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3D-QSAR

Notes

- Physical properties are measured for the molecule as a whole
- Properties are calculated using computer software
- No experimental constants or measurements are involved
- Properties are known as 'Fields'
- Steric field - defines the size and shape of the molecule
- Electrostatic field - defines electron rich/poor regions of molecule
- Hydrophobic properties are relatively unimportant

Advantages over QSAR

- No reliance on experimental values
- Can be applied to molecules with unusual substituents
- Not restricted to molecules of the same structural class
- Predictive capability

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