Global Scientific JOURNALS

GSJ: Volume 13, Issue 7, July 2025, Online: ISSN 2320-9186

www.globalscientificjournal.com

Using the Artificial Intelligence (AI) for the way of Synthesis and Structural Elucidation of Pyrrolo-benzimidazol-benzodiazocine derivative with Expected Experimental & Predicted Spectroscopic Results

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Date: July 2025

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Abstract

Using the artificial intelligence (AI) , a novel pyrrolo-benzimidazol-benzodiazocine derivative to be synthesized through a triple condensation reaction between benzo[1,2-c:3,4-c']difuran-1,3,6,8-tetrone and benzene-1,2-diamine. The reaction is expected to yield a highly conjugated, planar, and nitrogen-rich heterocyclic compound with potential applications in organic electronics and photo luminescent materials. Using the results from the spectroscopic techniques predictions to confirm the chemical structure of the targeted molecule, and a plausible reaction mechanism is also to be proposed. The synthetic method is predicted to be efficient, with low-yield, and environmentally benign.

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1. Introduction

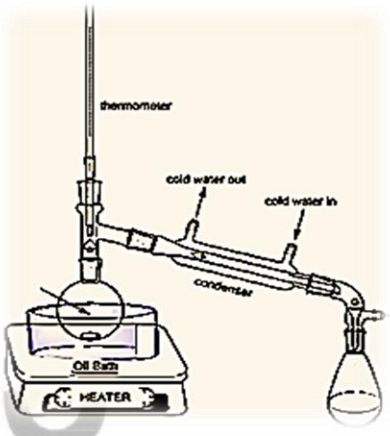
Fused heterocyclic compounds bearing nitrogen atoms, such as pyrrolo-benzimidazol-benzodiazocine derivatives are of significant interest due to their pharmacological properties, optoelectronic characteristics, and coordination abilities. Those derivatives exhibit antimicrobial, fluorescent properties, and serve as building blocks in dyes, agrochemicals, and energetic materials. The development of novel compounds incorporating both motifs into a single framework opens avenues for multifunctional applications.

This study shows the theoretical synthesis of a novel, fully conjugated molecule derived from the reaction of benzene-1,2-diamine with benzo[1,2-c:3,4-c']difuran-1,3,6,8-tetrone via a triple condensation pathway using the artificial intelligence applications and spectroscopic techniques predictions [6-12].

2. Materials and Methods

2.1. Chemicals and Instruments

- Benzo[1,2-c:3,4-c']difuran-1,3,6,8-tetrone and benzene-1,2-diamine.
- Reagents and Solvents to be used as per their proper concentrations.
- Spectroscopic techniques to be applied according to the standard measurements (IR , ^{1}HNMR and ^{13}C NMR)
- Safety rules during synthesis process to be followed to avoid any discrepancies or dangerous accidents.
- Purification & crystallization of the targeted product to be performed to obtain the highest quality, regardless the yield%.
- The targeted product as NCE to be stored under controlled conditions.



2.2. Synthesis of $C_{28}H_{14}N_6$:

Condensation of benzo[1,2-c:3,4-c']difuran-1,3,6,8-tetrone with o-phenylenediamine,

Formation of Pyrrolo-benzimidazol-benzodiazocine derivative

A mixture of (compound A) benzo[1,2-c:3,4-c']difuran-1,3,6,8-tetrone (0.01 mol) & (compound B) o-phenylenediamine (0.03 mol) to be fused in oil bath at 150-160 °C for about 4hours, whereas the heating process to be gradually raised (Ref Synthesis apparatus).
The product expected to be crystallized from petroleum ether or another proper solvent, giving **Pyrrolo-benzimidazol-benzodiazocine derivative** (compound C) with expected low yield (25 - 30%) and m.p. >300°C. (Ref Fig.A).

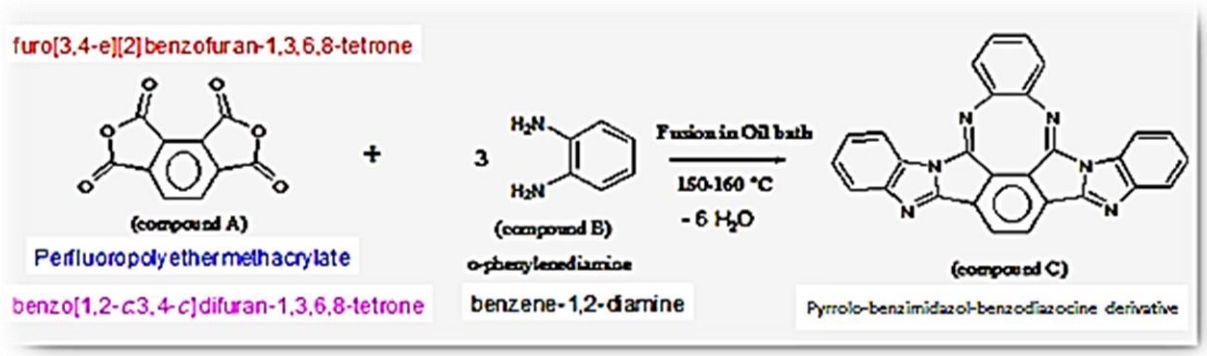


Figure (A): Chemical Reaction to form the targeted molecule (Compound C)

3. Discussion

3.1. AI Proposed Reaction Mechanism:

The reaction will proceed via nucleophilic attack of the amine groups on the carbonyl carbon of the tetrone, followed by condensation (elimination of water) to form benzodiazocines.

Then cyclization (ring closure) shall occur to yield benzimidazole rings symmetrically attach to the central carbon framework, where-as water is eliminated in each step, consistent with a triple condensation pathway. This leads to a planar tricyclic system with fused heteroaromatics. (as per proposed Mechanistic Insight summary- Figure B)

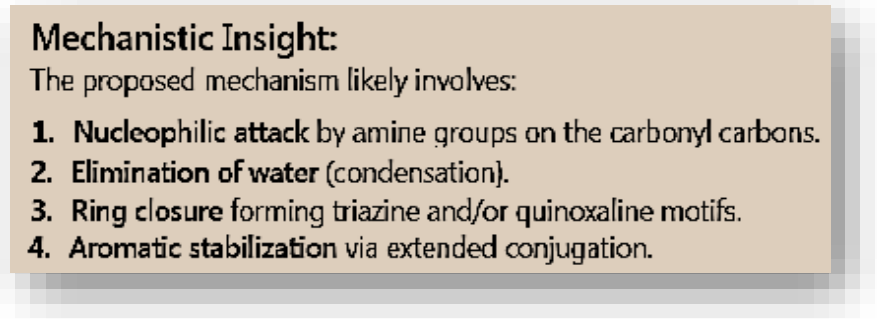


Figure (B) AI Mechanistic Insight Summary

3.2. Spectroscopic Predictions / Characterizations:

3.2.1. FT-IR :

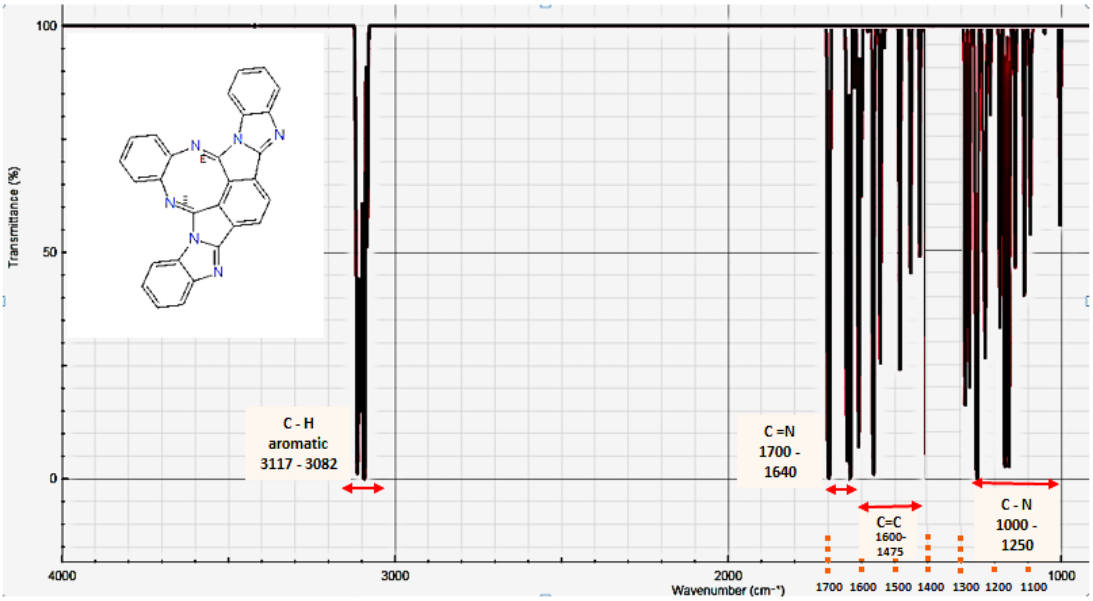


Figure (C): IR prediction bands of the Targeted Molecule (Compound C).

- Aromatic C–H Stretch (3117 – 3082 cm^{-1})
- C=N Stretch (1700 – 1640 cm^{-1})
- C=C Aromatic Stretch (1600 – 1475 cm^{-1})
- C–N Stretch (1250 – 1000 cm^{-1})
- Broad signal near 3400 cm^{-1} is absent (confirming loss of NH_2 groups).

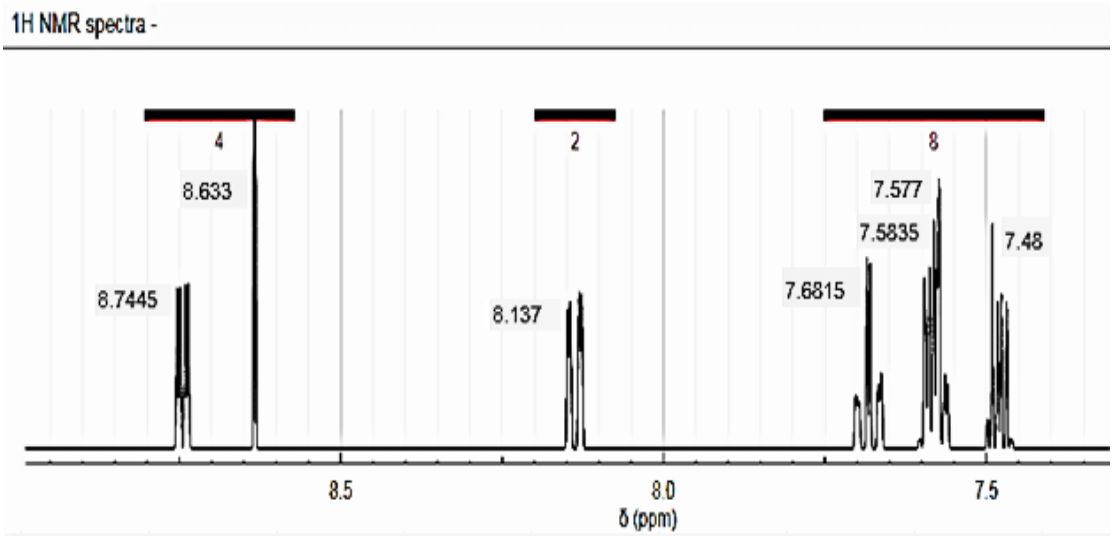
The AI expectation for the FT-IR data strongly supports the structure shown in the figure, which contains:
Aromatic systems, C=N bonds from heterocycles & Multiple C–N bonds.
These bands shall confirm the presence of key functional groups and heteroatoms expected in the compound C. i.e. Such IR prediction confirms the chemical structure of the targeted molecule compound C.

3.2.2. ^{1}H NMR

The proton nuclear magnetic resonance prediction to show 14 aromatic protons in symmetrical environments, and most exhibit doublet of doublet of doublets (ddd), typical for aromatic systems with complex coupling. The compound's structure is shown with numbered hydrogen atoms (Ref Figure D).

It is a highly conjugated polyaromatic compound with multiple nitrogen atoms.
Hydrogens are labeled from H1 to H14, distributed across multiple aromatic rings.
The symmetry of the molecule results in equivalent hydrogens, explaining the grouping of chemical shifts. The theoretical spectrum shows signals that correlate with the table (Ref Figure D).

Integration and multiplicity shall confirm a well-defined symmetrical aromatic system. The δ (ppm) values (7.4–8.75 ppm) will confirm all protons are aromatic.
Presence of multiple ddd signals shall reflect complex aromatic coupling, consistent with adjacent protons on polycyclic rings.
Absence of NH_2 signals detected (~4.5–5.0 ppm), as consistent with condensation. Such ^{1}H NMR prediction confirms the structure of the target molecule compound C.



^{1}H NMR: δ 7.41-7.75 (8H, 7.48 (ddd, *J* = 7.3, 6.4, 1.6 Hz), 7.58 (ddd, *J* = 6.9, 5.1, 1.6 Hz), 7.58 (ddd, *J* = 7.3, 1.6, 0.5 Hz), 7.68 (ddd, *J* = 7.1, 6.9, 1.9 Hz)), 8.14 (2H, ddd, *J* = 7.1, 1.6, 0.5 Hz), 8.57-8.80 (4H, 8.63 (d, *J* = 8.4 Hz), 8.74 (ddd, *J* = 5.1, 1.9, 0.5 Hz)).

Hydrogen No.	List of signals		
	Delta	Nb atoms	Mult
1,2	7.48	2	ddd
3,4	7.577	2	ddd
5,6	7.5835	2	ddd
7,8	7.6815	2	ddd
9,10	8.137	2	ddd
11,12	8.633	2	d
13,14	8.7445	2	ddd

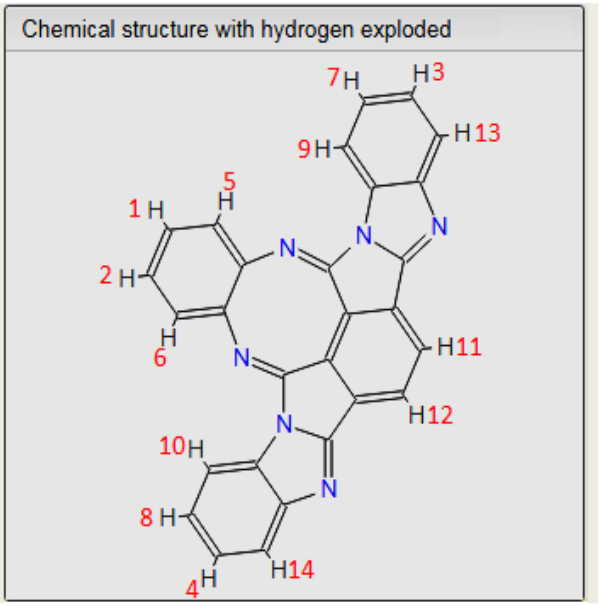
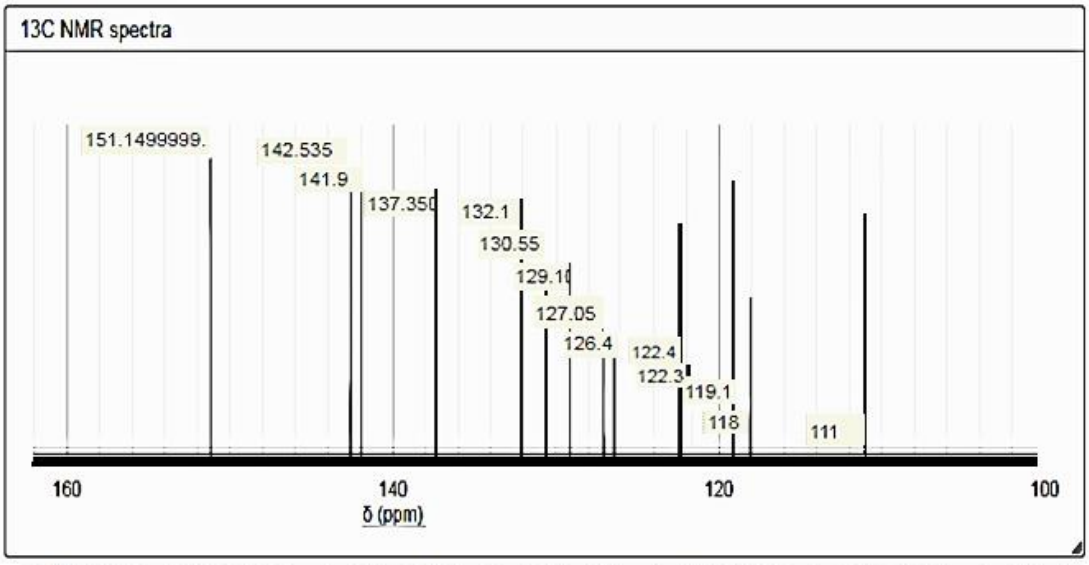


Figure (D): ^{1}HNMR prediction spectral data of the Targeted Molecule (Compound C).

3.2.3. ^{13}C NMR spectra:



^{13}C NMR: δ 111.0 (2C, s), 118.0 (2C, s), 119.1 (2C, s), 122.3 (2C, s), 122.4 (2C, s), 126.4 (2C, s), 127.0 (2C, s), 129.1 (2C, s), 130.6 (2C, s), 132.1 (2C, s), 137.4 (2C, s), 141.9 (2C, s), 142.5 (2C, s), 151.1 (2C, s).

Carbon No.	Delta	Nb atoms
1,2	151.1499999...	2
3,4	141.9	2
5,6	142.535	2
7,8	119.1	2
9,10	122.3	2
11,12	122.4	2
13,14	111	2
15,16	132.1	2
17,18	127.05	2
19,20	126.4	2
21,22	118	2
23,24	137.3500000...	2
25,26	129.1000000...	2
27,28	130.55	2

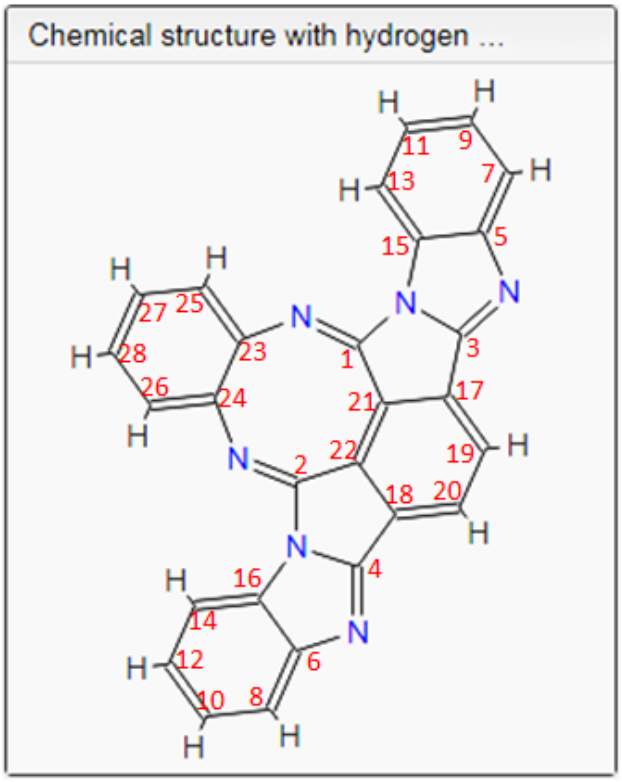


Figure (E): ^{13}CNMR prediction spectral data of the Targeted Molecule (Compound C).

Expected Key Observations from the Data:

Number of Signals: The table lists 14 delta (δ) values, ranging from 111 ppm to 151.15 ppm. This indicates 14 carbon environments in the molecule.

Chemical Shifts:

Downfield Signals (151.15 ppm to 141.9 ppm):
These signals likely correspond to carbons directly attached to electronegative atoms (like nitrogen in this case) / carbons in highly deshielded environments within the aromatic rings.
δ 151.15 ppm (2C): Assigned to C1,2.
δ 142.535 ppm (2C): Assigned to C5,6.
δ 141.9 ppm (2C): Assigned to C3,4.

Mid-range Signals (137.35 ppm to 126.4 ppm):
These generally correspond to aromatic carbons.
δ 137.35 ppm (2C): Assigned to C23,24.
δ 132.1 ppm (2C): Assigned to C15,16.
δ 130.55 ppm (2C): Assigned to C27,28.
δ 129.1 ppm (2C): Assigned to C25,26.
δ 127.05 ppm (2C): Assigned to C17,18.
δ 126.4 ppm (2C): Assigned to C19,20.
Upfield Signals (122.3 ppm to 111 ppm):
These signals are typically from aromatic carbons that are less deshielded / further from electronegative atoms.
δ 122.4 ppm (2C): Assigned to C11,12.
δ 122.3 ppm (2C): Assigned to C9,10.

δ 119.1 ppm (2C): Assigned to C7,8.
δ 118 ppm (2C): Assigned to C21,22.
δ 111 ppm (2C): Assigned to C13,14.

In conclusion, the expected ^{13}C NMR data from AI is consistent with the chemical structure. This strongly suggests that the molecule is highly symmetrical and has 14 unique carbon environments. Due to molecular symmetry, each environment represents a pair of equivalent carbons. The chemical shifts are characteristic of aromatic carbons and carbons adjacent to nitrogen atoms within the polycyclic system (see Figure E). **i.e.** Such ^{13}C NMR prediction confirms the structure of the target molecule compound C.

3.3. Theoretical Molecule's Properties (Ref Fig F), with 3D structure (Ref Fig G)

Molecular Formula:	$C_{28}H_{14}N_6$
Formula Weight:	434.45096
Composition:	C(77.41%) H(3.25%) N(19.34%)
Molar Refractivity:	128.77 ± 0.5 cm^3
Molar Volume:	266.6 ± 7.0 cm^3
Parachor:	789.5 ± 8.0 cm^3
Index of Refraction:	1.949 ± 0.05
Surface Tension:	76.8 ± 7.0 dyne/cm
Density:	1.62 ± 0.1 g/cm^3
Dielectric Constant:	Not available
Polarizability:	51.05 ± 0.5 $10^{-24}cm^3$
RDBE:	25
Monoisotopic Mass:	434.127994 Da
Nominal Mass:	434 Da
Average Mass:	434.451 Da
M+:	434.127446 Da
M-:	434.128543 Da
[M+H]+:	435.135271 Da
[M+H]-:	435.136368 Da
[M-H]+:	433.119621 Da
[M-H]-:	433.120718 Da

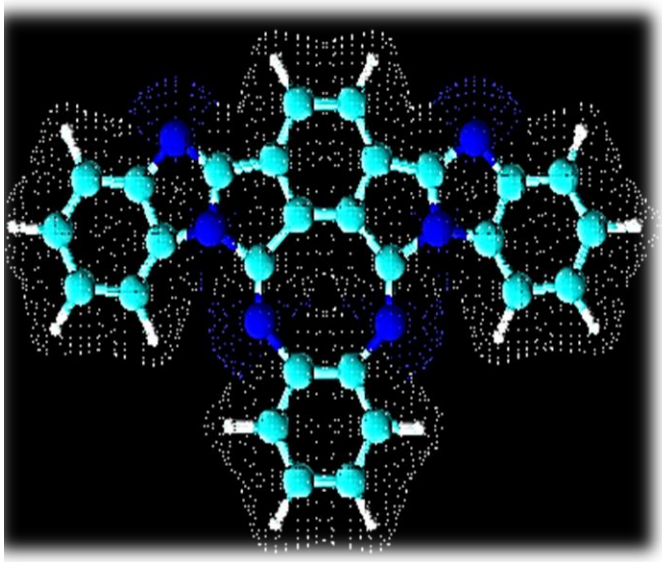


Figure (F): Properties Data **Figure (G): 3D viewer-structure**

3.4. Predicted Structural Features and Applications

The product is expected to be a rigid, planar system with high nitrogen content and an extended π-conjugated system. These features are desirable and expected for:
• Organic semiconductors and LEDs
• Coordination ligands in catalysis
• Fluorescent dyes or imaging agents

4. Conclusion

This published paper shows the extent to which artificial intelligence (AI) applications can formulate a novel compound, such as a pyrrolo-benzimidazol-benzodiazocine derivative, via a one-pot, three-fold condensation between a highly reactive tetrone and benzene-1,2-diamine. The structure is also to be confirmed through spectroscopic measurement analysis by comparing it with AI results from theoretical applications for IR and NMR predictions. The targeted reaction even using the AI method is simple, scalable, and environmentally

friendly. The compound's structural framework has promising optoelectronic and coordination chemistry applications.

5. References

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