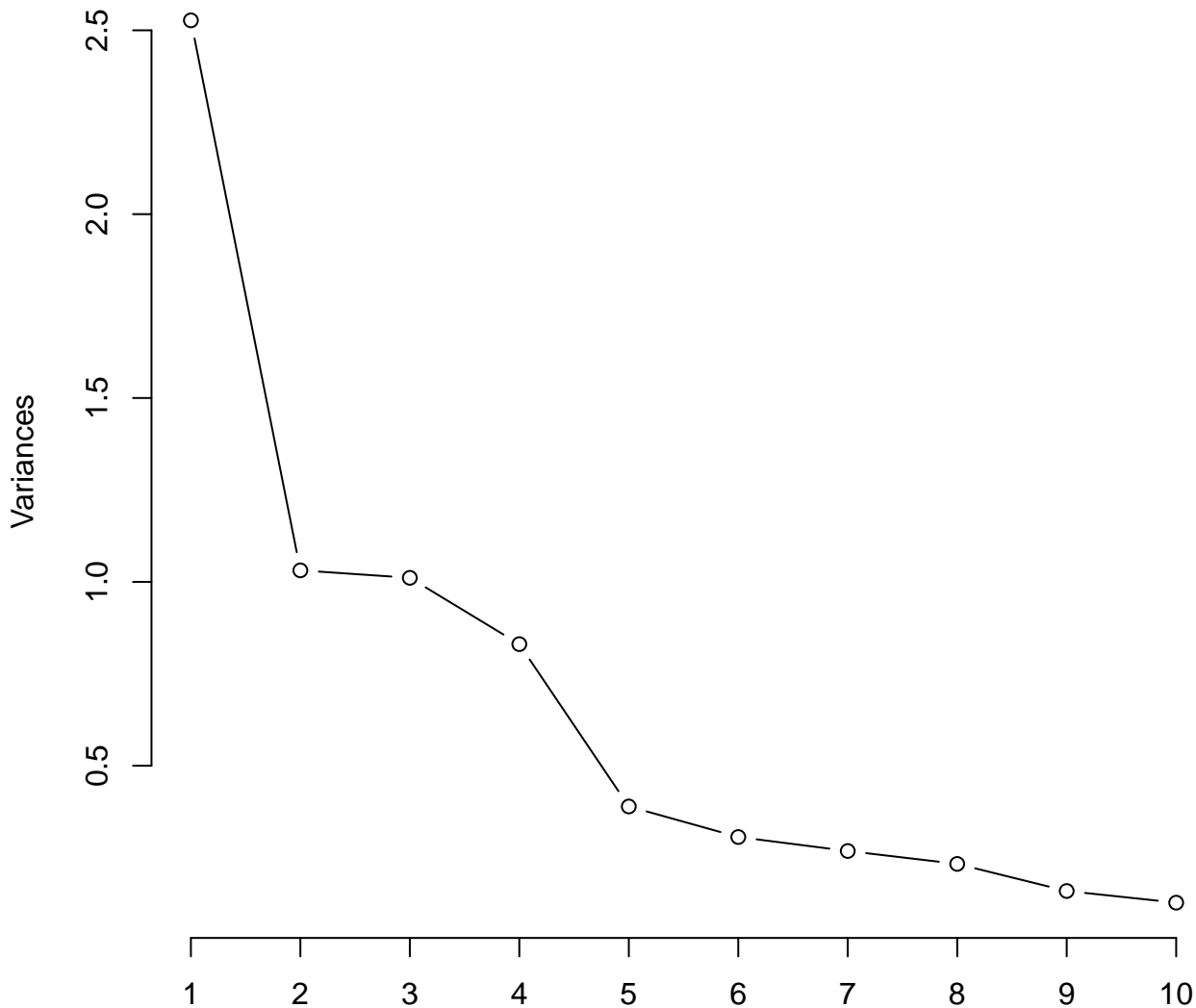
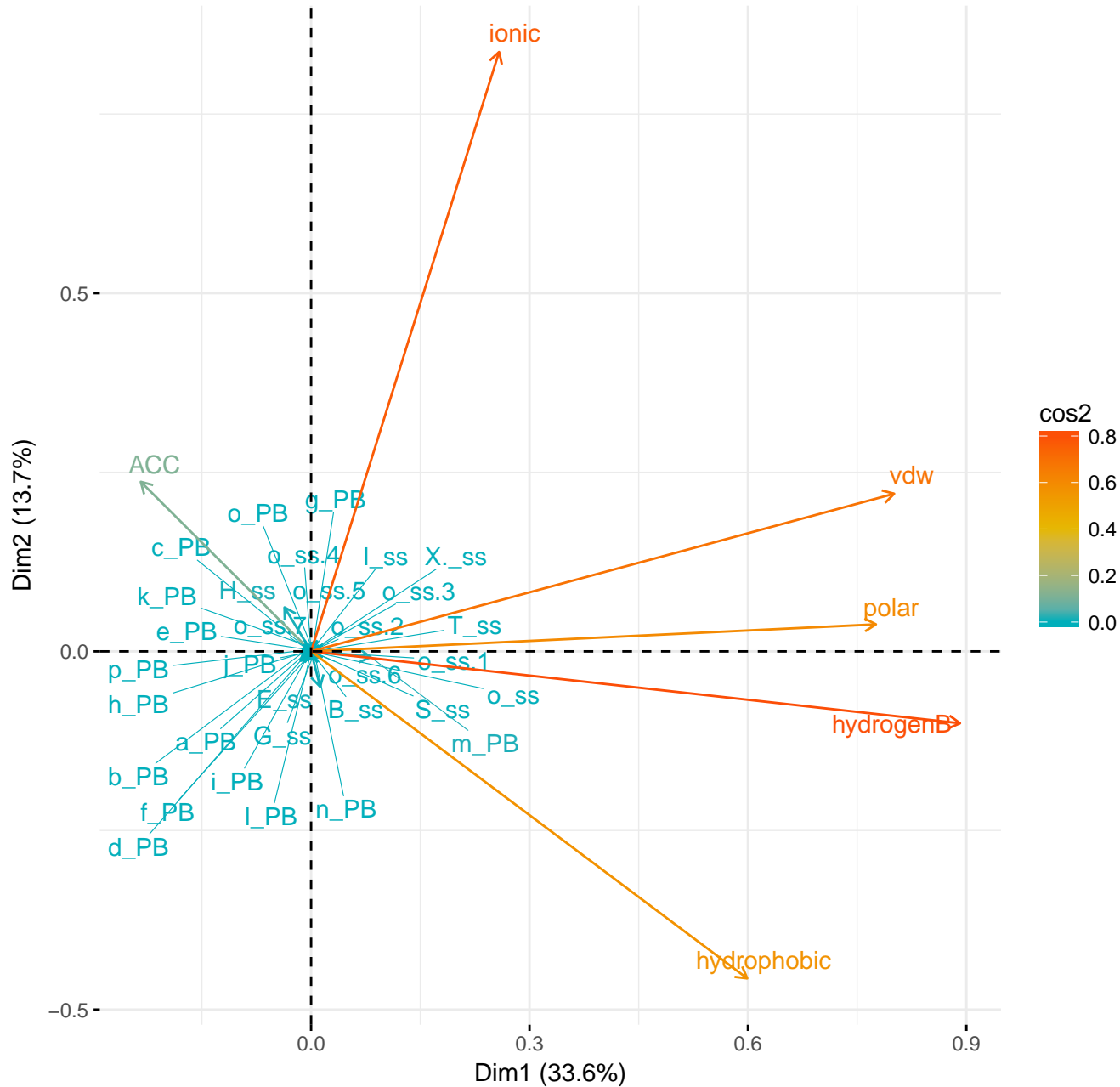


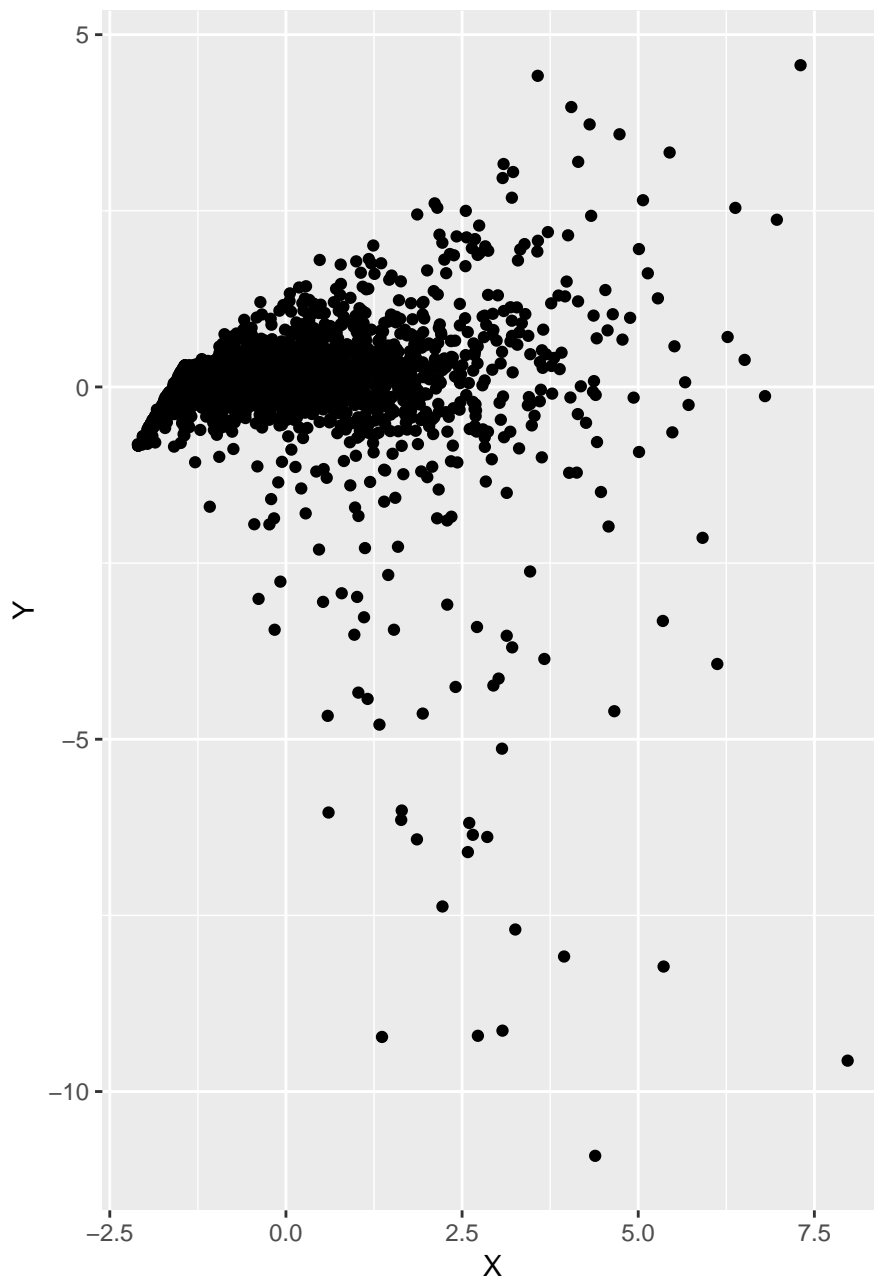
Variances en fonction des Composantes Principales



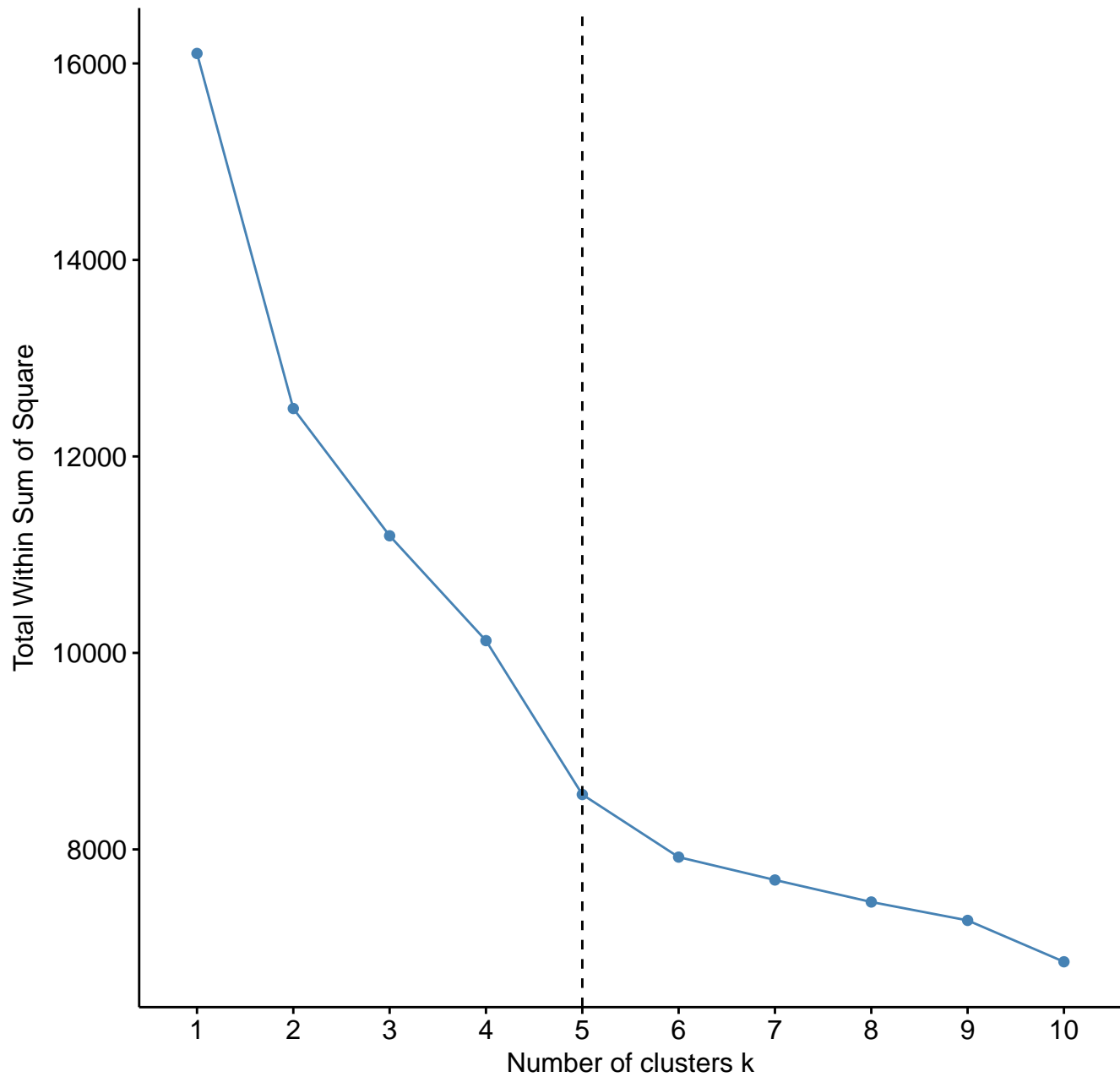
Variables – PCA



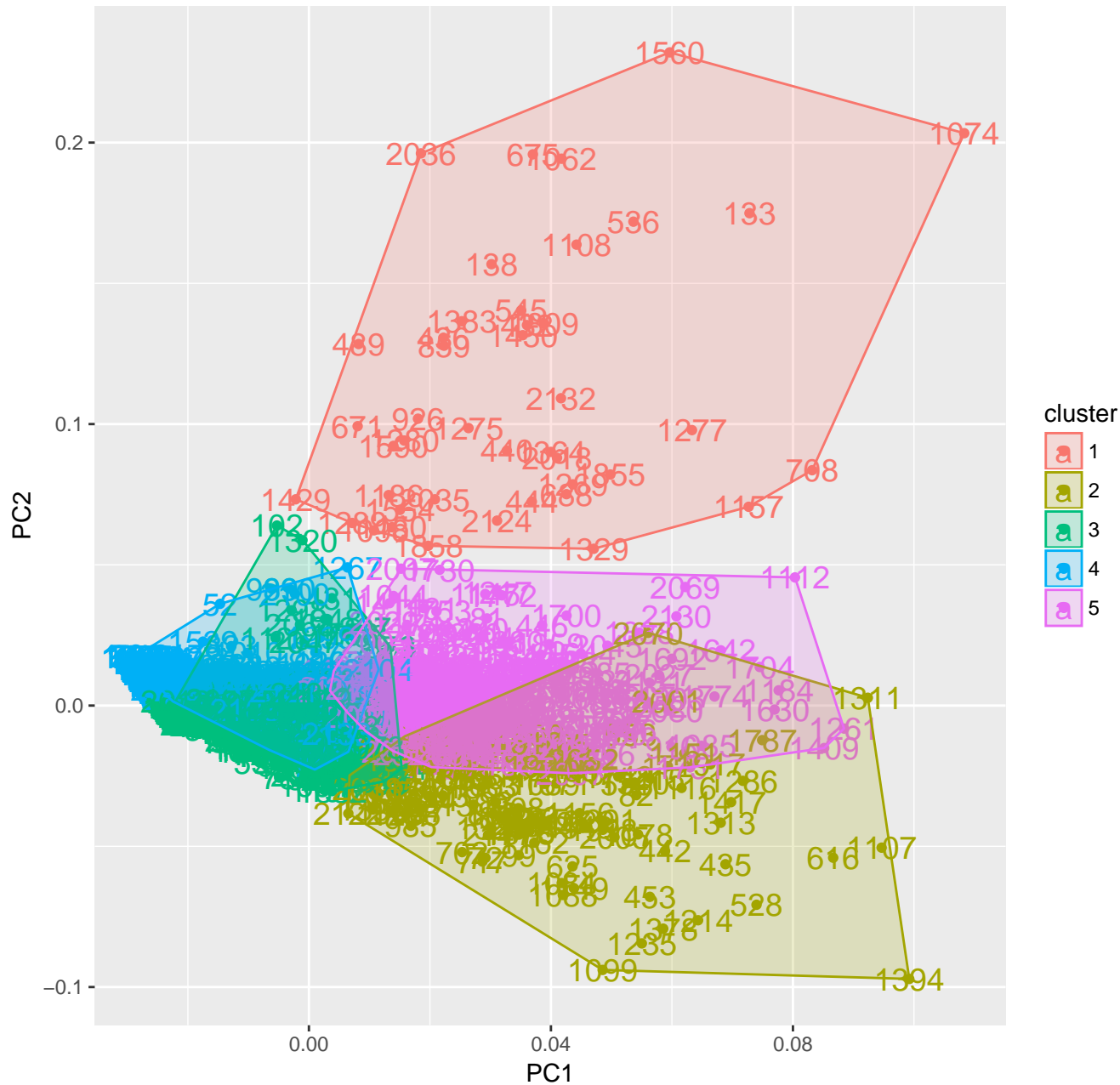
MDS with Shephard–Kruskal Stress 0.6



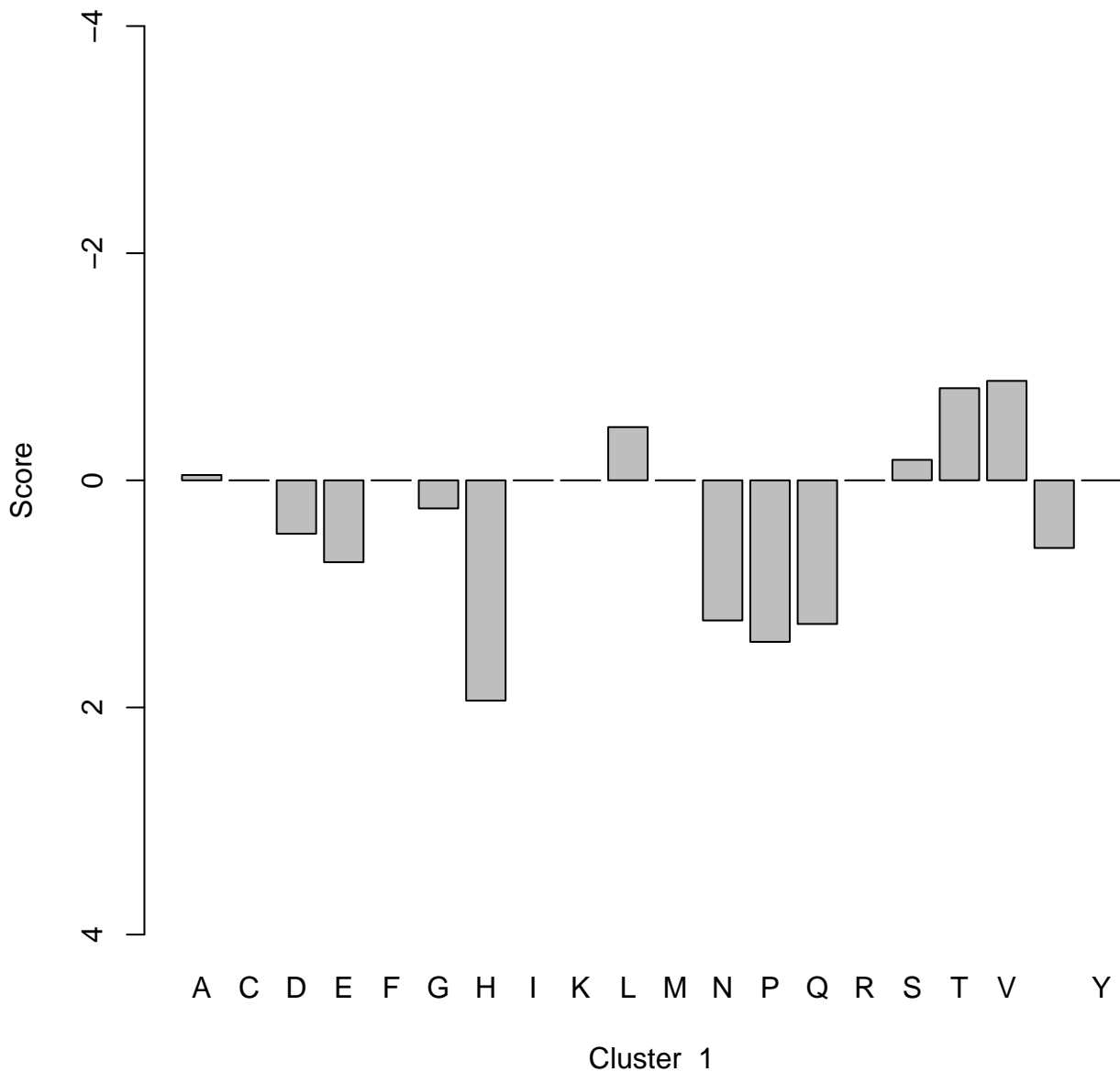
Optimal number of clusters



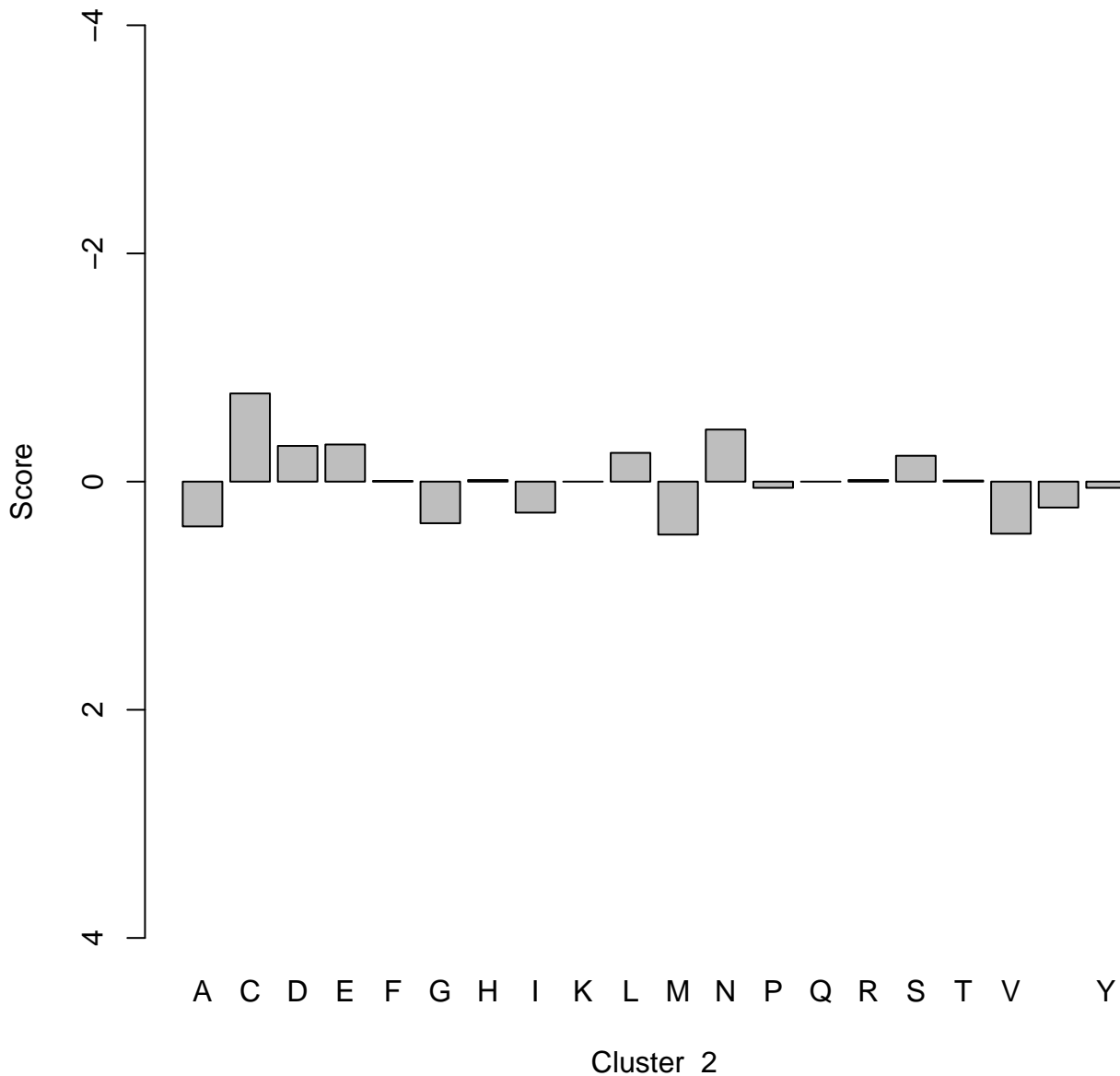
Clustering par Kmeans



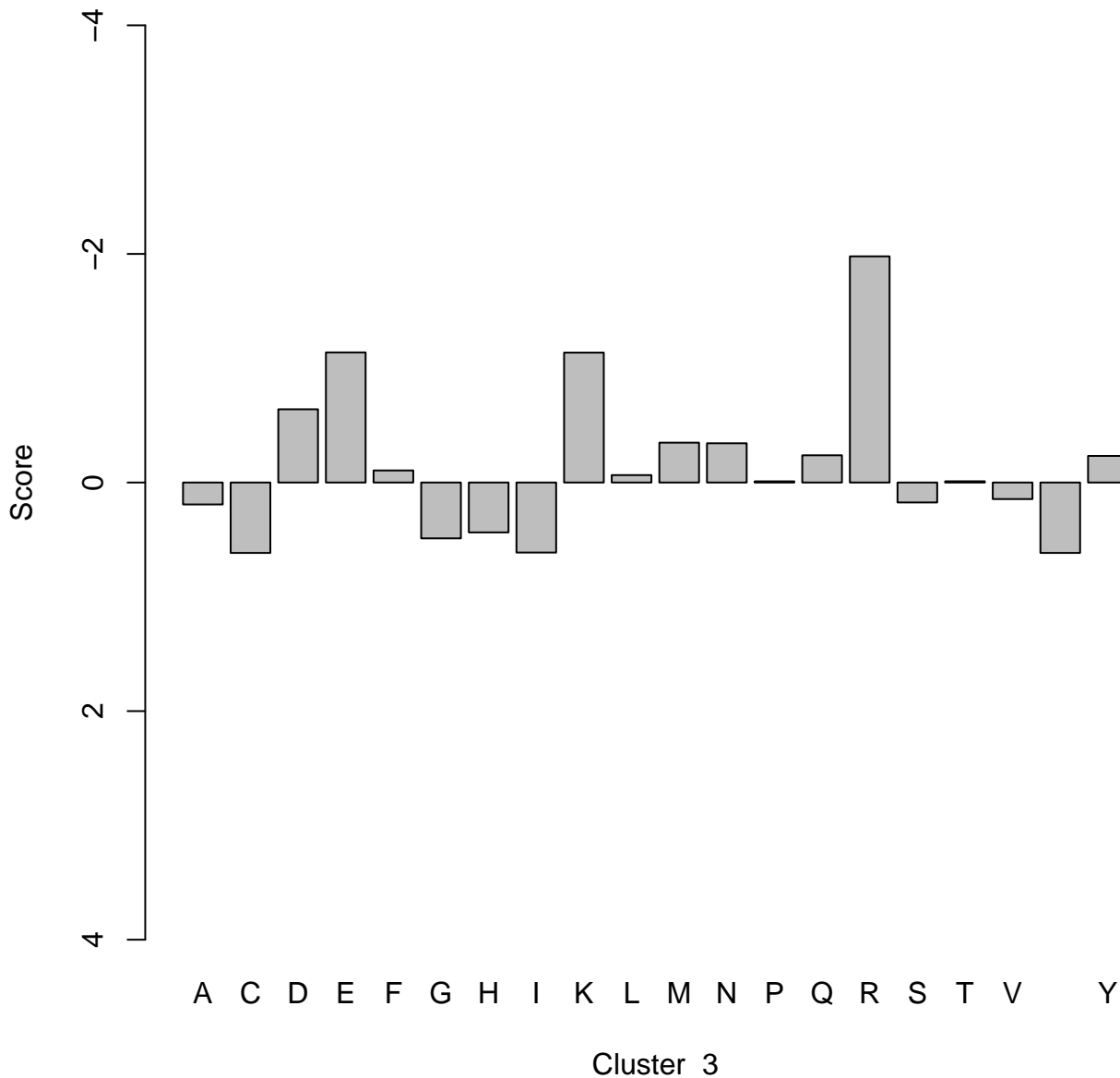
Distribution des scores (Méthodes Kmeans)



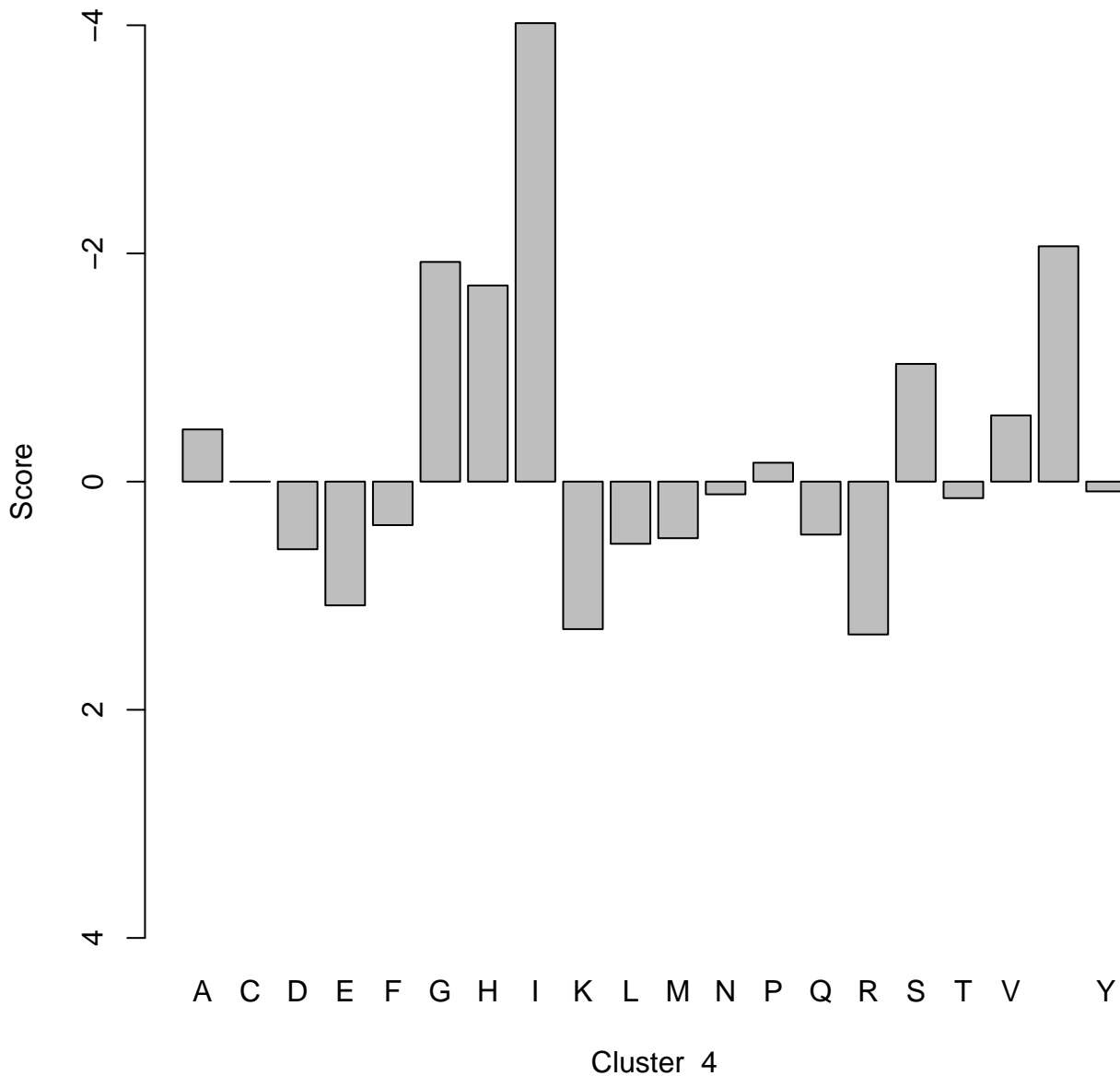
Distribution des scores (Méthodes Kmeans)



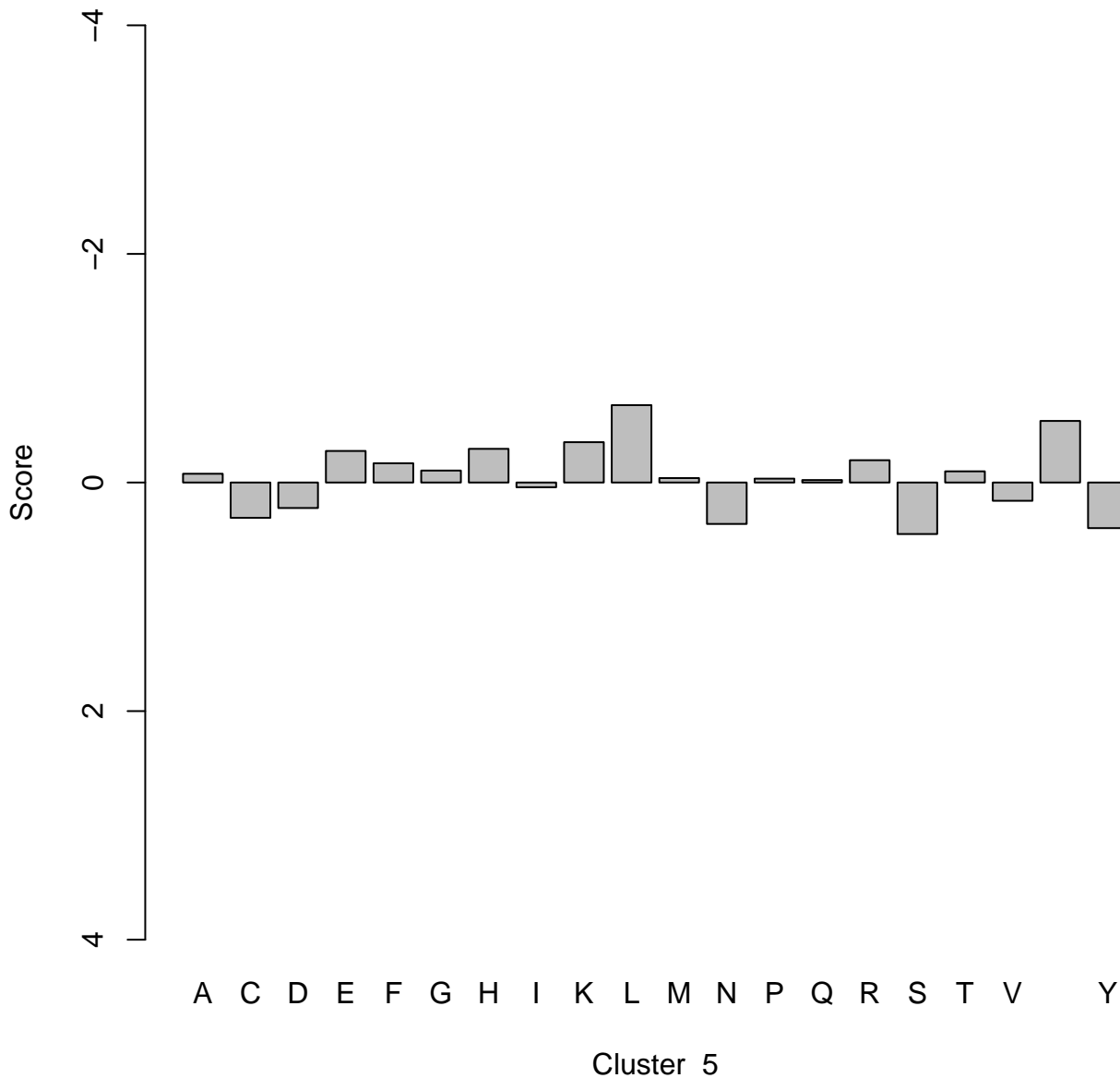
Distribution des scores (Méthodes Kmeans)



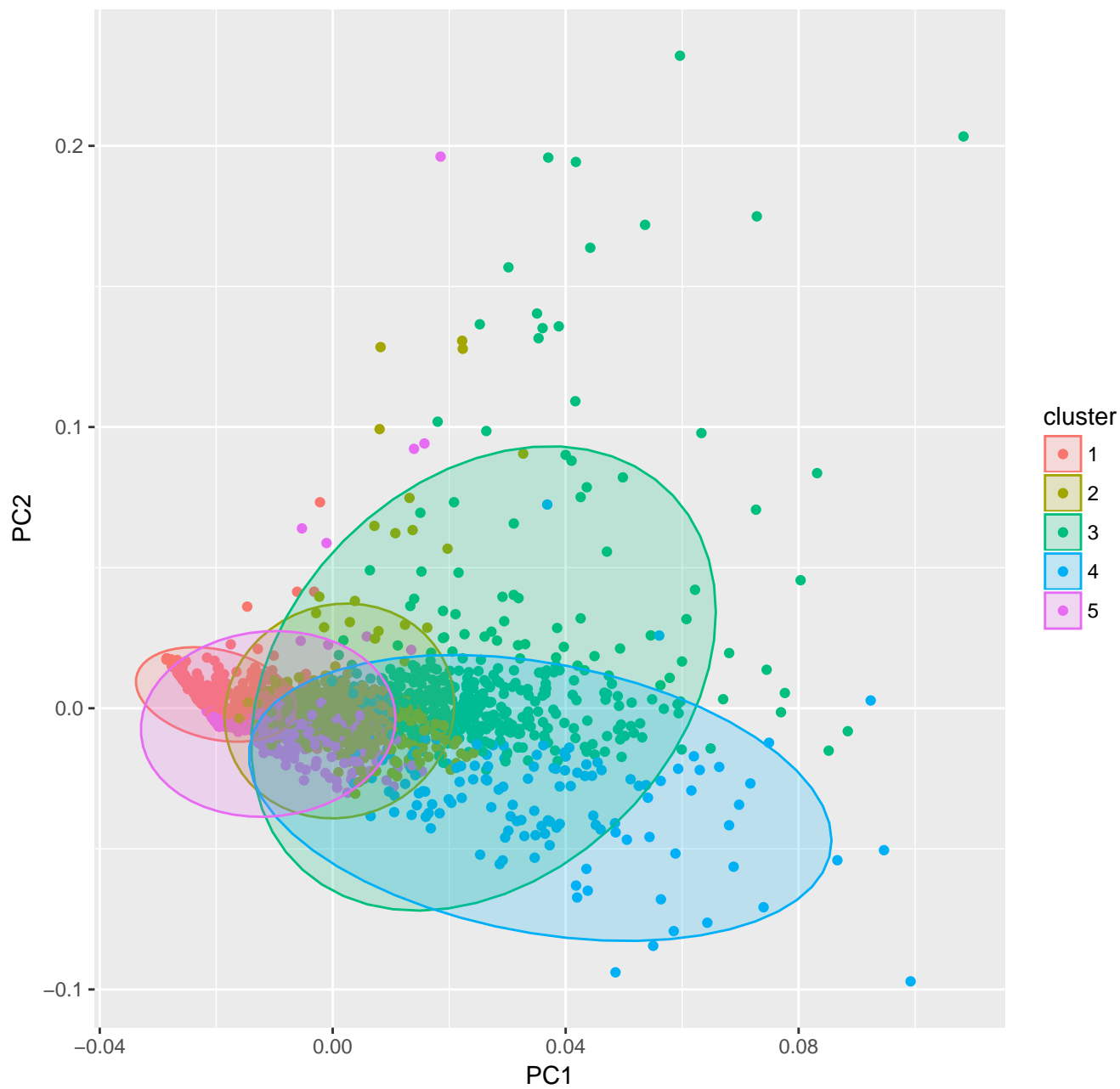
Distribution des scores (Méthodes Kmeans)



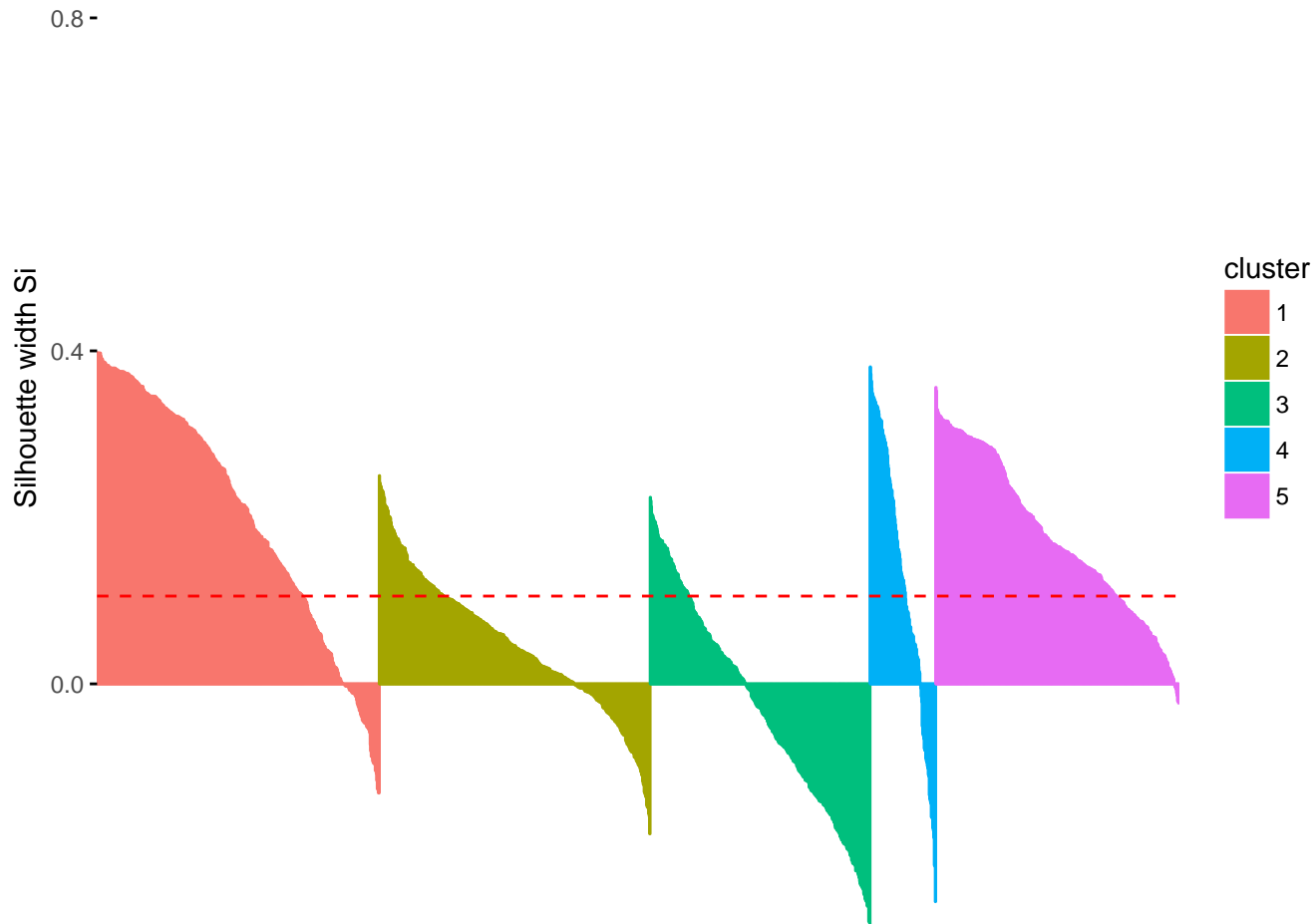
Distribution des scores (Méthodes Kmeans)



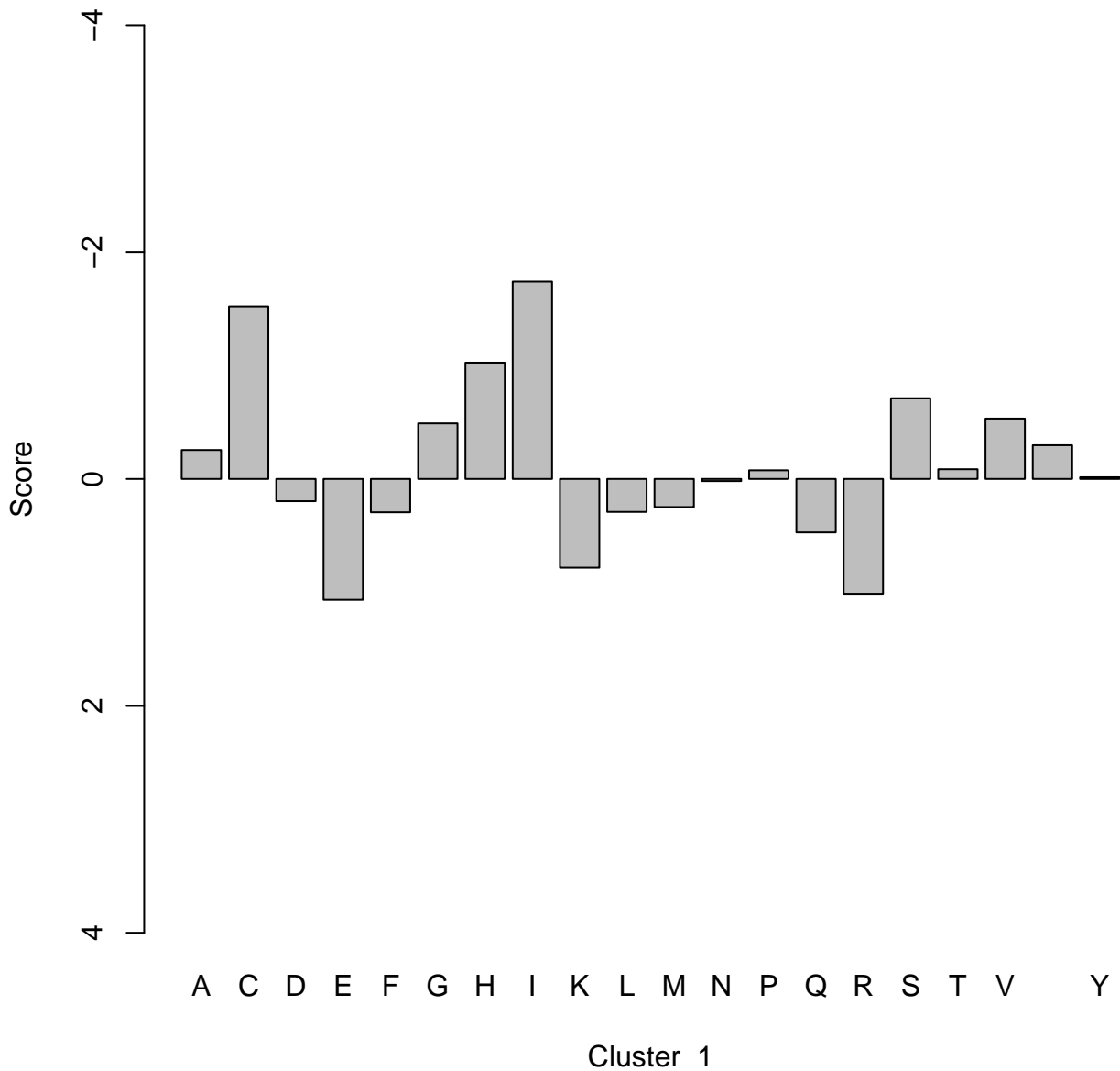
Clustering par Kmedoid(PAM)



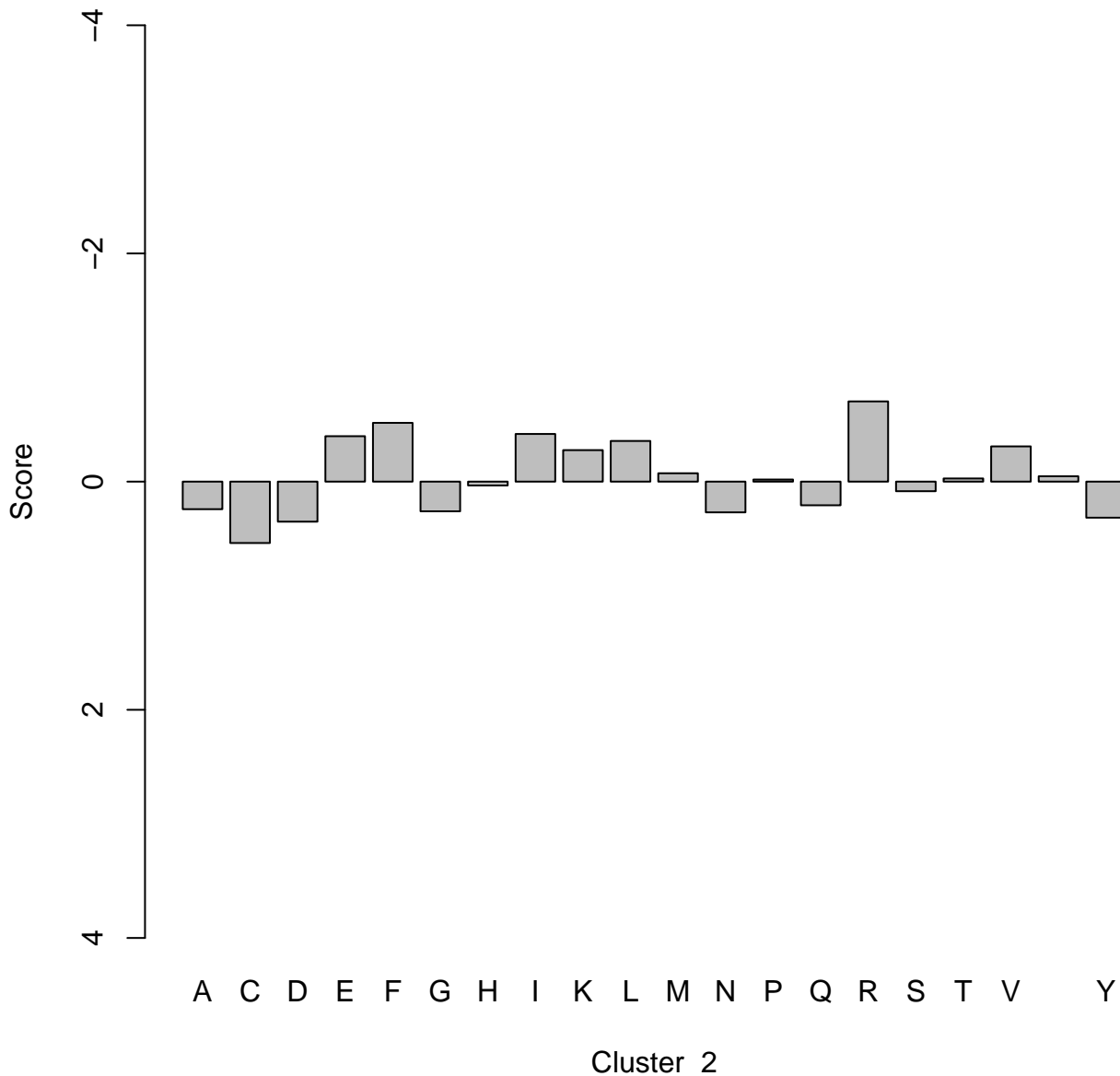
Clusters silhouette plot
Average silhouette width: 0.11



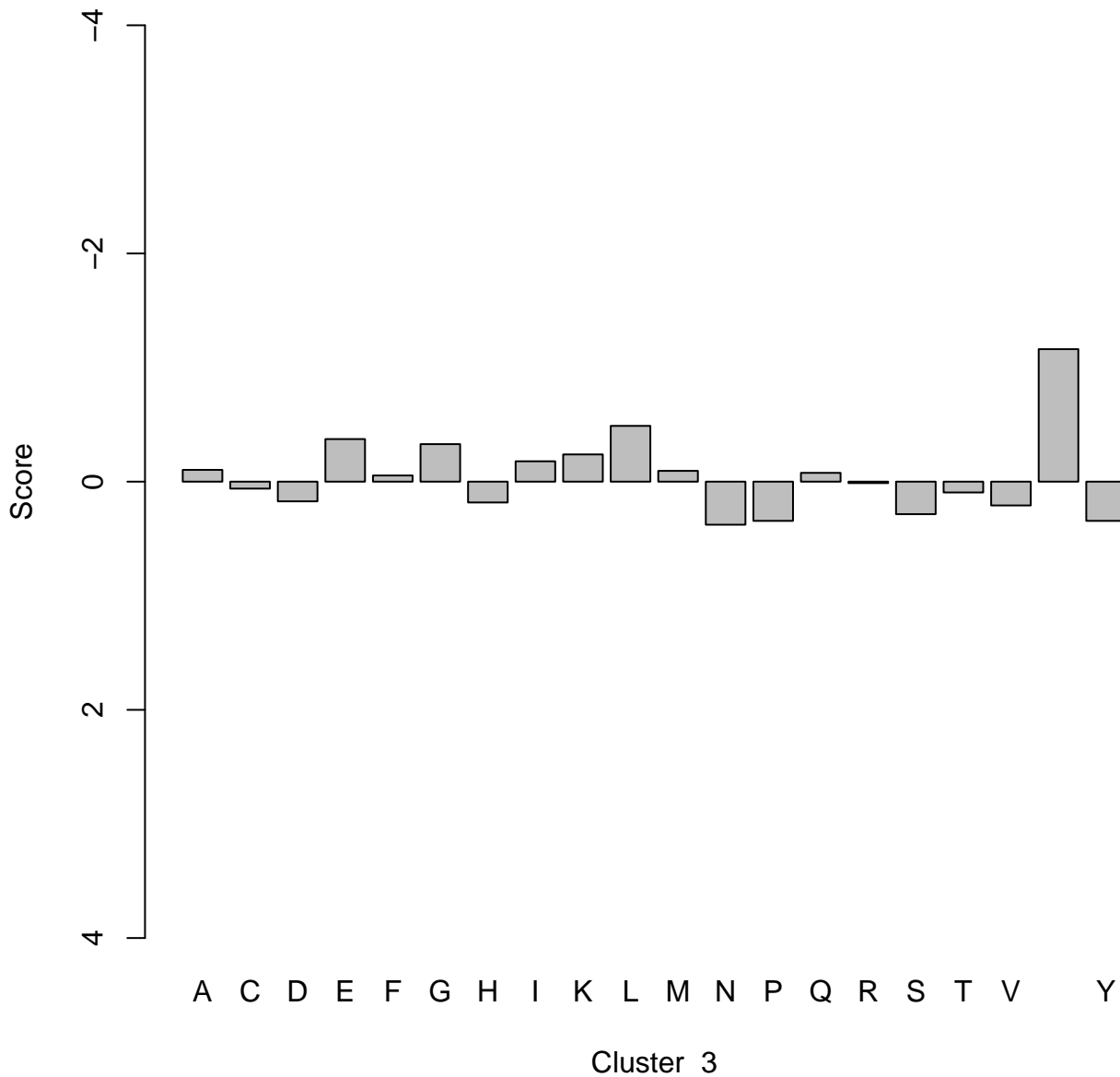
Distribution des scores (Méthode PAM)



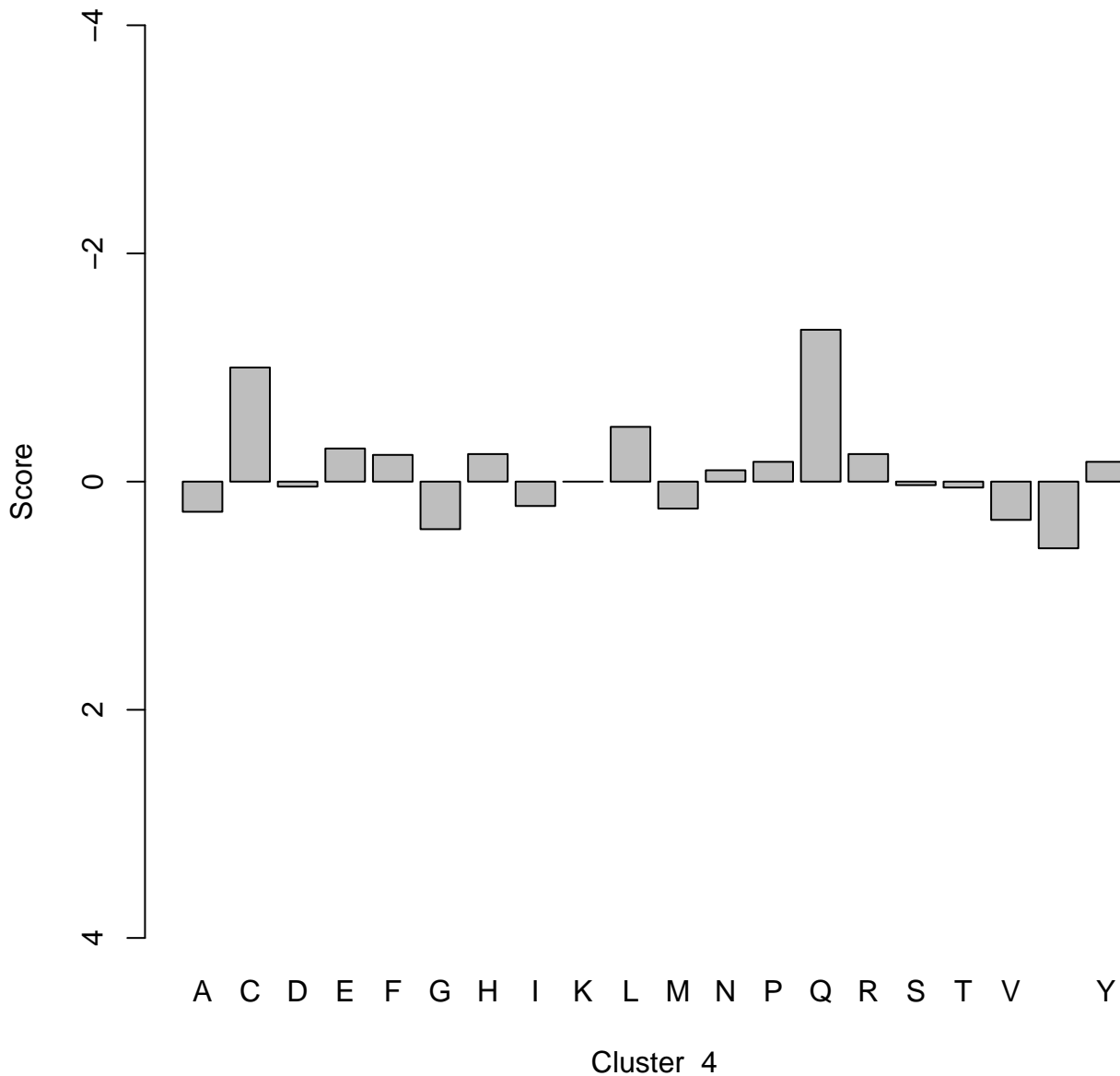
Distribution des scores (Méthode PAM)



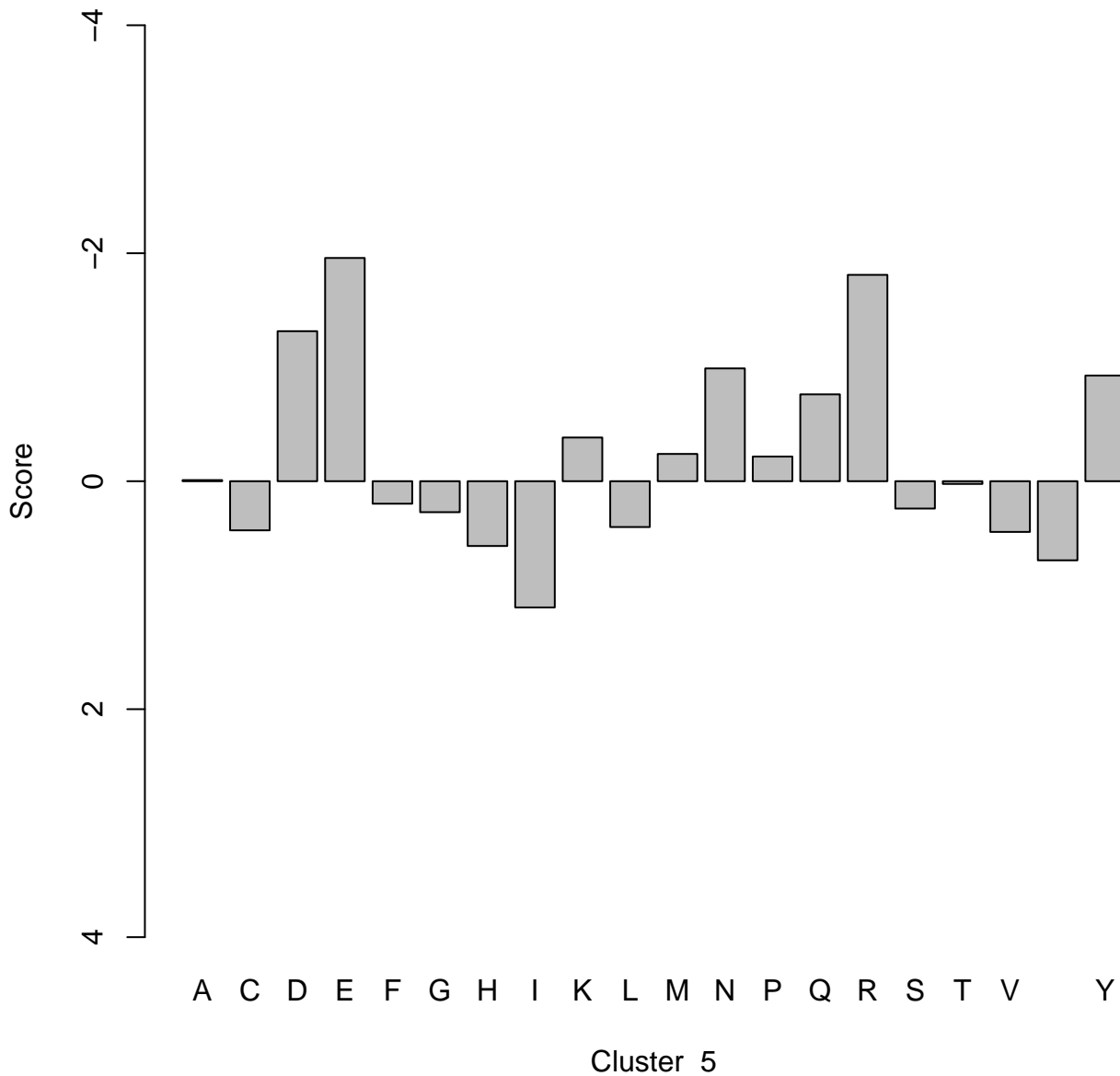
Distribution des scores (Méthode PAM)



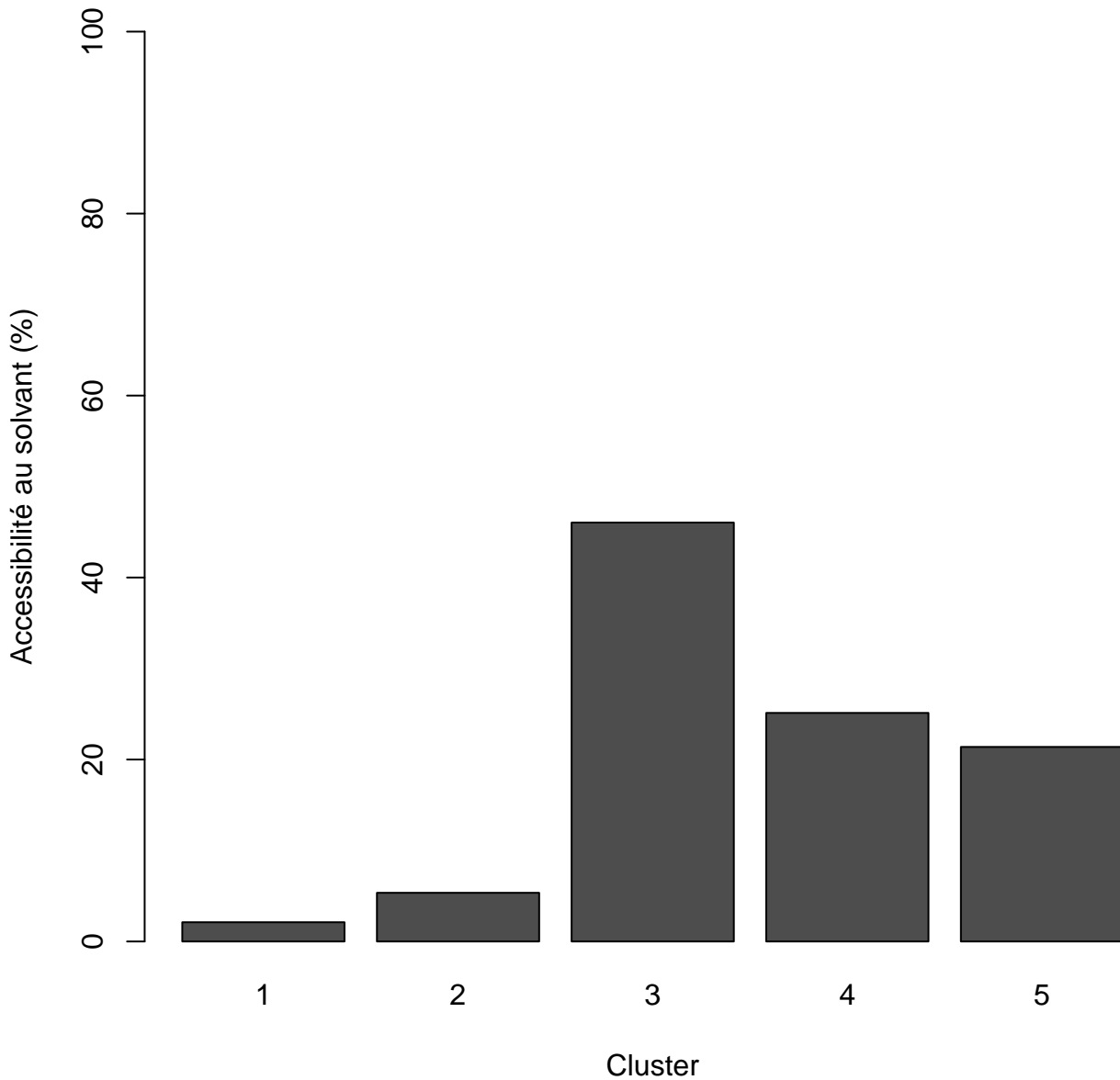
Distribution des scores (Méthode PAM)



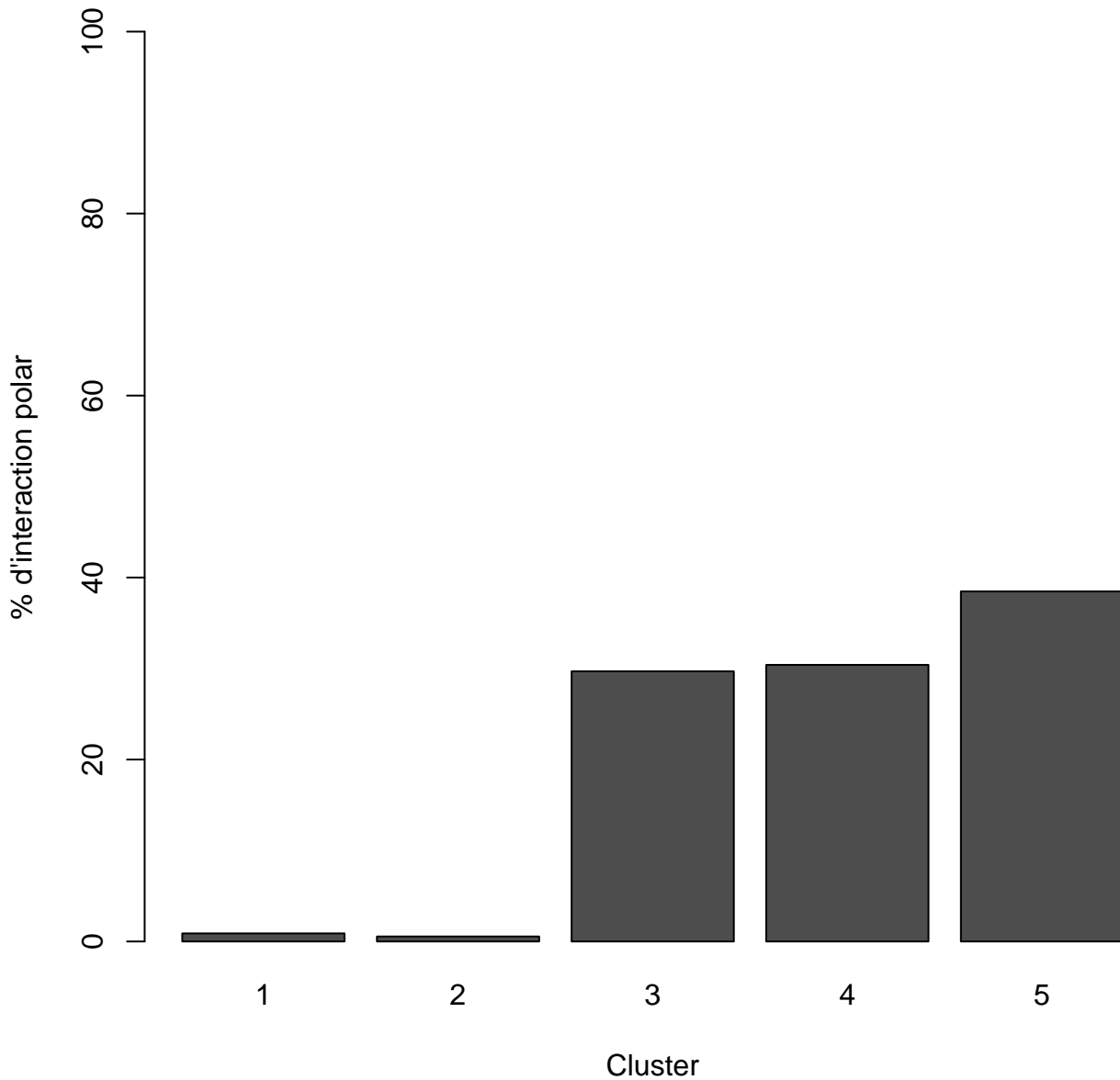
Distribution des scores (Méthode PAM)



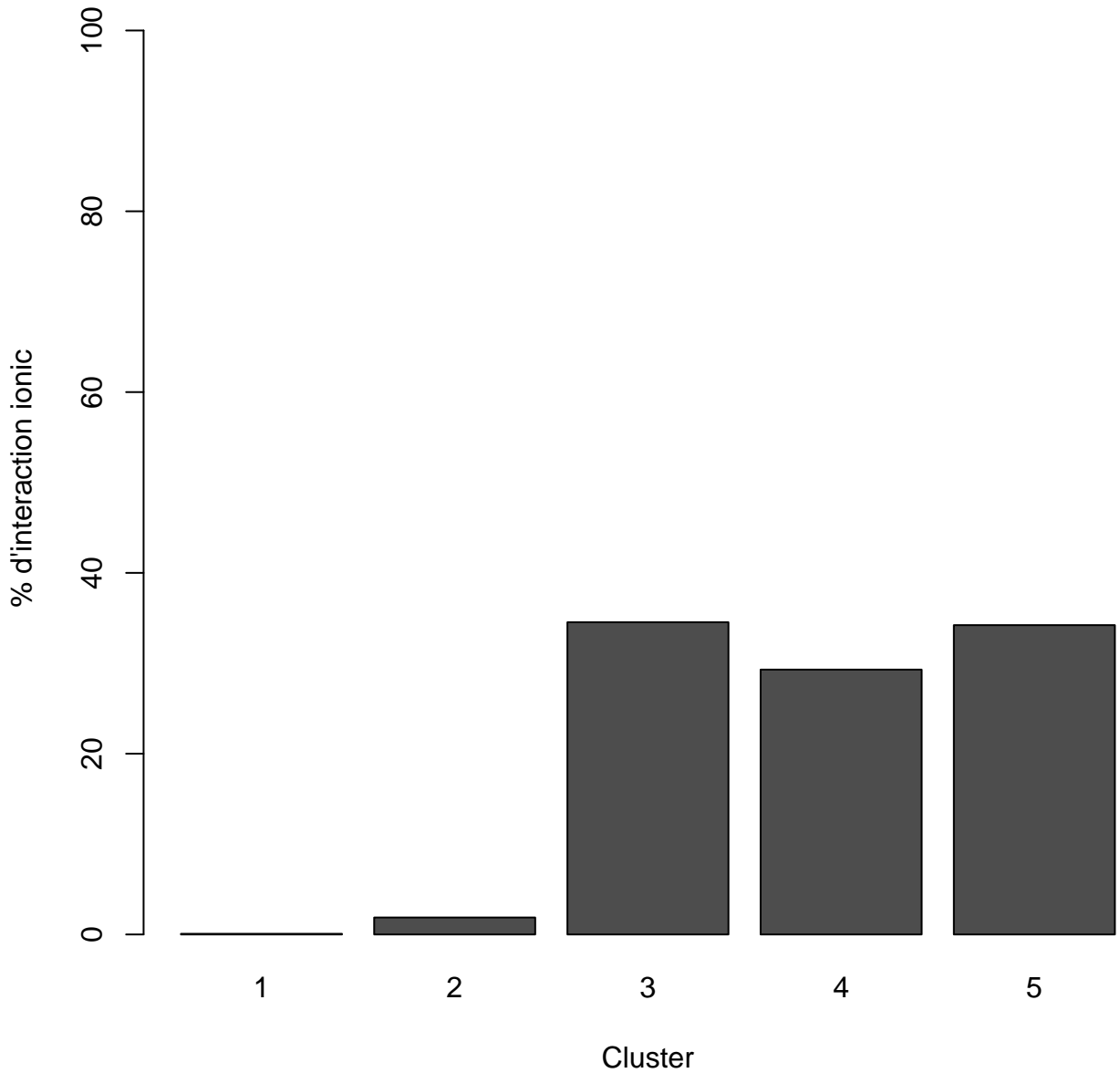
Accessibilité au solvant (%) Kmeans



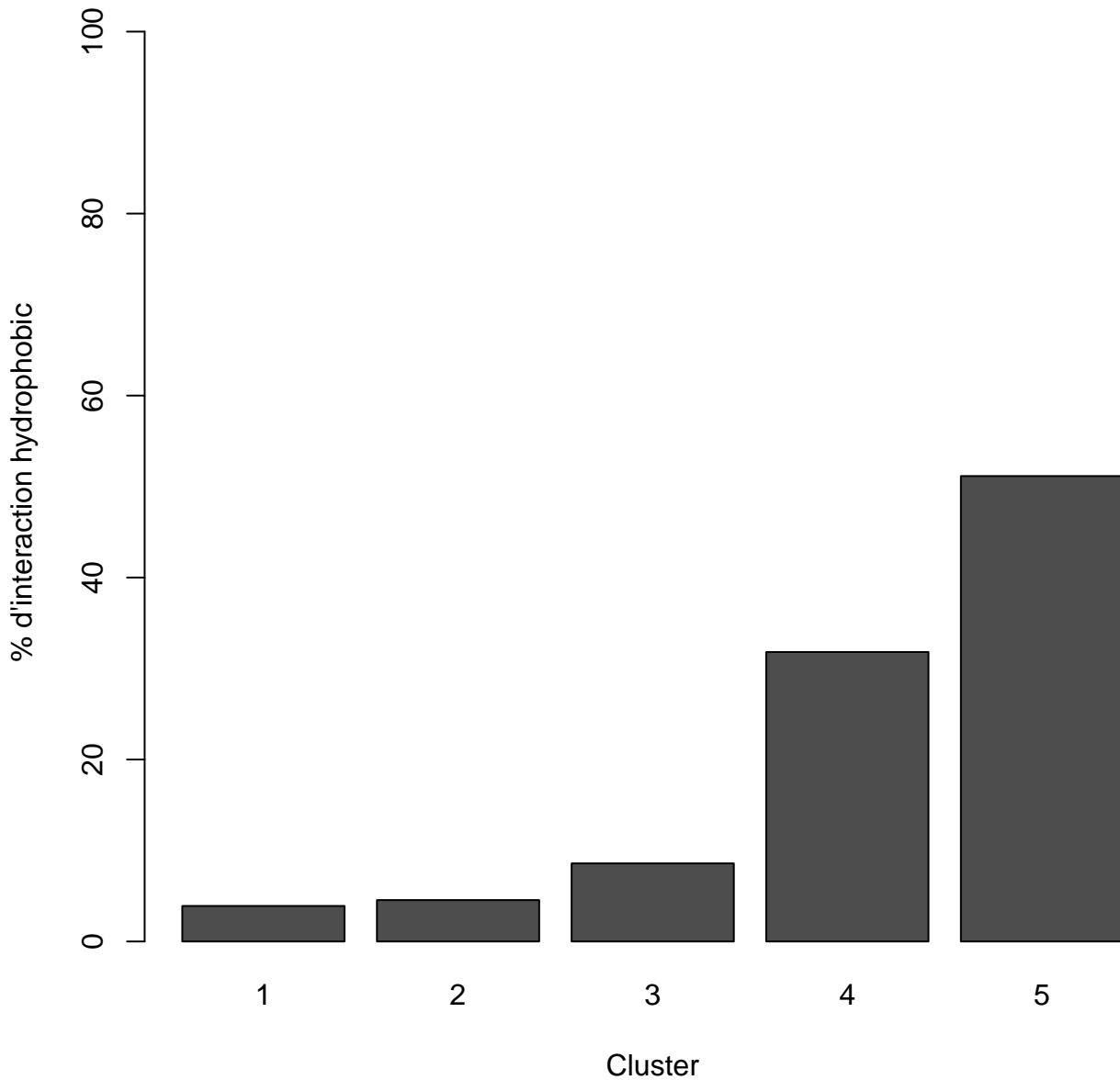
% d'interaction polar Kmeans



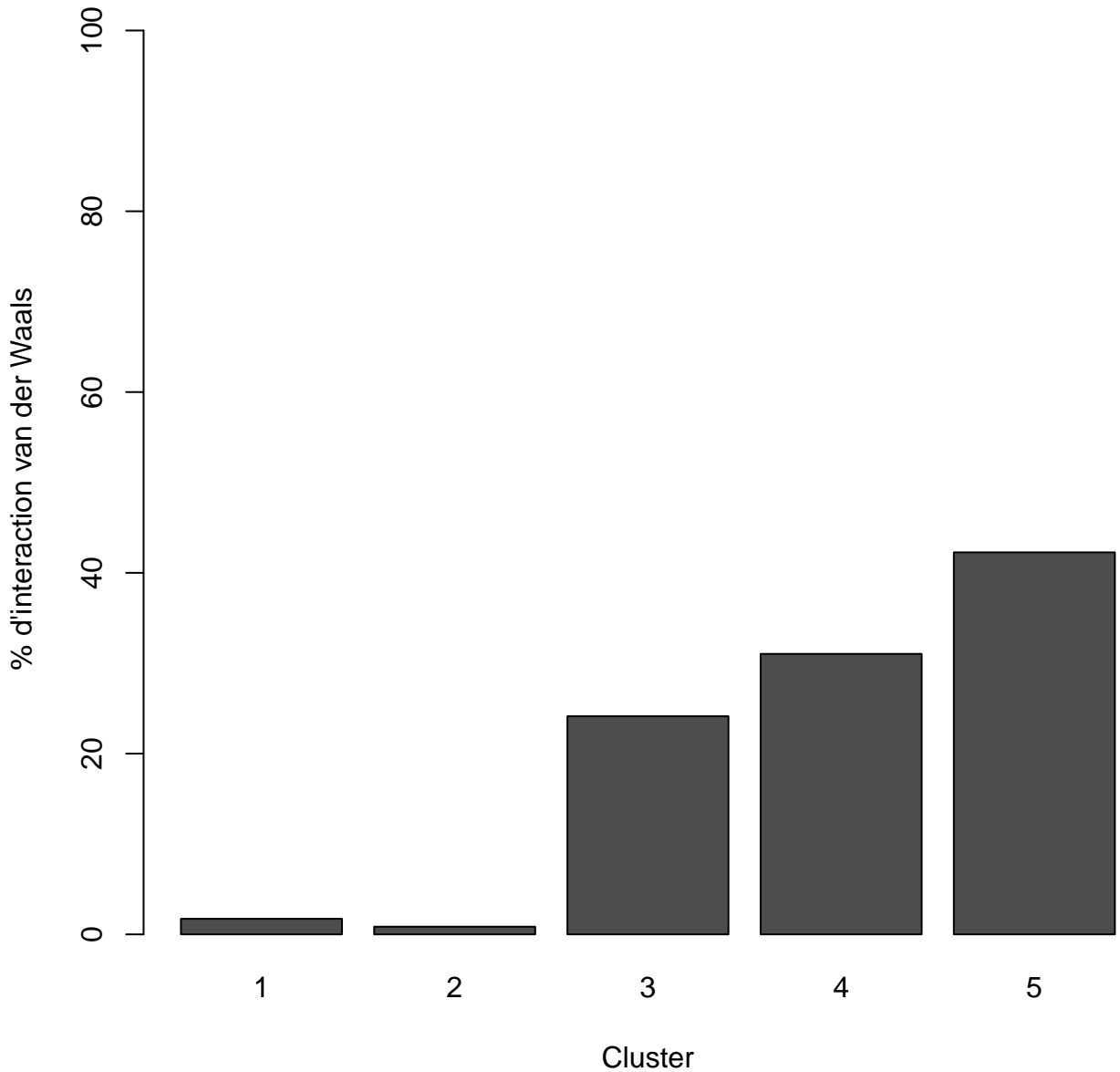
% d'interaction ionic Kmeans



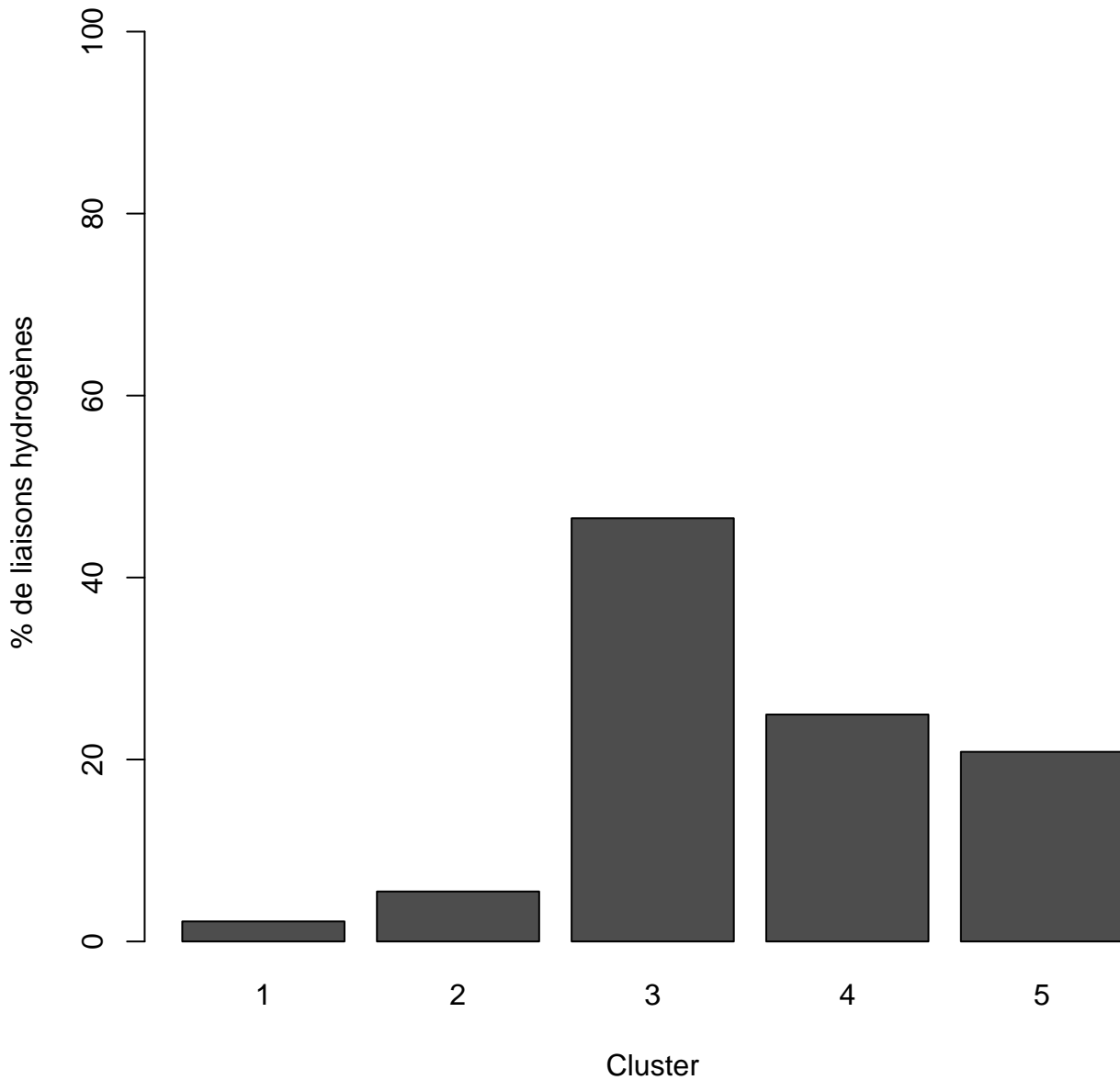
% d'interaction hydrophobic Kmeans



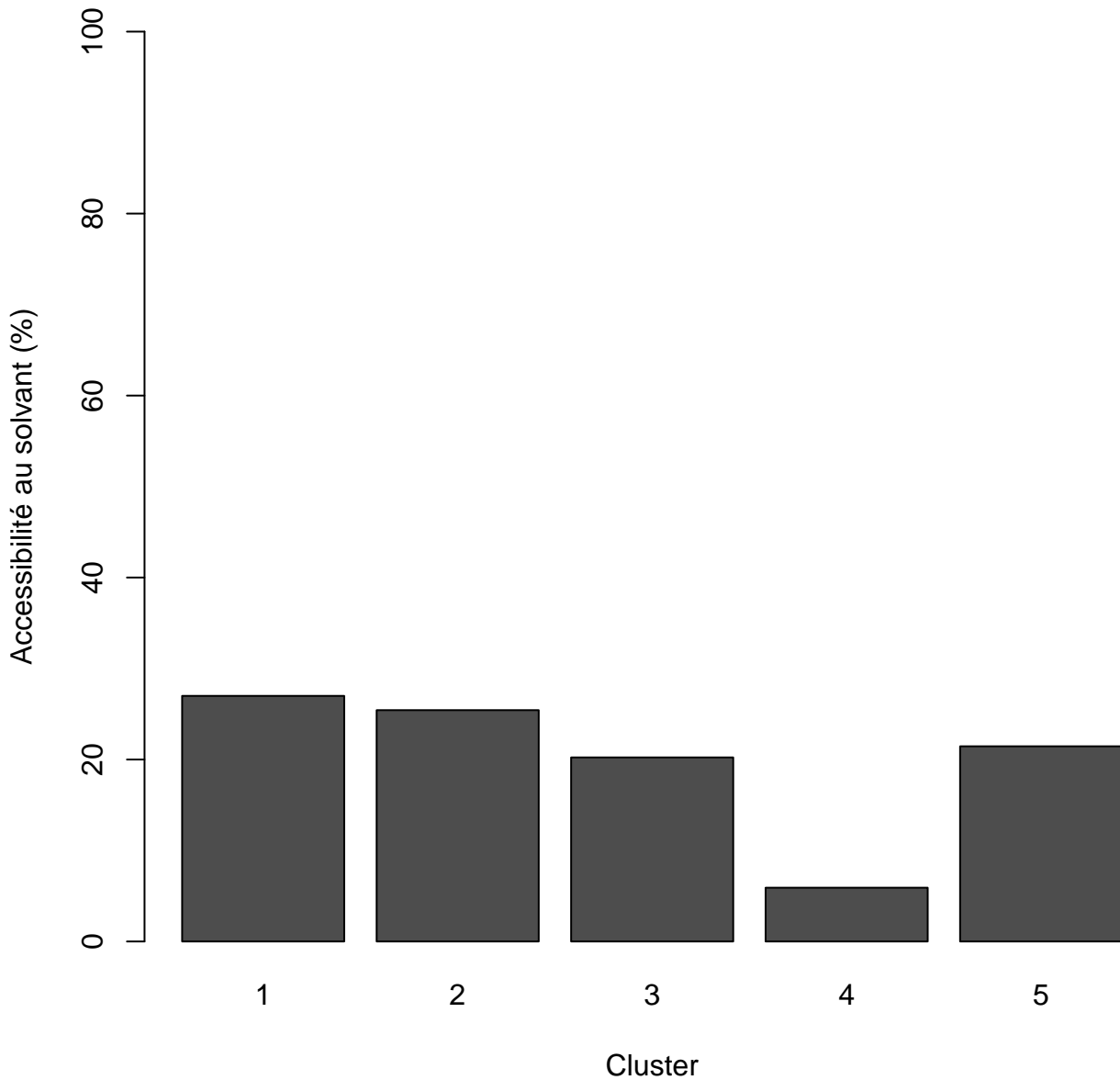
% d'interaction van der Waals Kmeans



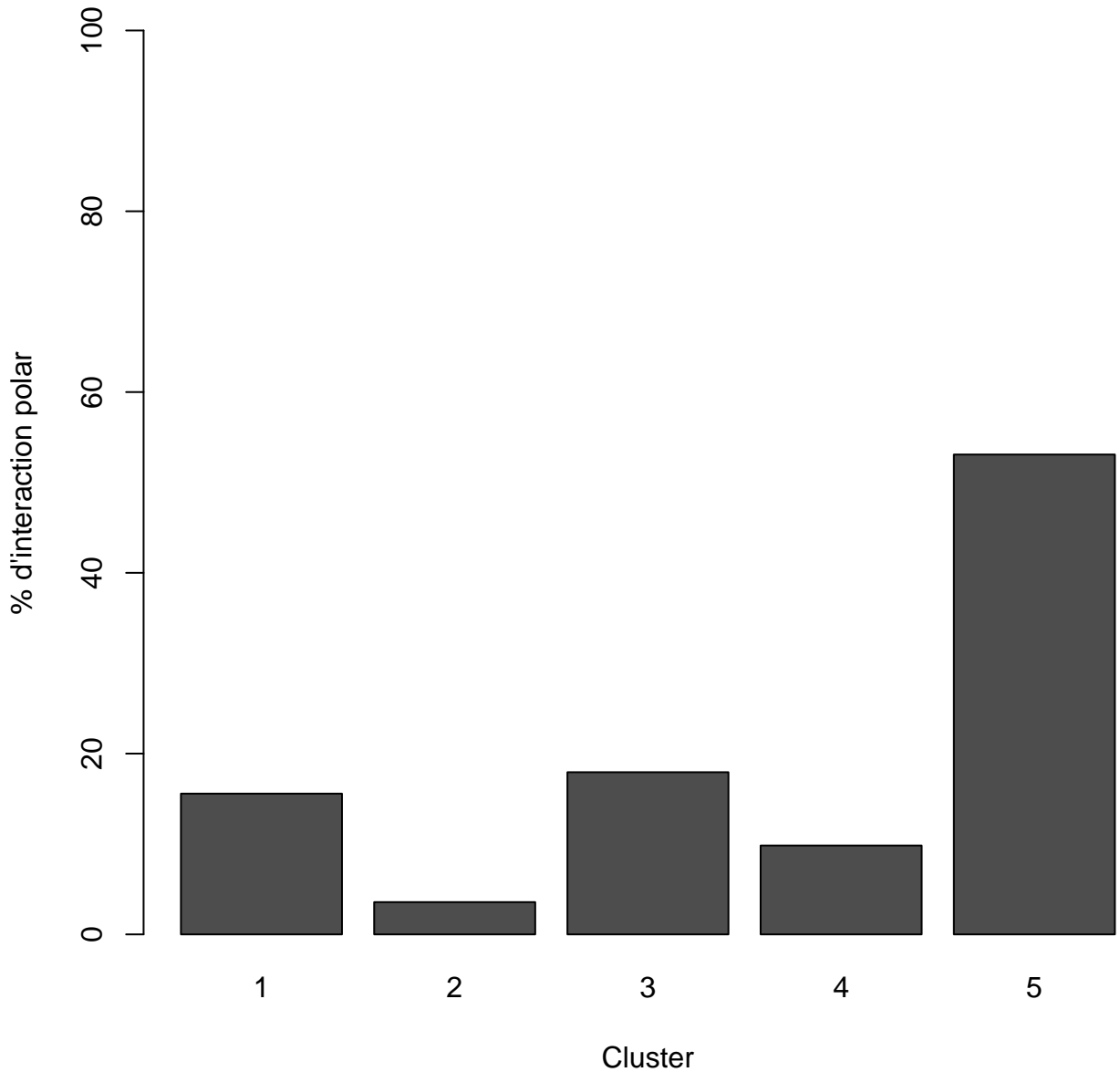
% de liaisons hydrogènes Kmeans



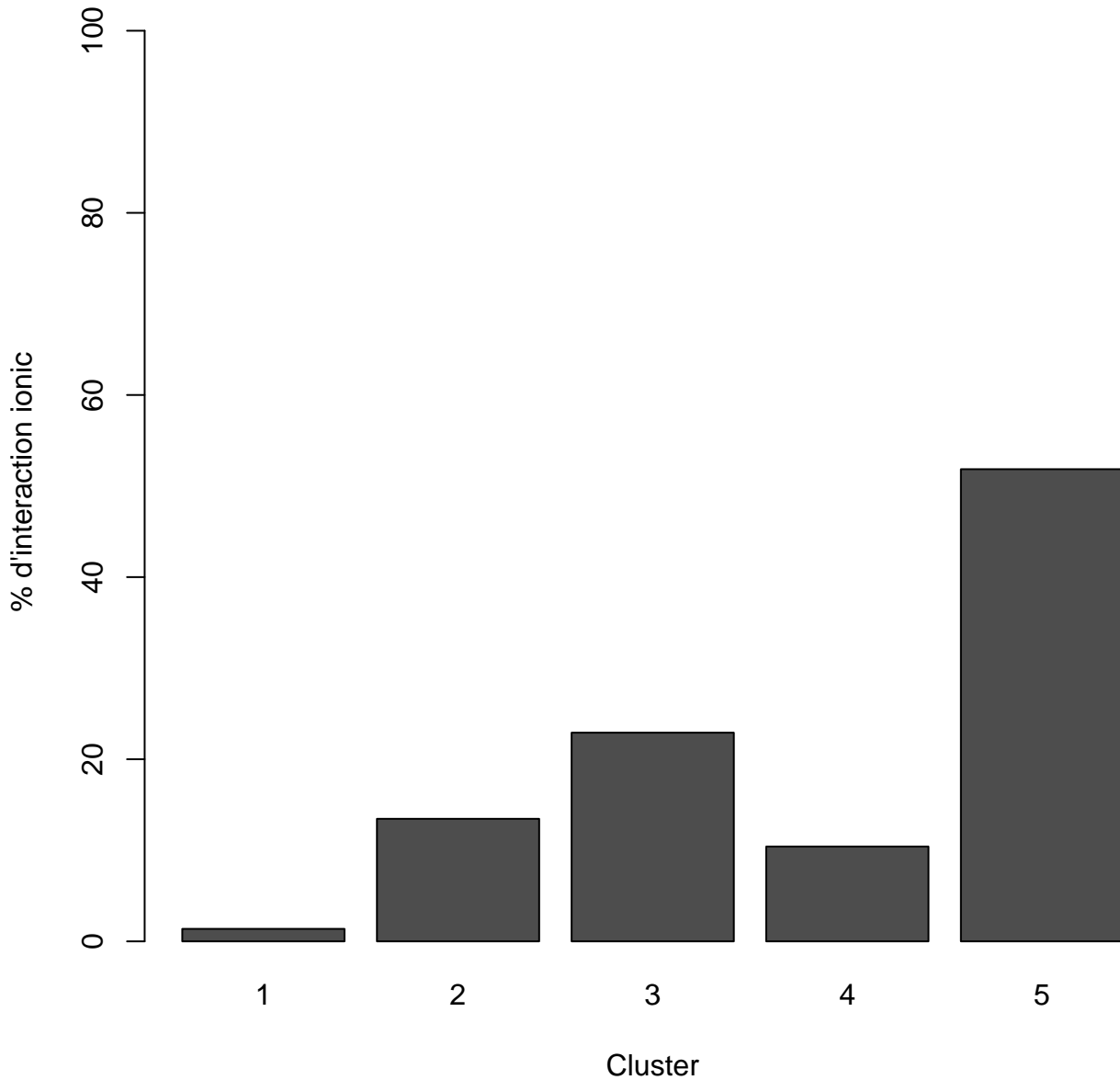
Accessibilité au solvant (%) Kmedoid



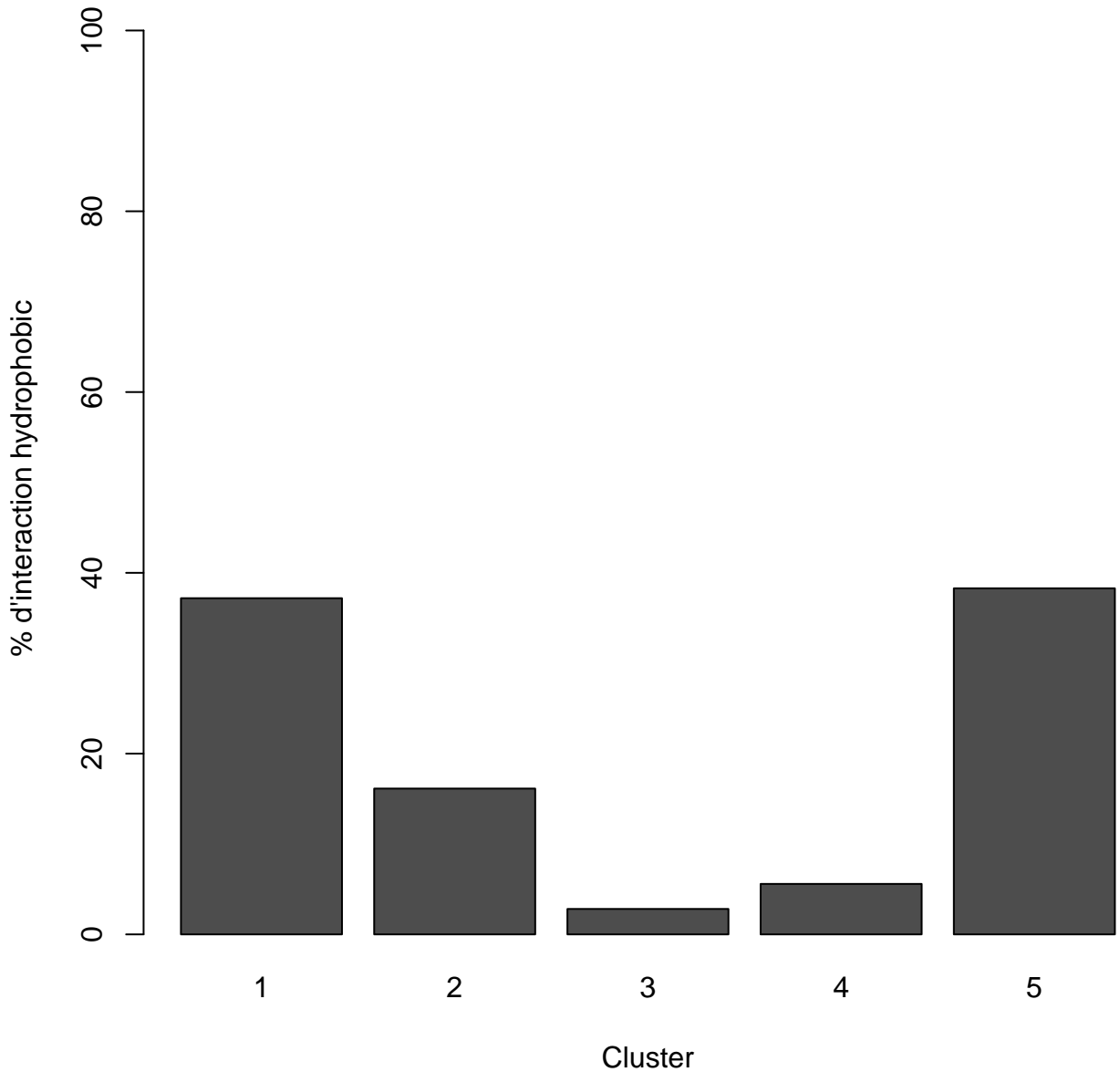
% d'interaction polar Kmedoid



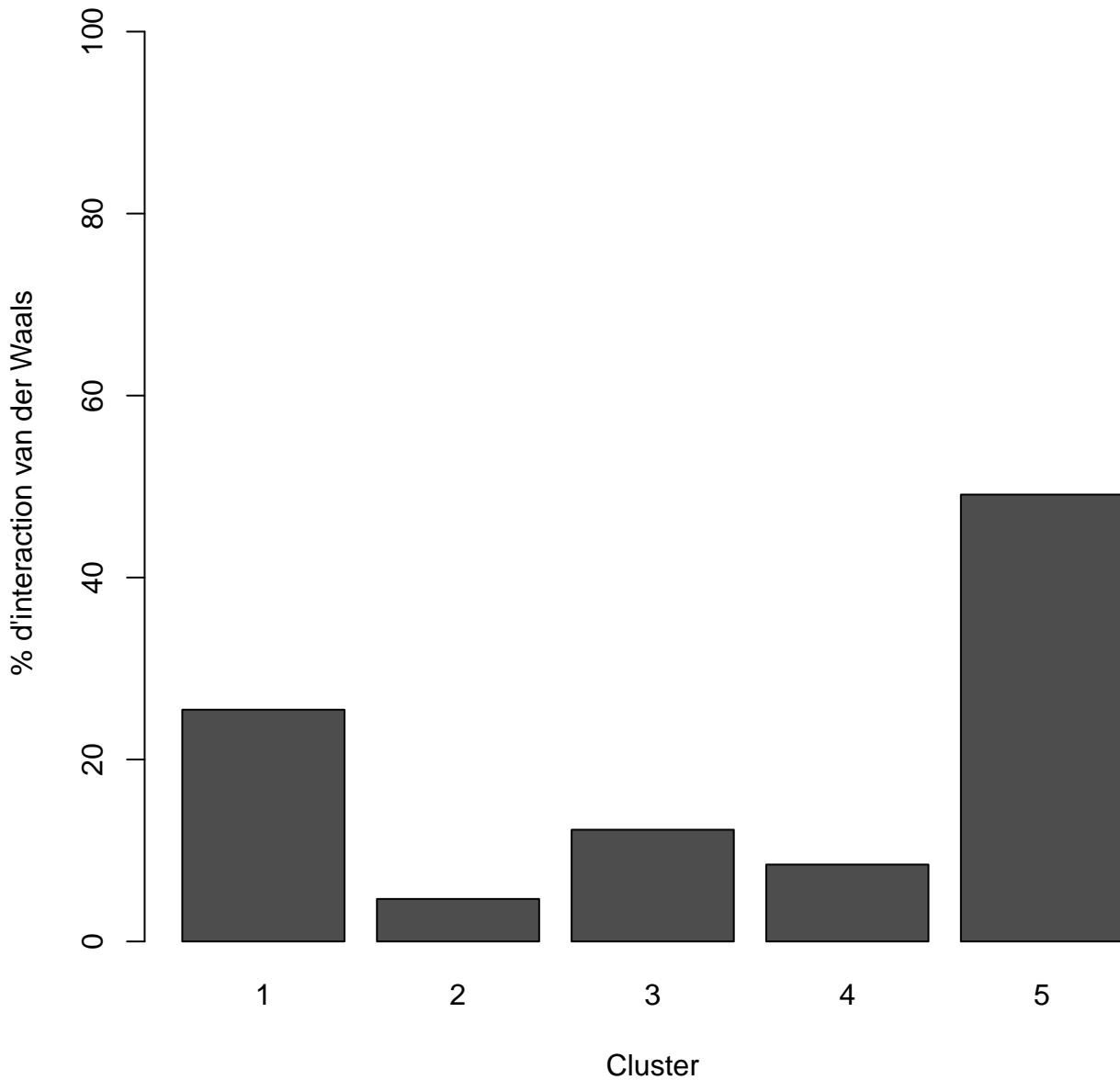
% d'interaction ionic Kmedoid



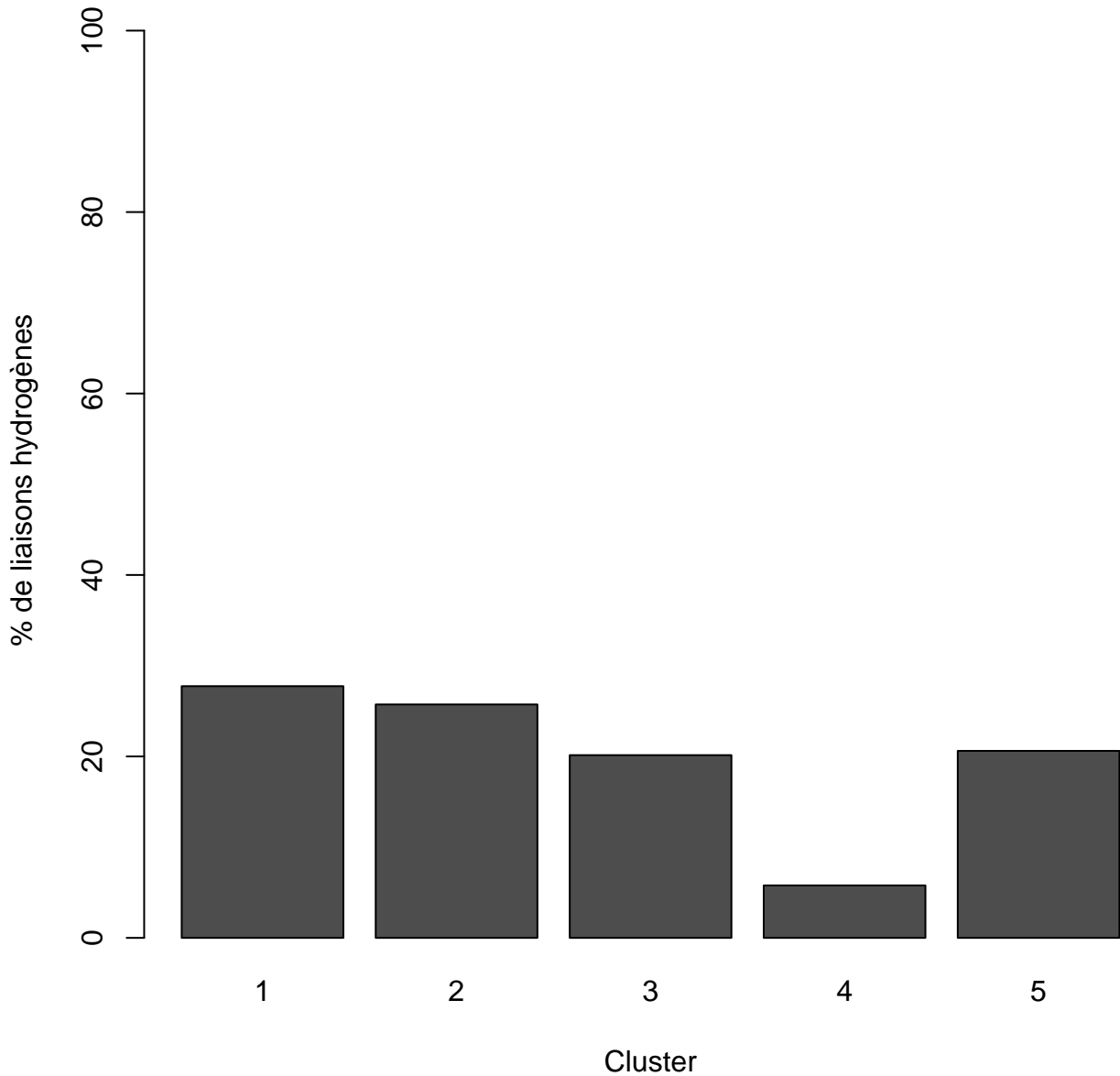
% d'interaction hydrophobic Kmedoid



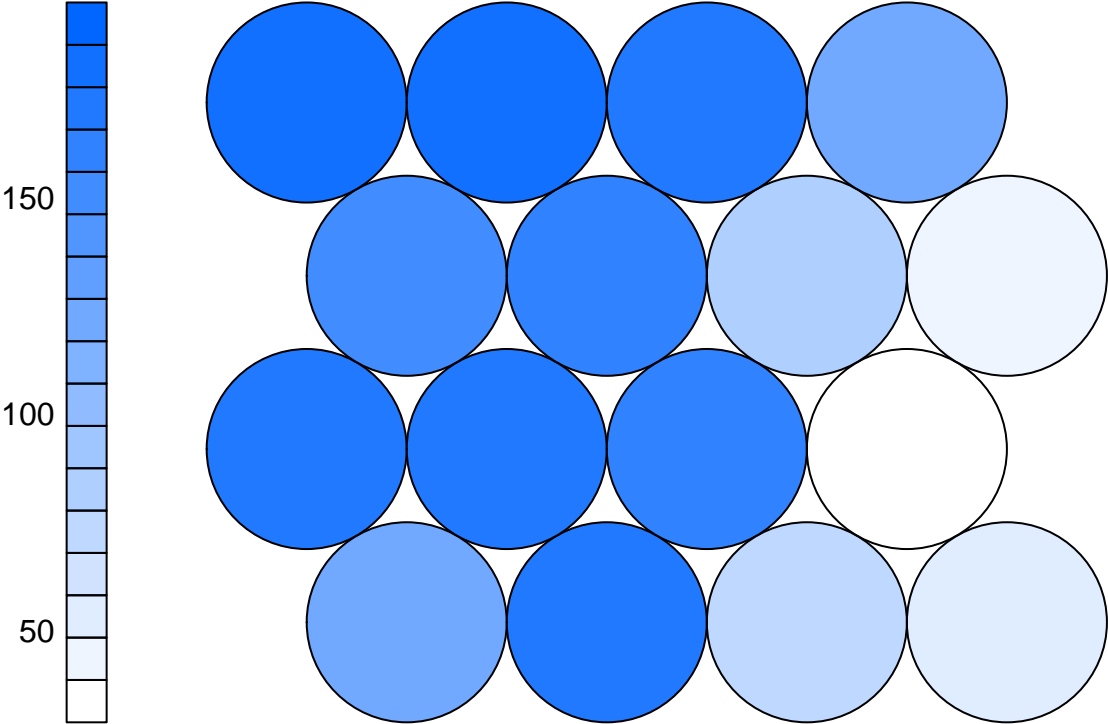
% d'interaction van der Waals Kmedoid



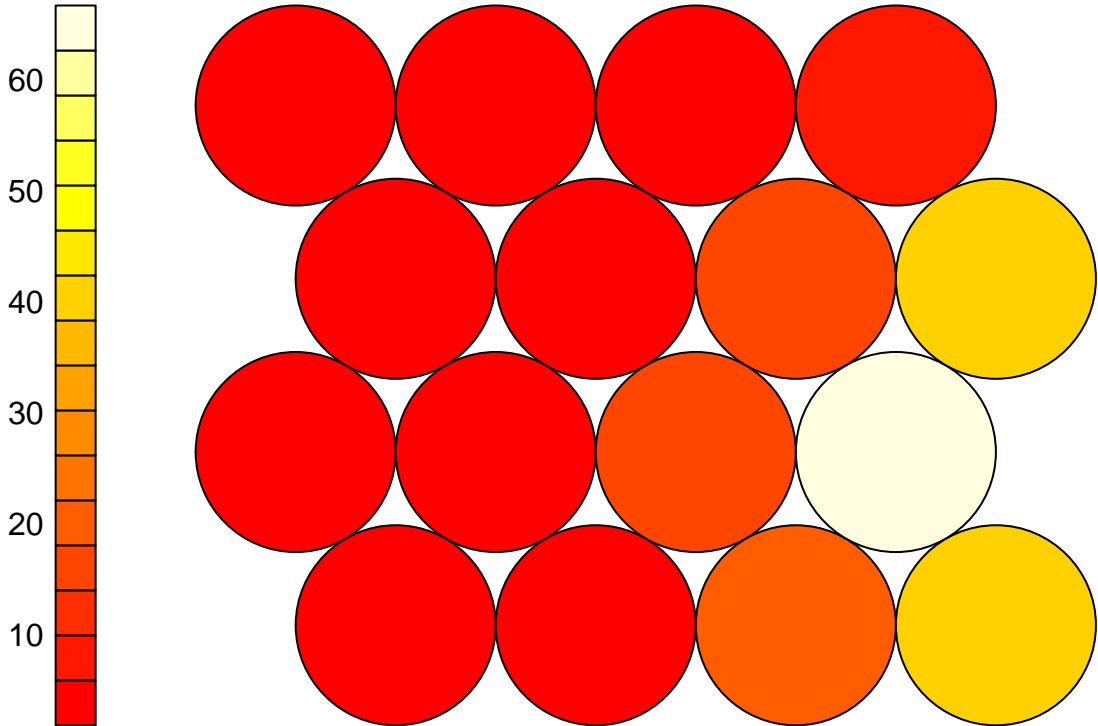
% de liaisons hydrogènes Kmedoid



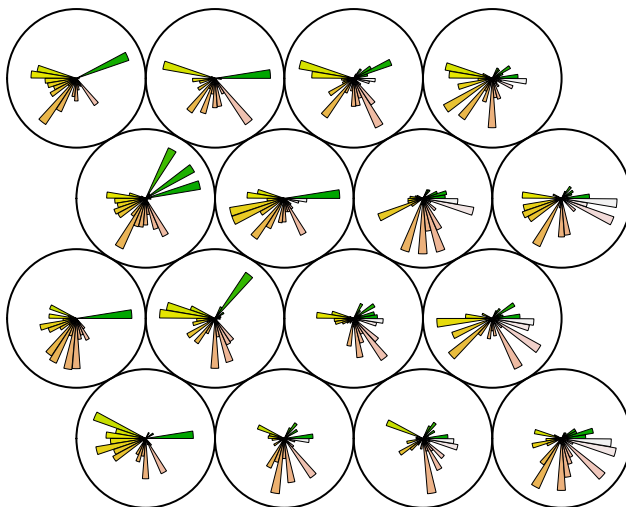
Carte de Kohonen n= 4



Neighbour distance plot

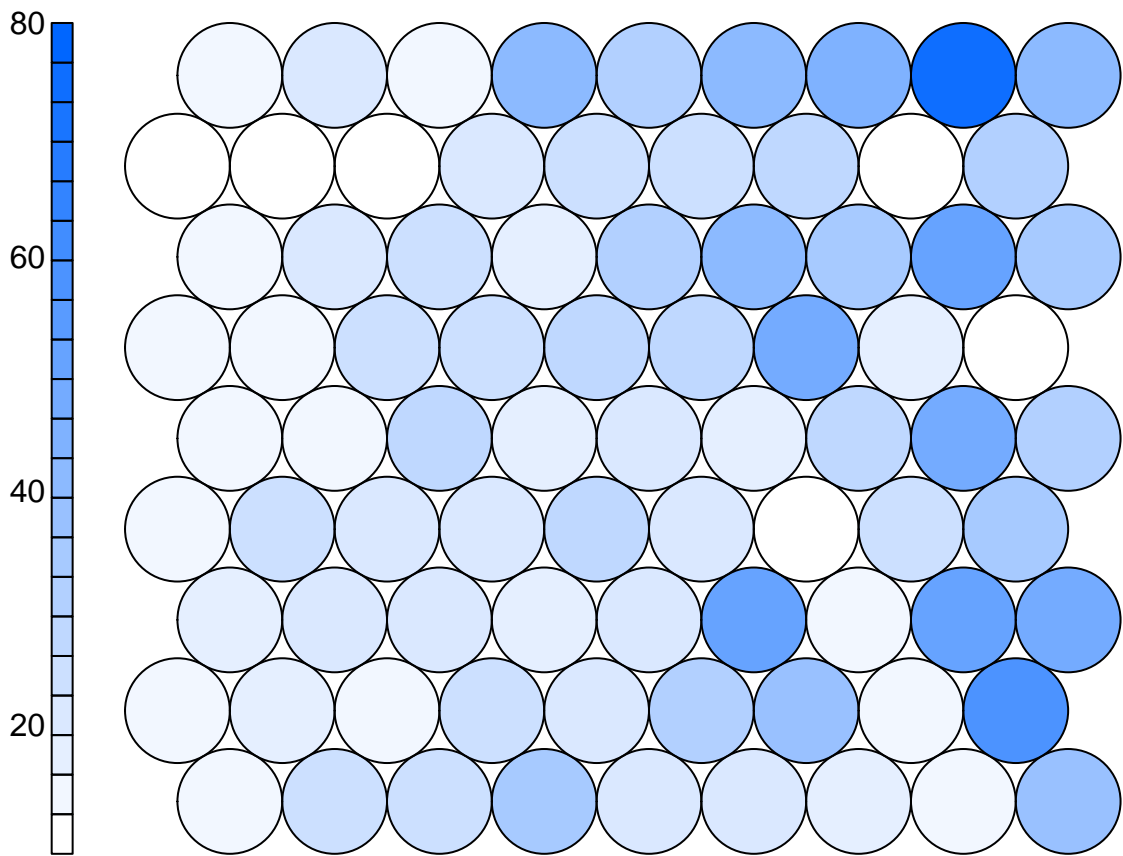


Codes plot

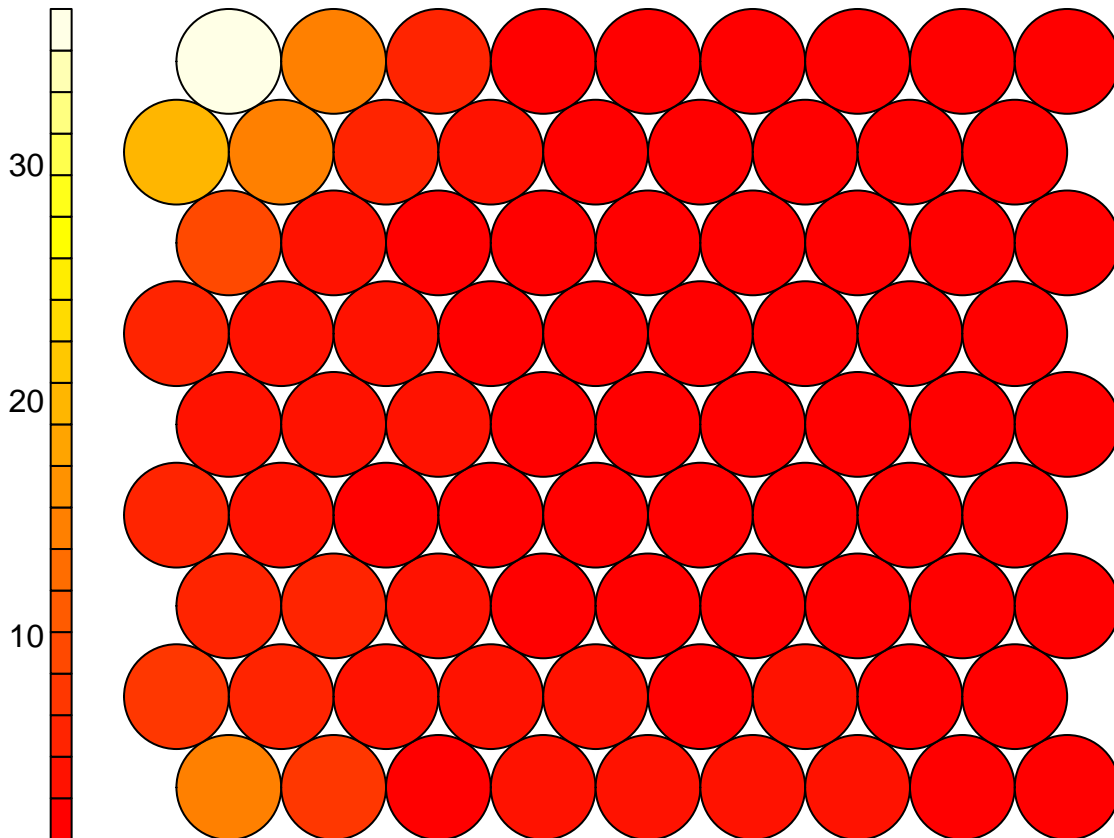


■ H_ss	■ c_PB
■ B_ss	■ d_PB
■ E_ss	■ e_PB
■ G_ss	■ f_PB
■ I_ss	■ g_PB
■ T_ss	■ h_PB
■ S_ss	■ i_PB
■ X._ss	■ j_PB
■ o_ss	■ k_PB
■ o_ss.1	■ l_PB
■ o_ss.2	■ m_PB
■ o_ss.3	■ n_PB
■ o_ss.4	■ o_PB
■ o_ss.5	■ p_PB
■ o_ss.6	■ polar

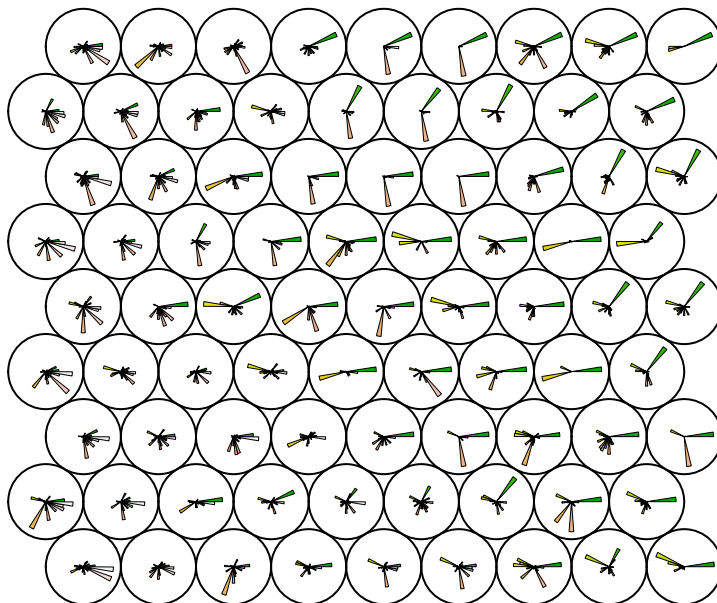
Carte de Kohonen n= 9



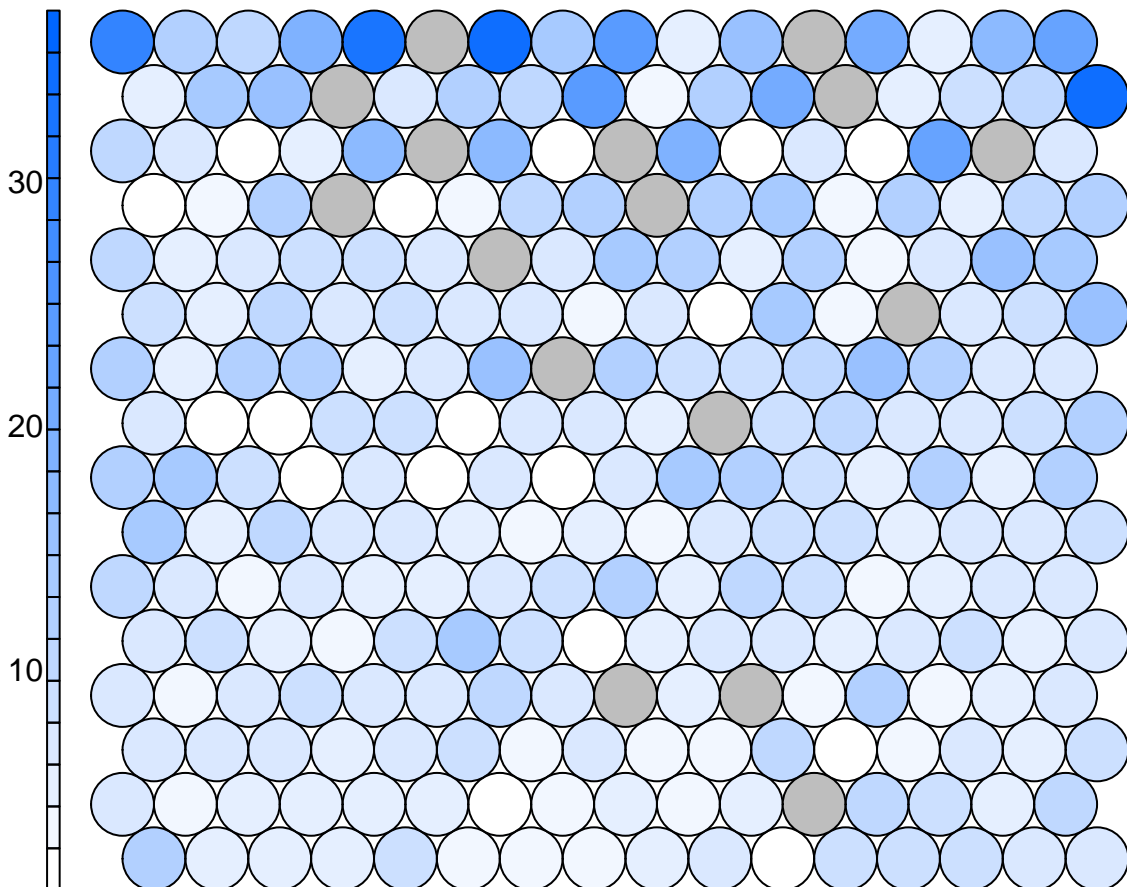
Neighbour distance plot



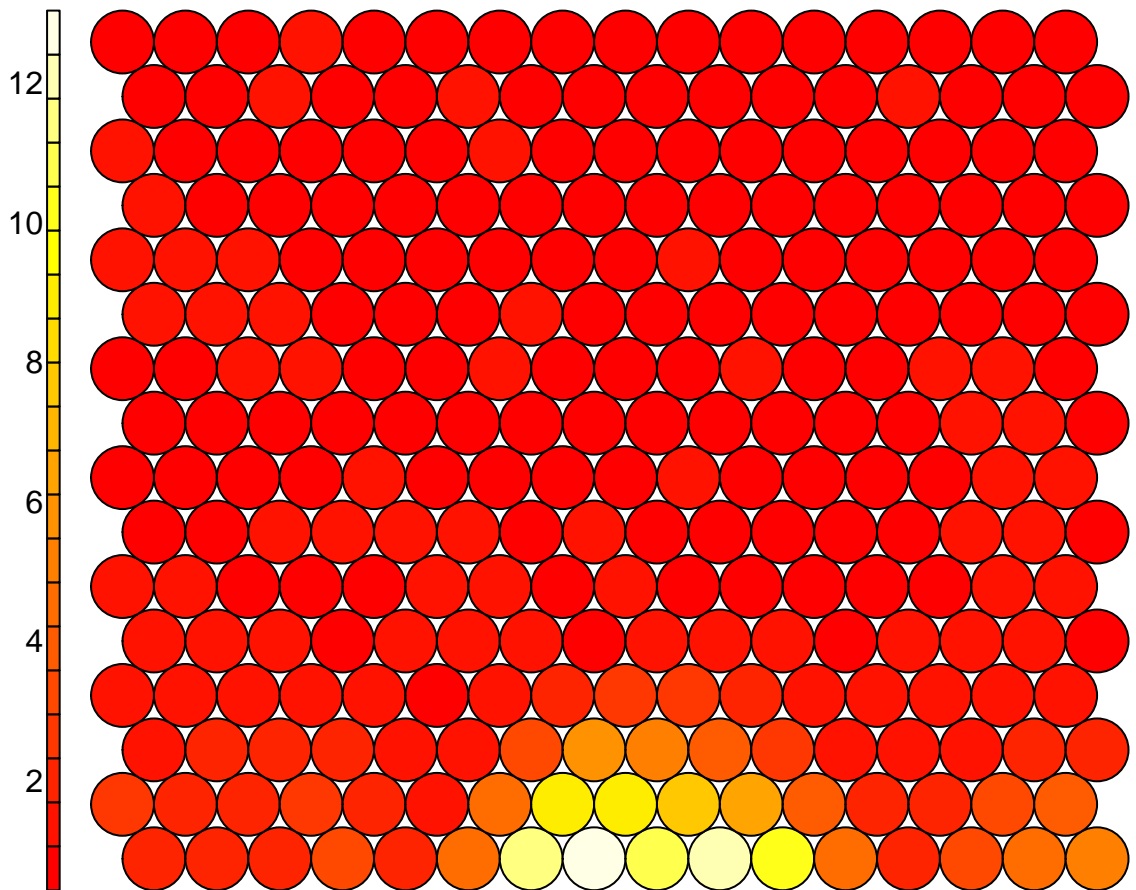
Codes plot



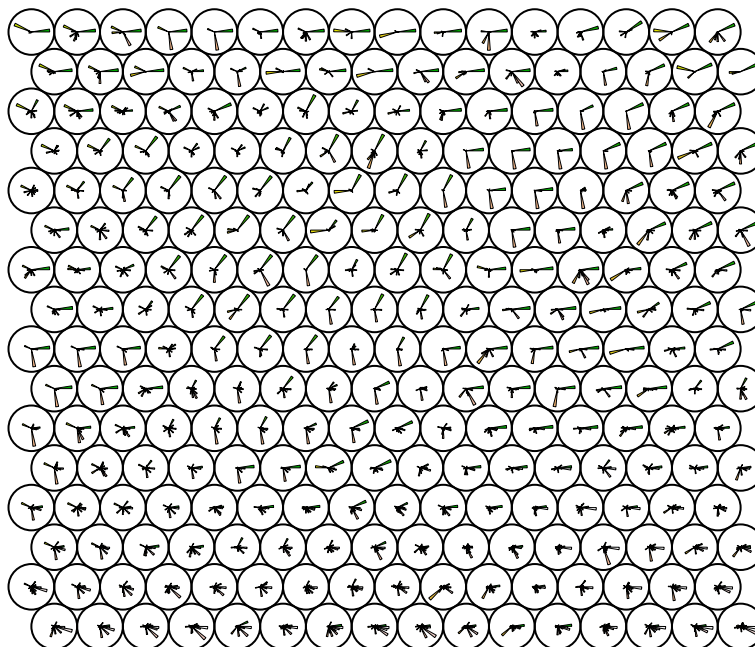
■ H_ss	■ c_PB
■ B_ss	■ d_PB
■ E_ss	■ e_PB
■ G_ss	■ f_PB
■ I_ss	■ g_PB
■ T_ss	■ h_PB
■ S_ss	■ i_PB
■ X._ss	■ j_PB
■ o_ss	■ k_PB
■ o_ss.1	■ l_PB
■ o_ss.2	■ m_PB
■ o_ss.3	■ n_PB
■ o_ss.4	■ o_PB
■ o ss.5	■ o PB





























A 2D visualization of a hexagonal lattice of particles. The particles are represented by circles, mostly red, with a color gradient from red to yellow/white at the bottom. A vertical color bar on the left indicates a scale from 2 to 12.

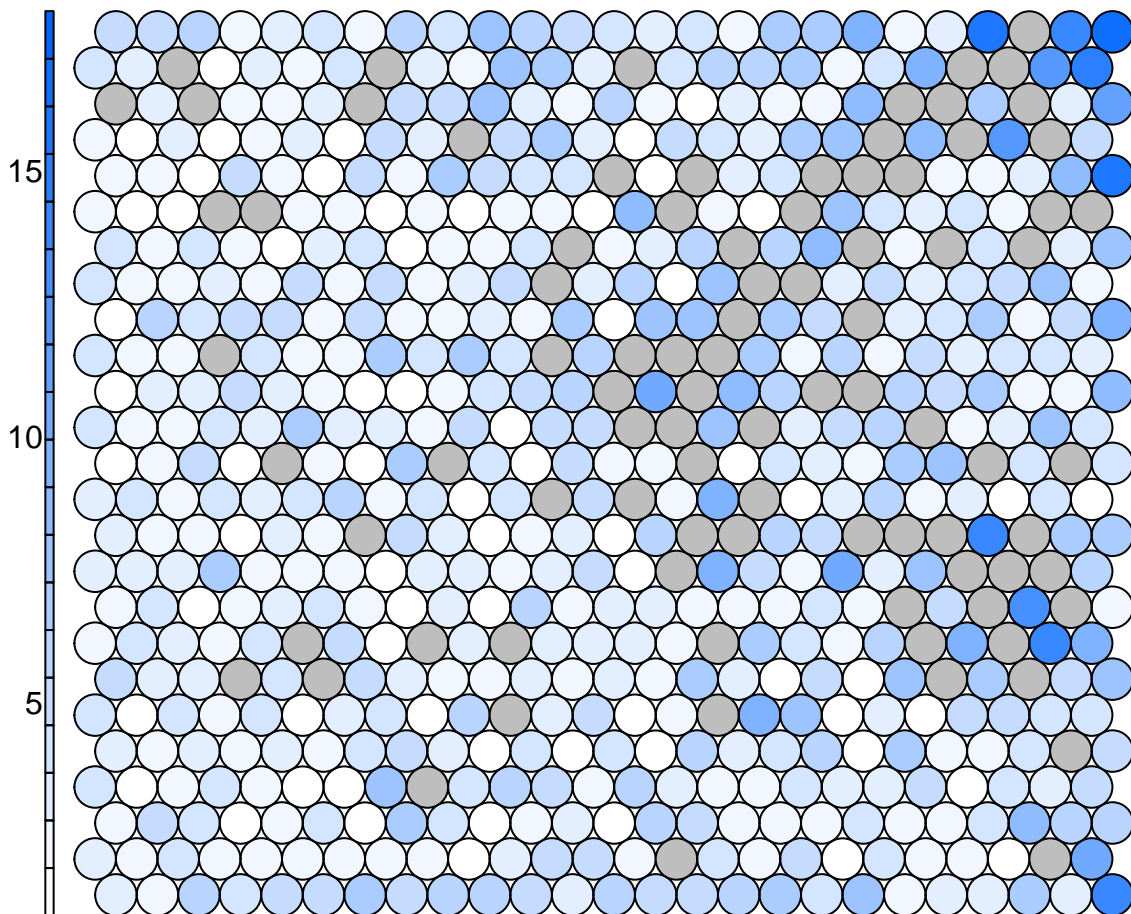


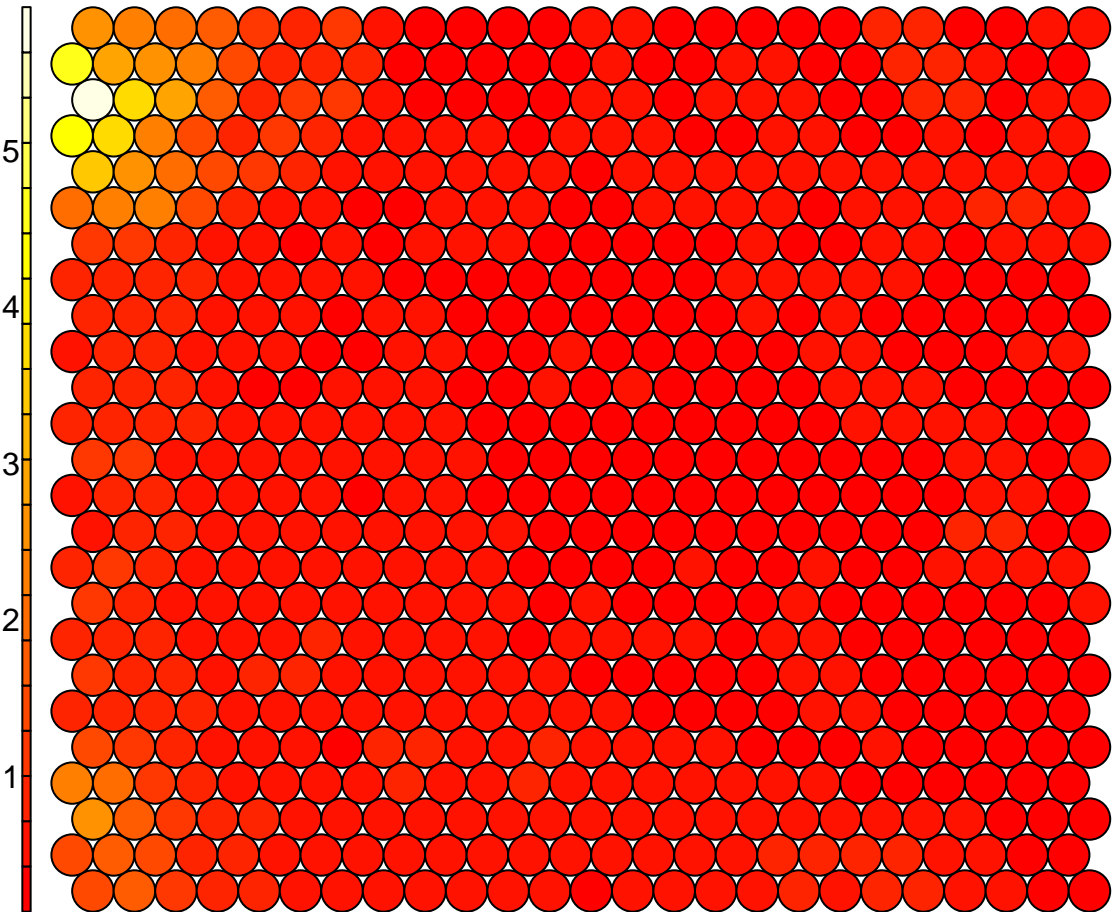
Codes plot



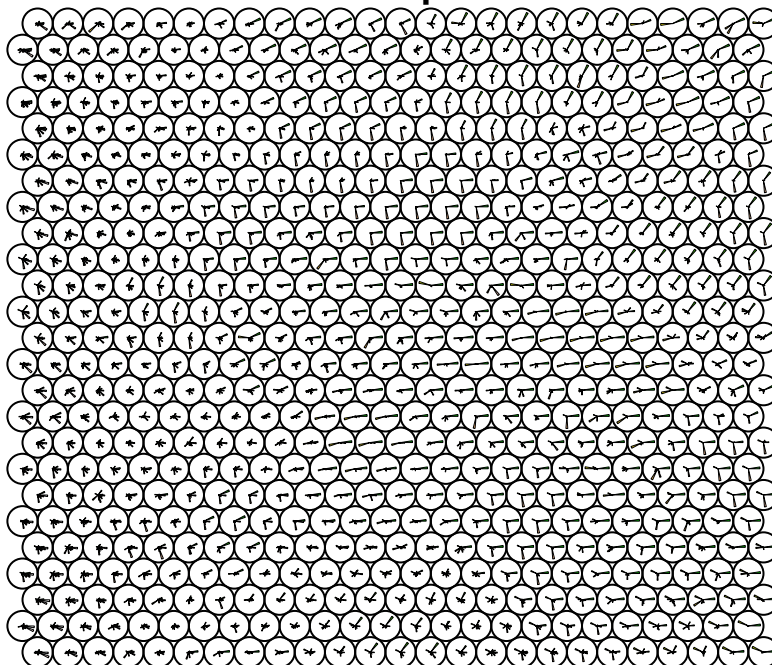
	H_ss		c_PB
	B_ss		d_PB
	E_ss		e_PB
	G_ss		f_PB
	I_ss		g_PB
	T_ss		h_PB
	S_ss		i_PB
	X_ss		j_PB
	o_ss		k_PB
	o_ss.1		l_PB
	o_ss.2		m_PB
	o_ss.3		n_PB
	o_ss.4		o_PB



























Carte de Kohonen n= 25



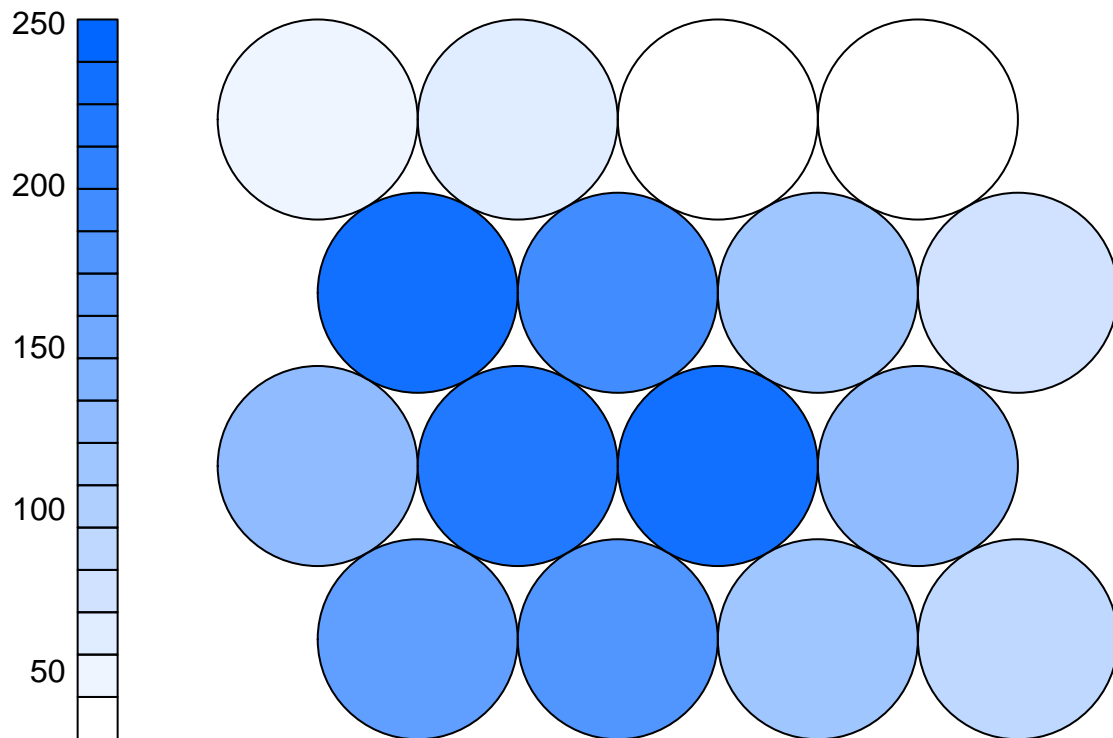


Codes plot

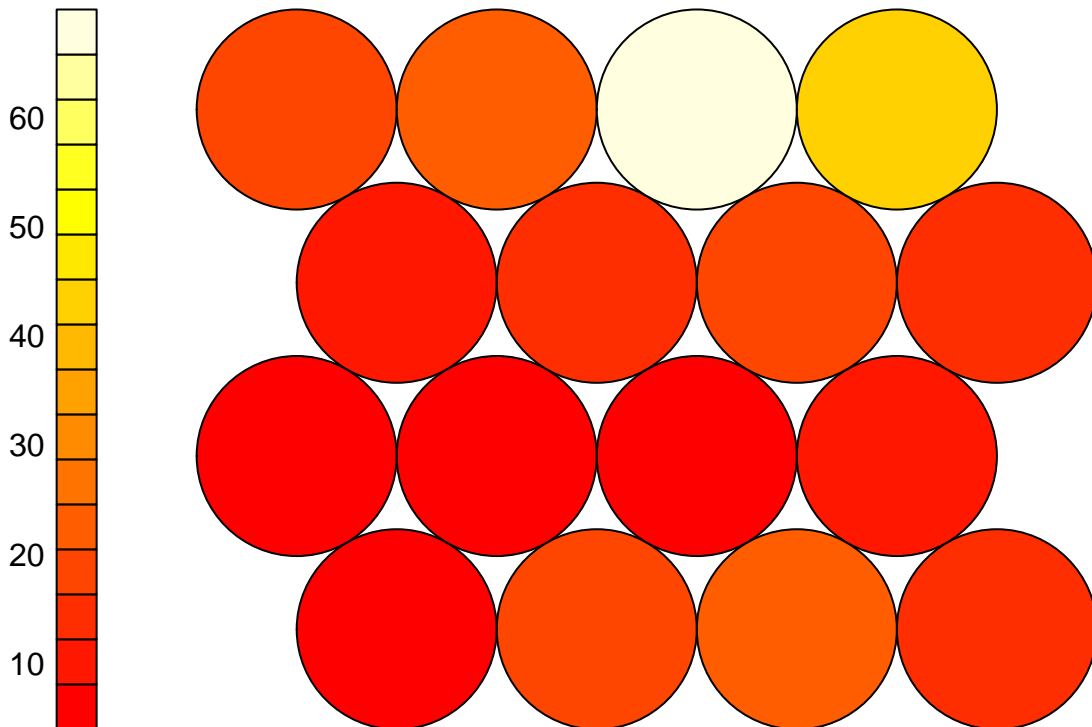


	H_ss		c_PB
	B_ss		d_PB
	E_ss		e_PB
	G_ss		f_PB
	I_ss		g_PB
	T_ss		h_PB
	S_ss		i_PB
	X_ss		j_PB
	o_ss		k_PB
	o_ss.1		l_PB
	o_ss.2		m_PB
	o_ss.3		n_PB
	o_ss.4		o_PB

Carte de Kohonen toroidal n= 4



Neighbour distance plot

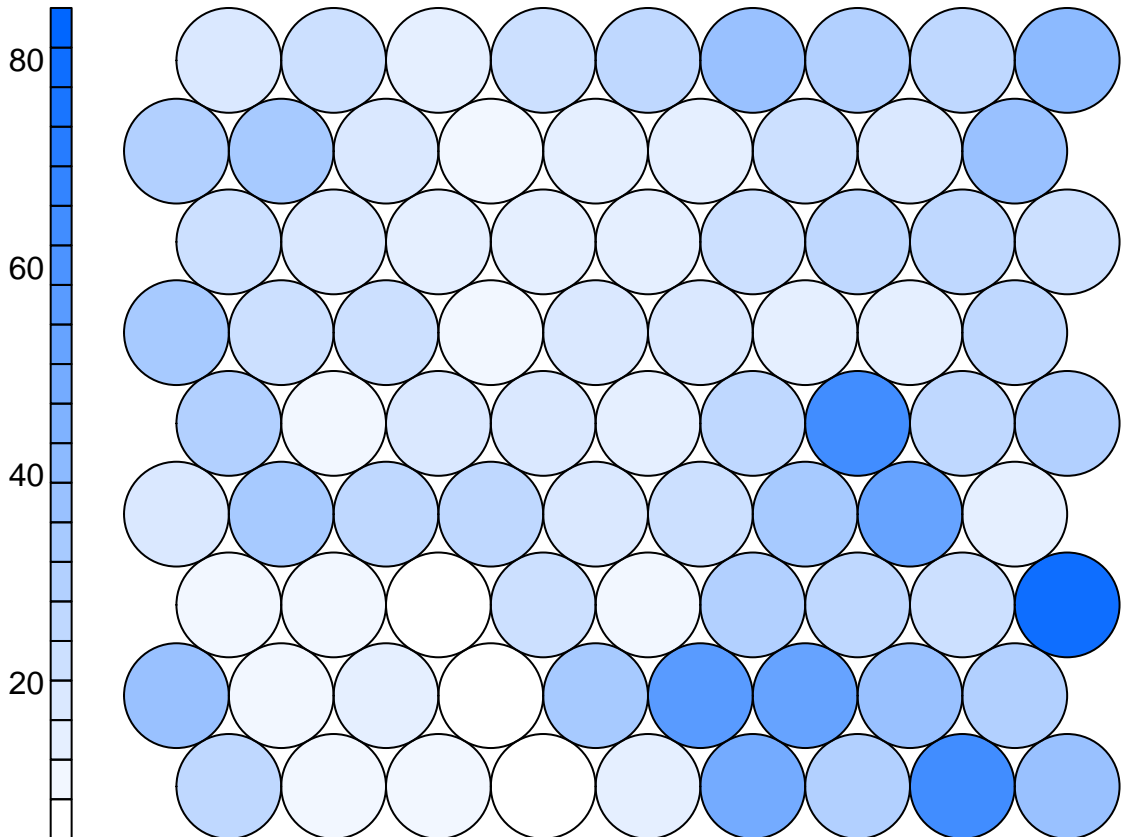


Codes plot

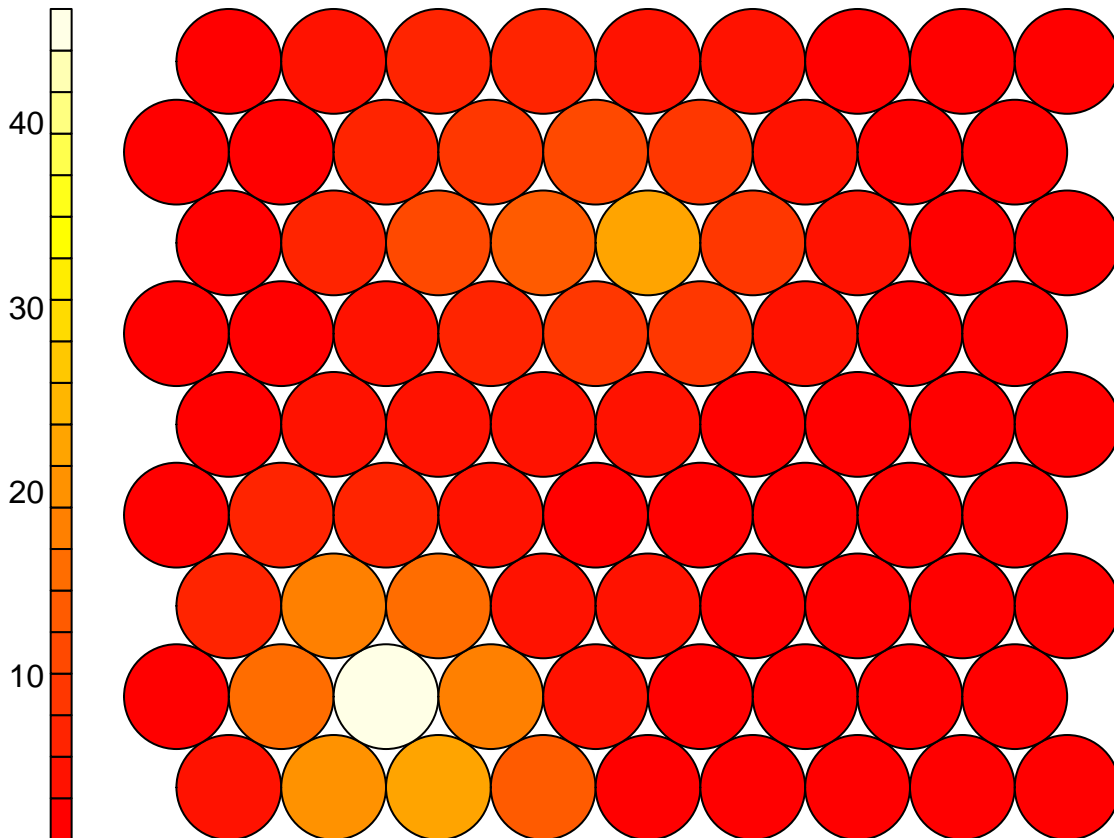


■ H_ss	■ c_PB
■ B_ss	■ d_PB
■ E_ss	■ e_PB
■ G_ss	■ f_PB
■ I_ss	■ g_PB
■ T_ss	■ h_PB
■ S_ss	■ i_PB
■ X._ss	■ j_PB
■ o_ss	■ k_PB
■ o_ss.1	■ l_PB
■ o_ss.2	■ m_PB
■ o_ss.3	■ n_PB
■ o_ss.4	■ o_PB
■ o_ss.5	■ p_PB
■ o_ss.6	■ polar

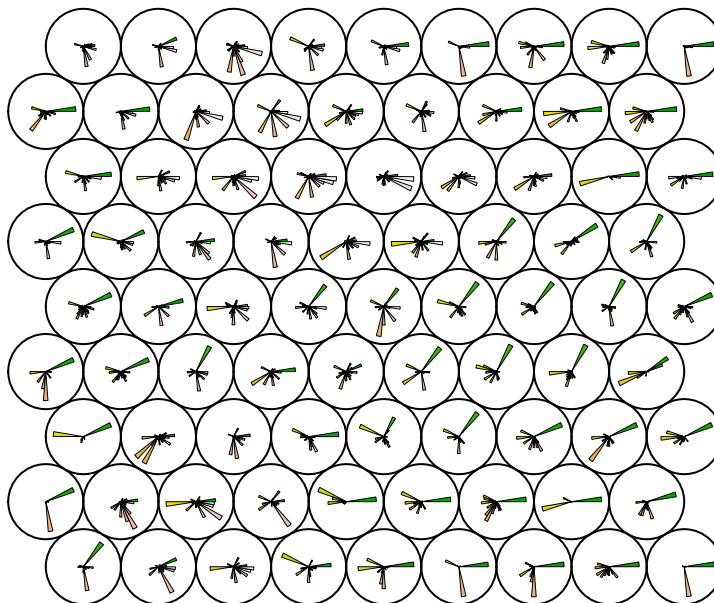
Carte de Kohonen toroidal n= 9



Neighbour distance plot

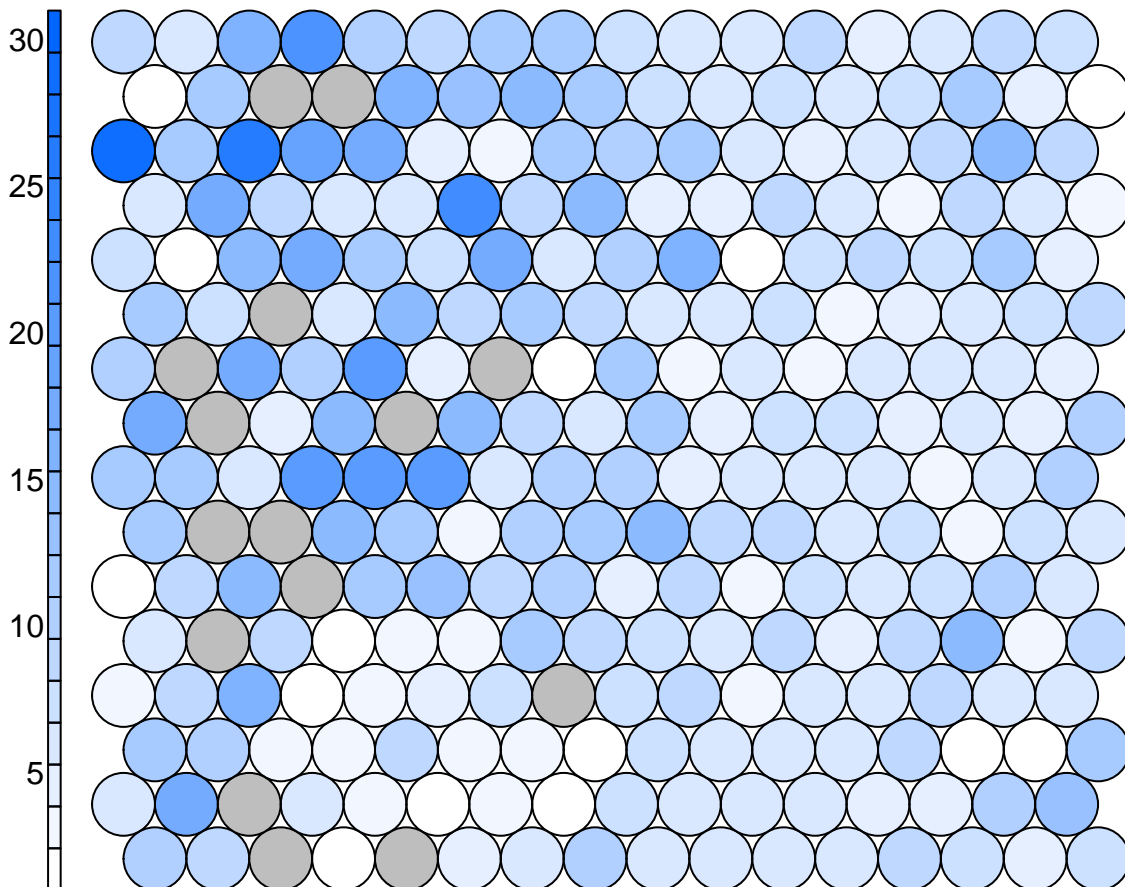


Codes plot

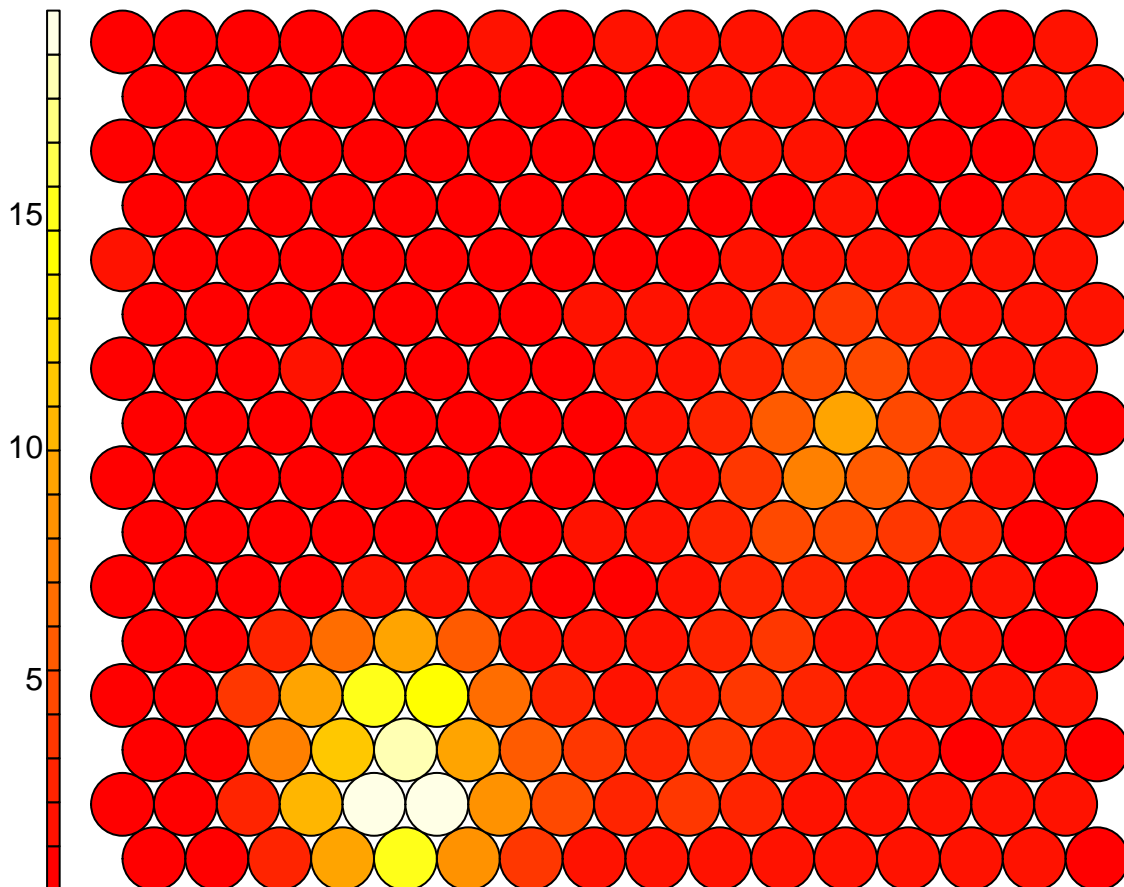


■ H_ss	■ c_PB
■ B_ss	■ d_PB
■ E_ss	■ e_PB
■ G_ss	■ f_PB
■ I_ss	■ g_PB
■ T_ss	■ h_PB
■ S_ss	■ i_PB
■ X_ss	■ j_PB
■ o_ss	■ k_PB
■ o_ss.1	■ l_PB
■ o_ss.2	■ m_PB
■ o_ss.3	■ n_PB
■ o_ss.4	■ o_PB
■ o ss.5	■ o PB

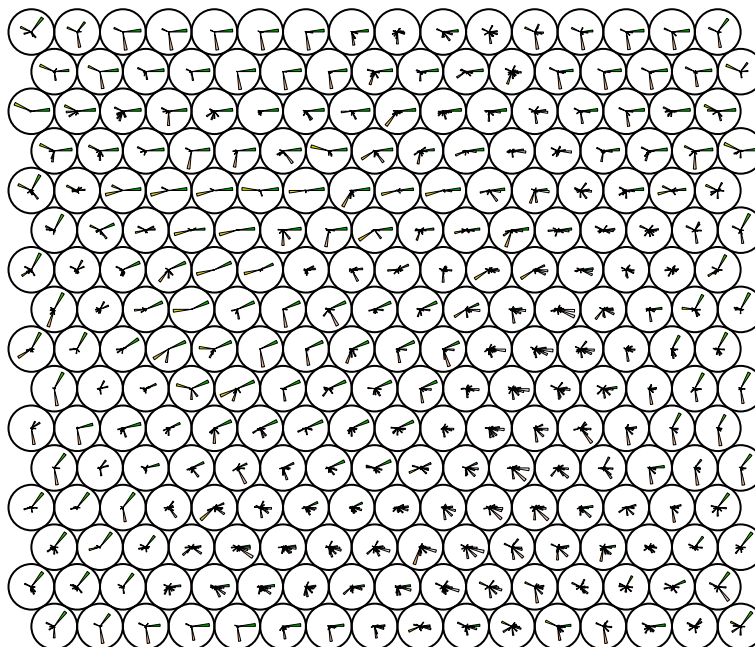
Carte de Kohonen toroidal n= 16





























Neighbour distance plot



Codes plot



	H_ss		c_PB
	B_ss		d_PB
	E_ss		e_PB
	G_ss		f_PB
	I_ss		g_PB
	T_ss		h_PB
	S_ss		i_PB
	X_ss		j_PB
	o_ss		k_PB
	o_ss.1		l_PB
	o_ss.2		m_PB
	o_ss.3		n_PB
	o_ss.4		o_PB

Carte de Kohonen toroidal n= 25

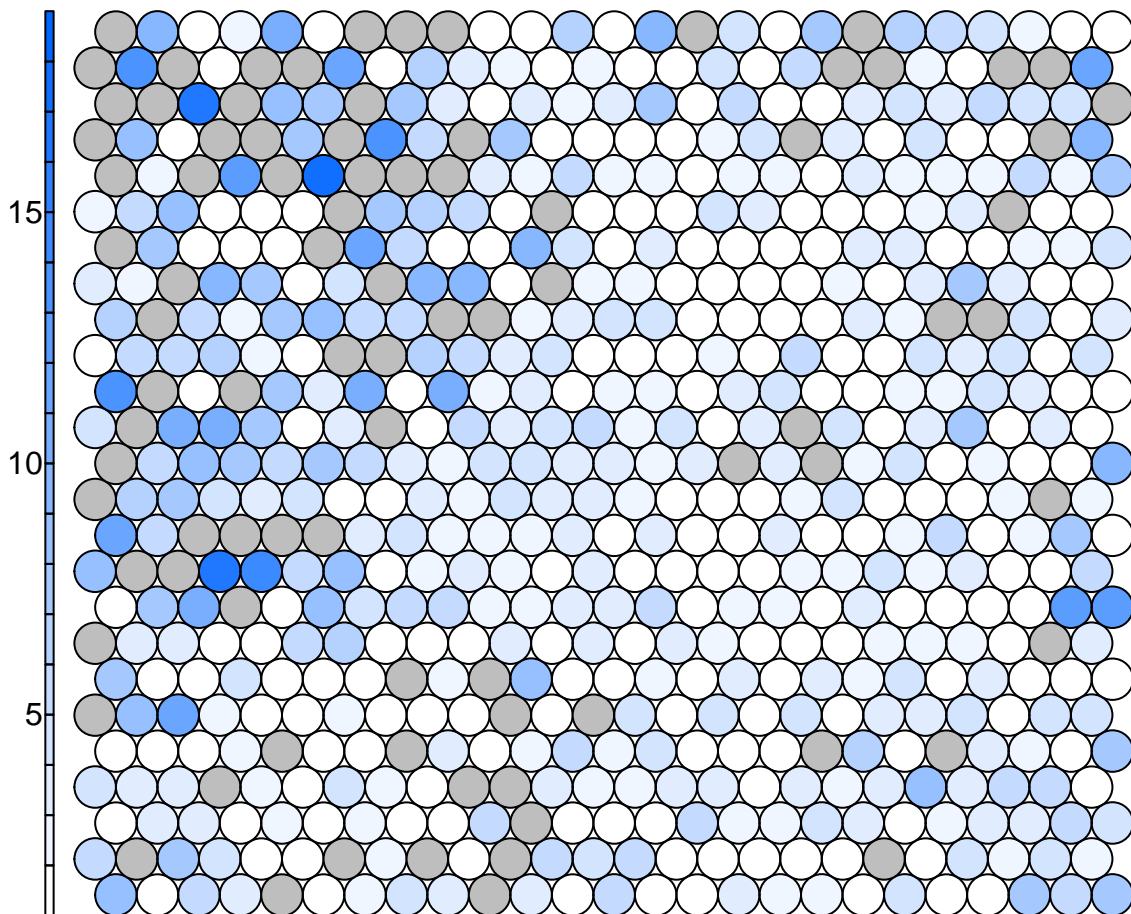
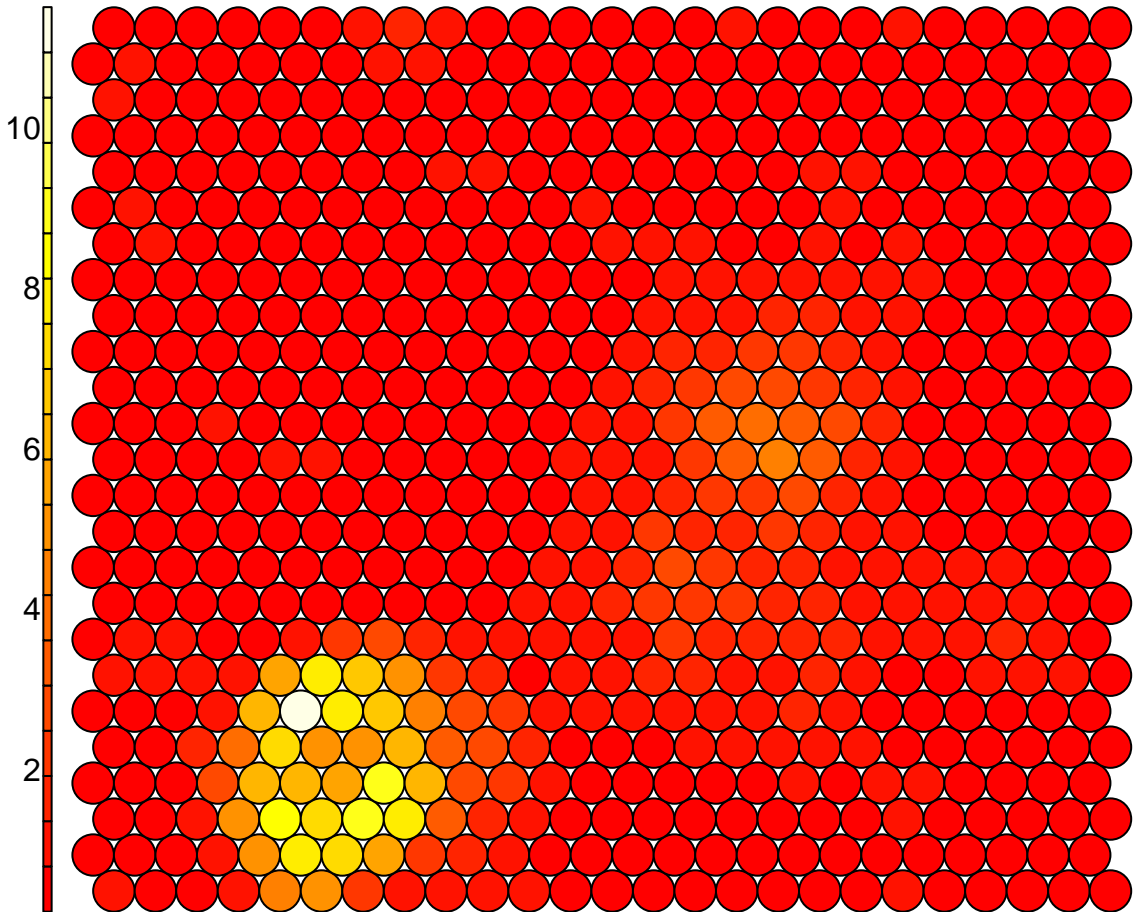
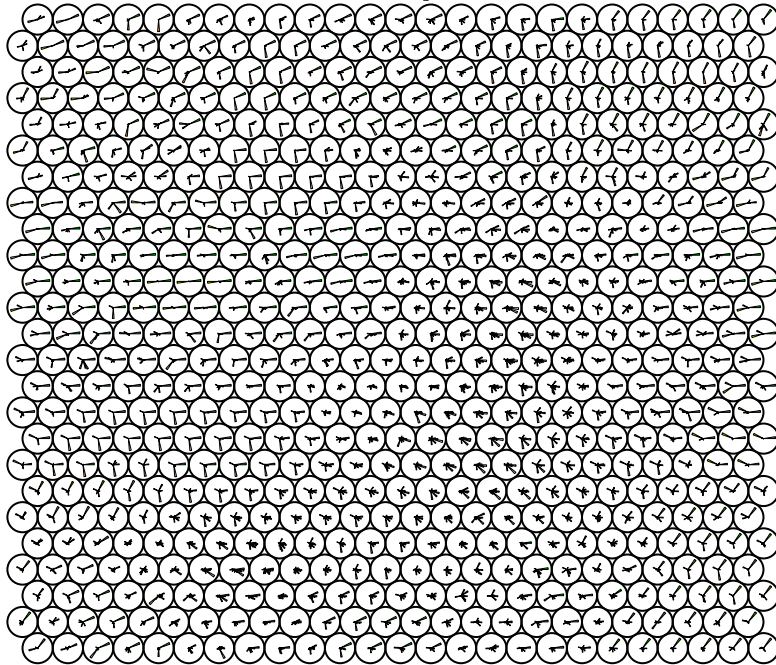




























Figure 1 shows a 2D visualization of a hexagonal lattice of particles. The lattice is composed of red circles, with a small cluster of yellow and white circles in the lower-left corner. A color bar on the left indicates the value of the parameter, ranging from 0 (dark red) to 10 (yellow).



Codes plot



	H_ss		c_PB
	B_ss		d_PB
	E_ss		e_PB
	G_ss		f_PB
	I_ss		g_PB
	T_ss		h_PB
	S_ss		i_PB
	X_ss		j_PB
	o_ss		k_PB
	o_ss.1		l_PB
	o_ss.2		m_PB
	o_ss.3		n_PB
	o_ss.4		o_PB