3D-QSAR TOOLS FOR THE STRUCTURE-ACTIVITY ANALYSIS OF SINGLE SITE POLYMERIZATION CATALYSTS

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The knowledge of structure-activity relationships is important to design more efficient catalyst systems. We present a well-established statistical technique known as 3D-QSAR\(^1\) aimed to find quantitative structure-activity relationships. This tool has been successfully used in the field of drug design and we have pioneered its application to single site polymerization catalysts\(^2\). We describe in some detail the main steps performed in the application of the 3D-QSAR methodology to the single site catalyst case. Then we review the main results obtained in our group with this chemometric technique in the case of metallocene and post-metallocene catalysts in olefin polymerization.\(^3\)