

ACS Symposium Series 2016 vol.1222, pages 243-267

Visualization of a multidimensional descriptor space

Gaspar H., Baskin I., Varnek A.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

© 2016 American Chemical Society. In this chapter, we review some concepts and techniques used to visualize chemical compounds represented as objects in a multidimensional descriptor space. Several modern dimensionality reduction techniques are compared with respect to their ability to visualize the data in 2D space, using as example a dataset of acetylcholinesterase inhibitors and their decoys.
