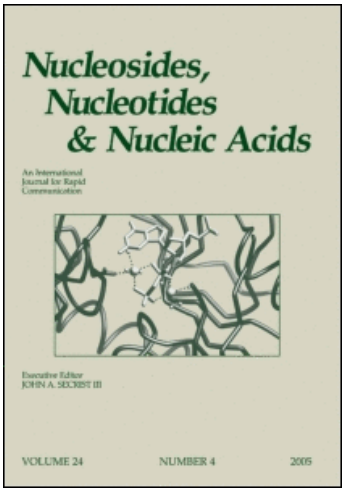

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ERRATUM

The following additional material was provided by Dr. Wilson when it was discovered that it was inadvertently not included in the draft that was published (N & N, 9, 479).

FURTHER COMMENTS ON THE CONTRIBUTION OF EXOCYCLIC SUBSTITUENTS TO BASE-PAIR PROPELLER TWIST

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Abstract

The arguments and results regarding base-pair propeller twisting calculated excluding the exocyclic base atoms are restated, updating the results given previously[1].

Introduction

In a recent paper[1], the propeller twists in a series of base-paired nucleic acid components were surveyed. It was found that the value of propeller twist was significantly affected by the exclusion of exocyclic base atoms from the calculations. The aim of this note is to amplify and clarify these previous results.

TABLE 1 - Selected average propeller twist (PT) values

Material	Type of Pair	Number of base-pairs	PT with exo atoms in planes	PT without exo atoms in planes
Nucleosides	All	54	14.7°	14.0°
and	R-R	38	15.7°	15.4°
Nucleotides	Y-Y	16	12.1°	10.5°
Nucleic	All	37	4.4°	4.3°
Acid	Homo	12	1.6°	1.3°
Bases	Hetero	25	5.8°	5.7°

Note - trends within the other classifications are discussed in the text

Results

Further analysis of the results presented previously[1] yielded the results shown in Table 1.

The most noticeable feature of the data, indicated in Table 1, is the very small but systematic reduction of the average propeller twist value in the base-pairs analysed when exocyclic atoms are removed from the base-pair system. This implies that the exocyclic atoms do tend to deviate slightly more than the others from the mean base plane.

The following general trends regarding the effect of removing exocyclic atoms from the calculated base-planes can also be discerned from the data for nucleosides and nucleotides (further to those given in Table 1) :

(i) Y-Y (pyrimidine-pyrimidine) pairs show a greater reduction (12.1° to 10.5°) than R-R (purine-purine) pairs (15.7° to 15.4°);

(ii) U-U pairs show the largest reduction of all (14.9° to 11.9°);

(iii) In the Wilson-Tollin (WT) classification[2], WT(I) [pyrimidine-pyrimidine] reduces most (12.1° to 10.5°, as in (i) above), with WT(VI) ["double-Hoogsteen"] next (15.5° to 14.0°);

(iv) For the Hobsza-Sandorfy (HS) classes[3], the TT(II) (22.8° to 18.0°) and TT(III) (16.9° to 15.0°) groups (comprised mainly of U-U pairs) show the most reduction, with AA(III) [exactly equivalent to WT(VI), see (iii) above, in these data] next.

The overall reduction in propeller twist value for nucleic acid bases is considerably smaller and consequently no notable trends in the reduction of twist in these materials can be discerned.

It is clear from these results that the average propeller twist decreases *more* on exclusion of exocyclic atoms for the least aromatic bases (pyrimidines) than for the more aromatic purines. This is as one would expect, since the additional deviation of exocyclic atoms from the base plane should tend to be more pronounced in the former case. The deviation of exocyclic atoms appears to be on average further out of the plane of the base-*pair*, as opposed to just the plane of the parent base, reflected in the systematic, if small, reduction in propeller twist value obtained when these atoms are excluded from the calculations.

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