

NMRbox Release Notes

NMRbox Release 3.0 (August 7, 2017)

Summary: Version 3.0 of the NMRbox VM includes 36 new and 18 updated NMR related software packages (see list below), including the commercial products MestraNova, dataChord Spectrum Analyst, and dataChord Spectrum Miner. The molecular visualization tools PyMOL, Chimera, and VMD are now fully functional and are backed by NVIDIA GPUs for increased performance. NAMD is our first program to take advantage of NVIDIA GPUs for CUDA computations with significant performance boosts over CPUs and more CUDA enabled packages are coming soon. Three MATLAB programs, compiled against the Matlab runtime libraries, have been added; ALATIS, GUARDD, and TITAN. Several additional packages were added to help with productivity including several new text editors, a virtual on-screen keyboard (xvkbd) to help with issues with keyboard mappings in RealVNC, additional Python packages, and updated tools for changing the screen resolution (resolution-changer.py) and shutting down VNC sessions that are not working properly (kill-vnc-server). We hope you enjoy the enhancements and please don't hesitate to email support@nmrbox.org with comments or suggestions to make NMRbox better.

Installed NMR Software Packages

	Title	Version	Status
1	4DSPOT	1.21	
2	ABACUS	2.5	Updated
3	Adapt NMR Enhancer	Build 4/8/2014	
4	ALATIS	1.01	Updated
5	Almost	2.1.0	
6	AmberTools	17	Updated
7	ARIA	2.3.1	
8	ArShift	Downloaded 11/15/2015	
9	ASDP	1.0	Added
10	AutoAssign	2.3.0	Added
11	Azara	2.8	
12	batman	1.2.1.03	Added
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	Updated
18	CCPNMR-Analysis	2.4.2	
19	CH3Shift	Downloaded 11/13/2015	
20	Chimera	1.11.2	
21	ClustalWX	2.1	Added
22	CNS	1.3	
23	CNS-ARIA	1.21	
24	COMPASS	1	
25	CPMG_FIT (Korzhnev)	9.0	
26	CSCDP	0.1	
27	CYRANGE	2.0	Added
28	DASHA	4.1	
29	dataChord Spectrum Analyst	9.2.0-b13	Added
30	dataChord Spectrum Miner	9.2.0-b13	Added

31	DYNAMO	7.2 rev 2013.047.09.17	
32	EISD	0.2	Added
33	ENSEMBLE	2.1	Added
34	FastModelFree	1.2	
35	GAMESS	20Apr2017	Added
36	GLOVE	Downloaded 10/3/2016	
37	GOAP	Downloaded 11/13/2015	
38	GUARDD	2012-04-21	Added
39	hmsIST	2.11	
40	IMP	2.7.0	Added
41	INCHI	1.05	Added
42	LARMORCA	1.00	Added
43	LARMORD	2.00	Added
44	localCIDER	0.1.14	Added
45	MATLAB-MCR	R2016b	
46	MestraNova	11	Added
47	MDAnalysis	0.16.2	Added
48	MDD	2.5_b06-22-2017	Updated
49	MESMER	1.0.0	Added
50	Modelfree	4.0	
51	Modeller	9.19-1	Updated
52	MOLMOL	2.1-2.6	
53	MoSART	1.0	Added
54	MVAPACK	Build 7/14/2015	
55	NAMD	2017-07-18	Added
56	NESSY	12.3.1	
57	NESTA-NMR	1.5	
58	NMRDraw	8.9 rev 2017.187.19.57	Updated
59	NMRFAM-Sparky	Build 07/07/2017	Updated
60	NMRfx Processor	10.1.6	Updated
61	nmrglue	0.7	Updated
62	NMRmix	Build 11/31/2015	
63	NMRPipe	8.9 rev 2017.187.19.57	Updated
64	nmrstarlib	2.0.2	Added
65	NMRViewJ	9.2.0-b12	Updated
66	nmr_wash	1.0.0	
67	nustool	1-2	Added
68	Open Babel	2.4.1	Added
69	PALES	2.1	
70	PANAV	2.1	Added
71	ParmEd	Downloaded 7/24/2017	Added
72	PLUQ	Downloaded 7/20/2016	
73	PONDEROSA	Build 06/22/2017	Updated
74	PPM/PPM_One	2015-07-09	Added
75	PROMEGA	1.40F1 rev 2012.029.12.03	
76	PyMOL	1.8.6.0	Updated
77	pynmrstar	2.3.4	Added
78	Pyshifts	Downloaded_2016-05-31	Added
79	RasMol	2.7.5.2	

80	RAW	1.1.0	
81	RCI	1n_10_6_12-A	
82	RDC Panda / RDC Analytic	1.0	Added
83	REDCAT	3	
84	REDCRAFT	Build 3/16/2015	
85	relax	4.0.3	Updated
86	RNAstrucutre	5.8.1	Added
87	rNMR	1.1.9	
88	RNMRTK	3.2 Build_2831	Updated
89	ROSETTA	2016.15.58628	
90	SHIFTS	5.1	
91	SHIFTX2	1.10	
92	SMILE	1.1_rev2017.153.15.06	Updated
93	SPARTA+	2.70F1 rev 2012.029.12.03	
94	Spectrum-Translator	1.1	
95	SQLite	3.14.2	
96	SSP	Downloaded 5/15/2016	
97	TALOS+	3.80F1 rev 20132.080.14.41	
98	TALOSN	4.12 rev 2015.147.15.40	
99	TINKER	6.3.3	Added
100	TITAN	1.3-3-g0e2b	Added
101	TOPSPIN	3.5p16	Added
102	TREND	1.1.0	Added
103	VMD	1.9.2	
104	VMD-Xplor	1.9.1	Added
105	XPLOR-NIH	2.45-updated	Updated
106	YESWORKFLOW	Build 248	

Additional Installed Software

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

Python Packages

	Title	Python Versions	Status
1	Biopython	2.7 & 3.5	Added
2	Matplotlib	2.7 & 3.5	
3	nose	2.7 & 3.5	Added
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	Added

NMR Software Packages that can be run as Python Modules

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

Text editors

	Title	Status
1	Atom	Added
2	Bluefish	Added
3	diffuse (diff)	Added
4	Emacs	
5	geany	Added
6	Gedit	
7	GVim	Added
8	jEdit	
9	meld (diff)	Added
10	nano	
11	NEdit	
12	pico	
13	Sublime Text	Added
14	Vi/Vim	
15	XEmacs	

Installed Tools

	Title	Status
1	Bonnie++	added
2	Calculator	
3	Chromium Browser	
4	CSH, TCSH shells	
5	FileZilla	
6	Firefox Web Browser	
7	Geary	Added
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	Added
22	POV-Ray	
22	R:Base	
23	ShellCheck	
24	Subversion	
25	Thunderbird Mail	
26	Xpdf	
27	xvkbd	Added

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 Certain python programs start very slow on first time use.