Fractal-like Self-Assembly in Citrate Synthase: Delineating Growth Patterns with Coarse Grained Simulations

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Fractals are complex, repeating and infinitely self-similar patterns. However, biomolecular fractals have been observed to be of limited range, and owing to physical realities, prone to exhibit imperfections. This talk will present the Sierpiński fractal like self-assembly of citrate synthase, a fractal captured recently with cryo-electron microscopy experiments. Atomistic re-modelling of the basic unit of growth, the initial dimer and hexamer, were further investigated for geometric, energetic, and dynamical responses that underlie hierarchical self-assembly of the oligomers. Coarse graining and subsequent analyses quantify deviations from ideal fractality and fluctuations with increasing fractal level. An in-house algorithm characterized the solvent-accessible regions lacking amino acid occupancy, the hallmark void of the Sierpiński fractal architecture. Finally, the underlying power law exponents of the structural and thermodynamic signatures of growth were determined. The framework underlying hierarchical assembly, structural fluctuations, and scaling behaviour were revealed contribute to the stability of protein fractal architectures. Combined, these lend insights into factors that limit realistic higher ordered fractalization in bio-molecular systems.