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Supporting Information

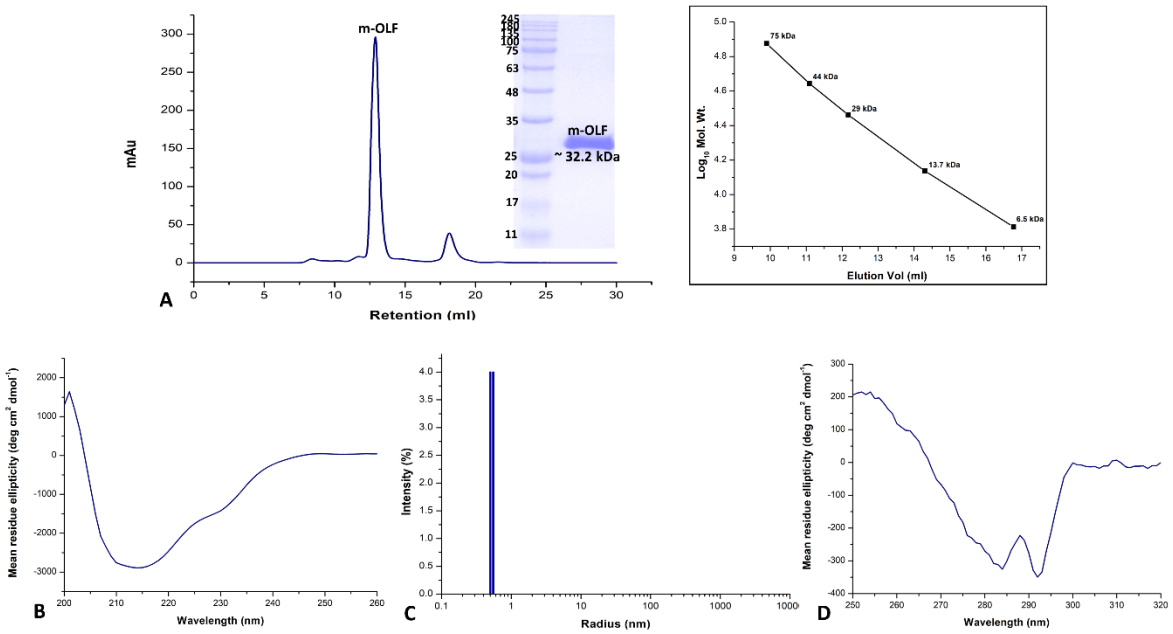
# Amyloid fibrillation of the glaucoma associated myocilin protein is inhibited by Epicatechin Gallate (ECG)

Ritika Sharma, [a] Anchala Kumari, [b] Bishwajit Kundu [c] and Abhinav Grover[*], [a]

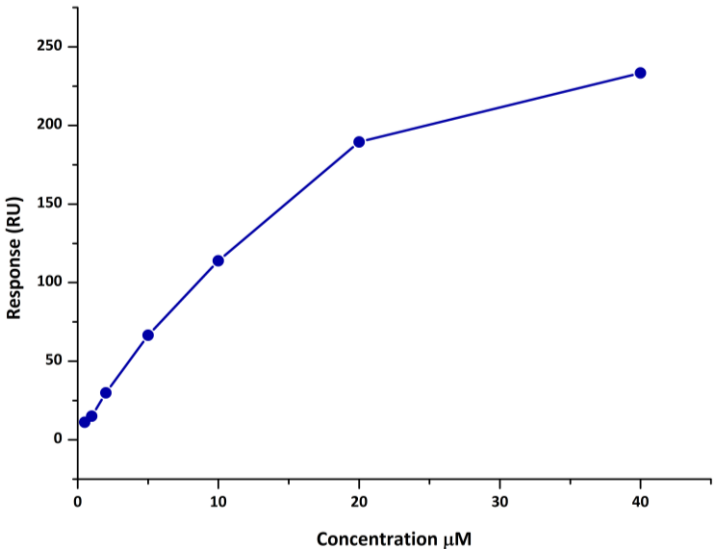
[a]School of Biotechnology, Jawaharlal Nehru University, New Delhi-110067, India

[b]Indian Council of Medical Research, International Health Division, New Delhi-110029, India

[c]Kusuma School of Biological Sciences, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, India – 110016




**Supplemental Figure S1. Purification and characterization of m-OLF.** (A) Size exclusion chromatogram of purified and refolded m-OLF (native m-OLF only corresponds to major peak fraction of the size exclusion chromatogram, and only this fraction was utilized for further analysis), also shown is the SDS PAGE analysis of recovered m-OLF along with the standard molecular weight markers; the inset on right is the calibration curve for Sup75. (B) Far UV CD spectra of the purified native m-OLF exhibits broad minimum at ~215 nm that is characteristic of antiparallel β sheet. (C) Analysis of the purified protein by dynamic light scattering revealing a homogenous solution with hydrodynamic radii of ~0.5nm (D) Near UV CD spectra of the purified native m-OLF displaying close double troughs at 282 nm and 291 nm.



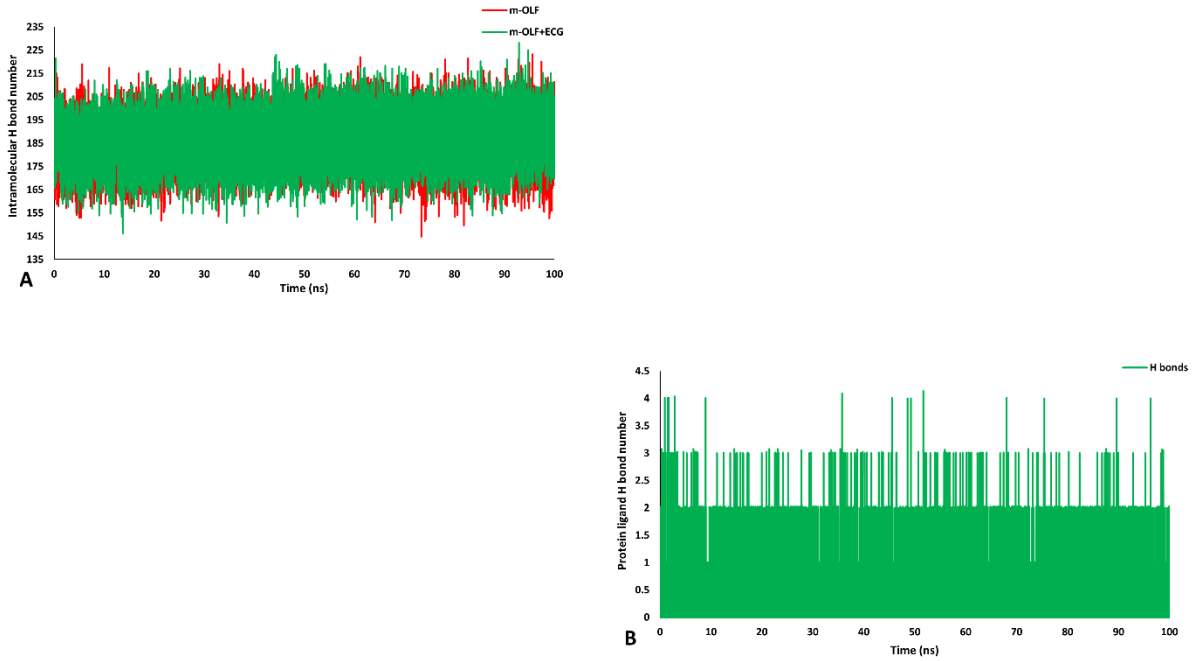

**Supplemental Figure S2. Dose-response plot for the binding of m-OLF with Epicatechin gallate (ECG).** The response values were obtained via extrapolation of the fitted response curves.

**Table S1: The estimated lag-times and apparent rate constants for m-OLF amyloid fibrillation reaction for each of the tested conditions.**

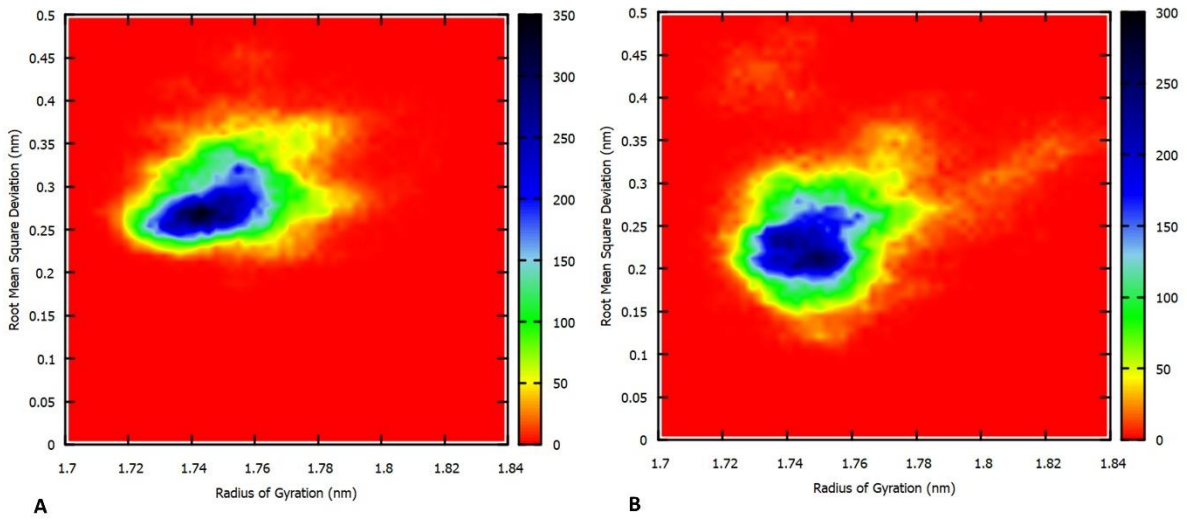
| Ratio | Lag-time (h) | $k_{app}$ rate constant ($h^{-1}$) |
|---|---|---|
| m-OLF alone | 20.3 | 0.09 |
| m-OLF + ECG 1:1 | 26.63 | 0.11 |
| m-OLF + ECG 1:5 | 29.31 | 0.12 |

**Table S2: Percentage of different secondary structural components in native and aggregated m-OLF.**

| Structural Component | Percentage content | | |
|---|---|---|---|
| | Native m-OLF | aggregated m-OLF (control) | Aggregated m-OLF (treated) |
| α helix | 1.9 | 0 | 0 |
| β sheet | 39.6 | 37.8 | 40.3 |
| Turn | 18.5 | 16.5 | 15.5 |
| Coil | 40 | 45.7 | 44.2 |




**Supplemental Figure S3. H bond analysis of the REMD simulation.** (A) Protein intramolecular H bonds are preserved in both the simulation systems. (B) The H bonding between the ligand (ECG) and the protein is maintained throughout the runtime of the REMD simulation.




**Supplemental Figure S4. Conformational sampling study via population density analysis.** Population density analysis was conducted for m-OLF in the absence (A) and presence of ECG (B) as a function of backbone (root mean square deviation) RMSD and radius of gyration (Rg). Blue regions indicate the heavily populated conformations, whereas yellow, green and red areas indicate decreasing levels of sampled conformations.