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研究简报

氨基酸描述子SZOTT用于多肽定量序效建模研究

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摘要 在相关研究的基础上, 提出一新的氨基酸描述子SZOTT, 该描述子所含信息量大, 且操作简便. 将其用于两类肽体系序列表征, 用偏最小二乘和正交信号纠正-偏最小二乘建模, 获得较好的建模结果.

关键词 氨基酸描述子(SZOTT) 肽 定量序效建模(QSAM) 偏最小二乘(PLS)

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Using SZOTT Descriptors for the Development of QSAMs of Peptides

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Abstract A new descriptor, namely scores vector of zero dimension，one dimension，two dimension and three dimension (SZOTT), was derived from principle components analysis of a matrix of 1 369 structural variables including 0D, 1D, 2D and 3D information for 20 coded amino acids. SZOTT scales were then employed to express structures of 20 thromboplastin inhibitors and 34 bactericidal peptides. The correlation coefficients of both whole calibration (R^2=R^2_{cu}) and of cross validation (Q^2=R^2_{cv}) for the multiple-variable models by classical partial least squares (PLS) and orthogonal signal correction-partial least squares (OSC-PLS) of 20 thromboplastin inhibitors were 0.989 and 0.748, 0.994 and 0.936, respectively. R^2 and Q^2 for the models by PLS and OSC-PLS of 34 bactericidal peptides were 0.619 and 0.406, 0.910 and 0.503, respectively. Satisfactory results obtained showed that structural information related to biological activity in both data sets could be described by SZOTT which included plentiful information related to biological activity, and which was conveniently operated and easy interpreted, also predictive capability of models were relative robust. There is a high prospect for SZOTT wide applications on quantitative sequence-activity modeling (QSAM) of peptides.

Key words SZOTT descriptor of amino acid; Peptide; Quantitative sequence-activity modeling(QSAM); Partial least squares(PLS)

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