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Article

Modeling and Virtual Screening of Antisense Peptides Targeting the Divergent Region of TumorÃƒÂ¢Ã‚Â€Ã‚Â•Associated MT1ÃƒÂ¢Ã‚Â€Ã‚Â•MMP Protein

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Correction added on 01 October 2015, after first online publication: ISSN (Print) has been corrected.

Abstract

Membrane typeÃƒÂ¢Ã‚Â€Ã‚Â•1 matrix metalloproteinase (MT1ÃƒÂ¢Ã‚Â€Ã‚Â•MMP; also known as MMP14) is a key enzyme involved in tumor invasion and metastasis, and is a potential target for drug discovery for cancer therapy. However, till now there is no MT1ÃƒÂ¢Ã‚Â€Ã‚Â•MMPÃƒÂ¢Ã‚Â€Ã‚Â• or MMPÃƒÂ¢Ã‚Â€Ã‚Â•based anticancer drugs in the market mainly because of the high conservation of the MMP family and also because there is no elucidated crystal structure for the mature MT1ÃƒÂ¢Ã‚Â€Ã‚Â•MMP. The modeling of the threeÃƒÂ¢Ã‚Â€Ã‚Â•dimensional structure of mature MT1ÃƒÂ¢Ã‚Â€Ã‚Â•MMP and the finding of MT1ÃƒÂ¢Ã‚Â€Ã‚Â•MMP targeted peptides by virtual screening are highly desired. In this study, the threeÃƒÂ¢Ã‚Â€Ã‚Â•dimensional structure of mature MT1ÃƒÂ¢Ã‚Â€Ã‚Â•MMP is constructed by homology and *de novo* modeling and later rationalized and optimized by molecular dynamics simulations. An antisense peptide library was constructed against the divergent sense peptide DEGTEEET in the specific region of MT1ÃƒÂ¢Ã‚Â€Ã‚Â•MMP, which was found by multiple alignment of the whole MMP family. The antisense peptide library was virtually screened against the constructed threeÃƒÂ¢Ã‚Â€Ã‚Â•dimensional model of MT1ÃƒÂ¢Ã‚Â€Ã‚Â•MMP. The top 20 novel peptides were further studied, which were found well docked with MT1ÃƒÂ¢Ã‚Â€Ã‚Â•MMP at the region of DEGTEEET, again confirming their specific binding to MT1ÃƒÂ¢Ã‚Â€Ã‚Â•MMP. Preliminary study of one of the topÃƒÂ¢Ã‚Â€Ã‚Â•ranked peptide SFLLSPFV showed that it could inhibit the viabilities of MG63 and MDAÃƒÂ¢Ã‚Â€Ã‚Â•MBÃƒÂ¢Ã‚Â€Ã‚Â•231 tumor cells. We thus not only successfully modeled the threeÃƒÂ¢Ã‚Â€Ã‚Â•dimensional structure of mature MT1ÃƒÂ¢Ã‚Â€Ã‚Â•MMP but also provided a new way for the finding of peptide candidates targeting MT1ÃƒÂ¢Ã‚Â€Ã‚Â•MMP based on antisense peptide library.

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