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# Yeast phenylalanine transfer RNA: atomic coordinates and torsion angles

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## ABSTRACT

The atomic coordinates of yeast phenylalanine transfer RNA (tRNA) as well as the torsion angles of the polynucleotide chain are presented as derived from an x-ray diffraction analysis of orthorhombic crystals. A comparison is made between the coordinates obtained from analysis of monoclinic crystals of the same material. It is concluded that the molecule has substantially the same form in the orthorhombic and the monoclinic lattices, except for differences found between residues at the 3' end of the polynucleotide chain. A number of observations are made concerning hydrogen bonding interactions which may account for many of the residues conserved in all tRNA sequences.

## INTRODUCTION

Approximately three years ago, the folding of the polynucleotide chain of yeast phenylalanine tRNA was described from a 4Å x-ray diffraction analysis of orthorhombic crystals (1). It was shown that the molecule was bent into an L-shape with the acceptor and TψC stems of the familiar tRNA cloverleaf forming one limb, while the D stem and the anticodon stem form the other limb. In this conformation, the 3' acceptor terminus is at one end of the L-shaped molecule 75Å from the anticodon at the other end. Somewhat over a year ago, the tertiary interactions in this molecule were described in an analysis at 3Å resolution of the orthorhombic crystals (2). At the same time, a similar 3Å resolution analysis of the monoclinic crystal form was reported in which most of the polynucleotide chain was traced with the exception of the interactions between the TψC and D loops at the corner of the L-shaped molecule (3).

X-ray diffraction data from orthorhombic crystals have been obtained to 2.5Å resolution (4). The 2.7Å data have been analyzed by two independent refinement methods to obtain preliminary atomic coordinates. The results of these analyses are presented here and in another paper (5). These two independent refinements have produced similar sets of atomic coordinates. Recently, atomic coordinates from the monoclinic crystal have been published (6). The coordinates from these two crystal forms are compared here and it is shown that the structures are almost identical in the orthorhombic and monoclinic lattices with the exception of the conformation near the 3' end of the polynucleotide chain.

## RESULTS

The atomic coordinates of yeast phenylalanine tRNA are presented in Table 1. The general conformation of the molecule including the secondary and tertiary interactions has been described earlier (1,2,7). Rough coordinates were measured in an optical comparitor and these coordinates were refined using a method similar to that described by Huber et al. (8), coupled with extensive idealization. At this stage in the refinement, the R factor is 0.33 at 3Å and 0.35 at 2.7Å. The positions of most of the residues in the polynucleotide chain are well defined, with the exception of residues 16, 17, 47 and 76 where the electron density is consistently weak and diffuse. Thus, it is possible that these may change their conformation slightly upon further refinement. We do not anticipate substantial changes in the atomic positions of the other residues. Most of the ribose residues in the molecule are in

Table 1. Atomic Coordinates of Yeast Phenylalanine tRNA

The Cartesian x, y, z coordinates, with distances in angstroms, correspond to the a, b and c axes of the orthorhombic unit cell (1). The origin of the unit cell is taken as the origin of the coordinate system. These coordinates have been deposited in the Protein Data Bank at Brookhaven National Laboratories, Upton, Long Island, New York (11). They can also be obtained upon request from the authors. The oxygen atoms attached to the phosphorus atom are labeled O1P and O2P, such that when the phosphate group is viewed from the O5' position, the atoms O3', O1P and O2P are organized in a clockwise arrangement. Methyl groups are designated as M, followed by the numbering of the atoms to which the methyl groups are attached.

Table 1

| | X | Y | Z |
|---|---|---|---|
| 1 | GUANOSINE | | |
| O1′ | 21.9 | 31.6 | 64.8 |
| C1′ | 20.8 | 30.7 | 65.2 |
| C2′ | 21.4 | 29.3 | 65.5 |
| O2′ | 21.8 | 29.4 | 66.9 |
| C3′ | 22.7 | 29.3 | 64.7 |
| O3′ | 23.7 | 28.5 | 65.2 |
| C4′ | 23.2 | 30.8 | 64.8 |
| C5′ | 24.1 | 31.3 | 63.7 |
| O5′ | 23.4 | 31.1 | 62.4 |
| P | 24.3 | 31.8 | 61.2 |
| O1P | 25.1 | 32.3 | 62.3 |
| O2P | 23.4 | 30.7 | 61.4 |
| N2 | 16.2 | 28.6 | 65.8 |
| O6 | 16.3 | 29.7 | 61.5 |
| C6 | 16.8 | 29.7 | 62.6 |
| N1 | 16.2 | 29.1 | 63.6 |
| C2 | 16.8 | 29.0 | 64.8 |
| N3 | 18.0 | 29.4 | 65.2 |
| C4 | 18.6 | 30.0 | 64.1 |
| C5 | 18.2 | 30.2 | 62.8 |
| N7 | 19.1 | 30.8 | 62.0 |
| C8 | 20.1 | 31.0 | 62.8 |
| N9 | 19.9 | 30.6 | 64.1 |
| 2 | CYTIDINE | | |
| O1′ | 20.2 | 25.2 | 66.5 |
| C1′ | 19.2 | 24.5 | 65.9 |
| C2′ | 19.8 | 23.1 | 65.5 |
| O2′ | 19.7 | 22.2 | 66.6 |
| C3′ | 21.3 | 23.5 | 65.3 |
| O3′ | 22.2 | 22.4 | 65.5 |
| C4′ | 21.5 | 24.5 | 66.5 |
| C5′ | 22.6 | 25.5 | 66.3 |
| O5′ | 22.5 | 26.1 | 65.0 |
| P | 23.9 | 27.0 | 64.7 |
| O1P | 25.1 | 26.5 | 65.4 |
| O2P | 23.8 | 27.0 | 63.3 |
| C6 | 19.2 | 26.6 | 64.3 |
| C5 | 18.9 | 27.2 | 63.2 |
| N4 | 17.7 | 27.1 | 61.0 |
| C4 | 18.0 | 26.6 | 62.3 |
| N3 | 17.5 | 25.4 | 62.7 |
| O2 | 17.2 | 23.7 | 64.1 |
| C2 | 17.7 | 24.7 | 63.8 |
| N1 | 18.7 | 25.3 | 64.7 |
| 3 | GUANOSINE | | |
| O1′ | 18.9 | 20.4 | 64.0 |
| C1′ | 18.1 | 20.2 | 62.8 |
| C2′ | 18.7 | 19.0 | 62.0 |
| O2′ | 18.0 | 17.9 | 62.4 |
| C3′ | 20.1 | 19.0 | 62.5 |
| O3′ | 20.7 | 17.8 | 62.4 |
| C4′ | 19.9 | 19.4 | 64.0 |
| C5′ | 21.2 | 20.0 | 64.6 |
| O5′ | 22.0 | 20.5 | 63.6 |
| P | 22.9 | 21.7 | 64.3 |
| O1P | 24.2 | 21.3 | 64.8 |
| O2P | 22.8 | 22.7 | 63.2 |
| N2 | 14.6 | 21.5 | 59.3 |
| O6 | 17.5 | 24.9 | 59.1 |
| C6 | 17.2 | 23.8 | 59.6 |
| N1 | 16.0 | 23.2 | 59.1 |
| C2 | 15.6 | 22.0 | 59.6 |
| N3 | 16.2 | 21.3 | 60.6 |
| C4 | 17.3 | 21.9 | 61.0 |
| C5 | 17.9 | 23.1 | 60.6 |
| N7 | 19.0 | 23.4 | 61.2 |
| C8 | 19.2 | 22.3 | 62.1 |
| N9 | 18.2 | 21.4 | 62.0 |
| 4 | GUANOSINE | | |
| O1′ | 17.2 | 17.2 | 59.6 |
| C1′ | 16.6 | 17.6 | 58.3 |
| C2′ | 17.2 | 16.5 | 57.3 |
| O2′ | 16.3 | 15.4 | 57.3 |
| C3′ | 18.5 | 16.1 | 58.0 |
| O3′ | 18.9 | 14.8 | 57.7 |
| C4′ | 18.0 | 16.1 | 59.5 |
| C5′ | 19.1 | 16.2 | 60.6 |
| O5′ | 20.3 | 16.8 | 59.9 |
| P | 21.4 | 17.2 | 61.1 |
| O1P | 22.2 | 16.1 | 61.5 |
| O2P | 22.0 | 18.4 | 60.4 |
| N2 | 14.8 | 20.0 | 54.2 |
| O6 | 17.8 | 22.9 | 55.9 |
| C6 | 17.2 | 21.8 | 55.9 |
| N1 | 16.3 | 21.5 | 55.0 |
| C2 | 15.7 | 20.3 | 55.0 |
| N3 | 15.8 | 19.3 | 55.9 |
| C4 | 16.7 | 19.6 | 56.8 |
| C5 | 17.5 | 20.8 | 56.9 |
| N7 | 18.3 | 20.8 | 58.0 |
| C8 | 18.1 | 19.6 | 58.6 |
| N9 | 17.1 | 18.9 | 58.0 |
| 5 | ADENOSINE | | |
| O1′ | 16.9 | 16.2 | 54.4 |
| C1′ | 16.9 | 17.2 | 53.4 |
| C2′ | 17.4 | 16.5 | 52.1 |
| O2′ | 16.2 | 16.0 | 51.5 |
| C3′ | 18.2 | 15.4 | 52.6 |
| O3′ | 18.3 | 14.3 | 51.7 |
| C4′ | 17.4 | 14.9 | 53.9 |
| C5′ | 18.2 | 14.1 | 54.9 |
| O5′ | 19.4 | 14.8 | 55.1 |
| P | 20.0 | 14.5 | 56.6 |
| O1P | 20.4 | 13.1 | 56.8 |
| O2P | 20.9 | 15.6 | 56.7 |
| N6 | 20.3 | 22.1 | 54.1 |
| C6 | 19.4 | 21.4 | 53.5 |
| N1 | 18.7 | 21.9 | 52.4 |
| C2 | 17.7 | 21.2 | 51.8 |
| N3 | 17.3 | 19.9 | 52.1 |
| C4 | 18.0 | 19.5 | 53.2 |
| C5 | 19.0 | 20.0 | 53.9 |
| N7 | 19.5 | 19.3 | 54.9 |
| C8 | 18.7 | 18.2 | 54.8 |
| N9 | 17.9 | 18.2 | 53.8 |
| 6 | URIDINE | | |
| O1′ | 18.1 | 17.0 | 48.8 |
| C1′ | 18.8 | 18.2 | 48.3 |
| C2′ | 19.6 | 17.7 | 47.0 |
| O2′ | 18.8 | 17.8 | 45.9 |
| C3′ | 19.8 | 16.2 | 47.4 |
| O3′ | 20.0 | 15.4 | 46.2 |
| C4′ | 18.4 | 15.9 | 48.0 |
| C5′ | 18.5 | 14.6 | 48.9 |
| O5′ | 19.7 | 14.5 | 49.5 |
| P | 19.6 | 13.8 | 51.0 |
| O1P | 19.5 | 12.3 | 50.9 |
| O2P | 20.6 | 14.5 | 51.7 |
| C6 | 19.9 | 17.9 | 50.6 |
| C5 | 20.8 | 18.2 | 51.5 |
| O4 | 22.6 | 19.7 | 52.0 |
| C4 | 21.7 | 19.3 | 51.2 |
| N3 | 21.5 | 20.0 | 50.0 |
| O2 | 20.5 | 20.3 | 48.0 |
| C2 | 20.5 | 19.6 | 49.1 |
| N1 | 19.8 | 18.6 | 49.4 |
| 7 | URIDINE | | |
| O1′ | 21.6 | 19.6 | 44.2 |
| C1′ | 23.1 | 19.7 | 44.1 |
| C2′ | 23.5 | 18.4 | 43.4 |
| O2′ | 24.6 | 18.7 | 42.6 |
| C3′ | 22.3 | 18.1 | 42.6 |
| O3′ | 22.2 | 18.9 | 41.4 |
| C4′ | 21.1 | 18.5 | 43.5 |
| C5′ | 20.8 | 17.4 | 44.6 |
| O5′ | 21.8 | 16.4 | 44.5 |
| P | 21.4 | 15.2 | 45.6 |
| O1P | 21.3 | 13.8 | 44.9 |
| O2P | 22.3 | 15.5 | 46.6 |
| C6 | 23.2 | 18.7 | 46.5 |
| C5 | 23.7 | 18.6 | 47.7 |
| O4 | 25.3 | 19.5 | 49.2 |
| C4 | 24.7 | 19.5 | 48.1 |
| N3 | 25.0 | 20.5 | 47.2 |
| O2 | 24.8 | 21.5 | 45.1 |
| C2 | 24.4 | 20.6 | 45.9 |
| N1 | 23.5 | 19.7 | 45.6 |
| 8 | URIDINE | | |
| O1′ | 25.8 | 15.4 | 39.9 |
| C1′ | 25.4 | 14.2 | 39.2 |
| C2′ | 25.3 | 14.5 | 37.7 |
| O2′ | 26.6 | 14.3 | 37.1 |
| C3′ | 24.9 | 16.0 | 37.7 |
| O3′ | 25.3 | 16.7 | 36.6 |
| C4′ | 25.8 | 16.5 | 38.9 |
| C5′ | 25.3 | 17.8 | 39.5 |
| O5′ | 24.0 | 17.6 | 39.9 |
| P | 23.4 | 19.1 | 40.4 |
| O1P | 24.4 | 19.9 | 41.1 |
| O2P | 22.8 | 19.5 | 39.2 |
| C6 | 23.3 | 14.6 | 40.5 |
| C5 | 22.0 | 14.3 | 40.9 |
| O4 | 20.4 | 12.6 | 40.7 |
| C4 | 21.5 | 13.0 | 40.5 |
| N3 | 22.4 | 12.2 | 39.8 |
| O2 | 24.3 | 11.8 | 38.8 |
| C2 | 23.7 | 12.5 | 39.4 |
| N1 | 24.1 | 13.8 | 39.8 |
| 9 | ADENOSINE | | |
| O1′ | 25.7 | 16.6 | 31.5 |
| C1′ | 24.7 | 16.6 | 30.6 |
| C2′ | 23.6 | 17.6 | 31.1 |
| O2′ | 23.1 | 18.3 | 29.9 |
| C3′ | 24.5 | 18.6 | 31.9 |
| O3′ | 25.3 | 19.4 | 31.1 |
| C4′ | 25.5 | 17.6 | 32.6 |
| C5′ | 24.9 | 16.9 | 33.8 |
| O5′ | 24.1 | 17.8 | 34.5 |
| P | 24.6 | 17.9 | 36.1 |
| O1P | 25.5 | 19.1 | 36.3 |
| O2P | 23.3 | 17.9 | 36.7 |
| N6 | 23.2 | 10.7 | 30.3 |
| C6 | 24.1 | 11.8 | 30.2 |
| N1 | 25.4 | 11.5 | 29.9 |
| C2 | 26.2 | 12.6 | 29.8 |
| N3 | 26.0 | 13.9 | 30.0 |
| C4 | 24.7 | 14.1 | 30.3 |
| C5 | 23.7 | 13.1 | 30.5 |
| N7 | 22.5 | 13.7 | 30.8 |
| C8 | 22.8 | 15.0 | 30.9 |
| N9 | 24.1 | 15.3 | 30.6 |
| 10 | 2m-GUANOSINE | | |
| O1′ | 22.5 | 22.7 | 29.1 |
| C1′ | 21.4 | 22.4 | 28.3 |
| C2′ | 20.1 | 22.6 | 29.2 |
| O2′ | 19.7 | 24.0 | 29.0 |
| C3′ | 20.7 | 22.5 | 30.6 |
| O3′ | 20.0 | 23.2 | 31.6 |
| C4′ | 22.1 | 23.1 | 30.5 |
| C5′ | 23.1 | 22.7 | 31.5 |
| O5′ | 23.3 | 21.3 | 31.4 |
| P | 24.9 | 20.9 | 30.8 |
| O1P | 25.0 | 21.2 | 29.4 |
| O2P | 25.6 | 21.7 | 31.8 |
| M2 | 16.8 | 21.2 | 27.6 |
| N2 | 17.2 | 19.9 | 27.2 |
| O6 | 20.4 | 16.8 | 26.8 |
| C6 | 20.0 | 18.0 | 27.1 |
| N1 | 18.7 | 18.3 | 27.0 |
| C2 | 18.3 | 19.5 | 27.3 |
| N3 | 19.1 | 20.6 | 27.7 |
| C4 | 20.4 | 20.3 | 27.7 |
| C5 | 20.9 | 19.0 | 27.4 |
| N7 | 22.3 | 19.1 | 27.5 |
| C8 | 22.5 | 20.3 | 27.9 |
| N9 | 21.4 | 21.0 | 28.0 |
| 11 | CYTIDINE | | |
| O1′ | 16.5 | 21.8 | 31.8 |
| C1′ | 15.8 | 20.6 | 31.7 |
| C2′ | 15.1 | 20.4 | 33.1 |
| O2′ | 13.8 | 21.0 | 33.0 |
| C3′ | 16.0 | 21.2 | 34.0 |
| O3′ | 15.4 | 21.7 | 35.1 |
| C4′ | 16.4 | 22.4 | 33.1 |
| C5′ | 17.6 | 23.2 | 33.5 |
| O5′ | 18.7 | 22.2 | 33.7 |
| P | 20.1 | 22.8 | 33.2 |
| O1P | 20.6 | 24.0 | 33.8 |
| O2P | 20.8 | 21.6 | 33.2 |
| C6 | 18.3 | 19.7 | 31.3 |
| C5 | 19.2 | 18.8 | 31.2 |
| N4 | 19.7 | 16.4 | 31.4 |
| C4 | 18.8 | 17.4 | 31.4 |
| N3 | 17.5 | 17.2 | 31.4 |
| O2 | 15.3 | 17.8 | 31.6 |
| C2 | 16.5 | 18.1 | 31.5 |
| N1 | 16.9 | 19.5 | 31.5 |
| 12 | URIDINE | | |
| O1′ | 13.5 | 17.2 | 35.4 |
| C1′ | 14.0 | 15.9 | 35.5 |
| C2′ | 14.0 | 15.5 | 37.1 |
| O2′ | 12.7 | 15.0 | 37.4 |
| C3′ | 14.2 | 16.9 | 37.7 |
| O3′ | 13.7 | 17.1 | 39.0 |
| C4′ | 13.3 | 17.8 | 36.7 |
| C5′ | 13.6 | 19.3 | 36.7 |
| O5′ | 15.0 | 19.4 | 36.5 |
| P | 15.4 | 21.0 | 36.5 |
| O1P | 14.6 | 21.8 | 37.4 |
| O2P | 16.8 | 20.9 | 36.8 |
| C6 | 16.2 | 17.0 | 34.9 |
| C5 | 17.5 | 17.0 | 34.5 |
| O4 | 19.2 | 15.5 | 33.9 |
| C4 | 18.0 | 15.7 | 34.2 |
| N3 | 17.2 | 14.6 | 34.3 |
| O2 | 15.2 | 13.6 | 34.8 |
| C2 | 15.9 | 14.6 | 34.7 |
| N1 | 15.4 | 15.9 | 35.0 |
| 13 | CYTIDINE | | |
| O1′ | 15.6 | 12.8 | 37.3 |
| C1′ | 16.7 | 11.8 | 37.3 |
| C2′ | 16.7 | 11.4 | 38.9 |
| O2′ | 15.8 | 10.3 | 39.0 |
| C3′ | 16.2 | 12.6 | 39.6 |
| O3′ | 15.5 | 12.3 | 40.8 |
| C4′ | 15.0 | 13.0 | 38.6 |
| C5′ | 14.6 | 14.5 | 38.7 |
| O5′ | 15.2 | 15.0 | 39.9 |
| P | 14.4 | 16.5 | 40.2 |
| O1P | 13.4 | 16.4 | 41.3 |
| O2P | 15.6 | 17.3 | 40.4 |
| C6 | 18.1 | 14.0 | 36.9 |
| C5 | 19.2 | 14.7 | 36.7 |
| N4 | 21.7 | 14.4 | 36.4 |
| C4 | 20.4 | 13.9 | 36.5 |
| N3 | 20.3 | 12.5 | 36.4 |
| O2 | 19.0 | 10.7 | 36.5 |
| C2 | 19.1 | 11.9 | 36.6 |
| N1 | 18.0 | 12.6 | 37.0 |
| 14 | ADENOSINE | | |
| O1′ | 18.0 | 8.6 | 39.5 |
| C1′ | 18.9 | 7.7 | 38.8 |
| C2′ | 19.1 | 6.5 | 39.7 |
| O2′ | 18.0 | 5.5 | 39.3 |

Table 1 (continued)

| | X | Y | Z |
|---|---|---|---|
| C3′ | 18.8 | 7.0 | 41.1 |
| O3′ | 18.4 | 6.1 | 42.0 |
| C4′ | 17.6 | 8.0 | 40.8 |
| C5′ | 17.4 | 9.1 | 41.8 |
| O5′ | 17.4 | 10.4 | 41.1 |
| P | 16.2 | 11.3 | 41.8 |
| O1P | 15.0 | 10.5 | 42.4 |
| O2P | 17.0 | 12.1 | 42.7 |
| N6 | 24.4 | 9.5 | 37.4 |
| C6 | 23.4 | 8.6 | 37.4 |
| N1 | 23.6 | 7.4 | 36.9 |
| C2 | 22.6 | 6.5 | 36.9 |
| N3 | 21.4 | 6.6 | 37.4 |
| C4 | 21.2 | 7.9 | 38.0 |
| C5 | 22.1 | 8.9 | 38.0 |
| N7 | 21.6 | 10.0 | 38.6 |
| C8 | 20.4 | 9.6 | 38.9 |
| N9 | 20.1 | 8.4 | 38.6 |
| **15** | **GUANOSINE** | | |
| O1′ | 22.2 | 5.1 | 40.6 |
| C1′ | 23.5 | 5.6 | 40.5 |
| C2′ | 24.4 | 4.8 | 41.5 |
| O2′ | 24.8 | 3.6 | 40.7 |
| C3′ | 23.4 | 4.4 | 42.5 |
| O3′ | 23.7 | 3.2 | 43.2 |
| C4′ | 22.1 | 4.1 | 41.6 |
| C5′ | 20.8 | 4.1 | 42.3 |
| O5′ | 20.7 | 5.4 | 43.0 |
| P | 19.1 | 5.8 | 43.3 |
| O1P | 18.4 | 4.7 | 44.0 |
| O2P | 19.3 | 7.0 | 43.9 |
| N2 | 27.6 | 8.5 | 39.5 |
| O6 | 24.7 | 11.3 | 41.6 |
| C6 | 25.0 | 10.2 | 41.1 |
| N1 | 26.2 | 10.0 | 40.6 |
| C2 | 26.5 | 8.8 | 40.1 |
| N3 | 25.8 | 7.6 | 40.1 |
| C4 | 24.6 | 7.9 | 40.7 |
| C5 | 24.1 | 9.1 | 41.2 |
| N7 | 22.9 | 9.0 | 41.7 |
| C8 | 22.6 | 7.7 | 41.5 |
| N9 | 23.5 | 7.0 | 40.9 |
| **16** | **DIHYDROURIDINE** | | |
| O1′ | 24.6 | 1.5 | 47.9 |
| C1′ | 23.7 | 0.6 | 48.5 |
| C2′ | 24.2 | -0.9 | 48.1 |
| O2′ | 25.1 | -1.4 | 49.0 |
| C3′ | 24.9 | -0.6 | 46.8 |
| O3′ | 25.9 | -1.5 | 46.4 |
| C4′ | 25.6 | 0.9 | 47.1 |
| C5′ | 25.9 | 1.8 | 45.9 |
| O5′ | 24.9 | 1.7 | 45.0 |
| P | 24.3 | 3.2 | 44.6 |
| O1P | 23.3 | 3.7 | 45.5 |
| O2P | 25.6 | 3.8 | 44.4 |
| C6 | 22.1 | 1.3 | 46.6 |
| C5 | 20.9 | 1.4 | 46.1 |
| O4 | 18.6 | 1.2 | 46.5 |
| C4 | 19.8 | 1.1 | 46.9 |
| N3 | 20.0 | 0.7 | 48.2 |
| O2 | 21.4 | 0.2 | 49.9 |
| C2 | 21.3 | 0.6 | 48.7 |
| N1 | 22.3 | 0.9 | 47.9 |
| **17** | **DIHYDROURIDINE** | | |
| O1′ | 29.3 | -5.3 | 45.3 |
| C1′ | 30.7 | -5.2 | 44.9 |
| C2′ | 31.2 | -3.9 | 45.6 |
| O2′ | 31.7 | -4.3 | 46.9 |
| C3′ | 30.0 | -3.1 | 45.8 |
| O3′ | 30.0 | -2.2 | 46.9 |
| C4′ | 28.9 | -4.2 | 46.1 |
| C5′ | 27.5 | -3.9 | 45.9 |
| O5′ | 27.4 | -2.9 | 44.8 |
| P | 26.1 | -2.0 | 44.9 |
| O1P | 26.2 | -0.8 | 44.1 |
| O2P | 25.1 | -3.0 | 44.7 |
| C6 | 30.7 | -3.7 | 42.8 |
| C5 | 30.9 | -3.5 | 41.5 |
| O4 | 31.1 | -4.7 | 39.4 |
| C4 | 30.9 | -4.7 | 40.7 |
| N3 | 30.8 | -5.9 | 41.3 |
| O2 | 30.7 | -7.2 | 43.1 |
| C2 | 30.7 | -6.1 | 42.6 |
| N1 | 30.7 | -5.0 | 43.3 |
| **18** | **GUANOSINE** | | |
| O1′ | 33.4 | 2.8 | 45.3 |
| C1′ | 34.7 | 2.2 | 45.1 |
| C2′ | 34.4 | 0.7 | 44.7 |
| O2′ | 35.4 | 0.4 | 43.7 |
| C3′ | 33.1 | 0.8 | 44.1 |
| O3′ | 33.1 | 1.3 | 42.8 |
| C4′ | 32.3 | 1.8 | 45.0 |
| C5′ | 31.8 | 1.3 | 46.4 |
| O5′ | 31.6 | -0.3 | 46.2 |
| P | 30.1 | -0.7 | 46.7 |
| O1P | 29.7 | -0.1 | 48.0 |
| O2P | 29.4 | -0.4 | 45.5 |
| N2 | 38.7 | 5.2 | 45.7 |
| O6 | 38.3 | 3.3 | 49.7 |
| C6 | 37.9 | 3.5 | 48.5 |
| N1 | 38.6 | 4.3 | 47.7 |
| C2 | 38.2 | 4.4 | 46.4 |
| N3 | 37.2 | 3.8 | 45.8 |
| C4 | 36.5 | 3.0 | 46.7 |
| C5 | 36.8 | 2.8 | 48.0 |
| N7 | 35.9 | 1.9 | 48.5 |
| C8 | 35.1 | 1.6 | 47.5 |
| N9 | 35.4 | 2.3 | 46.4 |
| **19** | **GUANOSINE** | | |
| O1′ | 37.0 | 2.7 | 40.1 |
| C1′ | 37.4 | 1.6 | 39.3 |
| C2′ | 36.1 | 1.2 | 38.4 |
| O2′ | 36.6 | 0.9 | 37.1 |
| C3′ | 35.4 | 2.5 | 38.4 |
| O3′ | 35.9 | 3.5 | 37.5 |
| C4′ | 35.6 | 3.1 | 39.8 |
| C5′ | 34.7 | 2.4 | 40.9 |
| O5′ | 34.0 | 1.3 | 40.3 |
| P | 33.3 | 0.4 | 41.5 |
| O1P | 31.9 | -0.1 | 41.1 |
| O2P | 34.3 | -0.5 | 41.9 |
| N2 | 41.6 | 1.8 | 42.1 |
| O6 | 39.9 | -2.3 | 43.0 |
| C6 | 39.9 | -1.2 | 42.4 |
| N1 | 40.9 | -0.3 | 42.6 |
| C2 | 40.8 | 0.9 | 41.9 |
| N3 | 39.9 | 1.4 | 41.0 |
| C4 | 38.9 | 0.4 | 40.9 |
| C5 | 38.8 | -0.9 | 41.5 |
| N7 | 37.7 | -1.6 | 41.1 |
| C8 | 37.1 | -0.7 | 40.3 |
| N9 | 37.8 | 0.5 | 40.1 |
| **20** | **GUANOSINE** | | |
| O1′ | 33.4 | 1.1 | 33.5 |
| C1′ | 32.1 | 1.7 | 33.2 |
| C2′ | 32.3 | 3.0 | 32.4 |
| O2′ | 32.4 | 2.6 | 31.0 |
| C3′ | 33.7 | 3.4 | 32.9 |
| O3′ | 34.4 | 4.1 | 32.0 |
| C4′ | 34.4 | 2.0 | 33.0 |
| C5′ | 35.6 | 1.9 | 33.9 |
| O5′ | 35.2 | 2.2 | 35.2 |
| P | 36 3 | 3.1 | 36.0 |
| O1P | 37.6 | 2.4 | 36.2 |
| O2P | 36.2 | 4.3 | 35.3 |
| N2 | 28.0 | 4.7 | 33.4 |
| O6 | 28.6 | 3.5 | 37.7 |
| C6 | 29.0 | 3.5 | 36.5 |
| N1 | 28.3 | 4.2 | 35.6 |
| C2 | 28.6 | 4.1 | 34.3 |
| N3 | 29.7 | 3.5 | 33.7 |
| C4 | 30.3 | 2.8 | 34.7 |
| C5 | 30.1 | 2.7 | 36.0 |
| N7 | 31.0 | 1.9 | 36.7 |
| C8 | 31.8 | 1.5 | 35.7 |
| N9 | 31.4 | 1.9 | 34.5 |
| **21** | **ADENOSINE** | | |
| O1′ | 30.5 | 7.2 | 34.2 |
| C1′ | 29.6 | 8.2 | 33.8 |
| C2′ | 29.2 | 7.9 | 32.3 |
| O2′ | 28.1 | 7.0 | 32.3 |
| C3′ | 30.5 | 7.1 | 31.9 |
| O3′ | 30.2 | 6.3 | 30.8 |
| C4′ | 30.8 | 6.3 | 33.1 |
| C5′ | 32.2 | 5.8 | 33.2 |
| O5′ | 33.0 | 6.4 | 32.1 |
| P | 34.5 | 5.7 | 32.1 |
| O1P | 35.3 | 6.2 | 30.9 |
| O2P | 34.9 | 6.0 | 33.4 |
| N6 | 31.3 | 13.8 | 34.9 |
| C6 | 30.5 | 12.8 | 34.9 |
| N1 | 29.3 | 13.0 | 35.5 |
| C2 | 28.4 | 12.0 | 35.6 |
| N3 | 28.5 | 10.7 | 35.1 |
| C4 | 29.7 | 10.6 | 34.6 |
| C5 | 30.7 | 11.5 | 34.4 |
| N7 | 31.8 | 11.0 | 33.7 |
| C8 | 31.5 | 9.8 | 33.5 |
| N9 | 30.2 | 9.5 | 33.9 |
| **22** | **GUANOSINE** | | |
| O1′ | 25.8 | 6.5 | 31.7 |
| C1′ | 24.6 | 6.8 | 32.4 |
| C2′ | 23.4 | 6.5 | 31.4 |
| O2′ | 23.1 | 5.2 | 31.5 |
| C3′ | 24.1 | 6.7 | 30.1 |
| O3′ | 23.6 | 6.0 | 29.0 |
| C4′ | 25.5 | 6.1 | 30.3 |
| C5′ | 26.7 | 6.6 | 29.4 |
| O5′ | 27.7 | 7.1 | 30.3 |
| P | 29.2 | 6.6 | 29.6 |
| O1P | 29.1 | 5.4 | 28.8 |
| O2P | 29.6 | 7.8 | 29.1 |
| N2 | 20.9 | 8.7 | 35.4 |
| O6 | 23.6 | 12.2 | 34.6 |
| C6 | 23.3 | 11.0 | 34.4 |
| N1 | 22.2 | 10.5 | 35.0 |
| C2 | 21.9 | 9.2 | 34.8 |
| N3 | 22.5 | 8.3 | 34.1 |
| C4 | 23.6 | 8.8 | 33.6 |
| C5 | 24.1 | 10.1 | 33.6 |
| N7 | 25.3 | 10.3 | 32.9 |
| C8 | 25.5 | 9.1 | 32.4 |
| N9 | 24.6 | 8.2 | 32.8 |
| **23** | **ADENOSINE** | | |
| O1′ | 19.6 | 6.5 | 31.1 |
| C1′ | 18.5 | 7.3 | 31.5 |
| C2′ | 17.4 | 7.2 | 30.4 |
| O2′ | 16.6 | 6.2 | 30.7 |
| C3′ | 18.3 | 6.8 | 29.2 |
| O3′ | 17.6 | 6.1 | 28.2 |
| C4′ | 19.3 | 5.8 | 29.9 |
| C5′ | 20.6 | 5.6 | 29.1 |
| O5′ | 21.1 | 6.9 | 28.6 |
| P | 22.6 | 6.7 | 28.0 |
| O1P | 22.6 | 5.9 | 26.8 |
| O2P | 22.9 | 8.1 | 27.9 |
| N6 | 19.8 | 13.1 | 32.5 |
| C6 | 19.0 | 12.0 | 32.7 |
| N1 | 18.0 | 12.0 | 33.5 |
| C2 | 17.2 | 10.9 | 33.7 |
| N3 | 17.4 | 9.7 | 33.1 |
| C4 | 18.5 | 9.7 | 32.3 |
| C5 | 19.3 | 10.8 | 32.0 |
| N7 | 20.3 | 10.4 | 31.2 |
| C8 | 20.1 | 9.1 | 30.9 |
| N9 | 19.0 | 8.7 | 31.6 |
| **24** | **GUANOSINE** | | |
| O1′ | 14.4 | 8.9 | 29.4 |
| C1′ | 14.1 | 10.3 | 29.5 |
| C2′ | 13.3 | 10.7 | 28.2 |
| O2′ | 11.9 | 10.5 | 28.5 |
| C3′ | 13.8 | 9.6 | 27.2 |
| O3′ | 12.9 | 9.3 | 26.2 |
| C4′ | 13.8 | 8.4 | 28.1 |
| C5′ | 14.8 | 7.3 | 27.6 |
| O5′ | 16.0 | 7.9 | 27.1 |
| P | 17.1 | 6.7 | 26.8 |
| O1P | 16.7 | 5.6 | 26.0 |
| O2P | 18.2 | 7.6 | 26.5 |
| N2 | 14.3 | 15.1 | 31.1 |
| O6 | 18.5 | 14.2 | 30.1 |
| C6 | 17.3 | 13.9 | 30.1 |
| N1 | 16.4 | 14.7 | 30.6 |
| C2 | 15.1 | 14.4 | 30.7 |
| N3 | 14.5 | 13.2 | 30.3 |
| C4 | 15.5 | 12.4 | 29.9 |
| C5 | 16.8 | 12.6 | 29.8 |
| N7 | 17.5 | 11.5 | 29.3 |
| C8 | 16.5 | 10.6 | 29.1 |
| N9 | 15.3 | 11.0 | 29.5 |
| **25** | **CYTIDINE** | | |
| O1′ | 12.9 | 14.2 | 27.3 |
| C1′ | 13.6 | 15.4 | 26.9 |
| C2′ | 13.1 | 15.8 | 25.5 |
| O2′ | 11.9 | 16.6 | 25.7 |
| C3′ | 12.7 | 14.4 | 24.9 |
| O3′ | 11.7 | 14.5 | 23.9 |
| C4′ | 12.1 | 13.7 | 26.2 |
| C5′ | 12.1 | 12.2 | 26.1 |
| O5′ | 13.0 | 11.8 | 25.1 |
| P | 12.8 | 10.2 | 24.8 |
| O1P | 11.5 | 9.8 | 24.2 |
| O2P | 14.0 | 9.9 | 24.2 |
| C6 | 15.6 | 13.8 | 26.9 |
| C5 | 16.9 | 13.5 | 26.7 |
| N4 | 19.2 | 14.4 | 26.3 |
| C4 | 17.8 | 14.6 | 26.6 |
| N3 | 17.3 | 15.9 | 26.7 |
| O2 | 15.6 | 17.3 | 27.0 |
| C2 | 16.0 | 16.1 | 26.9 |
| N1 | 15.1 | 15.1 | 26.9 |
| **26** | **2(2)m-GUANOSINE** | | |
| O1′ | 14.6 | 18.1 | 24.5 |
| C1′ | 15.9 | 18.4 | 24.2 |
| C2′ | 15.9 | 19.3 | 22.9 |
| O2′ | 15.7 | 20.6 | 23.3 |
| C3′ | 14.6 | 18.8 | 22.2 |
| O3′ | 14.0 | 19.7 | 21.4 |
| C4′ | 13.7 | 18.6 | 23.5 |
| C5′ | 12.5 | 17.6 | 23.3 |
| O5′ | 13.0 | 16.4 | 22.7 |
| P | 11.8 | 15.3 | 22.6 |
| O1P | 10.5 | 15.9 | 22.4 |
| O2P | 12.5 | 14.4 | 21.7 |
| M22 | 22.4 | 18.2 | 24.7 |
| M21 | 20.5 | 19.8 | 24.9 |
| N2 | 21.0 | 18.5 | 24.6 |
| O6 | 20.0 | 14.3 | 23.5 |
| C6 | 19.7 | 15.4 | 23.8 |
| N1 | 20.6 | 16.4 | 24.0 |
| C2 | 20.2 | 17.6 | 24.3 |
| N3 | 18.9 | 18.1 | 24.3 |
| C4 | 18.1 | 17.1 | 24.0 |
| C5 | 18.3 | 15.8 | 23.8 |
| N7 | 17.2 | 15.1 | 23.6 |
| C8 | 16.2 | 16.0 | 23.7 |

Table 1 (continued)

| | X | Y | Z |
|---|---|---|---|
| N9 | 16.7 | 17.3 | 24.0 |
| **27 CYTIDINE** | | | |
| O1′ | 19.1 | 20.1 | 20.4 |
| C1′ | 20.0 | 19.3 | 19.7 |
| C2′ | 19.8 | 19.6 | 18.2 |
| O2′ | 20.6 | 20.8 | 17.9 |
| C3′ | 18.3 | 20.1 | 18.2 |
| O3′ | 18.0 | 20.9 | 17.1 |
| C4′ | 18.3 | 20.9 | 19.5 |
| C5′ | 16.9 | 21.0 | 20.1 |
| O5′ | 16.2 | 19.8 | 19.9 |
| P | 14.5 | 20.1 | 20.0 |
| O1P | 14.2 | 21.5 | 19.8 |
| O2P | 14.1 | 19.0 | 19.1 |
| C6 | 18.7 | 17.5 | 20.9 |
| C5 | 18.3 | 16.2 | 21.1 |
| N4 | 18.6 | 13.8 | 20.4 |
| C4 | 19.0 | 15.2 | 20.4 |
| N3 | 20.1 | 15.6 | 19.6 |
| O2 | 21.4 | 17.1 | 18.8 |
| C2 | 20.5 | 16.9 | 19.5 |
| N1 | 19.7 | 17.9 | 20.0 |
| **28 CYTIDINE** | | | |
| O1′ | 21.7 | 18.7 | 15.8 |
| C1′ | 22.2 | 17.4 | 15.4 |
| C2′ | 22.0 | 17.3 | 13.8 |
| O2′ | 23.3 | 17.8 | 13.3 |
| C3′ | 20.9 | 18.3 | 13.6 |
| O3′ | 21.0 | 18.9 | 12.3 |
| C4′ | 21.3 | 19.4 | 14.6 |
| C5′ | 20.1 | 20.3 | 15.0 |
| O5′ | 18.9 | 19.5 | 15.1 |
| P | 17.7 | 20.4 | 15.7 |
| O1P | 17.3 | 21.6 | 14.9 |
| O2P | 16.7 | 19.3 | 15.9 |
| C6 | 20.2 | 16.7 | 17.0 |
| C5 | 19.2 | 15.9 | 17.4 |
| N4 | 18.4 | 13.5 | 17.4 |
| C4 | 19.3 | 14.5 | 17.1 |
| N3 | 20.4 | 14.1 | 16.3 |
| O2 | 22.3 | 14.6 | 15.1 |
| C2 | 21.4 | 15.0 | 15.8 |
| N1 | 21.2 | 16.4 | 16.1 |
| **29 ADENOSINE** | | | |
| O1′ | 22.3 | 15.5 | 11.0 |
| C1′ | 22.1 | 14.1 | 11.2 |
| C2′ | 21.7 | 13.5 | 9.8 |
| O2′ | 22.9 | 13.2 | 9.1 |
| C3′ | 21.1 | 14.7 | 9.1 |
| O3′ | 21.1 | 14.8 | 7.7 |
| C4′ | 22.0 | 15.9 | 9.7 |
| C5′ | 21.3 | 17.3 | 9.7 |
| O5′ | 20.1 | 17.2 | 10.4 |
| P | 19.9 | 18.6 | 11.2 |
| O1P | 19.9 | 19.8 | 10.3 |
| O2P | 18.7 | 18.3 | 11.9 |
| N6 | 18.1 | 11.9 | 15.1 |
| C6 | 19.2 | 11.8 | 14.3 |
| N1 | 19.9 | 10.6 | 14.2 |
| C2 | 20.9 | 10.5 | 13.4 |
| N3 | 21.5 | 11.5 | 12.6 |
| C4 | 20.8 | 12.6 | 12.8 |
| C5 | 19.7 | 12.9 | 13.5 |
| N7 | 19.3 | 14.2 | 13.4 |
| C8 | 20.1 | 14.7 | 12.5 |
| N9 | 21.0 | 13.8 | 12.1 |
| **30 GUANOSINE** | | | |
| O1′ | 20.9 | 10.1 | 8.8 |
| C1′ | 20.0 | 9.0 | 9.1 |
| C2′ | 19.5 | 8.5 | 7.7 |
| O2′ | 20.5 | 7.5 | 7.3 |
| C3′ | 19.7 | 9.7 | 6.8 |
| O3′ | 20.0 | 9.4 | 5.5 |
| C4′ | 21.0 | 10.3 | 7.4 |
| C5′ | 21.2 | 11.8 | 7.1 |
| O5′ | 19.9 | 12.5 | 7.2 |
| P | 20.1 | 14.1 | 6.8 |
| O1P | 20.5 | 14.3 | 5.4 |
| O2P | 18.8 | 14.5 | 7.3 |
| N2 | 17.4 | 6.1 | 12.4 |
| O6 | 15.1 | 10.0 | 12.5 |
| C6 | 16.1 | 9.3 | 12.0 |
| N1 | 16.2 | 8.0 | 12.4 |
| C2 | 17.2 | 7.2 | 11.9 |
| N3 | 18.1 | 7.5 | 11.0 |
| C4 | 18.0 | 8.8 | 10.7 |
| C5 | 17.0 | 9.7 | 11.1 |
| N7 | 17.2 | 10.9 | 10.4 |
| C8 | 18.3 | 10.8 | 9.7 |
| N9 | 18.8 | 9.5 | 9.8 |
| **31 ADENOSINE** | | | |
| O1′ | 17.2 | 6.9 | 6.9 |
| C1′ | 16.4 | 6.4 | 7.9 |
| C2′ | 15.4 | 5.3 | 7.2 |
| O2′ | 16.1 | 4.1 | 7.3 |
| C3′ | 15.4 | 5.8 | 5.8 |
| O3′ | 15.2 | 4.9 | 4.8 |
| C4′ | 16.9 | 6.3 | 5.6 |
| C5′ | 17.1 | 7.4 | 4.5 |
| O5′ | 17.5 | 8.6 | 5.1 |
| P | 18.8 | 9.2 | 4.4 |
| O1P | 19.4 | 8.3 | 3.4 |
| O2P | 18.4 | 10.5 | 4.1 |
| N6 | 12.7 | 10.0 | 11.1 |
| C6 | 13.3 | 8.8 | 10.8 |
| N1 | 13.1 | 7.7 | 11.6 |
| C2 | 13.7 | 6.6 | 11.4 |
| N3 | 14.5 | 6.2 | 10.4 |
| C4 | 14.8 | 7.3 | 9.6 |
| C5 | 14.2 | 8.6 | 9.7 |
| N7 | 14.7 | 9.4 | 8.8 |
| C8 | 15.5 | 8.7 | 8.1 |
| N9 | 15.6 | 7.4 | 8.5 |
| **32 CYTIDINE-O2′m** | | | |
| O1′ | 11.2 | 5.3 | 7.3 |
| C1′ | 10.1 | 6.2 | 7.5 |
| C2′ | 9.1 | 5.9 | 6.3 |
| O2′ | 8.3 | 4.8 | 6.7 |
| C2M | 7.8 | 3.7 | 6.3 |
| C3′ | 10.1 | 5.3 | 5.2 |
| O3′ | 9.5 | 4.5 | 4.3 |
| C4′ | 11.0 | 4.5 | 6.1 |
| C5′ | 12.4 | 4.3 | 5.4 |
| O5′ | 12.6 | 5.2 | 4.3 |
| P | 14.1 | 5.0 | 3.7 |
| O1P | 14.2 | 3.9 | 2.8 |
| O2P | 14.2 | 6.4 | 3.3 |
| C6 | 11.6 | 8.0 | 6.4 |
| C5 | 12.0 | 9.3 | 6.2 |
| N4 | 11.7 | 11.6 | 6.9 |
| C4 | 11.5 | 10.3 | 7.1 |
| N3 | 10.7 | 9.8 | 8.1 |
| O2 | 9.5 | 8.3 | 9.2 |
| C2 | 10.3 | 8.5 | 8.3 |
| N1 | 10.7 | 7.6 | 7.3 |
| **33 URIDINE** | | | |
| O1′ | 6.6 | 7.7 | 4.8 |
| C1′ | 6.4 | 9.1 | 4.6 |
| C2′ | 5.5 | 9.2 | 3.3 |
| O2′ | 4.1 | 9.1 | 3.6 |
| C3′ | 5.9 | 7.9 | 2.6 |
| O3′ | 5.0 | 7.4 | 1.7 |
| C4′ | 6.0 | 6.9 | 3.8 |
| C5′ | 6.9 | 5.7 | 3.6 |
| O5′ | 8.0 | 6.1 | 2.8 |
| P | 9.1 | 4.9 | 2.8 |
| O1P | 8.7 | 3.7 | 2.1 |
| O2P | 10.3 | 5.7 | 2.4 |
| C6 | 8.8 | 9.1 | 3.8 |
| C5 | 9.9 | 9.6 | 3.5 |
| O4 | 11.1 | 11.7 | 3.5 |
| C4 | 10.1 | 11.0 | 3.8 |
| N3 | 9.0 | 11.7 | 4.3 |
| O2 | 6.9 | 11.7 | 5.1 |
| C2 | 7.8 | 11.1 | 4.6 |
| N1 | 7.7 | 9.8 | 4.4 |
| **34 GUANOSINE-O2′m** | | | |
| O1′ | 3.5 | 11.0 | -1.9 |
| C1′ | 2.9 | 12.1 | -1.3 |
| C2′ | 4.1 | 13.0 | -0.7 |
| O2′ | 4.5 | 13.9 | -1.8 |
| C2M | 5.5 | 14.9 | -1.4 |
| C3′ | 5.1 | 12.0 | -0.5 |
| O3′ | 6.4 | 12.4 | -0.6 |
| C4′ | 4.9 | 11.0 | -1.8 |
| C5′ | 5.4 | 9.6 | -1.6 |
| O5′ | 5.5 | 9.3 | -0.2 |
| P | 5.0 | 7.8 | 0.2 |
| O1P | 3.6 | 7.5 | -0.4 |
| O2P | 6.0 | 7.0 | -0.5 |
| N2 | 0.4 | 15.5 | 1.7 |
| O6 | -0.8 | 11.6 | 3.5 |
| C6 | -0.2 | 12.3 | 2.6 |
| N1 | -0.3 | 13.6 | 2.7 |
| C2 | 0.5 | 14.3 | 1.8 |
| N3 | 1.3 | 13.9 | 0.8 |
| C4 | 1.4 | 12.5 | 0.8 |
| C5 | 0.7 | 11.7 | 1.7 |
| N7 | 1.0 | 10.4 | 1.4 |
| C8 | 1.8 | 10.5 | 0.3 |
| N9 | 2.1 | 11.7 | -0.2 |
| **35 ADENOSINE** | | | |
| O1′ | 5.4 | 15.7 | 1.9 |
| C1′ | 4.7 | 16.0 | 3.0 |
| C2′ | 5.7 | 16.4 | 4.1 |
| O2′ | 6.0 | 17.8 | 4.0 |
| C3′ | 7.0 | 15.6 | 3.6 |
| O3′ | 8.2 | 16.2 | 4.0 |
| C4′ | 6.8 | 15.8 | 2.1 |
| C5′ | 7.6 | 14.7 | 1.3 |
| O5′ | 7.3 | 13.4 | 1.8 |
| P | 7.5 | 12.3 | 0.7 |
| O1P | 8.8 | 12.3 | -0.1 |
| O2P | 7.0 | 11.2 | 1.4 |
| N6 | 1.1 | 11.9 | 5.6 |
| C6 | 1.6 | 13.2 | 5.5 |
| N1 | 1.1 | 14.2 | 6.3 |
| C2 | 1.6 | 15.4 | 6.1 |
| N3 | 2.6 | 15.8 | 5.3 |
| C4 | 3.0 | 14.8 | 4.5 |
| C5 | 2.6 | 13.5 | 4.5 |
| N7 | 3.2 | 12.8 | 3.6 |
| C8 | 4.0 | 13.6 | 3.0 |
| N9 | 4.0 | 14.9 | 3.5 |
| **36 ADENOSINE** | | | |
| O1′ | 5.4 | 16.7 | 7.8 |
| C1′ | 4.8 | 15.9 | 8.9 |
| C2′ | 5.8 | 15.8 | 10.0 |
| O2′ | 5.7 | 16.9 | 10.9 |
| C3′ | 7.1 | 15.9 | 9.2 |
| O3′ | 8.2 | 16.4 | 10.0 |
| C4′ | 6.8 | 17.0 | 8.2 |
| C5′ | 7.6 | 17.0 | 6.9 |
| O5′ | 8.0 | 15.7 | 6.6 |
| P | 9.0 | 15.7 | 5.3 |
| O1P | 10.1 | 16.6 | 5.4 |
| O2P | 9.1 | 14.3 | 5.1 |
| N6 | 2.5 | 10.5 | 7.5 |
| C6 | 2.6 | 11.7 | 8.3 |
| N1 | 1.8 | 11.8 | 9.3 |
| C2 | 1.9 | 12.9 | 10.1 |
| N3 | 2.7 | 14.0 | 9.9 |
| C4 | 3.4 | 13.8 | 8.8 |
| C5 | 3.5 | 12.7 | 8.0 |
| N7 | 4.4 | 12.9 | 7.0 |
| C8 | 4.9 | 14.1 | 7.2 |
| N9 | 4.4 | 14.7 | 8.3 |
| **37 Y NUCLEOSIDE** | | | |
| O1′ | 4.6 | 14.9 | 12.4 |
| C1′ | 4.0 | 13.7 | 13.0 |
| C2′ | 4.5 | 13.6 | 14.4 |
| O2′ | 3.7 | 14.3 | 15.2 |
| C3′ | 5.9 | 14.3 | 14.3 |
| O3′ | 6.3 | 14.8 | 15.5 |
| C4′ | 5.5 | 15.5 | 13.3 |
| C5′ | 6.7 | 16.0 | 12.6 |
| O5′ | 7.6 | 15.0 | 12.1 |
| P | 8.8 | 15.6 | 11.2 |
| O1P | 9.7 | 16.5 | 11.9 |
| O2P | 9.2 | 14.3 | 10.7 |
| C25 | -2.0 | 3.1 | 10.9 |
| O24 | -0.6 | 3.0 | 10.9 |
| O23 | -0.6 | 4.8 | 9.5 |
| C22 | 0.1 | 3.9 | 10.1 |
| N21 | 1.5 | 4.0 | 10.0 |
| C20 | 3.7 | 6.5 | 7.8 |
| O18 | 4.0 | 3.5 | 9.5 |
| O19 | 4.4 | 5.4 | 8.2 |
| C17 | 3.5 | 4.6 | 9.0 |
| C16 | 2.1 | 5.0 | 9.2 |
| C15 | 2.1 | 6.3 | 9.9 |
| C14 | 3.0 | 6.2 | 11.1 |
| C13 | 0.8 | 7.0 | 13.2 |
| C12 | 2.9 | 7.5 | 11.9 |
| C11 | 1.9 | 7.9 | 12.8 |
| N10 | 2.1 | 9.2 | 13.2 |
| O6 | 4.7 | 8.4 | 10.4 |
| C6 | 4.1 | 9.2 | 11.2 |
| N1 | 3.1 | 8.8 | 11.9 |
| C2 | 2.5 | 9.6 | 12.8 |
| N3 | 2.8 | 10.9 | 13.0 |
| C3 | 3.4 | 11.8 | 13.8 |
| C4 | 3.8 | 11.3 | 12.2 |
| C5 | 4.5 | 10.6 | 11.3 |
| N7 | 5.5 | 11.3 | 10.7 |
| C8 | 5.4 | 12.5 | 11.3 |
| N9 | 4.4 | 12.5 | 12.2 |
| **38 ADENOSINE** | | | |
| O1′ | 4.7 | 11.0 | 16.0 |
| C1′ | 4.8 | 9.6 | 15.6 |
| C2′ | 5.2 | 8.8 | 16.8 |
| O2′ | 4.0 | 8.4 | 17.5 |
| C3′ | 6.0 | 9.9 | 17.6 |
| O3′ | 6.0 | 9.6 | 19.0 |
| C4′ | 5.1 | 11.1 | 17.4 |
| C5′ | 5.8 | 12.5 | 17.6 |
| O5′ | 6.9 | 12.5 | 16.7 |
| P | 7.4 | 14.1 | 16.4 |
| O1P | 7.4 | 14.9 | 17.7 |
| O2P | 8.5 | 13.8 | 15.6 |
| N6 | 8.5 | 8.0 | 11.2 |
| C6 | 7.5 | 7.7 | 12.1 |
| N1 | 7.0 | 6.5 | 12.2 |
| C2 | 6.0 | 6.3 | 13.1 |
| N3 | 5.5 | 7.1 | 14.0 |
| C4 | 6.0 | 8.3 | 13.8 |
| C5 | 7.0 | 8.7 | 13.0 |
| N7 | 7.3 | 10.0 | 13.1 |
| C8 | 6.5 | 10.5 | 14.0 |
| N9 | 5.7 | 9.5 | 14.6 |
| **39 PSEUDOURIDINE** | | | |
| O1′ | 7.5 | 5.8 | 16.5 |
| C1′ | 8.7 | 5.4 | 15.7 |
| C2′ | 9.7 | 4.8 | 16.8 |
| O2′ | 9.4 | 3.5 | 17.0 |

Table 1 (continued)

| | X | Y | Z |
|---|---|---|---|
| C3′ | 9.3 | 5.6 | 18.1 |
| O3′ | 9.6 | 4.9 | 19.3 |
| C4′ | 7.7 | 5.6 | 17.9 |
| C5′ | 7.0 | 6.7 | 18.6 |
| O5′ | 7.9 | 7.8 | 18.8 |
| P | 7.2 | 9.0 | 19.7 |
| O1P | 6.7 | 8.5 | 21.0 |
| O2P | 8.2 | 10.0 | 19.6 |
| C6 | 8.8 | 7.9 | 15.3 |
| N1 | 9.4 | 9.0 | 14.8 |
| O2 | 11.3 | 9.8 | 13.6 |
| C2 | 10.6 | 8.8 | 14.1 |
| N3 | 11.0 | 7.5 | 13.9 |
| O4 | 10.9 | 5.3 | 14.2 |
| C4 | 10.4 | 6.4 | 14.4 |
| C5 | 9.3 | 6.6 | 15.1 |

40 5m-CYTIDINE

| | | | |
|---|---|---|---|
| O1′ | 12.6 | 2.8 | 15.8 |
| C1′ | 13.8 | 3.2 | 15.1 |
| C2′ | 15.0 | 2.8 | 16.0 |
| O2′ | 15.3 | 1.5 | 15.6 |
| C3′ | 14.4 | 2.8 | 17.4 |
| O3′ | 15.0 | 2.0 | 18.3 |
| C4′ | 12.9 | 2.2 | 17.0 |
| C5′ | 11.9 | 2.6 | 18.1 |
| O5′ | 11.8 | 4.0 | 18.2 |
| P | 11.0 | 4.4 | 19.6 |
| O1P | 10.7 | 3.2 | 20.5 |
| O2P | 11.7 | 5.5 | 20.0 |
| M5 | 11.8 | 7.6 | 16.3 |
| C6 | 12.8 | 5.5 | 15.6 |
| C5 | 12.8 | 6.8 | 15.6 |
| N4 | 14.1 | 8.8 | 14.9 |
| C4 | 13.9 | 7.5 | 14.9 |
| N3 | 14.9 | 6.7 | 14.3 |
| O2 | 15.7 | 4.7 | 13.7 |
| C2 | 14.8 | 5.3 | 14.3 |
| N1 | 13.7 | 4.8 | 15.0 |

41 URIDINE

| | | | |
|---|---|---|---|
| O1′ | 18.5 | 3.5 | 14.8 |
| C1′ | 19.4 | 4.5 | 14.7 |
| C2′ | 20.6 | 4.2 | 15.7 |
| O2′ | 21.5 | 3.4 | 15.0 |
| C3′ | 19.8 | 3.4 | 16.8 |
| O3′ | 20.6 | 2.6 | 17.5 |
| C4′ | 18.9 | 2.6 | 15.9 |
| C5′ | 17.6 | 2.1 | 16.6 |
| O5′ | 17.4 | 3.0 | 17.7 |
| P | 16.4 | 2.2 | 18.8 |
| O1P | 16.9 | 0.9 | 19.2 |
| O2P | 16.3 | 3.2 | 19.8 |
| C6 | 17.6 | 5.9 | 15.8 |
| C5 | 17.0 | 7.0 | 16.2 |
| O4 | 17.4 | 9.4 | 16.3 |
| C4 | 17.7 | 8.2 | 15.9 |
| N3 | 18.9 | 8.1 | 15.2 |
| O2 | 20.5 | 6.9 | 14.1 |
| C2 | 19.4 | 6.9 | 14.7 |
| N1 | 18.7 | 5.8 | 15.1 |

42 GUANOSINE

| | | | |
|---|---|---|---|
| O1′ | 23.3 | 5.5 | 16.0 |
| C1′ | 23.5 | 6.9 | 15.9 |
| C2′ | 24.8 | 7.1 | 16.9 |
| O2′ | 25.9 | 7.0 | 16.0 |
| C3′ | 24.7 | 5.9 | 17.8 |
| O3′ | 25.9 | 5.5 | 18.3 |
| C4′ | 24.2 | 4.8 | 16.8 |
| C5′ | 23.5 | 3.6 | 17.5 |
| O5′ | 22.6 | 4.1 | 18.4 |
| P | 21.4 | 3.0 | 18.8 |
| O1P | 22.0 | 1.7 | 19.3 |
| O2P | 20.5 | 3.8 | 19.5 |
| N2 | 22.8 | 11.9 | 15.0 |
| O6 | 19.3 | 10.8 | 17.6 |
| C6 | 20.4 | 10.4 | 17.0 |
| N1 | 21.1 | 11.4 | 16.3 |
| C2 | 22.2 | 11.1 | 15.7 |
| N3 | 22.9 | 9.9 | 15.7 |
| C4 | 22.1 | 9.0 | 16.3 |
| C5 | 20.9 | 9.1 | 17.0 |
| N7 | 20.5 | 8.0 | 17.6 |
| C8 | 21.4 | 7.1 | 17.2 |
| N9 | 22.4 | 7.6 | 16.5 |

43 GUANOSINE

| | | | |
|---|---|---|---|
| O1′ | 26.5 | 9.6 | 17.3 |
| C1′ | 26.1 | 11.0 | 17.5 |
| C2′ | 27.2 | 11.7 | 18.4 |
| O2′ | 28.2 | 12.2 | 17.5 |
| C3′ | 27.8 | 10.5 | 19.1 |
| O3′ | 29.2 | 10.7 | 19.5 |
| C4′ | 27.8 | 9.4 | 18.0 |
| C5′ | 27.9 | 7.9 | 18.5 |
| O5′ | 26.8 | 7.8 | 19.5 |
| P | 26.5 | 6.2 | 19.7 |
| O1P | 27.7 | 5.4 | 20.0 |
| O2P | 25.4 | 6.3 | 20.6 |
| N2 | 23.2 | 15.1 | 17.9 |
| O6 | 20.9 | 12.1 | 20.3 |
| C6 | 21.9 | 12.4 | 19.6 |
| N1 | 22.0 | 13.7 | 19.1 |
| C2 | 23.1 | 14.0 | 18.4 |
| N3 | 24.2 | 13.3 | 18.0 |
| C4 | 24.0 | 12.0 | 18.5 |
| C5 | 23.0 | 11.5 | 19.2 |
| N7 | 23.2 | 10.2 | 19.6 |
| C8 | 24.3 | 9.9 | 19.0 |
| N9 | 24.9 | 11.0 | 18.3 |

44 ADENOSINE

| | | | |
|---|---|---|---|
| O1′ | 27.9 | 15.3 | 19.2 |
| C1′ | 27.4 | 16.4 | 19.9 |
| C2′ | 28.6 | 16.9 | 20.8 |
| O2′ | 29.4 | 17.8 | 20.0 |
| C3′ | 29.4 | 15.6 | 21.0 |
| O3′ | 30.7 | 15.8 | 21.2 |
| C4′ | 29.2 | 15.0 | 19.5 |
| C5′ | 29.4 | 13.5 | 19.5 |
| O5′ | 29.3 | 12.9 | 20.8 |
| P | 29.6 | 11.3 | 20.8 |
| O1P | 31.0 | 11.0 | 21.0 |
| O2P | 28.6 | 10.9 | 21.8 |
| N6 | 23.3 | 13.7 | 23.3 |
| C6 | 24.4 | 13.7 | 22.5 |
| N1 | 25.0 | 12.6 | 22.2 |
| C2 | 26.1 | 12.6 | 21.4 |
| N3 | 26.7 | 13.6 | 20.8 |
| C4 | 26.0 | 14.8 | 21.2 |
| C5 | 24.9 | 14.9 | 21.9 |
| N7 | 24.5 | 16.2 | 22.0 |
| C8 | 25.4 | 16.9 | 21.3 |
| N9 | 26.3 | 16.1 | 20.7 |

45 GUANOSINE

| | | | |
|---|---|---|---|
| O1′ | 27.5 | 17.3 | 24.1 |
| C1′ | 26.7 | 16.9 | 25.2 |
| C2′ | 27.4 | 17.5 | 26.5 |
| O2′ | 26.9 | 18.9 | 26.7 |
| C3′ | 28.9 | 17.6 | 26.0 |
| O3′ | 29.6 | 18.6 | 26.6 |
| C4′ | 28.7 | 18.0 | 24.5 |
| C5′ | 29.9 | 17.7 | 23.6 |
| O5′ | 30.2 | 16.3 | 23.8 |
| P | 31.3 | 15.9 | 22.7 |
| O1P | 32.5 | 16.8 | 22.6 |
| O2P | 31.5 | 14.5 | 23.1 |
| N2 | 22.6 | 14.5 | 27.1 |
| O6 | 25.4 | 11.2 | 26.1 |
| C6 | 25.1 | 12.4 | 26.2 |
| N1 | 24.0 | 12.8 | 26.7 |
| C2 | 23.7 | 14.1 | 26.7 |
| N3 | 24.5 | 15.2 | 26.4 |
| C4 | 25.6 | 14.7 | 25.9 |
| C5 | 26.1 | 13.4 | 25.7 |
| N7 | 27.3 | 13.4 | 25.2 |
| C8 | 27.6 | 14.6 | 25.0 |
| N9 | 26.7 | 15.5 | 25.3 |

46 7m-GUANOSINE

| | | | |
|---|---|---|---|
| O1′ | 28.9 | 17.5 | 31.5 |
| C1′ | 29.4 | 16.6 | 32.6 |
| C2′ | 30.9 | 17.2 | 32.8 |
| O2′ | 30.8 | 18.2 | 33.8 |
| C3′ | 31.2 | 17.7 | 31.4 |
| O3′ | 32.2 | 18.8 | 31.5 |
| C4′ | 29.9 | 18.4 | 31.0 |
| C5′ | 29.7 | 18.6 | 29.5 |
| O5′ | 30.9 | 18.9 | 28.9 |
| P | 31.0 | 18.2 | 27.4 |
| O1P | 32.1 | 18.8 | 26.6 |
| O2P | 30.8 | 16.9 | 27.8 |
| M7 | 31.0 | 12.5 | 30.4 |
| N2 | 25.6 | 13.5 | 33.7 |
| O6 | 28.5 | 11.0 | 31.3 |
| C6 | 28.2 | 12.1 | 31.8 |
| N1 | 27.0 | 12.2 | 32.5 |
| C2 | 26.7 | 13.3 | 33.1 |
| N3 | 27.4 | 14.5 | 33.1 |
| C4 | 28.5 | 14.3 | 32.4 |
| C5 | 29.0 | 13.2 | 31.7 |
| N7 | 30.2 | 13.4 | 31.1 |
| C8 | 30.4 | 14.7 | 31.4 |
| N9 | 29.5 | 15.3 | 32.1 |

47 URIDINE

| | | | |
|---|---|---|---|
| O1′ | 34.8 | 20.3 | 35.8 |
| C1′ | 34.1 | 20.8 | 36.9 |
| C2′ | 33.6 | 19.6 | 37.7 |
| O2′ | 34.7 | 19.3 | 38.6 |
| C3′ | 33.5 | 18.5 | 36.6 |
| O3′ | 33.7 | 17.2 | 37.1 |
| C4′ | 34.8 | 18.9 | 35.8 |
| C5′ | 34.8 | 18.4 | 34.3 |
| O5′ | 33.7 | 19.1 | 33.6 |
| P | 33.6 | 18.6 | 32.1 |
| O1P | 34.5 | 19.3 | 31.2 |
| O2P | 33.7 | 17.2 | 32.3 |
| C6 | 32.2 | 21.2 | 35.2 |
| C5 | 31.1 | 21.8 | 34.7 |
| O4 | 29.4 | 23.3 | 35.3 |
| C4 | 30.5 | 22.8 | 35.6 |
| N3 | 31.2 | 23.1 | 36.7 |
| O2 | 32.9 | 22.9 | 38.2 |
| C2 | 32.3 | 22.5 | 37.1 |
| N1 | 32.8 | 21.6 | 36.3 |

48 CYTIDINE

| | | | |
|---|---|---|---|
| O1′ | 29.2 | 15.3 | 38.7 |
| C1′ | 29.3 | 14.3 | 39.8 |
| C2′ | 30.3 | 15.0 | 40.8 |
| O2′ | 29.9 | 14.7 | 42.1 |
| C3′ | 30.2 | 16.5 | 40.5 |
| O3′ | 29.0 | 17.0 | 41.0 |
| C4′ | 30.0 | 16.4 | 38.9 |
| C5′ | 31.3 | 16.3 | 38.1 |
| O5′ | 32.4 | 16.0 | 39.0 |
| P | 33.7 | 16.9 | 38.6 |
| O1P | 33.8 | 18.1 | 39.3 |
| O2P | 34.7 | 15.8 | 38.8 |
| C6 | 30.9 | 13.0 | 38.2 |
| C5 | 31.5 | 11.8 | 37.8 |
| N4 | 31.4 | 9.4 | 37.9 |
| C4 | 30.9 | 10.6 | 38.2 |
| N3 | 29.8 | 10.7 | 39.0 |
| O2 | 28.2 | 11.8 | 40.1 |
| C2 | 29.2 | 11.9 | 39.4 |
| N1 | 29.9 | 13.0 | 39.2 |
| C1′ | 27.9 | 21.3 | 43.5 |
| C1′ | 28.5 | 22.0 | 44.5 |
| C2′ | 30.0 | 22.2 | 44.0 |
| O2′ | 30.1 | 23.3 | 43.1 |
| C3′ | 30.2 | 20.9 | 43.1 |
| O3′ | 31.1 | 21.0 | 42.1 |
| C4′ | 28.8 | 20.9 | 42.4 |
| C5′ | 28.4 | 19.5 | 41.9 |
| O5′ | 28.2 | 18.6 | 43.0 |
| P | 28.8 | 17.1 | 42.6 |
| O1P | 30.1 | 16.8 | 43.2 |
| O2P | 27.6 | 16.4 | 42.8 |
| M5 | 27.1 | 18.0 | 47.0 |
| C6 | 27.8 | 20.1 | 45.9 |
| C5 | 27.9 | 19.3 | 47.0 |
| N4 | 28.9 | 19.0 | 49.2 |
| C4 | 28.7 | 19.7 | 48.0 |
| N3 | 29.4 | 20.9 | 47.9 |
| O2 | 29.9 | 22.7 | 46.7 |
| C2 | 29.3 | 21.7 | 46.8 |
| N1 | 28.5 | 21.2 | 45.7 |

50 URIDINE

| | | | |
|---|---|---|---|
| O1′ | 33.7 | 23.7 | 45.2 |
| C1′ | 34.5 | 23.6 | 46.4 |
| C2′ | 35.9 | 23.3 | 46.0 |
| O2′ | 36.6 | 24.6 | 45.8 |
| C3′ | 35.7 | 22.6 | 44.7 |
| O3′ | 36.8 | 22.7 | 43.8 |
| C4′ | 34.5 | 23.5 | 44.1 |
| C5′ | 33.7 | 22.8 | 43.0 |
| O5′ | 33.4 | 21.5 | 43.5 |
| P | 32.6 | 20.6 | 42.3 |
| O1P | 33.3 | 20.8 | 41.0 |
| O2P | 32.6 | 19.3 | 42.9 |
| C6 | 33.0 | 21.6 | 46.6 |
| C5 | 32.6 | 20.5 | 47.3 |
| O4 | 32.8 | 19.3 | 49.3 |
| C4 | 33.1 | 20.3 | 48.6 |
| N3 | 33.9 | 21.3 | 49.2 |
| O2 | 35.0 | 23.2 | 49.0 |
| C2 | 34.3 | 22.4 | 48.5 |
| N1 | 33.9 | 22.5 | 47.2 |

51 GUANOSINE

| | | | |
|---|---|---|---|
| O1′ | 38.5 | 23.0 | 48.2 |
| C1′ | 38.8 | 22.2 | 49.4 |
| C2′ | 40.2 | 21.6 | 49.2 |
| O2′ | 41.1 | 22.5 | 49.7 |
| C3′ | 40.3 | 21.6 | 47.7 |
| O3′ | 41.6 | 21.7 | 47.2 |
| C4′ | 39.6 | 23.0 | 47.3 |
| C5′ | 39.1 | 23.0 | 45.9 |
| O5′ | 38.6 | 21.7 | 45.5 |
| P | 38.1 | 21.8 | 43.9 |
| O1P | 39.1 | 22.4 | 43.0 |
| O2P | 37.6 | 20.5 | 43.8 |
| N2 | 37.2 | 20.2 | 53.8 |
| O6 | 34.9 | 17.9 | 50.8 |
| C6 | 35.8 | 18.8 | 51.1 |
| N1 | 36.1 | 19.0 | 52.4 |
| C2 | 37.0 | 19.9 | 52.7 |
| N3 | 37.7 | 20.7 | 51.8 |
| C4 | 37.3 | 20.5 | 50.6 |
| C5 | 36.4 | 19.5 | 50.1 |
| N7 | 36.3 | 19.6 | 48.7 |
| C8 | 37.2 | 20.5 | 48.4 |
| N9 | 37.8 | 21.1 | 49.4 |

52 URIDINE

| | | | |
|---|---|---|---|
| O1′ | 41.9 | 20.0 | 51.7 |
| C1′ | 41.6 | 18.8 | 52.5 |
| C2′ | 42.9 | 17.9 | 52.4 |
| O2′ | 43.7 | 18.3 | 53.5 |
| C3′ | 43.6 | 18.4 | 51.1 |
| O3′ | 45.0 | 18.3 | 51.1 |

Table 1 (continued)

| | X | Y | Z |
|---|---|---|---|
| C4′ | 43.2 | 20.0 | 51.2 |
| C5′ | 43.2 | 20.7 | 49.8 |
| O5′ | 42.6 | 19.9 | 48.9 |
| P | 42.7 | 20.5 | 47.4 |
| O1P | 44.0 | 21.1 | 47.1 |
| O2P | 42.2 | 19.4 | 46.6 |
| C6 | 40.1 | 18.4 | 50.5 |
| C5 | 39.2 | 17.7 | 49.8 |
| O4 | 37.9 | 15.8 | 49.8 |
| C4 | 38.7 | 16.6 | 50.4 |
| N3 | 39.1 | 16.3 | 51.7 |
| O2 | 40.3 | 16.7 | 53.5 |
| C2 | 40.0 | 17.0 | 52.4 |
| N1 | 40.5 | 18.1 | 51.7 |

53 GUANOSINE

| | | | |
|---|---|---|---|
| O1′ | 43.3 | 15.0 | 53.9 |
| C1′ | 42.4 | 14.0 | 54.1 |
| C2′ | 43.2 | 12.6 | 54.3 |
| O2′ | 43.4 | 12.6 | 55.7 |
| C3′ | 44.5 | 13.0 | 53.6 |
| O3′ | 45.6 | 12.3 | 54.1 |
| C4′ | 44.7 | 14.5 | 54.0 |
| C5′ | 45.6 | 15.3 | 53.0 |
| O5′ | 44.8 | 15.8 | 52.0 |
| P | 45.7 | 16.9 | 51.1 |
| O1P | 47.0 | 17.2 | 51.7 |
| O2P | 45.5 | 16.4 | 49.8 |
| N2 | 38.1 | 11.1 | 53.9 |
| O6 | 38.5 | 12.7 | 49.7 |
| C6 | 38.9 | 12.6 | 50.9 |
| N1 | 38.2 | 11.8 | 51.8 |
| C2 | 38.7 | 11.7 | 53.1 |
| N3 | 39.8 | 12.3 | 53.6 |
| C4 | 40.4 | 13.0 | 52.7 |
| C5 | 40.1 | 13.3 | 51.4 |
| N7 | 41.0 | 14.1 | 50.7 |
| C8 | 41.8 | 14.4 | 51.6 |
| N9 | 41.6 | 13.8 | 52.9 |

54 RIBOTHYMIDINE

| | | | |
|---|---|---|---|
| O1′ | 42.1 | 9.3 | 54.3 |
| C1′ | 41.3 | 8.4 | 53.6 |
| C2′ | 42.0 | 7.1 | 53.5 |
| O2′ | 41.6 | 6.3 | 54.7 |
| C3′ | 43.5 | 7.5 | 53.7 |
| O3′ | 44.3 | 6.6 | 54.3 |
| C4′ | 43.3 | 8.7 | 54.8 |
| C5′ | 44.4 | 9.7 | 54.8 |
| O5′ | 45.0 | 9.7 | 53.5 |
| P | 46.2 | 11.0 | 53.5 |
| O1P | 47.4 | 10.7 | 54.2 |
| O2P | 46.1 | 11.2 | 52.1 |
| M5 | 43.1 | 11.2 | 49.9 |
| C6 | 42.1 | 9.8 | 51.7 |
| C5 | 42.1 | 10.2 | 50.4 |
| O4 | 40.9 | 10.0 | 48.3 |
| C4 | 41.0 | 9.8 | 49.5 |
| N3 | 40.1 | 8.9 | 50.1 |
| O2 | 39.2 | 7.8 | 51.8 |
| C2 | 40.1 | 8.5 | 51.4 |
| N1 | 41.2 | 9.0 | 52.1 |

55 PSEUDOURIDINE

| | | | |
|---|---|---|---|
| O1′ | 42.8 | 4.8 | 50.8 |
| C1′ | 42.6 | 5.0 | 49.4 |
| C2′ | 43.5 | 3.9 | 48.7 |
| O2′ | 42.8 | 2.7 | 48.6 |
| C3′ | 44.6 | 3.7 | 49.8 |
| O3′ | 45.2 | 2.5 | 49.7 |
| C4′ | 43.8 | 3.7 | 51.1 |
| C5′ | 44.6 | 4.1 | 52.3 |
| O5′ | 45.2 | 5.3 | 52.1 |
| P | 45.6 | 6.0 | 53.6 |
| O1P | 46.2 | 5.1 | 54.6 |
| O2P | 46.3 | 7.2 | 53.1 |
| C6 | 43.8 | 7.1 | 50.0 |
| N1 | 44.3 | 8.3 | 49.7 |
| O2 | 44.6 | 9.8 | 47.9 |
| C2 | 44.1 | 8.8 | 48.4 |
| N3 | 43.4 | 8.0 | 47.5 |
| O4 | 42.2 | 6.1 | 47.1 |
| C4 | 42.8 | 6.8 | 47.9 |
| C5 | 43.1 | 6.4 | 49.1 |

56 CYTIDINE

| | | | |
|---|---|---|---|
| O1′ | 47.5 | 1.5 | 45.2 |
| C1′ | 46.4 | 1.8 | 44.3 |
| C2′ | 46.0 | 3.3 | 44.6 |
| O2′ | 46.7 | 4.1 | 43.8 |
| C3′ | 46.4 | 3.4 | 46.1 |
| O3′ | 46.7 | 4.7 | 46.4 |
| C4′ | 47.8 | 2.7 | 46.1 |
| C5′ | 48.3 | 2.2 | 47.4 |
| O5′ | 47.2 | 1.5 | 48.1 |
| P | 46.8 | 2.3 | 49.5 |
| O1P | 47.3 | 1.6 | 50.7 |
| O2P | 47.3 | 3.6 | 49.1 |
| C6 | 45.4 | -0.4 | 45.6 |
| C5 | 44.4 | -1.1 | 46.1 |
| N4 | 42.0 | -1.5 | 46.0 |
| C4 | 43.1 | -0.9 | 45.6 |
| N3 | 43.0 | 0.2 | 44.6 |
| O2 | 43.8 | 1.8 | 43.3 |
| C2 | 44.0 | 0.9 | 44.1 |
| N1 | 45.3 | 0.8 | 44.8 |

57 GUANOSINE

| | | | |
|---|---|---|---|
| O1′ | 43.0 | 4.1 | 43.0 |
| C1′ | 41.5 | 4.0 | 43.1 |
| C2′ | 41.1 | 5.5 | 43.0 |
| O2′ | 40.9 | 5.8 | 41.7 |
| C3′ | 42.3 | 6.3 | 43.5 |
| O3′ | 42.5 | 7.6 | 43.0 |
| C4′ | 43.5 | 5.4 | 42.9 |
| C5′ | 44.8 | 5.5 | 43.5 |
| O5′ | 44.7 | 5.6 | 45.0 |
| P | 46.1 | 6.0 | 45.7 |
| O1P | 47.1 | 6.5 | 44.8 |
| O2P | 45.5 | 6.8 | 46.8 |
| N2 | 37.8 | 0.6 | 43.7 |
| O6 | 39.3 | 1.2 | 47.9 |
| C6 | 39.3 | 1.5 | 46.6 |
| N1 | 38.5 | 0.9 | 45.8 |
| C2 | 38.5 | 1.2 | 44.5 |
| N3 | 39.3 | 2.1 | 43.8 |
| C4 | 40.2 | 2.6 | 44.7 |
| C5 | 40.3 | 2.5 | 46.1 |
| N7 | 41.2 | 3.2 | 46.6 |
| C8 | 41.8 | 3.8 | 45.6 |
| N9 | 41.2 | 3.5 | 44.4 |

58 1m-ADENOSINE

| | | | |
|---|---|---|---|
| O1′ | 37.3 | 7.4 | 44.0 |
| C1′ | 36.9 | 8.5 | 44.8 |
| C2′ | 37.9 | 9.7 | 44.4 |
| O2′ | 37.1 | 10.9 | 44.4 |
| C3′ | 38.1 | 9.3 | 42.9 |
| O3′ | 37.0 | 9.6 | 42.1 |
| C4′ | 38.3 | 7.8 | 43.0 |
| C5′ | 39.7 | 7.3 | 43.5 |
| O5′ | 40.3 | 8.3 | 44.3 |
| P | 41.7 | 8.8 | 43.6 |
| O1P | 41.6 | 9.8 | 42.5 |
| O2P | 42.4 | 9.1 | 44.8 |
| M1 | 35.3 | 4.7 | 49.6 |
| N6 | 37.4 | 6.4 | 50.2 |
| C6 | 36.8 | 6.4 | 49.0 |
| N1 | 35.8 | 5.6 | 48.7 |
| C2 | 35.3 | 5.7 | 47.4 |
| N3 | 35.6 | 6.5 | 46.4 |
| C4 | 36.7 | 7.3 | 46.8 |
| C5 | 37.3 | 7.3 | 48.0 |
| N7 | 38.3 | 8.3 | 48.0 |
| C8 | 38.2 | 8.8 | 46.8 |
| N9 | 37.3 | 8.2 | 46.2 |

59 URIDINE

| | | | |
|---|---|---|---|
| O1′ | 32.0 | 11.6 | 41.6 |
| C1′ | 30.8 | 11.1 | 42.3 |
| C2′ | 31.2 | 11.1 | 43.8 |
| O2′ | 30.8 | 12.3 | 44.3 |
| C3′ | 32.7 | 11.0 | 43.8 |
| O3′ | 33.3 | 11.6 | 44.9 |
| C4′ | 33.0 | 12.0 | 42.6 |
| C5′ | 34.4 | 11.7 | 42.0 |
| O5′ | 34.5 | 10.4 | 41.6 |
| P | 35.5 | 9.5 | 42.6 |
| O1P | 35.6 | 10.1 | 43.9 |
| O2P | 35.1 | 8.2 | 42.3 |
| C6 | 31.4 | 9.2 | 40.7 |
| C5 | 31.4 | 7.9 | 40.4 |
| O4 | 30.6 | 5.7 | 41.0 |
| C4 | 30.7 | 7.0 | 41.2 |
| N3 | 30.0 | 7.5 | 42.3 |
| O2 | 29.4 | 9.2 | 43.6 |
| C2 | 30.0 | 8.8 | 42.6 |
| N1 | 30.7 | 9.6 | 41.8 |

60 CYTIDINE

| | | | |
|---|---|---|---|
| O1′ | 29.3 | 8.7 | 47.0 |
| C1′ | 30.1 | 7.6 | 47.4 |
| C2′ | 31.1 | 8.2 | 48.4 |
| O2′ | 31.3 | 7.3 | 49.5 |
| C3′ | 30.4 | 9.4 | 48.9 |
| O3′ | 29.4 | 9.2 | 49.8 |
| C4′ | 29.7 | 9.9 | 47.6 |
| C5′ | 30.6 | 10.7 | 46.6 |
| O5′ | 31.8 | 10.0 | 46.5 |
| P | 33.1 | 11.0 | 46.4 |
| O1P | 33.0 | 12.2 | 47.3 |
| O2P | 34.2 | 10.1 | 46.5 |
| C6 | 32.1 | 7.5 | 45.7 |
| C5 | 32.8 | 6.9 | 44.7 |
| N4 | 32.8 | 5.1 | 43.0 |
| C4 | 32.2 | 5.9 | 44.0 |
| N3 | 30.8 | 5.6 | 44.3 |
| O2 | 29.0 | 5.8 | 45.6 |
| C2 | 30.2 | 6.2 | 45.3 |
| N1 | 30.8 | 7.0 | 46.2 |

61 CYTIDINE

| | | | |
|---|---|---|---|
| O1′ | 32.9 | 6.8 | 52.7 |
| C1′ | 34.2 | 7.4 | 53.0 |
| C2′ | 34.0 | 8.2 | 54.3 |
| O2′ | 34.2 | 7.4 | 55.4 |
| C3′ | 32.5 | 8.6 | 54.2 |
| O3′ | 31.9 | 8.9 | 55.4 |
| C4′ | 31.9 | 7.3 | 53.6 |
| C5′ | 30.6 | 7.4 | 52.9 |
| O5′ | 30.8 | 7.7 | 51.5 |
| P | 29.4 | 7.8 | 50.7 |
| O1P | 29.1 | 6.7 | 49.8 |
| O2P | 28.6 | 8.2 | 51.8 |
| C6 | 34.1 | 8.1 | 50.4 |
| C5 | 34.3 | 8.9 | 49.4 |
| N4 | 35.4 | 11.0 | 48.8 |
| C4 | 35.2 | 10.0 | 49.7 |
| N3 | 35.8 | 10.1 | 50.9 |
| O2 | 36.1 | 9.4 | 53.0 |
| C2 | 35.5 | 9.2 | 51.9 |
| N1 | 34.6 | 8.2 | 51.8 |

62 ADENOSINE

| | | | |
|---|---|---|---|
| O1′ | 34.5 | 9.8 | 56.9 |
| C1′ | 35.7 | 10.6 | 56.6 |
| C2′ | 35.7 | 11.7 | 57.7 |
| O2′ | 36.5 | 11.2 | 58.8 |
| C3′ | 34.3 | 11.8 | 58.1 |
| O3′ | 34.1 | 12.2 | 59.4 |
| C4′ | 33.8 | 10.3 | 58.1 |
| C5′ | 32.3 | 10.0 | 57.9 |
| O5′ | 31.8 | 11.0 | 57.0 |
| P | 31.2 | 10.2 | 55.7 |
| O1P | 29.8 | 9.9 | 55.8 |
| O2P | 31.6 | 11.1 | 54.7 |
| N6 | 35.9 | 13.8 | 51.5 |
| C6 | 36.4 | 13.4 | 52.7 |
| N1 | 37.6 | 13.9 | 53.1 |
| C2 | 38.0 | 13.5 | 54.3 |
| N3 | 37.5 | 12.7 | 55.2 |
| C4 | 36.3 | 12.1 | 54.7 |
| C5 | 35.7 | 12.4 | 53.5 |
| N7 | 34.6 | 11.7 | 53.3 |
| C8 | 34.5 | 11.0 | 54.5 |
| N9 | 35.5 | 11.2 | 55.3 |

63 CYTIDINE

| | | | |
|---|---|---|---|
| O1′ | 36.4 | 16.5 | 59.0 |
| C1′ | 36.4 | 17.6 | 58.1 |
| C2′ | 35.4 | 18.7 | 58.8 |
| O2′ | 36.2 | 19.5 | 59.7 |
| C3′ | 34.5 | 17.8 | 59.6 |
| O3′ | 33.9 | 18.4 | 60.7 |
| C4′ | 35.5 | 16.7 | 60.1 |
| C5′ | 34.8 | 15.4 | 60.5 |
| O5′ | 34.1 | 14.9 | 59.4 |
| P | 33.3 | 13.5 | 59.8 |
| O1P | 33.0 | 13.4 | 61.2 |
| O2P | 32.2 | 13.6 | 58.8 |
| C6 | 35.2 | 15.9 | 56.5 |
| C5 | 34.5 | 15.5 | 55.4 |
| N4 | 34.0 | 16.2 | 53.1 |
| C4 | 34.6 | 16.4 | 54.3 |
| N3 | 35.3 | 17.6 | 54.5 |
| O2 | 36.6 | 19.0 | 55.7 |
| C2 | 36.0 | 17.9 | 55.6 |
| N1 | 35.8 | 17.2 | 56.8 |

64 ADENOSINE

| | | | |
|---|---|---|---|
| O1′ | 35.6 | 21.6 | 58.1 |
| C1′ | 35.4 | 22.2 | 56.8 |
| C2′ | 34.5 | 23.5 | 57.0 |
| O2′ | 35.4 | 24.6 | 57.3 |
| C3′ | 33.7 | 23.1 | 58.2 |
| O3′ | 33.3 | 24.2 | 59.0 |
| C4′ | 34.8 | 22.4 | 59.1 |
| C5′ | 34.3 | 21.4 | 60.1 |
| O5′ | 33.2 | 20.7 | 59.6 |
| P | 32.7 | 19.5 | 60.6 |
| O1P | 32.5 | 19.9 | 61.9 |
| O2P | 31.7 | 18.9 | 59.7 |
| N6 | 33.1 | 19.0 | 52.2 |
| C6 | 33.8 | 20.1 | 52.8 |
| N1 | 34.4 | 20.9 | 51.9 |
| C2 | 35.1 | 22.0 | 52.4 |
| N3 | 35.4 | 22.3 | 53.7 |
| C4 | 34.8 | 21.3 | 54.5 |
| C5 | 34.0 | 20.3 | 54.2 |
| N7 | 33.6 | 19.6 | 55.2 |
| C8 | 34.1 | 20.2 | 56.3 |
| N9 | 34.8 | 21.3 | 55.9 |

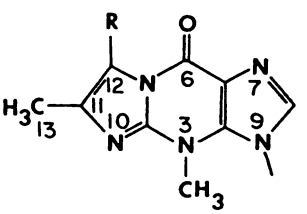
65 GUANOSINE

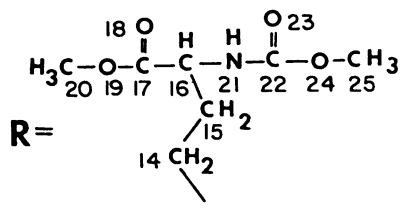
| | | | |
|---|---|---|---|
| O1′ | 33.5 | 25.7 | 54.6 |
| C1′ | 32.8 | 25.6 | 53.3 |
| C2′ | 31.7 | 26.7 | 53.3 |
| O2′ | 32.3 | 27.9 | 52.8 |
| C3′ | 31.4 | 26.9 | 54.8 |
| O3′ | 31.0 | 28.2 | 55.1 |
| C4′ | 32.9 | 26.8 | 55.4 |
| C5′ | 32.9 | 26.4 | 56.8 |
| O5′ | 31.9 | 25.5 | 57.1 |
| P | 31.9 | 25.0 | 58.7 |
| O1P | 31.9 | 26.1 | 59.7 |
| O2P | 31.0 | 23.9 | 58.6 |
| N2 | 31.3 | 23.7 | 48.8 |
| O6 | 30.1 | 20.5 | 51.7 |
| C6 | 30.6 | 21.7 | 51.5 |
| N1 | 30.6 | 22.1 | 50.2 |
| C2 | 31.1 | 23.3 | 50.0 |
| N3 | 31.7 | 24.2 | 50.8 |
| C4 | 31.6 | 23.7 | 52.1 |

Table 1 (continued)

| | X | Y | Z |
|---|---|---|---|
| C5 | 31.1 | 22.5 | 52.5 |
| N7 | 31.3 | 22.4 | 53.8 |
| C8 | 31.9 | 23.5 | 54.2 |
| N9 | 32.1 | 24.3 | 53.2 |
| 66 ADENOSINE | | | |
| O1' | 29.8 | 27.7 | 50.7 |
| C1' | 28.8 | 27.1 | 49.8 |
| C2' | 27.6 | 28.2 | 49.8 |
| O2' | 28.0 | 29.1 | 48.7 |
| C3' | 27.8 | 28.9 | 51.1 |
| O3' | 27.3 | 30.2 | 51.1 |
| C4' | 29.4 | 29.0 | 51.2 |
| C5' | 29.8 | 29.1 | 52.7 |
| O5' | 28.9 | 28.6 | 53.6 |
| P | 29.4 | 28.6 | 55.1 |
| O1P | 29.4 | 29.9 | 55.8 |
| O2P | 28.8 | 27.4 | 55.6 |
| N6 | 26.5 | 21.7 | 51.0 |
| C6 | 26.9 | 22.7 | 50.2 |
| N1 | 26.7 | 22.6 | 48.8 |
| C2 | 27.1 | 23.6 | 48.0 |
| N3 | 27.6 | 24.8 | 48.3 |
| C4 | 27.8 | 24.9 | 49.7 |
| C5 | 27.5 | 23.9 | 50.6 |
| N7 | 27.8 | 24.4 | 51.9 |
| C8 | 28.3 | 25.6 | 51.7 |
| N9 | 28.3 | 25.9 | 50.4 |
| 67 ADENOSINE | | | |
| O1' | 25.4 | 28.1 | 48.0 |
| C1' | 24.6 | 26.9 | 47.6 |
| C2' | 23.2 | 27.4 | 47.2 |
| O2' | 23.2 | 27.7 | 45.8 |
| C3' | 23.1 | 28.7 | 48.0 |
| O3' | 22.2 | 29.7 | 47.4 |
| C4' | 24.6 | 29.3 | 47.8 |
| C5' | 25.0 | 30.3 | 48.9 |
| O5' | 24.9 | 29.7 | 50.2 |
| P | 25.8 | 30.6 | 51.3 |
| O1P | 25.7 | 32.0 | 51.1 |
| O2P | 25.4 | 29.9 | 52.4 |
| N6 | 23.8 | 22.7 | 51.8 |
| C6 | 23.7 | 23.2 | 50.5 |
| N1 | 23.1 | 22.5 | 49.6 |
| C2 | 22.9 | 23.0 | 48.4 |
| N3 | 23.4 | 24.2 | 47.9 |
| C4 | 24.0 | 24.8 | 48.9 |
| C5 | 24.2 | 24.5 | 50.2 |
| N7 | 24.9 | 25.4 | 50.9 |
| C8 | 25.1 | 26.4 | 50.0 |
| N9 | 24.6 | 26.1 | 48.8 |
| 68 URIDINE | | | |
| O1' | 19.2 | 26.7 | 46.8 |
| C1' | 18.5 | 25.6 | 47.5 |
| C2' | 17.0 | 26.2 | 47.8 |
| O2' | 16.2 | 25.9 | 46.7 |
| C3' | 17.3 | 27.7 | 47.8 |
| O3' | 16.2 | 28.5 | 47.5 |
| C4' | 18.4 | 27.9 | 46.7 |
| C5' | 19.2 | 29.1 | 46.8 |
| O5' | 19.7 | 29.3 | 48.1 |
| P | 21.0 | 30.3 | 48.2 |
| O1P | 20.7 | 31.6 | 47.6 |
| O2P | 21.3 | 30.1 | 49.6 |
| C6 | 20.2 | 26.3 | 49.3 |
| C5 | 20.7 | 26.1 | 50.5 |
| O4 | 20.7 | 24.9 | 52.5 |
| C4 | 20.3 | 25.1 | 51.3 |
| N3 | 19.3 | 24.2 | 50.8 |
| O2 | 17.9 | 23.6 | 49.2 |
| C2 | 18.8 | 24.4 | 49.6 |
| N1 | 19.2 | 25.4 | 48.9 |
| 69 URIDINE | | | |
| O1' | 15.2 | 24.5 | 49.5 |
| C1' | 15.2 | 23.8 | 50.7 |
| C2' | 13.8 | 24.0 | 51.4 |
| O2' | 13.0 | 22.9 | 50.9 |
| C3' | 13.3 | 25.3 | 50.7 |
| O3' | 11.9 | 25.4 | 50.6 |
| C4' | 13.9 | 25.1 | 49.2 |
| C5' | 14.1 | 26.4 | 48.5 |
| O5' | 14.6 | 27.4 | 49.4 |
| P | 15.0 | 28.8 | 48.5 |
| O1P | 13.9 | 29.3 | 47.7 |
| O2P | 15.6 | 29.5 | 49.6 |
| C6 | 16.6 | 25.9 | 51.3 |
| C5 | 17.4 | 26.5 | 52.2 |
| O4 | 18.6 | 26.4 | 54.2 |
| C4 | 17.9 | 25.8 | 53.3 |
| N3 | 17.6 | 24.5 | 53.4 |
| O2 | 16.4 | 22.7 | 52.8 |
| C2 | 16.7 | 23.8 | 52.6 |
| N1 | 16.3 | 24.6 | 51.6 |
| 70 CYTIDINE | | | |
| O1' | 11.2 | 22.7 | 53.7 |
| C1' | 11.5 | 22.4 | 55.1 |
| C2' | 10.4 | 23.0 | 56.0 |
| O2' | 9.4 | 22.0 | 56.1 |
| C3' | 9.8 | 24.1 | 55.1 |
| O3' | 8.5 | 24.4 | 55.3 |
| C4' | 9.9 | 23.4 | 53.7 |
| C5' | 9.9 | 24.4 | 52.5 |
| O5' | 10.6 | 25.6 | 52.9 |
| P | 11.1 | 26.4 | 51.5 |
| O1P | 10.0 | 26.9 | 50.7 |
| O2P | 12.1 | 27.2 | 52.2 |
| C6 | 13.4 | 24.1 | 54.4 |
| C5 | 14.5 | 24.9 | 54.7 |
| N4 | 16.1 | 25.6 | 56.4 |
| C4 | 15.1 | 24.8 | 55.9 |
| N3 | 14.6 | 23.8 | 56.8 |
| O2 | 13.1 | 22.2 | 57.3 |
| C2 | 13.5 | 23.0 | 56.5 |
| N1 | 12.8 | 23.2 | 55.3 |
| 71 GUANOSINE | | | |
| O1' | 9.7 | 22.6 | 59.2 |
| C1' | 10.6 | 22.8 | 60.3 |
| C2' | 9.7 | 23.5 | 61.4 |
| O2' | 9.2 | 22.5 | 62.2 |
| C3' | 8.7 | 24.2 | 60.6 |
| O3' | 7.5 | 24.4 | 61.2 |
| C4' | 8.4 | 23.1 | 59.5 |
| C5' | 7.8 | 23.7 | 58.2 |
| O5' | 8.4 | 24.9 | 57.9 |
| P | 8.0 | 25.4 | 56.4 |
| O1P | 6.5 | 25.5 | 56.2 |
| O2P | 8.9 | 26.5 | 56.2 |
| N2 | 14.9 | 23.2 | 63.0 |
| O6 | 15.6 | 26.1 | 59.6 |
| C6 | 14.8 | 25.2 | 60.2 |
| N1 | 15.3 | 24.7 | 61.4 |
| C2 | 14.5 | 23.8 | 62.0 |
| N3 | 13.3 | 23.4 | 61.7 |
| C4 | 12.9 | 23.9 | 60.6 |
| C5 | 13.5 | 24.9 | 59.8 |
| N7 | 12.8 | 25.3 | 58.7 |
| C8 | 11.7 | 24.6 | 58.8 |
| N9 | 11.7 | 23.7 | 59.9 |
| 72 CYTIDINE | | | |
| O1' | 10.5 | 24.9 | 64.7 |
| C1' | 11.7 | 25.6 | 65.1 |
| C2' | 11.3 | 26.6 | 66.2 |
| O2' | 11.4 | 25.9 | 67.4 |
| C3' | 9.8 | 26.8 | 65.9 |
| O3' | 9.0 | 27.1 | 67.0 |
| C4' | 9.4 | 25.3 | 65.4 |
| C5' | 8.1 | 25.3 | 64.5 |
| O5' | 8.5 | 25.8 | 63.2 |
| P | 7.2 | 25.6 | 62.2 |
| O1P | 5.9 | 25.3 | 62.9 |
| O2P | 7.4 | 26.8 | 61.4 |
| C6 | 11.6 | 26.2 | 62.5 |
| C5 | 11.9 | 27.0 | 61.5 |
| N4 | 13.4 | 28.8 | 60.7 |
| C4 | 13.0 | 27.9 | 61.6 |
| N3 | 13.6 | 27.9 | 62.9 |
| O2 | 13.9 | 27.2 | 65.0 |
| C2 | 13.3 | 27.1 | 63.9 |
| N1 | 12.2 | 26.3 | 63.8 |
| 73 ADENOSINE | | | |
| O1' | 13.3 | 29.4 | 67.1 |
| C1' | 13.9 | 30.5 | 66.6 |
| C2' | 13.5 | 31.7 | 67.6 |
| O2' | 14.5 | 31.6 | 68.7 |
| C3' | 12.2 | 31.2 | 68.1 |
| O3' | 11.8 | 31.7 | 69.4 |
| C4' | 12.4 | 29.7 | 68.2 |
| C5' | 11.2 | 28.8 | 68.2 |
| O5' | 10.2 | 29.5 | 67.4 |
| P | 8.8 | 28.7 | 67.4 |
| O1P | 8.2 | 28.6 | 68.7 |
| O2P | 8.2 | 29.3 | 66.3 |
| N6 | 13.1 | 32.6 | 61.1 |
| C6 | 13.8 | 32.6 | 62.2 |
| N1 | 14.9 | 33.3 | 62.4 |
| C2 | 15.5 | 33.2 | 63.6 |
| N3 | 15.3 | 32.5 | 64.6 |
| C4 | 14.1 | 31.7 | 64.4 |
| C5 | 13.4 | 31.7 | 63.3 |
| N7 | 12.3 | 30.9 | 63.4 |
| C8 | 12.5 | 30.4 | 64.7 |
| N9 | 13.5 | 30.9 | 65.3 |
| 74 CYTIDINE | | | |
| O1' | 14.3 | 34.9 | 67.4 |
| C1' | 14.3 | 35.9 | 66.3 |
| C2' | 14.0 | 37.3 | 67.0 |
| O2' | 15.2 | 37.9 | 67.4 |
| C3' | 13.2 | 36.8 | 68.2 |
| O3' | 13.3 | 37.7 | 69.3 |
| C4' | 14.0 | 35.6 | 68.6 |
| C5' | 13.2 | 34.6 | 69.5 |
| O5' | 12.0 | 34.3 | 68.8 |
| P | 11.2 | 33.1 | 69.6 |
| O1P | 11.2 | 33.3 | 71.1 |
| O2P | 10.0 | 33.1 | 68.9 |
| C6 | 12.1 | 34.6 | 65.7 |
| C5 | 11.1 | 34.4 | 64.9 |
| N4 | 10.1 | 34.8 | 62.7 |
| C4 | 11.1 | 34.9 | 63.6 |
| N3 | 12.2 | 35.6 | 63.2 |
| O2 | 14.2 | 36.5 | 63.6 |
| C2 | 13.3 | 35.9 | 64.0 |
| N1 | 13.2 | 35.5 | 65.3 |
| 75 CYTIDINE | | | |
| O1' | 11.7 | 39.3 | 65.1 |
| C1' | 10.5 | 39.3 | 64.3 |
| C2' | 9.7 | 40.6 | 64.7 |
| O2' | 10.2 | 41.6 | 63.8 |
| C3' | 10.2 | 40.8 | 66.1 |
| O3' | 10.1 | 42.1 | 66.5 |
| C4' | 11.7 | 40.4 | 65.9 |
| C5' | 12.4 | 40.1 | 67.3 |
| O5' | 11.5 | 39.3 | 68.0 |
| P | 12.2 | 38.9 | 69.5 |
| O1P | 12.9 | 40.0 | 70.1 |
| O2P | 11.1 | 38.2 | 70.1 |
| C6 | 10.0 | 37.2 | 65.8 |
| C5 | 9.2 | 36.2 | 66.3 |
| N4 | 7.2 | 34.9 | 65.8 |
| C4 | 8.1 | 35.8 | 65.5 |
| N3 | 8.0 | 36.5 | 64.2 |
| O2 | 8.6 | 38.0 | 62.7 |
| C2 | 8.8 | 37.5 | 63.8 |
| N1 | 9.7 | 38.0 | 64.7 |
| 76 ADENOSINE | | | |
| O1' | 12.4 | 43.8 | 69.6 |
| C1' | 13.3 | 45.0 | 69.6 |
| C2' | 12.6 | 45.9 | 70.7 |
| O2' | 13.2 | 45.5 | 72.0 |
| C3' | 11.2 | 45.5 | 70.7 |
| O3' | 10.4 | 45.7 | 71.8 |
| C4' | 11.3 | 43.9 | 70.5 |
| C5' | 10.1 | 43.2 | 69.9 |
| O5' | 9.9 | 43.8 | 68.6 |
| P | 9.1 | 42.6 | 67.6 |
| O1P | 8.7 | 41.4 | 68.3 |
| O2P | 8.2 | 43.5 | 66.9 |
| N6 | 14.2 | 48.3 | 64.7 |
| C6 | 14.5 | 47.9 | 66.0 |
| N1 | 15.5 | 48.5 | 66.7 |
| C2 | 15.7 | 48.1 | 67.9 |
| N3 | 15.1 | 47.2 | 68.7 |
| C4 | 14.1 | 46.6 | 68.0 |
| C5 | 13.7 | 46.9 | 66.7 |
| N7 | 12.7 | 46.1 | 66.3 |
| C8 | 12.5 | 45.3 | 67.3 |
| N9 | 13.2 | 45.6 | 68.4 |

The base Y37 is numbered as follows:



the standard 3'-endo conformation; however, several are found which adopt the 2'-endo conformation: 7, 9, 18, 19, 48, 58 and 60. All of the purines and pyrimidines appear to be in the anti-conformation with the exception of residue A44. A44 is presented in the syn-conformation in Table 1 although it is possible to place the residue in the anti-conformation using the same electron density. Either conformation could form two hydrogen bonds to $m_2^2$G26. Further refinement should clarify this ambiguity.

The torsion angles in the polynucleotide chains are presented in Table 2, together with the angle $\chi$ which describes the conformation of the glycosyl linkage. The major torsional variations are in the two phosphoester linkages ($\beta, \gamma$) as had been suggested previously (9).

Table 2. Torsion Angles in the Polynucleotide Chain

| LINK | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ALPHA | | 204 | 218 | 195 | 209 | 224 | 198 | 162 | 265 | 213 | 271 | 210 | 188 | 155 | 232 | 210 | 250 | 218 | 199 |
| BETA | | 302 | 271 | 290 | 289 | 269 | 275 | 54 | 232 | 345 | 244 | 307 | 324 | 343 | 303 | 193 | 176 | 289 | 206 |
| GAMMA | 352 | 266 | 334 | 320 | 310 | 322 | 6 | 210 | 333 | 163 | 305 | 269 | 342 | 209 | 292 | 156 | 44 | 194 | 21 |
| DELTA | 175 | 189 | 151 | 171 | 153 | 151 | 184 | 186 | 235 | 114 | 142 | 184 | 194 | 137 | 158 | 126 | 207 | 233 | 171 |
| EPSILON | 50 | 50 | 55 | 51 | 55 | 46 | 52 | 54 | 41 | 42 | 41 | 46 | 46 | 39 | 48 | 57 | 50 | 70 | 14 |
| CHI | 9 | -10 | 21 | 9 | 5 | 2 | 55 | 12 | 117 | -28 | -10 | 21 | 12 | -5 | 12 | 35 | 95 | 68 | 110 |

| LINK | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ALPHA | 156 | 209 | 146 | 209 | 215 | 197 | 169 | 183 | 193 | 225 | 197 | 200 | 243 | 218 | 203 | 234 | 208 | 174 | 208 |
| BETA | 57 | 308 | 309 | 284 | 288 | 321 | 345 | 335 | 305 | 277 | 306 | 329 | 298 | 292 | 327 | 279 | 308 | 316 | 314 |
| GAMMA | 177 | 55 | 216 | 307 | 296 | 309 | 273 | 261 | 301 | 295 | 304 | 238 | 321 | 311 | 181 | 294 | 296 | 302 | 287 |
| DELTA | 217 | 188 | 139 | 172 | 167 | 192 | 177 | 202 | 171 | 146 | 183 | 127 | 175 | 166 | 138 | 157 | 181 | 174 | 159 |
| EPSILON | 56 | 50 | 54 | 49 | 42 | 45 | 51 | 55 | 47 | 56 | 49 | 55 | 50 | 47 | 52 | 51 | 49 | 49 | 62 |
| CHI | -17 | 45 | 7 | 21 | 18 | 8 | 17 | -6 | -10 | 13 | 30 | 5 | 38 | 30 | -1 | 5 | 18 | 13 | 0 |

| LINK | 39 | 40 | 41 | 42 | 43 | 44 | 45 | 46 | 47 | 48 | 49 | 50 | 51 | 52 | 53 | 54 | 55 | 56 | 57 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ALPHA | 211 | 162 | 179 | 199 | 198 | 199 | 204 | 234 | 168 | 122 | 175 | 203 | 191 | 178 | 176 | 209 | 233 | 235 | 137 |
| BETA | 322 | 333 | 327 | 297 | 297 | 287 | 338 | 233 | 266 | 110 | 137 | 302 | 313 | 319 | 330 | 295 | 292 | 232 | 17 |
| GAMMA | 295 | 254 | 291 | 298 | 294 | 329 | 288 | 45 | 157 | 334 | 350 | 281 | 294 | 278 | 238 | 317 | 287 | 137 | 253 |
| DELTA | 185 | 196 | 200 | 160 | 161 | 184 | 174 | 146 | 179 | 222 | 217 | 187 | 182 | 186 | 167 | 173 | 157 | 241 | 191 |
| EPSILON | 45 | 54 | 51 | 52 | 49 | 48 | 50 | 41 | 49 | 49 | 58 | 54 | 50 | 52 | 66 | 49 | 45 | 43 | 79 |
| CHI | 4 | 6 | 17 | 18 | 14 | -163 | 31 | 82 | 30 | 45 | -5 | 15 | 31 | 12 | 11 | 24 | 12 | -11 | 45 |

| LINK | 58 | 59 | 60 | 61 | 62 | 63 | 64 | 65 | 66 | 67 | 68 | 69 | 70 | 71 | 72 | 73 | 74 | 75 | 76 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ALPHA | 193 | 83 | 176 | 136 | 235 | 229 | 183 | 198 | 199 | 193 | 234 | 189 | 215 | 198 | 194 | 201 | 195 | 203 | 224 |
| BETA | 337 | 196 | 335 | 44 | 235 | 287 | 300 | 304 | 292 | 308 | 279 | 318 | 268 | 295 | 312 | 315 | 313 | 335 | 142 |
| GAMMA | 324 | 269 | 277 | 130 | 330 | 264 | 293 | 299 | 322 | 283 | 296 | 294 | 309 | 301 | 258 | 307 | 284 | 286 | 250 |
| DELTA | 237 | 253 | 218 | 180 | 119 | 187 | 170 | 177 | 172 | 159 | 161 | 173 | 159 | 169 | 172 | 184 | 175 | 180 | 151 |
| EPSILON | 42 | 84 | 21 | 59 | 51 | 51 | 43 | 51 | 44 | 45 | 52 | 51 | 53 | 56 | 52 | 48 | 49 | 52 | 46 |
| CHI | 111 | -16 | 91 | -28 | -7 | 9 | 15 | 17 | 22 | 0 | 11 | 25 | 2 | 18 | -9 | 11 | 20 | 13 | 10 |

.The system defining the torsion angles of the internucleotide linkage is described elsewhere (12). $\alpha$ refers to the torsion angle defined by C4', C3', O3', P; $\beta$ is defined by C3', O3', P, O5'; $\gamma$ is defined by O3', P, O5', C5'; $\delta$ is defined by P, O5', C5', C4'; $\epsilon$ is defined by O5', C5', C4', C3'. The angle $\chi$ describes the torsion angle about the glycosyl linkage. The internucleotide linkage has the same number as the nucleotide on the O5' side of the phosphorus atom.

Recent publication of the atomic coordinates for yeast phenylalanine tRNA in the monoclinic crystal (6) has made it possible to compare the conformation in these two crystal forms. In the initial description of the conformation in the monoclinic crystal, Robertus et al. (3) were unable to define the vital interactions between the D loop and the TΨC loop at the corner of the molecule. Inspection of the atomic coordinates in the monoclinic cell shows that they have confirmed the assignments which we made of the tertiary interactions in the orthorhombic unit cell somewhat over a year ago (2). Their coordinates indicate the interaction between Ψ55 and G18 as well as the stacking interactions of the other bases in the complex intertwining of these two loops (2, 7). In addition, they appear to have reinterpreted the conformation of the molecule in the segment lying between the acceptor stem and the D stem. In their initial description, $m_2^2$G26 was described as partially intercalated between the bases A44 and G45 (3). In their revised interpretation (6), they have adopted a geometry very similar to that which we described earlier, including appropriate modifications in the stacking interactions in this part of the molecule (2, 7). Thus the similarities in the conformation of the molecule in these two different crystal forms is greater than was initially apparent.

A comparison of the conformation of yeast phenylalanine tRNA in the two different crystal forms is shown in Figure 1. A projection is shown in which lines connect the group coordinates in the molecule as described in the figure legend. It can be seen that the conformation of the two molecules is quite similar with the exception of the two terminal residues at the end of the acceptor stem. Leaving out these two residues, the mean deviation in the positions of the atomic coordinates is 1.1Å while the mean difference in the positions of the group coordinates is 0.99Å. The residues for which there is a significant difference in conformation include D17, U47 and the side chain of Y37.

Using an independent refinement analysis on the orthorhombic data, another set of coordinates has been obtained (5). The group coordinates of the two different refinement analyses of the orthorhombic crystal form have a mean deviation of 0.96Å. This comparison makes

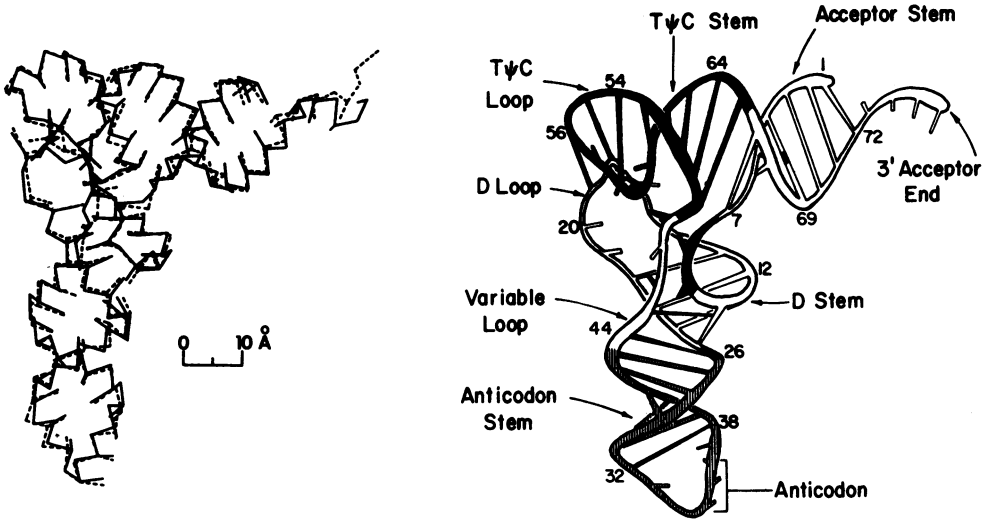



Figure 1. Comparison of the conformation of yeast phenylalanine tRNA in two crystal forms. The two molecules from the orthorhombic and monoclinic unit cells have been fitted by a least squares procedure (10). Three group coordinates are plotted: the position of the phosphorus atom, the centroid of the five atoms in the furanose ring of ribose, and the centroid of the six atoms which make up the six-membered ring in either pyrimidines or purines. The solid line connecting the group coordinates represents the conformation of the molecule in the orthorhombic unit cell, while the dashed line shows its conformation in the monoclinic unit cell. In the schematic diagram at the right, secondary and tertiary hydrogen bonds between bases are shown with different shading (2). The numbers refer to the residues in the polynucleotide chain.

it very clear that the conformations of the molecule in the monoclinic and the orthorhombic unit cells are essentially indistinguishable at this resolution except for the nucleotides at the 3' end of the molecule.

Several features of the hydrogen bonding interactions of yeast phenylalanine tRNA have been described recently (4). However, some additional observations can be made. It is interesting, for example, that both the orthorhombic and monoclinic analyses appear to show a GU base pair held together by two hydrogen bonds. Position 57 is always a purine (7). In the structure, there is a hydrogen bond between ribose 55 O2' and N7 of G57, a bond which can be preserved even if position 57 is adenine. In the present structure, G57 also has two other potential hydrogen bonds between the amino group N2 and O2' of

ribose 18 and O1' of ribose 19. These may further stabilize the structure.

Position 55 is always Ψ while position 33 is always uracil in tRNAs involved in polypeptide chain elongation (7). There may be structural reasons for these constancies. Both of these residues occur in a position where the polynucleotide chain turns a corner. As described previously (4), Ψ55 has P37 on top of the base while the N3 of Ψ55 forms a hydrogen bond to the phosphate group of P58. In a similar way, U33 is near the bend in the anticodon loop and it has P35 on top of the base U33, while N3 of U33 forms a hydrogen bond with phosphate P36. Thus the bases of both Ψ55 and U33 stabilize the corner in analogous ways. The geometry suggests a possible additional hydrogen bond from N1 of Ψ55 to phosphate 54, although the distance is too long at the present stage of refinement.

It is of interest that the anticodon loop is likely to be further stabilized by a hydrogen bond between N6 of A38 and O2 of C32. Since position 32 is always occupied by a pyrimidine containing O2 and position 38 usually has an appropriately positioned proton donor, it is possible that this interaction is of a general nature. The present coordinates show a hydrogen bonding distance between N4 of C61 and a phosphate oxygen of C60. If this distance remains after further refinement, it may provide an explanation for the constant GC pair found at the base of the TΨC stem. Finally, there is limited space around the constant pyrimidine site C60 and this may prevent insertion of a purine at this position in those tRNAs involved in the elongation of polypeptide chains.

With these observations, we can now give structural reasons for almost all of the base conservation in tRNA sequences.

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REFERENCES


1. Kim, S. H., Quigley, G. J., Suddath, F. L., McPherson, A., Sneden, D., Kim, J. J., Weinzierl, J. and Rich, A. (1973) Science 179, 285-288.
2. Kim, S. H., Suddath, F. L., Quigley, G. J., McPherson, A., Sussman, J. L., Wang, A. H.-J., Seeman, N. C. and Rich, A. (1974) Science 185, 435-440.
3. Robertus, J. D., Ladner, J. E., Finch, J. T., Rhodes, D., Brown, R. D., Clark, B. F. C. and Klug, A. (1974) Nature 250, 546-551.
4. Quigley, G. J., Wang, A. H.-J., Seeman, N. C., Suddath, F. L., Rich, A., Sussman, J. L. and Kim, S. H., Proc. Nat. Acad. Sci., Wash. (in press).
5. Sussman, J. L. and Kim, S. H., Biochem. Biophys. Res. Comm. (in press).
6. Ladner, J. E., Jack, A., Robertus, J. D., Brown, R. S., Rhodes, D., Clark, B. F. C. and Klug, A. (1975) Nucleic Acid Res. 2, 1629-1637.
7. Kim, S. H., Sussman, J. L., Suddath, F. L., Quigley, G. J., McPherson, A., Wang, A. H.-J., Seeman, N. C. and Rich, A. (1974) Proc. Nat. Acad. Sci. 71, 4970-4974.
8. Huber, R., Kukla, D., Bode, W., Schwager, P., Bartels, K., Diesenhofer, J. and Steigemann, W. (1974) J. Mol. Biol. 89, 73-101.
9. Seeman, N. C., Sussman, J. L., Berman, H. M. and Kim, S. H. (1971) Nature New Biol. 233, 90-92.
10. Nyburg, S. C. (1974) Acta Cryst. B30, 251-253.
11. Koetzle, T. F. (1973) Acta Cryst. B29, 1746.
12. Seeman, N. C., Rosenberg, J. M., Suddath, F. L., Kim, J. J. and Rich, A., J. Mol. Biol. (in press).