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Exploring the Bioaccumulation Potential of Monomers Through Experimental LogP Determination

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Objectives Hydrophobic organic compounds can accumulate across biological membranes. To explore the bioaccumulation potential of monomers commonly used in dental materials, we experimentally determined their octanol-water partition coefficient (logP) using the shake-flask method and compared it with *in-silico* computed values.
Methods Monomers BisEMA-3, BisEMA-6, BisEMA-10, BisGMA, HEMA, TEGDMA, and UDMA were added to the pre-saturated 1-octanol/water system. The mixture was then equilibrated for 24, 48, and 72 hours, respectively. Next, the samples were analyzed using UPLC-MS/MS and the logP value was calculated using the formula $\log P = \log(PeakArea_{octanol} \times V_{octanol} / PeakArea_{water} \times V_{water})$. In addition, three *in-silico* models, namely KOWWIN, ACD/LogP, and XLogP3, were used to compute the logP values. The relationship between experimental and computed values was explored using linear regression and mean absolute error.
Results Although there was no statistical difference between the logP values at different time points (*two-way ANOVA, $p>0.05$*), it can be considered that the final equilibrium was reached at the 72-hour time point. At this time point, the mean experimental logP values, from highest to lowest, were as follows: BisEMA10 > BisEMA3 > BisEMA6 > BisGMA > UDMA > TEGDMA > HEMA. In addition, a trend of lower experimental values than computed *in-silico* values was observed. This trend was more noticeable for more hydrophobic monomers. For BisEMA-3, -6, -10, BisGMA and UDMA, the difference between the experimental and predicted values varied by more than ±1 log unit. The mean absolute error between the experimental and computed logP was similar for all *in-silico* models; the lowest was for KOWWIN (1.38), followed by XLogP3 (1.46) and ACD/LogP (1.58).
Conclusions Valuable experimental logP values of monomers commonly used in dental materials were successfully determined with UPLC-MS/MS. Lower experimental values than the ones calculated are reassuring regarding bioaccumulation potential. The experimentally determined values could improve the *in-silico* models.