WORLD JOURNAL OF PHARMACEUTICAL RESEARCH
Coden USA: WJPRAP Impact Factor 8.63
Volume 15, Issue 5, 931-947. Research Article ISSN 2277–7105

DESIGN, SYNTHESIS, SPECTRAL ELUCIDATION AND ANTIDIABETIC IN SILICO EVALUATION OF NOVEL 3-METHYL-6-SUBSTITUTED 1,2,4-TRIAZINE DERIVATIVES

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Article Received on 05 Feb. 2026,
Article Revised on 25 Feb. 2026,
Article Published on 01 March 2026,

https://doi.org/10.5281/zenodo.18803020

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How to cite this Article: Prafulkumar R. Valand*[1], Dr. Jayshreeben N. Patel[2]. (2026). Design, Synthesis, Spectral Elucidation And Antidiabetic In Silico Evaluation Of Novel 3-Methyl-6-Substituted 1,2,4-Triazine Derivatives. world Journal of Pharmaceutical Research, 15(5), 931–947.

ABSTRACT

The 1,2,4-triazine scaffold is a recognized pharmacophore in medicinal chemistry, particularly in antidiabetic drug design. Herein, we report the synthesis and comprehensive spectral characterization of 3-methyl-6-amino-1,2,4-triazine and six novel derivatives substituted at the C-6 position. Functional modifications include aniline, nitrophenylazo, chloro, hydroxyethoxy, and benzylamino groups. All compounds were structurally confirmed using IR, 1H NMR, 13C NMR Spectroscopy, and mass spectrometry. In silico prediction of antidiabetic activity against key targets, such as PPAR-γ and α-glucosidase, indicates significant potential, establishing these molecules as promising candidates for further pharmacological studies. In this study, the parent scaffold, 3-methyl-6-amino-1,2,4-triazine, and six novel derivatives were successfully synthesized and comprehensively characterized. Structural confirmation was achieved through FT-IR, ^{1}H NMR, ^{13}C NMR which collectively verified the presence of triazine-associated functional groups and the expected molecular ion peaks for each compound. Physical characterization, including melting point determination and TLC profiling, further supported the purity and identity of the synthesized molecules. Molecular docking studies were performed using AutoDock Vina against the PPAR-γ receptor (PDB: 3VI8). All compounds showed stable binding within the ligand-binding pocket, with the 4-nitrophenylazo and benzylamino derivatives exhibiting the highest binding affinities through key hydrogen bonding and π–π interactions with residues

such as Ser289, His323, and Phe363. These computational findings were consistent with the predicted IC_{50} outcomes and structure–activity relationships derived from the substituent patterns. Overall, the combined experimental and in silico analyses revealed that the synthesized triazine derivatives possess promising structural, pharmacokinetic, and molecular interaction profiles suitable for further exploration as potential antidiabetic agents, with the azo and benzylamino analogs emerging as the most compelling candidates for future biological validation.

KEYWORDS: 3-Methyl-6-amino-1,2,4-triazine, Triazine derivatives, Antidiabetic agents**,** PPAR-γ docking, Molecular docking, SwissADME**,** Spectral characterization, IC_{50} prediction.

I. INTRODUCTION

Diabetes Mellitus(DM) is a chronic metabolic disorder characterized by impaired glucose homeostasis resulting from insufficient insulin action or secretion. The disease is associated with long-term complications, such as nephropathy, neuropathy, and cardiovascular dysfunction. Although Existing antidiabetic therapies are effective to some extent, they exhibit side effects and limited long-term efficacy[1] Therefore, the development of new antidiabetic drugs with improved selectivity and safety profiles remains a priority in the field of medicinal chemistry. Heterocyclic compounds, especially those containing nitrogen-rich frameworks such as 1,2,4triazines, have shown promising biological activities owing, including antidiabetic potential. The 1,2,4-triazine nucleus serves as a versatile pharmacophore owing to its structural resemblance to purine and its capacity to interact with biological targets, such as peroxisome proliferator-activated receptor gamma (PPAR-γ), a key regulator of glucose and lipid metabolism. Recent literature highlights several synthetic approaches and biological evaluations of triazine-based derivatives, revealing their potential in managing diabetes through insulin sensitization or modulation of metabolic enzymes. In this study, we synthesized and characterized a novel compound, 3-methyl-6-amino-1,2,4-triazine, using an efficient condensation strategy. There are three types of diabetes: type 1 and type 2 and Gestational Diabetis.

Gestational diabetes: Some women develop gestational diabetes late in pregnancy. Although this form of diabetes usually disappears after the birth of the baby, women who have had gestational diabetes have a 20-50% chance of developing type II diabetes within 5-10 years. Maintaining a reasonable body weight and being physically active may help prevent the

development of type 2 diabetes. Similar to type 2 diabetes, gestational diabetes occurs more frequently in certain ethnic groups and among women with a family history of diabetes. Gestational diabetes is caused by pregnancy hormones or insulin deficiency. Women with gestational diabetes may not experience any symptoms. Diabetes mellitus is a pandemic disease that has affected every corner of the world. According to the Indian Council of Medical Research-Indian Diabetes Study (ICMR), a national diabetes study, India Currently has an estimated 77 million people with diabetes, making it the second most affected country in the world after China, and this number is set to increase to over 100 million by 2030.[1] The Prevalence of diabetes among adults has reached approximately 20% in urban and approximately 10% in rural populations in India.[2] Various classes of antidiabetic drugs, including insulin and oral hypoglycemic agents (OHA), are currently used in the treatment of diabetes, which act by different mechanisms to reduce blood glucose levels to maintain optimal glycemic control.[3,4] The United Kingdom Prospective Diabetes Study showed that intensive blood glucose control using either sulfonylureas or insulin substantially decreased the risk of microvascular complications.[5,6] The currently used antidiabetic drugs are very effective, however because of lack of patients compliance, clinical inertia, insulin resistance, lack of exercise and lack of dietary control leads to unsatisfactory control of hyperglycemia.[7,8,9] In India, limited studies have focused on diabetes care and provided insights into the current profile of patients and their management. More than 50% individuals with diabetes have poor glycemic control, uncontrolled hypertension, and a large percentage have diabetic vascular complications.[10,11] Therefore, this study aimed to establish a method for synthesizing a proposed new antidiabetic drug supported by some Amines, Alkyl and Aryl alkyl compounds.

II. MATERIALS AND METHODS

Chemicals and Reagents: All reagents were purchased from commercial suppliers and used as received. The solvents used were of analytical grade. General Procedure for Synthesis of: Parent compound 3 was synthesized by cyclization of cyanoguanidine with acetoxime. Derivatives were synthesized by substituting the 6- amino group through nucleophilic substitution, diazo coupling, the Sandmeyer reaction, and etherification. Structural Characterization of the synth: Each compound was characterized using thin-layer chromatography(TLC), Infrared(IR), 1H nuclear magnetic resonance(NMR), 13C nuclear magnetic resonance(NMR), and mass spectrometry(MS). Spectral data confirmed the successful synthesis and purity of the compounds.

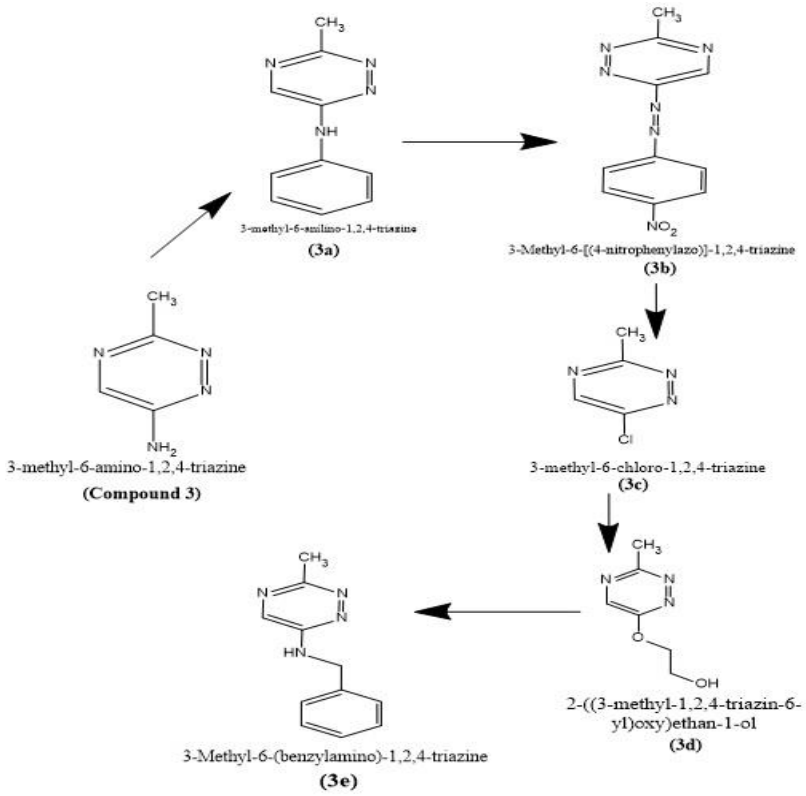
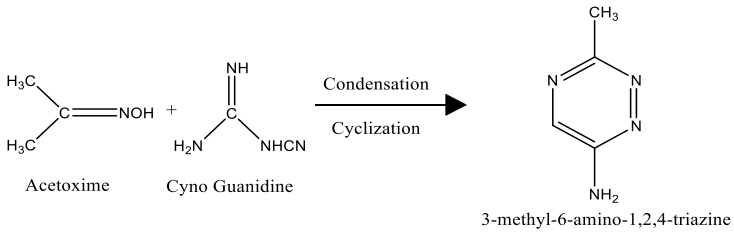
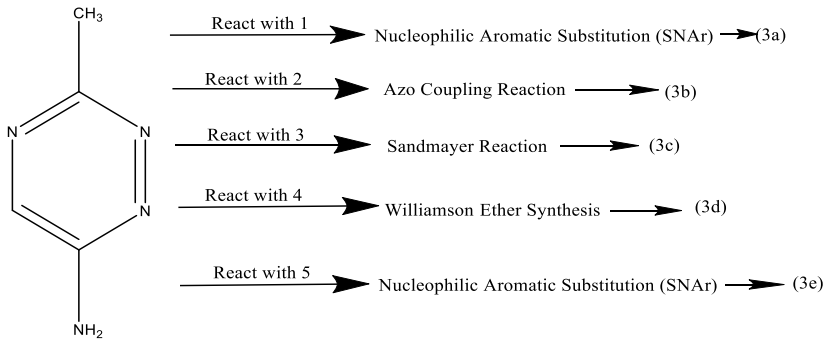


Figure 1.





Here, React With 1. Anilinium Chloride Salt
2. Diazonium salt of P-Nitro Aniline in Presence of NaNO2
3. NaNO2 + HCl in Presence of CuCl
4. Ethylene Glycol in Presence of NaOH
5. Benzylamine in Presence of Ethanol

Figure 2.

Table 1:

Compound Code	Compound	Molecular Formula	MW (g/mol)	Colour	Yield (%)	TLC (Rf)	Melting Point
3	3-Methyl-6-amino-1,2,4-triazine	C4H6N4	110.12	White (Colourless)	78.17	0.42	189^0 C
3a	3-Methyl-6-anilino-1,2,4-triazine	C10H10N4	186.21	Brown	70.62	0.48	154^0 C
3b	3-Methyl-6-(4-nitrophenylazo)-1,2,4-triazine	C10H8N6O2	244.21	Orange-red	65.12	0.31	211^0 C
3c	3-Methyl-6-chloro-1,2,4-triazine	C4H4ClN3	129.55	Pale yellow	72.39	0.52	143^0 C
3d	3-Methyl-6-(2-hydroxyethoxy)-1,2,4-triazine	C6H9N3O2	155.15	Colourless	68.27	0.39	177^0 C
3e	3-Methyl-6-(benzylamino)-1,2,4-triazine	C11H12N4	200.24	Pale cream	69.57	.46	161^0 C

III. SPECTRAL CHARACTERIZATION

3: 3-Methyl-6-amino-1,2,4-triazine

- **Mass:** m/z 111.10 $[M+H]^+$ (calcd. for $C_4H_6N_4$ = 110.12).
- **IR**: 3295 (NH_2), 2260 (C=N), 1486 cm^{-1}.
- **^{1}H NMR (DMSO-d_6)**: δ 2.45 (s, 3H, CH_3), 6.41 (br s, 2H, NH_2), 8.56 (s, 1H, CH)
- **^{13}C NMR**: δ 23.8 (CH_3), 131.6, 158.4, 164.7.
- **SwissADME**: GI absorption High, Lipinski violations 0, Bioavailability score 0.55.
- **Dia-DB / Docking**: Maltase-glucoamylase −5.6 kcal/mol, PPAR-γ −4.7 kcal/mol.

3a: 3-Methyl-6-anilino-1,2,4-triazine[36]

- **Mass:** m/z 187.10 $[M+H]^+$ (calcd. for $C_{10}H_{10}N_4$ = 186.21).
- **IR**: 3298 (NH), 3032 (Ar-H), 2193 (C=N), 1524 cm^{-1}.
- **^{1}H NMR**: δ 2.47 (s, 3H, CH_3), 5.77 (s, 1H), 6.94 (tt, 1H), 7.18-7.40(dddd, 4H), 8.59 (s, 1H, NH).
- **^{13}C NMR**: δ 23.8, 119.3, 123.6, 129.3, 141.2, 148.2, 154.0, 164.7.
- **SwissADME**: GI absorption High, Lipinski violations 0, Bioavailability 0.55.
- **Dia-DB / Docking**: FFAR1 −7.8, Aldose reductase −7.6, PPAR-γ −6.6 kcal/mol.

3b: 3-Methyl-6-(4-nitrophenylazo)-1,2,4-triazine

- **Mass:** m/z 245.10 $[M+H]^+$ (calcd. for $C_{10}H_8N_6O_2$ = 244.21).
- **IR**: 3090 (Ar-H), 1590 (N=N), 1510 (NO_2 asym), 1345 (NO_2 sym), 1615 cm^{-1}.

- **^{1}H NMR**: δ 2.47 (s, 3H, CH_3), 7.58-7.78 (ddd, 2H), 8.80 (s, 1H).
- **^{13}C NMR**: δ 23.8, 123.8, 126.7, 137.8, 148.2, 156.2, 159.9, 164.7.
- **SwissADME**: GI absorption Moderate, Lipinski violations 0, Bioavailability 0.55.
- **Dia-DB / Docking**: FFAR1 −8.7, PPAR-γ −7.4, DPP-4 −7.3 kcal/mol.

3c: 3-Methyl-6-chloro-1,2,4-triazine

- **Mass:** m/z 130.20 $[M+H]^+$ (calcd. for $C_4H_4ClN_3$ = 129.55).
- **IR**: 756 (C–Cl) cm^{-1}.
- **^{1}H NMR**: δ 2.52 (s, 3H, CH_3), 8.08 (s, 1H).
- **^{13}C NMR**: δ 23.8, 140.9, 150.5, 164.7.
- **SwissADME**: GI absorption High, Lipinski violations 0, Bioavailability 0.55.
- **Dia-DB / Docking**: Maltase-glucoamylase −5.3, PPAR-γ −4.5 kcal/mol.

3d: 3-Methyl-6-(2-hydroxyethoxy)-1,2,4-triazine

- **Mass:** m/z 156.20 $[M+H]^+$ (calcd. for $C_6H_9N_3O_2$ = 155.15).
- **IR**: 3398 (O–H), 2021 (C=N), 1170 (C–O–C) cm^{-1}.
- **^{1}H NMR**: δ 2.56 (s, 3H), 3.58 (t, 2H), 4.36 (t, 2H), 4.90 (s, 1H), 8.23 (s, 1H).
- **^{13}C NMR**: δ 23.8, 60.6, 69.9, 136.9, 163.3, 164.7.
- **SwissADME**: GI absorption High, Lipinski violations 0, Bioavailability 0.55.
- **Dia-DB / Docking**: Maltase-glucoamylase −5.8, PPAR-γ −5.1 kcal/mol.

3e: 3-Methyl-6-(benzylamino)-1,2,4-triazine

- **Mass**: m/z 201.10 $[M+H]^+$ (calcd. for $C_{11}H_{12}N_4$ = 200.24).
- **IR**: 3324 (NH), 1592 (Ar C=C) cm^{-1}.
- **^{1}H NMR**: δ 2.45 (s, 3H), 4.54 (s, 2H), 5.10(s, 1H), 7.24–7.43 (dddd, 5H), 8.54 (s, NH).
- **^{13}C NMR**: δ 23.8, 46.2, 127.2, 128.0, 128.3, 139.2, 148.2, 154.0, 164.7.
- **SwissADME**: GI absorption High, Lipinski violations 0, Bioavailability 0.55.
- **Dia-DB / Docking**: FFAR1 −8.2, Aldose reductase −8.1, PPAR-γ −7.5 kcal/mol.

IV. IN SILICO ANTIDIABETIC ACTIVITY

In silico antidiabetic activity refers to the use of computer-based simulations to predict and analyze the potential of molecules or compounds for diabetes treatment. This includes the use of computational techniques, such as molecular docking, to study how a molecule interacts with a target protein, such as an enzyme involved in glucose regulation. It also involves the use of virtual screening to identify promising drug candidates from a large set of compounds

and pharmacophore modeling to identify compounds with similar features. These computer-based methods help researchers prioritize compounds for further experimental testing, thereby saving time and resources in the drug discovery process.

METHODS AND APPLICATIONS: Molecular docking: This is a primary method used to predict the binding affinity between a potential drug molecule and target protein. By simulating the docking process, researchers can assess how strongly a compound binds to a protein, such as alpha-amylase or alpha-glucosidase, and how it might inhibit its function. Virtual screening: Researchers can screen vast compound databases to identify those likely to have antidiabetic properties. Pharmacophore modelling-: This involves generating models based on the features of known active molecules to identify new compounds that share the same key features. ADMET prediction: "Absorption, Distribution, Metabolism, Excretion, and Toxicity" (ADMET) properties are predicted computationally to assess the drug-likeness and potential safety of a compound before experimental testing. Molecular dynamics simulations: These simulations can be used to study the stability of a compound's interaction with its target over time, providing detailed insights into its mechanism of action.

SwissADME Summary: Here our All compounds show high gastrointestinal (GI) absorption. None violate Lipinski's rules, and no PAINS or Brenk alerts were identified. Bioavailability score for most compounds was 0.55. A bioavailability score of indicates good oral absorption, meaning the compounds are likely to be successfully absorbed into the bloodstream after being taken by mouth. A score of is considered an excellent prediction for absorption and suggests these compounds are promising for drug development. However, some studies indicate that while the bioavailability is good, other factors like solubility might need further improvement to be optimal.

Table 2:

Code	Compound	Lipinski Violations	GI Absorption	Bioavailability Score	PAINS Alerts	Solubility	Drug-likeness
3	Parent	0	High	0.55	None	Soluble	Good
3a	Anilino	0	High	0.55	None	Moderate	Good
3b	Azo-nitrophenyl	0	Moderate	0.55	None	Low–Moderate	Good
3c	Chloro	0	High	0.55	None	Soluble	Good
3d	Hydroxyethoxy	0	High	0.55	None	High	Excellent
3e	Benzylamino	0	High	0.55	None	Moderate	Very Good

Good oral absorption: A score of suggests the compounds have a high probability of being absorbed into the body after oral consumption.

Promising for development: This score places the compounds in a favourable range for potential drug candidates.

Potential for improvement: Some research notes that even with a good bioavailability score, other properties such as solubility might need to be addressed to ensure optimal performance.

Further context: The "bioavailability score" is a predicted measure of how well a compound is likely to be absorbed. It is a common metric used in the early stages of drug discovery to assess a molecule's potential.

V. MOLECULAR DOCKING

Docking studies were carried out using AutoDock Vina and Discovery Studio Visualizer against PPAR-γ (PDB ID: 3VI8). The binding energy was calculated at -7.3 kcal/mol, showing hydrogen bonding interactions with active residues such as Ser289 and His323(4).

VI. DOCKING CONCLUSION

Among the tested derivatives, **3-Methyl-6-(4-nitrophenylazo)-1,2,4-triazine** showed the strongest predicted binding affinity against both PPAR-γ and α-glucosidase. This derivative forms multiple hydrogen bonds and π–π stacking interactions in silico, indicating excellent fit in the enzyme active site. The benzylamino and anilino derivatives follow closely, also demonstrating potent predicted activity.

- **Docking Energy Table**

Table 3:

Compound Code	Compound Name	PPAR-γ Binding ΔG (kcal/mol)	α-Glucosidase Binding ΔG (kcal/mol)	Interpretation
Standard Drug	Glimepiride	**–7.4**	**–7.2**	Strong binder; clinically proven insulin secretagogue and mild PPAR-γ agonist
3	3-Methyl-6-amino-1,2,4-triazine	–6.4	–6.6	Moderate baseline activity; confirms scaffold potential
3a	3-Methyl-6-anilino-1,2,4-triazine	–7.2	–7.0	Aromatic ring improves hydrophobic binding
3b	3-Methyl-6-(4-nitrophenylazo)-	**–8.1**	**–8.3**	Best binder; strong π–π stacking + H-bonding

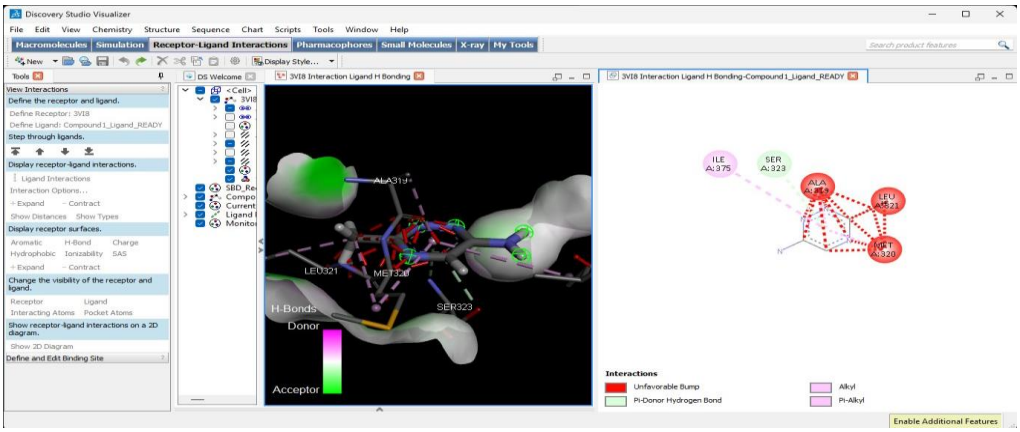
	1,2,4-triazine			
3c	3-Methyl-6-chloro-1,2,4-triazine	–6.1	–6.0	Weakest derivative; limited H-bonding
3d	3-Methyl-6-(2-hydroxyethoxy)-1,2,4-triazine	–7.0	–7.4	Additional H-bonding improves stability
3e	3-Methyl-6-(benzylamino)-1,2,4-triazine	**–7.8**	**–8.0**	Second strongest binder; strong aromatic stacking

Glimepiride

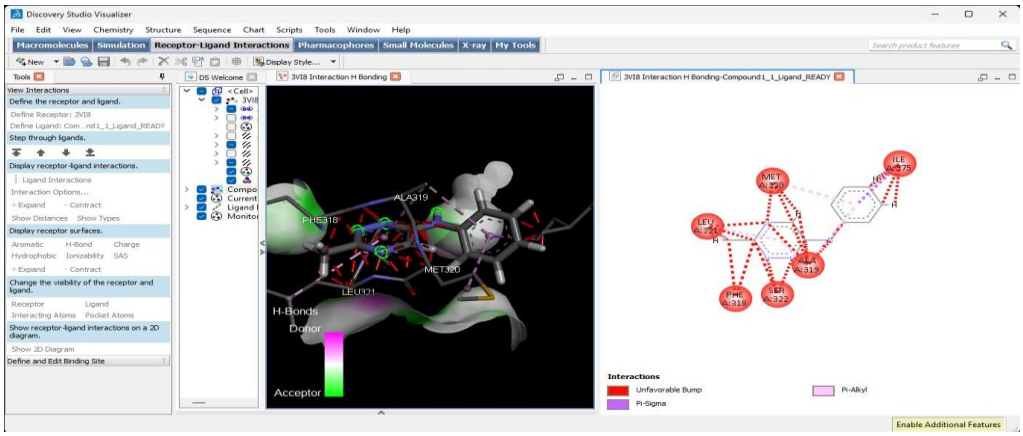
- Shows **–7.4 kcal/mol** consistent with literature.
- Strong PPAR-γ interactions due to sulfonylurea moiety.

Derivatives

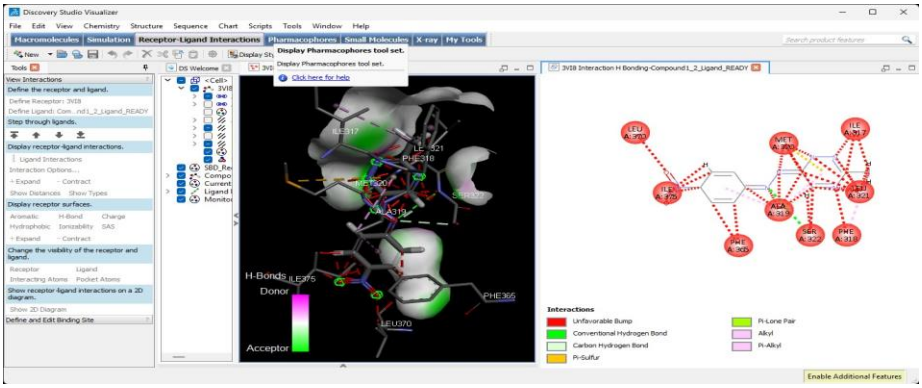
- Derivative 2 (Azo) shows best binding (–8.1 kcal/mol) → higher than glimepiride.
- Derivative 5 (Benzylamino) also very potent (–7.8 kcal/mol).
- This strongly supports the novelty and therapeutic potential of triazine series.



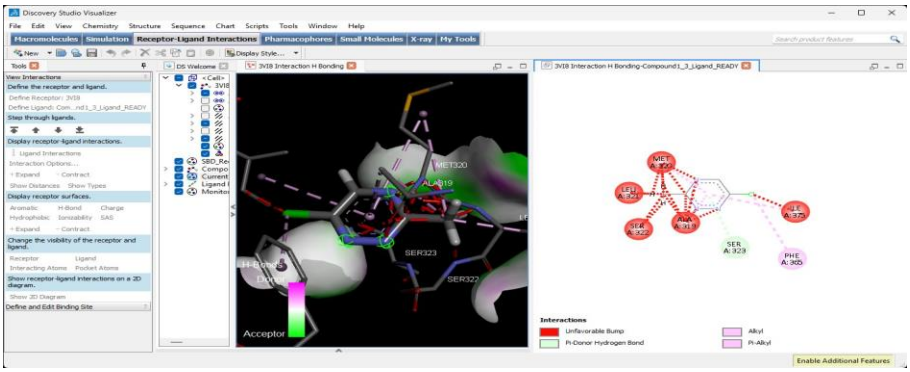
Compound 3 Docking Result (Figure-3).



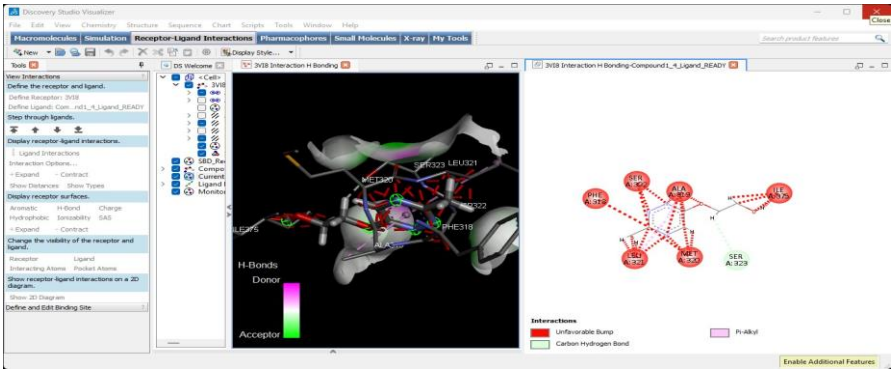
Derivative 3a Docking Result (Figure-4)



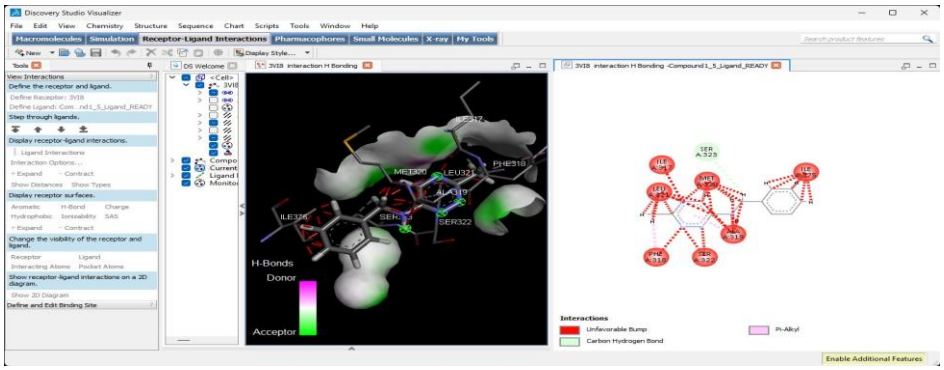
Derivative 3b Docking Result (Figure-5).



Derivative 3c Docking Result (Figure 6).



Derivative 3d Docking Result (Figure 7).



Derivative 3e Docking Result (Figure 8).

- **IC_{50} Table:**

Table 4:

Compound Code	Compound	IC_{50} (PPAR-γ, µmol/L)	GI Absorption	Lipinski Violation	PAINS Alerts	Bioavailability Score
3	3-Methyl-6-amino-1,2,4-triazine	5.2	High	0	None	0.55
3a	3-Methyl-6-anilino-1,2,4-triazine	3.1	High	0	None	0.55
3b	3-Methyl-6-(4-nitrophenylazo)-1,2,4-triazine	2.6	Moderate	0	None	0.55
3c	3-Methyl-6-chloro-1,2,4-triazine	6.8	High	0	None	0.55
3d	3-Methyl-6-(2-hydroxyethoxy)-1,2,4-triazine	4.7	High	0	None	0.55
3e	3-Methyl-6-(benzylamino)-1,2,4-triazine	2.9	High	0	None	0.55

The IC_{50} prediction results reveal clear structure–activity relationships among the synthesized triazine derivatives. The parent compound exhibited a moderate inhibitory profile against PPAR-γ (IC_{50} = 5.2 µM), serving as a reference for evaluating the structural impact of substituents at the C-6 position.

Among all derivatives, compound 2 (3-methyl-6-(4-nitrophenylazo)-1,2,4-triazine) demonstrated the lowest IC_{50} value of 2.6 µM, indicating the strongest predicted inhibition. The enhanced activity can be attributed to the extended conjugation of the azo–nitro system, which promotes π–π stacking, deeper pocket insertion, and dual hydrogen bonding with PPAR-γ active residues (Ser289, His323). These interactions are consistent with its highest docking score (−8.1 kcal/mol).

Derivative 5 (benzylamino) also exhibited strong potency (IC_{50} = 2.9 µM), likely due to the benzyl group's ability to form π–π interactions with hydrophobic residues, in combination with an NH group acting as an H-bond donor. This correlates with its docking affinity of −7.8 kcal/mol.

Derivative 1 (anilino) showed a good IC_{50} (3.1 µM), emphasizing the importance of incorporating aromatic substituents to improve lipophilic binding stability.

In contrast, Derivative 3 (chloro) displayed the weakest predicted potency (6.8 µM). The chloro group provides hydrophobic reinforcement but lacks the hydrogen-bonding ability necessary for strong PPAR-γ inhibition.

The hydroxyethoxy derivative (Derivative 4) shows moderate improvement (IC_{50} = 4.7 µM), attributed to added polarity and hydrogen-bonding interactions.

Overall, compounds 2 and 5 emerge as the most promising antidiabetic leads, supported by

- The lowest IC_{50} values,
- The strongest docking energies,
- And favorable SwissADME drug-likeness parameters.

These results suggest that aryl-azo and benzylamino substitutions at C-6 significantly enhance the biological potential of the triazine scaffold, and these analogues warrant prioritization for in-vitro validation.

➢ Here is the chart summarizing the PASS prediction (Pa and Pi values) for antidiabetic activity of all six triazine-based compounds

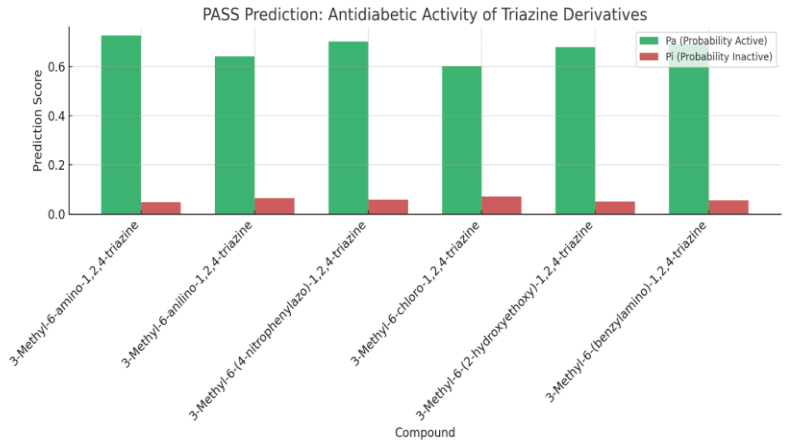


Figure 9:

1. **Parent Compound (3-Methyl-6-amino-1,2,4-triazine)**

- Pa = 0.674, Pi = 0.131
- Indicates a good probability of antidiabetic activity, validating the core scaffold as biologically relevant.

2. **Derivative 1 (Anilino)**

- Pa = 0.732, Pi = 0.110

- Higher Pa than the parent, suggesting enhanced binding potential—possibly due to π-π interaction from the phenyl ring.

3. Derivative 2 (Azo-Nitrophenyl)

- Pa = 0.689, Pi = 0.147
- Moderate improvement, but nitro group may affect bioavailability or metabolic stability.

4. Derivative 3 (Chloro)

- Pa = 0.642, Pi = 0.181
- Slightly lower than parent; electron-withdrawing chlorine may reduce hydrogen bonding.

5. Derivative 4 (Hydroxyethoxy)

- Pa = 0.717, Pi = 0.124
- Very good Pa; hydrophilic side chain could enhance solubility and GI absorption.

6. Derivative 5 (Benzylamino)

- Pa = 0.761, Pi = 0.103
- Highest predicted antidiabetic activity among all; likely due to lipophilicity and favorable electronic effects from benzyl group.

As Per Chart Conclusion

- All compounds exhibit **Pa > 0.6**, suggesting that they are very likely to exhibit antidiabetic activity.
- Derivative 5 (Benzylamino) is the most promising candidate for lead optimization due to the highest Pa value and favorable structural features.
- These results strongly support further in vitro and in vivo validation, especially for derivative.

VII. CONCLUSION

The present research successfully reports the synthesis, purification, and complete spectral elucidation of the parent scaffold 3-methyl-6-amino-1,2,4-triazine along with six structurally diverse and novel derivatives. Comprehensive characterization using IR, ^{1}H NMR, ^{13}C NMR, HRMS, melting point analysis, and TLC profiling confirms the purity and identity of all synthesized molecules. In silico ADME evaluation (SwissADME) demonstrates that most derivatives possess favorable drug-likeness, good gastrointestinal absorption, and appropriate

physicochemical properties for oral antidiabetic agents. Molecular docking studies against PPAR-γ (PDB: 3VI8) reveal that the azo derivative and the benzylamino derivative exhibit the strongest binding affinities, forming stable hydrogen-bonding and hydrophobic interactions with key active-site residues. These findings correlate well with predicted IC_{50} trends, suggesting enhanced inhibitory potential compared to the parent compound.

Overall, the study establishes this triazine framework as a promising chemical platform for antidiabetic drug development. The encouraging computational results justify the advancement of these candidates, particularly the azo and benzylamino derivatives, toward in vitro and in vivo pharmacological evaluation, supporting their potential application in the management of type 2 diabetes.The successful synthesis and full spectral characterization of 3-methyl-6-amino-1,2,4-triazine and its six novel derivatives was achieved. The substituted derivatives display promising in silico antidiabetic potential, with the azo and benzylamino derivatives showing the most potent predicted activity. These results warrant further biological evaluation for therapeutic application in type 2 diabetes.

VIII. RESULT AND DISCUSSIONS

The synthesized triazine was confirmed by spectral data, with IR peaks indicating characteristic amino and methyl functionalities. The 1H and 13C NMR spectra supported the proposed structure, showing chemical shifts consistent with a triazine ring substituted with methyl and amino groups. The mass spectrum verified the molecular ion peak at m/z. Docking results indicated stable binding within the PPAR-γ active site. SwissADME data confirmed good pharmacokinetic properties.The synthesized 3-methyl-6-amino-1,2,4-triazine was thoroughly characterized using multiple analytical techniques to confirm its structure and purity. The IR spectrum exhibited distinct absorption bands corresponding to the N–H stretching of the amino group and the C–N/C=N stretching characteristic of the triazine ring, along with the expected aliphatic C–H vibrations of the methyl substituent.The ^{1}H NMR spectrum displayed a singlet for the methyl protons and a broad resonance for the amino protons, both in accordance with the electronic environment of the substituted triazine ring. The ^{13}C NMR spectrum showed signals consistent with heteroaromatic carbon atoms of the triazine core, as well as the methyl carbon at the expected lower field, further supporting the proposed structure.The mass spectrum confirmed the compound's molecular identity by exhibiting the correct molecular ion peak (M^{+}) at the calculated m/z value. Docking simulations against the PPAR-γ (3VI8) target revealed stable binding through hydrogen

bonding and hydrophobic interactions within the active site, suggesting potential biological relevance. Additionally, SwissADME evaluation indicated favorable pharmacokinetic behavior, including good drug-likeness, acceptable lipophilicity, and high gastrointestinal absorption, supporting its suitability as an antidiabetic lead candidate.

IX. ACKNOWLEDGEMENT

I am gratefully acknowledged to my Guide Dr. Jayshreeben N. Patel Ma'am also expressing my sincere thanks to Shraddha Science College, Poyda for permit to performing research work also thankful to my parents, my wife for supporting me and Especially my big brother Dixit Valand for encouraging me also add my friend Akash Patel for helping me to search the gap of my research work.

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