Table S1. ADME properties predicted by QikProp and Dockig Score of Chelerythrine and 14 Chelerythrine like molecules found in Supernatural drug database.

SN. No	S	MW	QPlogP o/w	Q PlogS	Q PPCaco	Q PlogBB	PHOA	RO 5	Glide Dock Score
Chelerythrine (CHE)	2	349.385	4.591	-4.969	9514.447	0.426	100	0	-5.259
SN00288441(ONE)	2	379.412	4.34	-4.809	9729.842	0.375	100	0	-7.645
SN00375322(TWO)	1	349.385	4.257	-4.360	9729.750	0.436	100	0	-8.117
SN00155937(THREE)	2	349.385	4.018	-4.120	9487.679	0.426	100	0	-7.796
SN00361551	2	379.412	4.609	-4.991	9559.997	0.368	100	0	-7.55
SN00288491	3	393.438	4.18	-6.504	9906.038	-0.787	100	0	-7.53
SN00401299	0	335.359	3.716	-4.320	4236.699	0.110	100	0	-7.47
SN00388080	2	379.412	4.146	-4.891	9705.696	0.374	100	0	-7.44
SN00286890	2	393.395	3.525	-3.588	9678.933	0.434	100	0	-7.41
SN00000050	2	333.343	3.839	-3.990	9503.988	0.548	100	0	-7.36
SN00339333	2	363.369	3.519	-3.717	9740.327	0.497	100	0	-7.08
SN00276392	1	365.385	3.479	-4.042	4136.874	0.086	100	0	-6.97
SN00160090	2	363.369	3.941	-4.187	9621.772	0.492	100	0	-6.9
SN00160089	2	379.412	4.691	-5.158	9616.731	0.370	100	0	-6.78
SN00126678	4	189.213	2.558	-2.282	9631.381	0.554	100	0	-6.73

SN No.= Supernatural drug database ID

S (STARS) = Number of property/descriptor values falling outside the 95% range of similar values for known drugs. Recommended value 0-5.

MW = Molecular weight

QPlogPo/w = Predicted octanol / water partition coefficient. Recommended values –2.0 – 6.5.

QPlogS = Predicted aqueous solubility, log S. Recommended values –6.5 – 0.5.

QPPCaco = Predicted apparent Caco-2 cell permeability in nm/sec. Recommended values <25 poor, >500 great.

QPlogBB = Predicted brain/blood partition coefficient. Recommended values –3.0 – 1.2.

PHOA= Predicted human oral absorption on 0 to 100% scale.Recommended values >80% is high <25% is poor

RO5= Rule of Five,The rules are: mol_MW < 500, QPlogPo/w < 5, donorHB ≤ 5, and accptHB ≤ 10.

White color rows: Compounds selected for further analysis

Gray color rows: Compounds are not studied further

* The scores given are approximate values as predicted by the software and not measured experimentally.

Captions for Supplementary Fig.:

Fig. S1. Comparison of conformation of Chelerythrine bound to *Pu27* in its initial docked pose with that of the conformation obtained after 50 ns simulation.

Fig. S2. Comparison of conformation of THREE bound to *Pu27* in its initial docked pose with that of the conformation obtained after 50 ns simulation.

Fig. S3. Comparison of conformation of ONE bound to *Pu27* in its initial docked pose with that of the conformation obtained after 50 ns simulation.

Fig. S4. Comparison of conformation of TWO bound to *Pu27* in its initial docked pose with that of the conformation obtained after 50 ns simulation.

Fig. S5. Water grid density map of *Pu27* in different complexation states: (A) CHE-complex, (B) ONE-complex, (C) unbound PU27, (D) TWO-complex, (E) THREE-complex.

Fig. S6. Illustration of total number of water molecules in the inner and outer shell of ligand per unit time (ns), inner shell and outer shell represent the area within the radius of 3.4 Å and 5 Å from the centroid of the ligand respectively. (A) Number of water molecules in inner shell of CHE and ONE, (B) Number of water molecules in outer shell of CHE and ONE, (C) Number of water molecules in inner shell of TWO and THREE, (D) Number of water molecules in outer shell of TWO and THREE

Fig. S7. Porcupine plots of first (A-E) and second eigenvectors (F-J) of ONE-complex. Time frames are mentioned for respective plots. Blue color is for quadruplex structure and magenta color is for compound ONE. (Images are prepared in PyMOL)
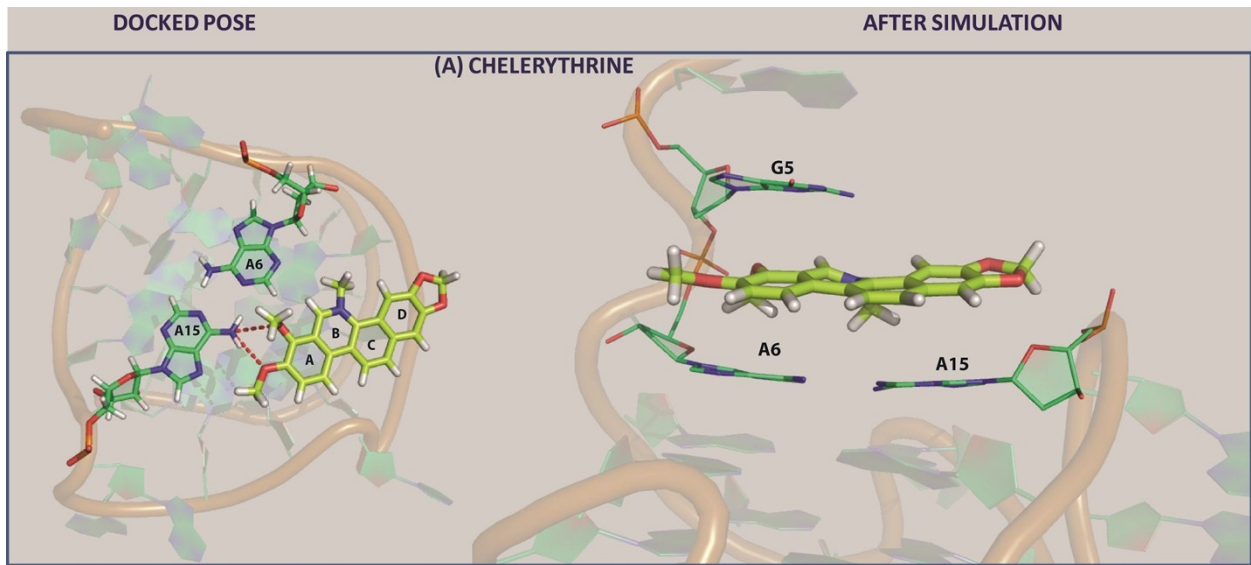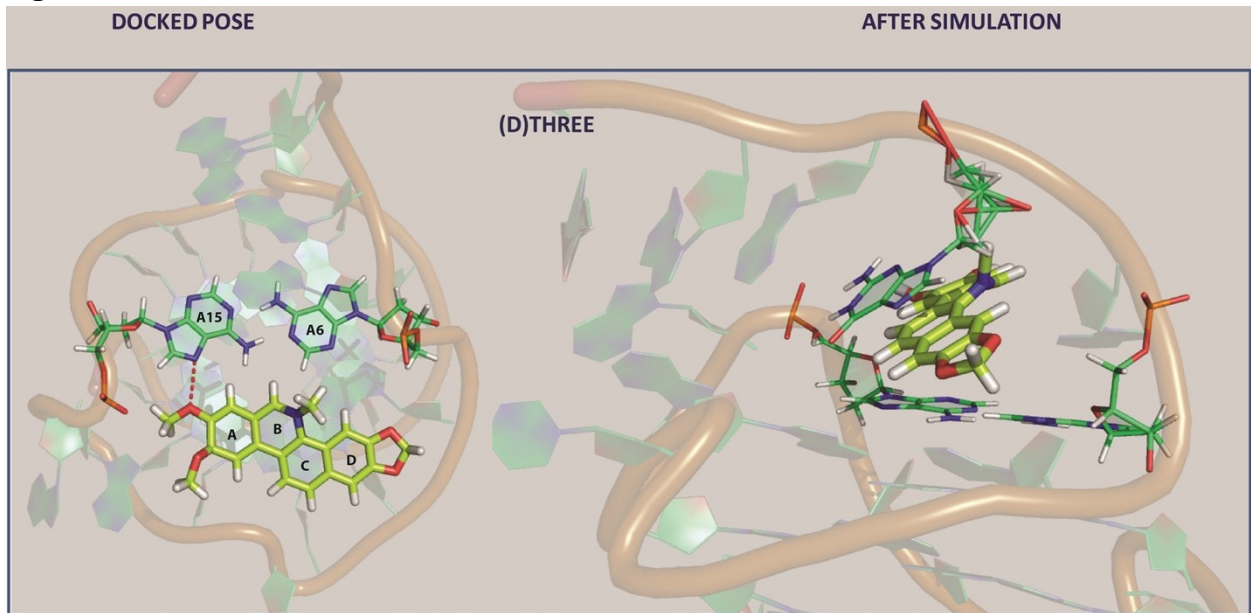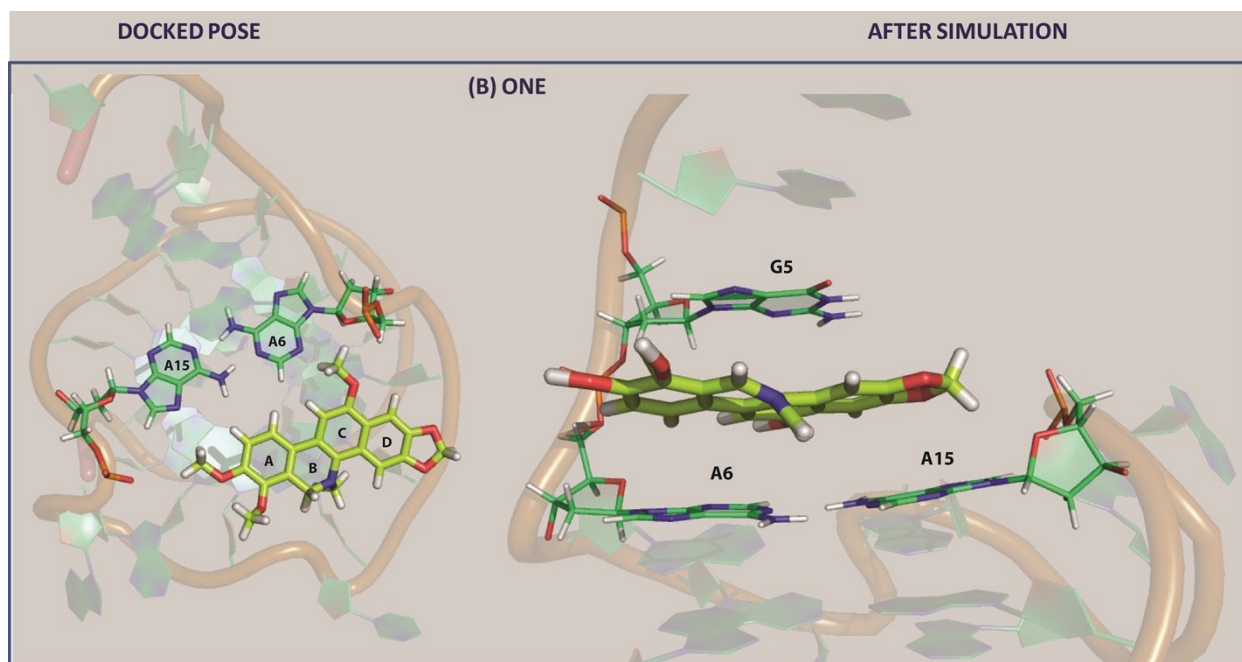
Fig. S1

DOCKED POSE   **AFTER SIMULATION**

(A) CHELERYTHRINE

Fig. S2

DOCKED POSE   **AFTER SIMULATION**

(D)THREE

Fig. S3

DOCKED POSE | AFTER SIMULATION

(B) ONE

Fig. S4

DOCKED POSE | AFTER SIMULATION

(C) TWO

Fig. S5

(A) Pu27-CHE   (B) Pu27-ONE   (C) Pu27   (D) Pu27-TWO   (E) Pu27-TWO

Fig. S6

Fig. S7

(A) 0-10 ns   (B) 11-20 ns   (C) 21-30 ns   (D) 31-40 ns   (E) 41-50 ns

(F) 0-10 ns   (G) 11-20 ns   (H) 21-30 ns   (I) 31-40 ns   (J) 41-50 ns