Table 1: The details of names and coding terms used of all modifications used in this work.

S. No.	Name Code	Base	Modification	Description
1	DC	Cytosine	No modification,	Deoxyribo Cytidine
2	DCS	Cytosine	Phosphorothioate (PS) modification	Deoxyribo Cytidine with PS modification
3	RC	Cytosine	No Modification,	Ribo Cytidine
4	RCS	Cytosine	Phosphorothioate (PS) modification	Ribo Cytidine with PS modification
5	LCC	Cytosine	Locked nucleic acid (LNA) modification	Cytidine with LNA modification
6	LCS	Cytosine	Locked nucleic acid (LNA) and phoshporothioate (PS) modification	Cytidine with LNA and PS modifications
7	CME	Cytosine	2'-O- methoxyethyl (MOE) modification	Ribo Cytidine with MOE modification
8	CMS	Cytosine	2'-O- methoxyethyl (MOE) and phosphorothioate (PS) modification	Ribo Cytidine with MOE and PS modifications
9	A1	Cytosine	N-linked LNA modification	Cytidine with N-linked LNA modifications
10	A2	Cytosine	Methoxy-N-linked LNA modification	Cytidine with methoxy-N-linked LNA modifications
11	A3	Cytosine	LNA linked to dimethyl amine modification	Cytidine with LNA linked to dimethyl amine modification
12	A4	Cytosine	LNA linked to N-diamide modification	Cytidine with LNA linked to N-diamide modification
13	A5	Cytosine	LNA linked to N-dihydroxy modification	Cytidine with LNA linked to N-dihydroxy modification

Table 2: The dihedral angles and PM6 energies of most stable conformations of all modifications.

S. No.	Name Code	Alpha (α)	Beta (β)	Gamma ($_{\gamma}$)	Delta (δ)	Epsilon (ε)	Chi (χ)	S1	S2	S3	S4	Energy (Kcal/mol)
1	**DC**	-56.87	-156.42	178.38	137.98	-151.78	-150.65					-97875.25
2	**DCS**	-56.37	-157.50	-151.91	138.40	-151.74	-151.05					-95371.76
3	**RC**	-65.66	-153.85	-176.09	84.17	-96.11	-143.53					-104619.98
4	**RCS**	-123.60	-124.81	124.33	84.39	-125.50	66.13					-104527.23
5	**LCC**	51.24	157.87	63.78	63.78	-166.75	-138.61					-107372.17
6	**LCS**	171.50	-142.58	-176.10	63.97	-167.18	-168.22					-107272.59
7	**CME**	-172.82	-152.69	-174.92	79.18	29.24	-134.54	93.72	-172.15	-93.97	97.51	-121758.93
8	**CMS**	98.05	-92.53	-174.55	79.48	30.46	47.06	124.96	-111.62	86.26	96.63	-121638.14
9	**A1**	50.08	157.40	63.57	63.75	-168.07	-139.36					-106966.52
10	**A2**	-43.76	-114.92	-86.64	64.54	-168.17	-170.02					-109241.72
11	**A3**	-131.55	96.15	-147.47	61.64	-166.85	-139.08					-109887.25
12	**A4**	-161.11	126.63	150.44	65.84	-166.30	-138.33					-112631.50
13	**A5**	46.17	155.53	63.62	65.63	-165.62	-138.70					-124924.12

Table 3: The electronic energy, dipole moment, polarizability, thermal energy and heat capacity of all the modifications obtained at the B3LYP/6-31G(d,p) level of theory are given.

S. No.	Name	Electronic Energy (hartree)	Dipole moment (Debye)	Polarizability (a.u)	Thermal Energy (Kcal/mol)	Heat Capacity cal/ mol-kelvin
1	DC	-1462.2522	6.561359	173.311667	212.828	83.289
2	DCS	-1785.2066	4.707803	187.250333	210.318	84.867
3	RC	-1537.4683	4.780571	174.736667	216.552	86.529
4	RCS	-1860.4220	4.629668	192.669667	214.053	87.869
5	LCC	-1575.5542	6.479880	181.739000	220.427	88.037
6	LCS	-1898.5040	6.349720	197.898333	217.775	89.822
7	CME	-1730.5920	1.959740	213.966667	276.589	104.445
8	CMS	-2053.5371	11.858483	224.859000	273.966	106.130
9	A1	-1591.5430	6.655189	178.414333	212.655	87.657
10	A2	-1706.0300	7.307183	196.298667	233.822	96.679
11	A3	-1709.5141	5.487077	212.611000	269.087	103.306
12	A4	-1741.545033	4.862393	206.580667	254.958	100.474
13	A5	-1781.237451	6.384333	198.818000	237.584	101.538

Table 4: The global quantum chemical descriptors HOMO, LUMO, HOMO-LUMO Gap, Ionization Potential, Electron Affinity, Global Hardness, Global Softness, Chemical Potential and Electrophilicity Index for gas phase calculations by B3LYP/6-31G(d,p) for all modifications.

S. No.	**Name**	**HOMO (eV)**	**LUMO (eV)**	**HOMO-LUM Gap(eV)**	**Ionization Potential** $I = -E_{HOMO}$	**Electron Affinity** $A = -E_{LUMO}$	**Global Hardness** $\eta = (I-A)/2$	**Global Softness** $S = 1/2n$	**Chemical Potential** $\mu = -(I+A)/2$	**Electro-negativity** $\chi = -\mu$	**Electrophilicity Index** $\omega = \mu^2/2n$
1	DC	-5.7386	-0.3785	**5.3601**	5.7386	0.3785	2.6800	0.1865	**-3.0585**	3.0585	**1.7452**
2	DCS	-5.9622	-0.6274	**5.3348**	5.9622	0.6274	2.6674	0.1874	**-3.2948**	3.2948	2.0348
3	RC	-6.0934	-0.7273	**5.3661**	6.0934	0.7273	2.6830	0.1863	-3.4103	3.4103	2.1673
4	RCS	-6.5263	-1.1311	**5.3952**	6.5263	1.1311	**2.6976**	0.1853	-3.8287	**3.8287**	**2.717**
5	LCC	-6.0063	-0.6767	**5.3296**	6.0063	0.6767	2.6648	0.1876	**-3.3415**	3.3415	2.095
6	LCS	-6.1715	-0.8587	**5.3128**	6.1715	0.8587	2.6564	**0.1882**	-3.5151	3.5151	2.3256
7	CME	-6.3484	-1.0269	**5.3215**	6.3484	1.0269	2.6607	0.1879	-3.6876	3.6876	2.5553
8	CMS	-6.4461	-1.1189	**5.3272**	6.4461	1.1189	2.6636	0.1877	-3.7825	3.7825	2.6857
9	A1	-6.0765	-0.7551	**5.3214**	6.0765	0.7551	2.6607	0.1879	-3.4158	3.4158	2.1925
10	A2	-6.4256	-1.0990	**5.3266**	6.4256	1.0990	2.6633	0.1877	-3.7623	**3.7623**	**2.6573**
11	A3	-5.8294	-0.8157	**5.0137**	5.8294	0.8157	2.5068	**0.1994**	**-3.3225**	3.3225	2.2018
12	A4	-6.2999	-0.9556	**5.3443**	6.2999	0.9556	2.6721	0.1871	-3.6277	3.6277	2.4625
13	A5	-6.0433	-0.6968	**5.3465**	6.0433	0.6968	**2.6732**	0.1870	-3.3700	3.3700	**2.1242**

Table 5: The global quantum chemical descriptors HOMO, LUMO, HOMO-LUMO Gap, Ionization Potential, Electron Affinity, Global Hardness, Global Softness, Chemical Potential and Electrophilicity Index for solvent phase calculations by B3LYP/6-311G(d,p) for all modifications.

S. No.	Name	HOMO (eV)	LUMO (eV)	**HOMO-LUMO Gap (eV)**	**Ionization Potential $I = -E_{HOMO}$**	**Electron Affinity $A = -E_{LUMO}$**	**Global Hardness $\eta = (I-A)/2$**	**Global Softness $S = 1/2\eta$**	**Chemical Potential $\mu = -(I+A)/2$**	**Electro-negativity $\chi = -\mu$**	**Electrophilicity Index $\omega = \mu^2/2n$**
1	DC	-6.8466	0.0198	**6.8665**	6.8466	-0.0198	3.4332	**0.1456**	**-3.4133**	3.4133	**1.6968**
2	DCS	-6.8784	-0.0043	**6.8741**	6.8784	0.0043	3.4370	0.1454	**-3.4414**	3.4414	1.7228
3	RC	-6.9293	-0.0416	**6.8877**	6.9293	0.0416	3.4438	0.1451	-3.4855	3.4855	1.7638
4	RCS	-7.4004	-0.2097	**7.1906**	7.4004	0.2097	**3.5953**	0.1390	-3.8051	**3.8051**	**2.0135**
5	LCC	-6.9152	-0.0446	**6.8706**	6.9152	0.0446	3.4353	**0.1455**	**-3.4799**	3.4799	1.7625
6	LCS	-6.9274	-0.0525	**6.8749**	6.9274	0.0525	3.4374	0.1454	**-3.4899**	3.4899	1.7716
7	CME	-6.9636	-0.0884	**6.8752**	6.9636	0.0884	3.4376	0.1454	-3.5260	3.5260	1.8083
8	CMS	-7.1576	-0.1346	**7.0229**	7.1576	0.1346	3.5114	0.1423	-3.6461	3.6461	1.8930
9	A1	-6.9555	-0.0729	**6.8825**	6.9555	0.0729	3.4412	0.1452	-3.5142	3.5142	1.7943
10	A2	-7.0053	-0.1099	**6.8953**	7.0053	0.1099	3.4476	0.1450	-3.5576	**3.5576**	**1.8355**
11	A3	-6.9277	-0.0459	**6.8817**	6.9277	0.0459	3.4408	0.1453	**-3.4868**	3.4868	1.7667
12	A4	-6.9644	-0.0821	**6.8823**	6.9644	0.0821	3.4411	0.1453	-3.5233	3.5233	1.8037
13	A5	-6.9410	-0.0672	**6.8738**	6.9410	0.0672	3.4369	0.1454	-3.5041	3.5041	1.7863

Table 6: The electronic energy of all monomers post base pairing and the corresponding base pairs along with their binding energies.

S. No.	Name	Electronic Energy (hartree)			Binding energies (kcal/mol)
		C (base)	G (base)	C-G (base-pair)	B.E = E(GC) - E(C) -E(G)
1	DC	-1462.6261	-1685.5267	-3148.1826	-18.700
2	DCS	-1785.5749	-1685.5267	-3471.1314	-18.700
3	RC	-1537.8634	-1685.5167	-3223.4096	-18.512
4	RCS	-1860.8121	-1685.5168	-3546.3583	-18.449
5	LCC	-1575.9554	-1685.5167	-3261.5017	-18.512
6	LCS	-1898.9042	-1685.5167	-3584.4504	-18.512
7	CME	-1731.0487	-1685.5167	-3416.5950	-18.574
8	CMS	-2053.9974	-1685.5167	-3739.5438	-18.637
9	A1	-1591.9510	-1685.5168	-3277.4971	-18.386
10	A2	-1706.4516	-1685.5168	-3391.9975	-18.261
11	A3	-1709.9545	-1685.5168	-3395.5006	-18.449
12	A4	-1741.9994	-1685.5168	-3427.5456	-18.512
13	A5	-1781.7078	-1685.5168	-3467.2538	-18.323