SUPPORTING INFORMATION FOR: Towards a Rationalization of Catalytic Activity Values by means of Local Hyper–Softness on the Catalytic Site. A Criticism About the Use of Net Electric Charges

Table 1: Relative reactivity descriptors on iron coming from: condensed nucleophilic Fukui function (r-f_{NN}^{+}{Fe}), condensed dual descriptor (r-f_{NNN}{Fe}), condensed nucleophilic local softness (r-s_{NN}^{+}{Fe}), condensed local hyper–softness (LHS, r-s_{NNN}{Fe}), global softness (r-S_{NN}) and global softness squared (r-S_{NN}^{2}). All of them are dimensionless.

	r-f_{NN}^{+}{Fe}	r-f_{NNN}{Fe}	r-s_{NN}^{+}{Fe}	r-s_{NNN}{Fe}	r-S_{NN}	r-S_{NN}^{2}
B3LYP:						
-NO$_2$	1.000	1.000	1.000	1.292	1.204	1.449
-H	1.168	1.170	1.026	1.167	1.058	1.119
-OCH$_3$	1.254	1.121	1.042	1.000	1.000	1.000
BP86:						
-NO$_2$	1.000	1.000	1.186	1.456	1.245	1.550
-H	1.052	1.067	1.056	1.110	1.053	1.108
-OCH$_3$	1.049	1.065	1.000	1.000	1.000	1.000
B97D:						
-NO$_2$	1.000	1.000	1.195	1.427	1.217	1.480
-H	1.018	1.020	1.047	1.078	1.047	1.096
-OCH$_3$	1.018	1.037	1.000	1.000	1.000	1.000
VSXC:						
-NO$_2$	1.000	1.000	1.187	1.543	1.254	1.572
-H	1.035	1.030	1.045	1.152	1.067	1.138
-OCH$_3$	1.056	1.019	1.000	1.000	1.000	1.000

Notice that, for every functional, sets of reactivity descriptors of the same type have been re defined according to the rule of dividing by the smallest value as explained in the article. This way of presenting different values, even of different order of magnitude in their original presentation allows one to realize qualitatively how better it is the relationship between a descriptor with the catalytic activity. So that, the descriptor that presents its closest relative value to the relative catalytic activity will be the best descriptor to explain catalytic activity values. As can be observed, the relative values of local hyper-softness (r-s_{NNN}{Fe}) reveals that local hyper-softness is the most appropriate descriptor that rationalizes the catalytic activity.
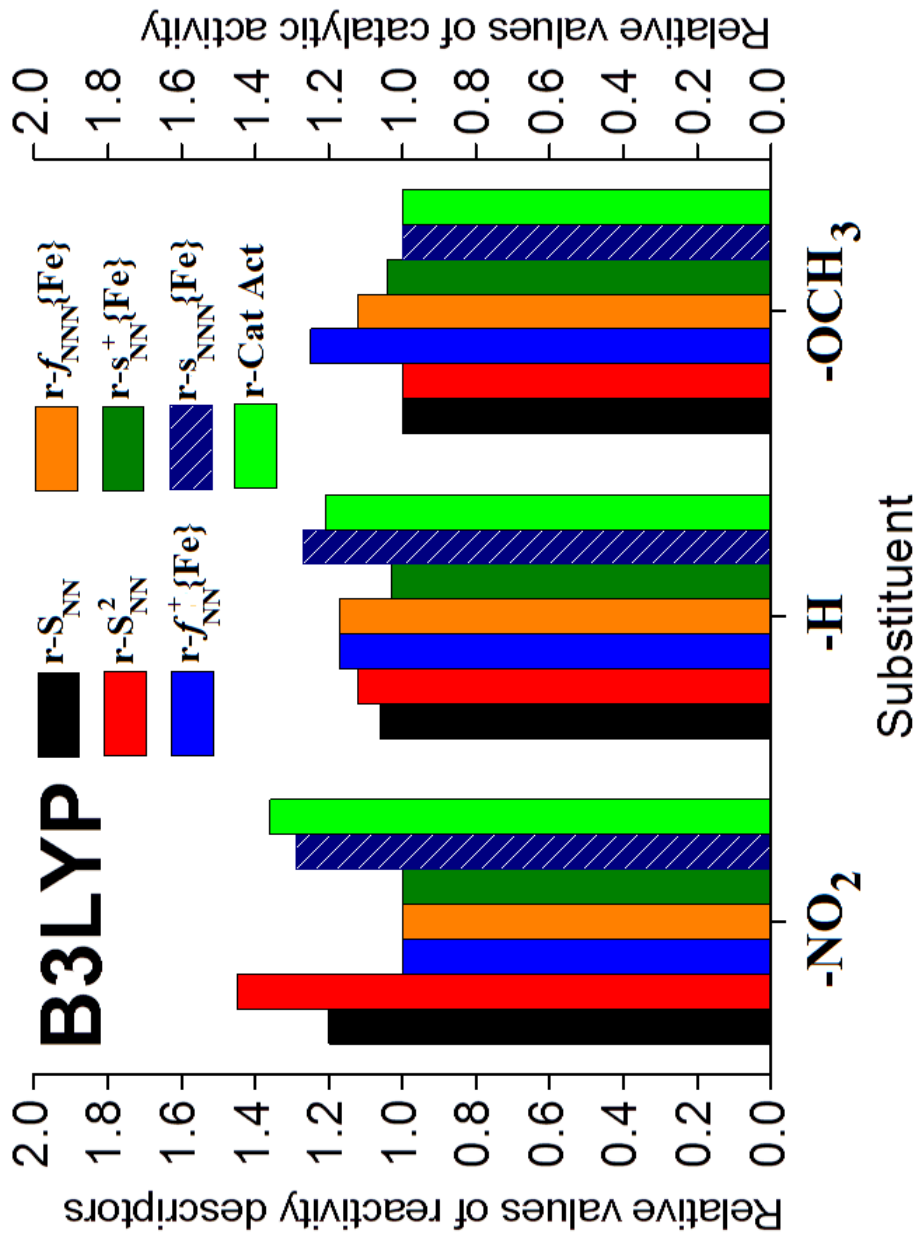
Figure 1: Bar graphs of relative descriptors condensed on iron atom along with relative catalytic activity (r-CatAct) at the B3LYP level of theory.
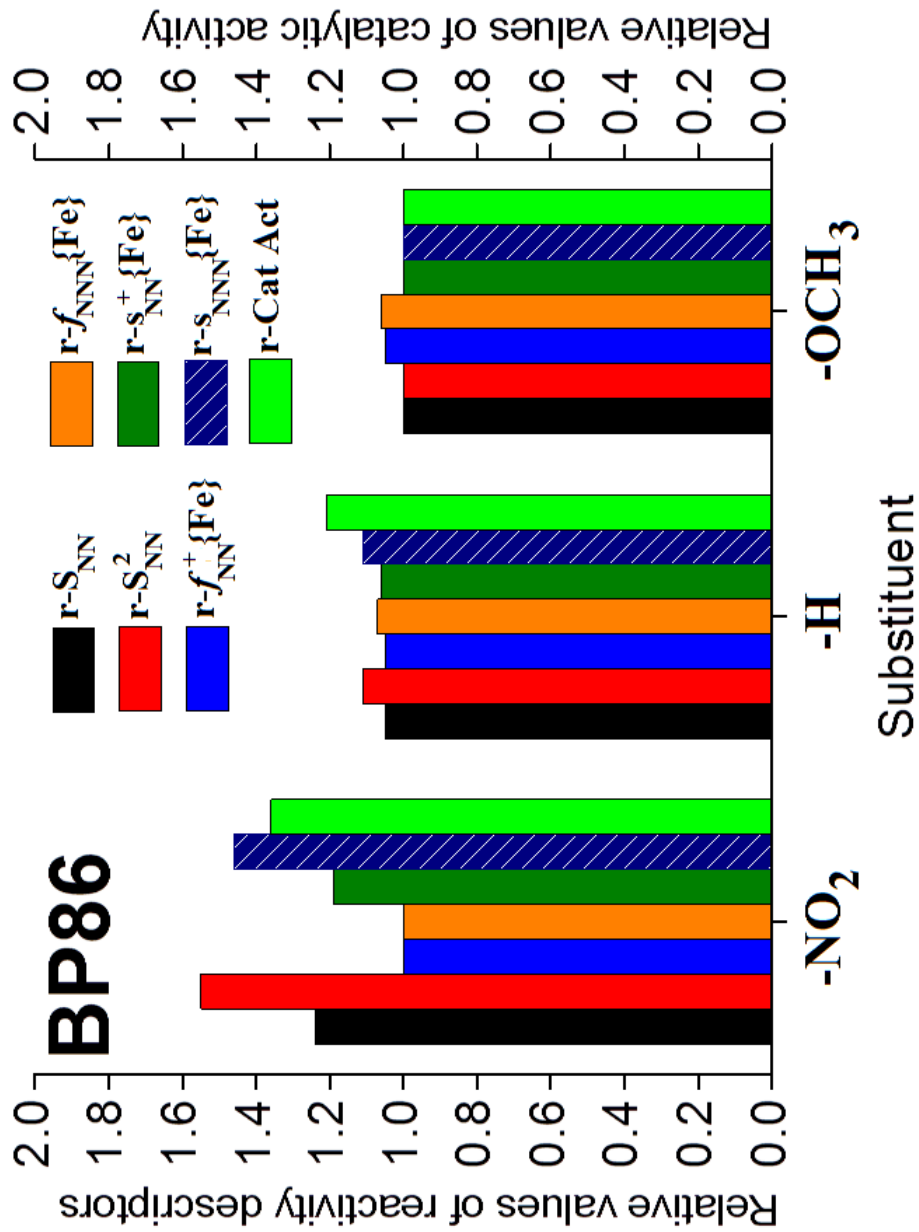
Figure 2: Bar graphs of relative descriptors condensed on iron atom along with relative catalytic activity (r-CatAct) at the BP86 level of theory.
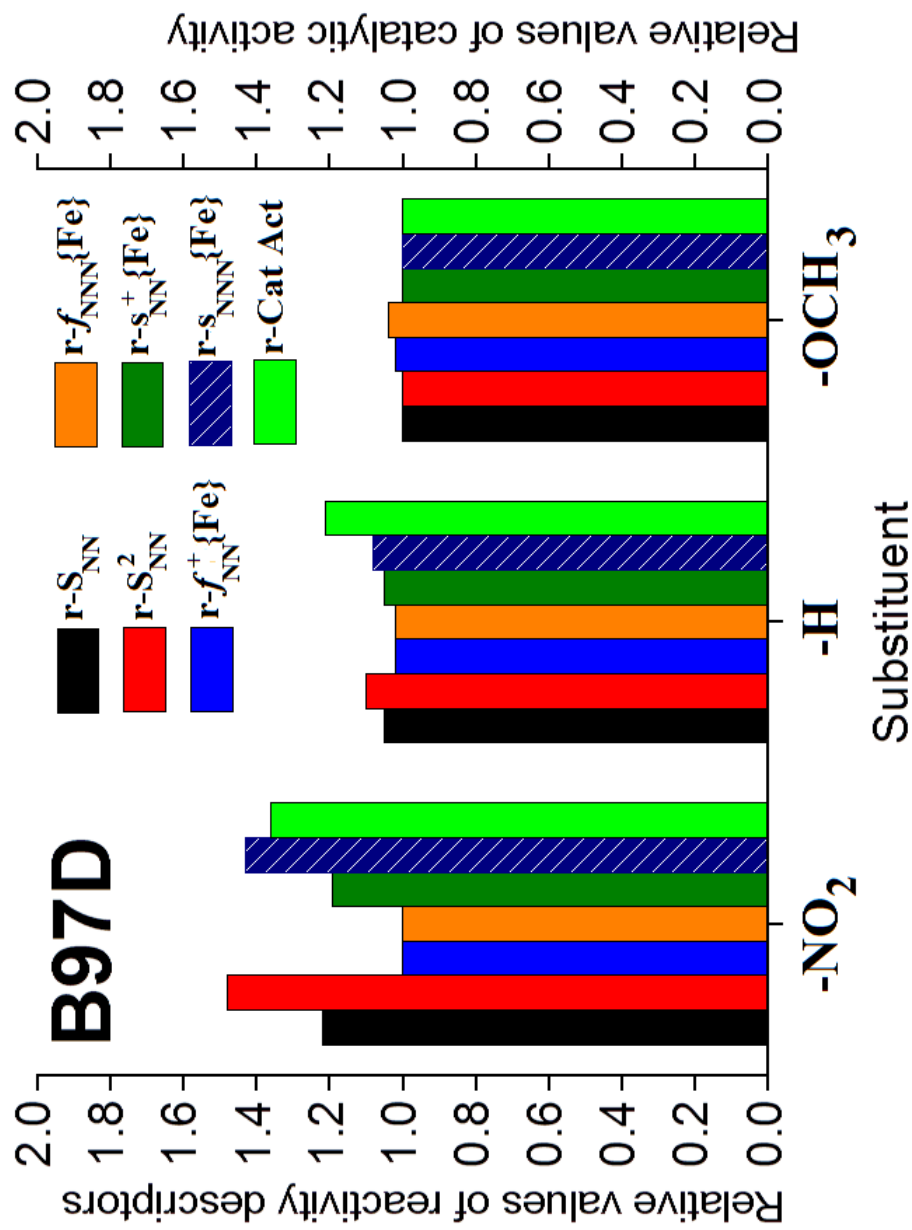
Figure 3: Bar graphs of relative descriptors condensed on iron atom along with relative catalytic activity (r-CatAct) at the B97D level of theory.
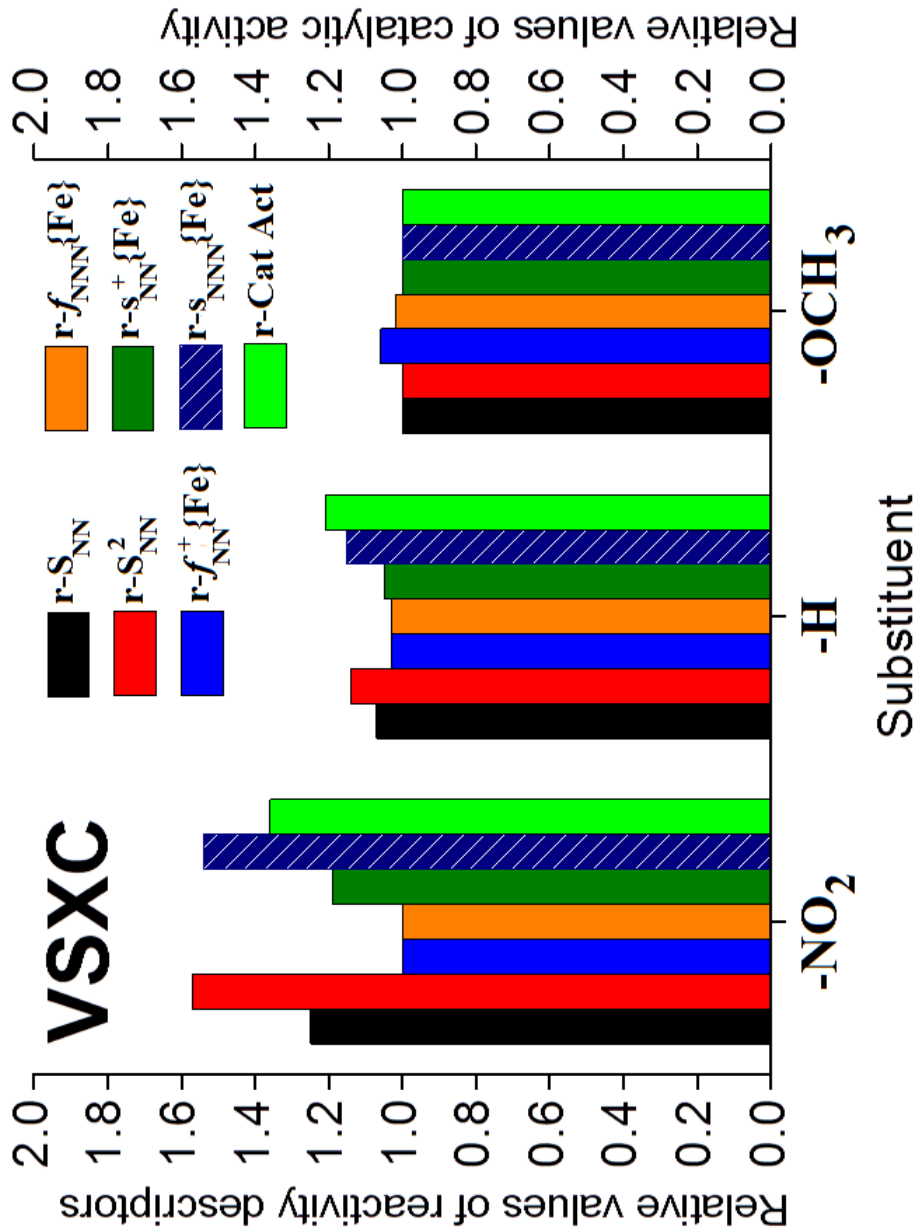
Figure 4: Bar graphs of relative descriptors condensed on iron atom along with relative catalytic activity (r-CatAct) at the VSXC level of theory.