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Characterization, Biological Studies And Application Of Novel Quaternary Ammonium Compound (Benzyldimethylphenylammonium Chloride)

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Abstract

Quaternary ammonium compounds (QACs) have proven to be highly beneficial in various applications, particularly as disinfectants, due to their potent antimicrobial properties. One such compound, benzyldimethylphenylammonium chloride (BDPAC), has garnered attention for its effectiveness during the COVID-19 pandemic, where the need for efficient disinfectants was paramount. This study synthesized and characterized BDPAC through UV-Visible and FT-IR spectroscopy, providing insights into its molecular structure and properties. The compound was incorporated into a hand sanitizer formulation, which was then tested for its antibacterial and antifungal efficacy against a range of microorganisms. The results showed that BDPAC exhibited strong antimicrobial activity, effectively inhibiting the growth of different bacteria and fungi, highlighting its broad-spectrum effectiveness. Additionally, the study investigated the pH variation of both the BDPAC compound and the prepared sanitizer, as pH entertains a critical role in assessing the product's effectiveness against microbes and its compatibility with skin. The findings suggest that BDPAC, with its proven disinfectant properties, can serve as a powerful agent in combating a various infectious diseases, making it a valuable addition to hand sanitizers and other disinfectant products used for hygiene and infection control.

Keywords: Benzyldimethylphenylammonium chloride, UV-visible, FT-IR, Bacteria, Fungi

Introduction

The COVID-19 pandemic significantly affected global public health, leading the World Health Organization (WHO) to release a set of urgent recommendations and guidelines designed to mitigate the transmission of the virus. These regulations included strict measures such as advising people to remain in their homes, the mandatory wearing of face masks, and most importantly, promoting

frequent hand-washing with soap and the use of sanitizers as part of enhanced hygiene protocols [1]. As the pandemic progressed, the demand for disinfectants, particularly hand sanitizers, increased exponentially due to the growing awareness of the virus's spread via surfaces and human contact. This surge in demand for sanitizers, alongside the growing understanding of the need for effective infection control measures, prompted the exploration of various disinfectant compounds that could be employed to prevent the spread of COVID-19 and other infectious diseases [2, 3, 4].

Among the promising candidates for this purpose are quaternary ammonium compounds (QACs), such as benzyldimethyphenylammonium chloride. These compounds have long been recognized for their potent antimicrobial properties, which include the ability to neutralize bacteria, viruses, and fungi by disrupting their cellular structures. Research has shown that QACs, particularly benzyldimethylphenylammonium chloride, possess broad-spectrum activity, making them ideal agents for use in disinfectants, sanitizers, and other cleaning products during infectious disease outbreaks [5, 6, 7, 8, 9, 10]. In this study, the primary focus was on the preparation and comprehensive analysis of benzyldimethylphenylammonium chloride as an active ingredient in sanitizers. The research involved a thorough spectral characterization of the compound using UV-Visible and FTIR spectroscopy, which helped identify its chemical structure, functional groups, and confirm its suitability for use in sanitizing products.

Beyond chemical analysis, the antimicrobial efficacy of both benzyldimethylphenylammonium chloride and the sanitizers formulated with it was carefully evaluated through antibacterial and antifungal studies. These experiments were carried out independently to evaluate the compound's effectiveness in suppressing the proliferation of five distinct bacterial species, encompassing both gram-positive and gram-negative strains, as well as two varieties of fungi. This allowed for an in-depth understanding of the compound's broad-spectrum antimicrobial activity, providing valuable insights into its effectiveness against a wide range of pathogens commonly associated with infections. The sanitizers were formulated to deliver maximum effectiveness without compromising user safety, and the study revealed that the sanitizers not only exhibited significant antimicrobial activity but also offered protection against a variety of infectious agents.

In addition to the antimicrobial studies, the pH variations of both the sanitizing solutions and the benzyldimethylphenylammonium chloride compound were carefully monitored. The pH of a solution can significantly affects its antimicrobial activity and stability, and understanding these variations is crucial in ensuring that the sanitizers remain effective over time while being safe for skin contact. The results indicated that the sanitizer solutions maintained a pH within a range suitable for both effective antimicrobial action and safe human use, highlighting their potential for widespread use in public health measures.

The findings of this research underscore the potential of benzyldimethylphenylammonium chloride as a highly effective and reliable disinfectant in the fight against infectious diseases. The study demonstrated that both the sanitizer and soap formulations prepared using this compound were active against a broad spectrum of bacterial and fungal pathogens. This research not only provides a valuable

contribution to the development of disinfectants for use during the COVID-19 pandemic but also has broader implications for future public health efforts in controlling infectious diseases. Now a days the environment plays an essential role in transmission of infectious diseases. The infectious diseases causing bacteria, fungi and viruses spread through the air droplets, mucus and during contact with person. In this pandemic situation, quaternary ammonium compounds based on alcohols that reduce the impact of microorganisms, WHO suggested that sanitizers reduce the level of microorganisms. The benzyldimethylphenylammonium chloride used sanitizers are developed in this study are safe for human use and offer an essential tool in preventing the spread of harmful pathogens, making them an important addition to global efforts to mitigate the impact of infectious outbreaks.

Materials and Methods

Chemicals

All chemicals utilized were of analytical grade. The substances N,N-Dimethyl aniline, Chlorobenzene, Isopropyl alcohol, and glycerin were acquired from Isochem Laboratory Chemicals, Pvt. Ltd in Kochi, India, and double-distilled water was employed consistently throughout the experiment.

Synthesis of Benzyldimethylphenylammonium chloride

In a clean dry reaction flask add N-N dimethylaniline typically in a molar excess add benzyl chloride dropwise to the reaction flask. The molar ratio of N-N dimethylaniline and benzyl chloride is typically 1:1. Slowly add conc. HCl dropwise to the mixture. The acid serves to protonate the amine group, forming the benzyldimethylphenylammonium chloride.

Experimental Section

A Li-2900 UV spectrometer was used to record the spectra to determine the produced benzyldimethylphenylammonium chloride's absorption wavelength. The Jasco FTIR-4600 is an instrument used to identify the presence of functional groups in quaternary ammonium compounds. Hand sanitizer and produced benzyldimethylphenylammonium chloride were measured for pH using a digital pH meter. The mean ± standard deviation was used to record the pH readings.

Biological Assay

In this study, two kinds of biological activity studies are employed. These studies are antifungal and antibacterial. Gram-positive and gram-negative bacteria have been the subjects of antibacterial and antifungal investigations using the disc diffusion method.

Results and Discussions

UV – Visible Spectroscopy

The synthesized compound's absorbance spectra are determined using UV spectroscopy. Eight distinct concentration solutions were made for this study, and the absorbance wavelength of each was determined. The absorbance wavelength was determined to have distinct peaks at 367nm, 366nm, 358nm, 354nm and 246nm at 0.1M to 0.8M concentrations. Table 1 shows the wavelength of UV absorptions. Figures 1 and 2 show the spectrum images for concentrations of 0.1M and 0.7M. The

0.1M concentration absorbed highest wavelength at 0.1M and 0.7M absorbed the least wavelength at 246nm.

Table.1. Absorbance wavelength of prepared quaternary ammonium compound

CONCENTRATION (Molarity)	ABSORBANCE WAVELENGTH (nm)
0.1M	367nm
0.2M	366nm
0.3M	366nm
0.4M	358nm
0.5M	366nm
0.6M	358nm
0.7M	246nm
0.8M	354nm

Fig.1.UV-Visible spectrum of Benzyldimethylammonium chloride at 0.1M concentration

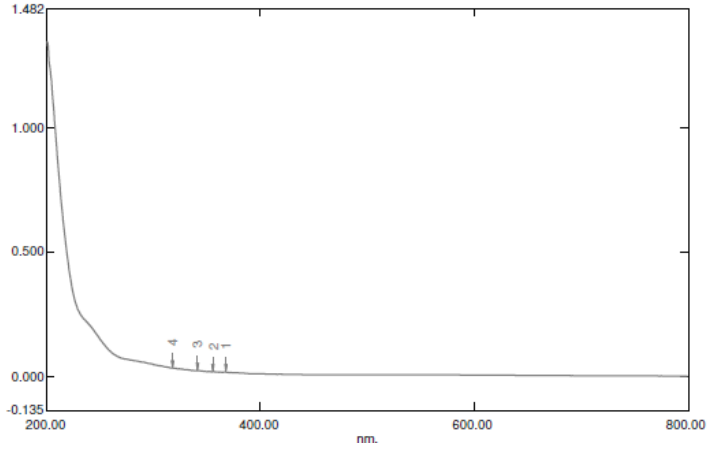
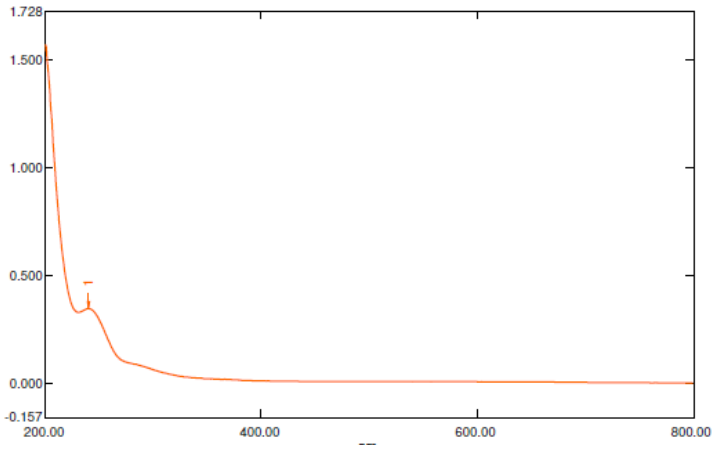


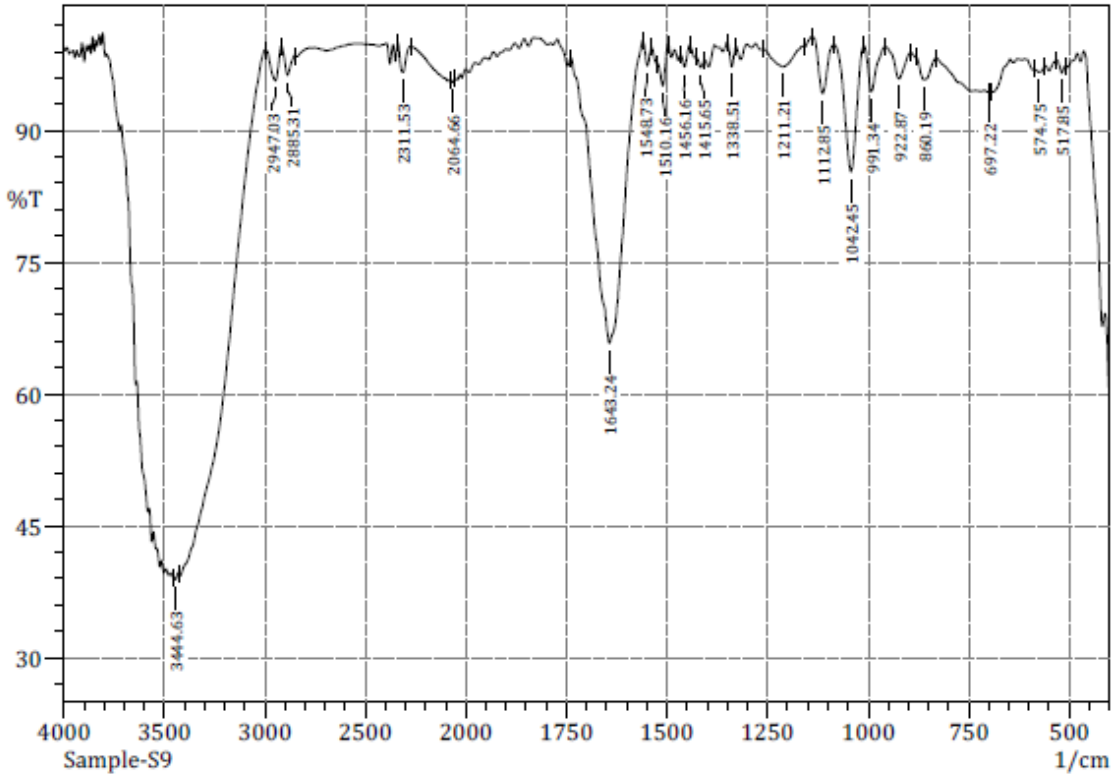
Fig. 2. UV-Visible spectrum of Benzyldimethylammonium chloride at 0.7M concentration



FT-IR Spectroscopy

One useful and non-destructive method for obtaining quantitative information about biological materials is FTIR spectroscopy. The 4000cm^{-1} to 500cm^{-1} range is covered by the FT-IR spectrum. There are numerous peaks identified for the synthesized BDPAC are shown in Fig. 3. The functional groups which whole peaks which belong to the ranges 2947cm^{-1}is C-H stretch of Aldehydes, 2885cm^{-1}C-H stretch of Alkanes, 2311cm^{-1}C=N stretch alkenes 574 cm^{-1}is C-Br stretching of Alkyl and aryl halides, 2064cm^{-1}C=C conjugated and C≡C,1643cm^{-1}is N-H bend of Primary amines, 1548cm^{-1} is NO_2 stretch Nitro compounds, 1510cm^{-1}is NO_2 stretch Nitro compounds, 517cm^{-1}is C-Br stretching of Alkyl and aryl halides.

Fig. 3 FT-IR spectrum of Benzyldimethylphenylammonium chloride



Antibacterial Assay

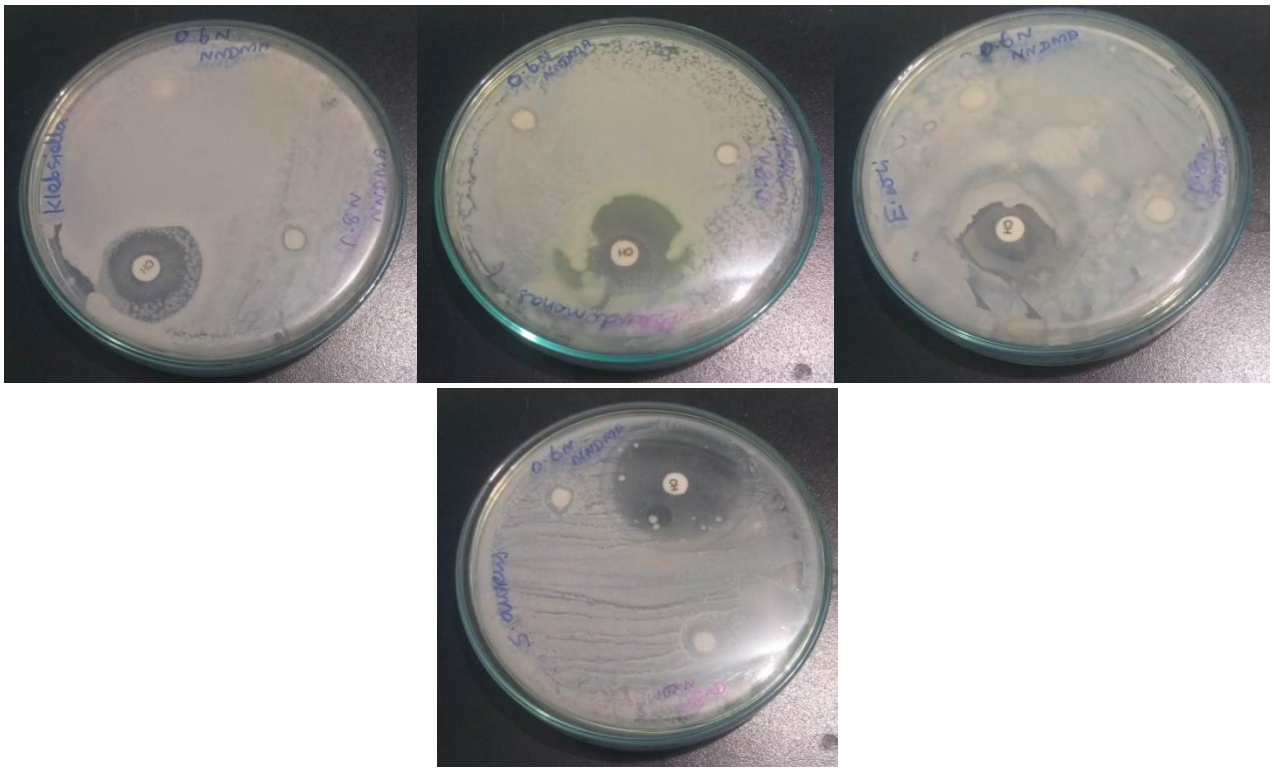
S. aureus, S. epidermidis, K. pneumoniae, E. coli, and P. aeruginosa were tested in the antibacterial testing of produced quaternary ammonium compounds [13,27,28,29,30]. The compounds' antibacterial activity at concentrations ranging from 0.1M to 0.8M. S. Aureus and S. Epidermidis bacteria have the strongest antibacterial activity in this solution out of the five species of bacteria tested. Both of these bacteria are classified as gram-positive. Therefore, compared to gram-negative bacteria, the benzyldimethylphenylammonium chloride is more active in gram-positive bacteria.

Table. 2 display the results of the antibacterial activity for BDPAC

Bacteria	**Zone of inhibition(mm)**								
	Concentration level								
	0.1	**0.2**	**0.3**	**0.4**	**0.5**	**0.6**	**0.7**	**0.8**	**Std**
Staphylococcus aureus	7	7	7	9	10	12	13	16	30
Staphylococcus epidermidis	7	7	9	9	10	12	12	12	15
Klebsiella pneumonia	7	7	7	7	12	12	13	15	25
Escherichia coli	7	7	9	15	13	12	12	12	30

Pseudomonas aeruginosa	7	7	7	9	9	9	10	11	25

Fig. 4. Antibacterial activity results for BDPAC



Antifungal Assay

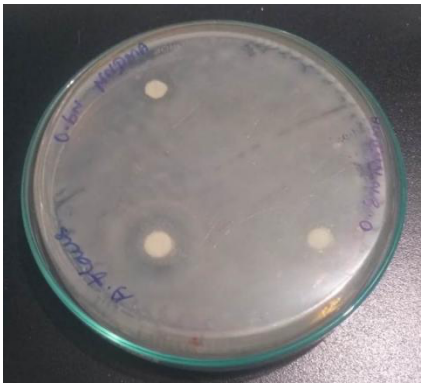
For the antifungal investigation, eight distinct normality solutions with concentrations ranging from 0.1M to 0.8M were provided. The effectiveness of these eight distinct treatments against two different fungal infections C. albicans and A. flavus was examined [13,29,30]. Upon completion of the research, it was discovered that when normalcy grows, so does activity. Compared to Candida albicans, this chemical is more effective against A. flavus infections. Thus, the results of the antifungal activity indicate that the chemical benzyldimethylphenylammonium chloride may be used to treat illnesses brought on by fungus like A. flavus and C. albicans.

Table 3 The Antifungal activity results for BDPAC

Fungi	**Zone of inhibition(mm)**								
	Concentration level								
	0.1	**0.2**	**0.3**	**0.4**	**0.5**	**0.6**	**0.7**	**0.8**	**std**

Aspergillus flavus	7	7	9	9	10	12	12	11	15
Candida albicans	7	7	7	7	8	9	10	14	24

Fig. 5. Antifungal activity results for BDPAC



Sanitizer

Benzyldimethylphenylammonium chloride, a quaternary ammonium compound, was utilized in the formulation of the disinfectant. The sanitizer was prepared using a solution with a concentration ranging from 0.1M to 0.8M. Studies on the produced sanitizer's antimicrobial properties were also carried out [8,15]. The research' findings demonstrate the effectiveness of sanitiser made with a Benzyldimethylphenylammonium chloride solution against both bacteria and fungus.

Table.4: The Antibacterial activity results for sanitizer prepared from BDPAC

Bacteria	**Zone of inhibition(mm)**								
	Concentration level								
	0.1	**0.2**	**0.3**	**0.4**	**0.5**	**0.6**	**0.7**	**0.8**	**Std**
S aureus	7	9	9	15	9	9	10	12	20
S epidermidis	-	-	7	9		7		10	16
K pneumonia	-	-	9	11		9		9	15
E coli	7	7	12	15		15		20	26
P aeruginosa	-	-	8	8		12		10	30

Fig. 6. Antibacterial activity results for sanitizer prepared from BDPAC

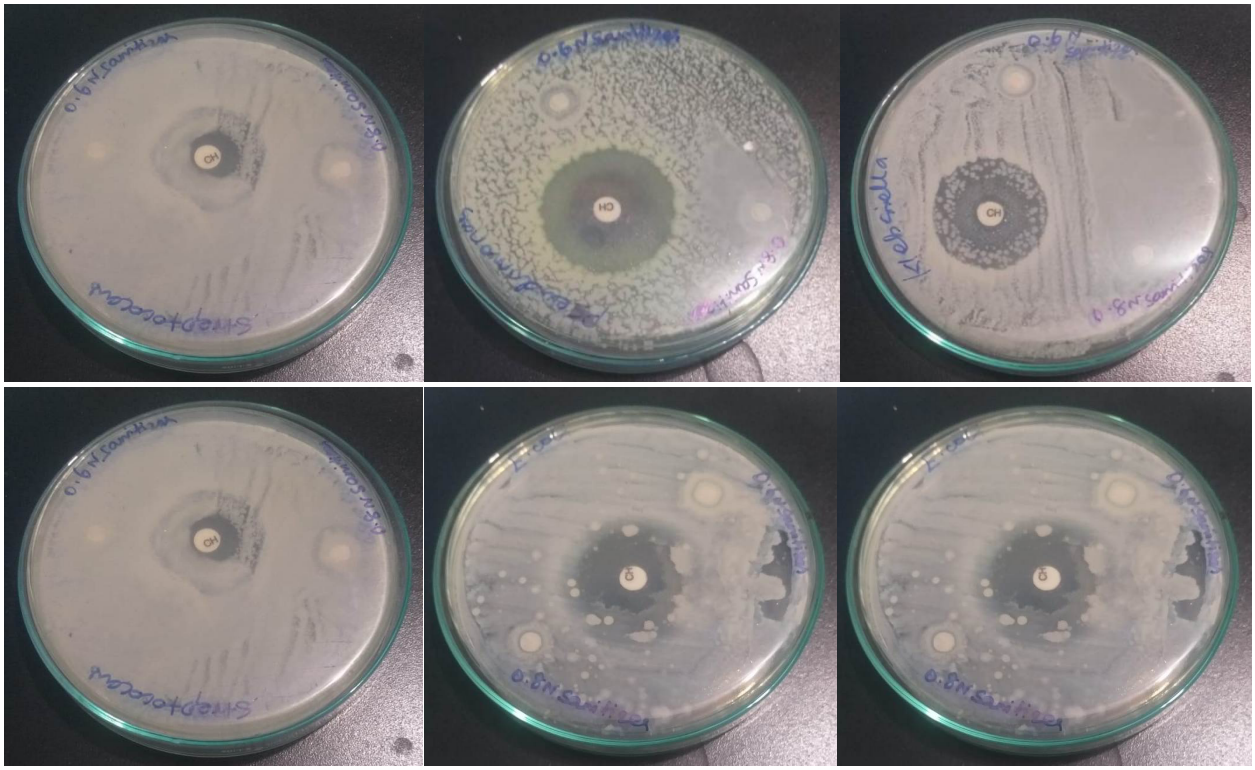
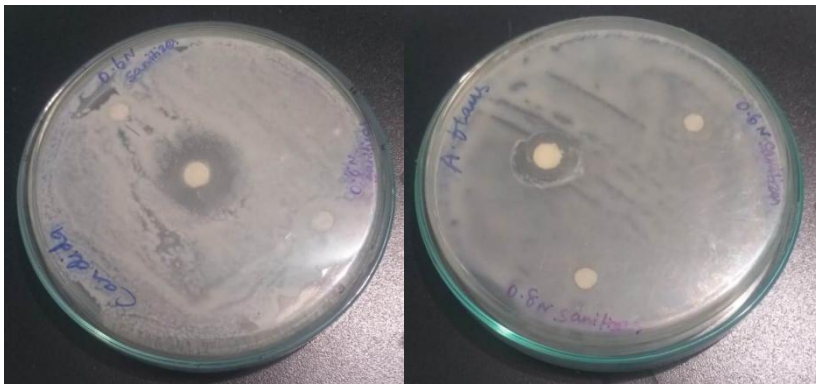


Table 5: The Antifungal activity results for sanitizer prepared from BDPAC

Fungi	Zone of inhibition(mm)								
	Concentration level								
	0.1	**0.2**	**0.3**	**0.4**	**0.5**	**0.6**	**0.7**	**0.8**	**std**
A flavus	9	9	13	15		9		10	15
C albicans	7	7	9	11		9		10	20

Fig. 7. Results of antifungal activity for the sanitizer formulated from BDPAC



pH Variation

A solution of benzyldimethylphenylammonium chloride is prepared with concentrations varying from 0.1M to 0.8M. Sanitizers were made independently using these eight concentration solutions at each of the eight concentrations. The produced chemical and sanitizer underwent distinct pH fluctuations. According to the findings of numerous research, sanitizers with pH values between 4 and 7 often do not harm skin. Furthermore, studies show that a pH of little over 7 is deemed safe for application to human skin [4,12,]. The produced sanitizer and compound have a pH value that is lower than or equal to 7. Therefore, people are not harmed by this sanitizer. Tables 4. and 5 show the pH variations of the chemical and sanitizer made in this study. Figures 5 and 6 depict the alterations in pH levels of the quaternary ammonium compound and the sanitizer derived from solutions of benzyldimethylphenylammonium chloride.

Table.6. pH fluctuations for the synthesized quaternary ammonium compound

Concentrations	pH variations
0.1M	2
0.2M	3
0.3M	4
0.4M	5
0..5M	5
0.6M	1
0.7M	1
0.8M	3

Table.7. pH fluctuations of sanitizer formulated from quaternary ammonium compounds

Concentrations	pH variations

0.1M	6
0.2M	5
0.3M	6
0.4M	5
0.5M	5
0.6M	4
0.7M	5
0.8M	5

Conclusion

This article presents the findings of several investigations that were conducted using the solution made with benzyldimethylphenylammonium chloride. The UV and FTIR spectral results have been utilized to ascertain the absorption wavelength and identify the functional groups. Compound and sanitizer pH fluctuations are measured independently. Based on the sanitizer's pH fluctuations, it has been determined that benzyldimethylphenylammonium chloride produced sanitizer is safe for human skin. Studies on antibacterial and antifungal properties have also examined the solution's ability to combat various bacterial and fungus species. According to the findings of these investigations, benzyldimethylphenylammonium chloride is a great disinfectant that has many applications for people.

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Author's contributions

The authors, S. Suba Jelin Goldy, C. Isac Sobana Raj, have made equal contributions to both the writing and reviewing of the manuscript.

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Availability of data and materials

Not applicable

Declarations

Ethical approval

When preparing this article, we perform the experiments contain FTIR, UV instrumentations, then pH variation, docking studies, antibacterial and antifungal activity.

Competing interests

The authors state that they possess no conflicts of interest.

REFERENCES

1) Cassandra. L., ACS Infectious Diseases., **2020**, 6, 1553-1557.
2) Deepthi. B V., Oriental Journal of Chemistry., **2024**, 6, 1570-1577.
3) Himasha M. Pera., Chemical Research in Toxicology., **2021**, 34, 672-674.
4) Alhassan H. Aodah., Saudi Pharmaceutical Journal., **2021**, 29, 807-814.
5) Hannah M. Dewey., ACS Chemical Health & Safety, **2021**, 10, 1-12.
6) Priya I. Hora., Environmental Science and Technology Letters., **2020**, 7, 622-631.
7) B.H. Ogilvie., Journal of Hospital Infection., **2020**, 108, 142-145.
8) Janee Lee Jia Jing., International Journal of Environmental Research and Public Health., **2020**, 17, 1-17.
9) Priya I. Hora., Environmental Science Process & Impacts., **2020**, 12, 1368-1381.
10) Zheng G., Environmental Science and Technology Letters., **2020**, 7, 760-765.
11) Renata Odzak., Pharmaceuticals., **2023**, 16, 1-23.
12) Ionidis, G. Hubscher., Infect. Dis., **2016**, 16, 77.
13) Fruzsina Demeter., International Journal of Molecular Sciences., **2023**, 24, 1-20.
14) Schrank, C.L., ACS Infectious Diseases., **2020**, 6, 1553-1557.
15) Sarah C. Marteinson., Environmental Reviews., **2023**, 31, 73-91.
16) Nikola Sakac., Sensors, **2023**, 2126.
17) Diya Patel., International Journal of Creative Research Thoughts., **2022**, 10, 1-12.
18) Deneke Shamebo Menamo., Ethiopian Journal of Science & Technology., **2017**, 10, 209-220.
19) Shivani Kushwaha., International Journal for Research in Applied Science & Engineering Technology., **2021**, 9, 1205-1214.
20) Deepthi B V., Res. J. Chem. Environ., **2024**, 28, 76-81.
21) Benarbia Abderrahim., World Journal of Environment Engineering., **2015**, 3, 95-110.
22) Deepthi B V., Acta Scientific Pharmaceutical Sciences., **2022**, 8, 32-39.
23) R. Anisha., Asian Journal of Chemistry., **2022**, 34, 3145-3150.
24) J. Jenisha., Indian Journal of Chemical Technology., **2023**, 30, 231-236.
25) S. Mahil Rani., Indian Journal of Biochemistry and Biophysics., **2020**, 57, 620-626.
26) Amit Kumar Sharma., The Journal of Biomedical Research., **2011**, 25, 335-347.
27) S. Sibmah., Indian Journal of Chemical Technology., **2022**, 29, 526-532.
28) Hasan A. Hemeg., Saudi Journal of Biological Science., **2020**, 27, 3221-3227.
29) Jeeffin Blessikha. R., Research Journal of Chemistry and Environment., **2023**, 27, 1-17.
30) R. Jeeffin Blessikha., Indian Journal of Chemical Technology., **2023**, 30, 385-391.