Question 1

In [189…

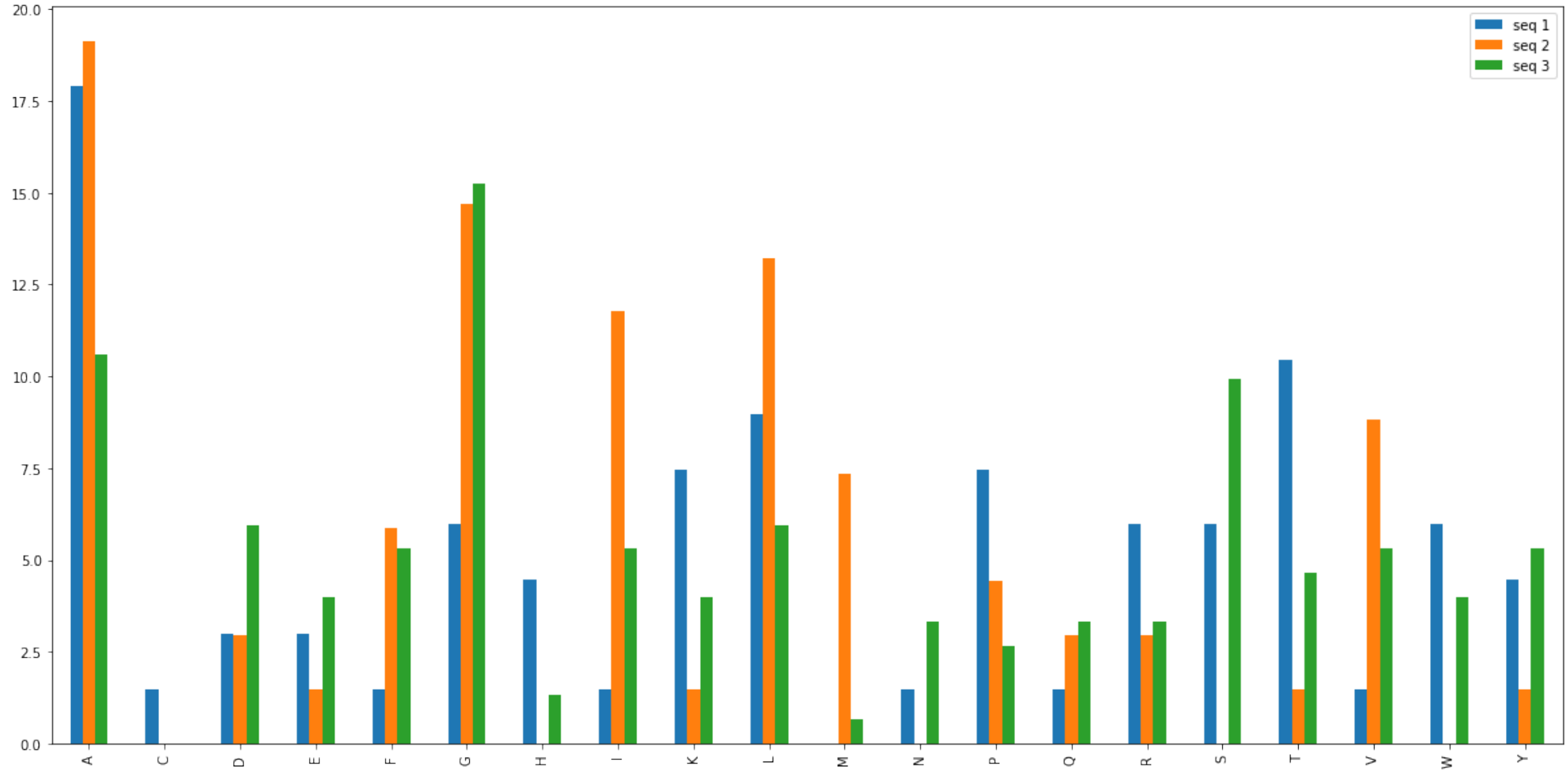
```
import pandas as pd
import string
import numpy as np
from collections import Counter
aas = set(string.ascii_uppercase) - set("BJOZXU")
res1 = "RATPTRWPVGCFNRPWTKWSYDEALDGIKAAGYAWTGLLTASKPSLHHATATPEYLAALKQKSRHAA"
res2 = "AAAVMMGLAAIGAAIGIGILGGKFLEGAARQPDLIPLLRTQFFIVMGLVDAIPMIAVGLGLYVMFAVA"
res3 = "AADVSAAVGATGQSGMTYRLGLSWDWDKSWWQTSTGRLTGYWDAGYTYWEGGDEGAGKHSLSFAPVFVYEFAGDSIKPFIEAGIGVAAFSGTRVGDQNLGSSLNFE
f1 = Counter(res1)
f1 = {r : f1[r] / len(res1) * 100 for r in sorted(aas)}
f2 = Counter(res2)
f2 = {r : f2[r] / len(res2) * 100 for r in sorted(aas)}
f3 = Counter(res3)
f3 = {r : f3[r] / len(res3) * 100 for r in sorted(aas)}
freq = []
for x in [f1,f2,f3]:
    freq.append(list(zip(*sorted(x.items())))[1])
df = pd.DataFrame(freq).T
df.index = sorted(aas)
df.columns = ['seq 1', "seq 2", "seq 3"]
df
```

Out[189…

	seq 1	seq 2	seq 3
A	17.910448	19.117647	10.596026
C	1.492537	0.000000	0.000000
D	2.985075	2.941176	5.960265
E	2.985075	1.470588	3.973510
F	1.492537	5.882353	5.298013
G	5.970149	14.705882	15.231788
H	4.477612	0.000000	1.324503
I	1.492537	11.764706	5.298013
K	7.462687	1.470588	3.973510
L	8.955224	13.235294	5.960265
M	0.000000	7.352941	0.662252
N	1.492537	0.000000	3.311258
P	7.462687	4.411765	2.649007
Q	1.492537	2.941176	3.311258
R	5.970149	2.941176	3.311258
S	5.970149	0.000000	9.933775
T	10.447761	1.470588	4.635762
V	1.492537	8.823529	5.298013
W	5.970149	0.000000	3.973510
Y	4.477612	1.470588	5.298013

In [197…

```
p = df.plot(kind = 'bar', figsize = (20,10))
```



- Sequence 1 has a high amount og Alanine and Threonine making some parts of it hydrophobic, while others hydrophillic
- Sequence 2 has a high amount of hyfrophobic residues, alanine, glycine, isoleucine etc. making it very hydrophobic
- Sequence 3 has higher glycine, serine and alanine making it slightly hydrophilic dues to the prescence of serine

Question 2

In [2]:

```
aa = "ACDEFGWHIKLMNYPQRSTV"
w = [85,115,130,145,160,70,200,150,125,145,125,143,130,175,110,140,170,100,115,110]
weights = {x : y for x,y in zip(aa,w)}
w1 = sum([y/100 * len(res1) * weights[x] for x,y in f1.items()]) - (len(res1)-1)*18
w2 = sum([y/100 * len(res2) * weights[x] for x,y in f2.items()]) - (len(res2)-1)*18
w3 = sum([y/100 * len(res3) * weights[x] for x,y in f3.items()]) - (len(res3)-1)*18

df = pd.DataFrame([w1,w2,w3])
df.index = ["seq 1", "seq 2", 'seq 3']
df.columns = ['Weight']
df
```

Out[2]:

	Weight
seq 1	7127.0
seq 2	6529.0
seq 3	15453.0

Question 3

In [167…

```
import re
s = """Ala: 8.47, 8.95 Phe: 3.91, 3.68 Lys: 5.76, 4.93 Pro: 4.63, 3.74
Asp: 5.97, 5.91 Gly: 7.82, 8.54 Leu: 8.48, 8.78 Gln: 3.82, 4.75
Cys: 1.39, 0.47 His: 2.26, 1.25 Met: 2.21, 1.56 Arg: 4.93, 5.24
Glu: 6.32, 4.78 Ile: 5.71, 4.77 Asn: 4.54, 5.74 Ser: 5.94, 8.05
Thr: 5.79, 6.54 Val: 7.02, 6.76 Trp: 1.44, 1.24 Tyr: 3.58, 4.13"""

mapping = {'CYS': 'C', 'ASP': 'D', 'SER': 'S', 'GLN': 'Q', 'LYS': 'K',
     'ILE': 'I', 'PRO': 'P', 'THR': 'T', 'PHE': 'F', 'ASN': 'N',
     'GLY': 'G', 'HIS': 'H', 'LEU': 'L', 'ARG': 'R', 'TRP': 'W',
     'ALA': 'A', 'VAL':'V', 'GLU': 'E', 'TYR': 'Y', 'MET': 'M'}

ress = re.findall("[A-z]{3}:.{11}",s)
comp = {}
for res in ress:
    r,w = res.split(': ')
    w = list(map(float,w.split(', ')))
    comp[r.upper()] = w
comp = {mapping[x] : y for x,y in comp.items()}
```

In [168…
```
dev_a = []
dev_b = []
for freq in [f1,f2,f3]:
    dev_a.append(sum([abs(comp[x][0] - freq[x]) for x in aas]))
    dev_b.append(sum([abs(comp[x][1] - freq[x]) for x in aas]))
```

In [187…
```
[abs(comp[x][0] - freq[x]) for x in aas])
```

Out[187…
```
{'A': 17.91044776119403,
 'C': 1.4925373134328357,
 'D': 2.985074626865714,
 'E': 2.985074626865714,
 'F': 1.4925373134328357,
 'G': 5.970149253731343,
 'H': 4.477611940298507,
 'I': 1.4925373134328357,
 'K': 7.462686567164178,
 'L': 8.955223880597014,
 'M': 0.0,
 'N': 1.4925373134328357,
 'P': 7.462686567164178,
 'Q': 1.4925373134328357,
 'R': 5.970149253731343,
 'S': 5.970149253731343,
 'T': 10.44776119402985,
 'V': 1.4925373134328357,
 'W': 5.970149253731343,
 'Y': 4.477611940298507}
```

In [179…
```
df = pd.DataFrame([dev_a,dev_b]).T
df.columns = ['Deviation from A', "Deviation from B"]
df.index = ['seq 1', 'seq 2', 'seq 3']
df['Group'] = ["A",'A','B']
df
```

Out[179…

	Deviation from A	Deviation from B	Group
seq 1	55.844030	58.523731	A
seq 2	74.514706	76.838235	A
seq 3	38.332252	32.597815	B

Question 4

In [6]:
```
def pairwise(res, type):
    p = [[0 for x in range(20)] for x in range(20)]
    for i,x in enumerate(sorted(aas)):
        for j,y in enumerate(sorted(aas)):
            if type == 1:
                p[i][j] = np.round(res.count(x+y) * 10**2 / (res.count(x) + res.count(y)) if res.count(x) + res.co
            elif type == 2:
                p[i][j] = np.round(res.count(x+y) * 10**2 / len(res), 2)
            elif type == 3:
                p[i][j] = np.round(res.count(x+y) * 10**2 / (res.count(x) * res.count(y)) if res.count(x) * res.co
    df = pd.DataFrame(p)
    df.columns = sorted(aas)
    df.index = sorted(aas)
    return df
```

Sequence 1, Formula 1

In [21]:
```
pairwise(res1,1)
```

Out[21]:

	A	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y
A	12.50	0.0	0.0	0.00	0.0	6.25	0.00	0.0	0.00	11.11	0.0	0.0	0.00	0.00	0.00	6.25	15.79	0.00	6.25	0.00
C	0.00	0.0	0.0	0.00	50.0	0.00	0.00	0.0	0.00	0.00	0.0	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
D	0.00	0.0	0.0	25.00	0.0	16.67	0.00	0.0	0.00	0.00	0.0	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
E	7.14	0.0	0.0	0.00	0.0	0.00	0.00	0.0	0.00	0.00	0.0	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	20.00
F	0.00	0.0	0.0	0.00	0.0	0.00	0.00	0.0	0.00	0.00	0.0	50.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
G	0.00	20.0	0.0	0.00	0.0	0.00	0.00	20.0	0.00	10.00	0.0	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	14.29
H	13.33	0.0	0.0	0.00	0.0	0.00	16.67	0.0	0.00	0.00	0.0	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
I	0.00	0.0	0.0	0.00	0.0	0.00	0.00	0.0	16.67	0.00	0.0	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K	5.88	0.0	0.0	0.00	0.0	0.00	0.00	0.0	0.00	0.00	0.0	0.0	10.00	16.67	0.00	11.11	0.00	0.00	11.11	0.00
L	5.56	0.0	12.5	0.00	0.0	0.00	11.11	0.0	9.09	8.33	0.0	0.0	0.00	0.00	0.00	0.00	7.69	0.00	0.00	0.00
M	0.00	0.0	0.0	0.00	0.0	0.00	0.00	0.0	0.00	0.00	0.0	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N	0.00	0.0	0.0	0.00	0.0	0.00	0.00	0.0	0.00	0.00	0.0	0.0	0.00	0.00	20.00	0.00	0.00	0.00	0.00	0.00
P	0.00	0.0	0.0	14.29	0.0	0.00	0.00	0.0	0.00	0.00	0.0	0.0	0.00	0.00	0.00	11.11	8.33	16.67	11.11	0.00
Q	0.00	0.0	0.0	0.00	0.0	0.00	0.00	0.0	16.67	0.00	0.0	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
R	6.25	0.0	0.0	0.00	0.0	0.00	14.29	0.0	0.00	0.00	0.0	0.0	11.11	0.00	0.00	0.00	0.00	0.00	12.50	0.00
S	0.00	0.0	0.0	0.00	0.0	0.00	0.00	0.0	11.11	10.00	0.0	0.0	0.00	0.00	12.50	0.00	0.00	0.00	0.00	14.29
T	10.53	0.0	0.0	0.00	0.0	9.09	0.00	0.0	8.33	0.00	0.0	0.0	16.67	0.00	9.09	0.00	0.00	0.00	0.00	0.00
V	0.00	0.0	0.0	0.00	0.0	20.00	0.00	0.0	0.00	0.00	0.0	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
W	0.00	0.0	0.0	0.00	0.0	0.00	0.00	0.0	0.00	0.00	0.0	0.0	11.11	0.00	0.00	12.50	18.18	0.00	0.00	0.00
Y	6.67	0.0	20.0	0.00	0.0	0.00	0.00	0.0	0.00	11.11	0.0	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Sequence 1, Formula 2

In [13]:
```
pairwise(res1,2)
```

Out[13]:

	A	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y
A	4.48	0.00	0.00	0.00	0.00	1.49	0.00	0.00	0.00	2.99	0.0	0.00	0.00	0.00	0.00	1.49	4.48	0.00	1.49	0.00
C	0.00	0.00	0.00	0.00	1.49	0.00	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
D	0.00	0.00	0.00	1.49	0.00	1.49	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
E	1.49	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.49
F	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0	1.49	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
G	0.00	1.49	0.00	0.00	0.00	0.00	0.00	1.49	0.00	1.49	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.49
H	2.99	0.00	0.00	0.00	0.00	0.00	1.49	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
I	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.49	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K	1.49	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0	0.00	1.49	1.49	0.00	1.49	0.00	0.00	1.49	0.00
L	1.49	0.00	1.49	0.00	0.00	0.00	1.49	0.00	1.49	1.49	0.0	0.00	0.00	0.00	0.00	0.00	1.49	0.00	0.00	0.00
M	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	1.49	0.00	0.00	0.00	0.00	0.00
P	0.00	0.00	0.00	1.49	0.00	0.00	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.00	1.49	1.49	1.49	1.49	0.00
Q	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.49	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
R	1.49	0.00	0.00	0.00	0.00	0.00	1.49	0.00	0.00	0.00	0.0	0.00	1.49	0.00	0.00	0.00	0.00	0.00	1.49	0.00
S	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.49	1.49	0.0	0.00	0.00	0.00	1.49	0.00	0.00	0.00	0.00	1.49
T	2.99	0.00	0.00	0.00	0.00	1.49	0.00	0.00	1.49	0.00	0.0	0.00	2.99	0.00	1.49	0.00	0.00	0.00	0.00	0.00
V	0.00	0.00	0.00	0.00	0.00	1.49	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
W	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.0	0.00	1.49	0.00	0.00	1.49	2.99	0.00	0.00	0.00
Y	1.49	0.00	1.49	0.00	0.00	0.00	0.00	0.00	0.00	1.49	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Sequence 1, Formula 3

In [14]:
```
pairwise(res1,3)
```

Out[14]:

	A	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y
A	2.08	0.0	0.00	0.0	0.0	2.08	0.00	0.0	0.00	2.78	0	0.0	0.00	0.0	0.00	2.08	3.57	0.0	2.08	0.00
C	0.00	0.0	0.00	0.0	100.0	0.00	0.00	0.0	0.00	0.00	0	0.0	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00
D	0.00	0.0	0.00	25.0	0.0	12.50	0.00	0.0	0.00	0.00	0	0.0	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00
E	4.17	0.0	0.00	0.0	0.0	0.00	0.00	0.0	0.00	0.00	0	0.0	0.00	0.0	0.00	0.00	0.00	0.0	0.00	16.67
F	0.00	0.0	0.00	0.0	0.0	0.00	0.00	0.0	0.00	0.00	0	100.0	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00
G	0.00	25.0	0.00	0.0	0.0	0.00	0.00	25.0	0.00	4.17	0	0.0	0.00	0.0	0.00	0.00	0.00	0.0	0.00	8.33
H	5.56	0.0	0.00	0.0	0.0	0.00	11.11	0.0	0.00	0.00	0	0.0	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00
I	0.00	0.0	0.00	0.0	0.0	0.00	0.00	0.0	20.00	0.00	0	0.0	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00
K	1.67	0.0	0.00	0.0	0.0	0.00	0.00	0.0	0.00	0.00	0	0.0	4.00	20.0	0.00	5.00	0.00	0.0	5.00	0.00
L	1.39	0.0	8.33	0.0	0.0	0.00	5.56	0.0	3.33	2.78	0	0.0	0.00	0.0	0.00	0.00	2.38	0.0	0.00	0.00
M	0.00	0.0	0.00	0.0	0.0	0.00	0.00	0.0	0.00	0.00	0	0.0	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00
N	0.00	0.0	0.00	0.0	0.0	0.00	0.00	0.0	0.00	0.00	0	0.0	0.00	0.0	25.00	0.00	0.00	0.0	0.00	0.00
P	0.00	0.0	0.00	10.0	0.0	0.00	0.00	0.0	0.00	0.00	0	0.0	0.00	0.0	0.00	5.00	2.86	20.0	5.00	0.00
Q	0.00	0.0	0.00	0.0	0.0	0.00	0.00	0.0	20.00	0.00	0	0.0	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00
R	2.08	0.0	0.00	0.0	0.0	0.00	8.33	0.0	0.00	0.00	0	0.0	5.00	0.0	0.00	0.00	0.00	0.0	6.25	0.00
S	0.00	0.0	0.00	0.0	0.0	0.00	0.00	0.0	5.00	4.17	0	0.0	0.00	0.0	6.25	0.00	0.00	0.0	0.00	8.33
T	2.38	0.0	0.00	0.0	0.0	3.57	0.00	0.0	2.86	0.00	0	0.0	5.71	0.0	3.57	0.00	0.00	0.0	0.00	0.00
V	0.00	0.0	0.00	0.0	0.0	25.00	0.00	0.0	0.00	0.00	0	0.0	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00
W	0.00	0.0	0.00	0.0	0.0	0.00	0.00	0.0	0.00	0.00	0	0.0	5.00	0.0	0.00	6.25	7.14	0.0	0.00	0.00
Y	2.78	0.0	16.67	0.0	0.0	0.00	0.00	0.0	0.00	5.56	0	0.0	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00

Sequence 2, Formula 1

In [15]:
```
pairwise(res2,1)
```

Out[15]:

	A	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y
A	15.38	0.0	0.0	0.0	0.00	0.00	0.0	14.29	0.00	0.00	0.00	0.0	0.00	0.00	6.67	0.0	0.00	15.79	0.0	0.0
C	0.00	0.0	0.0	0.0	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.0
D	6.67	0.0	0.0	0.0	0.00	0.00	0.0	0.00	0.00	9.09	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.0
E	0.00	0.0	0.0	0.0	0.00	9.09	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.0
F	5.88	0.0	0.0	0.0	12.50	0.00	0.0	8.33	0.00	7.69	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.0
G	8.70	0.0	0.0	0.0	0.00	5.00	0.0	11.11	9.09	21.05	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.0
H	0.00	0.0	0.0	0.0	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.0
I	4.76	0.0	0.0	0.0	0.00	16.67	0.0	0.00	0.00	5.88	0.00	0.0	18.18	0.00	0.00	0.0	0.00	7.14	0.0	0.0
K	0.00	0.0	0.0	0.0	20.00	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.0
L	4.55	0.0	0.0	10.0	0.00	10.53	0.0	5.88	0.00	5.56	0.00	0.0	0.00	0.00	9.09	0.0	0.00	6.67	0.0	10.0
M	0.00	0.0	0.0	0.0	11.11	13.33	0.0	7.69	0.00	0.00	10.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.0
N	0.00	0.0	0.0	0.0	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.0
P	0.00	0.0	20.0	0.0	0.00	0.00	0.0	0.00	0.00	8.33	12.50	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.0
Q	0.00	0.0	0.0	0.0	16.67	0.00	0.0	0.00	0.00	0.00	0.00	0.0	20.00	0.00	0.00	0.0	0.00	0.00	0.0	0.0
R	0.00	0.0	0.0	0.0	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	25.00	0.00	0.0	33.33	0.00	0.0	0.0
S	0.00	0.0	0.0	0.0	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.0
T	0.00	0.0	0.0	0.0	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	33.33	0.00	0.0	0.00	0.00	0.0	0.0
V	5.26	0.0	12.5	0.0	0.00	6.25	0.0	0.00	0.00	0.00	27.27	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.0
W	0.00	0.0	0.0	0.0	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.0
Y	0.00	0.0	0.0	0.0	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.0	0.00	14.29	0.0	0.0

Sequence 2, Formula 2

In [16]:
```
pairwise(res2,2)
```

Out[16]:

	A	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y
A	5.88	0.0	0.00	0.00	0.00	0.00	0.0	4.41	0.00	0.00	0.00	0.0	0.00	0.00	1.47	0.0	0.00	4.41	0.0	0.00
C	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.00
D	1.47	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	1.47	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.00
E	0.00	0.0	0.00	0.00	0.00	1.47	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.00
F	1.47	0.0	0.00	0.00	1.47	0.00	0.0	1.47	0.00	1.47	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.00
G	2.94	0.0	0.00	0.00	0.00	1.47	0.0	2.94	1.47	5.88	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.00
H	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.00
I	1.47	0.0	0.00	0.00	0.00	4.41	0.0	0.00	0.00	1.47	0.00	0.0	2.94	0.00	0.00	0.0	0.00	1.47	0.0	0.00
K	0.00	0.0	0.00	0.00	1.47	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.00
L	1.47	0.0	0.00	1.47	0.00	2.94	0.0	1.47	0.00	1.47	0.00	0.0	0.00	0.00	1.47	0.0	0.00	1.47	0.0	1.47
M	0.00	0.0	0.00	0.00	1.47	2.94	0.0	1.47	0.00	0.00	1.47	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.00
N	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.00
P	0.00	0.0	1.47	0.00	0.00	0.00	0.0	0.00	0.00	1.47	1.47	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.00
Q	0.00	0.0	0.00	0.00	1.47	0.00	0.0	0.00	0.00	0.00	0.00	0.0	1.47	0.00	0.00	0.0	0.00	0.00	0.0	0.00
R	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	1.47	0.00	0.0	1.47	0.00	0.0	0.00
S	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.00
T	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	1.47	0.00	0.0	0.00	0.00	0.0	0.00
V	1.47	0.0	1.47	0.00	0.00	1.47	0.0	0.00	0.00	0.00	4.41	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.00
W	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.0	0.00	0.00	0.0	0.00
Y	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.0	0.00	1.47	0.0	0.00

Sequence 2, Formula 3

In [17]:
```
pairwise(res2,3)
```

Out[17]:

	A	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y
A	2.37	0	0.00	0.00	0.00	0.00	0	2.88	0.0	0.00	0.00	0	0.00	0.0	3.85	0	0.0	3.85	0	0.00
C	0.00	0	0.00	0.00	0.00	0.00	0	0.00	0.0	0.00	0.00	0	0.00	0.0	0.00	0	0.0	0.00	0	0.00
D	3.85	0	0.00	0.00	0.00	0.00	0	0.00	0.0	5.56	0.00	0	0.00	0.0	0.00	0	0.0	0.00	0	0.00
E	0.00	0	0.00	0.00	0.00	10.00	0	0.00	0.0	0.00	0.00	0	0.00	0.0	0.00	0	0.0	0.00	0	0.00
F	1.92	0	0.00	0.00	6.25	0.00	0	3.12	0.0	2.78	0.00	0	0.00	0.0	0.00	0	0.0	0.00	0	0.00
G	1.54	0	0.00	0.00	0.00	1.00	0	2.50	10.0	4.44	0.00	0	0.00	0.0	0.00	0	0.0	0.00	0	0.00
H	0.00	0	0.00	0.00	0.00	0.00	0	0.00	0.0	0.00	0.00	0	0.00	0.0	0.00	0	0.0	0.00	0	0.00
I	0.96	0	0.00	0.00	0.00	3.75	0	0.00	0.0	1.39	0.00	0	8.33	0.0	0.00	0	0.0	2.08	0	0.00
K	0.00	0	0.00	0.00	25.00	0.00	0	0.00	0.0	0.00	0.00	0	0.00	0.0	0.00	0	0.0	0.00	0	0.00
L	0.85	0	0.00	11.11	0.00	2.22	0	1.39	0.0	1.23	0.00	0	0.00	0.0	5.56	0	0.0	1.85	0	11.11
M	0.00	0	0.00	0.00	5.00	4.00	0	2.50	0.0	0.00	4.00	0	0.00	0.0	0.00	0	0.0	0.00	0	0.00
N	0.00	0	0.00	0.00	0.00	0.00	0	0.00	0.0	0.00	0.00	0	0.00	0.0	0.00	0	0.0	0.00	0	0.00
P	0.00	0	16.67	0.00	0.00	0.00	0	0.00	0.0	3.70	6.67	0	0.00	0.0	0.00	0	0.0	0.00	0	0.00
Q	0.00	0	0.00	0.00	12.50	0.00	0	0.00	0.0	0.00	0.00	0	16.67	0.0	0.00	0	0.0	0.00	0	0.00
R	0.00	0	0.00	0.00	0.00	0.00	0	0.00	0.0	0.00	0.00	0	0.00	25.0	0.00	0	50.0	0.00	0	0.00
S	0.00	0	0.00	0.00	0.00	0.00	0	0.00	0.0	0.00	0.00	0	0.00	0.0	0.00	0	0.0	0.00	0	0.00
T	0.00	0	0.00	0.00	0.00	0.00	0	0.00	0.0	0.00	0.00	0	0.00	50.0	0.00	0	0.0	0.00	0	0.00
V	1.28	0	8.33	0.00	0.00	1.67	0	0.00	0.0	0.00	10.00	0	0.00	0.0	0.00	0	0.0	0.00	0	0.00
W	0.00	0	0.00	0.00	0.00	0.00	0	0.00	0.0	0.00	0.00	0	0.00	0.0	0.00	0	0.0	0.00	0	0.00
Y	0.00	0	0.00	0.00	0.00	0.00	0	0.00	0.0	0.00	0.00	0	0.00	0.0	0.00	0	0.0	16.67	0	0.00

Sequence 3, Formula 1

In [18]:
```
pairwise(res3,1)
```

Out[18]:

	A	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y
A	9.38	0.0	4.00	0.00	4.17	15.38	0.0	4.17	0.00	0.00	0.00	4.76	5.00	0.00	0.00	0.00	4.35	4.17	0.00	0.00
C	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
D	4.00	0.0	0.00	6.67	0.00	3.12	0.0	0.00	6.67	0.00	0.00	0.00	0.00	7.14	7.14	4.17	0.00	5.88	6.67	0.00
E	4.55	0.0	6.67	0.00	7.14	6.90	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	4.76	0.00	0.00	0.00	0.00
F	12.50	0.0	0.00	7.14	0.00	0.00	0.0	6.25	0.00	0.00	0.00	0.00	0.00	0.00	0.00	4.35	0.00	6.25	0.00	6.25
G	7.69	0.0	9.38	0.00	0.00	2.17	0.0	6.45	3.45	9.38	4.17	0.00	0.00	7.14	3.57	2.63	3.33	6.45	0.00	6.45
H	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	5.88	0.00	0.00	0.00	10.00
I	0.00	0.0	0.00	14.29	0.00	6.45	10.0	0.00	7.14	0.00	0.00	0.00	8.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K	0.00	0.0	0.00	0.00	7.14	0.00	12.5	7.14	0.00	0.00	0.00	0.00	10.00	9.09	0.00	4.76	0.00	0.00	0.00	0.00
L	0.00	0.0	0.00	0.00	5.88	6.25	0.0	0.00	13.33	0.00	0.00	7.14	0.00	0.00	0.00	8.33	6.25	0.00	0.00	0.00
M	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	12.50	0.00	0.00	0.00
N	4.76	0.0	7.14	0.00	7.69	3.57	0.0	0.00	0.00	7.14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
P	0.00	0.0	0.00	0.00	8.33	0.00	0.0	8.33	0.00	0.00	0.00	11.11	0.00	0.00	0.00	0.00	0.00	8.33	0.00	0.00
Q	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.00	0.00	0.00	0.00	10.00	11.11	0.00	0.00	10.00	8.33	0.00	0.00	0.00
R	4.76	0.0	0.00	0.00	0.00	0.00	0.0	7.69	0.00	14.29	0.00	0.00	0.00	0.00	0.00	0.00	0.00	7.69	0.00	0.00
S	3.23	0.0	0.00	0.00	4.35	5.26	0.0	4.35	0.00	12.50	0.00	5.00	0.00	0.00	0.00	3.33	4.55	4.35	9.52	4.35
T	0.00	0.0	0.00	0.00	0.00	10.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	8.33	4.55	0.00	0.00	13.33
V	4.17	0.0	0.00	0.00	6.25	9.68	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	7.69	4.35	0.00	0.00	6.25
W	0.00	0.0	20.00	8.33	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	9.09	0.00	0.00	0.00	0.00	8.33	0.00
Y	0.00	0.0	0.00	7.14	0.00	0.00	0.0	0.00	7.14	0.00	0.00	0.00	0.00	0.00	7.69	8.70	6.67	0.00	14.29	0.00

Sequence 3, Formula 2

In [19]:
```
pairwise(res3,2)
```

Out[19]:

	A	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y
A	1.99	0.0	0.66	0.00	0.66	3.97	0.00	0.66	0.00	0.00	0.00	0.66	0.66	0.00	0.00	0.00	0.66	0.66	0.00	0.00
C	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
D	0.66	0.0	0.00	0.66	0.00	0.66	0.00	0.00	0.66	0.00	0.00	0.00	0.00	0.66	0.66	0.66	0.00	0.66	0.66	0.00
E	0.66	0.0	0.66	0.00	0.66	1.32	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.66	0.00	0.00	0.00	0.00
F	1.99	0.0	0.00	0.66	0.00	0.00	0.00	0.66	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.66	0.00	0.66	0.00	0.66
G	1.99	0.0	1.99	0.00	0.00	0.66	0.00	1.32	0.66	1.99	0.66	0.00	0.00	1.32	0.66	0.66	0.66	1.32	0.00	1.32
H	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.66	0.00	0.00	0.00	0.66
I	0.00	0.0	0.00	1.32	0.00	1.32	0.66	0.00	0.66	0.00	0.00	0.00	0.66	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K	0.00	0.0	0.00	0.00	0.66	0.00	0.66	0.66	0.00	0.00	0.00	0.00	0.66	0.66	0.00	0.66	0.00	0.00	0.00	0.00
L	0.00	0.0	0.00	0.00	0.66	1.32	0.00	0.00	1.32	0.00	0.00	0.66	0.00	0.00	0.00	1.32	0.66	0.00	0.00	0.00
M	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.66	0.00	0.00	0.00
N	0.66	0.0	0.66	0.00	0.66	0.66	0.00	0.00	0.00	0.66	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
P	0.00	0.0	0.00	0.00	0.66	0.00	0.00	0.66	0.00	0.00	0.00	0.66	0.00	0.00	0.00	0.00	0.00	0.66	0.00	0.00
Q	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.66	0.66	0.00	0.00	1.32	0.66	0.00	0.00	0.00
R	0.66	0.0	0.00	0.00	0.00	0.00	0.00	0.66	0.00	1.32	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.66	0.00	0.00
S	0.66	0.0	0.00	0.00	0.66	1.32	0.00	0.66	0.00	1.99	0.00	0.66	0.00	0.00	0.00	0.66	0.66	0.66	1.32	0.66
T	0.00	0.0	0.00	0.00	0.00	1.99	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.66	0.66	0.00	0.00	0.00	1.32
V	0.66	0.0	0.00	0.00	0.66	1.99	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.66	0.66	0.00	0.00	0.00	0.66
W	0.00	0.0	1.99	0.66	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.66	0.00	0.00	0.00	0.00	0.66	0.00
Y	0.00	0.0	0.00	0.66	0.00	0.00	0.00	0.00	0.66	0.00	0.00	0.00	0.00	0.00	0.66	1.32	0.66	0.00	1.32	0.00

Sequence 3, Formula 3

In [20]:
```
pairwise(res3,3)
```

Out[20]:

	A	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y
A	1.17	0	0.69	0.00	0.78	1.63	0.00	0.78	0.00	0.00	0.00	1.25	1.56	0.00	0.00	0.00	0.89	0.78	0.00	0.00
C	0.00	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
D	0.69	0	0.00	1.85	0.00	0.48	0.00	0.00	1.85	0.00	0.00	0.00	0.00	2.22	2.22	0.74	0.00	1.39	1.85	0.00
E	1.04	0	1.85	0.00	2.08	1.45	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.11	0.00	0.00	0.00	0.00
F	2.34	0	0.00	2.08	0.00	0.00	0.00	1.56	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.83	0.00	1.56	0.00	1.56
G	0.82	0	1.45	0.00	0.00	0.19	0.00	1.09	0.72	1.45	4.35	0.00	0.00	1.74	0.87	0.29	0.62	1.09	0.00	1.09
H	0.00	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.33	0.00	0.00	0.00	6.25
I	0.00	0	0.00	4.17	0.00	1.09	6.25	0.00	2.08	0.00	0.00	0.00	3.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K	0.00	0	0.00	0.00	2.08	0.00	8.33	2.08	0.00	0.00	0.00	0.00	4.17	3.33	0.00	1.11	0.00	0.00	0.00	0.00
L	0.00	0	0.00	0.00	1.39	0.97	0.00	0.00	3.70	0.00	0.00	2.22	0.00	0.00	0.00	1.48	1.59	0.00	0.00	0.00
M	0.00	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	14.29	0.00	0.00	0.00
N	1.25	0	2.22	0.00	2.50	0.87	0.00	0.00	0.00	2.22	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
P	0.00	0	0.00	0.00	3.12	0.00	0.00	3.12	0.00	0.00	0.00	5.00	0.00	0.00	0.00	0.00	0.00	3.12	0.00	0.00
Q	0.00	0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	4.00	5.00	0.00	0.00	2.67	2.86	0.00	0.00	0.00
R	1.25	0	0.00	0.00	0.00	0.00	0.00	2.50	0.00	4.44	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.50	0.00	0.00
S	0.42	0	0.00	0.00	0.83	0.58	0.00	0.83	0.00	2.22	0.00	1.33	0.00	0.00	0.00	0.44	0.95	0.83	2.22	0.83
T	0.00	0	0.00	0.00	0.00	1.86	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.86	0.95	0.00	0.00	0.00	3.57
V	0.78	0	0.00	0.00	1.56	1.63	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.50	0.83	0.00	0.00	0.00	1.56
W	0.00	0	5.56	2.78	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.33	0.00	0.00	0.00	0.00	2.78	0.00
Y	0.00	0	0.00	2.08	0.00	0.00	0.00	0.00	2.08	0.00	0.00	0.00	0.00	0.00	2.50	1.67	1.79	0.00	4.17	0.00

Top pair preferences

In [78]:

```
def pref(res,type):
    if res == res1:
        s = 1
    elif res == res2:
        s = 2
    else:
        s = 3
    print(f'\t\tSequence {s}, Formula {type}\n')
    df = pd.DataFrame(sorted(zip(np.array(pairwise(res,type)).flatten(), [x+y for x in sorted(aas) for y in sorted
    df.columns = ['Preference', 'Residue']
    df.index = df.Residue
    return df.drop(axis = 1, columns = ['Residue']).T
```

In [85]:

```
for res in [res1,res2,res3]:
    for t in [1,2,3]:
        display(pref(res,t))
```

Sequence 1, Formula 1

Residue	FN	CF	DE	YD	VG	NR	GI	GC	EY	WT
Preference	50.0	50.0	25.0	20.0	20.0	20.0	20.0	20.0	20.0	18.18

Sequence 1, Formula 2

Residue	AT	AA	WT	TP	TA	HA	AL	YL	YD	YA
Preference	4.48	4.48	2.99	2.99	2.99	2.99	2.99	1.49	1.49	1.49

Sequence 1, Formula 3

Residue	FN	CF	VG	NR	GI	GC	DE	QK	PV	KQ
Preference	100.0	100.0	25.0	25.0	25.0	25.0	25.0	20.0	20.0	20.0

Sequence 2, Formula 1

Residue	TQ	RT	VM	RQ	GL	QP	PD	KF	IP	QF
Preference	33.33	33.33	27.27	25.0	21.05	20.0	20.0	20.0	18.18	16.67

Sequence 2, Formula 2

Residue	GL	AA	VM	IG	AV	AI	MG	LG	IP	GI
Preference	5.88	5.88	4.41	4.41	4.41	4.41	2.94	2.94	2.94	2.94

Sequence 2, Formula 3

Residue	TQ	RT	RQ	KF	YV	QP	PD	QF	LY	LE
Preference	50.0	50.0	25.0	25.0	16.67	16.67	16.67	12.5	11.11	11.11

Sequence 3, Formula 1

Residue	WD	AG	YW	RL	IE	TY	LK	SL	MT	KH
Preference	20.0	15.38	14.29	14.29	14.29	13.33	13.33	12.5	12.5	12.5

Sequence 3, Formula 2

Residue	AG	WD	VG	TG	SL	GL	GD	GA	FA	AA
Preference	3.97	1.99	1.99	1.99	1.99	1.99	1.99	1.99	1.99	1.99

Sequence 3, Formula 3

Residue	MT	KH	IH	HY	WD	QP	PN	RL	GM	YW
Preference	14.29	8.33	6.25	6.25	5.56	5.0	5.0	4.44	4.35	4.17

Question 5

In [147…

```
text = open("properties.txt").read()
order = re.search('Property.*',text).group(0)
order = [mapping[x.upper()] for x in order.split(' ') if x != '' and x != 'Property']
hgm = re.search('Hgm.*',text).group(0)
hgm = [float(x) for x in hgm.split(' ') if x != '' and x != 'Hgm']
et = re.search('Et.*',text).group(0)
et = [float(x) for x in et.split(' ') if x != '' and x != 'Et']
ca = re.search('Ca.*',text).group(0)
ca = [float(x) for x in ca.split(' ') if x != '' and x != 'Ca']
d = {x : (a,b,c) for x,a,b,c in zip(order,hgm,ca,et)}
```

In [154…

```
def prop(res,p):
    if p == 1:
        return sum([d[r][p-1] for r in res])/len(res)
    if p == 2 or p == 3:
        return sum([d[r][p-1] for r in res])
```

In [160…

```
for res in [res1,res2,res3]:
    for p,name in zip([1,2,3],['Average hydrophobicity', 'Helical contact area', 'Total non-bonded energy']):
        print(f"{name} : {prop(res,p)}")
    print('--------------')
```

```
Average hydrophobicity : 13.352537313432844
Helical contact area : 2156.0
Total non-bonded energy : 117.74000000000005
--------------
Average hydrophobicity : 13.77161764705882
Helical contact area : 2067.0
Total non-bonded energy : 126.66000000000003
--------------
Average hydrophobicity : 13.418675496688737
Helical contact area : 4616.0
Total non-bonded energy : 267.7500000000001
--------------
```

- Hydrophobicites of all sequences are similar
- Sequnece 3 appears to exist in a alpha helix
- Sequnece 3 has high non bounded enegry because of the prescence of glycine