

Brief information about the project

Name of the project	AP26100971 “Development of a technology for the production of fragrance compounds based on carboxylic acid esters via the utilization of unsaturated hydrocarbons from oil refinery gases using metal-complex carbonylation”.
Relevance	Kazakhstan has no domestic production of synthetic fragrance substances and is entirely dependent on imports from foreign countries. At the same time, existing oil refineries in Kazakhstan do not utilize valuable olefin raw materials from process gases. Incorporating refinery waste - unsaturated hydrocarbons and carbon monoxide - into the production of practically valuable products aligns with the principles of "green" chemistry, improves the environment, and has high economic significance. Developing cost-effective and innovative technologies for producing fragrance substances is a highly relevant task for the development of Kazakhstan's domestic perfume and cosmetics industry.
Purpose	To develop a technology for producing fragrance substances based on carboxylic acid esters via metal complex carbonylation of unsaturated hydrocarbons from oil refineries (alkenes, alkynes, and alkadienes) with carbon monoxide and alcohols in the presence of new modified catalysts, as well as to replace expensive catalysts with more accessible and effective heterogeneous analogues (magnetic, supported, etc.).
Objectives	Objective I (2025): Synthesis of new effective modified catalysts based on transition metal complexes. Includes synthesis of heterogeneous catalysts by the support impregnation method, synthesis of magnetically recoverable catalysts by precipitation, study of their reusability, and characterization by ICP-OES and BET methods. Objective II (2026): Synthesis of carboxylic acid esters via carbonylation of alkenes, alkynes, and alkadienes with various alcohols in the presence of new catalysts. Includes determination of optimal reagent ratios, optimal process parameters (pressure, temperature, duration), and analysis of products by GC, Mass-, IR-, and NMR-spectroscopy. Objective III (2027): Investigation of fragrance substance properties, determination of organoleptic characteristics and odor stability, toxicological testing at NUTRITEST laboratory, development of perfume compositions, creation of two original perfumes and three fragrance additives, and development of a laboratory-technological regulation for integration into the educational process at Al-Farabi Kazakh National University.
Expected and achieved results	Expected results upon project completion: innovative technology for synthesizing modified heterogeneous catalysts; synthesis of a series of carboxylic acid esters via single-stage carbonylation; two original perfumes and three fragrance additives; a laboratory-technological regulation integrated into the educational process; Achieved results for 2025:

	Activity 1.1 - Homogeneous palladium complexes $\text{PdCl}_2(\text{PPh}_3)_2$ and $\text{Pd}(\text{PPh}_3)_4$ were successfully synthesized and demonstrated high catalytic activity. In the carbonylation of cyclohexene, ethyl cyclohexanecarboxylate was obtained with a yield of 81.2% (catalyst $\text{PdCl}_2(\text{PPh}_3)_2$) and 79.5% (catalyst $\text{Pd}(\text{PPh}_3)_4$). In the carbonylation of cyclopentene, ethyl cyclopentanecarboxylate was obtained with yields of 83% and 82.6% respectively. Activity 1.2 - Heterogeneous supported catalysts were synthesized: 1% Pd/Polycarbonate and 1% Pd/Carbon. In the carbonylation of iodobenzene with methanol, methyl benzoate was obtained with a yield of 89.8% (Pd/PC catalyst) and 97.2% (Pd/C catalyst). Activity 1.3 - Magnetically recoverable catalysts Pd/Fe₃O₄/Polycarbonate and Pd/Fe₃O₄/Carbon were synthesized. Methyl benzoate was obtained with yields of 88.2% and 97.1% respectively. Separation of the solid catalyst from the reaction mixture was carried out using a permanent magnet with virtually no loss of palladium particles. Activity 1.4 - 12 carbonylation experiments of hexene-1 with ethanol were conducted, confirming the reusability of all four heterogeneous catalysts with product yields of at least 80%. Activity 1.5 - Specific surface areas of the catalysts were measured by the BET method: Pd/C - 950.8 m²/g; Pd/PC - 12.4 m²/g; Pd/Fe₃O₄/C - 721.2 m²/g; Pd/Fe₃O₄/PC - 20.8 m²/g. Additionally - preliminary studies on the carbonylation of alkadienes (1,3-butadiene, 1,5-hexadiene, 1,7-octadiene) were conducted. The highest yield of ethyl 8-nonenoate - 32.08% - was obtained in the carbonylation of 1,7-octadiene using the $\text{Pd}(\text{PPh}_3)_4$ catalyst.
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Usage	The project results are aimed at establishing domestic production of fragrance substances in Kazakhstan and reducing dependence on imports. The developed technologies will be integrated into the educational process at Al-Farabi KazNU with the opening of a new Master's program "Chemistry of Perfume and Cosmetics Production." The synthesized products will find application in Kazakhstan's perfume, cosmetics, and food industries. Upon project completion, commercialization of results is planned through the Science Fund JSC (RSTTD), which will create new jobs and supply the market with domestically produced goods.
Priority compared to real-world alternatives	The existing industrial method for producing carboxylic acid esters - esterification of organic acids with alcohols - has significant drawbacks: multi-stage process, duration of approximately 30 hours, low product yield (50-60%), and large volumes of industrial wastewater. The hydroalkoxycarbonylation method developed in this project provides a single-stage process with product yields of 95-98% in 4-5 hours at carbon monoxide pressure not exceeding 20 atm and temperature not exceeding 100°C. Accessible refinery waste is used as raw material. The production cost using the new method is 2-4 times lower than existing industrial analogues. The use of heterogeneous catalysts (supported and magnetic) solves the key problem of industrial homogeneous catalysis - the labor-intensive separation of catalyst from the reaction mixture - ensuring easy recovery and reuse with product yields of at least 80%.
List of publications with links to them	Azimbay A.M., Kudaibergenov N.Zh., Shalmagambetov K.M., Alikeyeva A.E., Bakytzhan Z., Zykai M.Kh. Regioselective hydroalkoxycarbonylation of 1.3-butadiene, 1.5-hexadiene, and 1.7-octadiene using palladium-phosphine catalytic systems. Chem. J. Kaz., 2025, 4(92), 138-148. DOI: https://doi.org/10.51580/2025-4.2710-1185.57
Patents	It is planned to receive a utility model based on the results of the project