

## Interfacial Design of Dentin Adhesive with a branched Carboxylic Acid Monomer

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**Statement of Purpose:** Water is ubiquitous in the mouths of normal, healthy individuals and under in vivo conditions, adhesives will experience physical phase separation at the interface with the wet tooth surface [1]. An increase of water miscibility can reduce the detrimental impact of phase separation, but hydrophilic monomers are plagued by problems such as increased water sorption and decreased mechanical properties [2,3]. A balance between hydrophobicity and hydrophilicity is required to promote the durability of dentin adhesives. In this work, a new glycerol-based dimethacrylate monomer with a vinyl and a carboxylate group is proposed as a dental comonomer that will provide improved water miscibility and mechanical properties. The objective of this work was to synthesize and characterize a new multifunctional monomer and to evaluate the properties of a dentin adhesive formulated with this new monomer under conditions that simulate the wet, oral environment.

### Methods:

Experimental adhesives contained 2-hydroxyethyl methacrylate (HEMA, Acros Organics, NJ), bisphenol-A diglycidyl ether dimethacrylate (bisGMA, Polysciences, Warrington, PA), and 4-((1,3-bis(methacryloyloxy)propan-2-yl)oxy)-2-methylene-4-oxobutanoic acid (BMPMOB), which was synthesized in our laboratory and used as a comonomer. To simulate the moist, oral environment, the adhesives control (HEMA/BisGMA 45/55 w/w) and experimental were formulated with 13 wt % water. The degree of conversion (DC) was determined by using a Spectrum 400 FTIR spectrometer (PerkinElmer, Waltham, MA). Dynamic mechanical analyses of cylindrical beam specimens (1mm x 15 mm) were performed using DMA Q800 (TA Instruments, New Castle, USA). The test temperature was varied from 0 to 200 °C with a ramping rate of 3 °C/min at a frequency of 1 Hz. The microscale morphologies of cured specimens were observed using X-ray  $\mu$ CT.

**Results:** The experimental formulations showed better water compatibility than the control (Fig. 1). With increased BMPMOB concentration, the maximum rate of polymerization and degree of conversion was decreased. Dynamic mechanical analyses in dry condition showed larger storage moduli and higher glass transition temperatures for the experimental formulations. In wet conditions, the copolymer with 25% BMPMOB showed improved mechanical properties as compared to lower concentrations and the controls.

**Conclusions:** By increasing the functionality of the comonomer, the balance between water sorption and mechanical properties can be controlled. The experimental adhesive copolymers had improved mechanical properties in both dry and wet conditions. These results indicate BMPMOB is a promising comonomer for improving dentin adhesives.

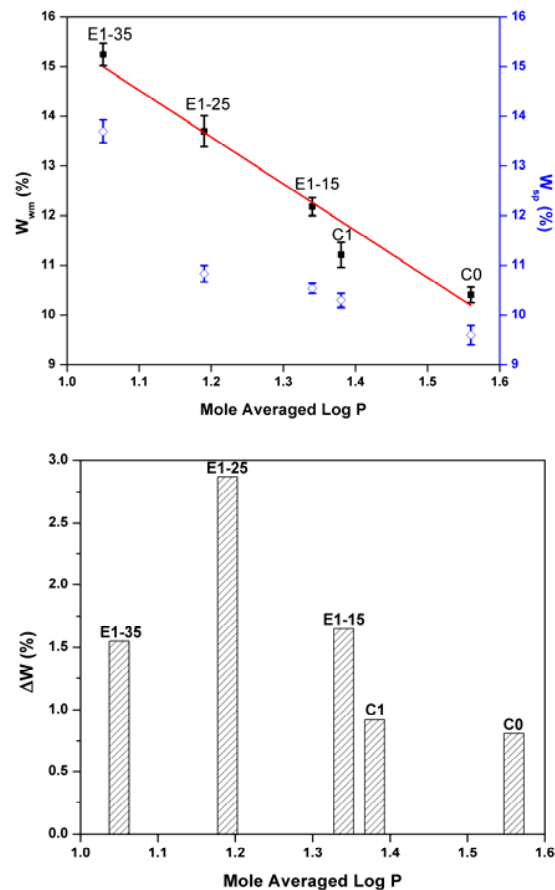


Figure 1. Relation between mole averaged log P and water miscibility of adhesive formulations, water sorption of copolymers contained BMPMOB.  $W_{wm}$  stands for water miscibility, and  $W_{sp}$  stands for water sorption. (■) represents the water miscibility value of liquid formulation; (◇) represents the water sorption of copolymer beam specimen, (▨) represents the difference between water miscibility of liquid formulation and water sorption of copolymer,  $\Delta W = W_{wm} - W_{sp}$ .

### References:

1. Spencer P, Wang Y. J Biomed Mater Res 2002, 62(3):447-456
2. Ye Q et al. J Dent Res 2011, 90(12):1434-1438
3. Ye Q et al. J Biomed Mater Res Part B 2012, 100B:1086-1092

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