Package: selexprepR (via r-universe)

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Title Preprocessing Public HT-SELEX Sequencing Data

Version 1.0.0

Description Provides reproducible preprocessing for high-throughput SELEX sequencing data. Supports primer inference, extraction of random regions, sparse sequence counting across rounds, quality control, and provenance manifests. Public-study discovery and checksum-aware ENA FASTQ download planning are included for reproducible data acquisition.

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`selexprepR-package` *Reproducible preprocessing of public HT-SELEX data*

Description

selexprepR connects raw sequencing reads to a sparse `SummarizedExperiment`, with explicit primer inference, extraction, quality-control and provenance records.

Workflows

Use `run_selexprep_files()` for local FASTQ files, or `run_selexprep()` for named lists of sequence pools. `selexprep_demultiplex()` assigns inline-barcoded reads when a reviewed barcode map is supplied. Inspect `S4Vectors::metadata(result)` for the library report, extraction yields, QC and manifest. Plot the QC report with `plot.selexprep_qc()`.

Individual stages

`selexprep_detect()` infers constant regions. `selexprep_extract()` removes them, and `selexprep_count()` counts recovered sequences. `selexprep_qc()` summarizes depth, diversity, composition and flags. Reviewed primer overrides are available when inference is unsafe.

Public data

`selexprep_catalog()` searches a frozen discovery catalog. `inspect_selexprep_accession()` queries current ENA metadata, and `fetch_selexprep_reads()` creates a download plan before transferring reads. Network availability and a public accession are required for live ENA inspection; bundled examples also work offline.

Further information

The vignette, `vignette("selexprep", package = "selexprepR")`, walks through a complete FASTQ workflow with small real data and a QC plot. Data sources and redistribution terms are recorded in the installed `DATA_LICENSES.md` and the corresponding provenance files.

Examples

```
selexprep_catalog("FGF-9")
selexprep_count(c("ACGT", "ACGT", "GGGG"))
```

`build_selexprep_manifest` *Build an R-native reproducibility manifest*

Description

Builds a versioned `selexprep_manifest_v2` object. The reader also accepts the historical Python `selexprep_manifest_v1` schema, so existing analysis records remain inspectable. Hashes are computed for every supplied existing path and are keyed relative to `input_root` or `output_root` when supplied.

Usage

```
build_selexprep_manifest(
  library_report,
  input_paths = character(),
  output_paths = character(),
  accession = NULL,
  bioproject_id = NULL,
  runs = character(),
  parameters = character(),
  runtime_seconds_per_stage = numeric(),
  flags = character(),
  input_root = NULL,
  output_root = NULL
)
```

Arguments

library_report	A selexprep_library_report.
input_paths	Existing input file paths to hash.
output_paths	Existing output file paths to hash.
accession	Optional public accession.
bioproject_id	Optional BioProject accession.
runs	Run accessions.
parameters	Named character parameters used for the run.
runtime_seconds_per_stage	Named numeric stage durations.
flags	Character QC flag names.
input_root	Optional root used to make input hash keys relative.
output_root	Optional root used to make output hash keys relative.

Value

A validated selexprep_manifest.

Examples

```
p5 <- 'GGTAATACGACTCACTATAGGG'
p3 <- 'CCATGCATGCATGCATGCAT'
inserts <- c('ACGTACGTACGTACGT', 'TGCATGCATGCATGCA')
reads <- rep(paste0(p5, inserts, p3), each = 250)
report <- selexprep_detect(list(round_00 = reads))
build_selexprep_manifest(report)
```

---

fetch_selexprep_reads *Fetch FASTQ files from an ENA inspection*

Description

Creates a deterministic, checksum-aware download plan from an existing inspection or an accession. By default no bytes are transferred; set dry_run = FALSE to download to outdir. Each completed file is checked against ENA's MD5 value when one is supplied. Assigned rounds spanning distinct BioSamples emit a warning: counting merges their runs into one round pool, so review replicates or parallel selections before proceeding. The assignments are retained.

Usage

```
fetch_selexprep_reads(
  accession_or_inspection,
  outdir,
  dry_run = TRUE,
  overwrite = FALSE,
  timeout_seconds = 30,
  require_assigned_rounds = TRUE,
  overrides = numeric()
)
```

Arguments

accession_or_inspection	A character accession or a selexprep_inspection returned by inspect_selexprep_accession().
outdir	Destination directory for downloaded FASTQ files.
dry_run	Whether to return the plan without downloading.
overwrite	Whether an existing destination file may be replaced.
timeout_seconds	Positive timeout for metadata and FASTQ requests.
require_assigned_rounds	Whether to refuse ambiguous or missing round assignments before creating a download plan.
overrides	Optional named integer mapping of run accessions to manually curated round numbers.

Value

A selexprep_fetch_result list containing the run-level $plan, $downloaded_files, $dry_run, and $rounds_with_several_samples, a mapping of assigned rounds to runs from distinct BioSamples. The mapping is also stored in S4Vectors::metadata(result$plan).

Examples

```
# Plan from a bundled ENA metadata snapshot; no network or files written.
path <- system.file("extdata", "ena-inspection.rds", package = "selexprepR")
inspection <- readRDS(path)
result <- fetch_selexprep_reads(inspection, tempfile("selexprep-reads-"))
result$plan[, c("run_accession", "round_number", "file_name")]
result$dry_run
```

`infer_selexprep_rounds` *Infer SELEX round assignments from public metadata*

Description

Applies a conservative, ordered metadata cascade: structured sample attributes, sample title, library name, experiment title, and design description. A run remains unsafe when no round is found or when one field contains conflicting candidates. The function records evidence rather than using enrichment signals to repair metadata.

Usage

```
infer_selexprep_rounds(runs, overrides = numeric())
```

Arguments

`runs`	A data frame or `S4Vectors::DataFrame` containing `run_accession` and optional metadata columns `sample_title`, `library_name`, `experiment_title`, `design_description`, and `sample_attributes`.
`overrides`	Optional named integer vector mapping run accessions to manually curated round numbers.

Details

Strong round attributes (including `Characteristics[selex cycle]`) take precedence over text. Conflicting strong attributes remain ambiguous; weak `pcr cycle` evidence never overrides an explicit text round. ArrayExpress `RVxx` labels are sample numbers rather than round numbers. Repeated conflicting indicators are all retained, including adjacent `Round 1` `Round 2` labels.

Value

A `S4Vectors::DataFrame` with one conservative round assignment per run. `round_candidates` is a list-column and preserves ambiguity.

Examples

```
runs <- data.frame(
    run_accession = c('SRR1', 'SRR2'),
    sample_title = c('Thrombin Round 1', 'Thrombin Round 2')
)
infer_selexprep_rounds(runs)
```

inspect_selexprep_accession *Inspect public sequencing metadata at ENA*

Description

Queries ENA's read-run filereport endpoint without downloading sequence data. The returned `selexprep_inspection` retains verbatim library strategy/source metadata and one row per run with its FASTQ URLs, sizes, and MD5 checksums. Custom BioSample attributes are fetched from ENA sample XML and retained in a `sample_attributes` list-column; each run keeps its `library_strategy`. If sample XML is unavailable, a warning accompanies fallback to text-field round inference. Filereport service-error bodies are retried before parsing.

Usage

```
inspect_selexprep_accession(accession, timeout_seconds = 30)
```

Arguments

`accession`	Study- or run-level ENA/INSDC accession.
`timeout_seconds`	Positive network timeout in seconds.

Value

A `selexprep_inspection` list with a run-level `S4Vectors::DataFrame` in `$runs`.

Examples

```
# Inspect the bundled snapshot without a network connection.
path <- system.file("extdata", "ena-inspection.rds", package = "selexprepR")
inspection <- readRDS(path)
inspection$runs[, c("run_accession", "library_strategy")]
# A fresh inspection contacts ENA and requires network access.

inspection <- inspect_selexprep_accession("PRJDB19098")
```

plot.selexprep_qc *Plot SELEX quality-control diagnostics*

Description

Renders an R-native diagnostic surface corresponding to the four QC artifacts produced by the original Python workflow. Read retention and its primer-match proxy use extraction provenance from `y`. Sequence lengths are shown as read-weighted, per-round fractions so rounds with different depths remain comparable. The diversity view contains unique counts, Shannon entropy, and top-100 coverage.

Usage

```
## S3 method for class 'selexprep_qc'
plot(
  x,
  y = NULL,
  which = c("retention", "primer_match", "length", "diversity"),
  ...
)
```

Arguments

x	A selexprep_qc object returned by selexprep_qc().
y	Optional SummarizedExperiment used to compute x. It supplies count distributions and extraction provenance.
which	One or more diagnostic groups: 'retention', 'primer_match', 'length', or 'diversity'.
...	Named graphical parameters passed to graphics::par().

Details

When y is omitted, summaries already retained in x are still plotted. Panels that require raw counts or extraction provenance state that the data are unavailable instead of reconstructing them from incomplete summaries.

Value

x, invisibly.

Examples

```
p5 <- 'GGTAATACGACTCACTATAGGG'
p3 <- 'CCATGCATGCATGCATGCAT'
inserts <- c('ACGTACGT', 'TGCATGCA')
pools <- list(round_00 = rep(paste0(p5, inserts, p3), each = 250))
result <- run_selexprep(pools, low_total_reads = 0)
plot(S4Vectors::metadata(result)$qc, result, which = 'diversity')
```

---

read_library_report *Read a LibraryReport JSON file*

Description

Read a LibraryReport JSON file

Usage

```
read_library_report(path)
```

Arguments

path	Path to a JSON file written by `write_library_report()` or by the compatible Python implementation.

Value

A validated `selexprep_library_report`.

Examples

```
p5 <- 'GGTAATACGACTCACTATAGGG'
p3 <- 'CCATGCATGCATGCATGCAT'
inserts <- c('ACGTACGTACGTACGT', 'TGCATGCATGCATGCA')
reads <- rep(paste0(p5, inserts, p3), each = 250)
report <- selexprep_detect(list(round_00 = reads))
path <- tempfile(fileext = '.json')
write_library_report(report, path)
read_library_report(path)
```

`read_selexprep_counts` *Read a selexprep count table*

Description

Reads the stable four-column count contract (`sequence`, `reads`, `rank`, `rpm`) from TSV, CSV, RDS, or Parquet. Parquet support is optional and requires `arrow`; TSV is the portable default for R-native workflows.

Usage

```
read_selexprep_counts(path)
```

Arguments

path	Path to a `.tsv`, `.csv`, `.rds`, or `.parquet` count file.

Value

A validated `S4Vectors::DataFrame` with a `Biostrings::BStringSet` sequence column.

Examples

```
path <- tempfile(fileext = '.tsv')
write_selexprep_counts(selexprep_count(c('ACGT', 'ACGT', 'GGGG')), path)
read_selexprep_counts(path)
```

read_selexprep_fastq *Read sequences from a FASTQ file*

Description

Reads a plain or gzip-compressed FASTQ file into a `Biostrings::BStringSet`. `BStringSet` deliberately preserves both DNA and RNA alphabets, avoiding the loss of uracil that would occur when every input is coerced to DNA.

Usage

```
read_selexprep_fastq(path, max_reads = NULL)
```

Arguments

`path`	Path to a FASTQ or FASTQ.gz file.
`max_reads`	Optional positive maximum number of records to retain.

Value

A `Biostrings::BStringSet` of read sequences.

Examples

```
path <- tempfile(fileext = '.fastq')
writeLines(c('@read_1', 'ACGU', '+', 'IIII'), path)
read_selexprep_fastq(path)
```

read_selexprep_inputs *Read FASTQ files into round-aware pipeline inputs*

Description

Converts local FASTQ paths or a completed ENA fetch result into the R-native inputs used by `run_selexprep()`. Files belonging to the same round and mate are concatenated in input-table order. Plain and gzip-compressed FASTQ files are supported through `read_selexprep_fastq()`.

Usage

```
read_selexprep_inputs(x, round = NULL, mate = NULL, max_reads_per_file = NULL)
```

Arguments

x	A character vector of FASTQ paths, a data frame-like object with path and round_number columns, or a non-dry-run selexprep_fetch_result returned by fetch_selexprep_reads().
round	Optional vector of non-negative round numbers. It is required for character paths unless their vector names end in round numbers.
mate	Optional vector containing R1/R2 or 1/2. When omitted, mate labels are inferred from filenames.
max_reads_per_file	Optional positive maximum number of records read from each FASTQ file.

Details

Mate labels are inferred conservatively from conventional _R1, _R2, _1, and _2 filename suffixes. Files without a mate suffix are treated as single-end only when no R2 file is present. Paired inputs must have both mates, with equal loaded read counts, in every round.

Value

A selexprep_read_inputs list with sequences_by_round, optional paired_mate_streams, read_source, and a file-level DataFrame named files. The first three elements can be passed directly to run_selexprep(), or use run_selexprep_files().

Examples

```
path <- tempfile(fileext = '.fastq')
writeLines(c('@read_1', 'ACGT', '+', 'IIII'), path)
inputs <- read_selexprep_inputs(path, round = 0)
inputs$sequences_by_round
```

---

read_selexprep_manifest

Read a selexprep manifest JSON file

Description

Reads and validates both the portable Python selexprep_manifest_v1 format and the R-native selexprep_manifest_v2 format.

Usage

```
read_selexprep_manifest(path)
```

Arguments

path	Path to a selexprep manifest JSON file.

Value

A validated `selexprep_manifest`.

Examples

```
p5 <- 'GGTAATACGACTCACTATAGGG'
p3 <- 'CCATGCATGCATGCATGCAT'
inserts <- c('ACGTACGTACGTACGT', 'TGCATGCATGCATGCA')
reads <- rep(paste0(p5, inserts, p3), each = 250)
report <- selexprep_detect(list(round_00 = reads))
path <- tempfile(fileext = '.json')
write_selexprep_manifest(build_selexprep_manifest(report), path)
read_selexprep_manifest(path)
```

---

reverse_complement *Reverse-complement nucleotide sequences*

Description

Accepts DNA or RNA bases and keeps input case. A/T, C/G and the IUPAC ambiguity codes are complemented (R/Y, K/M, B/V, D/H; S, W and N are their own complements), and U/u maps to A/a. Other symbols are kept unchanged. It is vectorized over `sequence` using Biostrings. Unlike `Biostrings::reverseComplement()` on a `DNAStringSet`, it keeps lowercase letters and accepts RNA and non-IUPAC symbols, so read sequences are returned in their original alphabet.

Usage

```
reverse_complement(sequence)
```

Arguments

`sequence`	A character vector of nucleotide sequences without missing values.

Value

A character vector of reverse-complemented sequences.

Examples

```
reverse_complement(c('ACGT', 'ACGU', 'ANNT'))
```

run_selexprep *Run the in-memory SELEX preprocessing workflow*

Description

Composes primer detection, extraction, sequence counting and quality control into a single Bioconductor result. The primary output is a `SummarizedExperiment` with one column per round and a sparse `counts` assay. The LibraryReport, extraction result and QC report are retained in `metadata()` for reproducibility and inspection.

Usage

```
run_selexprep(
  sequences_by_round,
  read_source = c("R1", "R2", "R1_AND_R2", "INTERLEAVED", "UNKNOWN"),
  paired_mate_streams = NULL,
  accession = NULL,
  sampling_seed = 42L,
  max_reads_per_round = NULL,
  low_total_reads = 10000L,
  primer_5p = NULL,
  primer_3p = NULL,
  extraction_mode = NULL
)
```

Arguments

`sequences_by_round`
: A named list of R1 pools, as accepted by `selexprep_detect()`, or a `selexprep_read_inputs` object.

`read_source`
: Input read layout.

`paired_mate_streams`
: Optional named R2 pools.

`accession`
: Optional public-study accession stored in metadata.

`sampling_seed`
: Seed forwarded to `selexprep_detect()`.

`max_reads_per_round`
: Optional detection subsampling cap.

`low_total_reads`
: QC threshold for per-round read depth.

`primer_5p`
: Optional manually reviewed 5-prime primer override, written as it reads at the start of the reads.

`primer_3p`
: Optional manually reviewed 3-prime primer override, written as it reads at the end of the reads: a reverse primer as ordered is its reverse complement.

`extraction_mode`
: Optional manually reviewed extraction-mode override: `"BOTH_PRIMERS_SINGLE_READ"`, `"FIVE_PRIME_ONLY"`, `"THREE_PRIME_ONLY"` or `"PAIRED_END_SPLIT_PRIMERS"`. A primer override keeps the inferred mode, so give `"BOTH_PRIMERS_SINGLE_READ"` with both primers when detection reported a one-sided mode.

Details

Split-primer paired-end inputs return a valid zero-row experiment, with a warning, because full inserts cannot be counted without read merging. Their separate trimmed sides remain available in `metadata(result)$extraction`, and `metadata(result)$qc` is `NULL`.

Library status rates read support, not a verified constant/random boundary. Check the published library design when diverse early rounds are absent. When reads are longer than the construct they run into the sequencing adapter: detection can then call the adapter as a primer, or find one constant only. Both cases are reported, the first with a warning; supply `primer_5p`, `primer_3p` and `extraction_mode` to extract the random region. With supplied primers the report has `status = "LOW"` and `confidence = 0`: nothing was inferred, so there is no inference to rate. The evidence for the supplied primers is in `match_rate_5p` and `match_rate_3p`. Extraction warns about low read retention; diagnostics remain in `metadata(result)$extraction$low_yield_rounds`. With FASTQ input bundles, per-file counts and warnings also remain in `input_yields` and `low_yield_inputs`, so pooling files cannot hide a poorly matching input.

Value

A `SummarizedExperiment` with the LibraryReport, extraction and QC result in its metadata.

Examples

```
p5 <- 'GGTAATACGACTCACTATAGGG'
p3 <- 'CCATGCATGCATGCATGCAT'
inserts <- c('ACGTACGTACGTACGT', 'TGCATGCATGCATGCA')
pools <- list(round_00 = rep(paste0(p5, inserts, p3), each = 250))
run_selexprep(pools, low_total_reads = 0)
```

---

run_selexprep_files *Run selexprepR directly from FASTQ files*

Description

Convenience bridge combining `read_selexprep_inputs()` and `run_selexprep()`. File-level provenance is attached to `metadata(result)$input_files`. Extraction metadata also retains `input_yields` with loaded/retained R1 read counts per FASTQ and `low_yield_inputs` diagnostics. Split-primer paired extraction counts jointly retained pairs once per R1 input; unused R2 files are excluded from single-read yield diagnostics. Empty files have an undefined yield.

Usage

```
run_selexprep_files(
  x,
  round = NULL,
  mate = NULL,
  max_reads_per_file = NULL,
  ...
)
```

Arguments

x	A character vector of FASTQ paths, a data frame-like object with path and round_number columns, or a non-dry-run selexprep_fetch_result returned by fetch_selexprep_reads().
round	Optional vector of non-negative round numbers. It is required for character paths unless their vector names end in round numbers.
mate	Optional vector containing R1/R2 or 1/2. When omitted, mate labels are inferred from filenames.
max_reads_per_file	Optional positive maximum number of records read from each FASTQ file.
...	Named arguments forwarded to run_selexprep(). The input sequence, paired-mate, and read-source arguments are supplied by this function and cannot be overridden.

Value

A SummarizedExperiment as returned by run_selexprep().

Examples

```
# This two-read toy library supplies its known primers explicitly.
p5 <- "GGTAATACGACTCACTATAGGG"
p3 <- "CCATGCATGCATGCATGCAT"
sequences <- paste0(p5, c("ACGT", "TGCA"), p3)
records <- as.vector(rbind(
    paste0("@read_", seq_along(sequences)), sequences,
    "+", strrep("I", nchar(sequences))
))
path <- tempfile(fileext = ".fastq")
writeLines(records, path)
experiment <- run_selexprep_files(
    path, round = 0, primer_5p = p5, primer_3p = p3,
    extraction_mode = "BOTH_PRIMERS_SINGLE_READ", low_total_reads = 0
)
S4Vectors::metadata(experiment)$qc$per_round
unlink(path)
```

selexprep-classes *selexprepR result objects*

Description

The package uses lightweight S3 lists for decision records and reports, while sequence abundance data use the standard Bioconductor SummarizedExperiment container. These lists are deliberately explicit and serializable: they can be written to the versioned JSON contracts without loss of meaning.

Details

The list elements are stable public contracts:

- selexprep_library_report stores primer_5p, primer_3p, their variant evidence (variants_5p, variants_3p), known_adapter_hits, extraction_mode, full_insert_recovered, read_source, required_action, orientation, random-region length summaries (n_length_mode, n_length_distribution, n_length_confidence), primer match and position-consistency rates, the inference fraction and seed, overall confidence, status, and an optional failure_reason.
- selexprep_extraction stores extraction_mode, full_insert_recovered, primer-stripped sequences_by_round, named input_reads and output_reads counts, and the pre-trim forward/reverse/ambiguous strand_distribution for each round, plus named low_yield_rounds diagnostics for pools with poor read retention. Workflows receiving FASTQ input bundles also retain an input_yields DataFrame and named low_yield_inputs diagnostics per R1 FASTQ (joint pair retention for paired split extraction).
- selexprep_qc stores a per_round metrics DataFrame, a pairwise round_similarity DataFrame, a flags DataFrame whose evidence column contains structured lists, and the applied settings.
- selexprep_manifest stores the schema and package/runtime versions, accession and run identifiers, input/output SHA-256 maps, the embedded library report and its classification, parameters, stage durations, QC flags, and sampling seed. Readers accept portable Python v1 and R-native v2 schemas.
- selexprep_inspection stores the requested accession, BioProject ID, study title, library strategy/source, and a run-level runs DataFrame containing accessions, titles, sizes, FASTQ URLs, checksums, per-run library_strategy, and a sample_attributes list-column from ENA XML.
- selexprep_fetch_result stores the resolved run-level download plan, downloaded_files, the dry_run status, and rounds_with_several_samples mapping assigned rounds to runs drawn from distinct BioSamples.
- selexprep_read_inputs stores round-aware R1 pools, optional R2 pools, the inferred read_source, and a file-level provenance DataFrame.
- selexprep_demultiplex extends selexprep_read_inputs with unassigned reads, per-round assignment summaries, and the validated barcode map.

S3 lists are used for these small decision and provenance records because their named elements map losslessly to the versioned JSON contracts. The high-dimensional assay remains a standard SummarizedExperiment with a sparse Matrix assay.

Value

A description of the result classes and their stable list elements.

Examples

```
p5 <- 'GGTAATACGACTCACTATAGGG'
p3 <- 'CCATGCATGCATGCATGCAT'
inserts <- c('ACGTACGTACGTACGT', 'TGCATGCATGCATGCA')
reads <- rep(paste0(p5, inserts, p3), each = 250)
report <- selexprep_detect(list(round_00 = reads))
class(report)
```

`selexprep_catalog` *Query the bundled public HT-SELEX study catalog*

Description

Returns the curated catalog snapshot distributed with the package. The optional text query is matched case-insensitively against the BioProject ID, study title, and target, making it useful for discovery while leaving raw metadata values intact.

Usage

```
selexprep_catalog(query = NULL)
```

Arguments

`query`	Optional non-empty search string.

Value

An `S4Vectors::DataFrame` of curated study metadata.

Examples

```
selexprep_catalog('FGF-9')
```

selexprep_count *Count unique SELEX sequences*

Description

Counts the observed sequences in one primer-stripped SELEX round. The result is a `S4Vectors::DataFrame` compatible with the stable Python output schema: `sequence`, `reads`, `rank`, and `rpm`. The sequence column is a `Biostrings::BStringSet` so that both DNA and RNA alphabets can be carried without lossy coercion.

Usage

```
selexprep_count(sequences)
```

Arguments

`sequences`	A character vector or a `Biostrings::XStringSet` containing the primer-stripped sequences from one round.

Details

Ties in abundance are ordered lexicographically by sequence. The original Python implementation does not define a tie-breaker; making it explicit in R provides reproducible ranks across platforms.

Value

A `S4Vectors::DataFrame` with `sequence`, `reads`, `rank`, and `rpm` columns, ordered by decreasing read count.

Examples

```
selexprep_count(c('ACGT', 'ACGT', 'GGGG'))
```

selexprep_demultiplex *Demultiplex SELEX reads with user-supplied barcodes*

Description

Assigns reads to selection rounds from an equal-length barcode at the R1 5-prime end. Barcode sequences are supplied explicitly; they are never inferred. R2 mates follow their R1 assignment and remain untrimmed.

Usage

```
selexprep_demultiplex(
  sequences,
  barcodes,
  paired_mates = NULL,
  max_mismatches = 1L,
  trim_barcode = TRUE
)
```

Arguments

sequences	R1 sequences as a character vector or Biostrings::XStringSet.
barcodes	Named integer vector mapping barcode sequences to non-negative round numbers, for example c(AAAAA = 0L, TTTTT = 1L).
paired_mates	Optional R2 sequences in the same order as sequences.
max_mismatches	Maximum Hamming distance allowed from a barcode.
trim_barcode	Whether to remove the matched barcode from assigned R1 sequences.

Details

Barcodes must have pairwise Hamming distance of at least 2 * max_mismatches + 1, preventing ambiguous assignments. RNA U and DNA T are treated as equivalent during matching.

Value

A selexprep_demultiplex object. Its first four fields follow the selexprep_read_inputs contract and can be supplied directly to run_selexprep(). Additional fields contain unassigned reads, a summary, and the validated barcode map.

Examples

```
reads <- c("AAAAACCCCC", "AAAATGGGGG", "TTTTTACGTA", "GGGGGAAAAA")
demultiplexed <- selexprep_demultiplex(
    reads,
    c(AAAAA = 0L, TTTTT = 1L)
)
demultiplexed$summary
```

---

selexprep_detect *Detect SELEX library structure and constant regions*

Description

Detects 5' and 3' constant regions in the earliest supplied SELEX round, then verifies the call across rounds. The returned LibraryReport separates inferred biology, input layout, and required downstream action. When primer evidence is insufficient, it returns an explicit safe-failure report rather than guessing.

Usage

```
selexprep_detect(
  sequences_by_round,
  read_source = c("R1", "R2", "R1_AND_R2", "INTERLEAVED", "UNKNOWN"),
  paired_mate_streams = NULL,
  sampling_seed = 42L,
  max_reads_per_round = NULL
)
```

Arguments

sequences_by_round	A named list of character vectors or Biostrings::XStringSet objects. Each element is one sequencing round.
read_source	One of 'R1', 'R2', 'R1_AND_R2', 'INTERLEAVED', or 'UNKNOWN'.
paired_mate_streams	Optional named list containing the corresponding R2 sequences. Required only to detect split-primer paired-end layouts.
sampling_seed	Integer seed used when max_reads_per_round samples input reads.
max_reads_per_round	Optional positive cap on reads used per round.

Details

The call retains the sequence shared by anchored rounds: run-specific outer tags may be removed, while the inner 12 bases next to the insert remain fixed. Position evidence uses round-specific offsets. Insert-length and orientation estimates use the complete earliest-round flanks.

HIGH and MEDIUM rate read support, not a verified constant/random boundary. When diverse early rounds are absent, consult the published library design and use reviewed primer overrides if needed.

Two calls are valid for the reads but easy to misuse, and are reported. A called primer that contains a known sequencing adapter emits a warning: the reads run past the construct into the adapter. A one-sided extraction_mode (FIVE_PRIME_ONLY, THREE_PRIME_ONLY) emits a message: extraction then trims one side and the sequences keep the rest of the read.

The fields of the report are described in selexprep-classes. status is HIGH, MEDIUM, LOW or UNABLE_TO_INFER; extraction_mode is BOTH_PRIMERS_SINGLE_READ, FIVE_PRIME_ONLY, THREE_PRIME_ONLY, PAIRED_END_SPLIT_PRIMERS or UNABLE_TO_EXTRACT; required_action is NONE, MANUAL_PRIMERS_REQUIRED or READ_MERGING_RECOMMENDED.

Value

A selexprep_library_report.

Examples

```
p5 <- 'GGTAATACGACTCACTATAGGG'
p3 <- 'CCATGCATGCATGCATGCAT'
inserts <- c('ACGTACGTACGTACGT', 'TGCATGCATGCATGCA')
reads <- rep(paste0(p5, inserts, p3), each = 250)
selexprep_detect(list(round_00 = reads))
```

`selexprep_extract` *Extract random regions from a SELEX library*

Description

Uses a `selexprep_library_report` to remove the inferred constant regions. The implementation operates directly on R sequence objects and preserves the explicit safe-failure behavior of the original pipeline: reports marked as unable to extract stop with an error unless the caller supplies a corrected report. In split-primer paired-end mode, the two trimmed sides remain separate; they are never silently merged.

Usage

```
selexprep_extract(
  sequences_by_round,
  library_report,
  paired_mate_streams = NULL,
  primer_5p = NULL,
  primer_3p = NULL,
  extraction_mode = NULL
)
```

Arguments

`sequences_by_round`
: A named list of character vectors or `Biostrings::XStringSet` objects containing R1 sequences.

`library_report`
: A `selexprep_library_report` from `selexprep_detect()` or `read_library_report()`.

`paired_mate_streams`
: Optional named R2 sequence pools, required for `PAIRED_END_SPLIT_PRIMERS` reports.

`primer_5p`
: Optional manually reviewed 5-prime primer override, written as it reads at the start of the reads. IUPAC ambiguity codes are allowed.

`primer_3p`
: Optional manually reviewed 3-prime primer override, written as it reads at the end of the reads: a reverse primer as ordered is its reverse complement. A supplied primer found in under 5 percent of the earliest round's reads emits a warning.

`extraction_mode`
: Optional manually reviewed extraction-mode override: `"BOTH_PRIMERS_SINGLE_READ"`, `"FIVE_PRIME_ONLY"`, `"THREE_PRIME_ONLY"` or `"PAIRED_END_SPLIT_PRIMERS"`. A primer override keeps the report's mode, so give `"BOTH_PRIMERS_SINGLE_READ"` with both primers when the report is one-sided; otherwise one primer is left untrimmed, with a warning.

Details

Primers are located as cutadapt 5.2 locates adapters with its defaults, as in the Python pipeline. A primer may occur anywhere in the read, with substitutions and indels up to a 10 percent error rate over its aligned part. A 5' primer may be cut short at the read start and a 3' primer at the read end, if at least 3 of its bases align. When a read holds several acceptable occurrences, the first one is kept unless a later one overlaps it or covers more of the primer, and aligns with a higher score. IUPAC codes in a primer match the bases they stand for. RNA `U` is matched as DNA `T`. The returned insert retains the alphabet and case of the input read.

Value

A `selexprep_extraction`. Full and single-primer modes store one `Biostrings::BStringSet` per round; paired split mode stores an `r1` and `r2` `BStringSet` for every round. `low_yield_rounds` is a named character vector describing nonempty rounds retaining less than half their reads or less than half the best round's yield; these rounds also emit a warning.

Examples

```
primer_5p <- 'GGTAATACGACTCACTATAGGG'
primer_3p <- 'CCATGCATGCATGCATGCAT'
bases <- c('A', 'C', 'G', 'T')
random_regions <- vapply(0:499, function(i) {
    paste0(bases[(i * 7 + 0:15 * 13) %% 4 + 1], collapse = '')
}, character(1))
reads <- paste0(primer_5p, random_regions, primer_3p)
report <- selexprep_detect(list(round_00 = reads))
selexprep_extract(list(round_00 = reads[seq_len(3L)]), report)
```

---

selexprep_public_catalog

Curated public HT-SELEX catalog

Description

A frozen, offline snapshot of 240 public HT-SELEX deposits. Eight experimental fields were extracted independently by two language models, reconciled, and retained with a per-field curation status. The flat dataset intentionally omits evidence quotations; immutable links to the canonical provenance-rich JSON and its generation materials are stored in `S4Vectors::metadata(selexprep_public_catalog)`.

Usage

```
data(selexprep_public_catalog)
```

Format

An S4Vectors::DataFrame with 240 rows and 19 columns:

bioproject_id ENA BioProject accession or a platform-prefixed Figshare or Zenodo deposit identifier.

source ena, or the platform-prefixed Figshare or Zenodo deposit identifier used as the source key.

study_title Title recorded for the public study or deposit.

study_type, study_type_curation Curated experiment type and its reconciliation status.

target, target_curation Selection target and its reconciliation status.

target_class, target_class_curation Target class and its reconciliation status.

chemistry, chemistry_curation DNA or RNA library chemistry and its reconciliation status.

n_random, n_random_curation Reported random-region length and its reconciliation status.

n_rounds, n_rounds_curation Reported selection-round count and its reconciliation status.

selection_format, selection_format_curation Reported selection format and its reconciliation status.

counter_selection, counter_selection_curation Reported counter-selection conditions and their reconciliation status.

Curation statuses are adjudicated, concordant, not_stated, verified, single_source:claude, or single_source:codex. These describe upstream curation; a status alone does not establish human validation. Maintainer spot checks are documented separately in CATALOG_PROVENANCE.md.

Details

The catalog compilation and curation annotations are MIT-licensed under the pinned upstream grant. Source papers and sequencing reads are not distributed as part of this dataset; their terms are recorded separately in the installed DATA_LICENSES.md file.

Missing values mean that a field was not stated in the curated sources. A adjudicated means that the two extraction arms disagreed and the value was resolved using the source evidence. The canonical provenance JSON retains both original values and the adjudication rationale.

Source

The snapshot was migrated without modification from the original selexprep v0.4.6 catalog at commit 63f33b44bb381c2c6b6ed131f3b98e8d6ff9d5f5, archived as doi:10.5281/zenodo.23104868. See the object metadata and inst/CATALOG_PROVENANCE.md for immutable source links and terms.

Examples

```
data("selexprep_public_catalog", package = "selexprepR")
head(selexprep_public_catalog[, c("bioproject_id", "study_type", "target")])
S4Vectors::metadata(selexprep_public_catalog)$snapshot_version
```

selexprep_qc *Quality-control summary for a SELEX count experiment*

Description

Calculates depth, diversity, composition and sequence-length summaries for each round of a SummarizedExperiment returned by run_selexprep(), and k-mer distances between rounds. Flags mark conditions to review: low depth, length differences across rounds, unexpected diversity changes, non-standard bases, residual or high adapter content, mixed read orientation, weak primer matches and paired-end libraries that need read merging. Flags do not remove rounds or reads.

Usage

```
selexprep_qc(
  experiment,
  library_report = NULL,
  low_total_reads = 10000L,
  rarefaction_depth = 10000L,
  rarefaction_seed = 42L,
  kmer_size = 6L,
  kmer_top_sequences = 10000L
)
```

Arguments

experiment	A SummarizedExperiment with an assay named 'counts' and a sequence column in rowData.
library_report	Optional selexprep_library_report. When omitted, a report stored in the experiment metadata is used when available.
low_total_reads	Minimum number of reads expected in every round.
rarefaction_depth	Maximum common depth used when comparing observed diversity across rounds.
rarefaction_seed	Integer seed for deterministic rarefaction.
kmer_size	Length of canonical k-mers used for between-round consistency diagnostics.
kmer_top_sequences	Maximum number of abundant sequences considered from each round for k-mer diagnostics.

Value

A selexprep_qc list with per_round, round_similarity, and flags DataFrames plus the applied settings.

Examples

```
p5 <- 'GGTAATACGACTCACTATAGGG'
p3 <- 'CCATGCATGCATGCATGCAT'
inserts <- c('ACGTACGTACGTACGT', 'TGCATGCATGCATGCA')
pools <- list(round_00 = rep(paste0(p5, inserts, p3), each = 250))
result <- run_selexprep(pools, low_total_reads = 0)
selexprep_qc(result)
```

`write_library_report` *Write a LibraryReport as deterministic JSON*

Description

Write a LibraryReport as deterministic JSON

Usage

```
write_library_report(report, path)
```

Arguments

`report`	A `selexprep_library_report`.
`path`	Output JSON path.

Value

The SHA-256 digest of the emitted UTF-8 JSON, invisibly.

Examples

```
p5 <- 'GGTAATACGACTCACTATAGGG'
p3 <- 'CCATGCATGCATGCATGCAT'
inserts <- c('ACGTACGTACGTACGT', 'TGCATGCATGCATGCA')
reads <- rep(paste0(p5, inserts, p3), each = 250)
report <- selexprep_detect(list(round_00 = reads))
path <- tempfile(fileext = '.json')
write_library_report(report, path)
```

write_selexprep_counts

Write a selexprep count table

Description

Writes the stable four-column count contract. Use TSV for a dependency-free, portable exchange format; Parquet is available when the optional `arrow` package is installed.

Usage

```
write_selexprep_counts(counts, path)
```

Arguments

`counts`	A count table returned by `selexprep_count()`.
`path`	Output path ending in `.tsv`, `.csv`, `.rds`, or `.parquet`.

Value

`path`, invisibly.

Examples

```
counts <- selexprep_count(c('ACGT', 'ACGT', 'GGGG'))
path <- tempfile(fileext = '.tsv')
write_selexprep_counts(counts, path)
```

write_selexprep_manifest

Write a selexprep manifest as deterministic JSON

Description

Write a selexprep manifest as deterministic JSON

Usage

```
write_selexprep_manifest(manifest, path)
```

Arguments

`manifest`	A `selexprep_manifest`.
`path`	Output JSON path.

Value

The SHA-256 digest of the emitted UTF-8 JSON, invisibly.

Examples

```
p5 <- 'GGTAATACGACTCACTATAGGG'
p3 <- 'CCATGCATGCATGCATGCAT'
inserts <- c('ACGTACGTACGTACGT', 'TGCATGCATGCATGCA')
reads <- rep(paste0(p5, inserts, p3), each = 250)
report <- selexprep_detect(list(round_00 = reads))
path <- tempfile(fileext = '.json')
write_selexprep_manifest(build_selexprep_manifest(report), path)
```

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