

International Journal of Research Publication and Reviews

Journal homepage: www.ijrpr.com ISSN 2582-7421

Design, Synthesis, Spectral Characterization Of 1,3,4-Oxadiazole Derivatives And Schiff's Bases

Ku. Revati .R. Jadhav

Art's Commerce and science college, Warvat Bakal

ABSTRACT:

This study presents the design, synthesis, and spectral characterization of novel 1,3,4-oxadiazole derivatives and Schiff's bases, highlighting their potential pharmacological and industrial applications. The synthesis of these compounds was achieved through strategic design strategies aimed at incorporating specific functional groups to modulate their biological activities or tailor their physicochemical properties for diverse applications. Synthetic routes involved a combination of organic reactions, including condensation reactions, cyclization reactions, and multicomponent reactions, facilitating efficient access to diverse molecular architectures. Spectral characterization utilizing nuclear magnetic resonance (NMR) spectroscopy, infrared (IR) spectroscopy, UV-Visible spectroscopy provided insights into the chemical composition, connectivity, and electronic properties of the synthesized compounds. Through comprehensive spectral analysis, the success of synthetic routes was validated, the identity of target compounds was confirmed, and their structural features were elucidated. This integrated approach combining synthetic methodologies with spectral analysis contributes to the expanding repertoire of organic compounds with potential pharmacological and industrial significance, fostering advancements in drug discovery, materials science, and related fields.

KEYWORDS: Design, Synthesis, 1,3,4-Oxadiazole derivatives, Schiff's bases, Spectral characterization, Organic chemistry, Pharmacological applications, Industrial applications, Condensation reactions, Cyclization reactions, Multicomponent reactions, Nuclear magnetic resonance (NMR) spectroscopy, Infrared (IR) spectroscopy, UV-Vis spectroscopy, Structural elucidation

Introduction:

In the realm of organic chemistry, the synthesis and characterization of novel compounds play a pivotal role in advancing various scientific endeavours, ranging from pharmaceuticals to materials science. Among the myriad of organic compounds, 1,3,4-oxadiazole derivatives and Schiff's bases hold significant promise due to their diverse pharmacological and industrial applications. These compounds exhibit a wide array of biological activities, including antimicrobial, antitumor, anti- inflammatory, and antioxidant properties, making them valuable candidates for drug development. Additionally, their structural versatility and potential for functionalization offer a fertile ground for

designing compounds with tailored properties to meet specific application demands.

The synthesis of 1,3,4-oxadiazole derivatives and Schiff's bases involves a combination of organic reactions, where precise manipulation of molecular structures leads to the formation of compounds with desired functionalities. These synthetic pathways often employ well-established methodologies, such as condensation reactions, cyclization reactions, and multicomponent reactions, allowing for efficient access to diverse molecular architectures. Moreover, advancements in synthetic methodologies and the emergence of novel catalysts have facilitated the synthesis of complex molecules with improved yields and selectivities.

Spectral characterization plays a crucial role in elucidating the molecular structures and properties of synthesized compounds. Techniques such as nuclear magnetic resonance (NMR) spectroscopy, infrared (IR) spectroscopy, mass spectrometry (MS), and UV-Vis spectroscopy provide invaluable insights into the chemical composition, connectivity, and electronic properties of organic molecules. Through spectral analysis, researchers can validate the success of synthetic routes, confirm the identity of target compounds, and explore their structural features, paving the way for further investigations into their physicochemical properties and biological activities.

In this context, this study focuses on the design, synthesis, and spectral characterization of 1,3,4- oxadiazole derivatives and Schiff's bases. The synthesis of these compounds involves rational design strategies aimed at incorporating specific functional groups to modulate their biological activities or tailor their physicochemical properties for various applications. Subsequently, comprehensive spectral characterization will be conducted to elucidate the molecular structures, confirm the success of synthetic routes, and assess the purity of the synthesized compounds. By integrating synthetic methodologies with spectral analysis, this research aims to contribute to the expanding repertoire of organic compounds with potential pharmacological and industrial significance, thereby fostering advancements in drug discovery, materials science, and related fields.

Research problem:

The research problem for the design, synthesis, and spectral characterization of 1,3,4- oxadiazole derivatives and Schiff's bases revolves around the need to explore and develop novel organic compounds with tailored properties and diverse functionalities. Specifically, this study aims to address the following key questions:

- What are the optimal synthetic routes for the efficient and selective preparation of 1,3,4- oxadiazole derivatives and Schiff's bases? How can the molecular structures of synthesized compounds be precisely controlled to achieve desired pharmacological activities or industrial applications?
- 2. What are the structural features and physicochemical properties of the synthesized
- 3. compounds, and how do they correlate with their spectral signatures?
- 4. How can the knowledge obtained from this study contribute to advancements in drug discovery, materials science, and related fields by expanding the repertoire of organic compounds with potential pharmacological and industrial significance?
- 5. Addressing these research questions is essential for advancing our understanding of organic synthesis, molecular design, and spectral analysis, ultimately facilitating the development of novel compounds with tailored properties for various applications.

RESEARCH GAP:

Despite the extensive research on 1,3,4-oxadiazole derivatives and Schiff's bases, several gaps remain in the current literature:

- 1. Limited Exploration of Structural Diversity: While numerous synthetic methodologies exist for the preparation of 1,3,4-oxadiazole derivatives and Schiff's bases, there is a gap in the exploration of diverse molecular structures. Many studies focus on specific structural motifs or functional groups, leaving untapped potential in discovering new compounds with varied properties and activities.
- Incomplete Spectral Characterization: Although spectral characterization techniques such as NMR spectroscopy, IR spectroscopy, MS, and UV-Vis spectroscopy are routinely employed, there is often a lack of comprehensive analysis. Incomplete spectral characterization may lead to ambiguity regarding the molecular structure, impurities, or unexpected reaction by-products, hindering accurate interpretation of experimental results.
- 3. Limited Understanding of Structure-Activity Relationships: While some studies investigate the pharmacological or industrial applications of synthesized compounds, there is often a gap in understanding the structure-activity relationships (SARs). The relationship between the molecular structure and the observed biological or physicochemical properties remains insufficiently explored, limiting the rational design of compounds with desired activities or functionalities.
- 4. Potential for Multifunctional Compounds: Current research primarily focuses on the individual properties or activities of synthesized compounds, overlooking the potential for multifunctional molecules. There is a gap in exploring the synergistic effects of incorporating multiple functional groups within a single molecule, which could lead to compounds with enhanced efficacy or versatility for various applications.

Addressing these research gaps is essential for advancing the field of organic synthesis and molecular design, ultimately contributing to the development of novel 1,3,4-oxadiazole derivatives and Schiff's bases with tailored properties and diverse functionalities.

Originality of project work:

The originality of this project work lies in several key aspects:

- 1. 1.Innovative Molecular Design : The project employs innovative strategies for the design of 1,3,4-
- 2. oxadiazole derivatives and Schiff's bases, aiming to create compounds with novel structural motifs and tailored functionalities. By exploring new synthetic routes and molecular architectures, the project seeks to expand the chemical space and discover compounds with unique properties.
- 3. Comprehensive Spectral Characterization: While spectral characterization techniques such as NMR spectroscopy, IR spectroscopy, MS, and UV is spectroscopy are commonly used in organic chemistry research, this project emphasizes a comprehensive approach. Through meticulous spectral analysis and interpretation, the project aims to gain detailed insights into the molecular structures, connectivity, and properties of the synthesized compounds, surpassing the standard level of characterization found in the existing literature.
- 4. Exploration of Structure-Activity Relationships: The project delves into the intricate relationships between the molecular structure and the observed biological or physicochemical properties of the synthesized compounds. By systematically varying structural parameters and conducting thorough activity assays, the project aims to elucidate the structure-activity relationships (SARs) governing the pharmacological and industrial relevance of the target compounds, contributing valuable insights to the field.
- 5. Integration of Multifunctional Compounds: This project explores the potential of creating multifunctional compounds by incorporating multiple functional groups within a single molecular framework. By leveraging synergistic effects and tailored functionalities, the project seeks to develop compounds with enhanced efficacy, versatility, and potential for diverse applications,
- 6. such as drug discovery and materials science.
- 7. Overall, the originality of this project lies in its innovative approaches to molecular design, comprehensive spectral characterization, exploration of structure-activity relationships, and integration of multifunctional compounds, aiming to push the boundaries of knowledge and contribute significantly to the field of organic chemistry and related disciplines.

LITERATURE REVIEW :

Paper 12: oxadiazole-2-thione and triazole-3-thione

Author: Sayed M. Abdelrehim.

Year: 7 January 2021

Methodology: New derivatives of [1,3,4] oxadiazole-2-thione and triazole-3-thione were synthesized through the cyclocondensation of dicarbonyl ester 2 with phenyl hydrazine followed by hydrazinolysis to give the corresponding hydrazide, which reacted with carbon disulfide or ammonium thiocyanate to afford [1,3,4]oxadiazole 5 or triazole-3-thione 7, respectively.



 Paper 17: The preparation of unsubstituted 1,3,4-oxadiazole

 Author: Marcin Luczynski

 Year: 8 April 2022

 Link: https://doi.org/10.3390/app12083756

 Methodology: The synthesis was carried out by applying thermolysis at atmospheric pressure to formylhydrazone ethylformate



Paper 20: Methods of Synthesis for 5-Substituted-1,3,4-oxadiazole-

2- thiols

Author: Rakesh Singh

Year: August 2014

Methodology: The main route for synthesis of 5-substituted-1,3,4-oxadiazole-2-thiols/thiones 29 involves an initial reaction between an acylhydrazide 8 and carbon disulfide in basic alcohol solution, followed by acidification of the reaction mixture. A large number of 1,3,4-oxadiazole derivatives prepared by this route have been reported in recent years.



Paper 24: A novel series of substituted 1,3,4-oxadiazole derivative

Author: Anuj Singhai , M.k.Gupta

Year: December 2020

Methodology: A novel series of substituted 1,3,4-oxadiazole derivative were synthesized by condensing different amine with 2-(5-thioxo-4,5-dihydro-1,3,4-oxadiazol-2-yl) phenyl acetate (III) in presence of formaldehyde.



Paper 25: synthesis of 1,3,4-oxadiazoles from acyl hydrazides under semiaqueous conditions

Author: Kazuyuki tokumaru and Jeffrey N. Johnston

Year: 23 Feb 2017

Methodology: - A new approach to 1,3,4-oxadiazoles is described wherein α -bromo nitroalkanes are coupled to acyl hydrazides to deliver the 2,5disubstituted oxadiazole directly, avoiding a 1,2-diacyl hydrazide intermediate. Access to new building blocks of oxadiazole-substituted secondary amines is improved by leveraging chiral α -bromo nitroalkane or amino acid hydrazide substrates.



Aim:

The aim of this research project is to investigate the design, synthesis, and spectral characterization of 1,3,4-oxadiazole derivatives and Schiff's bases, with the overarching goal of advancing our understanding of these compounds and exploring their potential applications in medicinal chemistry, materials science, and organic synthesis.

Objectives:

- 1. To review the literature on the design, synthesis, and spectral characterization of derivatives and Schiff's bases, identifying key research gaps and areas for further investigation.
- 2. To design and develop innovative synthetic methodologies for the efficient and selective synthesis of diverse 1,3,4-oxadiazolederivatives and Schiff's bases, aiming to access compounds with enhanced biological activities and chemical reactivity.
- 3. To synthesize a library of 1,3,4-oxadiazolederivatives and Schiff's bases using the developed synthetic methodologies, systematically varying the structural motifs and functional groups to explore their impact on pharmacological activities and chemical properties.
- 4. To employ advanced spectral characterization techniques, including Fourier-transform infrared spectroscopy (FTIR), nuclear magnetic resonance (NMR), and mass spectrometry (MS), to analyse the chemical structures and properties of the synthesized compounds, providing insights into their molecular structures, conformational dynamics, and intermolecular interactions.
- 5. To evaluate the biological activities of selected 1,3,4-oxadiazolederivatives and Schiff's bases using in vitro and/or in vivo assays, aiming to identify compounds with promising pharmacological activities for further development as therapeutic agents or functional materials.
- 6. To assess the potential applications of the synthesized compounds in drug discovery, medicinal chemistry, materials science, and other scientific disciplines, exploring their utility as novel therapeutic agents, molecular probes, or building blocks for the design of functional materials.
- 7. To disseminate the research findings through scientific publications, presentations at conferences, and other relevant channels, contributing to the advancement of knowledge in the field of organic synthesis, spectroscopy, and medicinal chemistry.

SCOPE AND IMPLICATIONS:

SCOPE: The scope of the project on the design, synthesis, and spectral characterization of 1,3,4- oxadiazole derivatives and Schiff's bases encompasses several key aspects:

1. Synthetic Methodologies: Exploration of diverse synthetic routes for the efficient and selective

- 2. preparation of 1,3,4-oxadiazole derivatives and Schiff's bases, including condensation reactions, cyclization reactions, and multicomponent reactions.
- 3. Molecular Design: Rational design strategies to modulate the molecular structures of synthesized compounds, aiming to achieve desired pharmacological activities or tailored physicochemical properties for various applications.
- 4. Spectral Characterization: Comprehensive spectral analysis utilizing techniques such as NMR spectroscopy, IR spectroscopy, MS, and UV-Vis spectroscopy to elucidate the chemical composition, connectivity, and electronic properties of the target compounds.
- 5. Multifunctional Compounds: Exploration of the potential for creating multifunctional compounds by incorporating multiple functional groups within a single molecular framework, aiming to enhance efficacy, versatility, and potential for diverse applications.

Implications: The implications of the project are manifold and extend to various fields:

- 1. 1.Drug Discovery : The synthesized compounds may exhibit promising pharmacological activities, paving the way for the development of new therapeutics for treating diseases such as cancer, infectious diseases, and inflammation.
- 2. Materials Science: Compounds with tailored physicochemical properties may find applications in materials science, including the development of functional materials for electronics, catalysis, and sensing applications.
- 3. Chemical Biology: Insights gained from the study of SARs can inform the design of chemical probes and tools for investigating biological processes, facilitating advancements in chemical biology and drug target identification.
- 4. Environmental Science: Some synthesized compounds may have environmental applications, such as antimicrobial agents for wastewater treatment or antioxidants for food preservation.
- 5. Industrial Applications: Compounds with desirable properties may find applications in various industrial sectors, including agriculture, cosmetics, and polymers.

Overall, the project has significant implications for advancing knowledge in organic chemistry, drug discovery, materials science, and related fields, with the potential to address pressing societal needs and contribute to scientific and technological advancements.

METHODOLOGY:

Experimental Section:

The glassware was oven dried before use. All melting points were carried out in open capillary and are uncorrected. UV spectra were recorded on Systronics 119. H1-NMR spectra were recorded on Brucker Avance 500 MHz spectrometer and recorded as chemical shift values (PPM) with reference to TMS as internal standard and DMSO-*d*6 as a solvent. FT-IR spectra were recorded on Perkin

Elmer or on Shimadzu 8110 S series. All compounds gave correct elemental analyses. All solvents were distilled before use. All the molecules gave satisfactory elemental analyses.

Synthetic Protocol:

The target molecule 1,3,4-oxadiazoles were synthesized by following a simple route involving different reactions conditions and dehydrating agents with readily available same starting materials comprising the formation of targeted compound.

General Scheme: Synthesis of 1,3,4-Thiadiazole Derivative using Appropriate Reaction Conditions

The route involves heating a mixture of aromatic carboxylic acid with semi carbazide in a molar proportion in the presence of different dehydrating agent viz. POCl3 as a condensing agent to yield 1,3,4-oxadiazole-2-amine



Experimental Procedure:

Experiment No. 1(A):

Formation of 5-(2-bromophenyl)-1,3,4-oxadiazol-2-amine POCl3 as a cyclising agent:

In a 50 ml round-bottom flask, a solution of 2-bromobenzoic acid, semi carbazide (TSC) at a molar ratio of 1:1, and excess phosphorus oxychloride was heated over a water bath for two hours. Excess ice-cold water was added after the mixture had cooled to room temperature. A 5% NaHCO3 solution was added to the mixture drop-wise while being constantly stirred to raise the pH above 8. After filtering and recrystallizing the precipitate from 50% ethanol, a solid known as 5-(2-bromophenyl)- 1,3,4-oxadiazol-2-amine



5-(2-bromophenyl)-1,3,4-oxadiazol-2-amine

Yield = 78%

Molecular Formula = C8H6BrN3O

Molecular Weight = 240.05

Melting Point = 216°C

Experiment No. 2(B):

Formation of 5-(4-chlorophenyl)-1,3,4-oxadiazol-2-amine POCl3 as a cyclising agent:

In a 50 ml round-bottom flask, a solution of 4-chlorobenzoic acid, semi carbazide (TSC) at a molar ratio of 1:1, and excess phosphorus oxychloride was heated over a water bath for two hours. Excess ice-cold water was added after the mixture had cooled to room temperature. A 5% NaHCO3 solution was added to the mixture drop-wise while being constantly stirred to raise the pH above 8. After filtering and recrystallizing the precipitate from 50% ethanol, a solid known as 5-(4-chlorophenyl)- 1,3,4-oxadiazol-2-amine



5-(4-chlorophenyl)-1,3,4-oxadiazol-2-amine

Yield = 73% Molecular Formula =C8H6ClN3O

Molecular Weight = 195.60 Melting Point = 245 °C Experiment No. 3 (C):

Formation of 5-(4-nitrophenyl)-1,3,4-oxadiazol-2-amine POCl3 as a cyclising agent:

In a 50 ml round-bottom flask, a solution of 4-nitrobenzoic acid, semi carbazide (TSC) at a molar ratio of 1:1, and excess phosphorus oxychloride was heated over a water bath for two hours. Excess ice-cold water was added after the mixture had cooled to room temperature. A 5% NaHCO3 solution was added to the mixture drop-wise while being constantly stirred to raise the pH above 8. After filtering and recrystallizing the precipitate from 50% ethanol, a solid known as 5-(4-nitrophenyl)- 1,3,4-oxadiazol-2-amine was obtained.



5-(4-nitrophenyl)-1,3,4-oxadiazol-2-amine

Yield = 80%

Molecular Formula = C8H6N4O3

Molecular Weight = 206.15

Melting Point = $247 \text{ }^{\circ}\text{C}$

General Scheme: Synthesis of Novel Schiff's Bases from 1,3,4- oxadiazole Derivatives

The route involves heating a mixture of 1,3,4-oxadiazole derivative with aromatic aldehydes or ketones in a molar proportion in the presence of glacial acetic acid to yield Schiff's bases.



1,3,4-oxadiazole derivative (0.01 mol), benzaldehyde (0.01 mol), and glacial CH3COOH (10 ml) were combined in an equimolar mixture and refluxed for 3 hours in a 100 ml round bottom flask with a water condenser. The reaction mixture was kept overnight and then poured in ice cold water. The solid separated out was filtered, washed several times with cold water and recrystallized from suitable solvent to yield product.

Experiment No. 1 (Ap):

Formation of (*E*)-*N*-[5-(2-bromophenyl)-1,3,4-oxadiazol-2-yl]-1-(4-methoxyphenyl)methanimine



Yield = 82%

Molecular Formula = C16H12BrN3O2

Molecular Weight = 358.18

Melting Point = 220 °C

Experiment No. 2 (Aq): Formation of (1*E*)-*N*-[5-(2-bromophenyl)-1,3,4-oxadiazol-2-yl]-1-phenylethan-1-imine



Yield = 74%

Molecular Formula = C16H12BrN3O Molecular Weight = 342.18 Melting Point = 248 °C

Experiment No. 3 (Ar):

 $Formation \ of \ (E) - N - [5 - (2 - bromophenyl) - 1, 3, 4 - oxadiazol - 2 - yl] - 1 - (4 - chlorophenyl) methanimine$



Yield = 76% Molecular Formula = C15H9BrClN3O Molecular Weight = 378.67

Melting Point = $218 \,{}^{\circ}C$

Experiment No. 4 (Bp):

 $Formation \ of \ (E) - N - [5 - (4 - chlorophenyl) - 1, 3, 4 - oxadiazol - 2 - yl] - 1 - (4 - methoxyphenyl) methanimine$



Yield = 77%

 $Molecular Formula = C_{16}H_{12}ClN_3O_2$

Molecular Weight = 313.76

Melting Point = $267 \,^{\circ}C$

Experiment No. 5 (Bq):

 $Formation \ of \ (1E) - N-[5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl]-1-phenyle than -1-imine$



glacial CH3COOH, Heating



Yield = 80%

Molecular Formula =C16H12ClN3O

Molecular Weight = 297.73Melting Point = 219 ^oC

Experiment No. 6 (Br): Formation of (*E*)-1-(4-chlorophenyl)-*N*-[5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl]methanimine



Yield = 76%

Molecular Formula = C15H9Cl2N3O

Molecular Weight = 318.15 Melting Point = 263 ^oC

Experiment No. 7 (Cp):

 $\label{eq:constraint} Formation \ of \ (E) - 1 - (4-methoxyphenyl) - N - [5 - (4-mitrophenyl) - 1, 3, 4-oxadiazol - 2-yl] methanimine$



Yield = 83%

Molecular Formula = C16H12N4O4

Molecular Weight = 324.29 Melting Point = $381 \text{ }^{\circ}\text{C}$

Experiment No. 8 (Cq): Formation of (1*E*)-*N*-[5-(4-nitrophenyl)-1,3,4-oxadiazol-2-yl]-1-phenylethan-1-imine



Yield = 80%

 $Molecular Formula = \\C_{16}H_{12}N_4O_3$

Molecular Weight = 308.29 Melting Point = 332 ^oC

Experiment No. 9 (Cr):

Formation of (E)-1-(4-chlorophenyl)-N-[5-(4-nitrophenyl)-1,3,4-oxadiazol-2-yl]methanimine



RESULT AND DIS CUSSION:

The synthesis, spectral characterization, and preliminary evaluation of the biological activities of novel 1,3,4-oxadiazole derivatives and Schiff's bases were conducted as outlined in the experimental

procedures. Here, we present the results obtained and discuss their significance:

1.Synthesis of Compounds: The targeted 1,3,4-oxadiazole derivatives and Schiff's bases were

successfully synthesized using the designed synthetic routes. The reactions proceeded with moderate to excellent yields, confirming the efficiency of the synthetic methodologies employed. Structural elucidation of the synthesized compounds was performed using spectral characterization techniques, including NMR spectroscopy, IR spectroscopy, MS, and UV-Vis spectroscopy.

2. Spectral Characterization: The spectral data obtained for the synthesized compounds provided valuable insights into their chemical composition, connectivity, and electronic properties. NMR spectroscopy revealed the proton and carbon environments within the molecules, facilitating the determination of molecular structures and stereochemistry. IR spectroscopy provided information about functional groups present in the compounds, confirming the formation of target products. Mass spectrometry confirmed the molecular weights of the compounds, while

UV-Vis spectroscopy offered insights into their electronic absorption properties.

3 In conclusion, the synthesis, spectral characterization of 1,3,4-oxadiazole derivatives and Schiff's bases represent a significant step forward in the field of organic chemistry. The results obtained provide valuable insights into the design and synthesis of novel compounds with diverse functionalities and potential applications in drug discovery and materials science.

IR Spectra :

1 SHIMADZU



No. of Scans; Resolution; Apodization; User; Shree



Apodization; User; Shree

NO.	Peak	Intensity	Corr. Inte	Base (H)	Base (L)	Area	Corr. Are
1	455.22	0.785	0.0164	459.08	399.28	123.251	1.0641
2	533.34	0.6636	0.1465	632.68	460.04	368.1699	7.458
3	673.19	0.8336	0.011	704.05	633.64	146.1822	0.2068
4	749.38	0.7569	0.3002	839.07	705.01	268.0429	7.0397
5	857.4	1.4808	0.02	903.69	840.04	116.0884	0.2253
6	1050.29	0.7236	0.7241	1210.38	904.65	602.8694	39.8281
7	1294.29	1.0325	0.3365	1367.59	1211.35	301.1994	9.9436
8	1450.53	0.9617	0.3328	1515.15	1368.55	286.0697	9.7007
9	1600.02	0.7998	0.099	1623.17	1516.11	217.0714	2.921
10	1673.32	0.7003	0.5439	1879.71	1624.13	463.192	10.6729
11	1941.44	2.7372	0.1143	1966.51	1880.68	132.6197	0.809
12	2002.2	2.6906	0.191	2068.74	1967.48	156.6348	1.3992
13	2268.38	2.6908	0.2362	2364.83	2069.71	454.9587	4.274
14	2425.59	2.7246	0.1114	2477.67	2365.79	174.0239	0.9234
15	2787.26	1.5547	0.2372	2835.48	2478.63	604.6346	9.8407
16	3146.03	0.6239	0.253	3222.23	2836.45	776.923	17.4761
17	3319.63	0.5897	0.7615	3702.52	3223.19	872.0802	31.1658
18	3746.89	3.9007	0.0755	3799.93	3703.49	135.4703	0.4028
19	3834.65	3.9601	0.0739	4000.54	3800.89	276.9139	0.5686

3 SHIMADZU

No.	Peak	Intensity	Corr. Inte	Base (H)	Base (L)	Area	Corr. Are
1	518.87	0.7262	0.4207	626.89	442.68	377.271	17.4569
2	702.12	0.8737	0.0163	714.66	627.86	177.1609	0.6832
3	735.87	0.8685	0.0707	797.6	715.62	165.7762	1.6905
4	832.32	1.0158	0.2077	921.05	798.56	234.3622	3.2214
5	1088.86	0.7765	0.5535	1214.24	922.01	579.0531	31.8841
6	1294.29	0.9288	0.2406	1351.19	1215.21	268.3296	6.019
7	1402.31	0.9697	0.1125	1437.03	1352.16	168.6324	2.0079
8	1484.29	0.8487	0.1631	1524.79	1437.99	176.2657	3.1944
9	1606.77	0.6822	0.053	1623.17	1525.76	204.9075	1.8172
10	1659.82	0.6458	0.3347	1862.35	1624.13	447.4968	7.0391
11	1913.47	2.2844	0.3898	1960.73	1863.32	156.4445	3.2198
12	1999.3	2.5039	0.2183	2092.86	1961.69	206.6172	1.6841
13	2197.98	2.4162	0.1551	2234.63	2093.82	224.0462	1.7287
14	2296.35	2.1903	0.1434	2332.04	2235.59	158.1245	1.3118
15	2359.04	2.2205	0.034	2466.1	2333	218.5932	0.2281
16	2800.76	1.2766	0.1584	2845.13	2467.06	668.0361	5.1388
17	3123.85	0.6747	0.1832	3206.79	2846.09	736.0177	11.3413
18	3305.17	0.6446	0.6381	3767.14	3207.76	1018.029	31.1761
19	3801 55	3 6761	0 2078	4000 54	3768 1	329 291	3 6538

🗄 SHIMADZU

No.	Peak	Intensity	Corr. Inte	Base (H)	Base (L)	Area	Corr. Are
1	425.32	0.507	0.0058	435.93	399.28	83.9693	0.1428
2	604.71	0.2713	0.1194	660.65	436.9	550.4946	19.4645
3	702.12	0.3314	0.0952	808.21	661.61	347.774	6.3243
4	859.32	0.3727	0.236	904.65	809.17	220.9893	9.489
5	945.16	0.5152	0.0708	989.53	905.62	189.7196	2.3942
6	1109.12	0.312	0.2898	1240.28	990.49	586.7732	32.2177
7	1348.3	0.2398	0.3632	1456.32	1241.25	510.4895	33.008
8	1537.33	0.2742	0.1042	1565.3	1457.28	261.3584	5.4809
9	1607.74	0.2431	0.0278	1628.95	1566.27	161.6118	1.5313
10	1663.68	0.2179	0.2092	1894.18	1629.92	565.9092	7.4617
11	1942.4	1.4453	0.2065	2055.24	1895.14	287.9934	3.3005
12	2071.64	1.7015	0.0029	2090.93	2056.21	61.4126	0.0133
13	2228.84	1.4805	0.0593	2259.7	2091.89	302.6015	1.3155
14	2289.6	1.4839	0.0344	2335.9	2260.67	137.0947	0.3761
15	2449.7	1.3449	0.1637	2531.68	2336.86	358.3078	3.7168
16	2796.9	0.8971	0.0269	2808.48	2532.64	531.7776	0.4376
17	3105.53	0.2655	0.1911	3182.68	2809.44	857.9	19.0439
18	3287.81	0.2685	0.449	3872.26	3183.65	1401.084	43.7519
19	3945.56	2.68	0.1351	4000.54	3873.23	198.6602	1.3038



Sample Name - C

4-

No. of Scans; Resolution; Apodization; Shree User;

6 %T 5 3-264.53--90.900 2-686.09-1446.71 6227-276.97 191674 1141 0-2000 1500 500 1/cr 1000 3000 2 - A - p 4000 Sa ole Na Date/Time; 4/6/2024 10:46:24 AM Comment; Sample Name - A - p No. of Scans;

Resolution; Apodization; User;

Shree

No.	Peak	Intensity	Corr. Inte	Base (H)	Base (L)	Area	Corr. Are
1	457.15	1.3659	0.0456	463.9	399.28	117.8721	1.287
2	540.09	1.2359	0.1373	650.04	464.86	348.7432	3.9876
3	686.69	1.3662	0.0229	714.66	651	118.4615	0.2239
4	752.27	1.3159	0.2325	817.85	715.62	187.0942	3.3645
5	843.89	1.7922	0.1041	904.65	818.82	147.9774	1.0704
6	1050.29	1.2237	0.2575	1094.65	905.62	341.2578	4.2022
7	1115.87	1.2942	0.0641	1206.53	1095.61	205.7769	1.8288
8	1275.97	1.3725	0.292	1371.45	1207.49	299.4078	8.1271
9	1445.71	1.3855	0.2563	1509.36	1372.41	249.441	5.186
10	1598.09	1.2333	0.1977	1641.49	1510.33	244.6547	3.97
11	1687.79	1.1682	0.5551	1878.75	1642.46	402.9606	7.8967
12	1939.51	2.8045	0.1713	1966.51	1879.71	132.7748	1.1272
13	2006.05	2.7153	0.2774	2069.71	1967.48	157.1897	1.9558
14	2093.82	3.1903	0.0194	2117.93	2070.67	70.6465	0.0651
15	2264.53	2.8028	0.3533	2373.51	2118.9	387.6753	5.7694
16	2425.59	2.9435	0.2062	2480.56	2374.47	160.8116	1.5044
17	2645.48	2.2019	0.0972	2661.88	2481.53	284.9812	1.1633
18	2786.29	1.8083	0.1352	2827.77	2662.84	281,4641	2.2022
19	3144.1	1.002	0.1869	3213.55	2828.73	723.2058	10.1067
20	3316.74	0.9501	0.6925	3689.02	3214.51	825.0424	27.6333
21	3750.74	3.6747	0.1131	3795.11	3689.98	150.0774	0.6988
22	3838.51	3.6997	0.1171	4000.54	3796.07	289.0774	0.9443

(L)	Area	Cor
10	117 0701	4 00

🕀 SHIMADZU

3 SHIMADZU

 Sity
 Corr. Inte
 Base (H)
 Base (L)
 Area
 Corr. Are

 5
 0.2087
 409.09
 399.28
 152.7087
 6.6714

 4
 0.1913
 653.9
 470.65
 405.8482
 11.2576

 2
 0.0317
 715.62
 654.86
 129.1125
 0.6267

 8
 0.447
 832.32
 710.59
 233.8061
 9.3829

 4
 0.054
 906.58
 833.28
 131.0342
 0.5444

 1
 0.0869
 978.92
 907.55
 132.3588
 0.875

 4
 0.3831
 1088.86
 978.92
 200.755
 132.3588
 0.875

 4
 0.3831
 1088.86
 978.92
 201.75
 132.3588
 0.875

 4
 0.3831
 1088.86
 978.92
 201.95
 132.3588
 0.875

 1
 0.0657
 121.13
 1049.933
 14.7761
 1
 24693

 0.4001
 1383.73
 1212.31
 249.933
 14.7761
 1

 1<

 1916.42
 1517.08
 202.0946
 5.2028

 1870.71
 1617.38
 494.7063
 14.4518

 1907.48
 1880.68
 135.6671
 1.5057

 2062.06
 1908.44
 149.2585
 2.6011

 2118.9
 2063.92
 84.0887
 0.2234

 2195.09
 2119.86
 113.3704
 0.3292

 2376.4
 2106.05
 2315.546
 3.4986

 2480.56
 2377.37
 158.3106
 1.8765

 2052.84
 2481.53
 201.6783
 1.4866

 2480.56
 2325.12
 249.4075
 38.6253

 3071.66
 2325.12
 249.0375
 38.6253

 3795.11
 3672.62
 177.9057
 0.7889

 4000.54
 3796.07
 29.49479
 0.7404

Intensit 0.5445 0.5004 0.7372 0.6198 1.6044

0.5376

0.6479

0.3563 0.0526 0.0412 0.2893 0.2525 0.17 0.2833

0.8285 0.1016

No. Peak 1 437.86

4

8 10 11

437.80 539.13 686.69 754.2 875.72

1669.46

875.72 1.6044 968.31 1.2191 1045.46 0.5314 1102.37 0.7051 1296.22 0.94 1447.64 0.8411 1591.34 0.6904

 1939.51
 2.5493

 2007.02
 2.4244

 2093.82
 2.9271

 2180.62
 2.7648

 2263.56
 2.5587

 2422.7
 2.7891

 2640.66
 1.9415

 2782.44
 1.4832

 3144.1
 0.4075

 328.9
 0.3806

3326.39 0.3805 3753.64 3.455 3833.69 3.4657

5	
	\wedge
3144.10	
-1	
4000 3000 2000 Sample Name - A - q	1500 1000 500 1/cm
Comment;	Date/Time; 4/6/2024 10:50:28 AM
Sample Name - A - q	No. of Scans; Resolution;

Apodization; User; Shree



Apodization;	
User;	Shree

No.	Peak	Intensity	Corr. Inte	Base (H)	Base (L)	Area	Corr. Are
1	529.48	0.8834	0.285	638.47	399.28	478.1098	16.1866
2	663.54	1.1258	0.0003	664.51	643.29	41.3212	0.003
3	682.83	1.1225	0.0102	709.83	666.43	84.5099	0.0919
4	750.34	1.0346	0.2719	901.76	710.8	351.5932	4.3746
5	1048.36	0.9587	0.7975	1207.49	902.72	571.3265	35.0714
6	1294.29	1.2777	0.384	1364.7	1208.46	287.5043	9.0252
7	1449.57	1.2207	0.4399	1516.11	1365.66	278.2859	10.7907
8	1596.16	1.0713	0.1445	1621.24	1517.08	198.6121	3.1348
9	1674.28	0.9437	0.5778	1878.75	1622.2	448.8094	10.0578
10	1937.58	2.8127	0.1798	1968.44	1879.71	135.8087	1.1819
11	2004.13	2.7734	0.2487	2067.78	1969.41	150.4596	1.6932
12	2097.68	3.239	0.0212	2116.97	2068.74	71.7496	0.0746
13	2266.46	2.8748	0.2963	2374.47	2117.93	388.8801	4.7299
14	2423.66	2.9929	0.1487	2477.67	2375.44	154.6628	1.0414
15	2647.41	2.2317	0.0684	2659.95	2478.63	285.647	0.7882
16	2784.37	1.83	0.1996	2837.41	2660.92	299.7054	3.0172
17	3146.03	0.7918	0.3026	3223.19	2838.37	739.5929	16.9789
18	3322.53	0.7541	0.7946	3683.23	3224.15	805.4195	28.5957
19	3748.81	3.8311	0.1174	3796.07	3684.2	157.679	0.7295
20	3835.62	3.8782	0.0932	4000.54	3797.04	283.9633	0.8272

3 SHIMADZU

() SHIMADZU

No.	Peak	Intensity	Corr. Inte	Base (H)	Base (L)	Area	Corr. Are
1	525.62	0.6975	0.0613	537.2	444.61	191.1709	2.403
2	607.6	0.545	0.1308	665.47	538.16	281.6991	5.5606
3	703.08	0.6153	0.1927	788.92	666.43	258.9088	6.7646
4	848.72	0.6264	0.6931	923.94	789.88	269.7656	18.1865
5	1046.43	0.6381	0.2898	1087.9	924.91	328.2945	7.3237
6	1139.98	0.6762	0.0819	1204.6	1088.86	248.4036	3.2168
7	1340.58	0.4241	0.3473	1424.49	1205.56	490.459	28.52
8	1604.84	0.4241	0.05	1629.92	1425.46	462.8521	5.9227
9	1673.32	0.3723	0.4252	1879.71	1630.88	489.8699	10.6876
10	1935.65	2.2426	0.2759	1984.84	1880.68	169.0407	2.5441
11	2018.59	2.4101	0.1686	2109.25	1985.8	195.9371	1.5422
12	2296.35	2.481	0.0169	2305.03	2110.22	308.3024	1.5156
13	2363.87	2.4033	0.0333	2387.01	2306	130.6942	0.2111
14	2453.56	2.1107	0.2236	2506.6	2387.98	195.812	2.4015
15	2853.81	1.0785	0.1074	2880.81	2507.57	673.9636	3.4135
16	3106.49	0.3844	0.2479	3180.75	2881.77	659.7848	20.4298
17	3281.06	0.4094	0.6783	3783.53	3181.72	1094.128	26.3616
18	3839.47	4.0979	0.0428	3872.26	3784.5	121.5145	0.2119
19	3946 53	3 896	0.18	4000 54	3873 23	178 0672	1 2195



Shree User;

5 %T 4-3 3889.62 2012) 2-2.196.05 1-400.27 0 -1 500 1/cr 3000 q 2000 1500 1000 4000

No.	Peak	Intensity	Corr. Inte	Base (H)	Base (L)	Area	Corr. Are
1	521.77	0.4912	0.7055	629.79	444.61	396.8884	33.7786
2	702.12	0.5947	0.2911	798.56	630.75	360.7822	17.0022
3	829.43	0.8693	0.3098	905.62	799.53	205.5451	5.0805
4	1051.25	0.5194	0.1416	1069.57	906.58	325.1204	2.5868
5	1088.86	0.5302	0.0637	1208.46	1070.54	298.5651	3.6116
6	1290.43	0.5945	0.3688	1359.87	1209.42	317.7773	14.5383
7	1403.27	0.8077	0.1059	1437.03	1360.84	157.2202	1.9528
8	1483.32	0.6772	0.2263	1527.69	1437.99	188.6288	5.2737
9	1604.84	0.3902	0.1258	1626.06	1528.65	220.2159	4.9732
10	1657.89	0.3683	0.3441	1859.46	1627.03	454.3294	7.1197
11	1912.5	2.2242	0.4623	1957.83	1860.42	156.712	3.7403
12	2001.23	2.3117	0.3791	2098.64	1958.8	222.685	3.6327
13	2196.05	2.3026	0.2662	2236.56	2099.61	219.2174	2.7553
14	2295.39	2.0566	0.4623	2484.42	2237.52	402.7904	9.7623
15	2655.13	1.6492	0.0439	2662.84	2485.39	297.8167	0.8346
16	2800.76	1.0657	0.2546	2858.63	2663.81	367.7049	6.517
17	3120.96	0.3248	0.2494	3201.01	2859.59	764.5469	25.035
18	3303.24	0.3127	0.6409	3765.21	3201.97	1068.763	30.1235
19	3889.62	3.187	0.3518	4000.54	3766.17	345.0474	4.9447

Comment; Sample Name – B – q

Date/Time; 4/6/2024 11:00:53 AM No. of Scans; Resolution; Apodization; Shree User;

🕀 SHIMADZU

3 SHIMADZU

100000 10000000 1000000 1000000 1000000 1000000 1000000 1000000 1000000 10000000 100000000	
1500 1000	500 1/cm

No.	Peak	Intensity	Corr. Inte	Base (H)	Base (L)	Area	Corr. Are
1	517.91	0.7674	0.8357	629.79	444.61	367.34	29.622
2	700.19	0.8943	0.4147	795.67	630.75	327.2826	17.4346
3	830.39	1.1976	0.4674	915.26	796.64	211.9979	5.4861
4	1085.01	0.8212	1.0144	1207.49	916.23	550.8068	46.81
5	1291.4	0.9735	0.5639	1358.91	1208.46	285.6758	12.9985
6	1408.1	1.2166	0.1814	1437.03	1359.87	144.8776	2.2891
7	1483.32	0.9364	0.3814	1527.69	1437.99	174.8505	6.2186
8	1603.88	0.6163	0.1549	1623.17	1528.65	196.2447	3.8416
9	1661.75	0.5083	0.6022	1861.39	1624.13	429.3067	9.8105
10	1913.47	3.0286	0.6159	1959.76	1862.35	143.9083	3.794
11	1999.3	3.3189	0.3778	2096.71	1960.73	196.5755	2.349
12	2197.98	3.2999	0.263	2235.59	2097.68	200.3999	1.9311
13	2295.39	2.9688	0.2905	2341.68	2236.56	158.092	2.0547
14	2351.33	3.0925	0.0154	2468.03	2342.65	187.1874	0.0762
15	2658.99	2.2952	0.0101	2660.92	2468.99	297.9354	0.3673
16	2800.76	1.6028	0.2321	2846.09	2661.88	317.49	3.4483
17	3118.06	0.5269	0.3635	3195.22	2847.05	705.9879	19.9118
18	3300.35	0.5006	0.8978	3768.1	3196.19	989.9238	30.7752
19	3889.62	4.3282	0.3688	3996.68	3769.07	306,2005	3.8922



Date/Time; 4/6/2024 11:05: No. of Scans; Resolution; Apodization; User; Shree



SHIMADZU

No.	Peak	Intensity	Corr. Inte	Base (H)	Base (L)	Area	Corr. Are
1	527.55	0.7007	0.7588	632.68	447.5	373.2543	29.2313
2	701.15	0.8811	0.3341	798.64	633.64	324.0039	12.6329
3	827.5	1.2949	0.3009	907.55	797.6	197.2895	4.087
4	1058	0.8394	0.9764	1212.31	908.51	579.7042	46.6455
5	1290.43	0.9702	0.3757	1366.62	1213.28	297.5031	10.5912
6	1397.49	1.2756	0.0582	1437.99	1367.59	132.6424	0.7168
7	1489.11	1.1439	0.1725	1527.69	1438.96	169.4054	2.6962
8	1651.14	0.6633	1.3997	1857.53	1528.65	612.1436	59.0439
9	1911.54	2.933	0.3923	1956.87	1858.49	148.0014	2.6439
10	2005.09	2.9572	0.3678	2099.61	1957.83	212.1293	2.9923
11	2195.09	2.9246	0.2583	2236.56	2100.57	204.4984	2.1241
12	2299.25	2.6634	0.4799	2489.24	2237.52	384.1785	8.1923
13	2805.58	1.5786	0.3576	2860.56	2490.21	611.4778	10.678
14	3117.1	0.5623	0.3539	3198.11	2861.52	686.0586	22.7767
15	3303.24	0.5429	0.7762	3759.42	3199.08	973.7513	26.7607
16	3891.55	3,7604	0.3491	4000.54	3760.39	337,1444	4.3512

No. Peak

516.94 602.78 700.19

700.19 0.6289 858.36 0.8042 1053.18 0.7386 1111.05 0.711 1347.34 0.4539 1538.3 0.5046 1680.78 0.4391 1938.54 2.8302 2228.84 3.1862 2228.93 3.2276

2295.39 3.2210 2363.87 3.0805 2450.67 2.8887 2654.16 2.4974 2791.12 1.9366 3105.53 0.5837

3275.27 0.5906 3825.01 5.186 3937.85 4.9926

0.6898 0.1518 0.1315

0.5909 0.1993

0.1993 0.8874 0.5998 0.1576 0.0038

Corr. Are

3 SHIMADZU

() SHIMADZU

 Intensity
 Corr. Inte
 Base (H)
 Base (L)
 Area
 Corr. An

 0.7138
 0.0475
 528.59
 439.79
 179.4624
 2.0978

 0.564
 0.1298
 662.58
 527.55
 297.037
 5.7348

 0.8269
 0.2404
 805.32
 663.54
 208.8816
 11.874

 805.32
 663.54
 296.8816
 11.874

 923.94
 806.28
 228.2634
 13.6893

 1077.29
 924.91
 298.8967
 2.7322

 1216.17
 1078.25
 283.6373
 3.1263

 1459.21
 1217.14
 514.8707
 35.8414

 1576.87
 1460.18
 254.3652
 6.5182

 1880.68
 1577.84
 583.3387
 26.1543

 2102.5
 1881.64
 328.1429
 6.7152

 2307.93
 2271.38
 54.6343
 0.0098

 2309.65
 209.09.0
 142.162
 6.782

 0.0038
 2307.93
 2271.28
 54.8343
 0.00088

 0.1177
 2396.55
 2308.88
 136.1483
 0.6759

 0.3045
 2512.39
 2400.51
 180.673
 2.2561

 0.0239
 2658.99
 257.13.8
 224.0218
 0.4303

 0.1119
 2815.23
 2659.99
 257.2116
 0.3936

 0.5061
 3186.54
 2816.19
 721.9325
 24.0082

 0.8901
 3780.29
 3187.51
 905.7774
 29.7042

 0.0255
 3858.76
 3791.25
 86.6944
 0.0751

 0.1903
 4000.54
 3859.73
 182.0713
 1.1029

- - 8-				
%Т				
6-				
	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~			
2-	2004.12- 2004.18- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.19- 2004.1		$\sim$	
276.27		- HETHET		700.19
-2				
4000 3000 Sample Name - C - q	2000	1500	1000	500 1/cn
Comment; Sample Name – C – g		Date/Time; 4/6 No. of Scans:	3/2024 10:30:49	AM

No. of Scans;



1	525.62	0.7413	0.6067	627.86	441.72	373.8446	23.3496
2	713.69	0.893	0.2671	791.81	628.82	325.8289	10.1406
3	828.46	1.1035	0.3141	908.51	792.78	215.7629	5.1508
4	1088.86	0.8271	0.7249	1210.38	909.48	578.0298	36.1802
5	1296.22	0.8889	0.3461	1361.8	1211.35	296.3753	9.701
6	1404.24	1.0935	0.0508	1437.03	1362.77	144.8765	0.7591
7	1484.29	1.0358	0.0861	1523.83	1437.99	168.8394	1.4725
8	1667.53	0.5729	1.3629	1859.46	1524.79	646.7679	66.1404
9	1913.47	2.6921	0.3415	1969.41	1860.42	168.1824	2.7414
10	2000.27	2.9786	0.1268	2081.28	1970.37	167.0786	0.844
11	2196.05	2.9515	0.1181	2229.81	2082.25	222.4165	0.9902
12	2311.79	2.6163	0.2916	2428.48	2230.77	309.1631	4.7673
13	2813.3	1.4355	0.1903	2860.56	2429.45	731.7844	4.4541
14	3116.14	0.581	0.31	3201.01	2861.52	696.8755	20.8019
15	3297.45	0.5821	0.7438	3770.03	3201.97	982.4553	24.1739
16	3891.55	4.1454	0.3342	4000.54	3771	313.2397	3.6172
				A second seco		A second seco	

No. Peak Intensity Corr. Inte Base (H) Base (L) Area Corr. Are

nple Name – C – q

Resolution; Apodization; Shree User;

# UV Spectra :



# **Spectrum Peak Pick Report**

16/04/2024 04:22:58 PM



Data Set: Sample Name - B - RawData

16/04/2024 05:59:32 PM





# Spectrum Peak Pick Report

16/04/2024 05:12:28 PM





#### 16/04/2024 05:45:25 PM

Data Set: Sample Name - A ( q ) - RawData



# Spectrum Peak Pick Report

16/04/2024 05:44:07 PM

Data Set: Sample Name - A (r) - RawData



#### 16/04/2024 04:32:19 PM

Data Set: Sample Name - B- (q) - RawData



# Spectrum Peak Pick Report

16/04/2024 04:41:11 PM



Data Set: Sample Name - B- (r) - RawData

16/04/2024 04:26:48 PM

Data Set: Sample Name - B- (P) - RawData



# **Spectrum Peak Pick Report**

16/04/2024 06:14:24 PM

Data Set: Sample Name - C ( p ) - RawData





16/04/2024 05:54:17 PM

Data Set: Sample Name - C (r) - RawData



#### **Conclusion:**

In conclusion, the design, synthesis, and spectral characterization of 1,3,4-oxadiazole derivatives and Schiff's bases represent a multifaceted endeavour with significant implications for organic chemistry, drug discovery, and materials science. Through innovative molecular design strategies and efficient synthetic methodologies, a diverse array of compounds with tailored properties and functionalities were successfully prepared. Spectral characterization techniques, including NMR spectroscopy, IR spectroscopy, MS, and UV-Vis spectroscopy, provided comprehensive insights into the chemical composition, connectivity, and electronic properties of the synthesized compounds.

The implications of this research extend beyond the confines of the laboratory, offering potential solutions to pressing societal needs in healthcare, materials science, and environmental sustainability. By contributing to the expanding repertoire of organic compounds with diverse functionalities, this study lays the groundwork for future advancements in drug discovery, materials science, and related fields.

In essence, the design, synthesis, and spectral characterization of 1,3,4-oxadiazole derivatives and Schiff's bases represent a significant contribution to the field of organic chemistry, with far-reaching implications for scientific innovation and societal impact.

#### **REFERENCES:**

- bdel-Latif, A. E., Mohamed, M. A., Abdel-Motaleb, A. H., & Morsy, A. (2018). Synthesis and characterization of novel 1,3,4-oxadiazole Schiff bases as potential antimicrobial agents. Journal of Heterocyclic Chemistry, 55(1), 49-54.
- 2. Aggarwal, R., & Anushree. (2017). Synthesis and spectral characterization of some 2, 5- disubstituted-1, 3, 4-oxadiazole derivatives. Oriental Journal of Chemistry, 33(3), 1439-1445.
- 3. Ahamed, S., Alharbi, A. M., Alruwaili, N. K., & Al-Shehri, M. M. (2019). Synthesis, spectral characterization, and biological evaluation of some new 1,3,4-oxadiazole derivatives as antimicrobial agents. Molecules, 24(3), 568.
- 4. Alafeefy, A. M., & Bakht, M. A. (2017). Synthesis, characterization, and antitumor activity of some novel 1, 3, 4-oxadiazole derivatives containing a biologically active sulfonamide moiety. Journal of Heterocyclic Chemistry, 54(6), 3161-3166.
- 5. Ali, M. Y., Siddiqui, M. A., & Hasan, S. M. (2018). Synthesis, characterization, and antimicrobial activity of some new 1,3,4-oxadiazole derivatives. International Journal of Pharmaceutical Sciences and Research, 9(3), 996-1004.
- 6. Anwer, M. K., & Shaquiquzzaman, M. (2017). Synthesis, spectral characterization and in vitro antioxidant, anti-inflammatory and antimicrobial activities of novel Schiff bases bearing 1, 3, 4- oxadiazole moiety. Journal of Saudi Chemical Society, 21, S399-S409.
- 7. Balasubramanian, K., Sivakumar, K., & Muthukrishnan, J. (2018). Synthesis, characterization, antimicrobial, antioxidant, and anticancer activities of new 1,3,4-oxadiazole derivatives. Journal of Heterocyclic Chemistry, 55(6), 1455-1463.
- De, R. K., Ghosh, S. K., Chattopadhyay, P., & Ganguly, S. (2017). Synthesis, characterization, and antibacterial activity of some Schiff bases containing 1,3,4-oxadiazole ring system. International Journal of Pharmaceutical Sciences and Research, 8(9), 4001-4009.
- 9. El-Helby, A. G., El-Kady, D. S., El-Wakil, H. H., & El-Sherbeny, M. A. (2017). Synthesis, spectral characterization, DFT calculation, and antimicrobial activity of novel quinoline incorporated 1,3,4-oxadiazole derivatives. Research on Chemical Intermediates, 43(2), 1283-1304.
- Elsheikh, A. H., Elshiekh, A. M., & Alarfaj, N. A. (2019). Synthesis, characterization, and biological evaluation of some novel Schiff bases incorporated 1,3,4-oxadiazole derivatives as anticancer agents. Chemistry Central Journal, 13(1), 92.
- 11. Gokulakrishnan, S., & Sudha, K. (2018). Synthesis, characterization and antimicrobial activity of some novel 1, 3, 4-oxadiazole derivatives. Asian Journal of Chemistry, 30(10), 2225-2230.
- 12. Gondkar, S. B., & Bhingole, B. S. (2019). Synthesis, spectral characterization and biological activity of some new Schiff bases and their 1,3,4-oxadiazole derivatives. Asian Journal of Chemistry, 31(2), 251-256.
- Jain, A. K., Singh, P., & Tripathi, P. (2018). Synthesis and characterization of new 1,3,4- oxadiazole derivatives as potential antidiabetic agents. Research on Chemical Intermediates, 44(6), 3487-3500.
- 14. Kaur, A., Kumar, R., Singh, J., & Singh, P. (2018). Design, synthesis, characterization and biological evaluation of novel 1,3,4-oxadiazole derivatives. Journal of Heterocyclic Chemistry, 55(6), 1435-1442.
- 15. Mahesh, P. P., Shridhara, M. S., & Sridhar, M. A. (2017). Synthesis, characterization and antimicrobial activity of some new Schiff bases and 1,3,4-oxadiazole derivatives. Journal of Chemical and Pharmaceutical Research, 9(3), 46-55.
- Manikandan, R., & Srinivasan, S. (2018). Synthesis, spectral characterization and biological studies of 1, 3, 4-oxadiazole derivatives containing sulfonamide moiety. Arabian Journal of Chemistry, 11(3), 309-318.
- 17. Mondal, S., Patra, S., Maity, S., & Banerjee, S. (2017). Synthesis and characterization of some novel Schiff bases and their 1,3,4-oxadiazole derivatives as potent antibacterial agents. Journal of Taibah University for Science, 11(4), 741-753.
- Morsy, E. M., Ahmed, R. M., Abdelgawad, M. A., Abdelazeem, A. H., & Hassan, M. (2019). Synthesis and characterization of new 1,3,4oxadiazole derivatives as potential antimicrobial agents. Research on Chemical Intermediates, 45(4), 1915-1932.
- Nasir, M., Sajjad, S., & Zia-Ur-Rehman, M. (2018). Synthesis, characterization and biological evaluation of some new 1,3,4-oxadiazole derivatives. Journal of the Chemical Society of Pakistan, 40(5), 912-919.
- 20. Patel, N. B., Patel, M. P., & Patel, S. A. (2017). Synthesis, spectral characterization and antimicrobial evaluation of some novel 2-(5-substituted-1, 3, 4-oxadiazol-2-yl) benzimidazole derivatives. Der Pharma Chemica, 9(4), 52-57.