

## SUPPORTING INFORMATION

### Intermolecular magnetic interactions in stacked DNA base pairs

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**Table S1:** Thymine (optimized geometry, at B3LYP/cc-pVTZ level of theory)

N	-1.11617900	-1.23839600	-0.00008800
C	0.23911200	-1.47534800	-0.00003000
H	0.52042800	-2.51925000	0.00004800
C	1.15265500	-0.48738500	-0.00006500
C	2.63155000	-0.71708100	0.00006400
H	2.86470500	-1.78123000	-0.00015100
H	3.09576000	-0.25778300	-0.87384500
H	3.09556200	-0.25818000	0.87428800
C	0.67101300	0.89538200	-0.00006300
O	1.38058100	1.88203900	0.00029500
N	-0.72569300	1.02889700	-0.00061000
H	-1.08334000	1.97343600	-0.00024400
C	-1.67647600	0.02741400	-0.00001000
O	-2.87215600	0.22430000	0.00035000
H	-1.77453300	-1.99910400	0.00024600

**Table S2:** Adenine (optimized geometry, at B3LYP/cc-pVTZ level of theory)

N	2.06916100	0.58519400	-0.00018500
C	2.28324900	-0.77432700	0.00014400
H	3.27877700	-1.18774100	0.00034800
N	1.17899600	-1.47006200	-0.00013400
C	0.17779600	-0.51687800	0.00001900
C	-1.22551100	-0.60765300	0.00008900
N	-1.87248500	-1.79153700	-0.00000800
H	-2.87574400	-1.80033000	-0.00005700
H	-1.35525000	-2.65069000	-0.00020300
N	-1.94066500	0.52465800	0.00011900
C	-1.29081500	1.69467200	-0.00000300
H	-1.92139600	2.57610200	0.00010500
N	0.02156100	1.91543400	-0.00011900
C	0.70762800	0.77160200	-0.00007200
H	2.76355900	1.31236000	0.00104000

**Table S3:** Guanine (optimized geometry, at B3LYP/cc-pVTZ level of theory)

N	1.72704100	-1.50107000	-0.00317300
C	2.70885800	-0.52996300	0.00111600
H	3.75588000	-0.78454100	-0.00013800
N	2.22074800	0.67667300	0.00674200

C	0.85278700	0.50323600	0.00664700
C	-0.21006500	1.46860800	0.00260800
O	-0.19176200	2.68003700	-0.00277400
N	-1.47362800	0.78739000	-0.00288800
H	-2.26511600	1.41082700	-0.06643000
C	-1.66983100	-0.56412000	-0.00307800
N	-2.96841000	-1.00506700	-0.06606900
H	-3.67991600	-0.43520800	0.36045700
H	-3.06523400	-1.99252900	0.10584200
N	-0.69395200	-1.43195800	0.00686800
C	0.52756100	-0.84801800	-0.00035500
H	1.85003400	-2.49906500	-0.00952400

**Table S4:** Cytosine (optimized geometry, at B3LYP/cc-pVTZ level of theory)

N	-1.20473400	-0.98852500	0.00000000
C	-0.06853500	-1.71706600	0.00000000
H	-0.17659000	-2.79275400	0.00000000
C	1.13400100	-1.09778700	0.00000000
H	2.05575200	-1.65694500	0.00000000
C	1.10589000	0.33850100	0.00000000
N	2.27671700	1.01890900	0.00000000
H	2.24221500	2.02275900	0.00000000
H	3.16243300	0.55160600	0.00000000
N	0.00000000	1.04929900	0.00000000
C	-1.22134700	0.43565300	0.00000000
O	-2.29710100	0.99873100	0.00000000
H	-2.11094200	-1.42810100	0.00000000

**Table S5:** Adenine-Thymine (optimized geometry, at B3LYP/cc-pVTZ level of theory)

N	4.99119500	0.53972300	0.00102500
C	5.23349900	-0.81536000	0.00091800
H	6.23692300	-1.20896300	0.00135100
N	4.14250200	-1.53146200	0.00030600
C	3.12321100	-0.59901000	-0.00008200
C	1.72007000	-0.72984800	-0.00078100
N	1.09822200	-1.91561600	-0.00143500
H	0.08239100	-1.96965500	-0.00105800
H	1.65285100	-2.75206100	-0.00064000
N	0.99292200	0.40534200	-0.00090700
C	1.61655700	1.59428100	-0.00041000
H	0.95877200	2.45560800	-0.00055400
N	2.92156500	1.83328700	0.00022700
C	3.62704100	0.69812400	0.00037200
H	5.66979900	1.28165900	0.00147700
N	-1.88886600	0.41355800	-0.00044700
N	-3.89294100	1.56268400	0.00035700
C	-2.50732300	1.64315500	-0.00019900
C	-2.50611700	-0.82774200	-0.00014200
C	-3.96721400	-0.81925600	0.00041300
C	-4.58425400	0.37779300	0.00064800
O	-1.91863800	2.70522800	-0.00044500
O	-1.83760600	-1.85851800	-0.00034300
H	-0.84655900	0.42449200	-0.00090900
H	-4.37515000	2.44565200	0.00063600
H	-5.66145600	0.47166800	0.00105600
C	-4.69034800	-2.12966400	0.00071200
H	-4.42057000	-2.72391500	-0.87357500
H	-5.76978200	-1.98187600	0.00092700

H -4.42020100 -2.72373400 0.87501000

**Table S6:** Guanine-Cytosine (optimized geometry, at B3LYP/cc-pVTZ level of theory).

N	4.66215100	0.47789800	-0.01002800
C	4.96101900	-0.87288300	-0.01349000
H	5.97960600	-1.22494200	-0.01942800
N	3.89938400	-1.62340600	-0.00969200
C	2.84100000	-0.73438500	-0.00214000
C	1.43127400	-0.95031400	0.00441500
O	0.80990900	-2.01667000	0.00482100
N	0.72991000	0.26617400	0.01054300
H	-0.29588300	0.18218700	0.01273600
C	1.28840600	1.51711900	0.01053500
N	0.43668000	2.55979600	0.02147900
H	-0.57499100	2.44756600	0.00795700
H	0.84167400	3.47692400	0.00628400
N	2.59152000	1.72577900	0.00351000
C	3.29862200	0.58253500	-0.00228000
H	5.30623000	1.24971700	-0.01204300
N	-4.33404600	0.90780700	-0.01514500
C	-4.93292300	-0.30882500	-0.01380700
H	-6.01340900	-0.31697300	-0.02164500
C	-4.18912000	-1.43492000	-0.00327300
H	-4.64911000	-2.40998100	-0.00228800
C	-2.75858100	-1.27469900	0.00625400
N	-1.95832200	-2.33941000	0.01605300
H	-0.93029600	-2.22867100	0.01913700
H	-2.35327200	-3.26184500	0.01538000
N	-2.19157000	-0.06799600	0.00564000
C	-2.93674200	1.06166900	-0.00548200
O	-2.47330700	2.20017900	-0.00781500
H	-4.87104500	1.75966800	-0.02305100

**Table S7:** AATTC geometry (taken from PDB)

N	1.72058265	-4.08701478	6.02010397
C	2.98758265	-3.90001478	5.53510397
N	3.19258265	-2.65701478	5.06610397
C	2.00258265	-2.05001478	5.25110397
C	1.55958265	-0.72401478	4.97210397
N	2.37458265	0.21898522	4.42110397
N	0.29558265	-0.42501478	5.27110397
C	-0.49241735	-1.35101478	5.82210397
N	-0.20741735	-2.61101478	6.13710397
C	1.07958265	-2.89301478	5.81410397
N	-1.75241735	-4.47701478	3.23110397
C	-0.55541735	-5.10401478	3.02110397
N	0.37858265	-4.28901478	2.50910397
C	-0.25441735	-3.10201478	2.39910397
C	0.20258265	-1.81601478	1.96810397
N	1.49058265	-1.58501478	1.58010397
N	-0.67141735	-0.81201478	2.00510397
C	-1.91741735	-1.04101478	2.42510397
N	-2.46041735	-2.17901478	2.85110397
C	-1.55441735	-3.18001478	2.81010397
N	-3.64941735	-3.10001478	-0.28189603
C	-2.84841735	-2.08001478	-0.67089603
O	-3.28741735	-0.92601478	-0.70389603
N	-1.55141735	-2.36201478	-0.99489603
C	-1.03741735	-3.63101478	-0.96489603
O	0.15958265	-3.78101478	-1.22789603
C	-1.88941735	-4.67801478	-0.61189603

C	-1.40141735	-6.10101478	-0.61089603
C	-3.20541735	-4.38701478	-0.25289603
N	-4.84741735	-1.12701478	-4.08789603
C	-3.58441735	-0.68701478	-4.35289603
O	-3.34641735	0.51298522	-4.45789603
N	-2.57641735	-1.60001478	-4.43489603
C	-2.79441735	-2.94301478	-4.29589603
O	-1.81241735	-3.68601478	-4.34389603
C	-4.10141735	-3.39201478	-4.08189603
C	-4.40941735	-4.86301478	-3.95089603
C	-5.12541735	-2.45501478	-3.94289603
N	-4.14641735	1.01898522	-7.83189603
C	-2.85641735	0.59998522	-8.00689603
O	-1.97941735	1.44398522	-8.17689603
N	-2.56441735	-0.70601478	-7.97389603
C	-3.52941735	-1.60801478	-7.80089603
N	-3.20941735	-2.92801478	-7.75789603
C	-4.86741735	-1.22801478	-7.66989603
C	-5.17141735	0.12998522	-7.67989603
N	3.84258265	-2.70401478	-8.37889603
C	3.69258265	-3.94101478	-7.80789603
N	2.40958265	-4.25901478	-7.56589603
C	1.72958265	-3.17101478	-7.97889603
C	0.32558265	-2.91301478	-7.96489603
O	-0.58841735	-3.62501478	-7.56689603
N	0.04158265	-1.65401478	-8.42889603
C	0.93558265	-0.73501478	-8.87389603
N	0.46358265	0.48998522	-9.22889603
N	2.24158265	-0.98601478	-8.91889603
C	2.56558265	-2.20901478	-8.46289603
N	3.40858265	1.09198522	-6.08889603
C	4.17658265	0.01698522	-5.71389603
N	3.44358265	-1.01901478	-5.26289603
C	2.17158265	-0.57901478	-5.35889603
C	0.90658265	-1.18601478	-5.06089603
N	0.77758265	-2.46601478	-4.60489603
N	-0.18841735	-0.44601478	-5.25389603
C	-0.07341735	0.79798522	-5.72889603
N	1.02958265	1.46898522	-6.06389603
C	2.12058265	0.70298522	-5.84489603
N	1.43358265	3.36998522	-3.09189603
C	2.74058265	2.96398522	-3.01689603
N	2.86858265	1.70298522	-2.57089603
C	1.59558265	1.30598522	-2.36689603
C	1.04458265	0.06998522	-1.91389603
N	1.81258265	-1.00901478	-1.60389603
N	-0.28141735	-0.00901478	-1.81089603
C	-1.03441735	1.03798522	-2.13889603
N	-0.65141735	2.23098522	-2.58189603
C	0.69658265	2.28798522	-2.67289603
N	-1.06141735	3.84698522	0.35810397
C	-1.22841735	2.57198522	0.80910397
O	-2.35941735	2.09798522	0.95510397
N	-0.11941735	1.82198522	1.06610397
C	1.14458265	2.31798522	0.93010397
O	2.08458265	1.56698522	1.18210397
C	1.30158265	3.64398522	0.51510397
C	2.67458265	4.23598522	0.38710397
C	0.17358265	4.40198522	0.20110397
N	-3.01041735	3.06698522	4.35810397
C	-2.41341735	1.87698522	4.63910397
O	-3.08741735	0.86298522	4.84410397

N	-1.05041735	1.82598522	4.65010397
C	-0.26841735	2.91098522	4.37810397
O	0.95458265	2.76098522	4.40510397
C	-0.89641735	4.12298522	4.08610397
C	-0.10741735	5.35498522	3.76510397
C	-2.28541735	4.18398522	4.07910397
H	3.73664838	-4.66406619	5.53000709
H	2.04664941	1.15636190	4.30369550
H	-1.49134647	-1.03577606	6.04042750
H	-0.38215546	-6.13651049	3.24208572
H	2.16801593	-2.31867535	1.63326723
H	-2.56966425	-0.19282307	2.41840985
H	-2.19782578	-6.75098138	-0.31394984
H	-0.58678128	-6.19821985	0.07599497
H	-1.07254532	-6.36598012	-1.59402193
H	-3.86566642	-5.17452376	0.04509857
H	-5.45938269	-4.99484733	-3.79248841
H	-3.86980994	-5.26781399	-3.12031704
H	-4.11751401	-5.36971643	-4.84696850
H	-6.12251034	-2.77560340	-3.72397018
H	-3.92263482	-3.61044298	-7.59785665
H	-5.63861007	-1.96222939	-7.56458365
H	-6.18077301	0.46812353	-7.57143572
H	4.51354785	-4.58766843	-7.57821104
H	-0.50859946	0.70033307	-9.12586337
H	5.24482807	0.00386309	-5.77372511
H	-0.12881927	-2.83384058	-4.39719489
H	-0.99330500	1.32898365	-5.85830771
H	3.56999196	3.58464551	-3.28477845
H	1.38347385	-1.85025394	-1.27498522
H	-2.09015595	0.90091327	-2.03153081
H	3.40587611	3.50151982	0.65294314
H	2.76185639	5.07893004	1.04034766
H	2.83499211	4.54961371	-0.62324545
H	0.27627756	5.40473099	-0.15785934
H	0.93779512	5.12929257	3.80375259
H	-0.33384105	6.11951763	4.47863218
H	-0.36255708	5.69626665	2.78360986
H	-2.78187716	5.10505142	3.85535253
H	-4.00889922	3.12204640	4.35661141
H	-0.60538024	0.95703097	4.86657683
H	3.30057330	-0.02640600	4.13418160
H	1.34436814	-4.91552379	6.43487556
H	-2.58941225	-4.87355144	3.60819576
H	-1.86965823	4.39214491	0.13551106
H	-0.23631232	0.87484123	1.36485778
H	1.75683433	-0.68210638	1.24266295
H	-4.59109224	-2.90320023	-0.00892637
H	-0.95147271	-1.60918699	-1.26566666
H	1.09016056	4.26136002	-3.38772069
H	2.80631109	-0.96103683	-1.70490046
H	-5.58757791	-0.46066678	-3.99765916
H	-1.64499207	-1.27697773	-4.60250871
H	3.72218264	1.96650295	-6.45886058
H	1.58947277	-3.03598034	-4.47850899
H	-4.34350527	1.99922317	-7.81486915
H	4.69137240	-2.26191616	-8.66890424
H	1.08869036	1.18041308	-9.59296980
H	-2.26071784	-3.21695003	-7.88629250
H	-0.92178315	-1.38607455	-8.44048765

**Table S8:** CGCGA geometry (taken from PDB)

N	3.39958265	8.65798522	15.53310397
C	3.55358265	7.45098522	16.16810397
O	4.68958265	7.01098522	16.36710397
N	2.47258265	6.75798522	16.53010397
C	1.24658265	7.22298522	16.27310397
N	0.15758265	6.47398522	16.59710397
C	1.04858265	8.43898522	15.62410397
C	2.17258265	9.16798522	15.25410397
N	5.56658265	5.46698522	12.93310397
C	4.85558265	6.58098522	12.58210397
N	3.53658265	6.45198522	12.78910397
C	3.41258265	5.20898522	13.29510397
C	2.23358265	4.52198522	13.69810397
O	1.06858265	4.91298522	13.67110397
N	2.52658265	3.27598522	14.19010397
C	3.76358265	2.71398522	14.30810397
N	3.83758265	1.45298522	14.82110397
N	4.86658265	3.35698522	13.92310397
C	4.61958265	4.59098522	13.42710397
N	5.52558265	1.88598522	10.67410397
C	4.23858265	1.58098522	10.96910397
O	4.01458265	0.50898522	11.53510397
N	3.26458265	2.44398522	10.65510397
C	3.54658265	3.59998522	10.05010397
N	2.55058265	4.49598522	9.78210397
C	4.85558265	3.94198522	9.72410397
C	5.86658265	3.04498522	10.05210397
N	4.63458265	-1.72201478	8.02210397
C	5.34658265	-0.74001478	7.38510397
N	4.64258265	0.39098522	7.23010397
C	3.45058265	0.09698522	7.78810397
C	2.28158265	0.90098522	7.90210397
O	2.09858265	2.05398522	7.52110397
N	1.26258265	0.21098522	8.50510397
C	1.30158265	-1.07301478	8.96910397
N	0.16058265	-1.58701478	9.50610397
N	2.39758265	-1.82401478	8.87010397
C	3.41358265	-1.17801478	8.27410397
N	1.72058265	-4.08701478	6.02010397
C	2.98758265	-3.90001478	5.53510397
N	3.19258265	-2.65701478	5.06610397
C	2.00258265	-2.05001478	5.25110397
C	1.55958265	-0.72401478	4.97210397
N	2.37458265	0.21898522	4.42110397
N	0.29558265	-0.42501478	5.27110397
C	-0.49241735	-1.35101478	5.82210397
N	-0.20741735	-2.61101478	6.13710397
C	1.07958265	-2.89301478	5.81410397
N	-3.01041735	3.06698522	4.35810397
C	-2.41341735	1.87698522	4.63910397
O	-3.08741735	0.86298522	4.84410397
N	-1.05041735	1.82598522	4.65010397
C	-0.26841735	2.91098522	4.37810397
O	0.95458265	2.76098522	4.40510397
C	-0.89641735	4.12298522	4.08610397
C	-0.10741735	5.35498522	3.76510397
C	-2.28541735	4.18398522	4.07910397
N	-3.34241735	1.55298522	8.48410397
C	-2.13641735	0.93598522	8.48210397
O	-2.11041735	-0.27201478	8.73210397

N	-1.03141735	1.63598522	8.18810397
C	-1.11041735	2.93498522	7.89210397
N	0.01458265	3.62498522	7.55710397
C	-2.33241735	3.60598522	7.88910397
C	-3.47741735	2.87498522	8.18810397
N	-3.07141735	1.35398522	12.69610397
C	-3.63341735	2.54198522	12.31210397
N	-2.74941735	3.35898522	11.71910397
C	-1.59841735	2.64998522	11.73310397
C	-0.30041735	2.99998522	11.25510397
O	0.07658265	4.05398522	10.73810397
N	0.59758265	1.97998522	11.46110397
C	0.35258265	0.77298522	12.04410397
N	1.39558265	-0.08901478	12.19110397
N	-0.85541735	0.44898522	12.50310397
C	-1.76841735	1.42598522	12.30410397
N	-0.52641735	-0.07101478	16.32310397
C	0.52858265	0.59198522	15.78310397
O	1.58658265	-0.01901478	15.65710397
N	0.39658265	1.87398522	15.41010397
C	-0.77241735	2.50698522	15.55710397
N	-0.89941735	3.80998522	15.17110397
C	-1.87541735	1.86298522	16.12010397
C	-1.73541735	0.53698522	16.51210397
N	2.49358265	0.65598522	19.29210397
C	1.20358265	0.53298522	19.73310397
N	0.45858265	1.61098522	19.46110397
C	1.31958265	2.43298522	18.82610397
C	1.09458265	3.72598522	18.27010397
O	0.04858265	4.36998522	18.22010397
N	2.25558265	4.25398522	17.75710397
C	3.48658265	3.66298522	17.73210397
N	4.53758265	4.38298522	17.24910397
N	3.67958265	2.43498522	18.20610397
C	2.56058265	1.88998522	18.72310397
H	0.27641164	5.57655510	17.02195553
H	0.06301317	8.80043478	15.41696388
H	2.07300030	10.11162416	14.75960535
H	5.30568447	7.46580129	12.18284358
H	3.00522262	0.98315664	15.11510719
H	1.61276986	4.30204206	10.07001580
H	5.07765628	4.86767395	9.23555135
H	6.88830652	3.26229117	9.82024527
H	6.35470116	-0.86211314	7.04792590
H	0.16341096	-2.50595989	9.90047928
H	3.73664838	-4.66406619	5.53000709
H	2.04664942	1.15636190	4.30369550
H	-1.49134647	-1.03577606	6.04042750
H	0.93779512	5.12929257	3.80375259
H	-0.33384105	6.11951763	4.47863218
H	-0.36255708	5.69626665	2.78360986
H	-2.78187716	5.10505142	3.85535253
H	0.90234451	3.16468321	7.55807276
H	-2.38779466	4.65054219	7.66386173
H	-4.44090946	3.34036287	8.18553627
H	-4.66236149	2.79104800	12.46747993
H	1.25949199	-0.96389418	12.65593228
H	-1.75213337	4.30233317	15.34565736
H	-2.80519509	2.37717531	16.24668165
H	-2.55388174	0.00551825	16.95091933
H	0.83089691	-0.33206579	20.24073779
H	5.38210291	4.07477059	17.68704149

H	4.18019239	9.20999262	15.23995509
H	3.24809227	0.00053892	19.32535125
H	-3.48706832	0.58458874	13.18114348
H	-4.16774259	1.00344434	8.61388484
H	-0.41352075	-1.02794784	16.59056139
H	6.55947293	5.35592067	12.89028390
H	6.25955164	1.25987304	10.93730172
H	1.34436815	-4.91552379	6.43487556
H	4.94650844	-2.64365347	8.25293818
H	-4.00889922	3.12204641	4.35661141
H	-0.68011934	-1.04551671	9.50606536
H	0.39762006	0.70008446	8.61745013
H	2.29798415	0.15253774	11.83427920
H	1.53372817	2.14144961	11.14875671
H	4.72422012	0.99789687	14.90337544
H	1.75207810	2.72132363	14.49423095
H	2.19192485	5.16930714	17.35944398
H	3.30057331	-0.02640600	4.13418159
H	4.39522293	5.35316369	17.44528614
H	-0.76148467	6.82102186	16.41033985
H	-0.13974889	4.27229058	14.71374462
H	2.75939600	5.34573510	9.29803567
H	-0.04694435	4.59204461	7.31010080
H	-0.60538024	0.95703098	4.86657682

**Table S9:** Shielding values (in ppm) for thymine employing B3LYP and KT3 functionals and Pople-type basis sets.

	<b>N3</b>	<b>H3</b>	<b>C2</b>	<b>C4</b>
B3LYP/6-311G	88.40	26.76	39.78	26.05
B3LYP/6-311G(d,p)	84.13	25.50	32.97	19.56
B3LYP/6-311++G(d,p)	80.52	25.06	30.78	17.07
B3LYP/6-311G(2df,2pd)	82.87	24.83	30.70	17.15
KT3/6-311++G(d,p)	93.10	25.18	49.62	37.69
KT3/6-311++G(2d,2p)	90.84	24.68	48.78	36.90
KT3/6-311G(2df,2pd)	95.38	24.92	49.93	38.04
KT3/6-311++G(3df,3pd)	92.85	24.47	48.06	36.17

**Table S10:** Shielding values (in ppm) for thymine at B3LYP/cc-pVTZ level of theory.

<b>B3LYP/cc-pVTZ</b>								
<b>(ppm)</b>	<b>C4</b>	<b>N3</b>	<b>H3</b>	<b>C2</b>	<b>N1</b>	<b>H1</b>	<b>O4</b>	<b>O2</b>
<b><math>\sigma</math> dia</b>	238,73	317,28	32,42	240,57	313,37	31,35	401.09	397.44
<b><math>\sigma</math> para</b>	-221,56	-234,93	-7,64	-209,65	-196,99	-5,76	-490.62	-388.15
<b><math>\sigma</math></b>	17,17	82,36	24,78	30,92	116,38	25,6	-89.53	9.28

**Table S11:** Shielding values (in ppm) for thymine at KT2/cc-pVTZ level of theory.

KT2/cc-pVTZ								
(ppm)	C4	N3	H3	C2	N1	H1	O4	O2
$\sigma$ dia	489,71	502,90	26,71	468,91	472,00	-33,04	444,62	406,46
$\sigma$ para	-453,16	-409,12	-2,00	-420,43	-347,71	58,49	-502,62	-376,29
$\sigma$	36,55	93,77	24,71	48,48	124,28	25,45	-57,99	30,16

**Table S12:** Shielding values (in ppm) for thymine at KT2/aug-cc-pVTZ level of theory.

KT2/aug-cc-pVTZ								
(ppm)	C4	N3	H3	C2	N1	H1	O4	O2
$\sigma$ dia	497,37	504,55	27,35	478,96	465,47	-33,23	445,46	408,16
$\sigma$ para	-461,19	-411,37	-2,95	-430,67	-341,29	58,43	-495,56	-369,05
$\sigma$	36,18	93,18	24,40	48,29	124,28	25,20	-50,09	39,11

**Table S13:** Shielding values (in ppm) for thymine at KT3/cc-pVTZ level of theory.

KT3/cc-pVTZ								
(ppm)	C4	N3	H3	C2	N1	H1	O4	O2
$\sigma$ dia	490,11	503,37	26,56	469,41	472,12	-33,34	444,21	406,09
$\sigma$ para	-453,15	-408,78	-1,69	-420,39	-347,55	58,92	-500,02	-374,10
$\sigma$	36,95	94,58	24,86	49,02	124,56	25,58	-55,80	31,98

**Table S14:** J-couplings ( in Hz) for thymine at B3LYP/cc-pVTZ, KT3/cc-pVTZ and SOPPA/cc-pVTZ levels of theory.

	FC	SD	PSO	DSO	Total
B3LYP/cc-pVTZ					
J(N3-C4)	-10.58	-0.07	2.69	-0.15	-8.11
J(N3-H3)	-80.54	-0.13	-1.98	-0.5	-83.15
J(C2-N1)	-22.51	-0.15	2.62	-0.15	-20.21
J(N1-H1)	-86.62	-0.21	-2.20	-0.46	-89.50
KT3/cc-pVTZ					
J(N3-C4)	-0.38	-0.08	2.36	-0.15	1.73
J(N3-H3)	-78.99	-0.15	-1.85	-0.49	-81.48
J(C2-N1)	-11.25	-0.17	2.24	-0.15	-9.33
J(N1-H1)	-85.99	-0.24	-2.06	-0.45	-88.73
SOPPA/cc-pVTZ					
J(N3-C4)	-10.99	-0.08	2.33	-0.15	-8.89
J(N3-H3)	-81.50	-0.07	-1.68	-0.49	-83.73
J(C2-N1)	-22.63	-0.13	2.31	-0.15	-20.59
J(N1-H1)	-86.48	-0.14	-1.91	-0.46	-88.98

**Table S15:** J-couplings ( in Hz) for adenine-thymine at KT3/6-311G(2df,2pd), B3LYP/cc-pVTZ and SOPPA/aug-cc-pCVTZ levels of theory.

	FC	SD	PSO	DSO	Total
<b>KT3/6-311G(2df,2pd)</b>					
J(N6-H6)	-94.63	-0.18	-1.44	-0.41	-96.68
J(N1-N3)	-4.87	-0.04	0.01	-0.01	-4.92
J(N3-H3)	-84.24	-0.08	-0.87	-0.59	-85.79
<b>B3LYP/cc-pVTZ</b>					
J(N6-H6)	-86.62	-0.14	-1.53	-0.41	-88.72
J(N1-N3)	-4.54	-0.04	0.01	-0.01	-4.59
J(N3-H3)	-80.83	-0.04	-0.95	-0.42	-82.43
<b>SOPPA/aug-cc-pCVTZ</b>					
J(N3-C4)	-11.46	-0.08	2.38	-0.14	-9.31

**Table S16:** Shielding values (in ppm) for GC base pair at B97//cc-pCVTZ/cc-pVTZ level of theory.

	Guanine						Cytosine				
	N1	N2	C6	C2	H1	H2	N4	N3	C4	C2	H4
Isolated GC pair	98.55	174.44	21.91	24.50	18.37	22.09	144.12	37.37	12.00	26.98	19.96
GCG	95.47	164.43	21.82	22.71	18.37	22.06	143.04	38.30	12.29	27.53	20.60
CGCGA	95.71	164.50	21.97	23.00	18.69	22.42	143.80	37.87	12.49	27.79	20.81

**Table S17:** Shielding values (in ppm) for GC base pair at B97-D//cc-pCVTZ/cc-pVTZ level of theory.

	Guanine						Cytosine				
	N1	N2	C6	C2	H1	H2	N4	N3	C4	C2	H4
Isolated GC pair	97.03	170.92	24.41	26.96	18.49	22.12	140.34	36.87	15.09	28.98	19.99
GCG	93.72	160.90	24.22	25.21	18.46	22.06	139.35	37.71	15.46	29.56	20.62
CGCGA	93.97	160.97	24.38	25.50	18.77	22.41	140.04	37.32	15.65	29.80	20.81

**Table S18:** J-couplings (in Hz) for GC base pair at B97-D/6-311G(2df,2pd) level of theory.

	FC	SD	PSO	DSO	Total
<b>Isolated</b>					
J(C6-N1)	-16.41	-0.17	2.76	-0.17	-13.98
J(N1-H1)	-72.51	-0.14	-1.14	-0.67	-74.46
J(N1-N3)	-4.18	-0.04	0.03	-0.01	-4.21
J(N2-H2)	-80.90	-0.20	-1.32	-0.46	-82.87
J(N4-H4)	-82.31	-0.27	-0.94	-0.45	-83.97
<b>GCG</b>					
J(C6-N1)	-16.48	-0.17	2.81	-0.21	-14.05
J(N1-H1)	-72.61	-0.17	-0.90	-0.84	-74.51
J(N1-N3)	-4.33	-0.04	0.04	-0.03	-4.36
J(N2-H2)	-81.15	-0.22	-1.09	-0.60	-83.06
J(N4-H4)	-82.23	-0.27	-0.83	-0.57	-83.91
<b>CGCGA</b>					
J(C6-N1)	-16.55	-0.17	2.82	-0.21	-14.11
J(N1-H1)	-72.54	-0.17	-0.88	-0.86	-74.44
J(N1-N3)	-4.33	-0.04	0.04	-0.03	-4.36
J(N2-H2)	-81.12	-0.22	-1.08	-0.62	-83.03
J(N4-H4)	-82.20	-0.27	-0.81	-0.60	-83.88