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*ga mlra genetic algorithm combined with multiple linear regression analysis technique was applied for the generation of two types of qsars first models containing exclusively 3d descriptors and second models consisting of physicochemical descriptors as expected 3d descriptor qsars have better statistical fits,* **first principles molecular structure search with a genetic** - *the algorithm is designed to work with first principles methods facilitated by the incorporation of local optimization and blacklisting conformers to prevent repeated evaluations of very similar solutions,* **genetic algorithms for chemical structure handling and** - *the genetic algorithm for conformational search h molecular conformational analysis has been a promising application area for gas with several published results lucasius et al 1991 blommers et al 1992 payne and glen 1993,* **survival of the fittest in drug design** - *genetic algorithms genetic algorithms gas allow computers to generate new random data when combined with a fitness function only the best data are randomly exchanged and mutated until a new generation of data is produced as with real genes genetic algorithms manipulate so called genetic material but instead of dna this genetic material is some other linear string of symbols in humans the genetic material is dna which is thought of in terms of its base pairs,* **genetic algorithms in molecular modeling by james** - 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