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Molecular modelling of amylose-lipid complexes (resistant starch 5) to identify fatty acid candidates for in vitro and in vivo studies

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Amylose, the linear fraction of starch, can form single helix inclusion complexes with a range of guest molecules including lipids, iodine, alcohols and flavour compounds[(1)]. Amylose-lipid complexes (ALCs) are known as resistant starch 5.

When eaten in food such as bread, potato or pasta, resistant starches withstand digestion by ensymes in the small intestine and pass into the colon where they act as substrates for fermentation by the gut microbiota[(2)]. Starch digestion in the small intestine is critical in determining post-prandial blood glucose and insulin concentrations, with wider health implications in development and management of metabolic and cardiovascular diseases[(3)]. This includes lower blood glucose and cholesterol levels, lower risk of colo-rectal cancers and cardiometabolic diseases, and increased satiety[(4)].

Enhancement of starchy foods, for example pasta, with ALCs would bring a host of health benefits, and molecular modelling can be used to gain greater understanding of the structure and behaviour of ALCs in order to optimise their incorporation into food matrices. The aim of this study was to use molecular modelling to identify whether ALCs were more stable with one or two fatty acids, and which fatty acid gave the most stable complex.

Molecular Mechanics was performed using the AMBER forcefield to build ALC molecules and measure their strain energy under static conditions. A 24 glucose-residue V-amylose helix was modelled with saturated fatty acids (even numbers C8-C22), and the complex binding energy calculated to determine the optimum amylose-fatty acid configuration.

Molecular Dynamics simulations were run on the same molecules solvated in a 55Å water cube, then the binding energy calculated.

When there is one saturated fatty acid in the complex, potential energy decreases as the hydrocarbon tail length increases, showing an increase in stability. However, when two fatty acids are in the complex, stability increases up to C16 (palmitic acid) then decreases for the longer chains.

Once solvated, single fatty acids reach an optimum at C12 (lauric acid) and then stability decreases. Double fatty acids increase in stability up to C20 (arachidic acid), then decrease at C22. Electrostatic interactions also peaked at C20 and dropped at C22, indicating that they have a stabilising effect on the complexes.

These results will inform which ALCs are produced in the lab to stand the greatest likelihood of being stable in foods, so they do not breakdown before reaching the small intestine of consumers. This optimum was C20 for ALCs containing two fatty acids. Further studies will look at the impact of the length of V-amylose polymers on formation of ALCs and on mixed combinations of fatty acids.

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