Design of transfection reagents in RNAi therapeutics by chemoinformatics approach

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RNAi is a natural biological process involving gene silencing or regulation with siRNA and expected to be applied in the therapeutics of gene disorders. The delivery of siRNA into the cell is demonstrated using cationic lipid. The lipid is called 'Transfection reagents' and the development of new reagents has recently advanced. Some relation exists between the chemical structures of the reagents and their properties, but it is not clear yet quantitatively and the development of new reagents depends on the experimental perception.

In this study we collected the data of the transfection reagents from the literature[123] and constructed statistical models between the structures of the reagents and their suppression efficiency of gene expression in order to predict the chemical structures of high efficient reagents in future.

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