

ScaLAPACK

Description: A subset of LAPACK routines for parallel calculations.

Site: <http://www.netlib.org/scalapack/>

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Open MPI

Description: Open Source MPI implementation (Version 3)

Site: <https://www.open-mpi.org/community/license.php>

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XCFun

Description: XCFun is a library of DFT exchange-correlation (XC) functionals.

Site: <http://dftlibs.org/xcfun/>

License:

A modified LGPL license that allows us to link ORCA statically with XCFun.

XCFun is copyright 2009-2017 Ulf Ekstrom and contributors.

The XCFun library is licensed under the LGPL license. This means that you may modify and distribute the library freely as long as you also release any changes made by you under the LGPL license. If you are just making modifications without distributing the modified library you are not obliged to release your changes. However, we do of course welcome all contributions as long as they are well tested and thought out.

Reference:

Ulf Ekström, Lucas Visscher, Radovan Bast, Andreas J. Thorvaldsen and Kenneth Ruud, *Arbitrary-Order Density Functional Response Theory from Automatic Differentiation*, [*Journal of Chemical Theory and Computation* 6, 1971 \(2010\)](#), DOI: [10.1021/ct100117s](https://doi.org/10.1021/ct100117s)

otool_smd

Description: otool_smd is a standalone code that, delivered a molecular geometry, computes the CDS energies and gradients. The code is a modification of parts of the GESOL code, which is redistributed with permission of C. J. Cramer and D. G. Truhlar.

Site: <https://comp.chem.umn.edu/gesol/>

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When publishing SMD results users shall cite:

Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. (2009) J. Phys. Chem. B, 113, 6378.

References:

GESOL Code: Marenich, A.; Hawkins, G.; Liotard, D.; Cramer, D., GESOL - version 2008.
<https://comp.chem.umn.edu/gesol>.

SMD Publication: Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. (2009) J. Phys. Chem. B, 113, 6378.

otool_gcp

Description: otool_gcp is used as an external tool that computes an energy correction in order to remove artificial overbinding effects from BSSE.

Site: <https://www.chemie.uni-bonn.de/pctc/mulliken-center/software/gcp/gcp>

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OpenBLAS

Description: OpenBLAS is an optimized BLAS library. It is used within the Windows executables.

Site: <https://www.openblas.net/>

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Intel® Math Kernel Library (Intel® MKL)

Description: Fastest and most used math library for Intel and compatible processors.

Site: <https://software.intel.com/en-us/intel-mkl>

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Libint

Description: libint is a library of C/C++ functions for efficient evaluation of several kinds of two-body molecular integrals over Gaussian functions and the optimizing compiler that generates a Libint library. Libint version 2 has been integrated into ORCA.

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