

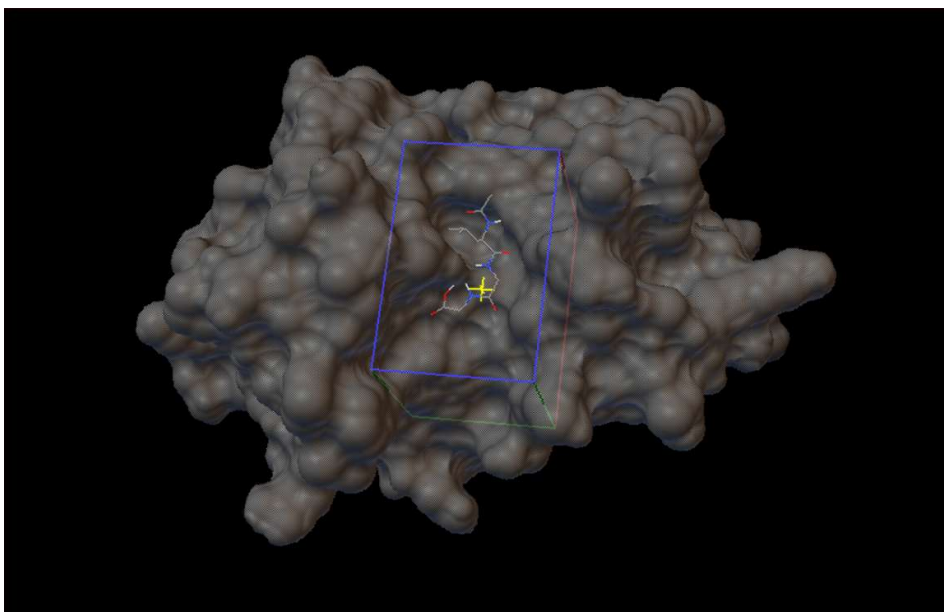
## Docking Parameters

### Grid box:

Coordinates of Central Grid Point of Maps = (-145.653, 127.771, -0.257)

Number of points in dimension = (32, 48, 40)

Grid Point Spacing (Angstrom) = 0.375



**Figure 1.** The grid box position in Cathepsin S

### Genetic Algorithm Parameters

Number of GA runs: 50

Population Size: 10

Maximum Number of evals: medium (2500000)

Maximum Number of generations: 27000

Maximum Number of top individuals that automatically survive: 1

Rate of Gene Mutation: 0.02

Rate of Crossover: 0.8

GA Crossover mode: twopt

Mean of Cauchy distribution for gene mutation: 0.0

Variance of Cauchy distribution for gene mutation: 1.0

Number of generations for picking worst individual: 10

**Docking Parameters**

For random number generator: Use defaults

For energy parameters: Use defaults

For step size parameters: Use defaults

For output format parameters: Use defaults