·····AlphaPept·····

·····GUI····AlphaPept settings·····FASTA·····DDA·····HDF····

AlphaPept ····· settings YAML ·····FASTA·····
····· GUI ····· CLI ···· workflow····
····· DDA ····· workflow ·····

····· settings

· AlphaPept GUI ·····DDA ···FASTA···· FDR ····· YAML·····
····· AlphaPept·Python ····· FAST
A ·····

··· | ···· | ····

file_paths | ····· | ·····

shortnames / groups | ····· | ·····

fasta_paths | ····· | ·····

results/database·· | ····· | ·····

····· workflow

··· YAML·····
····· HDF·····AlphaPept ·· CLI ···· workflow ····
YAML····· alphapept --help ·····

```
set -euo pipefail
: "${SETTINGS:?····GUI·····settings YAML}"
test -s "$SETTINGS"
mkdir alphapept-projectA-pilot-001
root="$PWD/alphapept-projectA-pilot-001"
cp "$SETTINGS" "$root/settings.yaml"
sha256sum "$root/settings.yaml" > "$root/settings.sha256"
alphapept --help > "$root/cli-help.txt" 2>&1
alphapept workflow "$root/settings.yaml"   > "$root/run.log" 2>&1
```

····· CLI ····· r
aw ····· HDF··· YAML ·····
·····

·····

AlphaPept ····· raw ····· *.ms_data.hdf····· results.hdf ····· YAML··· F
ASTA ····· HDF···· workflow ····· HDF ·· protei
n table····· peptide ····· FDR ·····

·····FASTA····· PSM/·····FDR·····
····· HDF···· YAML·····
·····

·····
·····

····

AlphaPept·····workflow·· https://github.com/MannLabs/alphapept/blob/master/README.md

AlphaPept··settings····· https://mannlabs.github.io/alphapept/settings.html

AlphaPept·····HDF·· https://mannlabs.github.io/alphapept/file_formats.html