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Investigation of the Experimental and Theoretical Release of Caffeine from Cosmetic Hydrogels and Patches

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Introduction:

Hydrogel formulations are well established for their use in cosmetic products, the release of cosmetic active ingredients depends on the hydrogel structure and their rheological properties, *In vitro* release testing by Franz cells is a commonly used experimental method to determine the release from cosmetic formulations.
Molecular docking (MD) is a widely used computational tool, which could provide a better understanding of the interactions in chemical systems by predicting the most probable type and location of binding.
A comparison between theoretical calculation and experimental results were performed in this study, aiming to find out whether and to which extent, the two sets of results would correlate. Thus, providing a 'proof of concept' that the in vitro release of caffeine from hydrogels could be predicted by using theoretical MD approach, for achieving a more efficient and sustainable cosmetic formulation development process.

Materials & Methods:

- MD studies of caffeine and gelling agents (GAs) were performed by the Autodock Vina software. The GAs and caffeine structures were optimised by the Density Functional Theory (DFT) calculations.

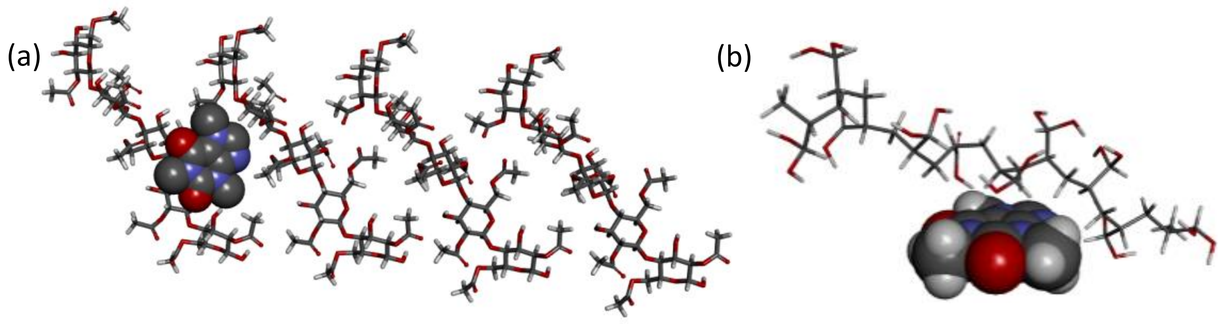

Figure 1. Examples of molecular docking visualisation - the most favourable binding site between (a) caffeine and membrane, (b) caffeine and gelling agent, xanthan gum.

- Fused Deposition Modelling 3D printing technology was employed for fabricating the patches for Franz cells where hydrogels were loaded onto. Two types of patches with different materials, namely inert polylactic acid (PLA), and swellable polyvinyl alcohol (PVA) patches. When PLA patches were used, due to the inert nature of PLA, it was assumed there was no interaction between formulations and the patch.
- 6 caffeine formulations were prepared with different gelling agents (GA), namely carrageenan (Carr), guar gum (GG), hydroxyethyl cellulose (HEC), Sodium carboxymethyl cellulose (NaCMC), sodium polyacrylate (NaPA) and xanthan gum (XG). The rheological properties of the hydrogels were characterised.
- IVRT of caffeine released from 6 hydrogels and hydrogel loaded patches were performed using vertical diffusion cells (Copley, UK), with cellulose acetate membrane, at 30 min, 1 h, 2 h, 3h, 5h, and 6 h. Each set of experiment was repeated 5 times.

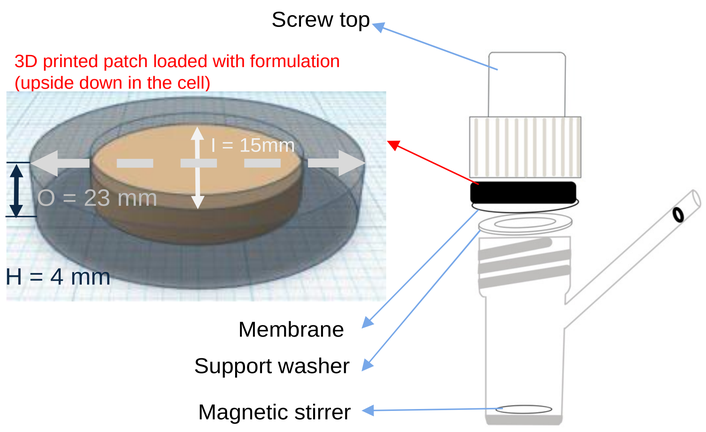

Figure 2. Schematic diagram of experimental set-up.

Results & Discussion:

Molecular Docking Results

- The binding energy (BE) for the caffeine-membrane system was −5.0 kcal/mol;
- The caffeine affinity towards membrane was higher than towards any GA.
- All GAs possess higher affinity towards membrane than towards caffeine. The difference between these affinities (membrane-GA and caffeine-GA) is almost identical.

Gelling agent	Binding energy (kcal/mol) towards		ΔE (kcal/mol)
	CA membrane	Caffeine	
XG	-6.3	-4.1	-2.2
NaCMC	-5.3	-3.1	-2.2
Carr	-6.0	-3.7	-2.3
NaPA	-4.1	-2.4	-2.3
HEC	-5.7	-3.4	-2.3
GG	-6.8	-4.3	-2.5

Experimental results

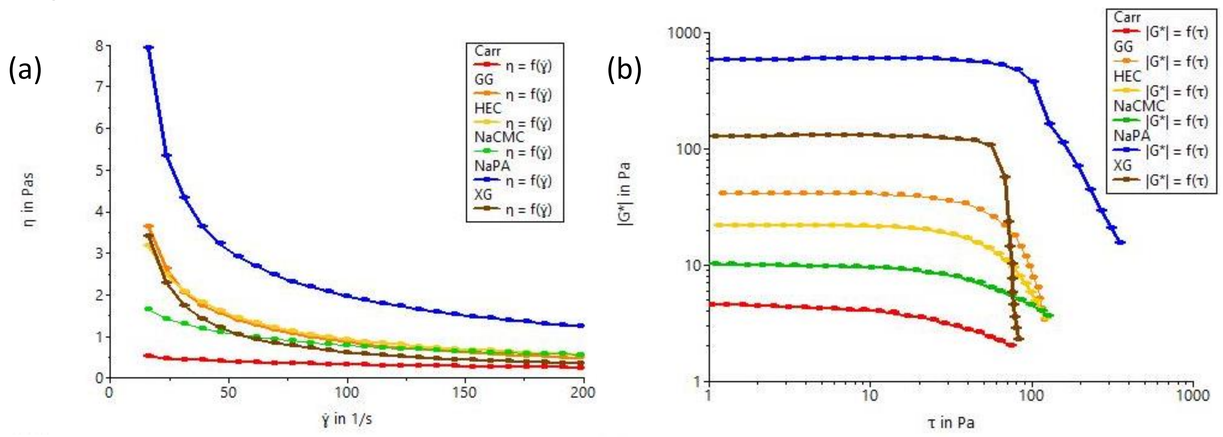

Figure 3. Rheological characterisation tests results, from (a) shear rate sweep, (b) the oscillatory stress sweep.

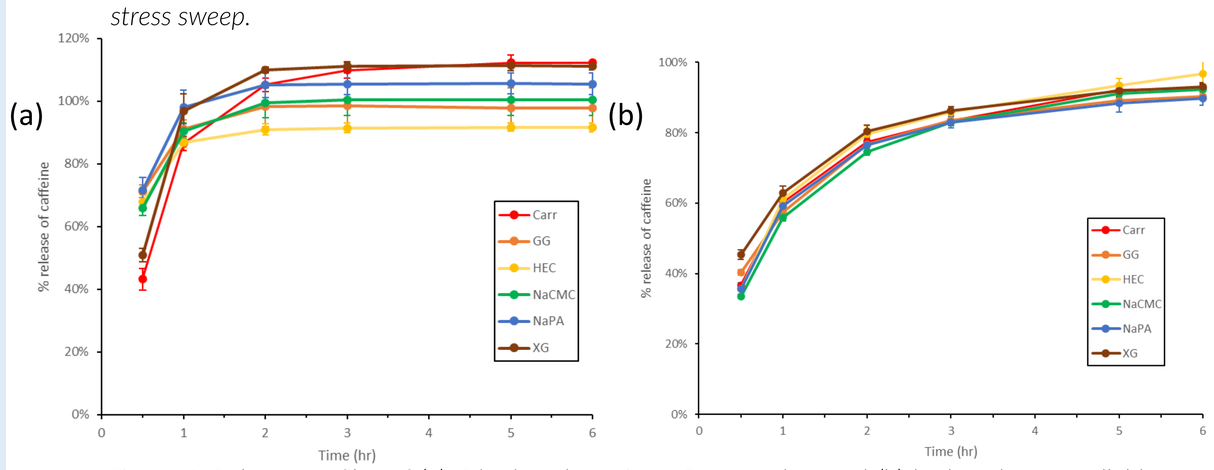

Figure 4. Release profiles of (a) 6 hydrogels on inert PLA patches and (b) hydrogels on swellable PVA patches, standard deviation was added as error bars.

- The MD results indicated that there would be no distinctive difference in caffeine kinetics among the hydrogels studied, which agrees with the experimental results. Theoretical calculation also indicates that the overall intermolecular forces would lead to the diffusion of caffeine from the hydrogel and its interaction with the membrane.

Conclusions:

Promising initial results were obtained, providing a 'proof of concept'. It was shown that molecular docking could partly explain how the chemical structure of gelling agents affects the release of caffeine from the hydrogels, loaded on two types of 3D-printed skin patches.
In common with other theoretical models, molecular docking suffers from over-simplifying the complex system of cosmetic active release. It is not likely to become a stand-alone solution for designing effective cosmetic formulations but, with further method development, it has the potential to assist researchers in the selection of excipients for the given active ingredient.

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