Rule and Root-based Metadata-Ecosystem for Structural Bioinformatics & Facebook

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Despite the widespread efforts to develop flexible formats such as PDB, mmCIF, CIF, to store and exchange data, the lack of best practice metadata pose major challenges. Readily adoptable methods with demonstrated usability across multiple solutions to create on-demand metadata are critical for the effective archive and exchange of data in a user-centric fashion. It is important that there exists a metadata-ecosystem where metadata of all structural and biological research evolve synchronously. Previously we described (Chem-BLAST, http://xpdb.nist.gov/chemblast/pdb.pl) a new ‘root’ based concept used in language development (Latin & Sanskrit) to simplify the selection or creation of terms for metadata for millions of chemical structures from the PDB and the PubChem. Subsequently we extended it to text-based data on Cell-image-data (BMC, doi:10.1186/1471-2105-12-487). Here we describe further extension of this concept by creating roots and rules to define an ecosystem for composing new or modifying existing metadata for demonstrated inter-operability. A major focus of the rules is to ensure that the metadata terms are self-explaining (intuitive), highly-reused to describe many experiments and also that they are usable in a federated environment to construct new use-cases. We illustrate the use of this concept to compose semantic terminology for a wide range of disciplines ranging from material science to biology. Examples of the use of such metadata to create demonstrated solutions to describe data on cell-image-data will also be presented. I will present ideas and examples to foster discussion on metadata architecture a) that is independent of formats and b) that is better suited for a federated environment c) that could be used readily to build components such as resource description framework (RDF) and Web services for Semantic web.