History of the developments of the R.E.D. tools

http://q4md-forcefieldtools.org/RED/

Last update of this document: September 28th, 2012

Ante_R.E.D. developments were initiated at TSRI in Professor D.A. Case's laboratory by
R. Lelong,[1,3] P. Cieplak[4] & F.-Y. Dupradeau[1,3]

Ante_R.E.D. 1.x were developed at the "UFR de Pharmacie" in Amiens by
F.-Y. Dupradeau[5] & P. Cieplak[4]

Ante_R.E.D. 2.x is currently developed at the "UFR de Pharmacie" in Amiens by
G. Klimerak,[5] P. Cieplak[4] & F.-Y. Dupradeau[5]

X R.E.D. I & R.E.D. I were developed at the "Faculté de Pharmacie" in Amiens by
A. Pigache,[1] P. Cieplak[2] & F.-Y. Dupradeau[1]

R.E.D. II was developed at TSRI in Professor D.A. Case's laboratory by
T. Zaffran,[1,3] P. Cieplak[4] & F.-Y. Dupradeau[1,3]

R.E.D. III.x developments were initiated at TSRI in Professor D.A. Case's laboratory
& are now carried out at the "UFR de Pharmacie" in Amiens by
F. Wang,[5] E. Garcia,[5] N. Grivel,[1,3] P. Cieplak[4] & F.-Y. Dupradeau[1,3 then 5]

R.E.D. IV is developed at the "UFR de Pharmacie" in Amiens by
F. Wang,[5] W. Rozanski,[5] E. Garcia,[5] D. Lelong,[5] P. Cieplak[4] & F.-Y. Dupradeau[5]

X R.E.D. III was developed at the "Faculté de Pharmacie" in Amiens by
C. Savineau,[1 then 5] P. Cieplak[4] & F.-Y. Dupradeau[1 then 5]
X R.E.D. III.x are now developed at the "UFR de Pharmacie" in Amiens by
F.-Y. Dupradeau[5] & P. Cieplak[4]

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[2] Accelrys Inc., San Diego, CA, USA
[3] The Scripps Research Institute, Dept. of Mol. Biology, La Jolla, USA
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We are grateful to T. A. D. Patko (California State University, Long Beach, CA, USA) for his contribution in porting R.E.D.-III.x on Mac OS & Windows/Cygwin

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Do you need a new feature which is not yet implemented in the R.E.D. III.5 tools?
contact the q4md force field tools team at contact@q4md-forcefieldtools.org
We will try to help you as much as possible.
Regularly look for bug fixes at the R.E.D. home page.

Need to perform more complex charge derivation and/or force field library building ?
See R.E.D. Server @ http://q4md-forcefieldtools.org/REDS/ to be able to interface R.E.D. IV.

Please, submit your force field library(ies) to R.E.DD.B. at http://q4md-forcefieldtools.org/REDDB/
to freely review & share your results within the scientific community.

Need help about the q4md force field tools ?
Please, ask your queries to the *q4md-forcefieldtools* mailing list @ http://lists.q4md-forcefieldtools.org/

We hope you will find the R.E.D.-III.5 tools useful...
The q4md force field tools team

*** Release of R.E.D. I & X R.E.D. I - December 3rd, 2003**

- Automatic RESP or ESP charge derivation for whole molecules using:
  . the Gaussian 03, 98 or 94 or GAMESS-US program (geometry optimization & MEP computation steps) &,
  . the RESP program (charge fitting step).
- Force field library building in the Tripos mol2 file format for whole molecules.
- Use of the PDB file format as input for R.E.D. execution.
- Implementation of the QMRA approach by controlling the molecular orientation of the optimized geometry using the re-reorientation algorithm available in the QM program.
- Development of the RBRA approach implementing a rigid-body re-orientation algorithm to control the molecular orientation of the optimized geometry. This allows derivation of highly reproducible RESP or ESP charge values independently of the QM program interfaced.
- Development of multiple-orientation RESP or ESP charge derivation for whole molecules.
- Handle parallel computing in QM calculations.

*** Release of R.E.D. II & X R.E.D. II - July 1st, 2005**

New features available:
- Bug corrections.
- Implementation of multiple conformation RESP or ESP charge derivation for whole molecules.
- Force field library building in the Tripos mol2 file format for multiple conformation.
- Development of multiple-orientation and/or multiple conformation RESP or ESP charge derivation for whole molecules.
- Chemical elements with a total number of electrons up to Z = 35 are automatically handled.

*** Release of the R.E.D. III tools - April 13th, 2007**

New features available:
- Bug corrections.
- Development of Ante_R.E.D.-1.
- Development of the P2N file format used as input (instead of the PDB file format) for the execution of R.E.D.
- Eight different charge derivation procedures are now available:
  . using different algorithms for MEP computation (Connolly surface or CHELPG algorithm) &
  . using different charge fitting procedures (with or without hyperbolic restraints).
- Introduction of multiple molecule charge derivation.
- Development of multiple-orientation and/or multiple conformation and/or multiple molecule RESP or ESP charge derivation.
- Handling of intra-molecular charge constraint, inter-molecular charge constraint and inter-molecular charge equivalencing during the charge fitting step.
- Introduction of charge derivation and force field library building for molecule fragments:
  . generation of the central & terminal fragments of amino-acids and the central fragment of nucleotides
- Tutorials are available @ http://q4md-forcefieldtools.org/Tutorial/ (Tutorials 1 & 2).

*** Release of the R.E.D. III.1 tools - January 12th, 2009**

New features available:
- Bug corrections.
- Better handling/display of system variables.
- Better interface to GAMESS-US and new interface to PC-GAMESS/Firefly in Ante_R.E.D., R.E.D. & X R.E.D.
- Portability on Mac OS X platforms.
- Better compatibility with R.E.D. Server.
- A new Mini-HowTo in the R.E.D tools distribution is available.

*** Release of the R.E.D. III.2 tools - April 1st, 2009**

New features available:
- Bug corrections.
- Better handling/display of system variables as well as code cleaning for R.E.D.
- Creation of a DEBUG mode in R.E.D. which allows:
  . quickly getting an idea of the tasks carried out by R.E.D.
  . debugging the source code & developing new functionalities.
- Correction and development of the Mini-HowTo.
- Increase compatibility with R.E.D. Server.

*** Release of the R.E.D. III.3 tools - October 1st, 2009**

New features available:
- Bug corrections.
- Portability on Windows platforms through the Cygwin environment making the R.E.D. tools fully functional on UNIX, MacIntosh and Windows operating systems.
- Interface of Gaussian 2009 is implemented (as for g03, g98 & g94).
- Improvement of GAMESS-US & PC-GAMESS interface and new interface for WinGAMESS,
- Implementation of a new Re_Fit mode for charge re-fitting and force field library re-building from a previous R.E.D. job,
- Development of the Mini-HowTo and creation of a History file summarizing the features implemented in the R.E.D. tools,
- Creation of a benchmark of charge values for models with an automatic checking procedure & connection with R.E.DD.B.
- New manuals are available in the PDF file format.

*** Release of the R.E.D. III.4 tools - July 6th, 2010**

New features available:
- Code cleaning and updates.
- Update of the Mini-HowTo & Tutorials.
- Charge reproducibility further demonstrated: differentiation between rotation, translation and re-orientation.
- Molecular fragments originating from the fusion between two molecules are reconstructed leading to correct geometries.
- Distribution of the R.E.D. III.4 tools under the GNU General Public License.

*** Release of the R.E.D. III.5 tools - February 20th, 2012**

New features available:
- Bug corrections and code cleaning.
- Update of the Mini-HowTo & Tutorials.
- Better handling of Gaussian, GAMESS and Firefly error messages.
- Rounding off errors automatically corrected at 10-6 up to 10-2 depending on the user choice.
- Handling geometrical constraints in the P2N file format (geometry optimization using the Gaussian program).
- Two new scripts for data submission in R.E.DD.B.
- New version for the RESP program : version 2.2 with updated documentation.
- Distribution of the R.E.D. III.5 tools under the GNU General Public License.

*** Release of the R.E.D. III.51 tools - February 20th, 2012**

New features available:
- Bug corrections related to the automatic rounding off error correction
See http://q4md-forcefieldtools.org/RED/popup/bugs-III.5.txt

*** Release of the R.E.D. III.52 tools - September 28th, 2012**

New features available:
- Handle the new installation procedure available in GAMESS version may 2012 R1
- Prevent the use of Gaussian 09 B.01
See http://q4md-forcefieldtools.org/RED/popup/bugs-III.5.txt

R.E.D. IV is available at R.E.D. Server - April 6th, 2009

- Charge derivation & force field library building for large sets of molecules and molecular fragments in a single R.E.D. job.
- Building of force field topology databases *i. e.* a set of force field libraries for whole molecules & molecular fragments.
- Introduction of a second format for handling inter-molecular charge equivalencing during the charge fitting step.
- Development of the tutorials @ http://q4md-forcefieldtools.org/Tutorial/ (Tutorial 3).

R.E.D. IV is available at R.E.D. Server - June, 2010

- Automatic generation of the different fragments for a new amino-acid or a new nucleoside
- Rounding off errors fully corrected at 10-6 up to 10-2 depending on the user choice
- Handling geometrical constraints in the P2N file format (for the Gaussian program)
- Development of a statistics module allowing
  . study of the impact of charge constraints during the fitting step,
  . comparison between ESP charges obtained in QM computation with RESP or ESP charges obtained after charge fitting,
  . comparison between Mulliken charges obtained in QM computation with charges obtained after charge fitting,
  . comparison between charges obtained from fitting and from averaging.

R.E.D. IV is available at R.E.D. Server Dev. - June, 2011

- Automatic generation of the different fragments for a new amino-acid or a new nucleoside
- Rounding off errors fully corrected at 10-6 up to 10-2 depending on the user choice
- Handling geometrical constraints in the P2N file format (for the Gaussian program)
- Development of a statistics module allowing
  . study of the impact of charge constraints during the fitting step,
  . comparison between ESP charges obtained in QM computation with RESP or ESP charges obtained after charge fitting,
  . comparison between Mulliken charges obtained in QM computation with charges obtained after charge fitting,
  . comparison between charges obtained from fitting and from averaging.
- Handing various values of atomic radii for metal centers in MEP computation
- Handling all the elements of the periodic table
- Handling new charge models based on DFT (RESP-X1, ESP-X1...)

Features currently developed in R.E.D. IV at R.E.D. Server

Under active development...
- Generation of united-carbon force field libraries (besides the regular all-atom force field libraries).
  . 3 different approaches are implemented & working on 2 new approaches
- Automatic handling of various approaches for charge equivalencing for chemically equivalent atoms.
- Handling extra-points & lone-pairs.
- Interface of the i_RESP program
- New charge models

For more information see http://q4md-forcefieldtools.org/REDS/popup/news.php
http://q4md-forcefieldtools.org/REDS-Development/popup/news.php

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