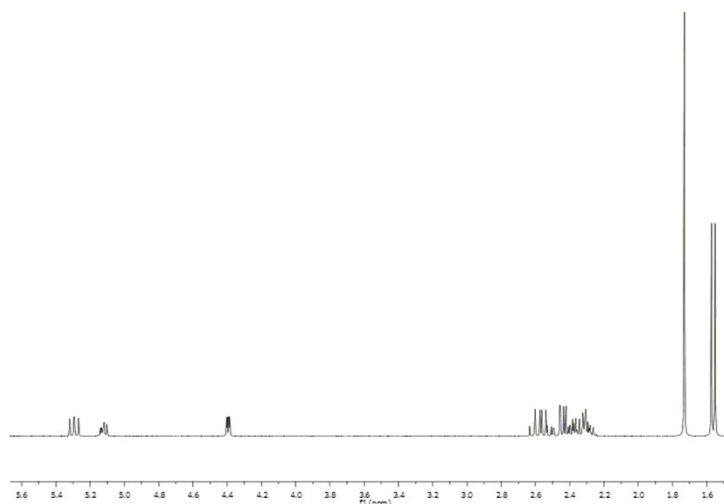


## Supplementary information

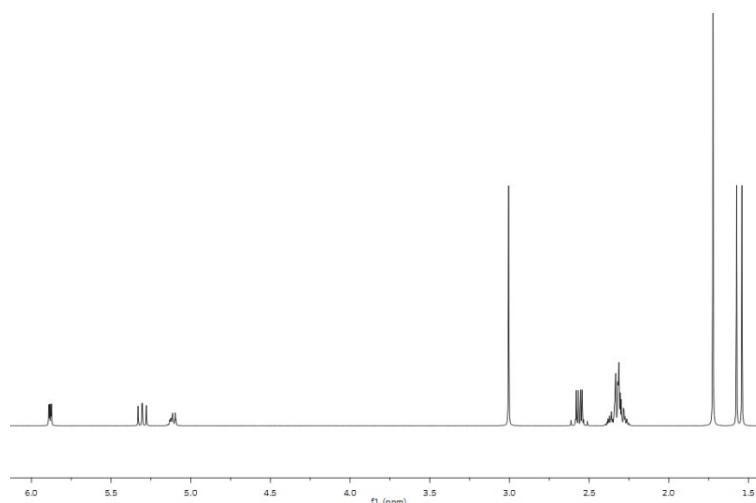
Title: Novel Anti-cancer Agents Based on Germacrone: Design, Synthesis, Biological activity, Docking Studies and MD Simulations

Authors: Lianbao Ye, Jie Wu, Weiqiang Chen, Yu Feng, Zhibing Shen

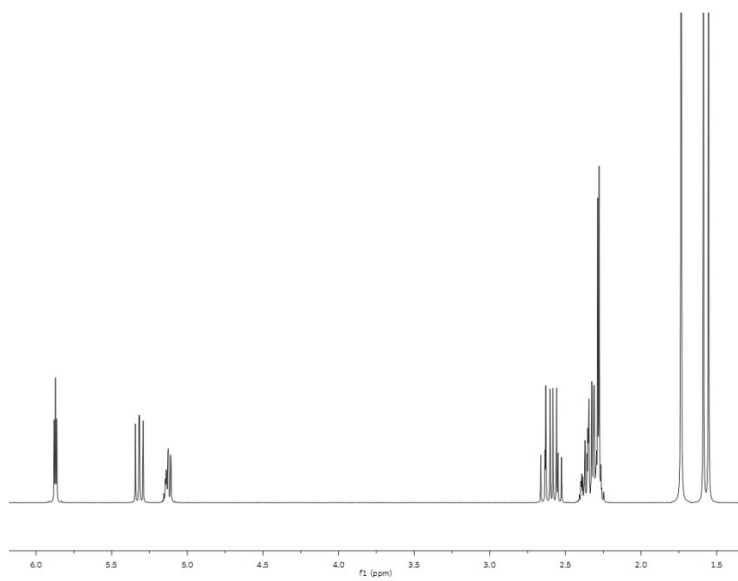
<sup>1</sup>HNMR and <sup>13</sup>C NMR of compounds



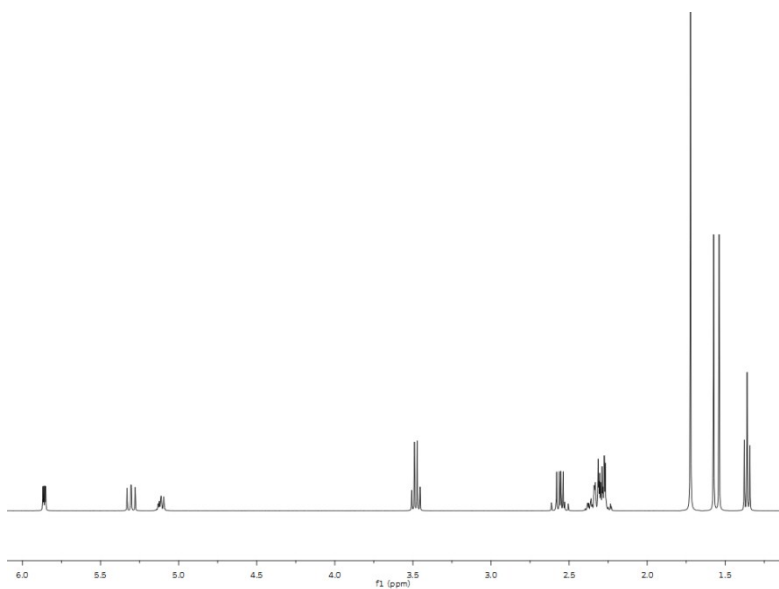
<sup>1</sup>HNMR of 2



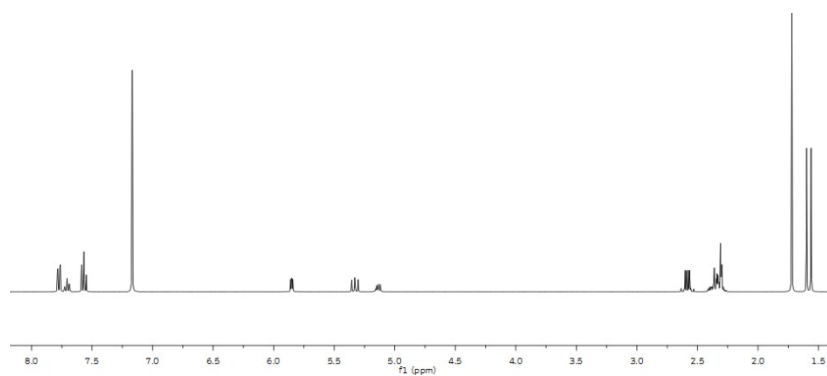
<sup>1</sup>HNMR of 3a



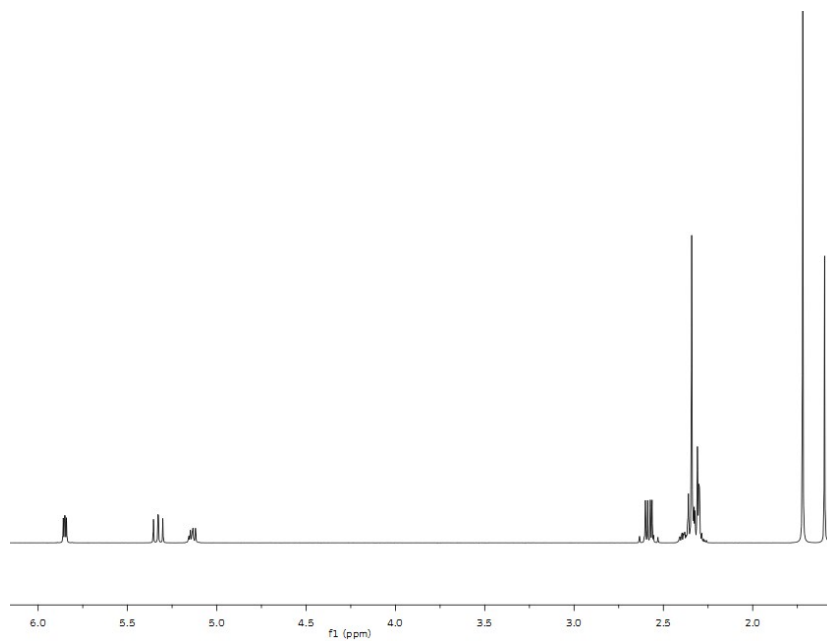
$^1\text{H}$ NMR of 3b



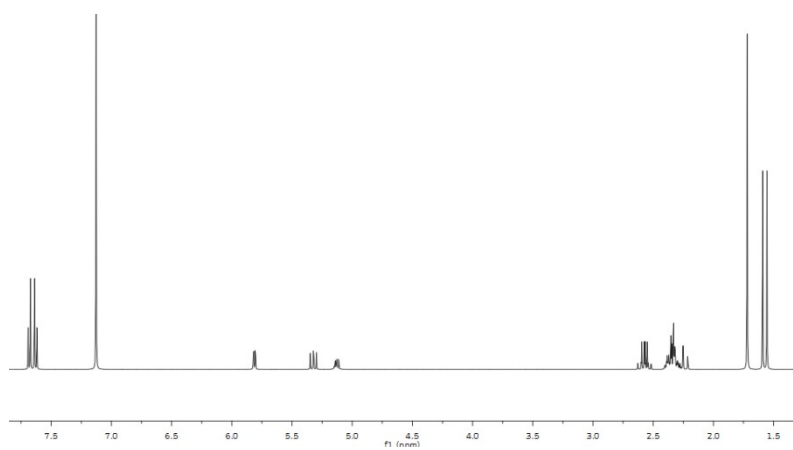
$^1\text{H}$ NMR of 3c



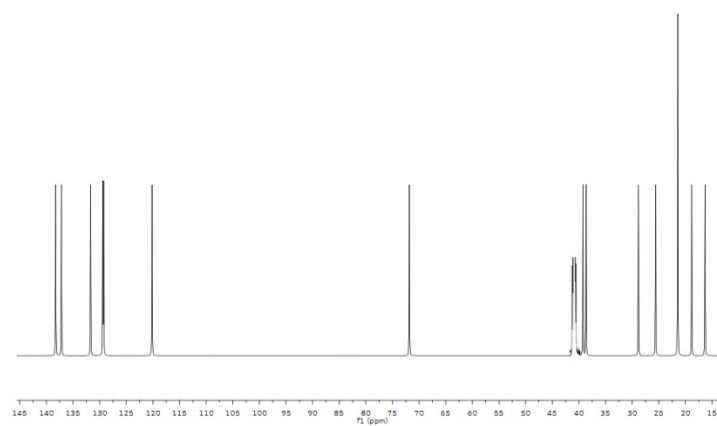
$^1\text{H}$ NMR of 3d



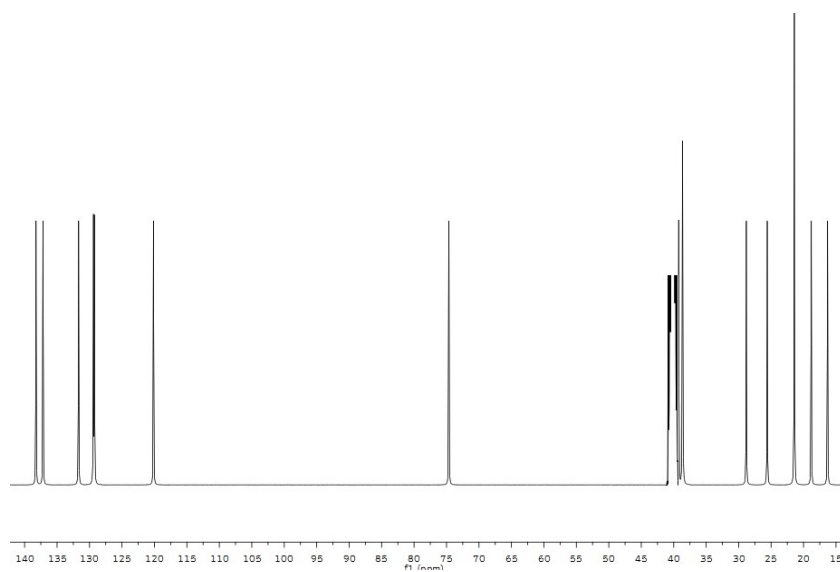
$^1\text{H}$ NMR of 3e



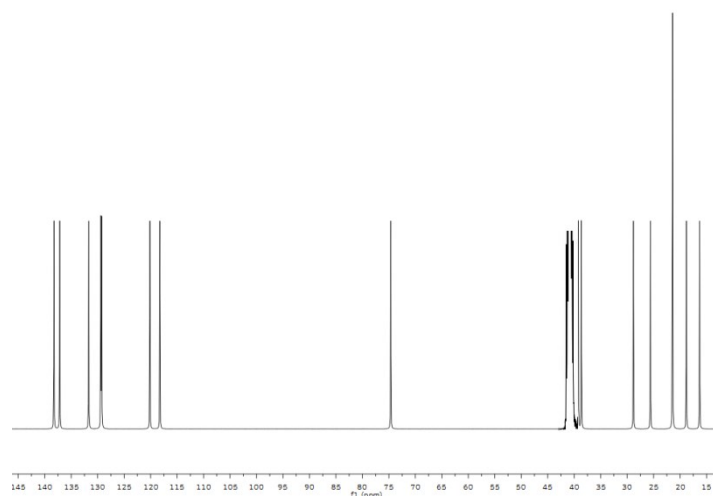
$^1\text{H}$ NMR of 3f



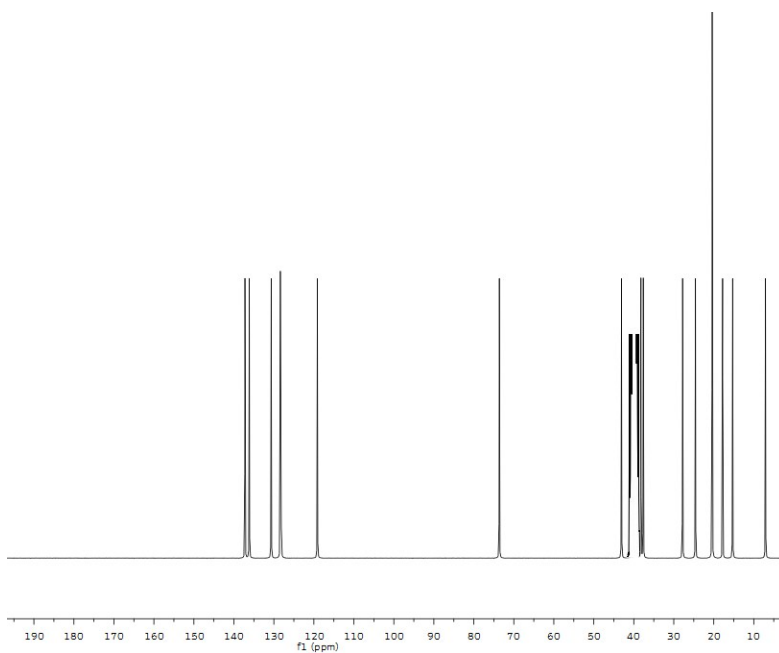
$^{13}\text{C}$  NMR of 2



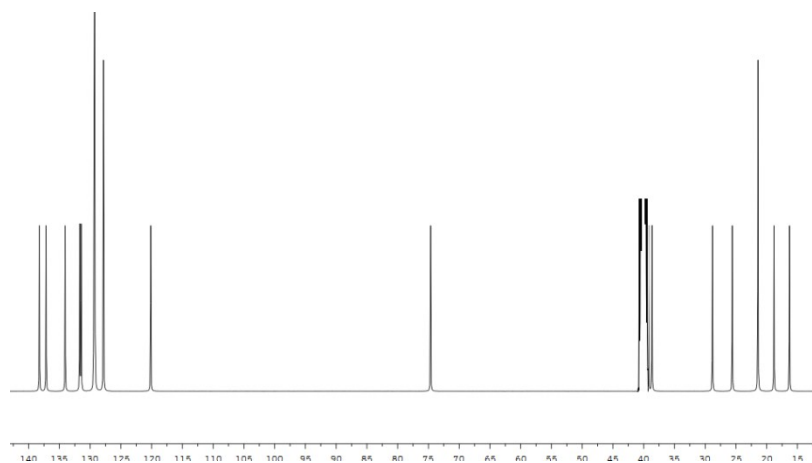
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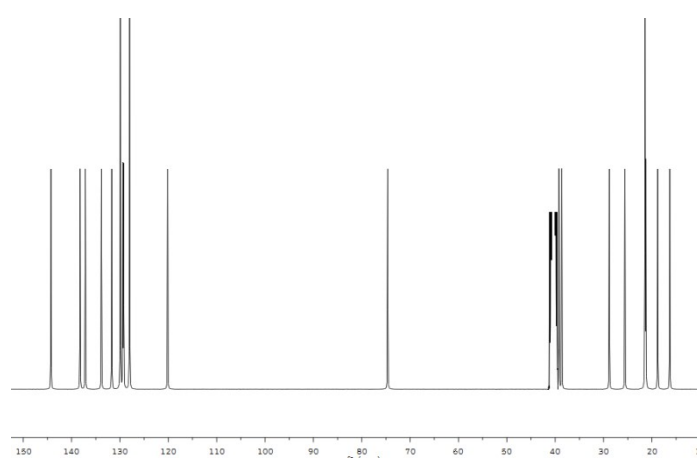
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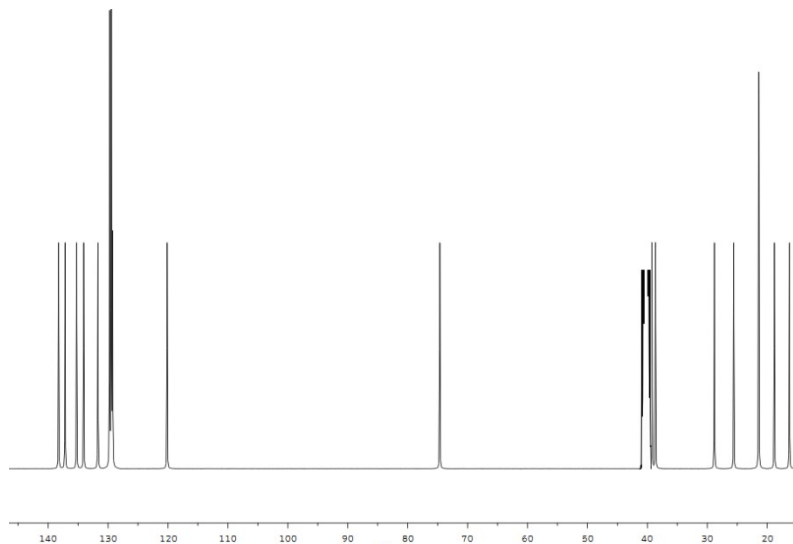
$^{13}\text{C}$  NMR of 3c



$^{13}\text{C}$  NMR of 3d



$^{13}\text{C}$  NMR of 3e



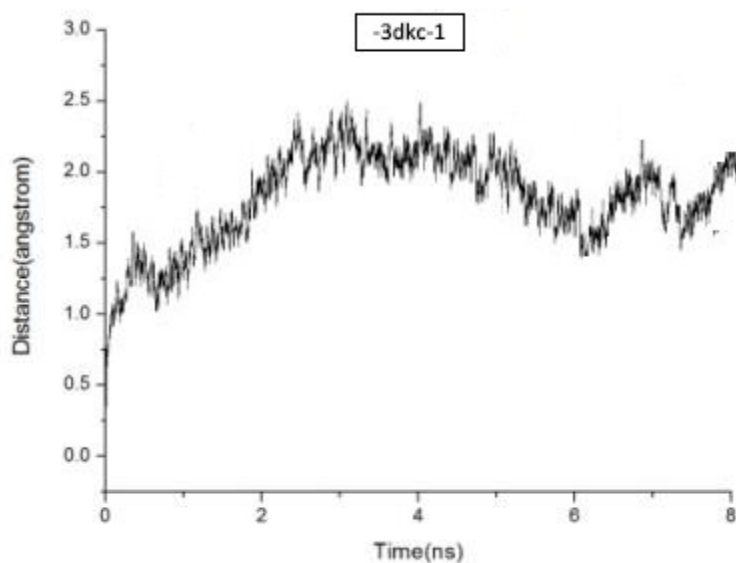
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## Supplementary information

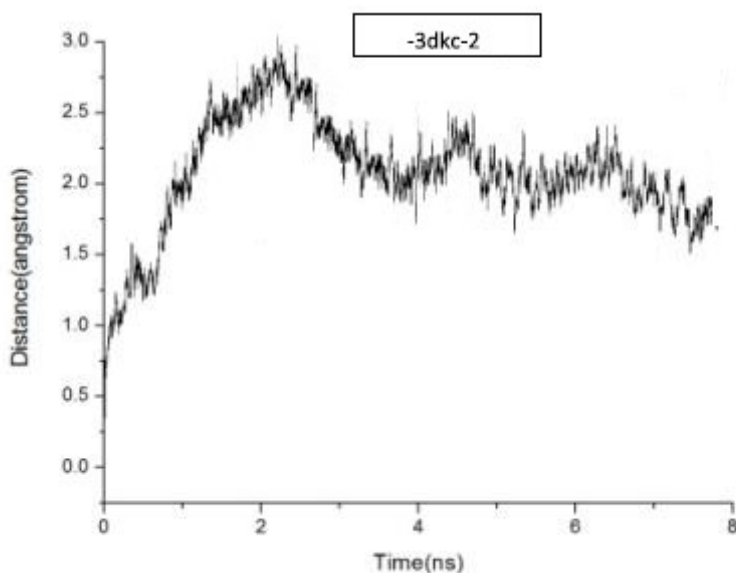
Title: Novel Anti-cancer Agents Based on Germacrone: Design, Synthesis, Biological activity, Docking Studies and MD Simulations

Authors: Lianbao Ye, Jie Wu, Weiqiang Chen, Yu Feng, Zhibing Shen

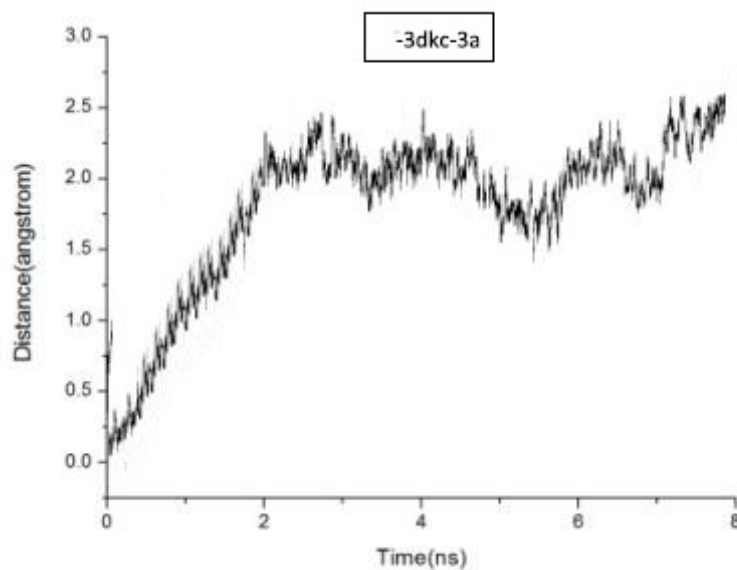
Figures of Plots of RMSD for all of the backbone atoms ( $\text{\AA}$ ) vs simulation time (ns) for 3DKC in complex with 1-3f



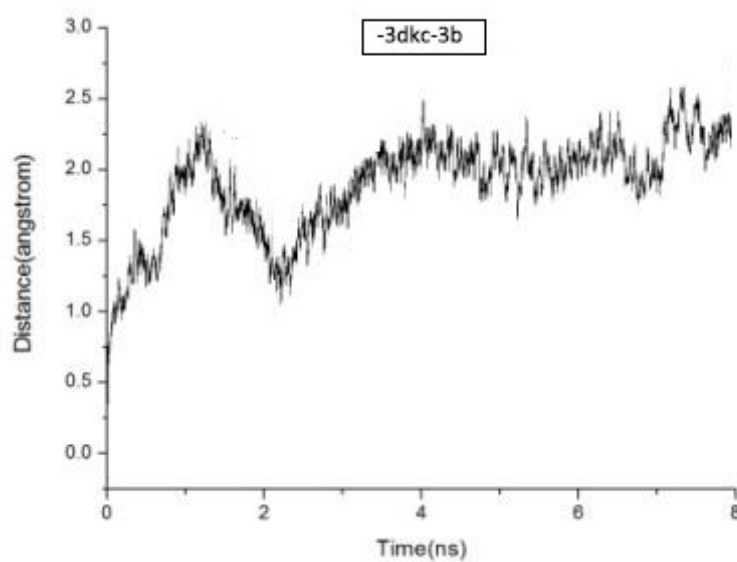
Figures of Plots of RMSD for all of the backbone atoms ( $\text{\AA}$ ) vs simulation time (ns) for 3DKC in complex with 1



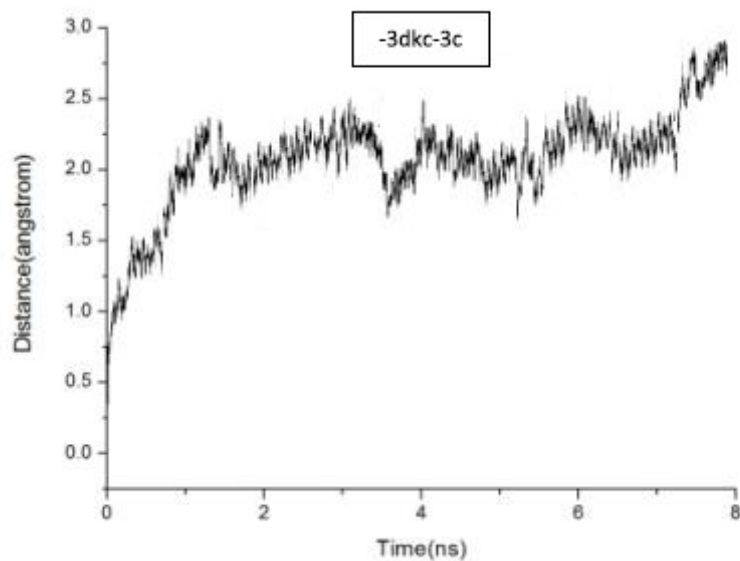
Figures of Plots of RMSD for all of the backbone atoms ( $\text{\AA}$ ) vs simulation time (ns) for 3DKC in complex with 2



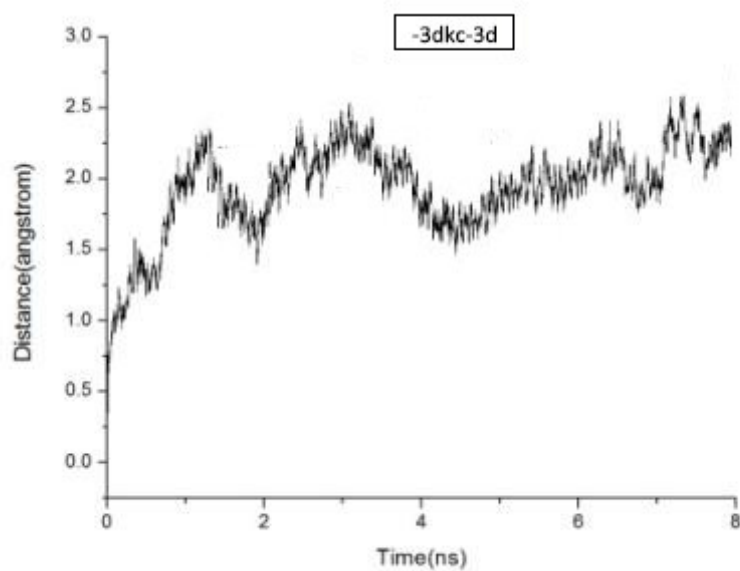
Figures of Plots of RMSD for all of the backbone atoms ( $\text{\AA}$ ) vs simulation time (ns) for 3DKC in complex with 3a



Figures of Plots of RMSD for all of the backbone atoms ( $\text{\AA}$ ) vs simulation time (ns) for 3DKC in complex with 3b

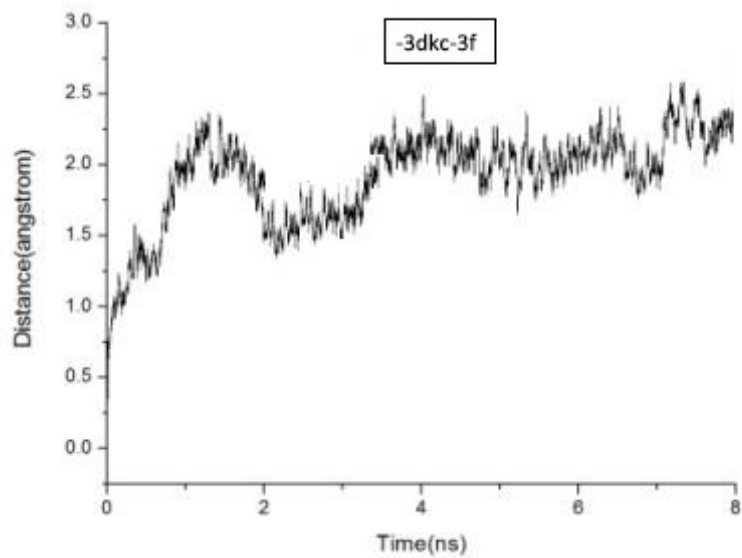


Figures of Plots of RMSD for all of the backbone atoms (Å) vs simulation time (ns) for 3DKC in complex with 3c



Figures of Plots of RMSD for all of the backbone atoms (Å) vs simulation time (ns) for 3DKC in complex with 3d





Figures of Plots of RMSD for all of the backbone atoms ( $\text{\AA}$ ) vs simulation time (ns) for 3DKC in complex with 3f