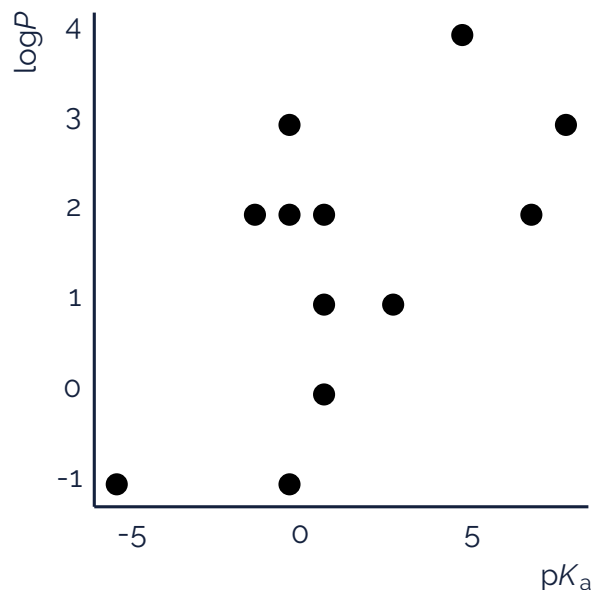


Clustering of compounds

You are developing an extraction method for analysis of pesticides. You have a bunch of analytes. All of the extraction methods (liquid-liquid extraction as well as SPE) you are thinking of could be affected by the polarity of the compound as well as its acid-base properties. Therefore, you would like to know if your analytes would need to be classified into different classes and treated separately or is it valid to assume one cluster. For this purpose, please perform (1) hierarchical clustering or (2) k-means clustering. Below is given a table with the $\log P$ and pK_a values as well as a rough visualization you can use.



Pesticide	pK_a	$\log P$
Aldicarb sulfoxide	1	0
Aldicarb sulphone	0	-1
Demeton-S-methyl sulfoxide	-5	-1
Carbendazim	7	2
Methomyl	1	1
Thiabendazole	8	3
Methiocarb sulfoxide	-1	2
Methiocarb sulphone	0	2
Aldicarb	3	1
Imazalil	5	4
Thiodicarb	1	2
Phorate sulfoxide		
Phorate sulphone		
Methiocarb	0	3