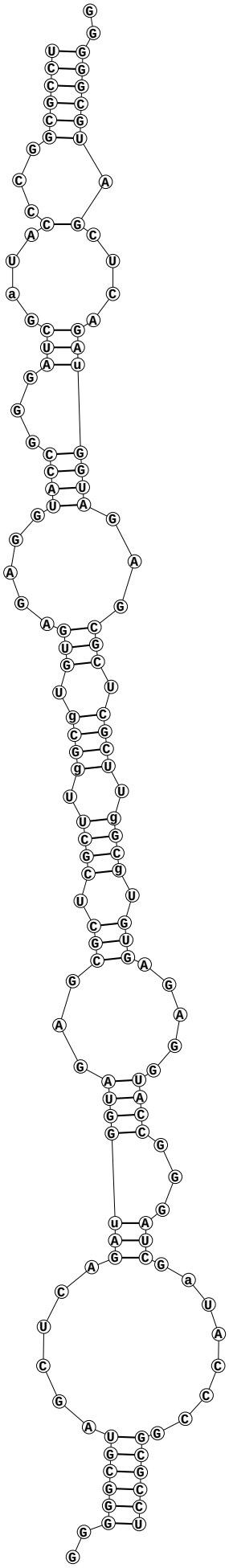

ENERGY = -46.1 ";exitmd5’w4p1t1_md5...