

## Carbonless DNA

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## Supplementary Information

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**Cartesian coordinates (in Å) of carbonless DNA(dimer) and DNA(hexamer)  
discussed in this work**

**Carbonless DNA(dimer)**

7	1.362537000	-0.919104000	-1.612997000
7	9.655691000	-2.709865000	-0.900763000
5	8.531223000	-0.708635000	0.283976000
8	8.880893000	-3.599703000	-0.165464000
7	5.293737000	-2.049433000	-1.204805000
8	7.705088000	-1.846359000	-1.773343000
7	2.265329000	0.028050000	-1.463808000
5	1.619142000	-2.434497000	-1.681201000
7	8.878128000	-1.523311000	-1.093249000
7	3.760592000	-3.778261000	-1.356121000
7	3.043902000	-2.593273000	-1.424750000
7	3.514387000	-0.139819000	-1.341255000
8	0.705208000	-3.291537000	-1.931187000
5	5.140865000	-3.481905000	-1.229238000
5	6.501171000	-1.199947000	-1.076647000
5	3.961150000	-1.529615000	-1.320954000
7	1.811827000	1.312886000	-1.514237000
7	7.051920000	-1.130170000	0.428251000
8	8.642364000	0.698546000	-0.153325000
1	0.383789000	-0.584648000	-1.669057000
1	9.747125000	-3.113083000	-1.838010000
1	9.277558000	-1.037559000	1.163965000
1	9.444445000	-0.914239000	-1.693055000
1	6.001886000	-4.315839000	-1.145338000
1	6.346617000	-0.068062000	-1.471603000
1	6.485988000	-0.491042000	0.987079000
1	6.982853000	-2.042376000	0.876732000
1	0.821894000	1.383973000	-1.244593000
1	2.437645000	1.897507000	-0.952221000
1	8.068412000	-3.748446000	-0.682564000
7	0.062010000	-1.176599000	1.423655000
7	5.758711000	2.411411000	-0.713945000
5	5.410207000	4.305785000	1.103499000
7	1.434458000	-3.222861000	1.542452000
8	6.342639000	1.786640000	0.400616000
7	3.430541000	1.218883000	2.021657000
8	3.634255000	2.908768000	0.198144000
7	-0.022481000	0.105378000	1.411318000
5	1.358035000	-1.819349000	1.613084000
7	4.865302000	3.408623000	-0.185060000
7	3.768242000	-1.080567000	2.143602000
1	4.075892000	-2.018290000	2.341723000
7	2.417674000	-0.893750000	1.872129000
7	0.866569000	1.027216000	1.547620000
5	4.395683000	0.192191000	2.267758000
5	3.540595000	2.690064000	1.744084000
8	8.527261000	3.126996000	-0.247067000
5	2.189847000	0.515950000	1.811831000
7	4.900947000	3.358317000	2.238175000
15	7.994252000	1.901382000	0.645838000
8	8.149113000	1.948738000	2.128171000
8	4.681481000	5.525719000	1.097808000
1	5.143445000	1.671945000	-1.086961000
1	6.618669000	4.411689000	1.041585000

1	-0.980444000	0.442908000	1.250071000
1	4.682472000	4.031314000	-0.973790000
1	5.553380000	0.313872000	2.557434000
1	2.597799000	3.339045000	2.131592000
1	4.719676000	3.907134000	3.073697000
1	5.613847000	2.663690000	2.466405000
1	0.605490000	-3.727466000	1.236736000
1	2.296762000	-3.710219000	1.358364000
1	5.238037000	6.280135000	0.912027000
5	-3.502876000	-1.449128000	0.969233000
8	-8.537494000	-3.336057000	1.592817000
7	-3.513422000	-5.813547000	0.425483000
8	-3.090293000	-0.127877000	1.129443000
1	-3.774030000	0.531687000	0.981171000
8	-8.614359000	0.792607000	0.561271000
7	-2.432857000	-2.379965000	1.030966000
5	-8.494421000	-0.681466000	0.442734000
7	-2.572606000	-3.714253000	0.859428000
7	-7.151373000	-1.107488000	-0.215554000
5	-5.101433000	-3.292618000	0.515898000
5	-3.809310000	-4.286561000	0.551002000
7	-4.866432000	-1.892969000	0.757955000
5	-6.016360000	-0.942426000	0.892388000
8	-1.480748000	-4.428519000	1.004656000
8	-6.816083000	-1.289587000	2.163077000
7	-8.186778000	-1.115480000	1.978248000
7	-8.891778000	-2.279495000	2.418293000
1	-1.452154000	-2.074308000	1.159392000
1	-9.475566000	-1.229879000	0.026462000
1	-7.206759000	-2.087917000	-0.495670000
1	-6.944830000	-0.572995000	-1.059440000
1	-6.257797000	-3.641749000	0.313602000
1	-5.699399000	0.232042000	0.913629000
1	-8.503800000	-0.362782000	2.597764000
1	-8.498099000	-2.480894000	3.342434000
1	-2.468674000	-5.751793000	0.645091000
1	-3.988298000	-6.404573000	1.103002000
1	-3.658148000	-6.203479000	-0.502291000
1	-7.566158000	-3.426201000	1.625735000
7	-1.835974000	0.871095000	-1.520041000
8	-6.783547000	2.164949000	-0.560684000
8	-8.540581000	1.195617000	-2.060006000
8	-1.021923000	1.704338000	-1.078228000
8	-4.505132000	5.579749000	-0.878054000
7	-1.464223000	-0.304988000	-1.793439000
8	-9.232601000	3.032217000	-0.244988000
5	-5.323892000	4.441065000	-1.089378000
5	-2.407644000	-1.359804000	-2.210930000
7	-4.619354000	3.422910000	-2.054163000
15	-8.376465000	1.742273000	-0.683860000
5	-4.144798000	0.368198000	-2.091901000
7	-3.786419000	-0.951880000	-2.375304000
7	-3.141157000	1.317712000	-1.676869000
5	-3.470587000	2.740071000	-1.197847000
8	-4.151843000	2.602510000	0.170966000
7	-5.210557000	3.492172000	0.294538000
7	-1.911550000	-2.636585000	-2.413559000
7	-6.405263000	2.808008000	0.643144000
1	-6.497428000	4.630196000	-1.316826000
1	-4.211554000	3.921451000	-2.840317000
1	-5.297401000	2.751518000	-2.413051000

1	-5.276690000	0.752412000	-2.185821000
1	-4.488488000	-1.622719000	-2.648295000
1	-2.539680000	3.488069000	-1.169976000
1	-5.007643000	4.106849000	1.087410000
1	-6.090245000	2.025106000	1.230370000
1	-0.921315000	-2.903313000	-2.225309000
1	-2.518316000	-3.406440000	-2.645515000
1	-5.014393000	6.387966000	-0.839881000
1	8.240085000	3.960921000	0.147194000
1	-9.284186000	3.673624000	-0.963049000
1	3.226420000	-4.621487000	-1.500621000

### Carbonless DNA(hexamer)

7	-4.620713000	0.871877000	-1.811076000
7	-3.336270000	2.739717000	-2.795761000
7	-5.478012000	0.451365000	-0.962836000
5	-4.306498000	2.302010000	-1.897738000
7	-5.134256000	4.464140000	-0.822075000
1	-4.666512000	5.031826000	-1.513653000
7	-5.113280000	3.094506000	-1.020956000
7	-6.208514000	1.061210000	-0.086676000
5	-6.026750000	2.493423000	-0.108370000
5	-8.584901000	4.782128000	3.645415000
8	-9.032646000	3.788927000	1.442532000
7	-9.508531000	4.777715000	2.297755000
7	-6.653719000	3.541204000	0.667953000
5	-6.097370000	4.760353000	0.166831000
1	-6.306531000	5.881570000	0.578748000
5	-7.597875000	3.356007000	1.788299000
7	-7.252313000	4.360230000	3.005231000
1	-7.619237000	2.210970000	2.200935000
1	-6.590532000	3.915456000	3.649011000
1	-6.783328000	5.186872000	2.627957000
8	-9.198404000	3.685663000	4.433622000
1	-8.623442000	5.867588000	4.174011000
1	-5.575656000	-0.573838000	-0.976072000
1	-10.430291000	4.453525000	2.615320000
1	-2.898588000	2.064493000	-3.424600000
1	-2.822239000	3.599014000	-2.684428000
8	-2.322046000	3.586668000	0.438553000
7	-4.442405000	0.878819000	2.936469000
5	-3.673885000	0.516659000	1.754933000
5	-4.520126000	2.259063000	3.304253000
5	-3.724149000	3.330710000	2.343061000
8	-3.478936000	-0.785171000	1.295977000
1	-3.667328000	-1.437066000	1.980343000
7	-3.022266000	1.495007000	0.963305000
7	-3.028587000	2.814839000	1.252875000
1	-2.402720000	1.212453000	0.175020000
7	-8.300231000	0.664108000	4.187340000
5	-6.615252000	-0.621170000	5.672285000
8	-7.547645000	1.720635000	4.743246000
8	-6.530806000	-0.527444000	3.235359000
7	-7.433498000	-0.480350000	4.276792000
5	-5.087101000	-0.238505000	3.705963000
7	-5.313812000	0.092644000	5.244809000
1	-4.472303000	-1.294830000	3.627482000
1	-5.418445000	1.108891000	5.344938000
1	-4.513839000	-0.180922000	5.821389000
8	-9.559916000	2.180212000	6.347922000

15	-8.366740000	2.920124000	5.552060000
8	-7.334066000	3.674153000	6.308868000
8	-6.420320000	-2.089677000	5.803064000
7	-3.498647000	4.870236000	2.242079000
1	-2.838830000	4.818572000	1.388984000
1	-3.057397000	5.323479000	3.040454000
1	-4.326513000	5.401825000	1.965480000
1	-8.274641000	0.890372000	3.176727000
1	-7.232072000	-0.131171000	6.590196000
1	-5.126089000	2.568558000	4.322185000
1	-8.066350000	-1.280384000	4.165322000
7	1.309945000	0.382516000	0.855155000
7	0.221157000	2.499486000	1.552600000
7	1.393677000	-0.896557000	0.890910000
5	0.342076000	1.092685000	1.684674000
7	-1.276264000	0.485636000	3.571086000
1	-1.558697000	1.447300000	3.699675000
7	-0.381050000	0.217911000	2.551952000
7	0.759653000	-1.778508000	1.580851000
5	-0.175873000	-1.191957000	2.506440000
7	-4.467128000	-3.957963000	4.424076000
5	-2.230552000	-5.031592000	5.136077000
8	-4.049593000	-3.051824000	5.425561000
8	-2.584430000	-3.699164000	3.094864000
7	-3.246725000	-4.547432000	3.954482000
7	-1.012336000	-1.817861000	3.510776000
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1	-2.411633000	-0.802306000	5.127570000
5	-1.180334000	-3.277643000	3.646236000
7	-1.310935000	-3.785555000	5.163624000
1	-0.320297000	-3.933183000	3.091010000
1	-0.384399000	-3.971446000	5.559558000
1	-1.754063000	-3.063833000	5.738041000
8	-5.775205000	-4.102519000	7.072601000
15	-5.176269000	-2.684830000	6.589215000
8	-4.465100000	-1.817024000	7.566916000
8	-1.563073000	-6.208657000	4.537358000
1	-4.727401000	-3.324134000	3.651456000
1	-2.848384000	-5.270332000	6.148504000
1	2.106045000	-1.259061000	0.237198000
1	-3.550932000	-5.370632000	3.421232000
1	0.811253000	2.877706000	0.808342000
1	-0.701595000	2.919916000	1.469788000
8	1.939415000	0.679274000	4.536579000
7	3.287604000	-3.292286000	3.920945000
5	3.691574000	-2.130689000	3.150512000
5	2.394683000	-3.101719000	5.029245000
5	1.876981000	-1.567225000	5.298470000
8	4.611162000	-2.172048000	2.094138000
1	4.976684000	-3.058510000	1.987330000
7	3.206890000	-0.835256000	3.438815000
7	2.342604000	-0.569310000	4.437562000
1	3.583908000	0.001203000	2.952376000
7	1.093962000	-6.320275000	2.876001000
5	3.436918000	-7.051651000	3.790508000
8	0.996373000	-5.949274000	4.231632000
8	3.055645000	-5.198011000	2.280979000
7	2.510292000	-6.413704000	2.609225000
5	3.867095000	-4.600983000	3.469071000
7	3.775821000	-5.758659000	4.554520000
1	5.011896000	-4.541088000	3.065749000

1	4.655407000	-5.892750000	5.060105000
1	3.049969000	-5.516136000	5.238602000
8	-0.171925000	-8.248025000	4.637078000
15	-0.174800000	-6.710178000	5.132167000
8	0.130549000	-6.398296000	6.553331000
7	0.859989000	-0.810837000	6.204521000
1	1.038525000	0.160873000	5.735931000
1	1.055123000	-0.790829000	7.203265000
1	-0.116980000	-1.068633000	6.055902000
1	0.832731000	-5.445534000	2.390319000
1	2.833883000	-7.913133000	4.396994000
1	2.091908000	-4.070940000	5.717341000
1	2.563573000	-7.003006000	1.772001000
7	5.274693000	0.687018000	1.078622000
8	9.102315000	3.648471000	-4.262405000
7	4.720938000	4.662915000	0.729073000
1	4.183107000	5.231955000	1.366315000
7	5.997622000	1.292152000	0.193161000
5	5.708923000	4.965949000	-0.233027000
5	8.366119000	4.789575000	-3.662742000
5	5.740033000	2.710853000	0.145890000
7	7.040246000	4.358841000	-3.020163000
5	3.999871000	2.522683000	1.914140000
7	4.758465000	3.305178000	0.990540000
7	6.350018000	3.753499000	-0.644405000
7	4.387259000	1.110414000	1.893640000
5	7.413113000	3.592296000	-1.649047000
7	3.009189000	2.972942000	2.799036000
8	8.681876000	4.342208000	-1.235798000
7	9.226713000	5.057885000	-2.297480000
1	5.884387000	6.072854000	-0.695330000
1	8.348825000	5.790113000	-4.338288000
1	6.493960000	5.190665000	-2.787067000
1	6.440935000	3.768707000	-3.606097000
1	7.670855000	2.428976000	-1.905722000
1	10.154533000	4.659995000	-2.498494000
1	2.609211000	2.278607000	3.432686000
1	2.323859000	3.653348000	2.501350000
1	5.407177000	-0.333991000	1.136408000
5	3.615158000	0.510332000	-1.790810000
8	3.449184000	-0.774054000	-1.271718000
1	3.618055000	-1.458724000	-1.929985000
8	7.526970000	1.608254000	-4.343374000
8	7.393561000	3.246786000	-6.244576000
7	3.298907000	4.819323000	-2.521667000
8	6.703659000	-2.228245000	-5.529400000
7	2.907118000	1.504560000	-1.074050000
5	6.848843000	-0.758747000	-5.381616000
7	2.869625000	2.803248000	-1.437440000
7	5.489311000	-0.056822000	-5.152113000
5	4.433962000	2.189955000	-3.419923000
5	3.579742000	3.284860000	-2.535108000
7	4.404453000	0.833209000	-2.969808000
5	5.064955000	-0.335192000	-3.645994000
8	2.106743000	3.588517000	-0.689800000
8	6.416969000	-0.730556000	-2.998594000
7	7.461156000	-0.598652000	-3.888359000
7	8.233633000	0.597096000	-3.669157000
1	2.270598000	1.234827000	-0.293019000
1	7.578997000	-0.267014000	-6.213607000
1	5.588768000	0.956169000	-5.284747000

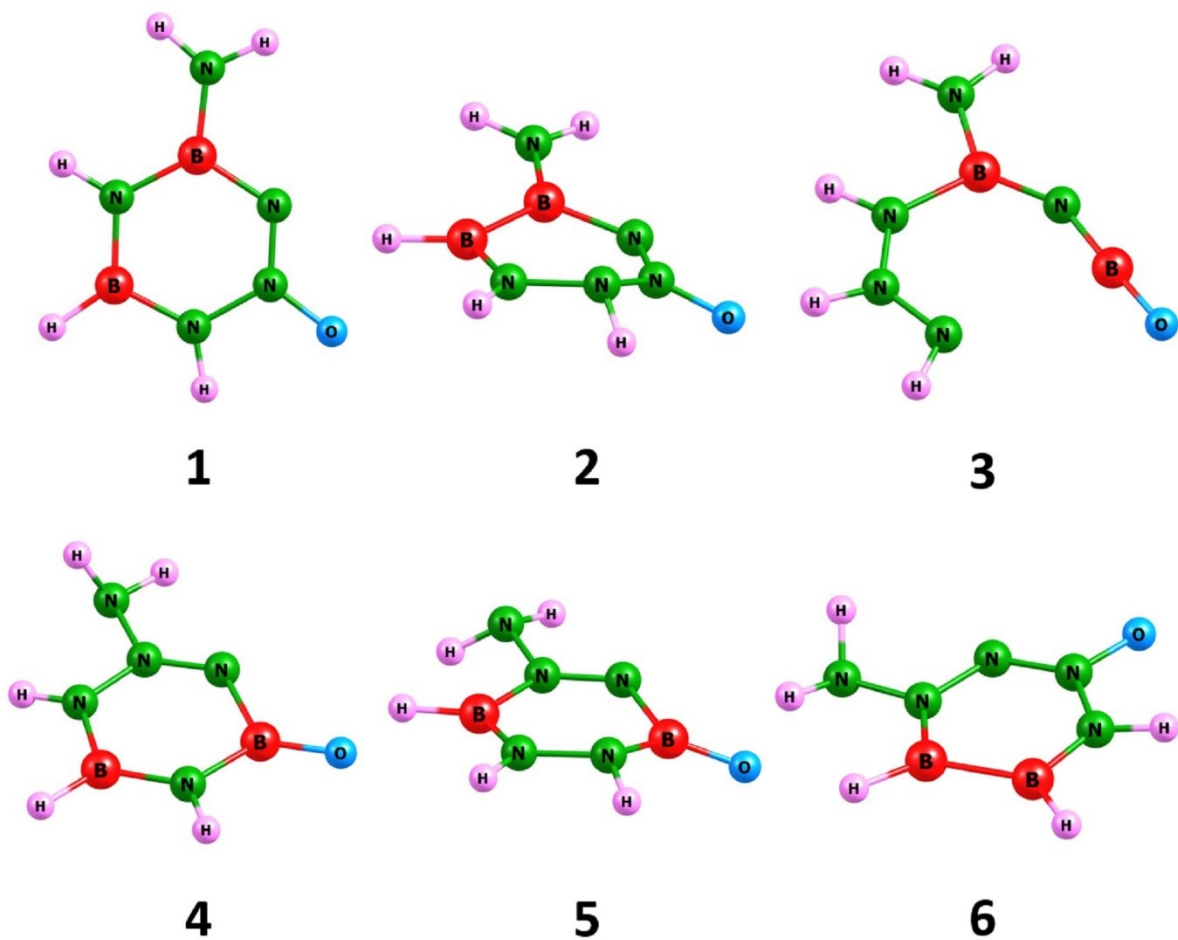
1	4.778510000	-0.371676000	-5.818327000
1	5.048717000	2.464002000	-4.443046000
1	4.382785000	-1.344414000	-3.611411000
1	8.116122000	-1.362651000	-3.690699000
1	8.044855000	0.822912000	-2.676808000
8	9.649982000	1.854341000	-5.861217000
15	8.383786000	2.677048000	-5.293989000
1	2.616939000	4.791536000	-1.686394000
1	4.097686000	5.397582000	-2.253260000
1	2.862623000	5.214237000	-3.353189000
7	-1.406957000	-0.944108000	-0.915849000
8	4.315735000	-3.161948000	-5.273105000
8	4.890044000	-2.052199000	-7.451649000
8	1.867266000	-6.291853000	-4.273077000
7	1.217617000	0.419282000	-3.650973000
1	1.479710000	1.383813000	-3.803144000
7	-0.716184000	-1.831467000	-1.544996000
5	1.711411000	-0.804478000	-4.160889000
5	2.507925000	-5.113102000	-4.897801000
5	0.198447000	-1.253505000	-2.496939000
7	1.542780000	-3.905675000	-5.006065000
5	-0.469898000	1.046421000	-1.834109000
7	0.324105000	0.159468000	-2.626207000
7	1.087890000	-1.887841000	-3.453090000
7	-1.404915000	0.336814000	-0.962978000
5	1.348182000	-3.338248000	-3.516923000
7	-0.413888000	2.462162000	-1.798430000
8	2.766631000	-3.642487000	-2.930458000
7	3.469609000	-4.538241000	-3.709223000
7	4.697729000	-3.964576000	-4.172268000
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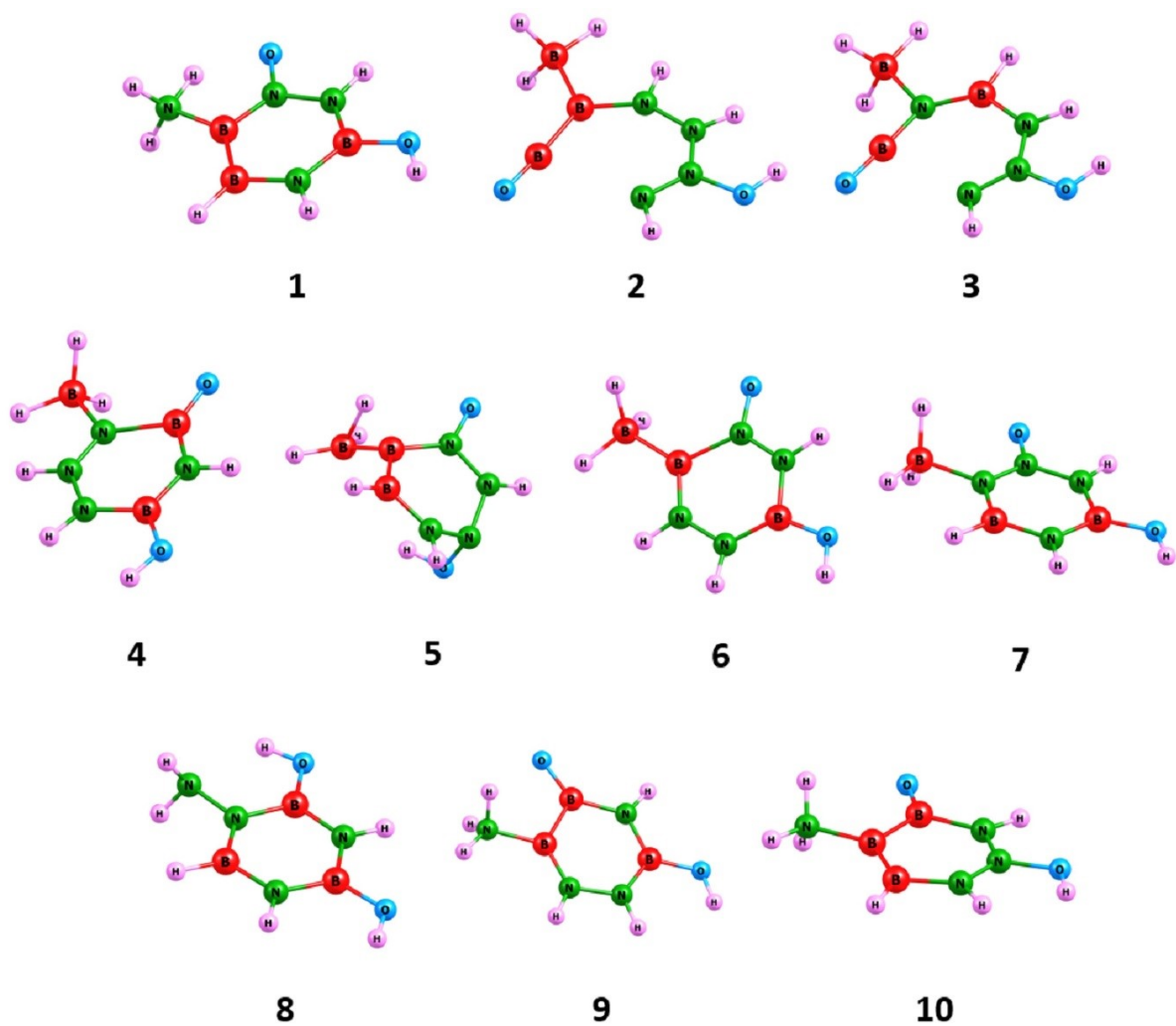


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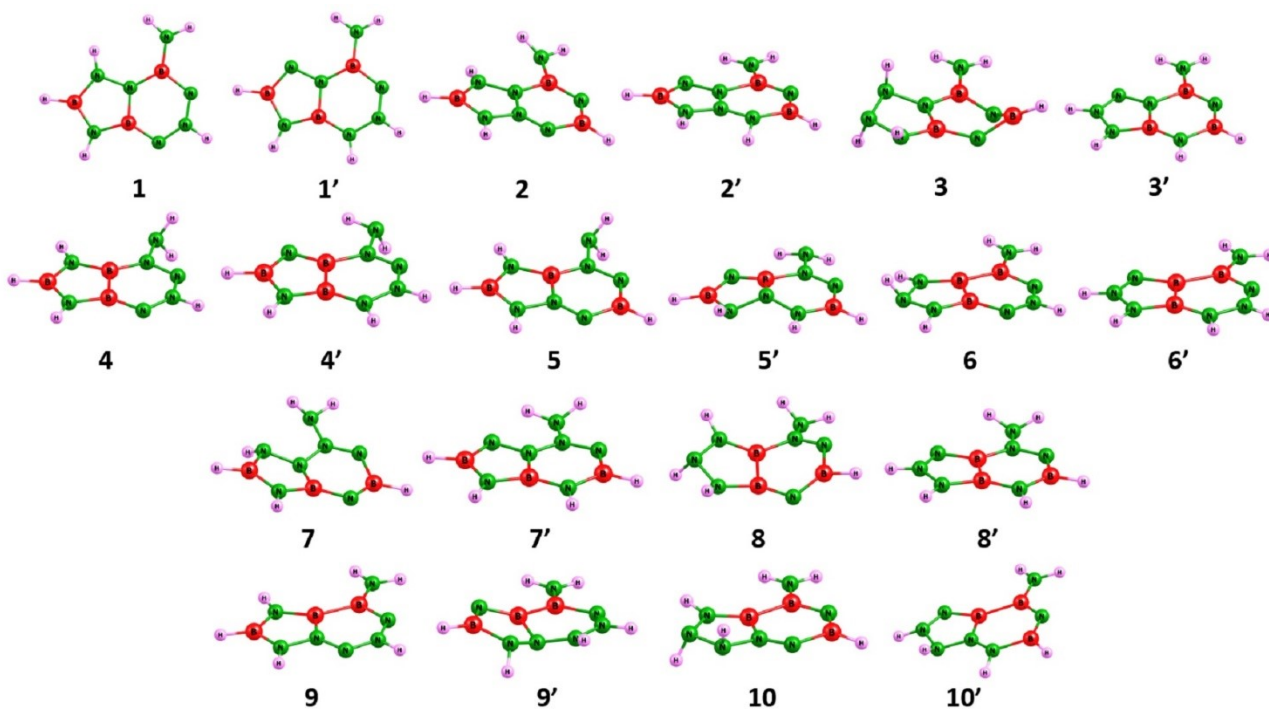
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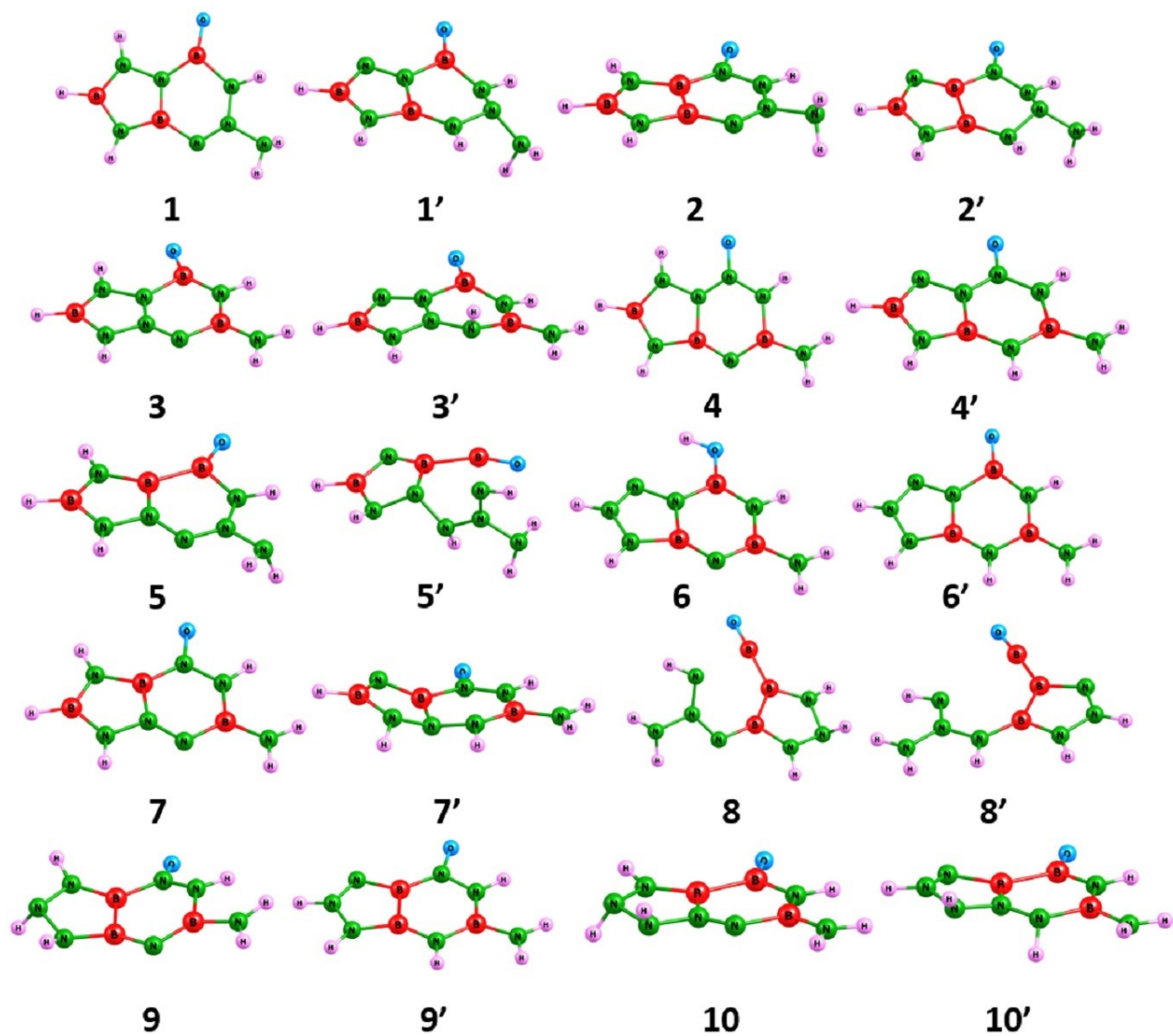
**Figure S1.** Isomeric structures of carbonless cytosine optimized at the  $\omega$ B97XD/aug-cc-pVDZ theory level.



**Figure S2.** Isomeric structures of carbonless thymine optimized at the  $\omega$ B97XD/aug-cc-pVDZ theory level.



**Figure S3.** Isomeric structures of carbonless adenine optimized at the  $\omega$ B97XD/aug-cc-pVDZ theory level.



**Figure S4.** Isomeric structures of carbonless guanine optimized at the  $\omega$ B97XD/aug-cc-pVDZ theory level.