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论文

用^{2}H-标记物和GC-MS分离鉴定联苯双酯在大鼠尿中的一个代谢产物

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摘要:

关键词: 联苯双酯 4,4′-甲氧基-5,6,5′,6′-二次甲氧基-2,2′-二甲氧羰基联苯 氘标记化合物 稳定性同位素 气相色谱—质谱

USE OF ^{2}H-LABELED COMPOUND AND GC- MS IN THE ISOLATION AND IDENTIFICATION OF A METABOLITE OF BIPHENYLDIMETHYL- DICARBOXYLATE IN RAT URINE

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Abstract:

Dimethyl-4, 4′-dimethoxy-5, 6, 5′, 6′-dimethylenedioxybiphenyl-2, 2′-dicarboxylate (biphenyldimethyldicarboxylate; BDD), a synthetic compound, has been used in the treatment of chronic hepatitis with good results in reducing s-GPT. Previous work in our laboratory studied its metabolites using ^{3}H-labeled compound in combination with TLC and found that its main methabolic pathway is demethylation followed by conjugation with glucuronic acid. This paper reports the isolation and identification of a metabolite of BDD from rat urine using ^{2}H-labeled compound and GC-MS. Rats fasted for 12h were intragastrically given a mixture of ^{2}H-labeled (consisting of monodeutero-and dideutero-BDD in the ratio about 1:1.3)and non-labeled BDD 150mg/kg and placed in metabolism cages for urine collection. The 24h urine was filtered and extracted three times each with 5ml of methylenedichloride. The extracts were pooled and evaporated to dryness under reduced pressure at 35℃. The residue was redissolved in chloroform and subjected to GC-MS analysis. The mass spectrum (m/z: 404, 405, 406; 373, 374, 375; 345, 346, 347; 330, 331, 332; etc)indicates that the molecular ionic and fragment peaks of the metabolite all have 14 amu less than those of BDD. This means that the metabolite isolated is mono-O-demethylated BDD. The result confirmed our findings reported previously.

Keywords: Dimethyl- 4, 4'- dimethoxy. 5,6, 5',6'- dimethylenedioxybiphenyl- 2, 2'- dicarboxylate Deuterium labeled compound Stable isotope Gas chromatography-mass spectrometry Biphenyldimethyldicarboxylate

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