B.1 FLAVORDB STATISTICS

**Figure B.1.1:** Category-wise statistics of entities/ingredients and flavor molecules. (A) A pie chart depicting the number of ingredients in each of the 34 categories. (B) Bar plot showing the total number of unique flavor molecules in each of the 34 categories.
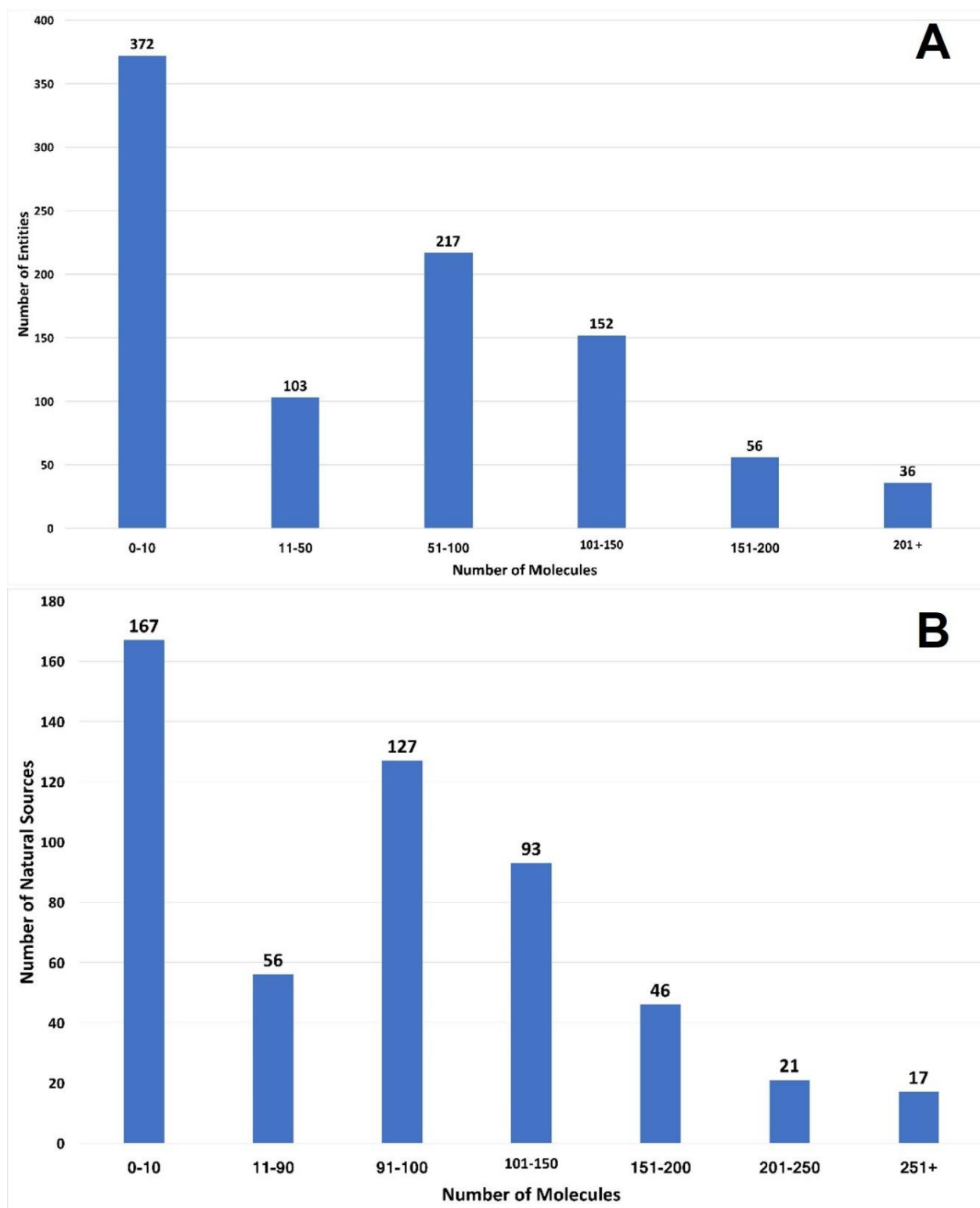
Figure B.1.2: Statistics of distribution of the number of flavor molecules across entities and their natural sources. Frequency distribution of the (A) number of Entities, and (B) the number of Natural Sources, across the range of 'Number of Flavor Molecules'.
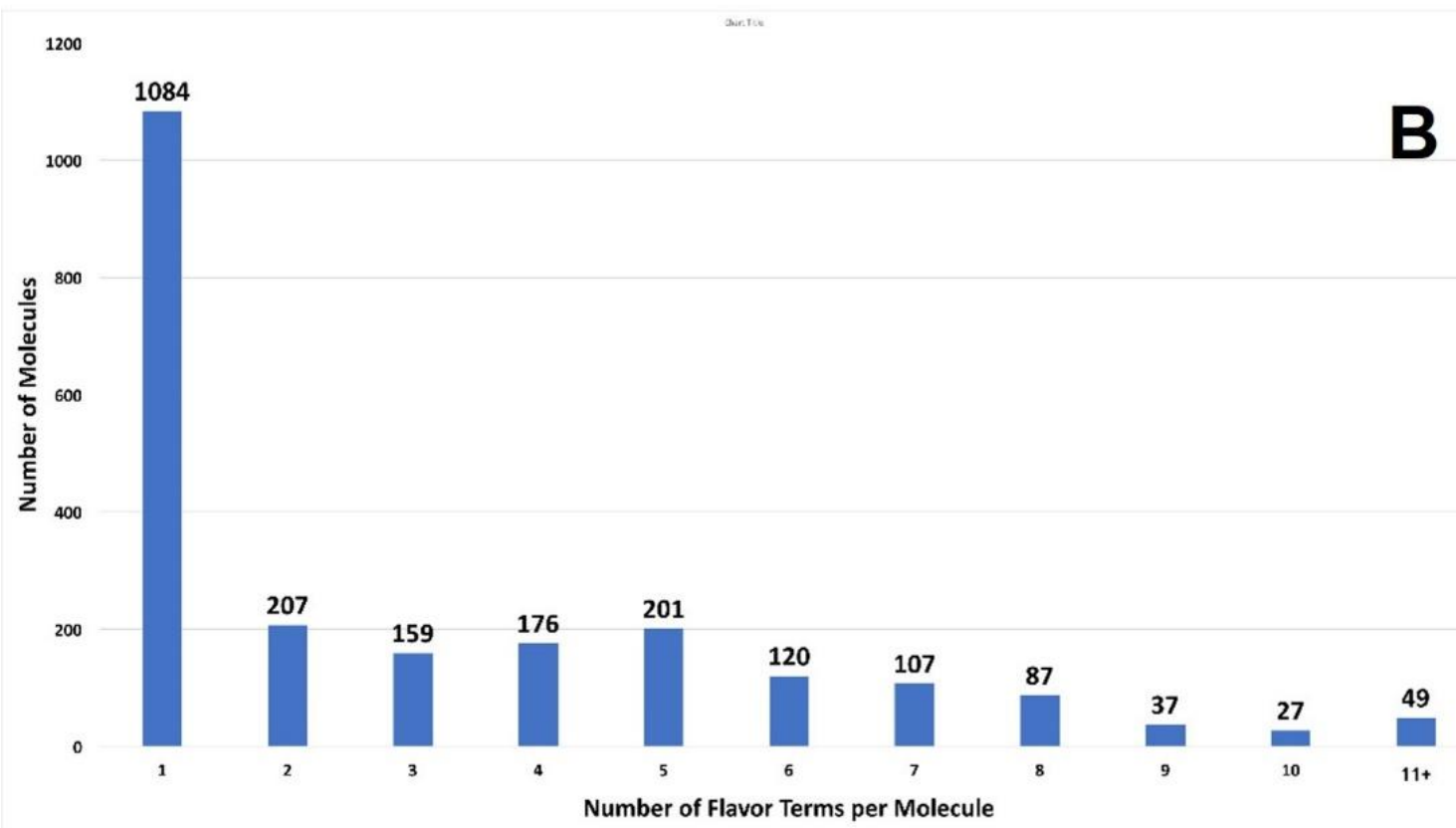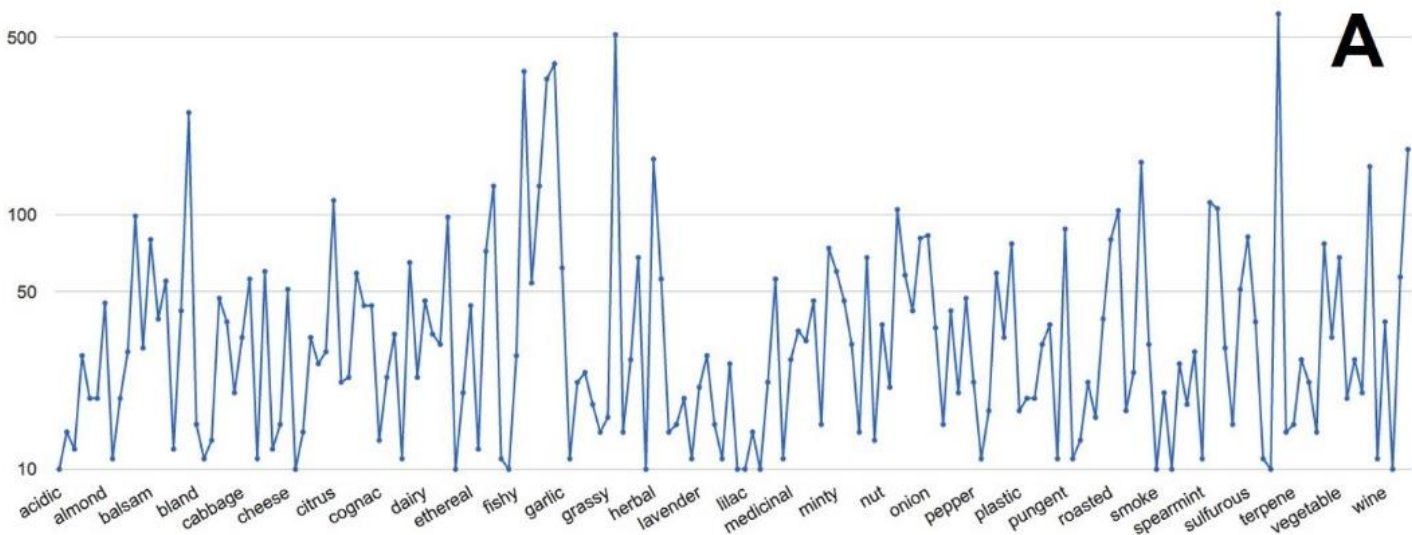
Figure B.1.3: Flavor Profile Statistics. (A) Frequency of occurrence of each 'flavor term' across naturally occurring flavor molecules (for clearer visualization only flavor terms occurring for ten or more times are shown). (B) Total number of flavor terms associated with each naturally occurring flavor molecule.
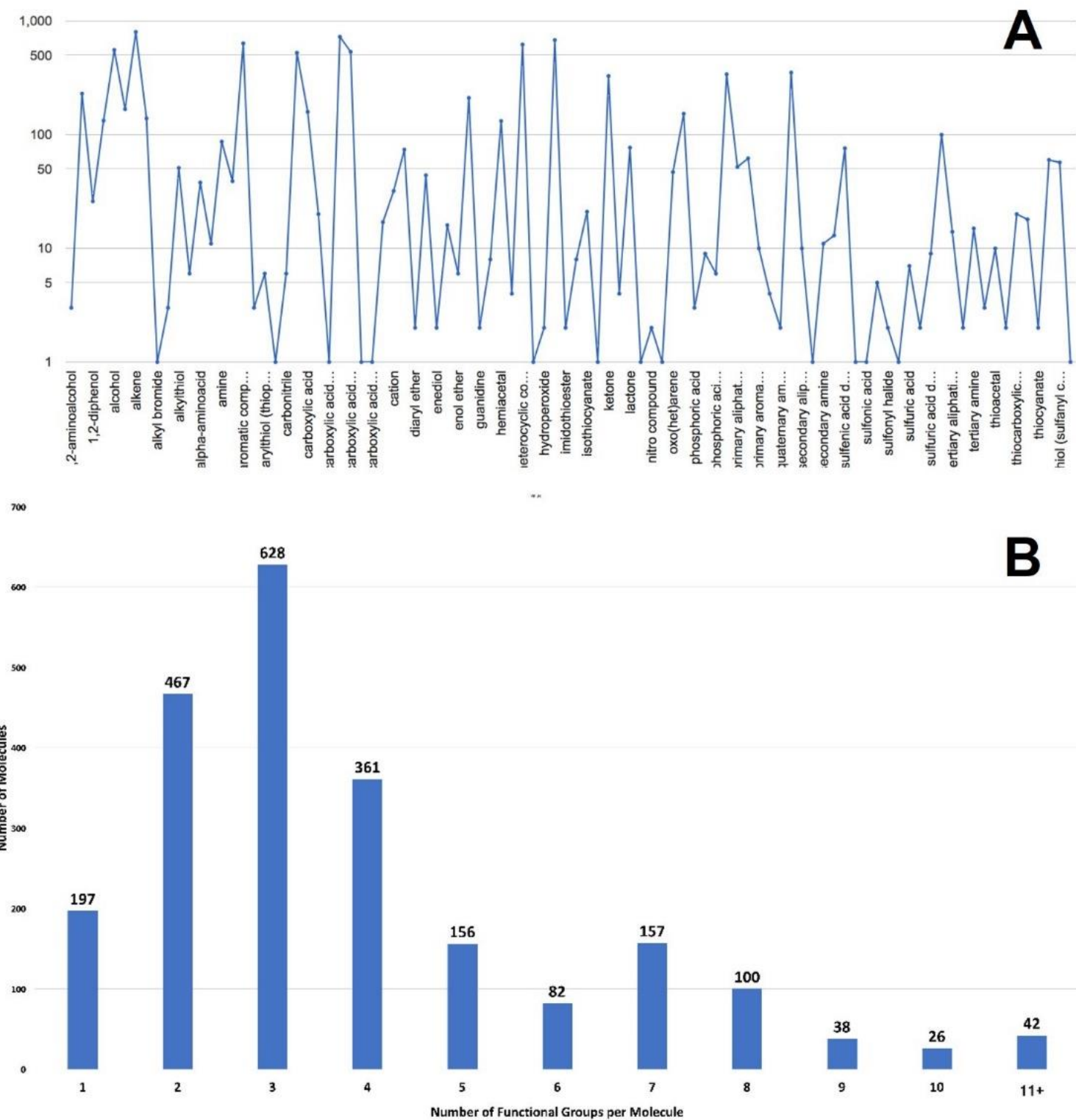
Figure B.1.4: Functional Group Statistics. (A) Frequency of occurrence of each functional group across naturally occurring flavor molecules. (B) The total number of functional groups associated with each naturally occurring flavor molecule.
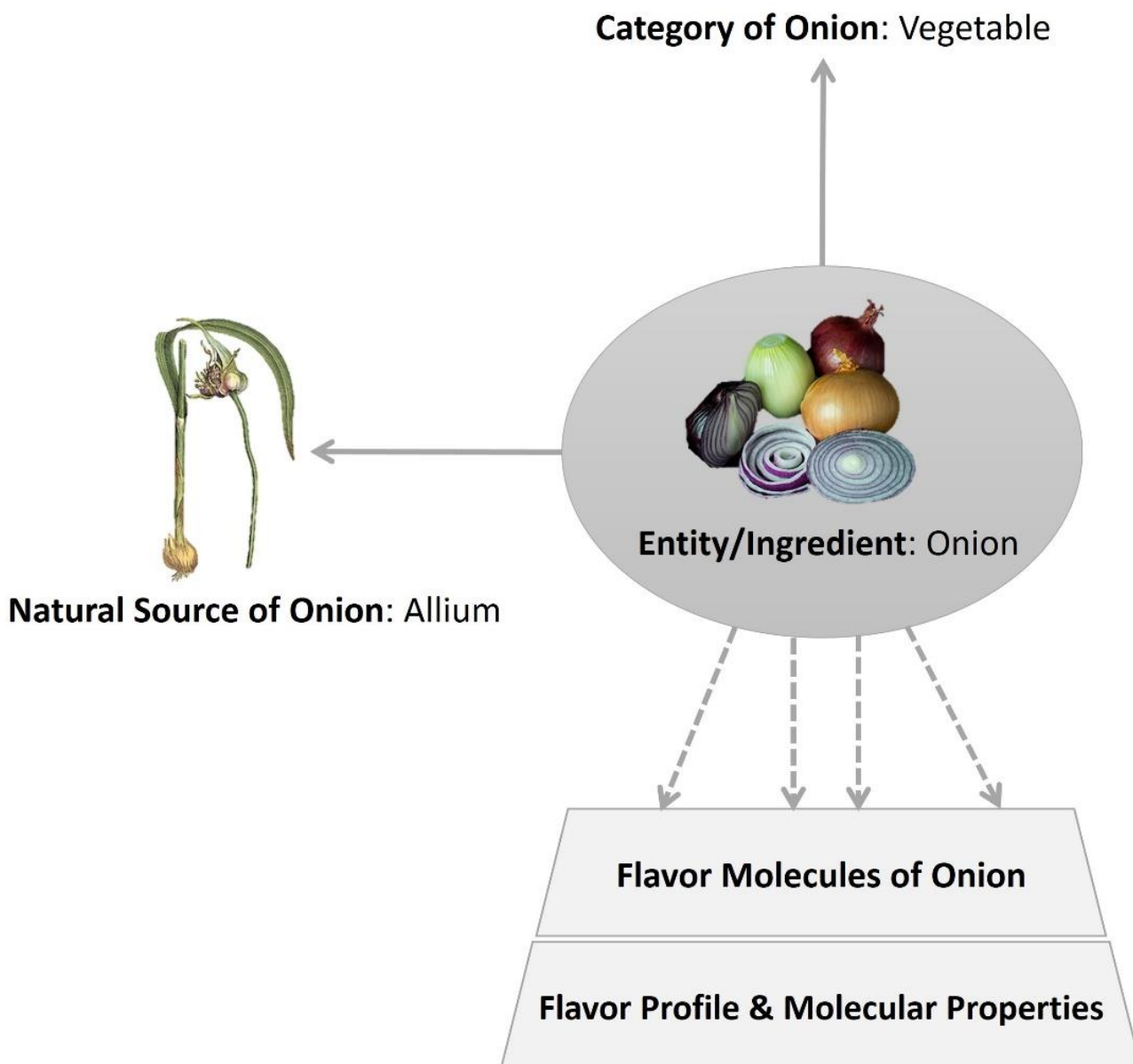
Figure B.1.5. Depiction of relationships among different concepts incorporated in FlavorDB. The Entity is synonymous to an Ingredient and is a key concept in the framework. In the illustration above, 'Onion' is an Entity/Ingredient, which is classified into the Category 'Vegetable'. The natural origin (plant or animal species/genus/family/kingdom) of an ingredient is referred to as the Natural Source, which in the case of onion is 'Allium'. Each ingredient comprises a set of flavor molecules. And further, each flavor molecule is characterized by a 'flavor profile' (a set of flavor terms) and by an array of 'molecular properties' (Physicochemical, 2D/3D and ADMET).

B.3. COMPARISON OF FLAVORDB WITH SIMILAR RESOURCES
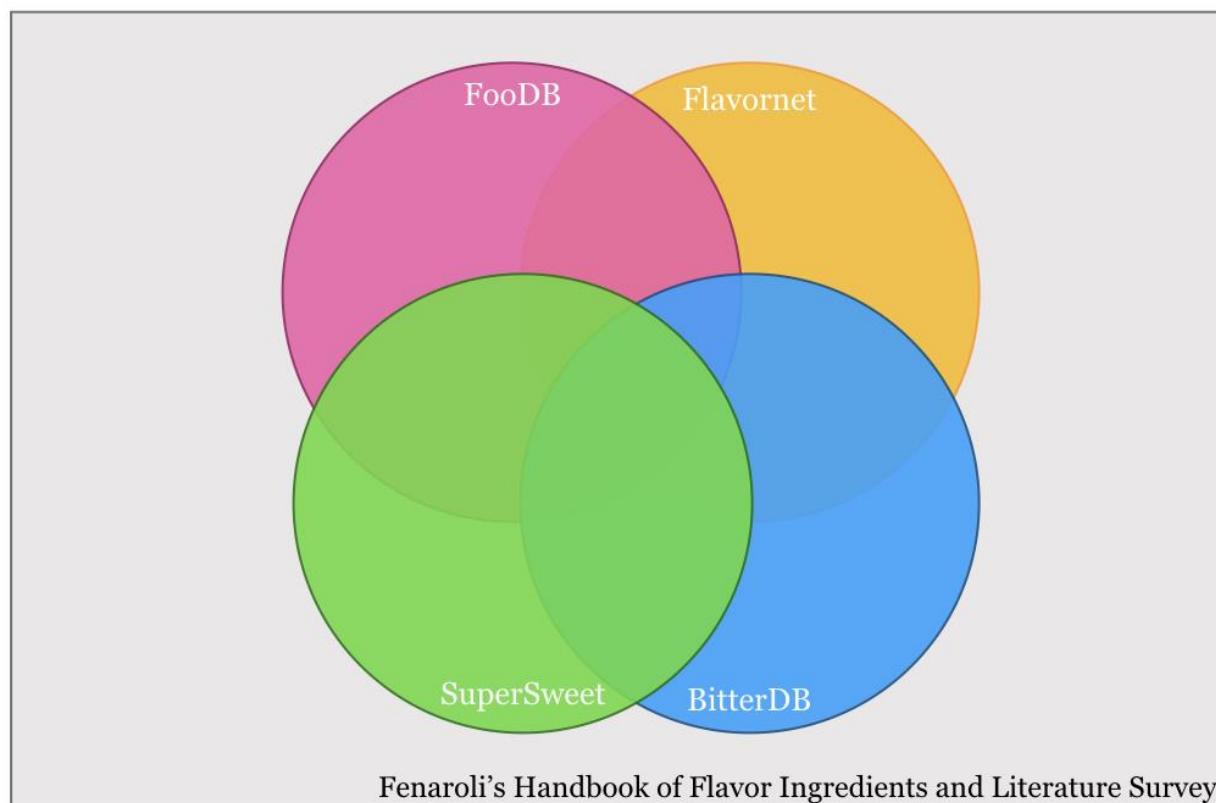
	FlavorDB	FooDB	Flavornet	SuperSweet	BitterDB
FlavorDB	**25595**	2681	627	21980	664
FooDB	2681	**2681**	579	25	190
Flavornet	627	579	**627**	1	38
SuperSweet	21980	25	1	**21980**	6
BitterDB	664	190	38	6	**664**

FlavorDB integrates data of flavor molecules available from various resources (FooDB, Flavornet, SuperSweet, BitterDB, Fenaroli's Handbook of Flavor Ingredients and Literature Survey) to create a comprehensive resource. It also embeds available information of flavors as well as ingredients linked with molecules from disparate sources. The above confusion matrix provides an overview of FlavorDB along with a comparison of coverage of flavor molecules available across other similar resources. Please note that molecular identifiers of flavor compounds were standardized to avoid degeneracy by mapping each molecule to its corresponding PubChem ID.

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