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Synthesis, characterization, antimicrobial activity and DFT studies of novel phthalazine-5,10-dione derivatives

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Abstract

1H-pyrazolo[1,2-b] phthalazine-5,10-dione derivatives (**5a-j**) were synthesized in good yields using microwave-ultrasonic techniques (MW/US) in an attempt to find possible antibacterial characteristics. They were then described using mass, FTIR, and ^{1}H-NMR spectra data. These antimicrobial compounds were further evaluated against two fungus strains, *C. albicans* and *A. fumigatus*, as well as *B. subtilis*, *B. sphaericus*, *S. aureus* (+ ve strains), and *P. aeruginosa.* Streptomycin is a reference treatment, while amphotericin B is a common antibiotic having antibacterial and antifungal qualities. The antibacterial and antifungal properties of compounds **5b, 5c**, **5e**, **5i**, and **5j** were comparable to those of the reference or control molecule. Moreover, to support the energy gap, polarizability, and binding site interactions, a DFT investigation was conducted successively.

Keywords: Pyrazolo[1,2-*b*]phthalazine-5,10-dione; MCRs; Anti-microbial activity; DFT.

1. Introduction

Heterocyclic compounds containing nitrogen have long been of interest due to their uses in agrochemicals, functional materials, and physiologically active medications [1-5]. The pharmacological characteristics and clinical uses of 1H-pyrazolo[1,2-*a*]pyridazine-5,8-diones and 1H-pyrazolo[1,2-*b*]phthalazine-5,10-diones, which contain a hydrazine moiety as bridgehead hydrazine heterocycles, have drawn a lot of attention among *N*-containing heterocyclic compounds.

Phthalazine derivatives have been reported to possess anticonvulsant [6], cardiotonic [7], antimicrobial [8], antifungal [9], anti-cancer [10] and anti-inflammatory [11] activities. Pyridazine derivatives were considered because they show properties such as anti-cancer [12], and also their numerous applications in chemiluminescent materials and photovoltaic materials [13].

One-pot chemical reactions using more than two starting ingredients are known as multicomponent reactions (MCRs), and the end product retains significant amounts of each component. A number of descriptive attributes, including atom economy, efficiency, convergence, and sustainability, are frequently linked to MCRs [12,13]. Because of its scaffold diversity and quick and simple access to physiologically relevant molecules, synthetic researchers in both industry and academia have acknowledged that MCRs are the favored approach for designing and discovering biologically active chemicals.Because of its scaffold diversity and quick and simple access to physiologically relevant molecules, synthetic researchers in both academia and industry have acknowledged that MCRs are the favored approach for designing and discovering biologically active chemicals [14-20].

In context of these discoveries and as a follow-up to our previous research work [21-26], we present here the synthesis of new phthalazine-5,10-dione derivatives from phthalazine dione deriative, malononitrile, and aromatic aldehydes. The computational chemistry shows a great importance in new modern chemistry as a type of green chemistry. Therefore, the compounds were also theoretically analyzed by density functional theory (DFT) and TD-DFT, or time-dependent density (DFT). (TD-DFT) expands the fundamental ideas of ground state density-functional theory (DFT) to address excitations, or more broadly speaking, time-dependent phenomena [27] .

2. Results and Discussion

2.1. Chemistry

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Creating an effective technique with a good to exceptional yield is the goal of the current investigation. The formation of all these new heterocyclic derivatives has been fully characterized by means of such spectroscopic techniques as FTIR, ^{1}H-NMR, mass spectroscopy, and elemental analysis that were in agreement with their proposed structures. A series of 1H-pyrazolo[1,2-*b*]phthalazine-5,10-dione derivatives (**5a-j**) were constructed with different techniques. The related 1H-pyrazolo[1,2-*b*]phthalazine-5,10-dione derivatives were produced from the reaction of 5-nitro-2,3-dihydrophthalazine-1,4-dione (**1**) with various biselectrophilic precursors, such as aromatic aldehydes (**2a-i**) in the presence of malononitrile or ethyl cyanoacetate *via* multi-component reaction technique. Additionlly, these derivatives (**5a-j)** prepared through the interaction between compound (**1**) with arylidine malononitriles (**3a-i**), and ethyl 2-cyano-3-aryl acrylate (**4**). The reaction of compound (**1**) and malononitrile with aromatic aldehydes as *p*-anisaldehyde, *p*-chlorobenzaldehyde, *o*-bromobenzaldehyde, thiophene-2-aldehyde, 1-hydroxy-2-naphthaldehyde, benzaldehyde, *m*-nitrobenzaldehyde, and 4-(dimethylamino)benzaldehyde were further transformed into 1H-pyrazolo[1,2-*b*]phthalazine-5,10-dione derivatives (**5a-i**), respectively as shown in **Scheme 1**.

On the other hand, the reaction of compound (**1**) under the same reaction condition in MW/US as before with ethyl cyanoacetate and as *p*-anisaldehyde afforded the desired 1H-pyrazolo[1,2-b]phthalazine-5,10-dione derivative **5j**. The target starting compound 5-nitro-2,3-dihydrophthalazine-1,4-dione (**1**) was prepared by the one pot reaction of the 3-nitrophthalic anhydride with hydrazine hydrate on a MW/US reaction condition for 10 min. Moreover, one pot reaction of the compound (**1**) with *p*-anisaldehyde in the presence of malononitrile in ethanol under ultrasonic irradiation (1h) yielded phthalazine-2-carbonitrile derivative (**5a**). The IR spectrum of **5a** revealed absorption bands at (3326, 3166), 2216, and 1661 attributed to NH_2, C≡N, and C=O groups, respectively. The ^{1}H-NMR spectrum showed three singlet signals at δ 3.46, 6.08 and 10.46 ppm attributed to O$C\underline{H}_3$, $C\underline{H}_{pyraz}$ and $N\underline{H}_2$ protons, respectively.

The evaluation of the cyclization reaction was continued through interaction with different aldehydes bearing electron-donating groups and electrons with drawing groups in their structures. The spectral data confirmed the formation of novel phthalazine-2-carbonitrile derivative (**5b-h**) (see Exp. section). The IR spectrum of (**5i**) revealed absorption bands at 3325, 3292, 3188 cm^{-1} related to (NH_2, NH) groups, 2200, and 1650 cm^{-1} attriubted to C≡N, and C=O groups, respectively, increase streching peaks in the NH_2 region due to symmetric and antisymmetric streching frequencies and NH_2=NH redox toutomerization leading to formation of the intra-molecular hydrogen bond as shown in the **Figure 1**. The structures of the two compounds were elucidated by their elemental and spectral analyses. ^{1}H-NMR spectrum of **5i** accounts two signals at δ 11.05 related to NH_2 group and at δ 12.65 related to NH group (50:50), respectively indicating the presence of the oxidation isomer. The presence of electron donating group (NMe_2) was enhanced the electron mobility with intra-molacular hydrogen bond and promoted the oxidation process.

DFT Study

High E_{HOMO} is recognized to imply a strong potential inclination for compounds to donate electrons. Good proficiencies will be purified by low energy gap values ($\Delta E=E_{LUMO}–E_{HOMO}$) since it will take less energy to remove an electron from LUMO.

A molecule's hardness or softness is determined by its ΔE value. Hard molecules are better at absorbing electrons when their ΔE values are high, and vice versa. The polarizability affinity distorted the original geometry of an electron cloud. When polarizability is higher, more inhibitor molecules will be accessible for absorption by an oxidized surface or radical through intramolecular electron transfer interactions [28,29]. As near as possible to the electron-donating group NMe_2, the authors noticed this in compound **5i**, where the cyano group's sp hybridization was twisted to create intramolecular hydrogen bonds and increase polarizability (**Figure 1** illustrates this). The computational chemical study can be helped us in the interpretation of the promotion of the oxidation process of amino group (E_{HO} = -8.20, E_{LU} = -1.18) and driving force to convert for the imino structure (E_{HO} = -8.49, E_{LU} -4.80) *via* formation of intra-molecular hydrogen bond with carbonyl of the phthalazine moiety.

From the optimized, HOMO and LUMO structures of the synthesized phthalazinone derivatives **5a-i** outlined in the **Fig. 1** to **Fig. 2**, the authors can be determined the binding energy, ionization potential, and electron affinity that be calculated hardness, softness and electrophilic index as shown in **Table 1**. The surface area, which supported the quantity of electron mobility and density in the produced phthalazinone, could be a reflection of these factors.

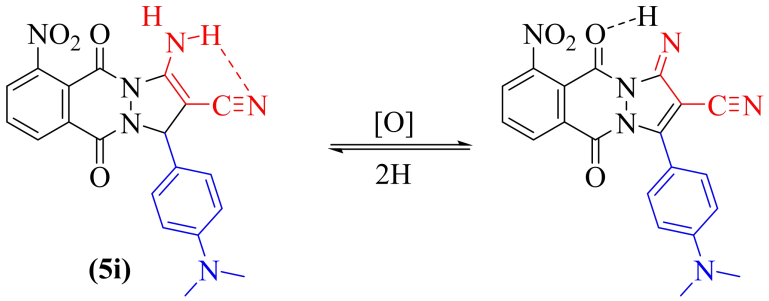
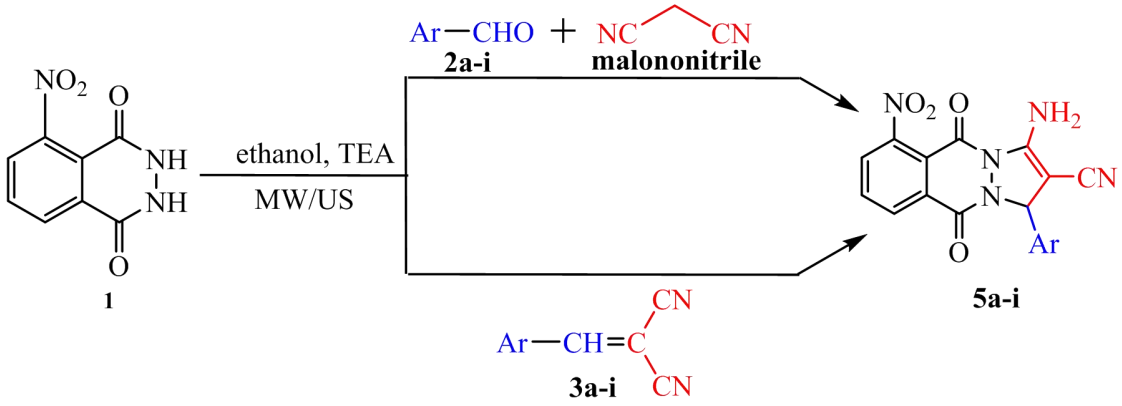
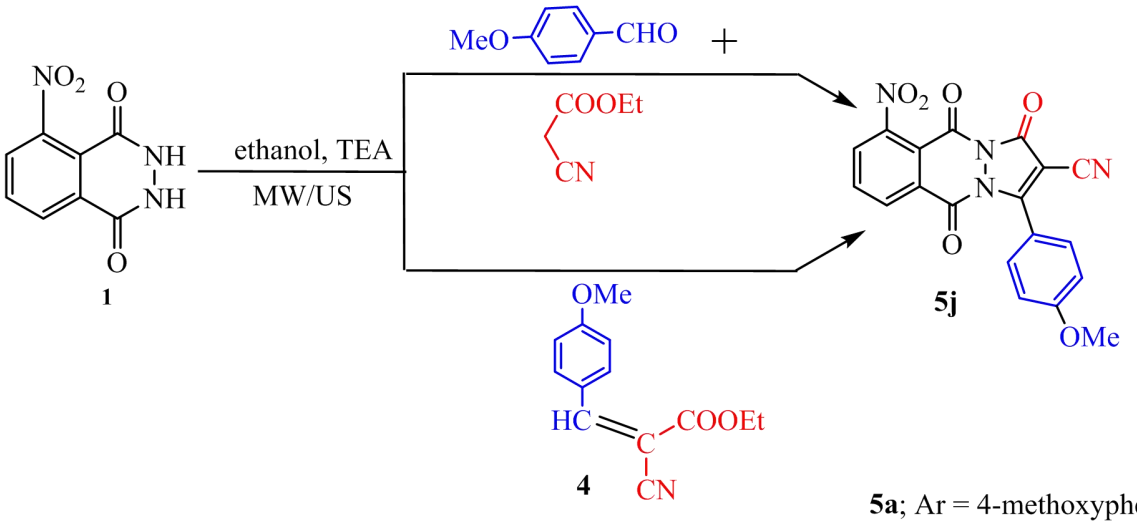


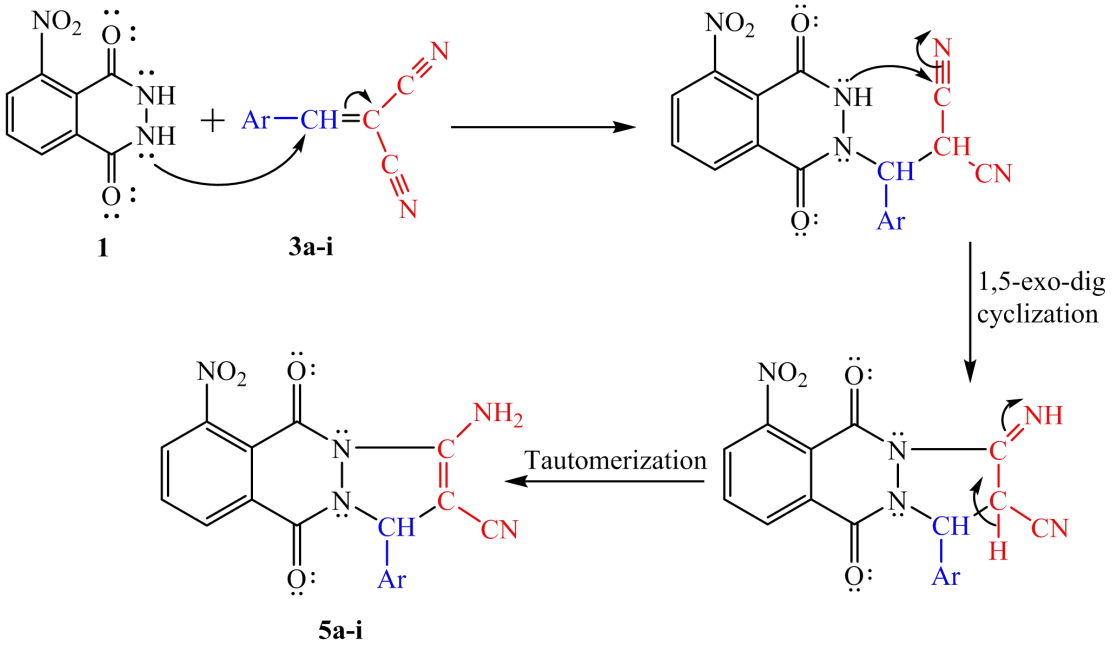
Figure 1. Outline the formation of the oxidation isomer due to enhancing the electron mobility by NMe_2 group supported by IR and ^{1}H-NMR spectra





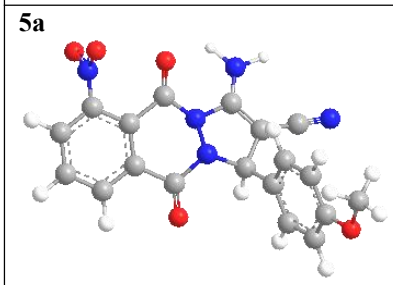
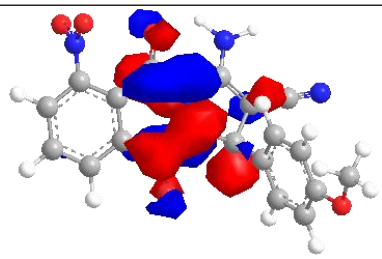
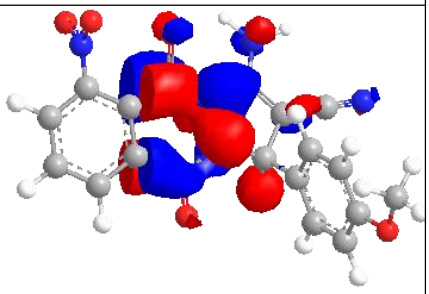
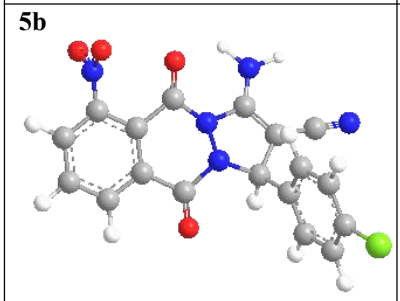
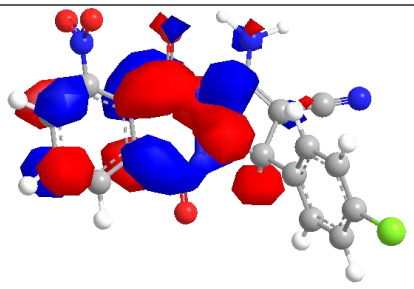
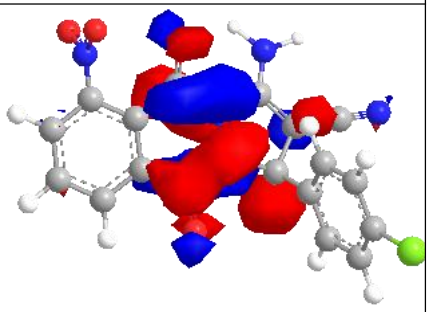
5a; Ar = 4-methoxyphenyl
5b; Ar = 4-chlorophenyl
5c; Ar = 2-bromophenyl
5d; Ar = 2-thiophenyl
5e; Ar = 1-hydroxy-2-naphthyl
5g: Ar = phenyl
5h; Ar = 3-nitrophenyl
5i; Ar = 4-(dimethylamino)phenyl

Scheme 1. Synthesis of 1H-pyrazolo[1,2-*b*]phthalazine-5,10 dione derivatives.



Scheme 2. The proposed mechanism of the formation of products (**5a-i)**

As outlined in the **Fig. 2**, the compound **5i** has full electron mobility and high surface area much more than the compound **5b** which serves and helps us in interpreting the antimicrobial results.
From the optimized, HOMO and LUMO structures of the synthesized phthalazinone derivatives **5a-j** outlined in the **Fig. 2**, the authors can be determined the binding energy, ionization potential, and electron affinity that be calculated hardness, softness and electrophilic index as shown in **Table 1**. These parameters could be reflected us the surface area that helped in strong-minded the amountof electron density and mobility in the synthesized phthalazinone. As outlined in the **Fig. 3**, the compound **5i** has full electron mobility and high surface area much more than the compound **5c** Which serves and helps us in interpreting the antimicrobial results.

Comp. No	HOMO	LUMO
5a			
5b			

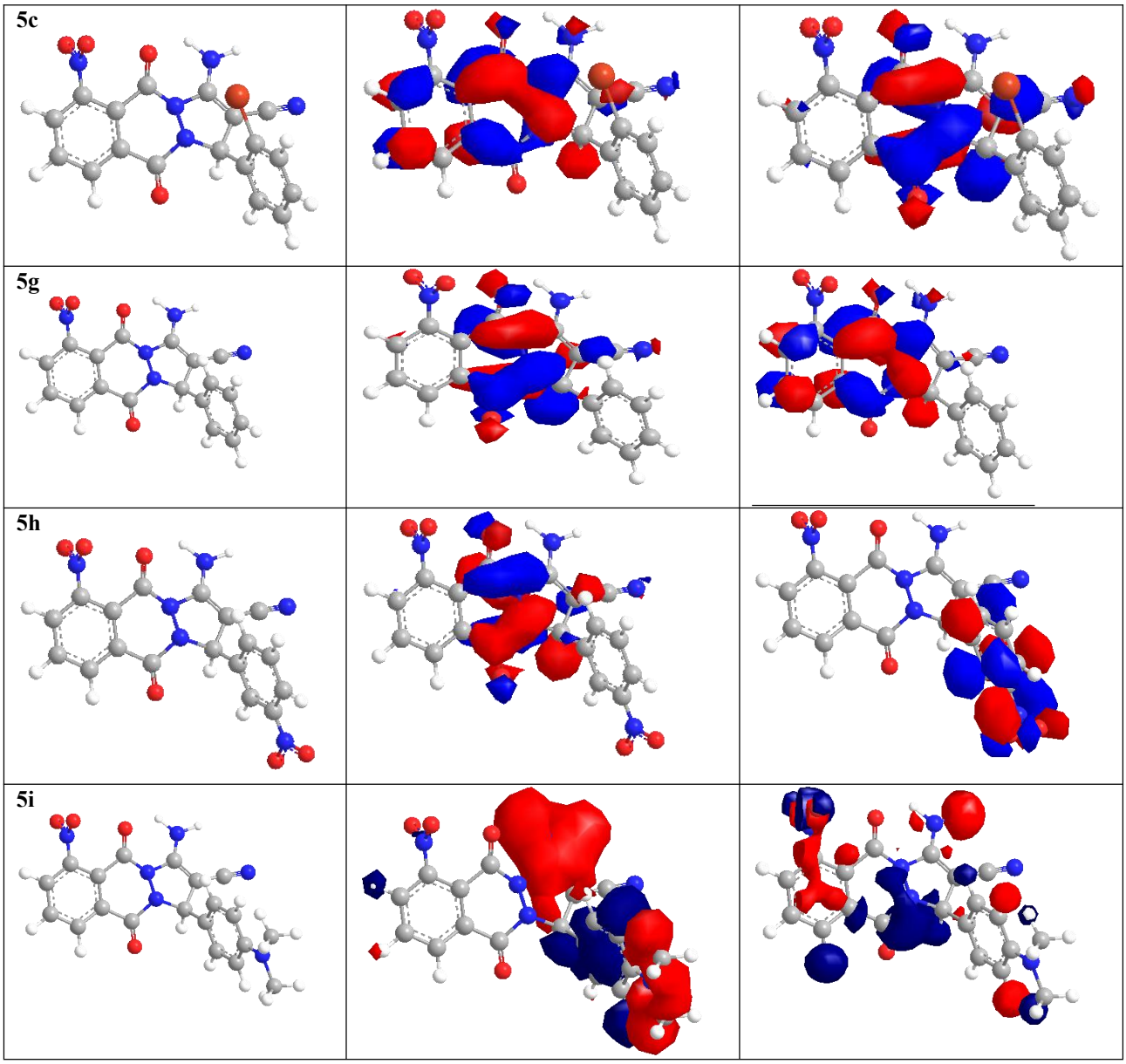


Fig. 2: HOMO-LUMO frontier orbital of the newly synthesized 1H-pyrazolo[1,2-*b*]phthalazine-5,10 dione derivatives (Red color represent positive phase while the blue the blue color points to the negative one).

Table 1: Global reactivity indices and energy level distribution of frontier orbitals

Comp. No	E_{HOMO}	E_{LUMO}	ΔE	I^a	A^b	μ^c	η^d	ω^e	ΔN	S^f	$A_{molec}(nm^2)$
5a	-8.57	-5.52	3.01	9.09	0.38	4.74	4.65	0.1068	0.26	8.790	597.443
5b	-5.57	-5.20	0.33	8.66	0.66	4.66	4.00	0.1491	0.38	12.139	590.401
5c	-8.13	-7.52	0.59	8.88	0.83	4.86	4.03	0.1300	0.34	11.558	442.608
5g	-3.47	-2.72	0.751	8.135	1.239	4.69	3.45	0.1281	0.31	9.395	519.866
5h	-7.54	-4.51	3.03	4.49	1.23	3.58	4.02	0.327	0.47	9.832	523.429
5i	-6.72	-6.52	0.20	6.69	6.38	0.74	2.65	0.1326	0.63	14.790	652.102

[a] Ionization potential, [b] Electron affinity, [c] Chemical potential, [d] Hardness, [e] Electrophilicity index, [f] Softness

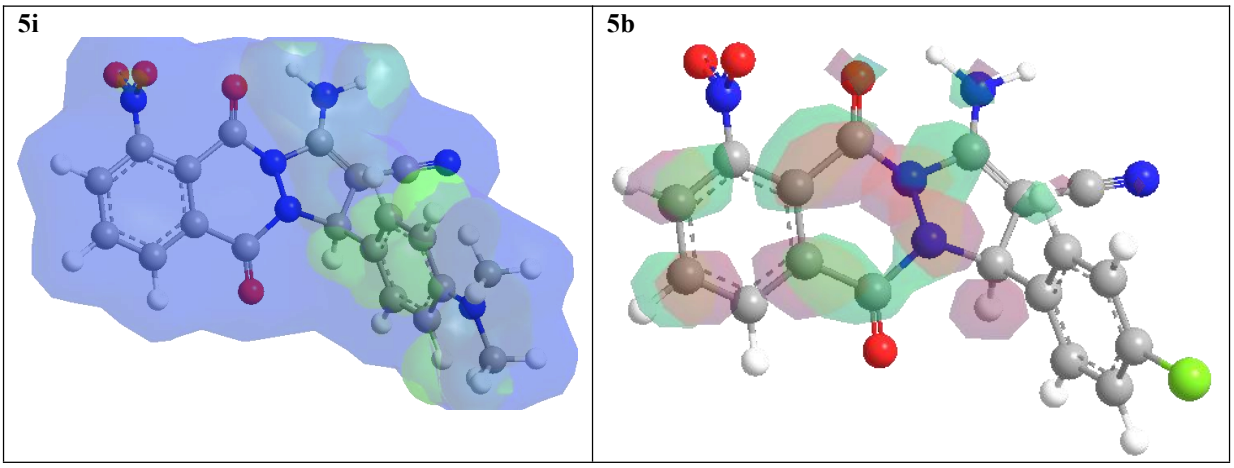


Fig. 3: Outline the electron denisty for the phthalazinone derivative **5b** and **5i** respectively

Antimicrobial studies

The disc diffusion method was utilized to assess the antibacterial assay of the synthesized **5a-j** compounds against four bacterial strains: *B. Subtilis* (MTCC 441), *B. Sphaericus* (MTCC 11), *S. Aureus* (MTCC 96) (+ve strains), and *P. Aeruginosa* (MTCC 741), in addition to two fungus strains, *C. Albicans* and *A. Fumigatus*.

Table 2, summarized the antibacterial and antifungal properties of the synthesized *1H*-pyrazolo[1,2-*b*]phthalazine-5,10-dione derivatives (**5a-j)**.

According to the antimicrobial data presented in **Table 2**, the majority of 1H-pyrazolo[1,2-*b*]phthalazine-5,10-dione derivatives had good effects, particularly **5a**, **5b**, **5c**, **5g**, **5h** and **5i**.

Table 2: Antibacterial and antifungal properties of the synthesized 1H-pyrazolo[1,2-b]phthalazine-5,10-dione derivatives **5a–j**.

3.

Compounds No.	MZI in 100 µg/mL (Mean Zone Inhibition)					
	A	B	C	D	E	F
5a	27	27	24	26	24	22
5b	32	30	32	27	27	28
5c	31	29	32	27	27	29
5d	15	13	17	12	0	5
5e	13	11	14	10	2	7
5g	22	20	18	20	22	18
5h	31	28	32	27	27	28
5i	32	31	33	30	[29]	31
5j	21	18	16	22	8	13
Amphotericin B	32	32	34	33	32	30
Streptomycin	32	31	33	28	-	-

Amphotericin B, Streptomycin and **5a-j** *compounds 100 µg/disc.* **A-** *B. Subtilis,* **B-** *B. Sphaericus,* **C-** *S. Aureus,* **D-** *P. Aeruginosa,* **E-** *C. Albicans, and* **F-** *A. Fumigatus*

Experimental

Unless otherwise indicated, all reactions involving reagents that were sensitive to air or moisture were conducted in flame-dried glassware in an argon environment. Prior to use, CH_2Cl_2, $(CH_3)_2CO$, MeOH, and dimethyl sulfoxide (DMSO) were distilled in accordance with normal procedures. Unless specified otherwise, additional reagents were bought and used just as supplied, requiring no additional purification. Thin layer chromatography

was used to monitor the reactions, which were magnetically stirred and used 0.15–0.2 mm pre-coated silica gel (10–40 μm) plates. Compounds were seen by heating them on a hot plate, staining them with ethanolic phosphomolybdic acid, or both. Under pressure, flash chromatography (FC) was carried out using silica gel (60–200 mesh). Using a CHN analyzer, elemental analyses were conducted, and all chemicals were found to be within ± 0.4 of their theoretical values. Using tetramethyl silane as the internal standard, nuclear magnetic resonance (NMR) spectra were captured using Bruker-250 or AMX 500 spectrometers in DMSO-d_6. Coupling constants (J) are given in Hz, and chemical shifts (δ) in ppm. These symbols denote multiplicity: s for singlet; d for doublet; t for triplet; q for quartet; m for multiplet; and br for broad. Mass spectra were recorded on a Shimadzu GC–MS-QP 1000X spectrometer operating at 70eV.

3-Amino-6-nitro-1-aryl-5,10-dioxo-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile5a-j

A mixture of the 5-nitro-2,3-dihydrophthalazine-1,4-dione (**1**) (2.07 g, 0.01 mol), different aromatic aldahydes (**2**) (0.01 mole), malononitrile (0.66 g, 0.01 mol) or ethyl-2-cyanoacetate (1.13 g, 0.01 mol) dissolved in (30 ml) absolute ethanol was refluxed for 30 min under microwave-ultrasonic irradiation. Then cooling, and the formed solid was filtered, washed with water, dried and recrystallized from ethanol to give compound (**5a-j**).

3-Amino-1-(4-methoxyphenyl)-6-nitro-5,10-dioxo-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile (5a)

Yield 90%, brown powder; mp 196–198 °C; IR (cm^{-1}) *ν*: 3326, 3166 (NH_2), 3061 (CH aromatic), 2898 (CH aliphatic), 2216 (C≡N), 1661 (C=O), 1602 (C=N); ^{1}H-NMR (DMSO-d_6, δ ppm): 3.46 (s, 3H, OCH_3), 6.08 (s, 1H, CH_{pyraz}), 6.98- 6.87 (m, 4H, Ar-H), 7.85-7.4 (d, J = 2.4, 2H, Ar-H), 7.86 (s, 1H, Ar-H); 10.46 (s, 2H, NH_2, D_2O exchangeable with D_2O). MS (m/z): 391 ($M^{\cdot+}$, 22.36%); Anal. Calcd for: $C_{19}H_{13}N_5O_5$: C, 58.31; H, 3.35; N, 17.90; Found: C, 58.11; H, 3.30; N, 17.83%.

3-Amino-1-(4-chlorophenyl)-6-nitro-5,10-dioxo-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile (5b)

Yield 85%; yellow crystals; mp. 220-222 °C. IR (cm^{-1}) *ν*: 3328, 3209 (NH_2), 2922 (CH aromatic), 2214 (C≡N), 1630 (C=N). ^{1}H-NMR (DMSO-d_6, δ ppm): 6.19 (s, 1H, CH_{pyraz}), 7.21-7.24 (m, 1H, Ar-H), 7.33-7.62 (m, 4H, Ar-H), 7.70-7.88 (m, 1H Ar-H), 8.02-7.92 (m, 1H Ar-H), 11.47 (s, 2H, NH_2, exchangeable with D_2O); MS (m/z): 395.8 ($M^{\cdot+}$, 19.29%); Anal. Calcd for: $C_{18}H_{10}ClN_5O_4$: C, 54.63; H, 2.55; N, 17.70; Found: C, 54.54; H, 8.90; N, 17.62%.

3-Amino-1-(2-bromophenyl)-6-nitro-5,10-dioxo-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile (5c)

Yield 85%; yellow crystals; mp. 210-212 °C; IR (cm^{-1}) *ν*: 3323, 3166 (NH_2), 2924 (CH aromatic), 2213 (C≡N), 1791, 1731 (C=O), 1618 (C=N). ^{1}H-NMR (DMSO-d_6, δ ppm): 6.20 (s, 1H, CH_{pyraz}), 6.78-8.37 (m, 7H, Ar-H), 11.65 (s, 2H, NH_2, exchangeable with D_2O); MS (m/z): 440.2 ($M^{\cdot+}$, 30.19%); Anal. Calcd for: $C_{18}H_{10}BrN_5O_4$: C, 49.11; H, 2.29; N, 15.91; Found: C, 49.00; H, 2.22; N, 15.81%.

3-Amino-6-nitro-5,10-dioxo-1-(thiophen-2-yl)-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile (5d)

Yield 68%; yellow crystals; mp. 216-219 ºC (MeOH). IR (cm^{-1}) *ν*: 3323, 3166 (NH_2), 3020 (CH aromatic), 2903 (CH aliphatic), 2209 (C≡N), 1662 (C=O), 1606 (C=N). ^{1}H-NMR (DMSO-d_6, δ ppm): 6.17 (s, 1H, $CH_{pyrazole}$), 6.41-6.86 (m, 3H, Ar-H), 7.31-8.86 (m, 3H, Ar-H), 11.65 (s, 2H, NH_2, exchangeable with D_2O). MS (m/z): 367.5 ($M^{\cdot+}$, 26.33%); Anal. Calcd for: $C_{16}H_9N_5O_4S$: C, 52.32; H, 2.47; N, 19.07; Found: C, 52.20; H, 2.40; N, 19.01%.

3-Amino-1-(1-hydroxynaphthalen-2-yl)-6-nitro-5,10-dioxo-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile (5e)

Yield 75%; yellow crystals; mp. 200-202 °C; IR (cm^{-1}) *ν*: 3354, 3214 (NH_2), 2923 (CH aromatic), 2201 (C≡N), 1662 (C=O), 1626 (C=N). ^{1}H-NMR (DMSO-d_6, δ ppm): 7.13-7.55 (m, 7H, Ar-H), 7.61-8.34 (m, 3H Ar-H), 10.73 (br. s, 2H, NH_2, exchangeable), 11.53 (br.s, 1H, OH, exchangeable with D_2O); MS (m/z): 433.5 ($M^{\cdot+}$, 27.32%); Anal. Calcd for: $C_{22}H_{13}N_5O_5$: C, 61.83; H, 3.07; N, 16.39; Found: C, 61.63; H, 3.00; N, 16.31%.

3-Amino-6-nitro-1-phenyl-5,10-dioxo-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile (5g)

Yield 80 %; yellow crystals; mp. 208-210 °C; IR (cm^{-1}) *ν*: 3104 (NH), 3015 (CH aromatic), 2933 (CH aliphatic), 2222 (C≡N), 1733, 1671 (2C=O), 1600 (C=N); ^{1}H-NMR (DMSO-d_6, δ ppm): 6.23 (s, 1H, CH_{pyraz}), 7.13-7.62 (m, 5H Ar-H), 7.61-7.64 (m, 1H, Ar-H), 7.70-7.88 (m, 1H Ar-H), 8.02-8.12 (m, 1H Ar-H), 11.47 (s, 2H, NH_2, exchangeable with D_2O); MS (m/z): 361 ($M^{\cdot+}$, 32.24%); Anal. Calcd for: $C_{18}H_{11}N_5O_4$: C, 52.81; H, 2.71; N, 17.11; Found: C, 52.61; H, 2.62; N, 17.05%.

3-Amino-6-nitro-1-(3-nitrophenyl)-5,10-dioxo-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile (5h)

Yield 78 %; yellow crystals; mp. 222-224 °C; IR (cm^{-1}) *ν*: 3164 (NH), 3017 (CH aromatic), 2899 (CH aliphatic), 2210 (C≡N), 1662 (C=O); ^{1}H-NMR (DMSO-d_6, δ ppm): 6.20 (s, 1H, CHpyraz), 7.38-7.77 (m, 3H, Ar-H), 7.78-

8.07 (m, 3H, Ar-H), 8.08-8.37 (m, 1H, Ar-H), 11.65 (s, 2H, NH_2, exchangeable with D_2O). MS (m/z): 406.2 (M^{+}, 25.16%); Anal. Calcd for: $C_{18}H_{10}N_6O_6$: C, 56.39; H, 2.47; N, 14.30; Found: C, 56.21; H, 2.40; N, 14.22%.

3-Amino-1-(4-(dimethylamino)phenyl)-6-nitro-5,10-dioxo-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2-carbonitrile (5i)

Yield 85%; yellow crystals; mp. 212-217 °C, IR (cm^{-1}) *v.* 3325, 3292 (NH_2), 3030 (CH aromatic), 2918(CH aliphatic), 2200 (C≡N), 1650 (C=O). ^{1}H-NMR (DMSO-d_6, δ ppm): 3.32 (s, 6H, $2CH_3$), 6.20 (s, 1H, CHpyraz), 6.78-7.37 (m, 4H, Ar-H), 7.38-7.87 (m, 3H, Ar-H), 11.05 (s, 2H, NH_2, exchangeable), 12.65 (s, 1H, NH, exchangeable with D_2O); MS (m/z): 404.2 (M^{+}, 19.36%); Anal. Calcd for: $C_{20}H_{16}N_6O_4$: C, 56.79; H, 2.90; N, 17.28; Found: C, 56.64; H, 2.81; N, 17.21%.

3-(4-Methoxyphenyl)-9-nitro-1,5,10-trioxo-5,10-dihydro-1H-pyrazolo[1,2-b]phthalazine-2 carbonitrile (5j)

Yield 88%; yellow crystals; mp. 242-245 °C (MeOH); IR (cm^{-1}) *v.* 3015 (CH aromatic), 2933 (CH aliphatic), 2222 (C≡N), 1733, 1671 (C=O), 1600 (C=N); ^{1}H-NMR (DMSO-d_6, δ ppm): 3.66 (s, 3H, OCH_3), 7.33-7.62 (m, 4H Ar-H), 7.70-7.88 (m, 1H, Ar-H), 7.92-8.02 (m, 2H, Ar-H). MS (m/z): 390.8 (M^{+}, 45.36%); Anal. Calcd for: $C_{19}H_{10}N_4O_6$: C, 52.81; H, 2.71; N, 17.11; Found: C, 52.67; H, 2.62; N, 17.02%.

4. Conclusion:

In an attempt to uncover potential antibacterial abilities, MW/US methods can aid in the synthesis, purification, and remarkable flexibility and generated in good yields of 1H-pyrazolo[1,2-*b*]phthalazine-5,10-dione derivatives. After that, they were described using mass, IR, and ^{1}H-NMR methods. In addition to two fungal strains, *C. Albicans* and *A. Fumigatus*, these antimicrobial compounds were additionally evaluated against *B. Subtilis* (MTCC 441), *B. Sphaericus* (MTCC 11), *S. Aureus* (MTCC 96) (+ve strains), and *P. Aeruginosa* (MTCC 741). In order to justify the energy gap, polarizability, and binding site interactions, computational chemistry was first determined. These results were obtained on a novel derivative (**5i**), which was arranged to a more bioactive oxidized structure.

Conflict of interest

No conflict of interest.

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