

TITLE

A Database Conundrum - MD, SAXS and NMR disorder data

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ABSTRACT

Neuroscience, immunology, and pathology research fields are progressing rapidly, while advancing research techniques make studying projects that include structural disorder easier. From neurodegenerative diseases to molecular toxicity, and infectious disease, disorder is becoming a prominent theme in structural science, a field classically driven by order. Disorder is equally as important as order, and the volume of published disorder data is growing. In parallel, research studying the driving factors of disorder, properties of protein aggregation, and small molecule tuning factors are defining what is disorder. It is necessary to define and archive disorder data well to understand and develop solutions important to applications of relevance. Current disorder data includes combinations of data from molecular dynamics (MD), small-angle X-ray scattering (SAXS), and nuclear magnetic resonance (NMR). The challenge is how to best and where to publicly deposit the data.