

NMRbox Release Notes

NMRbox Release 1.0 beta (July 2016), Initial release

Installed NMR Software Packages

	Title	Version	Status
1	4DSPOT	1.21	added
2	ABACUS	2.5	added
3	Adapt NMR Enhancer	Build 4/8/2014	added
4	Almost	2.1.0	added
5	AmberTools	16	added
6	ARIA	2.3.1	added
7	ArShift	Downloaded 11/15/2015	added
8	BMRB CS-Rosetta	0.3	added
9	CalRW	1.0	added
10	CalRW+	1.0	added
11	CARA	1.9.1.4	added
12	CCPNMR-Analysis	2.4.2	added
13	CH3Shift	Downloaded 11/13/2015	added
14	CNS	1.3	added
15	CNS-ARIA	1.21	added
16	COMPASS	1	added
17	CPMG_FIT (Korzhnev)	9.0	added
18	DASHA	4.1	added
19	DYNAMO	7.2 rev 2013.047.09.17	added
20	FastModelFree	1.2	added
21	GOAP	Downloaded 11/13/2015	added
22	hmsIST	2.11	added
23	Modelfree	4.0	added
24	Modeller	9.16-1	added
25	MOLMOL	2.1-2.6	added
26	NESSY	12.3.1	added
27	NESTA-NMR	1.0	added
28	NMRDraw	8.9 rev 2016.157.18.07	added
29	NMRFAM-Sparky	Build 5/27/2016	added
30	NMRfX Processor	10.0.0-b28	added
31	nmrGlue	0.4	added
32	NMRPipe	8.9 rev 2016.157.18.07	added
33	NMRViewJ	9.1.0-b58	added
34	PALES	2.1	added
35	PLUQ	Downloaded 7/20/2016	added
36	PONDEROSA	Build 5/27/2016	added
37	PROMEGA	1.40F1 rev 2012.029.12.03	added
38	RAW	0.99.9.14b	added
39	RCI	1n_10_6_12-A	added
40	relax	4.0.1	added
41	rNMR	1.1.9	added
42	RNMRTK	3.2-125	added
43	ROSETTA	2016.15.58628	added
44	SHIFTS	5.0.1	added

45	SHIFTX2	1.09A	added
46	SMILE	8.9 rev 2016.157.161.12.48	added
47	SPARTA+	2.70F1 rev 2012.029.12.03	added
48	Spectrum-Translator	1.1	added
49	SQLite	3.9.2	added
50	SSP	Downloaded 5/15/2016	added
51	TALOS+	3.80F1 rev 20132.080.14.41	added
52	TALOSN	4.12 rev 2015.147.15.40	added
53	XPLOR-NIH	2.40	added
54	YESWORKFLOW	Build 248	added

Additional Installed Software

	Title	Version	Status
1	Oracle Java	8	added
2	RStudio	0.99.878	added
3	RealVNC	5.3.1	added

Installed Ubuntu Tools

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

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

Notes

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

Patches

	Description
1	Program launcher for the BMRB CS-Rosetta portal fixed
2	Kernel parameters shmmax and shmall adjusted to allow larger data sets to be processed with RNMRTK