In [1]:
```python
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import gym
from gym import spaces
import torch
import torch.nn as nn
from torch.nn.utils.rnn import pad_sequence
import torch.optim as optim
from torch.nn.functional import one_hot
# from rdkit import Chem
# from rdkit.Chem import Crippen
import random
```

In [2]:
```python
state_size = 4
standard_amino_acids = ['A', 'R', 'N', 'D', 'C', 'Q', 'E', 'G', 'H', 'I',
action_space = np.arange(0, 20)
```

In [3]:
```python
class PolicyNetwork(nn.Module):
    def __init__(self, state_size, action_space):
        super(PolicyNetwork, self).__init__()
        self.fc1 = nn.Linear(state_size, 128)
        self.fc2 = nn.Linear(128, len(action_space))

    def forward(self, state):
        x = torch.relu(self.fc1(state))
        action_probs = torch.softmax(self.fc2(x), dim=0)
        return action_probs
```

In [4]:
```python
policy_net = PolicyNetwork(state_size, action_space)
policy_net #gives 20 probabilities for the 20 standard amino acids.
```

Out[4]:
```
PolicyNetwork(
  (fc1): Linear(in_features=4, out_features=128, bias=True)
  (fc2): Linear(in_features=128, out_features=20, bias=True)
)
```

In [5]:
```python
# s = [-1,-1,-1,0]
# se = []
# for i in range(3):
#     se.append(s)
#     for j in range(len(s)):
#         if s[j] == -1:
#             s[j] = 9
#             break
#     s[3] = s[3] + 1

# print(se)
```

In [6]:
```python
learning_rate = 0.001
num_episodes = 500
len_peptide = 3
max_steps = len_peptide
gamma = 0.99
```

In [7]:
```python
# Define your reward function
def compute_discounted_rewards(rewards, gamma):
```

```
        discounted_rewards = [rewards[-1]]
        for i in range(len(rewards) - 2, -1, -1):
            discounted_rewards.insert(0, rewards[i] + gamma * discounted_rewa
        return discounted_rewards
```

In [8]:
```python
# Define your training loop
def train():
    # Set up your optimizer
    optimizer = optim.Adam(policy_net.parameters(), lr= learning_rate)

    # Training loop
    for episode in range(num_episodes):
        # Initialize the state
        state = [-1,-1,-1,0]

        # Lists to store the trajectory
        states = []
        actions = []
        rewards = []

        # Collect trajectory by interacting with the environment
        for step in range(max_steps):
        # Convert the state to a PyTorch tensor

            state_tensor = torch.tensor(state, dtype=torch.float32)
            # Forward pass to get action probabilities

            action_probs = policy_net(state_tensor)

            # Sample an action from the action probabilities
            action = torch.multinomial(action_probs, 1).item()

            # Execute the action and observe the next state and reward
            next_state = action
            reward = action_probs[action].item()

            # Store the trajectory
            states.append(state)
            actions.append(action)
            rewards.append(reward)

            # Update the state
            for i in range(len(state)):
                if state[i] == -1:
                    state[i] = next_state
                    break
            state[3] = state[3] + 1

        # Compute discounted rewards
        discounted_rewards = compute_discounted_rewards(rewards, gamma)

        # Convert trajectory to tensors
        state_tensor = torch.tensor(states, dtype=torch.float32)
        action_tensor = torch.tensor(actions, dtype=torch.int64)
        reward_tensor = torch.tensor(discounted_rewards, dtype=torch.floa

        # Compute the loss
        action_probs = policy_net(state_tensor)
        selected_action_probs = action_probs.gather(1, action_tensor.unsq
        loss = -torch.mean(torch.log(selected_action_probs) * reward_tens
```

```python
        # Update the policy network
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

        # Print training progress
        print(f"Episode: {episode}, Loss: {loss}")
```

In [9]:
```python
train()
```

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Episode: 0, Loss: 0.2527870833873749
Episode: 1, Loss: 0.12812061607837677
Episode: 2, Loss: 0.4495612382888794
Episode: 3, Loss: 0.3946632444858551
Episode: 4, Loss: 0.31685808300971985
Episode: 5, Loss: 0.23426277935504913
Episode: 6, Loss: 0.2937659025192261
Episode: 7, Loss: 0.7505591511726379
Episode: 8, Loss: 0.10025864839553833
Episode: 9, Loss: 0.7924635410308838
Episode: 10, Loss: 0.47618845105171204
Episode: 11, Loss: 0.06063328683376312
Episode: 12, Loss: 0.8527063727378845
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Episode: 374, Loss: 0.07654281705617905
Episode: 375, Loss: 1.310839295387268
Episode: 376, Loss: 0.631199300289154
Episode: 377, Loss: 0.5950556397438049
Episode: 378, Loss: 0.7141851782798767
Episode: 379, Loss: 0.3360207974910736
Episode: 380, Loss: 0.7270687222480774
Episode: 381, Loss: 0.5255494117736816
Episode: 382, Loss: 0.25682058930397034
Episode: 383, Loss: 0.7961885929107666
Episode: 384, Loss: 0.5308642983436584
Episode: 385, Loss: 0.9629891514778137
Episode: 386, Loss: 1.6170930862426758
Episode: 387, Loss: 1.6472686529159546
Episode: 388, Loss: 0.11578001827001572
Episode: 389, Loss: 1.6380691528320312
Episode: 390, Loss: 0.3221895396709442
Episode: 391, Loss: 1.603181004524231
Episode: 392, Loss: 0.13771206140518188
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Episode: 395, Loss: 1.468990683555603
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Episode: 397, Loss: 1.5552153587341309
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Episode: 399, Loss: 1.3620686531066895
Episode: 400, Loss: 0.8335168957710266
Episode: 401, Loss: 1.7381114959716797
Episode: 402, Loss: 0.12033689022064209
Episode: 403, Loss: 1.6568942070007324
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Episode: 405, Loss: 0.12307638674974442
Episode: 406, Loss: 0.09705085307359695
Episode: 407, Loss: 0.6348535418510437
Episode: 408, Loss: 0.15254853665828705
Episode: 409, Loss: 0.4389707148075104
Episode: 410, Loss: 0.17266006767749786
Episode: 411, Loss: 0.5122812390327454
Episode: 412, Loss: 0.2827146351337433
Episode: 413, Loss: 0.3931431472301483
Episode: 414, Loss: 0.5106812715530396
Episode: 415, Loss: 0.174276769161224437
Episode: 416, Loss: 0.1979457587003708
Episode: 417, Loss: 0.12962807714939117
Episode: 418, Loss: 0.9693558216094971
Episode: 419, Loss: 0.09640253335237503
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Episode: 420, Loss: 0.12649756669999817
Episode: 421, Loss: 0.7457773089408875
Episode: 422, Loss: 0.19824965298175812
Episode: 423, Loss: 0.10253789275884628
Episode: 424, Loss: 0.12785392999649048
Episode: 425, Loss: 0.13540227711200714
Episode: 426, Loss: 0.3099653720855713
Episode: 427, Loss: 0.29794177412986755
Episode: 428, Loss: 0.2563778758049011
Episode: 429, Loss: 0.17373336851596832
Episode: 430, Loss: 0.5361964106559753
Episode: 431, Loss: 0.21357941627502441
Episode: 432, Loss: 0.21663261950016022
Episode: 433, Loss: 0.20381473004817963
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Episode: 435, Loss: 0.15092553198337555
Episode: 436, Loss: 0.4180103838443756
Episode: 437, Loss: 0.0981803610920906
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Episode: 439, Loss: 0.2989027500152588
Episode: 440, Loss: 0.137167826294899
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Episode: 462, Loss: 0.19463767111301422
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Episode: 467, Loss: 0.1984633356332779
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Episode: 471, Loss: 0.1551765352487564
Episode: 472, Loss: 0.19371511042118073
Episode: 473, Loss: 0.11127463728189468
Episode: 474, Loss: 0.16713188588619232
Episode: 475, Loss: 0.16778801381587982
Episode: 476, Loss: 0.154354065656662
Episode: 477, Loss: 0.10527190566062927
Episode: 478, Loss: 0.13037435710430145
Episode: 479, Loss: 0.45422014594078064
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Episode: 480, Loss: 0.15303516387939453
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Episode: 482, Loss: 0.6246637105941772
Episode: 483, Loss: 0.16732437908649445
Episode: 484, Loss: 0.1475726217031479
Episode: 485, Loss: 0.37256181240081787
Episode: 486, Loss: 0.5299069285392761
Episode: 487, Loss: 0.1537628173828125
Episode: 488, Loss: 0.11385353654623032
Episode: 489, Loss: 0.16902215778827667
Episode: 490, Loss: 0.17489682137966156
Episode: 491, Loss: 0.14753873646259308
Episode: 492, Loss: 0.16758771240711212
Episode: 493, Loss: 0.24398499727249146
Episode: 494, Loss: 0.1641007512807846
Episode: 495, Loss: 0.11850637197494507
Episode: 496, Loss: 0.1681807041168213
Episode: 497, Loss: 0.11412960290908813
Episode: 498, Loss: 0.16700617969036102
Episode: 499, Loss: 0.1281348615884781
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