Polymer Drug Interactions in Thiadiazolylthioacetamide Derivatives-Linear Dendritic Copolymer Nanoparticles: ONIOM Approach

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Abstract

The delivery of drugs for clinical treatment is a challenging problem. The programmed release of a drug at specified levels is important for various types of clinical treatments, including AIDS therapy. Various carriers have been shown to be useful in the targeted delivery of different classes of therapeutic agents. Among these carriers, biodegradable nanoparticles formulated from biocompatible polymers have shown the potential for the sustained intracellular delivery of different therapeutic agents. Theoretical investigation of the interaction between thiadiazolylthioacetamide derivatives (TTAs) and linear–dendrimer have been performed by the ONIOM2 (B3LYP/6-31G: UFF) method. The results showed that there are weak interactions containing hydrogen bonds and Vander Waals interactions, and clearly indicated that these complexes have relatively low stability; therefore, the PCA-PEG-PCA copolymer is a suitable drug delivery molecule for anti-HIV drugs. The interaction energies and NBO analysis of the anti-HIV drugs (TTAs derivatives)-polymer-tyrosine system indicated these nanocarriers can be utilised to improve the biological and anti-HIV activity of TTAs.

References

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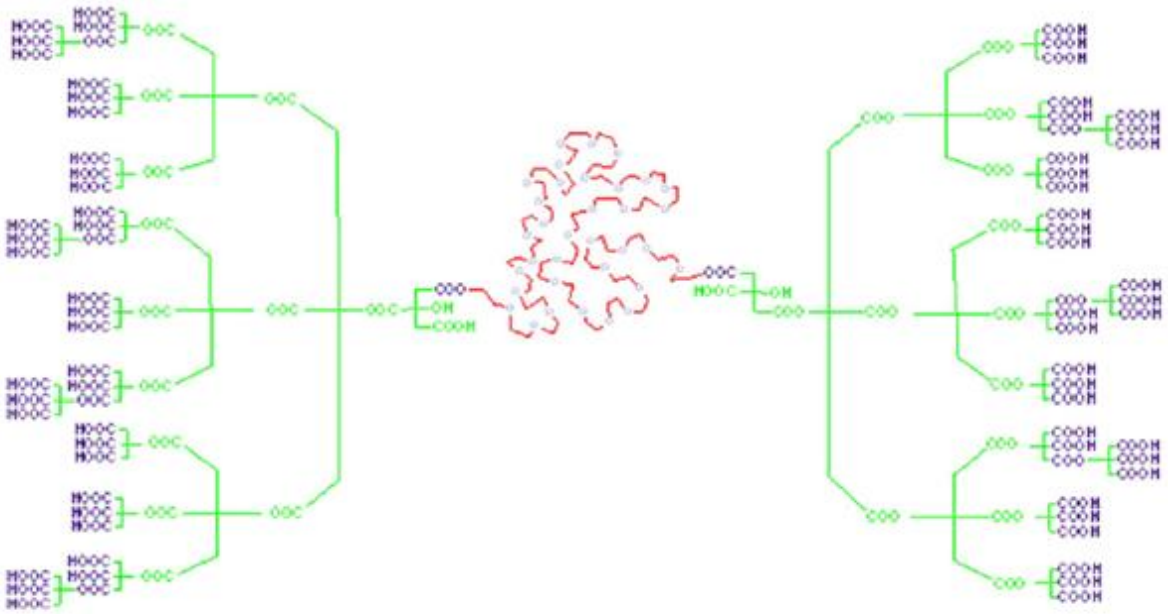

Figure 1 Triblock copolymer of (PCA)3-(PEG)10-(PCA)3

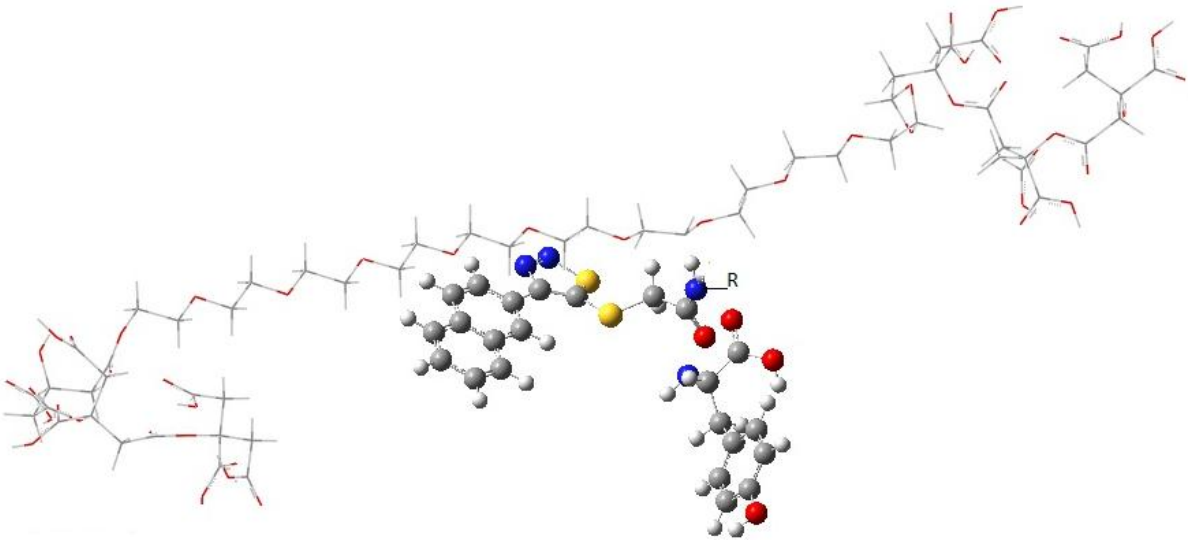

Figure 2 Tyrosine, TTA derivatives and (PCA)3-(PEG)10-(PCA)3 copolymer (ONIOM2)