

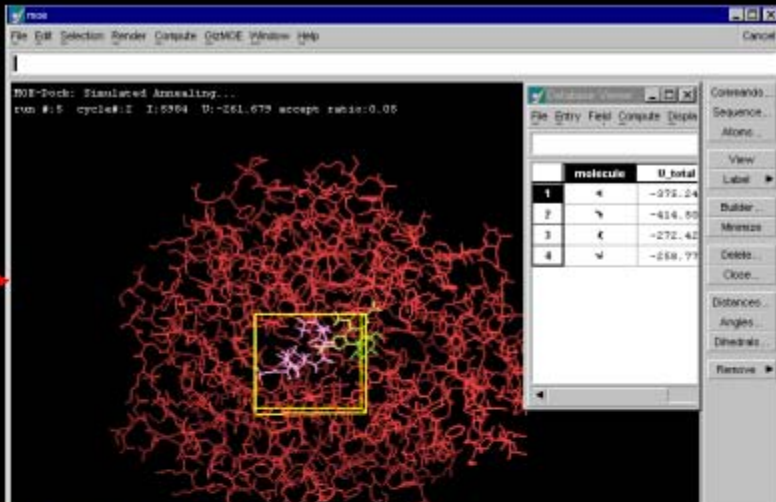
1<sup>st</sup> Generation of virtual peptide library  
(10 tetra peptides used 7 residues:  
P,G,D,R,E,S,K )

**Docking**  
MOE-Dock

4 rounds

**Evolution**  
**Genetic algorithm**  
- Selection  
- Crossover  
- Mutation(10~20%)

**Next  
generation**



### Genetic algorithm

| Sequence | Energy | Rank | Selection | Combination | Cross-over | Mutation |
|----------|--------|------|-----------|-------------|------------|----------|
| GEDG     | -99    | 1    | GERD      | GERD        | G D R G    | P D R G  |
| DSRD     | -114   |      | GERD      | SDRG        | S E R D    | S E R D  |
| GDGG     | -94    | 2    | DSRD      | GERD        | G E D G    | G E D G  |
| GERD     | -115   |      | DSRD      | GEDG        | G E R D    | G E R D  |
| GSRD     | -87    | 3    | SDRG      | DSRD        | D S R G    | P S R G  |
| DERD     | -79    |      | SDRG      | GDGG        | G D G D    | G D G D  |
| GDGP     | -71    | 4    | GEDG      | DSRD        | D D R G    | D E R G  |
| SDRG     | -109   | 5    | GGGG      | SDRG        | S S R D    | S S R D  |
| GEDP     | -41    | 6    | GDGG      | GGGG        | G G G D    | G G G D  |
| GGGG     | -98    | 7    | GSRD      | GSRD        | G S R G    | G S E G  |

Sequence

Ranking

Selection

Crossover

Mutation