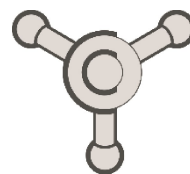




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ЧЕТВРТА КОНФЕРЕНЦИЈА МЛАДИХ ХЕМИЧАРА СРБИЈЕ КРАТКИ ИЗВОДИ РАДОВА

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Identifikacija i sinteza novih estara iz etarskog ulja hmelja (*Humulus lupulus* L.)

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Šišarke hmelja (*Humulus lupulus* L., Cannabaceae) se koriste za poboljšanje ukusa piva, a mnogi narodi ovu biljku koriste i u medicinske svrhe. Etarsko ulje hmelja se dobija hidrodestilacijom ženskih cvasti biljke (strobuli lupuli), u kojima se nalaze žlezde pune ulja. Do sada je identifikovano više od 200 različitih sastojaka ovog etarskog ulja, međutim, veliki broj jedinjenja je ostao neidentifikovan. Motivisani ovim, izolovano je etarsko ulje hidrodestilacijom svežih šišarki hmelja (prinos: 0,6%, w/w), sakupljenih u blizini Niša (jugo-istočna Srbija), a sastojaci etarskog ulja su preparativno razdvojeni gradijentnom "dry flash" hromatografijom na silika-gelu. Detaljna GC i GC-MS analiza dobijenih frakcija, pokazala je da je jedna od njih (eluirana sa 2% (v/v) dietil-etra u pentanu) bogata mnoštvom metil-estara alifatičnih karboksilnih kiselina normalnog i račvastog niza. Na osnovu njihovih masenih spektara i retencionih indeksa identifikovana je čitava serija metil-2-metilalkanoata (C₈-C₁₁). Kako metil-2-metilnonanoat i metil-2-metildekanoat nisu do sada identifikovani u etarskom ulju hmelja, izvršena je njihova sinteza. Odgovarajući litijum-enolati, dobijeni u reakciji metil-nonanoata i metil-dekanoata sa litijum-bis(trimetilsilil)amidom na -78 °C, alkilovani su metil-jodidom. GC ko-injekcija sintetisanih estara sa uzorkom etarskog ulja je potvrdila prisustvo metil-2-metilnonanoata i metil-2-metildekanoata u etarskom ulju hmelja.

Identification and synthesis of new esters from the essential oil of *Humulus lupulus* L.

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For hundreds of years strobiles from *Humulus lupulus* L. (Cannabaceae) have been used to flavor beer and in the ethnopharmacology of many nations. The essential oil is produced by the female inflorescences (strobuli lupuli) which contain the oil bearing glands. Up to now, more than 200 essential-oil constituents have been identified; however, a large number still remained unknown. Prompted by this, we subjected a sample of hydrodistilled essential oil of fresh hop cones (yield: 0.6%, w/w), collected from a wild-growing population of *H. lupulus* near the city of Niš (SE Serbia), to gradient "dry flash" SiO₂ chromatography. Initial GC and GC-MS analyses revealed a fraction (eluded with 2% (v/v) diethyl ether in pentane) that consisted of a myriad of methyl esters of normal and branched aliphatic carboxylic acids. A series of methyl 2-methylalkanoates (C₈-C₁₁) was tentatively identified based on their mass spectra and retention data. Since methyl 2-methylnonanoate and methyl 2-methyldecanoate were never previously reported for *H. lupulus*, we decided to prepare the two compounds by synthesis. The corresponding lithium enolates, obtained in the reaction of methyl nonanoate and methyl decanoate with lithium bis(trimethylsilyl)amide at -78 °C, were alkylated with methyl iodide. The subsequent co-injection experiments corroborated the initial tentative identifications, i.e. this is the first report on the occurrence of methyl 2-methylnonanoate and methyl 2-methyldecanoate in *H. lupulus* essential oil.

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