

# Package ‘pqsfinder’

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**Type** Package

**Title** Identification of potential quadruplex forming sequences

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**URL** <https://pqsfinder.fi.muni.cz>

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**Description** Pqsfinder detects

DNA and RNA sequence patterns that are likely to fold into an intramolecular G-quadruplex (G4). Unlike many other approaches, pqsfinder is able to detect G4s folded from imperfect G-runs containing bulges or mismatches or G4s having long loops. Pqsfinder also assigns an integer score to each hit that was fitted on G4 sequencing data and corresponds to expected stability of the folded G4.

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**biocViews** MotifDiscovery, SequenceMatching, GeneRegulation

**LazyData** TRUE

**Depends** Biostrings

**Imports** Rcpp (>= 0.12.3), GenomicRanges, IRanges, S4Vectors, methods

**Suggests** BiocStyle, knitr, rmarkdown, Gviz, rtracklayer, ggplot2, BSgenome.Hsapiens.UCSC.hg38, testthat, stringr, stringi

**LinkingTo** Rcpp, BH (>= 1.78.0)

**SystemRequirements** GNU make, C++11

**VignetteBuilder** knitr

**RoxygenNote** 7.1.2

**Encoding** UTF-8

**NeedsCompilation** yes

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|                                   |  |
|-----------------------------------|--|
| as.character,PQSViews-method      |  |
| <i>Coerce to character vector</i> |  |

---

Description

Coerce to character vector

Usage

```
## S4 method for signature 'PQSViews'  
as.character(x)
```

Arguments

x                      PQSViews object.

Value

Character vector representing PQS.

---

|                           |  |
|---------------------------|--|
| density,PQSViews-method   |  |
| <i>Get density vector</i> |  |

---

Description

Desity vector represents numbers of PQS (potential quadruplex forming sequences) overlapping at each position in input sequence.

Usage

```
## S4 method for signature 'PQSViews'  
density(x)
```

**Arguments**

x PQSViews object.

**Value**

Density vector.

**Examples**

```
pqs <- pqsfinder(DNAString("CCCCCGGGTGGGTGGGTGGGAAAA"))  
density(pqs)
```

---

|           |                                     |
|-----------|-------------------------------------|
| maxScores | <i>Get vector of maximal scores</i> |
|-----------|-------------------------------------|

---

**Description**

Get vector of maximal scores for a given object.

**Usage**

```
maxScores(x, ...)
```

**Arguments**

x An object.

... Additional arguments, for use in specific methods.

**Value**

Vector of maximal scores.

**Examples**

```
showMethods("maxScores")
```

---

```
maxScores, PQSViews-method
```

*Get vector of maximal scores*

---

### Description

For each sequence position it gives the maximal score of all PQS conformations which overlap that position.

### Usage

```
## S4 method for signature 'PQSViews'
maxScores(x)
```

### Arguments

x                      PQSViews object.

### Value

Vector of maximal scores.

### Examples

```
pqs <- pqsfinder(DNAString("CCCCCGGGTGGGTGGGTGGGAAAA"))
maxScores(pqs)
```

---

```
pqsfinder                      Identify potential quadruplex forming sequences.
```

---

### Description

Function for identification of all potential intramolecular quadruplex patterns (PQS) in DNA or RNA sequence.

### Usage

```
pqsfinder(
  subject,
  strand = "*",
  overlapping = FALSE,
  max_len = 50L,
  min_score = 47L,
  run_min_len = 2L,
  run_max_len = 11L,
  loop_min_len = 0L,
  loop_max_len = 30L,
  max_bulges = 3L,
  max_mismatches = 3L,
```

```

    max_defects = 3L,
    tetrad_bonus = 40L,
    mismatch_penalty = 28L,
    bulge_penalty = 20L,
    bulge_len_factor = 0.2,
    bulge_len_exponent = 1,
    loop_mean_factor = 6.6,
    loop_mean_exponent = 0.8,
    run_re = "G{1,10}. {0,9}G{1,10}",
    custom_scoring_fn = NULL,
    use_default_scoring = TRUE,
    deep = FALSE,
    verbose = FALSE
)

```

## Arguments

|                    |                                                                                                                                                                                   |
|--------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| subject            | DNAString or RNAString object.                                                                                                                                                    |
| strand             | Strand specification. Allowed values are "+", "-" or "*", where the last one represents both strands. Implicitly, the input DNAString object is assumed to encode the "+" strand. |
| overlapping        | If true, than all overlapping PQS will be reported.                                                                                                                               |
| max_len            | Maximal lenth of PQS.                                                                                                                                                             |
| min_score          | Minimal PQS score. The default value 52 shows the best balanced accuracy on G4 sequencing data provided by Chambers et al. 2015.                                                  |
| run_min_len        | Minimal length of quadruplex run.                                                                                                                                                 |
| run_max_len        | Maximal length of quadruplex run.                                                                                                                                                 |
| loop_min_len       | Minimal length of quadruplex loop. Unless the default scoring system is disabled, at most one loop can have zero length.                                                          |
| loop_max_len       | Maxmimal length of quadruplex loop.                                                                                                                                               |
| max_bulges         | Maximal number of runs with bulge.                                                                                                                                                |
| max_mismatches     | Maximal number of runs with mismatch.                                                                                                                                             |
| max_defects        | Maximum number of defects in total (max_bulges + max_mismatches).                                                                                                                 |
| tetrad_bonus       | Score bonus for one complete G tetrade.                                                                                                                                           |
| mismatch_penalty   | Penalization for a mismatch in tetrad.                                                                                                                                            |
| bulge_penalty      | Penalization for a bulge in quadruplex run.                                                                                                                                       |
| bulge_len_factor   | Penalization factor for a bulge length.                                                                                                                                           |
| bulge_len_exponent | Exponent of bulge length.                                                                                                                                                         |
| loop_mean_factor   | Penalization factor of loop length mean.                                                                                                                                          |
| loop_mean_exponent | Exponent of loop length mean.                                                                                                                                                     |
| run_re             | Regular expression specifying one run of quadruplex.                                                                                                                              |

|                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
|---------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| custom_scoring_fn   | Custom quadruplex scoring function. It takes the following 10 arguments: subject - Input DNAString or RNAString object, score - implicit PQS score, start - PQS start position, width - PQS width, loop_1 - start pos. of loop #1, run_2 - start pos. of run #2, loop_2 - start pos. of loop #2, run_3 - start pos. of run #3, loop_3 - start pos. of loop #3, run_4 - start pos. of run #4. Return value of the function has to be new score represented as a single integer value. Please note that if use_default_scoring is enabled, the custom scoring function is evaluated AFTER the default scoring system but ONLY IF the default scoring system resulted in non-zero score (for performance reasons). On the other hand, when use_default_scoring is disabled, custom scoring function is evaluated on every PQS. |
| use_default_scoring | Enables default internal scoring system. This option is particularly useful in case you intend to radically change the default behavior and specify your own scoring function. By disabling the default scoring you will get a full control above the underlying detection algorithm.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| deep                | Perform deep search. With this option enabled, <a href="#">maxScores</a> and <a href="#">density</a> vectors are computed. Deep search is much more computationally demanding.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| verbose             | Enables detailed output. Turn it on if you want to see all possible PQS found at each positions and not just the best one. It is highly recommended to use this option for debugging custom quadruplex scoring function. Each PQS is reported on separate row in the following format: start cnt pqs_sequence score, where start is the PQS starting position, pqs_sequence shows the PQS sequence structure with each run surrounded by square brackets and score is the score assigned to the particular PQS by all applied scoring functions.                                                                                                                                                                                                                                                                            |

## Details

Use [elementMetadata](#) function to get extra PQS features like number of tetrads (nt), bulges (nb), mismatches (nm) or loop lengths (ll1, ll2, ll3).

## Value

[PQSViews](#) object

## Examples

```
pv <- pqsfinder(DNAString("CCCCCGGGTGGGTGGGTGGGTAAAA"))
pv
elementMetadata(pv)
```

---

PQSViews

---

*PQSViews class constructor*


---

## Description

User friendly constructor for PQSViews class representing potential quadruplex forming sequences (PQS). PQSViews is a subclass of [XStringViews](#) class and adds two more slots to store PQS density and PQS score distribution.

**Usage**

```
PQSViews(  
  subject,  
  start,  
  width,  
  strand,  
  score,  
  density,  
  max_scores,  
  nt,  
  nb,  
  nm,  
  r11,  
  r12,  
  r13,  
  l11,  
  l12,  
  l13  
)
```

**Arguments**

|            |                                                         |
|------------|---------------------------------------------------------|
| subject    | DNASTring or RNASTring object.                          |
| start      | Start positions.                                        |
| width      | Lengths.                                                |
| strand     | Strand specifications.                                  |
| score      | Scores.                                                 |
| density    | Numbers of PQS overlapping at each position in subject. |
| max_scores | Score of the best PQS found at each position.           |
| nt         | Tetrad numbers.                                         |
| nb         | Bulge counts.                                           |
| nm         | Mismatch counts.                                        |
| r11        | Run 1 lengths.                                          |
| r12        | Run 2 lengths.                                          |
| r13        | Run 3 lengths.                                          |
| l11        | Loop 1 lengths.                                         |
| l12        | Loop 2 lengths.                                         |
| l13        | Loop 3 lengths.                                         |

**Details**

Use [elementMetadata](#) function to get extra PQS features like number of tetrads, bulges, mismatches or loop lengths.

**Value**

PQSViews object.

**Examples**

```
pv <- PQSViews(DNAString("GGTGGTGGTGG"), 1, 11, "+", 33, as.integer(rep(1, 11)),
               as.integer(rep(33, 11)), 2, 0, 0, 2, 2, 2, 1, 1, 1)

start(pv)
width(pv)
strand(pv)
score(pv)
density(pv)
maxScores(pv)
elementMetadata(pv)
```

PQSViews-class

*An S4 class to represent potential quadruplex forming sequences***Description**

Represents potential quadruplex forming sequences found by [pqsfinder](#) function. This is a subclass of [XStringViews-class](#) class and adds one more slot.

**Slots**

**density** Numbers of PQS (potential quadruplex forming sequences) overlapping at each position in input sequence.

**max\_scores** Score of the best PQS found at each position.

score,PQSViews-method *Get PQS score vector***Description**

Get PQS score vector

**Usage**

```
## S4 method for signature 'PQSViews'
score(x)
```

**Arguments**

**x** PQSViews object.

**Value**

Score vector.

**Examples**

```
pqs <- pqsfinder(DNAString("CCCCCGGGTGGGTGGGTGGGAAAA"))
score(pqs)
```

---

|                      |                    |
|----------------------|--------------------|
| show,PQSViews-method | <i>Show method</i> |
|----------------------|--------------------|

---

**Description**

Show method

**Usage**

```
## S4 method for signature 'PQSViews'  
show(object)
```

**Arguments**

|        |                  |
|--------|------------------|
| object | PQSViews object. |
|--------|------------------|

**Value**

PQSViews object printed.

---

|                        |                              |
|------------------------|------------------------------|
| strand,PQSViews-method | <i>Get PQS strand vector</i> |
|------------------------|------------------------------|

---

**Description**

Get PQS strand vector

**Usage**

```
## S4 method for signature 'PQSViews'  
strand(x)
```

**Arguments**

|   |                  |
|---|------------------|
| x | PQSViews object. |
|---|------------------|

**Value**

Strand vector.

**Examples**

```
pqs <- pqsfinder(DNAString("CCCCCGGGTGGGTGGGTGGGAAAA"))  
strand(pqs)
```

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