

What are field points?

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For computational efficiency, Cresset's field technology condenses the molecular fields down to a set of points around the molecule, termed "field points". Field points are the local extrema of the electrostatic, van der Waals and hydrophobic potentials of the molecule. They can be thought of as extended pharmacophores, with the advantages that their position is directly calculated from the molecule's physical properties, and they have size/strength information associated with them (so that e.g. not all H-bond donors are treated the same: some make stronger bonds than others). The generation of field points is described in detail in Cheeseright *et al*

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46,
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The four field types are used in unison to describe all the potential interactions that a ligand in a specified conformation can make to a protein.