Abstract:
The typical bitterness of fresh beer is well-known to decrease in intensity and to change in quality with increasing age. This phenomenon was recently shown to be caused by the conversion of bitter tasting trans-iso-alpha-acids into lingering and harsh bitter tasting tri- and tetracyclic degradation products such as tricyclocohumol, tricyclocohumene, isotricyclococumene, tetracyclocohumol, and epitetracyclocohumol. Interestingly, the formation of these compounds was shown to be trans-specific and the corresponding cis-iso-alpha-acids were found to be comparatively stable. Application of 18O stable isotope labeling as well as quantitative model studies combined with LC-MS/MS experiments, followed by computer-based molecular dynamics simulations revealed for the first time a conclusive mechanism explaining the stereospecific transformation of trans-iso-alpha-acids into the tri- and tetracyclic degradation products. This transformation was proposed to be induced by a proton-catalyzed carbon/carbon bond formation between the carbonyl atom C(1') of the isohexenoyl moiety and the alkene carbon C(2'') of the isoprenyl moiety of the trans-iso-alpha-acids.