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JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

J. Am. Chem. Soc., 1998, 120(17), 4230-4231, DOI:[10.1021/ja972607u](https://doi.org/10.1021/ja972607u)

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Supporting Information Table S1. <sup>13</sup>C Chemical Shifts and Structure Parameters of Crystalline Samples

| No. | REFCODE     | name*                           | C1'   | C2'   | C3'   | C3'-3.5 | C4'   | C5'   | C5'-3.5 | P     | V <sub>m</sub> | χ      | γ      | δ     | β     |
|-----|-------------|---------------------------------|-------|-------|-------|---------|-------|-------|---------|-------|----------------|--------|--------|-------|-------|
| 1   | BAFPAZ      | 5-bromo-2'-deoxycytidine        | na**  | 42.00 | 64.61 |         | na    | 58.84 |         | 16.9  | 37.1           | 156.7  | 55.7   | 79.6  |       |
| 2   | BEURID10-1  | uridine-1                       | 91.69 | 74.75 | 66.15 |         | 82.37 | 58.27 |         | 3.6   | 40.4           | -164.4 | 45.9   | 80.8  |       |
| 3   | IURIDN10-1  | 5-iodo-uridine-1                | 92.10 | na    | 66.59 |         | 84.03 | 59.40 |         | 8.8   | 36.0           | -164.3 | 62.2   | 76.2  |       |
| 4   | CYTIDI10    | cytidine                        | 92.90 | 76.00 | 67.00 |         | 84.50 | 60.50 |         | 9.0   | 38.0           | -162.8 | 47.1   | 83.0  |       |
| 5   | DXCYTD-1    | 2'-deoxycytidine-1              | 88.66 | 38.06 | 67.16 |         | 82.82 | 57.58 |         | 13.3  | 37.1           | -158.8 | 56.7   | 82.3  |       |
| 6   | MEURID      | 5-methyluridine                 | 90.38 | 77.23 | 67.29 |         | 83.99 | 59.03 |         | 15.2  | 40.8           | -154.2 | 49.4   | 82.1  |       |
| 7   | BEURID10-2  | uridine-2                       | 91.69 | 74.75 | 68.47 |         | 82.37 | 61.37 |         | 13.8  | 42.5           | -153.0 | 39.6   | 72.8  |       |
| 8   | ADPOSM      | adenosine 5'-phosphate          | 89.69 | 76.85 | 69.10 |         | 79.33 | 62.36 | 58.86   | 12.2  | 43.9           | -163.9 | 40.0   | 75.5  | 177.2 |
| 9   | SDGUNP01    | 2'-deoxygaunosine 5'-phosphate  | 84.40 | 42.94 | 70.60 |         | 81.70 | 66.90 | 63.40   | 83.8  | 40.8           | -123.3 | 176.9  | 93.4  | 112.4 |
| 10  | AZURID10-1  | 6-azauridine-1                  | 91.90 | 74.21 | 71.24 |         | 82.87 | 65.60 |         | 27.6  | 37.6           | -93.1  | -170.1 | 80.4  |       |
| 11  | AZURID10-2  | 6-azauridine-2                  | 91.90 | 74.21 | na    |         | 85.07 | 65.74 |         | 6.5   | 31.7           | -94.8  | -173.3 | 87.0  |       |
| 12  | TGUANS10    | 6-thioguanosine                 | 86.09 | 76.50 | 71.62 |         | 86.09 | 64.09 |         | 157.1 | 37.4           | -109.6 | -175.2 | 139.4 |       |
| 13  | ADENOS10    | adenosine                       | 92.70 | 75.50 | 71.80 |         | 85.40 | 63.30 |         | 6.9   | 36.8           | -171.4 | 176.9  | 83.3  |       |
| 14  | IDOCYT      | 5-iodo-2'-deoxycytidine         | 90.08 | 44.39 | 72.01 |         | 90.08 | 61.56 |         | 204.7 | 38.4           | -174.7 | 177.0  | 156.0 |       |
| 15  | CEZBIS      | 2'-deoxyadenosine               | 88.51 | 42.45 | 72.24 |         | 92.60 | 64.26 |         | 194.4 | 35.5           | -182.7 | 173.1  | 203.6 |       |
| 16  | THYDIN      | 2'-deoxythymidine               | 87.17 | 41.25 | 72.61 |         | 87.17 | 61.33 |         | 187.5 | 37.2           | -139.4 | 172.8  | 156.2 |       |
| 17  | BROXUR10    | 5-bromo-2'-deoxyuridine         | 88.00 | 41.30 | 72.80 |         | 88.00 | 64.10 |         | 145.5 | 41.2           | -138.9 | 166.7  | 142.5 |       |
| 18  | CLDOUR      | 5-chloro-2'-deoxyuridine        | 85.83 | 41.49 | 72.91 |         | 87.89 | 63.15 |         | 146.8 | 43.5           | -143.0 | 168.1  | 141.1 |       |
| 19  | GUOPNA01    | guanosine 5'-phosphate          | 86.88 | 79.08 | 73.24 |         | 86.88 | 66.05 | 62.55   | 170.5 | 35.2           | -122.6 | 54.8   | 147.3 | 172.1 |
| 20  | NAINSP      | inosine 5'-phosphate            | 87.64 | 77.81 | 73.26 |         | 87.64 | 65.17 | 61.67   | 160.0 |                | -130.0 | 56.0   |       | 172.0 |
| 21  | IDOXUR      | 5-iodo-2'-deoxyuridine          | 84.33 | 39.13 | 73.50 |         | 88.33 | 62.80 |         | 153.3 | 38.5           | -111.0 | 51.4   | 146.6 |       |
| 22  | DOURID-1    | 2'-deoxyuridine-1               | 88.42 | 40.47 | 73.83 |         | 87.00 | 62.57 |         | 173.0 | 38.6           | -153.6 | -69.2  | 156.6 |       |
| 23  | DOURID-2    | 2'-deoxyuridine-2               | 88.42 | 38.55 | 73.83 |         | 87.50 | 62.57 |         | 177.9 | 36.5           | -156.5 | -74.4  | 158.9 |       |
| 24  | CYTIAC      | cytidine 3'-phosphate           | 85.98 | 76.44 | 77.37 | 73.87   | 84.73 | 64.90 |         | 169.4 | 40.3           | -133.9 | 43.8   | 152.0 |       |
| 25  | ARBCYT10    | 1-β-D-arabinofuranosyl-cytosine | 89.63 | 78.89 | 74.68 |         | 89.63 | 64.09 |         | 162.3 | 37.3           | -150.0 | 51.6   | 145.4 |       |
| 26  | DOCYPO      | 2'-deoxycytidine 5'-phosphate   | 92.90 | 44.60 | 74.70 |         | 87.50 | 67.10 | 63.60   | 213.4 | 32.8           | -177.8 | 56.4   | 153.4 | 165.8 |
| 27  | INOSINE10-1 | inosine                         | 91.73 | 69.60 | 74.81 |         | 85.10 | 63.31 |         | 163.6 | 39.1           | -58.4  | 64.0   | 145.6 |       |
| 28  | DXCYTD-2    | 2'-deoxycytidine-2              | 87.12 | 44.28 | 75.76 |         | 87.12 | 63.63 |         | 168.8 | 39.0           | -137.7 | 62.4   | 148.2 |       |
| 29  | XDATA       | 3-deazauridine                  | 84.90 | 75.76 | 75.76 |         | 84.90 | 64.01 |         | 162.5 | 37.9           | -126.2 | 55.1   | 144.7 |       |
| 30  | IURIDN10-2  | 5-iodo-uridine-2                | 86.76 | na    | na    |         | 85.18 | 63.82 |         | 174.8 | 42.2           | -117.4 | -65.4  | 160.4 |       |
| 31  | HXURID      | 5-hydrouridine                  | 85.46 | na    | na    |         | 87.22 | 63.59 |         | 147.2 | 43.9           | -144.0 | 52.8   | 140.4 |       |

\* the content of sodium and water is not listed    \*\* not assignment

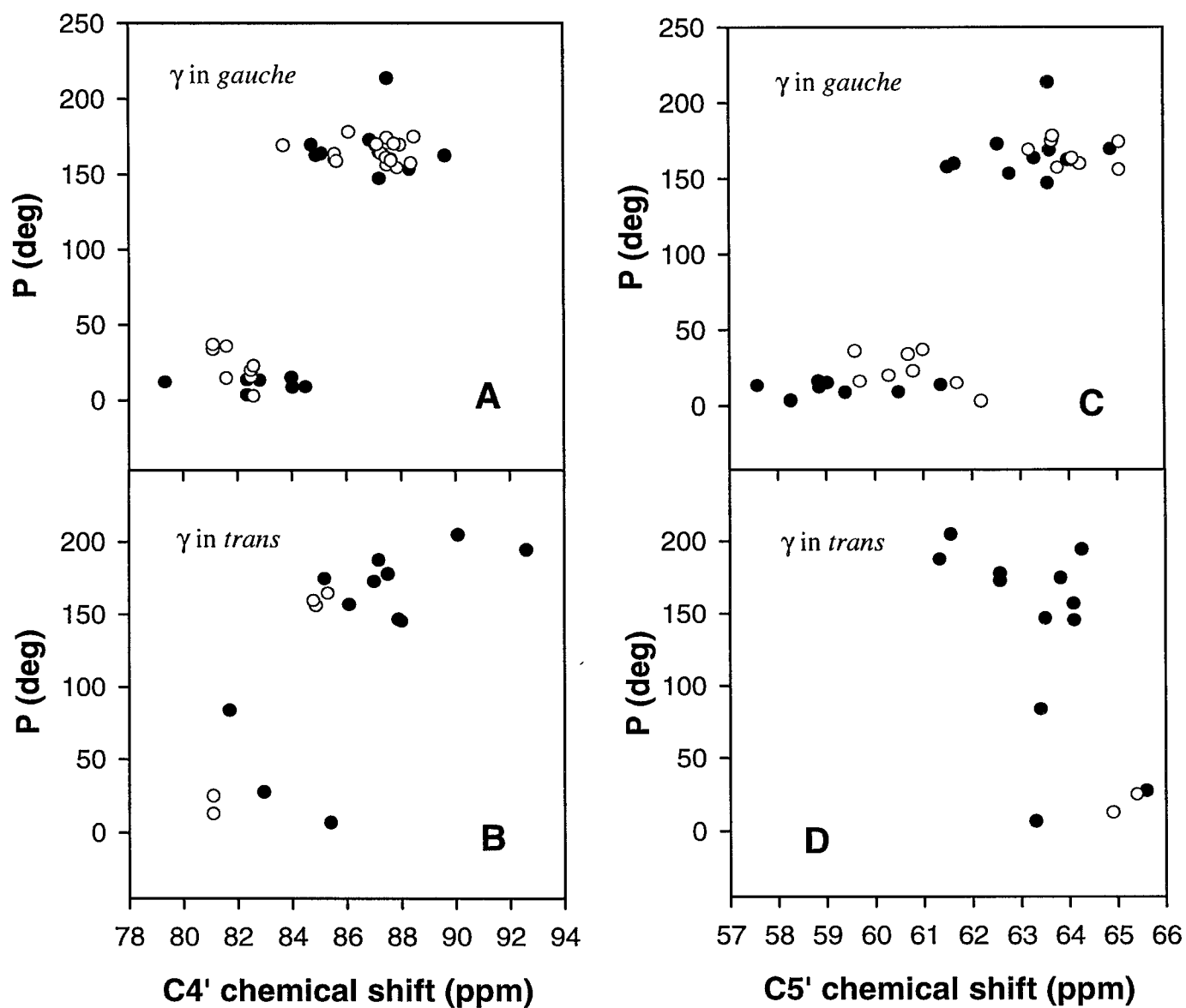
Supporting Information Table S2. <sup>13</sup>C Chemical Shifts and Structure Parameters of Solution Samples

| Name           | C1'   | C2'   | C3'       | C3'-3.5   | C4'       | C5'   | C5'-3.5 | P      | Vm    | χ       | γ       | δ      | α        | β        | ε         | ζ       |
|----------------|-------|-------|-----------|-----------|-----------|-------|---------|--------|-------|---------|---------|--------|----------|----------|-----------|---------|
| d(CGCGCG)2     |       |       |           |           |           |       |         |        |       |         |         |        |          |          |           |         |
| C1             | 88.20 | 39.63 | 78.00     | 74.50     | 88.39     | 63.80 |         | 157.25 | 34.00 | -145.31 |         | 131.98 |          |          | -157.48   | -134.25 |
| G2             | 84.47 | 40.11 | 79.85     | 76.35     | 87.50     | 68.58 | 65.08   | 174.06 | 37.03 | -112.61 | 65.03   | 157.19 | -67.23   | 154.74   | -157.22   | -110.40 |
| C3             | 86.50 | 39.90 | 76.80     | 73.30     | 85.58     | 67.76 | 64.26   | 160.04 | 33.53 | -132.40 | 51.17   | 128.52 | -75.40   | -177.76  | -177.01   | -89.72  |
| G4             | 84.53 | 40.30 | 79.95     | 76.45     | 87.50     | 68.58 | 65.08   | 156.09 | 35.17 | -96.34  | 73.36   | 137.64 | -105.17  | -156.51  | -155.85   | -123.89 |
| C5             | 86.50 | 39.90 | 76.80     | 73.30     | 85.58     | 67.60 | 64.10   | 163.39 | 31.71 | -133.23 | 57.76   | 116.39 | -64.43   | 158.33   | -163.11   | -100.89 |
| G6             | 84.80 | 41.90 | 73.50     |           | 88.50     | 67.18 | 63.68   | 174.74 | 28.99 | -94.06  | 48.15   | 137.55 | -75.81   | -160.93  |           |         |
| 5'GGACUUCGGUCC |       |       |           |           |           |       |         |        |       |         |         |        |          |          |           |         |
| G1             | 90.6  | 74.3  | 73.6      | 70.1      | 82.6      | 65.7  | 62.2    | 3.0    | 39.5  | -177.0  |         | 84.0   |          |          | -145.0    | -70.0   |
| G2             | 91.9  | 74.8  | 72.0/72.4 | 68.5/68.9 | 81.6      | 65.2  | 61.7    | 15.0   | 38.3  | -171.0  | 66.0    | 85.0   | -79.0    | 173.0    | -160.0    | -60.0   |
| A3             | 91.9  | 74.9  | 72.0/72.4 | 68.5/68.9 | 81.1      | 64.2  | 60.7    | 34.0   | 37.2  | -156.0  | 61.0    | 83.0   | -85.0    | -171.0   | -160.0    | -65.0   |
| C4             | 92.9  | 74.9  | 71.5      | 68.0      | 81.1/82.5 | 64.5  | 61.0    | 37.0   | 39.6  | -134.0  | 60.0    | 81.0   | -110.0   | -170.0   | -164.0    | -78.0   |
| U5             | 93.5  | 75.3  | 72.5      | 69.0      | 81.6      | 63.1  | 59.6    | 36.0   | 39.2  | -126.0  | 62.0    | 85.0   | -109.0   | -176.0   | 160.0     | -80.0   |
| U6             | 88.2  | 74.2  | 77.0      | 73.5      | 86.1      | 67.2  | 63.7    | 178.0  | 33.9  | -164.0  | 66.0    | 148.0  | -180.0   | 163.0    | -81.0     | -88.0   |
| C7             | 88.3  | 76.9  | 79.5      | 76.0      | 83.7      | 66.7  | 63.2    | 169.0  | 35.8  | -156.0  | 58.0    | 153.0  | -97.0    | 177.0    | -84.0     | 98.0    |
| G8             | 93.5  | 76.6  | 75.1      | 71.6      | 81.1/82.5 | 68.4  | 64.9    | 13.0   | 38.2  | 36.0    | 169.0   | 85.0   | 86.0     | -172.0   | -171/-112 | -29/-78 |
| G9             | 92.2  | 74.3  | 73.8      | 70.3      | 81.1/82.5 | 69.0  | 65.5    | 25.0   | 39.1  | -148.0  | 90.0    | 84.0   | -166/-34 | -116/122 | -166.0    | -68.0   |
| U10            | 93.3  | 74.5  | 71.4      | 67.9      | 81.1/82.5 | 63.2  | 59.7    | 16.0   | 39.9  | -152.0  | 69.0    | 82.0   | -90.0    | 172.0    | -165.0    | -67.0   |
| C11            | 92.9  | 74.9  | 71.6      | 68.1      | 81.1/82.5 | 63.8  | 60.3    | 20.0   | 40.1  | -163.0  | 69.0    | 81.0   | -84.0    | 176.0    | -164.0    | -67.0   |
| C12            | 91.9  | 76.8  | 69.2      |           | 82.6      | 64.3  | 60.8    | 23.0   | 38.4  | -159.0  | 60.0    | 80.0   | -84.0    | -174.0   |           |         |
| d(CGTACG)2     |       |       |           |           |           |       |         |        |       |         |         |        |          |          |           |         |
| C1             | 87.72 | na    | 77.83     | 74.33     | 87.98     | na    |         | 169.45 | 30.24 | -136.00 |         | 135.87 |          |          | -161.78   | -105.25 |
| G2             | 84.42 | na    | 79.71     | 76.21     | 87.22     | na    |         | 164.84 | 32.79 | -101.01 | 63.64   | 140.64 | -77.49   | 177.32   | 177.37    | -84.9   |
| T3             | 85.05 | na    | 77.62     | 74.12     | 85.66     | na    |         | 158.80 | 38.66 | -125.20 | 61.38   | 120.03 | -63.06   | 166.21   | -167.11   | -120.64 |
| A4             | 84.82 | na    | 79.55     | 76.05     | 87.30     | na    |         | 163.61 | 37.01 | -98.29  | 58.88   | 143.82 | -64.19   | 176.90   | 177.16    | -101.63 |
| C5             | 85.75 | na    | 75.82     | 72.32     | 84.87     | na    |         | 156.28 | 36.04 | -131.65 | 179.57  | 134.94 | 140.39   | 176.51   | -171.27   | -89.32  |
| G6             | 84.56 | na    | 73.44     |           | 87.77     | na    |         | 170.10 | 30.67 | -88.28  | 53.88   | 134.91 | -76.57   | -161.94  |           |         |
| d(CATATG)2     |       |       |           |           |           |       |         |        |       |         |         |        |          |          |           |         |
| C1             | 87.48 | na    | 77.26     | 73.76     | 87.88     | na    |         | 154.21 | 36.41 | -145.45 |         | 136.75 |          |          | 153.49    | -116.56 |
| A2             | 85.02 | na    | 79.51     | 76.01     | 87.14     | na    |         | 169.78 | 31.59 | -101.00 | 65.95   | 133.53 | -73.52   | 177.41   | -179.03   | -85.76  |
| T3             | 84.59 | na    | 76.88     | 73.38     | 85.30     | na    |         | 164.89 | 37.58 | -133.53 | -164.82 | 134.31 | 111.15   | -155.65  | -155.78   | -120.67 |
| A4             | 85.02 | na    | 78.70     | 75.20     | 87.48     | na    |         | 161.04 | 33.88 | -110.10 | 60.05   | 134.94 | -68.71   | 176.33   | -179.32   | -71.44  |
| T5             | 84.54 | na    | 75.92     | 72.42     | 84.77     | na    |         | 159.81 | 33.32 | -138.63 | -160.06 | 110.91 | 118.91   | -166.01  | -166.12   | -99.27  |
| G6             | 84.44 | na    | 72.95     |           | 87.66     | na    |         | 158.99 | 33.79 | -112.45 | 78.45   | 127.10 | -65.29   | 163.25   |           |         |

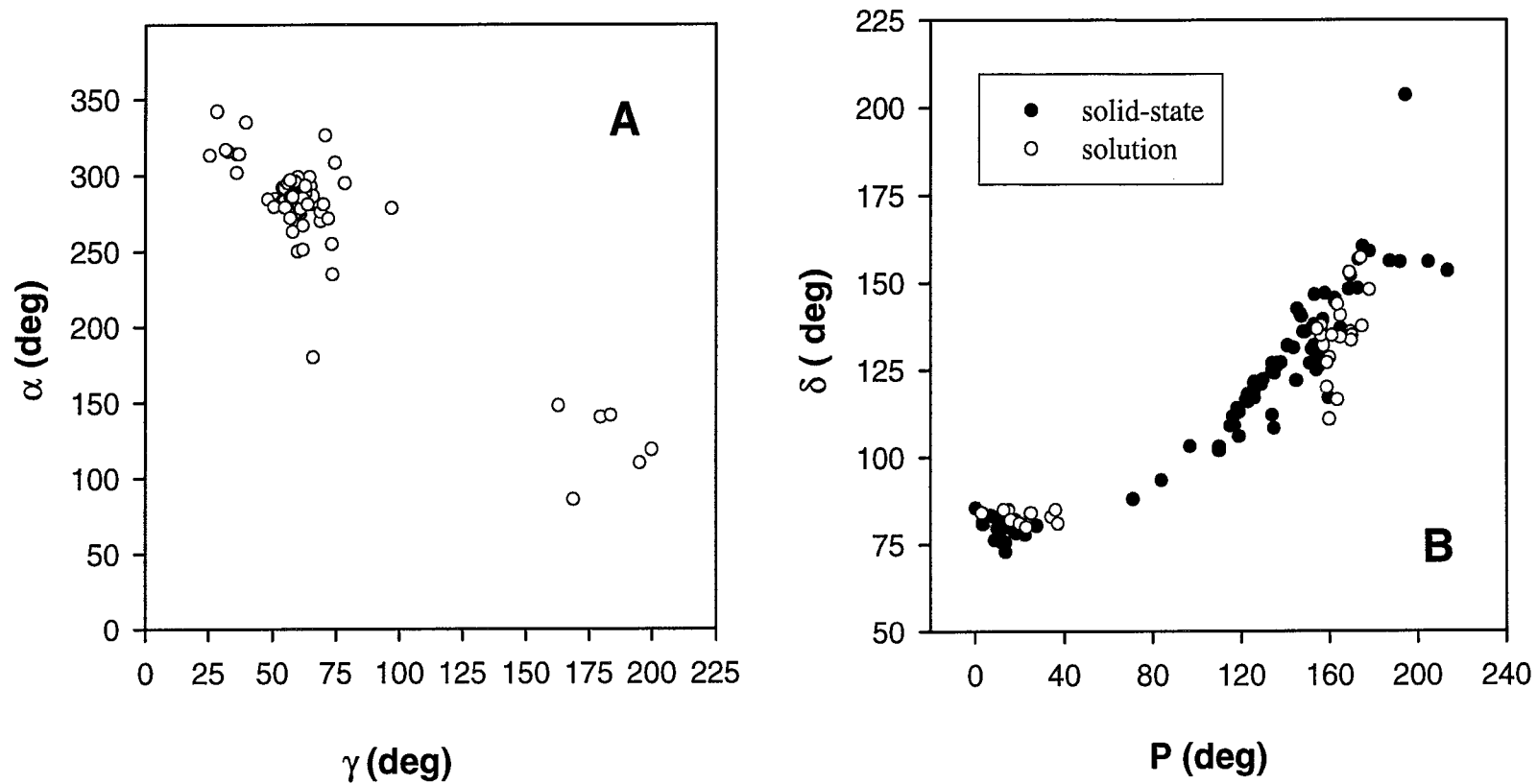
**Supporting Information Table S3. Structure Parameters of Solution Samples**

| Name             | P     | Vm | $\chi$ | $\gamma$ | $\delta$ | $\alpha$ | $\beta$ | $\varepsilon$ | $\zeta$ |
|------------------|-------|----|--------|----------|----------|----------|---------|---------------|---------|
| L10              |       |    |        |          |          |          |         |               |         |
| T1               | 155.3 |    | -126.6 | 62.1     | 136.9    |          |         | -174.5        | -86.7   |
| C2               | 135.1 |    | -107.4 | 55.8     | 124.1    | -72.4    | 187.1   | -180.9        | -88.9   |
| T3               | 117.7 |    | -115   | 57.6     | 112.4    | -65.7    | 174.9   | -177.6        | -96.8   |
| A4               | 129.1 |    | -105.9 | 62.5     | 120.9    | -65.9    | 172.1   | -185.5        | -93.1   |
| T5               | 129.7 |    | -115.9 | 61.5     | 122.1    | -62.3    | 172.1   | -177.8        | -98.7   |
| C6               | 126   |    | -111.1 | 61.5     | 121.5    | -67.3    | 175.1   | -175          | -91.8   |
| A7               | 159.5 |    | -111.2 | 57.7     | 117.1    | -72.4    | 174.7   | -181.5        | -99.3   |
| C8               | 143.8 |    | -109.6 | 60.5     | 131.3    | -68.5    | 177.4   | -184.3        | -89.5   |
| C9               | 122   |    | -116   | 59.4     | 116.4    | -63.6    | 176.6   | -172.2        | -90.5   |
| G10              | 96.9  |    | -116.8 | 50.6     | 103.2    | -80.7    | 179.3   |               |         |
| C11              | 134   |    | -115.6 | 67.4     | 124.9    |          |         | -173.5        | -91     |
| G12              | 138.1 |    | -106.5 | 55.9     | 127.1    | -74.7    | 182.7   | -178.8        | -102.3  |
| G13              | 125.6 |    | -116.4 | 55.6     | 118.1    | -71.5    | 182.8   | -178.9        | -84     |
| T14              | 116.1 |    | -113.1 | 57.1     | 111.7    | -63.9    | 170.7   | -174.7        | -91.5   |
| G15              | 125.7 |    | -108.3 | 55.7     | 117      | -67      | 174.9   | -185.4        | -92.1   |
| A16              | 125.8 |    | -112.5 | 56.7     | 118.8    | -64      | 178.2   | -176.9        | -92.1   |
| T17              | 116.4 |    | -116.9 | 59.1     | 111.5    | -62.7    | 169.7   | -173.4        | -104.1  |
| A18              | 136.1 |    | -102.5 | 64.5     | 126.1    | -61.1    | 166.3   | -177.6        | -91.7   |
| G19              | 130   |    | -106.7 | 58.7     | 122.3    | -67.2    | 171.1   | 178.1         | -102.7  |
| A20              | 134.7 |    | -100.8 | 61.2     | 108.3    | -71      | 166.7   |               |         |
| (rGCGGACGC)2     |       |    |        |          |          |          |         |               |         |
| G1               | 10    |    | -159.9 | 176.8    | 79.6     |          |         | -160.4        | -63.2   |
| C2               | 13.6  |    | -165   | 56.7     | 75.6     | -72.6    | 177.4   | -161.2        | -63.7   |
| G3               | 17.7  |    | -163.5 | 61       | 79.9     | -73.8    | 179.7   | -167.7        | -72.8   |
| G4               | 11.1  |    | -144.1 | 62.5     | 78.5     | -74.5    | 179.4   | -171.8        | -56.9   |
| A5               | 0.3   |    | -180.4 | -176.4   | 85.5     | 141.5    | 190.6   | -149.8        | -60     |
| C6               | 18.6  |    | -163   | 55.25    | 78.1     | -72      | 184.2   | -164.5        | -63.2   |
| G7               | 17.6  |    | -154.2 | 56.8     | 79       | -75.2    | 177.8   | -164          | -61.4   |
| C8               | 22.4  |    | -158.8 | 54.9     | 77.8     | -76.8    | 180.5   |               |         |
| d-GGATTGGCCAATCC |       |    |        |          |          |          |         |               |         |
| G1               | 121   |    | -132.7 | 30.8     |          |          | 208.5   | -179.6        | -84.8   |
| G2               | 152.6 |    | -109   | 32.7     |          | -44.5    | 204.2   | -193.6        | -98.9   |
| A3               | 180.2 |    | -110.9 | 25.5     |          | -46.6    | 219.7   | -201.4        | -103.3  |
| T4               | 139.9 |    | -135.7 | 74.6     |          | -51.5    | 190.7   | -198.6        | -98.3   |
| T5               | 119.1 |    | -126.7 | 71.9     |          | -88.3    | 208.7   | -199.8        | -82.8   |
| G6               | 156.3 |    | -111.6 | 36.9     |          | -46      | 215.1   | -66.5         | -186.1  |
| G7               | 168.1 |    | -119.4 | 73.6     |          | -125.2   | 140.4   | -174.9        | -97.3   |
| C8               | 129.4 |    | -134.9 | 55       |          | -68.2    | 216.1   | -164.2        | -117.7  |
| C9               | 126.5 |    | -134.4 | 97       |          | -81.5    | 164     | -196.3        | -113.6  |
| A10              | 164   |    | -110.8 | 39.4     |          | -25.2    | 193.6   | -194.2        | -115.6  |
| A11              | 161   |    | -125.3 | 28.3     |          | -18      | 181.7   | -182.8        | -141.5  |
| T12              | 177.4 |    | -128.6 | 70.7     |          | -33.5    | 160.7   | -176.4        | -91.9   |
| C13              | 122.5 |    | -119.2 | 31.7     |          | -43.2    | 186.6   | -190.3        | -85.6   |
| C14              | 148.8 |    | -99.8  | 36       |          | -58.3    | 210.4   | -360          | -360    |

| Name                        | P   | Vm | $\chi$ | $\gamma$ | $\delta$ | $\alpha$ | $\beta$ | $\epsilon$ | $\zeta$ |
|-----------------------------|-----|----|--------|----------|----------|----------|---------|------------|---------|
| d(CATTTGCATC).d(GATGCAAATG) |     |    |        |          |          |          |         |            |         |
| C1                          | 134 |    | -144   |          | 112      |          |         | -154       | -82     |
| A2                          | 162 |    | -102   | 59       | 135      | -73      | -175    | 169        | -84     |
| T3                          | 119 |    | -127   | 63       | 113      | -70      | 177     | -178       | -87     |
| T4                          | 118 |    | -126   | 63       | 114      | -72      | 174     | 173        | -84     |
| T5                          | 123 |    | -117   | 60       | 118      | -61      | 171     | -174       | -89     |
| G6                          | 151 |    | -121   | 163/61   | 127      | 148/-42  | -173    | -176       | -89     |
| C7                          | 115 |    | -138   | 62       | 109      | -93      | -177    | 171        | -85     |
| A8                          | 154 |    | -121   | 59       | 125      | -64      | -178    | -177       | -80     |
| T9                          | 110 |    | -129   | 56       | 102      | -65      | 166     | -174       | -81     |
| C10                         | 71  |    | -138   | 57       | 88       | -74      | 168     |            |         |
| G11                         | 165 |    | -105   |          | 137      |          |         | 180        | -94     |
| A12                         | 155 |    | -107   | 55       | 126      | -81      | -167    | 178        | -88     |
| T13                         | 119 |    | -131   | 56       | 106      | -65      | 168     | -179       | -91     |
| G14                         | 153 |    | -138   | 62       | 132      | -75      | 177     | -161       | -79     |
| C15                         | 123 |    | -107   | 57       | 116      | -88      | 177     | -174       | -104    |
| A16                         | 152 |    | -110   | 64       | 131      | -79      | 171     | -177       | -100    |
| A17                         | 155 |    | -113   | 63       | 129      | -67      | 176     | -179       | -101    |
| A18                         | 145 |    | -123   | 70       | 122      | -79      | 174     | -177       | -80     |
| T19                         | 110 |    | -136   | 57       | 103      | -63      | 163     | -174       | -82     |
| G20                         | 117 |    | -128   | 58       | 109      | -74      | 174     |            |         |
| d(C5-A6-A7).d(T16-A17-G18)  |     |    |        |          |          |          |         |            |         |
| C5                          | 134 | 40 | -121   | 57       | 127      | -71      | 179     | -155       | -128    |
| A7                          | 141 | 45 | -113   | 55       | 132      | -71      | 178     | -180       | -107    |
| T16                         | 126 | 40 | -122   | 58       | 121      | -70      | -179    | -172       | -102    |
| G18                         | 136 | 42 | -119   | 56       | 127      | -70      | -180    | -178       | -106    |
| A6                          | 153 | 40 | -90    | 62       | 138      | -71      | 164     | 180        | -111    |
| A17                         | 148 | 42 | -119   | 59       | 136      | -74      | 172     | -178       | -106    |
| A6                          | 152 | 41 | -97    | 60       | 137      | -75      | 168     | 176        | -102    |
| A17                         | 149 | 41 | -101   | 61       | 136      | -71      | 170     | 180        | -111    |



**Supp. Figure 1.** Plots of sugar pucker  $P$ (degree) versus  $^{13}\text{C}$  chemical shift (ppm) with different torsion angle  $\gamma$  for crystalline samples (●) and solution data (○). Sugar pucker  $P$  versus (A) C4' shift with  $\gamma$  in *gauche*. (B) C4' shift with  $\gamma$  in *trans*. (C) C5' shift with  $\gamma$  in *gauche*. (D) C5' shift with  $\gamma$  in *trans*.



**Supp. Figure 2.** Dependence of (A) torsion angle  $\alpha$  on  $\gamma$  and (B) torsion angle  $\delta$  on sugar pucker  $P$ .