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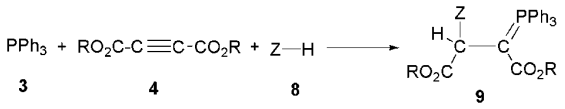
Contents

Graphical Abstracts



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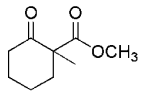
a		Me	80
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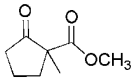
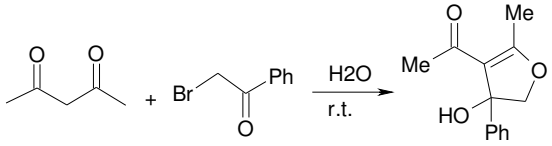
c		Me	90



The interaction between nucleic acid bases and a (10, 0) single-walled carbon nanotube (CNT) were investigated through calculations within density functional theory based treatments. It has been found that the guanine base adsorption is bound stronger to the outer surface of nanotubes in comparison to the other bases, consistent with the recent theoretical studies. In this work the insertion of nucleic acid bases inside the nanotubes has been also investigated for the first time. Our calculations reveal that the cytosine base exhibits a stronger binding to the inner surface of nanotubes side-wall. Furthermore, when nucleic acid bases were inserted inside the tube, the nanotube shape was deviated from cylinder.