

## Life cycle assessment of an optimized lab-scale production of thio-functionalized beta-cyclodextrins

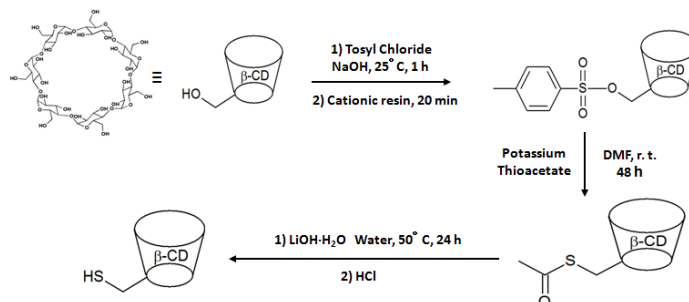
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Cyclodextrins (CD) form inclusion complexes and alter physical, chemical and biological properties of guest molecules, hence they are good candidates for drug delivery [1]. Furthermore, their complexing ability is enhanced by chemical modifications of their structure [2]. Polymers are good drug delivery vectors, due to their chemical modulation properties. They can be formulated as nanoparticles and applied to treat diverse diseases. Among them, poly(4-acryloylmorpholine) (PACM) is biocompatible and bio-eliminable (if its molecular weight is sufficiently low) and through controlled radical polymerization, we can insert chemical functions at the end of oligomers [3].

To further develop  $\beta$ -CD-PACM conjugates as components of pharmaceutical formulations, it is necessary to have a suitable large-scale production process. On the other hand, the continuous increase in awareness towards environmental issues leads civil society to demand less impacting products. Companies demonstrate the benefit of their products with life cycle assessment (LCA) while academics continue to develop the methods. Together, companies and universities respond to customers desires for greater environmental sustainability [4].

Here, we assessed the environmental burdens of the optimized laboratory synthesis of thio-functionalized  $\beta$ -CD with a life cycle analyses. SimaPro 8.1.1.16 modelled all the process. ILCD method calculated midpoint and endpoint impact categories. We measured electric consumption of all the pieces of equipment employed and calculated the standard deviation. A Monte-Carlo analyses calculated LCA results uncertainty.



**Figure 1.** Synthetic route for the preparation of mono-substituted  $\beta$ -CD-SH starting from  $\beta$ -CD.

We also compared the impact of a homogeneous vs a heterogeneous (weak acid resin) acidifier to precipitate the functionalized CD and evaluated the economic improvement. All the steps of the optimized synthesis had greater yield and purity. LCA demonstrated that the optimized synthesis is more favourable compared to the typical laboratory procedures. We encourage the spread of the environmental analyses about chemical lab-scale synthesis.

### References

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