

Supporting Information

An investigation of the use of spectral clustering for the analysis of molecular data

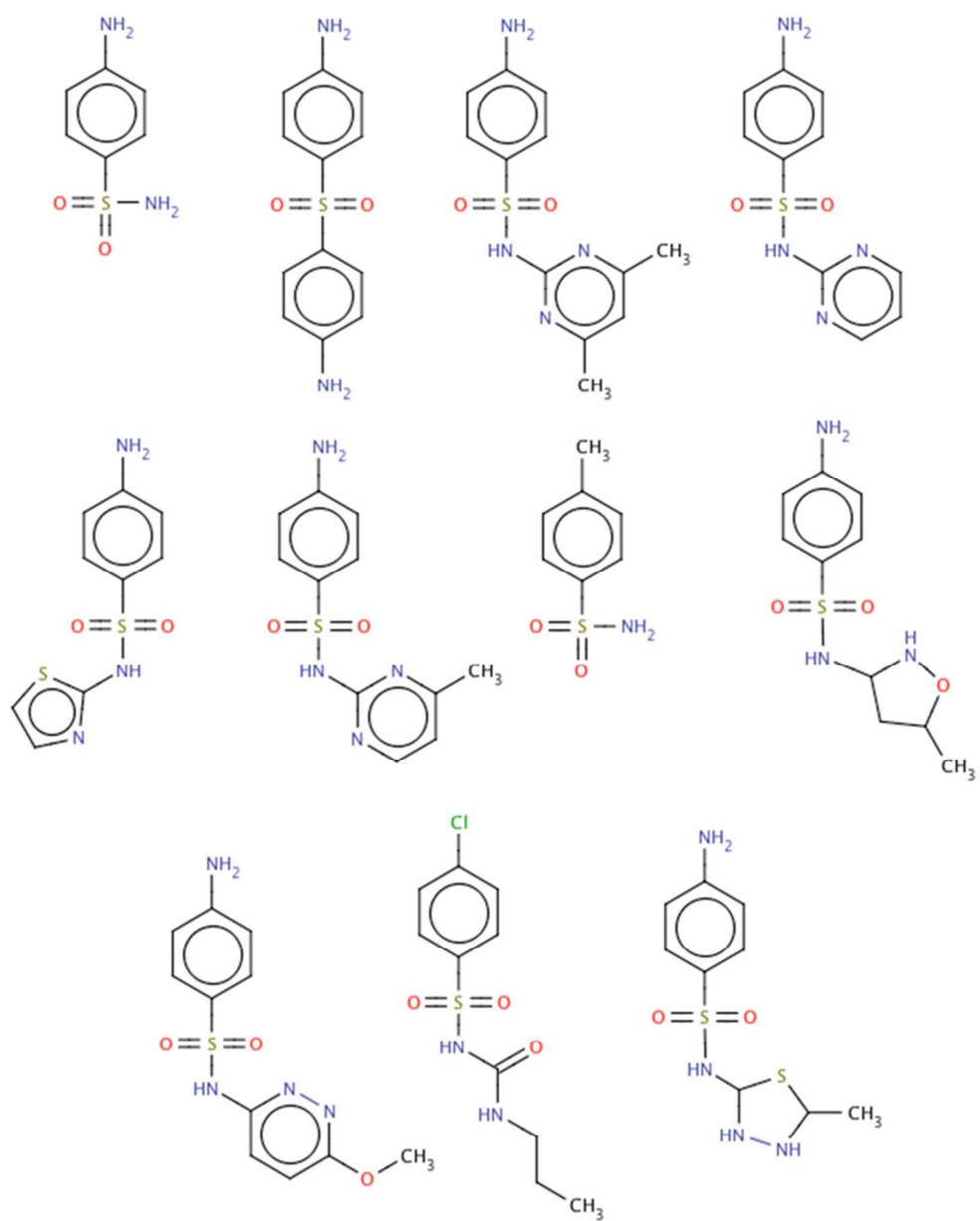
Sonny Gan¹, David A. Cosgrove², Eleanor J. Gardiner¹ and Valerie J Gillet^{1*}

¹ Information School, University of Sheffield, Regent Court, 211 Portobello Street, Sheffield
S1 4DP, United Kingdom.

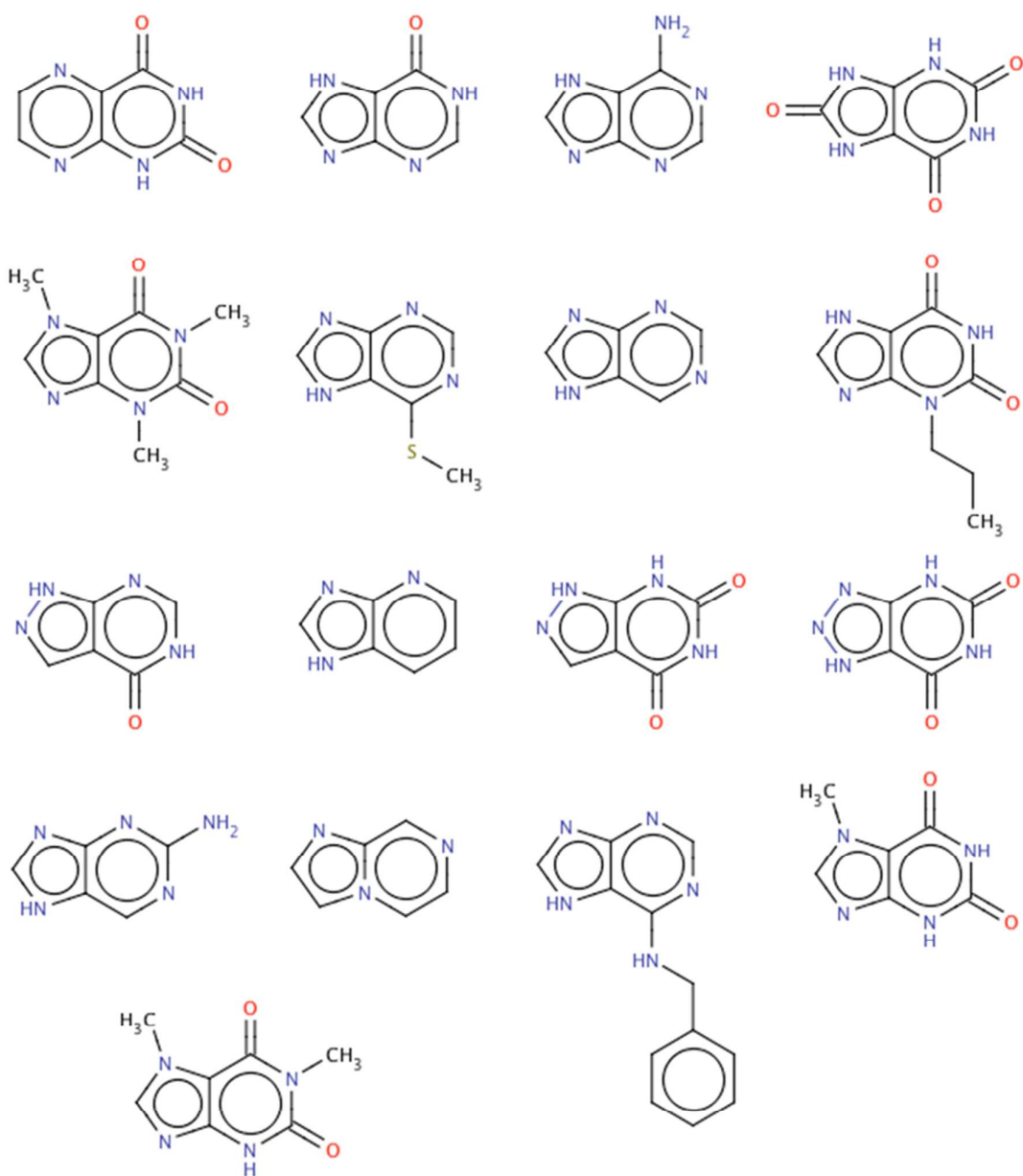
² AstraZeneca, Mereside, Alderley Park, Macclesfield SK10 4TG, United Kingdom.

* Author to whom all correspondence should be addressed: e-mail v.gillet@sheffield.ac.uk

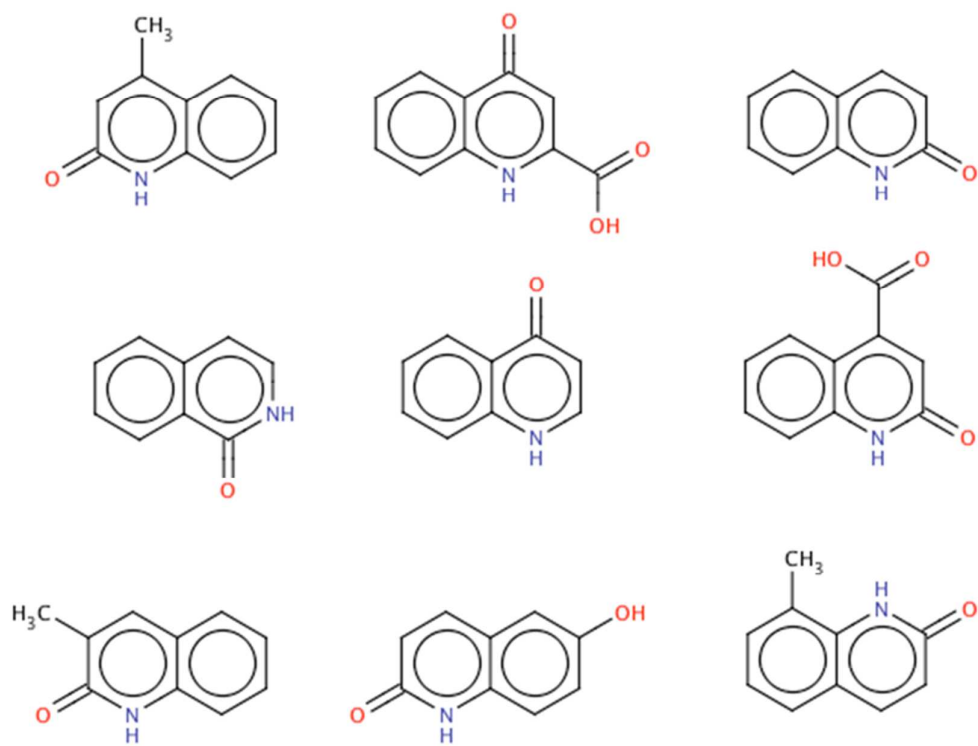
Ideal Clusters from DC100 Fragment Class



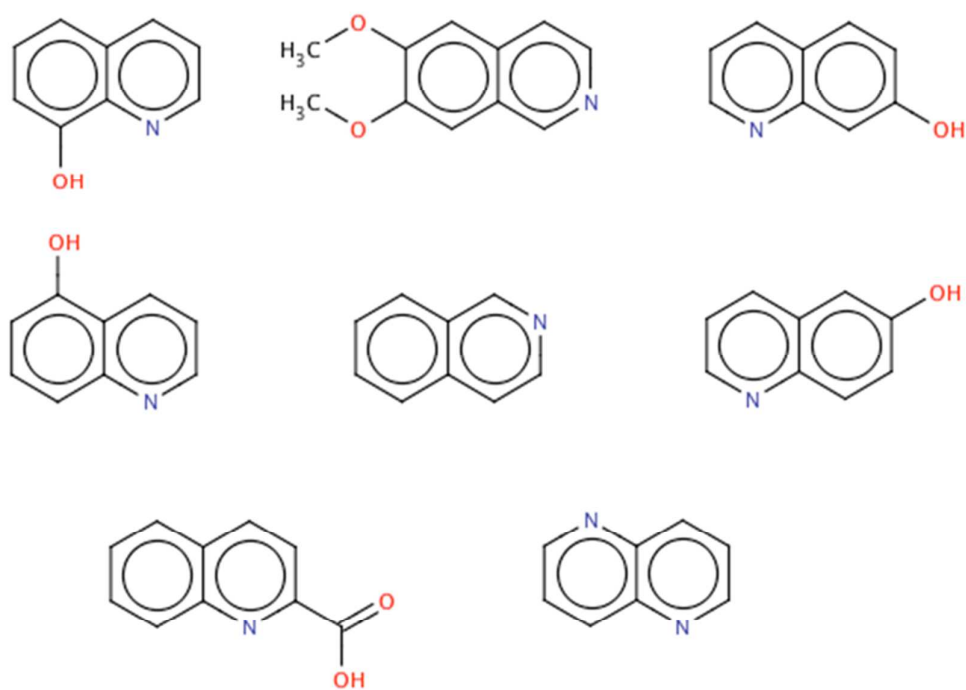
Cluster 1



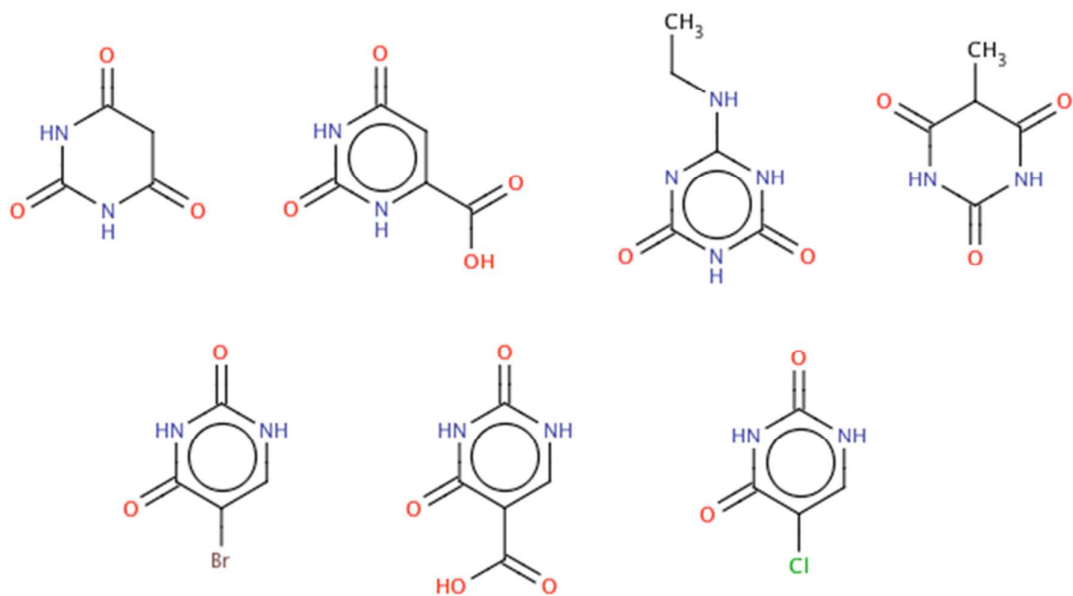
Cluster 2



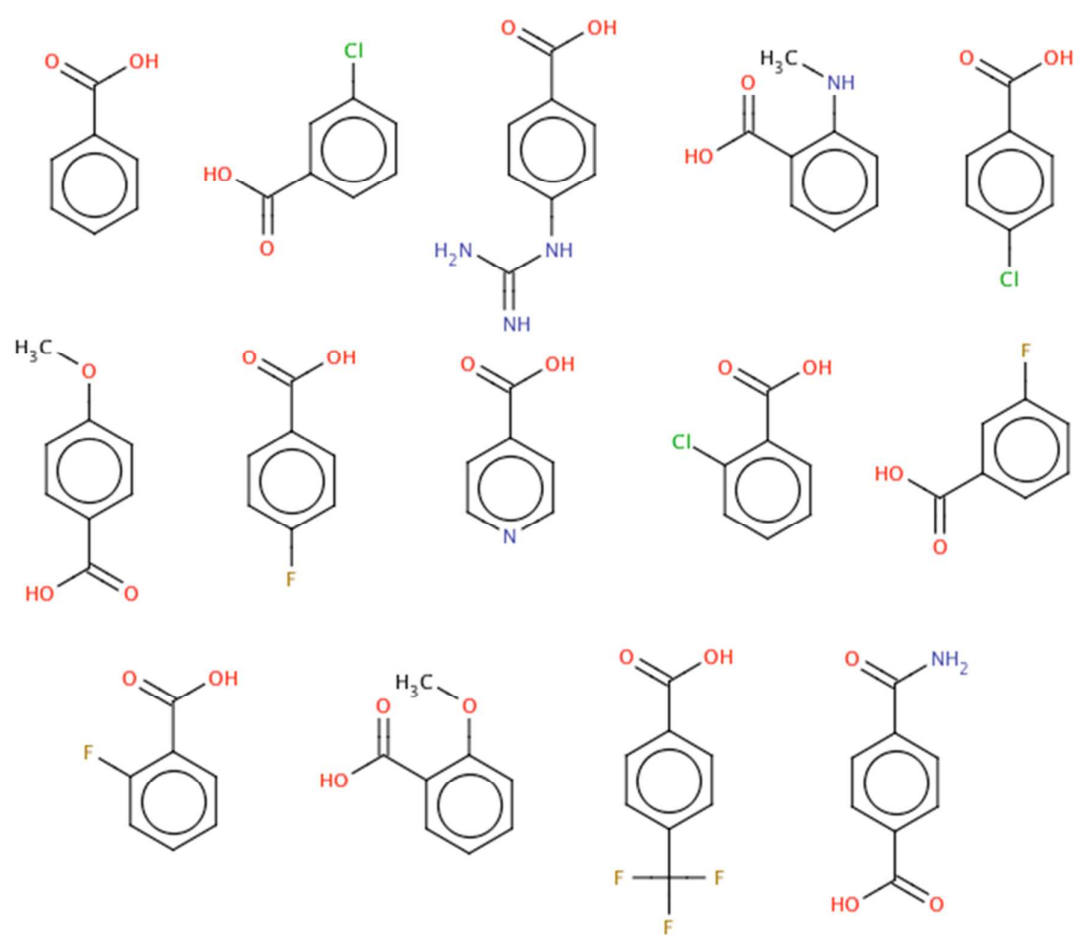
Cluster 3



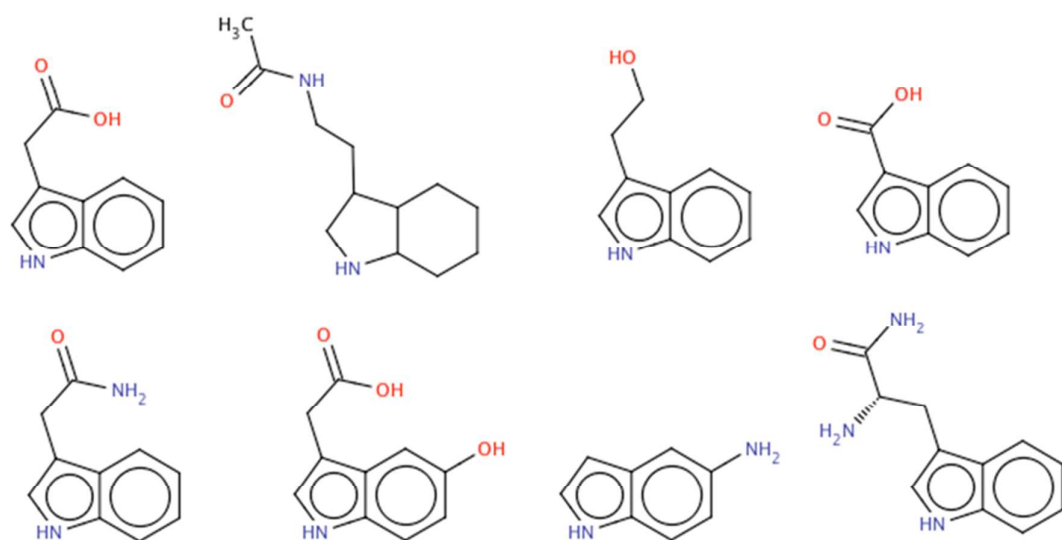
Cluster 4



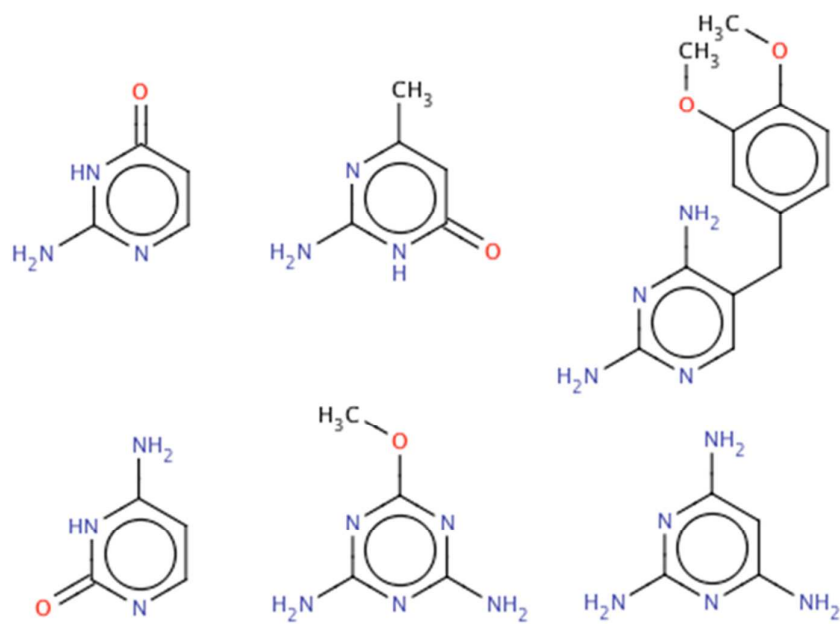
Cluster 5



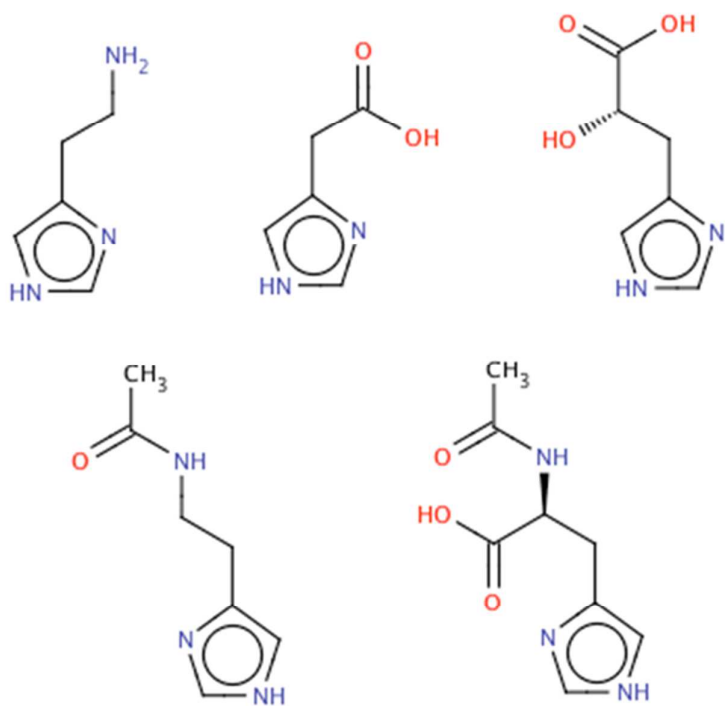
Cluster 6



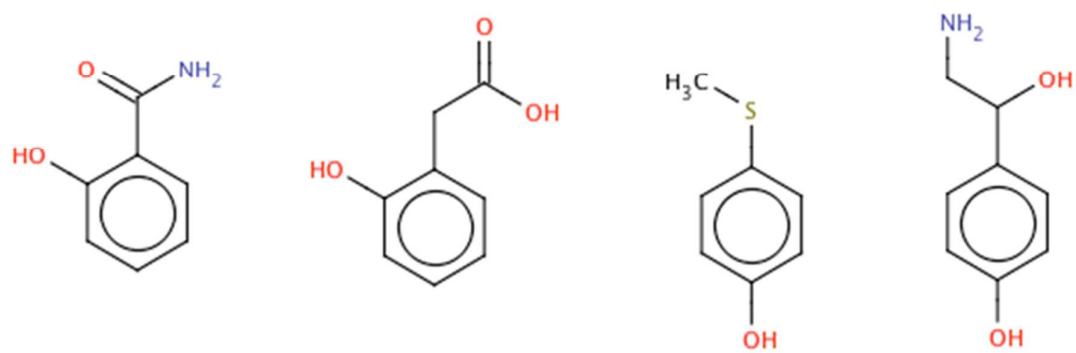
Cluster 7



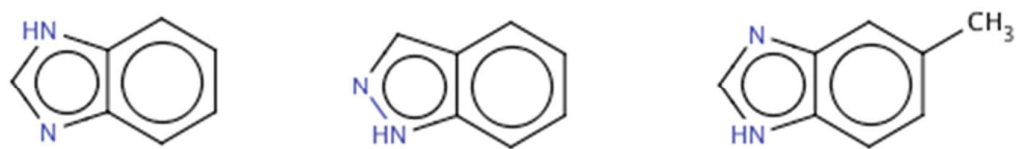
Cluster 8



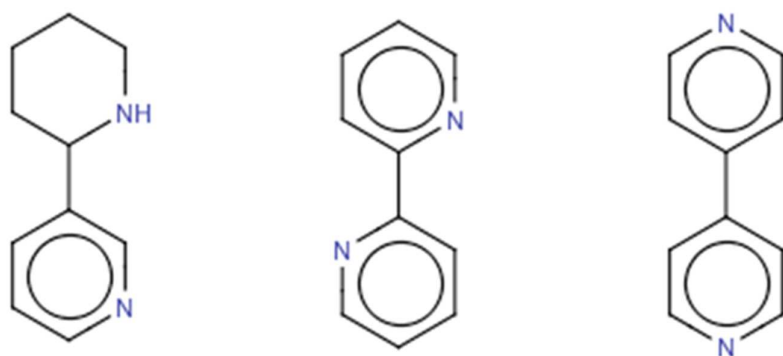
Cluster 9



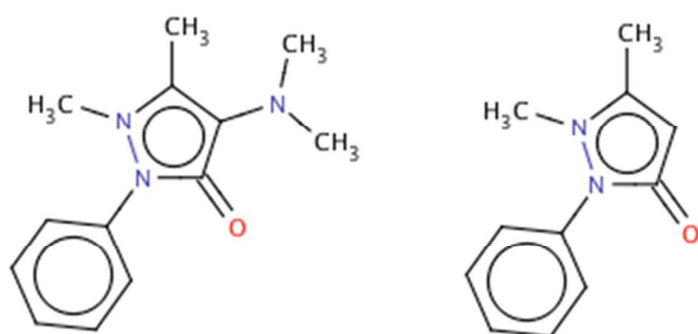
Cluster 10



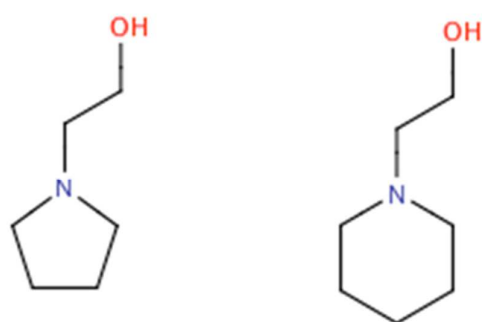
Cluster 11



Cluster 12



Cluster 13



Cluster 14