Determination of 2D pharmacophore with a new algorithm for determining emerging patterns. Application to 5-HT$_7$. 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$_{1A}$, 5-HT$_4$, 5-HT$_{5A}$, 5-HT$_6$ and 5-HT$_7$ receptors. Chemistry and molecular modelling activities on 5-HT$_7$ receptors have led to the design of different chemical families with an interesting affinity on this receptor[1]. The objective of this study is to visualize all our data in term of structure-activity relationship. Structural characteristics and physico-chemical properties[2] of the derivatives are encoded by specific descriptors. Among them, the chemical or pharmacophore fingerprints have yielded very interesting results[3]. Starting from 2D pharmacophore fingerprints[4], this poster will present a new approach using emerging patterns[5,6] of pharmacophoric pairs in order to characterize the active 5-HT$_7$ ligands. These results will be compared with the 3D pharmacophore already obtained[7].

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