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Exploring solvatochromism: a comprehensive analysis of research data of the solvent -solute interactions of 4-nitro-2-cyano-azo benzene-meta toluidine

Mahdi Shirali^{1*}, Shohre Rouhani², Kamaladin Gharanjig^{2,3} and Fatemeh Mirhashemi⁴

Abstract

This study investigates the solvatochromic behavior of a new D1 disperse dye, focusing on the 4-nitro-2-cyano-azo-Benzene-metaToluidine type. Using UV-visible spectroscopy, we analyze the dye's performance in single solvents and binary mixtures. Our analysis includes the evaluation of solvent polarity parameters and dye structure parameters, with emphasis on the longest wavelength intramolecular charge transfer absorption band. We identify nonlinear and linear patterns in the electronic transition energies plots with respect to solvent composition. Statistical analysis considers correlation coefficients, root mean squared error, mean absolute percentage error, and other parameters, providing insights into data accuracy and precision. This experimental and statistical study explores the absorption spectrum, wavelength characteristics, absorption energy, and polarity of a novel azo dye across various solvent and solute environments. These findings contribute to a comprehensive understanding of the dye's photophysical and photochemical properties, potentially enabling applications in optical sensors and advanced materials.

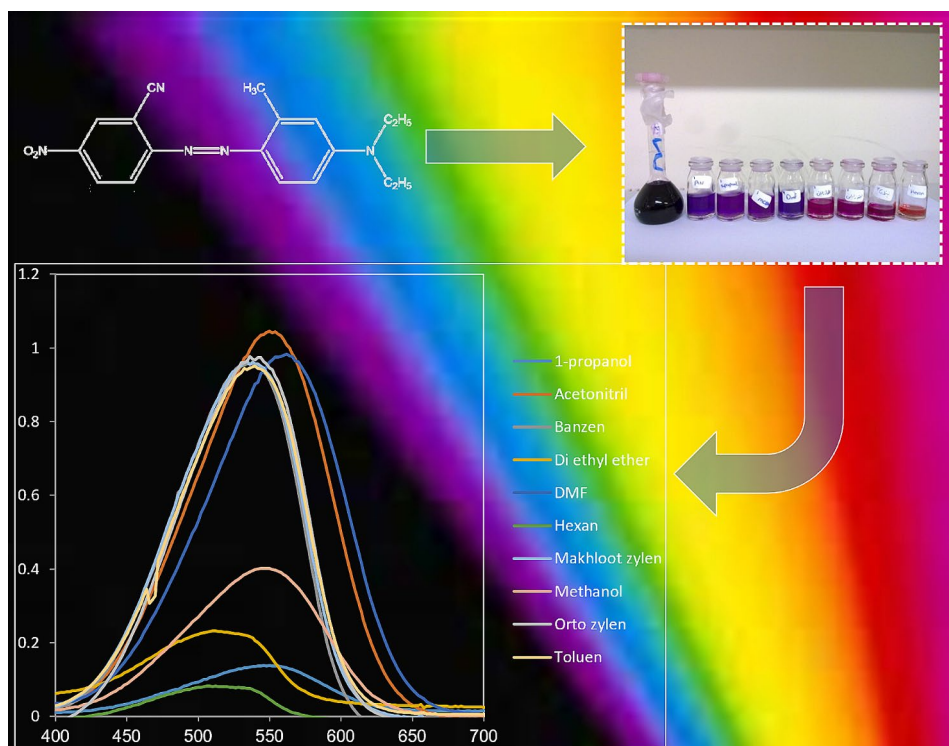
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Graphical abstract

Keywords Solvatochromic behavior, UV-visible spectroscopy, Statistical analysis

Introduction

It is declared that solvents properties including dielectric constant, refractive index values, the dipole moment and the most pivotal property in this regard, the solvent polarity have a significant effect on chemical and physical processes. The position of the absorption or emission spectra band of molecules can be adjusted by the solvent polarity [1–3].

Solvatochromism is a phenomenon that provides valuable information about the spectral shift of a solute induced by a change in the solvent polarity and describing the interactions that happen in the solvation shell of solute [4–7]. Solvatochromism estimates the local field of forces in the interior of liquids, indirectly, by the energy of the intermolecular interactions [8–11]. There are many several beneficial applications for this phenomenon in industrial and analytic purposes for instance they can be utilized to develop optical sensor materials to monitor pollutant levels in the environment [12–15] and also uses as a Lewis acid-base color indicator [16–21], imaging [22–25] and photo-switching [26, 27]. Conjugated molecules with electron-withdrawing and electron-donating groups can be considered an excellent solvatochromic probe because of the color change of these molecules can

be an indicator for solvent polarity. In these molecules, electron-withdrawing and electron-donating groups lead to charge transfer within the molecule itself [28]. Among the solvatochromic compounds Azo dyes have received great attention due to their wide application in the printing, plastics, textile, cosmetics and food industries [29, 30]. Furthermore, Azo dyes have been utilized as catalyzer exposing to ultraviolet light in photo-catalytic reactions [31]. Some azo dyes could be used as inhibitors for tumour-growth in biological systems [32–34]. The efficacy of azo colorants stems from the straightforwardness of their synthesis through diazotization and azo coupling processes. The versatility inherent in the myriad options available for the variation of both the diazo compound and coupling component contributes significantly to their success. Additionally, their typically high molar extinction coefficient, coupled with medium to high light and wet fastness properties, enhances their overall appeal [35].

ET (The electronic transition energy of the solute in maximum absorption) is a function of all types of interactions between solvent components and solute. These interactions are two types including nonspecific interactions such as polarity–polarizability interactions and

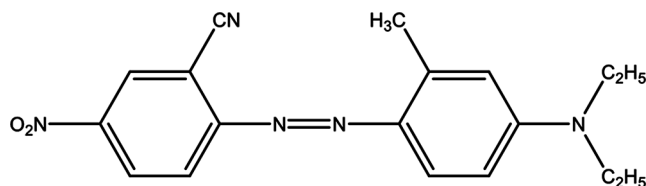


Fig. 1 Molecular structure of the azo dispersion dye used in the study

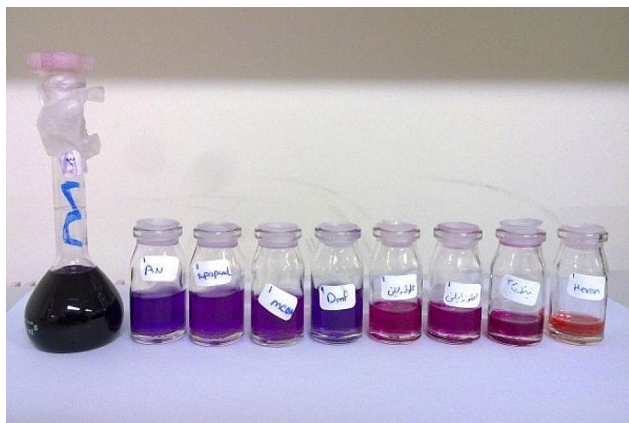


Fig. 2 D1 concentrations in various solvents

specific interactions such as hydrogen bonding and electron donor acceptor interactions [36–38]. ET parameters of a solute can be used in order to achieve information about the preferential solvation phenomena in the mixed solvent. Also, the change in position of the absorption maxima and therefore ET values upon changing the solvent composition can reveal the type of the solute-solvent as well as solvent-solvent interactions occurring in the solvent mixtures [39].

In this current research, an analytical exploration has been conducted utilizing both inductive and abductive approaches to analyze the structure of azo dye. Our

primary focus is on investigating changes in the absorption energy of a typical azo disperse dye in various polarities of aprotic, protic, and non-polar solvents. Through the calculation of statistical parameters such as correlation, standard deviation, standard error, p-value, T-critical, RMSE (root mean squared error), and MAPE (mean absolute percentage error), as well as the presentation of formulas in Figs. 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23 and 24; Tables 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22 and 23, a comprehensive evaluation and index of the interaction effect and changes in the studied components of the new azo dye structure have been obtained.

This study encompasses a spectroscopic examination and experimental as well as theoretical analysis of the statistical behavior of solvatochromism, along with inductive and analogical reasoning, concerning absorption changes, absorption energy, and wavelength shifts of the D1 disperse dye. Bathochromic and hypsochromic shifts are investigated in relation to the influence of intermolecular interactions, molecular polarizability, vibrational effects, and environmental screening across various solvents. These findings offer a comprehensive understanding of the solvatochromic and absorption characteristics of azo dyes in diverse solvent environments with distinct structural features. The primary objective of this research is to establish a conclusive link between data structure analysis and the combination of electron-donating

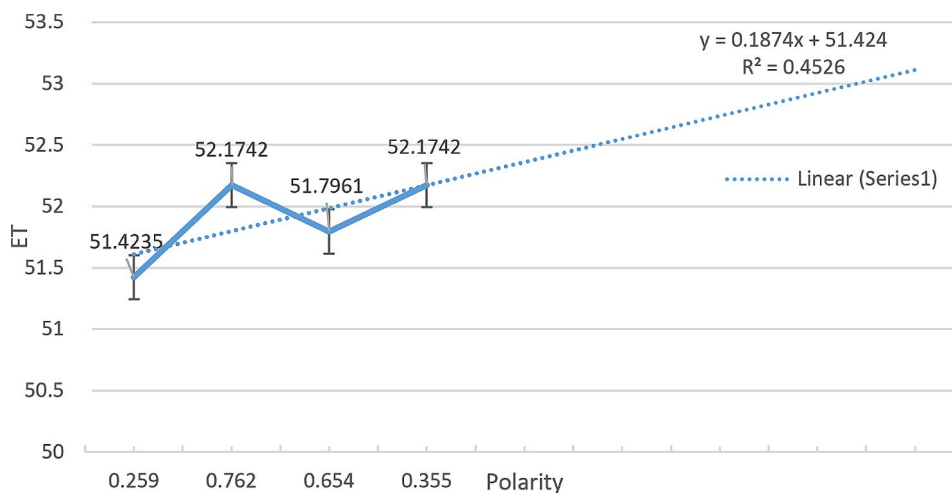


Fig. 3 Absorption energy changes of disperse dye D1 with solvent polarity variation (chloroform, methanol, ethanol, acetone)

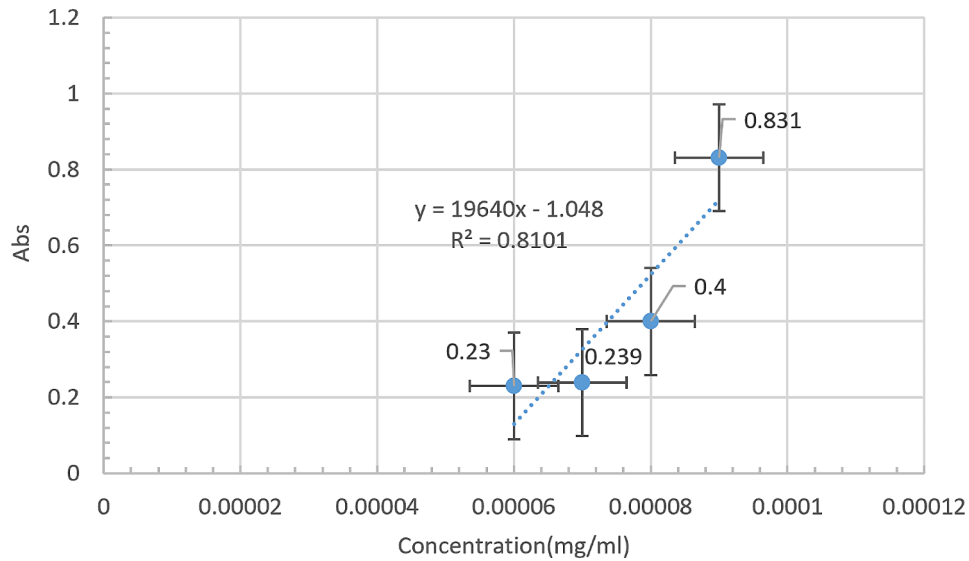


Fig. 4 Displays the absorption spectrum graph corresponding to varying concentrations of disperse azo dye D1

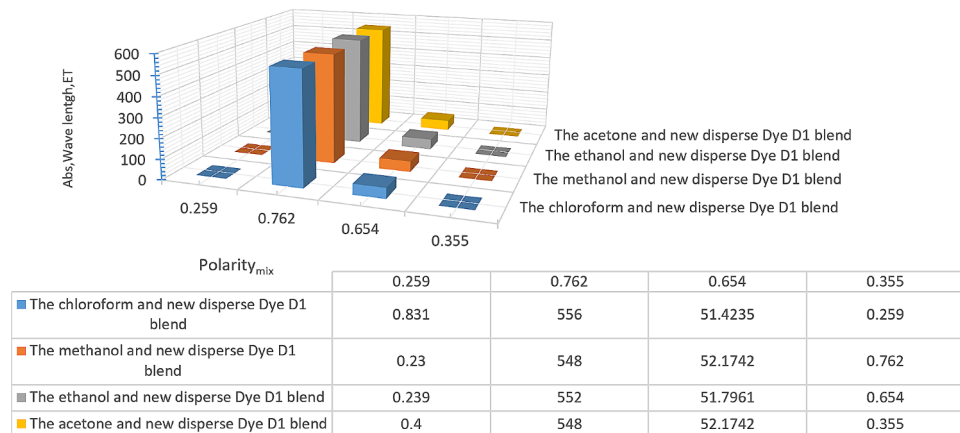


Fig. 5 3-D Column analyzing changes in absorption, absorption energy, and wavelength of disperse dye D1 in response to solvent polarity (chloroform, methanol, ethanol, and acetone)

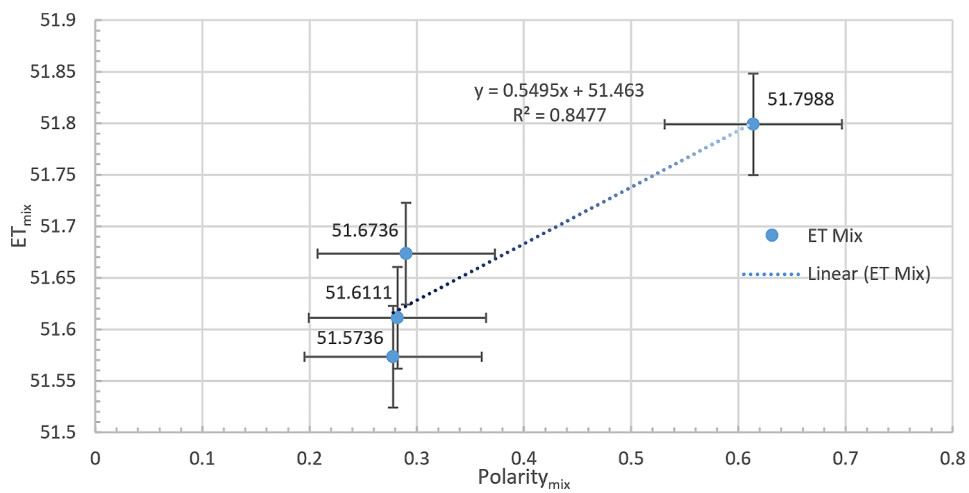
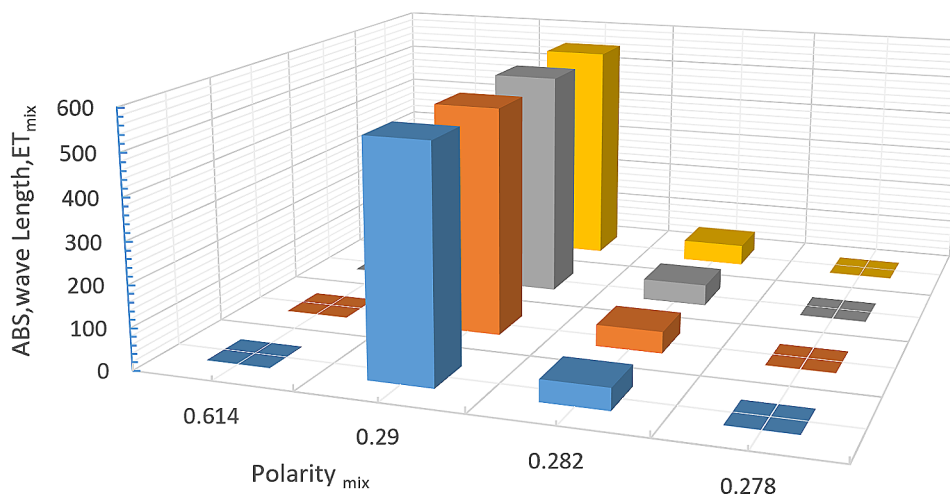


Fig. 6 Analysis of changes in absorption energy of disperse dye D1 in response to new polarity of chloroform-acetone mixtures with varying ratios



	0.614	0.29	0.282	0.278
■ The 1:1 ratio mixture of chloroform and acetone	0.311	552	51.7988	0.614
■ The 2:1 ratio mixture of chloroform and acetone	0.23	548	51.6736	0.29
■ The 3:1 ratio mixture of chloroform and acetone	0.232	552	51.6111	0.282
■ The 4:1 ratio mixture of chloroform and acetone	0.215	554	51.5736	0.278

Fig. 7 3-D column graph analyzing changes in absorption, absorption energy, and wavelength of disperse dye D1 in response to new polarity of chloroform-acetone mixtures with varying ratios

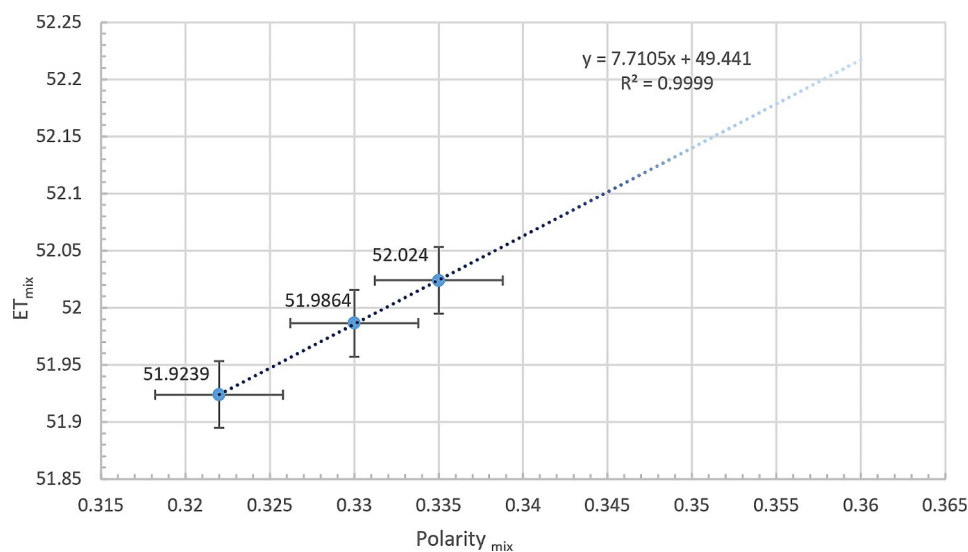


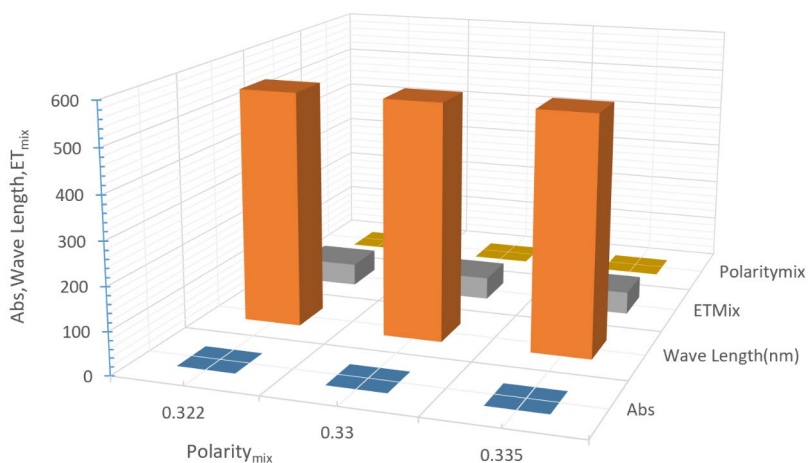
Fig. 8 Analysis of changes in absorption energy of disperse dye D1 in response to new polarity of acetone-chloroform mixtures with varying ratios

and electron-accepting substitutions within the azo dye structure. This aims to derive a pertinent and practical abstract concept that can serve as a model for the development of novel azo dye structures, laying the groundwork for the integration of artificial intelligence into the design of these new azo dyes.

Experimental methodology

Materials and reagents

All materials were sourced from Merck with a high degree of purity. The solvents used were as follows:



	0.322	0.33	0.335
Abs	0.286	0.31	0.312
Wave Length(nm)	552	552	552
ETmix	51.9239	51.9864	52.024
Polaritymix	0.322	0.33	0.335

Fig. 9 3-D Column graph analyzing changes in absorption, absorption energy, and wavelength of disperse dye D1 in response to new polarity of acetone-chloroform mixtures with varying ratios

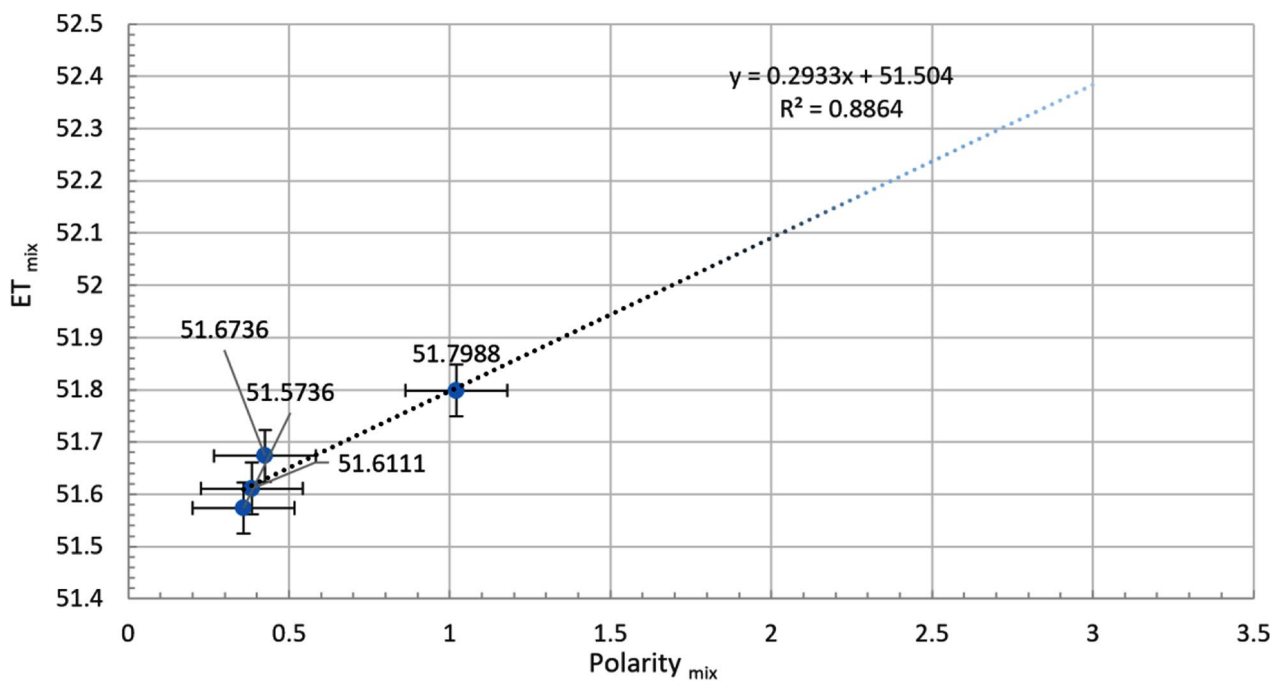


Fig. 10 Analysis of changes in absorption energy of disperse dye D1 in response to new polarity of methanol-chloroform mixtures with varying ratios

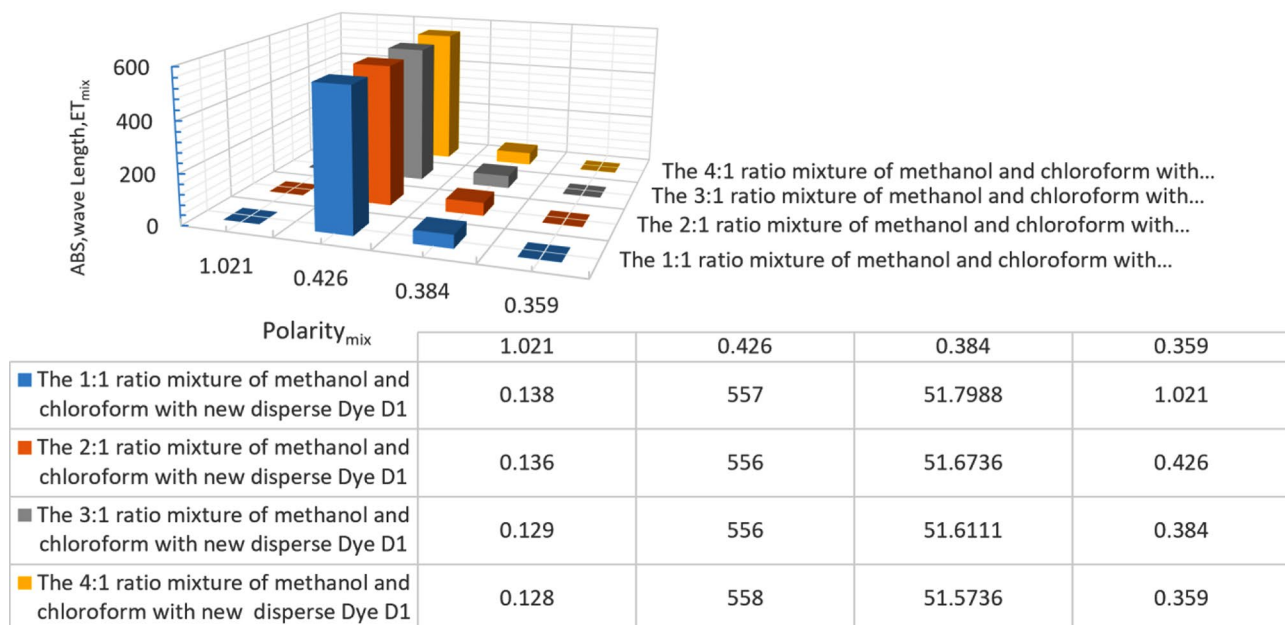


Fig. 11 3-D column graph analyzing changes in absorption, new absorption energy, and wavelength of disperse dye D1 in response to new polarity of methanol-chloroform mixtures with varying ratios

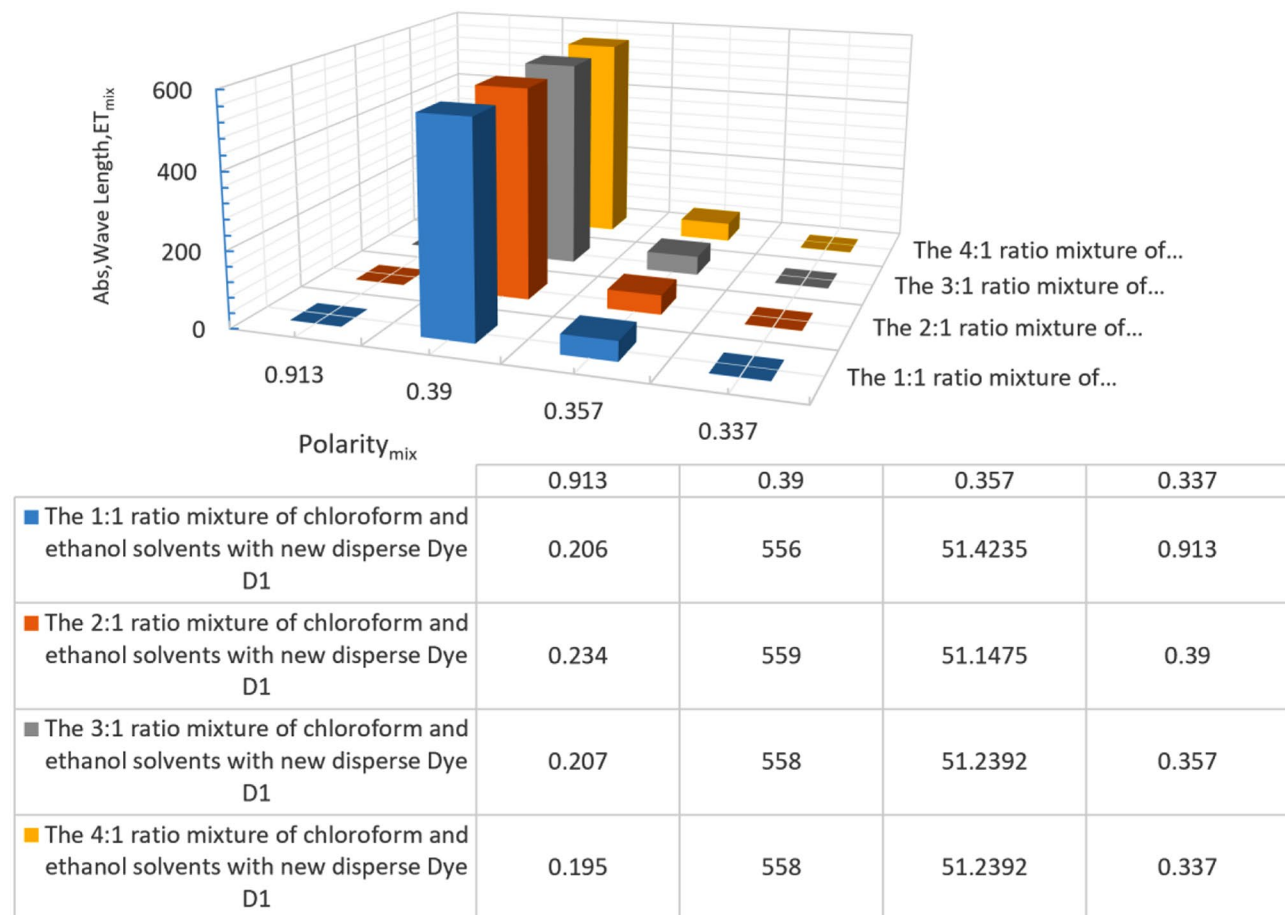


Fig. 12 3-D column graph analyzing changes in absorption, new absorption energy, and wavelength of disperse dye D1 in response to new polarity of chloroform-ethanol mixtures with varying ratios

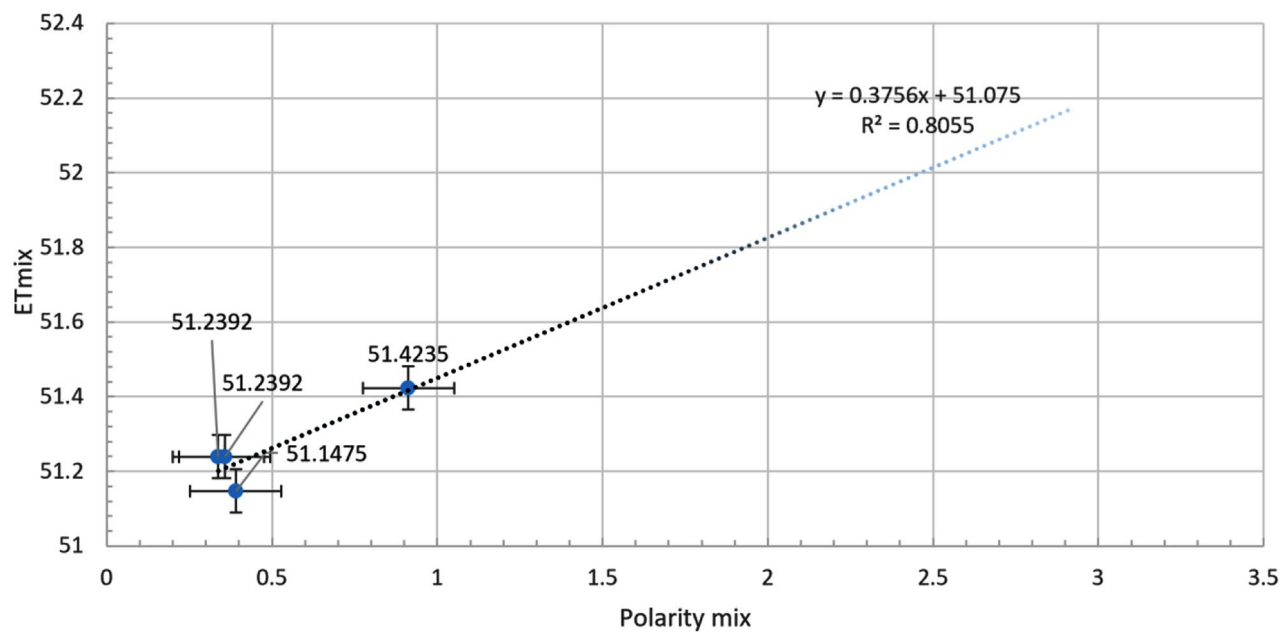


Fig. 13 Analysis of changes in absorption energy of disperse dye D1 in response to variations in the polarity of chloroform-ethanol mixtures with different ratios

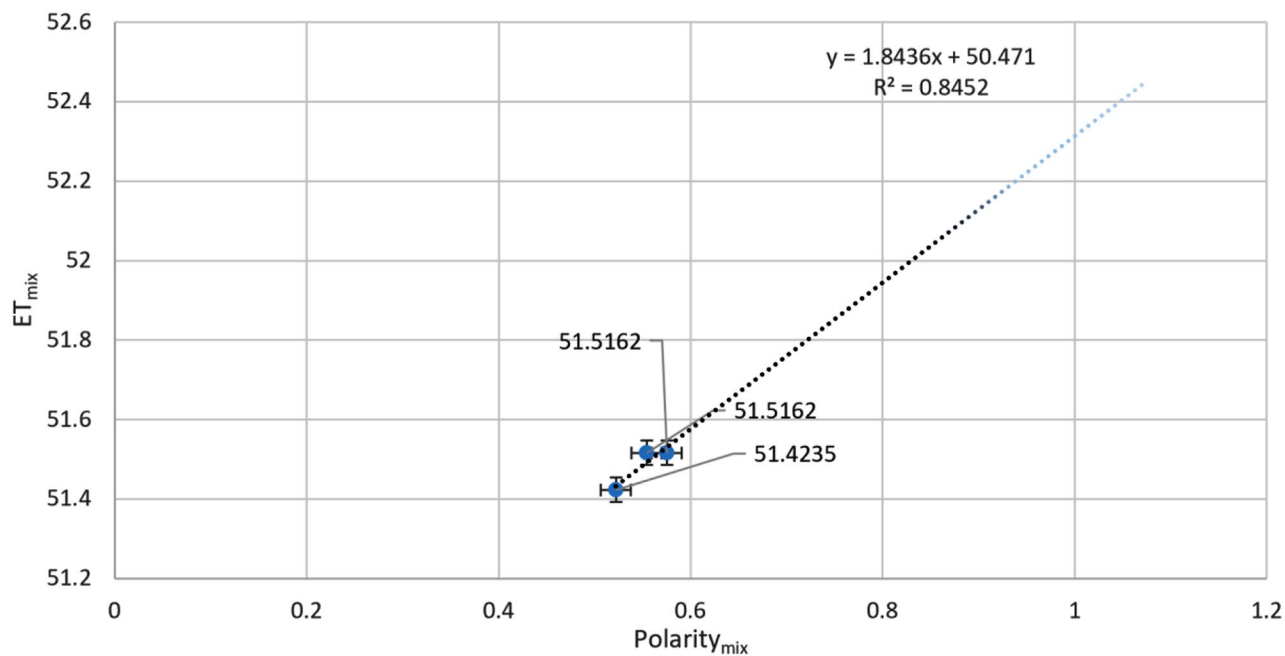
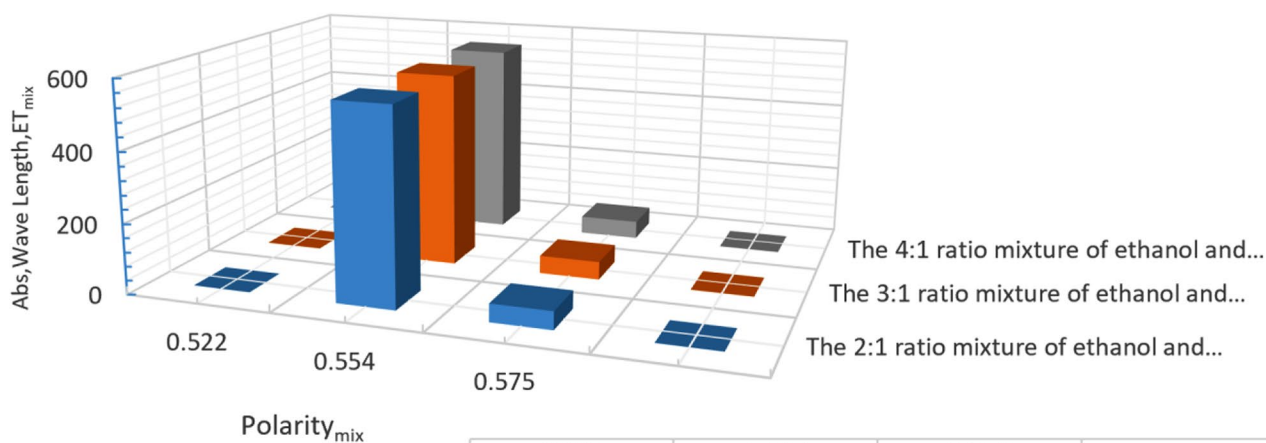


Fig. 14 Analysis of new absorption energy changes in response to altered polarity within ethanol-chloroform mixtures featuring different ratios for disperse dye D1



	0.522	0.554	0.575	
■ The 2:1 ratio mixture of ethanol and chloroform with new disperse Dye D1	0.267	556	51.4235	0.522
■ The 3:1 ratio mixture of ethanol and chloroform with new disperse Dye D1	0.273	555	51.5162	0.554
■ The 4:1 ratio mixture of ethanol and chloroform with new disperse Dye D1	0.302	555	51.5162	0.575

Fig. 15 Analysis of 3-D changes in absorption, new absorption energy, and wavelength of disperse dye D1 in response to altered polarity in ethanol-chloroform mixtures with varied ratios

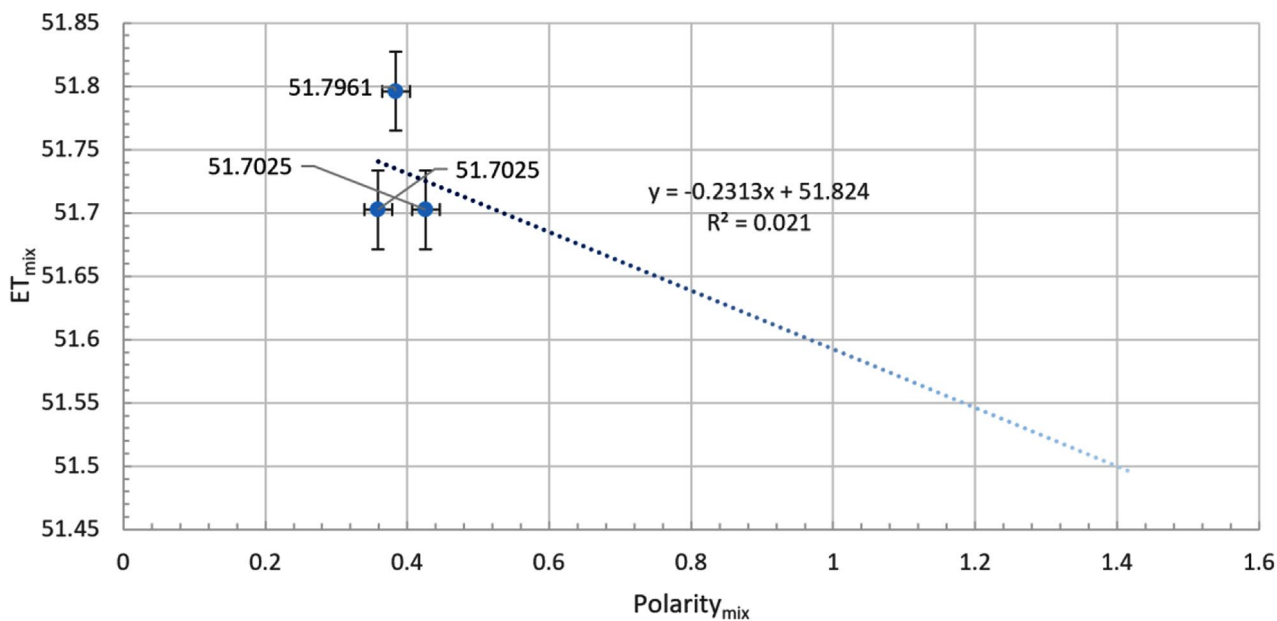


Fig. 16 Variations in new absorption energy of novel disperse Dye D1 with respect to the polarity of chloroform and methanol solvent mixture at various ratios

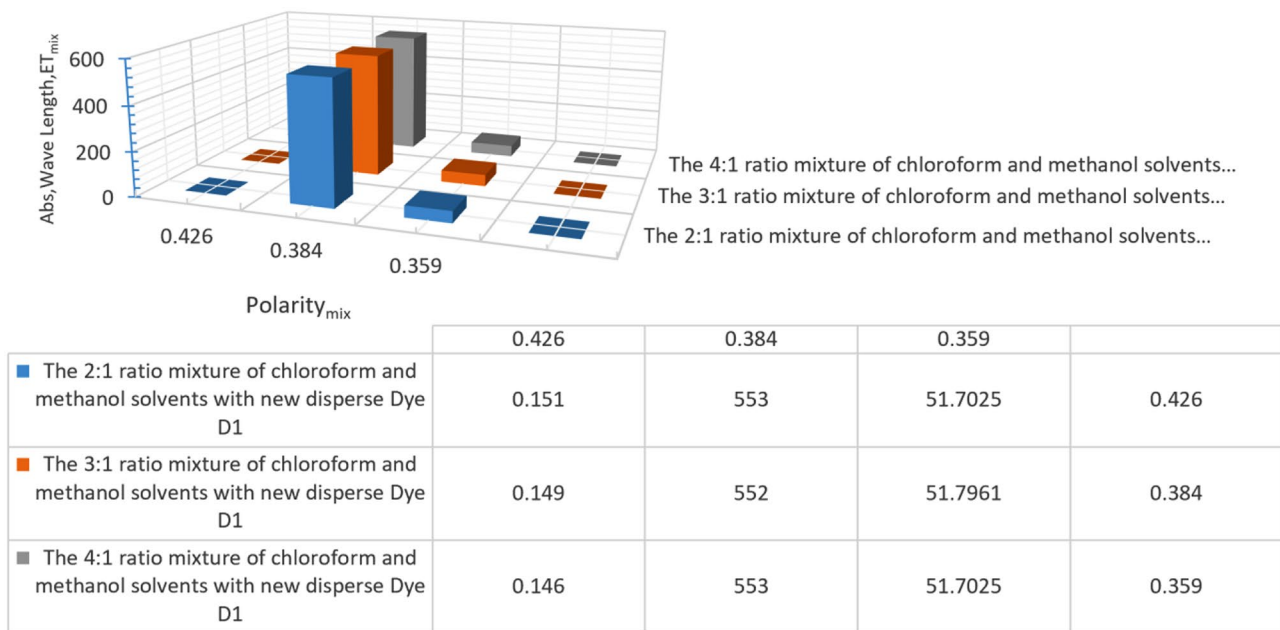


Fig. 17 3-D Column graph depicting changes in absorption, new absorption energy, and wavelength of novel Disperse Dye D1 with varying ratios of a chloroform-methanol solvent mixture

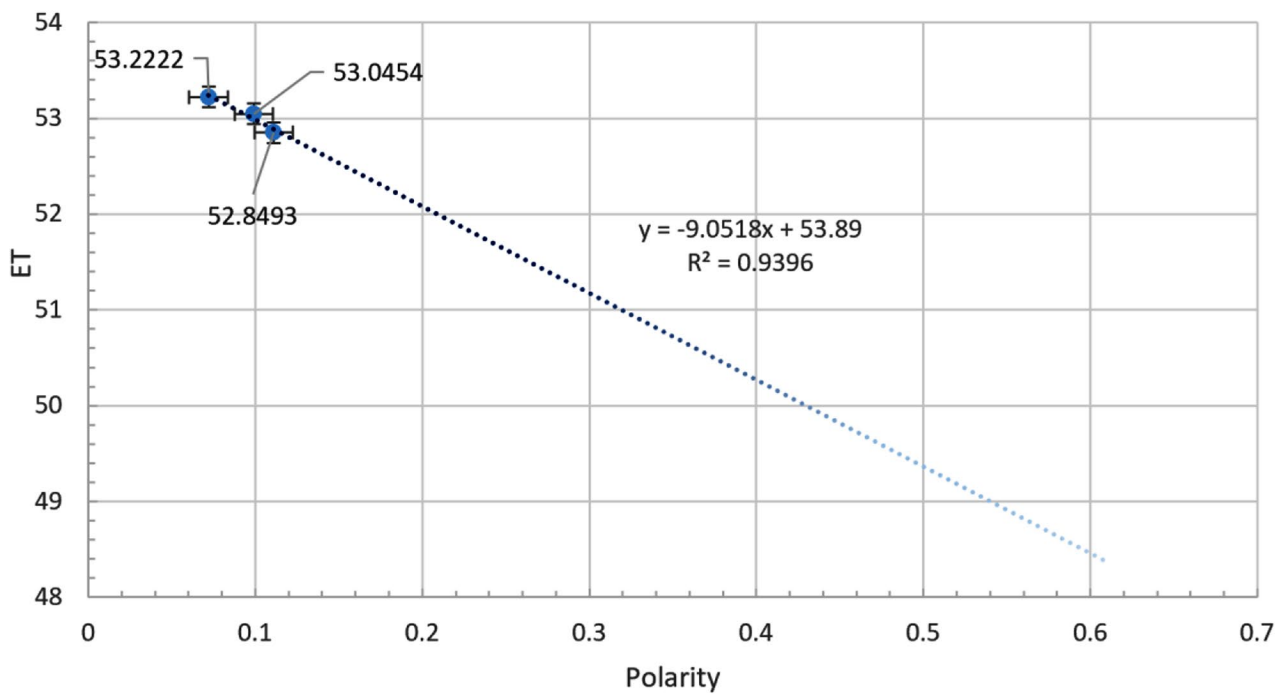


Fig. 18 Variations in absorption energy of new disperse dye D1 with polarity changes in benzene, toluene, and xylene solvents

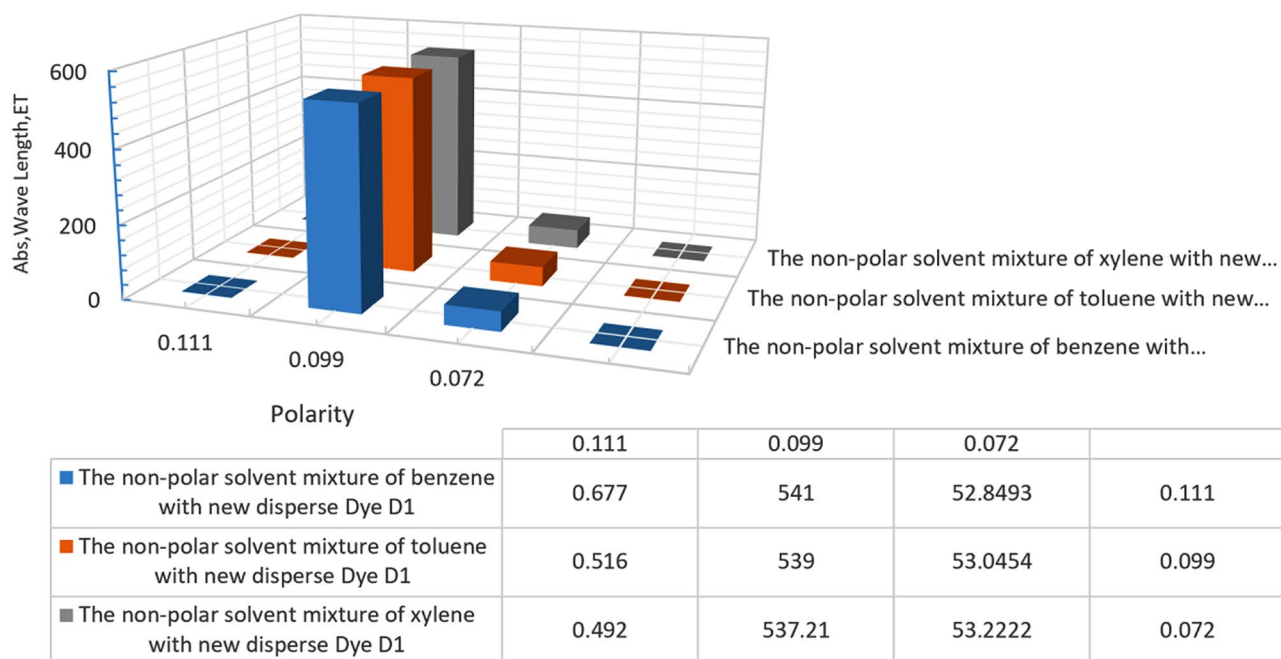


Fig. 19 Changes in absorption, absorption energy, and wavelength of typical dispersion dye D1 in response to polarity variations in non-polar solvents—benzene, toluene, and xylene

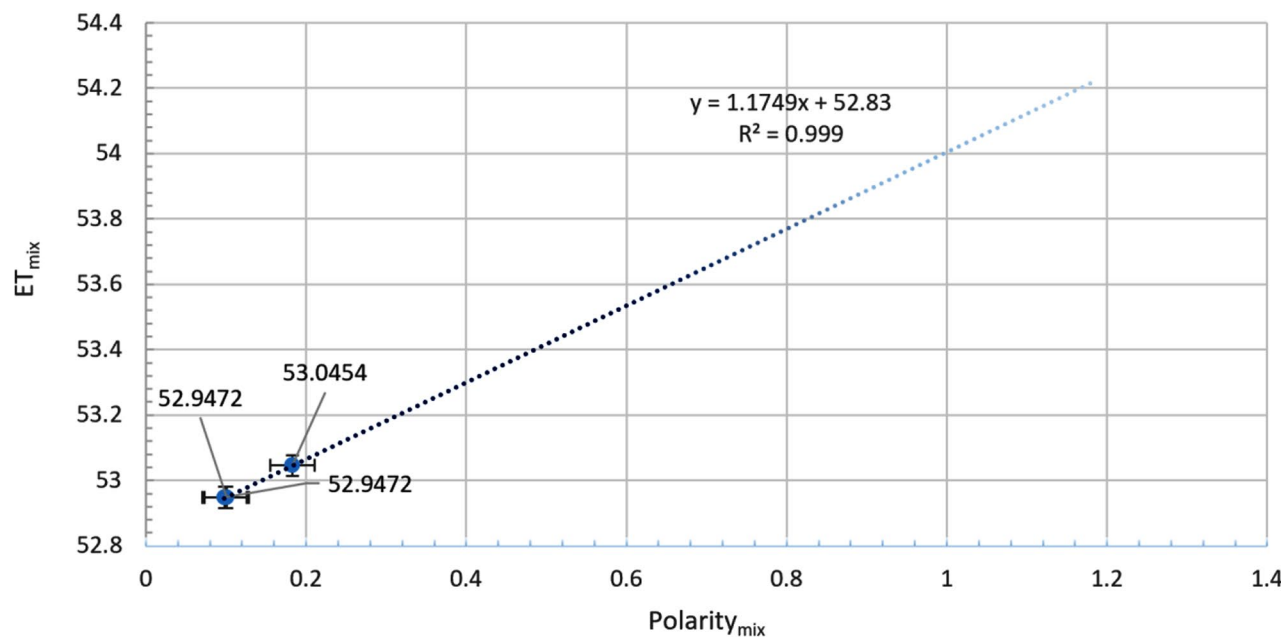


Fig. 20 Depicts the relationship between new polarity of non-polar solvents (benzene, toluene, and xylene) at various ratios and corresponding changes in new absorption energy for new dispersion dye D1

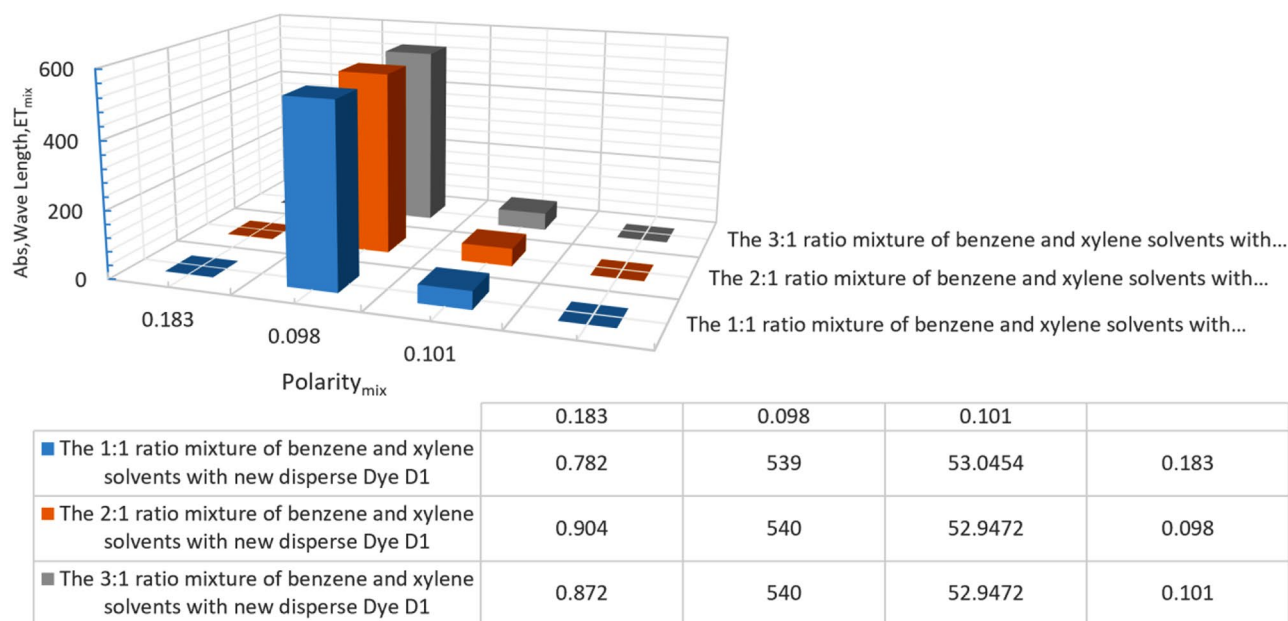


Fig. 21 3-D column graph exploring changes in absorption, new absorption energy, and wavelength of new dispersion dye D1. investigation emphasizes variations in polarity within non-polar solvents—benzene, toluene, and xylene—at different ratios

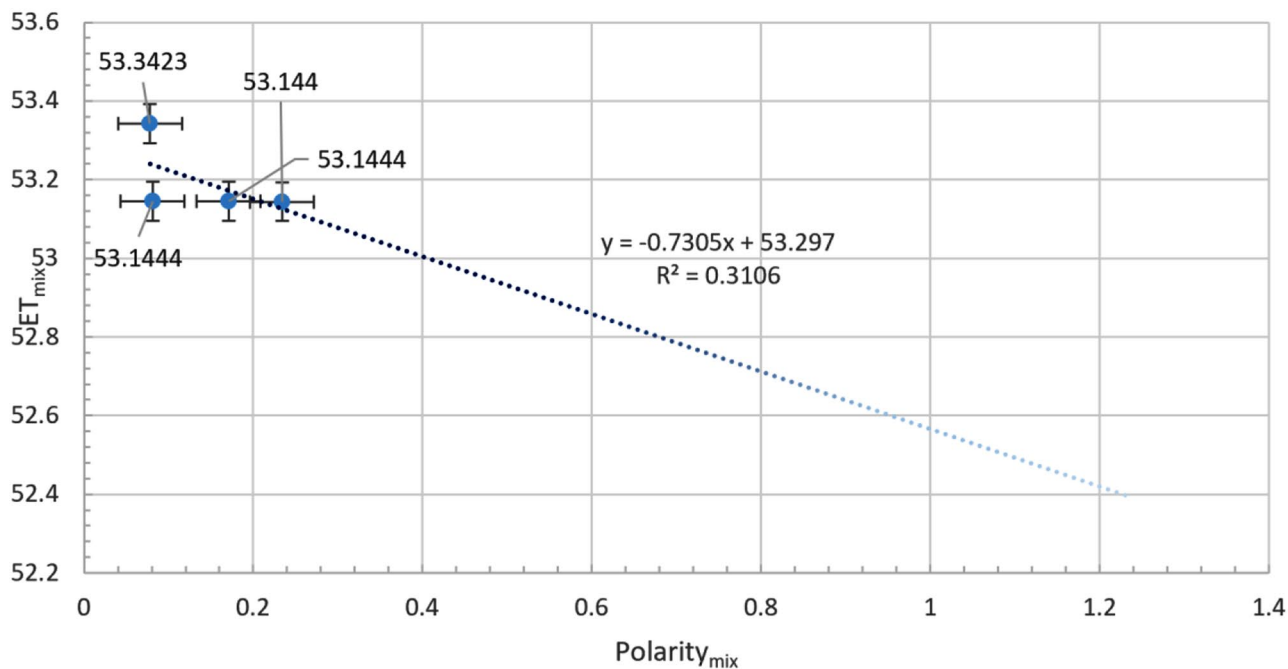


Fig. 22 Graphical analysis of changes in new absorption energy as new dispersion dye D1 is exposed to toluene and xylene solvents at different ratios. the graph highlights a linear relationship, emphasizing the impact of solvent polarity on the dye’s absorption energy

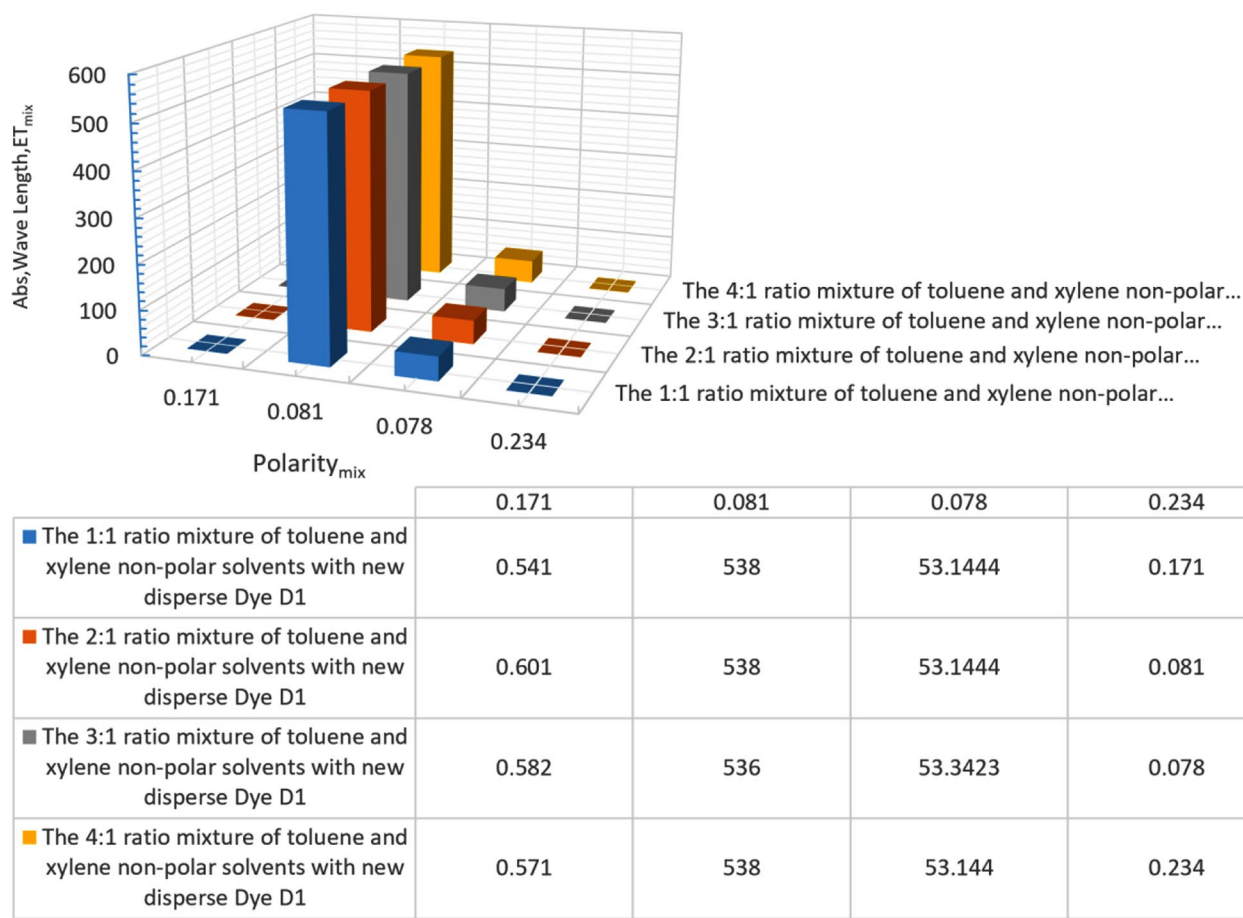


Fig. 23 3-D column graph illustrating changes in absorption, new absorption energy, and wavelength of novel dispersion dye D1 in response to varying polarity of non-polar solvents—toluene and xylene—at different ratios

Polar Aprotic Solvents: Acetone (purity>99.8%, ϵ : (dielectric constant): 20.7), Formaldehyde (purity>99.8%, ϵ : 38.3) and Acetonitrile (purity>99.8%, ϵ : 35.09).

Non-Polar Solvents: Chloroform (purity>99.5%, ϵ : 4.72), Hexane (purity>99.5%, ϵ : 2.02), Toluene (purity>99.5%, ϵ : 2.38), Benzene (purity>99.5%, ϵ : 2.15), Orthoxylene (purity>99.5%, ϵ : 2.57) and Diethyl Ether (purity>99.5%, ϵ : 4.33).

Polar protic solvent: Methanol (purity>99.8%, ϵ : 32.7), Propanol (purity>99.8%, ϵ : 20.1).

Totally, polar protic solvents contain hydrogen atoms connected directly to highly electronegative atoms like oxygen or nitrogen, enabling them to participate in hydrogen bonding. Polar aprotic solvents lack hydrogen atoms capable of hydrogen bonding, but still possess polar bonds. Nonpolar solvents lack significant dipole moments and do not readily interact with ionic compounds or polar molecules.

Experimental equipment

The following equipment was utilized for the experiments: Multi spec-1501 Shimadzu spectrophotometer

(The MultiSpec-1501 can acquire spectra over the entire wavelength range in just 100 milliseconds, company: Shimadzu Corporation), EQ-OC1-19 double-beam UV-Vis Spectrophotometer SP-LUV1910/SP-LUV1920 (Wavelength range: 190 nm~1100 nm, company: Infitek China), spectroluminescence device and T80 UV/vis spectrometer: (Wavelength range: 190 nm~1100 nm, company: Infitek China).

Statistical analysis of solvatochromism effects on new disperse dye D1 in single-solvent and dual-solvent systems

In this section, we delve into the statistical analysis of the solvatochromism behavior of new disperse dye D1 within both single-solvent and dual-solvent systems. Single-solvent and dual-solvent systems, comprising solvents with diverse structural and functional properties, encompass non-polar, polar aprotic, and polar protic solvents. Solutions containing electrolytes and more than one solvent are commonly referred to as mixed solvent systems. Also, Single solvent systems refer to a solvent system that consists of only one solvent, while dual solvent systems

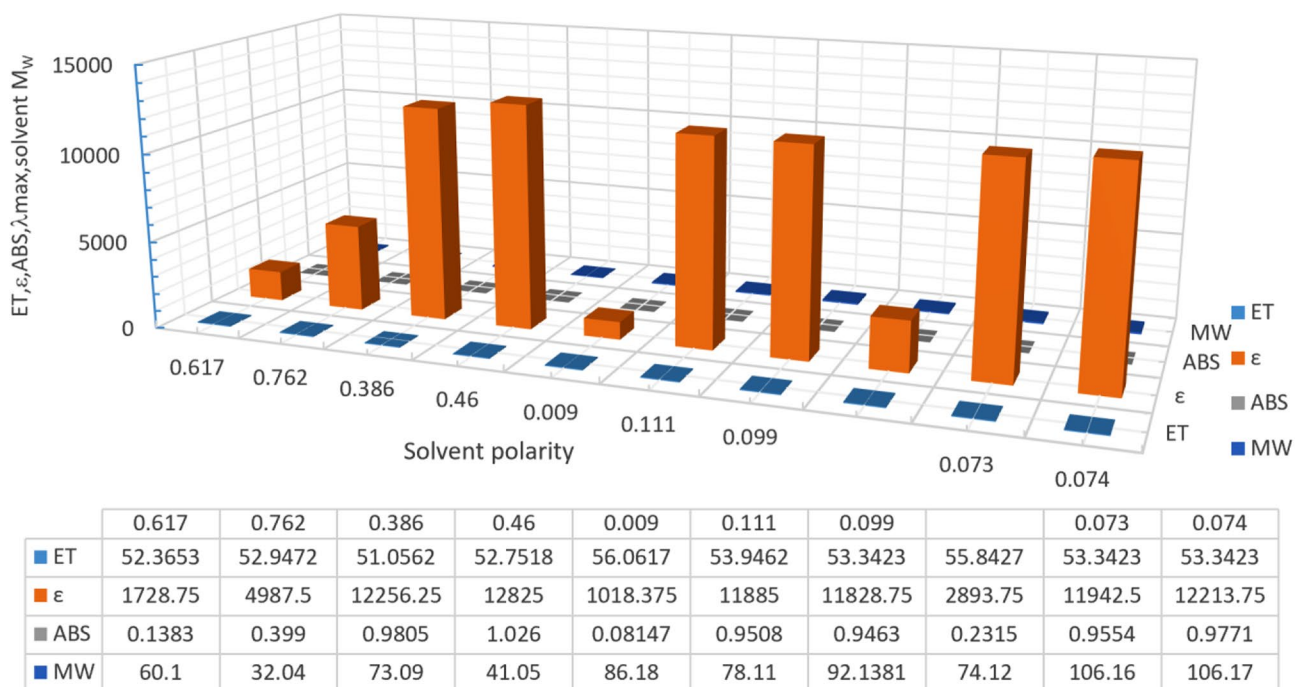


Fig. 24 Presents a comprehensive analysis of statistical data pertaining to various solvent structures and their influence on solvent polarity. This 3-D column graph visually depicts the intricate interaction between solvent polarity and crucial components, encompassing absorption energy, extinction coefficient, maximum wavelength, and molecular weight. The graph serves as a visual representation, illustrating how shifts in solvent polarity impact these essential parameters

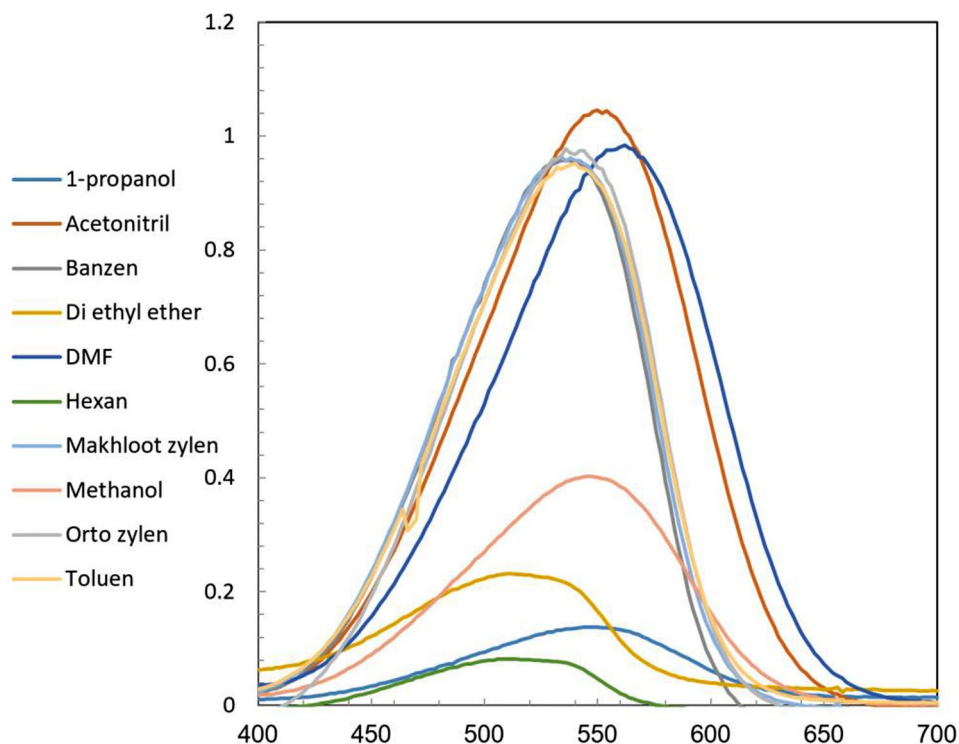


Fig. 25 Analysis of absorption test results measurement for new disperse dye D1 in various solvents (Fig. 25; Table 11)

Table 1 The measurement of variations in polarity, absorption energy, wavelength, and absorption of new disperse dye D1 in different solvents

The blending of diverse solvents with novel disperse dye D1	Abs	Wave Length(nm)	Et	Po-lar-ity*
The chloroform and novel disperse dye D1 blend	0.831	556	51.4235	0.259
The methanol and novel disperse dye D1 blend	0.23	548	52.1742	0.762
The ethanol and novel disperse dye D1 blend	0.239	552	51.796	0.654
The acetone and novel disperse dye D1 blend	0.4	548	52.1742	0.355

*The polarity of a solvent is determined by its solvation behavior, which in turn depends on the action of intermolecular forces (Coulomb, directional, inductive, dispersion, and charge transfer forces as well as hydrogen bonding forces) between the solvent and the solute

Table 2 The measurement of variations in polarity, absorption energy, wavelength, and absorption of disperse dye D1 in chloroform-acetone mixtures with varying ratios

The solvent-dye D1 mixture with varying ratios	Abs	Wave Length (nm)	Et _{mix}	Po-lar-ity _{mix}
The 1:1 ratio mixture of chloroform and acetone	0.311	552	51.7988	0.614
The 2:1 ratio mixture of chloroform and acetone	0.23	548	51.6736	0.29
The 3:1 ratio mixture of chloroform and acetone	0.232	552	51.6111	0.282
The 4:1 ratio mixture of chloroform and acetone	0.215	554	51.5736	0.278

Table 3 The measurement of variations in polarity, absorption energy, wavelength, and absorption of disperse dye D1 in acetone-chloroform mixtures with varying ratios

Mixture of solvents with novel dispersion dye D1 in different proportions	Abs	Wave Length (nm)	Et _{mix}	Po-lar-ity _{mix}
A mixture of acetone and chloroform with a ratio of 2:1	0.286	552	51.9239	0.322
A mixture of acetone and chloroform with a ratio of 3:1	0.31	552	51.9864	0.33
A mixture of acetone and chloroform with a ratio of 4:1	0.312	552	52.024	0.335

involve the use of two different solvents in a system. These systems are commonly used in various fields such as chemistry, pharmaceuticals, and material science for different purposes, including extraction, purification, and synthesis processes, this analysis aims to provide a comprehensive understanding of the dye's behavior in different solvent environments.

Table 4 The measurement of variations in new polarity, new absorption energy, wavelength, and absorption of disperse dye D1 in methanol-chloroform mixtures with varying ratios

The mixture of methanol and chloroform with novel disperse dye D1 in different proportions	Abs	Wave Length (nm)	Et _{mix}	Po-lar-ity _{mix}
The mixture of methanol and chloroform with novel disperse dye in a ratio of 1:1	0.138	557	51.7988	1.021
The mixture of methanol and chloroform with novel disperse dye with a ratio of 2:1	0.136	556	51.6736	0.426
The mixture of methanol and chloroform with novel disperse dye with a ratio of 3:1	0.129	556	51.6111	0.384
The mixture of methanol and chloroform with novel disperse dye in a ratio of 4:1	0.128	558	51.5736	0.359

Table 5 The measurement of variations in new polarity, new absorption energy, wavelength, and absorption of disperse dye D1 in chloroform-ethanol mixtures with varying ratios

The mixture of chloroform and ethanol solvents with new disperse dye D1 in different ratios	Abs	Wave Length (nm)	Et _{mix}	Po-lar-ity _{mix}
The mixture of chloroform and ethanol solvents with a new disperse dye with a ratio of 1:1	0.206	556	51.4235	0.913
The mixture of chloroform and ethanol solvents with a new disperse dye with a ratio of 2:1	0.234	559	51.1475	0.39
The mixture of chloroform and ethanol solvents with a new disperse dye with a ratio of 3:1	0.207	558	51.2392	0.357
The mixture of chloroform and ethanol solvents with a new disperse dye with a ratio of 4:1	0.195	558	51.2392	0.337

Investigation of solvatochromism's influence on solute-solvent interactions

In this study, we explored the impact of solvatochromism on solute-solvent interactions by employing spectroscopic statistical data analysis. Our focus was on the behavior of the well-established disperse dye, D1, when introduced to solvents with diverse structural and functional properties, encompassing non-polar, polar aprotic, and polar protic solvents.

By scrutinizing the alterations in absorption position, intensity, and spectral shape, and by examining the wavelength characteristics of the spectrophotometric device, we analyzed how the color attributes of the new

Table 6 Analysis of measurement variations in new polarity, new absorption energy, wavelength, and absorption of disperse dye D1 in ethanol-chloroform mixtures with varying ratios

The mixture of ethanol and chloroform with new disperse dye D1 in different proportions	Abs	Wave Length (nm)	Et _{mix}	Polarity _{mix}
The mixture of ethanol and chloroform with a new disperse dye at a ratio of 2:1	0.267	556	51.4235	0.522
The mixture of ethanol and chloroform with a new disperse dye at a ratio of 3:1	0.273	555	51.5162	0.554
The mixture of ethanol and chloroform with a new disperse dye at a ratio of 4:1	0.302	555	51.5162	0.575

Table 7 Analysis of measurement changes in new polarity, new absorption energy, wavelength, and absorption of novel disperse dye D1 in chloroform and methanol mixtures with varying ratios

The mixture of chloroform and methanol solvents with a novel disperse dye D1 in different proportions	Abs	Wave Length (nm)	Et _{mix}	Polarity _{mix}
The mixture of chloroform and methanol solvents with a novel disperse dye with a ratio of 2:1	0.151	553	51.7025	0.426
The mixture of chloroform and methanol solvents with a novel disperse dye with a ratio of 3:1	0.149	552	51.7961	0.384
The mixture of chloroform and methanol solvents with a novel disperse dye with a ratio of 4:1	0.146	553	51.7025	0.359

Table 8 Investigation of measurement changes in new polarity, new absorption energy, wavelength, and absorption disperse dye D1 in non-polar solvents (benzene, toluene, and xylene)

Mixture of non-polar solvents in novel disperse paint	Abs	Wave Length (nm)	Et	Polarity
Non-polar solvent mixture of benzene in novel disperse dye	0.677	541	52.8493	0.111
Non-polar solvent mixture of toluene in novel disperse dye	0.516	539	53.0454	0.099
Non-polar solvent mixture of xylene in novel disperse dye	0.492	537.21	53.2222	0.072

azo dispersion D1 evolved within solvents characterized by different polarities and distinct intermolecular interactions, including ion-dipole, dipole-dipole, induced dipole-dipole, and hydrogen bonding. Furthermore, we conducted both experimental and theoretical assessments of alterations in adsorption and desorption energies and other pertinent parameters associated with the novel structure of azo dye D1.

Table 9 Investigation of measurement changes in new polarity, new absorption energy, wavelength, and absorption of non-polar solvents (benzene and xylene) when mixed with typical dispersion dye D1 at various ratios

The mixture of benzene and xylene solvents with novel disperse dye D1 in different proportions	Abs	Wave Length (nm)	Et _{mix}	Polarity _{mix}
The mixture of benzene and xylene solvents with a novel dispersion color at a ratio of 1:1	0.782	539	53.0454	0.183
The mixture of benzene and xylene solvents with a novel dispersion color at a ratio of 2:1	0.904	540	52.9472	0.098
The mixture of benzene and xylene solvents with a novel dispersion color at a ratio of 3:1	0.872	540	52.9472	0.101

Table 10 Comprehensive analysis of measurement changes in new polarity, new absorption energy, wavelength, and absorption characteristics in non-polar solvents (toluene and xylene) interacting with new dispersion dye D1 at different ratios

The non-polar solvent mixture of toluene and xylene with a new disperse dye D1 in different ratios	Abs	Wave Length (nm)	Et _{mix}	Polarity _{mix}
The non-polar solvent mixture of toluene and xylene with a new dispersion dye with a ratio of 1:1	0.541	538	53.1444	0.171
The non-polar solvent mixture of toluene and xylene with a new dispersion color with a ratio of 2:1	0.601	538	53.1444	0.081
The non-polar solvent mixture of toluene and xylene with a new dispersion color with a ratio of 3:1	0.582	536	53.3423	0.078
The non-polar solvent mixture of toluene and xylene with a new dispersion color with a ratio of 4:1	0.571	538	53.144	0.234

Significance of absorption spectrum, absorption energy, solute-solvent interactions, and solvent-solvent behavior

The absorption spectrum and absorption energy of a dye are critical parameters that yield valuable insights into its structure and properties. In the case of a novel azo dye within a disperse dye, the absorption spectrum helps identify the wavelengths at which the dye absorbs light, revealing its color characteristics. Additionally, analyzing absorption energy provides a deeper understanding of the electronic transitions occurring within the dye molecule. When examining the dye's behavior in mixed solvents, it is essential to consider solute-solvent interactions. The interaction between the dye molecule and

Table 11 Comprehensive analysis of measurement changes and statistical summary of investigated components in conventional disperse dye D1 and corresponding solvent structures

Et	ϵ	Abs	λ_{max}	Solvent polarity	Solvent	Mw
Polarprotic solvent						
52.3653	1728.75	0.1383	546	0.617	1- Propanol	60.1
52.9472	4987.5	0.399	540	0.762	Methanol	32.04
Polaraprotic solvent						
51.0562	12256.25	0.9805	560	0.386	DMF	73.09
52.7518	12,825	1.026	542	0.46	Acetonitrile	41.05
Non-polar solvent						
56.0617	1018.375	0.08147	510	0.009	Hexane	86.18
53.9462	11,885	0.9508	530	0.111	Benzene	78.11
53.3423	11828.75	0.9463	536	0.099	Toluene	92.1381
55.8427	2893.75	0.2315	512	NO	Diethyl ether	74.12
53.3423	11942.5	0.9554	536	0.073	Mixture of xylene	106.16
53.3423	12213.75	0.9771	536	0.074	Ortho xylene	106.17

Table 12 Statistical analysis of adsorption energy data for various solvents interacting with representative disperse dye D1

Disperse dye D1	
Mean	53.4998
Standard Error	0.476670696
Median	53.3423
Mode	53.3423
Standard Deviation	1.507365093
Sample Variance	2.272149522
Kurtosis	0.351932208
Skewness	0.531790578
Range	5.0055
Minimum	51.0562
Maximum	56.0617
Sum	534.998
Count	10
Largest (1)	56.0617
Smallest (1)	51.0562
Confidence Level (95.0%)	1.078304029

Table 13 Statistical description of quenching absorption coefficient data from various solvents interacting with new disperse dye D1

Disperse dye D1	
Mean	8357.9625
Standard Error	1586.005023
Median	11856.875
Mode	-
Standard Deviation	5015.388253
Sample Variance	25154119.33
Kurtosis	-1.866458189
Skewness	-0.606275062
Range	11806.625
Minimum	1018.375
Maximum	12,825
Sum	83579.625
Count	10
Largest (1)	12,825
Smallest (1)	1018.375
Confidence Level (95.0%)	3587.792623

solvent molecules can significantly influence its solubility, stability, and optical attributes. Depending on the nature of the solvents, variations in the absorption spectrum and absorption energy may occur, resulting in solvatochromism behavior, which signifies changes in the dye's color or absorption properties in distinct solvent environments. Moreover, comprehending solvent-solvent interactions within dual-solvent systems is paramount for dye dissolution and application. The interactions between the two solvents, encompassing factors such as miscibility and preferential solvation, can directly impact the dye's solubility and stability. These aspects have far-reaching implications for the dye's utilization across various industries, including textile dyeing, ink formulation, and colorant production.

In summary, the investigation of the absorption spectrum, absorption energy, solute-solvent interactions, and

solvent-solvent behavior plays a pivotal role in understanding solvatochromism behavior and the dissolution of a novel azo dye structure. This knowledge serves as a foundation for optimizing the dye's performance and application in diverse solvent environments and industrial applications.

Experimental procedure

Experimental design

A concentrated stock solution of a new disperse dye D1, featuring an azo structure, was prepared with a concentration of 0.001 M in chloroform solvent. Subsequently, solutions with lower concentrations were derived from this stock solution for spectrophotometric analysis. To achieve this, the initial concentration of 0.001 M in various solvents was used as a starting point. For instance, 0.1 cc of the concentrated 0.001 M solution in chloroform

Table 14 Statistical overview of absorption rate data for new disperse dye D1 across various solvents

Disperse dye D1	
Mean	0.668637
Standard Error	0.126880402
Median	0.94855
Mode	-
Standard Deviation	0.40123106
Sample Variance	0.160986364
Kurtosis	-1.866458189
Skewness	-0.606275062
Range	0.94453
Minimum	0.08147
Maximum	1.026
Sum	6.68637
Count	10
Largest (1)	1.026
Smallest (1)	0.08147
Confidence Level (95.0%)	0.28702341

Table 15 Statistical analysis of maximum wavelength data for a solvent mixture in combination with novel disperse dye D1

Disperse dye D1	
Mean	534.8
Standard Error	4.715930449
Median	536
Mode	536
Standard Deviation	14.91308151
Sample Variance	222.4
Kurtosis	0.388680833
Skewness	-0.388984613
Range	50
Minimum	510
Maximum	560
Sum	5348
Count	10
Largest (1)	560
Smallest (1)	510
Confidence Level (95.0%)	10.66817584

was employed to create 10 cc solution with 0.001 M concentration in acetonitrile. The procedure involved transferring 0.1 cc of the stock solution to 10 cc volumetric flask, allowing complete evaporation of chloroform, and then adding acetonitrile to the flask to reach the desired volume. This methodology facilitated the generation of solutions with different solvents, eliminating the need to prepare separate solutions for each measurement. Consequently, we obtained solutions representing a range of solvents and the new azo dispersion dye D1. Furthermore, using the stock solution, a blend of polar aprotic, polar protic, and non-polar solvents was prepared in varying ratios, creating a spectrum of polarities for the D1 dye structure, as illustrated in Fig. 1.

Table 16 Statistical analysis of polarity data for polar protic, polar aprotic, and non-polar solvents

Disperse dye D1	
Mean	0.287888889
Standard Error	0.091970473
Median	0.111
Mode	-
Standard Deviation	0.275911419
Sample Variance	0.076127111
Kurtosis	-1.07004814
Skewness	0.723734372
Range	0.753
Minimum	0.009
Maximum	0.762
Sum	2.591
Count	9
Largest (1)	0.762
Smallest (1)	0.009
Confidence Level (95.0%)	0.212084291

Table 17 Statistical analysis of molecular weight for various solvents and the new disperse dye D1

Disperse dye D1	
Mean	98.74164545
Standard Error	24.87042184
Median	78.11
Mode	-
Standard Deviation	82.48585761
Sample Variance	6803.916705
Kurtosis	8.730363075
Skewness	2.817314674
Range	304.96
Minimum	32.04
Maximum	337
Sum	1086.1581
Count	11
Largest (1)	337
Smallest (1)	32.04
Confidence Level (95.0%)	55.41475316

In this experiment, we employed three distinct classes of solvents characterized by varying structures and functionalities: polar protic, polar aprotic, and non-polar solvents. Additionally, a new azo dispersion dye, D1 (depicted in Fig. 1), was utilized. The use of statistical data allowed us to integrate empirical and theoretical approaches comprehensively. Our objective was to analyze, predict, explain, and draw generalizations from the statistical data. This encompassed a thorough examination of the interaction between the diverse solvents and the D1 dye, offering insights into its behavior and performance.

The Fig. 1 illustrates the molecular structure and name of the new dispersive dye utilized in this study: 4-nitro-2-cyanoazobenzene-meta-toluidine, designated as D1.

Table 18 Results of two-sample t-test (assuming equal variances) for two sets of statistical data on absorption energy

	Variable 1	Variable 2
Mean	53.4998	54.0898
Variance	2.272149522	2.349873967
Observations	10	10
Pooled Variance	2.311011744	Pooled standard deviation 1.520201218
Hypothesized Mean Difference	0	
df	18	
t Stat	-0.867832555	
P(T<=t) one-tail	0.198454422	
t Critical one-tail	1.734063607	
P(T<=t) two-tail	0.396908844	
t Critical two-tail	2.10092204	

Table 19 Results of two-sample t-test (assuming equal variances) for two sets of statistical data on absorption

	Variable 1	Variable 2
Mean	0.668637	0.740967
Variance	0.160986	0.233107019
Observations	10	10
Pooled Variance	0.197047	Pooled standard deviation 0.443899416
Hypothesized Mean Difference	0	
df	18	
t Stat	-0.36435	
P(T<=t) one-tail	0.359921	
t Critical one-tail	1.734064	
P(T<=t) two-tail	0.719842	
t Critical two-tail	2.100922	

Table 20 Results of two-sample t-Test (assuming equal variances) for two statistical data series related to maximum wavelength

	Variable 1	Variable 2
Mean	534.8	541.1
Variance	222.4	228.9888889
Observations	10	10
Pooled Variance	225.6944444	Pooled standard deviation 15.02313031
Hypothesized Mean Difference	0	
df	18	
t Stat	-0.937702593	
P(T<=t) one-tail	0.18040492	
t Critical one-tail	1.734063607	
P(T<=t) two-tail	0.36080984	
t Critical two-tail	2.10092204	

Table 21 Statistical errors for 10 data related to absorption energy in a solvent mixture with novel disperse dye D1

Statistical Errors	
n	10
MAD	0.59
MSE	0.443
RMSE	0.6655825
MAPE	1.1040355

Table 22 Statistical errors for 10 data related to absorption in various solvent mixtures with novel dispersed dye D1

Statistical Errors	
n	10
MAD	0.07233
MSE	0.028632299
RMSE	0.169210812
MAPE	10.19100671

Table 23 Statistical errors for 10 data related to maximum wavelength in a solvent mixture with novel disperse dye D1

Statistical Errors	
n	10
MAD	6.3
MSE	47.3
RMSE	6.877499546
MAPE	1.179161087

The compound is a new azo purple disperse pigment with a molecular weight of 337 g/mol. It contains electron donor groups (CH_3 , $\text{N}(\text{C}_2\text{H}_5)_2$) and electron acceptor groups (N_2 , NO_2 , CN). The critical pressure (P_C) is 4328.25 KPa, the normal boiling point temperature (T_{boil}) is 620.57 K, the normal melting point temperature (T_{fus}) is 446.98 K, and the critical volume (V_C) is 0.430 m³/kmol.

The Fig. 2 illustrates the concentrations of new disperse dye D1 in solvents, including benzene, toluene, orthoxy-lene, acetonitrile, methanol, 1-propanol, and DMF.

Results and discussion

Results from tables and figures

The analogy reasoning of polarity changes correlates with variations in absorption energy, wavelength, and absorption of new azo dyes within single solvent environments

The table provides information on the highest and lowest absorption rates, wavelength, absorption energy and polarity for various solvent mixtures with novel disperse dye D1. The chloroform-D1 mixture exhibited the highest absorption rate, reaching 0.831, while the methanol-D1 mixture displayed the lowest absorption rate at 0.23. Additionally, the maximum wavelength (λ) recorded was 556 nm in the chloroform-D1 mixture, whereas the lowest wavelength, 548 nm, was observed in the methanol-D1 mixture. The data suggests that altering the polarity

of the solvent significantly influences both the absorption level and absorption energy. Notably, the absorption energy (ΔE_t) for individual mixtures was calculated, yielding a value of 0.7507. The maximum absorption energy (E) can be determined using the Eq. (1):

$$E(\text{kcal/mol}) = 28591.5/\lambda_{\text{max}} \quad (1)$$

The Eq. 1 allows the calculation of E based on the maximum wavelength (λ_{max}).

Figure 3 illustrates the variations in absorption energy of disperse dye D1 as a function of solvent polarity, specifically in chloroform, methanol, ethanol, and acetone solutions. In Fig. 3; Table 1, the highest absorption energy of 52.1742 was recorded for both the methanol-D1 and acetone-D1 mixtures, corresponding to the highest observed polarity of 0.762. Conversely, the lowest polarity value, 0.259, was observed in the chloroform-D1 mixture. Figure 3 presents the relationship between energy and solvent polarity, showed by the equation $Y=0.1874X+51.424$, with a correlation coefficient (R^2) value of 0.4526, a statistic is the standard deviation of its sampling distribution standard error (SE) has been calculated. The data analysis and processing were conducted through laboratory experimentation, yielding a low R^2 value and a high SE value, indicating increased uncertainty in the experimental and laboratory data. However, employing these statistical and theoretical calculations has enabled the analysis of experimental data and the inferential estimation of the dispersed dye Azo D1's interaction effects across various solvent and solute environments. Therefore, the absorption energy of a dye disperse solution is significantly influenced by the polarity of the system. In polar solvents, interactions between novel dye and solvent molecules can modify the electronic environment around the novel dye, causing shifts in absorption energy. This effect is due to changes in solvation energy and charge transfer interactions, impacting the absorption spectra of the novel dye disperse system. Overall, the absorption of energy in the solution can alter molecular interactions, affecting charge distribution and system polarity [40, 41].

The absorption spectrum graph in Fig. 4 has been computed and plotted based on different concentrations of new disperse azo dye D1. The formula $Y=19640x-1.048$ with an R^2 value of 0.8101 and a calculated standard error.

Figure 5 depicts a 3-D column graph that explores the variations in absorption, absorption energy, and wavelength of disperse dye D1 in relation to the polarity of the solvents: chloroform, methanol, ethanol, and acetone. An important observation from the absorption energy data is that the mixtures of methanol-D1 and acetone-D1 exhibit a hypsochromic shift, leading to shorter

wavelengths. In contrast, the mixtures of ethanol-D1 and chloroform-D1 display a bathochromic shift, resulting in longer wavelengths. The visualization and observability of the results from experimental tests, statistical data structuring, and inductive reasoning, along with the findings presented in Table 1; Figs. 3 and 5, collectively constitute an inferential model. This model suggests that the primary cause of the hypsochromic change is the solvent effect. Increasing solvent polarity facilitates electron transfer from the π^* molecular orbital to non-bonding pairs of electrons in n and π^* molecular orbitals, thus shifting absorption towards higher frequencies. The bathochromic shift is also attributed to solvent-induced structural changes. Increased solvent polarity facilitates electron transfer from the π and π^* molecular orbitals, causing a shift towards lower frequencies (longer wavelengths). This phenomenon arises from the polarizing forces between the solvent and the absorber, resulting in the lowering of energy levels of the π^* and π molecular orbitals, consequently amplifying the influence on π^* . The objectification of experimental and statistical data into a 3-D Column representation has facilitated the development of a computational, descriptive, and inferential model for the new disperse dye D1. This approach has led to a reduction in cognitive errors and uncertainty in the experimental results. Therefore, the polarity of the solution in a novel dye disperse system can significantly affect absorbance and wavelength characteristics. In such systems, changes in the polarity of the solvent can influence the solubility and dispersion of the novel dye molecules, leading to variations in absorbance levels and absorption wavelengths. The polarity of the solution can impact the electronic transitions within the new dye molecules, affecting their spectral properties and overall performance in the disperse system. This information is crucial for understanding the dye's behavior in various applications, such as in dye-sensitized solar cells, fluorescence imaging, or coloration processes.

The analogy reasoning explores how changes in polarity correlate with shifts in absorption energy and wavelengths of new azo dyes in dual solvent systems with different chloroform-acetone ratios

The adsorption energy in binary mixtures can be calculated using the following Eq. 2:

$$E_{12}(id) = x_1 E_{T1} = x_2 E_{T2} \quad (2)$$

The calculation of the new polarity in solvent mixtures is performed using Eq. 3:

$$P_{12}(id)x_1p_1 + x_2p_2 \quad (3)$$

Table 2 presents the findings from the analysis of chloroform and acetone mixtures with varying ratios. Notably, the mixture of chloroform and acetone with a 1:1 ratio exhibited the highest absorption rate, recording a value of 0.311, while the mixture with a 2:1 ratio displayed the lowest absorption rate at 0.23. In terms of wavelength, the mixture of chloroform and acetone with a 4:1 ratio showed the highest wavelength, measuring 554 nm, while the mixture with a 2:1 ratio had the lowest wavelength, at 548 nm. Additionally, the absorption energy (ΔE_t) for these binary mixtures was calculated, resulting in a value of 0.225.

The results further indicate that the mixture of chloroform and acetone with a 1:1 ratio exhibited the highest absorption energy at 51.7988. This resulted in a hypsochromic shift (shorter wavelength). Conversely, the mixture with a 4:1 ratio displayed the lowest absorption energy and a bathochromic shift (longer wavelength). It seems that the highest absorption levels and absorption energies are observed in solvents with the highest polarity.

This observation and the inductive reasoning from experimental data suggest that the increasing ratio of chloroform to acetone, along with the interactive effects of these solvents, contribute to the observed phenomenon. The interaction between chloroform (a non-polar solvent) and acetone (a polar aprotic solvent) gives rise to new molecular dipoles, consequently increasing the polarity of the solvent. This enhanced polarity facilitates electron transfer from the π^* molecular orbital to the π molecular orbital.

The test results and statistical inference presented in Table 2 support the assumption that the polarizing forces between the solvent and the absorber significantly influence the alignment of molecular orbitals, particularly impacting the π^* (unexcited) and π (excited) orbitals. This effect is more pronounced on the π^* orbital.

In Table 2; Fig. 6, the highest absorption energy value, 52.7988, was observed in the mixture of chloroform and acetone with a 1:1 ratio and disperse dye D1, while the lowest absorption energy value, 51.5736, was found in the mixture of chloroform and acetone with a 4:1 ratio and disperse dye D1. Furthermore, the highest new polarity value, 0.614, was recorded for the 1:1 mixture of chloroform and acetone with disperse dye D1, while the lowest new polarity value, 0.278, was observed in the 4:1 mixture of chloroform and acetone with disperse dye D1.

Figure 6 demonstrates a linear relationship in these changes, characterized by the equation $Y=0.5495x+51.463$, along with R^2 value of 0.8477. Additionally, a statistic the standard deviation of its sampling distribution SE has been calculated to assess the model's reliability. The data analysis and processing were conducted through laboratory experimentation,

resulting in an increase in the R^2 value and a decrease in the SE value. Consequently, a decrease in uncertainty was observed in the experimental and statistical data.

Figure 7 presents a 3-D column graph that investigates the alterations in absorption, absorption energy, and wavelength of disperse dye D1 in response to the changing polarity of chloroform and acetone mixtures with different ratios. Within Fig. 7, the analysis encompasses changes in absorption, new absorption energy, and wavelength for disperse dye D1 based on the new polarity of chloroform and acetone solutions with varying ratios. These changes are characterized by linear relationships. Remarkably, the investigation revealed that the mixture of chloroform and acetone with a 1:1 ratio displayed the highest new polarity and new absorption energy. Additionally, the effects of increasing the molecular weight of chloroform and acetone solvents on polarity and absorption energy are supposition within this concept. Furthermore, increasing the proportion of chloroform relative to acetone in the mixed solvents leads to a decrease in polarity, absorption, and absorption energy.

The analogy-based reasoning examines how changes in polarity correlate with variations in absorption energy and wavelengths of new azo dyes in dual solvent systems with varying acetone-chloroform ratios

Table 3 presents the findings obtained from the experiment. Notably, the mixture of acetone and chloroform with a 1:4 ratio exhibited the highest absorption energy at 52.024, resulting in a hypsochromic shift (shorter wavelength). Conversely, the mixture with a 2:1 ratio displayed the lowest absorption energy, measuring 51.9239, leading to a bathochromic shift (longer wavelength). The observed effects are attributed to the increasing ratio of acetone to chloroform and the interactive influence of acetone (a polar aprotic solvent) with chloroform (a non-polar solvent). This interaction results in the emergence of a new polarity marked by new molecular dipoles. Increasing the new polarity of the solvent induces a bathochromic shift and facilitates electron transfer from the π^* molecular orbital. This shift is assumed by the polarizing forces between the solvent and the absorber, which impact the molecular orbital levels of π (unexcited) and π^* (excited), with a greater effect on π^* . Additionally, the highest absorption rate, 0.312, was associated with the 4:1 mixture of acetone and chloroform with disperse dye D1, while the lowest absorption rate, 0.286, was related to the 2:1 mixture of acetone and chloroform with disperse dye D1. Minor changes in wavelength were also observed for the acetone-chloroform mixtures with different ratios. The calculated absorption energy (ΔE_t) for these binary mixtures yielded a value of 0.1001. These findings offer valuable theoretical and experimental insights into the impact of solvent-to-solute

ratios and intermolecular interactions, molecular polarizability, vibrational effects, and environmental screening on the absorption spectral properties. They enhance predictability regarding the behavior and performance of the D1 disperse dye [42].

Figure 8 explores the variations in absorption energy exhibited by disperse dye D1 in response to the dynamic polarity changes in acetone-chloroform mixtures with varying ratios. As detailed in Table 3 and illustrated in Fig. 8, the investigation identified the highest absorption energy value, 52.024, occurring in the 4:1 ratio mixture of acetone and chloroform with disperse dye D1. In contrast, the lowest absorption energy value, 51.9239, was observed in the 2:1 ratio mixture of acetone and chloroform with disperse dye D1.

Moreover, the analysis revealed the highest recorded new polarity value, 0.335, for the 4:1 mixture of acetone and chloroform with disperse dye D1, while the lowest new polarity value, 0.322, was observed in the 2:1 mixture of acetone and chloroform with the same dye. Figure 8 effectively depicts a linear relationship among these changes, represented by the equation $Y=7.7105x+49.441$, with R^2 value of 0.9999. Additionally, to ensure the model's reliability, a statistic is the standard deviation of its sampling distribution SE has been calculated and considered in the analysis. This rigorous examination contributes valuable insights to the understanding of absorption energy variations in disperse dye D1 within complex solvent mixtures. The data analysis and inductive reasoning processing were conducted through laboratory experience, resulting in an increase in the R^2 value and a decrease in the SE value. Consequently, a decrease in uncertainty was observed in the experimental and laboratory data.

Figure 9 introduces a 3-D column graph designed to assess the fluctuations in absorption, absorption energy, and wavelength of disperse dye D1 in response to the changing polarity of acetone-chloroform mixtures with varying ratios. The graphical representation within Fig. 9 accents a linear relationship in the alterations of absorption, new absorption energy, and wavelength. Remarkably, the 4:1 ratio mixture of acetone and chloroform solvents emerged with the highest new polarity and new absorption energy values.

Furthermore, this diagram not only illustrates linear changes but also offers valuable theoretical and experimental insights into the impact of molecular weight and new structures of acetone and chloroform solvent mixtures on polarity, absorption energy, absorption, wavelength, vibrational effects, and environmental screening. The structured presentation in Fig. 9 enhances the clarity and coherence of the data and findings, contributing to a more comprehensive understanding of the interaction between solvent composition and key color properties.

Through analogy reasoning, we explore the relationship between changes in polarity and shifts in absorption energy and wavelengths of new azo dyes in dual solvent systems with varying methanol and chloroform ratios

Table 4 summarizes the outcomes derived from an in-depth analysis of methanol and chloroform mixtures at varying ratios in conjunction with disperse dye D1. The findings reveal that the highest absorption energy was discerned in two instances: first, in the 1:1 ratio mixture of methanol (a polar protic solvent) and chloroform (a non-polar solvent), and second, in the mixture of methanol and chloroform with a 1:2 ratio. This observation assumed a hypsochromic shift, attributed to the escalating solvent polarity and the ensuing electron transfer from π^* to n molecular orbitals. This electron transfer prompts interaction between the solvent and non-bonding electron pairs in molecular orbitals, inducing a shift towards higher frequencies.

Conversely, elevating the ratio of chloroform (a non-polar solvent) in methanol (also a non-polar solvent) results in the emergence of new solvent structures with varying polarities. This precipitates a reduction in absorption energy, leading to a bathochromic shift. This shift is propelled by the polarizing forces between the solvent and the absorber, influencing the energy levels of the π (unexcited) and π^* (excited) molecular orbitals, with a supposed impact on the π^* molecular orbital. The observed phenomenon appears to stem from the intermolecular interactions within the novel solvent mixture structure, coupled with the altered polarizability and vibrational effects.

Additionally, the highest absorption rate, 0.138, corresponds to the 1:1 mixture of methanol and chloroform with disperse dye D1, while the lowest absorption rate, 0.128, is associated with the 4:1 mixture of methanol and chloroform with disperse dye D1. Minor fluctuations in wavelength were also noted for the methanol-chloroform mixtures at different ratios. The calculated absorption energy (ΔE_t) for these binary mixtures resulted in a value of 0.225. These findings offer nuanced insights into the intricate interaction of solvent ratios and interactions, delineating their profound impact on the absorption characteristics and behavior of disperse dye D1.

Figure 10 delves into the nuanced variations in absorption energy exhibited by disperse dye D1 in response to the changing polarity of methanol-chloroform mixtures with diverse ratios. The corresponding findings in Table 4; Fig. 10 reveal noteworthy insights. The highest absorption energy value, 51.7988, surfaced in the 1:1 mixture of methanol and chloroform with disperse dye D1, while the lowest absorption energy value, 51.5736, was identified in the 4:1 mixture of methanol and chloroform with the same dye.

Furthermore, the investigation unveiled the highest recorded new polarity value, 1.021, associated with the 1:1 mixture of methanol and chloroform with disperse dye D1, compared against the lowest new polarity value, 0.359, observed in the 4:1 mixture of methanol and chloroform with the same dye. Illustrating these changes, Fig. 10 summarizes the relationship between new absorption energy and new polarity, showed by the equation $Y=0.2933X+51.504$, showcasing a strong R^2 value of 0.8864. In the pursuit of model reliability, a statistic is the standard deviation of its sampling distribution SE has been meticulously calculated, fortifying the robustness of the findings. The data analysis and processing, conducted through laboratory experimentation, resulted in an increase in the R^2 value and a decrease in the SE value. This led to a reduction in uncertainty observed in the experimental and laboratory data.

Figure 11 introduces a 3-D column graph meticulously designed to assess the dynamic variations in absorption, new absorption energy, and wavelength of disperse dye D1 in response to the changing polarity of methanol-chloroform mixtures across various ratios. The analysis within Fig. 11 distinctly reveals a linear trend showing the alterations in absorption, new absorption energy, and wavelength.

Remarkably, the 1:1 ratio mixture of methanol and chloroform solvents emerges as a focal point, exhibiting the highest new polarity and new absorption energy values. This graphical representation not only elucidates the linear changes but also offers valuable insights into the impact of the molecular weight of methanol and chloroform solvents on new polarity, new absorption energy, absorption, wavelength and optimization of experimental design. By systematically exploring these interactions, Fig. 11 enhances our understanding of the interaction between solvent composition and key characteristics of the disperse dye D1, contributing to a more comprehensive interpretation of the experimental data and inductive reasoning.

By employing analogy reasoning, we explore how changes in polarity correlate with variations in absorption energy and wavelengths of new azo dyes in dual solvents with varying chloroform-ethanol ratios

Table 5 presents the findings obtained from the analysis of chloroform and ethanol mixtures with varying ratios in conjunction with new disperse dye D1. The results indicate that the highest absorption energy was observed in the 1:1 mixture of chloroform (a non-polar solvent) and ethanol (a polar protic solvent) with disperse dye D1, yielding an absorption energy of 51.4235. In contrast, the lowest absorption energy, 51.1475, was found in the 2:1 mixture of chloroform and ethanol with disperse dye D1. This trend is indicative of the impact of varying

solvent ratios on absorption energy. Furthermore, the new polarity of the solvent mixtures showed the highest value, 0.913, in the 1:1 mixture of chloroform and ethanol with disperse dye D1, while the lowest new polarity value, 0.337, was observed in the 4:1 mixture of chloroform and ethanol with disperse dye D1. These variations in new polarity are a consequence of changing solvent ratios. Additionally, the highest absorption rate, 0.234, was associated with the 2:1 mixture of chloroform and ethanol with disperse dye D1, while the lowest absorption rate, 0.195, was linked to the 4:1 mixture of chloroform and ethanol with disperse dye D1. Tiny changes in wavelength were observed for the different ratios of chloroform and ethanol solvents with disperse dye D1. The calculated absorption energy (ΔE_t) for these binary mixtures yielded a value of 0.276. These findings offer valuable insights into the influence of different ratios of chloroform and ethanol solvents on absorption properties, intermolecular interactions, polarizability in high solvent dielectric constants, and solvation behavior of the dispersed dye D1.

Figure 12 introduces a 3-D column graph designed to comprehensively and inductive reasoning assess variations in absorption, new absorption energy, and wavelength of disperse dye D1 in response to alterations in the polarity of chloroform-ethanol mixtures across diverse ratios. The analysis within Fig. 12 distinctly reveals a linear trend characterizing changes in absorption, new absorption energy, and wavelength.

Significantly, the 1:1 ratio mixture of chloroform and ethanol solvents stands out, exhibiting the highest new polarity and new absorption energy values. This graphical representation not only elucidates the linear changes but also provides valuable insights into the impact of the molecular weight of chloroform and ethanol solvents on new polarity, new absorption energy, absorption, and wavelength. This visualization enhances the presentation of the data structure and findings depicted in Fig. 12, thereby augmenting the interpretability and depth of the theoretical and experimental results.

Using analogy reasoning to examine how changes in polarity relate to shifts in absorption energy and wavelengths of new azo dyes in dual solvents with different ethanol-chloroform ratios

Table 6 succinctly summarizes significant findings derived from the comprehensive analysis of ethanol and chloroform mixtures across varying ratios in conjunction with disperse dye D1. The results highlight the highest observed new absorption energy, 51.4235, in the 2:1 mixture of ethanol (a polar protic solvent) and chloroform (a non-polar solvent) with disperse dye D1. In contrast, the lowest new absorption energy, 51.5162, was identified in the 4:1 and 3:1 mixture of ethanol and chloroform with

the same dye, showcasing a nuanced interaction with changes in solvent ratios.

Additionally, the analysis revealed the highest new polarity value, 0.575, in the 4:1 mixture of ethanol and chloroform with disperse dye D1, while the lowest new polarity value, 0.522, was observed in the 2:1 mixture of ethanol and chloroform with the dye. These fluctuations in new polarity underscore the sensitivity of the system to varying solvent ratios. Moreover, the highest absorption rate, 0.302, was attributed to the 4:1 mixture, while the lowest absorption rate, 0.267, was linked to the 2:1 mixture, indicating the distinct influence of different ratios on absorption characteristics.

Despite tiny changes in wavelength observed for the different ratios of ethanol and chloroform solvents in conjunction with disperse dye D1, it's crucial to note that the alterations in absorption energy, although relatively slight, result in bathochromic and hypsochromic shifts in the absorption spectra, as explained in previous sections (Tables 2 and 4, and 3). The calculated absorption energy (ΔE_t) for these binary mixtures yielded a value of 0.092, providing a quantitative measure of these subtle variations. These findings offer valuable theoretical and experimental insights into the intricate impact of varying ratios of ethanol and chloroform solvents on the absorption characteristics and behavior of the D1 disperse dye. Specifically, they display the changes in absorption, absorption energy, and the polarities of new mixed solvent structures across different levels (high/medium/low).

Figure 13 conducts a detailed analysis of the common relationship between changes in the absorption energy of disperse dye D1 and shifts in the polarity of chloroform-ethanol mixtures across different ratios. The graph serves as a valuable tool for understanding the dynamics between new absorption energy and the varying polarity of the solvent mixture. These changes are presented distinctly, revealing a clear linear trend within the graph.

The formulated equation, $Y=0.3756X+51.075$, summarizes the calculated alterations in new absorption energy corresponding to the changing polarity. The high $R^2=0.8055$ attests to the reliability and strength of the observed trend, while a statistic is the standard deviation of its sampling distribution SE quantifies the precision of the results. These clarifying's contribute to a more structured and clear presentation of the data and findings in Fig. 13, enhancing the interpretability and robustness of the observed trends. The data analysis and processing, conducted through laboratory experiments, resulted in an increase in the R^2 value and a decrease in the SE value, indicating a reduction in uncertainty observed in the experimental and laboratory data.

Figure 14 meticulously analyzes the impact of shifts in the polarity of ethanol-chloroform mixtures with varying

ratios on the new absorption energy of disperse dye D1. The graph distinctly portrays the trend of changes in new absorption energy in response to alterations in the polarity of the solvent mixture, presenting it as a clear and linear progression.

The formulated equation, $Y=1.8436X+50.471$, succinctly captures the calculated changes in new absorption energy corresponding to shifts in the polarity of the solvents. The high $R^2=0.8452$ attests to the reliability and robustness of the observed trend, while a statistic is the standard deviation of its sampling distribution SE quantifies the precision of the results. These clarifications contribute to a more structured and clear presentation of the data and findings in Fig. 14, facilitating enhanced interpretation and understanding of the observed trends. The data analysis and processing, conducted through laboratory experience, revealed an increase in the R^2 value and a decrease in the SE value, resulting in a decrease in uncertainty observed in the experimental and laboratory data.

Figure 15 undertakes a comprehensive evaluation of the absorption characteristics, encompassing new absorption energy and wavelength, of a typical diffuse dye (D1) within mixed solvents of ethanol and chloroform featuring diverse ratios. The ensuing graphs reveal a discernible linear trend, with the solvent mixture at a 4:1 ethanol to chloroform ratio demonstrating the highest new polarity and absorption energy.

Moreover, the analysis delves into the impact of the molecular weights of ethanol and chloroform on new polarity, absorption energy, absorption levels, and wavelength, emphasizing on the intricate interaction between solvent composition and key features of the disperse dye. These findings, abbreviated in Fig. 15, provide valuable insights into the nuanced effects of varying solvent ratios and molecular weights on the absorption properties of the disperse dye D1.

Using analogy reasoning, we explore how changes in polarity correspond to variations in absorption energy and wavelengths of new azo dyes in dual solvents with different chloroform-methanol ratios

Table 7 offers valuable insights into the nuanced changes in new polarity, new absorption energy, wavelength, and absorption of novel disperse dye D1 across various mixtures of chloroform and methanol. The results underscore that, despite variations in these parameters with changing ratios of chloroform and methanol, the differences in absorption energy remain relatively minor. The mixture of chloroform and methanol with a ratio of 3:1 exhibits the highest new absorption energy, while the lowest is observed in the 4:1 ratio mixture. This suggests that the composition of the solvent mixture, particularly the ratio of the non-polar solvent (chloroform) to the

polar protic solvent (methanol), has a subtle impact on the electronic transitions within the dye molecule.

Similarly, new polarity values vary with the ratios, peaking in the 2:1 mixture and reaching the lowest point in the 4:1 mixture. These changes in new polarity reflect alterations in the solvent environment, influencing the optical properties of the dye. Notably, despite these variations in new polarity and new absorption energy, the shifts in absorption are minor. These subtle changes align with bathochromic and hypsochromic shifts, consistent with the explanations provided in previous sections (Tables 2 and 4, and 3). Such shifts are influenced by alterations in the polarity of the solvent, impacting electron transitions within the dye molecule.

In summary, the data in Table 7 highlights the subtle yet discernible changes in the properties of new disperse dye D1 when exposed to different ratios of chloroform and methanol. While the differences in absorption energy are minimal, they can still exert influence on the color and optical characteristics of the dye. These findings are crucial for comprehending the solvatochromism behavior that occurs in response to alterations in solvent composition.

Figure 16 undertakes an examination of the changes in new absorption energy for novel disperse dye D1 regarding the new polarity of the mixture of chloroform and methanol solvents across various ratios. However, the data presented in Fig. 16 reveals a weak or nearly non-existent correlation between new polarity and new absorption energy. The formulated equation, $Y = -0.2313X + 51.824$, succinctly describes the calculated changes in new absorption energy corresponding to shifts in the polarity of the solvents. However, the low R^2 value of 0.021 indicates a minimal linear relationship between these two variables. This lack of a strong correlation suggests that changes in the polarity of the solvent mixture (chloroform and methanol) within the tested range have little impact on the absorption energy of new disperse dye D1. It implies that other factors may exert a more substantial influence on the absorption energy of the dye in this particular solvent mixture. Furthermore, considering the SE, which offers a measure of variability in the data, becomes relevant. If the standard error is relatively high, it indicates significant uncertainty in the relationship between new polarity and new absorption energy. In conclusion, Fig. 16 implies that the new polarity of the mixture of chloroform and methanol solvents, with different ratios, does not strongly correlate with new absorption energy for normal disperse dye D1. The observed relationship lacks statistical robustness, indicating that additional factors or interactions may contribute significantly to determining the absorption energy of the dye in this specific solvent mixture.

Figure 17 unfolds as a 3-D column graph, offering a visual representation of the changes in absorption, new absorption energy, and wavelength of a new disperse dye D1 in response to the new polarity of mixed solvents of chloroform and methanol across different ratios. The graph distinctly portrays linear changes in these parameters as a function of the new polarity. Notably, the solvent mixture of chloroform and methanol with ratios of 2:1 and 3:1 exhibits the highest new polarity and new absorption energy, it seems that increasing the ratio of chloroform to methanol increases the new polarity, absorption and absorption energy.

The observed linear relationships between new polarity, new absorption energy, and wavelength emphasize on the significance of changes in solvent composition, particularly the ratio of chloroform to methanol, in influencing the absorption characteristics of disperse dye D1. The graph supposes further exploration of the effects of the molecular weight of these solvents on new polarity, new absorption energy, absorption, and wavelength to achieve a comprehensive understanding of the dye's behavior in these solvent mixtures.

Using analogy reasoning, we explore how changes in polarity correlate with variations in absorption energy and absorption wavelengths of new azo dyes in single solvent systems

The notable high absorption energy observed in the mixture of toluene (a non-polar solvent) with disperse dye D1 has resulted in a hypsochromic shift. This shift is indicative of a transition towards shorter wavelengths in the absorption spectrum. The underlying mechanism for this hypsochromic shift lies in the solvent's interaction with the non-bonding electron pairs in the n molecular orbitals. By assuming these electron pairs, the solvent influences the electronic transitions within the dye molecule, causing a shift towards shorter wavelengths.

Conversely, in the case of benzene (also a non-polar solvent), a typical bathochromic shift is observed with disperse dye D1. This bathochromic shift signifies a shift towards longer wavelengths in the absorption spectrum. The reasons for these bathochromic and hypsochromic shifts have been elucidated in detail in the corresponding sections of Tables 2 and 4, and 3. Furthermore, these specific solvent ratios and changes in Gibbs's formation energy and enthalpy are hypothesized to have an effect on absorption spectroscopic properties, absorption energy, as well as solvent and solute polarity. For these binary mixtures, the absorption energy has been calculated, and $\Delta E_t = 0.372$ serves as a measure of the energy changes and polarity associated with these spectral shifts. This value quantifies the extent of energy change related to the observed shifts in absorption, wave length providing a comprehensive understanding of the spectral

behavior of disperse dye D1 in the presence of toluene and benzene solvents.

Figure 18 adeptly illustrates the trend of changes in absorption energy concerning the polarity of non-polar solvents, namely benzene, toluene, and xylene, when employed in conjunction with a novel dispersion dye D1. The observed changes display a linear nature, suggesting a systematic relationship between the solvents' polarity and the absorption energy of the dye.

The absorption energy is accurately modeled based on the solvents' polarity, as summarized in the formula $Y = -9.0518X + 53.89$. This mathematical representation provides a concise expression of the linear relationship, enabling predictions of absorption energy changes corresponding to alterations in solvent polarity. The model achieves a high degree of explanatory power, reflected in the R^2 value of 0.9396. Additionally, the SE has been calculated and presented, offering insights into the precision and reliability of the modeled relationship. The data analysis and processing, conducted through laboratory experience, resulted in an increased R^2 value and a decreased SE value, indicating a decrease in uncertainty observed in the experimental and laboratory data.

In summary, Fig. 18 not only visually portrays the linear trend of changes in absorption energy with respect to the polarity of non-polar solvents but also provides a quantifiable model that enhances the understanding of this relationship.

Figure 19 unfolds as a 3-D column graph, offering a comprehensive investigation into the changes in absorption, absorption energy, and wavelength of a novel dispersion dye D1. The analysis is centered around the degree of polarity in non-polar solvents, specifically benzene, toluene, and xylene. The graph visually abbreviates the variations in these parameters, providing a clear and intuitive representation of how they respond to the polarity of the solvents. The highest absorption energy of 53.2222 and the lowest polarity of 0.072 correspond to the non-polar solvent of xylene, whereas the lowest absorption energy of 52.8493 and the highest polarity of 0.111 are associated with the non-polar solvent of toluene containing the novel dispersed azo dye D1. Additionally, changes in solvent structure and variations in Gibb's energy and enthalpy of formation are assumed to impact the dye's absorption properties, particularly absorption energy, polarity, and wavelength.

Through analogy reasoning, we examine how changes in polarity correlate with variations in absorption energy and absorption wavelengths of new azo dyes in dual solvents with different benzene-xylene ratios

The data presented in Table 9 unveils several noteworthy findings regarding the behavior of the novel dispersion dye D1 in mixed solvents of benzene and xylene

at varying ratios. The highest absorption energy value, reaching 53.0454, is observed in the 1:1 mixture of benzene and xylene, both being non-polar solvents. In contrast, the lowest absorption energy value of 52.9472 is found in the 2:1 mixture of benzene and xylene with the same dispersion dye. This variation highlights the significant impact of changing solvent ratios on the absorption energy of the dye.

Additionally, the highest polarity value of 0.183 corresponds to a 1:1 mixture of benzene and xylene, while the lowest polarity value of 0.098 is observed in a 2:1 mixture of the same solvents with dispersion dye D1. These polarity values reflect the varying degrees of interaction between the dye and the solvents as the benzene to xylene ratio increases. They elucidate the complex dynamics within the solution structure and focus on the vibrational and screening effects of the environment on the properties of the absorption spectrum.

The data also includes information about absorption rates, with the lowest rate of 0.782 found in the 1:1 mixture of benzene and xylene, and the highest rate of 0.904 observed in the 2:1 mixture of the same solvents with the dispersion dye D1. These absorption rates provide insights into the efficiency of the dye-solvent interactions.

The absorption energy for binary mixtures, denoted as ΔE_t , is calculated to be 0.093. This calculated value summarizes the overall energy changes associated with the observed shifts in the absorption spectrum.

In summary, the findings in Table 9 collectively underscore how alterations in the ratios of benzene and xylene can significantly influence absorption energy, polarity, wavelength, and absorption rates of the dispersion dye D1. These insights contribute to a deeper understanding of the behavior of this dispersion dye in diverse solvent environments. The experimental and statistical data, along with the analysis and inductive reasoning presented in the previous tables and figures, have been generalized to elucidate the effects of changes in the interaction of various solvent and solute environments on the bathochromic and hypsochromic shifts of the new azo disperse dye.

Figure 20 illustrates the trend of changes in new absorption energy based on the new polarity of non-polar solvents, specifically benzene, toluene, and xylene, with the new dispersion dye D1 at varying ratios. The graph demonstrates a linear relationship between the new polarity and new absorption energy. The equation used to represent this relationship is $Y = -1.1749x + 52.83$, where Y represents the new absorption energy and x corresponds to the new polarity of the solvents. The high R^2 value of 0.999 indicates a strong correlation between new polarity and new absorption energy, underlining the reliability of the relationship depicted in the graph.

The SE, which measures the accuracy of the calculated values, has been computed and is also shown. These findings provide valuable insights into how changes in the polarity of non-polar solvents impact the absorption energy of the new dispersion dye D1, show its behavior in different solvent compositions. The data analysis and processing, conducted through laboratory experience, resulted in an increased R^2 value and a decreased SE value, indicating a decrease in uncertainty observed in the experimental and laboratory data.

Figure 21 shows a comprehensive analysis of the linear relationships among key parameters—new polarity, new absorption energy, absorption, and wavelength—and their dependency on the degree of new polarity in mixed solvents of benzene and xylene with the new dispersion dye D1. The graphs within Fig. 21 reveal a systematic and predictable connection between these parameters and the evolving polarity of the solvent mixtures.

The highest recorded new polarity value, standing at 0.183, corresponds to the 1:1 mixture of benzene and xylene with the dispersion dye D1. In contrast, the lowest new polarity value, measured at 0.098, is associated with the 2:1 mixture of the same solvents with the same dye. This distinct polarity gradient underscores the dye's sensitivity to variations in the proportion of non-polar solvents and offers valuable theoretical and experimental insights into how changes in polarity influence its absorption properties.

Examining new absorption energy, the highest value of 53.0454 is identified in the 1:1 mixture of benzene and xylene with the dispersion dye D1. On the other hand, the lowest new absorption energy value, measuring 52.9472, is observed in the 2:1 and 3:1 mixture of benzene and xylene with the same dye. These findings underscore the significant role played by varying ratios of non-polar solvents in influencing the absorption energy of the dispersion dye D1.

The exploration of the potential effects of the molecular weight of non-polar solvents such as benzene, toluene, and xylene on new polarity, new absorption energy, absorption, and wavelength opens avenues for further understanding the nuanced interactions within these solvent-dye systems.

Analogical reasoning explores how changes in polarity correlate with variations in absorption energy and absorption wavelengths of new azo dyes in dual solvents with different toluene-xylene ratios

The results presented in Table 10 demonstrate significant insights into the behavior of the novel dispersion dye D1 when exposed to non-polar solvents, specifically toluene and xylene, across varying ratios. Key findings from this analysis include: The highest new absorption energy, recorded at 53.3423, was observed in the 3:1 mixture of

toluene and xylene with new dispersion dye D1, indicating the impact of the solvent composition on the dye's absorption energy. Conversely, the lowest new absorption energy was 53.144, occurring in the 4:1 mixture of toluene (non-polar) and xylene (non-polar) with new dispersion dye D1, showcasing the variation in absorption energy under different conditions. New polarity values exhibited considerable differences, with the highest value of 0.234 found in the 4:1 mixture of toluene and xylene, while the lowest value of 0.078 was present in the 3:1 mixture, underlining the role of solvent ratios in influencing polarity. The wavelength experienced fluctuations, with the highest wavelength recorded at 538 nm in the 4:1, 2:1 and 1:1 mixture of toluene and xylene with new dispersion dye D1, while the lowest wavelength, 536 nm, was observed in the 3:1 mixture. The absorption rate also varied, with the highest rate of 0.601 associated with the 2:1 mixture of toluene and xylene, and the lowest rate of 0.541 found in the 1:1 mixture, emphasizing the role of solvent ratios in absorption characteristics. The calculated absorption energy for binary mixtures, $\Delta E_t = 0.198$, further emphasizes the variations in the behavior of new dispersion dye D1 when exposed to different ratios of toluene and xylene. These findings offer valuable theoretical and experimental insights for researchers and professionals exploring the interaction between dispersion dyes and non-polar solvents with novel structures and dielectric constants. They show new intermolecular interactions, vibrational effects, and molecular screening, emphasizing the significance of solvent composition in influencing spectrum characteristics and color absorption.

Figure 22 presents a graphical analysis of the changes in new absorption energy exhibited by novel dispersion dye D1 when exposed to toluene and xylene solvents at various ratios. The graph reveals a linear relationship, showcasing the influence of solvent polarity on the dye's absorption energy. The equation derived from the data is as follows: $Y = -0.7305x + 53.297$. However, $R^2 = 0.3106$ indicates that the correlation between the new absorption energy and solvent polarity, while linear, is not particularly strong. The standard error is not provided in the description, but it may offer additional insights into the accuracy of the model. This graph provides valuable information for researchers studying the behavior of new dispersion dyes in non-polar solvents, such as toluene and xylene, and highlights the relationship between solvent polarity and dye absorption energy. The data analysis and processing, conducted through laboratory experience, resulted in a decrease in the R^2 value and an increase in the SE value, indicating an increase in uncertainty observed in the experimental and laboratory data.

The graph reveals that the highest recorded new polarity value is 0.234, corresponding to the mixture of toluene and xylene with novel dispersion dye D1 at a 4:1

ratio. Conversely, the lowest observed new polarity value is 0.078, associated with the mixture of toluene and xylene with the same dye and a 3:1 ratio. In terms of new absorption energy, the highest value is 53.3423, obtained from toluene solvent with xylene and novel dispersion dye D1 at a 3:1 ratio. The lowest new absorption energy, 53.144, is related to toluene with xylene and novel dispersion dye D1 at a 4:1 ratio. This graph allows researchers to visualize the relationship between solvent polarity, new absorption energy, and wavelength changes in non-polar solvents, toluene and xylene, when exposed to normal dispersion dye D1 at various ratios. It also suggests that the molecular weight of these solvents can be a significant factor in influencing polarity, absorption energy, and other properties.

Analogical reasoning investigates how changes in polarity correlate with variations in absorption energy and absorption wavelengths of new azo dyes across polar protic, polar aprotic, and non-polar solvent environments MW dye D1:337.

In Table 11; Fig. 24, we meticulously examined the interaction between the statistical components and the data structure of new disperse dye D1 across various types of solvent structures. Our analysis involved careful calculations and the presentation of findings through visual aids and abductive reasoning. The components analyzed for novel disperse dye D1 included absorption energy, extinction absorption coefficient, maximum wavelength, absorption, and molecular weight. This study delves into the influence of solvent polarity on these components, revealing a clear and direct relationship between the quenching absorption coefficient and the levels of absorption energy, absorption, and molecular weight in the solvents.

In Fig. 25; Table 11, we examine the results of the absorption test for new disperse dye D1 in various solvents. Acetonitrile, a polar aprotic solvent with a polarity of 0.46, demonstrates the highest absorption at 1.026 and the highest extinction coefficient at 12,825. Similarly, DMF solvent, another polar aprotic solvent with a polarity of 0.386, exhibits the highest absorption of 0.9805 and the highest extinction coefficient of 12,256.25. Notably, both acetonitrile and DMF solvents display a noticeable tendency toward a bathochromic shift. Additionally, they demonstrate the highest dye aggregation in Fig. 25. In contrast, hexane and diethyl ether, non-polar solvents with a polarity of 0.009, present the lowest absorption at 0.08147 and the lowest extinction coefficient at 1,018.375. These solvents also feature the highest absorption energy at 56.0617. Similarly, diethyl ether, with a dielectric constant of 40.34, demonstrates the lowest absorption at 0.2315, the lowest extinction coefficient at 2,893.75, and the highest absorption energy at 55.8427. Hexane and

diethyl ether solvents exhibit a propensity for a hypsochromic shift, resulting in lower absorption. Additionally, they show the lowest dye aggregation in Fig. 25. Hence, in theoretical and experimental analysis, the influence of intermolecular interactions, molecular polarizability, vibrational effects, and molecular screening on the absorption spectrum properties of various solvents can be elucidated.

Computation of descriptive statistical indices for experimental data pertaining to the novel dispersed azo dye

Table 12 provides a thorough analysis of statistical criteria computed for the adsorption of the new structure of azo dye D1. This presentation encompasses vital statistical parameters: Mean: 53.4998, SE: 0.476670696, Standard Deviation: 1.507365093 and Confidence Level (95.0%): 1.078304029.

Moreover, the table functions as a valuable resource, given a comprehensive reference point for displaying additional relevant features derived from statistical experimental data of the typical azo disperse dye D1. This statistical information enhances our understanding, facilitating the interpretation and analysis of the intrinsic characteristics of the experimental data set in relation to the azo disperse dye D1.

Table 13 provides a full statistical examination of the extinction coefficient associated with the novel structure of azo dye D1. The analysis encompasses essential statistical parameters: Mean: 8357.9625, SE: 1586.005023, Standard Deviation: 5015.388253 and Confidence Level (95.0%): 3587.792623.

This table functions as a robust and comprehensive reference, presenting crucial features derived from statistical experimental data pertaining to the extinction coefficient of the new azo disperse dye D1. Beyond the basic statistical measures, it serves as a valuable tool for researchers, enriching our holistic understanding and facilitating the interpretation and analysis of the inherent characteristics within the experimental dataset. This statistical information significantly contributes to developing a theoretical perspective on the distinctive structure of azo dye D1.

Table 14 presents a detailed statistical analysis of absorption rates for the new azo dye D1 structure. This analysis includes key statistical measures: Mean: 0.668637, SE: 0.126880402, Standard Deviation: 0.40123106 and Confidence Level (95.0%): 0.28702341.

Additionally, Table 14 functions as a practical and comprehensive reference, offering insight into additional relevant features derived from statistical experimental data pertaining to the new azo disperse dye D1. This statistical information deepens our understanding and facilitates the interpretation and analysis of the basic aspects of the

experimental data set, contributing to a theoretical perspective on the new structure of azo dye D1.

Table 15 conducts an in-depth statistical scrutiny of the maximum wavelength associated with the novel structure of azo dye D1. The statistical metrics encompass fundamental measures: Mean: 534.8, SE: 4.715930449, Standard Deviation: 14.91308151 and Confidence Level (95.0%): 10.66817584.

Moreover, Table 15 serves as a pragmatic and comprehensive reference, providing insights into features derived from statistical experimental data concerning the maximum wavelengths of the prevalent azo scattering dye D1. This statistical information enriches our comprehension, facilitating the interpretation and analysis of the intrinsic features within the experimental dataset in connection to the new structure of azo dye D1. Consequently, it significantly contributes to shaping a theoretical perspective.

Table 16 brings an exhaustive statistical analysis of the polarity associated with diverse solvent structures. Key statistical metrics encompass: Mean: 0.287888889, SE: 0.091970473, Standard Deviation: 0.275911419 and Confidence Level (95.0%): 0.212084291.

Additionally, Table 16 serves as a pragmatic and comprehensive reference, providing insights into features derived from statistical experimental data related to the polarity of different types of solvent structures. This statistical information enhances our understanding, facilitating the interpretation and analysis of the intrinsic characteristics within the experimental datasets concerning various solvent structures. Consequently, it significantly contributes to shaping a theoretical perspective.

Table 17 presents a detailed statistical analysis of the molecular weight of various solvents and the new structure of disperse azo dye D1. Key statistical measures include: Mean: 98.74164545, SE: 24.87042184, Standard Deviation: 82.48585761 and Confidence Level (95.0%): 55.41475316.

Furthermore, Table 17 serves as a practical and comprehensive reference, providing insights into properties derived from the statistical data of the molecular weight of various solvent structures and the molecular weight of the new azo dye D1 structure. This statistical information deepens our understanding and aids in the interpretation and analysis of the essential attributes of the experimental data sets, pertaining to the molecular weights of various solvents and the new azo dye D1 structure, contributing to a theoretical perspective.

Conducting t-tests on statistical data concerning absorption energy, absorption, and wavelength of the novel dispersed azo dye

Table 18 presents the results of a two-sample t-test, assuming equal variances, for two separate sets of statistical data concerning the absorption energy values of

a solvent mixture with the new structure of new azo disperse dye D1. This analysis includes key statistical factors such as variance, combined standard deviation, degrees of freedom (df), t-statistics, and t critical value (one-tail, two-tail). The absence of a significant statistical discrepancy between the two data series is indicated by the low t Stat value of -0.867832555 when compared to the t critical value of (two-tail) 2.10092204. Therefore, there is no statistically significant difference between the two data series.

Table 19 displays the outcomes of a two-sample t-test, assuming equal variances, for two distinct sets of statistical data related to absorption values in different solvent mixtures featuring the new structure of the novel dispersed azo dye D1. This comprehensive analysis incorporates essential statistical parameters, including variance, combined standard deviation, degrees of freedom (df), t-statistics, and the t critical (one-tail, two-tail). The insignificance of statistically discernible differences between the two data series is evidenced by the low t Stat of -0.36435 when contrasted with the t critical value of (two-tail) 2.100922. Consequently, no statistically significant disparities are identified between the two data series.

In Table 20, the outcomes of a two-sample t-test, assuming equal variances, are presented for two distinct sets of statistical data relating to the maximum wavelength values in different solvent mixtures with the new dispersed azo dye D1. This analysis encompasses crucial statistical parameters, including variance, combined standard deviation, degrees of freedom (df), t-statistics, and the t critical (one-tail, two-tail). The insignificance of statistically significant differences between the two data series is evidenced by the low t Stat value of -0.937702593 when compared with the t critical value (two-tail) of 2.10092204. Consequently, there is no statistically significant discrepancy between the two data series.

Calculating the statistical errors in experimental data for novel dispersed azo dye

Table 21 showcases the computation and presentation of statistical errors, specifically RMSE=0.6655825 and MAPE=1.1040355, for 10 statistical data related to absorption energy in a solvent mixture with the new dispersed dye D1. These error calculations offer a thorough evaluation of the experimental data, providing valuable insights into the interaction effects of various solvents on the new structure of the dispersed azo dye D1. Consequently, this enhances the analysis, interpretation, and comprehension of the absorption energy data and the underlying theoretical patterns inherent in the new D1 dye structure.

In Table 22, statistical errors in the form of RMSE=0.169210812 and MAPE=10.19100671 are

calculated and presented for ten sets of statistical data related to the absorption in different solvent mixtures with the new dispersed dye D1. These error calculations provide a comprehensive assessment of the experimental data, enhancing the understanding of the interaction effects of various solvents on the new structure of the dispersed azo dye D1. This, in turn, facilitates the analysis and interpretation of the experimental adsorption data and a better grasp of the theoretical adsorption relationships and patterns for the new D1 dye structure.

Table 23 presents the calculation and presentation of statistical errors, specifically $RMSE=6.877499546$ and $MAPE=1.179161087$, for 10 statistical data related to the maximum wavelength in a solvent mixture with the new disperse dye D1. These error calculations offer a thorough assessment of the experimental data, providing valuable insights into the effects of various solvents on the new structure of the disperse dye D1. Consequently, this enhances the analysis and interpretation of the experimental maximum wavelength data, providing a clearer understanding of the theoretical absorption patterns associated with the new D1 dye structure.

Conclusions

In this paper, we conducted a comprehensive study of a new D1 disperse dye, 4-nitro-2-cyanoazobenzene-metaltoluidine (D1), within various polar aprotic polar, protic, and nonpolar solvents, each with different solvent ratios. Our investigation encompassed essential components of the D1 dye structure, including absorption energy, absorption wavelength, polarity, and other characteristics when placed in different solvent environments with diverse structures. To evaluate the impact of solvatochromism on the new structure of azo dye D1, in our analysis, we utilized statistical methods to calculate various types of errors, including $RMSE=0.6655825$ and $MAPE=1.1040355$, as well as $R^2=0.999$, $t\text{-test}=-0.36435$, and other relevant statistical factors. These analyses facilitated the comparison of experimental data with statistical and theoretical information. By integrating experimental data, statistical calculations, theoretical insights and inductive reasoning we gained a deeper understanding and predictive capacity regarding the interaction of different solvent structures on the novel azo disperse dye D1. This work contributes to a comprehensive framework for the photophysical and photochemical examination of the new D1 dye structure, enhancing our knowledge of its features.

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Author contributions

All authors contributed to the study conception, literature, analysis, and writing. Mahdi Shirali put forward the research ideas and finally approved the whole content. Shohre Rouhani, Kamaladin Gharanjig, Fatemeh Mirhashemi and Mahdi Shirali did the experiments and characterizations, analyzed the results and organized the writing framework.

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The authors declare no competing interests.

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References

1. Makitra RG, Reichardt C. Solvents and Solvent Effects in Organic Chemistry, Weinheim: Wiley-VCH, 2003, 630 p. Russian journal of general chemistry, 75(4), pp.664–664.
2. Ikram M, Rauf MA, Jabeen Z. Solvent effect on Si H stretching bands of substituted silanes. *Spectrochimica Acta Part A: Mol Spectrosc.* 1994;50(2):337–42.
3. Mishra A, Behera RK, Behera PK, Mishra BK, Behera GB. Cyanines during the 1990s: a review. *Chem Rev.* 2000;100(6):1973–2012.
4. Farajtabar A, Jaber F, Gharib F. Preferential solvation and solvation shell composition of free base and protonated 5, 10, 15, 20-tetrakis (4-sulfonatophenyl) porphyrin in aqueous organic mixed solvents. *Spectrochim Acta Part A Mol Biomol Spectrosc.* 2011;83(1):213–20.
5. Reichardt C. Solvatochromic dyes as solvent polarity indicators. *Chem Rev.* 1994;94(8):2319–58.
6. Reichardt C. Pyridinium N-phenolate betaine dyes as empirical indicators of solvent polarity: some new findings. *Pure Appl Chem.* 2004;76(10):1903–19.
7. Maitra A, Bagchi SJ. *Mol Liq.* 2008;137:131.
8. Nikolić J, Ušćumlić G, Krstić VV. Solvent effect on electronic absorption spectra of cyclohex-1-enylcarboxylic and 2-methylcyclohex-1-enylcarboxylic acids. *J Serb Chem Soc.* 2000;65(5–6):353–9.
9. Airinei A, Homocianu M, Dorohoi DO. Changes induced by solvent polarity in electronic absorption spectra of some azo disperse dyes. *J Mol Liq.* 2010;157(1):13–7.
10. Valentić N, Ušćumlić G, Radojković-Veličković M, Misić-Vuković M. Solvent effects on electronic absorption spectra of 3-N-(4-substituted-phenyl)-5-carboxy uracils. *J Serb Chem Soc.* 1999;64(3):149–54.
11. Suppan P, Ghoneim N. Solvatochromism the royal society of chemistry; 1997.
12. Golchoubian H, Rezaee E, Bruno G, Rudbari HA. Synthesis and solvatochromism studies of new mixed-chelate dinuclear copper (II) complexes with different counter ions. *Inorg Chim Acta.* 2011;366(1):290–7.
13. García-Ramos JC, Tovar-Tovar A, Hernández-Lima J, Cortés-Guzmán F, Moreno-Esparza R, Ruiz-Azuara L. A new kind of intermolecular stacking

- interaction between copper (II) mixed chelate complex (Casiopéina III-ia) and adenine. *Polyhedron*. 2011;30(16):2697–703.
- Valdez-Camacho JR, Pérez-Salgado Y, Espinoza-Guillén A, Gómez-Vidales V, Tavira-Montalvan CA, Meneses-Acosta A, Leyva MA, Vázquez-Ríos MG, Juaristi E, Höpfl H, Ruiz-Azuara L. Synthesis, structural characterization and antiproliferative activity on MCF-7 and A549 tumor cell lines of [Cu (NN)(β3-aminoacidate)] NO3 complexes (Casiopéinas®). *Inorg Chim Acta*. 2020;506:p119542.
 - Salarieh S, Golchoubian H, Moayyedi G, Rezaee E. Copper (II) complexes containing mixed-chelate ligand, solvatochromism and density functional theory studies. *J Mol Struct*. 2022;1250:131822.
 - Dorohoi DO, Airinei A, Dimitriu M. Intermolecular interactions in solutions of some amino-nitro-benzene derivatives, studied by spectral means. *Spectrochim Acta Part A Mol Biomol Spectrosc*. 2009;73(2):257–62.
 - Riahi S, Mousavi MF, Shamsipur M. Prediction of selectivity coefficients of a theophylline-selective electrode using MLR and ANN. *Talanta*. 2006;69(3):736–40.
 - Geary WJ. The use of conductivity measurements in organic solvents for the characterisation of coordination compounds. *Coord Chem Rev*. 1971;7(1):81–122.
 - Tsiamis C, Themeli M. Substituent and solvent effects in the spectra and structure of some mixed-ligand copper (II) chelates containing β-ketoenols. *Inorg Chim Acta*. 1993;206(1):105–15.
 - Mautner FA, Louka FR, LeGuet T, Massoud SS. Pseudohalide copper (II) complexes derived from polypyridyl ligands: synthesis and characterization. *J Mol Struct*. 2009;919(1–3):196–203.
 - Golchoubian H, Moayyedi G, Bruno G, Rudbari HA. Syntheses and characterization of mixed-chelate copper (II) complexes containing different counter ions; spectroscopic studies on solvatochromic properties. *Polyhedron*. 2011;30(6):1027–34.
 - Yamamoto R, Maruyama T. 1994. *Jpn. Kokai Tokyo Koho*, JP: 06073169.
 - Masuda Y, Inatsugu F. *Jpn Kokai Tokyo Koho*. 1975. JP: 50121176.
 - Golden ML, Yarbrough JC, Reibenspies JH, Bhuvanesh N, Lee PL, Zhang Y, Darenbourg MY. 2004. In: *The Proceedings of the 2004, 228th ACS National Meeting*, Philadelphia, PA, United State, August pp. 22–26.
 - Fontan CA, Olsina RA. 4-(3, 5-dichloro-2-pyridylazo)-1, 3-diaminobenzene as a metallochromic indicator for the complexometric determination of Cu (II) with EDTA. *Talanta*. 1989;36(9):945–9.
 - Sato O, Hayami S, Einaga Y, Gu ZZ. Control of the magnetic and optical properties in molecular compounds by electrochemical, photochemical and chemical methods. *Bull Chem Soc Jpn*. 2003;76(3):443–70.
 - Sato O. Optically switchable molecular solids: photoinduced spin-crossover, photochromism, and photoinduced magnetization. *Acc Chem Res*. 2003;36(9):692–700.
 - Sheng S, Liu B, Hou X, Wu B, Yao F, Ding X, et al. Aerobic biodegradation characteristic of different water-soluble azo dyes. *Int J Environ Res Public Health*. 2018;15(1):35.
 - Selvaraj V, Karthika TS, Mansiya C, Alagar M. An over review on recently developed techniques, mechanisms and intermediate involved in the advanced azo dye degradation for industrial applications. *J Mol Struct*. 2021;1224:129195.
 - Chung KT. Azo dyes and human health: a review. *J Env Sci Health Part C*. 2016;34(4):233–261.
 - Muruganandham M, Shobana N, Swaminathan M. Optimization of solar photocatalytic degradation conditions of reactive yellow 14 azo dye in aqueous TiO2. *J Mol Catalysis A Chem*. 2006;246(1–2):154–161.
 - Warwick GP. Relative rates of reduction of a series of azo compounds. *J Soc Dyers Colourists*. 1959;75(6):291–299.
 - Ross WCJ, Warwick GP. Reduction of cytotoxic azo compounds by hydrazine and by the xanthine oxidase–xanthine system. *Nature*. 1955;176(4476):298–299.
 - Farghaly TA, Abdallah ZA. Synthesis, azo-hydrazone tautomerism and antitumor screening of N-(3-ethoxycarbonyl-4, 5, 6, 7-tetrahydro-benzo [b] thien-2-yl)-2-arylhydrazono-3-oxobutanamide derivatives. *Arxivoc*. 2008;17:295–305.
 - Chen CC, Wang J. Synthesis of some pyridone azo dyes from 1-substituted 2-hydroxy-6-pyridone derivatives and their colour assessment. *Dyes Pigments* 1991;15(1):69–82.
 - El Seoud OA. Solvation in pure and mixed solvents: some recent developments. *Pure Applied Chem*. 2007;79(6):1135–1151.
 - Umadevi M, Suvitha A, Latha K, Rajkumar BJ, Ramakrishnan V. Spectral investigations of preferential solvation and solute–solvent interactions of 1, 4-dimethylamino anthraquinone in CH2Cl2/C2H5OH mixtures. *Spectrochimica Acta Part A Mol Biomolecular Spectroscopy*. 2007;67(3–4):910–915.
 - Giusti LA, Marini VG, Machado VG. Solvatochromic behavior of 1-(p-dimethylaminophenyl)-2-nitroethylene in 24 binary solvent mixtures composed of amides and hydroxylic solvents. *J Mol Liquids*. 2009;150(1–3):9–15.
 - Sayadian M, Khaleghian M, Yari M. Solvatochromism and preferential solvation in mixtures of methanol with ethanol, 1-propanol and 1-butanol. *Orient J Chem*. 2014;30(4):1897–1903.
 - Pérez-Salado Kamps, Á. Model for the Gibbs excess energy of mixed-solvent(chemical-reacting and gas-containing) electrolyte systems. *Ind Eng Chem Res*. 2005;44(1):201–225.
 - Thomsen K, Iliuta MC, Rasmussen P. Extended UNIQUAC model for correlation and prediction of vapor–liquid–liquid–solid equilibria in aqueous salt systems containing non-electrolytes. Part B. Alcohol (ethanol, propanols, butanols)–water–salt systems. *Chemical Eng Sci*. 2004;59(17):3631–3647.
 - Zhang W, Zhang Y, Su H, Zhu X, Wang L, Zhang J. The effects of dye aggregation on the performance of organic dyes in dye-sensitized solar cells: From static model to molecular dynamics simulation. *J Luminescence*. 2019;205:7–13.

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