

Error message:

```
xyz@mhcquantfinal-vm:~/mhcquant_run$ nextflow run ~/mhcquant/main.nf -profile singularity
-c ~/mhcquant_run/conf/xyz.config --input sample_sheet.tsv --fasta
HUMAN_2014_concat.fasta --skip_decoy_generation true --ms2pip_model timsTOF
--ms2pip_model_dir /home/xyz/ms2pip_models --outdir results_main -resume
```

N E X T F L O W ~ version 25.10.0

Launching `~/home/xyz/mhcquant/main.nf` [angry_lichterman] DSL2 - revision: e53fee5aa1



nf-core/mhcquant 3.1.0

Input/output options

```
input          : sample_sheet.tsv
outdir         : results_main
```

Database Options

```
fasta          : HUMAN_2014_concat.fasta
skip_decoy_generation : true
```

Database Search Settings

```
default_params_file_comet: /home/xyz/mhcquant_run/conf/comet_lowmem.txt
```

Rescoring settings

```
ms2pip_model   : timsTOF
ms2pip_model_dir : /home/xyz/ms2pip_models
```

Generic options

```
trace_report_suffix : 2025-11-26_19-42-58
```

Core Nextflow options

```
runName        : angry_lichterman
containerEngine : singularity
launchDir       : /home/xyz/mhcquant_run
workDir         : /home/xyz/mhcquant_run/work
```

```
projectDir      : /home/xyz/mhcquant
userName       : xyz
profile        : singularity
configFiles    : /home/xyz/mhcquant/nextflow.config,
/home/xyz/mhcquant_run/conf/xyz.config
```

!! Only displaying parameters that differ from the pipeline defaults !!

* The pipeline

<https://doi.org/10.1186/s13059-025-03763-8>

* The nf-core framework

<https://doi.org/10.1038/s41587-020-0439-x>

* Software dependencies

<https://github.com/nf-core/mhcquant/blob/master/CITATIONS.md>

WARN: The following invalid input values have been detected:

* --ms2pip_batch_size: 200

* --comet.spectrum_batch_size: 200

* --comet.extra_parameters: /home/xyz/mhcquant_run/conf/comet_lowmem.txt

executor > local (8)

```
[ -      ] NFCORE_MHCQUANT:MHCQUANT:PREPARE_SPECTRA:THERMORAWFILEPARSER -
[ -      ] NFCORE_MHCQUANT:MHCQUANT:PREPARE_SPECTRA:UNTAR             -
[ -      ] NFCORE_MHCQUANT:MHCQUANT:PREPARE_SPECTRA:UNZIP            -
[51/2661fd] NFCORE_MHCQUANT:MHCQUANT:PREPARE_SPECTRA:TDF2MZML (1)    | 1 of 1 ✓
[ -      ] NFCORE_MHCQUANT:MHCQUANT:PREPARE_SPECTRA:GUNZIP           -
[b5/d1a6b4] NFCORE_MHCQUANT:MHCQUANT:PYOPENMS_CHROMATOGRAMEXTRACTOR (1) | 1 of 1 ✓
[c2/1bcd1] NFCORE_MHCQUANT:MHCQUANT:OPENMSTHIRDPARTY_COMETADAPTER (1) | 1 of 1 ✓
[37/631aa3] NFCORE_MHCQUANT:MHCQUANT:OPENMS_PEPTIDEINDEXER (1)       | 1 of 1 ✓
[fd/bbc8f1] NFCORE_MHCQUANT:MHCQUANT:OPENMS_IDMASSACCURACY (1)       | 1 of 1 ✓
[bd/8088a6] NFCORE_MHCQUANT:MHCQUANT:OPENMS_IDMERGER (TTS1_10e6_test) | 1 of 1 ✓
[fb/b3ce83] NFCORE_MHCQUANT:MHCQUANT:RESCORE:MS2RESCORE (TTS1_10e6_test) | 0 of 1, retries:
1 ✘
[ -      ] NFCORE_MHCQUANT:MHCQUANT:RESCORE:OPENMS_PSMFEATUREEXTRACTOR -
[ -      ] NFCORE_MHCQUANT:MHCQUANT:RESCORE:OPENMS_PERCOLATORADAPTER -
[ -      ] NFCORE_MHCQUANT:MHCQUANT:RESCORE:OPENMS_IDFILTER_Q_VALUE  -
[ -      ] NFCORE_MHCQUANT:MHCQUANT:OPENMS_TEXTEXPORTER             -
[ -      ] NFCORE_MHCQUANT:MHCQUANT:SUMMARIZE_RESULTS                -
[ -      ] NFCORE_MHCQUANT:MHCQUANT:MULTIQC                          | 0 of 1
```

-[nf-core/mhcquant] Pipeline completed with errors-

ERROR ~ Error executing process > 'NFCORE_MHCQUANT:MHCQUANT:RESCORE:MS2RESCORE (TTS1_test)'

Caused by:

Process `NFCORE_MHCQUANT:MHCQUANT:RESCORE:MS2RESCORE (TTS1_test)` terminated **with** an error exit status (137)

Command executed:

```
ms2rescore_cli.py \  
  --psm_file TTS1_test.idXML \  
  --spectrum_path . \  
  --output_path TTS1_test_ms2rescore.idXML \  
  --processes 2 \  
  --ms2_tolerance 0.02 --ms2pip_model timsTOF --ms2pip_model_dir null  
--rescoring_engine percolator --feature_generators deeplc,ms2pip  
  
cat <<-END_VERSIONS > versions.yml  
"NFCORE_MHCQUANT:MHCQUANT:RESCORE:MS2RESCORE":  
  MS2Rescore: $(echo $(ms2rescore --version 2>&1) | grep -oP 'MS2Rescore \(\v\K[^\)]+')  
)  
END_VERSIONS
```

Command exit status:

137

Command output:

(empty)

Command error:

```
INFO: Environment variable SINGULARITYENV_NXF_TASK_WORKDIR is set, but  
APPTAINERENV_NXF_TASK_WORKDIR is preferred  
INFO: Environment variable SINGULARITYENV_NXF_DEBUG is set, but APPTAINERENV_NXF_DEBUG  
is preferred  
/usr/local/lib/python3.12/site-packages/pyopenms/__init__.py:49: UserWarning: Warning:  
OPENMS_DATA_PATH environment variable not found and no share directory was installed. Some  
functionality might not work as expected.  
warnings.warn(  
2025-11-17 12:00:02,921 INFO Percolator rescoring engine has been specified. Use the  
idXML containing rescoring features and run Percolator in a separate step.  
2025-11-17 12:00:02,921 INFO MS2Rescore config:  
2025-11-17 12:00:02,921 INFO {'$schema': './config_schema.json', 'ms2rescore':  
{'feature_generators': {'ms2pip': {'model': 'timsTOF', 'ms2_tolerance': 0.02, 'model_dir':  
'null'}, 'deeplc': {'deeplc_retrain': False, 'calibration_set_size': 0.15}},  
'rescoring_engine': {}}, 'config_file': None, 'psm_file': 'TTS1_10e6_test.idXML',  
'psm_file_type': 'infer', 'psm_reader_kwargs': {}, 'spectrum_path': '.', 'output_path':
```

```
'TTS1_10e6_test_ms2rescore.idXML', 'log_level': 'info', 'id_decoy_pattern': '^DECOY_',
'psm_id_pattern': None, 'spectrum_id_pattern': None, 'psm_id_rt_pattern': None,
'psm_id_im_pattern': None, 'lower_score_is_better': True, 'max_psm_rank_input': 10,
'max_psm_rank_output': 1, 'modification_mapping': {}, 'fixed_modifications': {},
'processes': 2, 'rename_to_usi': False, 'fasta_file': None, 'write_report': False,
'ms2pip_model_dir': 'null'}}
2025-11-17 12:02:18,988 INFO Removed 0 PSMs with rank >= 10.
2025-11-17 12:02:20,421 WARNING Removed 62 PSMs with invalid amino acids.
2025-11-17 12:02:22,524 INFO Found 502126 PSMs, of which 46.70% are decoys.
2025-11-17 12:02:26,838 WARNING Non-mapped modifications found: {'Oxidation',
'Carbamidomethyl'}
This can be ignored if they are Unimod modification labels.
2025-11-17 12:02:29,534 INFO Found 0 identified PSMs with rank <= 1 at 0.01 FDR before
rescoring.
2025-11-17 12:02:31,081 INFO Adding MS2PIP-derived features to PSMs.
2025-11-17 12:02:38,722 INFO Running MS2PIP for PSMs from run (1/1)
`20231208_TTS1_Neo_25cmIO_OBJ42567_C1R_A1101_YesLinker_10e6_iRT_thunderDDA_FX1_01_1_1_4847`
...
2025-11-17 12:02:41,571 INFO Downloading model_20240105_timsTOF_B.xgboost to
null/model_20240105_timsTOF_B.xgboost...
2025-11-17 12:03:57,245 INFO Downloading model_20240105_timsTOF_Y.xgboost to
null/model_20240105_timsTOF_Y.xgboost...
2025-11-17 12:05:04,254 INFO Processing spectra and peptides...
/usr/local/lib/python3.12/site-packages/pyopenms/__init__.py:49: UserWarning: Warning:
OPENMS_DATA_PATH environment variable not found and no share directory was installed. Some
functionality might not work as expected.
  warnings.warn(
/usr/local/lib/python3.12/site-packages/pyopenms/__init__.py:49: UserWarning: Warning:
OPENMS_DATA_PATH environment variable not found and no share directory was installed. Some
functionality might not work as expected.
  warnings.warn(
.command.sh: line 7: 41 Killed ms2rescore_cli.py --psm_file
TTS1_10e6_test.idXML --spectrum_path . --output_path TTS1_10e6_test_ms2rescore.idXML
--processes 2 --ms2_tolerance 0.02 --ms2pip_model timsTOF --ms2pip_model_dir null
--rescoring_engine percolator --feature_generators deepplc,ms2pip
INFO: Cleanup error: while stopping driver for /var/lib/apptainer/mnt/session/final:
fuse-overlayfs exited: fuse: reading device: Software caused connection abort

Work dir:
/home/xyz/mhcquant/work/fb/b3ce831d73ee9d700f01a25eca029f

Container:
/home/xyz/apptainer_cache/depot.galaxyproject.org-singularity-ms2rescore-3.1.5--pyhdfd78af_
1.img
```

Tip: you can replicate the issue by changing to the process work dir **and** entering the command ``bash .command.run``

-- Check `'.nextflow.log'` file **for** details

ERROR ~ Pipeline failed. Please refer to troubleshooting docs:

<https://nf-co.re/docs/usage/troubleshooting>

-- Check `'.nextflow.log'` file **for** details

WARN: Failed to render execution report -- see the log file **for** details

WARN: Failed to render execution timeline -- see the log file **for** details