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Regioselective synthesis, isomerisation, in vitro oestrogenic activity, and co-polymerisation of bisguaiacol F (BGF) isomers

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PURPOSE OF THE ABSTRACT
Bisguaiacol F (BGF), a potentially safer and renewable BPA replacement made from lignin derived vanillyl alcohol (VA), is a promising building block for future aromatic biopolymers. Unfortunately, like the synthesis of BPA, also this electrophilic condensation reaction is prone to regioselectivity issues, giving rise to m,p'- and o,p'-BGF by-products. In this work, the hitherto unconsidered influence of the m,p'-BGF regioisomer - the main isomeric byproduct of p,p'-BGF synthesis - on the physicochemical properties of poly(BGF carbonates) (BGF-PC) was systematically investigated by random copolymerization with different fractions of pure m,p'-BGF (25, 50 and 75 wt.%). To do so, the elusive m,p'-isomer was made in unparalleled regioselectivity (72%) by condensation of isovanillyl alcohol with guaiacol. Surprisingly, as supported by preliminary evidence, no isomeric scrambling as a result of acid-catalysed isomerisation was encountered for pure BGF isomers, which strongly facilitates their synthesis in contrast to petrochemical bisphenol F (BPF). Furthermore, to ensure safer chemical design, an in vitro hERalpha transactivation reporter assay was performed. Both the pure m,p'- and p,p'-BPF isomers display a significantly reduced potency (~90-96 times lower affinity than BPA) and efficacy (~37-48% of BPA's maximum activity). Interestingly, mutual comparison between p,p'-BPF and p,p'-BGF reveals and proofs the direct link between o-methoxy substitutions and reduced in vitro oestrogenic potency (for transactivation of hERalpha). In contrast to o,p'-BPA - the main byproduct of p,p'-BPA synthesis, m,p'-BGF is proven to be suitable for application in thermoplastics, avoiding time-consuming and labour-intensive recrystallizations to obtain isomerically pure p,p'-BGF.

FIGURES

FIGURE 1

FIGURE 2

KEYWORDS

BPA replacements | bisguaiacols | oestrogen activity | co-polycarbonates

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