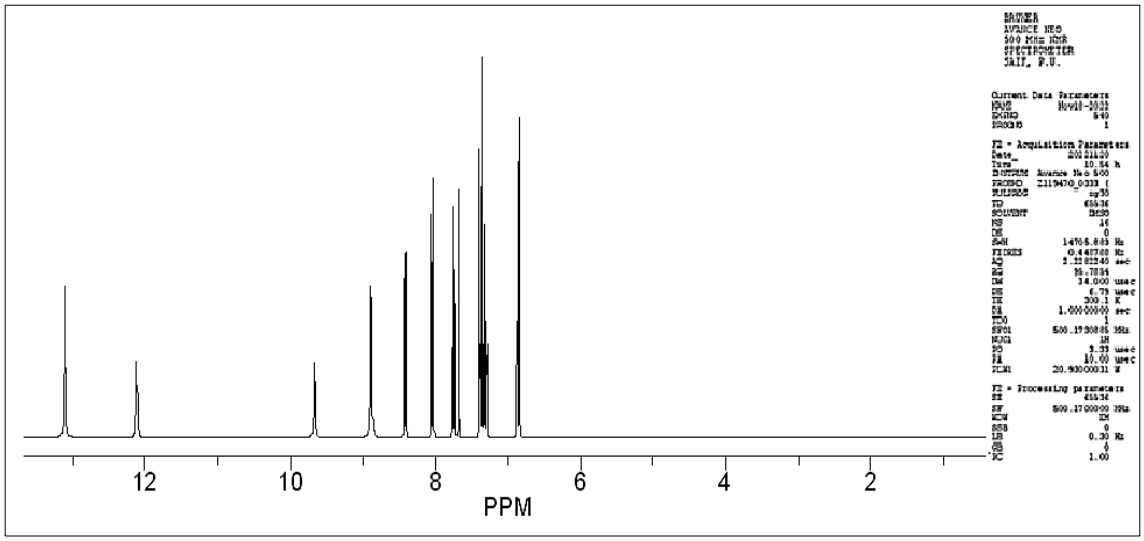


Fig 3.27: [1]HNMR spectrum of 3-((4-((2-carboxy phenyl) amino)-6-((4-(4-hydroxy phenyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydro pyrazine-2-carboxylic acid (Compound 6b)

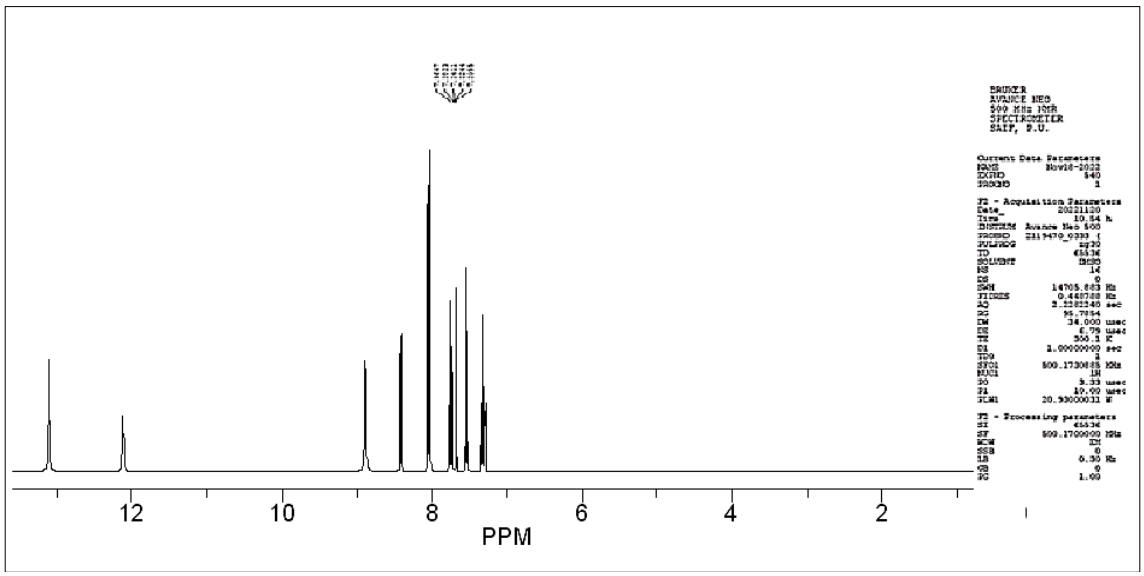


Fig 3.28: [1]HNMR spectrum of 3-((4-((2-carboxyphenyl) amino)-6-((4-(4-chlorophenyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydro pyrazine-2-carboxylic acid (Compound 6c)

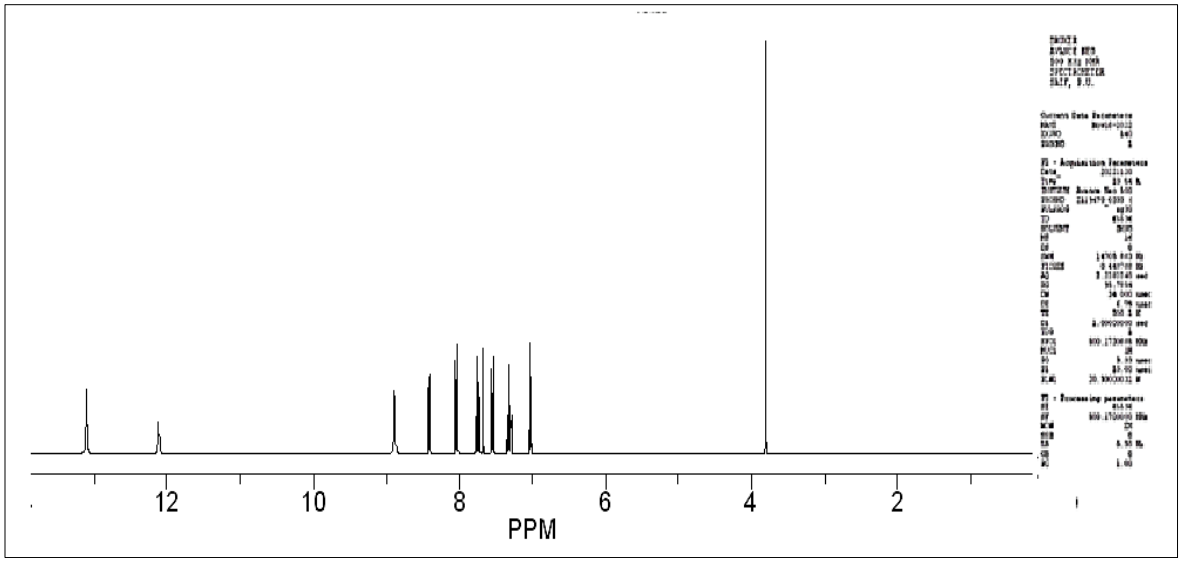


Fig 3.29 : [1]HNMR spectrum of 3-((4-((2-carboxyphenyl) amino)-6-((4-(4-methoxyphenyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydro pyrazine-2-carboxylic acid (compound 6d)

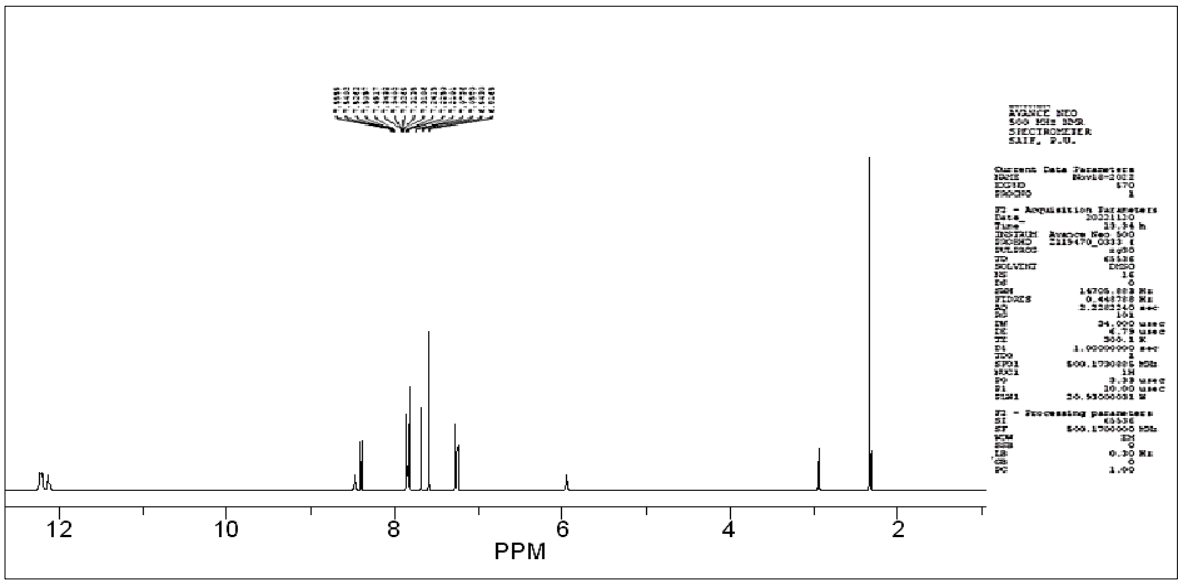


Fig 3.30: [1]HNMR spectrum of 3-((4-((2 carboxy phenyl) amino)-6-((4-(p-tolyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2-carboxylic acid (compound 6e)

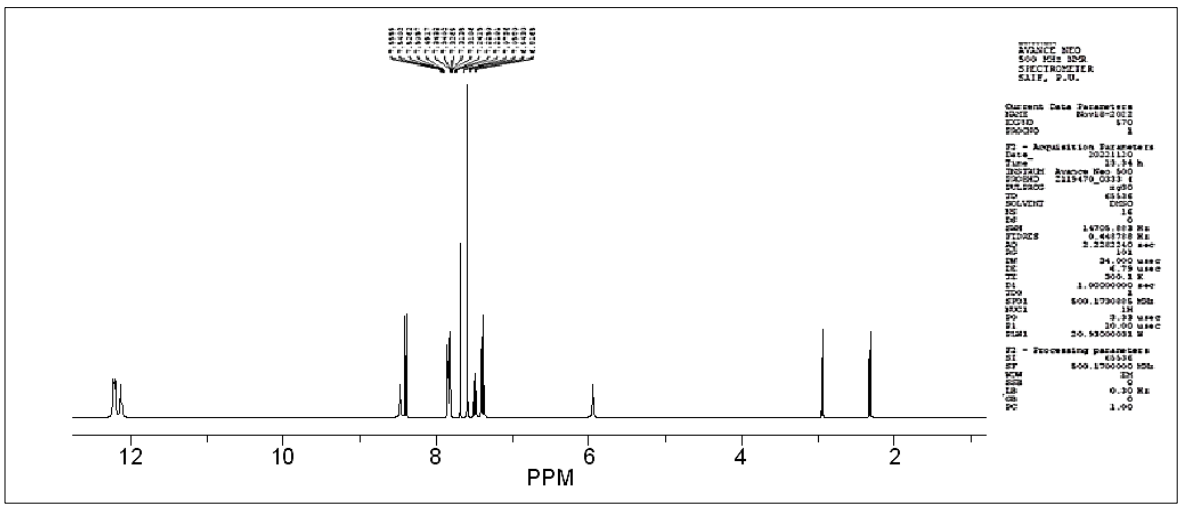


Fig 3.31: [1]HNMR spectrum of 3-((4-((2 carboxy phenyl) amino)-6-((4-(p-tolyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydro pyrazine-2-carboxylic acid (compound 6f)

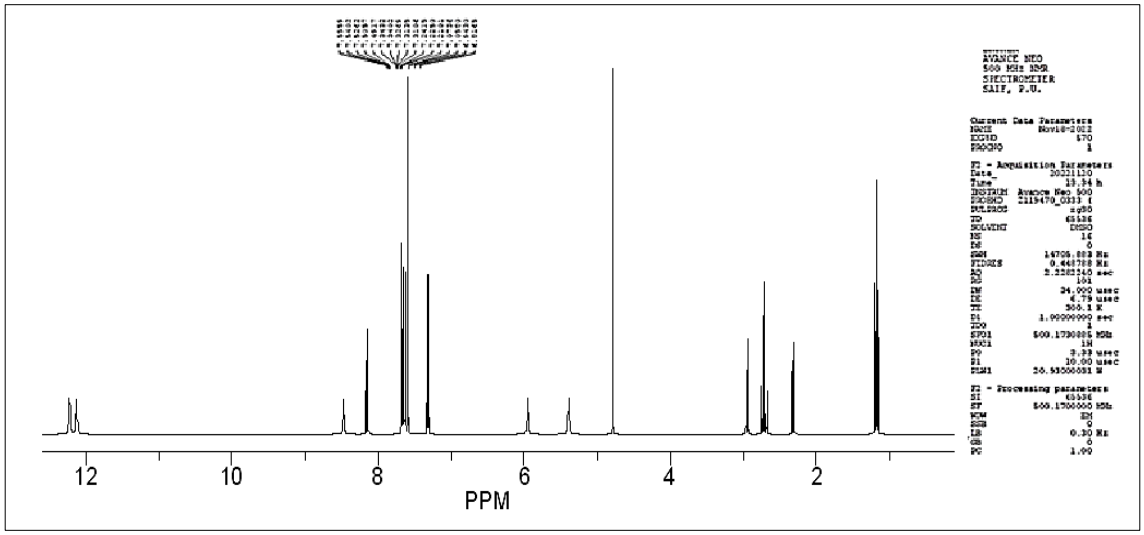


Fig 3.32: [1]HNMR spectrum of 3-((4-((2-carboxy phenyl) amino)-6-((4-(4-ethyl phenyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2-carboxylic acid (compound 6h)

From the above [1]H NMR data of newly synthesized 1,3,5-Triazine derivatives in DMSO revealed distinct proton environments. Compound 5a show characteristic peak pattern at 5.24 due to NH_2, Compound 5b show characteristic peak pattern at 9.67 due OH, Compound 5d show characteristic peak pattern at 3.98 due to OCH_3 Compound 5e show characteristic peak pattern at 2.34 due CH_3 Compound 5f show characteristic peak pattern at 7.39,7.49, 7.83 due to benzene ring. Compound 5g show characteristic peak pattern at δ 7.55,7.76, and Compound 5h show characteristic peak pattern at 2.73 due to CH_2 1.18 due to CH_3.and these values are good accord with literature survey [29-35].

The compound 6a show characteristic peak pattern at 5.42 due to NH_2 and patten of peak is singlet. Compound 6b show characteristic peak pattern at 9.67 due OH patten of peak is singlet, Compound 6d show characteristic peak pattern at 3.81 due to OCH_3 patten of peak is singlet Compound 6e show characteristic peak pattern at 2.34 due CH_3 and patten of peak is singlet Compound 6f show characteristic peak pattern at 7.86,7.39, 7.49 due to benzene ring and obtained patten of peak is dublet. Compound 6g show characteristic peak pattern at 7.76,7.55, and Compound 6h show characteristic peak pattern at 2.72 due to CH2 1.18 due to CH_3. patten of peak is triplet and quartet and these values are good accord with literature survey [36-40].

The [1]H NMR spectra of the synthesized 1,3,5-triazine derivatives displayed well-resolved proton signals consistent with the proposed molecular structures. The absence of ring protons in the triazine core was evident, while the characteristic chemical shifts corresponding to the substituted amines, aromatic, aliphatic, or heteroatom-linked protons confirmed successful substitution on the triazine nucleus. The splitting patterns and integration values matched the expected number of protons in each environment, thereby validating the structural framework.

Overall, the [1]H NMR spectral analysis strongly supports the successful synthesis and structural confirmation of the 1,3,5-triazine derivatives.

[13]C NMR Spectral Studies

[13]C Nuclear Magnetic Resonance (NMR) spectroscopy is a powerful analytical technique used to elucidate the carbon skeleton of organic molecules and to confirm the presence of specific structural moieties. In the case of 1,3,5-triazine derivatives, [13]C NMR provides critical information about the chemical environment of carbon atoms within the heteroaromatic ring as well as the attached substituents. The triazine ring typically shows characteristic downfield signals for the C=N carbons, which can be clearly distinguished from the resonances of the substituted aromatic or aliphatic carbons. The presence, position, and chemical shift of these signals serve as reliable markers for verifying successful substitution on the triazine nucleus.

Thus, [13]C NMR characterization not only complements FTIR, [1]H NMR, and mass spectral data but also offers definitive structural confirmation of the synthesized 1,3,5-triazine derivatives.

It is similar to [1]H NMR or proton NMR, the identification of carbon atoms in an organic molecule just as proton NMR identifies hydrogen atoms. [13]C NMR detects only the [13]C isotope. The main carbon isotope, [12]C is not detected although much less sensitive than [1]H NMR spectroscopy. The [13]C NMR spectra of all newly synthesized 1,3,5-triazine derivatives are shown below in Table No: 3.6 and Figure No: 3.33 to 3.48.

Table 3.6: [13]C NMR data of synthesised 1,3,5-Triazine Derivatives

Sr. No.	Compound	Chemical Shift (PPM) [13]C NMR (500MHz) DMSO	Figure No.
1.	Compound-5a	31.0, 25.5, 26.0, 38.0, 55.6, 164.1, 162.5, 160.6, 105.0, 150.2, 123.0, 128.3, 115.1, 145.6	3.33
2.	Compound-5b	31.0, 25.5, 26.0, 38.0, 55.6, 164.1, 162.5, 160.6, 105.0, 150.2, 125.6, 128.9, 116.4, 158.6	3.34
3.	Compound-5c	31.0, 25.5, 26.0, 38.0, 55.6, 164.1, 162.5, 160.6, 105.0, 150.2, 125.6, 128.9, 129.3,134.3	3.35
4.	Compound-5d	31.0, 25.5, 26.0, 38.0, 55.6, 164.1, 162.5, 160.6, 105.0, 150.2, 125.3, 128.5, 114.8, 160.6 and 55.8	3.36
5.	Compound-5e	31.0, 25.5, 26.0, 38.0, 55.6, 164.1, 162.5, 160.6, 105.0, 150.2, 130.0, 125.7, 129.5, 131.7, and 21.3	3.37
6.	Compound-5f	31.0, 25.5, 26.0, 38.0, 55.6, 164.1, 162.5, 160.6, 105.0, 150.2, 133.0, 127.5, 129.2, 128.7	3.38
7.	Compound-5g	31.0, 25.5, 26.0, 38.0, 55.6, 164.1, 162.5, 160.6, 105.0, 150.2, 132.0, 128.3, 132.1, 123.1	3.39

8.	Compound-5h	31.0, 25.5, 26.0, 38.0, 55.6, 164.1, 162.5, 160.6, 105.0, 150.2, 130.2, 125.7, 129.7, 144.3, 28.2, 14.5	3.40
9.	Compound-6a	145.0, 177.5, 72.7, 79.0, 164.1, 162.5, 160.6, 105.0, 150.2, 123.0, 128.3, 115.1 145.6	3.41
10.	Compound-6b	145.0, 177.5, 72.7, 79.0, 164.1, 162.5, 160.6, 105.0, 150.2, 126.2, 128.9, 116.4, 158.5	3.42
11.	Compound-6c	145.0, 177.5, 72.7, 79.0, 164.1, 162.5, 77.0, 103.3, 139.3, 132.3, 120.2, 128.7, 135.5.	3.43
12.	Compound-6d	145.0, 177.5, 72.7, 79.0, 164.1, 162.5, 77.0, 103.3, 139.3, 126.5, 129.7, 121.1, 159.8, 55.8.	3.44
13.	Compound-6e	145.0, 177.5, 72.7, 79.0, 164.1, 162.5, 77.0, 103.3, 139.3, 131.2, 129.0, 128.9, 21.3	3.45
14.	Compound-6f	145.0, 177.5, 72.7, 79.0, 164.1, 162.5, 77.0, 103.3, 139.3, 134.2, 128.3, 128.6, 127.9	3.46
15.	Compound-6g	145.0, 177.5, 72.7, 79.0, 164.1, 162.5, 77.0, 103.3, 139.3, 133.2, 128.6, 131.5, 122.3	3.47
16.	Compound-6h	145.0, 177.5, 72.7, 79.0, 164.1, 162.5, 77.0, 103.3, 139.3,131.4, 129.0, 127.6, 143.5, 28.2, 12.5	3.48

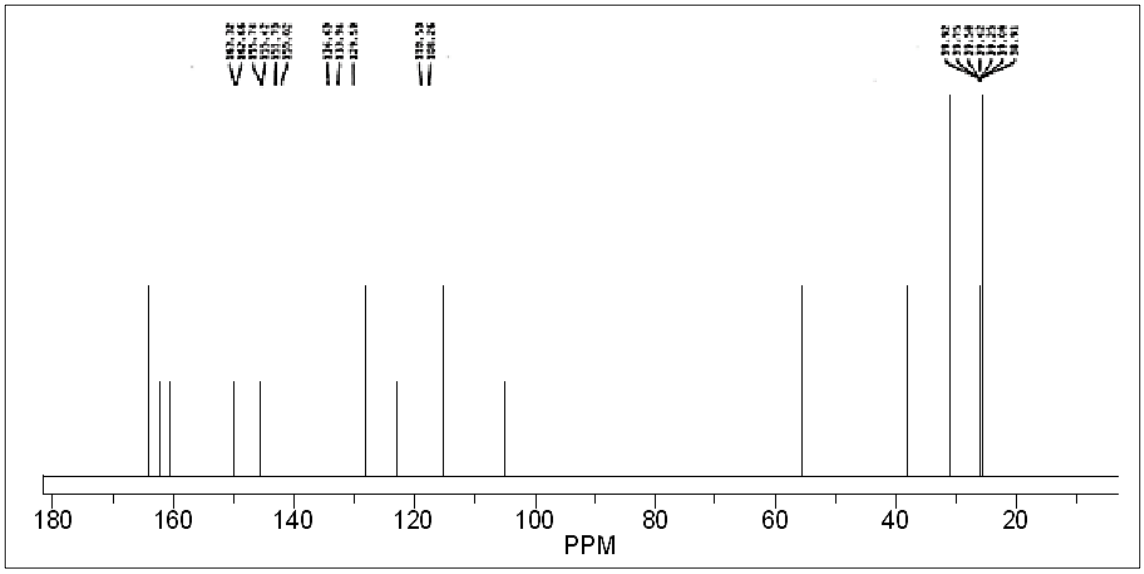


Fig 3.33: ^{13}C NMR Spectra N2-(4-(4-aminophenyl) thiazol-2-yl)-N4, N6-bis(cyclohexylmethyl)-1,3,5-triazine-2,4,6-triamine (Compound-5a)

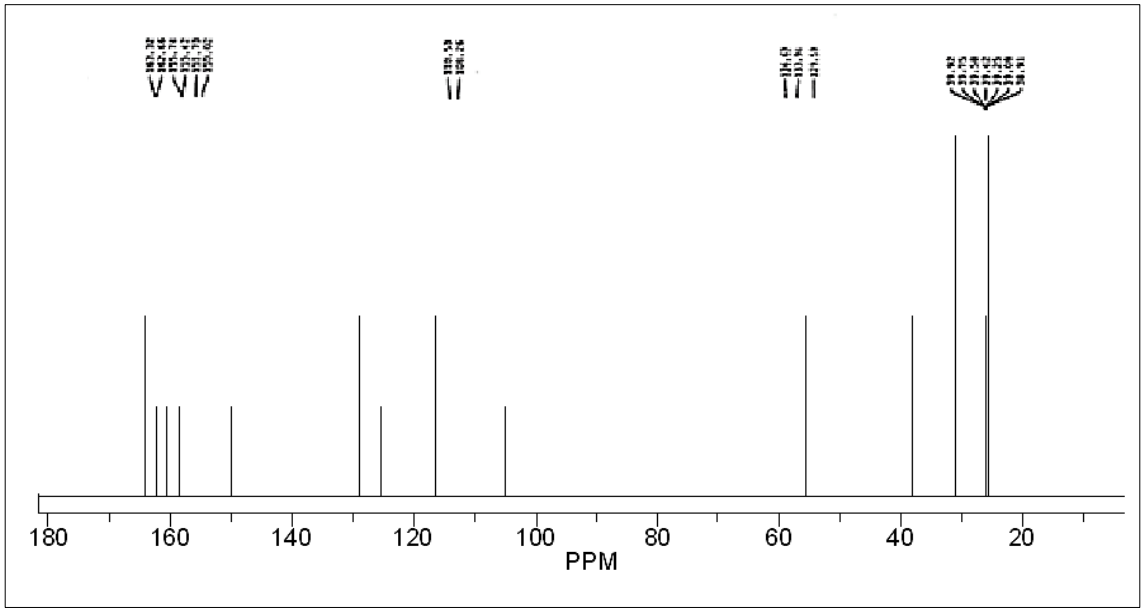


Fig 3.34: ^{13}C NMR Spectra of 4-(2-((4,6-bis((cyclohexylmethyl)amino)-1,3,5-triazin-2-yl) amino) thiazol-4-yl) phenol (Compound-5b)

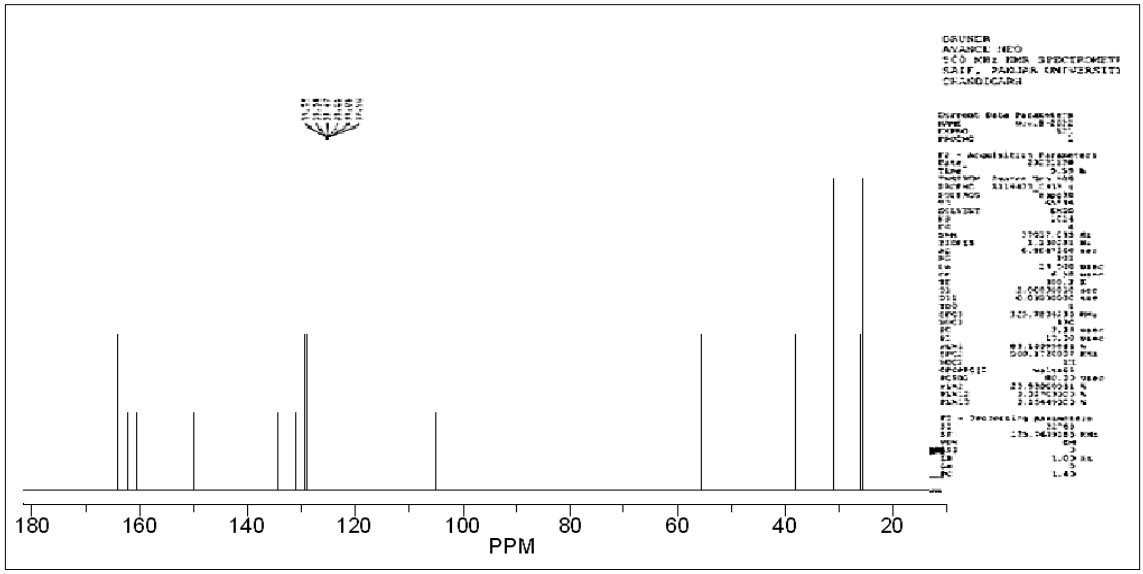


Fig 3.35: ^{13}C NMR Spectra of N2-(4-(4-chlorophenyl) thiazol-2-yl)-N4, N6-bis(cyclohexylmethyl)-1,3,5-triazine-2,4,6-triamine (Compound-5c)

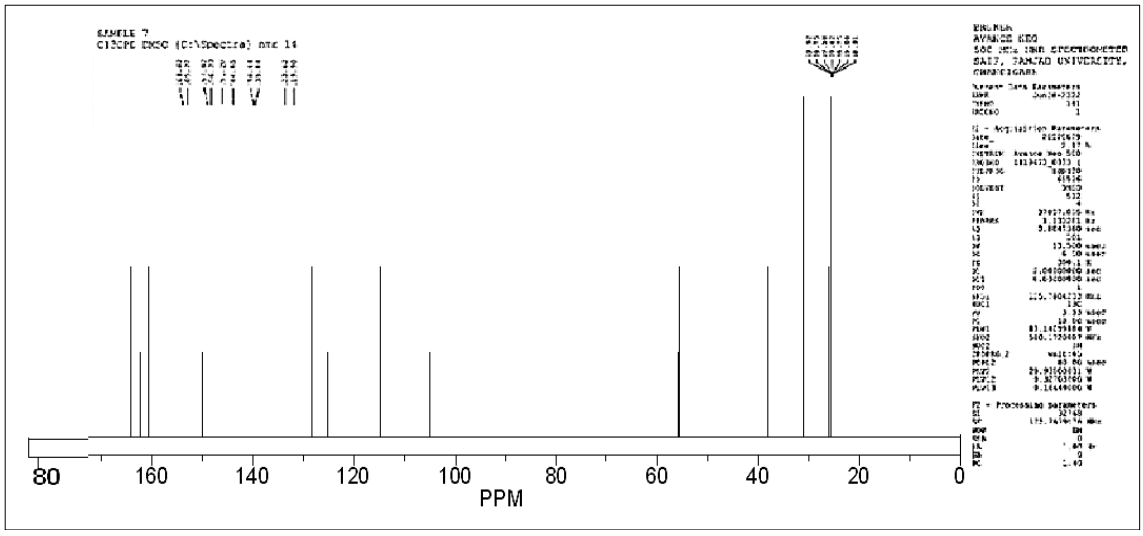


Fig 3.36: ^{13}C NMR Spectra of N2,N4-bis(cyclo hexyl methyl)-N6-(4-(4-methoxy phenyl)thiazol-2-yl)-1,3,5-triazine-2,4,6-triamine (Compound-5d)

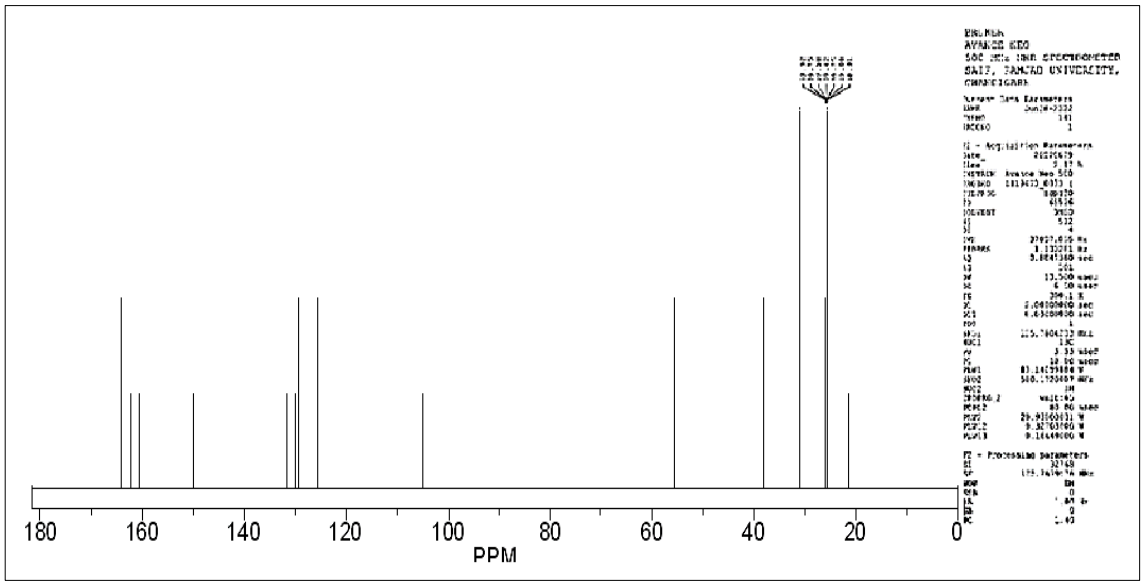


Fig 3.37: ^{13}C NMR Spectra of N2, N4-bis(cyclohexylmethyl)-N6-(4-(p-tolyl) thiazol-2-yl)-1,3,5-triazine-2,4,6-triamine (Compound-5e)

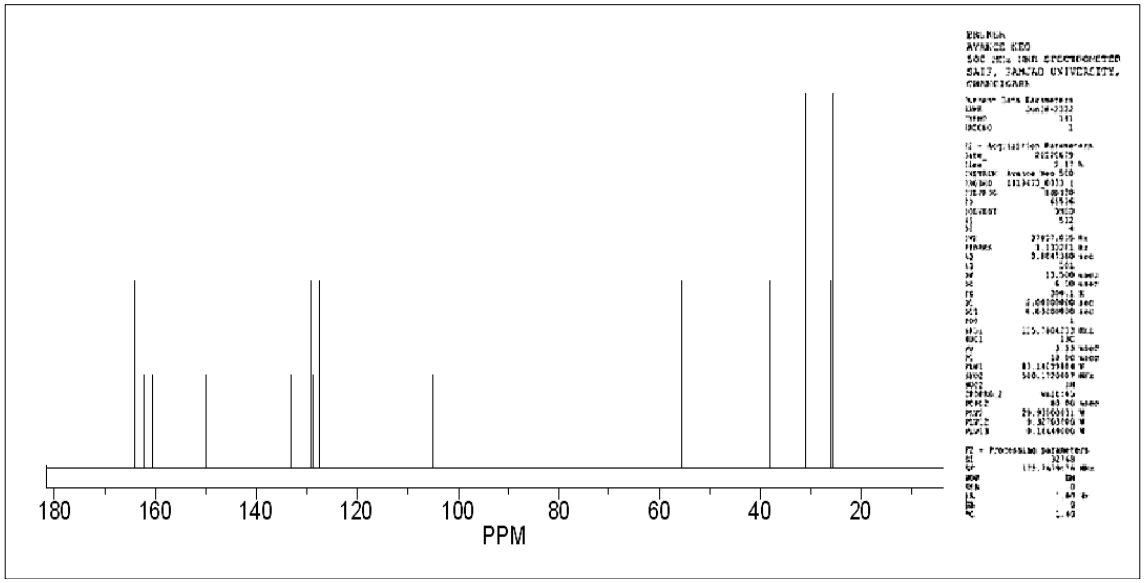


Fig 3.38: ^{13}C NMR Spectra of N2,N4-bis(cyclohexylmethyl)-N6-(4- phenylthiazol-2-yl)-1,3,5-triazine-2,4,6-triamine (Compound-5f)

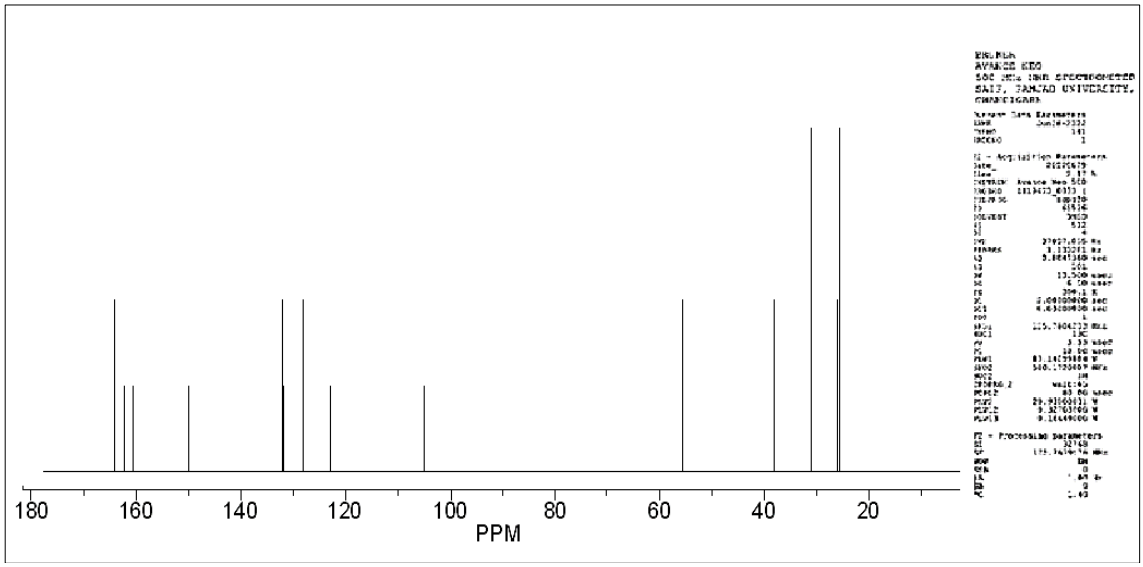


Fig 3.39: ^{13}C NMR Spectra of N2-(4-(4-bromophenyl) thiazol-2-yl)-N4, N6-bis(cyclohexylmethyl)-1,3,5-triazine-2,4,6-triamine (Compound-5g)

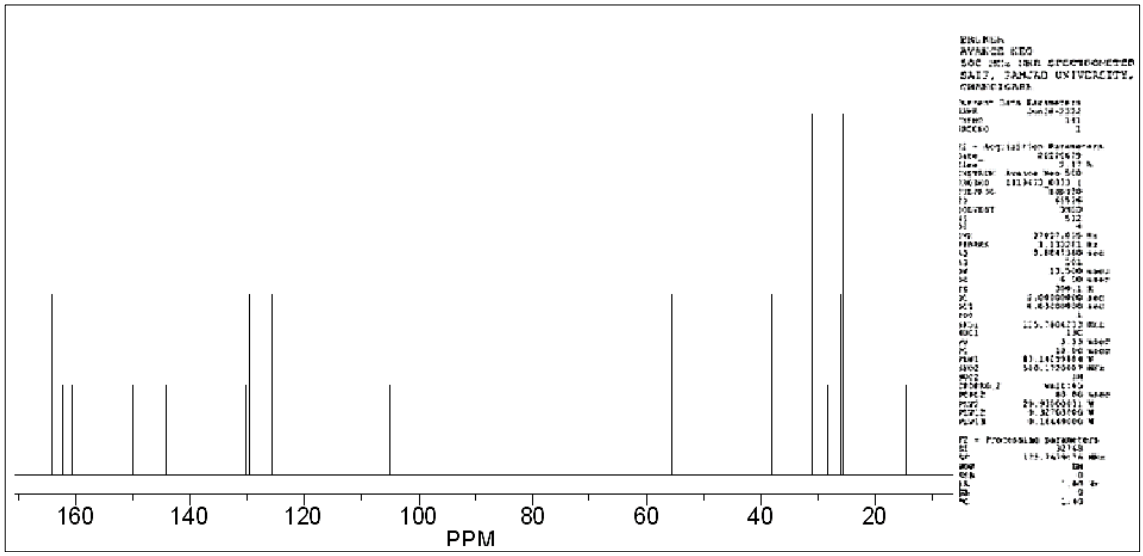


Fig 3.40: ^{13}C NMR Spectra of N2,N4-bis(cyclohexylmethyl)-N6-(4-(4-ethylphenyl)thiazol-2-yl)-1,3,5-triazine-2,4,6-triamine (Compound-5h)

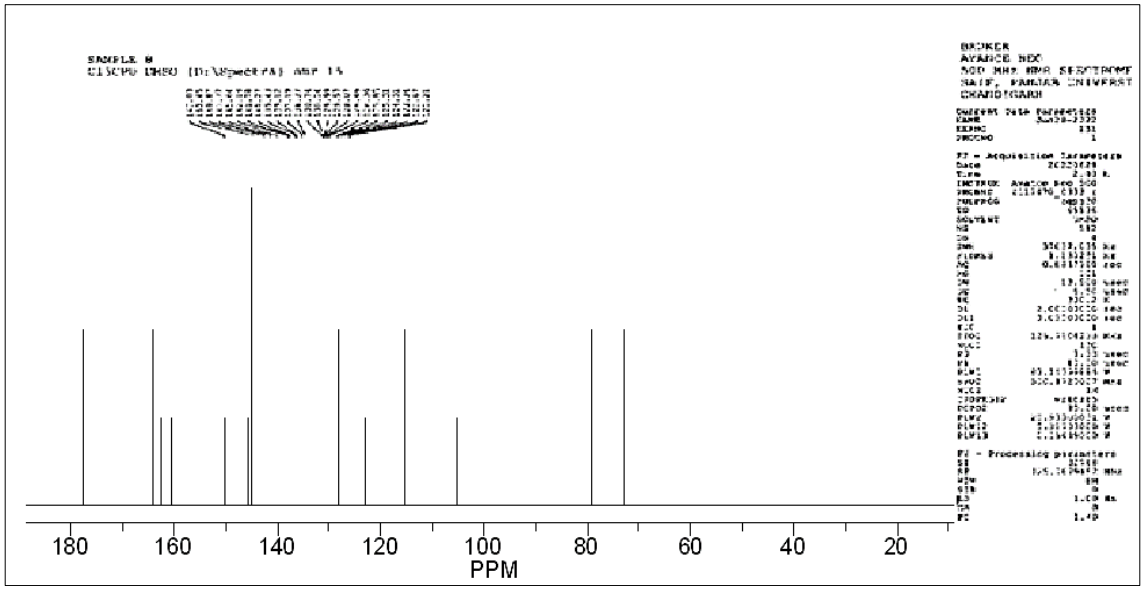


Fig 3.41: ^{13}C NMR Spectra of 3-((4-((4-(4-aminophenyl) thiazol-2-yl) amino) --((2-carboxyphenyl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2-carboxylic acid (Compound-6a)

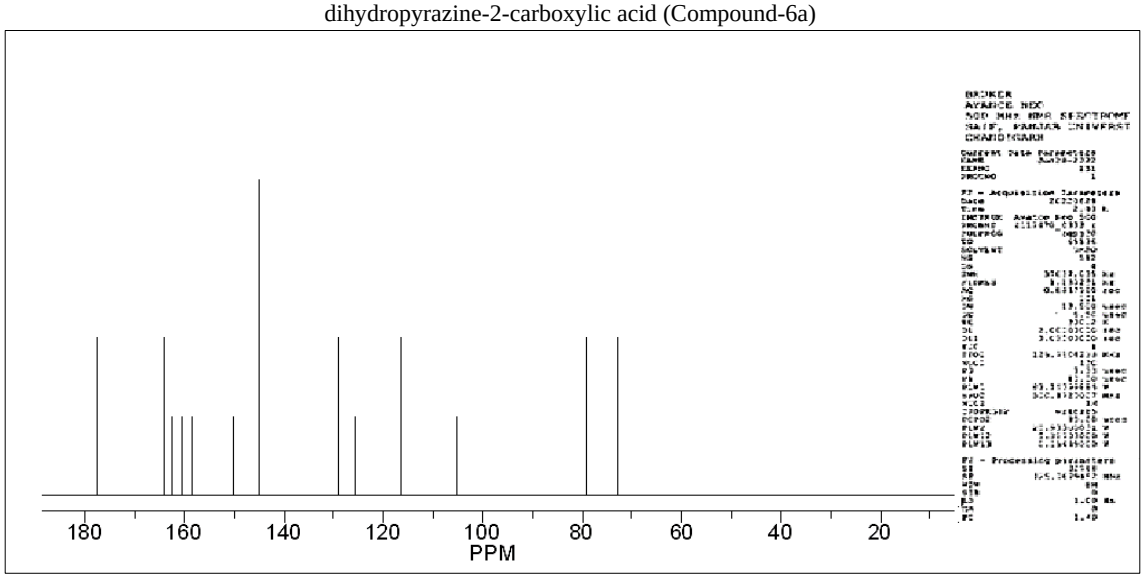


Fig 3.42: ^{13}C NMR Spectra of 3-((4-((2-carboxyphenyl) amino)-6-((4-(4-hydroxyphenyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2-carboxylic acid (Compound-6b)

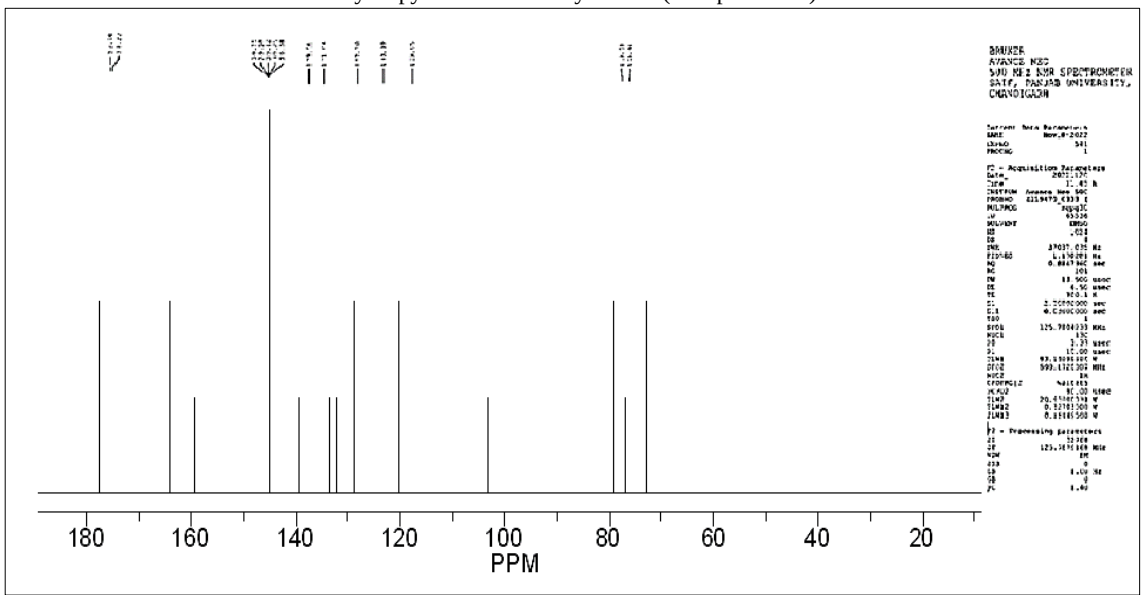


Fig 3.43: ^{13}C NMR Spectra of 3-((4-((2-carboxyphenyl) amino)-6-((4-(4-chlorophenyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2-carboxylic acid (Compound-6c)

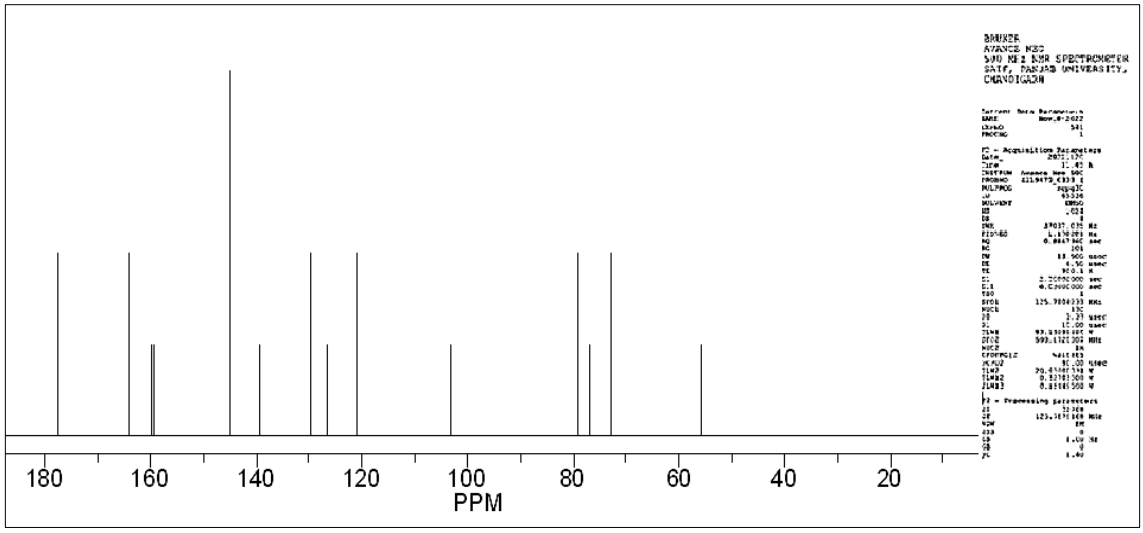


Fig 3.44: ^{13}C NMR Spectra of 3-((4-((2-carboxyphenyl) amino)-6-((4-(4-methoxyphenyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2-carboxylic acid (Compound-6d)

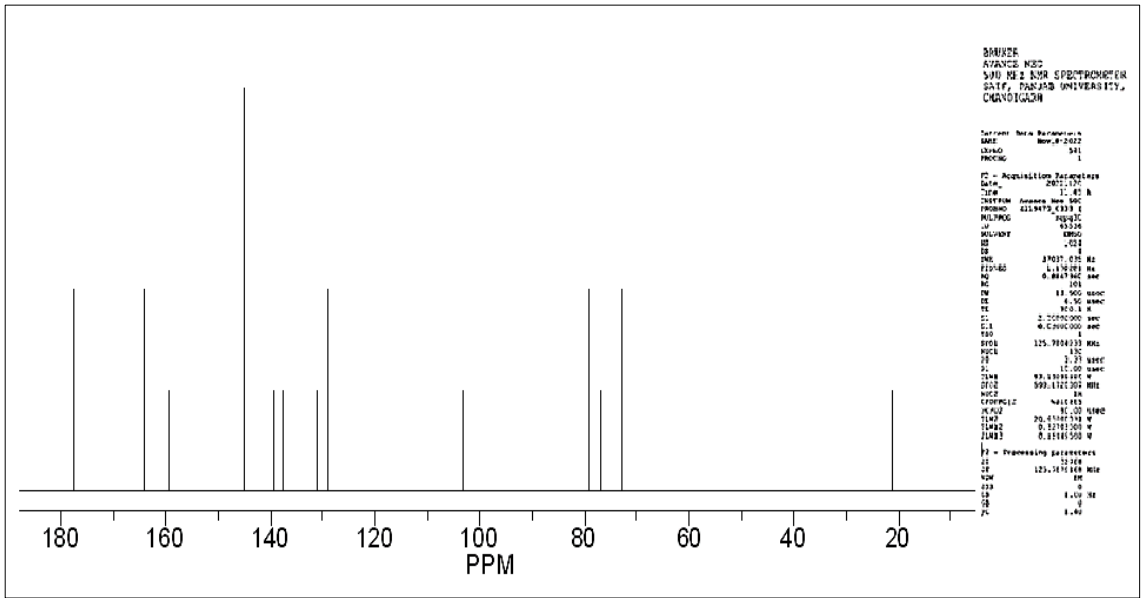


Fig 3.45: ^{13}C NMR Spectra of 3-((4-((2 carboxyphenyl) amino)-6-((4-(p-tolyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2-carboxylic acid (Compound-6e)

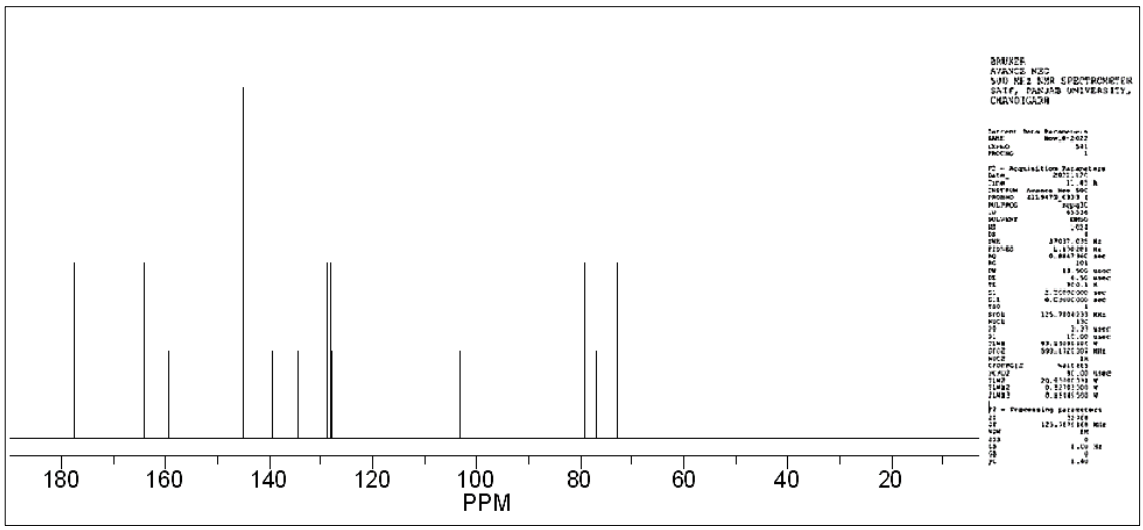


Fig 3.46: ^{13}C NMR Spectra of 3-((4-((2-carboxyphenyl) amino)-6-((4-phenylthiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2-carboxylic acid (Compound-6f)

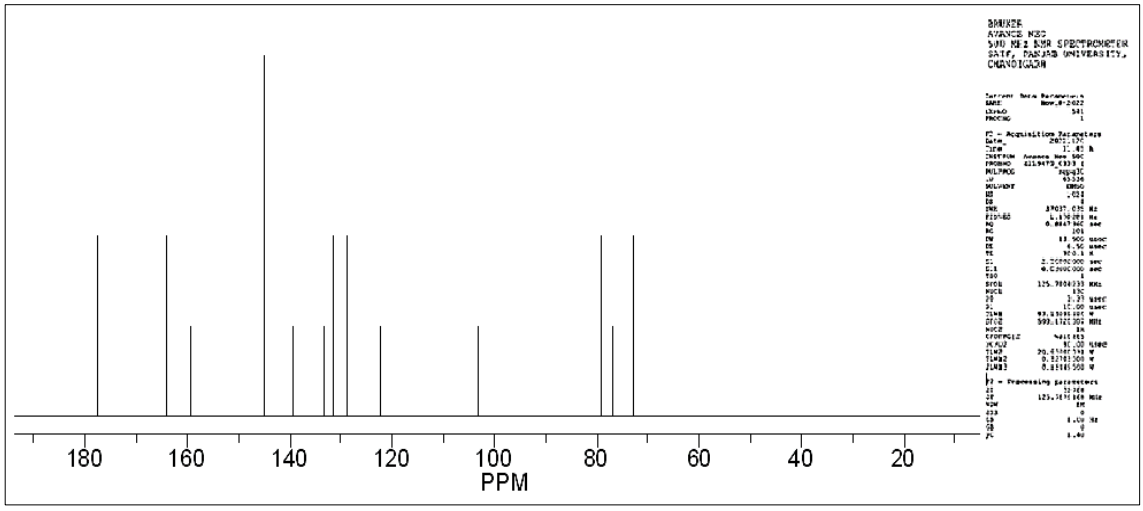


Fig 3.47: ^{13}C NMR Spectra of 3-((4-((4-(4-bromophenyl) thiazol-2-yl) amino)-6-((2-carboxyphenyl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2-carboxylic acid (Compound-6g)

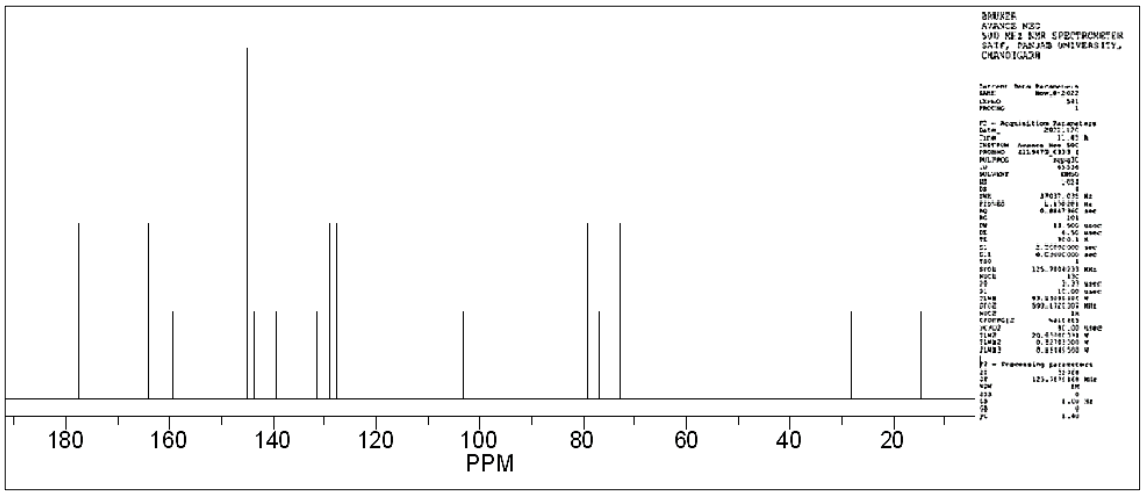


Fig 3.48: ^{13}C NMR Spectra of 3-((4-((2-carboxyphenyl) amino)-6-((4-(4-ethylphenyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2-carboxylic acid (Compound-6h)

The newly synthesized s-triazines derivatives with substituted amines analyzed for ^{13}C NMR spectral characterization. It is similar to proton NMR (^{1}H NMR). The identification of carbon atoms in an organic molecule just as proton NMR identifies hydrogen atoms. ^{13}C NMR spectrum of Compound-5a in DMSO showed that NH_2 attached carbons in the benzene ring gives characteristic peak at 123.0, 128.3, 115.1, 145.6 ppm, and peaks obtained at, 162.5, 160.6 due to triazines. peaks obtained at 164.1, due to imines. alco peak obtained due ethylene carbon at 31.0, 25.5 and 26.0. Compound-5b in DMSO showed that OH attached carbons in the benzene ring gives characteristic peak at 125.6, 128.9, 116.4, 158.6 ppm, and peaks obtained at, 162.5, 160.6 due to triazines. peaks obtained at 164.1, due to imines. alco peak obtained due ethylene carbon at 31.0, 25.5 and 26.0. Compound-5c in DMSO showed that Cl attached carbons in the benzene ring gives characteristic peak at 125.6, 128.9, 116.4, 158.6 ppm, and peaks obtained at, 162.5, 160.6 due to triazines. peaks obtained at 164.1, due to imines. alco peak obtained due ethylene carbon at 31.0, 25.5 and 26.0.

Compound-5d in DMSO showed that OCH_3 attached carbons in the benzene ring gives characteristic peak at 125.6, 128.9, 129.3,134.3 ppm, and peaks obtained at, 162.5, 160.6 due to triazines. peaks obtained at 164.1, due to imines. alco peak obtained due ethylene carbon at 31.0, 25.5 and 26.0. Compound-5e in DMSO showed that CH_3 attached carbons in the benzene ring gives characteristic peak at 131.7, and 21.3 ppm, and peaks obtained at, 162.5, 160.6 due to triazines. peaks obtained at 164.1, due to imines. alco peak obtained due ethylene carbon at 31.0, 25.5 and 26.0. Compound-5f in DMSO showed that carbons in the benzene ring gives characteristic peak at 127.5, 129.2, 128.7 ppm, and peaks obtained at, 162.5, 160.6 due to triazines. peaks obtained at 164.1, due to imines. alco peak obtained due ethylene carbon at 31.0, 25.5 and 26.0.

Compound-5g in DMSO showed that Br attached carbons in the benzene ring gives characteristic peak at 132.0, 128.3, 132.1, 123.1 ppm, and peaks obtained at, 162.5, 160.6 due to triazines. peaks obtained at 164.1, due to imines. alco peak obtained due ethylene carbon at 31.0, 25.5 and 26.0. Compound-5h in DMSO showed that ethylene attached carbons in the benzene ring gives characteristic peak at 129.7, 121.1, 159.8, 55.8 ppm, and peaks obtained at, 162.5, 160.6 due to triazines. peaks obtained at 164.1, due to imines. alco peak obtained due ethylene carbon at 31.0, 25.5 and 26.0. the above data obtained from ^{13}C NMR are good agreement with literature review [41

^{13}C NMR spectrum of Compound-6a in DMSO showed that NH_2 attached carbons in the benzene ring gives

characteristic peak at 123.0, 128.3, 115.1 145.6 ppm, and peaks obtained at, 164.1, 159.3, 160.6 due to triazines. peaks obtained at 145.0,72.7 and 79.0 due to carbon in imines. alco peak obtained due carboxyl carbon at 177.5 and peak obtained at 160.6 and 105.0 due to carbon in thiazole. ^{13}C NMR spectrum of Compound-6b in DMSO showed that OH attached carbons in the benzene ring gives characteristic peak at 126.2, 128.9, 116.4, 158.5 ppm, and peaks obtained at, 164.1, 159.3, 160.6 due to triazines. peaks obtained at 145.0,72.7 and 79.0 due to carbon in imines. alco peak obtained due carboxyl carbon at 177.5 and peak obtained at 160.6 and 105.0 due to carbon in thiazole. ^{13}C NMR spectrum of Compound-6c in DMSO showed that Cl attached carbons in the benzene ring gives characteristic peak at 120.2, 128.7, 135.5 ppm, and peaks obtained at, 164.1, 159.3, 160.6 due to triazines. peaks obtained at 145.0,72.7 and 79.0 due to carbon in imines. alco peak obtained due carboxyl carbon at 177.5 and peak obtained at 160.6 and 105.0 due to carbon in thiazole.

^{13}C NMR spectrum of Compound-6d in DMSO showed that OCH_3 attached carbons in the benzene ring gives characteristic peak at 121.1, 159.8, 55.8 ppm, and peaks obtained at, 164.1, 159.3, 160.6 due to carbon in triazines. peaks obtained at 145.0,72.7 and 79.0 due to carbon in imines. alco peak obtained due carboxyl carbon at 177.5 and peak obtained at 160.6 and 105.0 due to carbon in thiazole. ^{13}C NMR spectrum of Compound-6e in DMSO showed that CH_3 attached carbons in the benzene ring gives characteristic peak at 131.2, 129.0, 128.9, 21.3 ppm, and peaks obtained at, 164.1, 159.3, 160.6 due to carbon in triazines. peaks obtained at 145.0,72.7 and 79.0 due to carbon in imines. alco peak obtained due carboxyl carbon at 177.5 and peak obtained at 160.6 and 105.0 due to carbon in thiazole.

^{13}C NMR spectrum of Compound-6f in DMSO showed that carbons in the benzene ring gives characteristic peak at 134.2, 128.3, 128.6, 127.9 ppm, and peaks obtained at, 164.1, 159.3, 160.6 due to carbon in triazines. peaks obtained at 145.0,72.7 and 79.0 due to carbon in imines. alco peak obtained due carboxyl carbon at 177.5 and peak obtained at 160.6 and 105.0 due to carbon in thiazole. ^{13}C NMR spectrum of Compound-6g in DMSO showed that Br attached carbons in the benzene ring gives characteristic peak at 133.2, 128.6, 131.5, 122.3 ppm, and peaks obtained at, 164.1, 159.3, 160.6 due to carbon in triazines. peaks obtained at 145.0,72.7 and 79.0 due to carbon in imines. alco peak obtained due carboxyl carbon at 177.5 and peak obtained at 160.6 and 105.0 due to carbon in thiazole.

^{13}C NMR spectrum of Compound-6g in DMSO showed that ethyl attached carbons in the benzene ring gives characteristic peak at 129.0, 127.6, 143.5, 28.2, 12.5 ppm, and peaks obtained at, 164.1, 159.3, 160.6 due to carbon in triazines. peaks obtained at 145.0,72.7 and 79.0 due to carbon in imines. alco peak obtained due carboxyl carbon at 177.5 and peak obtained at 160.6 and 105.0 due to carbon in thiazole. the above data obtained from ^{13}C NMR are good agreement with literature review [24-28].

The ^{13}C NMR spectra of the synthesized 1,3,5-triazine derivatives provided conclusive evidence for the presence of the triazine nucleus and its substituents. The characteristic downfield signals observed for the C=N carbons of the triazine ring were consistent with the heteroaromatic environment, while the distinct chemical shifts for aromatic, aliphatic, and heteroatom-linked carbons confirmed the successful incorporation of the desired substituents. The number, intensity, and positions of the carbon signals matched well with the expected structural framework, and no extra peaks were observed, indicating good purity of the compounds.

Thus, ^{13}C NMR characterization strongly supports the successful synthesis and accurate structural confirmation of the 1,3,5-triazine derivatives.

Mass Spectrometry

The fragmentation patterns of all newly synthesized compound were reported in m/z values [29]. The Molecular Formulas and mass spectra details of all newly synthesized 1,3,5-triazine derivatives are shown below in Table No: 3.7 and 3.8 Figure No 3.49 To 3.64.

Table 3.7: Molecular Formulae and Molecular Weight of 1,3,5-Triazine Derivatives

Sr. No.	Compounds	Molecular Formula	Molecular Weight
1.	Compound-5a	$C_{26}H_{36}N_8S$	492.00
2.	Compound-5b	$C_{26}H_{35}N_7S$	494.00
3.	Compound-5c	$C_{26}H_{34}N_7ClS$	512.00
4.	Compound-5d	$C_{27}H_{37}N_7OS$	508.00
5.	Compound-5e	$C_{27}H_{37}N_7S$	491.71
6.	Compound-5f	$C_{26}H_{34}N_7S$	477.68
7.	Compound-5g	$C_{26}H_{34}N_7SBr$	556.58
8.	Compound-5h	$C_{28}H_{38}N_7S$	505.73
9.	Compound-6a	$C_{22}H_{20}N_{12}O_4S$	544.56
10.	Compound-6b	$C_{22}H_{19}N_{12}O_5S$	545.54
11.	Compound-6c	$C_{22}H_{18}N_{12}O_4SCl$	563.99
12.	Compound-6d	$C_{23}H_{21}N_{12}O_5S$	559.57
13.	Compound-6e	$C_{23}H_{21}N_{12}O_4S$	543.58
14.	Compound-6f	$C_{22}H_{18}N_{12}O_4S$	529.30
15.	Compound-6g	$C_{22}H_{18}N_{12}O_4SBr$	608.44
16.	Compound-6h	$C_{24}H_{23}N_{12}O_4S$	557.30

Table 3.8: Mass Spectrometric data of synthesised 1,3,5-Triazine Derivatives

S. No.	Compound.	Molecular ion peak (M+)	m/z Values	Figure No.
1.	Compound-5a	492	492, 477, 285, 209, 126, 111, 96	3.49
2.	Compound-5b	494	494, 478, 285, 208, 126, 111, 96	3.50
3.	Compound-5c	511	511, 478, 285, 208, 126, 111, 96	3.51
4.	Compound-5d	508	478, 285, 208, 126, 111, 96	3.52
5.	Compound-5e	492	478, 285, 208, 126, 111, 96	3.53
6.	Compound-5f	478	478, 285, 208, 126, 111, 96	3.54
7.	Compound-5g	557	478, 285, 208, 126, 111, 96	3.55
8.	Compound-5h	506	478, 285, 208, 126, 111, 96	3.56
9.	Compound-6a	548	533, 457, 333, 126, 209, 111, 96, 81.	3.57
10.	Compound-6b	549	549, 533, 457, 333, 126, 209, 111, 96, 81.	3.58
11.	Compound-6c	568	568, 533, 457, 333, 126, 209, 111, 96, 81.	3.59
12.	Compound-6d	564	564, 533, 457, 333, 126, 209, 111, 96, 81.	3.60
13.	Compound-6e	547	547, 533, 457, 333, 126, 209, 111, 96, 81.	3.61
14.	Compound-6f	533	533, 457, 333, 126, 209, 111, 96, 81.	3.62
15.	Compound-6g	612	612, 533, 457, 333, 126, 209, 111, 96, 81.	3.63
16.	Compound-6h	561	561, 533, 457, 333, 126, 209, 111, 96, 81.	3.64

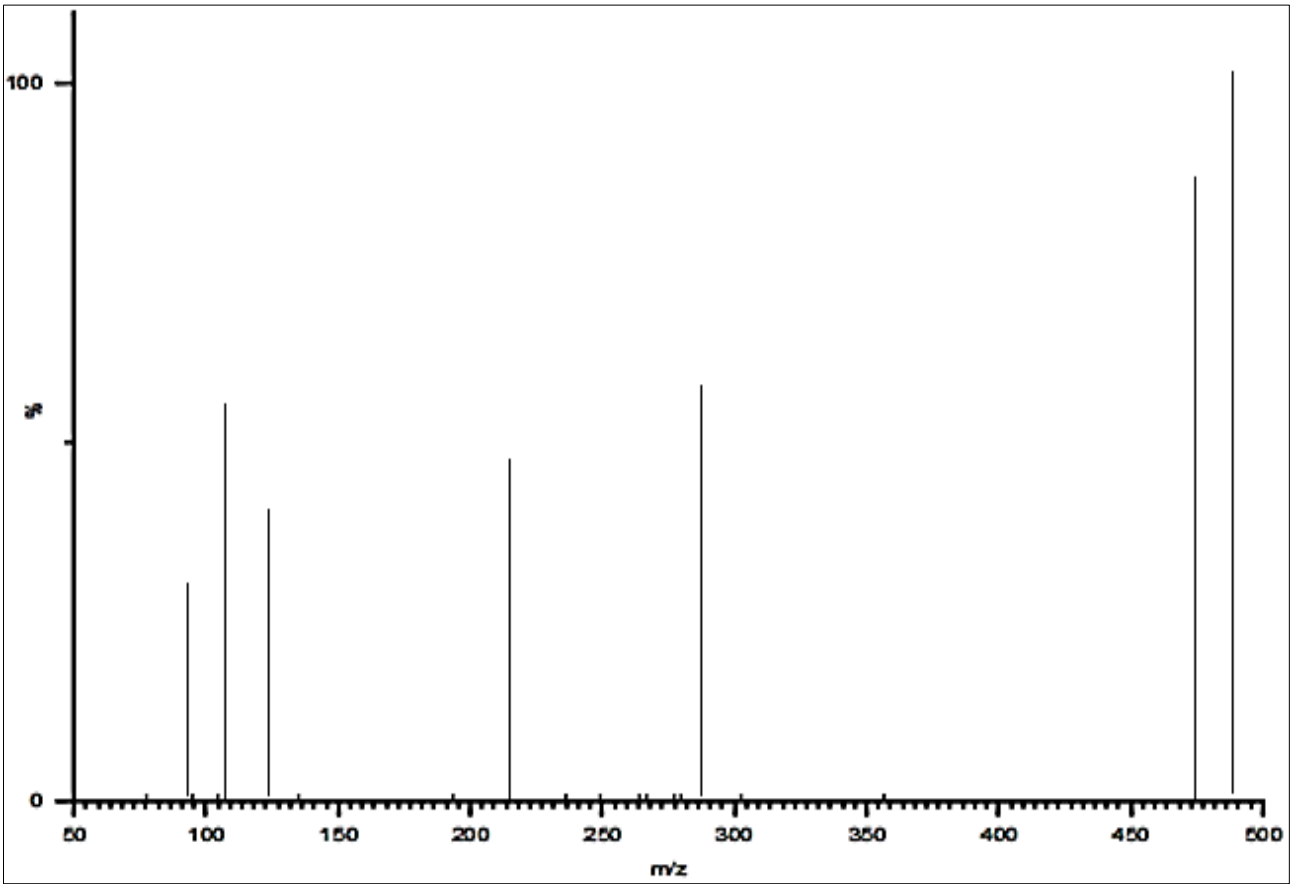


Fig 3.49: Mass spectrum of N2-(4-(4-amino phenyl) thiazol-2-yl)-N4, N6 bis (cyclohexyl methyl)-1,3,5-triazine-2,4,6-triamine

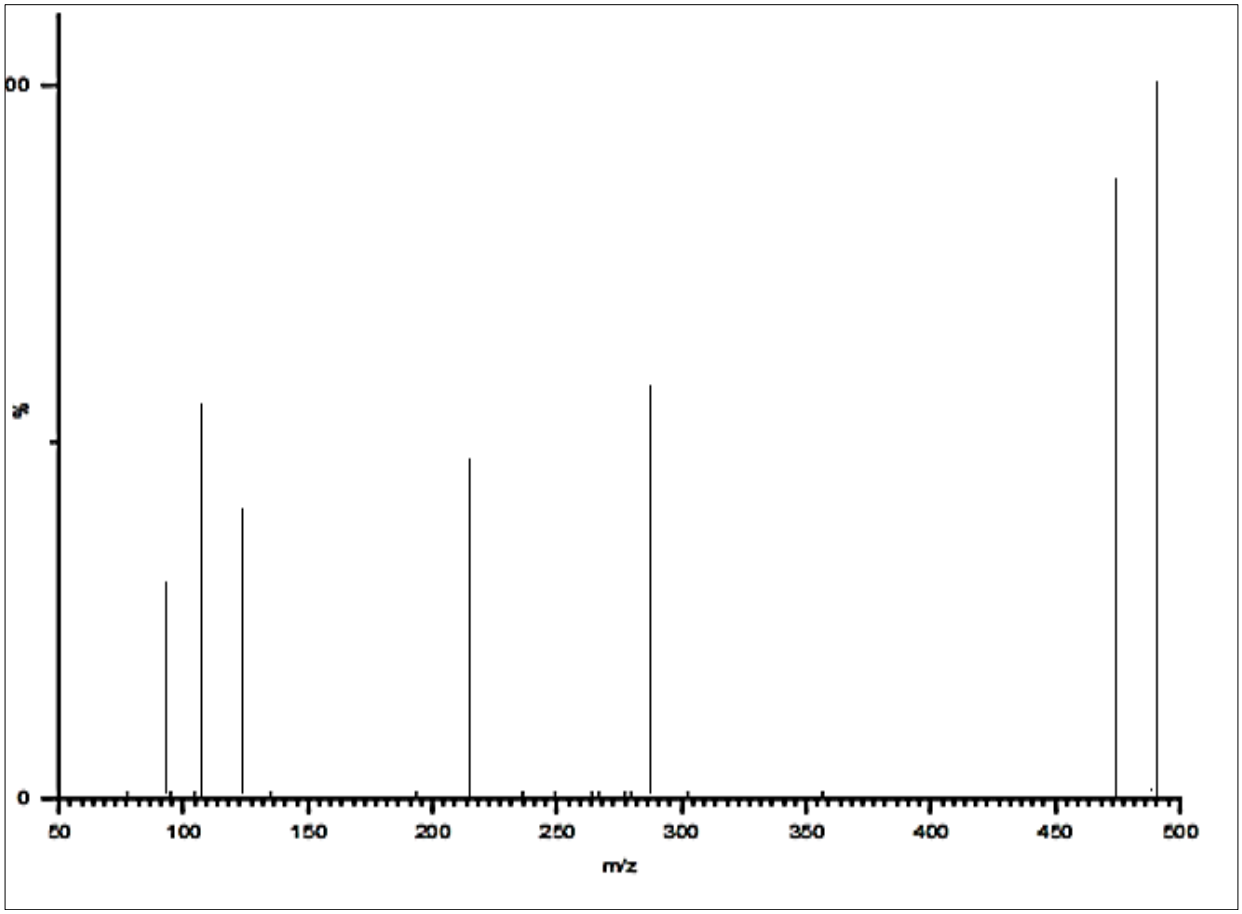


Fig 3.50: Mass spectrum of 4-(2-((4,6-bis((cyclohexylmethyl)amino)-1,3,5- triazin-2-yl) amino) thiazol-4-yl) phenol

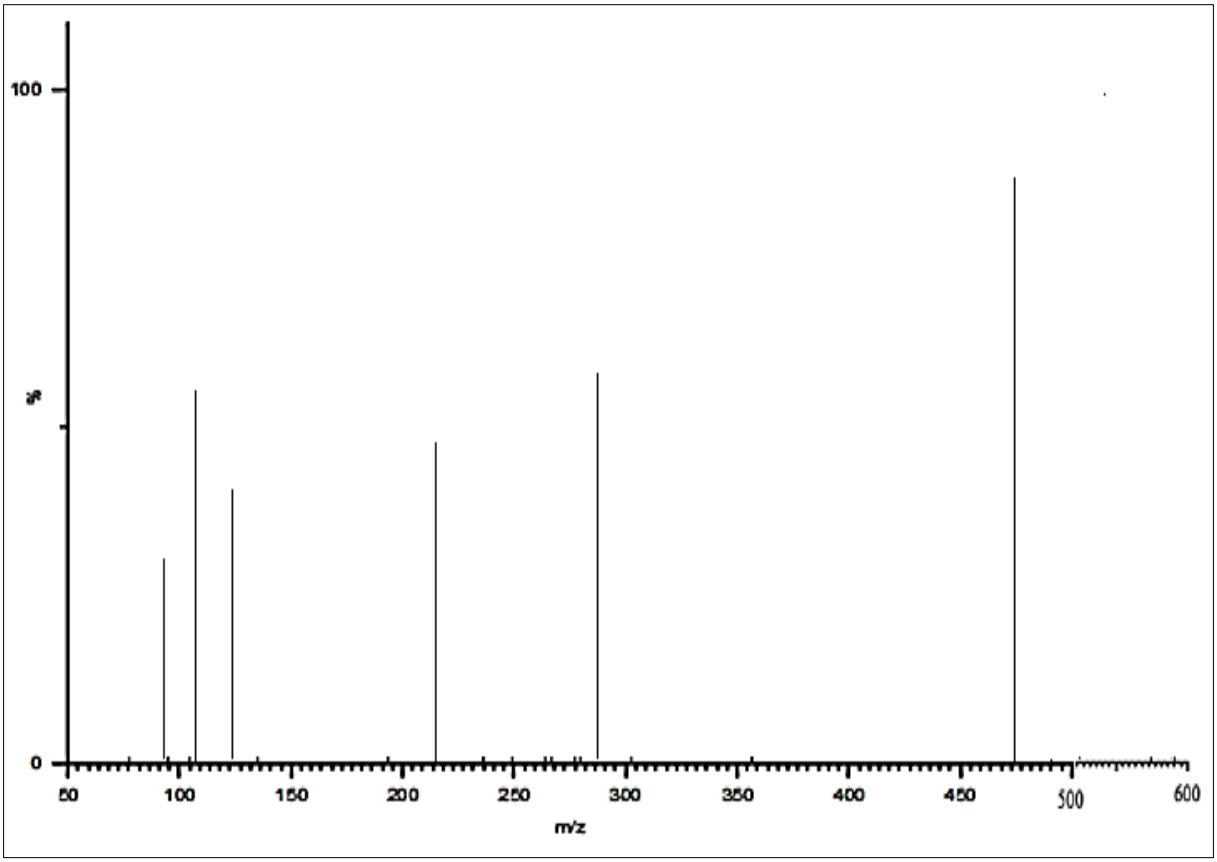


Fig 3.51: Mass spectrum of N2, N4-bis(cyclohexylmethyl)-N6-(4-phenylthiazol-2-yl)-1,3,5-triazine-2,4,6-triamine

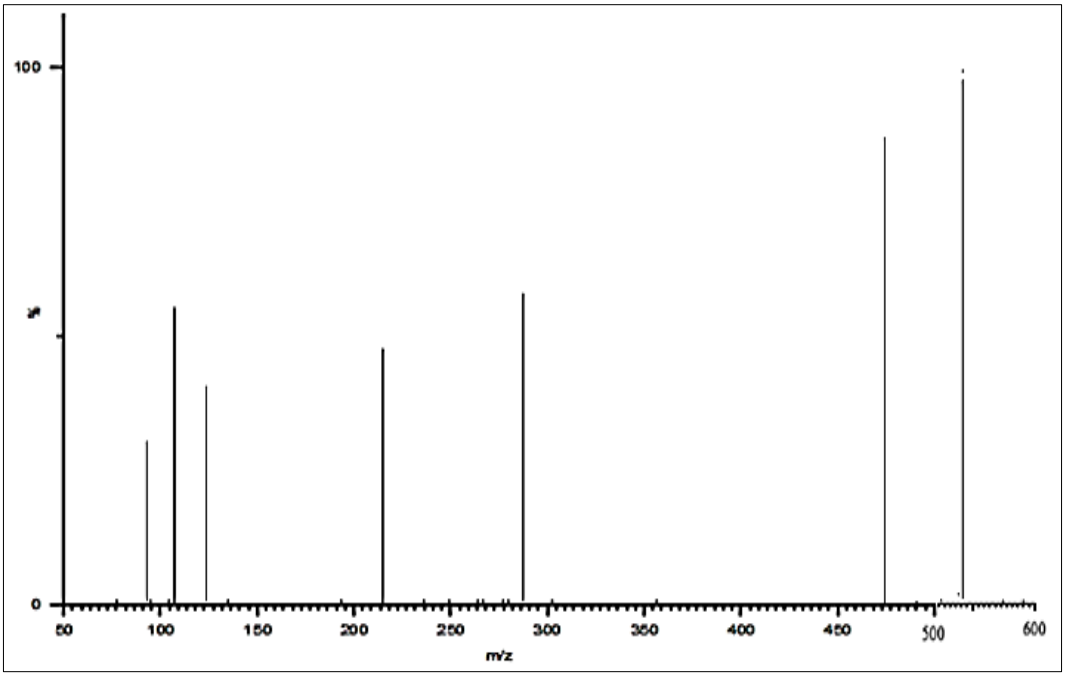
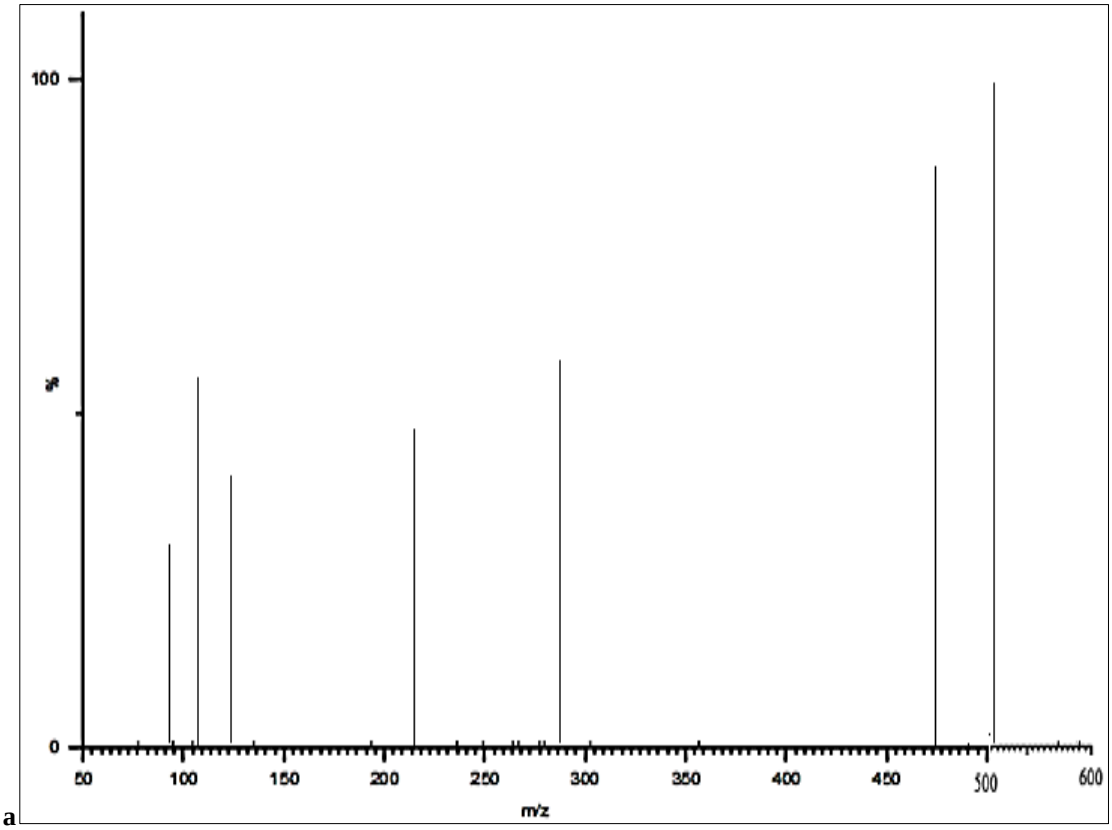


Fig 3.52: Mass spectrum of N2-(4-(4-chloro phenyl) thiazol-2-yl)-N4, N6- bis (cyclohexyl methyl)-1,3,5-triazine-2,4,6-triamine



a

Fig 3.53: Mass spectrum of N2, N4-bis (cyclohexyl methyl)-N6-(4-(4-methoxy phenyl) thiazol-2-yl)-1,3,5-triazine-2,4,6-triamine

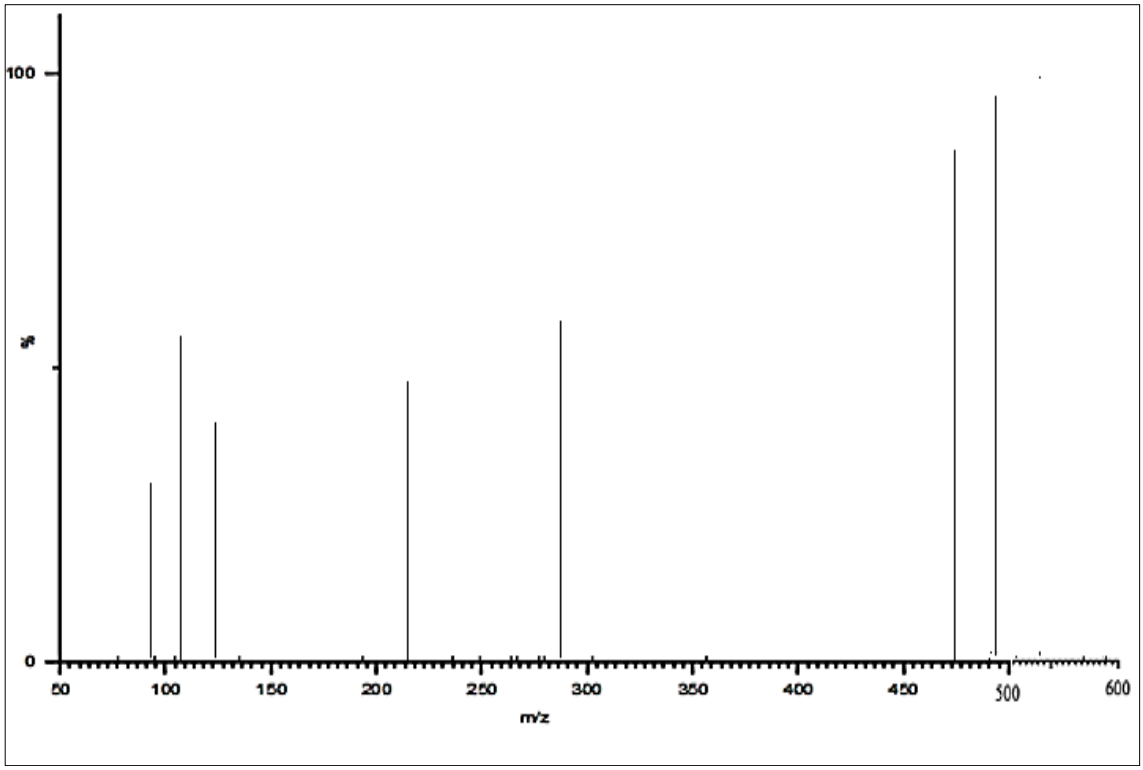


Fig 3.54: Mass spectrum of N2, N4-bis(cyclohexylmethyl)-N6-(4-(p-tolyl) thiazol-2-yl)-1,3,5-triazine-2,4,6-triamine

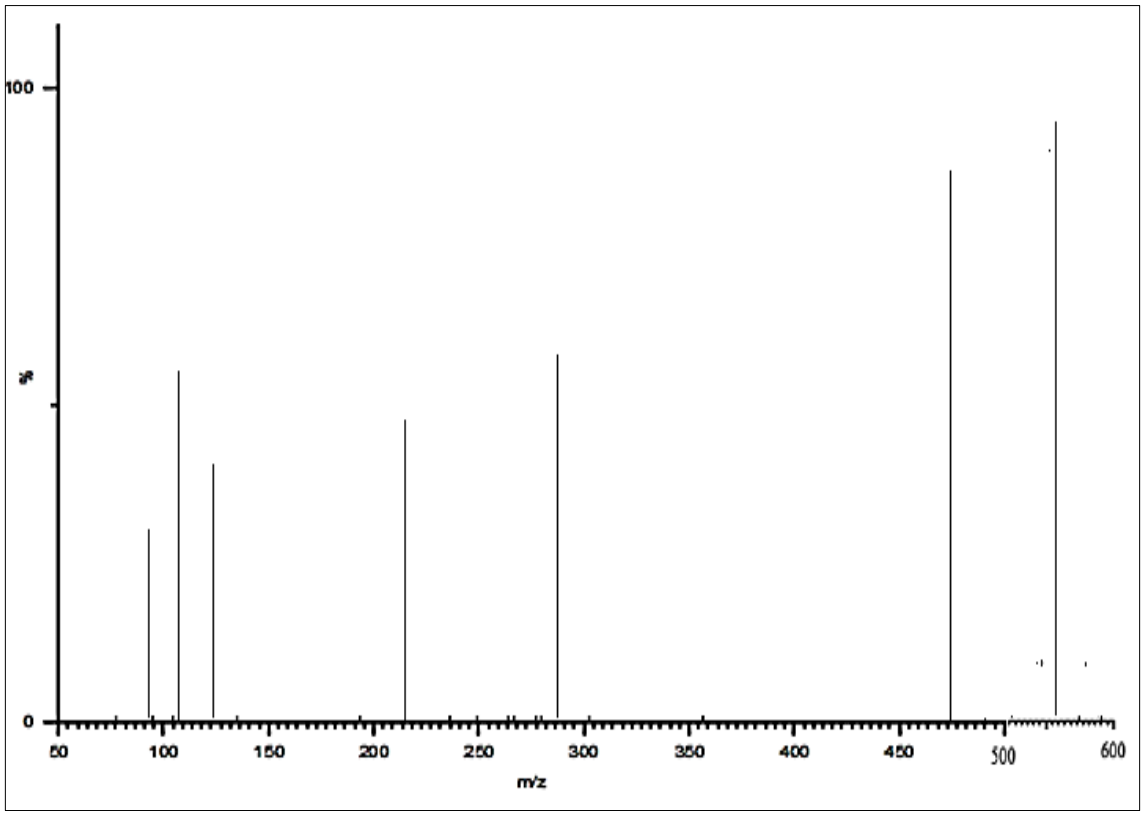


Fig 3.55: Mass spectrum of N2-(4-(4-bromo phenyl) thiazol-2-yl)-N4, N6-bis (cyclohexyl methyl)-1,3,5-triazine-2,4,6-triamine

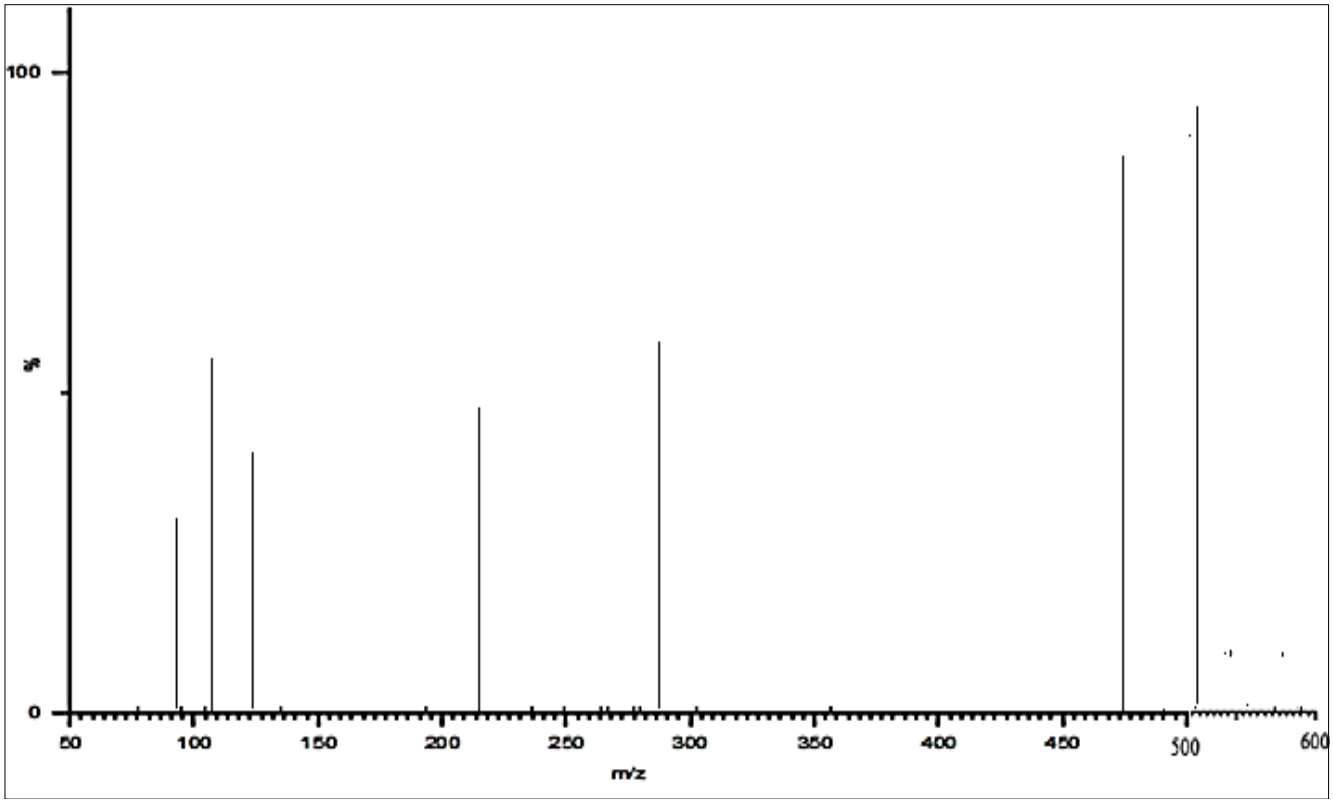


Fig 3.56: Mass spectrum of N2, N4-bis (cyclohexyl methyl)-N6-(4-(4-ethyl phenyl) thiazol-2-yl)-1,3,5-triazine-2,4,6-triamine

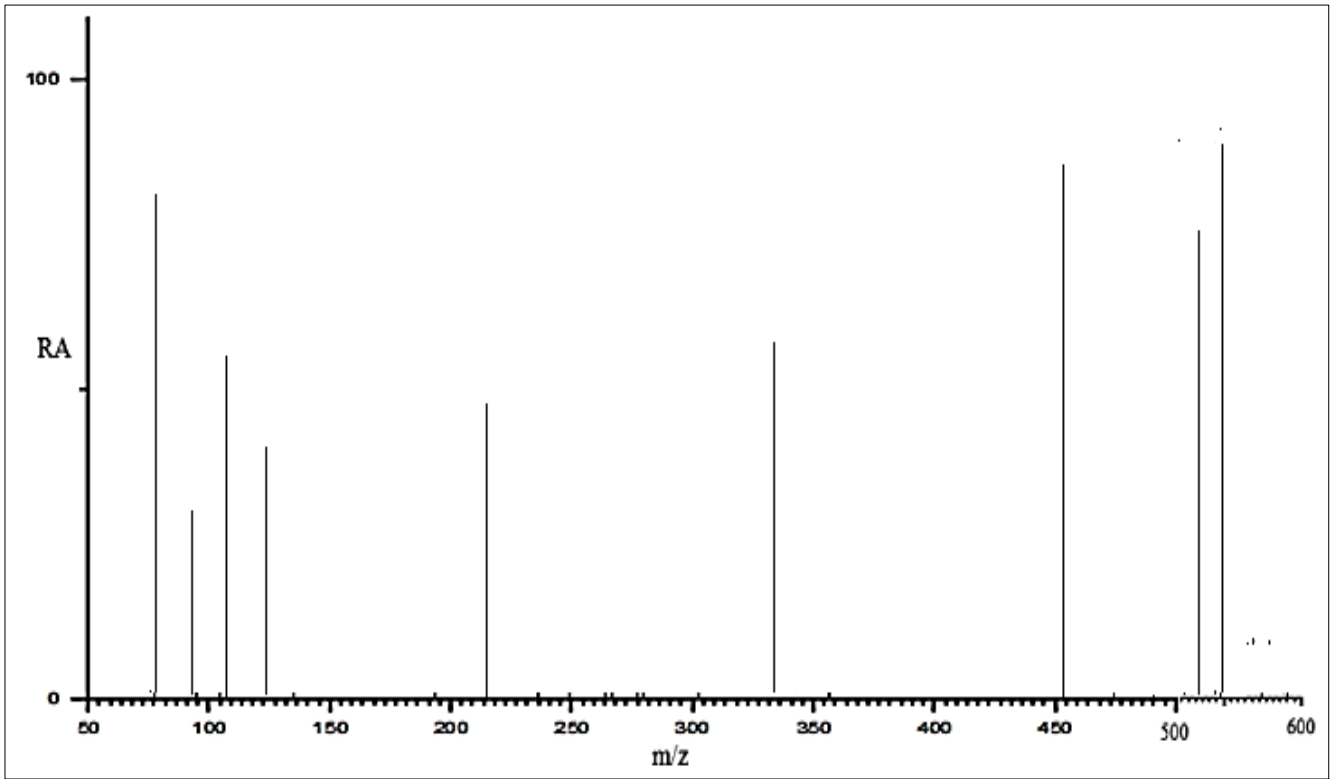


Fig 3.57: Mass spectrum of 3-((4-((2-carboxy phenyl) amino)-6-((4-(4-hydroxy phenyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2-carboxylic acid

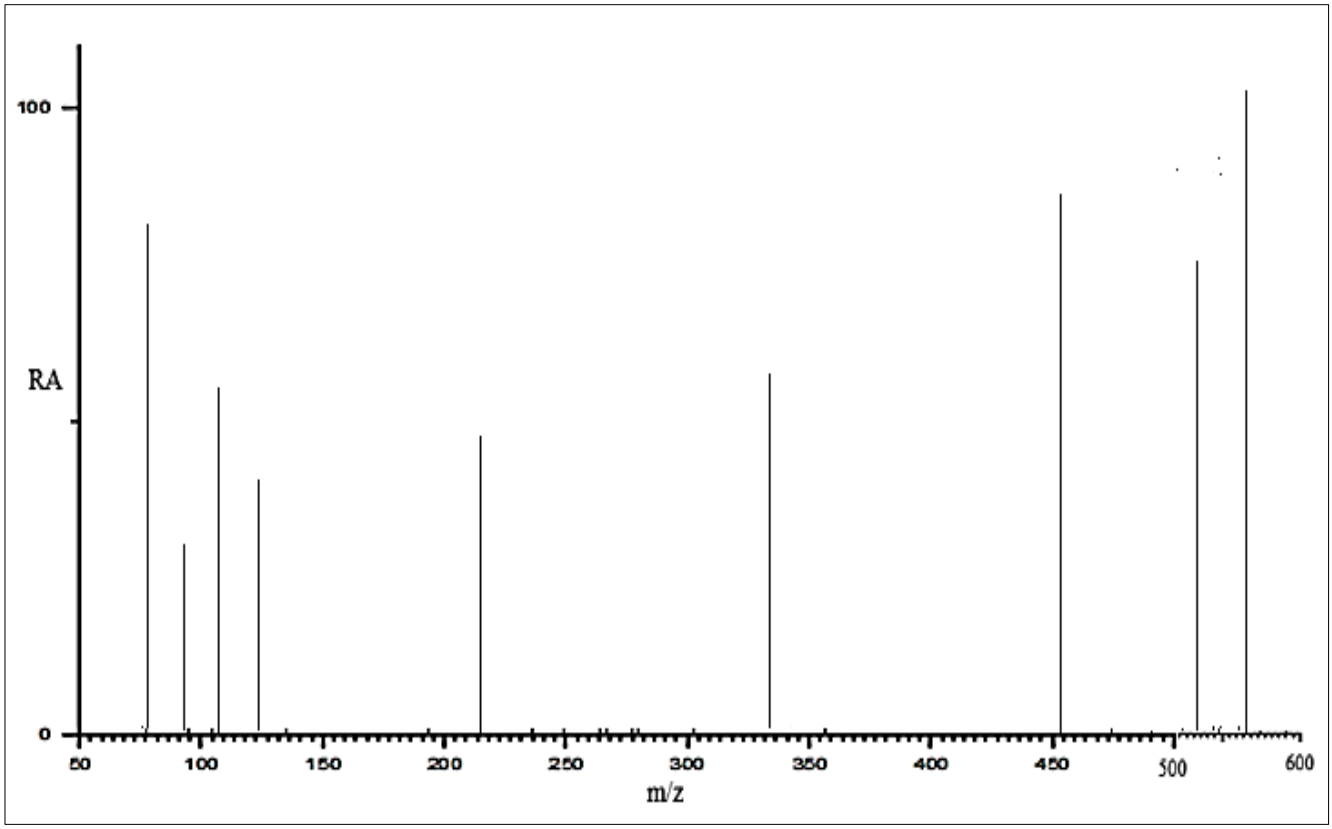


Fig 3.58: Mass spectrum of 3-((4-((2-carboxy phenyl) amino)-6-((4-(4-chloro phenyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl)amino)-2,3-dihydropyrazine- 2- carboxylic acid

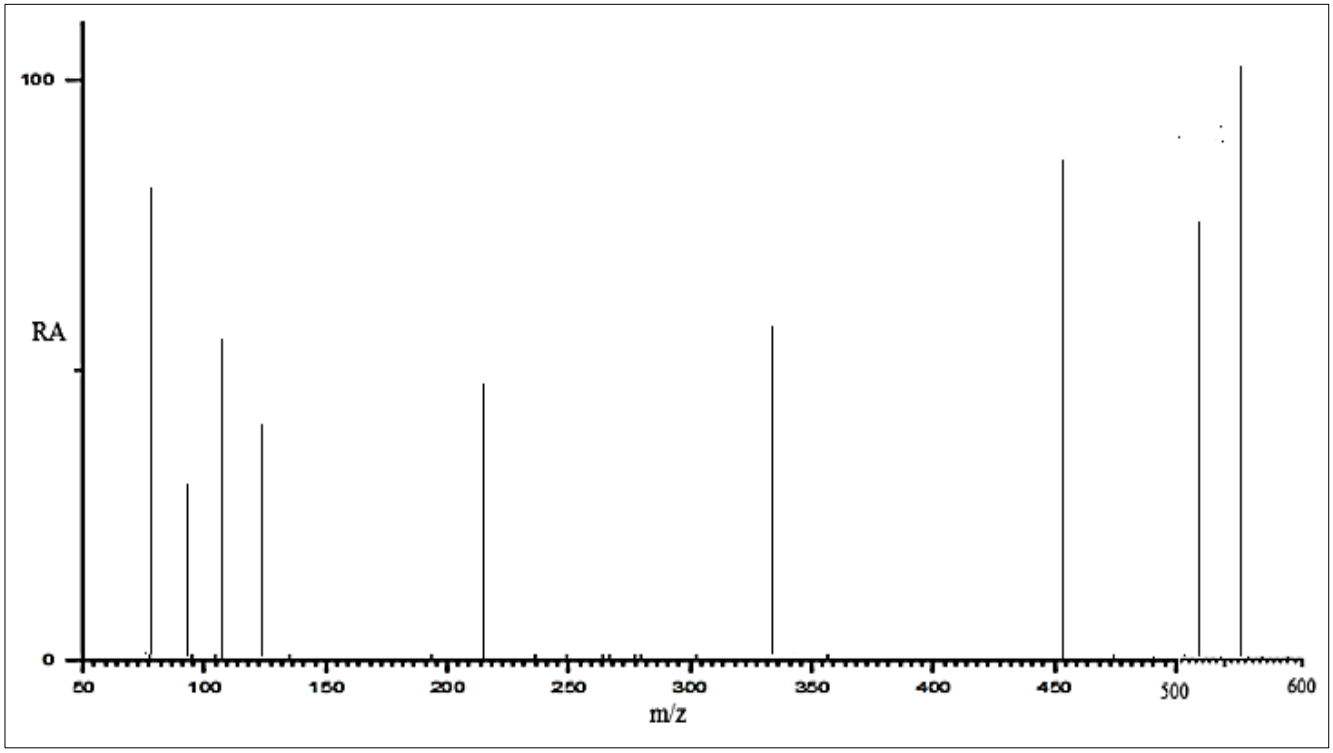


Fig 3.59: Mass spectrum of-((4-((2-carboxy phenyl) amino)-6-((4-(4-methoxy phenyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine- 2- carboxylic acid

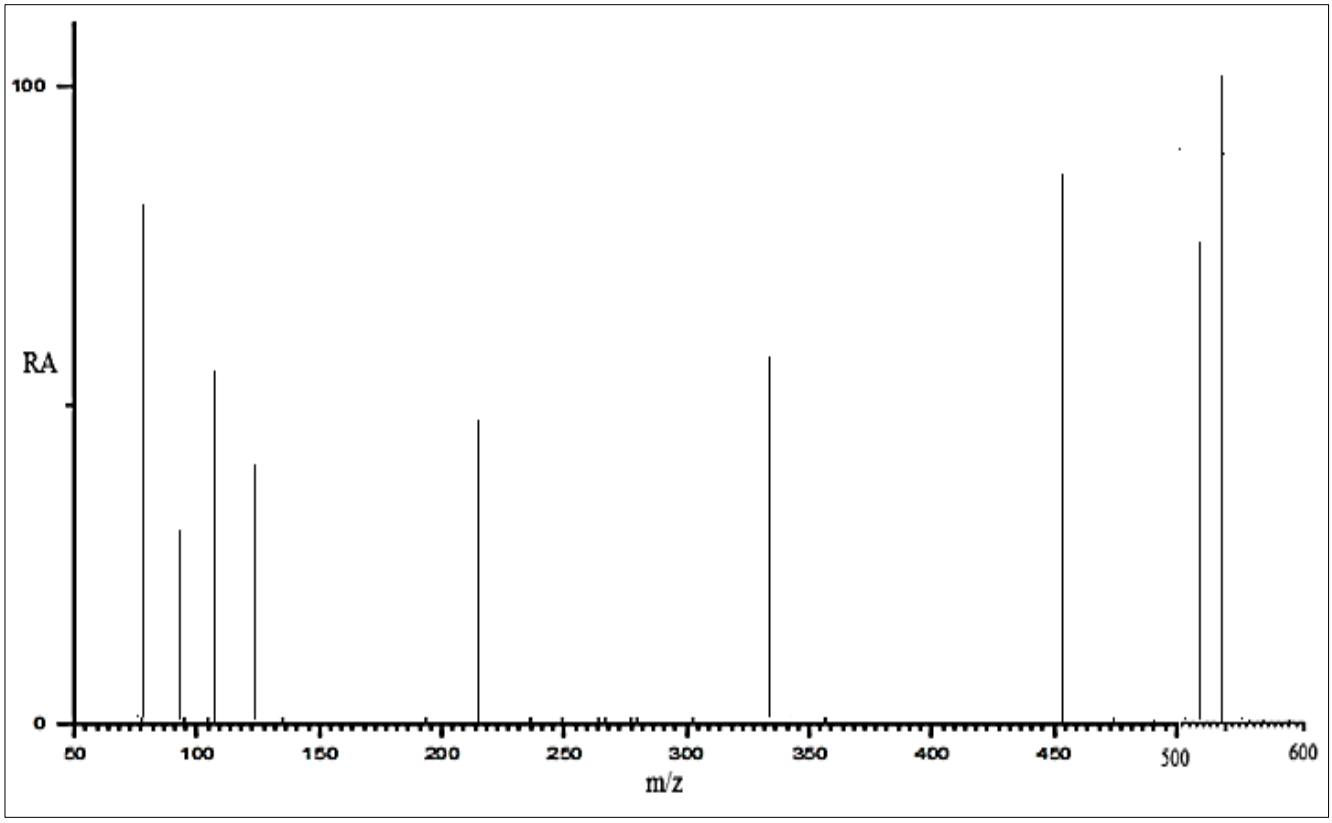


Fig 3.60: Mass spectrum of 3-((4-((2 carboxy phenyl) amino)-6-((4-(p-tolyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydropyrazine-2-carboxylic acid

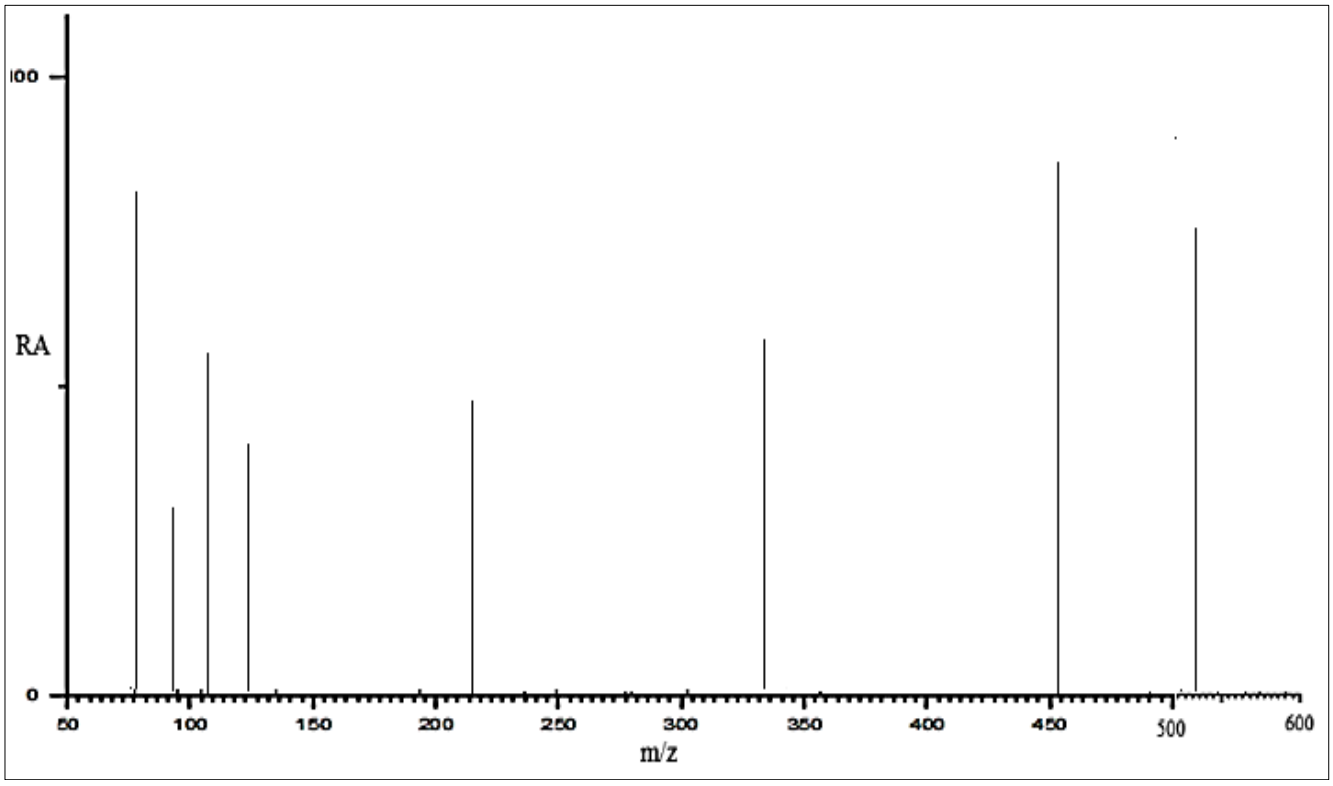


Fig 3.61: Mass spectrum of 3-((4-((2-carboxy phenyl) amino)-6-((4-phenyl thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydro pyrazine-2-carboxylic acid

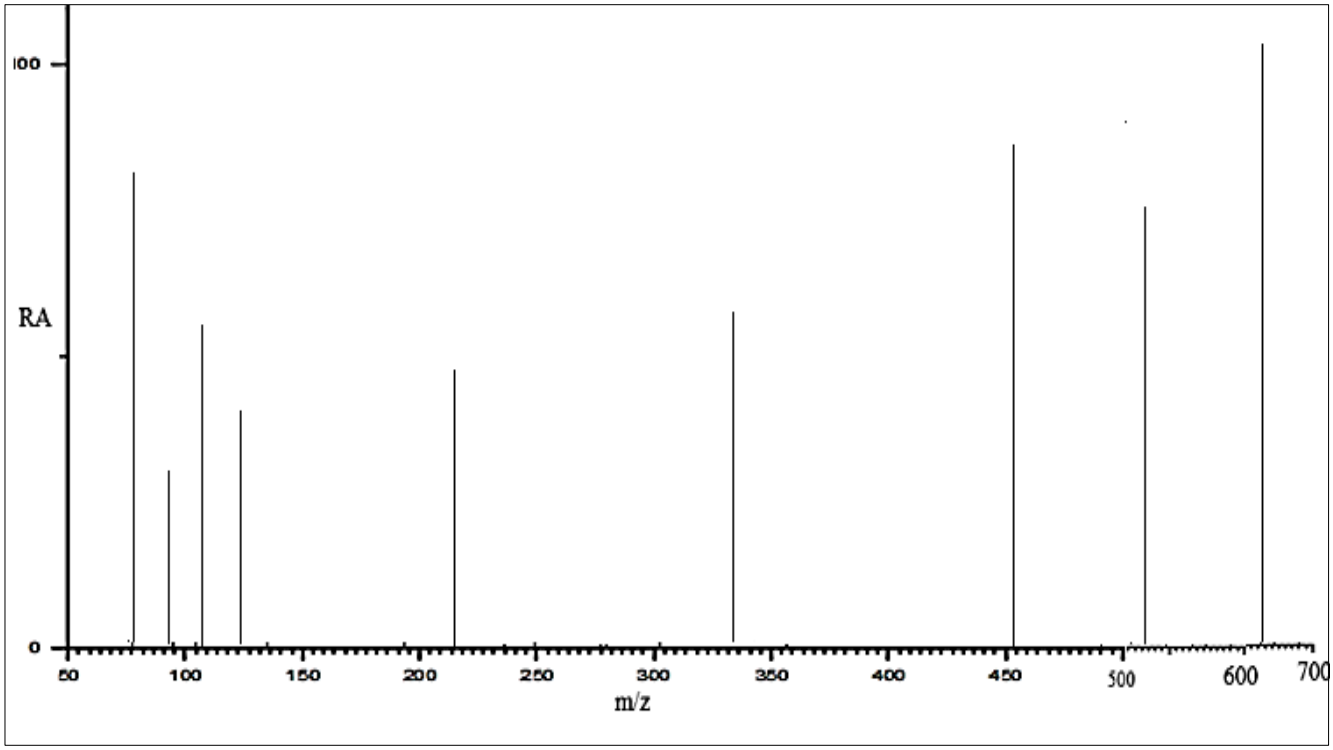


Fig 3.62: Mass spectrum of 3-((4-((4-(4-bromo phenyl) thiazol-2-yl) amino)-6-((2-carboxy phenyl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydro pyrazine-2-carboxylic acid

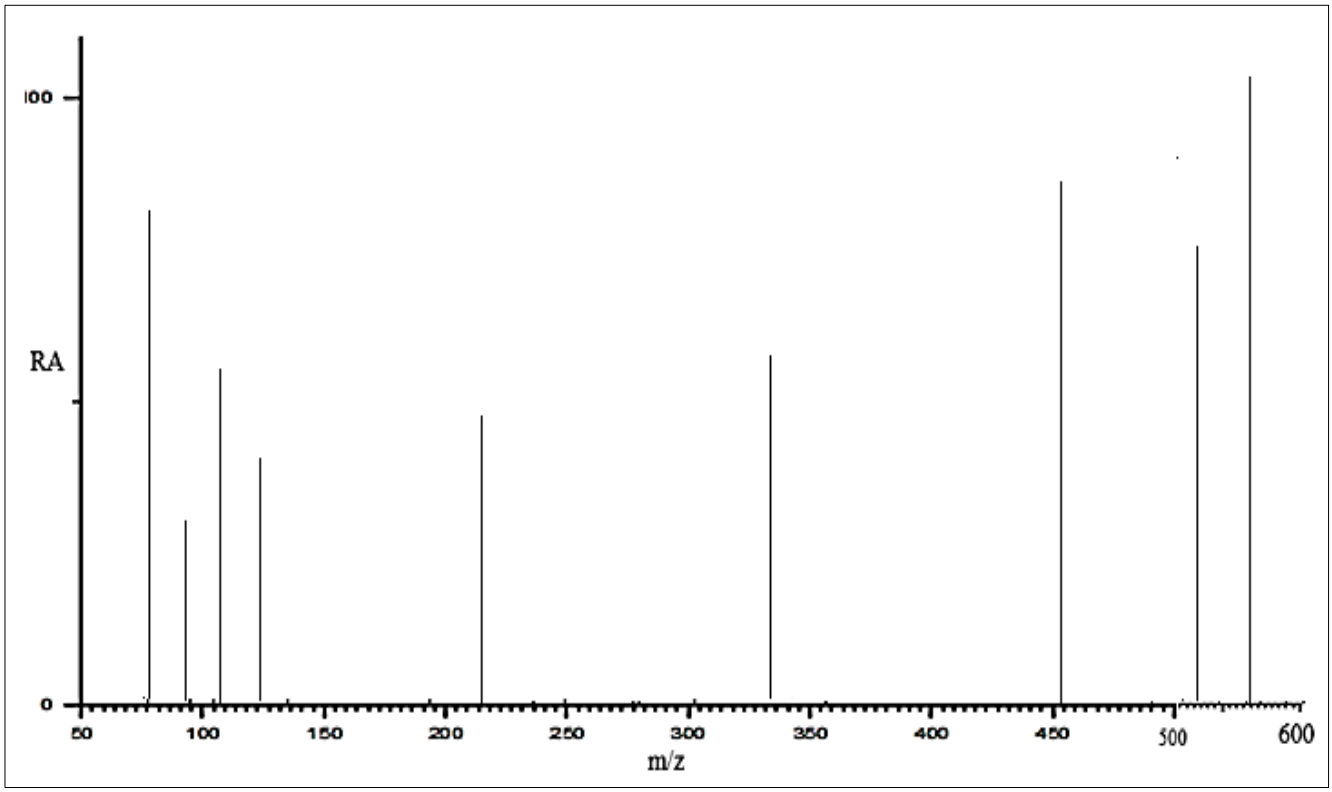


Fig 3.63: Mass spectrum of 3-((4-((2-carboxy phenyl) amino)-6-((4-(4-ethyl phenyl) thiazol-2-yl) amino)-1,3,5-triazin-2-yl) amino)-2,3-dihydro pyrazine-2-carboxylic acid

Mass Spectra of all newly synthesized 1,3,5 triazines derivatives were recorded on Alliance 2795, Q-TOF Micro mass- 2007 Mass spectrometer equipped with Electrospray Ionization (ESI) source (HRMS), mass range 50-2000 Dalton and Quadrupole analyzer with time of Flight. The newly synthesized s-triazines derivatives with substituted amines analyzed for mass spectral characterization. All the newly synthesized compounds give characteristic fragmentation at excepted m/z values, in the mass spectra gives base peak values and molecular ion peak values at excepted m/z values and fragmentation patten for all newly synthesized1,3,5 triazines derivatives is near about same.

Newly synthesized 135 triazines derivatives namely 5a to 5h gives molecular ions peak at 492,494, 511, 508, 492, 478, 557, 506 and for 6a to 6h gives molecular ions peak at 548,

549, 568, 564, 547, 533, 612 561 respectively and these values are good agreement with literature review [42].

The mass spectra of the synthesized 1,3,5-triazine derivatives provided definitive confirmation of their molecular weights and molecular formulas. The observed molecular ion peaks corresponded closely with the calculated molecular masses, validating the successful formation of the targeted compounds. Fragmentation patterns further supported the proposed structures by displaying characteristic cleavage of substituents and the triazine ring, consistent with known fragmentation behaviour of similar heterocyclic compounds. The absence of significant unexpected peaks indicated high purity of the synthesized derivatives.

Overall, mass spectral analysis corroborates the successful synthesis and structural integrity of the 1,3,5-triazine derivatives, complementing FTIR and NMR data in confirming their identity.

The synthesized 1,3,5-triazine derivatives were successfully characterized using FTIR, ^{1}H NMR, ^{13}C NMR, and mass spectrometry, providing conclusive evidence of their structures and purity. FTIR analysis confirmed the presence of the triazine ring through characteristic C=N stretching vibrations and identified functional groups introduced via substitution. ^{1}H NMR spectra displayed well-resolved proton signals with chemical shifts, splitting patterns, and integration consistent with the proposed substituents, while the absence of ring protons confirmed the triazine core. ^{13}C NMR spectra further supported the structure by showing downfield signals for the C=N carbons of the triazine nucleus along with resonances for aromatic, aliphatic, and heteroatom-linked carbons, consistent with the expected framework. Mass spectral data corroborated the molecular weights of the derivatives, with molecular ion peaks and fragmentation patterns aligning with the calculated structures and indicating high purity.

Collectively, these spectral techniques confirm the successful synthesis, structural integrity, and purity of the 1,3,5-triazine derivatives, providing a robust foundation for subsequent physicochemical and biological studies.

Conclusion

The spectral characterization of the synthesized 1,3,5-triazine derivatives confirms the successful incorporation of the desired substituents and validates the proposed structures. FT-IR spectra clearly indicated the presence of characteristic absorption bands corresponding to the triazine ring vibrations, C=N stretching, and functional groups of the substituted amines. ^{1}H-NMR and ^{13}C-NMR spectra provided detailed insights into the chemical environment of hydrogen and carbon atoms, showing well-defined signals consistent with the expected structural framework of the triazine nucleus and its substituents. The mass spectral data further corroborated the molecular weight of each compound, matching the calculated values, thereby confirming their purity and molecular integrity.

Overall, the combined spectral analyses FT-IR, NMR, mass spectrometry unequivocally establish the formation of the targeted 1,3,5-triazine derivatives and provide a reliable basis for further exploration of their physicochemical and biological properties.

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