In this example we will use the Profile Builder in StarDrop's MPO Explorer module to derive a multi-parameter scoring profile
, based on a data set initially described by Wager et al. [ACS Chem. Neurosci. 1 p. 435 (2010)]. Wager et al. used this data set to develop a multi-parameter optimisation method for selection of compounds intended for CNS indications. Wager's 'CNS MPO score' is calculated as the sum of the values of desirability functions for six physicochemical parameters, calculated logP (clogP), calculated logD at pH 7.4 (clogD), molecular weight (MW), topological polar surface area (TPSA), number of hydrogen bond donors (HBD) and the pKa of the most basic center (pKa), resulting in a value between 0 and 6. The authors compared the CNS MPO score for a set of 119 marketed drugs for CNS targets with 108 Pfizer CNS candidates and found that 74% of the marketed drugs achieved a desirability score of 4 compared with only 60% of the Pfizer candidates. The scoring profile derived by MPO Explorer will contain one or more rules that indicate combinations of properties that significantly increase the chances of identifying a drug and we will compare this with the results of the Wager et al. CNS MPO score.

To try this example yourself, please visit the Tutorials section of the Community. If you don't have access to StarDrop or the optional modules and would like to arrange a free trial license, please email us at
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