Defossilized building blocks for specialty chemicals

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Stefan Lundmark

Committed to setting science-based emission reduction targets, there will be a necessity for the chemical industry to source raw materials and create their products and intermediates based on renewable or recycled carbon atoms. A very interesting and promising building block for specialty chemicals is vanillin produced from the biomass component lignin. Given a highly efficient process, the applications for vanillin derivatives such as pentaerythritol spiro vanillin (PSV) in resins, coatings polymers and also engineered fluids have the potential to partly substitute chemicals such as for instance bis-phenol A (BPA) in epoxy systems and complement the family of rigid diols (CHDM, CBDO, isosorbide, hydrogenated BPA, etc.) for polyesters giving higher glass transition temperatures for packaging- and fiber applications, increased thermal and hydrolytic stabilities as well as introducing the acetal linkages suitable for chemical recycling at very low pH also for crosslinked materials.

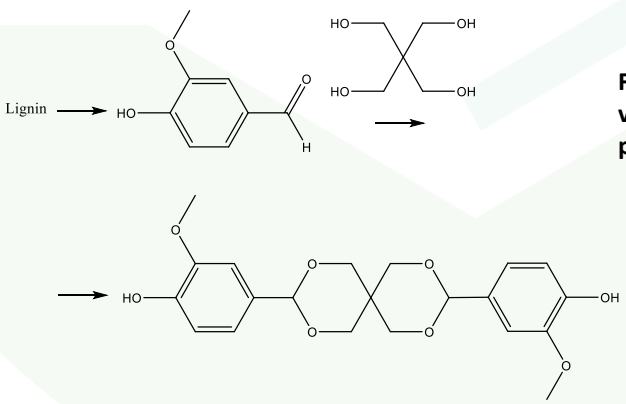

Figure 1. Conversion of lignin-based vanillin into pentaerythritol diacetal or pentaspirovanillin (PSV).

Novel straightforward two-step synthesis of diols with a spirocyclic acetal structure, starting from bio-based vanillin and pentaerythritol (Penta) as well as di-trimethylol propane (Di-TMP) has been developed. According to preliminary life cycle assessment (LCA), the greenhouse gas emissions from these bio-based diols are significantly lower than those of for instance bio-based 1,3-propanediol.

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Several copolymerizations of PSV rigid spiro-diol with neopentyl glycol (Neo), 1,6-hexanediol (HDO), terephthalic acid (TPA) and dimethyl terephthalate (DMT) by melt and solution polymerizations yielded a series of copolyesters, which showed improved glass transition temperatures and thermal stability upon the incorporation of the spiroacetal units. The crystallinity and melting point of copolyesters decreased with increasing content of the spirocyclic backbone structures. As an example, the copolyesters containing 10 % of the new PSV diol was semicrystalline, while those with 20 and 30 % spiro-diol incorporated were completely amorphous. Moreover, dynamic mechanical analysis indicated that the copolyesters showed storage moduli comparable to Akestra, a commercial fossil-based high-performance polyester. For the synthesis of glycidyl ethers, greener alternatives to the ubiquitously employed epichlorohydrin reagent has been developed. These functionalized monomers have been used in crosslinking reactions to form bio-based and potentially chemically recyclable thermosetting materials.

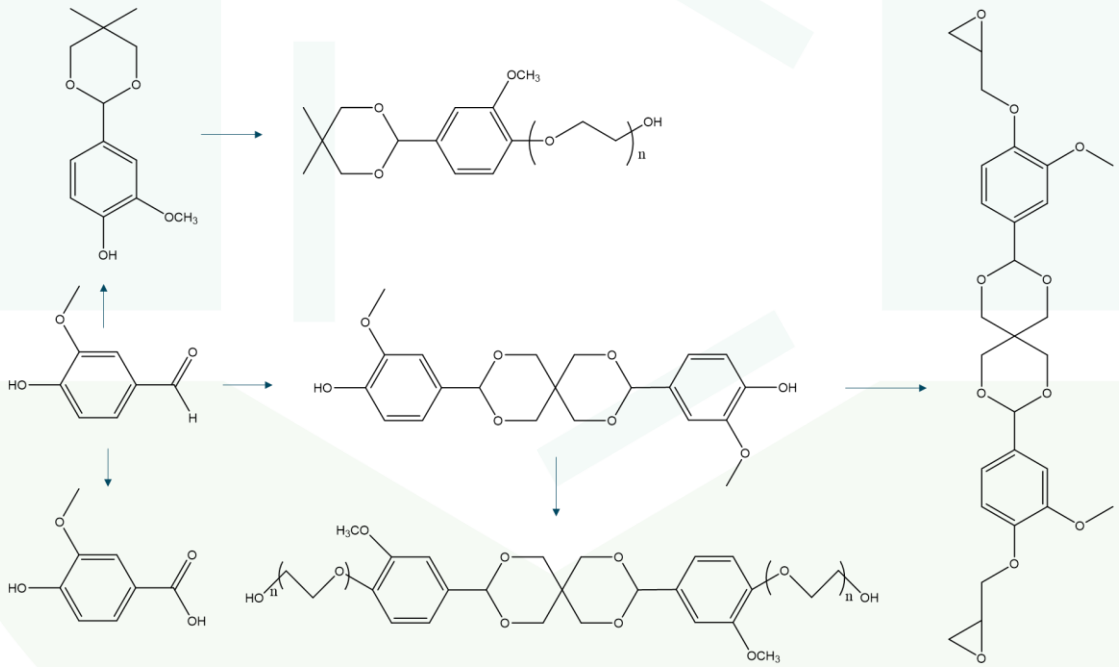

Figure 2. Summary of potential uses of vanillin and vanillin derivatives.

The interest in the use of vanillin for the preparation of renewable specialty chemicals towards applications in resins, coatings and polymers is based on that design parameters such as glass transition temperature, tensile strength, modulus, elongation at break, adhesion, pencil hardness properties and chemical resistance are comparable to or even better than those of conventional building blocks. Moreover, facilely recyclable materials can be designed using the acid-triggered structure of spiro diacetal functionality.

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