InChI Resolver and its Protocol

https://github.com/inchiresolver/inchiresolver

InChI Resolver: Project Goal

the specification of a common web API protocol for distributed InChI Resolver instances

referring to data & information of existing web resources

implementation of a network of federated InChI Resolvers

Benefits:

- web resources providing data & information based on InChI become findable & interlinked on the web
- their content is accessible in a generic way (JSON:API) for Web clients & applications
- (*long-term*) an autonomous client can find and collect information based on InChI

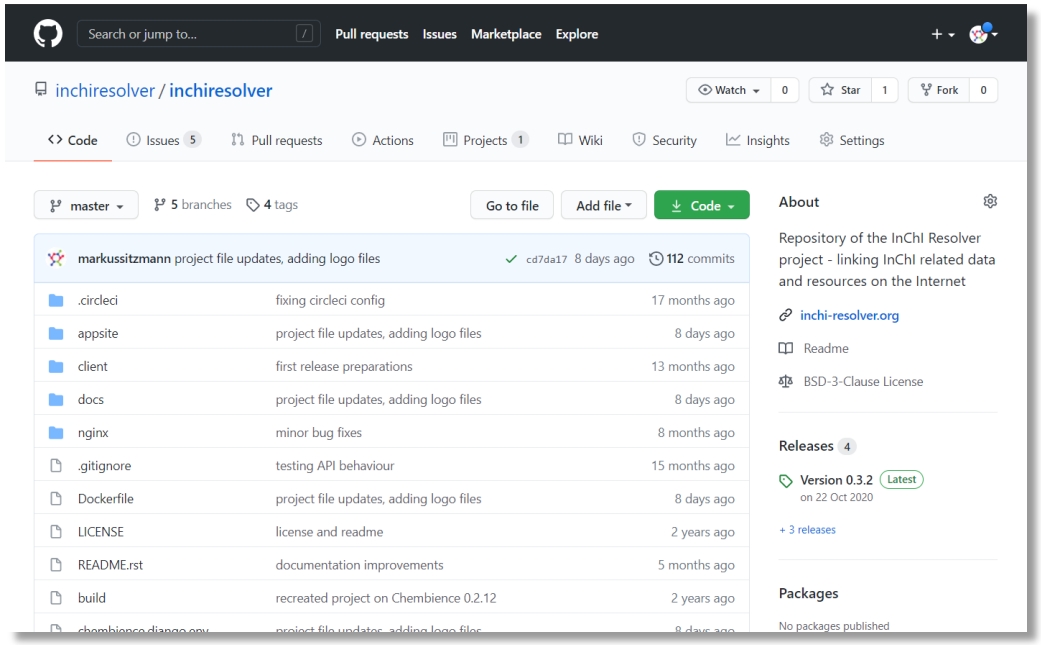
Goal of this Talk

make the project better known

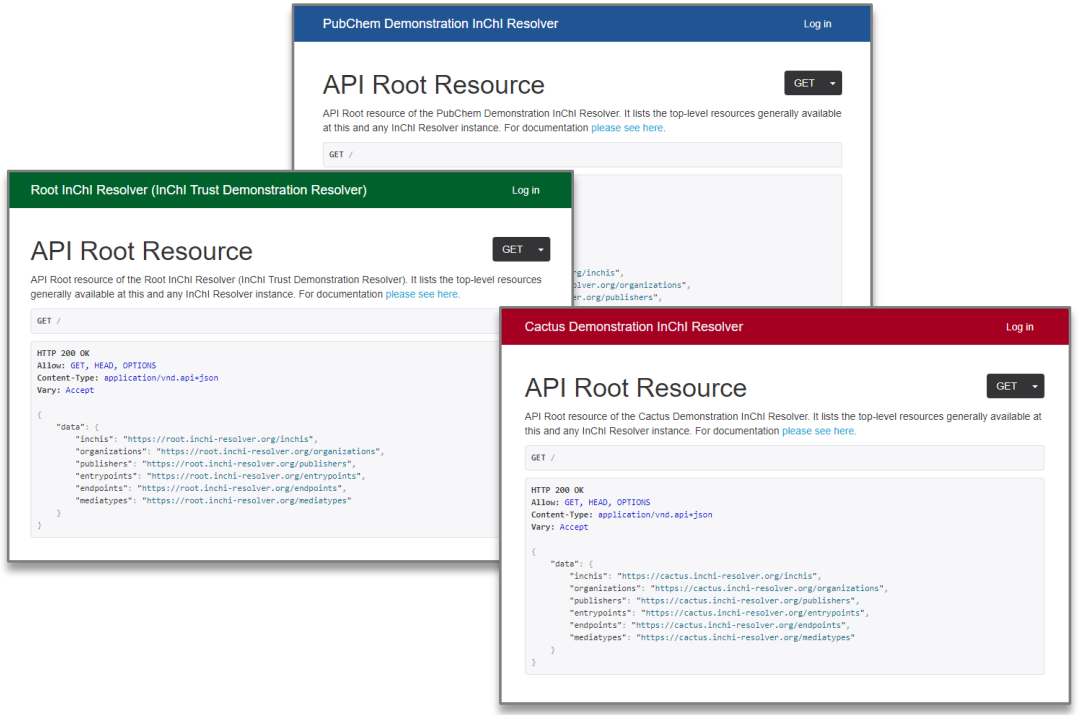
feedback and contributions

InChI Resolver Project – Current Status

InChI Resolver Protocol
specification



InChI Resolver Reference Implementation
downloadable & online



https://github.com/inchiresolver/inchiresolver

InChI Resolver Protocol – JSON:API

JSON:API

specification for how a **client** should request, fetch or modify server resources, and how a **server** should respond to those requests

designed to minimize both the number of requests and the amount of data transmitted between clients and servers

applies IANA-registered media type **application/vnd.api+json** for exchanging data

client and server implementations are available for a large number of **programming languages**

https://jsonapi.org/

based on

JSON Schema

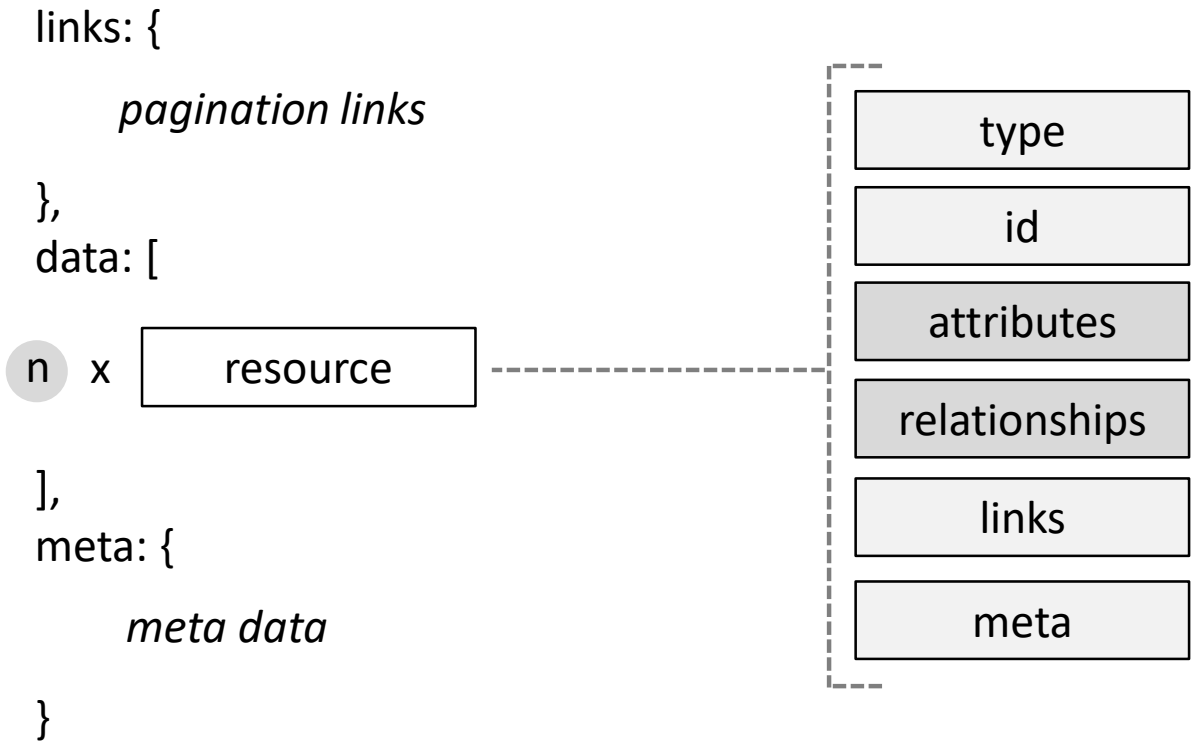
vocabulary that allows you to annotate and validate JSON documents

Internet Engineering Task Force (**IETF**) standard

https://json-schema.org/

InChI Resolver Protocol – JSON:API

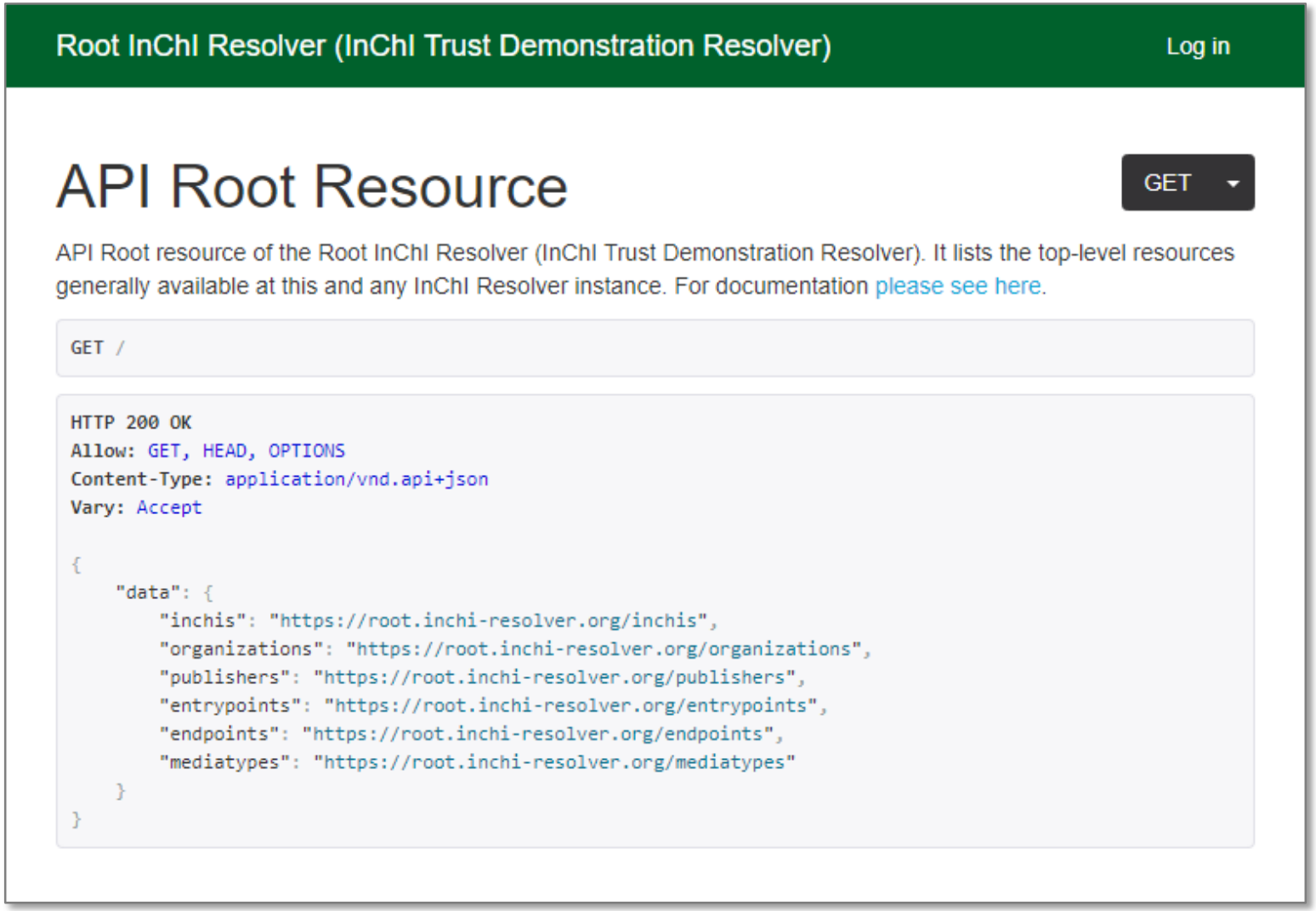
JSON:API Document Structure



InChI Resolver Resource Types

- /inchis
- /entrypoints
- /endpoints
- /publishers
- /organizations
- /mediatypes

InChI Resolver Protocol – JSON:API



InChI Resolver Resources: InChI

/inchis

attributes:

- string
- key
- version
- isStandard
- safeOptions


```
"attributes": {
  "string": "InChI=1S/C29H45N7O8S/c1-18(2)14-20(24(38)28-34-33- 27(44-
            28)19-12-10-9-11-13-19)31-26(40)22(16-43-8)32-
            25(39)21(35-45(41,42)36(6)7)15-23(37)30-17-
            29(3,4)5/h9-13,18,20-22,35H,14-17H2,1-
            8H3,(H,30,37)(H,31,40)(H,32,39)/t20-,21-,22-/m0/s1",
  "key": "SLTIZPMLXAYRIU-FKBYEOEOSA-N",
  "version": 1,
  "isStandard": true,
  "safeOptions": null
}
```


relationships: **entrypoints**

documentation: https://github.com/inchiresolver/inchiresolver/blob/master/docs/protocol.rst#**inchis-resource**

InChI Resolver Resources: Entrypoint

/entrypoints

attributes:

- name
- description
- category
- href
- entrypointHref

```
"attributes": {
   "name": "PubChem PUG REST",
   "description": "PUG (Power User Gateway), a web interface for accessing
                   PubChem data and services",
   "category": "service",
   "href": "https://pubchem.ncbi.nlm.nih.gov/rest/pug",
   "entrypointHref": null
}
```

site *service* *resolver* *self*

relationships: **publisher** **endpoints** **parent** **children**

documentation: https://github.com/inchiresolver/inchiresolver/blob/master/docs/protocol.rst#**entrypoints-resource**

InChI Resolver Resources: Endpoint

uri: IETF RFC 6570 - URI Template **fullPathUri:** entrypoint **href** + endpoint **uri**

/endpoints

attributes:

- uri
- fullPathUri
- description
- category
- requestMethods

```
"attributes": {
   "uri": "compound/inchikey/{inchi|inchikey}/cids,
   "fullPathUri": "https://pubchem.ncbi.nlm.nih.gov/rest/pug/
                                    compound/inchikey/{inchi|inchikey}/cids",
   "description": "resolve InChI or InChIKey to PubChem CID",
   "category": "uritemplate",
   "requestMethods": ["GET", "POST", "DELETE", ...]
}
```

schema *uritemplate* *documentation*

relationships: **entrypoint** **endpoints** (for response + request schemas) **mediatypes** (of accept headers + content)

documentation: https://github.com/inchiresolver/inchiresolver/blob/master/docs/protocol.rst#**endpoints-resource**

InChI Resolver Resources: Mediatype

/mediatypes

attributes:

- name
- description

```
"attributes": {
   "name": "text/xml",
   "description": "XML"
}
```

relationships: deliveringEndpoints acceptingEndpoints

documentation: https://github.com/inchiresolver/inchiresolver/blob/master/docs/protocol.rst#**mediatype-resource**

InChI Resolver Resources: Publisher

/publishers

attributes:

- name
- category
- email
- address
- href
- orcid

```
"attributes": {
   "name": "PubChem group",
   "category": "group",
   "email": "pubchem-help@ncbi.nlm.nih.gov",
   "address": "8600 Rockville Pike; Bethesda, MD  20894; USA",
   "href": "https://pubchemdocs.ncbi.nlm.nih.gov/contact",
   "orcid": null
}
```

entity *service* *network* *division* *person* *group* *none*

relationships: **entrypoints** **organization** **parent** **children**

documentation: https://github.com/inchiresolver/inchiresolver/blob/master/docs/protocol.rst#**publishers-resource**

InChI Resolver Resources: Organization

/organizations

attributes:

- name
- abbreviation
- category
- href

```
"attributes": {
   "name": "U.S. National Library of Medicine",
   "abbreviation": "NLM",
   "category": "government",
   "href": "https://www.nlm.nih.gov"
},
```

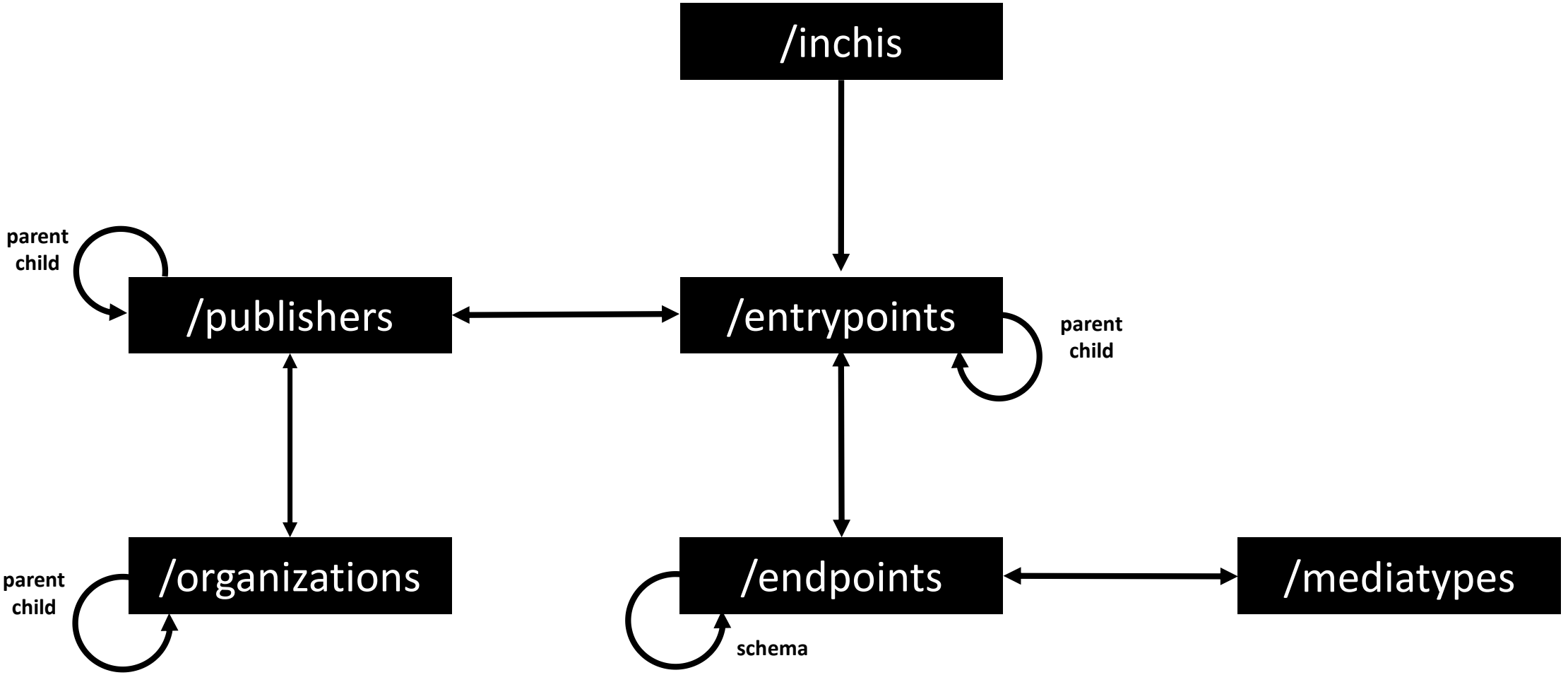
publishing *provider* *public* *society* *charity* *other* *none*

regulatory *government* *academia* *company* *vendor* *research*

relationships: **publishers** **parent** **children**

documentation: https://github.com/inchiresolver/inchiresolver/blob/master/docs/protocol.rst#**organizations-resource**

InChI Resolver: Resource Relationships



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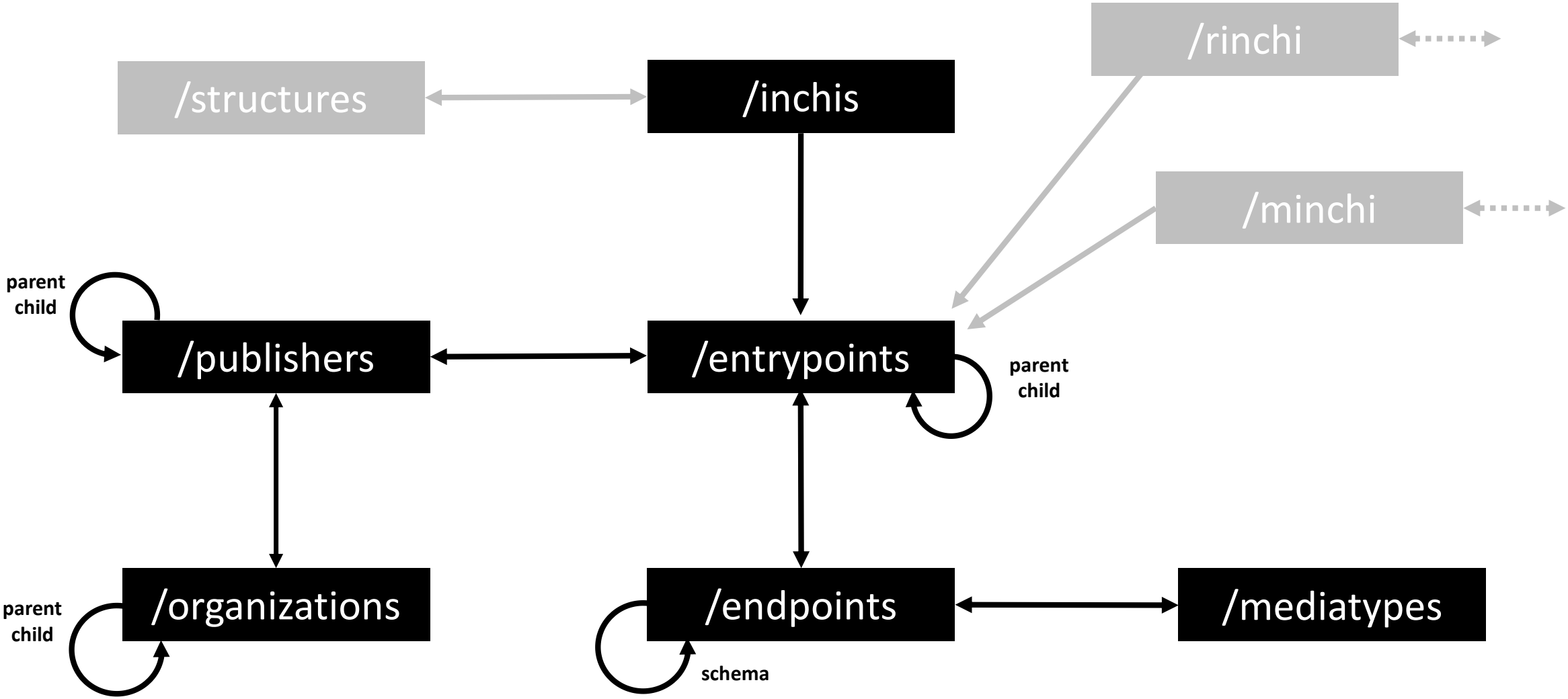
InChI Resolver: Resource Relationships



documentation: https://github.com/inchiresolver/inchiresolver/blob/master/docs/protocol.rst

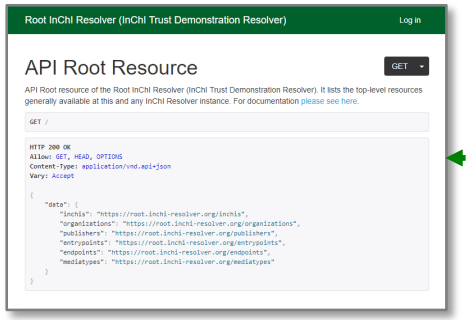
InChI Resolver Protocol – JSON:API Requests

InChI Resolver (JSON:API) resources

- support all HTTP methods
  GET, POST, PUT, PATCH, and DELETE
- allow **filtering** by attributes and **including** by relationship fields:

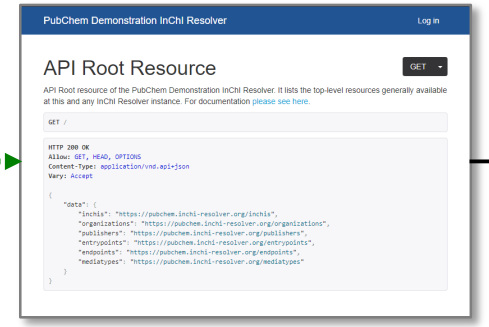
https://some.inchi-resolver.org/**inchis**
?**filter**[key]=LTCQRNQPODCPAS-CCVNUDIWSAN
&**include**=entrypoints.endpoints,entrypoints.publisher,entrypoints.publisher.organization

InChI Resolver: Reference Implementation (online)



https://root.inchi-resolver.org/

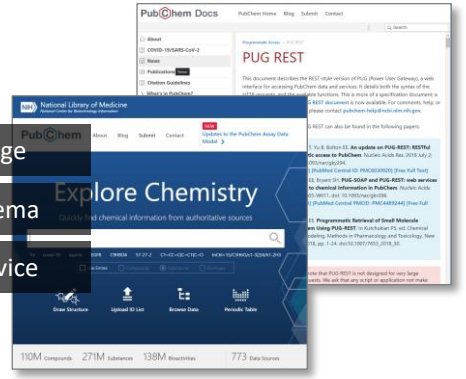
InChI Resolver protocol



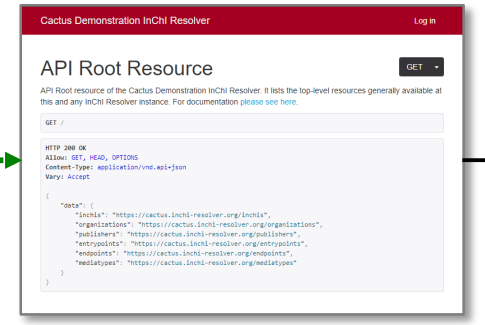
https://pubchem.inchi-resolver.org/

web page
XSD schema
web service

endpoint references



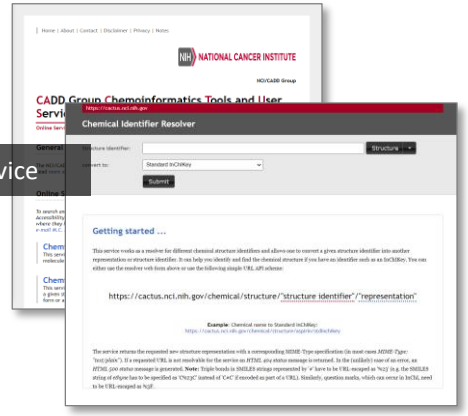
PubChem resources



https://cactus.inchi-resolver.org/

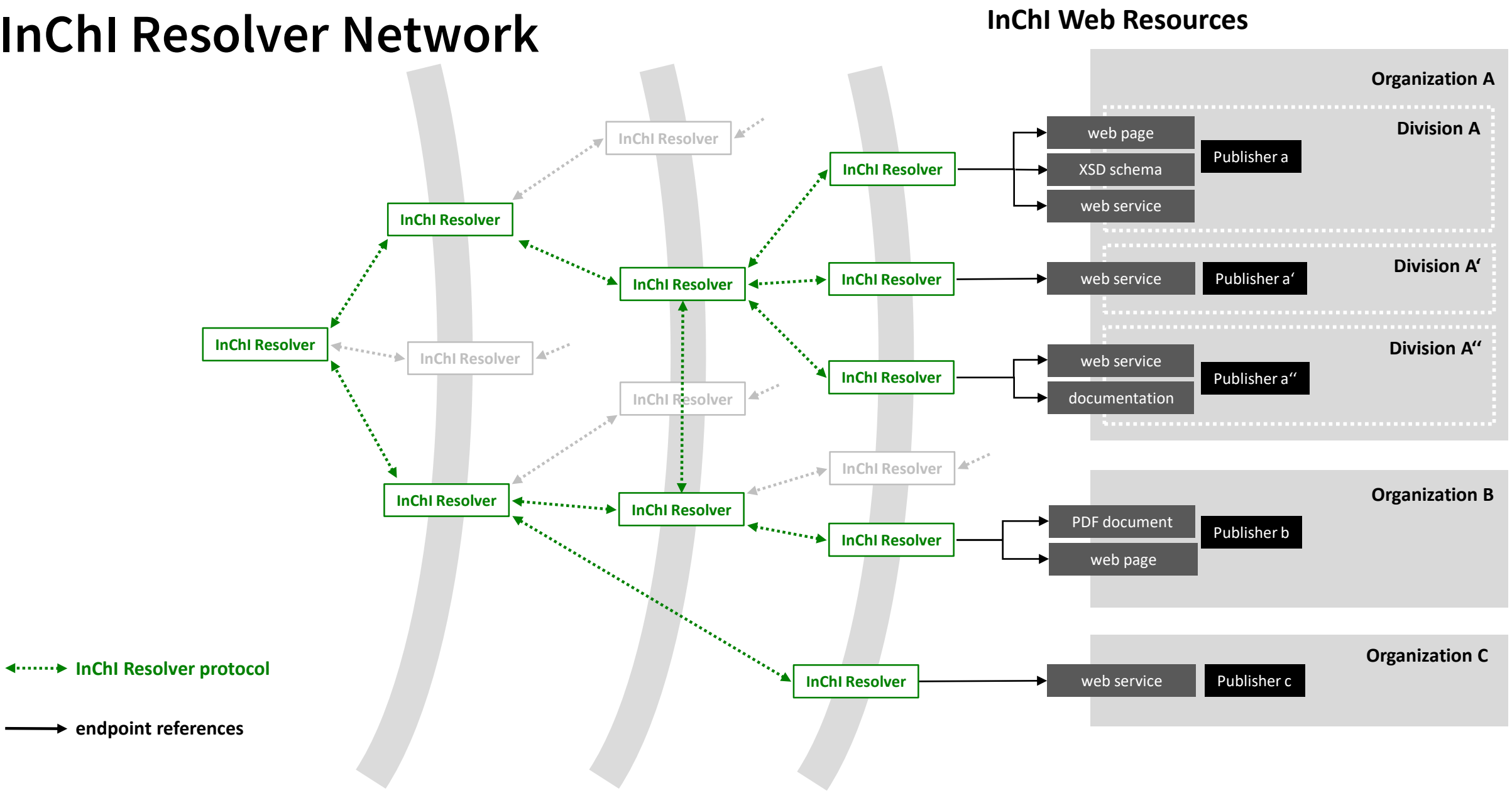
web service

endpoint references

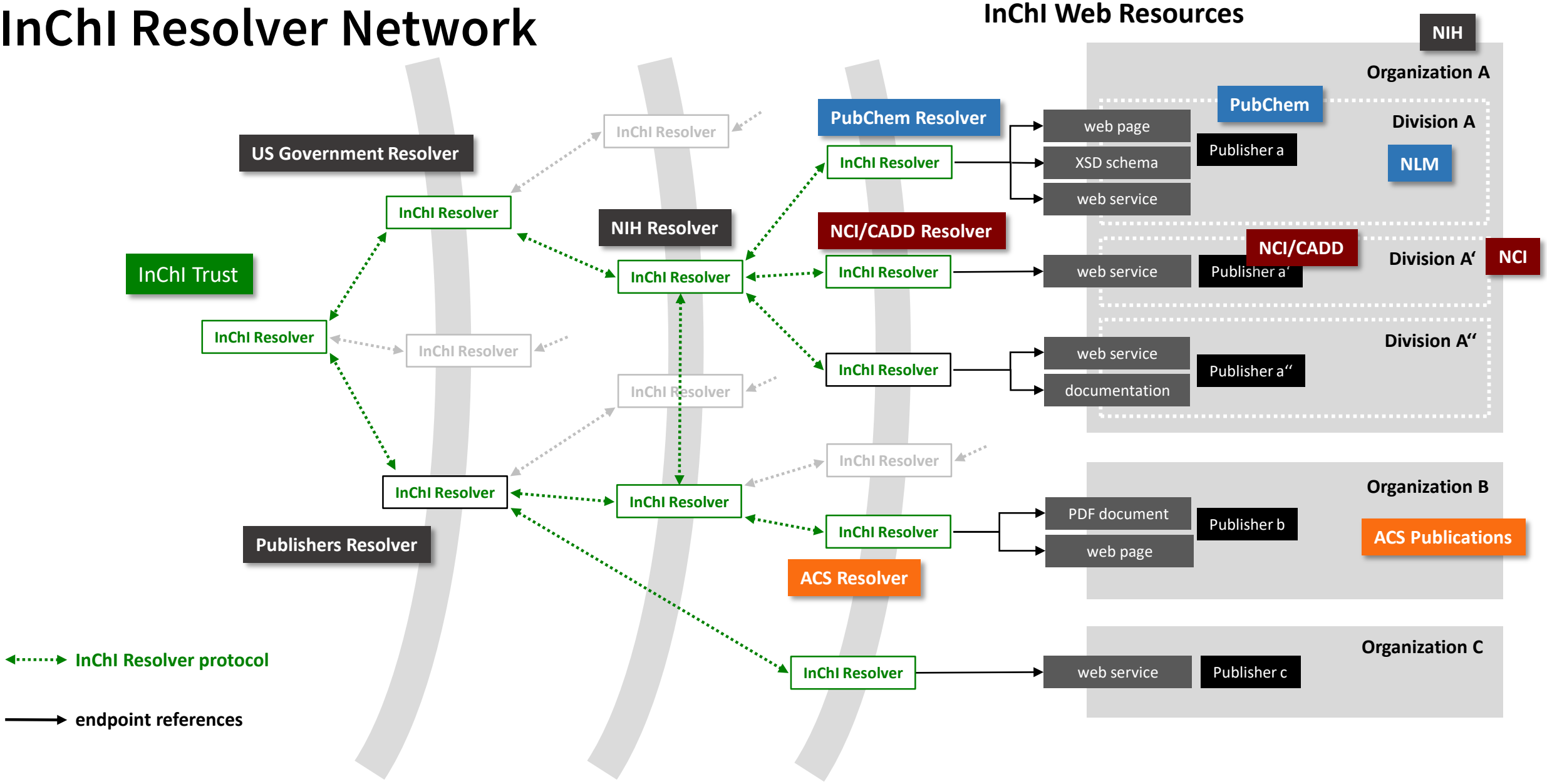


NCI/CADD resources

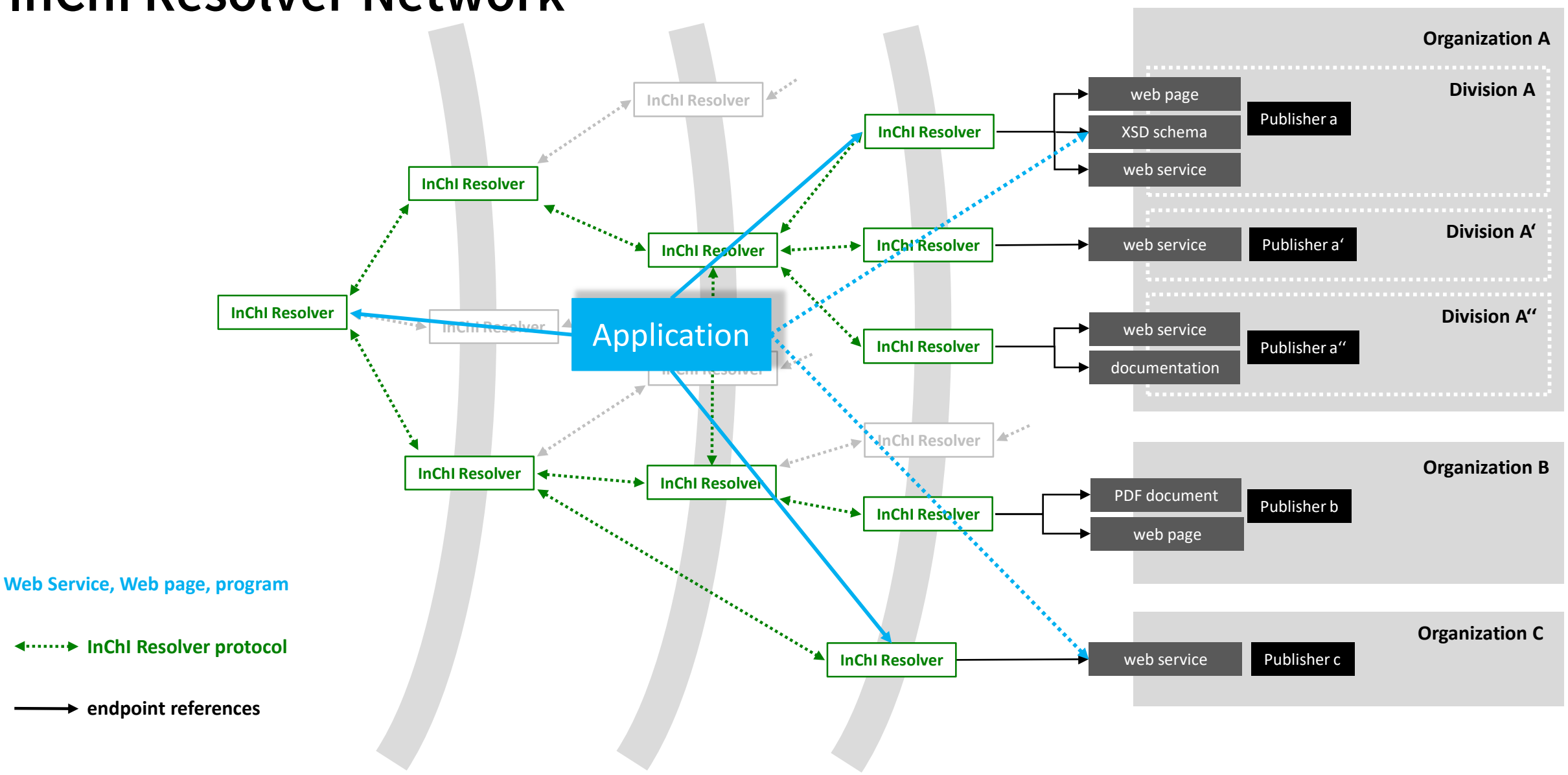
InChI Resolver Network



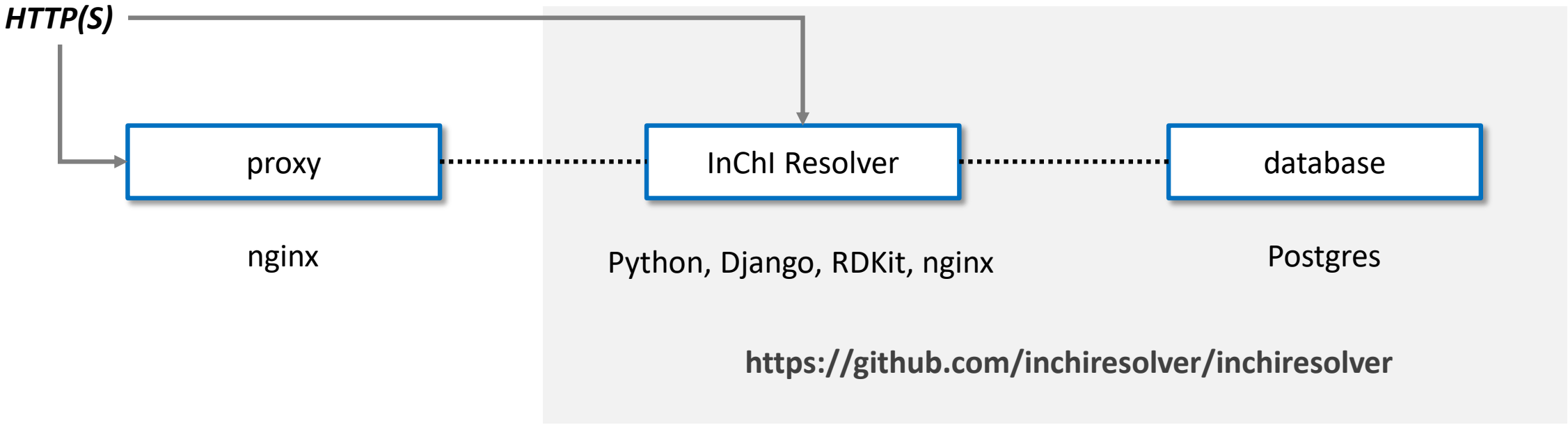
InChI Resolver Network



InChI Resolver Network



InChI Resolver: Reference Implementation – Technologies



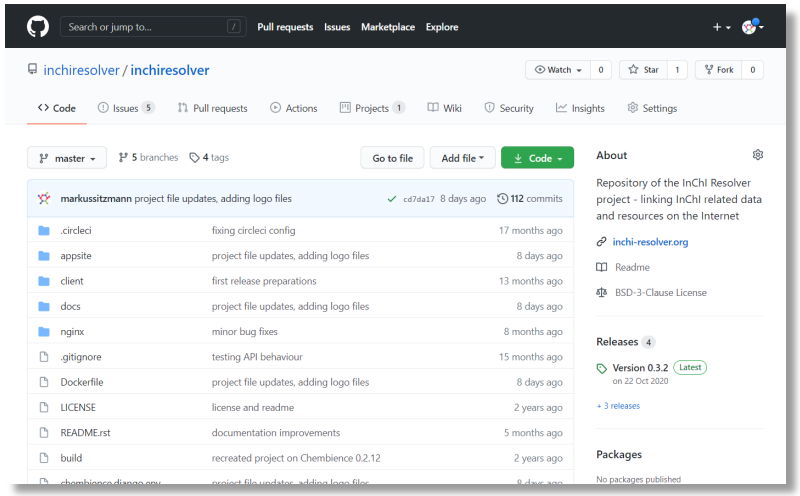
Docker Images available at Dockerhub

Chembience

https://github.com/chembience/chembience

InChI Resolver Project - Outlook

- representation of the InChI Resolver protocol as a single schema file
- more documentation
- loading more data
- definition of additional InChI Resolver resources (/minchi, /rinchi, /structure …)
- implementation of a InChI Resolver reference client
- unit tests



https://github.com/inchiresolver/inchiresolver

InChI Resolver and its Protocol

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