Molecules without sulfonamides 70000 Sage 2.0.0 Sage 2.1.0 Sage 2.2.0 60000 50000 40000 -30000 20000 10000 0 + -2.0-1.5-1.0-0.50.0 0.5 1.0 1.5 2.0 DDE (kcal/mol)