SUPPORTING INFORMATION

Crystal structure, stability and *in vitro* RNAi activity of oligoribonucleotides containing the ribo-difluorotoluyl nucleotide: insights into substrate requirements by the human RISC Ago2 enzyme

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FG RNA DUPLEX 1

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*****  CURVES 5.3 R.L. 1998  *****
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FILE : dftg_ab.pdb                          LIS  : dftg_ab
dna  :                                      axin :
axout:                                      daf  :
PDB  : dftg_ab_axis

acc  :    0.000  wid  :    0.750

maxn :   500  ior  :     0  ibond:     0  splin:     3  break:    -1
nleve:     3  nbac :     7

ends :     F  supp :     T  COMB :     T  DINU :     F  MINI :     T
rest :     F  line :     F  zaxe :     F  fit  :     F  test :     F
GRV  :     T  old  :     T  axonl:     F

Strand=    2 Nucleo=   24 Atoms =  508 Units =   24

Input   1) Xdisp=    0.00 Ydisp=    0.00 Inclin=    0.00 Tip=    0.00

Combined strands have   12 levels ...

Strand  1 has  12 bases (5'-3'): CGCFAAUUGGCG
Strand  2 has  12 bases (3'-5'): GCGGUUAAFCGC

FIRST SUM=  135.493 CPTS:    1.837  33.418   9.034  91.204

MINIMISATION: ACC =  0.100E-05 MAXN=  500 NVAR=   48

STEP    1 SUM=  135.493 DEL=  0.000E+00
STEP    2 SUM=  106.510 DEL= -0.290E+02
STEP    3 SUM=   88.866 DEL= -0.176E+02
STEP    4 SUM=   65.965 DEL= -0.229E+02
STEP    5 SUM=   64.832 DEL= -0.113E+01
STEP    6 SUM=   54.228 DEL= -0.106E+02
STEP    7 SUM=   49.681 DEL= -0.455E+01
STEP    8 SUM=   44.617 DEL= -0.506E+01
STEP    9 SUM=   38.645 DEL= -0.597E+01
STEP   10 SUM=   36.359 DEL= -0.229E+01
STEP   11 SUM=   35.030 DEL= -0.133E+01
STEP   12 SUM=   33.337 DEL= -0.169E+01
STEP   13 SUM=   31.467 DEL= -0.187E+01
STEP   14 SUM=   30.761 DEL= -0.707E+00
STEP   15 SUM=   29.737 DEL= -0.102E+01
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STEP   16 SUM=   28.387 DEL= -0.135E+01
STEP   17 SUM=   31.503 DEL=  0.312E+01
STEP   18 SUM=   28.074 DEL= -0.343E+01
STEP   19 SUM=   28.879 DEL=  0.805E+00
STEP   20 SUM=   28.005 DEL= -0.874E+00
STEP   21 SUM=   27.883 DEL= -0.122E+00
STEP   22 SUM=   27.686 DEL= -0.197E+00
STEP   23 SUM=   27.248 DEL= -0.438E+00
STEP   24 SUM=   26.761 DEL= -0.487E+00
STEP   25 SUM=   27.600 DEL=  0.839E+00
STEP   26 SUM=   26.630 DEL= -0.970E+00
STEP   27 SUM=   26.435 DEL= -0.195E+00
STEP   28 SUM=   26.110 DEL= -0.325E+00
STEP   29 SUM=   25.571 DEL= -0.539E+00
STEP   30 SUM=   25.159 DEL= -0.412E+00
STEP   31 SUM=   24.482 DEL= -0.677E+00
STEP   32 SUM=   23.714 DEL= -0.767E+00
STEP   33 SUM=   23.212 DEL= -0.502E+00
STEP   34 SUM=   22.963 DEL= -0.249E+00
STEP   35 SUM=   22.794 DEL= -0.168E+00
STEP   36 SUM=   22.638 DEL= -0.156E+00
STEP   37 SUM=   22.602 DEL= -0.361E-01
STEP   38 SUM=   22.562 DEL= -0.395E-01
STEP   39 SUM=   22.549 DEL= -0.131E-01
STEP   40 SUM=   22.535 DEL= -0.138E-01
STEP   41 SUM=   22.522 DEL= -0.127E-01
STEP   42 SUM=   22.521 DEL= -0.172E-02
STEP   43 SUM=   22.520 DEL= -0.607E-03
STEP   44 SUM=   22.520 DEL= -0.237E-03
STEP   45 SUM=   22.520 DEL= -0.137E-03
STEP   46 SUM=   22.520 DEL= -0.984E-04
STEP   47 SUM=   22.520 DEL= -0.570E-04
STEP   48 SUM=   22.519 DEL= -0.836E-04
STEP   49 SUM=   22.519 DEL= -0.813E-04
STEP   50 SUM=   22.519 DEL= -0.335E-04
STEP   51 SUM=   22.519 DEL= -0.225E-04
STEP   52 SUM=   22.519 DEL= -0.611E-05
STEP   53 SUM=   22.519 DEL= -0.106E-05
STEP   54 SUM=   22.519 DEL= -0.212E-06
STEP   55 SUM=   22.519 DEL= -0.940E-07
STEP   56 SUM=   22.519 DEL= -0.743E-07
STEP   57 SUM=   22.519 DEL= -0.446E-07
STEP   58 SUM=   22.519 DEL= -0.209E-07
STEP   59 SUM=   22.519 DEL= -0.506E-08
STEP   60 SUM=   22.519 DEL= -0.812E-09
STEP   61 SUM=   22.519 DEL= -0.976E-10
STEP   62 SUM=   22.519 DEL= -0.851E-11
STEP   63 SUM=   22.519 DEL= -0.352E-12
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STEP   64 SUM=   22.519 DEL= -0.142E-13
STEP   65 SUM=   22.519 DEL=  0.000E+00

FINAL SUM=   22.519 CPTS:    1.225  18.894   0.586   1.814

GRA=-0.45E-08 0.80E-08 0.16E-08-0.11E-08-0.56E-08-0.21E-08-0.22E-08-0.55E-09
GRA=-0.29E-08-0.16E-07-0.30E-10 0.58E-09 0.29E-08-0.74E-08 0.52E-09 0.18E-08
GRA= 0.26E-08-0.45E-08 0.15E-08-0.14E-09 0.26E-09 0.21E-07 0.96E-10-0.20E-08
GRA= 0.88E-09 0.92E-08-0.32E-08-0.41E-09-0.44E-08-0.97E-08-0.10E-08 0.83E-09
GRA=-0.33E-08 0.49E-08 0.16E-08 0.44E-09 0.56E-08-0.14E-07 0.26E-08 0.89E-09
GRA= 0.35E-08 0.47E-08 0.16E-08 0.18E-09 0.94E-09 0.22E-08-0.25E-08 0.32E-09

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|A| Global axis parameters |
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  1) U:   -0.069   0.995  -0.078  P:   -0.801 -13.863  15.983  D:    0.361
  2) U:   -0.040   0.995  -0.087  P:   -1.111 -11.132  15.891  D:    0.283
  3) U:   -0.062   0.995  -0.084  P:   -1.428  -8.271  15.575  D:    4.320
  4) U:   -0.019   0.999  -0.045  P:   -1.536  -5.384  15.015  D:    4.778
  5) U:    0.012   0.992  -0.125  P:   -1.101  -3.252  14.993  D:    0.095
  6) U:    0.012   0.991  -0.136  P:   -0.989  -0.531  14.717  D:    0.550
  7) U:   -0.056   0.984  -0.167  P:   -1.114   2.086  14.204  D:    0.331
  8) U:   -0.042   0.985  -0.169  P:   -1.161   4.788  13.853  D:    5.449
  9) U:   -0.081   0.989  -0.125  P:   -1.665   6.804  13.339  D:    5.307
 10) U:   -0.016   0.987  -0.163  P:   -1.525   9.842  12.692  D:    0.238
 11) U:   -0.019   0.991  -0.135  P:   -1.424  12.557  12.332  D:    0.808
 12) U:   -0.005   0.995  -0.104  P:   -1.446  15.150  12.315

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|B| Global Base-Axis Parameters |
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  1st strand      Xdisp    Ydisp   Inclin     Tip    Bc  Tc
                  (dx)     (dy)    (eta)    (theta)

  1) CT    1      -4.22     0.08    16.38    -2.18   3   0
  2) GA    2      -4.49    -0.19    14.78    -3.01   1  13
  3) CT    3      -4.38    -0.11    16.79    -3.53   3  -7
  4) FY    4      -2.81     0.23    15.70   -10.79   4 -27
  5) AE    5      -4.44    -0.17    19.61    -7.19   2  28
  6) AE    6      -4.49    -0.11    20.50    -8.70   2  24
  7) UI    7      -4.31     0.06    15.18   -10.70   4 -24
  8) UI    8      -4.37     0.22    15.19    -8.24   4 -26
  9) GA    9      -5.67     0.02    19.73   -10.12   1  11
 10) GA   10      -4.37     0.00    15.24    -9.96   1   5
 11) CT   11      -4.11     0.16    13.70   -12.09   3 -13
 12) GA   12      -4.35    -0.07    12.97    -7.89   1   0
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2nd strand	Xdisp (dx)	Ydisp (dy)	Inclin (eta)	Tip (theta)	Bc	Tc
1) GA 24	-4.32	0.15	10.13	-11.01	1	0
2) CT 23	-4.23	0.26	12.34	-12.32	3	-13
3) GA 22	-4.49	0.23	11.70	-9.26	1	5
4) GA 21	-5.56	0.28	14.77	-12.71	1	11
5) UI 20	-4.42	0.38	14.85	-11.87	4	-26
6) UI 19	-4.51	0.28	17.13	-11.30	4	-24
7) AE 18	-4.36	0.48	22.94	-14.31	2	24
8) AE 17	-4.36	0.07	21.30	-8.60	2	28
9) **F**Y 16	-2.63	0.30	14.97	-12.13	4	-27
10) CT 15	-4.35	-0.13	17.63	-7.03	3	-7
11) GA 14	-4.57	0.01	18.05	-7.38	1	13
12) CT 13	-4.14	0.31	17.86	-3.72	3	0

|C| Global Base pair-Axis Parameters |

Strand 1 with strand 2 ...

Duplex	Xdisp (dx)	Ydisp (dy)	Inclin (eta)	Tip (theta)	Bc	Tc
1) C 1-G 24	-4.27	-0.03	13.26	4.41	3	0
2) G 2-C 23	-4.36	-0.22	13.56	4.65	1	13
3) C 3-G 22	-4.44	-0.17	14.25	2.87	3	-7
4) **F** 4-G 21	-4.18	-0.02	15.23	0.96	4	-27
5) A 5-U 20	-4.43	-0.27	17.23	2.34	2	28
6) A 6-U 19	-4.50	-0.20	18.81	1.30	2	24
7) U 7-A 18	-4.33	-0.21	19.06	1.81	4	-24
8) U 8-A 17	-4.37	0.07	18.24	0.18	4	-26
9) G 9-**F** 16	-4.15	-0.14	17.35	1.01	1	11
10) G 10-C 15	-4.36	0.07	16.43	-1.47	1	5
11) C 11-G 14	-4.34	0.07	15.87	-2.36	3	-13
12) G 12-C 13	-4.24	-0.19	15.42	-2.09	1	0
Average:	-4.33	-0.10	16.23	1.13		

|D| Global Base-Base Parameters |

Strand 1 with strand 2 ...

Duplex	Shear	Stretch	Stagger	Buckle	Propel	Opening	Bc	T

	(Sx)	(Sy)	(Sz)	(kappa)	(omega)	(sigma)		
1) C 1-G 24	0.10	0.23	-0.16	6.25	-13.19	1.61	3	0
2) G 2-C 23	-0.26	0.07	0.03	2.44	-15.33	0.69	1	13
3) C 3-G 22	0.11	0.12	-0.08	5.09	-12.79	0.52	3	-7
4) **F** 4-G 21	2.75	0.52	-0.30	0.93	-23.50	7.69	4	-27
5) A 5-U 20	-0.02	0.21	-0.03	4.76	-19.07	3.32	2	28
6) A 6-U 19	0.02	0.17	-0.22	3.37	-20.00	1.20	2	24
7) U 7-A 18	0.06	0.54	-0.11	-7.76	-25.01	6.29	4	-24
8) U 8-A 17	0.00	0.29	0.16	-6.11	-16.84	4.10	4	-26
9) G 9-**F** 16	-3.04	0.32	-0.24	4.76	-22.24	6.01	1	11
10) G 10-C 15	-0.02	-0.12	-0.07	-2.39	-16.99	-2.33	1	5
11) C 11-G 14	0.45	0.16	-0.18	-4.35	-19.47	1.64	3	-13
12) G 12-C 13	-0.21	0.24	-0.08	-4.89	-11.61	2.07	1	0
Average:	-0.01	0.23	-0.11	0.18	-18.00	2.73		

|E| Global Inter-Base Parameters |

1st strand	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) C 1/G 2	-0.40	-0.43	2.84	-2.39	0.73	32.58	8
3) G 2/C 3	-0.02	0.21	2.83	1.67	-1.78	33.82	5
4) C 3/**F** 4	1.90	0.52	2.81	2.18	-7.96	45.36	-3
5) **F** 4/A 5	-1.83	-0.83	2.26	5.99	8.08	22.37	10
6) A 5/A 6	-0.16	0.04	2.64	1.20	-0.97	32.31	4
7) A 6/U 7	0.29	0.10	2.72	-5.21	2.30	37.21	7
8) U 7/U 8	-0.13	0.28	2.85	-0.03	1.64	34.01	-4
9) U 8/G 9	-1.14	-0.61	1.90	4.01	1.47	22.60	-9
10) G 9/G 10	1.02	0.21	3.18	-7.41	-3.00	40.25	1
11) G 10/C 11	0.36	0.27	2.68	-0.76	-0.70	37.64	5
12) C 11/G 12	-0.07	-0.46	2.62	0.34	5.81	32.77	8

2nd strand	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) G 24/C 23	-0.04	0.27	2.65	1.42	-2.87	33.51	8
3) C 23/G 22	-0.39	-0.15	2.94	-0.98	4.33	33.99	5
4) G 22/G 21	-0.74	-0.12	3.03	6.33	-2.75	38.20	1
5) G 21/U 20	0.95	0.52	1.99	2.16	-3.65	26.74	-9
6) U 20/U 19	-0.20	-0.08	2.83	2.59	0.03	34.43	-4
7) U 19/A 18	0.25	0.28	2.61	5.92	-7.31	32.12	7
8) A 18/A 17	-0.07	-0.53	2.59	-1.68	6.53	36.20	4
9) A 17/**F** 16	1.89	0.64	2.30	-6.86	-6.87	20.70	10
10) **F** 16/C 15	-2.00	-0.65	3.00	-0.26	8.26	48.59	-3

11) C 15/G 14	-0.11	0.02	2.79	1.20	-1.78	33.68	5
12) G 14/C 13	0.59	0.54	2.53	0.88	2.05	32.34	8

|F| Global Inter-Base pair Parameters |

Strand 1 with strand 2 ...

Duplex	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) C 1/G 2	-0.22	-0.35	2.74	-0.48	1.80	33.05	8
3) G 2/C 3	-0.21	0.18	2.89	0.35	-3.05	33.91	5
4) C 3/**F** 4	0.58	0.32	2.92	4.26	-2.61	41.78	-3
5) **F** 4/A 5	-0.44	-0.68	2.13	4.07	5.86	24.56	10
6) A 5/A 6	-0.18	0.06	2.73	1.89	-0.50	33.37	4
7) A 6/U 7	0.27	-0.09	2.67	0.35	4.80	34.67	7
8) U 7/U 8	-0.10	0.41	2.72	-0.86	-2.45	35.11	-4
9) U 8/G 9	0.37	-0.62	2.10	-1.43	4.17	21.65	-9
10) G 9/G 10	-0.49	0.43	3.09	-3.83	-5.63	44.42	1
11) G 10/C 11	0.12	0.13	2.74	0.22	0.54	35.66	5
12) C 11/G 12	0.26	-0.50	2.58	0.61	1.88	32.56	8
Average:	0.00	-0.07	2.66	0.47	0.44	33.70	

|G| Local Inter-Base Parameters |

1st strand	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) C 1/G 2	-0.19	-2.00	3.62	-0.93	9.36	31.10	8
3) G 2/C 3	0.22	-1.57	3.27	3.44	7.36	32.80	5
4) C 3/**F** 4	2.12	-1.41	3.09	7.55	4.84	43.16	-3
5) **F** 4/A 5	-1.36	-1.38	3.34	9.30	14.42	18.93	10
6) A 5/A 6	0.36	-1.42	3.34	5.32	9.99	29.79	4
7) A 6/U 7	0.93	-1.69	3.63	0.93	13.41	34.55	7
8) U 7/U 8	0.32	-1.51	3.27	5.33	10.34	32.74	-4
9) U 8/G 9	-0.74	-1.81	3.01	7.31	8.09	19.68	-9
10) G 9/G 10	1.58	-2.29	3.49	-0.36	9.03	40.12	1
11) G 10/C 11	0.90	-1.72	3.20	6.15	8.60	35.63	5
12) C 11/G 12	0.46	-2.20	3.27	5.86	13.04	31.17	8

2nd strand	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc

2) G 24/C 23	-0.56	-2.18	3.18	-5.24	9.22	32.26	8
3) C 23/G 22	-0.82	-1.75	3.20	-7.12	2.80	32.78	5
4) G 22/G 21	-1.19	-2.47	3.40	-0.92	11.28	38.00	1
5) G 21/U 20	0.44	-2.15	3.18	-3.34	10.39	24.58	-9
6) U 20/U 19	-0.69	-1.72	3.40	-4.12	9.32	32.86	-4
7) U 19/A 18	-0.38	-1.62	3.71	-0.88	17.84	29.49	7
8) A 18/A 17	-0.49	-1.10	3.15	-8.18	7.19	32.91	4
9) A 17/**F** 16	1.42	-1.03	3.27	-10.27	12.98	17.22	10
10) **F** 16/C 15	-2.30	-1.40	3.03	-8.13	5.48	46.87	-3
11) C 15/G 14	-0.56	-1.63	3.51	-2.76	11.88	31.64	5
12) G 14/C 13	0.35	-2.00	3.48	-2.04	7.87	30.22	8

|H| Local Inter-Base pair Parameters |

Strand 1 with strand 2 ...

Duplex	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) C 1/G 2	-0.39	-2.09	3.40	-3.11	9.31	31.89	8
3) G 2/C 3	-0.30	-1.66	3.27	-1.88	5.12	33.06	5
4) C 3/**F** 4	0.47	-1.87	3.48	3.49	8.23	40.91	-3
5) **F** 4/A 5	-0.47	-1.81	3.08	2.90	12.72	22.10	10
6) A 5/A 6	-0.15	-1.55	3.41	0.60	9.77	31.73	4
7) A 6/U 7	0.27	-1.63	3.74	0.11	15.65	32.63	7
8) U 7/U 8	-0.10	-1.28	3.24	-1.52	9.09	33.08	-4
9) U 8/G 9	0.37	-1.47	2.95	-1.36	10.94	18.65	-9
10) G 9/G 10	-0.38	-1.81	3.54	-4.34	7.31	44.12	1
11) G 10/C 11	0.18	-1.68	3.43	1.72	10.23	34.09	5
12) C 11/G 12	0.41	-2.10	3.36	1.86	10.53	30.80	8
Average:	-0.01	-1.72	3.35	-0.14	9.90	32.10	

|I| Global Axis Curvature |

Duplex	Ax	Ay	Ainc	Atip	Adis	Angle	Path	Dc
2) C 1/G 2	-0.13	-0.16	-0.79	1.56	0.21	1.75	2.75	8
3) G 2/C 3	-0.13	0.13	-0.34	-1.27	0.18	1.31	2.90	5
4) C 3/**F** 4	0.33	0.17	3.27	-0.70	0.37	3.34	2.94	-3
5) **F** 4/A 5	-0.19	-0.43	2.08	4.49	0.47	4.95	2.18	10
6) A 5/A 6	-0.11	-0.02	0.31	0.54	0.11	0.62	2.74	4
7) A 6/U 7	0.10	-0.07	0.11	4.30	0.13	4.30	2.67	7
8) U 7/U 8	-0.06	0.12	-0.04	-0.82	0.14	0.82	2.73	-4

9) U 8/G 9	0.15	-0.40	-0.54	3.34	0.43	3.38	2.14	-9
10) G 9/G 10	-0.28	0.22	-2.91	-3.16	0.35	4.30	3.11	1
11) G 10/C 11	0.10	0.12	0.78	1.43	0.16	1.63	2.74	5
12) C 11/G 12	0.17	-0.24	1.07	1.61	0.29	1.93	2.59	8

Overall axis bend ... UU= 3.93 PP= 6.15

Duplex	Offset	L.Dir ... wrt end-to-end vector
1) C 1	0.00	0.00
2) G 2	0.35	39.34
3) C 3	0.58	-9.15
4) **F** 4	0.56	-74.41
5) A 5	0.35	-28.07
6) A 6	0.43	-35.43
7) U 7	0.24	-77.14
8) U 8	0.23	-107.61
9) G 9	0.41	121.86
10) G 10	0.35	29.82
11) C 11	0.31	-35.40
12) G 12	0.00	0.00

Path length= 29.48 End-to-end= 29.25 Shortening= 0.78 %

|J| Backbone Parameters

1st strand	C1'-C2'	C2'-C3'	Phase	Ampli	Pucker	C1'	C2'	C3'
1)CT 1	-33.34	44.45	8.54	45.76	C3'-endo	105.7	100.5	99.7
2)GA 2	-36.19	47.32	7.32	48.87	C3'-endo	109.2	98.2	100.0
3)CT 3	-26.98	39.62	13.82	41.22	C3'-endo	106.4	101.4	101.7
4)**F**Y 4	-29.25	42.81	13.82	44.78	C3'-endo	105.7	99.8	101.4
5)AE 5	-35.77	45.95	5.62	47.10	C3'-endo	107.2	98.9	100.3
6)AE 6	-36.57	48.03	7.94	49.43	C3'-endo	105.9	99.4	98.7
7)UI 7	-31.65	45.56	13.54	47.49	C3'-endo	105.6	100.9	99.1
8)UI 8	-31.86	44.52	10.19	45.65	C3'-endo	105.7	100.2	101.1
9)GA 9	-32.72	45.32	10.30	46.75	C3'-endo	106.6	99.0	100.9
10)GA 10	-30.41	43.36	12.10	45.35	C3'-endo	108.1	98.0	102.1
11)CT 11	-30.50	45.31	15.17	47.56	C3'-endo	104.7	100.5	99.2
12)GA 12	-24.82	40.37	20.30	43.77	C3'-endo	107.2	101.1	101.2

Torsions	Chi C1'-N	Gamma C5'-C4'	Delta C4'-C3'	Epsil C3'-O3'	Zeta O3'-P	Alpha P-O5'	Beta O5'-C5'
1)CT 1	-165.15	59.60	80.30	-155.37	-70.55	-67.88	177.20

2)GA	2	-157.88	53.11	83.11	-147.49	-77.37	-62.56	167.19
3)CT	3	-162.08	53.54	80.54	-150.81	-62.00	-65.75	167.27
4)**F**Y	4	-157.31	51.79	79.53	-149.71	-82.91	-67.36	169.30
5)AE	5	-150.98	53.41	77.76	-156.52	-68.98	-68.86	172.24
6)AE	6	-154.12	54.95	79.94	-153.05	-68.43	-68.17	172.94
7)UI	7	-158.98	55.12	78.02	-154.18	-73.96	-61.81	170.60
8)UI	8	-158.35	48.54	75.20	-150.81	-74.88	-65.17	164.85
9)GA	9	-162.70	57.17	76.08	-151.00	-63.13	-67.03	173.61
10)GA	10	-164.95	58.70	76.29	-138.66	-75.32	-66.08	165.42
11)CT	11	-163.84	51.71	80.19	-155.18	-67.22	-66.40	-178.14
12)GA	12	-156.17	51.84	78.05	.....	.....	.....	.....

2nd strand		C1'-C2'	C2'-C3'	Phase	Ampli	Pucker	C1'	C2'	C3'
1)GA	24	-27.28	40.02	14.10	42.00	C3'-endo	108.4	100.5	101.9
2)CT	23	-33.16	44.88	9.16	46.30	C3'-endo	106.2	99.5	100.5
3)GA	22	-27.52	41.01	15.44	43.24	C3'-endo	105.5	101.1	100.3
4)GA	21	-34.04	46.81	11.05	48.84	C3'-endo	104.8	99.9	97.1
5)UI	20	-34.08	49.36	14.45	52.32	C3'-endo	108.0	97.2	98.3
6)UI	19	-27.68	42.05	16.37	44.70	C3'-endo	108.1	98.9	102.1
7)AE	18	-33.81	44.86	8.96	46.64	C3'-endo	106.3	99.8	98.8
8)AE	17	-34.41	44.11	5.52	45.33	C3'-endo	107.3	99.8	100.1
9)**F**Y	16	-30.68	44.10	12.31	45.41	C3'-endo	103.6	101.9	100.1
10)CT	15	-31.49	43.41	10.55	44.96	C3'-endo	107.5	100.3	100.1
11)GA	14	-32.90	43.98	9.06	45.86	C3'-endo	108.6	98.2	100.6
12)CT	13	-32.79	42.47	5.59	43.43	C3'-endo	106.0	100.2	101.1

Torsions		Chi C1'-N	Gamma C5'-C4'	Delta C4'-C3'	Epsil C3'-O3'	Zeta O3'-P	Alpha P-O5'	Beta O5'-C5'
1)GA	24	-157.69	54.08	80.21	.....	.....	.....	.....
2)CT	23	-163.17	53.20	80.72	-154.54	-65.51	-66.14	179.34
3)GA	22	-165.24	51.66	76.54	-147.30	-75.30	-60.97	165.31
4)GA	21	-166.91	59.49	72.21	-153.27	-63.53	-65.30	-178.45
5)UI	20	-159.12	47.93	78.54	-161.41	-70.67	-72.77	170.23
6)UI	19	-158.97	51.43	80.10	-150.89	-70.67	-66.05	170.12
7)AE	18	-153.00	52.36	79.79	-151.17	-70.24	-67.50	173.67
8)AE	17	-151.91	59.35	76.88	-158.20	-67.77	-68.64	172.95
9)**F**Y	16	-157.25	49.40	77.61	-147.07	-86.12	-65.67	161.05
10)CT	15	-160.92	54.85	82.73	-152.02	-64.80	-65.62	170.39
11)GA	14	-158.14	52.48	76.15	-143.06	-76.49	-61.72	163.33
12)CT	13	-165.13	57.38	81.96	-154.29	-72.20	-70.49	-179.57

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|K| Groove parameters |
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Atom defining backbone: P      12 levels,  3 sub-levels

 Levels          Minor groove                    Major groove
    i  n      Width    Depth  Angle       Width    Depth  Angle    Diam

C   1  0        --       --     --    C     --       --     --       --
    1  1        --       --     --          --       --     --       --
    1  2        --       --     --          --       --     --       --
G   2  0        --       --     --    G     --       --     --       --
    2  1        --       --     --          --       --     --       --
    2  2     10.21     0.51     31          --       --     --       --
C   3  0     10.17     0.48     27    C     --       --     --       --
    3  1     10.04     0.44     30          --       --     --    18.11
    3  2      9.94     0.62     31          --       --     --    18.17
F   4  0     10.00     0.61     33    F     --       --     --    18.17
    4  1     10.06     0.44     34          --       --     --    18.21
    4  2     10.16     0.26     34          --       --     --    18.33
A   5  0     10.22     0.36     30    A   2.94     8.76     28    18.36
    5  1     10.24     0.32     31        3.09     8.96     26    18.10
    5  2     10.29     0.33     31        3.18     9.33     24    17.76
A   6  0     10.36     0.40     30    A   3.22     9.56     28    17.45
    6  1     10.34     0.62     29        3.35     9.64     26    17.29
    6  2     10.37     0.55     32        3.39     9.52     27    17.17
U   7  0     10.50     0.62     31    U   3.36     9.34     26    17.19
    7  1     10.58     0.51     31        3.43     9.13     23    17.47
    7  2     10.67     0.44     30        3.42     8.85     29    17.84
U   8  0     10.72     0.43     28    U   3.27     8.79     26    18.03
    8  1     10.60     0.31     33          --       --     --    17.92
G   9  0     10.39     0.55     33    G     --       --     --    17.82
    9  1     10.13     0.65     31          --       --     --    17.79
    9  2      9.99     0.59     30          --       --     --    17.76
    9  3     10.06     0.61     28          --       --     --       --
G  10  0     10.18     0.56     26    G     --       --     --       --
   10  1     10.22     0.46     29          --       --     --       --
   10  2        --       --     --          --       --     --       --
C  11  0        --       --     --    C     --       --     --       --
   11  1        --       --     --          --       --     --       --
   11  2        --       --     --          --       --     --       --
G  12  0        --       --     --    G     --       --     --       --
```

FG RNA DUPLEX 2

```
************************************
*****  CURVES 5.3 R.L. 1998  *****
************************************

FILE : dftg_cd.pdb                          LIS  : dftg_cd
dna  :                                      axin :
axout:                                      daf  :
PDB  : dftg_cd_axis

acc  :    0.000  wid  :    0.750

maxn :   500  ior  :     0  ibond:     0  splin:     3  break:    -1
nleve:     3  nbac :     7

ends :     F  supp :     T  COMB :     T  DINU :     F  MINI :     T
rest :     F  line :     F  zaxe :     F  fit  :     F  test :     F
GRV  :     T  old  :     T  axonl:     F

Strand=    2 Nucleo=   24 Atoms =  508 Units =   24

Input   1) Xdisp=    0.00 Ydisp=    0.00 Inclin=    0.00 Tip=    0.00

Combined strands have   12 levels ...

Strand  1 has  12 bases (5'-3'): CGCFAAUUGGCG
Strand  2 has  12 bases (3'-5'): GCGGUUAAFCGC

FIRST SUM=  139.845 CPTS:    2.409  37.400   7.953  92.083

MINIMISATION: ACC =  0.100E-05 MAXN=  500 NVAR=   48

STEP    1 SUM=  139.845 DEL=  0.000E+00
STEP    2 SUM=  110.225 DEL= -0.296E+02
STEP    3 SUM=   88.526 DEL= -0.217E+02
STEP    4 SUM=   65.084 DEL= -0.234E+02
STEP    5 SUM=   71.167 DEL=  0.608E+01
STEP    6 SUM=   54.711 DEL= -0.165E+02
STEP    7 SUM=   52.502 DEL= -0.221E+01
STEP    8 SUM=   49.245 DEL= -0.326E+01
STEP    9 SUM=   44.806 DEL= -0.444E+01
STEP   10 SUM=   42.862 DEL= -0.194E+01
STEP   11 SUM=   41.230 DEL= -0.163E+01
STEP   12 SUM=   39.484 DEL= -0.175E+01
STEP   13 SUM=   37.408 DEL= -0.208E+01
STEP   14 SUM=   35.139 DEL= -0.227E+01
STEP   15 SUM=   42.262 DEL=  0.712E+01
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STEP   16 SUM=   34.698 DEL= -0.756E+01
STEP   17 SUM=   34.029 DEL= -0.669E+00
STEP   18 SUM=   33.657 DEL= -0.372E+00
STEP   19 SUM=   34.169 DEL=  0.513E+00
STEP   20 SUM=   33.547 DEL= -0.623E+00
STEP   21 SUM=   33.361 DEL= -0.185E+00
STEP   22 SUM=   33.036 DEL= -0.326E+00
STEP   23 SUM=   32.592 DEL= -0.444E+00
STEP   24 SUM=   31.575 DEL= -0.102E+01
STEP   25 SUM=   35.074 DEL=  0.350E+01
STEP   26 SUM=   31.388 DEL= -0.369E+01
STEP   27 SUM=   31.137 DEL= -0.251E+00
STEP   28 SUM=   30.749 DEL= -0.388E+00
STEP   29 SUM=   30.136 DEL= -0.613E+00
STEP   30 SUM=   30.023 DEL= -0.113E+00
STEP   31 SUM=   29.798 DEL= -0.225E+00
STEP   32 SUM=   29.236 DEL= -0.562E+00
STEP   33 SUM=   28.476 DEL= -0.759E+00
STEP   34 SUM=   28.381 DEL= -0.951E-01
STEP   35 SUM=   28.226 DEL= -0.156E+00
STEP   36 SUM=   28.012 DEL= -0.214E+00
STEP   37 SUM=   27.883 DEL= -0.128E+00
STEP   38 SUM=   27.825 DEL= -0.583E-01
STEP   39 SUM=   27.795 DEL= -0.300E-01
STEP   40 SUM=   27.774 DEL= -0.209E-01
STEP   41 SUM=   27.763 DEL= -0.112E-01
STEP   42 SUM=   27.756 DEL= -0.731E-02
STEP   43 SUM=   27.750 DEL= -0.545E-02
STEP   44 SUM=   27.749 DEL= -0.948E-03
STEP   45 SUM=   27.749 DEL= -0.476E-03
STEP   46 SUM=   27.749 DEL= -0.598E-04
STEP   47 SUM=   27.749 DEL= -0.576E-04
STEP   48 SUM=   27.749 DEL= -0.367E-04
STEP   49 SUM=   27.749 DEL= -0.458E-04
STEP   50 SUM=   27.749 DEL= -0.310E-04
STEP   51 SUM=   27.749 DEL= -0.259E-04
STEP   52 SUM=   27.749 DEL= -0.178E-04
STEP   53 SUM=   27.749 DEL= -0.581E-05
STEP   54 SUM=   27.749 DEL= -0.162E-05
STEP   55 SUM=   27.749 DEL= -0.612E-06
STEP   56 SUM=   27.749 DEL= -0.323E-06
STEP   57 SUM=   27.749 DEL= -0.179E-06
STEP   58 SUM=   27.749 DEL= -0.100E-06
STEP   59 SUM=   27.749 DEL= -0.310E-07
STEP   60 SUM=   27.749 DEL= -0.411E-08
STEP   61 SUM=   27.749 DEL= -0.655E-09
STEP   62 SUM=   27.749 DEL= -0.112E-09
STEP   63 SUM=   27.749 DEL= -0.171E-10
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STEP   64 SUM=   27.749 DEL= -0.170E-11
STEP   65 SUM=   27.749 DEL= -0.284E-13
STEP   66 SUM=   27.749 DEL=  0.000E+00

FINAL SUM=   27.749 CPTS:    1.331  21.947   1.054   3.417

GRA= 0.14E-07 0.46E-07-0.34E-08-0.59E-10-0.72E-08-0.17E-07 0.42E-08-0.40E-09
GRA= 0.87E-08-0.17E-07 0.32E-09 0.42E-09 0.21E-07-0.31E-07 0.72E-09-0.94E-09
GRA= 0.21E-07 0.35E-08 0.66E-08-0.61E-10 0.22E-07 0.23E-07-0.42E-08 0.30E-08
GRA=-0.34E-08-0.13E-07-0.43E-08-0.16E-08-0.15E-07-0.52E-07 0.23E-08-0.58E-08
GRA= 0.10E-07-0.93E-09 0.26E-08-0.57E-08-0.83E-08 0.79E-09 0.21E-08 0.12E-08
GRA=-0.15E-07 0.21E-07-0.83E-09 0.50E-08-0.22E-07-0.32E-07-0.44E-08-0.25E-08

---------------------------
|A| Global axis parameters |
---------------------------

  1) U:    0.021   0.994  -0.104  P:   14.577   1.159  39.695  D:    0.562
  2) U:    0.014   0.987  -0.162  P:   14.626   3.951  39.529  D:    0.678
  3) U:   -0.019   0.972  -0.233  P:   14.393   6.732  39.149  D:    6.068
  4) U:   -0.032   0.974  -0.226  P:   13.977   9.387  38.134  D:    7.131
  5) U:   -0.036   0.954  -0.297  P:   14.429  11.251  37.072  D:    0.255
  6) U:   -0.066   0.961  -0.267  P:   14.326  14.033  36.201  D:    0.554
  7) U:   -0.117   0.972  -0.204  P:   14.339  16.710  35.475  D:    0.630
  8) U:   -0.106   0.983  -0.151  P:   13.981  19.584  35.267  D:    6.026
  9) U:   -0.109   0.993  -0.040  P:   13.170  21.636  35.048  D:    4.759
 10) U:   -0.034   0.999   0.007  P:   13.141  24.544  34.715  D:    0.331
 11) U:   -0.034   0.999   0.008  P:   13.191  27.420  34.817  D:    0.757
 12) U:    0.030   0.999   0.039  P:   13.284  30.347  35.192

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|B| Global Base-Axis Parameters |
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  1st strand      Xdisp    Ydisp   Inclin     Tip    Bc  Tc
                  (dx)     (dy)    (eta)    (theta)

  1) CT    1      -4.20     0.84    18.63    -9.45   3   0
  2) GA    2      -4.32     0.67    14.97   -13.05   1  13
  3) CT    3      -4.36     0.32    11.96   -13.56   3  -7
  4) FY    4      -2.64     0.87    14.22   -13.77   4 -27
  5) AE    5      -3.96     0.73    17.65   -15.85   2  28
  6) AE    6      -3.88     0.68    16.36   -18.09   2  24
  7) UI    7      -4.19     0.48    12.38   -17.14   4 -24
  8) UI    8      -3.88     0.89    10.78   -16.77   4 -26
  9) GA    9      -5.06     0.86    11.28   -16.67   1  11
 10) GA   10      -4.00     0.55     7.77   -12.62   1   5
 11) CT   11      -3.69     0.54     9.11   -15.75   3 -13
```

12)	GA	12	-3.74	0.30	3.35	-13.46	1 0

2nd strand			Xdisp (dx)	Ydisp (dy)	Inclin (eta)	Tip (theta)	Bc	Tc
1)	GA	24	-4.21	-0.70	13.72	-4.17	1	0
2)	CT	23	-3.99	-0.51	14.50	-7.48	3	-13
3)	GA	22	-4.28	-0.76	17.60	-4.10	1	5
4)	GA	21	-5.62	-1.16	14.13	1.18	1	11
5)	UI	20	-3.85	-0.25	10.19	-3.44	4	-26
6)	UI	19	-3.93	-0.39	12.65	-7.72	4	-24
7)	AE	18	-4.03	-0.45	17.68	-7.30	2	24
8)	AE	17	-4.05	-0.68	17.21	-3.56	2	28
9)	**F**Y	16	-2.25	-0.12	10.87	-6.75	4	-27
10)	CT	15	-3.91	-0.55	11.15	-0.54	3	-7
11)	GA	14	-4.15	-0.42	7.88	0.26	1	13
12)	CT	13	-3.83	-0.07	11.44	0.10	3	0

|C| Global Base pair-Axis Parameters |

Strand 1 with strand 2 ...

Duplex			Xdisp (dx)	Ydisp (dy)	Inclin (eta)	Tip (theta)	Bc	Tc
1)	C	1-G 24	-4.21	0.77	16.17	-2.64	3	0
2)	G	2-C 23	-4.16	0.59	14.74	-2.79	1	13
3)	C	3-G 22	-4.32	0.54	14.78	-4.73	3	-7
4)	**F**	4-G 21	-4.13	1.01	14.18	-7.47	4	-27
5)	A	5-U 20	-3.90	0.49	13.92	-6.20	2	28
6)	A	6-U 19	-3.91	0.54	14.50	-5.19	2	24
7)	U	7-A 18	-4.11	0.47	15.03	-4.92	4	-24
8)	U	8-A 17	-3.97	0.79	14.00	-6.61	4	-26
9)	G	9-**F** 16	-3.65	0.49	11.07	-4.96	1	11
10)	G	10-C 15	-3.96	0.55	9.46	-6.04	1	5
11)	C	11-G 14	-3.92	0.48	8.50	-8.00	3	-13
12)	G	12-C 13	-3.79	0.18	7.40	-6.78	1	0
Average:			-4.00	0.57	12.81	-5.53		

|D| Global Base-Base Parameters |

Strand 1 with strand 2 ...

Duplex	Shear (Sx)	Stretch (Sy)	Stagger (Sz)	Buckle (kappa)	Propel (omega)	Opening (sigma)	Bc	T
1) C 1-G 24	0.01	0.14	-0.07	4.90	-13.62	0.35	3	0
2) G 2-C 23	-0.33	0.16	-0.07	0.47	-20.53	2.13	1	13
3) C 3-G 22	-0.08	-0.44	0.15	-5.64	-17.66	-5.77	3	-7
4) **F** 4-G 21	2.99	-0.30	0.43	0.09	-12.59	-2.24	4	-27
5) A 5-U 20	-0.12	0.48	0.06	7.46	-19.29	8.08	2	28
6) A 6-U 19	0.05	0.29	-0.10	3.71	-25.81	4.41	2	24
7) U 7-A 18	-0.15	0.03	-0.16	-5.31	-24.44	-0.14	4	-24
8) U 8-A 17	0.17	0.21	0.01	-6.43	-20.33	3.23	4	-26
9) G 9-**F** 16	-2.81	0.74	-0.20	0.41	-23.42	11.20	1	11
10) G 10-C 15	-0.09	0.00	0.05	-3.38	-13.15	-0.28	1	5
11) C 11-G 14	0.45	0.12	-0.02	1.23	-15.49	1.31	3	-13
12) G 12-C 13	0.09	0.23	-0.08	-8.09	-13.36	1.34	1	0
Average:	0.01	0.14	0.00	-0.88	-18.31	1.97		

|E| Global Inter-Base Parameters |

1st strand	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) C 1/G 2	-0.12	-0.38	2.79	-7.01	-3.96	34.42	8
3) G 2/C 3	-0.33	-0.37	2.92	-7.54	0.33	31.95	5
4) C 3/**F** 4	2.00	0.98	2.97	1.67	-0.80	44.30	-3
5) **F** 4/A 5	-0.96	-0.79	1.88	4.47	2.03	27.53	10
6) A 5/A 6	0.08	-0.12	2.84	-3.76	-2.26	32.68	4
7) A 6/U 7	-0.55	-0.32	2.73	-8.16	3.17	30.79	7
8) U 7/U 8	0.47	0.68	2.97	-4.65	1.10	38.49	-4
9) U 8/G 9	-0.86	-0.52	2.03	-3.10	5.40	26.31	-9
10) G 9/G 10	0.77	-0.15	3.04	-7.93	6.53	35.58	1
11) G 10/C 11	0.46	0.07	2.84	1.35	-3.12	34.64	5
12) C 11/G 12	0.16	-0.49	2.91	-5.44	6.37	32.56	8

2nd strand	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) G 24/C 23	0.22	0.40	2.79	-2.58	-2.95	32.64	8
3) C 23/G 22	-0.58	-0.23	2.69	-1.43	2.54	39.85	5
4) G 22/G 21	-1.07	-0.84	2.69	-4.07	5.87	40.77	1
5) G 21/U 20	2.14	1.57	2.25	-2.90	-8.73	17.21	-9
6) U 20/U 19	-0.09	-0.08	3.00	-0.01	-4.26	36.36	-4
7) U 19/A 18	-0.35	0.06	2.79	0.85	-1.80	35.34	7
8) A 18/A 17	0.14	-0.50	2.80	-3.52	3.01	35.13	4
9) A 17/**F** 16	2.12	1.05	2.25	-9.94	-8.49	18.34	10

10) **F** 16/C 15	-1.96	-0.59	2.78	-4.14	3.73	47.06	-3
11) C 15/G 14	-0.08	0.05	2.91	-3.27	0.78	33.04	5
12) G 14/C 13	0.52	0.60	2.97	3.88	-4.24	32.53	8

|F| Global Inter-Base pair Parameters |

Strand 1 with strand 2 ...

Duplex	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) C 1/G 2	0.05	-0.39	2.79	-4.80	-0.50	33.53	8
3) G 2/C 3	-0.45	-0.07	2.80	-4.48	-1.10	35.90	5
4) C 3/**F** 4	0.46	0.91	2.83	-1.20	-3.34	42.53	-3
5) **F** 4/A 5	0.59	-1.18	2.06	0.79	5.38	22.37	10
6) A 5/A 6	0.00	-0.02	2.92	-1.89	1.00	34.52	4
7) A 6/U 7	-0.45	-0.19	2.76	-3.66	2.48	33.06	7
8) U 7/U 8	0.31	0.59	2.89	-4.09	-0.95	36.81	-4
9) U 8/G 9	0.63	-0.79	2.14	-6.52	6.94	22.32	-9
10) G 9/G 10	-0.60	0.22	2.91	-6.04	1.40	41.32	1
11) G 10/C 11	0.19	0.01	2.87	-0.96	-1.95	33.84	5
12) C 11/G 12	0.34	-0.55	2.94	-0.78	5.31	32.55	8
Average:	0.10	-0.13	2.72	-3.06	1.33	33.52	

|G| Local Inter-Base Parameters |

1st strand	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) C 1/G 2	0.12	-1.99	3.49	-0.37	6.05	33.78	8
3) G 2/C 3	0.22	-2.01	3.53	-0.22	7.61	31.83	5
4) C 3/**F** 4	2.06	-1.03	2.86	11.54	8.96	41.92	-3
5) **F** 4/A 5	-0.62	-1.71	2.94	10.82	9.35	23.45	10
6) A 5/A 6	0.65	-1.42	3.33	5.46	7.38	31.01	4
7) A 6/U 7	0.20	-1.70	3.46	1.15	10.70	30.42	7
8) U 7/U 8	0.93	-1.41	3.19	6.43	8.68	37.38	-4
9) U 8/G 9	-0.41	-2.08	3.10	4.44	10.50	24.57	-9
10) G 9/G 10	1.19	-2.39	3.39	1.24	12.31	35.65	1
11) G 10/C 11	0.84	-1.77	3.03	9.53	2.02	32.97	5
12) C 11/G 12	0.79	-2.24	3.32	2.97	9.74	32.31	8

2nd strand	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc

2) G 24/C 23	-0.45	-2.01	3.26	-5.82	10.64	31.45	8
3) C 23/G 22	-1.32	-1.77	3.20	-5.38	8.48	37.72	5
4) G 22/G 21	-1.69	-1.83	3.24	-4.86	5.40	39.28	1
5) G 21/U 20	1.87	-2.38	3.19	-3.31	12.22	15.96	-9
6) U 20/U 19	-0.61	-1.79	3.32	-3.57	11.00	35.64	-4
7) U 19/A 18	-1.06	-1.67	3.34	-3.77	10.77	33.40	7
8) A 18/A 17	-0.49	-1.02	3.25	-6.63	7.45	32.86	4
9) A 17/**F** 16	1.77	-1.37	3.08	-11.75	12.42	15.70	10
10) **F** 16/C 15	-2.28	-1.31	3.10	-7.11	5.24	45.38	-3
11) C 15/G 14	-0.33	-1.84	3.25	-3.21	4.64	32.60	5
12) G 14/C 13	0.35	-2.26	3.66	3.81	9.57	31.44	8

|H| Local Inter-Base pair Parameters |

Strand 1 with strand 2 ...

Duplex	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) C 1/G 2	-0.17	-2.00	3.38	-3.10	8.37	32.89	8
3) G 2/C 3	-0.58	-1.89	3.44	-2.85	8.03	35.29	5
4) C 3/**F** 4	0.22	-1.49	3.23	3.41	6.93	40.84	-3
5) **F** 4/A 5	0.64	-2.06	2.90	3.83	10.98	19.79	10
6) A 5/A 6	0.02	-1.57	3.40	1.07	9.43	33.73	4
7) A 6/U 7	-0.43	-1.68	3.46	-1.34	10.78	32.68	7
8) U 7/U 8	0.22	-1.20	3.30	-0.12	8.21	35.66	-4
9) U 8/G 9	0.68	-1.79	2.88	-3.62	12.01	20.44	-9
10) G 9/G 10	-0.54	-1.76	3.49	-3.16	8.98	40.92	1
11) G 10/C 11	0.26	-1.80	3.18	3.19	3.36	33.00	5
12) C 11/G 12	0.58	-2.25	3.49	3.41	9.64	32.11	8
Average:	0.08	-1.77	3.29	0.06	8.79	32.49	

|I| Global Axis Curvature |

Duplex	Ax	Ay	Ainc	Atip	Adis	Angle	Path	Dc
2) C 1/G 2	0.00	-0.21	-3.36	-0.35	0.21	3.38	2.80	8
3) G 2/C 3	-0.29	-0.01	-4.53	0.84	0.29	4.61	2.82	5
4) C 3/**F** 4	0.27	0.43	-0.60	-0.59	0.51	0.84	2.87	-3
5) **F** 4/A 5	0.36	-0.66	1.04	4.11	0.75	4.24	2.19	10
6) A 5/A 6	0.00	-0.07	-2.47	-0.02	0.07	2.47	2.92	4
7) A 6/U 7	-0.25	-0.12	-4.18	2.22	0.28	4.73	2.77	7

8) U 7/U 8	0.16	0.26	-3.05	0.74	0.31	3.14	2.90	-4
9) U 8/G 9	0.32	-0.49	-3.59	5.30	0.58	6.40	2.22	-9
10) G 9/G 10	-0.29	0.16	-4.42	2.47	0.34	5.07	2.93	1
11) G 10/C 11	0.15	0.08	0.00	0.01	0.17	0.01	2.88	5
12) C 11/G 12	0.21	-0.25	0.32	4.09	0.32	4.10	2.95	8

Overall axis bend ... UU= 8.24 PP= 10.74

Duplex	Offset	L.Dir ... wrt end-to-end vector
1) C 1	0.00	0.00
2) G 2	0.31	104.80
3) C 3	0.32	50.57
4) **F** 4	0.37	-145.99
5) A 5	1.10	131.49
6) A 6	1.53	102.43
7) U 7	1.86	69.40
8) U 8	1.58	36.78
9) G 9	1.55	36.79
10) G 10	1.41	-1.36
11) C 11	0.85	-37.18
12) G 12	0.00	0.00

Path length= 30.25 End-to-end= 29.56 Shortening= 2.27 %

|J| Backbone Parameters |

1st strand	C1'-C2'	C2'-C3'	Phase	Ampli	Pucker	C1'	C2'	C3'
1)CT 1	-33.46	43.91	6.21	44.45	C3'-endo	104.7	102.3	100.2
2)GA 2	-33.18	45.30	10.50	47.45	C3'-endo	109.9	97.7	100.5
3)CT 3	-31.90	41.82	7.40	43.04	C3'-endo	108.1	100.6	101.2
4)**F**Y 4	-35.88	46.57	5.49	47.46	C3'-endo	104.4	99.7	99.5
5)AE 5	-32.57	45.12	10.48	46.87	C3'-endo	110.1	97.5	101.4
6)AE 6	-32.31	45.05	12.41	46.98	C3'-endo	105.2	101.9	98.3
7)UI 7	-35.89	48.67	10.21	50.56	C3'-endo	106.4	98.5	98.1
8)UI 8	-28.23	41.40	13.79	43.00	C3'-endo	105.8	101.2	101.3
9)GA 9	-25.39	41.33	20.34	44.93	C3'-endo	106.6	100.6	100.6
10)GA 10	-28.49	42.63	15.93	45.09	C3'-endo	105.5	101.4	99.3
11)CT 11	-29.03	41.86	13.49	43.89	C3'-endo	105.1	100.9	100.4
12)GA 12	-28.86	42.37	15.72	45.04	C3'-endo	106.8	100.9	99.1

Torsions	Chi	Gamma	Delta	Epsil	Zeta	Alpha	Beta
	C1'-N	C5'-C4'	C4'-C3'	C3'-O3'	O3'-P	P-O5'	O5'-C5'

1)CT	1	-167.11	49.18	82.37	-152.16	-71.54	-64.89	174.40
2)GA	2	-160.26	53.06	78.70	-153.10	-71.38	-60.75	173.96
3)CT	3	-158.91	52.41	83.59	-133.76	-64.56	-74.51	158.16
4)**F**Y	4	-158.47	58.80	76.10	-161.09	-72.49	-68.71	174.37
5)AE	5	-152.21	55.18	79.70	-154.38	-73.74	-63.24	163.28
6)AE	6	-157.70	58.23	84.69	-154.12	-74.11	-66.54	170.64
7)UI	7	-160.54	53.59	78.87	-146.81	-76.52	-63.98	169.34
8)UI	8	-158.42	51.39	79.87	-159.01	-66.13	-66.31	174.64
9)GA	9	-164.58	49.19	72.45	-150.55	-63.34	-65.34	178.01
10)GA	10	-165.43	52.11	75.35	-148.67	-71.78	-62.24	164.35
11)CT	11	-162.78	57.08	77.53	-154.34	-63.23	-68.13	176.52
12)GA	12	-161.60	56.88	79.80	.....	.....	.....	.....

2nd strand		C1'-C2'	C2'-C3'	Phase	Ampli	Pucker	C1'	C2'	C3'
1)GA	24	-29.47	41.63	11.89	43.08	C3'-endo	106.2	101.8	101.0
2)CT	23	-30.02	44.34	15.21	46.98	C3'-endo	107.3	98.7	99.8
3)GA	22	-32.71	43.88	8.60	45.17	C3'-endo	105.7	100.5	99.9
4)GA	21	-26.86	43.61	20.29	47.42	C3'-endo	107.3	99.4	100.4
5)UI	20	-28.72	43.82	15.66	45.87	C3'-endo	106.7	100.0	101.5
6)UI	19	-30.85	43.86	12.61	45.59	C3'-endo	106.1	100.3	99.5
7)AE	18	-29.98	43.45	12.50	45.24	C3'-endo	108.4	97.6	103.0
8)AE	17	-35.93	46.48	6.22	47.87	C3'-endo	108.4	98.4	100.5
9)**F**Y	16	-31.62	44.64	11.21	45.92	C3'-endo	103.9	100.5	100.3
10)CT	15	-30.09	45.09	16.02	47.80	C3'-endo	107.5	99.3	99.7
11)GA	14	-37.39	46.68	4.79	48.53	C3'-endo	109.9	96.2	100.6
12)CT	13	-36.06	46.71	7.64	48.41	C3'-endo	107.5	99.4	98.5

Torsions		Chi C1'-N	Gamma C5'-C4'	Delta C4'-C3'	Epsil C3'-O3'	Zeta O3'-P	Alpha P-O5'	Beta O5'-C5'
1)GA	24	-158.20	53.15	83.65	.....	.....	.....	.....
2)CT	23	-163.07	52.50	77.51	-151.84	-73.99	-58.39	173.06
3)GA	22	-163.82	59.07	80.16	-141.92	-68.64	-67.16	167.22
4)GA	21	-162.64	50.54	74.30	-151.06	-66.35	-63.79	167.43
5)UI	20	-163.21	52.69	78.68	-159.79	-71.90	-68.68	-179.04
6)UI	19	-161.89	56.35	80.11	-152.70	-71.57	-70.06	174.59
7)AE	18	-155.49	50.61	82.64	-145.23	-73.21	-66.66	168.89
8)AE	17	-148.59	54.88	78.64	-157.39	-70.29	-66.14	168.07
9)**F**Y	16	-158.91	52.28	80.93	-151.00	-84.30	-67.96	167.70
10)CT	15	-159.96	53.17	80.87	-151.62	-62.95	-68.28	167.83
11)GA	14	-159.90	51.22	84.57	-152.21	-70.15	-65.61	169.44
12)CT	13	-165.50	48.13	85.48	-157.50	-72.26	-69.02	-178.91

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|K| Groove parameters |
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Atom defining backbone: P      12 levels,  3 sub-levels
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Levels			Minor groove				Major groove			
	i	n	Width	Depth	Angle		Width	Depth	Angle	Diam
C	1	0	--	--	--	C	--	--	--	--
	1	1	--	--	--		--	--	--	--
	1	2	--	--	--		--	--	--	--
G	2	0	--	--	--	G	--	--	--	--
	2	1	10.19	0.81	33		--	--	--	--
	2	2	10.54	0.60	27		--	--	--	--
C	3	0	10.76	0.09	31	C	--	--	--	--
	3	1	10.78	-0.10	31		--	--	--	--
	3	2	10.74	-0.13	31		--	--	--	17.65
F	4	0	10.64	-0.14	32	**F**	--	--	--	17.92
	4	1	10.39	0.28	33		--	--	--	18.31
A	5	0	10.07	0.74	34	A	--	--	--	19.07
	5	1	9.80	1.06	30		3.59	8.04	27	19.11
	5	2	9.75	1.24	29		4.10	8.24	23	18.61
A	6	0	9.76	1.40	28	A	4.53	8.50	26	17.99
	6	1	9.82	1.19	31		4.78	9.18	22	17.63
	6	2	10.00	1.21	28		4.98	9.78	22	17.47
U	7	0	10.20	0.91	29	U	4.78	10.15	26	17.42
	7	1	10.33	0.72	34		4.12	9.76	29	17.49
	7	2	10.39	0.88	31		3.38	9.29	25	17.75
U	8	0	10.36	0.70	33	U	2.82	8.90	26	18.19
	8	1	10.28	0.67	35		--	--	--	18.35
	8	2	10.19	0.65	38		--	--	--	18.30
G	9	0	10.11	0.90	35	G	--	--	--	18.33
	9	1	10.06	0.70	34		--	--	--	18.56
	9	2	10.13	0.57	33		--	--	--	18.63
G	10	0	10.17	0.62	31	G	--	--	--	18.66
	10	1	10.09	0.72	34		--	--	--	--
	10	2	--	--	--		--	--	--	--
C	11	0	--	--	--	C	--	--	--	--
	11	1	--	--	--		--	--	--	--
	11	2	--	--	--		--	--	--	--
G	12	0	--	--	--	G	--	--	--	--

GA RNA DUPLEX

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**********************************
*****  CURVES 5.3 R.L. 1998  *****
**********************************

FILE : new_ga_C2.pdb                       LIS  : new_ga_C2
dna  :                                     axin :
axout:                                     daf  :
PDB  : new_ga_C2_axis

acc  :    0.000  wid  :    0.750

maxn :   500  ior  :     0  ibond:     0  splin:     3  break:    -1
nleve:     3  nbac :     7

ends :     F  supp :     T  COMB :     T  DINU :     F  MINI :     T
rest :     F  line :     F  zaxe :     F  fit  :     F  test :     F
GRV  :     T  old  :     T  axonl:     F

Strand=    2 Nucleo=   24 Atoms =  510 Units =   24

Input   1) Xdisp=    0.00 Ydisp=    0.00 Inclin=    0.00 Tip=    0.00

Combined strands have   12 levels ...

Strand  1 has  12 bases (5'-3'): CGCGAAUUAGCG
Strand  2 has  12 bases (3'-5'): GCGAUUAAGCGC

FIRST SUM=  106.511 CPTS:    3.410  14.151   9.274  79.676

MINIMISATION: ACC =  0.100E-05 MAXN=  500 NVAR=   48

STEP    1 SUM=  106.511 DEL=  0.000E+00
STEP    2 SUM=   82.610 DEL= -0.239E+02
STEP    3 SUM=   56.972 DEL= -0.256E+02
STEP    4 SUM=   43.613 DEL= -0.134E+02
STEP    5 SUM=   40.069 DEL= -0.354E+01
STEP    6 SUM=   36.200 DEL= -0.387E+01
STEP    7 SUM=   32.421 DEL= -0.378E+01
STEP    8 SUM=   28.211 DEL= -0.421E+01
STEP    9 SUM=   30.324 DEL=  0.211E+01
STEP   10 SUM=   26.528 DEL= -0.380E+01
STEP   11 SUM=   26.033 DEL= -0.495E+00
STEP   12 SUM=   25.202 DEL= -0.831E+00
STEP   13 SUM=   23.811 DEL= -0.139E+01
STEP   14 SUM=   21.740 DEL= -0.207E+01
STEP   15 SUM=   23.530 DEL=  0.179E+01
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STEP   16 SUM=   21.016 DEL= -0.251E+01
STEP   17 SUM=   19.746 DEL= -0.127E+01
STEP   18 SUM=   18.060 DEL= -0.169E+01
STEP   19 SUM=   42.530 DEL=  0.245E+02
STEP   20 SUM=   17.772 DEL= -0.248E+02
STEP   21 SUM=   17.884 DEL=  0.112E+00
STEP   22 SUM=   17.652 DEL= -0.232E+00
STEP   23 SUM=   17.468 DEL= -0.184E+00
STEP   24 SUM=   17.167 DEL= -0.300E+00
STEP   25 SUM=   16.821 DEL= -0.347E+00
STEP   26 SUM=   17.345 DEL=  0.524E+00
STEP   27 SUM=   16.722 DEL= -0.623E+00
STEP   28 SUM=   16.564 DEL= -0.158E+00
STEP   29 SUM=   16.301 DEL= -0.263E+00
STEP   30 SUM=   16.025 DEL= -0.275E+00
STEP   31 SUM=   15.728 DEL= -0.297E+00
STEP   32 SUM=   15.204 DEL= -0.524E+00
STEP   33 SUM=   14.511 DEL= -0.693E+00
STEP   34 SUM=   15.526 DEL=  0.102E+01
STEP   35 SUM=   14.081 DEL= -0.145E+01
STEP   36 SUM=   13.567 DEL= -0.514E+00
STEP   37 SUM=   13.073 DEL= -0.494E+00
STEP   38 SUM=   13.204 DEL=  0.130E+00
STEP   39 SUM=   12.863 DEL= -0.340E+00
STEP   40 SUM=   12.856 DEL= -0.729E-02
STEP   41 SUM=   12.791 DEL= -0.654E-01
STEP   42 SUM=   12.770 DEL= -0.208E-01
STEP   43 SUM=   12.738 DEL= -0.322E-01
STEP   44 SUM=   12.707 DEL= -0.310E-01
STEP   45 SUM=   12.700 DEL= -0.696E-02
STEP   46 SUM=   12.689 DEL= -0.104E-01
STEP   47 SUM=   12.685 DEL= -0.422E-02
STEP   48 SUM=   12.681 DEL= -0.399E-02
STEP   49 SUM=   12.681 DEL=  0.192E-03
STEP   50 SUM=   12.680 DEL= -0.138E-02
STEP   51 SUM=   12.680 DEL= -0.272E-03
STEP   52 SUM=   12.679 DEL= -0.226E-03
STEP   53 SUM=   12.679 DEL= -0.179E-04
STEP   54 SUM=   12.679 DEL= -0.324E-04
STEP   55 SUM=   12.679 DEL= -0.439E-04
STEP   56 SUM=   12.679 DEL= -0.540E-04
STEP   57 SUM=   12.679 DEL= -0.678E-04
STEP   58 SUM=   12.679 DEL= -0.255E-04
STEP   59 SUM=   12.679 DEL= -0.471E-05
STEP   60 SUM=   12.679 DEL= -0.862E-06
STEP   61 SUM=   12.679 DEL= -0.437E-06
STEP   62 SUM=   12.679 DEL= -0.108E-07
STEP   63 SUM=   12.679 DEL= -0.165E-07
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STEP   64 SUM=   12.679 DEL= -0.107E-07
STEP   65 SUM=   12.679 DEL= -0.236E-08
STEP   66 SUM=   12.679 DEL= -0.149E-08
STEP   67 SUM=   12.679 DEL= -0.650E-09
STEP   68 SUM=   12.679 DEL= -0.154E-09
STEP   69 SUM=   12.679 DEL= -0.106E-10
STEP   70 SUM=   12.679 DEL= -0.193E-11
STEP   71 SUM=   12.679 DEL= -0.213E-13
STEP   72 SUM=   12.679 DEL=  0.000E+00

FINAL SUM=   12.679 CPTS:    2.297   9.055   0.694   0.632

GRA= 0.36E-08-0.40E-07-0.14E-10-0.28E-08 0.11E-07 0.11E-07 0.12E-08 0.63E-09
GRA= 0.16E-07-0.52E-08 0.19E-09 0.10E-08-0.54E-09 0.64E-07 0.25E-09 0.25E-08
GRA=-0.96E-08-0.83E-08-0.48E-09-0.74E-09-0.50E-08 0.14E-08-0.18E-08-0.24E-09
GRA=-0.74E-08-0.11E-07-0.69E-09 0.13E-09-0.34E-08-0.56E-08-0.72E-11-0.15E-08
GRA= 0.29E-08-0.17E-07 0.28E-08-0.25E-09 0.17E-08-0.30E-08 0.74E-09-0.19E-09
GRA=-0.47E-09 0.43E-08-0.30E-09-0.45E-09 0.38E-09 0.13E-07-0.11E-08 0.27E-08

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|A| Global axis parameters |
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  1) U:    0.728  -0.009  -0.686  P:   30.506   0.617   9.916  D:    0.393
  2) U:    0.736   0.039  -0.676  P:   32.433   0.666   7.989  D:    0.376
  3) U:    0.712  -0.006  -0.702  P:   34.626   0.631   5.865  D:    2.493
  4) U:    0.735   0.037  -0.677  P:   36.226   0.762   3.989  D:    2.415
  5) U:    0.778  -0.025  -0.628  P:   38.035   0.833   2.667  D:    0.561
  6) U:    0.779   0.001  -0.627  P:   40.182   0.628   0.917  D:    0.221
  7) U:    0.779  -0.002  -0.627  P:   42.494   0.627  -0.915  D:    0.554
  8) U:    0.778   0.024  -0.628  P:   44.641   0.831  -2.665  D:    2.415
  9) U:    0.735  -0.037  -0.677  P:   46.454   0.759  -3.989  D:    2.496
 10) U:    0.712   0.006  -0.702  P:   48.052   0.629  -5.864  D:    0.368
 11) U:    0.736  -0.039  -0.676  P:   50.241   0.664  -7.988  D:    0.387
 12) U:    0.728   0.010  -0.686  P:   52.170   0.616  -9.917

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|B| Global Base-Axis Parameters |
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  1st strand      Xdisp    Ydisp   Inclin     Tip    Bc  Tc
                  (dx)     (dy)    (eta)    (theta)

  1) CYT   1      -4.20     0.53    17.12    -6.82   3   0
  2) GUA   2      -4.41     0.39    11.33    -5.99   1  13
  3) CYT   3      -4.20     0.21    10.92    -4.43   3 -13
  4) GUA   4      -4.53     0.58    18.55     1.22   1  10
  5) ADE   5      -4.13    -0.21    18.39    -5.86   2  18
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6)	ADE	6	-4.14	0.08	20.05	-12.64	2 24
7)	URI	7	-3.93	0.09	15.50	-13.23	4 -24
8)	URI	8	-4.27	0.10	15.22	-10.20	4 -28
9)	ADE	9	-4.40	0.55	15.89	-3.41	2 27
10)	GUA	10	-4.29	-0.27	16.17	-10.09	1 7
11)	CYT	11	-4.01	-0.01	15.14	-14.79	3 -13
12)	GUA	12	-4.24	-0.09	10.10	-13.00	1 0

2nd strand			Xdisp (dx)	Ydisp (dy)	Inclin (eta)	Tip (theta)	Bc	Tc
1)	GUA	24	-4.24	-0.10	10.11	-13.00	1	0
2)	CYT	23	-4.01	-0.01	15.16	-14.80	3	-13
3)	GUA	22	-4.29	-0.28	16.15	-10.04	1	7
4)	ADE	21	-4.40	0.55	15.90	-3.39	2	27
5)	URI	20	-4.26	0.10	15.21	-10.14	4	-28
6)	URI	19	-3.93	0.09	15.50	-13.24	4	-24
7)	ADE	18	-4.14	0.08	20.04	-12.61	2	24
8)	ADE	17	-4.13	-0.21	18.40	-5.89	2	18
9)	GUA	16	-4.53	0.58	18.54	1.25	1	10
10)	CYT	15	-4.19	0.21	10.92	-4.44	3	-13
11)	GUA	14	-4.40	0.39	11.35	-6.00	1	13
12)	CYT	13	-4.20	0.53	17.10	-6.81	3	0

|C| Global Base pair-Axis Parameters |

Strand 1 with strand 2 ...

Duplex			Xdisp (dx)	Ydisp (dy)	Inclin (eta)	Tip (theta)	Bc	Tc
1)	C 1-G	24	-4.22	0.31	13.61	3.09	3	0
2)	G 2-C	23	-4.21	0.20	13.25	4.40	1	13
3)	C 3-G	22	-4.24	0.24	13.54	2.80	3	-13
4)	G 4-A	21	-4.46	0.02	17.22	2.30	1	10
5)	A 5-U	20	-4.20	-0.15	16.80	2.14	2	18
6)	A 6-U	19	-4.03	-0.01	17.77	0.30	2	24
7)	U 7-A	18	-4.03	0.01	17.77	-0.31	4	-24
8)	U 8-A	17	-4.20	0.16	16.81	-2.15	4	-28
9)	A 9-G	16	-4.46	-0.02	17.22	-2.33	2	27
10)	G 10-C	15	-4.24	-0.24	13.55	-2.82	1	7
11)	C 11-G	14	-4.20	-0.20	13.24	-4.40	3	-13
12)	G 12-C	13	-4.22	-0.31	13.60	-3.10	1	0

Average:	-4.23	0.00	15.37	-0.01

|D| Global Base-Base Parameters

Strand 1 with strand 2 ...

Duplex	Shear (Sx)	Stretch (Sy)	Stagger (Sz)	Buckle (kappa)	Propel (omega)	Opening (sigma)	Bc	T
1) C 1-G 24	0.04	0.44	-0.08	7.00	-19.82	4.18	3	0
2) G 2-C 23	-0.40	0.39	-0.07	-3.83	-20.79	4.64	1	13
3) C 3-G 22	0.10	-0.07	0.25	-5.23	-14.47	-1.01	3	-13
4) G 4-A 21	-0.14	1.13	0.11	2.65	-2.17	-9.55	1	10
5) A 5-U 20	0.13	-0.11	0.08	3.18	-16.00	-3.13	2	18
6) A 6-U 19	-0.21	0.17	-0.02	4.55	-25.88	1.35	2	24
7) U 7-A 18	0.21	0.17	-0.03	-4.54	-25.85	1.36	4	-24
8) U 8-A 17	-0.14	-0.11	0.08	-3.18	-16.09	-3.10	4	-28
9) A 9-G 16	0.13	1.13	0.11	-2.65	-2.16	-9.58	2	27
10) G 10-C 15	-0.10	-0.07	0.25	5.26	-14.53	-1.01	1	7
11) C 11-G 14	0.40	0.39	-0.07	3.79	-20.79	4.66	3	-13
12) G 12-C 13	-0.04	0.44	-0.08	-7.00	-19.82	4.17	1	0
Average:	0.00	0.32	0.04	0.00	-16.53	-0.59		

|E| Global Inter-Base Parameters

1st strand	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) C 1/G 2	-0.22	-0.24	2.73	-5.92	3.71	34.56	8
3) G 2/C 3	0.13	-0.14	3.22	-0.93	-1.68	33.12	5
4) C 3/G 4	-0.57	0.24	2.38	9.67	8.02	23.31	8
5) G 4/A 5	0.55	-0.91	2.22	-2.24	-2.40	36.55	2
6) A 5/A 6	0.12	0.40	2.72	2.60	-7.94	37.68	4
7) A 6/U 7	0.21	-0.01	2.95	-4.54	-0.43	36.12	7
8) U 7/U 8	-0.47	0.12	2.82	-1.23	1.89	33.20	-4
9) U 8/A 9	-0.28	0.33	2.26	2.74	11.43	30.06	10
10) A 9/G 10	0.34	-0.96	2.52	-1.76	-4.30	31.90	3
11) G 10/C 11	0.36	0.31	2.89	-0.53	-7.90	38.76	5
12) C 11/G 12	-0.22	-0.18	2.72	-4.92	4.64	34.11	8

2nd strand	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) G 24/C 23	0.22	0.19	2.72	4.92	-4.68	34.09	8
3) C 23/G 22	-0.37	-0.31	2.89	0.47	8.01	38.78	5

4) G 22/A 21	-0.34	0.96	2.53	1.80	4.28	31.85	3
5) A 21/U 20	0.28	-0.33	2.25	-2.78	-11.43	30.13	10
6) U 20/U 19	0.47	-0.12	2.83	1.24	-1.94	33.20	-4
7) U 19/A 18	-0.21	0.01	2.95	4.54	0.46	36.11	7
8) A 18/A 17	-0.12	-0.40	2.72	-2.59	7.86	37.66	4
9) A 17/G 16	-0.55	0.91	2.22	2.21	2.50	36.54	2
10) G 16/C 15	0.57	-0.24	2.38	-9.67	-8.07	23.32	8
11) C 15/G 14	-0.13	0.14	3.21	0.94	1.63	33.10	5
12) G 14/C 13	0.22	0.23	2.73	5.88	-3.67	34.59	8

|F| Global Inter-Base pair Parameters |

Strand 1 with strand 2 ...

Duplex	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) C 1/G 2	0.00	-0.21	2.72	-0.50	4.20	34.32	8
3) G 2/C 3	-0.12	0.09	3.05	-0.23	-4.84	35.95	5
4) C 3/G 4	-0.45	-0.36	2.45	5.74	1.87	27.58	8
5) G 4/A 5	0.42	-0.29	2.24	-2.51	4.52	33.34	2
6) A 5/A 6	0.29	0.26	2.77	1.92	-3.00	35.44	4
7) A 6/U 7	0.00	-0.01	2.95	0.00	-0.45	36.12	7
8) U 7/U 8	-0.29	0.26	2.77	-1.91	-2.98	35.43	-4
9) U 8/A 9	-0.42	-0.29	2.24	2.47	4.47	33.30	10
10) A 9/G 10	0.46	-0.36	2.45	-5.72	1.89	27.61	3
11) G 10/C 11	0.12	0.08	3.05	0.21	-4.77	35.93	5
12) C 11/G 12	0.00	-0.21	2.73	0.48	4.16	34.35	8
Average:	0.00	-0.09	2.68	0.00	0.46	33.58	

|G| Local Inter-Base Parameters |

1st strand	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) C 1/G 2	-0.06	-2.02	3.56	-1.92	11.97	33.34	8
3) G 2/C 3	0.25	-2.00	3.39	2.01	4.62	33.10	5
4) C 3/G 4	-0.67	-0.88	2.92	10.16	13.75	21.86	8
5) G 4/A 5	0.57	-2.57	3.53	-1.17	8.96	33.25	2
6) A 5/A 6	0.65	-1.29	3.20	8.19	4.65	35.11	4
7) A 6/U 7	0.95	-1.53	3.46	3.38	10.45	34.57	7
8) U 7/U 8	0.13	-1.47	3.26	5.33	10.47	32.03	-4
9) U 8/A 9	-0.10	-1.24	3.09	5.83	19.13	27.52	10

10) A 9/G 10	0.67	-2.41	3.45	1.61	4.45	30.00	3
11) G 10/C 11	1.10	-1.66	3.07	7.58	2.73	37.45	5
12) C 11/G 12	0.64	-1.94	3.35	3.31	11.84	32.96	8

2nd strand	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) G 24/C 23	-0.64	-1.94	3.35	-3.31	11.88	32.94	8
3) C 23/G 22	-1.10	-1.65	3.07	-7.62	2.63	37.48	5
4) G 22/A 21	-0.66	-2.41	3.45	-1.56	4.46	29.96	3
5) A 21/U 20	0.09	-1.24	3.09	-5.86	19.14	27.58	10
6) U 20/U 19	-0.13	-1.47	3.26	-5.31	10.52	32.04	-4
7) U 19/A 18	-0.95	-1.53	3.46	-3.38	10.41	34.56	7
8) A 18/A 17	-0.65	-1.29	3.20	-8.18	4.72	35.09	4
9) A 17/G 16	-0.57	-2.57	3.53	1.14	8.87	33.25	2
10) G 16/C 15	0.68	-0.88	2.92	-10.15	13.80	21.87	8
11) C 15/G 14	-0.25	-2.00	3.40	-2.00	4.67	33.07	5
12) G 14/C 13	0.06	-2.02	3.56	1.88	11.93	33.37	8

|H| Local Inter-Base pair Parameters |

Strand 1 with strand 2 ...

Duplex	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (tau)	Roll (rho)	Twist (Omega)	Dc
2) C 1/G 2	-0.36	-1.97	3.47	-2.65	11.94	33.62	8
3) G 2/C 3	-0.45	-1.81	3.30	-2.85	3.71	35.60	5
4) C 3/G 4	-0.61	-1.65	3.15	4.49	8.85	25.90	8
5) G 4/A 5	0.28	-1.92	3.27	-3.76	13.92	30.36	2
6) A 5/A 6	0.27	-1.38	3.24	1.46	7.57	33.97	4
7) A 6/U 7	0.00	-1.52	3.59	0.00	10.47	35.45	7
8) U 7/U 8	-0.27	-1.38	3.24	-1.45	7.58	33.96	-4
9) U 8/A 9	-0.28	-1.92	3.28	3.73	13.87	30.33	10
10) A 9/G 10	0.62	-1.65	3.15	-4.46	8.87	25.93	3
11) G 10/C 11	0.45	-1.81	3.30	2.83	3.79	35.57	5
12) C 11/G 12	0.36	-1.97	3.47	2.64	11.90	33.65	8
Average:	0.00	-1.73	3.31	0.00	9.32	32.21	

|I| Global Axis Curvature |

Duplex	Ax	Ay	Ainc	Atip	Adis	Angle	Path	Dc

2)	C 1/G 2	-0.01	-0.10	-0.13	2.88	0.10	2.89	2.73	8
3)	G 2/C 3	-0.08	0.04	-0.52	-3.25	0.09	3.29	3.05	5
4)	C 3/G 4	-0.23	-0.14	2.05	2.37	0.27	3.13	2.47	8
5)	G 4/A 5	0.15	-0.11	-2.09	4.68	0.19	5.12	2.24	2
6)	A 5/A 6	0.13	0.11	0.95	-1.15	0.17	1.49	2.78	4
7)	A 6/U 7	0.00	-0.02	0.00	0.16	0.02	0.16	2.95	7
8)	U 7/U 8	-0.13	0.11	-0.95	-1.14	0.17	1.48	2.78	-4
9)	U 8/A 9	-0.15	-0.12	2.07	4.64	0.19	5.08	2.25	10
10)	A 9/G 10	0.24	-0.14	-2.05	2.38	0.27	3.14	2.47	3
11)	G 10/C 11	0.08	0.04	0.51	-3.19	0.09	3.23	3.05	5
12)	C 11/G 12	0.01	-0.10	0.12	2.85	0.10	2.86	2.73	8

Overall axis bend ... UU= 1.09 PP= 2.05

Duplex	Offset	L.Dir ... wrt end-to-end vector
1) C 1	0.00	0.00
2) G 2	0.13	80.41
3) C 3	0.21	28.99
4) G 4	0.53	17.61
5) A 5	0.34	4.38
6) A 6	0.10	-66.16
7) U 7	0.11	65.22
8) U 8	0.34	-0.92
9) A 9	0.53	-7.63
10) G 10	0.21	-27.71
11) C 11	0.13	-84.68
12) G 12	0.00	0.00

Path length= 29.49 End-to-end= 29.37 Shortening= 0.39 %

|J| Backbone Parameters |

1st strand	C1'-C2'	C2'-C3'	Phase	Ampli	Pucker	C1'	C2'	C3'
1)CYT 1	-34.07	45.23	8.81	46.69	C3'-endo	106.5	101.2	98.4
2)GUA 2	-34.74	45.56	8.49	47.63	C3'-endo	111.7	96.9	100.2
3)CYT 3	-29.78	43.77	13.36	45.31	C3'-endo	105.9	100.5	101.7
4)GUA 4	-33.42	46.82	11.31	48.52	C3'-endo	105.9	99.0	99.7
5)ADE 5	-26.06	41.29	19.09	44.25	C3'-endo	106.6	102.1	100.5
6)ADE 6	-29.34	41.39	12.65	43.53	C3'-endo	108.7	99.8	101.3
7)URI 7	-31.25	44.02	11.34	45.09	C3'-endo	104.7	102.7	99.9
8)URI 8	-32.03	45.86	12.92	48.08	C3'-endo	108.4	98.0	100.5
9)ADE 9	-27.95	44.99	20.57	48.79	C3'-endo	102.4	102.0	97.2
10)GUA 10	-30.73	42.97	11.83	44.94	C3'-endo	107.0	99.3	99.9

11)CYT	11	-27.91	42.04	16.01	44.38	C3'-endo	106.8	100.5	100.7
12)GUA	12	-24.92	40.15	20.13	43.44	C3'-endo	107.7	101.1	100.6

Torsions		Chi C1'-N	Gamma C5'-C4'	Delta C4'-C3'	Epsil C3'-O3'	Zeta O3'-P	Alpha P-O5'	Beta O5'-C5'
1)CYT	1	-164.71	60.48	78.52	-156.05	-71.56	-65.67	-179.39
2)GUA	2	-158.96	49.20	87.63	-152.58	-72.18	-64.23	177.91
3)CYT	3	-159.80	49.36	79.74	-128.42	-91.12	-66.23	145.28
4)GUA	4	-165.58	53.71	78.20	-159.76	-61.97	-68.36	179.01
5)ADE	5	-164.11	58.44	76.23	-147.03	-77.33	-62.00	170.12
6)ADE	6	-154.65	49.95	81.10	-153.32	-70.97	-63.12	168.76
7)URI	7	-159.27	52.92	81.33	-154.67	-70.31	-64.80	176.30
8)URI	8	-154.09	46.19	85.86	-138.99	-77.36	-77.74	162.66
9)ADE	9	-168.00	53.70	76.73	-162.96	-65.38	-64.03	175.43
10)GUA	10	-165.57	59.45	80.58	-148.08	-73.36	-63.23	165.89
11)CYT	11	-162.00	55.14	83.83	-149.66	-70.23	-61.74	173.64
12)GUA	12	-158.32	50.58	80.19	.....	.....	.....	.....

2nd strand		C1'-C2'	C2'-C3'	Phase	Ampli	Pucker	C1'	C2'	C3'
1)GUA	24	-24.91	40.14	20.17	43.44	C3'-endo	107.6	101.1	100.6
2)CYT	23	-27.91	42.03	16.01	44.38	C3'-endo	106.8	100.5	100.6
3)GUA	22	-30.72	42.99	11.85	44.95	C3'-endo	107.1	99.3	99.9
4)ADE	21	-28.03	45.07	20.51	48.86	C3'-endo	102.4	102.0	97.2
5)URI	20	-32.02	45.81	12.93	48.04	C3'-endo	108.4	98.0	100.5
6)URI	19	-31.25	44.02	11.34	45.09	C3'-endo	104.7	102.7	99.9
7)ADE	18	-29.34	41.39	12.65	43.53	C3'-endo	108.7	99.8	101.3
8)ADE	17	-26.08	41.29	19.08	44.25	C3'-endo	106.6	102.1	100.5
9)GUA	16	-33.45	46.87	11.29	48.56	C3'-endo	105.9	99.0	99.7
10)CYT	15	-29.80	43.78	13.34	45.31	C3'-endo	105.9	100.5	101.6
11)GUA	14	-34.71	45.57	8.51	47.62	C3'-endo	111.7	96.9	100.2
12)CYT	13	-34.06	45.25	8.81	46.69	C3'-endo	106.4	101.2	98.4

Torsions		Chi C1'-N	Gamma C5'-C4'	Delta C4'-C3'	Epsil C3'-O3'	Zeta O3'-P	Alpha P-O5'	Beta O5'-C5'
1)GUA	24	-158.35	50.60	80.19	.....	.....	.....	.....
2)CYT	23	-161.97	55.25	83.76	-149.68	-70.21	-61.76	173.68
3)GUA	22	-165.59	59.44	80.59	-148.08	-73.36	-63.26	165.85
4)ADE	21	-168.00	53.66	76.74	-162.98	-65.38	-64.07	175.44
5)URI	20	-154.13	46.33	85.78	-139.02	-77.31	-77.74	162.67
6)URI	19	-159.27	52.88	81.33	-154.67	-70.31	-64.86	176.27
7)ADE	18	-154.65	49.90	81.14	-153.32	-70.97	-63.07	168.72
8)ADE	17	-164.06	58.41	76.23	-146.98	-77.37	-61.96	170.16
9)GUA	16	-165.59	53.71	78.20	-159.73	-61.99	-68.32	179.00
10)CYT	15	-159.80	49.39	79.65	-128.43	-91.09	-66.23	145.28

11)GUA	14	-158.96	49.12	87.68	-152.54	-72.18	-64.20	177.87
12)CYT	13	-164.74	60.43	78.55	-156.00	-71.57	-65.65	-179.36

|K| Groove parameters |

Atom defining backbone: P 12 levels, 3 sub-levels

Levels			Minor groove				Major groove			
	i	n	Width	Depth	Angle		Width	Depth	Angle	Diam
C	1	0	--	--	--	C	--	--	--	--
	1	1	--	--	--		--	--	--	--
	1	2	--	--	--		--	--	--	--
G	2	0	--	--	--	G	--	--	--	--
	2	1	--	--	--		--	--	--	--
	2	2	10.32	0.92	32		--	--	--	--
	2	3	10.64	0.63	33		--	--	--	--
C	3	0	10.96	0.47	29	C	--	--	--	--
	3	1	11.20	-0.08	31		--	--	--	18.47
	3	2	11.34	-0.40	29		--	--	--	18.49
G	4	0	11.37	-0.48	28	G	--	--	--	18.50
	4	1	11.38	-0.56	29		--	--	--	18.38
	4	2	11.30	-0.29	30		--	--	--	18.27
A	5	0	11.15	0.13	31	A	--	--	--	18.17
	5	1	10.89	0.41	34		2.42	8.88	24	17.95
	5	2	10.62	0.77	33		2.76	8.90	25	17.56
A	6	0	10.35	1.27	28	A	2.93	8.88	32	17.05
	6	1	10.16	1.16	29		3.10	9.05	31	16.63
	6	2	10.17	1.09	30		3.10	9.05	32	16.63
U	7	0	10.37	1.33	28	U	2.92	8.81	35	17.05
	7	1	10.63	0.83	32		2.73	8.83	28	17.55
	7	2	10.91	0.34	35		2.41	8.84	26	17.95
U	8	0	11.17	0.15	30	U	--	--	--	18.17
	8	1	11.31	-0.26	29		--	--	--	18.27
	8	2	11.38	-0.50	28		--	--	--	18.38
A	9	0	11.38	-0.54	28	A	--	--	--	18.50
	9	1	11.33	-0.32	29		--	--	--	18.49
	9	2	11.19	0.00	30		--	--	--	18.47
G	10	0	10.93	0.44	30	G	--	--	--	--
	10	1	10.60	0.71	31		--	--	--	--
	10	2	10.28	1.00	32		--	--	--	--
	10	3	--	--	--		--	--	--	--
C	11	0	--	--	--	C	--	--	--	--
	11	1	--	--	--		--	--	--	--
	11	2	--	--	--		--	--	--	--
G	12	0	--	--	--	G	--	--	--	--

Table 1. Experimental t_m and thermodynamic data for melting of r(CGCUAAUUGGCG).

Experiment	0%	5%	10%	15%	20%	-ΔH (cal/mol) δα/δT_m	-ΔH (cal/mol) van't Hoff	-ΔS (eu) van't Hoff
Ethylene Glycol								
sm264A	57.1		56.3	54.1		47614	47750	119.7
sm264B1	57.9	55.7	56.0	53.4	53.1	47057	47560	119.0
sm264B2	57.6	55.6	55.9	53.5	53.2	48564	47700	119.7
sm264B3		55.5	56.0	53.7	53.0			
sm264B4		56.5	56.3	54.2	52.8			
sm264C	57.7		56.3	53.9		47045	47570	119.2
sm264D1	57.4		56.6	53.8		46337	49460	125.0
sm264D2	57.5		56.1	53.4	52.4	47262	49610	125.4
sm264E1	57.9	55.8	55.9	54.1	53.0	47215	47130	117.8
sm264E2		56.0	56.2	54.1	52.9			
sm264E3	57.8	55.6	56.2	54.5	52.7	49667	52080	132.7
sm264E4		56.3	56.3	53.5				
sm264F1	57.9	55.7	56.0	53.5	53.1	49584	49780	125.7
sm264F2	58.1	56.3	56.3	54.2	53.1	47062	48420	121.6
Average		**55.9**	**56.2**	**53.9**	**52.9**			
Standard Deviation		**0.4**	**0.2**	**0.4**	**0.2**			
Glycerol								
sm276A	57.6				53.5	51118	47660	119.6
sm276B1	57.5	56.3	55.5	55.1	53.3	49017	51460	130.9
sm276B2	57.6	56.9	55.8	54.7	53.7	48209	49350	124.5
sm276B3	57.8	56.6	55.5	55.0	53.0	47078	48830	122.7
sm276B4		57.0	55.8	54.4	53.7			
sm276C	57.9	56.1	55.5	54.4		48021	49440	124.7
Average		**56.6**	**55.6**	**54.7**	**53.4**			
Standard Deviation		**0.4**	**0.2**	**0.3**	**0.3**			
Acetamide								
sm279A	57.4	55.2	53.8	51.6	49.0	45866	49330	124.5
sm279B1	57.8	55.2	53.1	51.0	49.4	48349	49070	123.6
sm279B2	57.8	54.3	52.9	50.8	48.8	51273	54400	139.7
sm279B3		55.4	52.8	51.5	49.4			
sm279B4	57.6		53.1	50.7	48.4	49531	49940	126.4
sm279C	57.9	55.3	53.0	51.5	48.8	50393	52600	134.3
sm279D	57.8	55.1	53.1	50.9	48.9	47769	51540	132.0
sm279E1	57.5	54.8		50.8	49.3	49893	52080	132.9
sm279E2	57.9	54.9		51.0	49.2	46201	50700	128.4
sm279E3		54.9		51.2	48.5			
Average		**55.0**	**53.1**	**51.1**	**49.0**			
Standard Deviation		**0.3**	**0.3**	**0.3**	**0.4**			
Total Averages	**57.7**					**48266**	**49716**	**125.7**
Standard Deviation	**0.2**					**1548**	**1910**	**6**

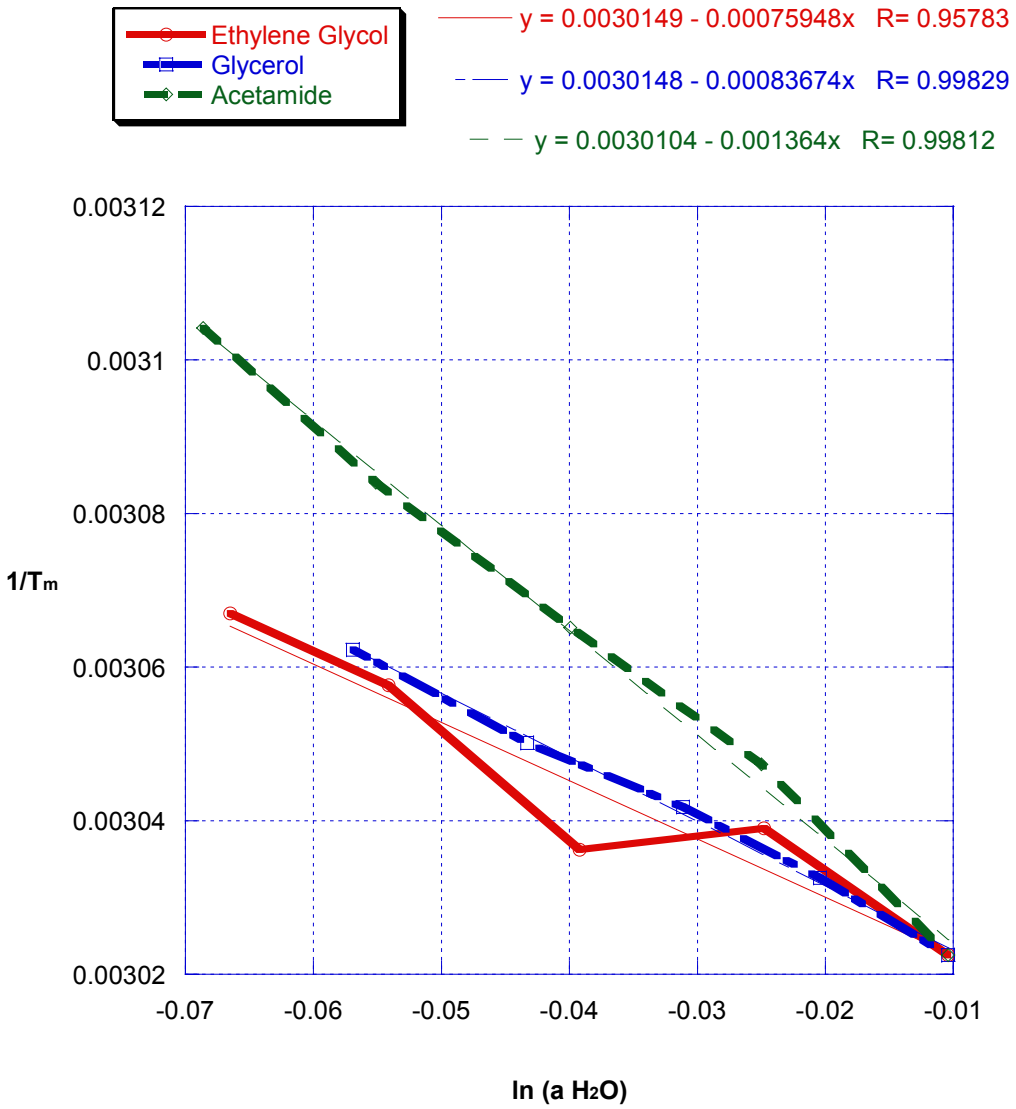

Figure 1. Reciprocal temperature of melting for r(CGCUAAUUGGCG) vs. the logarithm of water activity for small cosolutes.

Table 2. Calculations for r(CGCUAAUUGGCG).

Experiments	Cosolute	-ΔH (cal/mol)	-σH (cal/mol)	-Slope	-σSlope	Δn_w	σn_w
sm264	Ethylene Glycol	48266	1548	0.00075948	0.000119275	**18.5**	**3.0**
sm276	Glycerol	48266	1548	0.00083674	0.000136390	**20.3**	**3.4**
sm279	Acetamide	48266	1548	0.00136400	0.000116300	**33.1**	**3.0**

Table 3. Experimental t_m and thermodynamic data for melting of r(CGCFAAUUGGCG).

Experiment	0%	5%	10%	15%	20%	-ΔH (cal/mol) $\delta\alpha/\delta T_m$	-ΔH (cal/mol) van't Hoff	-ΔS (eu) van't Hoff
Ethylene Glycol								
sm270A1	55.0	52.4	53.2	51.3	49.7	38548	43070	106.6
sm270A2	55.1	52.3	53.5	51.6	49.6	40367	44260	110.2
sm270B1		52.2	52.7	51.3	50.3			
sm270B2			52.2	51.1	50.3			
sm270B3		52.3	52.8	51.3	49.8			
sm270B4			52.5	51.2	50.4			
sm270C	54.9	52.8	52.6	51.2	50.1	39339	39250	95.2
sm270D1	54.9	52.0	53.1	51.7	50.5	37650	39480	95.7
sm270D2	54.7	52.5	52.3	51.2	50.4	41835	43570	108.3
sm270D3		52.0	52.4	50.6	49.8			
sm270D4			52.4		50.2			
sm270E		52.9						
Average		**52.4**	**52.7**	**51.3**	**50.1**			
Standard Deviation		**0.3**	**0.4**	**0.3**	**0.3**			
Glycerol								
sm273A	54.8	53.9		49.7	49.0	42305	45370	113.6
sm273B1		53.2	52.8					
sm273B2	54.8	53.7	52.0	50.1	49.1	42662	44470	111.0
sm273B3			52.9		48.9			
sm273C		53.9	52.5	50.1				
sm273D1	55.4	53.1	52.9			43311	45170	112.8
sm273D2	54.9		52.1	50.1		41602	43340	107.4
sm273D3	54.6	53.0				42586	45180	113.2
sm273D4			52.6	49.7	48.3			
sm273E1	54.9				48.9	44274	42560	105.1
sm273E2		53.6	52.6	50.3	49.1			
Average		**53.5**	**52.6**	**50.0**	**48.9**			
Standard Deviation		**0.4**	**0.3**	**0.2**	**0.3**			
Acetamide								
sm284A	55.2	52.3	50.5	48.0	46.7	39738	45070	112.6
sm284B1	55.1	52.1	50.8	47.7	46.3	39891	42870	106.0
sm284B2		52.3	50.5	47.4	45.8			
sm284B3								
sm284B4			51.1	47.1	46.7			
sm284C1	54.7		51.2		46.2	40112	38660	93.4
sm284C2	54.6		50.3		46.8	39519	38380	92.5
sm284D1	55.1	52.8	51.1	47.4	46.9	37571	40440	98.5
sm284D2		52.3	51.1	47.4	46.5			
sm284D3		52.6	51.5	47.6	46.8			
sm284E1		52.4	51.1		46.2			

sm284E2		52.8	51.1	47.4	46.7			
sm284F					46.4			
Average		**52.5**	**50.9**	**47.5**	**46.5**			
Standard Deviation		**0.3**	**0.4**	**0.3**	**0.3**			
Total Averages	**54.9**					**40707**	**42571**	**105.1**
Standard Deviation	**0.2**					**2011**	**2504**	**8**

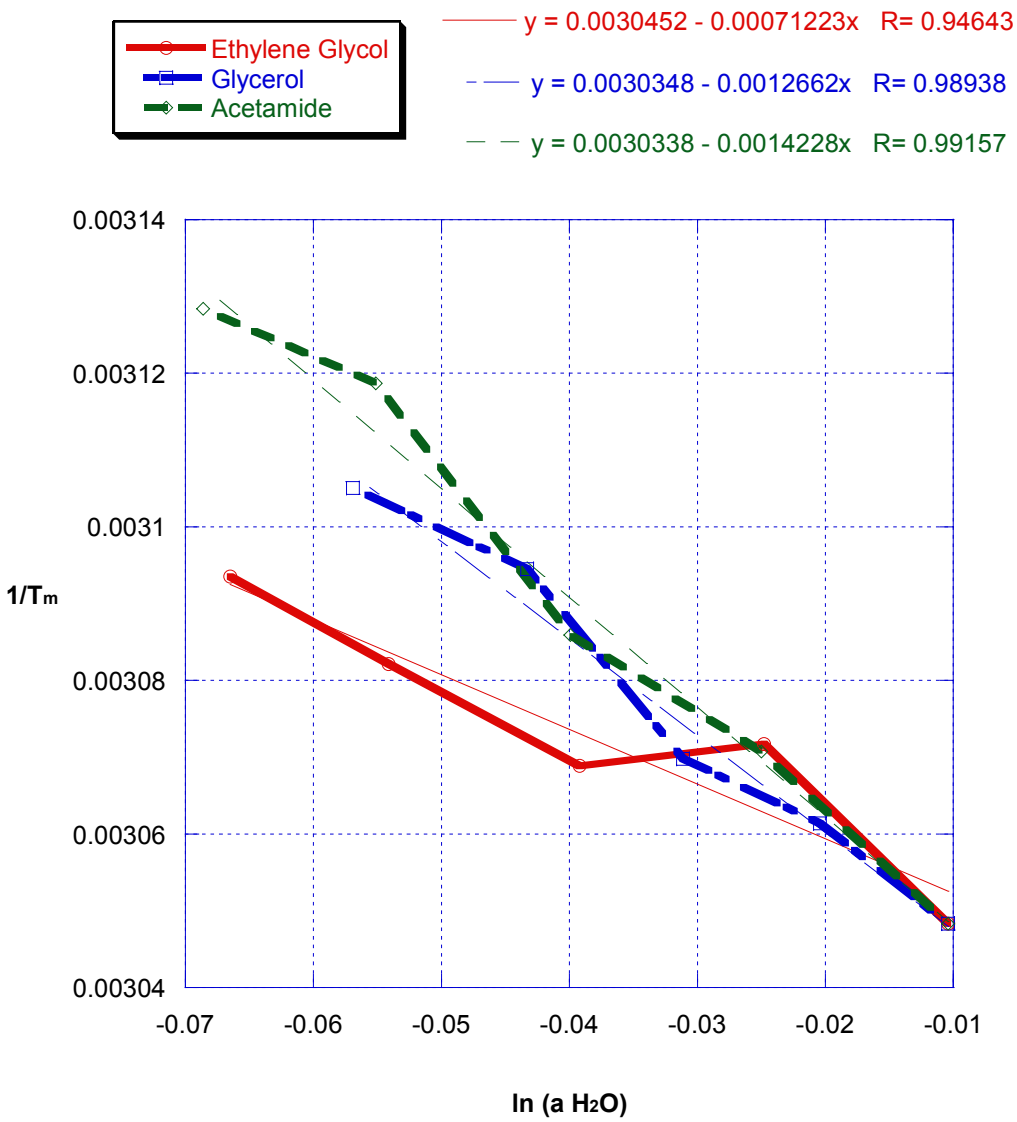

Figure 2. Reciprocal temperature of melting for r(CGCFAAUUGGCG) vs. the logarithm of water activity for small cosolutes.

Table 4. Calculations for r(CGCFAAUUGGCG).

Experiments	Cosolute	-ΔH (cal/mol)	-σH (cal/mol)	-Slope	-σSlope	Δn_w	σn_w
sm270	Ethylene Glycol	40707	2011	0.00071223	0.000094250	**14.6**	**2.1**
sm273	Glycerol	40707	2011	0.00126620	0.000147550	**26.0**	**3.3**
sm284	Acetamide	40707	2011	0.00142280	0.000095350	**29.2**	**2.4**

Table 5. Experimental t_m and thermodynamic data for melting of r(CGCGAAUUFGCG).

Experiment	0%	5%	10%	15%	20%	-ΔH (cal/mol) δα/δT_m	-ΔH (cal/mol) van't Hoff	-ΔS (eu) van't Hoff
Ethylene Glycol								
sm266A1	53.8	51.7		50.5	49.9	42524	41790	103.3
sm266A2	53.7	52.7	52.2	50.8	50.4	42897	43990	110.0
sm266B	54.1	52.0	51.6	50.5	50.0	43331	38780	94.1
sm266C1	53.4	52.7	52.6	51.0		43513	44850	112.7
sm266C2				50.8	50.4			
sm266C3	53.7		52.8	50.6	49.8	44344	46310	117.0
sm266D1	53.7	52.1	52.6	50.8	50.1	43663	45300	114.0
sm266D2	53.8	52.0	52.7	51.2		45332	42100	104.3
sm266E	53.8	52.7	52.5	50.7	50.1	47121	47890	121.9
sm266F1	53.6	52.6	52.9	50.7		45002	49900	128.1
sm266F2	54.5	53.0			49.7	44079	44820	112.3
sm266F3		52.8	53.0	51.0	50.1			
sm266F4	54.3	52.6		50.8		46017	44590	111.6
Average		**52.4**	**52.5**	**50.8**	**50.1**			
Standard Deviation		**0.4**	**0.4**	**0.2**	**0.2**			
Glycerol								
sm277A	54.1	52.4				44354	43830	109.3
sm277B1	53.4	52.0	50.9			39944	39500	96.4
sm277B2		52.6	50.7					
sm277B3								
sm277B4			51.0	50.3	48.6			
sm277C1	54.2	52.3	51.1	49.4		44983	45840	115.4
sm277C2	54.1	52.5	51.3		48.2	44478	47770	121.3
sm277C3			50.8	49.3	48.0			
sm277C4		52.9	50.7	50.0				
sm277D1	53.7	51.8	51.2	49.5	48.7	44126	47010	119.0
sm277D2				49.2	48.4			
Average		**52.4**	**51.0**	**49.6**	**48.4**			
Standard Deviation		**0.4**	**0.2**	**0.4**	**0.3**			
Acetamide								
sm283A	54.2	51.4	49.2	47.7	45.6	44158	44600	111.6
sm283B	54.2	51.0	49.0	46.9	45.5	40882	43400	108.0
sm283C1	53.5	50.7	49.2	47.2	45.0	42126	42750	106.2
sm283C2		50.5	49.5	47.7	45.6			
sm283C3		50.8	49.6		45.4			
sm283C4			49.9	46.9	45.0			
sm283D		51.2	49.3		45.8			
sm283E	53.3		49.3	47.5		41192	47080	119.5
sm283F1	54.0	50.8		47.0		41357	51700	133.3
sm283F2			49.6	47.4	45.1			

sm283F3			49.3	47.0	45.0			
sm283F4		51.1		47.2	45.8			
sm283G								
Average		**50.9**	**49.4**	**47.3**	**45.4**			
Standard Deviation		**0.3**	**0.3**	**0.3**	**0.3**			
Total Averages	**53.9**					**43592**	**44943**	**112.8**
Standard Deviation	**0.3**					**1779**	**3113**	**9**

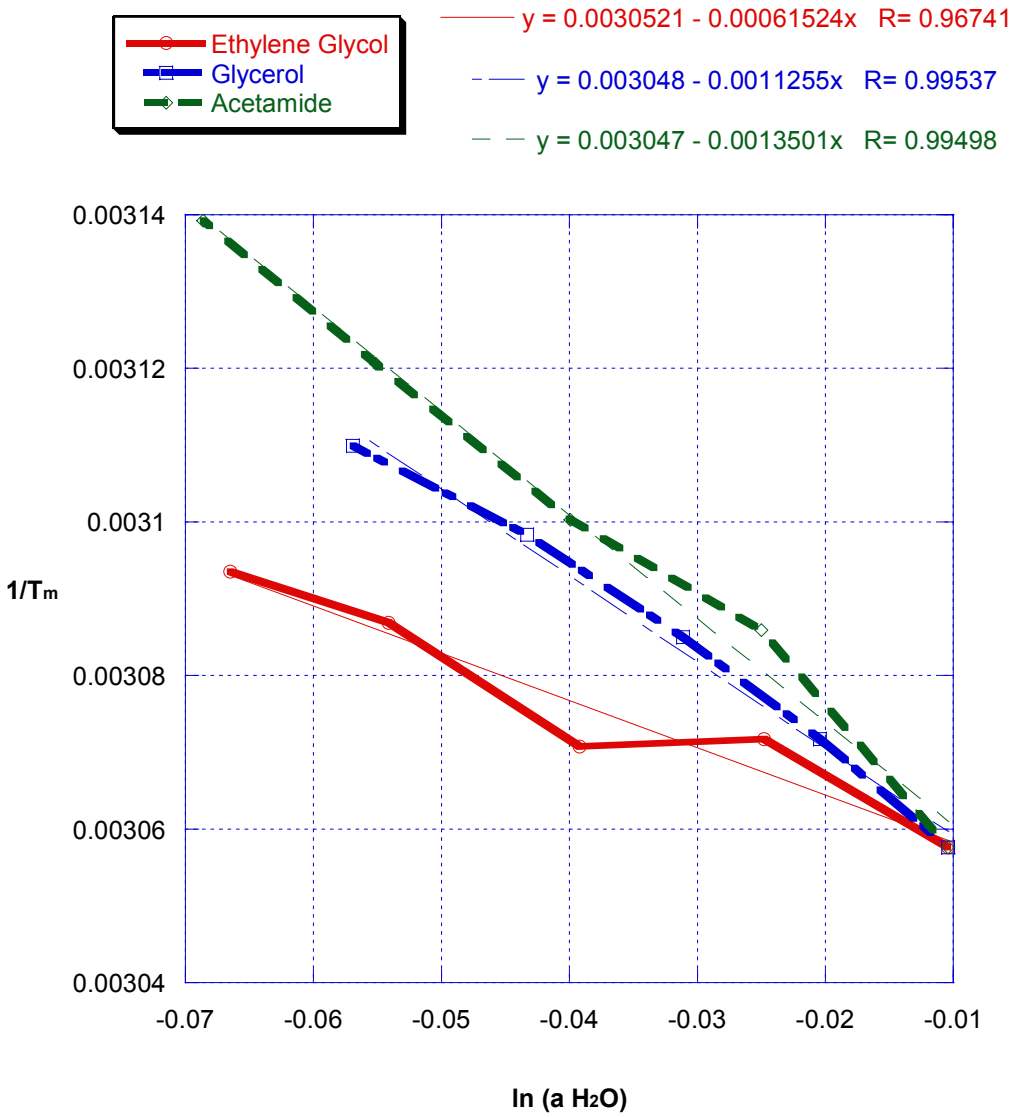

Figure 3. Reciprocal temperature of melting for r(CGCGAAUUFGCG) vs. the logarithm of water activity for small cosolutes.

Table 6. Calculations for r(CGCGAAUUFGCG).

Experiments	Cosolute	-ΔH (cal/mol)	-σH (cal/mol)	-Slope	-σSlope	Δn_w	σn_w
sm266	Ethylene Glycol	43592	1779	0.00061524	0.000107335	**13.5**	**2.4**
sm277	Glycerol	43592	1779	0.0011255	0.000163285	**24.7**	**3.7**
sm283	Acetamide	43592	1779	0.0013501	0.000131400	**29.6**	**3.1**

Table 7. Experimental t_m and thermodynamic data for melting of r(CGCFAAUUAGCG).

Experiment	0%	5%	10%	15%	20%	-ΔH (cal/mol) δα/δT_m	-ΔH (cal/mol) van't Hoff	-ΔS (eu) van't Hoff
Glycerol								
sm268A	53.7	51.9	51.5	49.8		37295	39410	96.0
sm268B	53.4	51.6	51.4	49.9		38246	40260	98.7
sm268C	52.9	52.2		49.6		37238	40490	99.6
sm268D1	53.3	52.5	51.8	50.8	49.6		40130	98.3
sm268D2		51.6	51.6	49.7	48.9			
sm268D3		52.6	51.6	50.1	48.2			
sm268E1	53.0	51.9	51.9	49.7	48.8	35024	38650	93.9
sm268E2	53.4	52.1		50.2	49.0	36512	36860	88.5
sm268E3				49.9	49.3			
sm268F1	52.9	51.1	51.2		49.8	37358	35880	85.6
sm268F2		51.8	51.6	49.3	49.1			
sm268F3					49.0			
sm268F4			51.2		48.7			
sm268G	53.0		51.8		49.2	34698	39250	95.6
Average		**51.9**	**51.6**	**49.9**	**49.1**			
Standard Deviation		**0.4**	**0.2**	**0.4**	**0.4**			
Glycerol								
sm278A	53.3	52.4				38629	43350	108.1
sm278B1	52.9	52.3	52.7	51.0		39662	39750	97.3
sm278B2	52.7	51.6			50.0	44676	43490	108.4
sm278B3	53.1		52.0	51.3		43408	41590	102.9
sm278B4				50.7	49.7			
sm278C	53.9	52.1	52.6		49.8	37346	42640	105.7
sm278D	53.2	52.4				46880	43800	109.6
sm278E1			52.4	50.8				
sm278E2		52.6	52.6	51.4	49.9			
sm278E3		52.3			49.1			
sm278E4					50.0			
Average		**52.2**	**52.5**	**51.0**	**49.8**			
Standard Deviation		**0.3**	**0.3**	**0.3**	**0.3**			
Acetamide								
sm285A1	53.1	50.7	48.9	47.6	45.4	35952	39890	97.6
sm285A2	52.9	50.9	49.5	46.5	45.7	38295	42480	105.6
sm285B1			49.3	47.4				
sm285B2		50.7	48.9	46.7	45.2			
sm285B3		50.5	48.7	47.4	46.0			
sm285B4		50.2	48.9	47.2	45.6			
sm285C1	53.1	50.2		47.0	45.8	34755	39660	96.9
sm285C2	53.2		49.9	46.7		33911	42820	106.5
sm285D1		50.8	48.8	47.2	45.4			

sm285D2		50.3	48.9	47.0				
sm285D3		50.4		47.1	45.5			
sm285D4			49.3	46.8	46.2			
sm285E1	53.5	51.1		46.9		37940	39620	96.7
sm285E2	53.3	50.6	49.6	47.1	45.6	38341	41820	103.4
sm285F	53.0		48.9			36999	41150	101.5
sm285G	53.1		48.9	46.7	45.4	37034	40720	100.1
sm285H1		51.3	49.2	47.1	45.2			
sm285H2			48.9	47.5				
sm285H3				47.2	46.0			
Average		**50.6**	**49.1**	**47.1**	**45.6**			
Standard Deviation		**0.3**	**0.3**	**0.3**	**0.3**			
Total Averages	**53.2**					**38105**	**40623**	**99.8**
Standard Deviation	**0.3**					**3264**	**2050**	**6**

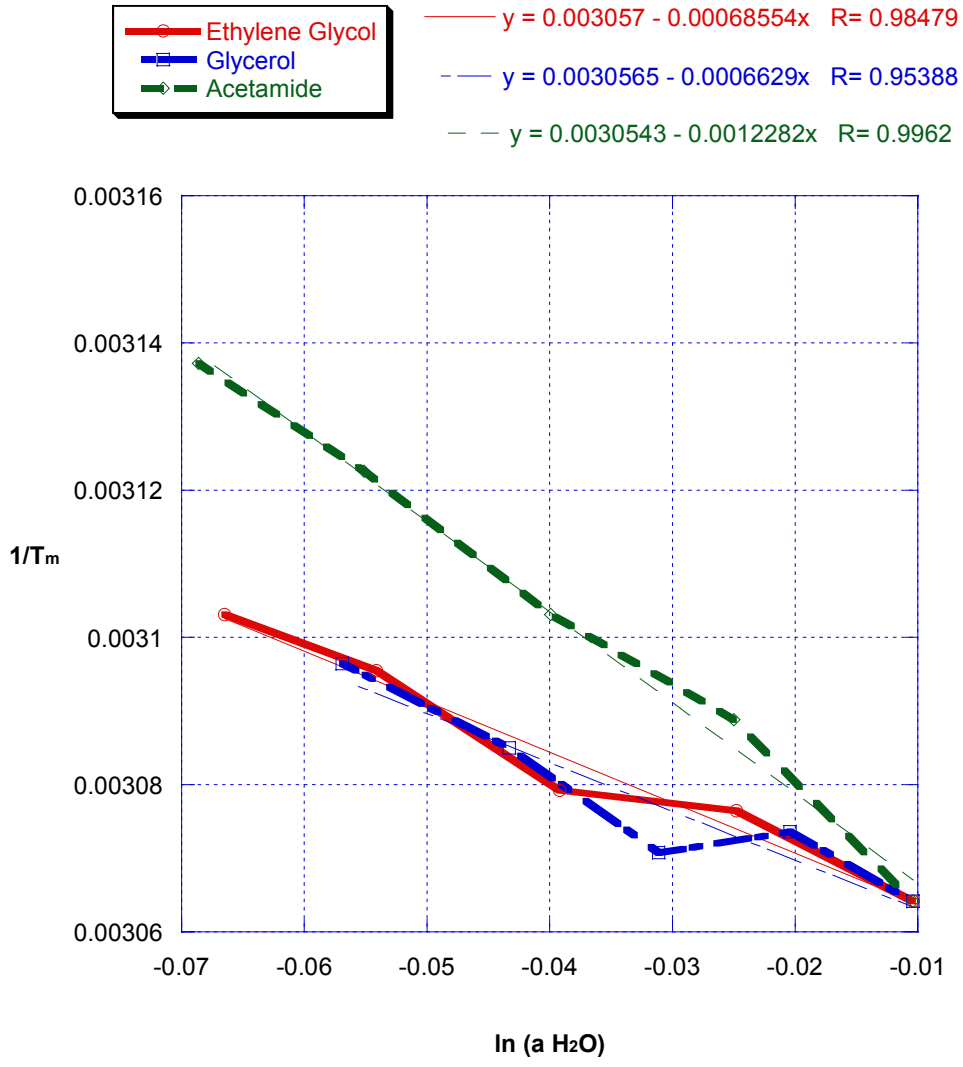

Figure 4. Reciprocal temperature of melting for r(CGCFAAUUAGCG) vs. the logarithm of water activity for small cosolutes.

Table 8. Calculations for r(CGCFAAUUAGCG).

Experiments	Cosolute	-ΔH (cal/mol)	-σH (cal/mol)	-Slope	-σSlope	Δn_w	σn_w
sm268	Ethylene Glycol	38105	3264	0.00068554	0.000148805	**13.2**	**3.1**
sm278	Glycerol	38105	3264	0.0006629	0.000162285	**12.7**	**3.3**
sm285	Acetamide	38105	3264	0.0012282	0.000105900	**23.6**	**2.9**

Table 9. Experimental t_m and thermodynamic data for melting of r(CGCGAAUUAGCG).

Experiment	0%	5%	10%	15%	20%	-ΔH (cal/mol) δα/δT_m	-ΔH (cal/mol) van't Hoff	-ΔS (eu) van't Hoff
Ethylene Glycol								
md115A1		56.5		54.6				
md115A2	58.1	57.0	55.2	54.2	53.1	50082	56180	145.1
md115B1	58.4	57.1	55.6	54.1		48099	53160	135.6
md115B2		57.3		54.7	52.6			
md115B3	57.9	56.5		54.3	53.2	55782	57030	147.5
md115B4			56.0	54.5	53.3			
md115C		56.5		54.6	53.3			
md115D1	58.2	56.5	55.9		52.8	50765	58820	152.8
md115D2			55.1	54.0	53.0			
md115D3	58.5			54.4	52.8	51419	60860	158.8
md115D4		56.6						
md115D5			55.7	55.1	52.9			
Average		**56.8**	**55.6**	**54.5**	**53.0**			
Standard Deviation		**0.3**	**0.4**	**0.3**	**0.2**			
Glycerol								
md116A2	58.0	57.1	55.8	54.3		49259	55580	143.2
md116A3	58.3		55.5	54.8		53256	57230	148.0
md116B1	58.3	57.4		54.8		49184	51100	129.4
md116B2	58.0	57.2	55.7	55.0	53.8	52112	56880	147.1
md116B3		57.1			53.1			
md116B4	58.5	57.2	55.9	54.8	53.5	48381	55750	143.3
md116D1			56.2		53.5			
md116D2			56.7		53.8			
md116D3			56.5		54.1			
Average		**57.2**	**56.0**	**54.7**	**53.6**			
Standard Deviation		**0.1**	**0.4**	**0.3**	**0.3**			
Total Averages	**58.2**					**50834**	**56259**	**145.1**
Standard Deviation	**0.2**					**2394**	**2720**	**8**

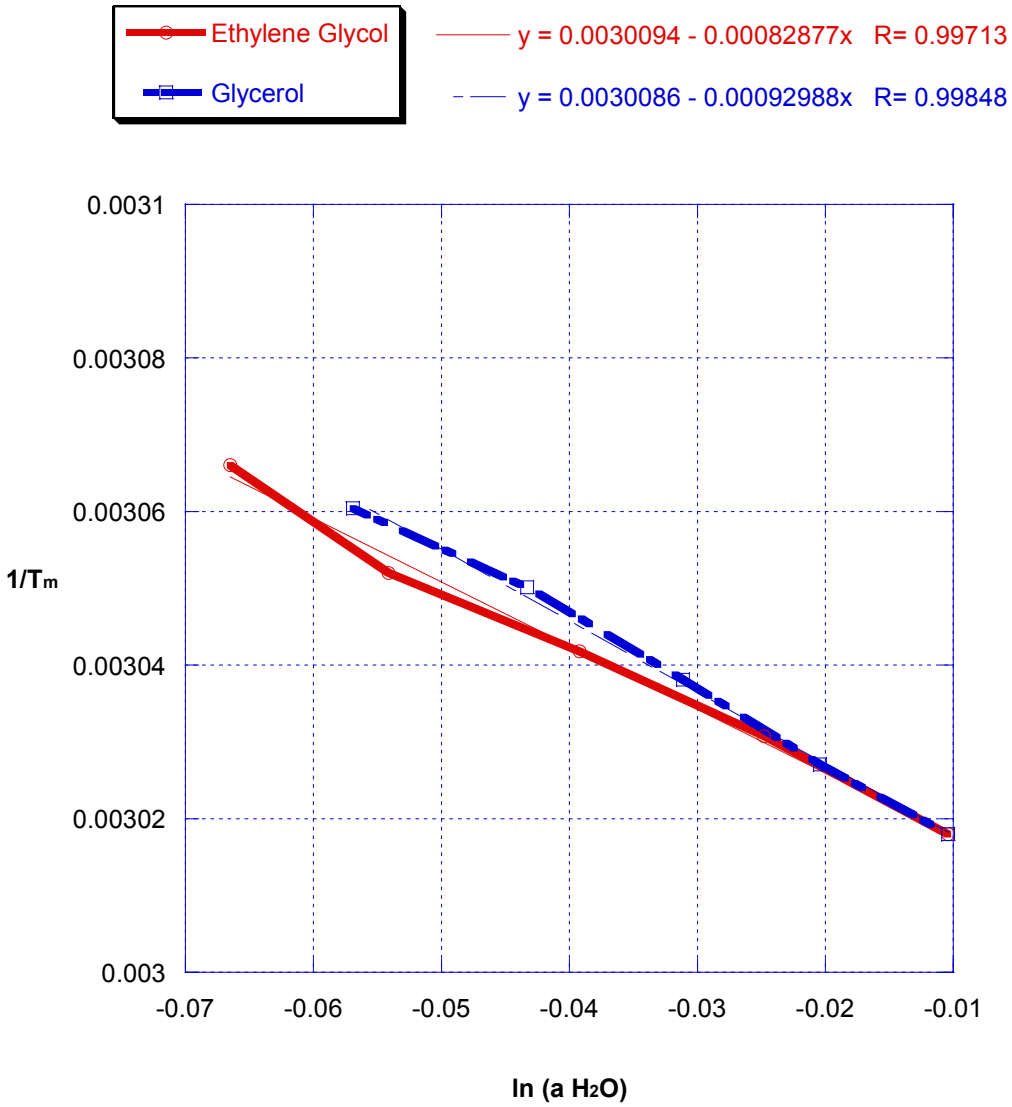

Figure 5. Reciprocal temperature of melting for r(CGCGAAUUAGCG) vs. the logarithm of water activity for small cosolutes.

Table 10. Calculations for r(CGCGAAUUAGCG).

Experiments	Cosolute	-ΔH (cal/mol)	-σH (cal/mol)	-Slope	-σSlope	Δn_w	σn_w
md115	Ethylene Glycol	50834	2394	0.00082877	0.000092390	**21.2**	**2.6**
md116	Glycerol	50834	2394	0.00092988	0.000110915	**23.8**	**3.1**