

## ANEXO 5

Reporte MOE de la ecuación lineal realizada considerando a los 43 ligandos.

Activity Field : pIC50

Observations : 43

Descriptors : 13

CORRELATION COEFFICIENT (R2) : 0.64942

ESTIMATED LINEAR MODEL

pIC50 =

$$\begin{aligned}
 &10.59311 \\
 &+0.07963 * a\_aro \\
 &-0.24708 * std\_dim2 \\
 &+0.00157 * VEGAsurfarea \\
 &-0.30023 * SPARCpka \\
 &-0.00660 * VEGApolararea \\
 &-0.01602 * SlogP_VSA1 \\
 &+0.63523 * KierFlex \\
 &+0.00327 * E\_sol \\
 &+1.12399 * PEOE_PC- \\
 &-0.12550 * a_nS \\
 &+0.03168 * a\_acc \\
 &-0.33294 * a\_hyd \\
 &+0.35142 * chi1_C
 \end{aligned}$$