

## Methacrylate Derivatives of Bile Acids for Use as Monomers for Dental Resins

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### Statement of Purpose:

The organic matrix of dental composites is typically a mix of two or more methacrylate monomers. The most common are 2,2-bis(4-(2-hydroxy-3-methacryloxypropoxy)phenyl)propane (BisGMA), 1,6-bis(methacryloyloxy-2-ethoxycarbonylamino)-2,4,4-trimethylhexane (UDMA) and triethyleneglycol dimethacrylate (TEGDMA). Despite their common use in dental composites, the high levels of stress produced during polymerization shrinkage and the release of organic leachates due to incomplete polymerization have prompted efforts towards improving the properties of the organic matrix. Current research trends focus on developing monomers that are less viscous, more biocompatible and shrink to a lesser extent during polymerization while maintaining high monomer conversion and mechanical properties. We have used bile acids, natural compounds in the body, for the design and preparation of new monomers for use as dental materials.

We report the preparation of multi-methacrylate monomers derived from cholic acid, the most abundant bile acid, the polymerization behavior in terms of conversion and shrinkage of these monomers in the presence of TEGDMA and the mechanical properties of the resulting polymers and composites. Our objective is to elucidate whether multi-methacrylate monomers based on cholic acid have potential as dental monomers, which would validate the evaluation of more complex formulations containing these monomers and further experimentation in clinically relevant experiments.

### Methods:

The monomers containing bile acids were synthesized as described previously.[13] Monomer mixtures were irradiated with an Optilux 401 visible-light gun. Post-curing of the polymers was done at 120°C for 24 h. Composites were prepared by initially incorporating the monomer mixture to the silanated filler consisting of a mix of the silanated SiO<sub>2</sub> and pyrogenic silica. The extent of silanization was ~6 wt% for both fillers as determined by thermogravimetric analysis.

Near-infrared spectra of the monomer mixtures and of the polymers were used to determine the degree of conversion. Dynamic mechanical properties of the polymers were measured between -50 and 150°C. All thermograms and stress-strain curves were recorded at in quintuplicate. Polymerization shrinkage was measured by axisymmetric drop analysis using a contact angle analyzer.

### Results:

The mixtures containing the commercial monomers BisGMA and UDMA exhibited higher shrinkage values

than most of the monomers containing bile acid derivatives. The polymers containing the cholic acid monomers have a more complex thermo-mechanical spectrum than their commercial counterparts, resulting from their more complex structure. The intensity of the transitions observed for these polymers are less intense, which results in a greater thermal stability.

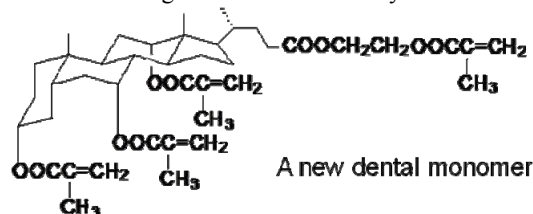


Figure 1. A methacrylate monomer based on cholic acid.

The elastic moduli of the commercial controls were comparable or inferior to those of all the polymers containing cholic acid derivatives. Polymers containing cholic acid-derived monomers had lower crosslinking density than the commercial monomers. The greater thermal stability of the polymers containing the cholic acid derivatives, despite their lower crosslinking density, demonstrates greater rigidity within the polymer network.

The polymers and composites containing cholic acid derivatives generally have moduli comparable to those containing BisGMA and UDMA. In general, differences between the composite formulations with respect to moduli and yield strengths were less pronounced than for the unfilled polymers.

### Conclusions:

This properties of the monomer and polymers were comparable to those prepared with the commercial models. The combined advantages of having multiple methacrylate groups and lower cytotoxicity make them promising candidates as dental resins. We plan to pursue further evaluation of such polymers in biological environments and characterize the nature, quantity, and toxicity of leachates from such materials.

### References:

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