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Designing effective anticancer-radiopeptide carriers A Molecular Dynamics study of their interaction with model tumor and healthy cell membranes

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We present in this talk an extensive Molecular Dynamics study of the interaction between a newly designed anticancer-radiopeptide and (models of) tumor and healthy cell membranes.
Inspired by the mechanism by which antimicrobial peptides interact with the negatively charged bacterial membranes, we have modified the human antimicrobial peptide LL-37 to get a functionalized radionuclide carrier capable of binding to the negatively charged tumor membranes but not to the neutral healthy ones. This selectivity property results from the fact that at the slight acidic pH surrounding tumor tissues the histidines belonging to the peptide get protonated thus making it positively charged.
Computation of the binding free-energy between the peptide and different kinds of membranes confirms that the affinity of the peptide to tumor membranes is significantly larger than to healthy tissues. These features (high affinity and generic tumor selectivity) recommend antimicrobial derived customized carriers as promising theranostic constructs in cancer diagnostic and therapy.

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