

最初にお読みください

Mascot Server version 3.0 for Linux Release Notes

新規インストール

インストールを行う前に、2頁の「最新の追加情報」及び3頁の「動作環境に対する注意点」をご覧ください。新規インストール手順はインストールDVDにある「Mascot_Server_v3.0_Lin_新規インストール手順.pdf」書類と、参照として「Mascot Server Installation and Setup」(インストールDVDの中の「manual.pdf」)の「2. Installation:Linux」をご覧ください。

アップグレード

バージョン2.8からversion 3.0にアップグレードする手順は、インストールDVDにある「Mascot_Server_v3.0_Lin_アップグレード手順.pdf」書類と、参照として「Mascot Server Installation and Setup」(インストールDVDの中の「manual.pdf」)の「2. Installation:Linux」をご覧ください。なお、旧バージョンで使用していたライセンスファイルはversion 3.0では使えなくなります。弊社が新たに提供するプロダクトキーを使ってversion 3.0用のライセンスファイルを取得してください。

新規サポート機能

インストールDVDにある別紙資料「ver. 3.0新機能紹介.pdf」をご覧ください。

バージョン 2.8 からの変更点

4頁以降にバージョン2.8.3からの変更点をまとめました。なお、この書類作成以降に追加された内容を含む最新の変更点に関しては、2頁の「最新の追加情報」並びに

「https://www.matrixscience.com/mascot_support_v3_0.html」をご覧ください。

最新の追加情報

データベースの圧縮

Mascot Server 3.0 に更新すると、すべての配列データベースが自動的にファイルの再圧縮を開始します。バージョン3.0では圧縮ファイル形式が変更されたためです。データベースの数が多い場合、完了まで非常に時間がかかる事があります。Database Status 画面における各データベースの” Status” 項目の情報から構築状況をご確認ください。

動作環境に対する注意点

サポートしている Linux カーネル/ディストリビューション

glibc 2.17 以降を含むディストリビューションで動作します。一般的なディストリビューションと最小バージョンの一覧は、弊社ウェブサイトに掲載されています。

https://www.matrixscience.com/help/pc_specs.html#LINUX

ソフトウェア RAID

ソフトウェア RAID (Lustre など) はサポートしていません。

ネットワークファイルシステム

GlusterFS はサポートしていません。

バージョン 2.8.3 からの変更点

以下の表並びに https://www.matrixscience.com/mascot_support_v3_0.html をご覧ください。
また、下記項目の詳細については弊社までお問い合わせください。

ID	Component	Description
6442	Daemon	Daemon assumes all new MDRO providers are files not folders
6486	nph-mascot.exe	Takes a long time to create the Fxxxxxx.dat.que.y files (Windows disk bottleneck in "Query prep time")
6847	master_results_2.pl	Browser performance improvements in Protein Family Summary
10876	master_results_2.pl	master_results_2.pl doesn't cope with missing mascot.dat
11568	Security	Remove references to Integra and Insight in Mascot Security
11865	nph-mascot.exe	Scaling with number of threads in SMP mode on yabby very disappointing (Windows disk bottleneck in "Searching... time")
12535	System	Slash the amount of time spent in preprocessing peak lists and postprocessing search results (soup to nuts)
12701	master_results_2.pl	Protein Family Summary should support tag searches
12743	Not determined	Searching for a sequence in a result file with a lot of identical sequences takes 30 minutes
12801	ms-status.exe	Link to error log produces a CGI error if ms-monitor.exe isn't running
12825	master_results_2.pl	Inconsistent treatment of DECOY=ON and DECOY=OFF
12892	Search results	Zero value for Observed in unassigned list for query whose only match is a chimeric duplicate
13106	Not determined	Add new method ms_inputquery::getQueryNumber()
13130	dbman_scan_for_library.pl	Failed to run dbman_msp_from_results_file.pl and crawl results on some Linux systems
13201	Documentation	ms-service.exe documentation is incorrect
13267	nph-mascot.exe	Allow user to select application-specific sub-set of mods for second pass of error tolerant search
13303	System	M00135 message is out of date
13345	Documentation	Search parameter help for instrument uses different row labels than Configuration Editor
13422	Import filters	MGF peak lists saved from Distiller Data import filter have peak picking parameters commented out.
13447	Search results	Add getPeakCharge method
13480	Search results	get_ms_mascotresults() defaults to old protein grouping for sequence tag searches
13483	nph-mascot.exe	Negative protein mass in MS/MS search
13486	master_results_2.pl	Repeat search of sequence tag from Protein Family Summary fails to pass through fixed and variable modifications
13516	master_results.pl	Show Mascot errors on the Wot no results page
13531	Performance	Reduce the time spent in caching search results
13632	nph-mascot.exe	Remove obsolete pip code from nph-mascot.exe
13678	Performance	Support new .msr file format
13765	Import filters	Output ion mobility values from MDRO if associated Mascot Server is 2.7 or later
13797	System	Update Boost to 1.79.0
13799	Percolator	Replace Percolator RT feature with MS2RescoreAdapter (DeepLC, MS2PIP)
13856	Perl interpreter	Update Perl on Windows to 5.38 and update prerequisites and modules
13858	Documentation	Roll-up of changes to Manual, release notes, and HTML pages for 3.0
13870	Percolator	Make sure Percolator is built with 64-bit, not 32-bit boost_regex
13872	Daemon	Review the need for 32-bit Parser
13976	Results display	Show more detailed information about search stage in addition to percentage
13988	ms-status.exe	Click on "view error log" when Mascot isn't running and get HTTP Error 502.2 - Bad Gateway

14017	export_dat_2.pl	New cache files are created when exporting a decoy search and a target FDR is set.
14033	System	Change from four-component to three-component versioning
14034	Installer	Migrate from WiX 3.7 to WiX 3.11 for Windows installer
14053	Documentation	Add documentation for setting up SSL
14058	ms-gettaxonomy.exe	ms-gettaxonomy.exe works correctly even when taxonomy block is disabled (Enabled=0)
14068	Installation	Remove directory gnu/7.2.0 from Linux shipper image
14109	Configuration files	MascotFileProcessingThreads set to -1 should automatically use all possible threads
14111	Search results	Rename ms_mascotresfile to ms_mascotresfile_dat
14117	nph-mascot.exe	nph-mascot.exe, write search results in MSR v0.9 format
14118	client.pl	Download .msr file using client.pl, and reconstruct full .dat from slim .dat and MSR
14119	export_dat_2.pl	Export MSR file in dat28 format (export_format=MascotDAT) and MSR format (export_format=MascotMSR)
14120	ms-createpip.exe	Create pip file from .dat or .msr results file
14121	Search results	New API for .msr results files, and implement parsing and interpretation of MSR v0.9 files
14125	Perl interpreter	Update Perl on Linux to 5.38 and update prerequisites and modules
14127	Building	Drop VS2012 and VS2013 shippers
14129	System	Compile Mascot with GCC11 and VS2019
14131	nph-mascot.exe	Uncaught exceptions are reported as meaningless exit code '-1073740791'
14133	Sample code	Update Parser examples for MSR files
14138	nph-mascot.exe	Crash in library search in cluster mode with fewer queries than SplitNumberOfQueries
14139	nph-mascot.exe	A search against a Spectral Library should always split by queries
14146	master_results_2.pl	Change the title of Percolator progress bar to "Refining with machine learning"
14147	master_results_2.pl	Display a warning in Protein Family Summary if Percolator is on and did not improve sensitivity
14152	nph-mascot.exe	The mass of the crosslinker is always unsigned in nph-mascot
14156	Installer	Ship Mascot with the latest VS2015-VS2022 redistributable
14157	Search results	Undefined behaviour in ms_fdr_query_processor::getThresholdForFDR()
14172	Database Manager	URL for PRIDE spectral libraries has changed
14173	Database Manager	UniProt REST URLs have changed
14179	Documentation	MinGW instructions
14181	MS1 Quantitation	Support target FDR in ms_distiller_data_search
14186	search_form.pl	Disallow TargetFDR and ET+Decoy on FORMVER=3 (Distiller 2.8)
14192	Installation	Upgrade Linux shippers to GCC 5.5.0 and MinGW to GCC 7.1.0
14208	Search results	ms_searchparams::getVarModsNeutralLosses() doesn't return satellite NLS
14211	nph-mascot.exe	Unexpected difference in query sort order in cluster mode
14217	Search results	Failing to read local mods NL string, fault introduced in Parser 2.7.0
14238	nph-mascot.exe	New command-line argument to nph-mascot.exe to specify output format
14239	search_form.pl	Specify output format as MSR when submitting a search
14240	Configuration files	New mascot.dat option SearchSubmitOutputFormat
14241	System	Script and help text for processing TMTpro complementary ions
14244	Documentation	Apache example config supplied with Mascot should include LimitRequestBody
14247	Configuration files	New mascot.dat option to diagnose MSR generation
14257	MS1 Quantitation	Move Quantlib/Distiller time alignment code to Parser and save/load in cdb/xml
14262	MS2 Quantitation	TMTpro 16-plex and 18-plex mod groups should be required=false
14265	nph-mascot.exe	Allow embedded config files in MIME format input
14274	Errors & warnings	Methods and classes not wrapped properly by SWIG for Perl, Python, Java and C#
14276	nph-mascot.exe	Memory leaks in nph-mascot searches
14280	System	View/process MSR format search results in Perl scripts
14282	Documentation	Add distiller_time_align_1.xsd to the website
14285	MS1 Quantitation	Implement New Imputation Methods in Parser
14287	nph-mascot.exe	Count all the accessions when creating the index files of a sequence database
14293	Threading	Further thread safety issues : getPeptideThreshold()
14300	peptide_view.pl	Peptide View, ET match, Use of uninitialized value in subroutine entry

14302	nph-mascot.exe	mzML file with a very large peak list segfaults nph-mascot.exe
14315	HTTP	Add getStage method to ms_http_client_search
14320	Documentation	Update Doxygen to version 1.9.6
14323	MS1 Quantitation	ms_ms1quantitation should allow a search without a quantitation method to load replicate or average results
14326	ms-config.exe	View modifications, linkers, quant method, crosslinking method from MSR file (ms-config.exe)
14331	System	Adapter interface for ML predictors, which inserts custom columns to pip file
14337	Documentation	Roll-up of changes to API doc and release notes for 2.9
14344	Installer	Unable to install on Windows 10 21H2 due to "QueryIISConfig: Failed to wait for child process (0x80070006)"
14357	External Processes	Ship Mascot Daemon Export Extender with Daemon
14361	Search results	ms_inputquery::getPeakMass(): Ions2 and Ions3 lines are missing the first peak
14362	export_dat_2.pl	pep_isbold field is confusing
14371	nph-mascot.exe	Heap Buffer Overflow when copying data from the nodes
14377	Search results	getQmatch() returns INT_MAX if called with non-existent query number, should return 0
14389	Search results	Implement schema changes for MSR v0.99; implement MSR parsing/processing for v0.99; fix bugs in MSR parsing/processing; implement schema changes for SDB v0.99; implement SDB writing/processing for v0.99; fix bugs in SDB parsing/processing; rename headers
14390	nph-mascot.exe	nph-mascot.exe, write search results in MSR v0.99 format
14392	Test harness	Add MSR files to the Parser test harness
14396	Parameters	When selecting data file format for Distiller, set processing option file to the default for that instrument
14415	client.pl	Add an interface to client.pl to remotely initiate percolator, and then track progress
14422	HTTP	Support MSR file download in ms_http_client_search::downloadResultsFile()
14423	search_form.pl	Add Percolator controls to the search form
14429	nph-mascot.exe	Embed a 'slim' .dat file in the Mascot Search Results (MSR) file
14432	Utilities	Add streaming decompression to ms_zip
14433	Errors & warnings	Parser should give a warning if reading a file from future version of Mascot
14441	Search results	New Parser class for retrieving MSR file in .dat format
14445	Configuration files	New option AlwaysCreateDat28ResultsFile
14446	Installer	Update SwissProt, PRIDE_contaminants and taxonomy files in shipper package for 3.0
14447	search_form.pl	Add clarification to "Peptide charge" search parameter that it's a fallback default
14457	ms-status.exe	ms-status.exe Show=RESULTFILE needs to print MSR in binary format
14462	System	Drop Windows Vista, 7, 8, Server 2008, Server 2008 R2 and Server 2012
14466	Installer	Ownership in shipper tar package on Linux should be root:root
14469	export_dat_2.pl	mzIdentML export specifies UseUnigeneClustering=1 and IncludeErrorTolerantMatches=1 when it shouldn't
14481	Search results	All methods of ms_inputquery should be const
14483	Search results	ms_inputquery::getNumUsed() always returns 0 despite docs say it always returns -1
14497	ms-searchcontrol.exe	Move results_file_mime2 implementation from client.pl to ms-searchcontrol.exe
14498	ms-searchcontrol.exe	New command ms-searchcontrol.exe --result_file_sql
14499	ms-searchcontrol.exe	ms-searchcontrol.exe --result_file_mime should return dat28 format stream if input is MSR
14501	ms-monitor.exe	Stop creating obsolete config files (mod_file, masses, substitutions) if CreateLegacyModAndSubstitutionFiles is false
14515	Results display	Hide the quantitation summary context menu if you don't have the "Task Database" node selected or allow the summary to be run by selecting specific searches
14516	Results display	Quantitation summary disabled for reporter datasets if you don't have the Daemon toolbox
14530	ms-makesearchlog.exe	Support MSR files in ms-makesearchlog.exe
14531	ms-searchcontrol.exe	Add MSR support for ms-searchcontrol.exe commands --create_results_cache, --results_cache_status, --results and --results_header
14532	client.pl	When using client.pl commands kill_job and nice_job from the command line, and if sessionID argument gives an invalid session, the script mistakenly defaults to the command line session
14533	client.pl	Switch from task-based to results-based permission check for client.pl commands result_file_mime, result_file_ini, results, xmlresults and results_header (only user spoofing)

		is affected)
14537	ms-searchcontrol.exe	Disallow downloading MSR file using client.pl?result_file_ini
14544	Masses	Change ms_modfile private member std::auto_ptr<ms_masses> to std::unique_ptr
14546	master_results_2.pl	Inadequate browser caching in Protein Family Summary when Mascot Security is enabled and using guest session or web authentication or IP/hostname/agent string authentication
14548	Search results	Clarify protein inference rules for multi-SL searches with same or different reference databases
14549	Search results	Display emPAI in integrated error tolerant searches
14551	Search results	ms_searchparams::getLIBRARY_SEARCH() returns -1 when LIBRARY_SEARCH=1 in search params
14552	System	Remove ms-lockmem.exe
14553	Configuration files	Remove ms_mascotoptions::getSeparateLockMem()
14554	Building	Compile SWIG modules with GCC11 and VS2019 (Perl, Python, C#, Java)
14558	Building	Update SWIG to 4.2.1
14560	System	Use the VS2019 and GCC 11 Perl modules with Mascot
14571	Search results	Unstable order of sameset accessions in integrated SL searches
14575	nph-mascot.exe	Incorrect fragment charge (Ions1_charge) when using Bruker XML input
14576	nph-mascot.exe	Automatic target-decoy by default
14577	Installation	Add wrapper for Perl 5.36 on Linux
14578	Search results	Add new method ms_mascotresfilebase::getSLExecCommand()
14584	Database Manager	Environmental_EST parse rule has changed; remove obsolete IPI databases; and SARS-CoV-2 is moved from pre-release to official Uniprot database
14588	MS2 Quantitation	Add accessor method ms_ms2quantitation::getPeptideSummary()
14590	MS1 Quantitation	Update mergeCdbFiles and mergeXmlFiles to support msr
14591	Daemon	Display and write a warning to the event log when the installation drive is low on space
14593	ms-searchcontrol.exe	Failing to fetch protein description for top hit in integrated spectral library search if top hit is not from SL
14596	export_dat_2.pl	If export_dat_2.pl ends with an error, the error message is duplicated in HTML output
14598	ms-status.exe	Remove BrowserSafe parameter from ms-status.exe; always use text/plain with Show=RESULTFILE when results file is dat28 format
14600	Daemon	Capture and check standard error if about to report MDS1129 with no error message
14604	nph-mascot.exe	Set SQLite application_id for MSR files
14605	nph-mascot.exe	Update Mascot Server version and schema version to final ones for beta release
14614	search_form.pl	Search form controls for Unimod classifications with error tolerant search
14615	Parameters	Search params for Unimod classifications with error tolerant search
14628	nph-mascot.exe	Support repeat searching from MSR file
14629	TaskDB	Allow user to delete multiple tasks from Daemon
14636	Utilities	ms_fileutilities::getLastModificationTime() fails on Windows if the file has been opened without shared read access
14637	Installation	Drop version-specific Python libraries and ship a single 'universal' library
14645	ms-createpip.exe	Median precursor error is missing the match to the last query
14647	Search results	New argument to ms_mascotresfilebase::setPercolatorFeatures(): a vector of ML adapter parameters
14649	Search results	ms_mascotresfilebase constructor, if XMLschemaDirectory is empty string, treat it the same as null pointer
14665	Configuration files	Add a ms_modification::getClassification() method
14667	master_results_2.pl	New format controls for activating MS2Rescore and selecting MS2PIP and DeepLC models
14673	Search results	ms_linker_site_vector fails to initialise alpha and beta peptide lengths to zero
14674	Configuration files	Add quantitation option to choose type of time alignment
14682	master_results.pl	Add a deprecation warning at the top of master_results.pl
14686	master_results_2.pl	Display machine learning quality report in Protein Family Summary
14691	System	Include new third-party Perl modules: TOML::XS, Devel::NYTprof, MIME::Lite, DBD::SQLite
14692	Installation	Internal shipper for Perl 5.38 built with VS2019 and GCC 11
14696	search_form.pl	Remove obsolete support for Isf.dat in the search form
14702	nph-mascot.exe	NA translation looks wrong in error tolerant decoy search against an NA database
14703	ms-createpip.exe	ms-createpip.exe should not write match data for chimeric duplicates

14704	ms-creatempip.exe	ms-creatempip.exe calculates -nan(ind) for RMS, RMSppm, meanAbsFragDa, meanAbsFragPPM
14707	Configuration files	ms_datfile::updateForInstaller(), Replace ResultsCache with a default
14714	Quantitation Summary	Support replicate quantitation via the quantitation summary
14716	peptide_view.pl	Default Peptide View to annotating all fragments, not just matched fragments
14718	System	Default to sequence FDR in Mascot Server
14721	System	Increase SplitNumberOfQueries to 2000
14732	get_params.pl	New CGI script get_ml_adapter_params.pl to list the available ML adapter parameters
14743	refine_results_with_ml.pl	New executable refine_results_with_ml.pl for backend use
14744	client.pl	client.pl?create_results_cache and client.pl?results should default to Percolator and ML adapter params specified as search parameters
14745	System	Default report scripts to Percolator and ML adapter parameters defined in the search form
14746	nph-mascot.exe	Pass through PERCOLATE and ML_ADAPTER_PARAM search parameters
14748	Search results	New methods ms_searchparams::getPERCOLATE() and ms_searchparams::getML_ADAPTER_PARAM()
14749	Search results	When setting Percolator flag in ms_mascotresfilebase::get_ms_mascotresults_params(), check the new search param PERCOLATE, then mascot.dat options
14750	Search results	ms_mascotresfile::get_ms_mascotresults_params() treats DECOY=-1 as DECOY=1 when deciding whether to set MSPEPSUM_PERCOLATOR
14752	Search results	ms_mascotresfilebase::get_ms_mascotresults_params() should not set MSPEPSUM_PERCOLATOR for error tolerant search
14754	MS2RescoreReport.py	Change machine learning quality report template so it has Matrix Science branding
14755	tidy_data.pl	tidy_data.pl needs to delete old pip and pop files
14759	nph-daemon_helper.pl	Remove nph-daemon_helper.pl (legacy script for ABI GPS Explorer)
14766	Installation	Update unimod.xml and unimod_xl.xml to the latest versions for 3.0
14775	Building	Python msparser library cannot be used with xgboost or tensorflow libraries
14776	Configuration files	ms_datfile::updateForInstaller(), change SplitNumberOfQueries from 1000 to 2000
14777	Configuration files	New option CreateLegacyModAndSubstitutionFiles
14778	Configuration files	New option AlwaysEnableAutoDecoySearch
14782	System	Ship unimod_tables.xml with Mascot
14783	master_results_2.pl	Always expand Sensitivity and FDR section in Protein Family Summary
14784	master_results_2.pl	Remove "Not what you expected" link
14785	Configuration files	ms_datfile::updateForInstaller(), set PercolatorUseRT to 0
14786	master_results_2.pl	Display a warning if percolate_rt=1 or PercolatorUseRT is enabled
14788	search_form.pl	Hide Monoisotopic/Average choice in search form
14789	Configuration files	New mascot.dat option SearchSubmitAcceptedFileTypes
14790	search_form.pl	Hide obsolete file formats from search form
14791	export_dat_2.pl	Remove DTASelect and pepXML as export format choices
14795	MS1 Quantitation	ms_ms1quant_time_align::getRToffset() looks in wrong part of array in some cases
14797	Configuration files	LabelAll option is obsolete
14798	ms-config.exe	ms-config.exe needs to download unimod_tables.xml when user clicks Check Unimod
14811	Configuration files	Quantitation method for TMT 32/35-plex
14812	ms-creatempip.exe	Percolator features based on matched fragments are incorrectly calculated.
14814	search_form.pl	Default target FDR to 1% in the search form
14818	search_form.pl	Javascript error in SQ search form
14820	Search results	Default to sequence FDR in get_ms_mascotresults_params()
14821	MS1 Quantitation	getRToffset() code is not treating the "to" consensus and "from" consensus properly
14825	Import filters	Make peak picking with the Distiller Daemon Toolbox Processor group aware on Windows 11 based systems
14829	Parameters	Daemon should take the list of peaklist formats from the SearchSubmitAcceptedFileTypes Mascot.dat option
14833	Search results	Change behavior of ms_mascotresfilebase::get_ms_mascotresults_params() to set the target FDR
14834	dbman_scan_for_library.pl	Set target FDR to zero when creating MSP file so that homology threshold (reported as hs=metadata field) is consistent
14837	master_results_2.pl	Prevent refining results if the search is sequence query with no MS/MS data
14842	ms-status.exe	ms-status.exe Show=MS_MODFILE should return mod_file contents from unimod.xml

14844	Configuration files	Add new method ms_masses::saveToString()
14848	ms-createpip.exe	The isoSysDMz feature is set to Inf when the query charge is unknown
14849	client.pl	Implicitly create pop files (refine results) when calling client.pl?result_file_pop
14850	ms-createpip.exe	ms-createpip.exe sometimes crashes when calculating the median precursor error
14858	System	Supply ms-win8-perl538.exe with Mascot on Windows to work around Perl 5.38 locale bug on Windows 8.1/Server 2012 R2 when active code page is not Latin1 or Unicode

何かお困りのことがありましたら support-jp@matrixscience.com (技術サポート)にご連絡ください。



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