ABSTRACT

The growing awareness of environmental issues and sustainable development is focused on obtaining materials from renewable sources. Lignocellulosic biomass represents the most important renewable source of organic carbon on earth, making it a natural source for the production of chemicals. In doctoral dissertation, we focused on the utilization of less utilized components of plant biomass from IAPS (lignin, ferulic acid, and secondary metabolites).

We investigated the oxidative cleavage of double and single C–C bonds, which is an important reaction for decomposition of complex molecules from biomass, from a synthetic point of view. Using the oxidant H_2O_2 and the catalyst V_2O_5, we developed a method for selective oxidative cleavage of C–C double bonds. The method allows selective conversion of cinnamic acid derivatives into benzaldehydes, benzoquinones or benzoic acids. The selectivity of the reaction depends on the solvent chosen. Derivatives of *p*-hydroxycinnamic acid were selectively converted to the corresponding benzaldehydes in DME and to benzoquinones in TFE. Cinnamic acid and styrene derivatives, which do not have a hydroxyl group at the *para* site, were selectively converted to benzoic acids in MeCN. The method allows selective conversion of ferulic acid to vanillin (91 %) in the presence of 7 eq. of 30 % H_2O_2 and 5 mol% catalyst. Oxidative cleavage of single C-C bonds plays an important role in the conversion of lignin to platform chemicals. A previously developed method based on H_2O_2/V_2O_5 was extended to various types of lignin. We used commercial lignin and real samples of kraft and organosolv lignin from Japanese knotweed, Staghorn sumac, and spruce. Due to the different structures of the lignin samples as determined by NMR spectroscopy, oxidative degradation was studied separately on all three sample types. In DME, commercial lignin and kraft lignin of spruce were successfully converted to vanillin (yields: 9.9% and 7.6%). Kraft lignin from Japanese knotweed was successfully depolymerized to a mixture of aromatic products.

IAPS are rich in various structural types of natural dyes, that have been isolated by extraction. Emodin isolated from Japanese knotweed was chemically modified by introducing various functional groups through nitration, sulfonation, and halogenation. Chemical modification of the emodin structure affected its color, binding, and antiviral and antibacterial properties. The emodin derivatives were photochemically characterized and used as photoredox catalysts for photoreduction of aryl halides. A Structure-Activity Relationship was performed with the emodin derivatives for antiviral activity against HCoV-NL63. Iodinated E-3I and brominated emodin E-2Br showed comparable antiviral activity as Remdesivir, which is already approved for use in emergency COVID-19 cases. Emodin derivatives were successfully bound to textile material (wool and polyamide). The functionalized textile material also showed antibacterial activity against *S. aureus*. Emodin, IAPS extracts, lignin and PHA were successfully incorporated into silane-type coatings, enabling the preparation of colored and transparent hydrophobic coatings for glass and wood.

Keywords: *Invasive alien plant species, H_2O_2, oxidation, green and sustainable chemistry, biomass, lignin, ferulic acid, vanillin, natural dyes, emodin, HCoV-NL63, coatings.*