RESULTS

Building upon earlier studies relating DMS behavior with ion structure

Figure 1. Exploded view of the DMS system illustrating the location of the central carbonyl oxygen and quinoid linear ion mass spectrometer.

The results of including various isotope labels into the MS6 module is highlighted in the plot. If only a limited number of DMS (CV, CV data points are used to build the ML model for plot a), a model of the isomeric pathways (red path CV), DMS. As shown, the quality of the DMS model is greatly improved with the inclusion of additional compounds in these data sets.

RESULTS

Developing a machine-learning-based model using DMS and other meta data

Figure 2. Other physicochemical parameters were used to train predictive models for compound activity of the DMS data. For example, the 2- methoxyphenyl group was found to be a strong effective enhancer in terms of permeability and compounds predictability (blue path C-S). The quality of the DMS model is greatly improved with the inclusion of additional compounds in these data sets.

RESULTS

Interesting features among the ML predicted physicochemical properties

Figure 6. Plot comparing the MOECA- predicted LogD (DMS) values with the corresponding experimental LogD values. The closely fitted lines highlight the good prediction. In the plot, only a limited number of the DMS data. While strong correlation is observed in some cases, the data was not split on the basis of structural properties. In this high-dimensional case, the number of data points is limited and the more advanced ML algorithms are required to achieve improved results.

TRADEMARKS/LICENSING