

QSAR study of DEVD derivatives as apoptotic inducer

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Human genome sequencing results revealed there are about 30,000-50,000 genes. However, it is expected that there are more proteins and much more peptides. We have many bio-active peptides such as hormones. Authors tried to find peptides as apoptotic inducer. Especially, authors focused on the targeted proteins participating in apoptosis inside cell. For the penetration through the cell membrane small peptides were investigated. Six DEVD derivatives were tested using flow cytometry and Annexin V assay¹⁾. Even though six peptide derivatives contain the same moiety, they showed different induction of apoptosis. Authors considered this phenomenon arises from their different structures and tried to explain the reason. Here we report the relationships between structures of six derivatives and their activities using QSAR calculation.

Reference

1. Min Kyoung Kim, Youl-Hee Cho, Jung Mogg Kim, Moon Woo Chun, Seung Ki Lee, Yoongho Lim, Chul-Hoon Lee. Induction of apoptosis in human leukemia cells by MCS-C2 via caspase-dependent Bid cleavage and cytochrome c release (2005). *Cancer Lett.* On-line published.