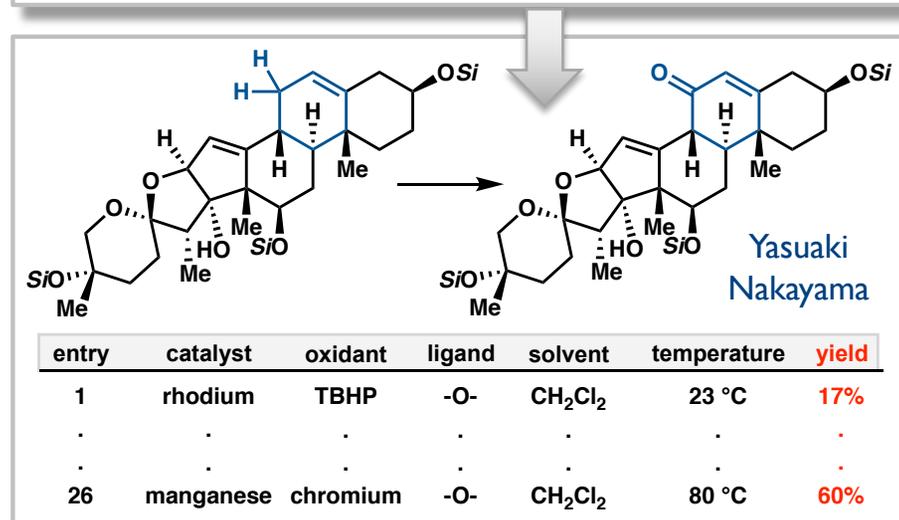
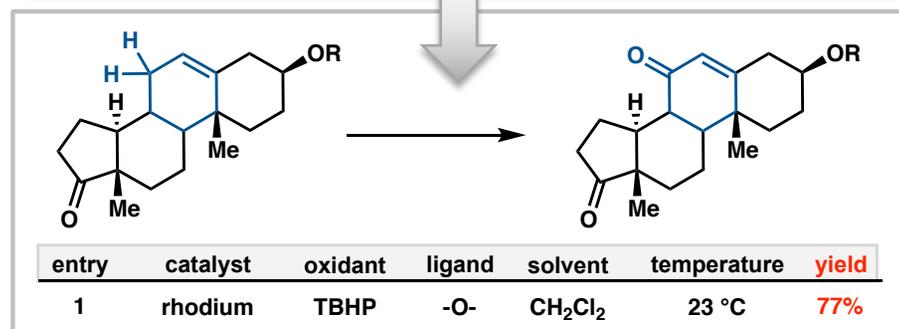
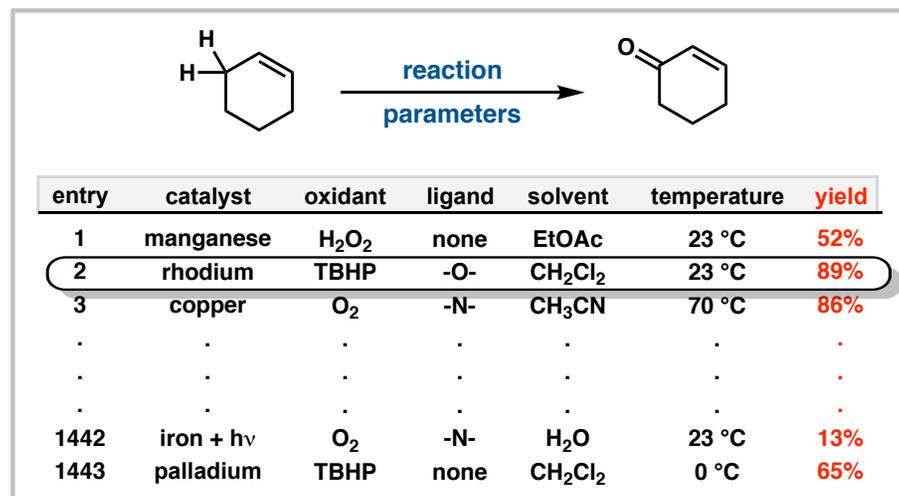


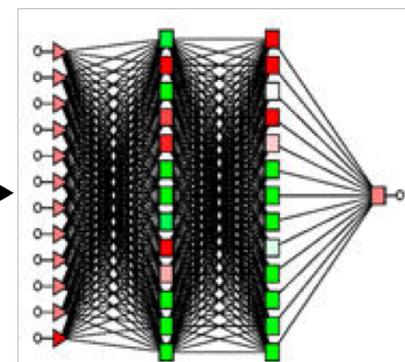
Machine Learning in Organic Chemistry



$$\Delta\text{Yld}(\%) = \sum_{q=1}^{q_{\max}} \sum_{g=1}^{g_{\max}} a_{q,g} \cdot \Delta V_k(m_q, m'_q)_g + \sum_{r=1}^{r_{\max}} b_r \cdot \Delta V(c_r, c'_r) + e_0$$



Train Test Loop



predictive model

