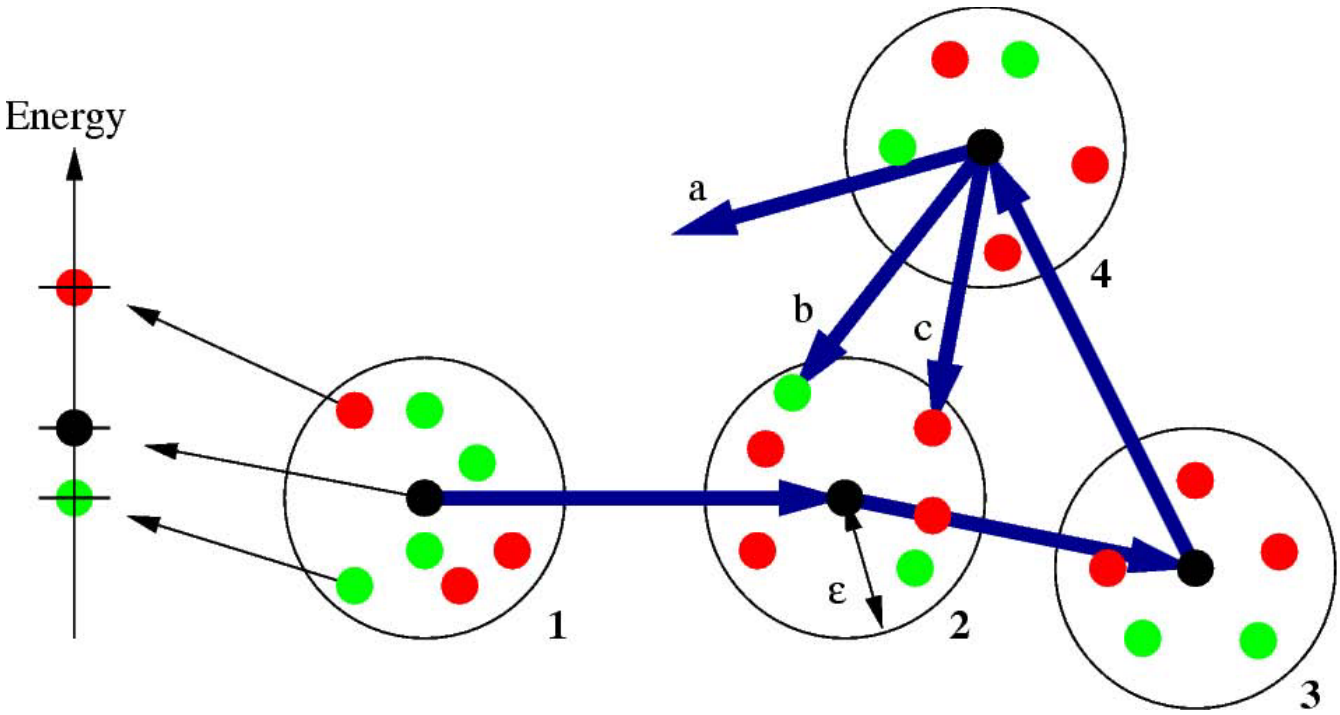

Figure 4
Explicit- and implicit tabu structures. Black points represent explicit tabu structures and red points represent implicit tabu structures.

Algorithm 1 Tabu Search

```
1: bestStructure, s ← random_conformation()
2: bestCost ← cost(bestStructure)
3: while not stop() do
4:    N ← compute_neighbours(s)
5:    sort N with respect to cost
6:    for all i ∈ N do
7:       if cost(N_i) < bestCost then
8:          bestCost ← cost(N_i)
9:          s, bestStructure ← N_i
10:         break loop
11:      end if
12:      if not Tabu(N_i, Q) then
13:         s ← N_i
14:         break loop
15:      end if
16:   end for
17:   pushback( Q, s )
18: end while
19: return bestStructure
```

Figure 5
Algorithm 1.

tabu difference. Each run is stopped after 15 minutes and the structure with the lowest observed HSE energy is reported. To get reasonable running times for these experiments, the HSE energy is based on the native structure of the small protein *Protegrin 1* (1PG1, 18 residues). Tables 1 and 2 show the results of the lattice experiments for the TS and MCS heuristics. There is a row for each lattice type and data columns show the average HSE energy found over the 20 runs for the various parameters. In the SCC lattice, structures with the same HSE energy are found in all 20 runs (tabu difference 0.4 and 0.5), but the best observed HSE energy is rather high. The reason is that the SCC lattice is very coarse grained and low energy structures therefore do not exist in this lattice. For lattices of increasing complexity, the ability to find structures with lower energy increases. TS and MCS seem to perform equally well in low complexity lattices. However, in high coordination lattices, the TS heuristic performs slightly better than MCS on average. For the lattice with highest complexity (HC8) TS found zero energy structures for all 20 runs, this robustness was not observed for the MCS heuristic. These results indicate that conformational search heuristics using the HSE measure require high complexity lattices or off-lattice models with a high degree of freedom. Furthermore, TS is slightly more robust that MCS in high coordination lattices. The results of experiments with variable tabu list size