Supporting information

to the paper

Structural and energetic factors controlling the enantioselectivity of dinucleotide formation under prebiotic conditions

by

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Calculation of HF/6-31G* dipoles for ImpA and ImpU

Explanation of the homochiral selectivity on the basis of dipole moment calculations has some apparent weaknesses. Namely, definition of molecular dipoles is unambiguous only for neutral systems, otherwise it becomes dependent on the choice of the reference coordinate system.\textsuperscript{S1} Accordingly, only for neutral molecules we can unambiguously calculate the dipole moment. Quantum chemical softwares enable calculation of molecular dipoles also for charged systems, and these so-called field independent dipoles are often used in chemistry. The dipoles derived in this way can be used to provide qualitative information regarding the asymmetry of the charge distribution in molecules and molecular ions.

Joshi et al.\textsuperscript{S2} used HF/6-31G* calculations to estimate the dipole moments of the anionic and zwitterionic forms of ImpA and ImpU. The dipoles derived from these calculations can be considered only as very approximate, since an accurate description of the electronic structure of highly polarizable anionic species would require at least inclusion of diffuse functions into the basis set. Notwithstanding, we have tried to reproduce their HF/6-31G* dipole moments computed on optimized geometries obtained at the same level. Unfortunately, our dipole moments shown on Figure S1 are entirely different from those reported by Joshi et al. Mainly, there is not much difference between the dipole moments when going from adenine to uracil, and the direction of the dipoles is mainly dictated by the total charge of the model (i.e. whether or not the imidazole ring is protonated). In addition, the dipole moment vectors of the corresponding zwitterionic and anionic species are not parallel, as was observed for ImpA by Joshi et al. We suspect that delicate conformational changes within the activated nucleotides might have a severe impact on the dipole moments, which could be also the reason for the difference between our computed results and those reported by Joshi et al. This, on the other hand, points at another weakness of the interpretation of the homochiral selectivity on the basis of dipole moments.

\textbf{Figure S1.} Computed HF/6-31G* dipole moments for the anionic (blue) and zwitterionic (red) forms of ImpA (left) and ImpU (right).

\textbf{References:}


Figure S2. Optimized geometry of the syn D,D c-di-AMP model computed at TPSS/TZVP level of theory.
Figure S3. Overlay of (a) D,L c-di-AMP (blue) and D,L c-UMP-AMP (red) as well as (b) D,D c-di-AMP (blue) and D,D c-AMP-UMP (red) computed at TPSS-D3(BJ)/def2-TZVPPD level of theory. In (a) the minor deviation of the two structures is caused by a subtle C2’-endo /C3’-endo conformational change at the L AMP unit.
Optimized geometries of all structures reported in the paper:

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D,L c-di-AMP, TPSS-D3(BJ)/def2-TZVPPD level, full optimization, gas-phase

H 0.8004 -0.5512 -1.4489
H 1.8762 -2.2748 -0.1209
H 3.8400 -3.1506 -0.8170
H -1.8832  2.2771 -0.0215
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics
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D,L c-di-AMP, TPSS-D3(BJ)/def2-TZVPPD level, full optimization, COSMO

\[
\begin{align*}
\text{C} & \quad 3.6428 \quad 1.3375 \quad 1.6668 \\
\text{N} & \quad 4.3270 \quad 0.3183 \quad 0.8512 \\
\text{C} & \quad 3.8776 \quad -0.9351 \quad 0.4793 \\
\text{N} & \quad 4.7394 \quad -1.5866 \quad -0.2840 \\
\text{C} & \quad 5.8093 \quad -0.7132 \quad -0.4238 \\
\text{C} & \quad 7.0374 \quad -0.8006 \quad -1.1131 \\
\text{N} & \quad 7.4203 \quad -1.8959 \quad -1.8039 \\
\text{N} & \quad 7.8824 \quad 0.2575 \quad -1.0512 \\
\text{C} & \quad 7.5200 \quad 1.3370 \quad -0.3368 \\
\text{H} & \quad 8.2401 \quad 2.1514 \quad -0.3244 \\
\text{N} & \quad 6.3895 \quad 1.5410 \quad 0.3558 \\
\text{C} & \quad 5.5718 \quad 0.4760 \quad 0.2746 \\
\text{H} & \quad 2.9147 \quad -1.3027 \quad 0.8065 \\
\text{H} & \quad 8.2410 \quad -1.8431 \quad -2.3921 \\
\text{H} & \quad 6.7519 \quad -2.6298 \quad -1.9916 \\
\text{H} & \quad 4.4071 \quad 1.8081 \quad 2.2896 \\
\text{O} & \quad 0.7518 \quad -1.0187 \quad 1.935 \\
\text{C} & \quad 0.3735 \quad -0.0409 \quad 2.1777 \\
\text{C} & \quad 1.3280 \quad 1.1285 \quad 2.0894 \\
\text{O} & \quad 2.6672 \quad 0.7083 \quad 2.4850 \\
\text{C} & \quad 1.5257 \quad 1.7118 \quad 0.6908 \\
\text{O} & \quad 0.4610 \quad 2.5946 \quad 0.3495 \\
\text{C} & \quad 2.9007 \quad 2.3747 \quad 0.7986 \\
\text{O} & \quad 2.7554 \quad 3.6047 \quad 1.5067 \\
\text{H} & \quad -0.6415 \quad 0.3214 \quad 1.9807 \\
\text{H} & \quad 0.4011 \quad -0.4776 \quad 3.1796
\end{align*}
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D,D c-di-UMP, TPSS-D3(BJ)/def2-TZVPPD level, full optimization, gas-phase
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D,D c-di-UMP, TPSS-D3(BJ)/def2-TZVPPD level, constrained optimization, gas-phase

| P  | 1.1887 | -2.9830 | -1.5255 |
| O  | 1.7127 | -3.7074 | -2.7146 |
| O  | 0.6823 | -3.6460 | -0.2712 |
| O  | -0.0298 | -1.9524 | -1.9753 |
| C  | 0.0807 | -1.3011 | -3.2516 |
| C  | -0.7151 | -0.0076 | -3.2330 |
| O  | -2.1285 | -0.2967 | -3.0760 |
| C  | -0.3416 | 0.9400  | -2.0940 |
| O  | 0.6786 | 1.8121  | -2.5671 |
| C  | -1.6801 | 1.6040  | -1.6666 |
| O  | -1.9008 | 2.8614  | -2.2701 |
| C  | -2.7435 | 0.6103  | -2.1749 |
| C  | -3.1530 | -1.9630 | 0.5250  |
| C  | -4.5047 | -1.7632 | 0.9834  |
| O  | -5.1092 | -2.3813 | 1.8632  |
| N  | -5.1658 | -0.7262 | 0.2884  |
| C  | -4.6920 | 0.0778  | -0.7380 |
| O  | -5.3920 | 0.9328  | -1.2736 |
| N  | -3.3708 | -0.1914 | -1.0874 |
| C  | -2.6531 | -1.1930 | -0.4750 |
| H  | 1.1281  | -1.0599 | -3.4677 |
| H  | -0.2889 | -1.9757 | -4.0311 |
| H  | -0.5659 | 0.5153  | -4.1866 |
| H  | 0.0305  | 0.3581  | -1.2467 |
| H  | -1.1804 | 3.4174  | -1.8634 |
| H  | -3.5650 | 1.1462  | -2.6504 |
| P  | 1.3576  | 2.9076  | -1.5229 |
| O  | 0.2364  | 3.6163  | -0.8092 |
| O  | 2.4430  | 3.5872  | -2.2798 |
| O  | 2.0046  | 1.8925  | -0.3827 |
| C  | 3.2228  | 1.2043  | -0.7107 |
| C  | 3.3233  | -0.0693 | 0.1107  |
| O  | 3.4376  | 0.2566  | 1.5203  |
| C  | 2.1131  | -0.9932 | -0.0194 |
| O  | 2.3670  | -1.9017 | -1.0847 |
| C  | 1.9256  | -1.6133 | 1.3930  |
| O  | 2.5316  | -2.8809 | 1.5342  |
| C  | 2.6436  | -0.6091 | 2.3161  |
| C  | 0.1305  | 2.0527  | 3.1420  |
| C  | -0.0789 | 1.8953  | 4.5591  |
| O  | -0.8165 | 2.5530  | 5.2974  |
| N  | 0.6967  | 0.8506  | 5.1093  |
| C  | 1.5975  | 0.0056  | 4.4778  |
| O  | 2.2276  | -0.8521 | 5.0903  |
| N  | 1.7087  | 0.2378  | 3.1089  |
| C  | 1.0021  | 1.2425  | 2.4888  |
D.D c-di-UMP, TPSS-D3(BJ)/def2-TZVPPD level, full optimization, COSMO

p  -0.96882817  -2.754665305 -2.113942619
o  -1.466509977 -3.258919635 -3.410145864
o  -0.933107261 -3.603103481 -0.903374591
o  -1.781394079 -1.407684461 -1.668482025
c -2.319360311 -0.477034838 -2.606444165
c -2.515819731  0.859317988 -1.934883564
o  -3.356796895  0.700201849 -0.773580859
c -1.255984045  1.528777325 -1.403582616
o -0.535156561  2.141015126 -2.44463182
o -1.828513187  2.467785048 -0.350638305
c -2.451459399  3.591929453 -0.959338755
c -2.913820416  1.560349174  0.24353468
o -1.540038745 -1.315345652  2.224928266
c -1.523932348 -0.776427497  3.53360348
o -1.189800467 -1.365655709  4.549950104
n -1.942269007  0.563054125  3.598114331
c -2.366736984  1.368704271  2.582651005
o -2.695536906  2.545758153  2.733443766
n -2.394309683  0.741316232  1.364299154
c -1.981417356 -0.556251222  1.20885035
h -1.634670394 -0.338107396 -3.434342172
h -3.271386951 -0.861315104 -2.975811862
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h -3.748909219  2.138289087  0.630169442
p  0.959764073  2.756234835 -2.123122423
o  0.907414571  3.614046071 -0.91891564
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c 1.257465562 -1.540625154 -1.38974847
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D,L c-di-UMP, TPSS-D3(BJ)/def2-TZVPPD level, full optimization, gas-phase

C 5.3434980 -1.6210180 -0.5141300
C 6.7343260 -1.2515690 -0.5916230
O 7.6722630 -1.9120260 -1.0481490
N 6.9881280 0.0288310 -0.0543790
C 6.0997310 0.9284240 0.5207550
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N 4.7796210 0.4850330 0.5027380
C 4.4415110 -0.7602940 0.0225050
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H 4.2279130 2.2205160 1.4762630
O 1.4582000 -1.4823880 0.8519410
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D,D c-AMP-UMP, TPSS-D3(BJ)/def2-TZVP/PP level, full optimization, gas-phase

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D,L c-UMP-AMP, TPSS-D3(BJ)/def2-TZVPPD level, full optimization, gas-phase

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Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics
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Sugar-phosphate ring model, Figure 4a, TPSS-D3(BJ)/def2-TZVPPD level, gas-phase

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Sugar-phosphate ring model, Figure 4b, TPSS-D3(BJ)/def2-TZVPPD level, gas-phase

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Sugar-phosphate ring model, Figure 4c, TPSS-D3(BJ)/def2-TZVPPD level, gas-phase

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics
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Sugar-phosphate ring model, Figure 4c, TPSS-D3(BJ)/def2-TZVPPD level, gas-phase

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Sugar-phosphate ring model, Figure 4d, TPSS-D3(BJ)/def2-TZVPPD level, gas-phase

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