··FragPipe·····

··FragPipe·····manifest·····DDA·····

FragPipe ····· workflow ·····DIA-NN/Python ·····
····· workflow ····· DDA ····· manifest ····· headless
·· dry-run ····· workflow ···

···· manifest ·····

FragPipe ·· headless manifest ·····experiment·bioreplicate · data type·····
·····experiment ·····DDA/DIA ··· workflow ·····
····· experiment·

```
from pathlib import Path

rows = []
seen = set()
for number, line in enumerate(Path('pilot.fp-manifest').read_text().splitlines(), 1):
    fields = line.split('\t')
    if len(fields) != 4:
        raise ValueError(f'·{number}···4·')
    raw, experiment, replicate, data_type = fields
    if not Path(raw).is_file():
        raise FileNotFoundError(f'·····{raw}')
    if not experiment or not replicate.isdigit() or int(replicate) < 1 or not data_type:
        raise ValueError(f'·{number}·····')
    if raw in seen:
        raise ValueError(f'·····{raw}')
    seen.add(raw)
    rows.append(fields)
if not rows:
    raise ValueError('manifest····')
print(f'manifest·····{len(rows)}····data type···workflow····')
```

·· workflow ··· headless ··

· GUI ····· workflow·····/····· headless ···
·····DIA-NN ····· Python ····· fragpipe --help ····· threads · ram ·
·····

```
set -euo pipefail
: "${FRAGPIPE:?FragPipe Linux·····}"
: "${WORKFLOW:?·····.workflow··}"
: "${MANIFEST:?·····.fp-manifest··}"
: "${TOOLS:?FragPipe····}"
: "${DIANN:?DIA-NN·····}"
: "${PYTHON_DIR:?FragPipe···Python··}"
test -s "$WORKFLOW" && test -s "$MANIFEST"
mkdir fragpipe-pilot-001
root="$PWD/fragpipe-pilot-001"
sha256sum "$WORKFLOW" "$MANIFEST" > "$root/input-config.sha256"
args=(--headless --workflow "$WORKFLOW" --manifest "$MANIFEST"
      --workdir "$root/results" --threads 4 --ram 16
      --config-tools-folder "$TOOLS" --config-diann "$DIANN"
      --config-python "$PYTHON_DIR")
"$FRAGPIPE" "${args[@]}" --dry-run > "$root/dry-run.log" 2>&1
"$FRAGPIPE" "${args[@]}" > "$root/run.log" 2>&1
```

Dry-run ····· headless ·····
workflow ·····FragPipe ·· workflow ·····
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·····FASTA·workflow ·····PSM/p
eptide/protein ·····FDR·····
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·····manifest | ····· | ·····

workflow···· | ·····FASTA····· | ···workflow·····

···· | FragPipe·Java·MSFragger··· | ·····

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·· workflow·manifest·FASTA/·····FragPipe ·····FragPipe headless ···
· threads/ram ·····
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FragPipe··headless····manifest·· https://fragpipe.nesvilab.org/docs/tutorial_headless.html

FragPipe····· https://fragpipe.nesvilab.org/docs/tutorial_fragpipe.html

FragPipe····· https://fragpipe.nesvilab.org/docs/tutorial_batch.html