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# Eco-design of new cosmetic ingredients by in silico fragment-based methods

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## PURPOSE OF THE ABSTRACT

The purpose of this study was to quickly get access to an active, safe and easily accessible candidate molecule for development, using innovative in silico methods to select new compounds having beneficial effects on healthy skin.

Through a process of fragmentation, functionalization, and recombination of 274 market approved molecules for cosmetic usage, we customized an in-house virtual library of 92,000 molecules ideally suited for virtual screening.

With this library in hand, we used cosmetophore*-based virtual screening to establish the proof of concept of our approach on a novel skin protein target. Hence, computational cosmetophore-based screening of this virtual library followed by a 3 month optimization phase led to the identification of an optimized lead with all its expected properties in hand to be developed as a candidate molecule for skin care in cosmetic applications.

This pilot project showcases the power of in silico approaches, allowing successful hit and lead discovery while reducing synthesis effort.

* A cosmetophore is an ensemble of steric and electronic features that are necessary for molecular recognition of a ligand by a cosmetic target.

## FIGURES


### FIGURE 1

From known cosmetics to new ingredients

Illustration of the in silico fragment-based tailor-made approach for cosmetics

### FIGURE 2


## KEYWORDS

in silico | virtual library | fragment-based | virtual screening


## BIBLIOGRAPHY