## Thermodynamics of Folding

## Thermodynamics of Folding: $\Delta G = \Delta H - T \Delta S$

- $\Delta G = 1.56 \text{ kcal/mol at } 54 \,^{\circ}\text{C}$
- $\Delta H = -35.10 \text{ kcal/mol}$
- $\Delta S = -112 \text{ cal/}(K \cdot \text{mol})$
- $T_m = 40$  °C assuming a 2 state model.
- linear DNA folding.
- Ionic conditions: [Na<sup>+</sup>] = 0.05 M, [Mg<sup>++</sup>] = 0 M.
- Standard errors are roughly  $\pm 5\%$ ,  $\pm 10\%$ ,  $\pm 11\%$  and 2-4 °C for free energy, enthalpy, entropy and  $T_m$ , respectively.

Structure 2  $0F_CGTGT_end$  $\Delta G = 1.56$ 

Structural element	δG	Information
External loop	-0.37	1 ss bases & 1 closing helices.
Stack	-0.70	External closing pair is a <sup>2</sup> -T <sup>31</sup>
Stack	-0.70	External closing pair is c <sup>3</sup> -G <sup>30</sup>
Stack	-0.70	External closing pair is a <sup>4</sup> -T <sup>29</sup>
Stack	-1.35	External closing pair is c <sup>5</sup> -G <sup>28</sup>
Helix	-3.45	5 base pairs.
Hairpin loop	5.38	Closing pair is g <sup>6</sup> -C <sup>27</sup>