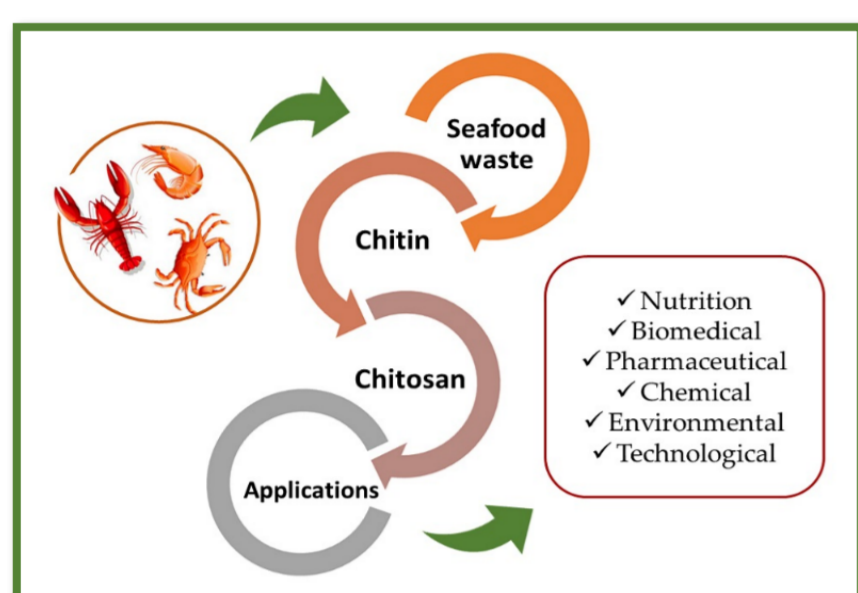




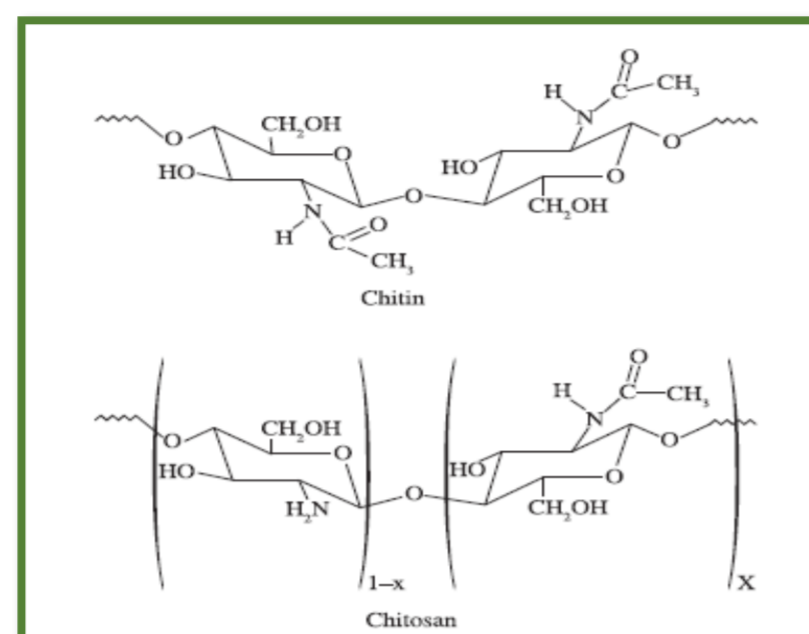
ABSTRACT

Antibacterial and antiviral filters greatly prevent the formation of harmful particles, infections and allergies that cause the spread of diseases. After the COVID-19 pandemic, which recently affected the whole world, it has been observed that the prevention of infectious diseases spread by air particles have been quite intensive. One of the strategy to prevent the spread of the infection is biocidal coating onto the air filters. In this study, it is emphasized that chitosan-based antibacterial membrane coating onto the air filter can enhance spreading of the microorganisms. Thus, chitosan was functionalized with polyethylene glycol units, methyl iodate and isobutryl aldehyde to enhance biocidal activity on the surface. Coating was applied to glass surfaces to provide biocidal activity. Afterwards, biocidal activity of the polypropylene coated surfaces was tested against to *E.coli* and *S.aureus*.

CHITOSAN

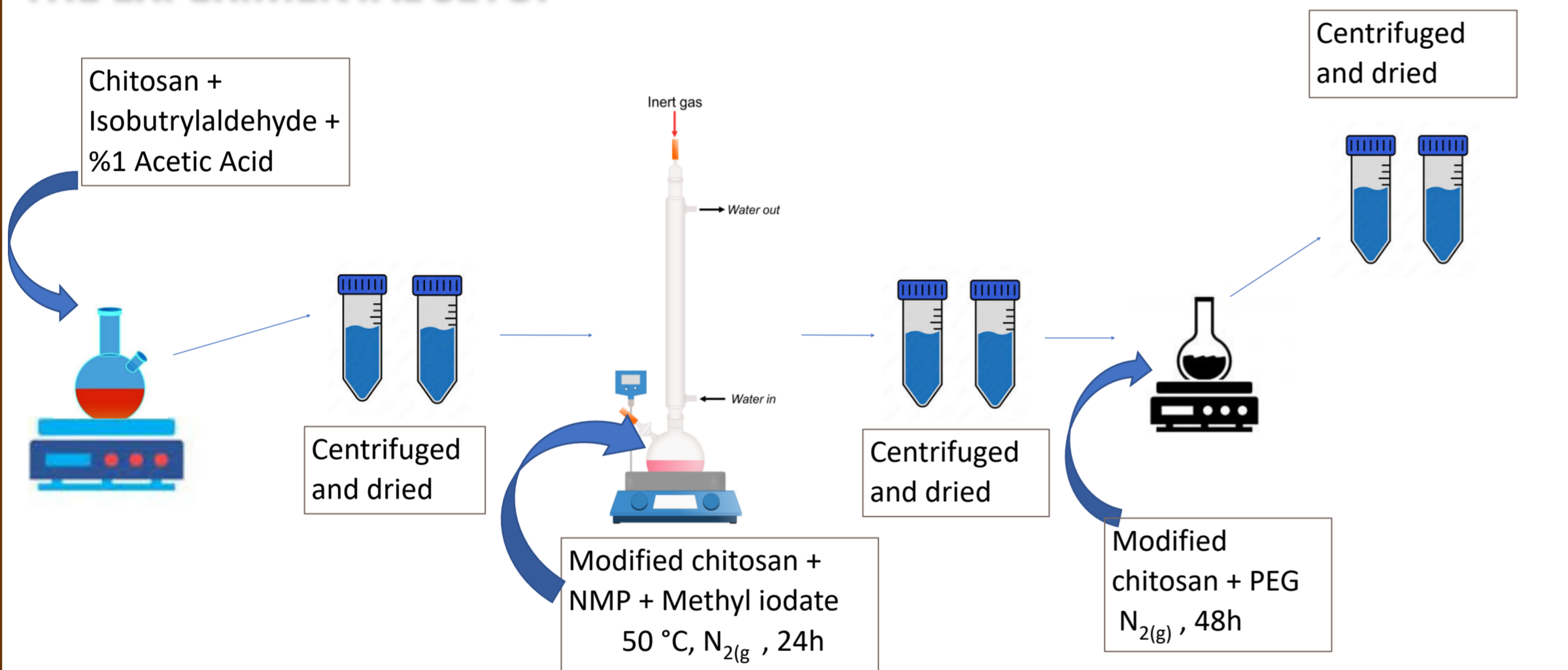


Chitosan Production Cycle [1]

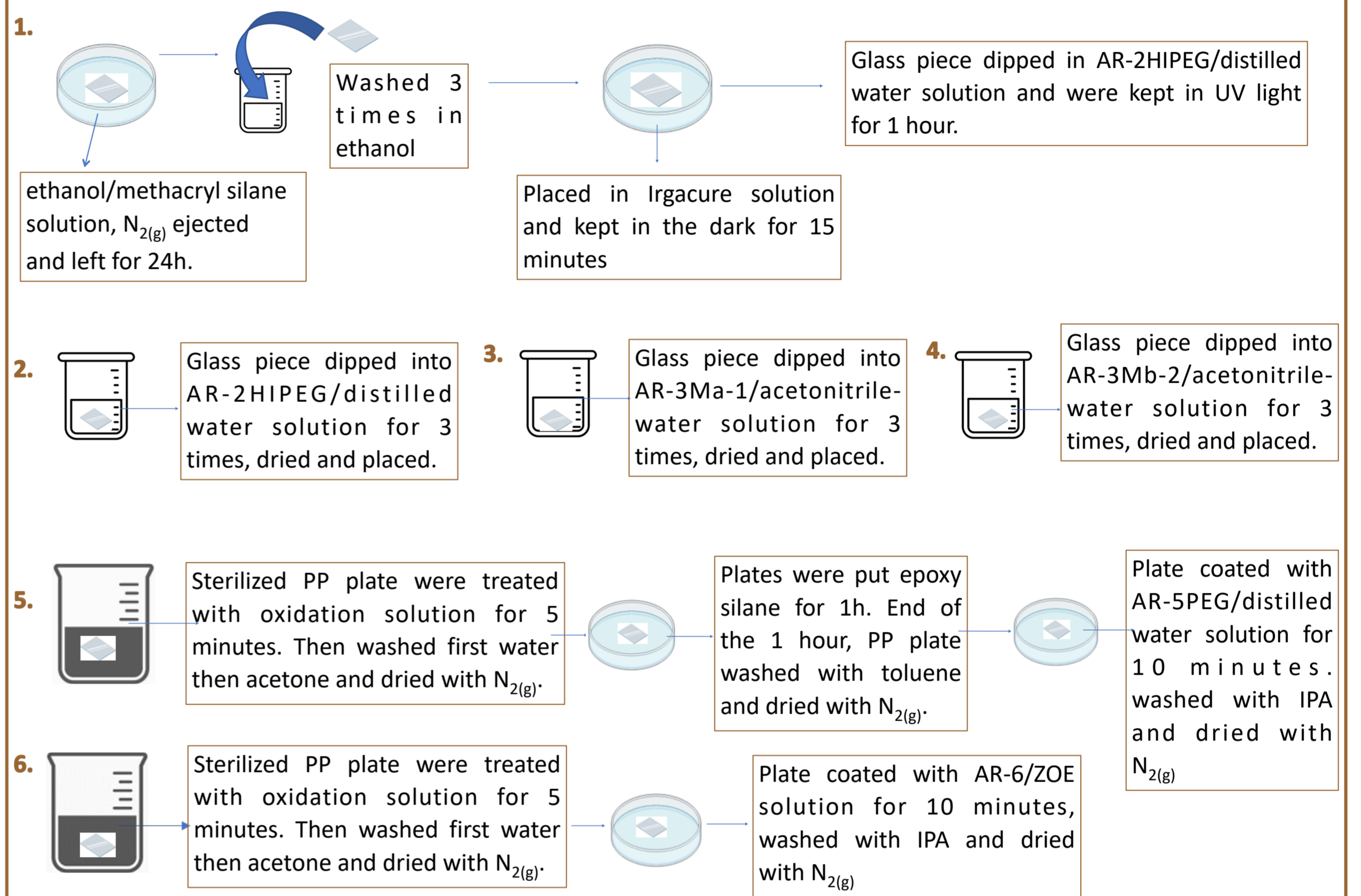


Schematically chemical structures of chitin and chitosan [2]

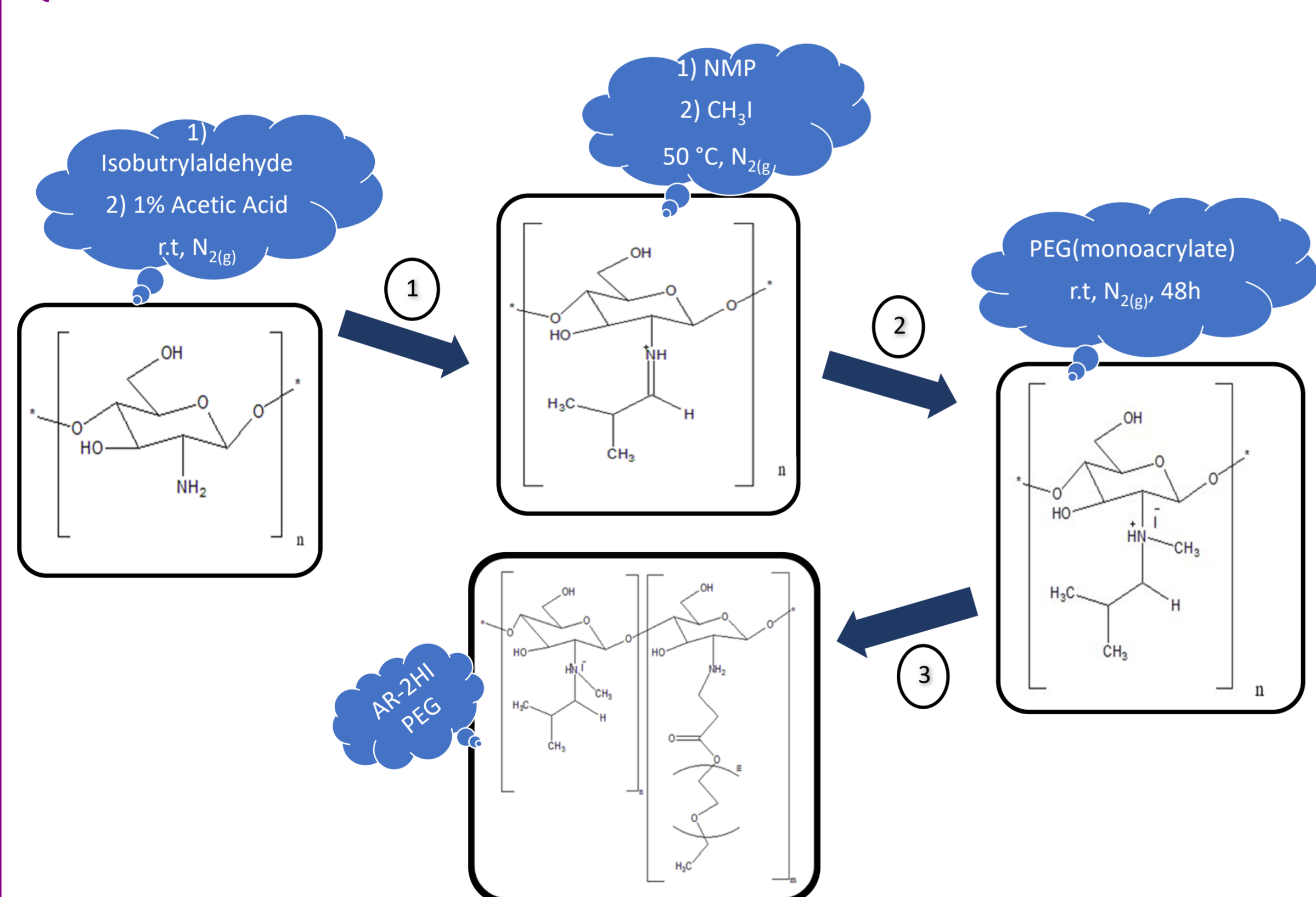
THE EXPERIMENTAL SETUP



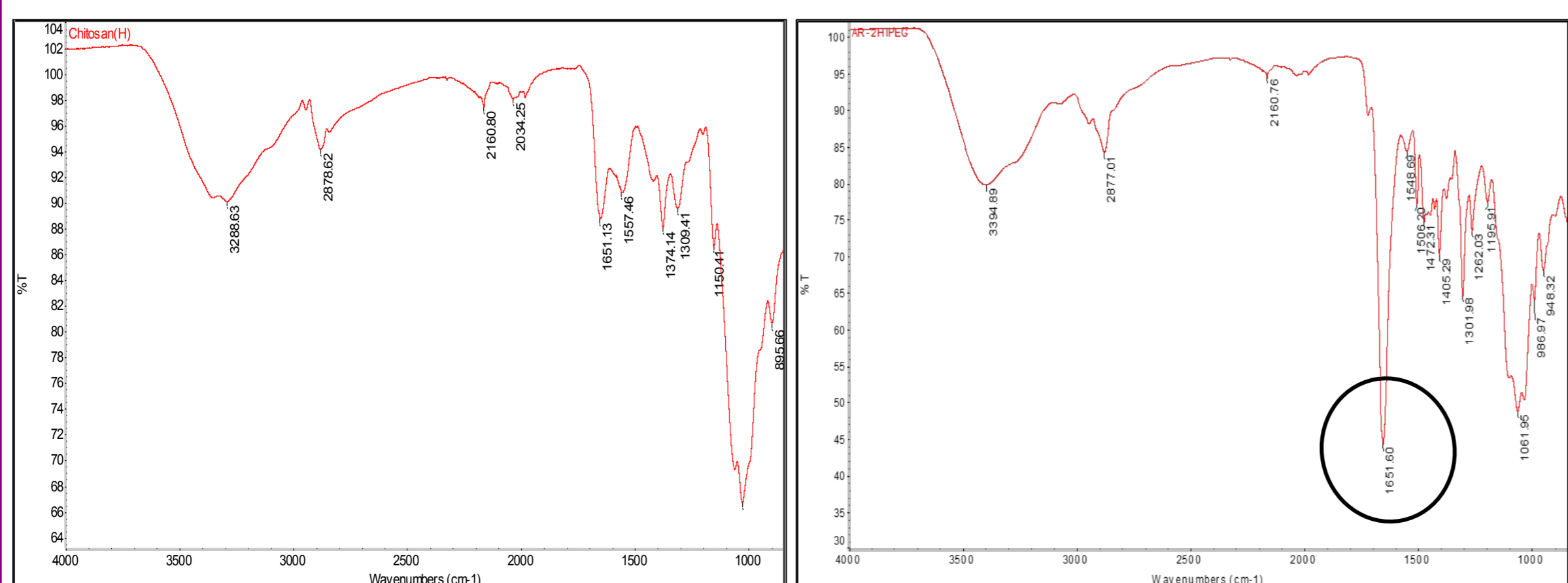
COATING SETUP



QUATERNIZED CHITOSAN

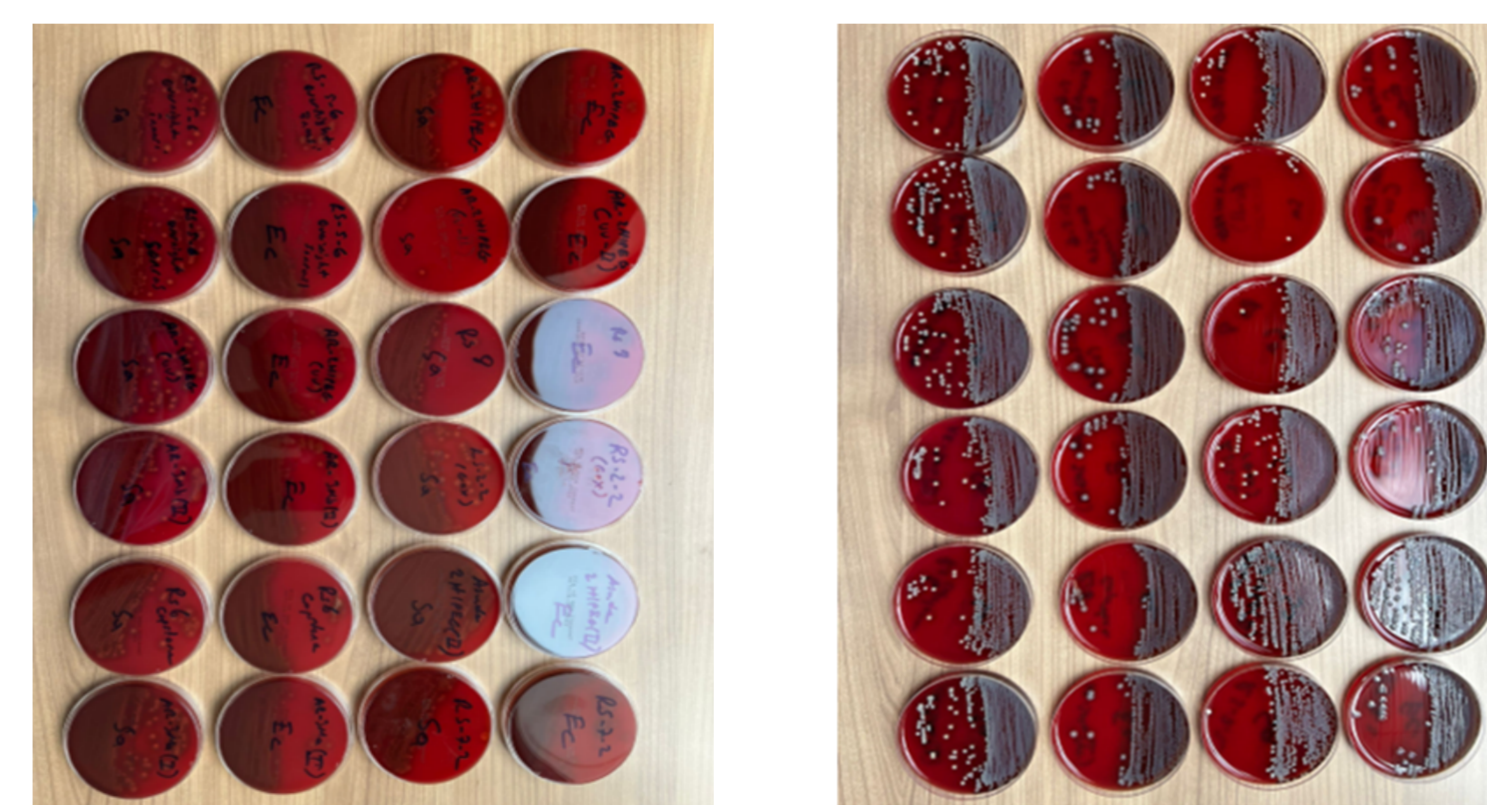


FTIR SPECTRA RESULT



BIOCIDAL ACTIVITY SURFACE TEST RESULTS

SAMPLE	E. COLI	S. AUREUS
AR-2HIPEG UV-1	no activity	no activity
AR-2HIPEG UV-2	no activity	%99.9 antibacterial activity
AR-2HIPEG-1	no activity	no activity
AR-2HIPEG-2	no activity	no activity
AR-3Ma-1	no activity	no activity
AR-3Mb-2	no activity	no activity



CONCLUSION

- In this research, biocidal surface was obtained by using chitosan derivatives. Quaternization through amine groups and PEG modification via Michael addition route were conducted.
- It was observed that bare PEG modification did not show any biocidal activity against *E.coli* and *S.aureus*. However, quaternization with methyl iodate resulted in 99.9% biocidal effectiveness against *S.aureus* bacteria.
- These surfaces are designed to minimize the spread of infections and maintain a more hygienic environment in various settings, including hospitals, air filters, public spaces, and households.

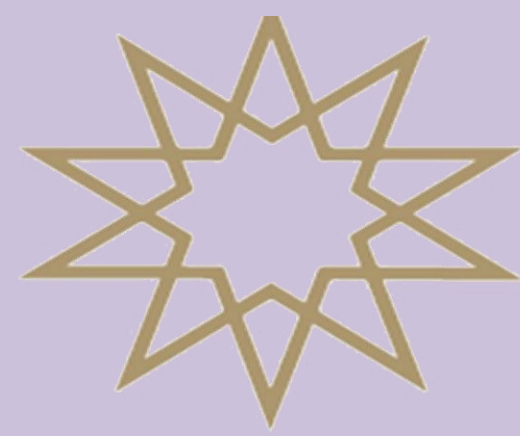
I would like to extend my appreciation to Arçelik R&D for their support in carrying out and collaboration with us in this research.

REFERENCES

[1] Teixeira-Costa, B. E., & Andrade, C. T. (2021, October 28). Chitosan as a Valuable Biomolecule from Seafood Industry Waste in the Design of Green Food Packaging. *Biomolecules*, 11(11), 1599.

[2] Goy, R. C., Britto, D. D., & Assis, O. B. G. (2009). A review of the antimicrobial activity of chitosan. *Polímeros*, 19(3), 241–247.

[3] Li, P., Poon, Y. F., Li, W., Zhu, H. Y., Yeap, S. H., Cao, Y., Qi, X., Zhou, C., Lamrani, M., Beuerman, R. W., Kang, E. T., Mu, Y., Li, C. M., Chang, M. W., Jan Leong, S. S., & Chan-Park, M. B. (2010, December 12). A polycationic antimicrobial and biocompatible hydrogel with microbe membrane suctioning ability. *Nature Materials*, 10(2), 149–156.



ABSTRACT

In this thesis, it was aimed to obtain antioxidant α -tocopherol from pumpkin seed shells grown in Nevşehir by using different extraction methods, including sCO₂ and traditional method. It is planned to recycle pumpkin seed shells, process this product with the most advantageous method with its beneficial properties, provide added value and export it as a product with high commercial value.

INTRODUCTION

Cucurbita pepo

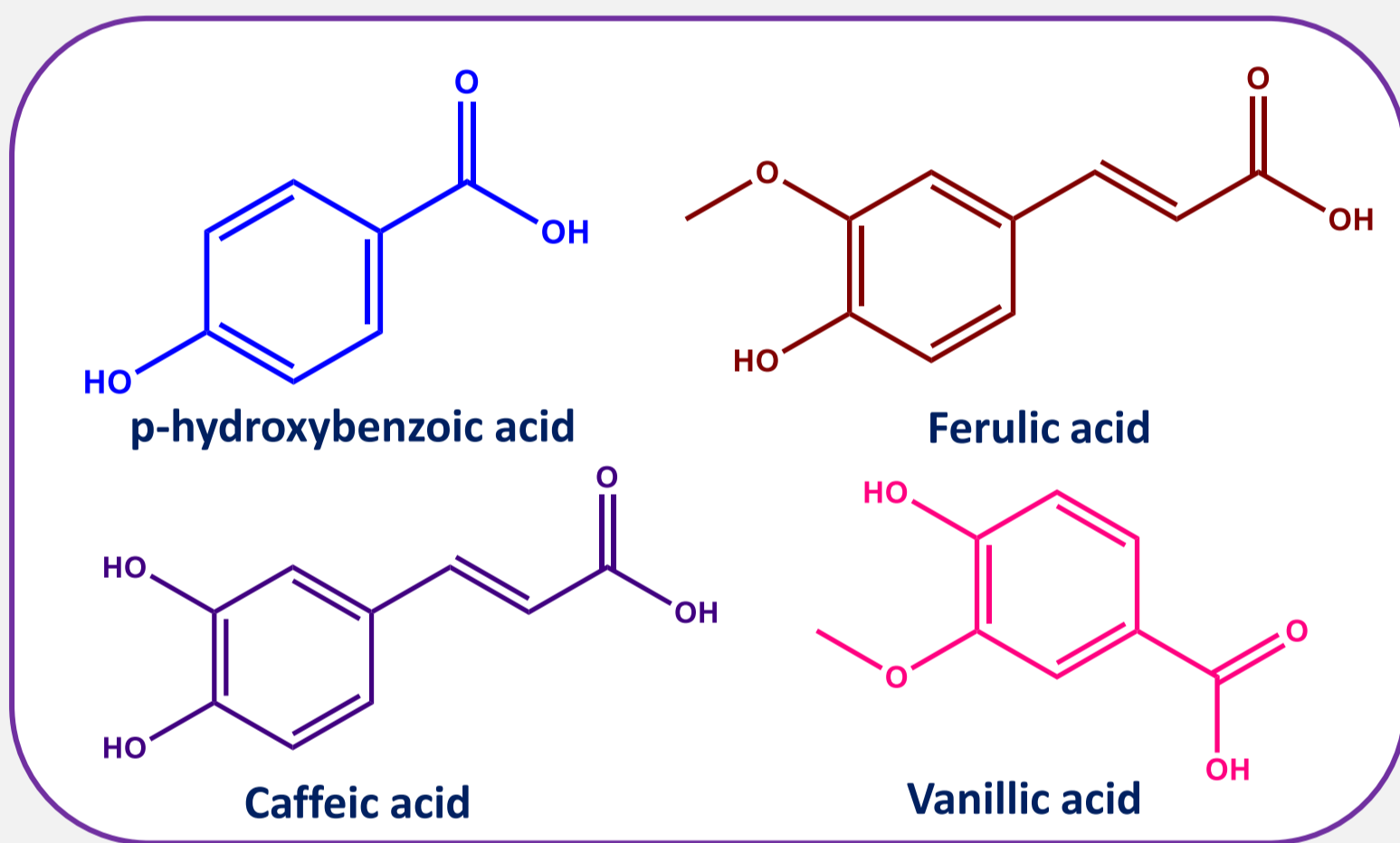
Cucurbita pepo is one of the earliest identified kinds of pumpkin. Native to the United States, it is found in the eastern and southwestern regions as well as northern Mexico. This plant offers nutritional and therapeutic properties. *Cucurbita pepo* has long been used as a traditional medicine in many nations to treat a variety of illnesses, inflammation, infections, diabetes, and antioxidants.

α -Tocopherol

Eight naturally occurring isoforms of vitamin E comprise four tocopherols and four tocotrienols. Because they perform antioxidant roles in biological membranes, tocopherols and tocotrienols are vital constituents. Vitamin E, which includes α -tocopherol and γ -tocopherol, is abundant in pumpkin seeds.

Phenolic Acids in *Cucurbita pepo* L.

Phenol, with one or more aromatic rings and hydroxyl groups, are widely found in plant tissues and have the functions of antioxidation, plant color formation. Although plant polyphenols have been extensively studied as natural antioxidants, there are few literatures on phenolic compounds in pumpkin seeds.



METHODS

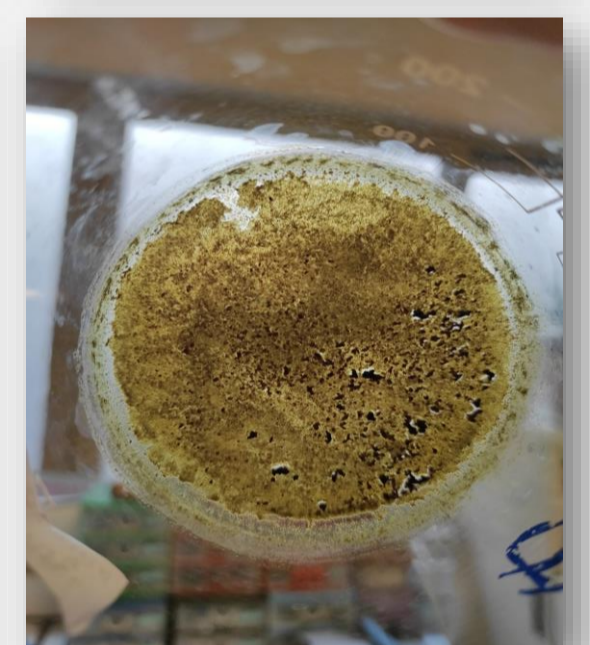
Supercritical CO₂ Extraction

50 grams of oven-dried pumpkin seed shells were extracted using 30 mL of ethanol as co-solvent. Extraction conditions were chosen as 50 °C and 25-30 MPa (250-300 bar). Extraction was done for 1 hour. As a result, 0,2706 grams of product were obtained.



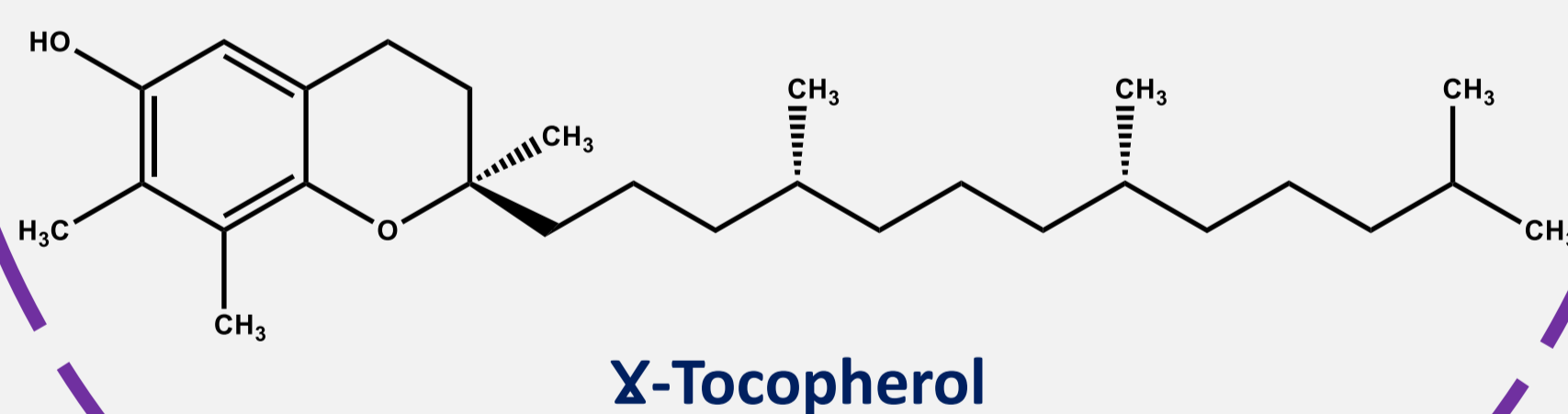
Soxhlet Extraction

31,05 g of dried pumpkin seed shells and 500 mL of ethanol were used for Soxhlet extraction system. Extraction process lasted for 4 hours and after the last siphon, the process ended. 0,978 grams of sample was obtained.



Cucurbita pepo

Pumpkin Seed Shells



α -Tocopherol

Cuprac Method

For the blank solution, 1 mL CuCl₂ solution, 1 mL Nc solution, 1 mL NH₄Ac solution and 1,1 mL water were added to the tube. To both extraction samples, 1 mL CuCl₂ solution, 1 mL Nc solution, 1 mL NH₄Ac solution, 0,850 mL water and 0,250 mL sample were added to three tubes. Yellow color was observed in the tubes. After sample addition, absorbance against the reference was recorded at 450 nm.

DPPH Method

Methanol was used for the blank solution. 2 mL DPPH solution and 2 mL methanol were used for the reference solution. For Soxhlet extract, 2 mL DPPH solution, 1,9 mL methanol and 0,1 mL sample solution were added. For sCO₂ extract, 2 mL DPPH solution, 1,5 mL methanol and 0,5 mL sample solution were added. A 30-minute period after the addition of DPPH was used to measure absorbance against methanol at 515 nm.



Folin-Ciocalteu Reagent

For the blank solution, 2,5 mL of Lowry C solution and 0,25 mL of Folin reagent and 2 mL of water were used. For Soxhlet extract, 2,5 mL Lowry C solution, 0,25 mL Folin solution, 1,9 mL water and 0,1 mL sample were added to the tube. For sCO₂ extract, 2,5 mL Lowry C solution, 0,25 mL Folin solution, 1,5 mL water and 0,5 mL sample were added to the tube. The tubes are left closed at room temperature for 30 minutes and their absorbance is measured at 750 nm against the sample-free reference.



RESULTS

In this thesis, Soxhlet extraction and sCO₂ were used to obtain *Cucurbita pepo* L. seed shells extracts. Antioxidant capacities of both extracts were measured. In order to obtain a commercial product from *Cucurbita pepo* L. seed shells, which are important for our country, it is aimed to purify these chemicals from the extracts obtained in subsequent research using HPLC device. The resulting product can be used in food supplements, pharmaceutical and cosmetic industries.

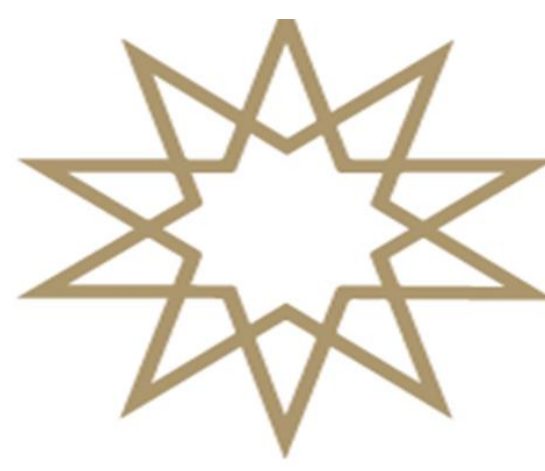
Antioxidant activities of both extracts were measured with CUPRAC method, DPPH method and Folin-Ciocalteu reagents. The reason why the total phenolic capacity is much higher than the total antioxidant capacity is that some phenolic compounds have antioxidant properties.

	TAC (mmol TR/g-Sample)	FRSC (mmol TR/g-Sample)	TPC (mmol TR/g-Sample)
Soxhlet Extraction	0,192±0,004	0,070±0,001	2,127±0,053
sCO ₂	0,008±0,001	0,004±0,001	0,228±0,004

REFERENCES

- [1] Apak, R., Güçlü, K., Özyürek, M., & Karademir, S. E. (2004). Novel total antioxidant capacity index for dietary polyphenols and vitamins C and E, using their cupric ion reducing capability in the presence of neocuproine: CUPRAC method. *Journal of Agricultural and Food Chemistry*, 52(26), 7970–7981.
- [2] Dotto, J. M., & Chacha, J. S. (2020). The potential of pumpkin seeds as a functional food ingredient: A review: Biofunctional ingredients of pumpkin seeds. In *Scientific African* (10).
- [3] Zygler, A., Stomińska, M., & Namieśnik, J. (2012). *Soxhlet Extraction and New Developments Such as Soxtec*.

We would like to express our gratitude to Bener Research Group, particularly Assoc. Prof. Mustafa BENER, for their valuable support in conducting this study.



ÖZET

Termoelektrik sistemler, ısı enerjisini doğrudan elektrik enerjisine çevirmenin en kolay ve en etkili yollarından biridir. termoelektrik malzemeler genellikle inorganik bileşiklerden oluşmaktadır. İnorganik bileşiklerin, yüksek maliyetli işlenmeleri ve zor üretim yöntemleri gibi dezavantajları bulunmaktadır. Bu dezavantajların üstesinden gelebilmek adına, organik yapıya sahip polimerler ortaya çıkmıştır. İletken polimerler, düşük maliyetli olmaları, kolay ve istenilen özellikte üretilmeleri, uzun ömürlü kullanılabilirliği gibi birçok avantaj sağlamaları birlikte, termoelektrik sistemlerde kullanılabilirliği için yeterli performans sağlayabilmeleri adına doping işlemi ile veya çeşitli maddelerle kompozit haline getirilerek daha üstün performanslar gösterebilmektedirler. Bu tez çalışmasında inorganik yapıya sahip çinko oksit sentezlenerek, iletken polimerlerden polipirol ile kütlece farklı oranlarda kompozitleri sentezlenmiştir. Üretilen kompozitlerden elde edilen pelletlerin termoelektrik performansları incelenmiştir.

İLETKEN POLİMERLER

İletken polimerler metaller ve yalıtkanlar arası bir iletkenliğe sahip polimerlerdir. Metaller ve yarı iletkenlerde doğal olarak var olmayan bazı malzeme özellikleri iletken polimerlerle kazanıldığı için iletken polimerler genellikle sentetik metal veya organik metal olarak da isimlendirilmektedir. Polimerler, ilk kullanımlarından bu yana elektriksel yalıtkanlığı iyi maddeler olarak bilinirler ve bu özelliklerinden dolayı elektriksel yalıtkanlığın arandığı kabloların kılıflanması gibi alanlarda önemli kullanım yerleri bulmuşlardır. Kolay işlenmeleri, esneklikleri, estetik görüntüleri, hafiflikleri ve kimyasal açıdan inert olmaları diğer üstün özellikleridir. İletken polimerleri, diğer polimerlerden ayıran temel özellik, sırayla değişen tek ve çift bağlardan oluşan konjuge zincir yapısına sahip olmaları ve yapılarındaki uzun konjuge çift bağlı zincirler nedeniyle iletkenlik özelliğine sahiptirler. Dolayısıyla sadece konjuge olmuş polimerler elektriği iletirler. Bu polimerler çok önceleri değişik metotlarla sentezlenmişler fakat iletkenliklerinin farkına varılmadığı için önemsenmemişlerdir. İlk kez, poliasetilen üzerine yapılan çalışmalarla, bir polimerin kendisinin doğrudan elektriği elektronlar üzerinden iletilebileceği anlaşılmıştır. Shirakawa sentezlediği poliasetilenin iletkenliğini katkılamaya (doplama) yoluyla büyük ölçüde artırarak iletken polimerlerin dikkat çekmesinde önemli bir araştırma olmuştur.

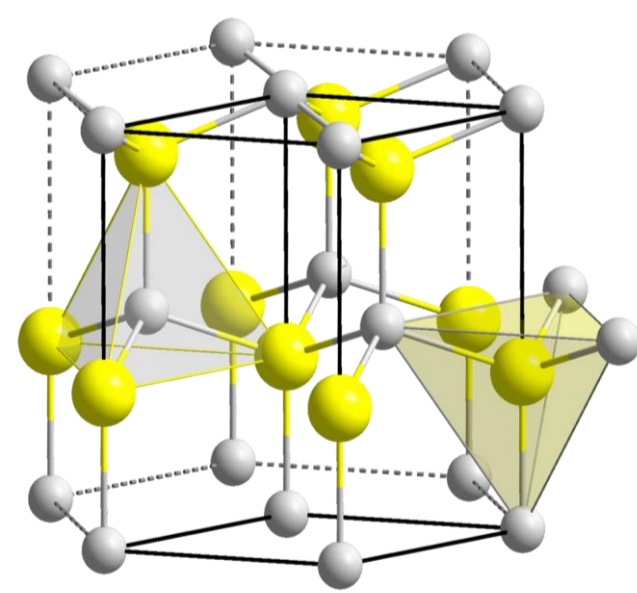
POLİPİROL

PPy, biyosensörlerde, gaz sensörlerinde, tellerde, antistatik kaplamalarda, katı elektrolit kondensatörlerde elektrokromik pencere ve vitrinlerde, ambalajlamada, polimer bataryalarda, elektronik cihazlarda ve fonksiyonel membranlarda potansiyel kullanıma sahiptir. 1937 yılında Pratsi, pirolü kimyasal olarak yükseltgeyerek siyah renkli bir bileşik elde etmiştir. Yapısını aydınlatamadığı bu bileşiğe pirol siyahı adını vermiştir. 1968 yılında Dall'olio sülfürik asit ortamında ilk defa elektrokimyasal yolla, pirolü yükseltgeyerek 8 S/cm iletkenliğe sahip polipirol (PPy) elde etmiştir. 1979 yılında Diaz ve arkadaşları tetraetilamoniyumtetrafloroborat destek elektrolit içerisinde %1'lik sulu asetonitril çözeltisinde pirolü yükseltgeyerek iletkenliği 10-100 S/cm arasında değişen iletken PPy filmi elde etmişlerdir. Bu çalışmadan sonra pirolün polimerleşme koşullarının optimizasyonu için birçok çalışma yapılmıştır. Elektrolit anyonları, elektrolit çözücülerini, çözeltinin pH'sı, polimerizasyon sıcaklığı, potansiyel-akım miktarları gibi birçok parametrenin optimizasyonu için hala çalışmalar devam etmektedir. PPy, iyi çevresel kararlılık, kolay sentezlenmesi ve diğer iletken polimerlerden daha yüksek iletkenliğe sahip olması, kolay sentezlenmesi ve zehirleyici etkilerinin az olmasından dolayı ticari uygulamalarda umut vaat eden bir polimerdir [1].

Polimer	Yapısı
Poliasetilen	
Polipirol	
Politiyolen	
Poli-parafenilen	
Polanilin	

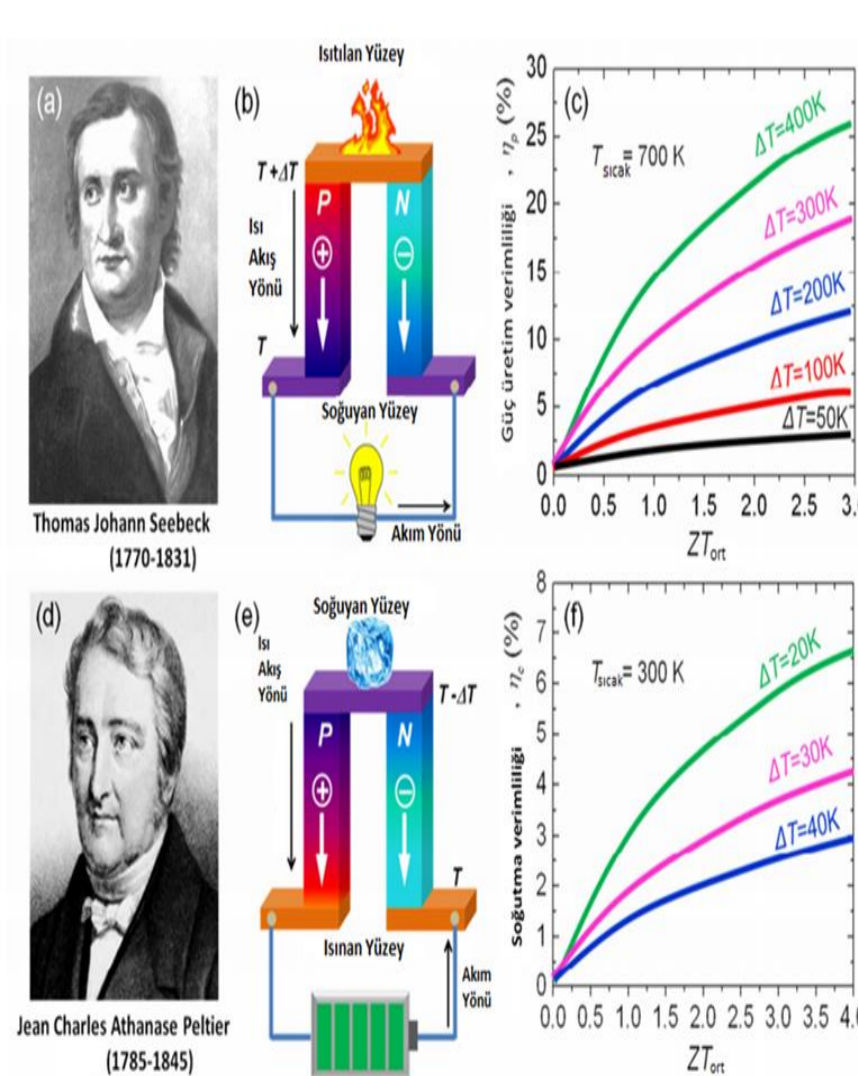
ÇİNKO OKSİT

ZnO formülü ile gösterilen bir inorganik bileşik suda çözünmeyen beyaz bir tozdur ve yaygın olarak kauçuk, plastik, seramik, cam, çimento, yağlayıcı, boya, merhem, yapıştırıcı, sızdırmazlık maddesi, pigment, yiyecekler, bataryalar, ferritler, yangın geciktiriciler ve ilk yardım bantları gibi kullanım alanlarına sahiptir. Mineral çinko, doğal olarak meydana gelmesine rağmen, çoğu çinko oksit sentetik olarak üretilir. ZnO, II-VI grubunda bulunan geniş bantlı bir yarı iletkenidir. Oksijen boşluğuna veya çinko geçiş maddelerine bağlı olarak yarı iletkenlerin doğal yüklenmeleri n tipidir. Bu yarı iletken, iyi şeffaflık, yüksek elektron hareketliliği, geniş bant aralığı ve oda sıcaklığında güçlü ışıltama dahil olmak üzere çeşitli avantajlara sahiptir. Çinko oksit, iki ana formda, altıgen wurtzite ve kübik çinkoblend halinde kristalleşir. Wurtzite yapısı, ortam koşullarında en kararlı ve bu nedenle en yaygın olanıdır.



TERMOELEKTRİK MALZEMELER

Termoelektrik (TE) kavramı, 19. yüzyılın başlarına kadar uzanan çeşitli TE etkilerinin keşfedilmesiyle, yarı iletkenlerde gözlemlenen en eski özelliklerden biridir. TE sistemler, atık ısıdan veya çevre sıcaklığına göre düşük sıcaklık gradyanlı ısı kaynaklarından ısı enerjisini, doğrudan elektrik enerjisine çevirmenin en etkili yoludur. Halen yaygın olan enerji dönüşüm teknolojileri, küresel ısınmaya neden olan ısı emisyonu ve kirlilik konularını beraberinde getirmektedir. Bu nedenle, termal gradyanı faydalı elektrik enerjisine dönüştüren TE enerji üretimi, bu alanda temiz ve yeşil bir seçenek sağlama amacına daha iyi hizmet edebilir. TE malzemelerin özellikleri, birimsiz bir ölçüt olan ZT performans katsayısına göre belirlenmektedir. ZT katsayısı, $ZT = \sigma S^2 T / \kappa$ eşitliği ile belirlenmekte olup, elektriksel iletkenliği (σ , n-tipi için yük taşıyıcı elektronlar ve p-tipi malzemeler için boşluklar ile birlikte), Seebeck katsayısına (S, p-tipi için pozitif ve n-tipi için negatif), mutlak sıcaklığa (T, (K)) ve ısı iletkenliğe (κ) bağlı olarak değişir. Termogüç olarak da adlandırılan Seebeck katsayısı ($\Delta V / \Delta T$), potansiyel farkın (ΔV) sıcaklık farkına (ΔT) oranıyla belirlenmektedir. Çoğu koşulda, σ , S ve κ birbirine bağlıdır. Artmış elektrik iletkenliği, azalmış bir Seebeck katsayısı ve artmış termal iletkenlik değeri verir [2,3].



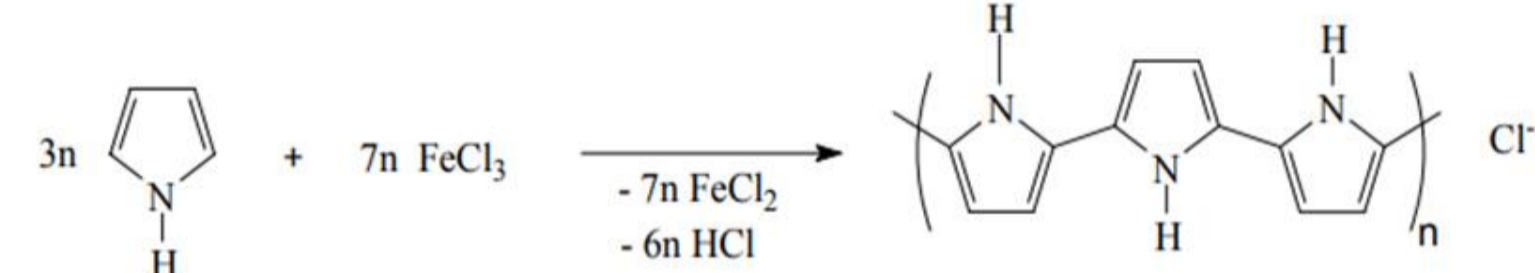
DENEYSSEL KISIM

ZnO Nanopartikül Sentezi

Çinko oksit nanopartikülleri, öncül olarak $ZnSO_4 \cdot 7H_2O$ ve NaOH kullanılarak doğrudan çöktürme yöntemiyle hazırlandı. Kısaca 200 mL distile su içerisinde 5,76 gr $ZnSO_4 \cdot 7H_2O$ ilave edilerek hazırlandı ve bu çözeltiye sürekli karıştırılarak eşit hacimde 8 gr NaOH damla damla ilave edildi. manyetik karıştırıcı üzerinde sürekli karıştırıldı. Sentezlenen ürün, etonolle ile yıkanarak safsızlıklar uzaklaştırıldı. Çökelti bir gün oda sıcaklığında bekletildikten sonra 350 °C'de 3 saat bekletildi. Daha sonra ZnO nanopartiküllerinin beyaz bir çökeltisi elde edildi.

PPy Sentezi

İletken polimerler, kimyasal polimerizasyon yöntemi ile sentezlenebilirler. Monomerin $FeCl_3$, $RuCl_3$, $MoCl_5$ gibi geçiş metal klorürleri varlığındaki yükseltgenme reaksiyonu ile. başlatıcı radikaller $FeCl_3$ gibi yükseltgeyici bir reaktif tarafından oluşturulur. Daha sonra bu başlatıcılar, monomer ile reaksiyona girerek serbest radikalleri veya iyonları oluşturur ve devam eden zincir büyümesi reaksiyonları ile polimer elde edilir. Başlatıcı olarak $FeCl_3$ kullandığımız polipirol sentezinde, ilk olarak 40,55 gr $FeCl_3$ 100 mL metonolde çözüldü. 2,5 M 25 mL $FeCl_3$ çözeltisine 1,75 mL pirolün damla damla ilave edildi ve 20 dakika sonunda reaksiyon sonlandırıldı. Elde edilen koyu yeşil polipirol, süzülür ve metonolle yıkanarak vakum etüvünde 60°C de kurutuldu.



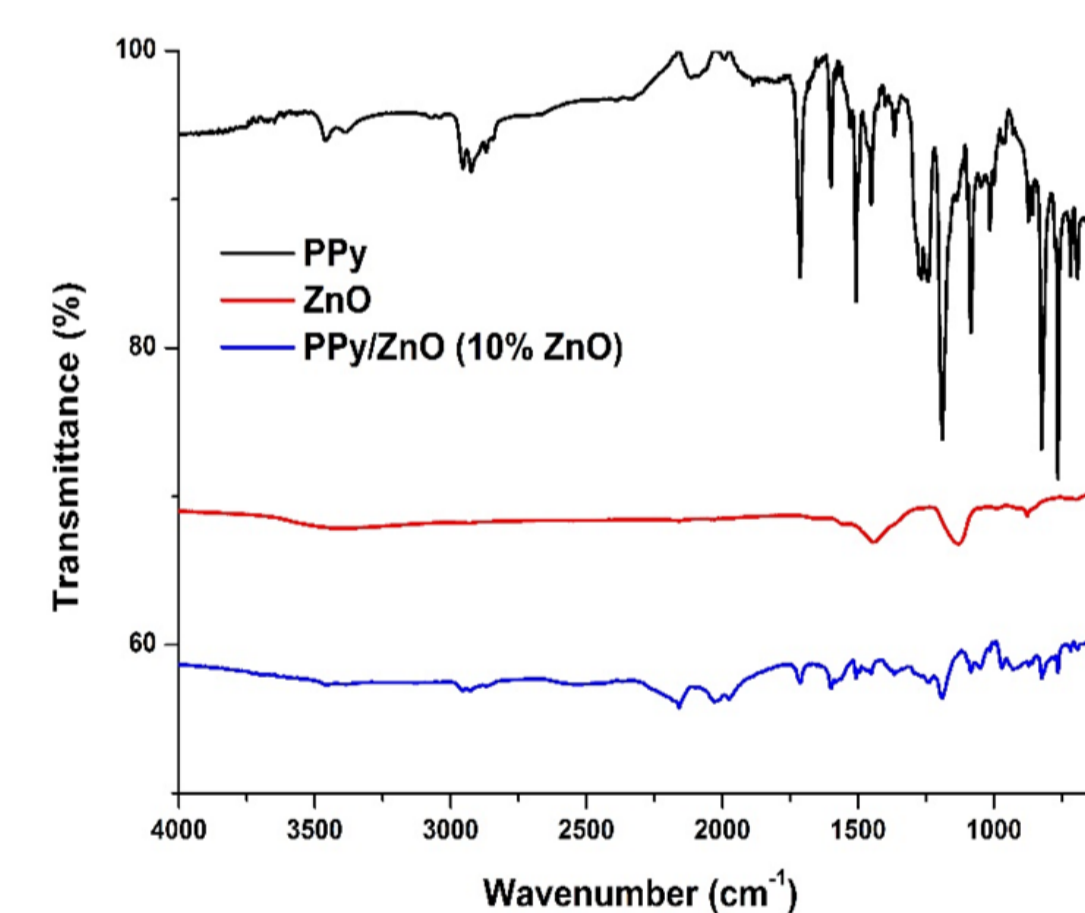
Şekil 1. Pirolün $FeCl_3$ varlığındaki kimyasal polimerizasyon reaksiyonu

PPy/ZnO Kompozitlerin Sentezi

Kompozitler *in-situ* teknikle sentezlendi. Polimerizasyon reaksiyonları PPy'ye benzer şekilde gerçekleştirildi. Ayrıca prosenin ikinci adımında monomer ilavesinden sonra ortama çeşitli ağırlık oranlarında (polimer ağırlığına göre %10 ve %15) ZnO ilave edildi. Kurutulan numuneler pellet haline getirilerek elektriksel iletkenlik ve Seebeck katsayısı ölçümleri gerçekleştirildi.

SONUÇLAR

Saf PPy için 1550 cm^{-1} ve 1470 cm^{-1} 'deki tepe noktaları temel PPy halka titreşimlerine atanırken, 1290 cm^{-1} ve 1050 cm^{-1} 'deki bant $=C-H$ düzlem içi titreşimlere atfedilir. 1190 cm^{-1} 'deki pik C-N titreşimlerine karşılık gelir ve 970 cm^{-1} 'deki pik polimerize pirolün varlığını doğrular. Kompozit için neredeyse saf PPy'ye benzer bir spektrum elde edildi. Bu, ZnO parçacıklarının çoğunlukla PPy ile kaplandığını gösterir.



Şekil 2. Saf PPy, ZnO ve PPy/ZnO kompozitinin FTIR-ATR spektrumları

Örneklerin güç faktörü değerleri ölçülen elektriksel iletkenlikleri ve Seebeck katsayıları ile $P = \sigma S^2$ eşitliği ile hesaplanmıştır.

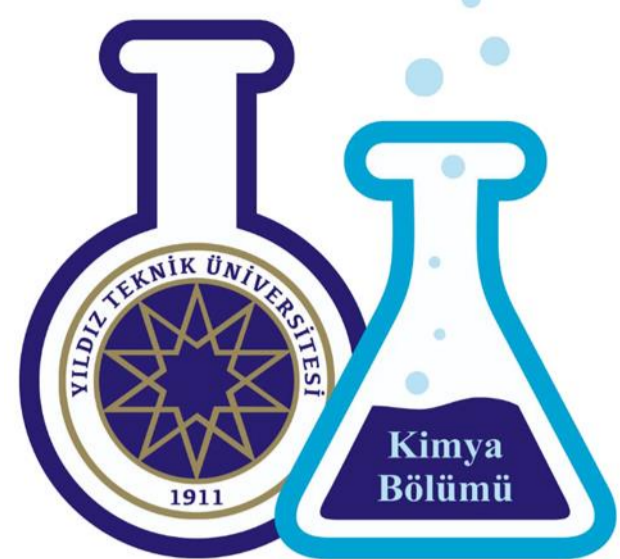
Elde edilen verilerden saf PPy'nin iletkenliğinin yaklaşık 15 kat kadar arttığı gözlemlendi. Bunun yanı sıra, her iki kompozit de saf PPy'ye kıyasla daha yüksek iletkenlik ve güç faktörü değeri göstermiştir.

Numune	İletkenlik ($S \cdot cm^{-1}$)	Seebeck Katsayısı ($\mu V \cdot K^{-1}$)	Güç Faktörü ($\mu W \cdot m^{-1} \cdot K^{-2}$)
PPy	3,90	6	0,014
ZnO	65,51	--	0,20
PPy/ZnO -%10	52,83	7,8	0,32
PPy/ZnO -%15	58,66	6,7	0,26

Sonuç olarak bu çalışmada, kompozitlerin kimyasal yapılarını incelemek amacıyla yapılan FTIR analizleri sonucunda kompozitlerin başarı ile sentezlendiği belirlenmiştir. Termoelektrik analizler sonucunda saf PPy'ye ait iletkenlik değerinin, ZnO eklemesi ile 3,90 S/cm değerinden 52 S/cm değerine arttığı, Seebeck katsayısı değerlerinin ise 6,7 $\mu V/K$ ile 7,8 $\mu V/K$ arasında değiştiği gözlemlenmiştir.

KAYNAKÇA

- Pratsi, G. (1937). XXV. The Manufacture of Polypyrroles and Other Nitrogenous Compounds from Pyrrole and its Homologues. Journal of the Chemical Society
- Morelli, D.T., *Thermoelectric Materials*, in *Springer Handbook of Electronic and Photonic Materials*. 2017, Springer. p
- Du, Y., et al., *Research progress on polymer-inorganic thermoelectric nanocomposite materials*. Progress in Polymer Science, 2012. 37(6): p. 820-841

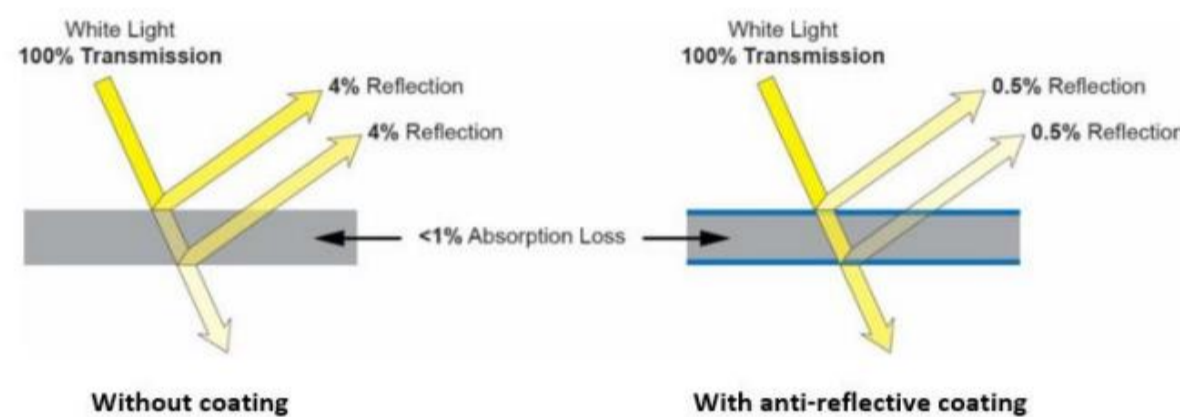


Abstract

In today's world, there is a significant shift towards clean energy sources to reduce environmental damage and preserve nature. Clean energy refers to the form of energy obtained from naturally occurring and self-renewable sources such as wind, solar, and wave. Various systems exist for harnessing clean energy sources, one of which is solar panels used to harness energy from sunlight. The importance of anti-reflective coatings is growing in tandem with initiatives to boost solar panel efficiency. The anti-reflective coating process, which improves the mechanical and light transmission qualities of glass, has an impact on the use and efficacy of solar panels. The sol-gel approach, which incorporates the Stöber method, is one of these coating methods. Creating consistent and manageable silica nanoparticles is a significant challenge. In this thesis, we used the sol-gel process to synthesize silica nanoparticles. The amount of tetraethyl orthosilicate (TEOS) and polyacrylic acid (PAA) used in the sol-gel process and film formation properties were analyzed.

Introduction

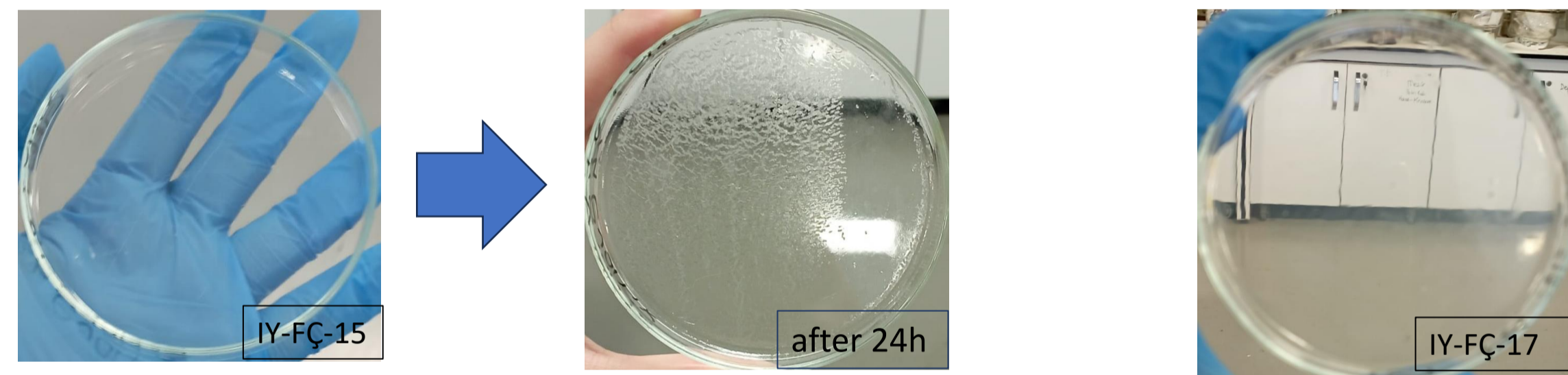
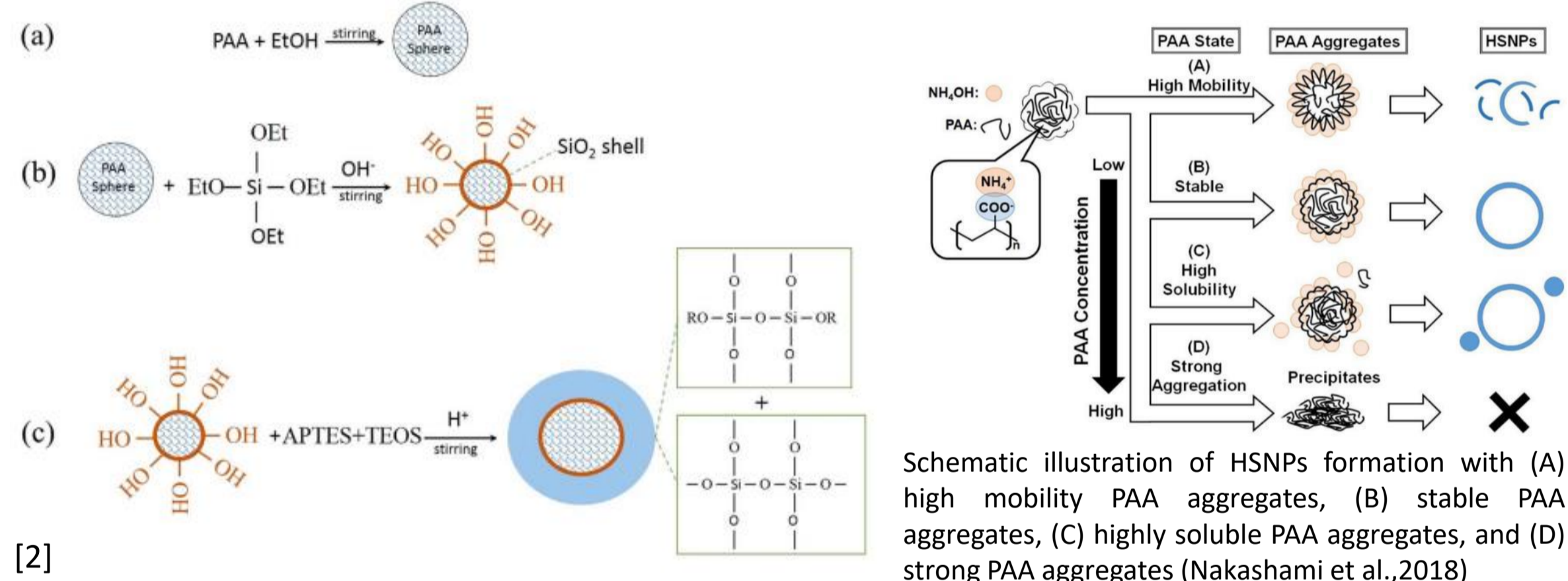
One of the most basic optical phenomena is reflection, which happens when light travels across a boundary between two media with different refractive indices. Because of this natural phenomenon, some living things evolved with a physical feature that has anti-reflective surfaces. [1]



Solid Content and film Properties of Sol-Gel

	IY-FÇ-6	IY-FÇ-7	IY-FÇ-8	IY-FÇ-9	IY-FÇ-10	IY-FÇ-11	IY-FÇ-12	IY-FÇ-13	IY-FÇ-14	IY-FÇ-15	IY-FÇ-17	IY-FÇ-18	IY-FÇ-19	IY-FÇ-20	IY-FÇ-21
GK4	10 mL	10 mL	10 mL	10 mL	10 mL	10 mL	10 mL	10 mL	10 mL	10 mL	10 mL	10 mL	10 mL	10 mL	10 mL
IY-H3															
Evonik Silicone	0.2 mL		0.2 mL				0.2 mL				0.4 mL	0.4 mL	0.4 mL		
Tegostab		0.2 mL													
PGMEA			0.1 mL	0.1 mL		0.1 mL	0.5 mL	0.5 mL			0.1 mL				
BYK					0.2 mL	0.1 mL		0.2 mL							
Acrylic resin 5000				0.1 mL						1 drop					
Silane 750													0.2 mL		
Silane P2-AR									0.2 mL						0.2 mL
Solid content	4.56%	4.62%	4.28%	5.06%	4.27%	3.47%	2.24%	3.0%	3.01%	6.01%	6.81%	5.44%	4.09%	3.76%	3.77%

Morphology of Silica Nanoparticles using PAA



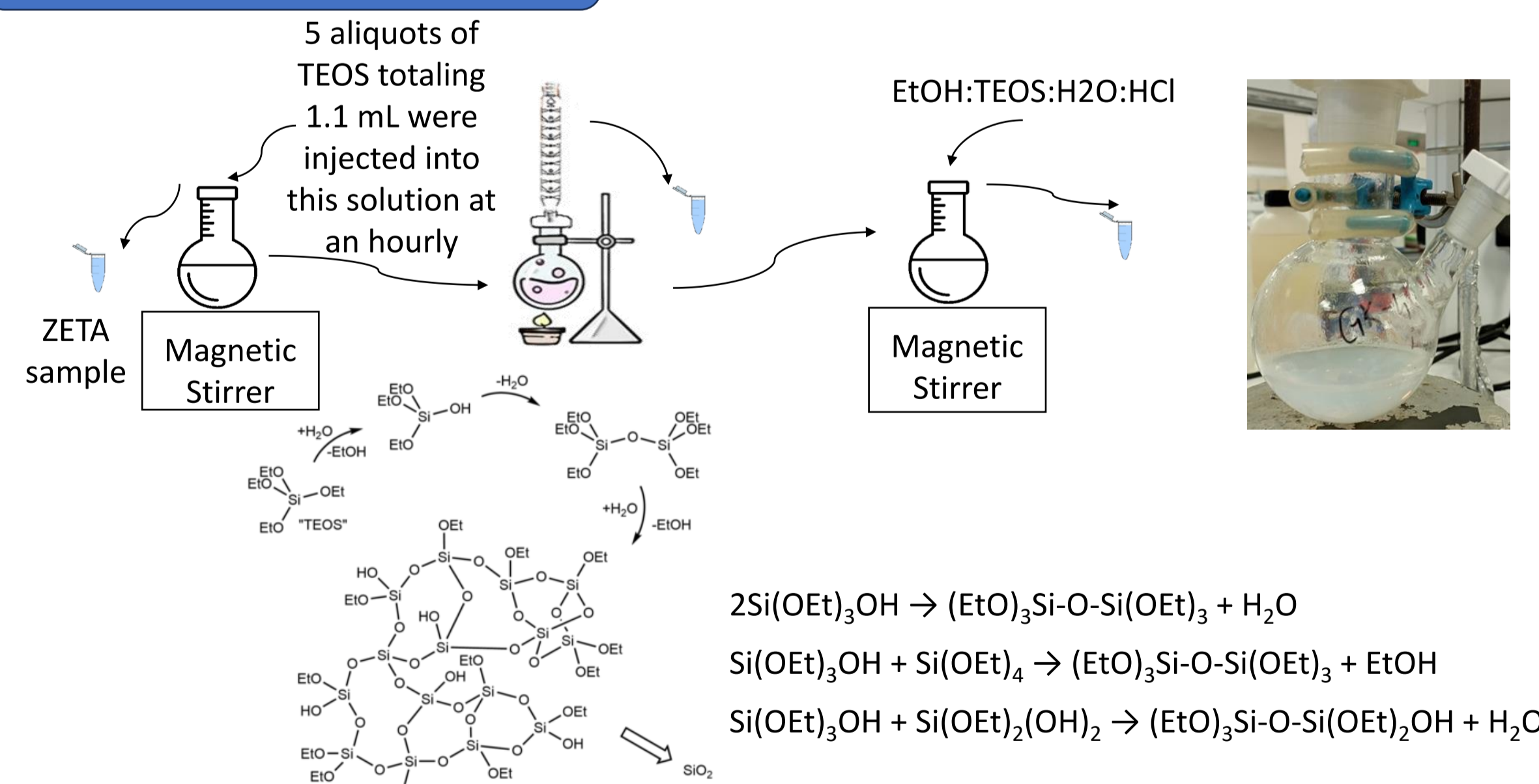
	Step C with HCl	Step C with acetic acid	Step C with phosphoric acid
GK4-IY1	+		
GK4-IY2		+	
GK4-IY3			+



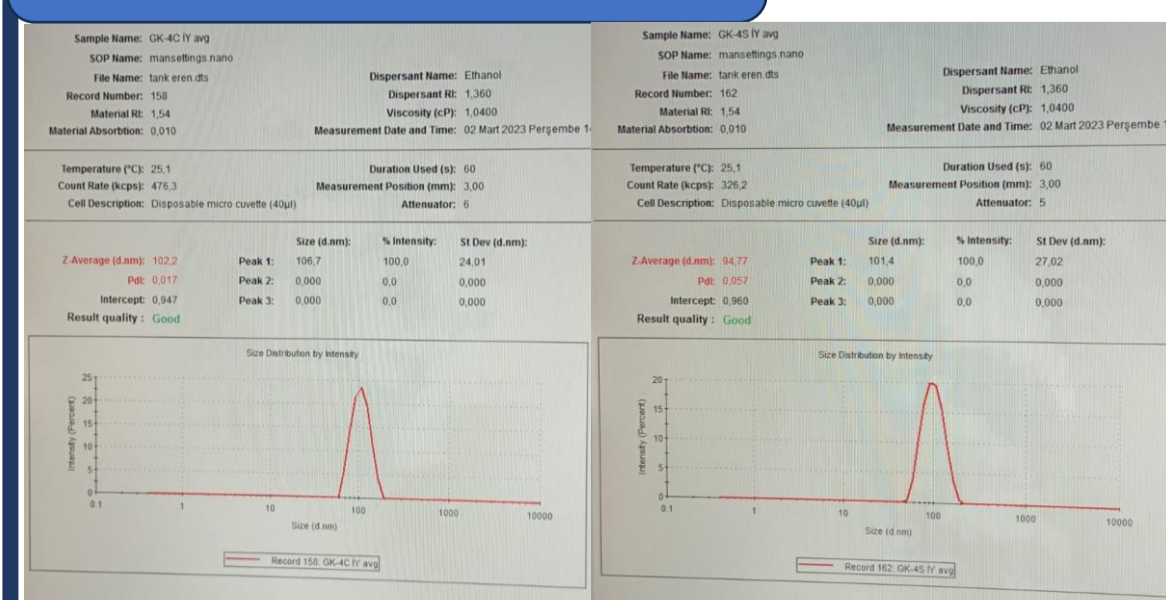
	Solid PAA (g)	NH3 (mL)	EtOH (mL)	TEOS (mL)
IY-H1	0.27	4.5	90	2.25
IY-H2	0.15	4.5	90	2.25
IY-H3	0.10	4.5	90	2.25



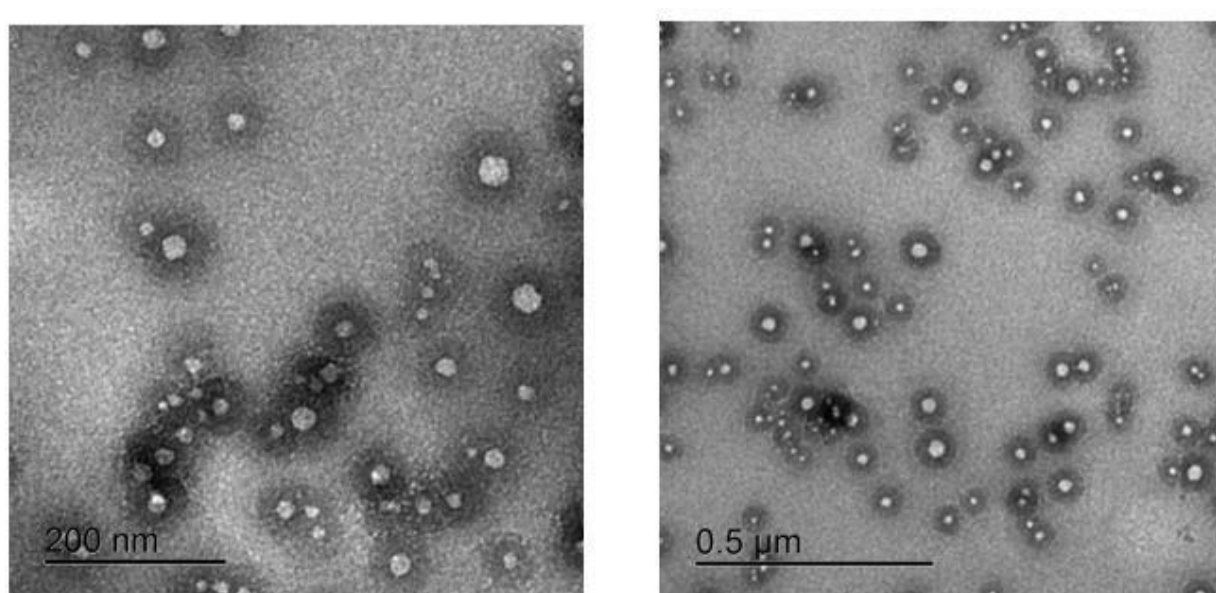
The Experimental SETUP



Particle Size



DLS results of GK4



TEM results of GK4

After the reflux (on the right), the particle size increased to 94.77 nm and the Pdl value was 0.057. After Step C (on the left), the Pdl value decreased to 0.017 and the particle size was 102.2 nm

Conclusion

- Particle size increased with increasing PAA solids content. Particle size can be affected by the polyacrylic acid dropping rate into the solvent, the TEOS dropping rate, and the speed at which the magnet stirrer rotates.
- The film structures which contain Evonik silicone were observed to be more transparent in studies. Additionally, it was observed that films with a higher amount of solid material exhibited less fragility and created a more transparent image.

References

- Xiao Li, Xinhong Yu & Yanchun Han (2013). Polymer thin films for antireflection coatings. J. Mater. Chem. C, 2013, 1, 2266. DOI: 10.1039/c2tc00529h
- Guo, Z. Q., Liu, Y., Tang, M. Y., Wang, J. H., & Su, X. P. (2017). Super-durable closed-surface antireflection thin film by silica nanocomposites. Solar Energy Materials and Solar Cells, 170, 143–148.
- Yi Du, Lunet E. Luna, Wui Siew Tan, Michael F. Rubner, and Robert E. Cohen (2010) Hollow Silica Nanoparticles in UV-Visible Antireflection Coatings for Poly(methyl methacrylate) Substrates ACS Nano Volume 4, 4308–4316



KİMYA BÖLÜMÜ

SYNTHESIS, CHARACTERIZATION AND INVESTIGATION OF MESOMORPHIC PROPERTIES OF 2,4,6-TRIS(E)-3,4-BIS(DODECYLOXY)STYRYL)-1,3,5-TRIAZINE

Duygu CANSEVEN 1802D041
Advisor : Prof. Dr. Huriye AKDAŞ KILIÇ



ABSTRACT

Liquid crystals are substances that are frequently used in many areas today, especially in digital goods. For example, they are given a lot of space in watches, computer screens and thermometers. Liquid crystals make our lives much easier because they show both liquid and solid phase properties, show different mesophase properties with the bonded side chains and chirality they have, and thus enable the existence of much higher quality and useful products. Liquid crystals were discovered by Friedrich Reinitzer and Otto Lehmann.

Triazine is a substance first synthesized by Ulric Nef. Although there are many isomers, 1,3,5 triazine is the most common. Since it is a substance that requires many electrons, it is used as an electron carrier. Triazine molecules enable supramolecular interactions thanks to the sigma and pi electrons they contain. Triazine core systems are used in OLED, semiconductor systems and solar panels.

In liquid crystals with a triazine core, the 1,3,5-triazine structure acts as a rigid core and flexible side chains are attached to the 2,4,6 positions. Since triazine molecules can make hydrogen bonds within themselves, this results in low molecular weight molecules. Liquid crystals with triazine nuclei exhibit columnar mesophase. Thanks to the triazine nucleus, the mobility of electrons in liquid crystals increases and enables the formation of luminescent columnar liquid crystals.

In this study, the liquid crystal properties of molecules with triazine nuclei were examined. For this study, 2,4,6-tris((E)-3,4-bis(dodecyloxy)styryl)-1,3,5-triazine (**2**) was synthesized. The mesomorphic properties of this compound were examined by DSC and polarization microscopy (PM), and its molecular structures were examined by ¹H-NMR, ¹³C-NMR spectroscopic methods. Since the pi bonds in both the triazine and the benzene rings substituted with alkoxy groups, which are the side groups in this compound, add luminescence properties, the compound was also examined by UV-VIS spectroscopy.

1. INTRODUCTION

Friedrich Reinitzer and Otto Lehmann discovered liquid crystals in the late 19th century. Liquid crystals can flow like a fluid but they have the molecular order of the solid crystal. Liquid crystals have both liquid and solid state properties. Liquid crystal state shows the phase called as 'mesophase'. The molecules showing this phase is called as 'mesogene'. Liquid crystals can be divided into two parts as **thermotropic liquid crystals** and **lyotropic liquid crystals** depending on the types of formation of mesophases. Thermotropic liquid crystals form mesophases with the effect of temperature. Lyotropic liquid crystals form mesophases with the effect of temperature and solvent system. Thermotropic liquid crystals show a diversity depending on the geometrical structures of mesogenes. These are **discotic**, **banana-shaped** and **calamitic**. Liquid crystals are used in watches, computer screens and thermometers, mobile phones.

1,3,5 triazine was firstly synthesized by **Ulric Nef** in 1895. Triazines are the six-membered heterocycles that include nitrogen. Its molecular formula is C₃H₃N₃. It has three isomeric forms. These are 1,2,3 triazine, 1,2,4 triazine and 1,3,5 triazine but 1,3,5 triazine isomer is the most common one. When aromatic ring nomenclature is considered, **1,3,5 triazine** is sometimes shown with **-sym** or **-s** as its symmetric abbreviation. In liquid crystals with a triazine core, the 1,3,5-triazine structure acts as a rigid core and flexible side chains are attached to the 2,4,6 positions. Since triazine molecules can make hydrogen bonds within themselves, this results in low molecular weight molecules. Liquid crystals with triazine nuclei exhibit columnar mesophase. Thanks to the triazine nucleus, the mobility of electrons in liquid crystals increases and enables the formation of luminescent columnar liquid crystals.

2. SYNTHESIS SCHEME

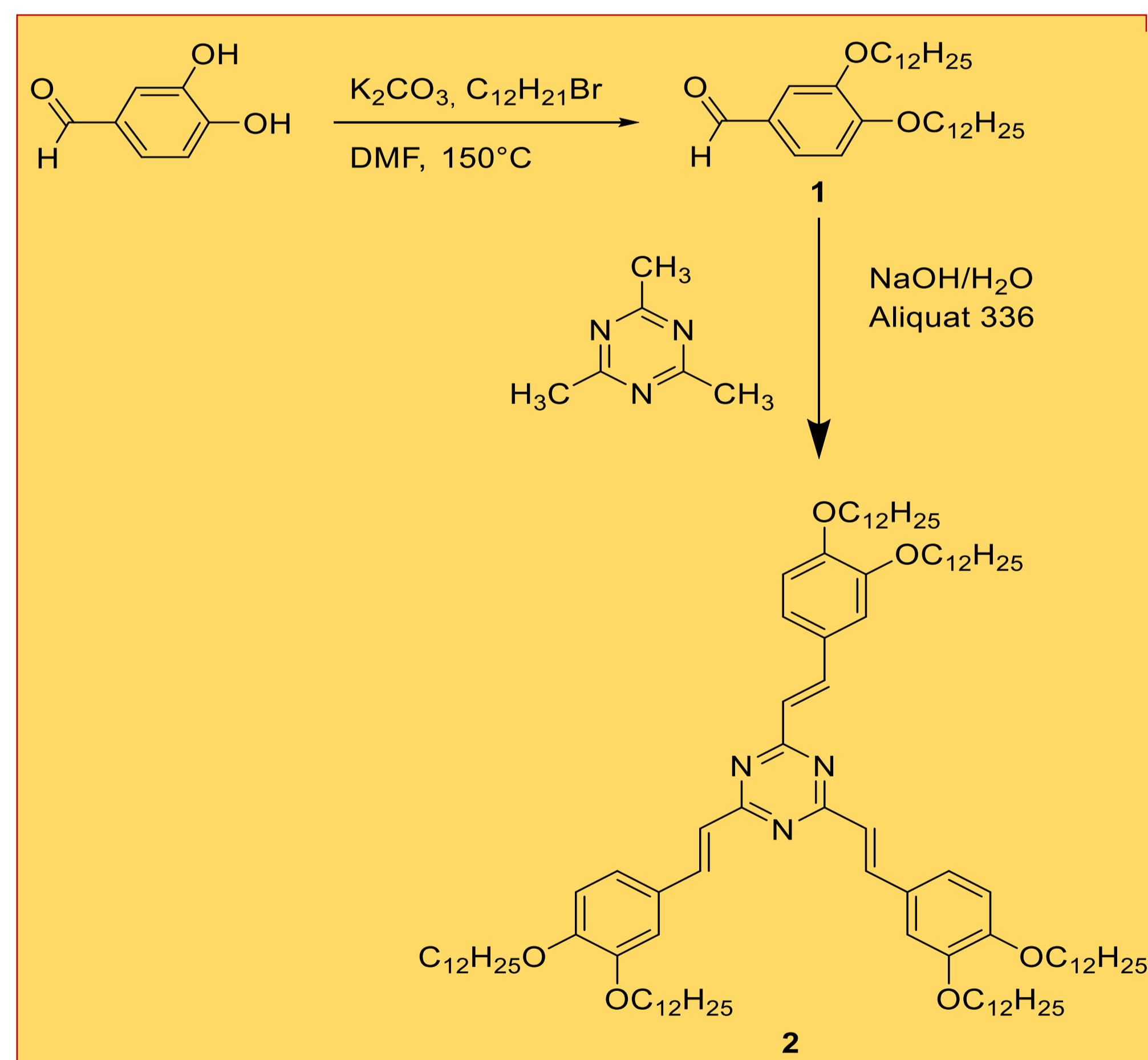


Figure 1. The synthesis scheme of 2,4,6-tris((E)-3,4-bis(dodecyloxy)styryl)-1,3,5-triazine (**2**).

5. CONCLUSION

As a result of the examinations, it was determined that the synthesized new triazole derivative molecule (**2**) did not exhibit liquid crystal properties. However, if desired, liquid crystal properties can be achieved with various contributions to the molecule, such as binding different side chains.

6. REFERENCES

- Bhagavath, P., Shetty, R. and Sunil, D., (2020). "1,3,5-Triazine-Based Liquid Crystals: An Up-to-Date Appraisal of Their Synthetic Design and Mesogenic Properties," *Critical Reviews in Solid State And Materials Sciences*, vol. 45, (no. 5), pp. 378–409.
- Collings, P. J., Hird, M., (1997). "Introduction to Liquid Crystals Chemistry and Physics." Taylor & Francis, Londra
- Kelker, H., (1973). "History of Liquid Crystals," *Molecular Crystals and Liquid Crystals*, vol. 21, (no.1), pp. 1-48

3. STRUCTURAL CHARACTERIZATION

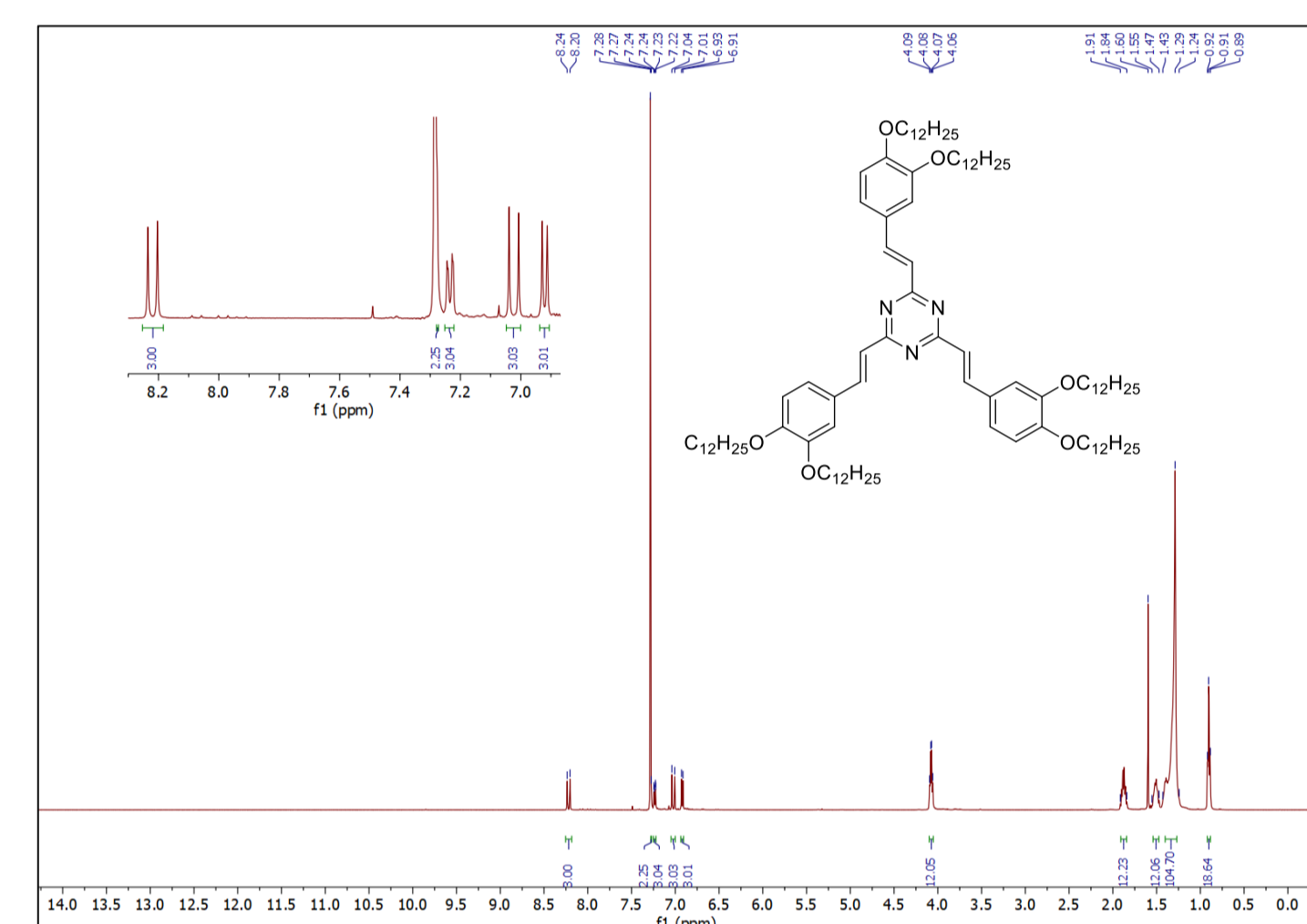


Figure 2. ¹H-NMR (CDCl₃) spectrum of compound **2**.

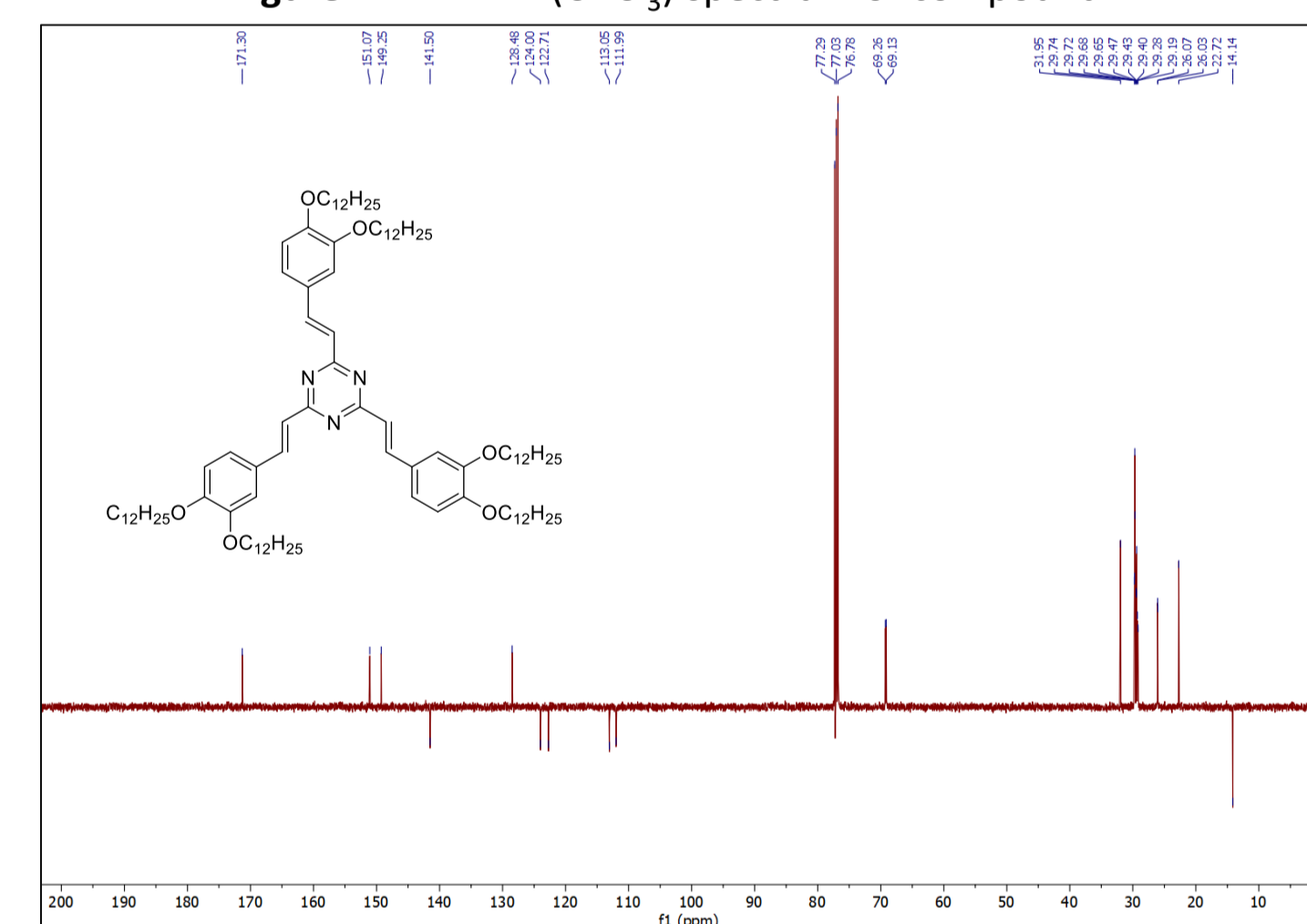


Figure 3. ¹³C-NMR (APT) (CDCl₃) spectrum of compound **2**.

4. OPTICAL & MESOMORPHIC PROPERTIES

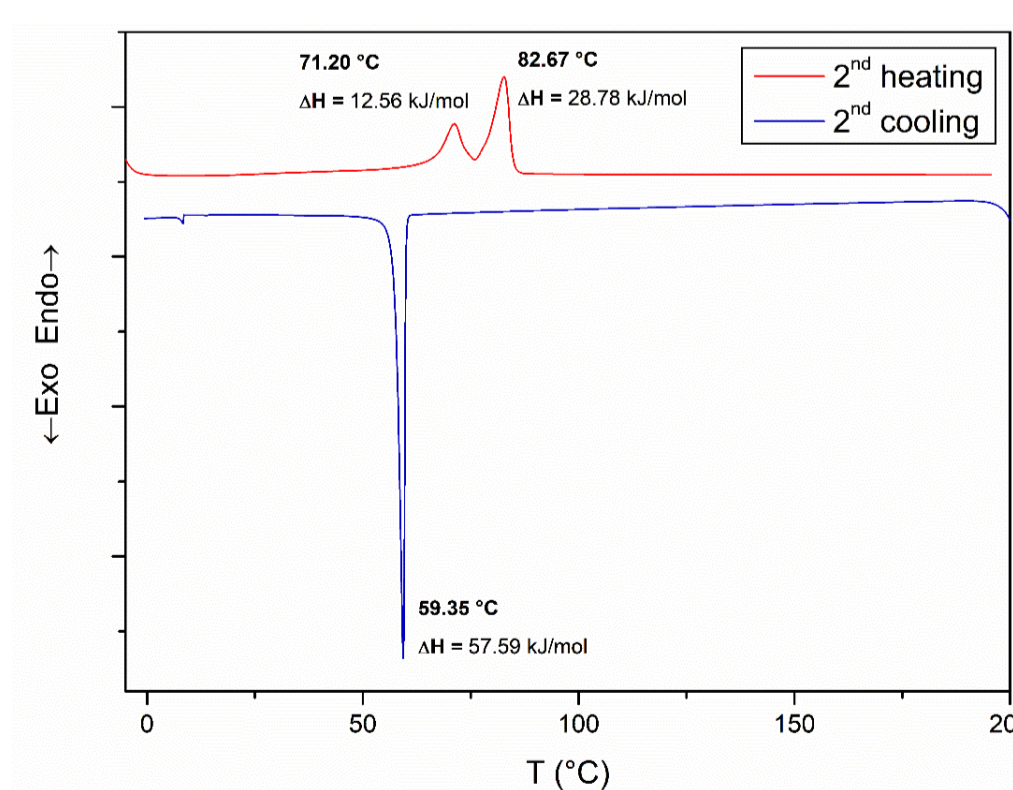


Figure 4. the DSC thermogram of compound **2**.

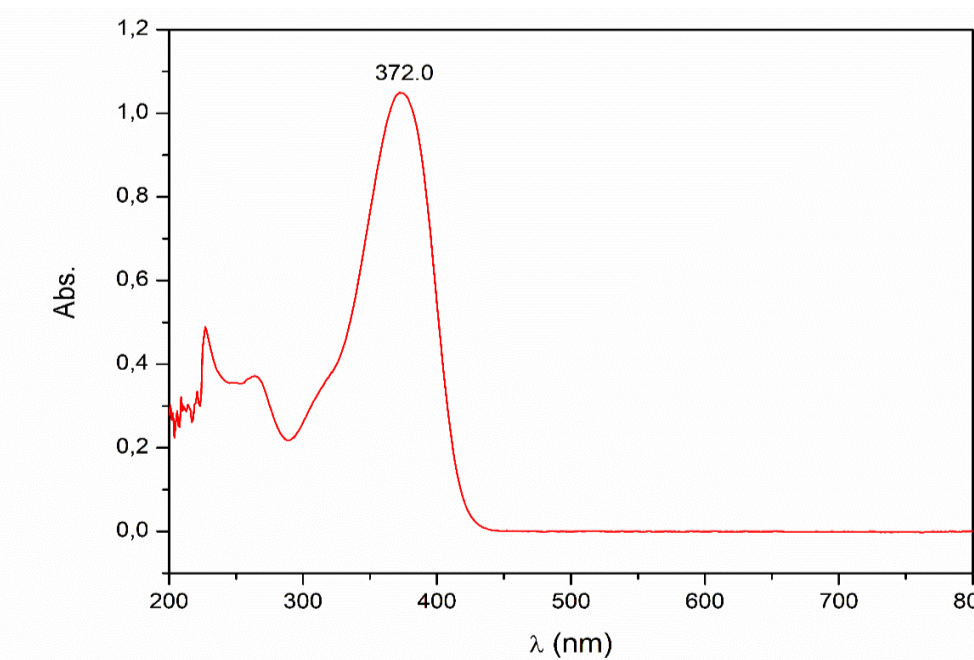


Figure 5. the UV-VIS spectrum of compound **2**.

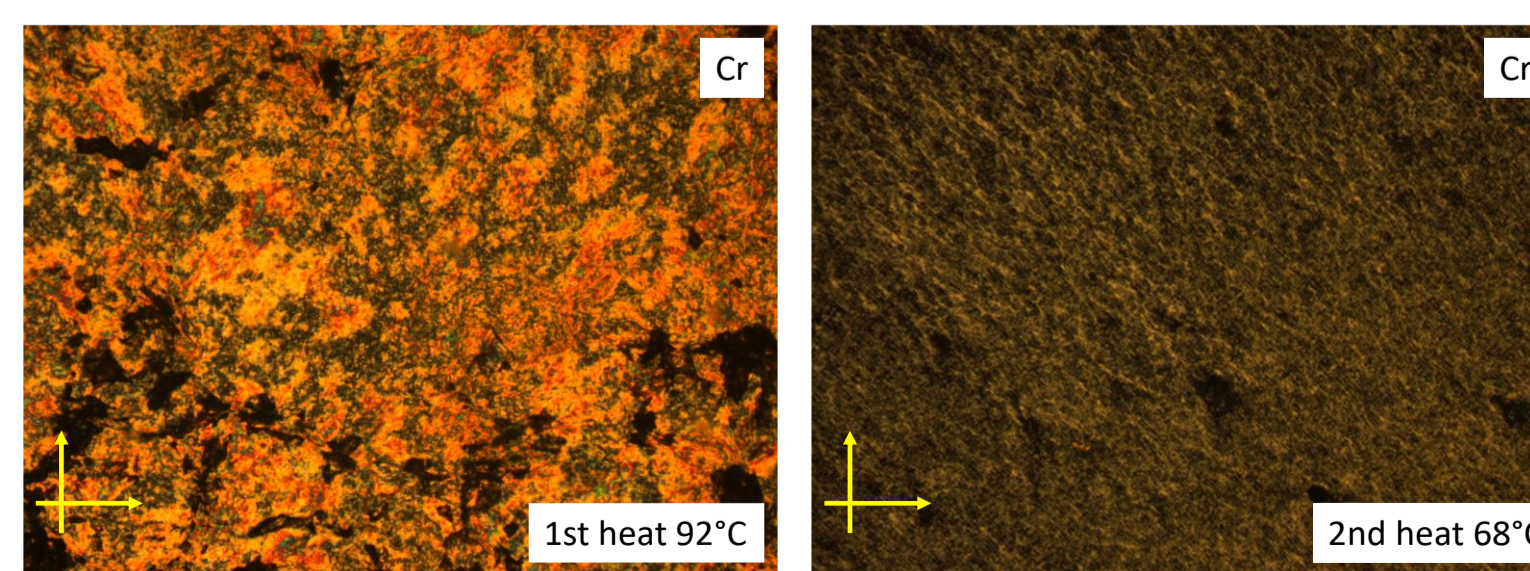


Figure 6. Optical photographs of compound **2** under optical polarization microscope

Phase transition temperatures and enthalpies T / °C [ΔH kJ/mol] ^a				
Compound	Solvent	Conc. (mol/L)	λ _{max} (abs) (nm)	ε _{max} (L mol ⁻¹ cm ⁻¹)
2	CH ₂ Cl ₂	1.3392x10 ⁻⁵	372.0	78361

Heating → Cr₁ 72.20 [12.56] Cr₂ 82.67 [28.78] Iso
Cooling → Iso 59.35 [57.59] Cr

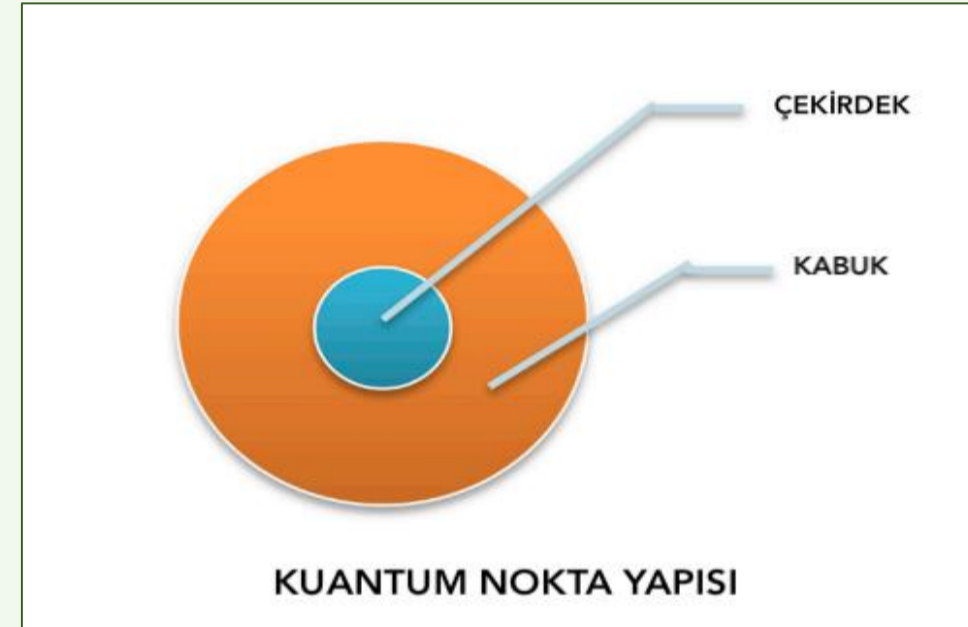
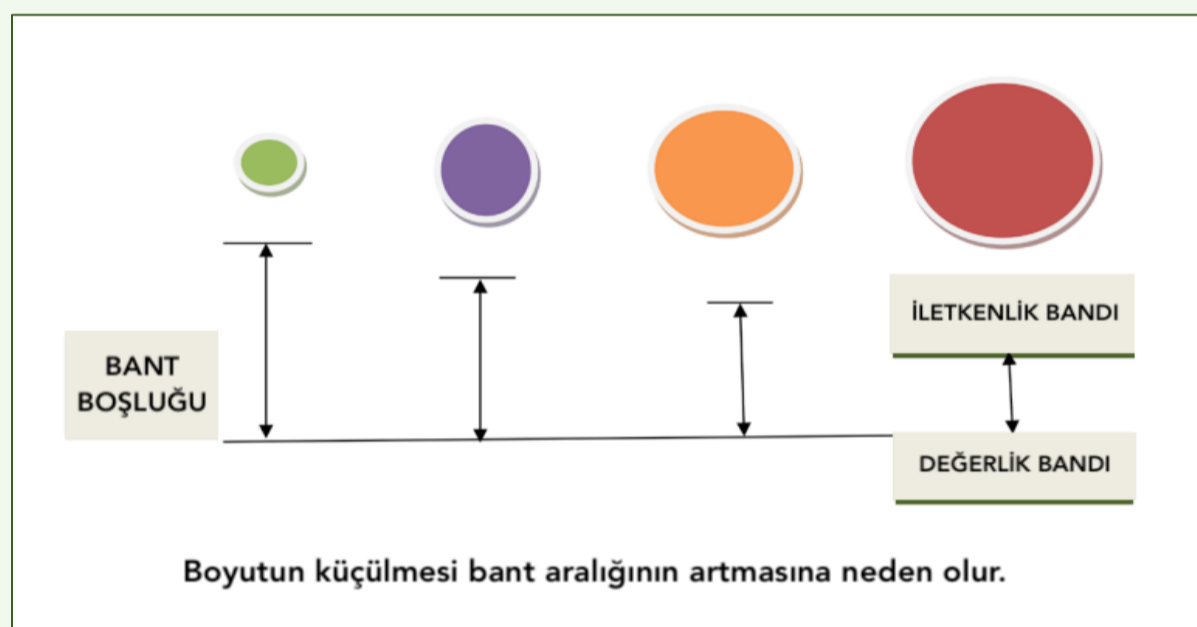
Table 1. & 2. Mesophases, phase transition temperatures and associated enthalpies of the compound **2** on heating and cooling (1), optical properties of compound **2** (2).



1980'li yılların başında keşfedilen kuantum noktalarının, sahip oldukları üstün optik özellikler ile popülerleşmiş ve kısa sürede uygulama alanları genişlemiştir. Kuantum noktaları, boyutları ayarlanabilen, boyutlarıyla birlikte yaydığı renk ve parlaklıkları da değişebilen yarıiletken, 2-10 nm boyutlarında nanoparçacıklardır. Bu özellikleri sayesinde biyogörüntüleme, ekran teknolojileri, güneş panelleri, tedavi süreçleri gibi uygulama alanlarında büyük rol oynamaktadırlar.

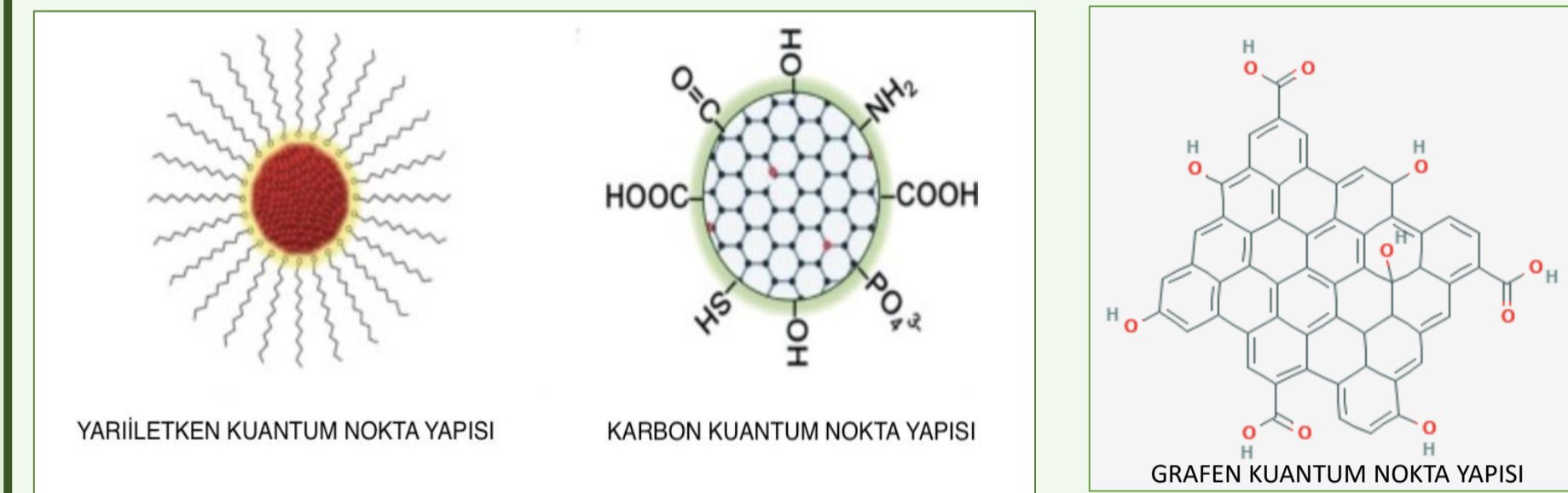
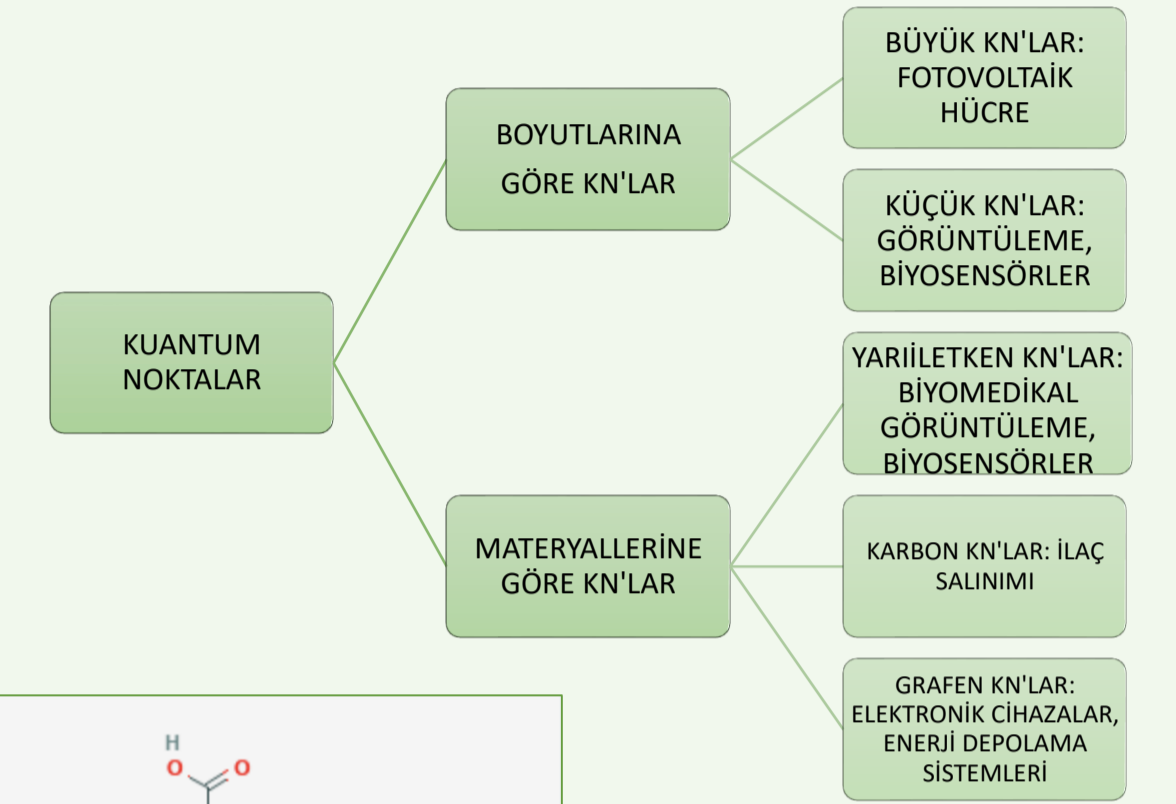
KUANTUM NOKTALARI

Kuantum noktaları (KN) 2-10 nm arasında boyutlara sahiptirler ve bu değer KN'nın sahip olduğu iletkenlik bandı ve değerlik bandı arasındaki bant genişliği mesafesidir. Yarı iletken bir malzeme veya bir metal, nanometrik boyutlara indirildiğinde bant aralığı da değişecektir. KN'nın bant genişliği, uyarılan elektronun iletkenlik bandına geçmesi için gereken enerjiyi ve dalgaboyunu etkilediğinden yansıyacak ışığın rengini de etkileyecektir [1]. Bununla birlikte KN'lar ışığı absorblayabilirler ve temel duruma geldiklerinde ışık fotonlarını serbest bırakabilirler. Bu da yine KN'nın boyutuna bağlıdır. KN ne kadar küçükse emisyon dalga boyu o kadar kısa olur.



KUANTUM NOKTALARININ KARAKTERİZASYONU

Kuantum noktalar, bileşimlerine/yapılarına göre, boyutlarına göre, üretildikleri materyale göre karakterize edilirler ve türlerine göre farklı uygulama alanlarında kullanılırlar. KN'ların bu özelliklerine göre karakterize edilmesi için spektroskopi, mikroskopi, saçılma, elektriksel teknikler kullanılmaktadır [3].



KUANTUM NOKTALARININ FİZİKOKİMYASAL ÖZELLİKLERİ

1. AYARLANABİLİR IŞIK EMİSYONU

KN'nın boyutları, çekirdeklerinin kimyasal bileşiminden etkilenmektedir. Örneğin, Kadmiyum sülfür'ün emisyon dalga boyu aralığı mavi ışık bölgesinde iken, Kadmiyumtellür'ün emisyonu ise kırmızı ışık bölgesinde ışına yapar.

Kuantum noktaları	Boyut yarıçapı (nm)	Emisyon aralığı (nm)
CdS	2.8-5.4	410-460
CdTe	3.1-9.1	520-750
CdSe	2-8	480-680
CdTe/CdSe	4-9.2	650-840
InP	2.5-4.5	610-710
InAs	3.2-6	860-1270
PbSe	3.2-4.1	1100-1310
Dt-Ag2S	5.4-10	1000-1300

2. EŞSİZ ABSORBSİYON SÖNÜMLEME KATSAYISI

Bir maddenin verilen dalgaboyunda ışığı ne kadar absorbladığının ölçüsüdür. Bu özellik, ışık yoğunluğunun az olduğu koşullarda, az sayıda fotonun minimum düzeyde absorblanmasına ve minimum düzeyle parlaklığa ulaşılmasına sebep olur.

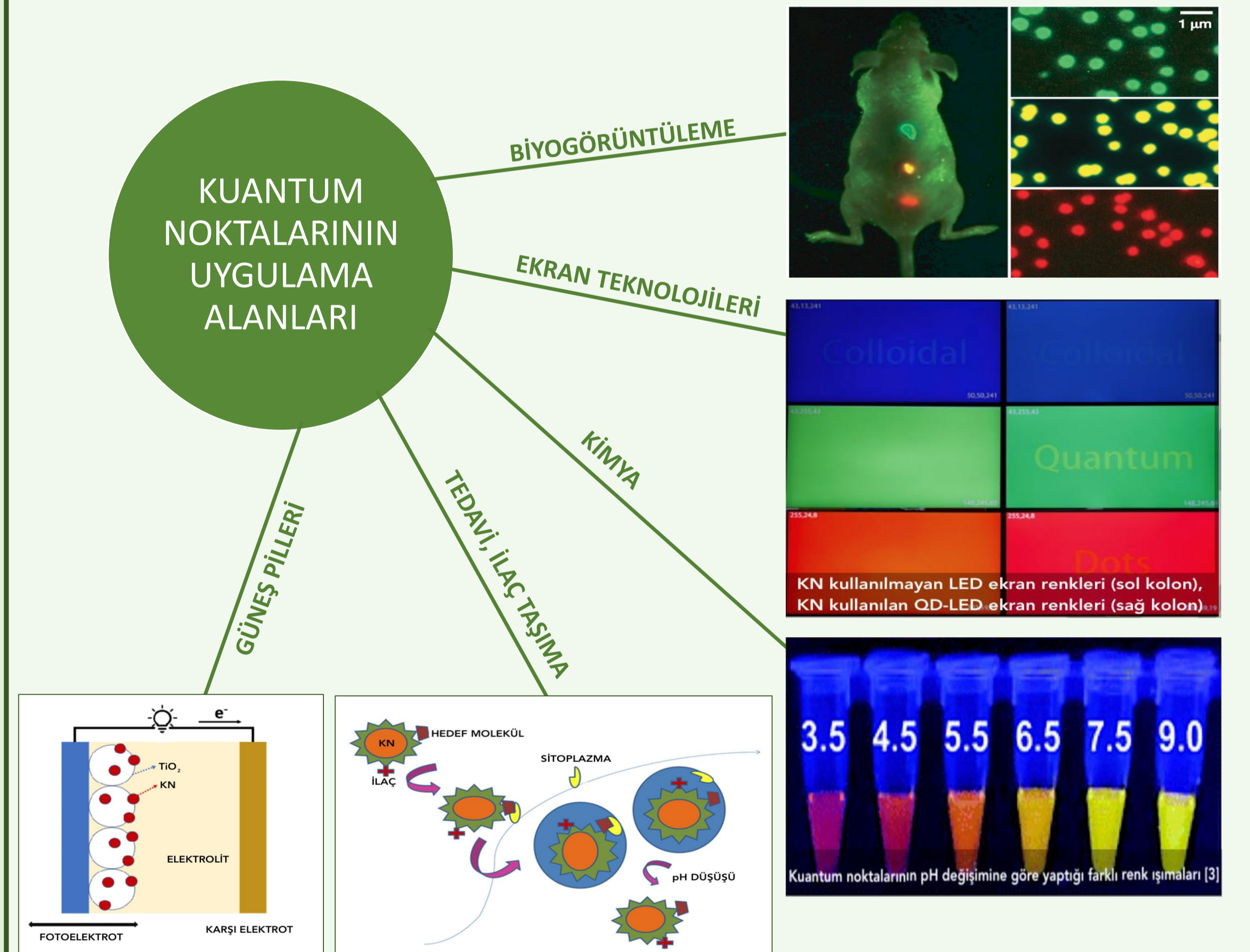
3. YÜKSEK FLORESANS KUANTUM VERİMİ

Floresans kuantum verimi, emilen fotonların yayılan fotonlara oranı olarak tanımlanır. KN'nın floresans özelliği güçlüdür ve bu da ekran teknolojilerinde yüksek parlaklık ve yüksek çözünürlük gibi avantajlara yol açar.

4. FOTOKİMYASAL DAYANIKLILIK

KN, inorganik doğası nedeniyle, foto ve kimyasal bozulmaya karşı son derece dirençlidirler. Bu özellik, onları uzun süre boyunca mükemmel ve etkili görüntüleme problemlerine haline getirir.

KUANTUM NOKTALARININ UYGULAMA ALANLARI



KUANTUM NOKTALARININ SENTEZ YÖNTEMLERİ

Kuantum noktaları, II-VI veya III-V grup elementlerinden oluşurlar. Genel olarak CdS, CdSe, CdSe/ZnS, CdTe elementleri, yapay bir şekilde nanometrik boyutlara küçültülürler. Bu elementler arasında CdS, KN'larda daha kararlı bir yapı göstermesinden dolayı çok fazla tercih edilmektedir [2]. Kuantum noktaları temel olarak iki farklı yöntem ile sentezlenirler. Bu iki teknik: yukarıdan aşağıya işleme (up-down) ve aşağıdan yukarıya işleme (bottom-up) olarak genelleştirilebilir.

YUKARIDAN AŞAĞIYA İŞLEME YÖNTEMLERİ

- Moleküler Işın Epitaksisi
- İyon implantasyonu
- Litografi
- Mekanik Öğütme

AŞAĞIDAN YUKARIYA İŞLEME YÖNTEMLERİ

- Püskürtme
- Sprey Piroлиз
- Plazma Arki

Kuantum noktalarının güçlü optik ve elektriksel özellikleri, onları birçok uygulama alanında kullanılabilir hale getirmiştir. Sağlık, kimya, görüntüleme teknolojileri ve güneş pilleri gibi hayatımızda çok önemli rolü olan alanlarda sıklıkla kuantum nokta teknolojisine rastlanmaktadır. Kanser hücrelerinin görüntülenmesi, ilaç taşıma sistemiyle kanser ve bulaşıcı hastalıkların tedavisi, kimyasal analizlerde sensör görevi, elektriksel gücüne odaklanılarak güneş pillerindeki enerji tasarrufu gibi görevleri ve daha fazlasıyla geniş bir uygulama alanına hizmet etmektedir.

SONUÇ

Kuantum noktaları, nano boyutlu malzemeler olup, 20. yüzyılın son çeyreğinde sentezlenmişlerdir. Optik özellikleri ve floresans davranışlarıyla dikkat çeken bu malzemeler, düşük maliyetli ve hızlı sentez yöntemleriyle önem kazanmıştır. Sağlık alanında görüntüleme teknolojilerinde sıklıkla kullanılmalarına rağmen, içerdikleri ağır metaller nedeniyle sentez yöntemleri üzerinde odaklanılmıştır. Teşhis ve tedavi uygulamalarında etkili rol oynamışlar, aynı zamanda QLED TV'ler ile yenilenebilir enerji uygulamalarında kullanılmışlardır. Bilimsel çalışmalarda 1985'te başlayan kuantum nokta araştırmaları, hızla artarak popülerlik kazanmıştır. Bu çalışmaların, kuantum noktalarının uzun vadeli popülerliğini sürdüreceği ve çeşitli alanlarda insanlığa önemli katkılar sağlayacağı öngörülmektedir.

KAYNAKÇA

- [1] P. Sun, Z. Xing, Z. Li and W. Zhou, Recent advances in quantum dots photocatalysts, *Chem. Eng. J.*, 2023, 458 141399, <https://doi.org/10.1016/j.cej.2023.141399>
- [2] William W. Yu, E. Chang, R. Drezek, V. L. Colvin, Water-soluble quantum dots for biomedical applications, *Biochemical and Biophysical Research Communications*, 2006, 348(3), 781-786, <https://doi.org/10.1016/j.bbrc.2006.07.160>
- [3] B. Gidwani, V. Sahu, S. S. Shukla, R. Pandey, V. Joshi, V. K. Jain, A. Vyas, Quantum dots: Prospectives, toxicity, advances and applications. *Journal of Drug Delivery Science and Technology*, 2021, 61, 102308, <https://doi.org/10.1016/j.jddst.2020.102308>



**YTU FEN EDEBİYAT
FAKÜLTESİ**

DEPARTMENT OF CHEMISTRY

**SYNTHESIS AND CHARACTERIZATION OF NOVEL SCHIFF BASES AND
DETERMINATION OF THEIR ANTIFUNGAL EFFECTS**

GRG
GUNKARA RESEARCH GROUP

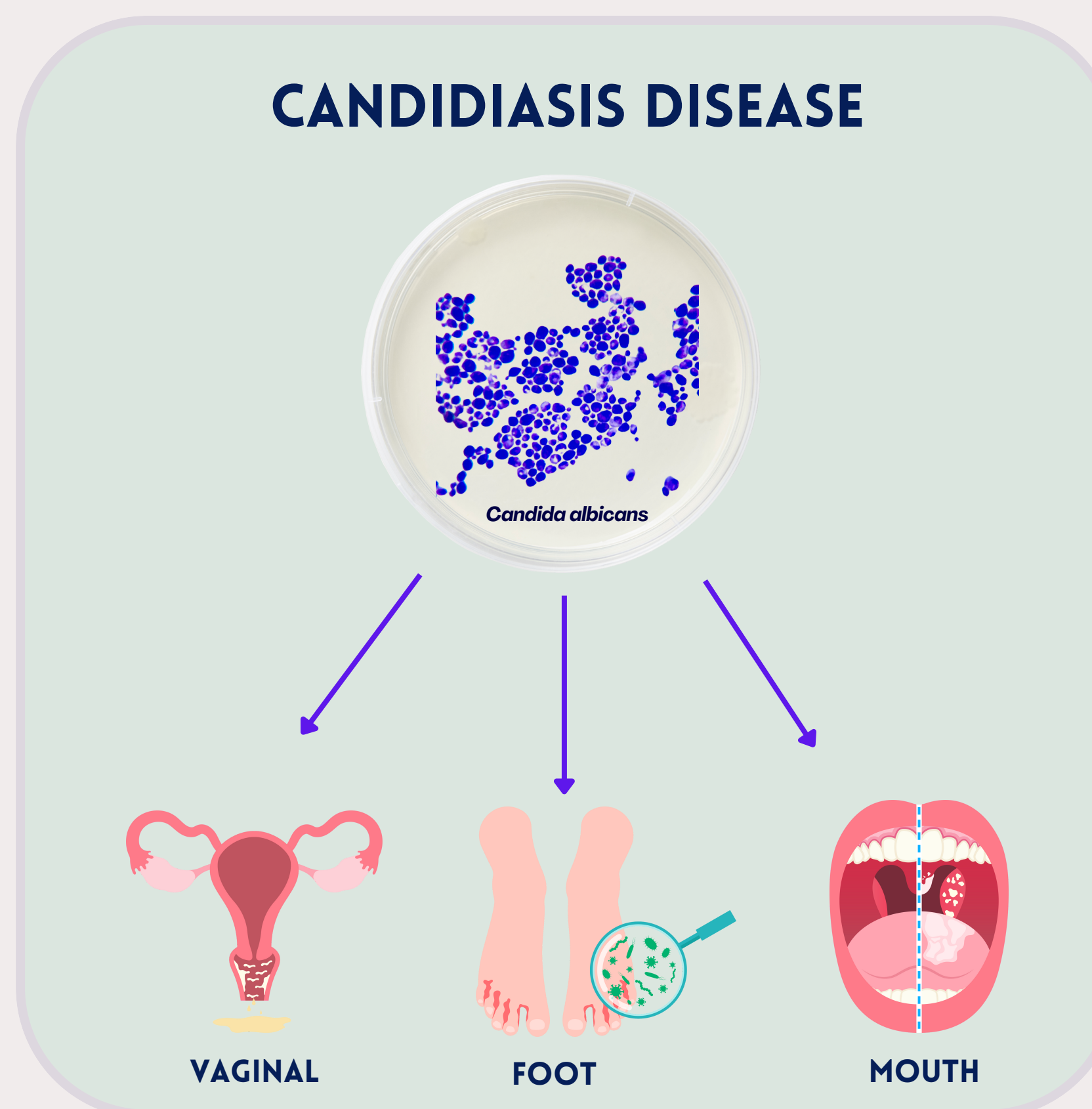
MELİKE AKDEMİR 19024088

ASSOC. PROF. ÖMER TAHİR GÜNKARA

ABSTRACT

Fungi are organisms that can be found on internal and external surfaces in the environment and have more than 5 M species. Some pathogenic and disease-causing species of fungi significantly threaten and negatively affect human and animal health. Since the 20th century, antifungal medicines have been used to control these diseases. There are 5 main classes of antifungal drugs. However, some fungi can exhibit resistance to these drugs. Therefore, the synthesis of new organic molecules with high biological activity and reliable antifungal properties is sought in the literature. Schiff bases stand out in the literature as alternative antifungal drugs due to their properties. Easy synthesis, and mild reaction conditions are among the advantages of Schiff bases. In this study, two Schiff bases with high antifungal activity were synthesized according to the results of docking studies, and their results were evaluated.

CANDIDIASIS DISEASE

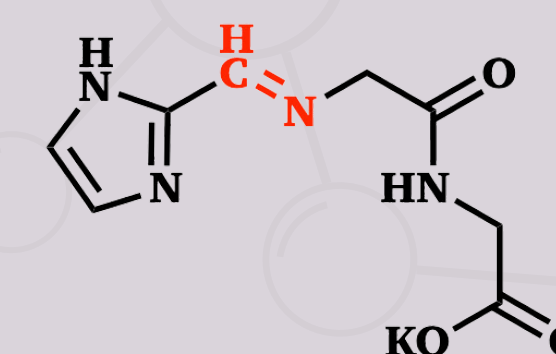


ANTIFUNGAL DRUGS

Classes of antifungal drugs that can be used for fungal infections:

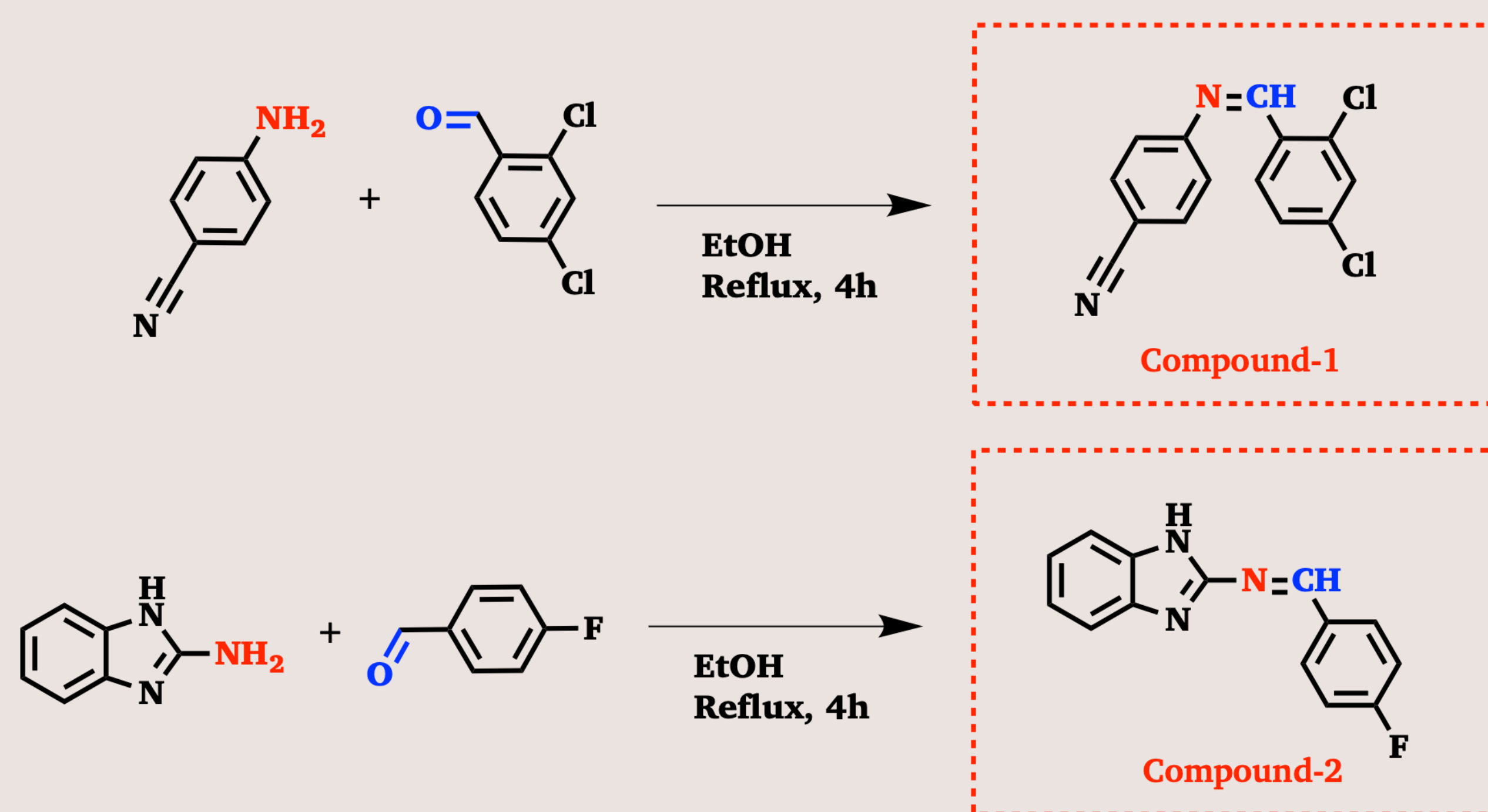
- 1949 Polyenes
- 1957 Pyrimidine analogues
- 1969 Azoles
- 1974 Allylamines
- 1987 Echinocandins

Resistance to antifungal drugs is a significant problem in the worldwide. Thus, new molecules are being investigated in the literature as alternatives to these drugs. Schiff bases are one of them.

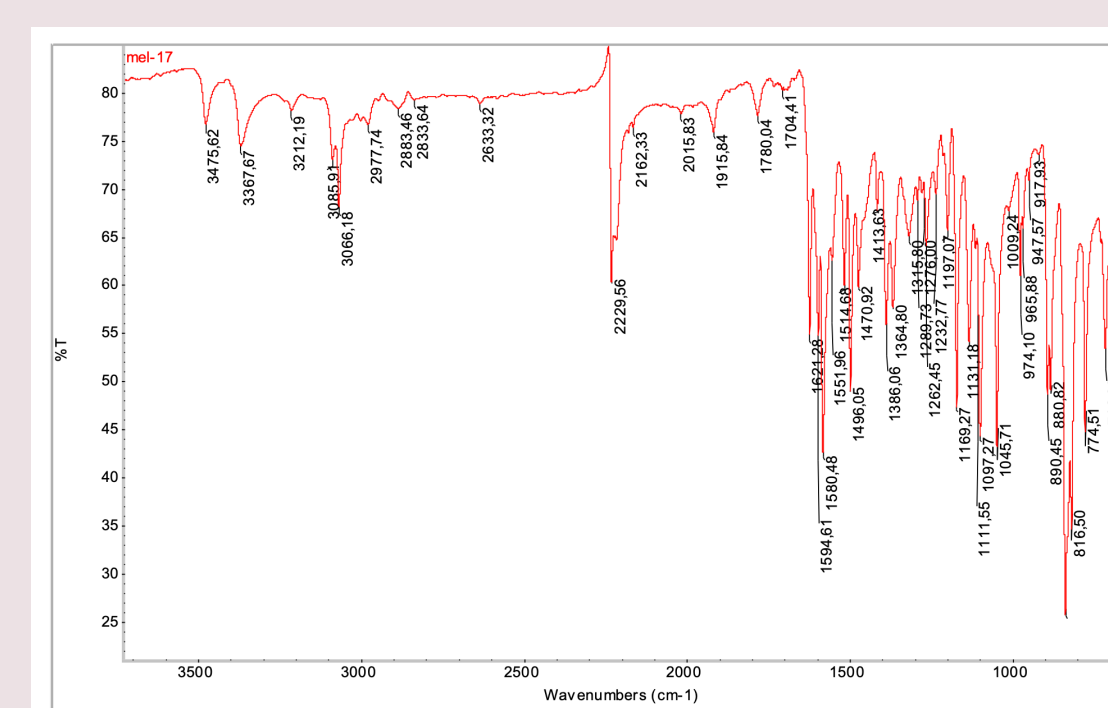


Antifungal Schiff base synthesized by Joseyphus and Nair.

SYNTHESIS

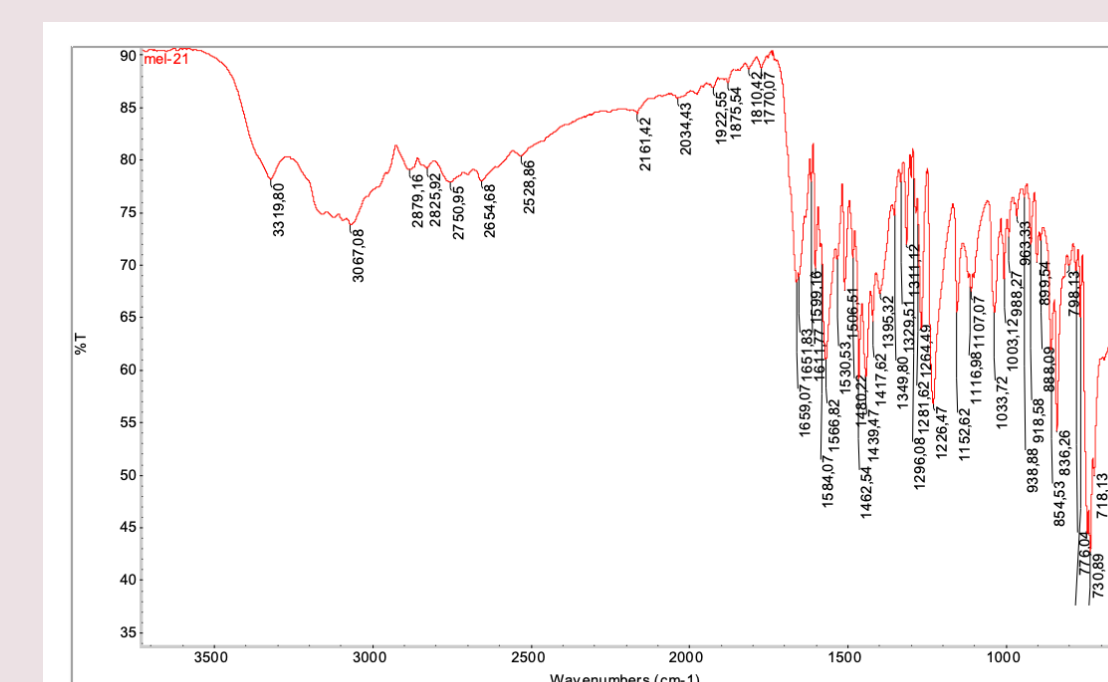


CHARACTERIZATION



FTIR (ATR) SPECTRUM OF COMPOUND-1

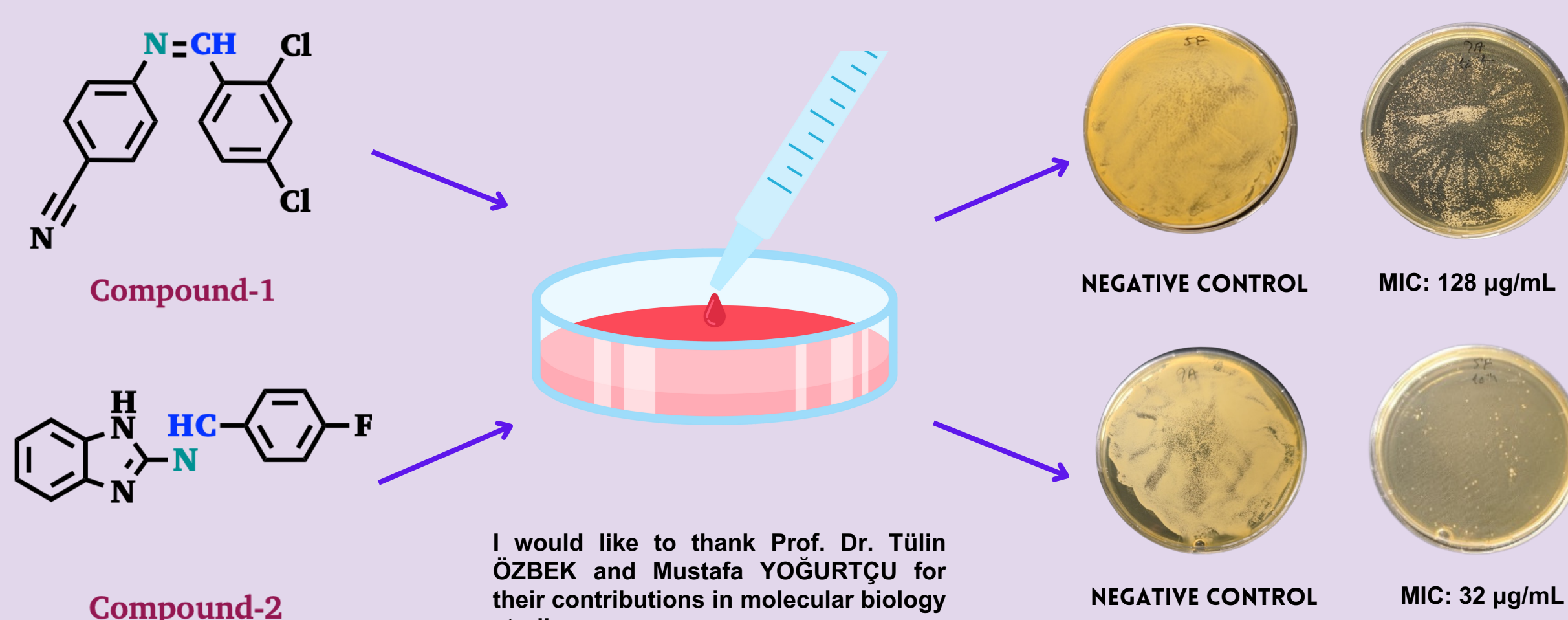
$\nu = 3066$ (aromatic C-H stretching), 2977 and 2883 (aliphatic C-H stretching), 2229 (CN stretching), 1580 (aromatic C=C stretching), 1620 (C=N stretching), 816 (C-Cl stretching) cm^{-1} .



FTIR (ATR) SPECTRUM OF COMPOUND-2

$\nu = 3319$ (secondary N-H stretching), 3067 (aromatic C-H stretching), 2879 (aliphatic C-H stretching), 1584, 1611, and 1650 (N-H bending), 1659 and 1651 (C=N stretching), 1003 (C-F stretching) cm^{-1} .

BROTH-MICRODILUTION METHOD

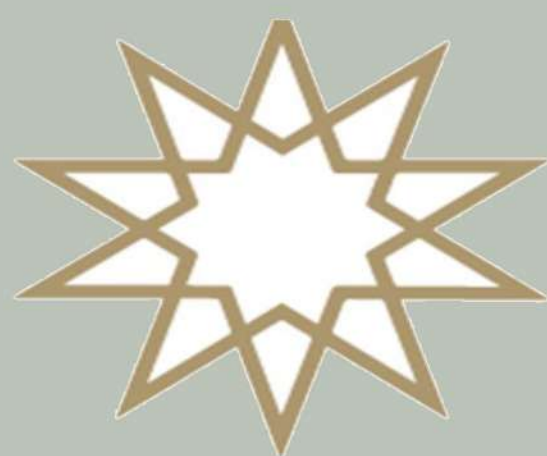


I would like to thank Prof. Dr. Tülin ÖZBEK and Mustafa YOĞURTCU for their contributions in molecular biology studies.

CONCLUSION

Fungal diseases can damage ecosystems as they also infect animals and plants. Numerous studies in the literature are focused on minimizing the serious risk that fungi. However, considering the capacity of some fungal species to resist antifungal drugs as a disadvantage, the synthesis of new organic molecules that can show antifungal activity has come to the fore. When the antifungal properties of compound-1 synthesized in this study were examined, it was determined that it showed an antifungal effect under high concentration conditions (128 $\mu\text{g/mL}$). On the other hand, the high antifungal effect of compound-2 synthesized under very low concentration conditions (32 $\mu\text{g/mL}$) was determined. According to these results, it can be said that the antifungal activity of compound 2 is very high compared to compound 1.

1) Casadevall, A. (2018). Fungal diseases in the 21st century: The near and far horizons. *Pathogens and Immunity*, 3(2), 183–196. <https://doi.org/10.20411/pai.v3i2.249>
2) Joseyphus, R. S., & Nair, M. S. (2008). Antibacterial and Antifungal Studies on Some Schiff Base Complexes of Zinc(II). *Mycobiology*, 36(2), 93. <https://doi.org/10.4489/myco.2008.36.2.093>
3) Kaur, J., & Nobile, C. J. (2023). Antifungal drug-resistance mechanisms in *Candida* biofilms. In *Current Opinion in Microbiology* (Vol. 71). Elsevier Ltd. <https://doi.org/10.1016/j.mib.2022.102237>



Abstract

This thesis explores the role of green solvents in minimizing environmental impacts in accordance with the principles of green chemistry. Green solvents are materials designed to reduce ecological effects, widely applied in various industries to replace traditional solvents. The study emphasizes the general classification, advantages, and industrial examples of green solvents, highlighting their contribution to environmental sustainability. By underscoring the role of green chemistry and green solvents in future environmentally friendly chemical practices, the thesis supports the increased use of green solvents as a significant step in reducing environmental impacts.

Green Chemistry

The history of chemistry spans 150 years, with green chemistry emerging in 1990 as part of the pollution prevention movement. The U.S. Environmental Protection Agency (EPA) introduced strategies for pollution prevention, leading to the incorporation of green chemistry. Despite its recent inception, green chemistry has become integral in academia and industry, aligning with consumer demands for sustainable practices. Green chemistry principles are applied across various sectors, influencing material selection, reagent use, and synthesis processes. Choosing non-harmful and renewable materials is emphasized, and reagent selection considers potential harms. Catalysts play a crucial role, reducing energy requirements and improving selectivity. Solvents, often hazardous, require careful selection; alternatives like water, supercritical carbon dioxide, and ionic liquids are recommended. Implementing green chemistry principles reduces raw material, product, solvent, reagent, and by-product quantities, leading to cost savings and risk mitigation. Anastas & Warner's principles serve as a foundation for defining green chemistry, contributing to sustainable development goals for the environment and the economy.

The Twelve Principles of Green Chemistry



Green Solvents

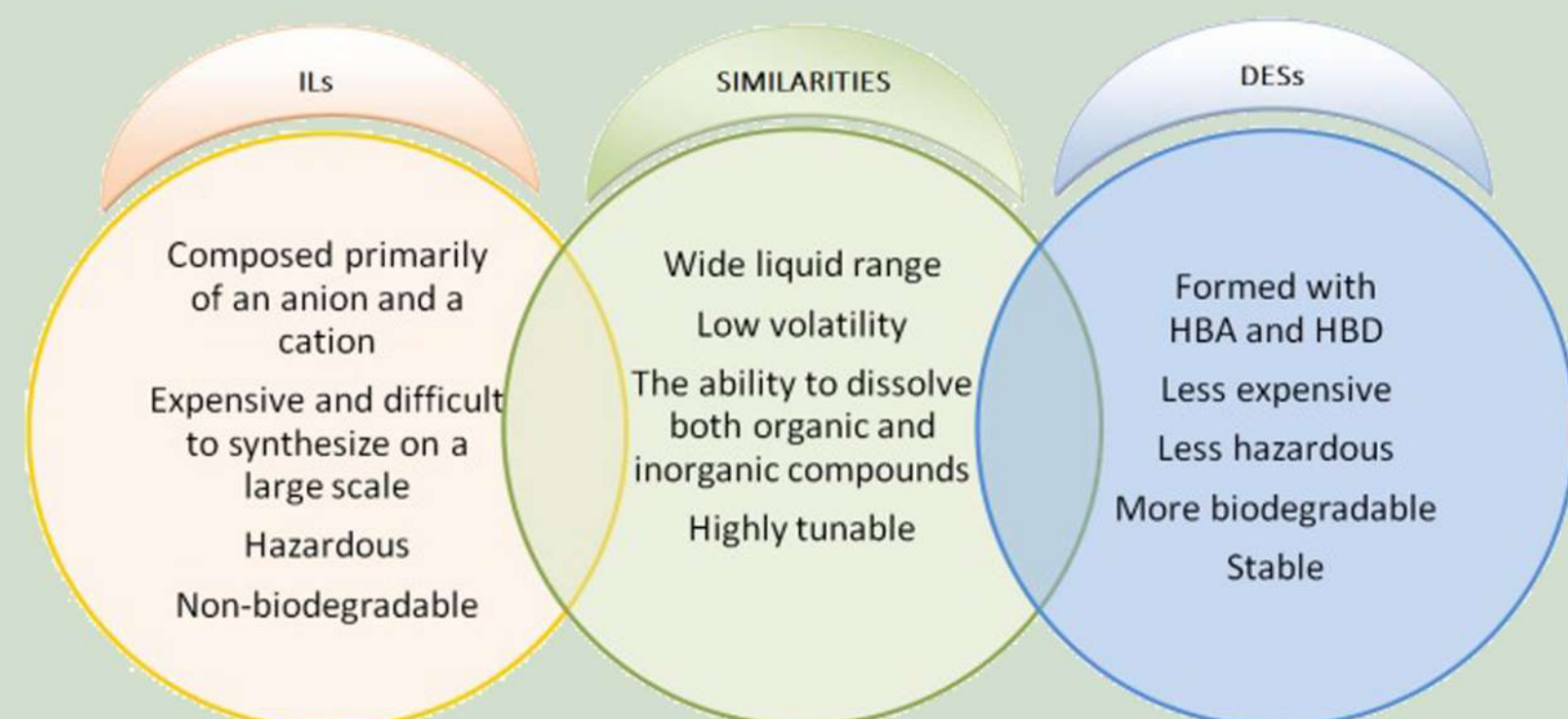
Green chemistry is dedicated to establishing sustainable processes, mitigating risks linked to chemical substances, and pioneering innovative synthetic methods. Current research places significant emphasis on substituting conventional solvents with safer, environmentally friendly alternatives sourced from agricultural crops, such as ethyl acetate derived from corn processing. These green solvents, offering heightened safety for both human health and the environment, prove to be versatile and suitable for a wide range of applications.



Classification of Green Solvents

Ionic Liquids (ILs)

In recent years, ionic liquids (ILs), predominantly composed of organic salts with low melting points, have garnered significant interest. Among the environmental and technological advantages of ILs are low volatility, non-flammability, and thermal, chemical, and electrochemical stability. These characteristics make them customizable solvents for various applications. ILs serve as environmentally friendly options, particularly in bio-based extraction processes, owing to their special features that have minimal impact on air quality and enable effective separation of diverse substances.



Deep Eutectic Solvents (DES)

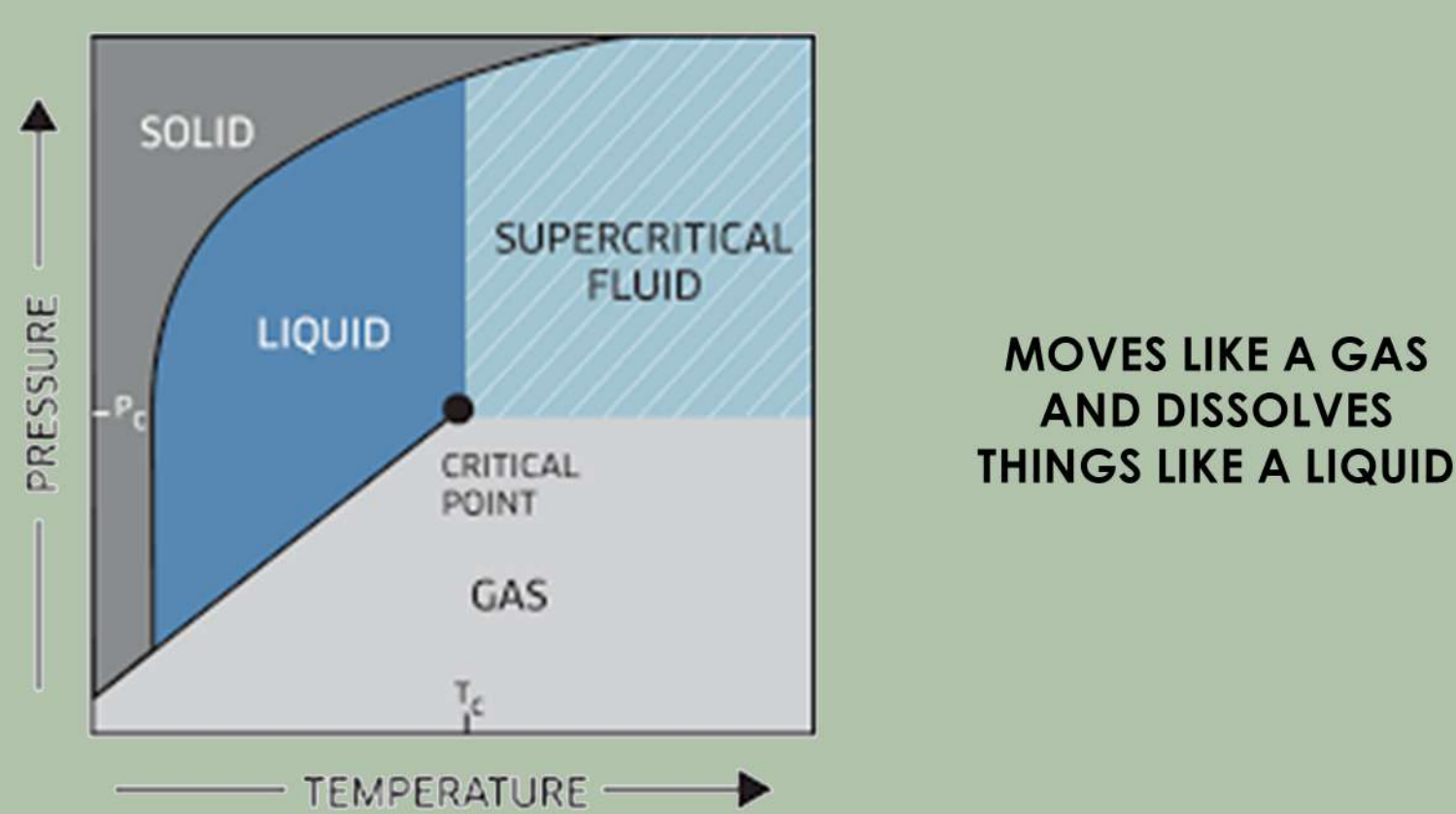
Deep Eutectic Solvents (DES) are unique solvents formed by eutectic mixtures, usually composed of a hydrogen bond donor and a hydrogen bond acceptor. Notable features include low toxicity, low volatility, high thermal stability, and tunable properties. DESs are cost-effective, biodegradable, biocompatible, and can be derived from renewable resources. They offer environmental, economic, and functional benefits, finding applications in green chemistry and pharmaceuticals. DESs are simpler and more cost-effective than Ionic Liquids, with potential in various fields, including organic synthesis, catalysis, and biomedical applications.

Water

Recent research focuses on using water as a substitute for organic solvents in various organic reactions due to its non-toxic, safe, eco-friendly, and cost-effective properties. Water can be the sole solvent or combined with others to form two-phase emulsions in "aqueous reactions," leading to faster reaction rates compared to organic solvents. However, challenges include water's high heat of vaporization and the need for extensive wastewater treatment to comply with regulations. Despite these challenges, water is recognized as a favorable solvent in certain organic reactions, such as Diels-Alder reactions, where its hydrophobic nature proves advantageous.

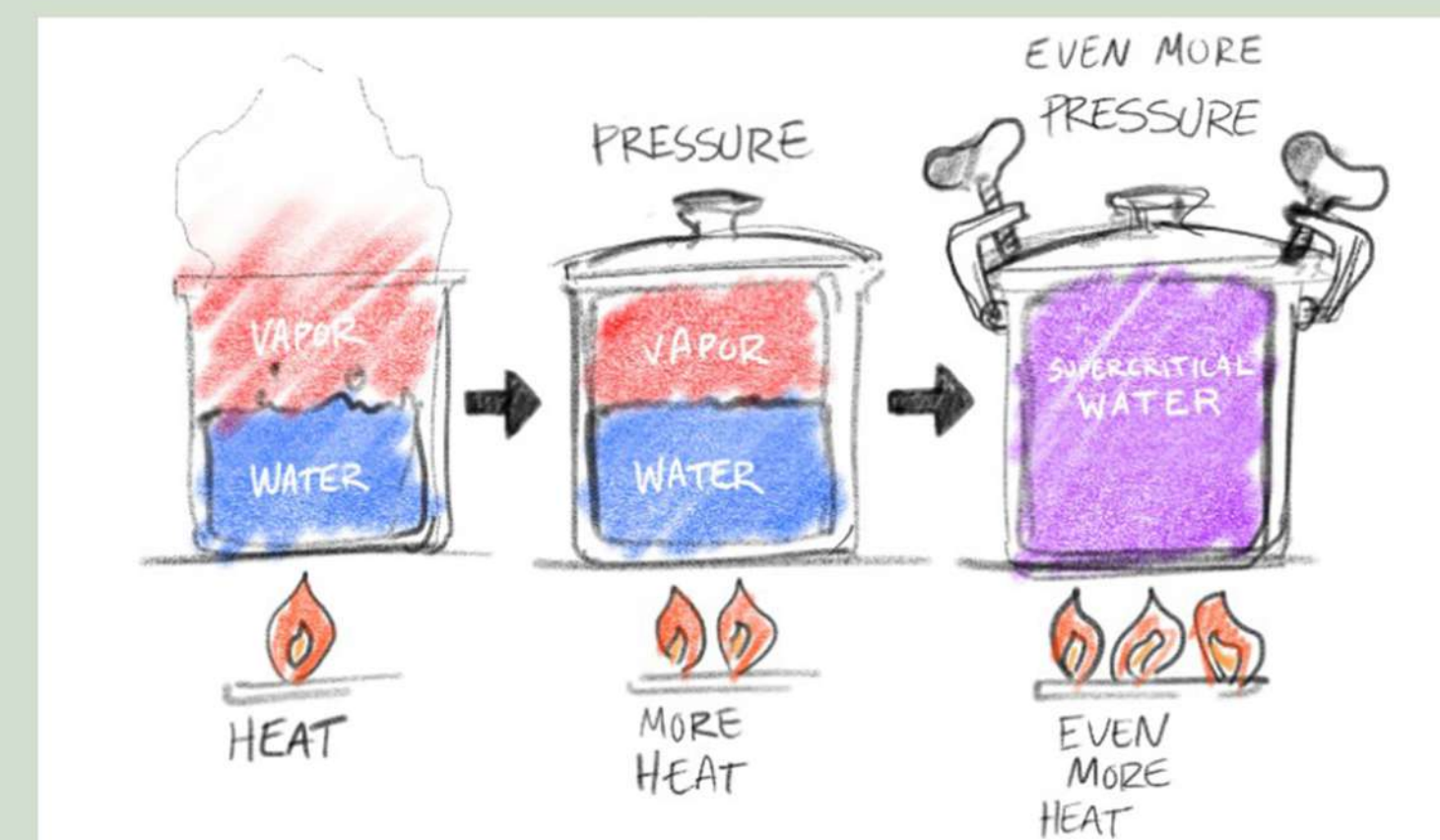
Supercritical and Subcritical Fluids

Classical thermodynamics defines supercritical fluids (SCFs) as fluids heated and compressed beyond the critical point. SCFs exhibit properties between gases and liquids, with densities resembling liquids and viscosities similar to gases. Retrograde behavior, where solute solubility decreases with rising temperature, is observed in supercritical fluids, influencing their phase behavior.



Various compounds are explored as supercritical extraction solvents, with carbon dioxide (CO₂) and water being noteworthy. CO₂, a commonly used supercritical fluid, has low toxicity, is non-explosive, and is environmentally benign. Recent developments include CO₂-expanded liquids, reducing solvent consumption. Supercritical fluids, such as supercritical CO₂, offer advantages like low toxicity, non-flammability, and easy separation from extracted components, facilitating efficient recovery. Their ability to dissolve both polar and non-polar compounds allows selective extraction, contributing to environmental sustainability. Supercritical CO₂ has distinct properties, including a small, linear molecule structure and high solvating power. It is considered a clean technology, with applications in extracting non-polar and moderately polar compounds. Its low critical temperature enables extraction of heat-sensitive compounds, and it is environmentally friendly.

Supercritical water (scH₂O) exhibits unique properties, such as variable density and high polarity. Operating under high temperature and pressure, scH₂O enhances solubility and diffusivity, making it effective for extracting polar and ionic compounds. It can generate reactive hydroxyl radicals, offering potential in waste treatment.



Overall, supercritical fluids, including scCO₂ and scH₂O, are versatile and efficient extraction solvents with applications in diverse fields, ranging from essential oils to environmental remediation. They offer advantages such as selectivity, environmental friendliness, and suitability for heat-sensitive substances.

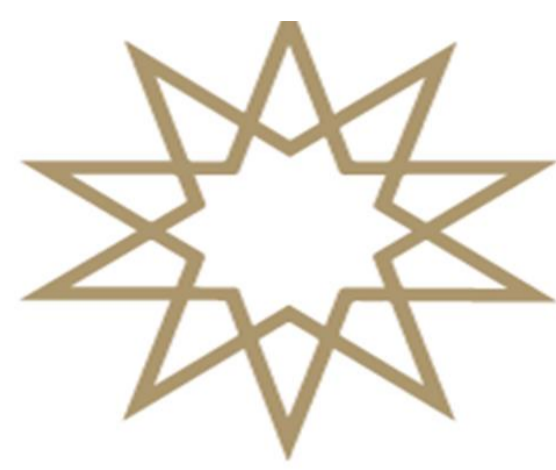
Biosolvents

Biosolvents have emerged as a green alternative to volatile organic compounds that are harmful to the environment and human health. These solvents, derived from natural sources, encompass chemical structures such as acids, fatty acid esters, bioethanol, terpenic compounds, isosorbide, and glycerol. They find applications in various industries, including agriculture, cosmetics, cleaning, paint, and agricultural chemicals. For these solvents to be viable, they must meet specific technical, environmental, and ecological criteria. Derived from diverse sources, these solvents contribute to sustainable chemi-



References

- [Chen, Y., & Mu, T. (2021). Revisiting greenness of ionic liquids and deep eutectic solvents. *Green Chemical Engineering*, 2(2), 174-186.
Pathak, M., Singh, L., Kumar, A., & Upadhyay, G. Green solvents and their importance in medicinal chemistry: An overview. *Chemistry*, 14, 15
Usman M, Cheng S, Boonyubol S, Cross JS. Evaluating green solvents for bio-oil extraction: Advancements, challenges, and future perspectives. *Energies*. 2023; 16(15):5852. .



Artificial leather, also known as synthetic or faux leather, has emerged as a significant alternative to traditional animal-derived leather, offering a myriad of benefits that extend beyond its aesthetic appeal. This versatile material is primarily composed of polymeric substances, often polyurethane or polyvinyl chloride, which are engineered to mimic the look and feel of genuine leather. One key characteristic lies in its sustainability, as it reduces reliance on animal resources and minimizes environmental impact. Moreover, artificial leather boasts enhanced durability and resistance to wear and tear, making it a viable choice for various applications, from fashion to upholstery. In terms of customization, artificial leather offers a wide range of textures and colors, providing designers and manufacturers with creative flexibility. This adaptability contributes to its popularity in the fashion industry, allowing for the creation of diverse and stylish products. Additionally, the production process of artificial leather tends to be more cost-effective compared to traditional leather, making it an economically viable choice. From a scientific perspective, studying the composition and structure of artificial leather sheds light on the intricate engineering behind its properties. Understanding the chemical processes involved in its production contributes to advancements in materials science and polymer chemistry. In conclusion, artificial leather stands as a testament to the intersection of technology, sustainability, and design. Its characteristics, ranging from Eco friendliness and durability to aesthetic versatility, make it a compelling subject of study with implications for both the fashion industry and scientific research in material engineering.

INTRODUCTION

- Artificial leather, or synthetic leather, is made from polymers like polyurethane (PU) and polyvinyl chloride (PVC). PU offers flexibility, breathability, and durability, mimicking genuine leather. It's popular for comfort and longevity. PVC is water-resistant and cost-effective, suitable for moisture-resistant applications like bags and outerwear. However, PVC may be less breathable, and its environmental impact raises concerns.
- Various factors affect artificial leather characteristics, including polymer choice, manufacturing processes (calendering, coating, embossing), and additives (plasticizers, stabilizers). Tanning methods enhance durability, but artificial leather uses chemical treatments, posing environmental concerns.
- Environmental considerations are crucial in artificial leather production due to petrochemical-based materials and chemicals, raising worries about resource depletion and pollution. Efforts focus on sustainable alternatives and eco-friendly processes to minimize environmental impact.
- In conclusion, artificial leather characteristics depend on polymers, manufacturing, additives, tanning, and environmental factors. Ongoing research aims to improve performance while addressing environmental concerns.

APPLICATION AREAS

- Fashion and Apparel
- Automotive Industry
- Furniture
- Accessories
- Sports Equipment
- Medical Industry
- Aviation and Marine
- Promotional Items
- Interior Design
- Super Capacitors



Polymers Used During the Production of Artificial Leather

- Polyvinyl Chloride (PVC)
- Polyurethane (PU)
- Polyamide (Nylon)
- Polyester
- Polycarbonate (PC)

Production Methods

- Coating Method
- Embossing
- Treatment and Finishing
- Quality Control and Inspection

Materials Needed

- Fabric Base
- Polymer Coating
- Additives and Chemicals
 - Plasticizers
 - Stabilizers
- Colorants and Pigments
- UV Inhibitors
- Flame Retardants
- Foaming Agents
- Tackifiers
- Biocides and Antimicrobial Agents
- Water and Solvent-Based Adhesives
- Cross-Linking Agents
- Release Agents



DISCUSSION AND REVIEWS

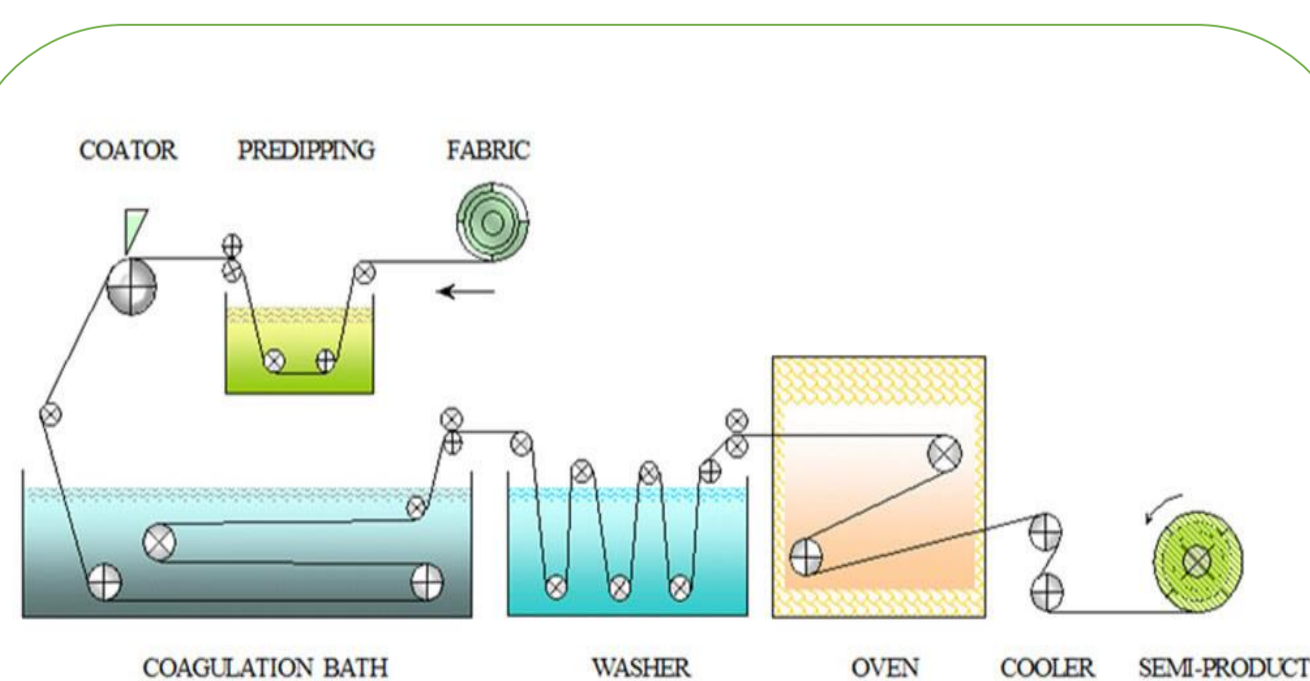
- This exploration reveals artificial leather as a complex material intersecting polymer science, material engineering, and environmental sustainability. Emphasizing the pivotal role of polyurethane (PU) and polyvinyl chloride (PVC), the discussion delves into their molecular structures and impact on mechanical, tactile, and durability properties.
- A comparative analysis guides tailored applications for industries from fashion to automotive, offering valuable insights for scientists, engineers, and manufacturers.
- The environmental discourse stresses the need to consider the ecological impact of artificial leather. Sustainable practices, including life cycle analysis and exploration of eco-friendly alternatives like bio-based polymers, signal a promising direction for future research and industry practices.
- In the broader context of interdisciplinary research, this thesis bridges chemistry, material science, and environmental studies, providing a holistic understanding of artificial leather. Amid evolving consumer preferences and environmental consciousness, the research contributes to responsible material choices and sustainable practices.

STOPPING LIMITS

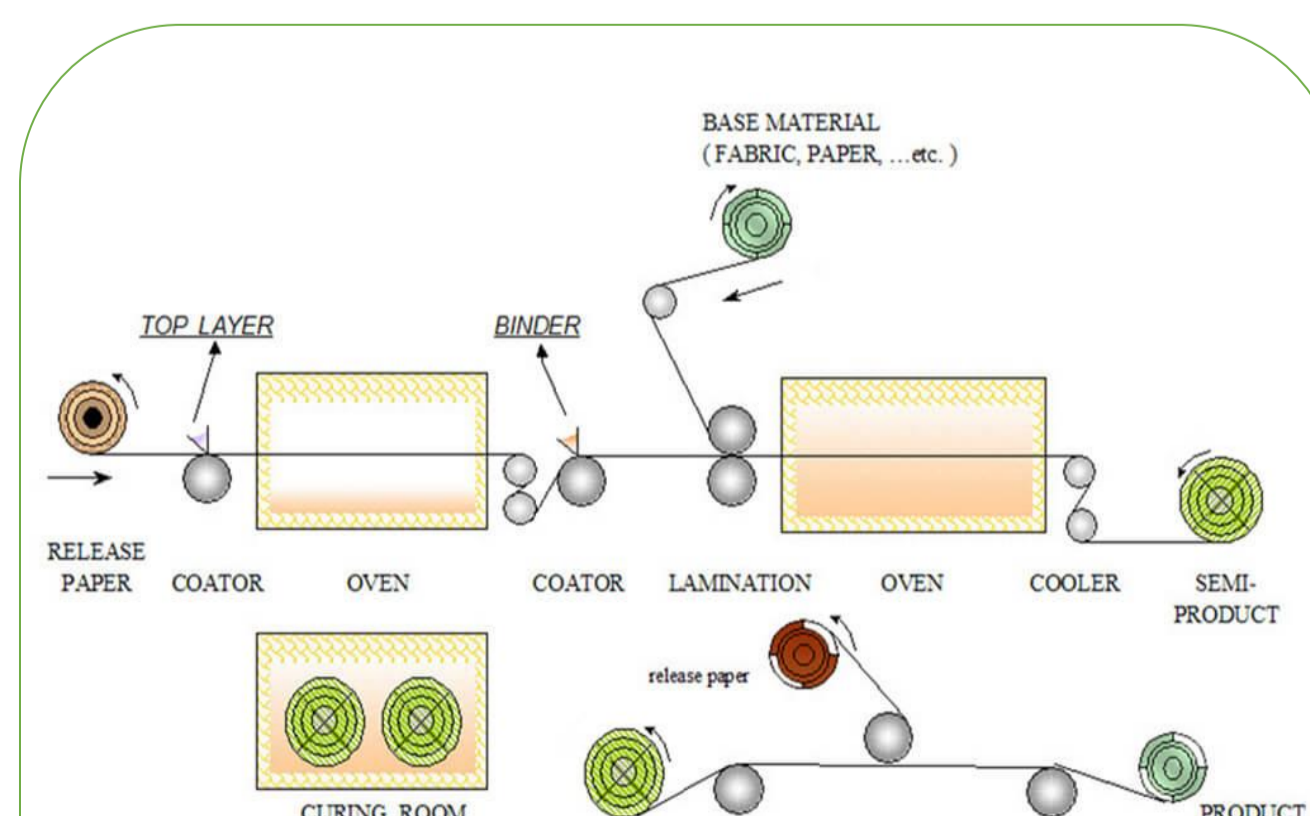
- Acknowledging study limitations, the focus on PU and PVC provides foundational insights, leaving the broader landscape of polymers in synthetic leather unexplored. Environmental considerations could benefit from a more comprehensive life cycle assessment.
- The dynamic nature of technological advancements implies potential research outdatedness, emphasizing the need for ongoing inquiry.
- The study primarily explores technical and environmental facets, leaving room for future investigations into cultural perceptions, consumer behavior, and market dynamics related to artificial leather.
- Recognizing these limits sets the stage for more holistic approaches that integrate scientific, environmental, social, economic, and cultural dimensions, encouraging continued research in the dynamic field of synthetic materials.

REFERENCES

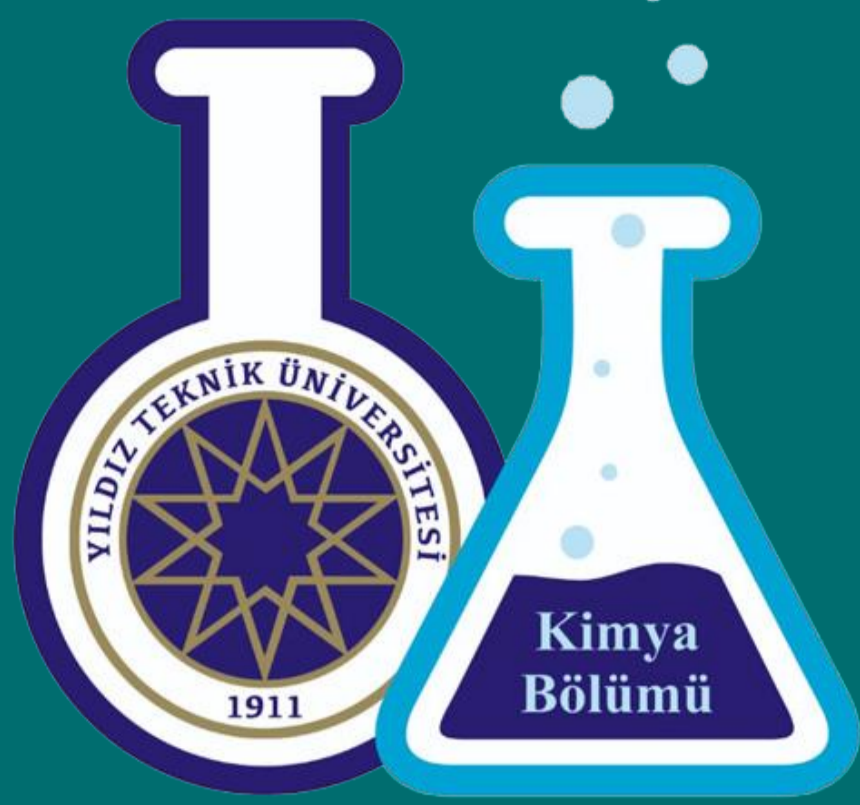
- [1] Kovalenko, G. M., Bokova, E. S., Novikova, Yu. E., & Petrova, E. K. (2021). Development Of Conditions for Obtaining Artificial And Synthetic Leather Coatings Based On Environmental Latex Compositions
- [2] Lee, S. S., Choi, K. H., Kim, S. H., & Lee, S. Y. (2018). Wearable supercapacitors printed on garments. *Advanced Functional Materials*, 28(11), 1705571
- [3] Lin, Z., Sun, Z., Xu, C., Zhang, A., Xiang, J., & Fan, H. (2021). A self-mating waterborne polyurethane coating with admirable abrasion-resistance. *Rsc Advances*, 11(44), 27620-27626



Wet Process Enhance hand-feel and get strong physical properties



Dry Process To get colors, effects, and texture.

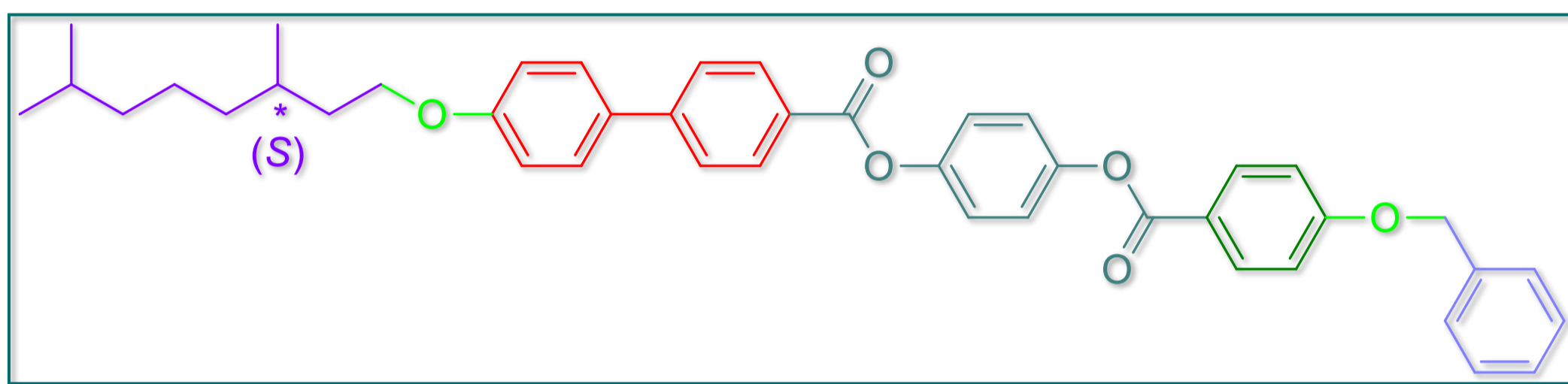


ABSTRACT

Liquid crystals are organic molecules that have the properties of both crystalline solids and liquids. A liquid crystal is fluid, like an isotropic liquid, and at the same time the molecules show orientational or positional order, as in solid crystals. Liquid crystals form organized structures formed between these two phases. In this study, the synthesis, structural and mesomorphic characterization of a new terephthalate-based rod-like molecule with a (S)-3,7-dimethyloctyloxy chiral terminal chain have been carried out.

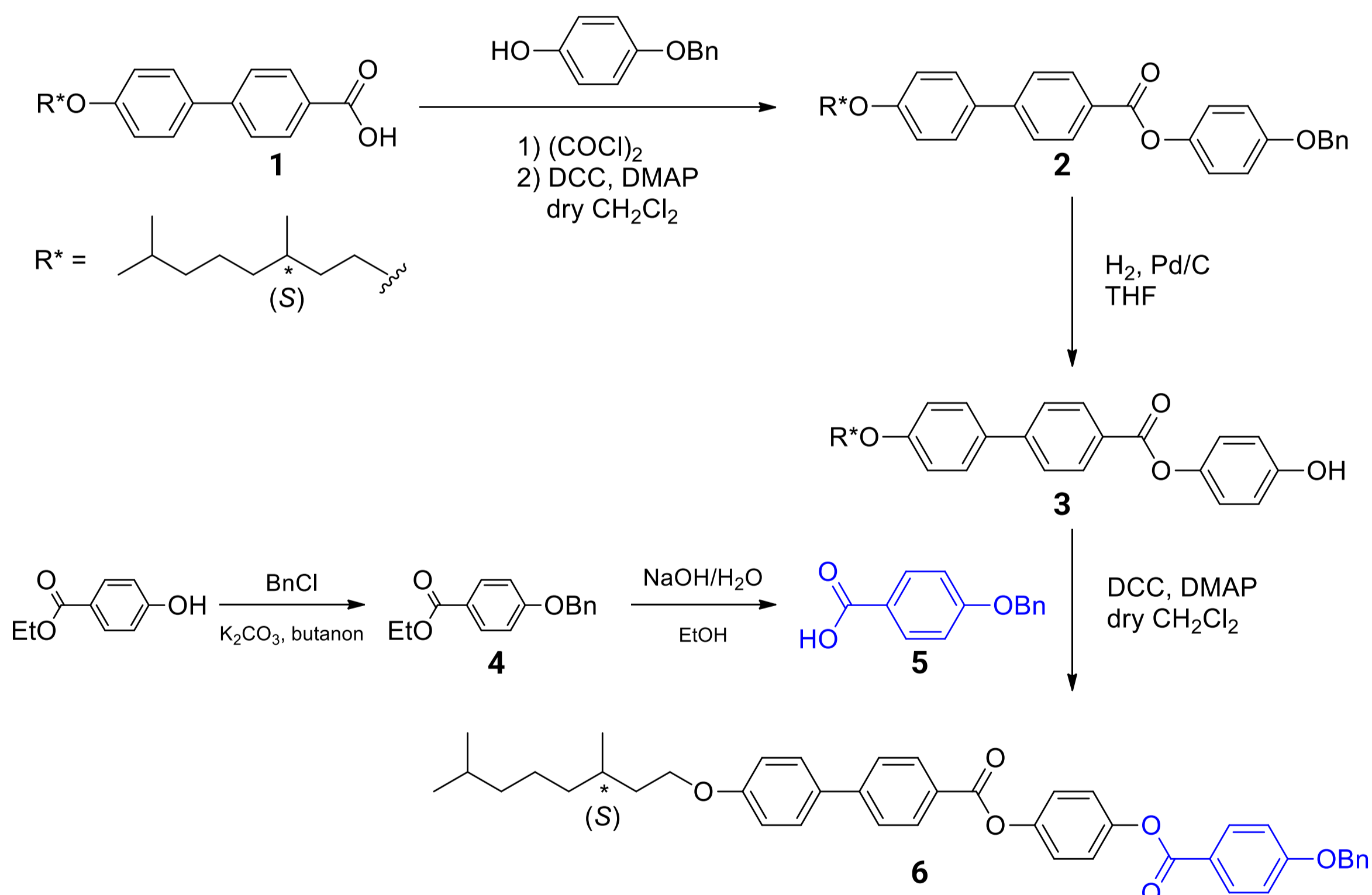
CALAMITIC (ROD-LIKE) LIQUID CRYSTALS

Liquid crystal molecules are typically 'rod shaped' – long and thin with a rigid center that allows them to maintain their shape. They also have flexible ends, which means that they can still flow past each other with ease. Molecules with this shape are known as calamitic liquid crystals. The units used in this general structure affect the physical properties of the liquid crystal molecule. The length of the liquid crystal molecule and its side chains also significantly affects the mesophase structure. In the crystalline state, the molecule is held together by very strong intramolecular interactions, which gives the molecule a rod-like (calamitic) geometry.



SYNTHESIS

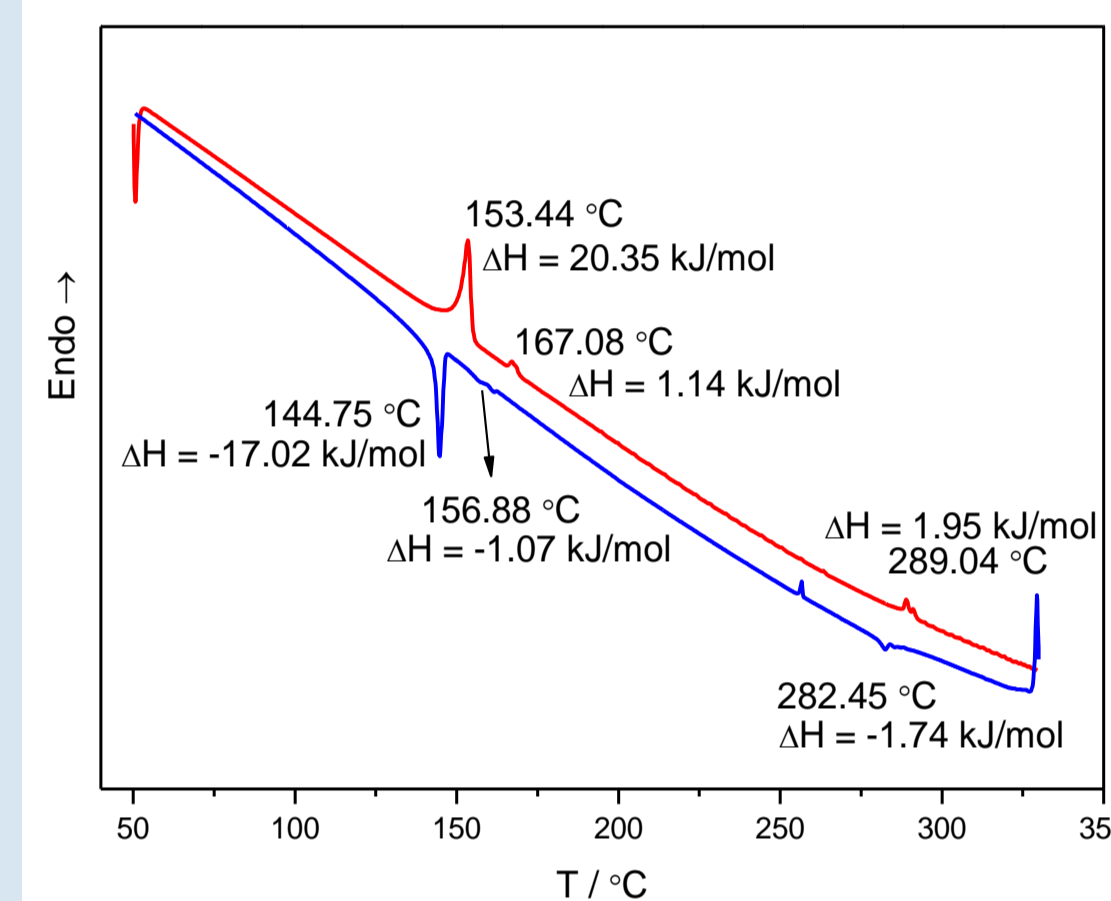
In this study, a new terephthalate derivative compound with (S)-3,7-dimethyloctyloxy chiral chain, containing ester linking groups, with a new rod-like geometry has been designed. Synthesis of new liquid crystals exhibiting mesophases that meet practical needs is important in terms of literature.



MESOMORPHIC PROPERTIES

The mesomorphic properties of the chiral calamitic liquid crystal with a benzyloxy terminal unit were examined. The newly synthesized compound exhibited **enantiotropic** liquid crystal mesophases. On cooling from the isotropic phase, **N*** phase was firstly appeared, which was characterized by traditional focal-conic texture. By further cooling, **SmC*** phase occurred as a low temperature phase.

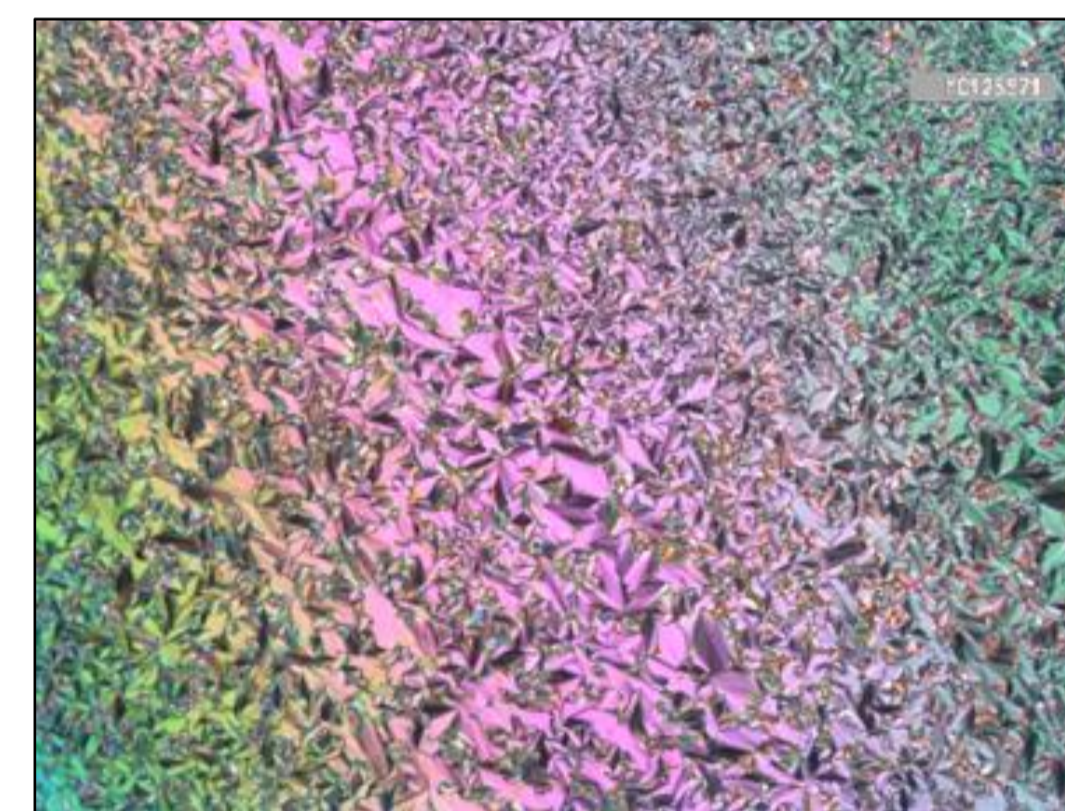
DSC thermogram of heating and cooling of synthesized molecule



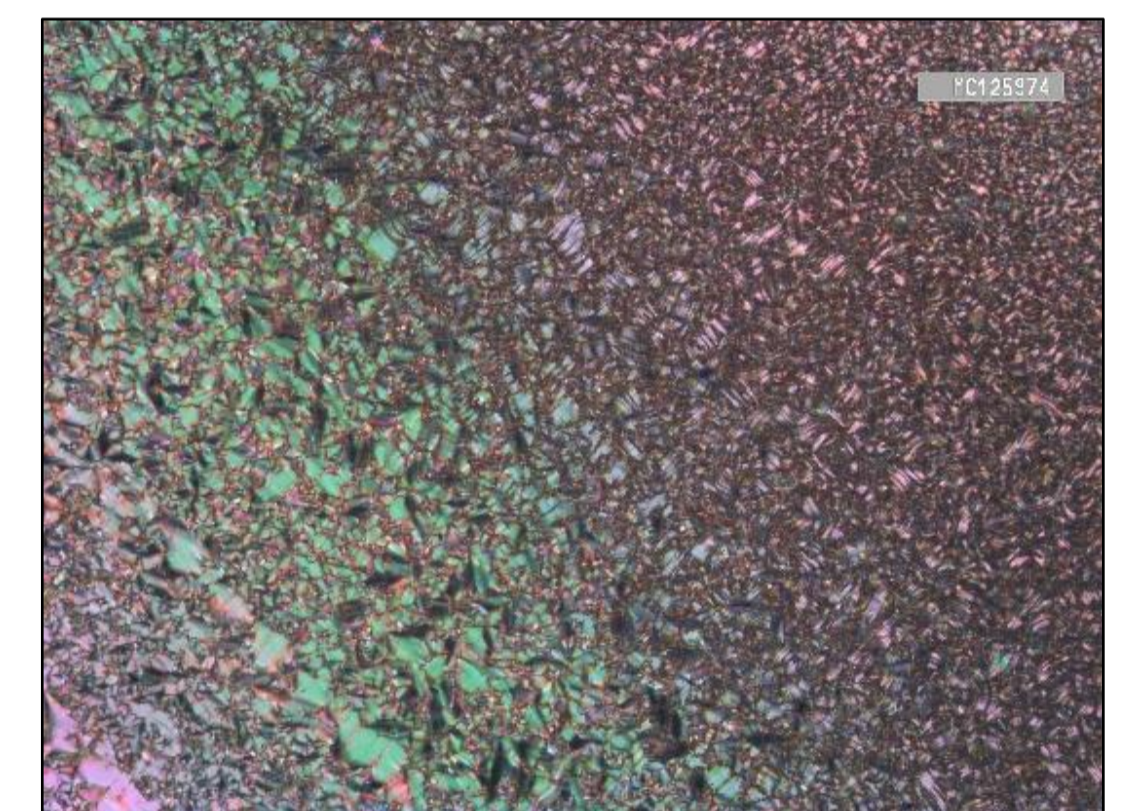
T/°C [ΔH kJ/mol]	
H →	Cr 153.44 [20.35] SmC* 167.08 [1.14] N* 289.04 [1.95] Iso
C →	Iso 282.45 [-1.74] N* 156.88 [-1.07] SmC* 144.75 [-17.02] Cr

Enthalpy values in brackets taken from the 2nd heating and 2nd cooling scans at a rate of 10°C min⁻¹;
Abbreviations: Cr = crystalline, SmC* = chiral tilted smectic phase, N* = chiral nematic phase, Iso = isotropic liquid phase.

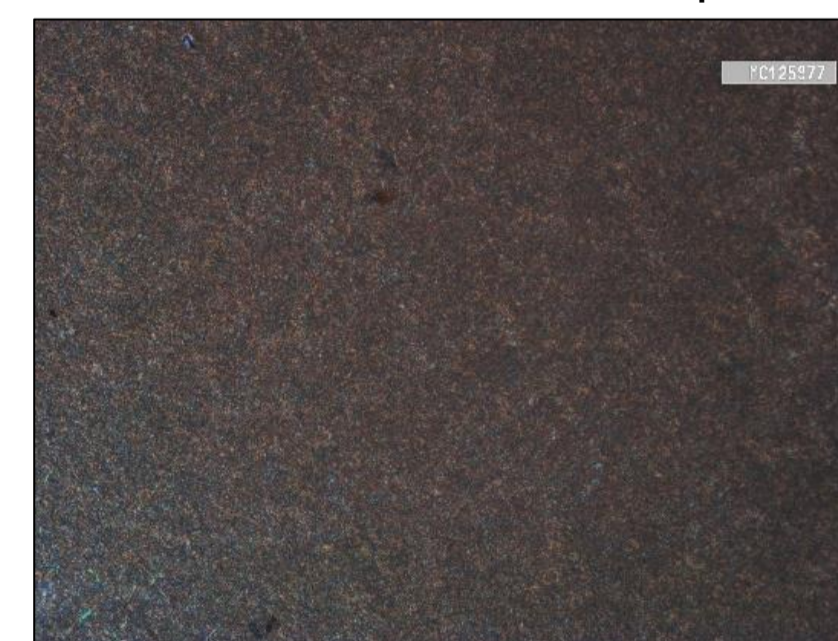
Optical photographs of synthesized molecule on cooling under optical polarization microscope



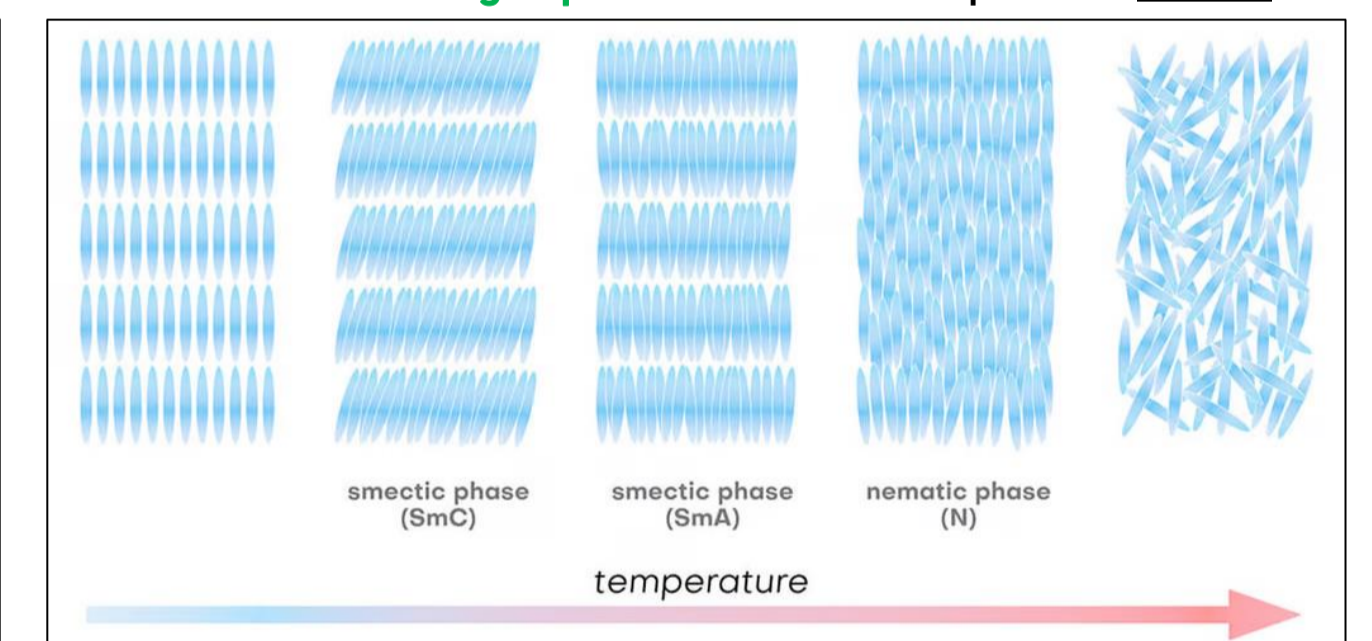
The focal-conic texture of N* phase at 190.1 °C



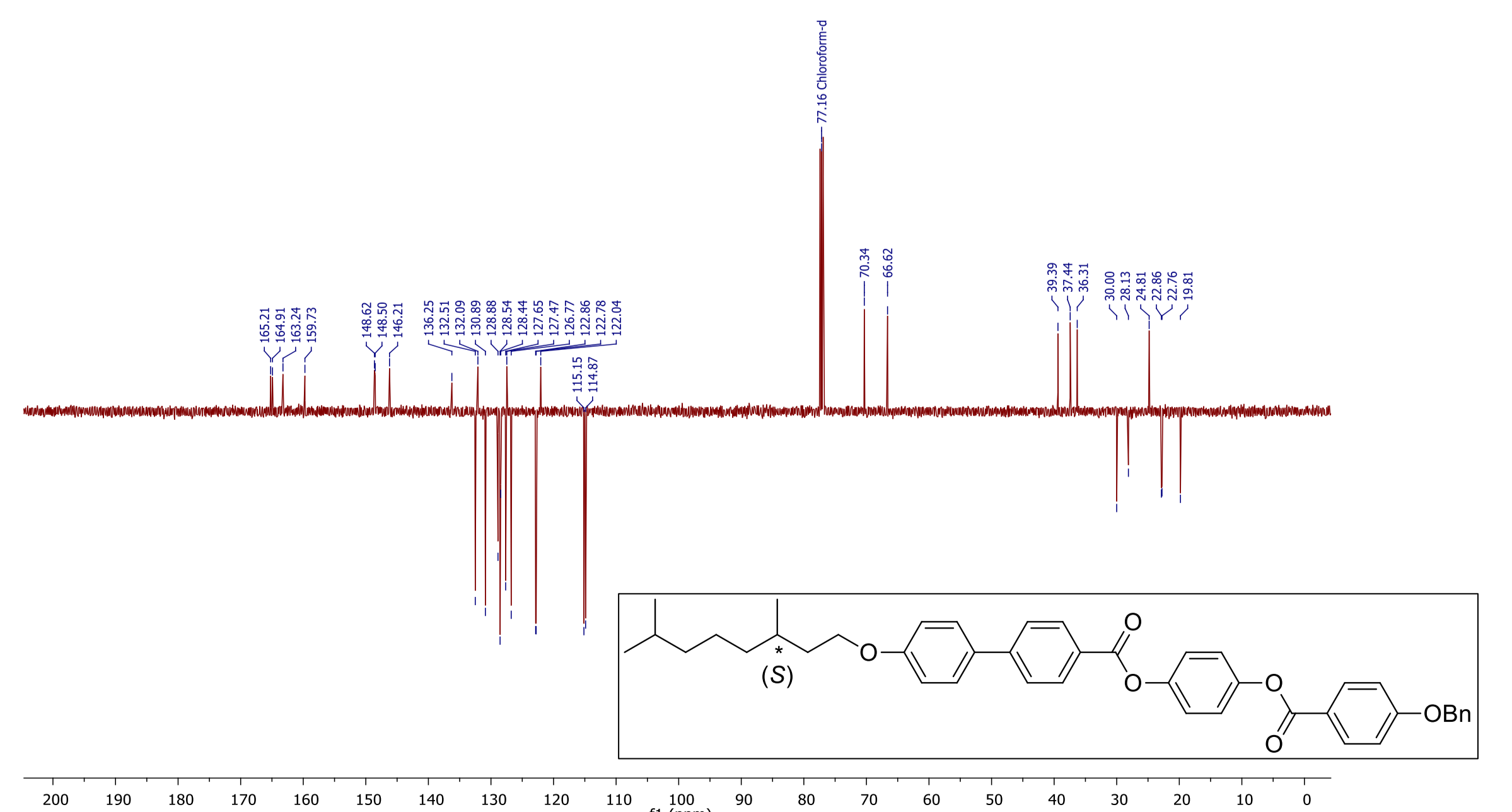
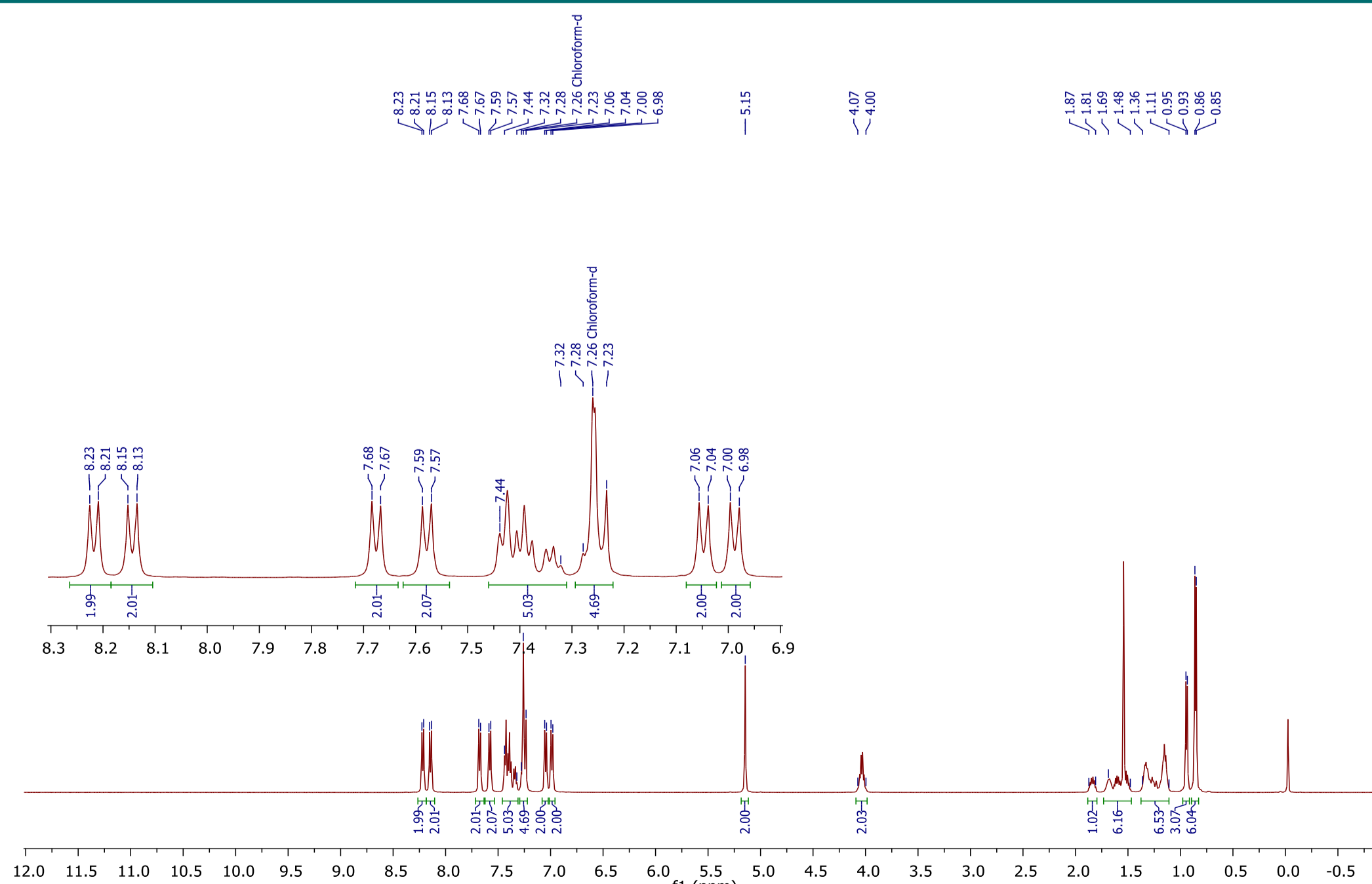
The finger-print texture of SmC* phase at 150.7 °C

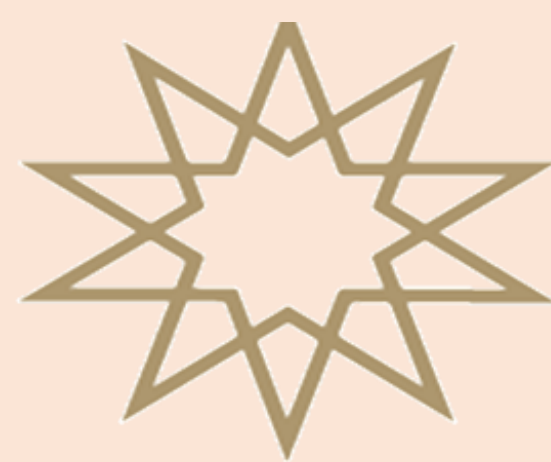


Crystalline state at 131.3 °C



CHARACTERIZATION

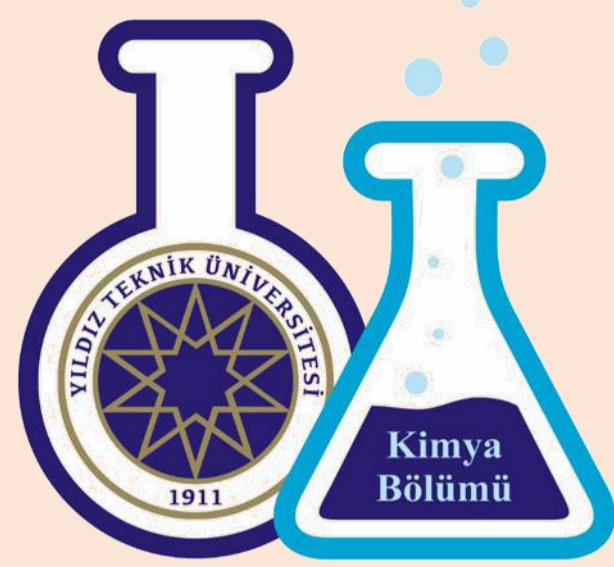




SYNTHESIS OF [E]-1-(4-((NAPHTHALEN-2-YLMETHYLENE)AMINO)PHENYL)ETHAN-1-ONE AND ITS INVESTIGATION OF PHOTOPHYSICAL AND PHOTOCHEMICAL PROPERTIES

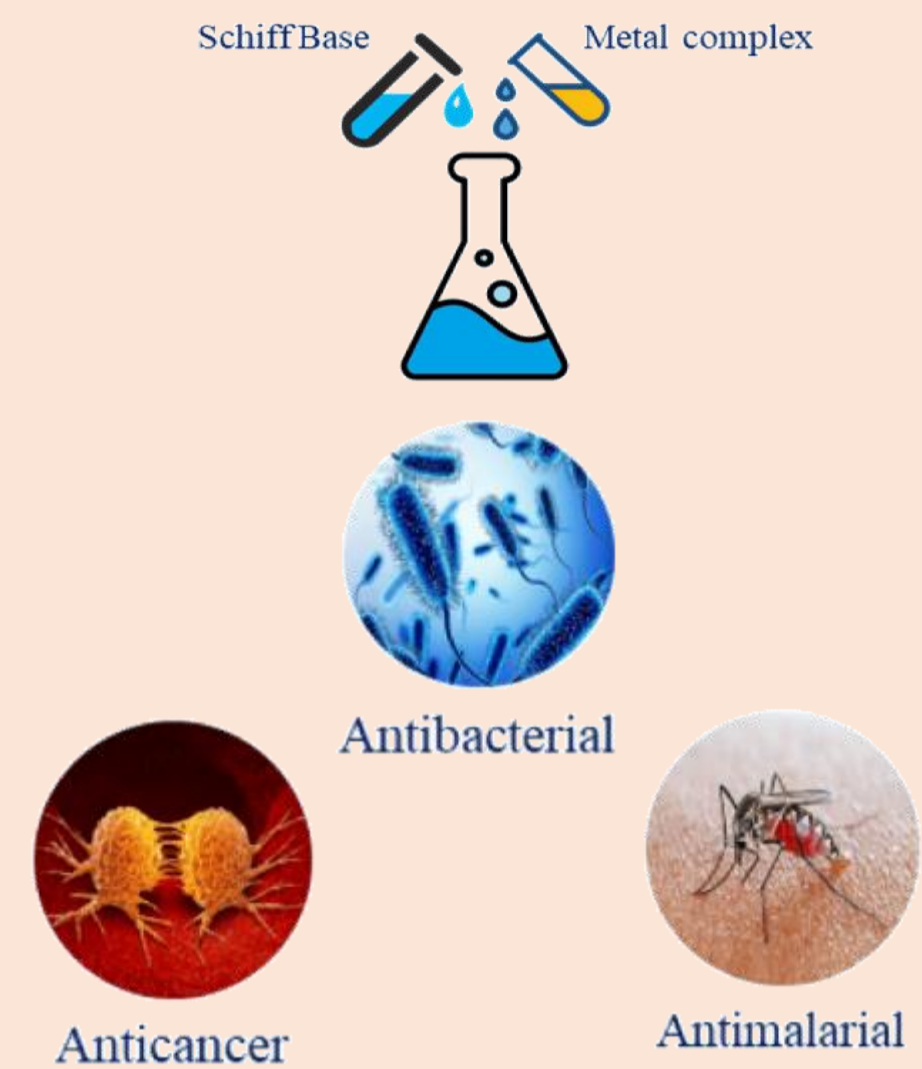
Cansu KILIÇUZAR 1802D030

Advisor: Prof.Dr.Nergis ARSU



ABSTRACT

The formation of the Schiff bases which was discovered by Hugo Schiff is another variation of nucleophilic addition to the carbonyl group, where the nucleophile is amine. Imine group of schiff bases can bind with different metal centers involving various coordination sites and allow formation of metal complexes of different geometries which are biologically active compounds. In this study a novel Schiff base [E]-1-4NMAPE-one was synthesized and its photophysical and photochemical properties were investigated. UV Spectroscopy, NMR, FTIR were used for the characterization. Photobleaching studies were performed with the synthesized Schiff base with NMDEA, 5200 seconds was sufficient for the Schiff base to totally get bleached. Formulation including the schiff base, NMDEA, TPGDA was prepared for UV-Curing and Photo-DSC measurements.



SYNTHESIS

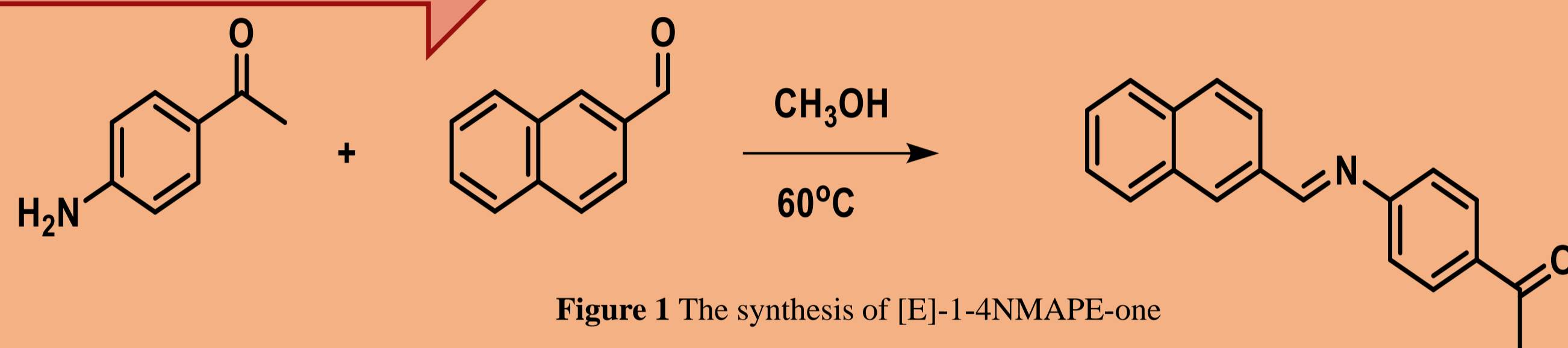


Figure 1 The synthesis of [E]-1-4NMAPE-one

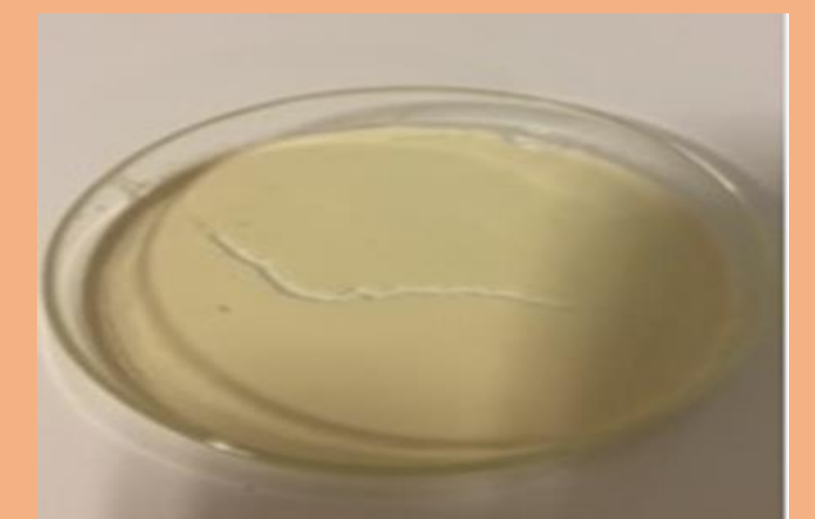


Figure 2 The precipitation process and the dried form of the Schiff base [E]-1-4NMAPE-one

CHARACTERIZATION STUDIES

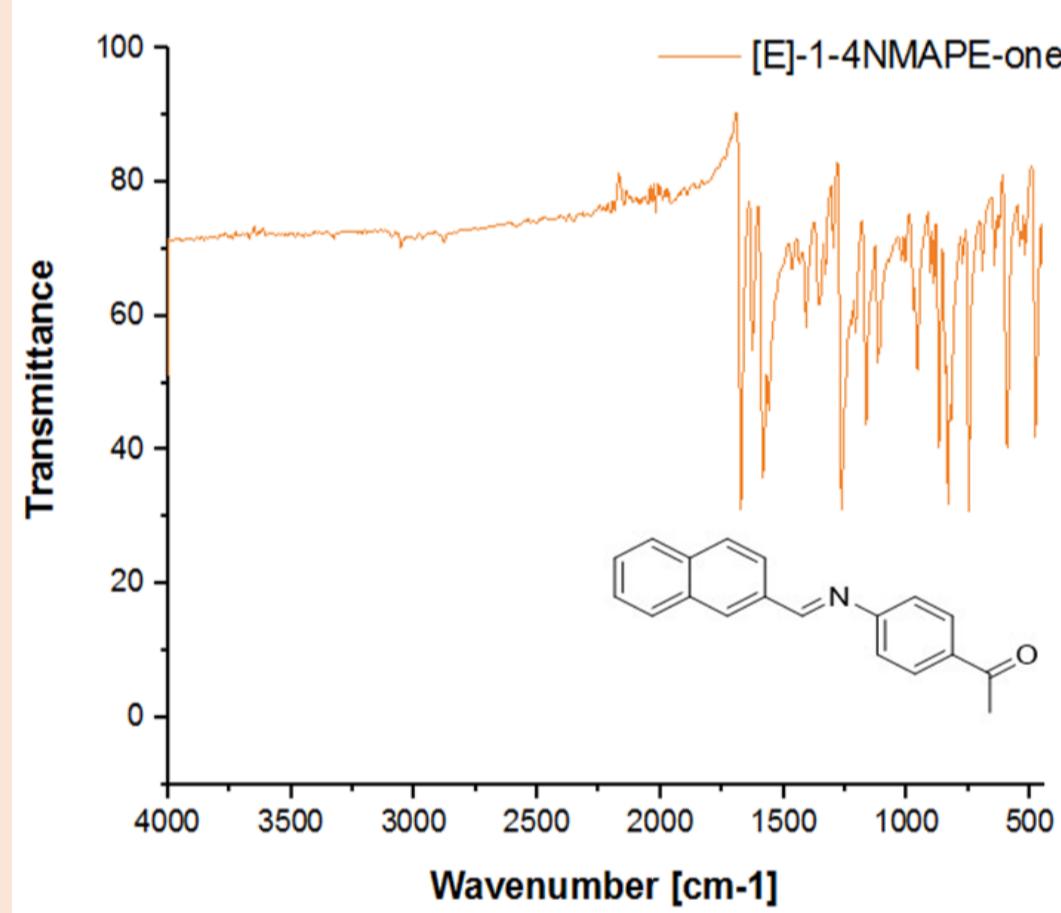


Figure 3 The FT-IR spectrum of [E]-1-4NMAPE-one

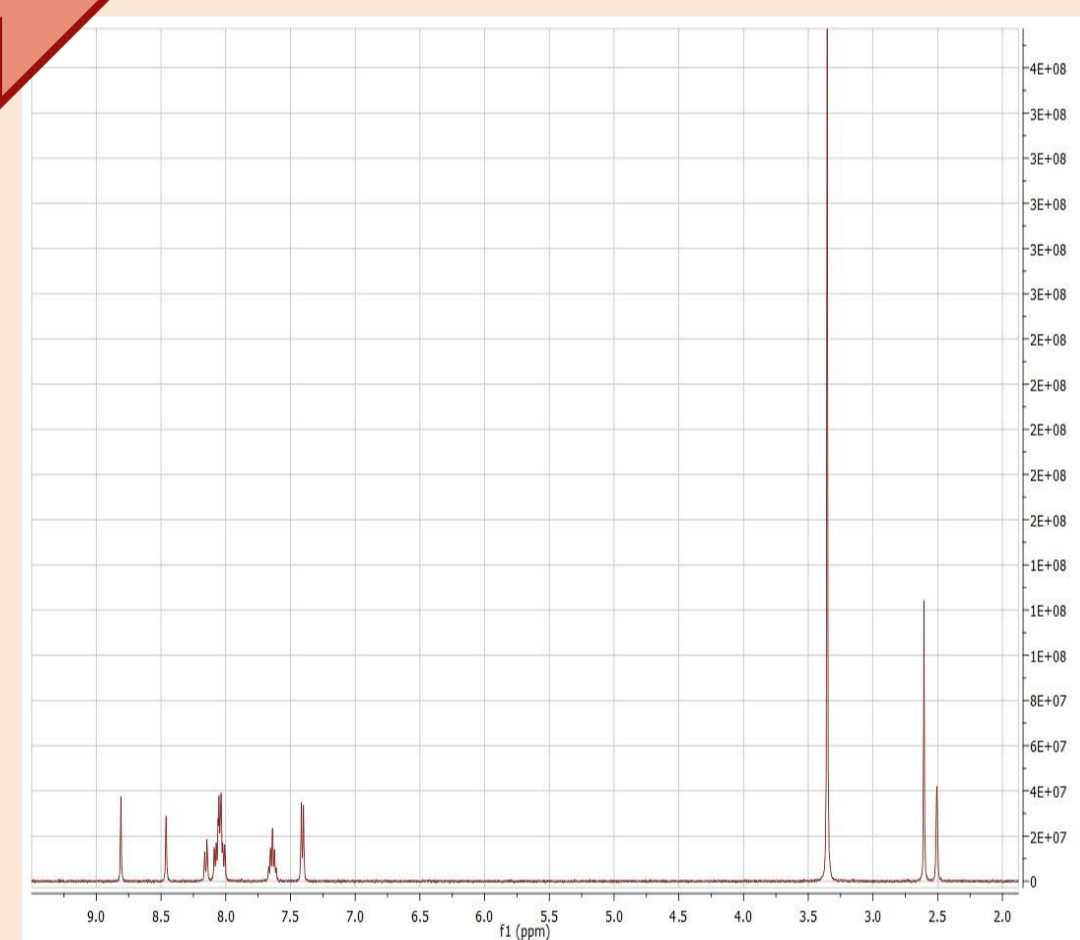


Figure 4 ¹H Nuclear magnetic resonance of [E]-1-4NMAPE-one (Solvent: DMSO-d₆)

PHOTOPHYSICAL PROPERTIES

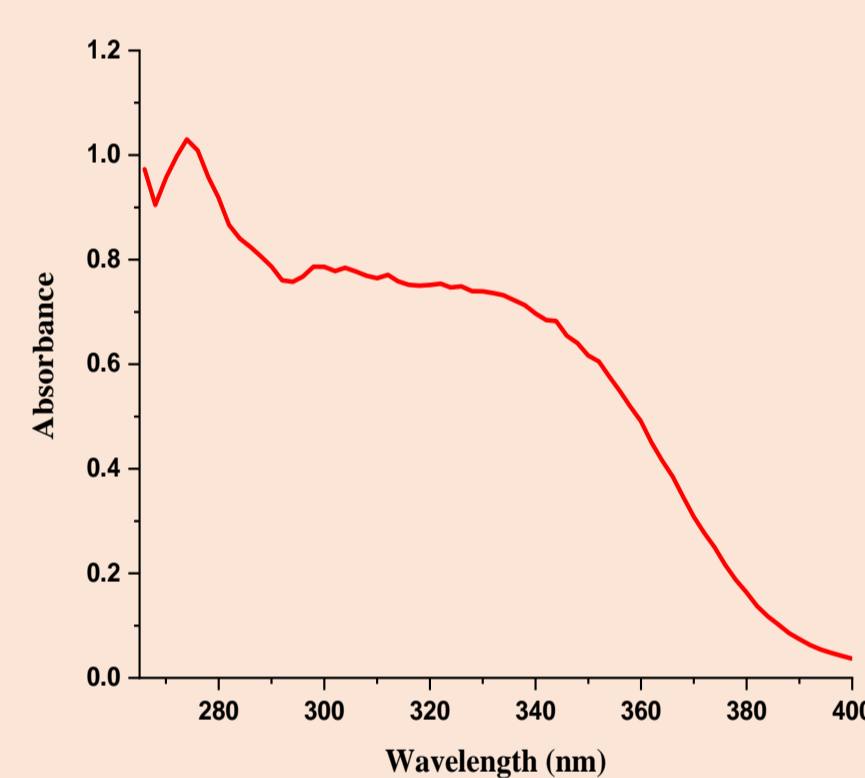


Figure 5 UV-Vis absorption spectrum of [E]-1-4NMAPE-one ($4 \times 10^{-5} \text{M}$) in DMF. Molar absorptivity coefficient was measured as $\epsilon = 9615 \text{ L} \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$ at 365nm.

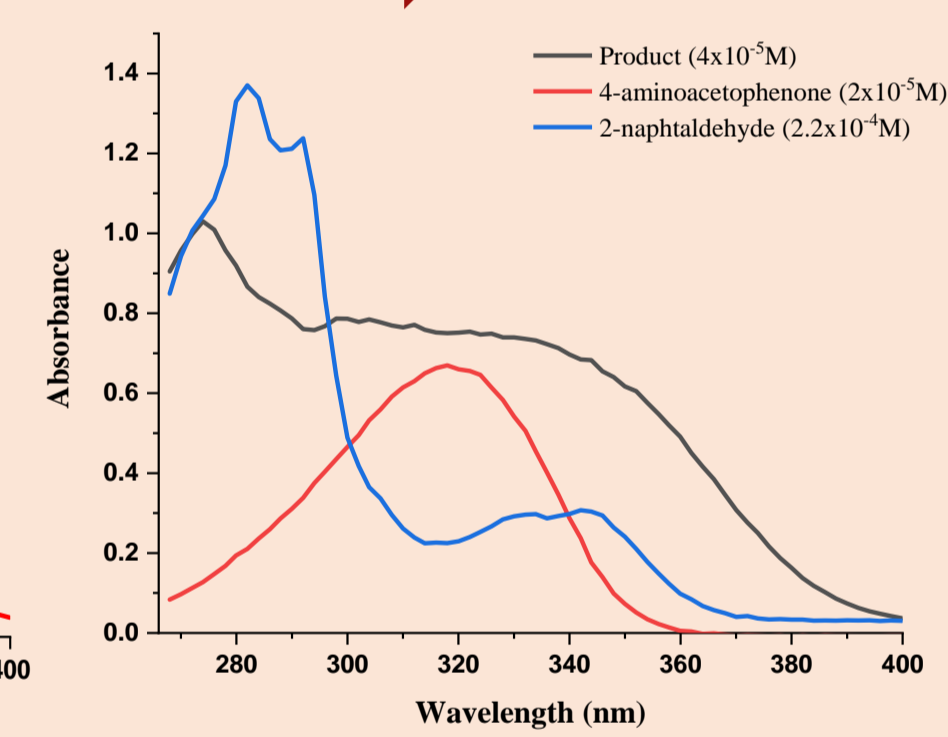


Figure 6 UV-VIS absorption spectrum of comparison of the reactants and the product. At 365nm, ϵ value for 4-aminoacetophenone is $74 \text{ L} \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$ and for 2-naphthaldehyde $257 \text{ L} \cdot \text{mol}^{-1} \cdot \text{cm}^{-1}$.

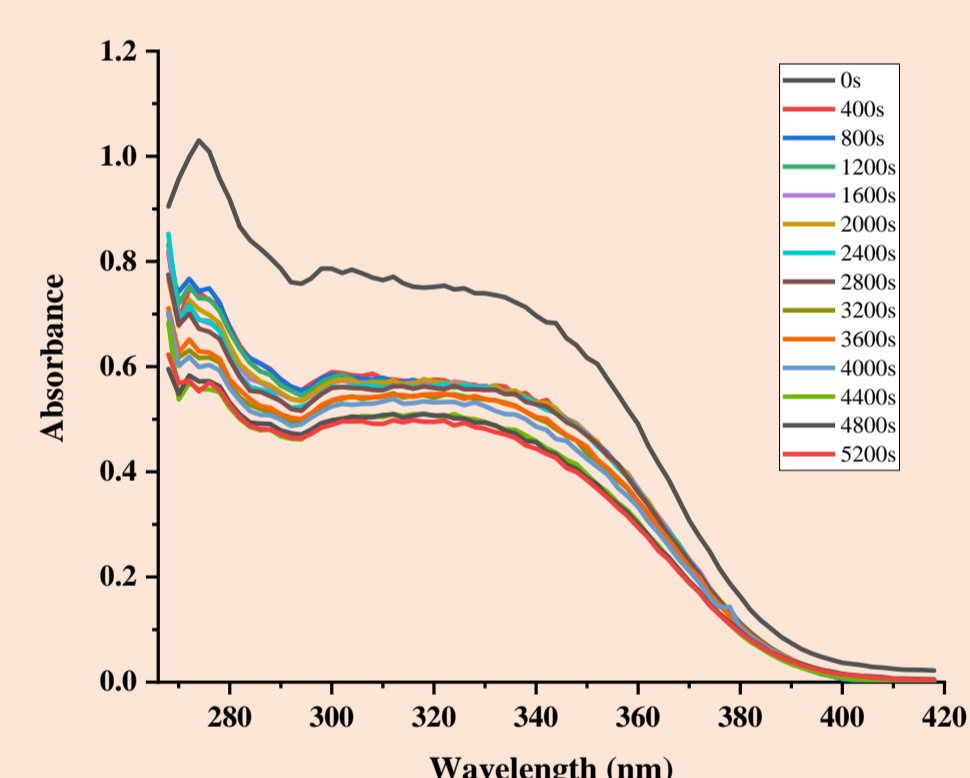


Figure 7 Photobleaching of $4 \times 10^{-5} \text{M}$ [E]-1-4NMAPE-one in the presence of NMDEA in DMF.

PHOTO-DSC STUDIES

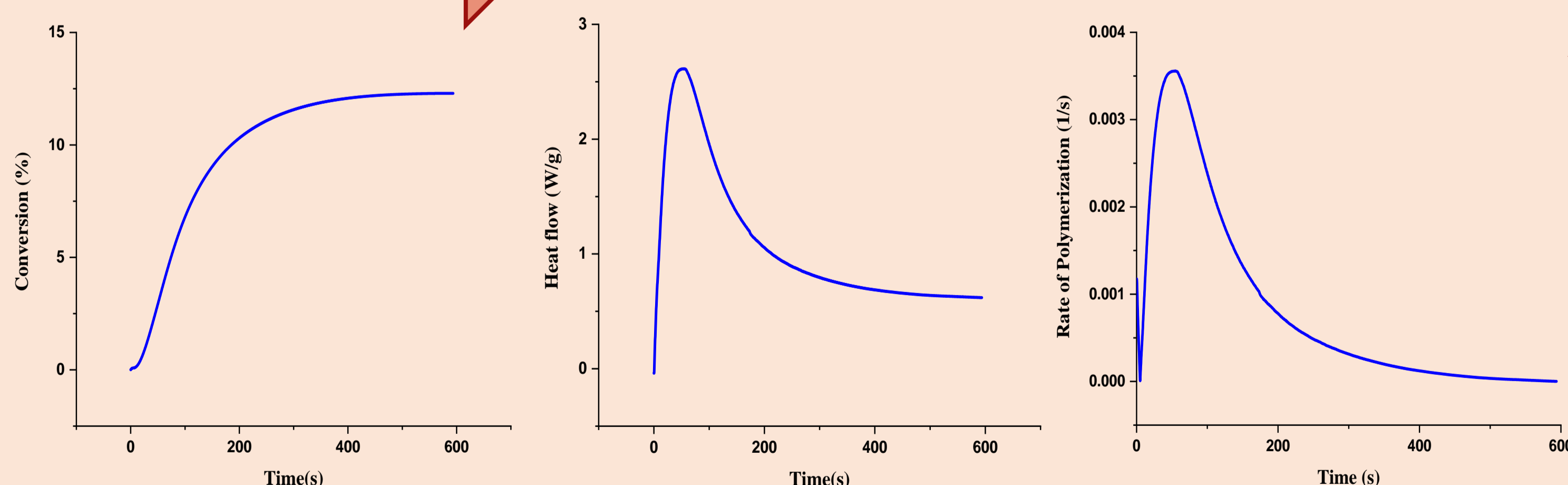


Figure 8 Photo - DSC results -the conversion %, the heat flow and the rate of polymerization- of the formulation of 0.1% w/w of [E]-1-4NMAPE-one, %99 TPGDA, %1 NMDEA.

SOLUTION PHOTOPOLYMERIZATION AND UV-CURING APPLICATION

Table 1 Photopolymerization of MMA (methyl methacrylate) in DMF in the presence of [E]-1-4NMAPE-one with and without NMDEA.

[PI]	NMDEA	Conversion %
10^{-3}M	10^{-2}M	—
10^{-4}M	10^{-3}M	—
10^{-3}M	—	—



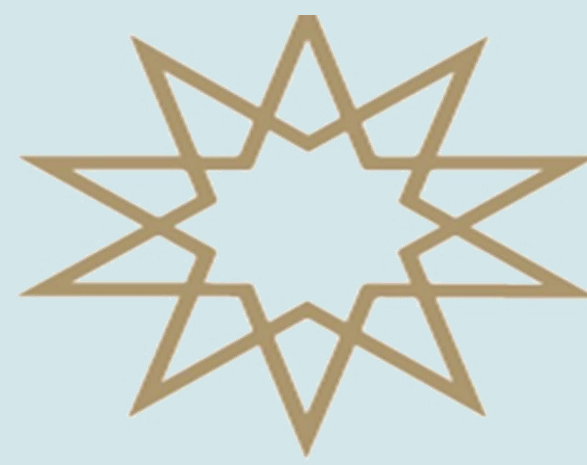
Figure 9 UV cured formulation of 0.1% w/w of [E]-1-4NMAPE-one, %99 TPGDA, %1 NMDEA and irradiation time is 135 seconds.

CONCLUSION

In this study a novel Schiff base synthesis was achieved. Photophysical properties such as UV-Vis absorption spectrum was recorded and high molar absorptivity value was calculated in the near visible region. Photolysis was performed in DMF with NMDEA during 5200s of irradiation time. Photopolymerization and Photo-DSC experiments were conducted both mono and diacrylates in the presence of [E]-1-4NMAPE-one with and without NMDEA. Possible pharmacological activities of this schiff base such as anticancer, antibacterial, antimicrobial, antiviral will be analyzed as future studies.

REFERENCES

- [1] Sadia, M., Khan, J., Naz, R., Zahoor, M., Shah, S. W. A., Ullah, R., ... & Sohaib, M. (2021). Schiff base ligand L synthesis and its evaluation as anticancer and antidepressant agent. *Journal of King Saud University-Science*, 33(2), 101331.
- [2] Nagar, S., Raizada, S., & Tripathi, N. (2023). A review on various green methods for synthesis of Schiff base ligands and their metal complexes. *Results in Chemistry*, 101153.
- [3] Adesina, A. D. (2022). Synthesis of Schiff Bases by Non-Conventional Methods. In *Schiff Base in Organic, Inorganic and Physical Chemistry*. IntechOpen.



TÜBİTAK 2209-A
PROJECT

SYNTHESIS OF NOVEL TETRAZINE DERIVATIVE COMPOUND AND DETERMINATION OF THEIR ANTIFUNGAL ACTIVITIES

ZEHRA YILDIZ KÖK 19024081

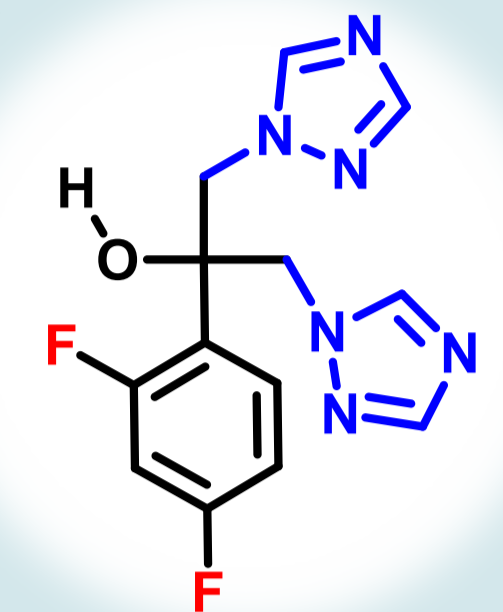
Assoc. Prof. ÖMER TAHİR GÜNKARA

ABSTRACT

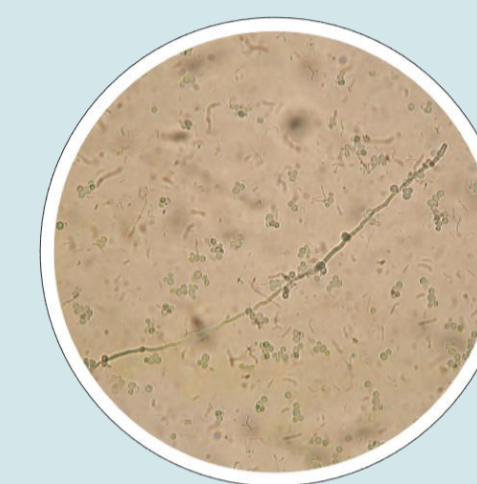
Fungi are unicellular or multicellular eukaryotic organisms that also include microorganisms such as yeast and mold. Fungi are one of the microorganisms that people are frequently exposed to today. Thousands of fungal species can cause infection in humans. The fact that fungi cause illness or death to millions of people worldwide despite existing treatments is related to the inadequacy of drugs and the resistance of fungi to existing drugs. For this reason, antifungal drug development studies continue. Heterocyclic compounds are used as pharmaceutical raw materials or as starting materials in syntheses. Heterocyclic compounds are also used in the production of drugs for fungal diseases. Novel tetrazine and their derivatives can be synthesized by ring-closing reactions of haloamides and azides. Nitrogen-containing cyclic compounds have a very important place in biological activity. The fluconazole molecule, which is one of the important members of the antifungal drug class and contains nitrogen and fluorine atoms in its structure, is effective on fungi. In this thesis study inspired by the fluconazole molecule; A tetrazine derivative, which is not included in the literature, contains fluorine and heterocyclic structure in its structure, is pharmacologically important and has antifungal effect, has been synthesized.



Flucon



Fluconazole



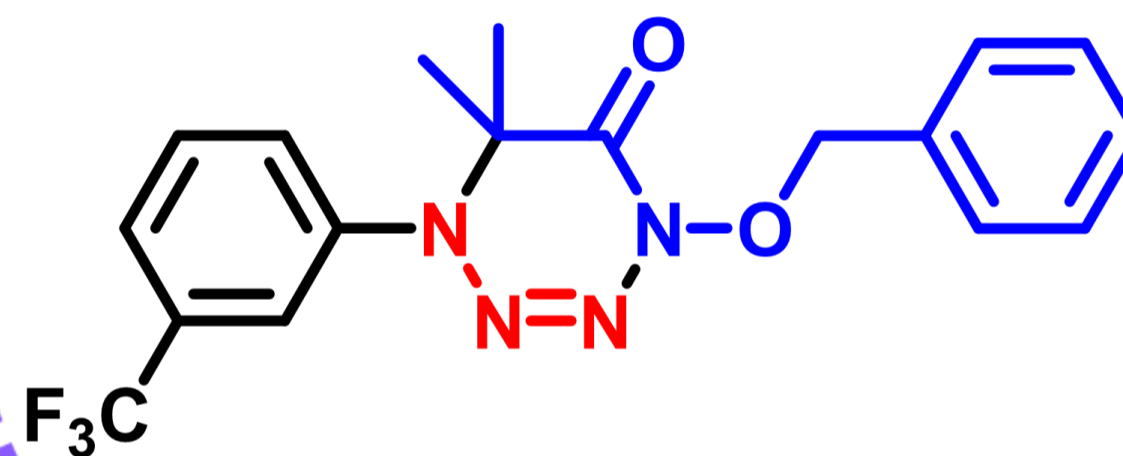
Candida
albicans

The most common fungal cell that causes infections today is *Candida albicans*. *Candida albicans* can cause infection in the mouth (thrush), vagina (vaginal candidiasis), places where the skin folds (hips, armpits), between the fingers and around the lips.

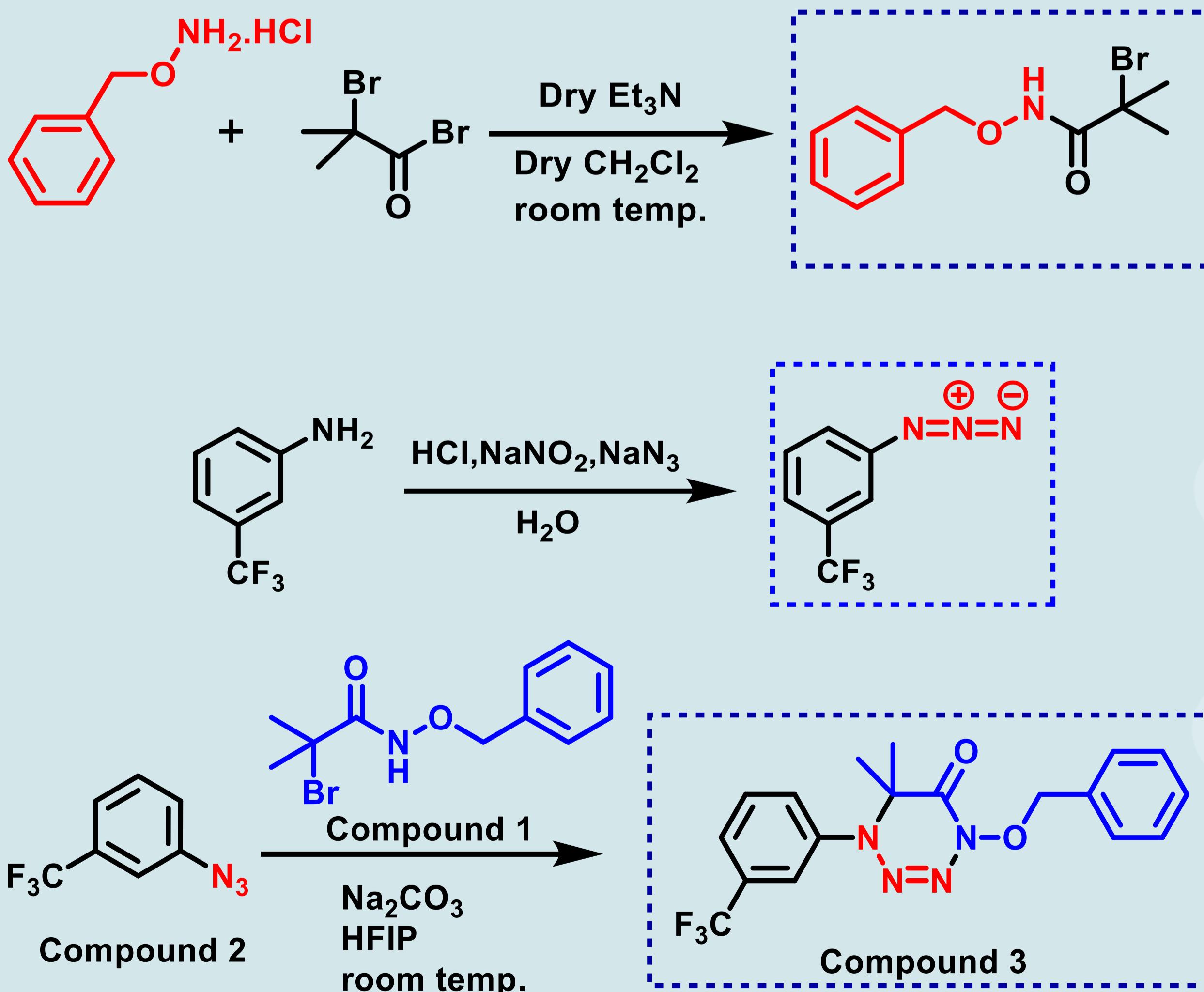
METHOD

The reaction will be carried out in the Schlenk system. Weighed *N*-(benzyloxy)-2-bromo-2-methylpropanamide (Compound 1) (0.375 mmol), 1-azido-3-(trifluoromethyl) benzene (Compound 2) (0.25 mmol) and Na₂CO₃ (0,75 mmol) are placed sequentially in the Schlenk tube. The air in the tube is removed with the help of vacuum and the entire tube is filled with nitrogen gas. 1.0 mL of hexafluoro isopropanol (HFIP) solvent is added to the reaction medium. The reaction mixture is stirred under nitrogen at room temperature for 12 hours. The reaction is terminated according to the TLC result and filtered through celite. The solvent is removed under vacuum. Yield 11%.

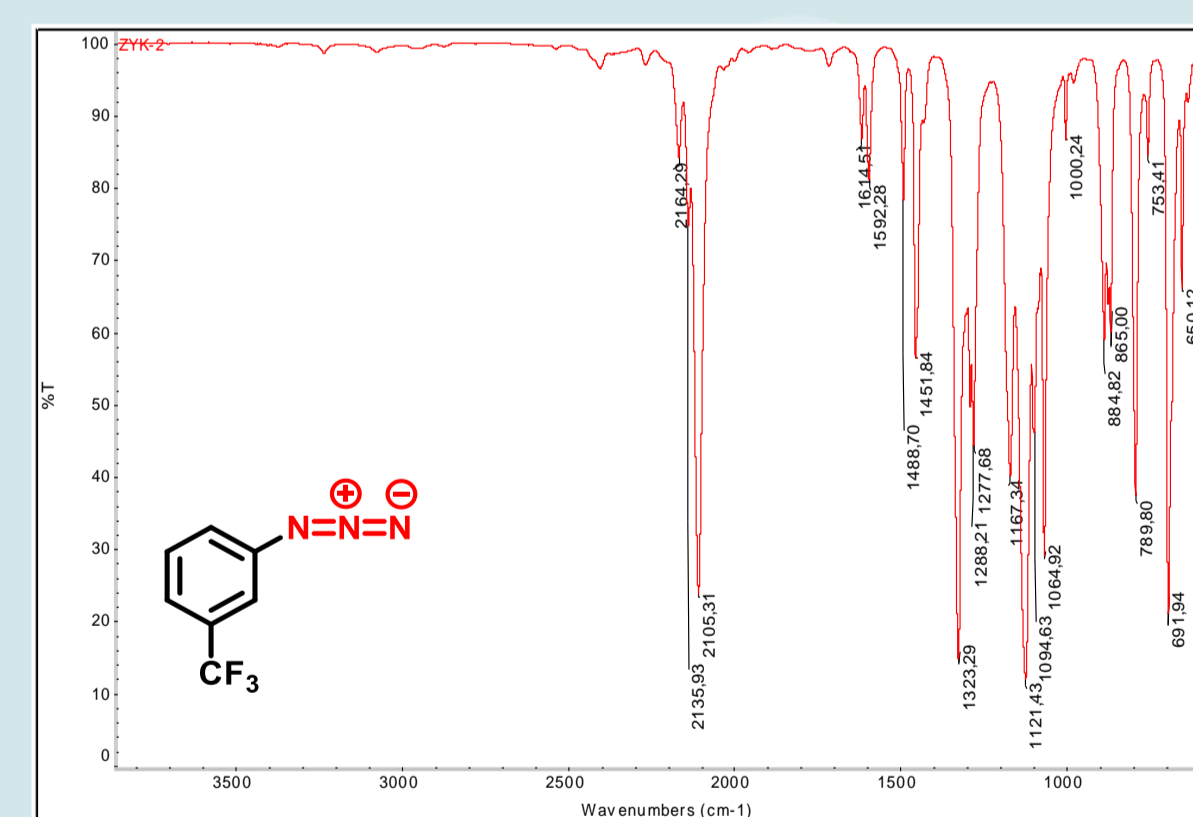
COMPOUND-3



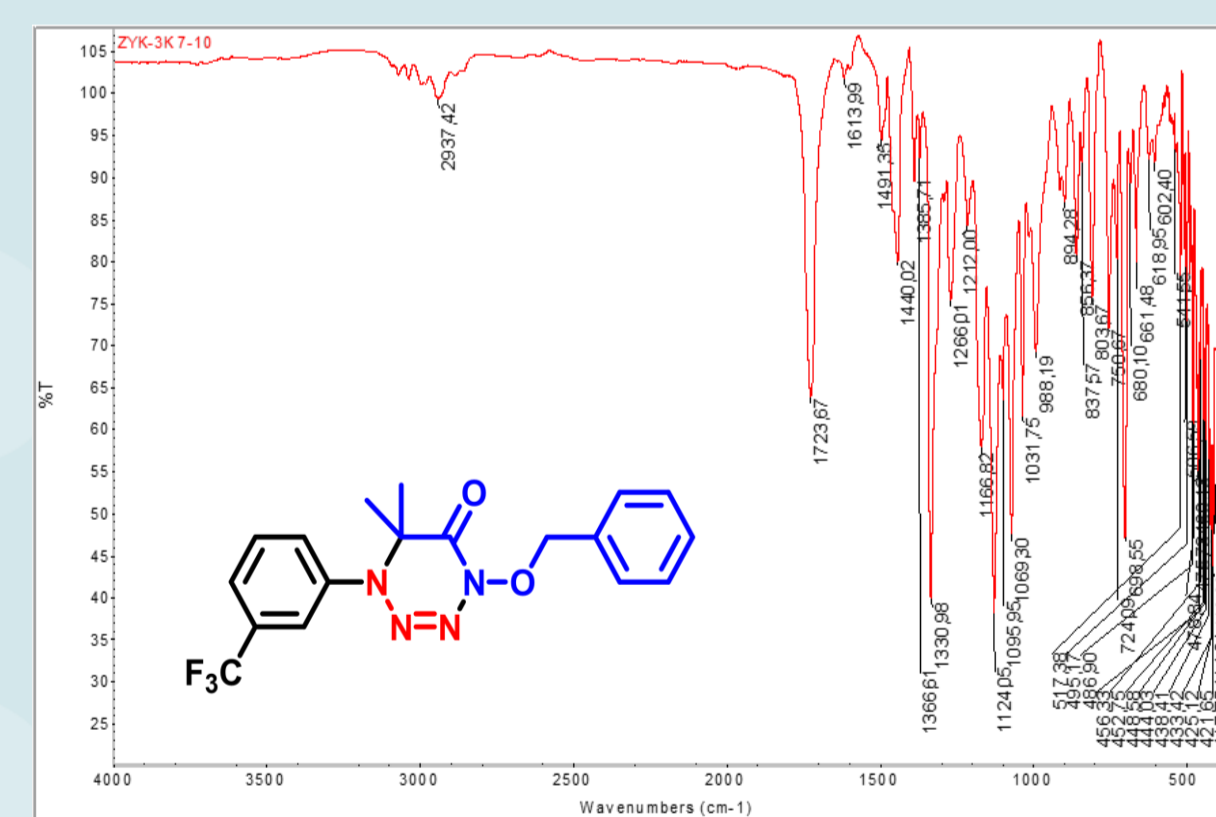
SYNTHESIS



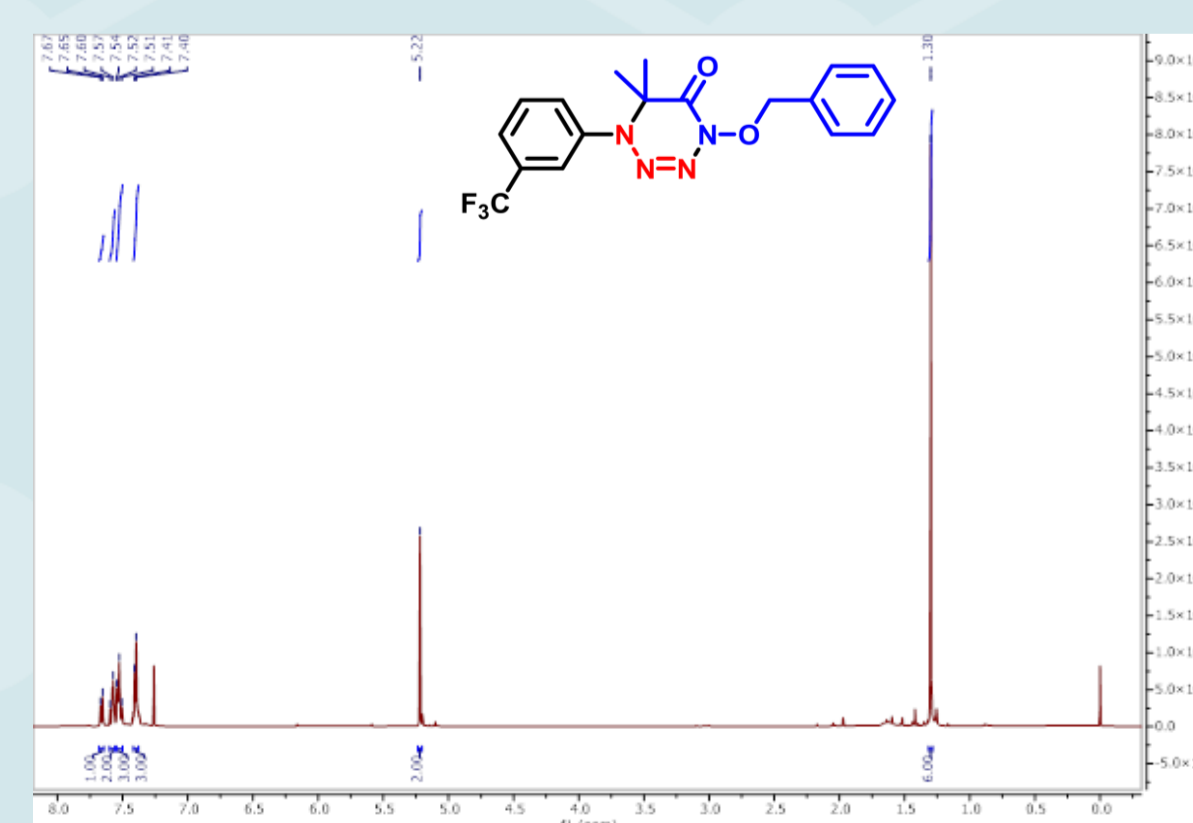
RESULTS



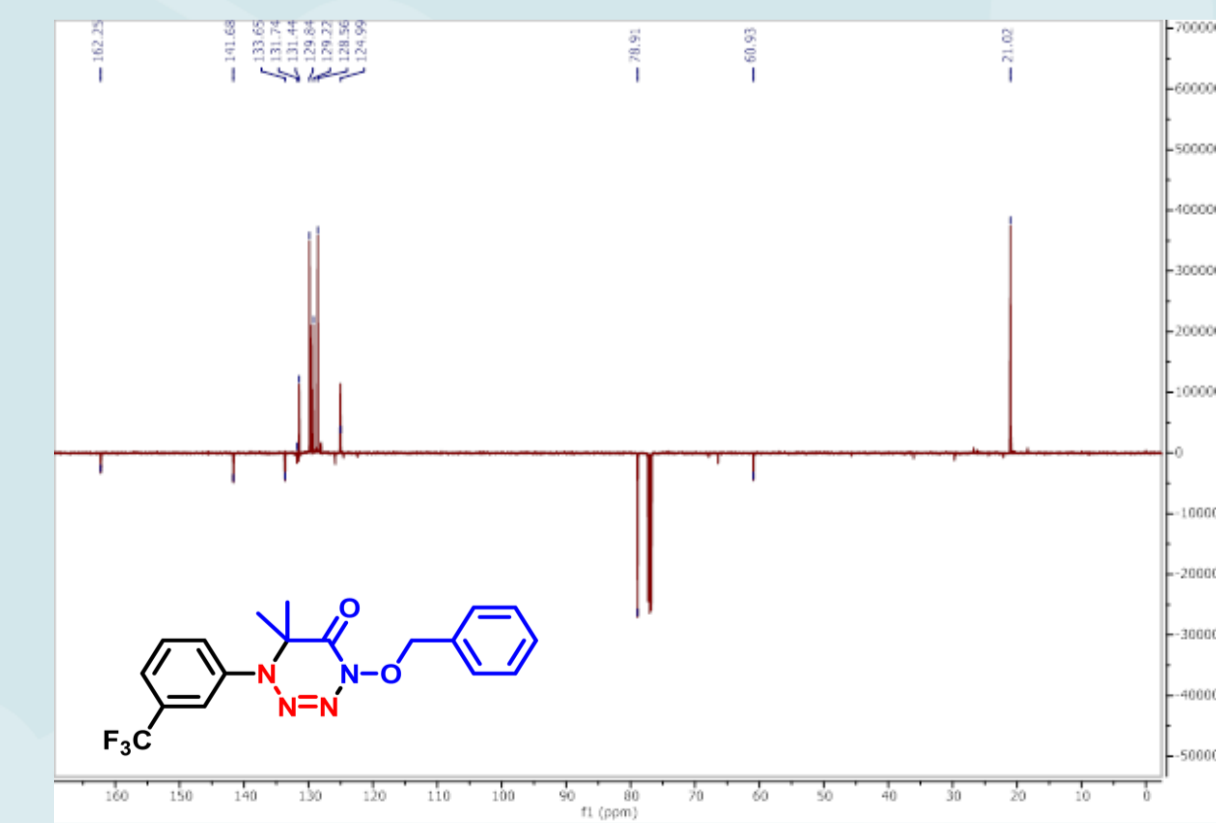
IR(ATR) Spectrum of Compound-2



IR(ATR) Spectrum of Compound-3



¹H-NMR Spectrum of
Compound-3 (CDCl₃)



¹³C-NMR (APT) Spectrum of
Compound-3 (CDCl₃)

CONCLUSION

In this study, a new tetrazine derivative was synthesized and its structure was characterized based on spectral data such as FTIR, ¹H NMR, ¹³C NMR (APT), respectively. Anti-fungal activity studies of the new derivative are ongoing. I would like to thank Prof. Dr. Tülin ÖZBEK and Mustafa YOĞURTCU from the Department of Molecular Biology and Genetics for their support in antifungal studies.

REFERENCES

- [1] Eyllcim, O., Gunay, F., GÜNKARA, Ö. T., Ng, Y. Y., Uluçan, O., & Erden, I., (2023). Design and synthesis of novel 1,2,3,4-tetrazines as new anti-leukemia cancer agents. *Chemical Biology and Drug Design*, vol.102, no.5, 1186-1201.
- [2] Arora, P., Arora, V., Lamba, H. S., & Wadhwa, D. (2012). Importance Of Heterocyclic Chemistry: A Review. *IJPSR*, 3(9), 2947-2954.
- [3] Cowen, L. E., Sanglard, D., Howard, S. J., Rogers, P. D., & Perlin, D. S. (2015). Mechanisms of Antifungal Drug Resistance. *Cold Spring Harbor Perspectives in Medicine*, 5(7), a019752.