## Sander Su

Integrated Dietary Supplement Knowledge Base
Data Analysis

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## Background

The first step would be to create a data parser, following the instructions here:

https://docs.biothings.io/en/latest/doc/studio.html#part-1-single-datasource. In this case, the primary key for the document should be a concept identifier for a dietary ingredient, and the document should contain all the relationships stated in the database.

For example, here is a set of lines from MRREL . RRF, which contains these relationships:

```
DR1378627|DC0477352|is_effective_for|DC0478476|NMCD
DR1378629|DC0477352|has_adverse_effect_on|DC0478449|NMCD
DR1378613|DC0477352|is_effective_for|DC0478466|NMCD
```

this snippet declares that DC0477352 has three relationships, that it is is\_effective\_for - DC0478476, that it has\_adverse\_effect\_on - DC0478449, and that it is\_effective\_for - DC0478466. All of those facts were originally sourced from the "NMCD" database. Those concept identifiers can be resolved in the MRC0NSO. RRF file using either UMLS or MEDDRA identifiers:

```
$ egrep 'DC0477352|DC0478476|DC0478466|DC0478449' MRCONSO.RRF | egrep 'UMLS|MEDDRA'
DC0477352|DA0137592|7-oxodehydroepiandrosterone|SY|UMLS|C0525091|Y
DC0477352|DA0137591|7-oxodehydroepiandrosterone|SY|UMLS|C0525091|Y
DC0478449|DA0170196|Nervous system disorders|SY|MEDDRA|10029205|Y
DC0478466|DA0170257|Obesity, NOS|SY|UMLS|C0028754|Y
DC0478476|DA0170285|RAYNAUD PHENOMENON|SY|UMLS|C0034735|Y
DC0478476|DA0170283|RAYNAUD PHENOMENON|SY|UMLS|C0034735|Y
```

So the dietary ingredient 7-oxodehydroepiandrosterone (UMLS: C0525091) is related to RAYNAUD PHENOMENON (UMLS: C0034735) because 7-oxodehydroepiandrosterone is\_effective\_for (treating) RAYNAUD PHENOMENON. Similarly, that ingredient has\_adverse\_effect\_on - Nervous systems disorders, and it is\_effective\_for - Obesity, NOS.

Background

```
"UMLS:C0525091": {
 "name": "7-oxodehydroepiandrosterone",
 "umls": "UMLS:C0525091",
 "is_effective_for": [
     "name": "RAYNAUD PHENOMENON",
     "umls": "UMLS:C0034735",
     "source": [
          "name": "iDISK",
          "record": "DR1378627"
          "name": "NMCD"
      "name": "Obesity, NOS",
     "umls": "UMLS:C0028754",
     "source": [
          "name": "iDISK",
          "record": "DR1378613"
          "name": "NMCD"
  "has_adverse_effect_on": [
     "name": "Nervous systems disorders",
      "meddra": "MEDDRA:0029205",
```

• Source: <a href="https://conservancy.umn.edu/handle/11299/204783">https://conservancy.umn.edu/handle/11299/204783</a>

File View/Open	Description	Size	Format
README.md	Decription of the data file formats (TXT)	4.712Kb	text/markdown
README.htm	Description of the data file formats (HTML)	81.73Kb	HTML
idisk-rrf-1.0.1-2020-01-28.zip	iDISK RRF	9.565Mb	application/zip

- Main files
  - MRREL: Relation file of concepts (708,164 records)
    - 919 concepts
  - MRCONSO: Detail of concept (209,499 records)
    - Sources (UMLS or MEDDRA): 10,527 records

## - MRREL (similar to UMLS concept)

rui	cui1	rel	cui2	sab
DR0000007	DC0001355	has_ingredient	DC0478167	DSLD
DR0000013	DC0001355	has_ingredient	DC0478268	DSLD
DR0000015	DC0001355	has_ingredient	DC0477973	DSLD
DR0000019	DC0001355	has_ingredient	DC0483034	DSLD
DR0000009	DC0001355	has_ingredient	DC0483298	DSLD
DR0000011	DC0001355	has_ingredient	DC0482716	DSLD
DR0000003	DC0001355	has_ingredient	DC0483261	DSLD
DR0000017	DC0001355	has_ingredient	DC0483608	DSLD
DR0000005	DC0001355	has_ingredient	DC0482541	DSLD
DR0000023	DC0001357	has_ingredient	DC0478191	DSLD
DR0000025	DC0001358	has_ingredient	DC0477963	DSLD

#### - MRCONSO

cui	aui	str	tty	sab	scode	ispref v
DC0478122	DA0159849	Rose Hip	SY	DSLD	118	Υ
DC0478122	DA0159871	ROSE HIPS	SY	UMLS	C0772037	Υ
DC0478122	DA0159872	ROSE HIPS	SY	UMLS	C0772037	Υ
DC0478122	DA0159873	ROSE HIPS	SY	UMLS	C0772037	Υ
DC0478122	DA0159898	Rose hips	SN	NHPID	3972	Υ
DC0478122	DA0159843	Rose Hip	SY	NMCD	839	Υ
DC0478122	DA0159920	Rose hip	SN	NHPID	0432	Υ
DC0478122	DA0159904	Rosehips	SY	DSLD	118	N
DC0478122	DA0159858	Rose Hips fruit powder	SY	DSLD	118	N
DC0478122	DA0159891	Hop Fruit	SY	NMCD	839	N
DC0478122	DA0159881	Satapatrika	SY	NMCD	839	N

#### Steps:

- 1. Find unique cui1s and their cui2s from MRREL file
- 2. Find cuis with UMLS or MEDDRA sources only from MRCONSO file
- 3. Loop cui1s and cui2s from step 1 to get the detail of cui2 from step 2
- 4. Combine findings from step 1 and step 3 as JSON objects

JSON Output

```
"_id": "DSLD:30552",
"name": "Douglas Laboratories - L-Lysine 500 mg",
"dsld": "DSLD:30552",
"has_ingredient": [
        "name": "AjiPure pharmaceutical grade L-Lysine HCl",
        "ispref": "N",
        "dsld": "DSLD:172",
        "source": [
                "name": "iDisk",
                "record": "DR0000001"
            },
                "name": "DSLD"
    },
        "name": "Hydrochlorure de L-Lysine",
        "ispref": "N",
        "nmcd": "NMCD:237",
        "source": [
                "name": "iDisk",
                "record": "DR0000001"
            },
                "name": "DSLD"
    },
```

# Thank you