



تقييم تحويل الزيوت النباتية المحفزة بواسطة النيكل الثنائي المدعوم بحمض لويس لإنتاج عوامل مضادة
لمسببات الأمراض من خلال نمذجة العلاقة بين التركيب والنشاط

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Lewis Acid-Supported Ni(II)-Catalyzed conversion of vegetable oils for
producing anti-pathogen agents and evaluated by structure-activity modeling.

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(تاريخ الاستلام: 2026/5/20م، تاريخ المراجعة: 2026/5/29م، تاريخ القبول: 2026/7/12م)

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Abstract:

Redox-active transition metal catalysts such as Pd(II), Fe(II), and Ni(II) are well known to cooperate with Lewis acids in the functionalization of organic molecules and the synthesis of pharmaceutical candidates. This study focuses specifically on Ni(II) catalysts within an advanced synthetic framework. We demonstrate that $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ -catalyzed isomerization, enhanced by the Lewis acidity of $\text{Zn}(\text{Otf})_2$, promotes the hydrogenation of olefins as a key step. While bivalent metal catalysts like Pd(II), Fe(II), or Ni(II) alone show limited activity, the combination of Ni(II) with alkali-earth-modified Lewis acids (e.g., Al^{3+} , Sc^{3+} , or Zn^{2+}) significantly improves catalytic efficiency. Notably, Ni(II)/alkali-earth-modified zeolites catalyze alkene dimerization even in the absence of redox metals such as Cu^{2+} or Brønsted acids. The resulting products were characterized by NMR, GC, and GC-MS, and reaction kinetics were monitored by GC and UV-vis spectroscopy. The inclusion of alkali-earth modifiers substantially enhanced Ni(II)-catalyzed isomerization and dimerization of vegetable oils. These catalytic modifications yield high-value intermediates with potential efficacy as antipathogenic agents, as evaluated by in vitro assays.

Keywords: vegetable oils, Homogeneous-catalysis, Coordination, Membrane disruption, dimerization.

المخلص:

من المعروف أن المحفزات المعدنية الانتقالية النشطة في تفاعلات الأكسدة والاختزال، مثل البلاتينيوم (II) والحديد (II) والنيكل (II)، تتعاون بشكل قوي مع أحماض لويس في إضافة المجموعات الوظيفية إلى الجزيئات العضوية وخاصة في تخليق المركبات الصيدلانية. تركز هذه الدراسة تحديداً على محفزات النيكل (II) ضمن إطار تخليقي متطور، ونود التوضيح أن عملية التماثل المحفزة بواسطة كلوريد النيكل الثنائي المائي $[\text{NiCl}_2 \cdot 6\text{H}_2\text{O}]$ ، والمعززة بحموضة لويس لـ الزنك ثلاثي فلورو ميثان سلفونات $[\text{Zn}(\text{Otf})_2]$ ، والتي تعزز هدرجة الأوليفينات كخطوة أساسية. في حين أن استخدام المحفزات المعدنية ثنائية التكافؤ مثل البلاتينيوم أو الحديد أو النيكل منفردة، تُظهر نشاطاً محدوداً للغاية. لكن من خلال دمج النيكل (II) مع أحماض لويس المعدلة بعناصر قلوية ترابية خاصة مع الألمنيوم، السكندينيوم، أو الزنك يُحسن الكفاءة التحفيزية بشكل ملحوظ. تجدر الإشارة إلى أن الزيوليتات المعدلة بالنيكل (II)/الفلزات القلوية الترابية تحفز عملية ازدواج الألكينات حتى في غياب المعادن المؤكسدة والمختزلة مثل أيونات النحاس الثنائي Cu^{2+} أو أحماض البرونستد H^+ . وقد تم توصيف المنتجات الناتجة من التفاعلات باستخدام تقنيات الرنين المغناطيسي النووي NMR، والكروماتوغرافيا الغازية (GC)، والكروماتوغرافيا الغازية مع مطياف الكتلة (GC-MS). تمت مراقبة حركية التفاعل باستخدام الكروماتوغرافيا الغازية ومطيافية الأشعة فوق البنفسجية والمرئية. وقد أدى إضافة الفلزات القلوية الترابية إلى تعزيز كبير لعملية التماثل والازدواج المحفزة بالنيكل (II) للزيوت النباتية. تنتج عن هذه التعديلات التحفيزية وسائط عالية القيمة ذات فعالية محتملة كعوامل مضادة للميكروبات الممرضة، تم تقييمها من خلال الفحوصات المخبرية والنمذجة الحاسوبية، بما في ذلك التفاعلات الحيوية الجزيئية باستخدام نموذج الالتحام الجزيئي.

الكلمات المفتاحية: الزيوت النباتية، التحفيز المتجانس، التنسيق، النمذجة الحاسوبية، التضاعف.

1. Introduction

Linear alkenes like vegetable oils are ubiquitous renewable feedstocks utilized extensively in the food, cosmetic, and chemical industries. Their utility is largely defined by the degree of unsaturation (carbon-carbon double bonds) present in their fatty acid chains (Lligadas et al., 2010). While unsaturation natural products are essential oils for industrial nutritional benefits (Chaura et al., 2026), it renders the oils susceptible to oxidative rancidity and limits their thermal stability (Biermann et al., 2021). Consequently, partial hydrogenation/isomerization is a critical industrial process employed to increase the melting point and oxidative stability of these oils (Biermann et al., 2021). However, conventional hydrogenation processes often lack selectivity and can lead to the formation of undesirable trans fatty acids, prompting the search for more controlled catalytic systems (Hassan, 2007). This study investigates the use of non-redox metal ions, functioning as Lewis acids, to modulate the activity and selectivity of a nickel(II) catalyst for the hydrogenation of functionalized olefines, aiming for improved product quality (Klausfelder & Kempe, 2023).

Nickel and alkali-earth-modified based zeolites catalyze catalysts accelerated the dimerization of linear alkenes. Raney nickel and nickel(0/II) complexes are environmentally friendly, vital, and therapeutics, including Ni(II)Cl₂ facilitates key C-C and C-heteroatom cross-coupling reactions in drug synthesis (Derosa et al., 2020) (Ehrmaier et al., 2019). They contributed to the synthesis of complex as biologically active molecules (e.g., 3-functionalized 4-hydroxycoumarins) following the mechanism of Suzuki/Heck reactions and hydrogenation, often under milder/light-activated and aqueous conditions (Al-Qadisy et al., 2021; Ebrahim et al., 2023).

Hetero-organometallic LA/Ni(II) catalysis represents an advanced level in drug-molecular synthesis, focusing on catalytic complexes that involve Ni-heteroatom bonds (such as M-S, M-O, M-N, M-P, or M-Si) and/or traditional metal-carbon (M-C) bonds. While the Ni(II)/alkali-earth-modified zeolite catalyst is applied in the catalytic coupling formation of C-C or C-H bonds (Senan et al., 2026; Zheng et al., 2014). Use Ni(II)/LA catalysis more broadly in pharmaceutical synthesis, not just for traditional cross-couplings, including a dimerization pathway that enables direct heteroatom incorporation (e.g., N, O, S) into organic frameworks. One of the industrial procedures is direct functionalization of molecules and streamlined access to potential drug candidates. Using inexpensive Lewis acids (e.g., ZnCl₂, AlCl₃, BF₃, or lanthanides), recyclable or heterogeneous LA would be preferred (Zheng et al., 2014). In parallel with the application of this catalytic system in industrial processing, the biological activity of metal complexes has garnered significant attention. The structural complexity introduced by partially isomerized/hydrogenated olefins and their potential to interact with biological membranes. This research evaluates the antipathogenic efficacy of chemicals from catalytic systems and, through catalytic modification combined with biological screening in pharmaceutical synthesis, establishes a dual-purpose application that unlocks Lewis acid-assisted nickel catalysis.

2. Materials and Ni(II) catalyzed vegetable oils

2. 1. Chemical materials

All chemicals were purchased from commercial suppliers and arranged in the laboratory store; (9Z,12Z)-octadecadienoic acid methyl ester (Methy linoleate -ML), linolic acid, olic acid, methyl olate and linolenic acid were purchased from (Aladdin Ltd., Shanghai, China). Ni-Dichloride hexahydrate

($\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$), Bis(cyclooctadiene)nickel [$\text{Ni}(\text{COD})_2$] and Iron (III) citrate monohydrate ($\text{C}_6\text{H}_5\text{O}_7 \cdot \text{H}_2\text{O}$) and ferrous chloride tetrahydrate ($\text{FeCl}_2 \cdot 4\text{H}_2\text{O}$) were purchased from (Nanjing Chemlin Chemical Co., Ltd.), (FeCl_3) was purchased from (Aladdin Ltd., Shanghai, China) and, $\text{Ba}(\text{OTf})_2$, $\text{Zn}(\text{OTf})_2$, $\text{Y}(\text{OTf})_3$ and $\text{Sc}(\text{OTf})_3$ the others Lewis acids were purchased from (Accela Chembio Co., Ltd., Shanghai, China), methanol (MeOH) and dichloromethane (DCM): (Sinopharm Chemical Reagent Co., Ltd., Shanghai, China). NMR was performed on an AV400 MHz instrument (Bruker, Beijing, China). Using the GC (HP-1, DB-1, CP-Sil 5 CB-) column for analysis. Gas chromatography (GC) analysis a 9750 GC (Fuli, Zhejiang, China), GC-MS analysis is Agilent-B-WAX spectrometer utilized for determine the products and UV-Vis spectra were recorded on an Analytikjena-specord 205 UV-Vis spectrophotometer (Senan, Zhang, Zeng, et al., 2017).

2.2 Functionalization vegetable oils (e.g., the original methyl-linoleate) were reacted under hydrogen pressure (10 atm) at 70-90 °C in the presence of a Ni-based catalyst (2 mM,). Various Lewis acids List them, e.g., LiBH_4 , AlCl_3 , $\text{Zn}(\text{OTf})_2$, $\text{Ba}(\text{OTf})_2$, $\text{Sc}(\text{OTf})_3$ and SiO_2 were added as promoters. The 100 mM of Methyl Progress of this reaction was monitored by advanced analytical methods such as NMR, and GC-MS spectroscopy. The result of ^1H NMR spectra with chemical shifted, δ 5.4 – 5.10 (m, 4H vinylic), 3.93 (s, 3H, O- CH_3), 2.7 (t, signal of bis-allylic proton, 2H), [2.30 (t, $J = 7.6$ Hz, 2H, OCCH_2), 2.05 (q, $J = 6.8$ Hz, 4H) allylic], 1.69 – 1.55 (m, 2H, OCCH_2CH_2), 1.40 – 1.24 (m, 14H, $-(\text{CH}_2)_7$), 0.89 (t, $J = 6.8$ Hz, 3H, CH_3CH_2), in **figure 1**.

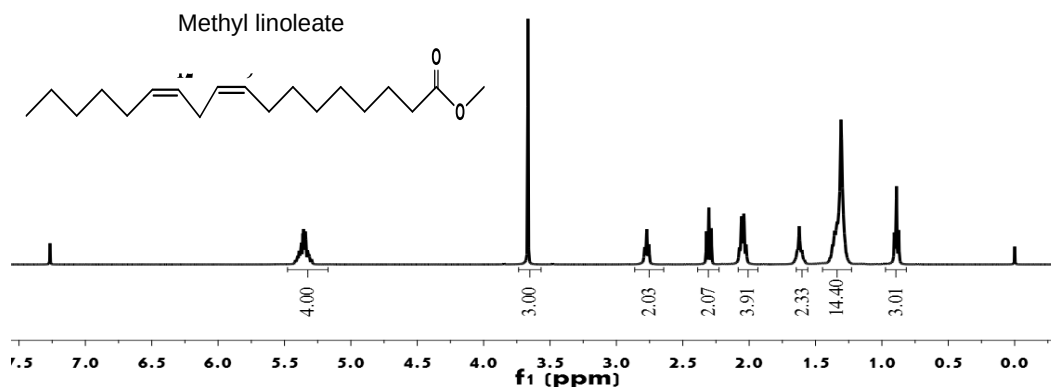


Figure 1. ^1H NMR spectra of original methyl linoleate (SOY-oils) substrate ^1H NMR (400 MHz, CDCl_3) (Senan, Zhang, Zeng, et al., 2017).

Using $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ (11.88 mg, 0.05 mmol) and $\text{Zn}(\text{OTf})_2$ (36.4 mg, 0.10 mmol) were dissolved in 3 mL of acetonitrile t. BuOH (9:1, v/v) in a glass tube; methyl linoleate (53.0 mg, 0.30 mmol) was added to the above solution, and the reaction mixture was magnetically stirred at 110 °C in an oil bath for 9 h. Conjugated diene mixtures as the total products were determined by GC analysis with an internal standard method. Next, the solvent was removed under reduced pressure, and the remaining mixtures were dissolved in CH_2Cl_2 . The result is determined by NMR, and ^1H NMR (400 MHz, CDCl_3) δ 5.99 (d, $J = 13.8$ Hz, 1H), 5.74 – 5.46 (s, 1H), 5.46 – 4.85 (m, 2H), 3.66 (s, 3H), 2.30 (t, $J = 7.5$ Hz, 2H), 2.07 –

1.92 (m, 4H), 1.61 (dd, $J = 15.7, 8.8$ Hz, 2H), 1.42 – 1.20 (m, 16H. $-(CH_2)_8$), 0.89 (dd, $J = 13.4, 7.1$ Hz, 3H, CH_3CH_2) **Figure 2.**

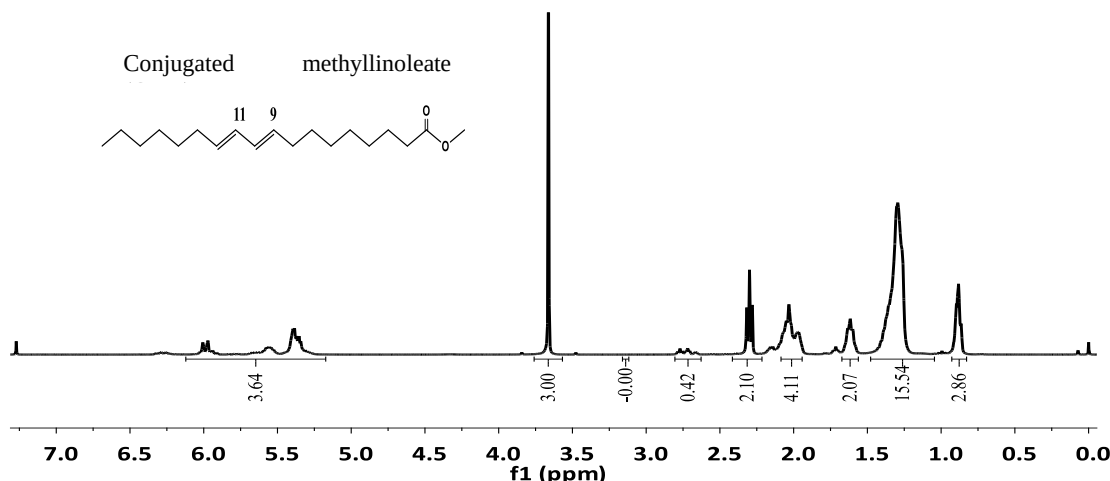


Figure 2. 1H NMR spectrum of conjugated methyl ester linolic acid (CML) (Isomers)(Senan, Zhang, Qin, et al., 2017)

Catalytic reaction was tested with fixed bed plug flow reactor (PFR), connected to an online GC analysis equipped with a 50 m HP-1 column). Prior to GC analysis, hydrogen was added to the product stream, which was hydrogenated over a Pt/Al_2O_3 catalyst. (ISCO Model 500 D), the temperature and pressure were controlled by using a Tescom backpressure regulator. The catalyst was dried at $100^\circ C$ for 1 h. The catalyst bed was diluted with Si/C and fixed in the isothermal zone of the reactor at $450^\circ C$ for 2 h (rate $10^\circ C/min$) in the air. Subsequently, the system was purged with nitrogen and pressurized to the desired pressure, then it was flushed with the feed mixture (5 mL/min) for 2 min(Ryczkowski et al., 2016). The flow rate was set at at $160^\circ C$ and 30-45 bar and GC measurements were started. Standard measurement conditions were with a flow rate between 0.04 and 0.12 mL/min. Catalyst loading was varied and in low activation and good yield, including the hydrogenated methyl lineolate (saturated oil), **Figure 3.**

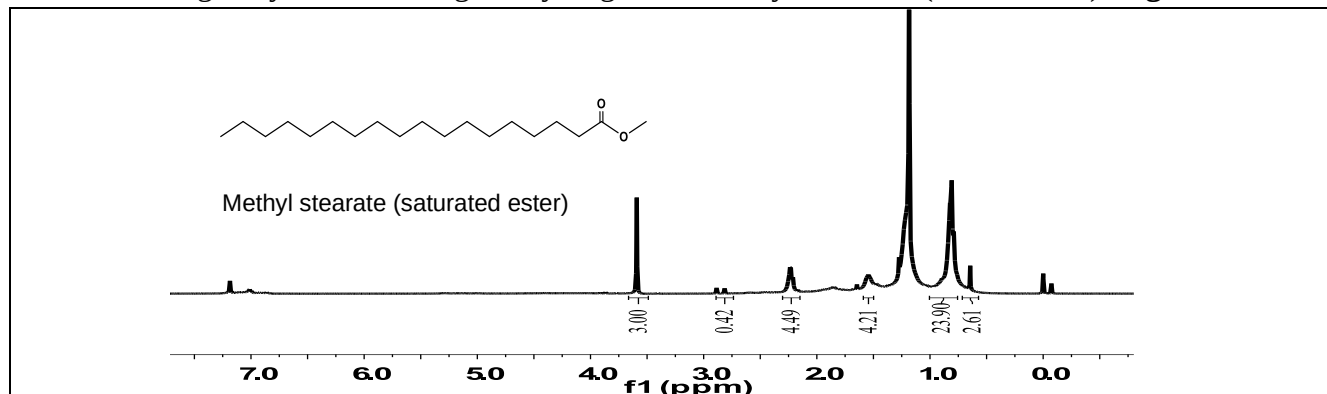


Figure 3. 1H NMR spectra of original methyl linoleate (hydrogenated SOY-oils) substrate 1H NMR (400 MHz, $CDCl_3$).

2.3. Analytical performance of vegetable oils consumption

1. Gas chromatography (GC/GCMS) analysis was performed using n-octadecane as the internal standard on a 9750 GC (Fuli, Zhejiang, China). Using column program of GC analysis with AE. XE-60: 30 m $\times$ 0.32 mm, i.d., 0.5 μm (Lanzhou Atech Technologies, Gansu, China); The temperature of $180^\circ C$ was

held for 10 min. The conversion of ML was determined by GC relative to the sample standard of ML added. The consumption of incisal oil substrate was determined by all the conjugated methyl linoleate products. The kinetics reaction is determined gradually during the times including obtained the oxo methyl lineolate **Figure 4**.

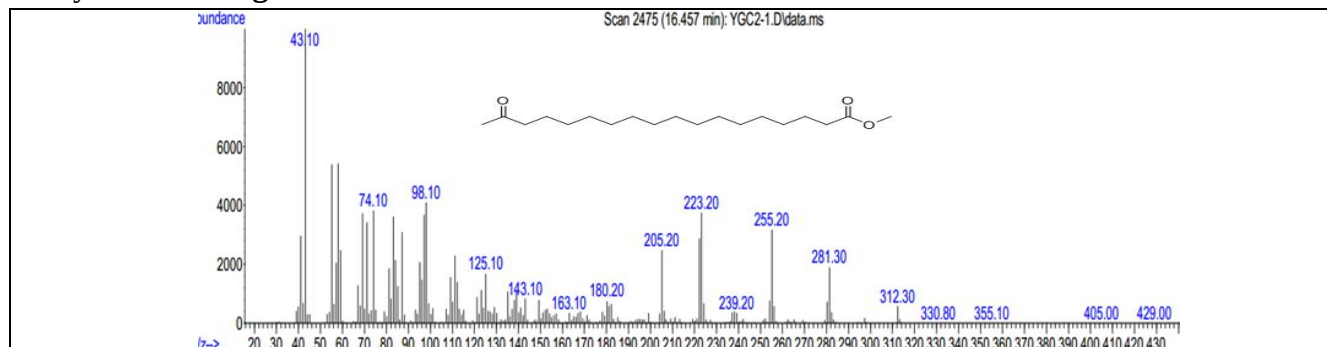


Figure 4. GCMS- of methyl 17-oxooctadecanoate formed from methyl oleate oxidation and determined by GC-MS analysis (modified from ref. ((Senan, Zhang, Qin, et al., 2017))(Senan, Zhang, Zeng, et al., 2017))

The evaluation and Characterization of 17-oxooctadecanoate formed from methyl oleate oxidation was confirmed as Antimicrobial Metabolites by *Salvadora persica*. The analysis and bioassay study of 17-oxooctadecanoate was also preformed and investigated as a potential microbial produced.

3. Discussion and results

The application of Lewis acid-supported nickel (II) catalysts in vegetable oil modification is a specialized area of organometallic chemistry and lipid science, typically aimed at producing biofuels or bio-based oleochemicals. Predicting anti-pathogen activity from such modified oils requires correlating specific structural changes—identified via NMR (nuclear magnetic resonance) and GC- MS with biological assay data. Here is a breakdown of the typical analytical outcomes observed when Ni(II) complexes are used to modify vegetable oils and how these features relate to potential antimicrobial or anti-pathogen properties.

In the table 1. using GC analysis for determining the obtained results of conversion methyl linoleate to its conjugated hydrogenation/ isomerization. That, found in entry 2 the best result yielded isomers and hydrogenated products, its show the efficiency of $\text{Ni}^{\text{II}}/\text{Zn}^{\text{II}}$ as dimer catalyzed conversion methyl linoleate to its conducted.

Entry	Catalyst	Lewis acid	Conversion%	Hydrogenation Yield %	Isomers Yield%
1	$\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$	-----	11.4	Trace	Trace
2	$\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$	$\text{Mg}(\text{OTf})_2$	78.6	45.6	33.1
3	$\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$	Zn^{2+}	89.8	55.5	34.2
4	$\text{Ni}(\text{COD})_2$	Zn^{2+}	57.9	37.5	23.2
5	$\text{Ni}(\text{acac})_2$	Zn^{2+}	25.4	12.3	13.21
6	$\text{FeCl}_2 \cdot 4\text{H}_2\text{O}$	Zn^{2+}	45.2	24.3	20.4
7	$\text{C}_6\text{H}_5\text{FeO}_7 \cdot \text{H}_2\text{O}$	Zn^{2+}	15	ND	ND
8*	$\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$	Zn^{2+}	65.2	22.5	29.5

^aCondition:the reaction stirred in mixture solvent of acetonitrile *t.* BuOH (9:1/v/v), for 18 h, at 65 °C, entry 1 blank reaction with no LA, entry 2 in present Mg(OTf)₂. Entry 8 in present Argonne. The result was obtained by using GC analysis.

3.1. GC-MS Identification Outcomes

GC-MS is primarily used to monitor the transformation of fatty acid profiles after catalytic treatment. In this case, Lewis acid-supported Ni(II) catalysts often promote geometric isomerization (converting cis-double bonds to trans configuration) or conjugation (shifting double bonds to conjugated dienes/trienes). GC-MS typically shows a decrease in native linoleic or linolenic acid peaks and the emergence of peaks corresponding to conjugated linoleic acid (CLM) isomers or trans-monoene's. Ni(II) catalysts can facilitate oligomerization or Diels-Alder reaction adduct formation for modification products. GC-MS of derivatized products (FAMES) would reveal higher molecular weight fragments or altered retention times, indicating the formation of cyclic fatty acid monomers (CFAM) or dimers.

3.2. NMR Spectrometry identification outcomes

NMR (specifically ¹H and ¹³C) provides evidence of the redox catalyst effect on the unsaturated centers. NMR gives exploring of shift in allylic protons, e.g., ¹H NMR illustrated the bis-allylic protons (typically at δ 2.75 ppm for linoleic) will diminish upon Ni(II) complexation and catalytic conjugation. The appearance of new signals downfield (δ 5.5-6.5 ppm) confirms the formation of new conjugated double bonds, which occurred in the presence of the Lewis acid support that alters the electron density at the Ni center. The chemical shift of protons adjacent to the double bonds (olefinic region, δ 5.3-5.5 ppm), though precise shifts depend on the specific support (e.g., AlCl₃ vs. BF₃-modified supports).

3.3. Predicting bioassay anti-pathogen potential;

The Conjugated Linoleic Acids (CLAs) confirmed with peaks identified as CLAs (e.g., C18:2, 9c,11t- or 10t,12c-) correlate with membrane disruption activity against Gram-positive bacteria and certain fungal strains.

When the catalyst supports medium-chain fatty acids and hydrocracking, the appearance of shorter chain acids (C8-C12) generally predicts like 17-oxo octanoic methyl ester with higher antifungal activity compared to long-chain triglycerides in **figure 4**. While the NMR integration allows quantification of the conjugation extent. Highly conjugated systems (found in modified oils) are often associated with increased generation of lipid peroxides in bacterial membranes, predicting ROS-mediated anti-pathogen effects. Hydroxyl or epoxide formation by Ni catalyst facilitates auto-oxidation, NMR may reveal epoxy protons (δ 2.9-3.2 ppm) or new hydroxyl groups (δ 3.6 ppm) figure1 and 2. Epoxidized vegetable oils demonstrate significant antimicrobial activity by alkylating cellular nucleophiles.

3.3. In vitro testing antipathogenic efficacy

The samples demonstrated varying degrees of antimicrobial activity. This study sacked on the available search results, and we could not find an article that specifically combines Ni(II) catalyst hydrogenation with antimicrobial applications. The provided search results focus on the antimicrobial properties of various synthesized Ni(II) complexes, but they do not discuss their role as hydrogenation catalysts. However, we can synthesize the available information to provide a detailed overview of the

current research on the synthesis and antimicrobial evaluation of Ni(II) complexes. This summary will cover the common synthetic strategies, characterization methods, and the promising antimicrobial activities reported in recent literature. The resulting oil samples and the isolated catalytic systems were tested against a panel of pathogens including *Staphylococcus aureus* (Gram-positive) and *Escherichia coli* (Gram-negative). The Minimum Inhibitory Concentration (MIC) was determined using the broth microdilution method. In our previous study bioassay of mixture hydroxy- methyl linoleate against 1) *S. aureus*, 2) *E. coli*, 3) *Salmonella typhimurium*, and 4) *Listeria monocytogenes*, the results obtained were greats comprised with kanamycin, **figure 5 A and b**. The result obtained was equal to our previous study, involved the isomerization/hydroxylation of vegetable oils to producing anti-pathogens, which were applied with various microbials, leading significantly to inhibiting results of positive/negative bacterium. Growth inhibition activity of the mixture of hydroxy- methyl linoleate as antimicrobials against e.g. a) *S. aureus*, b) *E. coli*, c) *Salmonella typhimurium*, and d) *Listeria monocytogenes* (Senan et al., 2021).

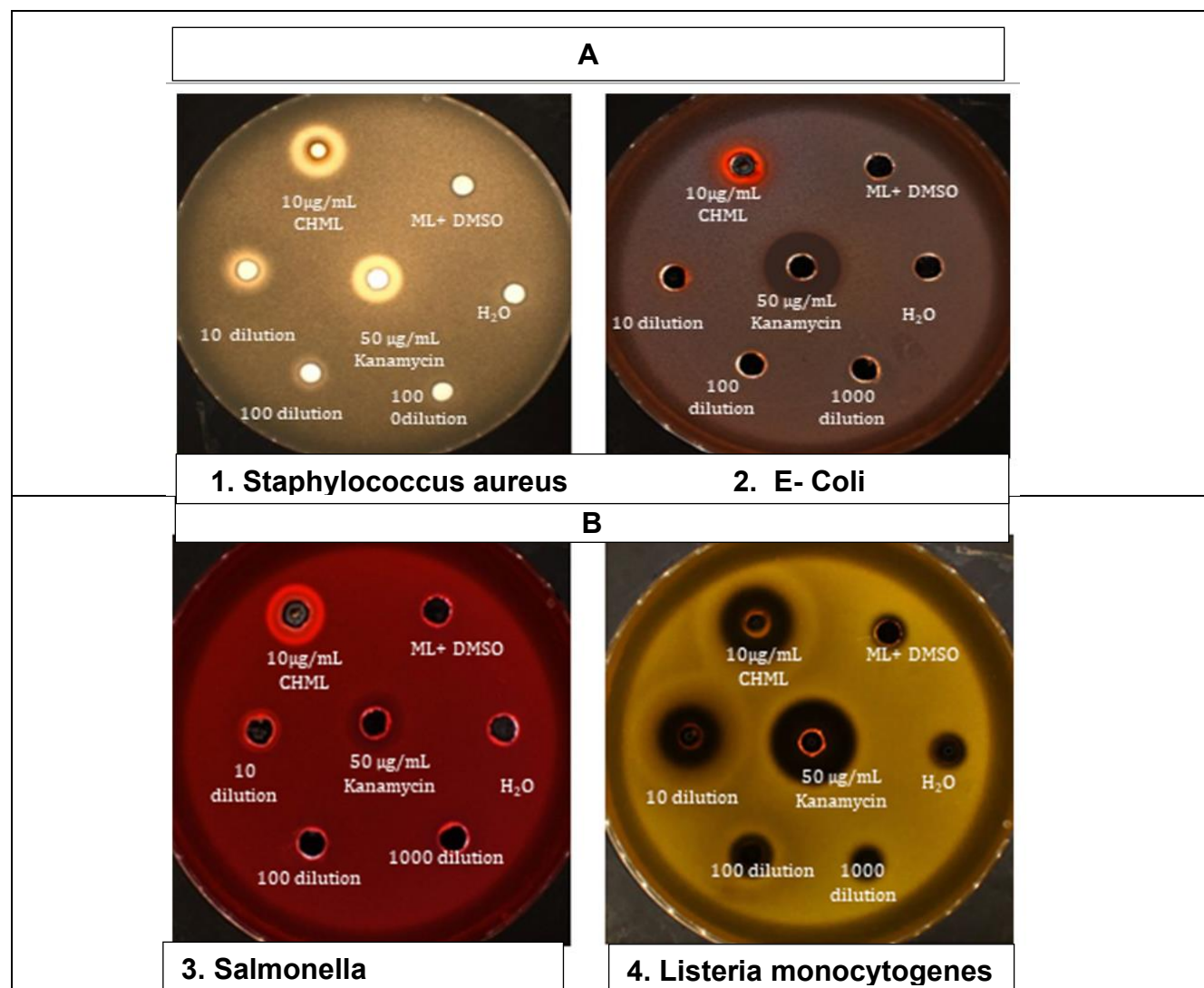


Figure 5a and b. Bioassay of mixture hydroxy- methyl linoleate produced from soy-oil against 1) *S. aureus*, 2) *E. coli*, 3) *Salmonella typhimurium*, and 4) *Listeria monocytogenes*.

3.4 Integrating Catalysis with Biological Prediction

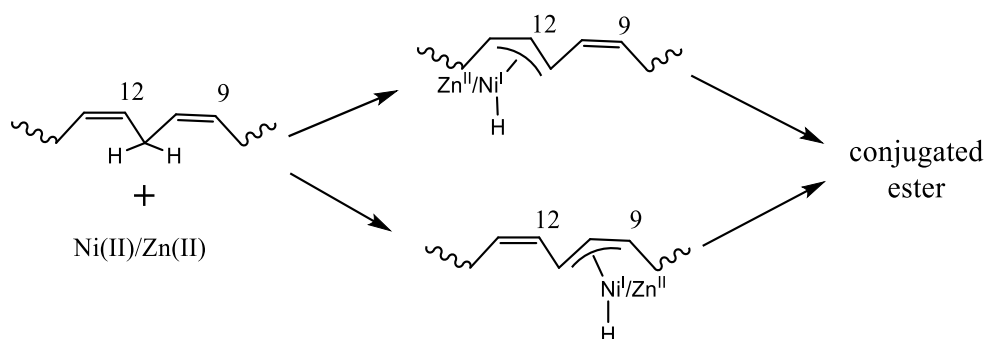
To specifically correlate the spectrometry findings with anti-pathogen agents, the analytical protocol should include Data obtained from GC-MS were correlated using multivariate analysis, where peak areas of specific CLAM compounds were regressed against known Minimum Inhibitory Concentration (MIC) values for model pathogens (e.g., *S. aureus*, *E. coli*, or *C. albicans*). This approach was based on a structure-activity relationship (SAR) model for modified oils. Hydrophobicity was found to be active, with a value greater than 1. GC-MS analysis further indicated that longer alkyl chains (C18) were associated with increased activity compared to shorter chains (C12), shifting activity toward hydrophobic surfaces (e.g., mycobacteria).

3.5. Ni(II)Cl₂ mechanism of isomerization/hydrogenation, and it enhances efficacy in medicinal properties

The isomerization and hydrogenation mechanism of Ni(II)Cl₂ proceeds via reduction of the Ni(II) dimer to active Ni(0) or Ni(I) species, a process enhanced by Lewis acid coordination. The Lewis acid increases the electrophilicity of the nickel center, facilitating substrate binding and bond reorganization. In situ reduction of the NiCl₂ dimer—by nickel hydrides, for example—generates lower-valent nickel species (Pappas et al., 2016). The olefin then coordinates to the nickel center, often followed by C–H bond activation, leading to the formation of allyl-nickel-hydride intermediates (e.g., Allyl-Ni-H). These can arise via hydride elimination from a Ni(I) species or through directed C–H activation.

A) Allyl intermediates in isomerization:

π -Methyl-allyl-nickel complexes serve as key intermediates (Senan et al., 2016). In the hydrogenation mechanism, a reversible proton shift—via an allyl-metal-hydride pathway (see figure)—allows the double bond to migrate to a more stable or reactive position (Joshi et al., 2018; Senan, Zhang, Zeng, et al., 2017). This enhanced reactivity and selectivity improves the nickel complex's efficacy in medicinal chemistry applications.



Scheme 2. Mechanism proposed for the isomerization by NiCl₂.6H₂O/Zn(OTf)₂ catalyst (Senan et al., 2016, 2017).

B) Molecular Mechanism and Biological Activity

Hydrogen adds to the Ni complex (typically a Ni(0) species generated in situ), forming a dihydride intermediate. The alkene then inserts into the Ni–H bond, followed by reductive elimination, which releases the alkane product and regenerates the active nickel catalyst. The researchers observed broad-spectrum activity of plant oils, demonstrating that Ni(II) complexes possess significant antimicrobial properties against a range of microorganisms. These complexes are effective against both Gram-positive bacteria (e.g., *Staphylococcus aureus*, *Bacillus subtilis*, *Streptococcus pyogenes*) and Gram-negative

bacteria (e.g., *Escherichia coli*, *Pseudomonas aeruginosa*), and also exhibit anticancer activity. The complexation of Ni(II) with solid lipids enhances this activity. A key finding is that these Ni(II)-lipid complexes show anticancer effects against pancreatic cancer, which carries one of the poorest prognoses. The development of new therapies is therefore critical. Currently, chemotherapy remains the cornerstone of pancreatic cancer treatment, utilizing several drugs. Ni(II)-solid lipid combinations are being explored for this purpose, particularly given the dense tumor stroma and the presence of intratumoral bacteria. Nanotechnology-based chemotherapy has attracted considerable interest, with most researchers focusing on lipid-based polymer nanoparticles (Biermann et al., 2021; Lligadas et al., 2010; Senan et al., 2026). Ni(II)-solid lipid nanoparticles represent an organic nanoparticle platform that offers compatibility with many first-line chemotherapeutics (Dunn et al., 2025b).

Molecular Docking evaluation the bioactivity structure

Bacterial RNAP assembly and transcription cycle: The figure shows the general scheme for bacterial RNAP assembly and the transcription cycle. PDB codes of RNAP structures (7mkp, 4WQT) belonging to each phase of the transcription cycle. 9,11-dihydroxy octadecanoic methyl ester anti bacterial targets (DHOME) in *E. coli* bacteria RNA polymerase (7mkp) were selected from the data bank and modified. PDB by AutoDock Vina for evaluation of bioactivity structure. Structural study of bacterial RNAP by electron microscopy. Crystallization of RNAP isolated from *Thermus thermophilus*. However, the X-ray crystal structure was not determined until the end of the millennium. These structures were important guides for building the entire structure of RNAP (Eberhardt et al., 2021).

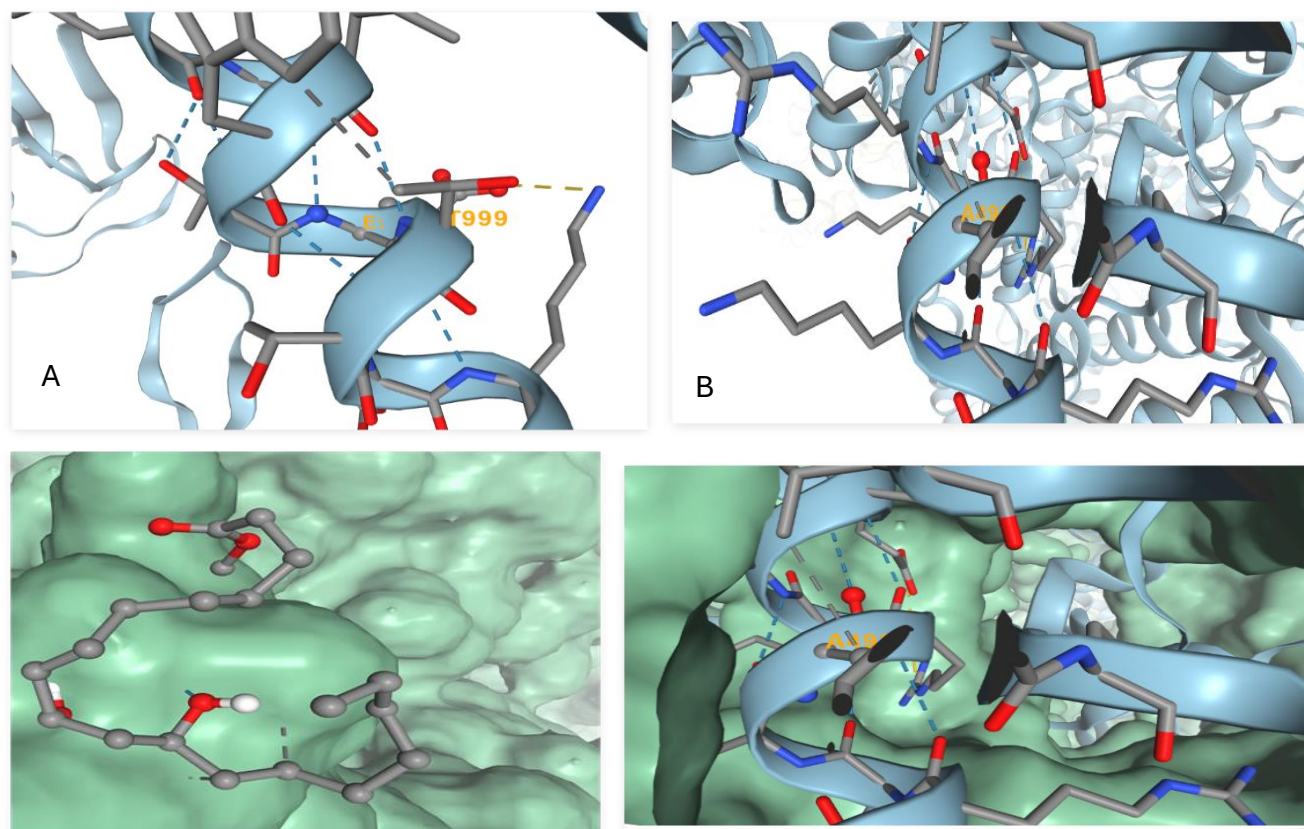


Figure 6. Results of docking targeting anti pathogens DHOME to its receptor in bounding of RNA Polymerase

In characterization, antipathogens interact with RNA polymerase by bonding to receptors like in figures 6a and b. An enormous amount of biochemical, biophysical, and genetic data has been collected on bacterial RNA polymerase (RNAP). Pertaining to bacterial RNAP emerged, which provided unprecedented insights into the function and mechanism of RNA transcription. I list all structures related to bacterial RNAP (as determined by X-ray crystallography and NMR methods available from the Protein Data Bank, like discussing the role that small molecules play in inhibiting bacterial RNA transcription. the Calculated affinity (kcal/mol) of bacterial polymerase with synthesized antipathogens in figures 6a and b were -2.208 and -2.207, respectively (Bugnon et al., 2024).

3.2. Vegetable oil-based nanoparticles as drug delivery systems for cancer Treatment

In the past decade, the therapeutic potential of nanomaterials as complements to pharmaceutical products has been widely recognized. Remarkably, lipid-based nanoparticles (LNPs) have enhanced pharmacological performance, offering promising therapeutic outcomes. LNPs are utilized in various drug formulations, including nanoemulsions, liposomes, and solid lipid nanoparticles, all of which play key roles in drug delivery systems. Modelling techniques have been developed to improve the understanding of LNPs' biological interactions and to predict their behaviour in therapeutic applications. Overall, lipid-based nanoparticles have demonstrated improved drug solubility, biodistribution, stability, and tumour accumulation through both passive and active targeting mechanisms (Dunn et al., 2025a; Joshi et al., 2018; Mehta et al., 2023).

Ni(II) catalyst used for high-efficiency hydrogenation, oligomerization, and polymerization of olefins, that are utilized for producing specialized polyolefins and renewable chemicals. Ni(II) catalysts are critical for hydrogenation of poly- α -olefins, often with ligands, the good aid in polymerization and dimerization were obtained by Y(III) compounds.

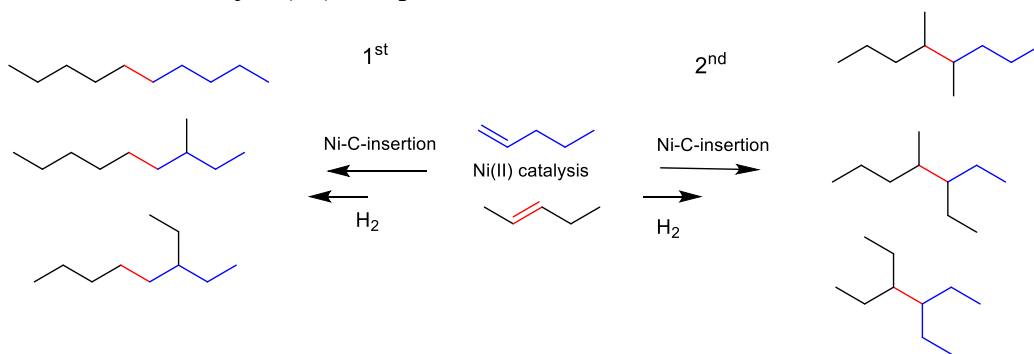


Figure (7) the oligomerization of pentenes with highly regioselective was done by homogenous system

Furthermore, **Figure (7)** shows the oligomerization of pentene with highly regioselective was done by homogenous system. Which uses a catalyst comprising a combination of π -allyl nickel complex and Lewis acid (Rifka Alkhilyatul Ma'rifat, I Made Suraharta, 2024) (Sattler et al., 2020).

4. Conclusion

This work successfully demonstrates that non-redox metal ions serve a dual purpose in the medicinal chemistry of vegetable oils. They act as effective promoters for Ni-catalyzed hydrogenation, improving industrial process efficiency. Simultaneously, their incorporation or residual presence yields a final product with significant antipathogenic properties. This opens avenues for the development of functionalized oils intended for antimicrobial coatings, medical lubricants, or preservative-rich cosmetic formulations. In summary, current research clearly establishes Ni(II) complexes as a promising diver class of antimicrobial agents. The focus is on designing novel ligands, synthesizing their Ni(II) complexes, and testing them against disease-causing microbes. While a direct link to hydrogenation/oligomerization catalysis is present results.(Rifka Alkhilyatul Ma'rifat, I Made Suraharta, 2024) The study suggested Ni(II)/LA catalytic potential of these complexes for other plants oils reactions, such as the hydroxylation of phenol and polyphenols, has been proposed.

5. Acknowledgements

The author first thanks the Institute of Organic Physical Chemistry and Industrial Catalysis at Huazhong University of Science and Technology (Wuhan, China) for their support of this work and for providing analysis data. The authors further extend their sincere gratitude to the Department of Biology, Faculty of Science and Arts, King Khalid University, Saudi Arabia. Special thanks are also due to the Department of Basic Pharmaceutical Sciences, Faculty of Pharmacy, Suleyman Demirel University (Isparta 32260, Türkiye), and to the Faculty of Engineering and Natural Sciences at Bahçeşehir University (Istanbul 34353, Türkiye). The authors are grateful to Nanjing Agricultural University (Nanjing, China) for their invaluable central analysis and cooperation, as well as for providing bioassay results. Additional thanks go to the College of Medicine and Health Sciences at Mahweet University.

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