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==> amber03

"info" : ["Duan et al. (2003), J. Comp. Chem. 24, 1999-2012",

"Parameters converted from those at

<http://amber.scripps.edu/amber9.ffparms.tar.gz>",

"Bugfix from

<http://amber.scripps.edu/bugfixes/9.0/bugfix.5> applied to correct torsion assignments"]

==> amber94

"info" : ["Cornell et al. (1995), JACS 117, 5179-5197",

"Parameters converted from those at

<http://amber.scripps.edu/amber9.ffparms.tar.gz>"]

==> amber96

"info" : ["Kollman (1996), Acc. Chem. Res. 29, 461-469",

"Parameters converted from those at

<http://amber.scripps.edu/amber9.ffparms.tar.gz>"]

==> amber99

"info" : ["Wang et al. (2000), J. Comp. Chem. 21, 1049-1074",

"Parameters converted from those at

<http://amber.scripps.edu/amber9.ffparms.tar.gz>"]

==> amber99SB

"info" : ["Wang et al. (2000), J. Comp. Chem. 21, 1049-1074",

"Hornak et al. (2006), Proteins: Structure, Function and Genetics, 3:712-725.",

"Parameters converted from those at

<http://amber.scripps.edu/amber9.ffparms.tar.gz>"]

APBS (Adaptive Poisson-Boltzmann Solver)

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C and C++ Libraries for Parsing PDB Records

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CHARMM Force Field Parameters

==> charmm22

"info" : ["MacKerell et al. (1998), J. Phys. Chem. B. 102,
3586-3616 (proteins)",

"Beglov et al. (1994), J. Chem. Phys. 100,
9050-9063 (ions)",

"parameters generated from

http://www.pharmacy.umaryland.edu/faculty/amackere/param/toppar/toppar_c31b1.tar.gz"

==> charmm27

"info" : ["MacKerell et al. (2004), J. Comp. Chem. 25,
1400-1415 (protein cmap)",

"MacKerell et al. (1998), J. Phys. Chem. B. 102,
3586-3616 (proteins)",

"Beglov et al. (1994), J. Chem. Phys. 100,
9050-9063 (ions)",

"parameters generated from

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ClustalW v. 2.0.11

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ConfigObj

ConfigObj ver. 4

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epydoc

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2006-Jan-27

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FTGL

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Pfam-A-seed.gz

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pytz

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PyYAML

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scipy ver. 0.5.2

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setuptools

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simplejson

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Version 2, June 1991

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virtualenv

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==> spce

"info" : ["Berendsen et al. (1987) J. Phys. Chem. 91, 6269."]

==> spc

"info" : ["Berendsen et al. in Intermolecular Forces, edited by B. Pullman (Reidel, Dordrecht,1981), p. 331."]

==> tip3p_charmm

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"Parameters as tabulated in: Mahoney et al (2000)
J. Chem. Phys. 112, 8910"]

==> tip4pew

"info" : ["Horn et al. (2004) J. Chem. Phys. 120, 9665"]

==> tip4p

"info" : ["Jorgensen et al. (1985) Mol. Phys. 56, 1381",
"Parameters as tabulated in: Mahoney et al.
(2000) J. Chem. Phys. 112, 8910"]

==> tip5p

"info" : ["Mahoney et al. (2000) J. Chem. Phys. 112, 8910"]

Water Site Analysis Software

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zlib. h

zlib.h -- interface of the 'zlib' general purpose compression library
version 1.1.3, July 9th, 1998

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