Cresset KNIME nodes

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KNIME UGM 2014
Cresset summary

> Founded in 2002 by Dr. Andy Vinter – initial Welcome Trust funding
> Located in Cambridge, UK
> Primary market pharmaceutical and biotech R&D
> 13 of the top 20 pharmaceutical companies use Cresset technology in their research programmes
> 160 collaborative projects delivered to global clients
> Other markets include flavour and fragrance, agrochemical and chemicals
Biologically Relevant Molecular Comparisons

Bioisosteres

Bioisosteric groups

blaze

forge

torch

spark
Focused towards MedChem - easy to use interfaces

Power Users & CompChem - more features and more complicated
XED Force Field

> Detailed Electrostatics

> Improved intermolecular interactions

> Accurate reproduction of bioactive conformations
What Can You do with Cresset Nodes?

> 3D Ligand Alignment (Forge Align)
  > SAR interpretation
  > Library Design/Evaluation
> 3D QSAR (Forge Build, Forge Score)
> Activity Cliff detection (Activity Miner)
  > 3D based similarity (shape, electrostatics)
  > 2D fingerprints
> Similarity Matrix (Activity Miner)
  > 3D, 2D
> Ligand Based Virtual Screening (Forge Align)

> Bioisostere generation (Spark)
  > Find new cores for your molecules
  > Screen all possible R groups from available reagents

> Conformation exploration (XedeX)
> Ligand Minimisation (XedMin, FREE)
  > 2D->3D conversion
  > Ligand minimisation in vacuo or in a (fixed) protein cavity
Activity Cliffs

> Regions in the SAR where you get a larger change in activity relative to the change in structure
> Usually measure change in structure using fingerprints
> Activity Miner node adds measurement in 3D – shape and electrostatics
  > More activity cliffs
  > Explanation for observed SAR

Also has an effect here!

Has an effect here!
Activity Miner in KNIME
More to Come

> REST interface to cloud based virtual screening
> Access from KNIME using the KREST nodes
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