

**Supplementary Table 1 | The calculated energies of the various conformations of PF846.**

Molecule name	Energy (kcal/mol)
Optimized_X-ray_molecule_1	-1110331.97
Optimized_X-ray_molecule_2	-1110333.04
Pose 1	-1110331.49
Pose 2	-1110331.64
Pose 3	-1110333.24
Pose 4	-1110333.59