

Alchemical Pathways

What are alchemical pathways?

- Alchemical pathways are a series of thermodynamic states where intermediate states do not necessarily model a physical system. For example,
 - a drug lead can be morphed into a similar proposed compound
 - harmonic restraints can be added to keep atoms in a certain position
 - states whose energy is a linear interpolation between states 0 and 1 can be defined as, $U_{\lambda}(r^N) = (1 - \lambda)U_0(r^N) + \lambda U_1(r^N)$