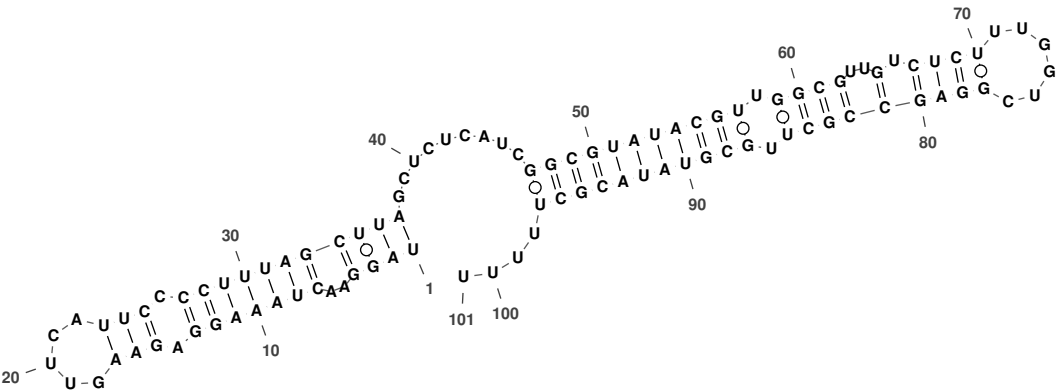

[initially -35.70] 5 (E=-35.70 kcal/mol)