FlavourDB

Molecule Search: Allows users to search for specific molecules by name, CAS number, or chemical structure. This type of search is useful for finding detailed information about particular flavor molecules.
Food Search: Enables users to search for foods by name. This search provides information about the flavor molecules found in each food and how they contribute to the overall flavor profile.
Flavor Profile Search: Allows users to search for flavor profiles by combining different flavor notes. Users can explore which foods or molecules match a specific combination of flavors.
Molecular Descriptor Search: Users can search based on molecular descriptors such as molecular weight, hydrogen bond donors, or acceptors. This search is particularly useful for researchers looking for molecules with specific chemical properties.
Similarity Search: A search option that allows users to find molecules similar to a given molecule based on structural or flavor profile similarity.
Advanced Search: Combines multiple search parameters for a more refined search, allowing users to filter results based on various criteria like molecule type, food type, flavor notes, and molecular properties.

1. Molecule Search API

Endpoint: `/api/molecule-search`

Methods:

- **GET**: Search for molecules by name, CAS number, or chemical structure.

Parameters:

- `name` (string): Name of the molecule.
- `cas_number` (string): CAS number of the molecule.
- `structure` (string): Chemical structure represented in SMILES, InChI, or other formats.

```
{
  "molecules": [
    {
      "id": 1,
      "name": "Vanillin",
      "cas_number": "121-33-5",
      "structure": "C8H8O3",
      "properties": {
        "molecular_weight": 152.15,
        "hydrogen_bond_donors": 1,
        "hydrogen_bond_acceptors": 3
      },
      "flavor_profile": ["vanilla", "sweet"]
    },
    ...
  ]
}
```


2. Food Search API

Endpoint: `/api/food-search`

Methods:

- **GET**: Search for foods by name.

Parameters:

- `name` (string): Name of the food.

```
{
  "foods": [
    {
      "id": 1,
      "name": "Chocolate",
      "flavor_molecules": [
        {
          "name": "Vanillin",
          "contribution": "vanilla flavor"
        },
        {
          "name": "Theobromine",
          "contribution": "bitter taste"
        }
      ]
    },
    ...
  ]
}
```


3. Flavor Profile Search API

Endpoint: `/api/flavor-profile-search`

Methods:

- **GET**: Search for flavor profiles by combining different flavor notes.

Parameters:

- `flavor_notes` (string): Comma-separated list of flavor notes (e.g., "sweet,vanilla,fruity").

```
{
  "results": [
    {
      "type": "food",
      "name": "Strawberry",
      "flavor_profile": ["sweet", "fruity", "tart"]
    },
    {
      "type": "molecule",
      "name": "Ethyl butyrate",
      "flavor_profile": ["fruity", "pineapple"]
    },
    ...
  ]
}
```


4. Molecular Descriptor Search API

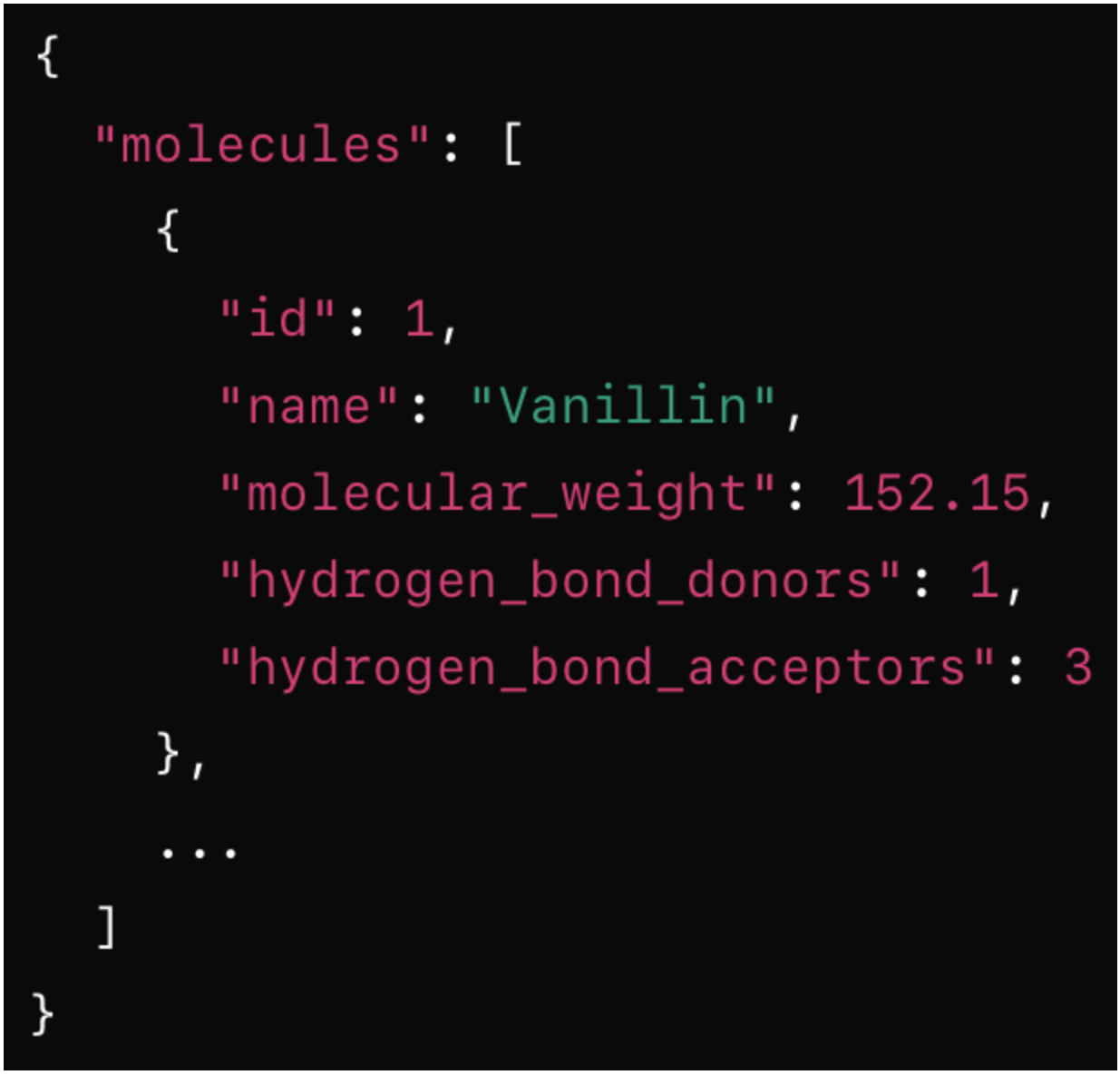
Endpoint: `/api/molecular-descriptor-search`

Methods:

- **GET**: Search based on molecular descriptors such as molecular weight, hydrogen bond donors, or acceptors.

Parameters:

- `molecular_weight_min` (float): Minimum molecular weight.
- `molecular_weight_max` (float): Maximum molecular weight.
- `h_bond_donors` (integer): Number of hydrogen bond donors.
- `h_bond_acceptors` (integer): Number of hydrogen bond acceptors.



5. Similarity Search API

Endpoint: `/api/similarity-search`

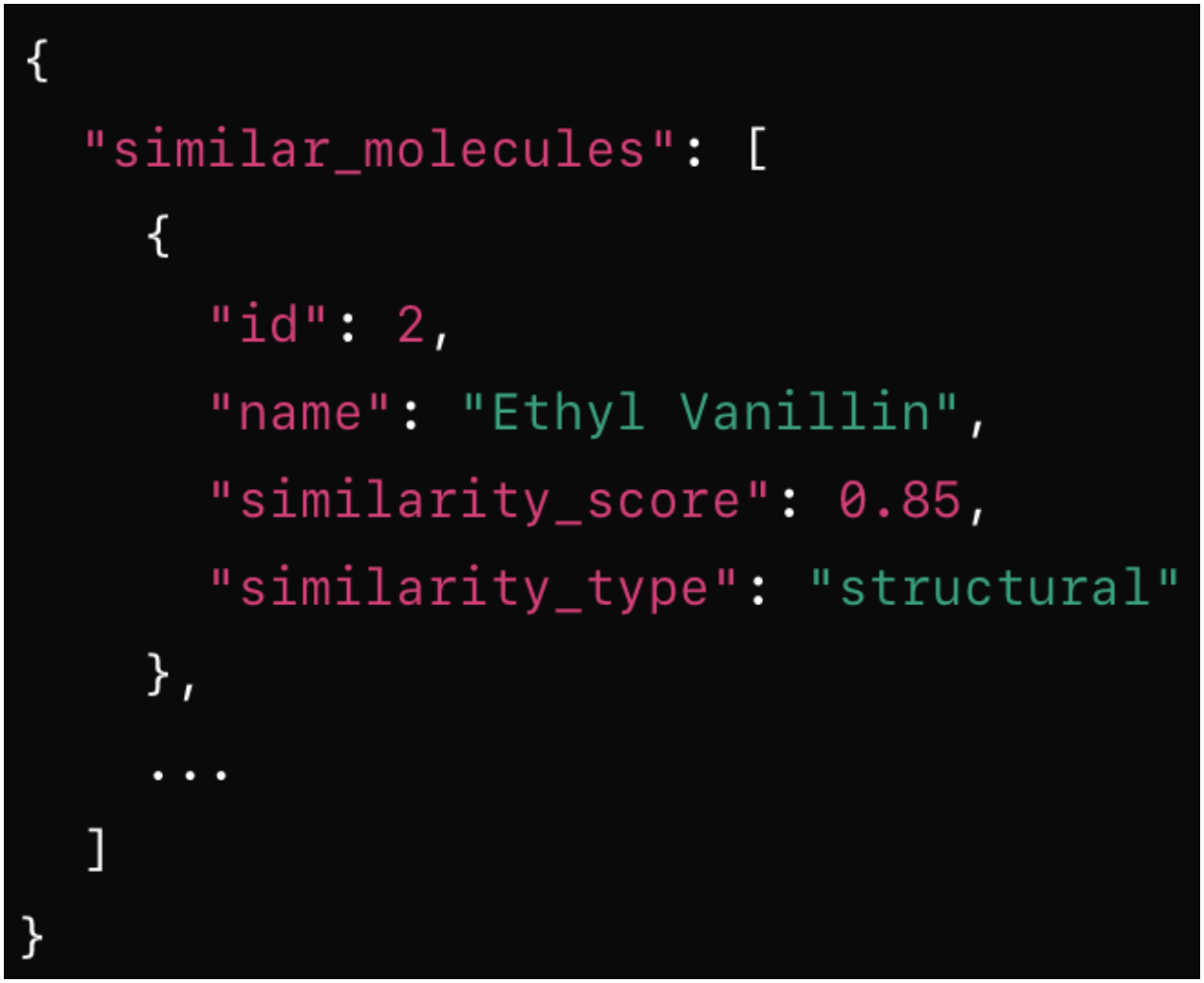
Methods:

- **GET**: Find molecules similar to a given molecule based on structural or flavor profile similarity.

Parameters:

- `reference_molecule_id` (integer): ID of the reference molecule.

- `similarity_type` (string): Type of similarity ("structural", "flavor").



6. Advanced Search API

Endpoint: `/api/advanced-search`

Methods:

- **GET**: Combines multiple search parameters for a more refined search.

Parameters:

- `molecule_type` (string): Type of molecule (e.g., "aromatic", "terpenoid").
- `food_type` (string): Type of food (e.g., "fruit", "spice").
- `flavor_notes` (string): Comma-separated list of flavor notes.
- `molecular_properties` (string): Comma-separated list of molecular properties (e.g., "molecular_weight>150", "h_bond_donors<2").

```
{
  "results": [
    {
      "type": "molecule",
      "name": "Linalool",
      "molecular_properties": {
        "molecular_weight": 154.25,
        "h_bond_donors": 1,
        "h_bond_acceptors": 1
      },
      "flavor_profile": ["floral", "citrus"]
    },
    {
      "type": "food",
      "name": "Cinnamon",
      "flavor_molecules": [
        {
          "name": "Cinnamaldehyde",
          "contribution": "spicy, warm flavor"
        }
      ]
    },
    ...
  ]
}
```


FlavourDB2

Search by Alternative IDs:

- Search using common name, IUPAC, SMILES, CAS Number, FEMA Number, FL Number, NAS Number, EINECS Number, or JFCFA Number.

Search by Food Category:

- Find compounds used in specific food categories, showing usual and maximum concentrations. Combine multiple categories using `@` (AND) or `!` (OR).

Search by Regulatory Status:

- Search based on IOFI (natural, artificial, etc.) and COE (approved, provisional, etc.) values.

Search by Synthesis:

- Search for compounds using specific chemicals or processes in their synthesis. Combine searches using `@` (AND) or `!` (OR).

1. Search by Alternative IDs API

Endpoint: `/api/alternative-id-search`

Methods:

- **GET**: Search using various alternative identifiers like common name, IUPAC, SMILES, CAS Number, FEMA Number, FL Number, NAS Number, EINECS Number, or JFCFA Number.

Parameters:

- `common_name` (string): Common name of the molecule.
- `iupac_name` (string): IUPAC name of the molecule.
- `smiles` (string): SMILES notation of the molecule.
- `cas_number` (string): CAS number of the molecule.
- `fema_number` (string): FEMA number of the molecule.
- `fl_number` (string): FL number of the molecule.
- `nas_number` (string): NAS number of the molecule.
- `einecs_number` (string): EINECS number of the molecule.
- `jfca_number` (string): JFCFA number of the molecule.

```
{
  "molecules": [
    {
      "id": 1,
      "name": "Limonene",
      "alternative_ids": {
        "common_name": "Limonene",
        "iupac_name": "1-Methyl-4-(1-methylethenyl)-cyclohexene",
        "smiles": "CC1=CCCC2=C1C(=CC=C2)C",
        "cas_number": "138-86-3",
        "fema_number": "2175",
        "fl_number": "5",
        "nas_number": "105-92-5",
        "einecs_number": "205-341-0",
        "jfca_number": "1234"
      }
    },
    ...
  ]
}
```


2. Search by Food Category API

Endpoint: `/api/food-category-search`

Methods:

- **GET**: Find compounds used in specific food categories, showing usual and maximum concentrations. Combine multiple categories using `@` (AND) or `!` (OR).

Parameters:

- `categories` (string): Comma-separated list of food categories with logical operators (`@`, `!`). (e.g., "fruit@spice", "beverage!candy")

```
"compounds": [
  {
    "id": 1,
    "name": "Cinnamonaldehyde",
    "food_categories": [
      {
        "category": "spice",
        "usual_concentration": "0.5%",
        "maximum_concentration": "1.5%"
      }
    ]
  },
  {
    "id": 2,
    "name": "Vanillin",
    "food_categories": [
      {
        "category": "dessert",
        "usual_concentration": "0.2%",
        "maximum_concentration": "1.0%"
      },
      {
        "category": "beverage",
        "usual_concentration": "0.1%",
        "maximum_concentration": "0.5%"
      }
```


3. Search by Regulatory Status API

Endpoint: `/api/regulatory-status-search`

Methods:

- **GET**: Search based on IOFI (natural, artificial, etc.) and COE (approved, provisional, etc.) values.

Parameters:

- `iofi_status` (string): IOFI regulatory status (e.g., "natural", "artificial").
- `coe_status` (string): COE regulatory status (e.g., "approved", "provisional").


```
{
  "compounds": [
    {
      "id": 1,
      "name": "Ethyl Vanillin",
      "regulatory_status": {
        "iofi_status": "artificial",
        "coe_status": "approved"
      }
    },
    {
      "id": 2,
      "name": "Limonene",
      "regulatory_status": {
        "iofi_status": "natural",
        "coe_status": "approved"
      }
    },
```


4. Search by Synthesis API

Endpoint: `/api/synthesis-search`

Methods:

- **GET**: Search for compounds using specific chemicals or processes in their synthesis. Combine searches using `@`(AND) or `!` (OR).

Parameters:

- `chemicals` (string): Comma-separated list of chemicals used in synthesis with logical operators (`@`, `!`). (e.g., "benzene@ethyl_alcohol", "acetone!ethanol")
- `processes` (string): Comma-separated list of synthesis processes with logical operators.


```
"compounds": [
  {
    "id": 1,
    "name": "Cinnamaldehyde",
    "synthesis": {
      "chemicals": ["cinnamon", "aldehyde"],
      "processes": ["oxidation", "distillation"]
    }
  },
  {
    "id": 2,
    "name": "Linalool",
    "synthesis": {
      "chemicals": ["linalyl_acetate", "terpene"],
      "processes": ["hydrolysis", "fermentation"]
    }
```

A. Searching Flavor Compounds by Alternative IDs

- **Overview**: FlavorDB2 allows users to search for flavor compounds using various molecular identifiers or nomenclature systems.
- **Search Parameters**: Users can search using:
    - **Common Name**: The everyday name of a compound.
    - **IUPAC**: The International Union of Pure and Applied Chemistry naming convention.
    - **SMILES**: Simplified Molecular Input Line Entry System, a notation to describe a chemical structure using ASCII strings.
    - **CAS Number**: Unique numerical identifiers assigned by the Chemical Abstracts Service.
    - **FEMA Number**: Assigned by the Flavor and Extract Manufacturers Association for flavoring substances.
    - **FL Number**: Flavor numbers that identify substances for regulatory purposes.
    - **NAS Number**: Numbers provided by the National Academy of Sciences for identifying flavor substances.
    - **EINECS Number**: European Inventory of Existing Commercial chemical Substances number.
    - **JFCFA Number**: Japanese Food Chemistry and Food Additives number.
- **Benefit**: This flexibility allows users to find flavor compounds in the database regardless of which identifier they have or prefer.

B. Flavor Compounds Used in Food Category

- **Overview**: Users can search the database based on food categories to identify all flavor compounds associated with those categories.
- **Details Provided**: For each compound found in a particular food category, the database lists:
    - **Usual Concentration**: The typical concentration at which the compound is used.
    - **Maximum Concentration**: The highest concentration at which the compound is safely used.
- **Advanced Search**: Users can perform advanced queries by combining multiple food categories using:
    - **@ (AND) Operator**: To search for compounds associated with all specified categories.
    - **! (OR) Operator**: To search for compounds associated with any of the specified categories.

C. Flavor Compounds Based on Regulatory Status

- **Overview**: This search allows users to find flavor compounds based on their regulatory status.
- **Search Parameters**:
    - **IOFI Values**: International Organization of the Flavor Industry classifications, which indicate the nature of the compound (natural, artificial, nature identical, not nature identical, artificial, and identical).
    - **COE Values**: Council of Europe classifications, which specify regulatory status such as approved, approved in some quantity, used provisionally, or unknown.
- **Functionality**: By specifying these values, users can generate a list of flavor molecules that match the regulatory criteria they are interested in.

D. Flavor Compound Synthesis

- **Overview**: Users can search for flavor compounds based on the chemicals used in their synthesis process.
- **Search Options**:
    - **Chemical Name**: Searching by a specific chemical (e.g., ‘acetic acid’) will display a list of flavor compounds synthesized using that chemical.
    - **Compounded Queries**: Users can refine their searches further by adding multiple chemicals using the **@ (AND)** or **! (OR)** operators.
    - **Processes and Terms**: Searches can also be performed based on chemical processes (e.g., ‘esterification’, ‘distillation’) or other related terms in the synthesis field.
- **Purpose**: This search functionality helps users understand the synthesis processes of flavor compounds and the chemicals involved.