

Supplementary material

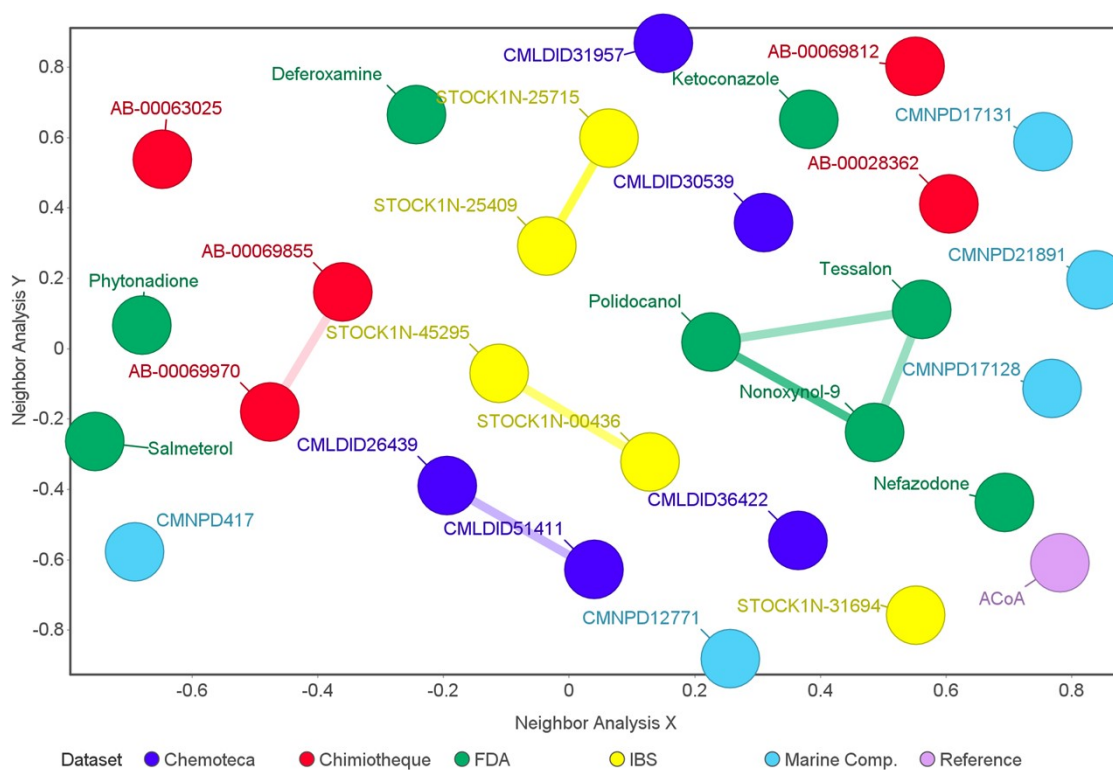


Figure S1. Similarity chart calculated using the SkelSpheres Descriptor of Datawarrior.

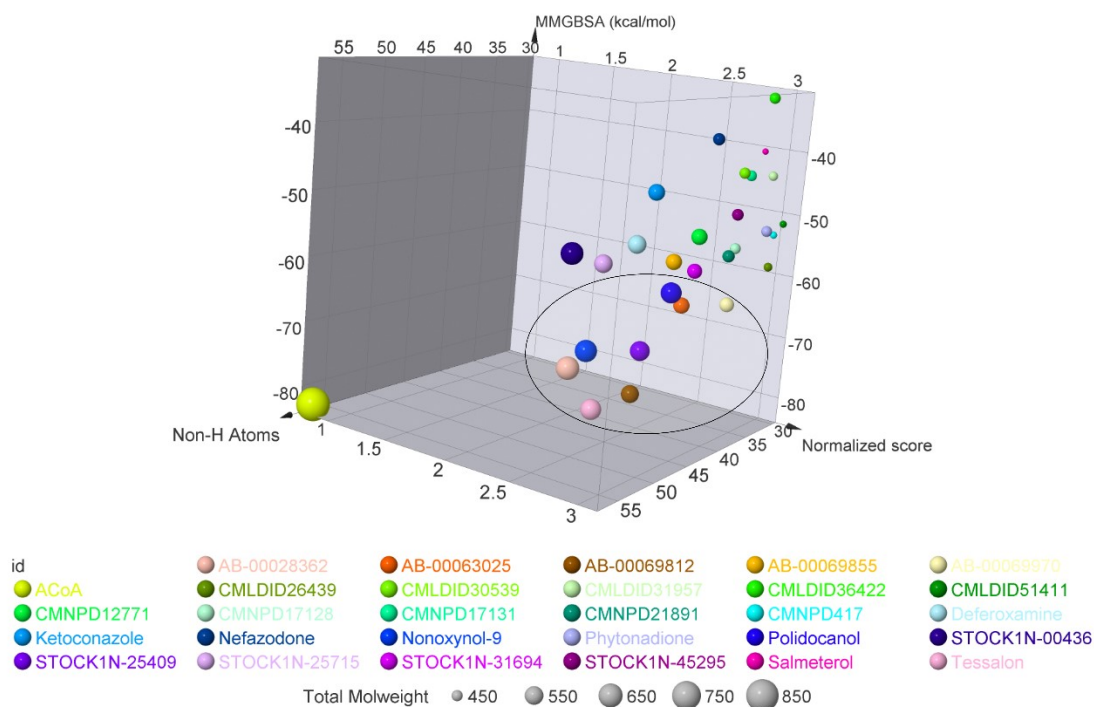


Figure S2. 3D graphic showing the results with the normalized ChemPLP score (x axis), MMGBSA (kcal/mol - estimated binding free energies) values (y axis) and number of heavy atoms (z axis). The size of the sphere represents the total molecular weight (g/mol). The compounds selected for experimental testing are Tessalon, AB-00069812, AB-00028362, Nonoxynol-9, STOCK1N-25409, AB-00069970, AB-00063025 and Polidocanol, even though they present a slightly lower normalized score, because they present more negative binding free energies.