

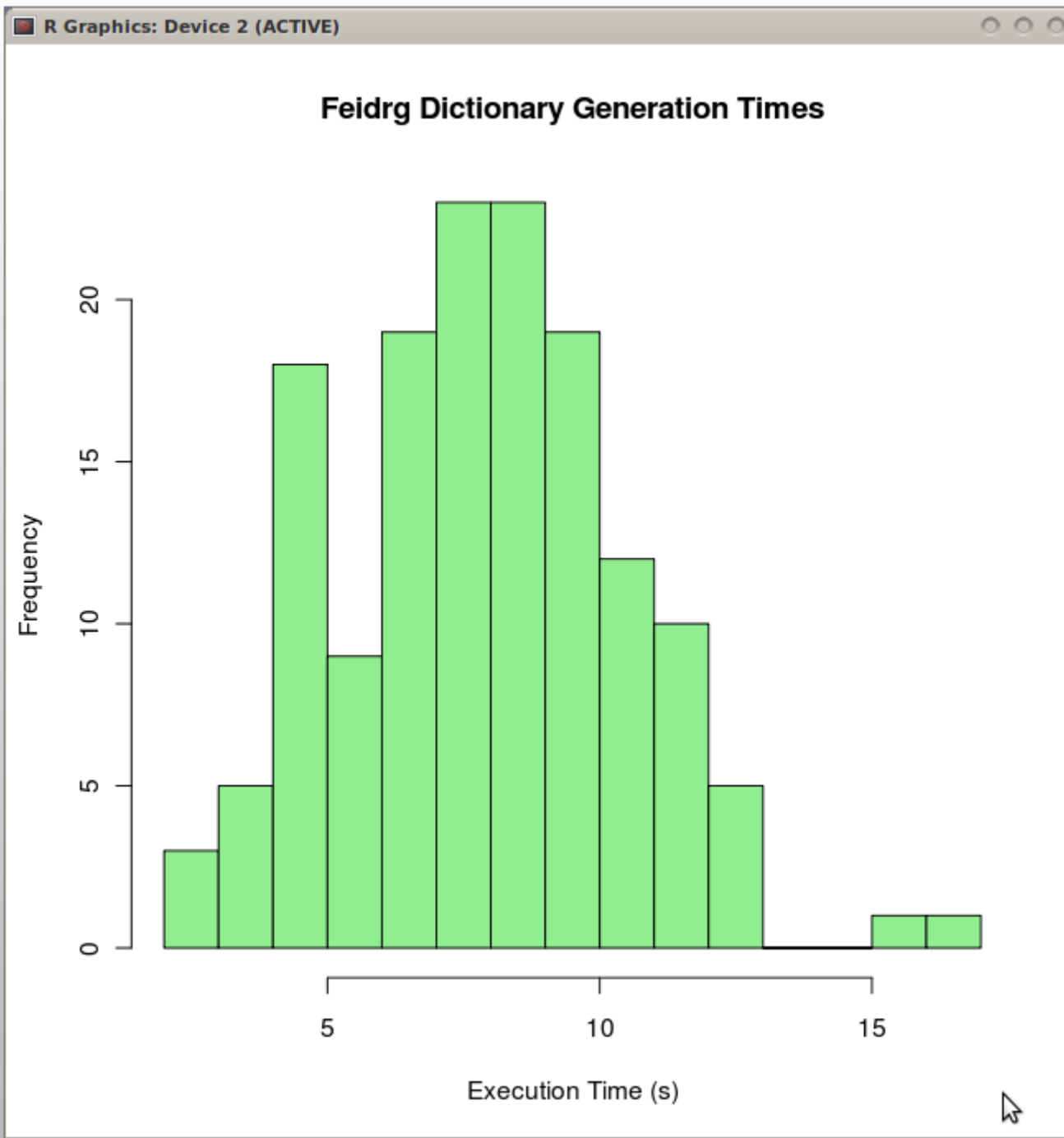
Comparing Dictionaries

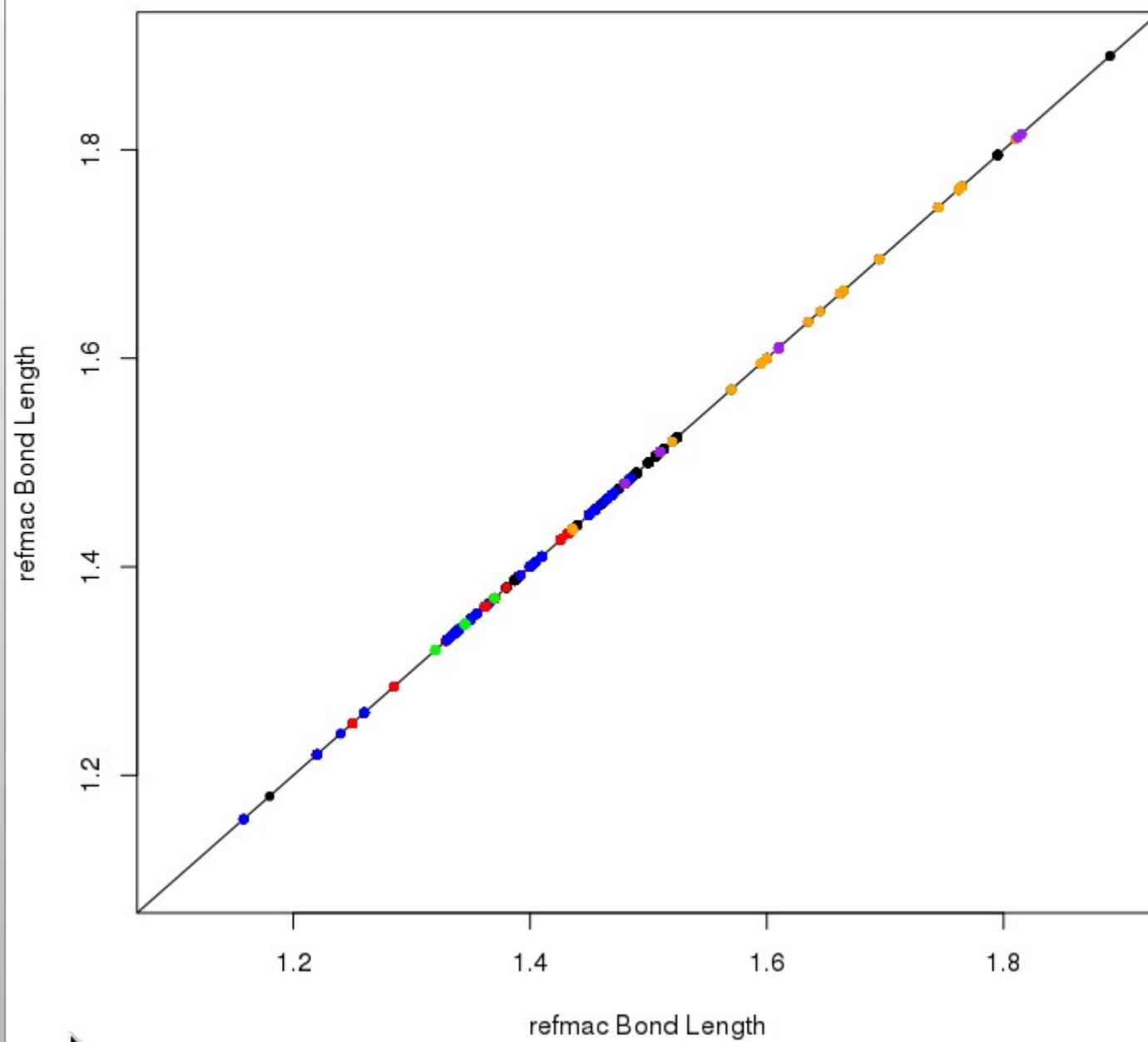
Comparisons include:

- Comparisons include:
 - Refmac
 - Feidrg
 - Grade
 - Pyrogen
 - Phenix.elbow
- 148 compounds
 - no metals
- 170,000 geometric comparisons

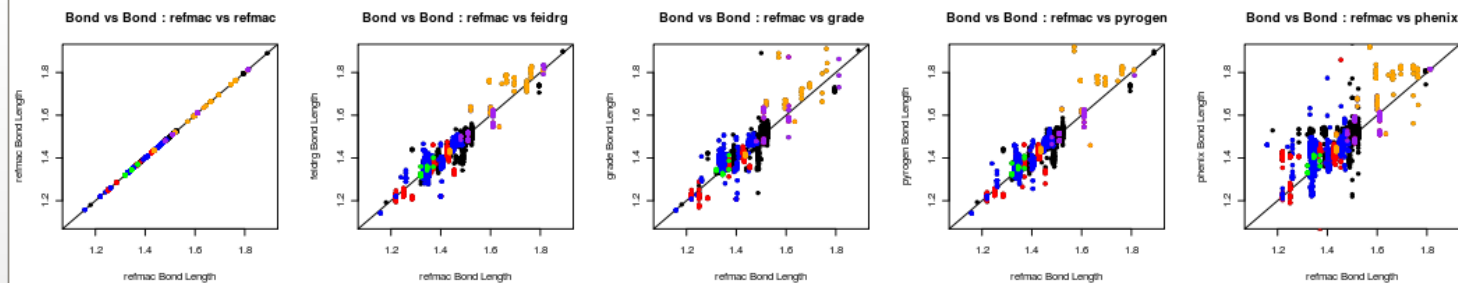
Comparisons include:

- Note: Phenix.elbow, Grade & Pyrogen use Mogul
 - Feidrg does not, of course
- Phenix.elbow & Grade use QM
 - Feidrg and Pyrogen do not
- Dictionaries that are close to each other are close to the truth?
- Dictionaries can differ in many ways
 - bond lengths, atom names, atom energy types, partial charges, bond length esd, angles, angle esds, chiral atoms, plane definitions, torsion definitions

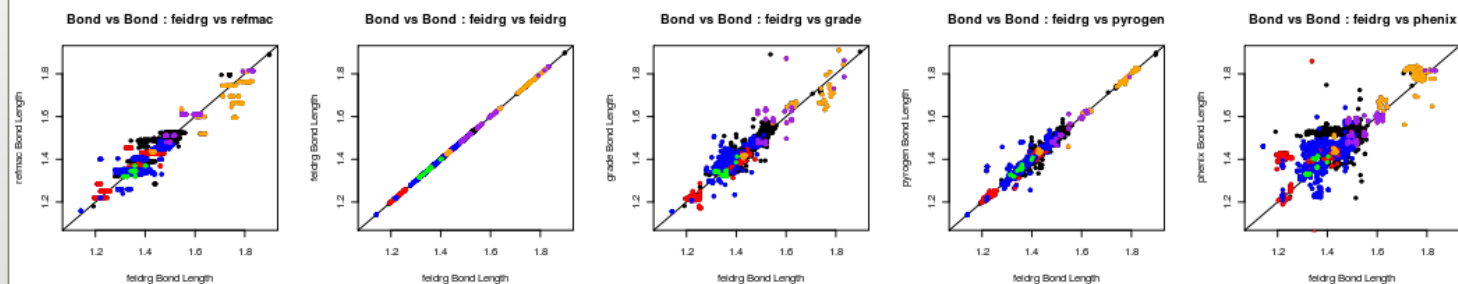


Bond vs Bond : refmac vs refmac

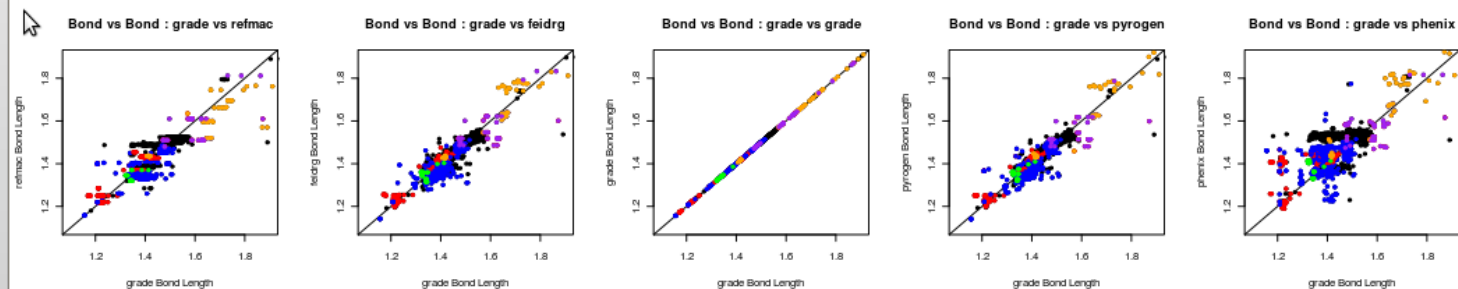
Refmac



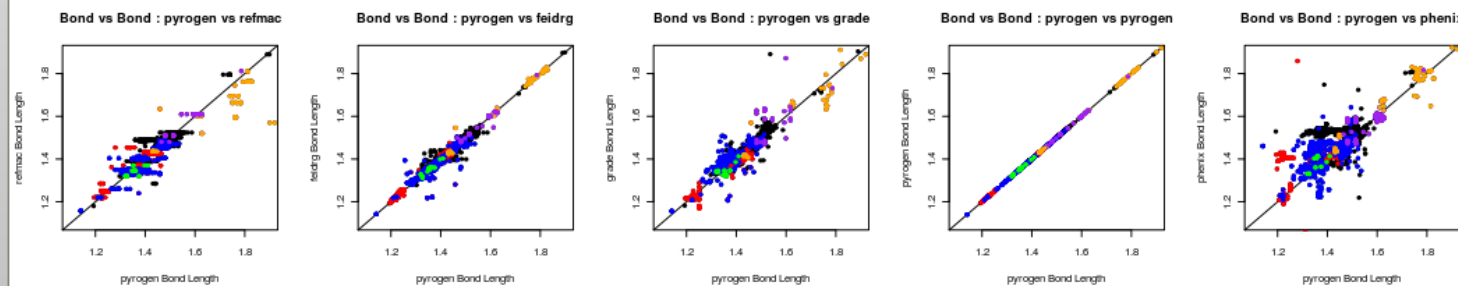
Feidrg



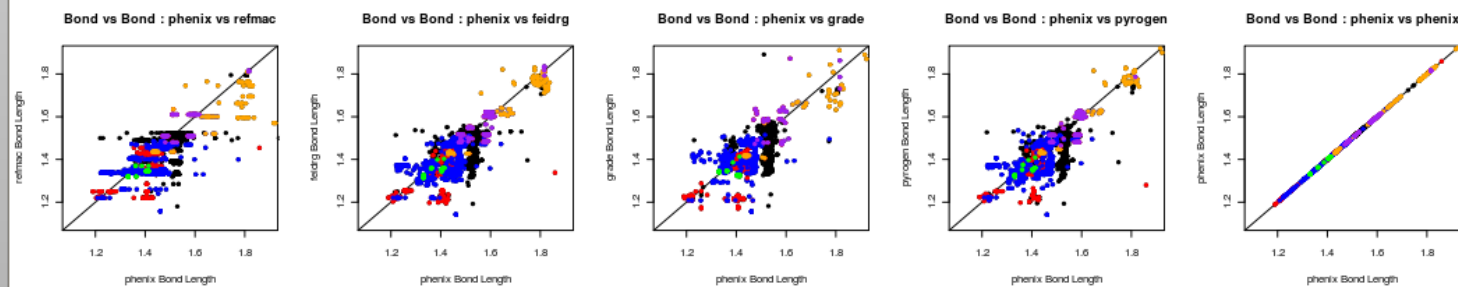
Grade



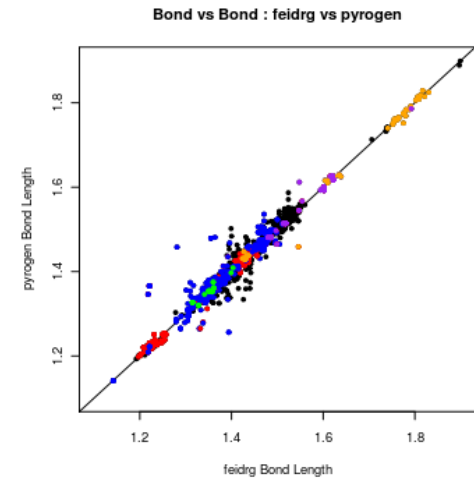
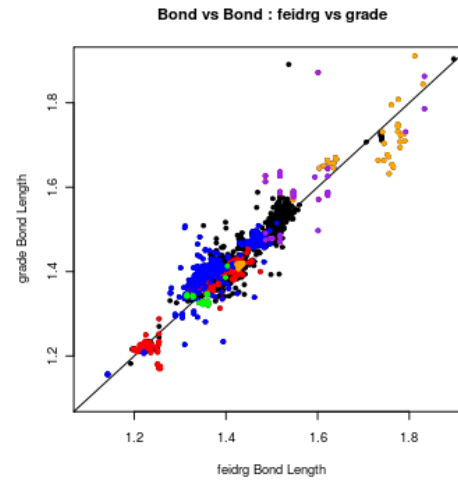
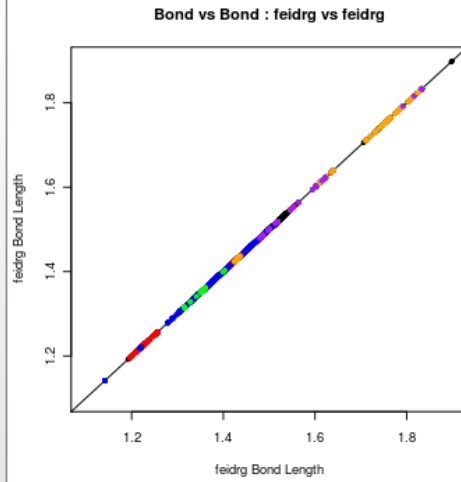
Pyrogen



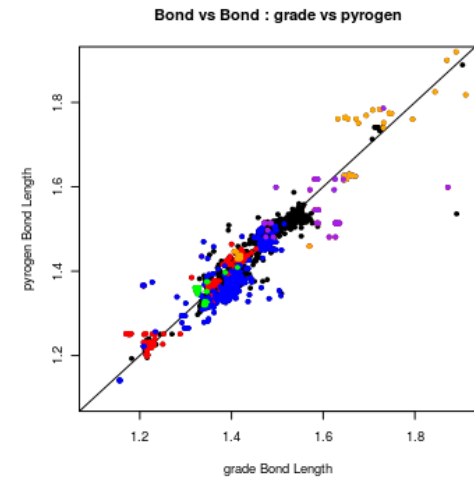
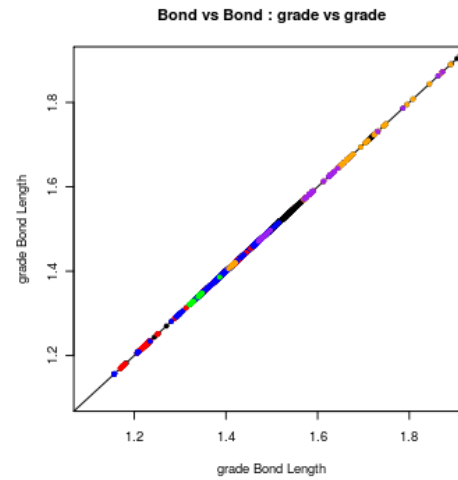
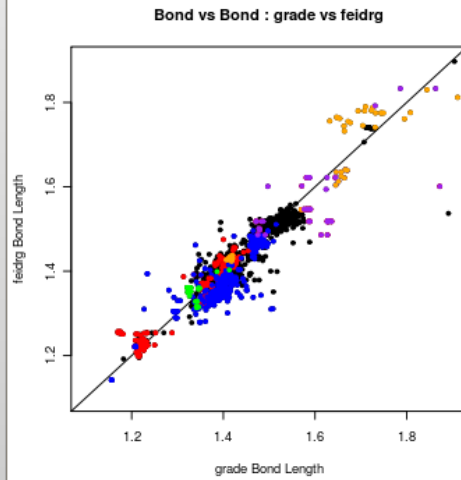
Phenix



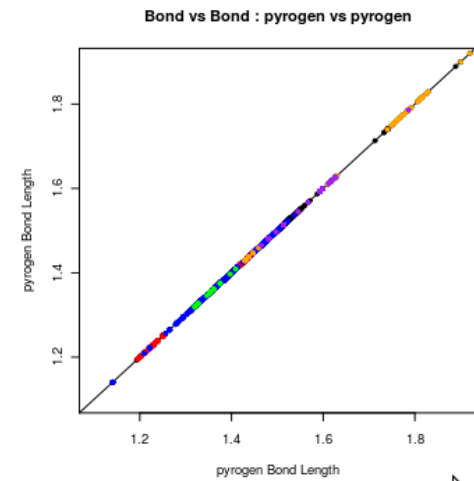
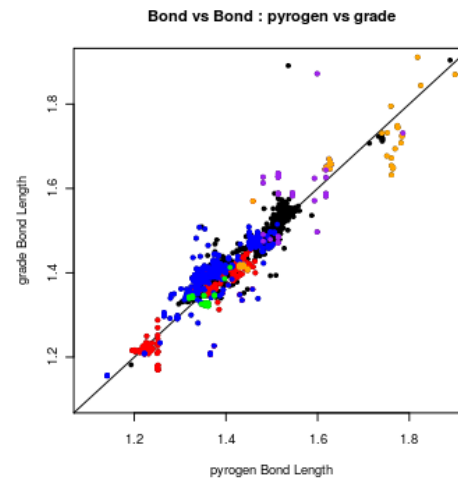
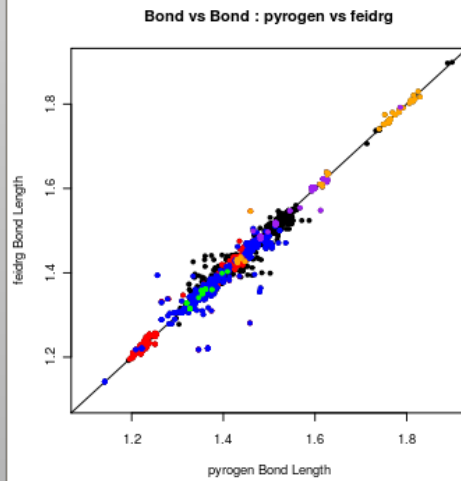
Feidrg



Grade

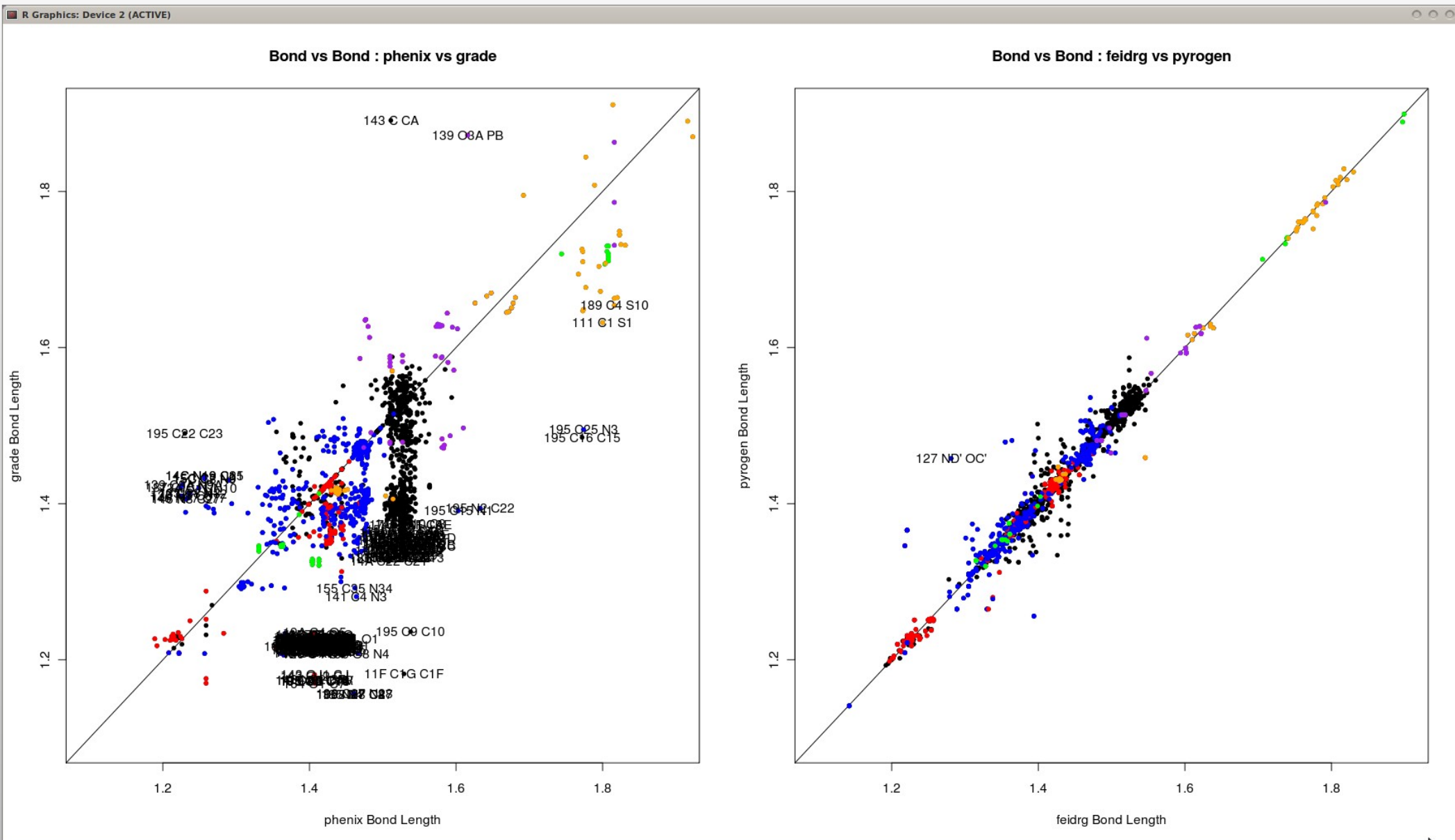


Pyrogen

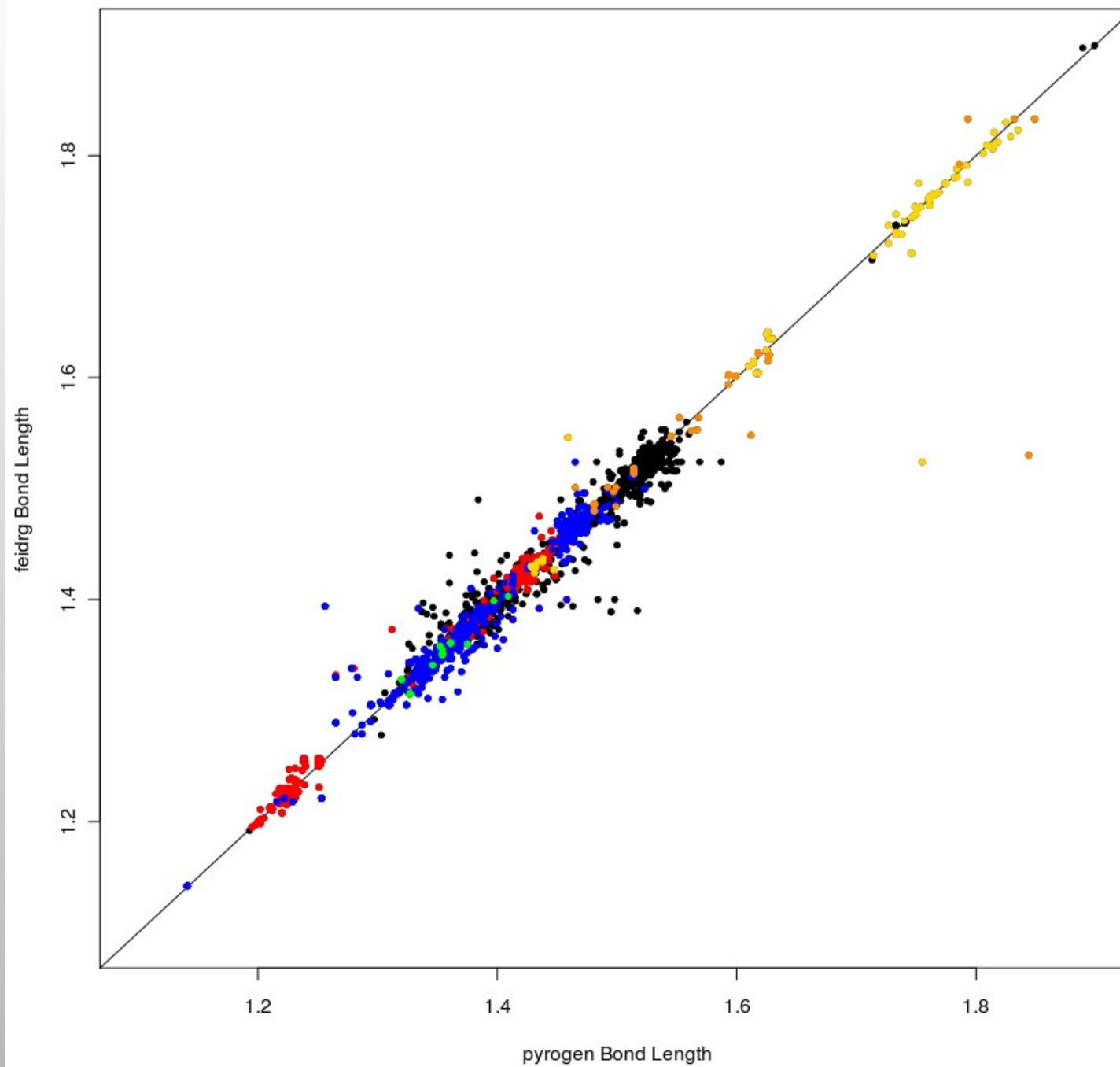


Phenix vs Grade

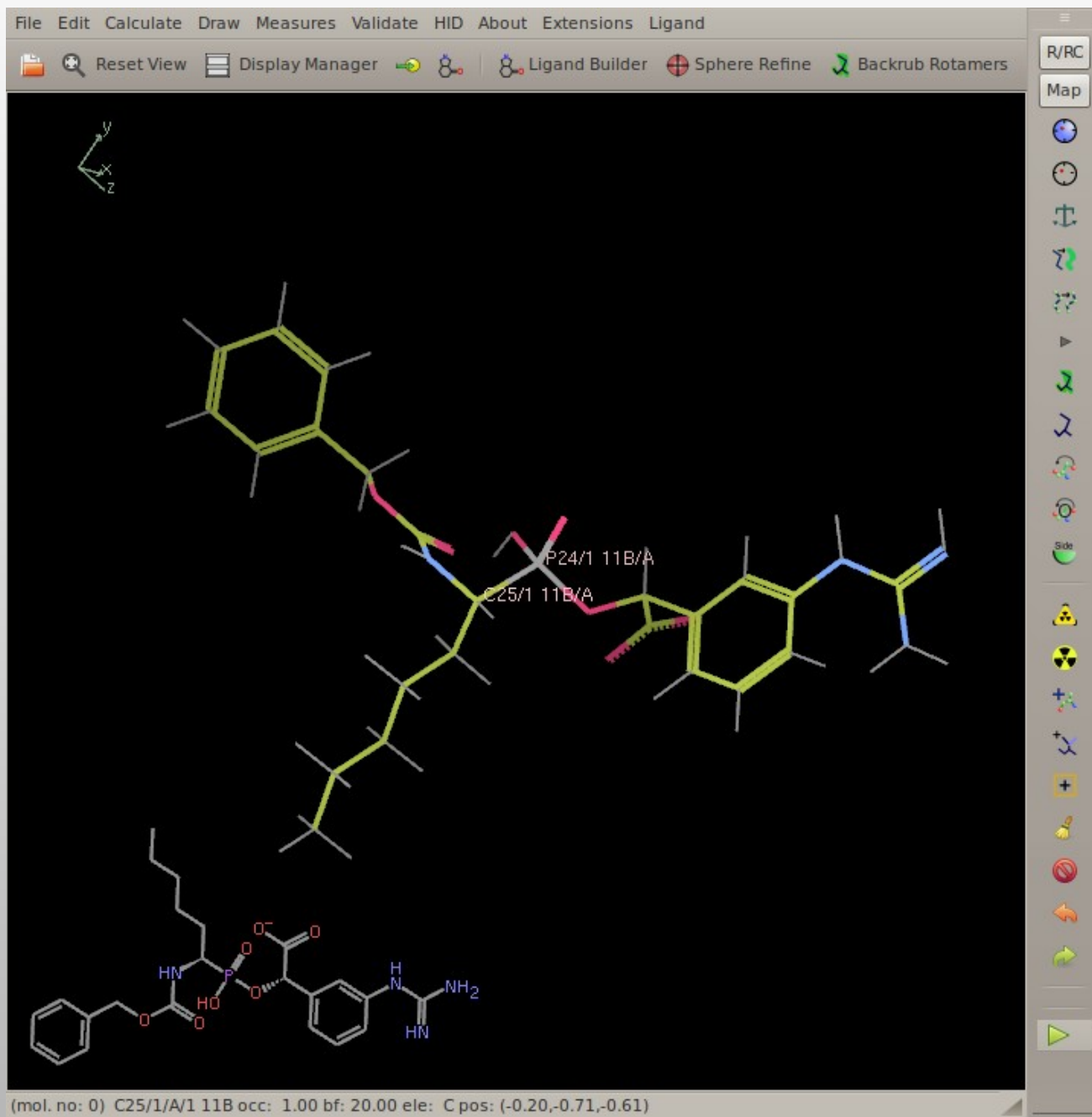
Pyrogen vs Feidrg



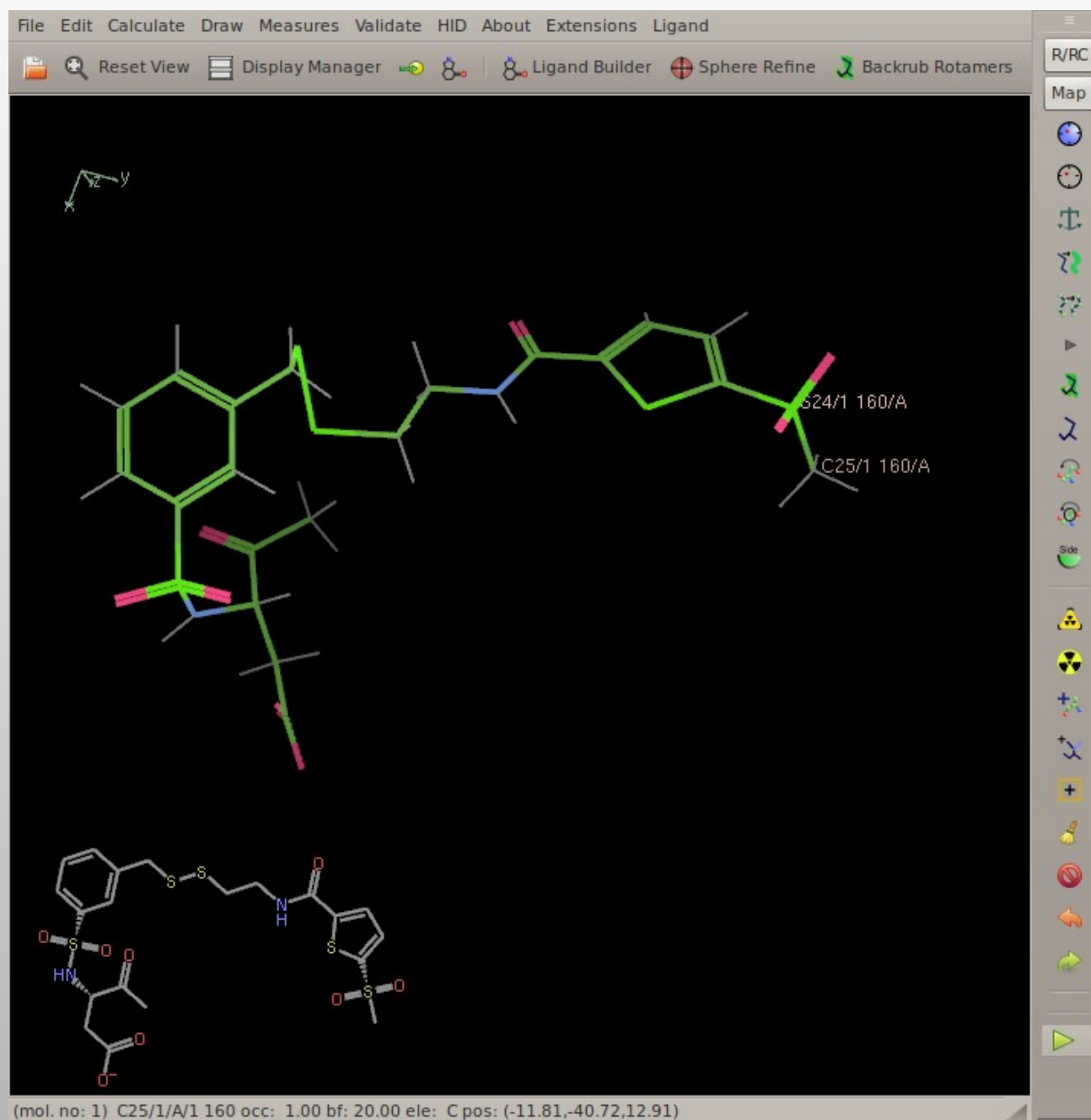
Bond vs Bond : pyrogen vs feidrg



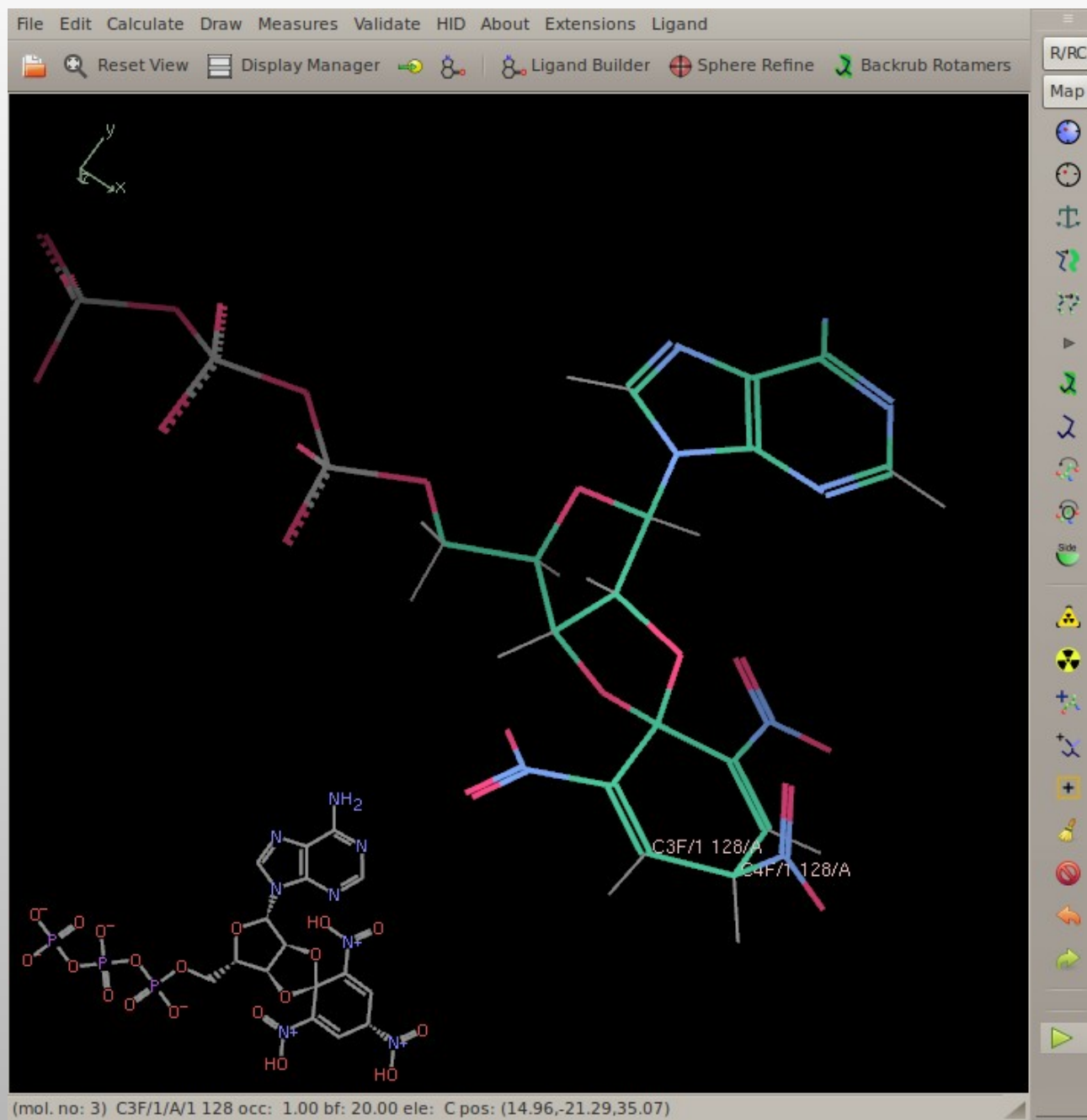
Acedrg's Biggest Bond Outliers: 1



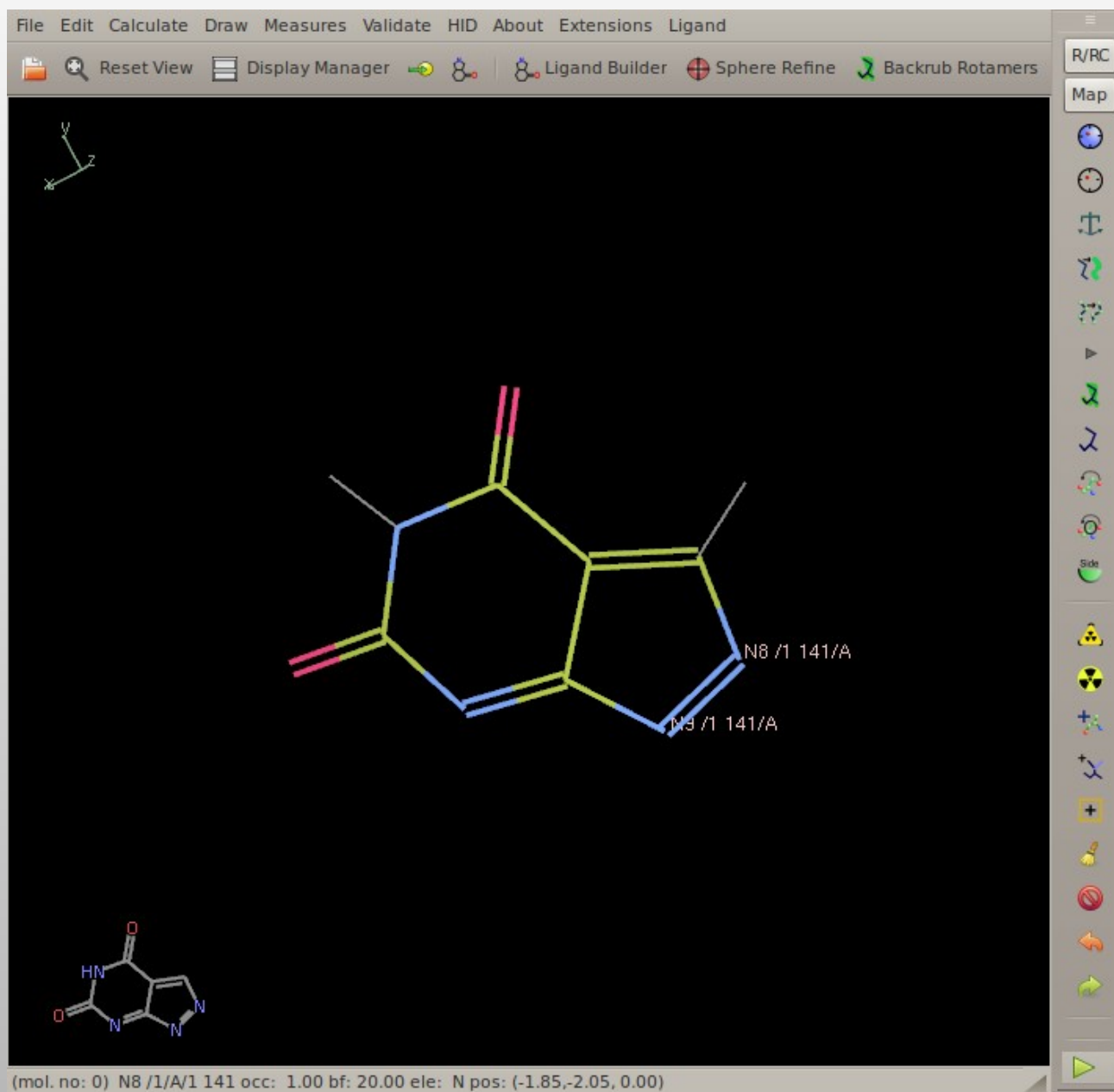
Acedrg's Biggest Bond Outliers: 2



Acedrg's Biggest Bond Outliers: 3

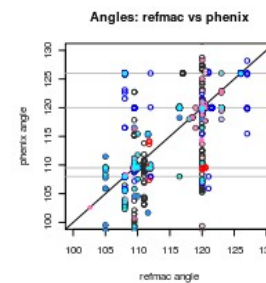
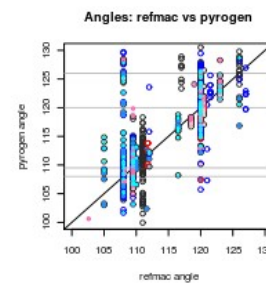
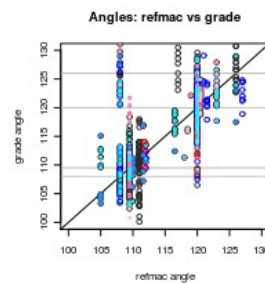
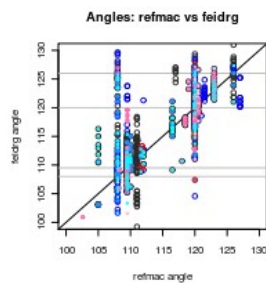
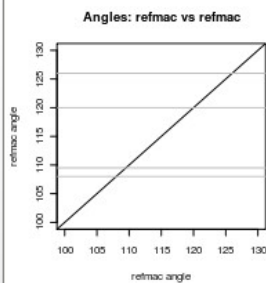


Acedrg's Biggest Bond Outliers: 4

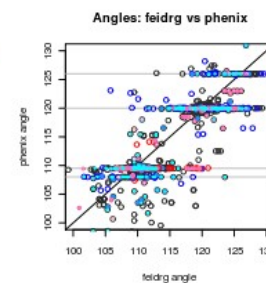
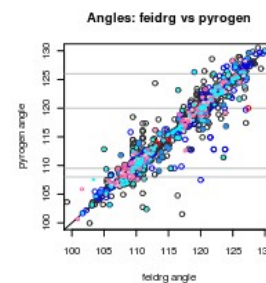
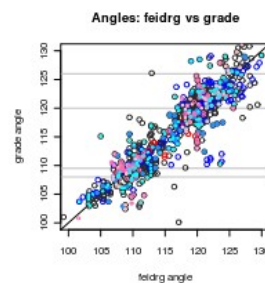
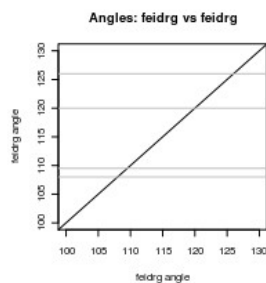
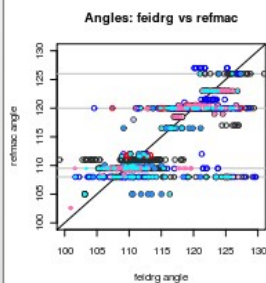


Angles...

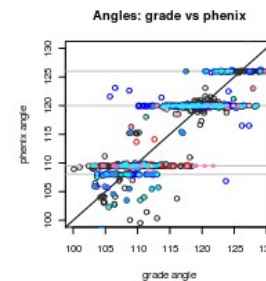
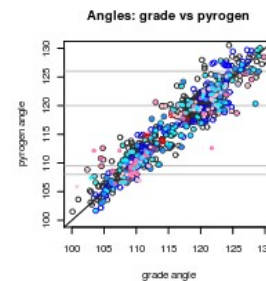
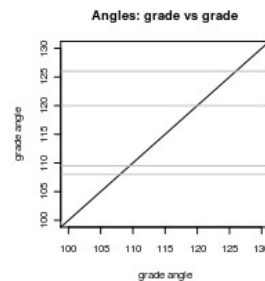
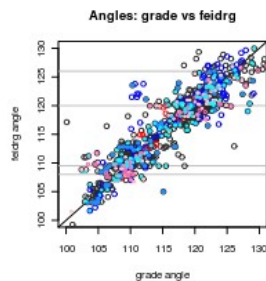
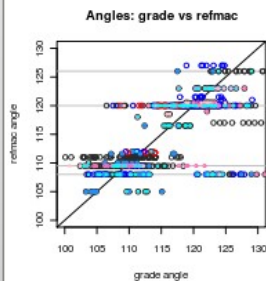
Refmac



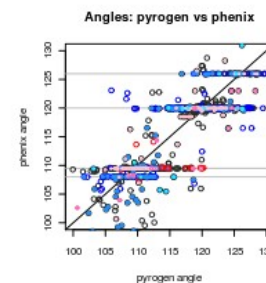
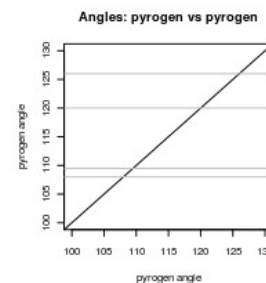
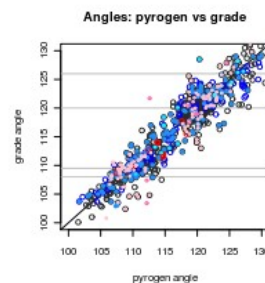
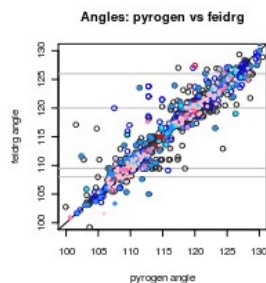
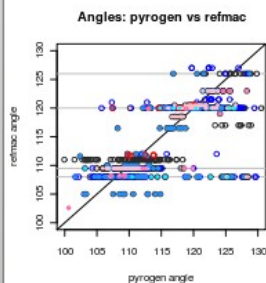
Feidrg



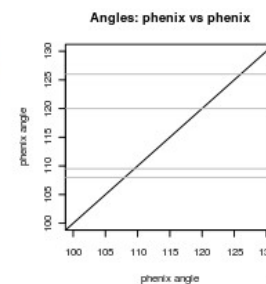
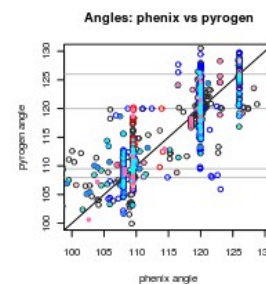
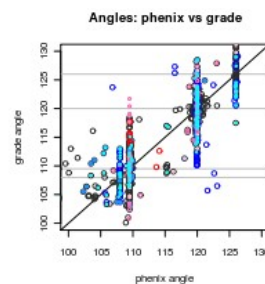
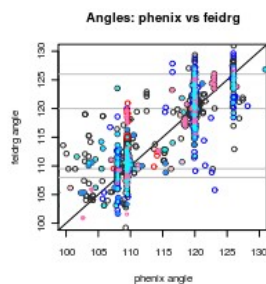
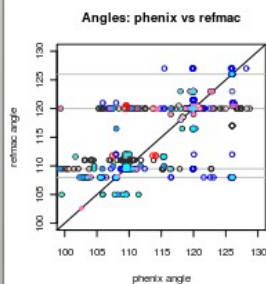
Grade



Pyrogen



Phenix



Different Dictionary Generators are different

- Feidrg and Pyrogen are most closely related for bonds and angles
 - One uses CSD (currently), other used COD
 - Neither use QM