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# Prediction API

The API used for prediction will be RESTful and will allow the prediction of an NMR spectrum and NMR data from a molecule described in the SMILES format.

## 1. Functional Objectives

- Allow users to submit a molecule (SMILES format) and other parameters
- Generate and return the simulated NMR spectrum and data corresponding to the molecule
- Provide a structured response according to the format described below

## 2. Endpoints

- **/predict** [POST]
  - **Description**: Triggers an NMR spectrum prediction
  - **HTTP Status Codes :**
    - **200 OK :** Always returned, whether the request is successful or a prediction error occurred.
    - **Errors are not indicated by HTTP status**, but instead by a JSON field:

```
{
  "error": "Description of the error"
}
```

    - **Important :** Any HTTP status code other than 200 OK (e.g. 400, 500) is treated by the system as an unexpected error
  - **JSON Request :**

```
{
  "smiles": "CCO",
  {
    "key": "type",
    # Supported Values : "1H", "13C" or "Unknown"
    "value": "13C"
  },
}
```

- **JSON Response :**


```
{
  "smiles": "CCOC",
  "spectrum": [
    {
      "ppm": 65.4,
      "intensity": 0.89,
      "atomID": [3]
    },
            ...
  ],
  "peaksInfos": [
    {
      "assignement": [1, 2],
      "delta": 58.2,
      "nbAtoms": 2,
      "multiplicity": "t",
      "coupling": [7.2]
    },
            ...
  ],
  "metadata": {
    "nucleusType": "13C"
  }
}
```