MetumpX - A Metabolomics Support Package for Untargeted Mass Spectrometery

Supplementary Tables

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version v2.1

A specific criteria is used for enclosure of tools in MetumpX. Softwares which are included are due to these specific reasons:

- Publication Date (later then 2010)
- Freeware License
- Linux based
- Offline

Table I shows the selection criterion.

TABLE I: MetumpX Selection Criteria

Sr. no	Software Tool Name	Pub. Date (2010-)	Offline	Linux based	Free	Installed
1	ProbMetab[1]	✓	✓	✓	✓	✓
2	intCor[2]	✓	✓	✓	✓	✓
3	CorrectOverloadedPeaks[3]	✓	✓	✓	✓	✓
4	iMet-Q[4]	✓	✓		✓	
5	AnalyzerPro[5]	✓	✓	✓		
6	ADAP-GC[6]	✓	✓	✓	✓	✓
7	ChromGenius[7]	✓	✓	✓		
8	ChromA[8]	✓		✓	✓	
9	X13CMS[9]	✓	✓	✓	✓	✓
10	MET-COFEA[10]	✓	✓		✓	
11	MET-XAlign[11]	✓	✓		✓	
12	batchCorr[12]	✓	✓	✓	✓	✓
13	MZMine[13]	✓	✓	✓	✓	✓
14	MET-IDEA[14]	✓	✓		✓	
15	PyMS[15]	✓	✓	✓	✓	✓
16	MassCascade[16]		✓	✓	✓	
17	Mnova-MS[17]	✓	✓	✓		
18	XCMS[18]	✓	✓	✓	✓	✓
19	flagme[19]	✓	✓	✓	✓	✓
20	Elm. Metabolomics[20]	✓	✓		✓	
21	MetCirc[21]	✓	✓	✓	✓	✓
22	mzAccess[22]	✓	✓	✓		
23	SpeckTackle[23]		✓	✓	✓	
24	COMSPARI[24]		✓	✓	✓	
25	DAVE[25]	✓		✓	✓	
26	TargetSearch[26]	✓	✓	✓	✓	✓
27	HCor[27]	✓	✓	✓	✓	✓
28	MS-DIAL[28]	✓	✓		✓	
29	MaxEnt[29]	✓	✓	✓	✓	✓
30	RANSY/RAMSY[30]	✓		✓	✓	
31	UniDec[31]	✓	✓		✓	
32	Metab[32]	✓	✓	✓	✓	✓
33	decoMS2[33]	✓	✓	✓	✓	✓
34	GAGdecon[34]	✓	✓	✓	✓	✓
35	TMTc+[35]	✓	✓	✓		
36	BernetAl2018[36]		✓	✓	✓	
37	BUPID-Top-Down[37]	✓		✓	✓	
38	PicaudEtAl2018[38]	✓		✓	✓	
39	msXpertSuite[39]	✓	✓	✓	✓	✓
40	proFIA[40]	✓	✓	✓	✓	✓
41	apLCMS[41]	✓	✓	✓	✓	✓
42	yamss[42]	✓	✓	✓	✓	✓
43	cosmiq[43]	✓	✓	✓	✓	✓
44	AMDIS[44]	✓	✓		✓	
45	mzMatch-ISO[45]	✓	✓	✓	✓	✓
46	Elgen-MS[46]		✓	✓	✓	
47	MetaQuant[47]		✓	✓	✓	
48	CAMERA[48]	✓	✓	✓	✓	✓
49	MS-FLO[49]	✓		✓	✓	
50	JumPm[50]	✓	✓	✓		
51	FastChrom[51]	✓	✓		✓	
52	GridMass[52]		✓	✓	✓	
53	KMMDA[53]	✓	✓	✓	✓	✓
54	HayStack[54]	✓		✓	✓	
55	msPeak[55]	✓	✓	✓	✓	✓
56	GC-Aanlyzer[56]	✓	✓	✓		
57	MsXelerator[57]	✓	✓	✓		
58	MarkerLynx[58]	✓	✓	✓		
59	GCxGCAnalyzer[59]	✓	✓	✓		
60	MetNorm[60]	✓	✓	✓	✓	✓
61	MetTailor[61]	✓	✓	✓	✓	✓
62	MetaPre[62]	✓		✓	✓	
63	NOREVA[63]	✓		✓	✓	
64	crmn[64]	✓	✓	✓	✓	✓
65	Normalizer[65]	✓		✓	✓	
66	metaX[66]	✓		✓	✓	
67	MetabR[67]		✓	✓	✓	
68	LowessNormalization[68]	✓	✓		✓	
69	MSPrep[69]	✓	✓	✓	✓	✓
70	AIoutput [70]	✓	✓		✓	
71	Ionwinze[71]	✓	✓		✓	
72	MPP [72]	✓	✓	✓		
73	R2DGC[73]	✓	✓	✓	✓	✓
74	mSPA[74]	✓	✓	✓	✓	✓
75	Maui-VIA[75]	✓	✓		✓	
76	SECIMTools[76]	✓	✓	✓	✓	✓
77	BatMass[77]	✓	✓	✓	✓	✓
78	MetaboQC[78]	✓	✓	✓		
79	QCScreen[79]	✓	✓	✓	✓	✓
80	QC-RFSC[80]		✓	✓	✓	
81	mscompare[81]		✓	✓	✓	
82	PYQUAN[82]	✓	✓		✓	
83	MINMA[83]	✓	✓	✓	✓	✓
84	MetaboloDerivatizer[84]	✓	✓		✓	
85	SIRIUS[85]	✓	✓	✓	✓	✓
86	HAMMER[86]	✓	✓		✓	
87	ISDB-MN[87]		✓	✓	✓	
88	SweetSubstitute [88]	✓	✓		✓	
89	MetFrag[89]	✓		✓	✓	
90	MetFusion[90]	✓		✓	✓	
91	iontree[91]	✓	✓	✓	✓	✓
92	ACD/MS Fragmenter[92]		✓	✓	✓	
93	MassFrontier[93]	✓	✓	✓		
94	MWASTools[94]	✓	✓	✓	✓	✓
95	RegScan[95]		✓	✓	✓	
96	InCroMAP[96]	✓	✓	✓	✓	✓
97	PathVisio[97]	✓	✓	✓	✓	✓
98	CHem-SMP[98]	✓	✓	✓		
99	cPath[99]	✓	✓	✓	✓	✓
100	MetaMapp[100]		✓	✓	✓	
101	Mapping Tool[101]	✓	✓	✓	✓	✓
102	BLASTX [102]	✓		✓	✓	
103	PSSAlib [103]	✓	✓	✓		
104	iPath [104]	✓		✓	✓	
105	MetExplore [105]	✓		✓	✓	
106	CATABOL[106]		✓	✓	✓	
107	Paintomics[107]	✓		✓	✓	
108	ProtienLounge[108]	✓		✓	✓	
109	CellMLTools[109]		✓	✓	✓	
110	FCF[110]		✓	✓	✓	
111	PathPred[111]	✓		✓	✓	
112	SABIO-RK[112]	✓		✓	✓	
113	OptCom[113]		✓	✓	✓	
114	Subpathway-GM[114]	✓		✓	✓	
115	IPAVS[115]	✓		✓	✓	
116	GAM[116]	✓		✓	✓	
117	GLAMM[117]	✓		✓	✓	
118	PASMet[118]	✓		✓	✓	
119	NICElips[119]		✓	✓	✓	
120	MetaMapR[120]	✓		✓	✓	
121	PAPi[121]	✓	✓	✓	✓	✓
122	ReactPRED[122]	✓	✓	✓	✓	✓
123	JigCell[123]		✓	✓	✓	
124	Cell++[124]		✓	✓	✓	
125	MetNetter[125]		✓	✓	✓	
126	MEMOSys[126]	✓		✓	✓	
127	MonaLisa[127]	✓	✓	✓	✓	✓
128	QSSPN[128]	✓	✓	✓	✓	✓
129	NetSeed[129]	✓		✓	✓	
130	tEFMA[130]	✓	✓	✓		
131	NetCmpt[131]	✓		✓	✓	
132	SED-ED [132]	✓	✓	✓	✓	✓
133	MetNetMaker [133]	✓	✓		✓	
134	RxnSim [134]	✓	✓	✓	✓	✓
135	MetExploreViz[135]	✓		✓	✓	
136	CorrelationCalculator[136]		✓	✓	✓	
137	WebMetabase [137]	✓		✓	✓	
138	MoDitify[138]	✓	✓	✓	✓	✓
139	MetaboSignal[139]	✓	✓	✓	✓	✓
140	JMassBalance[140]	✓	✓	✓	✓	✓
141	MetaDiff[141]	✓	✓	✓	✓	✓
142	FTA [142]		✓	✓	✓	
143	PySCeSToolbox[143]	✓	✓	✓	✓	✓
144	MEBS[144]	✓	✓	✓	✓	✓
145	Subpathway-GMir[145]	✓	✓	✓	✓	✓
146	ProI[146]	✓		✓	✓	
147	MetaNetSam[147]	✓	✓	✓	✓	✓
148	lumpGEM [148]		✓	✓	✓	
149	redGEM[149]		✓	✓	✓	
150	CCC[150]	✓	✓	✓		
151	HuEtAl2018[151]	✓	✓	✓		
152	Kamneva[152]	✓	✓	✓	✓	✓
153	XeDetect[153]		✓	✓	✓	
154	ReactomePA[154]	✓	✓	✓	✓	✓
155	IPPAD[155]	✓		✓	✓	
156	MMinte[156]	✓	✓	✓	✓	✓
157	SED-ML[157]		✓	✓	✓	
158	NetCooperate[158]	✓		✓	✓	
159	PathRings[159]	✓		✓	✓	
160	IntPath [160]	✓		✓	✓	
161	EvoMS[161]	✓		✓	✓	
162	phraSED-ML[162]	✓	✓	✓	✓	✓
163	CARMEN[163]	✓		✓	✓	
164	ScrumPy[164]	✓	✓	✓	✓	✓
165	Pybrn[165]	✓	✓	✓	✓	✓
166	Pyabolism[166]	✓	✓	✓	✓	✓
167	KEGGREST[167]	✓	✓	✓	✓	✓
168	VIENNA-RNL[168]		✓	✓	✓	
169	Fbar[169]	✓	✓	✓	✓	✓
170	MetaCore[170]	✓		✓	✓	
171	PathwayLab[171]	✓	✓	✓		

172	MetScape[172]	✓	✓	✓	✓	✓
173	MPEA[173]	✓		✓	✓	
174	IMPaLA[174]	✓		✓	✓	
175	MBRole[175]	✓		✓	✓	
176	zeroSum[176]	✓	✓	✓	✓	✓
177	ChemRICH[177]	✓		✓	✓	
178	FELLA[178]	✓	✓	✓	✓	✓
179	BinChE[179]	✓		✓	✓	
180	MetaboliteIDConv.[180]	✓	✓	✓	✓	✓
181	MetaboAnalyst[181]	✓	✓	✓	✓	✓
182	MapMan[182]		✓	✓	✓	
183	3Omics[183]	✓		✓	✓	
184	integrOmics[184]	✓	✓	✓	✓	✓
185	MetDisease[185]	✓	✓	✓	✓	✓
186	MetaBridge[186]	✓		✓	✓	
187	MetMask[187]	✓	✓	✓	✓	✓
188	ProMeTra [188]		✓	✓	✓	
189	MAGI[189]	✓		✓	✓	
190	KPIC2[190]	✓	✓	✓	✓	✓
191	MarVis-Suite[191]	✓	✓		✓	
192	MSClust[192]		✓	✓	✓	
193	MetMSLine[193]	✓	✓	✓	✓	✓
194	SimExTargid [194]	✓	✓	✓	✓	✓
195	MetaboliteDetector [195]		✓	✓	✓	
196	specmine[196]	✓	✓	✓	✓	✓
197	W4M [197]	✓		✓	✓	
198	MeltDB [198]	✓	✓		✓	
199	xMSAnalyzer [199]	✓	✓	✓	✓	✓
200	ChromaTOF[200]	✓	✓	✓		
201	MetabolmeExpress[201]	✓		✓	✓	
202	Metabox [202]	✓	✓	✓	✓	✓
203	PiMP[203]	✓		✓	✓	
204	MET-COFEI[204]	✓	✓		✓	
205	MAIT [205]	✓	✓	✓	✓	✓
206	BinVestigate[206]	✓		✓	✓	
207	CEU Mass Mediator [207]	✓		✓	✓	
208	MAGMa[208]	✓		✓	✓	
209	CSI:FingerID [209]	✓		✓	✓	
210	MS2LDA_SUPPORT [210]	✓		✓	✓	
211	MetExtract [211]	✓	✓		✓	
212	T-BioInfo [212]	✓		✓	✓	
213	MetAlign[213]	✓	✓		✓	
214	CFM-ID [214]	✓		✓	✓	
215	Ideom [215]		✓	✓	✓	
216	AStream [216]		✓	✓	✓	
217	PUTMEDID-LCMS[217]	✓	✓	✓	✓	✓
218	DECOMP [218]		✓	✓	✓	
219	MetiTree[219]	✓		✓	✓	
220	MIA [220]	✓	✓	✓	✓	✓
221	MFSearcher[221]	✓	✓		✓	
222	ChemDistiller[222]		✓	✓	✓	
223	MSeasy[223]	✓	✓	✓	✓	✓
224	SIMPLE[224]		✓	✓	✓	
225	MAVEN[225]		✓	✓	✓	
226	SpectConnect [226]	✓		✓	✓	
227	RAMClustR[227]	✓	✓	✓	✓	✓
228	Molfind[228]	✓	✓	✓	✓	✓
229	MS2Analyzer [229]	✓	✓	✓	✓	✓
230	MS-FINDER [230]	✓	✓		✓	
231	geoRge[231]	✓	✓	✓	✓	✓
232	MetFamily[232]	✓		✓	✓	
233	eRAH[233]	✓	✓	✓	✓	✓
234	IsoMS [234]	✓	✓		✓	
235	MetDIA [235]		✓	✓	✓	
236	iMET[236]	✓		✓	✓	
237	MIDAS[237]		✓	✓	✓	
238	InterpretMSSpectrum [238]	✓	✓	✓	✓	✓
239	AssayR[239]	✓	✓	✓	✓	✓
240	MCID[240]	✓		✓	✓	
241	compMS2Miner[241]	✓		✓	✓	
242	MetShot [242]	✓	✓	✓	✓	✓
243	MINE[243]	✓		✓	✓	
244	NP-StructurePred. [244]	✓	✓	✓		
245	MetaboSearch[245]	✓	✓	✓	✓	✓
246	ALLocator[246]	✓		✓	✓	
247	PROFANCY[247]	✓	✓		✓	
248	SpiderMass[248]	✓	✓		✓	
249	MZedDB[249]	✓		✓	✓	
250	BinBase [250]		✓	✓	✓	
251	PowerGet[251]	✓	✓		✓	
252	AMDORAP [252]	✓	✓	✓	✓	✓
253	MBIdent [253]	✓	✓	✓	✓	✓
254	peakANOVA[254]	✓	✓	✓	✓	✓
255	MI-Pack[255]	✓	✓	✓	✓	✓
256	SetupX [256]		✓	✓	✓	
257	FeatureFinderMetabo [257]		✓	✓	✓	
258	MassMetaSite[258]		✓	✓	✓	
259	MetDNA[259]	✓		✓	✓	
260	DASI[260]	✓	✓	✓		
261	MetaboList[261]	✓	✓	✓	✓	✓
262	MetaMS[262]	✓	✓	✓	✓	✓
263	SIEVE[263]	✓	✓	✓		
264	SimMet[264]	✓		✓	✓	
265	Apex[265]	✓	✓	✓		
266	Nontarget[266]	✓	✓	✓	✓	✓
267	NIST MS Search[267]	✓	✓		✓	
268	El-Maven [268]	✓	✓	✓	✓	✓

Metabolomics Softwares are mainly workflows and one software can lie in more then one metabolomic pipeline category. Table II shows a software categorization scheme. The software is placed in the lowest category it is present.

TABLE II: MetumpX Software Categorization Scheme

Sr. No.	Software	Noise Filtering	Chromatogram Alignment	Peak Alignment	Retention Time Correction	Spectral Deconvolution	Peak Detection	Data Normalization	Statistical Analysis	Quality Control	Metabolite Quantification	Data Imputation	In-silico Fragmentation	Metabolite Identification	Spectral Visualization	Clustering Analysis	mGWAS	Mapping	Network Analysis	Enrichment Analysis	Integrative Analysis
1	**CorrectOverloadedPeaks**[3]	✓																			
2	specmine[196]	✓					✓	✓	✓			✓		✓							
3	intCor[2]	✓	✓	✓																	
4	**batchCorr**[12]		✓																		
5	**mSPA**[74]			✓																	
6	AMDORAP[252]	✓	✓	✓			✓														
7	MI-Pack[255]			✓																	
8	**Metab**[32]					✓															
9	decoMS2[28]					✓								✓							
10	GAGdecon[34]					✓															
11	msXpertSuite[39]					✓															
12	ADAP-GC[6]					✓	✓														
13	MaxEnt[29]					✓															
14	**HCor**[27]				✓																
15	MetMSLine[193]	✓	✓				✓								✓						
16	**X13CMS**[9]		✓				✓														
17	proFIA[40]	✓					✓								✓						
18	cosmiq[43]		✓				✓				✓										
19	mzMatch-ISO[45]						✓							✓							
20	PyMS[15]						✓							✓							
21	TargetSearch[26]						✓							✓							
22	msPeak[55]						✓							✓							
23	Metabox[202]							✓	✓										✓	✓	✓
24	**MetNorm**[60]	✓						✓													
25	crmn[64]	✓						✓													
26	**KMMDA**[53]						✓		✓												
27	MSPrep[69]							✓	✓			✓									
28	flagme[19]		✓				✓		✓		✓				✓						
29	SECIMTools[76]							✓	✓	✓											
30	**QCScreen**[79]									✓											
31	**MetTailor**[61]		✓								✓										
32	MetaQuant[47]						✓	✓			✓			✓							
33	apLCMS[41]		✓				✓				✓			✓							
34	**MINMA**[83]											✓									
35	**SIRIUS**[85]												✓								
36	iontree[91]												✓								
37	MetShot[242]													✓							
38	Molfind[228]													✓							
39	MIA[220]													✓							
40	MetaMS[262]													✓							
41	MSeasy[223]													✓							
42	RAMClustR[227]													✓							
43	MetaboSearch[245]													✓							
44	El-Maven[268]													✓							
45	**geoRge**[231]													✓							
46	eRAH[233]													✓							
47	MetaboList[261]t													✓							
48	InterpretMSSpectrum[238]													✓							
49	AssayR[239]													✓							
50	MS2Analyzer[229]													✓							
51	Nontarget[266]													✓							
52	MetMask[187]													✓							
53	peakANOVA[254]													✓							
54	PUTMEDID-LCMS[217]													✓							
55	SimExTargid[194]	✓	✓	✓			✓	✓			✓			✓	✓	✓					
56	MetaboAnalyst[181]							✓	✓					✓		✓			✓		✓
57	CAMERA[48]						✓							✓		✓					
58	**KPIC2**[190]		✓				✓				✓					✓					
59	**MWASTools**[94]																✓				
60	**InCroMAP**[96]																	✓			
61	PathVisio[97]																	✓			
62	Mapping Tool[101]																	✓			
63	ChemDistiller[222]																	✓			
64	PycesToolbox[143]																		✓		
65	MetaDiff[141]																		✓		
66	ReactomePA[154]																		✓		
67	MEBS[144]																		✓		
68	RxnSim[134]																		✓		
69	phraSED-ML[162]																		✓		
70	ScrumPy[164]																		✓		
71	Subpathway-GMir[145]																		✓		
72	Kamneva[152]																		✓		
73	MetaboSignal[139]																		✓		
74	ReactPRED[122]																		✓		
75	Mminte[156]																		✓		
76	**PAPi**[121]																		✓		
77	MetaNetSam[147]																		✓		
78	Fbar[169]																		✓		
79	SED-ED[132]																		✓		
80	QSSPN[128]																		✓		

81	JMassBalance[140]																	✓		
82	Pyabolism[166]																	✓		
83	Pybrn[165]																	✓		
84	MonaLisa[127]																	✓		
85	MoDitify[138]																	✓		
86	CorrelationCalculator[136]																	✓		
87	KEGGREST[167]																	✓		
88	**integrOmics**[184]																			✓
89	MetScape[172]																	✓	✓	✓
90	cPath[99]																	✓	✓	✓
91	MetDisease[185]																	✓		✓
92	**zeroSum**[176]																		✓	
93	FELLA[178]																		✓	
94	MetaboliteIDConvertor[180]																		✓	
95	MZMine[13]	✓	✓			✓	✓	✓			✓			✓	✓					
96	XCMS[18]		✓	✓			✓	✓			✓			✓	✓					
97	yamss[42]		✓				✓													
98	R2DGC[73]		✓	✓			✓							✓	✓					
99	**BatMass**[77]									✓					✓					
100	MAIT[205]		✓				✓		✓			✓		✓	✓			✓		
101	ProbMetab[1]	✓	✓				✓		✓					✓	✓					
102	MetCirc[21]			✓										✓	✓					
103	xMSAnalyzer[199]		✓			✓	✓			✓				✓	✓					

List of software tools and plugins included in MetumpX package are shown in the following table. Software which are recommended are also mentioned in the table by using a bold text. Download size, version and Latest update of each software is mentioned for user convenience.

TABLE III: The table enumerates software packaged in MetumpX in accordance with their categories.

Sr. No.	Software Name	Size (MB)	Version	Latest Update
Data Pre-processing				
Noise Filtering				
1	**C.O.Peaks**[3]	4.8	1.2.17	2019
2	specmine[196]	15.2	2.0.3	2018
3	intCor[2]	3.0	1.03.0	2014
Chromatogram Alignment				
4	**batchCorr**[12]	17.2	0.2.1	2018
Peak Alignment				
5	**mSPA**[74]	0.1	1.0.0	2011
6	AMDORAP[252]	40.9	1.0.6	2012
7	MI-Pack[255]	28.9	1.0.0	2015
Spectral Deconvolution				
8	**Metab**[32]	3.2	1.18.0	2019
9	decoMS2[28]	5.2	0.1.0	2013
10	GAGdecon[34]	0.1	1.0.0	2018
11	msXpertSuite[39]	0.7	4.1.0	2019
12	ADAP-GC[6]	3.2	3.0.0	2017
13	MaxEnt[29]	12.4	3.4.1	2017
Retention Time Correction				
14	**HCor**[27]	0.1	1.01.0	2014
Data Processing				
Peak Detection				
15	MetMSLine[193]	1.6	1.2.1	2017
16	**X13CMS**[9]	0.1	1.4.0	2014
17	proFIA[40]	2.0	1.10.0	2019
18	cosmiq[43]	17.5	1.18.0	2019
19	mzMatch-ISO[45]	0.1	1.0.0	2019
20	PyMS[15]	0.45	1.0.0	2012
21	TargetSearch[26]	0.69	1.40.3	2019
22	msPeak[55]	32.3	1.0.0	2013
Data Normalization				
23	Metabox[202]	53.0	1.2.0	2016
24	**MetNorm**[60]	0.5	0.1.0	2015
25	crmn[64]	2.4	0.0.20	2014
Statistical Analysis				
26	**KMMDA**[53]	0.5	1.0.0	2018
27	MSPrep[69]	1.0	0.0.2	2018
28	flagme[19]	22.0	1.40.0	2019
Quality Control				
29	SECIMTools[76]	0.6	1.0.0	2018
30	**QCScreen**[79]	12.1	1.0.0	2018
Metabolite Quantification				
31	**MetTailor**[61]	0.9	2.0.0	2015
32	MetaQuant[47]	12.0	1.0.0	2010

33	apLCMS[41]	14.1	6.6.3	2019
Data Imputation				
34	**MINMA**[83]	2.6	0.1.0	2017
In-silico Fragmentation				
35	**SIRIUS**[85]	37.0	4.0.1	2019
36	iontree[91]	0.9	1.23.1	2018
Metabolite Identification				
sr	MetShot[242]	0.9	0.3.2	2018
37	Molfind[228]	36.2	1.9.0	2013
38	MIA[220]	2.7	1.0.0	2017
39	MetaMS[262]	3.7	1.20.0	2019
40	MSeasy[223]	5.8	5.3.3	2013
41	RAMClustR[227]	51.6	0.4.1	2019
42	MetaboSearch[245]	45.7	1.0.0	2012
43	El-Maven[268]	91.4	9.0.0	2019
44	**geoRge**[231]	13.7	1.0.0	2017
45	eRAH[233]	3.7	1.1.0	2018
46	MetaboList[261]	0.3	1.4.0	2019
47	I.MSSpect.[238]	0.2	1.2.0	2018
48	AssayR[239]	71.6	0.0.9	2017
49	MS2Analyzer[229]	3.0	2.1.0	2016
50	Nontarget[266]	3.5	1.9.0	2019
51	MetMask[187]	4.43	0.5.3	2017
52	peakANOVA[254]	0.5	1.0.0	2015
53	PUTMEDID[217]	191.2	1.0.0	2011
Data Clustering Analysis				
54	SimExTargid[194]	49.8	0.2.1	2017
55	MetaboAnalyst[181]	49.3	4.0.0	2019
56	CAMERA[48]	2.1	1.40.0	2019
57	**KPIC2**[190]	15.7	2.4.0	2019
Data Network Analysis				
mGWAS				
58	**MWASTools**[94]	56.3	1.8.0	2019
Metabolite Mapping				
59	**InCroMAP**[96]	54.6	1.5.0	2012
60	PathVisio[97]	17.6	3.3.0	2019
61	Mapping Tool[101]	15.0	1.3.0	2013
62	ChemDistiller[222]	133.2	0.1.0	2018
Metabolic Network Analysis				
63	PySCeSToolbox [143]	5.1	0.9.6	2018
64	MetaDiff[141]	6.0	1.0.0	2016
65	ReactomePA[154]	11.6	1.28.0	2019
66	MEBS[144]	73.2	1.0.0	2017
67	RxnSim[134]	21.6	1.0.3	2013
68	phraSED-ML[162]	1.8	1.0.3	2018
69	ScrumPy[164]	1093.9	1.0.0	2018
70	Subpathway[145]	1.7	3.0.0	2013
71	Kamneva 2016[152]	101.8	1.0.0	2016
72	MetaboSignal[139]	169.1	1.14.0	2019
73	ReactPRED[122]	52.4	1.0.0	2016
74	Mminte[156]	52.2	1.0.0	2017
75	**PAPi**[121]	0.6	1.24.0	2019
76	MetaNetSam[147]	3.8	1.1.0	2015
77	Fbar[169]	2.1	0.5.2	2018
78	SED-ED[132]	6.4	2.2.3	2016
79	QSSPN[128]	2.1	1.0.0	2015
80	JMassBalance[140]	3.7	1.0.0	2013
81	Pyabolism[166]	0.4	1.0.0	2017
82	Pybrn[165]	0.6	0.4.3	2016
83	MonaLisa[127]	17.8	5.1.0	2016
84	MoDentify[138]	0.6	0.99.0	2019
85	C.Calculator[136]	16.4	1.0.0	2010
86	KEGGREST[167]	13.67	1.24.0	2019
Data Integration Analysis				
87	**integrOmics**[184]	0.1	2.55.0	2012
88	MetScape[172]	17.2	3.1.3	2017
89	cPath[99]	1.32	2.0.0	2019
90	MetDisease[185]	15.2	1.1.0	2014
Data Enrichment Analysis				
91	**zeroSum**[176]	1.0	2.0.0	2019
92	FELLA[178]	3.1	1.4.1	2019
93	M.IDConvertor[180]	0.2	1.0.0	2010
Data Visualization				
94	MZMine[13]	148.7	2.0.0	2019
95	XCMS[18]	3.5	3.7.1	2018
96	yamss[42]	15.5	1.9.1	2018
97	R2DGC[73]	0.6	1.0.3	2017
98	**BatMass**[77]	0.1	0.3.0	2018
99	MAIT[205]	36.2	1.18.0	2019
100	ProbMetab[1]	0.2	1.0.0	2013
101	MetCirc[21]	5.0	1.14.0	2017
102	xMSAnalyzer[199]	38.9	2.0.6	2019

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