

SUPPORTING INFORMATION

Synthesis of novel calix[4]arene *p*-benzazole derivatives and investigation of their DNA binding and cleavage activities with molecular docking and experimental studies

Seyda Cigdem Ozkan^{a,b}, Fatma Aksakal^c, Aydan Yilmaz^{*b}

^aDepartment of Chemical and Chemical Processing Technologies, Acigol Vocational School of Technical Sciences, Nevsehir Hacı Bektaş Veli University, Nevsehir, Turkey

^bDepartment of Chemistry, Faculty of Science, Selcuk University, 42075, Konya, Turkey

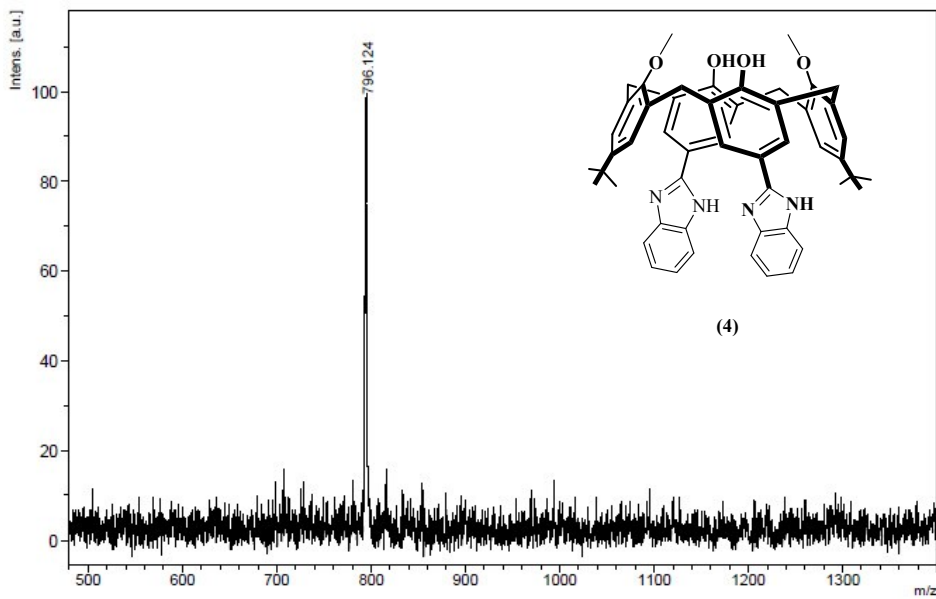
^cDepartment of Chemistry, Faculty of Science, Hacettepe University, Ankara, Turkey

†*E-mail: aydan@selcuk.edu.tr; Tel.: +90 332 2233866; Fax: +90 332 2412499

CONTENTS

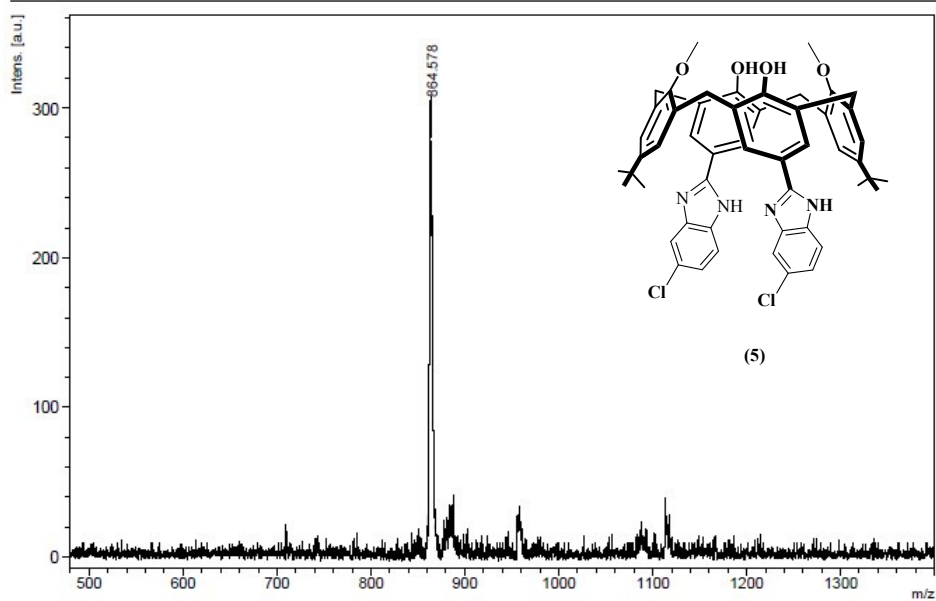
MALDI-TOF MS Spectra of the compounds 4 and 5	S1
MALDI-TOF MS Spectra of the compounds 6 and 7	S2
MALDI-TOF MS Spectra of the compounds 10 and 11	S3
MALDI-TOF MS Spectra of the compound 12	S4
Molecular Docking Results for the compounds 4 , 6 , 7 and 11	S5

Compound 4



m/z	SN	Quality Fac	Res.	Intensity	Area
796.124				23.33	

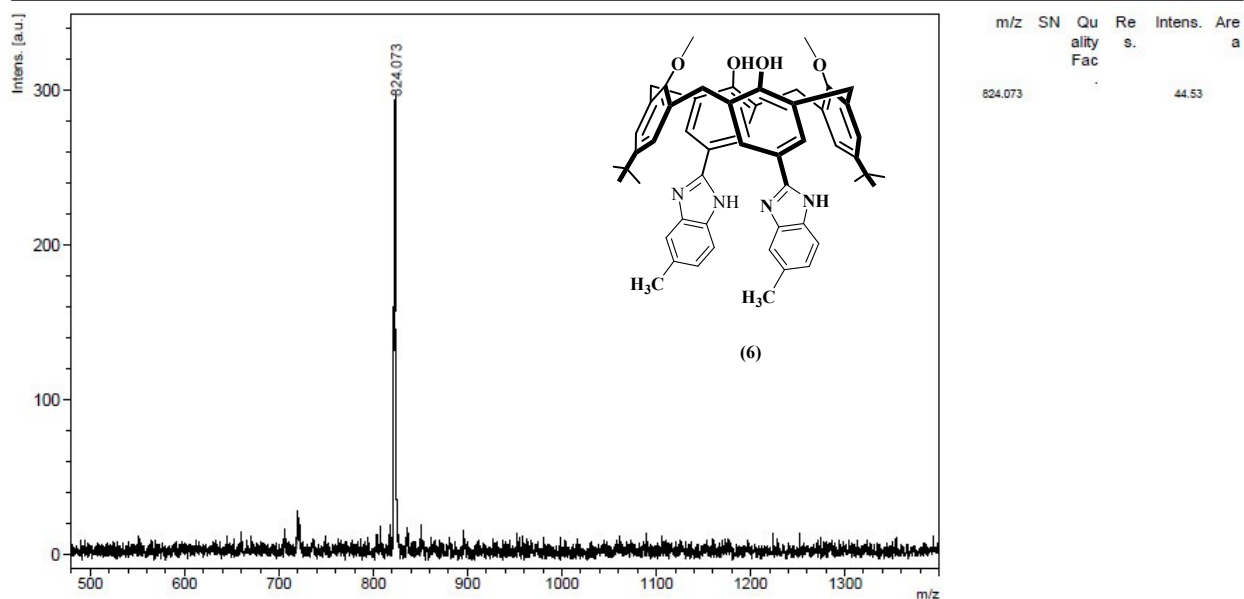
Compound 5



m/z	SN	Quality Fac	Res.	Intensity	Area
864.578				278.00	

Figure S1. MALDI-TOF MS spectra of compounds 4 and 5

Compound 6



Compound 7

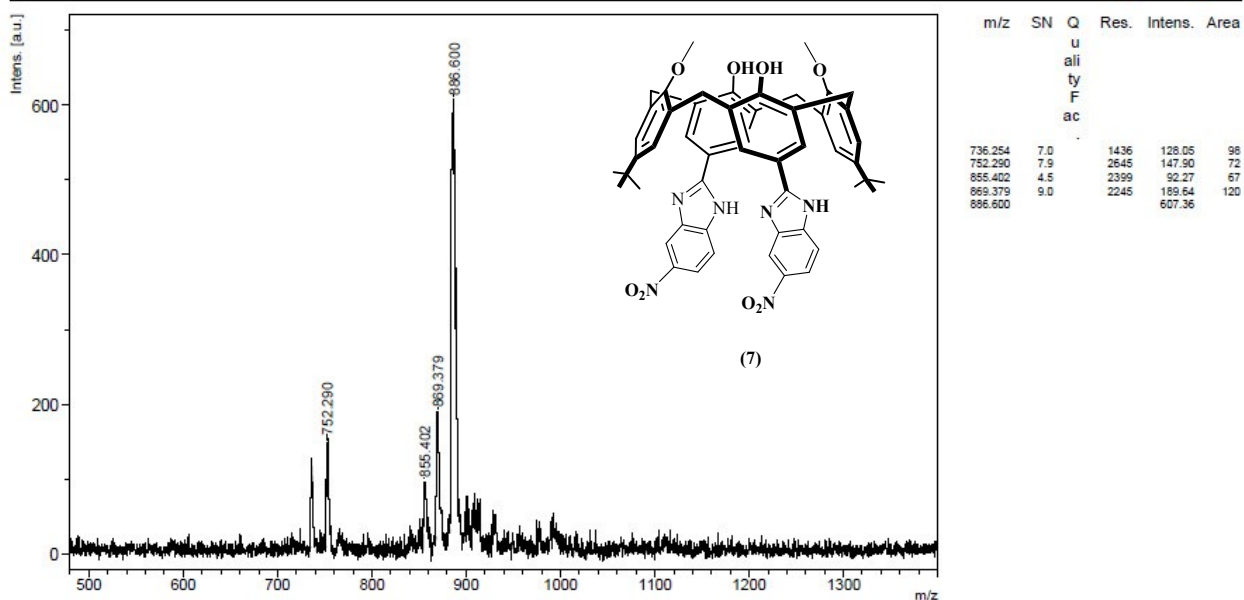
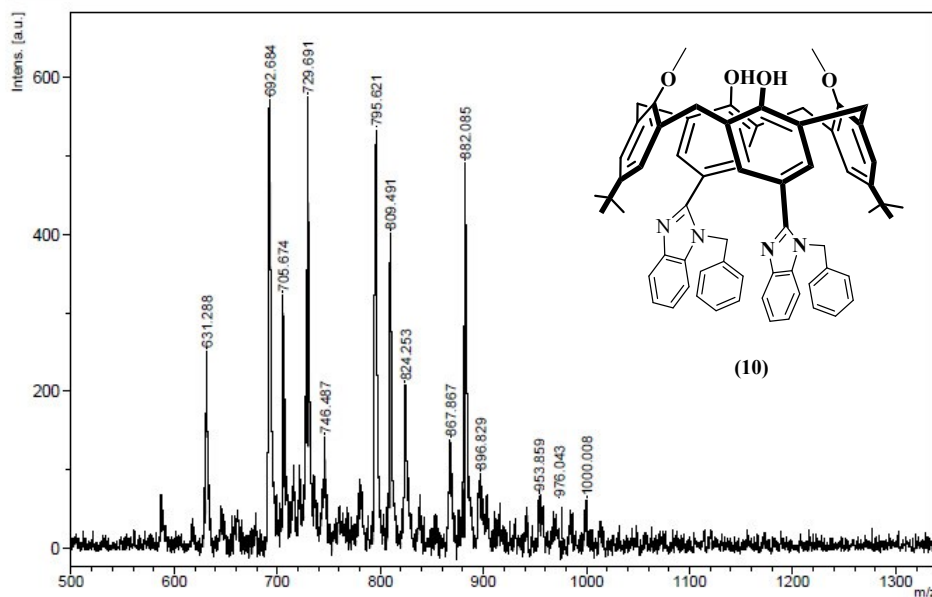


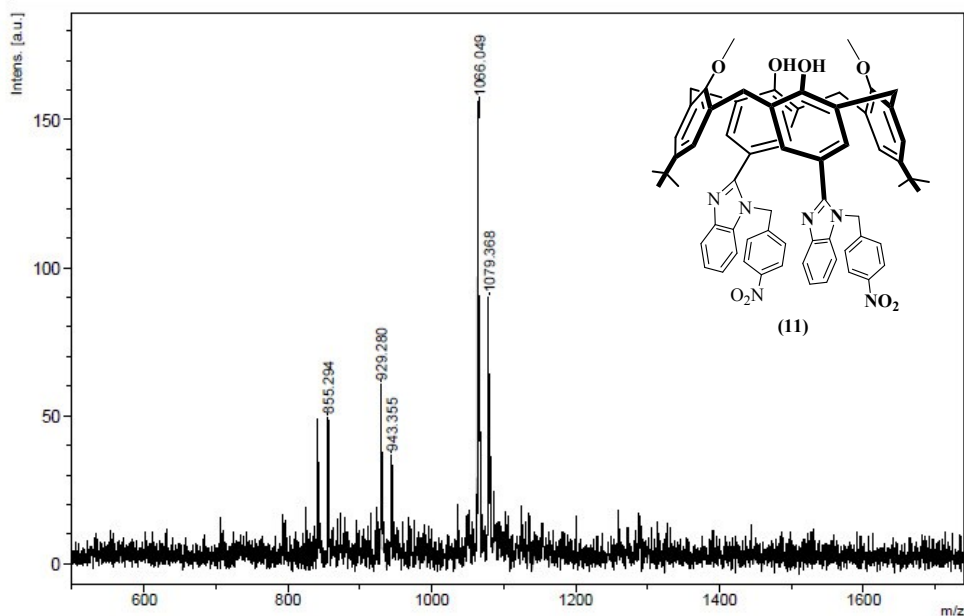
Figure S2. MALDI-TOF MS spectra of compounds 6 and 7

Compound 10



m/z	SN	Q	Res.	Intens.	Area
631.288	8.7		1432	250.95	166
692.684	17.0		778	570.31	833
705.674	9.3		673	321.66	402
729.691	15.8		660	574.24	951
746.487	3.7		2104	141.83	87
795.621	14.7		1759	532.46	395
809.491	11.0		728	400.44	511
824.253	5.8		1259	208.20	218
867.867	3.9		1444	137.23	111
882.085	14.0		732	490.61	722
896.829	2.8		1004	94.85	99
942.695	1.7		1786	54.15	36
953.859	2.2		2459	67.52	41
976.043				4.48	
984.511				49.66	
1000.008				61.32	

Compound 11



m/z	SN	Q	Res.	Intens.	Area
841.399	6.2		1833	48.61	27
855.294	6.2		2351	49.08	22
929.280	7.1		2336	60.35	46
943.355	4.2		2407	36.07	21
1066.049				50.67	
1079.368				59.07	

Figure S3. MALDI-TOF MS spectra of compounds 10 and 11

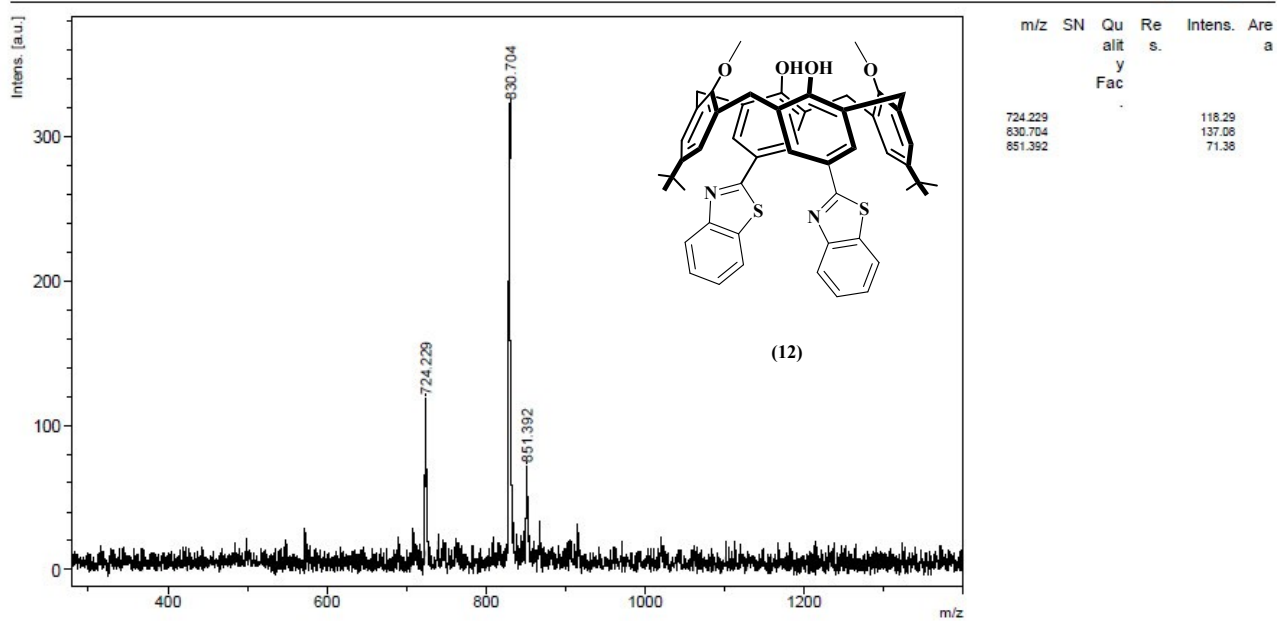


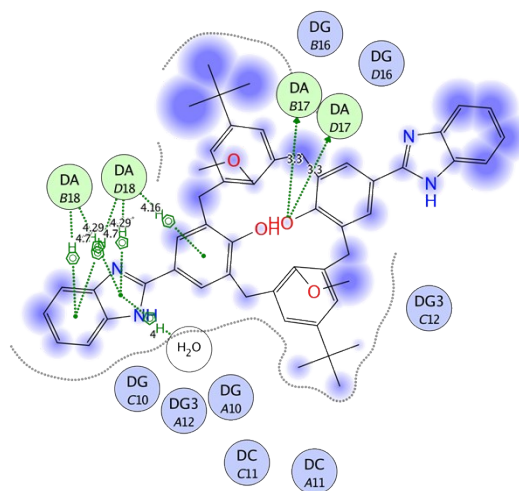
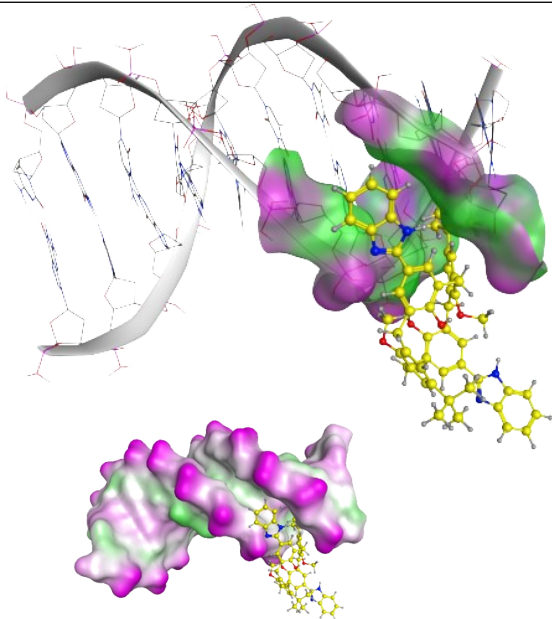
Figure S4. MALDI-TOF MS spectra of compound 12

Compound

(a)

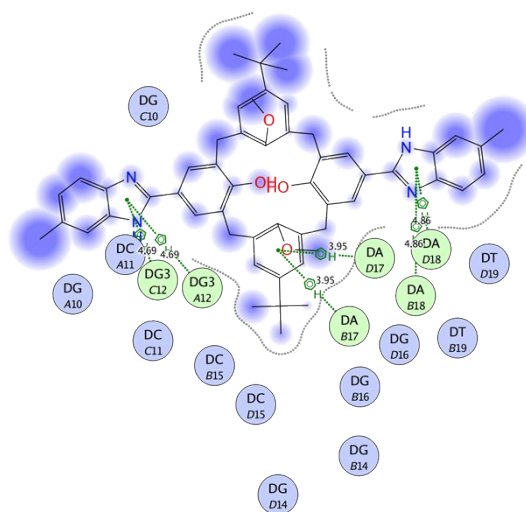
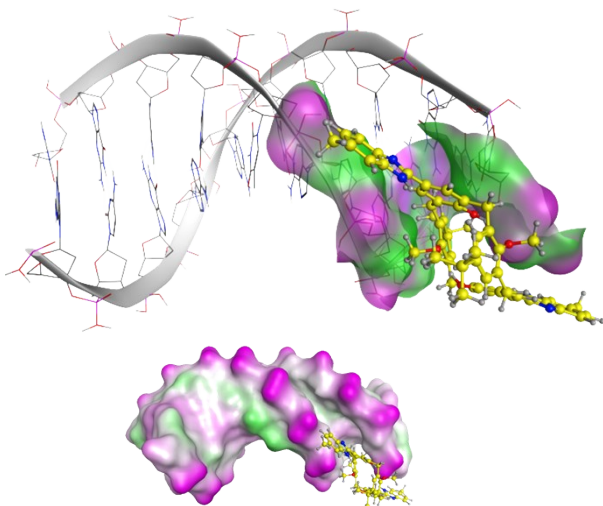
(b)

4

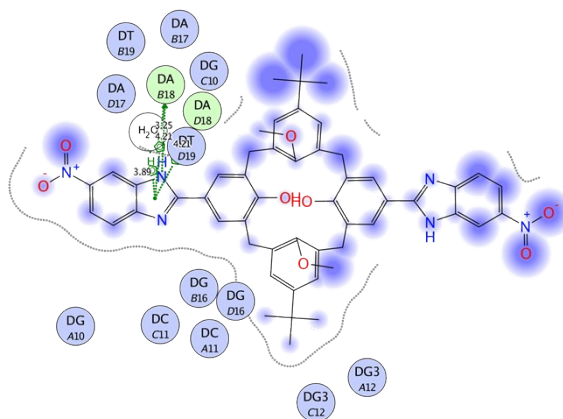
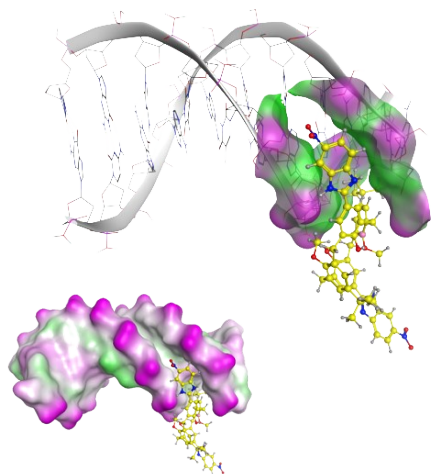


- polar
- acidic
- basic
- greasy
- proximity contour
- sidechain acceptor
- sidechain donor
- backbone acceptor
- backbone donor
- solvent residue
- metal complex
- solvent contact
- metal/ion contact
- ligand exposure
- receptor exposure
- arene-arene
- arene-H
- arene-cation

6



7



11

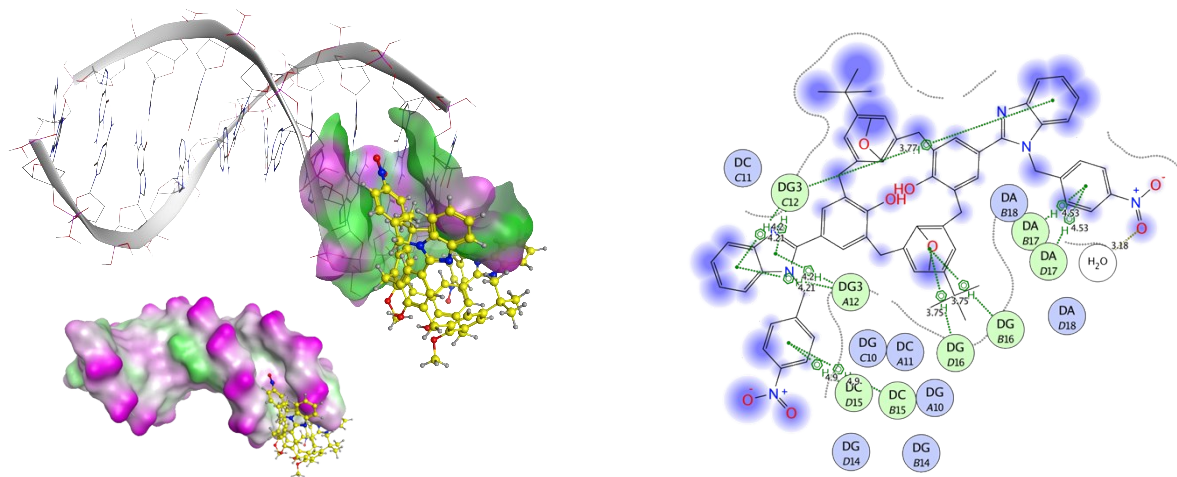


Figure S5. Three-dimensional (3D) docked structures with molecular surface representations (a) and two-dimensional (2D) interaction plots (b) obtained for the most energetically profitable poses of compound-DNA complexes (PDB ID: 1BNA).