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Trainor:discoveryandidentificationofleadcompoundsfromcombinational
Indeed every single chemist reported properties that were never identified as important by our SNB or RF classifiers. The question of consensus among chemists is a complex one; accordingly we approached it in a number of ways.

Manyofthesedescriptorsweredirectlycalculatedwithstandardcomponent
of Medicinal Chemistry 54 : - Part 6 Topics in drug design and discovery: macromolecular X-ray crystallography and NMR as tools for structure-based drug design, J.