Documentation for Atomic Charge Calculator II - API

Atomic Charge Calculator II is a web tool designed for calculation of partial atomic charges. In order to be able to control this tool automatically, we have made API available.

This short documentation serves as a guideline to a simple workflow.

API runs under URL:

```
http://78.128.250.156/
```

All responses are in JSON format. To see if the request was successfull, you need to check **`status_code`** of JSON response. In case that your request was not successfull, you can display error message of JSON response.

Example of error response (usage of non-existent identifier gcnyaulugl):

```
{
  "status_code": 400,
  "message": "Structure ID gcnyaulugl does not exist."
}
```

1. Uploading structure

Please note, that it is possible to upload only files of max size 10 MB.

Assume that you would like to get partial atomic charges of structure with PDB ID 1NER.

First you need to upload this structure to the server. The structure is saved under specific identifier called **`structure_id`**, which is obtained in request response. Use this **`structure_id`** identifier for operations related to specific structure.

API provides three options for uploading structure to the server. If the structure is in the PDB database, it is possible to specify its PDB ID to pid[] parameter of **`/pdb_id`** endpoint.

```
curl -X POST http://78.128.250.156/pdb_id?pid[]=1ner
```

If the structure is in the Pubchem database, use **`/pubchem_cid`** endpoint and specify compound CID of your structure to cid[] parameter (1NER is not available in Pubchem, therefore 2244 CID is used for demonstration purposes).

```
curl -X POST http://78.128.250.156/pubchem_cid?cid[]=2244
```

If you would like to upload the file from local storage, it is possible to use **`/send_files`** endpoint.

```
curl -X POST -F file[]=@1ner.pdb http://78.128.250.156/send_files
```

API enables to upload more than one structure in the same time. In that case, dictionary containing the structure identifiers under the structure names is obtained.

Please, be aware, that if you use **/pdb_id** endpoint, protein structure in .cif format will be uploaded to the server. In case, that you would like, for any reason, upload structure in .pdb format, you have to use **/send_files** endpoint and upload structure from your local storage.

If your request is successfull, response in JSON format is received.


```
{
  "message": "OK",
  "status_code": 200,
  "structure_ids": {
    "1ner": "1ner7ozsxew5"
  }
}
```


2. Adding hydrogens to structure (WIP: Works just for structures in .pdb format)

If the protein structure has no hydrogens and you would like to add them, use **/add_hydrogens** endpoint.

Hydrogens are added by PropKa (pdb2pqr) programme.

Specify identifier of input structure without hydrogens and obtain new identifier representing structure with added hydrogens.

```
curl -X POST http://78.128.250.156/add_hydrogens?structure_id=1ner7ozsxew5
```

3. Choice of calculation method

If you are not sure, which method for calculation of partial atomic charges is suitable for your dataset, you can use **/suitable_methods** endpoint.

```
curl "http://78.128.250.156/suitable_methods?structure_id=1ner7ozsxew5"
```

API response contains list of methods suitable for calculation partial atomic charges. Every method also contains list of suitable parameters. If parameters is null, method does not require any parameters.


```
{
"suitable_methods": {
    "denr": [
      "DENR_00_from_QEq"
```

```
    ],
    "eqeq": null,
    "formal": null,
    "mgc": null,
    "qeq": [
      "QEq_00_original"
    ],
    "tsef": [
      "TSEF_00_from_QEq"
    ],
    "veem": null
  },
  "message": "OK",
  "status_code": 200
}
```


4. Calculation of charges

The main purpose of Atomic Charge Calculator II is calculation of partial atomic charges.

To get partial atomic charges, use **`/calculate_charges`** endpoint. You can specify several parameters

- mandatory:
  - **`structure_id`** – identifier of your structure
- optional:
  - **`method`** – calculation method
  - **`parameters`** – parameters set by specific method
  - **`read_hetatm`** - use in case that you would like to read not only the protein, but also ligands.
    Default: True
  - **`ignore_water`** - use in case, that you would like to ignore water molecules.
    Default: False

Calculate partial atomic charges of uploaded 1NER structure. For the purpose of this tutorial, ‚denr' method is used.

```
curl
"http://78.128.250.156/calculate_charges?structure_id=1ner7ozsxew5&method=denr&parameters=DENR_00_from_QEq"
```

API response contains list of partial atomic charges.


```
{
  "charges": [
    -0.1108,
    0.0257,
    0.0512,
    -0.1958,
    0.0114,
    …
    0.0753
  ],
  "message": "OK",
  "method": "denr",
  "parameters": "DENR_00_from_QEq",
  "status_code": 200
}
```


In case, that you would not specify method, first method of suitable methods for your dataset is used. Parameters are retrieved in similar way.

Be aware, that if you want to use method that was in response of **`/suitable_methods`**, you have to set read_hetatm and ignore_water as you set in **`/suitable_method`** endpoint. Otherwise you may get an error message, that the method is not suitable for your dataset.

Please note, that calculated partial atomic charges can vary, when using different methods.