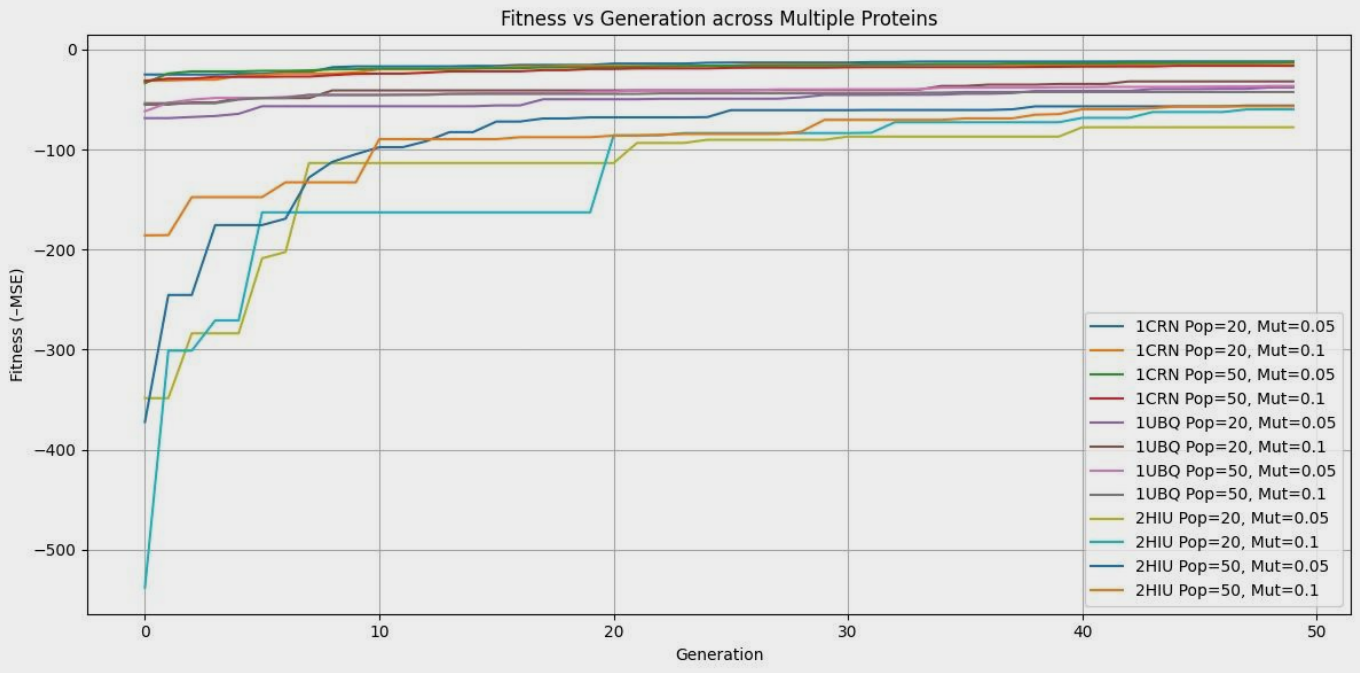
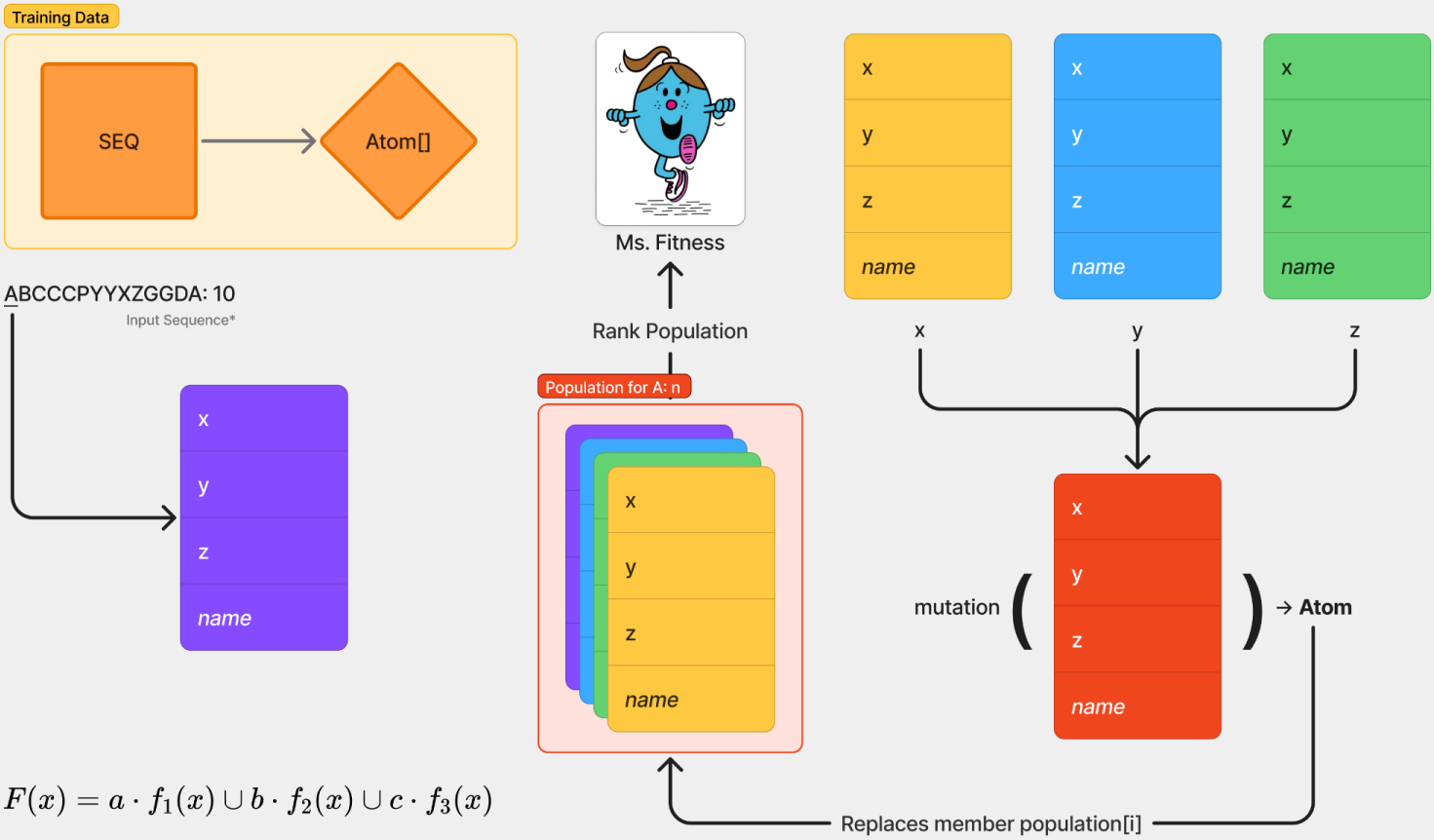
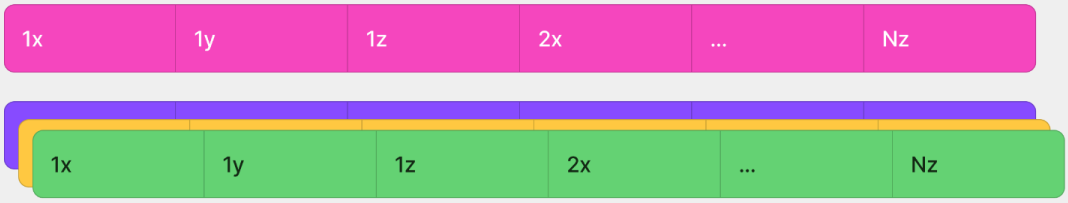


Protein	Population	Mutation	Algorithm	Crossover	Final Fitness
1CRN	20	0.05	GA	OnePoint	-39.7086
1CRN	20	0.05	GA	TwoPoint	-91.5643
1CRN	20	0.05	GA	Uniform	-71.8795
1CRN	20	0.05	PSO	OnePoint	-59.8793
1CRN	20	0.05	PSO	TwoPoint	-20.0417

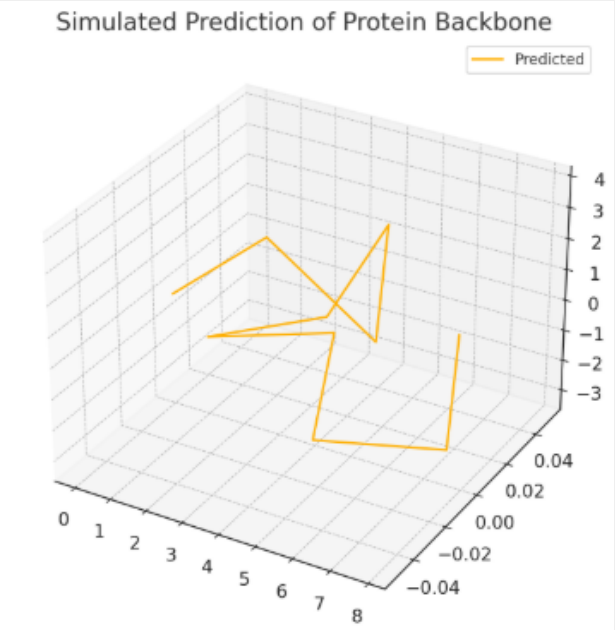


$$F(x) = a \cdot f_1(x) \cup b \cdot f_2(x) \cup c \cdot f_3(x)$$

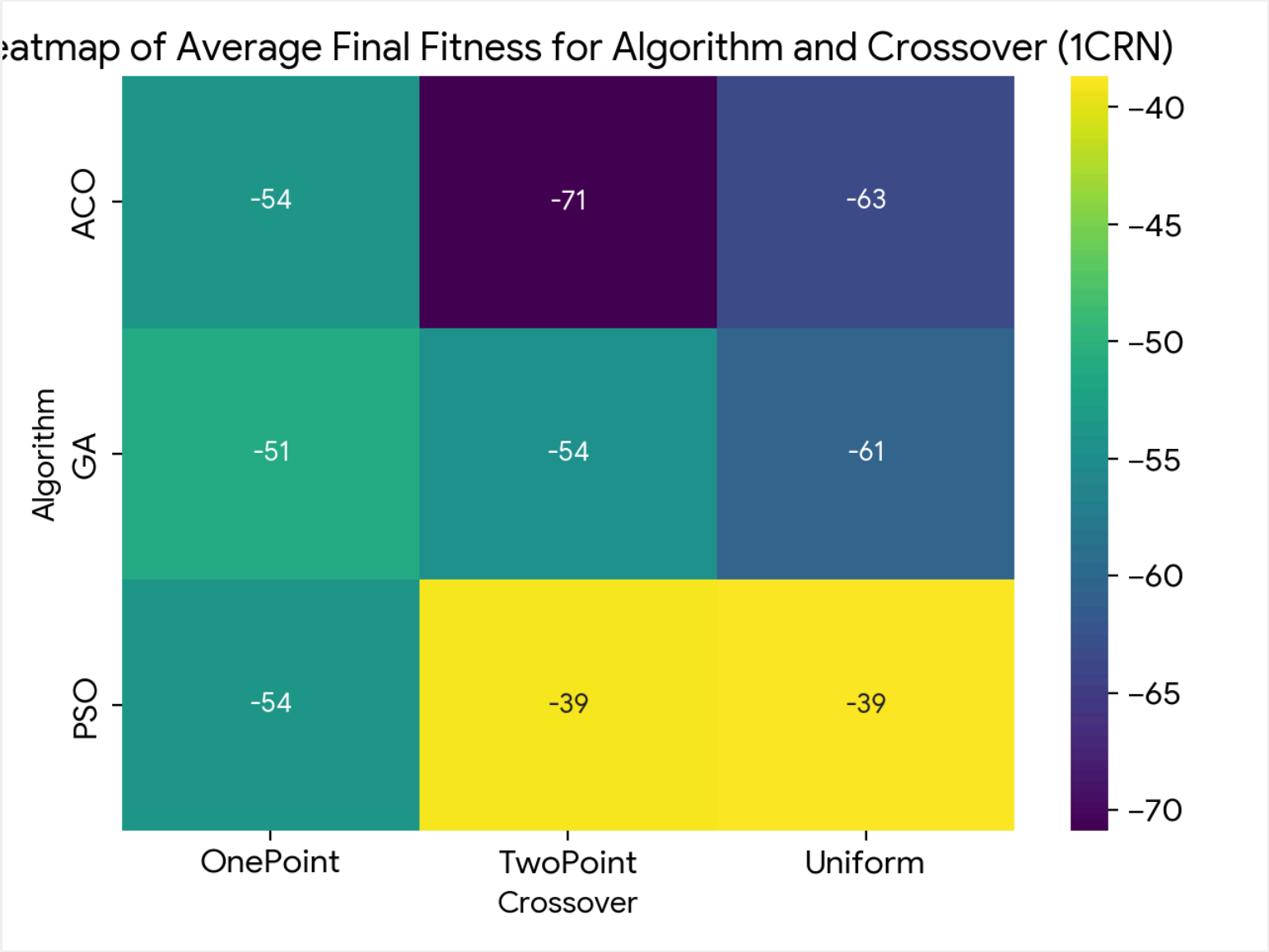


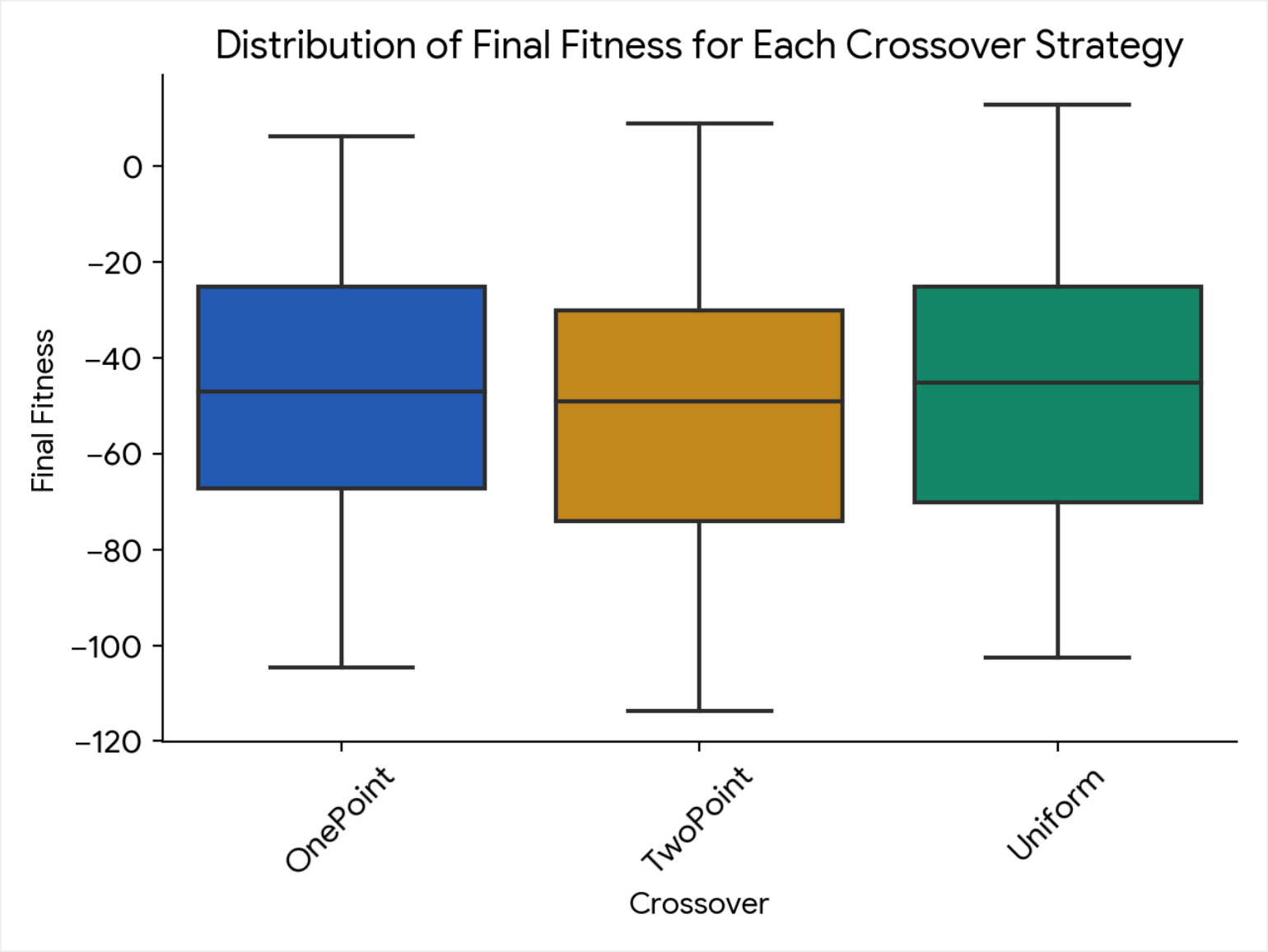
Actual Chromosome Implementation

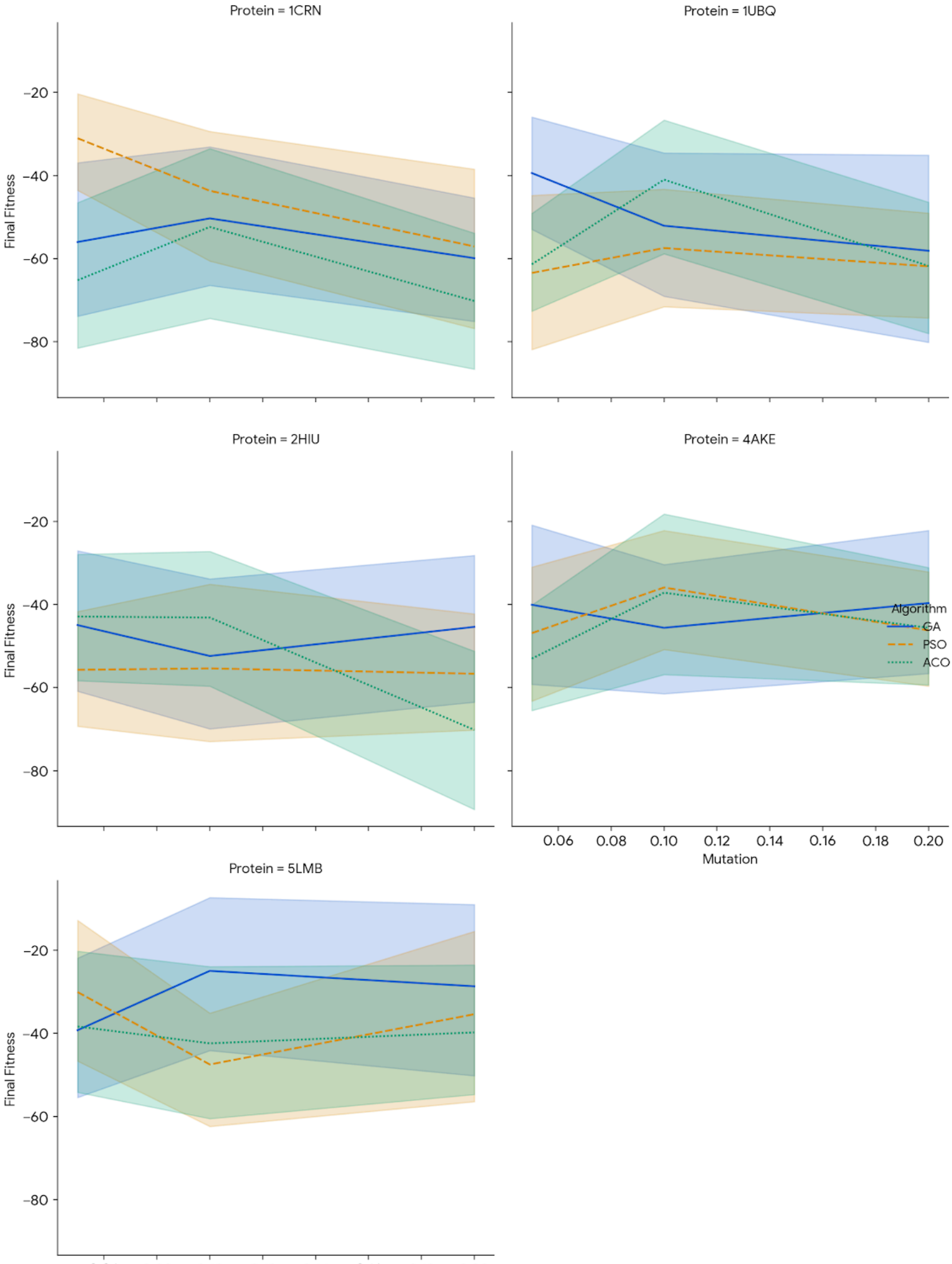
We flattened the data-structure to 1-dimension for EA to mutate and learn

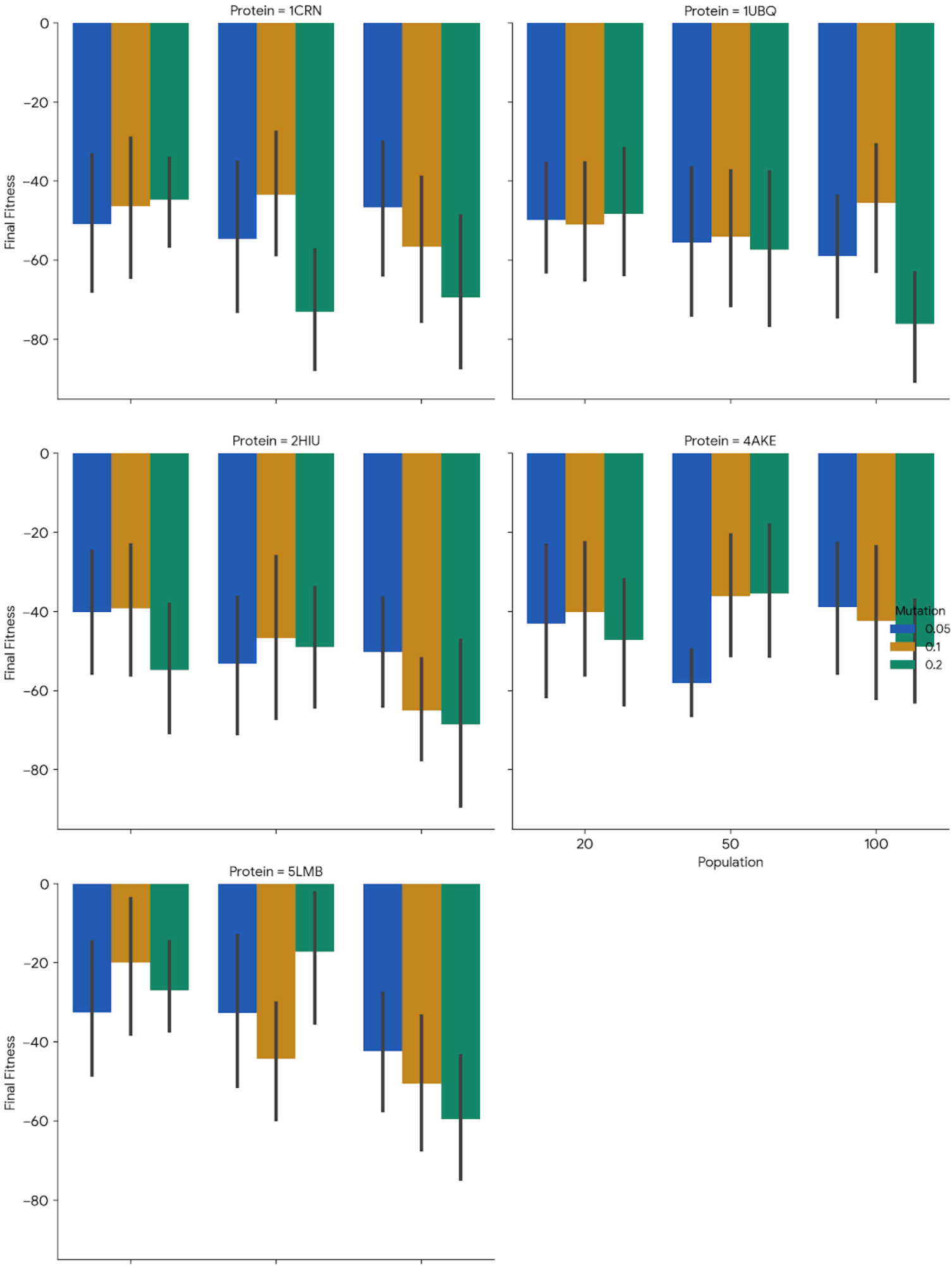


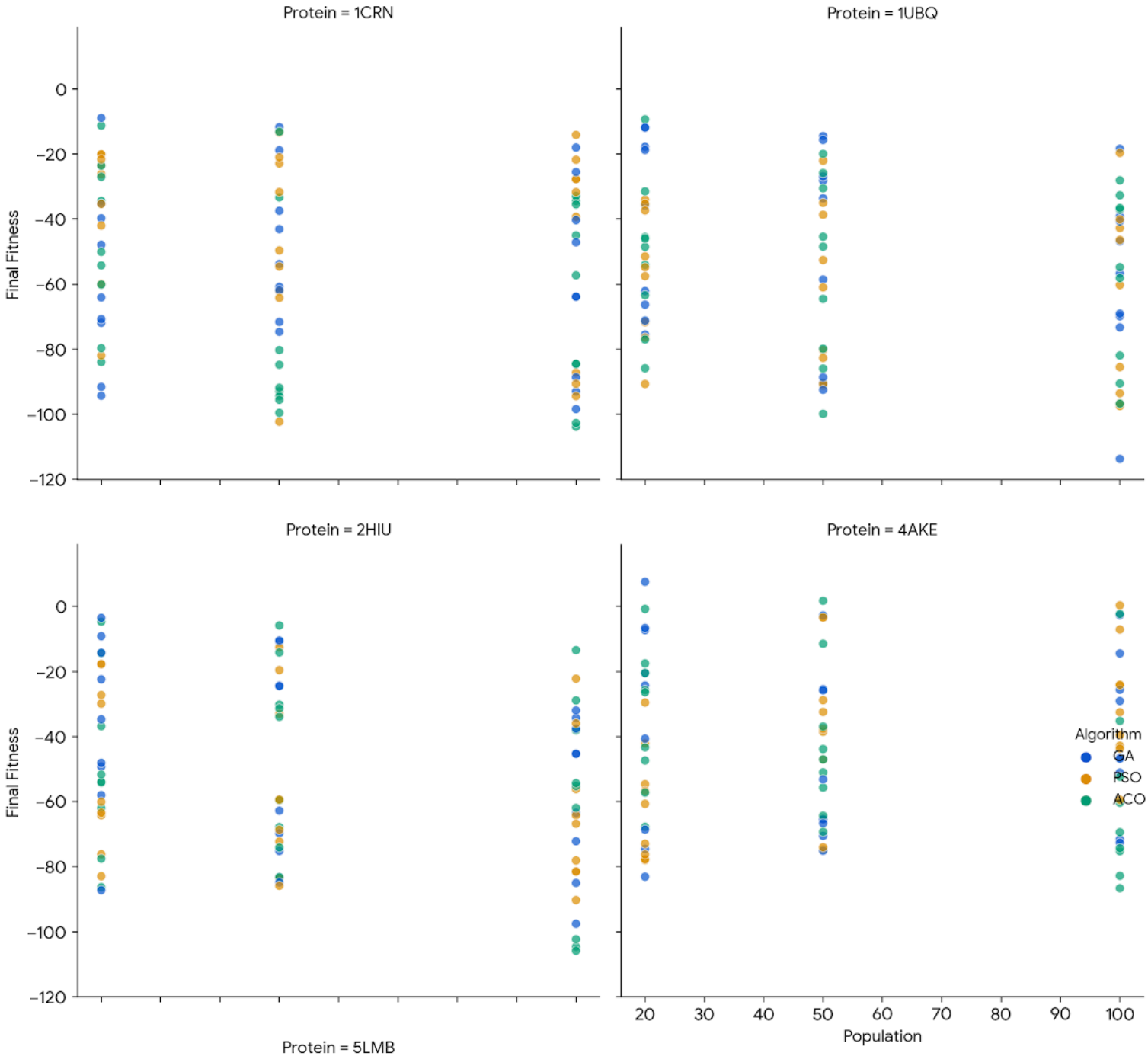

```
ATOM  17406  O   SER C 514     207.108 194.732 247.224  1.00124.90           O
ATOM  17407  CB  SER C 514     209.289 194.744 249.512  1.00124.90           C
ATOM  17408  OG  SER C 514     209.656 194.065 248.326  1.00124.90           O
ATOM  17409  N   LYS C 515     206.154 193.833 249.057  1.00121.97           N
ATOM  17410  CA  LYS C 515     205.352 192.887 248.285  1.00121.97           C
ATOM  17411  C   LYS C 515     204.389 193.594 247.338  1.00121.97           C
ATOM  17412  O   LYS C 515     204.156 193.119 246.220  1.00121.97           O
ATOM  17413  CB  LYS C 515     204.596 191.953 249.234  1.00121.97           C
ATOM  17414  CG  LYS C 515     203.594 192.660 250.130  1.00121.97           C
ATOM  17415  CD  LYS C 515     202.910 191.719 251.106  1.00121.97           C
ATOM  17416  CE  LYS C 515     201.885 190.851 250.411  1.00121.97           C
ATOM  17417  NZ  LYS C 515     201.125 190.004 251.370  1.00121.97           N
ATOM  17418  N   SER C 516     203.819 194.726 247.760  1.00114.35           N
ATOM  17419  CA  SER C 516     202.819 195.405 246.942  1.00114.35           C
ATOM  17420  C   SER C 516     203.383 195.893 245.616  1.00114.35           C
ATOM  17421  O   SER C 516     202.615 196.137 244.680  1.00114.35           O
ATOM  17422  CB  SER C 516     202.220 196.582 247.713  1.00114.35           C
ATOM  17423  OG  SER C 516     201.433 197.399 246.864  1.00114.35           O
ATOM  17424  N   LYS C 517     204.705 196.039 245.514  1.00119.17           N
ATOM  17425  CA  LYS C 517     205.330 196.530 244.293  1.00119.17           C
ATOM  17426  C   LYS C 517     205.162 195.580 243.115  1.00119.17           C
ATOM  17427  O   LYS C 517     205.315 196.016 241.969  1.00119.17           O
ATOM  17428  CB  LYS C 517     206.818 196.787 244.541  1.00119.17           C
```

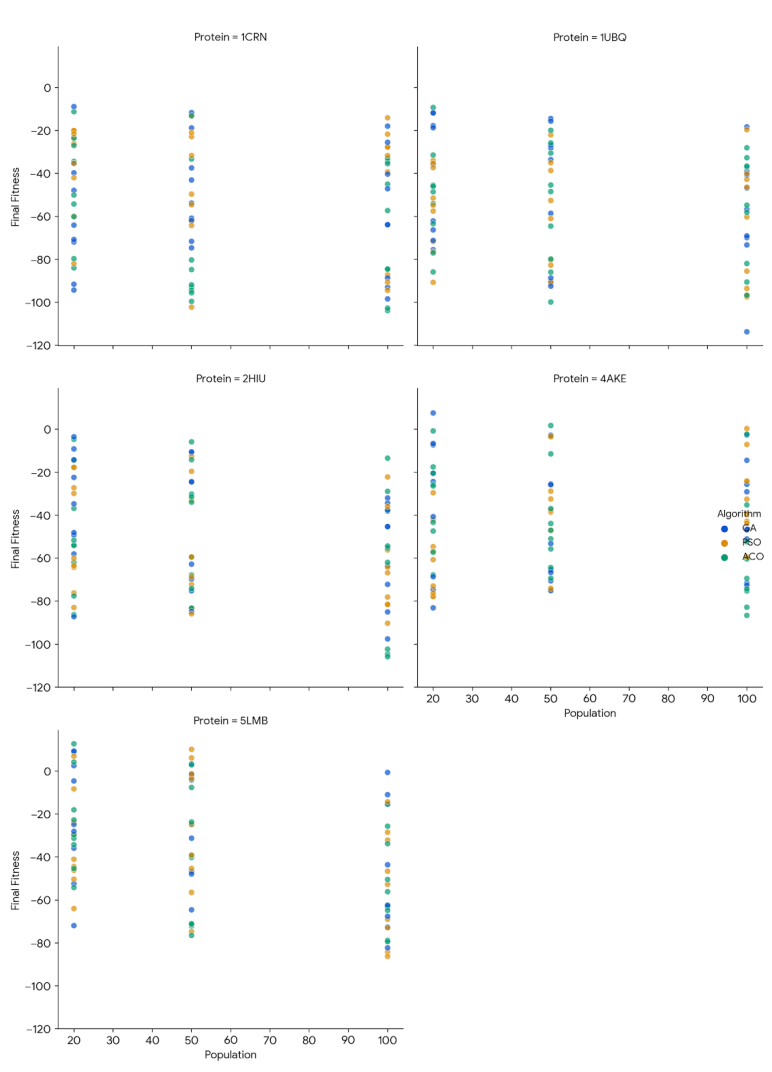

eatmap of Average Final Fitness for Algorithm and Crossover (1CRN)
ACO
GA
PSO
Algorithm
-54
-71
-63
-51
-54
-61
-54
-39
-39
OnePoint
TwoPoint
Uniform
Crossover
−40
−45
−50
−55
−60
−65
−70


Distribution of Final Fitness for Each Crossover Strategy
Final Fitness
0
−20
−40
−60
−80
−100
−120
OnePoint
TwoPoint
Uniform
Crossover


Protein = 1CRN
Protein = 1UBQ
Protein = 2HIU
Protein = 4AKE
Protein = 5LMB
Final Fitness
−20
−40
−60
−80
0.06
0.08
0.10
0.12
0.14
0.16
0.18
0.20
Mutation
Algorithm
GA
PSO
ACO


Protein = 1CRN
Protein = 1UBQ
Protein = 2HIU
Protein = 4AKE
Protein = 5LMB
Final Fitness
0
−20
−40
−60
−80
20
50
100
Population
Mutation
0.05
0.1
0.2


Protein = 1CRN
Protein = 1UBQ
Protein = 2HIU
Protein = 4AKE
Protein = 5LMB
Final Fitness
0
−20
−40
−60
−80
−100
−120
20
30
40
50
60
70
80
90
100
Population
Algorithm
GA
PSO
ACO



Fitness Proportional Selection Data

Individual	Fitness	Selection Probability (Proportional)
Ind_1	43.7086	0.0769351
Ind_2	95.5643	0.168211
Ind_3	75.8795	0.133562
Ind_4	63.8793	0.112439
Ind_5	24.0417	0.0423177
Ind_6	24.0395	0.0423139
Ind_7	15.2275	0.0268032
Ind_8	87.9559	0.154818
Ind_9	64.1004	0.112828
Ind_10	73.7265	0.129772

Rank-Based Selection Data (Linear Ranking)

Individual	Fitness	Rank	Selection Probability (Rank-Based Linear)
Ind_7	15.2275	1	0.06
Ind_6	24.0395	2	0.07
Ind_5	24.0417	3	0.08
Ind_1	43.7086	4	0.09
Ind_4	63.8793	5	0.10
Ind_9	64.1004	6	0.11
Ind_10	73.7265	7	0.12
Ind_3	75.8795	8	0.13
Ind_8	87.9559	9	0.14
Ind_2	95.5643	10	0.15

Binary Tournament Selection Data

Individual	Tournament Wins
Ind_1	4
Ind_2	0
Ind_3	1
Ind_4	1
Ind_5	4
Ind_6	4
Ind_7	1
Ind_8	1
Ind_9	3
Ind_10	1