

Supplementary Material

Stacking with the unnatural DNA base 6-ethynylpyridone

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Computation of geometrical parameters

Table S1. Cartesian coordinates (in Å) of the optimised base pairs

Table S2. Cartesian coordinates (in Å) of the optimised dinucleotides

Table S3. Cartesian coordinates (in Å) of the stacked base pairs extracted from the optimised dinucleotides

Table S4. Cartesian coordinates (in Å) of the optimised dinucleotide duplexes

Table S5. Cartesian coordinates (in Å) of the stacked base pairs extracted from the optimised dinucleotide duplexes

Computation of geometrical parameters

The Rise is calculated as the scalar product of the vector ($\overline{m_1 m_2}$) connecting the midpoints of the base rings of the stacked bases and the plane vector of one of the bases. This corresponds to the component of $\overline{m_1 m_2}$ that is perpendicular to the base plane. As the two bases are not completely parallel in the optimised structures, this scalar product depends on which base's plane vector is used. The vertical distance presented herein is therefore computed as the average of the two values obtained when using the first or the second base's plane vector. The midpoints are calculated as the average of the atomic coordinates of C2, C4 and C6 for pyrimidine bases and 6-ethynylpyridone or the average of the atomic coordinates of C4 and C5 for purine bases. The base plane is defined by the C2, C4 and C6 atoms (pyrimidines) or C4, C5 and C2 atoms (purines). In H-bonded base pairs consisting of two pyrimidine bases, the direction of C2→C4→C6 is clockwise for one base and counterclockwise for the other base. This means if the plane vectors are defined by C2, C4, C6 (both in this order), a base pair with unflipped pyrimidine bases would have a tilt between 90 and 180°. To facilitate comparison with mixed pyrimidine/purine base pairs, where a pair with unflipped bases has a tilt between 0 and 90°, the tilt for pyrimidine/pyrimidine base pairs is converted to the 0-90° range by subtracting the value of the original tilt from 180°.

The Tilt is calculated as the angle between the plane vectors of the two H-bonded or stacked bases.

The Twist for stacked bases is calculated as the dihedral defined by the points C4(upper)-midpoint(upper)-midpoint(lower)-C4(lower).

Table S1. Cartesian coordinates (in Å) of the optimised base pairs

35			
CG			
H	6.57985900	-1.07029200	0.01903300
H	5.41030600	-2.04963300	-0.90161000
H	5.39114600	-2.07971600	0.88070600
C	5.56022300	-1.45503900	0.00155900
C	3.28041300	-0.40351300	-0.00340300
N	2.55191800	-1.54027300	-0.02802800
H	0.75361400	-3.26689600	-0.03708700
H	-0.63571700	-2.18903700	-0.02142200
N	0.37835000	-2.33001500	-0.07618700
C	1.25030500	-1.30830100	-0.03693000
H	-0.32462800	0.05917400	-0.01997900
N	0.70691200	-0.04474500	-0.01992000
O	0.83224600	2.23572100	0.01680800
C	1.42920000	1.14974500	0.00465500
C	2.83673200	0.91612700	0.01289200
N	3.90425200	1.79136800	0.03646700
H	5.98634200	1.34160200	0.04937700
C	4.95527600	1.01234100	0.03442700
N	4.64282600	-0.32792200	0.01080900
N	-4.35887300	-0.69495300	0.01980700
C	-4.96509600	0.52151300	-0.00428700
H	-6.04955800	0.51169600	-0.00522300
C	-4.24797400	1.67161400	-0.02504200
H	-4.73341400	2.63845000	-0.04335500
C	-2.82093000	1.54169600	-0.01971900
N	-2.03814700	2.62434500	-0.03606800
H	-1.01883800	2.52299500	-0.02181300
H	-2.44181200	3.55011300	-0.04903200
N	-2.22696000	0.34435400	0.00136800
C	-2.96575300	-0.79155800	0.02173300
O	-2.45405400	-1.92325800	0.04258300
C	-5.12936200	-1.93693600	0.04279300
H	-4.88943800	-2.53694300	-0.83640100
H	-4.88429200	-2.50686100	0.94030400
H	-6.18925700	-1.68560500	0.04155300
35			
EA			
H	-6.59040900	1.28086500	-0.05959100
H	-5.49984000	2.00372700	1.15015900
C	-3.31124700	0.51370700	0.10882200
N	-2.53204200	1.55972400	0.43629200
H	-0.54767900	2.00022000	0.74425000
C	-1.25303900	1.21363100	0.48858100
N	-0.70243500	0.00665900	0.26464300
H	-1.57046400	-3.02762100	-0.44224800
H	0.02907800	-2.40474500	-0.06891600
N	-0.96092500	-2.23852300	-0.27665600
C	-1.50254700	-1.03362400	-0.05275000
C	-2.89077500	-0.78842500	-0.14739100
N	-3.96212500	-1.60332500	-0.44517200
H	-6.02620800	-1.08438100	-0.54094700
C	-4.99620100	-0.79889100	-0.36813000
N	-4.67186400	0.49122600	-0.03757400
H	-5.31261300	2.40994900	-0.57637300

C	-5.57248800	1.62032700	0.13082800
C	4.41627800	0.59070700	-0.12417100
C	3.05259900	0.74206500	-0.06080000
C	2.65838600	-1.64559300	0.21792700
C	4.08882100	-1.81724800	0.15808500
C	4.91155200	-0.74240800	-0.00491800
H	4.47204800	-2.82764800	0.24535200
H	5.98775300	-0.89430500	-0.04920400
N	2.22934400	-0.34548500	0.10896800
H	1.20463600	-0.19157000	0.16896800
O	1.83231000	-2.57182800	0.35653500
C	5.36691800	1.73940400	-0.31065500
H	4.84016100	2.69403600	-0.36039000
H	6.08138800	1.78360400	0.51775900
H	5.94197200	1.61610300	-1.23436500
C	2.39346100	2.01085100	-0.16735900
C	1.83627000	3.07859500	-0.26074100
H	1.34408300	4.02585300	-0.34421800

33

EC

H	-5.13248200	1.74828100	-0.26972600
H	-3.67927300	2.67635400	0.18968300
H	-4.54869200	1.73216600	1.41704000
C	-4.24924200	1.76280500	0.36789700
O	-1.92767200	1.28159800	1.61591900
C	-2.22065800	0.44590800	0.75823600
N	-1.43188800	-0.62415600	0.46001200
H	-1.24828000	-3.28186300	-1.33340600
H	-0.14644700	-2.67869100	-0.10988300
N	-0.99783500	-2.56409300	-0.66846800
C	-1.81739800	-1.52790300	-0.44294400
H	-3.36366300	-2.13346100	-1.89542900
C	-3.05100700	-1.40379700	-1.16019400
H	-4.75824200	-0.12627400	-1.36674900
C	-3.81016300	-0.31628100	-0.87493900
N	-3.42621400	0.59846100	0.05194200
C	3.40831800	0.89634300	-0.27353600
C	2.04784600	0.80673800	-0.10679200
C	2.13797900	-1.54799200	0.51686100
C	3.56881800	-1.46189000	0.36223900
C	4.15729200	-0.29022600	-0.01386400
H	4.14498000	-2.36151900	0.54702400
H	5.23802900	-0.24875300	-0.13097200
N	1.46480300	-0.37186700	0.29187300
H	0.43734900	-0.39530600	0.43771600
O	1.50613000	-2.58156800	0.82344500
C	4.10355600	2.15512900	-0.70963800
H	3.39928600	2.97949600	-0.83613200
H	4.85382900	2.45446500	0.02939400
H	4.62323100	1.99874400	-1.66077700
C	1.14140900	1.89216300	-0.34175200
C	0.35531600	2.78676200	-0.54270800
H	-0.34175700	3.58115200	-0.71340300

36

EG

H	-6.80779800	-0.69013400	-0.41938900
H	-6.15074300	0.94879300	-0.65695100
H	-6.25290500	0.25752300	0.98409500

C	-6.07193700	0.03301700	-0.06860700
C	-3.56492900	0.06459400	0.06571500
N	-3.42015700	1.31418600	0.56514000
H	-2.61763100	3.43055900	1.55129300
H	-0.95997400	3.04452700	1.64897800
N	-1.84352100	2.89502900	1.17818800
C	-2.16377700	1.64452700	0.75119200
H	-0.16245300	1.13944900	0.60253700
N	-1.11385000	0.79992300	0.47918500
O	-0.19563300	-1.16283000	-0.24989000
C	-1.21555800	-0.50026500	-0.03709900
C	-2.57819200	-0.86573200	-0.24715700
N	-3.13856400	-2.02904900	-0.72932800
H	-5.19949500	-2.48786600	-1.01148400
C	-4.42622700	-1.79623700	-0.70298900
N	-4.74687700	-0.54455900	-0.23116800
C	4.47840100	0.70727500	-0.25977000
C	3.13834800	0.42831400	-0.35160600
C	3.40090800	-1.84918100	0.49803900
C	4.81615100	-1.56076600	0.59613400
C	5.31081400	-0.34490400	0.23346600
H	5.45649900	-2.35233600	0.96919600
H	6.37866100	-0.15470800	0.31741500
N	2.64398900	-0.80149600	0.01621400
H	1.63091500	-0.96178700	-0.06195900
O	2.86394900	-2.92436600	0.80540000
C	5.07734800	2.02960100	-0.64740800
H	4.31507600	2.73437600	-0.98461600
H	5.60540600	2.47510500	0.20205500
H	5.80557400	1.89963100	-1.45488800
C	2.16803900	1.36977300	-0.83188200
C	1.35006800	2.15945400	-1.24228800
H	0.62844200	2.85936700	-1.61241700

35

ET

H	-3.97845400	3.20407400	1.06926100
H	-2.40710500	3.52637600	0.30738800
H	-2.47003500	2.90921600	1.95842700
C	-2.94914500	2.85029600	0.97609200
O	-0.54334800	1.33215800	0.50053800
C	-1.63163200	0.80419500	0.25928700
H	-0.80241500	-0.97826700	-0.35408900
N	-1.68665100	-0.48887000	-0.23287200
O	-2.75881200	-2.37139900	-0.95369200
C	-2.81636700	-1.22203200	-0.53892700
H	-6.07901000	-0.62205300	-0.45592500
H	-5.30685300	-2.17148300	-0.02695900
H	-5.23193200	-1.57498900	-1.70216400
C	-5.23401200	-1.27986600	-0.65180700
H	-5.02014700	1.15468700	0.26100800
C	-4.02674800	0.73436400	0.14205900
N	-4.00262400	-0.55308800	-0.33930100
C	-2.91851600	1.44623000	0.45207900
C	3.90848700	-1.00812700	0.08993400
C	2.61758100	-0.59815000	0.30765800
C	3.03431200	1.65984600	-0.53322200
C	4.39817800	1.23312500	-0.76373800
C	4.79655600	-0.03406400	-0.46344400

H	5.07982200	1.96445700	-1.18365600
H	5.82757100	-0.32865600	-0.64725200
N	2.22080300	0.68306800	0.00245900
H	1.24113700	0.94322900	0.17437500
O	2.58412500	2.78987200	-0.77639400
C	4.40131200	-2.39233100	0.40403000
H	3.60666100	-3.02069200	0.81047700
H	4.79277400	-2.87423900	-0.49789900
H	5.21566100	-2.35327100	1.13509300
C	1.60202400	-1.44763300	0.86020700
C	0.74555600	-2.15917100	1.33052100
H	-0.00960000	-2.79129700	1.75191800

36

GEb

N	-1.11574300	-1.12931800	0.48946000
C	-1.99572800	-1.65018400	-0.47461200
C	-3.12864600	-0.78796700	-0.64600500
C	-3.19749600	0.37543100	0.11112800
N	-2.31915600	0.83417100	1.03815000
C	-1.29018600	0.03732200	1.18467800
N	-4.35958100	0.98559400	-0.25883700
C	-4.93166500	0.17533600	-1.20965900
N	-4.22662800	-0.89748200	-1.47099500
C	-4.87037100	2.24285100	0.26401800
O	-1.73715500	-2.70969700	-1.04119600
N	-0.26229800	0.38469900	2.03106100
O	1.51748500	-1.87929700	1.27004200
C	2.44467300	-1.27530000	0.68533500
C	3.65160700	-1.88392100	0.19147000
C	4.60015300	-1.13294700	-0.43825600
C	4.45944600	0.27283000	-0.63993600
C	3.30803200	0.84740200	-0.16221500
N	2.35634000	0.07900400	0.46957900
C	3.00415500	2.24265300	-0.27229400
C	2.72781800	3.41550000	-0.35300400
C	5.53654300	1.05125000	-1.34054700
H	1.51822300	0.53683600	0.83899100
H	5.28297700	2.11010300	-1.41614700
H	6.48514600	0.96180100	-0.80139400
H	5.69416900	0.66169900	-2.35146200
H	-5.87478900	0.43892300	-1.67064300
H	-5.81886600	2.46043600	-0.22663300
H	-5.02702600	2.16019500	1.34099800
H	3.76606600	-2.95146100	0.34029900
H	2.48796300	4.45627300	-0.42728700
H	-0.51820600	1.10932300	2.69330800
H	0.24246700	-0.39364500	2.45029500
H	-0.24449200	-1.64924100	0.65671000
H	5.50378100	-1.61367800	-0.80594900
H	-4.16061800	3.04618600	0.05861000

36

TA

H	6.87446900	-1.07437400	-0.00009600
H	5.72529500	-2.10352600	0.89184400
C	3.55120100	-0.50405700	-0.00001500
N	2.81635400	-1.63060100	-0.00006400
H	0.83852800	-2.21118400	-0.00012900
C	1.51772400	-1.36150100	-0.00009200

N	0.91757400	-0.15826900	-0.00007400
H	1.62178800	3.00054100	0.00004200
H	0.04624300	2.22169900	-0.00002300
N	1.06604900	2.15683000	-0.00000200
C	1.66973600	0.96130100	-0.00002200
C	3.07351800	0.80453800	0.00000900
N	4.11330000	1.70956800	0.00006200
H	6.20618900	1.31241200	0.00010500
C	5.18517600	0.95235100	0.00006900
N	4.91516800	-0.39138900	0.00002100
H	5.72512200	-2.10369000	-0.89162000
C	5.86716400	-1.49052700	0.00004100
N	-3.99116400	-1.26715100	0.00003600
C	-4.65299000	-0.06229300	0.00004400
H	-5.73562000	-0.13916200	0.00007700
C	-4.03018300	1.13902400	0.00001500
C	-4.75363100	2.45180900	0.00002000
H	-4.48663500	3.04331500	0.88160900
H	-4.48675100	3.04326200	-0.88164000
H	-5.83521500	2.29696800	0.00009400
C	-2.57735000	1.14025600	-0.00003100
O	-1.88094200	2.16173900	-0.00007100
N	-1.98044700	-0.10468500	-0.00002700
H	-0.94000800	-0.13455600	-0.00005700
C	-2.61338700	-1.32510300	-0.00000300
O	-1.99668600	-2.38553300	-0.00001400
C	-4.71209400	-2.53957600	0.00006400
H	-4.44954800	-3.11465300	-0.88947700
H	-4.44948700	-3.11464700	0.88959100
H	-5.78049900	-2.32947900	0.00010100
34			
TC			
H	5.30814400	1.88788400	0.54232500
H	4.04202300	2.50850300	1.62144100
H	4.03696200	2.95834200	-0.08330400
C	4.24710400	2.13904400	0.61162200
O	1.36464900	2.14050500	0.59921700
C	1.95304700	1.08531000	0.33818100
H	0.19807300	0.00777800	0.13785000
N	1.23005600	-0.05979600	0.05673000
O	1.02981300	-2.24760500	-0.57321100
C	1.74103200	-1.28792800	-0.30047200
H	4.79195600	-2.54937900	-0.66595300
H	3.39220900	-2.92563900	-1.70485200
H	3.38562100	-3.41623000	0.00496500
C	3.70799800	-2.64654500	-0.69815400
H	4.96771400	-0.44518100	-0.08713400
C	3.89817600	-0.26810500	-0.03294400
C	3.39786800	0.94430700	0.29836400
N	3.11838700	-1.35957200	-0.33011800
N	-3.84624300	-0.56223000	0.13662100
C	-4.28644500	0.49017900	-0.59912900
H	-5.32515600	0.45233600	-0.90955600
C	-3.47123100	1.52670600	-0.91712300
H	-3.82742700	2.36756500	-1.49740200
C	-2.12322800	1.44964400	-0.43939300
N	-1.25061300	2.43356800	-0.70222000
H	-0.33049400	2.42363000	-0.25763600

H	-1.54796500	3.26593100	-1.19088100
N	-1.68216900	0.40800000	0.26698100
C	-2.51798700	-0.61728700	0.59121700
O	-2.16383400	-1.58816800	1.26544100
C	-4.72706500	-1.67323700	0.48773000
H	-4.32325600	-2.60543500	0.08921300
H	-4.80358300	-1.75627000	1.57320700
H	-5.71137700	-1.48401600	0.06080600

37

TG

H	-7.03518400	-0.58530200	0.10128500
H	-6.34919200	0.79496700	-0.79248600
H	-6.29578400	0.77045700	0.98985100
C	-6.23909300	0.15886100	0.08758300
C	-3.73187200	0.05304200	0.01011500
N	-3.48874800	1.38439600	0.02222400
H	-2.46060500	3.64924300	0.18604400
H	-0.82112700	3.15681400	0.19226600
N	-1.77701900	2.94849900	-0.07048100
C	-2.20330500	1.65828100	-0.01458100
H	-0.23864900	1.00751700	-0.07635100
N	-1.22361100	0.70192400	-0.05379900
O	-0.45613300	-1.44542300	-0.08510100
C	-1.42915400	-0.67852400	-0.05830600
C	-2.81919500	-0.99848300	-0.02844500
N	-3.47257700	-2.21267400	-0.02265200
H	-5.56819500	-2.58958500	0.03361300
C	-4.74078700	-1.89191400	0.01788900
N	-4.96171600	-0.53443700	0.03977200
N	3.69981100	1.31373500	0.01088800
C	4.77145300	0.44687600	0.03691400
H	5.74306000	0.92946300	0.06057900
C	4.64671800	-0.89808500	0.03374500
C	5.81033000	-1.84182300	0.06228600
H	5.76374500	-2.48778500	0.94478000
H	5.80294300	-2.49265000	-0.81781400
H	6.75421000	-1.29223200	0.08182200
C	3.30159300	-1.45679000	0.00070500
O	3.03959900	-2.65542300	-0.00532900
N	2.27503600	-0.51727000	-0.02519500
H	1.30771100	-0.87902700	-0.04935300
C	2.41367300	0.84480500	-0.02088700
O	1.44355700	1.61200800	-0.04419300
C	3.88768600	2.76557200	0.01675400
H	3.44810500	3.19986200	-0.88241500
H	3.40969700	3.19785200	0.89716800
H	4.95657300	2.97098900	0.04006900

36

TT

H	6.40719100	0.66268400	0.00001500
H	5.59185700	1.97094800	0.88160600
H	5.59186000	1.97095600	-0.88156800
C	5.53780800	1.32430800	0.00001600
O	2.88380600	2.47139900	0.00001100
C	2.99857700	1.24908100	0.00001500
H	0.94680900	0.90691900	-0.00000200
N	1.86706000	0.44106200	0.00000100
O	0.78012900	-1.56776500	-0.00001800

C	1.83617900	-0.92871000	-0.00001000
H	4.10402500	-3.34867300	-0.00001200
H	2.55946300	-3.38812500	-0.88980100
H	2.55945500	-3.38813500	0.88976500
C	3.06808000	-3.01385000	-0.00001400
H	5.13341400	-1.41591400	0.00000400
C	4.22672600	-0.81964200	0.00000400
C	4.26645700	0.53089400	0.00001100
N	3.05852500	-1.55043200	-0.00000600
N	-4.16176100	-0.55442300	0.00000800
C	-4.22652700	0.81803100	0.00000000
H	-5.23266900	1.22504000	0.00000000
C	-3.13890500	1.62319600	-0.00000800
C	-3.20977200	3.12045100	-0.00001700
H	-2.70940000	3.53336800	0.88161600
H	-2.70940600	3.53335800	-0.88165800
H	-4.24884000	3.45791900	-0.00001500
C	-1.83500500	0.98628900	-0.00000900
O	-0.76175100	1.60082900	-0.00001700
N	-1.84443100	-0.39500300	-0.00000100
H	-0.92944800	-0.86876300	-0.00000300
C	-2.95168900	-1.21477400	0.00001100
O	-2.86608400	-2.43670500	0.00001100
C	-5.36898700	-1.38094900	0.00001600
H	-5.38526700	-2.01285000	-0.88947200
H	-5.38526500	-2.01283500	0.88951500
H	-6.23596700	-0.72234000	0.00001200

Table S2. Cartesian coordinates (in Å) of the optimised dinucleotides

62

A-E_dinucleotide

C	2.75443600	-4.24503000	-0.11012300
O	1.85373400	-4.17819900	0.98796900
C	2.81314000	-2.88586000	-0.77968600
O	1.55989800	-2.58718400	-1.41097200
C	3.08736000	-1.72813700	0.18758000
O	3.86481400	-0.75927900	-0.51736000
C	1.68871200	-1.21353800	0.50827500
C	0.92176500	-1.48298300	-0.78681800
N	-3.99390300	-0.44751800	-1.97316800
C	-2.84099700	0.03158700	-2.47208900
N	-1.59660600	-0.28322900	-2.13086900
C	-1.56677400	-1.22782000	-1.17941900
C	-2.67415500	-1.85677000	-0.60952100
C	-3.93699100	-1.38881000	-1.02048600
N	-5.09035200	-1.87368200	-0.49121700
N	-2.28570800	-2.81892300	0.30150400
C	-0.97773500	-2.75261100	0.29235200
N	-0.47834500	-1.80142200	-0.56788500
P	4.47066800	0.54088000	0.29319600
C	2.71630500	2.05187700	-0.93191400
O	3.17593700	1.55365600	0.31745400
C	1.36159500	2.69544000	-0.75504000
O	0.39861300	1.71158200	-0.39189000
C	1.26703100	3.81176700	0.32071700
O	1.06524800	5.09227900	-0.26571100
C	0.01073200	3.43008700	1.10766400
C	-0.69193500	2.44330900	0.16431300
C	-3.01187600	1.58017600	0.58697600
N	-3.86407600	0.70690700	1.22097500
C	-3.48201300	-0.32152600	2.06569000
O	-4.33166600	-1.10565900	2.50806600
C	-2.06166500	-0.35988200	2.34160100
C	-1.20855900	0.51108000	1.73621300
O	5.52891600	1.11442100	-0.60215700
O	4.72779200	0.16933200	1.72321500
H	-2.94950500	0.78518800	-3.24853300
H	-5.03563500	-2.25678200	0.44746500
H	-5.92943300	-1.34214500	-0.69131100
H	-0.30422900	-3.37651000	0.86807800
H	0.92425000	-0.61810100	-1.45629900
H	1.26752100	-1.79818900	1.33019500
H	1.67964800	-0.15323600	0.76214000
H	3.62981800	-2.05335500	1.07953900
H	3.58614500	-2.91282300	-1.55457300
H	2.41913800	-4.98877400	-0.84307900
H	3.76310700	-4.51380100	0.22981800
H	1.81133000	-5.04712000	1.41286100
H	2.63761300	1.23456900	-1.66066500
H	3.42293900	2.79453300	-1.32305700
H	1.06899700	3.14446000	-1.71829300
H	2.15851500	3.82716700	0.95606800
H	0.28080000	2.91623200	2.03591300
H	-0.59627400	4.30596300	1.34939100
H	-1.19929300	2.99625900	-0.63964700

H	1.87712700	5.36398600	-0.72048700
H	-4.85931000	0.76942800	1.02302500
H	-0.14324700	0.45515100	1.94459400
C	-1.66232900	1.50430500	0.81559600
C	-3.62890800	2.54351400	-0.27543100
C	-4.17497500	3.35145200	-0.98767500
H	-4.65274400	4.06836200	-1.62342900
H	-1.71363000	-1.12594500	3.02539800

63

A-T_dinucleotide

C	2.26629600	-4.40851900	-0.18462000
O	1.36161800	-4.26159300	0.90241400
C	2.48160900	-3.05401400	-0.83128900
O	1.28043900	-2.61312000	-1.48017400
C	2.85904500	-1.94497300	0.15760200
O	3.74128900	-1.05250300	-0.52357600
C	1.51483900	-1.29425500	0.46623400
C	0.74813500	-1.45972600	-0.84661700
N	-4.02632000	-0.00192800	-2.17698700
C	-2.82136600	0.40729500	-2.60964200
N	-1.61813700	-0.00342300	-2.22316300
C	-1.69752100	-0.97115800	-1.29676200
C	-2.87071600	-1.52040500	-0.78049300
C	-4.07853700	-0.96164800	-1.24233000
N	-5.28368900	-1.37718600	-0.78147400
N	-2.59382700	-2.51672700	0.13460500
C	-1.28558100	-2.55652700	0.17185300
N	-0.68083200	-1.63804900	-0.65624200
P	4.45369800	0.17822600	0.30777300
C	2.89856200	1.85565100	-0.96520200
O	3.26494300	1.31564200	0.29620900
C	1.61487400	2.63745100	-0.82780700
O	0.54317200	1.75865800	-0.48773900
C	1.60189600	3.75824500	0.24613900
O	1.67656000	5.04989500	-0.33893800
C	0.23319500	3.58628100	0.91440000
C	-0.48493300	2.61239900	-0.02486400
N	-1.52494300	1.80636800	0.59451800
C	-2.84091900	2.04058300	0.23849200
O	-3.18924400	2.89530200	-0.56301400
N	-3.74880800	1.22686900	0.88227700
C	-3.48932200	0.21596500	1.80410500
O	-4.41127200	-0.45691300	2.25063400
C	-2.08310800	0.06279900	2.16228400
C	-1.18715500	0.85869800	1.54150100
C	-1.71788500	-0.96120400	3.19300400
O	5.58745200	0.64453700	-0.55626000
O	4.62881600	-0.21574300	1.74372200
H	-2.84074800	1.18558500	-3.36837500
H	-5.30384700	-1.84079300	0.11933700
H	-6.08194200	-0.79203600	-0.99568100
H	-0.68555500	-3.24010000	0.76124500
H	0.85089500	-0.58949800	-1.50109400
H	1.02200000	-1.84962900	1.26823300
H	1.61276200	-0.24469600	0.74464300
H	3.35195200	-2.33572200	1.05192700
H	3.26182000	-3.15258500	-1.59293500
H	1.86411800	-5.10043800	-0.93436100

H	3.23481200	-4.78955300	0.16459000
H	1.20745900	-5.12951600	1.30281000
H	2.75756600	1.05098000	-1.69840200
H	3.68847100	2.52144300	-1.33425200
H	1.39423700	3.11023000	-1.79785200
H	2.41785100	3.62059600	0.96218500
H	0.33742800	3.13354800	1.90491000
H	-0.28972700	4.53979700	1.01447400
H	-0.95689200	3.13241200	-0.86352500
H	2.58221500	5.20777800	-0.64615500
H	-4.72089100	1.37099600	0.62133200
H	-2.08791200	-1.94788100	2.89871300
H	-0.63334700	-1.01407300	3.31906200
H	-2.16802000	-0.71544600	4.16068100
H	-0.12293000	0.79283500	1.74499400

60

C-E_dinucleotide

C	2.09670200	-4.37914900	0.09560800
O	1.12197600	-4.17186500	1.11045200
C	2.29872600	-3.07702600	-0.65413300
O	1.11367700	-2.75357300	-1.39276500
C	2.57952500	-1.87543400	0.26014800
O	3.51086100	-1.02814700	-0.41611200
C	1.21115100	-1.21716300	0.39186000
C	0.57210800	-1.50824700	-0.96450900
P	4.22353200	0.21053800	0.40252600
C	2.72015500	1.91256500	-0.90583800
O	3.05389300	1.36476400	0.36319600
C	1.43157900	2.69388000	-0.79298500
O	0.36469500	1.80021400	-0.49515900
C	1.39771000	3.79833000	0.29890900
O	1.24287500	5.09420800	-0.26884000
C	0.13573500	3.46624200	1.09676300
C	-0.65525900	2.58279200	0.12322800
C	-2.99288200	1.68596900	0.37337700
N	-3.88380500	0.83098100	0.97586300
C	-3.56818600	-0.13335800	1.91831400
O	-4.44631900	-0.89302000	2.34507200
C	-2.17374300	-0.14204000	2.30394100
C	-1.28661800	0.72136400	1.73833600
O	5.37502000	0.64676600	-0.45498400
O	4.38064800	-0.16342500	1.84662200
H	0.79152200	-0.72765700	-1.69344400
H	0.65295900	-1.69784200	1.20031800
H	1.27715100	-0.14485900	0.57465200
H	2.99804800	-2.17907500	1.22354400
H	3.12625700	-3.20377600	-1.36047000
H	1.76507300	-5.15068800	-0.60975900
H	3.05452800	-4.68838400	0.53378400
H	0.97717500	-5.00392900	1.58360800
H	2.59121900	1.10972800	-1.64352700
H	3.52310100	2.57486400	-1.25156000
H	1.23658100	3.17911700	-1.76276600
H	2.29664200	3.76860800	0.92323400
H	0.39431000	2.89287800	1.99238700
H	-0.40064600	4.36956900	1.39664200
H	-1.13882700	3.21267300	-0.63706500
H	2.05344200	5.32810300	-0.74668900

H	-4.85668000	0.85873200	0.68359200
H	-0.24426900	0.69081200	2.04425800
C	-1.67431000	-0.88341800	-1.83839600
C	-1.45241300	-2.52156700	-0.07802100
C	-2.79675300	-2.64141800	0.02146600
H	-0.75679700	-3.13169000	0.49321100
C	-3.57221500	-1.75583100	-0.79804200
H	-3.25976700	-3.34606000	0.70012200
N	-0.88313600	-1.62061800	-0.92936200
N	-3.02949200	-0.94083700	-1.68773900
O	-1.13614200	-0.21324100	-2.72056000
N	-4.91876300	-1.76589500	-0.68889500
H	-5.43954100	-1.05835200	-1.19189100
H	-5.34214600	-2.13581400	0.15265000
C	-1.67179500	1.66758800	0.73963400
C	-3.54451200	2.55495000	-0.62312300
C	-4.04512500	3.26848000	-1.45869100
H	-4.48013400	3.90534300	-2.20137500
H	-1.87277100	-0.87230800	3.04714600

61

C-T_dinucleotide

C	1.68189900	-4.47653300	0.02082100
O	0.67627800	-4.19671900	0.98739500
C	2.04949100	-3.18538400	-0.68398700
O	0.94089500	-2.72983600	-1.47138000
C	2.39637800	-2.03634900	0.27318700
O	3.42001700	-1.25432500	-0.34643500
C	1.08568400	-1.26549700	0.36635400
C	0.50182300	-1.44818100	-1.03245400
P	4.15383600	-0.05240800	0.50813300
C	2.83505700	1.71560800	-0.91307500
O	3.06316000	1.17348400	0.38013300
C	1.60141800	2.58747500	-0.88127500
O	0.45980100	1.78454800	-0.59261500
C	1.59974900	3.73287400	0.16825000
O	1.71082500	5.00926100	-0.44498100
C	0.21961600	3.61370700	0.82250400
C	-0.53243300	2.67918900	-0.12968900
N	-1.59892300	1.89788000	0.47782000
C	-2.90049600	2.07961900	0.04514800
O	-3.23007100	2.88889700	-0.80908900
N	-3.81902900	1.27464900	0.68517700
C	-3.57992000	0.29069300	1.63917300
O	-4.50718800	-0.38276100	2.07363600
C	-2.18480500	0.16133300	2.04489000
C	-1.28255900	0.96789100	1.45003500
C	-1.83375900	-0.86667500	3.07600300
O	5.38354500	0.30177800	-0.27432000
O	4.18777600	-0.41508500	1.96277800
H	0.84100100	-0.67404600	-1.72106000
H	0.44491100	-1.72696900	1.12292600
H	1.24106000	-0.21328600	0.59910600
H	2.74886300	-2.39658800	1.24333700
H	2.89591800	-3.37853300	-1.35171700
H	1.31746200	-5.19736500	-0.72098100
H	2.57970600	-4.88649000	0.50124900
H	0.42818400	-5.02001000	1.43227400
H	2.69156800	0.90981400	-1.64459300

H	3.69649600	2.31713800	-1.22802100
H	1.47614800	3.04802500	-1.87357600
H	2.40324200	3.59453600	0.89837400
H	0.29922500	3.15176800	1.81078900
H	-0.26230200	4.58797000	0.92680600
H	-0.98337100	3.22465600	-0.96355400
H	2.61947900	5.13224200	-0.75962900
H	-4.77992600	1.37911200	0.37123200
H	-2.09260500	-1.87113900	2.72164200
H	-0.76494400	-0.84026900	3.30241800
H	-2.39090700	-0.69567200	4.00253200
H	-0.22769900	0.92540100	1.69927500
C	-1.61230900	-0.57955600	-2.01917800
C	-1.66301300	-2.27168800	-0.29549500
C	-3.01622100	-2.26193400	-0.28232000
H	-1.06824100	-2.96402400	0.29635600
C	-3.65006600	-1.28751900	-1.12433100
H	-3.58546900	-2.93735300	0.34356900
N	-0.95541300	-1.41001100	-1.08139200
N	-2.97258600	-0.50228400	-1.94896600
O	-0.95619300	0.04651000	-2.85130800
N	-4.98965600	-1.16321200	-1.09931500
H	-5.42872800	-0.43995300	-1.65366100
H	-5.54133800	-1.62245200	-0.38823100

62

E-A_dinucleotide

C	1.60345700	4.56822400	-0.27769100
O	0.71127900	4.20633300	-1.32417300
C	1.94365800	3.32790000	0.52617600
O	0.78877900	2.88031300	1.24121900
C	2.40885800	2.14639700	-0.33326200
O	3.43987900	1.47129800	0.39189400
C	1.14738300	1.29639800	-0.46433200
C	0.43111900	1.53929000	0.86563300
P	4.35037900	0.32862700	-0.36126200
C	3.13086600	-1.52345000	1.03984500
O	3.38139800	-0.99520600	-0.25591200
C	2.03741000	-2.56289800	0.93710700
O	0.79630100	-1.91008400	0.64396200
C	2.26147900	-3.60679500	-0.18694500
O	1.91680000	-4.91962700	0.23757300
C	1.24177400	-3.19167100	-1.23957000
C	0.12390800	-2.66886300	-0.34650300
O	5.55325700	0.12952400	0.51371700
O	4.45479400	0.64155600	-1.82483400
H	0.80306400	0.84126200	1.62560800
H	0.54784500	1.66979100	-1.30005100
H	1.37566500	0.23936000	-0.61142100
H	2.80152300	2.46871000	-1.30144600
H	2.72787500	3.58659500	1.24721900
H	1.14241200	5.30890700	0.38740300
H	2.53088900	4.99055300	-0.68665300
H	0.48978100	4.99843000	-1.83466400
H	2.81189000	-0.72529600	1.72310100
H	4.04128500	-1.98593600	1.43937600
H	1.94974000	-3.08007400	1.90231800
H	3.28912100	-3.58001400	-0.56222800
H	1.65511700	-2.38037300	-1.84505500

H	0.93725000	-4.02293200	-1.87797800
H	-0.42834800	-3.49328200	0.11985500
H	2.56238800	-5.22018600	0.89538400
C	-1.82335700	0.69635600	1.64963300
C	-3.93650300	1.61954800	0.79737500
C	-1.07159200	1.47538500	0.80851500
C	-3.13294900	2.42496400	-0.09581000
C	-1.77407600	2.35039700	-0.07771900
O	-5.17017100	1.64330300	0.87944300
H	-1.18115400	2.99217500	-0.72748000
H	-3.66455500	3.10192700	-0.75615300
N	-3.19803500	0.76659300	1.60287600
H	-3.73572300	0.18665800	2.24116500
C	-1.28371400	-0.18570900	2.64120200
C	-0.87164400	-0.92204600	3.50475300
H	-0.49273000	-1.57969000	4.25979600
N	-0.87048600	-1.84166100	-0.98567700
C	-2.19196300	-1.78176200	-0.60599000
C	-0.73476900	-0.94266700	-2.02026700
N	-2.80677300	-2.48114500	0.35559800
C	-2.77746500	-0.84618800	-1.45486100
N	-1.84586000	-0.32695200	-2.33351200
H	0.21407500	-0.79026900	-2.51668100
C	-4.10550200	-2.19669600	0.41226400
C	-4.15735300	-0.62492200	-1.27767500
N	-4.80365000	-1.33145200	-0.33784900
H	-4.68053600	-2.73293900	1.16341100
N	-4.85926600	0.24773200	-2.04331500
H	-4.32770600	0.93612700	-2.56226200
H	-5.72904400	0.58285600	-1.64486600

60

E-C_dinucleotide

C	-1.03597100	4.64276500	0.01815800
O	-0.14453900	4.29875600	1.07127600
C	-1.47307100	3.37364500	-0.68807700
O	-0.35824900	2.79283800	-1.37012100
C	-2.01316800	2.29500600	0.25952900
O	-3.08809700	1.63326700	-0.41522800
C	-0.81115100	1.37659800	0.45298000
C	-0.11355700	1.45341100	-0.90662600
P	-4.05267400	0.58881800	0.40981400
C	-2.99390900	-1.43356600	-0.88420400
O	-3.16962800	-0.79767200	0.37383200
C	-1.85871900	-2.42579600	-0.78758800
O	-0.65008300	-1.72739600	-0.53038300
C	-1.92994300	-3.45101900	0.35278200
O	-2.70934400	-4.58994700	0.04014400
C	-0.45906900	-3.84388500	0.52099900
C	0.32083600	-2.68825500	-0.14651400
N	1.27498800	-2.00778200	0.71929200
C	2.64712100	-1.98822900	0.38609100
O	3.04666000	-2.64332300	-0.58039900
N	3.47681600	-1.23393100	1.15437000
C	3.00589600	-0.54351300	2.18304400
C	1.62390800	-0.56989800	2.56954200
C	0.80485500	-1.31897100	1.79606900
O	-5.27649000	0.41155800	-0.44096400
O	-4.11985700	0.99062600	1.85382100

H	-0.57292700	0.74067100	-1.60183300
H	-0.17042100	1.78231700	1.24118700
H	-1.10421100	0.35650500	0.70079100
H	-2.38196800	2.71513300	1.19937800
H	-2.24389600	3.63403900	-1.42313400
H	-0.54357000	5.30247600	-0.70707700
H	-1.92485400	5.15357500	0.41171700
H	0.13687300	5.10906800	1.51980500
H	-2.75545500	-0.69318100	-1.65891300
H	-3.91375000	-1.95468000	-1.17694500
H	-1.78917500	-2.97029300	-1.74449200
H	-2.31289200	-2.95815300	1.25404900
H	-0.17058600	-3.98176300	1.56557800
H	-0.27594600	-4.78170300	-0.01117500
H	0.88794400	-3.02195000	-1.01664100
H	-3.64473800	-4.38544500	0.18764700
H	-0.26283400	-1.39856500	1.97693000
C	2.02320100	0.33543900	-1.67129900
C	4.23234700	1.00160300	-0.83335500
C	1.37545600	1.24317300	-0.87339100
C	3.54287200	1.98240100	-0.02217600
C	2.18596300	2.08241000	-0.04516500
O	5.45721900	0.82528100	-0.86909300
H	1.68038400	2.83523600	0.55799100
H	4.15670200	2.61980200	0.60503700
N	3.39519000	0.24241300	-1.63004300
H	3.84211000	-0.49788300	-2.16383900
C	1.37692400	-0.52602800	-2.61748500
C	0.87808500	-1.25179700	-3.44379000
H	0.42239000	-1.89791700	-4.16568000
H	1.25155300	-0.01623400	3.42190400
N	3.88191100	0.19136400	2.89034300
H	3.57182900	0.82707600	3.61124900
H	4.83103100	0.28027300	2.55128700

61

E-E_dinucleotide

C	-2.28780500	-4.35411500	0.14774200
O	-1.28298300	-4.28130900	-0.85561100
C	-2.45003600	-2.98472300	0.77938800
O	-1.25596200	-2.64466600	1.49271700
C	-2.68499000	-1.85594500	-0.23409700
O	-3.58126300	-0.91812900	0.37286000
C	-1.29115400	-1.26621100	-0.40772400
C	-0.71016000	-1.41106700	1.00013700
P	-4.20516200	0.31928300	-0.51293800
C	-2.58668900	1.95923900	0.74683600
O	-2.97683900	1.41211500	-0.50490900
C	-1.23190100	2.61613500	0.60542400
O	-0.27807000	1.64391300	0.21175900
C	-1.12444300	3.76440500	-0.43309900
O	-0.98106400	5.03353700	0.19322700
C	0.16602900	3.43523400	-1.19281400
C	0.83157000	2.36984600	-0.30772200
C	3.05970400	1.25254200	-0.66481200
N	3.83958900	0.32720600	-1.31766700
C	3.40174300	-0.53960900	-2.30551700
O	4.17794200	-1.37070800	-2.78944000
C	2.01158300	-0.36315400	-2.67123200

C	1.23531800	0.56150700	-2.04444900
O	-5.34576000	0.85775500	0.30146900
O	-4.36160800	-0.10588900	-1.94341000
H	-1.05298500	-0.58483700	1.63435300
H	-0.72750200	-1.87743900	-1.11901500
H	-1.30620700	-0.22824200	-0.73689900
H	-3.11958700	-2.21930600	-1.16973800
H	-3.28858800	-3.02428700	1.48471800
H	-2.00574200	-5.07301300	0.92704400
H	-3.24910700	-4.66266200	-0.28417700
H	-1.17448500	-5.15714700	-1.25322100
H	-2.52633400	1.16762300	1.50485500
H	-3.32322800	2.70048000	1.08208500
H	-0.94510500	3.03215100	1.58684100
H	-1.99363800	3.77366800	-1.09959000
H	-0.06612000	3.01059500	-2.17419600
H	0.78534900	4.32431200	-1.33301200
H	1.36623100	2.85268200	0.52386500
H	-1.82019000	5.27509600	0.61437300
H	4.79630900	0.18675200	-1.00032400
H	0.18888600	0.66200800	-2.32242300
C	1.46543800	-2.50148600	0.29733400
C	3.64682100	-1.64211700	0.97704700
C	0.78819300	-1.49142800	1.04843200
C	1.55895700	-0.63430000	1.78886600
O	4.88385300	-1.57600200	0.93938900
C	1.74221800	1.40468900	-1.00726800
C	3.71374400	1.99628000	0.37096600
C	4.29125100	2.59306000	1.24803600
H	4.79818700	3.13060800	2.02324200
H	1.62071700	-1.01253200	-3.44668700
H	0.85318700	-3.21435400	-0.25347900
C	2.82406600	-2.58908700	0.25867700
H	3.33840700	-3.34338900	-0.32658600
N	2.93077000	-0.74361300	1.74758400
H	3.48599200	-0.07056300	2.26994200
C	1.05544600	0.40345000	2.63940900
C	0.69265900	1.27988300	3.38727700
H	0.35914600	2.05429700	4.04723900

63

E-G_dinucleotide

C	0.45094600	4.55593700	-0.64708500
O	-0.44006200	3.81873800	-1.47429500
C	1.03851900	3.61666200	0.38809600
O	0.00362500	3.18778400	1.28160700
C	1.65832100	2.34554200	-0.21299800
O	2.83464800	2.03170400	0.53655800
C	0.56490400	1.30561600	-0.00564100
C	-0.09786500	1.76251300	1.29560500
P	3.99333600	1.08298900	-0.14043500
C	3.14616700	-0.97683400	1.25680800
O	3.31661600	-0.41306000	-0.03637500
C	2.45306600	-2.31816200	1.12303300
O	1.11597400	-2.13043000	0.64625100
C	3.11336100	-3.28630400	0.12688300
O	2.86506500	-4.64026700	0.48208000
C	2.34858500	-3.01400200	-1.16097400
C	0.94713300	-2.72365900	-0.63131400

O	5.16903500	1.16016400	0.78855000
O	4.09951600	1.37397800	-1.60826700
H	0.44069500	1.36875800	2.16731000
H	-0.15475900	1.37828800	-0.82663800
H	0.94681900	0.28335000	0.05333600
H	1.92325900	2.47788300	-1.26623600
H	1.80004100	4.15856400	0.96076300
H	-0.07828200	5.36819200	-0.13339800
H	1.26833200	4.98723300	-1.23990500
H	-0.81013000	4.41228900	-2.14373300
H	2.52683300	-0.31554700	1.87927900
H	4.11979700	-1.10695200	1.74409100
H	2.39851600	-2.77645400	2.11810000
H	4.18786900	-3.09914600	0.02538900
H	2.77775800	-2.13515100	-1.64268800
H	2.37030100	-3.86554800	-1.84327200
H	0.35570600	-3.63766200	-0.51956900
H	3.34580000	-4.84851900	1.29783700
C	-2.01183700	0.36510100	2.16503300
C	-4.26269100	0.50141800	1.20605900
C	-1.54662100	1.36590300	1.35496000
C	-3.78166500	1.60407300	0.40938700
C	-2.47789300	1.99203800	0.47112100
O	-5.39302700	-0.01227100	1.12341900
H	-2.10343000	2.78782500	-0.17110200
H	-4.48758400	2.05971600	-0.27667400
N	-3.33196500	-0.02102100	2.08088100
H	-3.65303600	-0.78235500	2.67345000
C	-1.20773700	-0.34295700	3.11478400
C	-0.55001900	-0.95111100	3.92463000
H	0.03961500	-1.48756800	4.63958000
N	0.15367900	-1.82896800	-1.45723400
C	-1.19553300	-1.65849800	-1.29397400
C	0.53816900	-0.92705300	-2.43028800
N	-1.97761200	-2.33745000	-0.42101100
C	-1.55739100	-0.66511500	-2.19329200
N	-0.45866000	-0.22487100	-2.90172300
H	1.56616300	-0.83454600	-2.75070300
C	-3.23967500	-1.98166900	-0.48783200
C	-2.93240900	-0.26375400	-2.25197600
N	-4.17630300	-2.60134900	0.28396600
N	-3.70648500	-1.01943600	-1.34989800
O	-3.46371600	0.59526000	-2.94901600
H	-3.78236700	-3.18637900	1.01188900
H	-4.96623500	-2.03321100	0.58817000
H	-4.69869900	-0.79312200	-1.33386600

62

E-T dinucleotide

C	-1.25396300	4.60191100	-0.08818200
O	-0.31435600	4.27945100	0.92957500
C	-1.66913800	3.32432200	-0.79233600
O	-0.55523800	2.79077100	-1.51555100
C	-2.13706500	2.21848200	0.16248000
O	-3.20132600	1.51341400	-0.48468300
C	-0.89435700	1.34776200	0.31042200
C	-0.24972500	1.45927300	-1.07334000
P	-4.09838900	0.43155800	0.36870600
C	-2.95248000	-1.56823100	-0.88989200

O	-3.13770900	-0.90367200	0.35157800
C	-1.78757200	-2.52413300	-0.77760900
O	-0.58819300	-1.78477300	-0.58640200
C	-1.80328000	-3.49529600	0.41156500
O	-2.55570100	-4.66850800	0.16990500
C	-0.31848000	-3.83878100	0.56652400
C	0.41187400	-2.70505900	-0.18679800
N	1.37945800	-1.96201300	0.61373100
C	2.70421600	-1.93402800	0.22403700
O	3.15513200	-2.56822800	-0.72068300
N	3.50009100	-1.11623500	0.99706500
C	3.11197200	-0.29353700	2.05191400
O	3.93931700	0.41045000	2.61718700
C	1.69491000	-0.36303400	2.38978300
C	0.91837900	-1.19513000	1.66629600
C	1.18088600	0.50684300	3.49567100
O	-5.31660500	0.16828300	-0.46710300
O	-4.17410900	0.85696500	1.80528600
H	-0.70608100	0.73465500	-1.75884800
H	-0.24189300	1.77536500	1.07769700
H	-1.13861500	0.31650700	0.56282400
H	-2.49385300	2.61688800	1.11635700
H	-2.47184800	3.56208900	-1.50016200
H	-0.81062900	5.28565600	-0.82266200
H	-2.14611300	5.07646800	0.34145700
H	-0.04714900	5.09440600	1.37854300
H	-2.74454500	-0.84332800	-1.68791500
H	-3.85807900	-2.12548600	-1.15879700
H	-1.72616100	-3.10986500	-1.70983400
H	-2.18068200	-2.97090300	1.29684400
H	-0.00213100	-3.90466800	1.61003800
H	-0.11924400	-4.80114500	0.08694800
H	0.95881200	-3.07408300	-1.05698100
H	-3.49323800	-4.48306600	0.32908000
H	4.47793800	-1.06651300	0.71613100
H	1.36550500	1.56279800	3.26758300
H	0.10605700	0.36390100	3.63176300
H	1.68813000	0.28422200	4.43969000
H	-0.14598000	-1.29577300	1.85803400
C	1.89686100	0.37331900	-1.85615300
C	4.09265600	1.03090400	-0.97703400
C	1.24427100	1.29396500	-1.07818000
C	3.40395000	2.05803600	-0.22726600
C	2.04733100	2.16143900	-0.27217000
O	5.30412300	0.77680300	-0.91679600
H	1.53421000	2.92850700	0.30676500
H	4.01195000	2.70269400	0.39746500
N	3.27011200	0.28248700	-1.79842300
H	3.72454300	-0.46440800	-2.31787300
C	1.26263600	-0.52133900	-2.77815800
C	0.78044800	-1.28363900	-3.58092700
H	0.33863800	-1.95989900	-4.28373700

63

G-E_dinucleotide

C	4.76207300	-2.87472900	-0.32212100
O	3.99205300	-3.49608900	0.69760400
C	4.06891700	-1.60055400	-0.76542700
O	2.80243300	-1.91552300	-1.36613200

C	3.75058400	-0.60814500	0.36188800
O	3.78377900	0.69339100	-0.22941400
C	2.34267300	-1.02571200	0.76071800
C	1.74312700	-1.36659100	-0.59803500
C	-2.33534000	-0.86554700	-1.73720400
N	-1.03769200	-0.91283000	-1.55535400
C	-0.63023200	-2.04890500	-0.95425600
C	-1.37782300	-3.15503900	-0.57530800
C	-2.79191300	-3.12223800	-0.80068200
N	-0.57675800	-4.09189500	0.05138800
C	0.61504600	-3.55212500	0.05980500
N	0.64524000	-2.30846000	-0.53913300
P	3.21570100	2.02092900	0.56398500
C	1.34333400	2.53240600	-1.24922600
O	1.64634800	2.06385600	0.06232400
C	-0.01585700	3.21079700	-1.26116100
O	-1.06136200	2.25677600	-1.04884100
C	-0.19534500	4.27988400	-0.17123300
O	-1.07051700	5.31673000	-0.60057400
C	-0.90879200	3.51777000	0.93631500
C	-1.79469600	2.54040600	0.15443400
C	-3.33426000	0.73069800	1.01227600
N	-3.51376600	-0.48247900	1.63716300
C	-2.50407600	-1.29254800	2.13465600
C	-1.17190400	-0.75900300	1.93765700
C	-0.98318500	0.44130000	1.32608700
O	3.94593300	3.19263000	-0.02246500
O	3.16710900	1.74866400	2.03792200
H	1.51953800	-3.99215900	0.46281300
H	1.33913400	-0.47683500	-1.09251600
H	2.39415400	-1.91887000	1.38816700
H	1.80177000	-0.23886200	1.28418300
H	4.46641700	-0.66096300	1.18728600
H	4.69442600	-1.11165200	-1.51940600
H	4.86120900	-3.53758400	-1.19034700
H	5.76620800	-2.62172500	0.04291200
H	4.42267900	-4.32449600	0.95353700
H	1.33552100	1.68718400	-1.94928100
H	2.10323600	3.25311800	-1.57125700
H	-0.15789600	3.65584100	-2.25446200
H	0.76689500	4.69320500	0.15289600
H	-0.17397600	2.98012800	1.54053600
H	-1.49067200	4.18276600	1.57844500
H	-2.74004600	3.02313200	-0.11977300
H	-0.63713400	5.82726100	-1.30142600
H	-4.45896800	-0.84129600	1.74188800
H	0.02173000	0.82104800	1.14888400
O	-3.64469900	-3.96691900	-0.54181300
N	-2.88308500	0.23533100	-2.32098400
H	-2.30061500	1.06643100	-2.21314800
H	-3.87505100	0.40052300	-2.19689900
C	-2.07240700	1.23905600	0.85696900
C	-4.52555500	1.36383900	0.52899800
C	-5.54573800	1.86051000	0.11519400
H	-6.44671700	2.30937500	-0.25006300
H	-0.34393900	-1.37109200	2.28347500
O	-2.78295400	-2.36571800	2.67914600
N	-3.17503700	-1.89826600	-1.39389900

H	-4.17248900	-1.80377600	-1.56457800
64			
G-T	dinucleotide		
C	4.67378200	-3.03903100	-0.26932800
O	3.85901300	-3.63639400	0.72975900
C	4.03113800	-1.74357000	-0.72620300
O	2.76990100	-2.02111100	-1.35740100
C	3.71826400	-0.74378300	0.39713500
O	3.82247200	0.56121500	-0.17942100
C	2.28508000	-1.10871900	0.75329600
C	1.71182800	-1.43545300	-0.61821800
C	-2.38559400	-0.79371100	-1.66960400
N	-1.08896800	-0.85513700	-1.47491600
C	-0.69312400	-2.03039700	-0.94213200
C	-1.45294800	-3.14973000	-0.62784500
C	-2.86550200	-3.09525600	-0.86011000
N	-0.65720000	-4.14468600	-0.09272900
C	0.54552400	-3.62759100	-0.07101400
N	0.58516200	-2.34499200	-0.57708800
P	3.19088500	1.88545000	0.56916800
C	1.38844400	2.33134000	-1.32829900
O	1.64182800	1.87482500	-0.00158600
C	0.14715800	3.20221500	-1.34556400
O	-1.02632900	2.40673700	-1.12190300
C	0.13179700	4.28448300	-0.25031000
O	-0.57589600	5.44240900	-0.67421000
C	-0.69160800	3.63895100	0.85633700
C	-1.70533600	2.82581600	0.05412200
C	-3.59650700	1.39602700	0.62186400
N	-3.99945100	0.20496100	1.18268300
C	-3.20703000	-0.76482100	1.79303300
C	-1.78484400	-0.45050800	1.83695000
C	-1.37605400	0.70575200	1.27172900
O	3.91522600	3.06525100	-0.00666700
O	3.08391900	1.63824700	2.04410900
H	1.45083200	-4.10676200	0.28289700
H	1.34549700	-0.53649700	-1.12326300
H	2.28292400	-2.00024800	1.38584700
H	1.75160300	-0.29968400	1.24895400
H	4.40720000	-0.82993400	1.24249100
H	4.68792600	-1.27274400	-1.46486800
H	4.77346800	-3.70387600	-1.13596600
H	5.67586900	-2.81807700	0.12100500
H	4.26212600	-4.47321800	1.00264900
H	1.23537600	1.46871400	-1.98779800
H	2.23791400	2.91881800	-1.69249900
H	0.05857100	3.66138400	-2.33731500
H	1.14654900	4.54055600	0.07432300
H	-0.05059400	2.99964500	1.46584700
H	-1.17540000	4.38328200	1.49152100
H	-2.57364100	3.42811400	-0.21452100
H	-0.06513500	5.89231900	-1.36456900
H	-4.99561300	0.01124700	1.12308500
H	-0.32314700	0.97051900	1.20247400
O	-3.72192500	-3.95303700	-0.66874700
N	-2.92154000	0.32940300	-2.21333200
H	-2.32028500	1.14978900	-2.14836000
H	-3.91503100	0.50483500	-2.12770600

O	-3.71848000	-1.78817300	2.23037600
N	-3.23652300	-1.83395800	-1.37739800
H	-4.23030600	-1.72867400	-1.56284400
N	-2.23631000	1.63874200	0.71780900
O	-4.39116900	2.15325000	0.08150100
C	-0.87205300	-1.44222300	2.49263100
H	-0.84659600	-2.38828300	1.93927000
H	0.14290400	-1.04848100	2.56587600
H	-1.22544300	-1.66932000	3.50345800

63

T-A_dinucleotide

C	-1.01320600	4.57051600	-0.03250400
O	-0.20908700	4.15695400	1.06551200
C	-1.56035900	3.33744900	-0.72468000
O	-0.50635000	2.63821900	-1.39874300
C	-2.19830900	2.32945900	0.23910600
O	-3.33620900	1.76477900	-0.41468200
C	-1.09399100	1.29675900	0.45399900
C	-0.32712800	1.33070000	-0.86651900
P	-4.37017200	0.81932000	0.45212600
C	-3.63973300	-1.32055700	-0.88009500
O	-3.63154300	-0.64753200	0.37125700
C	-2.58857300	-2.40550000	-0.87528700
O	-1.29578300	-1.80640100	-0.84164300
C	-2.57514500	-3.35213200	0.32895900
O	-3.51600300	-4.40250000	0.23543600
C	-1.15397900	-3.90767900	0.25770000
C	-0.35394500	-2.78842400	-0.44166500
O	-5.64230400	0.77217600	-0.34119100
O	-4.32346900	1.22052700	1.89638300
H	-0.69963800	0.58093500	-1.56544300
H	-0.46363400	1.59316100	1.29634200
H	-1.50937200	0.30669100	0.63676000
H	-2.51497500	2.79879300	1.17384500
H	-2.29657000	3.65257500	-1.47162200
H	-0.42344600	5.15334700	-0.75014600
H	-1.85560400	5.18297800	0.31422300
H	0.16616900	4.93900000	1.49560700
H	-3.42547300	-0.61991600	-1.69716500
H	-4.62501200	-1.76717700	-1.05979100
H	-2.70530800	-3.00495000	-1.79230500
H	-2.73077800	-2.77105800	1.24566000
H	-0.73350000	-4.16613400	1.23135400
H	-1.16246800	-4.80624500	-0.36685100
H	0.20689300	-3.15599700	-1.30583700
H	-4.38110500	-4.08196800	0.53115000
C	1.72650800	0.27975100	-1.69812900
C	1.86090500	1.92549600	0.05796100
C	3.20956600	1.97615600	0.05890700
H	1.26845000	2.58558100	0.68552600
C	3.92446400	1.13392300	-0.89008500
N	1.11506300	1.09103200	-0.75528800
O	1.12239800	-0.42588400	-2.49165500
N	3.10681100	0.32283400	-1.67232600
H	3.56847400	-0.26853000	-2.35775200
O	5.14084800	1.11222800	-1.03915200
C	4.00317300	2.90075700	0.93203000
H	4.57015100	3.61608100	0.32708400

H	3.34373200	3.45702500	1.60270800
H	4.72708900	2.34375600	1.53553600
N	0.62915700	-2.13654000	0.40410500
C	0.39295700	-1.38325400	1.52833500
C	1.99119900	-2.13616300	0.22286600
H	-0.61223800	-1.24420800	1.90490100
N	1.47710600	-0.88162300	2.06555700
C	2.49376400	-1.34707900	1.25550900
N	2.70653200	-2.76988000	-0.71685900
C	3.89525300	-1.19296100	1.29529700
C	4.01077900	-2.56240900	-0.55971500
N	4.51185900	-0.46045100	2.24648000
N	4.63573100	-1.82790700	0.37350800
H	4.66290100	-3.05081000	-1.27998400
H	5.49429000	-0.24835800	2.13152700
H	3.96255700	0.15398000	2.83242200

61

T-C_dinucleotide

C	-0.30424200	4.60285700	-0.14231000
O	0.52165400	4.12144900	0.91099500
C	-0.99567600	3.42097700	-0.79315900
O	-0.03447700	2.61486900	-1.48717000
C	-1.69502200	2.49192000	0.20878800
O	-2.89698700	2.01890300	-0.40269700
C	-0.68127800	1.37073400	0.40827700
C	0.00935800	1.29732400	-0.95136500
P	-3.97131200	1.15144800	0.49657400
C	-3.42797000	-1.01799700	-0.86736300
O	-3.35132100	-0.36923200	0.39498300
C	-2.46347800	-2.17991700	-0.89954800
O	-1.13545400	-1.68437000	-0.78717600
C	-2.56117000	-3.20765200	0.23272300
O	-3.56413100	-4.18297500	0.02721500
C	-1.17592500	-3.85375200	0.17356200
C	-0.27826000	-2.76777800	-0.46160100
C	2.12094400	-2.49126700	0.14368900
N	3.05059000	-1.92409100	0.95898500
C	2.68168200	-1.20940100	2.01347500
C	1.30590100	-1.00638700	2.36997600
C	0.38949600	-1.55473600	1.53942100
O	-5.26580600	1.20085400	-0.26003100
O	-3.85219600	1.54630700	1.93847900
H	-0.49069700	0.59468200	-1.61894200
H	0.02164900	1.64385000	1.19913500
H	-1.16465100	0.42713900	0.65556300
H	-1.94140300	3.00450100	1.14209300
H	-1.72380100	3.79636000	-1.52005300
H	0.29397000	5.12812600	-0.89650700
H	-1.06754600	5.28967400	0.24577200
H	0.98522000	4.86887200	1.31559000
H	-3.16885200	-0.31969900	-1.67335100
H	-4.44775500	-1.38127800	-1.04319200
H	-2.59515200	-2.70828800	-1.85809900
H	-2.72003300	-2.68629600	1.18462900
H	-0.80364300	-4.17604900	1.14844700
H	-1.22783500	-4.72840000	-0.48200100
H	0.24502500	-3.12024800	-1.34991800
H	-4.41910700	-3.82674000	0.31124800

H	-0.67987500	-1.45936600	1.70122400
C	1.85296400	-0.08901200	-1.79218700
C	2.29603100	1.59078500	-0.11790600
C	3.62298000	1.35144100	-0.07360300
H	1.83926700	2.39860400	0.44879800
C	4.15166500	0.28394700	-0.91400300
N	1.40792000	0.87270500	-0.90007500
O	1.13024700	-0.69195700	-2.57148400
H	1.01305000	-0.44544400	3.24815500
N	3.20984700	-0.33026100	-1.72946100
H	3.53050600	-1.11135500	-2.29501600
O	5.32785000	-0.06179300	-0.95835100
C	4.57856100	2.13627700	0.77293600
H	5.33079300	2.63446700	0.15246600
H	4.04548100	2.89483500	1.35157800
H	5.11244800	1.48130200	1.46850800
N	0.75890900	-2.25073800	0.42885500
O	2.42291500	-3.19000000	-0.82675200
N	3.65249000	-0.66822900	2.76724300
H	3.44656500	-0.11671900	3.58769000
H	4.62005000	-0.83656700	2.52585800

62

T-E_dinucleotide

C	1.23233000	-4.55889600	-0.08117200
O	0.32976900	-4.19275300	0.95544200
C	1.70569800	-3.29944700	-0.77966000
O	0.61846700	-2.70081600	-1.49825900
C	2.23200600	-2.22088600	0.17769000
O	3.31501200	-1.55819300	-0.47806700
C	1.03061600	-1.29812900	0.35139600
C	0.34742600	-1.39292700	-1.01116800
P	4.27879900	-0.53358100	0.37889600
C	3.22533800	1.53870700	-0.84198200
O	3.38847800	0.84702800	0.38944700
C	2.07057600	2.50718500	-0.72737600
O	0.86404800	1.78517500	-0.54589000
C	2.09082200	3.47336200	0.46360100
O	2.87425300	4.63235700	0.23993100
C	0.61091500	3.84844200	0.60192300
C	-0.13995000	2.73595200	-0.17802800
C	-2.52679300	2.07467700	0.30216600
N	-3.44195600	1.38407600	1.06419700
C	-3.14051800	0.57411000	2.14777000
O	-4.04111100	-0.02637200	2.74275800
C	-1.72974900	0.53017800	2.47663700
C	-0.81938600	1.22456200	1.74275200
O	5.49920400	-0.32718900	-0.46894300
O	4.34630300	-0.98586600	1.80751900
H	0.72294300	-0.63912500	-1.70469700
H	0.38381500	-1.68262900	1.14468100
H	1.32067300	-0.27241900	0.57617100
H	2.58190800	-2.64321100	1.12351900
H	2.48794800	-3.56934700	-1.49701200
H	0.74010800	-5.21073600	-0.81293000
H	2.10415300	-5.08381600	0.33035300
H	0.00551600	-4.99475500	1.39021400
H	3.01789100	0.83078200	-1.65481900
H	4.14303400	2.08620400	-1.08965500

H	2.02501300	3.10170000	-1.65611500
H	2.44332200	2.93794900	1.35271000
H	0.29419000	3.90630100	1.64617400
H	0.44176800	4.82532700	0.13965000
H	-0.58389100	3.14890600	-1.09209800
H	3.80595200	4.42120500	0.40094300
H	-4.42447000	1.42346600	0.80287600
H	0.23483600	1.18175800	2.00828000
C	-1.69914600	-0.31114300	-1.83441900
C	-1.85662700	-2.03882200	-0.15835800
C	-3.20021300	-1.96528600	-0.04526700
H	-1.27383600	-2.77940600	0.38516400
C	-3.88995800	-0.95650700	-0.83679300
N	-1.10300400	-1.21324800	-0.97267300
O	-1.09807900	0.38208400	-2.64096600
C	-1.19447000	2.01484300	0.61118200
C	-3.06798000	2.81842000	-0.79616500
C	-3.56053500	3.42395600	-1.71776200
H	-3.98844600	3.96726600	-2.53536600
H	-1.44193500	-0.07810200	3.32696800
N	-3.07349200	-0.24238400	-1.70629100
H	-3.52616400	0.45275800	-2.29433500
O	-5.09165600	-0.71090400	-0.78403900
C	-4.01082000	-2.84947100	0.85371100
H	-4.76249000	-3.40353400	0.28204600
H	-3.36537200	-3.56652900	1.36731400
H	-4.53429700	-2.24909600	1.60437000

64

T-G_dinucleotide

C	-2.87210600	-4.18425900	-0.17481300
O	-1.78453500	-4.04215400	-1.07983100
C	-3.09543700	-2.86083300	0.53125700
O	-1.95631100	-2.55760700	1.34985000
C	-3.26366600	-1.66452700	-0.41720800
O	-4.14389300	-0.73370200	0.22063300
C	-1.85033000	-1.10639400	-0.49692400
C	-1.36859800	-1.33026100	0.93357600
P	-4.64402800	0.60740900	-0.59538200
C	-2.98201000	2.09395800	0.80218000
O	-3.33266500	1.59746100	-0.48074900
C	-1.56565800	2.62193000	0.78381000
O	-0.64412500	1.56708400	0.51893500
C	-1.21406800	3.65837900	-0.29030200
O	-1.62427200	4.97140000	0.03501800
C	0.31501600	3.56788600	-0.31554600
C	0.61089000	2.17682800	0.29276500
O	-5.76261500	1.17858900	0.22414000
O	-4.77787900	0.28701400	-2.05397500
H	-1.68278500	-0.52092000	1.59257900
H	-1.27117400	-1.69271100	-1.21298800
H	-1.82711400	-0.05405300	-0.76949100
H	-3.67266800	-1.95380800	-1.38916500
H	-3.97722800	-2.94973300	1.17492200
H	-2.65339600	-4.95297500	0.57621900
H	-3.79057000	-4.46275000	-0.70774800
H	-1.61918400	-4.89419000	-1.50861300
H	-3.06298500	1.30256500	1.55837100
H	-3.66018300	2.90660700	1.09083200

H	-1.35757200	3.06036800	1.77407400
H	-1.64306900	3.34141200	-1.24784500
H	0.73517700	3.66599500	-1.31849400
H	0.73191400	4.35714800	0.31652600
H	1.17237300	2.25442600	1.23140600
H	-2.55140300	5.08824000	-0.22047000
C	0.69433100	-0.69303600	2.08541200
C	0.79626800	-2.25391700	0.24823600
C	2.14205200	-2.34595600	0.25543600
H	0.18319300	-2.86082600	-0.41322800
C	2.87312100	-1.52548200	1.21136600
N	0.07677200	-1.41775200	1.08186800
O	0.10421300	-0.03410200	2.92880600
N	2.07310100	-0.76754500	2.05948600
H	2.55362700	-0.19888700	2.75120400
O	4.09507700	-1.47670000	1.31333700
C	2.91735800	-3.22949500	-0.67310800
H	3.56188500	-3.91620500	-0.11522000
H	2.23978100	-3.81546600	-1.29894200
H	3.56214400	-2.63218600	-1.32765100
N	1.38508100	1.29618600	-0.56382400
C	0.96214100	0.64683700	-1.70591500
C	2.73613400	1.09011300	-0.48131100
H	-0.07567700	0.67178100	-2.00889900
N	1.93120900	0.03312400	-2.33425000
C	3.05409000	0.30212200	-1.58089300
N	3.55446000	1.55680400	0.48916400
C	4.42190600	-0.07900800	-1.77311500
C	4.80530900	1.19491600	0.31392300
O	4.91840600	-0.76297200	-2.66434500
N	5.23531700	0.46065100	-0.76121600
N	5.75977200	1.61615100	1.18725100
H	6.22167400	0.22947100	-0.83795200
H	6.60388600	1.06485000	1.28143600
H	5.39812000	1.97409500	2.06299700

63

T-T_dinucleotide

C	-0.74161400	4.59590600	-0.15936500
O	0.15291100	4.14602000	0.85104900
C	-1.36553000	3.38582100	-0.82636200
O	-0.36819600	2.67178700	-1.57083500
C	-1.96468700	2.37758800	0.16348900
O	-3.12946300	1.81447000	-0.44328100
C	-0.85627600	1.34168100	0.31166800
C	-0.21464100	1.34928900	-1.07377000
P	-4.11019100	0.83888900	0.45228100
C	-3.32314000	-1.26938000	-0.89972800
O	-3.33026500	-0.60712500	0.35728600
C	-2.27200200	-2.35450700	-0.89426300
O	-0.97840200	-1.76404200	-0.80913200
C	-2.29255600	-3.33864700	0.28130200
O	-3.22121300	-4.39205000	0.11897500
C	-0.86275400	-3.88328300	0.25314500
C	-0.05787100	-2.79281400	-0.48951900
N	1.01192800	-2.18946000	0.30494900
C	2.32787000	-2.41045200	-0.05155700
O	2.67464700	-3.09371600	-1.00490600
N	3.24386500	-1.78016400	0.76511700

C	2.99198200	-0.94113200	1.84851300
O	3.92219800	-0.42688100	2.45643000
C	1.57890000	-0.76573500	2.16657700
C	0.67885500	-1.41196700	1.39770600
C	1.21088800	0.12901000	3.31007200
O	-5.39863600	0.75157600	-0.31024500
O	-4.03808100	1.24484000	1.89394500
H	-0.68777100	0.62932600	-1.74296700
H	-0.14932900	1.66676200	1.07946600
H	-1.24871000	0.35763400	0.56147300
H	-2.23730200	2.84314600	1.11420100
H	-2.13943900	3.72694000	-1.52199200
H	-0.20958700	5.18631500	-0.91491900
H	-1.53968300	5.21205800	0.27440700
H	0.57484000	4.91315000	1.26430200
H	-3.10144100	-0.56003300	-1.70755900
H	-4.30559700	-1.71548400	-1.09576700
H	-2.36463500	-2.92742400	-1.83117700
H	-2.49030200	-2.78855700	1.20890300
H	-0.45739200	-4.08518900	1.24708100
H	-0.85029300	-4.81519000	-0.31955500
H	0.42012500	-3.17221700	-1.39383000
H	-4.09860600	-4.08903100	0.39645200
H	4.21961400	-1.91238600	0.50789700
H	1.57648900	1.14702900	3.13061200
H	0.12630600	0.16640300	3.43891700
H	1.66444900	-0.21885400	4.24343100
H	-0.38845400	-1.34185600	1.58344200
C	1.68692300	0.07660500	-1.96829300
C	2.06854700	1.76874500	-0.29061600
C	3.40259800	1.56999400	-0.23164300
H	1.58039700	2.56000200	0.27426100
C	3.96436400	0.50381300	-1.05020300
N	1.20978100	1.02054900	-1.07590600
O	0.99312600	-0.54639800	-2.75646700
N	3.05090700	-0.13028700	-1.88490500
H	3.40843000	-0.87883100	-2.47327000
O	5.13818400	0.14643700	-1.04110900
C	4.32506200	2.36908900	0.63776900
H	5.09865700	2.86019400	0.03871100
H	3.76811500	3.13431800	1.18446700
H	4.82461500	1.71686100	1.36079900

Table S3. Cartesian coordinates (in Å) of the stacked base pairs extracted from the optimised dinucleotides

35

A-E

N	-0.55202700	0.87128600	2.26266400
C	-0.25365800	-0.42679500	2.44599000
N	0.68193400	-1.15430600	1.84643700
C	1.39920300	-0.42394600	0.98011300
C	1.24399700	0.93939900	0.72743600
C	0.17774700	1.57862000	1.38860400
N	-0.11853200	2.88729500	1.17633300
N	2.18174800	1.38677600	-0.18199700
C	2.86809700	0.31246900	-0.48210900
N	2.43768200	-0.81931400	0.17208200
C	-1.86227300	-0.46884400	-0.58650700
N	-1.67760800	0.84595100	-0.94430200
C	-0.68382100	1.32078100	-1.78341900
O	-0.55580400	2.53906600	-1.96192900
C	0.12955200	0.28230900	-2.37922200
C	-0.05495500	-1.02534200	-2.04923600
H	-0.87245200	-0.94645300	3.17373100
H	0.15295200	3.27651500	0.27873200
H	-1.01380300	3.20360800	1.52997700
H	3.71591600	0.26562800	-1.15540800
H	-2.27642700	1.55233100	-0.52474000
H	0.57731200	-1.78848300	-2.49563900
C	-1.05437400	-1.44084700	-1.11732700
C	-2.93414800	-0.72493300	0.32891700
C	-3.85016600	-0.91458700	1.09258300
H	-4.65884900	-1.08909400	1.77227800
H	0.90141200	0.59833000	-3.07198700
C	-1.18174800	-2.88323700	-0.71058400
H	-0.62282100	-3.06704800	0.21543600
H	-2.22365300	-3.16200800	-0.53251500
H	-0.77593800	-3.53781400	-1.48622500
C	2.97763100	-2.16513400	0.07040800
H	3.38714900	-2.47857000	1.03275200
H	2.18909500	-2.85740800	-0.23282100
H	3.76765100	-2.16535400	-0.68053200

36

A-T

N	0.13916900	2.70555000	-0.43603100
C	-0.15580400	2.16098300	-1.62893200
N	-0.91141600	1.10003200	-1.89207700
C	-1.43360500	0.57254400	-0.77398700
C	-1.24749200	1.04797900	0.52366800
C	-0.38543500	2.15281300	0.66698500
N	-0.08753800	2.67762100	1.88077500
N	-1.95063000	0.28889800	1.43806400
C	-2.53648800	-0.62489500	0.70577500
N	-2.25363800	-0.52178900	-0.63751900
N	1.41697700	-1.18137700	-1.11939700
C	2.07920300	-0.04912600	-0.68022500
O	2.72524900	0.68944900	-1.40920500
N	1.96247500	0.17808500	0.67462000
C	1.25632700	-0.57266400	1.61097200
O	1.20838900	-0.20589400	2.77944700

C	0.62517100	-1.77557200	1.07820300
C	0.73852400	-2.00967900	-0.24614900
C	-0.10586700	-2.67616000	2.02629600
H	0.29595000	2.65180700	-2.48729900
H	-0.21199100	2.08076000	2.69013700
H	0.69317300	3.32128300	1.92178300
H	-3.20649500	-1.39688200	1.06605000
H	2.42755300	1.01570800	1.01505800
H	-0.87550300	-2.11724300	2.56697100
H	-0.58072900	-3.50096300	1.48860300
H	0.58014000	-3.09596500	2.76965000
H	0.28389300	-2.87568000	-0.71697600
C	1.46247500	-1.45125900	-2.55610500
H	0.94568100	-0.65302400	-3.09452500
H	2.49988900	-1.50456100	-2.88989900
H	0.96787700	-2.40338100	-2.74452700
C	-2.76691400	-1.34834100	-1.71794300
H	-3.53336500	-0.80858900	-2.27836700
H	-1.94884200	-1.61563200	-2.38925800
H	-3.19468400	-2.25495400	-1.28972800

33

C-E

C	-1.94108700	-0.16954700	-0.01600200
N	-1.65598900	1.17357400	-0.06570600
C	-0.93334700	1.81062700	-1.06055700
O	-0.68185200	3.01821300	-0.96665200
C	-0.53098900	0.93871500	-2.14274400
C	-0.83485800	-0.38778600	-2.12160000
H	-1.94987600	1.76120600	0.70953400
H	-0.51727000	-1.02044300	-2.94614700
C	1.42211300	-1.07568700	1.03305200
C	2.49465500	0.32072800	-0.61962900
C	2.09501900	1.44202800	0.02418000
H	3.13569900	0.33536200	-1.49785900
C	1.24561000	1.24752400	1.16342200
H	2.37797100	2.42943800	-0.31704600
N	2.12035600	-0.91673800	-0.18471600
N	0.94901600	0.05030900	1.64199600
O	1.25142100	-2.20137800	1.50281300
N	0.74437100	2.32618200	1.80409700
H	0.06029900	2.16778500	2.53333500
H	0.69831000	3.21169800	1.31621200
C	-1.55093200	-0.99065100	-1.04228500
C	-2.64815000	-0.61059400	1.14932800
C	-3.24115500	-0.94476100	2.14662000
H	-3.76704300	-1.25052200	3.02773200
H	0.03046600	1.38809400	-2.95456700
C	-1.80888200	-2.47260100	-1.02372500
H	-0.95216200	-3.00974900	-0.59962400
H	-2.68734500	-2.72006000	-0.42315300
H	-1.96743000	-2.84597900	-2.03901000
C	2.55078500	-2.12855800	-0.87601000
H	3.25256000	-2.68964400	-0.25505000
H	1.68333700	-2.75747800	-1.08456100
H	3.02896100	-1.84429800	-1.81307300

34

C-T

N	-0.82897400	1.90051300	0.26266900
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C	-1.24641100	1.45552800	-0.97912000
O	-1.11725400	2.09418400	-2.01291100
N	-1.85421400	0.21810500	-0.95332800
C	-2.03038000	-0.62867100	0.13634500
O	-2.54434200	-1.73055700	-0.01800100
C	-1.56718800	-0.08806000	1.40948000
C	-1.00219100	1.13634100	1.40118000
C	-1.72531600	-0.92620000	2.64063600
H	-2.15390500	-0.13646900	-1.85735100
H	-1.16745800	-1.86455600	2.54161500
H	-1.36032200	-0.39365300	3.52239500
H	-2.77577400	-1.18842800	2.80152600
H	-0.63227400	1.60003300	2.30936400
C	2.08119100	0.12304600	-0.60003100
C	1.48020100	-1.57818500	1.00669000
C	0.77533700	-2.25641200	0.07147900
H	1.63345700	-1.94737700	2.01841300
C	0.67016600	-1.63272700	-1.21700100
H	0.30167000	-3.20482900	0.29083300
N	2.06555200	-0.37936800	0.72206600
N	1.30146600	-0.50898900	-1.52404400
O	2.77448300	1.10143900	-0.87752900
N	-0.08504600	-2.20810100	-2.17051200
H	-0.19996500	-1.73888600	-3.05922900
H	-0.70493400	-2.97508100	-1.95057000
C	2.83722700	0.34712300	1.72664600
H	3.90281600	0.30712000	1.48932600
H	2.51933700	1.39099400	1.74406000
H	2.65617800	-0.10672500	2.70083600
C	-0.14019000	3.19085800	0.30409900
H	0.79222400	3.13074000	-0.26223500
H	-0.77763100	3.96482600	-0.12587400
H	0.07731200	3.43079500	1.34403300

35

E-A

C	0.49697800	1.75547600	0.47050600
C	-1.93253500	1.52804800	0.17083200
C	0.71001200	1.92133100	-0.87362100
C	-1.69321000	1.68880900	-1.24657900
C	-0.43488600	1.87900800	-1.72912800
O	-3.03849100	1.38628400	0.70562300
H	-0.27458000	2.03897800	-2.79419500
H	-2.56322100	1.67448400	-1.89451200
N	-0.77968500	1.54081500	0.94054800
H	-0.91605500	1.42897200	1.94141700
C	1.51863100	1.83249600	1.47186200
C	2.34397800	1.91330700	2.34935500
H	3.08770600	1.97687000	3.11681100
N	1.80075700	-1.67023000	-0.45659200
C	0.66111600	-1.60796400	0.31242900
C	1.37349300	-1.64602200	-1.76572300
N	0.56524900	-1.61320500	1.64756000
C	-0.39391900	-1.56095400	-0.59498000
N	0.07317100	-1.58165700	-1.89533500
H	2.07249100	-1.68988900	-2.59000200
C	-0.70406800	-1.58865200	2.04637300
C	-1.68829800	-1.51955900	-0.04062800
N	-1.81418500	-1.54956900	1.29481500

H	-0.86832500	-1.60155000	3.12122000
N	-2.80774000	-1.48563900	-0.80620600
H	-2.69452400	-1.21710000	-1.77616400
H	-3.64116800	-1.12882000	-0.35270600
C	2.07867600	2.13473300	-1.45808200
H	2.13586500	3.09920400	-1.97385200
H	2.85305700	2.11031000	-0.68861900
H	2.30335900	1.35511400	-2.19447300
C	3.16754100	-1.66702600	0.03735700
H	3.36513400	-0.73542600	0.57347600
H	3.32113000	-2.51473400	0.70750100
H	3.84301400	-1.74848600	-0.81424700

33

E-C

N	0.63321700	2.02915000	-0.14466500
C	0.01088900	1.30387800	-1.18427200
O	0.66234500	1.00090800	-2.18763200
N	-1.29580500	0.96379300	-1.02784400
C	-1.95854100	1.30763500	0.06722200
C	-1.36599100	2.07475300	1.12570000
C	-0.06386600	2.40410000	0.96370500
H	0.49697700	2.96351000	1.70633400
C	1.12399500	-1.35485500	0.12489600
C	-1.06276200	-2.09616300	-0.70863700
C	0.66648700	-1.24029600	1.41244200
C	-1.52719100	-2.00818400	0.65954300
C	-0.69830800	-1.59406400	1.65613200
O	-1.74307800	-2.44633300	-1.68189600
H	-1.05558900	-1.54741400	2.68391200
H	-2.56136000	-2.27736700	0.84527200
N	0.27044900	-1.76782500	-0.87190500
H	0.61069000	-1.75806000	-1.82942900
C	2.47794700	-1.12002000	-0.28346700
C	3.61103200	-0.95720400	-0.66810500
H	4.61719600	-0.79941300	-0.99825700
H	-1.92034200	2.36577600	2.00871400
N	-3.24431400	0.92567100	0.16003000
H	-3.76983300	1.05501900	1.01272200
H	-3.62137300	0.30400500	-0.54356900
C	2.01702900	2.45322000	-0.34665300
H	2.64019400	1.58407600	-0.55657800
H	2.07446200	3.14593100	-1.18964600
H	2.36481500	2.94808400	0.56012900
C	1.57059900	-0.76590900	2.51893400
H	2.43289000	-1.42867400	2.64664600
H	1.95673700	0.23856100	2.31000400
H	1.02765200	-0.72750900	3.46602200

34

E-E

C	-0.78258800	1.56892500	0.01536000
N	-1.91242700	0.86736700	-0.33384300
C	-2.62354700	0.02115900	0.50112200
O	-3.59762100	-0.60336100	0.06690400
C	-2.11240500	-0.03809100	1.85487600
C	-1.00587900	0.66580000	2.21623500
H	-2.21439600	0.88389500	-1.30559300
H	-0.62898200	0.58968900	3.23335300
C	0.21487400	-2.48744800	0.34902200

C	-0.29808300	-1.29206200	-1.71662000
C	1.38220700	-1.69200800	0.56728500
C	1.70535200	-0.77110500	-0.39421700
O	-1.00718300	-0.98995600	-2.68716300
C	-0.29735400	1.49749200	1.29427400
C	-0.17526500	2.33149400	-1.03507500
C	0.31984200	2.94945800	-1.94716300
H	0.76120900	3.50484200	-2.74942800
H	-2.63874400	-0.68089600	2.55169800
H	-0.01727900	-3.25349500	1.08774100
C	-0.59041300	-2.31259600	-0.73540200
H	-1.48668700	-2.90290800	-0.89121000
N	0.88668500	-0.61474400	-1.49005400
H	1.12048800	0.10398700	-2.17040800
C	2.86126700	0.07579400	-0.37104900
C	3.82649300	0.80038600	-0.41904200
H	4.68601600	1.43817300	-0.45052000
C	2.20075400	-1.88233800	1.81345600
H	3.10885000	-1.27613000	1.79491600
H	1.61851400	-1.59742500	2.69744400
H	2.48802500	-2.93182400	1.93310100
C	0.94451400	2.21689300	1.74087300
H	1.38621600	2.80149400	0.93140500
H	0.72143300	2.89063500	2.57494700
H	1.69534900	1.49761900	2.08829700

36

E-G

C	-1.69187300	1.46326500	-0.23067100
C	-2.60857900	-0.80522500	-0.09317200
C	-1.26020900	1.27390200	-1.51643000
C	-2.20701500	-0.97419100	-1.47024300
C	-1.54226900	0.01460200	-2.12974800
O	-3.09932900	-1.68627700	0.63208400
H	-1.19342800	-0.13531400	-3.15020300
H	-2.40423300	-1.93863800	-1.92515800
N	-2.35597800	0.44997300	0.42285200
H	-2.58028400	0.57043300	1.40754300
C	-1.49673400	2.66924300	0.51697800
C	-1.34951500	3.67540300	1.16854500
H	-1.21271700	4.57006600	1.74070600
N	2.93689400	0.60896900	0.21627200
C	1.85805500	-0.16472500	0.55318600
C	3.43161800	0.08435000	-0.96190000
N	1.07845400	0.00061700	1.64765400
C	1.76758300	-1.12983000	-0.44067200
N	2.76635200	-0.96132900	-1.37721300
H	4.28807100	0.51221700	-1.46312600
C	0.12344600	-0.89767500	1.72906900
C	0.72836400	-2.11234200	-0.34709100
N	-0.79295500	-0.82214200	2.72937600
N	-0.05075900	-1.90124300	0.80881000
O	0.46468400	-3.04242000	-1.10249700
H	-0.53458900	-0.24156200	3.51755500
H	-1.36049700	-1.63127000	2.94747900
H	-0.85571500	-2.51860100	0.90648300
C	3.41936600	1.76798600	0.94921600
H	2.65100700	2.54372900	0.96893900
H	3.67361000	1.47993900	1.97082700

H	4.30848900	2.14781600	0.44636900
C	-0.49115400	2.31878600	-2.27672500
H	-0.42774800	3.25695500	-1.72238500
H	0.52851500	1.96893600	-2.47478000
H	-0.96388300	2.51966900	-3.24326000

35

E-T

N	0.29007200	-1.95116200	-0.53070700
C	0.18219100	-0.98036900	-1.50719800
O	-0.70217600	-0.95303900	-2.35288200
N	1.16885000	-0.01933000	-1.45544700
C	2.18972300	0.10915900	-0.51657400
O	2.97032300	1.05028700	-0.58419100
C	2.22468300	-0.94203400	0.49378500
C	1.28904200	-1.91072200	0.42273000
C	3.27377500	-0.87247700	1.56077100
H	1.09827400	0.71696800	-2.15577300
H	3.18026100	0.06099700	2.12738900
H	3.17528400	-1.71100200	2.25459100
H	4.27841200	-0.89055800	1.12674800
H	1.25062000	-2.72290100	1.14289400
C	-1.81124300	0.58159100	0.46493800
C	-0.44995400	2.32636400	-0.59780500
C	-1.10577400	0.66294000	1.63728800
C	0.22987000	2.46687600	0.67088200
C	-0.08118700	1.65809000	1.72075500
O	-0.16653200	2.92721800	-1.64398600
H	0.44529000	1.75998300	2.66906400
H	1.01867600	3.20860400	0.72712200
N	-1.48320300	1.40785200	-0.58724000
H	-1.96187100	1.26995900	-1.47383400
C	-2.91692200	-0.29876700	0.23000300
C	-3.86391700	-1.00710300	-0.01392500
H	-4.69777500	-1.64661600	-0.21929100
C	-1.37400900	-0.23803700	2.80972000
H	-1.64936400	0.34513000	3.69464700
H	-2.17887700	-0.94500500	2.59846200
H	-0.47265400	-0.80933400	3.05978300
C	-0.68132200	-3.04578300	-0.56949700
H	-1.69317100	-2.64046500	-0.53792300
H	-0.55140800	-3.62801500	-1.48433100
H	-0.51438800	-3.68336200	0.29744300

36

G-E

C	-0.15191600	-0.07983200	-1.81544300
N	0.68927700	0.86443300	-1.46909200
C	1.73150900	0.40410200	-0.74802200
C	2.04193000	-0.90136100	-0.39392000
C	1.14301100	-1.94106000	-0.79702300
N	3.18128600	-0.93505300	0.38894700
C	3.53285600	0.31923400	0.51159800
N	2.68853800	1.18133900	-0.15945600
C	-2.36195900	0.05229500	0.67525700
N	-1.63966400	-0.90470200	1.35124200
C	-0.44604300	-0.69091000	2.02410400
C	0.02699900	0.67674200	1.96145000
C	-0.68146100	1.63168000	1.30073200
H	4.39128000	0.69842800	1.05327200

H	-1.98563600	-1.86039900	1.35969000
H	-0.30358000	2.65011600	1.22659900
O	1.20399100	-3.15024700	-0.59235300
N	-1.25929900	0.25026800	-2.53479300
H	-1.53103800	1.22602800	-2.40960400
H	-2.03479100	-0.40176900	-2.54762800
C	-1.92028000	1.34803300	0.64673000
C	-3.53945300	-0.41490400	0.00530800
C	-4.51332100	-0.84456000	-0.56536600
H	-5.38117100	-1.21738300	-1.06984000
H	0.97441500	0.88924100	2.44828900
O	0.11723900	-1.62814600	2.59876700
N	0.04879500	-1.40564400	-1.51313600
H	-0.63779900	-2.09206700	-1.81377200
C	-2.65092600	2.44481400	-0.07534500
H	-3.47898300	2.05666100	-0.67275300
H	-3.05812100	3.17207500	0.63559100
H	-1.96642300	2.99025300	-0.73527400
C	2.79164900	2.62772200	-0.25479000
H	2.95619300	2.92404200	-1.29256800
H	1.87443600	3.09122900	0.11327200
H	3.63325100	2.95423300	0.35581300

37

G-T

C	-0.07890500	-0.33127900	-1.75549000
N	0.60826900	0.74881200	-1.46544200
C	1.71665900	0.48717700	-0.74100500
C	2.21880200	-0.73729200	-0.31964600
C	1.48391700	-1.92074600	-0.65371600
N	3.38049300	-0.56351300	0.40821100
C	3.55964100	0.73321400	0.43670300
N	2.58041000	1.42327600	-0.24715300
C	-2.91385200	-0.19201800	0.10346700
N	-2.20730400	-1.14430600	0.80308600
C	-1.08060500	-0.95902500	1.60130100
C	-0.62131300	0.42059700	1.69633700
C	-1.29481900	1.35976100	0.99785000
H	4.37209900	1.26492200	0.91799500
H	-2.54667200	-2.09744200	0.70419700
H	-0.96550000	2.39603300	0.96311100
O	1.73571700	-3.09433400	-0.39846100
N	-1.21362400	-0.21664000	-2.49270000
H	-1.60619500	0.72380500	-2.50705500
H	-1.88594400	-0.97364200	-2.50196600
O	-0.55136000	-1.91927000	2.14713200
N	0.31331000	-1.59302000	-1.37371000
H	-0.25660000	-2.39129100	-1.64025600
N	-2.43445300	1.09838800	0.25607000
O	-3.87382800	-0.48819500	-0.59480500
C	0.57849000	0.69819900	2.55074500
H	1.47744000	0.22001800	2.14438900
H	0.75678600	1.77133100	2.63520600
H	0.42613200	0.29572800	3.55723600
C	-3.16088600	2.17037200	-0.42391400
H	-3.39873900	1.86722600	-1.44445600
H	-4.09297000	2.38790300	0.10293100
H	-2.53185500	3.05927200	-0.44081800
C	2.46712300	2.86272100	-0.41933300

H	2.44686300	3.10778900	-1.48270100
H	1.55397600	3.22691300	0.05600000
H	3.33174600	3.33476400	0.04692800

36

T-A

C	-0.17990300	1.46889200	-1.19351800
C	1.15554800	1.87460200	0.77176800
C	2.17309200	1.07924400	0.38001500
H	1.21502600	2.46381800	1.68272400
C	2.05750400	0.40795000	-0.90723900
N	-0.01041400	2.05731000	0.04987300
O	-1.15347400	1.64646400	-1.90989100
N	0.85717400	0.63953000	-1.57349800
H	0.74538800	0.20011300	-2.48293100
O	2.91942000	-0.30033500	-1.41489700
C	3.43925100	0.90742000	1.16382500
H	4.30004300	1.28056800	0.59910500
H	3.38199800	1.44970800	2.11079400
H	3.62710800	-0.14988300	1.37677300
N	-2.48761600	-0.31690600	0.52327400
C	-2.07219100	-0.06735300	1.80867900
C	-1.50662100	-1.08753300	-0.05273400
H	-2.68519100	0.50764500	2.49070500
N	-0.90469900	-0.58656800	2.09677600
C	-0.53440600	-1.23375200	0.93468400
N	-1.47917500	-1.61775200	-1.28338400
C	0.59470500	-2.00426600	0.58694600
C	-0.37683000	-2.33509100	-1.48101900
N	1.60610600	-2.22961100	1.45170700
N	0.64082500	-2.55749800	-0.63492400
H	-0.28193400	-2.80726600	-2.45602200
H	2.45908800	-2.64424600	1.09975900
H	1.66317000	-1.68315500	2.30065600
C	-3.71077000	0.12785400	-0.12572800
H	-3.45462500	0.71208200	-1.01263100
H	-4.31572300	-0.73458000	-0.41241800
H	-4.26996600	0.74736700	0.57606800
C	-1.05726600	2.96451700	0.51624700
H	-0.98109400	3.93163900	0.01259500
H	-2.03244500	2.52636200	0.30055000
H	-0.94648600	3.09636100	1.59225000

34

T-C

C	1.39633600	0.76469000	-1.12195200
N	0.29732300	1.55039900	-0.96237700
C	0.05804300	2.15451400	0.19374300
C	0.93410100	2.03876800	1.32520300
C	2.01124500	1.23635500	1.16332300
H	2.73789700	1.06416400	1.95145600
C	0.06221200	-1.87786200	-0.21240500
C	-1.44694900	-0.83265800	1.35321600
C	-2.27659400	-0.35666900	0.40182800
H	-1.66569200	-0.72307000	2.41270900
C	-1.92853000	-0.60380100	-0.99212400
N	-0.27937400	-1.52541700	1.08294900
O	1.02979900	-2.56371400	-0.50667200
H	0.74697000	2.55752500	2.25659500
N	-0.78908300	-1.37667100	-1.17538200

H	-0.48689100	-1.53070200	-2.13336600
O	-2.57187600	-0.21105200	-1.95999400
C	-3.54116400	0.38896700	0.70285400
H	-4.41137800	-0.14093700	0.30165500
H	-3.67068300	0.50595600	1.78171900
H	-3.52635400	1.38320800	0.24556600
N	2.23966400	0.57545300	-0.00512900
O	1.67182600	0.21287000	-2.19002400
N	-1.05209500	2.90479200	0.28420400
H	-1.29559700	3.39800500	1.13105000
H	-1.65149300	3.00341600	-0.52435700
C	0.60044700	-1.99295000	2.15138400
H	0.54244200	-3.07957000	2.24830400
H	1.63054200	-1.71074500	1.92267900
H	0.29289900	-1.52082000	3.08352300
C	3.41376400	-0.27737600	-0.18423200
H	3.09080300	-1.27722300	-0.48001100
H	4.06033700	0.13904900	-0.95945600
H	3.95571600	-0.32484300	0.76056500

35

T-E

C	1.48182600	-1.13732200	0.27065900
N	0.32053500	-1.87648300	0.28426700
C	-0.47286500	-2.15091700	-0.81856600
O	-1.51527900	-2.80022100	-0.68651300
C	0.04521600	-1.62120400	-2.06409500
C	1.20203600	-0.90669300	-2.09191400
H	-0.02608900	-2.22576500	1.17479000
H	1.57646100	-0.52086200	-3.03777300
C	0.19118100	1.89409700	0.56561100
C	-1.72655400	1.34500600	-0.79071600
C	-2.27809400	0.51694200	0.12226800
H	-2.22634100	1.58225700	-1.72743900
C	-1.54106100	0.28626500	1.35655500
N	-0.50802200	1.97755700	-0.62431700
O	1.22509700	2.49758700	0.80892400
C	1.95535000	-0.62789600	-0.90849300
C	2.11445400	-0.95068200	1.54239900
C	2.61211700	-0.80644700	2.63334100
H	3.06296000	-0.67632800	3.59593100
H	-0.53087000	-1.82123400	-2.96076500
N	-0.38113100	1.04084300	1.48993500
H	0.14531900	0.92486800	2.35210100
O	-1.86736100	-0.49751200	2.24335200
C	-3.59007900	-0.18187600	-0.07106300
H	-4.29123500	0.07547200	0.72952800
H	-4.03561100	0.10016000	-1.02841400
H	-3.44732600	-1.26695600	-0.05726700
C	0.07739100	2.80753700	-1.67611200
H	0.15591600	3.84352300	-1.34098600
H	1.07344300	2.43380300	-1.92544000
H	-0.56230200	2.75090200	-2.55545600
C	3.21614300	0.19583300	-0.95284300
H	3.09902100	1.12112400	-0.37790800
H	4.06637900	-0.35214400	-0.53424100
H	3.45858600	0.46307900	-1.98415600

37

T-G

C	-2.36726900	-0.59980800	-1.00057000
C	-1.98694800	1.62205200	-0.13997200
C	-0.80467500	1.78378700	-0.76904600
H	-2.44411500	2.42206100	0.43684600
C	-0.29694400	0.66858100	-1.55642500
N	-2.73213200	0.45834300	-0.18762800
O	-3.04357600	-1.60188600	-1.18003600
N	-1.13895000	-0.43682500	-1.61040000
H	-0.82121800	-1.22445100	-2.16846900
O	0.77416200	0.65462300	-2.15516600
C	0.01369900	3.03573300	-0.68639500
H	0.21855900	3.43766600	-1.68374400
H	-0.50924800	3.79712200	-0.10248200
H	0.97914000	2.83626800	-0.20776000
N	-0.28705900	-1.14334600	1.61283400
C	-0.40797100	-0.07829400	2.48228400
C	0.84427200	-0.91336800	0.87675400
H	-1.22204700	-0.02861700	3.19242600
N	0.54070200	0.81037200	2.33794400
C	1.33845400	0.30189500	1.33504200
N	1.33786700	-1.71423600	-0.09497600
C	2.54239200	0.81218600	0.74915500
C	2.43536700	-1.23592000	-0.63627300
O	3.14605600	1.85226300	0.99903700
N	3.03436700	-0.07262900	-0.22648400
N	3.07552400	-1.94431700	-1.60555800
H	3.89062400	0.22867700	-0.68285200
H	3.66270900	-1.44294100	-2.26066600
H	2.51826700	-2.67842200	-2.02556100
C	-4.02905400	0.36326200	0.48271200
H	-4.84089500	0.40813400	-0.24710100
H	-4.08991500	-0.57946000	1.02761900
H	-4.11507000	1.19291400	1.18281700
C	-1.12224100	-2.33204700	1.54278900
H	-1.24484900	-2.62348800	0.49833100
H	-0.66344300	-3.15347600	2.09801500
H	-2.09835300	-2.10187300	1.97144200

36

T-T

N	2.08541000	0.67009400	-0.23355000
C	1.39904500	0.46182100	-1.41387000
O	1.79051200	-0.26593900	-2.31559300
N	0.20518500	1.14811400	-1.49730000
C	-0.38144800	1.96810200	-0.53571400
O	-1.47166400	2.48281700	-0.74977200
C	0.40934400	2.14478100	0.67761100
C	1.59691300	1.50964300	0.74934400
C	-0.14683600	3.00170000	1.77302700
H	-0.32748500	0.99259800	-2.35041700
H	-1.10088200	2.59462400	2.12843700
H	0.54650600	3.05041600	2.61636600
H	-0.34028700	4.01848500	1.41720500
H	2.24681600	1.60613700	1.61356300
C	0.32583000	-2.05441300	0.25553800
C	-1.39022800	-0.83627300	1.43656700
C	-2.16466300	-0.64772500	0.34689900
H	-1.70705300	-0.51955500	2.42791700
C	-1.66411700	-1.13581200	-0.93121900

N	-0.15521400	-1.45909300	1.40846100
O	1.35902900	-2.70142500	0.18771000
N	-0.46665400	-1.83840700	-0.85599700
H	-0.08814500	-2.19654400	-1.72937100
O	-2.20836200	-0.96534000	-2.01767700
C	-3.49170500	0.04744100	0.37967400
H	-4.28500500	-0.60742600	0.00507000
H	-3.74037000	0.34893800	1.40041300
H	-3.46772100	0.94044700	-0.25253800
C	0.65494800	-1.60313800	2.61730400
H	0.64912700	-2.63985600	2.96148000
H	1.68265400	-1.30407300	2.40214600
H	0.24135600	-0.95389600	3.38780700
C	3.37977000	-0.00246600	-0.09583300
H	3.23750000	-1.08280700	-0.16182000
H	4.05588600	0.32815500	-0.88657600
H	3.79877700	0.25653200	0.87570600

Table S4. Cartesian coordinates (in Å) of the optimised dinucleotide duplexes

124

5C3C-5G3G

O	-3.76128800	-0.13467300	1.85400000
N	-5.00235200	-2.01065300	1.29730100
C	-2.65234600	-3.42495900	1.29865500
H	-6.03073300	-3.80383300	0.98068100
C	-3.89866900	-4.11699500	1.10328300
C	-5.03933700	-3.37228100	1.10759600
C	-3.76541200	-1.35819100	1.59133100
H	-5.10480900	0.88785200	-1.12591000
H	-6.73654100	4.89820900	-2.74834500
H	-2.55355400	3.23471600	-0.17296500
H	-3.41598300	4.81896000	-1.71334300
H	-3.31240500	3.45232000	-2.85254100
H	-5.69307600	2.93108300	-2.48984200
H	-5.60977200	4.68500200	0.00530000
H	-7.78764200	3.81853300	-0.30980900
H	-7.03825600	2.82694500	0.96767300
H	-8.59808500	-4.93863600	0.97678100
H	-10.11243300	-3.19388800	1.59736000
H	-8.87375900	-3.56877400	2.83476400
H	-9.16705500	-1.13563900	2.37621300
H	-9.18109000	-1.64505500	-0.36733900
H	-6.69912700	-0.67688400	-0.87079000
H	-6.92186700	-2.40200200	-0.50155800
H	-5.96247000	-0.18644000	1.39046600
O	-8.84907300	0.35909000	-2.20603200
O	-9.82179200	2.35722700	-0.66542600
C	-4.08809100	0.54120100	-1.28798400
C	-3.78515400	-0.75054300	-1.60380200
C	-2.39764000	-1.10805700	-1.68413500
O	-0.87239600	2.04006000	-1.30570100
C	-1.73626800	1.13289500	-1.33810800
N	-3.10223800	1.47569400	-1.12324300
C	-3.42800100	2.88426900	-0.72586500
C	-3.76819200	3.80002300	-1.92127900
O	-5.79152800	5.02236000	-2.54444700
C	-5.30350600	3.80274500	-1.94727300
O	-4.57888800	2.86280200	0.12998800
C	-5.65285500	3.67822700	-0.44432100
O	-7.24127100	1.88169700	-0.90308700
C	-7.00703000	3.07171900	-0.10564200
P	-8.81687500	1.24034000	-0.95552100
C	-6.25209800	-1.22552200	1.21489800
C	-7.01935600	-1.38568500	-0.10769900
O	-8.81643500	0.25879000	0.43336400
C	-8.47688700	-1.15354400	0.31361900
O	-7.15506800	-1.66598400	2.26144100
C	-8.52261600	-1.75480400	1.73710700
O	-8.31828000	-4.01514100	0.84724200
C	-9.03028000	-3.19379200	1.81121400
H	8.76784800	-4.95998700	-1.37608700
H	10.31391700	-3.16462300	-1.67741800
H	9.15917200	-3.37604000	-3.02830400
H	9.40385500	-1.03239000	-2.31805100
H	9.39631700	-1.70631800	0.36387600

H	6.84102100	-1.02901500	0.94620800
H	7.16438400	-2.65771600	0.29956300
H	6.17441200	-0.20430000	-1.24086200
N	5.22924000	-2.01071100	-1.40744600
N	3.78988400	-3.74746600	-1.61412400
C	1.68249500	-2.26574800	-1.71042000
C	3.08446400	-2.53988000	-1.63424900
C	3.96566500	-1.45203700	-1.51372500
N	3.67865200	-0.13674200	-1.48132400
C	2.36900400	0.12185700	-1.52537000
C	6.46217900	-1.26038400	-1.20852600
C	7.21450800	-1.58537200	0.08763600
O	7.38609000	-1.54911900	-2.29337300
C	8.74142200	-1.70241400	-1.75265000
O	8.47306600	-4.05893800	-1.15433100
C	9.24705900	-3.13056600	-1.95786900
C	8.65671100	-1.22095400	-0.28505700
O	8.91044300	0.21857200	-0.32231900
P	8.51793900	1.24999900	0.96580900
C	6.55986000	2.59455800	-0.39041400
O	6.89382200	1.61300500	0.62443600
C	5.46494900	3.54718600	0.10333600
O	4.15295300	2.90116500	0.18557900
C	5.71643800	4.13251500	1.51464500
O	5.10248600	5.44025100	1.67528500
C	4.97110700	3.15686300	2.43226500
C	3.77986700	2.67870000	1.57411400
O	9.37474800	2.49892000	0.74306200
O	8.46955000	0.46768300	2.28032200
H	6.20627000	2.07520300	-1.29290600
H	7.44739300	3.19114200	-0.64507700
H	5.36888000	4.35271700	-0.63938600
H	6.79052500	4.17924200	1.74197900
H	5.63097200	2.32324200	2.68321500
H	4.63724000	3.64188600	3.35485000
H	2.86833800	3.25209700	1.77521900
H	5.57632700	6.06681700	1.09754800
N	3.41426500	1.27497200	1.76434900
C	2.11580700	0.77736500	1.77734000
C	4.25988600	0.15813800	1.74424700
N	0.98011200	1.50764600	1.79288300
C	2.25346700	-0.62257300	1.78524300
N	3.60342500	-0.98510800	1.76721900
H	5.33183900	0.28379300	1.67406900
C	-0.12893400	0.75777300	1.78712800
C	1.06849300	-1.42192800	1.74147000
N	-2.62117400	-2.09853700	1.55166300
N	-1.47811200	-4.07975400	1.24221400
H	-1.45821100	-5.07314100	1.04274800
H	-0.58457400	-3.57965000	1.39069000
H	-3.93466300	-5.19181300	0.95164600
O	0.98062300	-2.67364200	1.70157600
N	-0.10341800	-0.62691900	1.73226100
H	-1.01145400	-1.14753700	1.68163400
N	-1.34332300	1.34968800	1.85914000
H	-2.22678700	0.81568200	1.83985300
H	-1.36750200	2.36099800	1.82079300
N	-1.42629900	-0.17639400	-1.56162100

N	-2.02284500	-2.38642400	-1.88993900
H	-2.72224100	-3.11974200	-1.89977600
H	-1.02338000	-2.65172100	-1.86131300
H	-4.56530700	-1.49405700	-1.72550700
O	0.74089600	-3.08909900	-1.82355200
N	1.40969900	-0.87550100	-1.63269800
H	0.39609100	-0.60851200	-1.62060800
N	1.94759200	1.41329000	-1.48971500
H	2.63303400	2.07564300	-1.12512600
H	0.94840100	1.63016900	-1.35980800
C	5.05690100	-3.39632000	-1.47217900
H	5.91387400	-4.06028500	-1.42879500

125

5C3T-5A3G

O	-3.16320400	-0.13905500	1.16027100
N	-4.60907800	-1.93727700	0.94082400
C	-2.39161100	-3.54009600	0.71536300
H	-5.79841300	-3.64525600	0.72042700
C	-3.70116200	-4.11307000	0.56846500
C	-4.77126300	-3.28532100	0.72372300
C	-3.29702100	-1.37555000	1.01761800
H	-5.50473500	1.20084800	-1.91882200
H	-4.78956500	-1.76887900	-3.78194100
H	-6.09371700	-1.03310500	-2.81944400
H	-5.05880400	-2.30681900	-2.12419600
H	-0.80091400	0.06437300	-1.73991400
H	-7.74805200	5.20751700	-2.20276600
H	-3.19653400	3.64383000	-0.56708900
H	-4.31089700	5.06759500	-2.05129100
H	-4.46299400	3.67093800	-3.14126500
H	-6.71500100	3.22318300	-2.32668300
H	-6.03888700	4.77106000	0.21361700
H	-8.26776200	3.95996900	0.30134700
H	-7.29076200	2.87266600	1.31970500
H	-8.13464300	-4.85810700	1.31254900
H	-9.41709500	-3.21763100	2.49715500
H	-7.86505400	-3.65049900	3.27905000
H	-8.34112600	-1.18645000	3.10508700
H	-9.00221900	-1.59955000	0.40091800
H	-6.78377100	-0.26023100	-0.51575000
H	-6.85372200	-2.03381900	-0.42286700
H	-5.41486800	-0.10206300	1.44458500
O	-9.65580900	0.33154800	-1.22437700
O	-10.26410300	2.21316400	0.61986800
C	-5.07161500	-1.42385100	-2.77748000
C	-4.46674600	0.87899200	-1.91925800
C	-4.10231800	-0.38092900	-2.28578000
O	-2.24564800	-1.88708000	-2.40060900
C	-2.69428400	-0.74174100	-2.17364900
N	-1.83314100	0.28812500	-1.78721700
O	-1.34432400	2.43778200	-1.13251700
C	-2.18401900	1.58250300	-1.44771000
N	-3.56591000	1.83987800	-1.49255100
C	-4.06011700	3.15920700	-1.02965600
C	-4.69218100	4.04261300	-2.13829200
O	-6.77901000	5.31222300	-2.20121700
C	-6.19601800	4.04728400	-1.81996600
O	-5.08617800	2.91436400	-0.04211400

C	-6.21296000	3.80391300	-0.29129000
O	-7.90036500	2.06713000	-0.52981600
C	-7.47999100	3.19214000	0.28322200
P	-9.29293000	1.23188700	-0.04097500
C	-5.80129000	-1.10578600	1.25047200
C	-6.88738900	-1.10949000	0.16036200
O	-8.67113000	0.28793900	1.23123800
C	-8.21414100	-1.06190900	0.93861400
O	-6.41909300	-1.63214800	2.45107100
C	-7.87079300	-1.74280400	2.28281800
O	-7.92182800	-3.91663600	1.18410000
C	-8.32020600	-3.19922100	2.38383900
N	0.94524500	-0.35650000	-1.71476500
H	8.04277700	-4.35533500	-2.03388800
H	9.56743200	-2.73089800	-2.85652500
H	8.04304700	-2.81475100	-3.79232200
H	8.81334900	-0.50730900	-3.17618700
H	9.24165300	-1.37279900	-0.55894900
H	7.04757100	-0.07065700	0.47651700
H	6.98845100	-1.79866300	0.03261300
H	5.83417500	0.58946900	-1.45438900
H	5.65556900	-3.24992100	-1.31448400
N	4.89038100	-1.23549600	-1.39937000
C	4.77151900	-2.62380600	-1.36027400
N	3.51797300	-3.04423500	-1.43129300
C	1.36875300	-1.65234200	-1.62323800
C	2.76546900	-1.87599400	-1.52847600
C	3.59621400	-0.73977500	-1.52585200
N	3.19289100	0.54566900	-1.62627000
C	1.85637800	0.64212600	-1.71329600
C	6.13810400	-0.46300000	-1.46810000
C	7.14076200	-0.78317800	-0.34405400
O	6.80546800	-0.75673600	-2.72283300
C	8.20767200	-1.11209300	-2.48781600
O	7.89605300	-3.42785500	-1.77620200
C	8.47536300	-2.58295900	-2.80615600
C	8.51496500	-0.70270000	-1.03188900
O	9.05893100	0.64816300	-1.07266400
P	9.72230900	1.32277200	0.33817500
C	7.56347900	2.91437400	0.47322400
O	8.32553300	1.86899500	1.12835500
C	6.23192400	3.09469500	1.18560800
O	5.37139800	1.94249000	0.91307600
C	6.32435300	3.23042000	2.74403700
O	5.52352000	4.33645900	3.24246400
C	5.68128900	1.93275400	3.24631100
C	4.65257500	1.65006100	2.13977300
O	10.53684200	2.52319100	-0.15035300
O	10.28079600	0.22091200	1.24157600
H	7.38046200	2.65322200	-0.57993500
H	8.11898400	3.86472000	0.50400000
H	5.74573400	3.99855100	0.78208300
H	7.36587900	3.33451600	3.07328000
H	6.43542300	1.13892700	3.27366700
H	5.22933200	2.04691400	4.23655200
H	3.78297000	2.31595500	2.23372100
H	5.92920300	5.16561400	2.92854600
N	4.11910800	0.30120100	2.08147800

C	2.78177600	-0.02494200	1.86966000
C	4.79997400	-0.91602400	2.20998400
N	1.76372400	0.84499900	1.70088800
C	2.73318200	-1.42961200	1.89823500
N	4.00714200	-1.96372200	2.10160100
H	5.86739200	-0.95326500	2.38166800
C	0.57668900	0.24407200	1.54998600
C	1.47010100	-2.07223300	1.69649000
H	1.43672500	1.64654200	-1.77880100
N	0.45210500	-2.64038000	-1.61528100
H	-0.53988600	-2.43478400	-1.79054000
H	0.75391700	-3.60104200	-1.50871100
N	-2.22527200	-2.21764400	0.92730700
N	-1.28749300	-4.31317900	0.64845400
H	-0.36809500	-3.93528400	0.93095500
H	-1.38734000	-5.31980100	0.57883800
H	-3.84063900	-5.17636600	0.39692500
O	1.22910800	-3.30135200	1.62960000
N	0.42241000	-1.13285100	1.54751800
H	-0.52433900	-1.52545500	1.32830500
N	-0.54813500	0.98995700	1.42384600
H	-1.46059500	0.54463300	1.24059300
H	-0.43211500	1.93961500	1.08511700

124

5C3E-5A3G

O	3.26779400	-0.10212900	-1.44155100
N	4.72238100	-1.87798200	-1.13895200
C	2.52024100	-3.48789100	-0.84646900
H	5.92902500	-3.53256800	-0.71584500
C	3.83144700	-4.03027200	-0.62086000
C	4.89619800	-3.19970000	-0.80311000
C	3.41080000	-1.33149000	-1.24203900
H	5.72356900	0.11521900	2.31721100
H	0.88664300	-0.44361400	1.96385700
H	5.98963800	6.01539400	1.82997800
H	3.66821700	3.28266000	1.95939900
H	5.31735300	3.24646400	3.78881700
H	6.34947700	2.09816400	2.88673600
H	7.35135500	4.15270400	2.19095700
H	5.56140200	4.50209200	-0.02525700
H	7.84903700	4.08146000	-0.52292200
H	6.91373300	2.72837600	-1.21899800
H	8.40709700	-4.58608200	-0.52705600
H	9.74772100	-3.10080900	-1.82208800
H	8.34463400	-3.76699800	-2.71397800
H	8.67218800	-1.28546800	-2.92868200
H	8.98606300	-1.17610400	-0.13220800
H	6.61536300	0.19293500	0.21323600
H	6.74553700	-1.56602600	0.48643500
H	5.51343500	-0.11849300	-1.88504100
O	10.08276100	0.81017100	0.91146700
O	10.08823900	2.64817600	-1.06954900
C	4.64684500	-0.00854600	2.23771000
C	4.11483400	-1.27298600	2.29248000
O	2.13396200	-2.61354500	2.22646400
C	2.69285100	-1.48662600	2.18715600
N	1.93047300	-0.32020300	2.03647500
C	2.45856200	0.95500900	1.97882300

C	4.45159700	2.51357700	1.88725100
C	5.63058000	2.91926500	2.79161000
O	5.58865900	5.29068400	2.34442400
C	6.27657900	4.05748400	1.98920600
O	5.03495000	2.55846500	0.53949200
C	6.00948300	3.64442700	0.50555200
O	8.01435800	2.26380900	0.51412100
C	7.23751700	3.19990900	-0.27794700
P	9.39069100	1.59195000	-0.20845400
C	5.91248600	-1.04123400	-1.45530900
C	6.83915500	-0.76719100	-0.25660800
O	8.69678900	0.51316500	-1.32597600
C	8.25750000	-0.79164800	-0.85375300
O	6.70300000	-1.74146600	-2.44261500
C	8.12372300	-1.72061500	-2.08214400
O	8.10885400	-3.66349900	-0.61741100
C	8.64626100	-3.13835600	-1.86164600
N	-0.95205600	-0.74350300	1.84376600
H	-8.22426800	-4.43515100	1.44359500
H	-9.71837100	-2.84051200	2.37298200
H	-8.24350400	-3.09217000	3.35688800
H	-8.89144500	-0.69959700	2.96164400
H	-9.22902800	-1.26566600	0.25008300
H	-6.94087600	0.04698700	-0.54349300
H	-6.96828200	-1.71918400	-0.28771800
H	-5.79409500	0.44113700	1.50187100
H	-5.76221200	-3.36644100	0.96150400
N	-4.92157300	-1.40665600	1.28380600
C	-4.85660200	-2.78768300	1.10528900
N	-3.62454800	-3.26701700	1.17843600
C	-1.43061200	-2.00169000	1.59361600
C	-2.83146500	-2.14842200	1.42463400
C	-3.61451600	-0.98445200	1.50877500
N	-3.16109300	0.26307400	1.76118500
C	-1.82657200	0.28657100	1.91471400
C	-6.13952800	-0.59215900	1.38469200
C	-7.09991900	-0.74431000	0.19045600
O	-6.87603600	-0.99043700	2.56972200
C	-8.27892200	-1.25478600	2.23845100
O	-8.02834300	-3.49314300	1.29413300
C	-8.62008600	-2.73751300	2.38447100
C	-8.50130200	-0.68024400	0.82334700
O	-8.99611700	0.68028200	0.98534500
P	-9.59996200	1.51081800	-0.36787600
C	-7.38631700	3.03127200	-0.34129800
O	-8.16517500	2.05954500	-1.08403700
C	-6.03906700	3.22707700	-1.01933800
O	-5.20733200	2.04135600	-0.80746400
C	-6.10271100	3.46215800	-2.56740900
O	-5.26649900	4.57622200	-2.98314500
C	-5.48432600	2.18133100	-3.14011200
C	-4.47654300	1.80997400	-2.04112800
O	-10.36743300	2.69952500	0.21603800
O	-10.19043100	0.52236000	-1.37616100
H	-7.22734900	2.68784000	0.69209300
H	-7.91618800	3.99593700	-0.30932300
H	-5.54046300	4.09242200	-0.55195100
H	-7.13555000	3.61347200	-2.90522300

H	-6.25744300	1.40978400	-3.22197900
H	-5.01798900	2.34339600	-4.11689800
H	-3.59470200	2.46509200	-2.08239600
H	-5.66015600	5.39473800	-2.62843700
N	-3.96593700	0.45164000	-2.05586600
C	-2.64158700	0.09390700	-1.81425400
C	-4.65558300	-0.74595800	-2.28591400
N	-1.62205800	0.94044900	-1.55739100
C	-2.60757700	-1.30702100	-1.92729000
N	-3.87888900	-1.80877600	-2.21466800
H	-5.71589900	-0.75786800	-2.50028500
C	-0.44567600	0.31581200	-1.40937500
C	-1.35544700	-1.97609400	-1.73371100
H	-1.37809400	1.25849600	2.11518100
N	-0.57146800	-3.03455600	1.51986100
H	0.43732200	-2.90455000	1.69923100
H	-0.92169400	-3.94513000	1.24774400
N	2.34663900	-2.17732000	-1.11979400
N	1.42377800	-4.27024500	-0.80347600
H	1.51516400	-5.26409900	-0.62843000
H	0.50111800	-3.89799400	-1.07749400
H	3.97829900	-5.07465500	-0.36196800
O	-1.12198100	-3.20842200	-1.75223800
N	-0.30601500	-1.05983100	-1.48929800
H	0.64714000	-1.47232000	-1.33848300
N	0.67252100	1.02987900	-1.15381300
H	1.61690700	0.61534300	-1.20739200
H	0.58009000	2.03587800	-1.08438800
C	3.83715900	1.14904000	2.07243300
C	1.52825200	2.02866300	1.85865100
C	0.73945400	2.94704400	1.77716400
H	0.04136000	3.75300900	1.69145700
H	4.73958100	-2.15446700	2.41095000

126

5T3T-5A3A

H	3.43090900	-5.67926800	0.52458200
H	4.88224300	-5.62738500	-0.50695100
H	3.27627100	-5.93958900	-1.21473200
C	3.81985300	-5.36253700	-0.45363900
O	1.22964300	-4.03814900	-0.52498100
H	1.19621100	-1.55336600	-0.89852400
N	2.16755500	-1.96489900	-0.84111400
O	2.99815700	0.13873400	-1.23791900
N	4.48679600	-1.65020100	-1.03775100
C	2.26546100	-3.34604300	-0.65695900
H	5.67935700	-3.36227300	-0.94351800
C	3.61925100	-3.88206700	-0.65474200
C	4.65006200	-3.01727700	-0.86534400
C	3.20294200	-1.06716800	-1.05874000
H	5.41371100	1.15414600	1.86692900
H	4.89458700	-1.88283500	3.70065500
H	6.12436000	-1.06245000	2.70882400
H	5.11627100	-2.35821500	2.01607000
H	0.75262200	-0.12498900	1.96243700
H	7.44805600	5.27131300	2.31696000
H	2.98015900	3.52123600	0.62365400
H	4.01904700	4.97581300	2.13886300
H	4.23356100	3.56782200	3.20432200

H	6.50736500	3.23754300	2.38181700
H	5.74239700	4.82256800	-0.11225900
H	8.01734200	4.15389100	-0.22977100
H	7.09920800	3.05073100	-1.28460900
H	7.96178800	-4.56689000	-1.74272100
H	9.20958900	-2.86477400	-2.88317600
H	7.61808600	-3.23736800	-3.61495600
H	8.13139400	-0.79139700	-3.31121800
H	8.90818600	-1.36842800	-0.67199800
H	6.73658300	-0.11005500	0.43604700
H	6.79246900	-1.87085800	0.20680500
H	5.29593600	0.20655300	-1.45058100
O	9.58834700	0.48383100	1.06368400
O	10.09496600	2.49164500	-0.67567300
C	5.11884000	-1.49592800	2.69715800
C	4.38904900	0.79500100	1.90857800
C	4.08712100	-0.48160600	2.27746400
O	2.28483000	-2.04446800	2.49623300
C	2.68793700	-0.88781800	2.24227000
N	1.77645100	0.11214900	1.89110800
O	1.18622300	2.23265100	1.22693600
C	2.06738200	1.41619300	1.52279700
N	3.43981400	1.72510000	1.52620900
C	3.86679500	3.07494500	1.08112900
C	4.44891300	3.96889900	2.20966800
O	6.47517200	5.33054300	2.31750900
C	5.95205600	4.05196400	1.89797700
O	4.90801900	2.90311200	0.09530500
C	5.97895500	3.85383500	0.36369700
O	7.76953700	2.21145600	0.52785800
C	7.27625300	3.34055200	-0.23741600
P	9.16896600	1.44581500	-0.05025700
C	5.67369900	-0.81430000	-1.34550800
C	6.80463200	-0.90552600	-0.30598600
O	8.53365200	0.56754500	-1.36227500
C	8.09481100	-0.80146700	-1.13728100
O	6.23351200	-1.26014700	-2.60548600
C	7.69013400	-1.39427700	-2.50598300
O	7.77145800	-3.63267100	-1.54525500
C	8.11948800	-2.84545700	-2.71651900
N	-1.00413100	-0.58833800	2.17520700
H	-7.98136200	-4.63132800	0.77786600
H	-9.63734500	-3.24636900	1.76571600
H	-8.23373900	-3.54987000	2.83568200
H	-8.98382500	-1.16103800	2.69145500
H	-9.08997800	-1.38233500	-0.08707800
H	-6.82585300	0.11772000	-0.53043800
H	-6.76726700	-1.66627900	-0.48603400
H	-5.87015400	0.31265400	1.64381600
H	-5.54900400	-3.40444100	0.70317200
N	-4.86332100	-1.44027100	1.27080300
C	-4.69592700	-2.79183200	0.97345200
N	-3.44375300	-3.20396300	1.10035200
C	-1.37576600	-1.85256900	1.81248100
C	-2.74365000	-2.06966500	1.50882800
C	-3.60635000	-0.96381800	1.62827400
N	-3.25807500	0.28816200	1.99830700
C	-1.94055900	0.38372700	2.24440100

C	-6.13697100	-0.71433300	1.36842900
C	-6.99260400	-0.76423800	0.08995700
O	-6.93106300	-1.30291100	2.42913400
C	-8.28887700	-1.58763100	1.95571900
O	-7.82909300	-3.66965800	0.76612800
C	-8.55173300	-3.09165600	1.88592900
C	-8.43788400	-0.84535800	0.61088700
O	-9.01044500	0.46245900	0.89937400
P	-9.61592200	1.40054300	-0.38074900
C	-7.48664500	3.02613900	-0.15577400
O	-8.19013000	2.07886500	-0.99847700
C	-6.15464800	3.38540700	-0.79868800
O	-5.23470100	2.24974300	-0.68853000
C	-6.23289800	3.75060800	-2.31769800
O	-5.41266400	4.90513200	-2.64307500
C	-5.60211100	2.53136700	-3.00143800
C	-4.55354900	2.11012500	-1.96256900
O	-10.45046700	2.49025900	0.29664000
O	-10.13586900	0.49414900	-1.49913700
H	-7.30483600	2.59439400	0.84023600
H	-8.08561100	3.94181600	-0.03392700
H	-5.72353400	4.23611400	-0.24664200
H	-7.27014700	3.91523900	-2.63541100
H	-6.36306000	1.75235700	-3.11581100
H	-5.16963800	2.77618700	-3.97633300
H	-3.67833100	2.77426900	-1.99365000
H	-5.81605600	5.68758000	-2.22376500
N	-4.03378200	0.75615600	-2.06724200
C	-2.74058200	0.37416400	-1.71384100
C	-4.71101300	-0.42358300	-2.37566000
N	-1.71376900	1.16612300	-1.34187200
C	-2.71757300	-1.02525200	-1.84368100
N	-3.96080000	-1.50552000	-2.25569200
H	-5.74734600	-0.41865900	-2.68697300
C	-0.59842600	0.45463100	-1.10474500
C	-1.49427000	-1.67381000	-1.53532300
N	-0.43938500	-0.88521500	-1.18160800
H	0.28543800	1.01128300	-0.79690100
H	-1.56534200	1.36912700	2.52220400
N	-0.43816400	-2.82206000	1.77625900
H	0.54722100	-2.58822500	1.95256400
H	-0.64468900	-3.69753100	1.30986400
N	-1.32009500	-3.01398200	-1.58863500
H	-0.45490900	-3.41958100	-1.20723900
H	-2.14364700	-3.60361300	-1.64385700

125

5E3T-5A3A

O	-0.85433900	-4.19645100	0.42568100
H	-1.04569200	-1.73976100	0.88615300
N	-1.98037300	-2.23055400	0.84472200
C	-1.96023900	-3.60428500	0.60772200
H	-5.37011500	-4.01494600	0.86717500
C	-3.25471700	-4.23867600	0.59922200
C	-4.39944400	-3.51848600	0.85339000
C	-3.11952400	-1.49792700	1.12747600
H	-5.53076200	1.52225500	-1.71118600
H	-5.16243200	-1.16446500	-4.00672800
H	-6.32466100	-0.54411700	-2.80889800

H	-5.29545200	-1.94799300	-2.43085700
H	-0.90797900	0.17221400	-2.15695400
H	-7.65262400	5.45983700	-1.42642300
H	-2.95694500	3.69837300	-0.34866500
H	-4.21600900	5.34422700	-1.44502800
H	-4.41356600	4.13533700	-2.73508300
H	-6.61841200	3.53012500	-1.88143900
H	-5.91980500	4.71506600	0.83048500
H	-8.07530200	3.68183300	0.80582200
H	-6.97538100	2.58600900	1.68296100
H	-8.01342700	-5.14454300	1.03550300
H	-9.37798500	-3.55760500	2.17676200
H	-7.92652800	-4.06099400	3.09699900
H	-8.32525900	-1.59053300	3.03671800
H	-8.77911500	-1.80919800	0.26953400
H	-6.48269200	-0.49499000	-0.41986200
H	-6.55600600	-2.27341800	-0.35914900
H	-5.42926000	-0.34646700	1.72846100
O	-9.14588500	0.27983000	-1.30661100
O	-10.00546400	1.98492200	0.60583900
C	-5.32545400	-0.97415900	-2.93635200
C	-4.51387000	1.16765300	-1.85912000
C	-4.25743500	-0.05674700	-2.39973000
O	-2.50968600	-1.64208700	-2.81811200
C	-2.87230500	-0.50506700	-2.44567400
N	-1.91890100	0.43128900	-2.02720100
O	-1.24480900	2.45042600	-1.16089900
C	-2.16055300	1.69594000	-1.51412100
N	-3.52342400	2.03140800	-1.41913300
C	-3.89476800	3.31219200	-0.75421300
C	-4.59288300	4.33977000	-1.67559400
O	-6.68510900	5.57505500	-1.44880000
C	-6.07763800	4.27456100	-1.28325600
O	-4.80840700	3.01087100	0.31687900
C	-6.02036400	3.81711500	0.19681800
O	-7.51717400	1.95373200	-0.24932300
C	-7.21064900	3.01089400	0.69456400
P	-8.94488000	1.06712500	-0.00921300
C	-5.65050800	-1.37516900	1.41042800
C	-6.64094300	-1.35519900	0.23047600
O	-8.47396500	0.01698400	1.24125600
C	-8.02316200	-1.32741400	0.89941100
O	-6.36170300	-2.05326300	2.50111700
C	-7.79558900	-2.10113100	2.21872700
O	-7.75134100	-4.20766900	0.99751500
C	-8.27454000	-3.55218000	2.18401500
N	0.83983900	-0.39554300	-2.39621900
H	7.42920900	-4.82865800	-0.66637600
H	9.19204500	-3.60956500	-1.69661400
H	7.75536100	-3.81857600	-2.74506300
H	8.71256300	-1.49966300	-2.66048200
H	8.81116800	-1.66121800	0.12143800
H	6.67729800	0.02743200	0.53456300
H	6.47672600	-1.74384300	0.53726900
H	5.72617800	0.24944400	-1.63509400
H	5.12038200	-3.38481300	-0.52720400
N	4.58902300	-1.41365000	-1.22572400
C	4.32158900	-2.73435200	-0.86504000

N	3.05364200	-3.07590300	-1.03072600
C	1.11120500	-1.65131300	-1.92738800
C	2.44506000	-1.92624400	-1.53266700
C	3.38208300	-0.88522500	-1.67482600
N	3.13400000	0.35453300	-2.15153900
C	1.84127200	0.50980500	-2.48083800
C	5.91430600	-0.78913400	-1.34018200
C	6.77013500	-0.87920200	-0.06427300
O	6.65717000	-1.45686700	-2.39284900
C	7.98600300	-1.84802100	-1.91409900
O	7.36749500	-3.85691300	-0.66912700
C	8.12173400	-3.36695600	-1.80973600
C	8.20177500	-1.08973900	-0.58769100
O	8.88011100	0.15804700	-0.91250600
P	9.53419600	1.10033800	0.33977500
C	7.52212400	2.84423500	-0.03502600
O	8.15787800	1.92400100	0.88724100
C	6.19931700	3.31362600	0.55522400
O	5.23560100	2.20859200	0.53763900
C	6.28141500	3.80714200	2.03464300
O	5.45145600	4.97707100	2.26620600
C	5.66387000	2.64522600	2.82126300
C	4.59445300	2.15018400	1.83861200
O	10.47341000	2.08381100	-0.36246200
O	9.95040600	0.20944800	1.51263300
H	7.33454000	2.35160000	-1.00104500
H	8.17031400	3.71721700	-0.20938300
H	5.80769800	4.12572900	-0.07780200
H	7.31887800	4.00643600	2.33249100
H	6.42977700	1.87889100	2.97676100
H	5.25048900	2.96326100	3.78314400
H	3.71564100	2.80997400	1.84570900
H	5.84054800	5.72403600	1.77497000
N	4.08742000	0.80233800	2.05250300
C	2.82026000	0.37134500	1.66563000
C	4.73854900	-0.32564100	2.55245800
N	1.83028200	1.10152400	1.11333200
C	2.78086000	-0.99920300	1.97309400
N	3.99276600	-1.41726500	2.52314700
H	5.75450400	-0.27939100	2.92286600
C	0.73403700	0.35978800	0.88517400
C	1.57789100	-1.68732200	1.67087000
N	0.55720100	-0.95769900	1.13479200
H	-0.11388600	0.87332300	0.43573300
H	1.54891100	1.49234900	-2.85276300
N	0.11517500	-2.56354500	-1.88800500
H	-0.82982000	-2.26846700	-2.16394600
H	0.18245200	-3.35583400	-1.25017600
N	1.38912300	-3.00838300	1.90759600
H	0.61933300	-3.48741300	1.41694900
H	2.21340200	-3.56288900	2.11629500
C	-2.92457100	-0.11814300	1.42041300
C	-2.74429000	1.05145900	1.68509900
H	-2.60989700	2.09181800	1.88773100
C	-4.36459200	-2.12025400	1.12835800
H	-3.28311900	-5.30799300	0.40241300

Table S5. Cartesian coordinates (in Å) of the stacked base pairs extracted from the optimised dinucleotide duplexes

70

5C3C-5G3G

N	-2.35530500	-1.87533000	0.57759600
O	-3.27651000	0.01264400	1.49246000
N	-4.73521000	-1.55596200	0.59905700
C	-2.52916800	-3.06014900	-0.04683300
H	-5.93563700	-3.09189600	-0.16324600
C	-3.84188300	-3.54365700	-0.37678400
C	-4.90525900	-2.77385600	-0.01667500
C	-3.42010200	-1.09083900	0.92036600
H	-5.55391400	2.39624800	-0.39681300
C	-4.52786700	2.16437200	-0.67097000
C	-4.20251300	1.17348200	-1.55032000
C	-2.81104100	0.87053900	-1.72053500
N	-1.85550100	1.64037000	-1.15542000
O	-1.32606200	3.44827400	0.16041600
C	-2.18587300	2.68265100	-0.34508300
N	-3.55637400	2.89279200	-0.03800700
H	5.51211200	-1.94975500	-2.31997400
N	4.81457200	-0.03220900	-1.60913600
C	4.64859200	-1.33194700	-2.10033300
N	3.38126900	-1.65576100	-2.28323200
C	1.25813300	-0.27215400	-1.86280600
C	2.66540600	-0.52075600	-1.89917300
C	3.53929200	0.50418900	-1.48835200
N	3.22397500	1.74619700	-1.05973100
C	1.90822800	1.96771800	-1.00410000
N	4.04225000	0.22874400	2.22354200
C	2.69887200	-0.01195600	1.94706400
C	4.72101900	-0.95639400	1.91513800
N	1.67621300	0.85276500	2.12052400
C	2.64666000	-1.34270000	1.49711700
N	3.92224400	-1.90917200	1.47713600
H	5.79223200	-1.04384200	2.03679100
C	0.48256900	0.32534000	1.81968100
C	1.37485800	-1.89638000	1.14683900
O	0.32487000	-1.03920900	-2.20441200
O	1.12931900	-3.04286800	0.70164900
N	0.96562400	1.02033700	-1.36406600
H	-0.05352900	1.25952100	-1.28756000
N	0.32445700	-0.97014000	1.35311300
H	-0.63548800	-1.28991800	1.07848800
N	1.43956200	3.18578300	-0.61478300
H	2.11752300	3.79108600	-0.16355200
H	0.45268100	3.29184800	-0.33168100
N	-0.64499300	1.05668300	1.99861800
H	-1.56658800	0.68691600	1.71966900
H	-0.54012200	2.06607500	2.02256200
H	-4.97133300	0.58448800	-2.03914800
H	-3.98856200	-4.50450300	-0.86134100
N	-1.43322000	-3.78385900	-0.34810900
H	-0.49842100	-3.49541400	-0.01321600
H	-1.53521200	-4.69915700	-0.77156600
N	-2.41083200	-0.19312500	-2.44893700
H	-3.10304900	-0.85541700	-2.78114900

H	-1.42528200	-0.50319900	-2.39933100
C	6.05363500	0.64302000	-1.26912000
H	6.20846500	1.50378600	-1.92324200
H	6.01665400	0.97982000	-0.23004100
H	6.87750100	-0.06049800	-1.39119300
C	4.59987900	1.48678200	2.68627300
H	4.41254100	2.27008200	1.94761400
H	4.14662200	1.76819900	3.63903000
H	5.67483100	1.36116200	2.81976600
C	-3.88123300	3.94286100	0.92318700
H	-3.38573200	3.73368500	1.87309600
H	-3.54203600	4.91058000	0.54938800
H	-4.96105300	3.95866800	1.06709700
C	-5.86948900	-0.77546000	1.08198700
H	-5.89183500	-0.78327200	2.17434200
H	-5.77705900	0.25381200	0.73723100
H	-6.78664100	-1.21485000	0.69052200

70

5C3E-5G3A

H	-1.00947900	-1.80636200	-1.90285300
H	-2.70733400	-2.23437900	-2.11430300
N	-1.99235400	-1.51895200	-2.05036600
H	-4.50760600	-0.56446700	-2.22988600
H	-3.65882300	3.07900600	1.93864000
C	-3.70730500	2.02361900	1.77814900
C	-3.77774400	0.83805700	1.53279300
H	-1.80740200	-0.79080200	1.46028200
N	-2.72057500	-1.29396700	1.31267600
H	-3.89901900	-4.38650400	0.65083100
H	-6.01977500	-3.07476800	0.49940900
O	-1.53660100	-3.26746900	1.16312600
C	-5.07354800	-2.57982400	0.72122600
C	-3.91178000	-3.31034100	0.80794000
C	-5.09150600	-1.16948600	0.92590900
C	-2.64657700	-2.67386100	1.09670500
C	-3.88622100	-0.55260600	1.24950900
H	-5.04978300	1.85091100	-1.81837500
C	-4.02846600	1.48084500	-1.84905200
C	-3.72667000	0.16859300	-2.06049100
C	-2.34947500	-0.22266000	-1.96112300
N	-1.37337800	0.69186200	-1.77014800
O	-0.78882000	2.89651500	-1.49608300
C	-1.67101000	2.01567000	-1.62709100
N	-3.04356200	2.40244100	-1.60904300
C	2.42267300	0.89355300	-1.40414100
N	3.71269800	0.60058500	-1.21859100
C	3.95762100	-0.72219600	-1.14878100
C	3.05247000	-1.78846700	-1.28026300
C	1.67516600	-1.47978800	-1.50986100
N	3.71035000	-3.01285300	-1.12704400
C	4.97279000	-2.69150200	-0.89964100
N	5.18762800	-1.31038800	-0.90070800
H	5.79933700	-3.37810000	-0.75010500
O	0.72282300	-2.28211700	-1.66475300
N	2.04206500	2.19837900	-1.48935000
H	2.71295300	2.85568700	-1.08990800
H	1.04371500	2.44267300	-1.42900500
N	1.44345700	-0.07971000	-1.54171300

H	0.44185700	0.21516000	-1.63701300
N	3.33925700	2.06553300	1.94077500
C	2.04904900	1.56165000	1.81434400
C	4.17198300	0.95529100	2.08636700
N	0.90601300	2.25007500	1.61461000
C	2.17834600	0.16571500	1.91353900
N	3.51557000	-0.19440000	2.08617700
H	5.24451200	1.07595000	2.15261000
C	-0.15259500	1.43184400	1.50733900
C	0.99059600	-0.59975300	1.77460900
N	-0.17845500	0.08161600	1.58136700
H	-1.11557100	1.90482000	1.33126500
N	0.96139200	-1.94945700	1.82998500
H	1.84214400	-2.45218800	1.81703800
H	0.09623900	-2.45090800	1.57335700
C	3.72110100	3.46728300	1.93951000
H	3.07468400	4.00999900	1.24810500
H	3.61569400	3.89468600	2.93931600
H	4.75746100	3.55166400	1.61102500
C	6.44577500	-0.60765600	-0.72722200
H	6.76664300	-0.16342600	-1.67223700
H	6.32466400	0.17960100	0.01866800
H	7.19730900	-1.31935600	-0.38503500
C	-3.34460800	3.81175300	-1.37925700
H	-2.84602800	4.14613900	-0.46789700
H	-2.98969200	4.41558300	-2.21733400
H	-4.42338700	3.92407900	-1.27232100
C	-6.36217200	-0.37086300	0.82243100
H	-6.54833500	0.20846500	1.73226600
H	-6.31604900	0.33810200	-0.01246600
H	-7.21624700	-1.03126600	0.65652000

71

5C3T-5G3A

H	-1.11845700	-1.60096500	-2.00835100
H	-2.82483800	-1.88808200	-2.35184000
N	-2.06787000	-1.23409800	-2.19023000
O	-0.57698400	3.02094900	-1.23503100
N	-2.85067400	2.70634100	-1.46127600
H	-3.81961300	-4.60692800	-0.06243100
H	-5.43816300	-4.40117300	0.65349200
H	-4.01839800	-4.69632800	1.68920000
C	-4.37273900	-4.17971500	0.78606200
O	-1.76173900	-2.94162600	1.14496100
H	-1.67192700	-0.44249600	1.36559100
N	-2.64554400	-0.82333100	1.20457600
H	-4.49989100	-0.07078400	-2.40599300
O	-3.43179800	1.32986300	1.32813300
N	-4.93271900	-0.40515100	0.88701900
C	-2.77349500	-2.20792400	1.07684700
H	-6.17944700	-2.06854600	0.69314000
C	-4.13492500	-2.69431500	0.88605300
C	-5.13707500	-1.77528500	0.80490600
C	-3.65425900	0.12587500	1.15935600
H	-4.87392900	2.34527700	-1.81190100
C	-3.88649100	1.89187800	-1.82358700
C	-3.67498500	0.57977600	-2.13481400
C	-2.33767300	0.07467600	-2.00773300
N	-1.30755000	0.89240300	-1.69961000

C	-1.51352000	2.21882300	-1.46140600
C	2.48906600	0.85452400	-1.37694300
N	3.76242600	0.47507200	-1.23991500
C	3.92237500	-0.86224200	-1.21337500
C	2.94659800	-1.86492700	-1.34337900
C	1.58667300	-1.46213100	-1.52977800
N	3.52880900	-3.13230300	-1.24054900
C	4.81567600	-2.89799300	-1.04449800
N	5.11858900	-1.53388900	-1.01939700
H	5.60041000	-3.63914700	-0.93572400
O	0.57971700	-2.19518000	-1.68369600
N	2.19041000	2.18236000	-1.40756300
H	2.91639500	2.78301100	-1.01492300
H	1.21176500	2.48411900	-1.29181500
N	1.44648500	-0.05009500	-1.51591500
H	0.46285000	0.30867900	-1.58257400
N	3.59348700	1.95116700	1.97719800
C	2.26765900	1.53871700	1.87961900
C	4.35431400	0.78389900	2.05765700
N	1.16703800	2.30880100	1.75135200
C	2.30942700	0.13296400	1.92320900
N	3.62415600	-0.31946500	2.04052600
H	5.43418100	0.83126700	2.09203100
C	0.05282200	1.56740600	1.64092300
C	1.07319500	-0.54554900	1.77594000
N	-0.04845800	0.21951900	1.64505200
H	-0.89089800	2.09771400	1.51869600
N	0.94892100	-1.89316700	1.76444300
H	1.78783000	-2.45642700	1.67673900
H	0.04561700	-2.31016100	1.50372500
C	-3.06245700	4.09457700	-1.06567600
H	-2.68948300	4.24384600	-0.05027700
H	-2.53057400	4.76354500	-1.74429300
H	-4.13095500	4.30579800	-1.09869900
C	-6.05141500	0.53229700	0.86460500
H	-6.28329800	0.87848200	1.87516100
H	-5.78840200	1.39139400	0.24727800
H	-6.91818900	0.02885700	0.43796000
C	4.06649300	3.32421500	2.01541500
H	3.50923200	3.91784200	1.28887600
H	3.92463800	3.74980000	3.01142500
H	5.12585700	3.33729600	1.75829400
C	6.42157600	-0.91542100	-0.85629500
H	6.72334700	-0.41857400	-1.78104200
H	6.38133800	-0.18237100	-0.04879800
H	7.14584300	-1.69090600	-0.60651100

71

5E3T-5A3A

H	-3.72970700	-3.99928300	-1.17274700
H	-5.19462500	-4.11390900	-0.16480200
H	-3.65283300	-4.81382400	0.39252200
C	-4.10829300	-3.96796800	-0.14117000
O	-1.38493900	-3.05797300	0.38095800
H	-1.09846400	-0.74622600	1.31480100
N	-2.10661900	-1.04778200	1.22389800
O	-2.70796300	0.93285100	2.21995300
N	-4.37486400	-0.57489200	1.58681600
C	-2.34500700	-2.31297600	0.68064100

H	-5.74915600	-2.01055200	0.94517400
C	-3.75025400	-2.65996500	0.51566800
C	-4.68435100	-1.78832800	0.98692900
C	-3.04043100	-0.14855300	1.71728600
H	-5.70540400	1.89900700	-1.43346800
H	-0.94451600	0.84459800	-1.55571700
C	-4.64492000	1.65979000	-1.44105500
C	-4.24967400	0.40558100	-1.84019400
O	-2.41021500	-1.08688200	-2.21200600
C	-2.85527300	0.03924900	-1.86912200
N	-1.97373400	1.05182900	-1.46760200
C	-2.36410000	2.30501200	-1.04064500
N	0.84718100	0.46735900	-1.86189600
H	5.52463200	-2.50359800	-1.57446700
N	4.78984400	-0.47693500	-1.64265800
C	4.65002500	-1.86324900	-1.60099700
N	3.38789100	-2.26309500	-1.64113900
C	1.25678000	-0.83758500	-1.81241800
C	2.65153900	-1.08222200	-1.72221600
C	3.50008500	0.03841000	-1.73071900
N	3.11483800	1.33166100	-1.80081400
C	1.77716000	1.44905900	-1.85558800
N	4.36693700	1.09852700	2.07107300
C	3.01356600	0.83144400	1.87222200
C	5.01432900	-0.13518300	2.00952000
N	1.98825300	1.70854000	1.85835500
C	2.92991300	-0.56318000	1.70955200
N	4.19268900	-1.14858600	1.79604300
H	6.08525800	-0.22081300	2.13704600
C	0.81021400	1.08873100	1.67666600
C	1.63770300	-1.10117600	1.47915000
N	0.58921200	-0.23034500	1.49159300
H	-0.08341200	1.71141400	1.66644400
H	1.37990500	2.46278000	-1.89159600
N	0.33644700	-1.81835900	-1.86566100
H	-0.67030600	-1.59717400	-1.89881500
H	0.62110900	-2.77258000	-1.68028600
N	1.39012600	-2.41450100	1.26671100
H	0.45340500	-2.69054400	0.94131800
H	2.17322400	-3.01950800	1.04199100
C	-3.71534000	2.65232400	-1.02206900
H	-4.96764900	-0.35201400	-2.14319200
C	-1.31891700	3.18168800	-0.62756100
C	-0.41097500	3.89999400	-0.26495800
H	0.39379100	4.52350700	0.06293200
C	4.95929100	2.40971400	2.27296100
H	4.76200800	3.04405400	1.40611900
H	4.54079300	2.87343000	3.16830100
H	6.03548500	2.28700600	2.39601900
C	6.01735500	0.29703500	-1.58699900
H	6.17045600	0.83224700	-2.52647700
H	5.96207700	1.01458300	-0.76492900
H	6.85018400	-0.38525900	-1.41526500
C	-5.41103600	0.34783700	2.04150200
H	-5.28543000	0.55668600	3.10546600
H	-5.34564600	1.28490800	1.48219400
H	-6.38337300	-0.11239300	1.87040200
C	-4.16776200	3.99963000	-0.52867200

H	-4.14798700	4.04330000	0.56669000
H	-3.52459100	4.80116100	-0.90265400
H	-5.19145700	4.20037400	-0.85354300

72

5T3T-5A3 A

H	3.57698900	-4.42032900	1.00471700
H	4.91789500	-4.55075200	-0.16065100
H	3.27312400	-5.07309400	-0.60725600
C	3.85161000	-4.31940100	-0.05495700
O	1.19259000	-3.14034000	-0.14275700
H	0.97682300	-0.80753100	-1.05173500
N	1.97185500	-1.15989200	-1.00794800
O	2.63500700	0.82797600	-1.94668900
N	4.23914300	-0.81402300	-1.51426500
C	2.16837500	-2.45900300	-0.53387100
H	5.53443400	-2.41592300	-1.17015400
C	3.54555200	-2.93117100	-0.55657300
C	4.49866100	-2.09973100	-1.06162500
C	2.92689400	-0.29781300	-1.52759100
H	5.27088800	2.60682500	0.58192200
H	5.10926900	0.04707600	3.08728800
H	6.18833300	0.66564000	1.81366900
H	5.19728700	-0.78898600	1.53609200
H	0.72393000	1.21442400	1.45223700
C	5.21368000	0.20461800	2.00503500
C	4.27789300	2.22953300	0.81053300
C	4.08850400	1.05950300	1.48293600
O	2.41084700	-0.47753000	2.23236600
C	2.71881500	0.60542400	1.68720800
N	1.72048800	1.46621000	1.22196900
O	0.94531100	3.35846200	0.17101500
C	1.89738200	2.66267700	0.54521300
N	3.24321700	3.01387800	0.33452400
N	-0.97408600	0.74790600	1.94746100
H	-5.46389200	-2.49119100	1.62638300
N	-4.84467100	-0.42598000	1.66880300
C	-4.62669500	-1.80278700	1.66219900
N	-3.34595100	-2.12981900	1.74369400
C	-1.30313200	-0.57823800	1.91531100
C	-2.67846500	-0.90788200	1.81413500
C	-3.58977000	0.16427600	1.77646100
N	-3.28251600	1.47930200	1.82088500
C	-1.95552500	1.67579600	1.89852900
N	-4.46809900	0.98628800	-2.14153300
C	-3.12680600	0.74135900	-1.85150300
C	-5.10064300	-0.25639800	-2.10734100
N	-2.11789500	1.63365500	-1.77526900
C	-3.03352500	-0.64933900	-1.66981100
N	-4.27973600	-1.25515700	-1.83095100
H	-6.16037600	-0.35965100	-2.30029000
C	-0.94491700	1.03523200	-1.50609700
C	-1.75020900	-1.16646400	-1.35698200
N	-0.71494100	-0.28055800	-1.30067500
H	-0.07024000	1.67878900	-1.42473800
H	-1.61451200	2.71144000	1.90974200
N	-0.31754000	-1.49611500	1.99551100
H	0.66458900	-1.19287400	2.01010200
H	-0.51538300	-2.46134000	1.75923800

N	-1.50293300	-2.47669100	-1.13026300
H	-0.58289400	-2.75377600	-0.76246800
H	-2.29167400	-3.09297000	-0.96583000
C	-6.11128000	0.27591000	1.55723400
H	-6.30463500	0.85161900	2.46465200
H	-6.08481400	0.94968200	0.69752900
H	-6.90353200	-0.45941600	1.41577200
C	-5.06440800	2.28626500	-2.39675300
H	-4.92703500	2.93488300	-1.52895300
H	-4.59949400	2.74383000	-3.27220600
H	-6.12970700	2.14722900	-2.58170300
C	3.49167500	4.21897000	-0.45220100
H	3.10304500	4.08547600	-1.46448700
H	2.99988300	5.07486600	0.01263400
H	4.56648700	4.39068600	-0.49156000
C	5.29292500	0.04481700	-2.04632700
H	5.13884000	0.21782500	-3.11373100
H	5.27965000	1.00372700	-1.52382000
H	6.25281000	-0.44467100	-1.88644000