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Electronic Supplementary Information

Structure optimization of dendritic lipopeptide based gene vectors with the assistance from molecular dynamic simulation

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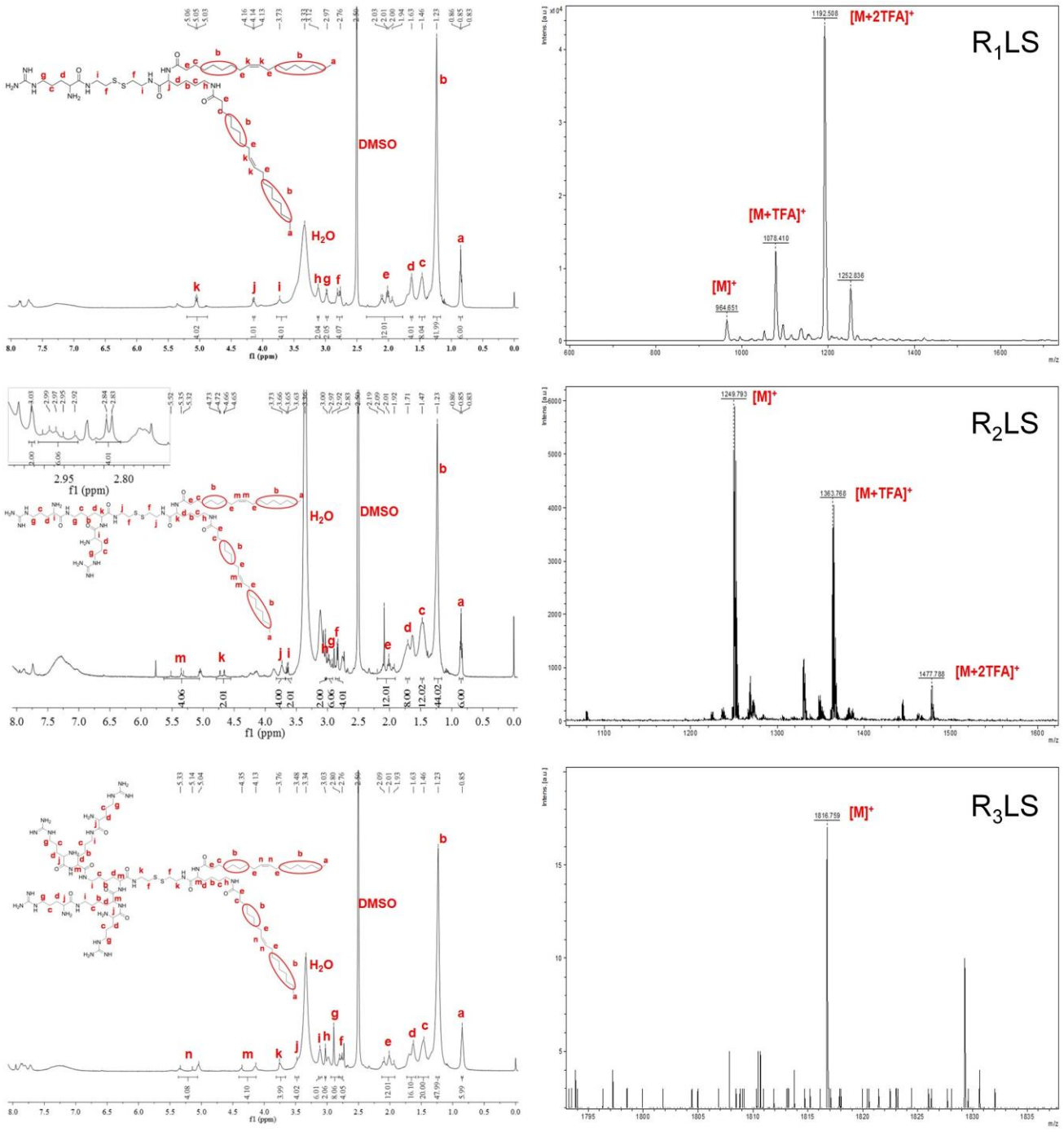

Fig. S1 Nuclear magnetic resonance (^{1}H NMR) and mass spectrometry (MALDI-TOF-MS) of $R_{1/2/3}$LS molecules.

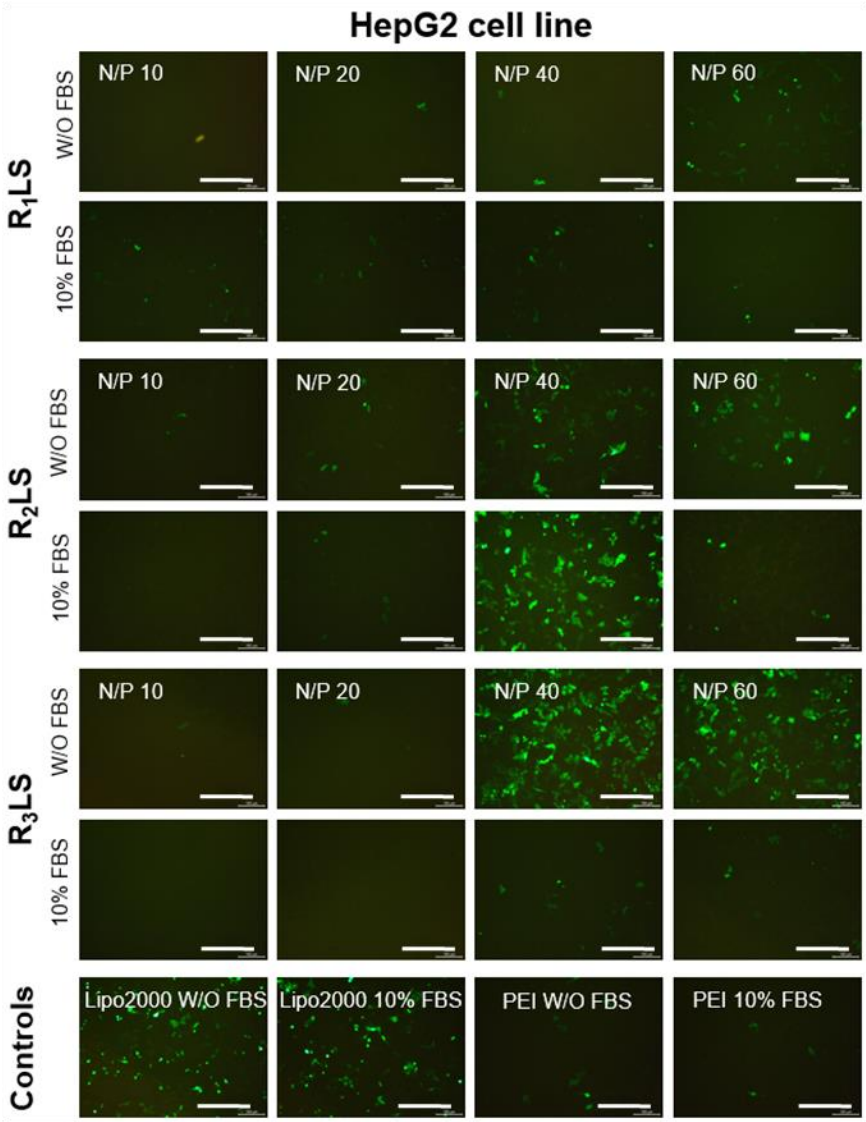

Fig. S2 *In vitro* transfection efficiency of different generation dendritic peptides. Green fluorescence proteins were expressed on HepG2 cell lines with 10 % FBS or without FBS. The N/P ratio of PEI/DNA was 10. Scale bar is 100 μm.

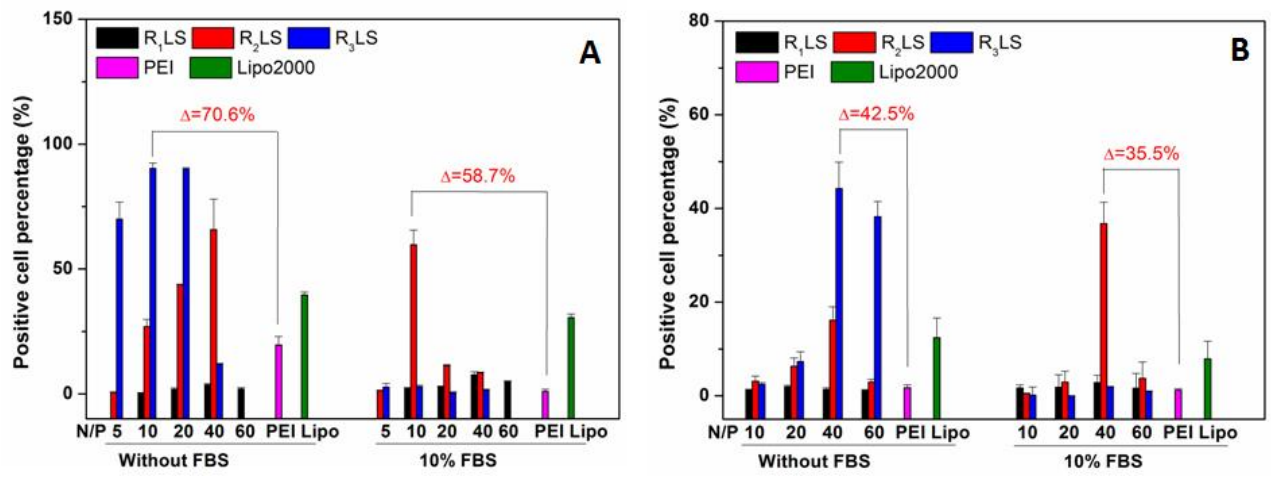

Fig. S3 The semi-quantitative evaluation of transfection efficiency *in vitro*. (A) Hela cell lines, (B) HepG2 cell lines. "Δ" represents the difference value.

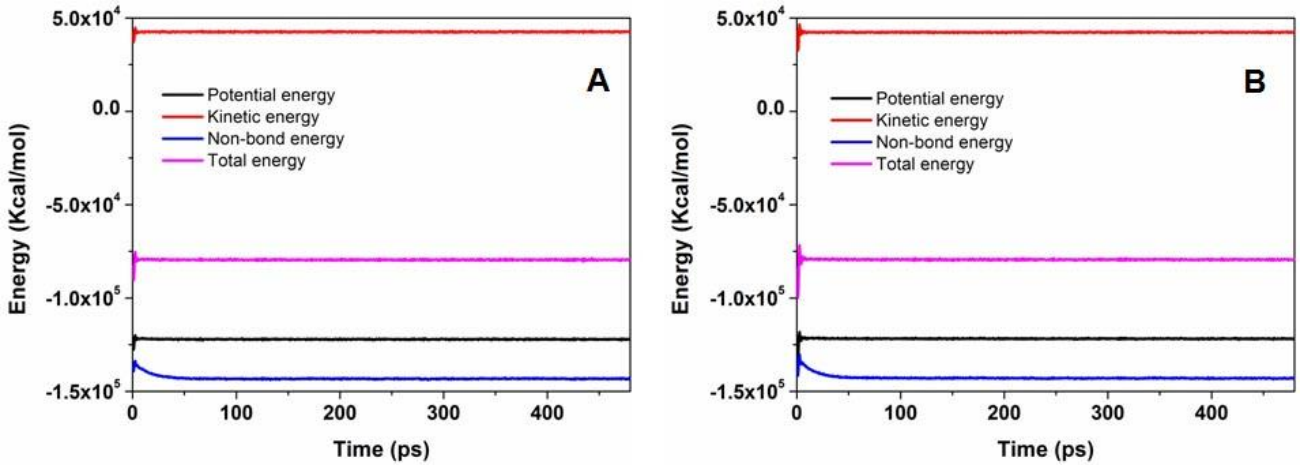

Fig. S4 The tendency of energy change for R_2LS system during 500 ps, (A) a couple of molecular system; (B) multiple molecular system. (R_1LS and R_3LS system were similar as R_2LS system.)

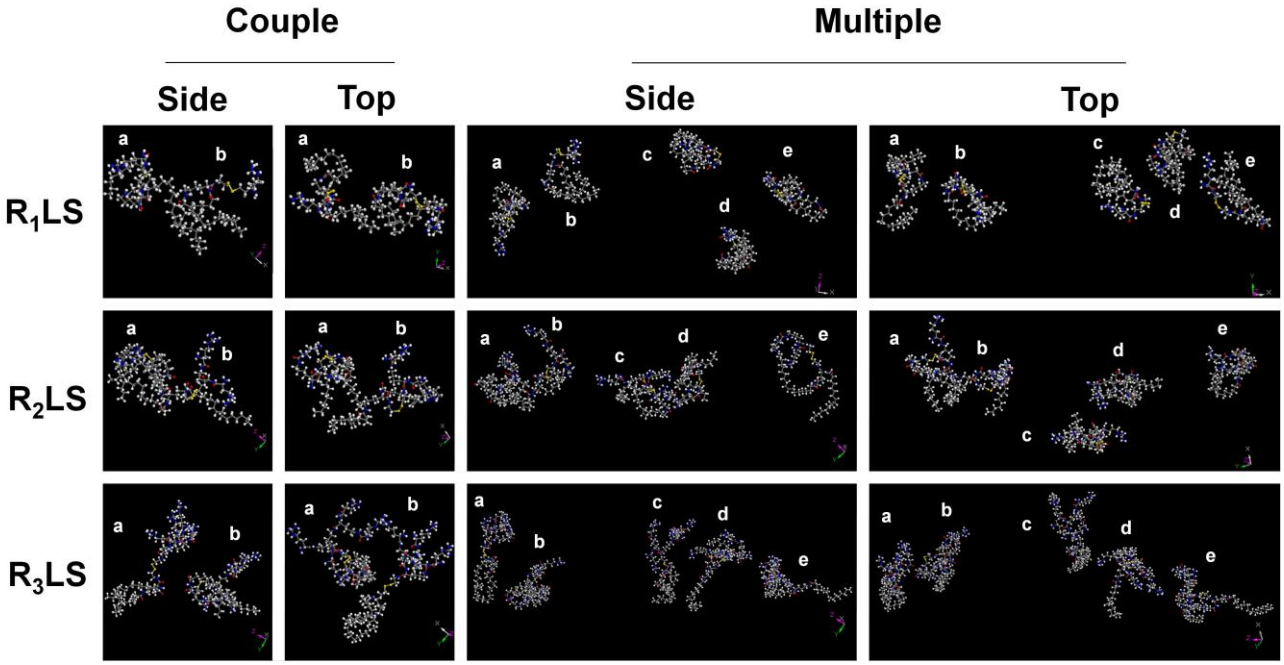

Fig. S5 The results of intermolecular interaction at 500 ps by molecular dynamic simulation. The left two lines were the intermediate states of couple molecules simulation for $R_{1/2/3}LS$ (the two molecules were marked by a and b). The right two lines were the intermediate states of five molecules simulation for $R_{1/2/3}LS$ (the five molecules were marked by a, b, c, d, e, respectively).