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MASS SPECTROMETRY FOR BIO POLYESTER ANALOGUES

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The direct evidence of the ring-opening polymerization (ROP) mechanism of β-lactones initiated with strong nucleophiles was provided by ESI-MS^n over 15 years ago. The polymer chain growth proceeds regioselectively and stereoselectively entirely via carboxylate anions. Propagation on carboxylate active centers (much less sensitive to impurities than any other anionic species) enables the scaling up of the anionic ROP polymerization process towards PHA biopolyester analogues. The specific synthetic method based on the carbonylation of the respective epoxides under CO at ambient pressure opens up new opportunities for exploring the utility of substituted β-lactones as monomers for the synthesis of new PHA analogues with desired properties. Results of the further studies regarding this area will be presented. Special emphasis will be given to PHA analogues with the desired molecular structure, including the structure of the end groups. The molecular level structures of synthetic analogues of PHA will be discussed based on the ESI-MS fragmentation experiments, preferably used because of distinct fragmentation pathways along the PHA chain.

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