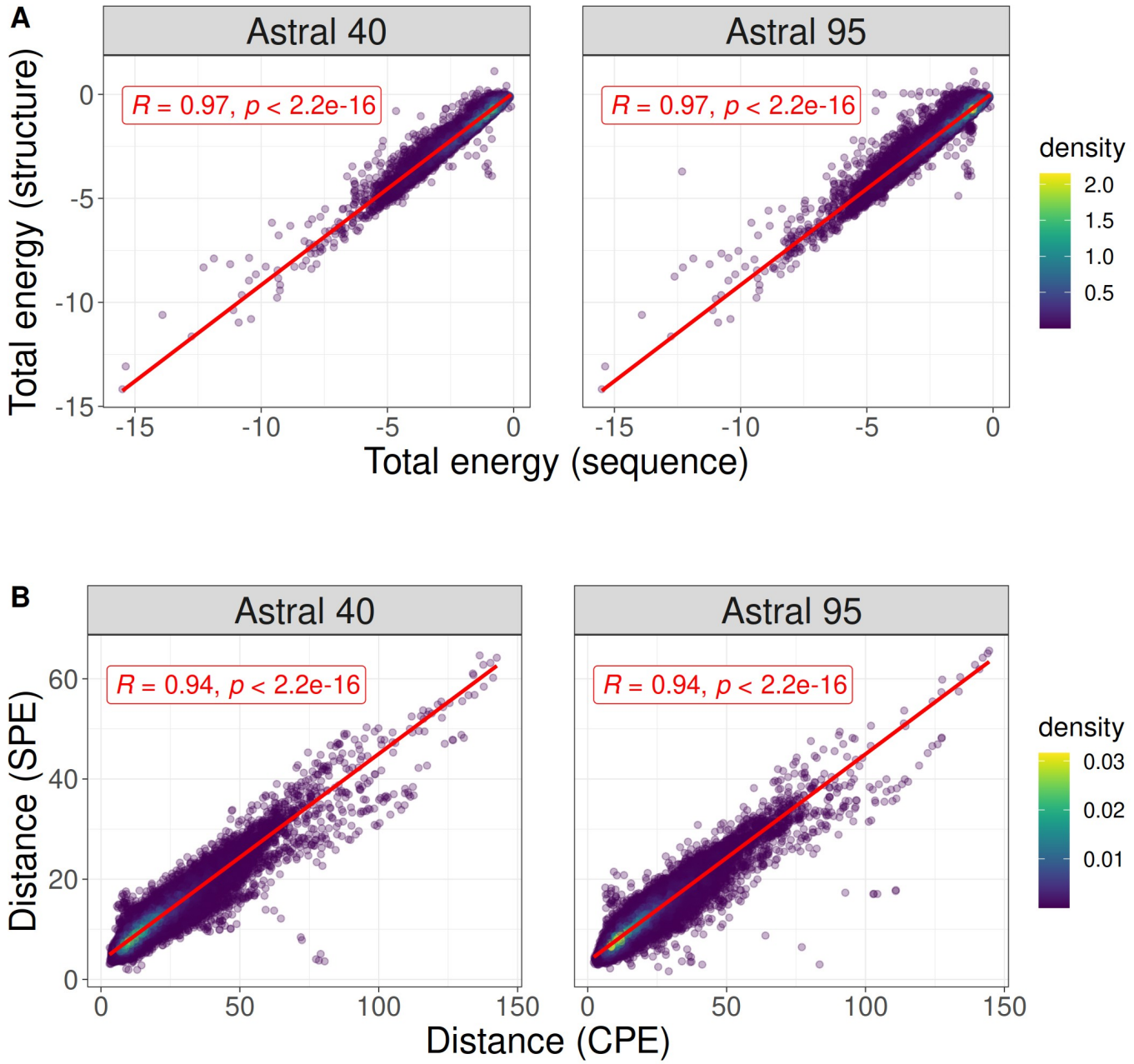
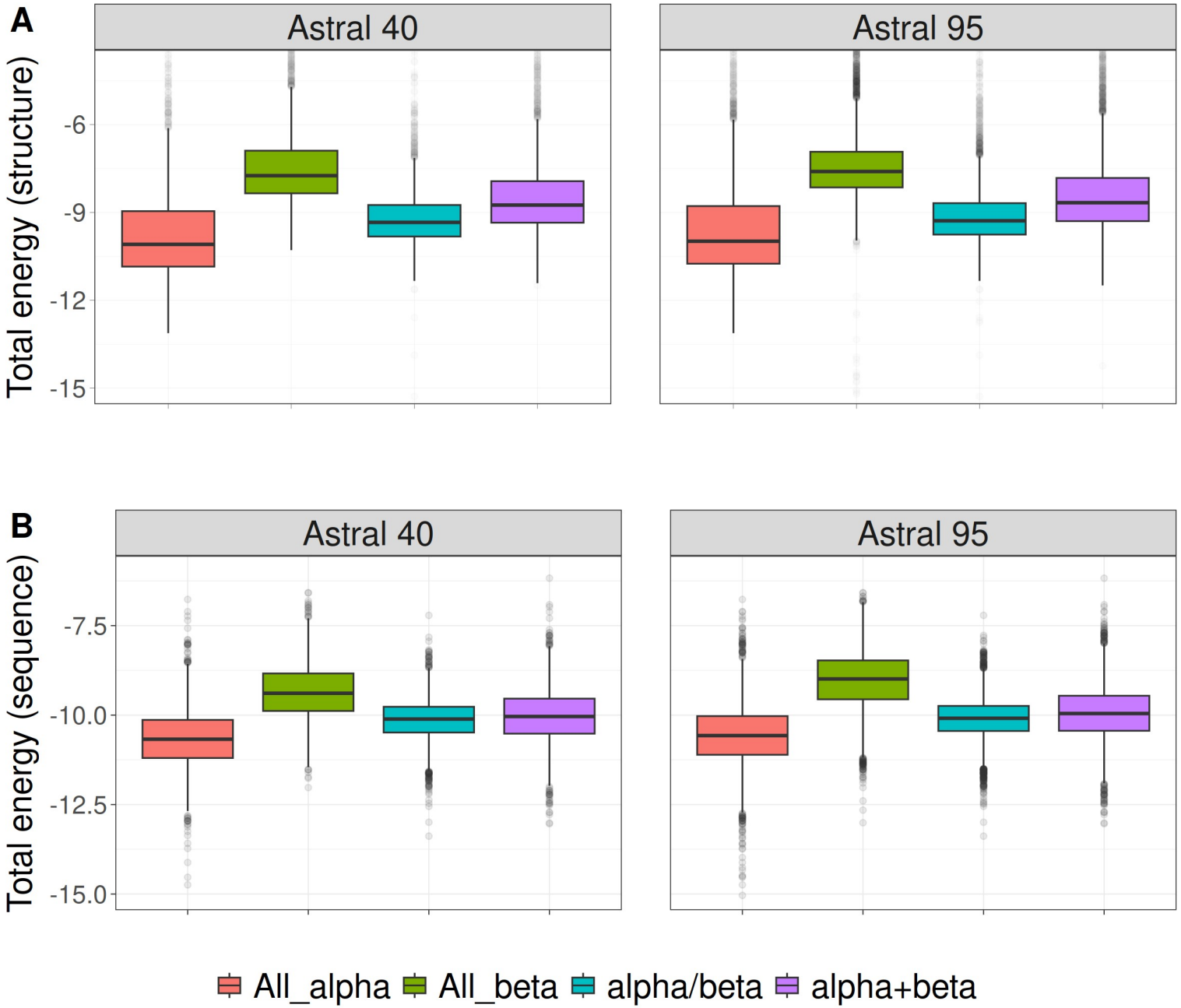
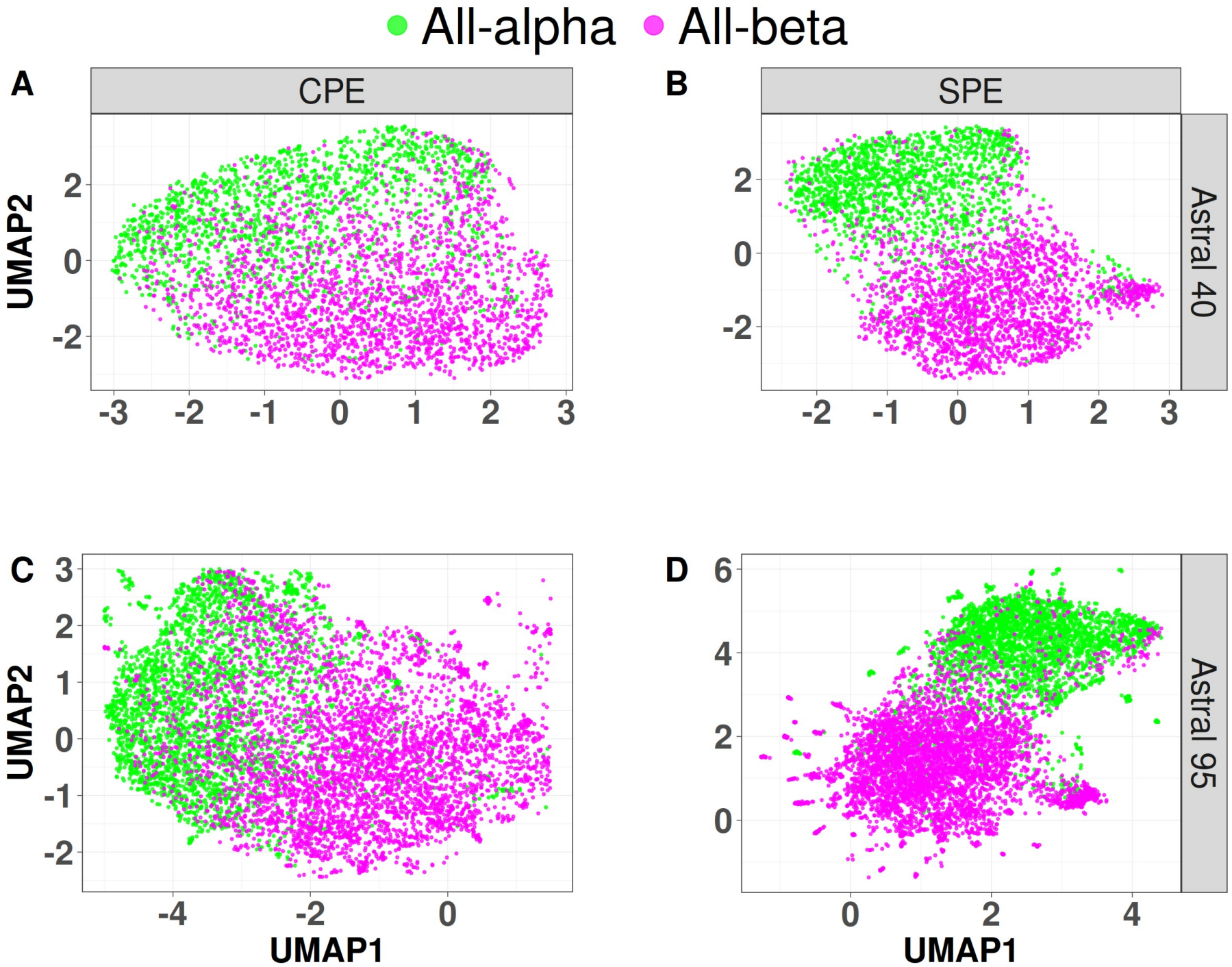
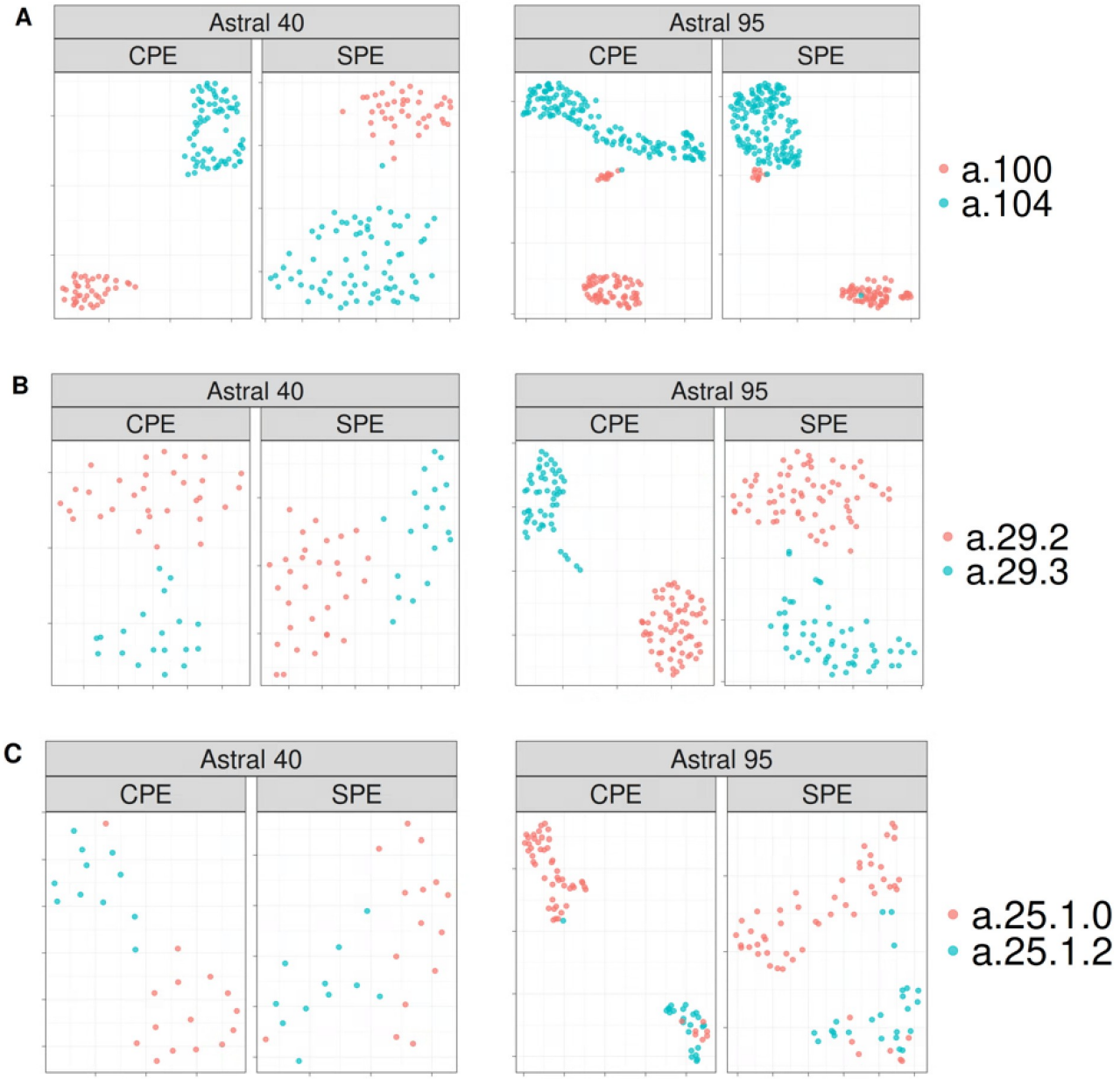
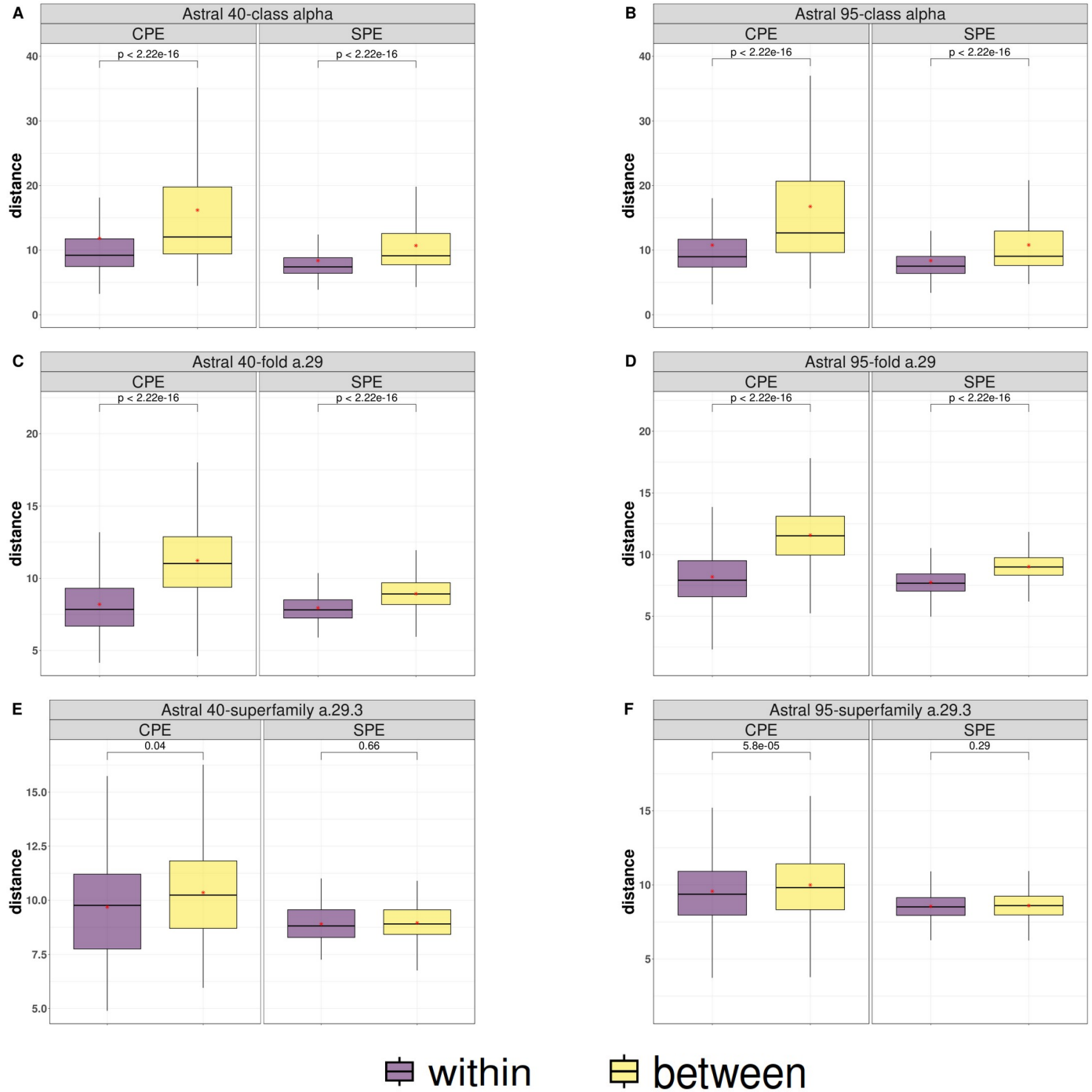

A
Astral 40
Astral 95
R = 0.97, p < 2.2e-16
R = 0.97, p < 2.2e-16
Total energy (structure)
Total energy (sequence)
density
2.0
1.5
1.0
0.5
B
Astral 40
Astral 95
R = 0.94, p < 2.2e-16
R = 0.94, p < 2.2e-16
Distance (SPE)
Distance (CPE)
density
0.03
0.02
0.01

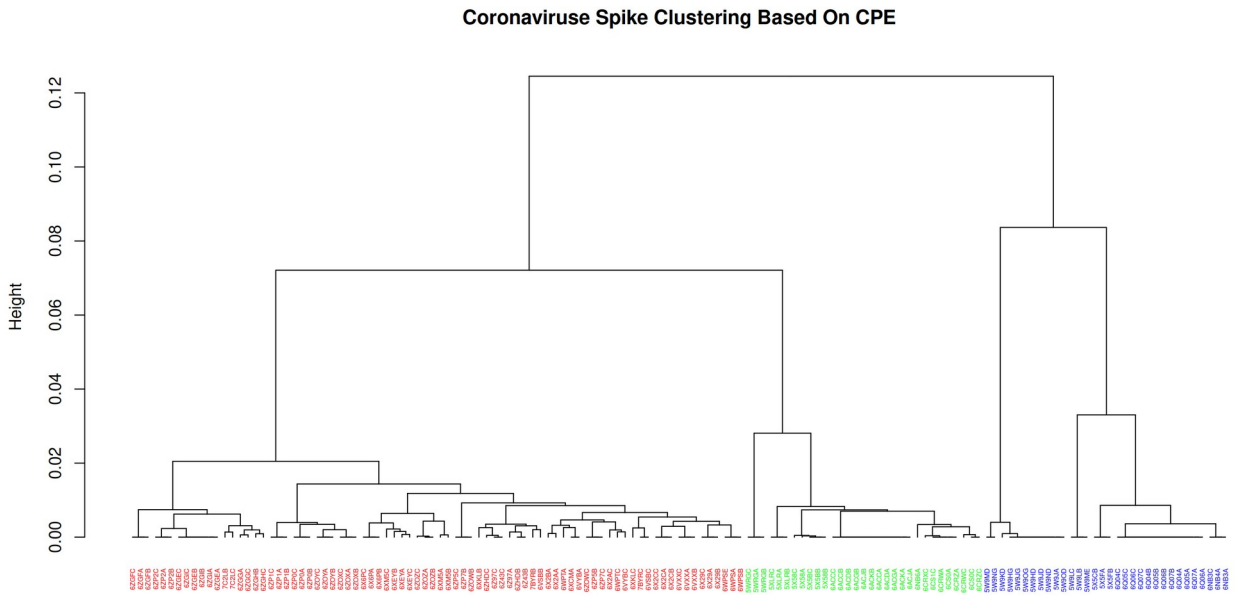

A
Astral 40
Astral 95
Total energy (structure)
-6
-9
-12
-15
B
Astral 40
Astral 95
Total energy (sequence)
-7.5
-10.0
-12.5
-15.0
All_alpha
All_beta
alpha/beta
alpha+beta


All-alpha
All-beta
A
CPE
B
SPE
Astral 40
C
D
Astral 95
UMAP1
UMAP2

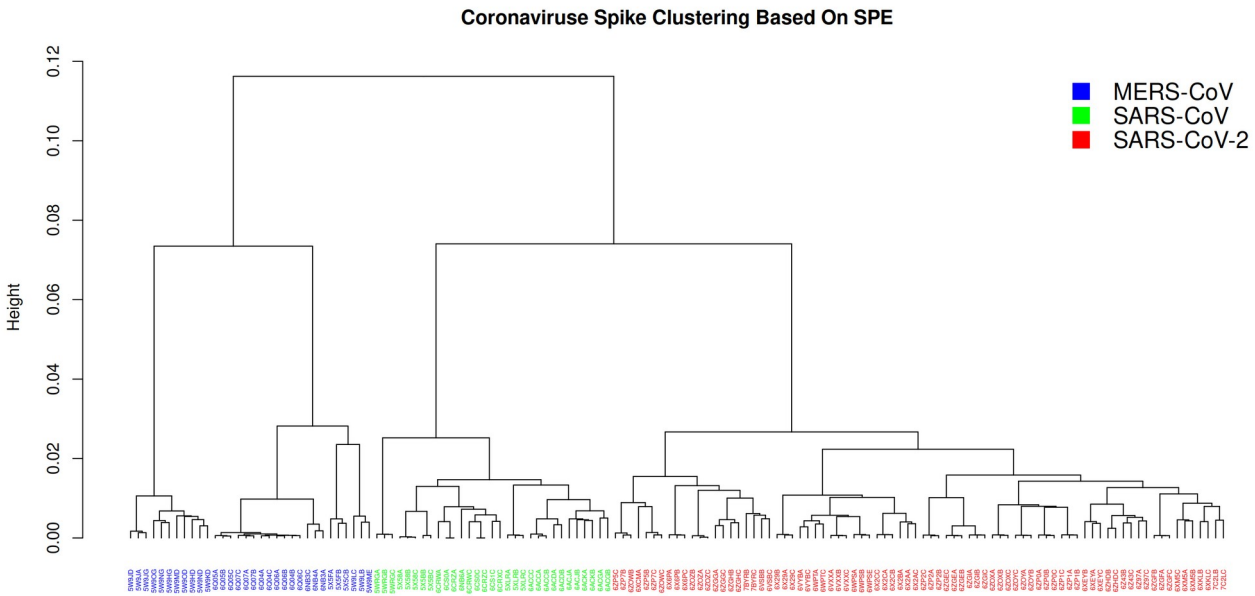

A
Astral 40
CPE
SPE
Astral 95
CPE
SPE
a.100
a.104
B
Astral 40
CPE
SPE
Astral 95
CPE
SPE
a.29.2
a.29.3
C
Astral 40
CPE
SPE
Astral 95
CPE
SPE
a.25.1.0
a.25.1.2

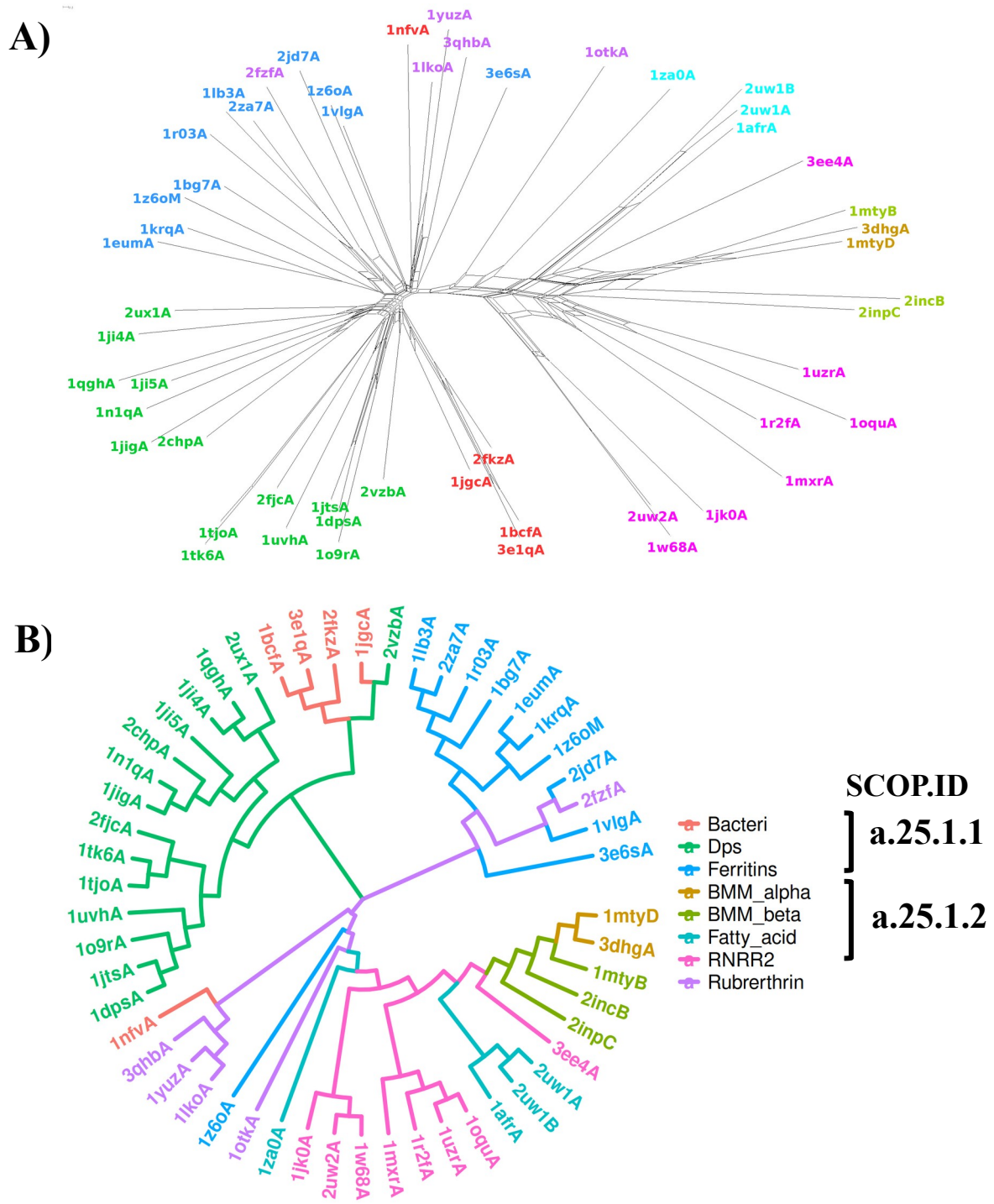

A
Astral 40-class alpha
CPE
SPE
p < 2.22e-16
p < 2.22e-16
distance
B
Astral 95-class alpha
CPE
SPE
p < 2.22e-16
p < 2.22e-16
distance
C
Astral 40-fold a.29
CPE
SPE
p < 2.22e-16
p < 2.22e-16
distance
D
Astral 95-fold a.29
CPE
SPE
p < 2.22e-16
p < 2.22e-16
distance
E
Astral 40-superfamily a.29.3
CPE
SPE
0.04
0.66
distance
F
Astral 95-superfamily a.29.3
CPE
SPE
5.8e-05
0.29
distance
within
between

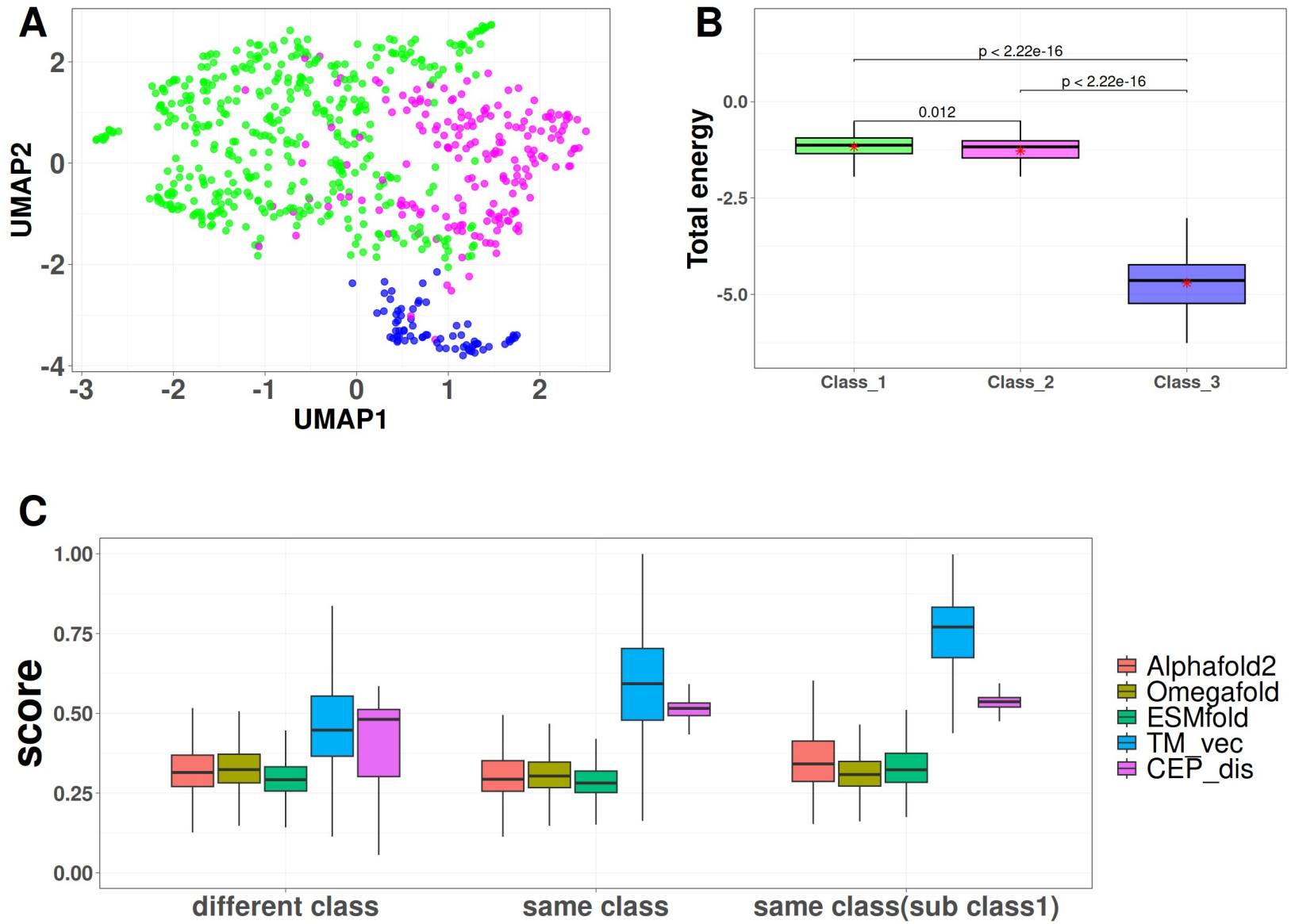
A)

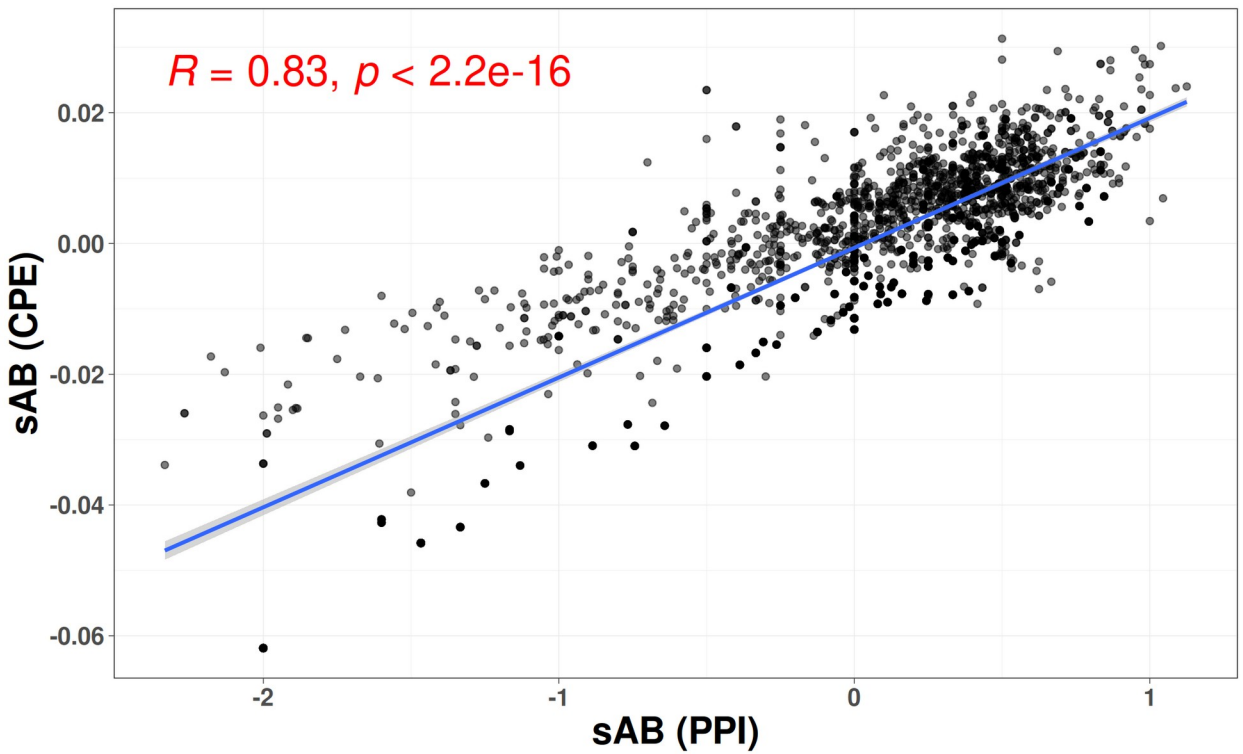

Coronaviruse Spike Clustering Based On CPE
Height
0.00
0.02
0.04
0.06
0.08
0.10
0.12

B)


Coronaviruse Spike Clustering Based On SPE
Height
0.00
0.02
0.04
0.06
0.08
0.10
0.12
MERS-CoV
SARS-CoV
SARS-CoV-2


A)
1yuzA
1nfvA
3qhbA
1lkoA
3e6sA
1otkA
1za0A
2uw1B
2uw1A
1afrA
3ee4A
1mtyB
3dhgA
1mtyD
2incB
2inpC
1uzrA
1r2fA
1oquA
1mxrA
1jk0A
2uw2A
1w68A
2fkzA
1jgcA
1bcfA
3e1qA
2vzbA
2fjcA
1jtsA
1dpsA
1o9rA
1uvhA
1tjoA
1tk6A
2ux1A
1ji4A
1qghA
1ji5A
1n1qA
1jigA
2chpA
2jd7A
2fzfA
1lb3A
2za7A
1z6oA
1vlgA
1r03A
1bg7A
1z6oM
1krqA
1eumA
B)
Bacteri
Dps
Ferritins
BMM_alpha
BMM_beta
Fatty_acid
RNRR2
Rubrerthrin
SCOP.ID
a.25.1.1
a.25.1.2


A
UMAP2
UMAP1
2
0
-2
-4
-3
-2
-1
0
1
2
B
Total energy
p < 2.22e-16
p < 2.22e-16
0.012
0.0
-2.5
-5.0
Class_1
Class_2
Class_3
C
score
1.00
0.75
0.50
0.25
0.00
different class
same class
same class(sub class1)
Alphafold2
Omegafold
ESMfold
TM_vec
CEP_dis


R = 0.83, p < 2.2e-16
0.02
0.00
-0.02
-0.04
-0.06
sAB (CPE)
-2
-1
0
1
sAB (PPI)