# MS30-P05 | SEPARATION AND RESOLUTION OF METHYLCYCLOHEXANONES BY ENCLATHRATION WITH DEOXYCHOLIC ACID

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Molecular selectivity by host-guest procedures is a method which can be applied to the separation of enantiomers. The resolution of methycyclohexanones (MCH) by enclathration has been studied using a variety of chiral hosts[1,2]. For the analysis reported here, deoxycholic acid (DCA) was used as a host to separate and resolve the different isomers of (MCH) whose normal boiling points range from 162 to 169℃. Competition experiments of these isomers resulted in a preference of DCA towards 2MCH with the following trend 2MCH>3MCH>4MCH. This trend was then confirmed by differential scanning calorimetry results. Additionally, DCA resolved 2MCH by enclathrating the S-conformer, but 3MCH remained unresolved. However, competition experiments of rac-2MCH/rac-3MCH resulted in both guests been resolved yielding to (S)-conformers, this suggested that 2MCH had a templating effect on the final structures. This was then proven along a selectivity curve of 2MCH vs 3MCH with 2MCH mole fraction varying from 0 to 1. This is shown in figure 1.
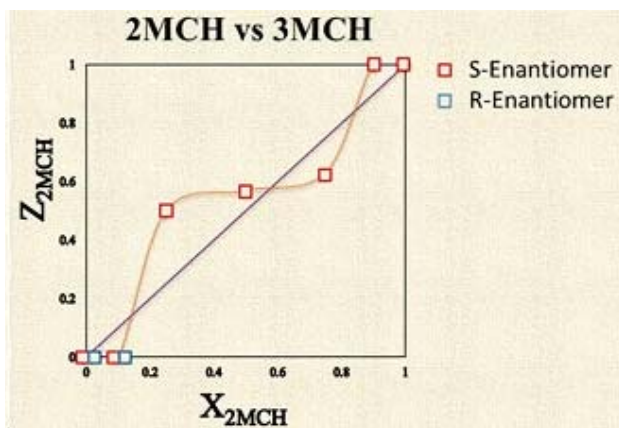
Figure 1. Competition experiment of 2MCH vs 3MCH with S-enantiomer represented in red while the R-enantiomer is represented in blue.

[1] Weber, E.; Reutel, C.; Foces-Foces, C.; Llamas-Saiz, A. L. J. Alanine-derived hosts comprising a roof-shaped carbonimide framework. Synthesis, inclusion formation and X-ray crystal structures of racemic and optically resolved free hosts, and their crystalline complexes with 3-methylcyclohexanone. Soc. Perkin Trans.2 1994, 1455-1461.
[2] Batisai, E.; Nassimbeni, L.R.; Weber, E. Inclusion compounds of a borneol dumb-bell host with methylcyclohexanones and 2-butanols: structures and resolutions. CrystEngComm. 2015, 17, 4205-4209.