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Novel flavonoid extracted from Coriandrum sativum in treatment of diabetic nephropathy

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Objectives: It has been known that renin-angiotensin system (RAS) pathway is involved in the kidney diseases especially diabetic nephropathy. It is important to identify the novel ACE inhibitors from herbs that can inhibit the enzymes that are involved in the pathway. Therefore, our objective of this study was to investigate the insilico therapeutic role of plant flavonoids extracted from *coriandrum sativum* (a herb) in targeting the angiotensin- converting enzyme (ACE) inhibition.

Methods: The three-dimensional structure of ACE used for the present docking study was taken from Protein Data Bank (PDB ID: 1O86). The ligands used in the study were apigenin, daidzein, and luteolin, pectolinarigenin, pinocembrin, pseudobaptigenin, quercetin extracted from *coriandrum sativum* and the standard drug remipril 3D structure of were retrieved from PubChem Compound Database. Consequently, the ligands were docked to ACE protein using "Autodock 4.2." The final figures were generated with the help of Discovery Studio Visualizer (Accelrys San Diego, CA, USA).

Results: Our result shows that ACE Inhibition of pseudobaptigenin to be most effective and can provide their possible clinical significance against hypertension and nephropathy. Further, we have calculated based on minimum inhibition constant, Ki and highest negative free energy of binding with the maximum interacting surface area in the docking studies. We reported that the binding energy was highest in pseudobaptigenin (-5.77 kcal/mol). The free binding energies were (- 5.45 kcal/mol), (- 5.24 kcal/mol) and (-4.9 kcal/mol, (-4.82 kcal/mol, (- 4.77 kcal/mol, (- 4.75 kcal/mol) using apigenin, pinocembrin, daidzein, pectolinarigenin, quercetin, and luteolin compared to the standard drug (- 3.66 kcal/mol), respectively.

Conclusions: This study may provide the clue that pseudobaptigenin, apigenin, pinocembrin could provide the best therapeutic potential compared with other selected herbs in the treatment of hypertension and related morbidities such as diabetic nephropathy.