## Score vs RMSD for tested proteins 2jam 2qfa 3e7o 3elj -8.0 **-**-7.5 **-**-3.0 **-**\_8 **-**-8.5 **-**-3.5 **-**-8.0 **-**\_9 **-**-9.0 **-**-4.0 **-**-8.5 **-**-10 **-**-9.5 **-**-4.5 **-**-11· -9.0 **-**4x21 3npc 3sx0 4agl -3.5 **-**−9.0 **-**-7.0 **-**-11 **-**-3.7 **-**−7.5 **-**−9.5 **-**-3.9 **-**-8.0 **-**-10.0 **-**-12 **-**-8.5 **-**-4.1 **-**-10.5 **-**Tool -9.0 **-**-4.3 **-**–13 ledock 514q 6e43 6q9y 6s1j smina -8.0 **-**\_9 **-**-8 vina -8.5 **-**\_8 **-**-10 **-**-9.0 **-**-10 **-**-9.5 **-**-11 **-**\_9 **-**-12 **-**-10.0 **-**-10.5 **-**0.0 2.5 5.0 7.5 10.0 12.5 0.0 2.5 5.0 7.5 10.0 12.5 0.0 2.5 5.0 7.5 10.0 12.5 6y4q -4.5 **-**-5.0 **-**-5.5 **-**

Score [Kcal/mol]

-6.0 **-**

-6.5 **-**

0.0 2.5 5.0 7.5 10.0 12.5