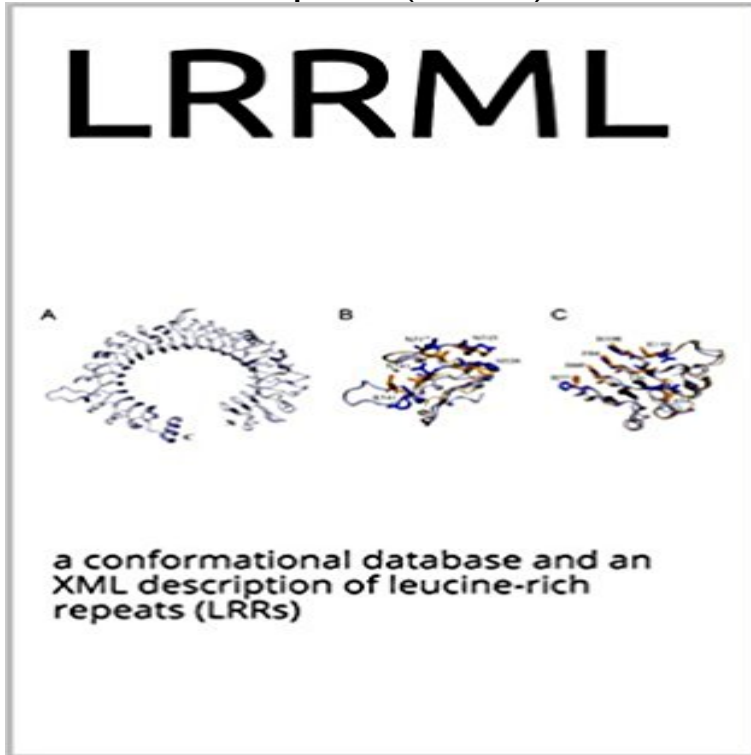


LRRML: a conformational database and an XML description of leucine-rich repeats (LRRs)



Background Leucine-rich repeats (LRRs) are present in more than 6000 proteins. They are found in organisms ranging from viruses to eukaryotes and play an important role in protein-ligand interactions. To date, more than one hundred crystal structures of LRR containing proteins have been determined. This knowledge has increased our ability to use the crystal structures as templates to model LRR proteins with unknown structures. Since the individual three-dimensional LRR structures are not directly available from the established databases and since there are only a few detailed annotations for them, a conformational LRR database useful for homology modeling of LRR proteins is desirable.

Description We developed LRRML, a conformational database and an extensible markup language (XML) description of LRRs. The release 0.2 contains 1261 individual LRR structures, which were identified from 112 PDB structures and annotated manually. An XML structure was defined to exchange and store the LRRs. LRRML provides a source for homology modeling and structural analysis of LRR proteins. In order to demonstrate the capabilities of the database we modeled the mouse Toll-like receptor 3 (TLR3) by multiple templates homology modeling and compared the result with the crystal structure.

Conclusion LRRML is an information source for investigators involved in both theoretical and applied research on LRR proteins. It is available at <http://zeus.krist.geo.uni-muenchen.de/~lrrml>.

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