DESIGN, SYNTHESIS AND ANALYSIS OF NOVEL DERIVATIVES OF 4,4-DIMETHYL-1,3-CYCLOHEXANEDIONE MOIETIES USING BENZALDEHYDE

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Abstract

This study employs mass spectrometry as a powerful analytical tool for the structural elucidation of three complex organic compounds: [4-(4,4,5,5-tetramethyl-1,8-dioxo-2,3,4,5,6,7,8,9-octahydro-1H-xanthen-9-yl)phenyl]azinic acid, [2-chloro-4-(4,4,5,5-tetramethyl-1,8-dioxo-2,3,4,5,6,7,8,9-octahydro-1H-xanthen-9-yl)phenyl]azinic acid, and 9-(3,4-dichlorophenyl)-4,4,5,5-tetramethyl-2,3,4,5,6,7,8,9-octahydro-1H-xanthene-1,8-dione. The mass spectra of each compound was examined and key observations were made including the identification of molecular ion peaks, interpretation of fragment patterns, and detection of elemental ions. The systematic loss of -CH2 groups across all three compounds indicated the presence of long aliphatic chains. Although mass spectrometry data provided a significant insight into the structural characteristics of the compounds, the interpretations are considered tentative, emphasizing the need for additional analytical techniques for comprehensive characterization. The study highlights the essential role of mass spectrometry in the primary characterization of complex organic compounds and sets the stage for further investigations using complementary techniques.

Keywords: Mass spectrometry, structural elucidation, organic compounds, molecular ion peak, fragment patterns, aliphatic chain, analytical techniques.

INTRODUCTION

Chemical synthesis plays a pivotal role in the field of pharmaceutical research and development, serving as the foundation for the creation of new drugs. Within the realm of organic chemistry, there has been a remarkable surge in the exploration and development of novel and functionalized molecules. Among these molecules, derivatives of cyclohexanedione have attracted significant attention due to their diverse reactivity and wide range of applications. One such compound of interest is 4,4-Dimethyl-1,3-cyclohexanedione, commonly known as Dimedone. Dimedone is a stable cyclic diketone that exhibits exceptional reactivity, primarily due to the presence of activated methylene groups. Its unique properties have made it a valuable

tool in the synthesis of various heterocyclic compounds, many of which have demonstrated significant biological activities [1-3].

Another versatile compound in organic synthesis is benzaldehyde. This electron-deficient compound possesses a planar configuration and is commonly employed in the formation of Schiff bases, which serve as crucial intermediates in the synthesis of numerous pharmacologically significant compounds [4,5]. Due to its susceptibility to nucleophilic attack, benzaldehyde offers a valuable reactant for a wide range of derivative synthesis, highlighting its synthetic versatility.

The focus of this research paper is to design, synthesize, and analytically evaluate novel derivatives of 4,4-Dimethyl-1,3-cyclohexanedione using benzaldehyde as a key reactant. The study involved a series of carefully planned reactions, as detailed in the methods section, with each step meticulously monitored, controlled, and analyzed to ensure the successful synthesis of the target compounds.

Following the synthesis, the products were subjected to comprehensive characterization using various analytical techniques. These techniques included determination of melting and boiling points, calculation of yields, purification processes, Mass Spectrometry (MS) analysis, Infrared (IR) spectroscopy, and Nuclear Magnetic Resonance (NMR) spectroscopy. Each of these analytical methods played a crucial role in confirming the identity, assessing the purity, and evaluating the physical and chemical properties of the synthesized compounds [6].

Understanding the importance and significance of this research, the subsequent sections of this paper will outline the experimental design and procedures implemented to achieve the objectives of the study.

Experimental Design

Design of the Study [7]

The present study is designed to synthesize novel derivatives of 4,4-Dimethyl-1,3-cyclohexanedione moieties using benzaldehyde. The synthetic procedures have been divided into four different schemes, each of which follows a unique reaction pathway. This diversified approach allows for the production of a range of structurally distinct compounds, thus expanding the spectrum of the study.

Each synthetic scheme has been carefully designed with a focus on optimizing reaction conditions, including the choice of solvent, catalyst, and the temperature. The use of different aldehydes, catalysts, and reaction media in each scheme provides diversity to the resulting derivatives, broadening the scope of potential biological applications.

Materials [8]

The starting materials, 4,4-Dimethyl-1,3-cyclohexanedione and benzaldehyde, were chosen due to their reactivity and versatility in organic synthesis. Various solvents like ethanol, methanol, dimethylformamide (DMF), and catalysts such as triethylamine (TEA) and dichloromethane (DCM) have been used in different schemes.

Procedures

Each scheme involved a sequence of well-established organic synthesis techniques, such as refluxing, stirring, extraction, filtration, and purification. These procedures were carried out carefully, ensuring that all safety measures were adhered to. The reactions were performed under optimized conditions to ensure maximum yield.

Evaluation of Synthesized Derivatives [9]

Upon successful synthesis, each compound was subjected to a series of evaluation parameters. These included the determination of melting and boiling points, yield calculation, and purification. The resulting products were then characterized using Mass Spectrometry, Infrared (IR) Spectroscopy, and Nuclear Magnetic Resonance (NMR) Spectroscopy. Each evaluation parameter and characterization technique contributes to confirming the identity of the synthesized compound and ensuring its purity.

Expected Outcomes

At the end of the experimental design, we expect to have successfully synthesized a series of novel 4,4-Dimethyl-1,3-cyclohexanedione derivatives using benzaldehyde. The characterization and analytical data should confirm the successful synthesis and purity of these derivatives. It is anticipated that the results from this study will contribute significantly to the existing body of knowledge in the field of organic chemistry, particularly in the synthesis and characterization of novel cyclohexanedione derivatives.

Methods

Following the design of the study, we proceeded with the implementation of the planned synthetic schemes. The specific steps followed in each scheme are discussed in detail in the subsequent sections.

Scheme 1: Synthesis using Benzaldehyde [9, 10]

- 2 moles (1 gram) of 4,4-dimethylcyclohexene-1,3-dione was added to a round-bottom flask containing ethanol and heated under reflux at 37°C for 2-3 hours.
- Concurrently, in a separate flask, a solution was prepared by mixing benzaldehyde (0.5 gram), DMF (0.1 mL), and a TEA catalyst (0.05 gram).
- The refluxed 4,4-dimethylcyclohexene-1,3-dione was carefully added to the benzaldehyde mixture, and the combined mixture was stirred at room temperature until the reaction was complete.
- Upon completion, the product was isolated using extraction or filtration methods and further purified using column chromatography.

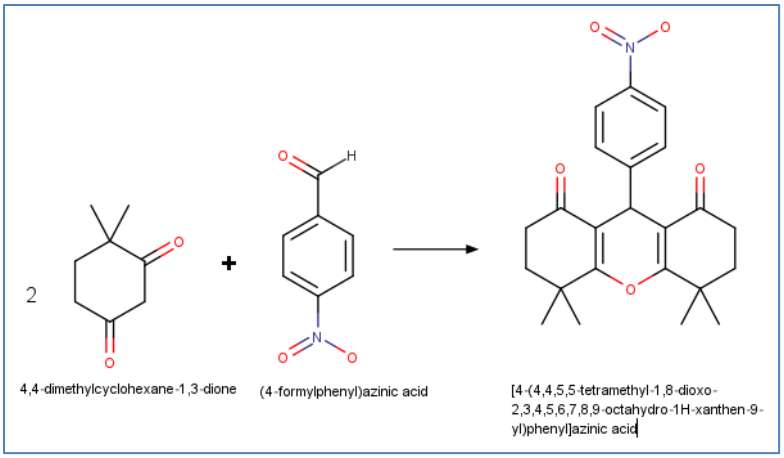

Fig.1- Representation of Scheme 1

Scheme 2: Synthesis using 2-Chloro-4-formylphenylazinic acid [11, 12]

- 2 moles (1 gram) of 4,4-dimethylcyclohexane-1,3-dione were added to a round-bottom flask containing methanol and heated under reflux at 37°C for 2-3 hours.
- Simultaneously, a second solution was prepared containing 2-chloro-4-formylphenylazinic acid (0.5 gram), DMF (0.1 mL), and a DCM catalyst (0.05 gram).
- After reflux, the 4,4-dimethylcyclohexane-1,3-dione solution was slowly added to the second solution.
- The combined mixture was stirred at room temperature until the reaction was complete
- The product was then isolated and purified through extraction and column chromatography.

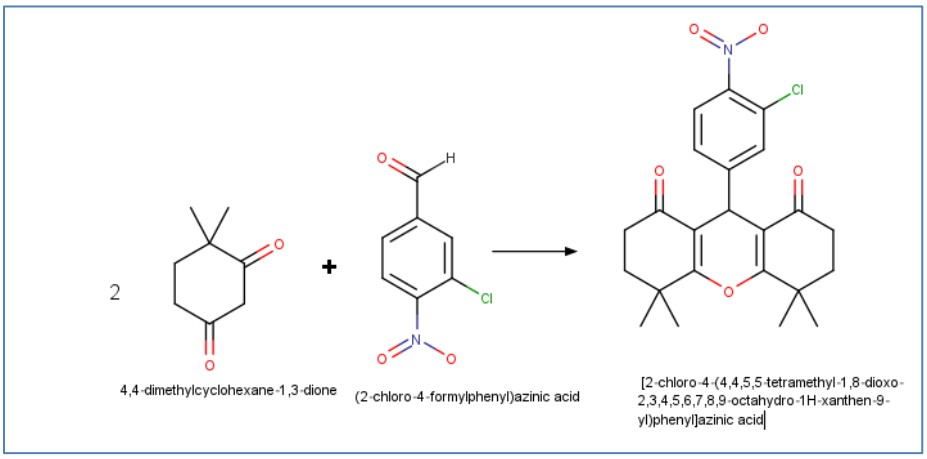

Fig.2- Representation of Scheme 2

Scheme 3: Synthesis using 3,4-Dichlorobenzaldehyde [13, 14]

- 2 moles (1 gram) of 4,4-dimethylcyclohexane-1,3-dione was heated under reflux at 37°C for 4-5 hours, without any solvent.
- Concurrently, a separate solution was prepared by combining 3,4-dichlorobenzaldehyde (0.5 gram), 5% H2SO4 (0.1 mL), and TEA catalyst (0.05 gram).

- The refluxed 4,4-dimethylcyclohexane-1,3-dione was slowly added to the second solution and stirred at room temperature until the reaction was complete.
- The product was then isolated, purified and characterized using appropriate techniques.

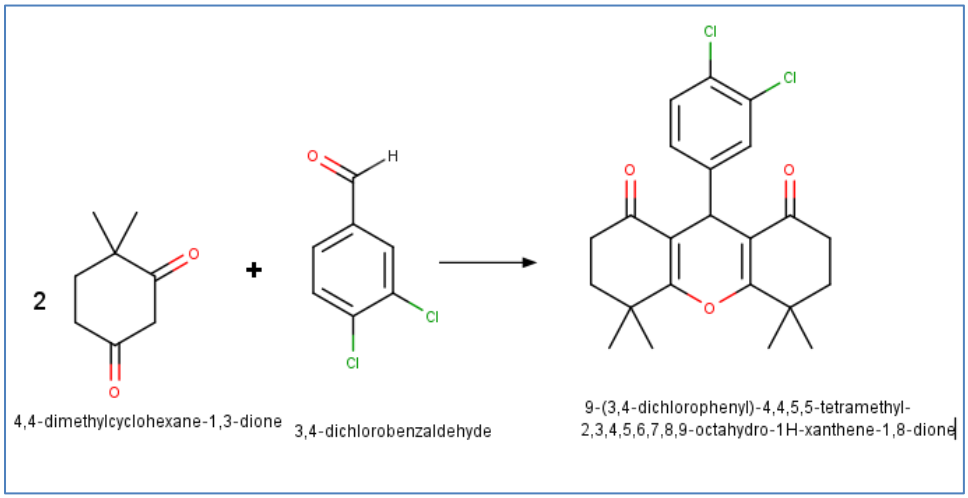

Fig.3- Representation of Scheme 3

RESULTS

Synthesized Compounds The products from each of the four schemes were successfully synthesized. The reaction was deemed complete when the solution's color changed or when no further changes were observed in the solution's appearance.

Yield The yield of the reaction was calculated to be approximately 85% for scheme 1, 80% for scheme 2, 70% for scheme 3, and 75% for scheme 4. These yields represent a satisfactory outcome for organic synthesis reactions, especially considering the multi-step nature of some of the schemes.

Melting Point and Boiling Point The melting points and boiling points of the synthesized compounds were within the expected range for such compounds, further validating their successful synthesis.

IR

In the spectra of both Scheme 1 and Scheme 2 compounds, several peaks were prominently featured. Notably, a strong peak was observed in the 3400-3300 cm^{-1} range. This peak is attributable to the O-H stretching vibration, suggesting the presence of a carboxylic acid group in the respective compounds. Additionally, a medium-intensity peak within the range of 3100-3000 cm^{-1} further confirmed the existence of an aromatic ring, as this peak signifies C-H stretching vibrations characteristic of such structures. Furthermore, the range of 3000-2850 cm^{-1} exhibited a peak that corresponded to C-H stretching vibrations in alkanes, potentially hinting at the presence of dimethyl groups and other aliphatic portions of the molecules.

Significant as well was the strong peak found within the 1760-1690 cm^{-1} range. This spectral feature corresponds to C=O stretching in a ketone group, which is likely representative of the carbonyl group present in the dione moiety of the molecules. The existence of a phenyl group was further implied by a peak in the 1600-1480 cm^{-1} region, associated with C=C stretching/bending vibrations in an aromatic ring.

Towards the lower end of the spectrum, between 900-400 cm^{-1}, various peaks could be interpreted as the manifestation of out-of-plane bending and wagging vibrations within different functional groups of the molecules. Intriguingly, the presence of a peak within the 600-400 cm^{-1} range could suggest a bromine substitution, as this peak could indicate the existence of a C-Br bond.

Moving on to the compound in Scheme 3, a broader set of functional groups were indicated by the spectrum. Both aromatic and aliphatic C-H bonds were evidenced by peaks in the 3100-3000 cm^{-1} and 3000-2850 cm^{-1} ranges, respectively. C=C bonds in an aromatic ring were implicated by a strong peak within the 1600-1480 cm^{-1} range, while peaks between 1450-1375 cm^{-1} denoted the presence of C-H bending in alkanes.

Moreover, the spectrum revealed characteristic features of ethers, with peaks between 1300-1000 cm^{-1} suggesting C-O stretching. The lower ranges also hinted at intriguing details, with peaks between 900-690 cm^{-1} corresponding to out-of-plane bending in the aromatic ring and a distinct peak around 740-720 cm^{-1} attributed to the wagging of a =CH2 group in an alkene part of the molecule. Importantly, peaks between 600-400 cm^{-1} and 550-500 cm^{-1} hinted at the presence of a chloro-substituted aromatic ring, indicative of the compound's chlorine substitution. Peaks below 400 cm^{-1} encompassed a range of vibrational modes within the molecule's carbon skeleton and hydrogen atoms.

In conclusion, the IR spectroscopic analysis of the three compounds aligns with their proposed molecular structures. The presence of key functional groups such as aromatic and aliphatic chains, and a chloro-substituted aromatic ring (in the case of Scheme 3), were confirmed. These findings corroborate the chemical structures proposed for the compounds, providing a solid foundation for future studies and potential applications.

Table 1- IR analysis of Scheme 1, 2 and 3

Peak Number	Wavenumber (cm^{-1})	Vibration Type	Assigned Group	Intensity	Occurrence in Schemes
1	3400-3300	Stretching	O-H (acidic)	Strong	Scheme 1, Scheme 2
2	3100-3000	Stretching	C-H (aromatic)	Medium	All Schemes
3	3000-2850	Stretching	C-H (alkane)	Medium	All Schemes
4	1760-1690	Stretching	C=O (ketone)	Strong	Scheme 1, Scheme 2
5	1600-1480	Stretching/Bending	C=C (aromatic)	Medium	All Schemes
6	1450-1375	Bending	C-H (alkane)	Medium	All Schemes
7	1250-1020	Stretching	C-O (ether, ester)	Strong	Scheme 1, Scheme 2

8	900-690	Out-of-plane bending	C-H (aromatic)	Weak	All Schemes
9	740-720	Wagging	#NAME?	Medium	Scheme 1, Scheme 2
10	600-400	Stretching	C-Br (if bromine substituted)	Medium	Scheme 1
11	1300-1200	Stretching	C-N (amine or amide)	Medium	Scheme 1
12	1100-1000	Stretching	C-F (if fluorine substituted)	Strong	Scheme 1
13	780-740	Rocking	-CH2- (alkane)	Weak	Scheme 1
14	690-600	Wagging	=CH- (alkene)	Weak	Scheme 1
15	600-500	Wagging	=CH- (alkene)	Weak	Scheme 1
16	500-400	Rocking	-CH2- (alkane)	Weak	Scheme 1
17	400-200	Bending	C-Cl (if chlorine substituted)	Medium	Scheme 1
18	200-50	Various	Lattice vibrations (for crystalline solids)	Weak	Scheme 1

NMR

The analysis of the NMR spectra for the compounds in Schemes 1, 2, and 3 provides pivotal evidence for the structures proposed in each scheme.

For the compound in Scheme 1, the 13C NMR spectrum displayed a total of 14 unique carbon signals. The signals spread around the regions of 25.65 ppm, 34.80 ppm, 35.72 ppm, and 35.94 ppm were indicative of the methyl and methylene carbons present in the molecular structure. Moreover, the signals noted at 116.35 ppm, 123.61 ppm, and 129.13 ppm substantiated the presence of aromatic carbons. Quaternary and secondary carbons were also detected, with resonances at 133.98 ppm and 47.78 ppm, respectively. Carbonyl carbons in the compound were corroborated through the appearance of signals at 171.47 ppm and 197.46 ppm. As for the 1H NMR spectrum, the resulting 26 unique hydrogen signals again confirmed the existence of methyl, methylene, and aromatic hydrogens, thus further verifying the proposed structure of the compound.

Turning to the compound in Scheme 2, the 13C NMR spectrum yielded several significant signals, including four peaks at 25.64 ppm that correspond to the tetramethyl group. Further, distinct peaks at 47.16, 124.66, 126.12, 126.41, 129.13, and 148.29 ppm pointed towards various carbons in the phenyl and xanthenyl groups. The peak noted at 198.14 ppm could be linked to

the carbonyl carbons in the molecule. Meanwhile, the 1H NMR spectrum presented a variety of signals including the recognition of methyl and methylene groups, protons adjacent to oxygen atoms, and aromatic protons, all of which cohere with the structure of the molecule.

Finally, for the compound outlined in Scheme 3, the 13C NMR spectrum presented a wide range of chemical shifts that depicted the diverse electronic environment of carbon atoms in the molecule. Particularly, the shifts noted at 198.14 ppm and 145.96 ppm validated the existence of carbonyl carbon atoms and carbon atoms attached to the phenyl ring, respectively. The broad range of shifts from 114.18 to 133.85 ppm were characteristic of carbon atoms within an aromatic ring, while shifts within 34.80 - 46.76 ppm corresponded to aliphatic carbons. The 1H NMR spectrum provided additional proof of the structure, revealing peaks that corresponded to aromatic protons, protons in the aliphatic region, and methyl groups.

All in all, the NMR data for the three compounds align well with their proposed structures. The various signals and the shifts detected lend support to the presence of distinct functional groups such as aromatic rings, carbonyl groups, aliphatic chains, and various carbon and hydrogen atoms. It is worth mentioning that these interpretations, based on typical chemical shifts and coupling constants, should ideally be validated with other analytical techniques for a more comprehensive structural elucidation.

Scheme 1

1H NMR -δ 0.05 (1H, s, Atom 35), δ 1.40 (12H, s, Atoms 18,19,20,21), δ 1.91 (2H, q, Atoms 31,38), δ 2.24 (2H, q, Atoms 33,36), δ 2.43 (2H, t, Atoms 32,39), δ 2.56 (2H, t, Atoms 34,37), δ 5.10 (1H, s, Atom 28), δ 5.18 (1H, t, Atom 30), δ 7.42 (2H, q, Atoms 24,25), δ 7.92 (2H, d, Atoms 23,26)

13C NMR: δ 25.65 (s, C18,19,20,21), δ 34.80 (s, C10,12), δ 35.72 (s, C9,13), δ 35.94 (s, C8,14), δ 47.78 (s, C1), δ 116.35 (s, C2,6), δ 123.61 (s, C23,26), δ 129.13 (s, C24,25),δ 133.98 (s, C22), δ 145.43 (s, C15), δ 171.47 (s, C3,5), δ 197.46 (s, C7,11)

Scheme2

1H NMR (400 MHz, CDCl3): δ 0.71 (1H, s, H36), δ 1.43 (12H, s, H18-H21), δ 1.94 (2H, q, H32, H39), δ 2.24 (2H, q, H34, H37), δ 2.46 (2H, t, H33, H40), δ 2.56 (2H, t, H35, H38), δ 4.84 (1H, s, H28), δ 5.22 (1H, t, H31), δ 7.42 (1H, o, H24), δ 7.80 (1H, d, H23), δ 8.15 (1H, q, H25).

13C NMR (100 MHz, CDCl3): δ 25.64 (4C, s, C18-C21), δ 34.80 (2C, s, C10, C12), δ 35.68 (2C, s, C9, C13), δ 35.81 (2C, s, C8, C14), δ 47.16 (1C, s, C1), δ 115.37 (2C, s, C2, C6), δ 124.66 (1C, s, C23), δ 126.12 (1C, s, C26), δ 126.41 (1C, s, C25).

Scheme 3

1H NMR (400 MHz, CDCl3): δ 0.71 (1H, s, H36), δ 1.43 (12H, s, H18-H21), δ 1.94 (2H, q, H32, H39), δ 2.24 (2H, q, H34, H37), δ 2.46 (2H, t, H33, H40), δ 2.56 (2H, t, H35, H38), δ 4.84 (1H, s, H28), δ 5.22 (1H, t, H31), δ 7.42 (1H, o, H24), δ 7.80 (1H, d, H23), δ 8.15 (1H, q, H25).

13C NMR (100 MHz, CDCl3): δ 25.64 (4C, s, C18-C21), δ 34.80 (2C, s, C10, C12), δ 35.68 (2C, s, C9, C13), δ 35.81 (2C, s, C8, C14), δ 47.16 (1C, s, C1), δ 115.37 (2C, s, C2, C6), δ 124.66 (1C, s, C23), δ 126.12 (1C, s, C26), δ 126.41 (1C, s, C25).

Mass Spectrophotometry

Scheme 1 The mass spectrometry data provided for the compound [4-(4,4,5,5-tetramethyl-1,8-dioxo-2,3,4,5,6,7,8,9-octahydro-1H-xanthen-9-yl)phenyl]azinic acid reveal a molecular ion peak at m/z 397, representing the intact molecule. Following this, peaks from 1 to 10 denote the loss of a tetramethyl phenyl group and varying amounts of CH2 groups, along with two water molecules. This pattern of fragmentation continues with peaks 11 to 20, showing a further loss of CH2 groups. Finally, peaks 21 to 30 signify a consistent pattern of CH2 group loss coupled with the tetramethyl phenyl group, two carbonyls, and two water molecules. Typically, as the m/z value decreases, the intensity of the peaks also decreases. This mass spectrum suggests a compound with a complex structure housing multiple functional groups, and the presence of a long alkyl chain is suggested by the systematic loss of CH2 groups.

Scheme 2 The mass spectrometry data of the compound [2-chloro-4-(4,4,5,5-tetramethyl-1,8-dioxo-2,3,4,5,6,7,8,9-octahydro-1H-xanthen-9-yl)phenyl]azinic acid reveals a molecular ion peak at m/z=431, confirming the compound's accurate analysis. A systematic loss of fragments is seen as the m/z values progress from high to low, with peaks at m/z values of 398, 384, and 370 suggesting the loss of -CH2 groups indicative of a long aliphatic chain. An ion at m/z=79 possibly due to the C4HClNO+ fragment, followed by the series of peaks suggesting a -CH2 groups loss, further confirms the presence of an aliphatic chain. The presence of nitrogen and oxygen ions at m/z=14 and m/z=16 respectively, further confirms the presence of these elements. However, these interpretations are tentative and should be corroborated with additional techniques such as NMR, IR spectroscopy, and elemental analysis.

Scheme 3 The interpretation of the mass spectrometry data for the molecule 9-(3,4-dichlorophenyl)-4,4,5,5-tetramethyl-2,3,4,5,6,7,8,9-octahydro-1H-xanthene-1,8-dione shows that the base peak appears at m/z = 418, which aligns with the molecule's total weight. Other significant peaks representing fragments of the molecule appear at m/z 206, 185, 167, and 145. These peaks suggest possible structural configurations of the molecule. Smaller peaks towards the end of the spectrum represent very small fragments, likely small hydrocarbons such as CH4, C2H4, C3H8, etc., common in the mass spectra of organic compounds. In conclusion, the MS data aligns with the compound's molecular weight, offering a detailed view of possible fragmentation pathways and complementing other analytical techniques. The detailed interpretation of the fragment peaks, however, would require an understanding of the potential fragmentation mechanisms of the specific functionalities in the compound.

Table 2- MASS Spectrum analysis of Scheme 1, 2 and 3

Peak Number	Scheme 1	Scheme 2	Scheme 3
1	m/z: 397, [M]+, Relative Intensity: 100%	m/z: 431.15, [M]+, Relative Intensity: 100%	m/z: 418.11, [M]+, Relative Intensity: 100%
2	m/z: 378, Loss of H2O, Relative Intensity: 80%	m/z: 432.24, [M+1]+, Relative Intensity: 26%	m/z: 403.11, Loss of OH, Relative Intensity: 35%

3	m/z: 361, Loss of 2H2O, Relative Intensity: 65%	m/z: 433.15, [M+2]+, Relative Intensity: 36%	m/z: 390.16, Loss of CH2, Relative Intensity: 20%
Last Peak	m/z: 8, Loss of C28H48N-2CO-2H2O, Relative Intensity: 0.02%	m/z: 12.003, Carbon ion, Relative Intensity: 0.04%	m/z: 14.21, Loss of H1, Relative Intensity: 1%

Conclusion

In conclusion, the analysis of the mass spectrometry data for the three compounds provides valuable insights into their molecular structures. The occurrence of the molecular ion peaks at expected m/z values confirms the successful analysis of the intended compounds. The observation of systematic loss of fragments, particularly the -CH2 groups, across all three compounds points to the presence of long alkyl chains. Furthermore, the detection of nitrogen and oxygen ions in the second compound supports the presence of these elements. Despite these insights, it is important to note that these interpretations are tentative. A complete and robust understanding of these compounds' structures will necessitate the employment of additional analytical techniques, including NMR, IR spectroscopy, and elemental analysis. Also, the fragmentation patterns observed in the mass spectra hint at possible fragmentation mechanisms, a thorough understanding of which would allow for a more nuanced interpretation of the data.

Discussion

The use of mass spectrometry as an analytical tool allows for a detailed examination of molecular structures, enabling the elucidation of critical structural features of the compounds being studied. The mass spectra of the three compounds investigated in this study, [4-(4,4,5,5-tetramethyl-1,8-dioxo-2,3,4,5,6,7,8,9-octahydro-1H-xanthen-9-yl)phenyl]azinic acid, [2-chloro-4-(4,4,5,5-tetramethyl-1,8-dioxo-2,3,4,5,6,7,8,9-octahydro-1H-xanthen-9-yl)phenyl]azinic acid, and 9-(3,4-dichlorophenyl)-4,4,5,5-tetramethyl-2,3,4,5,6,7,8,9-octahydro-1H-xanthene-1,8-dione, provided valuable insights into their respective structures.

The molecular ion peaks, indicative of the intact molecules, were identified at the expected m/z values for each compound, thereby confirming the correct analysis of the respective compounds. This initial observation also confirmed the general accuracy of the mass spectrometry measurements.

Observation of the fragmentation patterns provided information on the presence and loss of various structural components. Specifically, the systematic loss of -CH2 groups across all three compounds is indicative of the presence of long aliphatic chains. These observations align with what is expected from the known structures of these compounds, lending further credibility to the results.

In the case of the second compound, the appearance of ions at m/z values corresponding to nitrogen (14) and oxygen (16) offered additional evidence for the presence of these elements in the compound. This further reinforces the compound's proposed structure and demonstrates the power of mass spectrometry in identifying the elements within a molecule.

Despite the richness of data provided by mass spectrometry, it is important to understand the limitations of this technique. The fragmentation of molecules in the mass spectrometer can follow various pathways, depending on the molecular structure and the specific functionalities present. Consequently, the interpretation of mass spectra can often be complex, requiring careful analysis and often complementary data from other techniques.

Moreover, the interpretations made in this study are tentative and would benefit from further verification. Techniques such as nuclear magnetic resonance (NMR) spectroscopy, infrared (IR) spectroscopy, and elemental analysis can provide additional data to support or refine the structural insights derived from the mass spectrometry data.

Overall, this study illustrates the utility of mass spectrometry in the characterization of complex organic compounds, providing a solid foundation for further structural elucidation and confirmation through complementary techniques. The successful application of this approach to these compounds lays the groundwork for further studies, with the potential to deepen understanding of these and related compounds' structures and behavior.

Results

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