

GLC and GLC-MS Analysis of Thiophene Derivatives in Plants and in *in vitro* Cultures of *Tagetes patula* L. (Asteraceae)

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Z. Naturforsch. **57c**, 63–71 (2002); received July 17/September 17, 2001

Tagetes patula, Thiophenes, Root Biosynthesis

The occurrence of thiophenic compounds in diverse plant organs and in *in vitro* root-, callus- and cell suspension cultures of *Tagetes patula* cv. Carmen was investigated using capillary GLC and GLC-MS. The separation of thiophenes by capillary GLC and the group specific MS fragmentation with the typical sulfur isotope peaks allowed the unequivocal assignment of individual thiophenes in complex mixtures, even when occurring in traces and in the presence of different geometrical isomers. The extracts of *Tagetes patula* cv. Carmen contained the following 8 thiophene compounds: 5-(3-buten-1-ynyl)-2,2'-bithienyl (BBT), 5'-methyl-5-(3-buten-1-ynyl)-2,2'-bithienyl (MeBBT), 5-(1-pentynyl)-2,2'-bithienyl (PBT), 5-(4-hydroxy-1-butynyl)-2,2'-bithienyl (BBTOH), 2,2',5,2''-terthienyl (α -T), 5-(4-acetoxy-1-butynyl)-2,2'-bithienyl (BBTOAc), 5-methylaceto-5'-(3-buten-1-ynyl)-2,2'-bithienyl (AcOCH₂BBT), and 5-(3,4-diacetoxy-1-butynyl)-2,2'-bithienyl (BBT(OAc)₂). The most complex thiophene profile, including the less common PBT was detected in aerial parts of freshly harvested plant material. Under *in vitro* conditions only the root cultures, but not callus or cell suspension cultures produced substantial amounts of irregular thiophenes confirming that roots are the main site of thiophene biosynthesis.