Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary information:

Table S1: Calculated Binding Energy of Ligand 1, 2 and 3 with random DNA sequences as ligand receptor sites.

Duplex Receptor	**DNA Sequence**	**Binding Energy (Kcal/mole)**		
		Ligand 1	**Ligand 2**	**Ligand 3**
Receptor 1	ATATTAATAT	-10.3	-6.8	-5.2
Receptor 2	GCGCCGGCGC	-8.3	-6.8	-5.7
Receptor 3	GTCATATCTA	-10.3	-6.7	-5.2
Receptor 4	ACGTAGCTTC	-10.1	-6.8	-5
Receptor 5	TAAGAGTGCG	-8.3	-7.1	-5.5
Receptor 6	GACACCAGCG	-10	-7	-6.5
Receptor 7	ATGGGCTGTG	-10.1	-6.8	-5.1
Receptor 8	GAAGGCCCAACAACT	-9.7	-7	-5.2
Receptor 9	ACGGACCTAGGTGAG	-10.1	-6.9	-5.2
Receptor 10	CAGAGTCAACTCGAG	-10.1	-7.2	-6

Table S2: Binding Energies of best five docking modes determined by Autodock Vina simulation between Ligand 1, 2, 3 and Dickerson Dodecamer, DNA Pol I

Ligand	Best Five Docking Mode Binding Energies (kcal/mole)									
	with Dickerson Dodecamer					with DNA Pol I				
Ligand 1	9.9	9.8	9.7	9.2	9.2	10.6	9.5	9	9	8.8
Ligand 2	8.1	8	7.9	7.8	7.8	9.6	9.3	9.2	9.2	8.7
Ligand 3	6.3	6.2	6.1	6	5.9	6.4	6.3	6.3	6.3	6.2

Supplementary information and figures:

1. Synthesis and characterization of complexes 1, 2 and 3

Chemicals for the synthesis of the Ligand 1, 2 and 3 and for Complex 1, 2 and 3 were procured from standard commercial sources (Sigma Aldrich- USA, S.D. Fine chemicals - India, Invitrogen - India) and all were used directly without further purification. A Thermo Finnigan FLASH EA 1112 CHNS analyzer was used to perform Elemental analyses. Perkin-Elmer Lambda 35 was used for the infrared spectroscopy. For absorption spectra, Perkin–Elmer Lambda 650 was used.

1.1 Synthesis of Complex 1

Ligand 1 (0.718 g, 2.0 mmol) dissolved in a methanol solution (25 mL), was added dropwise to a methanolic solution (25 mL) of $FeCl_2$ (0.125 g; 1.0 mmol). The stirring of the reaction mixture was continued to obtain a deep purple colored solution. The solvent was evaporated and the residue was washed with cold ethanol several times, followed by cold diethyl ether, and finally dried in vacuum over anhydrous P_4O_{10}. The synthesized complexes were characterized by CHN analysis, mass spectrometry, infrared spectroscopy (FT-IR) and UV-visible spectroscopy. The major results are summarized below:

Complex 1: $[Fe(pydppz)_2]Cl_2$: [Yield: 0.76 g, 90%] Analysis: Calculated for $C_{46}H_{26}Cl_2FeN_{10}$: C, 65.34; H, 3.10; N, 16.57. Found: C, 65.67; H, 3.31; N, 16.55. ESIMS in 10% aqueous MeOH: m/z: 387.63 $[M\text{-}2Cl]^{2+}$. IR/ cm^{-1}: 3045(w), 2912(w), 1607(s), 1539(w), 1480(w), 1401(s), 1343(vs), 1254(m), 1118(m), 1041(m), 725(s), 590(w) (br, broad; s, strong; vs, very strong, m, medium; w, weak). UV-vis (DMF) [λ_{max}/ nm (ε/ M^{-1} cm^{-1})]: 556 (4250), 388sh (20740), 367 (30690), 289 (62320) (sh, shoulder peak).

1.2. Synthesis of Complex 2 and 3:

Complexes 2 and 3 were prepared by following a general synthetic procedure. Briefly, methanolic solutions of ligands (0.41 g, 1.0 mmol for Ligand 2; 0.29 g, 1.0 mmol for Ligand 3) were added to methanolic solutions of ferric chloride (0.16 g, 1.0 mmol). The solution was stirred for 30 min until the precursor complex [Fe(L)Cl_3] (L = Ligand 2 or Ligand 3) precipitated, which was filtered thereafter and air dried before calculating the yield [Yield: 0.52 g (90%) for Ligand 2; 0.39 g (85%) for Ligand 3]. A solution of benzhydroxamic acid (0.14 g, 1.0 mmol) and triethylamine(0.10 g, 1.0 mmol), in methanol, was added drop wise to solution of the precursor complex (L: 0.57 g, 1.0 mmol for Ligand 2; 0.45 g, 1.0 mmol for Ligand 3), to obtain a deep purple colored solution. The solvent was evaporated slowly to get a solid. Once the solid residue was isolated, it was thoroughly washed with diethyl ether and dried in a vacuum over P_4O_{10} to obtain the final complex.[10] The detailed synthesis schemes of the three iron complexes are depicted in Supplementary **Figures S1A, B and C**. We briefly present below the CHN analysis, UV-visible, FT-IR, and mass spectral characterization of these complexes.

Complex 2: [Fe(BHA)(pydpa)Cl]Cl.H_2O: Yield: 0.54 g (79%). Analysis: Calculated for $C_{36}H_{31}Cl_2FeN_4O_3$ (MW: 694.41): C, 62.27; H, 4.50; N, 8.07. Found: C, 62.50; H, 4.76; N, 8.21%. ESIMS in MeOH, m/z: 636.27 $[M\text{-}2Cl^- + MeO^-]^+$, 604.47 $[M\text{-}2Cl^-\text{-}H^+]^+$, 640.07 $[M\text{-}Cl^-]^+$. IR (solid phase, cm1): 3377 (br), 2933 (m), 2666 (m), 1603 (s), 1490 (s), 1448 (s), 1345 (m), 1140 (m), 1070 (m), 1030 (m), 913 (m), 850 (s), 768 (s), 685 (s), 553 (w), 490 (w). UV–Vis (DMF) λ_{max}, nm (ε, M^{-1} cm^{-1}): 466 (1530), 345 (22,100), 328 (15,800), 315 (8340), 277 (24,190), 267 (18,480).

Complex 3: [Fe(BHA)(phdpa)Cl]Cl.H_2O: Yield: 0.42g(75%). Analytical Calculation for $C_{26}H_{27}Cl_2FeN_4O_3$ (MW: 570.27): C, 54.76; H, 4.77; N, 9.82. Found: C, 54.49; H, 5.07; N, 9.53%. ESIMS in MeOH, m/z: 512.17 $[M–2Cl^- + MeO^-]^+$, 480.52 $[M-2Cl^- -H^+]^+$. IR (solid phase, cm^{-1}): 3397 (br), 2944 (m), 2600 (m), 2490 (m), 1604 (s), 1480 (s), 1438 (s), 1345 (m), 1150 (s), 1026 (s), 913 (s), 810 (s), 760 (s), 706 (s), 540 (w), 479 (w). UV–Vis (DMF) λ_{max}, nm (ε, M^{-1} cm^{-1}): 454 (1420), 268 (6380).

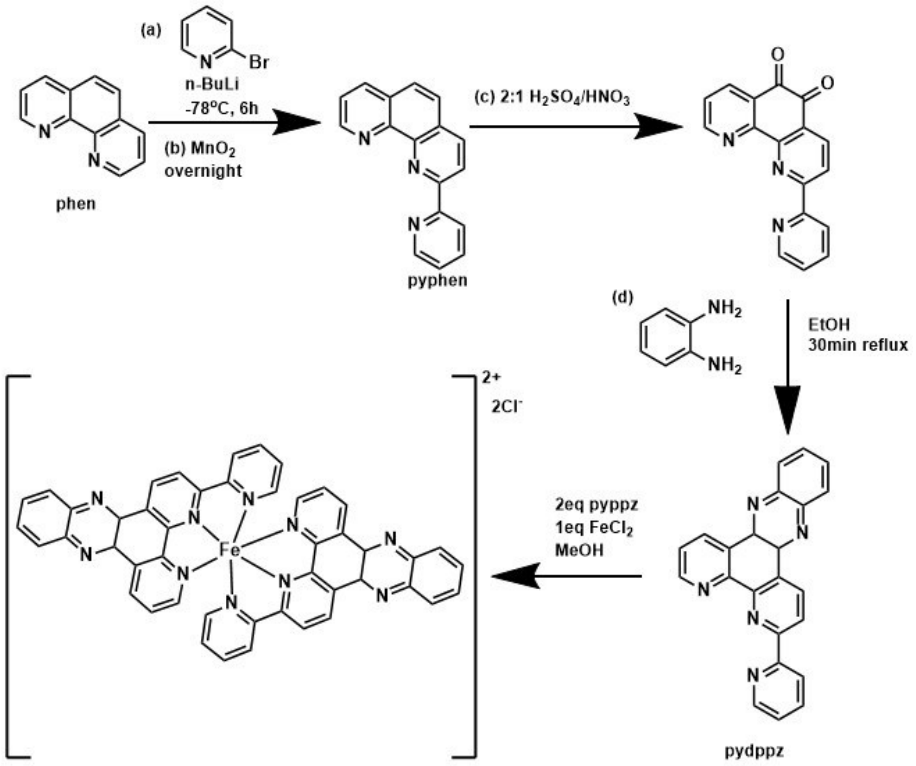


Fig. S1A: Synthesis scheme for complex1. (a) reaction done in dry THF, followed by basic alumina column chromatographic purification using eluent THF/hexane (1:5) (c) after reaction, reaction mixture was normalized with NaOH and purified by silica column chromatography (100-200 mesh) with DCM as eluent.

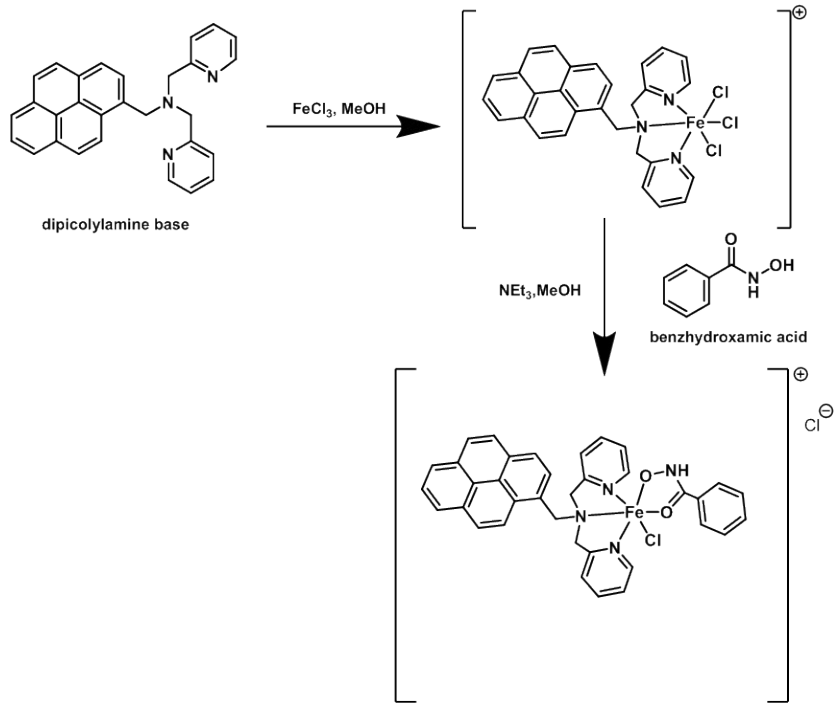


Fig. S1B: Synthesis scheme for complex2

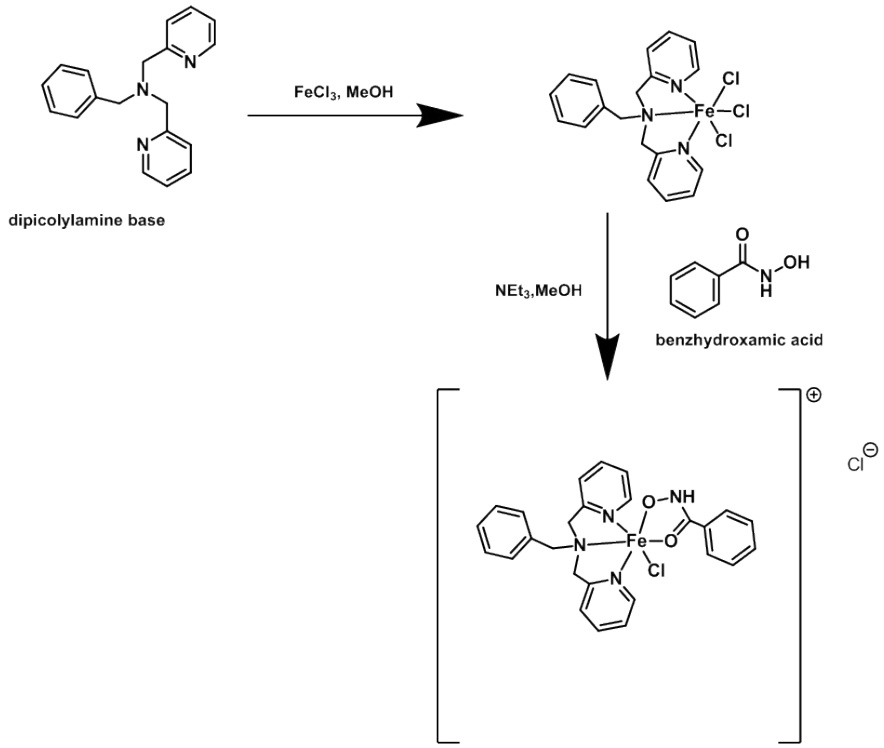


Fig. S1C: Synthesis scheme for complex3

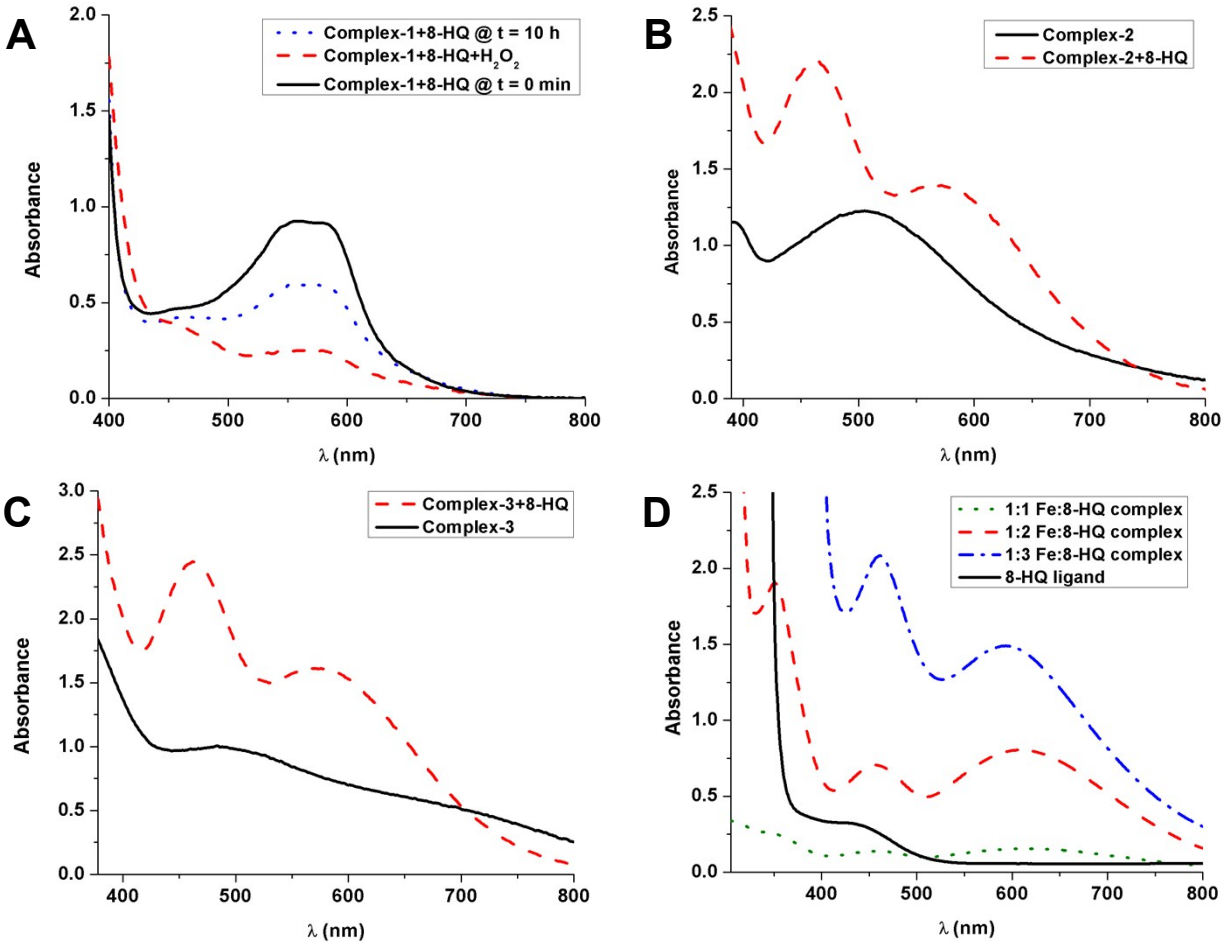


Fig. S2: Ligand exchange reactions of the three iron complexes (A-C) with 8-hydroxyquinoline (8-HQ). (D) UV-Vis absorption spectra of Fe: 8-HQ complexes in 1:3, 1:2 and 1:1 mole ratios.

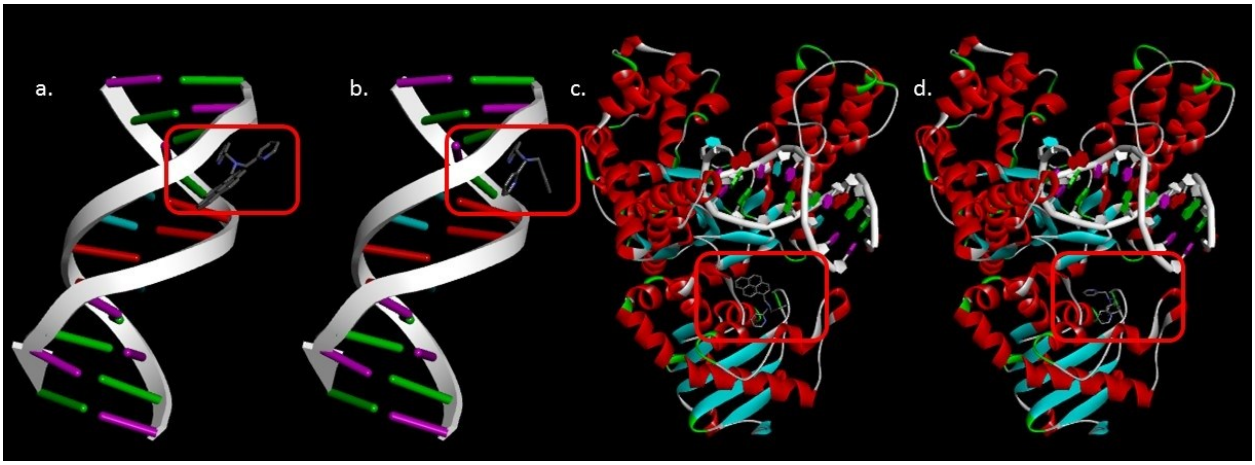
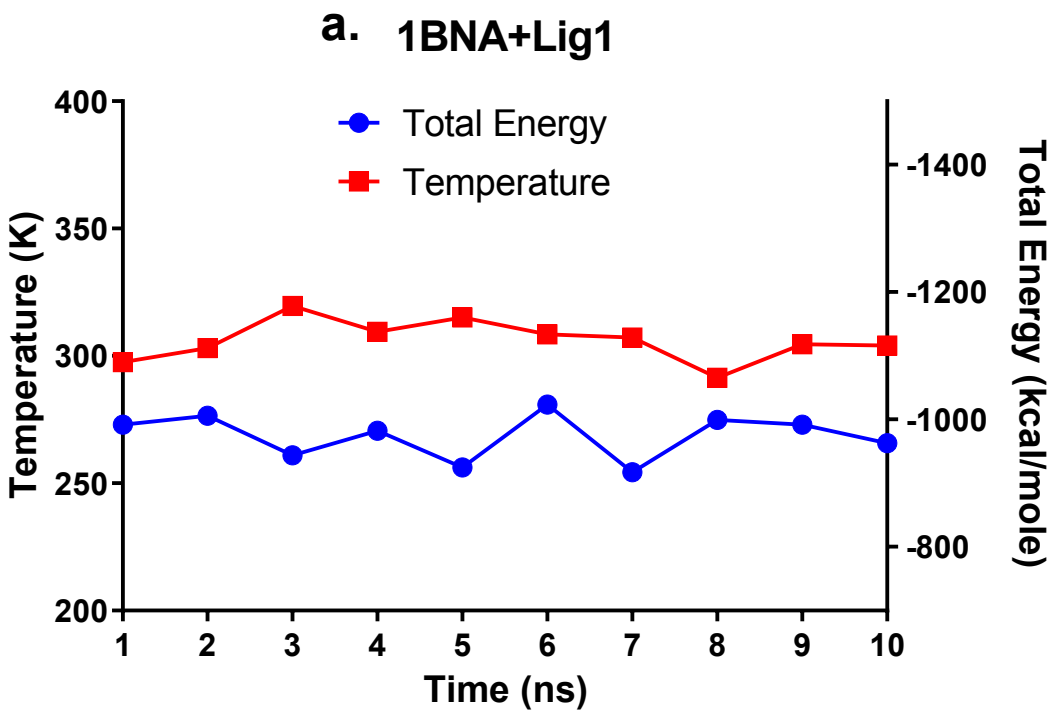
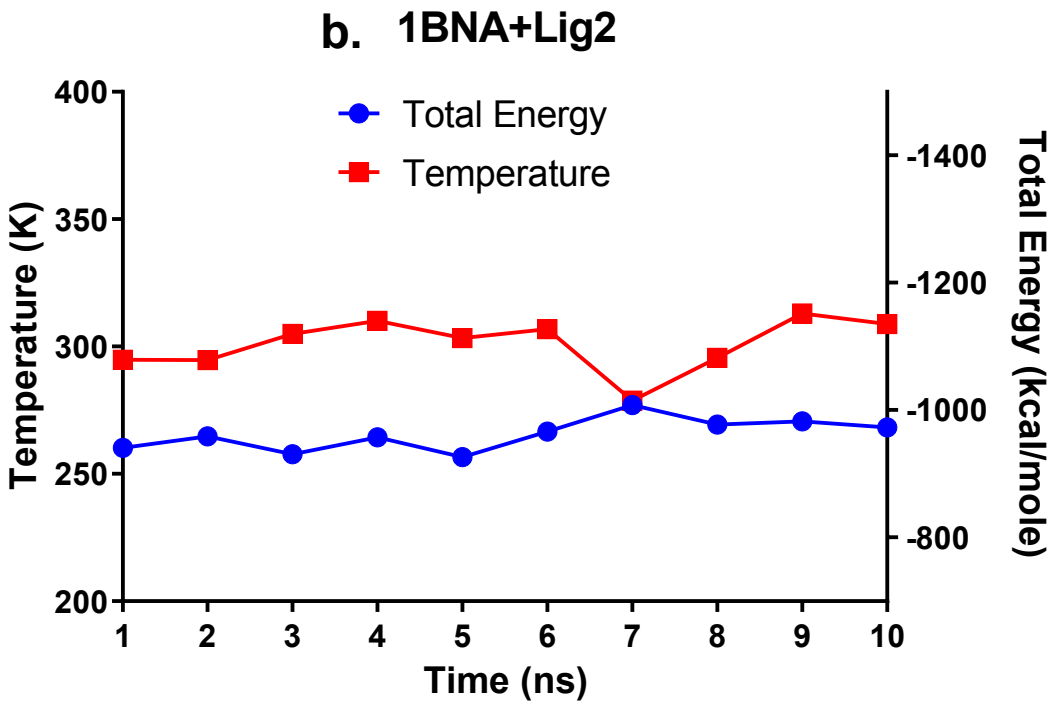


Fig. S3: Best binding mode of Dickerson dodecamer (1BNA) with a. Ligand2 and b. Ligand3. Best binding mode of DNA Pol I (3EYZ) with c. Ligand2 and d. Ligand3.


a. 1BNA+Lig1
Total Energy
Temperature
Temperature (K)
Total Energy (kcal/mole)
Time (ns)
400
350
300
250
200
-1400
-1200
-1000
-800
1
2
3
4
5
6
7
8
9
10


b. 1BNA+Lig2
Total Energy
Temperature
Temperature (K)
Total Energy (kcal/mole)
Time (ns)
400
350
300
250
200
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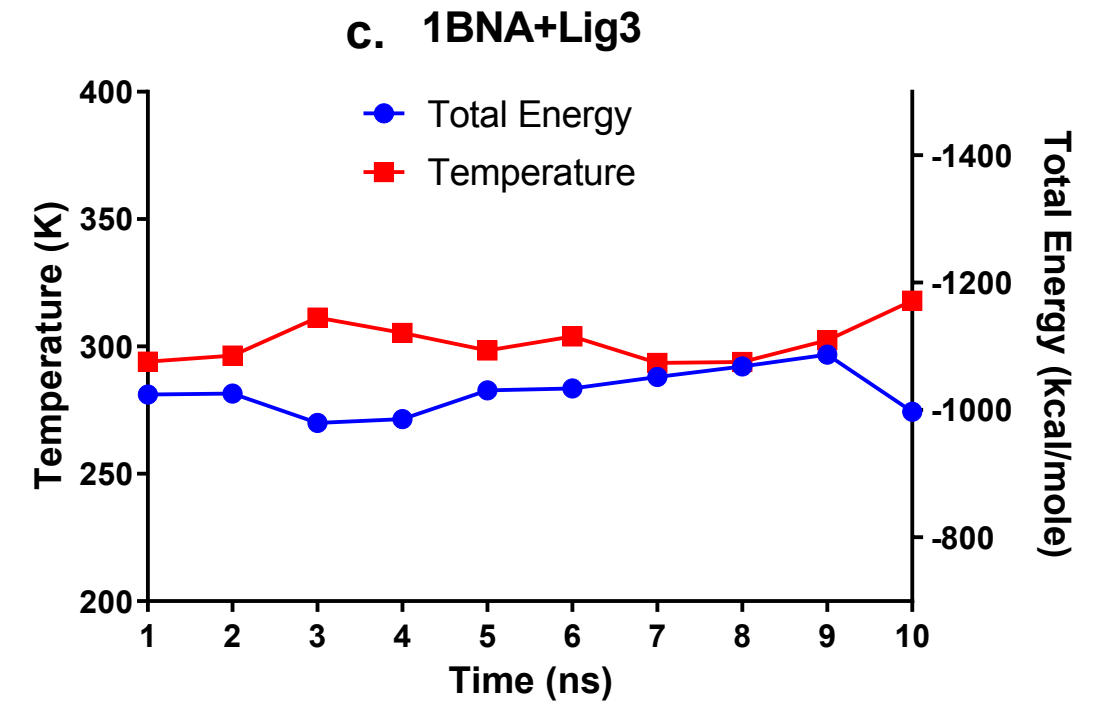
-1000
-800
1
2
3
4
5
6
7
8
9
10


c. 1BNA+Lig3
Total Energy
Temperature
Temperature (K)
Total Energy (kcal/mole)
Time (ns)
400
350
300
250
200
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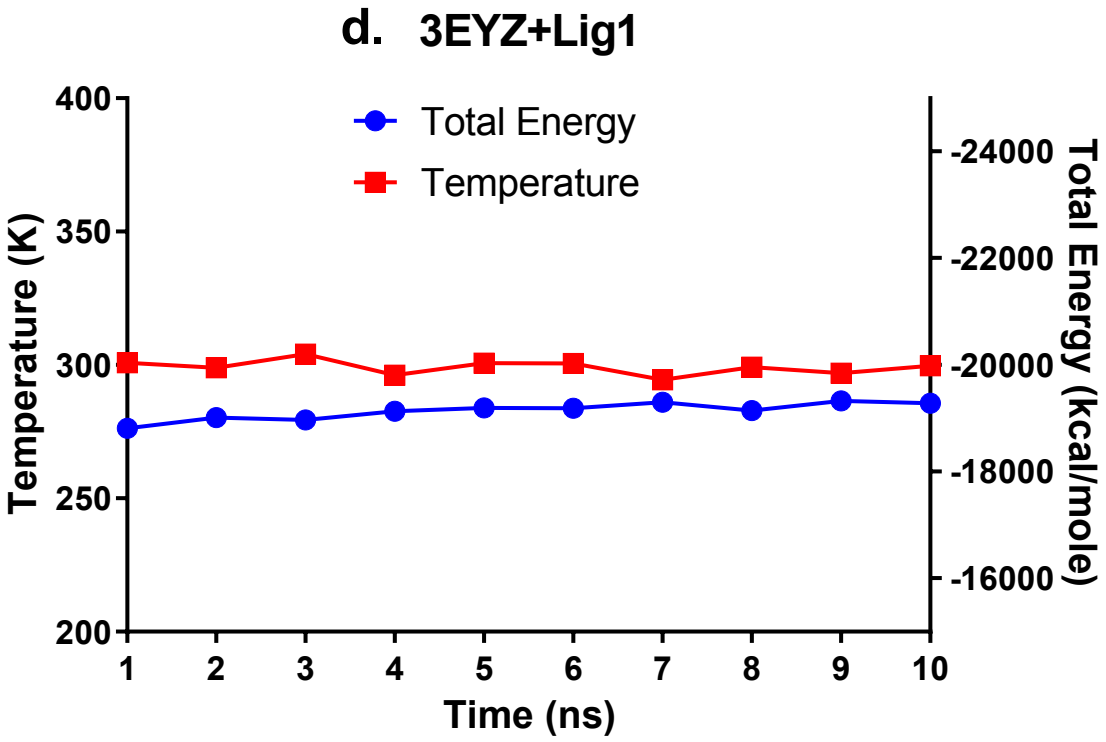
-800
1
2
3
4
5
6
7
8
9
10


d. 3EYZ+Lig1
Total Energy
Temperature
Temperature (K)
Total Energy (kcal/mole)
Time (ns)
400
350
300
250
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-20000
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1
2
3
4
5
6
7
8
9
10

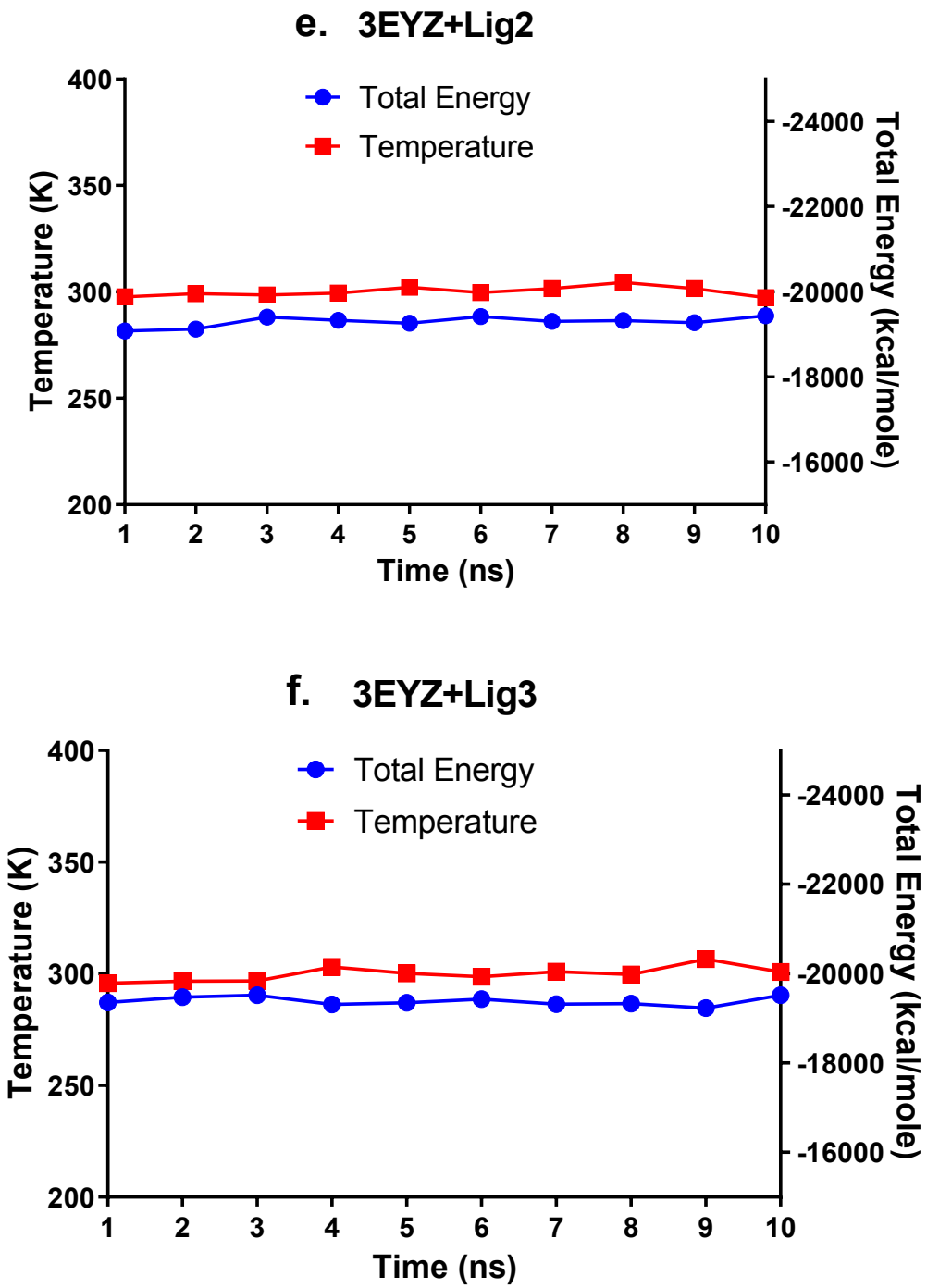


Fig S4: Molecular Dynamics: The best binding modes from docking results were subjected to a standard molecular dynamics cascade prior to a 10ns NAnoscale Molecular Dynamics (NAMD) simulation with NVT model and time step of 2fs. Here we report 'Total Energy vs Time' and 'Temperature vs Time' graphs as an evidence of stable simulation. a. 1BNA+Ligand1, b. 1BNA+Ligand2, c. 1BNA+Ligand3, d. 3EYZ+Ligand1, e. 3EYZ+Ligand2 and f. 3EYZ+Ligand3 (1BNA- Dickerson Dodecamer, 3EYZ-DNA Pol I).

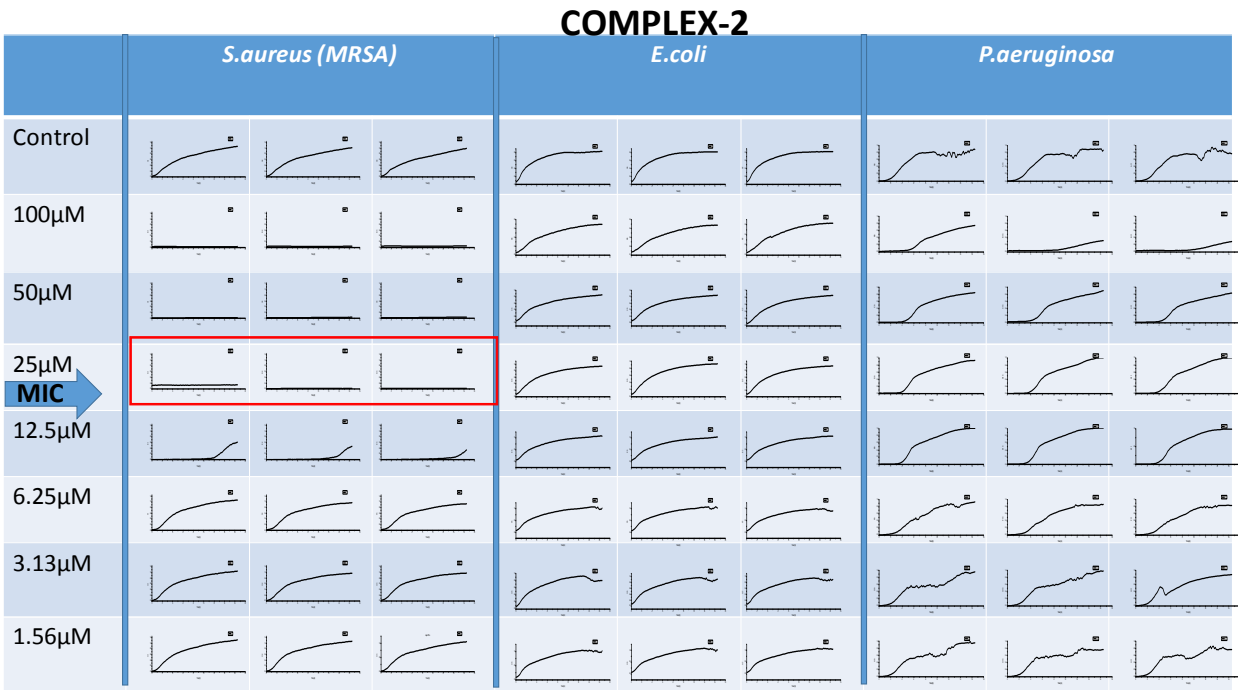


Fig. S5: MIC determination of complex-2 against representative bacterial strains. For each graph, the X-axis scale corresponds to time (0 – 18 h) and the Y-axis scale corresponds to optical density (OD @ 600 nm) ranging from 0 – 1.25 (a.u), as indicated in the inset below.

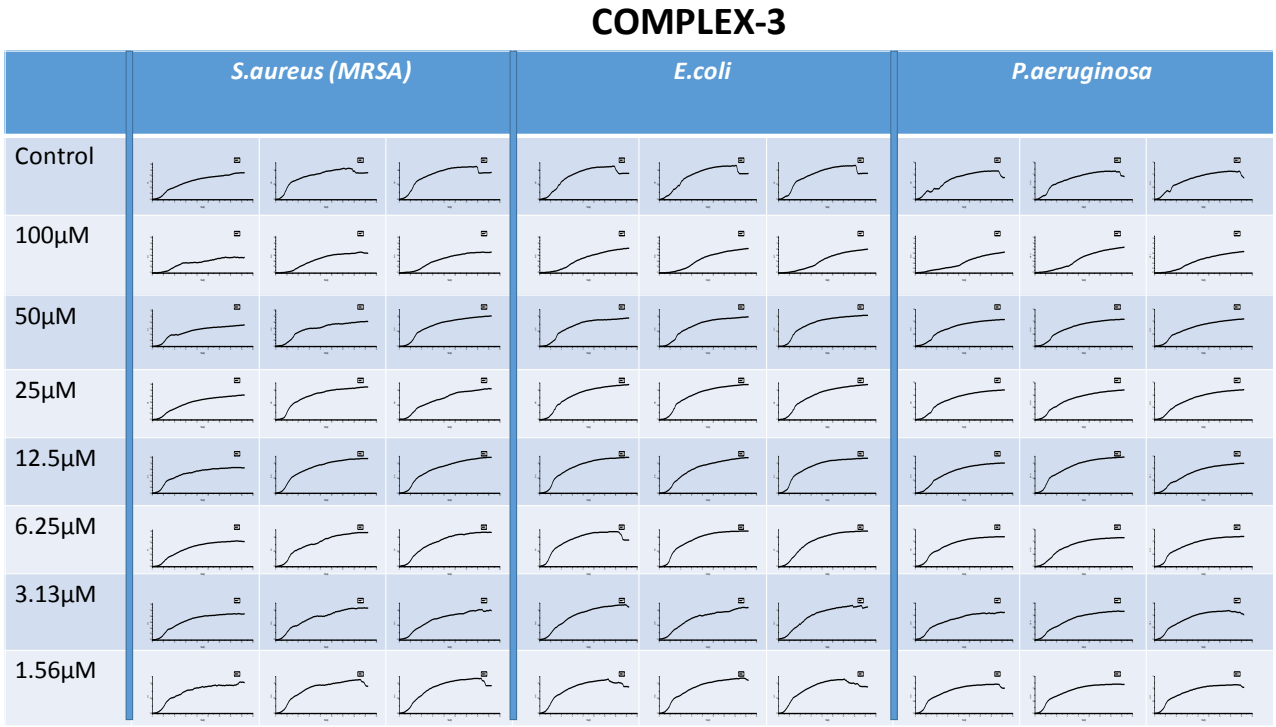
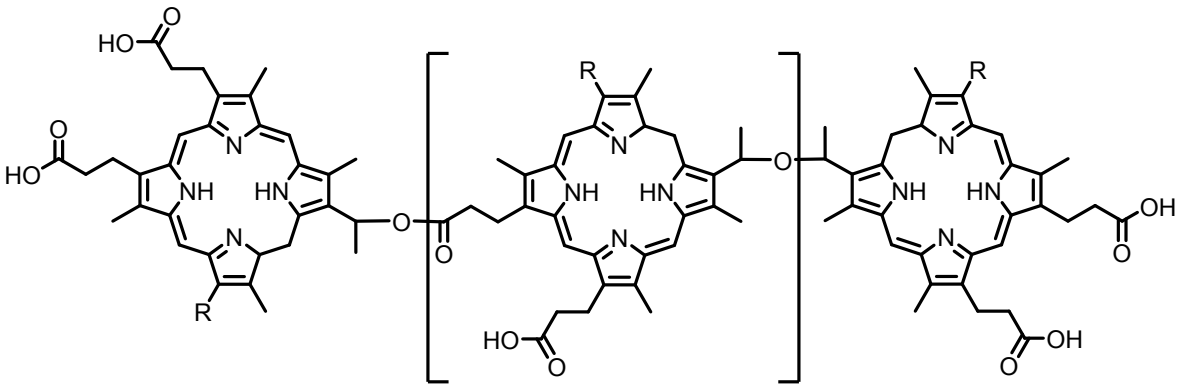
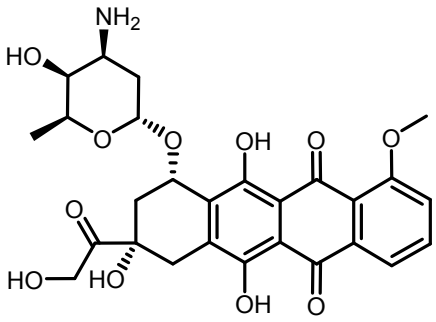


Fig. S6: MIC determination of complex-3 against representative bacterial strains. For each graph, the X-axis scale corresponds to time (0 – 18 h) and the Y-axis scale corresponds to optical density (OD @ 600 nm) ranging from 0 – 1.25 (a.u), as indicated in the inset below.



Porfimer (DB00707)



Doxorubicin (DB00997)

Fig. S7: Molecular structures of Porfimer, a photodynamic therapy drug and doxorubicin, an anticancer/ antibiotic.