# Exploring C-Chem with numeric MM and Ab-Initio methods

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- **Abstract**
  - Computational chemistry is no new subject – however, the idea of taking the process from including a human being in the loop between ab initio methods and general rule making for molecular mechanics (MM) calculations to excluding that same being via AI seems to be unimplemented. This project revolves around the idea that molecular mechanics is an incredibly fast and viable way of calculating the geometry of molecules and that as such, given the proper parameterizations and generalities, can be as accurate as or more accurate than ab initio methods.
- **Process**
  - The project is split into three parts – one part for MM, one part for Ab-initio methods, and one part for the AI that will take the output of the ab-initio methods and generate molecular mechanics rules.
- **Code and Development/ Methodology**
  - The MM section is based on the concept of a 'Rule,' a generalized data structure governing the interaction of molecular constituent 'Identities' (such as atoms and functional groups and specific atoms within specific functional groups). The system minimizes the energy of a set of 'Constituents' based on the specified 'Rules' of the system applicable to the 'Constituents's 'Identities.
  - <Ab initio and AI sections to go here>

<Images Here>