22nd March, 2018

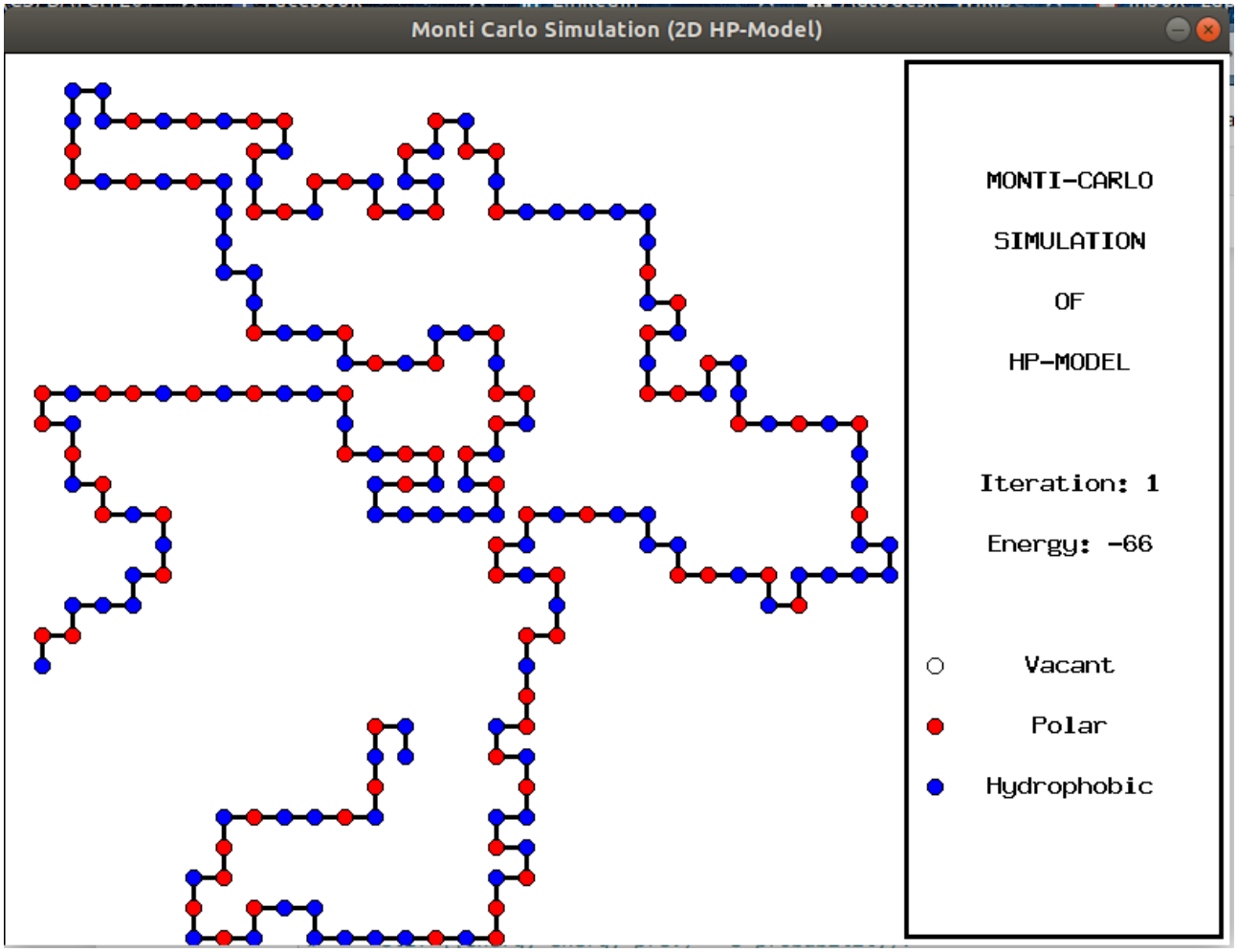
3D Modeling & Simulations in Bioinformatics (CS06F)

ASSIGNMENT: 01

METROPOLIS MONTI CARLO SIMULATION

OF

2D Hyperbolic-Polar model of Proteins



Name: ZEESHAN ALI, **Roll No:** I14-1623

Instructor: PROF. HAMMAD NAVEED

Main Block

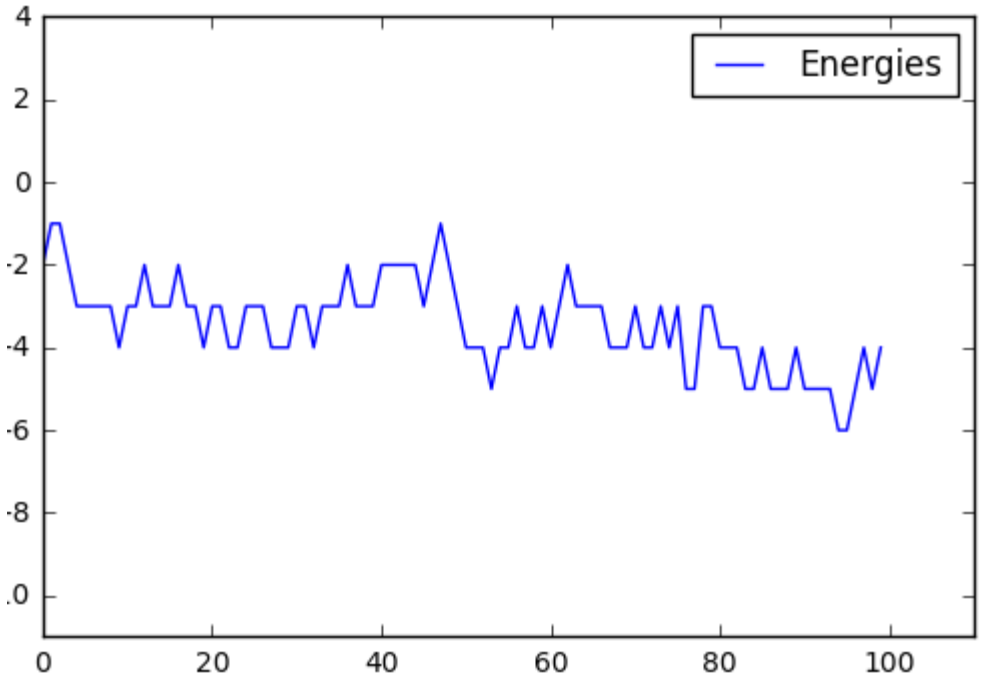
```
probability = 0.5
NUM_OF_ITERATIONS = 1000
hyper_parameter = 6

energy = calculate_Energy(residue_position)

energies = []
rpositions = []
mutation_type = []

for iteration in range(NUM_OF_ITERATIONS):
    rp_, m_type = random_mutation(residue_position)
    residue_position_updated = np.copy(rp_)

    if (residue_position_updated != []):
        energy_updated = calculate_Energy(residue_position_updated)
        if (energy_updated < energy):
            energy = energy_updated
            residue_position = np.copy(residue_position_updated)
        elif ((energy_updated-energy) < hyper_parameter*probability):
            energy = energy_updated
            residue_position = np.copy(residue_position_updated)

    energies.append(energy)
    rpositions.append(residue_position)
    mutation_type.append(m_type)
```

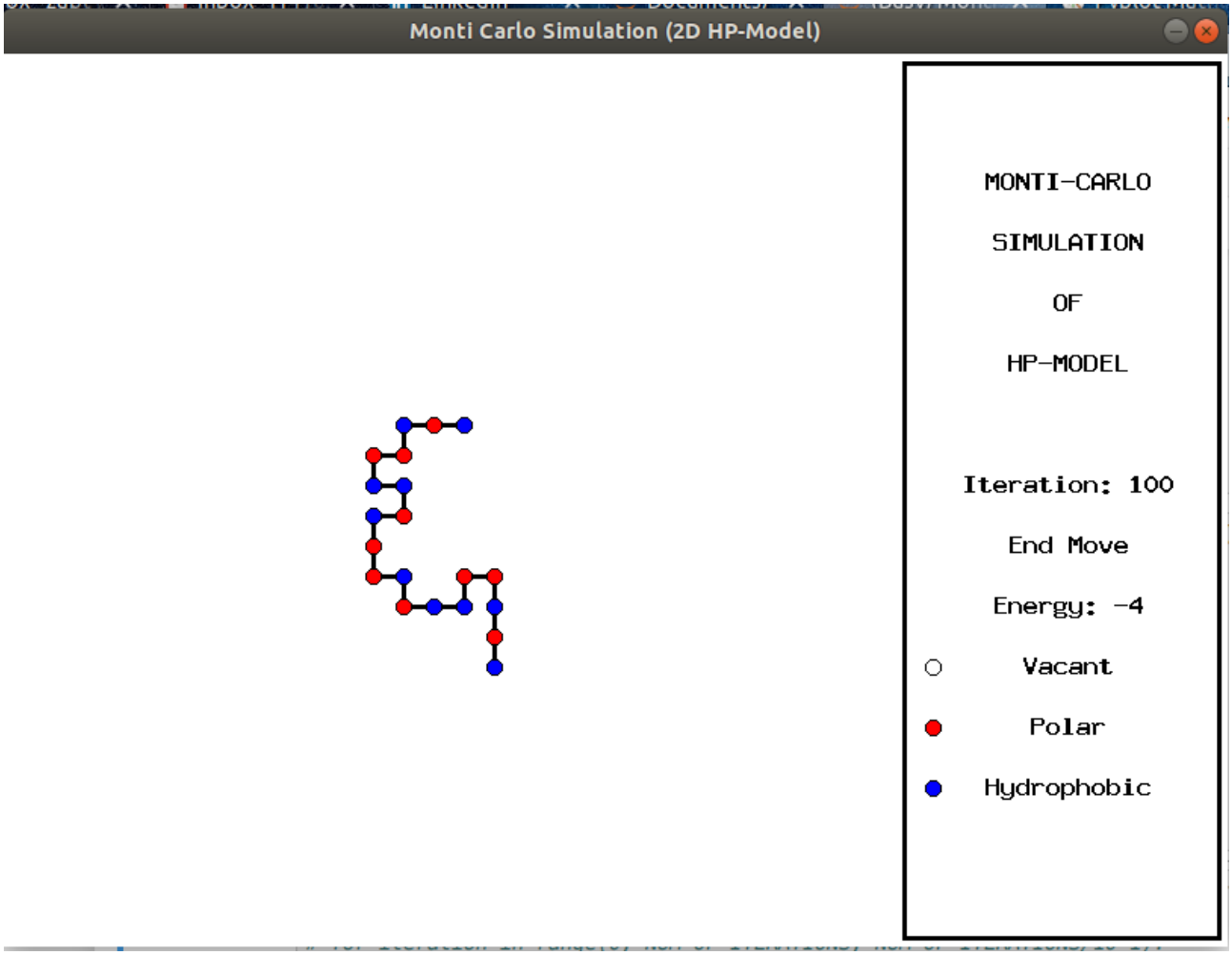
Results of the algorithm on different protein sequences

(Observed that the performance was better for longer sequences)

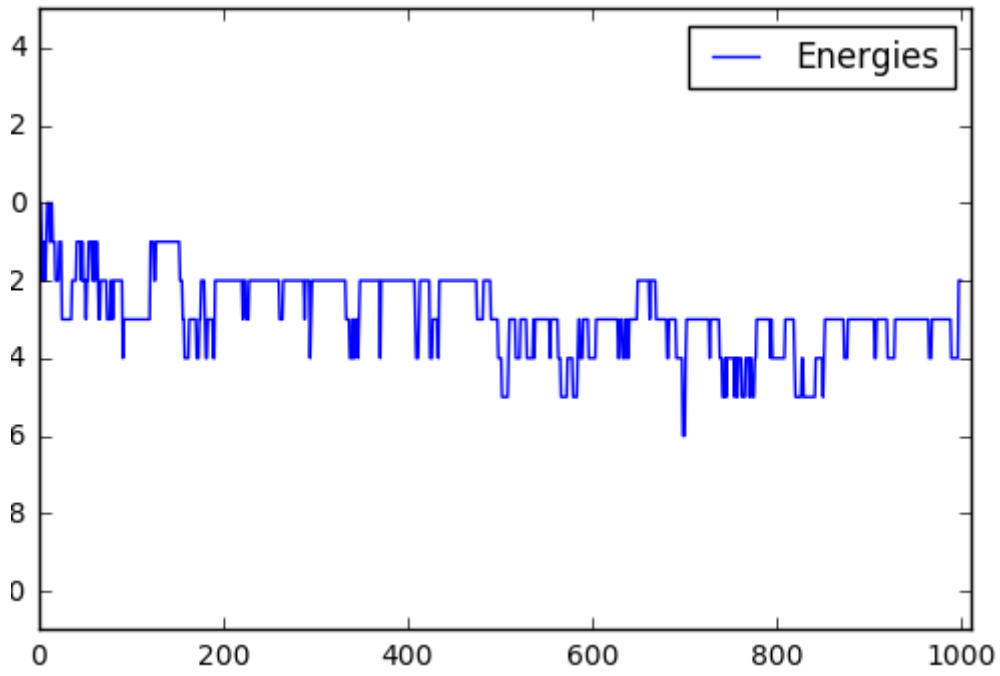
S#	Length	Sequence	Energy
01	20	HPHPPHHPHPPHPHHPPHPH	-4
02	24	PPHPPHHPPPPHHPPPPHHPPPPHH	-2
03	25	PPHPPHHPPPPHHPPPPHHPPPPHH	-2
04	36	PPPHHPPHHPPPPPHHHHHHHPPHHPPPPHHPPHPP	-5
05	48	PPHPPHHPPHHPPPPPHHHHHHHHHHPPPPPPPPHHPPHHHPPHHHH	-16
06	51	HHPHPHPHPHHHHPHPPPHPPPHPPPPHPPPHPPPHPHPHHHHHPHPHPHH	-16
07	60	PPHHHPHHHHHHHHPPPHHHHHHHHHHHPHPPPHHHHHHHHHHHHHPPPPHHHHHHPHHPHP	-31
08	64	HHHHHHHHHHHHPHPHPPHHPPHHPPHPPHHPPHHPPHPPHHPPHHPPHPHPHHHHHHHHHH	-40
09	85	HHHHPPPPHHHHHHHHHHHHPPPPPPHHHHHHHHHHHHPPPHHHHHHHHHHHHPPPHHHHHHHHHHHPPPHPPH HPPHHPPHPH	-59
10	100	PPPHHPPHHHPPHHHPHHPHHPHHHHPPPPPPPHHHHHHPPHHHHHPPPPPPPPPHPHHPHHHHHHHHHHP PHHHPHHPHPPHPHHHPPPPPPHHH	-33
11	100	PPPPPPHPHHPPPPPHHHPHHHHHPHHPPPPHHPPHHPHHHHHPHHHHHHHHHHPHHPHHHHHHPPPPPPPPPP PHHHHHHHPPHPHHHPPPPPPHPHH	

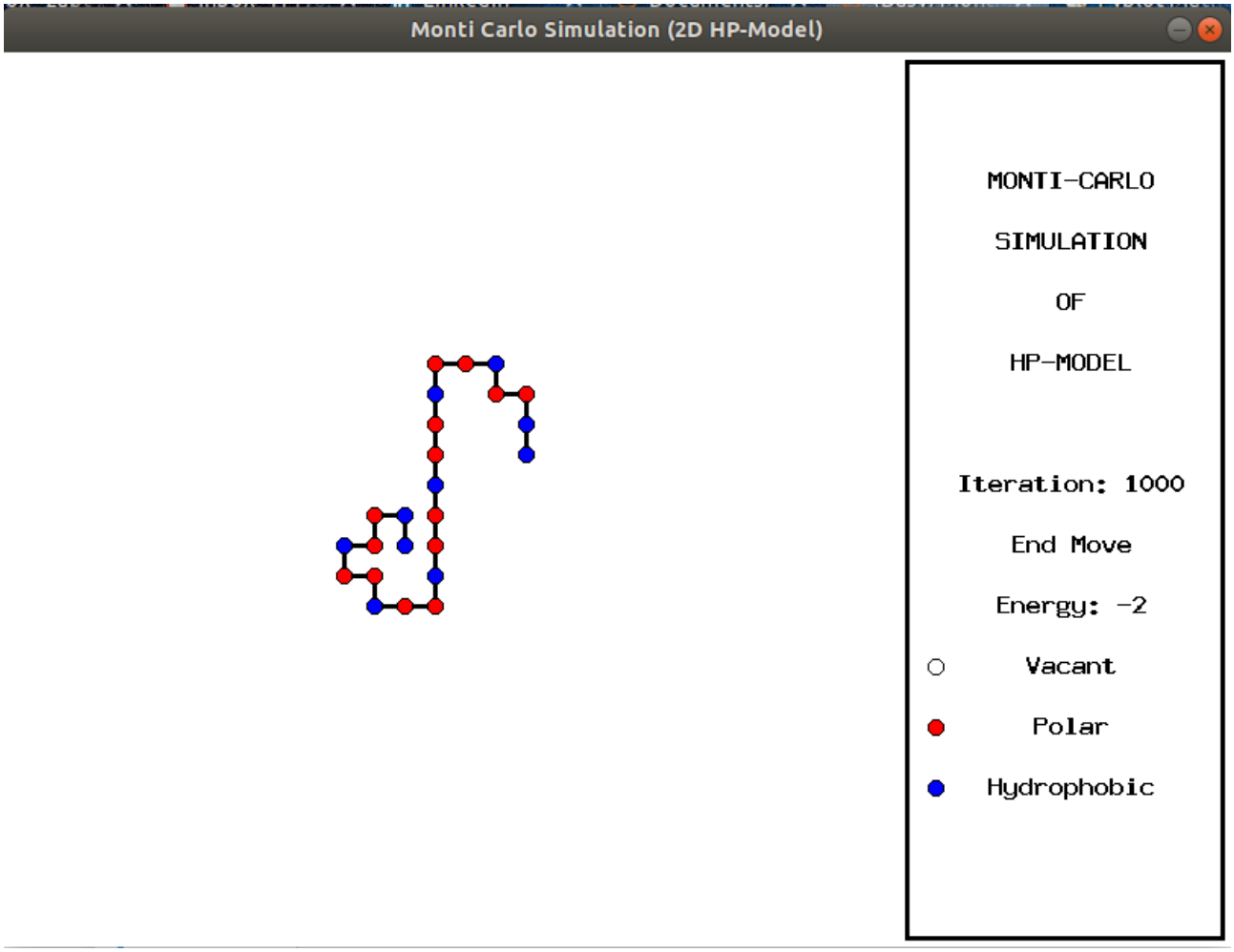
➔ STRING_01 = "HP"*2+"P"+"H"*2+"P"+"H"+"P"*2+"H"+"P"+"H"*2+"P"*2+"HPH"



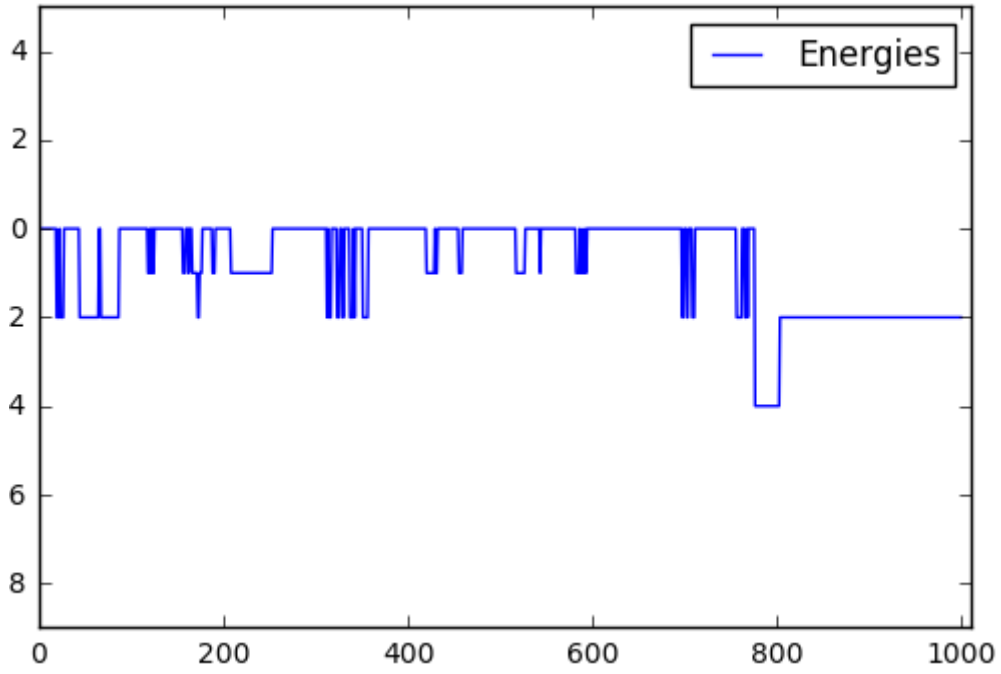


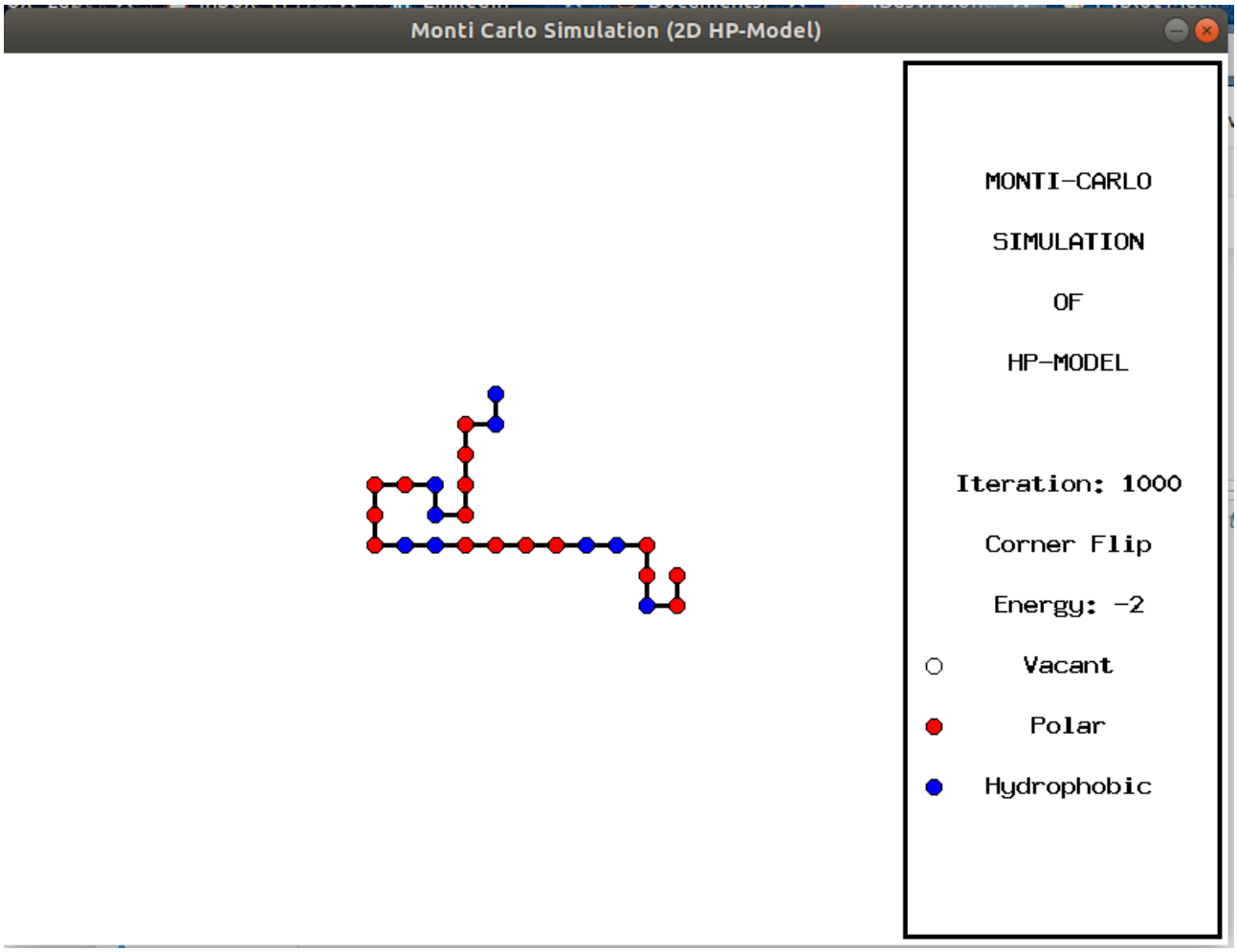
➔ STRING_02 = "H"*2+("P"*2+"H")*7+"H"



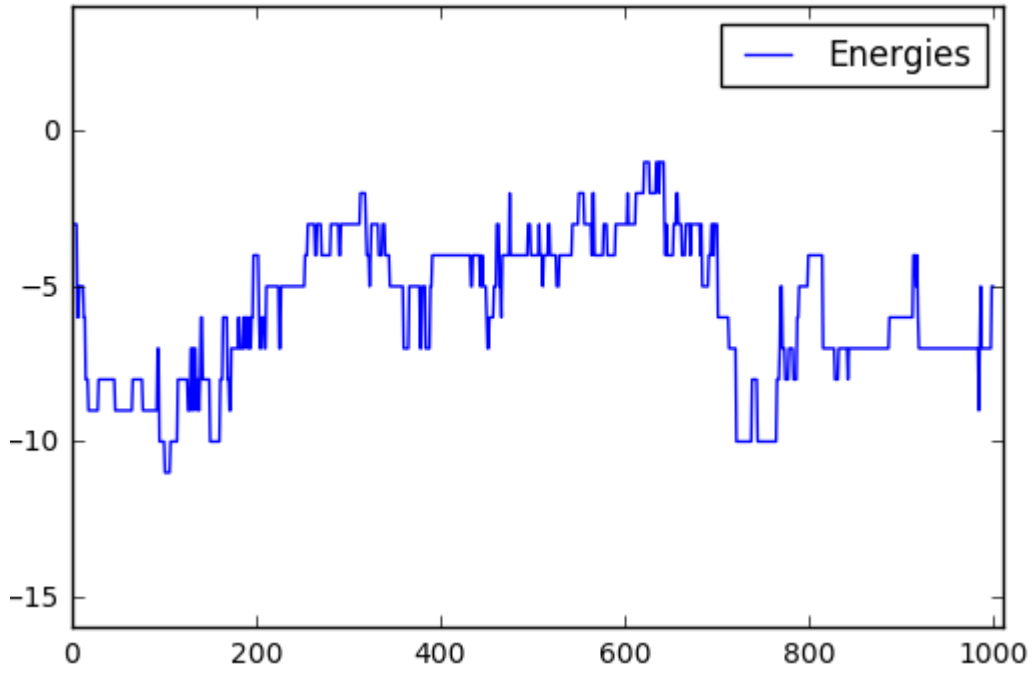


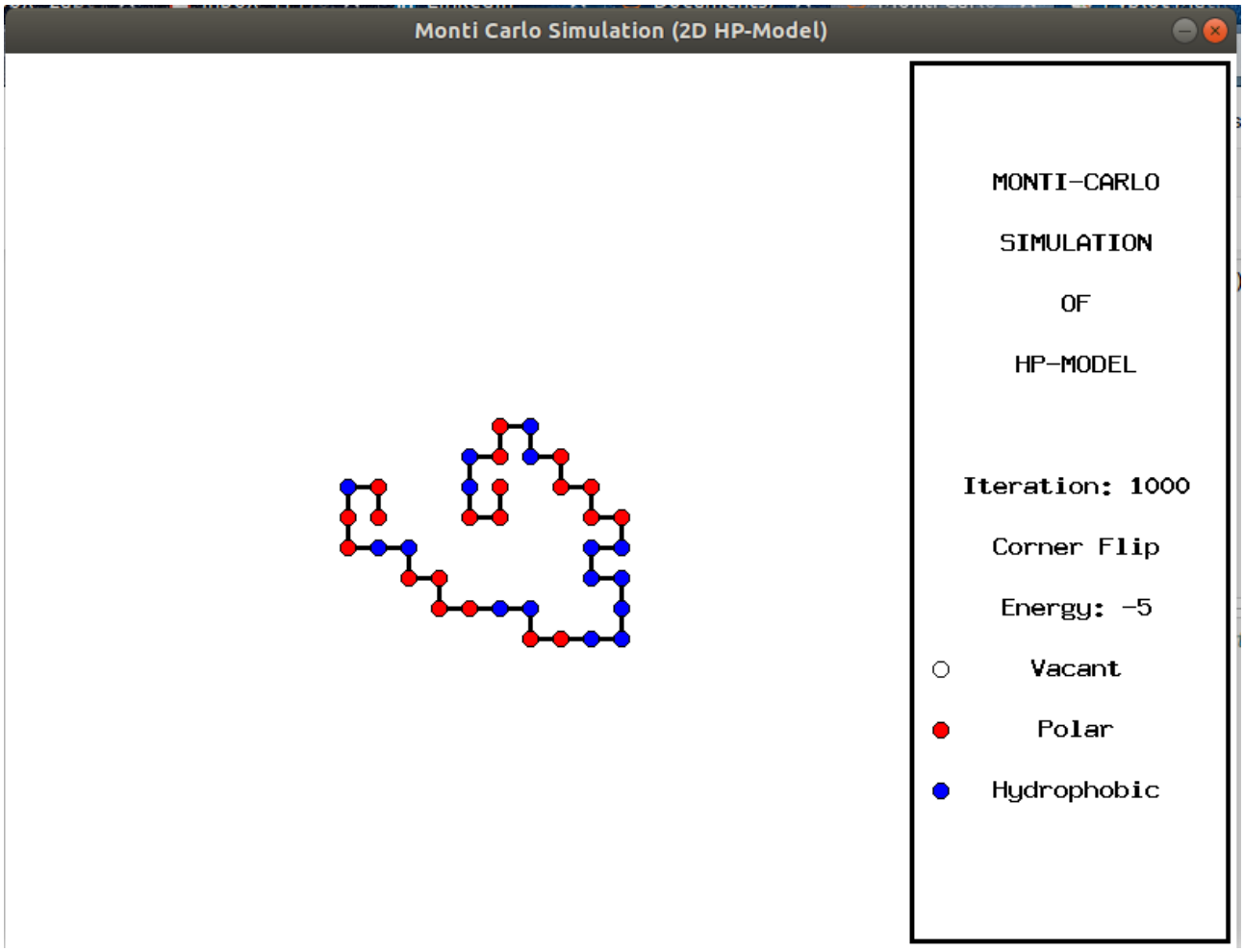
➔ STRING_03 = "P"*2+"H"+"P"*2+("H"*2+"P"*4)*3+"H"*2



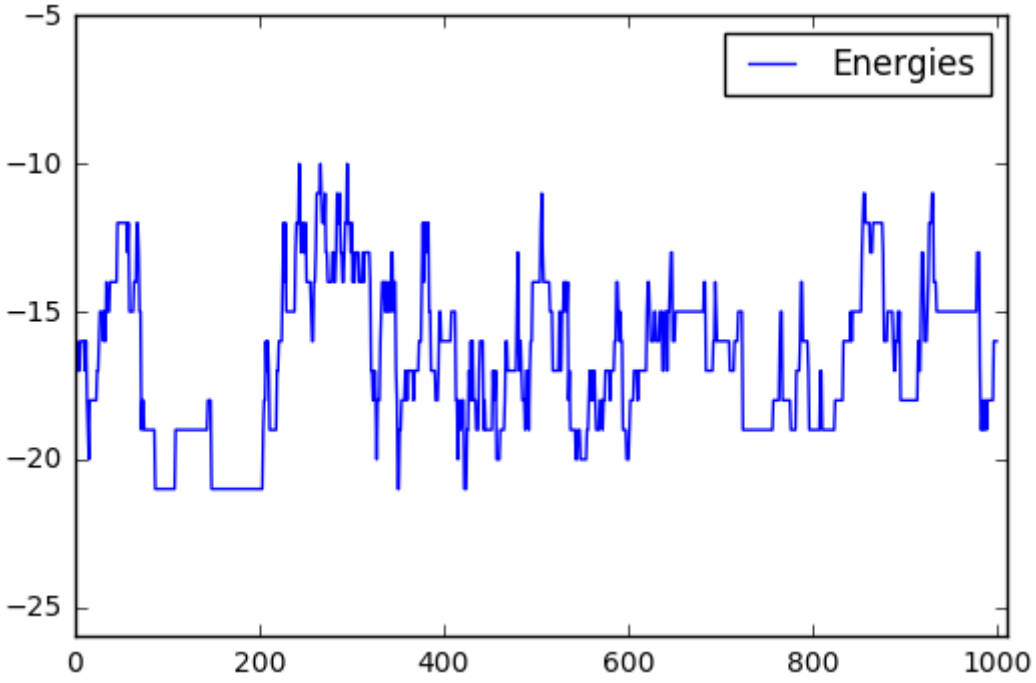


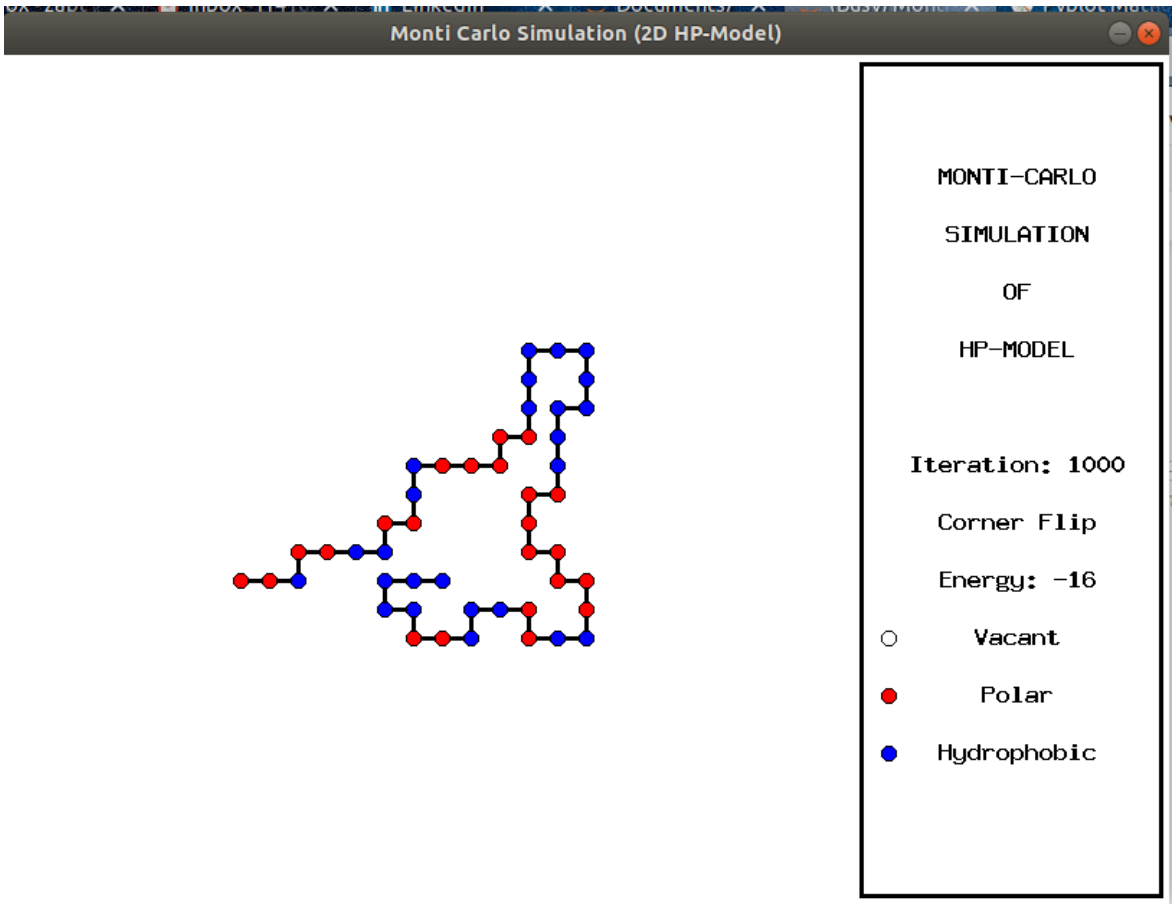
➔ STRING_04 = "PPPHH"+"P"*2+"H"*2+"P"*5+"H"*7+"P"*2+"H"*2+"P"*4+"HHPPHPP”



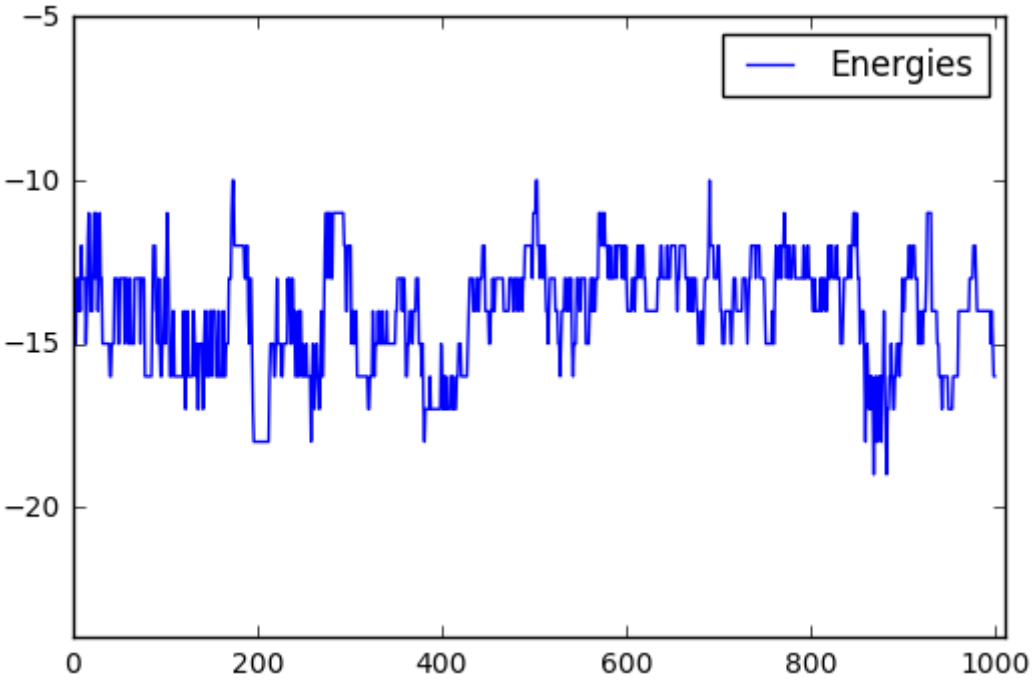


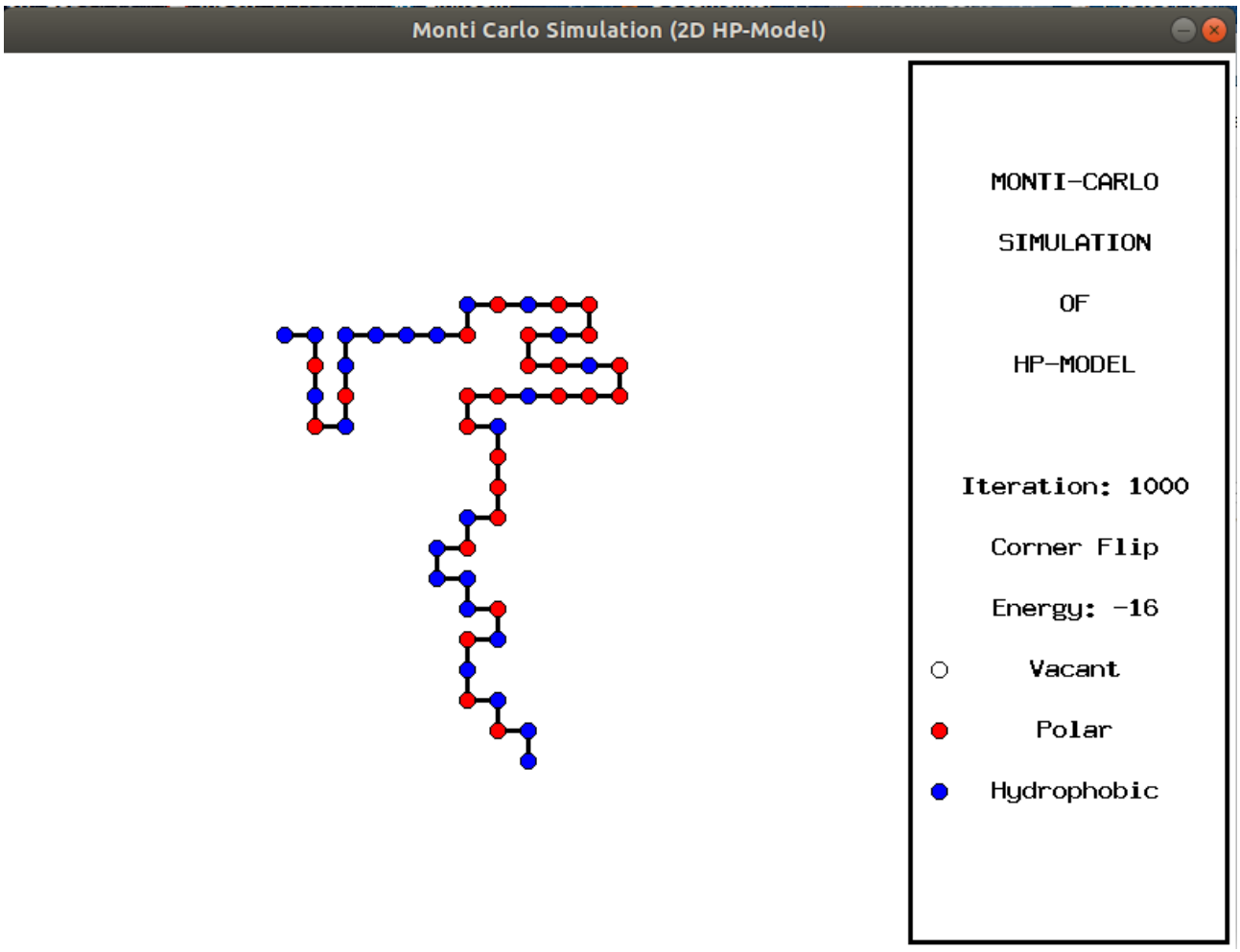
➔ STRING_05 = "P"*2+"H"+("P"*2+"H"*2)*2+"P"*5+"H"*10+"P"*6+
("P"*2+"H"*2)*2+"H"+"P"*2+"H"*5



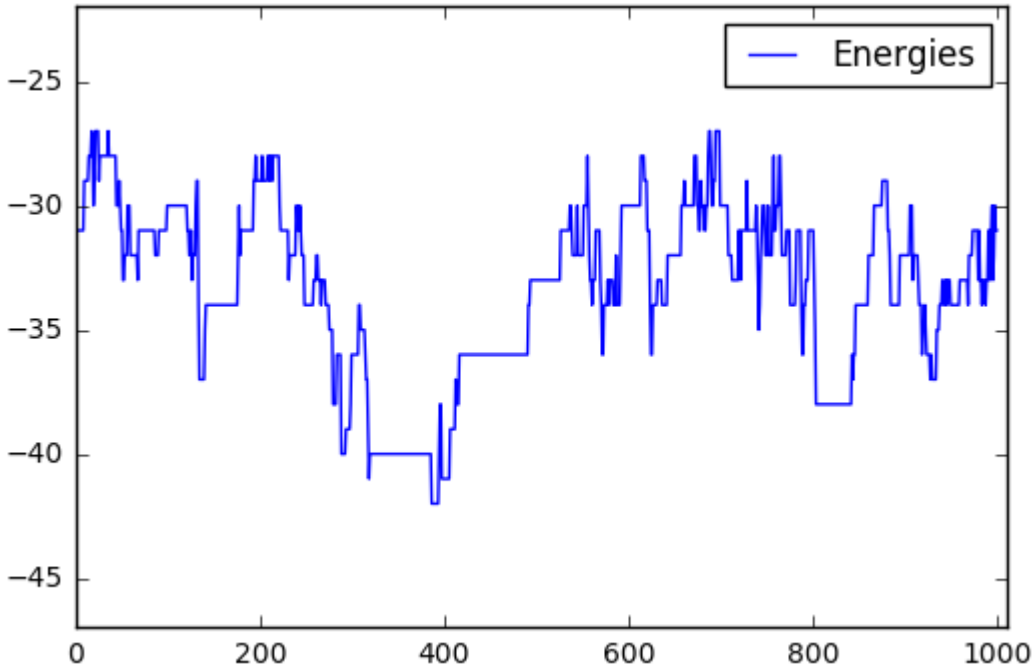


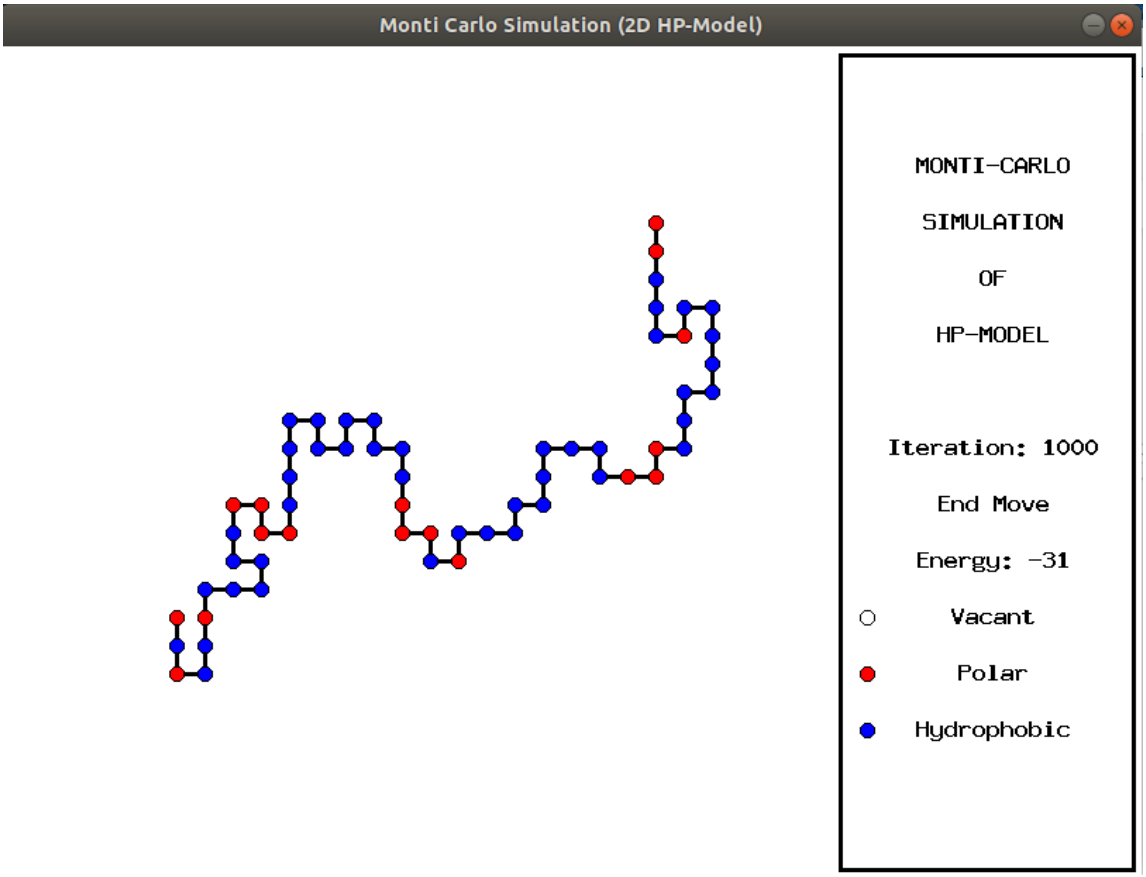
➔ STRING_06 = "H"*2+"PH"*3+"P"+"H"*4+"PH"+("P"*3+"H")*2+"P"*4+"H"+("P"*3+"H")*2+"PHP"+"H"*4+"HP"*3+"H"*2



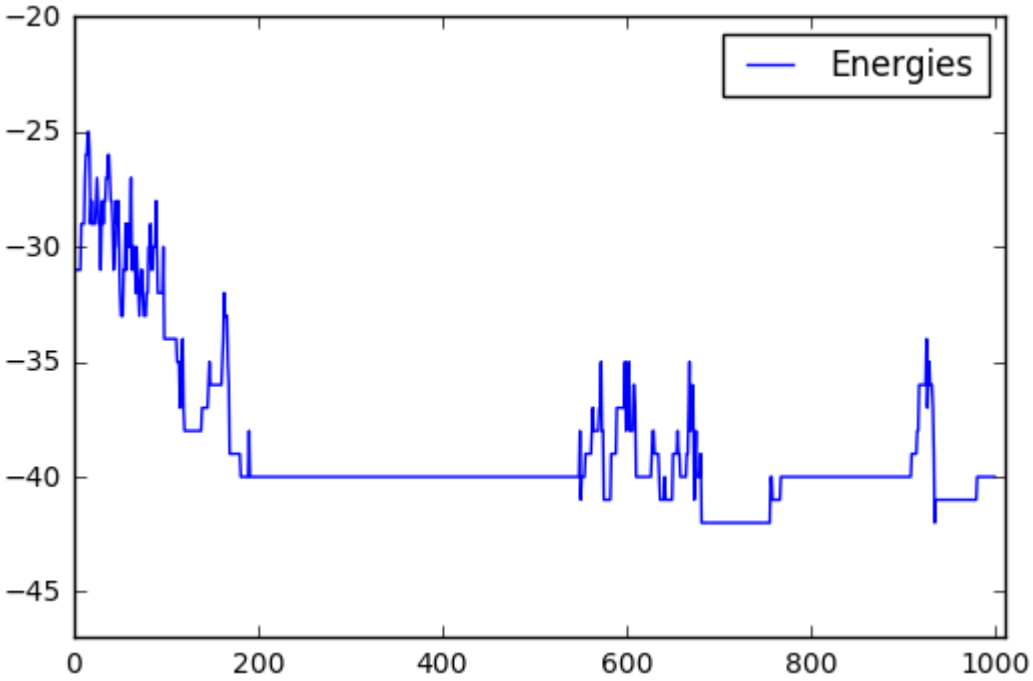


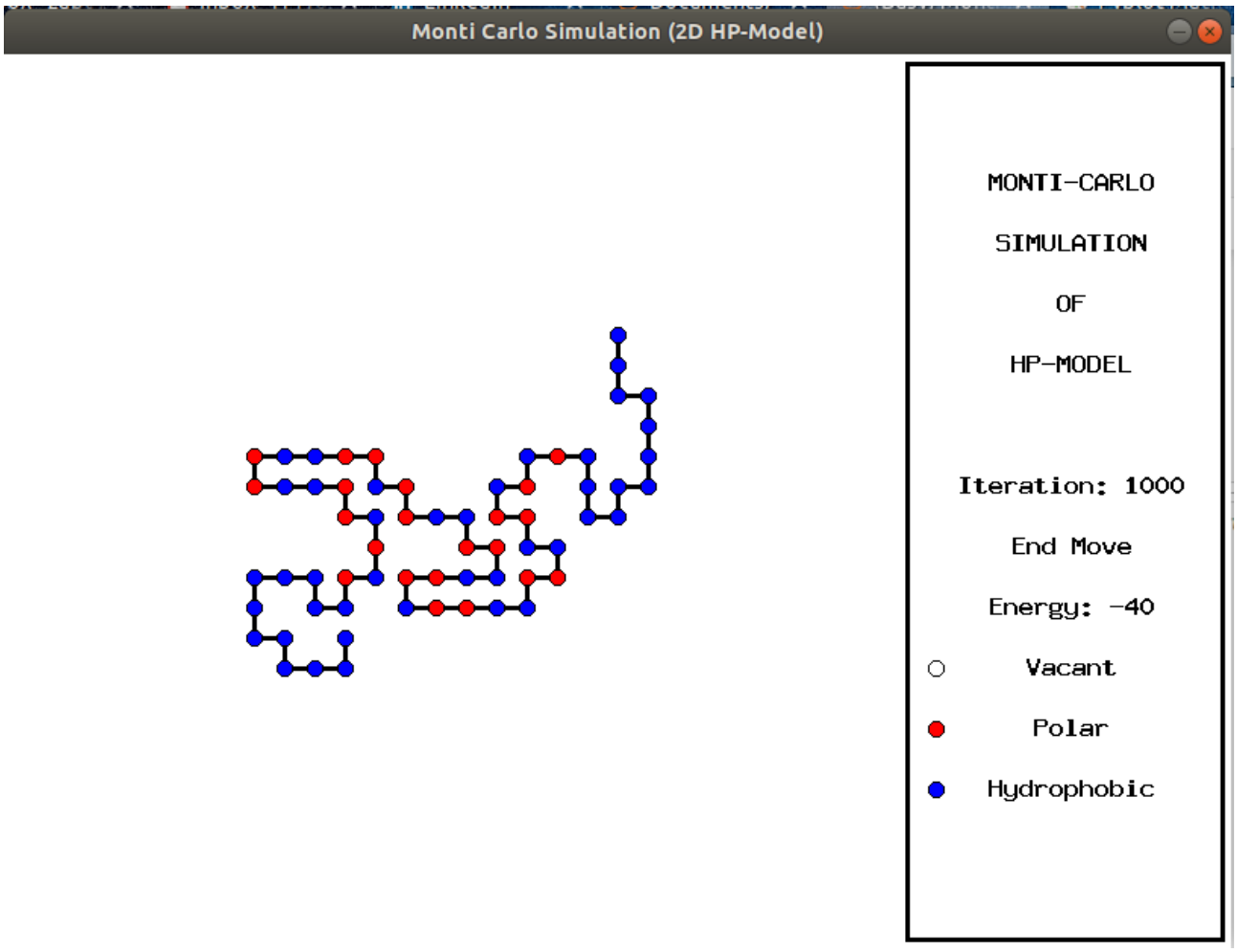
➔ STRING_07 = "PPHHHPHHHHHHHHPPPHHHHHHHHHHPHPPPHHHHHHHHHHPPPPHHHHHHPHHPHP"



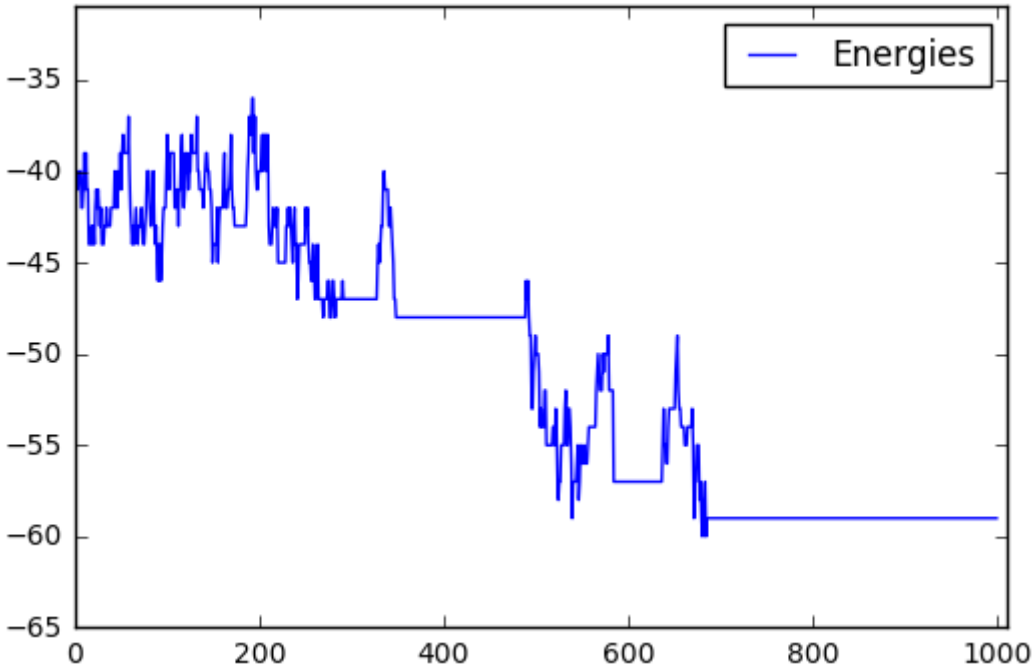


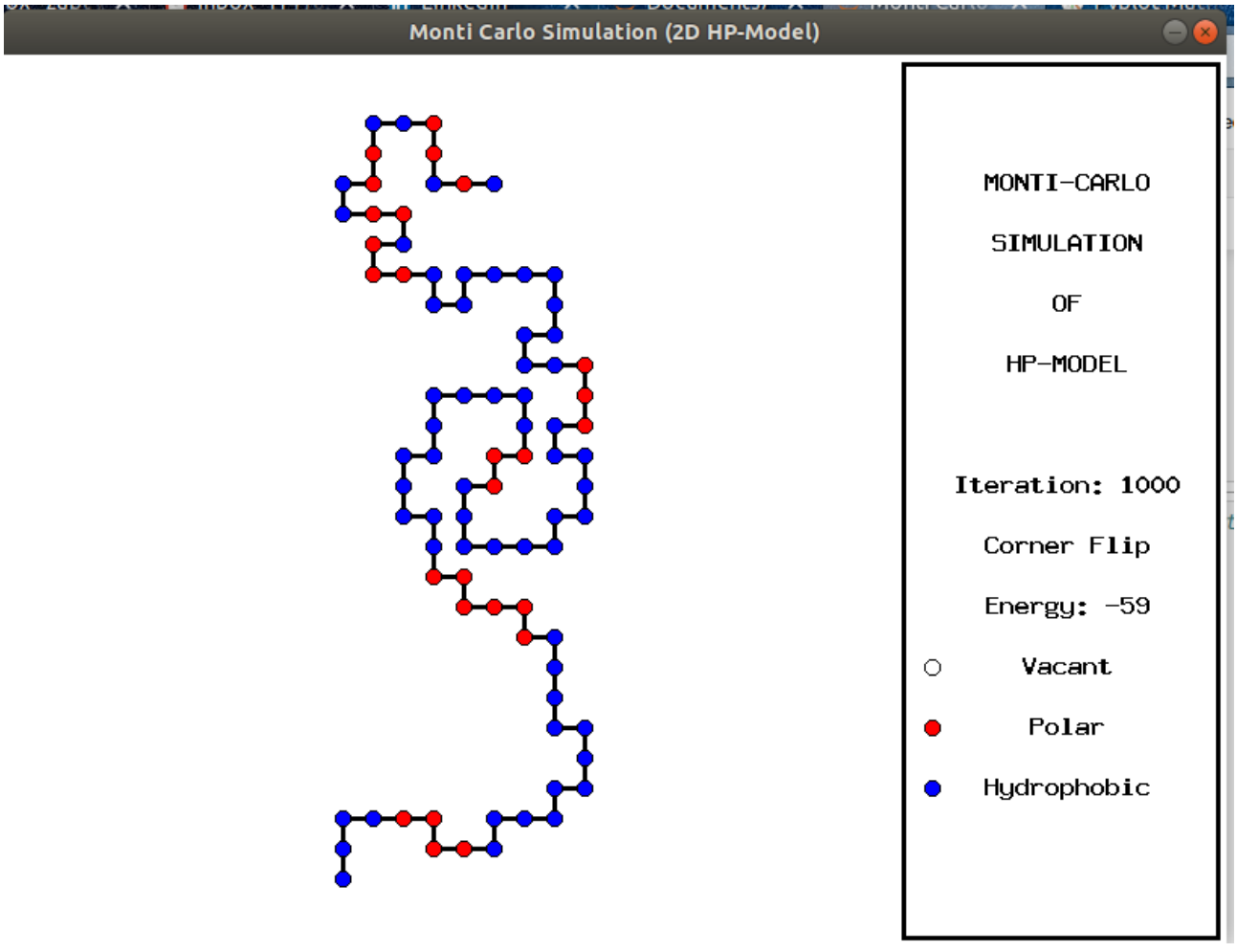
➔ STRING_08 =
"H"*12+"PH"*2+"PPHH"*2+"PPHPPHHPPHHPPHPPHHPPHHPPHPHP"+"H"*12



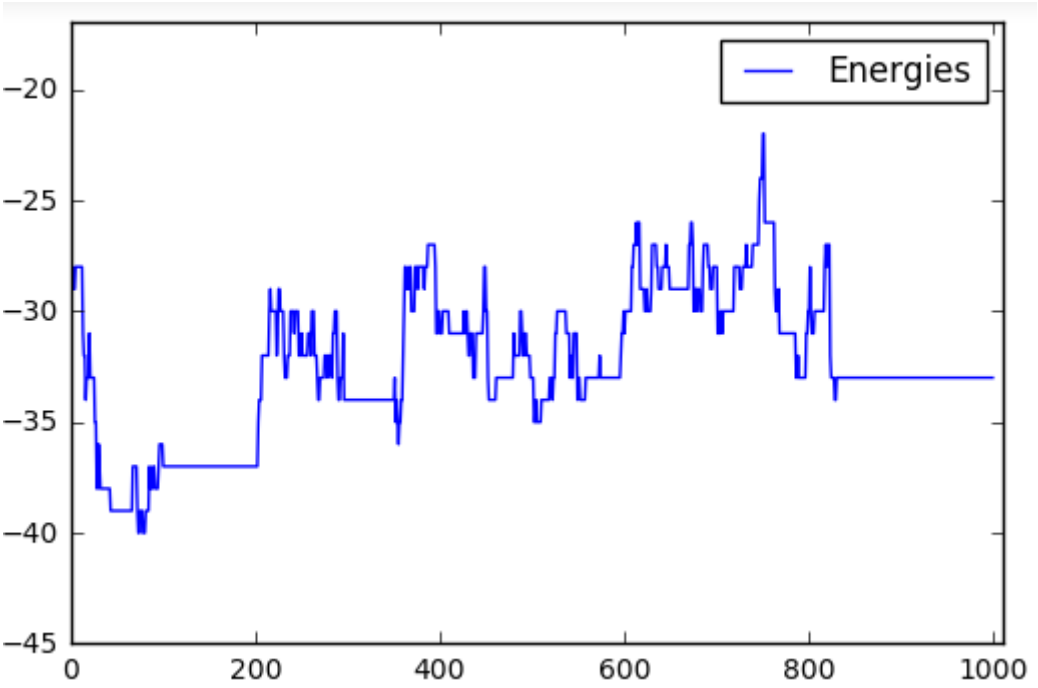


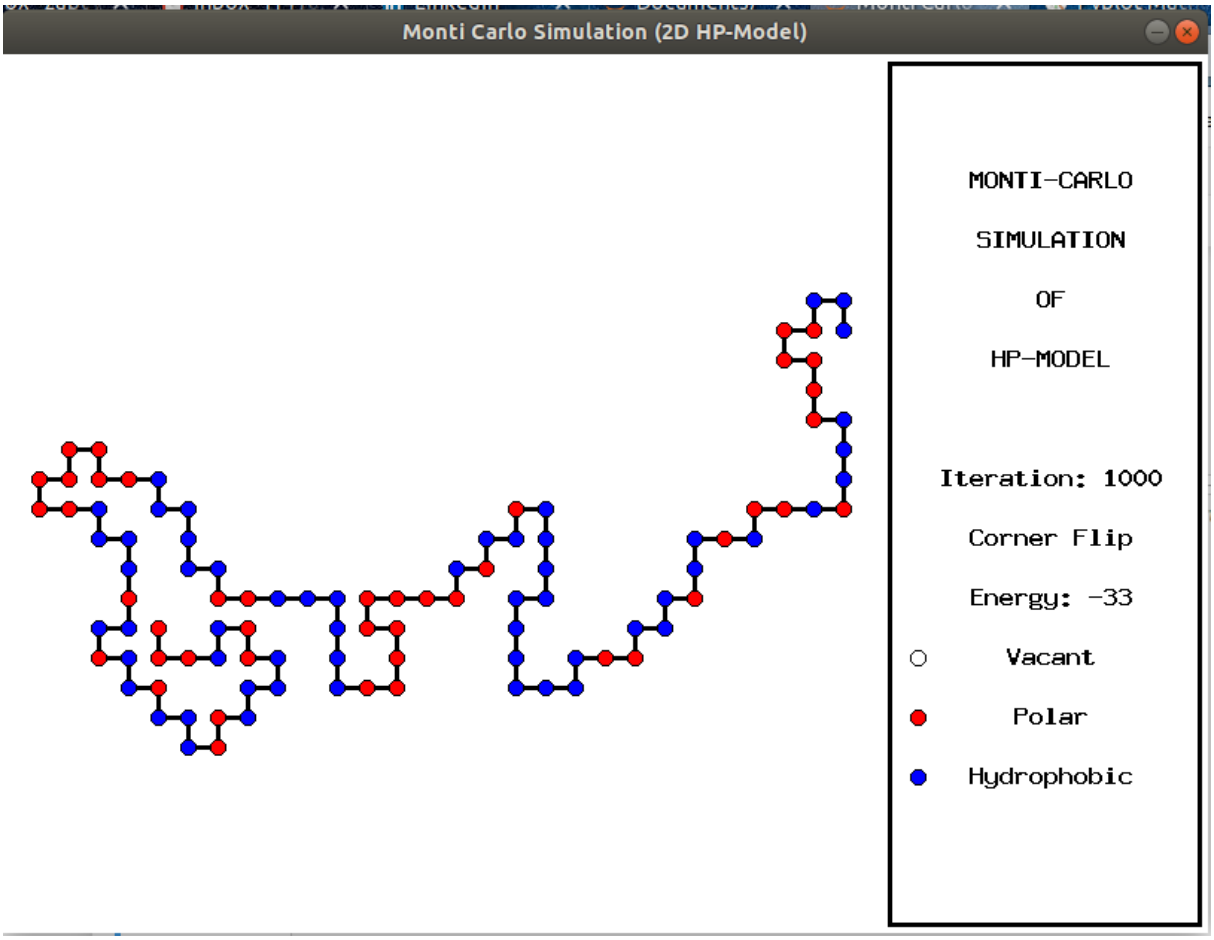
➔ STRING_09 = "HHHHPPPPHHHHHHHHHHHHPPPPPP"+("H"*12+"P"*3)*3+
"HPPHHPPHHPPHPH"





➔ STRING_10 =
"PPPHHPPHHHHPPHHHPHHPHHPHHHHPPPPPPPPHHHHHHPPHHHHHHPPPPPPPPPHPHHPHHHHHHHHHHHHHPPHHHPHHPHPPHPHHHPPPPPPHHH"





➔ STRING_11 =
"PPPPPPHPHHPPPPPHHHPHHHHHPHHPPPPHHPPHHPHHHHHPHHHHHHHHHHPH
HPHHHHHHHPPPPPPPPPPHHHHHHHHPPHPHHHPPPPPPHPHH"