

ORIGINAL RESEARCH ARTICLE

Synthesis, Structural Characterization, and IPCE Performance Evaluation of Novel Naphthalimide-Substituted Azo Dyes for Dye-Sensitized Solar Cells

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ABSTRACT

This study presents the synthesis, characterization, and photovoltaic evaluation of novel naphthalimide-substituted azo dyes for dye-sensitized solar cells (DSSCs). The dyes were synthesized through nitration, amination, diazotization, and azo-coupling reactions to obtain highly conjugated donor- π -acceptor systems. Structural characterization using FT-IR, UV-Vis, Mass spectrometry, and ¹H/¹³C NMR confirmed successful dye formation. The dyes exhibited good thermal stability with melting points of 170–173°C and 175–178°C. UV-Vis analysis showed strong visible-light absorption with λ_{max} values of 467 and 517 nm for Dye 1 and 459 and 504 nm for Dye 2 in ethanol and DMSO, respectively. Dye 2 showed higher molar absorptivity ($6.58 \times 10^4 \text{ Lmol}^{-1}\text{cm}^{-1}$) than Dye 1 ($5.28 \times 10^4 \text{ Lmol}^{-1}\text{cm}^{-1}$), indicating improved light-harvesting ability. FT-IR spectra confirmed the presence of characteristic absorption bands corresponding to N-H/O-H stretching vibrations at frequency range of 3254–3608 cm^{-1} , azo linkages (-N=N-) appeared at 1505–1569 cm^{-1} , strong carbonyl absorptions were detected between 1654 and 1729 cm^{-1} , and cyano groups were identified within 2278–2288 cm^{-1} , confirming successful incorporation of electron donor and electron acceptor functionalities into the dye framework essential for DSSC sensitization. Mass spectrometric fragmentation patterns verified the presence of stable conjugated aromatic systems containing amino, azo, cyano, and imide groups. The ¹H and ¹³C NMR spectra further validated the molecular structures and strong donor-acceptor interactions. IPCE studies revealed efficient photon-to-current conversion, with Dye 1 achieving 53% at 520 nm and Dye 2 showing 48.7% at 550 nm, thus demonstrating that structural modification of the naphthalimide core confirms that photons from the sun have been converted into electricity.

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INTRODUCTION

The rapid increase in global energy demand and the environmental consequences of fossil fuel consumption have spurred extensive research into renewable and sustainable energy technologies. Among renewable energy sources, solar energy remains one of the most abundant and environmentally friendly options for electricity generation. In recent years, dye-sensitized solar cells (DSSCs) have emerged as promising third-generation photovoltaic devices due to their low fabrication cost, simple manufacturing process, flexibility, transparency, and good performance under low-light conditions. Michael Grätzel first introduced the modern DSSC concept in 1991, leading to significant advances in sensitizer chemistry and photovoltaic materials (Grätzel, 2003).

Dye-sensitized solar cells operate through photo-induced electron transfer processes involving a semiconductor, an

electrolyte, a counter electrode, and a photosensitizing dye. Among these components, the dye sensitizer is considered the heart of the DSSC because it determines the extent of light absorption, electron injection efficiency, and overall photovoltaic performance. Consequently, the design and synthesis of efficient organic sensitizers with broad absorption spectra, strong charge-transfer capability, suitable energy levels, and excellent thermal stability remain important research priorities (Hagfeldt *et al.*, 2020)

Organic dyes containing donor- π -acceptor (D- π -A) architectures have attracted considerable attention as alternatives to expensive ruthenium-based sensitizers because of their tunable electronic properties, high molar extinction coefficients, environmental compatibility, and relatively low production cost. Among the various organic chromophores investigated, naphthalimide derivatives

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have emerged as highly promising materials for optoelectronic and photovoltaic applications due to their excellent photostability, strong fluorescence behavior, broad visible-light absorption, electron-deficient imide core, and ease of structural modification (Wang *et al.*, 2020).

Furthermore, naphthalimide-based dyes exhibit remarkable optical and electrochemical properties that make them attractive candidates for solar energy conversion applications (Liu *et al.*, 2021). Their rigid aromatic framework enhances light-harvesting and charge-separation, which are essential parameters for improving photocurrent generation and overall power conversion efficiency in DSSCs. Recent studies have shown that structural engineering of naphthalimide derivatives through substitution with electron-donating amines and conjugated linkers can significantly improve absorption characteristics and photovoltaic performance (Chen *et al.*, 2022)

Despite considerable progress in DSSC technology, challenges such as dye aggregation, limited spectral absorption, charge recombination, and long-term operational stability continue to limit device efficiency. Therefore, the synthesis of novel naphthalimide-substituted amines with improved photo-physical and electrochemical properties remains an active area of investigation. The development of efficient metal-free organic sensitizers is particularly desirable because they offer environmental sustainability, structural versatility, and reduced production costs compared with conventional metal-complex dyes (Zhang *et al.*, 2022)

In this study, naphthalimide-substituted azo dyes were synthesized and characterized for application in dye-sensitized solar cells. The synthesized compound was characterized using spectroscopic and analytical

techniques such as Fourier Transform Infrared Spectroscopy (FT-IR), Ultraviolet-Visible Spectroscopy (UV-Vis), Nuclear Magnetic Resonance Spectroscopy (^1H and ^{13}C NMR), and Incident Photon-to-Current Conversion Efficiency (IPCE) in order to determine the efficiency with which absorbed photons are converted into electrical current, thereby reflecting the light harvesting ability and electron injection efficiency of the dyes in Dye Sensitized Solar Cell (DSSC) applications (Yang and Cao, 2020).

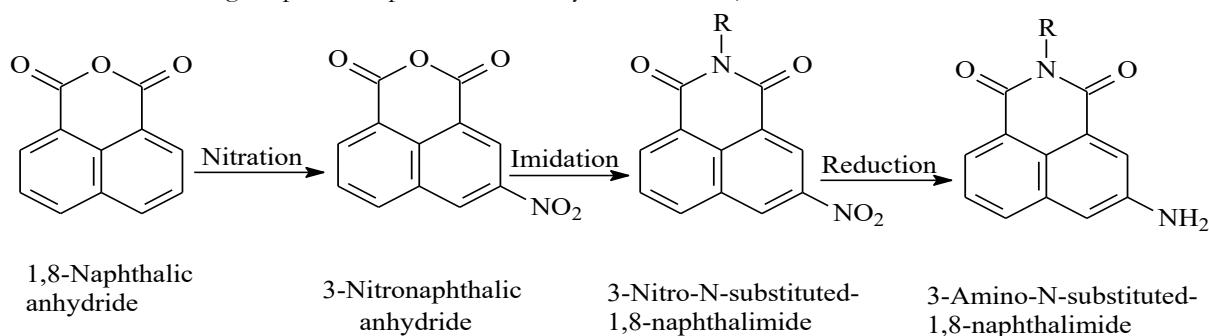
MATERIALS AND METHODS

Chemicals/Reagents and Equipment

Analytical-grade reagents and chemicals used for the synthesis of intermediates and dyes were purchased from Bijoe Chemical Company and Weifang Senya Chemical Company Limited, China. Most of the chemicals used in this research work are Propylamine, 3-Aminobenzoic acid, 3,4-Diaminobenzoic acid, Tetracyanoethylene, 1,8-naphthalic anhydride, Tetrahydrofuran, Iodine-iodide electrolyte, Titanium oxide, propionic acid, acetic acid, Agilent CARY 300 UV-visible spectrophotometer, Agilent CARY 630 FT-IR, Agilent Gas chromatography-mass spectrometry (7890B GC System). Agilent (^1H and ^{13}C NMR) 300 MHz spectrometer and Gallenkamp melting point apparatus, Newport 2636-R IPCE measurement system.

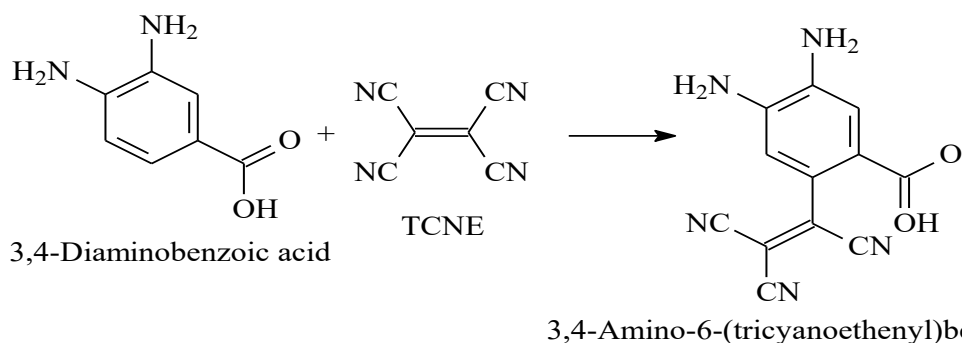
Synthesis of N-Substituted Naphthalimide Derivatives

The synthesis of the N-Substituted Naphthalimide Derivatives was achieved following the procedure reported in the work of Fed'ko and Anikin (2015), as outlined in the reaction Scheme 1 (Fed'ko and Anikin, 2015):

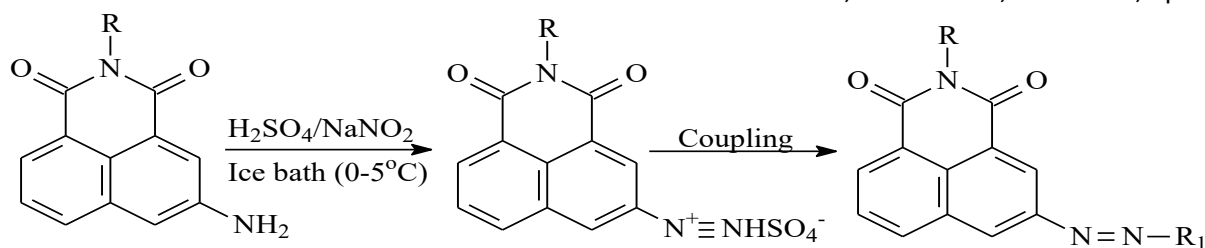


Scheme 1: Synthesis of Naphthalimide Intermediates

Where R represent $(-\text{CH}_2)_2\text{CH}_3$



Scheme 2: Tricyanovinilation of 3,4-Diaminobenzoic acid



Scheme 3: Diazotization and Coupling Reaction

Where R represent propyl amine ($-(\text{CH}_2)_2\text{CH}_3$) and R_1 represent the cyanorated coupling components

Synthesis of 3-nitro-1, 8- naphthalic anhydride

Sodium nitrate (1.30 g, 15 mmol) was added portionwise to a solution of 1,8-naphthalic anhydride (3.00 g, 15 mmol) in 30 mL of concentrated sulfuric acid. The reaction mixture was heated for 2 h on a water bath, then poured onto ice; the precipitate was filtered, washed with water, and dried at 110°C . The crude product was purified by crystallization from acetic acid to obtain 3-nitronaphthalic anhydride as yellow solid crystals.

Synthesis of 3-nitro-propyl-1, 8-naphthalimide (a)

A suspension of 3-nitro-1, 8- naphthalic anhydride (0.02 mol, 4.86 g) and propylamine (0.02 mol, 4.71 g) was stirred under reflux for 7 hours in ethanol (100 ml). The cooled suspension was filtered, and the filtrate was recrystallized from ethanol to obtain yellow crystals.

Synthesis of 3-amino-propyl-1, 8-naphthalimide (1)

A solution of 3-nitropropyl-1,8-naphthalimide (1.00 g, 4 mmol) in ethanol (100 ml) and hot water (50 ml) was prepared. Sodium dithionite (0.55 g) was added portionwise while stirring. The reaction mixture was refluxed for 3 h and concentrated on a water bath. Hydrochloric acid (10 ml) was added to the residue, and the precipitate was filtered and dried. The crude product was purified by crystallization from ethanol as brown crystals.

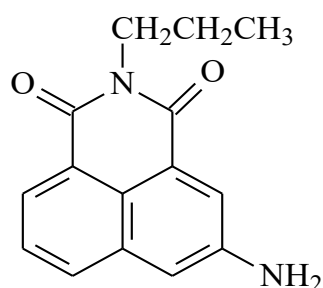


Figure 1: Structures of 3-Amino-2-Propyl-1H-Benzo[de]Isoquinoline-1,3(2H)-Dione

Synthesis of Cyanorated Coupling Components

A solution of the requisite benzoic acid derivative (0.01 mol, 3 g) and (0.01 mol, 0.8 g) tetracyanoethylene (TCNE) in dimethylformamide (DMF) (20 ml) were stirred at 70°C for 6 hr. The solvent was removed and the residual solid was collected and recrystallized from toluene/chloroform mixture (1:3) [9]. The reaction is presented in [Scheme 2](#):

Procedure for diazotization

Dry sodium nitrite (1.5 mmol, 0.104 g) was added to cold conc. H_2SO_4 (98 %, 1.1 ml) at such a rate that yellow fume was not evolved. The reaction temperature was gradually increased to 65°C using a water bath until the sodium nitrite was dissolved. The resulting solution was cooled to $0-5^\circ\text{C}$ and then added dropwise at $5-20^\circ\text{C}$ to a mixture of propionic acid and acetic acid (10 ml, 1.5:8.5). The finely ground powder of 3-amino-N-substituted-1,8-naphthalimide was added portion-wise at less than 10°C , and the mixture was stirred for 3 hours. The obtained clear solution was used immediately in coupling reactions as shown in reaction [scheme 3](#) ([Obadahun et al., 2023](#))

Coupling reactions

The cyanorated coupling components, 3-amino-6-(tricyanoethynyl)benzoic acid and 3,4-diamino-6-(tricyanoethynyl)benzoic acid (0.02 mol, 0.53 g), were each dissolved with potassium hydroxide solution (0.02 mol, 2.54 g) at $0-5^\circ\text{C}$. The previously prepared diazonium solution of the 3-amino-N-substituted-1,8-naphthalimide was added over 30-40 minutes with vigorous stirring. The mixture was stirred for a further 1 hour under $0-5^\circ\text{C}$ and the pH of the solution was adjusted to 4-5 using 10 % sodium acetate, and thereafter stirred for 1 hour. The resulting product was collected by filtration, washed with warm water, then cold water, and dried. The crude product was purified several times by recrystallizing from dimethyl sulfoxide (DMSO). Thin-layer chromatography was thereafter carried out to ascertain the dyes' purity ([Agho et al., 2017](#)).

Characterization of the Synthesized Dyes

The synthesized dyes were characterized by melting point determination, UV-visible spectroscopy, Mass spectrometry (MS), Fourier transform infrared spectroscopy (FT-IR), $^1\text{H-NMR}$, and $^{13}\text{C-NMR}$. The Photo-physical properties of the synthesized dyes, including the Incident Photon-to-Current Conversion Efficiency (IPCE), which represents the efficiency with which absorbed photons are converted into electrical current, thereby reflecting the light-harvesting ability and electron-injection efficiency of the dyes in Dye-Sensitized Solar Cell (DSSC) applications, were determined.

Photo-Electrochemical Measurement of Incident Photon to Current Conversion Efficiency

The incident light intensity was calibrated using a reference Si solar cell (Newport Oriel, 91150 V) to set 1

Sun (100 mW/cm²). The incident monochromatic photon-to-current conversion efficiency measurement was fully controlled using the Newport 2636-R IPCE measurement system, equipped with a 75 W short-arc Xenon lamp as the light source, connected to a monochromator. Calibration of the incident light was performed before measurements using a silicon photodiode.

RESULTS AND DISCUSSION

The physicochemical properties presented in Table 1 provide important evidence for the successful synthesis and purity of the prepared naphthalimide azo dyes intended for Dye-Sensitized Solar Cell (DSSC) applications. The empirical formulas and molecular weights obtained for Dye 1 (C₂₇H₁₇N₇O₄, 503.48 g/mol)

and Dye 2 (C₂₇H₁₈N₈O₄, 518.49 g/mol) are consistent with the proposed molecular structures containing imide, azo, amino, and cyano functional groups.

The melting point ranges of 170-173°C for Dye 1 and 175-178°C for Dye 2 indicate the formation of relatively thermally stable, good-purity, and highly conjugated aromatic compounds. The percentage yields of 72.0% for Dye 1 and 70.0% for Dye 2 demonstrate that the diazotization and azo coupling reactions proceeded successfully with appreciable synthetic efficiency, while the dark brown appearance of both dyes is characteristic of highly conjugated azo chromophores with extended π -electron delocalization. Such coloration suggests strong absorption within the visible region of the electromagnetic spectrum, which is an essential requirement for effective DSSC sensitizers (Mishra *et al.*, 2020).

Table 1: Physical Properties of the Synthesized Dyes

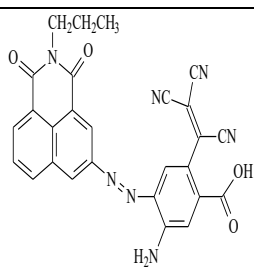
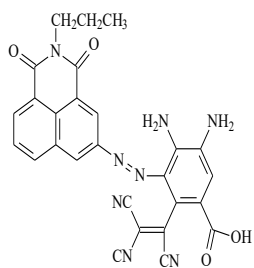
Dye No	Emperical formula	Molecular weight (g/mol)	Melting point (°C)	Percentage yield (%)	Appearance	Dye Structure
Dye 1	C ₂₇ H ₁₇ N ₇ O ₄	503.48	170-173	72.0	Dark brown	
Dye 2	C ₂₇ H ₁₈ N ₈ O ₄	518.49	175-178	70.0	Dark brown	

Table 2: Visible absorption Spectroscopy of Dyes

Dye No	Ethanol λ_{\max} (nm)	DMSO λ_{\max} (nm)	ϵ_{\max} in DMSO $\times (10^4 \text{ Lmol}^{-1}\text{cm}^{-1})$
Dye 1	467.00	517.00	6.58
Dye 2	459.00	504.00	5.28

Table 3: The Infra-Red Spectra of the Synthesized Dyes

Dye No	Vibrational frequencies (cm ⁻¹)
Dye 1	N-H/OH str. 3608, 3350, 3254; C-H str. Ar. 2963; C-H str. Aliphatic 2929; C=O str. 1654; C-N str. 1390; -N=N str. 1505, 1569; CN str. 2278
Dye 2	N-H/OH str. 3380; C-H str. Ar. 2970; C-H str. Aliphatic 2933; C=O str. 1729; C=C str. 1610; C-N str. 1319; -N=N str. 1513; CN str. 2288

The summarized UV-Visible Absorption Spectroscopy of the synthesized naphthalimide-substituted dye sensitizers is presented in Table 2. Both dyes exhibited strong absorption within the visible region, as presented in Table 2, confirming the presence of extended π -conjugation arising from the naphthalimide core, azo linkage (-N=N-), and electron-withdrawing cyano substituents. Such broad visible absorption is essential for efficient solar light harvesting in DSSC systems. Dye 1 showed absorption maxima (λ_{\max}) at 467 nm in ethanol and 517 nm in

DMSO, while Dye 2 exhibited λ_{\max} values at 459 nm and 504 nm, respectively. The observed bathochromic shift (red shift) in DMSO relative to ethanol indicates solvent polarity effects on the dyes' electronic transitions. This behavior suggests strong intramolecular charge transfer (ICT) within the dye molecules, a desirable feature for DSSC sensitizers. The molar extinction coefficients (ϵ_{\max}) obtained in DMSO further demonstrate the excellent light-absorbing properties of the synthesized dyes. Dye 1 exhibited a higher molar absorptivity ($6.58 \times$

$10^4 \text{ L mol}^{-1} \text{ cm}^{-1}$) than Dye 2 ($5.28 \times 10^4 \text{ L mol}^{-1} \text{ cm}^{-1}$). The high molar absorptivity values ($\epsilon_{\text{max}} > 5 \times 10^4 \text{ L mol}^{-1} \text{ cm}^{-1}$) are consistent with highly conjugated D- π -A naphthalimide dyes (Zhang *et al.*, 2022). For comparison,

perylene diimide dyes (a class of highly conjugated organic dyes) exhibit ϵ up to $8 \times 10^4 \text{ L mol}^{-1} \text{ cm}^{-1}$ (Mishra *et al.*, 2020). Thus, indicating stronger photon harvesting efficiency (Kuang *et al.*, 2007).

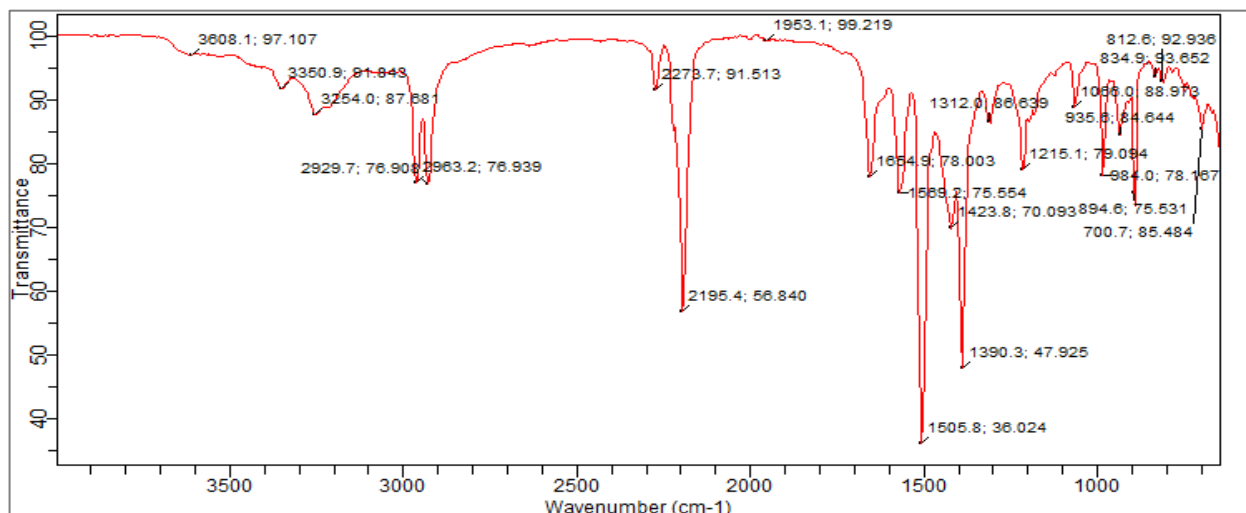


Figure 2: FT-IR of Dye 1

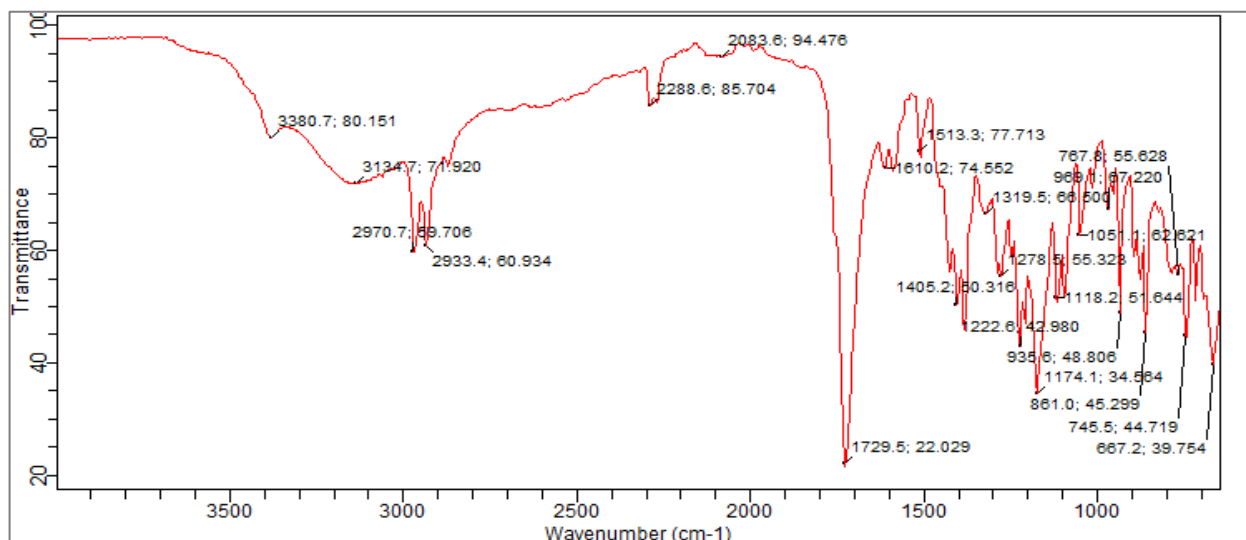


Figure 3: FT-IR of Dye 2

Table 4: MS Fragmentations of the Synthesized Dyes

Dye No	Molecular Formula	Experimental values of m/z fragment	Corresponding positive charge fragment	Theoretical value
Dye 1	$\text{C}_{27}\text{H}_{17}\text{N}_7\text{O}_4$	55.1, 93.1, 150.0, 207.0, 503.0	$\text{C}_3\text{H}_5\text{N}^+$, C_3HO_2^+ , $\text{C}_8\text{H}_{12}\text{N}_3^+$, $\text{C}_{11}\text{N}_3\text{O}_2^+$, M	503.48
Dye 2	$\text{C}_{27}\text{H}_{18}\text{N}_8\text{O}_4$	74.0, 143.1, 298.2, 515.7	C_5N^+ , $\text{C}_8\text{H}_5\text{N}_3^+$, $\text{C}_{14}\text{H}_{13}\text{N}_4\text{O}_4^+$, M	518.49

The FT-IR spectra of the dyes are presented in Figures 2 and 3, and the observed data are summarized in Table 3. The results confirm the successful synthesis of the naphthalimide-substituted azo dyes, as evidenced by characteristic functional group absorptions corresponding to the proposed molecular structures. The observed absorption bands provide strong evidence for the incorporation of amino/hydroxyl (N-H and O-H stretching vibrations at $3254 - 3380 \text{ cm}^{-1}$), azo ($-\text{N}=\text{N}-$) at the frequency range of 1505 and 1569 cm^{-1} , imide carbonyl ($\text{C}=\text{O}$ stretching vibration) at the vibrational frequency range of $1610-1654 \text{ cm}^{-1}$, aromatic/aliphatic

(C-H stretching vibrations) appears at $2929-2970 \text{ cm}^{-1}$, and cyano functionalities ($\text{C}\equiv\text{N}$) appears at the vibrational frequency range of $2278-2288 \text{ cm}^{-1}$ respectively, which are essential structural features for efficient Dye Sensitized Solar Cell (DSSC) sensitizers. The FT-IR results thus suggest successful formation of highly conjugated naphthalimide azo dyes containing donor and acceptor functional groups necessary for efficient intramolecular charge transfer. The presence of azo, carbonyl, amino, and cyano groups is particularly important for enhancing visible-light absorption, electron transfer, and anchoring in DSSC applications (Nagarajan *et al.*, 2020).

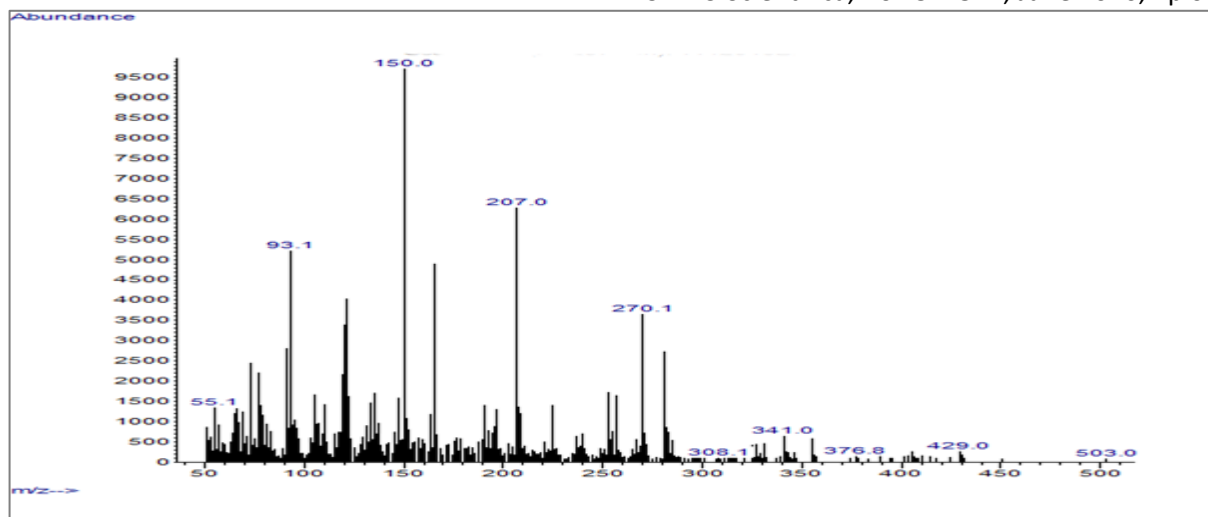


Figure 4: MS Spectrum of Dye 1

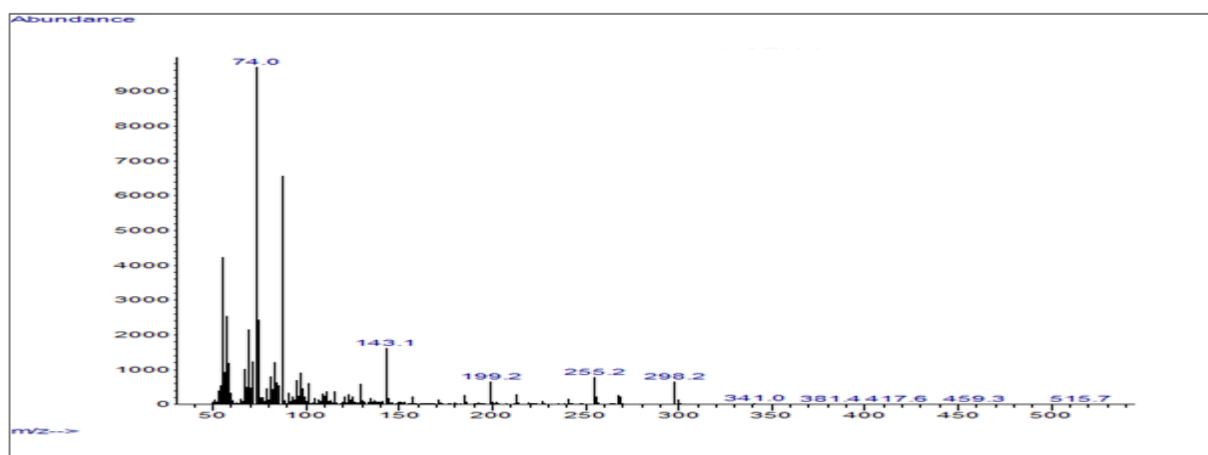


Figure 5: MS Spectrum of Dye 2

 Table 5: ^1H and ^{13}C -NMR (300 MHz, MeO- d_4): δH (ppm) Data of the Synthesized Dyes

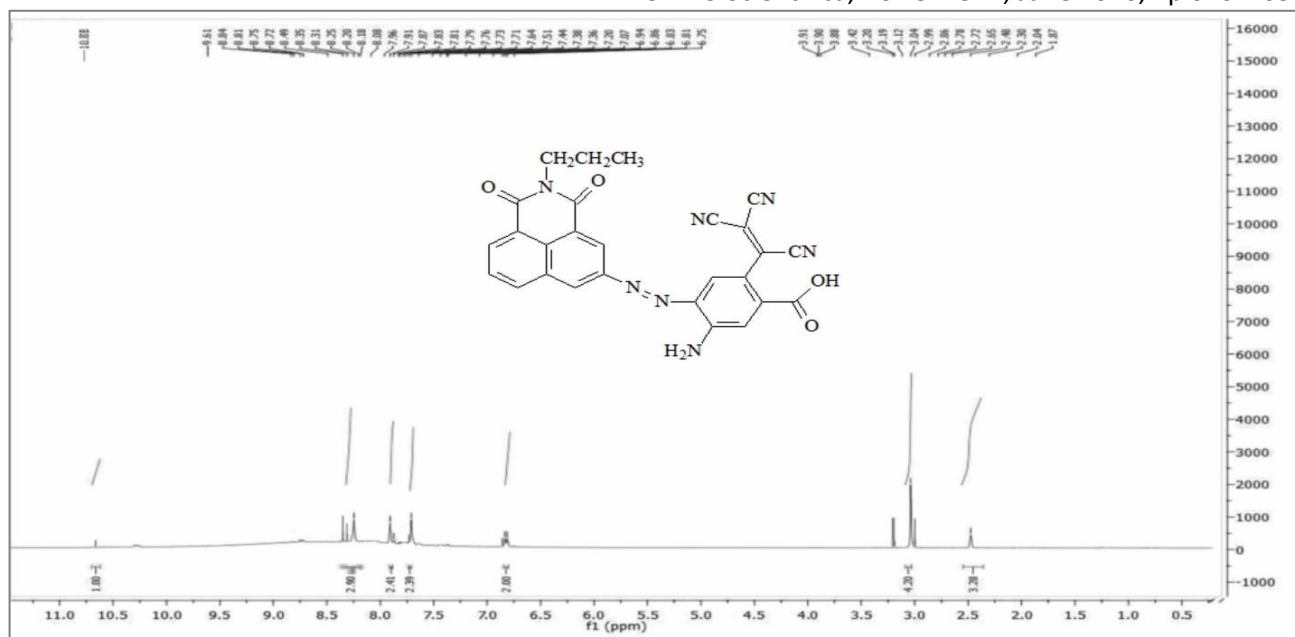
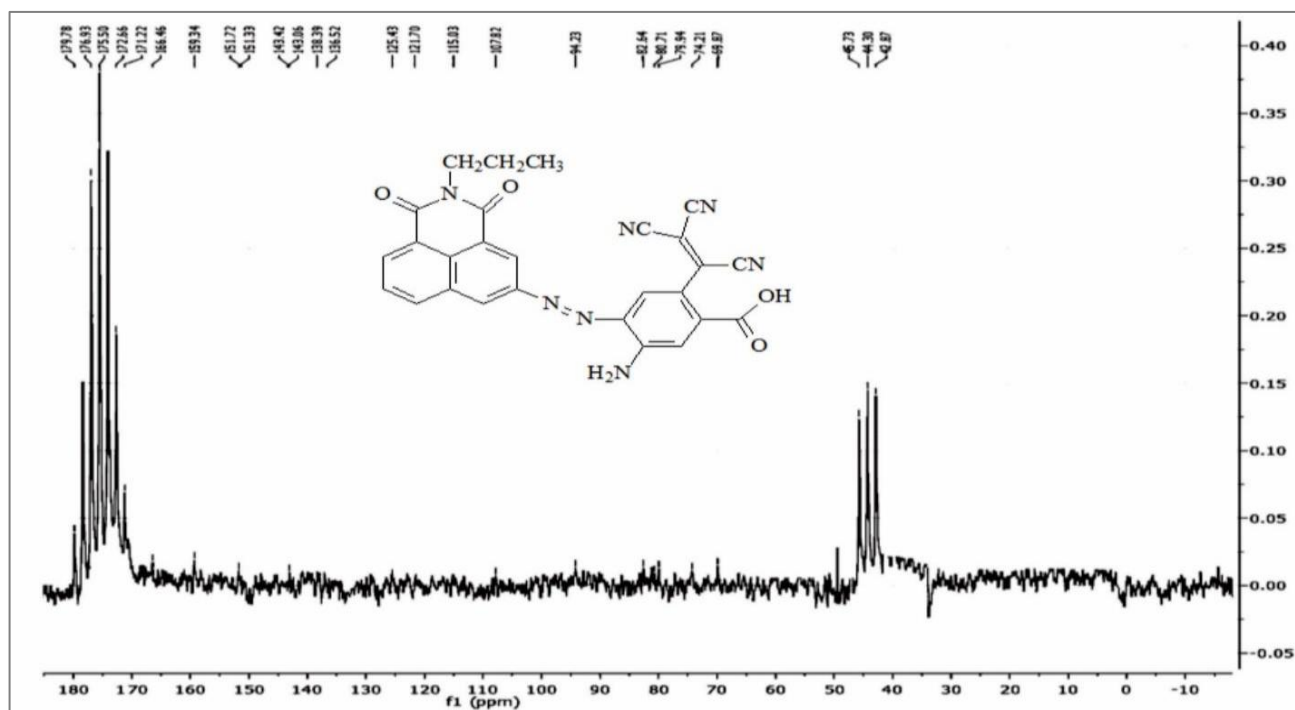
Dye No	^1H and ^{13}C -NMR
Dye 1	10.88(S, 1H, COOH), 8.20(d, 1H, J=2H ₂), 8.18(d, 1H, J=2H ₂), 8.08(d, 1H), 7.87(S, 1H), 7.73(S, 2H, NH ₂), 3.04(t, 2H, CH ₂), 2.99(m, 2H, CH ₂), 2.04(t, 3H, CH ₃); ^{13}C -NMR(400 MHz, MeO- d_4): δ (ppm) 179.78, 176.93, 175.50, 172.66, 171.22, 166.46, 159.34, 151.72, 151.33, 143.42, 143.06, 138.39, 136.52, 125.43, 121.70, 115.03, 107.82, 94.23, 82.64, 80.71, 79.94, 74.21, 69.87, 45.73, 44.30, 42.87
Dye 2	11.96(S, 1H, COOH), 10.69(S, 1H, OH), 8.10(d, 1H), 7.95 (d, 2H), 7.91(S, 1H), 7.87(d, 1H), 7.83(S, 1H), 7.76(d, 2H), 7.64(d, 1H), 7.44(d, 1H), 7.09(d, 1H), 6.87(S, 2H, NH ₂); ^{13}C -NMR(400 MHz, MeO- d_4): δ (ppm) 185.80, 184.27, 179.84, 178.40, 176.96, 175.53, 174.12, 172.68, 171.22, 170.80, 167.16, 153.93, 153.48, 142.13, 139.55, 134.87, 133.93, 130.00, 125.31, 122.50, 118.94, 114.74, 113.27, 106.45, 103.75, 100.84, 96.18, 93.19, 85.10

The MS spectra of the dyes are presented in Figures 4 and 5, and the observed data are summarized in Table 4. For Dye 1 with molecular formula $\text{C}_{27}\text{H}_{17}\text{N}_7\text{O}_4$, several characteristic fragment ions were observed at m/z values of 55.1, 93.1, 150.0, 207.0, and 503.0. The fragment at m/z 55.1 corresponding to $\text{C}_3\text{H}_5\text{N}^+$ indicates cleavage involving nitrogen-containing aliphatic moieties, while the fragment at m/z 93.1 (C_5HO_2^+) may be attributed to aromatic oxygen-containing fragments derived from the carboxyl or imide portions of the molecule. The fragments at m/z 150.0 and 207.0 further confirm the stability of nitrogen-rich aromatic intermediates generated during fragmentation. The molecular ion peak observed at m/z 503.0 closely matches the molecular mass of the

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synthesized dye, confirming the successful synthesis of the target compound.

Similarly, Dye 2 with molecular formula $\text{C}_{27}\text{H}_{18}\text{N}_8\text{O}_4$ exhibited significant fragment ions at m/z 74.0, 143.1, 298.2, and 515.7. The fragment at m/z 74.0 assigned to C_5N^+ and the peak at m/z 143.1 corresponding to $\text{C}_8\text{H}_5\text{N}_3^+$ suggest fragmentation involving cyano and azo-containing aromatic regions of the dye. The larger fragment at m/z 298.2 indicates the presence of stable conjugated aromatic segments incorporating nitrogen and oxygen functionalities. The molecular ion peak at m/z 515.7 further supports the successful formation of the synthesized dye structure.


 Figure 6: ^1H NMR of Dye 1

 Figure 7: ^{13}C NMR of Dye 1

The fragmentation behavior of both dyes demonstrates the presence of stable aromatic conjugated systems, which is characteristic of naphthalimide azo chromophores. The abundance of nitrogen-containing fragments confirms successful incorporation of amino, azo, and cyano groups into the dye framework. These structural features are highly beneficial for DSSC applications because they promote strong electron delocalization, intramolecular charge transfer, and efficient light harvesting properties. The mass spectrometric results validate the molecular integrity and structural composition of the synthesized dyes, supporting their suitability as potential sensitizers for Dye-Sensitized Solar Cells and further confirming the successful formation of the proposed highly conjugated dye molecules containing naphthalimide, azo, amino, and cyano functionalities (Chiu *et al.*, 2017).

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The ^1H and ^{13}C spectrum of the dye is presented in Figures 6, 7, 8, and 9, and the observed data is summarized in Table 5. The NMR spectral data confirm the successful synthesis and structural integrity of the naphthalimide azo dyes. The presence of conjugated aromatic systems, donor amino groups, electron-withdrawing carbonyl and cyano functional groups, and carboxylic acid anchoring groups indicates that the synthesized dyes possess favorable electronic structures for efficient light harvesting and electron transfer in DSSC applications. The observed chemical shifts are consistent with the proposed molecular frameworks, which contain aromatic rings, amino groups, azo linkages, cyano substituents, carboxylic acid groups, and the naphthalimide moiety.

transfer in DSSC applications. The aliphatic carbon signals around δ 42.87-45.73 ppm correspond to the propyl substituent carbons. The ^{13}C -NMR spectrum of Dye 2 showed several downfield signals between δ 167.16 and 185.80 ppm, attributable to carbonyl carbons of the imide and carboxylic groups. Aromatic and conjugated

carbon resonances appearing between δ 85.10-153.93 ppm confirm the presence of electron-rich and electron-deficient carbons within the conjugated dye backbone. These results suggest enhanced electron delocalization and donor-acceptor interactions within the molecule (Nwanya *et al.*, 2011).

Table 6: Incident photon-to-current conversion efficiency (IPCE) of the photo-sensitizers

Dyes No.	Wavelength λ_{max} (nm)	IPCE (%)
1	520	53.0
2	550	48.7

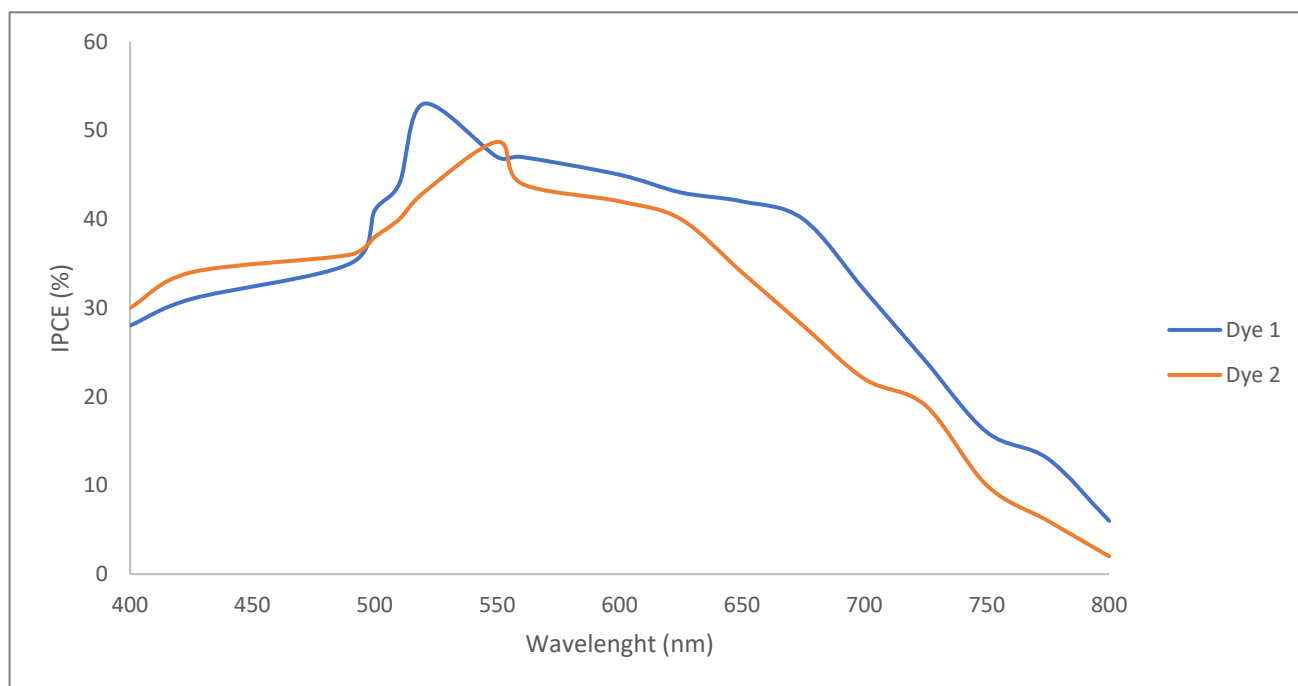


Figure 10: Spectrum of Incident photon-to-current conversion efficiency (IPCE) of the photo-sensitizers

The Incident Photon-to-Current Conversion Efficiency (IPCE) spectrum is shown in Figure 10, and the results are summarized in Table 6. The IPCE represents the efficiency with which absorbed photons are converted into electrical current, thereby reflecting the light-harvesting ability and electron-injection efficiency of the dyes in Dye-Sensitized Solar Cell (DSSC) applications. The IPCE results demonstrate that the synthesized naphthalimide-substituted azo dyes exhibit effective light-harvesting and photoelectrochemical properties. The enhanced performance of Dye 1 suggests that its molecular architecture provides more favorable donor- π -acceptor interactions, enabling efficient solar energy conversion in DSSC devices (Hosseinnazhad *et al.*, 2024a).

From Figure 10, both dyes exhibited broad photoresponse across the visible region (400-800 nm), confirming that the synthesized dyes are capable of harvesting a significant portion of solar radiation. This broad absorption behavior is attributed to the extended π -conjugation in the dye molecules, arising from the naphthalimide core, azo linkage ($-\text{N}=\text{N}-$), amino groups, and electron-withdrawing cyano substituents.

Dye 1 showed superior photovoltaic performance compared to Dye 2 across most of the visible spectrum. The maximum IPCE value of Dye 1 reached 53% at 520

nm, whereas Dye 2 exhibited a slightly lower maximum value of 48.7% at 550 nm. The higher IPCE response of Dye 1 suggests more efficient light absorption, electron excitation, and electron injection into the TiO_2 conduction band. This may be attributed to better molecular alignment, stronger electronic communication between donor and acceptor groups, or reduced charge recombination within the DSSC system. Nevertheless, both dyes displayed appreciable IPCE responses, confirming their suitability as sensitizers for DSSC applications (Hosseinnazhad *et al.*, 2024b).

CONCLUSION

The study successfully synthesized and characterized two novel naphthalimide-substituted azo dyes (Dye 1 and Dye 2) for use in Dye-Sensitized Solar Cell (DSSC) applications. Both dyes were synthesized with high yields (72.0% for Dye 1 and 70.0% for Dye 2) and exhibited strong thermal stability, with melting points ranging from 170°C to 178°C. The dyes showed strong absorption across the visible light spectrum (400-800 nm), which is essential for solar energy conversion. FT-IR spectra confirmed the presence of characteristic absorption bands corresponding to N-H/O-H stretching vibrations at frequency range of 3254-3608 cm^{-1} , azo linkages ($-\text{N}=\text{N}-$) appeared at 1505-1569 cm^{-1} , strong carbonyl

absorptions were detected between 1654 and 1729 cm^{-1} , and cyano groups were identified within 2278–2288 cm^{-1} , confirming successful incorporation of electron donor and electron acceptor functionalities into the dye framework. essential for DSSC sensitization. Mass spectrometric fragmentation patterns verified the presence of stable conjugated aromatic systems containing amino, azo, cyano, and imide groups. The ^1H and ^{13}C NMR spectra further validated the molecular structures and strong donor-acceptor interactions. Dye 1 showed a higher molar extinction coefficient, suggesting a greater ability to harvest photons than Dye 2. Despite Dye 2's better photon harvesting, Dye 1 achieved a higher Incident Photon-to-Current Conversion Efficiency (IPCE) of 53% at 520 nm, compared to 48.7% for Dye 2 at 550 nm. The enhanced IPCE performance of Dye 1 is attributed to more efficient electron injection into the TiO_2 conduction band and reduced charge recombination losses within the solar cell system. Thus, the synthesized naphthalimide-based azo dyes are promising, cost-effective, metal-free organic sensitizers for advancing DSSC technology.

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