Electronic Supplementary Information

to

Structural and electronic properties of barbituric acid and melamine–containing ribonucleosides as plausible components of prebiotic RNA: Implications for prebiotic self-assembly

Sarabjeet Kaur,[a] Purshotam Sharma*[a] and Stacey D. Wetmore*[b]

[a] *Computational Biochemistry Laboratory, Department of Chemistry and Centre for Advanced Studies in Chemistry, Panjab University, Chandigarh, 160014, India.*
E-mail: psharma@pu.ac.in

[b] *Department of Chemistry and Biochemistry, University of Lethbridge, Alberta, T1K 3M4, Canada.*
Email: stacey.wetmore@uleth.ca

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S1. Details of Molecular Mechanics Conformational Search. The initial structures for the α– and β–anomers of BA (denoted α– BA and β–BA respectively, Figs. 1c and 1d) and MM (denoted α–MM and β–MM respectively, Figs. 1e and 1f), and their 5′–methoxy counterparts (denoted methoxy–α–BA, methoxy–β–BA, methoxy–α–MM and methoxy–β–MM, respectively) were fully optimized and their Mulliken atomic charges calculated at the B3LYP-D3/6-31G(d,p) level of theory. Thereafter, a conformational search was performed on each system using Hyperchem 8.0.7,[1] the AMBER 99 molecular mechanics force field[2] and the default AMBER atom types. Conformational analyses were carried out by considering rotation about the nucleoside backbone torsions (i.e., α ∠(O3′–P–O5′–C5′), β ∠(H–O5′–C5′–C4′), γ ∠(O5′–C5′–C4′–C3′), δ ∠(C5′–C4′–C3′–O3′) and ζ ∠(C4′–C3′–O3′–H)), the 2′–OH torsion, the endocyclic sugar torsions (namely ν_0 ∠(C4′–O4′–C1′–C2′), ν_1 ∠(O4′–C1′–C2′–C3′), ν_2 ∠(C1′–C2′–C3′–C4′), ν_3 ∠(C2′–C3′–C4′–O4′) and ν_4 ∠(C3′–C4′–O4′–C1′)), as well as the χ glycosidic torsional angle (∠(O4'–C1'–C1–C2) for BA and ∠(C1–N1–C1′–C2′) for MM), and the additional ϕ torsion angle (∠(O4'–C1'–N1–C2)) in the MM rNs (Figure 1). A usage directed search consisting of 10,000 iterations or 1,000 optimizations was used to generate conformations. The ten lowest energy conformations obtained from the conformational search were fully optimized at the B3LYP-D3/6-31G(d,p) level of theory, and their relative energies were calculated with B3LYP-D3/6-311+G(2df,p). The lowest energy conformation thus obtained was then used for the glycosidic torsional and deglycosylation scans.

References.

1. HyperChem(TM) Professional 8.0.7, Hypercube, Inc., 1115 NW 4th Street, Gainesville, Florida 32601, USA.
2. J. Wang, P. Cieplak and P. A. Kollman, *J. Comput. Chem.* 2000, **21**, 1049-1074.

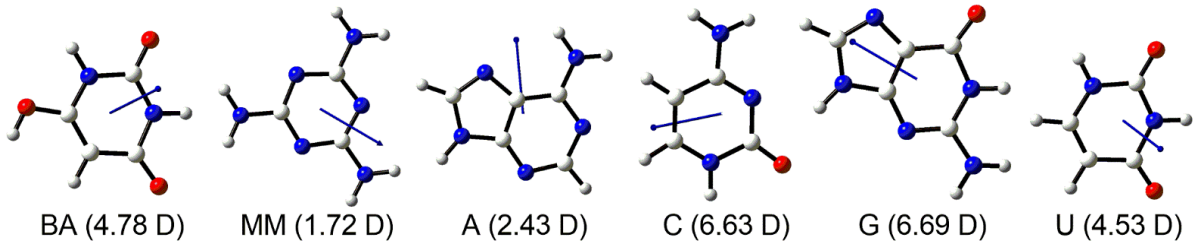

Figure S1. B3LYP-D3/6-31G(d,p) alignment and magnitude (Debye) of the dipole moments in the prebiotic and canonical nucleobases.

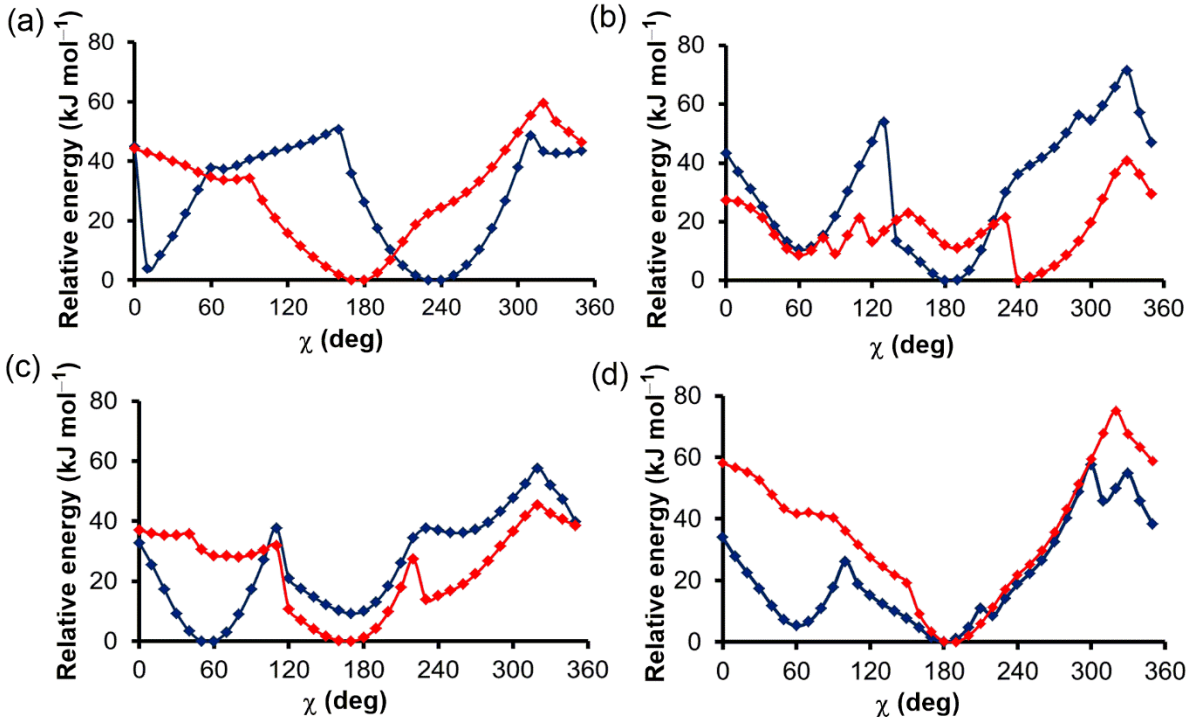

Figure S2. B3LYP-D3/6-31G(d,p) relative energies (kJ mol^{-1}) as a function of rotation about the χ glycosidic torsion angle for the free model (blue) and the polymer model (red) of the biologically-relevant β–anomer of (a) adenosine, (b) cytidine (c) guanosine and (d) uridine.

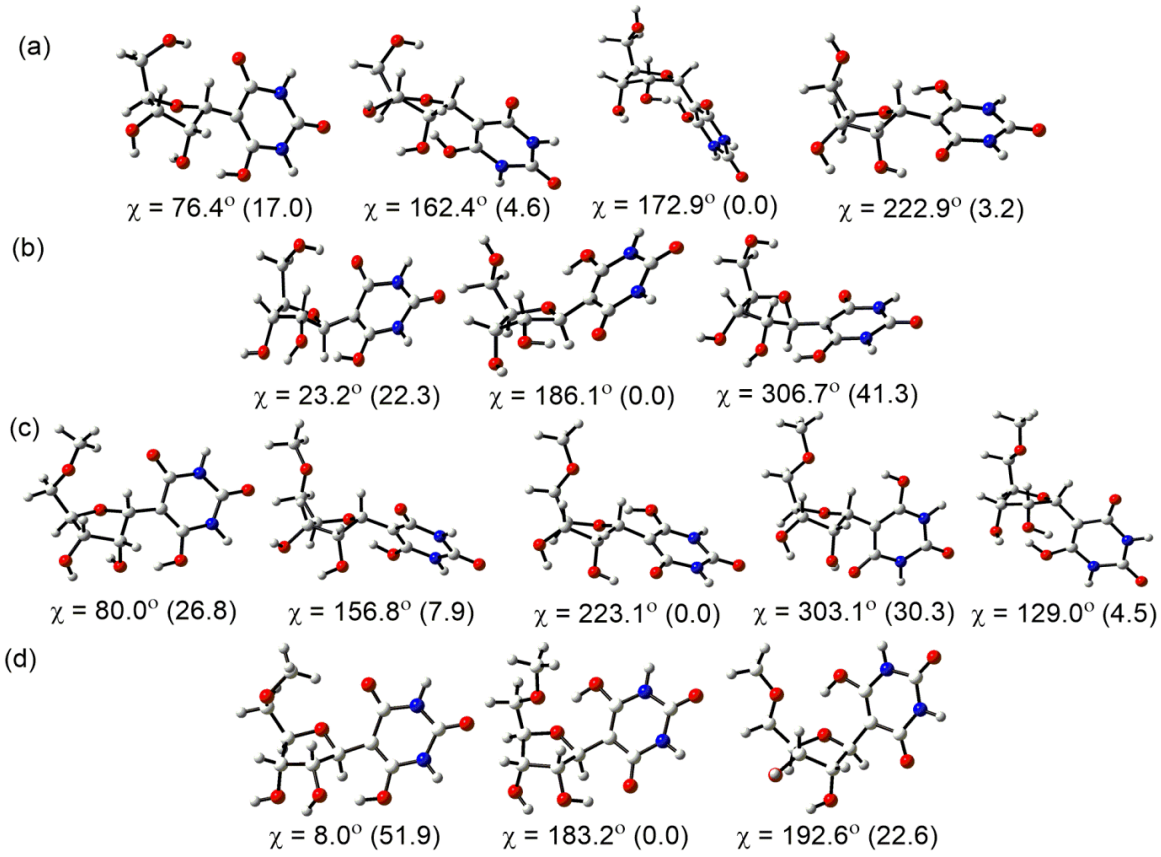

Figure S3. B3LYP-D3/6-31G(d,p) optimized structures and B3LYP-D3/6-311+G(2df,p) relative energies (kJ mol^{-1}, parentheses) for BA-containing rNs obtained by scanning the χ torsion angle for the (a) α–BA free model, (b) β–BA free model, (c) α–BA polymer model and (d) β–BA polymer model.

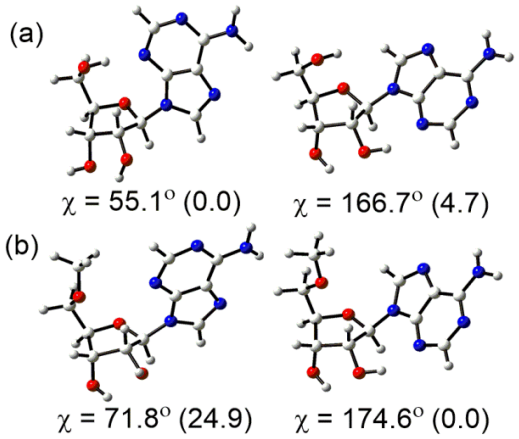

Figure S4. B3LYP-D3/6-31G(d,p) optimized structures and B3LYP-D3/6-311+G(2df,p) relative energies (kJ mol^{-1}, parentheses) obtained by scanning the χ torsion angle for (a) the free model and (b) the polymer model of the biologically–relevant β–anomer of adenosine.

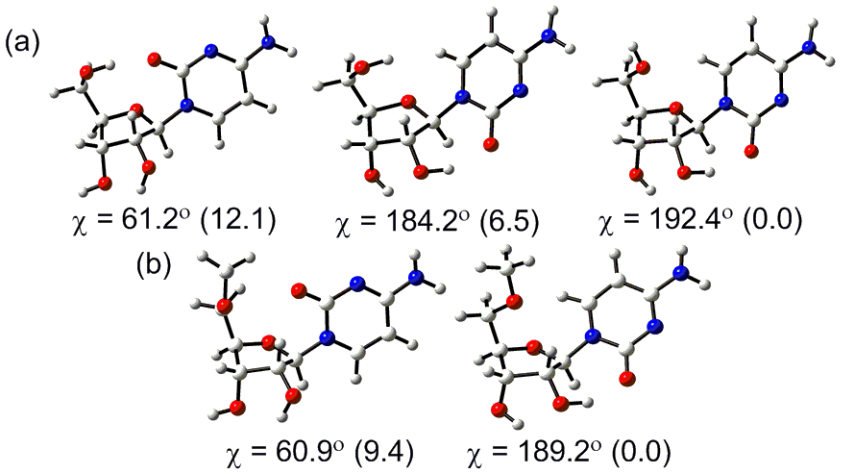

Figure S5. B3LYP-D3/6-31G(d,p) optimized structures and B3LYP-D3/6-311+G(2df,p) relative energies (kJ mol^{-1}, parentheses) obtained by scanning the χ torsion angle for (a) the free model and (b) the polymer model of the biologically–relevant β–anomer of cytidine.

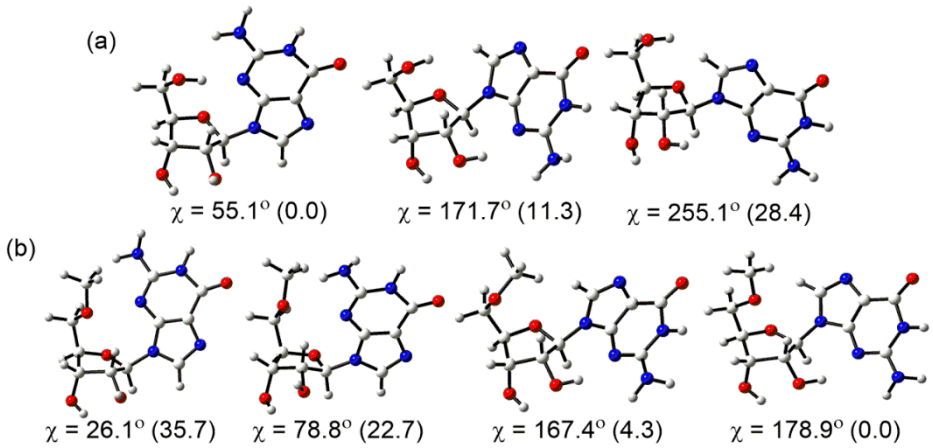

Figure S6. B3LYP-D3/6-31G(d,p) optimized structures and B3LYP-D3/6-311+G(2df,p) relative energies (kJ mol^{-1}, parentheses) obtained by scanning the χ torsion angle for (a) the free model and (b) the polymer model of the biologically-relevant β–anomer of guanosine.

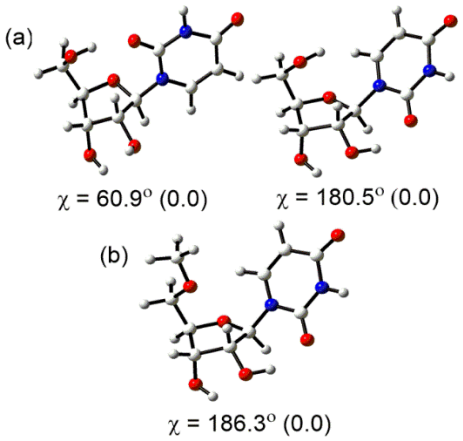

Figure S7. B3LYP-D3/6-31G(d,p) optimized structures and B3LYP-D3/6-311+G(2df,p) relative energies (kJ mol^{-1}, parentheses) obtained by scanning the χ torsion angle for (a) the free model and (b) the polymer model of the biologically-relevant β–anomer of uridine.

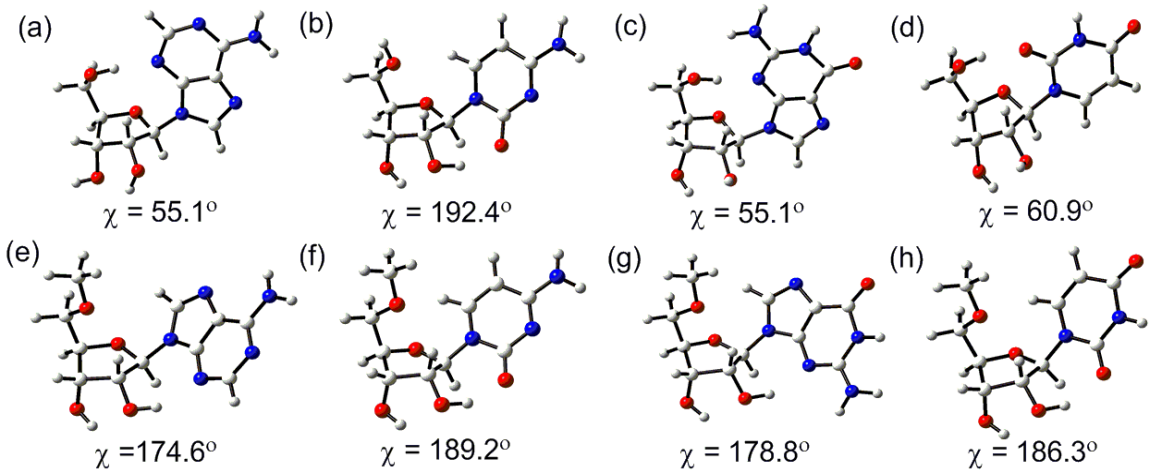

Figure S8. B3LYP-D3/6-31G(d,p) optimized global minima identified from glycosidic torsion scans corresponding to the free model of adenosine, cytosine, guanosine and uridine (a-d), and the polymer model of the biologically-relevant β–anomers of the canonical rNs (e-h).

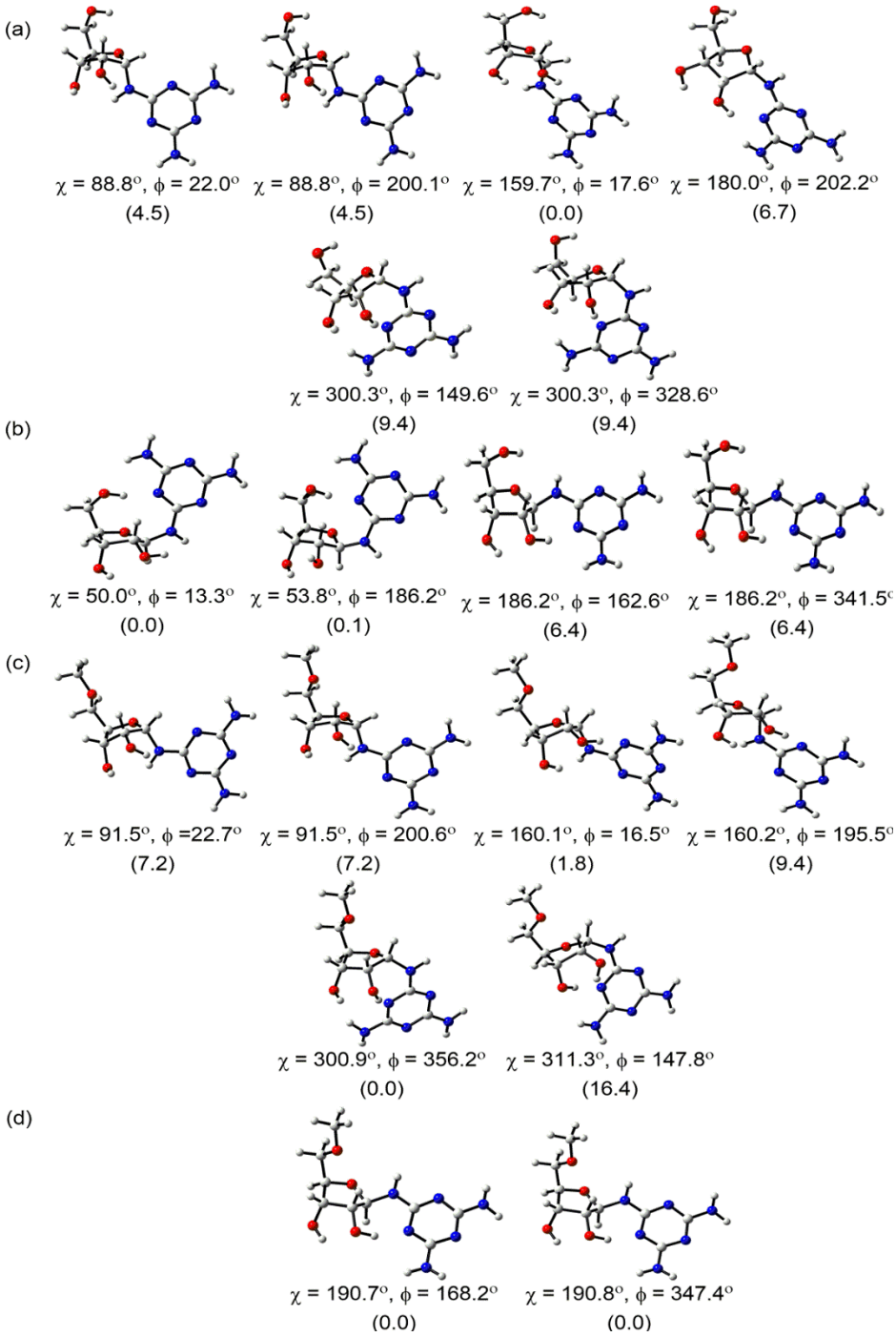

Figure S9. B3LYP-D3/6-31G(d,p) optimized structures and B3LYP-D3/6-311+G(2df,p) relative energies (kJ mol^{-1}, parentheses) for MM-containing rNs obtained by scanning the χ and ϕ torsion angles for the (a) α–MM free model, (b) β–MM free model, (c) α–MM polymer model and (d) β–MM polymer model.

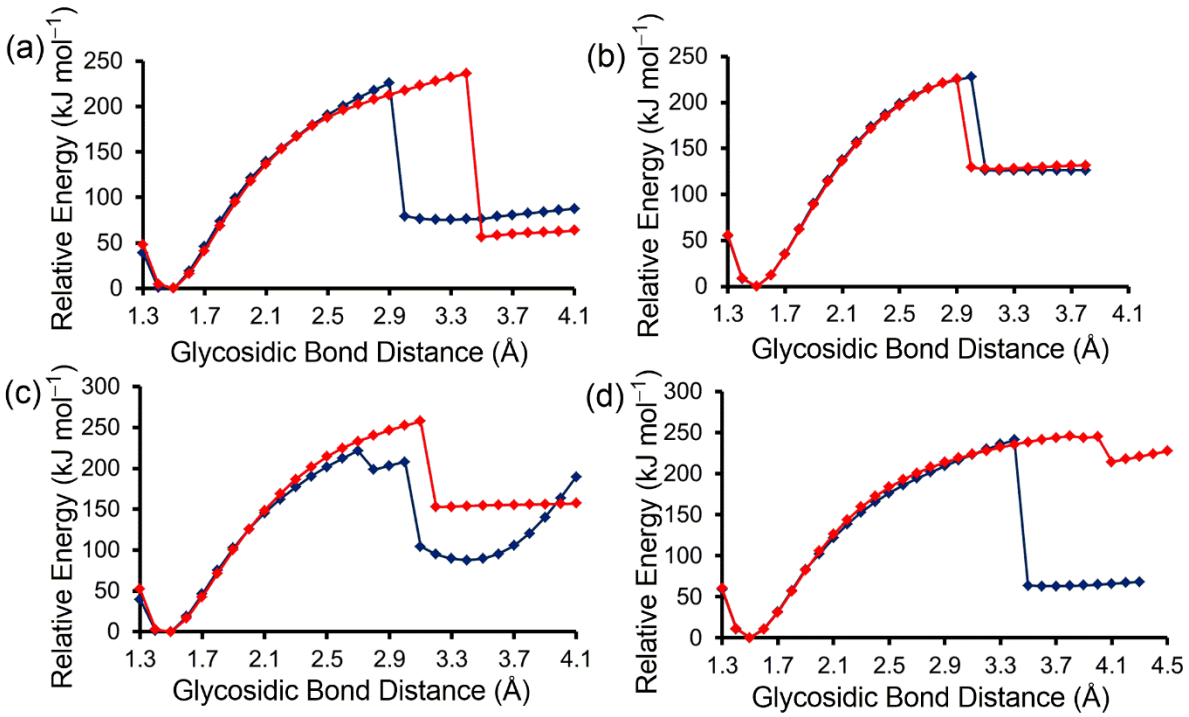

Figure S10. B3LYP-D3/6-31G(d,p) relative energy (kJ mol^{-1}) as a function of the glycosidic bond distance for the free model (blue) and the polymer model (red) of the biologically-relevant β-anomers of (a) adenosine, (b) cytidine, (c) guanosine and (d) uridine.

Table S1. B3LYP/6-311+G(2df,p) stacking energies (kJ mol^{-1}) as a function of the angle of rotation (α, deg) for prebiotic:prebiotic nucleobase dimers.[a]

α	BA–BA	MM–MM	BA–MM
0°	8.2	–1.8	–27.8
30°	–12.5	–16.9	–24.7
60°	–28.8	–16.3	–18.9
90°	–23.8	–14.7	–27.1
120°	–19.5	–4.7	–26.6
150°	–28.6	–17.6	–22.9
180°	–34.9	–16.1	–17.2
210°	–28.6	–17.6	–25.3
240°	–19.5	–4.7	–26.9
270°	–23.8	–14.7	–26.0
300°	–27.9	–16.3	–17.4
330°	–12.5	–16.9	–26.3

[a]α is defined as 0° when the glycosidic bonds of the interacting monomers align, and increases when the first monomer is rotated with respect to the second in an anti-clockwise direction.

Table S2. B3LYP/6-311+G(2df,p) stacking energies (kJ mol^{-1}) as a function of the angle of rotation (α, deg) for BA stacked with a canonical nucleobase.[a]

α	BA–A	BA–U	BA–C	BA–G
0°	–35.2	–16.6	–6.9	–21.8
30°	–33.3	–17.0	–14.5	–26.1
60°	–26.1	–21.6	–19.5	–43.8
90°	–23.5	–4.1	–14.2	–48.3
120°	–25.6	–1.5	–14.7	–37.3
150°	–27.3	–14.7	–24.1	–28.2
180°	–22.4	–29.3	–33.5	–22.7
210°	–20.9	–28.9	–38.3	–19.7
240°	–21.3	–15.1	–34.2	–16.1
270°	–24.1	–18.4	–36.2	–16.4
300°	–14.5	–31.7	–26.1	–24.9
330°	–21.4	–31.1	–14.5	–28.9

[a]α is defined as 0° when the glycosidic bonds of the interacting monomers align, and increases when the first monomer is rotated with respect to the second in an anti-clockwise direction.

Table S3. B3LYP/6-311+G(2df,p) stacking energies (kJ mol^{-1}) as a function of the angle of rotation (α, deg) for MM stacked with a canonical nucleobases.[a]

(α)	MM–A	MM–U	MM–C	MM–G
0°	–22.1	–27.4	–23.3	–23.8
30°	–24.8	–24.5	–21.8	–23.4
60°	–19.2	–19.9	–16.4	–25.3
90°	–22.1	–26.1	–23.6	–27.2
120°	–23.6	–26.4	–20.9	–23.8
150°	–24.1	–23.2	–20.2	–23.0
180°	–18.2	–19.3	–16.6	–24.4
210°	–20.9	–23.7	–21.4	–27.1
240°	–21.8	–26.9	–23.4	–25.2
270°	–25.1	–26.7	–24.2	–24.3
300°	–15.7	–20.6	–19.6	–22.5
330°	–20.3	–25.5	–23.3	–25.4

[a]α is considered as 0° when the glycosidic bonds of the interacting monomers align, and increases when the first monomer is rotated with respect to the second in an anti-clockwise direction.

Table S4. Cartesian coordinates of the optimized hydrogen-bonded A:U pair.

Energy (in hartrees) = –882.4877718

Atom	X	Y	Z
N	4.59917900	0.80701900	–0.00059200
C	4.96873600	–0.52392700	–0.00044300
H	6.00902000	–0.82008800	–0.00071000
N	3.94756600	–1.34621600	0.00006800
C	2.84515500	–0.50913200	0.00023900
C	1.45547700	–0.77013900	0.00074400
N	0.93752400	–2.00907000	0.00156100
H	1.56583300	–2.79576100	0.00018300
H	–0.07295300	–2.15008300	0.00065900
N	0.62631200	0.29757900	0.00068100
C	1.13318500	1.54645800	0.00019100
H	0.38394100	2.33518400	0.00007500
N	2.41497700	1.90985700	–0.00025300
C	3.22282300	0.83782700	–0.00019900
H	5.20483000	1.61365500	–0.00095100
N	–4.07073100	–1.21098300	–0.00040800
C	–4.85810000	–0.08097300	0.00018400
H	–5.92788700	–0.25809800	0.00043400
C	–4.31659200	1.15517600	0.00035000
H	–4.92602800	2.04784900	0.00076000
C	–2.86199400	1.30894500	0.00003700
O	–2.26406600	2.37700800	0.00018600
N	–2.15489600	0.09555500	–0.00056400
H	–1.10397600	0.16340600	–0.00022000
C	–2.67983000	–1.16616900	–0.00064300
O	–2.01258300	–2.20123000	–0.00097000
H	–4.47226000	–2.13687400	–0.00017400

Table S5. Cartesian coordinates of the optimized hydrogen-bonded G:C pair.

Energy (in hartrees) = –937.8832716

Atom	X	Y	Z
N	–4.33329200	0.89928200	0.00006600
C	–4.92648700	–0.32586100	0.00008000
H	–6.01075900	–0.34181300	0.00014200
C	–4.16913800	–1.45051200	0.00008400
H	–4.62049700	–2.43402800	0.00020700
C	–2.73448500	–1.27693900	–0.00005500
N	–1.92318200	–2.33688900	0.00001500
H	–0.89000900	–2.21802600	0.00029300
H	–2.31043700	–3.26635000	0.00020600
N	–2.17231400	–0.06042700	–0.00015200
C	–2.93209900	1.06583000	0.00005500
O	–2.48313000	2.21628900	–0.00019000

H	–4.87345600	1.75298000	0.00003900
N	4.65510400	0.50443400	–0.00008100
C	4.96603500	–0.84808400	0.00008500
H	5.99210000	–1.18994200	0.00008500
N	3.90776600	–1.61404900	0.00000400
C	2.84155500	–0.72958100	–0.00006700
C	1.43016900	–0.96085300	–0.00016200
O	0.82592300	–2.04511900	–0.00010200
N	0.71145900	0.24905400	–0.00003100
H	–0.31979400	0.15570400	–0.00005300
C	1.26097500	1.51058700	0.00021900
N	0.39738700	2.54696000	–0.00009500
H	–0.61811900	2.42976700	–0.00004400
H	0.80047900	3.46857900	0.00009000
N	2.56831000	1.73912800	0.00020000
C	3.28631000	0.59799700	0.00010400
H	5.29246600	1.28581600	–0.00017400

Table S6. Cartesian coordinates of the optimized hydrogen-bonded BA:MM pair.

Energy (in hartrees) = –936.9377723

Atom	X	Y	Z
C	–2.14669900	–1.14245900	0.02677500
N	–1.42067000	–0.00028600	0.01658800
C	–2.15864700	1.13590300	–0.00627100
C	–4.09616100	–0.01471500	–0.02033800
N	–3.48980500	–1.21225500	0.00977600
N	–3.50320400	1.18905300	–0.02336200
N	–5.45723100	–0.02345300	–0.07676600
H	–5.92266600	–0.89104400	0.13464000
H	–5.93251800	0.84466100	0.10906700
N	–1.49638900	2.30687400	–0.01073300
H	–0.47859700	2.34712500	0.01005600
H	–2.04646500	3.14878400	–0.03016700
N	–1.47317500	–2.30876300	0.06614800
H	–0.45819400	–2.33881000	0.02981600
H	–2.01418600	–3.15583700	0.02766100
C	2.03361200	–1.18434900	–0.01575700
N	3.42811000	–1.13098000	–0.02361900
C	4.13731000	0.04043000	–0.00943100
C	3.50503100	1.24228100	0.01324500
C	2.05743500	1.28198600	0.02156800
N	1.41465800	0.03554100	0.00726900
O	1.45776600	–2.26772000	–0.02911500
O	1.40137700	2.32435900	0.03976300
O	5.46596700	–0.17680200	–0.02096700
H	4.04318500	2.18011500	0.02424400
H	3.91453000	–2.01670800	–0.04068600
H	0.35689100	0.02670600	0.01348300

H	5.92981100	0.67173600	–0.01143100

Table S7 Cartesian coordinates of the optimized hydrogen-bonded MM:U pair.

Energy (in hartrees) = –861.6781694

Atom	X	Y	Z
C	1.79770600	1.13904600	0.01533800
N	1.06317800	0.00045400	0.01167200
C	1.79369400	–1.13933200	–0.00020300
C	3.73940900	–0.00407000	–0.01518700
N	3.14188400	1.19734700	0.00339800
N	3.13709900	–1.20393600	–0.01195100
N	5.10032100	–0.00671600	–0.06594300
H	5.57273400	0.85931700	0.13584300
H	5.56910600	–0.87723100	0.12462800
N	1.12492700	–2.30847800	0.00258800
H	0.10952100	–2.34302800	0.01055300
H	1.67011000	–3.15346300	–0.01470600
N	1.13250700	2.30846600	0.03891000
H	0.11525300	2.34602700	0.02029700
H	1.68019000	3.15180200	0.01357600
N	–3.78430600	–1.15543900	–0.00012900
C	–4.49893900	0.01774700	–0.01341200
H	–5.57790700	–0.08879200	–0.01952300
C	–3.87508800	1.21456200	–0.01830900
H	–4.41852500	2.14847800	–0.02871900
C	–2.41811000	1.26648800	–0.00936700
O	–1.77132000	2.31324900	–0.01285600
N	–1.77735000	0.02377900	0.00409000
H	–0.71880100	0.01678000	0.00933300
C	–2.39279600	–1.20339300	0.00891200
O	–1.80407500	–2.28062700	0.02039300
H	–4.24160100	–2.05548900	0.00334000

Table S8. Cartesian coordinates of the optimized hydrogen-bonded A:BA pair

Energy (in hartrees) = –957.748272

Atom	X	Y	Z
N	4.97538500	–0.79567600	0.00056500
C	5.33781700	0.53724600	0.00052000
H	6.37645700	0.83915300	0.00077300
N	4.31209300	1.35381500	0.00004600
C	3.21411600	0.51090000	–0.00011100
C	1.82254100	0.76572600	–0.00035800
N	1.29714300	1.99971300	–0.00052400
H	1.92169300	2.78954300	–0.00042800
H	0.28268100	2.13493800	–0.00036800
N	0.99876500	–0.30786000	–0.00043200

C	1.51358500	–1.55279800	–0.00018700
H	0.77074800	–2.34745700	–0.00030400
N	2.79705900	–1.91043000	0.00012000
C	3.59913300	–0.83368900	0.00016000
H	5.58530500	–1.59904200	0.00084100
C	–2.46257900	–1.25879100	–0.00026600
N	–3.85736300	–1.11294000	–0.00031700
C	–4.48714500	0.10154900	0.00030600
C	–3.78310200	1.26537200	0.00040100
C	–2.33630000	1.21341300	–0.00007300
N	–1.78142300	–0.06684500	–0.00051800
O	–1.93902500	–2.36071600	–0.00023500
O	–1.60791300	2.21165700	–0.00009700
O	–5.82865300	–0.02659100	0.00069100
H	–4.26584600	2.23305800	0.00070700
H	–4.40192700	–1.96412200	0.00033400
H	–0.73155800	–0.14470200	–0.00060500
H	–6.23283300	0.85183100	0.00124400

Table S9. Cartesian coordinates of the MM–MM stacked dimer with α = 0°.

Energy (in hartrees) = –446.67049890

Atom	X	Y	Z
C	1.65587100	1.24599300	–0.36112900
N	1.65174100	0.33157700	–1.34614800
C	1.65656400	–0.93571400	–0.89843500
C	1.65605600	–0.31029600	1.25951100
N	1.65184900	1.00000900	0.96018100
N	1.65214400	–1.33166600	0.38591000
N	1.68506300	–0.63550700	2.58015900
N	1.68507000	–1.91679200	–1.84045600
N	1.68536300	2.55235900	–0.73968100
H	1.50180100	–1.59290000	2.83130300
H	1.50179100	0.09569900	3.24725900
H	1.50195800	–2.86013200	–1.54070100
H	1.50163900	2.76464400	–1.70636500
H	1.50227700	3.24845500	–0.03598200
H	1.50097600	–1.65554000	–2.79497600
C	–1.64412900	1.24599300	–0.36112800
N	–1.64825900	0.33157800	–1.34614800
C	–1.64343600	–0.93571400	–0.89843400
C	–1.64394400	–0.31029600	1.25951200
N	–1.64815100	1.00001000	0.96018200
N	–1.64785600	–1.33166500	0.38591100
N	–1.61493700	–0.63550700	2.58016000
N	–1.61493000	–1.91679100	–1.84045500
N	–1.61463700	2.55235900	–0.73968100
H	–1.79819900	–1.59289900	2.83130400

H	–1.79820900	0.09570000	3.24725900
H	–1.79804200	–2.86013200	–1.54070000
H	–1.79836100	2.76464400	–1.70636500
H	–1.79772300	3.24845600	–0.03598100
H	–1.79902400	–1.65553900	–2.79497500

Table S10. Cartesian coordinates of the BA–BA stacked dimer with α = 0°.

Energy (in hartrees) = –490.23578420

Atom	X	Y	Z
C	1.64998400	–0.46089300	1.36247700
N	1.65005100	0.87905600	0.96298000
C	1.65036300	1.28452400	–0.34722000
C	1.65000300	0.39204200	–1.37149400
C	1.64999600	–1.03033400	–1.08659400
N	1.64976100	–1.33813000	0.29758800
H	1.64913500	0.70454500	–2.40673300
O	1.65001400	–0.78784500	2.53385700
O	1.65018800	–1.93091400	–1.91023200
O	1.64971100	2.62791500	–0.45036400
H	1.65091000	1.56777100	1.70235700
H	1.64939100	–2.32171900	0.53584400
H	1.65050800	2.87761000	–1.38456000
C	–1.65001600	–0.46089200	1.36247700
N	–1.64994900	0.87905700	0.96298100
C	–1.64963700	1.28452500	–0.34722000
C	–1.64999700	0.39204300	–1.37149400
C	–1.65000400	–1.03033300	–1.08659300
N	–1.65023900	–1.33813000	0.29758800
H	–1.65086500	0.70454600	–2.40673200
O	–1.64998600	–0.78784400	2.53385800
O	–1.64981200	–1.93091300	–1.91023200
O	–1.65028900	2.62791600	–0.45036300
H	–1.64909000	1.56777200	1.70235700
H	–1.65060900	–2.32171800	0.53584400
H	–1.64949200	2.87761100	–1.38456000

Table S11. Cartesian coordinates of the BA–MM stacked dimer with α = 0°.

Energy (in hartrees) = –446.67049210

Atom	X	Y	Z
C	1.67592700	0.49696500	–1.32801800
N	1.69848300	–0.84395400	–0.93243100
C	1.67431000	–1.25382500	0.37617600
C	1.62502400	–0.36517300	1.40259000
C	1.59748300	1.05775300	1.12179300
N	1.62608400	1.37024100	–0.26104200

H	1.60461600	–0.68118500	2.43656200
O	1.69872300	0.82787200	–2.49806500
O	1.55382800	1.95521000	1.94768100
O	1.70402800	–2.59717600	0.47548500
H	1.73575500	–1.52987600	–1.67346200
H	1.60776100	2.35434300	–0.49645500
H	1.68639600	–2.85001000	1.40867100
C	–1.66803900	1.23229700	–0.32507900
N	–1.62467200	0.37374200	–1.35824900
C	–1.59900400	–0.91583200	–0.98030700
C	–1.66882000	–0.41053200	1.20776900
N	–1.69863800	0.91381200	0.98030100
N	–1.62530200	–1.38198500	0.27999000
N	–1.66439700	–0.80727800	2.50903300
N	–1.52240600	–1.84252100	–1.97333600
N	–1.66211400	2.55787800	–0.63095900
H	–1.82963300	–1.78115300	2.70273800
H	–1.88254200	–0.11853600	3.20997600
H	–1.68905400	–2.80504700	–1.73034000
H	–1.82709300	2.81870200	–1.58910900
H	–1.88009800	3.20955900	0.10460800
H	–1.68929100	–1.53349900	–2.91668500

Table S12. Cartesian coordinates of the BA–U stacked dimer with α = 0°.

Energy (in hartrees) = –414.97633630

Atom	X	Y	Z
N	0.75685600	2.09310400	–1.29525600
C	1.14159200	2.63683400	–0.08526400
H	1.00653400	3.68882400	0.12727100
N	1.66567300	1.76041500	0.73699100
C	1.62413100	0.57168500	0.02694700
C	2.03120800	–0.74283700	0.34046300
N	2.58856800	–1.05701100	1.53196600
H	2.86270100	–2.00908900	1.70896100
H	2.72493000	–0.34429800	2.22886900
N	1.85857800	–1.71266500	–0.57613200
C	1.30302700	–1.38218400	–1.75461900
H	1.18710100	–2.20419300	–2.45768000
N	0.87560100	–0.18805000	–2.17894600
C	1.06312400	0.75060600	–1.24248100
H	0.33631400	2.57094000	–2.07755300
C	–0.93871700	–0.89532200	1.56883700
N	–1.31450200	–1.55992100	0.39744700
C	–1.94076000	–0.94911600	–0.65884400
C	–2.24599500	0.37457100	–0.64034600
C	–1.90709600	1.17505500	0.52098700
N	–1.26388500	0.44540200	1.55277400

H	–2.73863600	0.86293300	–1.46991600
O	–0.38449200	–1.46634700	2.48850800
O	–2.12517100	2.36731300	0.66378100
O	–2.18877700	–1.81829900	–1.65801800
H	–1.10145900	–2.54666700	0.35328300
H	–1.01144400	0.97086400	2.38004300
H	–2.62983100	–1.35533700	–2.38342100

Table S13. Cartesian coordinates of the BA–A stacked dimer with α = 0°.

Energy (in hartrees) = –490.23576490

Atom	X	Y	Z
N	0.75685600	2.09310400	–1.29525600
C	1.14159200	2.63683400	–0.08526400
H	1.00653400	3.68882400	0.12727100
N	1.66567300	1.76041500	0.73699100
C	1.62413100	0.57168500	0.02694700
C	2.03120800	–0.74283700	0.34046300
N	2.58856800	–1.05701100	1.53196600
H	2.86270100	–2.00908900	1.70896100
H	2.72493000	–0.34429800	2.22886900
N	1.85857800	–1.71266500	–0.57613200
C	1.30302700	–1.38218400	–1.75461900
H	1.18710100	–2.20419300	–2.45768000
N	0.87560100	–0.18805000	–2.17894600
C	1.06312400	0.75060600	–1.24248100
H	0.33631400	2.57094000	–2.07755300
C	–0.93871700	–0.89532200	1.56883700
N	–1.31450200	–1.55992100	0.39744700
C	–1.94076000	–0.94911600	–0.65884400
C	–2.24599500	0.37457100	–0.64034600
C	–1.90709600	1.17505500	0.52098700
N	–1.26388500	0.44540200	1.55277400
H	–2.73863600	0.86293300	–1.46991600
O	–0.38449200	–1.46634700	2.48850800
O	–2.12517100	2.36731300	0.66378100
O	–2.18877700	–1.81829900	–1.65801800
H	–1.10145900	–2.54666700	0.35328300
H	–1.01144400	0.97086400	2.38004300
H	–2.62983100	–1.35533700	–2.38342100

Table S14. Cartesian coordinates of the BA–C stacked dimer with α = 0°.

Energy (in hartrees) = –490.23577460

Atom	X	Y	Z
N	1.43964600	–1.26124100	1.21950200
C	1.18075700	–0.16668300	1.97582600
H	0.83435700	–0.33912100	2.98959800

C	1.36030200	1.07539100	1.45426900
H	1.17208900	1.96783900	2.03675400
C	1.82639700	1.12864800	0.09057500
N	2.05733400	2.34548500	–0.47788300
H	2.25462900	2.34945800	–1.46743700
H	1.68039400	3.18263800	–0.06550800
N	2.07462200	0.06554900	–0.65084700
C	1.90320800	–1.19444700	–0.13223400
O	2.10613500	–2.24167100	–0.72369500
H	1.31584300	–2.19701200	1.58019100
C	–1.33930600	1.31124900	–0.86271800
N	–1.78034000	1.03901600	0.43591200
C	–1.94828200	–0.22744600	0.93481200
C	–1.69134600	–1.33080900	0.18499000
C	–1.22724600	–1.18038900	–1.18113800
N	–1.08855400	0.16887600	–1.59459400
H	–1.82046500	–2.33222400	0.57212700
O	–1.20084600	2.44685400	–1.27534300
O	–0.96246700	–2.08475900	–1.95665900
O	–2.38121300	–0.20430500	2.21049700
H	–1.98063100	1.83964900	1.01890100
H	–0.76609300	0.31395600	–2.54284600
H	–2.48887100	–1.11100700	2.52888900

Table S15. Cartesian coordinates of the BA–G stacked dimer with α = 0°.

Energy (in hartrees) =–490.23576120

Atom	X	Y	Z
N	0.19775500	1.92798700	–1.70204900
C	0.84744700	2.71913400	–0.76917500
H	1.63815600	3.39822300	–1.05691300
N	0.39847300	2.54251000	0.44666900
C	–0.59447200	1.59076400	0.31436900
C	–1.45652300	1.00135100	1.30662900
O	–1.54226300	1.18176600	2.50800700
N	–2.33895000	0.05614900	0.67203800
H	–3.01969900	–0.34226300	1.30727800
C	–2.37691800	–0.25694600	–0.66291000
N	–3.34308400	–1.15155200	–1.06601100
H	–3.58959100	–1.89114100	–0.42323000
H	–3.21702000	–1.45989900	–2.02020000
N	–1.58297300	0.28260900	–1.55810800
C	–0.73561600	1.19570800	–1.01688700
H	0.36027800	1.88468400	–2.69665200
C	1.13293100	–1.08122600	1.59722300
N	2.10102000	–0.31744400	0.93805500
C	2.33522900	–0.38257800	–0.41173600
C	1.62627700	–1.21226600	–1.22084900
C	0.59178400	–2.05772100	–0.65573600

N	0.43329800	–1.91130200	0.74574300
H	1.80477900	–1.26799700	–2.28593500
O	0.94995800	–1.00031000	2.79680800
O	–0.11282400	–2.84308500	–1.26905100
O	3.32005400	0.45771000	–0.78506500
H	2.64597000	0.30968900	1.51315400
H	–0.28026700	–2.48541300	1.17636300
H	3.45838200	0.38546200	–1.73938000

Table S16. Cartesian coordinates of the MM–U stacked dimer with α = 0°.

Energy (in hartrees) = –414.97634340

Atom	X	Y	Z
C	–1.13227100	–0.06118700	1.51933100
N	–1.26490100	1.17892800	1.01837200
C	–1.66914600	1.19675500	–0.26333300
C	–1.77030200	–1.04367200	–0.39799800
N	–1.37239100	–1.21557300	0.87425700
N	–1.94659000	0.12887900	–1.03079900
N	–2.00088800	–2.17086700	–1.12392900
N	–1.79467700	2.41877100	–0.84783800
N	–0.69329300	–0.15823500	2.80332700
H	–2.47318300	–2.07113100	–2.00724600
H	–2.05716400	–3.04485300	–0.62768800
H	–2.26910700	2.46804600	–1.73427000
H	–0.68639100	0.67972400	3.36106700
H	–0.76379500	–1.05442600	3.25624500
H	–1.77607600	3.22840700	–0.25001300
N	1.47510000	1.15377900	–1.26155000
C	1.22222900	–0.00609200	–1.95748900
H	0.89828100	0.12931000	–2.98343400
C	1.37040800	–1.22274700	–1.39198400
H	1.17326800	–2.13574900	–1.93542200
C	1.81019200	–1.33308100	–0.00317400
O	1.98058600	–2.36839200	0.61771000
N	2.03962300	–0.08247800	0.61360100
H	2.34624200	–0.10898400	1.57855800
C	1.89856800	1.18236700	0.06760900
O	2.11624900	2.21865000	0.66669000
H	1.36129100	2.06111100	–1.68885200

Table S17. Cartesian coordinates of the MM–A stacked dimer with α = 0°.

Energy (in hartrees) = –446.67049560

Atom	X	Y	Z
N	–0.44303000	–2.26158600	–1.07022900
C	–0.61771900	–2.73639400	0.21498900
H	–0.25277300	–3.71126400	0.50916400

N	–1.25048800	–1.89756600	0.99910900
C	–1.50768000	–0.80839000	0.18270500
C	–2.15401900	0.42525000	0.41150600
N	–2.67600500	0.74983900	1.61616600
H	–3.12758300	1.64201600	1.73029900
H	–2.61078500	0.10409500	2.38492600
N	–2.25306800	1.30482300	–0.60193200
C	–1.72852400	0.96540100	–1.79203000
H	–1.83674800	1.71288400	–2.57496700
N	–1.09531700	–0.15894700	–2.14358800
C	–1.01580300	–1.00895700	–1.11190600
H	0.00915200	–2.72838300	–1.84146400
C	2.16864000	–0.01165000	–0.68020500
N	2.12053900	–0.69145300	0.47823800
C	1.50181900	–0.02129500	1.46544200
C	1.07231200	1.75879900	0.16364700
N	1.66206900	1.21130700	–0.91290100
N	0.94903300	1.20078900	1.38012500
N	0.56442600	3.01163200	0.01141200
N	1.44334700	–0.63534200	2.67798300
N	2.81076000	–0.61477700	–1.71687500
H	–0.03877000	3.36417300	0.73606900
H	0.47776600	3.37193400	–0.92450800
H	0.83060200	–0.24262800	3.37339200
H	3.03119500	–1.59281400	–1.62660200
H	2.69951200	–0.21442600	–2.63372100
H	1.67840800	–1.61321500	2.71996500

Table S18. Cartesian coordinates of the MM–C stacked dimer with α = 0°.

Energy (in hartrees) = –446.67047760

Atom	X	Y	Z
N	1.40057200	1.31547600	–1.19682600
C	1.19627300	0.21890400	–1.96682600
H	0.85772700	0.38729800	–2.98392700
C	1.41772500	–1.02007200	–1.45408700
H	1.27351600	–1.91358600	–2.04739400
C	1.86613600	–1.06803300	–0.08428000
N	2.13726200	–2.28020900	0.47633500
H	2.32046800	–2.28596400	1.46858400
H	1.79987300	–3.12762000	0.05086400
N	2.06124500	–0.00317300	0.67037600
C	1.84716100	1.25400400	0.16086300
O	1.99977700	2.30266200	0.76477500
H	1.24472800	2.24905400	–1.55071100
C	–1.73842000	–1.07647500	–0.46995600
N	–1.95920800	0.13413600	–1.01042900
C	–1.72815800	1.14890600	–0.15992700
C	–1.12608800	–0.22146800	1.51562200

N	–1.31635800	–1.33050200	0.78053100
N	–1.30497600	1.04787800	1.11170600
N	–0.72931900	–0.40284000	2.80418500
N	–1.96169000	2.40454200	–0.62851000
N	–1.98430200	–2.15418300	–1.26295800
H	–0.40347600	0.40279800	3.31215200
H	–0.41189000	–1.31965700	3.07243800
H	–1.62243400	3.17933900	–0.08273600
H	–2.11830300	–1.99121700	–2.24722500
H	–1.65321800	–3.05173100	–0.94982000
H	–2.09555400	2.51753600	–1.61975400

Table S19. Cartesian coordinates of the MM–G stacked dimer with α = 0°.

Energy (in hartrees) = –446.67051340

Atom	X	Y	Z
N	–0.18866300	1.84980500	1.79437600
C	–0.82183000	2.69949500	0.90252700
H	–1.60391300	3.37395100	1.22288900
N	–0.36927300	2.58162200	–0.31909000
C	0.60884700	1.60937400	–0.23379000
C	1.46720000	1.06117000	–1.25252600
O	1.56175400	1.30445200	–2.44209800
N	2.33233600	0.07017400	–0.66579100
H	3.01039100	–0.30375500	–1.31855400
C	2.35883300	–0.31460000	0.65056900
N	3.30963100	–1.24391900	1.00922900
H	3.54850800	–1.95158300	0.32873300
H	3.17414200	–1.60107300	1.94492700
N	1.56834100	0.18800800	1.57000100
C	0.73732100	1.14141800	1.07492900
H	–0.35690800	1.75566300	2.78450400
C	–1.62522000	–1.24556500	1.02899300
N	–0.66969900	–2.02246500	0.49062100
C	–0.50748200	–1.83178500	–0.82991800
C	–2.10422700	–0.25434200	–0.92971500
N	–2.37668700	–0.33701200	0.38384800
N	–1.18179300	–0.96323700	–1.60274900
N	–2.84968300	0.62292500	–1.65456900
N	0.42203500	–2.60779500	–1.45002700
N	–1.86885900	–1.40806300	2.35752600
H	–2.54383400	0.83742200	–2.58929100
H	–3.40935900	1.29083900	–1.15065700
H	0.69181800	–2.35788000	–2.38706200
H	–1.20291200	–1.93817100	2.89492600
H	–2.43948900	–0.71788700	2.81720200
H	1.06307100	–3.12442200	–0.87087100

Table S20. Cartesian coordinates of the optimized global minimum of α–BA at χ = 172.9°.

Energy (in hartrees) = –986.4352208

Atom	X	Y	Z
O	–3.92384900	0.47496100	–1.12909800
C	–3.84080900	–0.81132800	–0.53206900
H	–4.64830600	–0.97565300	0.20004900
H	–3.89599000	–1.61119500	–1.28498100
C	–2.51138700	–0.94507000	0.19242600
H	–2.49489100	–1.91225400	0.70741200
O	–1.42131800	–0.94617800	–0.76945700
C	–0.69007900	0.31323100	–0.73041400
C	1.30816200	–1.17326800	–0.15910700
H	3.00754600	–2.26259800	0.25127400
C	3.59977300	–0.31559300	–0.01948700
C	1.67036900	1.18714600	–0.50787500
O	1.31831500	2.35779000	–0.71973600
C	–2.16355900	0.15957500	1.18220400
H	–3.05672900	0.57470400	1.66983500
C	–1.44881500	1.20344800	0.31158100
H	–2.18884500	1.80611800	–0.22259500
O	–0.63938600	1.99390200	1.15367500
H	0.00427700	2.45666400	0.58233600
O	–1.25021200	–0.37851800	2.12361800
H	–0.65320200	0.35856100	2.33856200
C	0.77511000	0.06393500	–0.42749700
O	0.63492700	–2.31361600	–0.09055400
H	–0.29959100	–2.06651400	–0.33084300
N	2.65672500	–1.33531600	0.05336300
O	4.78869000	–0.49529600	0.16200800
N	3.02965800	0.90980600	–0.31738300
H	3.66246300	1.69833600	–0.36276400
H	–0.77538900	0.76545800	–1.72384600
H	–4.71594500	0.51013100	–1.67852400

Table S21. Cartesian coordinates of the optimized global minimum of β–BA at χ = 186.1°.

Energy (in hartrees) = –986.440161

Atom	X	Y	Z
O	1.75585500	–1.91079200	1.41803500
C	2.74187700	–2.02323500	0.39910400
H	2.57141000	–2.91257100	–0.22779300
H	3.76050400	–2.09259900	0.81112300
C	2.65582300	–0.78522000	–0.47926900
H	3.38331500	–0.86860900	–1.29348900
O	1.32687000	–0.72492000	–1.06441600
C	0.63970800	0.47559000	–0.64011700
H	0.72788500	1.22822400	–1.43481000

C	–1.37068500	–1.06936200	–0.36244700
H	–3.08682800	–2.18766100	–0.12906500
C	–3.61591200	–0.22165800	0.13386700
C	–1.66013100	1.31241800	–0.06996900
O	–1.27356600	2.48620900	0.02539300
C	2.86299300	0.55036100	0.24226300
H	3.47940200	0.43014300	1.14491700
C	1.43147300	0.99843500	0.58175400
H	1.08475100	0.48975600	1.48873900
O	1.40499800	2.40306600	0.70653200
H	0.48935000	2.68765800	0.50365000
O	3.44431800	1.46472700	–0.66722200
H	3.04928400	2.32417300	–0.43621200
C	–0.81608300	0.18611000	–0.37010600
O	–0.72620300	–2.20741300	–0.58735700
H	0.21479300	–1.93998100	–0.76662400
N	–2.71164800	–1.24906500	–0.11781900
O	–4.79848800	–0.41504500	0.34014900
N	–3.01670600	1.02632400	0.12829100
H	–3.61933900	1.81130700	0.34045000
H	1.75929400	–2.71796200	1.94643400

Table S22. Cartesian coordinates of the optimized global minimum of 5′-methoxy α–BA at χ = 223.1°.

Energy (in hartrees) = –1025.722764

Atom	X	Y	Z
O	3.06752000	–1.47035800	0.69072900
C	3.32038700	–0.96885200	–0.61018000
H	3.22062700	–1.77095800	–1.36015300
H	4.34034900	–0.55609500	–0.69062100
C	2.31912500	0.13769100	–0.88912300
H	2.46940900	0.52707600	–1.90170200
O	0.97756400	–0.38525000	–0.80749100
C	0.31903900	0.19075500	0.35580500
C	–1.61369300	–1.22044500	–0.23742800
H	–3.22973300	–2.42694300	–0.66359600
C	–3.96788800	–0.62007700	–0.01252400
C	–2.14396700	1.03293300	0.46384000
O	–1.91919800	2.20796800	0.78111500
C	2.39456100	1.31605800	0.12529800
H	2.91930500	0.98058000	1.02451300
C	0.91289900	1.59396300	0.46178100
H	0.78171900	2.00638700	1.46898200
O	0.43918600	2.47876700	–0.53211200
H	–0.44960700	2.74522600	–0.22781900
O	3.06892200	2.44279300	–0.37576500
H	2.38443600	2.96024300	–0.83370900
C	–1.16655400	0.01334100	0.17574400

O	–0.82678700	–2.23523000	–0.58741700
H	0.07932600	–1.86132700	–0.73774400
N	–2.94770700	–1.51846100	–0.32093000
O	–5.14649600	–0.90597200	–0.09230900
N	–3.48377800	0.61559800	0.37499800
H	–4.18164000	1.31972500	0.57926300
H	0.65391300	–0.37953100	1.23756300
C	3.97690200	–2.48011500	1.08427900
H	3.93645200	–3.35015300	0.41038300
H	5.01316500	–2.10907500	1.10751700
H	3.69212700	–2.79837300	2.08969400

Table S23. Cartesian coordinates of the optimized global minimum of 5′-methoxy β–BA at χ = 155.4°.

Energy (in hartrees) = –1025.726573

Atom	X	Y	Z
O	2.43162300	1.40408300	0.17888500
C	3.15351000	0.67249500	–0.81030600
H	4.15500000	0.40951700	–0.44685000
H	3.24404100	1.28190800	–1.72104100
C	2.38405400	–0.60471100	–1.10931600
H	2.82334900	–1.06408100	–2.00417500
O	1.01270800	–0.25937000	–1.39067100
C	0.12548700	–1.11497900	–0.61699900
C	–1.34191600	0.92016900	–0.29442100
H	–2.65033800	2.48397000	0.01962200
C	–3.73332500	0.74999900	0.21208800
C	–2.33098300	–1.29198000	–0.14764000
O	–2.30494100	–2.51872300	–0.15605500
C	2.35139600	–1.63323400	0.07217500
H	2.45620800	–2.64242000	–0.34079700
C	0.92891400	–1.45487700	0.64805300
H	0.54387500	–2.35907200	1.12246600
O	0.92278800	–0.44218300	1.64144500
H	1.25636700	0.37999400	1.23479200
O	3.36593900	–1.44839000	1.03046600
H	2.94825200	–0.93256300	1.74162400
C	–1.18841600	–0.43517900	–0.39094400
O	–0.39107900	1.84234700	–0.45836800
H	0.42691600	1.38242600	–0.75547000
N	–2.56792500	1.47768500	–0.02027900
O	–4.79943200	1.28079300	0.46277800
N	–3.53743300	–0.61402100	0.12096200
H	–4.34791700	–1.19283300	0.29954100
H	–0.05601200	–2.04794300	–1.16695600
C	3.05485300	2.62001800	0.57125700
H	4.02873900	2.43303600	1.04346800
H	3.19823000	3.28537900	–0.29107900

H	2.38850500	3.10226400	1.28856000

Table S24. Cartesian coordinates of the optimized global minimum of α–MM at χ = 159.7° and ϕ = 17.6°.

Energy (in hartrees) = –942.83164

Atom	X	Y	Z
C	1.35408700	–0.46643200	–0.23154700
N	1.60160000	0.86442400	–0.26762300
C	2.91270100	1.18092700	–0.22179200
C	3.53941000	–0.97513300	–0.08266400
N	2.27791000	–1.43489300	–0.13515200
N	3.92897600	0.31446600	–0.13522600
N	4.52395200	–1.90170900	0.00354800
N	3.22188400	2.50176200	–0.23315400
N	0.05681500	–0.84251700	–0.27790200
H	5.46358100	–1.58855800	0.18141400
H	4.26739100	–2.85882400	0.17944200
H	4.18990000	2.75857500	–0.33466800
H	–0.13546700	–1.83291300	–0.25331200
H	2.50355000	3.16576200	–0.46986200
O	–4.43167500	0.81622800	–1.09292700
C	–4.44299900	–0.49750400	–0.55283400
H	–5.19266600	–0.51131200	0.24469700
H	–4.73955700	–1.23993800	–1.30945800
C	–3.08283900	–0.88467400	0.01571400
H	–3.10354200	–1.91796200	0.38144000
O	–2.12962500	–0.78965800	–1.08893900
C	–1.03617200	0.02213500	–0.72669800
C	–2.55486000	0.03345200	1.12555800
H	–3.36964800	0.60230900	1.59499100
C	–1.58245200	0.96276600	0.37485500
H	–2.16210700	1.75389100	–0.12033100
O	–0.62514900	1.48516500	1.26401100
H	0.23132700	1.53259600	0.78262700
O	–1.85164700	–0.74015100	2.08027400
H	–1.10183900	–0.17796900	2.34272000
H	–0.70182000	0.57715200	–1.61089500
H	–3.76354200	0.80057200	–1.79314500

Table S25. Cartesian coordinates of the optimized global minimum of β–MM at χ = 50.1° and ϕ = 13.4°.

Energy (in hartrees) = –942.83529

Atom	X	Y	Z
C	1.24476700	–0.82987200	–0.17460900
N	2.43260600	–1.41750200	–0.38087800

C	3.48650600	–0.61782100	–0.13120100
C	2.19874300	1.13958800	0.42312300
N	1.06037100	0.43090700	0.23827200
N	3.44229600	0.66842400	0.26097700
N	2.04946700	2.42644100	0.81004200
N	4.71635900	–1.16753400	–0.28124800
N	0.15001400	–1.62793200	–0.39662800
H	2.87075200	3.00758200	0.83599200
H	1.12950800	2.84665000	0.77278200
H	5.51813900	–0.55998700	–0.24935400
H	0.39422100	–2.47266100	–0.89335900
H	4.78656100	–2.07180000	–0.71737000
O	–1.00653800	2.22369800	0.34221600
C	–1.90299700	2.16351800	–0.75190700
H	–1.42611300	2.48162800	–1.69285000
H	–2.73036800	2.85349400	–0.54608600
C	–2.45951600	0.75708500	–0.95931100
H	–3.23180000	0.76925300	–1.73814000
O	–1.37254600	–0.09895000	–1.39484900
C	–1.22138600	–1.18615000	–0.49264200
C	–3.04115100	0.10611200	0.30837000
H	–3.37518400	0.85689300	1.03657500
C	–1.85977800	–0.71758800	0.82901400
H	–1.16939000	–0.07589700	1.38147800
O	–2.33296300	–1.79126600	1.62830500
H	–1.57515800	–2.34841700	1.84979700
O	–4.10342300	–0.75366700	–0.08425200
H	–4.15468000	–1.44428100	0.59421200
H	–0.34607700	1.49799900	0.21277400
H	–1.79556800	–2.05782400	–0.83659400

Table S26. Cartesian coordinates of the optimized global minimum of methoxy α–MM at χ = 300.9° and ϕ = 356.2°.

Energy (in hartrees) = –982.11929

Atom	X	Y	Z
C	–1.51412100	–0.82915000	–0.00495900
N	–2.64257600	–1.56035000	–0.02080200
C	–3.76424600	–0.84010100	–0.17443500
C	–2.66100900	1.11240600	–0.27822300
N	–1.46166200	0.50860400	–0.14288900
N	–3.84853400	0.49892800	–0.30714800
N	–2.64749200	2.46319300	–0.41728200
N	–4.93538300	–1.52291400	–0.17472800
N	–0.36661200	–1.53515500	0.15751200
H	–3.52978600	2.94444900	–0.35768500
H	–1.79894200	2.96817100	–0.21321800
H	–5.77662000	–1.03223500	–0.42765800
H	–0.52114200	–2.52995900	0.21072700

H	–4.90451900	–2.52792800	–0.21275000
O	3.98911200	–0.56956300	–0.02884900
C	3.60926200	0.30718100	–1.07644100
H	4.22856600	1.22131000	–1.06390300
H	3.74331300	–0.18046200	–2.05521900
C	2.14234300	0.68541500	–0.91490000
H	1.89208900	1.42144200	–1.68675700
O	1.29160400	–0.44947800	–1.11696000
C	0.99482700	–1.06846900	0.13839500
C	1.75966400	1.24118500	0.46527600
H	2.57491500	1.80170000	0.93045900
C	1.40335000	–0.04200700	1.26554300
H	2.30451700	–0.43036600	1.74393400
O	0.43467000	0.16638400	2.25805600
H	–0.05150000	0.96107000	1.98346400
O	0.63782100	2.10263800	0.38647500
H	–0.09820600	1.54149000	0.01738600
H	1.61010600	–1.96841800	0.24408700
C	5.32496100	–1.01896400	–0.13720500
H	5.49300000	–1.57368100	–1.07350700
H	6.04074300	–0.18280500	–0.09828500
H	5.51343200	–1.68474100	0.70820400

Table S27. Cartesian coordinates of the optimized global minimum of methoxy β–MM at χ = 190.7° and ϕ = 168.2°.

Energy (in hartrees) = –982.12039

Atom	X	Y	Z
C	–1.58841400	–0.49267500	–0.36820100
N	–1.88513900	0.74879400	0.08406400
C	–3.18591500	0.92628800	0.39422800
C	–3.71350100	–1.19607900	–0.12949300
N	–2.46126700	–1.50563700	–0.50001100
N	–4.14827800	–0.00070900	0.31558500
N	–4.63504600	–2.18950200	–0.19520900
N	–3.55558500	2.16505500	0.80860300
N	–0.30319200	–0.74188500	–0.70083400
H	–5.60551600	–1.94520800	–0.08782100
H	–4.38227000	–3.04076800	–0.66914800
H	–4.47651000	2.27015400	1.20154000
H	–0.08660200	–1.65701400	–1.06739100
H	–2.84290900	2.83746200	1.03929000
O	3.18355900	–1.37474600	0.90752100
C	3.85454500	–0.92029700	–0.25248700
H	3.96991700	–1.73733200	–0.98322500
H	4.86292800	–0.54706100	–0.00240600
C	3.05266700	0.20122000	–0.89094300
H	3.64113400	0.63409700	–1.70857300
O	1.83243800	–0.34333100	–1.44169500

C	0.71241200	0.28564200	–0.85469200
H	0.32817600	1.09112200	–1.50024200
C	2.63593700	1.32344900	0.07276700
H	3.30517700	1.38198700	0.94244600
C	1.20890400	0.91392100	0.46503800
H	1.23681400	0.13871300	1.23946300
O	0.46625600	2.05131000	0.85314500
H	–0.46955100	1.81319400	0.65678200
O	2.59774800	2.54957000	–0.63787800
H	1.83858500	3.02479900	–0.25716000
C	3.84415600	–2.44866100	1.54452700
H	3.24730000	–2.72505400	2.41681400
H	3.93276000	–3.32382000	0.88149800
H	4.85536700	–2.16736400	1.87954700