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ACCEPTED MANUSCRIPT

New insights into the efficiency of thymol synergistic effect with p-cymene in inhibiting advanced glycation end products: A multi-way analysis based on spectroscopic and electrochemical methods in combination with molecular docking study

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Highlights

• The inhibitory activity of thymol and its synergistic effect with p-cymene were linked to its antioxidant property to reduce the formation of AGEs.

• A multi-way analysis based on spectroscopic and electrochemical methods shows that inhibitors have antiglycated activities in a concentration-dependant manner.

• Molecular docking study reveals that thymol has protective effects toward arginin or lysine modification.

• Thymol and p-cymene are a part of diet in the form of spices and thus thay have major benefits in preventing

the non-enzymatic glycation in vivo.

ABSTRACT

Protein glycation in the body is one of the main reasons of diabetes complications. The electrochemical studies on the inhibitory mechanism of glycation are rather scarce. Thus, it is important to investigate the role of electrochemistry in the glycation process with basic chemometric frameworks. The aim of the current study is to investigate the anti-glycation effects of candidate compounds from thyme species i.e. thymol and p-cymene. To gain this objective, the electrochemical and absorption responses of glycated bovine serum albumin (BSA) in the absence and presence of inhibitors were recorded after 20 day of incubation. Due to the presence of multiple binding sites on BSA for the interaction with glucose, there are overlapping between the signals of these sites. Therefore, it is reasonable to use chemometric

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