Structure determination of cyclodextrin derivatives and cyclodextrin complexes by NMR spectroscopy: comparative analysis of the molecular architectures

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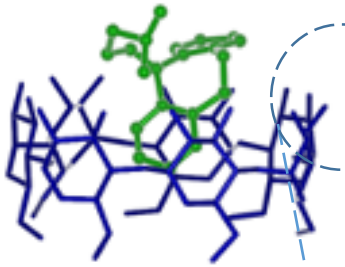
Synthesis/method/protocol: The structure and *in vitro* efficacy of modified cyclodextrins and their drug complexes were determined. For cyclodectrin's modification peptides and glycopeptides were designed.

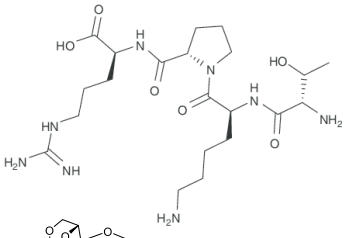
Scientific Goal: Evaluation of structure – activity relations in order to design optimized drug - cyclodextrin complexes.

Result: Using high-resolution ^{1}H- and ^{13}C-NMR (optimized NOESY, ROESY) the formation of molecular complexes was detected through the changes in the chemical shifts and intermolecular interactions. In our "pilot study" polarity and size of the guest molecules were described. We have proved that cyclodextrins are promising candidates as target cell specific delivery vehicles.



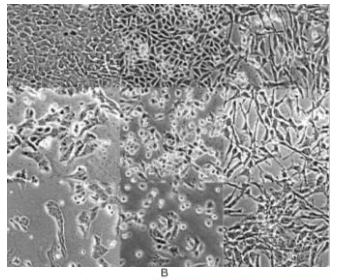
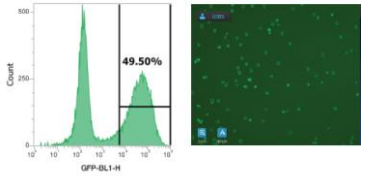
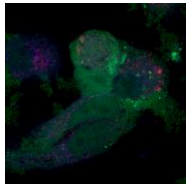
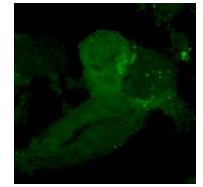



MODIFICATIONS:
CELL SURFACE SPECIFIC
PEPTIDES, GLYCOPEPTIDES
GLYCOCOMPOUNDS



Brucker DRX 500 NMR



ROESY SPECTRUM OF A CYCLODEXTRIN COMPLEX WITH HETEROCYCLIC ANTITUBERCULAR COMPOUND