## CONCLUSION

From the results of the evaulation of both drugs, chloroquines and mefloquines, our linear modellings may serve as a useful basis for further drug design and evaluation. However, the agreement of observed and calculated activities is not yet very satisfactory and improvement of the models seems desirable.

Large variations in the values of the parameters within models for the same series of compounds indicate that other factors chould still play an important role, most probably geometrical effects which are not by our nonoptimized geometry input. Efficient methods of geometry optimization within CNDO framework might help in the future to reveal these factors. Changes in geometry will also lead to changes in atomic net charges.

Besides these methodical error sources one should also be in mind the inaccuracy of drug activity data which will not allow any model to fit beyond these experimentally determined.

Semiempirical CNDO calculations seem to be accurate enough for searching of electronic structure - activity relations. High computer effort for the ab initio work does not improve results. Models using atomic charge parameters seem to be sufficient. Geometry optimization of drugs, although very time consuming, might be the best way to improve data. Approaches like force-optimized geometries should be examined for this purpose in the future.