

NMRbox Release Notes

NMRbox Release 2.0 (December 19, 2016)

Installed NMR Software Packages

	Title	Version	Status
1	4DSPOT	1.21	
2	ABACUS	2.5	
3	Adapt NMR Enhancer	Build 4/8/2014	
4	Almost	2.1.0	
5	AmberTools	16	
6	ARIA	2.3.1	
7	ArShift	Downloaded 11/15/2015	
8	Azara	2.8	added
9	BMRB CS-Rosetta	0.3	
10	CalRW	1.0	
11	CalRW+	1.0	
12	CAMERA	Downloaded 10/25/2016	added
13	CARA	1.9.1.4	
14	CCPNMR-Analysis	2.4.2	
15	CH3Shift	Downloaded 11/13/2015	
16	Chimera	1.11.2	added
17	CNS	1.3	
18	CNS-ARIA	1.21	
19	COMPASS	1	
20	CPMG_FIT (Korzhnev)	9.0	
21	CSCDP	0.1	added
22	DASHA	4.1	
23	DLV	Build 12/17/2012	added
24	DYNAMO	7.2 rev 2013.047.09.17	
25	FastModelFree	1.2	
26	GLOVE	Downloaded 10/3/2016	added
27	GOAP	Downloaded 11/13/2015	
28	hmsIST	2.11	
29	MATLAB-MCR	R2016b	added
30	MD2NOE	1.0	added
31	MDD	2.5	added
32	Modelfree	4.0	
33	Modeller	9.17-1	updated
34	MOLMOL	2.1-2.6	
35	MVAPACK	Build 7/14/2015	added
36	NESSY	12.3.1	
37	NESTA-NMR	1.5	updated
38	NMRDraw	8.9 rev 2016.157.18.07	updated
39	NMRFAM-Sparky	Build 5/27/2016	updated
40	NMRfX Processor	10.0.0-b36	updated
41	nmrglue	0.5	updated
42	NMRmix	Build 11/31/2015	added
43	NMRPipe	8.9 rev 2016.157.18.07	updated
44	NMRViewJ	9.2.0-b2	updated

45	nmr_wash	1.0.0	added
46	PALES	2.1	
47	PLUQ	Downloaded 7/20/2016	
48	PONDEROSA	Build 8/3/2016	updated
49	PROMEGA	1.40F1 rev 2012.029.12.03	
50	PyMOL	1.8.2.1	added
51	RasMol	2.7.5.2	added
52	RAW	1.1.0	updated
53	RCI	1n_10_6_12-A	
54	REDCAT	3	added
55	REDCRAFT	Build 3/16/2015	added
56	relax	4.0.2	updated
57	rNMR	1.1.9	
58	RNMRTK	3.2-125	
59	ROSETTA	2016.15.58628	
60	SHIFTS	5.1	updated
61	SHIFTX2	1.10	updated
62	SMILE	8.9 rev 2016.157.161.12.48	updated
63	SPARTA+	2.70F1 rev 2012.029.12.03	
64	Spectrum-Translator	1.1	
65	SQLite	3.14.2	updated
66	SSP	Downloaded 5/15/2016	
67	TALOS+	3.80F1 rev 20132.080.14.41	
68	TALOSN	4.12 rev 2015.147.15.40	
69	TREND	1.1.0	added
70	VMD	1.9.2	added
71	XPLOR-NIH	2.43	updated
72	YESWORKFLOW	Build 248	

Additional Installed Software

	Title	Version	Status
1	Oracle Java	8	
2	RStudio	0.99.878	
3	RealVNC	5.3.1	
4	VirtualGL	2.5	added
5	DropBox	2015.10.28	added

Installed Ubuntu Tools

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

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

Installed Utility Scripts

	Title	Description	Status
1	resolution-changer	Change VNC resolution	
2	kill-vnc-server	Manually kill VNC server	
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	added

Patches

Description
1

Known issues

Issue
1 Chimera does not work properly through VNC. Must be run via ssh with X11 graphics.
2 PyMOL does not work properly through VNC. Must be run via ssh with X11 graphics.
3 Certain python programs start very slow on first time use.