

NMRbox Release Notes

NMRbox Release 5.0 (September 24, 2018)

Summary: Version 5.0 of the NMRbox VM includes 46 new and 38 updated NMR related software packages for a total of 153 (see list below). 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	
3	Adapt NMR Enhancer	Build 4/8/2014	
4	ALATIS	4.1	updated
5	Almost	2.1.0	
6	AmberTools	18	updated
7	ANATOLIA	1.0	added
8	ARIA	2.3.1	
9	ArShift	Downloaded 06/01/2018	updated
10	ASDP	2.0	updated
11	AutoAssign	2.3.0	
12	Azara	2.8	
13	batman	1.2.1.11	updated
14	BMRB CS-Rosetta	0.31	updated
15	CalRW	1.0	
16	CalRW+	1.0	
17	Cambridge-CS	1.02	added
18	CAMERA	Downloaded 10/25/2016	
19	CARA	1.9.1.7	updated
20	CATIA	0.52p	added
21	CCPNMR-Analysis	2.4.2	
22	CH3Shift	Downloaded 06/01/2018	updated
23	Chemex	0.6.1	
24	ClustalWX	2.1	
25	CNS	1.3	
26	CNS-ARIA	1.21	
27	COMPASS	1	
28	CPMG_FIT (Korzhnev)	9.0	
29	CSCDP	0.1	
30	CS-GAMDY	1.0	
31	CTFFIND	4.1.10	added
32	CYRANGE	2.0	
33	CYTOSCAPE	3.6.1	added
34	DANGLE	1.1.1	added
35	DASHA	4.1	
36	dataChord Spectrum Analyst	9.2.0-b17	updated
37	dataChord Spectrum Miner	9.2.0-b17	updated
38	DATAWARRIOR	4.7.2	added
39	DOSY Toolbox	2.7	

40	drawnmr	0.24	added
41	DYNAMO	7.2 rev 2013.047.09.17	
42	EISD	0.2	
43	ENSEMBLE	2.1	
44	FastModelFree	1.3	updated
45	FuDA	1.0	added
46	Gctf	1.18	added
47	Geometric-Approximation	Downloaded 12/08/2017	added
48	GISSMO	1.2	added
49	GLOVE	Downloaded 10/3/2016	
50	GNAT	1.1.1	added
51	GOAP	Downloaded 11/13/2015	
52	GREMLIN	2.01	added
53	GROMACS	2018.2	added
54	GUARDD	2012-04-21	
55	hmsIST	2.11	
56	HullRad	3	added
57	IMP	2.9.0	updated
58	INCHI	1.05	
59	Jellyfish	2018-08-29	added
60	Jupyter	1.0.0	added
61	Kd-calc		added
62	LARMORCA	1.00	
63	LARMORD	2.00	
64	localCIDER	0.1.14	
65	MATLAB-MCR	R2016b	
66	MestraNova	12.0.2-20910	updated
67	Metscape	3.1.3	added
68	MDAnalysis	0.18.0	updated
69	MddNMR	2.6	updated
70	MESMER	1.0.0a	updated
71	MetaboAnalystR	1.0.1	added
72	MMTSB	2018-08-01	added
73	Modelfree	4.20	
74	Modeller	9.20	updated
75	mol2sphere	1.0	added
76	Molib	1.0.9	updated
77	MOLMOL	2.1-2.6	
78	MolProbity	4.4	added
79	MoSART	1.0	
80	MotionCor2	1.1.0	added
81	MVAPACK	0.4.1	
82	NAMD	2.12	updated
83	NESSY	12.3.1	
84	NESTA-NMR	1.5	
85	NMRDraw	9.6 rev 2018.184.13.26	updated
86	NMRFAM-Sparky	Build 08-17-2018	updated
87	NMRfx Analyst	10.2.15	added
88	NMRfx Processor	10.2.15	updated

89	NMRfX Structure	10.2.15	added
90	nmrplug	0.7	
91	NMRmix	Build 11/31/2015	
92	NMRPipe	9.6 rev 2018.184.13.26	updated
93	nmrstarlib	2.1.1	updated
94	NMRViewJ	9.2.0-b20	updated
95	nmr_wash	1.0.0	
96	nus-tool	1-2	
97	Open Babel	2.4.1	
98	OpenMM	7.2.2	added
99	OpenVnmrJ	1.1_RevA_06-18-18	added
100	OSPNEY	3.0b1	added
101	PALES	2.1	
102	PANAV	2.1	
103	ParmEd	3.0.3	updated
104	PINT	2.1.0	added
105	PLUQ	0.2.1	updated
106	PONDEROSA	Build 04/26/2018	updated
107	PPM/PPM_One	2015-07-09	
108	PROMEGA	1.40F1 rev 2012.029.12.03	
109	PyMOL	2.1.0	updated
110	pynmrstar	2.5.1	updated
111	Pyshifts	Downloaded_2016-05-31	
112	Qhull	7.2.0	added
113	RasMol	2.7.5.2	
114	RAW	1.1.0	
115	RCI	1n_10_6_12-A	
116	RDC Panda / RDC Analytic	1.0	
117	REDCAT	3	
118	REDCRAFT	Build 3/16/2015	
119	relax	4.0.3	
120	Relion	2.1.0	added
121	ResMap	1.1.4	added
122	RNAstructure	6.0.1	updated
123	rNMR	1.1.9	
124	RNMRTK	3.2.2 Build_4983	updated
125	ROSETTA	2016.15.58628	
126	RUNER	1.03	added
127	SEER	2018-08-01	added
128	SHIFTS	5.5	updated
129	SHIFTX	1.0	
130	SHIFTX2	1.10	
131	SHIMpanzee	2018-08-29	added
132	SIMPSON	4.2.1	added
133	SpinDrops	2.0.4	added
134	SMILE	2.0 beta Rev 2018.094.15.20	updated
135	SPARTA+	2.70F1 rev 2012.029.12.03	
136	Spectrum-Translator	2.4	updated
137	SQLite	3.14.2	

138	ssNake	0.6	added
139	SSP	Downloaded 5/15/2016	
140	tameNMR	2018-01-24	added
141	tiger	2018-08-29	added
142	TALOS+	3.80F1 rev 20132.080.14.41	
143	TALOSN	4.12 rev 2015.147.15.40	
144	TITAN	1.4-1-g97af	updated
145	TREND	1.1.0	
146	Unblur	1.0.2	added
147	VMD	1.9.3	updated
148	VMD-Xplor	1.9.1	
149	XDrawChem	1.10.2	added
150	XEASY	1.3.11	added
151	XPLOR-NIH	2.48	updated
152	xyza2pipe	1.0.3	added
153	YESWORKFLOW	Build 248	