Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Info

Syntheses, spectroscopic and crystallographic characterizations of cis- and trans-dispirocyclic ferrocenylphosphazenes: Molecular dockings, cytotoxic and antimicrobial activities

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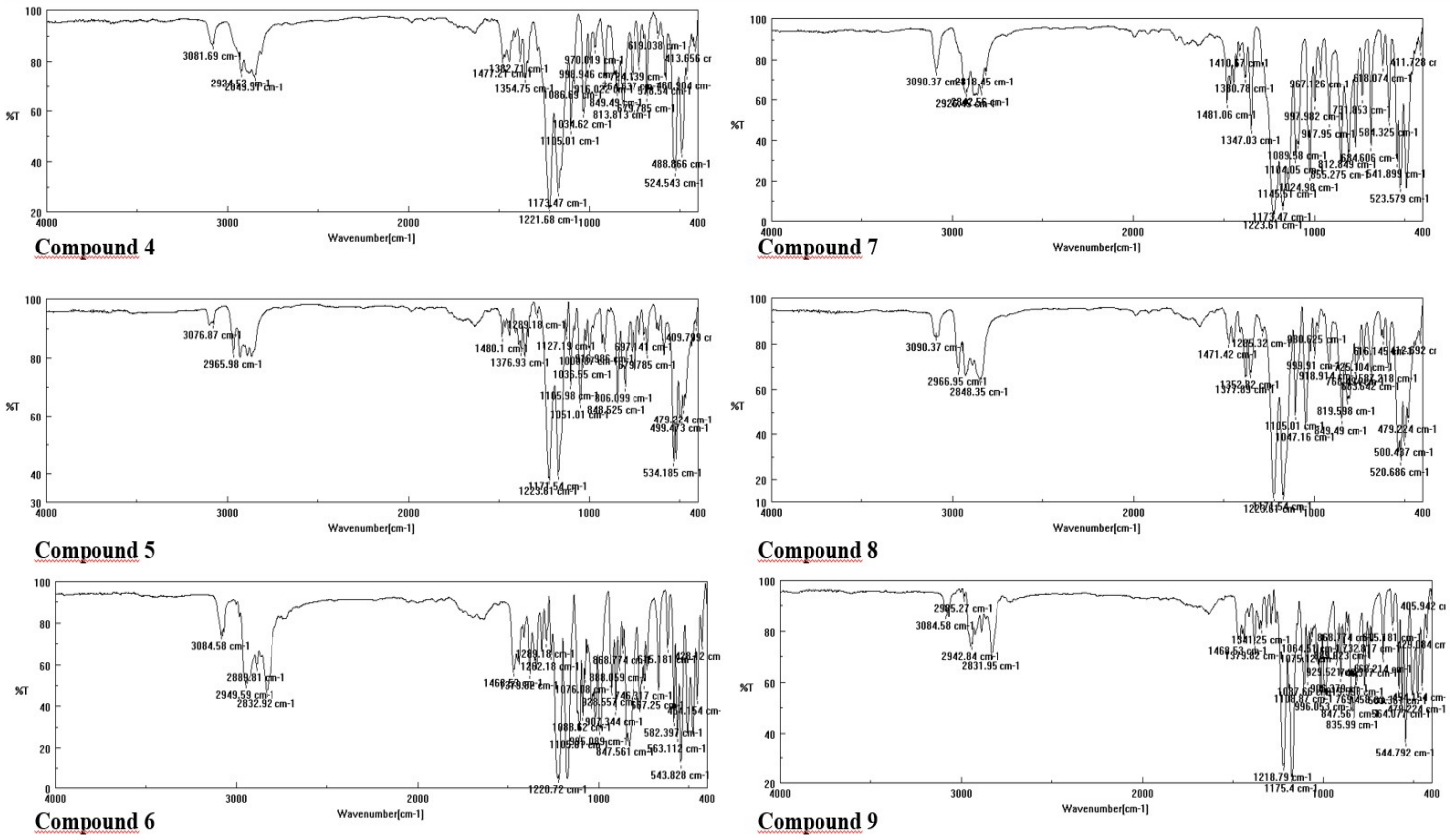


Fig. S1. The IR spectra of the cis- and trans-phosphazenes.

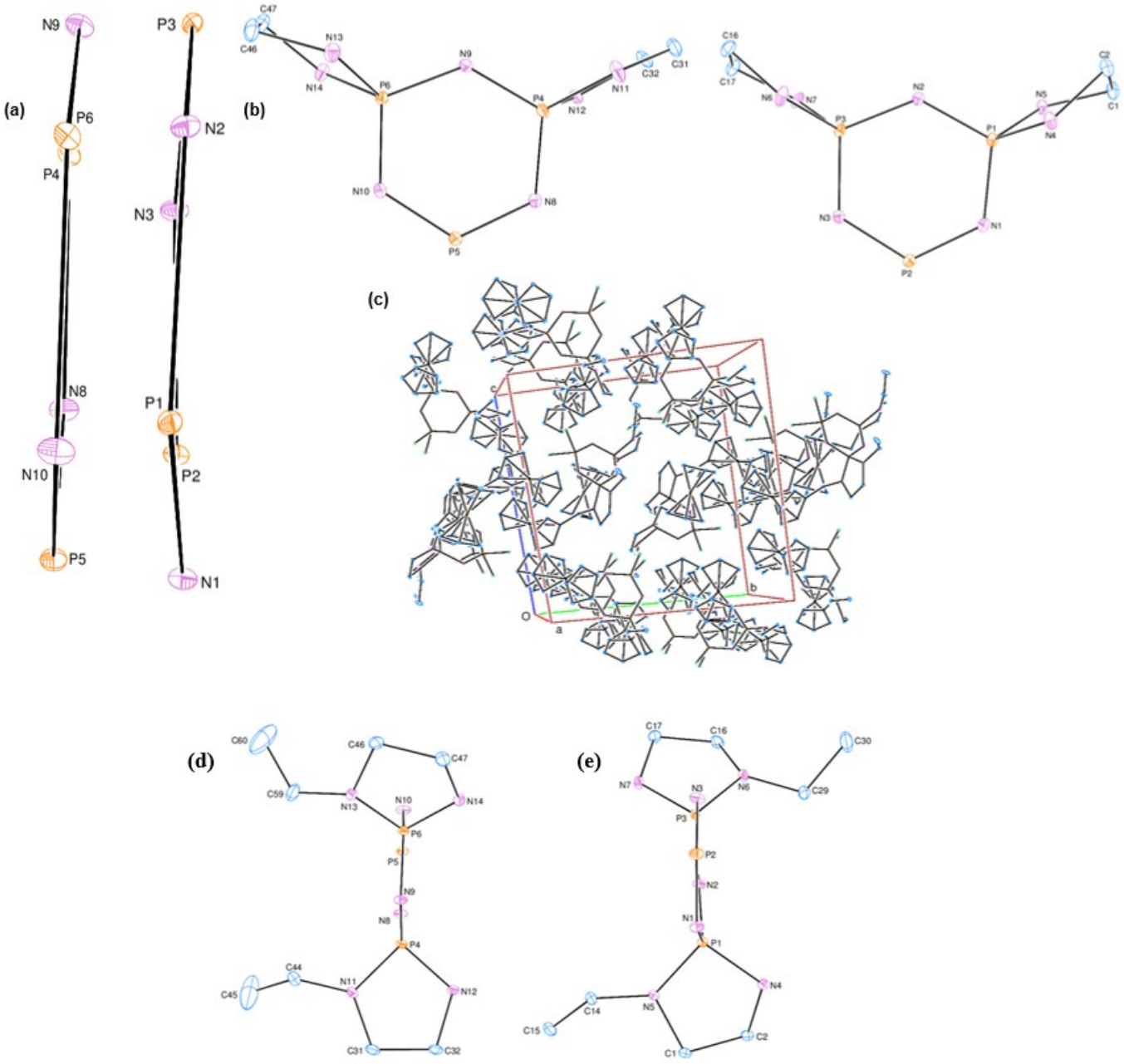


Fig. S2. The conformations of (a) the phosphazene rings, (b) the five-membered spiro-rings, (c) the packing diagram and independent molecules in the unit cell of (d) **5** and (e) **8**.

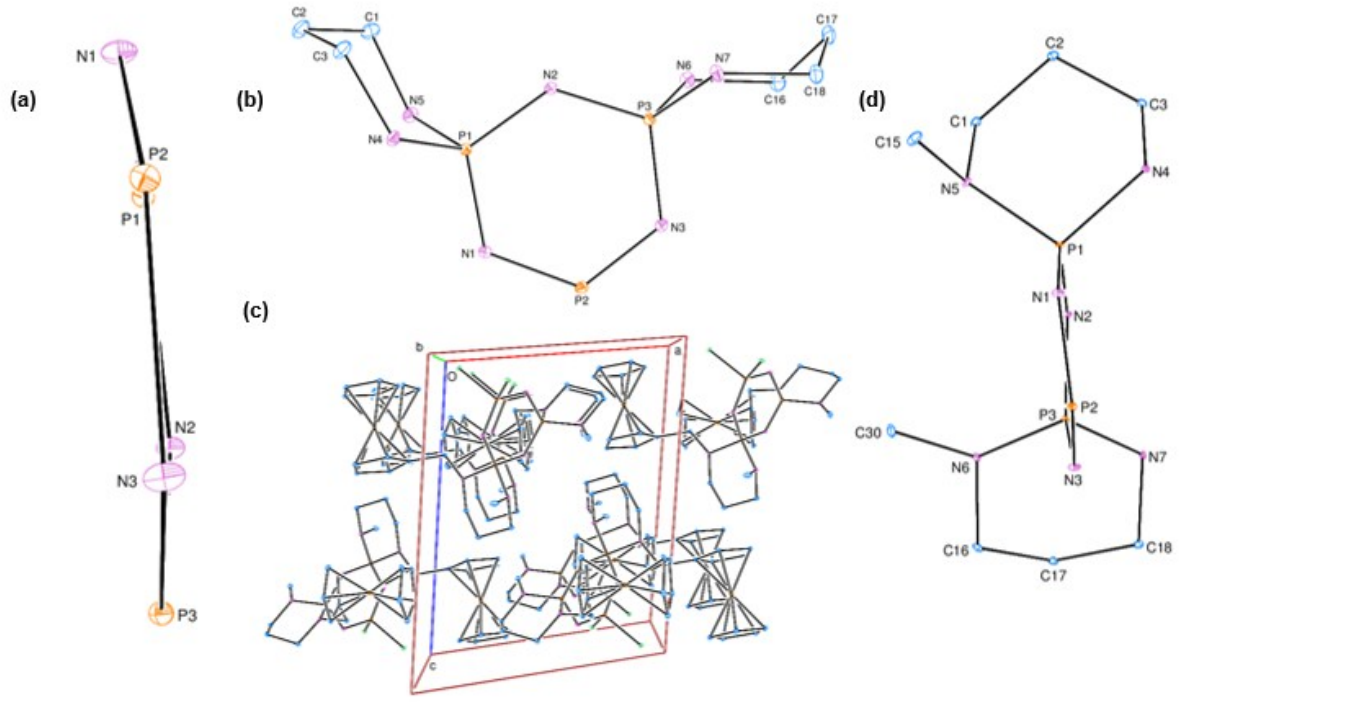


Fig. S3. The conformations of (a) the phosphazene ring, (b) the six-membered spiro-ring, (c) the packing diagram of **6** and **(d)** cis isomer-compound **6.**

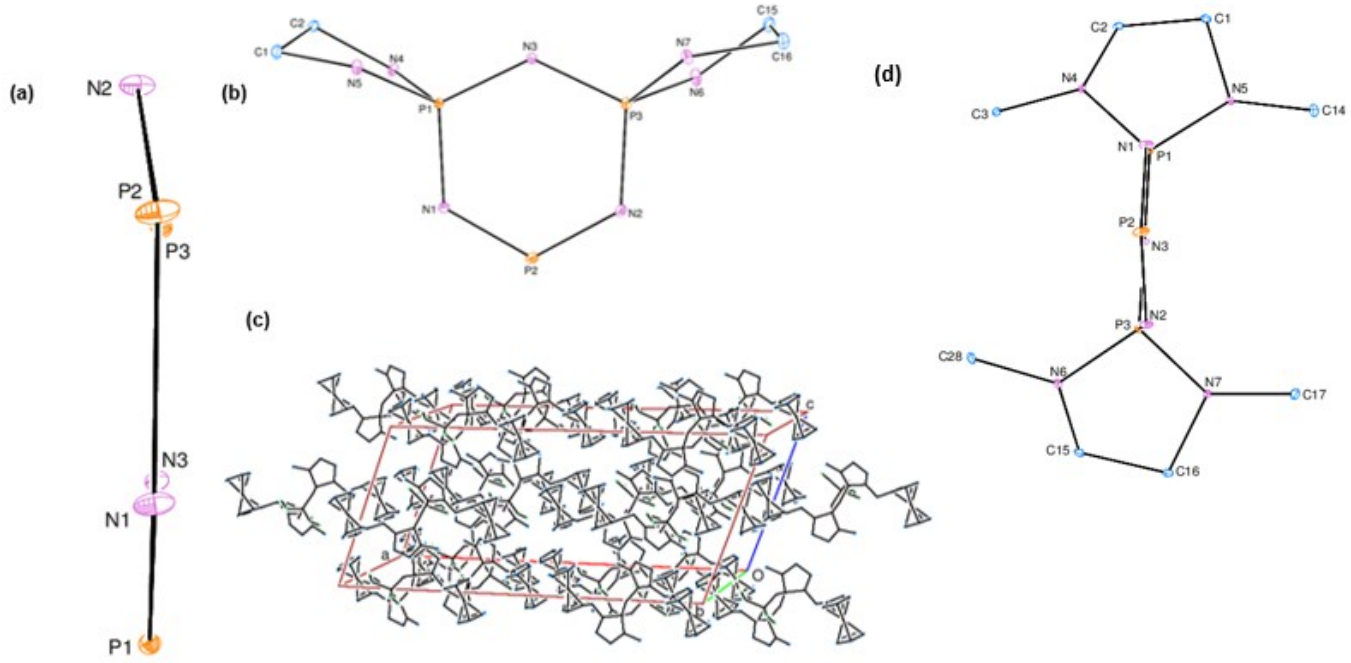


Fig. S4. The conformations of (a) the phosphazene ring, (b) the five-membered spiro-ring, (c) the packing diagram of **7** and (d) trans isomer-compound **7**.

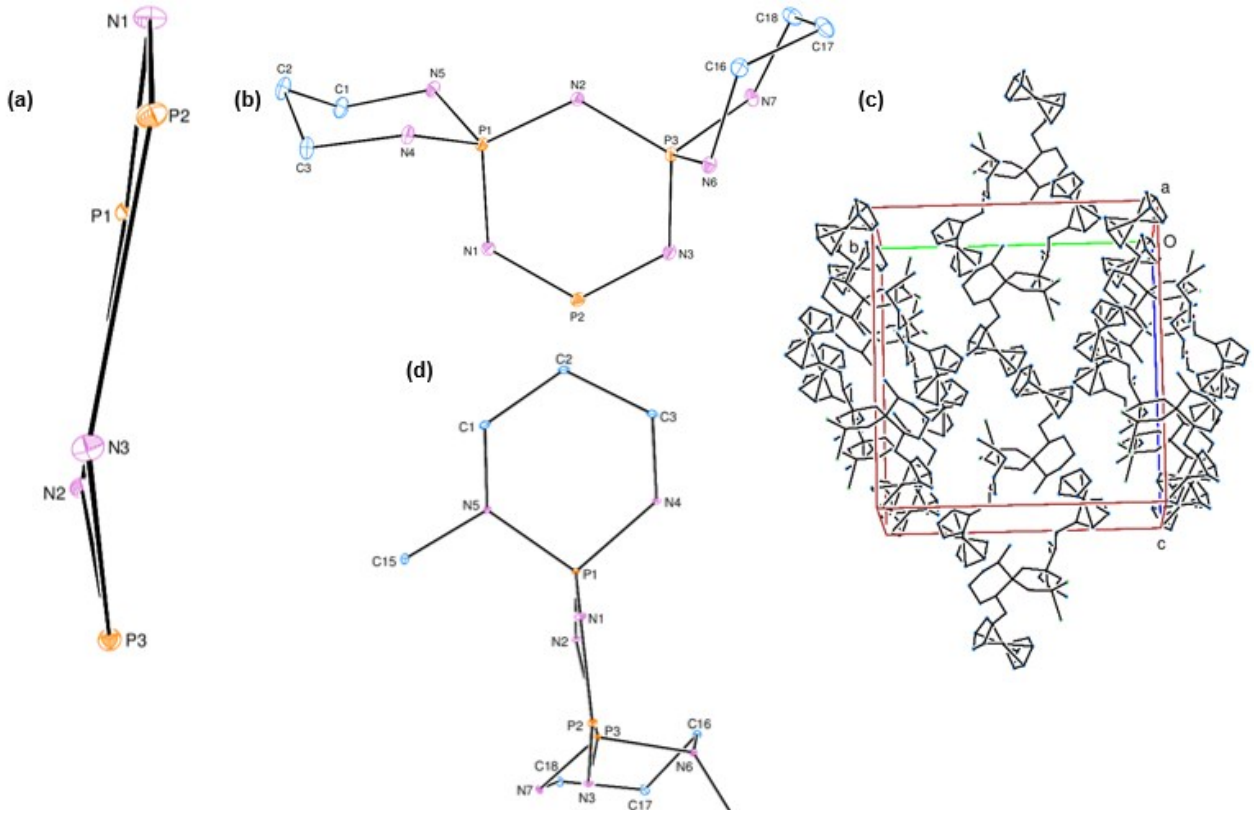
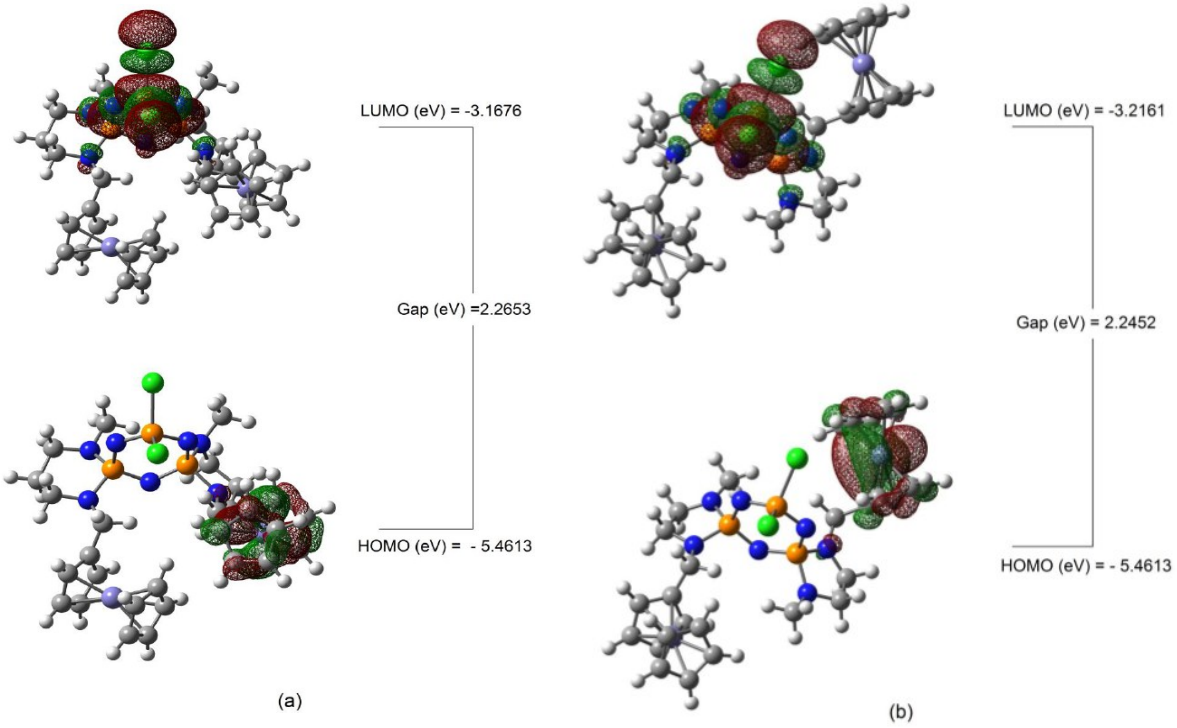


Fig. S5. The conformations of (a) the phosphazene ring, (b) the six-membered spiro-ring, (c) the packing diagram of **9** and **(d)** trans isomer-compound **9**.



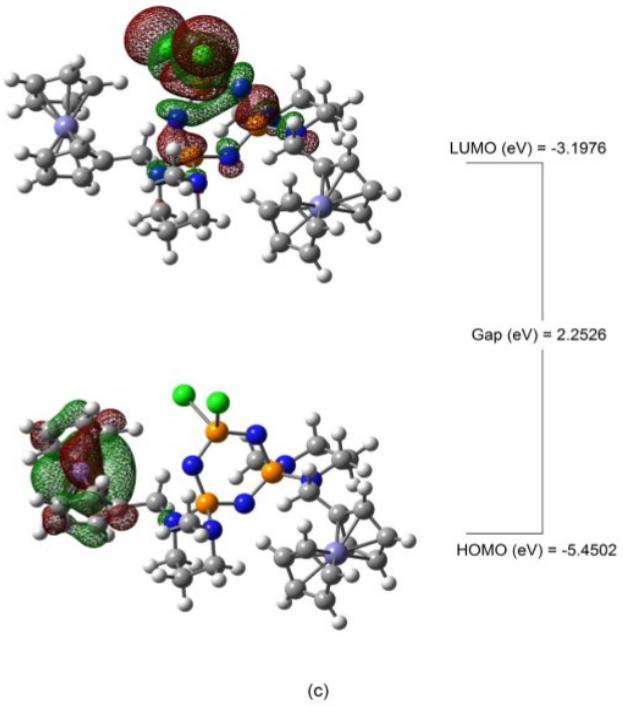


Fig. S6. Molecular orbital surfaces and energy levels are given for the HOMO and LUMO of (a) **6**, (b) **7** and (c) **9**.

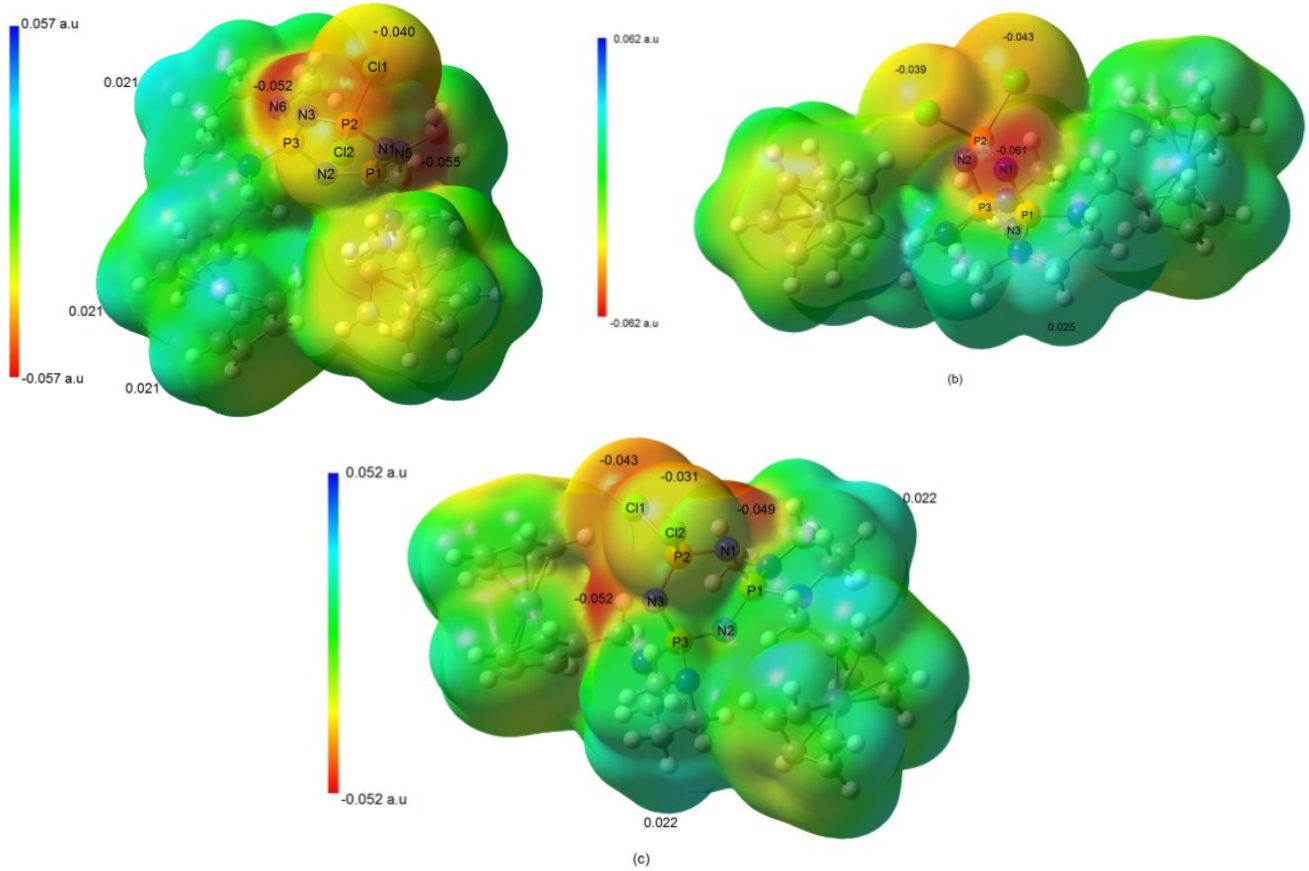


Fig. S7. Molecular electrostatic potential (MEP) map for (a) **6**, (b) **7** and (c) **9**.

Table S1 Calculated total energies and chemical parameters of the compounds **6**, **7** and **9** at DFT/B3LYP/LANL2DZ level.

Compounds	**6**	**7**	**9**
E_{TOTAL}(Hartee)	-1846.3853	-1767.7703	-1846.3852
E_{HOMO} (eV)	-5.4330	-5.4613	-5.4502
E_{LUMO}(eV)	-3.1676	-3.2161	-3.1976
ΔE_{Gap}(eV)	2.2653	2.2452	2.2526
I (eV)	5.4330	5.4613	5.4502
A(eV)	3.1677	3.2161	3.1976
μ (Debye)	7.5196	7.3287	7.1570
η (eV)	1.1327	1.1226	1.1263
χ (eV)	4.3004	4.3387	4.3239
σ (eV)	0.8829	0.8908	0.8879
μ_p(eV)	-4.3004	-4.3387	-4.3239
ω	10.4733	10.5663	10.5285

E_{TOTAL}: Total energy, E_{HOMO} and E_{LUMO}: Energy values of HOMO and LUMO, μ: Total molecular dipole moments, ΔE_{Gap} = (E_{LUMO} – E_{HOMO}): gap of energy, I: Ionization potential, A: Electron affinity, η: Absolute hardness, (I-A)/2, χ: Electronegativity, (I+A)/2, σ: Softness, 1/η, μ_p: Chemical potential, -(I+A)/2, ω: Electrophilicity, $\mu_p^2/2\eta$.

Table S2 Binding affinity of different poses of the compounds **6**, **7** and **9** as predicted Autodock Vina.

Compound/DNA	Mode	Affinity (kcal/mol)	Distance from best mode RMSD l.b.	RMSD u.b.
(6)/A-DNA				
	1	-9.1	0.000	0.000
	2	-9.1	6.090	11.266
	3	-9.0	4.331	6.691
	4	-9.0	3.633	8.308
	5	-9.0	8.121	11.571
	6	-8.9	4.942	8.945
	7	-8.8	3.645	7.424
	8	-8.7	3.323	7.671
	9	-8.5	5.269	9.607
(6)/B-DNA				
	1	-7.9	0.000	0.000
	2	-7.8	4.906	9.203
	3	-7.7	3.633	5.917
	4	7.6	4.777	9.690
	5	-7.5	3.271	5.667
	6	-7.4	5.578	10.374
	7	-7.3	3.169	9.111
	8	-7.3	4.496	9.529
	9	-7.2	5.748	10.523
(7)/A-DNA				
	1	-9.0	0.000	0.000
	2	-9.0	1.160	8.712
	3	-8.8	1.122	8.831
	4	-8.8	2.390	8.545
	5	-8.8	3.391	9.890
	6	-8.7	1.623	2.772
	7	-8.6	2.484	3.954
	8	-8.6	4.272	6.276
	9	8.5	3.866	9.729
(7)/B-DNA				
	1	-7.9	0.000	0.000
	2	-7.6	3.706	10.782
	3	-7.5	0.870	1.998
	4	-7.2	2.033	9.658
	5	-7.1	2.365	3.268
	6	-7.0	3.934	10.436
	7	-6.6	3.120	4.558
	8	-6.6	3.949	5.785
	9	-6.6	2.701	9.344
(9)/A-DNA				
	1	-9.1	0.000	0.000
	2	-9.1	1.473	9.110
	3	-9.0	1.744	9.357
	4	-9.0	2.676	10.117
	5	-8.7	1.210	2.154
	6	-8.6	1.796	9.053
	7	-8.5	3.076	9.877
	8	-8.5	2.036	8.918
	9	-8.5	5.427	9.596
(9)/B-DNA				
	1	-7.0	0.000	0.000

2	-7.0	7.436	10.602
3	-6.8	1.658	2.640
4	-6.8	8.610	14.636
5	-6.7	7.279	10.344
6	-6.6	6.002	11.023
7	-6.6	6.031	9.186
8	-6.4	9.001	14.884
9	-6.3	6.856	11.946

Table S3 Binding interactions of the compounds **6**, **7** and **9** with A-DNA and B-DNA (DG: Guanosine, DC: Cytosine, DA: Adenosine, DT: Thymidine)

Compound-DNA	Name	Distance (Å)	Bonding types	Biding site of DNA	Biding site of Ligand	Binding mode DNA→ Ligand
(**6**)-A-DNA	UNK0:C-B:DC4:OP2	3.37	C-H bond (Hydrogen)	B:DC4:OP2	(**6**):C15	OP2-Acceptor → C-Donor
(**6**)-A-DNA	UNK0:C-B:DC4:OP2	3.39	C-H bond (Hydrogen)	B:DC4:OP2	(**6**):C30	OP2-Acceptor → C-Donor
(**6**)-A-DNA	UNK0:Cl-B:DC4	3.75	π-σ (hydrophobic)	B:DC4	(**6**):UNK0:Cl1	C-H → π Orbitals
(**6**)-A-DNA	B:DC3:UNK0	5.48	π-Alkyl (hydrophobic)	B:DC3	(**6**):UNK0	π Orbitals → π Alkyl
(**6**)-B-DNA	UNK0:C-B:DA17:OP2	3.36	C-H bond (Hydrogen)	B:DA17:OP2	(**6**):C15	OP2-Acceptor → C-Donor
(**6**)-B-DNA	UNK0:C-B:DA17:N7	3.19	C-H bond (Hydrogen)	B:DA17:N7	(**6**):C16	N7-Acceptor → C-Donor
(**6**)-B-DNA	B:DA18:UNK0	4.66	π-Alkyl (hydrophobic)	B:DA18	(**6**):UNK0	π Orbitals → π Alkyl
(**6**)-B-DNA	B:DA17:UNK0	5.38	π-Alkyl (hydrophobic)	B:DA17	(**6**):UNK0	π Orbitals → π Alkyl
(**7**)-A-DNA	UNK0:C-B:DG5:OP2	3.33	C-H bon (Hydrogen)	B:DG5:OP2	(**7**):C28	OP2-Acceptor → C-Donor
(**7**)-A-DNA	UNK0:C-B:DG6:N7	3.29	C-H bond (Hydrogen)	B:DG6:N7	(**7**):C15	N7-Acceptor → C-Donor
(**7**)-A-DNA	UNK0:C-A:DG5:OP2	3.01	C-H bond (Hydrogen)	A:DG5:OP2	(**7**):C14	OP2-Acceptor → C-Donor
(**7**)-A-DNA	UNK0:C-A:DG6:N7	3.64	C-H bond (Hydrogen)	B:DG6:N7	(**7**):C1	N7-Acceptor → C-Donor
(**7**)-A-DNA	B:DC4:N4-UNK0	3.70	π-Donor (electrostatic)	A:DC4:N4	(**7**):UNK0	N4 → π Orbitals
(**7**)-B-DNA	UNK0:C-B:DA17:N7	3.75	C-H bond (Hydrogen)	B:DA17:N7	(**7**):C17	N7-Acceptor → C-Donor
(**7**)-B-DNA	UNK0:C-B:DA5:N7	3.78	C-H bond (Hydrogen)	B:DA5:N7	(**7**):C15	N7-Acceptor → C-Donor
(**7**)-B-DNA	A:DC3:OP2-UNK0	4.80	π-Anion (electrostatic)	A:DC3:OP2	(**7**):UNK0	Negative → π Orbitals
(**7**)-B-DNA	B:DT19:C7-UNK0	3.77	π-σ (hydrophobic)	B:DCT19	(**7**):UNK0	C-H → π Orbitals
(**9**)-A-DNA	UNK0:C-B:DG6:N7	3.72	C-H bond (Hydrogen)	B:DG6:N7	(**9**):C15	N7-Acceptor → C-Donor

(**9**)-A-DNA	UNK0:C-B:DG6:N7	3.37	C-H bond (Hydrogen)	B:DG6:N7	(**9**):C1	N7-Acceptor → C-Donor
(**9**)-A-DNA	UNK0:C-B:DC4:OP2	3.45	C-H bond (Hydrogen)	B:DC4:OP2	(**9**):C4	OP2-Acceptor → C-Donor
(**9**)-A-DNA	A:DG6:UNK0	4.78	π-Alkyl (hydrophobic)	B:DG6	(**9**):UNK0	π Orbitals → π Alkyl
(**9**)-A-DNA	A:DG5:OP2-UNK0	4.46	π-Anion (electrostatic)	A:DG5:OP2	(**9**):UNK0	Negative → π Orbitals
(**9**)-A-DNA	A:DG5:UNK0	4.86	π-Alkyl (hydrophobic)	B:DG5	(**9**):UNK0	π Orbitals → π Alkyl
(**9**)-A-DNA	A:DC4:UNK0	4.61	π-Alkyl (hydrophobic)	B:DC4	(**9**):UNK0	π Orbitals → π Alkyl
(**9**)-B-DNA	A:DG4:UNK0	5.12	π-Alkyl (hydrophobic)	B:DG4	(**9**):UNK0	π Orbitals → π Alkyl
(**9**)-B-DNA	A:DC3:UNK0	5.02	π-Alkyl (hydrophobic)	B:DC3	(**9**):UNK0	π Orbitals → π Alkyl