Table 1: Number of steps for H_2O and Paracetamol geometry optimization

Molecule	Method	i-pi Calls	lammp Calls	Ratio	Final Energy	RMSD
H_2O	`bfgs`	10	14	1.4	-3.54380971e-05	0
	`bfgstrm`	9	11	1.22222222	-3.54380818e-05	0
	`lbfgs`	9	14	1.55555556	-3.54380677e-05	0
	`cg`	3	130	43.3333333	-3.54388591e-05	**Ref**
	`sd`	10000	69001	6.9	-3.54336644e-05	0
Paracetamol	`bfgs`	351	460	1.31054131	-0.465428777	**Ref**
	`bfgstrm`	344	346	1.00581395	-0.465428771	0
	`lbfgs`	251	278	1.10756972	-0.465428666	0.001
	`cg`	111	2768	24.9369369	-0.465265918	0.055
	`sd`	200000	410584	2.05292	-0.462710144	0.144

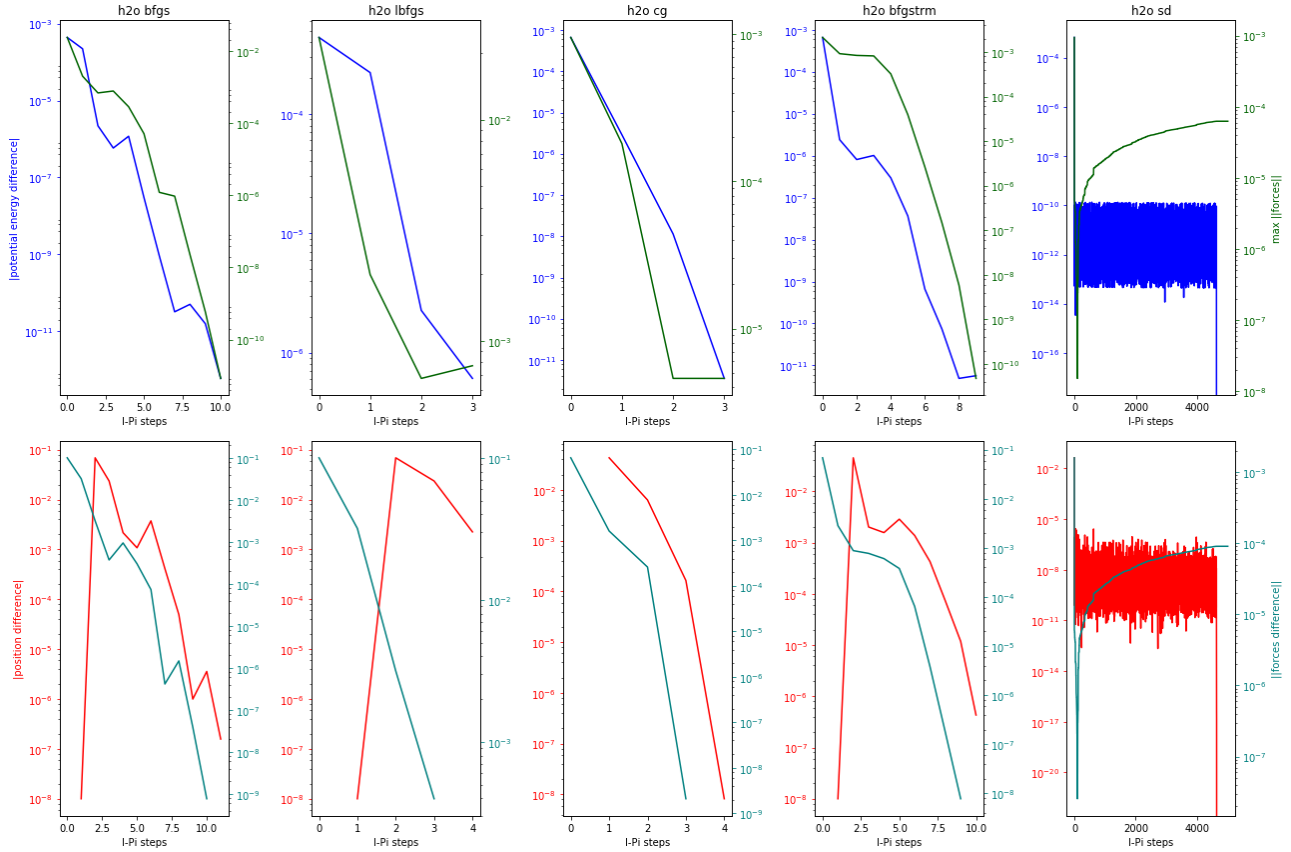

Figure 1: H_2O results

For the two molecule the steepest descent optimization ran until the maximum number of steps was reached. For paracetamol it appears that going further than 500 steps doesn't change the structure nor the numerical output of i-Pi. For water this limit is reached around 4500 steps.

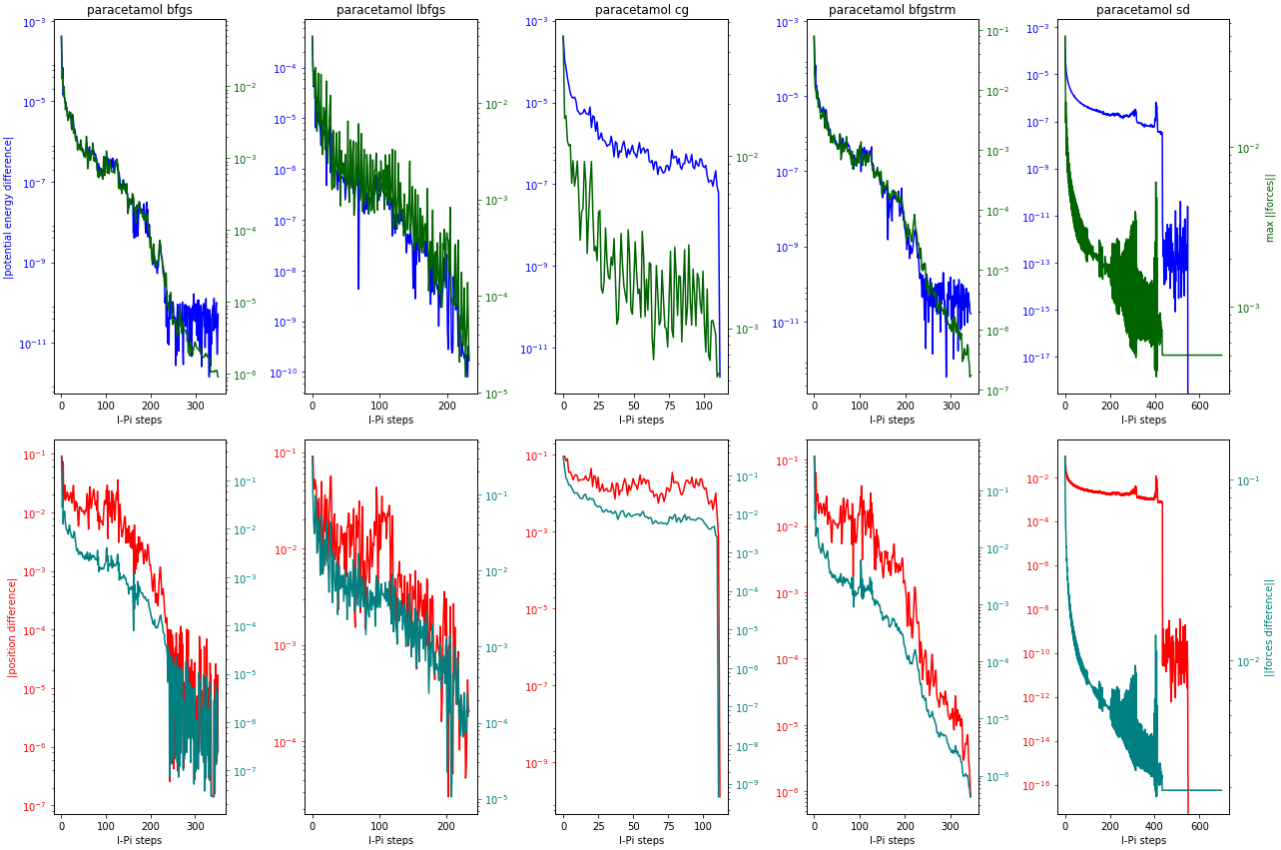

Figure 2: Paracetamol results