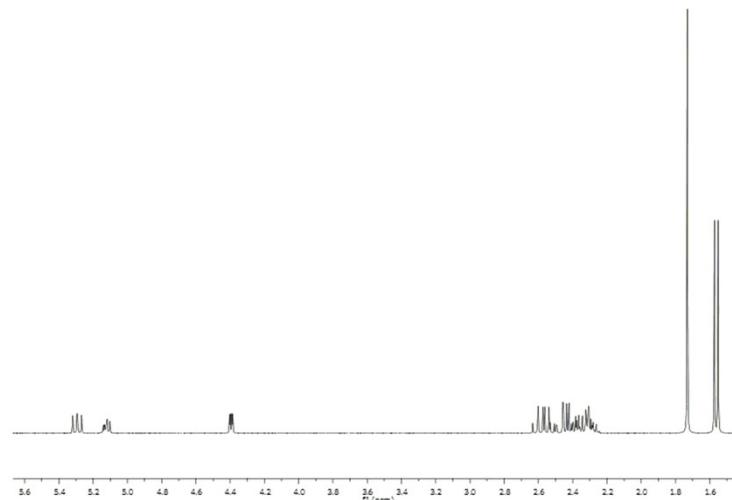


Supplementary information

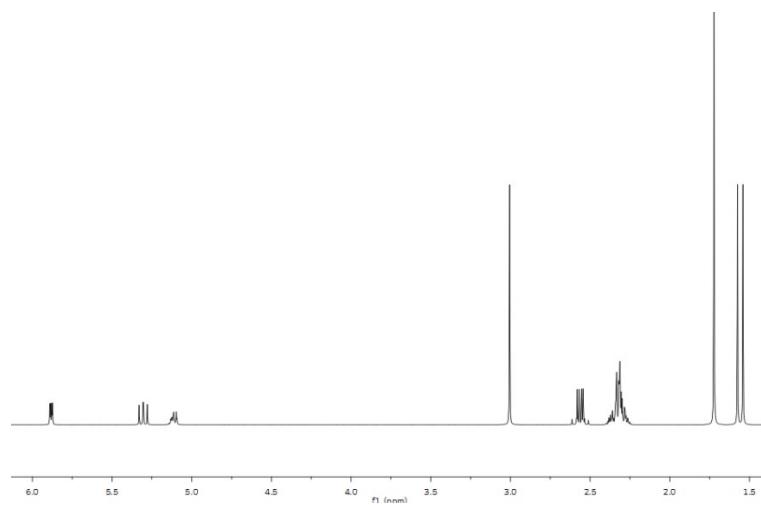
Title: Novel Anti-cancer Agents Based on Germacrone: Design, Synthesis, Biological activity, Docking Studies and MD Simulations

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

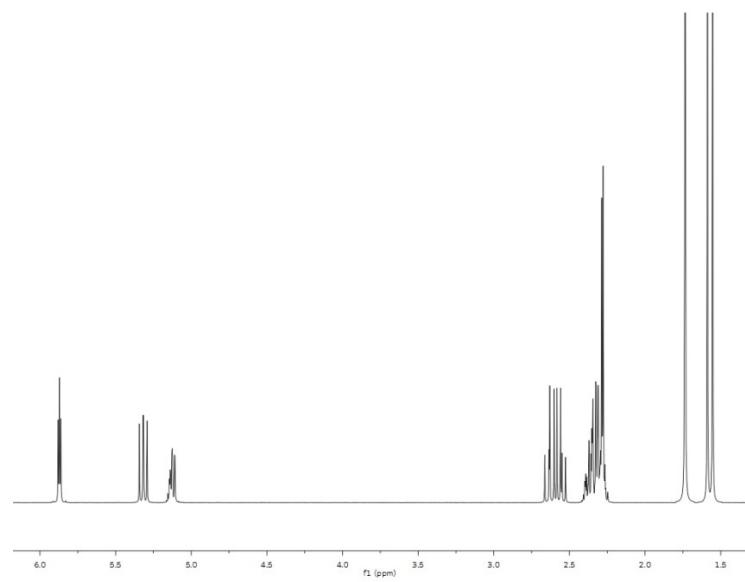
^1H NMR and ^{13}C NMR of compounds



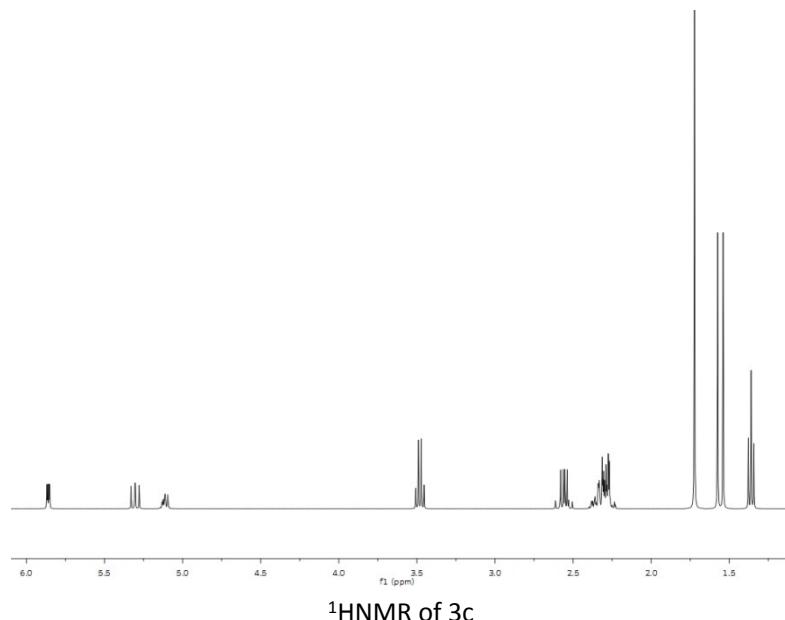
^1H NMR of 2



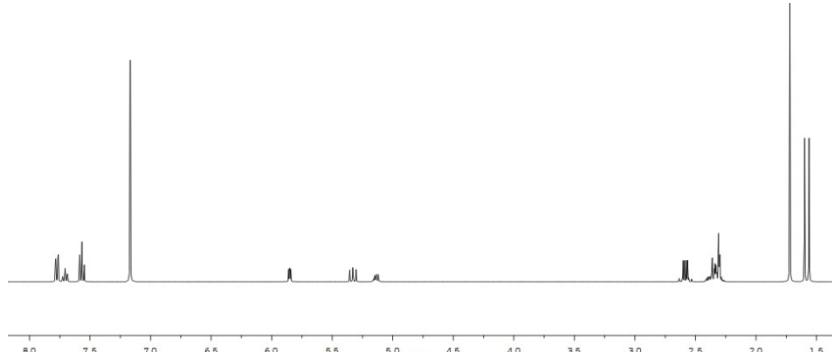
^1H NMR of 3a



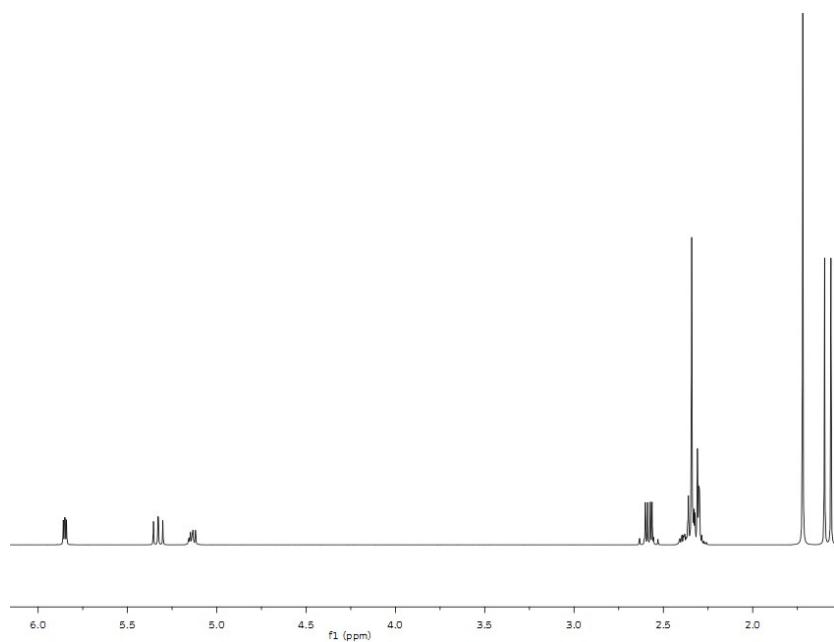
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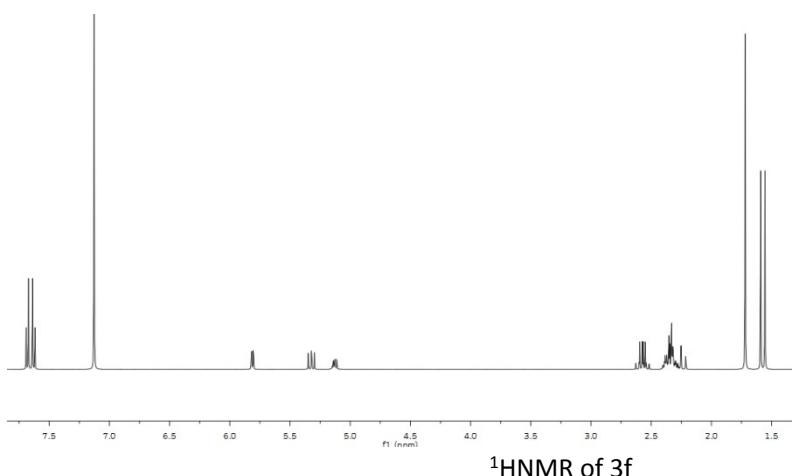
^1H NMR of 3c



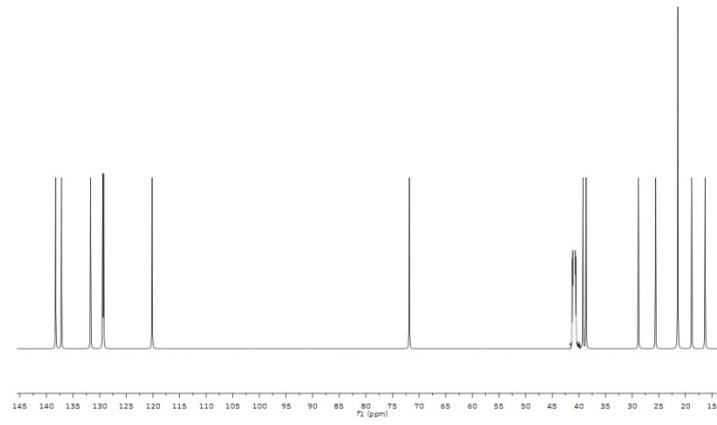
^1H NMR of 3d



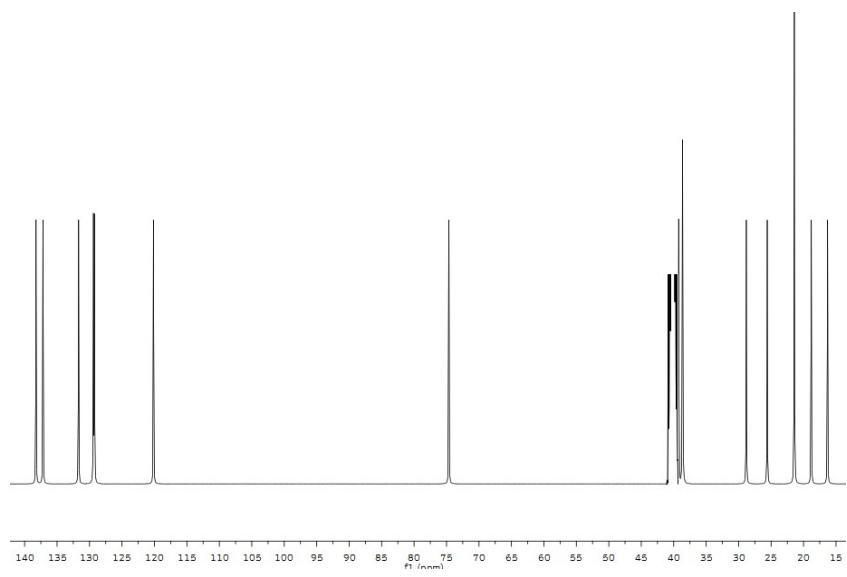
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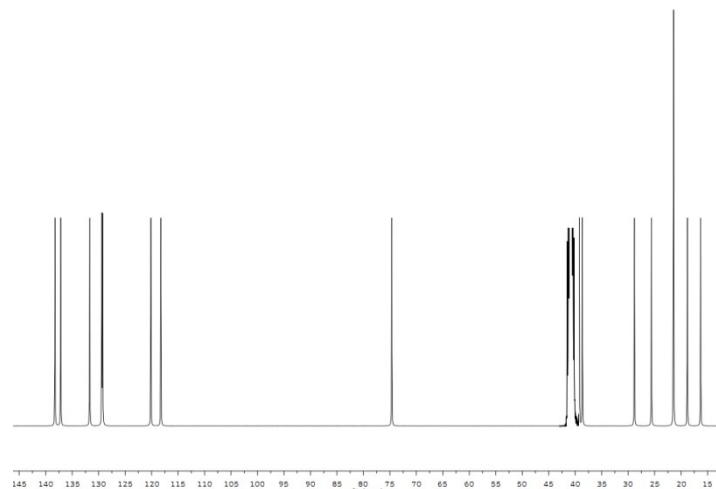
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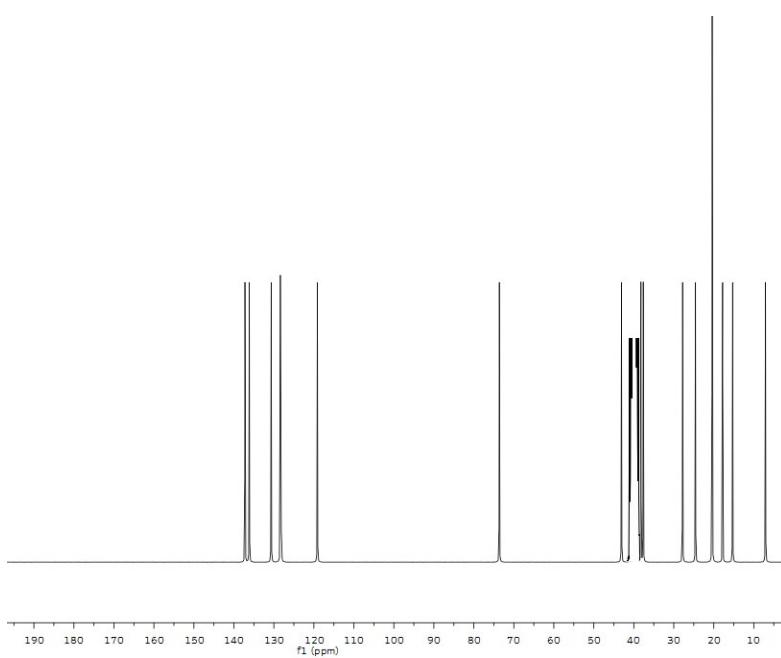
^{13}C NMR of 2



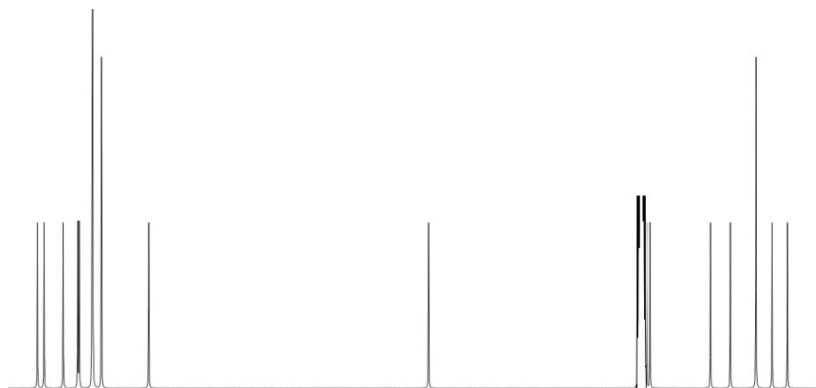
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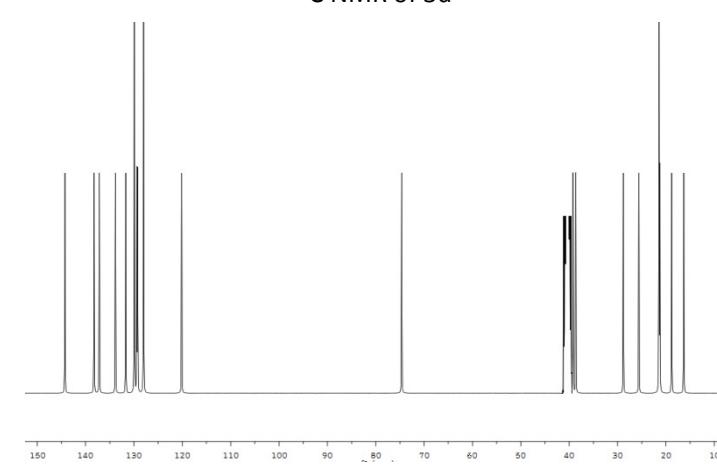
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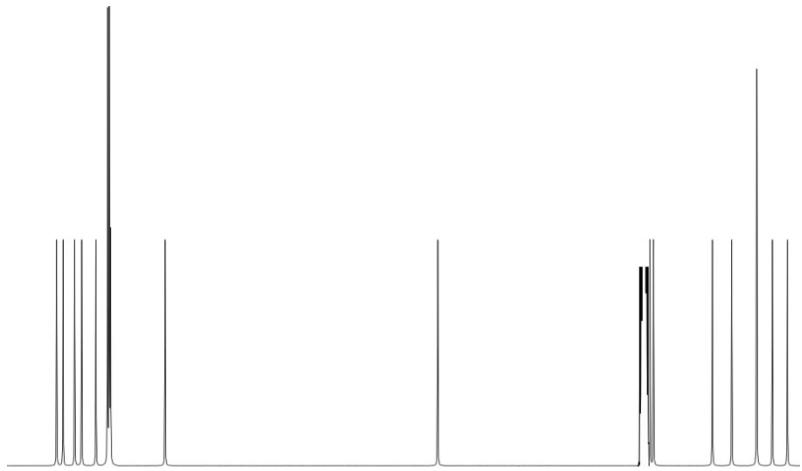
¹³C NMR of 3c



¹³C NMR of 3d



¹³C NMR of 3e



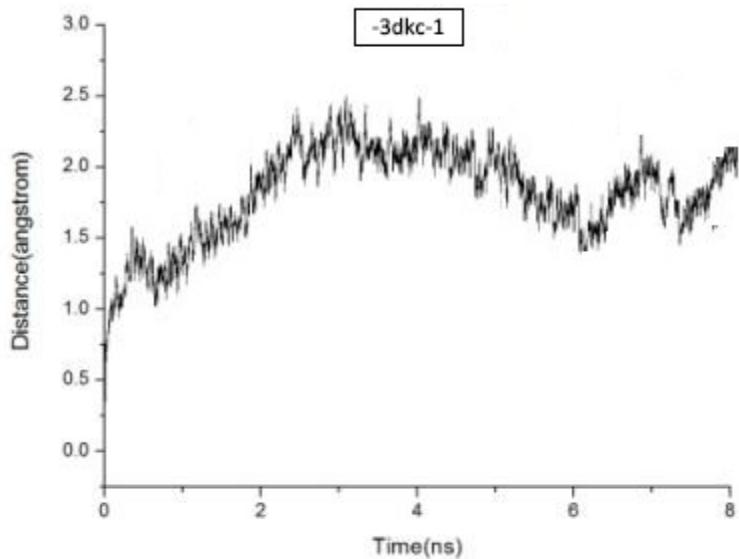
¹³C NMR of 3f

Supplementary information

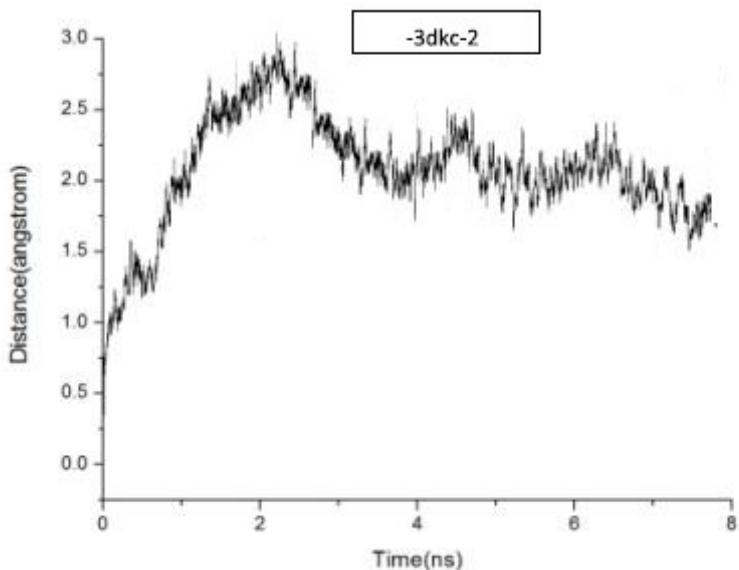
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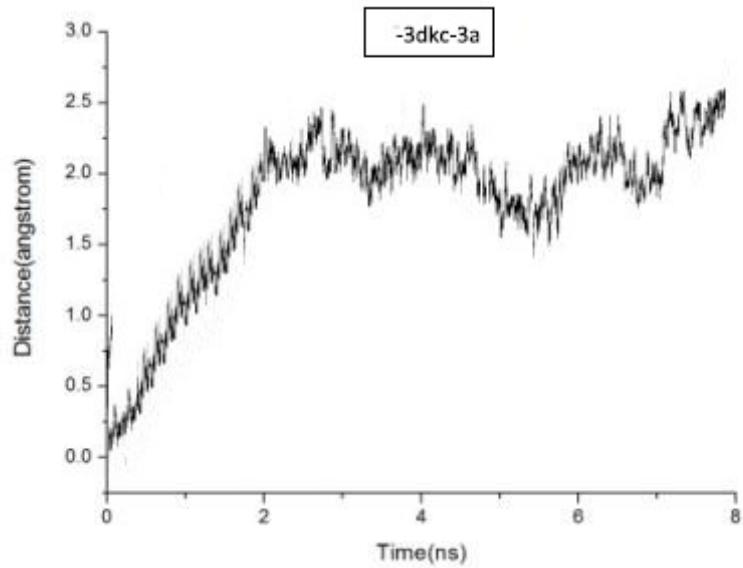
Figures of Plots of RMSD for all of the backbone atoms (\AA) vs simulation time (ns) for 3DKC in complex with 1-3f



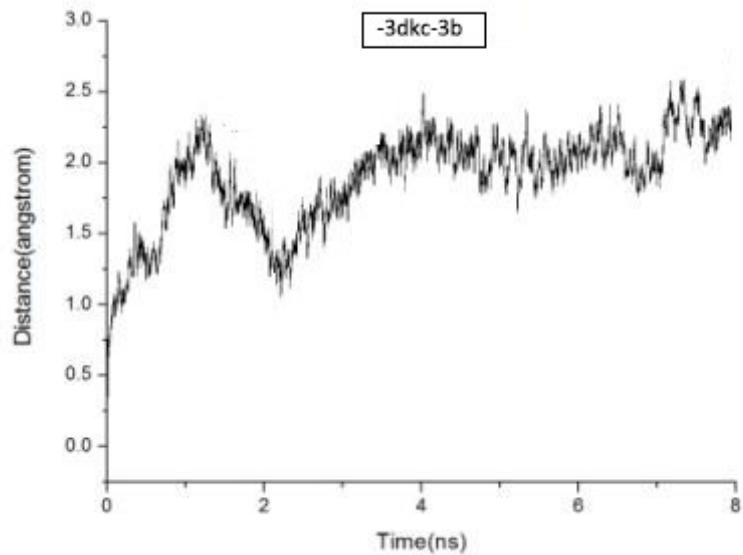
Figures of Plots of RMSD for all of the backbone atoms (\AA) vs simulation time (ns) for 3DKC in complex with 1



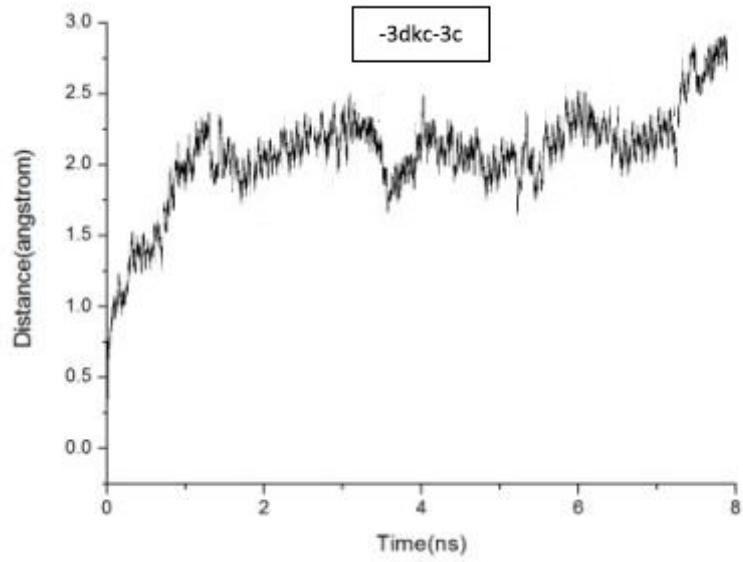
Figures of Plots of RMSD for all of the backbone atoms (\AA) vs simulation time (ns) for 3DKC in complex with 2



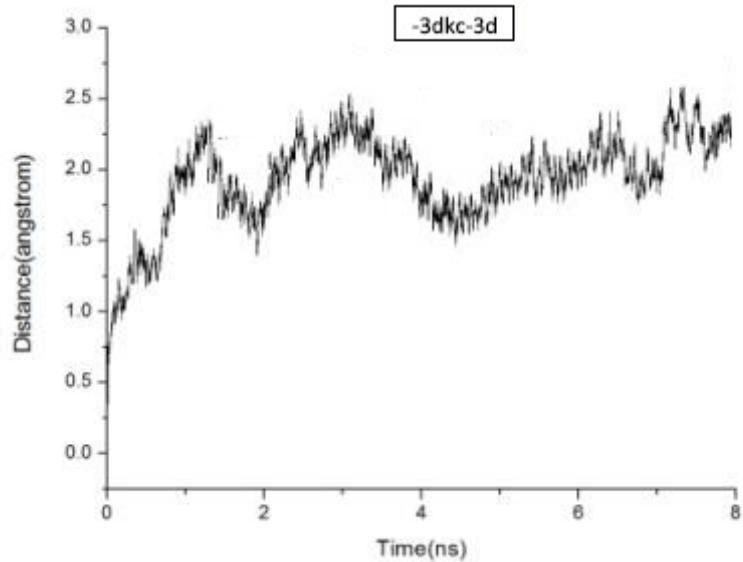
Figures of Plots of RMSD for all of the backbone atoms (\AA) vs simulation time (ns) for 3DKC in complex with 3a



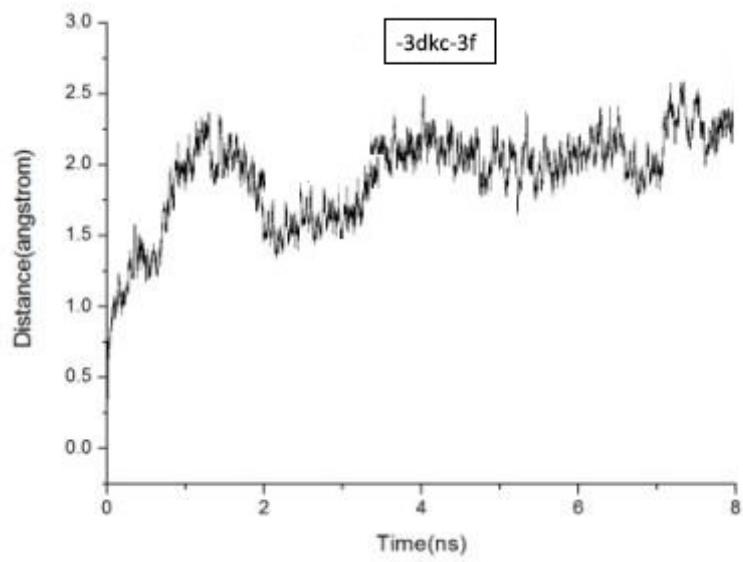
Figures of Plots of RMSD for all of the backbone atoms (\AA) vs simulation time (ns) for 3DKC in complex with 3b



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



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



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