Determination of 2D pharmacophore with a new algorithm for determining emerging patterns. Application to 5-HT\textsubscript{7} ligands.

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Since many years, our laboratory (CERMN) has built a structure named ATBI which allows to test compounds on 5-HT\textsubscript{1A}, 5-HT\textsubscript{4}, 5-HT\textsubscript{5A}, 5-HT\textsubscript{6} and 5-HT\textsubscript{7} receptors. Chemistry and molecular modelling activities on 5-HT\textsubscript{7} receptors have led to the design of different chemical families with an interesting affinity on this receptor\textsuperscript{1}. The objective of this study is to visualize all our data in term of structure-activity relationship. Structural characteristics and physico-chemical properties\textsuperscript{2} of the derivatives are encoded by specific descriptors. Among them, the chemical or pharmacophore fingerprints have yielded very interesting results\textsuperscript{3}. Starting from 2D pharmacophore fingerprints\textsuperscript{4}, this poster will present a new approach using emerging patterns\textsuperscript{5,6} of pharmacophoric pairs in order to characterize the active 5-HT\textsubscript{7} ligands. These results will be compared with the 3D pharmacophore already obtained\textsuperscript{7}.