

Advanced
Chemistry
Development

ACD/Labs

What's New with ACD/Labs NMR Predictors Version 12.0

*Featuring ACD/HNMR Predictor, CNMR Predictor,
NNMR Predictor, FNMR Predictor, and PNMR
Predictor*

For more than a decade, ACD/Labs has been fully dedicated to building integrated solutions that enable data transfer and connection within chemical organizations. We remain committed to the adoption and creation of the latest technological and industrial advances, empowering our customers' research and development efforts with the foremost chemical capabilities. Each year, we release newer versions of our software to provide enhanced capabilities and superior integration between existing and new technologies.

New capabilities for ACD/Labs NMR Predictors 12.0 have resulted from collaboration with our users, as well as feedback from industry experts. We appreciate your input and encourage you to contact us with ideas or suggestions for new features by visiting support.acdlabs.com. In addition, we invite you to join us at one of the seminars we will be holding throughout the year to discuss our products and learn more about the current version. Visit www.acdlabs.com/events/ for a list of upcoming events.

Among the key features of ACD/Labs NMR Predictors presented below, are:

- All NMR Predictors now include 1D NMR Processing capability
- Internal database expansions
- Update or change structure in XNMR Predictor databases
- Neural network and incremental algorithms for ^{15}N , ^{19}F , and ^{31}P NMR predictions



Now Includes 1D NMR Processing Capability

All NMR Predictors now come with all of the features previously available in ACD/1D NMR Processor. This gives the end-user the flexibility to process their 1D NMR data and predict spectra within the same interface and application. In addition, it gives all users of NMR Predictors access to our cutting edge verification algorithms that provide the ability to automatically evaluate the correspondence between a proposed structure and experimental spectrum as well as auto-assignment of 1D NMR Spectrum.

For more information on how the processing and prediction applications work together visit:

<http://www.acdlabs.com/verification>

For more information on the processing capabilities and features available visit:

<http://www.acdlabs.com/nmrprocessor>

Internal Database Expansions

The annual expansion of our internal databases continues to provide even more support for diverse chemical structures.

ACD/HNMR Predictor now contains over 210,700 chemical structures.

Year	2002	2003	2004	2005	2006	2007	2008
Release	Version 6.0	Version 7.0	Version 8.0	Version 9.0	Version 10	Version 11	Version 12
# of Chemical Shifts	1,200,000	1,320,000	1,384,000	1,440,000	1,578,505	1,666,199	1,755,262

ACD/CNMR Predictor now contains over 200,100 chemical structures.

Year	2002	2003	2004	2005	2006	2007	2008
Release	Version 6.0	Version 7.0	Version 8.0	Version 9.0	Version 10	Version 11	Version 12
# of Chemical Shifts	1,700,000	1,850,000	2,017,000	2,160,000	2,351,827	2,430,218	2,547,046

ACD/NNMR now contains 9287 chemical structures with over 21,700 ¹⁵N chemical shifts.

Year	2002	2003	2004	2005	2006	2007	2008
Release	Version 6.0	Version 7.0	Version 8.0	Version 9.0	Version 10	Version 11	Version 12
# of Chemical Shifts	15,270	17,950	18,540	20,320	20,698	21,435	21,782

ACD/FNMR now contains over 17,000 chemical structures with over 35,300 ¹⁹F chemical shifts.

Year	2002	2003	2004	2005	2006	2007	2008
Release	Version 6.0	Version 7.0	Version 8.0	Version 9.0	Version 10	Version 11	Version 12
# of Chemical Shifts	26,140	27,200	29,300	31,225	32,790	35,014	35,349

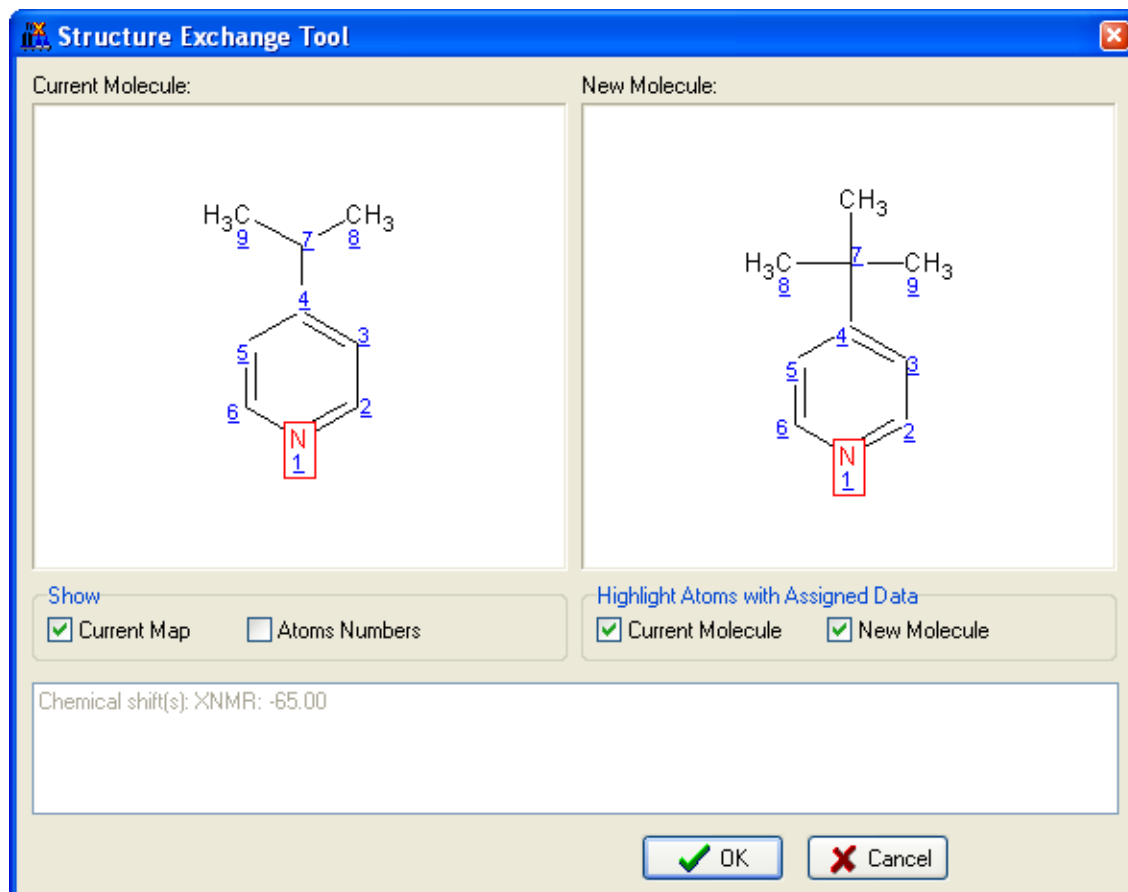
ACD/PNMR now contains over 27,500 chemical structures with over 34,000 ³¹P chemical shifts.

Year	2002	2003	2004	2005	2006	2007	2008
Release	Version 6.0	Version 7.0	Version 8.0	Version 9.0	Version 10	Version 11	Version 12
# of Chemical Shifts	24,680	25,940	28,190	31,420	32,474	33,695	34,020



Update or Change Structure in XNMR Predictor Database

In some cases, it may be necessary to change or update a structure in the predictor database. This is now possible in version 12 using the structure exchange tool. Users can simply double-click on the structure in the database record, modify the structure in ChemSketch, and the structure will be updated and existing assignments in the database will be retained.



Neural Network and Incremental Algorithms for ^{15}N , ^{19}F , and ^{31}P NMR Predictions

In addition to standard HOSE code algorithm, users can now view prediction results for new proprietary algorithms using the neural network and incremental approach.

The screenshot shows the ACD/XNMR software window. On the left is a chemical structure of a fluorinated amide with atoms numbered 1 through 18. The nitrogen atom in the amide group is highlighted in red and labeled '10'. On the right, there are two tables: 'Chemical Shifts' and 'Coupling Constants'. Below the tables is a text box for the 'Reference Compound: CH3NO2 (default)'. At the bottom of the window are buttons for 'Report', 'OK', and 'Help'.

Chemical Shifts:

X	N1	Value(ppm)	Error	Neural Net	Incr. Value
15N	10	-284.93	29.22	-247.31	-240.38
15N	18	-121.8	5.0	-114.29	-131.06
15N	14	-121.8	5.0	-114.29	-131.06

Reference Compound: CH3NO2 (default)

Coupling Constants:

X	J	N1	N2	Valu...	Error
15N	2J	3	10	-4.83	3.11
15N	3J	3 H	10	-3.32	2.28
15N	3J	2	10	-2.83	2.08
15N	4J	2 H	10	-0.69	0.5
15N	1J	4	10	-11.4	27.96
15N	4J	1	10	0.9	0.89
15N	2J	5	10	-4.83	3.11
15N	3J	5 H	10	-3.32	2.28
15N	3J	6	10	-2.83	2.08

To learn more about this product, please download our catalog from <http://www.acdlabs.com/download/catalogs/nmrcat.pdf> or visit our Web site (http://www.acdlabs.com/predict_nmr/).

Because ACD/Labs software is highly integrated, new features in connected modules may also be relevant. In particular, you may want to review information about ACD/1D NMR Manager and ACD/NMR Workbook (and ACD/Labs NMR Content Databases).



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