

## First results

- first table shows scoring after correlation docking with 20 degree stepsize
- second table shows scoring after refinement with 1000 steps and uniformly distributed recreation of rotation

```
julia> include("src/dockings/main.jl")
1375.255305 seconds (15.24 G allocations: 713.790 GiB, 6.59% gc time, 1.69% compilation time: 5% of which was recompilation)
5x5 DataFrame
  Row  α      β      γ      R      score
     Float32 Float32 Float32 Tuple... Float32
-----
  1    6.0    0.0    5.0  (140.0, 20.0, -40.0)  83.0
  2    6.0    0.0    5.0  (140.0, 20.0, -40.0)  83.0
  3   -4.0    1.0   -2.0  (120.0, 40.0, 140.0)  83.0
  4   -4.0    1.0   -2.0  (120.0, 40.0, 140.0)  83.0
  5    0.0    2.0    3.0  (-180.0, 40.0, 120.0)  82.0
710.719024 seconds (4.20 G allocations: 196.651 GiB, 2.84% gc time, 0.12% compilation time)
8x5 DataFrame
  Row  α      β      γ      R      score
     Float32 Float32 Float32 Tuple... Float32
-----
  1   -4.0   -6.0   -1.0  (125.369, 39.8656, -42.4324)  93.0
  2   -2.0    0.0   -1.0  (135.999, 39.8246, -50.8895)  85.0
  3   -1.0    0.0    3.0  (144.674, 39.9662, -32.0736)  84.0
  4    6.0    0.0    5.0  (140.0, 20.0, -40.0)  83.0
  5    6.0    0.0    5.0  (140.0, 20.0, -40.0)  83.0
  6   -4.0    1.0   -2.0  (120.0, 40.0, 140.0)  83.0
  7   -4.0    1.0   -2.0  (120.0, 40.0, 140.0)  83.0
  8    0.0    2.0    3.0  (-180.0, 40.0, 120.0)  82.0
```