With Lead Discovery, I can answer all of my questions

- Alkyl substitution at R6 is optimal. Unsubstituted beta-position is key.
- Chiral center (R) enantiomer 15x more active.
- Optimal activity when R5 is ortho substituted.
- R1 and R2 must be H, loss of all activity with substitution.
- Increased activity when R3 is electron W/D. Increased pIC50 stability and activity against target when R4 does not equal H.

With Lead Discovery I can:
- Identify SAR patterns hidden to the human eye
- Visualize Matched Molecular Pair Analysis (MMPA)
- Calculate chemical properties

Click here to learn more about Lead Discovery powered by TIBCO Spotfire®

@PKI_Informatics Follow us on Twitter for all the latest news and events around TIBCO Spotfire®, ChemDraw and Elements.