

桢楠木精油中两种主要化合物的分离纯化及其结构 定

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摘要:【目的】对桢楠木精油中的主要化学成分进行分离纯化, 并通过核磁共振技术确定其分子结构。

【方法】以四川桢楠木材为研究对象, 采用超临界 CO₂ 流体萃取获得桢楠木精油, 依次利用硅胶柱层析、硝酸银硅胶柱层析及 C18 制备型高效液相色谱 (HPLC) 法分离纯化得到高纯度天然化合物, 并进一步根据核磁共振波谱 (NMR) 解析主要化合物的化学结构。【结果】桢楠木精油中的主要化合物 I、II 不仅稳定存在于不同产地的桢楠木材中, 且两者的相对含量均显著高于其他化合物, 在所有化合物中占有绝对优势。制备型高效液相色谱分离纯化后的化合物 I、II 的纯度分别为 96.6% 和 95.1%, 这是目前分离纯化或人工合成可实现的最高纯度。【结论】通过结构分析, 获知化合物 I 的化学名称为 2-((2R,8R,8aS)-8,8a-Dimethyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl)propan-2-ol, 英文为 Valerianol, 中文称作缬草醇; 化合物 II 的化学名称为 2-((2R,5R,10R)-6,10-Dimethylspiro[4.5]dec-6-en-2-yl)propan-2-ol, 英文为 Agarospirol, 中文称作沉香螺醇。缬草醇 Valerianol (化合物 I) 与沉香螺醇 Agarospirol (化合物 II) 对桢楠木精油的功效和用途有重大影响, 有必要进一步研究其生物活性与毒理。

关 词: 桢楠木精油; 分离纯化; 硅胶柱层析; 制备型高效液相色谱; 结构鉴定

Separation, purification, and structural identification of two main compounds in *Phoebe Zhennan* Essential Oil

Abstract: [Objective] To isolate and purify the main chemical components in *Phoebe Zhennan* wood's essential oil and determine its molecular structure using the nuclear magnetic resonance (NMR) technique. [Methods] Sichuan Zhennan wood was used as the research material. *Phoebe Zhennan* wood essential oil obtained by supercritical CO₂ fluid extraction was purified by methods such as silica gel column chromatography, silver nitrate silica gel column chromatography, and preparative high-performance liquid chromatography (HPLC) with C18 to isolate and purify the high-purity natural compounds. The chemical structures of the main compounds were further determined and analyzed by NMR spectroscopy. [Results] The main compounds in *Phoebe Zhennan* wood essential oil, compounds I and II, remain stable in *Phoebe Zhennan* wood from different sources. Still, their relative contents are significantly higher than other compounds, showing absolute dominance among all compounds. The purity of the compounds I and II after preparation-type high-performance liquid chromatography purification is 96.6% and 95.1%, respectively, the highest purity achievable through current separation purification or artificial synthesis. [Conclusion] Through structural analysis, it was determined that the chemical name of compound I is 2-((2R,8R,8aS)-8,8a-Dimethyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl)propan-2-ol, known in English as Valerianol, the chemical name of compound II is 2-((2R,5R,10R)-6,10-Dimethylspiro[4.5]dec-6-en-2-yl)propan-2-ol, known in English as Agarospirol. Valerianol (compound I) and Agarospirol (compound II) significantly affect the efficacy and usage of *Phoebe Zhennan* wood essential oil, warranting further research into their biological activities and toxicology.

Keywords: *Phoebe Zhennan* wood essential oil, Isolation and purification, Silica gel column chromatography, Preparative high-performance liquid chromatography, Structural identification