Looking at Molecules with Smart Computers

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The ability to reason with new information and learn from it is a fundamental aspect of intelligence. It is also at the heart of the challenge to build smarter computers and computing software. The wealth of information on molecular structures, rapidly growing in the crystallographic databases, offers a singular opportunity to assess new computing approaches and their ability to mimic human intelligence. In this presentation, we will describe methodologies, based on artificial intelligence and machine learning techniques, that can assist in the discovery of new knowledge and its application to the reconstruction, analysis and interpretation of molecular scenes. These methodologies were developed, as part of the Molecular Scene Analysis project, and are used for data mining and automated molecular image interpretation.