Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Getting SMART in Drug Discovery: Chemoinformatics Approaches for Mining Structure-Multiple Activity Relationships

Fernanda Saldívar-González, J. Jesús Naveja, Oscar Palomino-Hernández, José L. Medina-Franco

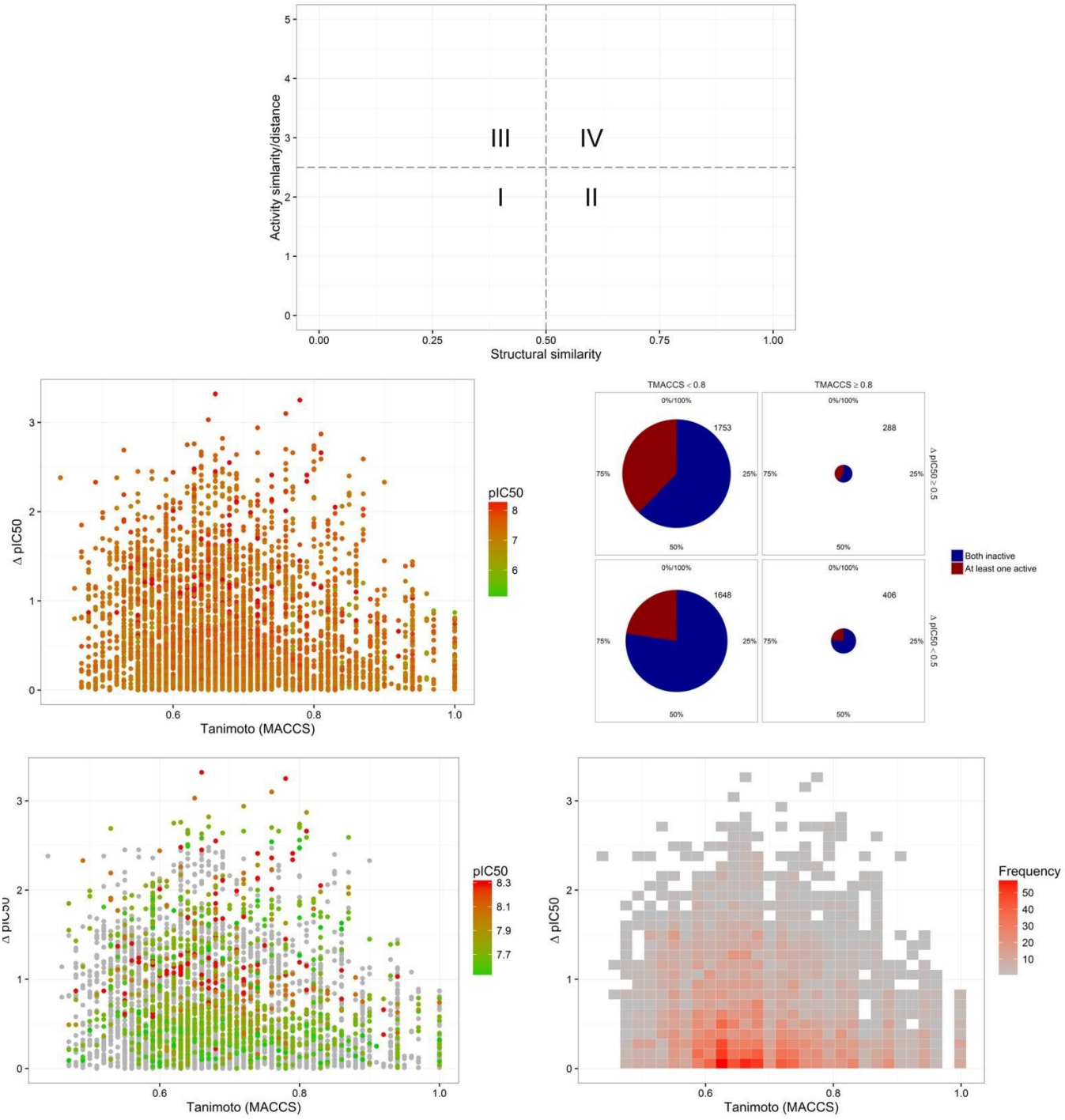

Figure S1. A) General form of the structure–activity similarity (SAS) maps showing four major regions. Regions I and II are associated with scaffold hopping and smooth SAR, respectively. Region III does not provide relevant information and region IV indicates discontinuous SAR and activity cliffs. Actual (B) and simplified SAS maps for a data set of 91 compounds tested against *Giardia intestinalis*: C) Categorical map showing the distribution of the data point in each of the four quadrants of the SAS map; D) Filtered map displaying the 'active regions' of the landscape i.e., pairs of compounds that contain at least one active molecular in the pair; and E) Density map that shows the amount of data points in each region using a continuous color scale from red (more data points) to gray color (less data points). The simplified SAS maps are designed to aid in the visual representation and interpretation of the SAS maps.

Cluster A

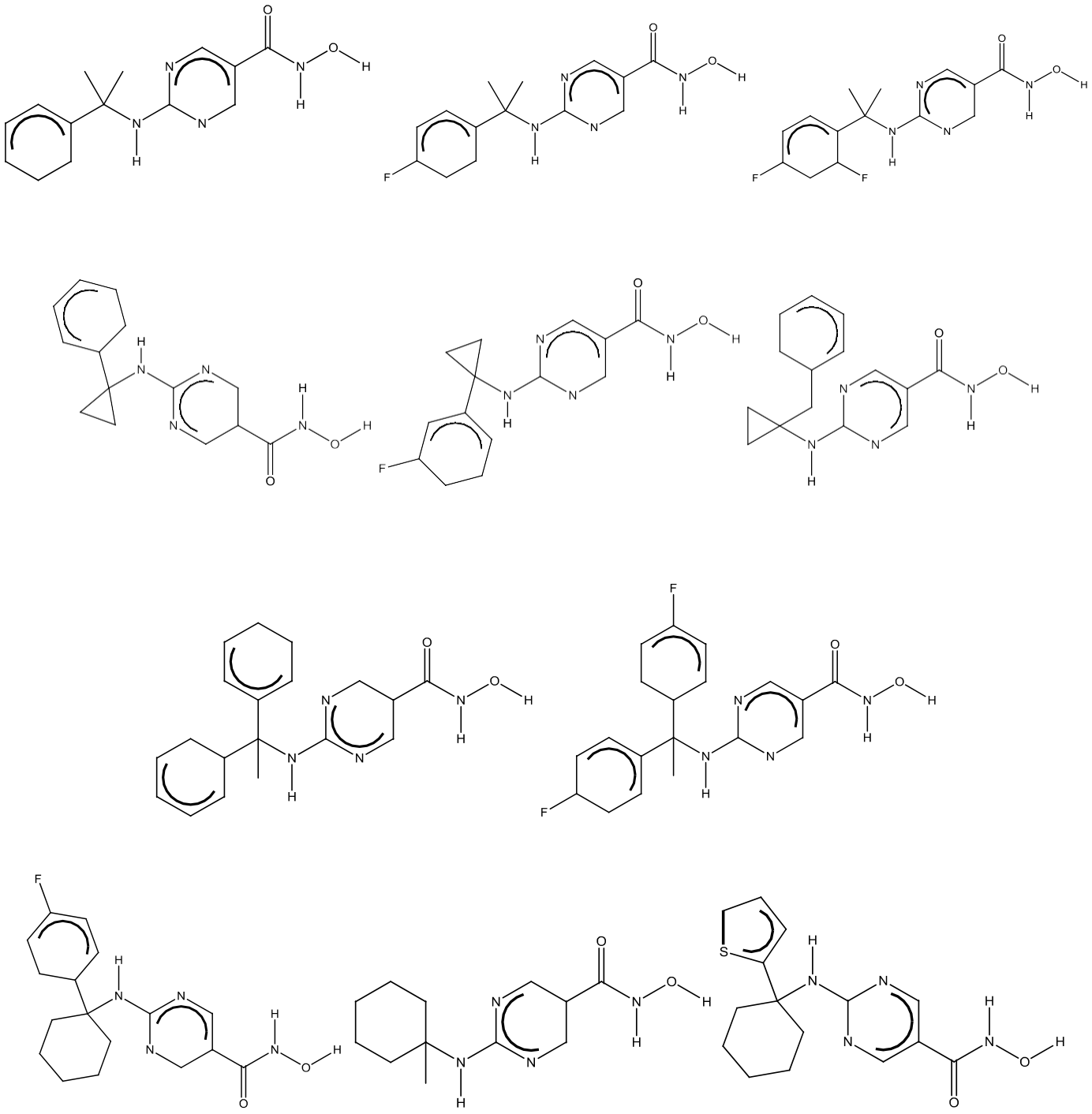

Figure S2. Chemical structures of the two main clusters obtained in the visual representation of the chemical space of 140 pyrimidine hydroxyl amide compounds (continued in next page).

Cluster B

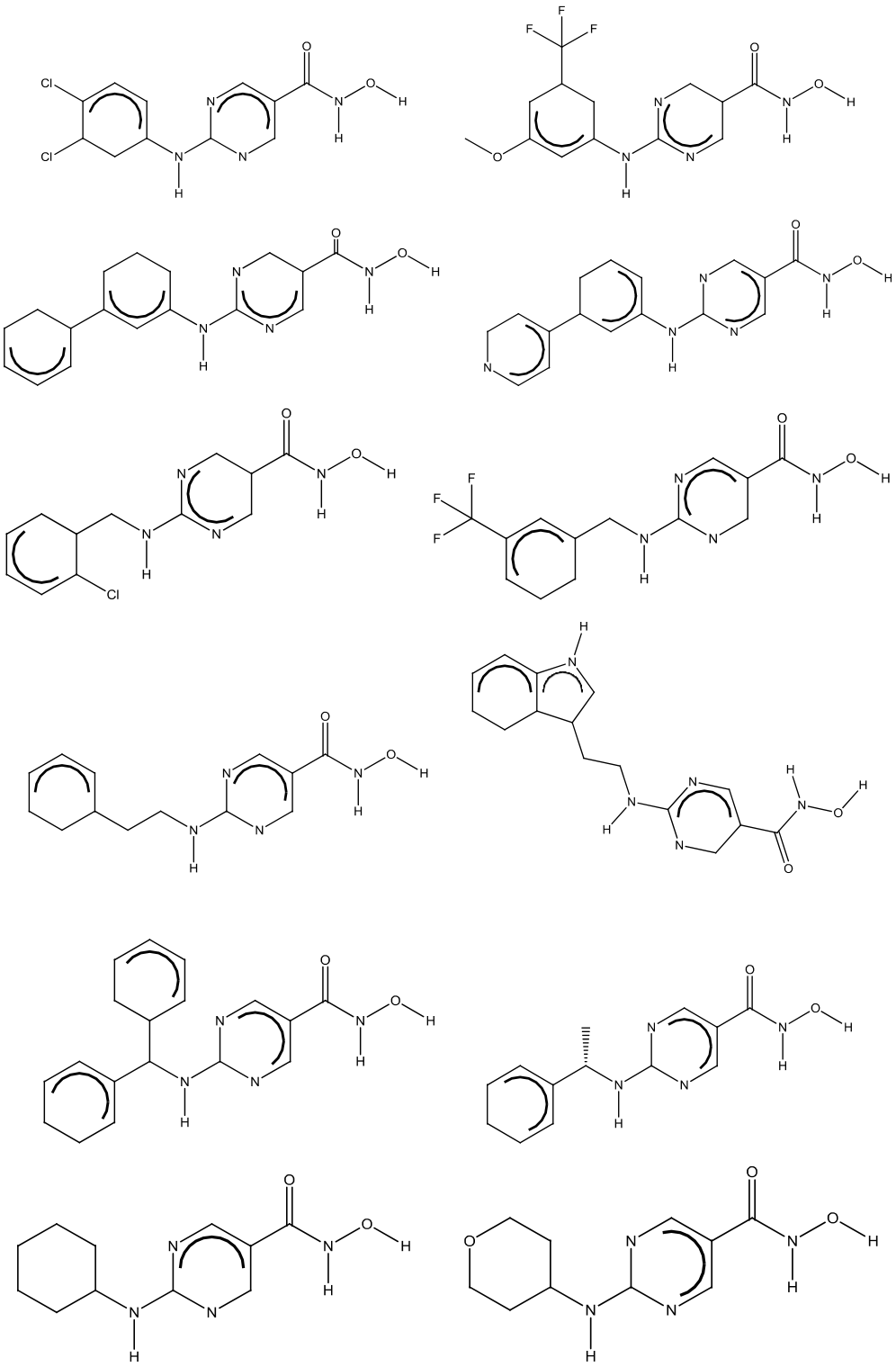

Figure S2 (contd.)