

Abstract ID: - 178

Abstract Topic: - Omics technologies

Abstract Title: - Satvik Dietary Phytonutrients as a Potential Modulators of Anti-Citrullinated Protein Antibodies in Rheumatoid Arthritis: A computational technologies

Presenting author name: - Dhavalkumar Solanki

Presenting author institute: - Department of Zoology, Biomedical Technology, Human Genetics and Wildlife Biology & Conservation , University School of Sciences, Gujarat University, Ahmedabad - 380 009. Gujarat, India.

Co-authors name: - Janvi Mistry, Mohammadfesar Ghanchi, Dr. Gaurankumar Sindhav, Pooja Trivedi

Co-authors institute: - Department of Zoology, Biomedical Technology, Human Genetics and Wildlife Biology & Conservation , University School of Sciences, Gujarat University, Ahmedabad - 380 009. Gujarat, India., Department of Zoology, Biomedical Technology, Human Genetics and Wildlife Biology & Conservation , University School of Sciences, Gujarat University, Ahmedabad - 380 009. Gujarat, India., Department of Zoology, Biomedical Technology, Human Genetics and Wildlife Biology & Conservation , University School of Sciences, Gujarat University, Ahmedabad - 380 009. Gujarat, India., Department of Zoology, Biomedical Technology, Human Genetics and Wildlife Biology & Conservation , University School of Sciences, Gujarat University, Ahmedabad - 380 009. Gujarat, India., , , , ,

Aims: - Green gold – diet, nature’s most efficient remedy and our multibillion economy. New-emerging large scale health issues clearly associated with our life style, especially during such far progress scientists too signify the healthy, complete, timely and “Satvik” diet is unavoidable domain as well as mandatory to have health acuity. Distraction and self-centered living all around the world are impacted many health anomalies, which are a global health threat. One of prominent alteration is in our unique system that is immune may be due to unceasing and over used. Rheumatoid Arthritis (RA; OMIM#180300), characterized by the redundant formation of autoantibodies viz. Rheumatoid Factor (RF) and Anti-Citrullinated Protein Antibodies (ACPAs) and downstream cascade impairment. With these the present study thought to explore with dietary phytonutrients, may be used as a palliative for the available Disease-Modifying Anti-Rheumatic Drugs (DMARDs). Given the foregoing, the purpose of this study is to evaluate the therapeutic potential of satvik dietary phytonutrients in alleviating Rheumatoid Arthritis (RA) by investigating their functional property to modulate Anti-Citrullinated Protein Antibodies and reduce inflammation.

Methods: - Various dietary phytonutrients such as taxifolin, stigmaterol, apigenin, rutin and curcumin have exhibited potential in both restraining ACPA production and mitigating inflammation also intoned and incorporated in our routine diet since long. In this context, we employed YASARA (Yet Another Scientific Artificial Reality Application), a high-throughput computational tool, for conducting Molecular Docking (MD). Primary objective was to scrutinize the intricate interplay and molecular mechanisms governing the influence of dietary phytochemicals on ACPA. Consequently, we conducted molecular

docking of ACPA antibodies with a comprehensive catalogue of 150 routinely practised dietary phytochemicals.

Results: - MD analysis concluded that stigmasterol, cholecalciferol, curcumin, apigenin, taxifolin and rutin with scores of 8.08, 7.87, 7.2, 7.1, 6.95, and 6.8 kcal/mol respectively, were chosen based on their docking scores and their interactions with the key molecule/s present in the ATP binding pocket. Such compounds act as potential suppressors and/or regulatory of ACPA antibodies through their unique molecular interactions with the ACPA-binding pocket.

Conclusions: - These insights shed light on the molecular mechanisms by which these nature's gift could be harnessed as complementary management. Further additional experimental confirmation is indeed required, this computational perspective provides a foundation for comprehending the molecular underpinnings, diet practice enhancements, options for amelioration and holds substantial potential for enhancing one's quality of life.

Keywords: - MD analysis concluded that stigmasterol, cholecalciferol, curcumin, apigenin, taxifolin and rutin with scores of 8.08, 7.87, 7.2, 7.1, 6.95, and 6.8 kcal/mol respectively, were chosen based on their docking scores and their interactions with the key molecule/s present in the ATP binding pocket. Such compounds act as potential suppressors and/or regulatory of ACPA antibodies through their unique molecular interactions with the ACPA-binding pocket.