Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Influence of Size and Charge of Gold Nanocluster on Complexation with siRNA: A Molecular Dynamics Simulation Study

Sathish Kumar Mudedla [a, b], Ettayapuram Ramaprasad Azhagiya Singam[a], Kanagasabai Balamurugan[a] and Venkatesan Subramanian[a, b, *]

[a] *Chemical Laboratory, CSIR-Central Leather Research Institute, Adyar, Chennai-600 020, India*

[b] *Academy of Scientific and Innovative Research (AcSIR), CSIR-CLRI Campus, Chennai 600 020, India*

* To whom correspondence should be addressed. Tel.: +91 44 24411630. Fax: +91 44 24911589. E–mail: subuchem@hotmail.com, subbu@clri.res.in.

Table S1 The Width of Minor and Major Grooves of siRNA for the Complexes AU38, AU102, 2AU38 and 2AU102

Model	Starting value		Averaged value	
	Major(Å)	Minor(Å)	Major(Å)	Minor(Å)
AU38	19.7	15.6	19.1	14.1
AU102	19.7	15.6	20.2	15.4
2AU38	19.7	15.6	20.3	15.3
2AU102	19.7	15.6	20.1	15.2

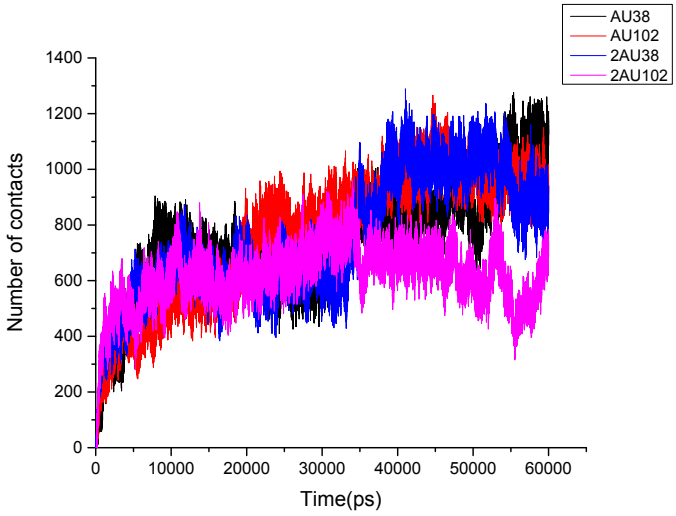


Fig. S1 The number of contacts between gold nanocluster and siRNA.

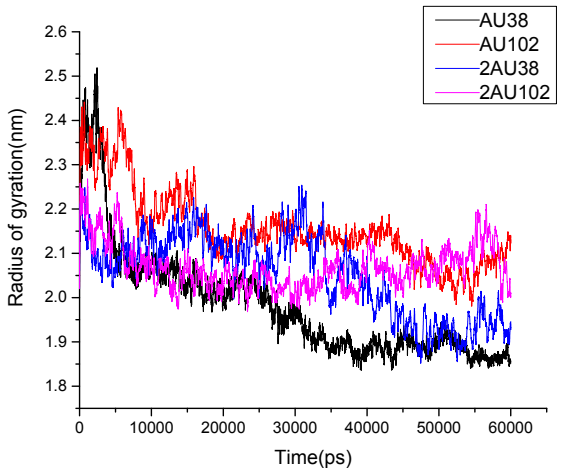


Fig. S2 The radius of gyration for the complexes of siRNA with AU38, AU102, 2AU38 and 2AU102.

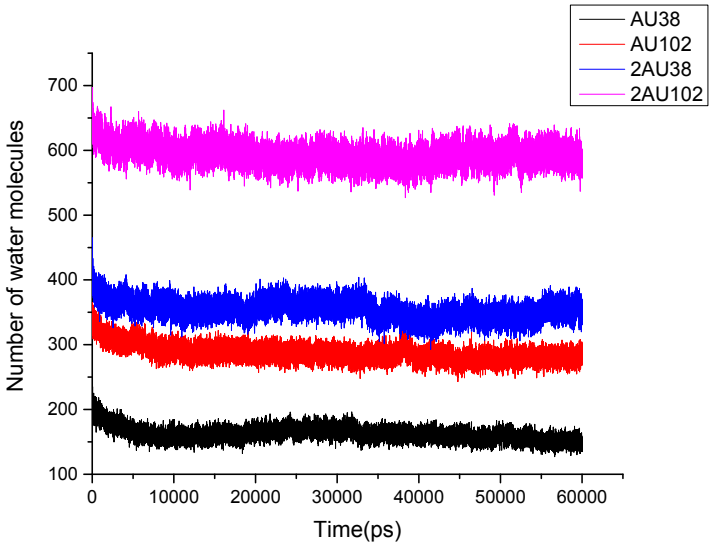
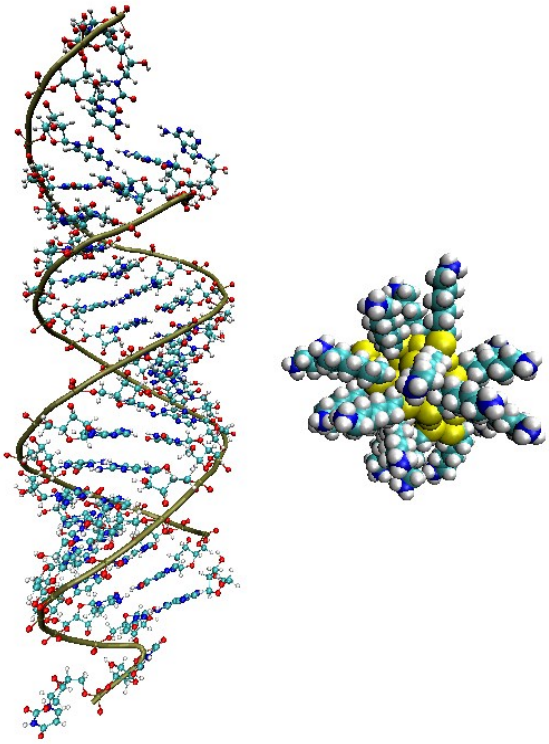
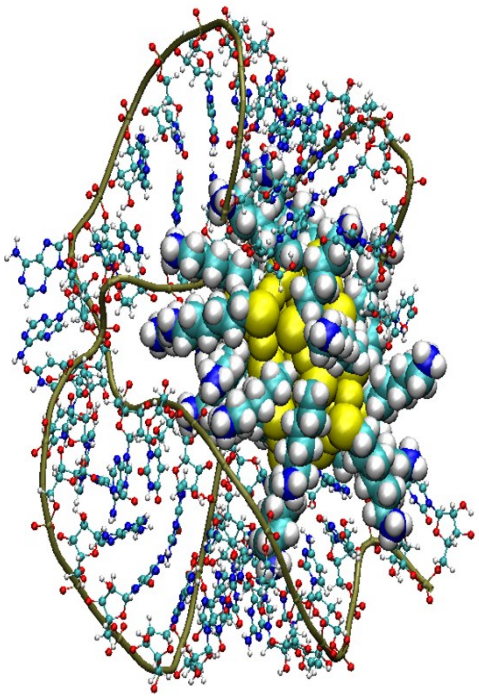


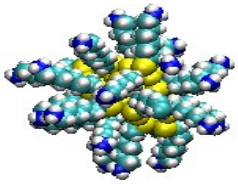
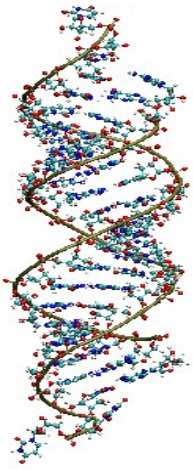
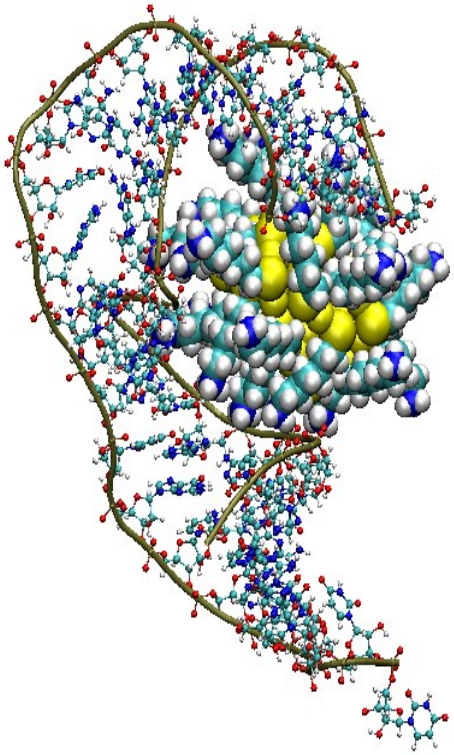
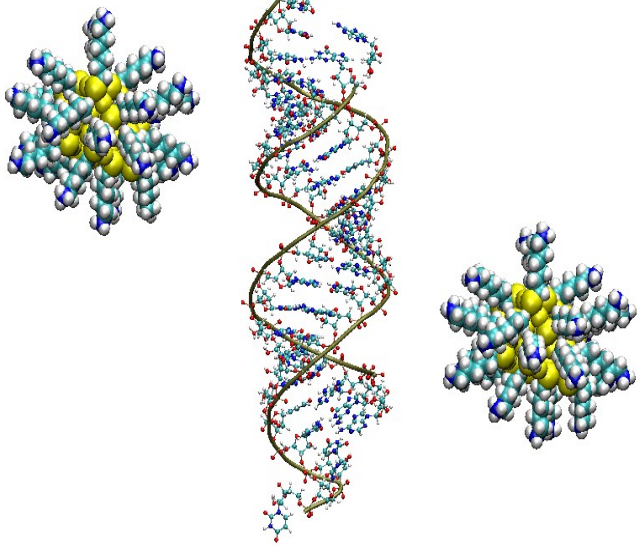
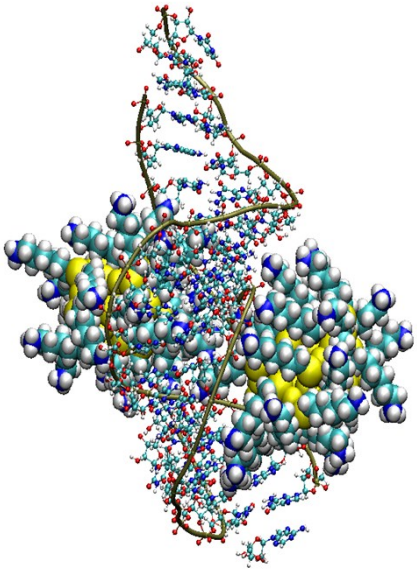
Fig. S3 The number of water molecules in all the systems.

AU38-configuration-1

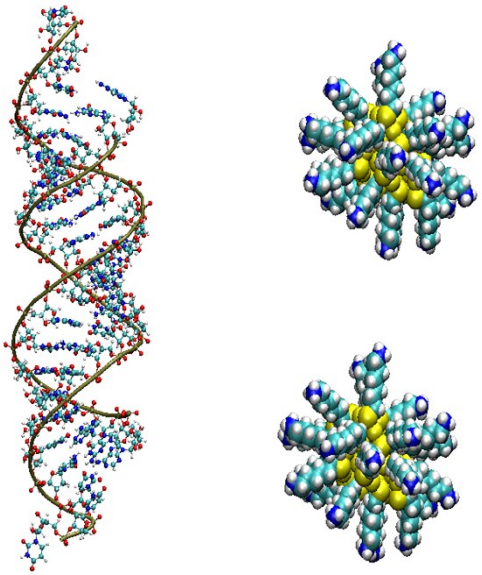




60 ns

0 ns	
AU38-configuration-2   0 ns	 60 ns
2AU38-configuration-1  0 ns	 60 ns

2AU38-configuration-2



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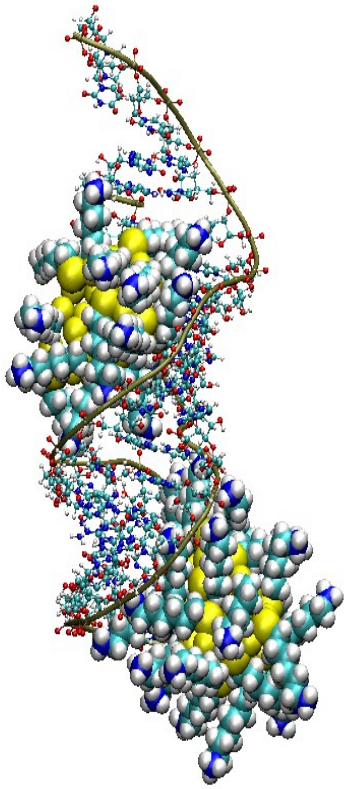

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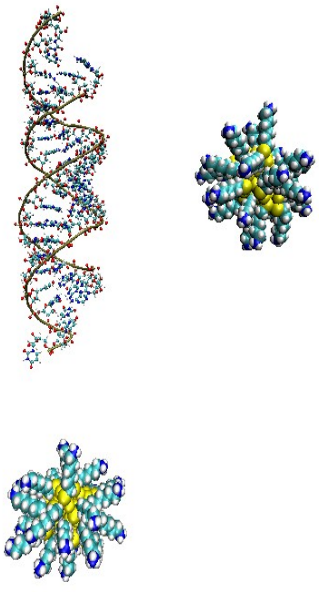
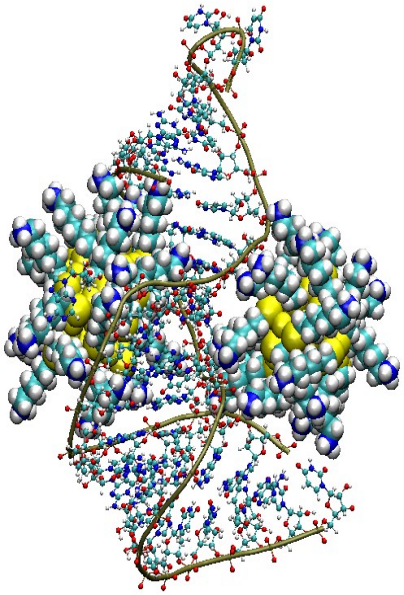
2AU38-configuration-3



0 ns



60 ns

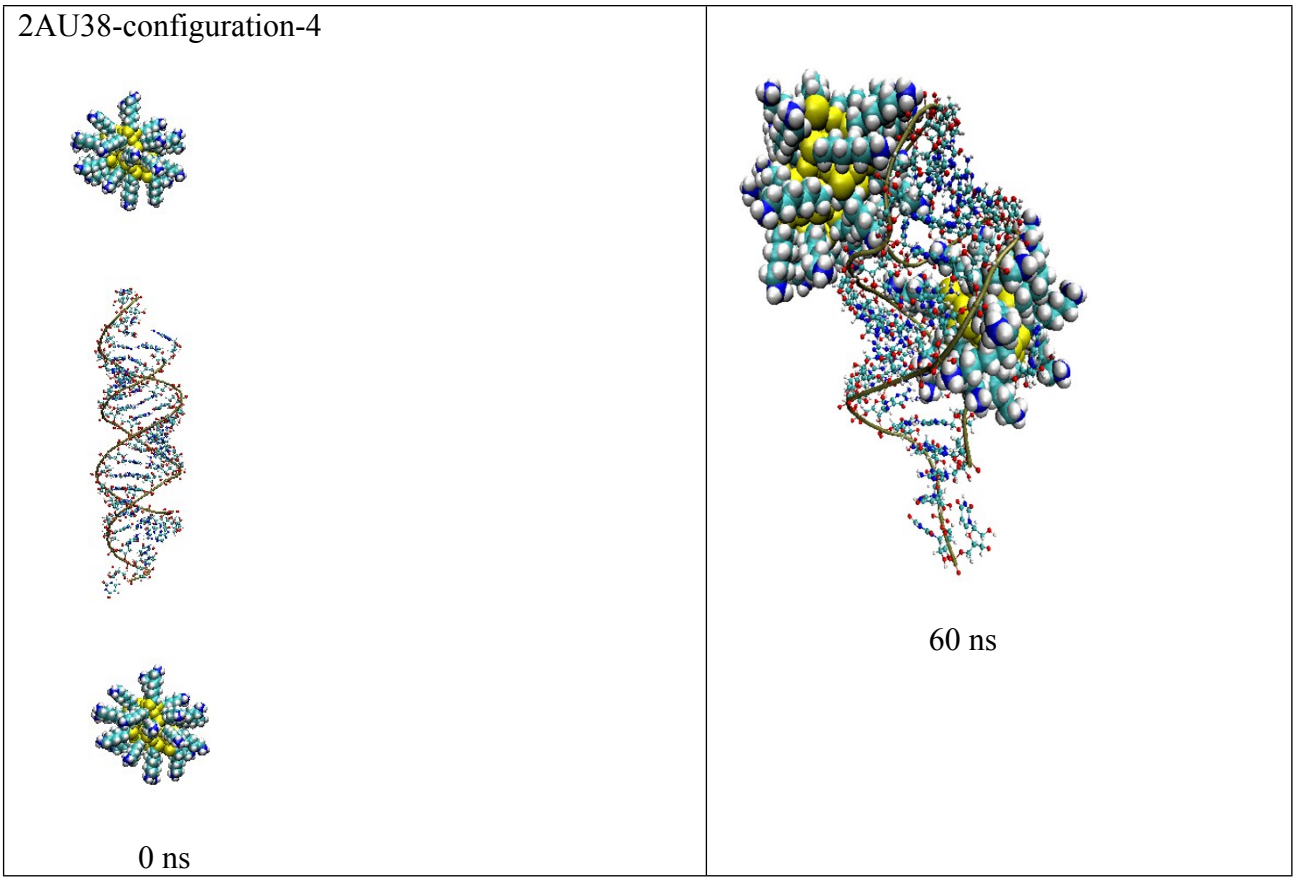


Fig. S4 The snapshots of the initial and final geometries of the simulated systems (AU38 and 2AU38 with siRNA, respectively).

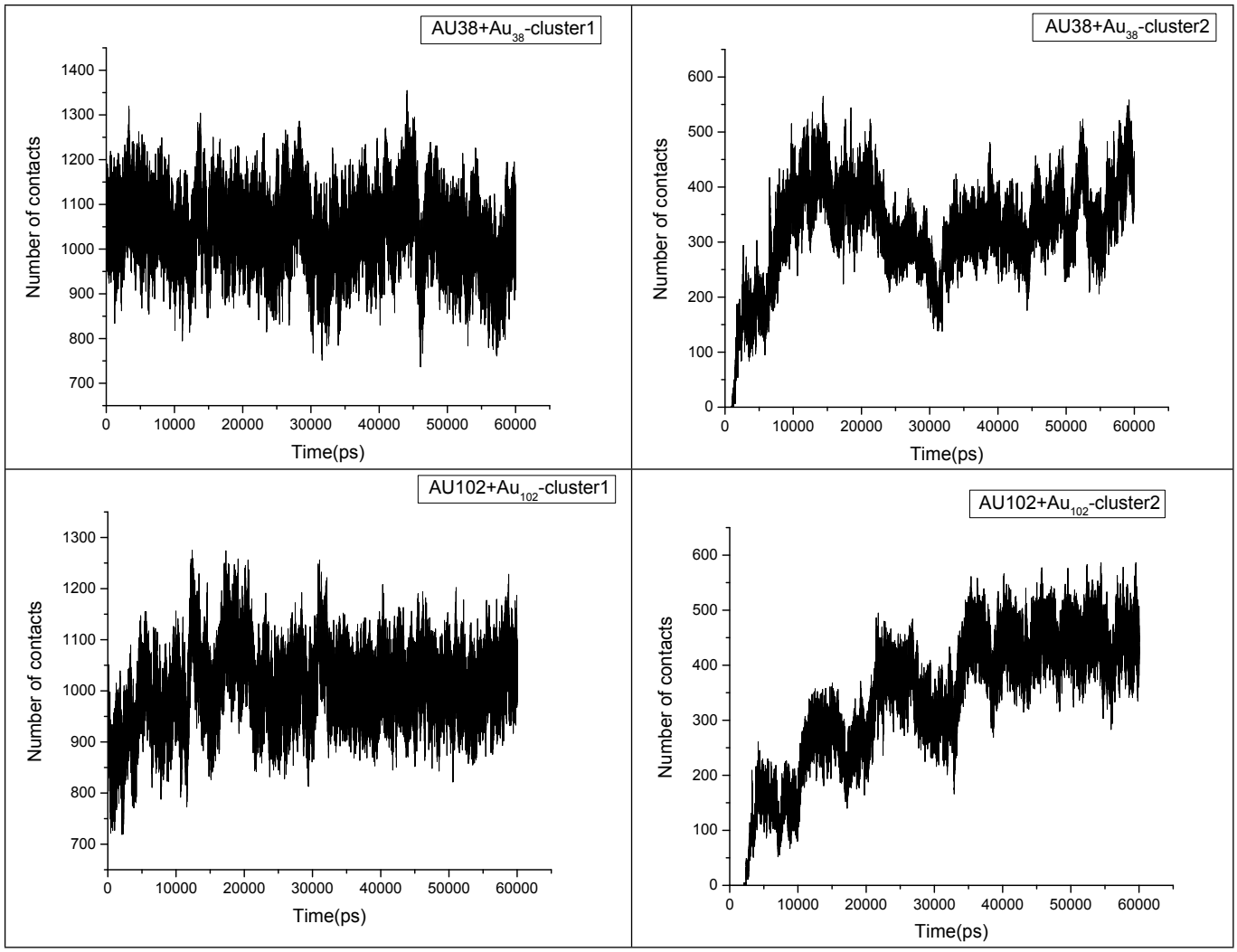
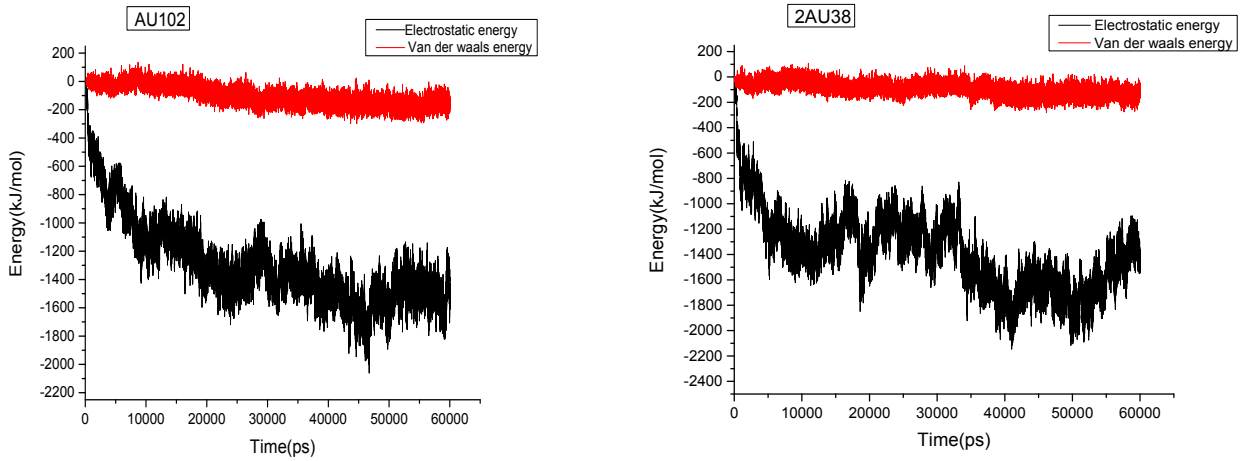


Fig. S5 The number of contacts between gold nanocluster and siRNA in AU38+Au_{38} and AU102+Au_{102} model.



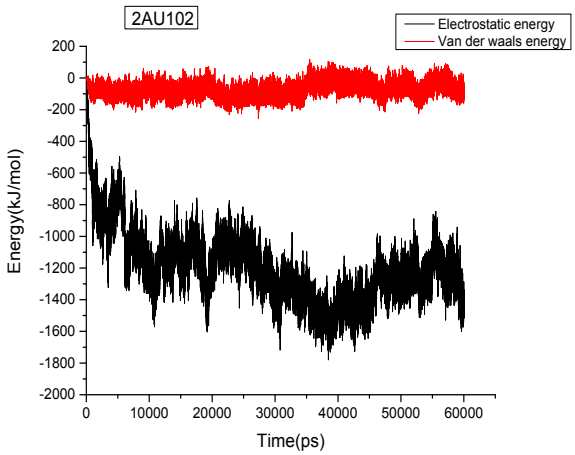


Fig. S6 The electrostatic and van der Waals interaction energy between positively charged gold nanoclusters and siRNA in AU102, 2AU38 and 2AU102 models.

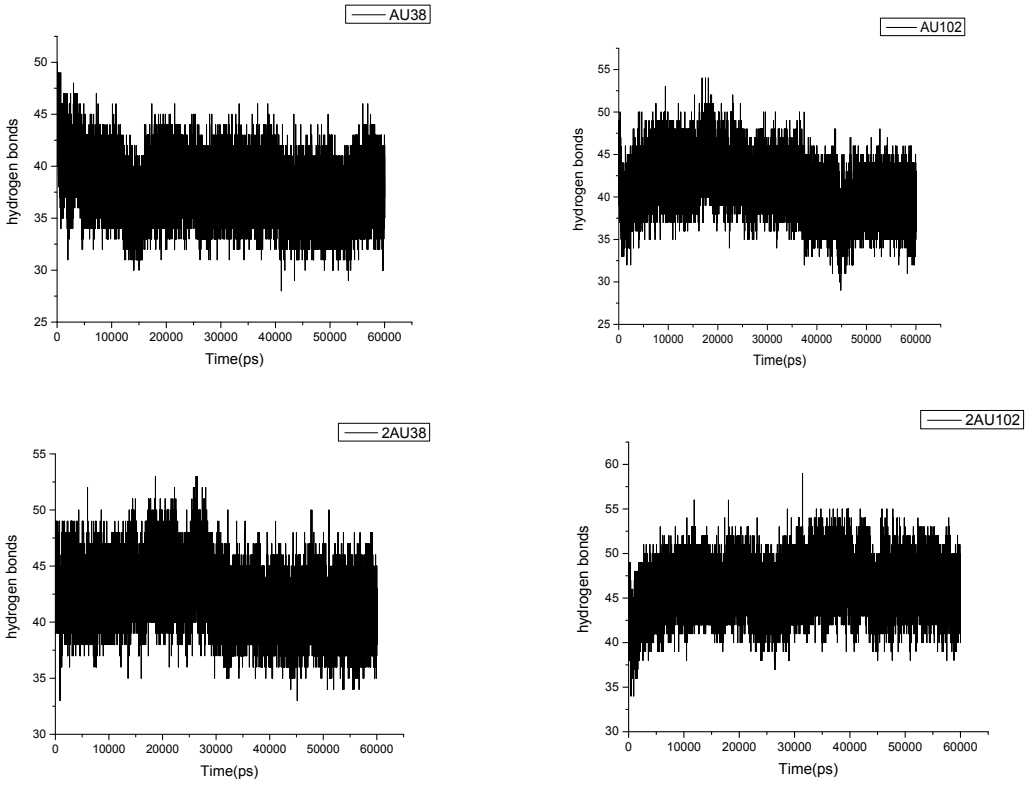
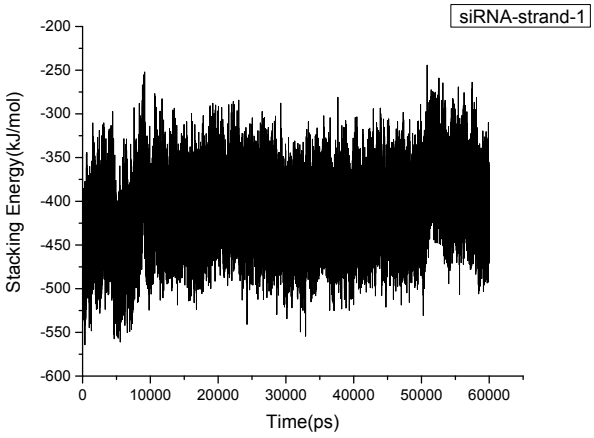
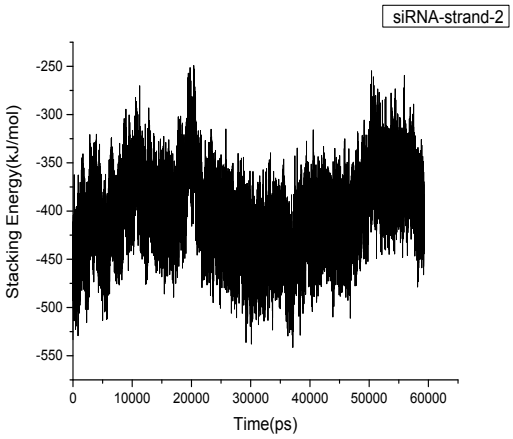
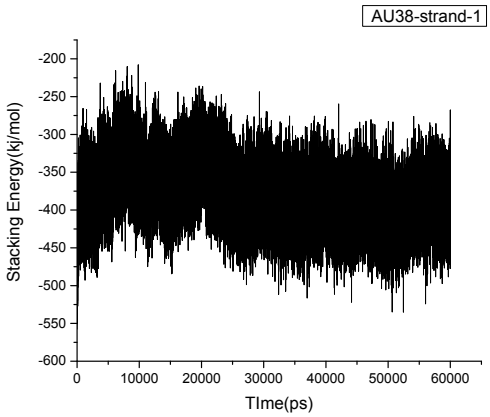
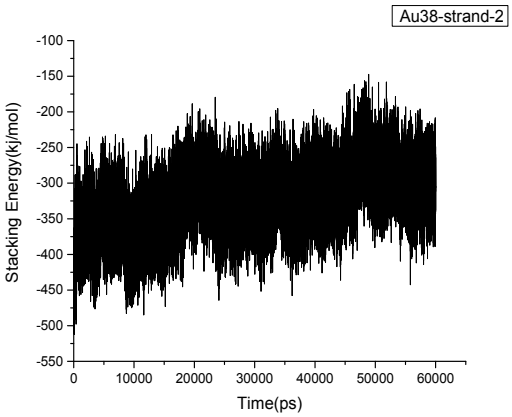


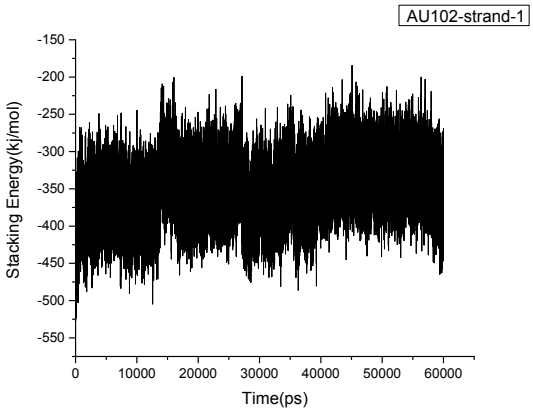
Fig. S7 The number of hydrogen bonds in siRNA for all the complexes of siRNA and gold nanoclusters.

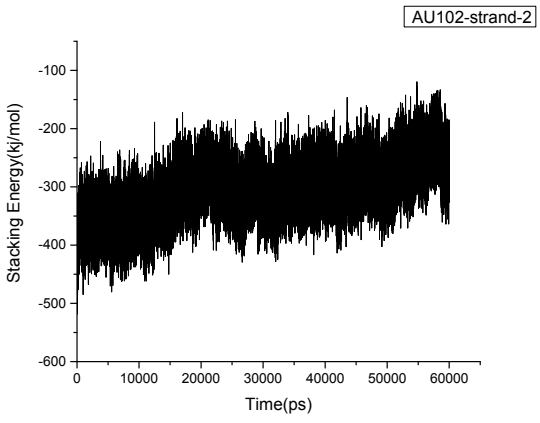

siRNA-strand-1
Stacking Energy(kJ/mol)
-200
-250
-300
-350
-400
-450
-500
-550
-600
0
10000
20000
30000
40000
50000
60000
Time(ps)


siRNA-strand-2
Stacking Energy(kJ/mol)
-250
-300
-350
-400
-450
-500
-550
0
10000
20000
30000
40000
50000
60000
Time(ps)


AU38-strand-1
Stacking Energy(kj/mol)
-200
-250
-300
-350
-400
-450
-500
-550
-600
0
10000
20000
30000
40000
50000
60000
TIme(ps)


Au38-strand-2
Stacking Energy(kj/mol)
-100
-150
-200
-250
-300
-350
-400
-450
-500
-550
0
10000
20000
30000
40000
50000
60000
Time(ps)


AU102-strand-1
Stacking Energy(kj/mol)
-150
-200
-250
-300
-350
-400
-450
-500
-550
0
10000
20000
30000
40000
50000
60000
Time(ps)


AU102-strand-2
Stacking Energy(kj/mol)
-100
-200
-300
-400
-500
-600
0
10000
20000
30000
40000
50000
60000
Time(ps)

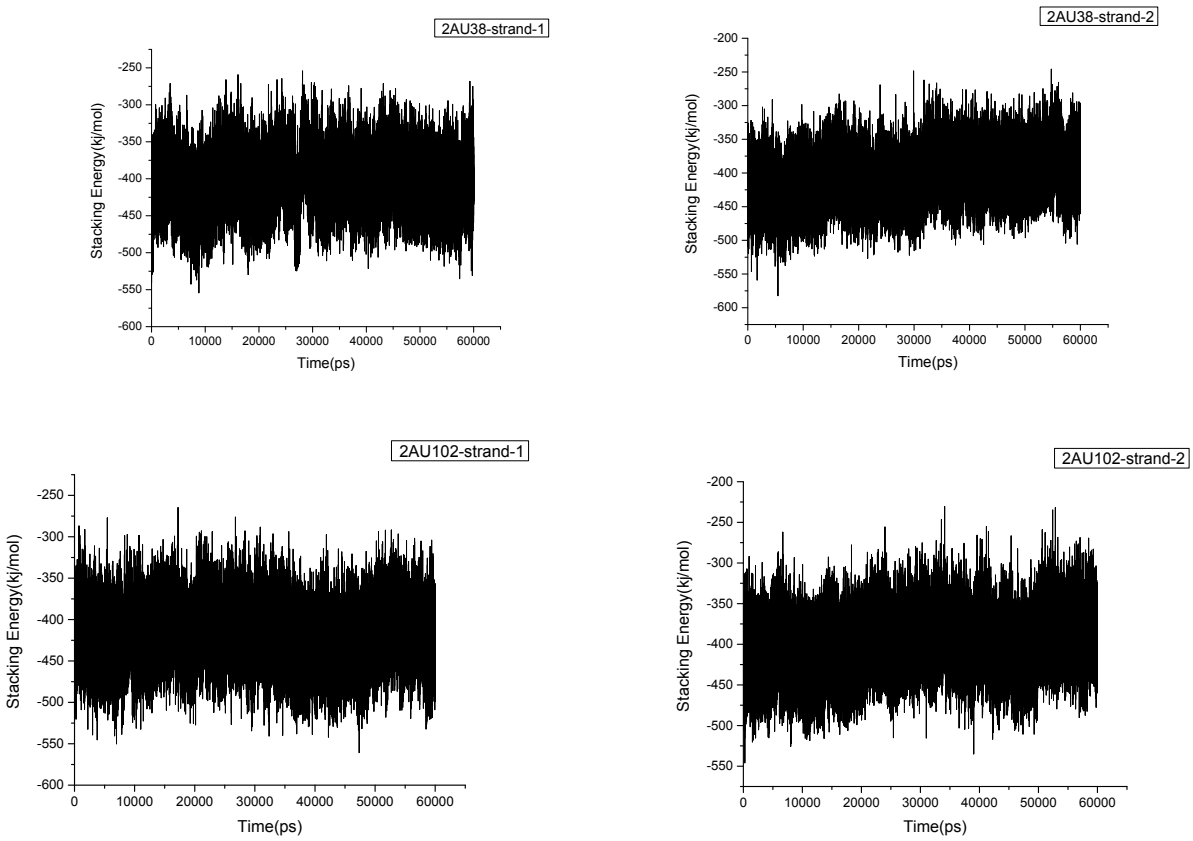
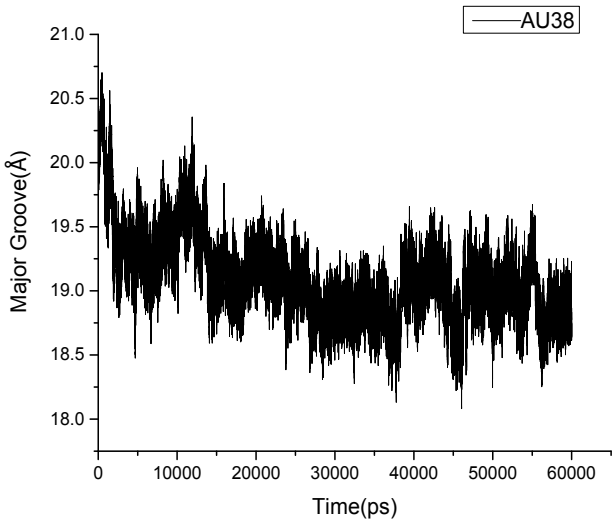
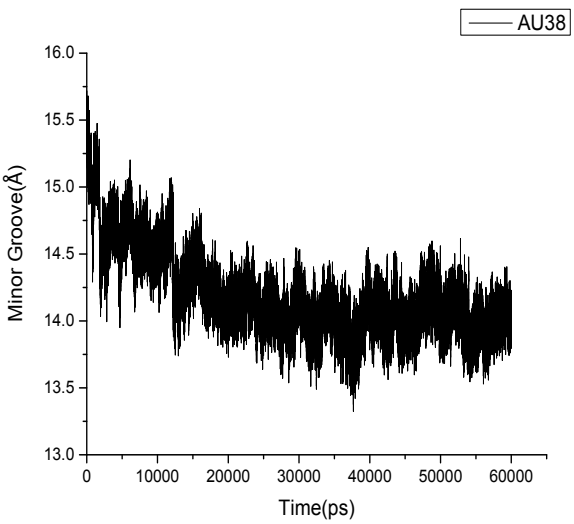
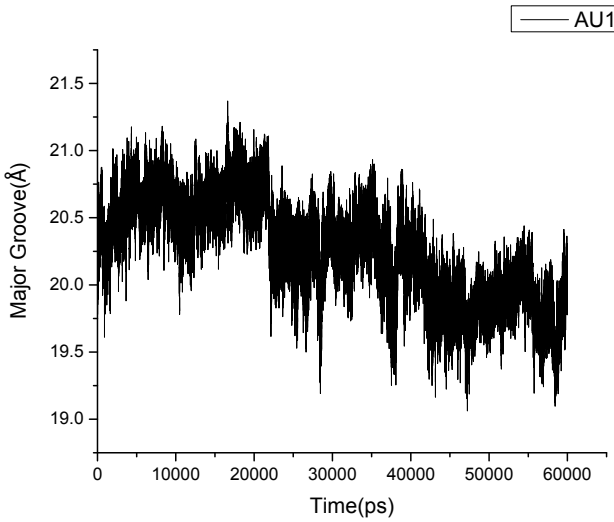
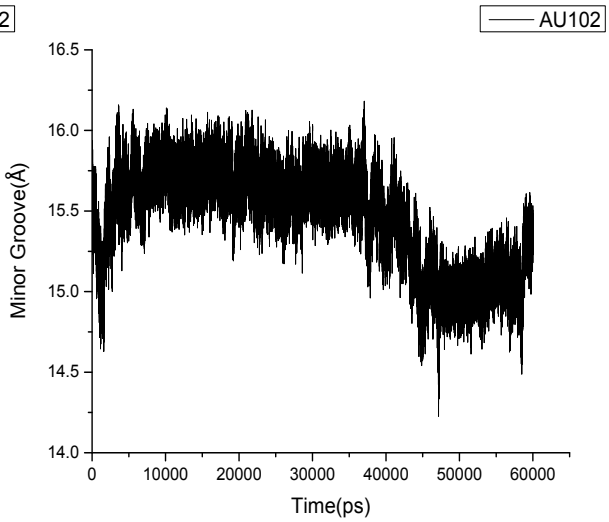


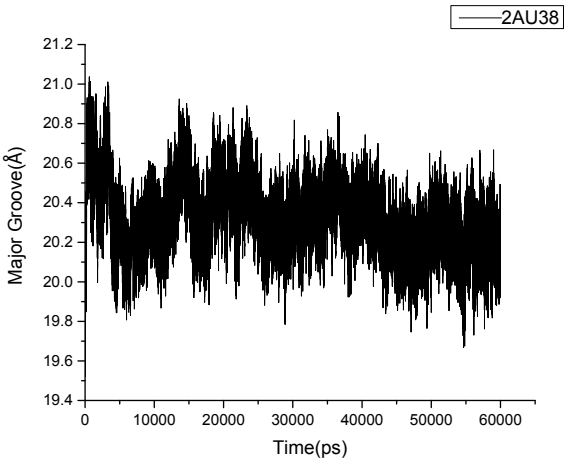
Fig. S8 Stacking energy in each strand of siRNA for all the models (siRNA, AU38, AU102, 2AU38 and 2AU102).

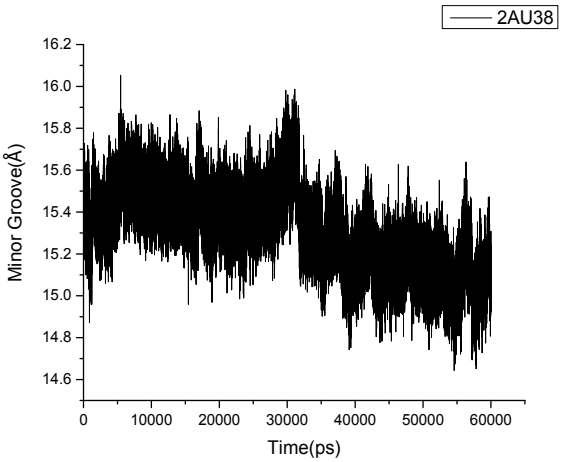

AU38
Major Groove(Å)
Time(ps)


AU38
Minor Groove(Å)
Time(ps)


AU102
Major Groove(Å)
Time(ps)


AU102
Minor Groove(Å)
Time(ps)


2AU38
Major Groove(Å)
Time(ps)


2AU38
Minor Groove(Å)
Time(ps)

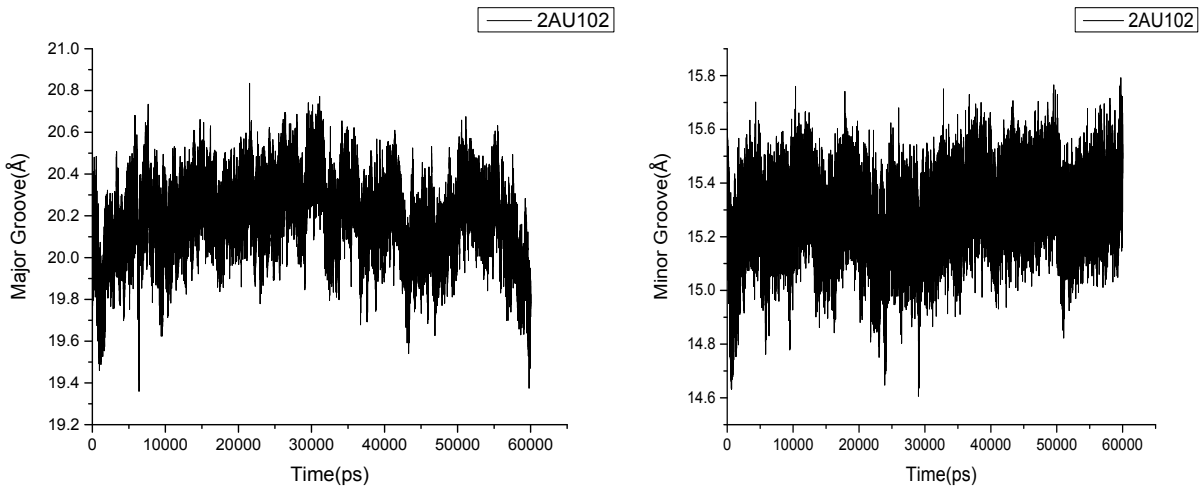
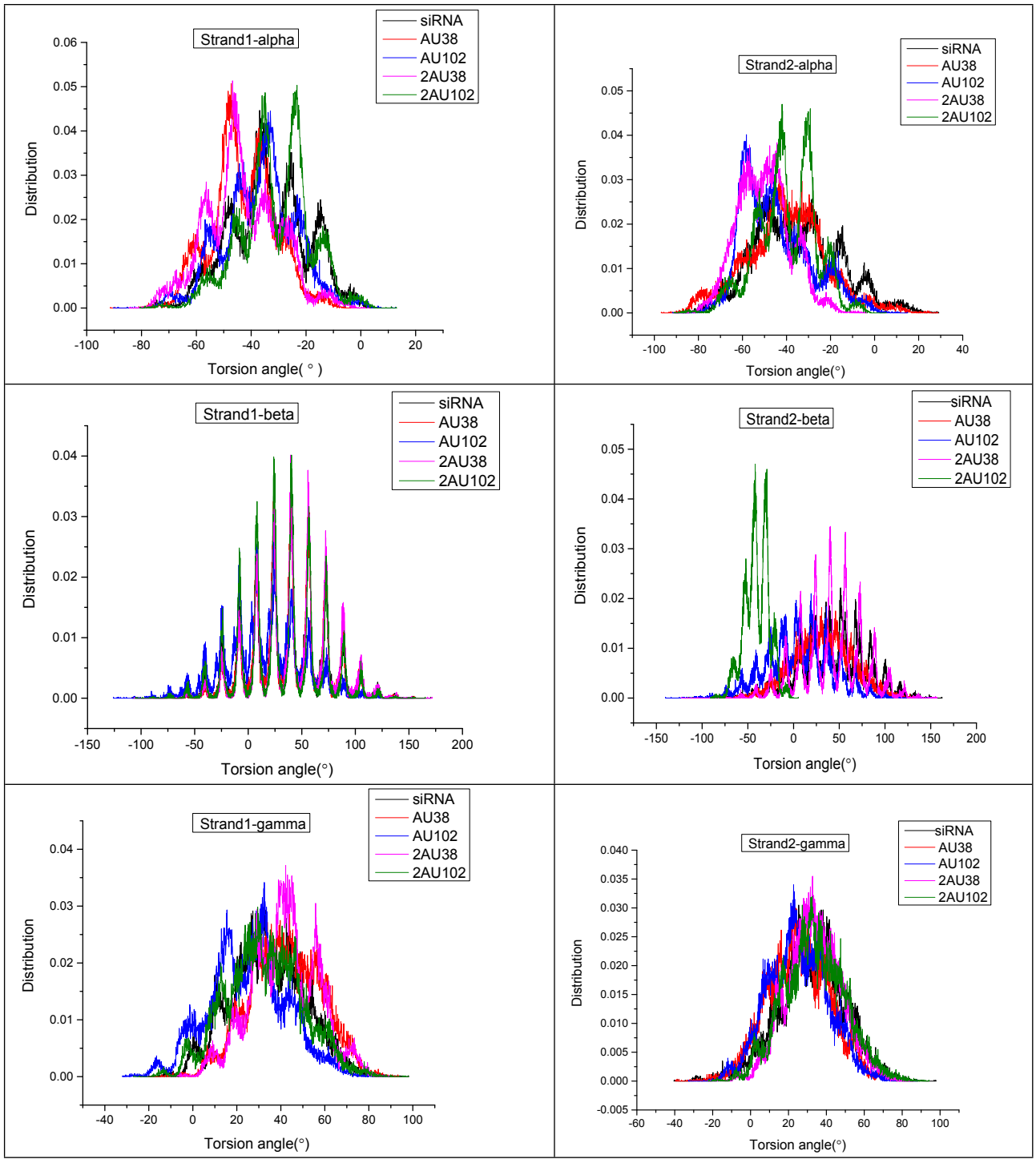


Fig. S9 The width of minor and major grooves of siRNA for all the complexes as a function of time.


Strand1-alpha
siRNA
AU38
AU102
2AU38
2AU102
Distribution
Torsion angle(°)
Strand2-alpha
siRNA
AU38
AU102
2AU38
2AU102
Distribution
Torsion angle(°)
Strand1-beta
siRNA
AU38
AU102
2AU38
2AU102
Distribution
Torsion angle(°)
Strand2-beta
siRNA
AU38
AU102
2AU38
2AU102
Distribution
Torsion angle(°)
Strand1-gamma
siRNA
AU38
AU102
2AU38
2AU102
Distribution
Torsion angle(°)
Strand2-gamma
siRNA
AU38
AU102
2AU38
2AU102
Distribution
Torsion angle(°)

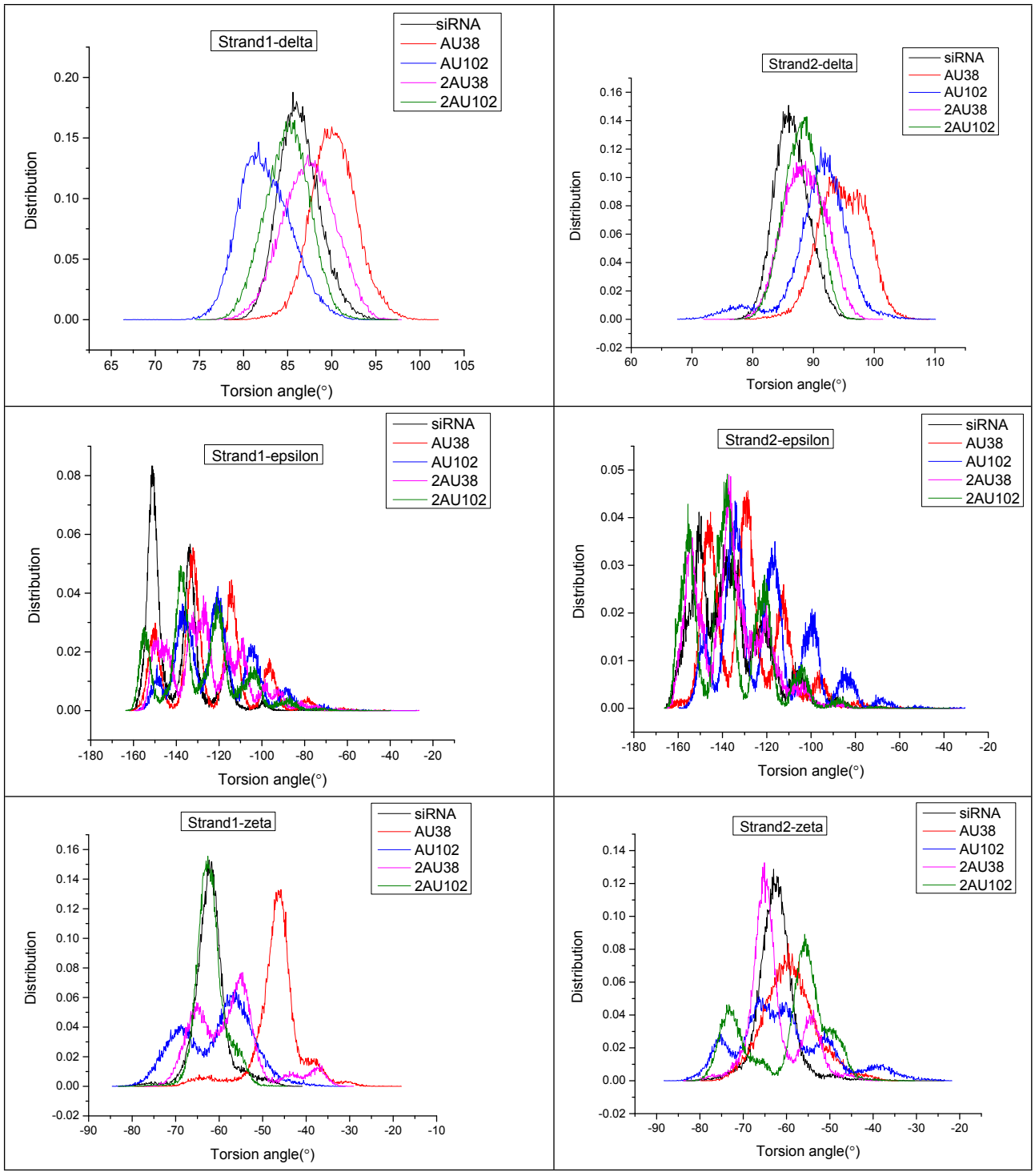


Fig. S10 The distribution of average torsion angles along the strand-1 and strand-2 of siRNA in all the models.

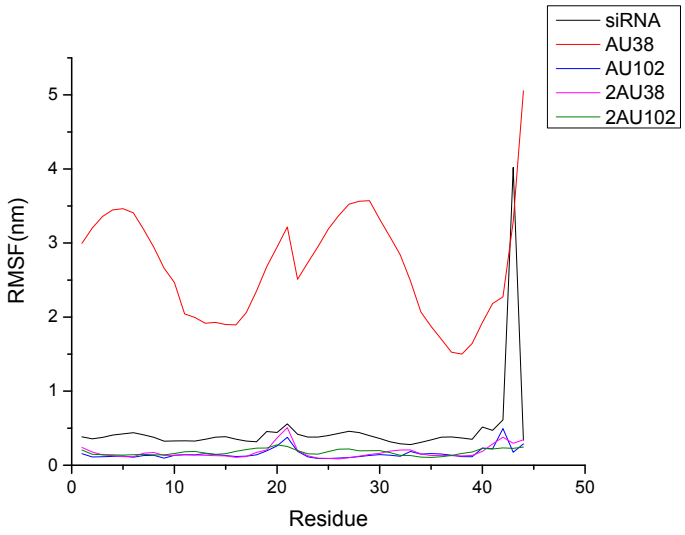
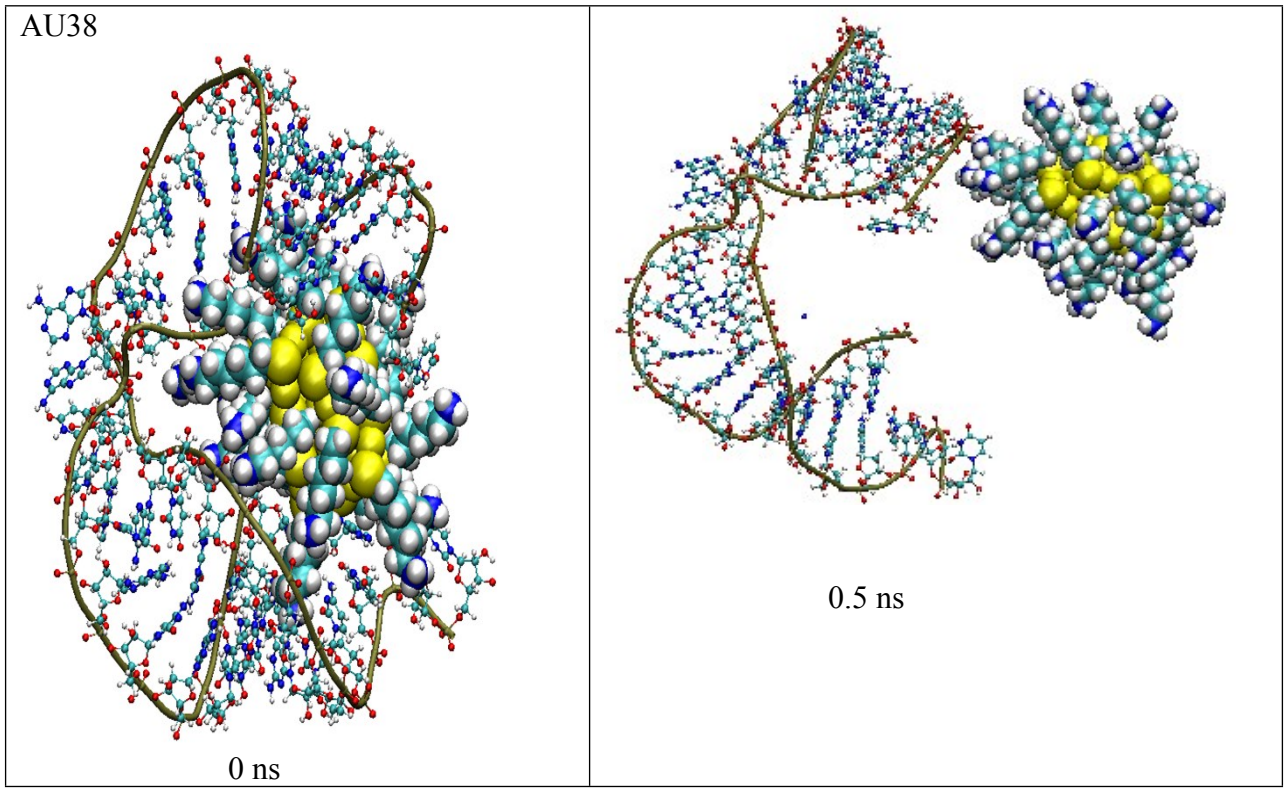
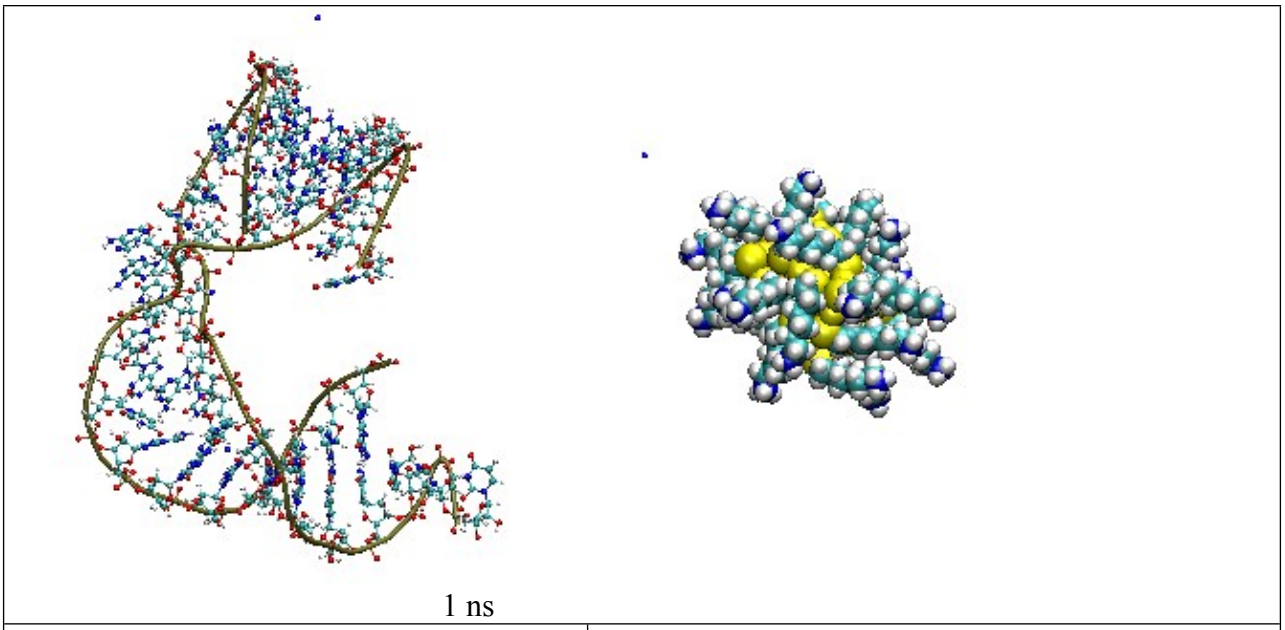


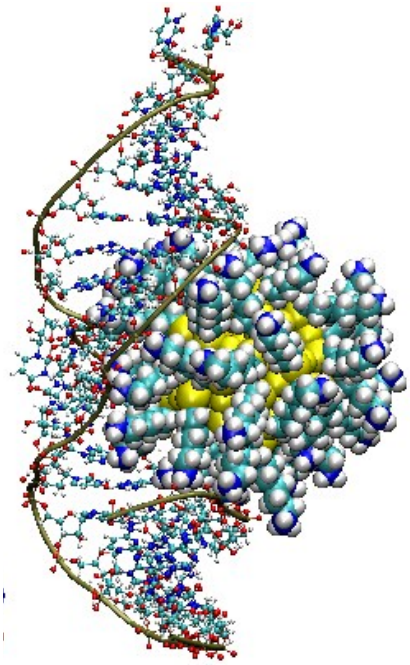
Fig. S11 The root mean square fluctuation of siRNA for all the models (siRNA, AU38, AU102, 2AU38 and 2AU102).



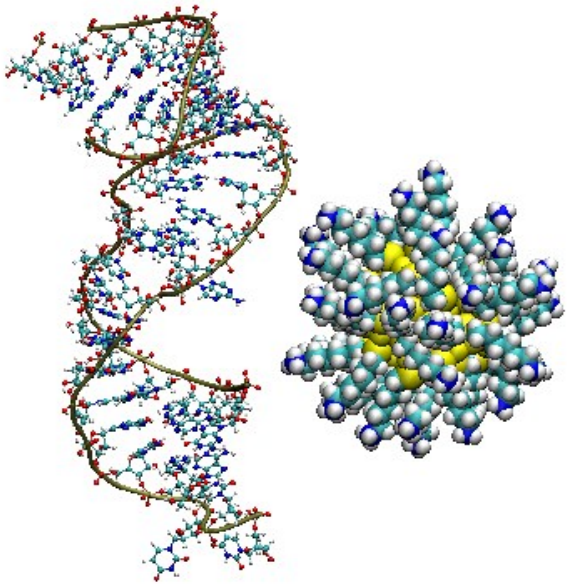


1 ns

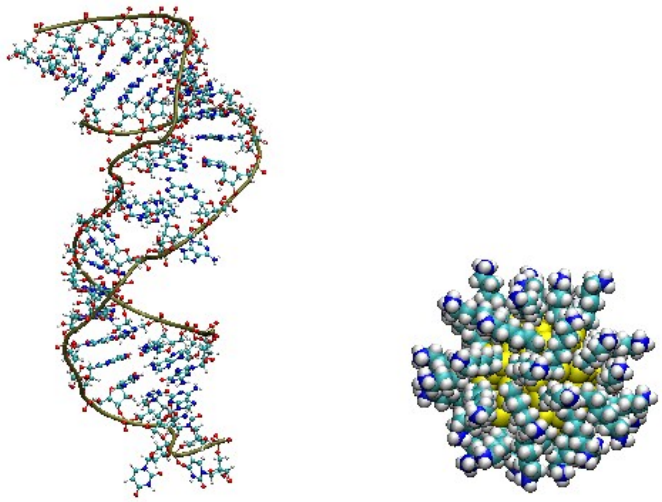
AU102



0 ns

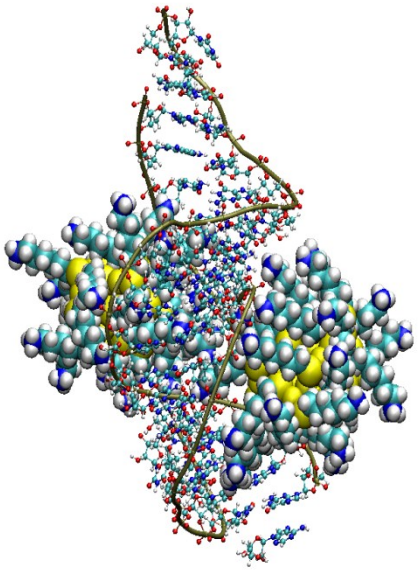


0.5 ns

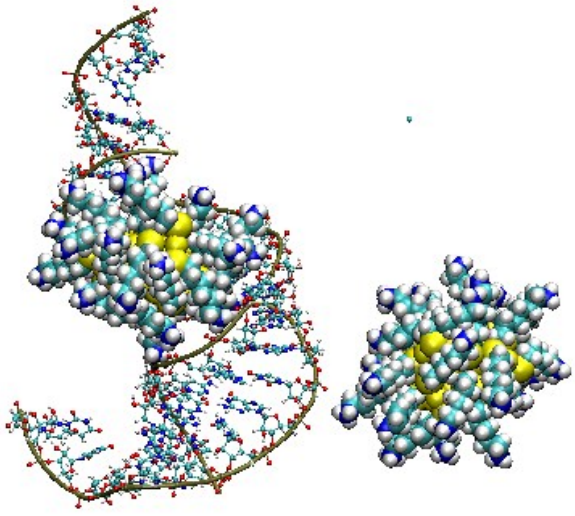


1 ns

2AU38-1



0 ns



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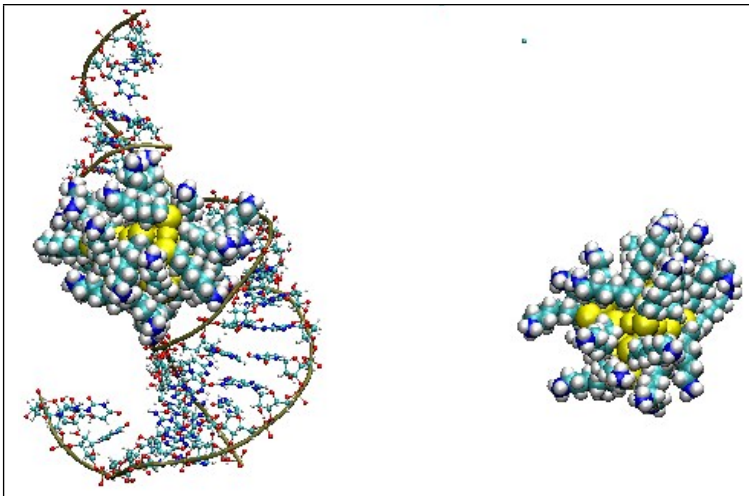
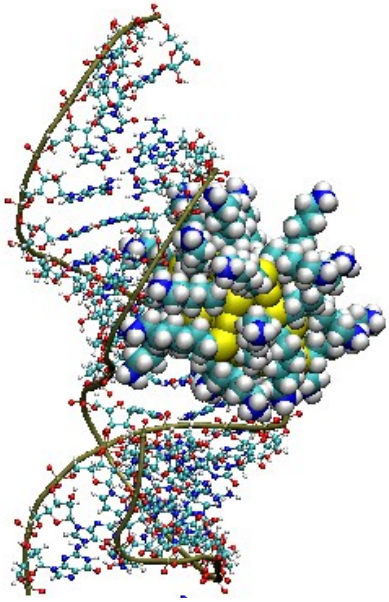
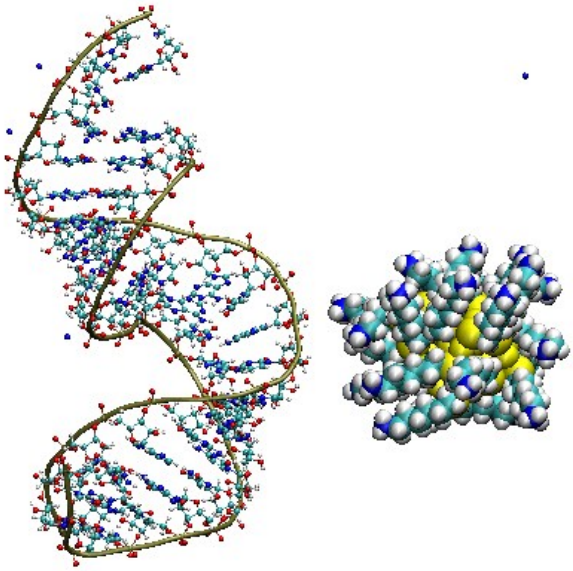


1 ns

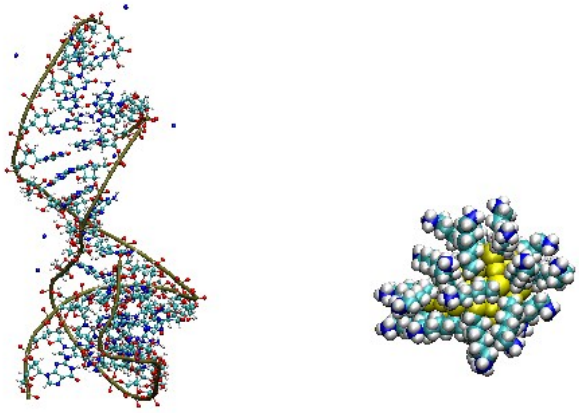
2AU38-2



0 ns

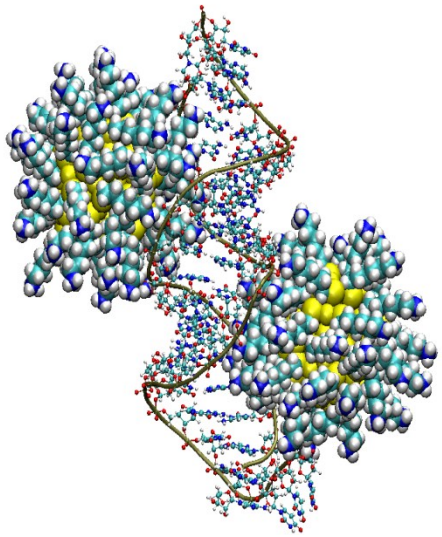


0.5 ns

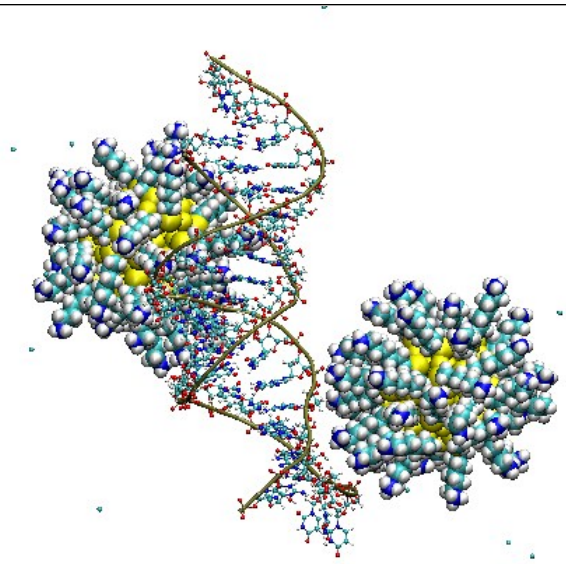


1 ns

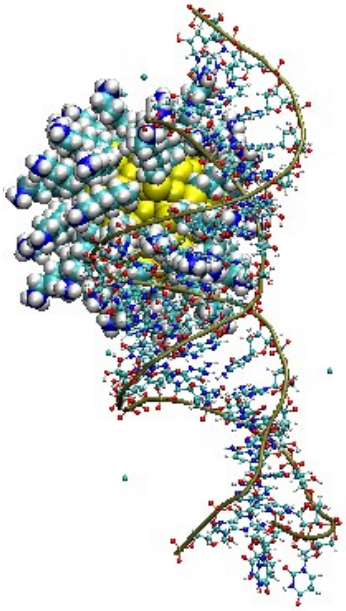
2AU102-1

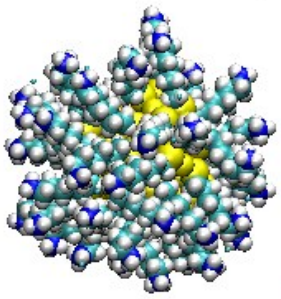


0 ns



0.5 ns





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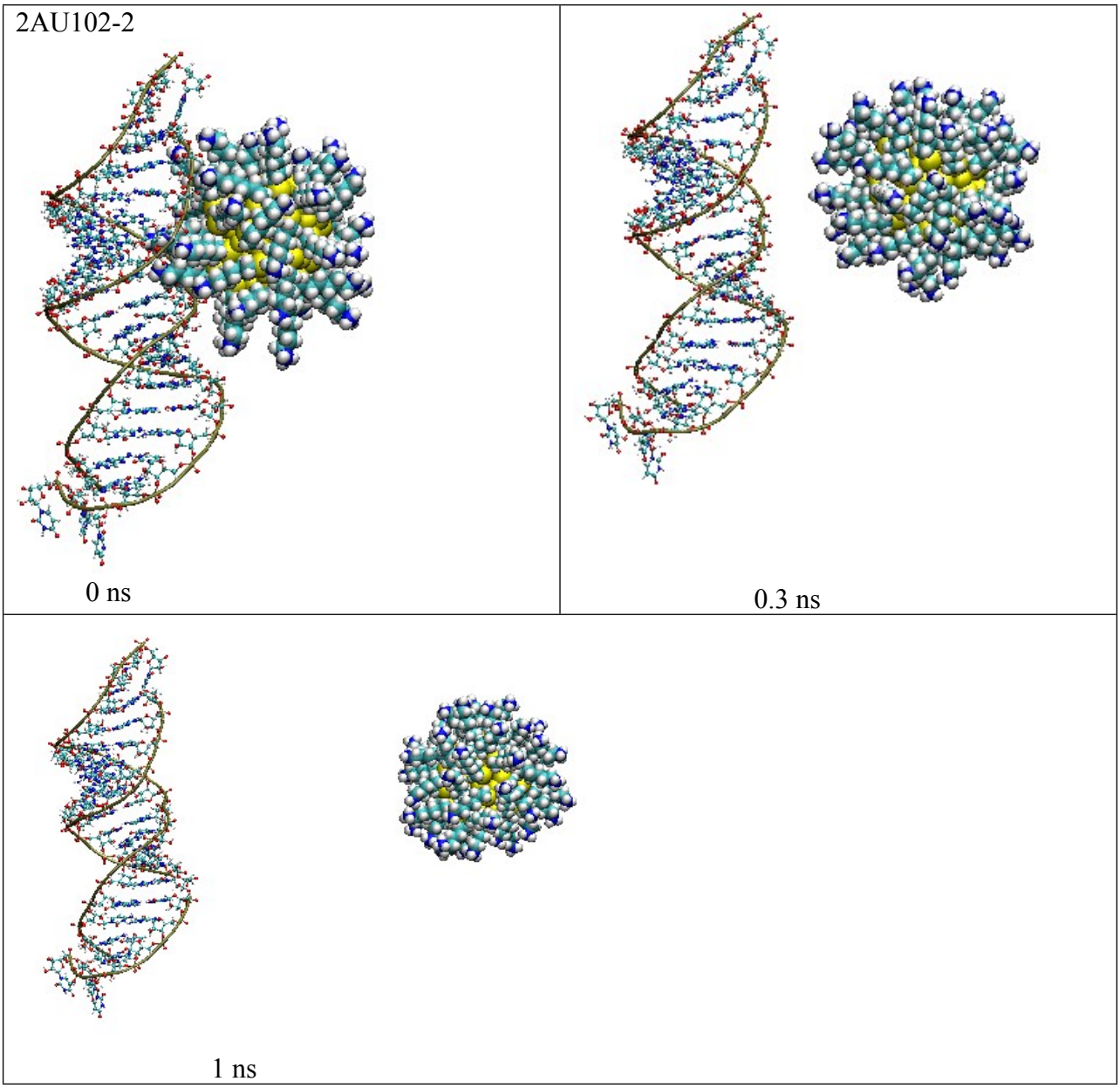

Fig. S12 The snapshots for the dissociation of gold nanocluster from the complexes of siRNA and gold nanocluster.