Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

yDNA versus yyDNA pyrimidines: Computational analysis of the effects of unidirectional ring expansion on the preferred sugar–base orientation, hydrogen-bonding interactions and stacking abilities

Purshotam Sharma, Linda A. Lait and Stacey D. Wetmore*

Department of Chemistry and Biochemistry, University of Lethbridge, 4401 University Drive West, Lethbridge, Alberta, Canada T1K 3M4

*Corresponding author S.D.W.: E-mail: stacey.wetmore@uleth.ca; Phone: 403-329-2323; Fax: 403-329-2057.

Supporting Information (10 pages)

Table S1-S4. Cartesian coordinates of hydrogen-bonded base pairs containing expanded pyrimidines.

Table S1. A:yT

Calculated energy (in Hartrees)= -1114.47875470

Atom	X	Y	Z
C	-6.41802500	-2.11676600	0.00001200
H	-5.70117200	-2.93874300	0.00249000
N	-5.65885600	-0.87674800	0.00097500
C	-6.13504700	0.41993200	0.00250400
H	-7.19832000	0.62273900	0.00361100
N	-5.19320600	1.33462000	0.00255800
C	-4.02206400	0.60005600	0.00091300
C	-2.65942000	0.97786500	0.00017100
N	-2.25195600	2.25777100	0.00110100
H	-1.25760900	2.48587000	0.00002700
H	-2.94671900	2.98644900	0.00205200
N	-1.73810400	-0.01334900	-0.00148300
C	-2.14003300	-1.29978700	-0.00222500
H	-1.33124800	-2.02709700	-0.00336000
N	-3.38582200	-1.77010700	-0.00164400
C	-4.28438300	-0.77257100	-0.00009700
H	-7.04918900	-2.18728900	0.89045000
H	-7.04470400	-2.18895900	-0.89348900
O	0.66947400	2.71382700	-0.00201100
C	1.45880500	1.76824600	-0.00159600
N	2.82288600	1.97610800	-0.00075900
N	1.06649800	0.44994500	-0.00212800
C	3.77422500	0.96192700	-0.00003500
H	3.10520800	2.94580700	-0.00020900
C	1.89381300	-0.67124800	-0.00125800
H	0.03186900	0.27675900	-0.00214400
C	3.34134800	-0.37353300	-0.00029100
C	5.14797900	1.24257500	0.00090600
O	1.42289800	-1.80132800	-0.00134700
C	4.28189800	-1.41106400	0.00042600
C	6.05998800	0.19613000	0.00160100
H	5.49178700	2.27326400	0.00109600
C	5.64925700	-1.15126400	0.00136800
H	3.90206200	-2.42797700	0.00022100
H	7.12231900	0.42735200	0.00234200
C	6.66712100	-2.26676300	0.00205800
H	7.31646400	-2.21595700	0.88362700
H	6.18081000	-3.24540700	0.00253300
H	7.31660800	-2.21690900	-0.87946600

Table S2. A:yyT

Calculated energy (in Hartrees)= -1268.12531063

Atom	X	Y	Z
N	-1.55221000	2.26526800	0.00095000
C	-2.22580300	-0.05206300	-0.00050000
C	-2.58208300	1.32714300	0.00048700
C	-0.79694500	-0.44055800	-0.00127100
O	-0.40320100	-1.59951400	-0.00242500
N	0.10042700	0.62169600	-0.00051200
H	1.12196900	0.38202700	-0.00187100
C	-0.20743600	1.96363800	0.00072600
O	0.64506300	2.85251200	0.00185800
C	-3.91252100	1.70211900	0.00108300
C	-4.93315600	0.72252000	0.00088200
H	-4.18397400	2.75470700	0.00180300
C	-3.21234100	-1.01817800	-0.00084400
C	-4.58051300	-0.66883900	-0.00009500
H	-2.90559300	-2.05955300	-0.00162800
H	-1.76284600	3.25305200	0.00207400
C	-6.94453300	-1.29995400	0.00052700
C	-7.27969300	0.08595500	0.00143000
C	-5.61194100	-1.64873800	-0.00022600
C	-6.31442400	1.06273000	0.00162900
H	-8.32909300	0.37080500	0.00195100
H	-5.32462500	-2.69743700	-0.00091400
H	-6.59734100	2.11199300	0.00232700
C	-8.04056400	-2.33636000	0.00057300
H	-8.68400800	-2.23457600	0.88243600
H	-8.68605800	-2.23244800	-0.87947100
H	-7.63205400	-3.35022000	-0.00110500
H	8.01446100	-2.55554200	-0.88959000
C	7.39384300	-2.44036500	0.00356200
H	6.62339500	-3.21232000	0.00670400
N	6.71995500	-1.15210400	0.00272800
H	8.01851100	-2.55211300	0.89431700
C	7.28222100	0.10961700	0.00346100
C	5.35560500	-0.95566100	0.00016500
H	8.35673200	0.24058600	0.00547500
N	6.40387800	1.08551500	0.00177700
C	5.18603700	0.43130900	-0.00047400
N	4.39221200	-1.89075900	-0.00124600
C	3.85182300	0.89990500	-0.00299500
C	3.18090000	-1.33790700	-0.00328100
N	3.53132500	2.20415700	-0.00532000
N	2.86605800	-0.02723100	-0.00416400
H	2.32525100	-2.00941300	-0.00425500
H	2.55459000	2.49828300	-0.00224400
H	4.27341400	2.88452300	-0.00001200

Table S3. G:yC

Calculated energy (in Hartrees)= -1209.15821051

Atom	X	Y	Z
N	5.95821500	-0.43088500	0.02767200
C	6.29057800	0.91664700	0.04714900
H	7.32523700	1.23389000	0.06677500
N	5.25335400	1.71268400	0.03843600
C	4.16747500	0.85531700	0.01193900
C	2.76224400	1.11596100	-0.00685900
O	2.17868400	2.21338300	-0.00289600
N	2.01816300	-0.07754700	-0.03193600
H	0.98942500	0.03539400	-0.03896900
C	2.53911200	-1.35103400	-0.03804700
N	1.64985400	-2.36490800	-0.07326500
H	0.63685000	-2.21691300	-0.04491900
H	2.02786300	-3.29667200	-0.04341300
N	3.84059400	-1.60552100	-0.01855900
C	4.58510500	-0.48054000	0.00505200
C	6.85211900	-1.57482900	0.03270200
H	7.45423900	-1.59731300	0.94630300
H	6.23749800	-2.47463500	-0.01192300
H	7.51889300	-1.55205300	-0.83457700
H	0.48694000	2.43035200	-0.02833900
N	-0.54383200	2.58948300	-0.03789500
C	-1.37449500	1.53936100	-0.02419700
H	-0.89423100	3.53318700	-0.01918600
N	-0.87407100	0.31321800	-0.02554800
N	-2.72571500	1.78218100	-0.01208900
C	-1.69530900	-0.78858100	-0.01226300
C	-3.65492400	0.74168600	0.00010200
H	-3.05890100	2.73420800	-0.01462500
O	-1.22386100	-1.93476200	-0.01062000
C	-3.16234500	-0.56992200	0.00064800
C	-5.04103700	0.99890400	0.01171700
C	-4.05934100	-1.64522800	0.01317400
C	-5.89455200	-0.10077200	0.02391600
C	-5.43311000	-1.43112800	0.02515500
H	-3.64164500	-2.64664500	0.01313700
H	-6.96705100	0.08238200	0.03278100
C	-6.41347300	-2.57983700	0.04077800
H	-5.89490500	-3.54151300	0.02111800
H	-7.04217200	-2.55750000	0.93847000
H	-7.08604900	-2.54439900	-0.82390600
C	-5.57042400	2.41264900	0.01072600
H	-5.23684600	2.97802700	0.89126700

H	-5.25281500	2.97084700	-0.88024100
H	-6.66258900	2.41752300	0.02052600

Table S4. G:yyC

Calculated energy (in Hartrees)= -1323.48402481

Atom	X	Y	Z
C	2.70242900	1.37130600	-0.00605900
C	0.34204800	1.90451900	-0.02204700
N	-0.59872000	2.85546500	-0.02986200
H	-1.60666100	2.58516600	-0.01973300
H	-0.35439900	3.83214200	-0.01063900
N	-0.02553600	0.63008400	-0.02625200
C	0.90680900	-0.37667300	-0.01882500
O	0.56277400	-1.56676600	-0.02060700
C	4.02699700	1.76225900	0.00245100
C	5.05348000	0.78896300	0.00945300
H	4.29121200	2.81713400	0.00396600
C	3.34037000	-0.96329500	-0.00110400
C	4.70661400	-0.60420300	0.00790100
H	3.04141300	-2.00674600	-0.00289600
C	2.34580500	-0.00510500	-0.00812000
N	1.65726500	2.29623000	-0.01239200
H	1.88414100	3.28004100	-0.01368000
C	6.43274400	1.13707400	0.01823700
C	7.40318500	0.16568100	0.02516500
H	6.71018900	2.18786200	0.01943900
C	5.74419800	-1.57789800	0.01531800
C	7.07483000	-1.22192000	0.02390500
H	8.45104100	0.45583800	0.03185100
H	5.46267600	-2.62813200	0.01406600
C	8.17641700	-2.25254700	0.03193500
H	8.82590700	-2.14696400	-0.84498600
H	8.81462200	-2.14519200	0.91688200
H	7.77343400	-3.26848800	0.03035400
H	-8.09194900	-2.16266100	0.96270200
C	-7.50862000	-2.06915000	0.04141900
N	-6.74156100	-0.83648200	0.03441500
H	-8.18612900	-2.11059500	-0.81670600
H	-6.80265700	-2.89818700	-0.01929600
C	-7.21555700	0.46797100	0.05742100
C	-5.37123800	-0.73951400	0.00773700
H	-8.27807200	0.67293000	0.08072400
N	-6.26911700	1.37002300	0.04702500
N	-4.51094400	-1.77872100	-0.02017300
C	-5.09820800	0.63331700	0.01584700

C	-3.24429700	-1.38693200	-0.04309300
C	-3.72884800	1.04194200	-0.00703400
N	-2.86203300	-0.06519400	-0.03611000
N	-2.25142500	-2.29942200	-0.08310300
O	-3.26488300	2.19522000	-0.00341300
H	-1.85154000	0.15757900	-0.04712000
H	-1.26119600	-2.04119300	-0.05724500
H	-2.52560500	-3.26679700	-0.05340300

Table S5-S12. MP2/6-31G(d) optimized monomers used to build dimers for center-of-mass stacking calculations.

Table S5. Thymine (T).

Calculated energy (in Hartrees)= -452.80601731

Atom	X	Y	Z
N	0.14415400	-1.66631700	0.00000000
C	-1.08610300	-1.04128900	0.00000000
H	-1.94395700	-1.70796900	0.00000000
C	-1.21462700	0.30706100	0.00000000
C	-2.52945400	1.02192800	0.00000000
H	-2.61589200	1.66653800	0.87905200
H	-2.61589200	1.66653800	-0.87905200
H	-3.36103700	0.31207600	0.00000000
C	0.00000000	1.12147500	0.00000000
O	0.02537700	2.35108200	0.00000000
N	1.19251000	0.38116700	0.00000000
H	2.05291600	0.92395400	0.00000000
C	1.35681800	-0.99517800	0.00000000
O	2.44355100	-1.56009500	0.00000000
H	0.21597900	-2.67696300	0.00000000

Table S6. y-thymine (yT).

Calculated energy (in Hartrees)= -566.80370113

Atom	X	Y	Z

N	0.28292100	-1.62395900	0.00000000
C	0.00000000	0.76807700	0.00000000
C	0.84536200	-0.35164900	0.00000000
C	-1.46319400	0.58467300	0.00000000
O	-2.28821200	1.49348100	0.00000000
N	-1.86198200	-0.75213300	0.00000000
H	-2.86512100	-0.92104300	0.00000000
C	-1.06938200	-1.89743600	0.00000000
O	-1.53173600	-3.03120200	0.00000000
C	2.23581100	-0.17552100	0.00000000
C	2.76379500	1.11073000	0.00000000
H	2.89299400	-1.04302000	0.00000000
C	0.54298800	2.05785200	0.00000000
C	1.92130300	2.23154500	0.00000000
H	-0.14191000	2.90156300	0.00000000
H	2.34614200	3.23143800	0.00000000
H	0.87763500	-2.44598300	0.00000000
H	3.84317000	1.24183000	0.00000000

Table S7. yy-thymine (yyT).

Calculated energy (in Hartrees)= -719.95956709

Atom	X	Y	Z
N	2.36141600	0.42347800	0.00000000
C	0.00000000	0.93246500	0.00000000
C	1.04324400	-0.03063400	0.00000000
C	0.32582900	2.37493500	0.00000000
O	-0.50173300	3.28106000	0.00000000
N	1.69198500	2.64397800	0.00000000
H	1.95769300	3.62582700	0.00000000
C	2.75676700	1.74312000	0.00000000
O	3.92784000	2.10069000	0.00000000
C	0.74044200	-1.38055800	0.00000000
C	-0.60478900	-1.81271800	0.00000000
H	1.54050200	-2.12099100	0.00000000
C	-1.32120900	0.53032700	0.00000000
C	-1.66022300	-0.84007600	0.00000000
H	-2.09545500	1.29584700	0.00000000
H	3.12738100	-0.24209800	0.00000000
H	-4.34233900	-2.95500600	0.00000000
C	-3.30596500	-2.62599800	0.00000000
C	-2.26678600	-3.58840900	0.00000000
C	-3.01058200	-1.28001100	0.00000000
C	-0.94686000	-3.19126300	0.00000000
H	-2.51438400	-4.64740700	0.00000000
H	-3.80552100	-0.53614700	0.00000000

H	-0.14974700	-3.93328900	0.00000000

Table S8. Cytosine (C).

Calculated energy (in Hartrees)= -393.76465490

Atom	X	Y	Z
N	-1.20108300	-0.98917800	0.00000000
C	-0.06095200	-1.72627900	0.00000000
H	-0.17406900	-2.80633000	0.00000000
C	1.14480600	-1.09954900	0.00000000
H	2.07294400	-1.65835900	0.00000000
C	1.10708900	0.33798200	0.00000000
N	2.27881800	1.02414500	0.00000000
H	2.23508000	2.03358800	0.00000000
H	3.17527400	0.56464200	0.00000000
N	0.00000000	1.05811100	0.00000000
C	-1.22732900	0.43056000	0.00000000
O	-2.31501300	0.99848200	0.00000000
H	-2.11496600	-1.42923500	0.00000000

Table S9. y-cytosine (yC).

Calculated energy (in Hartrees)= -586.09190502

Atom	X	Y	Z
C	0.00000000	0.60177900	0.00000000
C	1.93078600	-0.82464500	0.00000000
N	3.29198900	-0.88279100	0.00000000
H	3.70416800	-1.80394200	0.00000000
H	3.88902300	-0.07154100	0.00000000
N	1.25827900	-1.94461600	0.00000000
C	-0.13601700	-1.90081500	0.00000000
O	-0.81087600	-2.93118800	0.00000000
C	-0.57479100	1.88736600	0.00000000
C	-1.96661600	1.96626100	0.00000000
C	-2.17940100	-0.44162800	0.00000000
C	-2.76819100	0.81588500	0.00000000
H	-2.43509000	2.94915000	0.00000000
H	-2.76568200	-1.35621400	0.00000000

H	-3.85077700	0.91395700	0.00000000
C	-0.78430900	-0.55894500	0.00000000
N	1.38406700	0.43380500	0.00000000
H	1.98141000	1.25074600	0.00000000
C	0.29176900	3.11814600	0.00000000
H	0.93525600	3.16154500	0.88721900
H	0.93525600	3.16154500	-0.88721900
H	-0.32628200	4.01903600	0.00000000

Table S10. yy-cytosine (yyC)

Calculated energy (in Hartrees)= -700.07570399

Atom	X	Y	Z
C	1.01634300	-0.04846300	0.00000000
C	2.60746700	1.75434000	0.00000000
N	3.92561500	2.09267900	0.00000000
H	4.13781500	3.07939700	0.00000000
H	4.67817500	1.42286700	0.00000000
N	1.72021400	2.71519700	0.00000000
C	0.36638800	2.38944500	0.00000000
O	-0.50575500	3.25814900	0.00000000
C	0.70815400	-1.39673500	0.00000000
C	-0.64236700	-1.81034400	0.00000000
H	1.49975300	-2.14697800	0.00000000
C	-1.32503900	0.54747000	0.00000000
C	-1.68173700	-0.81876800	0.00000000
H	-2.08734900	1.32462000	0.00000000
C	0.00000000	0.93933300	0.00000000
N	2.33381400	0.41061900	0.00000000
H	3.08633600	-0.26794500	0.00000000
C	-1.00601700	-3.18369800	0.00000000
C	-2.33146100	-3.56115300	0.00000000
H	-0.22034200	-3.93808100	0.00000000
C	-3.03835700	-1.24131000	0.00000000
C	-3.35533600	-2.58218500	0.00000000
H	-2.59513000	-4.61631700	0.00000000
H	-3.82193300	-0.48554300	0.00000000
H	-4.39701600	-2.89427500	0.00000000

Table S11. Adenine (A)

Calculated energy (in Hartrees)= -465.94705721

Atom	X	Y	Z
N	-2.15072700	0.12906000	0.00000000
C	-1.90629800	1.47894600	0.00000000
H	-2.71140600	2.20310400	0.00000000
N	-0.61545400	1.78364100	0.00000000
C	0.00000000	0.54736400	0.00000000
C	1.35914600	0.17264500	0.00000000
N	2.35303400	1.09016300	0.00000000
H	3.31214000	0.77561900	0.00000000
H	2.13618400	2.07562900	0.00000000
N	1.67232800	-1.13335000	0.00000000
C	0.66248400	-2.03283700	0.00000000
H	0.97426900	-3.07513600	0.00000000
N	-0.65923100	-1.81786100	0.00000000
C	-0.92510300	-0.50063200	0.00000000
H	-3.05221200	-0.33370200	0.00000000

Table S12. Guanine (G)

Calculated energy (in Hartrees)= -540.99345585

Atom	X	Y	Z
N	-2.17314700	0.73436300	0.00000000
C	-1.83295800	2.06736500	0.00000000
H	-2.58196200	2.84872600	0.00000000
N	-0.52471700	2.26447100	0.00000000
C	0.00000000	0.98937000	0.00000000
C	1.37499700	0.56303300	0.00000000
O	2.42012800	1.20302100	0.00000000
N	1.42180900	-0.86801500	0.00000000
H	2.37168900	-1.23106700	0.00000000
C	0.35157100	-1.73014400	0.00000000
N	0.63350200	-3.06395200	0.00000000
H	1.57216900	-3.42861500	0.00000000
H	-0.14509800	-3.70474100	0.00000000
N	-0.90303500	-1.33902100	0.00000000
C	-1.00287800	0.02113100	0.00000000
H	-3.10309200	0.33208300	0.00000000