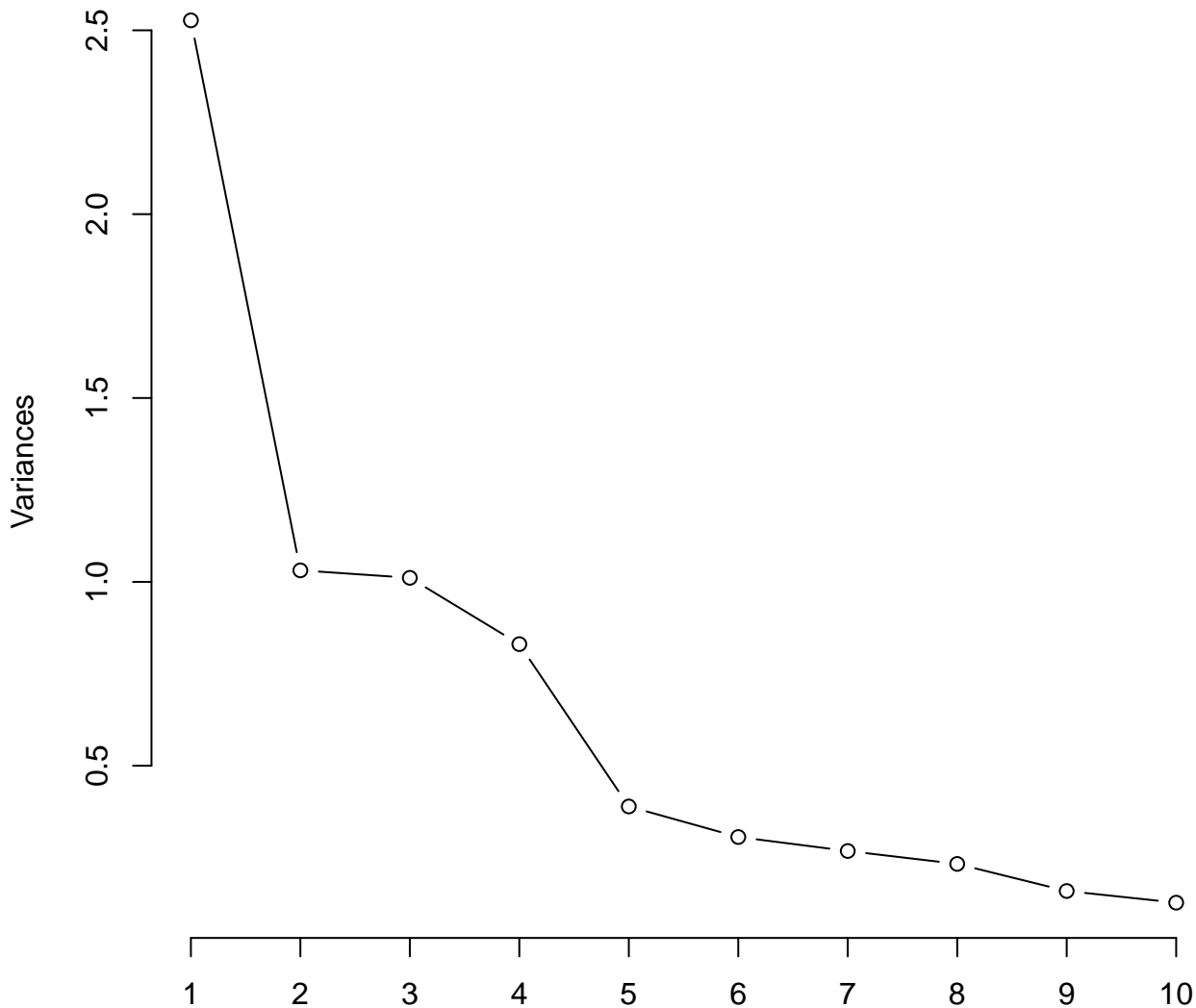
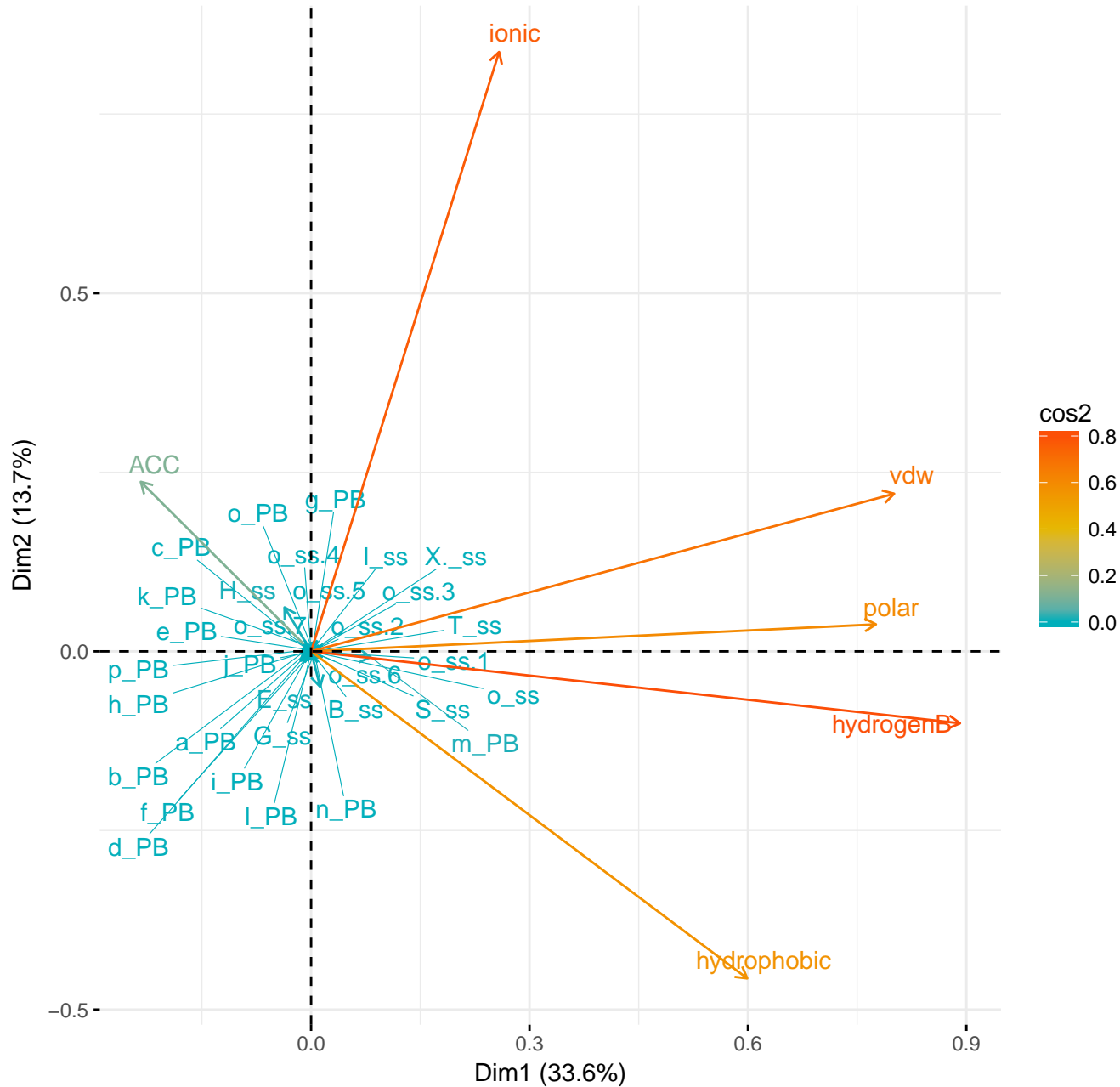


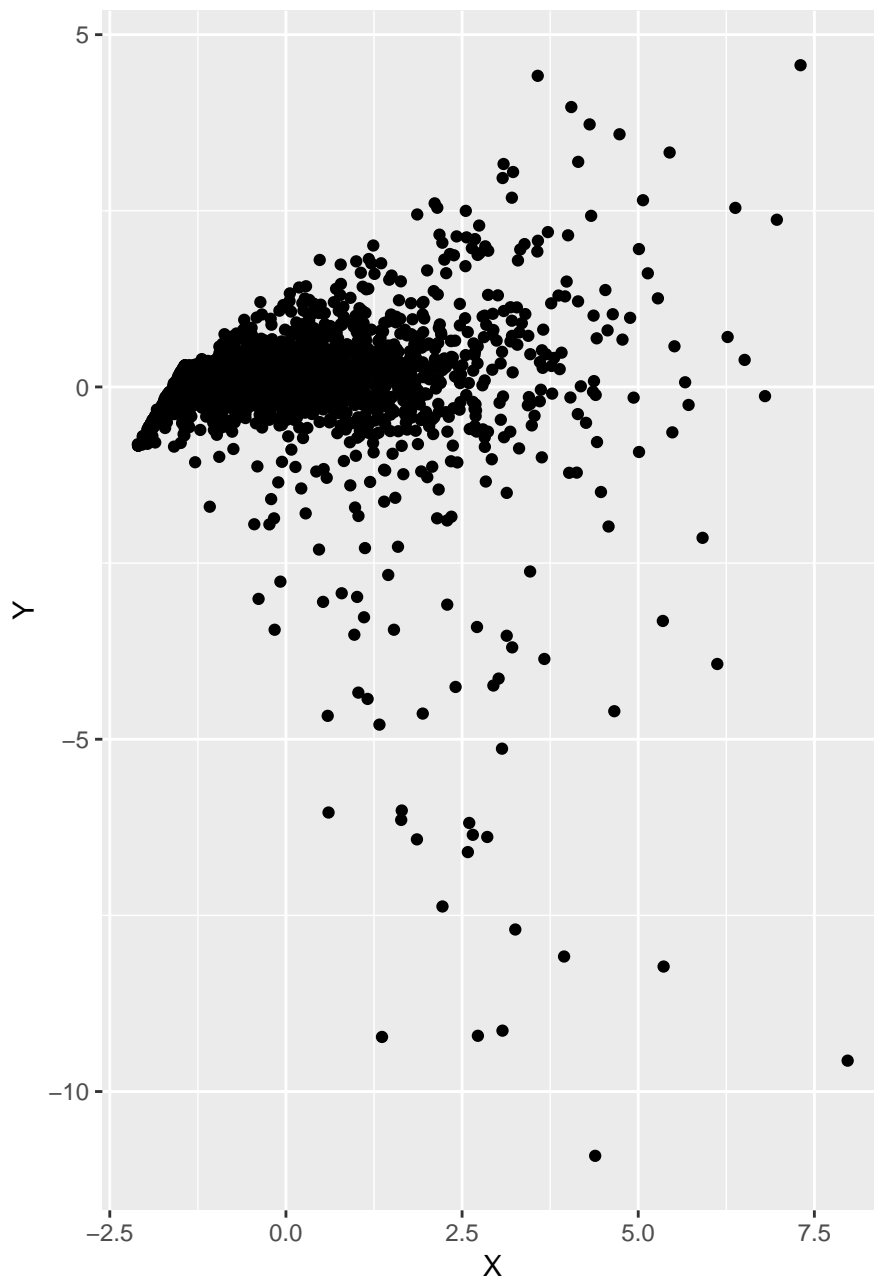
## Variances en fonction des Composantes Principales



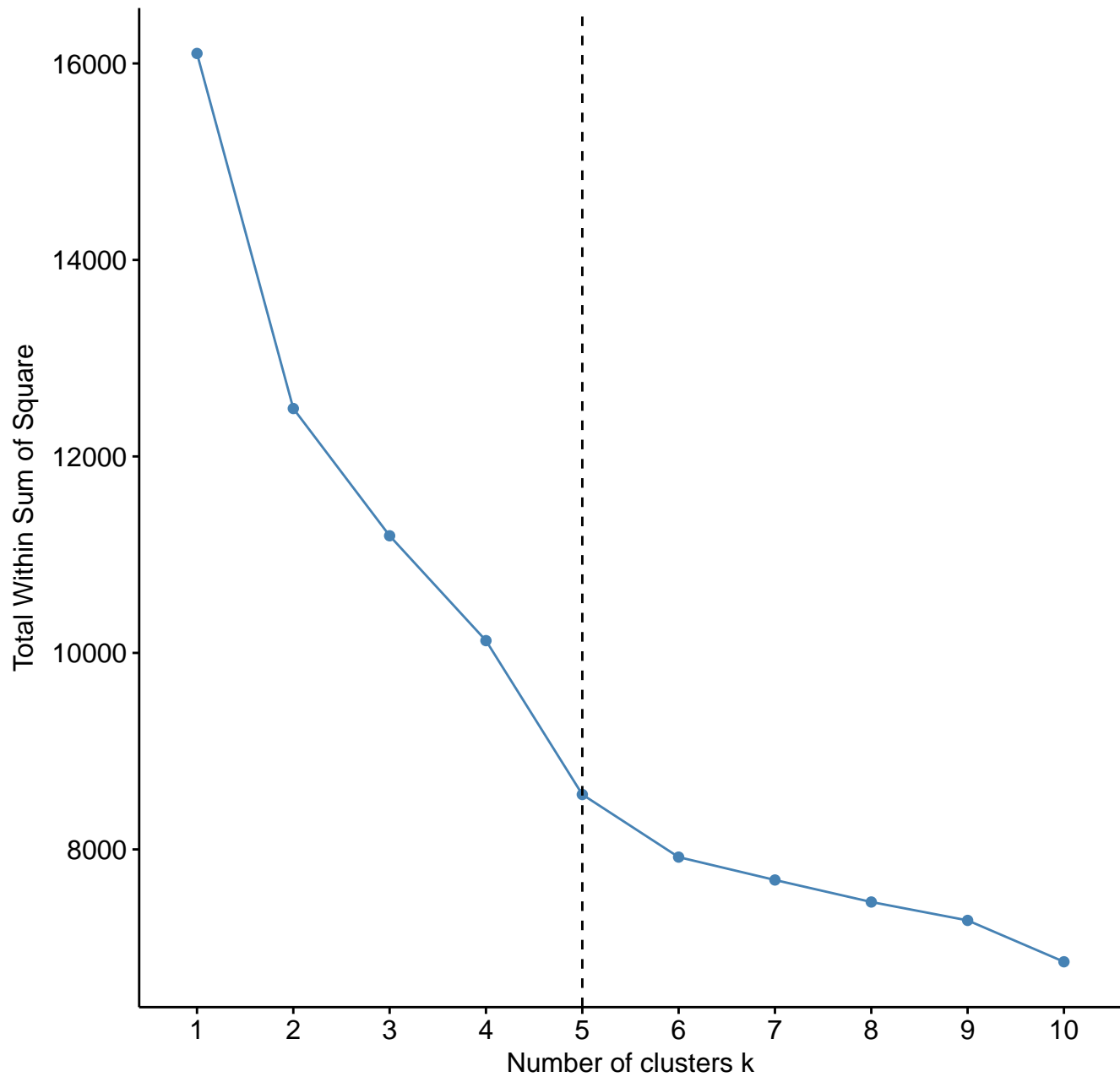
# Variables – PCA



MDS with Shephard–Kruskal Stress 0.6



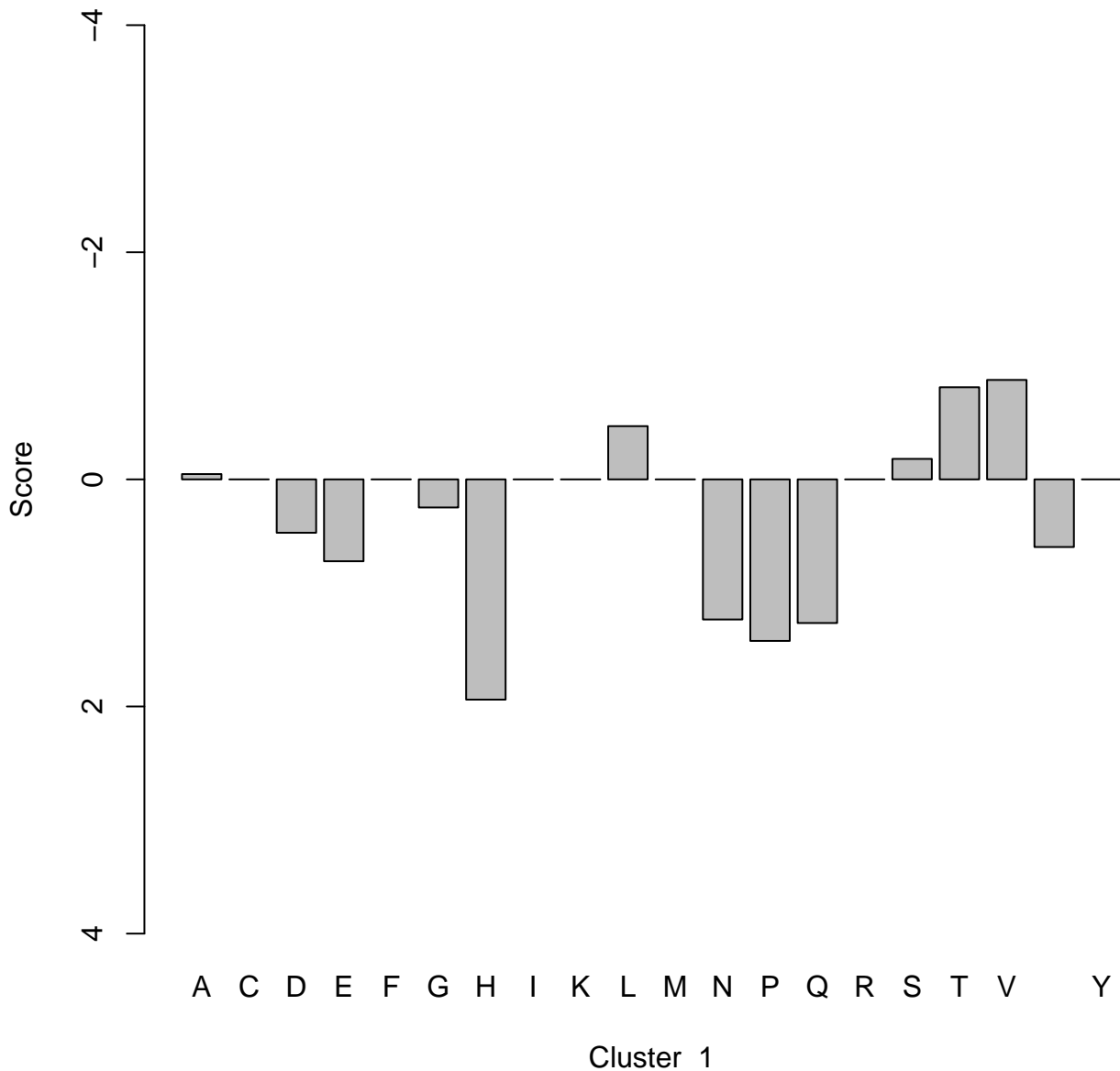
Optimal number of clusters



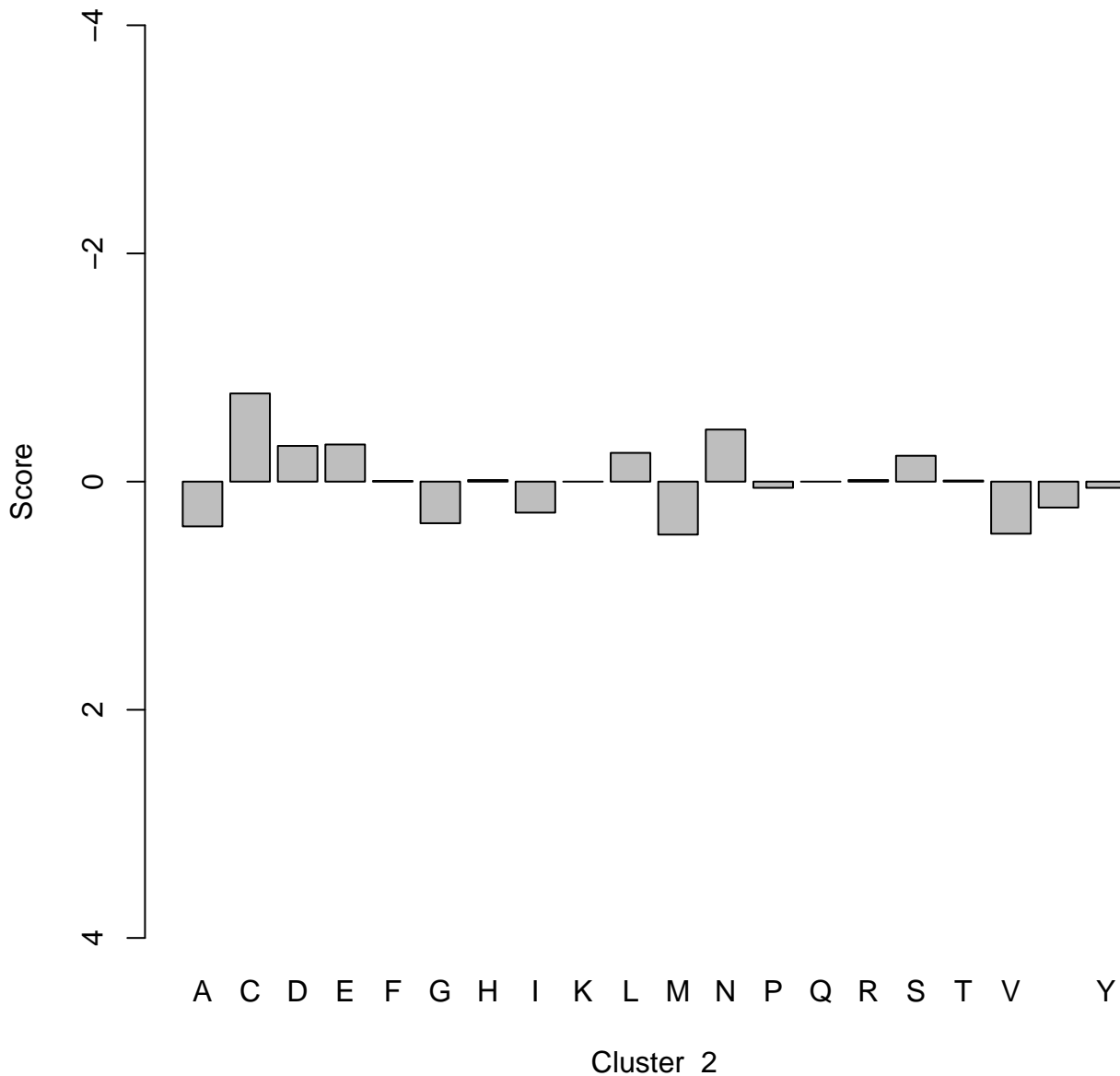
A PCA plot showing the distribution of 1000 random numbers. The x-axis is labeled 'PC1' and ranges from 0.00 to 0.08. The y-axis is unlabeled but ranges from approximately -0.02 to 0.06. The data points are colored based on their value, with a gradient from blue (low values) to red (high values). Four overlapping convex hulls are drawn around the data, representing different value ranges: a red hull for high values (top right), a blue hull for low values (bottom left), a green hull for intermediate values (center), and a yellow hull for intermediate values (bottom right). The hulls are semi-transparent, allowing overlapping areas to appear darker. The red hull is the largest and most central, while the blue hull is the smallest and most peripheral.



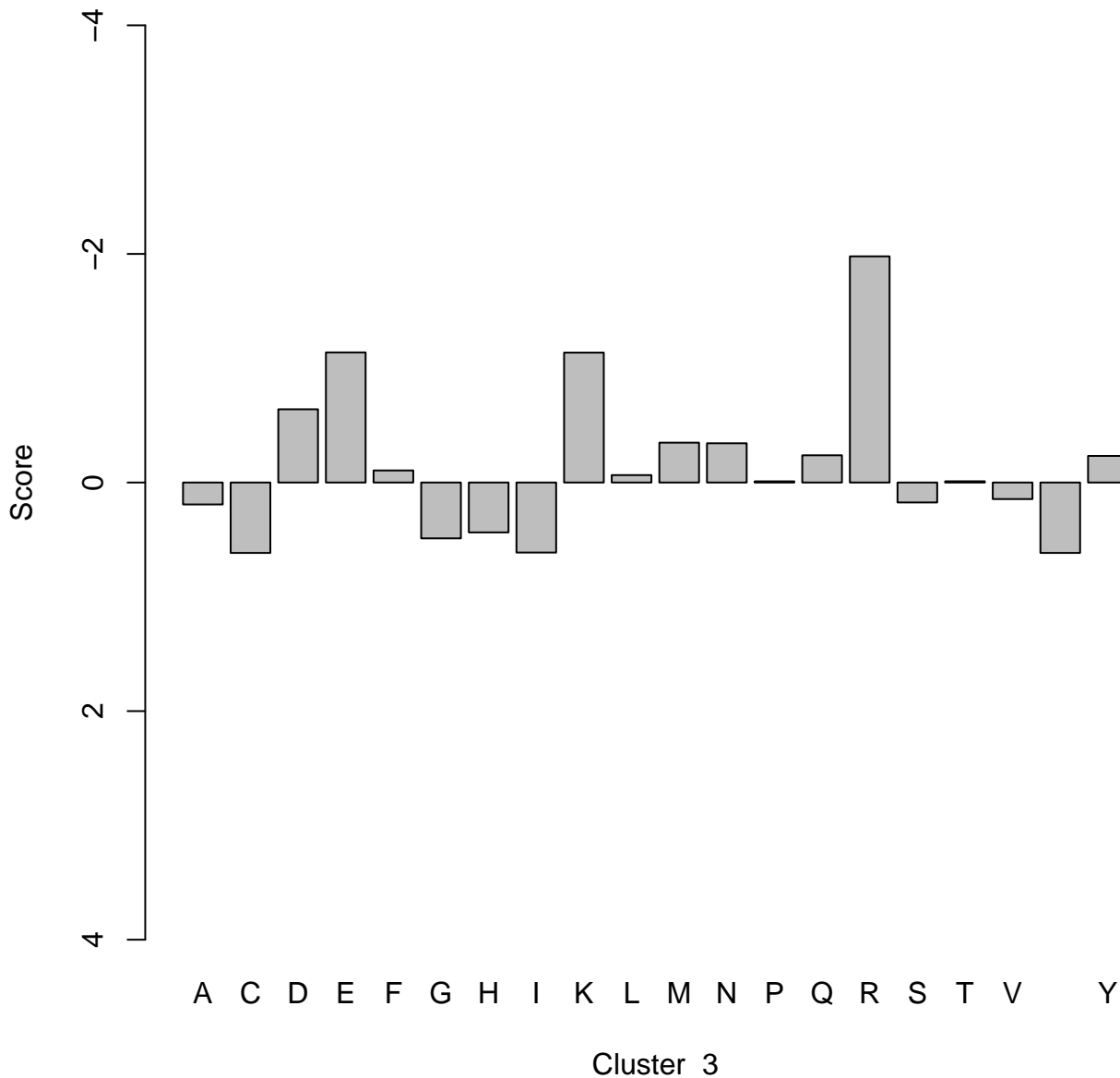
## Distribution des scores (Méthodes Kmeans)



## Distribution des scores (Méthodes Kmeans)

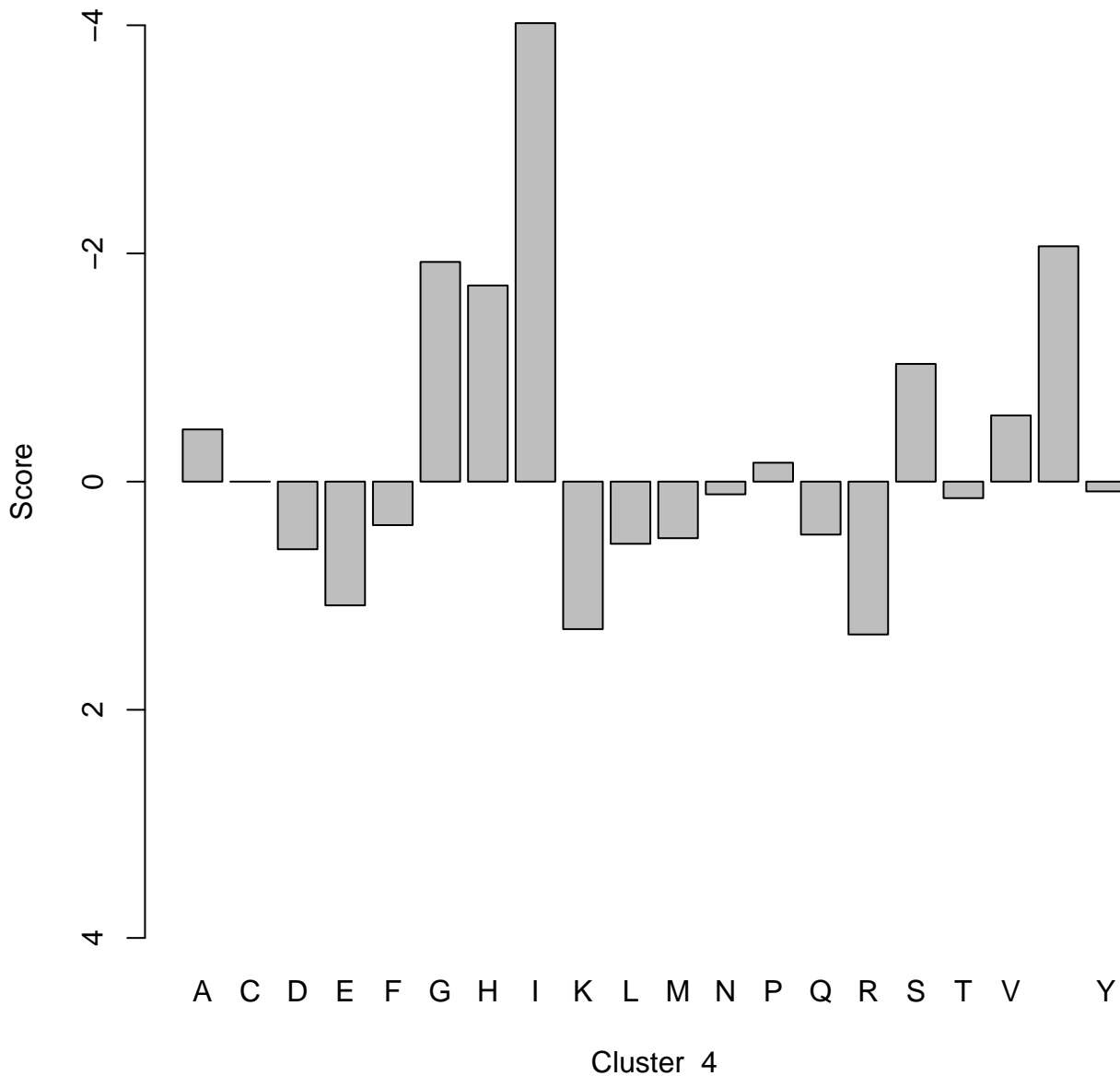


## Distribution des scores (Méthodes Kmeans)

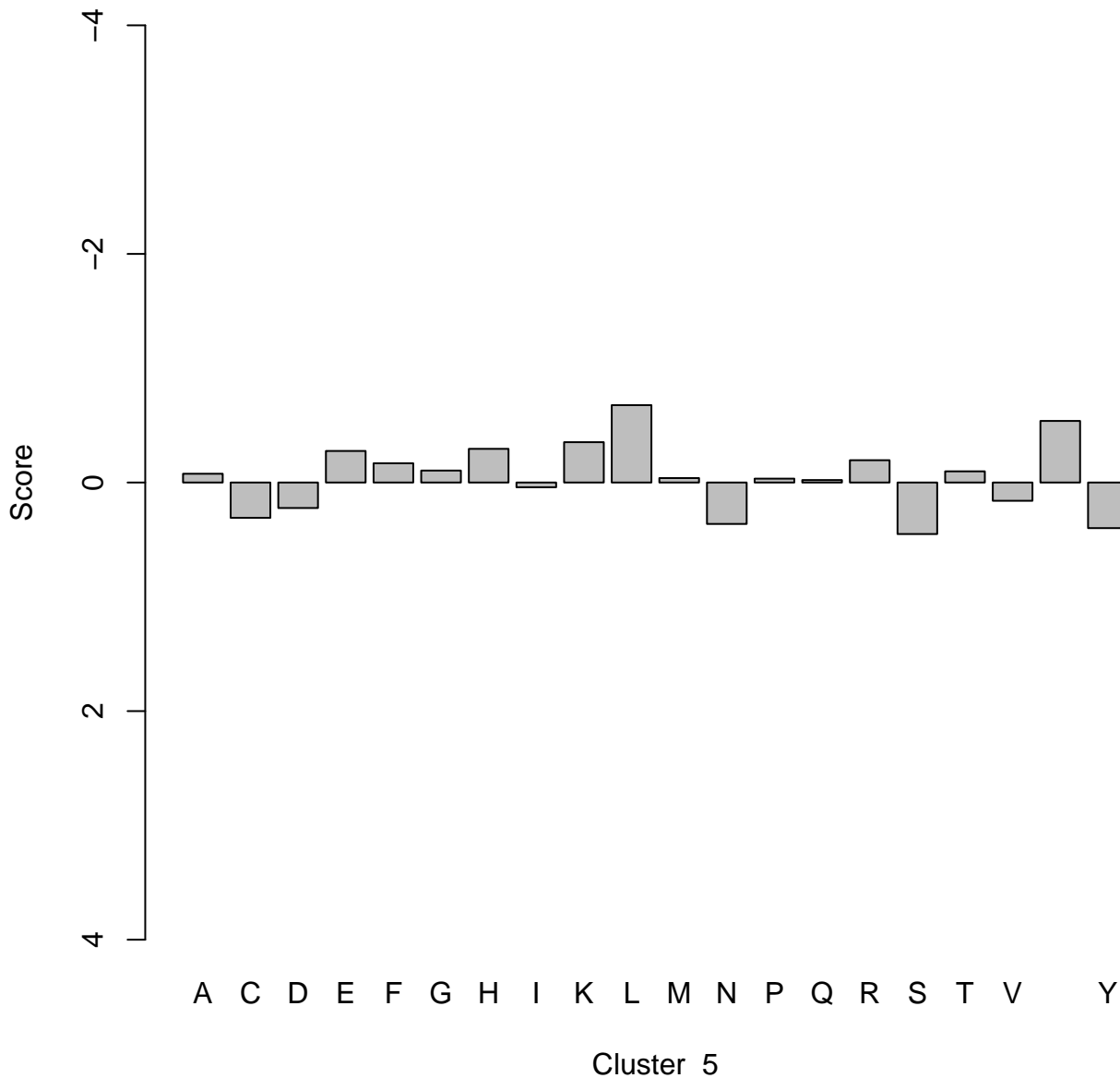




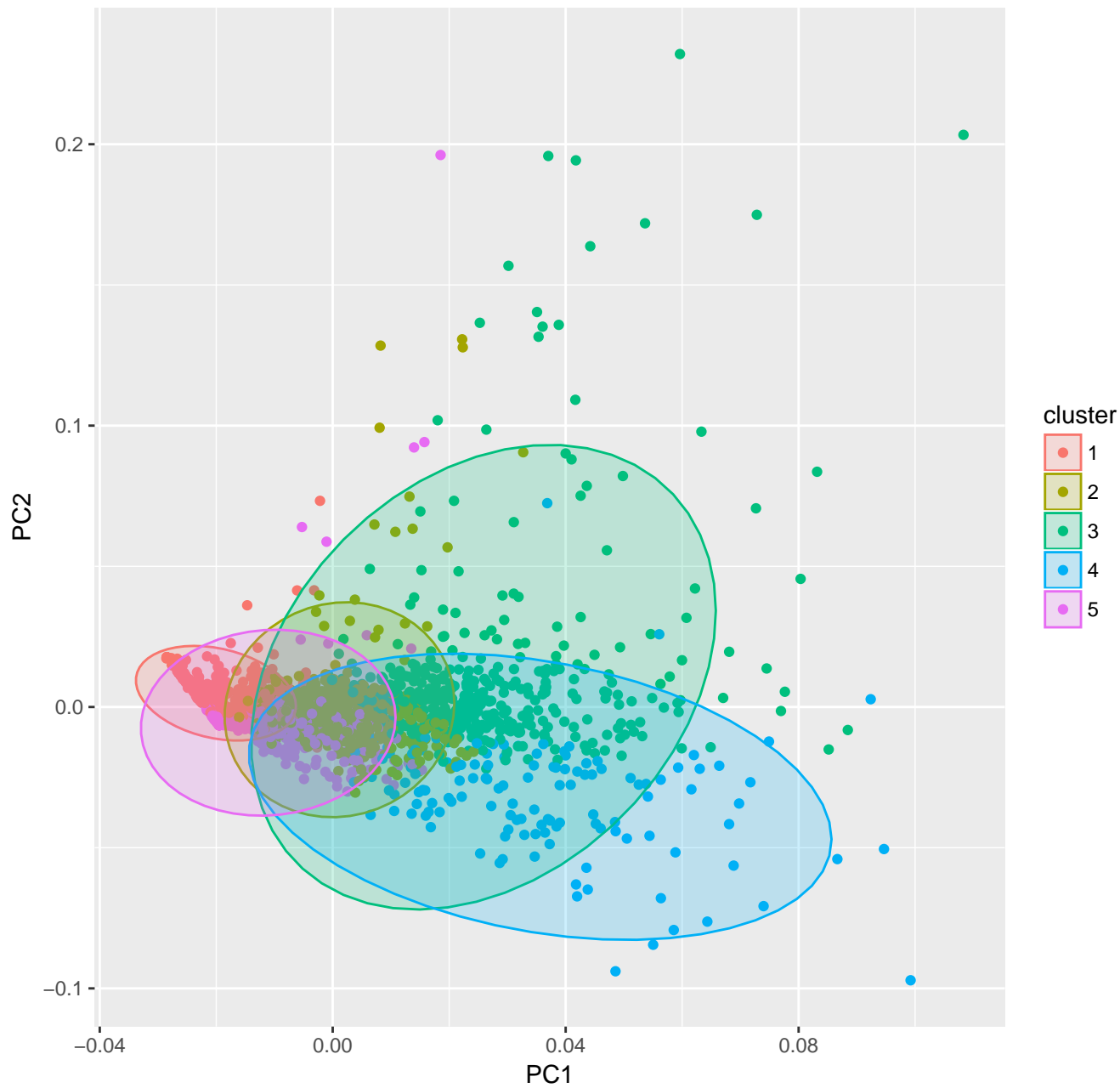
## Distribution des scores (Méthodes Kmeans)



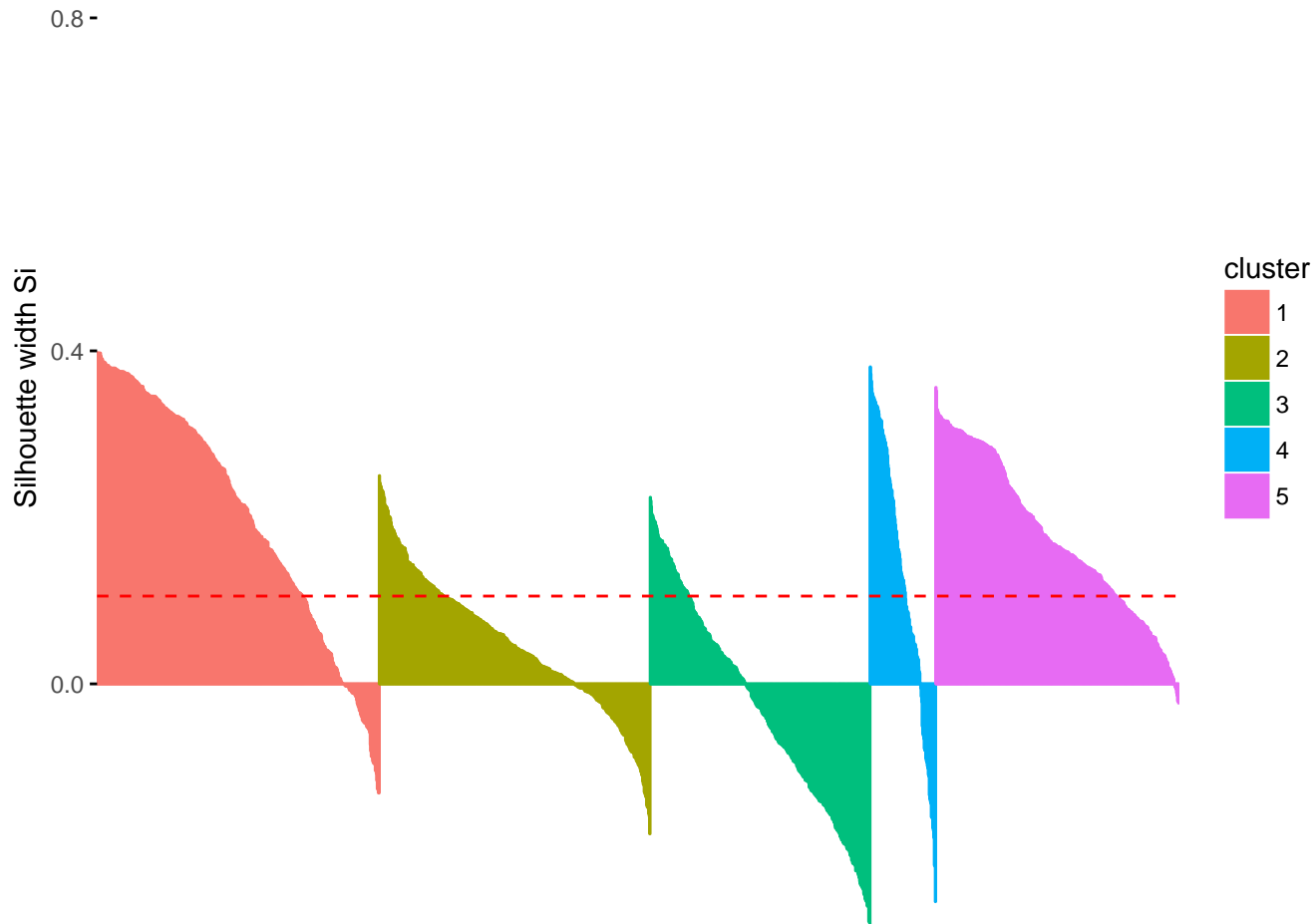
## Distribution des scores (Méthodes Kmeans)



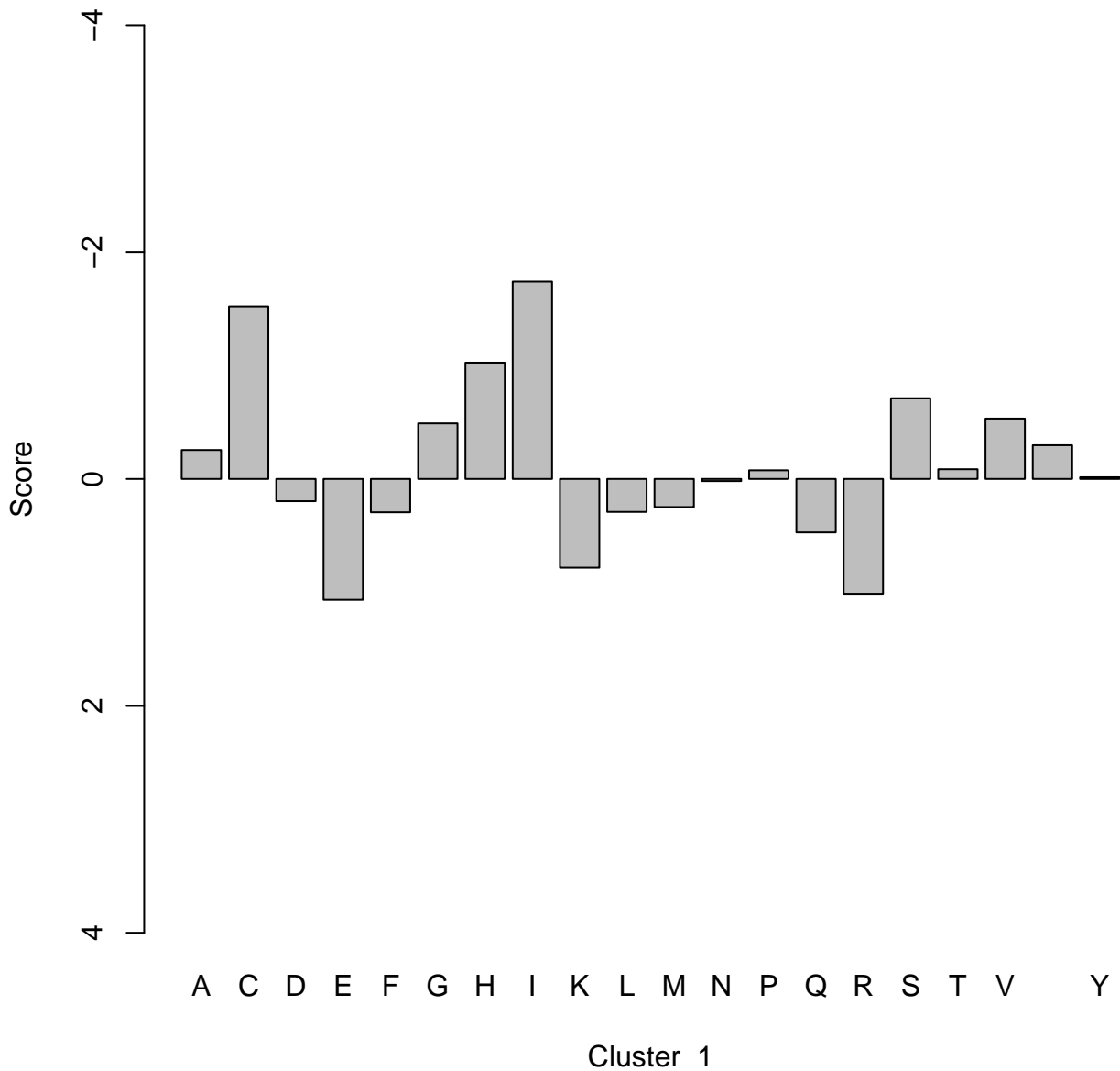
Clustering par Kmedoid(PAM)



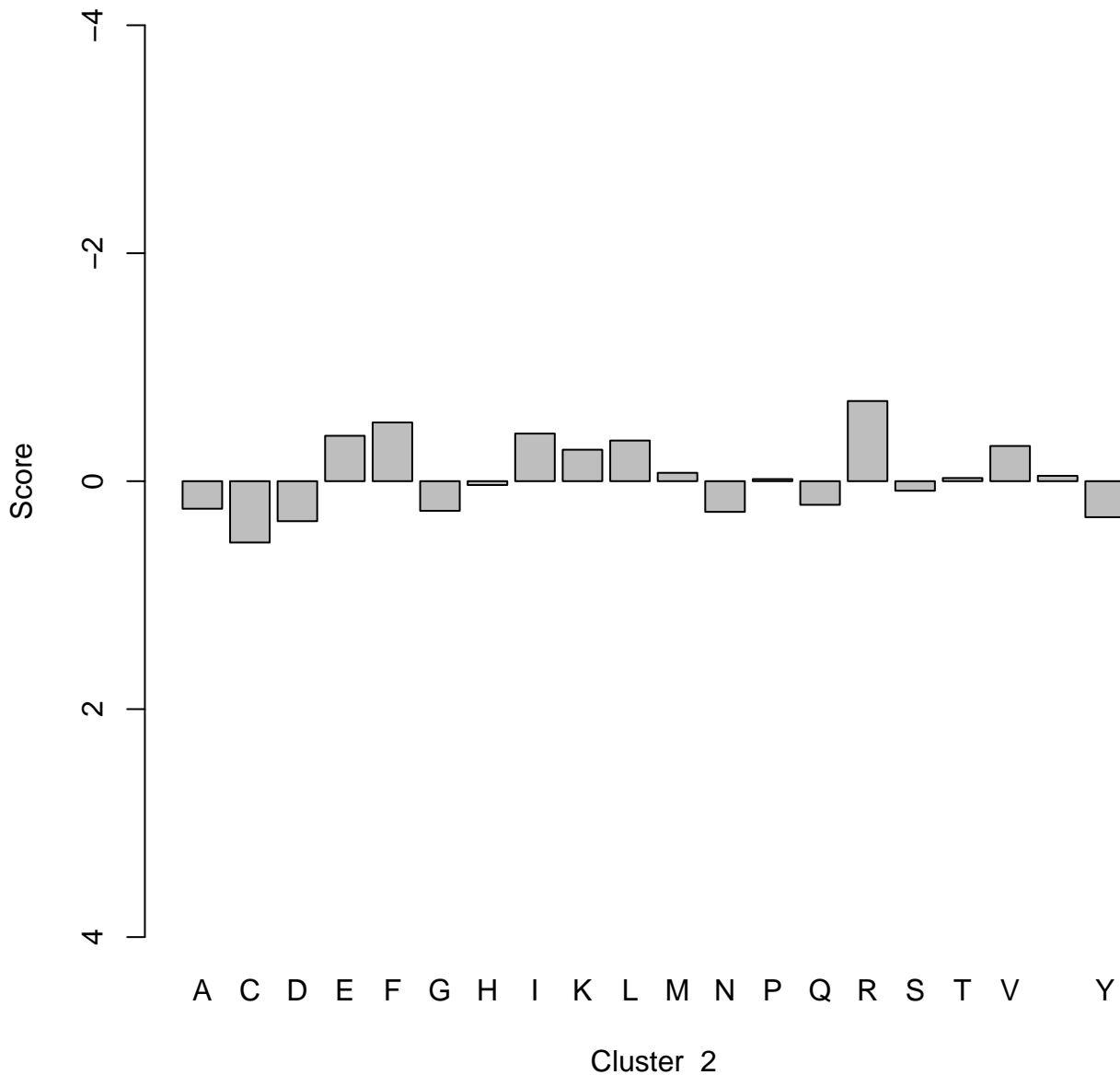
Clusters silhouette plot  
Average silhouette width: 0.11



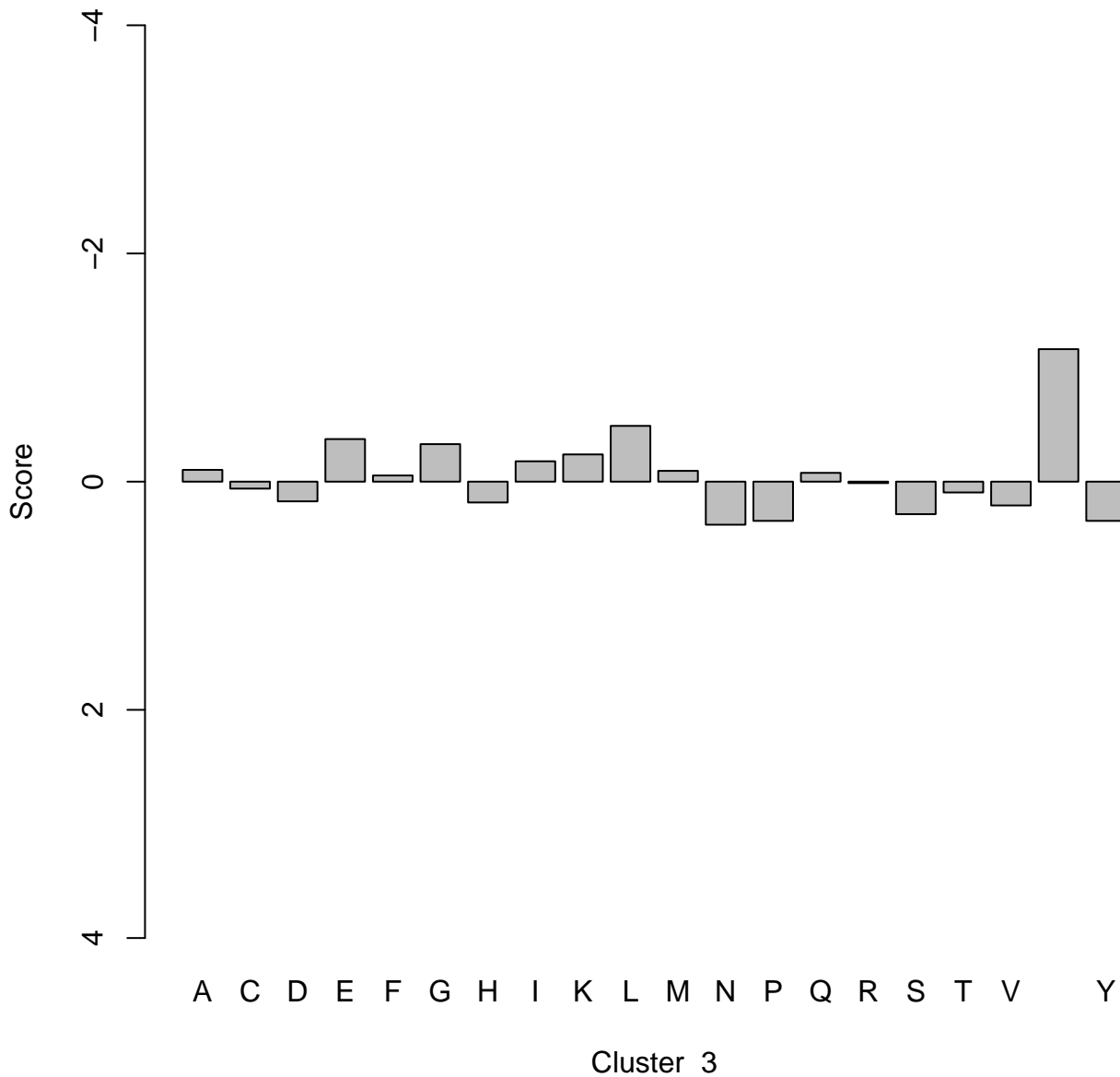
## Distribution des scores (Méthode PAM)



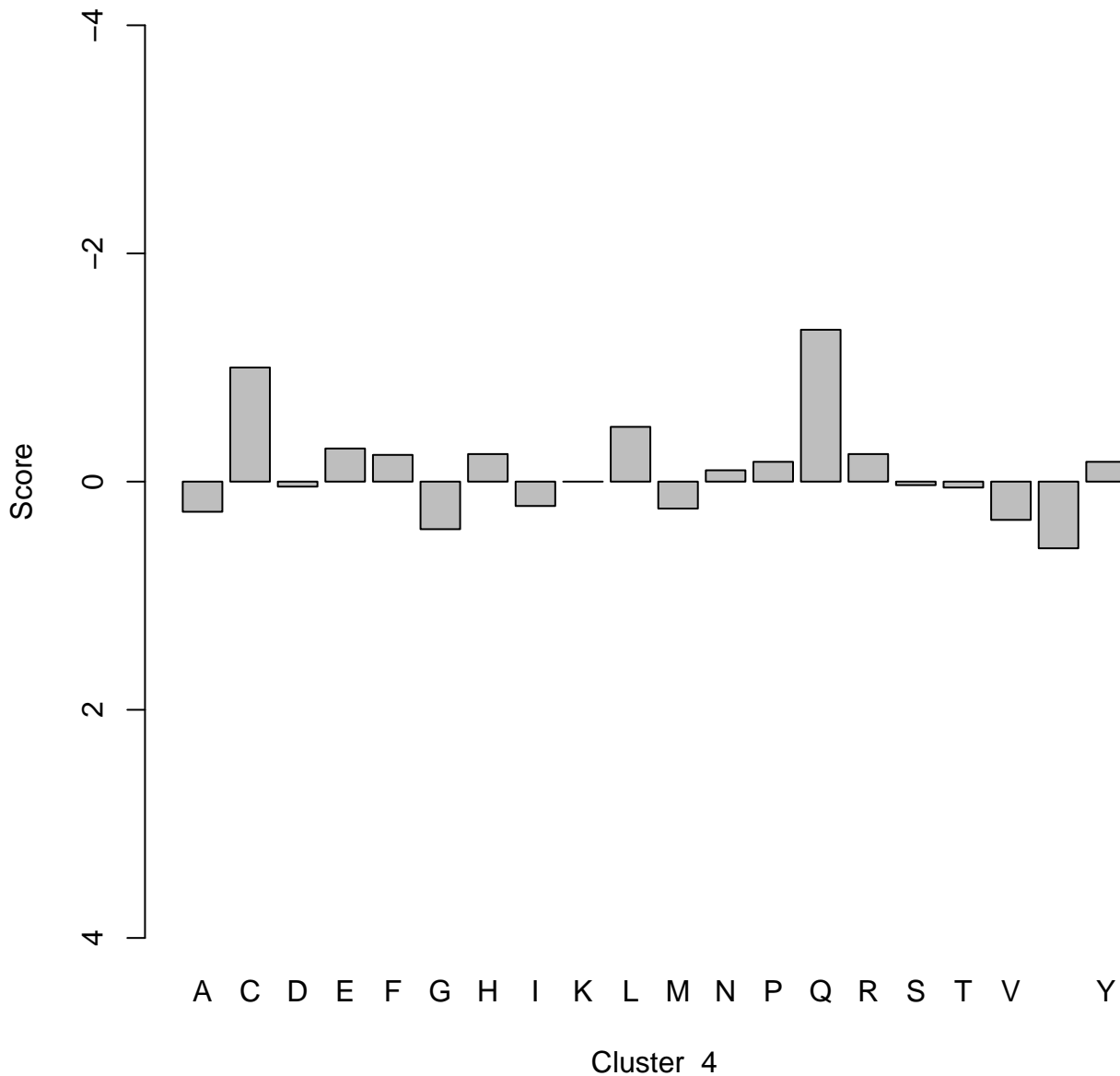
## Distribution des scores (Méthode PAM)



# Distribution des scores (Méthode PAM)

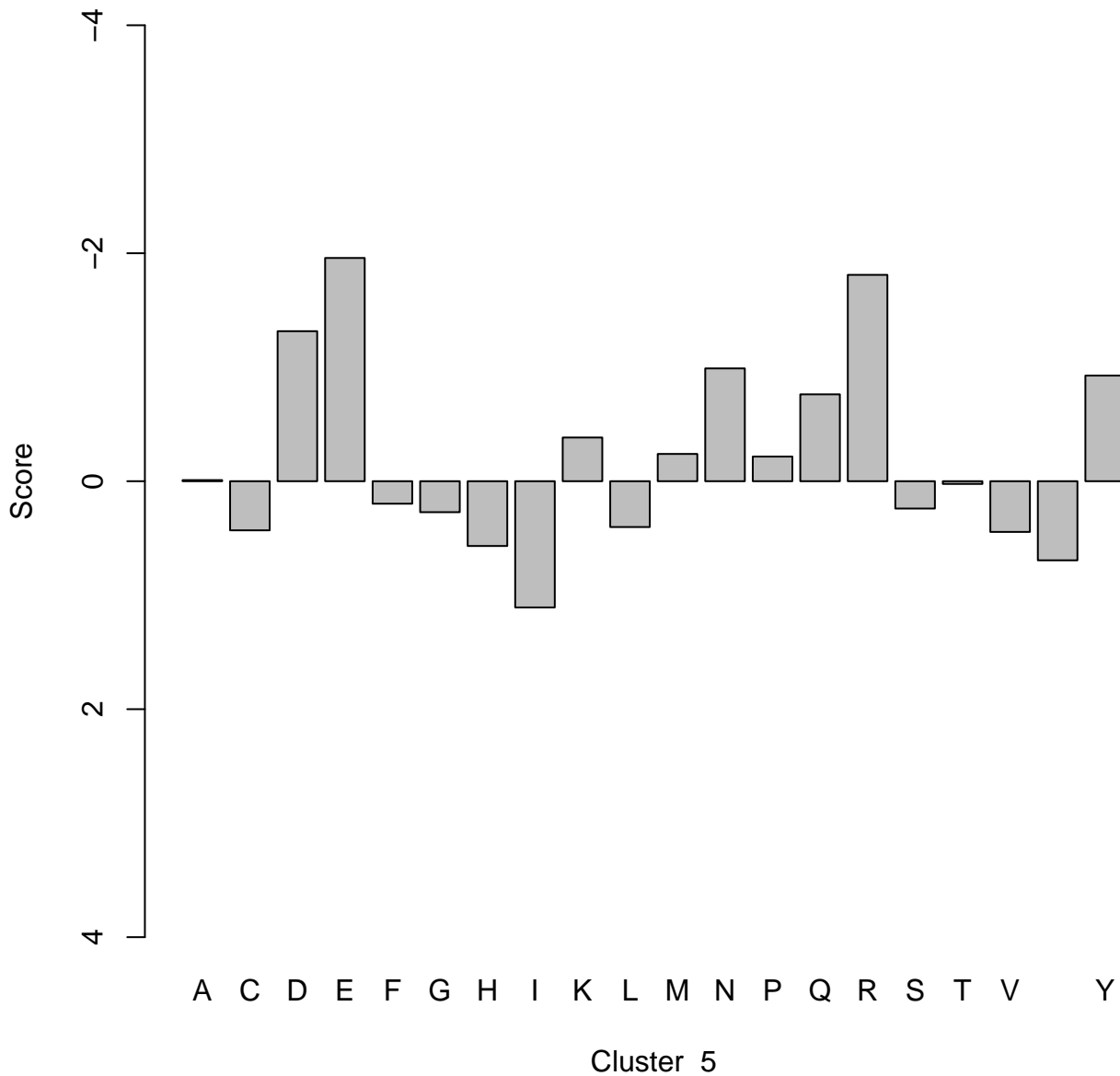


# Distribution des scores (Méthode PAM)

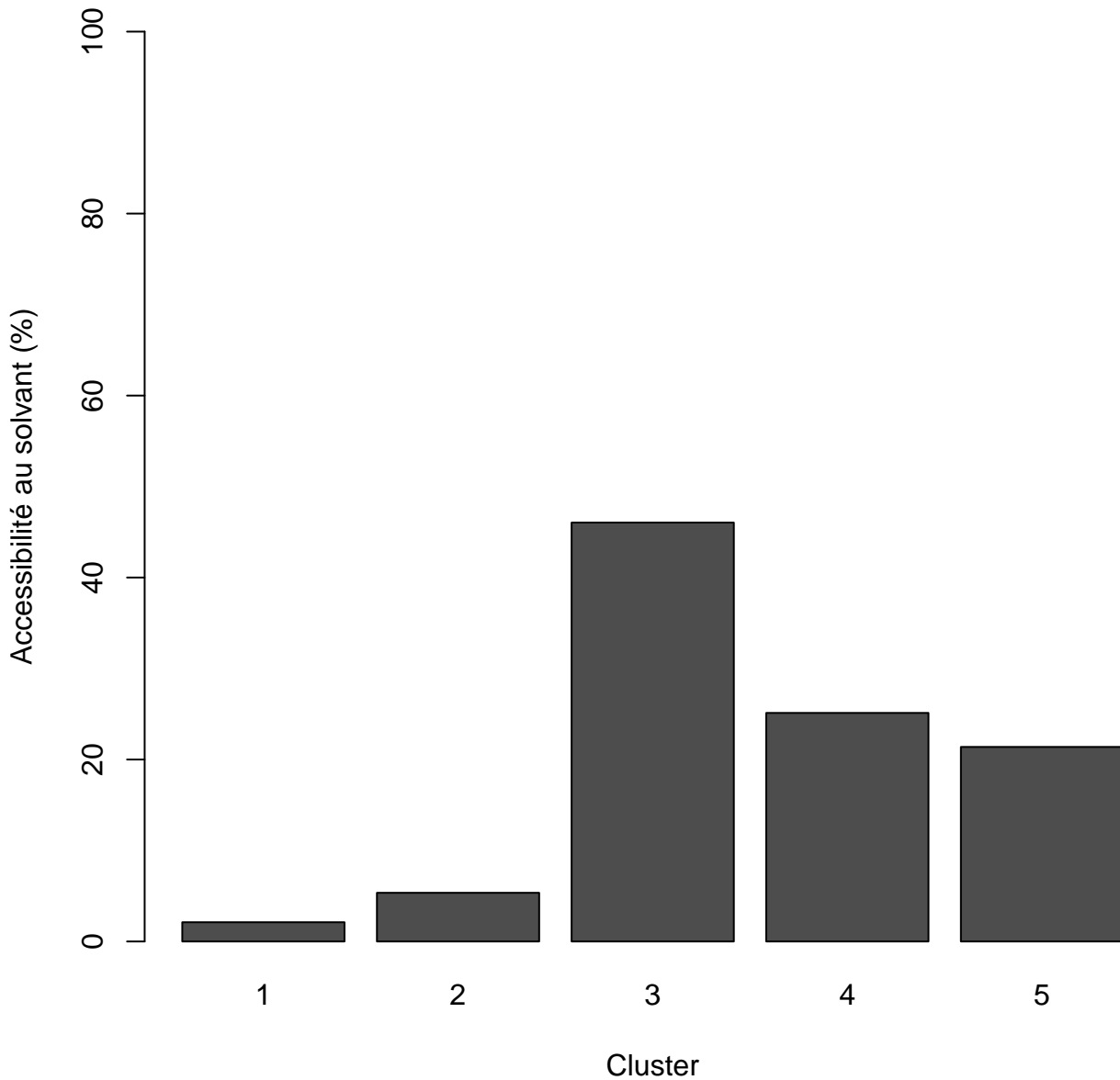




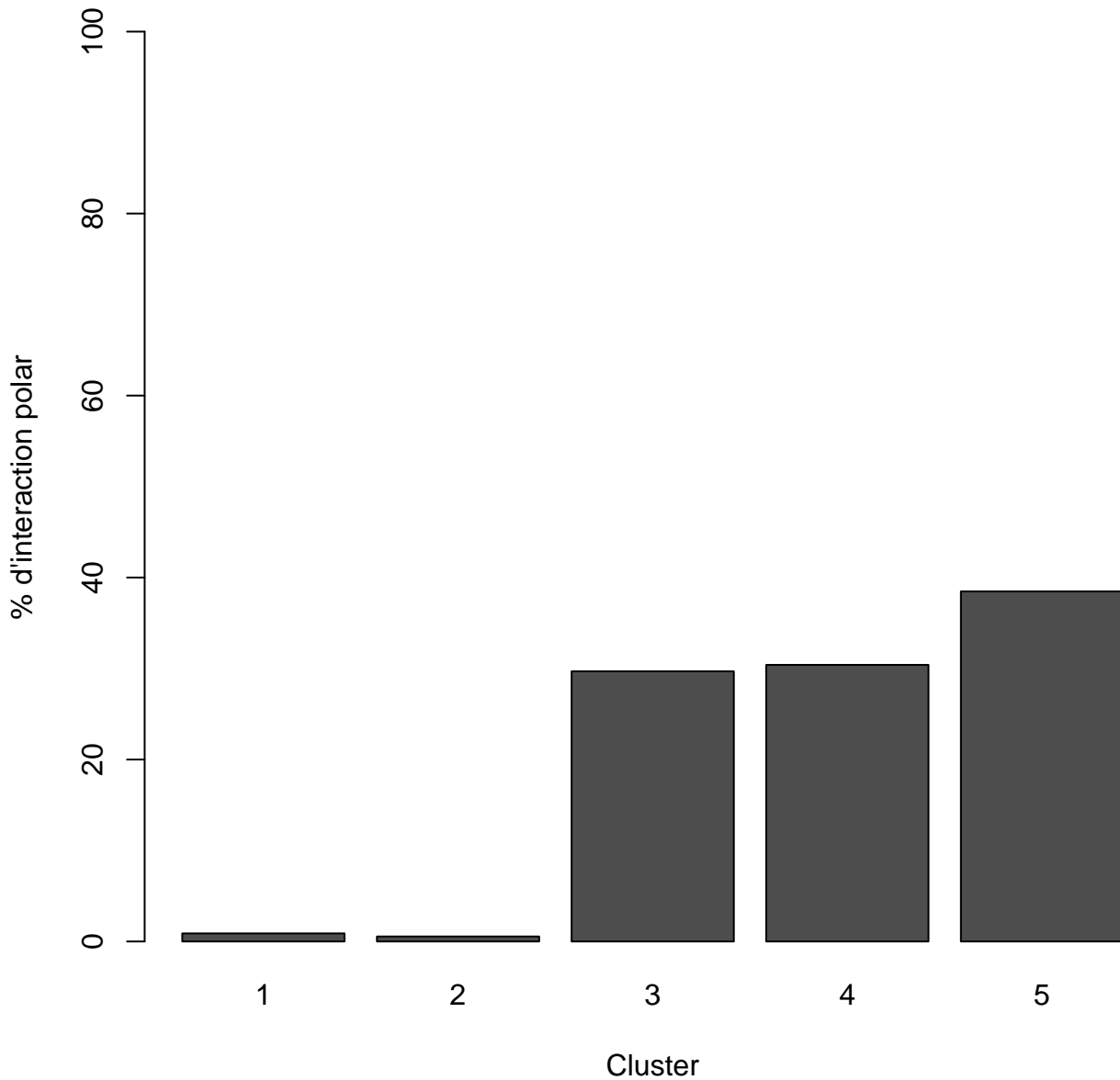
## Distribution des scores (Méthode PAM)



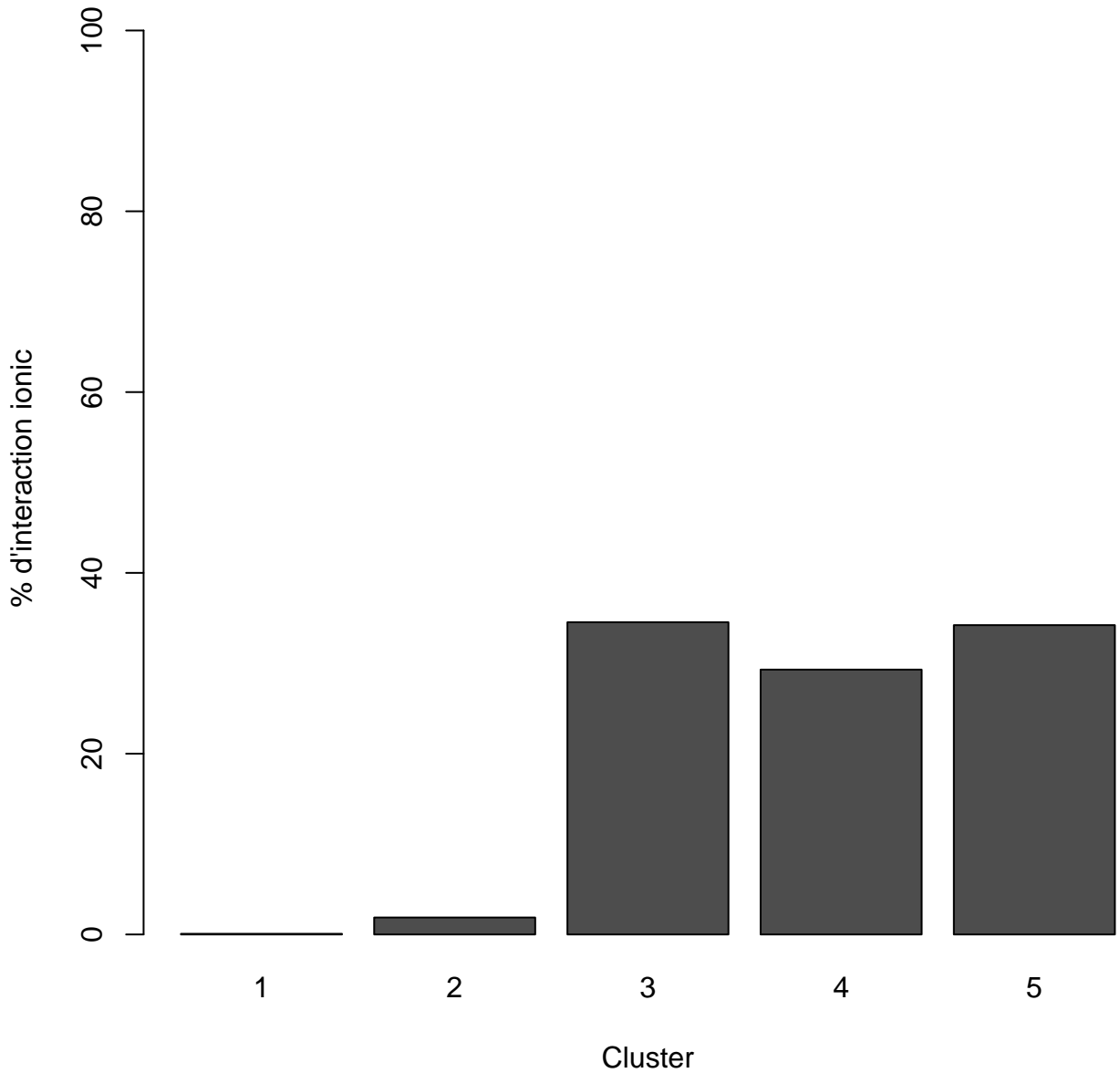
**Accessibilité au solvant (%) Kmeans**



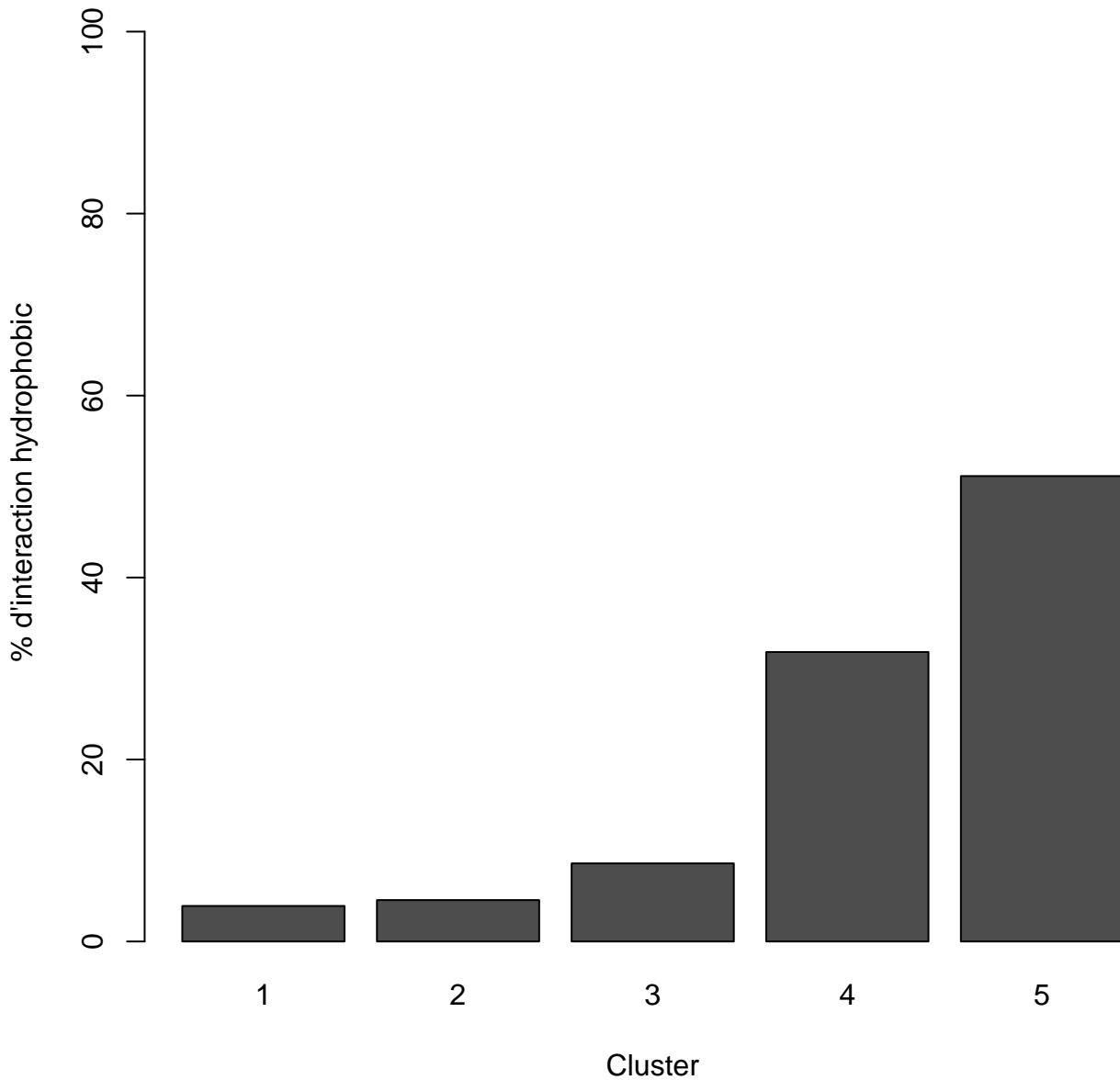
# **% d'interaction polar Kmeans**



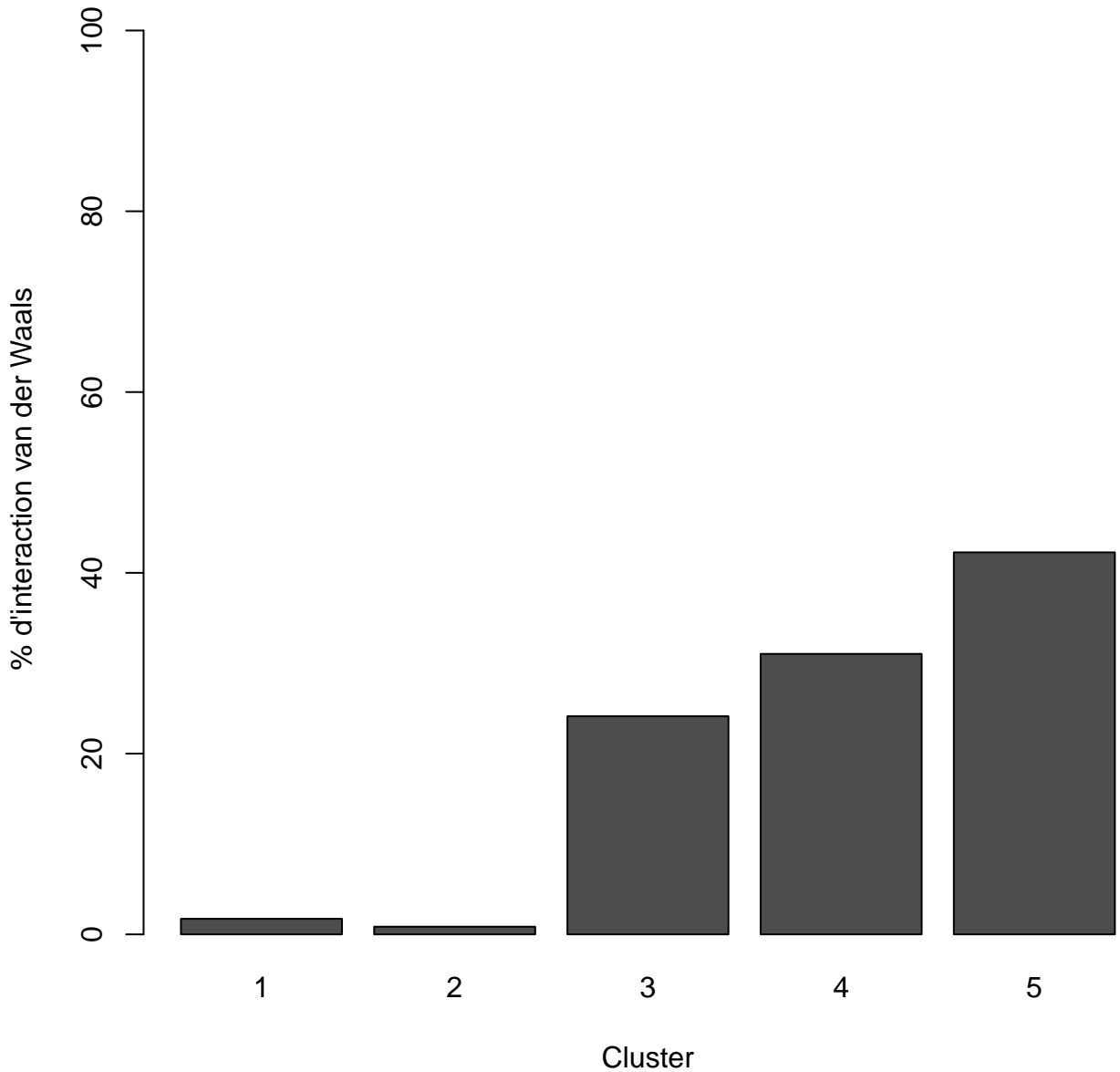
# **% d'interaction ionic Kmeans**



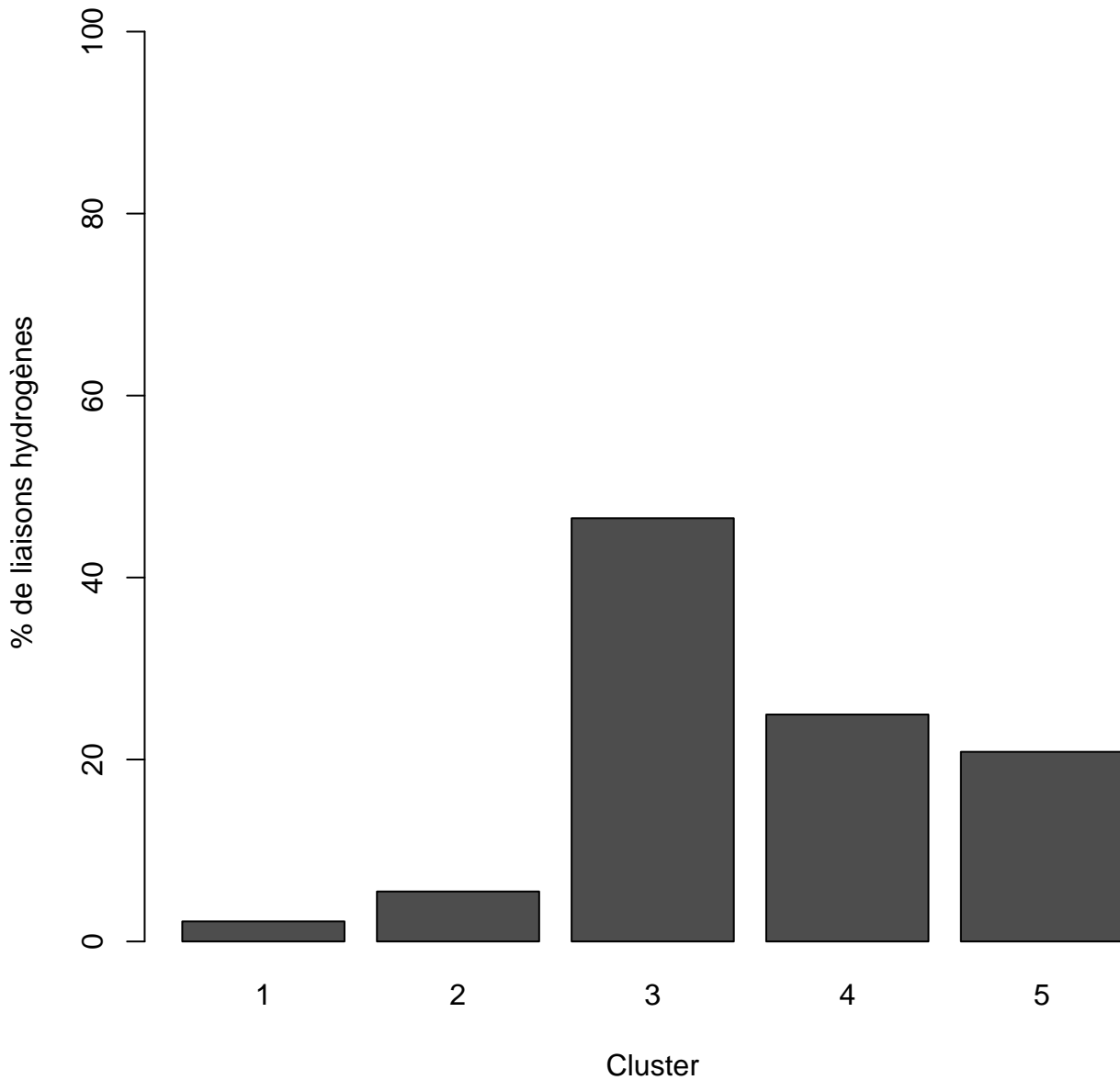
**% d'interaction hydrophobic Kmeans**



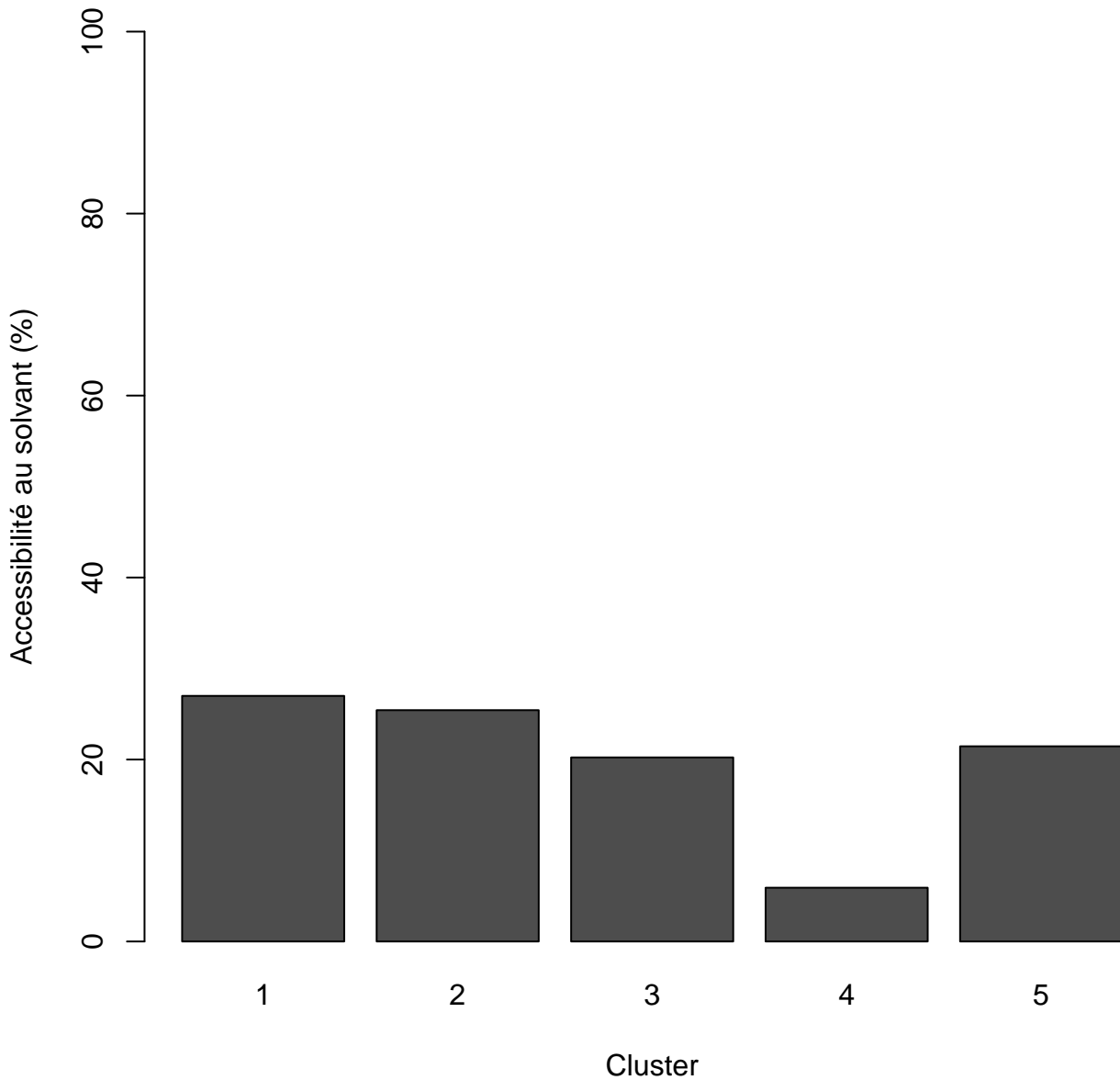
## % d'interaction van der Waals Kmeans



## % de liaisons hydrogènes Kmeans

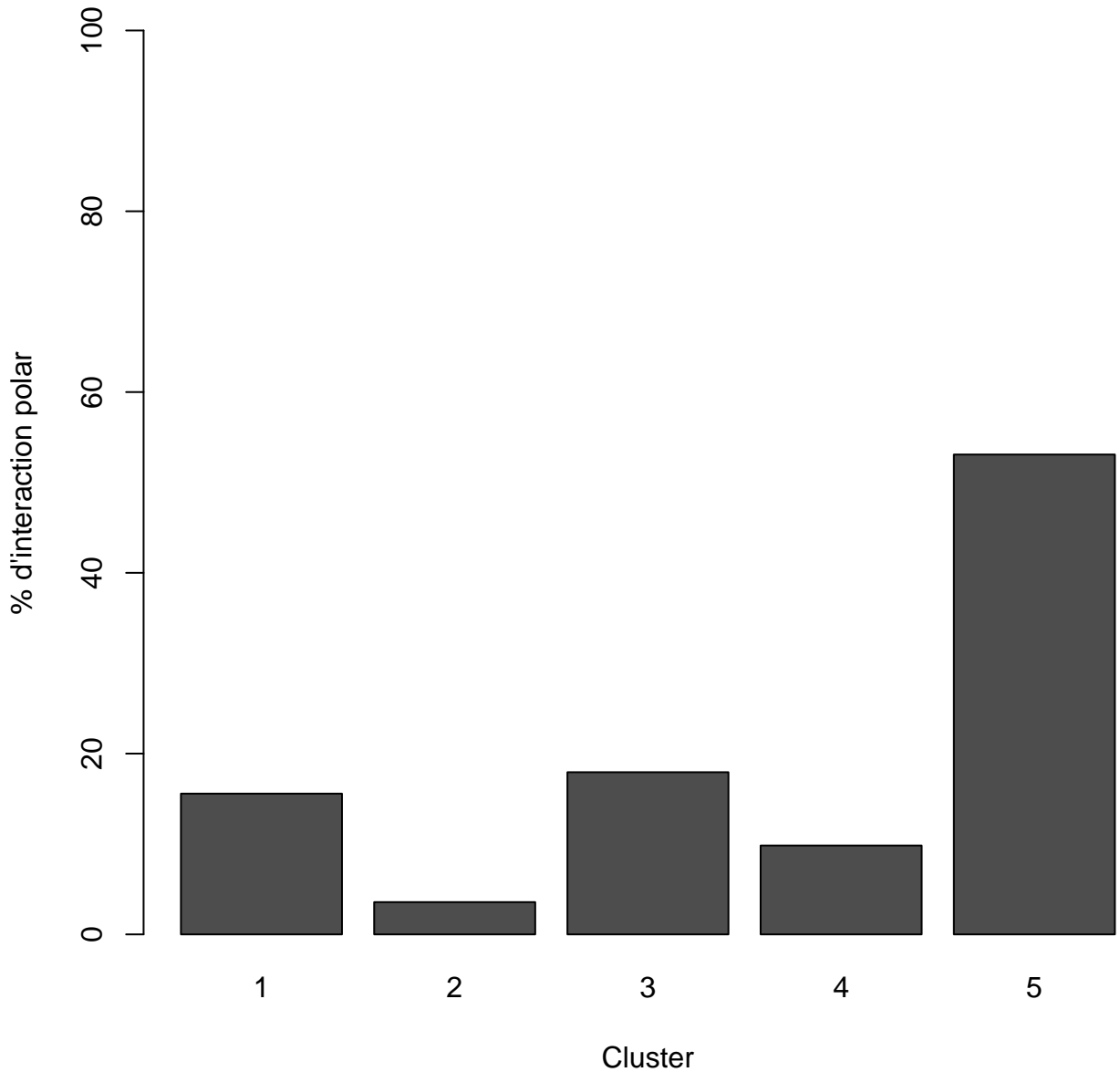


## Accessibilité au solvant (%) Kmedoid

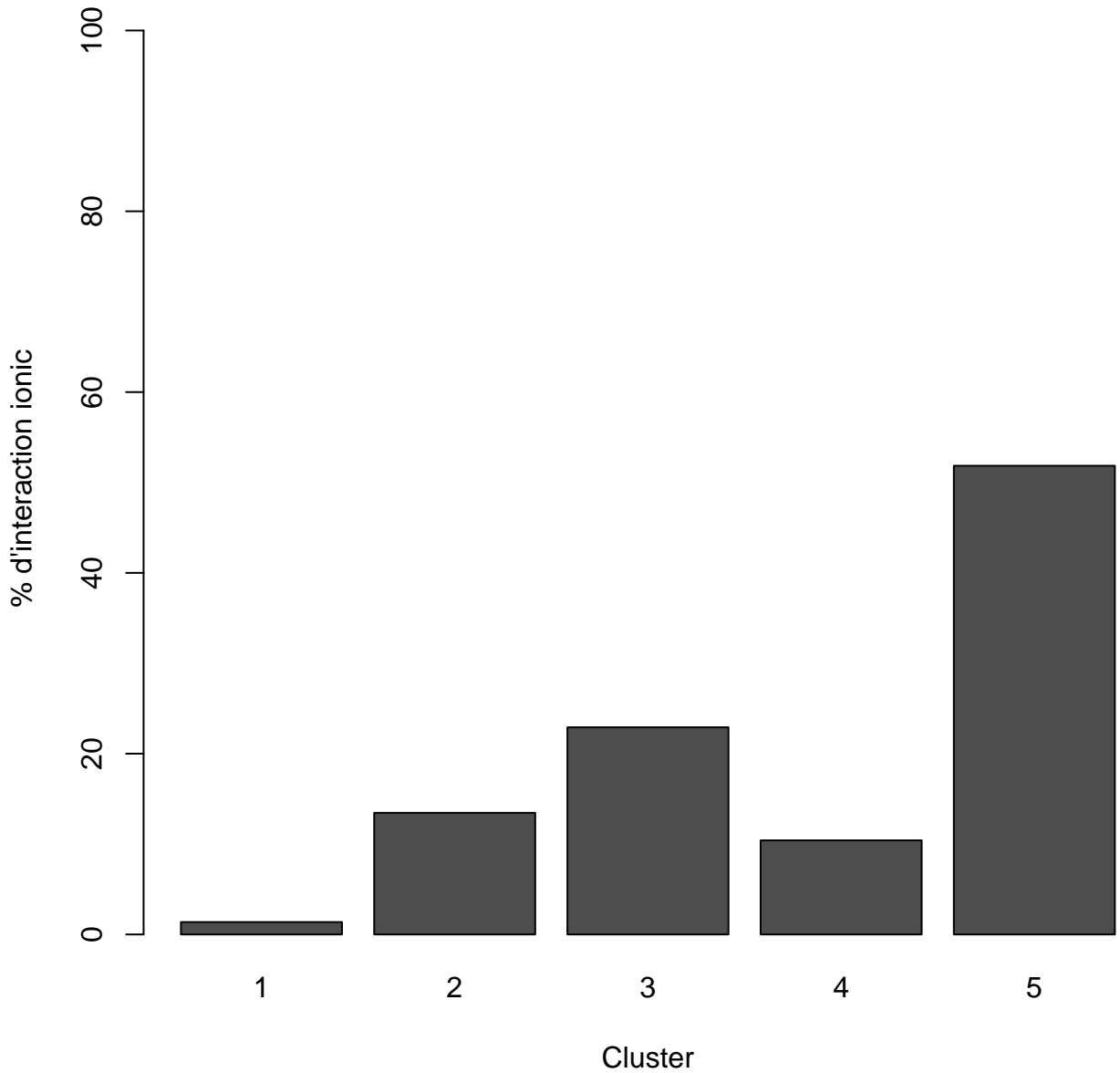




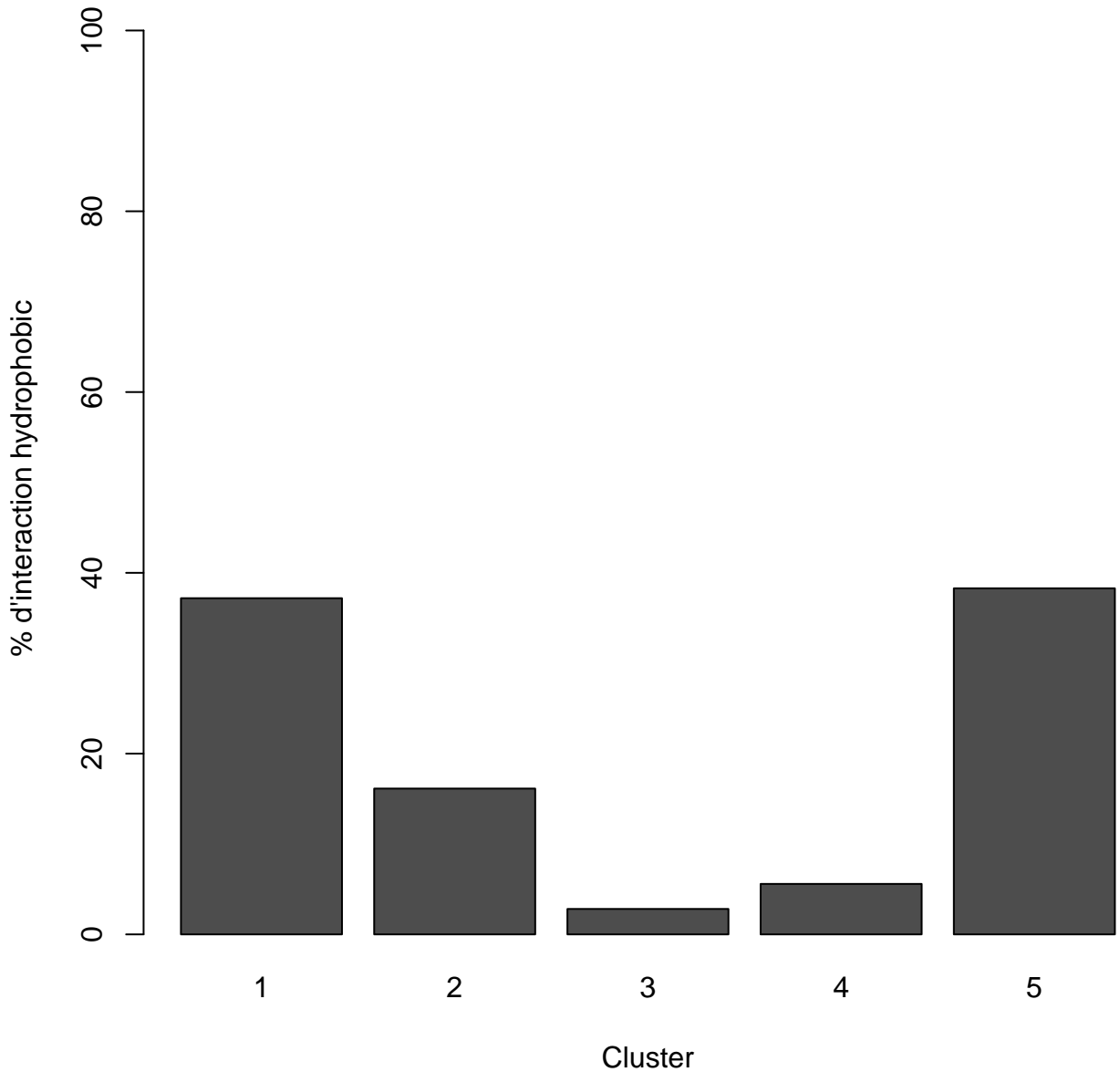
# **% d'interaction polar Kmedoid**



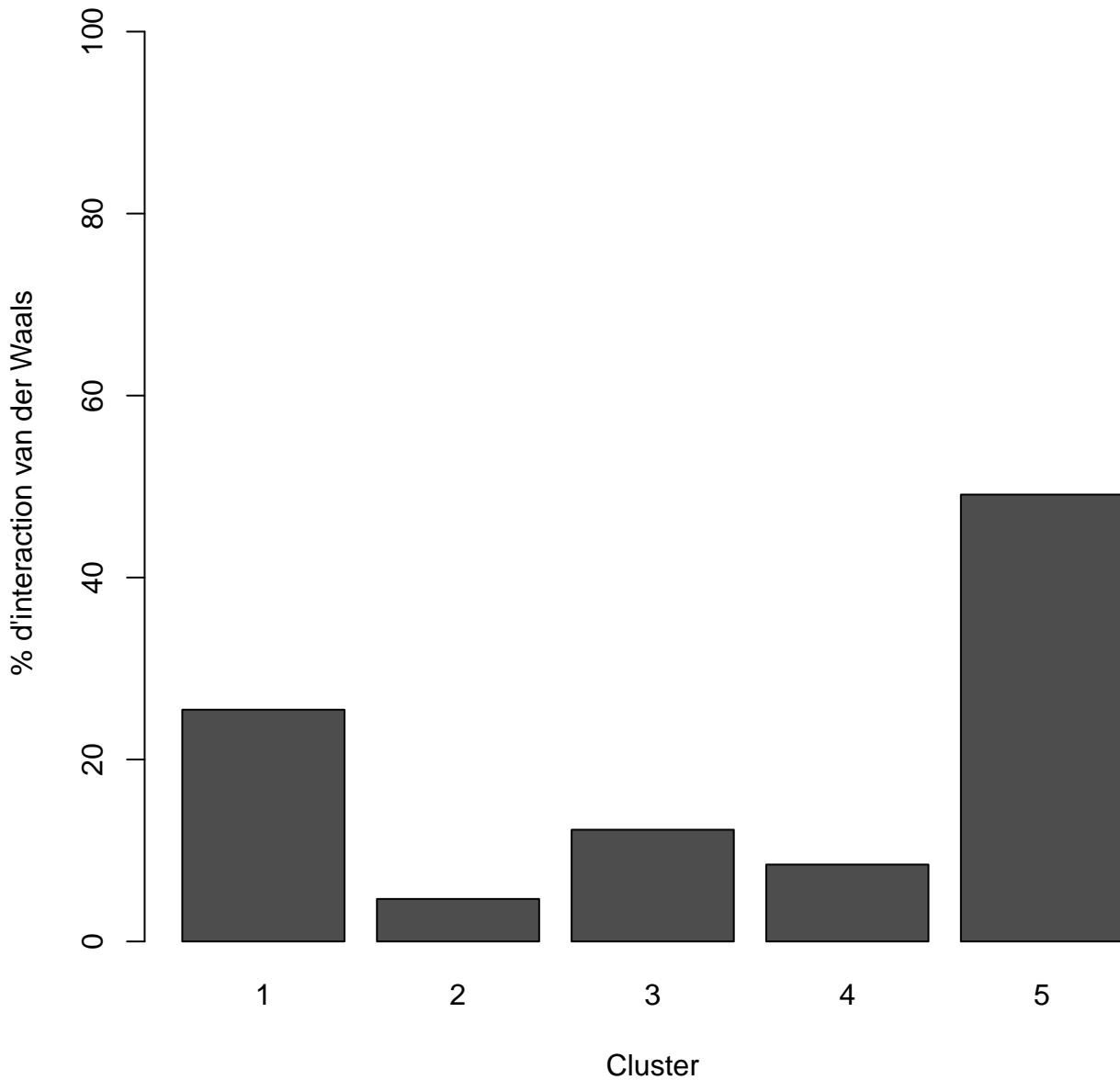
# **% d'interaction ionic Kmedoid**



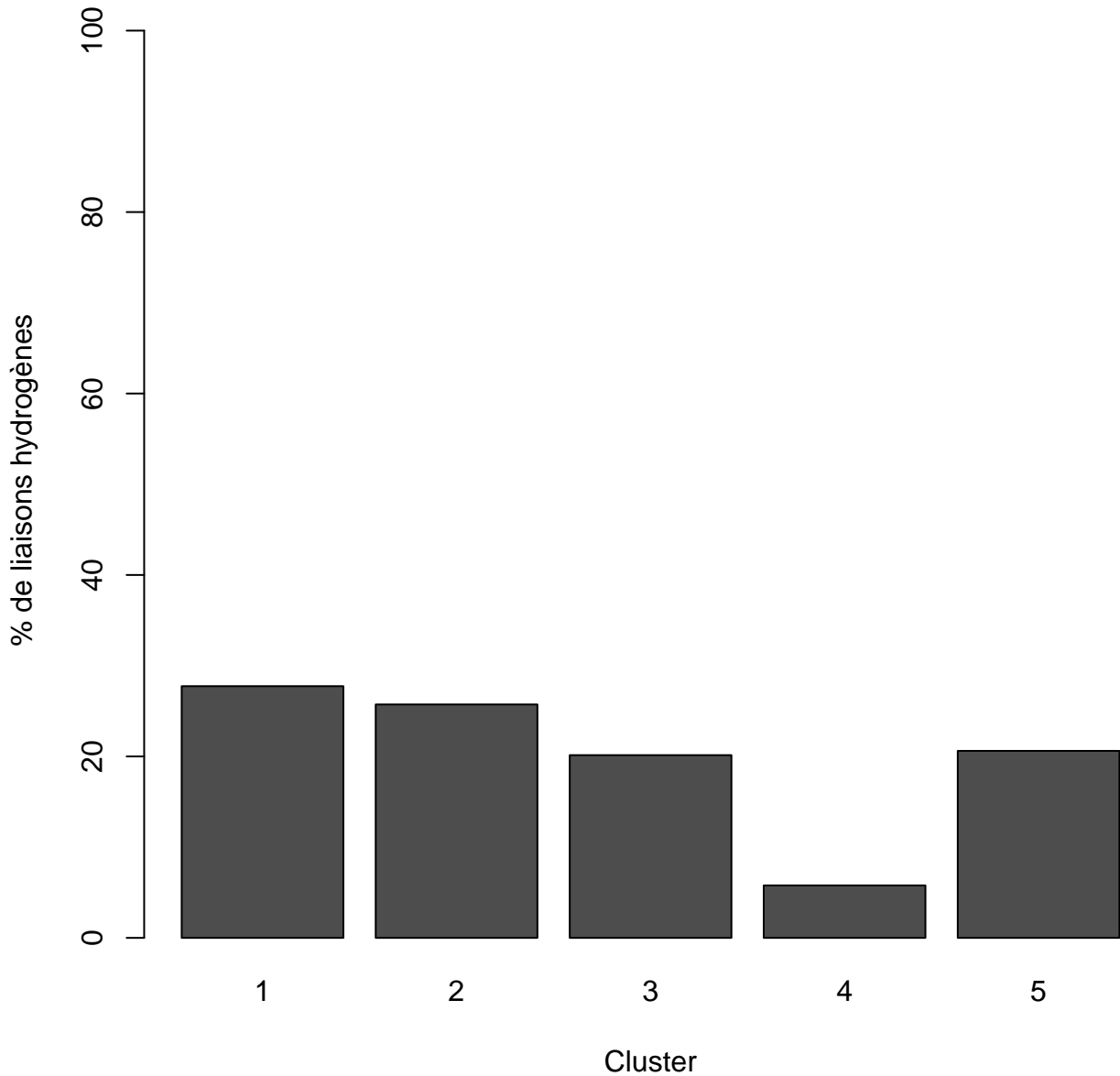
# % d'interaction hydrophobic Kmedoid



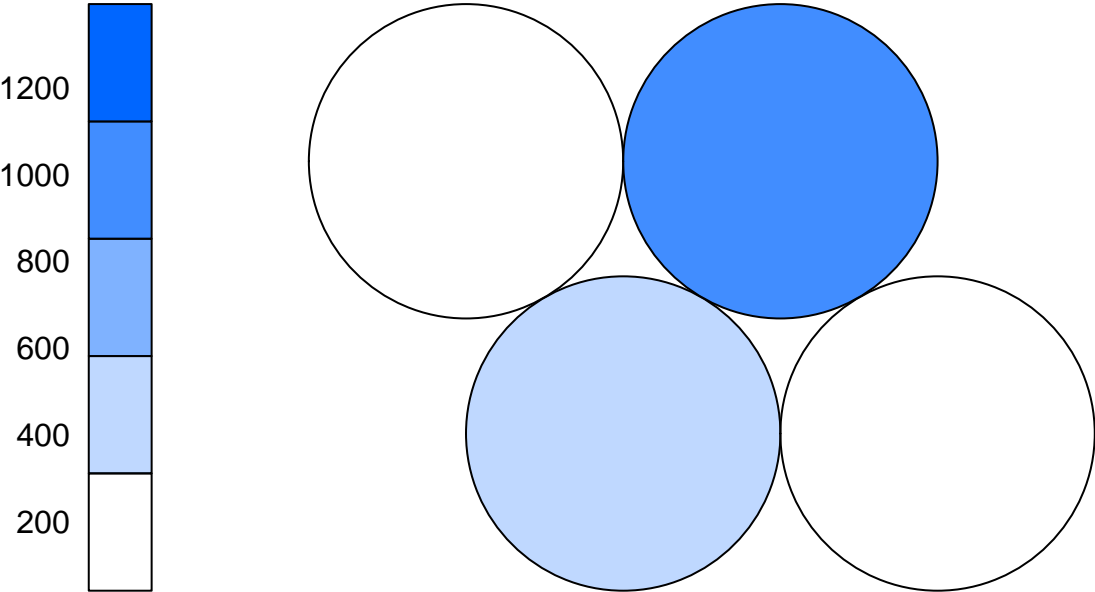
## % d'interaction van der Waals Kmedoid



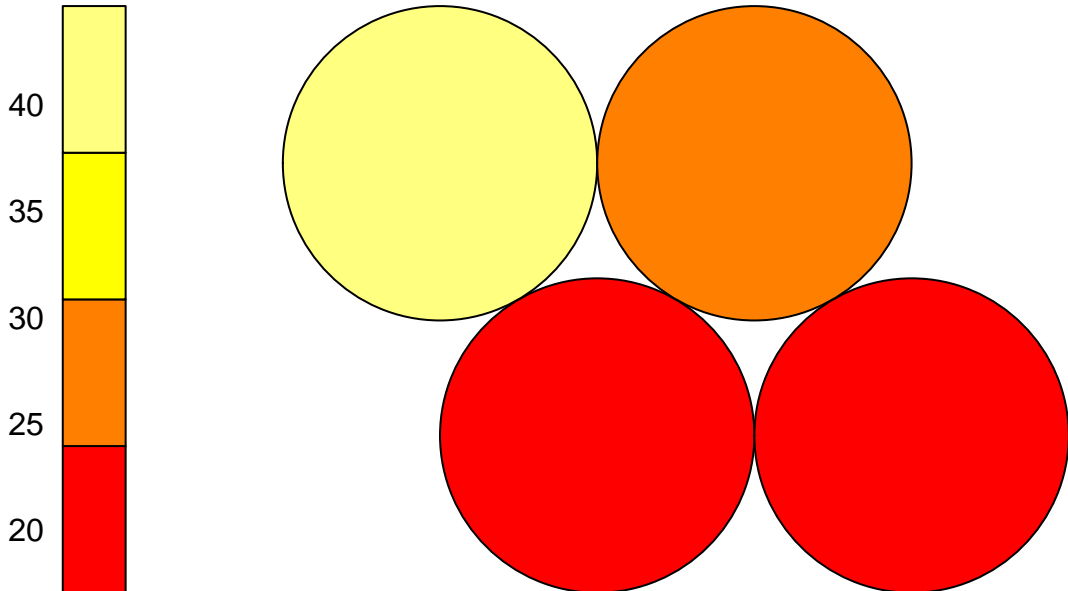
## % de liaisons hydrogènes Kmedoid



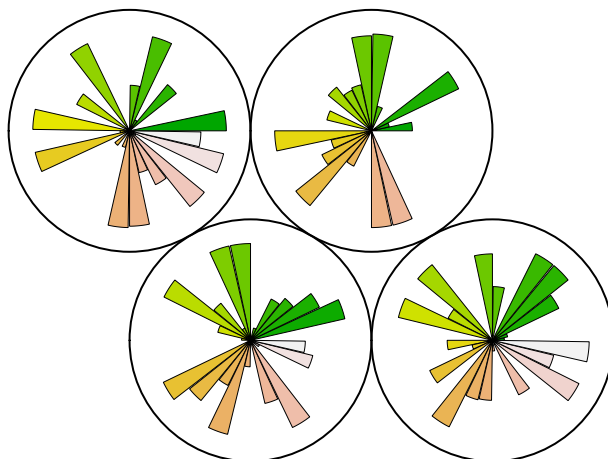
**Carte de Kohonen n= 4**































## Neighbour distance plot



# Codes plot

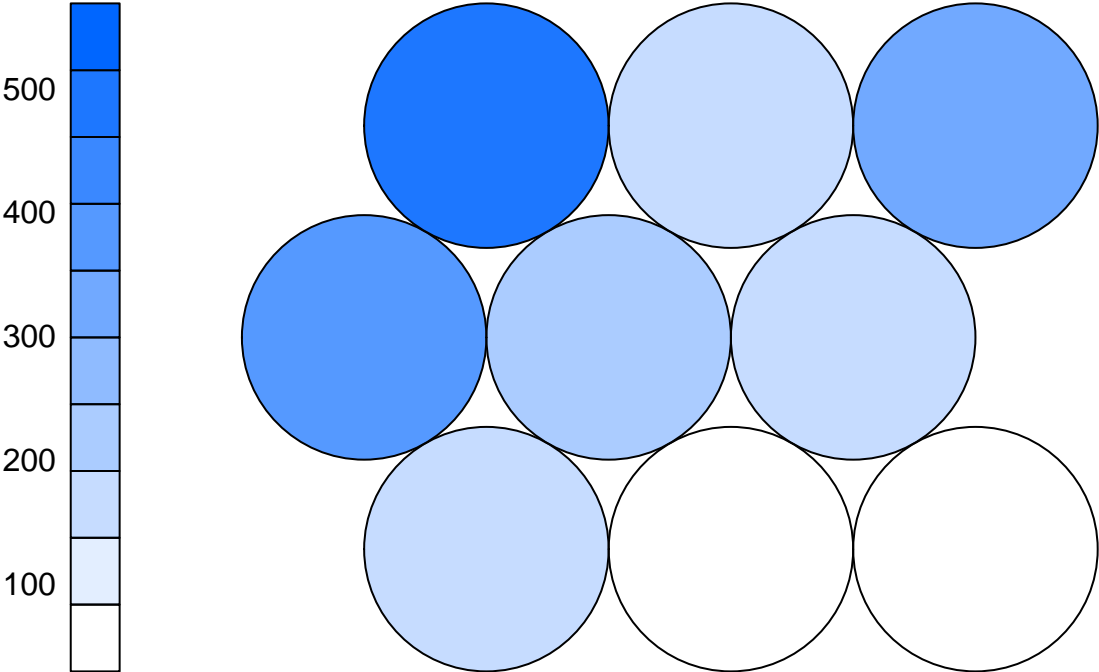


|   |      |   |             |
|---|------|---|-------------|
|    | H_ss |    | h_PB        |
|    | B_ss |    | i_PB        |
|    | E_ss |    | j_PB        |
|    | G_ss |    | k_PB        |
|    | T_ss |    | l_PB        |
|    | S_ss |    | m_PB        |
|   | ACC  |   | n_PB        |
|  | a_PB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

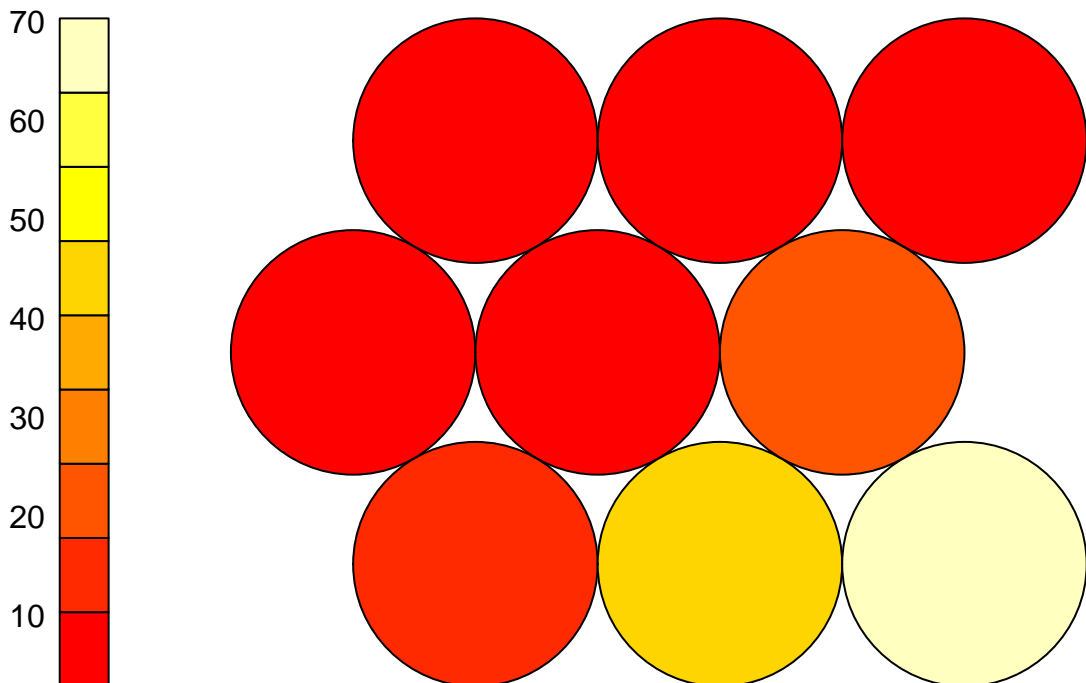




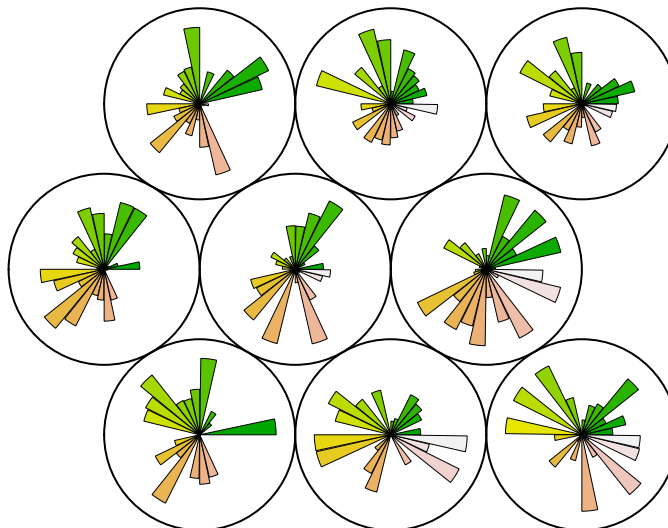
**Carte de Kohonen n= 9**



## Neighbour distance plot



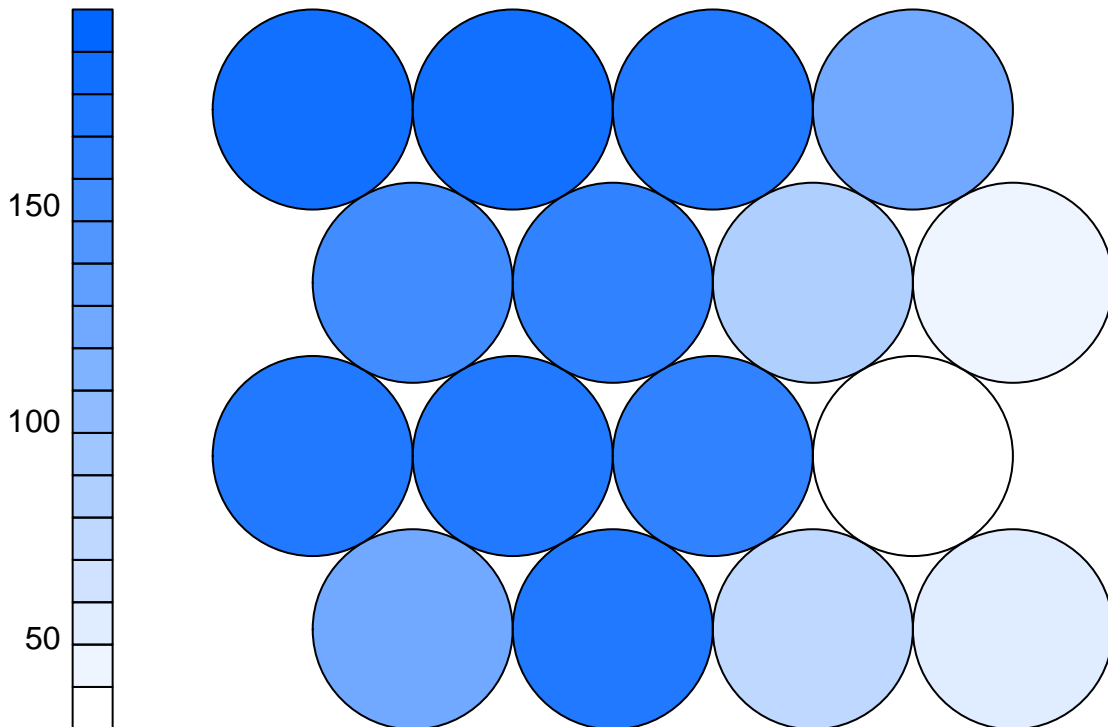
# Codes plot



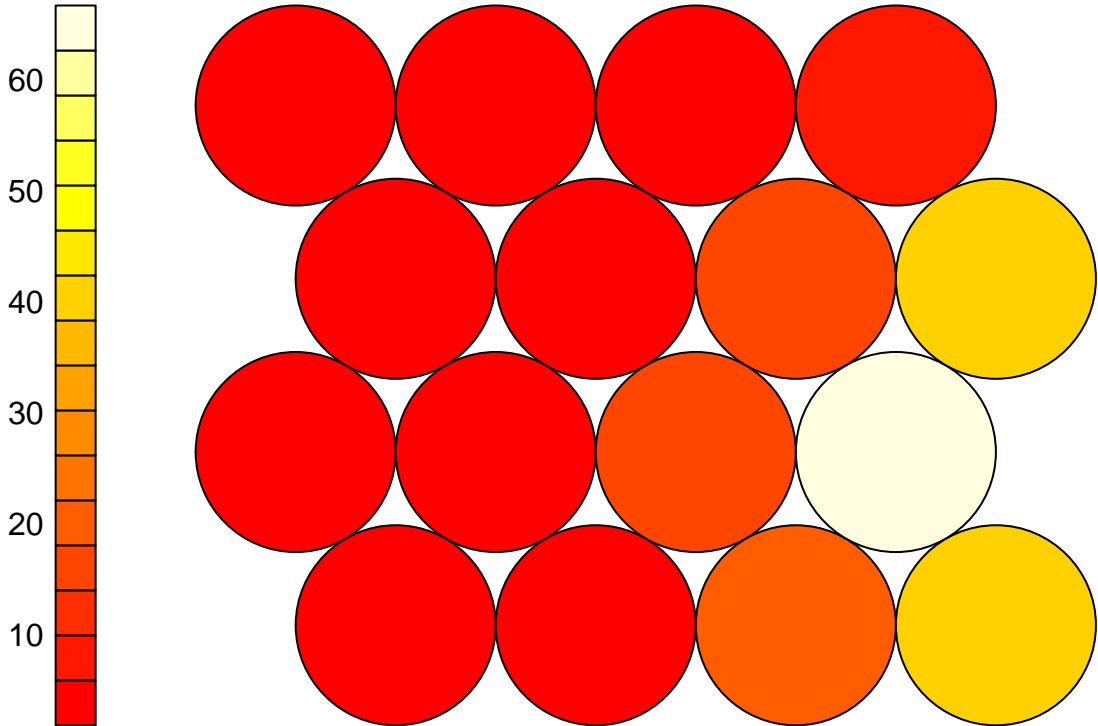
|   |   |
|---|---|
| <span style="color: green;">■</span> H_ss | <span style="color: yellow;">■</span> h_PB        |
| <span style="color: green;">■</span> B_ss | <span style="color: yellow;">■</span> i_PB        |
| <span style="color: green;">■</span> E_ss | <span style="color: orange;">■</span> j_PB        |
| <span style="color: green;">■</span> G_ss | <span style="color: orange;">■</span> k_PB        |
| <span style="color: green;">■</span> T_ss | <span style="color: orange;">■</span> l_PB        |
| <span style="color: green;">■</span> S_ss | <span style="color: orange;">■</span> m_PB        |
| <span style="color: green;">■</span> ACC  | <span style="color: orange;">■</span> n_PB        |
| <span style="color: green;">■</span> a_PB | <span style="color: orange;">■</span> o_PB        |
| <span style="color: green;">■</span> b_PB | <span style="color: orange;">■</span> p_PB        |
| <span style="color: green;">■</span> c_PB | <span style="color: orange;">■</span> polar       |
| <span style="color: green;">■</span> d_PB | <span style="color: orange;">■</span> ionic       |
| <span style="color: green;">■</span> e_PB | <span style="color: orange;">■</span> hydrophobic |
| <span style="color: green;">■</span> f_PB | <span style="color: orange;">■</span> vdw         |
| <span style="color: green;">■</span> g_PB | <span style="color: orange;">■</span> hydrogenB   |



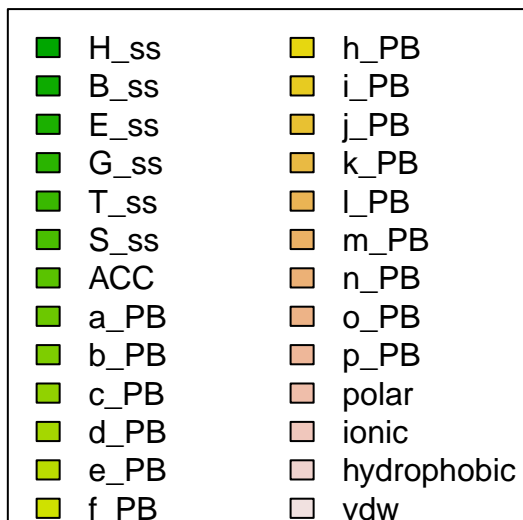
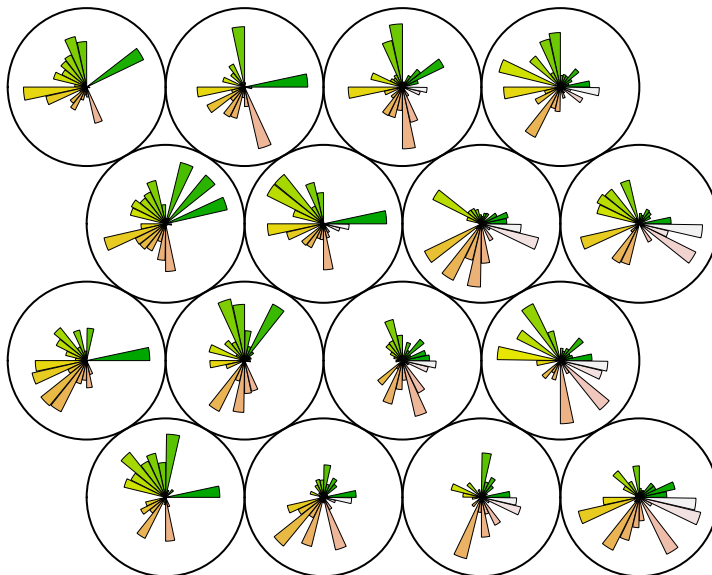
**Carte de Kohonen n= 16**



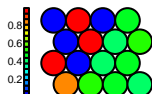
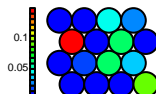
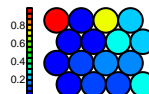
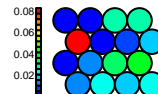
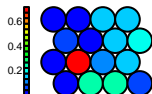
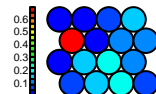
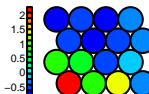
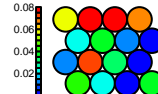
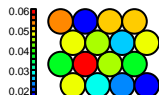
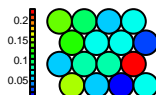
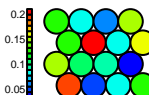
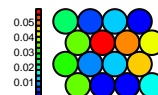
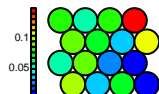
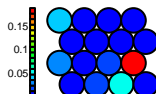
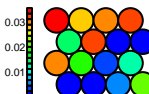
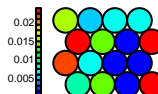
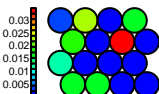
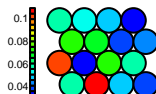
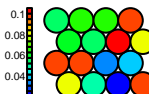
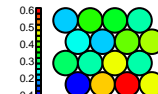
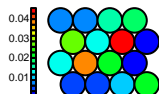
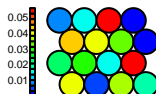
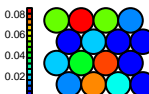
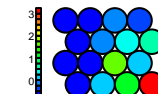
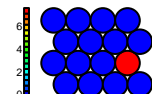
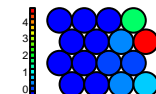
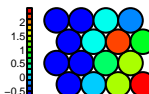
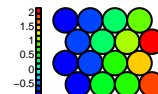
**Neighbour distance plot**



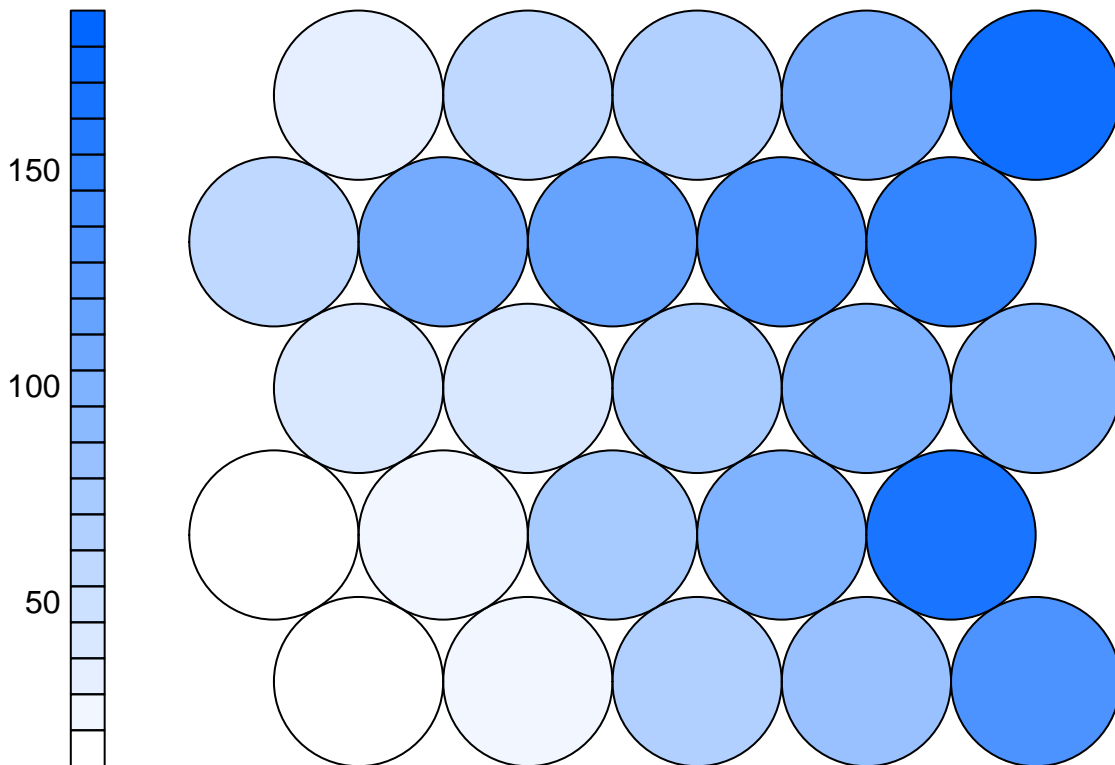
# Codes plot



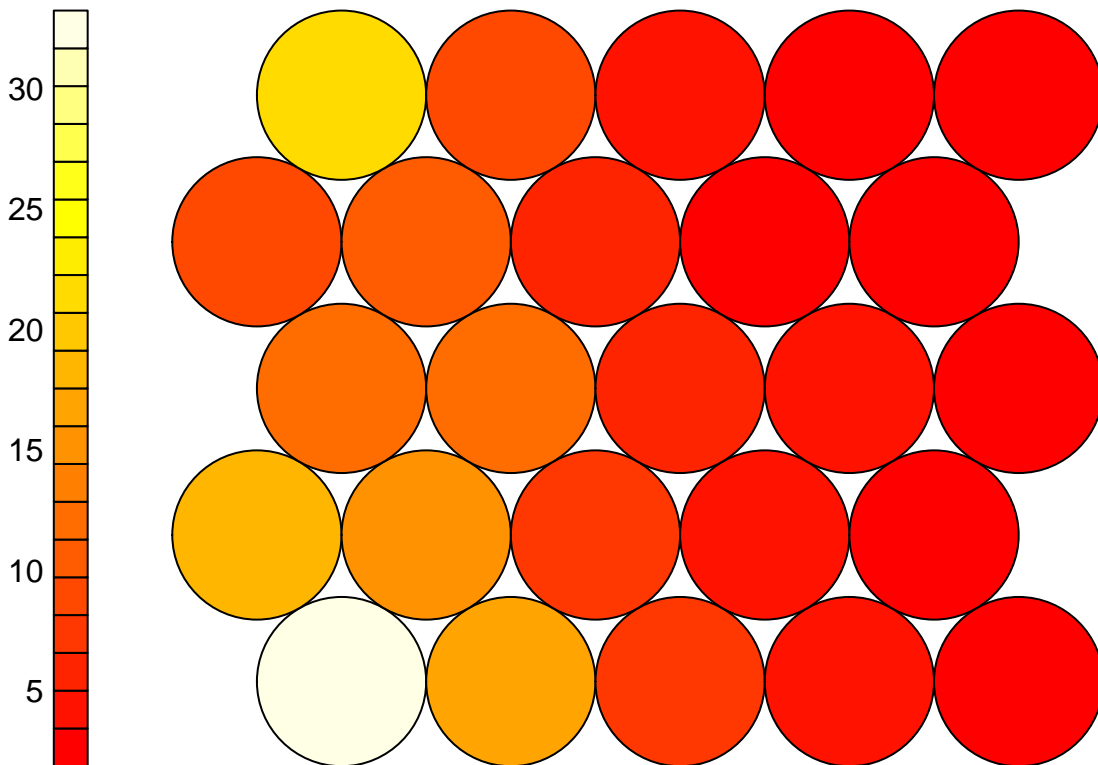


**H\_ss****B\_ss****E\_ss****G\_ss****T\_ss****S\_ss****ACC****a\_PB****b\_PB****c\_PB****d\_PB****e\_PB****f\_PB****g\_PB****h\_PB****i\_PB****j\_PB****k\_PB****l\_PB****m\_PB****n\_PB****o\_PB****p\_PB****polar****ionic****hydrophobic****vdw****hydrogenB**

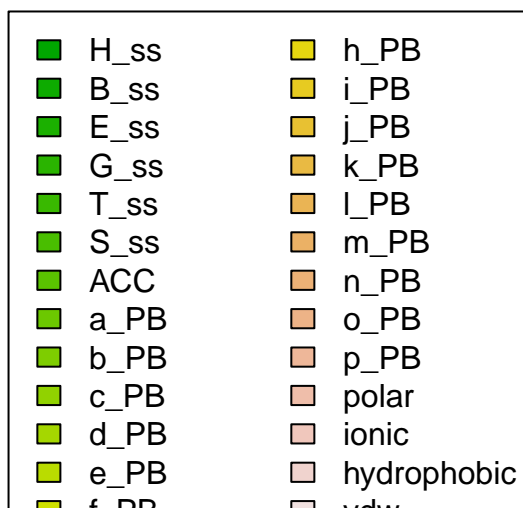
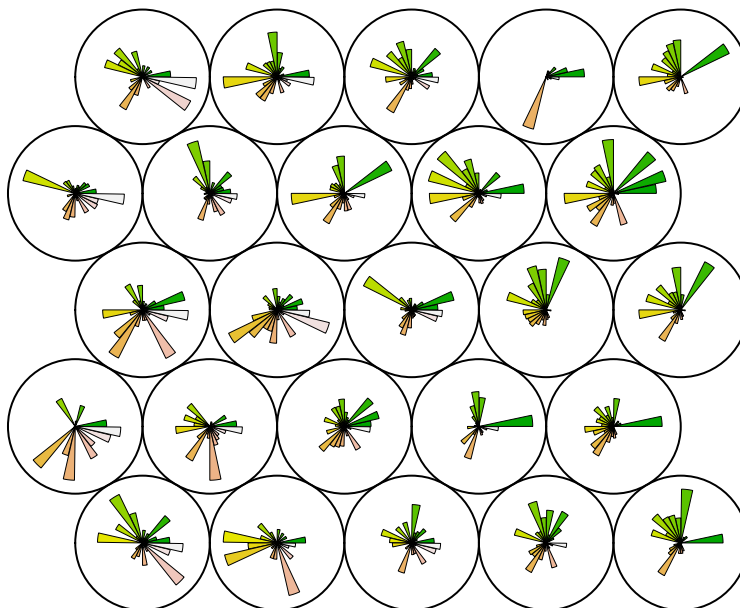
**Carte de Kohonen n= 25**



Neighbour distance plot

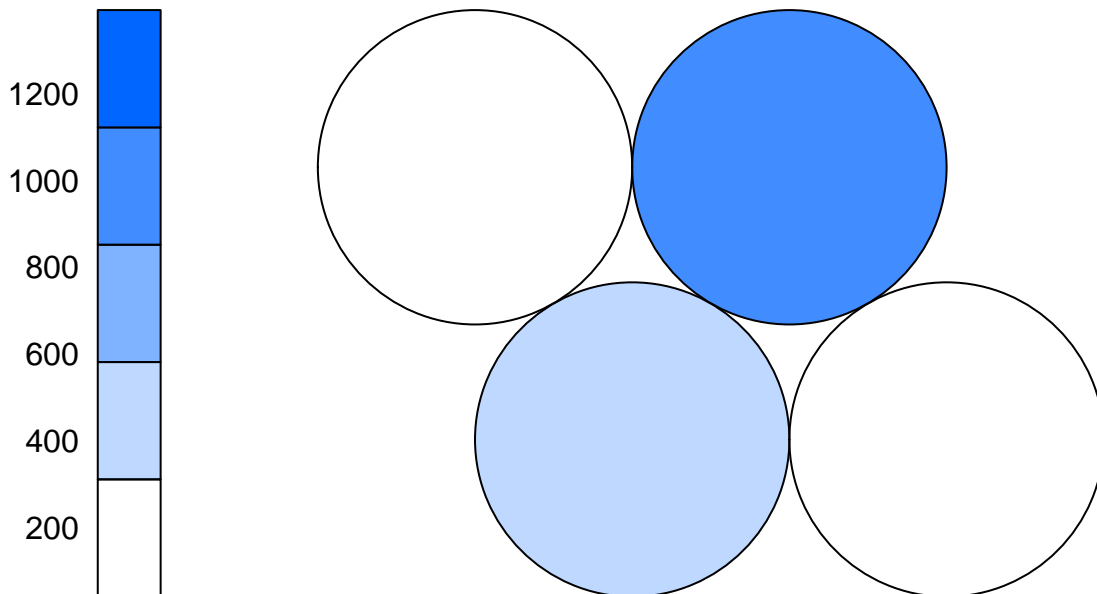


# Codes plot

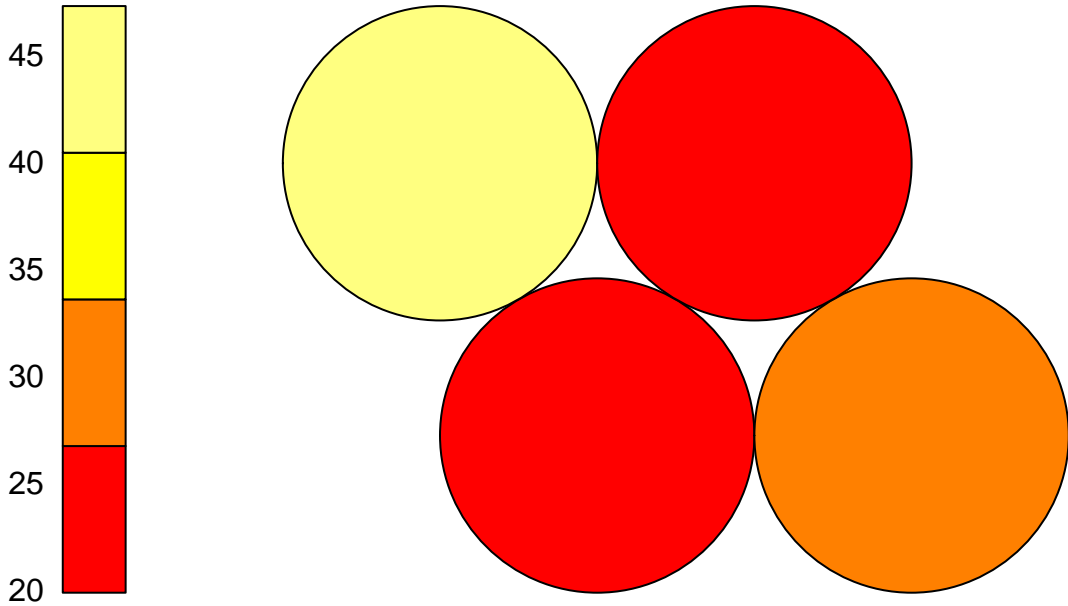




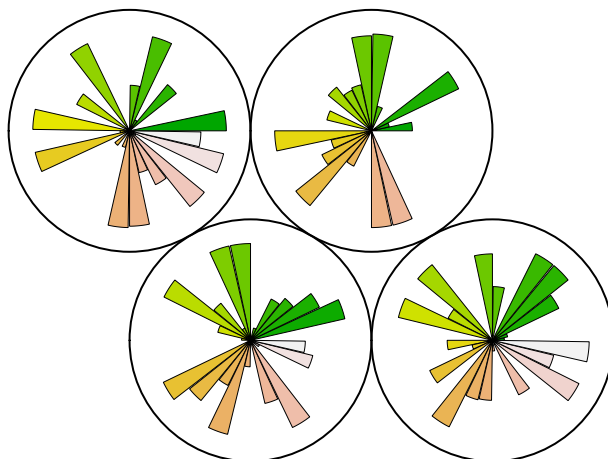
## Carte de Kohonen toroidal n= 4































## Neighbour distance plot



# Codes plot

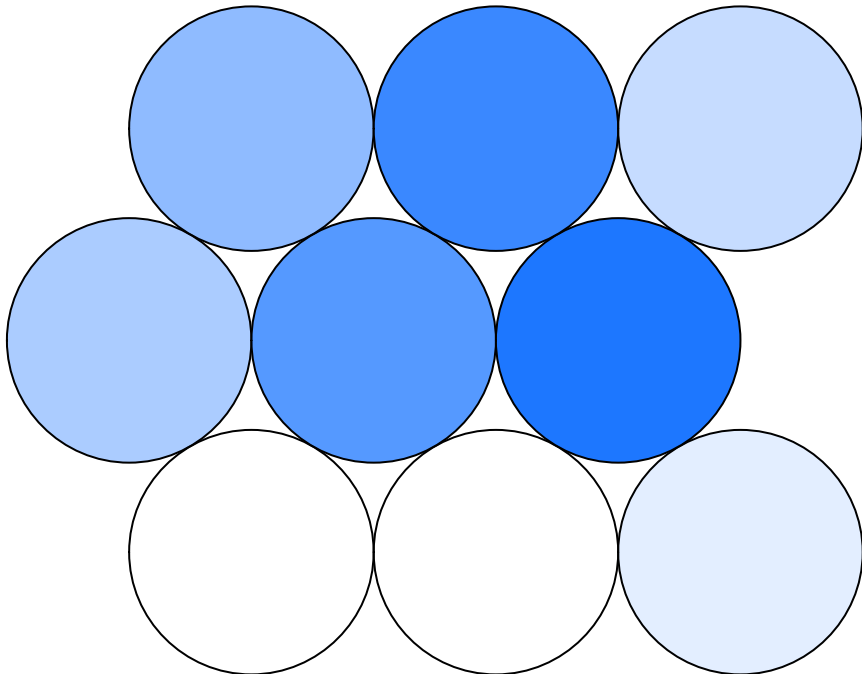
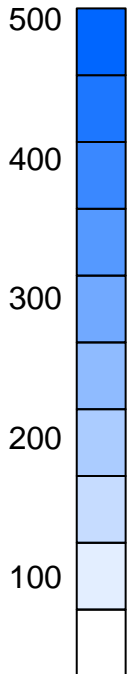


|   |      |   |             |
|---|------|---|-------------|
|    | H_ss |    | h_PB        |
|    | B_ss |    | i_PB        |
|    | E_ss |    | j_PB        |
|    | G_ss |    | k_PB        |
|    | T_ss |    | l_PB        |
|    | S_ss |    | m_PB        |
|   | ACC  |   | n_PB        |
|  | a_PB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

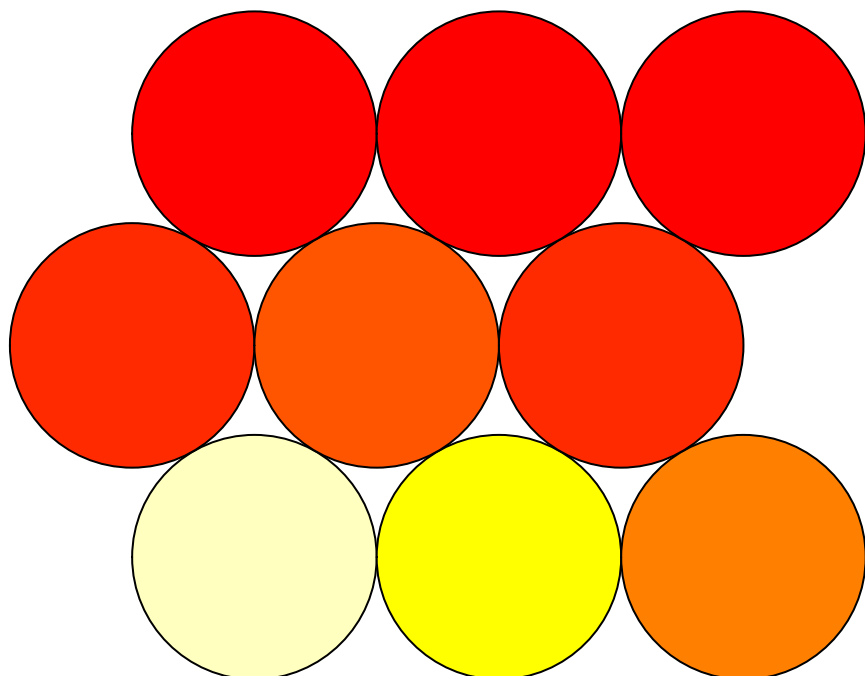
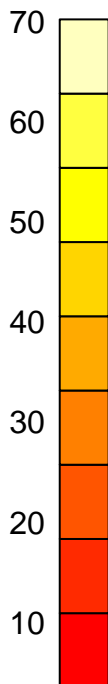




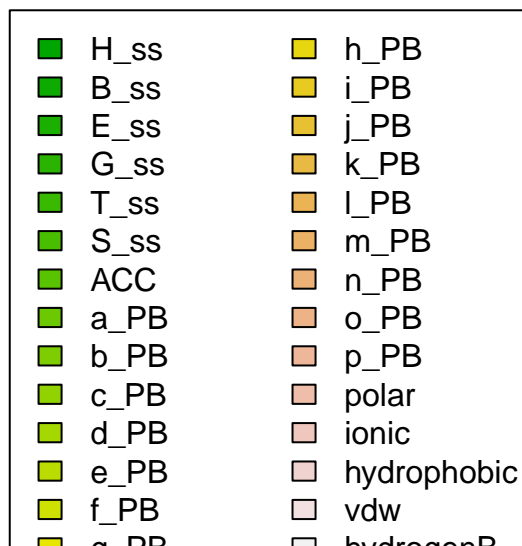
# Carte de Kohonen toroidal n= 9



## Neighbour distance plot

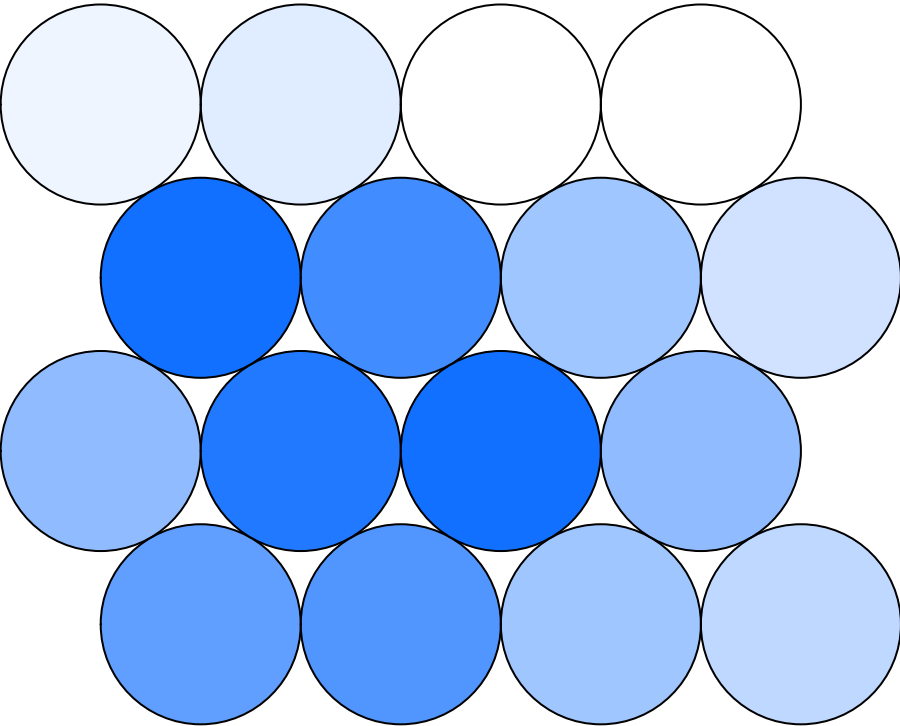
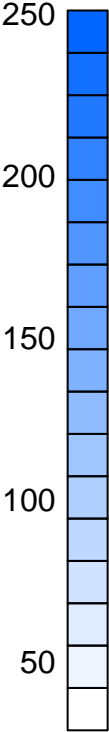


# Codes plot

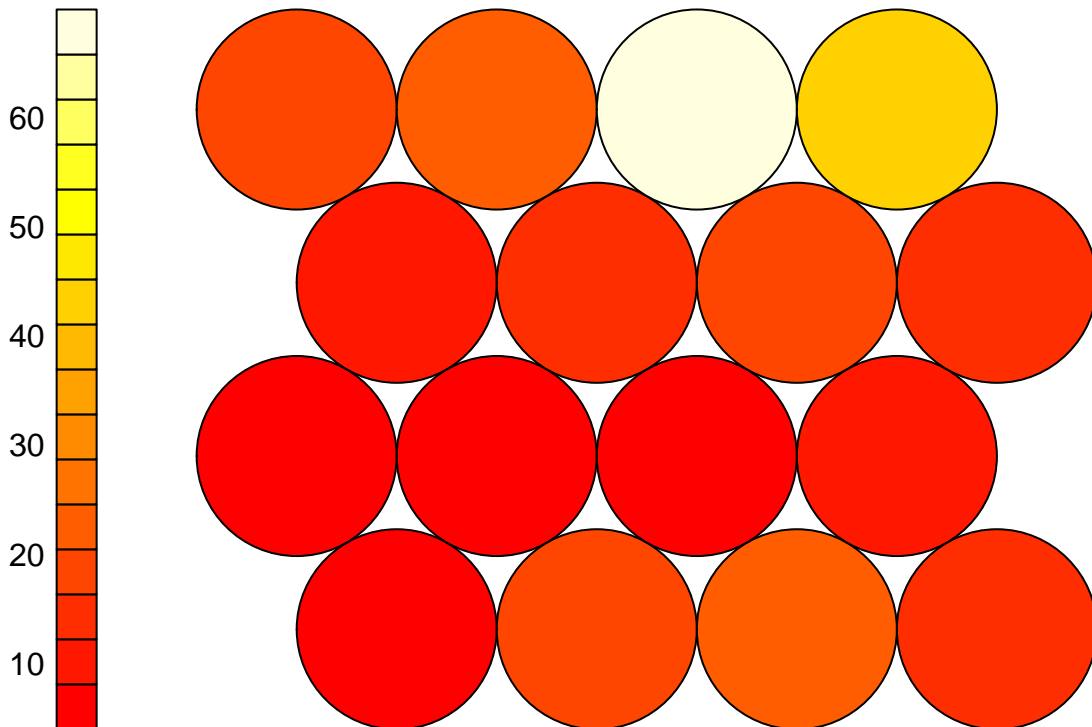




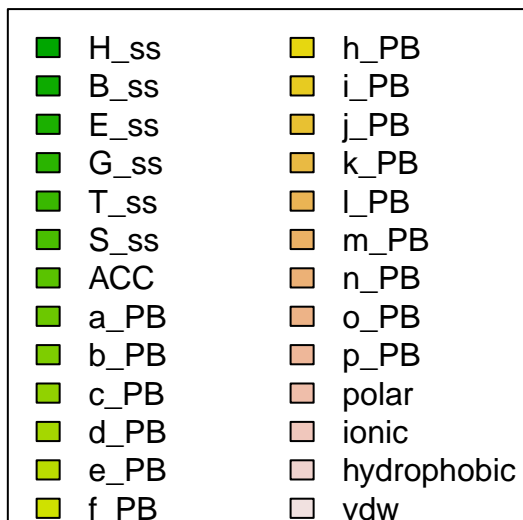
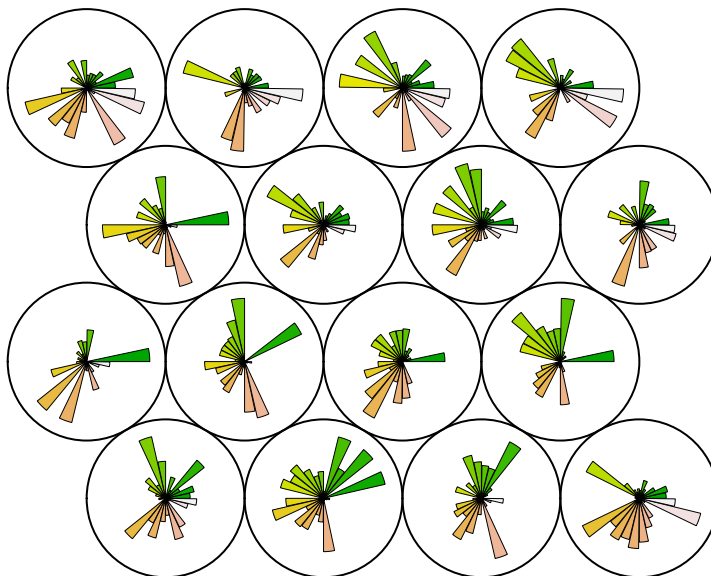
**Carte de Kohonen toroidal n= 16**



**Neighbour distance plot**



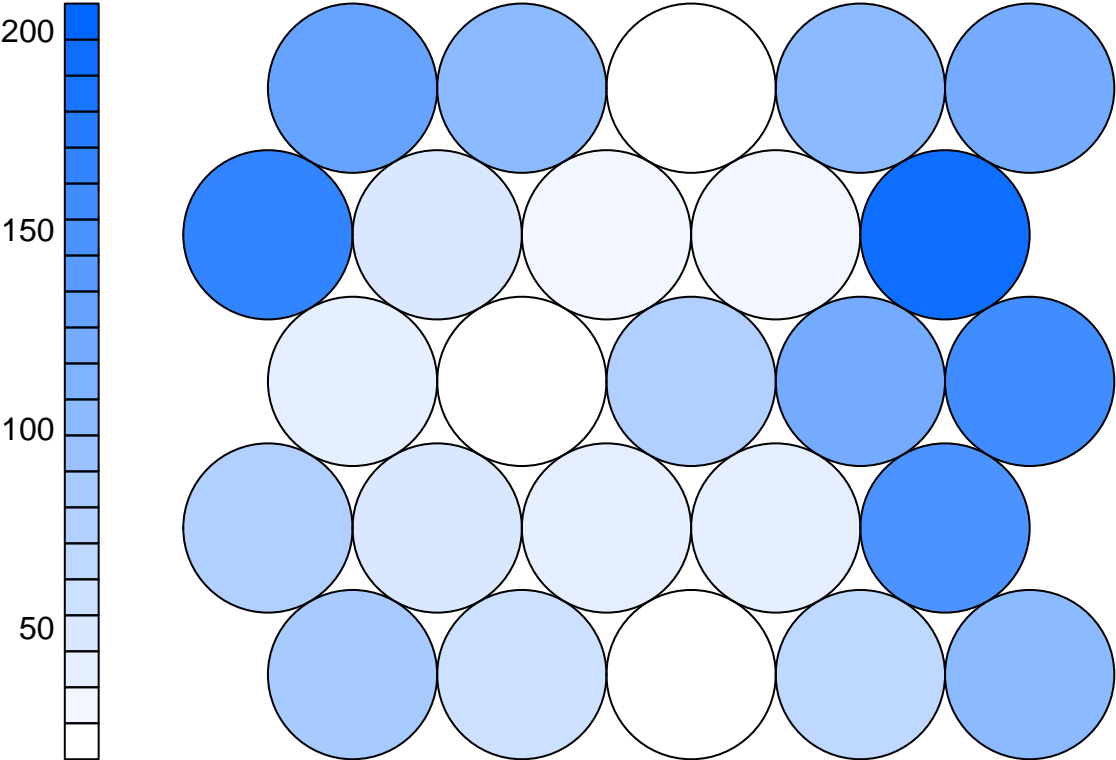
# Codes plot



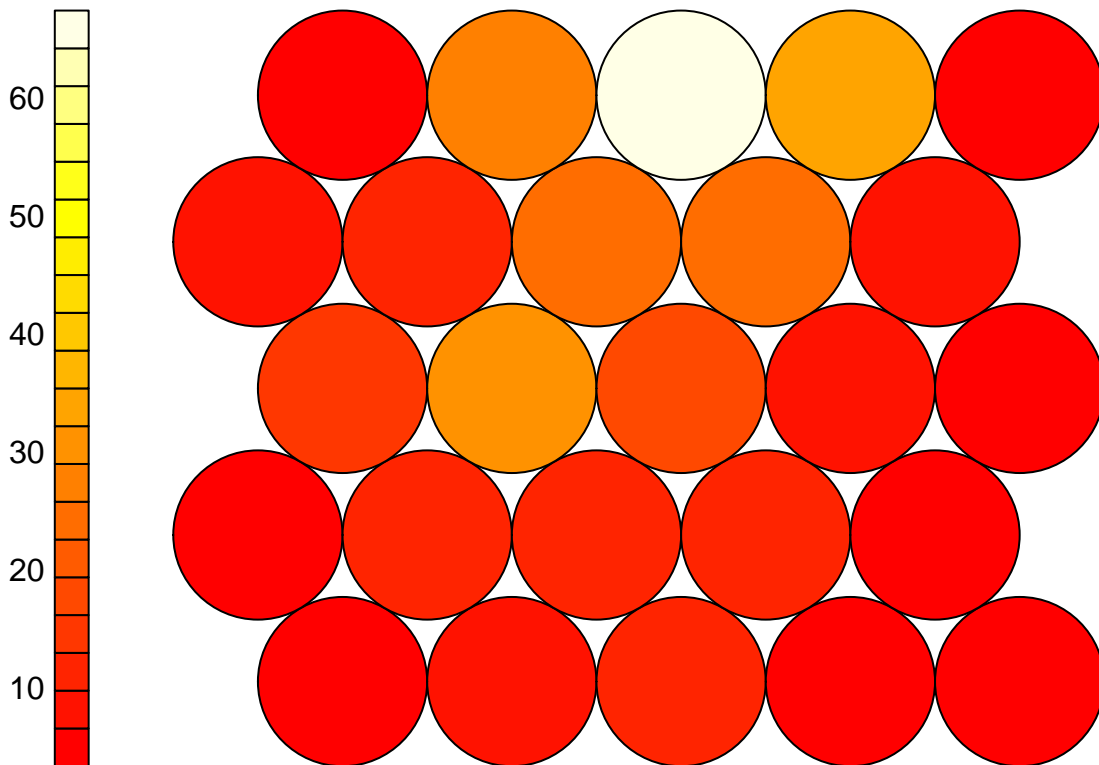




**Carte de Kohonen toroidal n= 25**



Neighbour distance plot



# Codes plot

