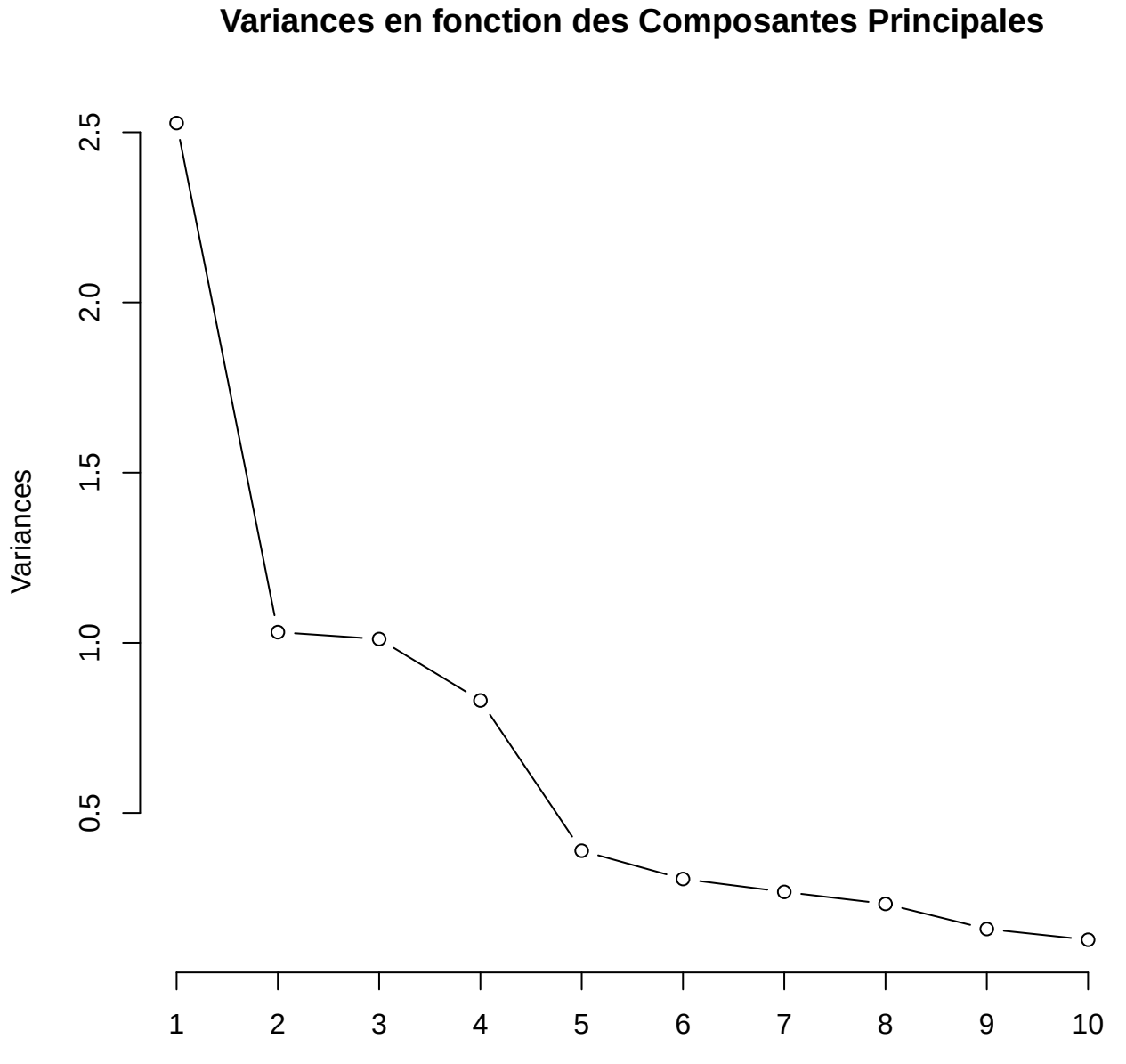
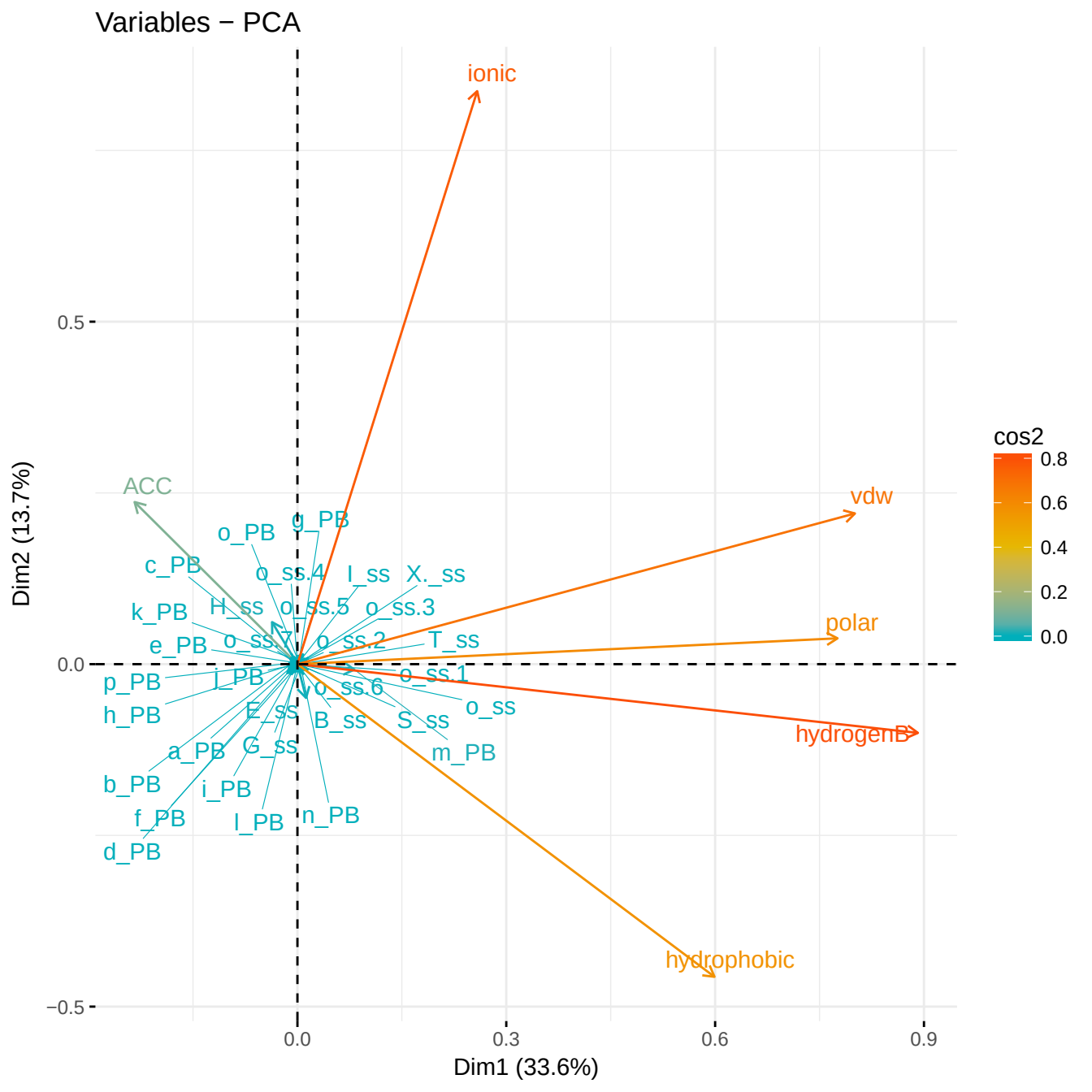
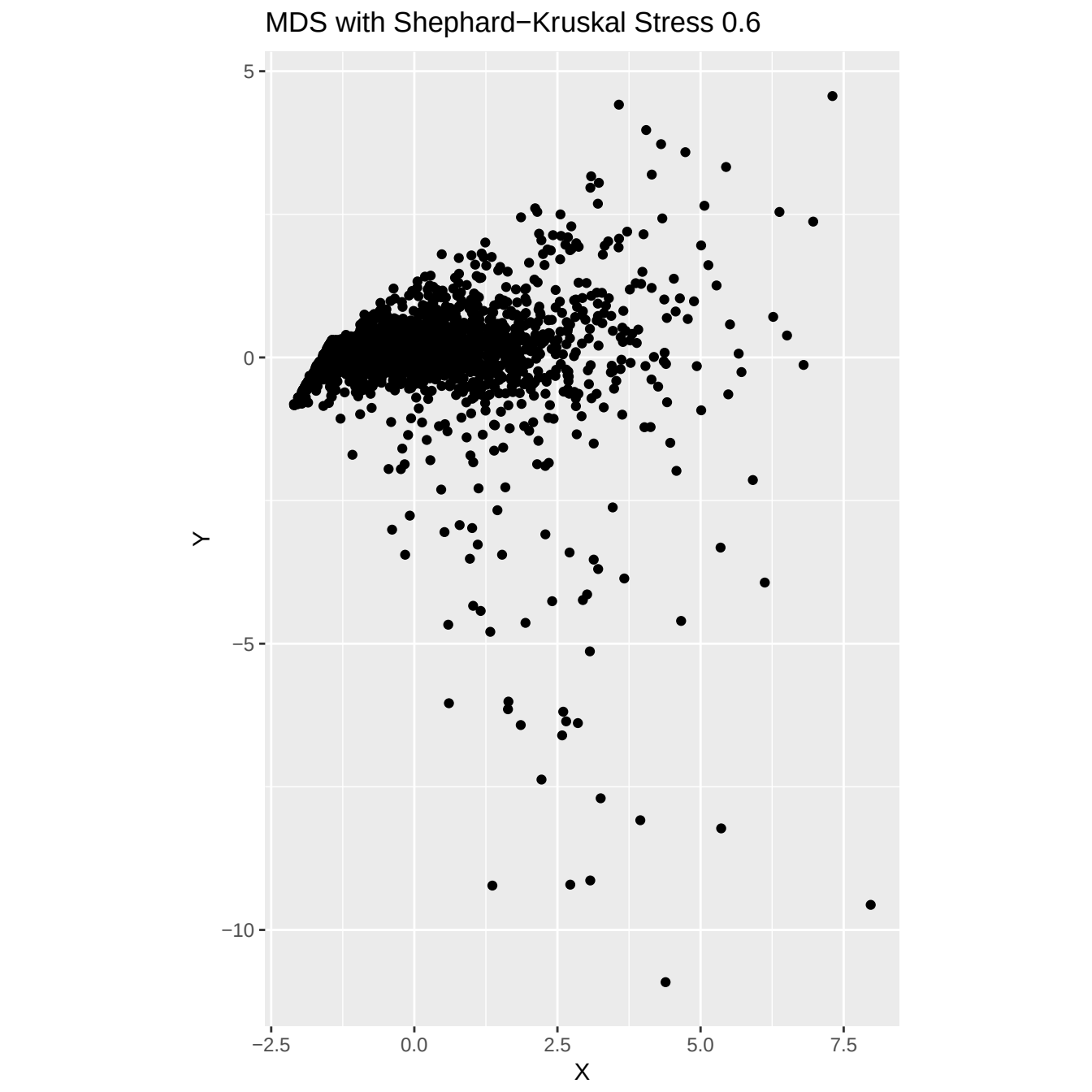
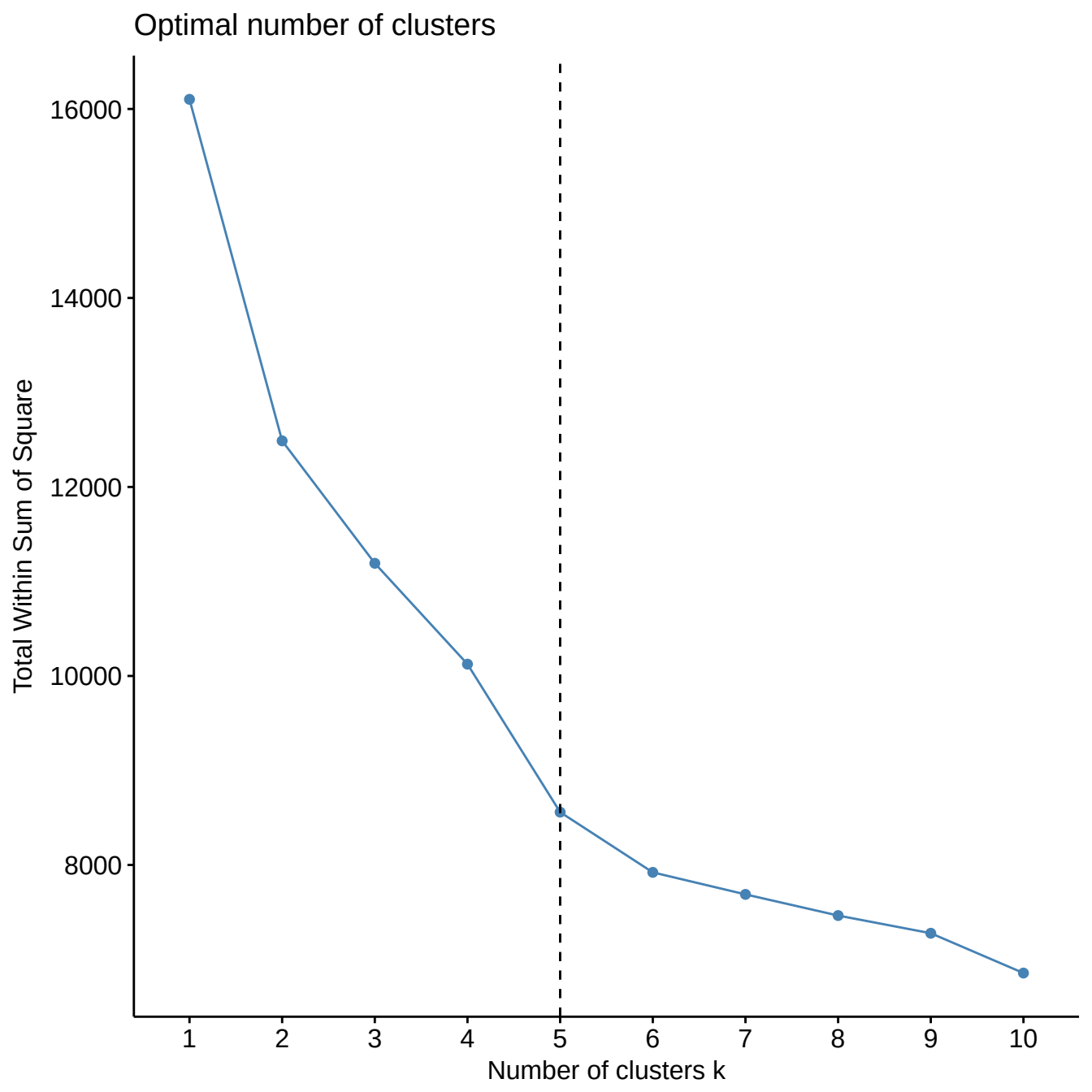
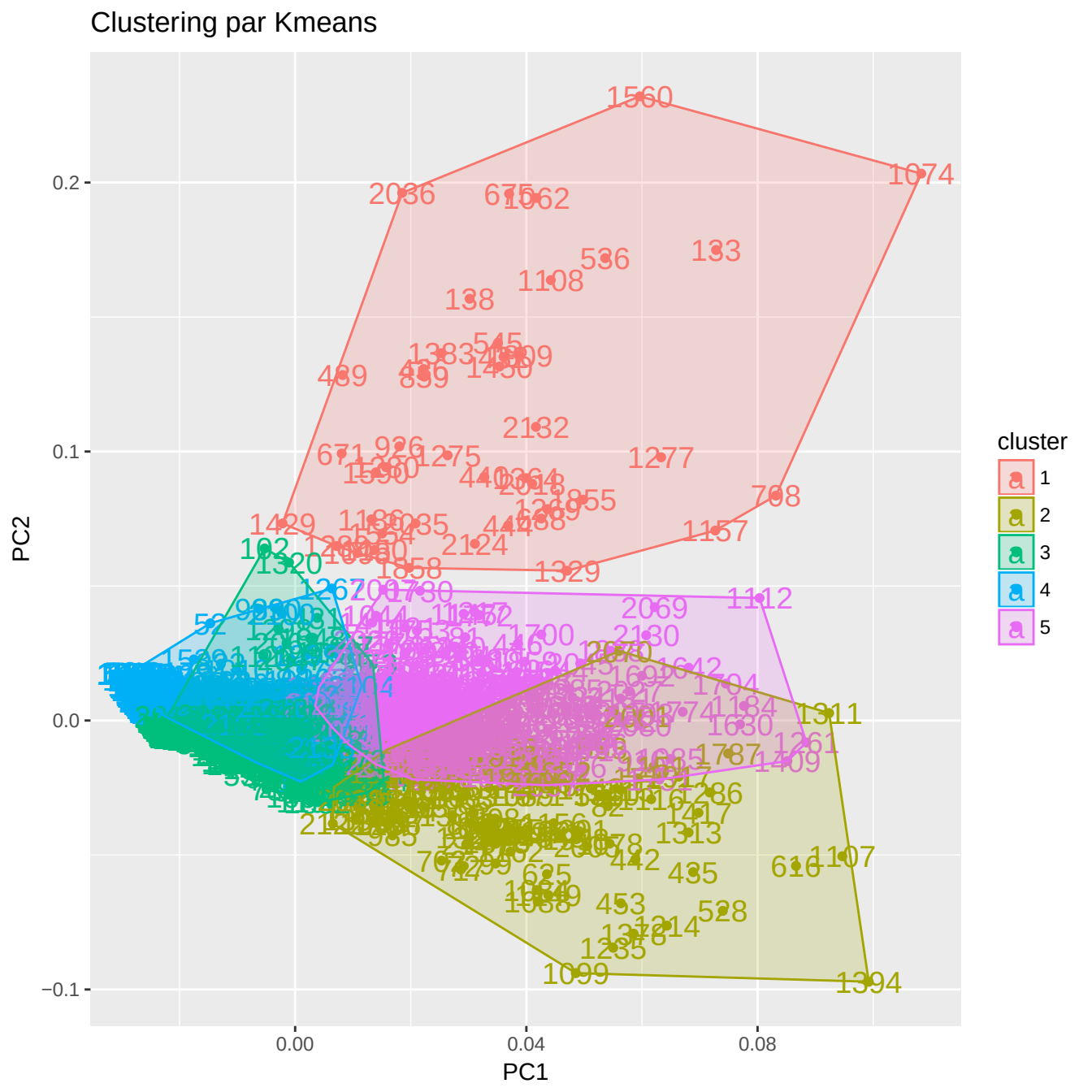
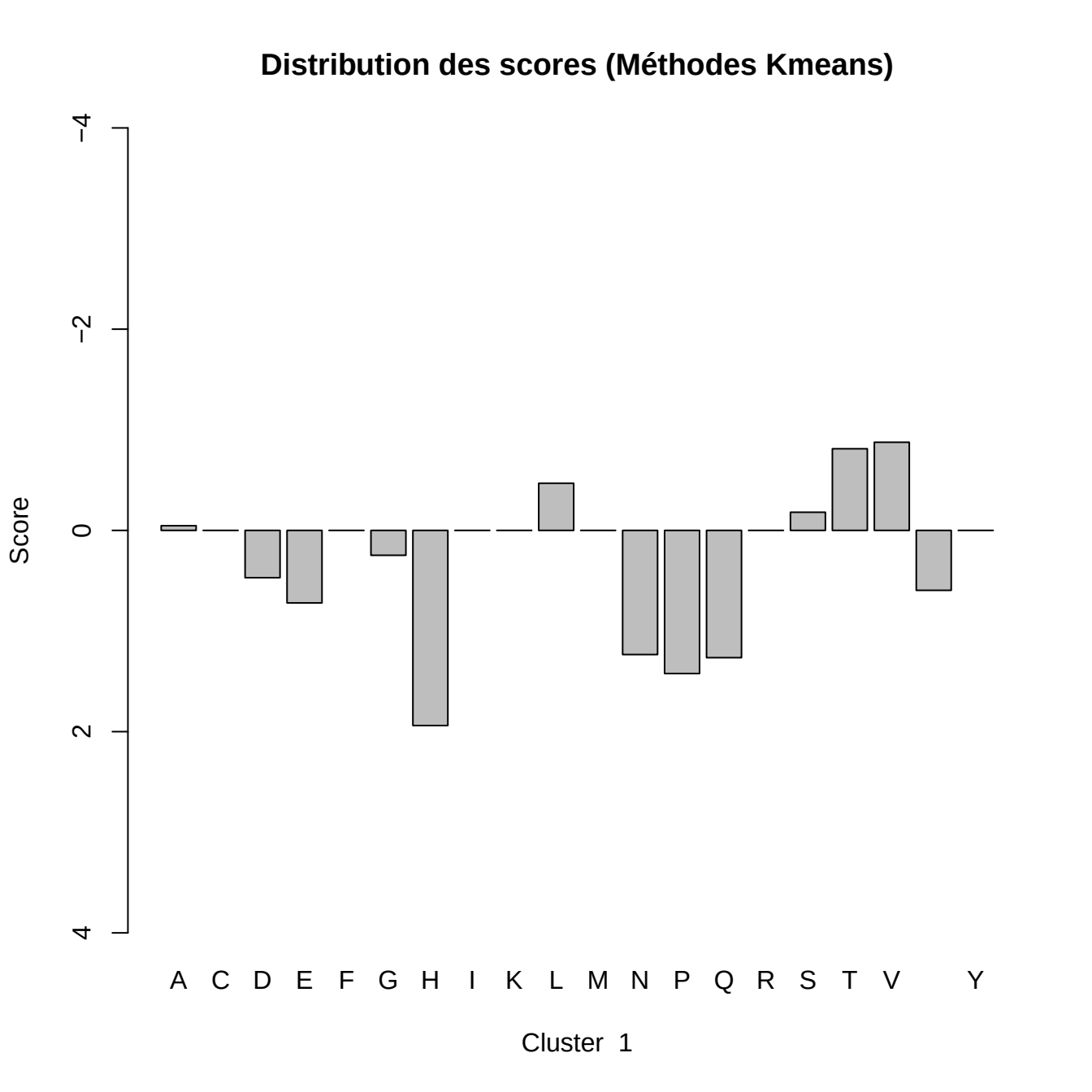

Variances en fonction des Composantes Principales
Variances
0.5
1.0
1.5
2.0
2.5
1
2
3
4
5
6
7
8
9
10

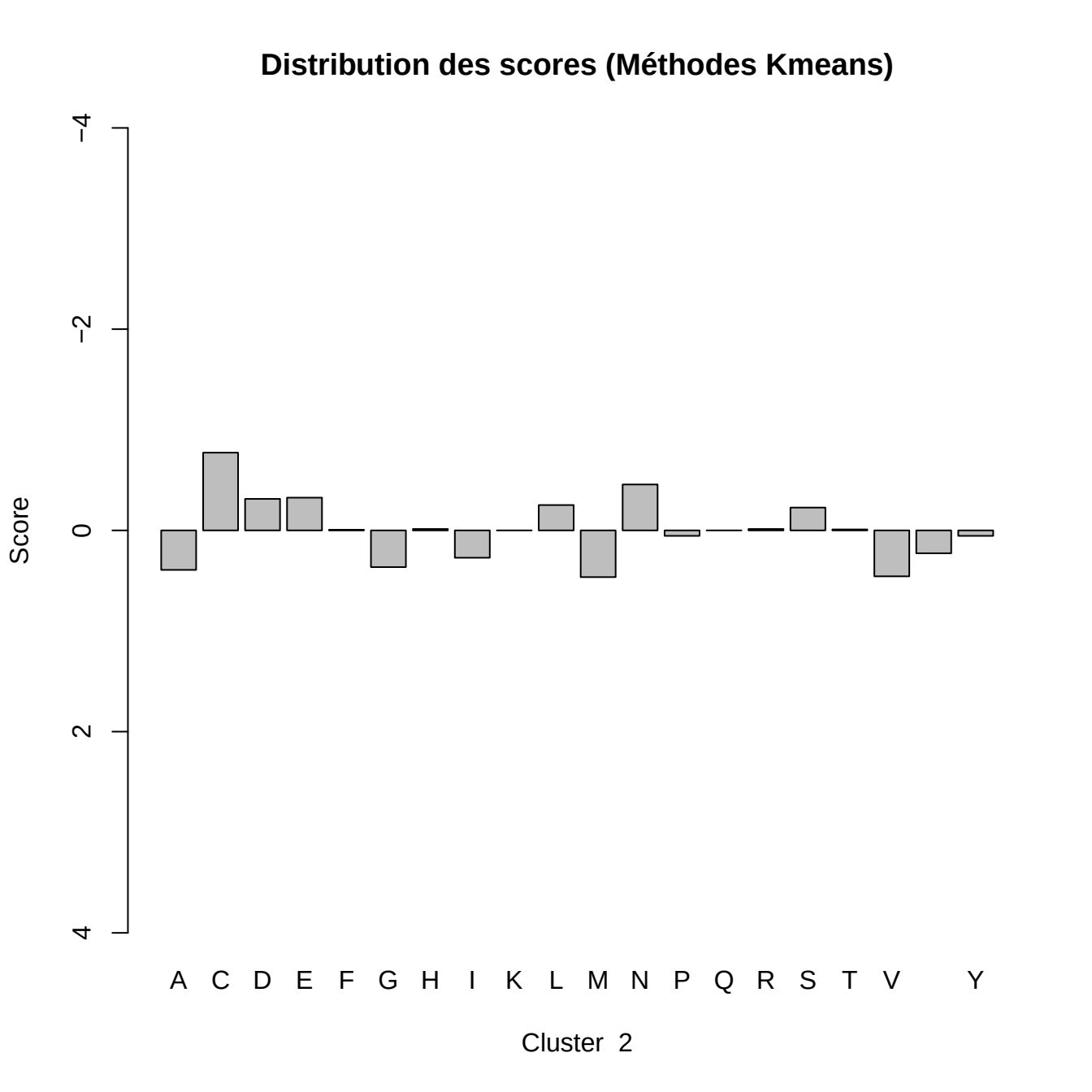

Variables − PCA
ionic
vdw
polar
hydrogenB
hydrophobic
ACC
o_PB
g_PB
c_PB
o_ss.4
l_ss
X._ss
k_PB
H_ss
o_ss.5
o_ss.3
e_PB
o_ss.7
o_ss.2
T_ss
p_PB
l_PB
o_ss.1
o_ss.6
h_PB
E_ss
B_ss
S_ss
o_ss
a_PB
G_ss
m_PB
b_PB
i_PB
f_PB
l_PB
n_PB
d_PB
cos2
0.8
0.6
0.4
0.2
0.0
0.5
0.0
−0.5
Dim2 (13.7%)
0.0
0.3
0.6
0.9
Dim1 (33.6%)

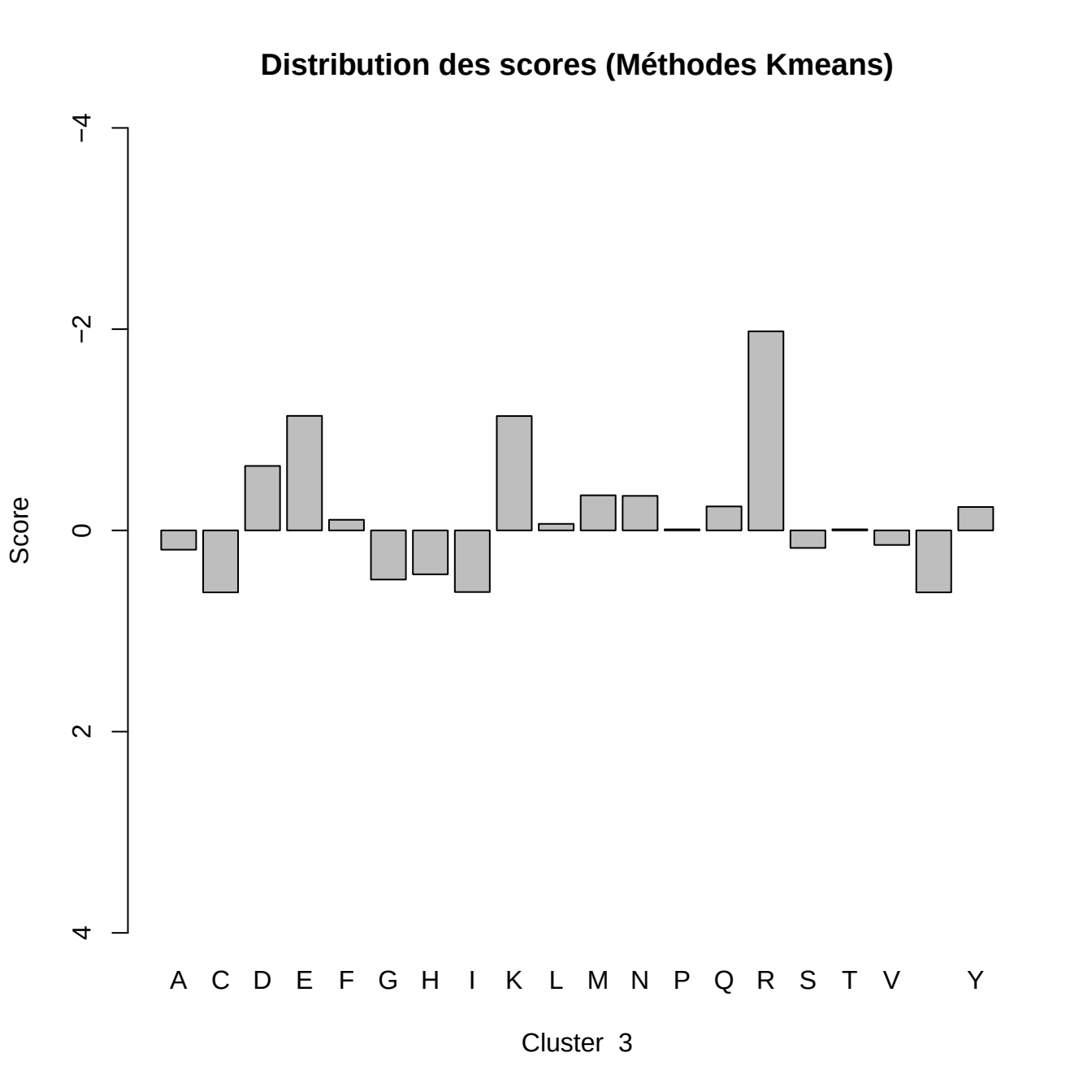

MDS with Shephard−Kruskal Stress 0.6
5
0
−5
−10
Y
−2.5
0.0
2.5
5.0
7.5
X

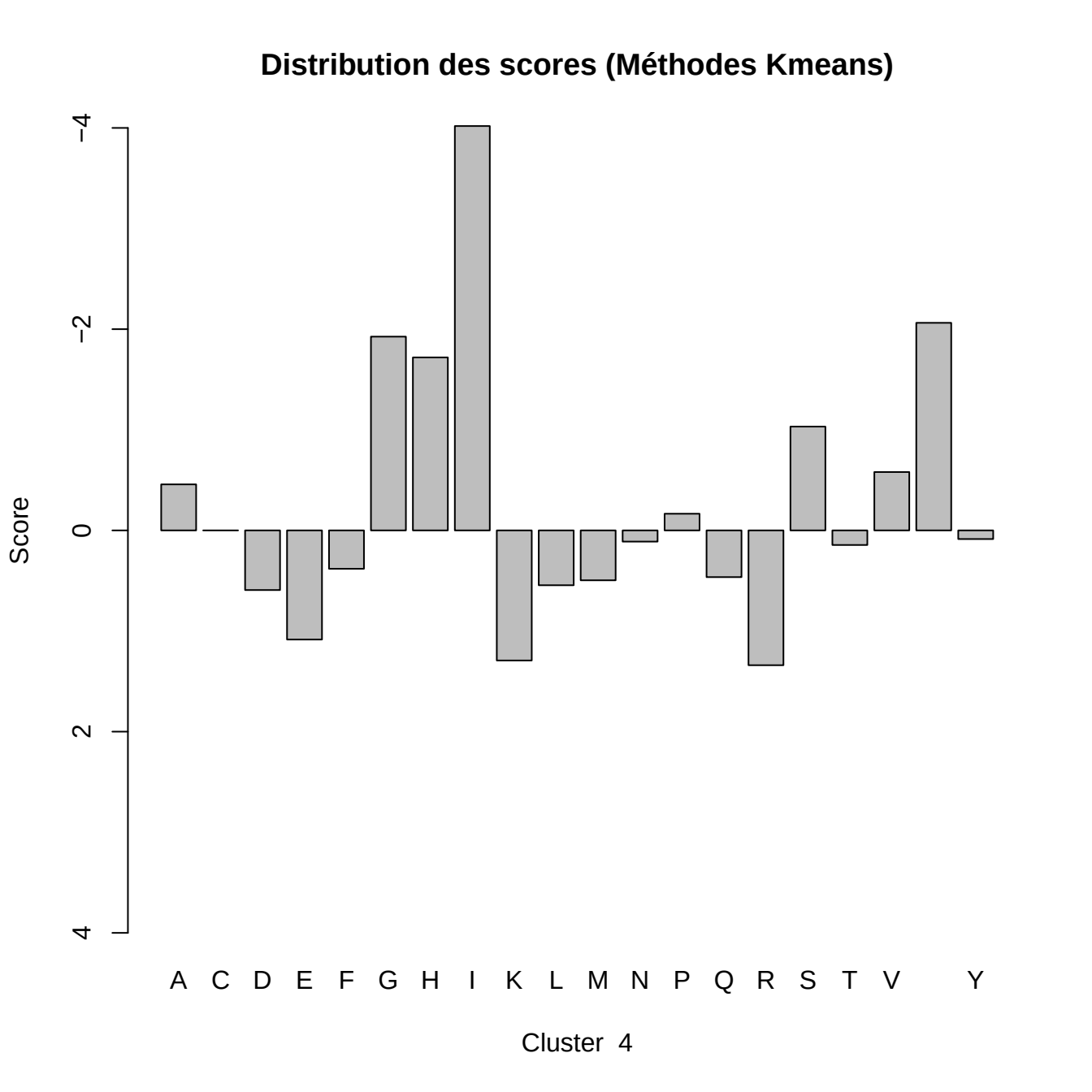

Optimal number of clusters
Total Within Sum of Square
16000
14000
12000
10000
8000
1
2
3
4
5
6
7
8
9
10
Number of clusters k

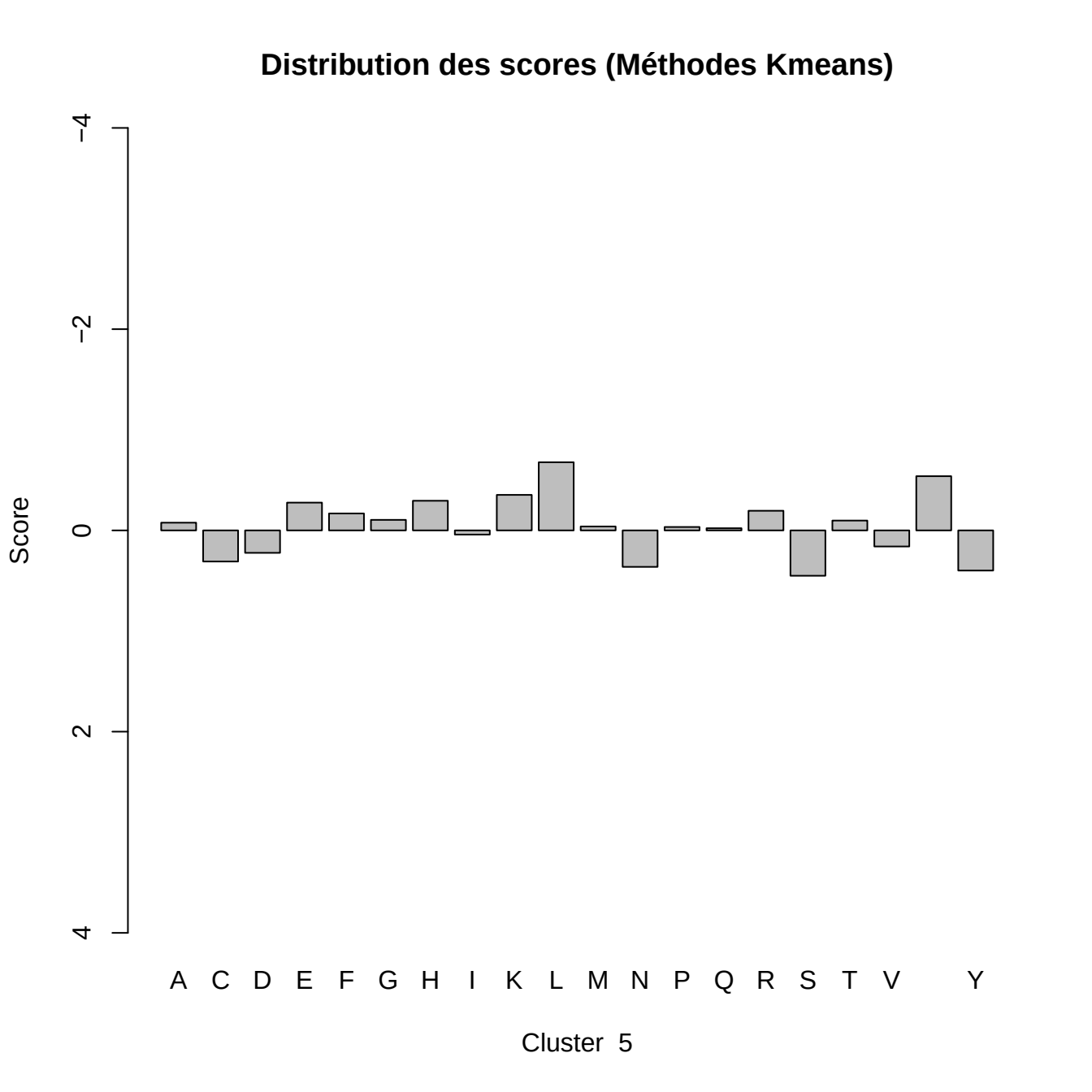

Clustering par Kmeans
PC2
PC1
0.2
0.1
0.0
−0.1
0.00
0.04
0.08
cluster
1
2
3
4
5

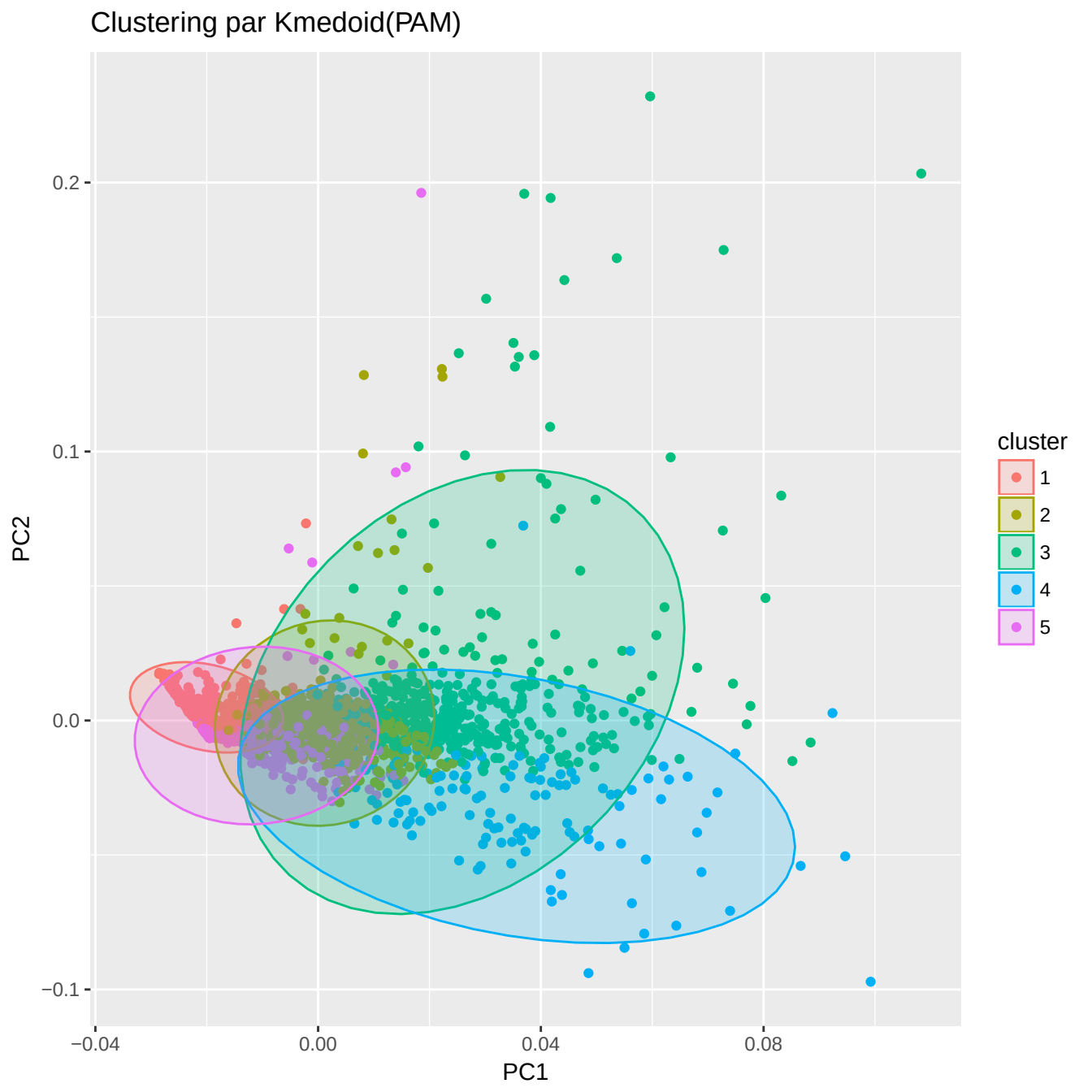

Distribution des scores (Méthodes Kmeans)
Score
−4
−2
0
2
4
A C D E F G H I K L M N P Q R S T V Y
Cluster 1

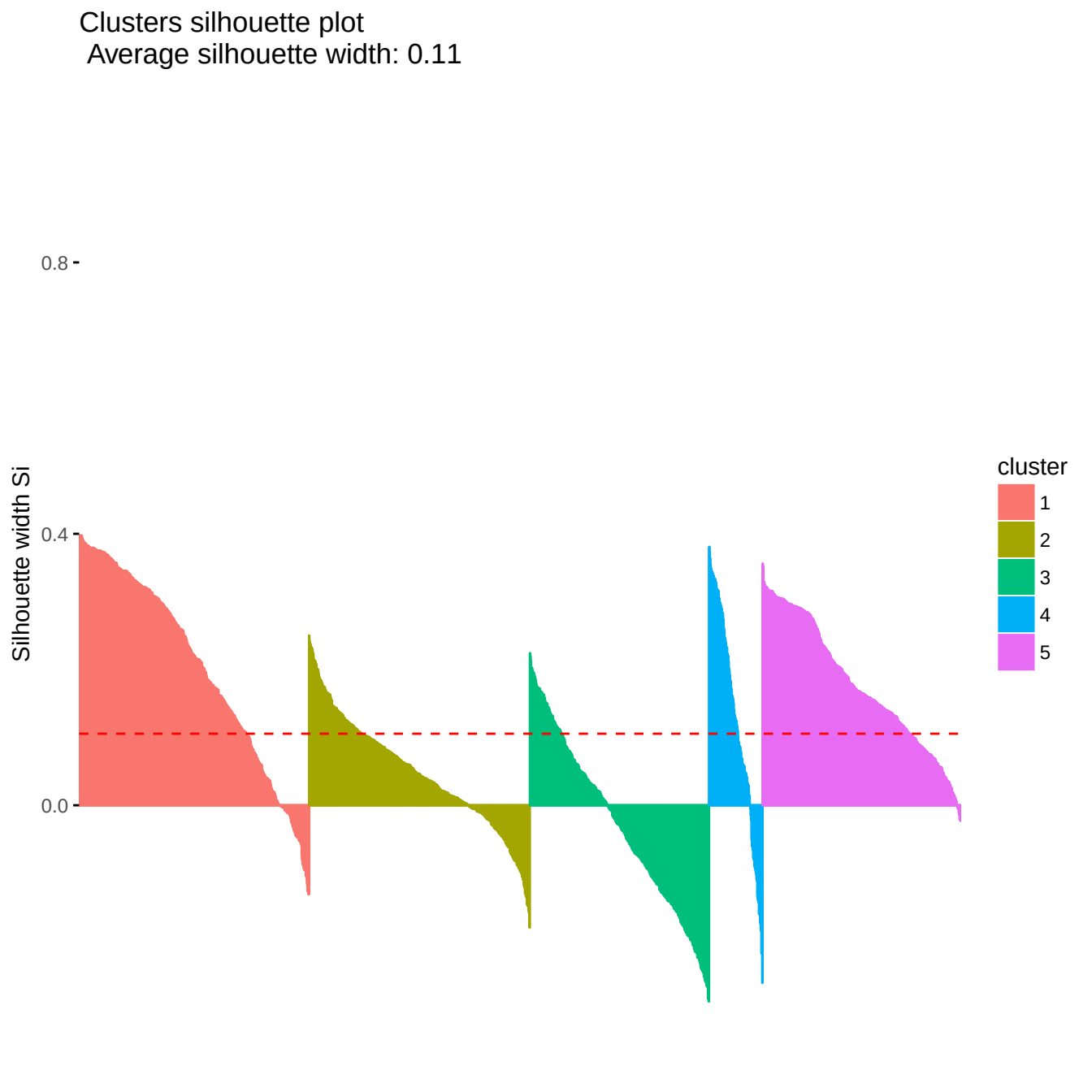

Distribution des scores (Méthodes Kmeans)
Score
−4
−2
0
2
4
A C D E F G H I K L M N P Q R S T V Y
Cluster 2

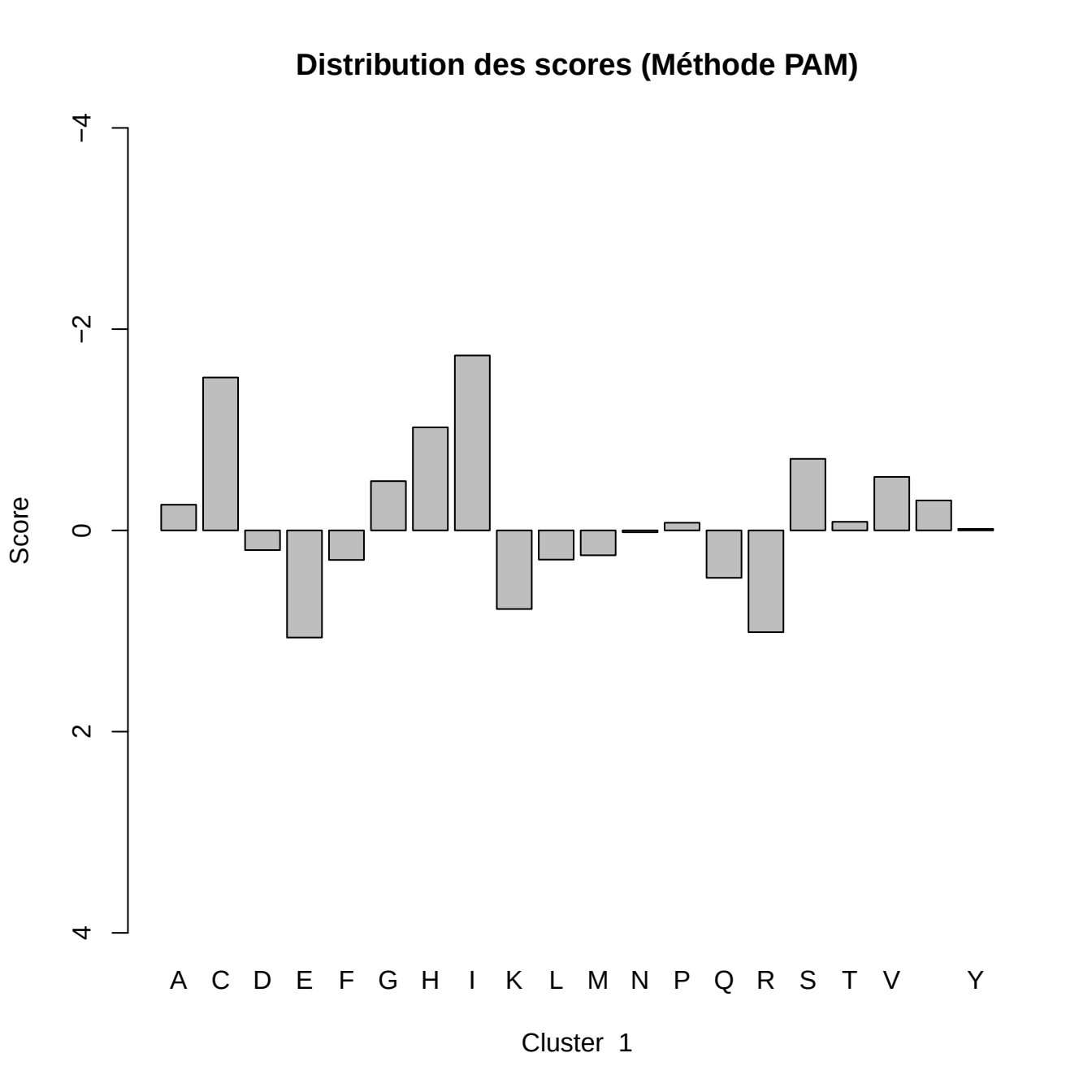

Distribution des scores (Méthodes Kmeans)
Score
−4
−2
0
2
4
A C D E F G H I K L M N P Q R S T V Y
Cluster 3

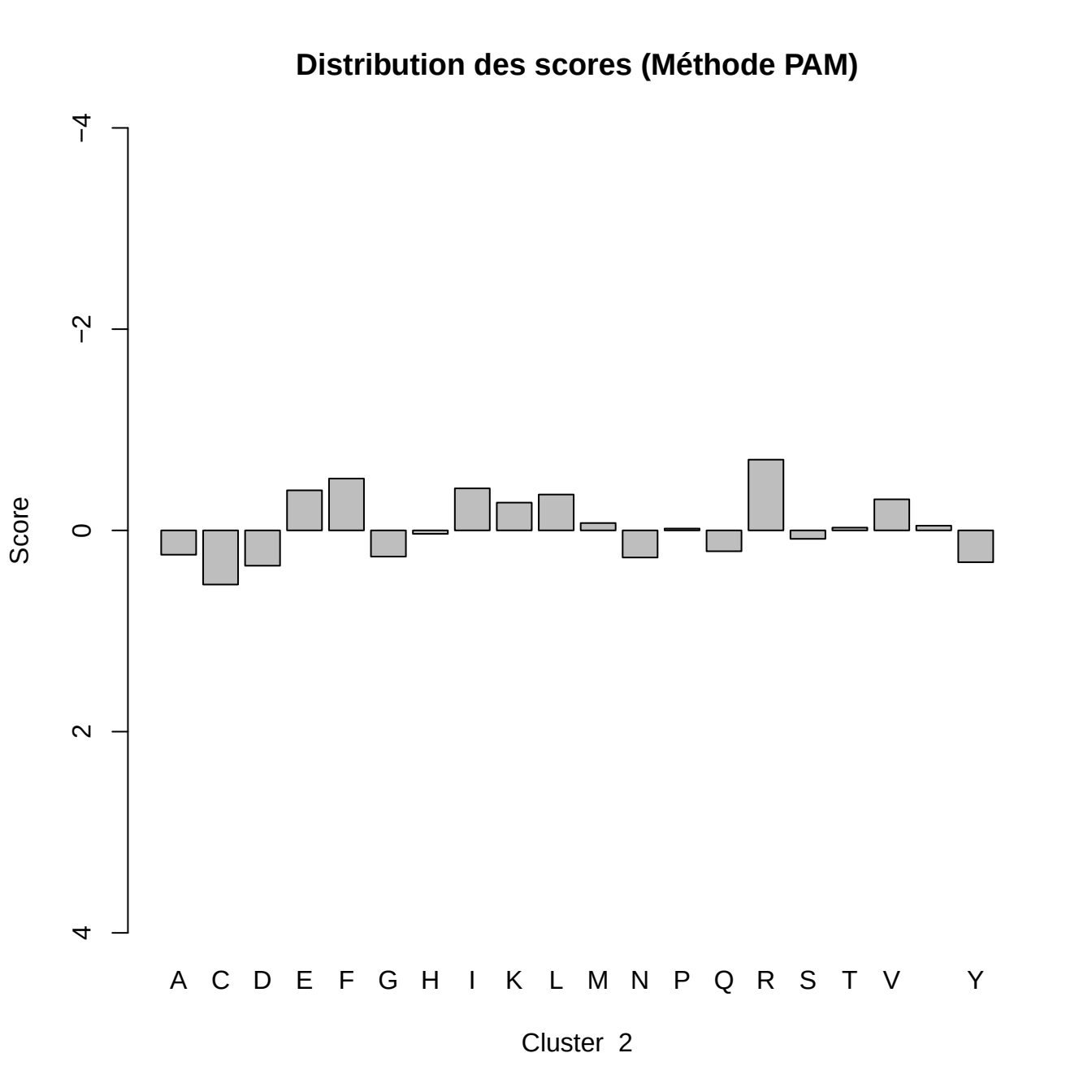

Distribution des scores (Méthodes Kmeans)
Score
−4
−2
0
2
4
A C D E F G H I K L M N P Q R S T V Y
Cluster 4

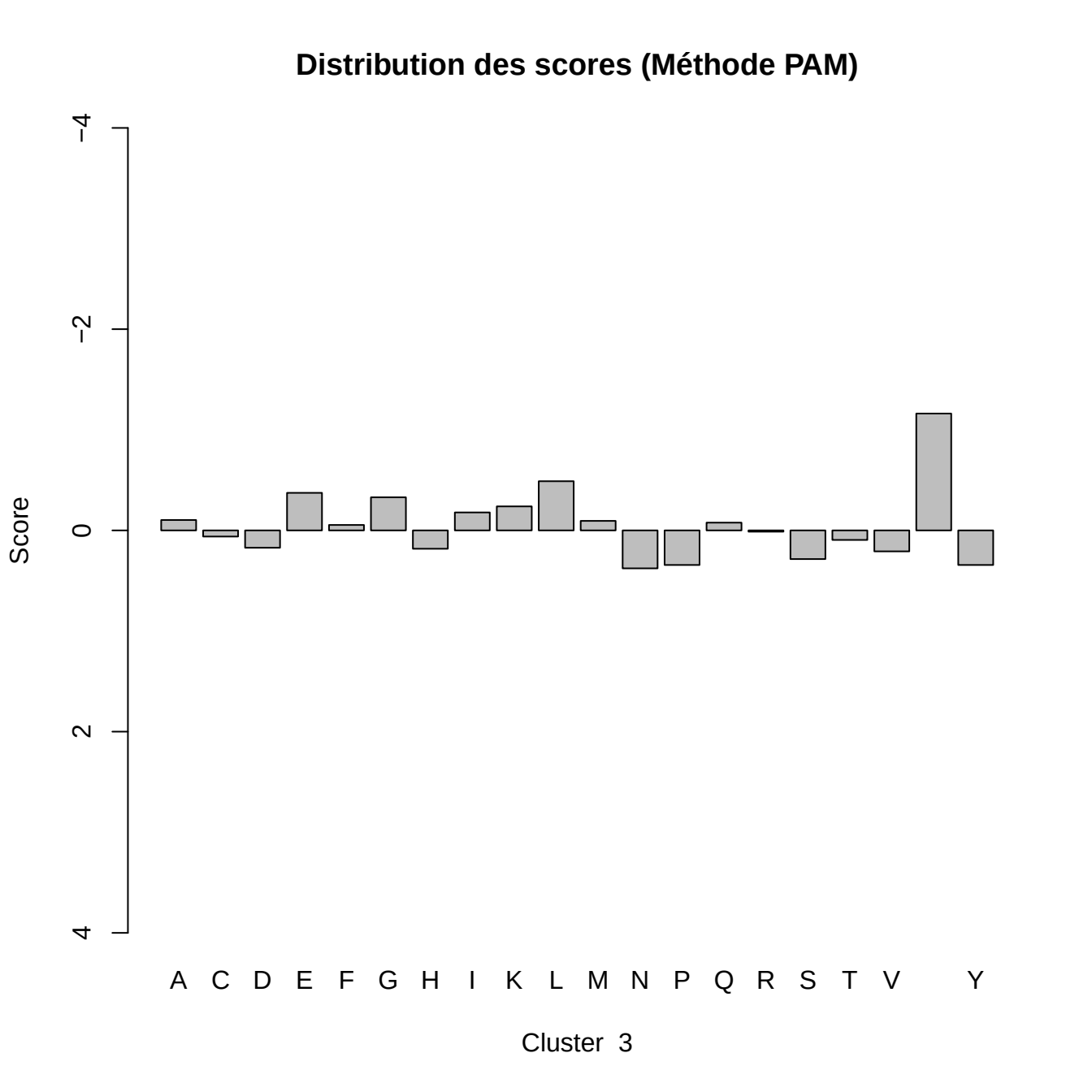

Distribution des scores (Méthodes Kmeans)
Score
−4
−2
0
2
4
A C D E F G H I K L M N P Q R S T V Y
Cluster 5

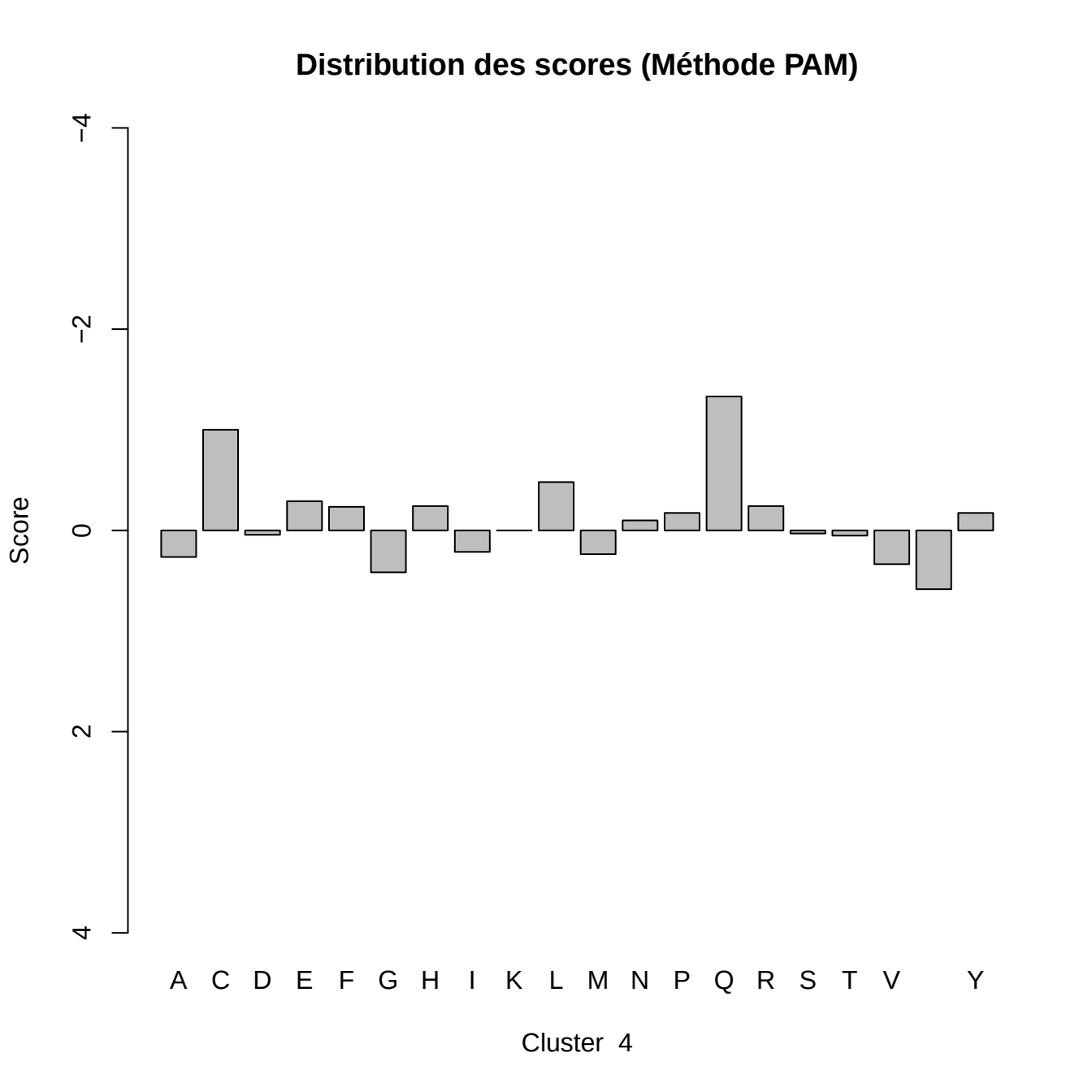

Clustering par Kmedoid(PAM)
PC2
PC1
0.2
0.1
0.0
−0.1
−0.04
0.00
0.04
0.08
cluster
1
2
3
4
5

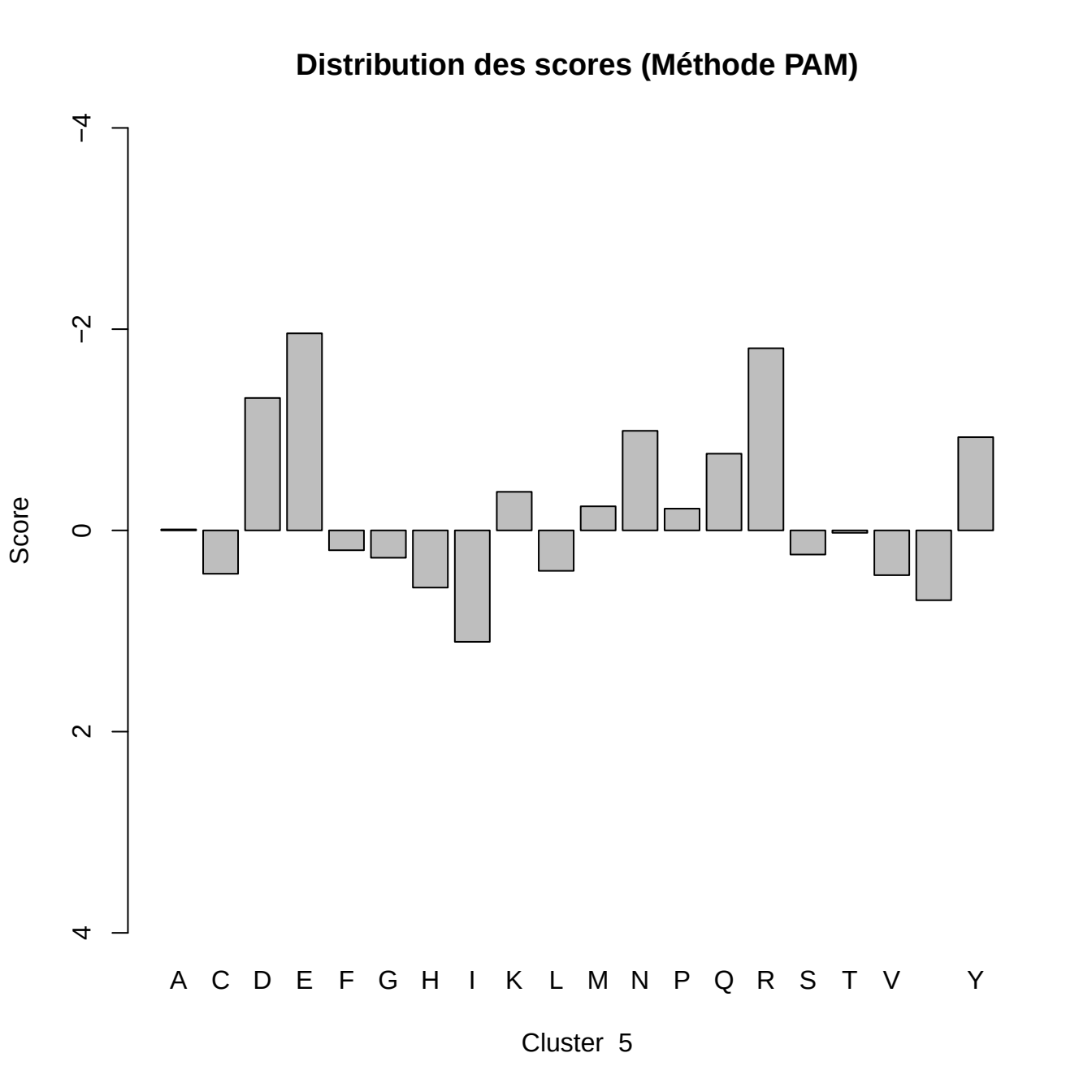

Clusters silhouette plot
Average silhouette width: 0.11
Silhouette width Si
0.8
0.4
0.0
cluster
1
2
3
4
5

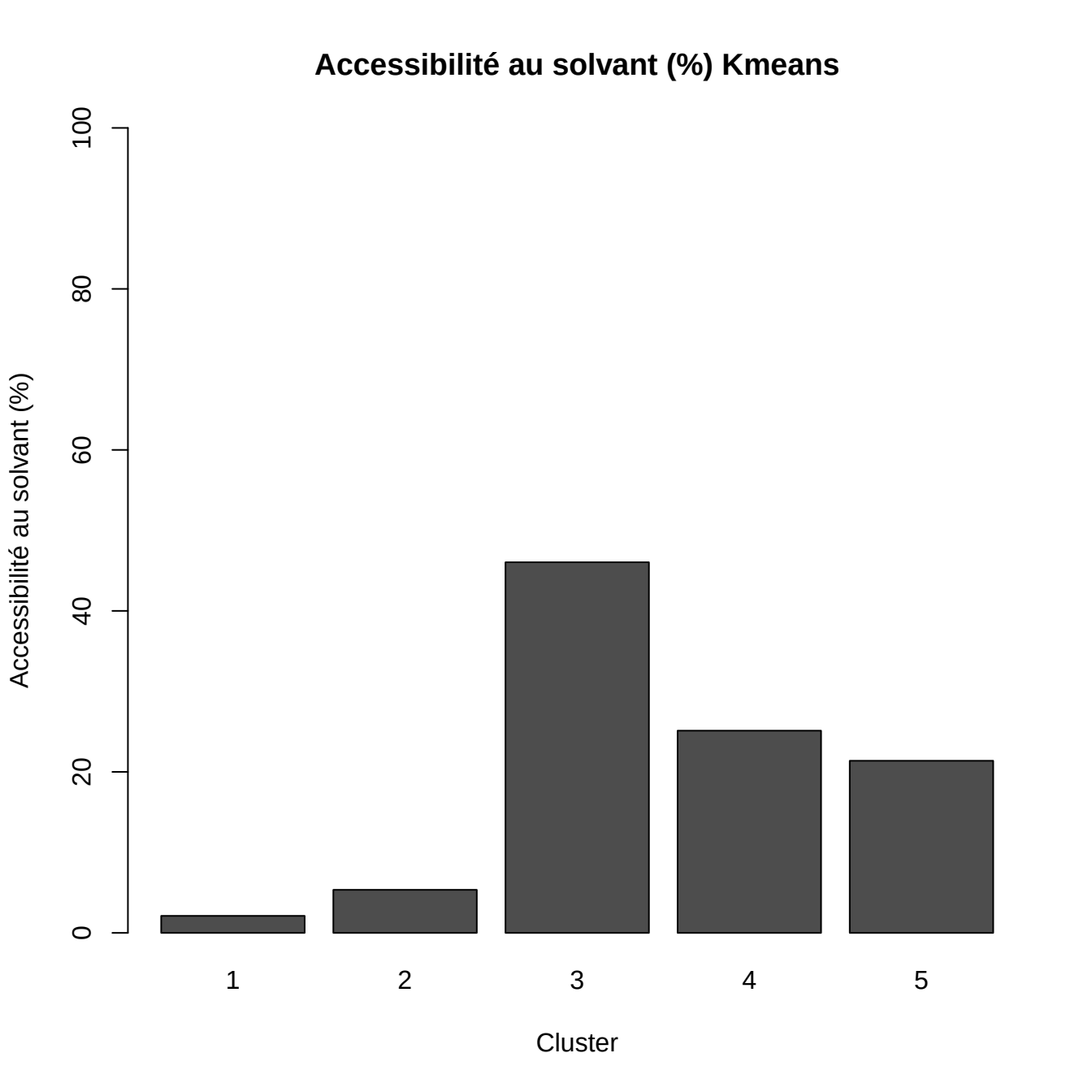

Distribution des scores (Méthode PAM)
Score
−4
−2
0
2
4
A C D E F G H I K L M N P Q R S T V Y
Cluster 1

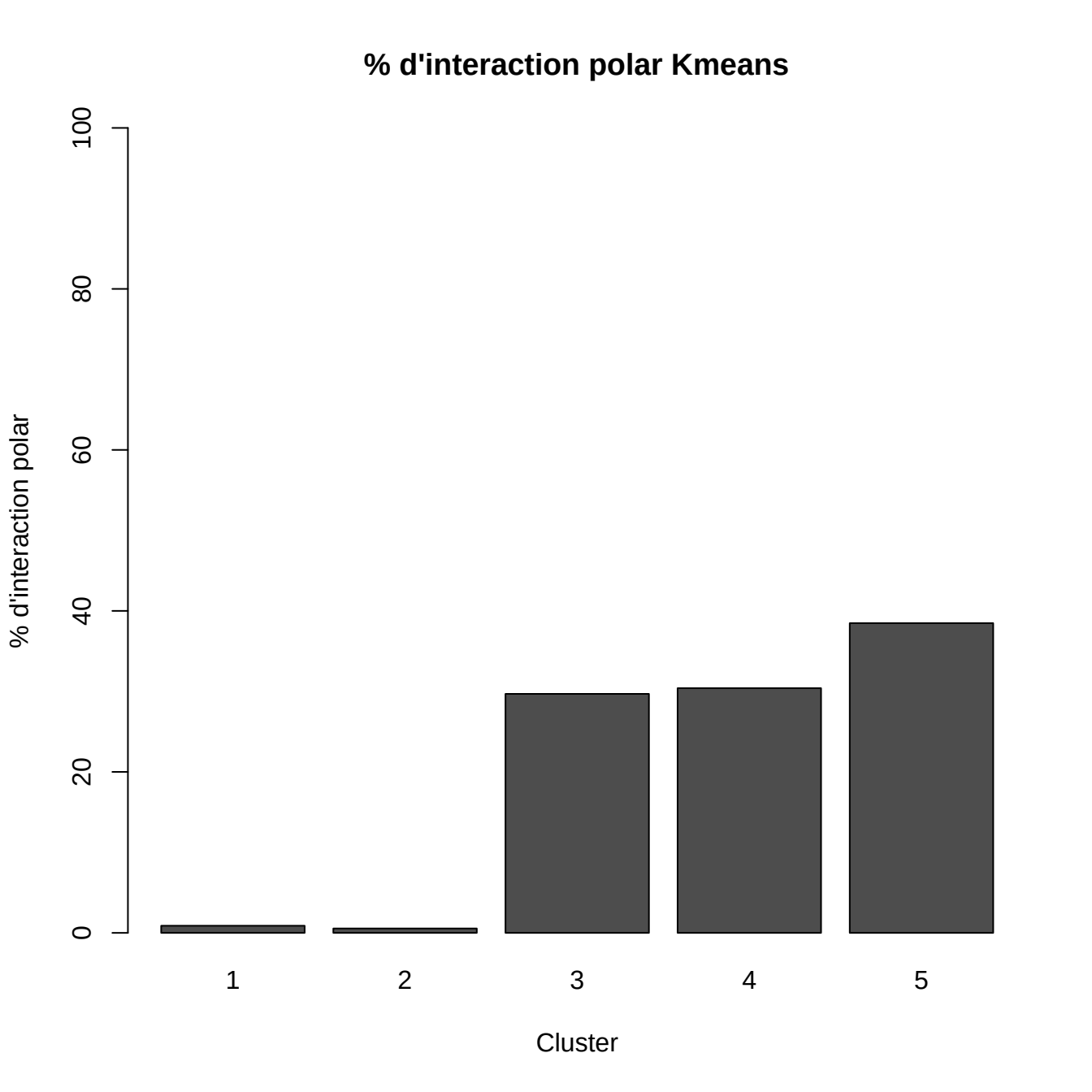

Distribution des scores (Méthode PAM)
Score
−4
−2
0
2
4
A C D E F G H I K L M N P Q R S T V Y
Cluster 2

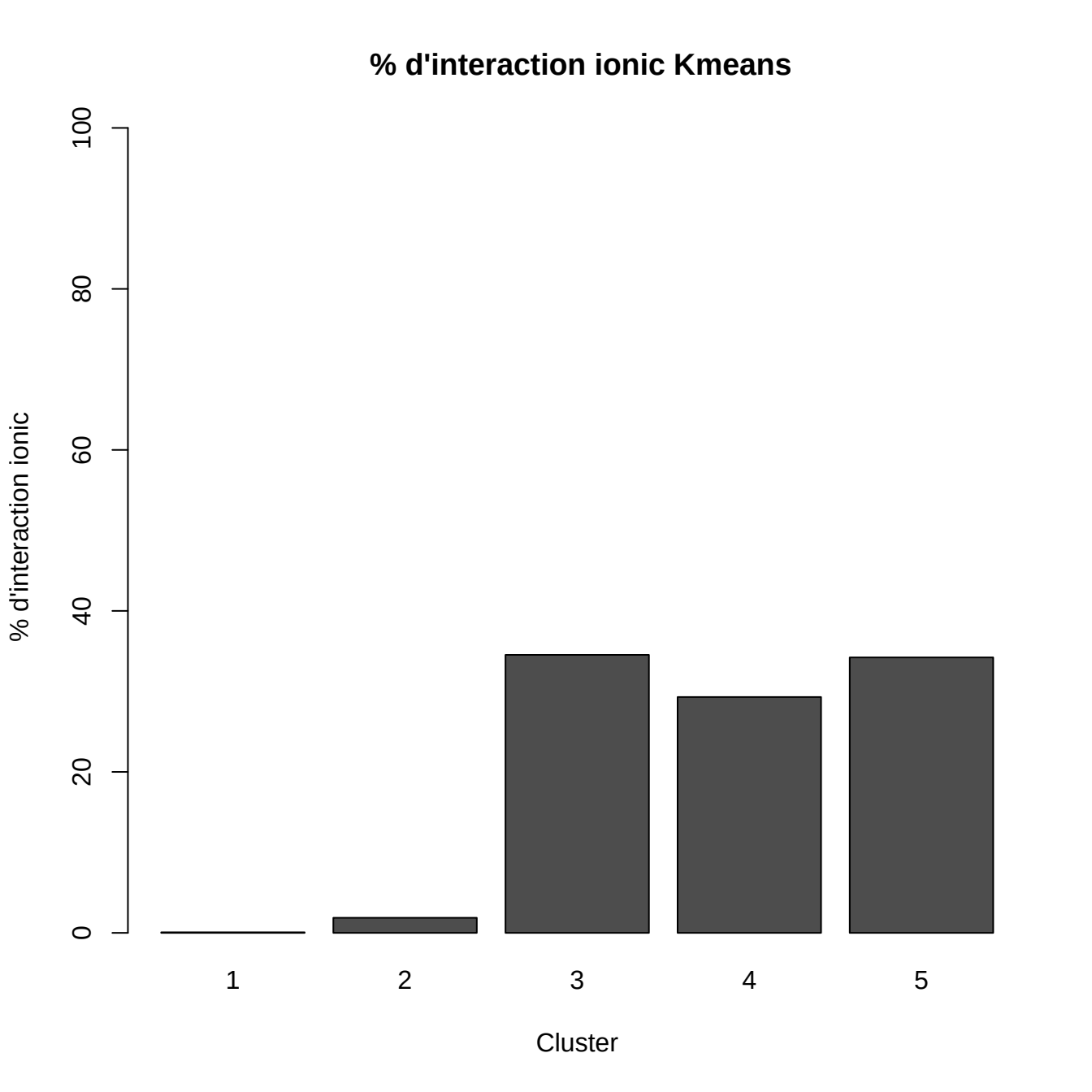

Distribution des scores (Méthode PAM)
Score
−4
−2
0
2
4
A C D E F G H I K L M N P Q R S T V Y
Cluster 3

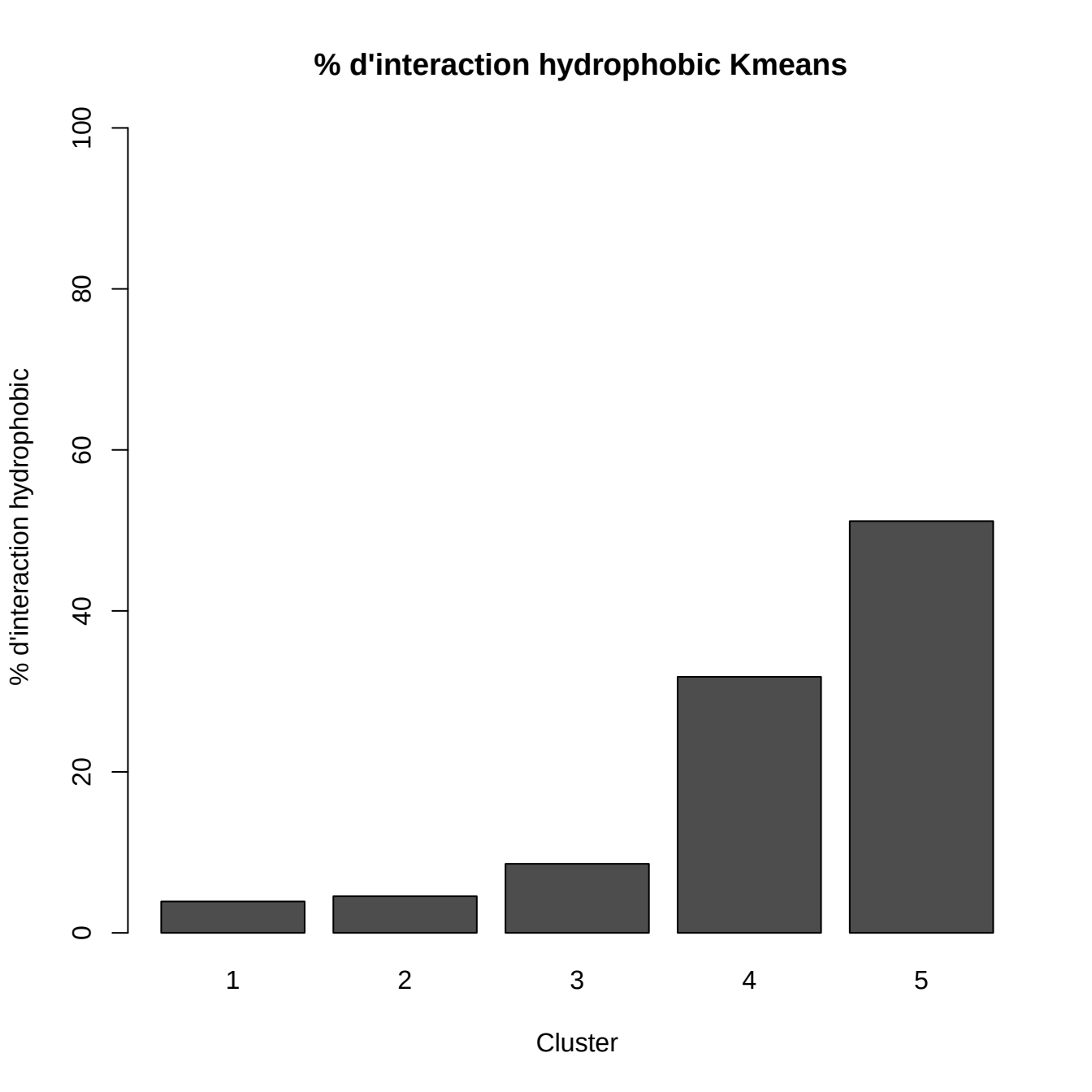

Distribution des scores (Méthode PAM)
Score
−4
−2
0
2
4
A C D E F G H I K L M N P Q R S T V Y
Cluster 4

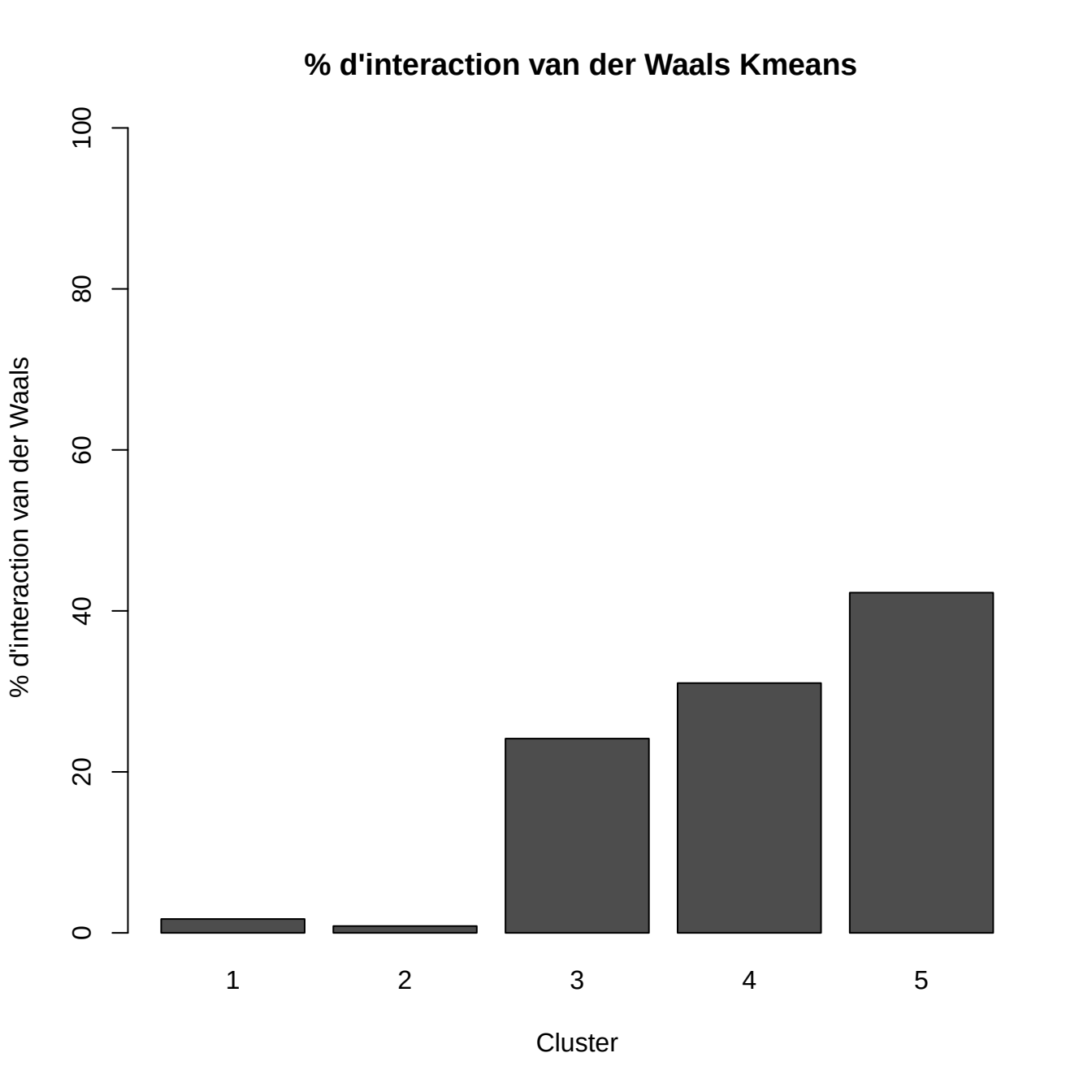

Distribution des scores (Méthode PAM)
Score
−4
−2
0
2
4
A C D E F G H I K L M N P Q R S T V Y
Cluster 5

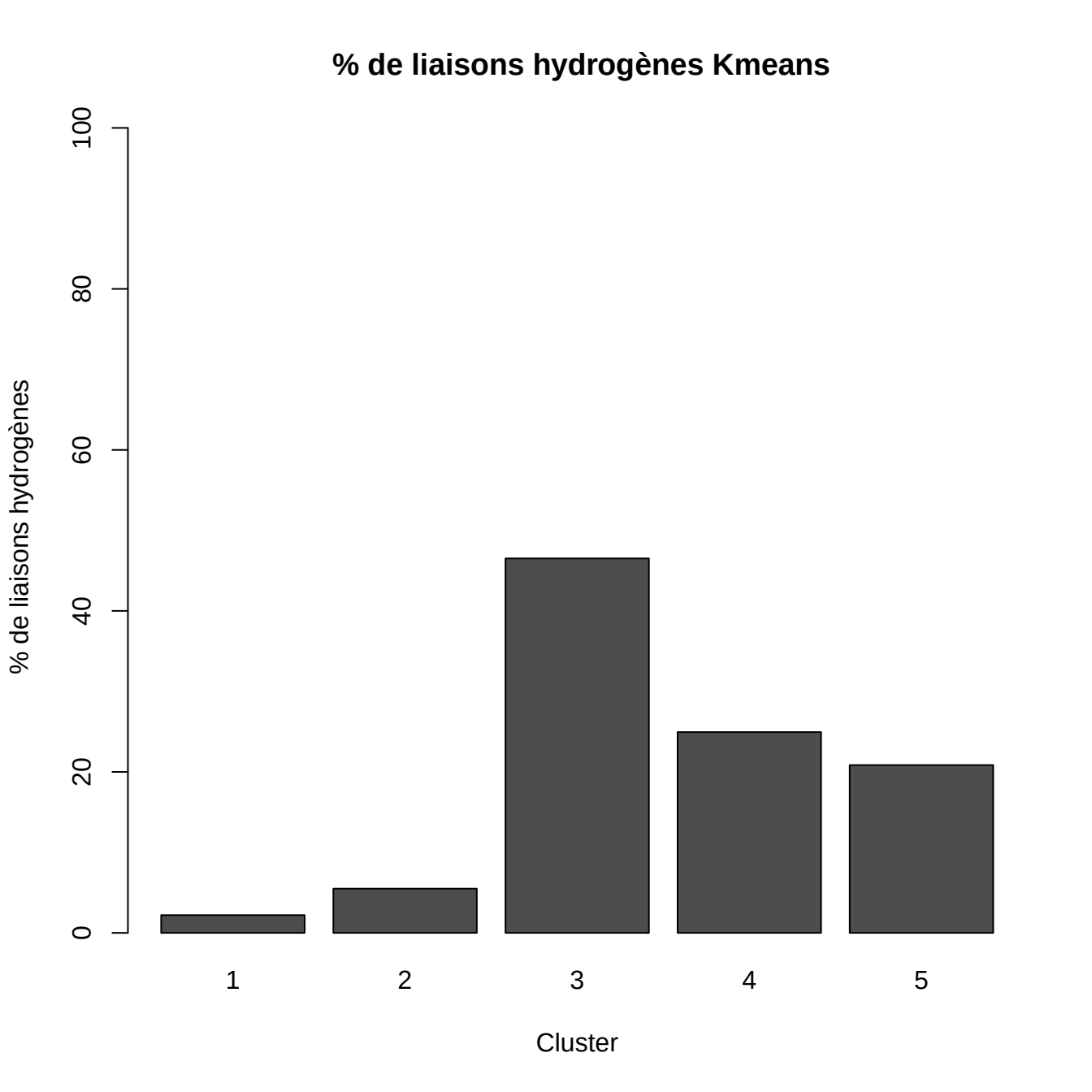

Accessibilité au solvant (%) Kmeans
Accessibilité au solvant (%)
0
20
40
60
80
100
1
2
3
4
5
Cluster

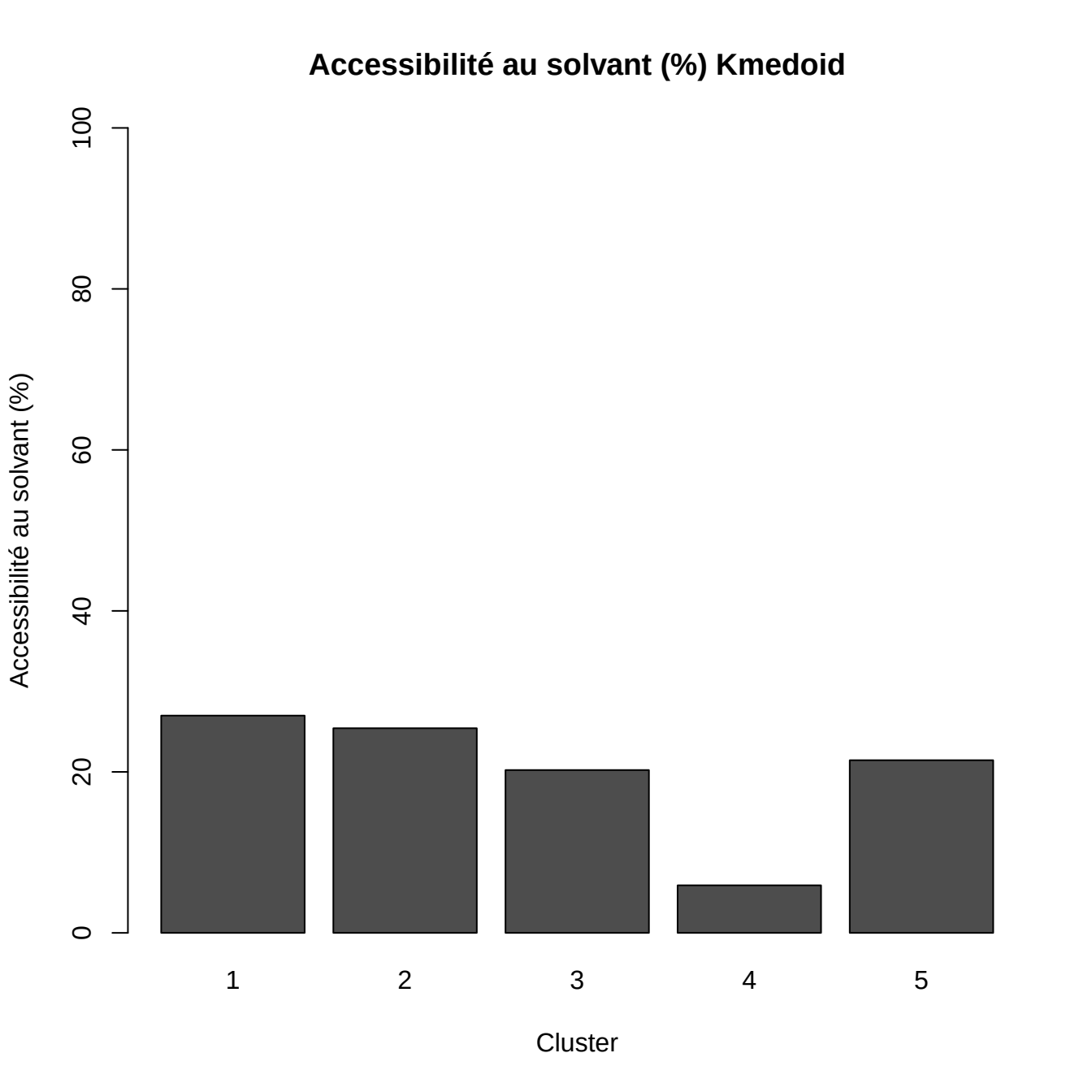

% d'interaction polar Kmeans
% d'interaction polar
0
20
40
60
80
100
1
2
3
4
5
Cluster

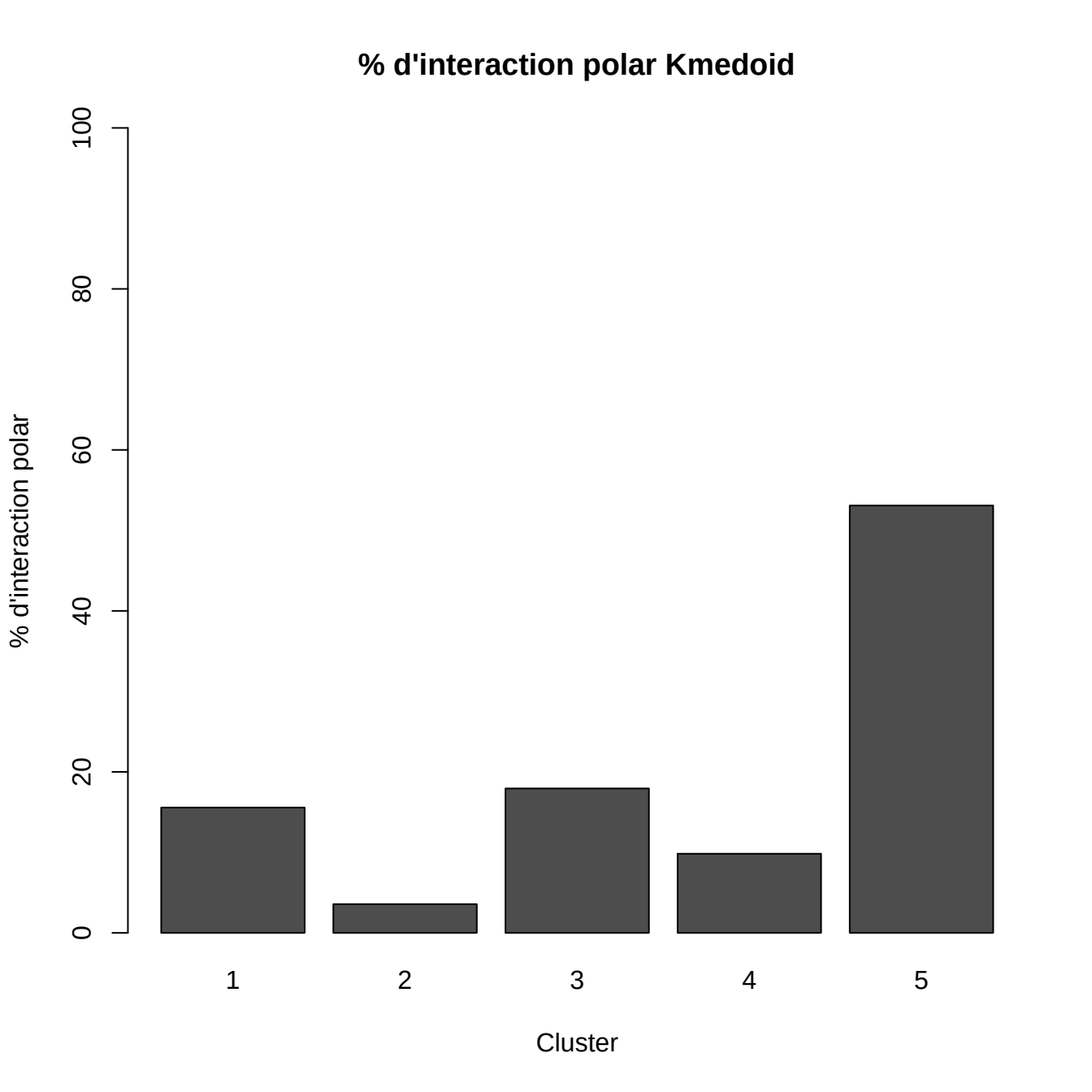

% d'interaction ionic Kmeans
% d'interaction ionic
0
20
40
60
80
100
1
2
3
4
5
Cluster

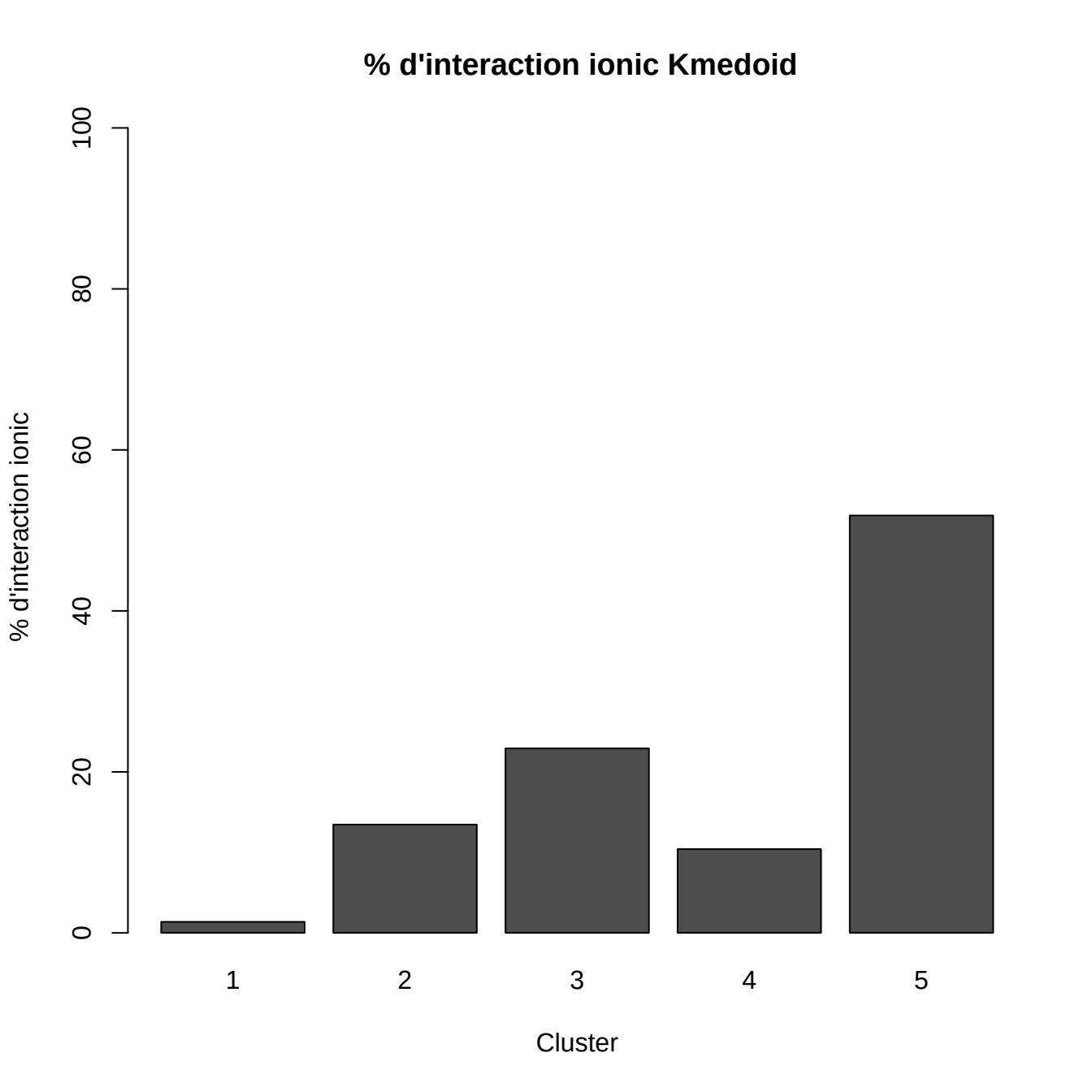

% d'interaction hydrophobic Kmeans
% d'interaction hydrophobic
0
20
40
60
80
100
1
2
3
4
5
Cluster

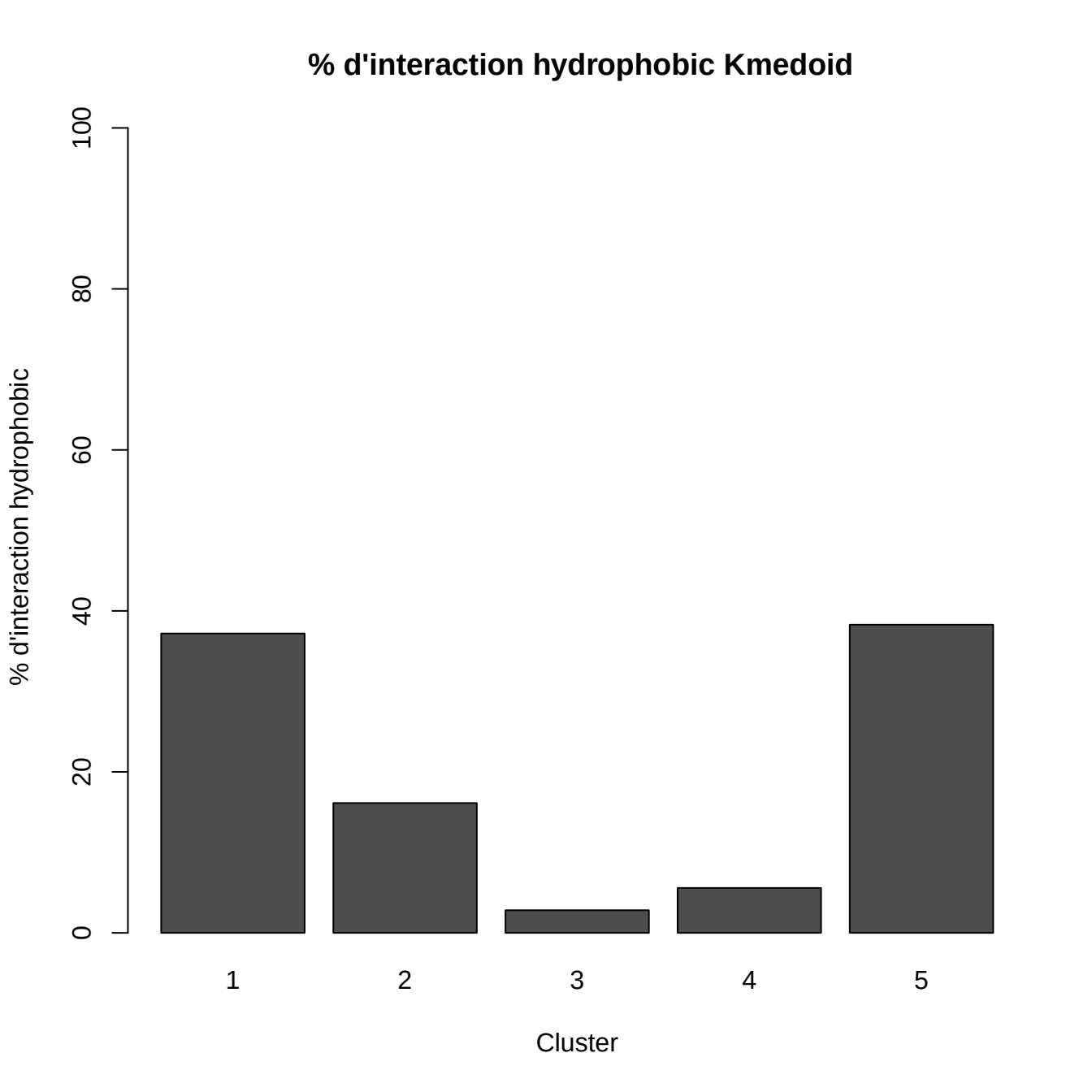

% d'interaction van der Waals Kmeans
% d'interaction van der Waals
0
20
40
60
80
100
1
2
3
4
5
Cluster

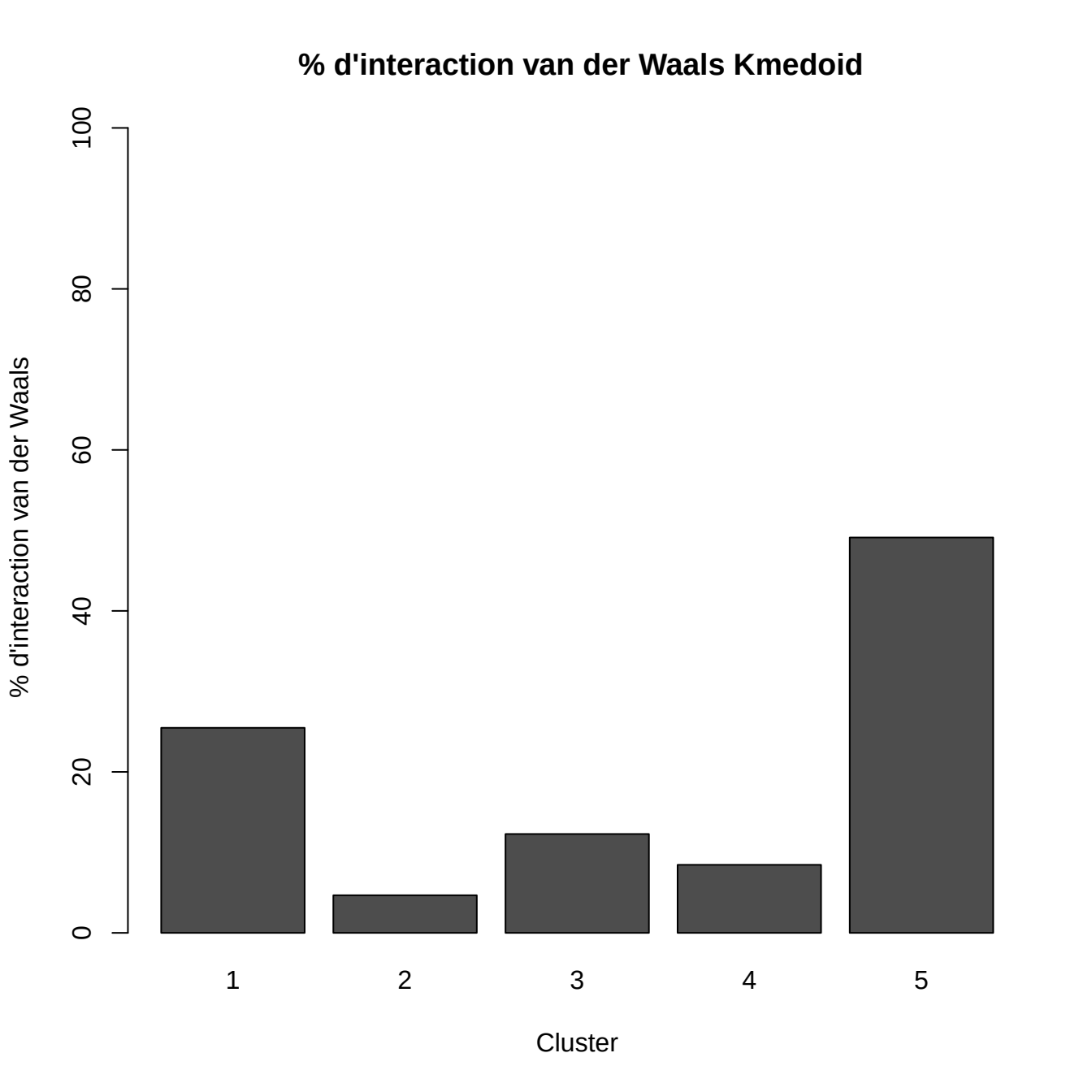

% de liaisons hydrogènes Kmeans
% de liaisons hydrogènes
0
20
40
60
80
100
1
2
3
4
5
Cluster

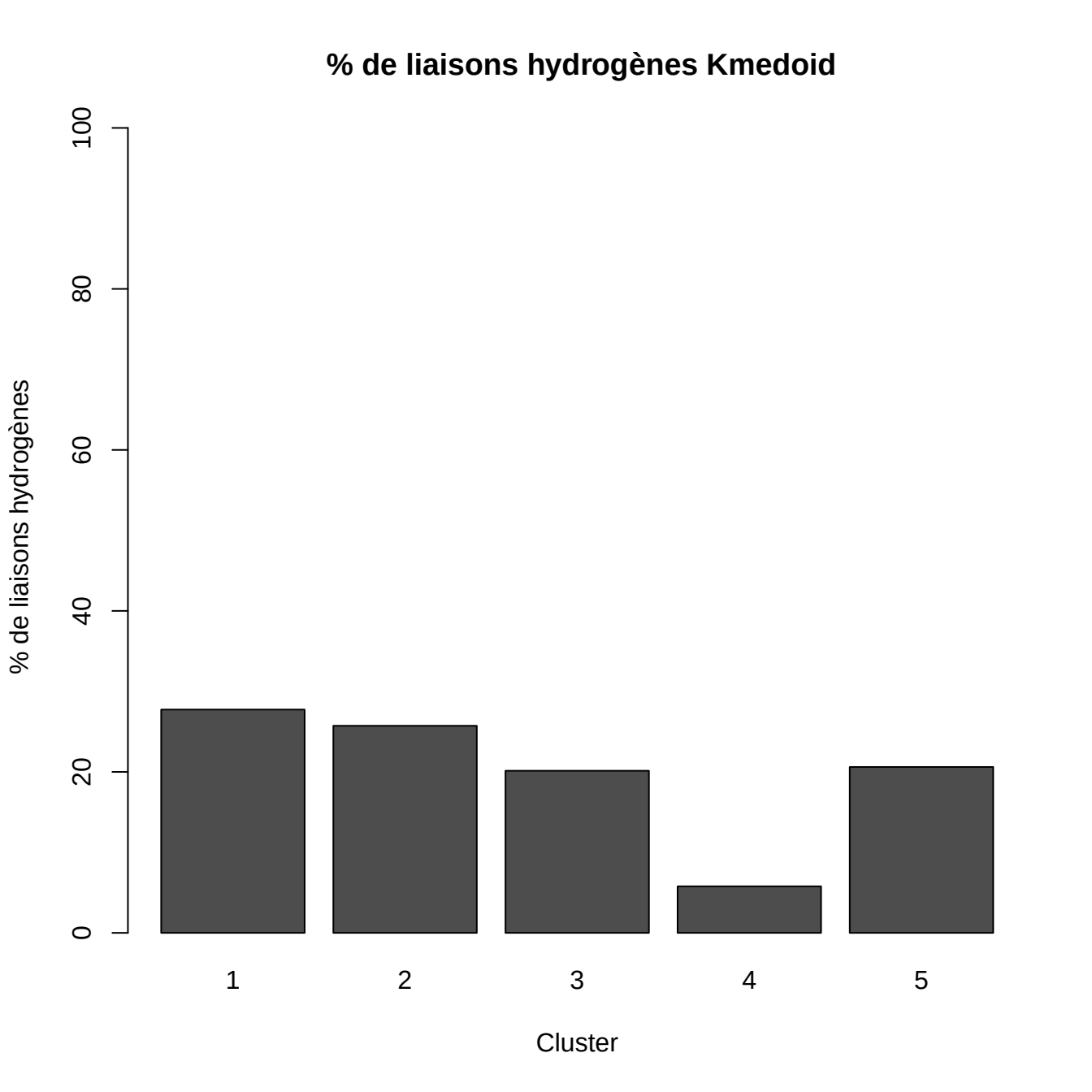

Accessibilité au solvant (%) Kmedoid
Accessibilité au solvant (%)
0
20
40
60
80
100
1
2
3
4
5
Cluster

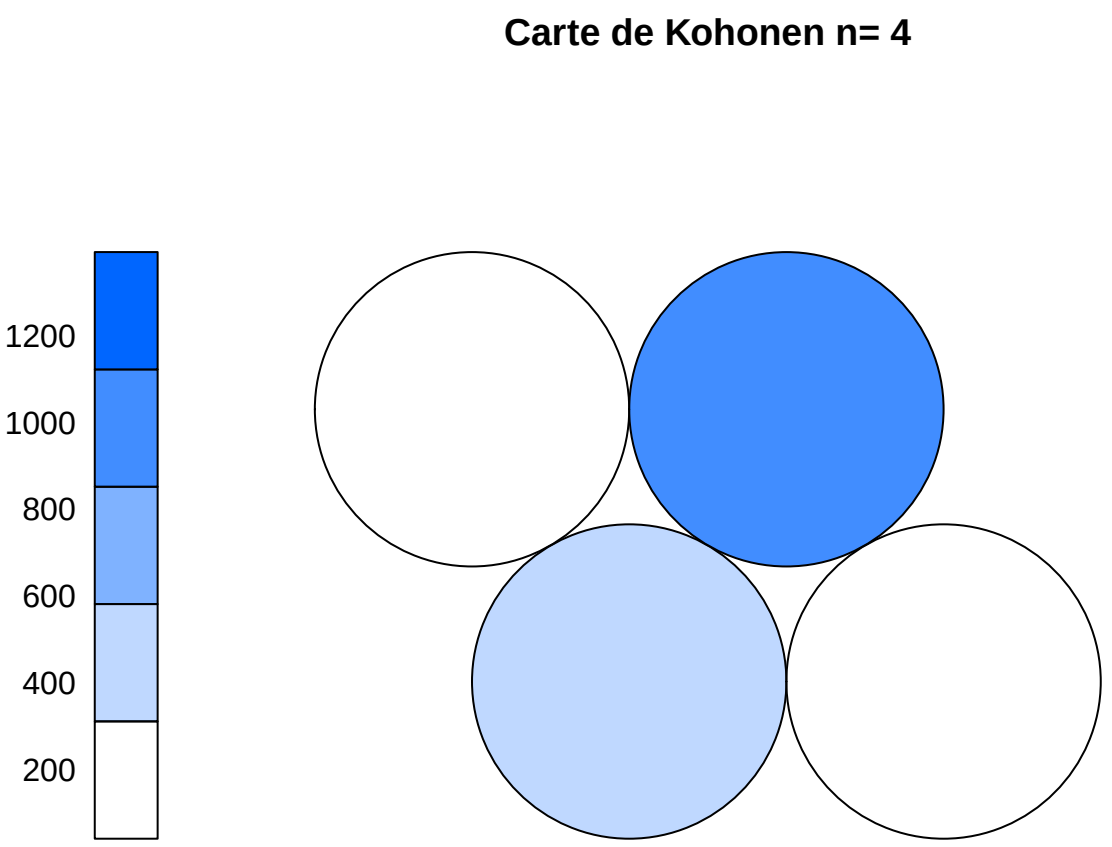

% d'interaction polar Kmedoid
% d'interaction polar
0
20
40
60
80
100
1
2
3
4
5
Cluster

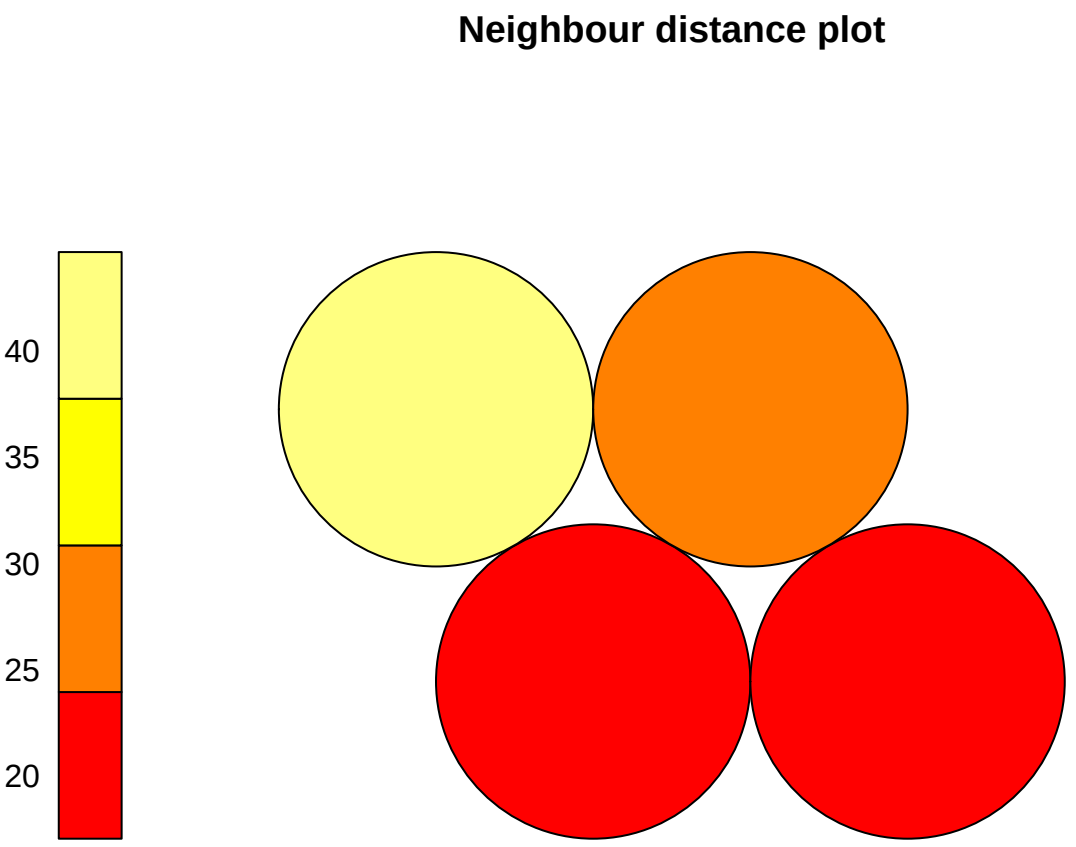

% d'interaction ionic Kmedoid
% d'interaction ionic
0
20
40
60
80
100
1
2
3
4
5
Cluster


% d'interaction hydrophobic Kmedoid
% d'interaction hydrophobic
0
20
40
60
80
100
1
2
3
4
5
Cluster

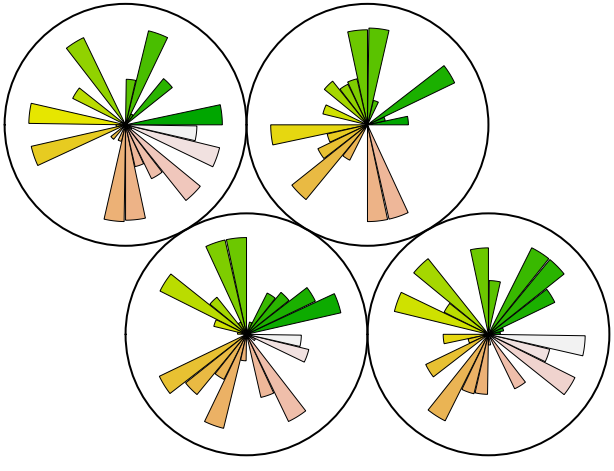

% d'interaction van der Waals Kmedoid
% d'interaction van der Waals
0
20
40
60
80
100
1
2
3
4
5
Cluster

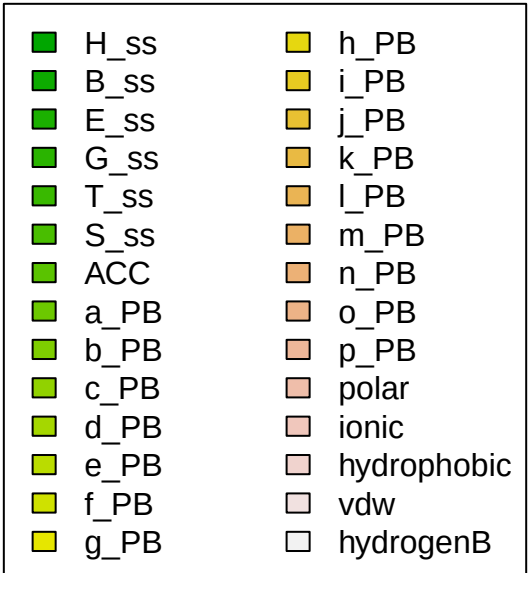

% de liaisons hydrogènes Kmedoid
% de liaisons hydrogènes
0
20
40
60
80
100
1
2
3
4
5
Cluster

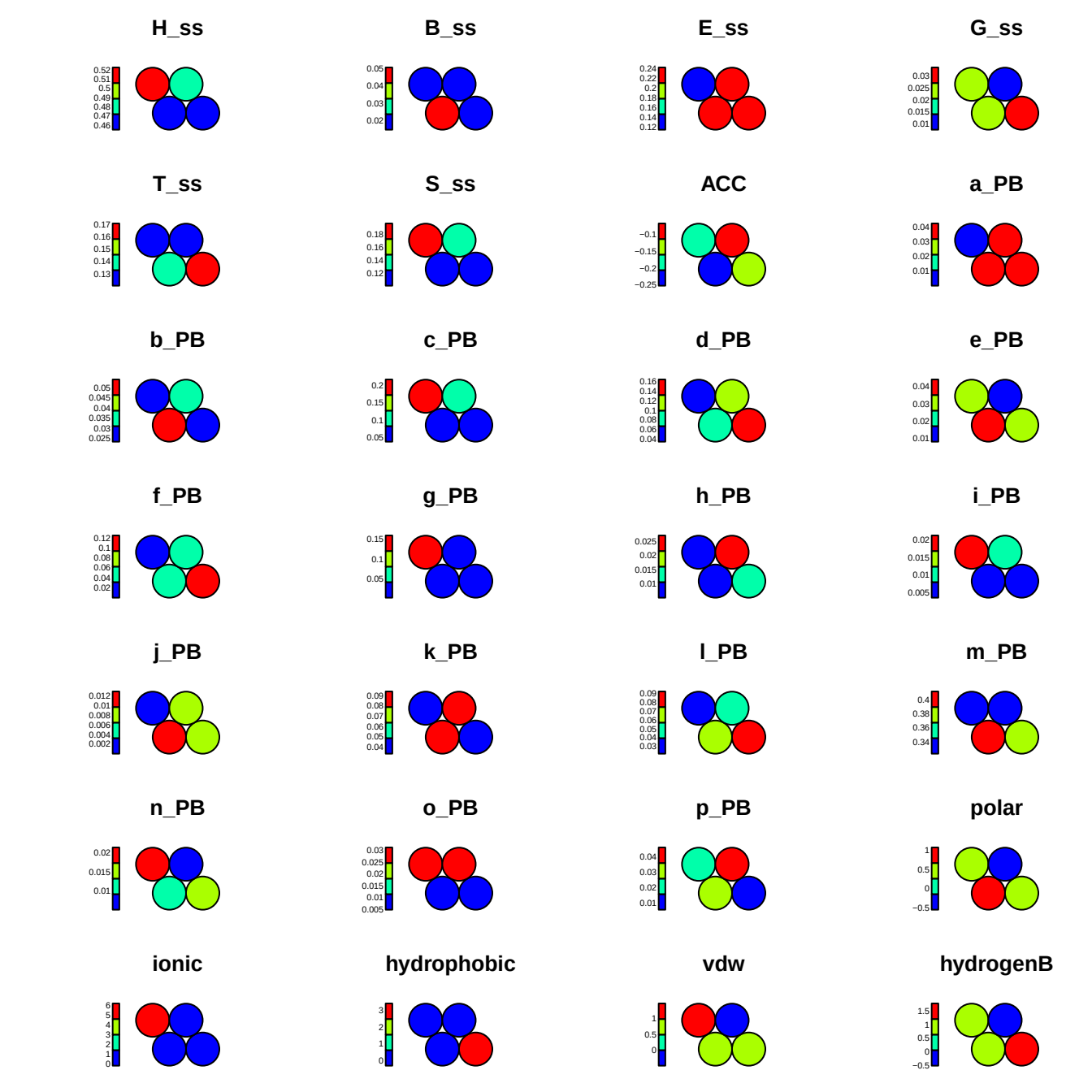

Carte de Kohonen n= 4
1200
1000
800
600
400
200

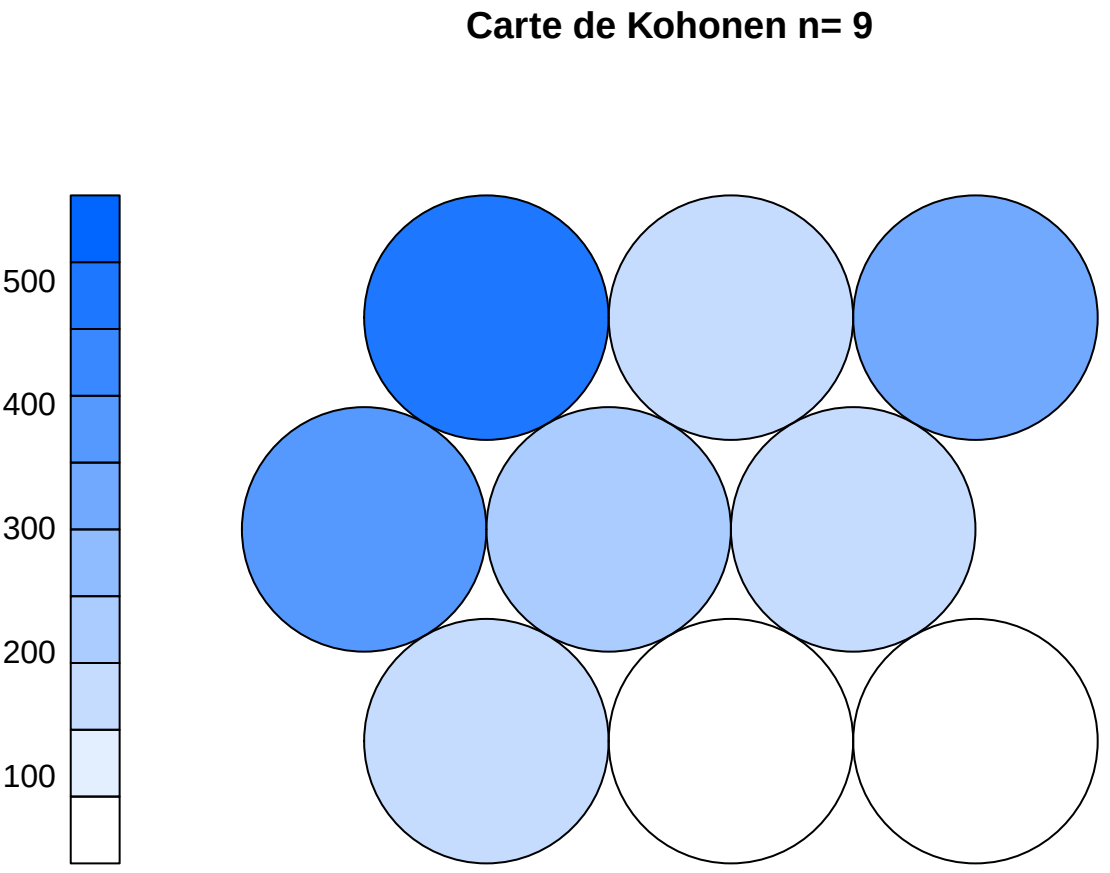

Neighbour distance plot
40
35
30
25
20

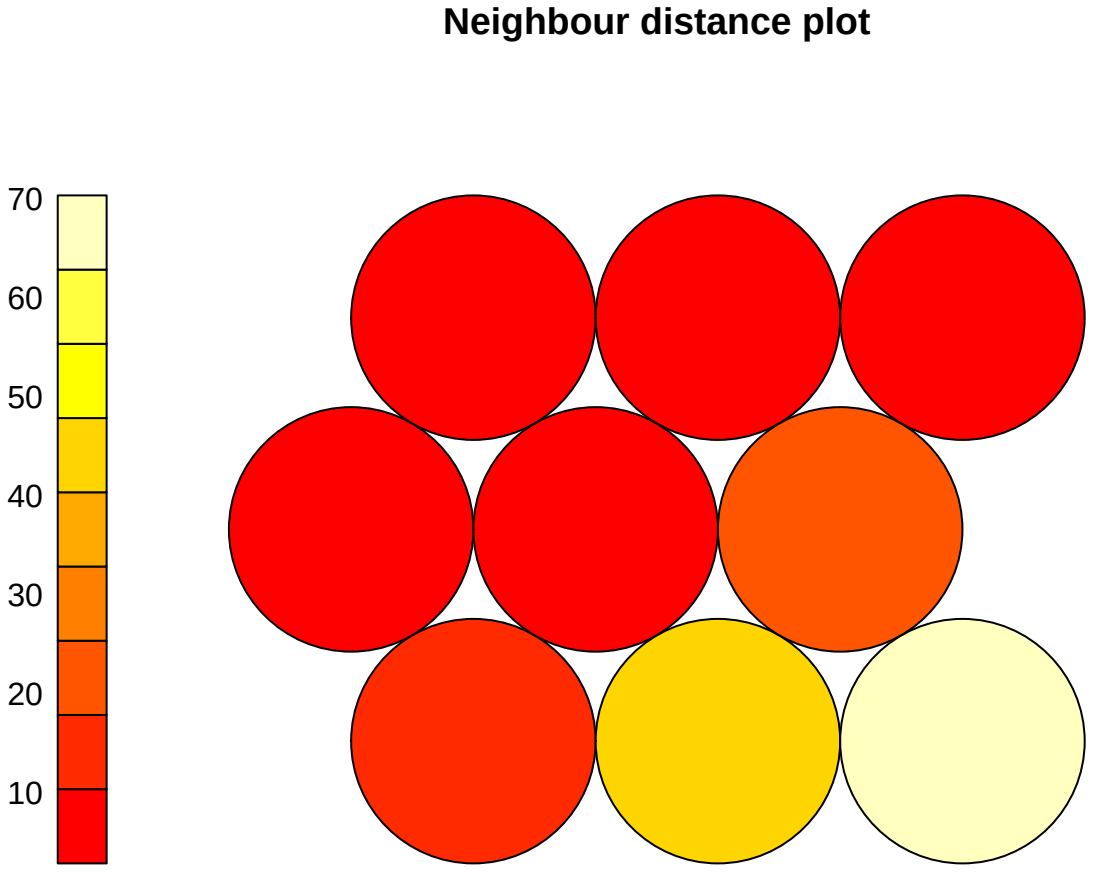
Codes plot



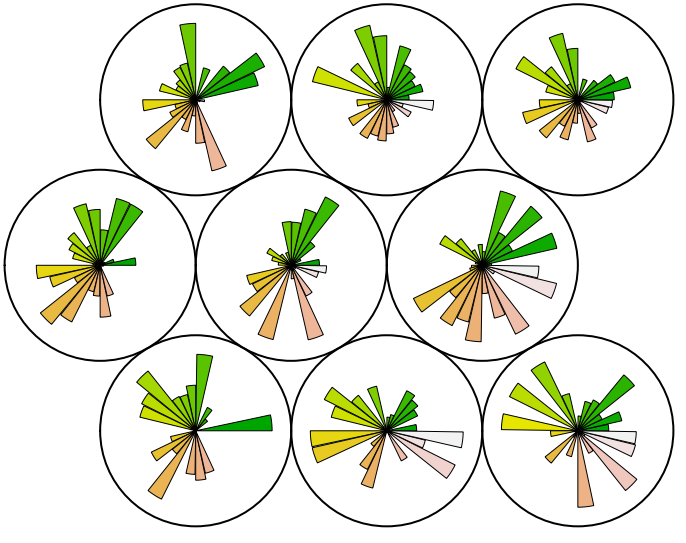

H_ss
B_ss
E_ss
G_ss
T_ss
S_ss
ACC
a_PB
b_PB
c_PB
d_PB
e_PB
f_PB
g_PB
h_PB
i_PB
j_PB
k_PB
l_PB
m_PB
n_PB
o_PB
p_PB
polar
ionic
hydrophobic
vdw
hydrogenB

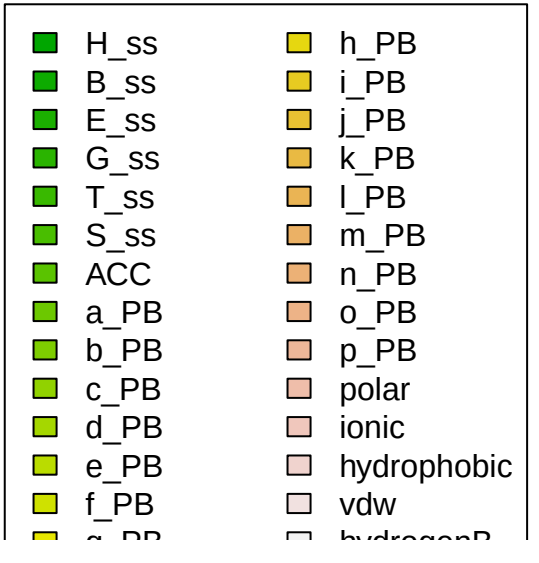

H_ss
B_ss
E_ss
G_ss
T_ss
S_ss
ACC
a_PB
b_PB
c_PB
d_PB
e_PB
f_PB
g_PB
h_PB
i_PB
j_PB
k_PB
l_PB
m_PB
n_PB
o_PB
p_PB
polar
ionic
hydrophobic
vdw
hydrogenB


Carte de Kohonen n= 9
500
400
300
200
100

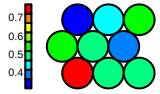

Neighbour distance plot
70
60
50
40
30
20
10

Codes plot

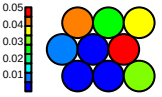



H_ss
B_ss
E_ss
G_ss
T_ss
S_ss
ACC
a_PB
b_PB
c_PB
d_PB
e_PB
f_PB
h_PB
i_PB
j_PB
k_PB
l_PB
m_PB
n_PB
o_PB
p_PB
polar
ionic
hydrophobic
vdw

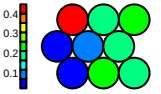
H_ss



B_ss



E_ss



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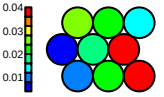

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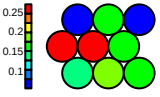

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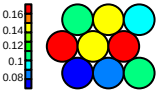

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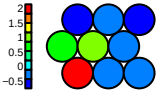

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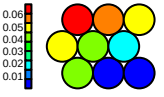

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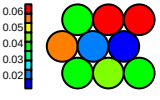

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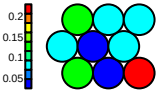

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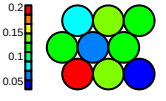

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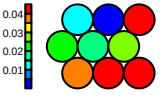

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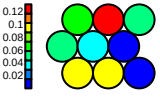

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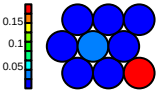

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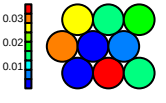

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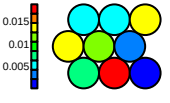

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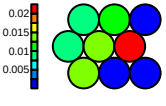

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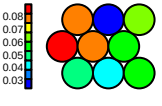

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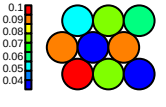

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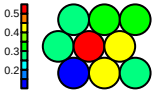

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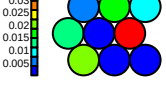

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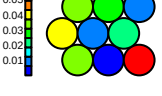

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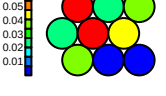

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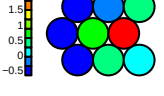

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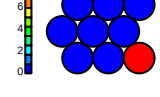

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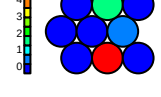

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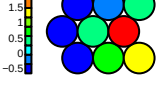

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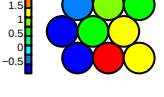

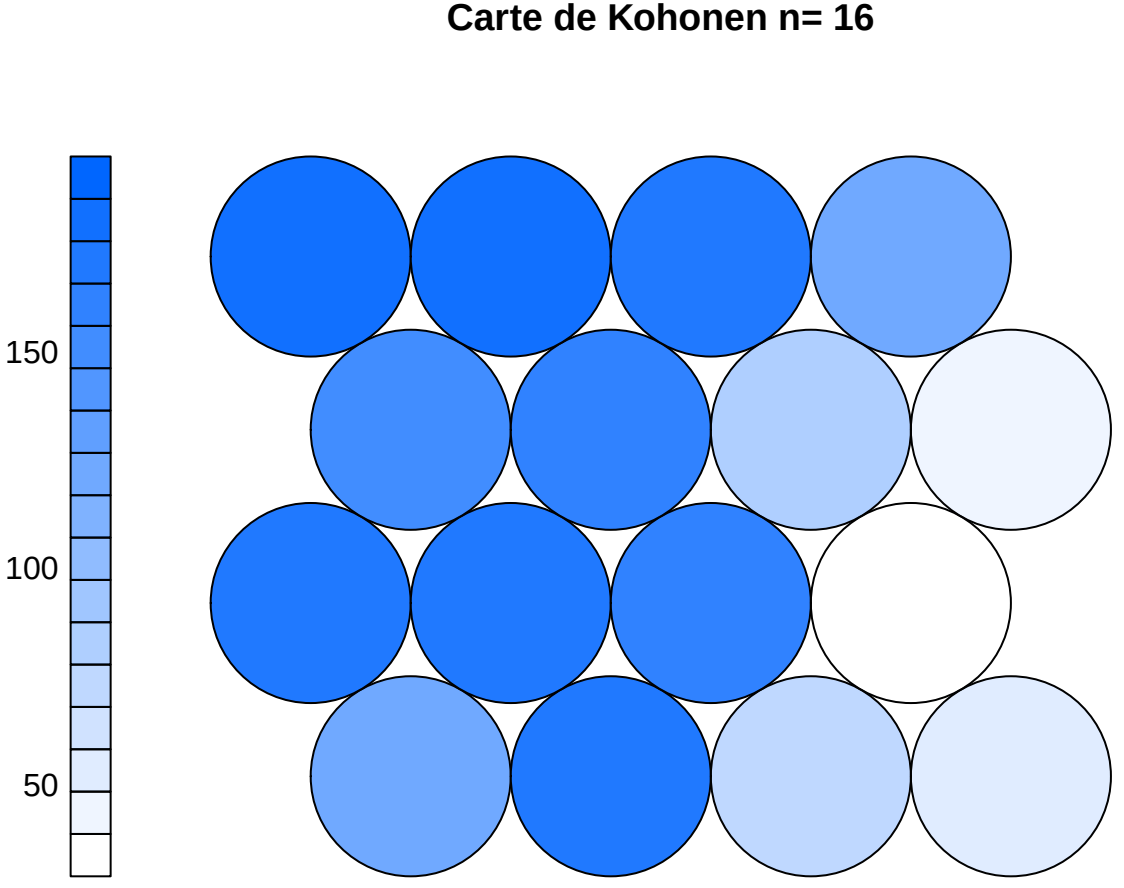
Carte de Kohonen n= 16
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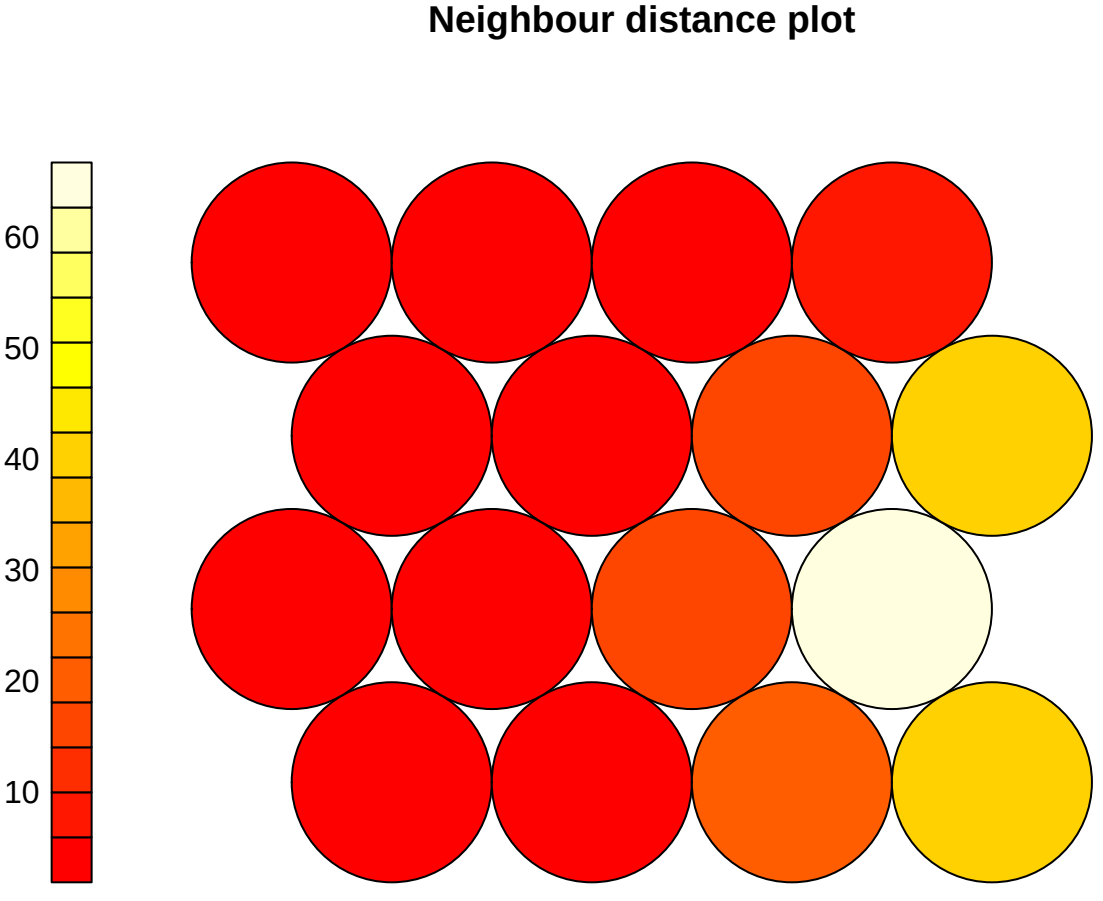
100
50


Neighbour distance plot
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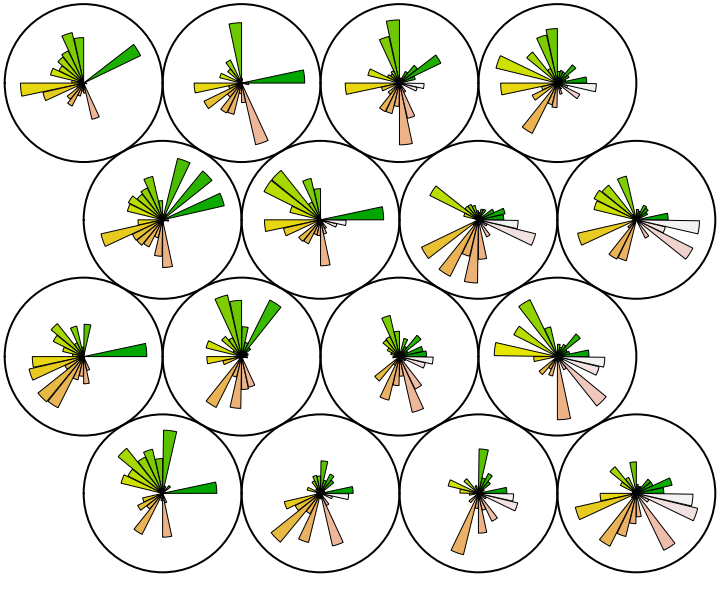
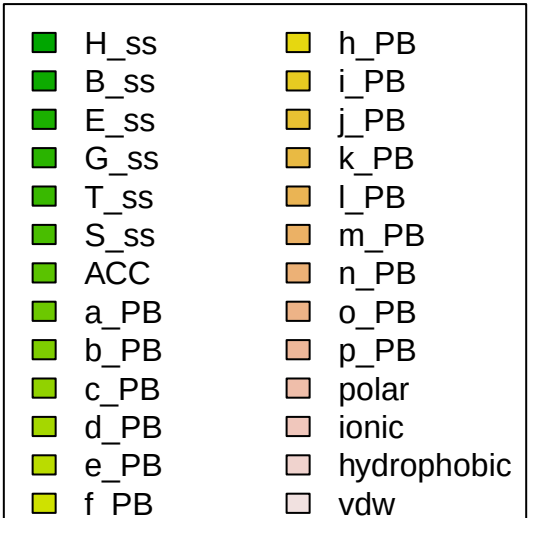
50
40
30
20
10

Codes plot

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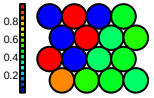
H_ss



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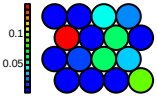

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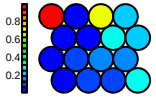

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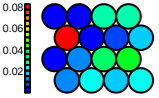

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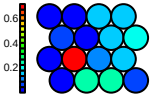

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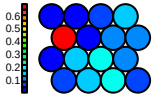

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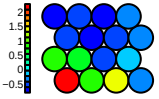

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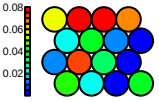

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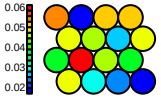

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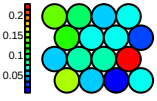

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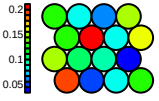

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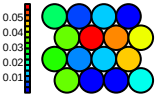

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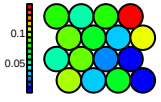

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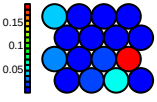

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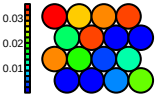

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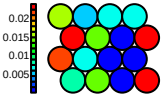

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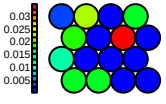

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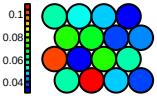

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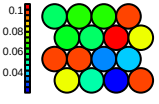

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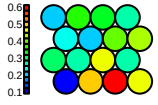

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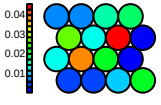

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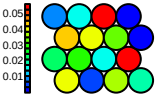

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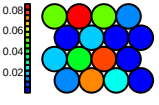

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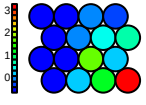
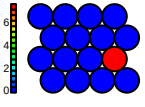
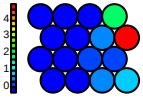


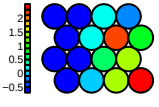
ionic



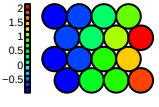
hydrophobic

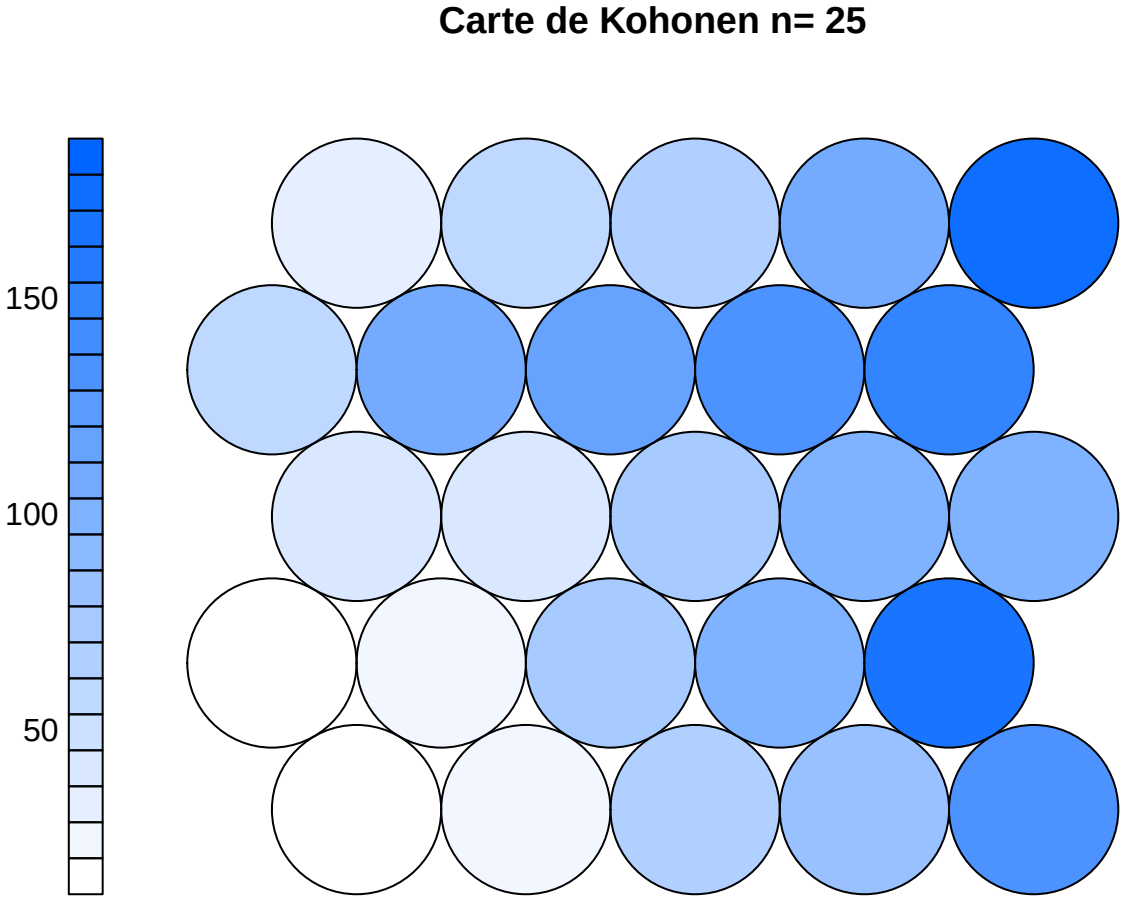


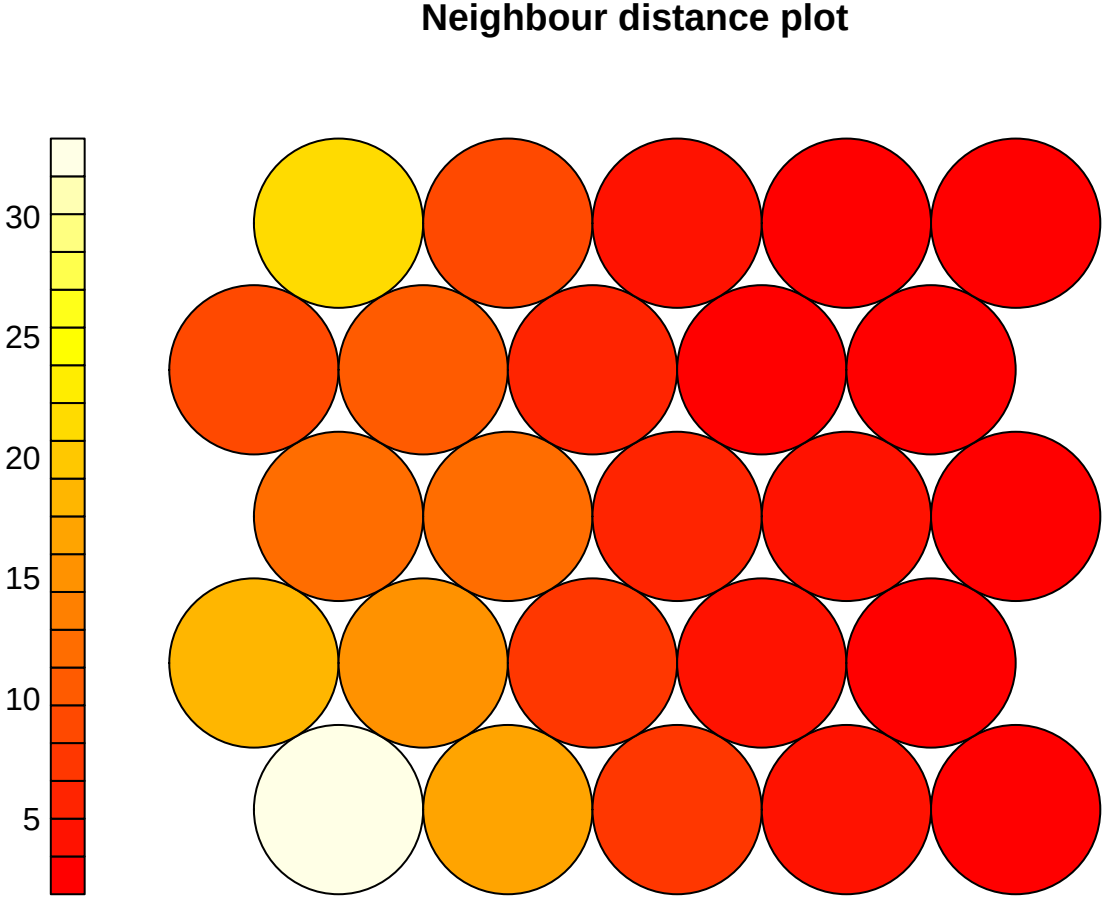
vdw



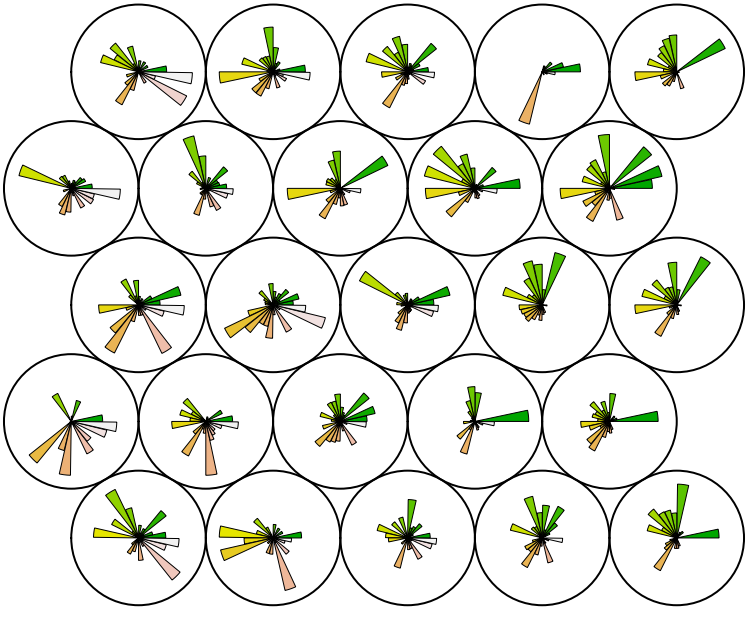
hydrogenB

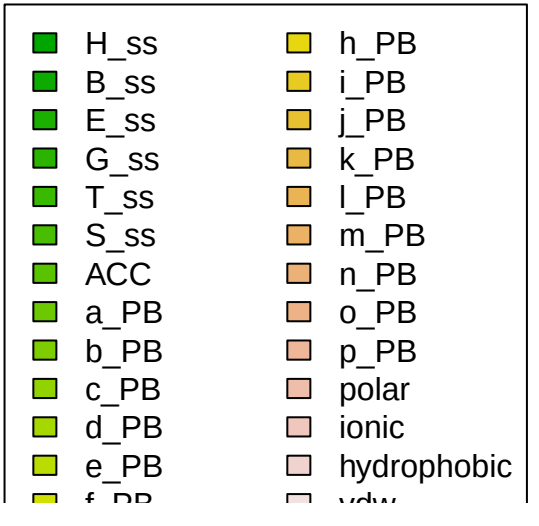



Carte de Kohonen n= 25
150
100
50


Neighbour distance plot
30
25
20
15
10
5

Codes plot




H_ss
B_ss
E_ss
G_ss
T_ss
S_ss
ACC
a_PB
b_PB
c_PB
d_PB
e_PB
h_PB
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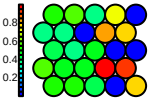
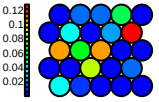
j_PB
k_PB
l_PB
m_PB
n_PB
o_PB
p_PB
polar
ionic
hydrophobic

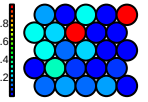
H_ss



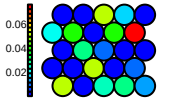
B_ss



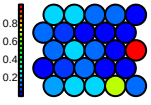
E_ss



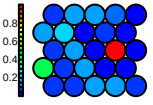
G_ss



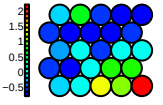
T_ss



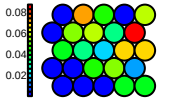
S_ss



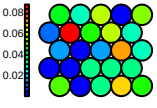
ACC



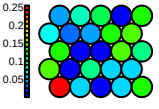
a_PB



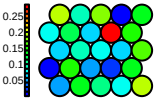
b_PB



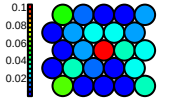
c_PB



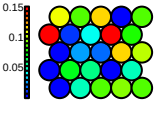
d_PB



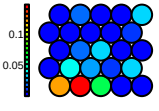
e_PB



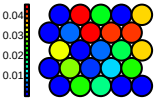
f_PB



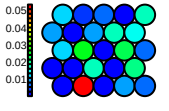
g_PB



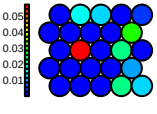
h_PB



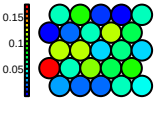
i_PB



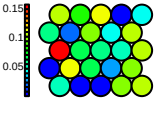
j_PB



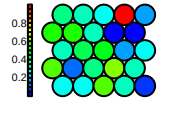
k_PB



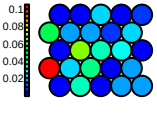
l_PB



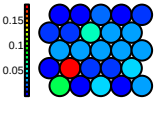
m_PB



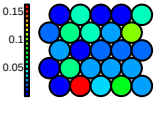
n_PB



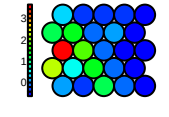
o_PB



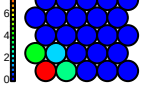
p_PB



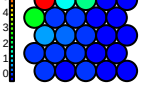
polar



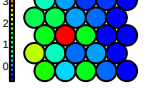
ionic



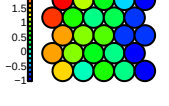
hydrophobic

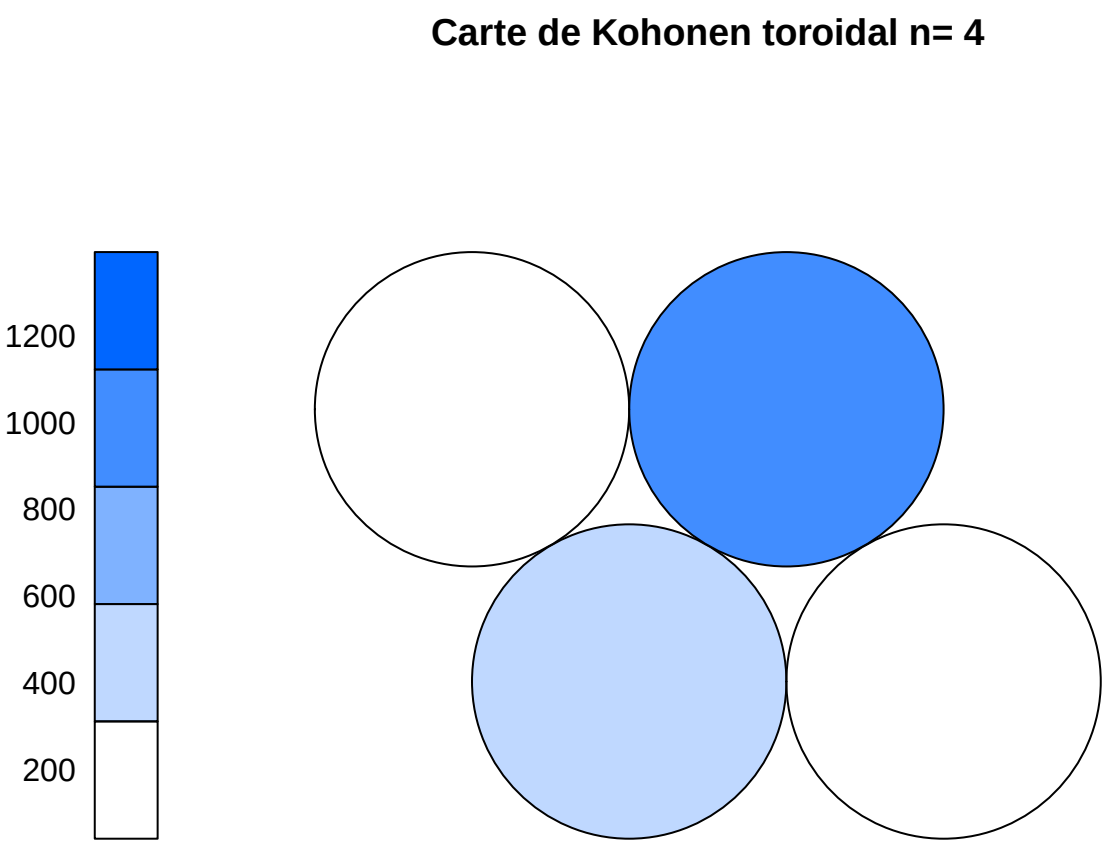


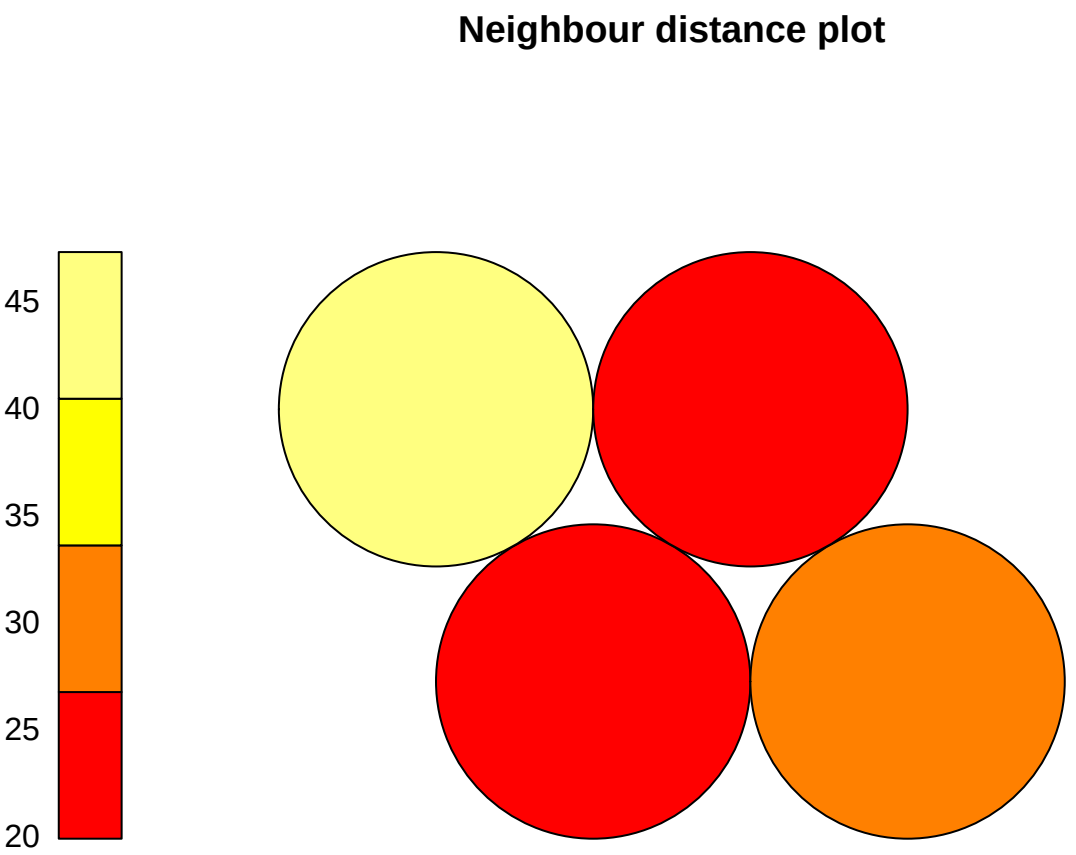
vdw



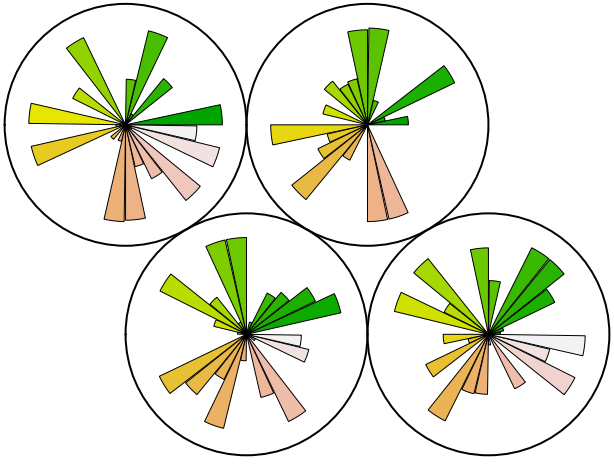
hydrogenB

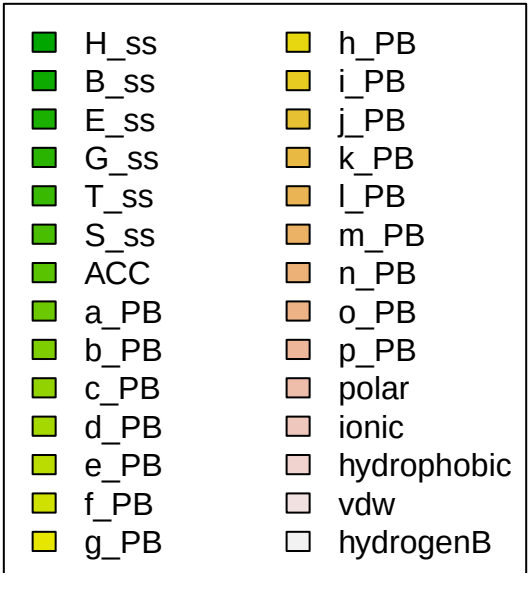



Carte de Kohonen toroidal n= 4
1200
1000
800
600
400
200


Neighbour distance plot
45
40
35
30
25
20

Codes plot




H_ss
B_ss
E_ss
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ACC
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p_PB
polar
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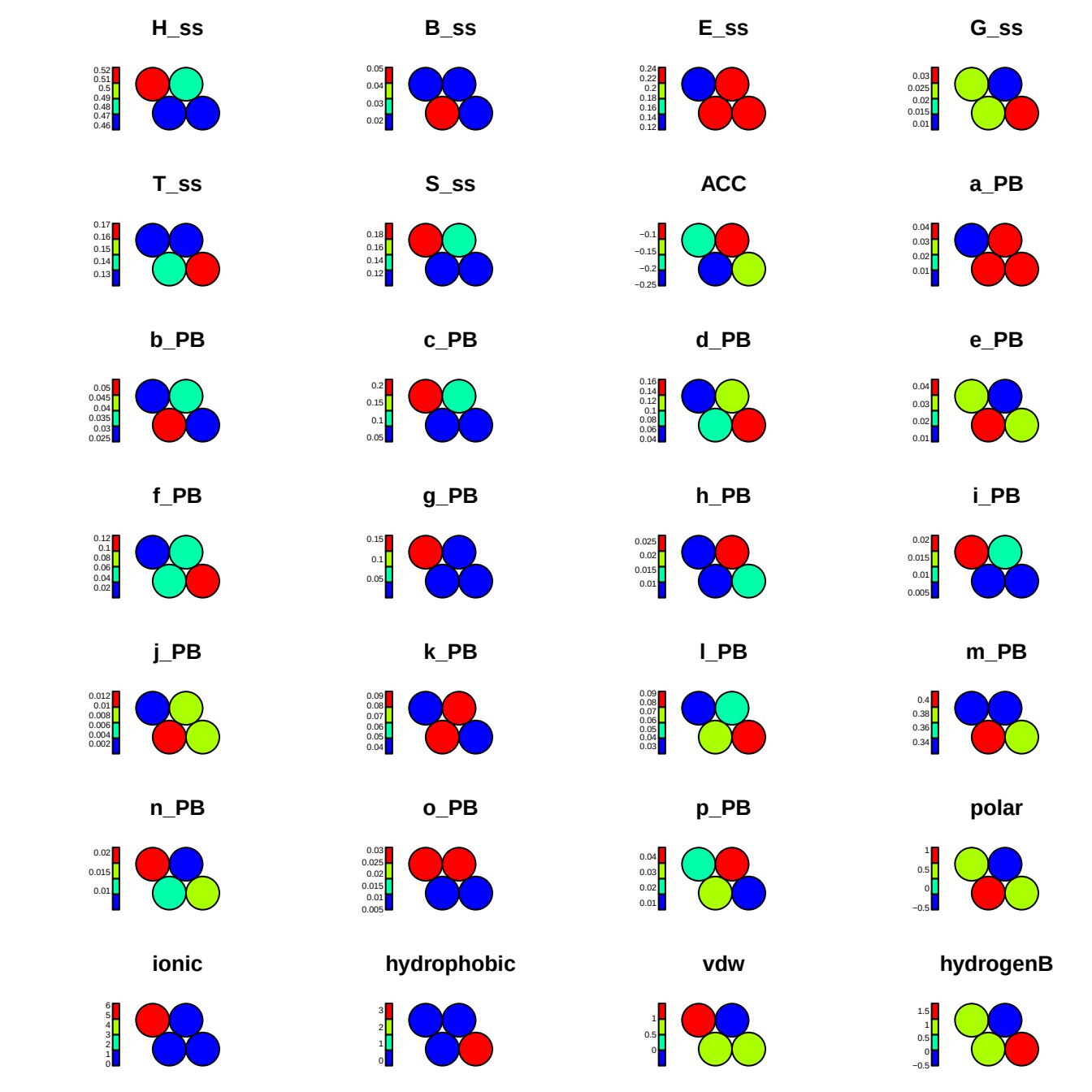
hydrophobic
vdw
hydrogenB


H_ss
B_ss
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G_ss
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c_PB
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g_PB
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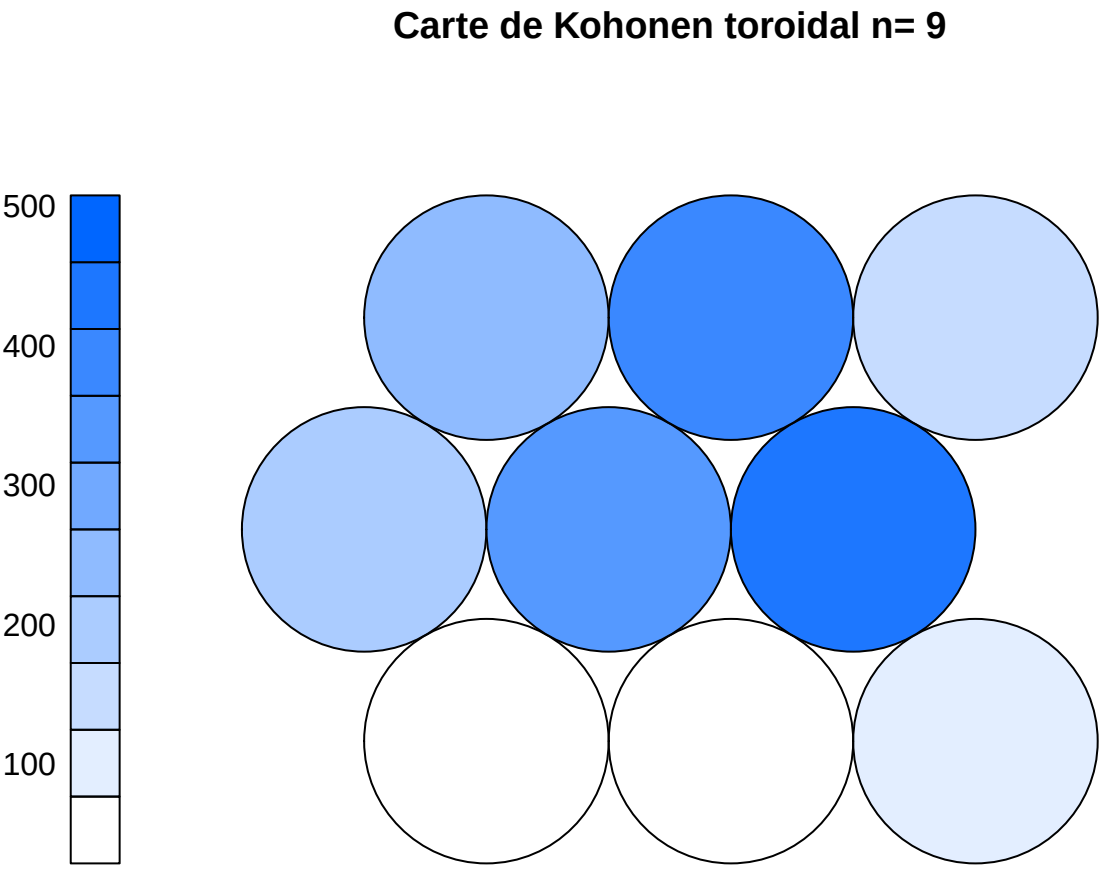
polar
ionic
hydrophobic
vdw
hydrogenB


Carte de Kohonen toroidal n= 9
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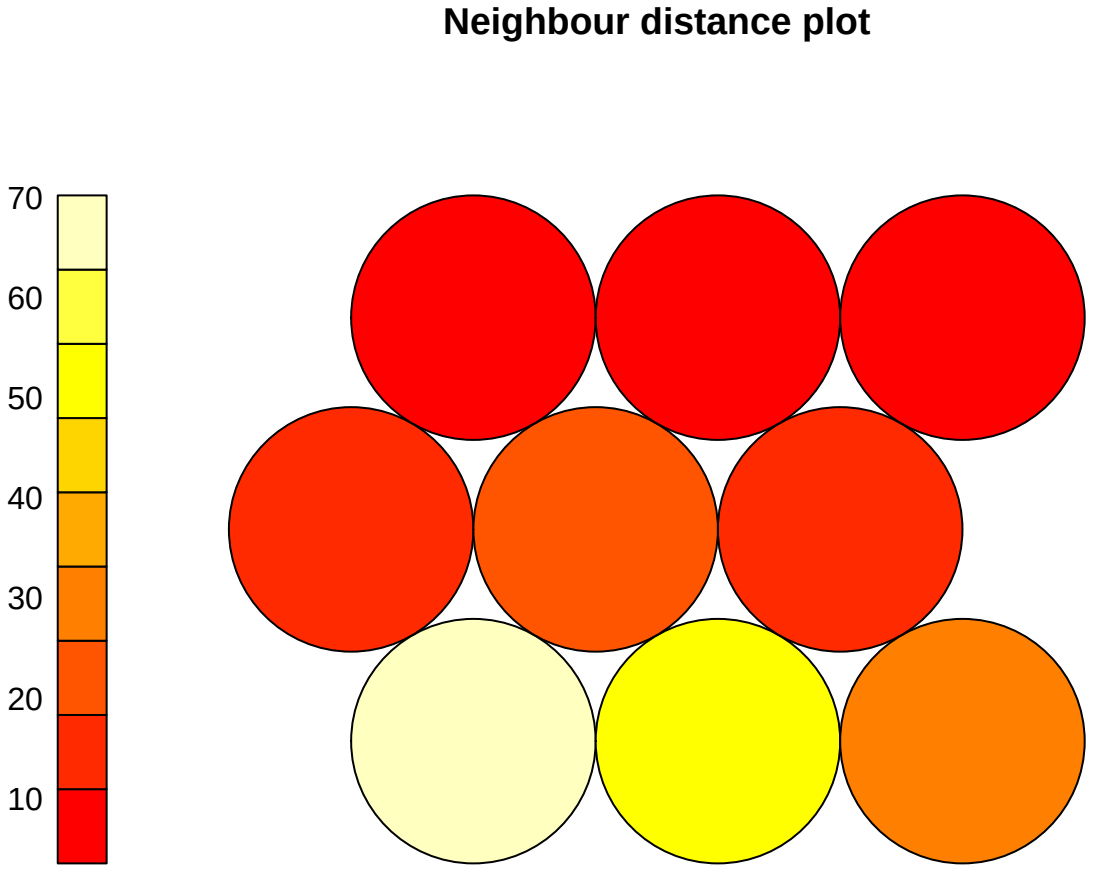
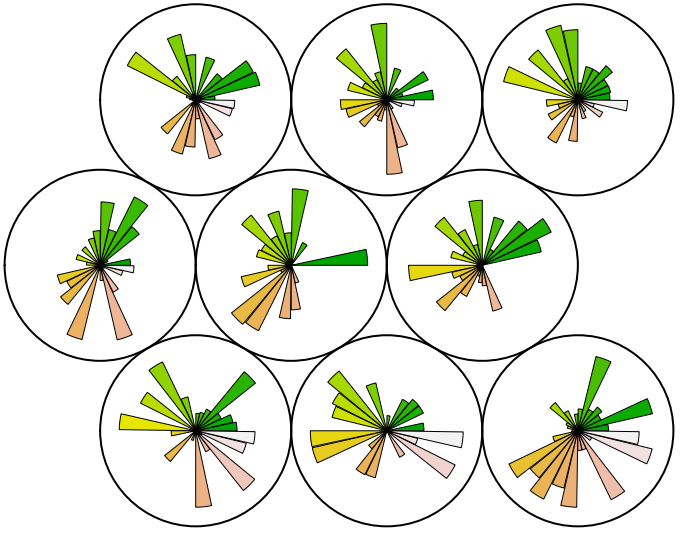
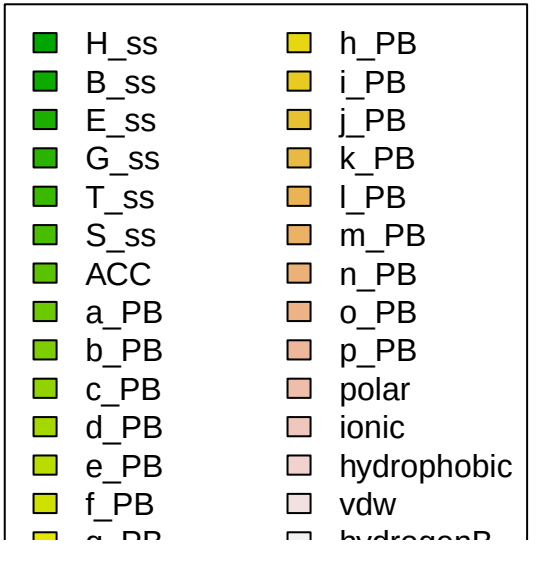
400
300
200
100


Neighbour distance plot
70
60
50
40
30
20
10

Codes plot




H_ss
B_ss
E_ss
G_ss
T_ss
S_ss
ACC
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b_PB
c_PB
d_PB
e_PB
f_PB
h_PB
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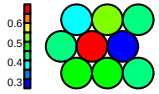
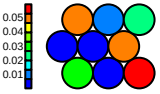
m_PB
n_PB
o_PB
p_PB
polar
ionic
hydrophobic
vdw

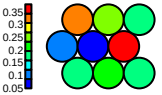
H_ss



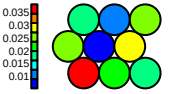
B_ss



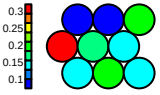
E_ss



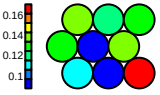
G_ss



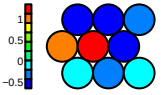
T_ss



S_ss



ACC



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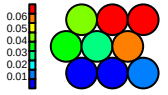

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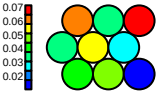

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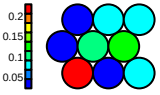

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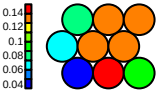

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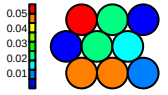

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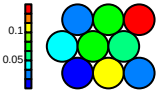

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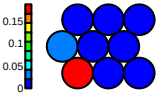

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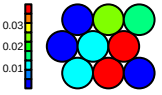

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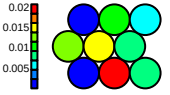

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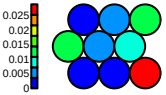

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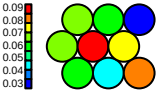

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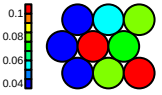

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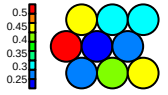

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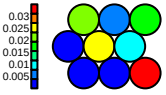

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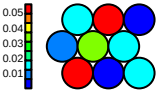

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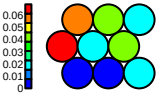

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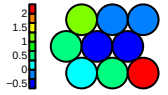

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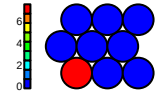
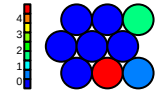


hydrophobic



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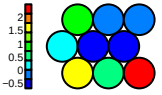
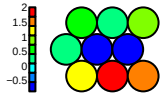
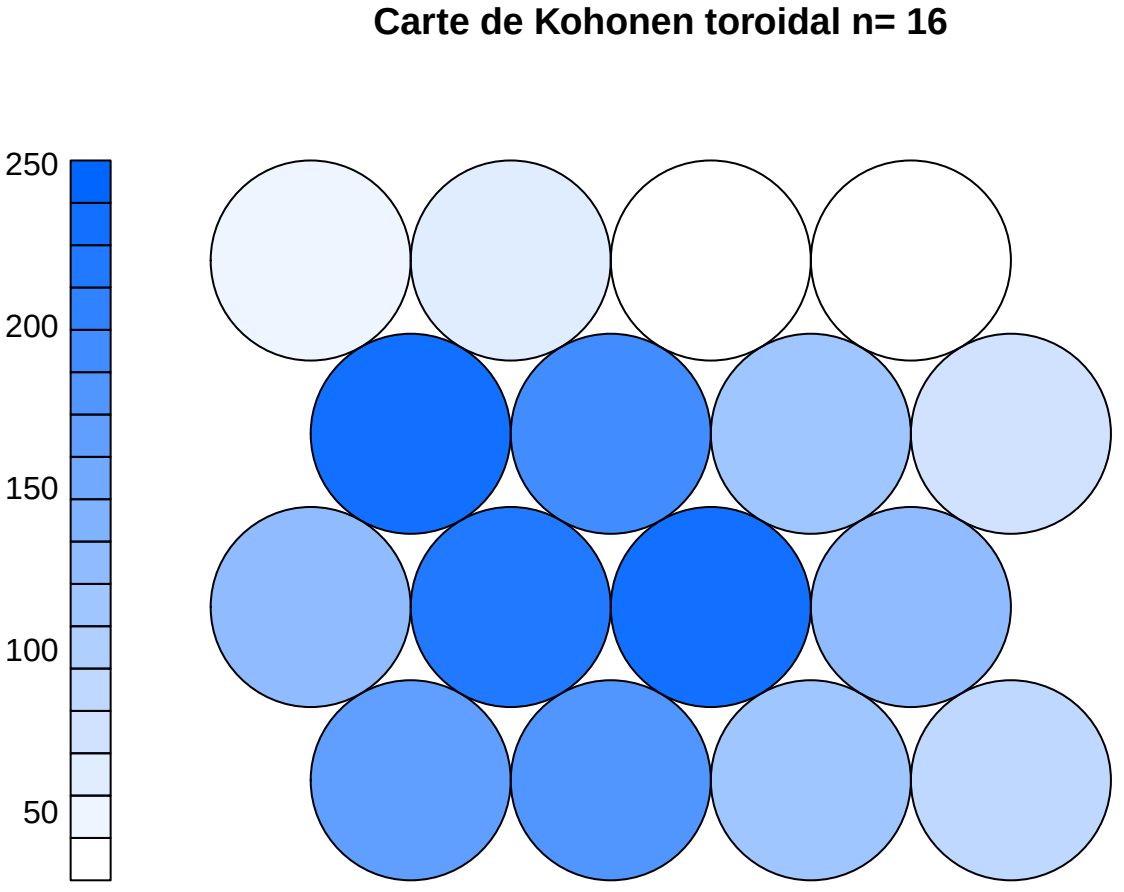


hydrogenB

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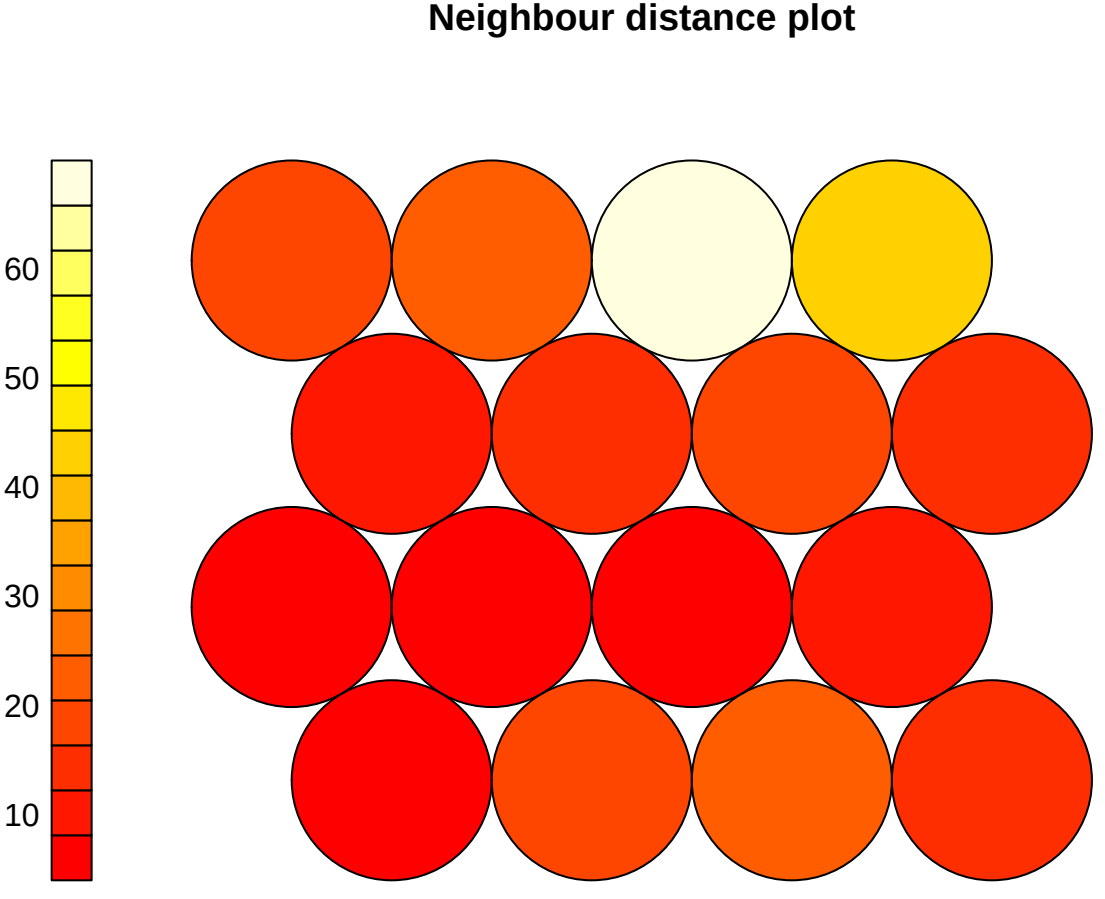
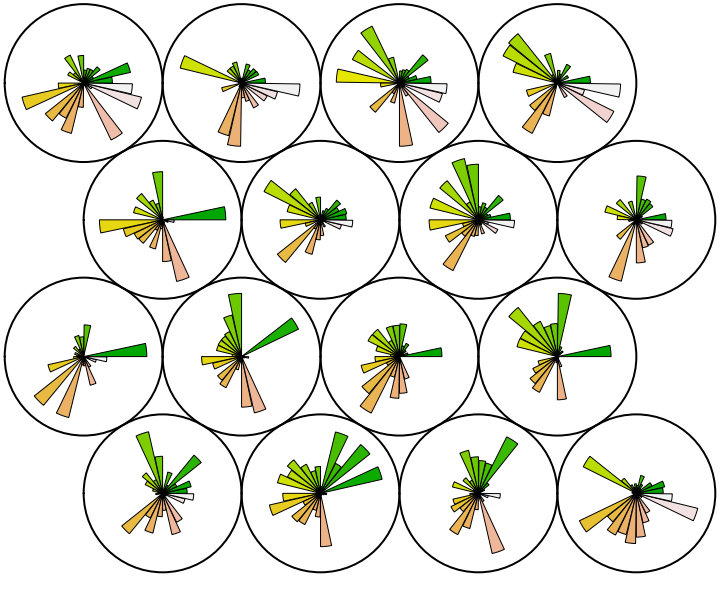
150
100
50


Neighbour distance plot
60
50
40
30
20
10

Codes plot



H_ss
B_ss
E_ss
G_ss
T_ss
S_ss
ACC
a_PB
b_PB
c_PB
d_PB
e_PB
f_PB
h_PB
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polar
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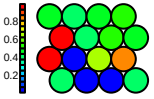
hydrophobic
vdw

H_ss



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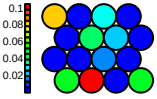

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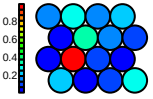

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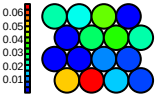

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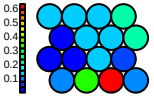
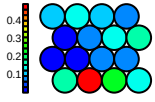


S_ss



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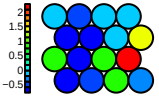

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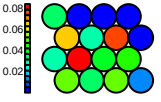

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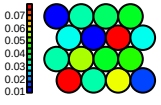

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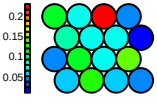

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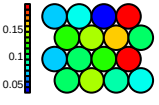

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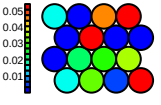

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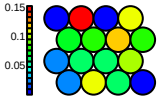
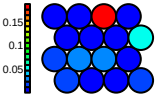


g_PB



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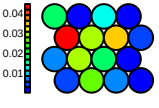

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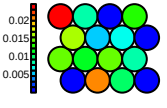

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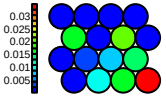
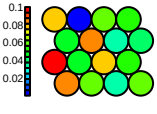


k_PB



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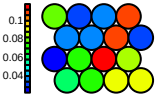

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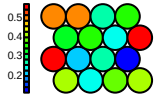

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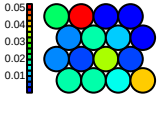

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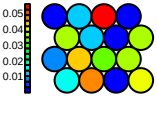

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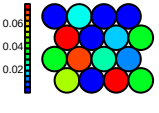
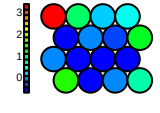
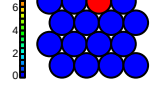


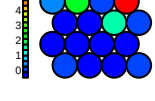
polar



ionic



hydrophobic



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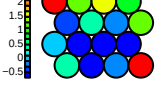

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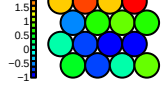
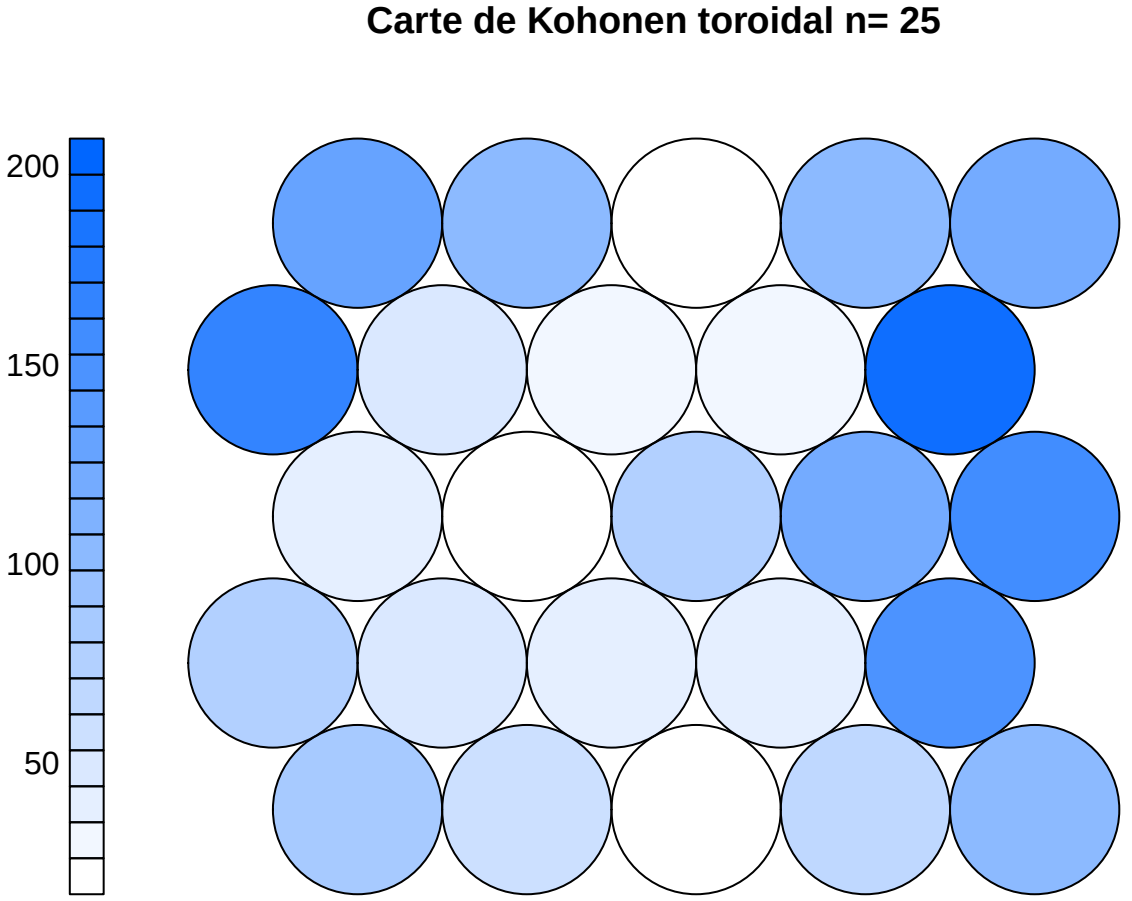
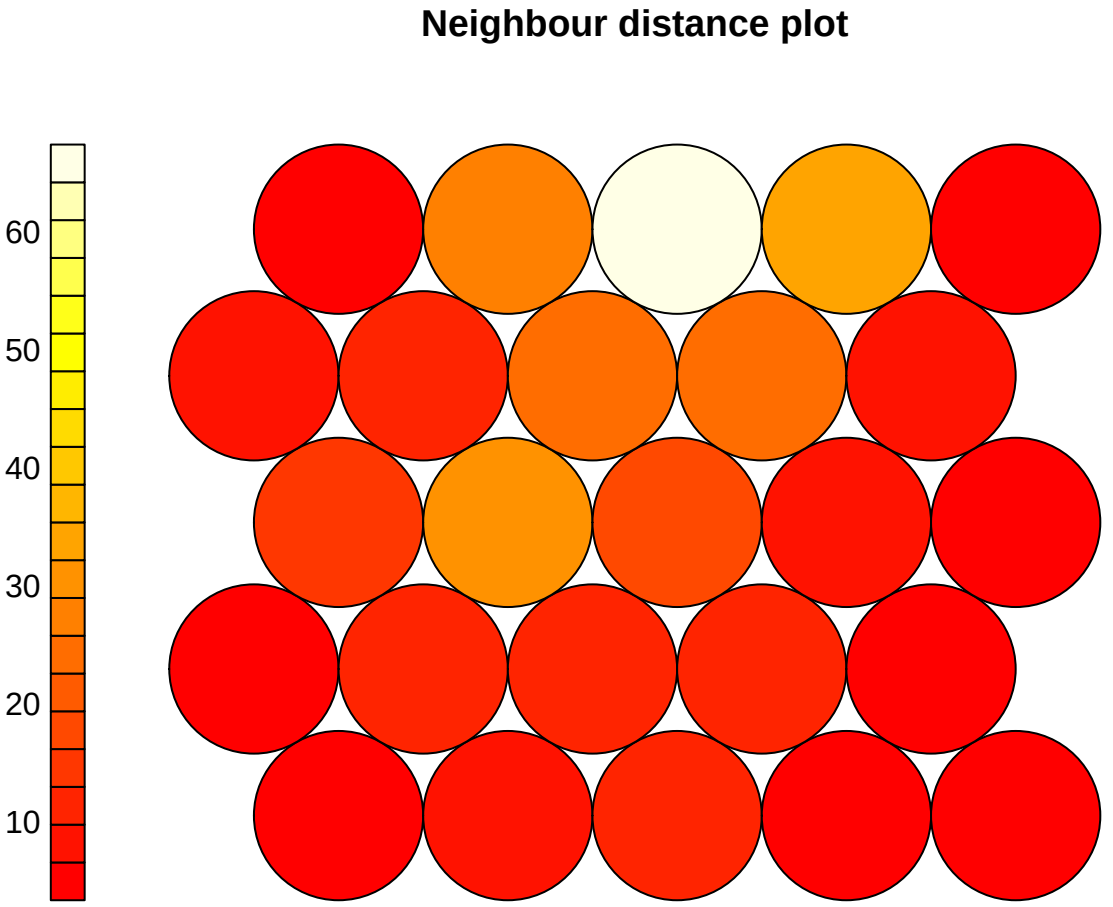



Carte de Kohonen toroidal n= 25
200
150
100
50


Neighbour distance plot
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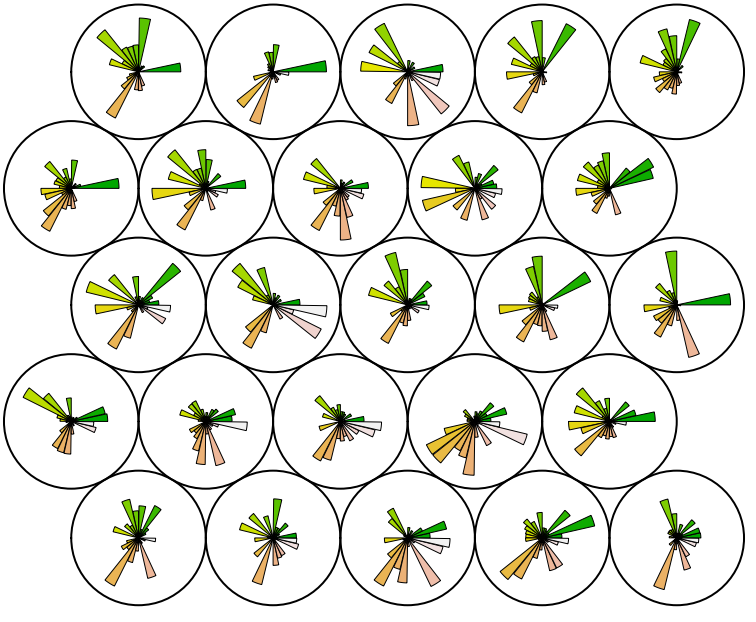
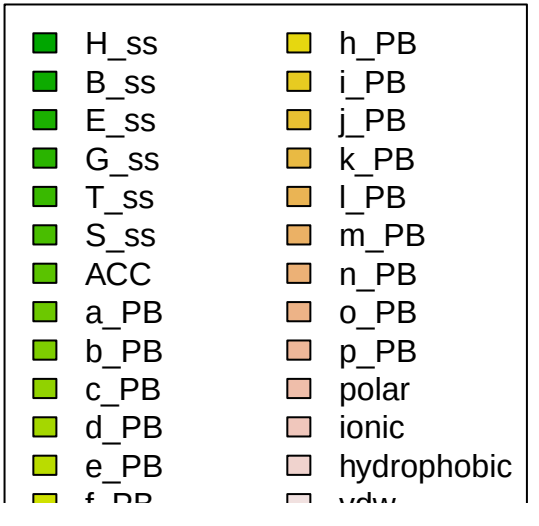
50
40
30
20
10

Codes plot




H_ss
B_ss
E_ss
G_ss
T_ss
S_ss
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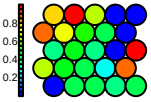
polar
ionic
hydrophobic

H_ss



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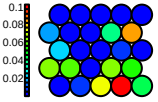
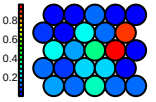


E_ss



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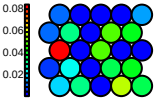

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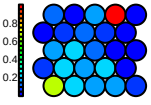
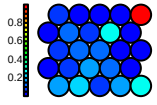


S_ss



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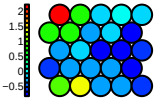

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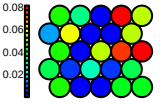

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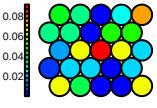

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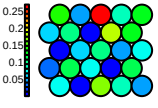

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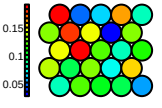

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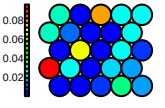
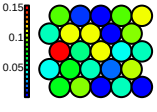


f_PB



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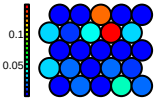
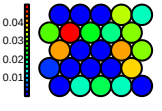


h_PB



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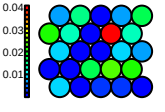

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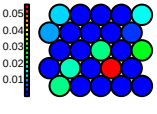
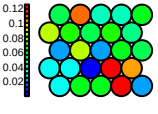


k_PB



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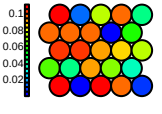

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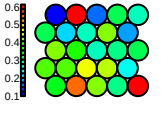

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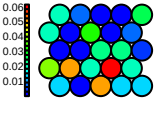

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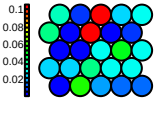
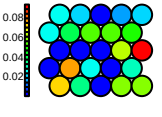


p_PB



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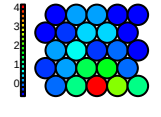

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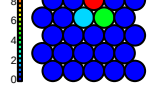

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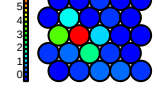

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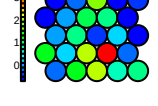
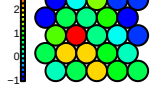
hydrogenB