Molecular interaction fields : applications in drug discovery and ADME prediction

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Abstrak

This unique reference source, edited by the world's most respected expert on molecular interaction field software, covers all relevant principles of the GRID force field and its applications in medicinal chemistry. Entire chapters on 3D-QSAR, pharmacophore searches, docking studies, metabolism predictions and protein selectivity studies, among others, offer a concise overview of this emerging field.