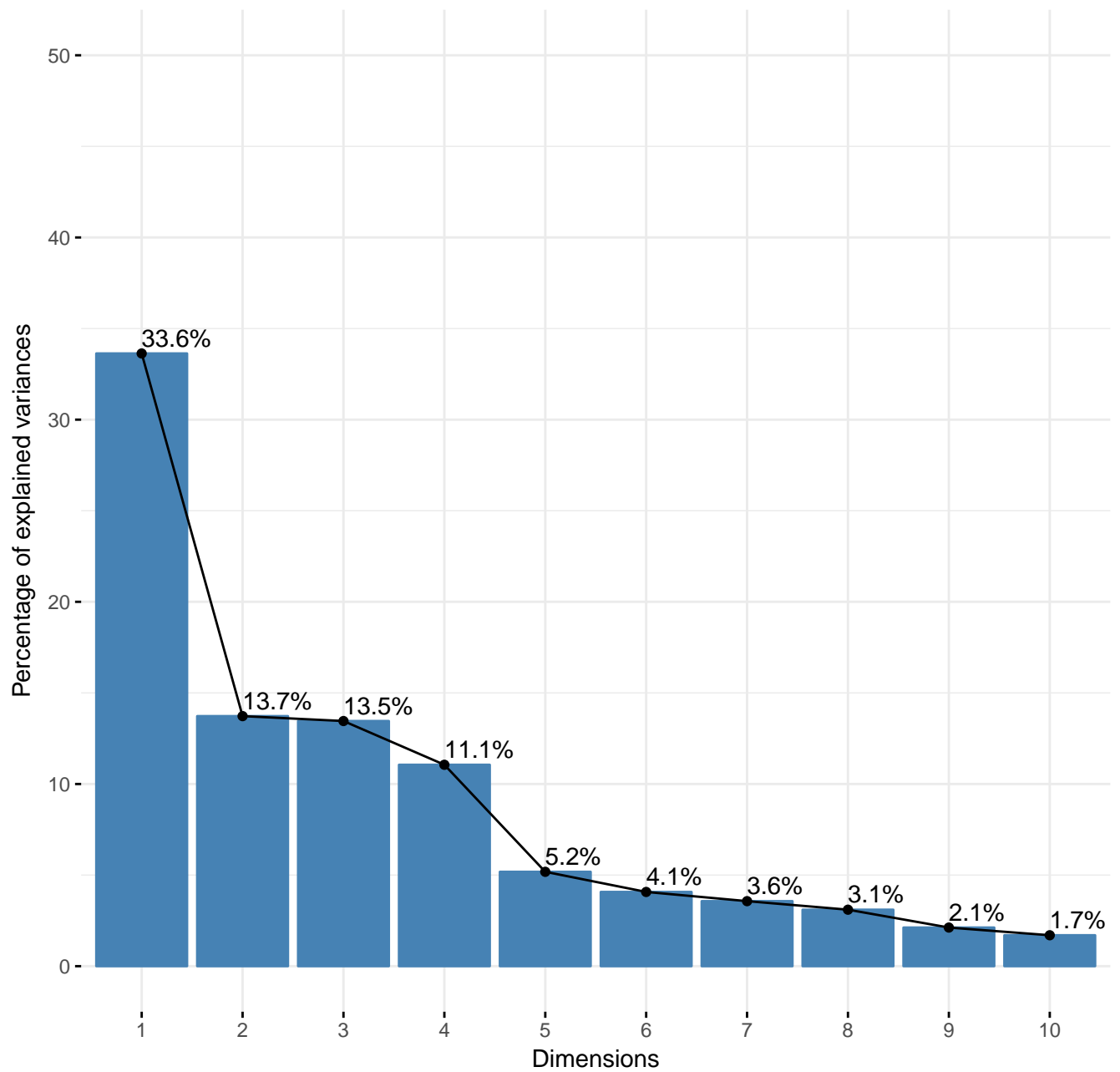
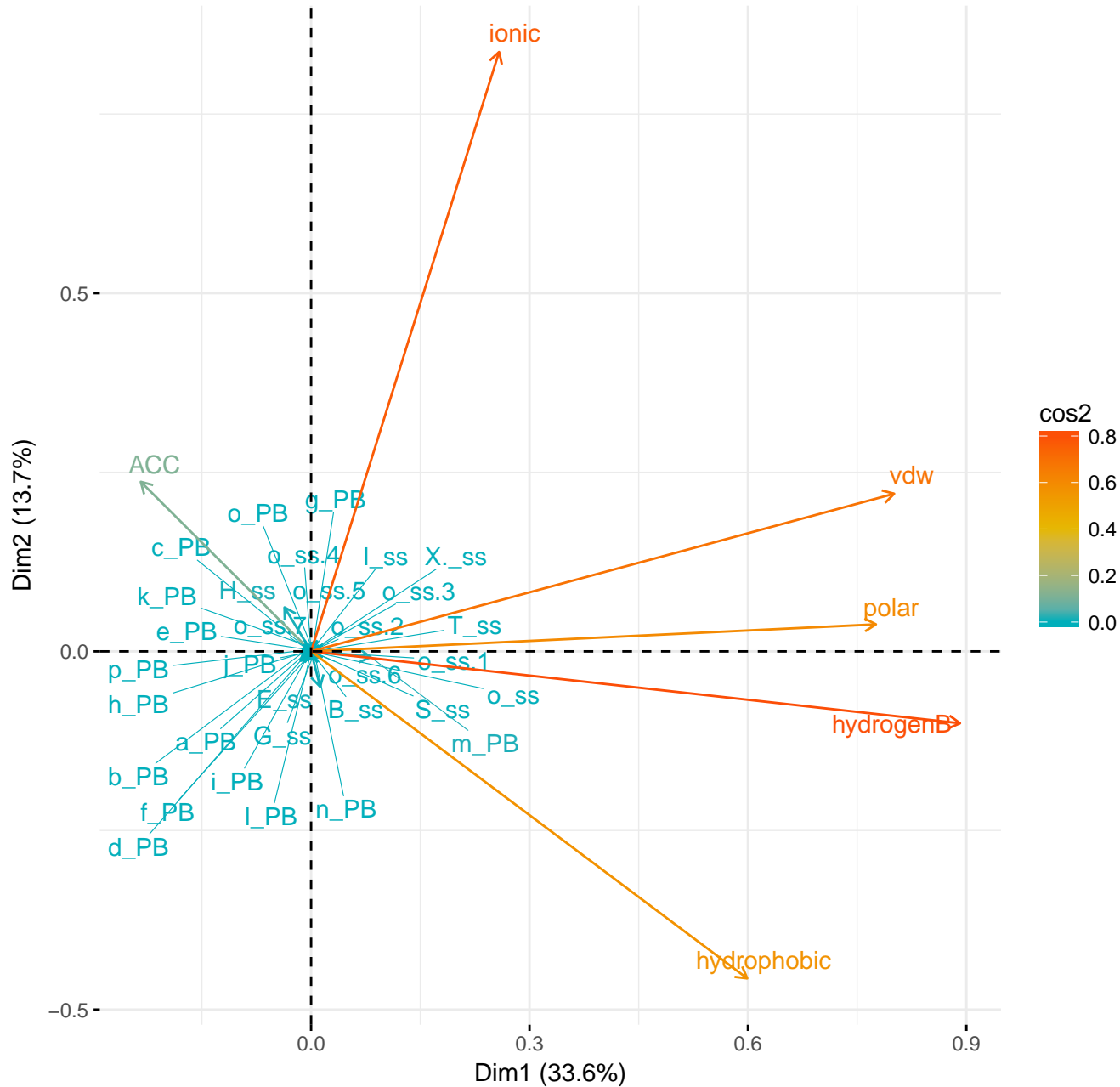


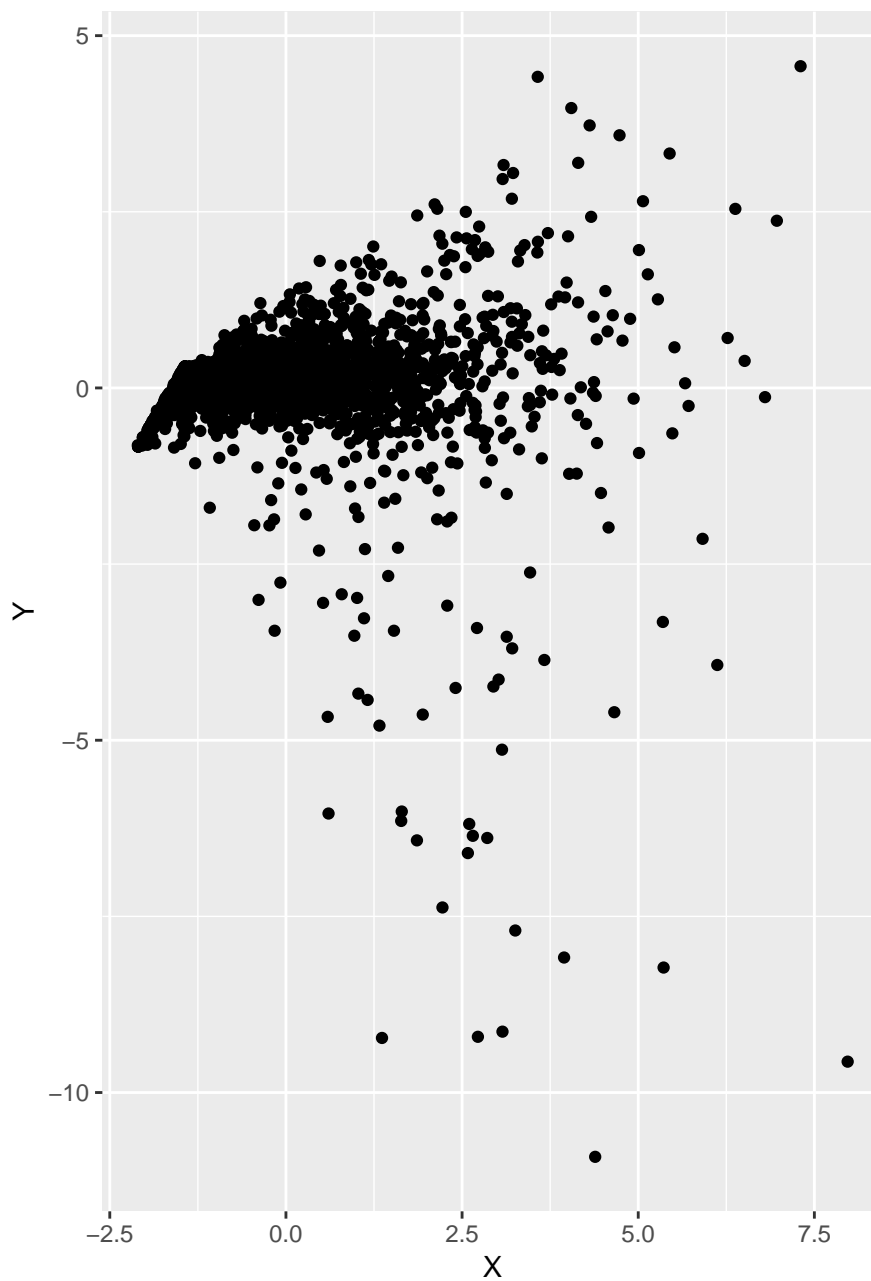
Scree plot



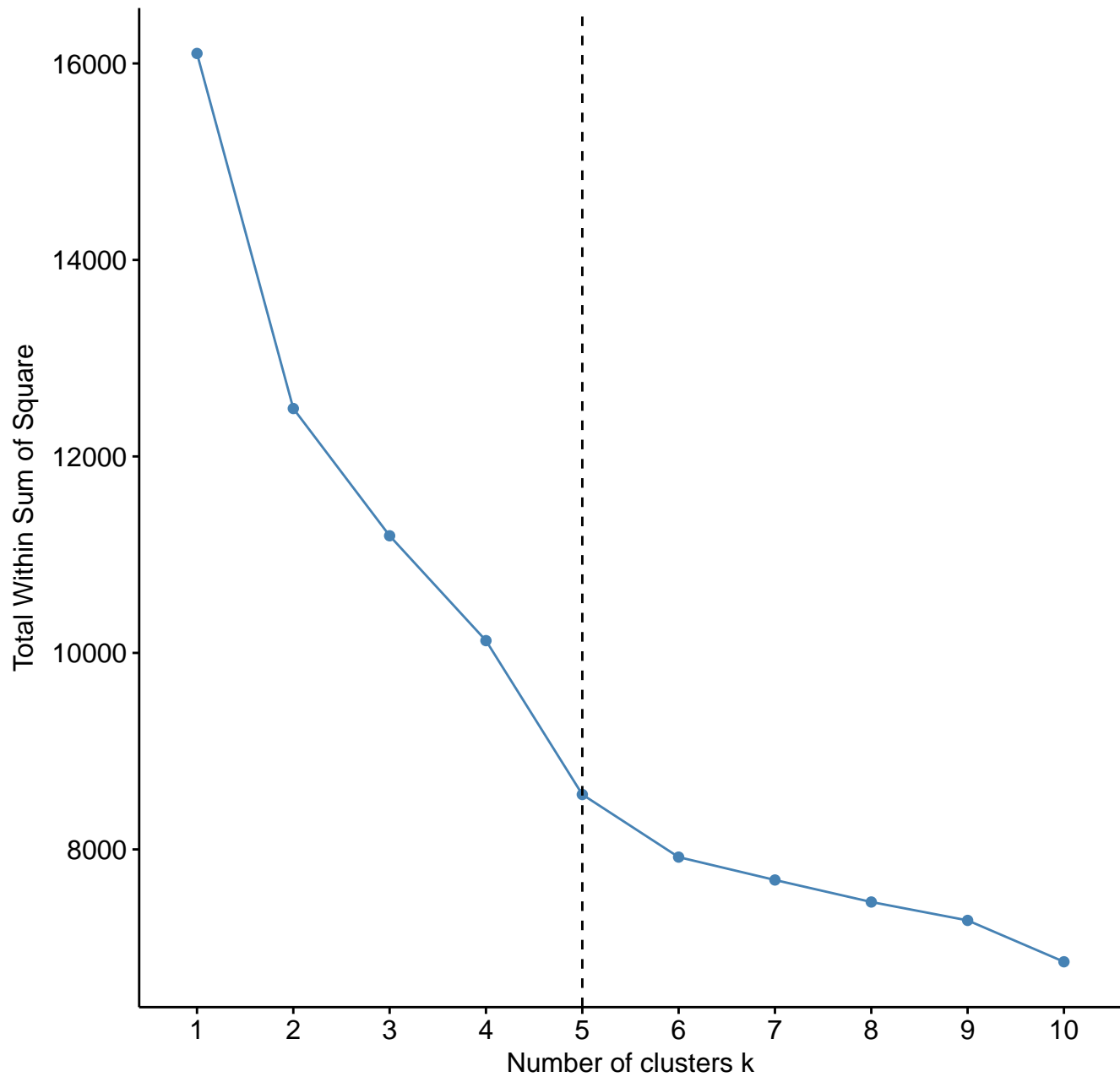
Variables – PCA



MDS with Shephard–Kruskal Stress 0.6



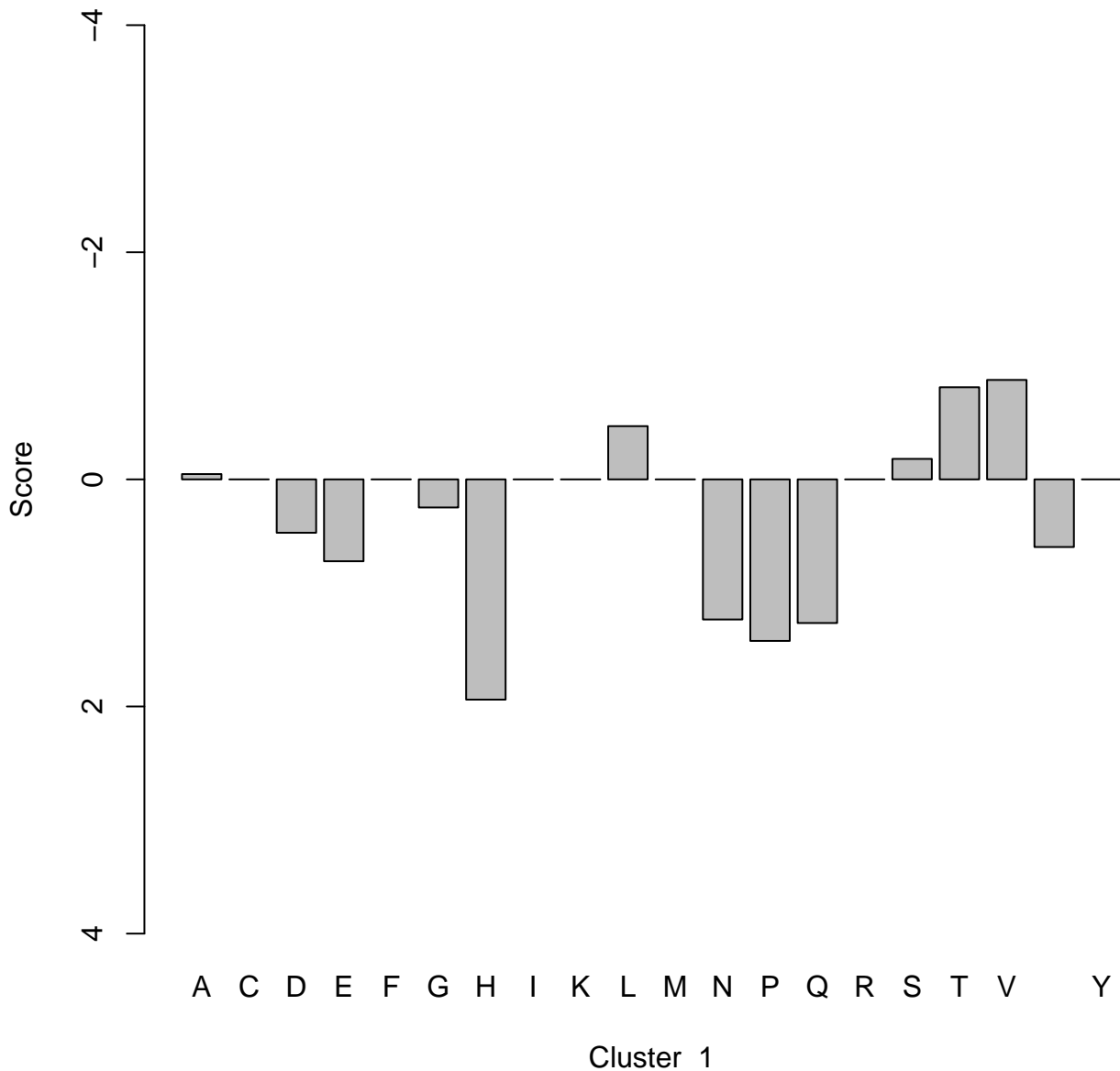
Optimal number of clusters



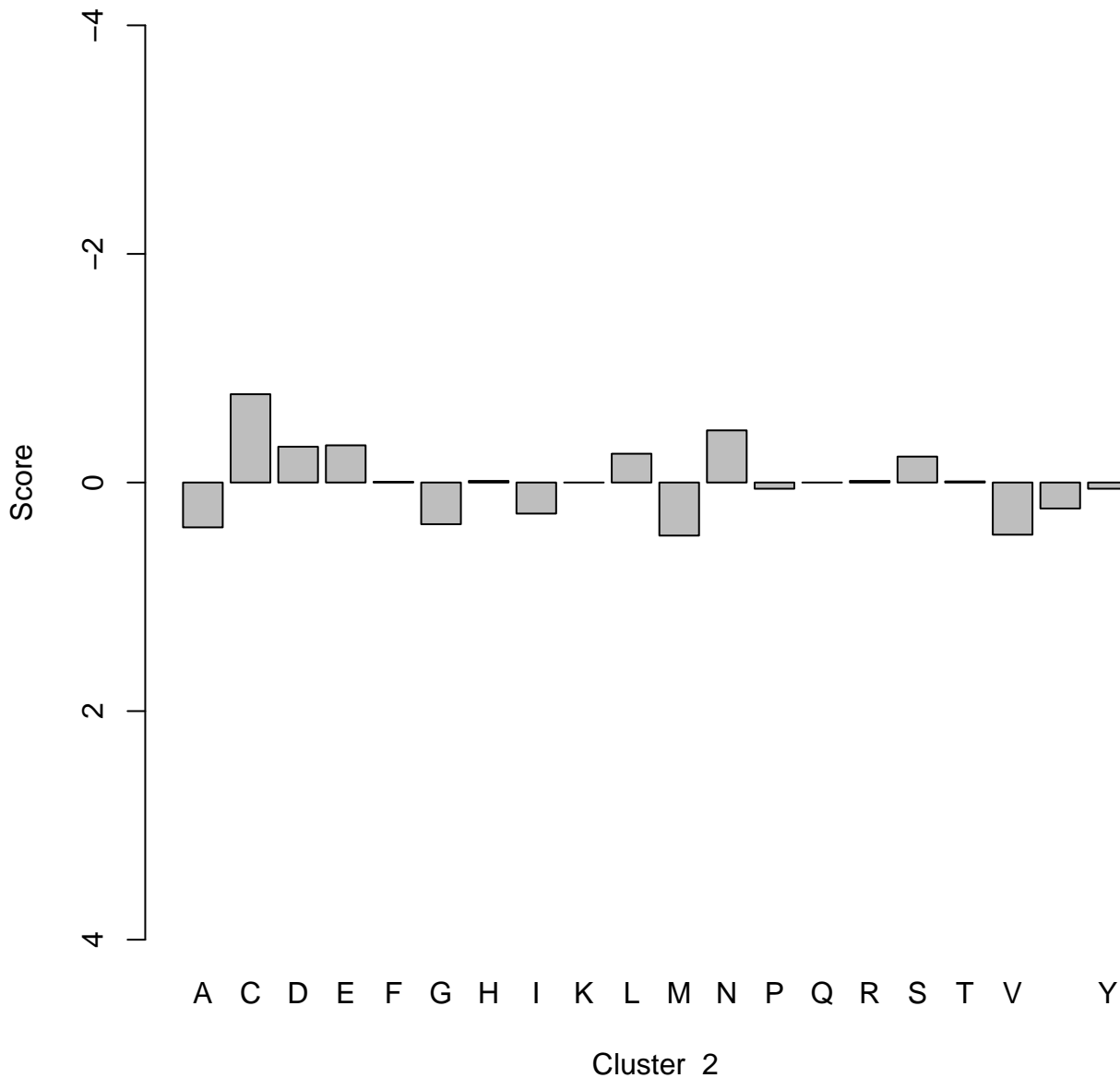
A PCA plot showing the distribution of 1000 random numbers. The x-axis is labeled 'PC1' and ranges from 0.00 to 0.08. The y-axis is unlabeled but ranges from approximately -0.02 to 0.06. The data points are colored based on their value, with a color scale from blue (low values) to red (high values). Four overlapping convex hulls are drawn around the data, representing different ranges of values: a red hull for the highest values (top right), a purple hull for the middle values (center), a green hull for the lower values (bottom left), and a yellow-green hull for the lowest values (bottom right). The hulls overlap significantly, indicating that the principal components do not perfectly separate the data by value.



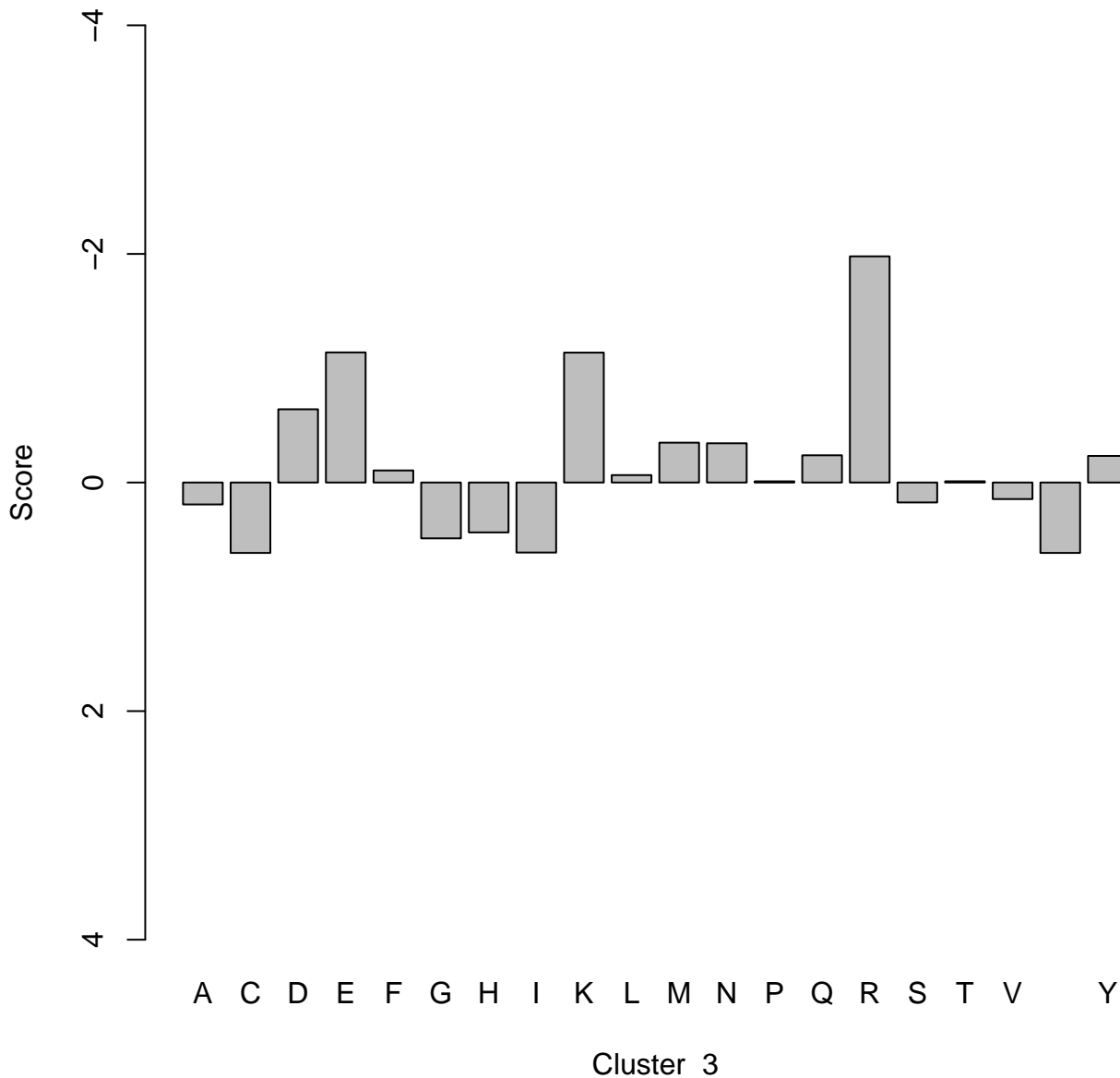
Distribution des scores (Méthodes Kmeans)



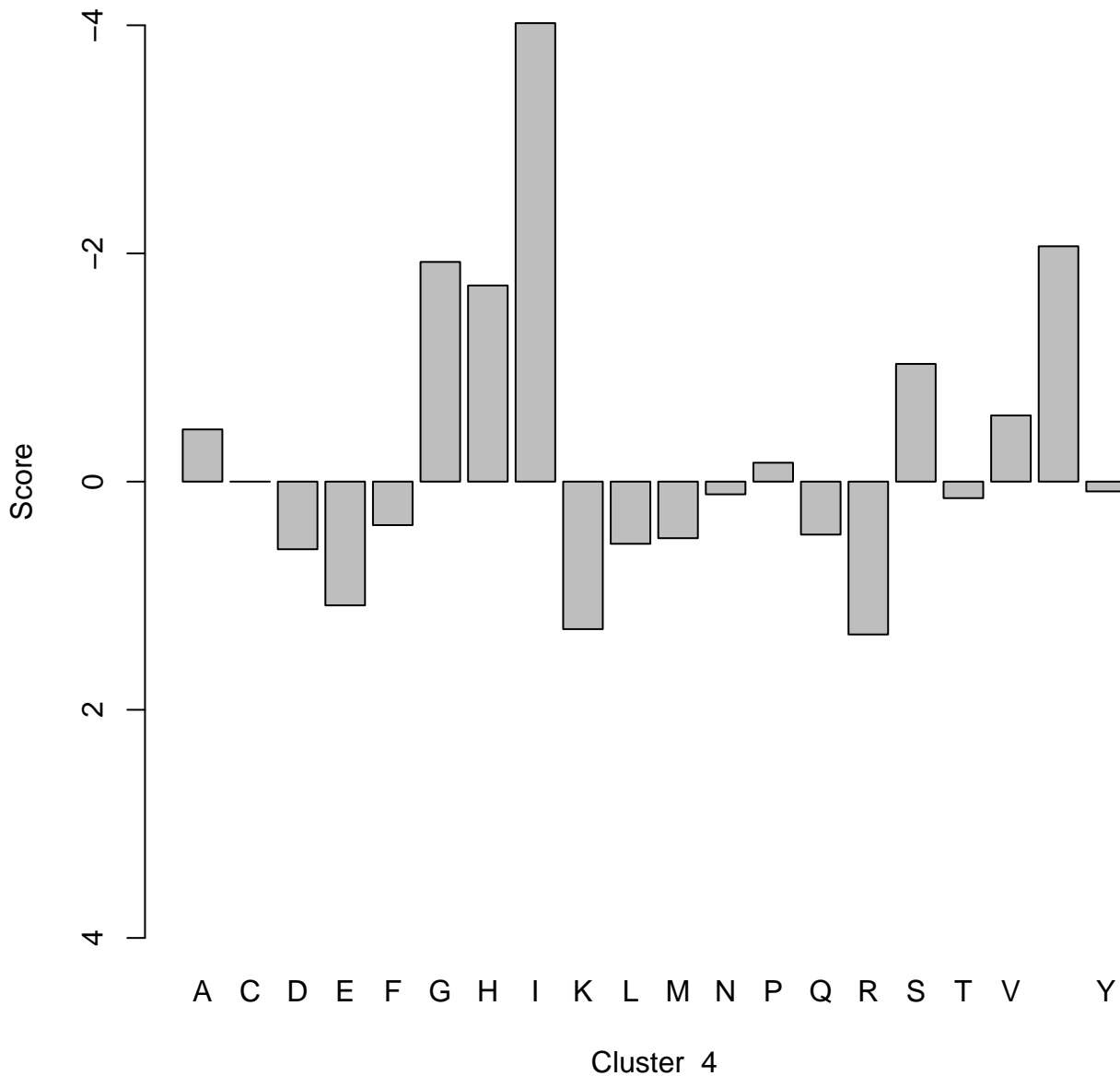
Distribution des scores (Méthodes Kmeans)



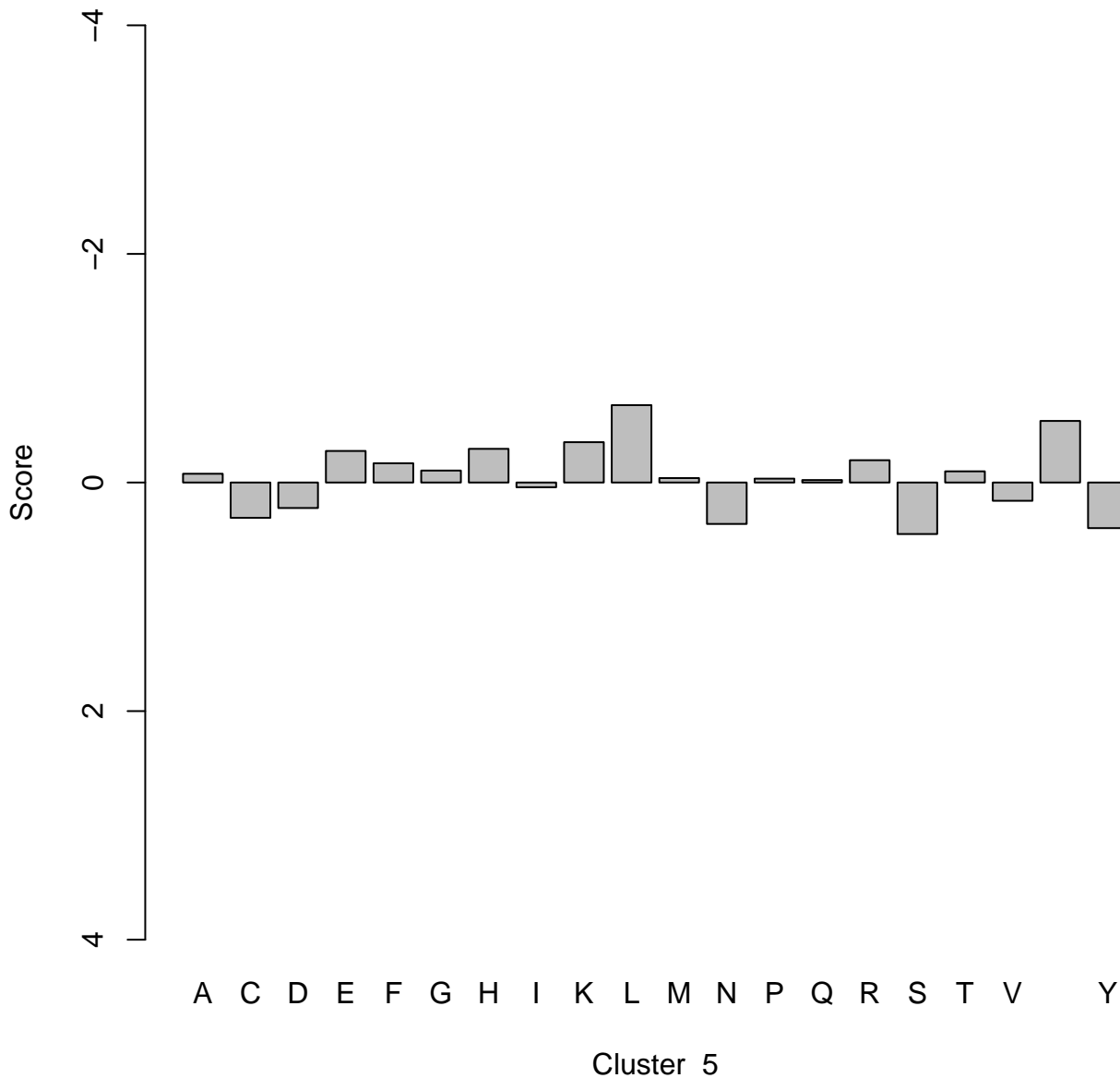
Distribution des scores (Méthodes Kmeans)



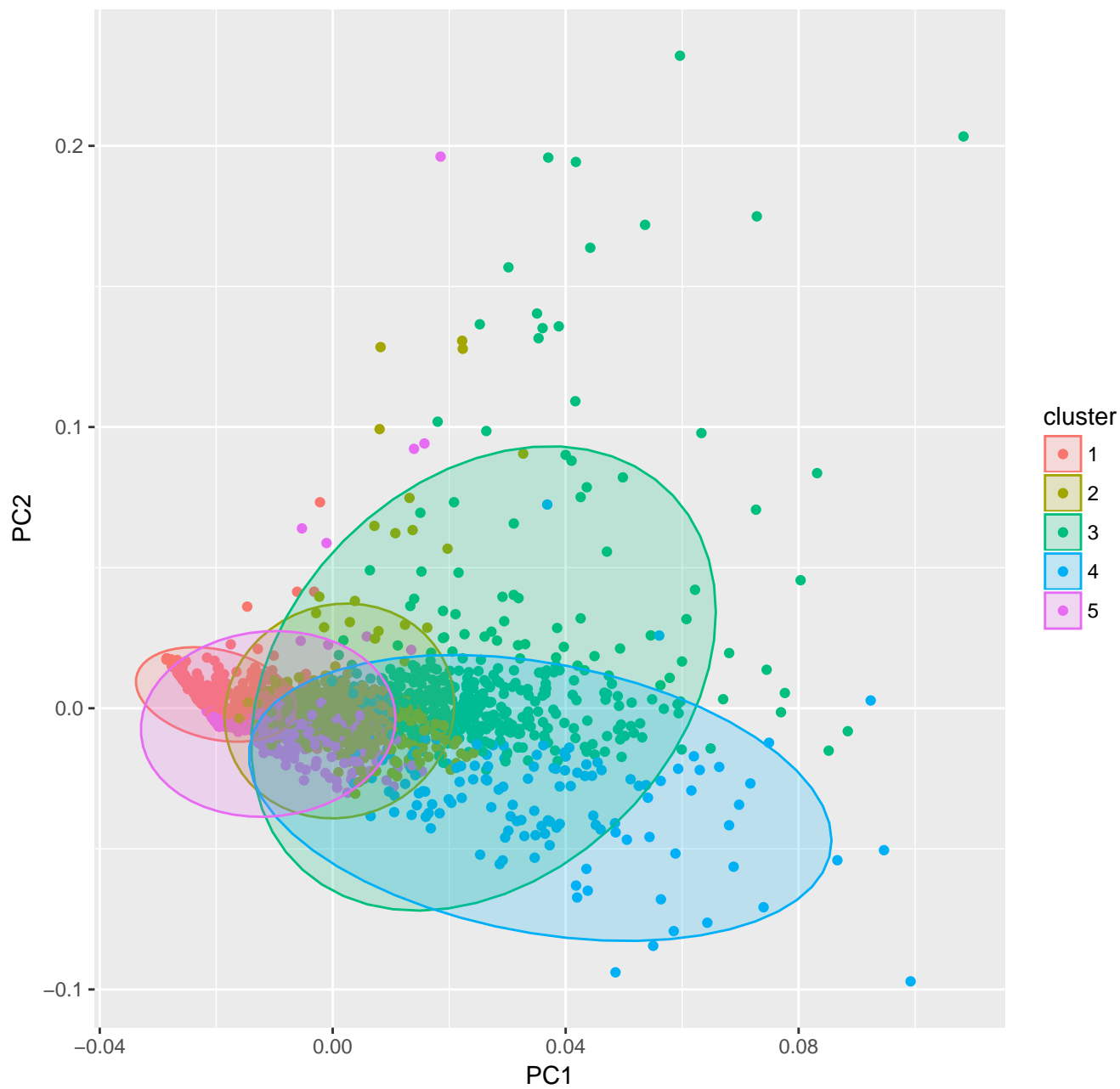
Distribution des scores (Méthodes Kmeans)



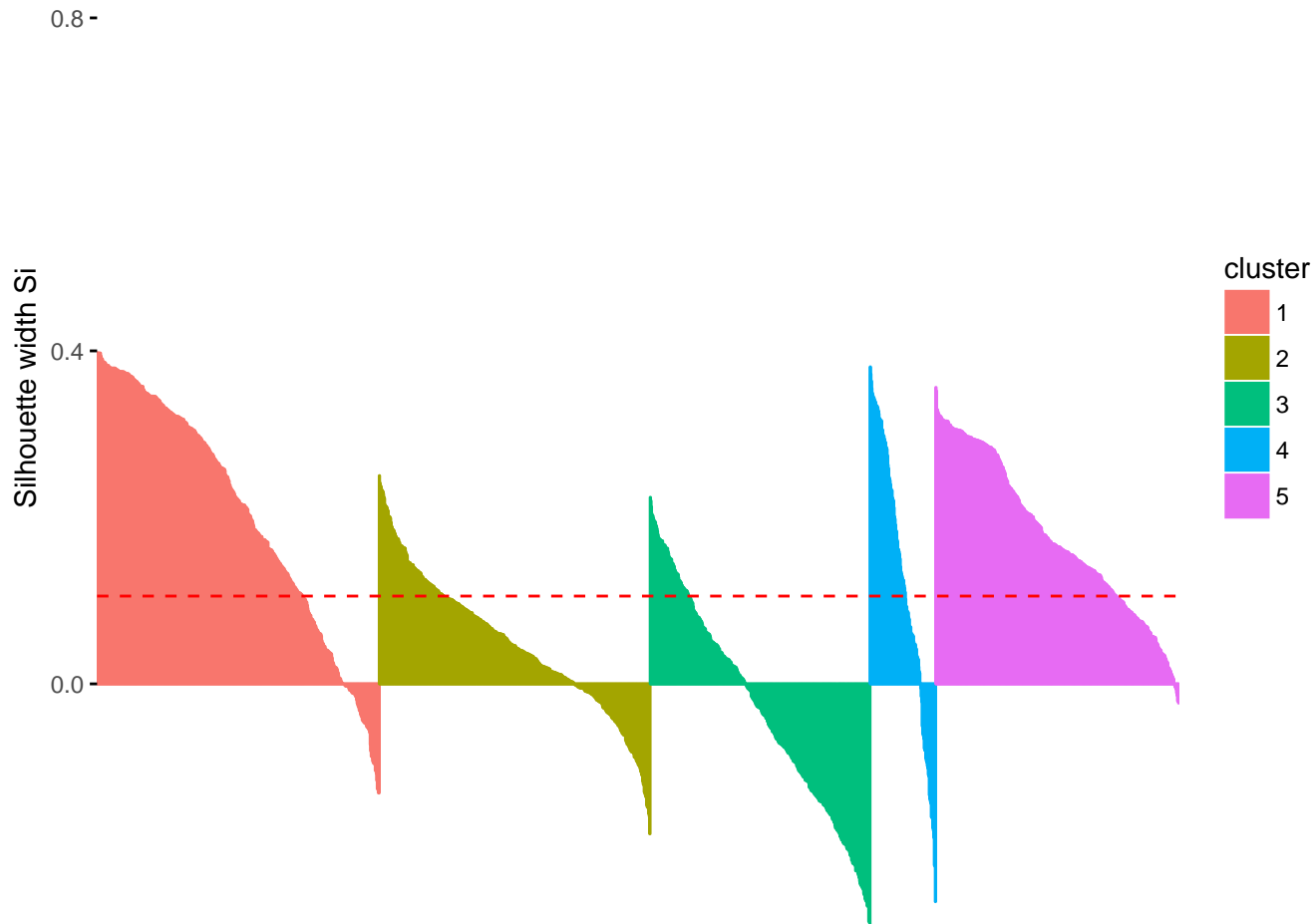
Distribution des scores (Méthodes Kmeans)



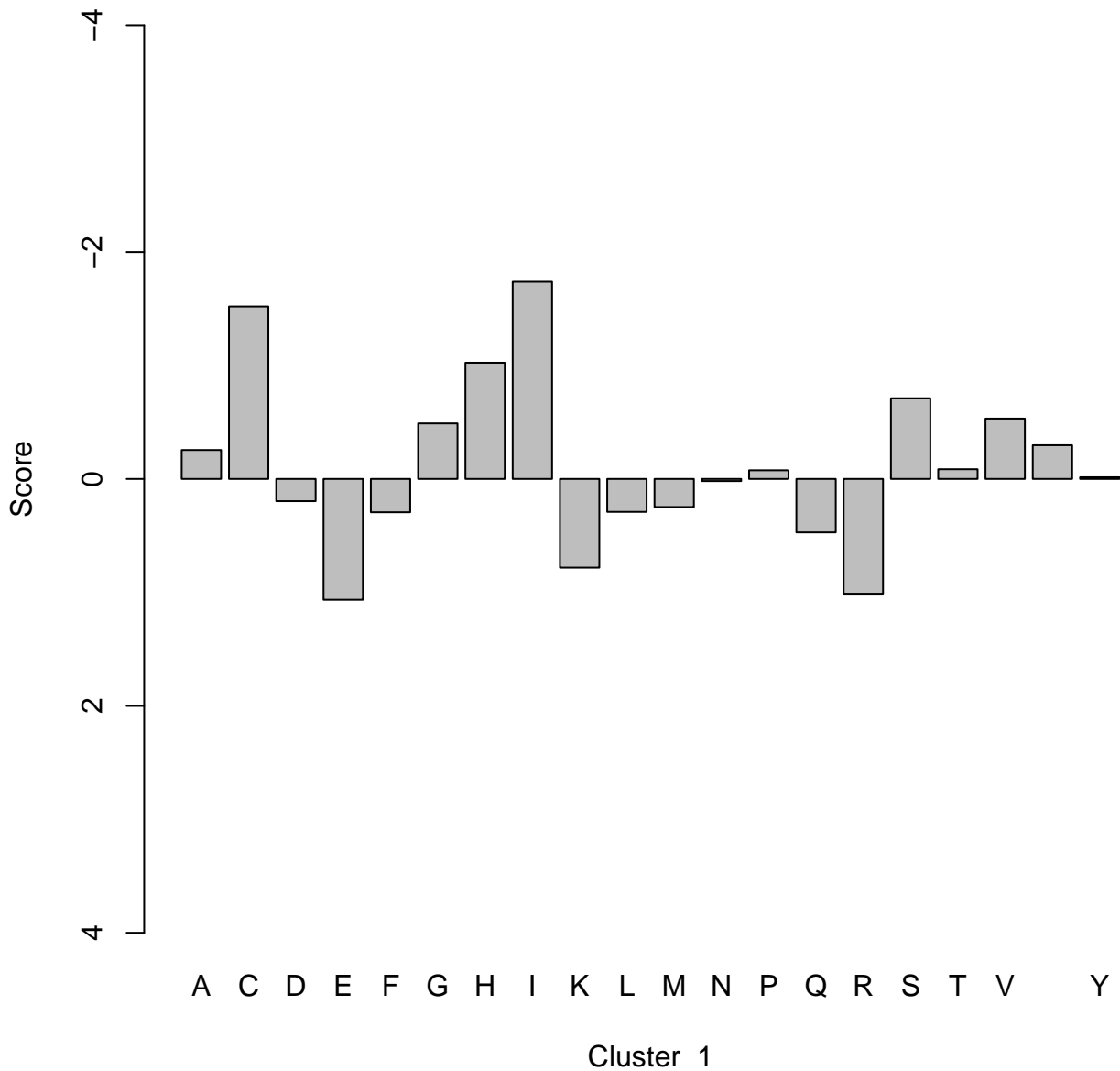
Clustering par Kmedoid(PAM)



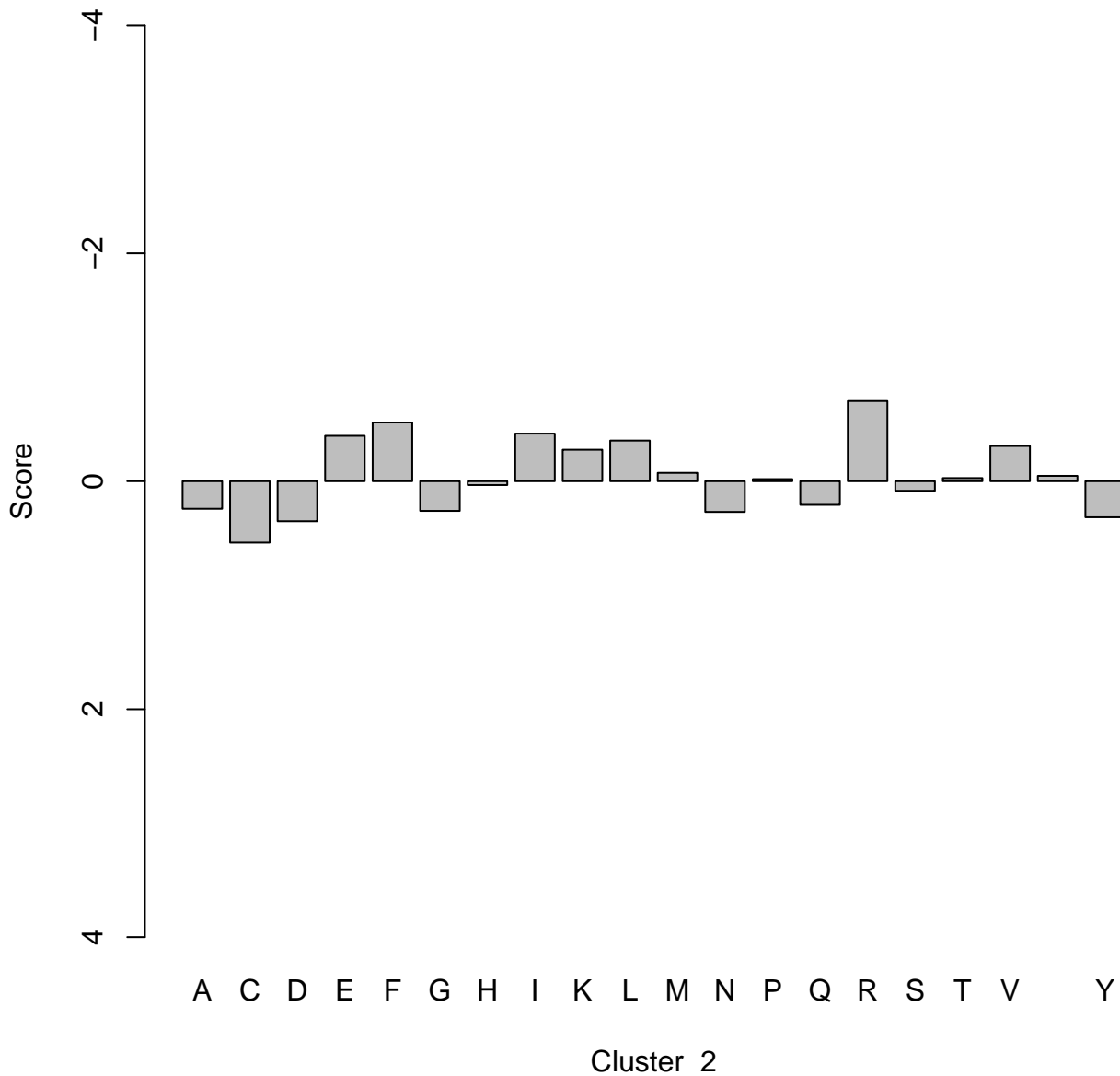
Clusters silhouette plot
Average silhouette width: 0.11



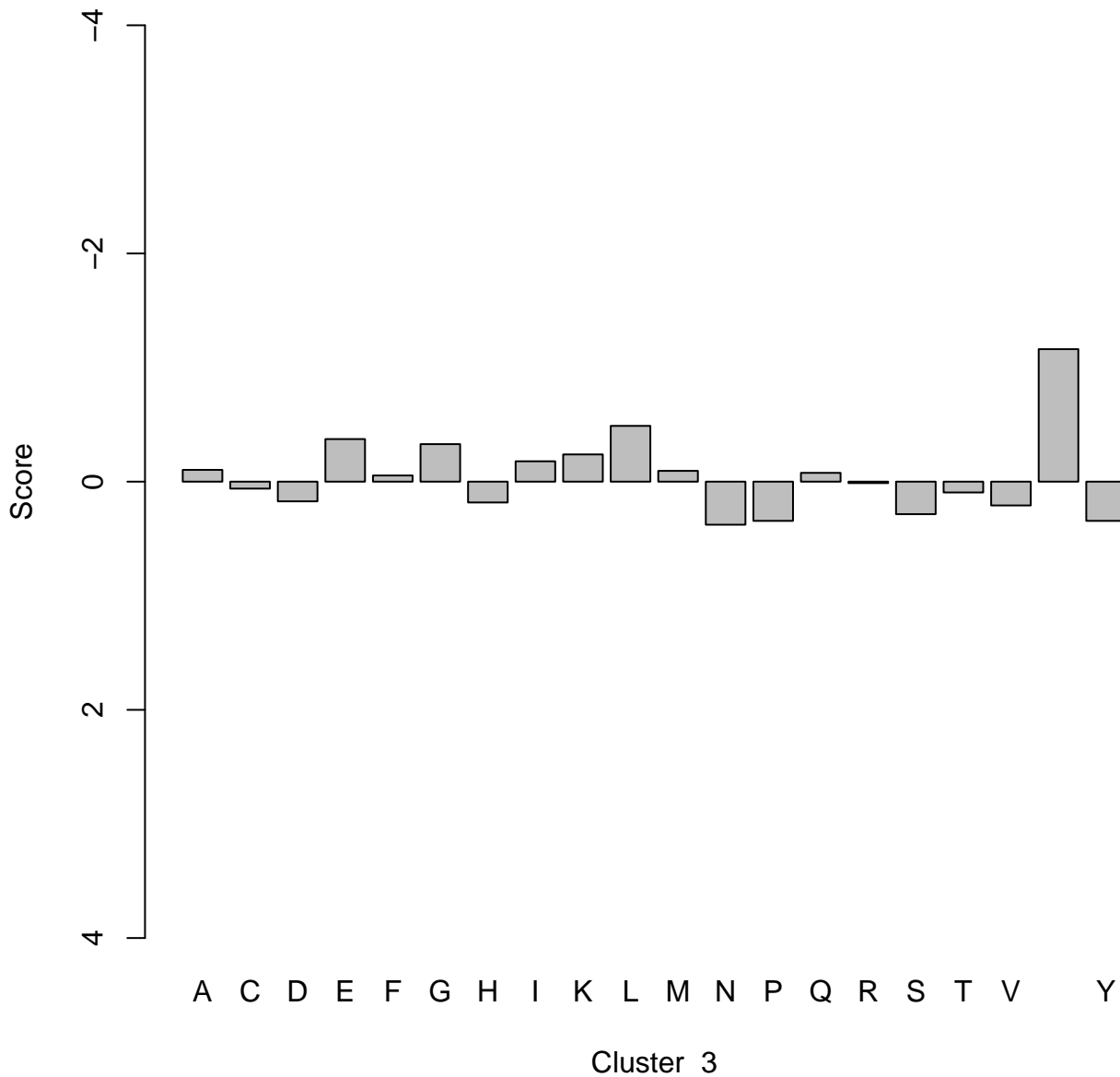
Distribution des scores (Méthode PAM)



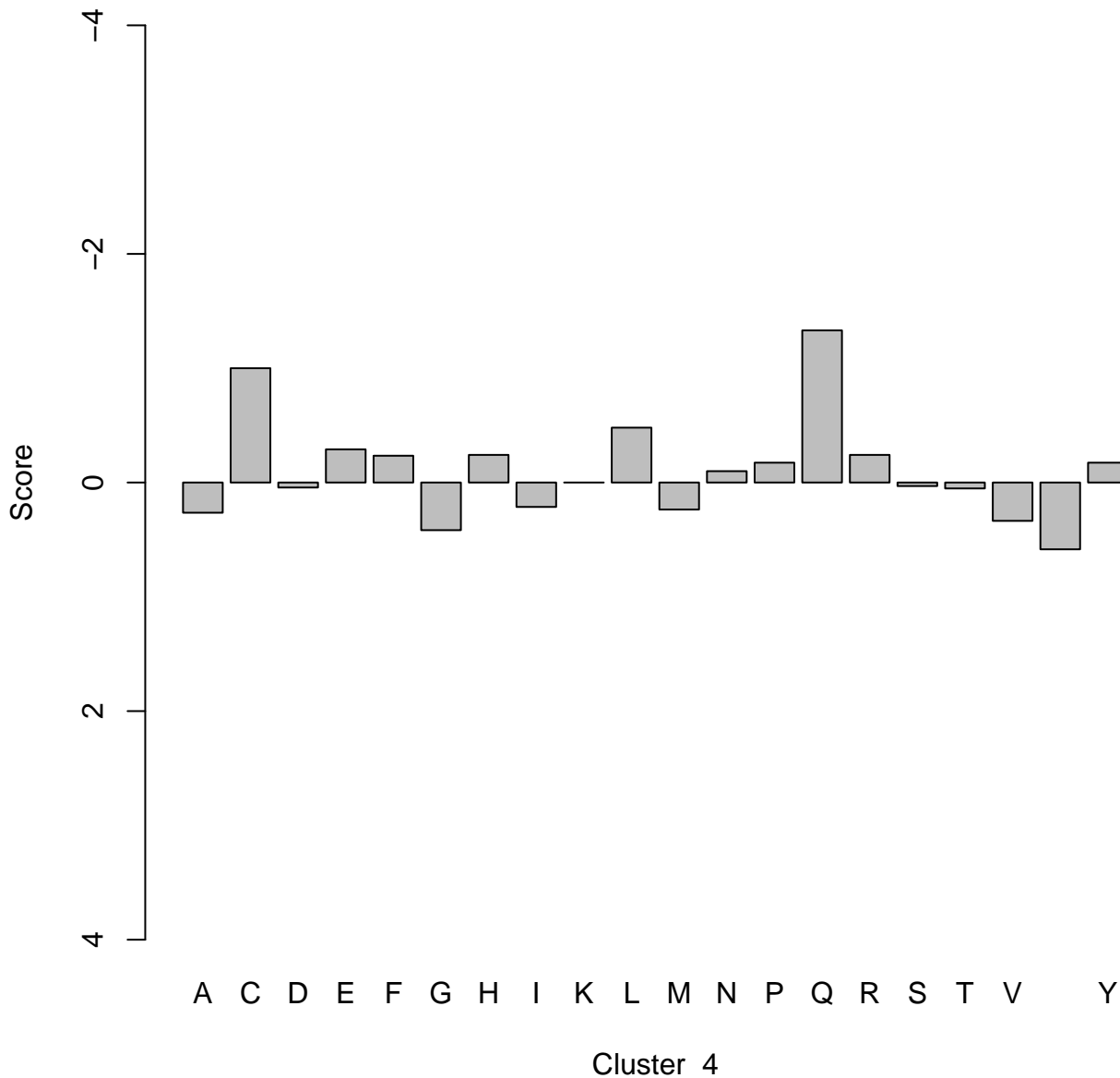
Distribution des scores (Méthode PAM)



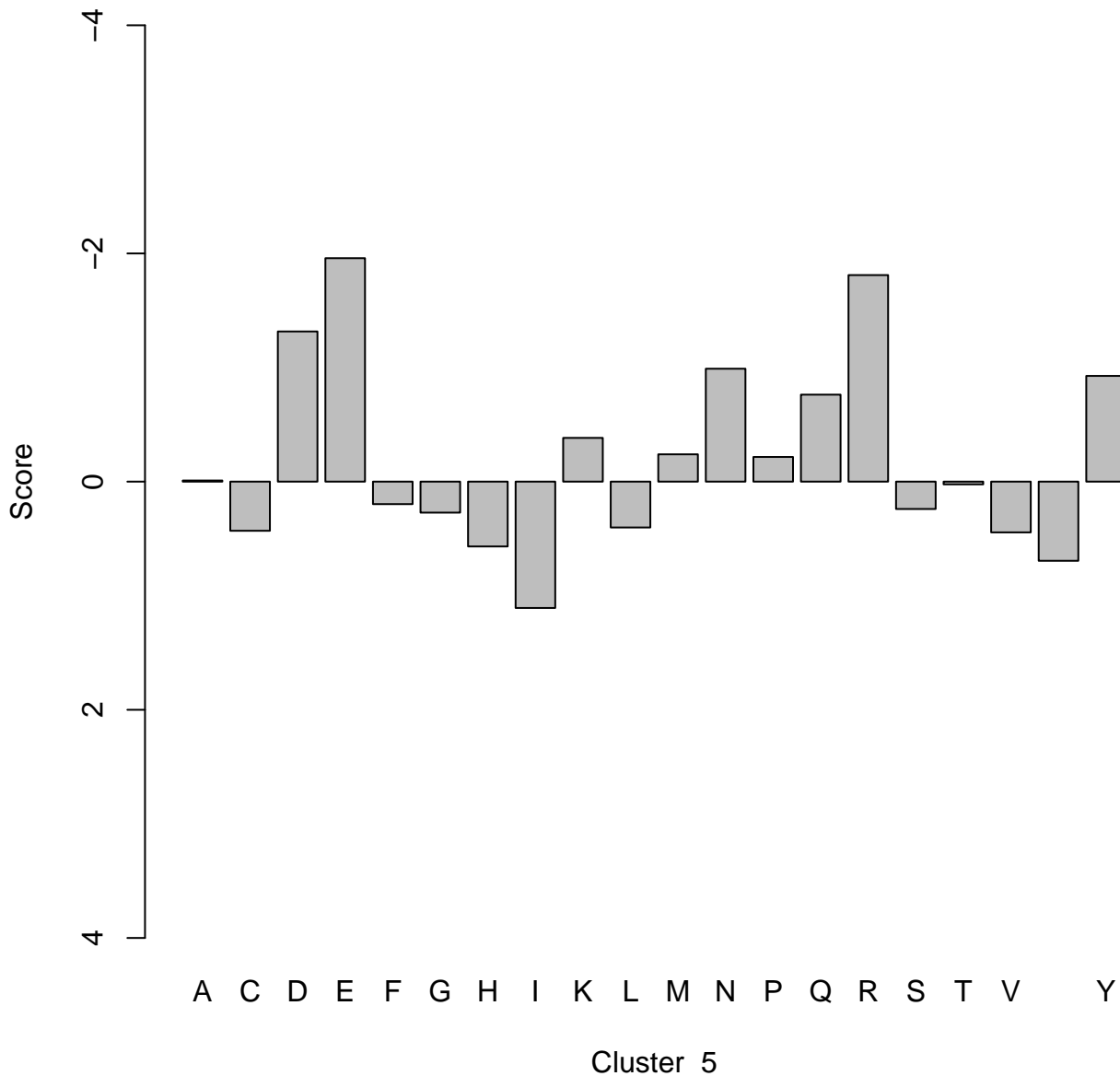
Distribution des scores (Méthode PAM)



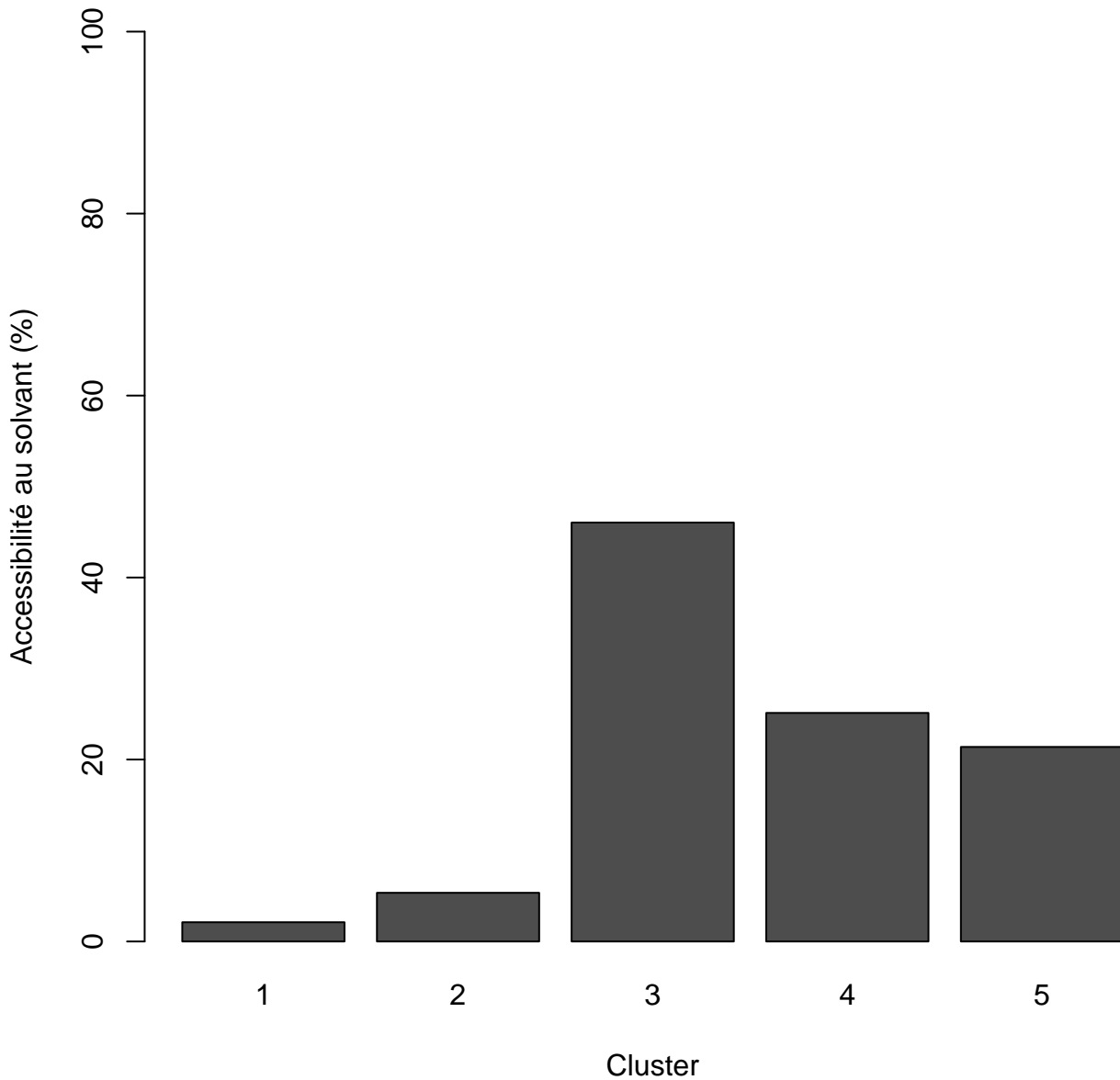
Distribution des scores (Méthode PAM)



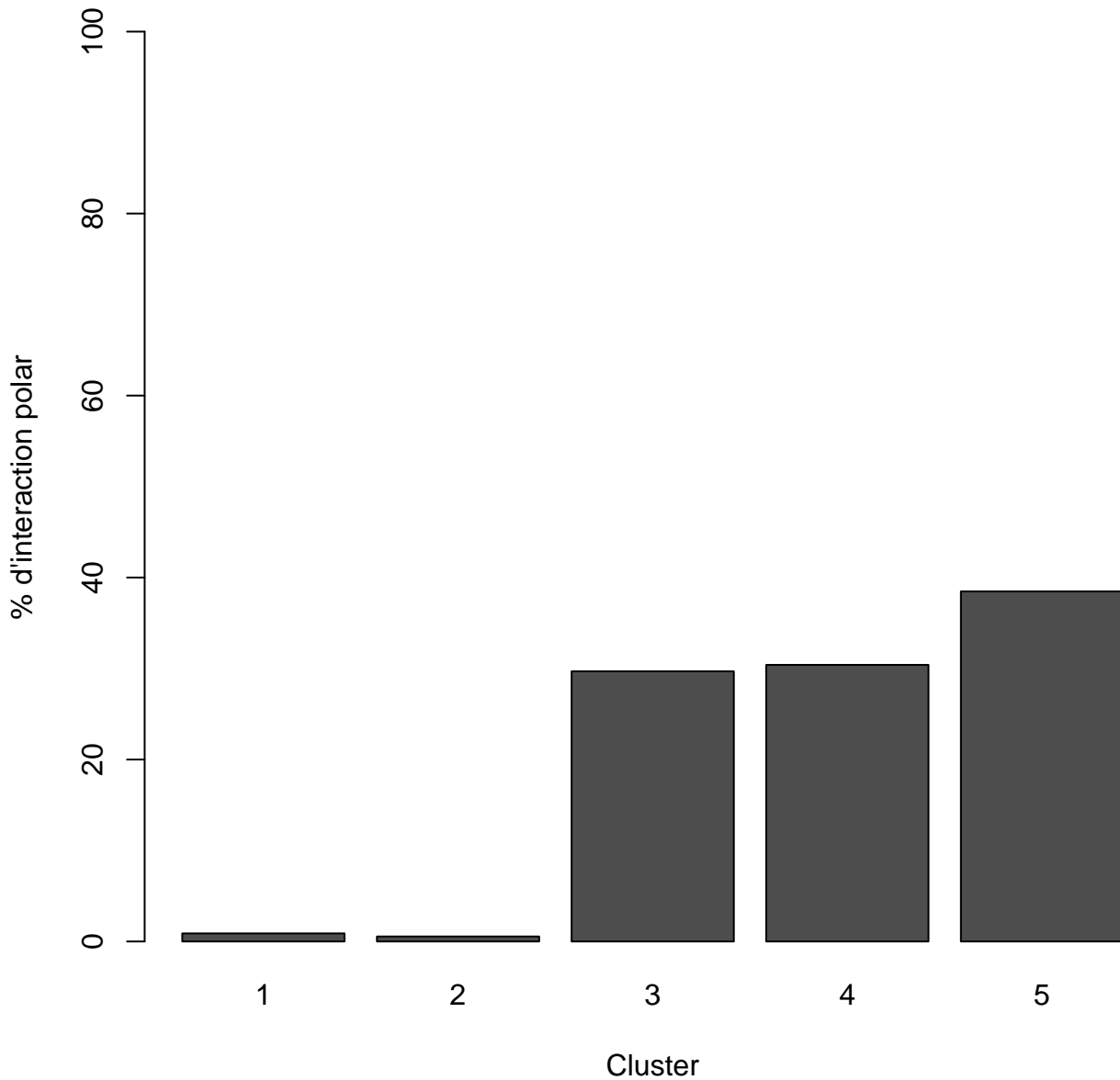
Distribution des scores (Méthode PAM)



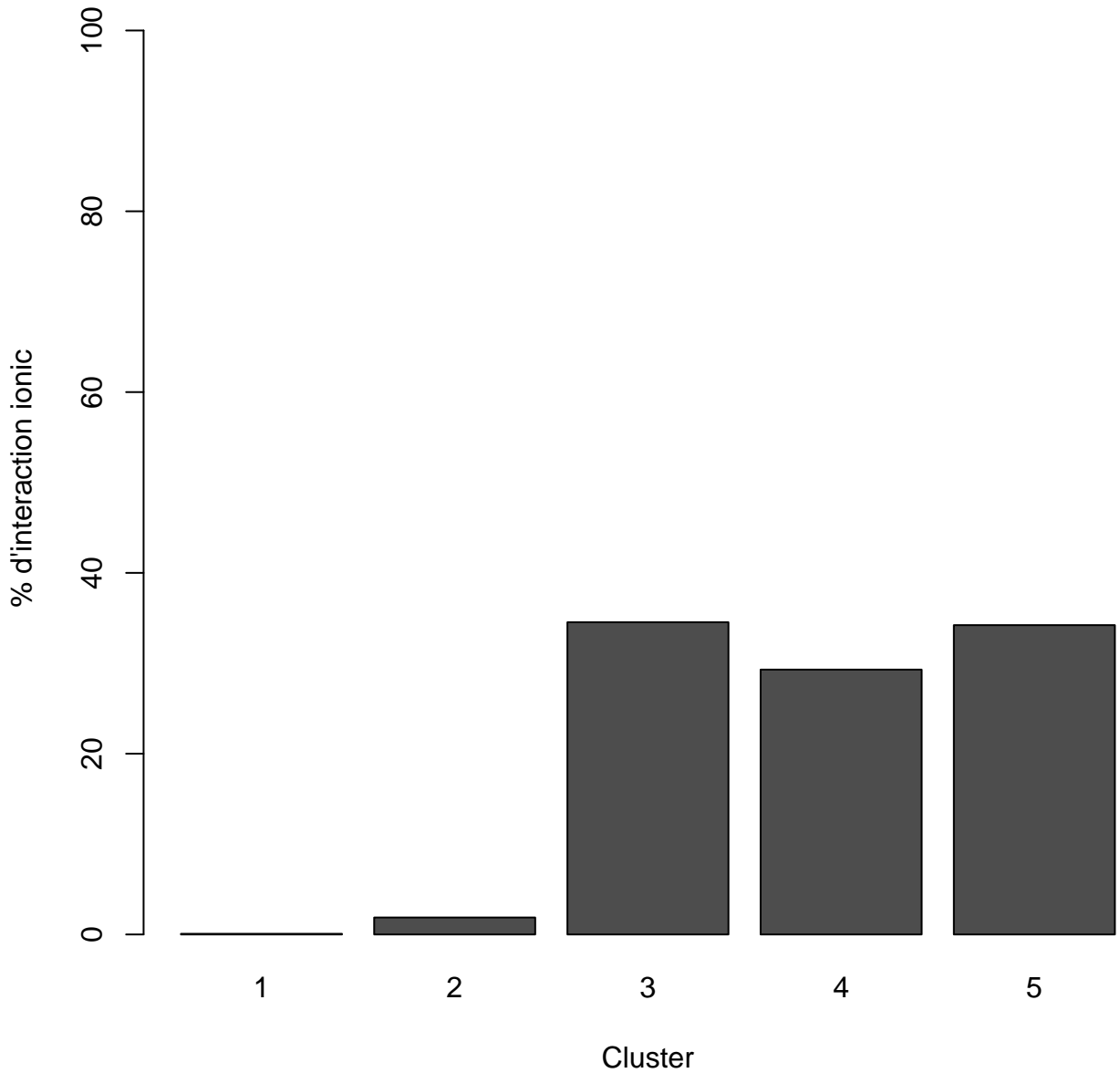
Accessibilité au solvant (%) Kmeans



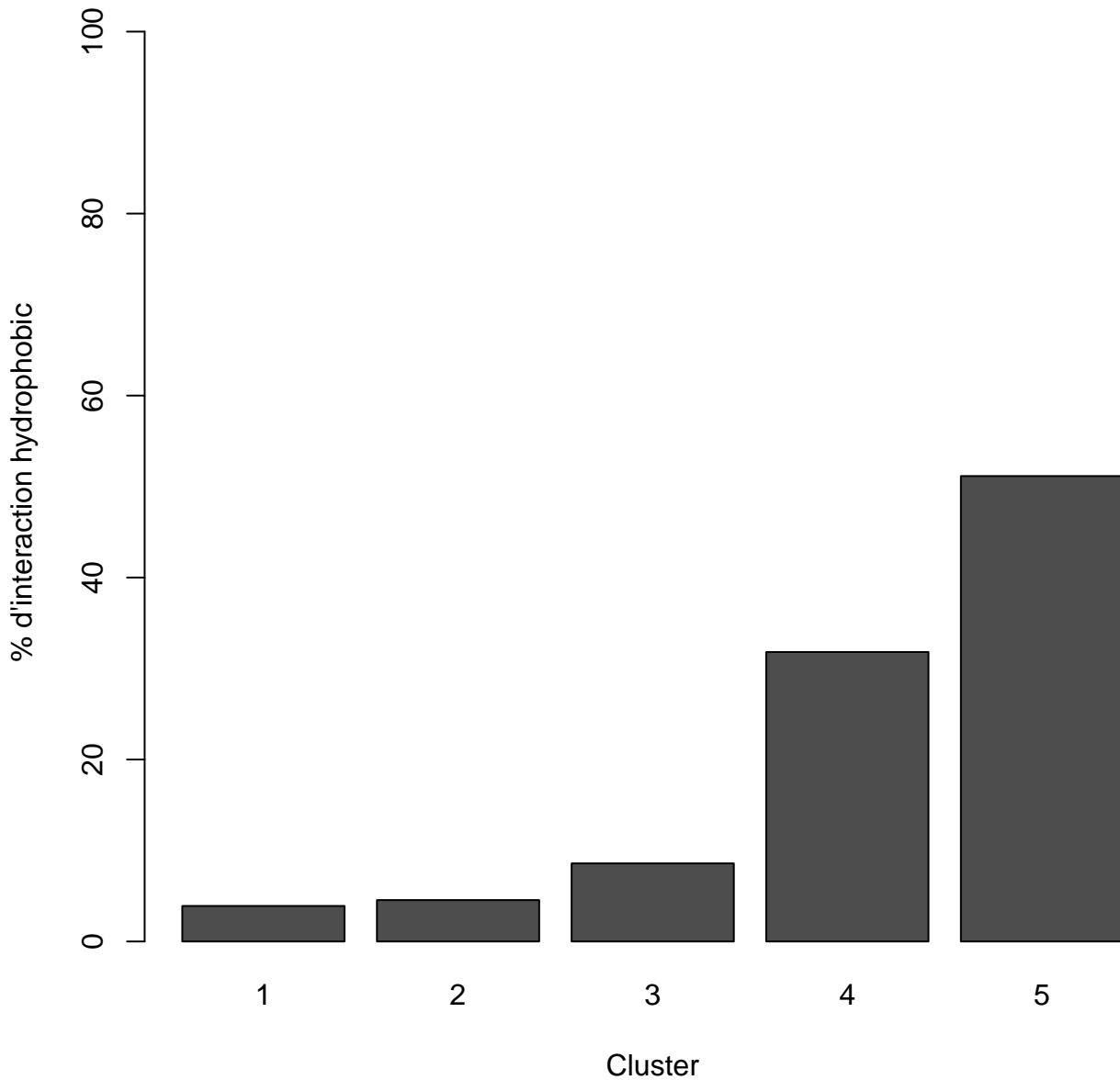
% d'interaction polar Kmeans



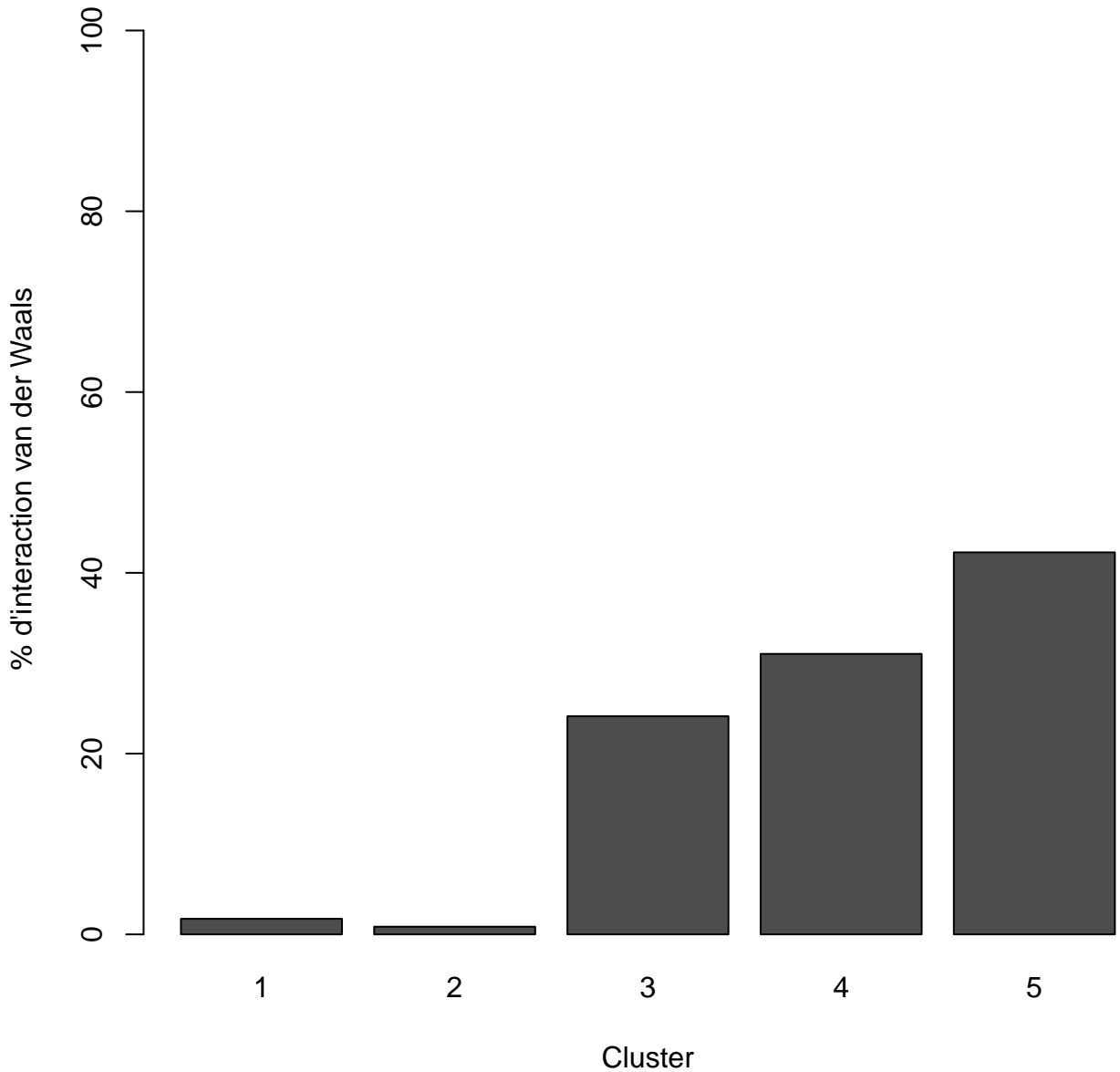
% d'interaction ionic Kmeans



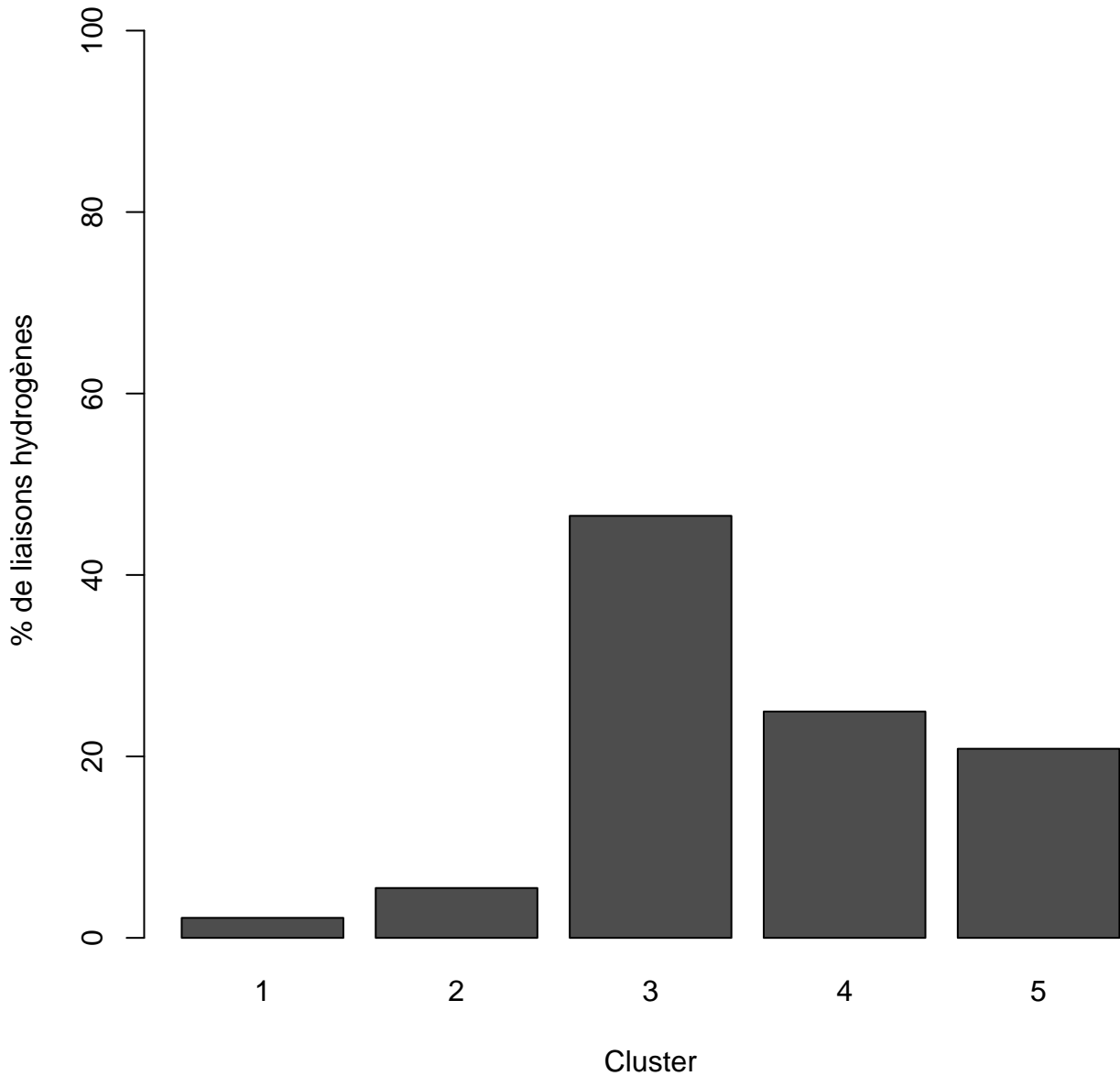
% d'interaction hydrophobic Kmeans



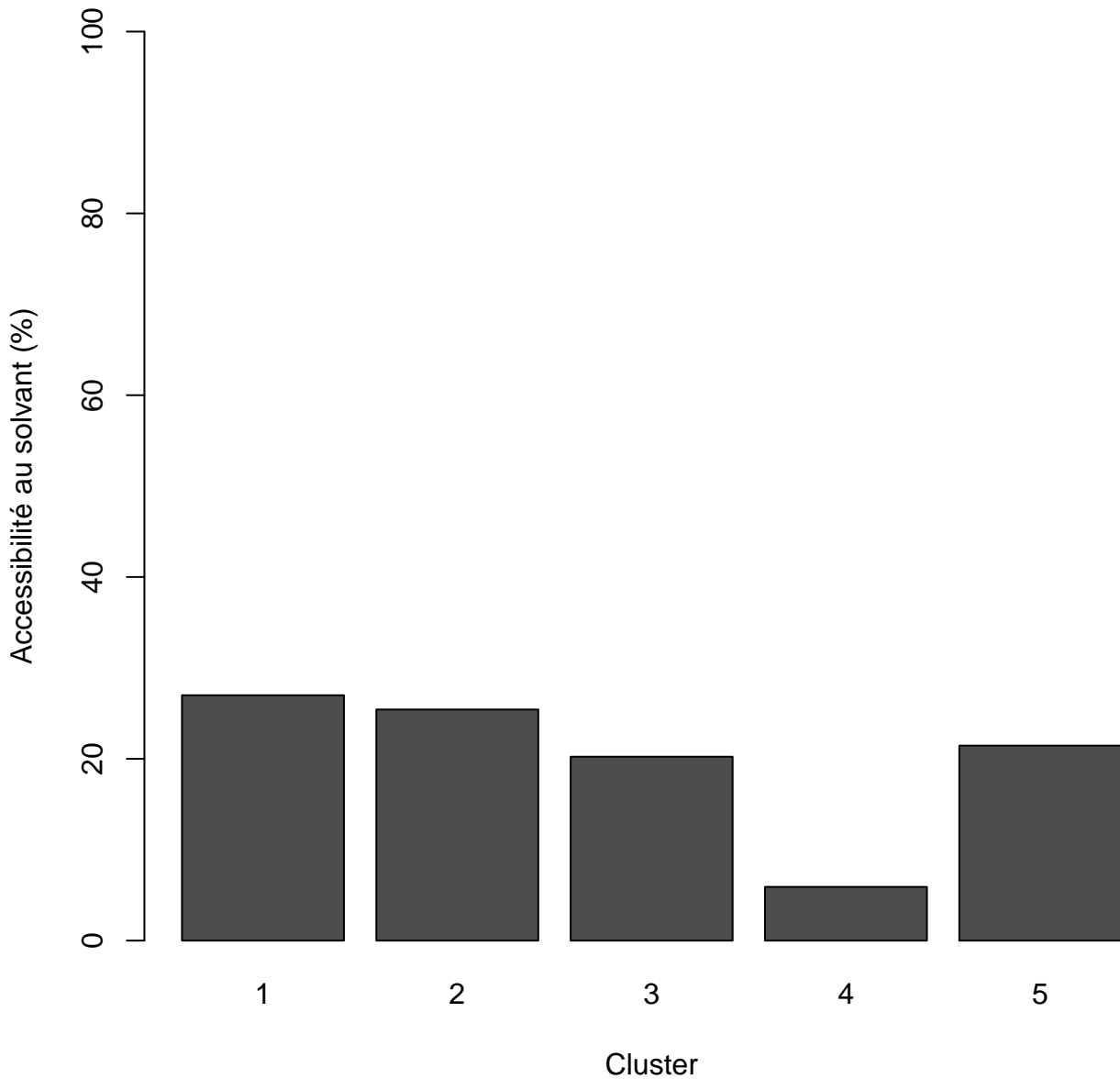
% d'interaction van der Waals Kmeans



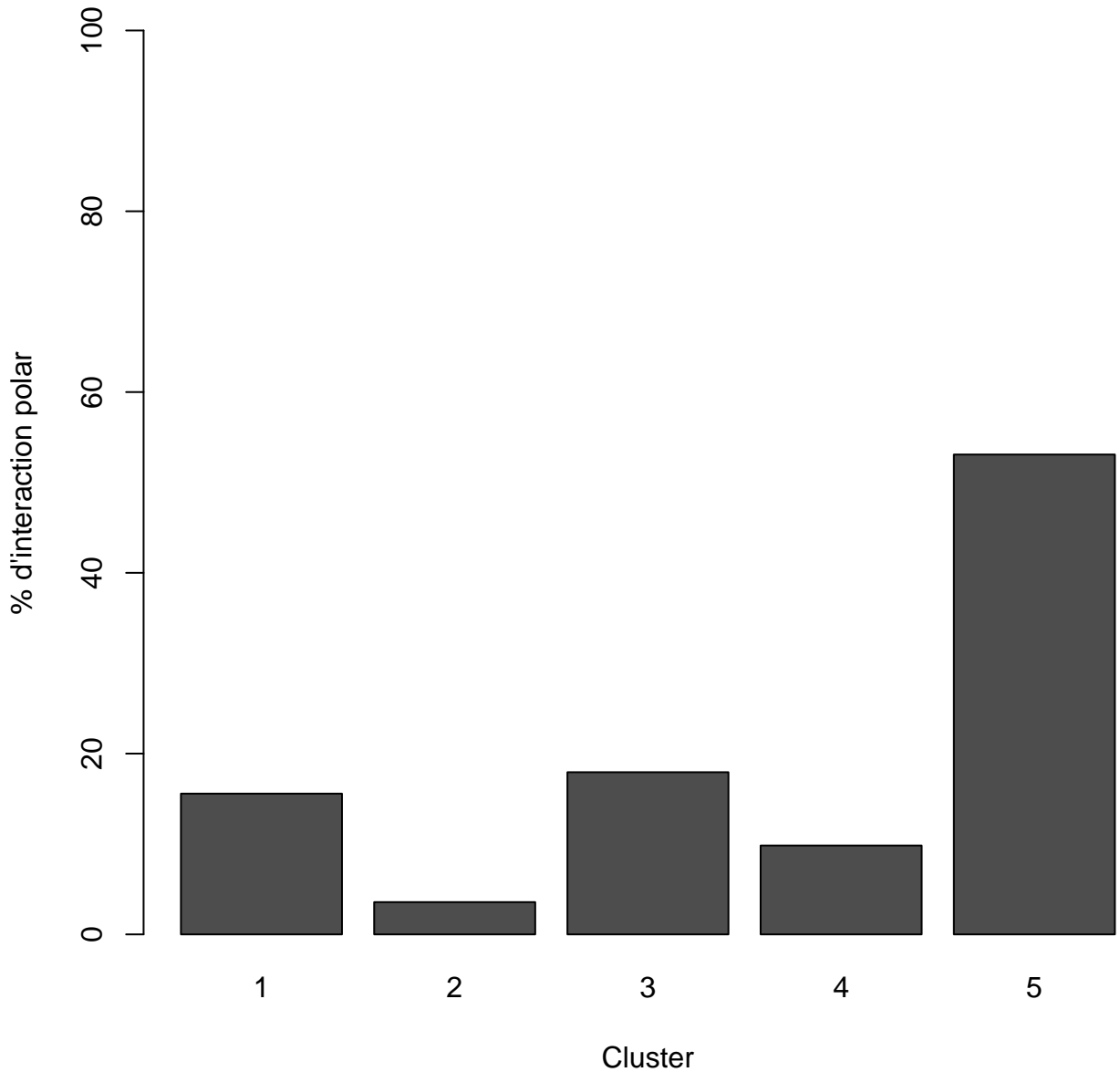
% de liaisons hydrogènes Kmeans



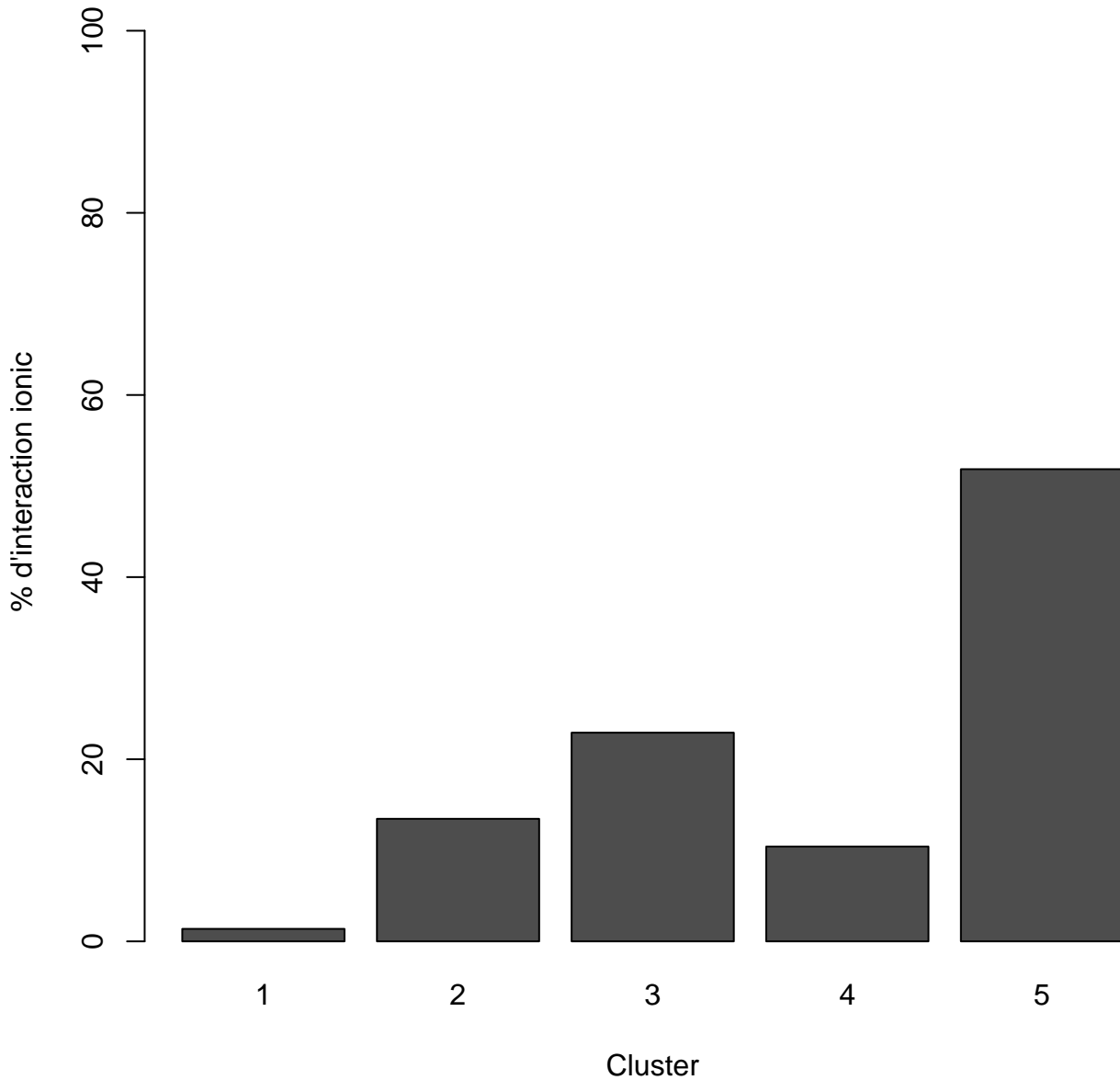
Accessibilité au solvant (%) Kmedoid



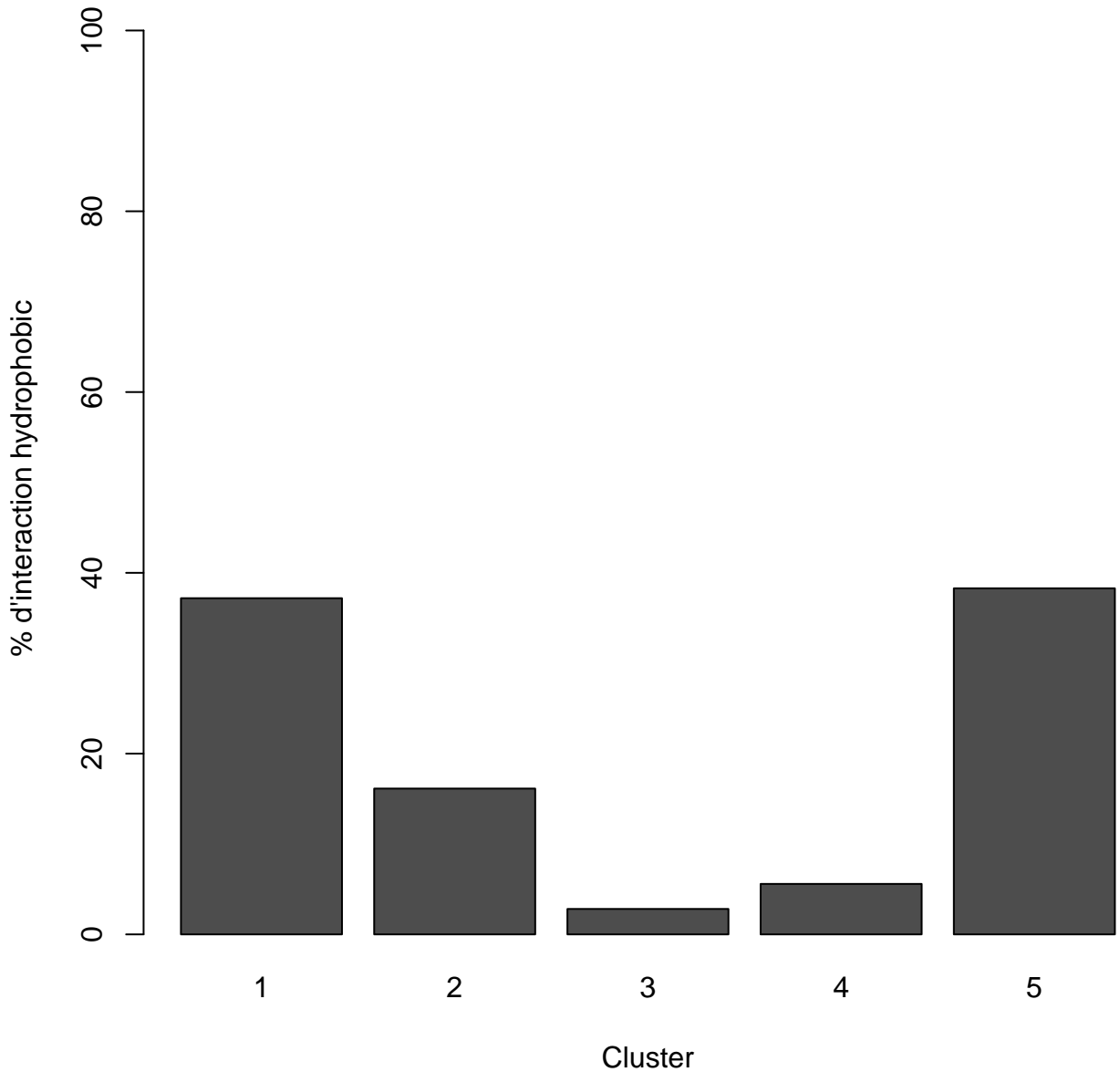
% d'interaction polar Kmedoid



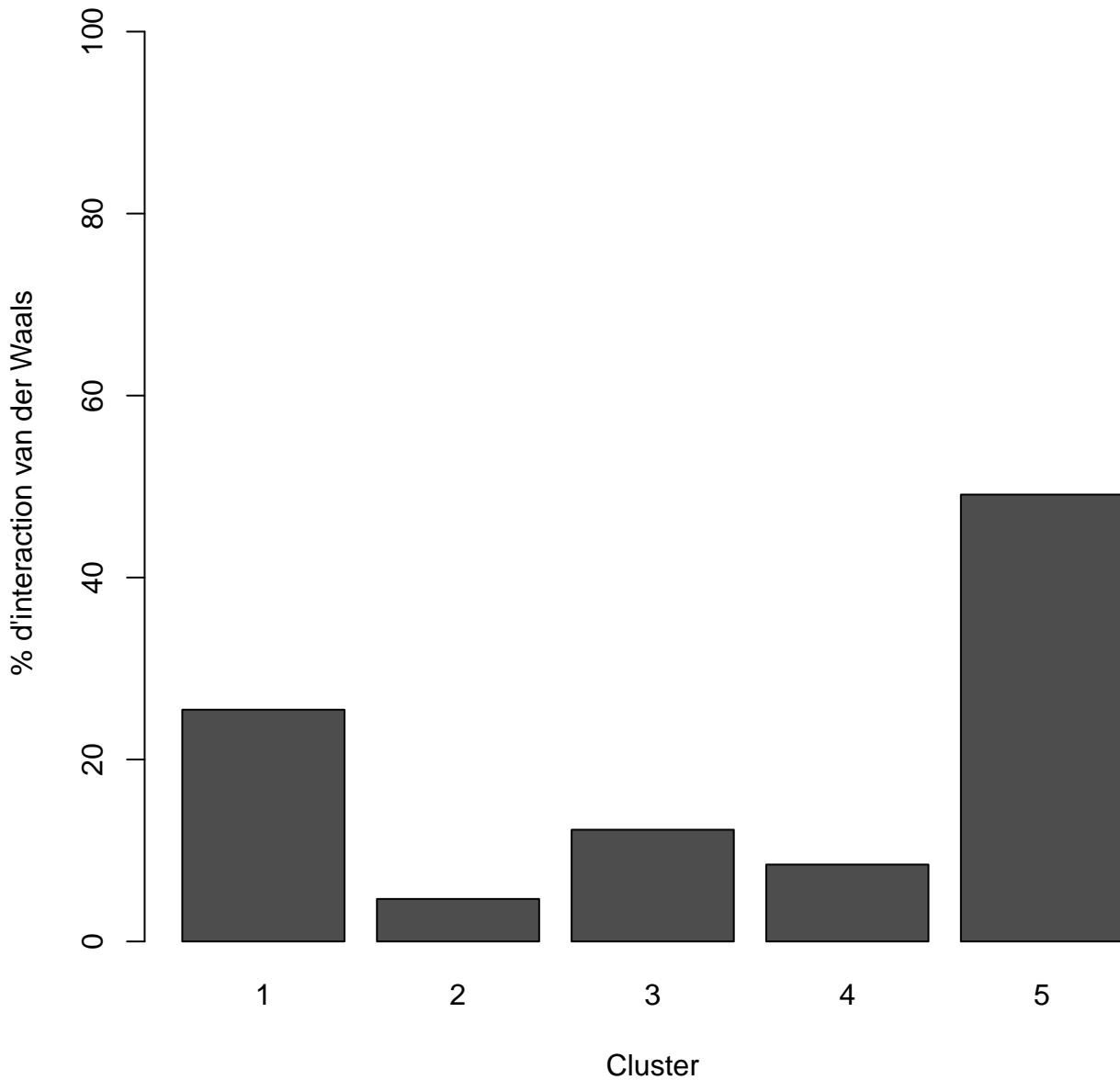
% d'interaction ionic Kmedoid



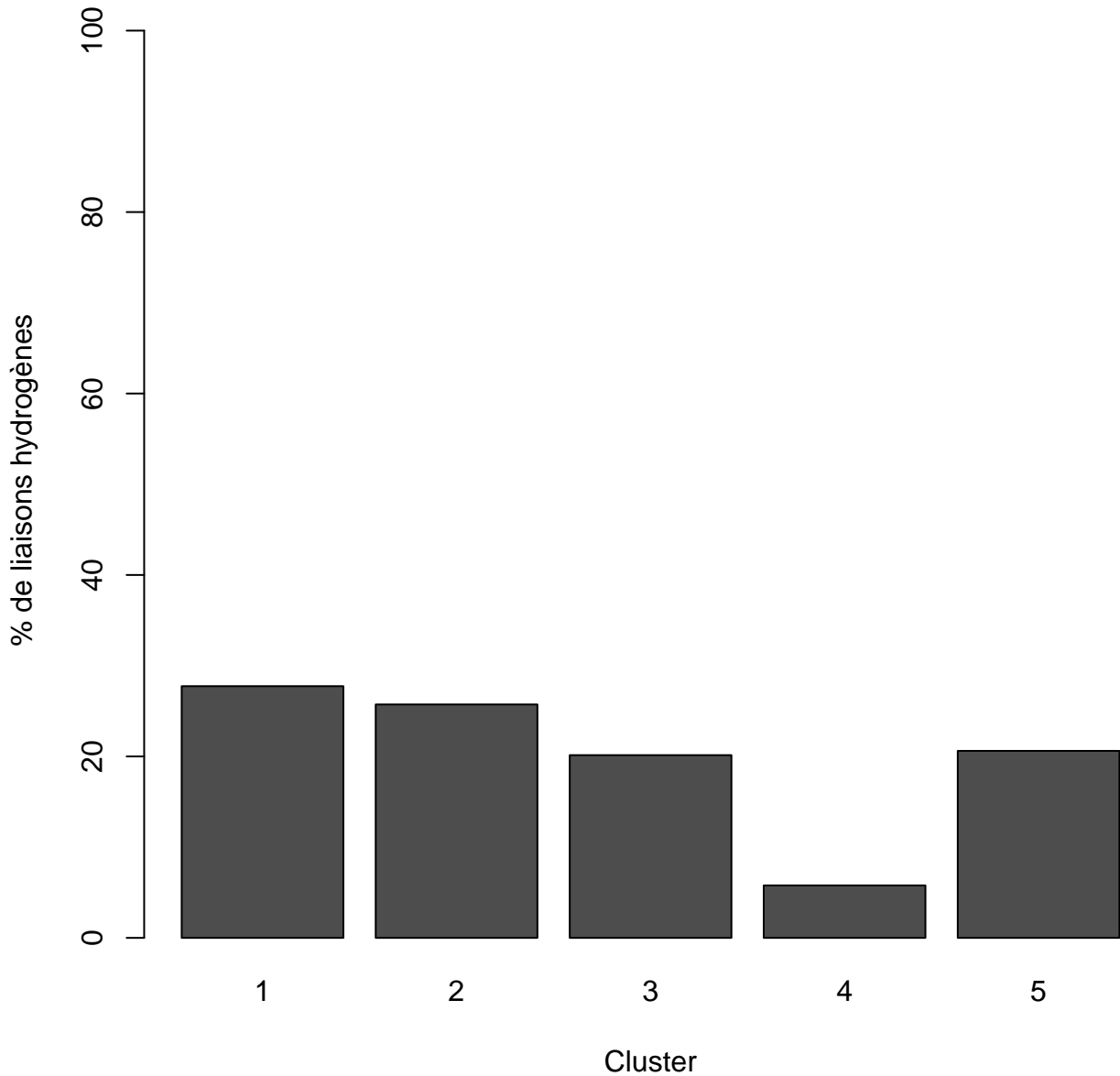
% d'interaction hydrophobic Kmedoid



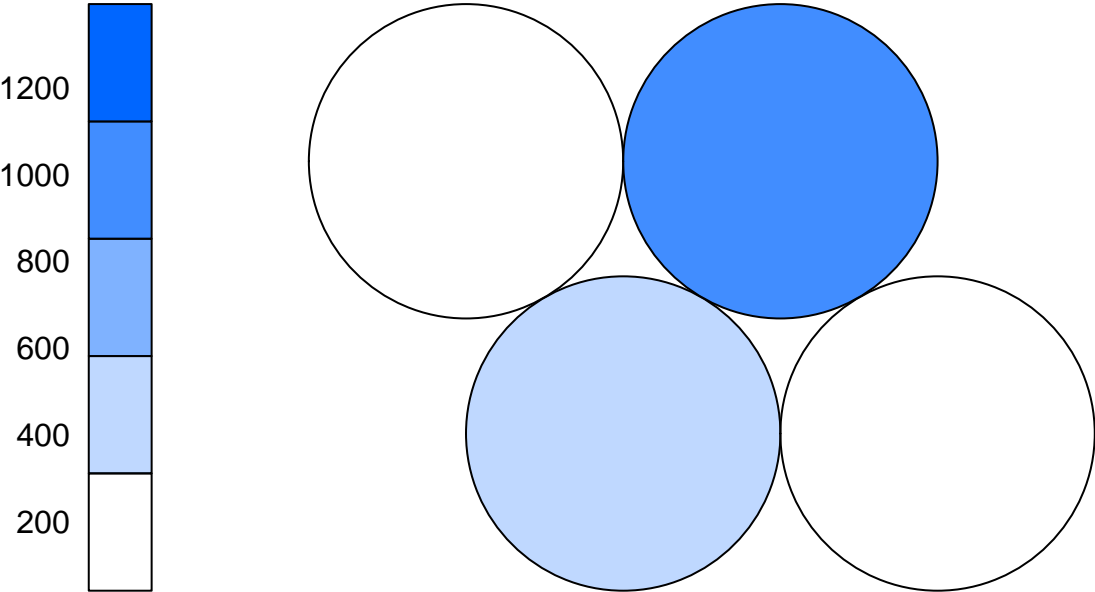
% d'interaction van der Waals Kmedoid



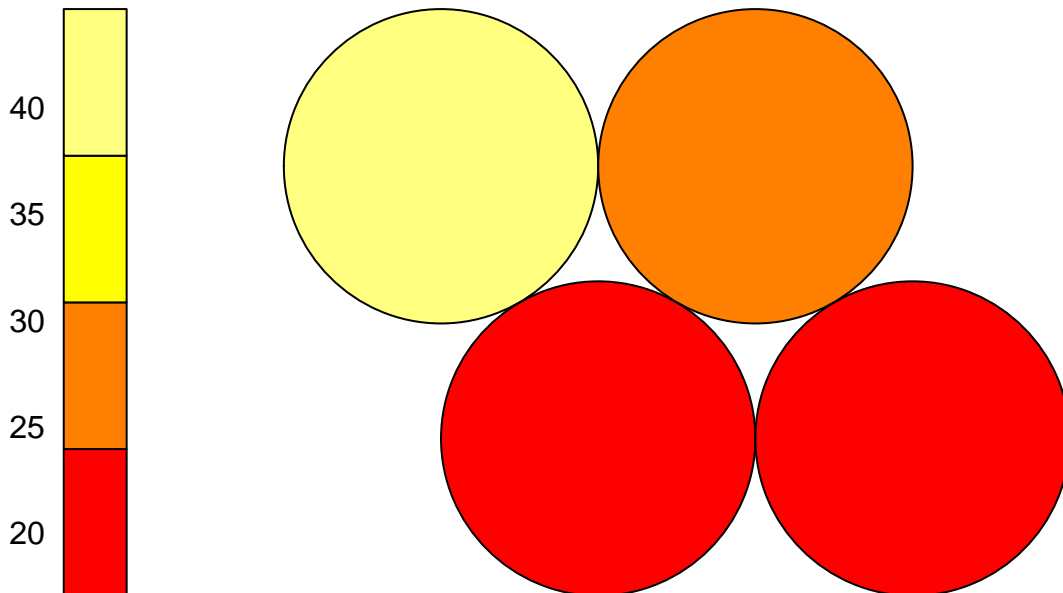
% de liaisons hydrogènes Kmedoid



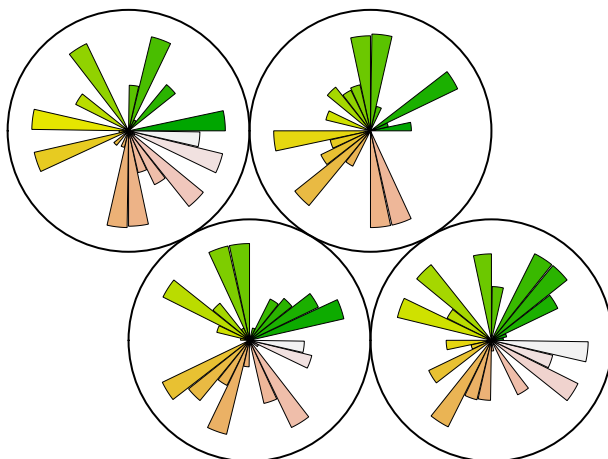
Carte de Kohonen n= 4































Neighbour distance plot

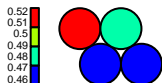


Codes plot

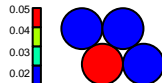


	H_ss		h_PB
	B_ss		i_PB
	E_ss		j_PB
	G_ss		k_PB
	T_ss		l_PB
	S_ss		m_PB
	ACC		n_PB
	a_PB		o_PB
	b_PB		p_PB
	c_PB		polar
	d_PB		ionic
	e_PB		hydrophobic
	f_PB		vdw
	g_PB		hydrogenB

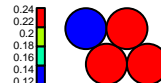
H_ss



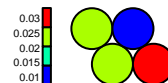
B_ss



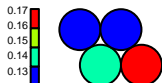
E_ss



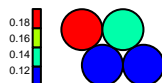
G_ss



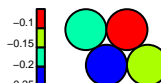
T_ss



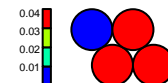
S_ss



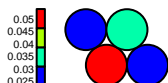
ACC



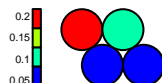
a_PB



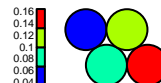
b_PB



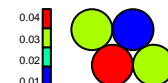
c_PB



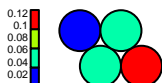
d_PB



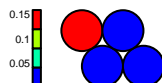
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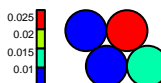
f_PB



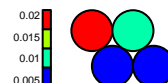
g_PB



h_PB



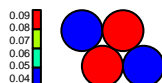
i_PB



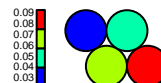
j_PB



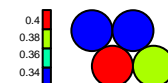
k_PB



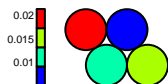
l_PB



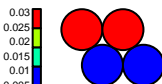
m_PB



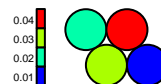
n_PB



o_PB



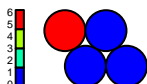
p_PB



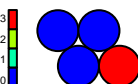
polar



ionic



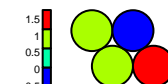
hydrophobic



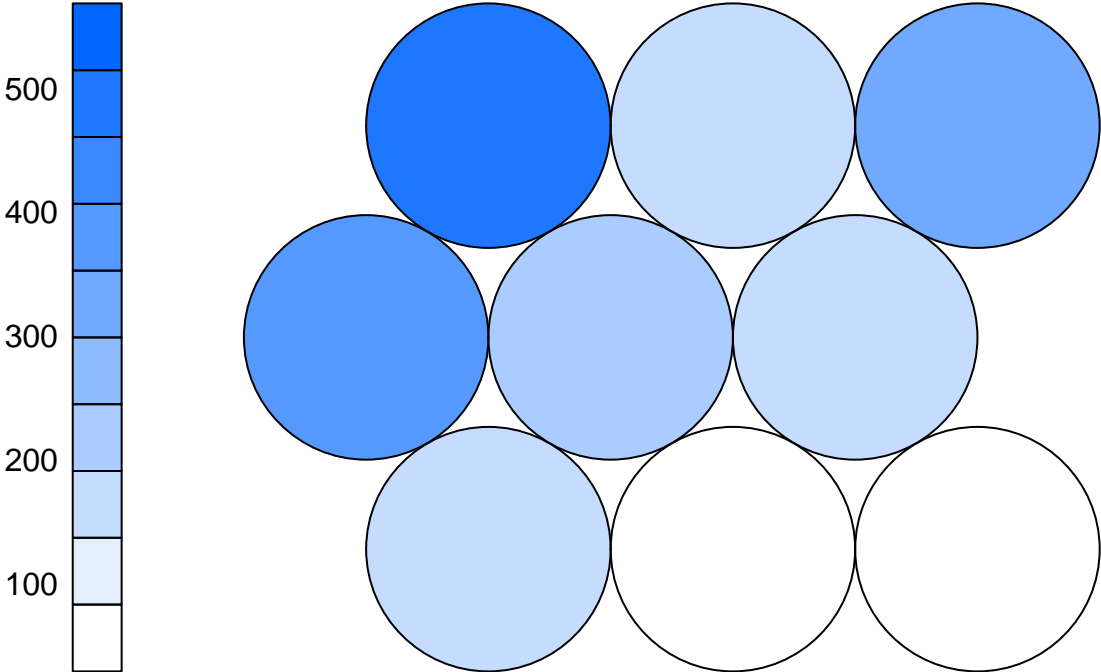
vdw



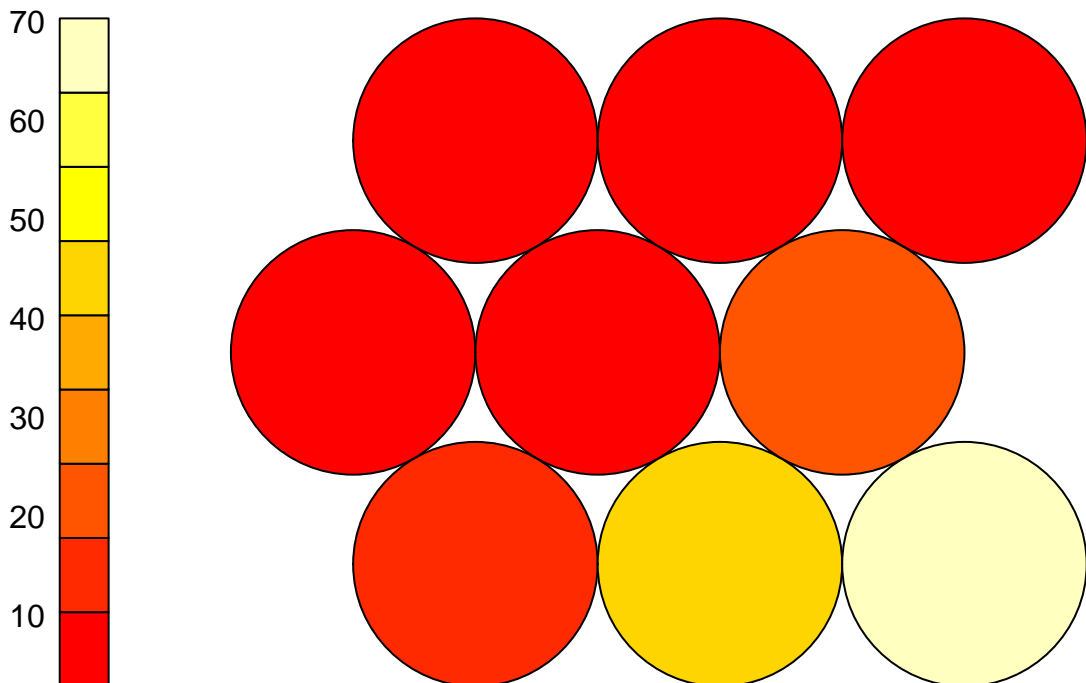
hydrogenB



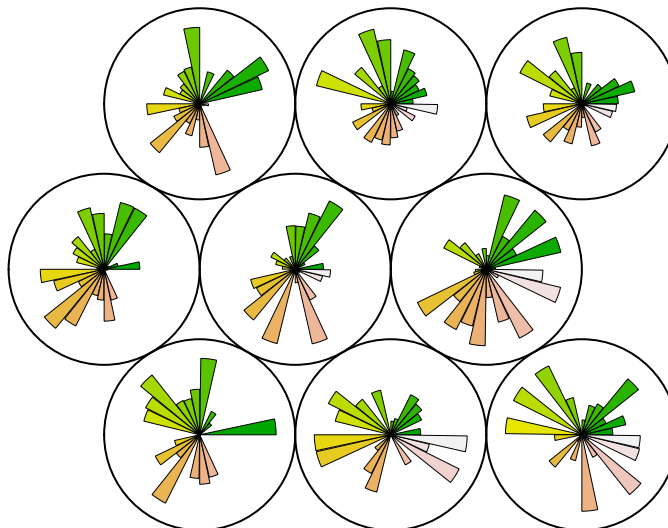
Carte de Kohonen n= 9



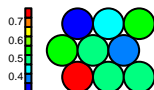
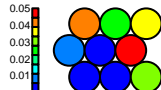
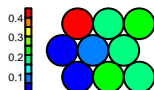
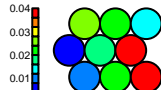
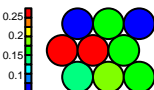
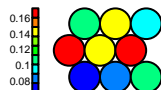
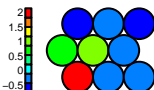
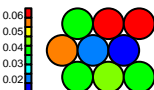
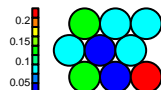
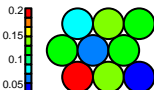
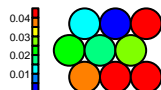
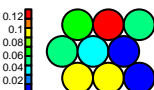
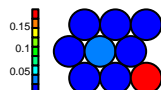
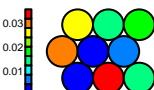
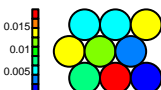
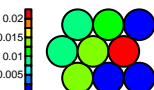
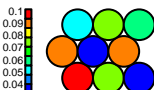
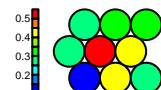
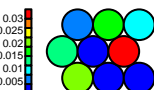
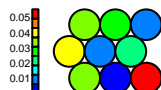
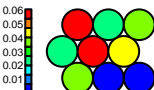
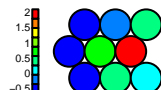
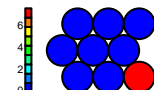
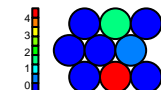
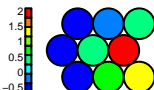
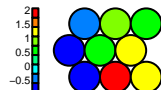
Neighbour distance plot



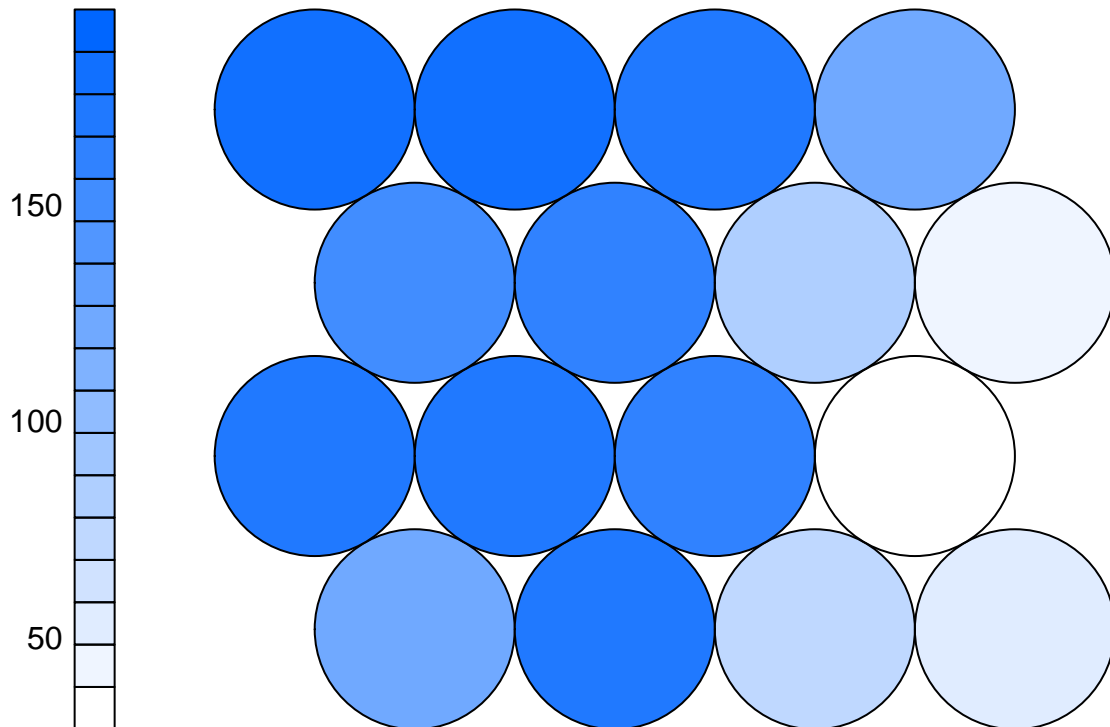
Codes plot



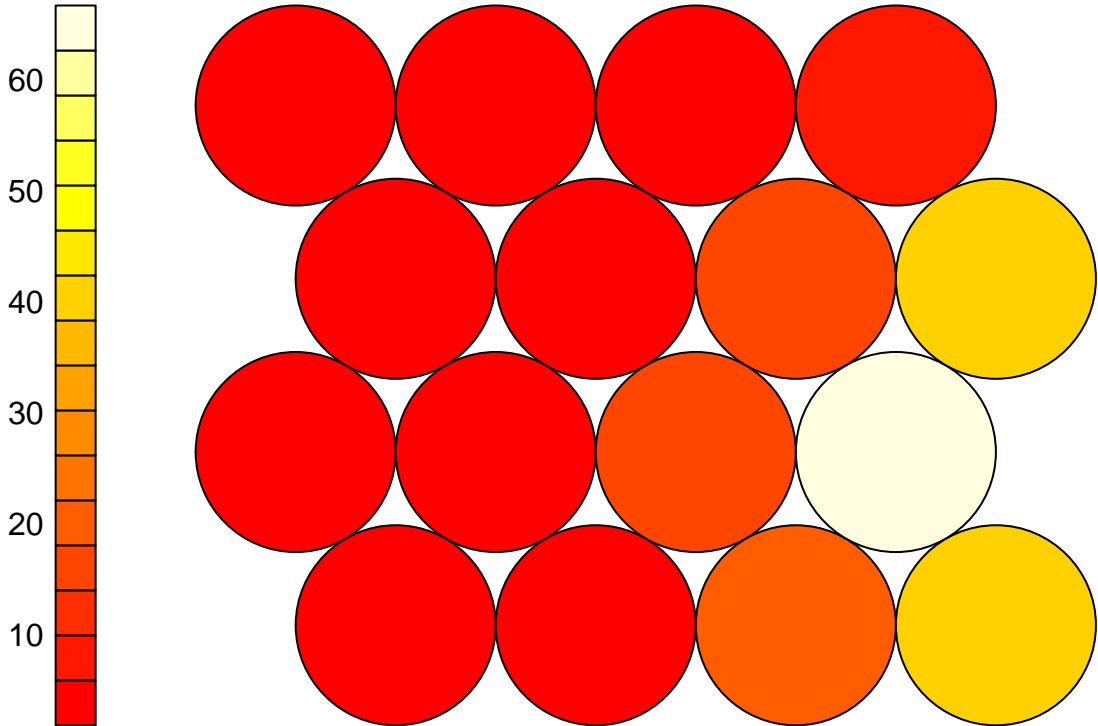
■ H_ss	■ h_PB
■ B_ss	■ i_PB
■ E_ss	■ j_PB
■ G_ss	■ k_PB
■ T_ss	■ l_PB
■ S_ss	■ m_PB
■ ACC	■ n_PB
■ a_PB	■ o_PB
■ b_PB	■ p_PB
■ c_PB	■ polar
■ d_PB	■ ionic
■ e_PB	■ hydrophobic
■ f_PB	■ vdw
■ g_PB	■ hydrogenB

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**

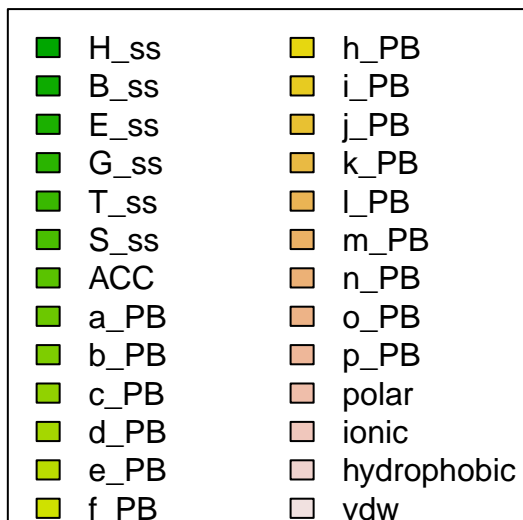
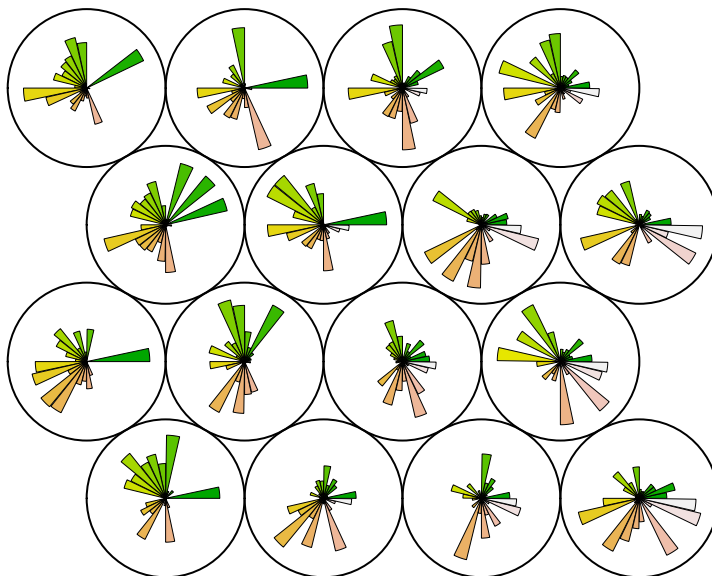
Carte de Kohonen n= 16

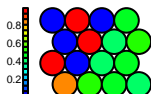
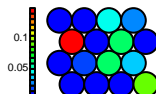
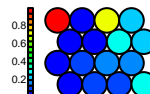
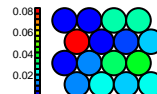
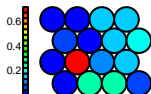
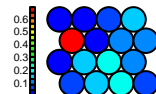
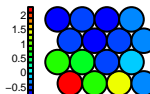
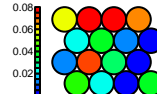
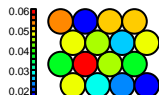
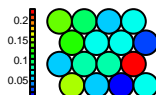
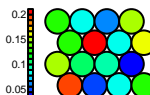
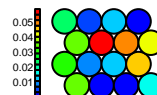
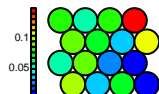
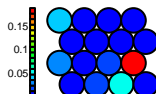
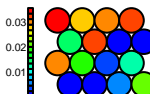
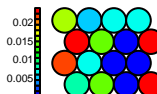
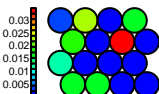
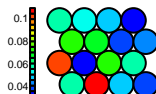
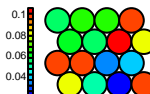
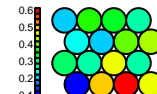
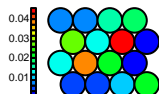
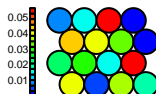
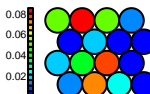
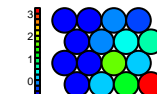
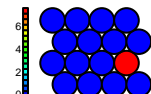
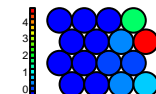
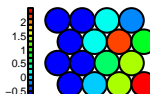
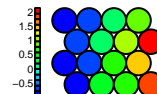


Neighbour distance plot

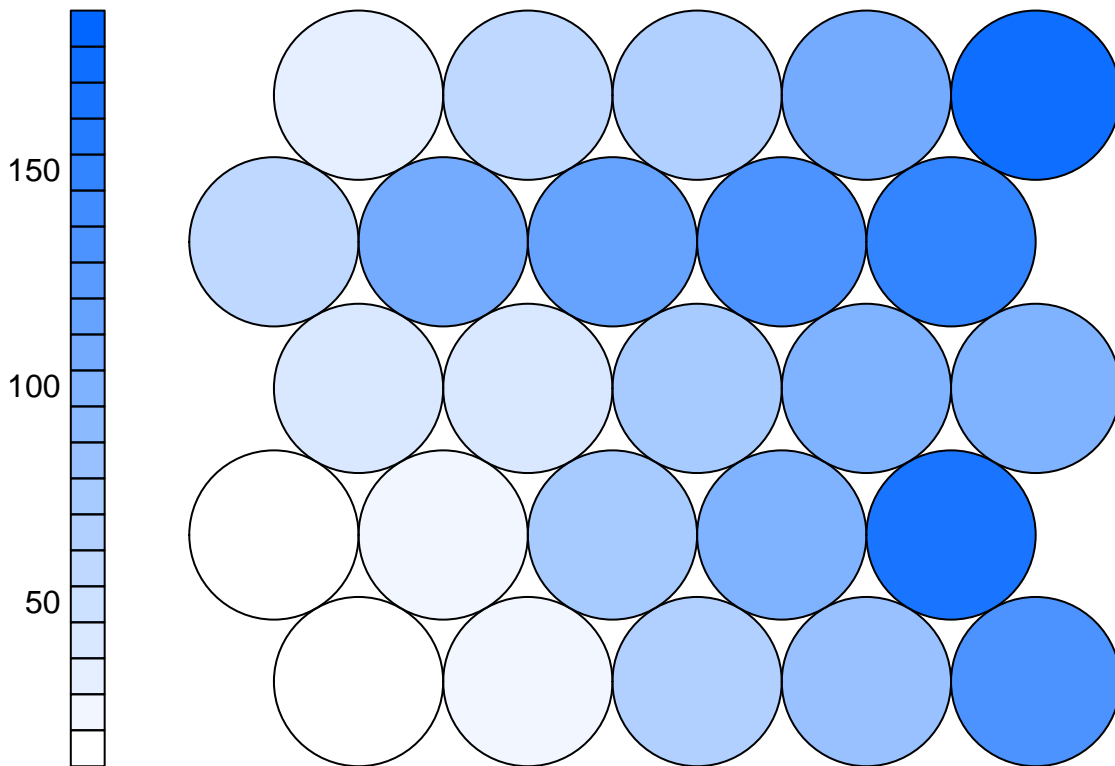


Codes plot

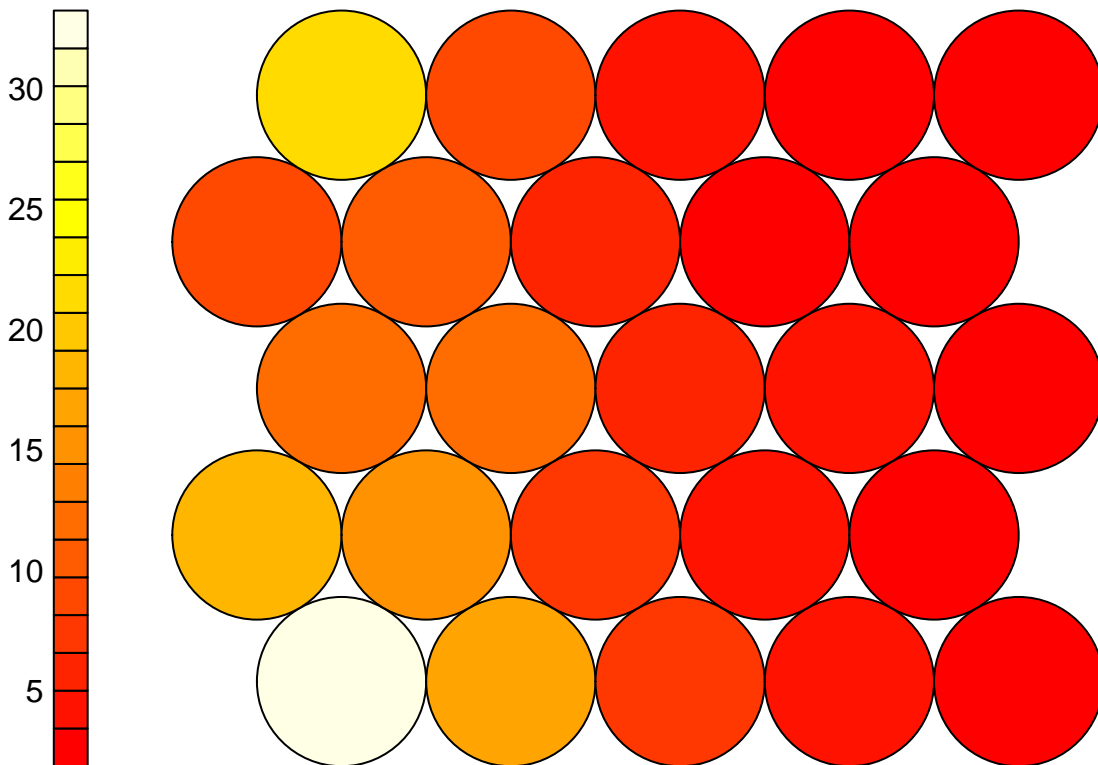


H_ss**B_ss****E_ss****G_ss****T_ss****S_ss****ACC****a_PB****b_PB****c_PB****d_PB****e_PB****f_PB****g_PB****h_PB****i_PB****j_PB****k_PB****l_PB****m_PB****n_PB****o_PB****p_PB****polar****ionic****hydrophobic****vdw****hydrogenB**

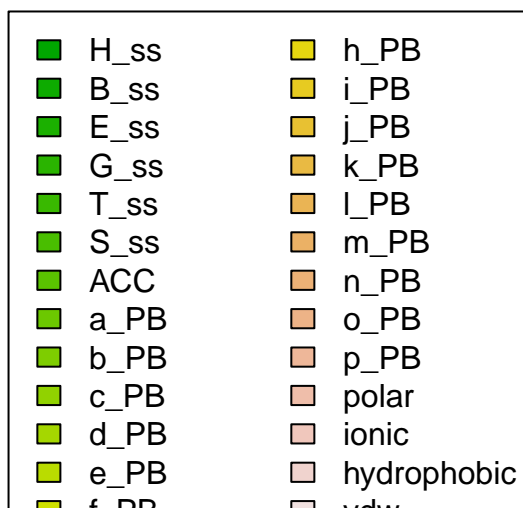
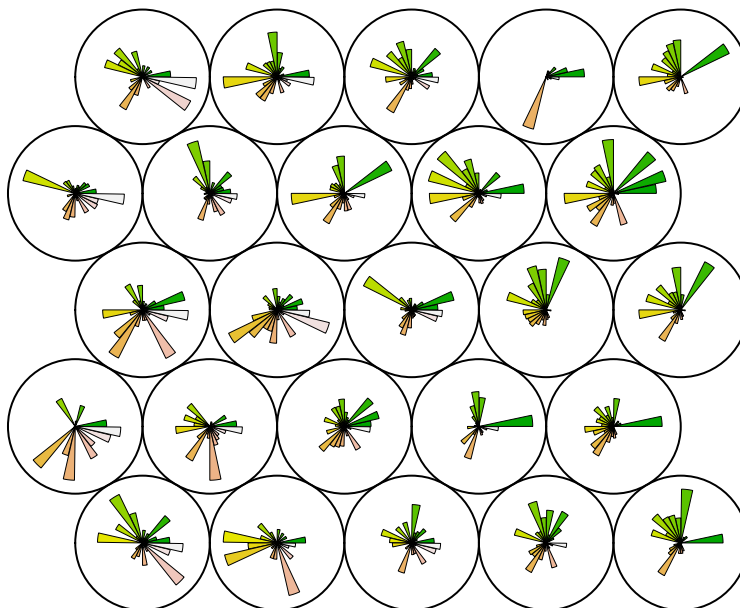
Carte de Kohonen n= 25



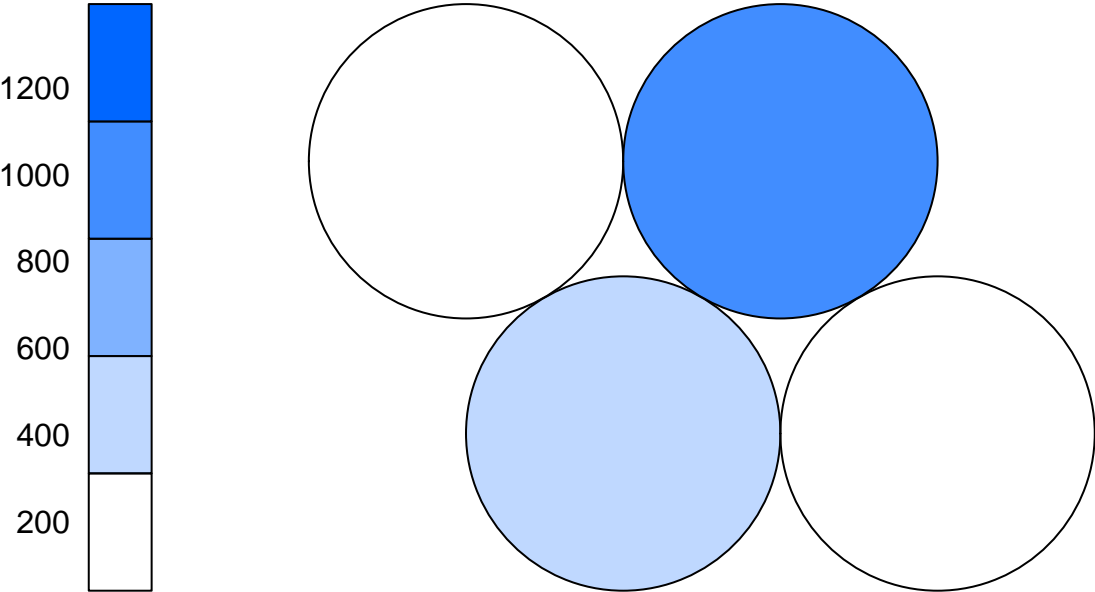
Neighbour distance plot



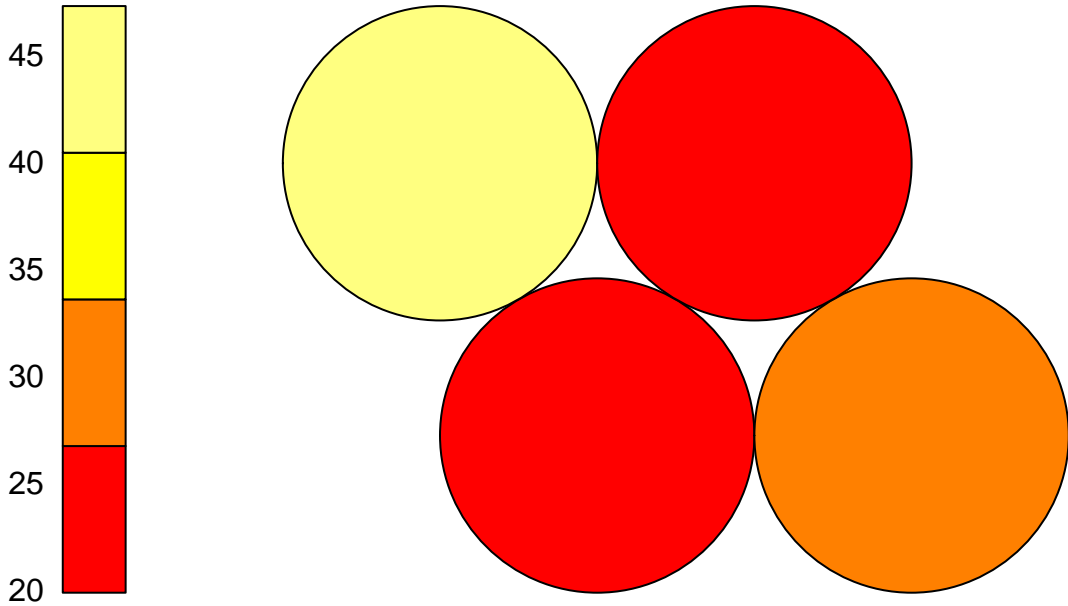
Codes plot



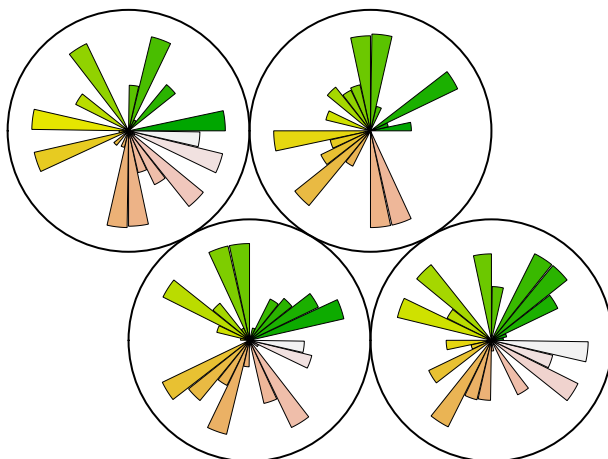
Carte de Kohonen toroidal n= 4































Neighbour distance plot

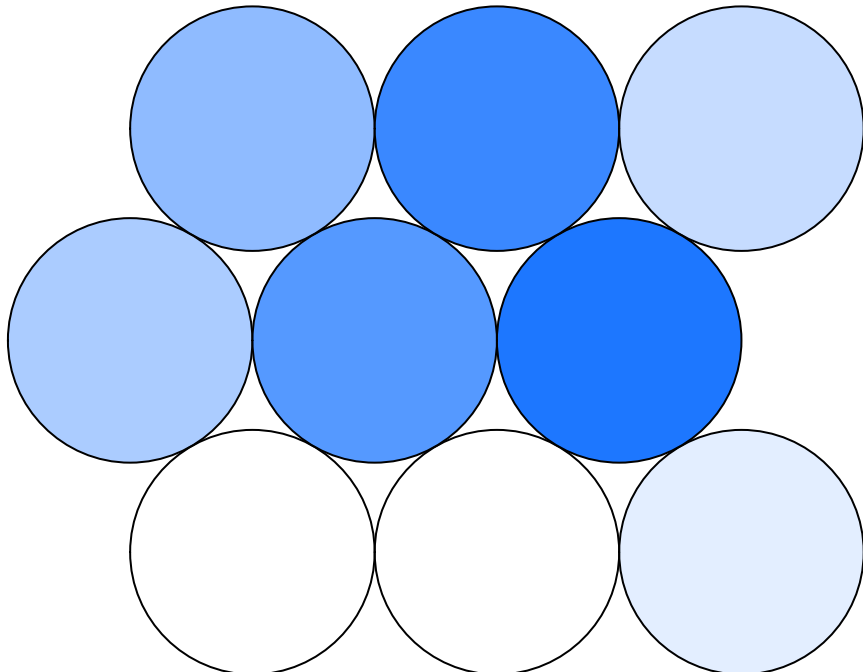
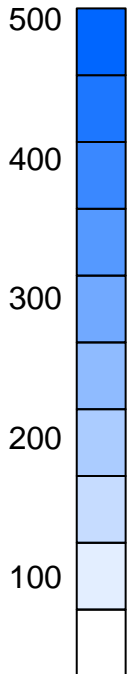


Codes plot

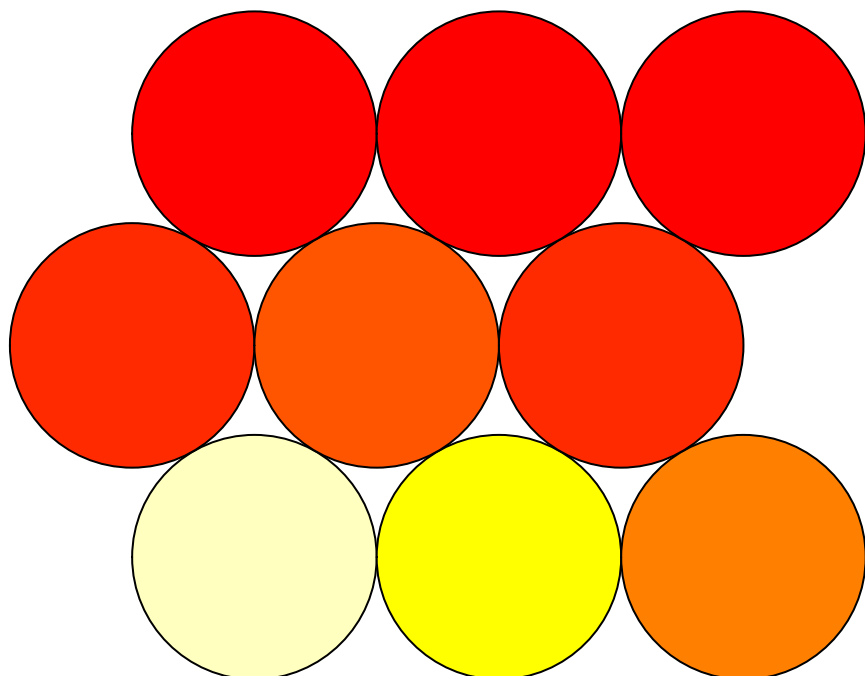
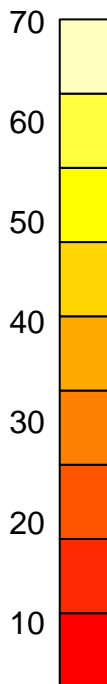


	H_ss		h_PB
	B_ss		i_PB
	E_ss		j_PB
	G_ss		k_PB
	T_ss		l_PB
	S_ss		m_PB
	ACC		n_PB
	a_PB		o_PB
	b_PB		p_PB
	c_PB		polar
	d_PB		ionic
	e_PB		hydrophobic
	f_PB		vdw
	g_PB		hydrogenB

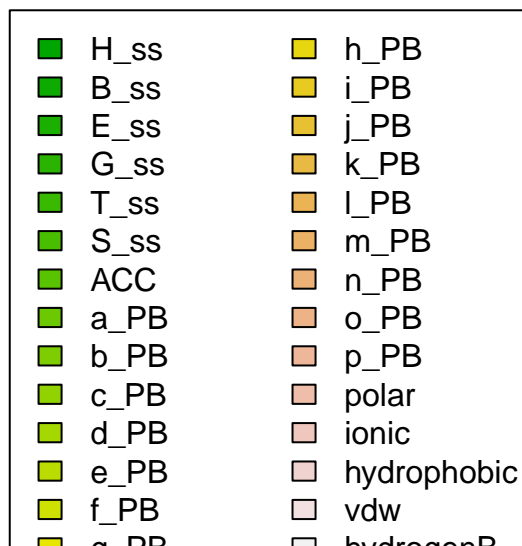
Carte de Kohonen toroidal n= 9



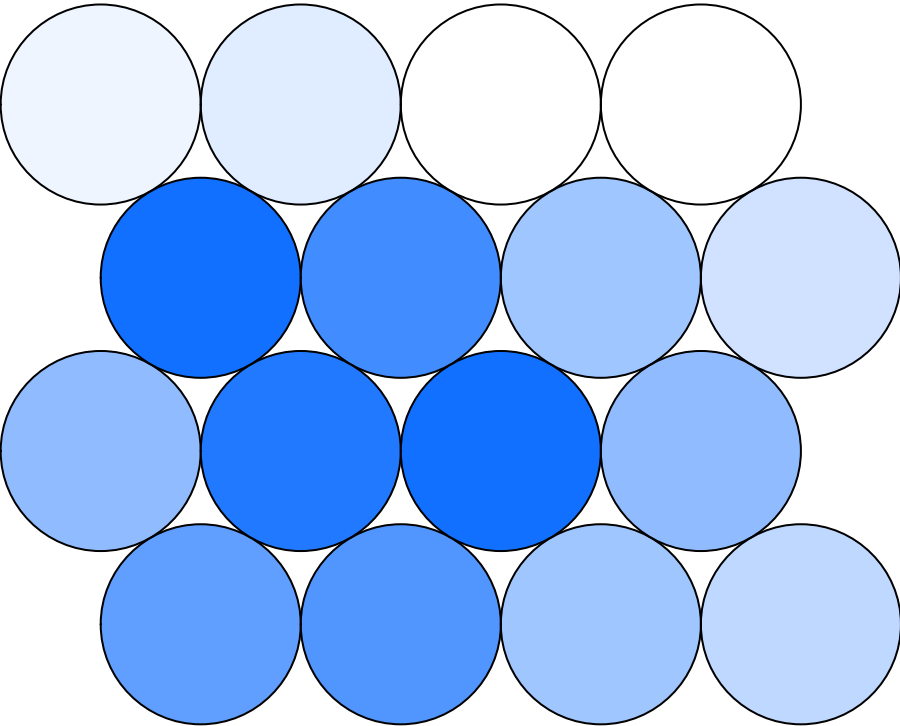
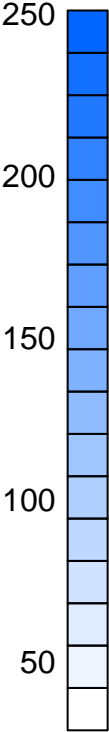
Neighbour distance plot



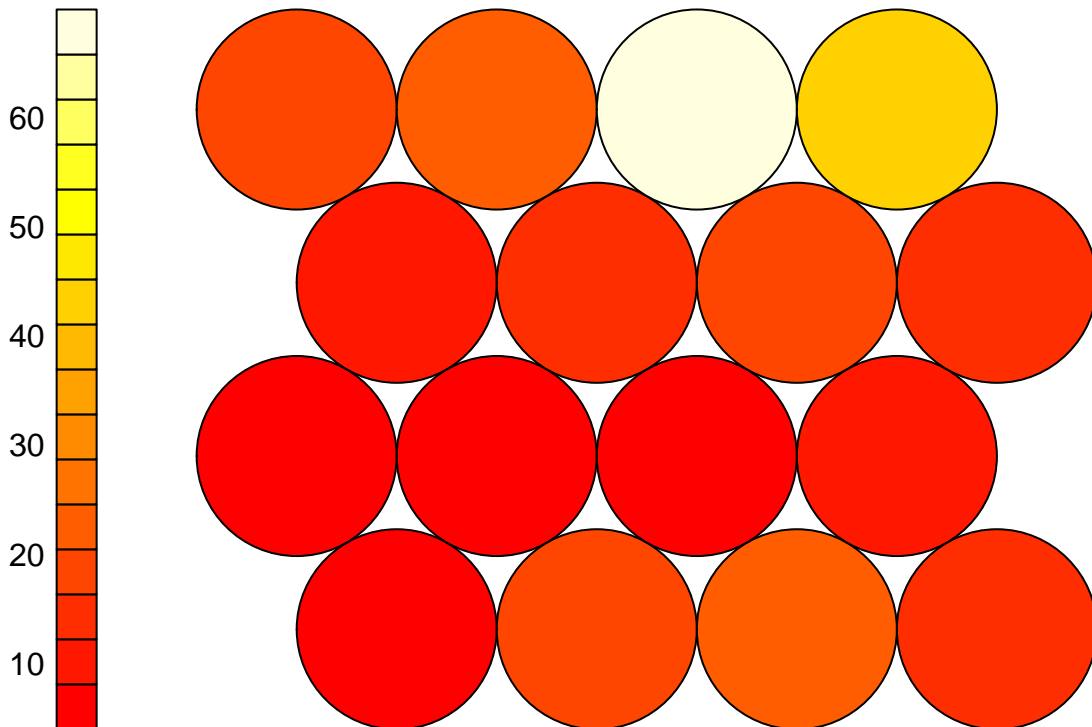
Codes plot



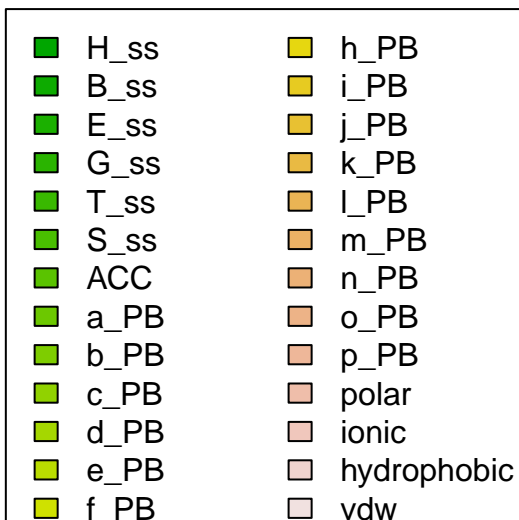
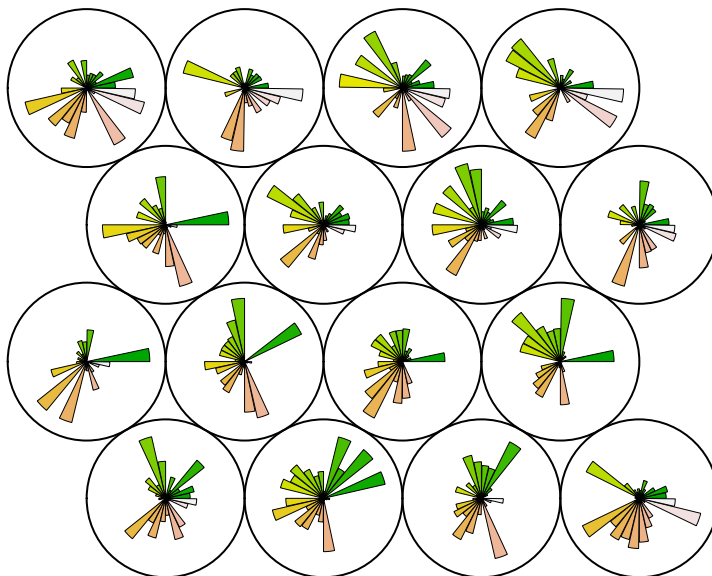
Carte de Kohonen toroidal n= 16



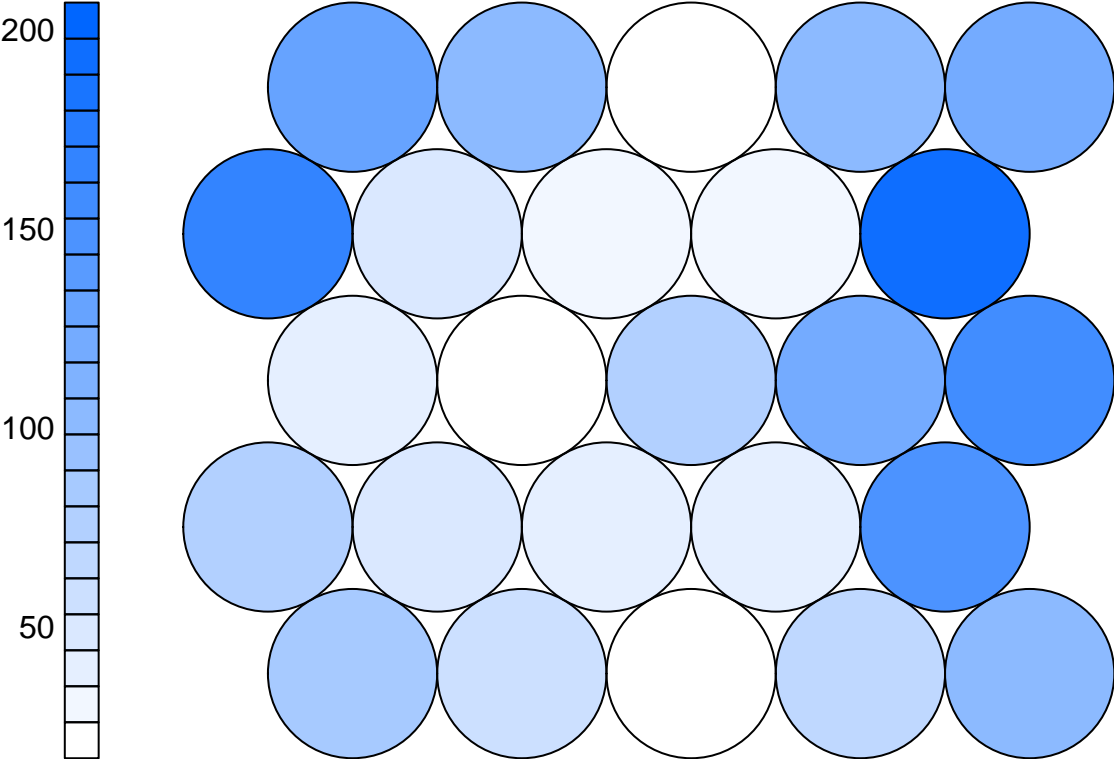
Neighbour distance plot



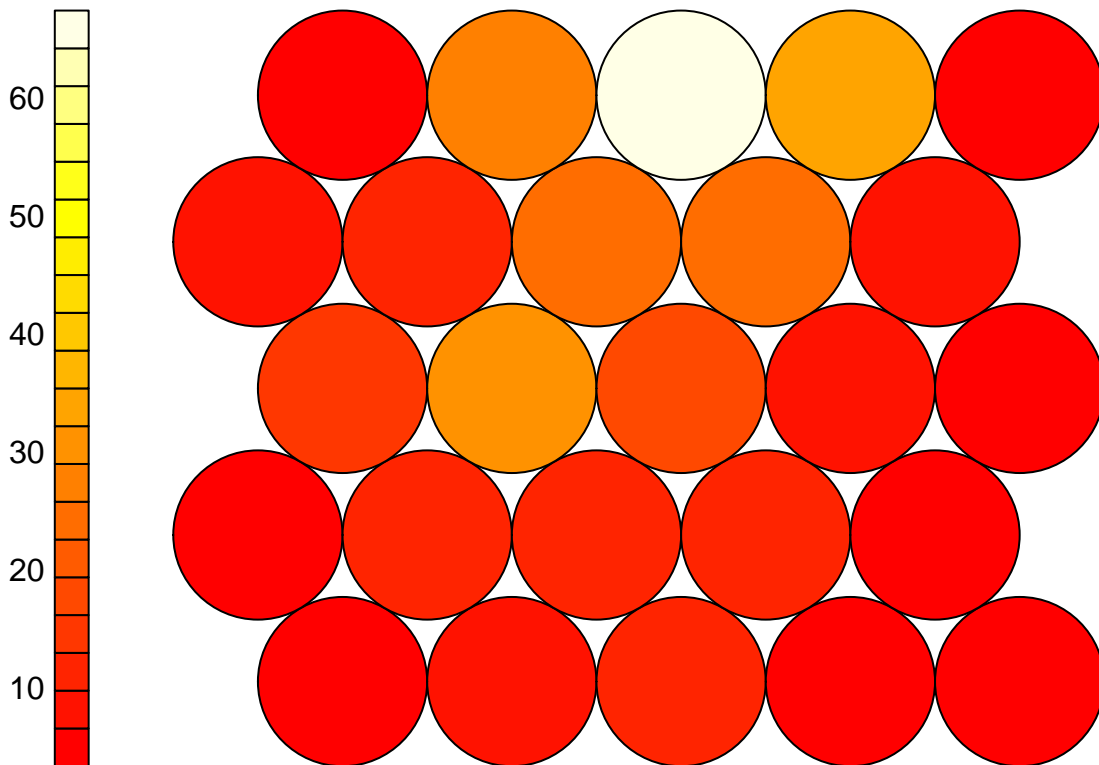
Codes plot



Carte de Kohonen toroidal n= 25



Neighbour distance plot



Codes plot

