

NMRbox Release Notes

NMRbox Release 4.0 (December 16, 2017)

IMPORTANT: Please Cite and Acknowledge NMRbox in your publications! See <https://nmrbox.org/acknowledge-us> for details.

Software: Version 4.0 of the NMRbox VM includes 10 new and 19 updated NMR related software packages (see list below). Unfortunately, a few programs were removed as we attempt to work out licensing agreements with the developers.

Hardware: NMRbox VMs are equipped with 32 CPUs and 188 GB of RAM along with two NVIDIA GPUs for increased drawing performance. When processing jobs which utilize high numbers of CPUs please use the nice command by simply placing the word “nice” in front of your command (i.e. nice xplor < refine.inp > refine.out).

Storage: Home folders are located at /home/nmrbox/username and are backed up regularly. Currently there are no storage quotas, but we reserve the right to impose quotas if storage becomes limited. In addition, users have a second home folder located at /nmr/archive/username which is located on a highly reliable storage appliance. There is a folder located at /public for sharing files with other users and tutorial data from our workshops can be found at /tutorial.

Scratch disk: We have added a scratch disk to the VMs with dramatic speed improvements for data processing where high disk input/output (I/O) is needed. Please read the scratch disk policies **VERY CAREFULLY** which can be found in the NMRbox VM at /scratch/username/README. **The scratch disk is for transient files and files older than 48 hours WILL BE DELETED** to ensure all users have available space on the scratch disk. These policies may be altered based on usage. In addition, the scratch disk is local to a single VM and thus files are not shared across different NMRbox VMs as your home, archive, and public folders are.

Google Group: The NMRbox project has a Google Group for support questions, comments, and requests at <https://groups.google.com/forum/#!forum/nmrbox>. Questions pertaining to your personal account should be sent by email to support@nmrbox.org.

FAQ: The NMRbox team has a FAQ at <https://nmrbox.org/faq> with answers to frequent questions.

Installed NMR Software Packages

	Title	Version	Status
1	4DSPOT	1.21	
2	ABACUS	2.5	
3	Adapt NMR Enhancer	Build 4/8/2014	
4	ALATIS	1.01	
5	Almost	2.1.0	
6	AmberTools	17u8	Updated
7	ARIA	2.3.1	
8	ArShift	Downloaded 11/15/2015	
9	ASDP	2.0	Updated
10	AutoAssign	2.3.0	
11	Azara	2.8	
12	batman	1.2.1.03	
13	BMRB CS-Rosetta	0.3	
14	CalRW	1.0	
15	CalRW+	1.0	
16	CAMERA	Downloaded 10/25/2016	

17	CARA	1.9.2a5	
18	CCPNMR-Analysis	2.4.2	
19	CH3Shift	Downloaded 11/13/2015	
20	ChemEx	0.6.1	Added
	Chimera	1.11.2	Removed
21	ClustalWX	2.1	
22	CNS	1.3	
23	CNS-ARIA	1.21	
24	COMPASS	1	
25	CPMG_FIT (Korzhnev)	9.0	
26	CSCDP	0.1	
27	CS-GAMDY	1.0	Added
28	CYRANGE	2.0	
29	DASHA	4.1	
30	dataChord Spectrum Analyst	9.2.0-b17	Updated
31	dataChord Spectrum Miner	9.2.0-b17	Updated
32	DOSY Toolbox	2.7	Added
33	DYNAMO	7.2 rev 2013.047.09.17	
34	EISD	0.2	
35	ENSEMBLE	2.1	Added
36	FastModelFree	1.2	
	GAMESS	20Apr2017	Removed
37	Geometric Approximation	Downloaded 12/8/2017	Added
38	GLOVE	Downloaded 10/3/2016	
39	GNAT	0.96	Added
40	GOAP	Downloaded 11/13/2015	
41	GUARDD	2012-04-21	
42	hmsIST	2.11	
43	IMP	2.7.0	
44	INCHI	1.05	
45	Kd-Calc	2.0	Added
46	LARMORCA	1.00	
47	LARMORD	2.00	
48	localCIDER	0.1.14	
49	MATLAB-MCR	R2016b	
50	MestraNova	12	Updated
51	MDAnalysis	0.16.2	
52	MDD	2.5_b06-22-2017	
53	MESMER	1.0.0	
54	Modelfree	4.20	Updated
55	Modeller	9.19-1	
56	Molib	1.0.6	Added
57	MOLMOL	2.1-2.6	
58	MoSART	1.0	
59	MVAPACK	Build 7/14/2015	
	NAMD	2017-07-18	Removed
60	NESSY	12.3.1	
61	NESTA-NMR	1.5	
62	NMRDraw	9.4 rev 2017.335.16.23	Updated

63	NMRFAM-Sparky	Build 12/08/2017	Updated
64	NMRfx Processor	10.1.18	Updated
65	nmrplug	0.7	
66	NMRmix	Build 11/31/2015	
67	NMRPipe	9.4 rev 2017.335.16.23	Updated
68	nmrstarlib	2.0.6	Updated
69	NMRViewJ	9.2.0-b17	Updated
70	nmr_wash	1.0.0	
71	nustool	1-2	
72	Open Babel	2.4.1	
73	PALES	2.1	
74	PANAV	2.1	
75	ParmEd	Downloaded 7/24/2017	
76	PLUQ	0.2.1	Updated
77	PONDEROSA	Build 09/27/2017	Updated
78	PPM/PPM_One	2015-07-09	
79	PROMEGA	1.40F1 rev 2012.029.12.03	
80	PyMOL	1.8.6.0	
81	pynmrstar	2.5.1	Updated
82	Pyshifts	Downloaded_2016-05-31	
83	RasMol	2.7.5.2	
84	RAW	1.1.0	
85	RCI	1n_10_6_12-A	
86	RDC Panda / RDC Analytic	1.0	
87	REDCAT	3	
88	REDCRAFT	Build 3/16/2015	
89	relax	4.0.3	
90	RNAstrucutre	6.0	Updated
91	rNMR	1.1.9	
92	RNMRTK	3.2 Build_2831	
93	ROSETTA	2016.15.58628	
94	SHIFTS	5.3	Updated
95	SHIFTX	1.0	Added
96	SHIFTX2	1.10	
97	SMILE	1.1_rev2017.153.15.06	
98	SPARTA+	2.70F1 rev 2012.029.12.03	
99	Spectrum-Translator	1.1	
100	SQLite	3.14.2	
101	SSP	Downloaded 5/15/2016	
102	TALOS+	3.80F1 rev 20132.080.14.41	
103	TALOSN	4.12 rev 2015.147.15.40	
	TINKER	6.3.3	Removed
104	TITAN	1.3-3-g0e2b	
105	TOPSPIN	3.5p17	Updated
106	TREND	1.1.0	
	VMD	1.9.2	Removed
	VMD-Xplor	1.9.1	Removed
107	XDrawChem	1.10.2	Added
108	XPLOR-NIH	2.46	Updated

Additional Installed Software

	Title	Version	Status
1	DropBox	2015.10.28	
2	HTCondor		
3	Open JDK	8	Added
	Oracle Java	8	Removed
4	RealVNC	6.0.2	
5	RStudio	1.0.143	
6	Sublime Text	3-3126	
7	VirtualGL	2.5	

Python Packages

	Title	Python Versions	Status
1	Biopython	2.7 & 3.5	
2	Matplotlib	2.7 & 3.5	
3	nose	2.7 & 3.5	
4	NumPy	2.7 & 3.5	
5	pandas	2.7 & 3.5	
6	pip	2.7 & 3.5	
7	SciPy	2.7 & 3.5	
8	SymPy	2.7 & 3.5	

NMR Software Packages that can be run as Python Modules

1	AmberTools	2.7	Updated
2	ChemEx	2.7	Added
3	COMPASS	2.7	
4	EISD	2.7	
5	localCIDER	2.7 & 3.5	
6	MDAnalysis	2.7	
7	Modeller	2.7 & 3.5	
8	mollib	2.7 & 3.5	Added
9	nmrplug	2.7 & 3.5	
10	nmrstarlib	2.7 & 3.5	Updated
11	ParmEd	2.7	
12	Pluq	2.7 & 3.5	Updated
13	pynmrstar	2.7 & 3.5	Updated

Text editors

	Title	Status
1	Atom	
2	Bluefish	
3	diffuse (diff)	

4	Emacs
5	geany
6	Gedit
7	GVim
8	jEdit
9	meld (diff)
10	nano
11	NEdit
12	pico
13	Sublime Text
14	Vi/Vim
15	XEmacs

Installed Tools

	Title	Status
1	Bonnie++	
2	Calculator	
3	Chromium Browser	
4	CSH, TCSH shells	
5	FileZilla	
6	Firefox Web Browser	
7	Geary	
8	GIMP	
9	Git	
10	gnuplot	
11	Grace	
12	Graphviz	
13	HTCondor	
14	Inkscape	
15	IPython	
16	JMol	
17	Julia	
18	Libre Office	
19	littler	
20	Octave	
21	OpenDX	
22	POV-Ray	
22	R:Base	
23	ShellCheck	
24	Subversion	
25	Thunderbird Mail	
26	Xpdf	
27	xvkbd	

Note: Many additional Ubuntu packages installed. Packages with interest to NMRbox users listed above.

Installed Utility Scripts

	Title	Description	Status
1	resolution-changer.py	Change VNC resolution	Updated
2	kill-vnc-server	Manually kill VNC server	Updated
3	res.prl	Predict assignment based on CA, CB chemical shifts	
4	bruker2sbtools.prl	Extract relevant information for processing from Bruker acqu* files	
5	procpa.prl	Extract relevant information for processing from Varian procpa file	
6	sample_schedule_changer.prl	Change sample schedules	

Notes

	Category	Details	Status
1	User storage	Mount point for home folders created at /home/nmrbox/	
2	User storage	Mount point for user archive folders created at /nmr/archive/	
3	User storage	Mount point for sharing data created at /public	
4	Backups	User home folders automatically backed up daily to geo-dispersed storage system	
5	Tutorial	Directory for tutorial data created and populated at /tutorial	

Patches

Description
1

Known issues

Issue
1