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In silico discovery and rational prediction of differential peptide mimetic active inhibitors against LINE1 and LINE2 conserved retro-transposition mechanism on the CD133/AID/APOBEC cancer stem cell derived protein motif like binding domains by annotating tetrahedral meshes in a QM Index Dynamic Unified Theorem

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Identification and solution structure of a highly conserved C-terminal domain within ORF1p is required for retro-transposition of long interspersed nuclear element-1. Retrotransposons constitute almost half of the human genome and are considered to be one of the major driving forces in the evolution of eukaryotic genomes. They are classified into two major types, long terminal repeat (LTR) retrotransposons, which include retroviruses and non-LTR retrotransposons. The non- LTR retrotransposon LINE1 (L1) and LINE2 (L2) clades, which are widespread among vertebrates, differ in two important structural and functional characteristics. Second, unlike the L1 reverse transcriptase that can mobilize other RNA species, the L2 enzyme is specific for its own 3' UTR. Furthermore, while both L1 and L2 elements are present in fish, amphibians and reptiles, only the L1 retrotransposon clade has greatly expanded in mammals, reaching 17% of the human genome. In contrast, the L2 retrotransposons are inactive in placental mammals, with only highly defective copies present in the human genome. It has also been shown that an elevated expression of the stem cell marker CD133 was associated with Line-1 demethylation in hepatocellular carcinoma. That relationship of Line-1 demethylation and the CD133 expression of cancer stem cells were discussed in hepatocellular carcinoma (HCC). Cancer cells are also characterized by expression of active LINE-1 elements (L1s, long interspersed nuclear elements-1). Several million small- like poly-pharmacophore molecules will be designed in-silico in a single HTS campaign within the cell populations for screening could easily invalidate an entire campaign. As a result in this scientific drug discovery approach we have introduced an in silico discovery and rational prediction of the solution structure of differential peptide mimetic active inhibitors of LINE1 and LINE2 conserved retro-transposition mechanism in the host defense stem cell marker CD133/AID/APOBEC by identifying QM Fragment LINE1 and LINE2 conserved retro-transposition mechanism utilizing URLs 3D structure precision utilities of QM Based Structure CD133/LINE-1 AID/APOBEC Protein/Ligand Complexes on Model derivation and symbolic representation of LINE1-AID to the retro-transposition locus. We finally, generated in-silico experimental procedures and network specifications of stem cell marker CD133/APOBEC3s LINE-1 retro-transposition physiological targets based on a Line-1, Line-2 QM index dynamic unified theorem for multiple entities as an efficient and versatile tool for the lead structure generation and optimization of a dynamic simulated in-silico druggable database of experimentally measured effects of mutations on structurally defined protein-ligand complexes of transposable elements for assessing and comparing protein–small molecule affinities by predicting binding affinities and scoring values on simulated importing and annotating tetrahedral meshes in reverse transcriptase LINE1 assays and L1 constructs for the discovery of chemical probes for fragment-based drug discovery by binding homology search according to ligand and receptor similarity to or better than other binding-homology methods with higher computational efficiency online.

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