3D-QSAR (three-dimensional quantitative structure-activity relationships)

Three-dimensional quantitative structure-activity relationships (3D-QSAR) involve the analysis of the quantitative relationship between the biological activity of a set of compounds and their three-dimensional properties using statistical correlation methods.

Source:

PAC, 1997, 69, 1137 (Glossary of terms used in computational drug design (IUPAC Recommendations 1997)) on page 1142