



# Design and Synthesis of Novel Organic Compounds: A Comprehensive Study on Structural Elucidation and Characterization

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This study involved aniline subordinates in cold acidic corrosive as the dissolvable to orchestrate nitro-subbed phthalimide analogs (1a-1e) and (2a-2e). With a focus on structural elucidation and characterization through a variety of approaches, the chapter provides a thorough description of the synthetic process, including methodology, analytical characterization, and reaction attempts. As displayed in Plan 1, the last segment gives a careful show of the ghastly information essential for the characterization of the combined compounds. These synthetic substances were made by responding 3-nitrophthalic anhydride at high temperatures with various toluidine subordinates. Section chromatography was utilized to filter the combined items while thin-layer chromatography (attention) was utilized to follow the responses' advancement. Despite regular assessment and condensing point affirmation, the reach characterization contained infrared (IR), proton nuclear magnetic resonance ( $^1\text{H}$  NMR), and carbon-13 nuclear magnetic resonance ( $^{13}\text{C}$  NMR) assessments. To summarize, this examination surveys the expected antibacterial action of novel nitro-subbed phthalimide analogs and offers bits of knowledge into their design, synthesis, and characterization. The outcomes highlight expected utilizes for these substances, particularly in the treatment of bacterial and contagious sicknesses, which calls for more examination to explain their methods of activity and expand their helpful adequacy.

**Keywords:** Novel Organic Compounds, nuclear magnetic resonance, Minimum Inhibitory Concentration, including infrared, carbon-13, Design And Synthesis, maximal electroshock, thin-layer chromatography, Structural Elucidation And Characterization.

## 1. Introduction

The examination concerning novel organic compounds is a key pursuit in contemporary logical exploration, offering significant experiences into structural elucidation, characterization techniques, and their noteworthy ramifications on natural frameworks. Within the space of pharmacology, the investigation of natural movement expects principal significance, requiring a complicated examination of the nuanced balance between the invaluable and unfriendly impacts of drug specialists on living creatures (Wade, 2008). This investigation includes the careful measurement of medication communications with cell parts,

integrating contemplations like partiality, adequacy, and complicated elements across different tissues under factor conditions. Within the broad scene of organic synthesis, our center meets upon a particular class of compounds that assumes a significant part in the development of naturally dynamic atoms - Phthalimides. Perceived as subsidiaries of isoindoline-1,3-dione, Phthalimides stand as imperative elements within organic manufactured science, filling in as primary substrates. This talk tries to highlight the essentialness of Phthalimides in our examination, explaining their manufactured pathways, sub-atomic construction, and their considerable commitments to the age of a different cluster of naturally dynamic particles (McMurry, 2012).

The synthesis of Phthalimides, usually accomplished through different organic strategies using phthalic anhydride, yields a compound with an unmistakable cyclic, fragrant imide structure lodging two carbonyl gatherings fastened to an amine practical gathering. The remarkableness of Phthalimides lies in their critical occupation as building blocks for the association of a lot of organically unique blends, each depicted by the general design - CO-N(R)- CO-. This talk plans to unwind the nuanced complexities of Phthalimides in the more extensive setting of organic synthesis, with accentuation on their hydrophobic and nonpartisan credits, delivering them important in the making of different bioactive particles (Nagarkar, 2014).

➤ **Biological Activity in Pharmacology:**

Natural action in pharmacology is a nuanced idea, enveloping the valuable and unfriendly impacts of medications on living organic entities. The power or concentration expected for a particular sub-atomic element to evoke a characterized natural impact is a basic measure. Organic action is surveyed through measures that uncover how medications collaborate with cell parts, including proteins, compounds, receptors, nucleic acids, and bio films (Ranganathan, 2013). The intricacy of medication conduct in various tissues under different circumstances is affected by elements like proclivity, viability, and the cell climate. This conversation underscores the measurement of organic action as well as investigates the difficulties looked by pharmacologists in foreseeing drug impacts in helpful settings, resolving issues like tissue-explicit medication ways of behaving and naturally prompted fluctuation (Maharana, 2011).

➤ **Microorganisms and Their Influence on Human Life:**

Microorganisms apply significant effects on human existence, forming the climate and impacting different parts of society. They assume vital parts in the creation of food, meds, and synthetic substances. While offering various advantages, microorganisms are additionally connected with illnesses that influence people, creatures, and plants (Chauhan, 2020). Understanding their exercises is vital, taking into account their job in food decay, sicknesses like Guides and flu, and their authentic importance in fighting, religion, and populace relocations. The message features the double idea of microorganisms, recognizing their expected risks while perceiving their fundamental commitments to mankind's set of experiences and day to day existence (Kumari, 2009).

➤ **Bioactive Compounds and Drug Development:**

The conversation on natural movement stretches out to bioactive compounds, stressing their cooperation with cell tissues in the human body. During the time spent growing new

medications, a compound's not entirely settled by meeting the ADME (Retention, Dissemination, Digestion, and Discharge) prerequisites notwithstanding its capacity to focus on a goal successfully). The text focuses on the significance of bioactive substances having appropriate ADME properties to be viewed as compelling medications. Also, the measurements subordinate nature of movement and the likely scope of impacts, from valuable to unfriendly, are urgent contemplations in drug improvement and clinical applications. This knowledge gives a more exhaustive comprehension of the complexities engaged with creating bioactive compounds for helpful use (Varaprasad, 2011).

By digging further into these particular perspectives, we improve our appreciation of the diverse idea of organic action, microorganisms, and the advancement of bioactive compounds in the area of pharmacology (Harisha M. B., 2019).

### 1.1. Phthalimides

Phthalimides, likewise perceived as subordinates of isoindoline-1,3-dione, are blended through different organic strategies, regularly using phthalic anhydride simultaneously. Addressed in Figure 1, phthalimide is a translucent white strong with feeble sharpness, highlighting a cyclic, fragrant imide structure with two carbonyl gatherings connected to an amine utilitarian gathering. For organic synthesis scientific experts, this substance is a fundamental structure block since it very well might be utilized to make various naturally dynamic compounds with the overall recipe - CO-N(R)- CO-. These compounds are unbiased and hydrophobic (Prathap, 2011).

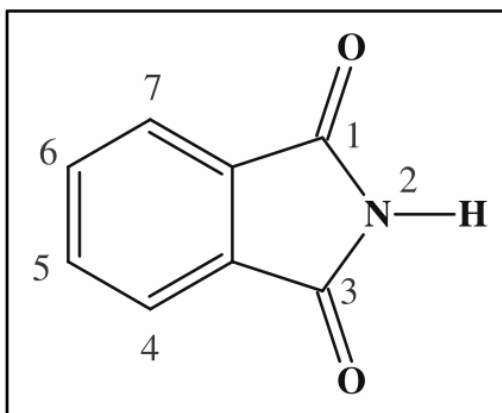


Figure 1: Phthalimide (isoindoline-1,3-dione)

Notable nucleophilic characteristics of the phthalimide anion allow it to be treated with intense potassium hydroxide solution ( $K_a = 5 \times 10^{-9}$ ) to generate a potassium salt. This potassium salt is used in the Gabriel Synthesis, a chemical process that turns primary alkyl halides into primary amines and is shown in Scheme 1 (Prathap, 2014).

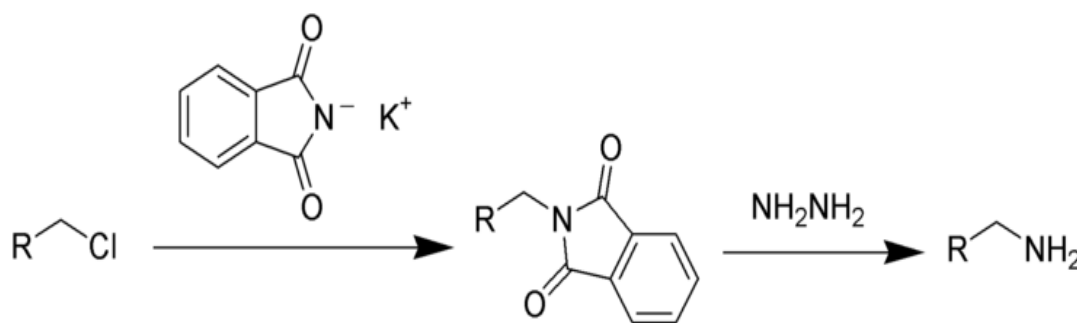


Figure 2: Gabriel synthesis

The Gabriel Synthesis is important because it can yield primary amines without contaminating secondary or tertiary amines, works with a broad variety of functional groups, and uses gentle conditions in both stages (Prathap, 2011).

Phthalimides provide exceptional mechanical characteristics, heat resistance, solvent resistance, and oxidative stability. On the other hand, they proceed through the Hofmann reaction (Scheme 2), which results in N-haloamides through hydrolytic ring-opening. These are created by rearranging either free imides or N-haloimides to produce anthranilic acids (Hirsch, 2005).

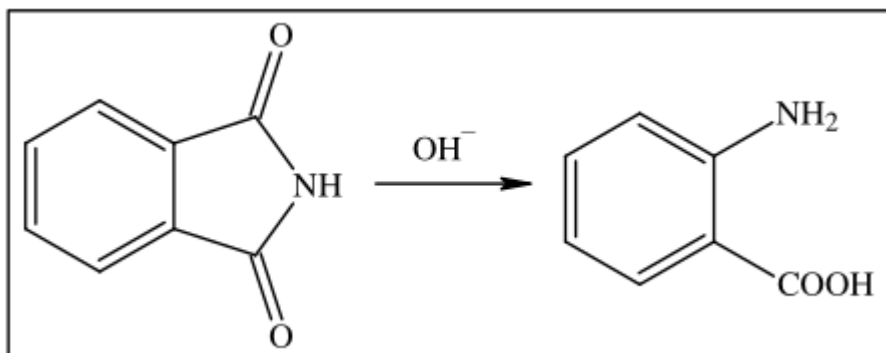


Figure 3: Hoffmann degradation of phthalimide

#### ➤ Applications:

Because of their biological and pharmacological properties, heterocyclic molecules containing nitrogen have garnered a lot of attention. Phthalimides and their N-substituted derivatives are heterocyclic compounds with an imide ring that have a variety of biological functions. Also known as isoindoline-1,3-dione, phthalimide is a naturally occurring substance that is necessary for life (Nishy, 2011).

Important intermediates in the synthesis of functionalized natural products and alkaloids, such as nuevamine, chilenine, lennoxamine, and magallanesine, have been these substances. A growing body of research in medicinal chemistry has focused on isoindole-1,3-dione derivatives because of their important medicinal properties, which include analgesic,

antifungal, antibacterial, antimicrobial, antitumor, anticonvulsant, anti-inflammatory, hypoglycemic, androgen receptor antagonistic, anxiolytic, anti-HIV-1, anthelmintic, anticancer, and antiviral properties. The following highlights a number of medical uses along with illustrative illustrations (Duan, 2013).

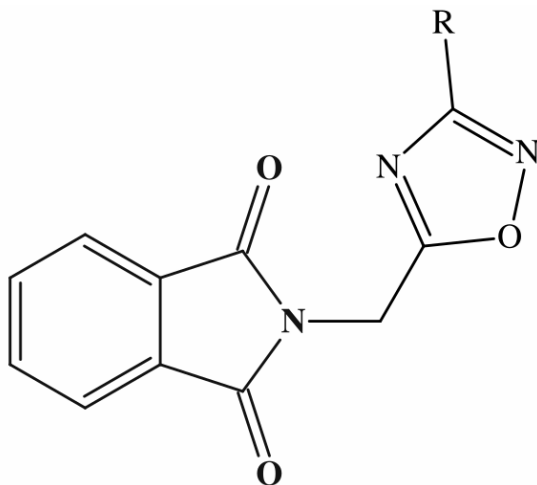


Figure 4: Isoindoline-1,3-dione based analgesic compounds

Jeong et al.'s synthesis of compound 10, which exhibits increased anticancer activity, shows that phthalimide-based polymers are effective antitumor agents (Park, 2015).

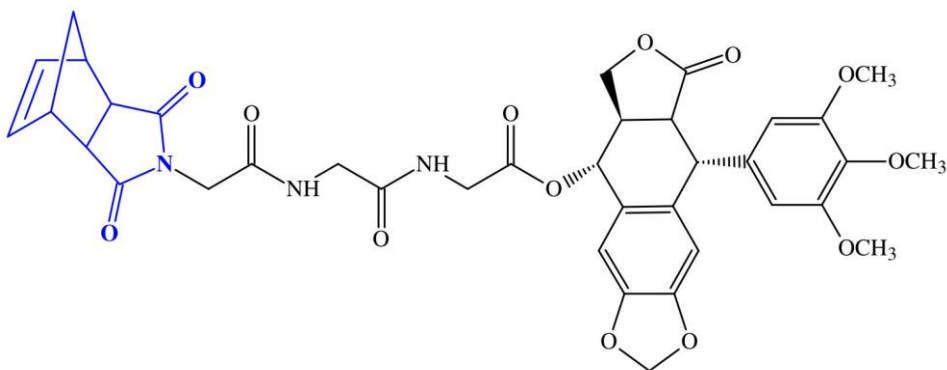


Figure 5: Phthalimide based antitumor compounds

The maximal electroshock (MES) test has demonstrated strong activity for a number of N-phenyl phthalimides. Displays two instances of anticonvulsant drugs based on phthalimides (11, 12).

Using streptozocin-induced hyperglycemic rats, S. P. Mahapatra synthesised 3-phthalimidoethyl 4-substituted cinnamoyl substituted benzanilides (Bazan, 2007). These compounds were then tested for their hypoglycemic efficacy in vivo. These compounds showed notable hypoglycemic action in vivo (Harisha, 2014).

Thalidomide's phthalimide component, a sedative and glutamic acid derivative, is known to

*Nanotechnology Perceptions* Vol. 20 No.S4 (2024)

have anti-HIV properties. This activated monocytoid cell line shown anti-HIV efficacy. The 1950s saw the development of thalidomide, also known as  $\alpha$ -N-(phthalimido) glutarimide,  $C_{13}H_{10}N_2O_4$ , by the West German pharmaceutical company "Grünenthal." Its strong anti-myeloma action has been confirmed by several recent clinical trials, and early trials suggest that it may be useful in treating a number of malignant illnesses (Harisha M. B., 2019).

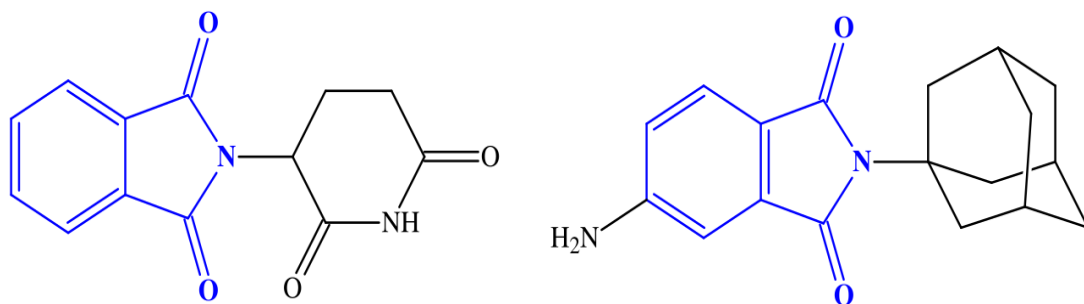


Figure 6: Phthalimide based anti-HIV compounds

N-phenyl phthalimide subordinates having perceptible selectivity files against human cells and inhibitory impacts against *Plasmodium falciparum* (touchy and safe strains) in the low micromolar range have been blended by V. S. Bolzani. *Pneumocystis jirovecii* pneumonia is dealt with and forestalled with quinone antimicrobial medication atovaquone. Its sluggish acting system is similar to that of atovaquone, the best inhibitor, 4-amino-2-(4-methoxyphenyl) isoindoline-1,3-dione (Harisha M. B., 2018).

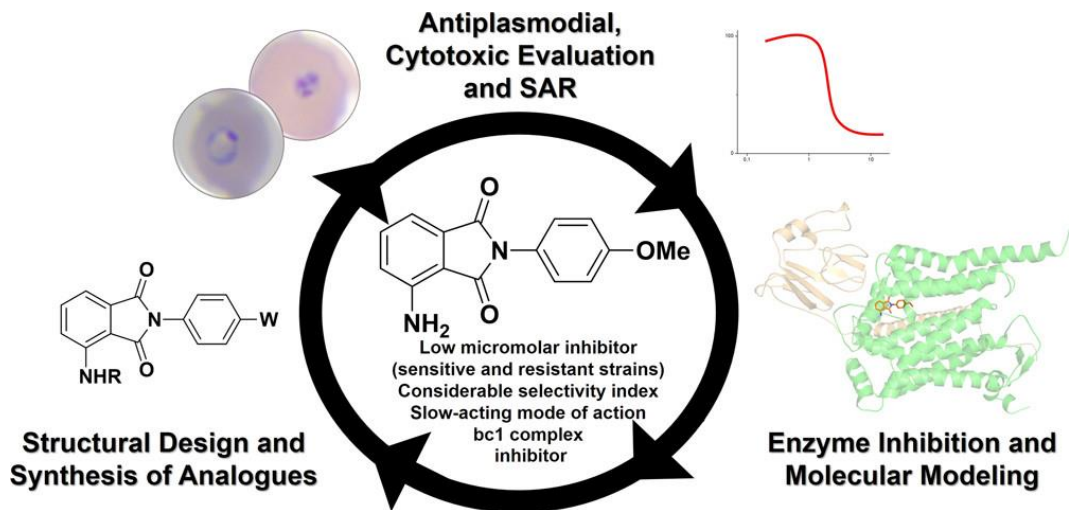


Figure 7: Phthalimide analogue exhibiting antiviral bioactivity

Source: <https://doi.org/10.1021/acsomega.8b01062>

### Significance of the study

The study of the design and synthesis of novel organic compounds, in conjunction with exhaustive structural elucidation and characterization, is of great importance in the advancement of scientific knowledge and practical applications. The discovery of unique  
*Nanotechnology Perceptions* Vol. 20 No.S4 (2024)

properties and reactivities is the result of the expansion of the chemical space by researchers through the development of innovative chemical structures. This examination is fundamental for the progression of drug improvement, as it works with the ID of novel medications with upgraded adequacy and designated treatments with decreased incidental effects. The improvement of cutting edge materials with particular properties, like upgraded conductivity and novel optical attributes, is worked with by it in the field of material science. Also, it is fundamental for the execution of nanotechnology.

Another basic viewpoint is the natural effect, as the improvement of ecologically harmless compounds advances economical substance cycles and contamination control, in this manner adding to cleaner air and water. In the horticultural area, the advancement of new compounds can bring about the improvement of plant development control and the improvement of additional powerful pesticides and herbicides, subsequently expanding agrarian efficiency. Headways in polymer science and upgraded adequacy and cost-viability in substance fabricating are beneficial to modern applications.

This study is an important asset for the schooling of future researchers, as it advances an interdisciplinary methodology that consolidates science, science, physical science, and materials science to prepare them in organic synthesis and characterization strategies. This exploration likewise invigorates innovative headways, including the improvement of novel impetuses for synthetic responses and the progression of adaptable hardware and OLEDs. In general, the design and synthesis of new organic compounds, as well as their structural elucidation and characterization, are essential for the advancement of science and society, with a significant impact on industrial technology, agriculture, healthcare, and environmental sustainability.

## **2. Literature Review**

Das, S., Heasman, P., Ben, T., & Qiu, S. (2017) To track down reasonable applications and give a careful comprehension of the essential development of the plan and engineered approaches of permeable natural materials with tunable qualities, blend the new huge leap forwards and the customary capabilities and practices in the field of permeable natural materials. With an emphasis on the geographies of translucent and shapeless permeable natural materials, this work gives an exhaustive examination of the plan philosophies. Aside from explaining the connection among structure and capability and the latest purposes of permeable natural materials, we likewise talk about the snags and impediments that substitute the approach to creating permeable natural materials with redid models and attributes for pragmatic purposes (Das, 2017).

Liu, Y., Huang, Y., Zhu, R., Farag, M. A., Capanoglu, E., & Zhao, C. (2023) The constraints of the current technologies and the necessary future advancements for overcoming these limitations and enhancing identification score and/or yield were taken into consideration in conclusion. There has been a sharp increase in interest in carbohydrates and how they affect human health. A more accurate evaluation of carbohydrates and their pharmacological effects has been made possible by significant advancements in analytical techniques. Creating a method for measuring carbs would undoubtedly help us comprehend how diet affects our



intake of carbohydrates. It is now more practical to synthesise these chemicals rather than isolate them because to advancements in characterisation and complex structure discovery technology. Improved analytical instruments, glycomics, and automation technologies, among other technological advancements, have created new avenues for the worldwide evaluation of the majority of carbs in samples that are anticipated. The primary analytical techniques used on carbohydrates are explained (Liu, 2023).

Salardón-Jiménez, N., Zagrodzki, P., Paško, P., Domínguez-Álvarez, E., Sevilla-Hernández, C., Sanmartín, C.,... & Gorinstein, S. (2022) This work aimed to synthesise many novel organic selenium compounds (selenoesters), assess their efficacy in providing selenium to Brassica sprouts, and look into the metabolism of these compounds in sprouts. Our findings demonstrated that the fortified sprouts had a selenium level several orders of magnitude higher than the unfortified ones. The dosages of selenium that sprouts received from various selenium compounds varied significantly. Seleno-L-methionine, Se(IV), and Se-methylselenocysteine were added to the sprouts in small amounts (less than 10%) as supplemented selenium. Various other low molecular weight species of selenium were also identified, varying in amounts based on the compound utilised in the fortification process. Finally, it can be said that new selenium-containing compounds were effectively used to strengthen kale sprouts. Their low molecular weight metabolites and derivatives have not been previously described in the Brassica genus. This includes their identification, screening, and characterisation (including the elucidation of their structures) (Zagrodzki, 2022).

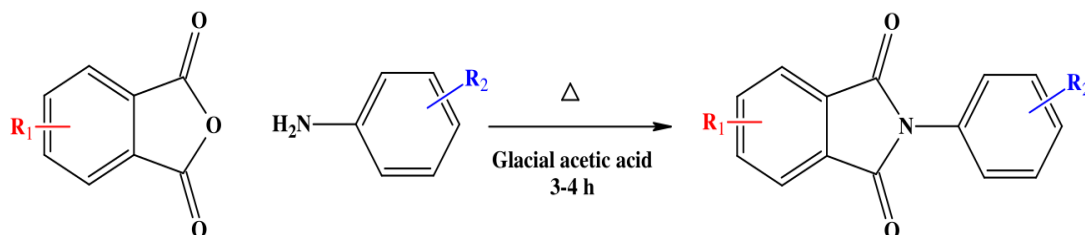
Henson, Z. B., Bazan, G. C., Welch, G. C., and Coughlin, J. E. (2014) The utilization of natural semiconductors in sunlight based cells with a bulk heterojunction (BHJ) design holds potential as a greener answer for the world's developing energy requests. Throughout the course of recent years, natural sunlight based cells based on the BHJ engineering have shown a consistent improvement in gadget execution, with power change efficiencies outperforming 10%. An enormous part of this accomplishment might be credited to formed polymer/fullerene pairings, where major mechanical forward leaps have been made conceivable by improved polymer plan strategies, engineered conventions, gadget fabricating systems, and characterisation methods. Since they are simpler to functionalize, more amiable to traditional natural cleansing and portrayal strategies, and have less cluster to-bunch fluctuation than their polymer counterparts. (Coughlin, 2014).

Mirza, M. U., and Froeyen, M. (2020) Potential medications that especially target Nsp12 RNA polymerase, Nsp13 helicase, and the essential protease — all fundamental SARS-CoV-2 proteins — were accounted for in the review. Finding conceivable restricting modes and the going with mixtures' good atomic association profile has been made more straightforward by an incorporated virtual screening and sub-atomic elements reproductions method. Moreover, in light of remaining energy disintegration examination, the overall significance of ligand restricting is featured by the distinguishing proof of basically huge restricting site buildups in preserved themes inside the dynamic site. The underlying information from this computational work has opened the entryway for the advancement of explicit inhibitors to address the Coronavirus flare-up, even though the ongoing review requires trial approval (Mirza, 2020).



### 3. Methodology

Our objective was to make the nitro-subbed phthalimide analogs (1a-1e) and (2a-2e) by involving frosty acidic corrosive as a dissolvable and aniline subordinate. Detailing the synthetic process, including technique, analytical characterization, and attempted reactions, is the main focus of this chapter. The spectrum data that help the characterization of the synthesized compounds are included in the latter section (Scheme 1).



Scheme 1: Isoindoline-1,3-dione analogues replaced with nitro

#### 3.1. Materials and Methods

The mixtures were noticeable under UV light and iodine, and the responses were followed utilizing tender loving care examination on silica gel plates (eluent: petrol ether - ethyl acetic acid derivation in various proportions).

Three nicothalic anhydride (0.50 g, 2.59 mmol), a subsidiary of toluidine (0.28 g, 2.59 mmol) (p-, m-, or o-toluidine), chilly acidic corrosive (15 ml), ethyl acetic acid derivation, petrol ether, Buchner channel, tender loving care plate, and the right solvents for attention investigation are the materials required.

Utilizing squeezed KBr pellets, IR spectra of all mixtures were obtained utilizing a Bruker FT-IR spectrometer. JEOL (600 MHz) and Bruker (300 MHz) spectrometers gave the  $^1H$  and  $^{13}C$  NMR spectra, and TMS was utilized as an inner reference to report compound changes in parts per million. The Carlo Erba instrument EA-1108 basic analyzer was utilized to do essential investigations. Liquefying focuses are estimated utilizing an uncorrected Lab-Hosp dissolving point gadget.

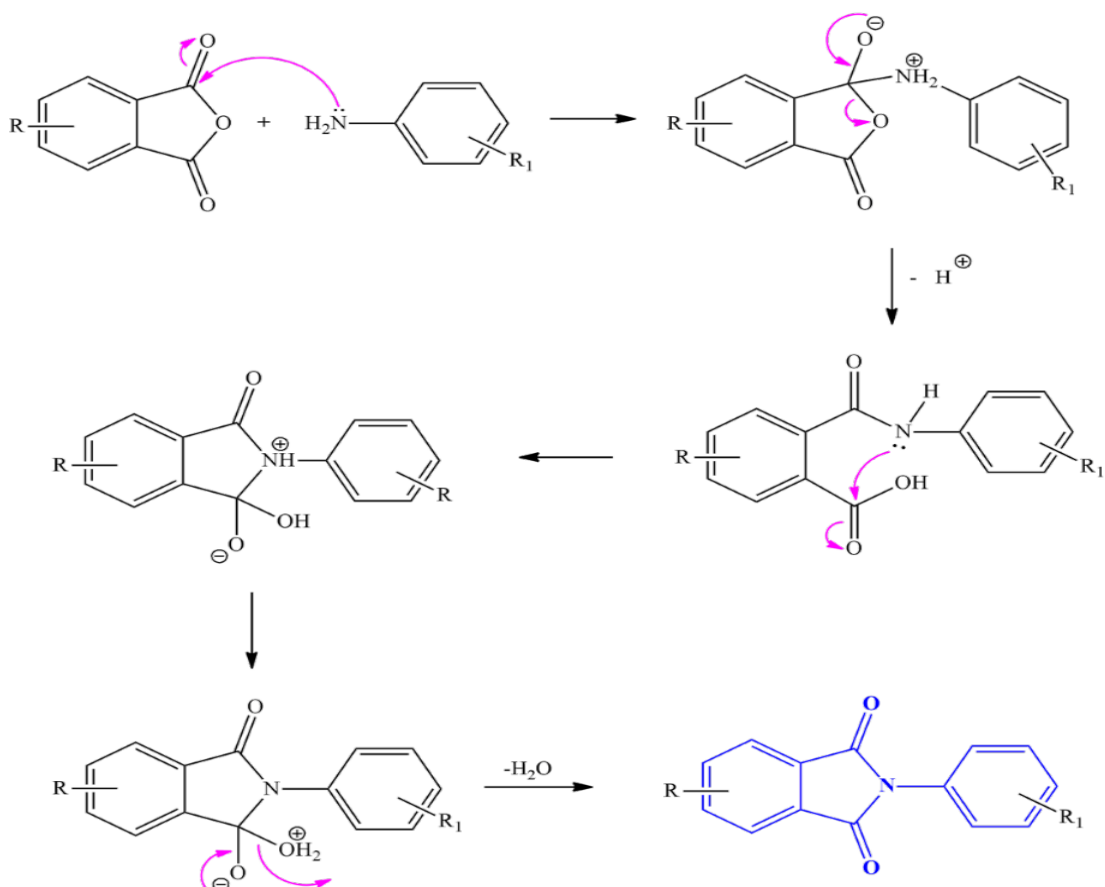
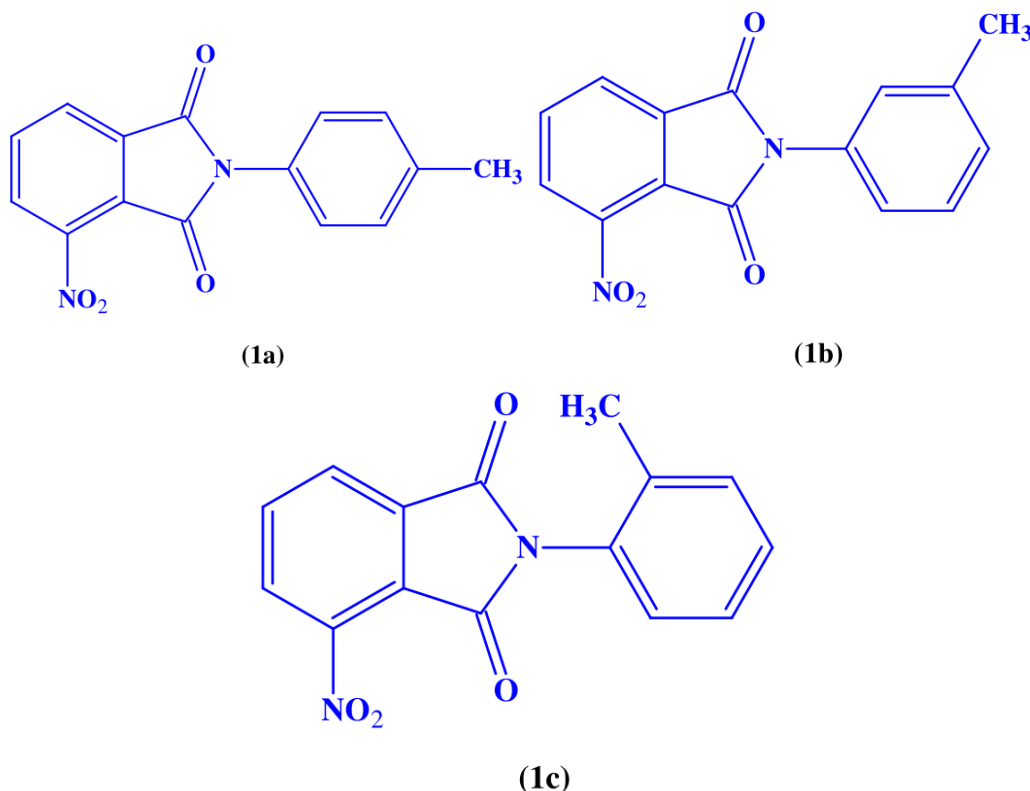


Figure 8: A believable process for isoindoline-1,3-dione synthesis

According to the suggested mechanism, which is depicted in Figure, the first addition of aromatic amine to phthalic anhydride yields the intended end product. The water molecule is removed during the subsequent cyclization of the unstable intermediate in an acidic reaction, resulting in the creation of cyclic imides (isindoline-1,3-dione).

#### 4. RESULT AND DISCUSSION



Synthesis of 4-nitro-2-(p-tolyl) isindoline-1,3-dione (1a): In this technique, a solitary necked round-base jar was loaded up with 15 ml of icy acidic corrosive and 0.50 g of 3-nitrophthalic anhydride (2.59 mmol). A warming mantle with a reflux condenser and magnetic stirrer was essential for the device. After adding 0.28 g (2.59 mmol) of p-toluidine to the mixture, the reaction continued for 3–4 hours at 80°C. TLC was used to track the reaction's progress, and once it was finished, the liquid was poured over ice-cold water. Following filtering and a water wash, the precipitated solid was processed using column chromatography to obtain the crude product. With the use of ethyl acetate: petroleum ether (15:85) for the elution, pure compound (1a) with a melting point of 215°C and a yield of 0.47 g (64%) was isolated.

Striking groups were found at specific wavenumbers in Range 1 of the infrared (IR) examination did in potassium bromide (KBr): 2923 cm<sup>-1</sup> for CH extending, 1777 cm<sup>-1</sup> for C=O extending, 1734 cm<sup>-1</sup> for another C=O extending, and 1536 cm<sup>-1</sup> for N-O extending. Continuing on toward Range 2 of the proton nuclear magnetic resonance (1H NMR) examination, various pinnacles showed up at 2.41 (singlet, 3H, - CH<sub>3</sub>), 7.30 (doublet, 1H, C-3, Ar'- H), 7.94 (trio, 1H, C-3, Ar-H), 8.15 (doublet, 1H, C-4, Ar-H), and 8.21 (doublet, 1H, C-2, Ar'- H). The information was recorded at  $\delta$ , ppm, involving a recurrence of 300 MHz in CDCl<sub>3</sub>. Moreover, tops were recognized at various situations in Range 3 of the carbon-13 nuclear magnetic resonance (13C NMR) examination, which was recorded at  $\delta$ , ppm, with a recurrence of 75 MHz in CDCl<sub>3</sub>. These positions included 21.24 (- CH<sub>3</sub>), 123.44 (C-2, Ar-

CH), 126.39 (C-6, Ar-C), 127.33 (C-2, Ar'-CH), 128.23 (C-3, Ar'-CH), 128.78 (C-1, Ar'-C), 129.90 (C-4, Ar-CH), 133.84 (C-5, Ar-C), 135.63 (C-3, Ar-CH), 138.86 (C-4, Ar'-C), 145.41 (C-1, Ar-C), 162.03 (C=O), and 164.99 (C=O). The accompanying results were gotten from the basic investigation of the substance having the atomic equation  $C_{15}H_{10}N_2O_4$ : Found: C, 63.43; H, 3.25; O, 23.10; N, 9.70; Determined: C, 63.83; H, 3.57; O, 22.67; N, 9.92.

Combination of 4-nitro-2-(m-tolyl) isoindoline-1,3-dione (1b): In a solitary necked round-base carafe, chilly acidic corrosive, 3-nitrophthalic anhydride, and m-toluidine were blended utilizing a comparative system. Under tender loving care checking, the response was done for three to four hours at 80°C. Reactant utilization was trailed by the pouring of response combination over super cold water. Subsequent to separating and washing the hastened strong, the item was dried in a hot air broiler under hoover. With a yield of 0.51 g (70%) and a liquefying point of 210°C, compound (1b) was created.

Unmistakable groups were found at specific wavenumbers in the KBr-based infrared (IR) study (Range 19): 2919  $cm^{-1}$  for CH extending, 1774  $cm^{-1}$  for C=O extending, 1715  $cm^{-1}$  for another C=O extending, and 1535  $cm^{-1}$  for N-O extending. Involving a recurrence of 600 MHz in  $CDCl_3$ , the proton nuclear magnetic resonance ( $^1H$  NMR) examination in Range 20 was then changed to. Tops were found at 2.43 (singlet, 3H, -CH<sub>3</sub>), 7.21-7.27 (multiplet, 4H, Ar'-H), 8.14 (doublet, 1H, C-4, Ar-H), 8.66 (singlet, 1H, C-1, Ar-H), and 8.76 (doublet, 1H, C-3, Ar-H). Besides, tops were seen at different situations in Range 21 of the carbon-13 nuclear magnetic resonance ( $^{13}C$  NMR) examination, recorded at  $\delta$ , ppm, with a recurrence of 150 MHz in  $CDCl_3$ . These positions included 21.37 (-CH<sub>3</sub>), 119.11 (C-1, Ar-CH), 123.48 (C-4, Ar'-CH), 124.95 (C-6, Ar'-CH), 126.98 (C-3, Ar-CH), 129.11 (C-4, Ar-CH), 129.54 (C-5, Ar'-CH), 129.62 (C-2, Ar'-CH), 130.80 (C-1, Ar'-C), 133.13 (C-6, Ar-C), 136.12 (C-5, Ar-C), 139.42 (C-3, Ar'-CH), 151.94 (C-2, Ar-C), 164.98 (C=O), and 165.24 (C=O). The accompanying results of an essential investigation were acquired for the particle having the substance recipe  $C_{15}H_{10}N_2O_4$ : Found: C, 64.15; H, 3.65; N, 9.50; O, 22.25; Determined: C, 63.83; H, 3.57; N, 9.92; O, 22.67.

Synthesis of 4-nitro-2-(m-tolyl) isoindoline-1,3-dione (1b): 3-nitrophthalic anhydride, frigid acidic corrosive, and o-toluidine were responded at 80°C for three to four hours utilizing a similar trial device. Following the finish of the response, which was followed by attention, the response blend was continuously added to super cold water. Following separating and washing, the accelerated strong was permitted to air dry prior to being additionally refined to eliminate any excess ethanol. With a yield of 0.45 g (62%) and a softening mark of 200°C, unadulterated compound (1c) was delivered.

Significant groups were found at specific wavenumbers in the KBr-based infrared (IR) study (Range 22): 2919  $cm^{-1}$  for CH extending, 1782  $cm^{-1}$  for C=O extending, 1726  $cm^{-1}$  for extra C=O extending, and 1538  $cm^{-1}$  for N-O extending. Continuing on toward the proton nuclear magnetic resonance ( $^1H$  NMR) examination in Range 23, recorded at  $\delta$ , ppm, at a recurrence of 600 MHz in  $CDCl_3$ , the accompanying pinnacles were noted: 2.20 (singlet, 3H, -CH<sub>3</sub>); 7.20-7.43 (multiplet, 4H, Ar'-H); 8.15 (doublet, 1H, C-4, Ar-H); 8.67 (singlet, 1H, C-6, Ar-H); and 8.77 (doublet, 1H, C-3, Ar-H). Besides, tops were seen at various situations in Range 24 of the carbon-13 nuclear magnetic resonance ( $^{13}C$  NMR) examination, which was recorded at  $\delta$ , ppm, with a recurrence of 150 MHz in  $CDCl_3$ . These positions included 17.97

(- CH<sub>3</sub>), 119.18 (C-1, Ar-CH), 125.02 (C-3, Ar-CH), 127.04 (C-4, Ar-CH), 128.39 (C-4, Ar'-CH), 129.52 (C-3, Ar'-CH), 129.85 (C-6, Ar-CH), 131.92 (C-6, Ar-C), 133.32 (C-2, Ar'-C), 136.29 (C-5, Ar-C), 151.93 (C-2, Ar-C), 164.91 (C=O), and 165.17 (C=O). Following a basic examination of the atom with the synthetic equation C<sub>15</sub>H<sub>10</sub>N<sub>2</sub>O<sub>4</sub>, the accompanying results were acquired: C, 63.83; H, 3.57; N, 9.92; O, 22.67, were determined.

Huge groups were found at 2923 (CH extending), 1777 (C=O extending), 1734 (an extra C=O extending), and 1536 (N-O extending) in KBr, as per the IR examination (Range 1).

There were a few critical tops in the <sup>1</sup>H NMR study (Range 2) at δ, ppm, 300 MHz, CDCl<sub>3</sub>: 2.41 (s, 3H, -CH<sub>3</sub>), 7.30 (d, 1H, C-3, Ar'-H), 7.94 (t, 1H, C-3, Ar-H), 8.15 (d, 1H, C-4, Ar-H), and 8.21 (d, 1H, C-2, Ar-H).

Tops were found at 21.24 (-CH<sub>3</sub>), 123.44 (C-2, Ar-CH), 126.39 (C-6, Ar-C), 127.33 (C-2, Ar'-CH), 128.23 (C-3, Ar'-CH), 128.78 (C-1, Ar'-C), 129.90 (C-4, Ar-CH), 133.84 (C-5, Ar-C), 135.63 (C-3, Ar-CH), 138.86 (C-4, Ar'-C), 145.41 (C-1, Ar-C), 162.03 (C=O), and 164.99 (C=O) in the <sup>13</sup>C NMR examination (Range 3) at δ, ppm, 75 MHz, CDCl<sub>3</sub>.

#### 4.1. Analysis of the elements for C<sub>15</sub>H<sub>10</sub>N<sub>2</sub>O<sub>4</sub>:

- Calculated: C, 63.83; H, 3.57; O, 22.67; N, 9.92
- Found: C, 63.43; H, 3.25; O, 23.10; N, 9.70;

#### 4.2. Biological Activity

##### ➤ Assessment Techniques

Certain requirements must be met in order to evaluate antibacterial activity, including:

1. Ensuring that the drug being evaluated and the test organisms have close contact.
2. Creating ideal conditions for microbe development.
3. Keeping the study's surroundings consistent.
4. Maintaining a sterile and aseptic environment.

Over time, a number of techniques have been used to evaluate antimicrobial activity, including:

1. The turbidimetric technique
2. The dilution method of Agar streak
3. The process of serial dilution
4. The Agar diffusion method, which includes the Paper Disc, Agar Ditch, and Agar Cup methods.

Successive Weakening and the board Refined: During both essential and optional screenings, a calculated strategy including the formation of sequential weakenings is utilized to decide the Minimum Inhibitory Concentration (MIC). Prior to being infused, the anti-toxin free control tube is subcultured. This implies separating the material similarly across one-fourth of a plate that is medium-appropriate for the living being's development, and afterward hatching it at

37°C all evening long.

**MIC Affirmation and Documentation:** to affirm the accuracy of the medication concentrations, the MIC is confirmed by perusing the MIC of the control creature. The least concentration that stops a living being's development is known as the minimum inhibitory concentration, or MIC. How much development from the control tube, which goes about as a kind of perspective for the underlying inoculum, is basically looked at.

**Supplies and Procedures:** For antimicrobial test methods, all synthetic medicines are used. Numerous control strategies are used, including drug control, vehicle control, organism control, agar control, and control with recognised antibacterial agents. Crucial elements include utilising Mueller Hinton Broth as the nutritional media and testing against MTCC cultures. The Institute of Microbial Technology in Chandigarh provides strains, and the inoculum size is set at  $10^8$  Colony Forming Units per millilitre.

**Finding the IC<sub>50</sub> Value:** Measuring the percentages of bacterial growth inhibition are necessary to find the median inhibitory concentration (IC<sub>50</sub>). The linear relationship between the concentration logarithm and inhibitory probability is the basis for calculating the IC<sub>50</sub> values. Three separate experiments' means plus or minus standard deviations are taken into account in the computation.

**Essential and Optional Screening:** Every engineered drug is weakened to a stock arrangement concentration of 2000 micrograms for each milliliter for the essential screening. In the principal screening, concentrations of 1000 µg/mL, 500 µg/mL, and 250 µg/mL are used. The microorganisms in the optional screen are all exposed to a second round of weakening for dynamic prescriptions that were tracked down in this step. For this situation, 200 µg/mL, 100 µg/mL, 50 µg/mL, 25 µg/mL, 12.5 µg/mL, and 6.25 µg/mL are utilized as concentrations.

**Reading of the MIC Results:** The MIC is defined as the greatest dilution that exhibits at least a 99% inhibitory zone. The sensitivity of this determination to the inoculum's size highlights the requirement that the test combination comprise  $10^8$  organisms/mL.

#### 4.3. Evaluation of Biological Effects

In vitro screening was utilized to assess the natural action of recently blended heterocyclic mixtures from Series-1, 2, and 3 against Gram-positive and Gram-negative bacterial strains, explicitly *S. aureus* and *E. Coli*. Besides, the growth strain *A. brasiliensis* was utilized to evaluate their in vitro antifungal adequacy. The agar weakening strategy was utilized for the underlying assessments of the antibacterial and antifungal properties. The assessed drugs were weakened with DMSO to get the objective concentration when tried against standard strains. The typical distance across of the hindrance zones (IZ) of bacterial or contagious development encompassing the plates, estimated in millimeters, was recorded for each tried substance (Table 1).

Table 1: Agar dilution with DMSO as a vehicle to test Series-1, 2, and 3 heterocyclic compounds for antibacterial and antifungal activity against *S. aureus*, *E. coli*, and *A. brasiliensis* strains."

Compound	GRAM +VES. aureus (ATCC 6538)			GRAM –VEE. coli (ATCC 8739)			FUNGIA. brasiliensis (ATCC 16404)		
	1 g	0.5 g	DMSO	1 g	0.5 g	DMSO	1 g	0.5 g	DMSO
	(Per 100µl)			(Per 100µl)			(Per 100µl)		
1a	0	0	0	0	0	0	0	0	0
1b	0	0	0	12	14	0	0	0	0
1c	0	0	0	9	11	0	8	10	0

#### 4.4. Biological Activity Screening Results

##### 1) 4-nitro-2-(p-tolyl) 1,3,-dione-isoindoline (1a)



##### 2) 4-nitro-2-(m-tolyl) 1,3,-dione-isoindoline (1b)





3) 4-nitro-2-(o-tolyl) 1,3,-dione-isoindoline (1c)



Testing the antibacterial action against Gram-positive *Staphylococcus aureus* (ATCC 6538), Gram-negative *Escherichia coli* (ATCC 8739), and the growth *Aspergillus brasiliensis* (ATCC 16404) was a critical part of the exploration discoveries on the plan and creation of novel natural mixtures. For each substance, three concentrations were inspected: one gram, a portion of a gram, and DMSO (per 100 $\mu$ l). The compound's all's tried portions meaningfully affected *Staphylococcus aureus* (0 mm hindrance zone width).

In two experiments, the chemical exhibited modest effectiveness against *Escherichia coli*, with inhibition zone widths of 12 mm and 14 mm at the highest concentration (1 gramme). Nevertheless, no inhibition was seen at 0.5 grammes. The chemical demonstrated a moderate level of efficacy against *Aspergillus brasiliensis*. In two trials, inhibition zone widths of 8 mm and 10 mm were noted at the maximum concentration (1 gramme), although no inhibition was detected at 0.5 grammes. Overall, the substance was ineffective against *Staphylococcus aureus* but shown encouraging antibacterial action against *Escherichia coli* and *Aspergillus brasiliensis*. It is necessary to conduct more research into its potential as an antibacterial agent.

## 5. Conclusion

Using aniline derivatives in glacial acetic acid as the solvent, the study's main focus was on the synthesis of nitro-substituted phthalimide analogues (1a-1e) and (2a-2e). The synthetic pathway was described in detail, along with the analytical characterisation, attempted reactions, and methodology. The characterisation of the synthesised compounds was supported by spectral data. According to the theorised mechanism, aromatic amine was added to phthalic anhydride, and then the mixture underwent acidic conditions for cyclization, resulting in the formation of cyclic imides (isoindoline-1,3-dione).

Antimicrobial screening was performed on the synthesised compounds against *Aspergillus brasiliensis*, *Escherichia coli*, and *Staphylococcus aureus*. At the highest tested concentration, there was moderate action against *Escherichia coli* and *Aspergillus brasiliensis*, but no inhibitory impact against *Staphylococcus aureus*. Specifically, *Aspergillus brasiliensis* showed hindrance zone sizes of 8 mm and 10 mm, while *Escherichia coli* showed restraint zone breadths of 12 mm and 14 mm. The viability contrasted at lower dosages, however, with *Aspergillus brasiliensis* and *Escherichia coli* both appearance no restraint at 0.5 grams.

The consequences of this study show a promising antibacterial movement against *Aspergillus brasiliensis* and *Escherichia coli*, demonstrating potential purposes for the combined compounds. To more readily grasp their antimicrobial systems and boost their viability for a more extensive scope of helpful applications, more exploration is encouraged.

### 5.1 Recommendations

A few critical proposals can be made in light of the discoveries of the concentrate on the design and synthesis of novel organic compounds and their natural assessment. The in vitro screening showed that the blended heterocyclic compounds from Series-1, 2, and 3 showed various degrees of antibacterial and antifungal movement. All the more exactly, the compounds shown empowering viability against Gram-negative *Escherichia coli* and the organism strain *Aspergillus brasiliensis*, but they showed no adequacy against Gram-positive *Staphylococcus aureus*. In view of these discoveries, it is suggested that future examinations focus on refining the synthetic creations to work on their viability against microbes and organisms. Modifying the substituents on the phthalimide analogs can possibly upgrade their viability against a more extensive assortment of microbial strains, including Gram-positive microscopic organisms. Besides, researching different dissolvable frameworks and response conditions might bring about the development of additional strong compounds. It is urgent to perform careful robotic examinations to fathom the particular manners by which these synthetic substances apply their antibacterial properties. This information can possibly educate the creation regarding more proficient particles and pinpoint imminent focuses for helpful turn of events. By integrating other hazardous microorganisms and parasites into the natural assessment, we can actually assess the colossal capability of these synthetic compounds.

Besides, it is prudent to lead in vivo examinations to evaluate the pharmacokinetics, poisonousness, and helpful adequacy of the most positive substances. These examinations are pivotal for surveying the reasonable attainability of the compounds as restorative specialists. Participating in organizations with microbiologists and pharmacologists will be favorable in advancing these ventures. It is prudent to consider protecting the new compounds that have

eminent antibacterial properties to defend licensed innovation and advance future financial headway. Communicating with drug organizations to investigate the chance of creating and showcasing drugs in view of these revelations could be an essential move toward changing over these outcomes into pragmatic use in clinical medicines.

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