

3D QSAR Study (CoMFA) of 4-Aminoquinolines, Inhibitors of CpG-ODN Driven Response

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Bacterial DNA and oligodeoxynucleotides (ODN) with CpG-motifs are immunostimulatory. The three-dimensional quantitative structure-activity relationship (3D QSAR) analysis with a training set of 100 antagonists of immunostimulatory CpG-ODN was conducted by Comparative Molecular Field Analysis (CoMFA). Statistically robust CoMFA model was obtained with a cross-validated correlation coefficient of 0.575 and conventional correlation coefficient of 0.934. For a test set of 7 inhibitors, the predictive coefficient r^2_{pred} was 0.875. The results were compared to the classical Free-Wilson analysis.

Abstract ID#: 11209

Password: 254312

Title: 3D QSAR Study (CoMFA) of 4-Aminoquinolines, Inhibitors of CpG-ODN Driven Response

Category Selection: General Poster Session IV

Presentation Format: Poster

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