SUPPORTING INFORMATION

Measurement and Theory of Hydrogen Bonding Contribution to Isosteric DNA Base Pairs

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Synthesis of DNA oligonucleotides.

Phosphoramidite derivatives of 2,4-dichloro-5-toluene-1-β-D-deoxyriboside (dL) and 2,3-dichloro-5-toluene-1-β-D-deoxyriboside ($d^{23}L$) were prepared as previously described.[1,2] The Phosphoramidite derivative of 2,4-difluoro-5-toluene-1-β-D-deoxyriboside (dF) was obtained from Glen Research.

DNA oligonucleotides were synthesized on an Applied Biosystems 394 synthesizer using standard β-cyanoethylphosphoramidite chemistry. Oligonucleotides were synthesized in DMT-on mode and were cleaved and deprotected in concentrated NH_4OH at 55°C for overnight. The oligonucleotides were semi-purified and DMT-deprotected by Poly-Pack II column (Glen Research) and were further purified using reverse phase HPLC (C_{18} column 22 x 250 mm; solvent A: 0.1 M aq. triethylammonium acetate (pH 8), solvent B: acetonitrile; Gradient 0–30% solvent B.) Oligonucleotides were all characterized by MALDI-TOF mass spectrometry.

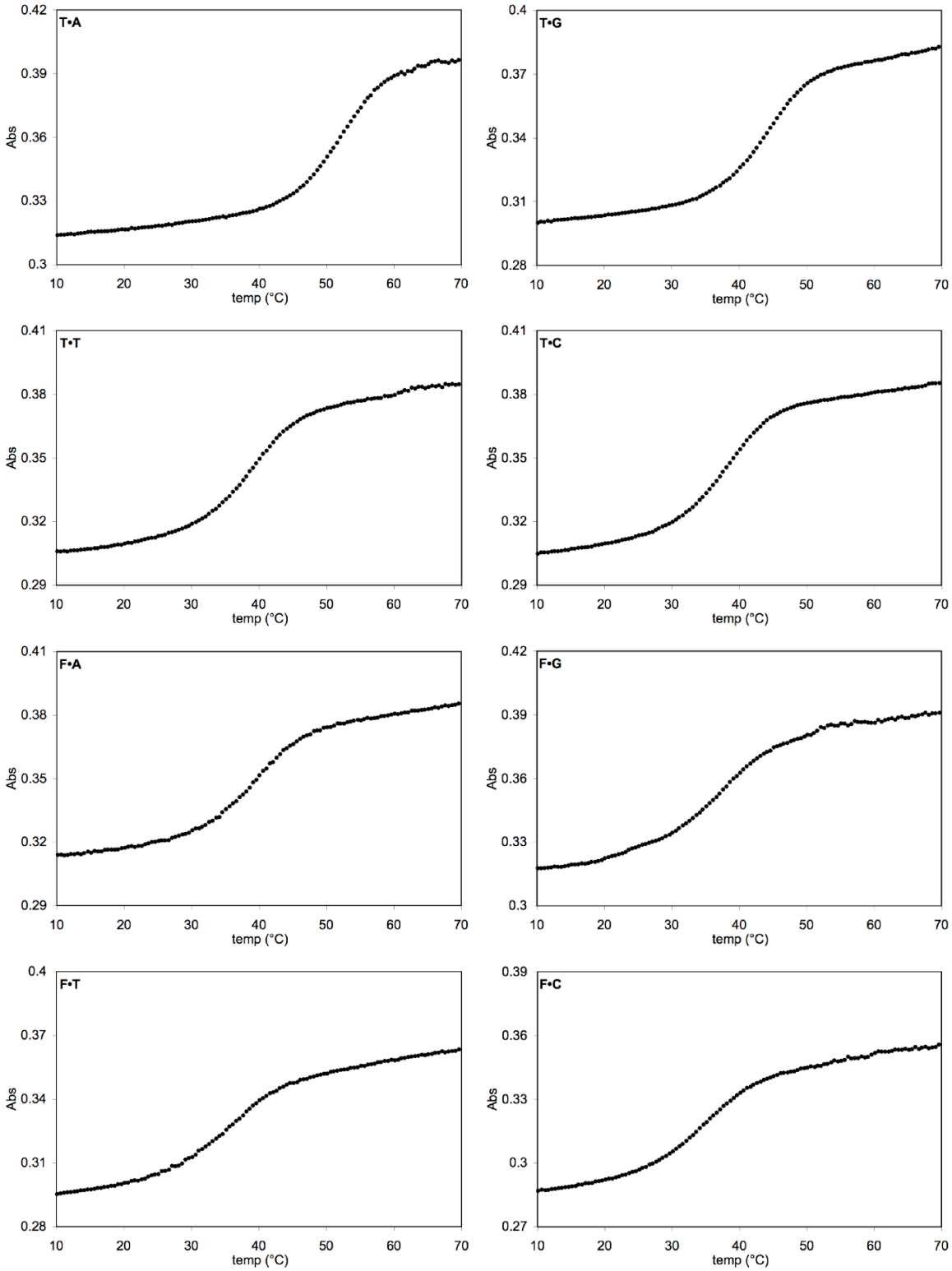
The oligonucleotides were quantified by measuring absorbance at 260 nm at 90 °C. The corresponding molar extinction coefficients were calculated by summing up the individual extinction coefficients for all the bases in the sequence. The molar extinction coefficients for dA, dG, dT, dC, dF, dL, and $d^{23}L$ were taken as 15400, 11500, 8700, 7400, 1200, 250, and 250, $M^{-1}\cdot cm^{-1}$ at 260 nm, respectively.

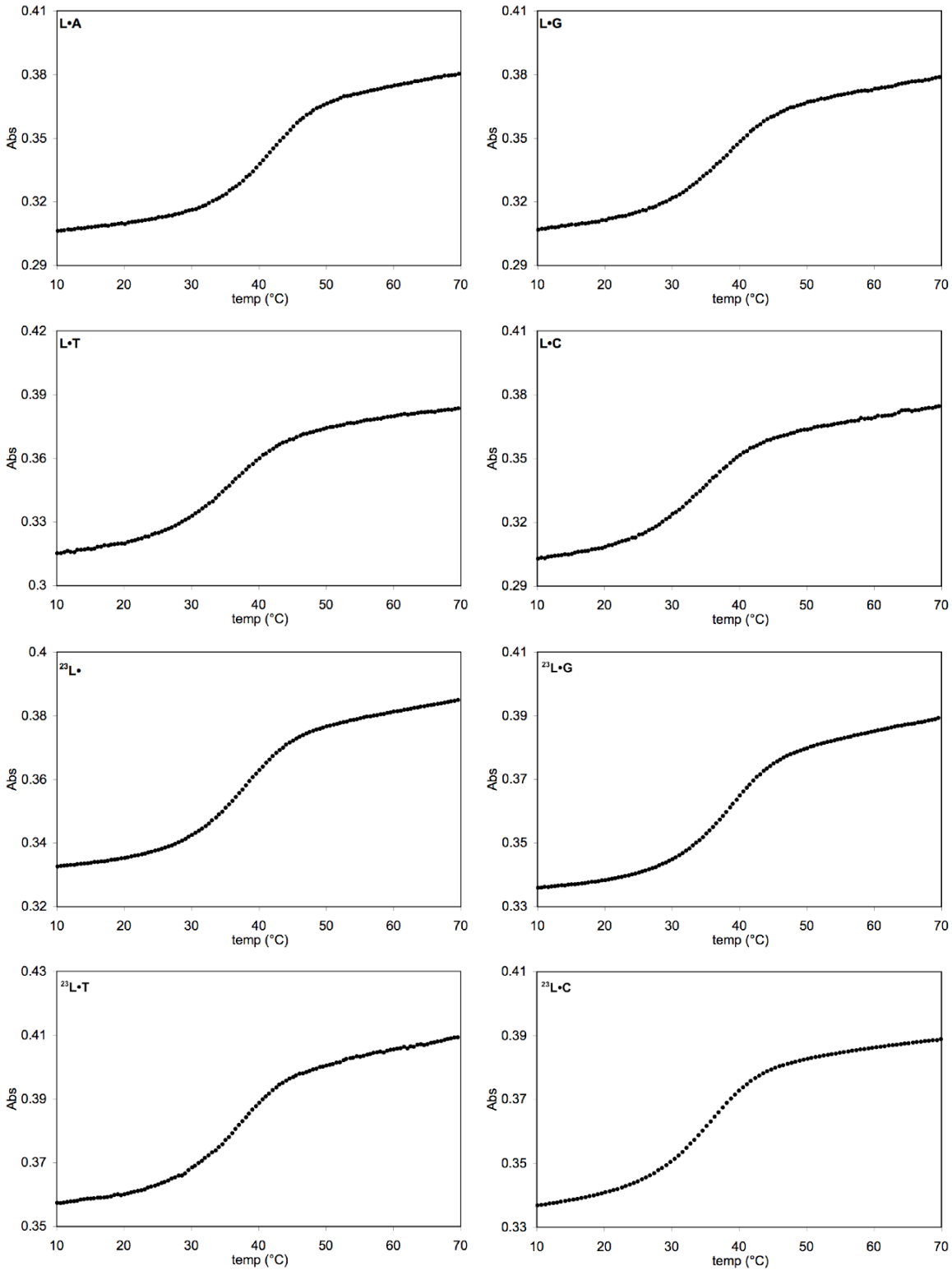
[1] Kim, T. W.; Kool, E. T. *J. Org. Chem.* **2005**, *70*, 2048–2053.
[2] Sintim, H. O.; Kool, E. T. *Angew. Chem. Int. Ed.* **2006**, *45*, 1974–1979.

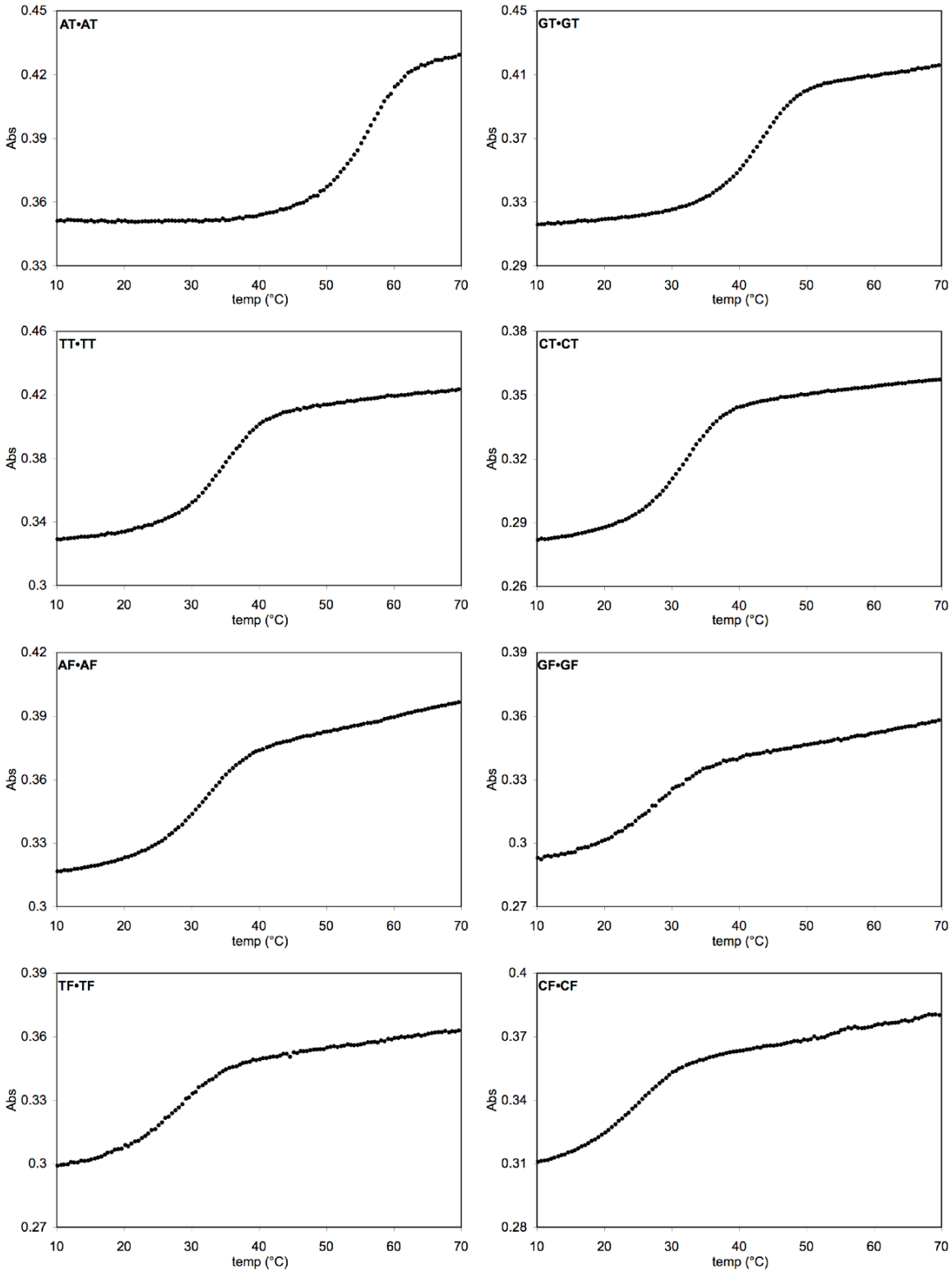
Table S1. MALDI-MS data for modified DNAs.

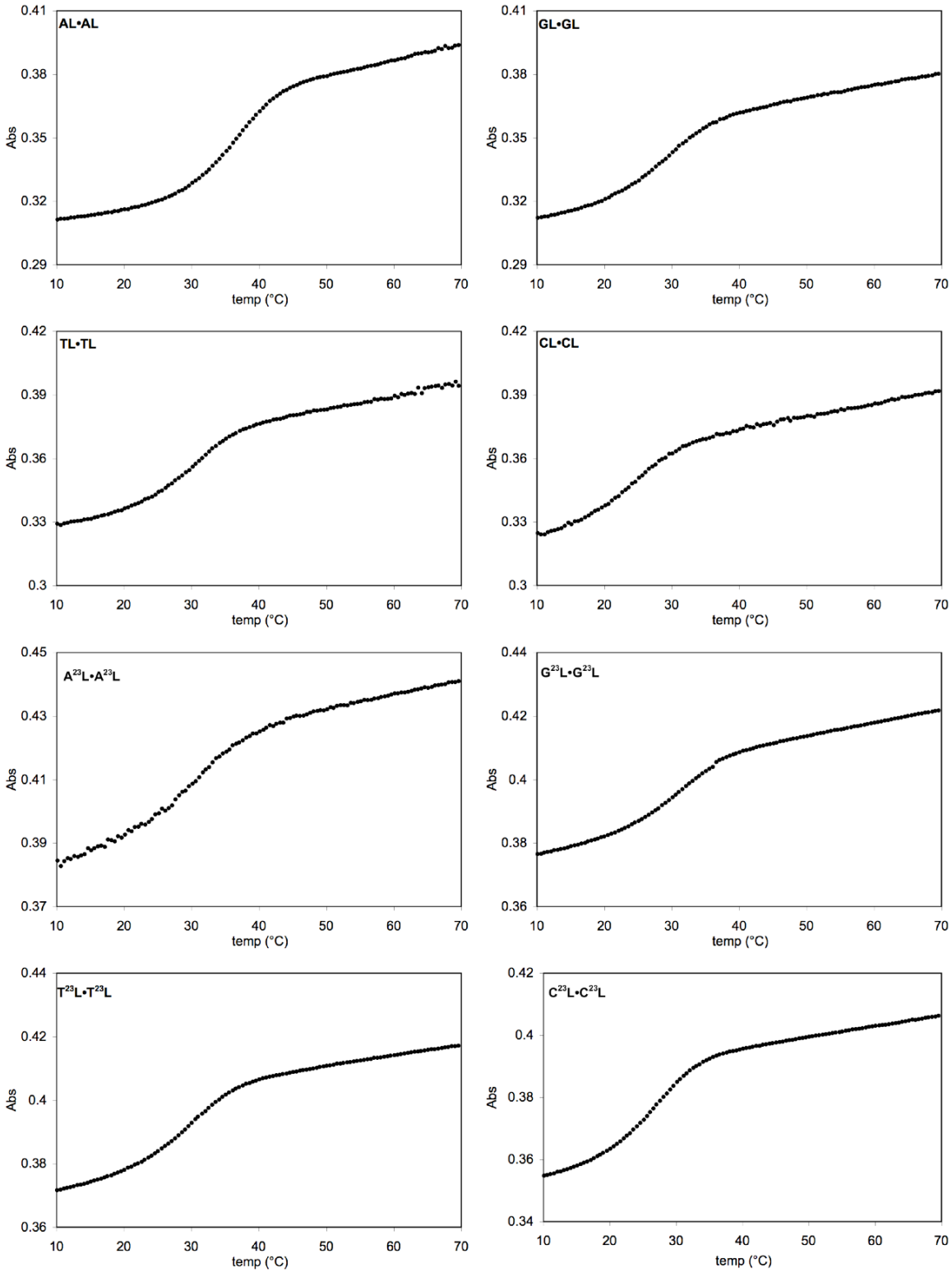
Oligonucleotide	Mass (Calc.)	Mass (found)
5'-TGTAT**T**CGTGCG	3667.4	3666.4
5'-TGTAT**F**CGTGCG	3669.4	3669.7
5'-TGTAT**L**CGTGCG	3701.3	3700.5
5'-TGTAT^{23}**L**CGTGCG	3701.3	3700.7
5'-CGCACG**A**ATACA	3623.4	3624.1
5'-CGCACG**G**ATACA	3639.4	3640.2
5'-CGCACG**T**ATACA	3614.4	3614.1
5'-CGCACG**C**ATACA	3599.4	3601.0
5'-GGTGG**A**AT**T**CGGAG	4383.9	4383.2
5'-GGTGG**A**AT**F**CGGAG	4385.9	4385.2
5'-GGTGG**A**AT**L**CGGAG	4417.8	4418.2
5'-GGTGG**A**AT^{23}**L**CGGAG	4417.8	4417.3
5'-GGTGG**G**AT**T**CGGAG	4399.9	4399.7
5'-GGTGG**G**AT**F**CGGAG	4401.9	4400.7
5'-GGTGG**G**AT**L**CGGAG	4433.8	4435.5
5'-GGTGG**G**AT^{23}**L**CGGAG	4433.8	4431.5
5'-GGTGG**T**AT**T**CGGAG	4374.9	4374.2
5'-GGTGG**T**AT**F**CGGAG	4376.9	4375.1
5'-GGTGG**T**AT**L**CGGAG	4408.8	4408.8
5'-GGTGG**T**AT^{23}**L**CGGAG	4408.8	4408.6
5'-GGTGG**C**AT**T**CGGAG	4359.9	4360.0
5'-GGTGG**C**AT**F**CGGAG	4361.9	4361.7
5'-GGTGG**C**AT**L**CGGAG	4393.8	4396.5
5'-GGTGG**C**AT^{23}**L**CGGAG	4393.8	4391.5
5'-CTCCG**A**AT**T**CCACC	4143.7	4143.0
5'-CTCCG**A**AT**F**CCACC	4145.7	4145.8
5'-CTCCG**A**AT**L**CCACC	4177.6	4178.7
5'-CTCCG**A**AT^{23}**L**CCACC	4177.6	4177.9
5'-CTCCG**G**AT**T**CCACC	4159.7	4158.2
5'-CTCCG**G**AT**F**CCACC	4161.7	4161.5
5'-CTCCG**G**AT**L**CCACC	4193.6	4193.0
5'-CTCCG**G**AT^{23}**L**CCACC	4193.6	4193.9
5'-CTCCG**T**AT**T**CCACC	4134.7	4133.8
5'-CTCCG**T**AT**F**CCACC	4136.7	4135.4
5'-CTCCG**T**AT**L**CCACC	4168.6	4168.4
5'-CTCCG**T**AT^{23}**L**CCACC	4168.6	4169.6
5'-CTCCG**C**AT**T**CCACC	4119.7	4119.0
5'-CTCCG**C**AT**F**CCACC	4121.7	4121.2
5'-CTCCG**C**AT**L**CCACC	4153.6	4153.2
5'-CTCCG**C**AT^{23}**L**CCACC	4153.6	4155.4
5'-CGCGCG	1793.2	1792.8
5'-CGCGCGA	2106.4	2106.0
5'-TCGCGCG	2097.4	2097.2
5'-FCGCGCG	2099.4	2100.3
5'-TCGCGCGA	2410.6	2409.2
5'-FCGCGCGA	2412.6	2413.9

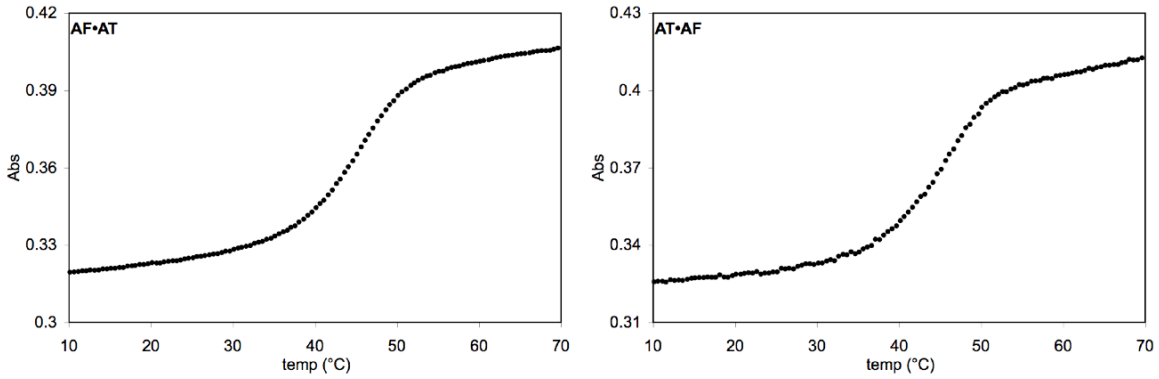
Fig. S1. Representative melting curves obtained for DNA duplexes at 3 μM total DNA concentration.




L•A
L•G
L•T
L•C
^{23}L•
^{23}L•G
^{23}L•T
^{23}L•C
Abs
temp (°C)


AT•AT
GT•GT
TT•TT
CT•CT
AF•AF
GF•GF
TF•TF
CF•CF
Abs
temp (°C)


AL•AL
GL•GL
TL•TL
CL•CL
A23L•A23L
G23L•G23L
T23L•T23L
C23L•C23L
Abs
temp (°C)



The following melting curves are obtained at 6 μM for the self-complementary DNAs:

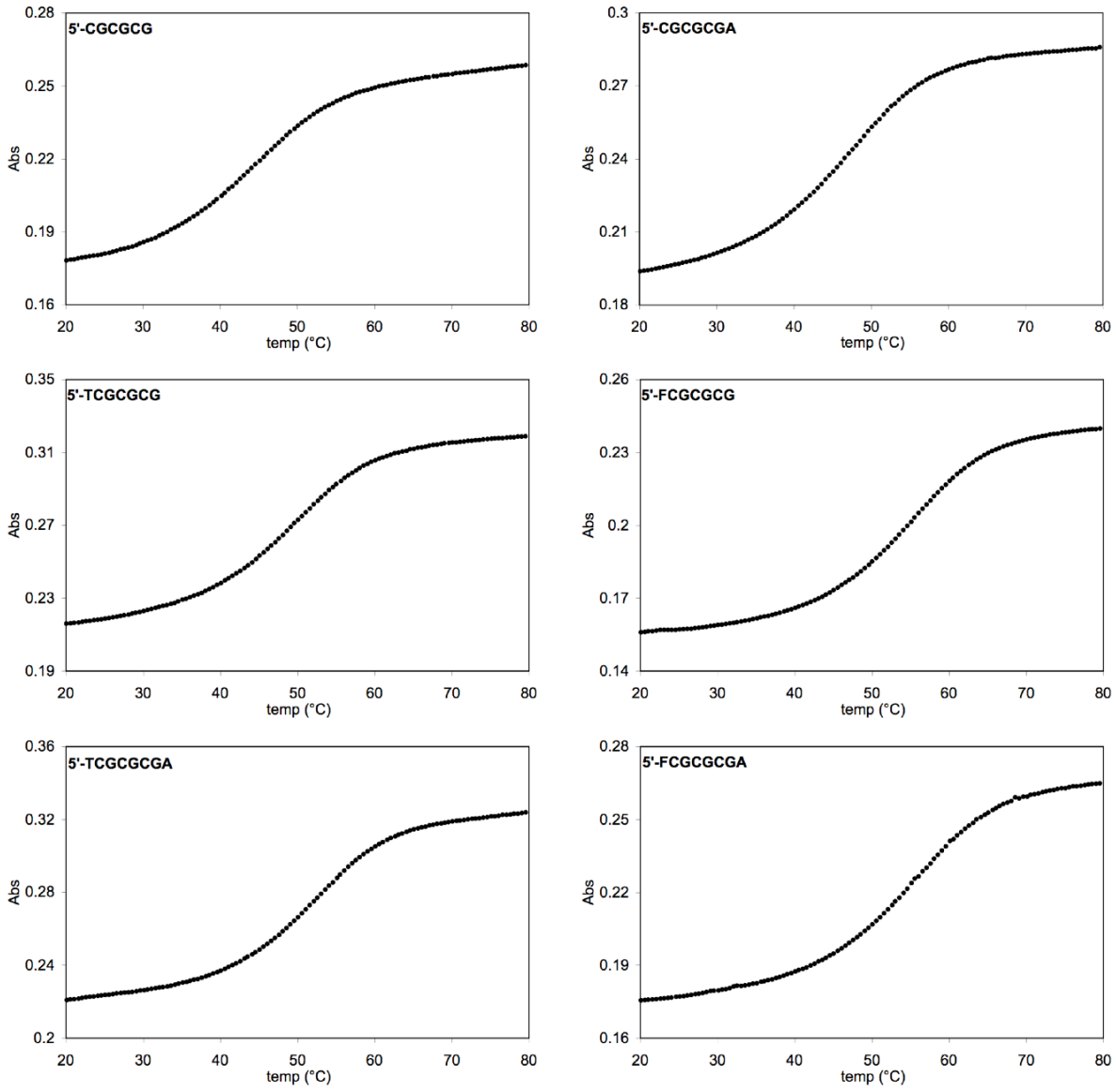
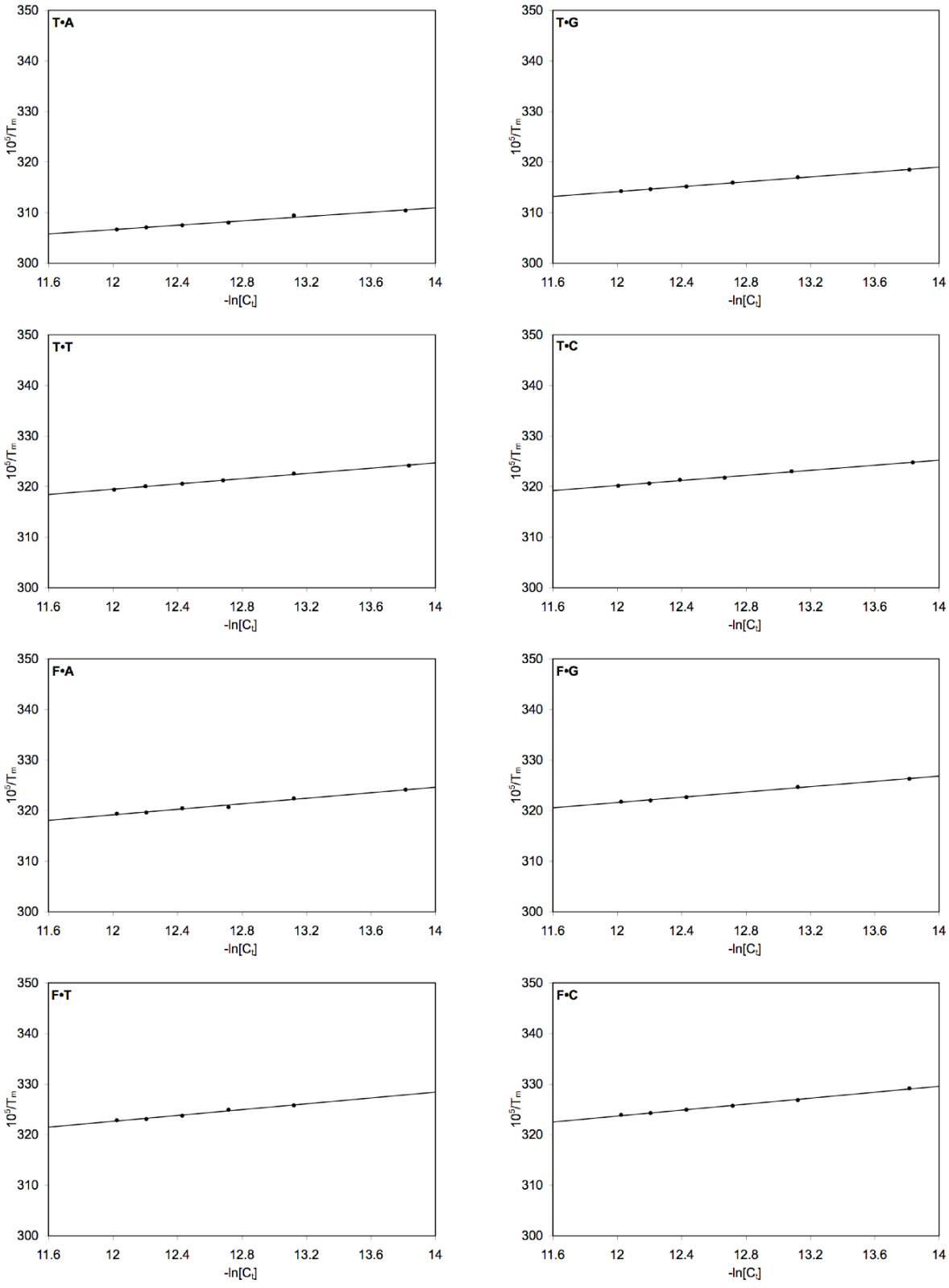
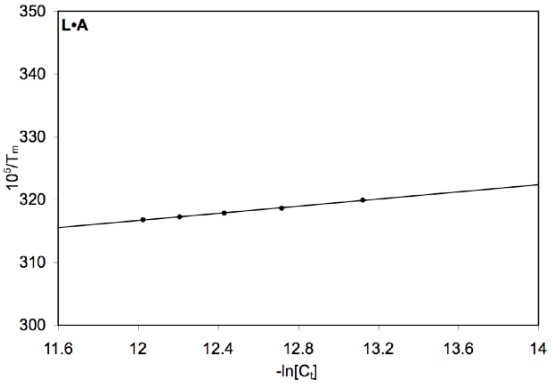
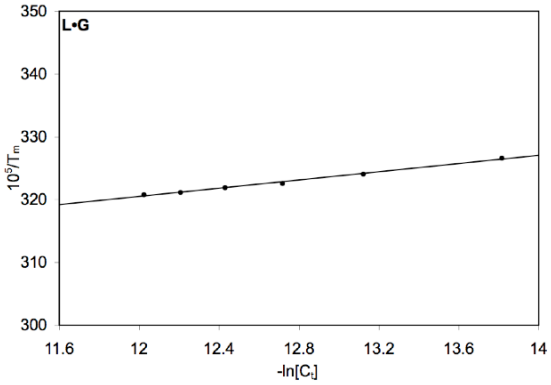
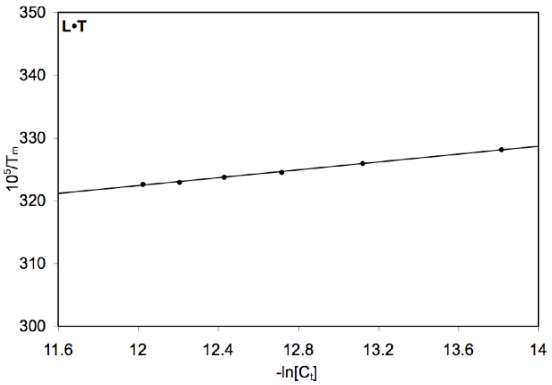


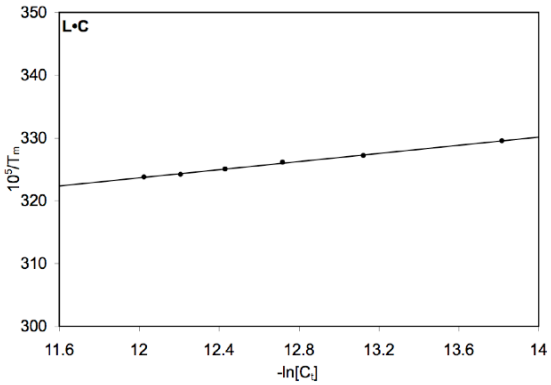
Fig. S2. Van't Hoff plots for the modified DNA duplexes.

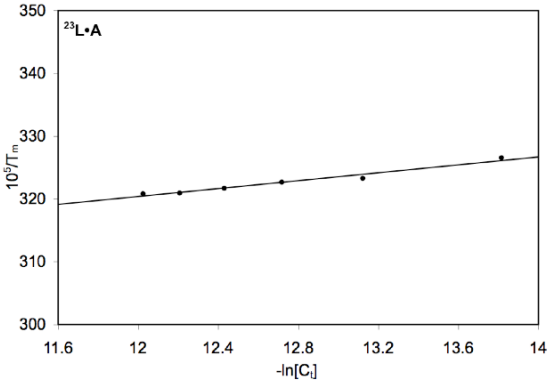


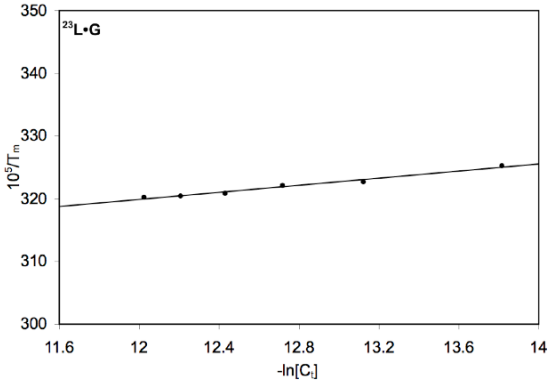

L•A
350
340
330
320
310
300
$10^5/T_m$
11.6
12
12.4
12.8
13.2
13.6
14
-ln[C_t]

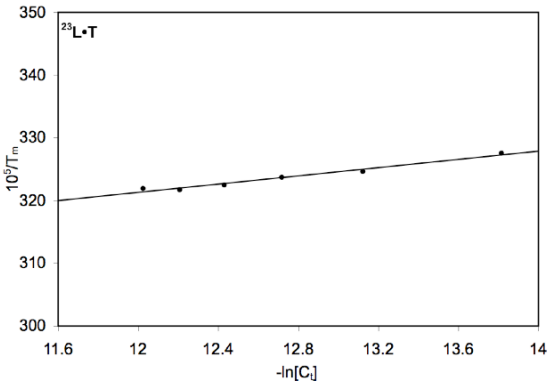

L•G
350
340
330
320
310
300
$10^5/T_m$
11.6
12
12.4
12.8
13.2
13.6
14
-ln[C_t]

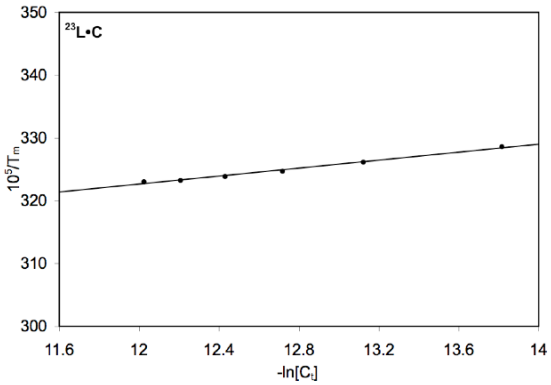

L•T
350
340
330
320
310
300
$10^5/T_m$
11.6
12
12.4
12.8
13.2
13.6
14
-ln[C_t]

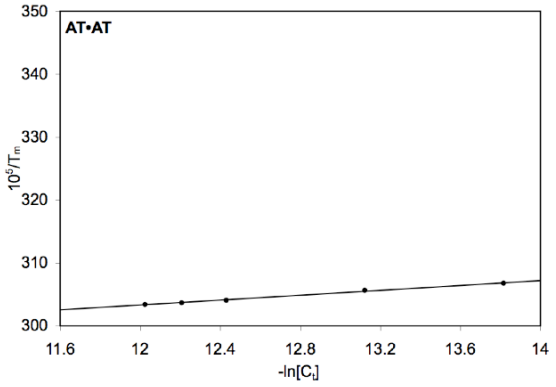

L•C
350
340
330
320
310
300
$10^5/T_m$
11.6
12
12.4
12.8
13.2
13.6
14
-ln[C_t]

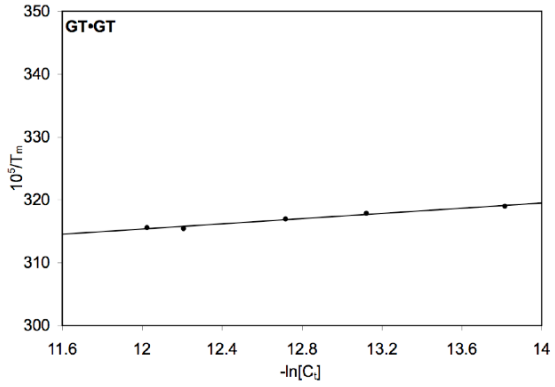

^{23}L•A
350
340
330
320
310
300
$10^5/T_m$
11.6
12
12.4
12.8
13.2
13.6
14
-ln[C_t]

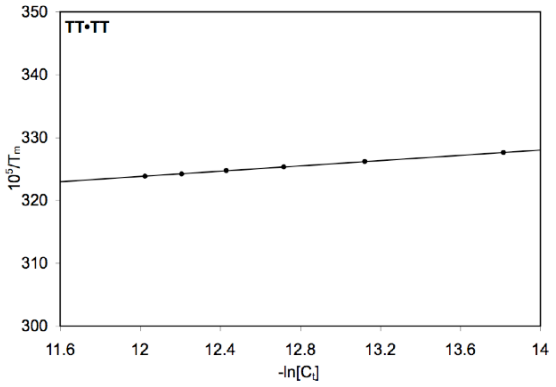

^{23}L•G
350
340
330
320
310
300
$10^5/T_m$
11.6
12
12.4
12.8
13.2
13.6
14
-ln[C_t]


^{23}L•T
350
340
330
320
310
300
$10^5/T_m$
11.6
12
12.4
12.8
13.2
13.6
14
-ln[C_t]


^{23}L•C
350
340
330
320
310
300
$10^5/T_m$
11.6
12
12.4
12.8
13.2
13.6
14
-ln[C_t]


AT•AT
350
340
330
320
310
300
$10^5/T_m$
11.6
12
12.4
12.8
13.2
13.6
14
-ln[C_t]


GT•GT
350
340
330
320
310
300
$10^5/T_m$
11.6
12
12.4
12.8
13.2
13.6
14
-ln[C_t]


TT•TT
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340
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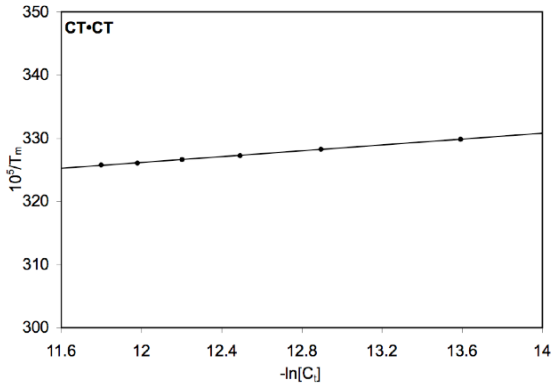
12.4
12.8
13.2
13.6
14
-ln[C_t]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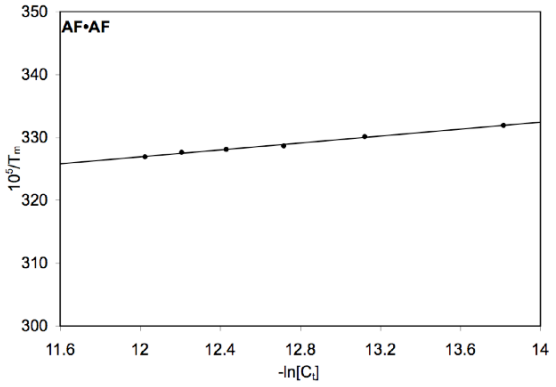
13.6
14
-ln[C_t]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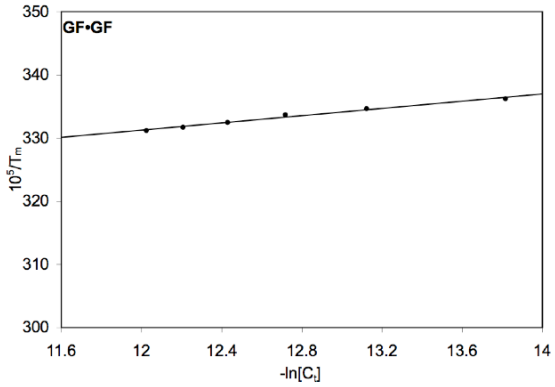
13.6
14
-ln[C_t]


GF•GF
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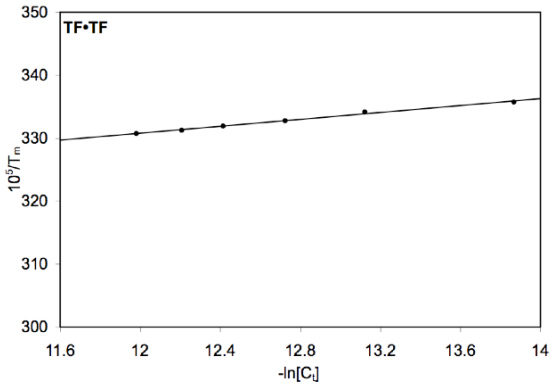
-ln[C_t]


TF•TF
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310
300
$10^5/T_m$
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12.4
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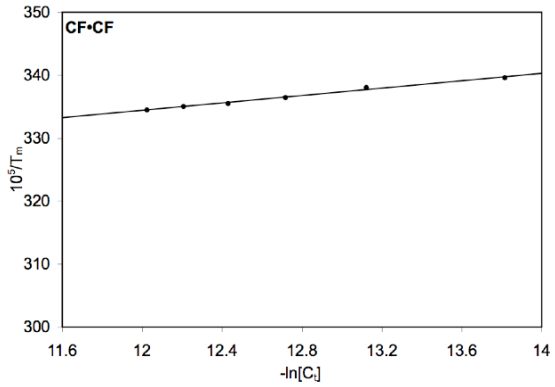
13.6
14
-ln[C_t]


CF•CF
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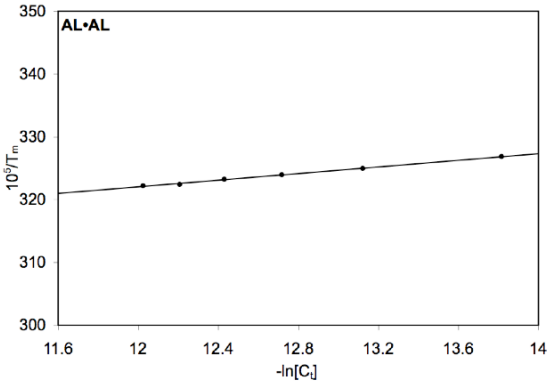
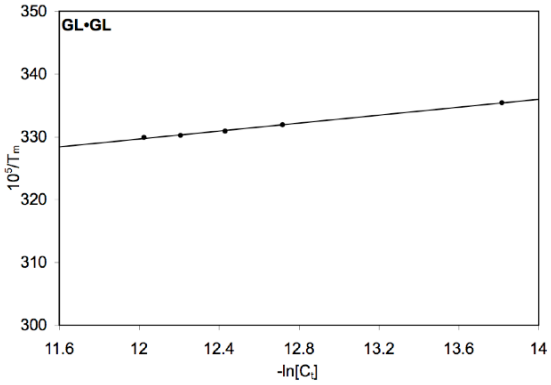
340
330
320
310
300
$10^5/T_m$
11.6
12
12.4
12.8
13.2
13.6
14
-ln[C_t]


AL•AL
350
340
330
320
310
300
$10^5/T_m$
11.6
12
12.4
12.8
13.2
13.6
14
-ln[C_t]


GL•GL
350
340
330
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310
300
$10^5/T_m$
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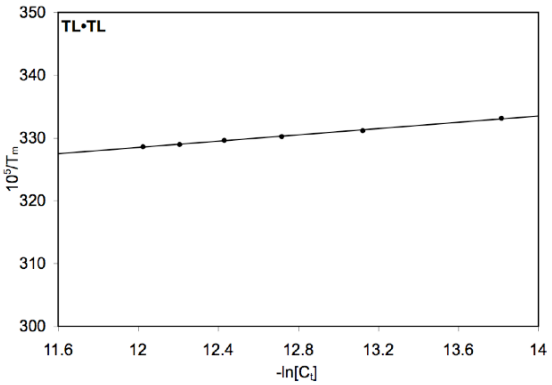
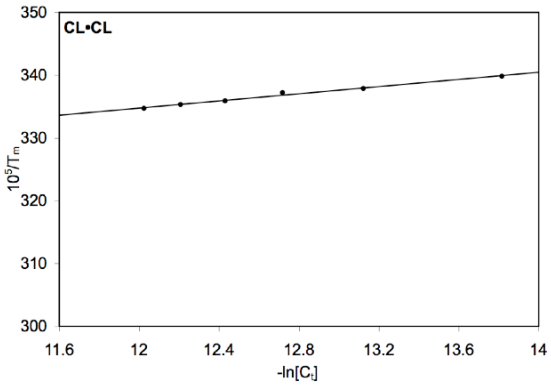
12
12.4
12.8
13.2
13.6
14
-ln[C_t]


TL•TL
350
340
330
320
310
300
$10^5/T_m$
11.6
12
12.4
12.8
13.2
13.6
14
-ln[C_t]


CL•CL
350
340
330
320
310
300
$10^5/T_m$
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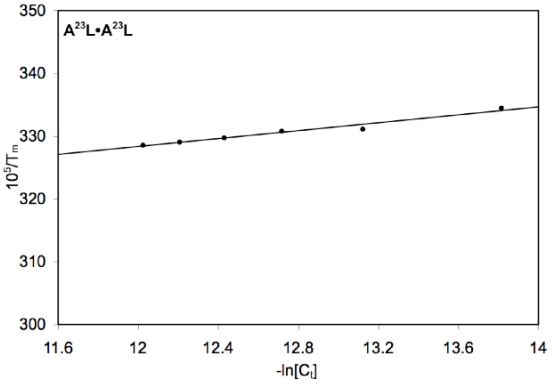
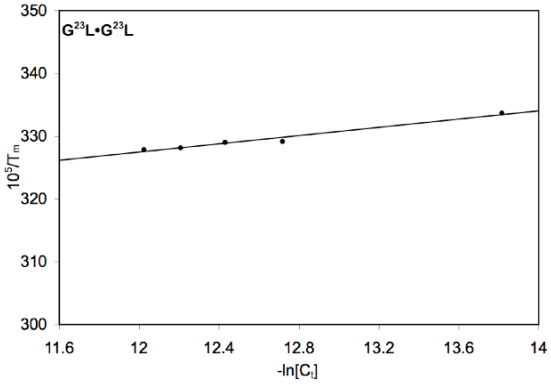
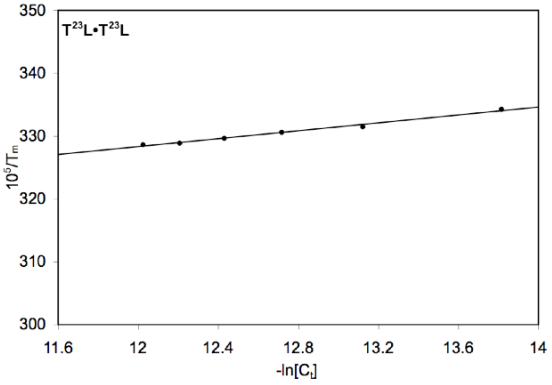
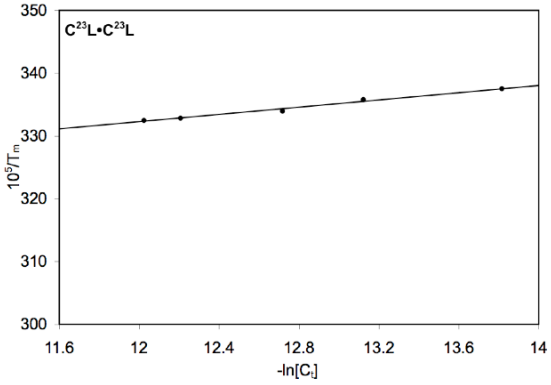
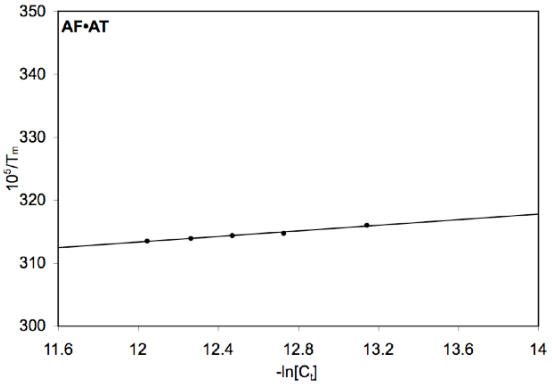
12
12.4
12.8
13.2
13.6
14
-ln[C_t]

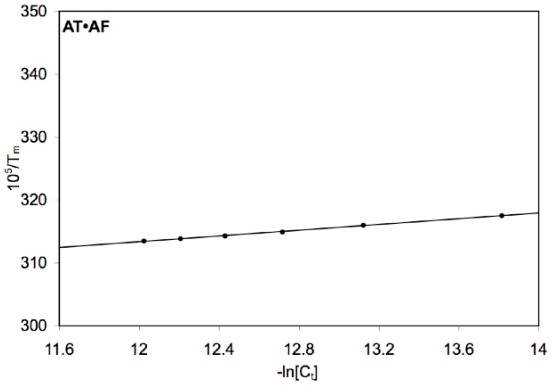

$A^{23}L•A^{23}L$
350
340
330
320
310
300
$10^5/T_m$
11.6
12
12.4
12.8
13.2
13.6
14
-ln[C_t]

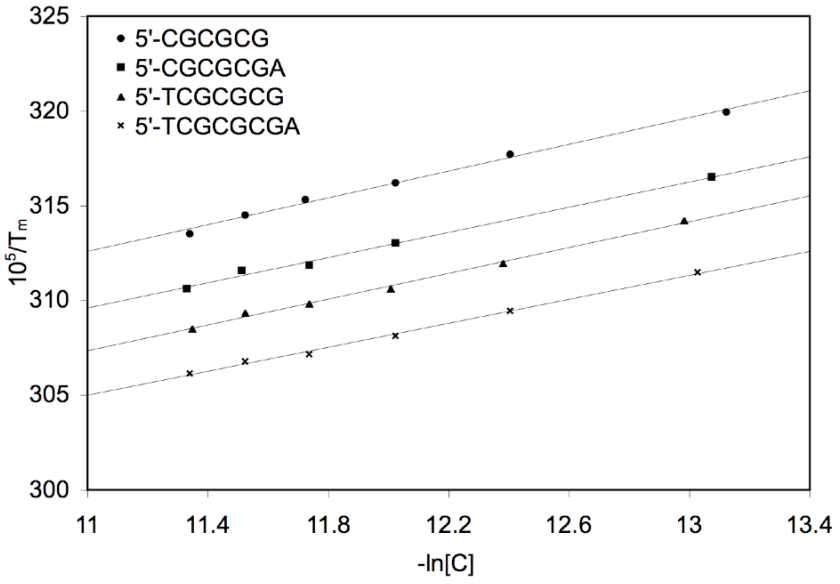

$G^{23}L•G^{23}L$
350
340
330
320
310
300
$10^5/T_m$
11.6
12
12.4
12.8
13.2
13.6
14
-ln[C_t]


$T^{23}L•T^{23}L$
350
340
330
320
310
300
$10^5/T_m$
11.6
12
12.4
12.8
13.2
13.6
14
-ln[C_t]


$C^{23}L•C^{23}L$
350
340
330
320
310
300
$10^5/T_m$
11.6
12
12.4
12.8
13.2
13.6
14
-ln[C_t]


AF•AT
350
340
330
320
310
300
$10^5/T_m$
11.6
12
12.4
12.8
13.2
13.6
14
-ln[C_t]


AT•AF
350
340
330
320
310
300
$10^5/T_m$
11.6
12
12.4
12.8
13.2
13.6
14
-ln[C_t]


5'-CGCGCG
5'-CGCGCGA
5'-TCGCGCG
5'-TCGCGCGA
325
320
315
310
305
300
$10^5/T_m$
11
11.4
11.8
12.2
12.6
13
13.4
-ln[C]

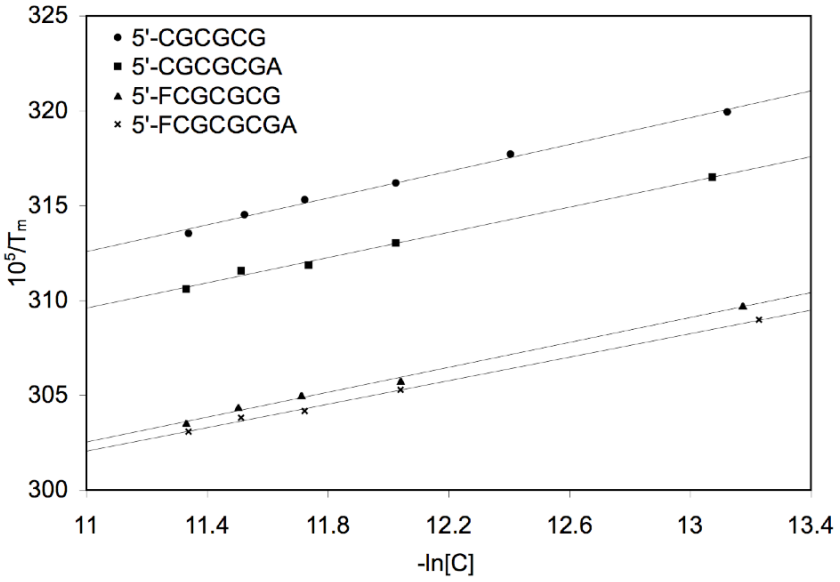

5'-CGCGCG
5'-CGCGCGA
5'-FCGCGCG
5'-FCGCGCGA
325
320
315
310
305
300
$10^5/T_m$
11
11.4
11.8
12.2
12.6
13
13.4
-ln[C]

Table S2. Thermodynamic parameters for heterodimers obtained by thermal melting studies.

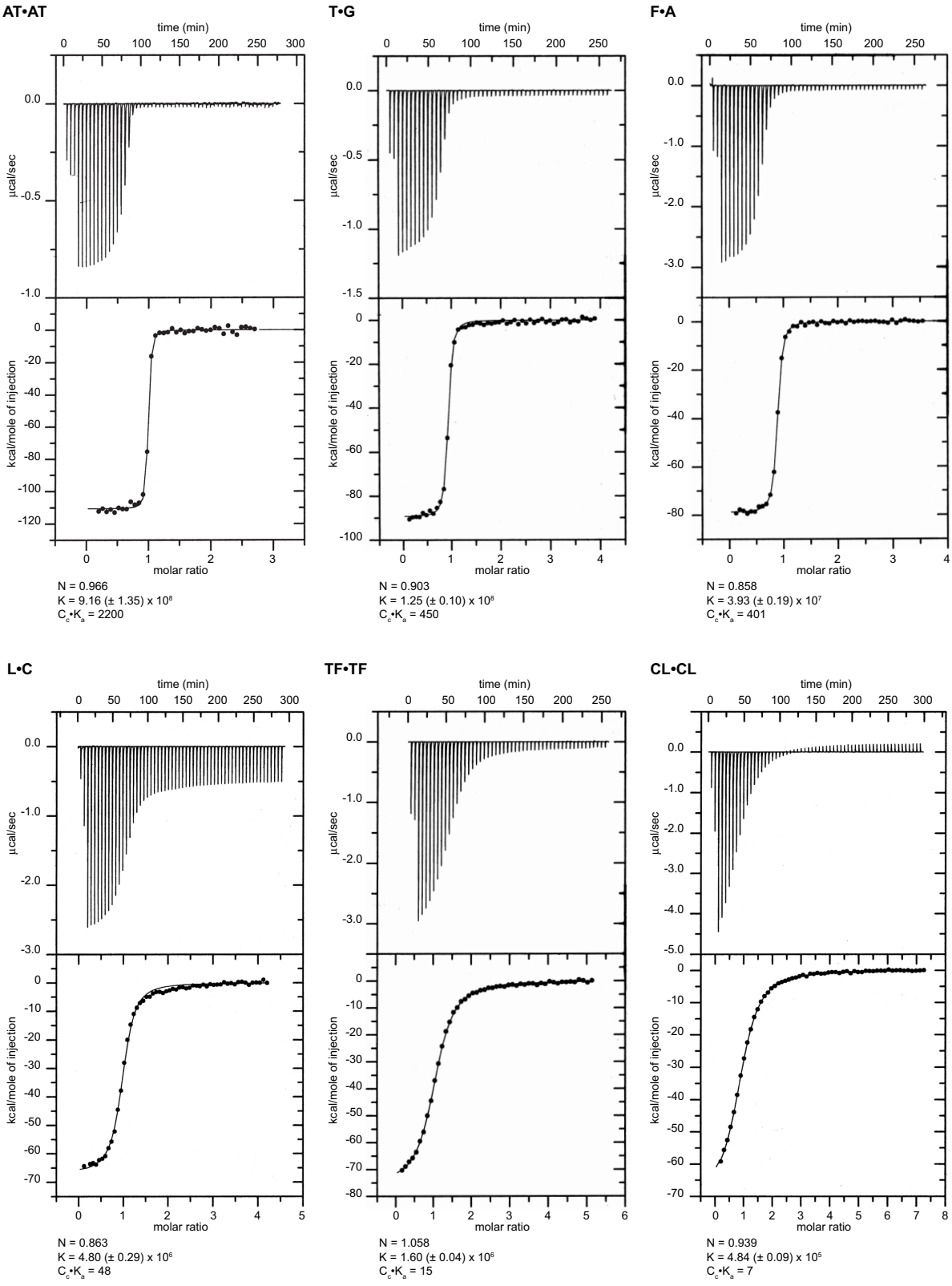
DNA Duplex	T_m @ 3 μM (°C)	$\Delta H°_{37,melt}$ (kcal/mol)	$\Delta S°_{37,melt}$ (cal/k.mol)	$\Delta G°_{37,melt}$ (kcal/mol)
T•A	51.3	-94.60 (± 4.41)	-263.60 (± 13.60)	-12.85 (± 0.20)
T•G	43.4	-83.56 (± 2.19)	-235.94 (± 6.94)	-10.38 (± 0.04)
T•T	38.1	-76.46 (± 2.14)	-217.66 (± 6.85)	- 8.95 (± 0.02)
T•C	37.4	-79.38 (± 1.71)	-227.58 (± 5.52)	- 8.80 (± 0.02)
L•A	40.7	-73.04 (± 1.46)	-204.76 (± 4.65)	- 9.54 (± 0.03)
L•G	36.8	-63.61 (± 3.58)	-177.30 (± 11.53)	- 8.62 (± 0.03)
L•T	35.0	-62.70 (± 3.00)	-175.53 (± 9.82)	- 8.26 (± 0.05)
L•C	33.5	-62.79 (± 1.48)	-176.65 (± 4.80)	- 8.00 (± 0.02)
F•A	38.7	-73.17 (± 3.54)	-206.92 (± 11.32)	- 9.00 (± 0.07)
F•G	36.0	-72.34 (± 1.74)	-205.97 (± 5.64)	- 8.46 (± 0.03)
F•T	34.6	-66.92 (± 3.97)	-189.30 (± 12.86)	- 8.22 (± 0.07)
F•C	33.9	-67.29 (± 2.83)	-191.22 (± 9.30)	- 7.98 (± 0.06)
^{23}L•A	36.8	-66.74 (± 4.46)	-187.33 (± 14.41)	- 8.64 (± 0.13)
^{23}L•G	37.3	-72.27 (± 4.62)	-204.66 (± 15.01)	- 8.80 (± 0.09)
^{23}L•T	35.8	-62.78 (± 5.40)	-175.16 (± 17.50)	- 8.46 (± 0.10)
^{23}L•C	34.8	-64.92 (± 2.98)	-182.89 (± 9.65)	- 8.20 (± 0.04)
AT•AT	55.0	-99.87 (± 2.85)	-276.28 (± 8.69)	-14.18 (± 0.16)
GT•G T	42.4	-94.26 (± 6.18)	-270.62 (± 19.55)	-10.32 (± 0.15)
TT•T T	34.2	-91.23 (± 1.96)	-268.76 (± 6.39)	- 7.87 (± 0.03)
CT•CT	31.9	-84.90 (± 1.72)	-250.26 (± 5.68)	- 7.28 (± 0.04)
AL•AL	35.6	-75.82 (± 2.36)	-217.57 (± 7.64)	- 8.34 (± 0.02)
GL•G L	29.2	-63.50 (± 2.38)	-182.74 (± 7.90)	- 6.82 (± 0.07)
TL•T L	29.7	-76.74 (± 1.89)	-225.42 (± 6.22)	- 6.82 (± 0.04)
CL•CL	23.4	-67.14 (± 3.00)	-198.09 (± 10.06)	- 5.70 (± 0.14)
AF•AF	30.9	-73.60 (± 2.58)	-214.02 (± 8.43)	- 7.22 (± 0.04)
GF•G F	26.8	-69.24 (± 3.22)	-202.80 (± 10.69)	- 6.35 (± 0.11)
TF•T F	27.3	-72.68 (± 3.15)	-213.85 (± 10.47)	- 6.36 (± 0.10)
CF•CF	24.0	-68.34 (± 3.09)	-201.94 (± 10.94)	- 5.70 (± 0.13)
A^{23}L•A^{23}L	29.1	-64.93 (± 5.06)	-186.63 (± 16.76)	- 7.04 (± 0.19)
G^{23}L•G^{23}L	30.6	-62.91 (± 5.06)	-179.43 (± 16.64)	- 7.26 (± 0.17)
T^{23}L•T^{23}L	29.3	-66.64 (± 3.79)	-192.28 (± 12.21)	- 7.01 (± 0.10)
C^{23}L•C^{23}L	26.3	-68.73 (± 3.52)	-201.76 (± 11.75)	- 6.16 (± 0.13)

Table S3. ITC concentrations and association constants obtained for the modified DNA duplexes

DNA Duplex	C_s (μM)	C_c (μM)	C_s/C_c	K_a (M^{-1})	$C_c \bullet K_a$
T•A	30.1	2.2	13.7	2.67 (± 0.38) x 10^{8} [a]	587
T•A	48.8	2.3	21.2	3.49 (± 0.54) x 10^{8} [a]	803
T•G	70.2	3.6	19.5	1.25 (± 0.10) x 10^{8}	450
T•T	89.7	5.6	16.0	4.96 (± 0.28) x 10^{7}	278
T•C	113.3	6.5	17.4	2.92 (± 0.16) x 10^{7}	190
L•A	70.1	5.1	13.7	5.66 (± 0.43) x 10^{7}	190
L•G	103.5	6.3	16.4	1.70 (± 0.12) x 10^{7}	107
L•T	188.8	10.1	16.4	9.04 (± 0.46) x 10^{6}	91
L•C	190.1	10.1	18.8	4.80 (± 0.29) x 10^{6}	48
F•A	195.1	10.2	19.1	3.93 (± 0.19) x 10^{7}	401
F•G	200.1	10.0	20.0	1.51 (± 0.07) x 10^{7}	150
F•T	199.4	10.1	19.7	1.07 (± 0.04) x 10^{7}	108
F•C	191.2	10.2	18.7	1.01 (± 0.04) x 10^{7}	103
AT•AT	42.5	2.4	17.7	9.16 (± 1.35) x 10^{8}	2198
GT•GT	99.8	4.8	20.8	1.10 (± 0.08) x 10^{8}	528
TT•TT	196.8	9.5	20.7	2.72 (± 0.06) x 10^{7}	258
CT•CT	244.6	12.5	19.6	7.63 (± 0.26) x 10^{6}	95
AL•AL	181.7	8.8	20.6	1.28 (± 0.07) x 10^{7}	113
GL•GL	304.0	11.8	25.8	1.68 (± 0.05) x 10^{6}	20
TL•TL	241.6	9.9	24.4	2.38 (± 0.05) x 10^{6}	24
CL•CL	481.1	15.1	31.9	4.84 (± 0.09)x 10^{5}	7
AF•AF	185.4	9.2	20.2	7.48 (± 0.18) x 10^{6}	69
GF•GF	232.0	9.3	24.9	1.90 (± 0.06) x 10^{6}	18
TF•TF	244.2	9.2	26.5	1.60 (± 0.04) x 10^{6}	15
CF•CF	234.3	10.7	21.9	7.86 (± 0.20) x 10^{5}	8
AF•AT	45.2	3.0	15.1	1.74 (± 0.15) x 10^{8}	522
AT•AF	43.3	3.0	14.4	1.56 (± 0.15) x 10^{8}	468

[a] K_a for T•A in this paper was calculated from averaging K_a values obtained from two experiments.

Fig. S3. Representative ITC curves for the modified DNA duplexes obtained at 25 °C.

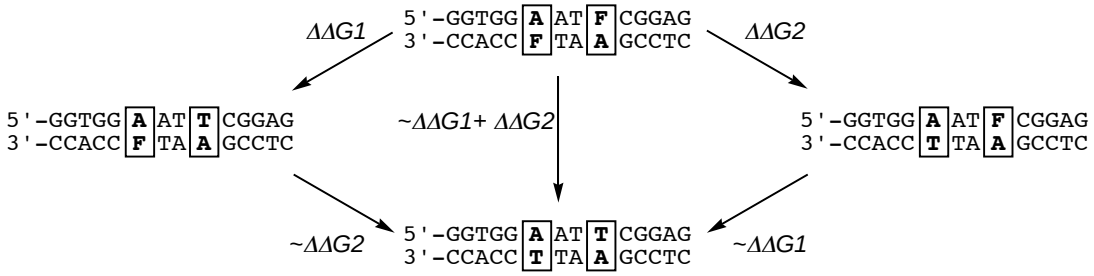


Estimation of $\Delta G°_{itc}$ for AT•AT and T•A duplexes

As mentioned in the paper, an accurate measurement of K_a and $\Delta G°$ for AT•AT duplex was not possible, because the experimentally obtained K_a was outside of the optimal range ($1000/C_c > K_{a,25} > 1/C_c$) and appeared to be underestimated (see plots below). To fit K_a within the optimal range, one can decrease C_c as low as possible but still yield a measurable hybridization heat. However, our ITC measurement with the lowest possible C_c of the AT duplex (2.4 μM) provided a K_a value that still did not fit within the optimal range. To solve this issue, we instead indirectly determined the desired thermodynamic values for the double-substituted duplex by summing the stabilization of two half-substituted duplexes.

To do this, we prepared two new 14-bp duplexes, AT•AF and AF•AT, each containing one T/A and one F/A (Table 1). We worked under the assumption that the difference between the $\Delta G°$ of these duplexes and that of AF•AF duplex ($\Delta\Delta G°_1$ and $\Delta\Delta G°_2$, respectively*)* could be summed to provide a more accurate hybridization $\Delta G°$ value, and consequently K_a, for the full AT•AT duplex. The additivity of the $\Delta\Delta G°$ values was first verified by thermal denaturation experiments. We then estimated the $\Delta G°_{25,itc}$ and $K_{a,25}$ for AT•AT duplex using the sum of the $\Delta\Delta G°_{itc}$ values:

$$\Delta G°_{25,itc} \text{ for AT•AT} = \Delta G°_{25,itc} \text{ for AF•AF} + \Delta\Delta G°_{1,itc} + \Delta\Delta G°_{2,itc}$$



Thermal denaturation experiments verified that the replacement of the two F/A base pairs in AF•AF duplexes with T/A base pairs changes the hybridization thermodynamic values largely in an additive manner. These experiments show that AF•AT and AT•AF duplexes are 3.5–3.6 kcal/mol more stable than AF•AF duplex and 3.4–3.5 Kcal/mol less stable than AT•AT duplex at 37 °C. With respect to the fully substituted AF•AF duplex, the AT•AT duplex displays twice the stabilization as the monosubstituted AF•AT and AT•AF duplexes. We thus estimated the $\Delta G°_{25,itc}$ of AT•AT and T•A duplexes as below:

$\Delta G°_{25,itc}$ of AT•AT = $\Delta G°_{25,itc}$ of AF•AF + ($\Delta G°_{25,itc}$ of AF•AT - $\Delta G°_{25,itc}$ of AF•AF) + ($\Delta G°_{25,itc}$ of AT•AF - $\Delta G°_{25,itc}$ of AF•AF) = -13.04 Kcal/mol

We similarly used the average of these $\Delta\Delta G°_{itc}$ values to better determine the K_a and $\Delta G°$ for 12mer T•A duplex, which also appeared to be underestimated by a direct ITC measurement, from those for F•A 12mer duplex:

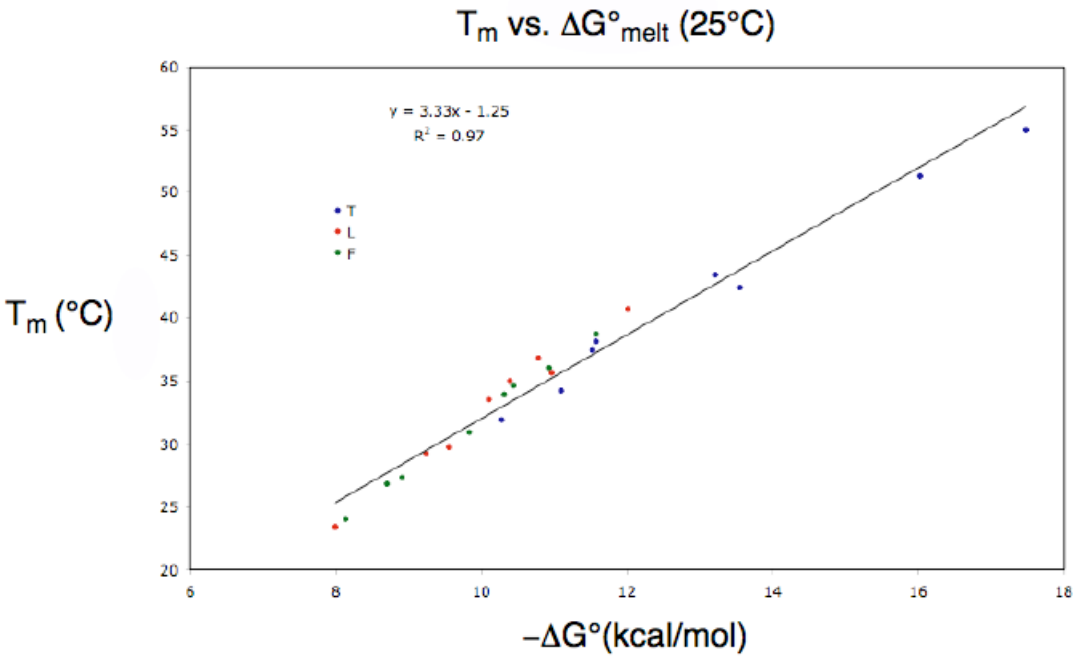
$$\Delta G°_{25,itc} \text{ for T•A} = \Delta G°_{25,itc} \text{ for F•A} + (\Delta\Delta G°_{1.itc} + \Delta\Delta G°_{2,itc})/2$$

or

$$\Delta G°_{25,itc} \text{ of T•A} = \Delta G°_{25,itc} \text{ of F•A} + [(\Delta G°_{25,itc} \text{ of AF•AT} - \Delta G°_{25,itc} \text{ of AF•AF}) + (\Delta G°_{25,itc} \text{ of AT•AF} - \Delta G°_{25,itc} \text{ of AF•AF})]/2 = -12.22 \text{ Kcal/mol}$$

Plotted fits to the melting vs. ITC free energy data show that these indirectly measured values for the all-A/T duplexes better fit the entire data set (see plots below), thus providing confidence that (a) the originally measured values were indeed underestimated and (b) that the values estimated form the half-substitutions are more reliable.

Fig. S4. Correlation plots of T_m vs ΔG_{melt25} and ΔG_{melt37}



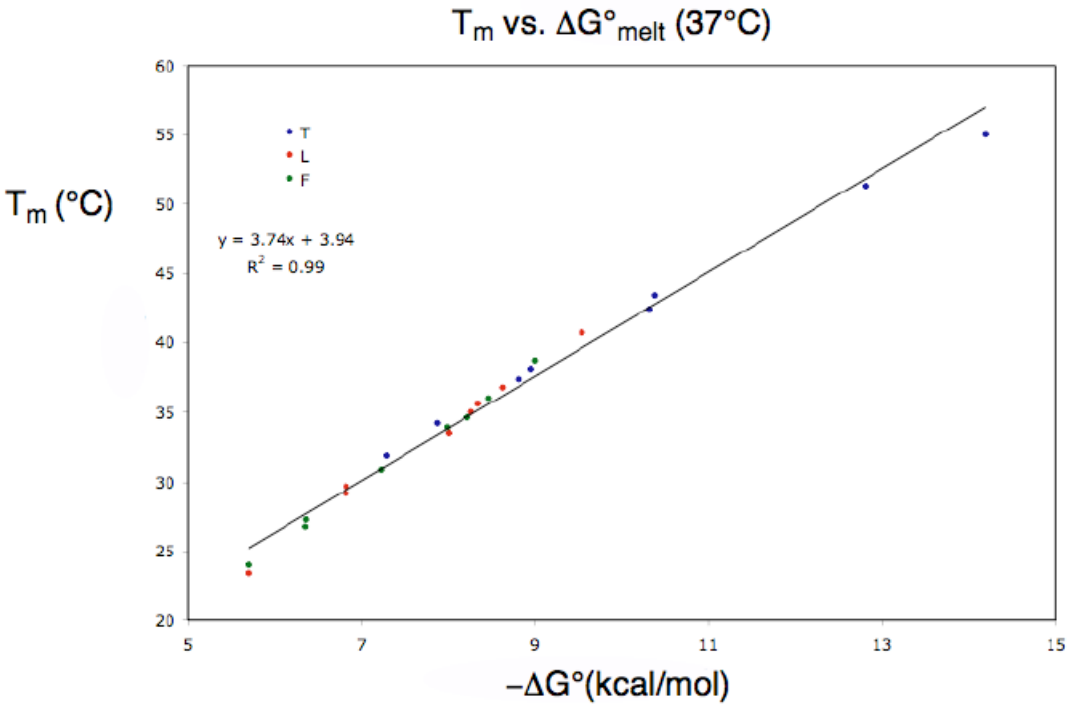
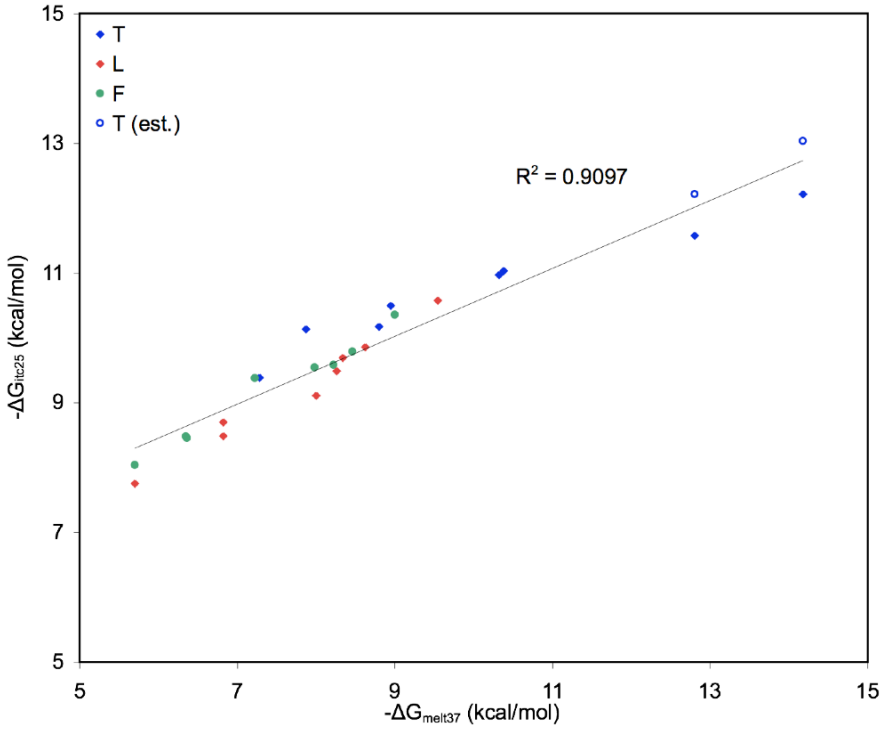
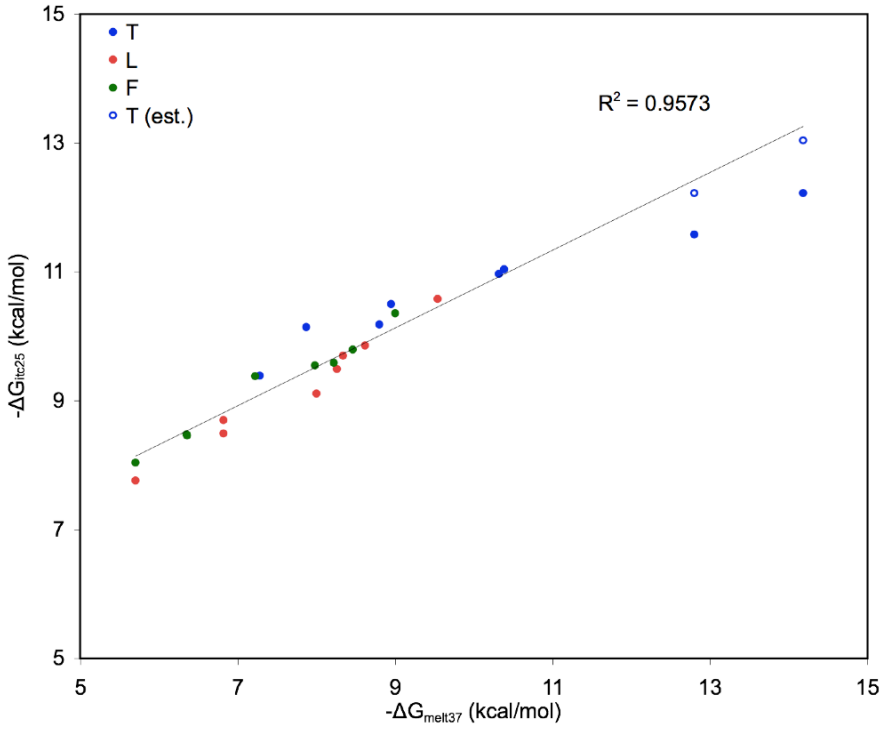


Fig. S5. Plots of ΔG_{melt37} *vs* ΔG_{itc25}

Fit using all experimental data



Fit of experimental data excluding duplexes with T/A base pairs, showing better fit to the data and showing better fit to estimated values for T/A duplexes (open circles)



Full Citation for Gaussian09:

Gaussian 09, Revision A.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

Fig. S6. Optimized structures for the pairs in this study. H…X distances (in Å) are listed in black, and heavy atom distances (X…H…X) are in blue.

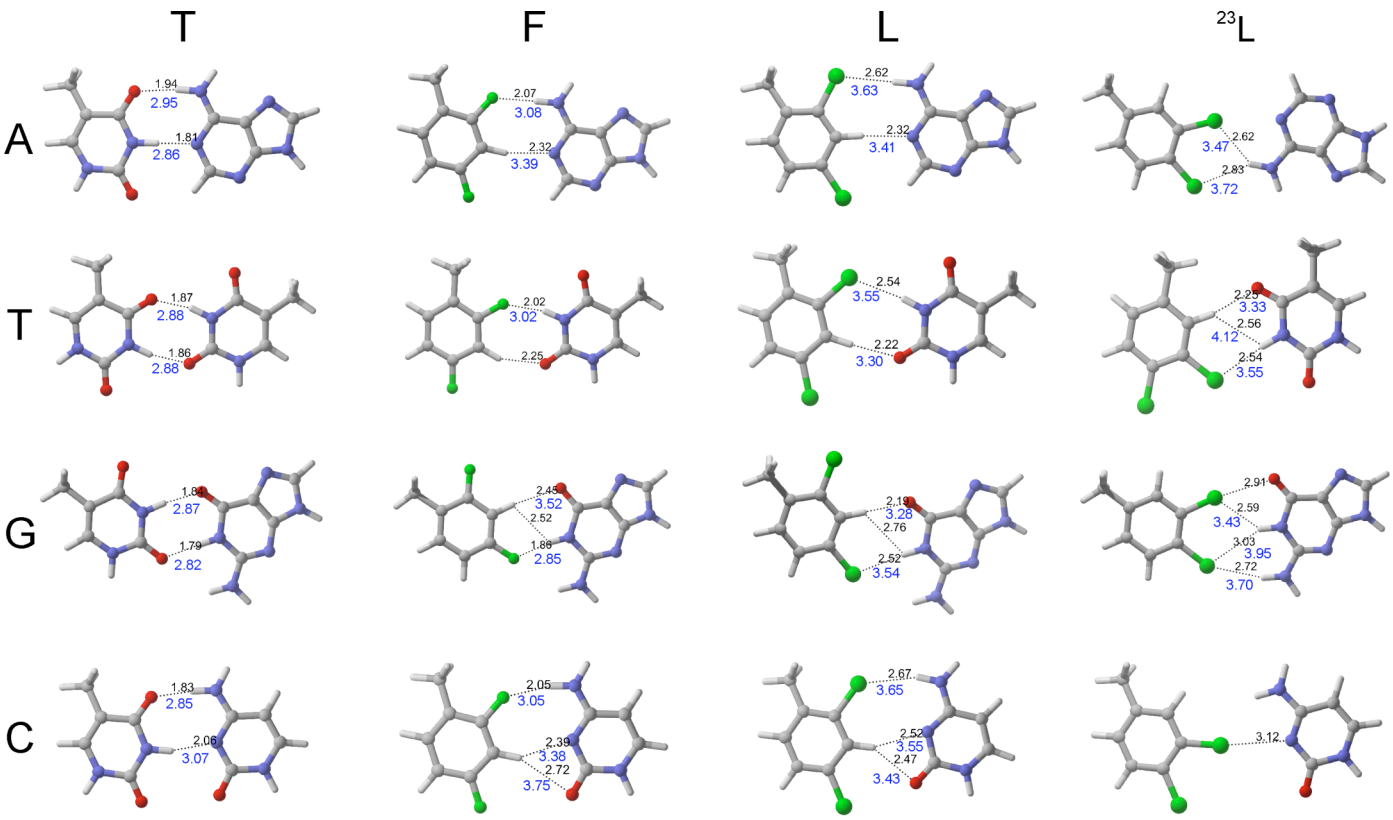


Table S4. M06-2X/6-31+G(*d*) absolute energies (hartree) in the gas phase, and in water (CPCM).

	Gas Phase			Water (CPCM)		
	Dimer	**Monomer1**	**Monomer2**	**Dimer**	**Monomer1**	**Monomer2**
TA	–921.14783	–453.96836	–467.15576	–921.15109	–453.97331	–467.16066
TC	–848.77403	–453.96836	–394.78482	–848.78623	–453.97331	–394.79945
TG	–996.36074	–453.96836	–542.36535	–996.37391	–453.97331	–542.38235
TT	–907.95677	–453.96836	–453.96836	–907.96245	–453.97331	–453.97331
FA	–937.03085	–469.86776	–467.15576	–937.02319	–469.85926	–467.16066
FC	–864.66132	–469.86776	–394.78482	–864.66307	–469.85926	–394.79945
FG	–1012.24391	–469.86776	–542.36535	–1012.24650	–469.85926	–542.38235
FT	–923.84330	–469.86776	–453.96836	–923.83610	–469.85926	–453.97331
LA	–1657.74431	–1190.58207	–467.15576	–1657.73715	–1190.57380	–467.16066
LC	–1585.37314	–1190.58207	–394.78482	–1585.37419	–1190.57380	–394.79945
LG	–1732.95535	–1190.58207	–542.36535	–1732.95779	–1190.57380	–542.38235
LT	–1644.55610	–1190.58207	–453.96836	–1644.54901	–1190.57380	–453.97331
^{23}LA	–1657.73629	–1190.57793	–467.15576	–1657.73126	–1190.57004	–467.16066
^{23}LC	–1585.36476	–1190.57793	–394.78482	–1585.36985	–1190.57004	–394.79945
^{23}LG	–1732.95321	–1190.57793	–542.36535	–1732.95458	–1190.57004	–542.38235
^{23}LT	–1644.55338	–1190.57793	–453.96836	–1644.54580	–1190.57004	–453.97331

M06-2X/6-31+G(d) Optimized Cartesian Coordinates (Å)
Gas-Phase

```
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C        0.6602150       -2.0270920        0.0000000
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C       -0.9217550       -0.4955690        0.0000000
C        0.0000000        0.5477780        0.0000000
C        1.3576280        0.1677090        0.0000000
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H        3.3102090        0.7650410        0.0000000
H        2.1400180        2.0659980        0.0000000
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C        1.3731940        0.5563050        0.0000000
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H 1.2219490 -2.9160000 0.0000000
C 0.3614150 3.4438670 0.0000000
C 2.0889150 1.8497520 0.0000000
C 3.0824480 2.8239830 0.0000000
C 2.6419870 4.1491960 0.0000000
C 4.5371430 2.4388890 0.0000000
H 0.0000000 1.2982830 0.0000000
H 3.3810470 4.9460420 0.0000000
H 5.1674610 3.3315670 0.0000000
H 4.7884590 1.8405980 0.8815490
H 4.7884590 1.8405980 -0.8815490
H -4.3107730 -4.2951230 0.0000000
H 0.9450340 5.5050300 0.0000000
F 2.4881640 0.5489630 0.0000000
F -0.9513110 3.7456920 0.0000000
C 0.7296060 2.1064480 0.0000000
C 1.2862600 4.4757220 0.0000000

28
FC
N -1.7372570 -0.7963680 0.0000000
C -2.7895680 0.0755140 0.0000000
N -4.0855770 -0.4957610 0.0000000
C -4.3049700 -1.8322830 0.0000000
C -3.2598700 -2.6943640 0.0000000
C -1.9463120 -2.0968340 0.0000000
N -0.8571360 -2.8926790 0.0000000
H 0.0554990 -2.4530910 0.0000000
H -0.9294070 -3.8970710 0.0000000
C 2.8481790 2.7576750 0.0000000
C 1.5029760 2.4214510 0.0000000
F 0.5930030 3.4101090 0.0000000
C 1.0568390 1.1066860 0.0000000
C 2.0416170 0.1341770 0.0000000
F 1.6572760 -1.1723640 0.0000000
C 3.4107760 0.3862640 0.0000000
C 3.7897110 1.7298760 0.0000000
C 4.4007080 -0.7474060 0.0000000
H 0.0000000 0.8503580 0.0000000
H 4.8484580 1.9759720 0.0000000
H 5.4228690 -0.3604240 0.0000000
H 4.2751880 -1.3841690 0.8817210
H 4.2751880 -1.3841690 -0.8817210
H 3.1402230 3.8020790 0.0000000
O -2.6856210 1.2893170 0.0000000
H -3.4057420 -3.7667150 0.0000000
H -5.3406890 -2.1559350 0.0000000
H -4.8498530 0.1680470 0.0000000

31
FG

N	-0.9823540	1.3253140	0.0000000
C	-1.3223090	2.6513240	0.0000000
N	-2.5573490	3.0861160	0.0000000
C	-3.4563240	2.0695980	0.0000000
C	-3.2367730	0.6964500	0.0000000
C	-1.8785710	0.2242940	0.0000000
N	-4.4276460	0.0039890	0.0000000
C	-5.3434830	0.9297080	0.0000000
N	-4.8140480	2.2054630	0.0000000
H	-6.4114340	0.7593900	0.0000000
C	3.9995420	-0.2313250	0.0000000
C	2.6173890	-0.2434320	0.0000000
F	1.9642590	0.9582390	0.0000000
C	1.8569670	-1.4007800	0.0000000
C	2.5704920	-2.5897930	0.0000000
F	1.8793470	-3.7436100	0.0000000
C	3.9625920	-2.6695190	0.0000000
C	4.6593230	-1.4604320	0.0000000
C	4.6437760	-4.0109300	0.0000000
H	0.7674160	-1.3900820	0.0000000
H	5.7458290	-1.4803230	0.0000000
H	5.7296980	-3.8889580	0.0000000
H	4.3610190	-4.5958410	0.8807930
H	4.3610190	-4.5958410	-0.8807930
H	-5.3158160	3.0824370	0.0000000
H	4.5372000	0.7102350	0.0000000
N	-0.2940140	3.5376510	0.0000000
H	-0.5173820	4.5207670	0.0000000
H	0.6711980	3.2468560	0.0000000
O	-1.4286310	-0.9083720	0.0000000
H	0.0000000	1.0659620	0.0000000

30
FT

N	-3.1783830	1.6829540	0.0000000
C	-2.0222950	0.9280610	0.0000000
O	-2.0331240	-0.2900240	0.0000000
N	-0.8730370	1.6866240	0.0000000
C	-0.7741390	3.0835970	0.0000000
O	0.3137520	3.6266520	0.0000000
C	-2.0595510	3.7958850	0.0000000
C	-3.1888530	3.0626140	0.0000000
C	-2.0214820	5.2931280	0.0000000
H	0.0000000	1.1623640	0.0000000
H	-4.1754560	3.5154280	0.0000000
H	-3.0322440	5.7099530	0.0000000
H	-1.4857750	5.6644430	0.8790900
H	-1.4857750	5.6644430	-0.8790900
H	-4.0390130	1.1520340	0.0000000
C	0.6816830	-3.7639540	0.0000000
C	1.6073030	-1.6027350	0.0000000
C	2.9122040	-2.0863290	0.0000000
C	3.0516130	-3.4756400	0.0000000
C	4.0814940	-1.1392110	0.0000000
H	-0.5216060	-1.9519910	0.0000000
H	4.0518260	-3.9008910	0.0000000
H	5.0221510	-1.6953840	0.0000000
H	4.0650360	-0.4897330	-0.8809000
H	4.0650360	-0.4897330	0.8809000
H	2.0564720	-5.4063060	0.0000000
C	0.4713610	-2.3925460	0.0000000
C	1.9475540	-4.3273750	0.0000000
F	1.4445810	-0.2527040	0.0000000
F	-0.3920360	-4.5770360	0.0000000

```
30
TA
N       -0.7736160       -0.7128480        0.0000000
C       -2.1193700       -0.7479570        0.0000000
N       -2.9094960       -1.8120190        0.0000000
C       -2.1965130       -2.9478030        0.0000000
C       -0.8105010       -3.0698740        0.0000000
C       -0.0757270       -1.8634400        0.0000000
N        1.2629130       -1.8310310        0.0000000
N       -0.4187980       -4.3931180        0.0000000
C       -1.5444210       -5.0550250        0.0000000
N       -2.6541570       -4.2411610        0.0000000
H       -2.6018220        0.2272210        0.0000000
H       -1.6338940       -6.1332190        0.0000000
H        1.7637560       -0.9407040        0.0000000
H        1.7744500       -2.7012450        0.0000000
N        0.2512720        4.1657370        0.0000000
C       -0.4010640        2.9427340        0.0000000
O       -1.6138770        2.8461360        0.0000000
N        0.4541920        1.8645020        0.0000000
C        1.8366790        1.8974240        0.0000000
O        2.4867040        0.8546400        0.0000000
C        2.4487220        3.2289350        0.0000000
C        1.6214360        4.2940070        0.0000000
C        3.9439790        3.3173560        0.0000000
H        0.0000000        0.9223380        0.0000000
H        1.9909630        5.3149890        0.0000000
H        4.2736060        4.3599580        0.0000000
H        4.3603650        2.8161100        0.8792370
H        4.3603650        2.8161100       -0.8792370
H       -3.6242800       -4.5241100        0.0000000
H       -0.3516170        4.9777540        0.0000000

28
TC
N       -1.5970820       -0.7822170        0.0000000
C       -2.7539150       -0.0489300        0.0000000
N       -3.9686150       -0.7776370        0.0000000
C       -4.0214280       -2.1309440        0.0000000
C       -2.8779960       -2.8544480        0.0000000
C       -1.6411760       -2.1068630        0.0000000
N       -0.4767340       -2.7705940        0.0000000
H        0.3990750       -2.2405660        0.0000000
H       -0.4550510       -3.7778530        0.0000000
N        2.3027230        2.8217020        0.0000000
C        1.0014060        2.3281000        0.0000000
O        0.0396690        3.0606760        0.0000000
N        0.9420440        0.9425530        0.0000000
C        2.0217890        0.0759760        0.0000000
O        1.8615780       -1.1431930        0.0000000
C        3.3530230        0.6858980        0.0000000
C        3.4240790        2.0318600        0.0000000
C        4.5423640       -0.2248530        0.0000000
H        0.0000000        0.5147070        0.0000000
H        4.3705040        2.5642870        0.0000000
H        5.4724250        0.3504450        0.0000000
H        4.5317760       -0.8763660        0.8794220
H        4.5317760       -0.8763660       -0.8794220
H        2.3699630        3.8307120        0.0000000
O       -2.8038530        1.1660910        0.0000000
H       -2.8885220       -3.9366430        0.0000000
H       -5.0089510       -2.5809510        0.0000000
H       -4.8073920       -0.2114220        0.0000000
```

31
TG
N -1.0279370 1.2832830 0.0000000
C -1.6570870 2.4956600 0.0000000
N -2.9603150 2.6468190 0.0000000
C -3.6059700 1.4555880 0.0000000
C -3.0800720 0.1661710 0.0000000
C -1.6527970 0.0245070 0.0000000
N -4.0833490 -0.7787780 0.0000000
C -5.1844950 -0.0847920 0.0000000
N -4.9591510 1.2785720 0.0000000
H -6.1860100 -0.4930510 0.0000000
N 3.8236390 0.2656240 0.0000000
C 2.4507940 0.2289540 0.0000000
O 1.7918500 1.2725170 0.0000000
N 1.9097890 -1.0227610 0.0000000
C 2.6217910 -2.2355510 0.0000000
O 2.0372760 -3.2978300 0.0000000
C 4.0885580 -2.1048870 0.0000000
C 4.6151120 -0.8679820 0.0000000
C 4.8917910 -3.3682810 0.0000000
H 0.8745560 -1.0875240 0.0000000
H 5.6847170 -0.6842320 0.0000000
H 5.9634800 -3.1520270 0.0000000
H 4.6511150 -3.9745170 0.8786760
H 4.6511150 -3.9745170 -0.8786760
H -5.6472390 2.0183520 0.0000000
H 4.2327190 1.1901350 0.0000000
N -0.8441640 3.5817240 0.0000000
H -1.2676960 4.4962400 0.0000000
H 0.1609840 3.4903260 0.0000000
O -0.9607620 -0.9900360 0.0000000
H 0.0000000 1.2559000 0.0000000

30
TT
N -3.2290270 1.0741290 0.0000000
C -1.9535240 0.5544280 0.0000000
O -1.7562650 -0.6555590 0.0000000
N -0.9599630 1.4957780 0.0000000
C -1.1234700 2.8869280 0.0000000
O -0.1593640 3.6270800 0.0000000
C -2.5190450 3.3532680 0.0000000
C -3.4964820 2.4283310 0.0000000
C -2.7531890 4.8322890 0.0000000
H 0.0000000 1.1232860 0.0000000
H -4.5497250 2.6908970 0.0000000
H -3.8226410 5.0598310 0.0000000
H -2.2923390 5.2938510 0.8788240
H -2.2923390 5.2938510 -0.8788240
H -3.9736820 0.3899220 0.0000000
N 2.1962530 -3.8688050 0.0000000
C 0.8770710 -3.4403870 0.0000000
O -0.0590540 -4.2122000 0.0000000
N 0.7508650 -2.0647000 0.0000000
C 1.7790170 -1.1351990 0.0000000
O 1.5387120 0.0683580 0.0000000
C 3.1395810 -1.6766100 0.0000000
C 3.2765950 -3.0177240 0.0000000
C 4.2805230 -0.7059810 0.0000000
H -0.2067800 -1.6866770 0.0000000
H 4.2484660 -3.5017490 0.0000000
H 5.2392500 -1.2317450 0.0000000
H 4.2343990 -0.0555960 -0.8788650
H 4.2343990 -0.0555960 0.8788650
H 2.3194050 -4.8725790 0.0000000

15
A
N 1.6634880 -1.1347290 0.0000000
C 0.6602150 -2.0270920 0.0000000
N -0.6503780 -1.8056760 0.0000000
C -0.9217550 -0.4955690 0.0000000
C 0.0000000 0.5477780 0.0000000
C 1.3576280 0.1677090 0.0000000
N 2.3515760 1.0797100 0.0000000
N -0.6269150 1.7780380 0.0000000
C -1.8990750 1.4819110 0.0000000
N -2.1449990 0.1283710 0.0000000
H 0.9681320 -3.0695610 0.0000000
H -2.7057310 2.2029150 0.0000000
H 3.3102090 0.7650410 0.0000000
H 2.1400180 2.0659980 0.0000000
H -3.0441170 -0.3328050 0.0000000

```
13
C
N        0.0000000        1.0543690        0.0000000
C       -1.2203020        0.4327720        0.0000000
N       -1.2054260       -0.9868320        0.0000000
C       -0.0679600       -1.7196450        0.0000000
C        1.1374060       -1.1008390        0.0000000
C        1.1038530        0.3412520        0.0000000
N        2.2756870        1.0194880        0.0000000
H        2.2434950        2.0291070        0.0000000
H        3.1677750        0.5523670        0.0000000
O       -2.2982520        0.9961290        0.0000000
H        2.0650500       -1.6581220        0.0000000
H       -0.1817190       -2.7988540        0.0000000
H       -2.1183930       -1.4239490        0.0000000

15
F
C        1.2618830       -0.9989890        0.0000000
C        0.0000000        0.9971020        0.0000000
C       -1.2075800        0.3022250        0.0000000
C       -1.1218440       -1.0912680        0.0000000
C       -2.5151290        1.0469710        0.0000000
H        2.1585300        0.9690020        0.0000000
H       -2.0410180       -1.6711610        0.0000000
H       -3.3534660        0.3460250        0.0000000
H       -2.6034820        1.6903340        0.8810850
H       -2.6034820        1.6903340       -0.8810850
H        0.1676150       -2.8400600        0.0000000
F       -0.0455260        2.3448230        0.0000000
F        2.4554380       -1.6227840        0.0000000
C        1.2437130        0.3879460        0.0000000
C        0.1033060       -1.7577900        0.0000000

16
G
N        1.4251250       -0.8716190        0.0000000
C        0.3528240       -1.7260380        0.0000000
N       -0.8918360       -1.3268470        0.0000000
C       -0.9998330        0.0272540        0.0000000
C        0.0000000        0.9912240        0.0000000
C        1.3731940        0.5563050        0.0000000
N       -0.5347690        2.2600740        0.0000000
C       -1.8236100        2.0711420        0.0000000
N       -2.1669230        0.7336910        0.0000000
H       -2.5744270        2.8493520        0.0000000
H       -3.0952270        0.3345520        0.0000000
N        0.6256340       -3.0573860        0.0000000
H       -0.1553610       -3.6958820        0.0000000
H        1.5616670       -3.4285020        0.0000000
O        2.4095160        1.1866420        0.0000000
H        2.3711600       -1.2373660        0.0000000

15
T
N        0.1548320       -1.6637860        0.0000000
C        1.3575030       -0.9817700        0.0000000
O        2.4368840       -1.5371500        0.0000000
N        1.1975030        0.3910610        0.0000000
C        0.0000000        1.1168550        0.0000000
O        0.0156520        2.3328180        0.0000000
C       -1.2180010        0.2961030        0.0000000
C       -1.0771840       -1.0433630        0.0000000
C       -2.5348430        1.0100530        0.0000000
H        2.0555340        0.9337190        0.0000000
H       -1.9298860       -1.7151900        0.0000000
H       -3.3648380        0.2984610        0.0000000
H       -2.6228570        1.6557070        0.8792340
H       -2.6228570        1.6557070       -0.8792340
H        0.2334300       -2.6719470        0.0000000
```

30
LA

N	-0.6727890	-1.3086070	0.0000000
C	-1.9988580	-1.5262730	0.0000000
N	-2.6490370	-2.6845000	0.0000000
C	-1.7995840	-3.7189400	0.0000000
C	-0.4090030	-3.6582160	0.0000000
C	0.1524340	-2.3646490	0.0000000
N	1.4837840	-2.1656540	0.0000000
N	0.1533970	-4.9191920	0.0000000
C	-0.8763420	-5.7223010	0.0000000
N	-2.0834960	-5.0620600	0.0000000
H	-2.6136500	-0.6297040	0.0000000
H	-0.8231680	-6.8029300	0.0000000
H	1.8506770	-1.2234510	0.0000000
H	2.1132440	-2.9542170	0.0000000
C	-0.7585240	2.9361930	0.0000000
C	1.5624780	2.4131590	0.0000000
C	1.9214410	3.7646820	0.0000000
C	0.8731560	4.6889660	0.0000000
C	3.3584880	4.2091650	0.0000000
H	0.0000000	0.9111330	0.0000000
H	1.1120770	5.7492760	0.0000000
H	3.4211140	5.2999000	0.0000000
H	3.8881850	3.8318390	0.8809610
H	3.8881850	3.8318390	-0.8809610
H	-3.0075120	-5.4711690	0.0000000
H	-1.2607870	5.0271710	0.0000000
Cl	2.8349720	1.2055070	0.0000000
Cl	-2.4256800	2.4227550	0.0000000
C	0.2440560	1.9727000	0.0000000
C	-0.4612960	4.2938400	0.0000000

28
LC

N	-1.7875030	-1.2513110	0.0000000
C	-2.7301540	-0.2619300	0.0000000
N	-4.0847380	-0.6735790	0.0000000
C	-4.4627930	-1.9739160	0.0000000
C	-3.5275030	-2.9539320	0.0000000
C	-2.1528790	-2.5159730	0.0000000
N	-1.1677980	-3.4389830	0.0000000
H	-0.2113090	-3.1096400	0.0000000
H	-1.3566450	-4.4280720	0.0000000
C	2.4498480	2.9065700	0.0000000
C	1.1782070	2.3433240	0.0000000
Cl	-0.2105130	3.3906370	0.0000000
C	0.9975280	0.9618850	0.0000000
C	2.1383660	0.1654450	0.0000000
Cl	1.9467870	-1.5799460	0.0000000
C	3.4394540	0.6793800	0.0000000
C	3.5614480	2.0707610	0.0000000
C	4.6523360	-0.2107750	0.0000000
H	0.0000000	0.5264720	0.0000000
H	4.5564430	2.5086290	0.0000000
H	5.5654220	0.3895410	0.0000000
H	4.6654880	-0.8614430	0.8807510
H	4.6654880	-0.8614430	-0.8807510
H	2.5636950	3.9855570	0.0000000
O	-2.4819330	0.9308110	0.0000000
H	-3.7993460	-4.0014300	0.0000000
H	-5.5296520	-2.1716620	0.0000000
H	-4.7636380	0.0773280	0.0000000

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31
LG
N       -0.2320410       -2.1275570        0.0000000
C       -0.6576050       -3.4291320        0.0000000
N        0.1506630       -4.4586870        0.0000000
C        1.4554460       -4.0867640        0.0000000
C        2.0086170       -2.8115710        0.0000000
C        1.1181930       -1.6828440        0.0000000
N        3.3850270       -2.8678850        0.0000000
C        3.6590980       -4.1408750        0.0000000
N        2.5266470       -4.9317380        0.0000000
H        4.6510790       -4.5716350        0.0000000
C       -2.9031410        3.0507950        0.0000000
C       -2.0491730        1.9561190        0.0000000
Cl       -2.7565530        0.3465080        0.0000000
C       -0.6678790        2.0942160        0.0000000
C       -0.1509900        3.3876020        0.0000000
Cl       1.5813620        3.5710380        0.0000000
C       -0.9617470        4.5288580        0.0000000
C       -2.3441340        4.3252370        0.0000000
C       -0.3757750        5.9137210        0.0000000
H        0.0000000        1.2346270        0.0000000
H       -3.0013630        5.1908790        0.0000000
H       -1.1678020        6.6663730        0.0000000
H        0.2560200        6.0721840        0.8801060
H        0.2560200        6.0721840       -0.8801060
H        2.4780670       -5.9410220        0.0000000
H       -3.9787910        2.9105150        0.0000000
N       -2.0001800       -3.6327890        0.0000000
H       -2.3315770       -4.5851290        0.0000000
H       -2.6674790       -2.8783530        0.0000000
O        1.3501490       -0.4872660        0.0000000
H       -0.9133870       -1.3723500        0.0000000

30
LT
N        3.5457120       -1.3066370        0.0000000
C        2.2360400       -0.8707540        0.0000000
O        1.9324410        0.3084810        0.0000000
N        1.3189780       -1.8982850        0.0000000
C        1.5766520       -3.2745210        0.0000000
O        0.6605470       -4.0739730        0.0000000
C        3.0007960       -3.6359330        0.0000000
C        3.9059530       -2.6387770        0.0000000
C        3.3451390       -5.0935770        0.0000000
H        0.3412720       -1.6144030        0.0000000
H        4.9752200       -2.8257800        0.0000000
H        4.4286520       -5.2394680        0.0000000
H        2.9214510       -5.5888330        0.8791400
H        2.9214510       -5.5888330       -0.8791400
H        4.2435470       -0.5747020        0.0000000
C       -1.0998490        3.2533490        0.0000000
C       -2.1454200        1.1137980        0.0000000
C       -3.4243090        1.6792380        0.0000000
C       -3.4892860        3.0752660        0.0000000
C       -4.6701240        0.8362300        0.0000000
H        0.0000000        1.3914950        0.0000000
H       -4.4659860        3.5522290        0.0000000
H       -5.5600840        1.4700520        0.0000000
H       -4.7074010        0.1867370       -0.8808100
H       -4.7074010        0.1867370        0.8808100
H       -2.4186230        4.9513850        0.0000000
C       -0.9771660        1.8678540        0.0000000
C       -2.3462690        3.8688730        0.0000000
Cl       -2.0021730       -0.6347720        0.0000000
Cl        0.3408920        4.2327430        0.0000000
```

```
15
L
C         0.5435530       -1.3737490        0.0000000
C         0.0000000        0.9537980        0.0000000
C        -1.3720070        0.6808000        0.0000000
C        -1.7449890       -0.6662570        0.0000000
C        -2.3985820        1.7798840        0.0000000
H         2.0195740        0.2005720        0.0000000
H        -2.8032140       -0.9143140        0.0000000
H        -3.4078600        1.3616120        0.0000000
H        -2.2883800        2.4211570        0.8806660
H        -2.2883800        2.4211570       -0.8806660
H        -1.1208900       -2.7348910        0.0000000
Cl         0.5461750         2.6127430         0.0000000
Cl         1.7354910        -2.6440790         0.0000000
C         0.9641460       -0.0489140        0.0000000
C        -0.8086520       -1.6959910        0.0000000
```

30
23ClA

N	-0.0393290	-2.0133890	0.0000000
C	-1.2487180	-2.5951160	0.0000000
N	-1.5449030	-3.8908920	0.0000000
C	-0.4376780	-4.6420260	0.0000000
C	0.8799170	-4.1907090	0.0000000
C	1.0487270	-2.7912790	0.0000000
N	2.2683940	-2.2156180	0.0000000
N	1.7756450	-5.2417950	0.0000000
C	1.0145490	-6.3029730	0.0000000
N	-0.3298540	-6.0110090	0.0000000
H	-2.0916590	-1.9081790	0.0000000
H	1.3708510	-7.3245540	0.0000000
H	2.3373050	-1.2085610	0.0000000
H	3.1018230	-2.7838060	0.0000000
C	-1.2621800	3.4654890	0.0000000
C	1.1490010	3.4886550	0.0000000
C	1.1627820	4.8846700	0.0000000
C	-0.0599500	5.5580390	0.0000000
C	2.4740790	5.6292640	0.0000000
H	-0.0781710	6.6446250	0.0000000
H	2.3128660	6.7104090	0.0000000
H	3.0696590	5.3763810	0.8834080
H	3.0696590	5.3763810	-0.8834080
H	-1.1005010	-6.6646400	0.0000000
H	-2.2111870	5.3827950	0.0000000
Cl	-2.7792370	2.6213690	0.0000000
C	-0.0466210	2.7750030	0.0000000
C	-1.2618010	4.8569150	0.0000000
H	2.0840750	2.9341960	0.0000000
Cl	0.0000000	1.0408820	0.0000000

28
23ClC

N	-1.0793210	-2.5781110	0.0000000
C	-2.3910280	-2.9712350	0.0000000
N	-2.6286210	-4.3712750	0.0000000
C	-1.6395540	-5.2945720	0.0000000
C	-0.3432320	-4.9006460	0.0000000
C	-0.1181640	-3.4755900	0.0000000
N	1.1544110	-3.0157390	0.0000000
H	1.3011290	-2.0148110	0.0000000
H	1.9475860	-3.6360270	0.0000000
C	0.8008640	4.2915130	0.0000000
C	0.1085070	3.0841830	0.0000000
Cl	-1.6248740	3.1007300	0.0000000
C	0.8223560	1.8817550	0.0000000
C	2.2144630	1.9085730	0.0000000
C	2.9197490	3.1133510	0.0000000
C	2.1921790	4.3044580	0.0000000
C	4.4277680	3.1092180	0.0000000
H	2.7154340	5.2569390	0.0000000
H	4.8239440	4.1280170	0.0000000
H	4.8199920	2.5947460	0.8835670
H	4.8199920	2.5947460	-0.8835670
H	0.2372870	5.2190210	0.0000000
O	-3.3508190	-2.2248410	0.0000000
H	0.4703020	-5.6143400	0.0000000
H	-1.9435200	-6.3363410	0.0000000
H	-3.6047150	-4.6393180	0.0000000
H	2.7532420	0.9642150	0.0000000
Cl	0.0000000	0.3540760	0.0000000

31
23ClG
N -0.5093970 1.8203520 0.0000000
C 0.1780840 3.0048760 0.0000000
N -0.3954800 4.1821120 0.0000000
C -1.7492240 4.0933270 0.0000000
C -2.5575220 2.9637840 0.0000000
C -1.9270670 1.6699210 0.0000000
N -3.8914710 3.3085310 0.0000000
C -3.8919430 4.6108230 0.0000000
N -2.6185090 5.1455060 0.0000000
H -4.7711550 5.2405850 0.0000000
C 3.2178130 -3.2422340 0.0000000
C 2.1876890 -2.3087120 0.0000000
Cl 2.6023140 -0.6132030 0.0000000
C 0.8572880 -2.7317360 0.0000000
C 0.5769900 -4.0957170 0.0000000
C 1.5981800 -5.0476160 0.0000000
C 2.9213400 -4.6016240 0.0000000
C 1.2614170 -6.5170300 0.0000000
H 3.7346170 -5.3221280 0.0000000
H 2.1668760 -7.1291200 0.0000000
H -2.3579960 6.1216980 0.0000000
H 4.2466190 -2.8969710 0.0000000
N 1.5331430 2.9253900 0.0000000
H 2.0553880 3.7877290 0.0000000
H 2.0251260 2.0468270 0.0000000
O -2.4116230 0.5547270 0.0000000
H 0.0000000 0.9396140 0.0000000
H -0.4640040 -4.4084690 0.0000000
Cl -0.4583360 -1.6051720 0.0000000
H 0.6718000 -6.7834170 0.8831740
H 0.6718000 -6.7834170 -0.8831740

30
23ClT
N -3.4998840 -3.0517940 0.0000000
C -2.1319770 -2.8396230 0.0000000
O -1.3209290 -3.7414390 0.0000000
N -1.7937300 -1.4989090 0.0000000
C -2.6566570 -0.4034410 0.0000000
O -2.2142300 0.7345790 0.0000000
C -4.0853840 -0.7335150 0.0000000
C -4.4302620 -2.0364180 0.0000000
C -5.0630330 0.4014730 0.0000000
H -0.7935030 -1.3031150 0.0000000
H -5.4663590 -2.3605060 0.0000000
H -6.0914600 0.0304110 0.0000000
H -4.9174910 1.0361600 0.8796080
H -4.9174910 1.0361600 -0.8796080
H -3.7837580 -4.0225570 0.0000000
C 3.4006210 1.0614700 0.0000000
C 1.0224110 1.5031390 0.0000000
C 1.2542070 2.8773430 0.0000000
C 2.5778130 3.3304040 0.0000000
C 0.0974700 3.8441510 0.0000000
H 2.7822260 4.3984220 0.0000000
H 0.1299550 4.4911030 0.8832210
H 0.1299550 4.4911030 -0.8832210
H -0.8568360 3.3112480 0.0000000
H 4.6662840 2.7881520 0.0000000
C 2.0849340 0.6020260 0.0000000
C 3.6398290 2.4354640 0.0000000
Cl 4.7470010 -0.0339820 0.0000000
Cl 1.7350710 -1.1056800 0.0000000
H 0.0000000 1.1326400 0.0000000

15
23Cl
C 0.8420650 -0.4399250 0.0000000
C -1.3811840 0.5038890 0.0000000
C -1.9500140 -0.7711500 0.0000000
C -1.0974350 -1.8764390 0.0000000
C -3.4495260 -0.9302280 0.0000000
H -1.5148900 -2.8796810 0.0000000
H -3.7334990 -1.9857050 0.0000000
H -3.8942810 -0.4602070 0.8832920
H -3.8942810 -0.4602070 -0.8832920
H 0.9440740 -2.5768190 0.0000000
Cl 2.5679880 -0.2686220 0.0000000
C 0.0000000 0.6746530 0.0000000
C 0.2847210 -1.7147860 0.0000000
Cl 0.6447130 2.2862470 0.0000000
H -2.0147920 1.3869020 0.0000000

Water (CPCM)

```
30
FA
N       -1.1635850       -0.7150870        0.0000000
C       -2.5059840       -0.7240270        0.0000000
N       -3.3279920       -1.7659490        0.0000000
C       -2.6539220       -2.9264010        0.0000000
C       -1.2705590       -3.0787120        0.0000000
C       -0.5113050       -1.8898760        0.0000000
N        0.8308030       -1.9045890        0.0000000
N       -0.9137150       -4.4113820        0.0000000
C       -2.0611020       -5.0441090        0.0000000
N       -3.1432990       -4.2044630        0.0000000
H       -2.9746090        0.2564940        0.0000000
H       -2.1845140       -6.1169030        0.0000000
H        1.3581130       -1.0410080        0.0000000
H        1.3234100       -2.7851750        0.0000000
C        0.2275870        3.3788030        0.0000000
C        2.0492610        1.8989160        0.0000000
C        2.9782260        2.9325030        0.0000000
C        2.4556510        4.2270660        0.0000000
C        4.4520570        2.6447950        0.0000000
H        0.0000000        1.2135580        0.0000000
H        3.1447390        5.0652170        0.0000000
H        5.0139030        3.5796190        0.0000000
H        4.7402900        2.0659600        0.8811850
H        4.7402900        2.0659600       -0.8811850
H       -4.1169380       -4.4774090        0.0000000
H        0.6792870        5.4727360        0.0000000
F        2.5273000        0.6259700        0.0000000
F       -1.1063540        3.5951280        0.0000000
C        0.6766040        2.0669220        0.0000000
C        1.0821560        4.4676810        0.0000000

28
FC
N       -1.7211010       -0.7826590        0.0000000
C       -2.7768400        0.0709900        0.0000000
N       -4.0585330       -0.4849200        0.0000000
C       -4.2801800       -1.8228900        0.0000000
C       -3.2362130       -2.6859200        0.0000000
C       -1.9262100       -2.0956970        0.0000000
N       -0.8408450       -2.8829560        0.0000000
H        0.0759970       -2.4537240        0.0000000
H       -0.9171260       -3.8880540        0.0000000
C        2.7721110        2.7684670        0.0000000
C        1.4432730        2.3809410        0.0000000
F        0.4867650        3.3362390        0.0000000
C        1.0432990        1.0534500        0.0000000
C        2.0593440        0.1145620        0.0000000
F        1.7138860       -1.2000110        0.0000000
C        3.4169270        0.4161210        0.0000000
C        3.7474380        1.7724400        0.0000000
C        4.4449920       -0.6788330        0.0000000
H        0.0000000        0.7497330        0.0000000
H        4.7956280        2.0518420        0.0000000
H        5.4498940       -0.2537340        0.0000000
H        4.3355850       -1.3170140        0.8795160
H        4.3355850       -1.3170140       -0.8795160
H        3.0313160        3.8193910        0.0000000
O       -2.6611980        1.3004090        0.0000000
H       -3.3794760       -3.7567590        0.0000000
H       -5.3149920       -2.1388280        0.0000000
H       -4.8329940        0.1667930        0.0000000
```

```
31
FG
N       -0.9735760        1.2298470        0.0000000
C       -1.2535330        2.5733620        0.0000000
N       -2.4766250        3.0563710        0.0000000
C       -3.4158830        2.0820060        0.0000000
C       -3.2437140        0.7009320        0.0000000
C       -1.9105300        0.1851090        0.0000000
N       -4.4606810        0.0506720        0.0000000
C       -5.3427820        1.0148910        0.0000000
N       -4.7669680        2.2621140        0.0000000
H       -6.4148830        0.8891640        0.0000000
C        3.9768150       -0.1996600        0.0000000
C        2.5952770       -0.2106600        0.0000000
F        1.9372050        0.9846060        0.0000000
C        1.8377270       -1.3704940        0.0000000
C        2.5524920       -2.5568740        0.0000000
F        1.8581190       -3.7150770        0.0000000
C        3.9419880       -2.6385530        0.0000000
C        4.6368870       -1.4284460        0.0000000
C        4.6208770       -3.9788380        0.0000000
H        0.7497440       -1.3628480        0.0000000
H        5.7211760       -1.4491320        0.0000000
H        5.7042490       -3.8547430        0.0000000
H        4.3359640       -4.5607590        0.8801990
H        4.3359640       -4.5607590       -0.8801990
H       -5.2513370        3.1501850        0.0000000
H        4.5164820        0.7389250        0.0000000
N       -0.1913220        3.4011760        0.0000000
H       -0.3516320        4.3967640        0.0000000
H        0.7582190        3.0590370        0.0000000
O       -1.5189230       -0.9810660        0.0000000
H        0.0000000        0.9390240        0.0000000

30
FT
N       -3.0352040        1.9940750        0.0000000
C       -2.0378260        1.0550740        0.0000000
O       -2.2515490       -0.1511200        0.0000000
N       -0.7705490        1.5908510        0.0000000
C       -0.4297110        2.9423090        0.0000000
O        0.7487060        3.2766670        0.0000000
C       -1.5555560        3.8687370        0.0000000
C       -2.8004790        3.3488970        0.0000000
C       -1.2661470        5.3360080        0.0000000
H        0.0000000        0.9240900        0.0000000
H       -3.6874090        3.9697630        0.0000000
H       -2.1966240        5.9052580        0.0000000
H       -0.6824120        5.6158220        0.8809150
H       -0.6824120        5.6158220       -0.8809150
H       -3.9820260        1.6374710        0.0000000
C        0.1948820       -3.5671690        0.0000000
C        1.5292090       -1.6337040        0.0000000
C        2.7102670       -2.3668780        0.0000000
C        2.5701750       -3.7560910        0.0000000
C        4.0475790       -1.6827640        0.0000000
H       -0.6309840       -1.5595930        0.0000000
H        3.4667200       -4.3663450        0.0000000
H        4.8486460       -2.4239550        0.0000000
H        4.1636700       -1.0461560       -0.8800960
H        4.1636700       -1.0461560        0.8800960
H        1.2161900       -5.4507680        0.0000000
C        0.2595220       -2.1825020        0.0000000
C        1.3197050       -4.3732370        0.0000000
F        1.6271440       -0.2757090        0.0000000
F       -1.0253360       -4.1472020        0.0000000
```

```
30
TA
N       -0.7514250       -0.7237240        0.0000000
C       -2.0926510       -0.7974700        0.0000000
N       -2.8502930       -1.8845640        0.0000000
C       -2.1057420       -3.0041490        0.0000000
C       -0.7150080       -3.0797770        0.0000000
C       -0.0179990       -1.8526170        0.0000000
N        1.3172710       -1.7699900        0.0000000
N       -0.2849630       -4.3896050        0.0000000
C       -1.3944190       -5.0862310        0.0000000
N       -2.5211880       -4.3071430        0.0000000
H       -2.5999420        0.1647380        0.0000000
H       -1.4573810       -6.1637870        0.0000000
H        1.7827840       -0.8596110        0.0000000
H        1.8643510       -2.6178820        0.0000000
N        0.0997570        4.1355230        0.0000000
C       -0.4812640        2.8911160        0.0000000
O       -1.6938560        2.7134470        0.0000000
N        0.4188840        1.8557750        0.0000000
C        1.7961020        1.9533770        0.0000000
O        2.4862240        0.9286390        0.0000000
C        2.3395340        3.3041670        0.0000000
C        1.4590740        4.3289570        0.0000000
C        3.8253150        3.4792580        0.0000000
H        0.0000000        0.8991090        0.0000000
H        1.7784400        5.3640230        0.0000000
H        4.0858370        4.5385470        0.0000000
H        4.2704740        3.0083810        0.8800830
H        4.2704740        3.0083810       -0.8800830
H       -3.4766780       -4.6386410        0.0000000
H       -0.5312600        4.9263660        0.0000000

28
TC
N       -1.5929670       -0.8265070        0.0000000
C       -2.7987690       -0.1940120        0.0000000
N       -3.9502080       -0.9849970        0.0000000
C       -3.9161120       -2.3411000        0.0000000
C       -2.7266670       -2.9844940        0.0000000
C       -1.5467420       -2.1622580        0.0000000
N       -0.3462330       -2.7463030        0.0000000
H        0.5004530       -2.1726150        0.0000000
H       -0.2684690       -3.7522690        0.0000000
N        2.1814490        2.9209630        0.0000000
C        0.9235760        2.3654140        0.0000000
O       -0.0921770        3.0435870        0.0000000
N        0.9199930        0.9852340        0.0000000
C        2.0417630        0.1715550        0.0000000
O        1.9241360       -1.0554990        0.0000000
C        3.3344300        0.8390570        0.0000000
C        3.3407750        2.1884350        0.0000000
C        4.5652850       -0.0121060        0.0000000
H        0.0000000        0.5129490        0.0000000
H        4.2548620        2.7695300        0.0000000
H        5.4614940        0.6094470        0.0000000
H        4.5864140       -0.6593880        0.8798300
H        4.5864140       -0.6593880       -0.8798300
H        2.2154670        3.9323190        0.0000000
O       -2.9272320        1.0318220        0.0000000
H       -2.6590830       -4.0623410        0.0000000
H       -4.8719420       -2.8497660        0.0000000
H       -4.8328960       -0.4894300        0.0000000
```

31
TG
N -1.0321300 1.2173730 0.0000000
C -1.6753580 2.4259410 0.0000000
N -2.9862810 2.5553280 0.0000000
C -3.6172110 1.3606020 0.0000000
C -3.0645090 0.0812190 0.0000000
C -1.6429740 -0.0326600 0.0000000
N -4.0516590 -0.8839190 0.0000000
C -5.1675580 -0.2047070 0.0000000
N -4.9644520 1.1547850 0.0000000
H -6.1626300 -0.6241500 0.0000000
N 3.7982070 0.3785420 0.0000000
C 2.4360690 0.3163480 0.0000000
O 1.7366420 1.3357080 0.0000000
N 1.9167690 -0.9485900 0.0000000
C 2.6464570 -2.1377140 0.0000000
O 2.0618390 -3.2141880 0.0000000
C 4.0983770 -1.9872310 0.0000000
C 4.6037600 -0.7372500 0.0000000
C 4.9391340 -3.2241910 0.0000000
H 0.8846330 -1.0285110 0.0000000
H 5.6678300 -0.5364830 0.0000000
H 5.9988410 -2.9660450 0.0000000
H 4.7263490 -3.8364230 0.8799420
H 4.7263490 -3.8364230 -0.8799420
H -5.6788270 1.8713650 0.0000000
H 4.2041750 1.3061640 0.0000000
N -0.8774630 3.5112580 0.0000000
H -1.2971360 4.4280130 0.0000000
H 0.1294330 3.4312710 0.0000000
O -0.9431150 -1.0564580 0.0000000
H 0.0000000 1.2151460 0.0000000

30
TT
N -3.2243240 1.1212870 0.0000000
C -1.9880640 0.5409760 0.0000000
O -1.8347970 -0.6823830 0.0000000
N -0.9423060 1.4231650 0.0000000
C -1.0323400 2.8133720 0.0000000
O -0.0136770 3.4945160 0.0000000
C -2.3875090 3.3559680 0.0000000
C -3.4157530 2.4834530 0.0000000
C -2.5529910 4.8425050 0.0000000
H 0.0000000 1.0027940 0.0000000
H -4.4501230 2.8040930 0.0000000
H -3.6103660 5.1102450 0.0000000
H -2.0777560 5.2831610 0.8799940
H -2.0777560 5.2831610 -0.8799940
H -4.0152740 0.4901280 0.0000000
N 2.0298040 -3.8541380 0.0000000
C 0.7545210 -3.3446850 0.0000000
O -0.2469390 -4.0465660 0.0000000
N 0.7064910 -1.9687870 0.0000000
C 1.7866770 -1.1063980 0.0000000
O 1.6032240 0.1152250 0.0000000
C 3.1034740 -1.7234080 0.0000000
C 3.1585300 -3.0731560 0.0000000
C 4.3042890 -0.8310240 0.0000000
H -0.2330020 -1.5437000 0.0000000
H 4.0942440 -3.6193410 0.0000000
H 5.2209160 -1.4219210 0.0000000
H 4.3035370 -0.1838590 -0.8801720
H 4.3035370 -0.1838590 0.8801720
H 2.1068950 -4.8635480 0.0000000

15
A
N 1.6650980 -1.1334900 0.0000000
C 0.6629780 -2.0255900 0.0000000
N -0.6466380 -1.8060870 0.0000000
C -0.9244070 -0.4936010 0.0000000
C 0.0000000 0.5474310 0.0000000
C 1.3597400 0.1736610 0.0000000
N 2.3511810 1.0798270 0.0000000
N -0.6294520 1.7753490 0.0000000
C -1.9046420 1.4750390 0.0000000
N -2.1444830 0.1265660 0.0000000
H 0.9728740 -3.0653350 0.0000000
H -2.7148530 2.1892560 0.0000000
H 3.3129290 0.7739460 0.0000000
H 2.1478110 2.0679790 0.0000000
H -3.0507300 -0.3226450 0.0000000

```
13
C
N        0.0000000        1.0510440        0.0000000
C       -1.2081490        0.4283840        0.0000000
N       -1.2158660       -0.9694280        0.0000000
C       -0.0827690       -1.7144320        0.0000000
C        1.1273890       -1.1066500        0.0000000
C        1.1150860        0.3294890        0.0000000
N        2.2800820        0.9956710        0.0000000
H        2.2754230        2.0052200        0.0000000
H        3.1667400        0.5157450        0.0000000
O       -2.2889950        1.0235530        0.0000000
H        2.0494560       -1.6696060        0.0000000
H       -0.2126290       -2.7886700        0.0000000
H       -2.1258850       -1.4128690        0.0000000

15
F
C        1.2590890       -0.9960940        0.0000000
C        0.0000000        0.9951230        0.0000000
C       -1.2066010        0.3024500        0.0000000
C       -1.1213880       -1.0904140        0.0000000
C       -2.5144610        1.0413760        0.0000000
H        2.1578180        0.9710520        0.0000000
H       -2.0400820       -1.6669280        0.0000000
H       -3.3452550        0.3342770        0.0000000
H       -2.6037420        1.6823130        0.8800320
H       -2.6037420        1.6823130       -0.8800320
H        0.1657230       -2.8371990        0.0000000
F       -0.0478310        2.3457930        0.0000000
F        2.4564960       -1.6211860        0.0000000
C        1.2448660        0.3900160        0.0000000
C        0.1037110       -1.7570050        0.0000000

16
G
N       -1.4301950       -0.8650580        0.0000000
C       -0.3618190       -1.7288710        0.0000000
N        0.8900170       -1.3257570        0.0000000
C        1.0054250        0.0214960        0.0000000
C        0.0000000        0.9815040        0.0000000
C       -1.3609520        0.5411860        0.0000000
N        0.5331020        2.2545600        0.0000000
C        1.8260270        2.0652600        0.0000000
N        2.1672360        0.7341920        0.0000000
H        2.5791570        2.8396910        0.0000000
H        3.1027890        0.3499540        0.0000000
N       -0.6390730       -3.0460650        0.0000000
H        0.1325290       -3.6960280        0.0000000
H       -1.5781920       -3.4132750        0.0000000
O       -2.3953050        1.2015100        0.0000000
H       -2.3735440       -1.2389710        0.0000000

15
T
N        0.1553230       -1.6604050        0.0000000
C        1.3454480       -0.9789580        0.0000000
O        2.4370330       -1.5284980        0.0000000
N        1.1936950        0.3910690        0.0000000
C        0.0000000        1.1114640        0.0000000
O        0.0231750        2.3361750        0.0000000
C       -1.2120480        0.3000320        0.0000000
C       -1.0724340       -1.0418020        0.0000000
C       -2.5358970        0.9976890        0.0000000
H        2.0533710        0.9300960        0.0000000
H       -1.9233960       -1.7113450        0.0000000
H       -3.3497310        0.2704500        0.0000000
H       -2.6370930        1.6371400        0.8800760
H       -2.6370930        1.6371400       -0.8800760
H        0.2187480       -2.6700970        0.0000000
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30
LA
N       -0.6276780       -1.2954290        0.0000000
C       -1.9373280       -1.5871110        0.0000000
N       -2.5201580       -2.7801350        0.0000000
C       -1.6138910       -3.7702400        0.0000000
C       -0.2285930       -3.6260900        0.0000000
C        0.2604550       -2.3031690        0.0000000
N        1.5727140       -2.0193680        0.0000000
N        0.4021080       -4.8532890        0.0000000
C       -0.5847840       -5.7146870        0.0000000
N       -1.8200110       -5.1233810        0.0000000
H       -2.5978370       -0.7246150        0.0000000
H       -0.4761880       -6.7889220        0.0000000
H        1.8848570       -1.0567600        0.0000000
H        2.2593950       -2.7590260        0.0000000
C       -0.8962520        2.8296520        0.0000000
C        1.4532360        2.4725320        0.0000000
C        1.7139870        3.8452750        0.0000000
C        0.6030390        4.6930230        0.0000000
C        3.1147790        4.3876880        0.0000000
H        0.0000000        0.8660030        0.0000000
H        0.7665550        5.7656230        0.0000000
H        3.0993050        5.4778430        0.0000000
H        3.6657710        4.0443320        0.8800160
H        3.6657710        4.0443320       -0.8800160
H       -2.7137780       -5.5971550        0.0000000
H       -1.5480900        4.8800390        0.0000000
Cl       2.8019860        1.3557020        0.0000000
Cl      -2.5183350        2.1806450        0.0000000
C        0.1703240        1.9403600        0.0000000
C       -0.7010790        4.2047050        0.0000000

28
LC
N       -1.8032500       -1.2275430        0.0000000
C       -2.6337660       -0.1518980        0.0000000
N       -4.0103610       -0.3898510        0.0000000
C       -4.5437580       -1.6368780        0.0000000
C       -3.7286800       -2.7179080        0.0000000
C       -2.3168400       -2.4518910        0.0000000
N       -1.4577380       -3.4832190        0.0000000
H       -0.4647480       -3.2971190        0.0000000
H       -1.7787530       -4.4392180        0.0000000
C        2.6219710        2.7730910        0.0000000
C        1.3154320        2.3005070        0.0000000
Cl      -0.0012860        3.4469680        0.0000000
C        1.0288700        0.9388320        0.0000000
C        2.1044690        0.0575130        0.0000000
Cl       1.7691470       -1.6614050        0.0000000
C        3.4397700        0.4750750        0.0000000
C        3.6664740        1.8535520        0.0000000
C        4.5772350       -0.5049900        0.0000000
H        0.0000000        0.5822830        0.0000000
H        4.6903360        2.2134070        0.0000000
H        5.5333990        0.0197070        0.0000000
H        4.5343890       -1.1521370        0.8796660
H        4.5343890       -1.1521370       -0.8796660
H        2.8179450        3.8385750        0.0000000
O       -2.2330830        1.0156140        0.0000000
H       -4.1137280       -3.7274020        0.0000000
H       -5.6238250       -1.6991580        0.0000000
H       -4.6060030        0.4279820        0.0000000
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31
LG
N -0.3168920 -2.2492000 0.0000000
C -0.6616990 -3.5791810 0.0000000
N 0.2218960 -4.5541960 0.0000000
C 1.4958870 -4.1040350 0.0000000
C 1.9545590 -2.7906730 0.0000000
C 0.9916420 -1.7362090 0.0000000
N 3.3339980 -2.7494350 0.0000000
C 3.6959400 -4.0049170 0.0000000
N 2.6250860 -4.8665340 0.0000000
H 4.7115410 -4.3704500 0.0000000
C -2.8880010 3.0872910 0.0000000
C -2.0356870 1.9914980 0.0000000
Cl -2.7229520 0.3817610 0.0000000
C -0.6546050 2.1330020 0.0000000
C -0.1404840 3.4247170 0.0000000
Cl 1.5975660 3.6080180 0.0000000
C -0.9470400 4.5667220 0.0000000
C -2.3295630 4.3624770 0.0000000
C -0.3592560 5.9484850 0.0000000
H 0.0000000 1.2648930 0.0000000
H -2.9820610 5.2291430 0.0000000
H -1.1488490 6.7016230 0.0000000
H 0.2724980 6.1020500 0.8789730
H 0.2724980 6.1020500 -0.8789730
H 2.6647350 -5.8768290 0.0000000
H -3.9623210 2.9487830 0.0000000
N -1.9761890 -3.8699700 0.0000000
H -2.2550450 -4.8392730 0.0000000
H -2.6948100 -3.1632550 0.0000000
O 1.1694270 -0.5193790 0.0000000
H -1.0474830 -1.5396660 0.0000000

30
LT
N -3.2598850 1.8991270 0.0013030
C -2.0448110 1.2668830 0.0006800
O -0.9746380 1.8625590 0.0009490
N -2.1353210 -0.1062460 -0.0003450
C -3.2970380 -0.8767460 -0.0007160
O -3.2194820 -2.0993070 -0.0017100
C -4.5432090 -0.1182950 0.0001030
C -4.4601240 1.2283480 0.0010440
C -5.8386990 -0.8681700 -0.0003090
H -1.2508850 -0.6122780 -0.0008040
H -5.3382750 1.8611140 0.0016770
H -6.6799460 -0.1731530 0.0001680
H -5.9154160 -1.5099620 -0.8810220
H -5.9153500 -1.5111160 0.8795660
H -3.2390420 2.9107160 0.0021100
C 3.0300050 1.2459990 -0.0006050
C 2.1508970 -0.9635130 0.0003680
C 3.4282010 -1.5300690 0.0004870
C 4.5049400 -0.6390510 0.0000640
C 3.6351490 -3.0173020 0.0009960
H 0.9127860 0.8126960 -0.0001380
H 5.5135850 -1.0394290 0.0001520
H 4.6990320 -3.2556720 0.0010540
H 3.1743300 -3.4748990 0.8806110
H 3.1742790 -3.4755170 -0.8782720
H 5.1724920 1.4133570 -0.0008750
C 1.9222930 0.4074550 -0.0001070
C 4.3237590 0.7404430 -0.0004850
Cl 0.7552920 -2.0240520 0.0007500
Cl 2.7825690 2.9735850 -0.0015720

15
L
C 0.5430250 -1.3696140 0.0000000
C 0.0000000 0.9517030 0.0000000
C -1.3710010 0.6798740 0.0000000
C -1.7447230 -0.6669540 0.0000000
C -2.3965310 1.7765240 0.0000000
H 2.0202670 0.2046850 0.0000000
H -2.8014860 -0.9128080 0.0000000
H -3.4028440 1.3558970 0.0000000
H -2.2822230 2.4159030 0.8788960
H -2.2822230 2.4159030 -0.8788960
H -1.1183710 -2.7327620 0.0000000
Cl 0.5420330 2.6118140 0.0000000
Cl 1.7358040 -2.6425720 0.0000000
C 0.9671910 -0.0468570 0.0000000
C -0.8073530 -1.6953300 0.0000000

30
23ClA
C 0.9836380 -3.9852620 0.0000000
C 2.3625390 -4.1782370 0.0000000
C 0.5428310 -2.6449040 0.0000000
N 0.3104440 -5.1904740 0.0000000
N 3.3032170 -3.2213080 0.0000000
N 2.5219810 -5.5376820 0.0000000
N 1.4643540 -1.6670500 0.0000000
N -0.7606220 -2.3197290 0.0000000
C 1.2673700 -6.0856370 0.0000000
C 2.7619340 -2.0084840 0.0000000
H 3.3988950 -6.0413100 0.0000000
H -1.0390460 -1.3483970 0.0000000
H -1.4697330 -3.0376670 0.0000000
H 1.1222840 -7.1558530 0.0000000
H 3.4589860 -1.1759860 0.0000000
Cl 0.0000000 1.1064240 0.0000000
C -1.0519890 2.4928480 0.0000000
C -0.5387520 3.7911410 0.0000000
C -2.4276570 2.2892780 0.0000000
Cl 1.1739950 4.0838170 0.0000000
C -1.4121920 4.8731380 0.0000000
C -3.3144990 3.3671830 0.0000000
H -2.8054570 1.2715620 0.0000000
C -2.7866360 4.6593980 0.0000000
H -1.0073200 5.8785720 0.0000000
C -4.8001580 3.1314450 0.0000000
H -3.4582060 5.5112610 0.0000000
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H -5.1062980 2.5630790 0.8818370
H -5.1062980 2.5630790 -0.8818370

28
23ClC
N -0.7469750 -2.6752580 0.0000000
C -1.9699760 -3.2678110 0.0000000
N -2.0128250 -4.6651760 0.0000000
C -0.8992020 -5.4391730 0.0000000
C 0.3257730 -4.8616740 0.0000000
C 0.3503760 -3.4251400 0.0000000
N 1.5323410 -2.7890280 0.0000000
H 1.5539510 -1.7778650 0.0000000
H 2.4053390 -3.2934930 0.0000000
C 0.1852420 4.3372070 0.0000000
C -0.3089050 3.0374420 0.0000000
Cl -2.0284000 2.7851500 0.0000000
C 0.5818580 1.9626810 0.0000000
C 1.9528600 2.1954340 0.0000000
C 2.4611170 3.4962070 0.0000000
C 1.5581310 4.5606560 0.0000000
C 3.9483670 3.7240330 0.0000000
H 1.9299330 5.5799740 0.0000000
H 4.1808250 4.7899660 0.0000000
H 4.4114440 3.2729430 0.8812170
H 4.4114440 3.2729430 -0.8812170
H -0.5119140 5.1670990 0.0000000
O -3.0365780 -2.6466090 0.0000000
H 1.2348960 -5.4451120 0.0000000
H -1.0560500 -6.5101660 0.0000000
H -2.9344440 -5.0845070 0.0000000
H 2.6283550 1.3456920 0.0000000
Cl 0.0000000 0.3232300 0.0000000

31
23ClG
N -0.5199880 1.7856800 0.0000000
C 0.1677190 2.9754310 0.0000000
N -0.4173830 4.1529990 0.0000000
C -1.7664640 4.0643530 0.0000000
C -2.5612900 2.9243730 0.0000000
C -1.9218060 1.6454020 0.0000000
N -3.9004510 3.2555500 0.0000000
C -3.9110350 4.5621340 0.0000000
N -2.6478120 5.1035150 0.0000000
H -4.7914470 5.1861320 0.0000000
C 3.2369920 -3.1676120 0.0000000
C 2.1852190 -2.2595930 0.0000000
Cl 2.5493190 -0.5556560 0.0000000
C 0.8689060 -2.7209400 0.0000000
C 0.6151200 -4.0883200 0.0000000
C 1.6609750 -5.0134160 0.0000000
C 2.9720860 -4.5330990 0.0000000
C 1.3724020 -6.4901660 0.0000000
H 3.7998430 -5.2345360 0.0000000
H 2.3011400 -7.0626290 0.0000000
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H 4.2556860 -2.7978660 0.0000000
N 1.5118510 2.8988360 0.0000000
H 2.0431090 3.7559230 0.0000000
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H 0.0000000 0.9098430 0.0000000
H -0.4159820 -4.4279200 0.0000000
Cl -0.4695080 -1.6129240 0.0000000
H 0.7931820 -6.7754380 0.8817990
H 0.7931820 -6.7754380 -0.8817990

30
23ClT
N -3.4857360 -2.9652520 0.0000000
C -2.1334930 -2.7369710 0.0000000
O -1.2967940 -3.6278280 0.0000000
N -1.8012920 -1.3991930 0.0000000
C -2.6714270 -0.3123750 0.0000000
O -2.2274690 0.8314550 0.0000000
C -4.0882510 -0.6522380 0.0000000
C -4.4223030 -1.9597480 0.0000000
C -5.0871480 0.4618250 0.0000000
H -0.8025120 -1.2003160 0.0000000
H -5.4529970 -2.2914790 0.0000000
H -6.1029860 0.0629440 0.0000000
H -4.9574920 1.0963610 0.8797280
H -4.9574920 1.0963610 -0.8797280
H -3.7778380 -3.9339020 0.0000000
C 3.3965160 0.9659480 0.0000000
C 1.0319880 1.4692970 0.0000000
C 1.3028840 2.8363060 0.0000000
C 2.6382700 3.2542150 0.0000000
C 0.1770310 3.8343140 0.0000000
H 2.8707290 4.3140930 0.0000000
H 0.2313420 4.4786050 0.8808220
H 0.2313420 4.4786050 -0.8808220
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H 4.7095400 2.6553850 0.0000000
C 2.0705290 0.5418130 0.0000000
C 3.6753770 2.3315040 0.0000000
Cl 4.7132400 -0.1670630 0.0000000
Cl 1.6786220 -1.1558100 0.0000000
H 0.0000000 1.1253500 0.0000000

15
23Cl
C 0.8364920 -0.4452570 0.0000000
C -1.3811480 0.5118510 0.0000000
C -1.9548510 -0.7615770 0.0000000
C -1.1066190 -1.8702870 0.0000000
C -3.4524450 -0.9147200 0.0000000
H -1.5285260 -2.8700040 0.0000000
H -3.7371490 -1.9678150 0.0000000
H -3.8912820 -0.4394880 0.8808970
H -3.8912820 -0.4394880 -0.8808970
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C 0.0000000 0.6721070 0.0000000
C 0.2762510 -1.7179060 0.0000000
Cl 0.6595150 2.2797750 0.0000000
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