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## *In-silico* Analysis of the Potential Inhibitory Effects of Curcumin and Chlorogenic Acid on the Pathological Aggregation of Prevalent Mutants of Human Superoxide Dismutase 1

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Familial amyotrophic lateral sclerosis (ALS) has been linked with mutant misfolded superoxide dismutase (SOD) aggregates in motor neurons. Although the aggregation pathway has not yet been fully elucidated, the use of naturally occurring polyphenols to inhibit this deleterious process shows pharmacologic potential for intervention. Curcumin, the polyphenolic active component of turmeric, has been demonstrated to have inhibitory properties against the aggregation of a broad spectrum of misfolded proteins. Using Autodock Vina, Autodock tools and Discovery Studio Visualizer, both the keto and enol forms of curcumin as well as chlorogenic acid, a curcuminoid, were docked with A4V and I113T, two prevalent mutants of SOD and the protein in its wild type configuration, comparing metal bound versus apo versions of the protein. Putative binding sites as well as ligand binding affinities and protein bound configurations were determined and analyzed. The results indicate that the ligands form stable complexes with these proteins, with chlorogenic acid exhibiting higher levels of binding affinities for the two mutants and wild type SOD.

### Biography

James Villanueva is the recipient of the DuPont – National Academy of Science and Technology Young Scientist Award in 2003 and has been teaching Medical Biochemistry, Genetics and Nutrition at IAU since 2005. He received the IAU Faculty of the Year Award in 2006 and was appointed as the Dean of Student Affairs in 2007 and elected Chairman of the Admissions Committee in 2008. His research interests include protein folding/misfolding, protein spectroscopy, development of immunoliposomes and biodesulfurization. He has completed Post-Doctoral research work at Notre Dame University in Indiana; The Institute for Protein Research, Osaka University, Japan and Bari University, Italy. Over the years, he has consistently made outstanding contribution to student success in NBME Shelf exams and is closely associated with the university student community as the Faculty Advisor to the Student Government Association (SGA). He was promoted to full Professor of Biochemistry, Genetics and Nutrition in September of 2011 and then as the Dean of Basic Sciences in 2014, he continues to inspire and be inspired by academia.

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