Compounds **7**, **9** were examined for antibacterial activity against ESKAPE pathogens. Some compounds were found to be active against *Acinetobacter baumannii* and *Candida albicans*. Antimicrobial screening was performed by CO-ADD (The Community for Antimicrobial Drug Discovery), funded by the Wellcome Trust (UK) and The University of Queensland (Australia).

References

1. *Kollenz G., Penn G., Ott W., Peters K., Peters E.-M., von Schnering H. G.* // Chemische berichte. 1984. Vol. 117. P. 1310−1329.
2. *Konovalova V. V., Shklyaev Yu. V., Maslivets A. N.* // Arkivoc. 2015. i. P. 48–69.
3. *Konovalova V., Maslivets A.* // Mini-Reviews in Organic Chemistry. 2018. Vol. 16. P. 173–192.

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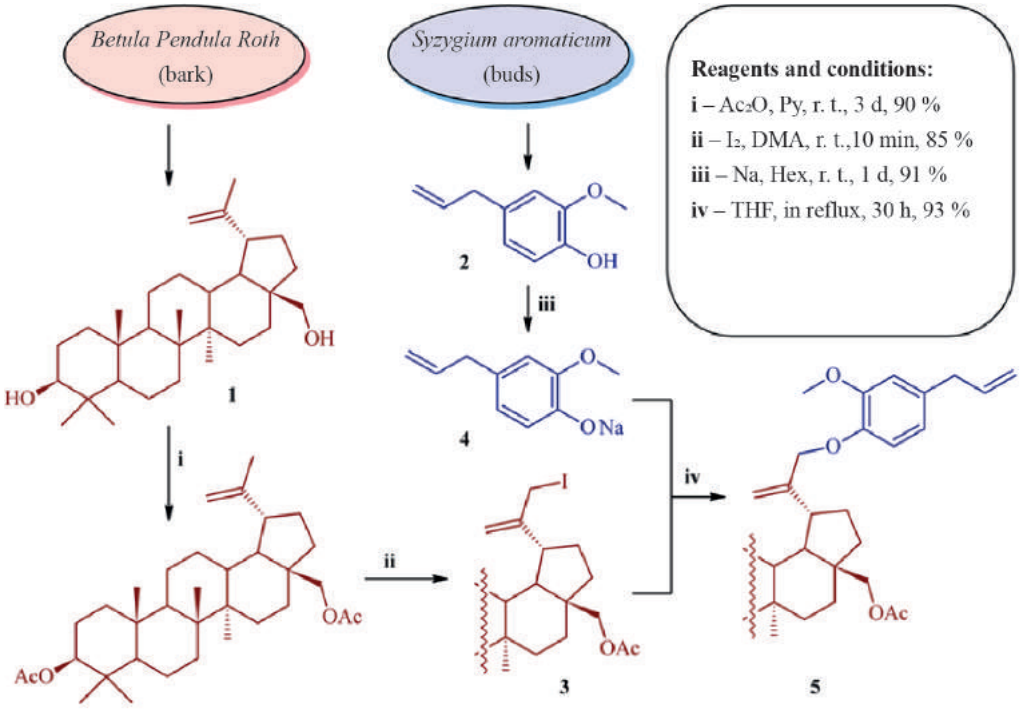
SYNTHESIS OF (3,28-DIACETYLLUP-20(29)-EN-30-YL)EUGENOL

Keywords: eugenol, betulin, natural compounds, biological activity.

Natural compounds play an important role in development of new pharmaceuticals. Biologically active compounds from renewable plant sources serve as a target structure for different synthetic approaches to be applied. As a result of these chemical modifications a large variety of substances with valuable properties has been synthesized. The list of natural products being researched is limited according to several criteria: the compound should be simply isolated from

a plant material* (extraction, distillation, etc.); the content of the compound allows it to be isolated in a sufficient quantity; the compound possess a wide range of biological activity.

Two objects that match the restrictions were chosen. The first is betulin **1** – pharmacologically active lupane type triterpenoid. It forms up to 30 % of the dry weight of birch bark of *Betula Pendula* species. It shows a wide spectrum of biological and pharmacological properties, such as anti-HIV, anti-inflammatory and cytotoxic [1]. The second is eugenol **2** – phenylpropaniod and the main component of essential oil of *Syzygium aromaticum* (up to 80 %). The application of **2** is growing fast as modern scientific methods have revealed antifungal, anesthetic, antibacterial, cytotoxic, antioxidant, and insecticidal activity of this compound [2]. Combining chemical structures of **1** and **2** may lead to new substances with improved or different properties. To implement this approach we carried out alkylation of **2** with 30-iodo-3,28-diacetylbetulin **3**. Compound **3** was synthesized by acetylation of **1** followed by electrophilic monoiodation** [3]. To accelerate the final stage we turned **1** into sodium eugenolate **4**. Alkylation was proceeded in THF solution with an excess of **4** (scheme 1).



Scheme 1. Synthetic route to compound **5** based on isolated **1** and **2**

The yield of resulting ether **5** was 93 %. The final product was isolated by column chromatography on silica (gradient elution with ethyl acetate/hexane). The structure of **5** is proven by ^{1}H, ^{13}C NMR spectroscopy and mass spectrometry. To evaluate biological activity of synthesized (3,28-diacetyllup-20(29)-en-30-yl)eugenol **5** PASS prediction service was used. Under the same evaluation method compound **5** showed estimated probability of antiprotozoal activity similar to artemisinin*** (table 1), though compounds **1, 2** do not demonstrate such Pa values for this type of activity.

Table 1

Biological activity of 5 calculated by PASS service

Pa	Pi	Activity name
0.945	0.002	Antiprotozoal (Leishmania)
0.937	0.003	Caspase 3 stimulant
0.909	0.002	Hepatoprotectant
0.910	0.005	Antineoplastic

Pa – probability «to be active», Pi – probability «to be inactive»

* as long as full synthesis is not available or too expensive; ** modification of **1** at C(3) and C(28) positions via nucleophilic deoxyhalogenation is hardly to be carried out due to strong tendency of the triterpenoid to elimination and isomerization processes; *** sesquiterpenoid known for its strong *in vivo* antiprotozoal activity (against *Plasmodium falciparum*)

References

1. *Tolstikov G. A., Flekhter O. B., Shultz E. E., Baltina L. A., Tolstikov A. G.* // Chem. Sustain. Develop. 2005. Vol. 13. P. 1–29.
2. *Ramawat K. G., Merillon J.-M.* Natural Products. Phytochemistry, Botany and Metabolism of Alkaloids, Phenolics and Terpenes. Berlin; Heidelberg: Springer-Verlag, 2013. P. 2673–2683.
3. *Yemets S. V., Shubina T. E., Krasutsky P. A.* // Org. Biomol. Chem. 2018. Vol. 11. P. 2891–2897.

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SYNTHESIS OF 7-FORMYL METHYL ABIETATE VIA VILSMEIER-HAACK REACTION

Keywords: Vilsmeier-Haack reaction, formylation, abietane diterpenoids, methyl abietate.

The Vilsmeier-Haack reaction is one of the widely useful general methods employed for the formylation of various electron-rich aromatic, aliphatic, and heteroaromatic substrates [1]. The reaction goes *via* the formation of efficient and mild electrophilic halomethyleneiminium intermediates, which has attracted great attention in synthetic organic chemistry [2]. Previously, we found that both the carboxyl group