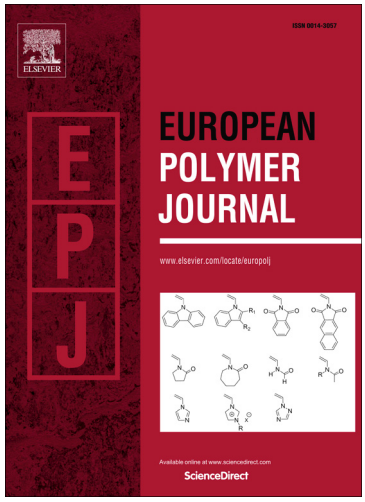

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The influence of a methyl substituent on molecularly imprinted polymer morphology and recognition – acrylic acid *versus* methacrylic acid

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Abstract: In this report, we have investigated factors contributing to the morphology and template recognition of bupivacaine-imprinted copolymers of methacrylic acid (MAA) and ethyleneglycol dimethacrylate (EGDMA). To this end, MAA, the most commonly used functional monomer in non-covalent molecular imprinting protocols, was compared and contrasted with the closely related acrylic acid (AA) in terms of polymer morphologies, recognition characteristics, and molecular level events in the corresponding pre-polymerization mixtures. Two series of analogous bupivacaine-imprinted EGDMA-copolymers containing increasing fractions of either AA or MAA were studied through all-component MD simulations in the pre-polymerization phase, equilibrium binding experiments on corresponding synthesized polymers and morphology characterization by N_2-sorption measurements. A higher degree of hydrogen bonding frequency between respective functional monomer and bupivacaine was recorded for the mixtures containing AA compared to those containing MAA. In contrast, results from binding experiments demonstrated higher binding capacities for the polymers prepared with MAA than for those prepared with AA, which is explained by differences in polymer morphology. The surface areas and pore volumes of the AA-polymers were higher than for the MAA-polymers and the overall