The ability to understand and manipulate metabolism is of great value in the chemical industry, as it opens the door to engineering organisms to make valuable small molecule chemicals and intermediates. However, even simple organisms like bacteria and yeast have extremely complex metabolic networks, consisting of typically well-characterized stoichiometric relationships and often poorly-characterized regulatory relationships. We will discuss applications of machine learning in two areas that are important to developing a predictive understanding of cellular metabolism: the analysis of systems-scale measurement of small molecules (a field known as metabolomics), and the development of dynamic, systems-scale models of metabolism. In the first area, we address the task of imputing missing values in large metabolomics datasets, which may be due to a near-zero measurement or an analytical error. We consider mixtures of both of these models of missingness and develop an imputation technique based on the k-nearest-neighbors approach that uses information that is otherwise typically discarded in such analyses. We show that for datasets with missingness that reasonably represents that of real datasets, our approach performs equal to or better than existing methods. In the second area, we address the task of identifying the unknown regulatory structure in a metabolic network using dynamic measurements of metabolite levels and a novel dynamic modeling framework we have developed. By training on a few simple models, we are able to substantially prune the large search space of candidate regulatory interactions in other simple models, and we have had reasonable success at identifying the true interactions from that search space. Taken together, these applications of machine learning in systems biology and metabolic engineering can help move towards more comprehensive and predictive models of metabolism at the systems scale.