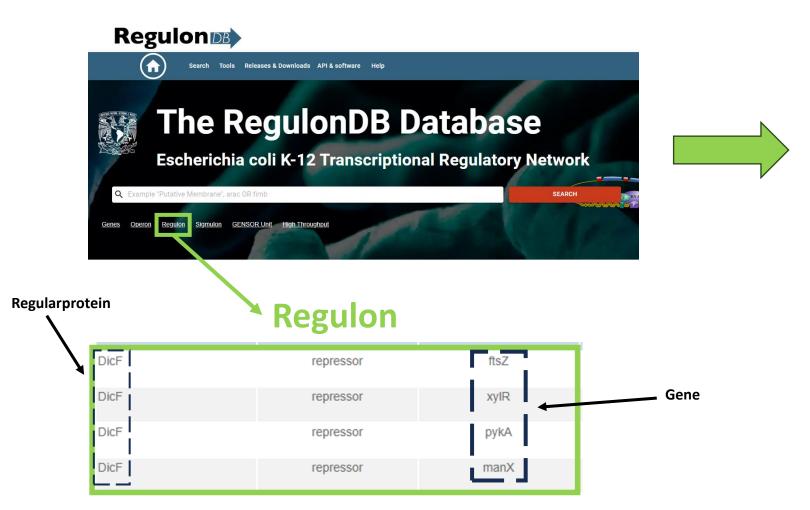
# Molekulare Daten von Bakterien in einen Knowledge Graph überführen

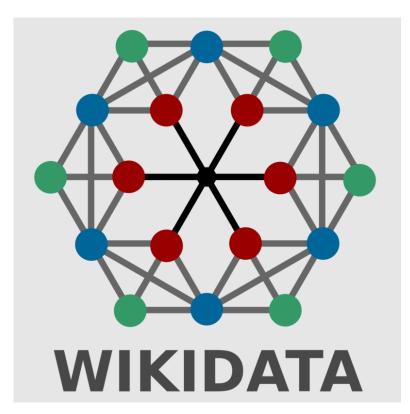
Gruppe 4

Kerem & Tim

31.07.2024

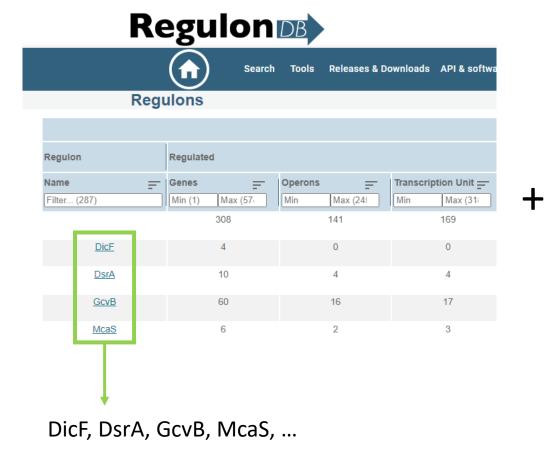
### Ziel



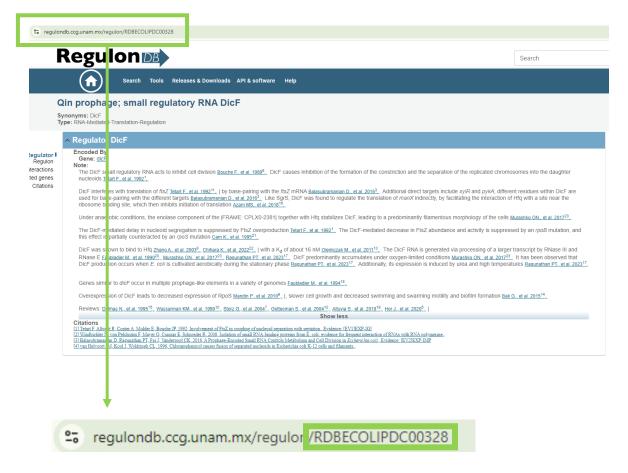


#### Schritt 1 – Daten sammeln

#### 1. Regulon Kennzeichnung



#### 2. Link zum DB Eintrag

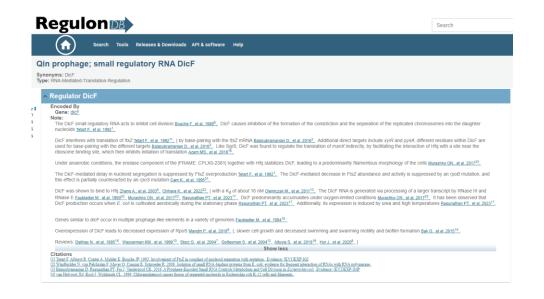


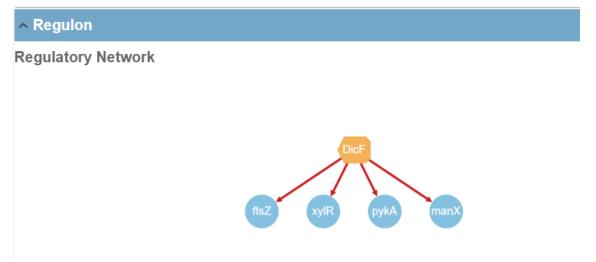
#### Schritt 1 – Daten sammeln

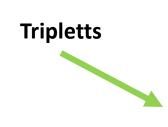
```
chrome options = webdriver.ChromeOptions()
#chrome options.add argument("--headless")
chrome options.add argument("--no-sandbox")
chrome options.add argument('--window-size=1920,1080')
chrome_options.add_experimental_option("prefs", {
    "download.prompt_for_download": False,
    "download.directory_upgrade": True,
    "safebrowsing.enabled": True
driver = webdriver.Chrome(options=chrome_options)
actions = ActionChains(driver)
def click_button_wait(XPATH):
    WebDriverWait(driver, 10).until(EC.element_to_be_clickable((By.XPATH, XPATH))).click()
def find next page button():
    driver.execute script("window.scrollTo(0, document.body.scrollHeight);") # scroll down
    button_xpath = "/html/body/div[1]/div/div[2]/div/div[2]/div/div[3]/div/table/tbody/tr[19]/td/div/div/button[3]"
    button = WebDriverWait(driver, 10).until(EC.element_to_be_clickable((By.XPATH, button_xpath)))
    button.click()
# seite aufrufen
driver.get("https://regulondb.ccg.unam.mx/regulon")
# Cookies Rejecten
click_button_wait('/html/body/div[1]/div/div[4]/div/div[3]/button[2]')
is_last_page = False
regulon_links = {}
    while True:
       # Get Table Body
        table_body = WebDriverWait(driver, 10).until(EC.visibility_of_element_located((By.XPATH,'/html/body/div[1]/div/di
        # jedes tr (zeile der tabelle) sammeln
        elements = table_body.find_elements(By.XPATH,".//*[contains(@id, 'tr')]")
        for i in range(0, len(elements)):
                link = elements[i].find elements(By.XPATH,".//*")[0].find element(By.XPATH,"div/div/a").get attribute("hr
                name = elements[i].find elements(By.XPATH,".//*")[0].find element(By.XPATH,"div/div/a").get attribute("te
                regulon_links[name] = link
            except:
                pass
        find_next_page_button()
    print("finished")
```

```
{'DicF': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC00328',
 'DsrA': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC00358',
 'GcvB': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC03275',
 'McaS': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC03411',
 'GadY': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC03413',
 'MicF': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC03508',
 'OxyS': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC03909',
 'ChiX': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04122',
 'SgrS': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04132',
 'IstR-1': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04134'
 'RseX': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04142',
 'RydC': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04143',
 'OhsC': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04144',
 'SvmR': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04148',
 'MgrR': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04149',
 'FnrS': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04150',
 'ArrS': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04151',
 'SdsN': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04154',
 'AgrB': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04160',
```

### Schritt 2 – Daten abfragen

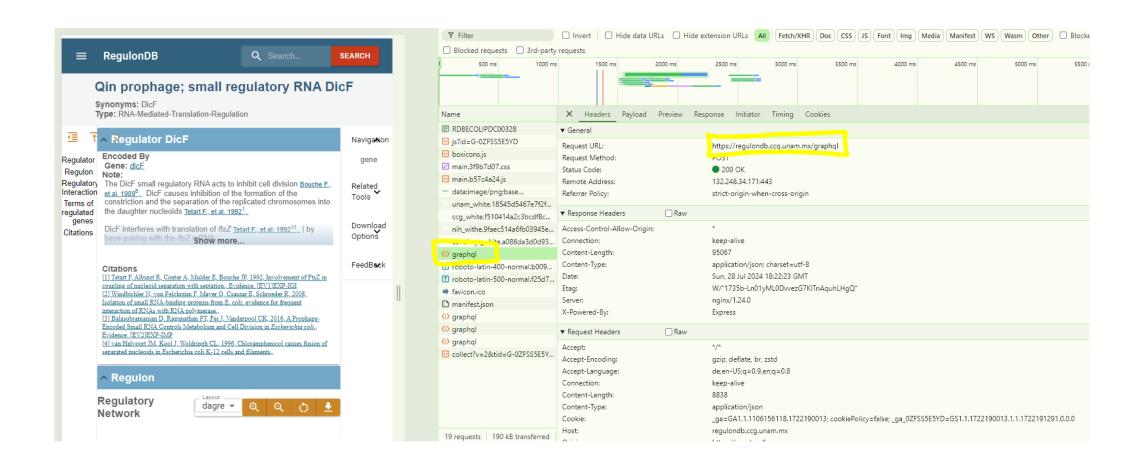






^ Regulatory Interactions							
Active Conformation Name Filter (1)	Function =	Regulated Entity Name =	Regulated Entity Type == Filter (1)	First Gene Min (-15 Max (42)		Regulated Genes =	RBS
DicF	repressor	ftsZ	gene	-15		ftsZ	105277
DicF	repressor	xyIR	gene	13		xyIR	3734988
DicF	repressor	pykA	gene	-10		<u>pykA</u>	1937631
DicF	repressor	manX	gene	42		manX	1902082

### Schritt 2 – Daten abfragen



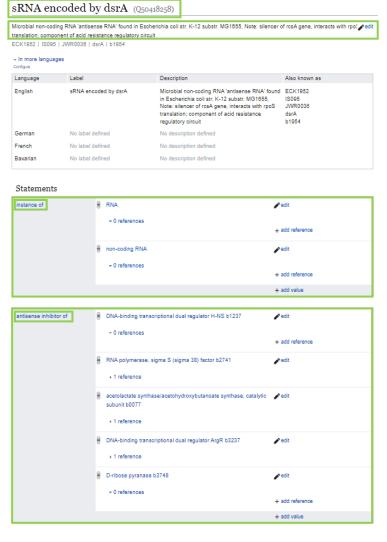
### Schritt 2 – Daten abfragen

```
url = "https://regulondb.ccg.unam.mx/graphql"
  request1["variables"]["advancedSearch"] = "RDBECOLIPDC00328[_id]"
  response = json.loads(requests.post(url = url, json = request1, verify = False).content)
C:\Anaconda\lib\site-packages\urllib3\connectionpool.py:1061: InsecureRequestWarning: Unverified HTTPS request is being made
to host 'regulondb.ccg.unam.mx'. Adding certificate verification is strongly advised. See: https://urllib3.readthedocs.io/en/
1.26.x/advanced-usage.html#ssl-warnings
  warnings.warn(
  response
  {'data': {'getRegulonBy': {'data': [{'_id': 'RDBECOLIPDC00328'.
       'aligmentMatrix': {'aligment': None,
        'consensus': None,
        'matrix': None,
       'urlMatrixOualityResult': None,
        'urlPWMLogo': None,
        '__typename': 'AligmentMatrix'},
       'allCitations': [{'evidence': {'_id': 'RDBECOLIEVC00062',
         'additiveEvidenceCodeRule': None,
         'code': 'EXP-IGI',
         'name': 'Inferred from genetic interaction',
          'type': 'W'.
          '__typename': 'Evidence'},
         'publication': {' id': 'RDBECOLIPRC06277',
          'authors': ['Tetart F',
          'Albigot R',
           'Conter A',
           'Mulder E'.
           'Bouche JP'],
          'citation': 'Tetart F, Albigot R, Conter A, Mulder E, Bouche JP, 1992, Involvement of FtsZ in coupling of nucleoid s
  eparation with septation.',
          'pmid': '1552861',
          'title': 'Involvement of FtsZ in coupling of nucleoid separation with septation.',
```

#### Graphql Endpoint

```
{'DicF': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC00328'
'DsrA': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC00358',
'GcvB': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC03275',
'McaS': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC03411',
'GadY': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC03413',
'MicF': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC03508',
'OxyS': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC03909',
'ChiX': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04122',
'SgrS': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04132',
'IstR-1': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04134'
'RseX': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04142',
'RydC': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04143',
'OhsC': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04144',
'SymR': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04148',
'MgrR': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04149',
'FnrS': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04150',
'ArrS': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04151',
'SdsN': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04154',
'AgrB': 'https://regulondb.ccg.unam.mx/regulon/RDBECOLIPDC04160',
```

### Schritt 3 – Daten Preparen





#### **UPLOAD REGULONS**

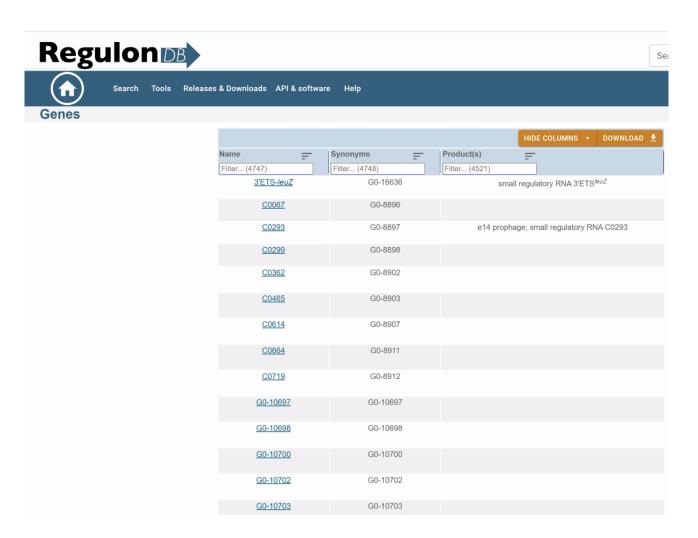
- 1. kurze beschreibung des items
- konstant: instance of [P31] (RNA [Q11053] / non-coding RNA [Q427087])
- 3. konstant: found in taxon [P703] (Escherichia coli str. K-12 substr. MG1655 [Q21102938])
- 4. statements für gene: inhibitor / repressor / dual
- 5. strand orientation [P2548] (reverse [Q22809711] / forward [Q22809680])
- 6. genomic start [P644] / genomic end [P645]

```
1 list(regulon data.values())[0]
{'beschreibung': 'The DicF small regulatory RNA acts to inhibit cell division.',
 'left position': 1649382,
 'right position': 1649434,
 'strand orientation': '022809711'}
 1 list(triplets.values())[0]
[{'subjekt': 'DicF', 'predikat': 'repressor', 'objekt': 'ftsZ'},
 {'subjekt': 'DicF', 'predikat': 'repressor', 'objekt': 'xylR'},
 {'subjekt': 'DicF', 'predikat': 'repressor', 'objekt': 'pykA'},
 {'subjekt': 'DicF', 'predikat': 'repressor', 'objekt': 'manX'}]
 1 print(gene_ids["ftsZ"])
 2 print(gene_ids["xylR"])
 3 print(gene ids["pykA"])
 4 print(gene_ids["manX"])
0127734188
Q127735541
0127735563
Q127735585
```

# Schritt 4 – Daten hochladen (PyWikiBot)

#### Genes erzeugen

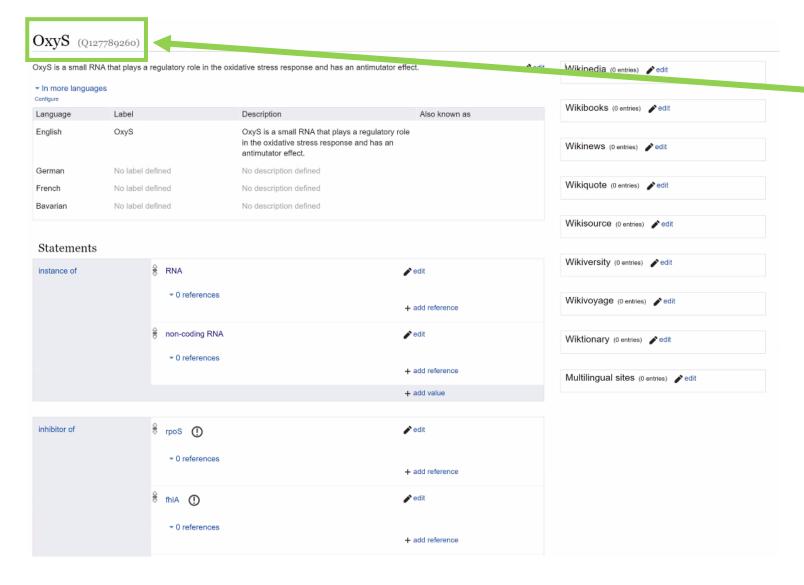
```
: 1 i = 0
   2 for key, value in list(gene_descriptions.items())[6:]:
          label = key
          description = value
          # Create Item
          data = {
              'labels': {'en': {'language': 'en', 'value': label}},
               'descriptions': {'en': {'language': 'en', 'value': str(description)}}
  10
  11
          new_item = pywikibot.ItemPage(repo)
  12
          new_item.editEntity(data, summary=f'Creating new item: {label}')
  13
  14
          # Create Statement
  15
          claim = pywikibot.Claim(repo, "P31") # instance of
          target = pywikibot.ItemPage(repo, "Q7187") # gene
  17
          claim.setTarget(target)
  18
          new item.addClaim(claim, summary='Adding education information')
  19
  20
          gene ids[key] = new item.getID()
  21
          print(key, i, "/", len(gene_descriptions))
= Sieeping for 9.4 seconds, 2024-07-24 15:43:27
  citR 2686 / 2697
  Sleeping for 9.3 seconds, 2024-07-24 15:43:38
  Sleeping for 9.6 seconds, 2024-07-24 15:43:47
  glsB 2687 / 2697
 Sleeping for 9.4 seconds, 2024-07-24 15:43:57
  Sleeping for 9.3 seconds, 2024-07-24 15:44:08
  yneG 2688 / 2697
  Sleeping for 9.2 seconds, 2024-07-24 15:44:18
  Sleeping for 9.4 seconds, 2024-07-24 15:44:27
  sfmC 2689 / 2697
  Sleeping for 9.4 seconds, 2024-07-24 15:44:37
  Sleeping for 9.5 seconds, 2024-07-24 15:44:47
```



# Schritt 4 – Daten hochladen (PyWikiBot)

```
def generate claims(regulon, info):
  label - regulon
  if info["beschreibung"] != None:
      description = info["beschreibung"]
       description = "description: " + regular
                                                                                                                                                   Item wird erzeugt
  if len(str(description)) >= 250:
      description = str(description[:249])
       'labels': {'en': {'language': 'en', 'value': label}},
       "descriptions": {'en': {'language': 'en', 'value': str(description)}}
  new item = pywikibot.ItemPage(repo)
  new_item.editEntity(data, summary=f'Creating new item: {label}')
  claims = []
  # claims für instance of
  instance_of_rna = {'mainsnak': {'snaktype': 'value', 'property': "P31", 'datavalue': {'entity-type': 'iten', 'numeric-id': "11053"}, 'type': 'wikibase-entityid'}}, 'type': 'statement', 'rank': 'normal'}
  claims.append(instance of rna)
  instance_of_non_coding_rna = {'mainsnak': {'snaktype': 'value', 'property': "P31", 'datavalue': {'value': {'entity-type': 'item', 'numeric-id': "427087"}, 'type': 'wikibase-entityid'}}, 'type': 'statement', 'rank': 'normal'}
  claims.append(instance_of_non_coding_rna)
   # claims für funktionen der gene (repressor, activator, dual)
  for i in range(0, len(triplets[regulon])):
       value = triplets[regulon][i]
       if value["predikat"] -- "repressor":
           repressor = {'mainsnak': {'snaktype': 'value', 'property': "P3776", 'datavalue': {'value': {'entity-type': 'item', 'numeric-id': str(gene_ids[value["objekt"]][1:])}, 'type': 'wikibase-entityid'}}, 'type': 'statement', 'rank': 'normal'}
          claims.append(repressor.copy())
       elif value["predikat"] == "activator":
           activator_of = {"mainsnak": {"snaktype": "value", 'property': "P3771", 'datavalue': {'value': ('entity-type': 'item', 'numeric-id': str(gene_ids[value["objekt"]][1:])), 'type': 'wikibase-entityid'}), 'type': 'statement', 'rank': 'normal')
           claims.append(activator_of.copy())
       elif value["predikat"] == "dual":
           dual = {'mainsnak': ('snaktype': 'value', 'property': "P1322", 'datavalue': ('value': ('entity-type': 'item', 'numeric-id': str(gene_ids[value["objekt"]][1:])}, 'type': 'wikibase-entityid'}}, 'type': 'statement', 'rank': 'normal'}
           claims.append(dual.copy())
   # claim für found in taxon
   found_in_taxon = {'mainsnak': {'snaktype': 'value', 'property': "P703", 'datavalue': {'value': {'entity-type': 'iten', 'numeric-id': 21102938}, 'type': 'wikibase-entityid'}}, 'type': 'statement', 'rank': 'normal'}
   claims.append(found_in_taxon)
  # claims für strand orientation
  if info["left position"] != None:
       genomic_start = ('mainsnak': {'snaktype': 'value', 'property': "P644", 'datavalue': {'value': str(info["left_position"]), 'type': 'string'}, 'type': 'wikibase-entityid'}, 'type': 'statement', 'rank': 'normal'}
      claims.append(genomic start)
  if info["right position"] |- None:
       genomic_end = {'mainsnak': {'snaktype': 'value', 'property': "P645", 'datavalue': {'value': str(info["right_position"]), 'type': 'string'}, 'type': 'wikibase-entityid'}, 'type': 'statement', 'rank': 'normal'}
       claims.append(genomic_end)
   if info["strand_orientation"] |- None and info["left_position"] |- None and info["right_position"] |- None:
      switch = {"22809711" : "22809680", "22809680" : "22809711"}
      so = switch[str(info["strand_orientation"][1:])]
       strand_orientation = {'mainsnak': {'snaktype': 'value', 'property': "P2548", 'datavalue': {'value': {'entity-type': 'item', 'numeric-id': so}, 'type': 'wikibase-entityid'}}, 'type': 'statement', 'rank': 'normal'}
      claims.append(strand orientation)
  data = { 'claims': claims}
  new_item.editEntity(data, summary='Adding multiple claims in one request')
  return new item.getID()
```

# Ergebnis



```
regulon qids
{'0xyS': 'Q127789260'
 'ChiX': 'Q127789264',
 'SgrS': 'Q127789265',
 'IstR-1': 'Q127789266',
 'RseX': 'Q127789268',
 'RydC': '0127789270',
 'OhsC': 'Q127789272',
 'SymR': 'Q127789274',
 'MgrR': 'Q127789276',
 'FnrS': 'Q127789277',
 'ArrS': 'Q127789278',
 'SdsN': 'Q127789281',
 'AgrB': '0127789283',
 'RalA': 'Q127789285',
 'MicL-S': 'Q127789288',
 'CpxQ': 'Q127789289',
 'SdhX': '0127789292',
 'C0293': '0127789294',
```