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

Table S1. Sequence of MYC Pu27 (WT), Pu24 (PDB id: 2MGN) and Pu22 (PDB id: 5W77). Substituted bases for Pu24 (G13T) and Pu22 (G14T/G23T) are underlined. The 3' parts for Pu24 and Pu22 are highlighted in yellow while the top, middle, and bottom G-tetrads are colored red, green, and orange respectively.

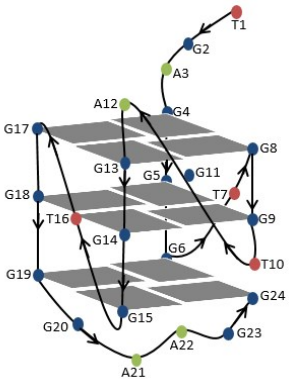
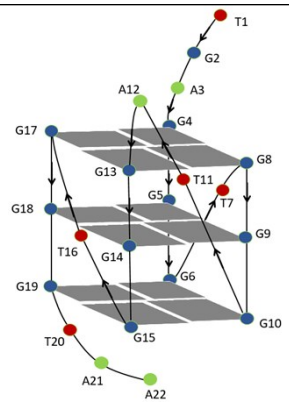
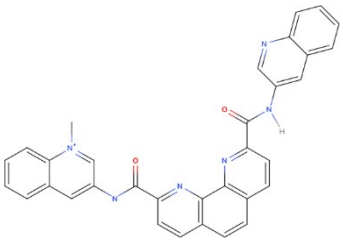
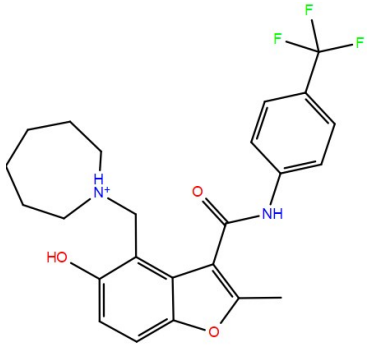
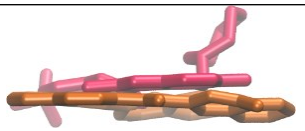
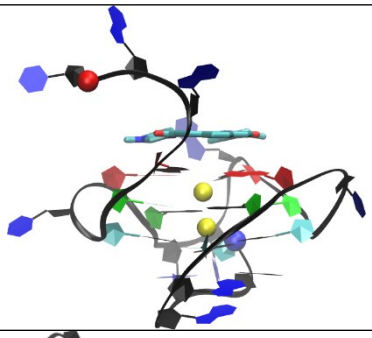
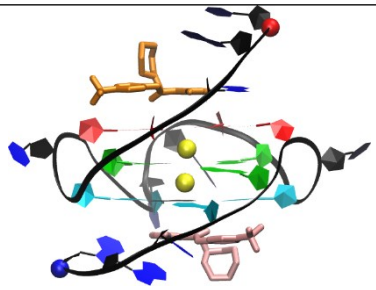
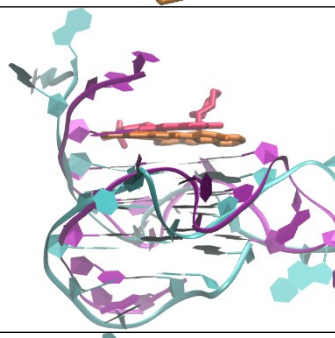
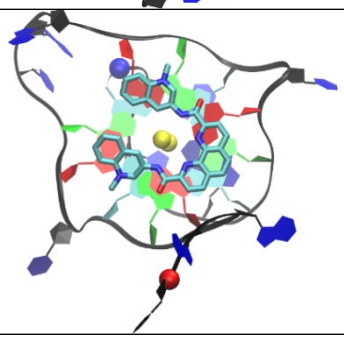
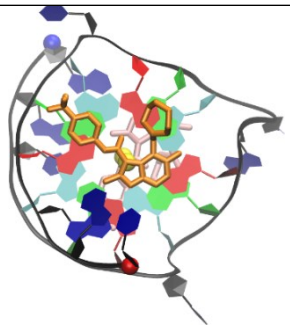
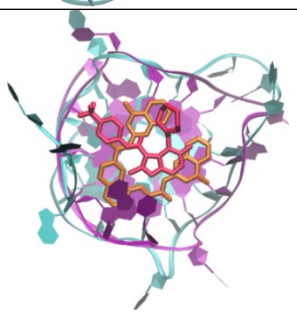
Name	Sequence
Pu27 (WT)	5'-TGGGGAG G G TG G GGAG G G TG G G GAAGG -3'
Pu24	5'-TGAG^{1}G^{1}G^{1}TG^{2}G^{2} T GAG^{3}G^{3}G^{3}TG^{4}G^{4}G^{4}GAAGG^{2}-3'
Pu22	5'-TGAG^{1}G^{1}G^{1}TG^{2}G^{2}G^{2} T AG^{3}G^{3}G^{3}TG^{4}G^{4}G^{4} T AA-3'

Table S2. Oxygen to Potassium Distance. Values are reported in Å. Colors refer to G4 layer: top (red); middle (green); bottom (blue). Values in red represent outliers from the data trend.

Residue:Oxygen:Pottasium	Apo form	Top Binding	Bottom Binding	Side Binding
G4:O6:K1	2.67±0.11	2.67±0.01	2.67±0.01	2.67±0.01
G8:O6:K1	2.69±0.12	2.68±0.00	2.68±0.01	2.69±0.01
G13:O6:K1	2.71±0.12	2.68±0.00	2.67±0.01	2.68±0.01
G17:O6:K1	2.70±0.13	2.70±0.00	2.70±0.01	2.70±0.01
G5:O6:K1	2.81±0.18	2.82±0.02	2.86±0.05	2.85±0.01
G9:O6:K1	2.78±0.18	2.83±0.01	2.83±0.04	2.82±0.02
G14:O6:K1	2.75±0.15	2.82±0.01	2.84±0.01	2.83±0.01
G18:O6:K1	2.81±0.19	2.75±0.01	2.77±0.02	2.77±0.01
G5:O6:K2	2.87±0.22	2.88±0.02	2.86±0.03	2.86±0.01
G9:O6:K2	2.92±0.26	2.87±0.02	2.86±0.03	2.87±0.04
G14:O6:K2	2.85±0.21	2.89±0.02	2.89±0.02	2.89±0.01
G18:O6:K2	2.91±0.25	2.83±0.01	2.82±0.02	2.81±0.03
G6:O6:K2	2.76±0.16	2.68±0.01	2.68±0.00	2.68±0.00
G15:O6:K2	2.72±0.13	2.74±0.00	2.75±0.01	2.74±0.01
G19:O6:K2	2.75±0.14	2.69±0.00	2.69±0.01	2.69±0.00
G24:O6:K2	2.73±0.19	2.73±0.01	2.73±0.01	2.73±0.02

Table S3. Oxygen to Oxygen Distance. Values are reported in Å. Colors refer to G4 layer: top (red); middle (green); bottom (blue).

Residue:Oxygen-Residue:Oxygen	Apo form	Top Binding	Bottom Binding	Side Binding
G4:O6-G8:O6	3.39±0.19	3.32±0.02	3.38±0.02	3.37±0.03
G8:O6-G13:O6	3.27±0.18	3.27±0.02	3.33±0.02	3.31±0.03
G13:O6-G17:O6	3.37±0.20	3.36±0.03	3.40±0.05	3.39±0.04
G17:O6-G4:O6	3.29±0.18	3.29±0.01	3.34±0.02	3.33±0.02
G5:O6-G9:O6	2.97±0.16	2.98±0.01	2.98±0.02	2.97±0.01
G9:O6-G14:O6	3.03±0.17	3.02±0.01	3.02±0.02	3.01±0.01
G14:O6-G18:O6	2.98±0.15	2.99±0.01	2.99±0.01	2.99±0.01
G18:O6-G5:O6	3.29±0.18	3.29±0.01	3.34±0.02	3.33±0.02
G6:O6-G15:O6	3.35±0.18	3.36±0.01	3.36±0.01	3.36±0.01
G15:O6-G19:O6	3.29±0.19	3.28±0.00	3.28±0.01	3.29±0.01
G19:O6-G24:O6	3.37±0.18	3.36±0.01	3.37±0.01	3.36±0.01
G24:O6-G6:O6	3.39±0.17	3.39±0.00	3.39±0.02	3.39±0.01
G4:O6-G5:O6	3.27±0.23	3.35±0.02	3.29±0.02	3.30±0.02
G8:O6-G9:O6	3.47±0.25	3.49±0.02	3.47±0.04	3.51±0.03
G13:O6-G14:O6	3.39±0.24	3.39±0.03	3.35±0.02	3.37±0.04
G17:O6-G18:O6	3.35±0.25	3.38±0.02	3.38±0.01	3.36±0.05
G5:O6-G6:O6	3.18±0.20	3.22±0.02	3.21±0.01	3.20±0.02
G9:O6-G15:O6	3.42±0.24	3.43±0.01	3.44±0.02	3.44±0.03
G14:O6-G19:O6	3.30±0.22	3.30±0.01	3.27±0.02	3.29±0.02
G18:O6-G24:O6	3.40±0.22	3.39±0.01	3.38±0.02	3.39±0.02

G-Quadruplex			
Ligands			 
Side View			
Top View			

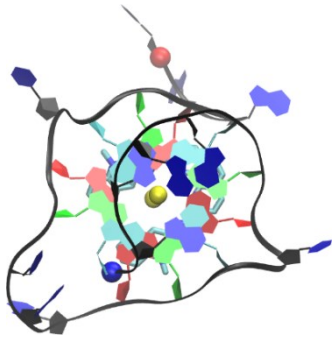
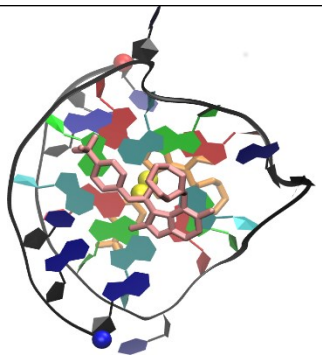
Bottom View			
	Pu24 (PDB ID: 2MGN)	Pu22 (PDB ID: 5W77)	(2MGN/5W77)

Figure S1: High-resolution structures of MYC G-quadruplex derivatives Pu24 (PDB ID : 2MGN) and Pu22 (PDB ID : 5W77) complexed with the ligands Phen-DC3 and DC-34, respectively. Cartoon representations for each G-quadruplex are displayed in the first row. Side, top and bottom binding representations for 2MGN, 5W77 and their superimpositions are displayed. 2MGN and 5W77 are colored cyan and purple, respectively. Phen-DC3 is colored orange and DC-34 is colored orange/red and pink for top and bottom binding positions, respectively. 5'- and 3'- ends are represented as red and blue spheres, respectively. Potassium ions are represented as yellow spheres.

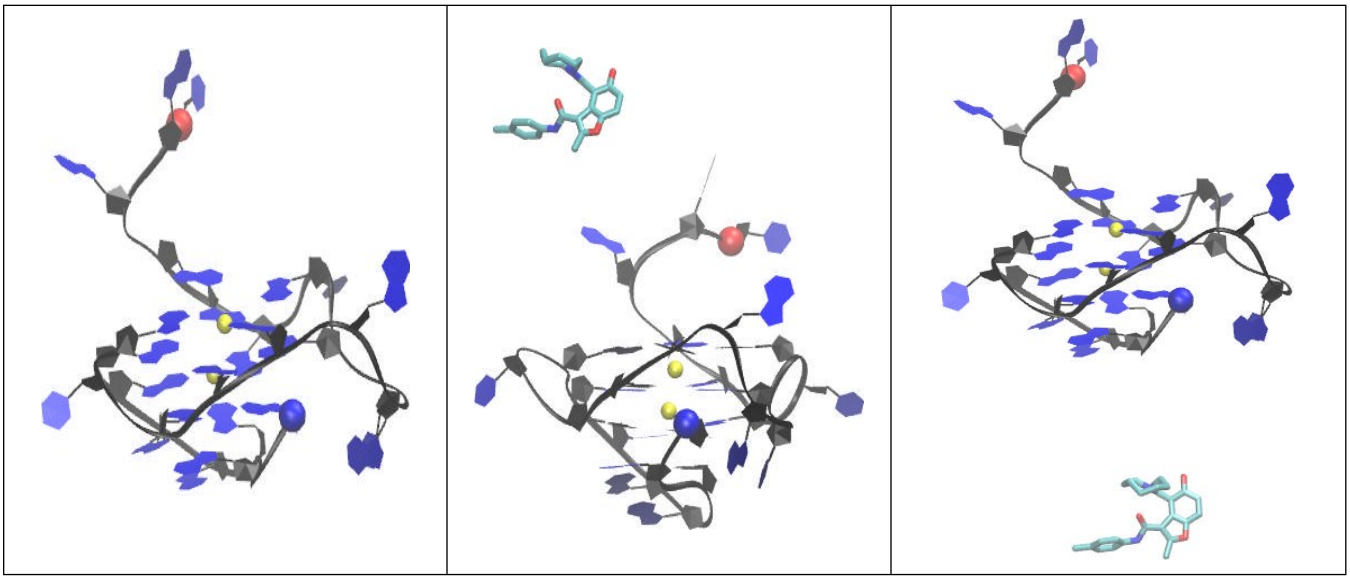


Figure S2. Apo form (left) of Pu24 and unbound complex (middle and right) of Pu24 plus a ligand DBD1 as the starting conformation of MD simulations. 5` and 3` of the DNA and K+ ions is represented as a red, blue and yellow spheres, respectively.

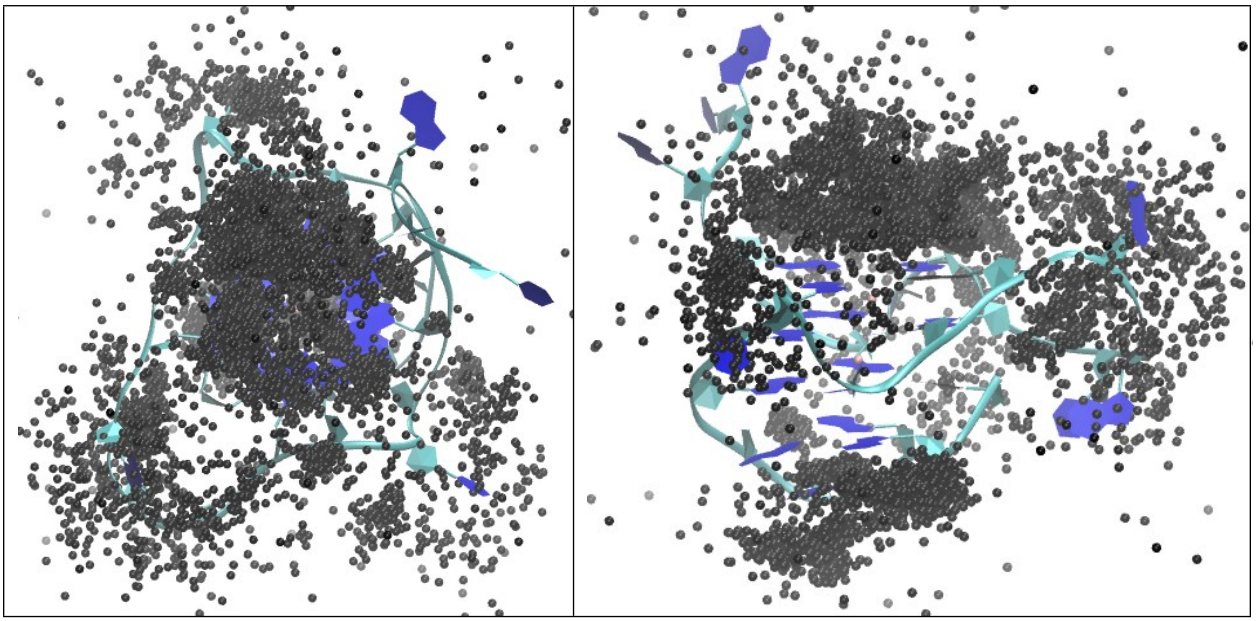
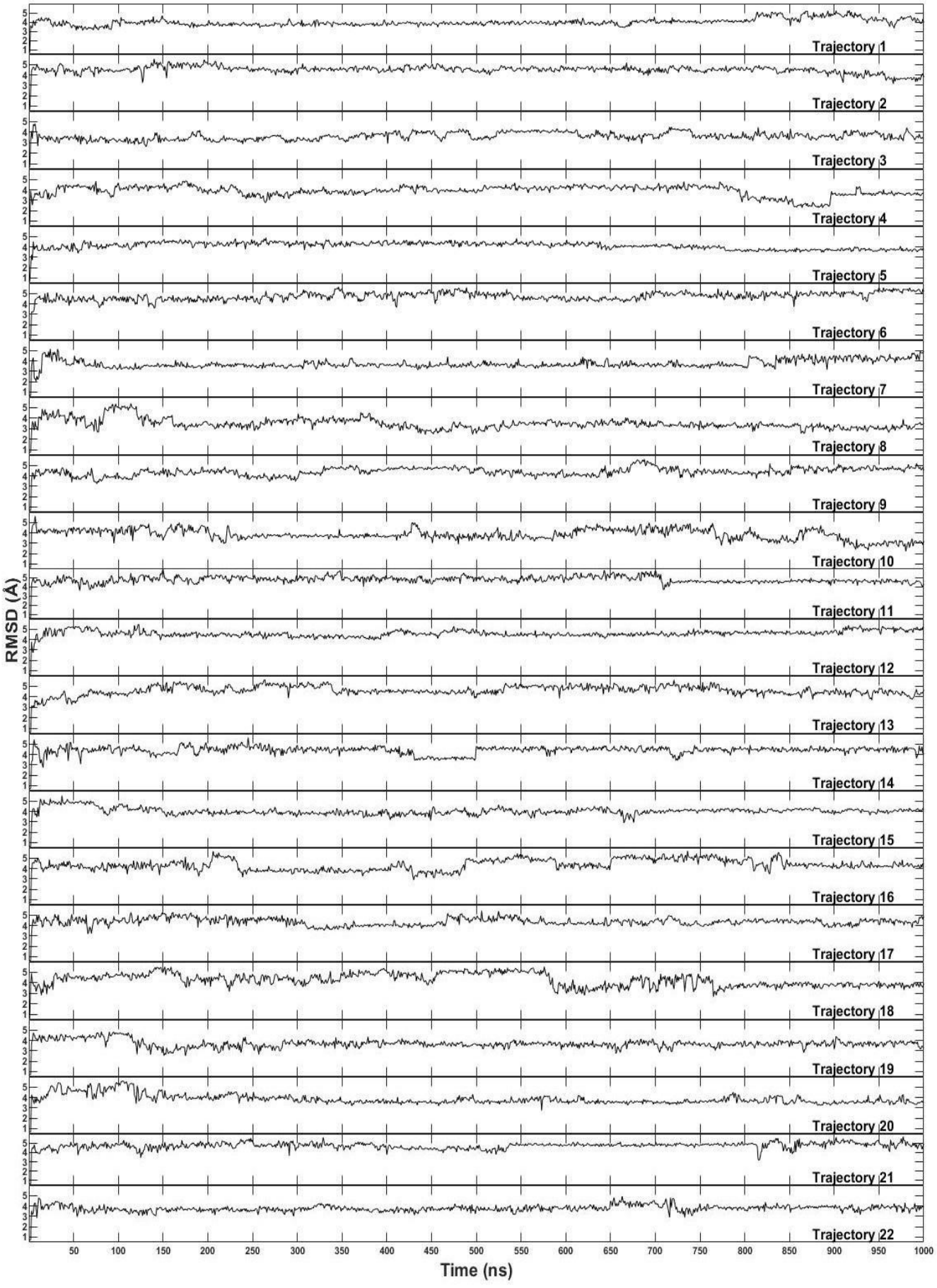


Figure S3. Top and side views of the distribution of the ligand DBD1 positions over all 33 free ligand binding trajectories to the Pu24 G-quadruplex.


RMSD (Å)
Trajectory 1
Trajectory 2
Trajectory 3
Trajectory 4
Trajectory 5
Trajectory 6
Trajectory 7
Trajectory 8
Trajectory 9
Trajectory 10
Trajectory 11
Trajectory 12
Trajectory 13
Trajectory 14
Trajectory 15
Trajectory 16
Trajectory 17
Trajectory 18
Trajectory 19
Trajectory 20
Trajectory 21
Trajectory 22
Time (ns)

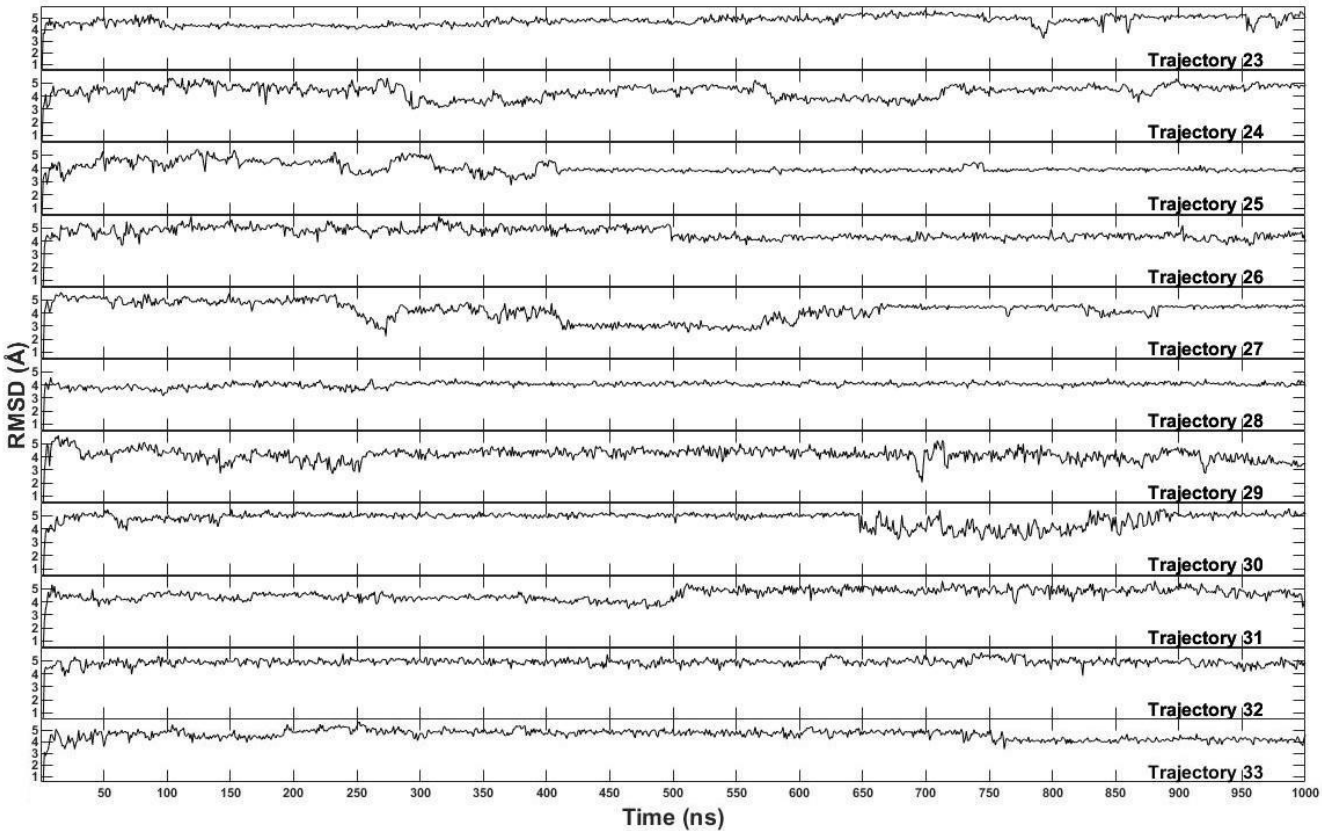
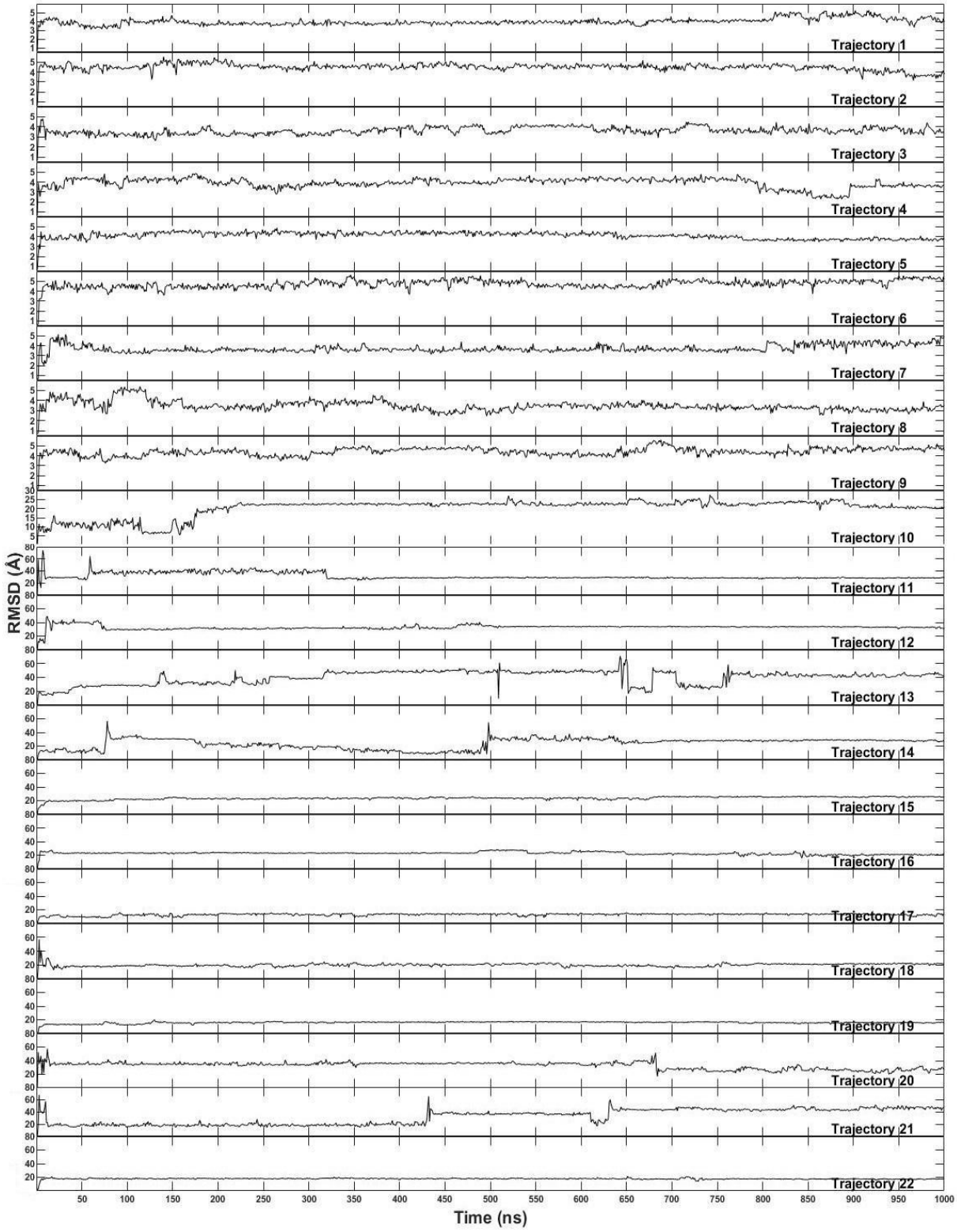


Figure S4. RMSD of the Pu24 G-quadruplex in the 33 free ligand binding simulations.


RMSD (Å)
Trajectory 1
Trajectory 2
Trajectory 3
Trajectory 4
Trajectory 5
Trajectory 6
Trajectory 7
Trajectory 8
Trajectory 9
Trajectory 10
Trajectory 11
Trajectory 12
Trajectory 13
Trajectory 14
Trajectory 15
Trajectory 16
Trajectory 17
Trajectory 18
Trajectory 19
Trajectory 20
Trajectory 21
Trajectory 22
50 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000
Time (ns)

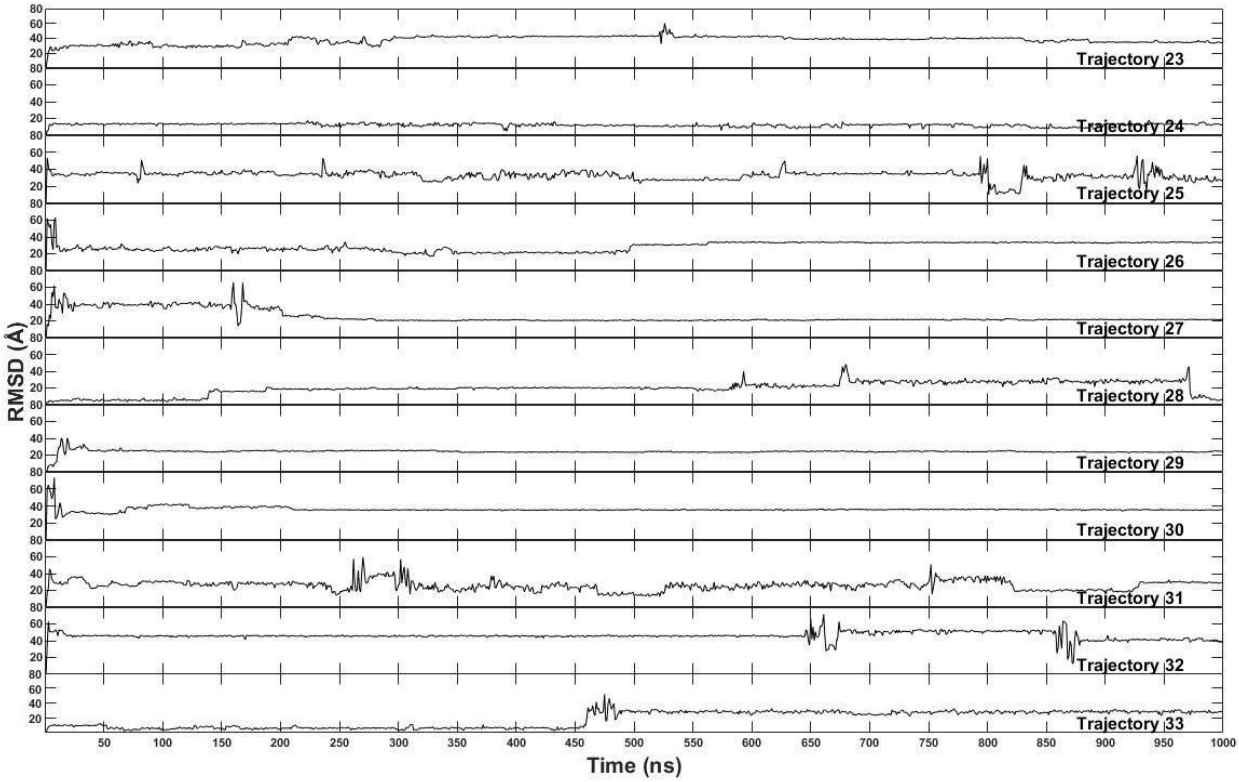
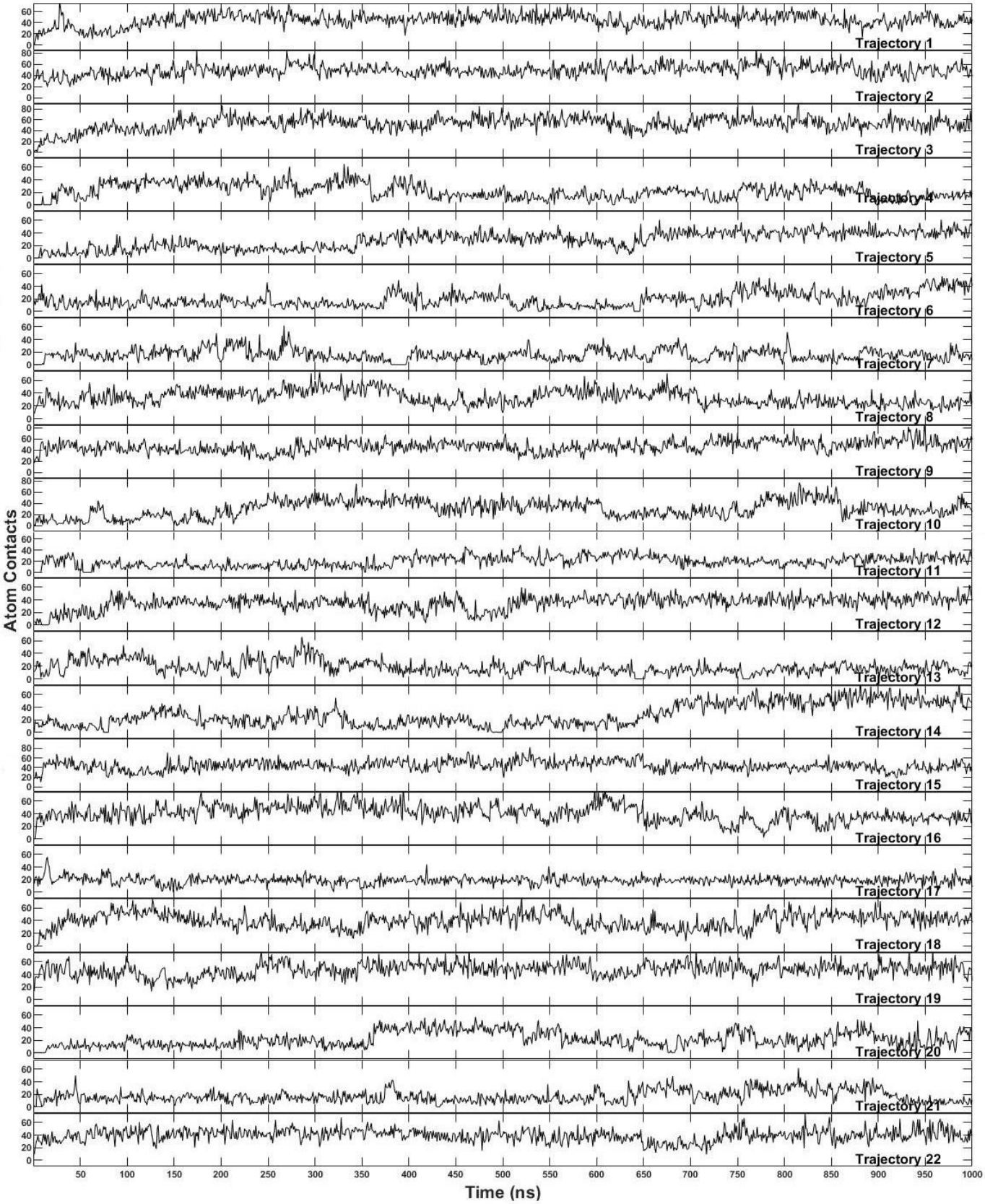


Figure S5. Ligand RMSD in the 33 free ligand binding simulations of DBD1 to the Pu24 G-quadruplex.


Atom Contacts
Trajectory 1
Trajectory 2
Trajectory 3
Trajectory 4
Trajectory 5
Trajectory 6
Trajectory 7
Trajectory 8
Trajectory 9
Trajectory 10
Trajectory 11
Trajectory 12
Trajectory 13
Trajectory 14
Trajectory 15
Trajectory 16
Trajectory 17
Trajectory 18
Trajectory 19
Trajectory 20
Trajectory 21
Trajectory 22
Time (ns)

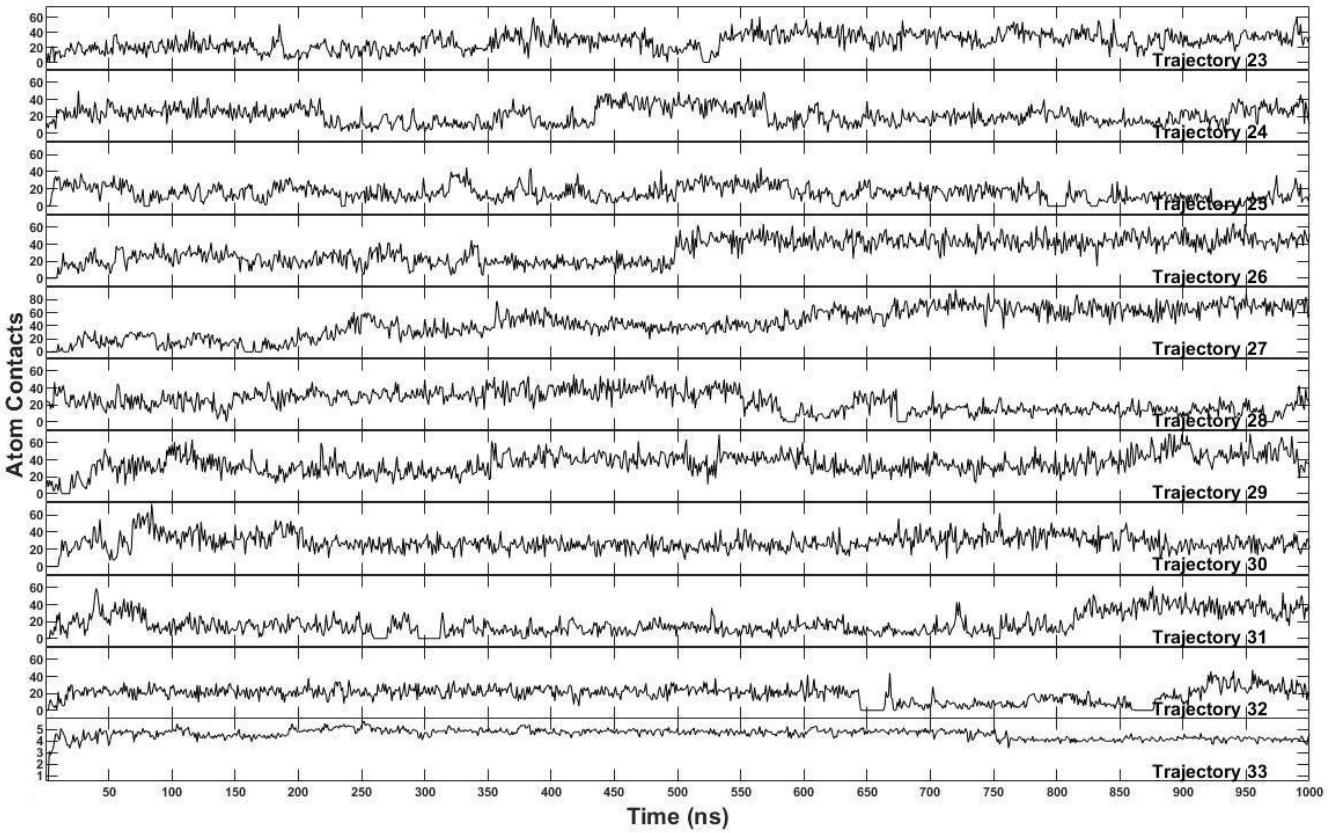
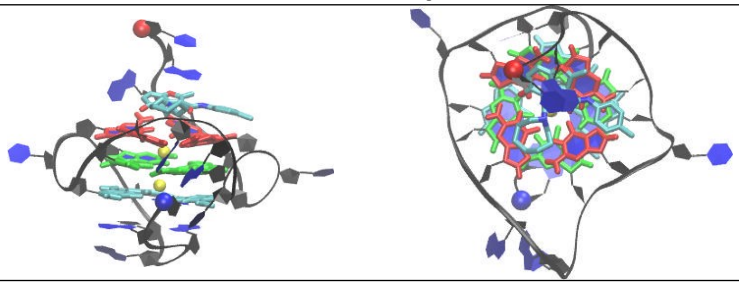
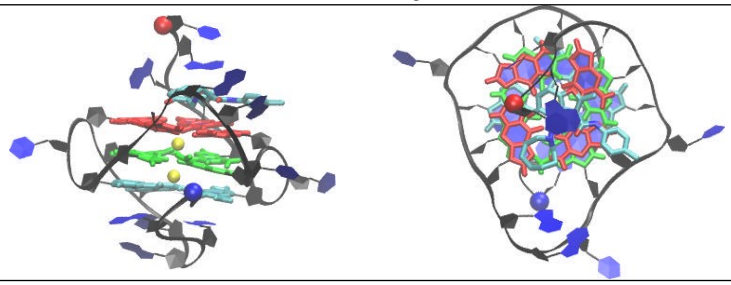
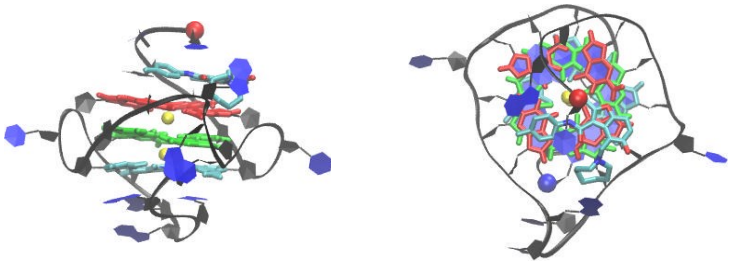
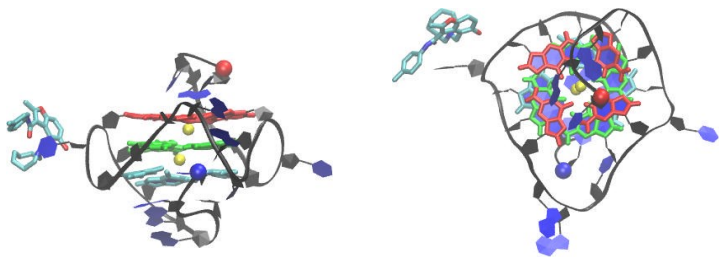


Figure S6: Atom contacts between DBD1 and the Pu24 G-quadruplex in the 33 free ligand binding simulations.

01 - Top	02 - Top
	
03 - Top	**04 - Side**
	
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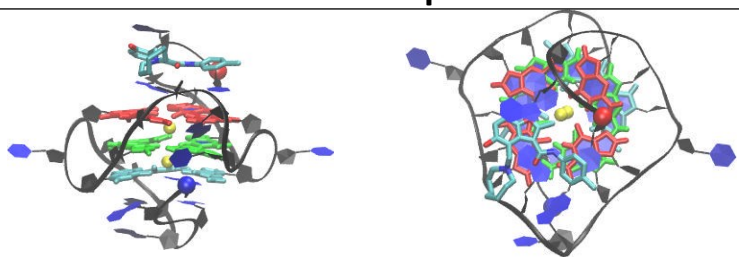
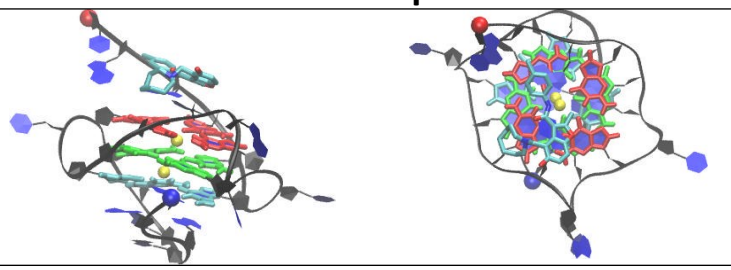
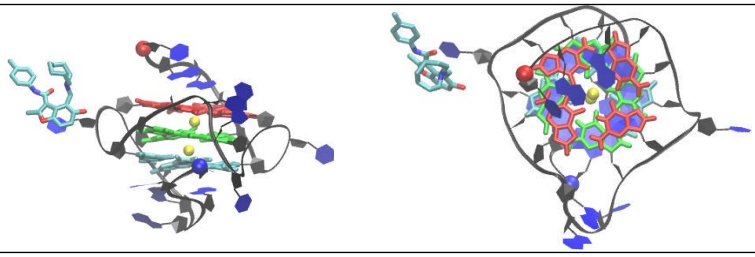
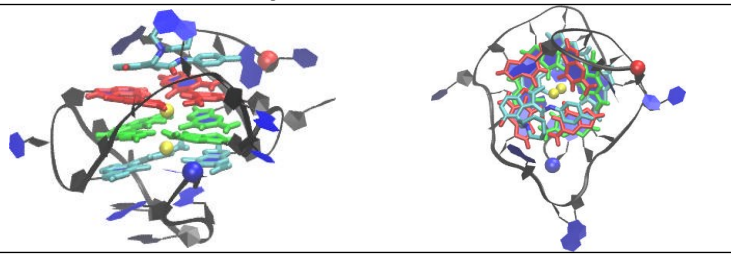
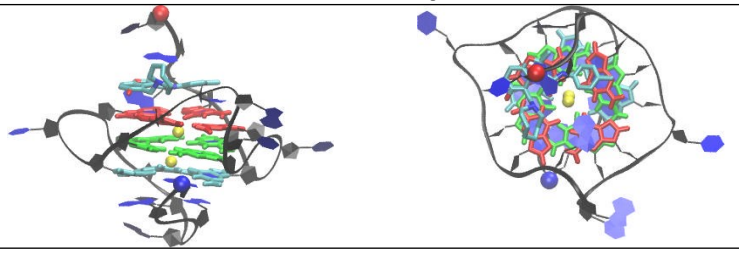
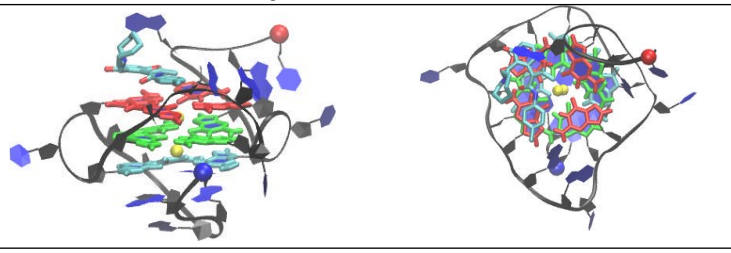
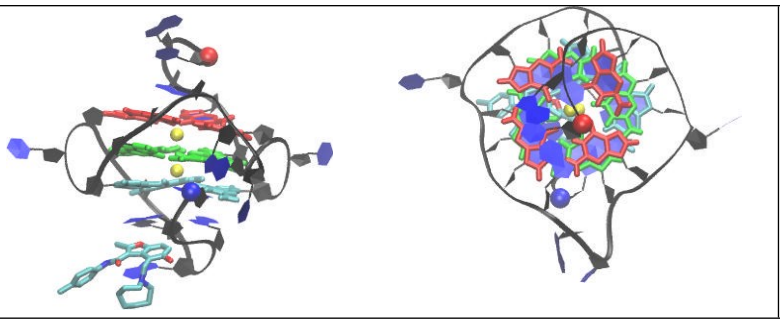
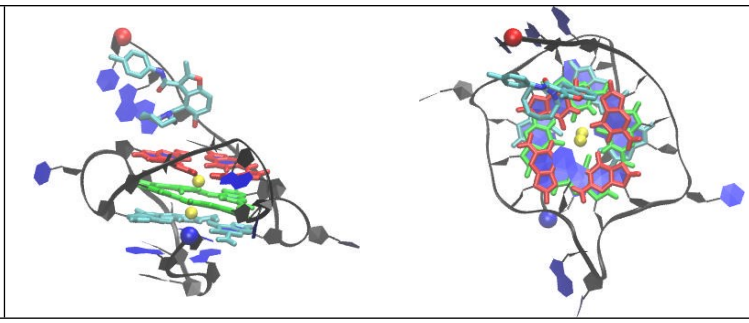
	
07 - Side	**08 - Top/No intercalation**
	
09 – Top	**10 - Top/No intercalation**
	
11 - Bottom	**12 - Top/No intercalation**



13 - Bottom



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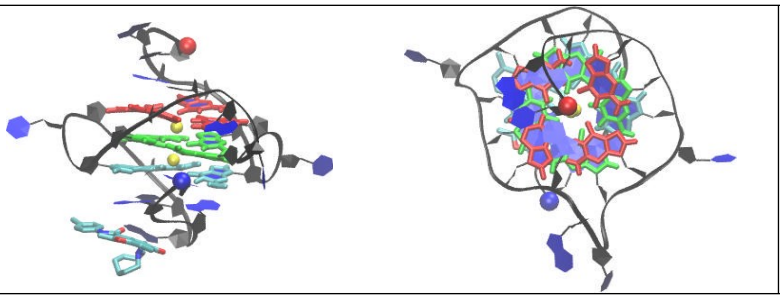
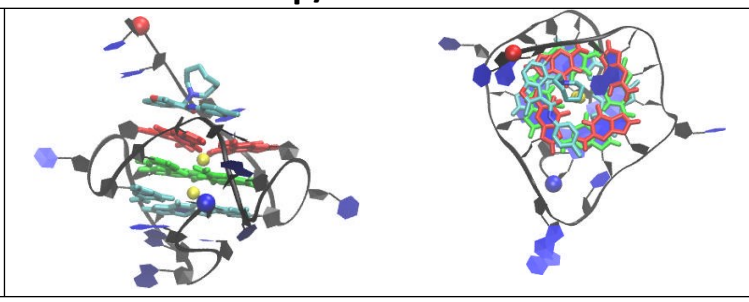
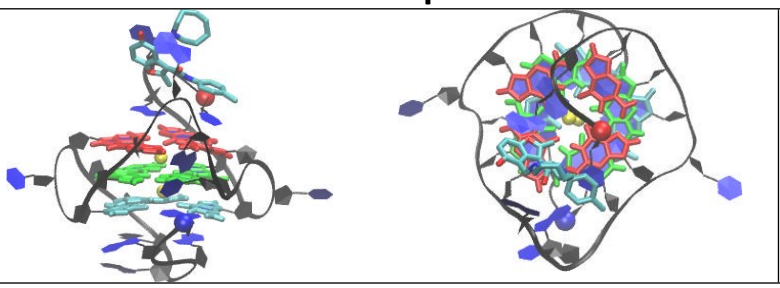


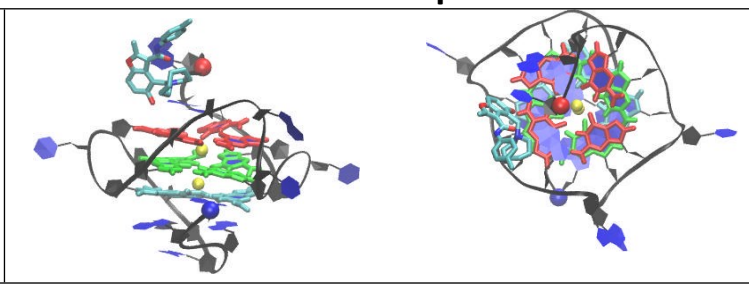
15 - Top



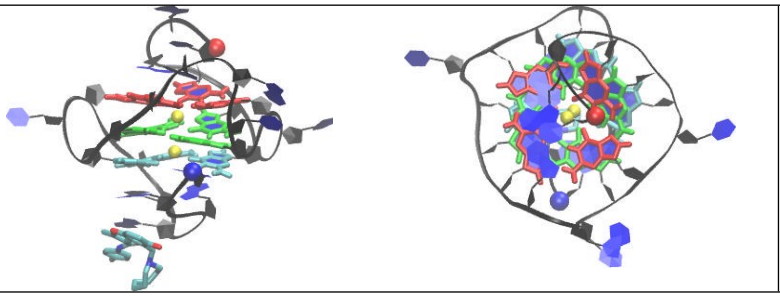
16 - Top



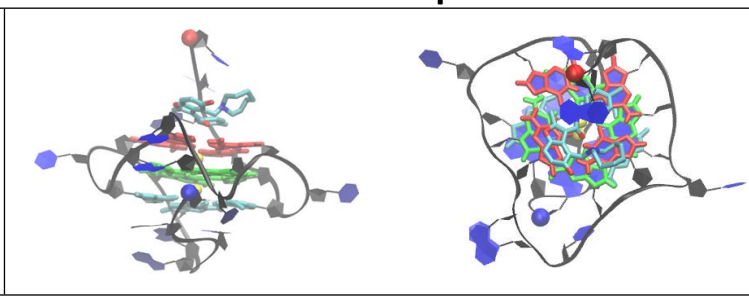
17 - Bottom



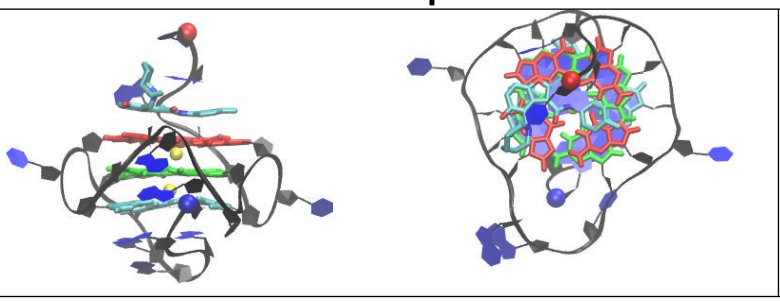
18 - Top



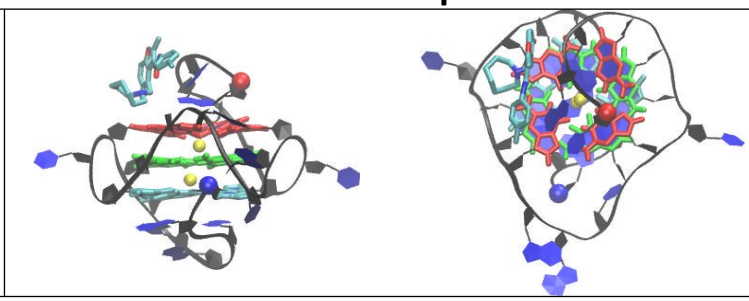
19 – Top



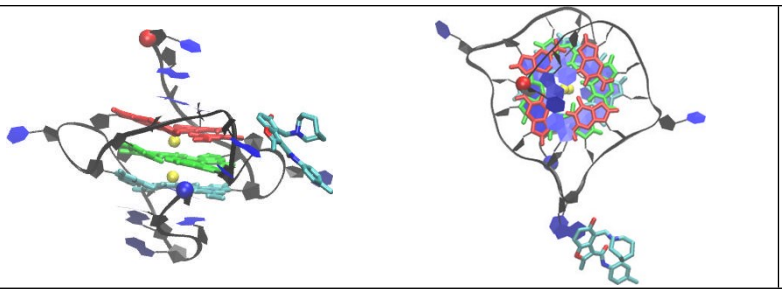
20 – Top



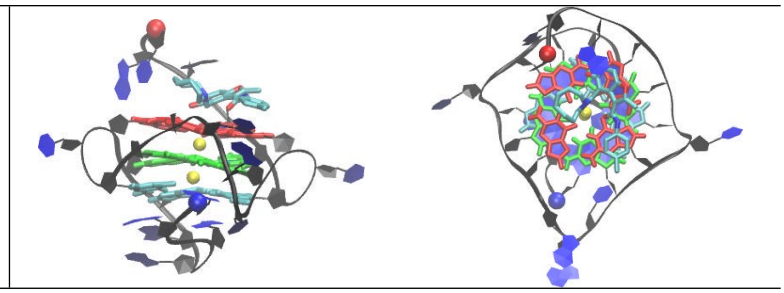
21 - Side



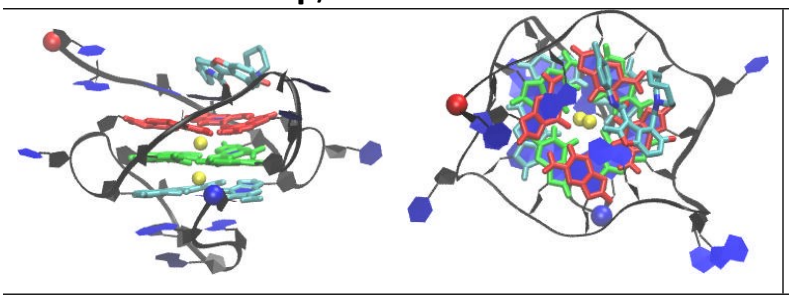
22 - Top/No intercalation



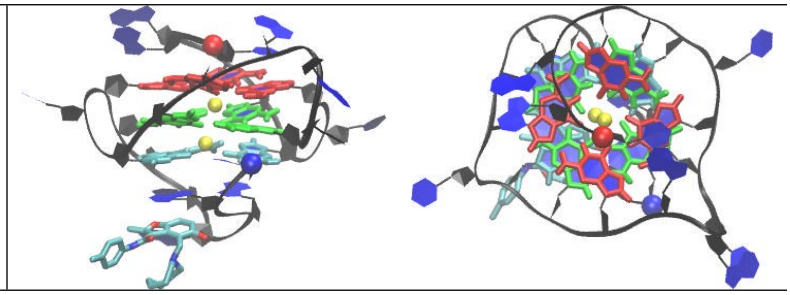
23 - Top/No intercalation



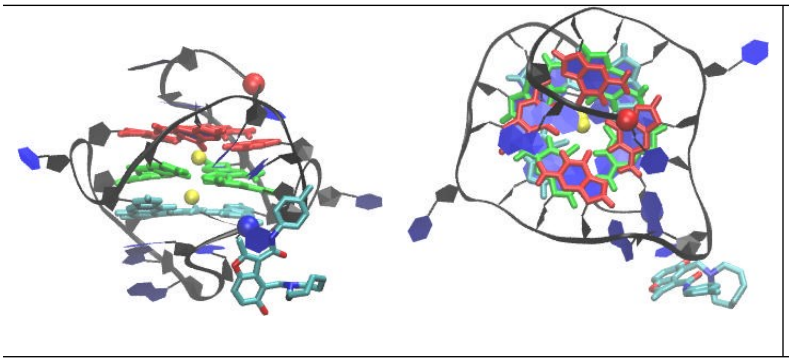
24 - Bottom



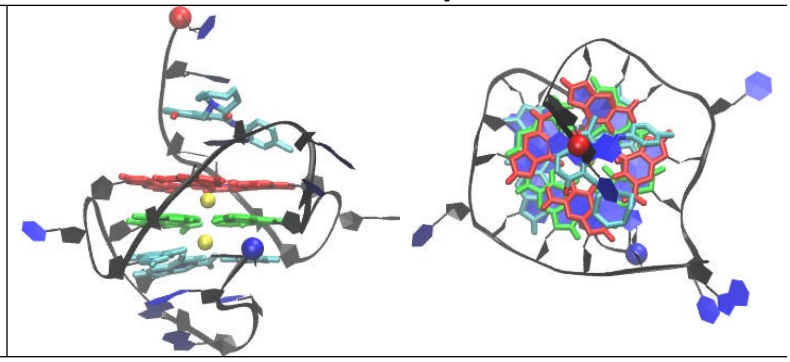
25 - Bottom/Side



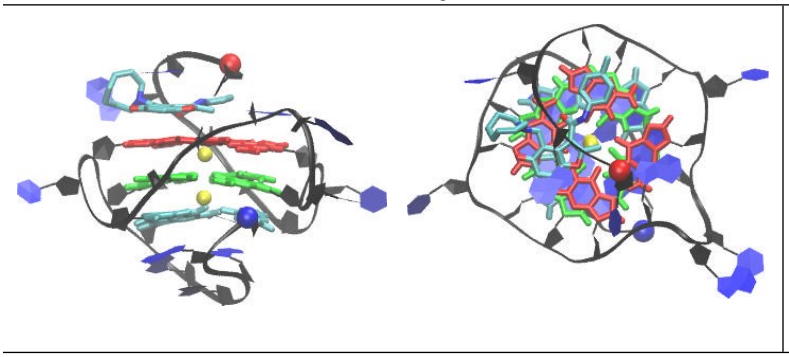
26 - Top



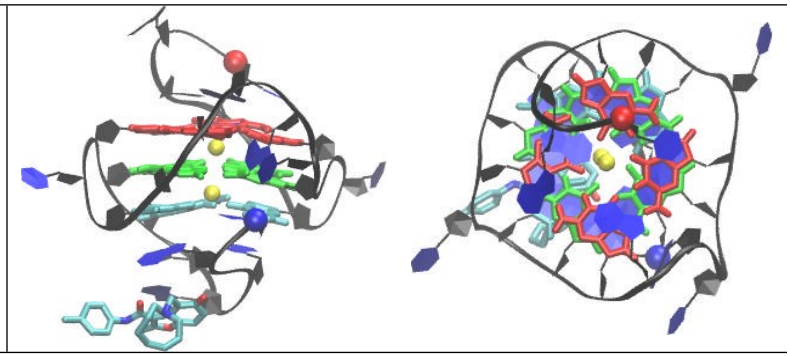
27 - Top



28 - Bottom



29 - Top



30 - Top/No intercalation

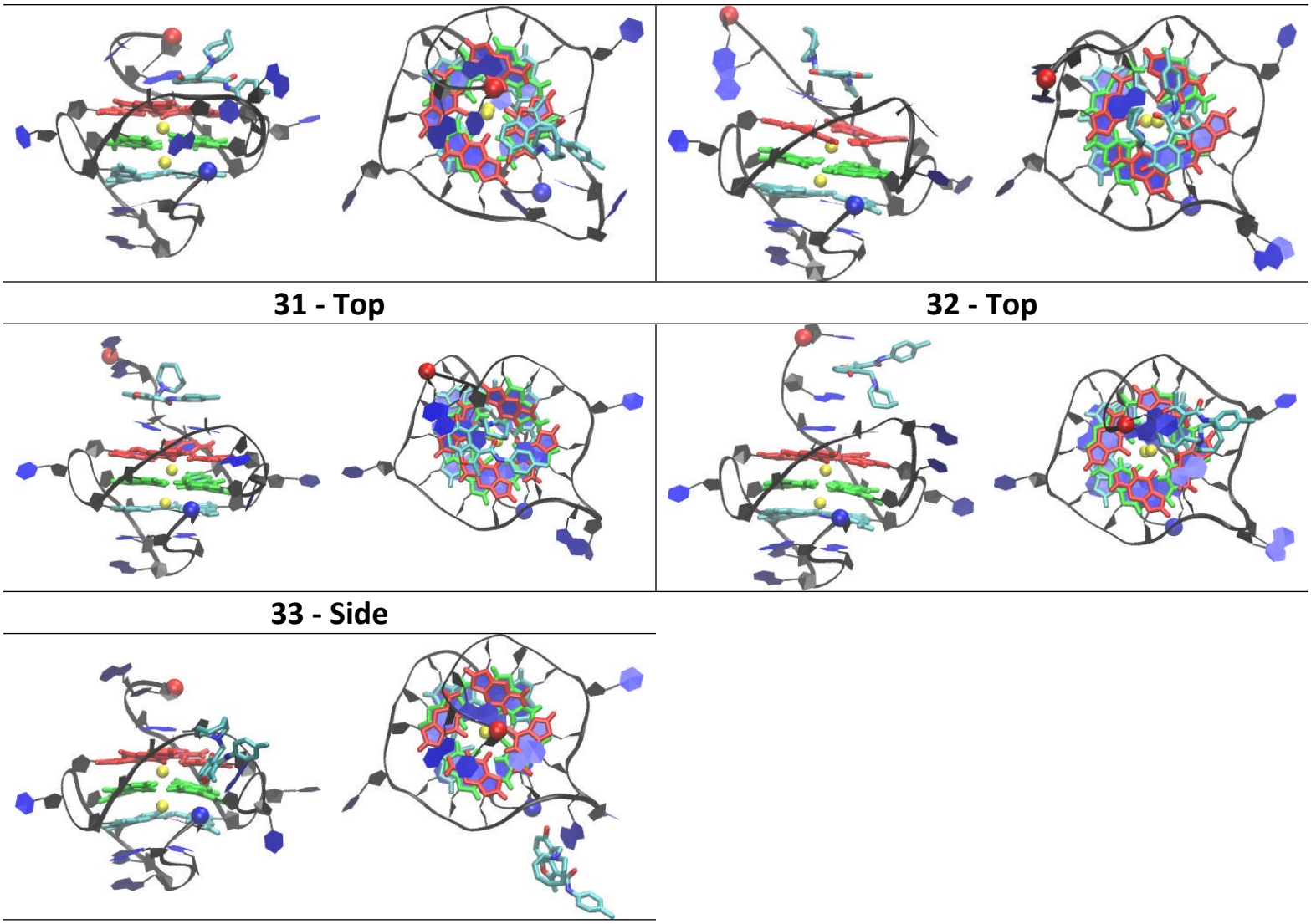


Figure S7. Last snapshot of the 33 free ligand binding simulations of DBD1 to the Pu24 G-quadruplex.

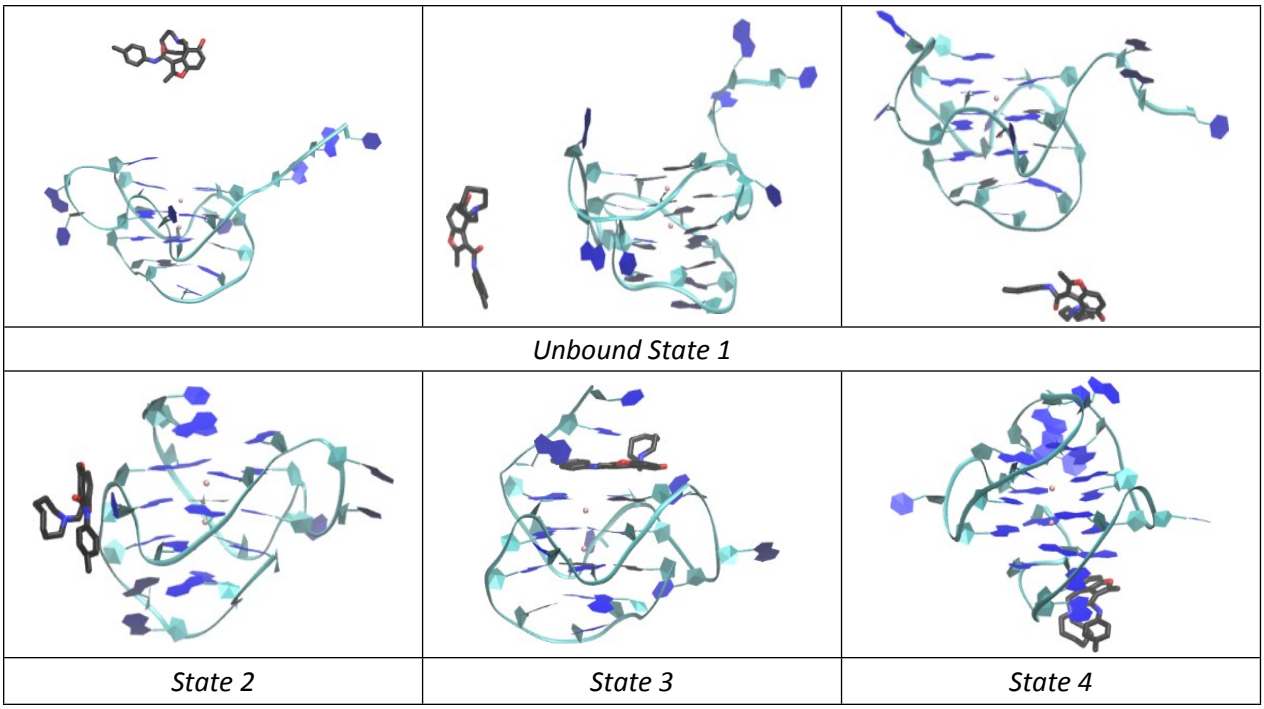


Figure S8. Four major states observed in the MSM analysis. Unbound State 1: three representative structures of unbound state 1. States 2 (side binding) and 4 (bottom binding): intermediate states. State 3: the most stable state (top binding). DBD1 and the Pu24 G-quadruplex are colored black and blue/cyan, respectively. Potassium Ions are represented as yellow spheres.

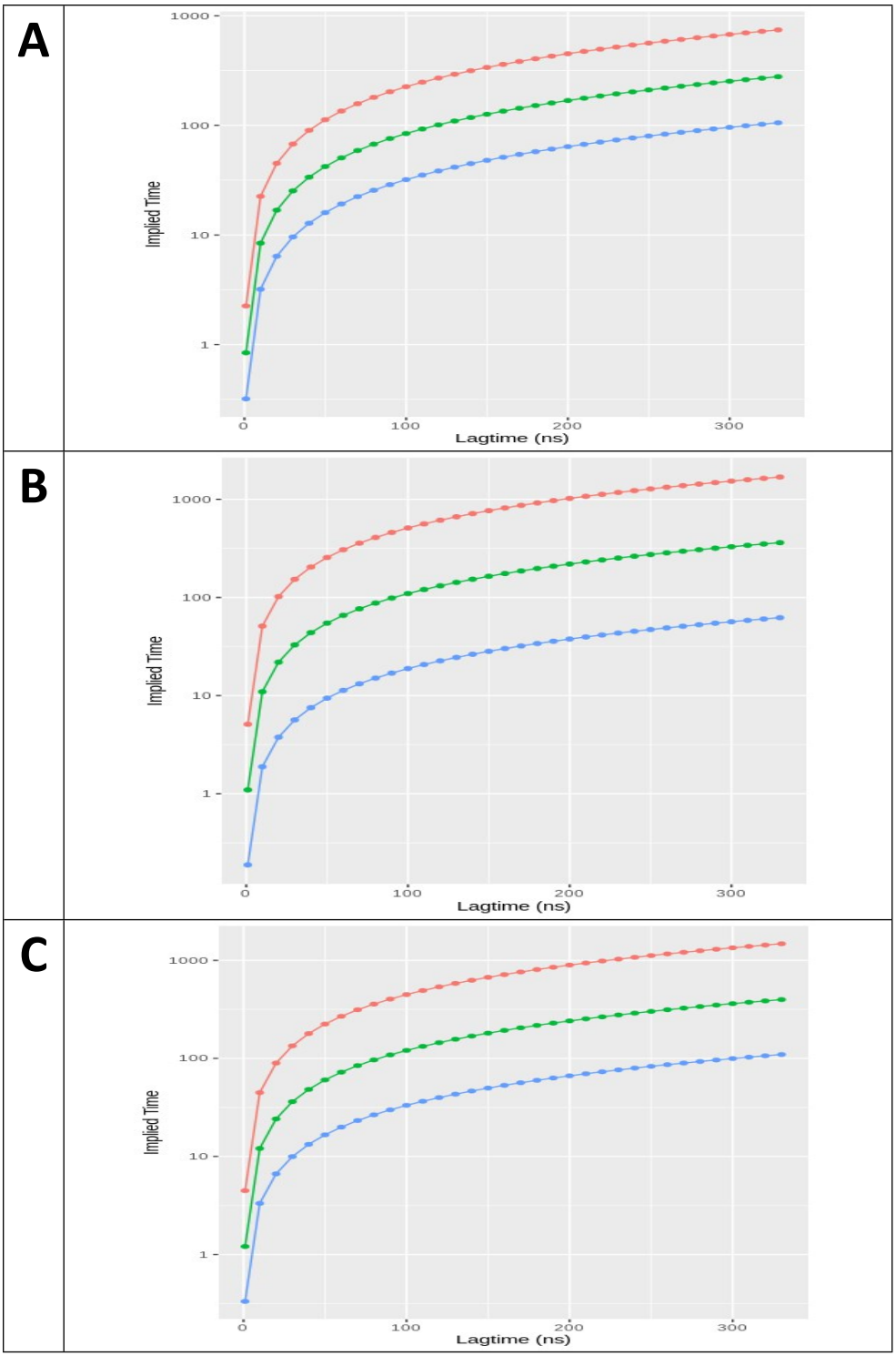


Figure S9. Implied timescale plots for side (red), top (green) and bottom (blue) binding states of G4 with bound ligand determined using three blocks of simulation data. Each block (**A, B and C**) shows approximately 333.3 ns of simulation data. **A** represents simulation block between 0 to 333.3 ns. **B** represents simulation block between 333.3 to 666.7 ns. **C** represents simulation block between 666.7 to 1000.0 ns. All three colored lines have stabilized and all three bound states have converged roughly at lagtime 250 ns.

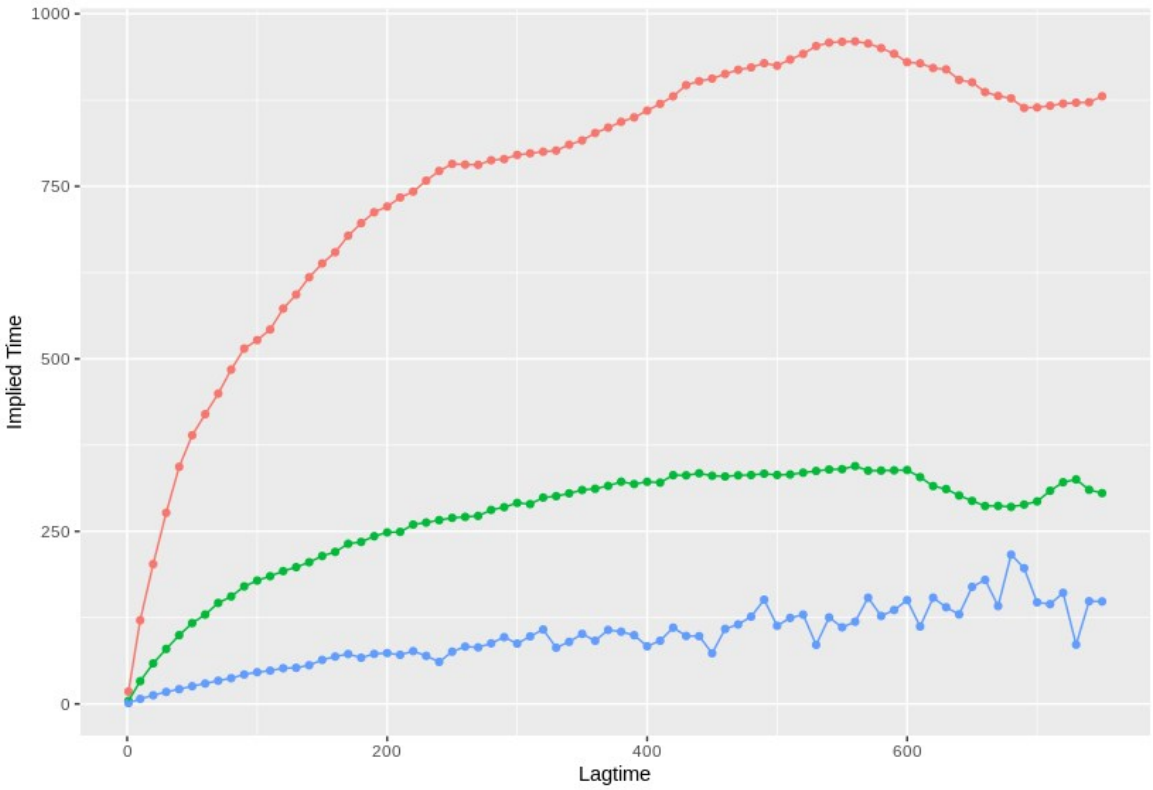


Figure S10. Plot of the implied timescales for the side (red), top (green) and bottom (blue) binding states of G4 with bound ligand. All three lines have stabilized and all three bound states have converged by roughly 250 ns. Timescales are only shown up until 750 ns as the transition matrices after that are significantly less reliable.

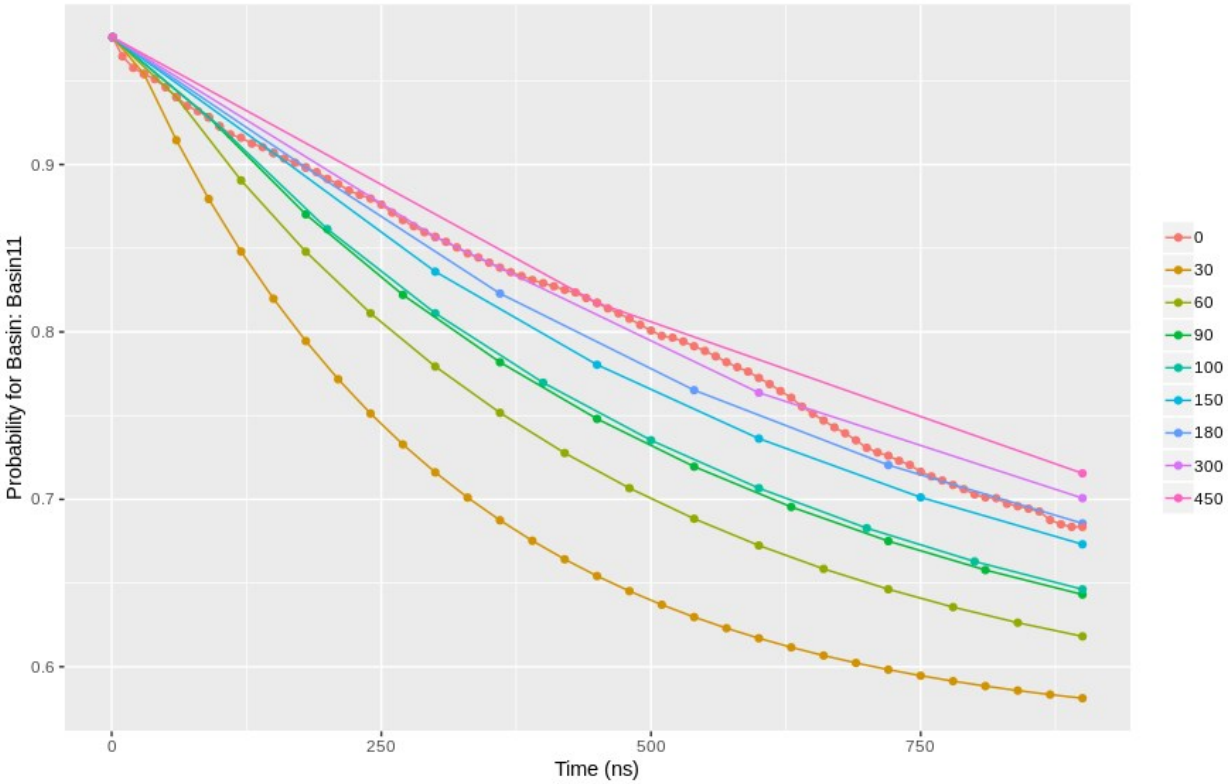


Figure S11. Plot of the Chapman-Kolmogorov test of the probability for Basin 11. Basin 11 is indicative of the probability that the simulation will remain in cluster 3, the most stable state (top binding mode, **Figure S8**). Each line denotes the approximation of a model for that given lag time. The line for 0 ns is the actual simulation data. As the line for 0 ns falls between the lines from 180 ns and 450 ns, it is clear that the model closely approximates the simulation between lag times of 180 ns and 450 ns.

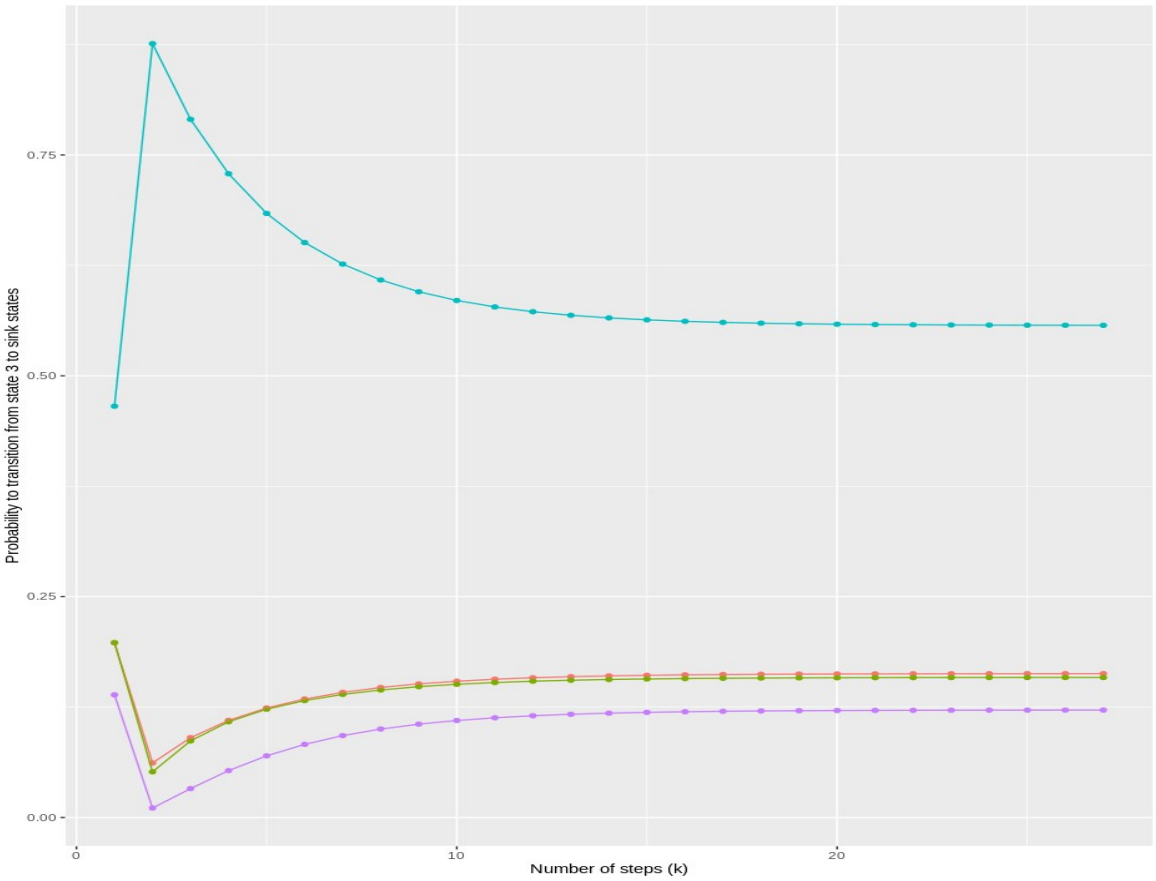


Figure S12: Distribution of the apo-form (red), side (green), top (blue) and bottom (purple) binding states changing as a function of increasing steps (250 ns per step). The first data point of each state represents the state's initial distribution probability within the first 250 ns of simulation time (0.1976970, 0.1979394, 0.4655758 and 0.1387879 for apo-form, side, top and bottom states, respectively). The last data point for each state represents that state's distribution probability at equilibrium (0.1628341, 0.1584603, 0.5571244 and 0.1215812 for apo-form, side, top and bottom, respectively).

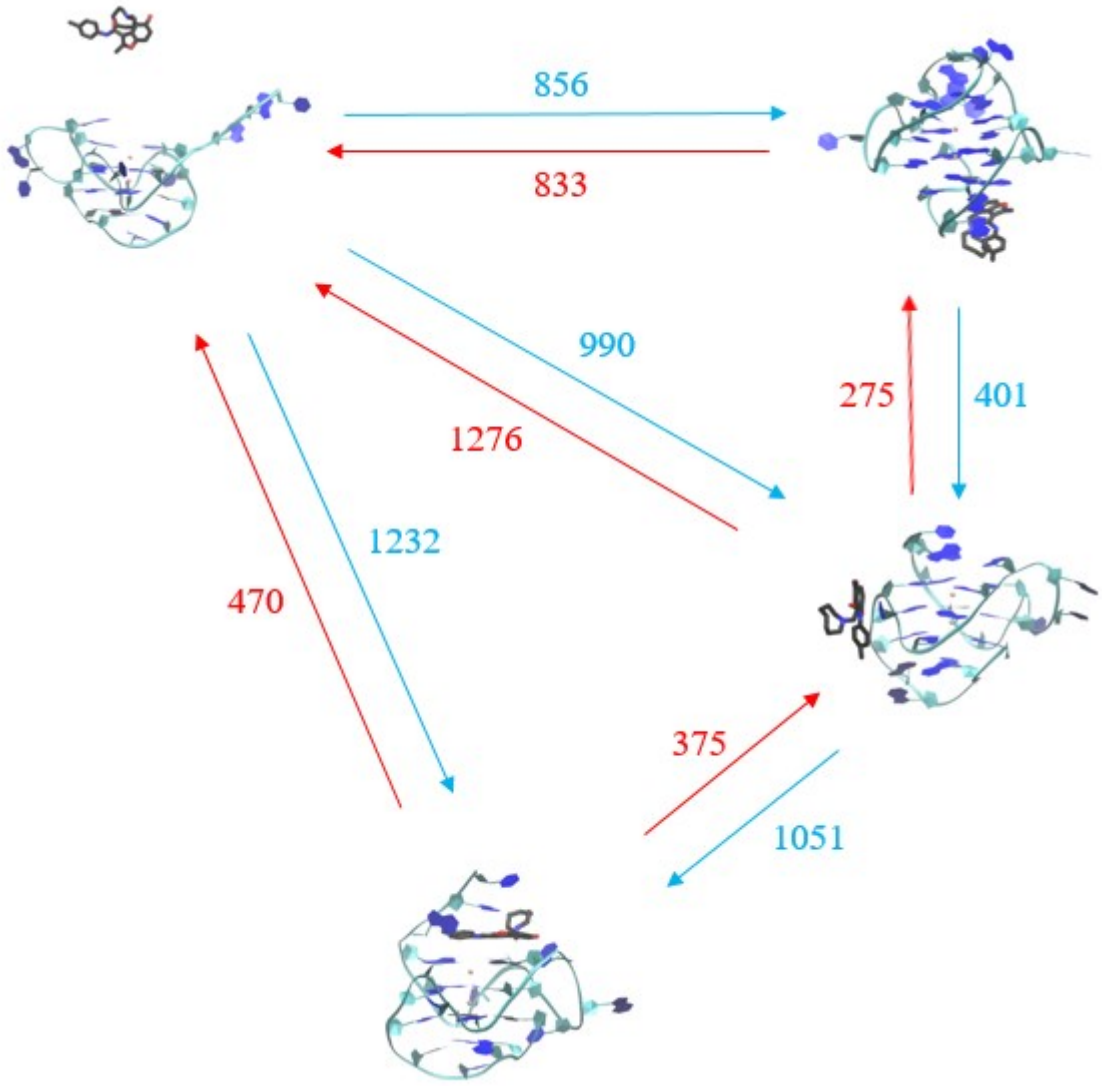
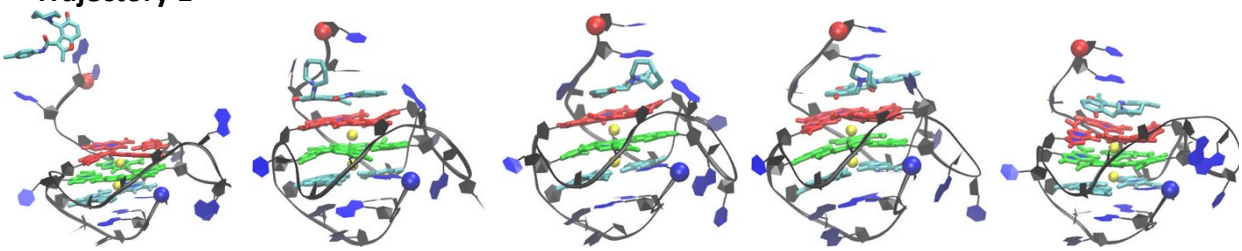


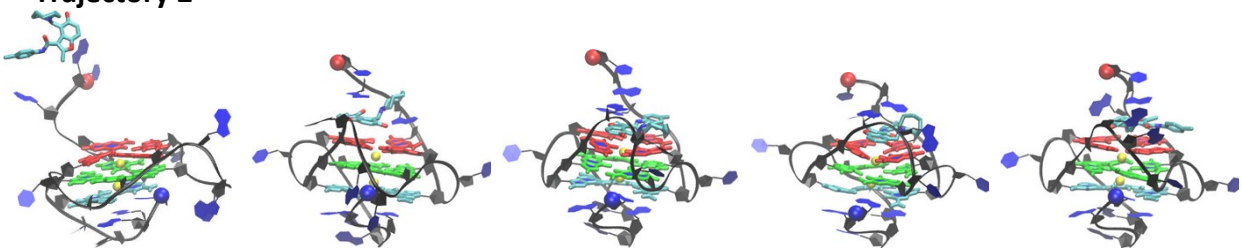
Figure S13: MSM model of observed transitions for a lag time of 250ns between the four states (unbound, top, side, and bottom). Directional arrows are labelled with the number of observed transitions in the same color. DBD1 and the Pu24 G-quadruplex are colored black and blue/cyan respectively. Potassium ions are represented as yellow spheres.

Trajectory 1



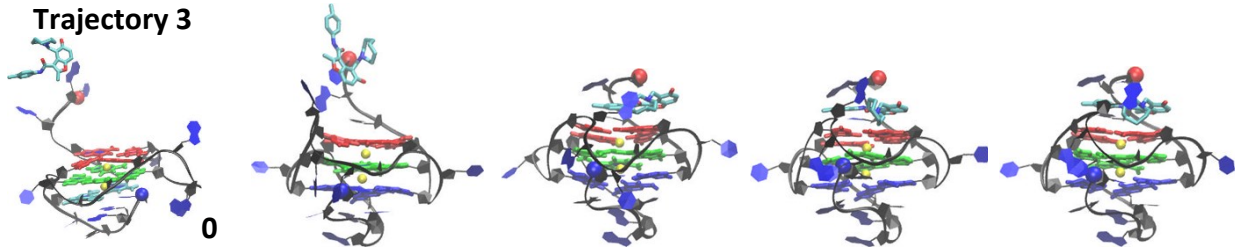
00ns 35ns 151ns 552ns 1001ns

Trajectory 2



00ns 10ns 421ns 639ns 1001ns

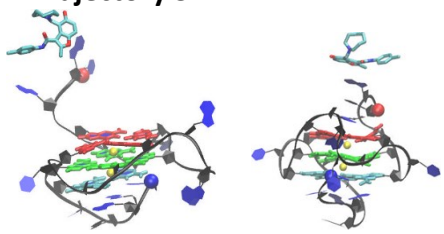
Trajectory 3



0

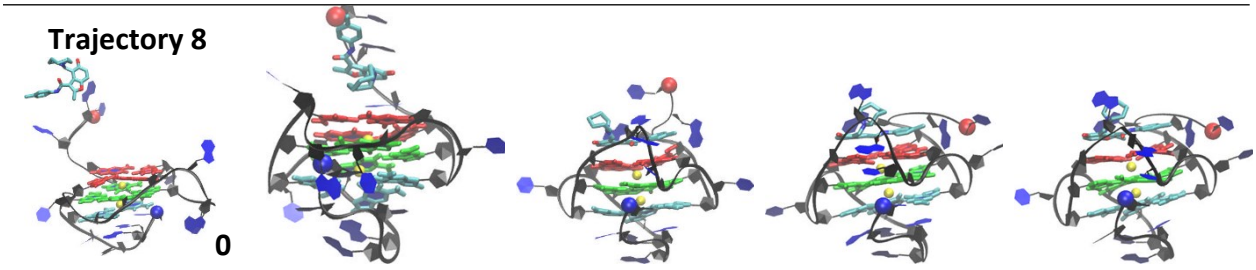
0ns 08ns 297ns 684ns 1001ns

Trajectory 5



00ns 20ns 500ns 652ns 1001ns

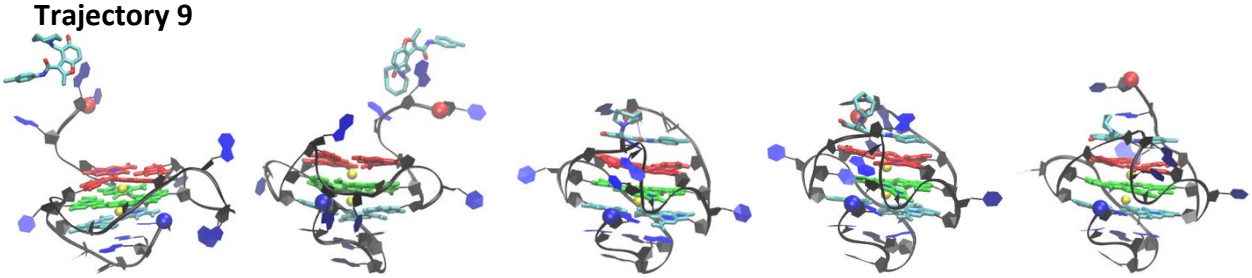
Trajectory 8



0

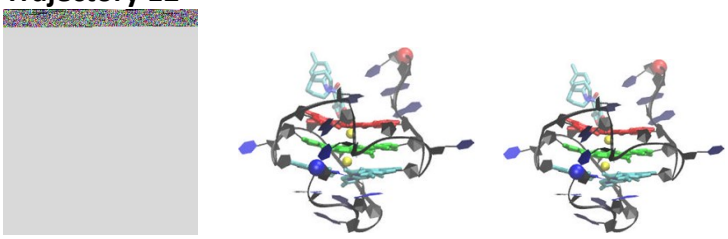
0ns 12ns 386ns 750ns 1001ns

Trajectory 9



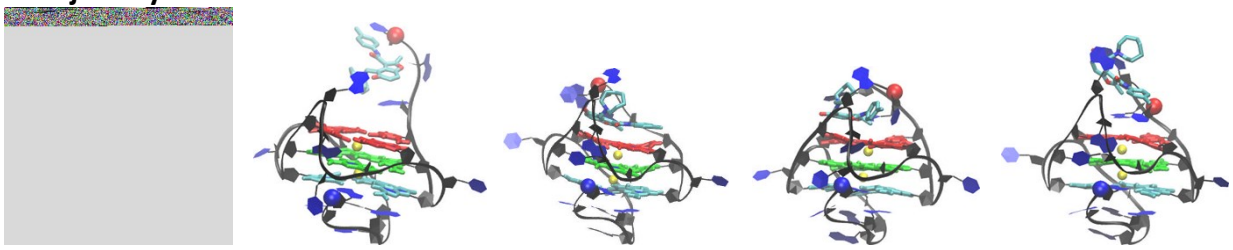
00ns 02ns 156ns 506ns 1001ns

Trajectory 12



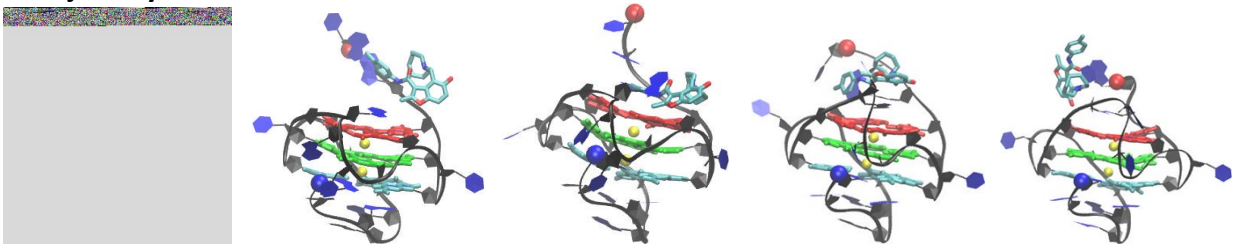
00ns 18ns 515ns 856ns 1001ns

Trajectory 15



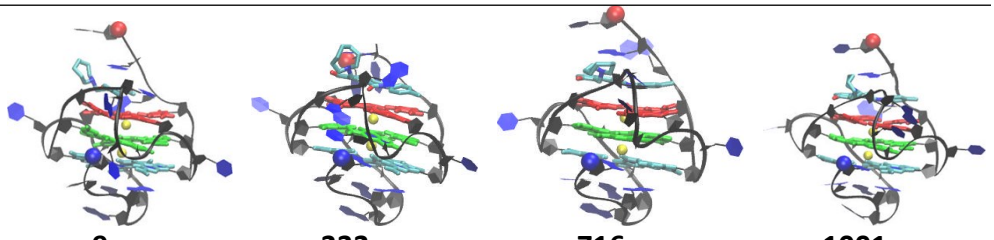
00ns 04ns 100ns 396ns 1001ns

Trajectory 16



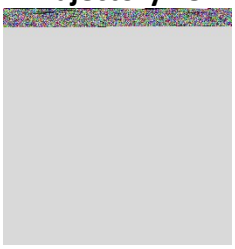
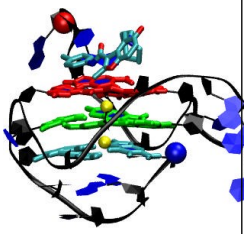
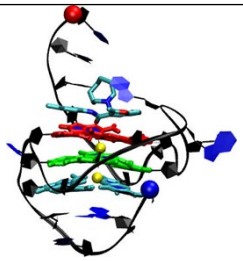
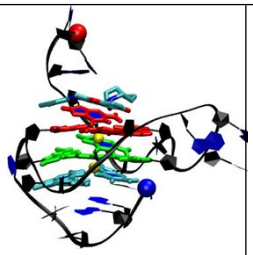
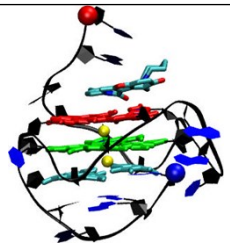
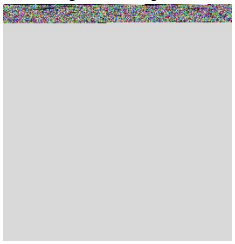
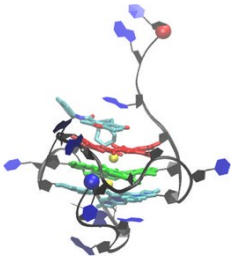
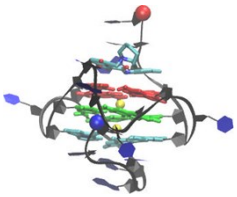
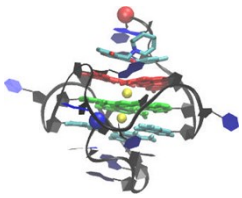
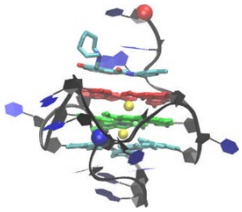
00ns 04ns 127ns 543ns 1001ns

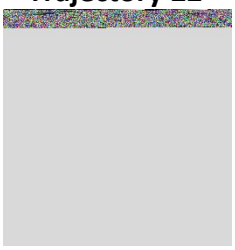
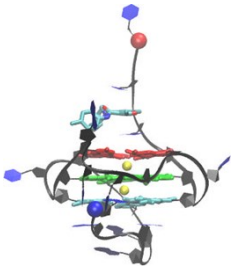
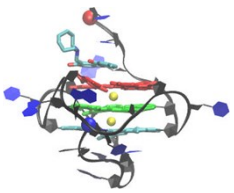
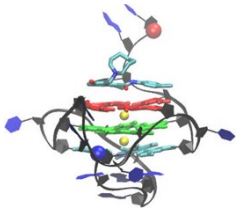
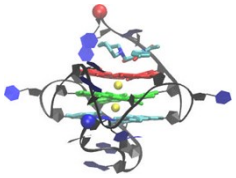
Trajectory 17 (Top)



9ns 333ns 716ns 1001ns

00ns

Trajectory 18				
				
00ns	34ns	368ns	602ns	1001ns
Trajectory 19				
				
00ns	03ns	228ns	748ns	1001ns

Trajectory 20				
				
00ns	120ns	486ns	687ns	1001ns
Trajectory 22				
				
00ns	05ns	488ns	715ns	1001ns

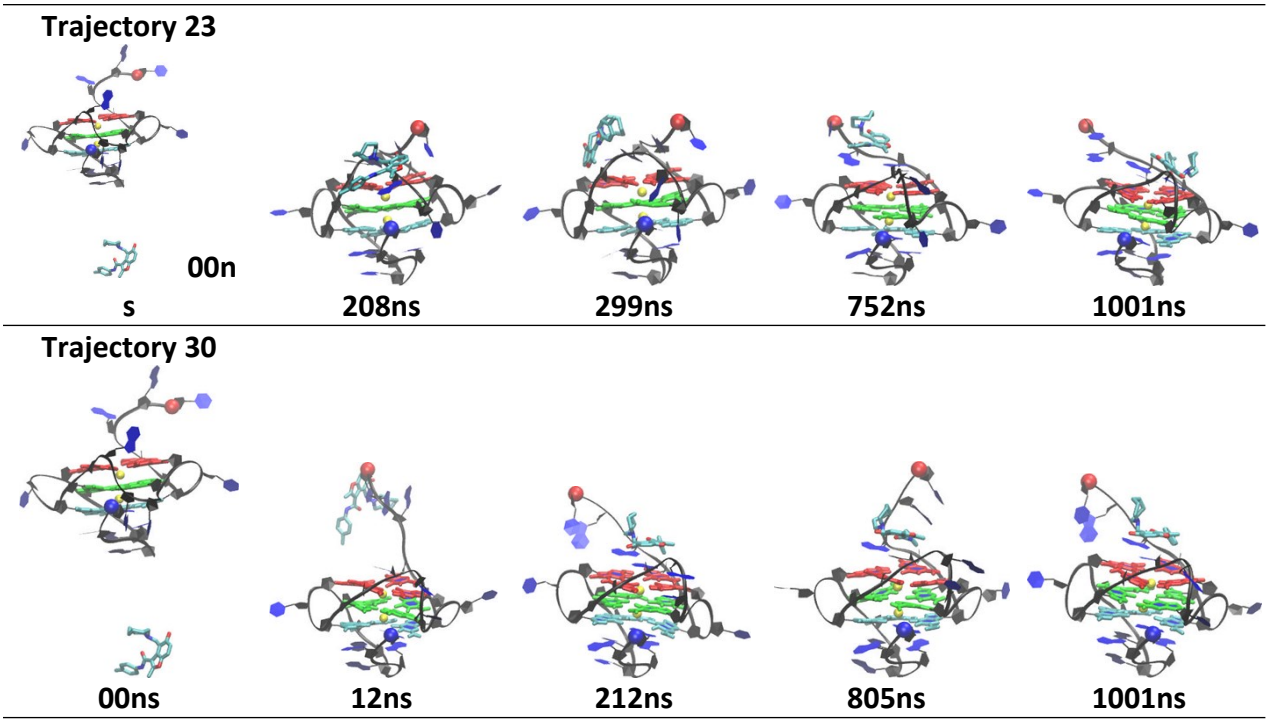
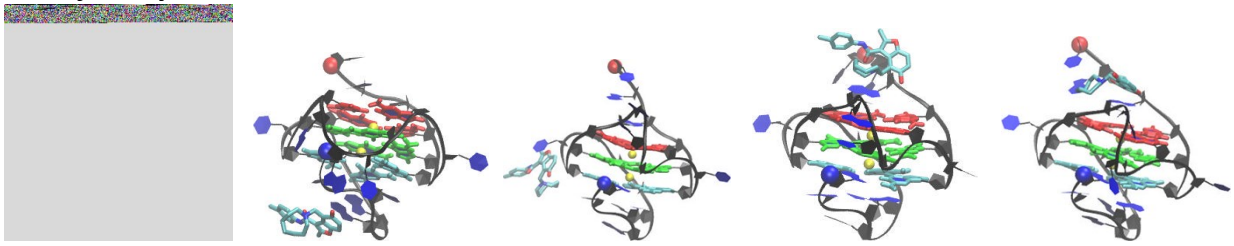


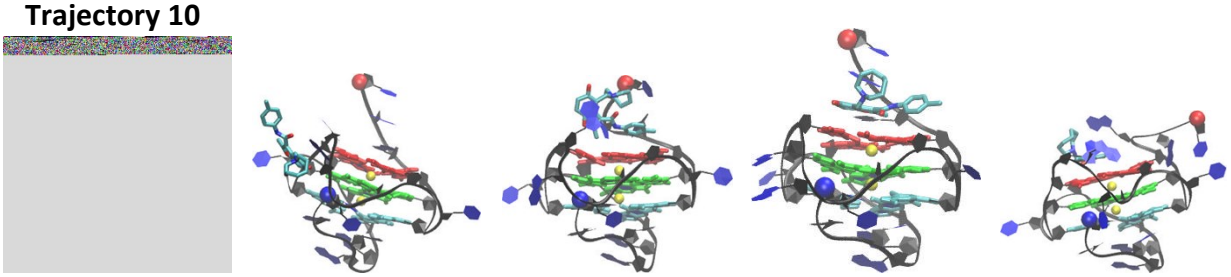
Figure S14. Trajectories of the primary binding pathway of DBD1 to the top site of the Pu24 G-quadruplex.

Trajectory 6



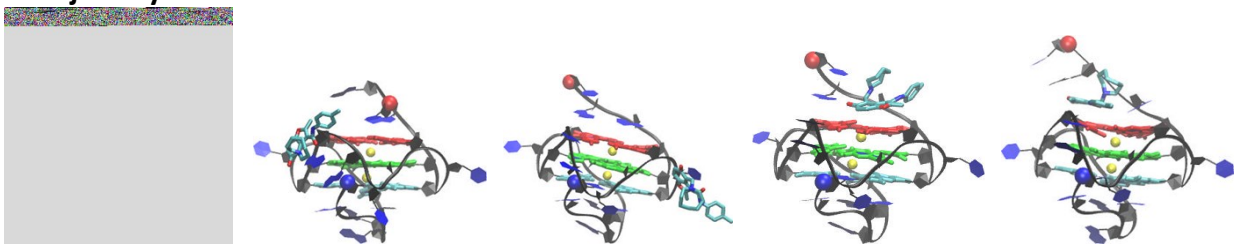
00ns 09ns 524ns 722ns 1001ns

Trajectory 10



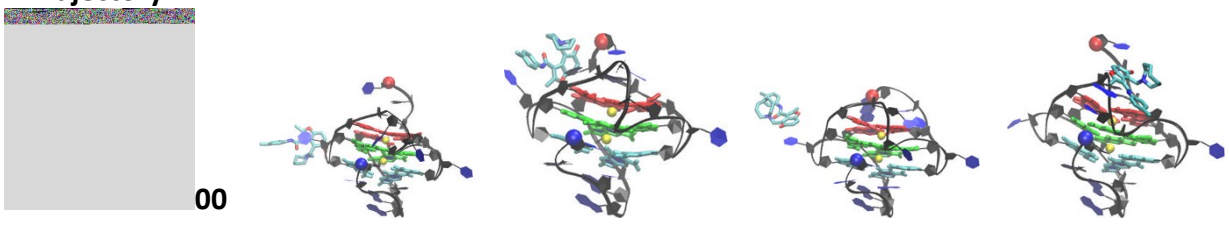
00ns 24ns 238ns 675ns 1001ns

Trajectory 14



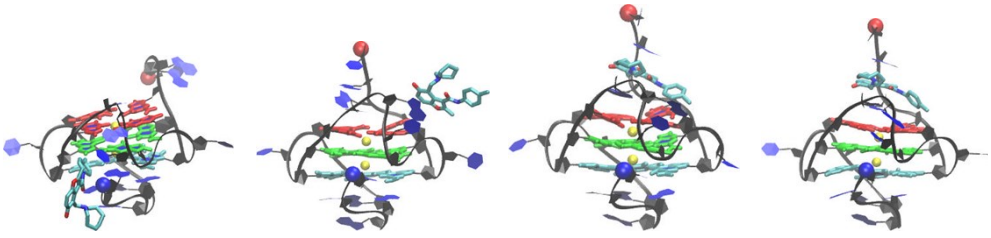
00ns 57ns 503ns 647ns 1001ns

Trajectory 21

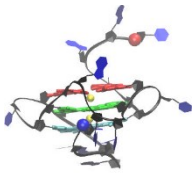


00

ns 15ns 379ns 617ns 1001ns



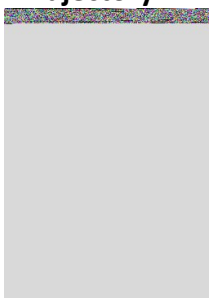
Trajectory 26 11ns 292ns 580ns 1001ns

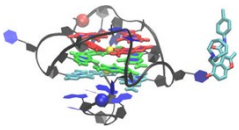


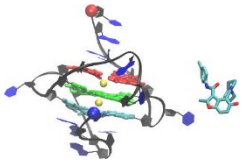
00

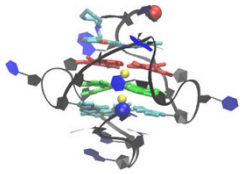
ns

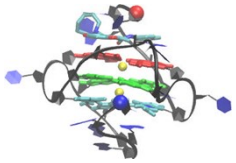
Trajectory 27





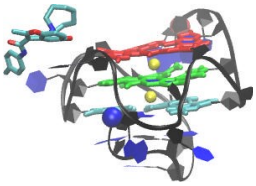


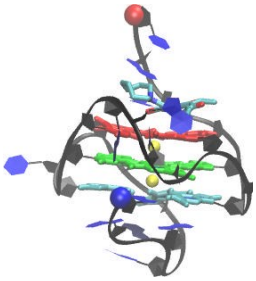


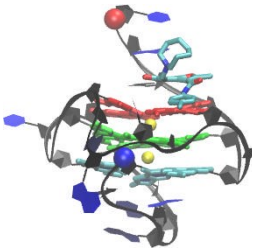


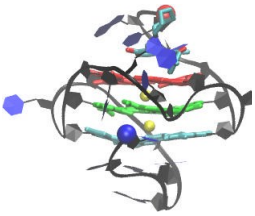
00ns 20ns 172ns 621ns 1001ns

Trajectory 29



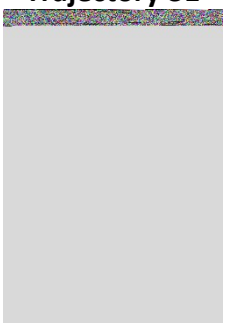


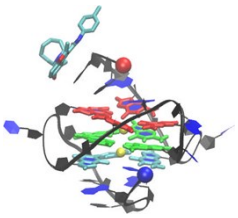


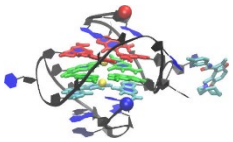


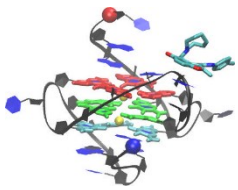
00ns 22ns 500ns 740ns 1001ns

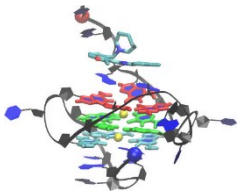
Trajectory 31











00ns 83ns 277ns 739ns 1001ns

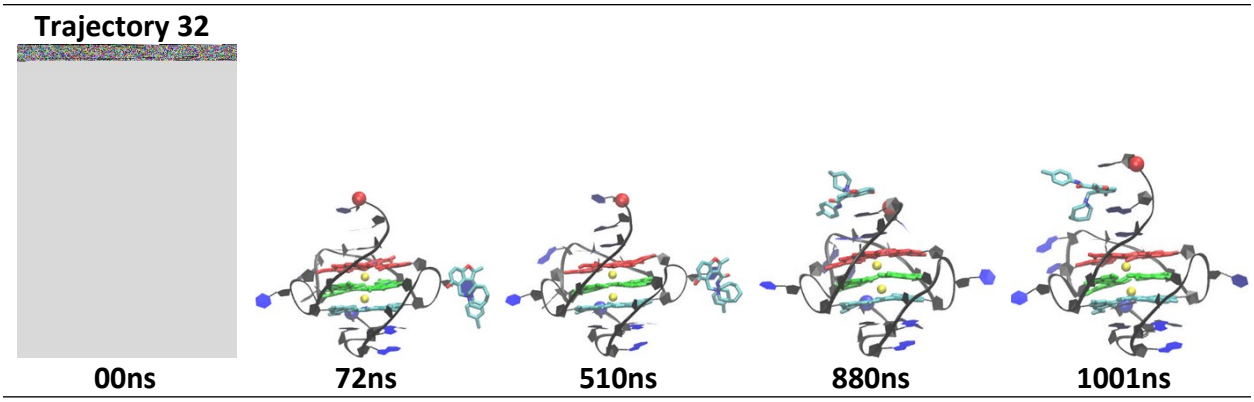


Figure S15 Trajectories of the secondary binding pathway of DBD1 to the top site of the Pu24 G-quadruplex via a side binding.

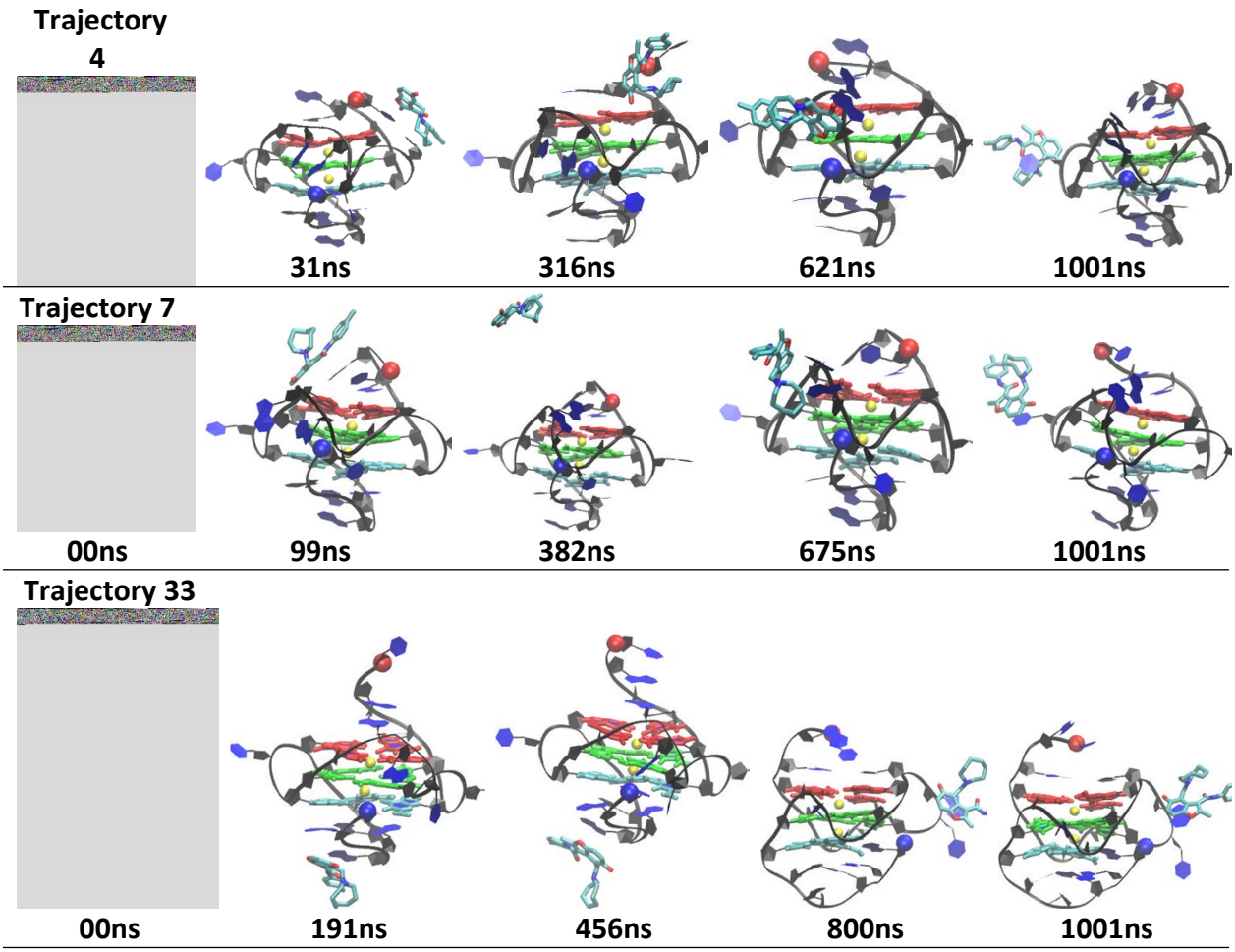


Figure S16. Trajectories of the binding pathway of DBD1 to the side site of the Pu24 G-quadruplex via a bottom/top binding.

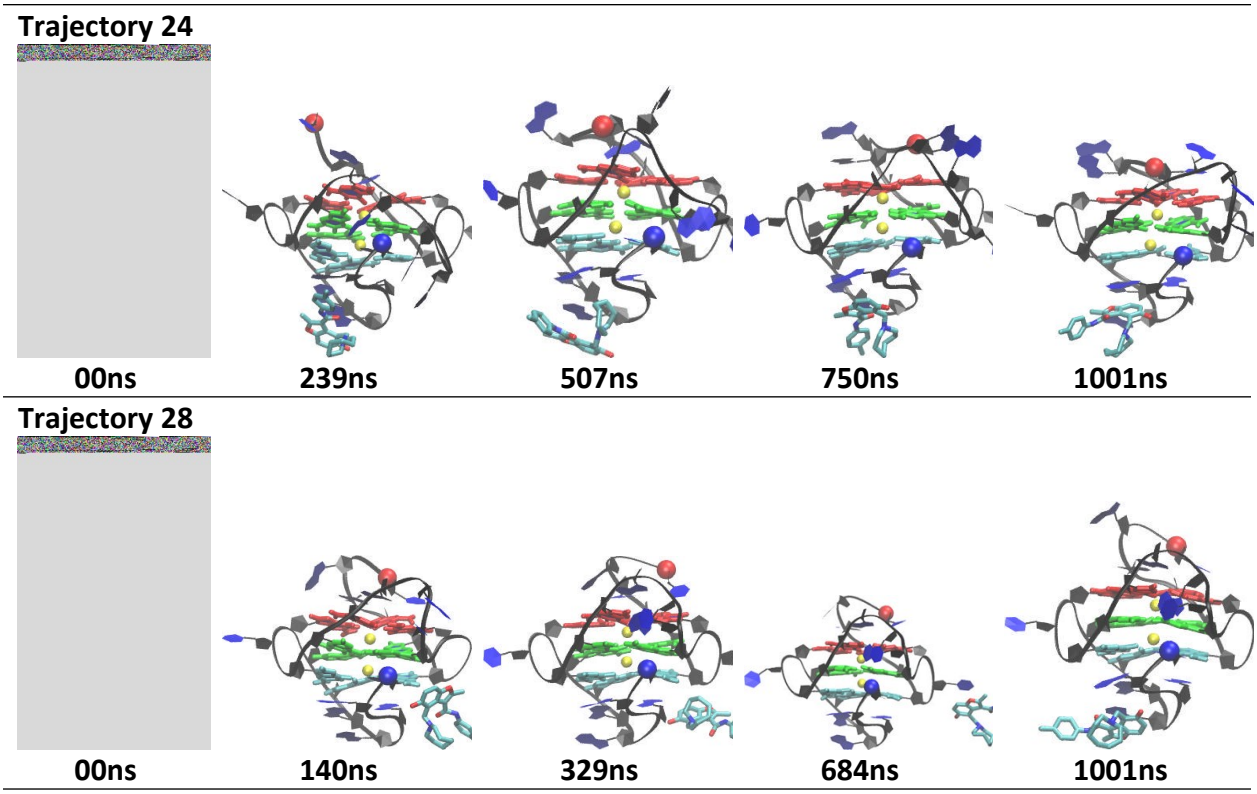


Figure S17. Trajectories of the binding pathway of DBD1 to the bottom site of the Pu24 G-quadruplex.

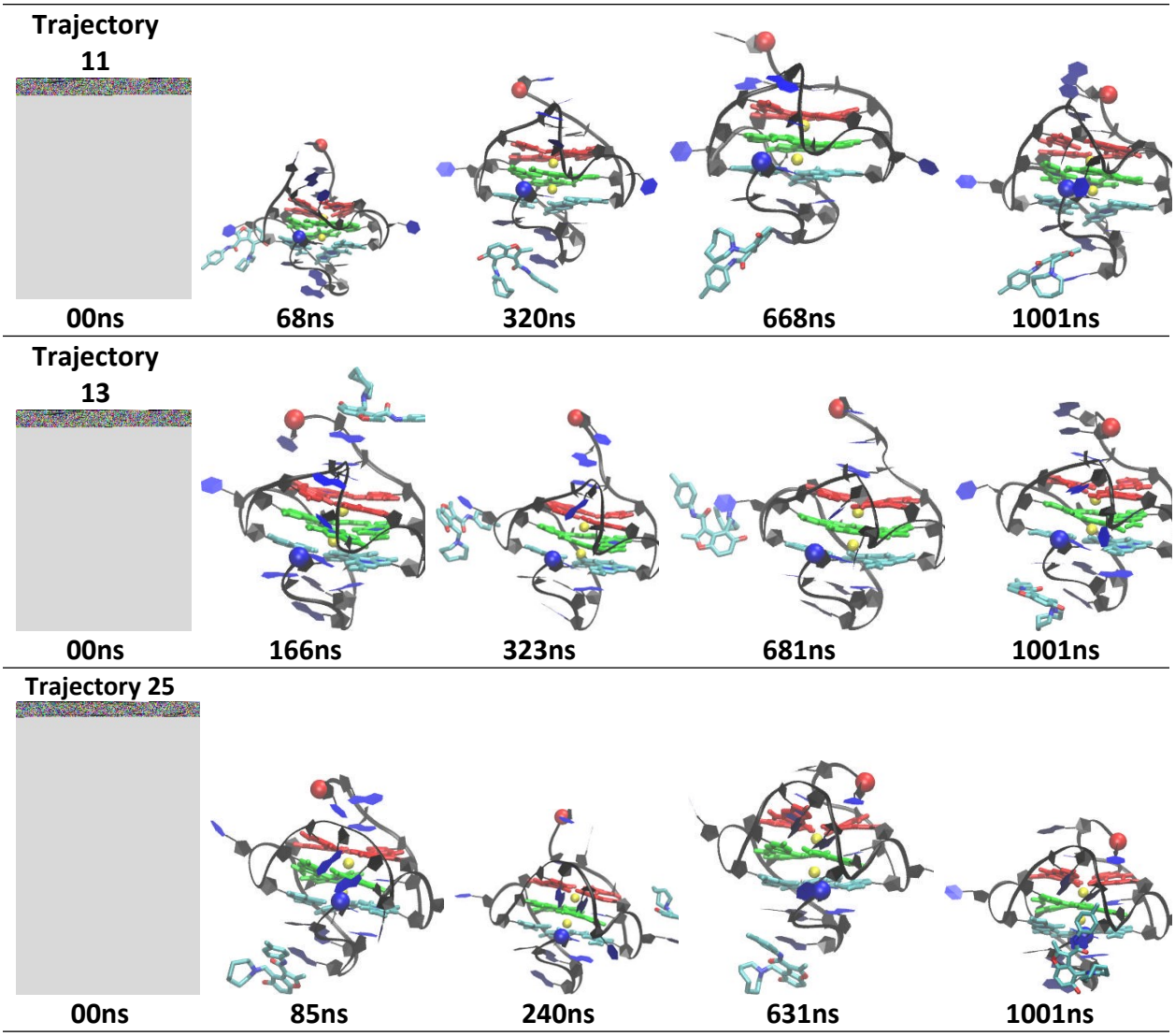


Figure S18. Trajectories of the binding pathway of DBD1 to the bottom site of the Pu24 G-quadruplex via side binding.

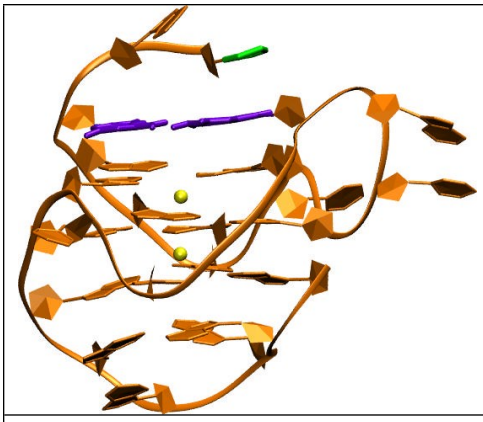
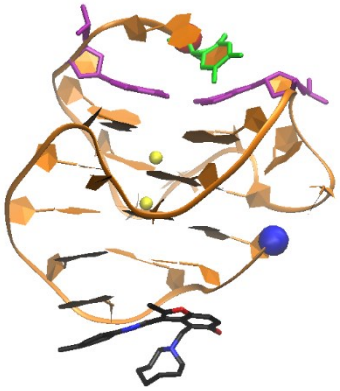
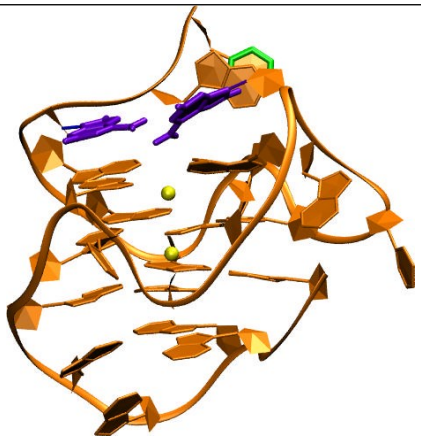
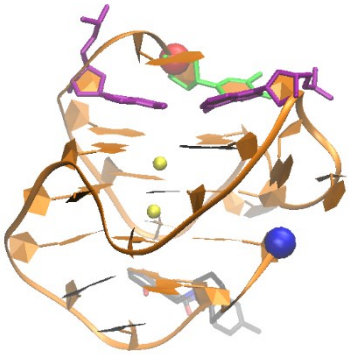
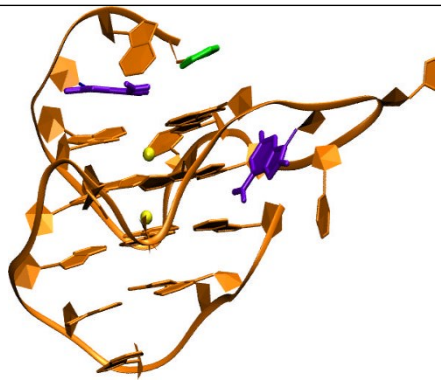
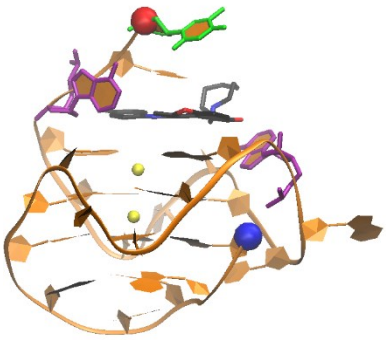
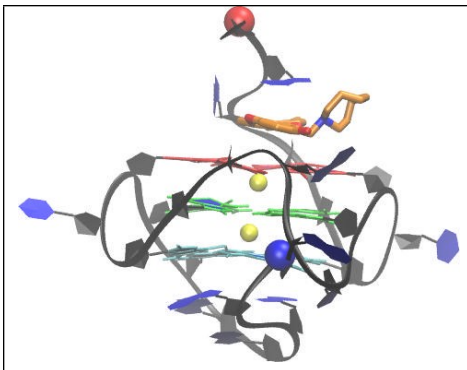
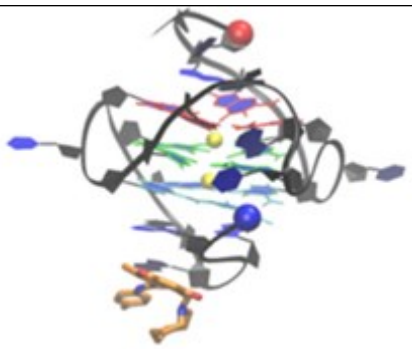
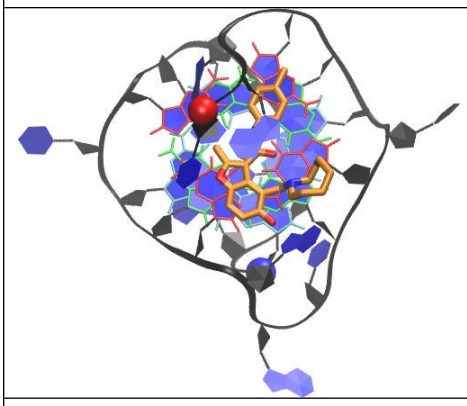
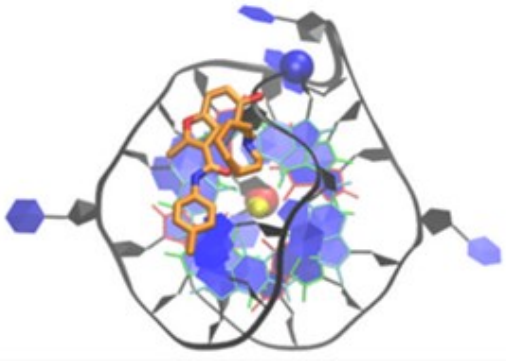
	
Cluster 1 (84.2 %) **A**	Bottom (12.1 %) **B**
	
Cluster 2 (14.8 %) **C**	Side (15.6 %) **D**
	
Cluster 3 (1.0 %) **E**	Top (55.9 %) **F**

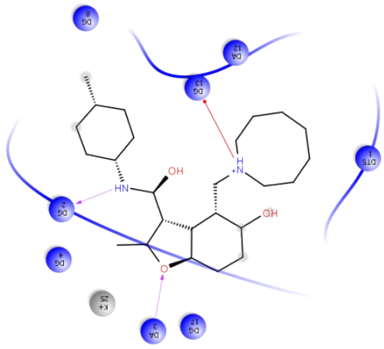
Figure S19: Conformational comparison of the apo-form (left column) and ligand-bound (right column) forms of Pu24 G-quadruplex structures. Each cluster is titled with their respective population counts. **A** and **B** represent the apo-form and bound conformations of Pu24 before and after bottom-binding occurs, respectively. **C** and **D** represent the apo-form and bound conformations of Pu24 before and after side-binding occurs, respectively. **E** and **F** represents the apo-form and ligand-bound conformations of Pu24 before and after top-binding occurs, respectively. Nucleotide T1 is shown in green and nucleotides A3 and A12 are shown in purple, respectively. 5’ and 3’ ends of Pu24 are shown as red and blue spheres, respectively. Potassium ions are shown as yellow spheres, respectively. Ligand DBD1 is shown in black.

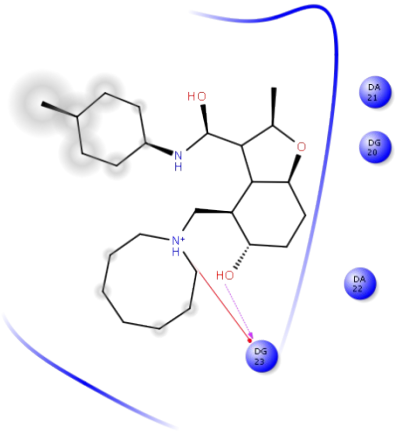









OH
HN
H
N
OH
O


HO
N
H
O
N+
H
HO

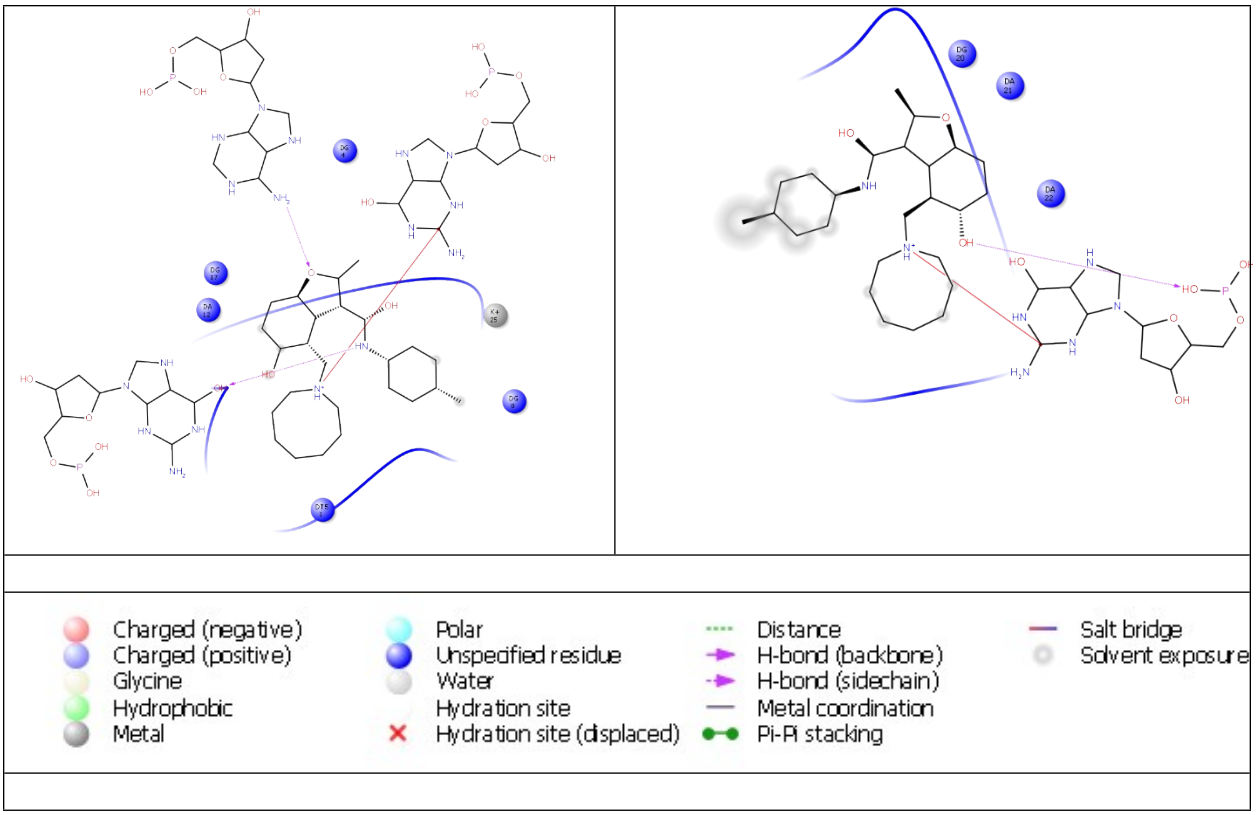
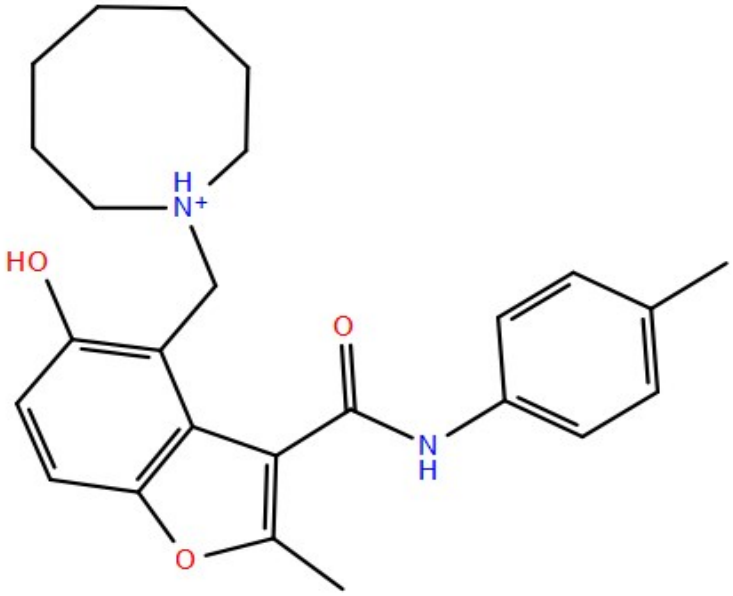
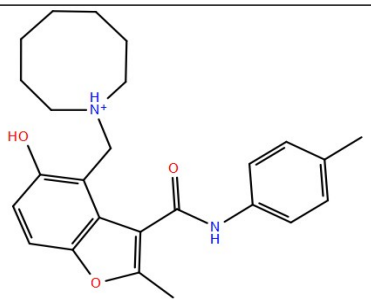
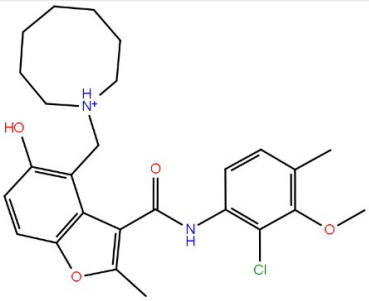
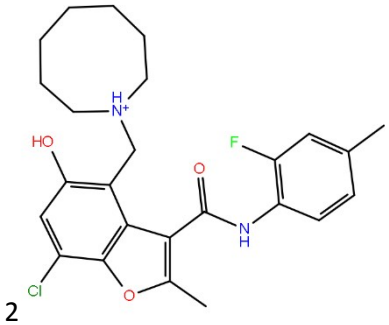
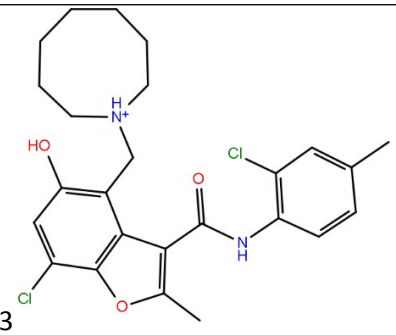
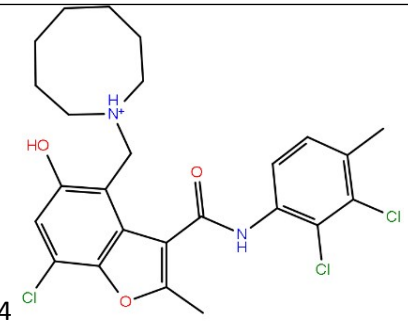
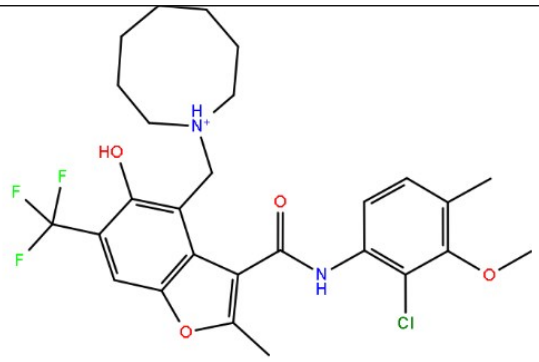
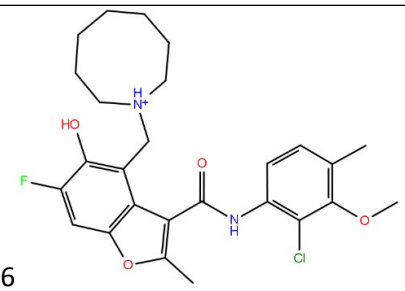
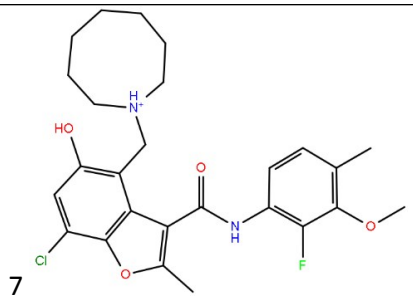
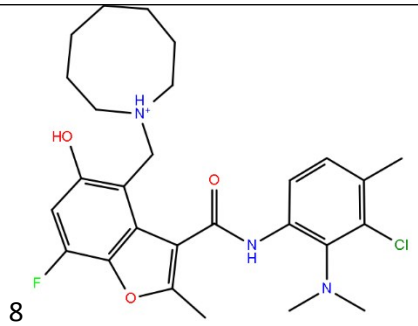
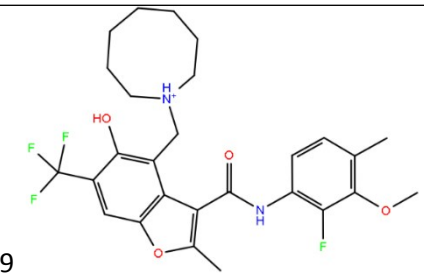
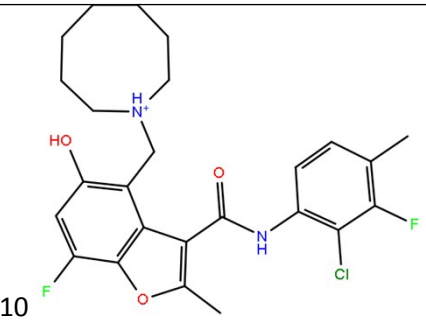
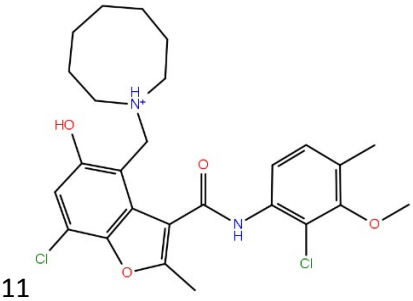
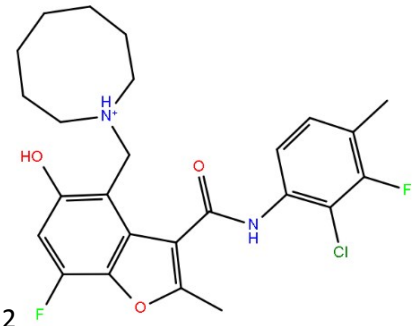
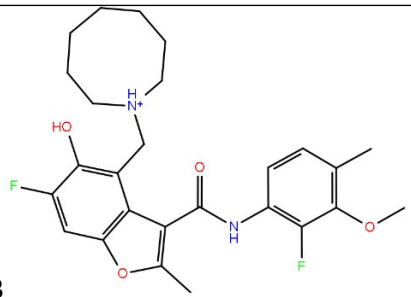
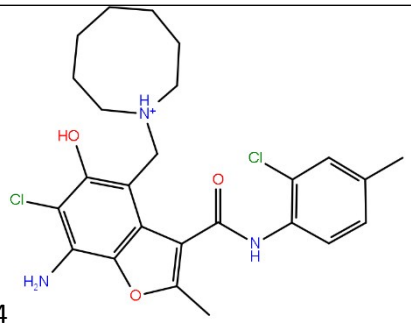
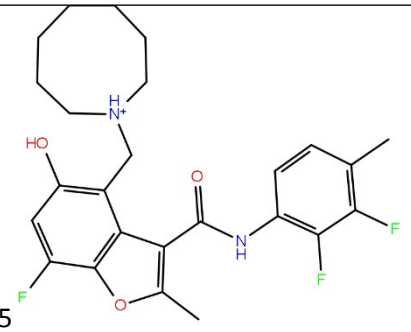
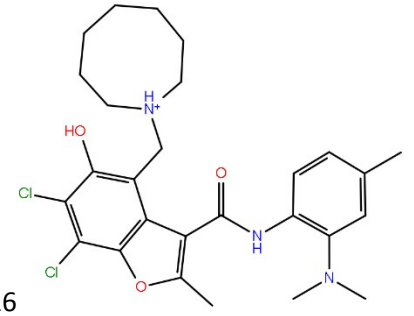


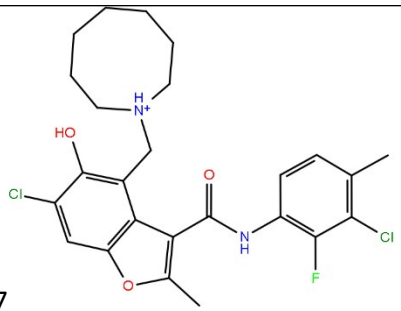
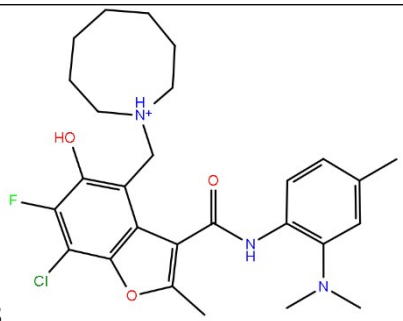
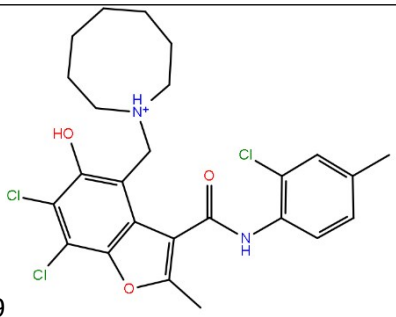
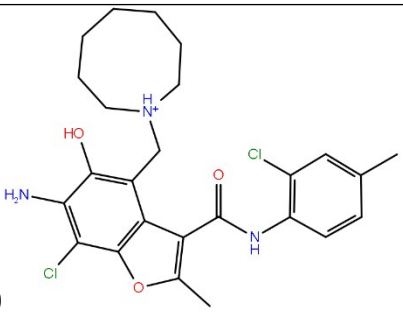
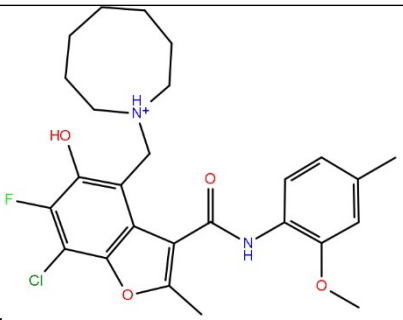
Figure S20. 2D interaction diagrams of MD structure top binding position (top-left), MD structure bottom binding position (top-right), 2MGN top binding position (bottom-left), and 5W77 bottom binding position (bottom-right).

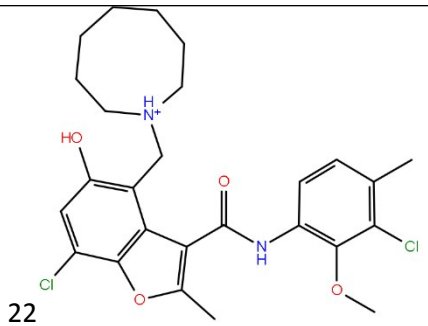
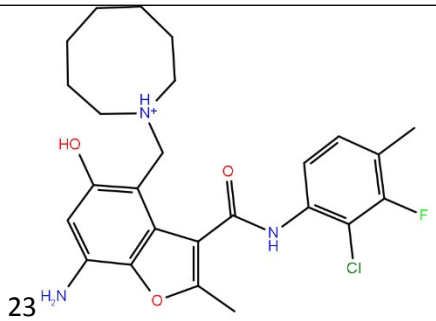
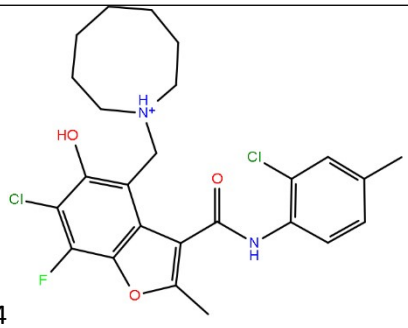
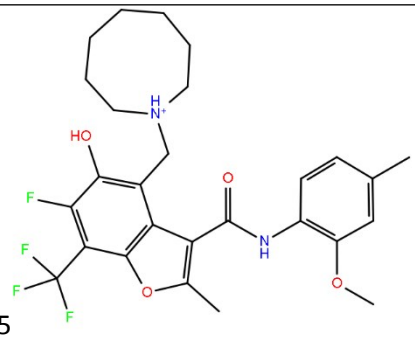
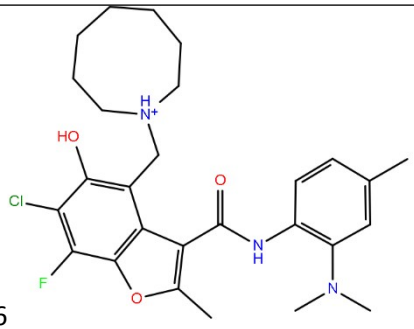
Chemical Structure of DBD1: Substitution Sites Marked		
 **S1-S2 =H, F, Cl, OMe, NMe2** **S3-S4=H, F, Cl, NH2, CF3**		
Chemical Structure of Ligand	**Docking Score (kcal/mol)**	**Docking Score Change with Reference to DBD1 (kcal/mol)**
 **DBD1**	-8.891	0
 1	-9.281	-0.390

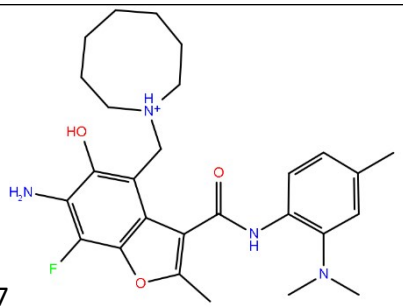
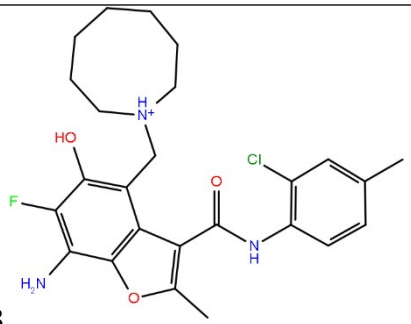
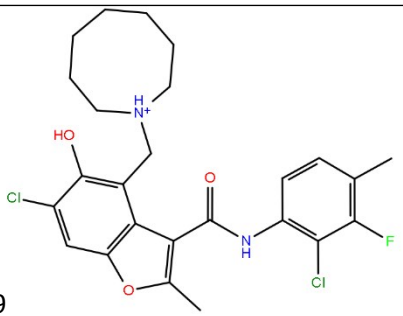
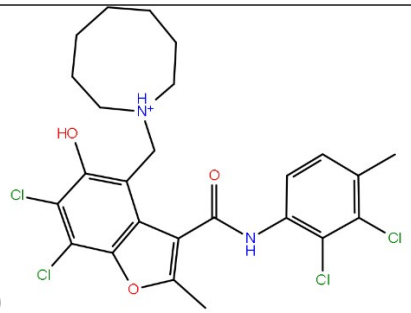
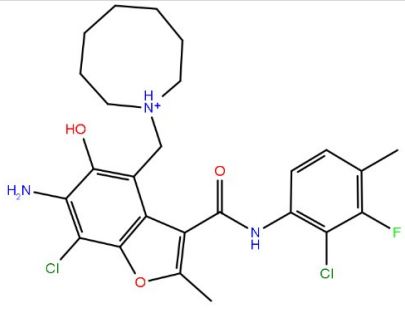
 2	-9.255	**-0.364**
 3	-9.155	-0.264
 4	-9.565	**-0.596**
 **5**	-9.487	**-0.674**
 6	-9.377	-0.486

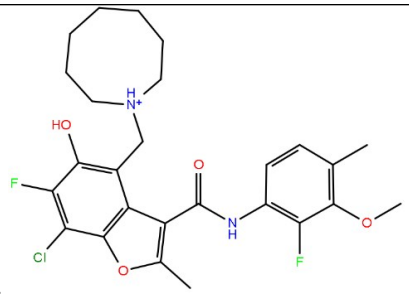
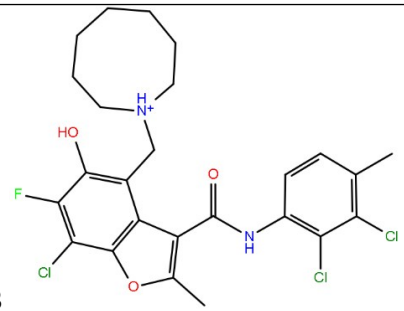
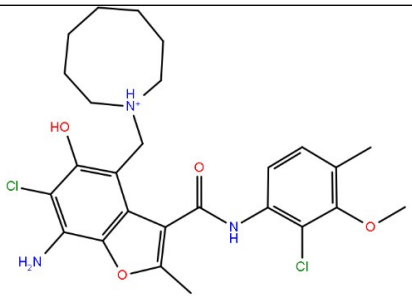
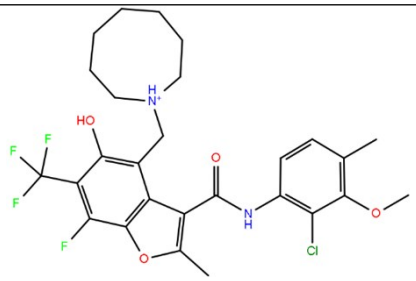
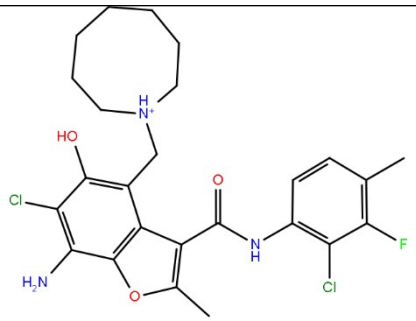
7 	-9.349	-0.458
8 	-9.309	-0.418
9 	-9.298	-0.407
10 	-9.296	-0.405
11 	-9.296	-0.405

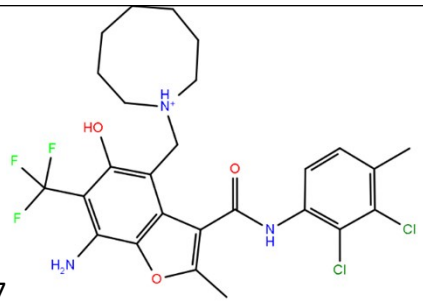
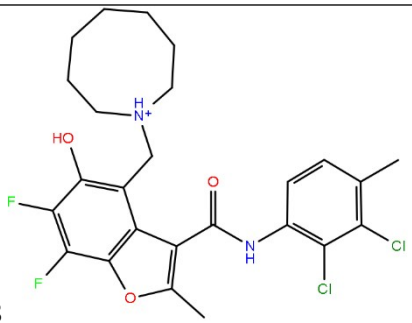
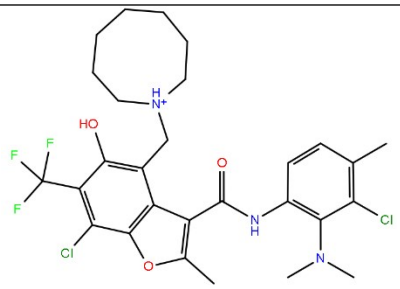
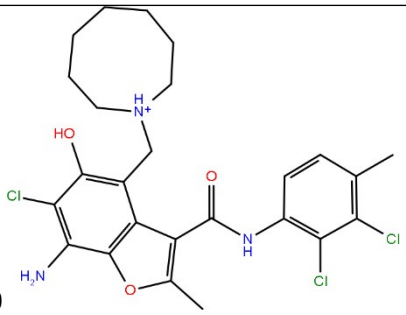
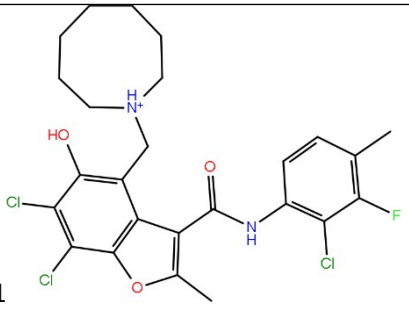
 12	-9.296	-0.405
 13	-9.264	-0.373
 14	-9.214	-0.323
 15	-9.212	-0.321
 16	-9.193	-0.302

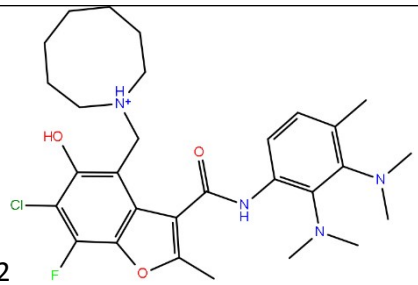
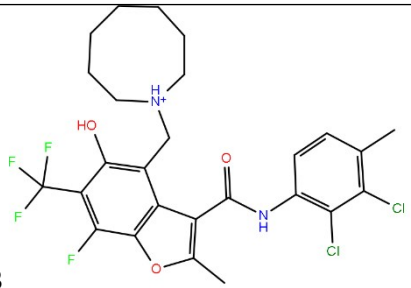
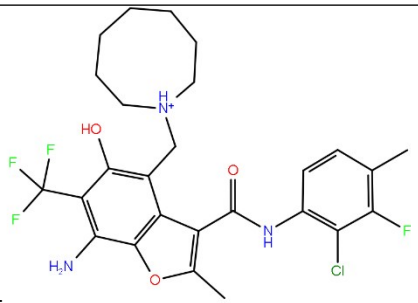
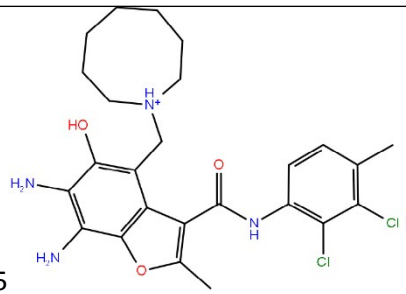
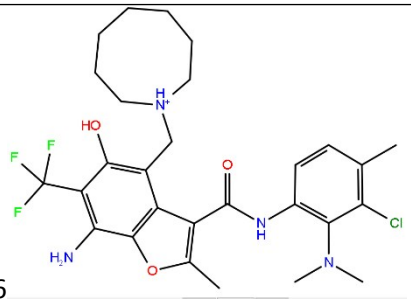
 17	-9.192	-0.301
 18	-9.184	-0.293
 19	-9.181	-0.290
 20	-9.166	-0.275
 21	-9.163	-0.272

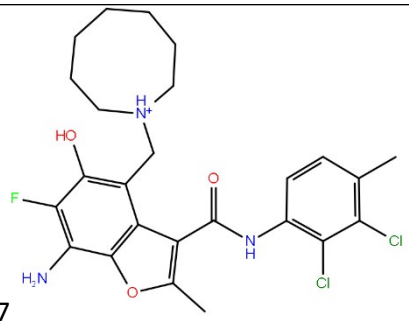
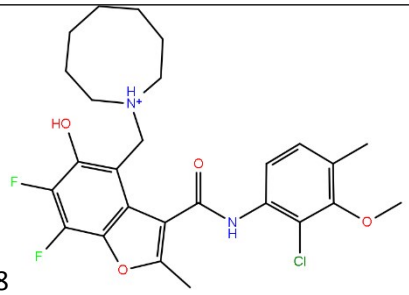
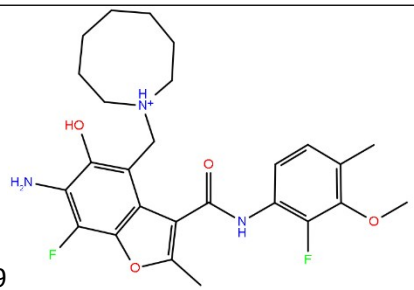
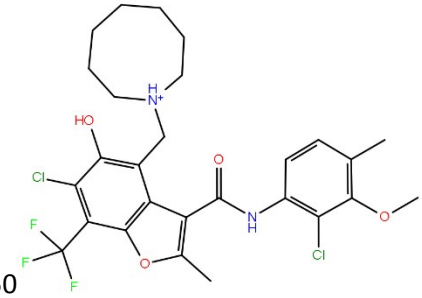
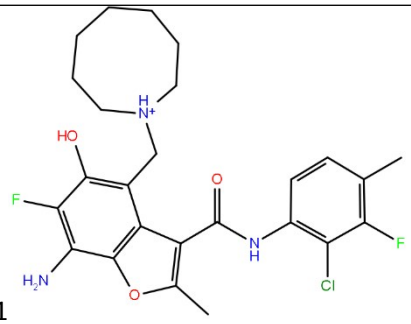
 22	-9.149	-0.258
 23	-9.146	-0.255
 24	-9.131	-0.240
 25	-9.126	-0.235
 26	-9.111	-0.220

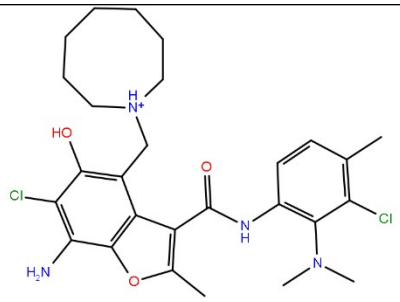
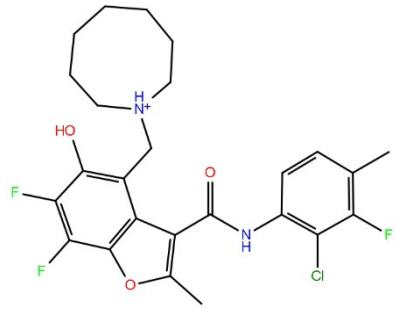
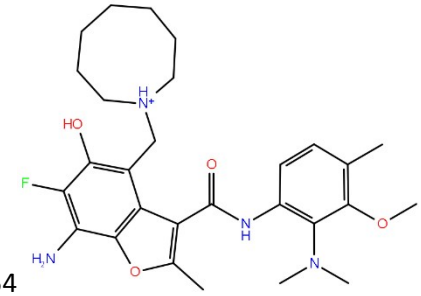
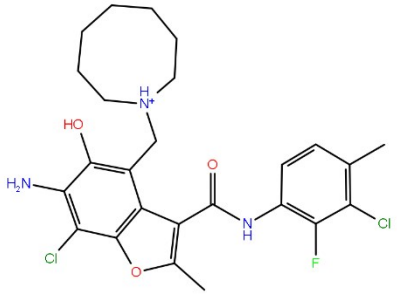
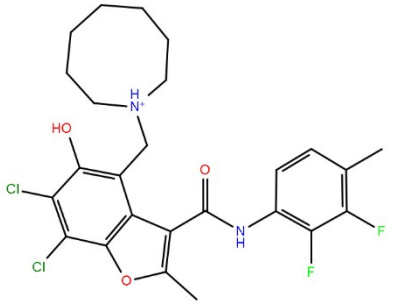
27 	-9.107	-0.216
28 	-9.098	-0.207
29 	-9.097	-0.206
30 	-9.415	-0.524
31 	-9.388	-0.497

32 	-9.381	-0.490
33 	-9.359	-0.468
34 	-9.358	-0.467
35 	-9.357	-0.466
36 	-9.317	-0.426

37 	-9.301	-0.410
38 	-9.295	-0.404
39 	-9.289	-0.398
40 	-9.286	-0.395
41 	-9.249	-0.358

 42	-9.236	-0.345
 43	-9.236	-0.345
 44	-9.228	-0.337
 45	-9.203	-0.312
 46	-9.202	-0.311

 47	-9.193	-0.302
 48	-9.192	-0.301
 49	-9.174	-0.283
 50	-9.151	-0.260
 51	-9.144	-0.253

52 	-9.144	-0.253
53 	-9.117	-0.226
54 	-9.106	-0.215
55 	-9.105	-0.214
56 	-9.096	-0.205

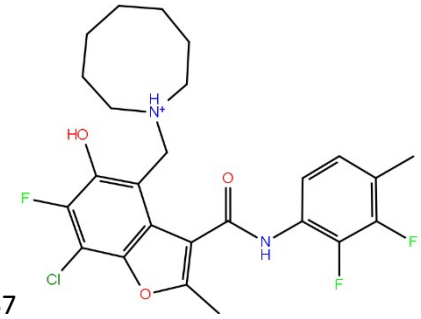
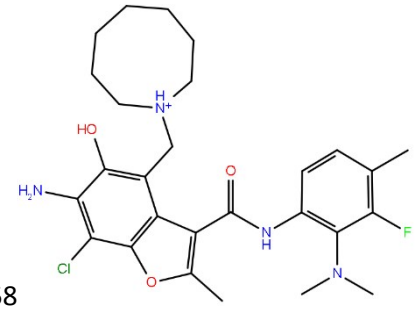
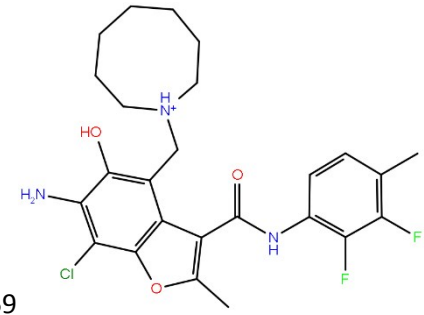
 57	-9.095	-0.204
 58	-9.095	-0.204
 59	-9.091	-0.200

Figure S21. Chemical structure of DBD1 and additional derivative compounds defined through virtual screening, including their docking scores. For DBD1, red arrows indicate substitution sites for derivatives in this table. Substitution sites (S1-S2) contain either H, F, Cl, OMe and NMe2 atoms/groups and substitution sites (S3-S4) contain either H, F, Cl, NH2 and CF3 atoms/groups. Docking scores are provided for each derivative, as well as the difference in docking scores compared to the reference DBD1 ligand. Derivative compounds are listed in decreasing docking score and increasing amount of substitution sites.

Figure S22. AMBER GAFF2 force field of the ligand DBD1 (+1) in Mol2 format.

@<TRIPOS>MOLECULE

DBD

61 64 1 0 0

SMALL

Current Charge

@<TRIPOS>ATOM

1	C1	4.0160	-2.6980	0.0670	ca	1 DBD	-0.125600
2	H31	4.5890	-3.5180	0.4560	ha	1 DBD	0.195300
3	C2	2.6690	-2.5760	0.3310	ca	1 DBD	0.187600
4	C3	1.8700	-1.5500	-0.1440	ca	1 DBD	-0.107100
5	C4	2.4500	-0.5520	-0.9520	ca	1 DBD	-0.035800
6	C5	3.8100	-0.6730	-1.2180	ca	1 DBD	0.281700
7	C6	4.5850	-1.7220	-0.7170	ca	1 DBD	-0.336400
8	H32	5.6330	-1.7650	-0.9540	ha	1 DBD	0.198500
9	C7	0.5360	-1.8800	0.3590	cc	1 DBD	-0.099500
10	C8	0.6780	-3.0180	1.0800	cd	1 DBD	0.281700
11	O9	1.9420	-3.4460	1.0710	os	1 DBD	-0.266500
12	C10	1.6700	0.5530	-1.6210	c3	1 DBD	-0.055000
13	H33	2.2250	0.9480	-2.4570	hx	1 DBD	0.117100
14	H34	0.7230	0.1830	-1.9790	hx	1 DBD	0.117100
15	N11	1.3320	1.7230	-0.7290	n4	1 DBD	-0.047200
16	H61	0.7240	1.3180	-0.0260	hn	1 DBD	0.213800
17	C12	2.5380	2.3390	-0.0570	c3	1 DBD	-0.085000
18	H35	3.4040	1.8360	-0.4480	hx	1 DBD	0.111100
19	H36	2.5950	3.3690	-0.3730	hx	1 DBD	0.111100
20	C13	2.4900	2.2370	1.4670	c3	1 DBD	-0.052800
21	H37	2.0660	1.2780	1.7540	hc	1 DBD	0.053300
22	H38	3.5180	2.2210	1.8140	hc	1 DBD	0.053300

23	C14	1.7680	3.3800	2.1870	c3	1 DBD -0.059200
24	H39	1.8590	3.1880	3.2510	hc	1 DBD 0.046100
25	H40	2.3080	4.3070	2.0050	hc	1 DBD 0.046100
26	C15	0.2810	3.5970	1.8700	c3	1 DBD -0.038900
27	H41	-0.2550	2.6520	1.9270	hc	1 DBD 0.025600
28	H42	-0.1160	4.2030	2.6760	hc	1 DBD 0.025600
29	C16	-0.0580	4.3220	0.5450	c3	1 DBD -0.051400
30	H43	-0.8750	5.0040	0.7500	hc	1 DBD 0.050400
31	H44	0.7700	4.9540	0.2330	hc	1 DBD 0.050400
32	C17	-0.5370	3.4490	-0.6270	c3	1 DBD -0.023900
33	H45	-1.2610	2.7250	-0.2700	hc	1 DBD 0.044900
34	H46	-1.0680	4.0870	-1.3280	hc	1 DBD 0.044900
35	C18	0.4960	2.7210	-1.4820	c3	1 DBD -0.186800
36	H47	1.1780	3.4020	-1.9720	hx	1 DBD 0.131400
37	H48	-0.0300	2.1720	-2.2490	hx	1 DBD 0.131400
38	C19	-0.2510	-3.8480	1.9020	c3	1 DBD -0.137400
39	H49	0.2190	-4.0660	2.8530	hc	1 DBD 0.076700
40	H50	-0.4450	-4.7940	1.4080	hc	1 DBD 0.076700
41	H51	-1.1880	-3.3420	2.0820	hc	1 DBD 0.076700
42	C20	-0.6960	-1.0670	0.2240	c	1 DBD 0.191300
43	N21	-1.8390	-1.7400	0.0240	n	1 DBD -0.066600
44	H52	-1.7630	-2.7100	-0.1870	hn	1 DBD 0.209600
45	C22	-3.1340	-1.1590	-0.1260	ca	1 DBD 0.004600
46	C23	-3.9280	-1.5650	-1.1820	ca	1 DBD -0.144900
47	H53	-3.5520	-2.2760	-1.8980	ha	1 DBD 0.133600
48	C24	-5.2100	-1.0560	-1.3230	ca	1 DBD -0.194000
49	H54	-5.8160	-1.3870	-2.1470	ha	1 DBD 0.164600
50	C25	-5.7150	-0.1270	-0.4250	ca	1 DBD 0.091000
51	C26	-4.8960	0.2730	0.6290	ca	1 DBD -0.111600

```
      52 H55       -5.2640    0.9870    1.3450 ha       1 DBD     0.138000
      53 C27       -3.6230   -0.2390    0.7900 ca       1 DBD    -0.218400
      54 H56       -3.0150    0.0740    1.6160 ha       1 DBD     0.170300
      55 C28       -7.1120    0.4290   -0.5660 c3       1 DBD    -0.225600
      56 H57       -7.1040    1.5140   -0.5570 hc       1 DBD     0.085100
      57 H58       -7.7440    0.1000    0.2530 hc       1 DBD     0.085100
      58 H59       -7.5730    0.1050   -1.4910 hc       1 DBD     0.085100
      59 O29        4.3760    0.2860   -1.9900 oh       1 DBD    -0.579100
      60 H60        5.2700    0.0640   -2.2180 ho       1 DBD     0.458700
      61 O30       -0.6510    0.1460    0.2950 o        1 DBD    -0.317000
@<TRIPOS>BOND
     1    1    2 1
     2    1    3 ar
     3    1    7 ar
     4    3    4 ar
     5    3   11 1
     6    4    5 ar
     7    4    9 1
     8    5    6 ar
     9    5   12 1
    10    6    7 ar
    11    6   59 1
    12    7    8 1
    13    9   10 2
    14    9   42 1
    15   10   11 1
    16   10   38 1
    17   12   13 1
    18   12   14 1
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19 12 15 1

20 15 16 1

21 15 17 1

22 15 35 1

23 17 18 1

24 17 19 1

25 17 20 1

26 20 21 1

27 20 22 1

28 20 23 1

29 23 24 1

30 23 25 1

31 23 26 1

32 26 27 1

33 26 28 1

34 26 29 1

35 29 30 1

36 29 31 1

37 29 32 1

38 32 33 1

39 32 34 1

40 32 35 1

41 35 36 1

42 35 37 1

43 38 39 1

44 38 40 1

45 38 41 1

46 42 43 1

47 42 61 2

48 43 44 1

49 43 45 1

50 45 46 ar

51 45 53 ar

52 46 47 1

53 46 48 ar

54 48 49 1

55 48 50 ar

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57 50 55 1

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59 51 53 ar

60 53 54 1

61 55 56 1

62 55 57 1

63 55 58 1

64 59 60 1

@<TRIPOS>SUBSTRUCTURE

1 DBD 1 TEMP 0 **** **** 0 ROOT