# Resource Summary Report

Generated by RRID on Sep 19, 2026

## RESP ESP charged Database

RRID:SCR_007883
Type: Tool

### Proper Citation

RESP ESP charged Database (RRID:SCR_007883)

### Resource Information

**URL:** http://q4md-forcefieldtools.org/REDDB

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**Description:** A new source of RESP or ESP atomic charge values for small structures or model systems. Its goals are multiple. R.E.DD.B. freely stores and distributes derived RESP or ESP charges of high quality and high reproduciblility within force field library(ies) in the scientific community. However, R.E.DD.B. can also be seen as a tool devoted to reproduce, compare, criticize and improve the different RESP and ESP models. As indicated by its name, R.E.DD.B. deals _only_ with RESP or ESP charges, and not with other types of atomic charges (Mulliken, Gasteiger or Bader analysis...). As previously said, many different procedures are used to derive such RESP or ESP charges, and the charge values are affected by many parameters (Quantum Mechanics programs, algorithms, molecular orientation, molecular conformation, human errors, etc..). Thus, R.E.DD.B. not only stores RESP or ESP charge values, but also the structures and information about the procedure used to derive the reported charge values. Two types of "projects" can be found in R.E.DD.B. - A WHOLE MOLECULE "project", which corresponds to an intact (un-broken) molecule. Examples are small organic or inorganic molecules such as solvent (DMSO, ethanol, cyclohexane etc...), and ligands of proteins or nucleic acids. - A MOLECULE FRAGMENT "project", which corresponds to a part (or fragment) of an organic or inorganic macro-molecule. This means that some atoms have to be removed from the structure(s) used in the charge derivation process to lead to the target fragment(s). Examples are amino-acid (AA) fragments 'NH-CH(R)-CO' where the atomic charges are generally derived using capped amino acids 'ACE-AA-NME', nucleotide fragments originating from the fusion between dimethylphosphate and the corresponding nucleosides, or monosaccharide fragments. These fragments are generally compatible with previously existing ones (available in force field topology databases), and used to construct macro-molecules such as proteins, nucleic acids or polysaccharides.

**Synonyms:** R.E.DD.B.

**Resource Type:** data or information resource, database

**Resource Name:** RESP ESP charged Database

**Resource ID:** SCR_007883

**Alternate IDs:** nif-0000-03384

**Record Creation Time:** 20220129T080244+0000

**Record Last Update:** 20260912T200154+0000

## Ratings and Alerts

No rating or validation information has been found for RESP ESP charged Database.

No alerts have been found for RESP ESP charged Database.

## Data and Source Information

**Source:** SciCrunch Registry

## Usage and Citation Metrics

We found 3 mentions in open access literature.

**Listed below are recent publications.** The full list is available at RRID .

Wang Z, et al. (2020) Cyclodextrin complexation studies as the first step for repurposing of chlorpromazine. International journal of pharmaceutics, 584, 119391.

Amato F, et al. (2014) Exploitation of a very small peptide nucleic acid as a new inhibitor of miR-509-3p involved in the regulation of cystic fibrosis disease-gene expression. BioMed research international, 2014, 610718.

Hamon F, et al. (2014) Synthesis and characterization of a new photoinduced switchable ??-cyclodextrin dimer. Beilstein journal of organic chemistry, 10, 2874.