

ANNEX

list of software, databases, websites on QSARs and REACH

Here it will be presented a list of currently available software with their reference websites.

Accord for Excel (Accelrys Inc., San Diego, CA, USA)

<http://www.accelrys.com/products/accord>

ADAPT (Prof. P.C. Jurs, PennState University, University Park, PA 16802, USA)

<http://research.chem.psu.edu/pcjgroup/adapt.html>

CODESSA (Semichem Inc. – 7204 Mullen, Shawnee, KS 66216, USA)

<http://www.semichem.com>

DRAGON (Talete srl, via Pisani 13, 20124 Milano, Italy)

<http://www.talete.mi.it>

GRIN/GRID (Molecular Discovery Ltd. – West Way House, Elms Parade, Oxford OX2 9LL, UK)

No indication are available about the reference website.

HYBOT-PLUS (Prof. O. Raevsky – Russian Academy of science, IPAC)

<http://molpro.ipac.ac.ru/hybot.html>

MOLCONN-Z (Prof. L.H. Hall – 2 Davis Street, Quincy, MA 02170, USA)

<http://molpro.ipac.ac.ru/hybot.html>

<http://www.eslc.vabiotech.com/molconn/manuals/310s/preface1.html>

OASIS (Laboratory of Mathematical Chemistry. Prof. O. Mekenyan – Bourgas University, 8010 Bourgas, Bulgaria)

<http://www.oasis-lmc.org>

POLLY (Prof. S. Basak – University of Minnesota, 5013 Miller Trunk Highway, Duluth, MN 55811, USA)

No indication are available about the reference website.

SYBYL/QSAR (Tripos Inc. – 1699 South Hanley Rd., St. Louis, MO 63144-2913, USA)

http://www.serc.iisc.ernet.in/broadcast_messages/msg02517.html

TSAR (Accelrys Inc., San Diego, CA, USA (formerly Oxford Molecular Ltd, UK))

<http://www.accelrys.com>

A list of current tools/databases, either publicly or commercially available, will be shown below with their reference websites.

FREE AVAILABLE TOOLS

Ambit

<http://ambit.acad.bg>

Danish QSAR database

<http://ecbqsar.jrc.it>

Toxtree

<http://ecb.jrc.it/qsar/qsar-tools>

Toxmatch

<http://ecb.jrc.it/qsar/qsar-tools>

JRC QSAR Model Database

<http://qsar.db.jrc.it>

DART

<http://ecb.jrc.it/qsar/qsar-tools>

OECD QSAR Application Toolbox

<http://oecd-toolbox-march-2008.software.informer.com/>

AIM

<http://www.epa.gov/oppt/sf/tools/methods.htm>

OncoLogic®

<http://www.epa.gov/oppt/newchems/tools/oncologic.htm>

ECOSAR

<http://www.epa.gov/oppt/newchems/tools/21ecosar.htm>

EPI Suite

<http://www.epa.gov/oppt/exposure/pubs/episuite.htm>

COMMERCIALY AVAILABLE TOOLS

Leadscope®

<http://www.leadscope.com>

Derek

<http://www.lhasalimited.org>

HazardExpert

<http://www.compudrug.com>

TOPKAT

<http://www.accelrys.com>

The CASE family of methods

<http://www.multicase.com>

TIMES

<http://www.multicase.com>

TerraQSAR™

<http://www.terrabase-inc.com>