

利用分子识别包结结晶法选择性分离小茴香挥发油中的化学组分

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摘要 用GC-MS方法测定了小茴香挥发油的全组分,其中对-丙烯基茴香醚的含量为82.65%。采用包结结晶法对小茴香挥发油中的对-丙烯基茴香醚进行了选择性分离,以1,1,6,6-四苯基-2,4-己二炔-1,6-二醇(简称D.D)作为主体分子,小茴香挥发油中的对-丙烯基茴香醚作为客体分子,D.D选择性地与之形成超分子包结物晶体。采用IR,¹H NMR,单晶XRD确定了包结物的形成及其主客体分子摩尔比为2:1。包结物晶体属于P1空间群,晶胞参数:a=1.2972(2) nm,b=1.5119(2) nm,c=1.6799(2) nm, $\alpha=100.57(1)^\circ$, $\beta=104.89(1)^\circ$, $\gamma=113.58(1)^\circ$,Z=2。利用Kugelrohr真空蒸馏技术从包结物晶体中蒸出被分离的化学组分,用IR,¹H NMR和MS方法,确定了反式对-丙烯基茴香醚。用GC方法测定了选择分离出的挥发油化学,GC分析结果表明,分离的反式对-丙烯基茴香醚的化学纯度为97%,回收率为75.28%。

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Selective isolation of chemical component from volatile oil of xiaohuixiang by molecular cognition inclusion crystalline method

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Abstract The chemical components of volatile oil from *Foeniculum Vulgare* Mill were determined by GC-MS. Anethole accounted for 82.65% of the whole oil. Selective isolation of anethole from the volatile oil was carried out using an inclusion crystalline method with 1,1,6,6-tetraphenylhexa-2,4-diyne-1,6-diol inclusion complex with anethole. The crystal structure of the inclusion complex was determined by IR, ¹H NMR and single crystal XRD techniques. The host-guest molar ratio in complex was found to be 2:1. Crystal structure of inclusion compound belong to space group P1, a=1.2972(2) nm, b=1.5119(2) nm, c=1.6799(2) nm, $\alpha=100.57(1)^\circ$, $\beta=104.89(1)^\circ$, $\gamma=113.58(1)^\circ$, Z=2. The isolated chemical component was isolated from the inclusion crystal complex by using Kugelrohr vacuum distillation technique and was identified to be trans-anethole by means of IR, ¹H NMR, and MS spectroscopy. The results of GC analysis showed that chemical purity of trans-anethole isolated from volatile oil was 97% and the yield was 75.28%.

Key words [MOLECULAR RECOGNITION](#) [CRYSTALLIZE](#) [SEPARATION](#) [CHROMATOGRAPHY-MASS SPECTROGRAPHY](#)

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