

FingerprintsStringUtil

SYNOPSIS

```
use Fingerprints::FingerprintsStringUtil;

use Fingerprints::FingerprintsStringUtil qw(:all);
```

DESCRIPTION

FingerprintsStringUtil module provides the following functions:

AreFingerprintsStringValuesValid, GenerateFingerprintsBitVectorString, GenerateFingerprintsString, GenerateFingerprintsVectorString, GetDefaultBitStringFormat, GetDefaultBitsOrder, GetDefaultVectorStringFormat, GetFingerprintsStringDelimiter, GetFingerprintsStringTypeAndDescription, GetFingerprintsStringValues, ParseFingerprintsBitVectorString, ParseFingerprintsString, ParseFingerprintsVectorString

The current release of MayaChemTools supports the following types of fingerprint bit-vector and vector strings:

```
FingerprintsVector;AtomNeighborhoods:AtomicInvariantsAtomTypes:MinRadi
us0:MaxRadius2;41/AlphaNumericalValues;ValuesString;NR0-C.X1.B01.H3-AT
C1:NR1-C.X3.B03.H1-ATC1:NR2-C.X1.B01.H3-ATC1:NR2-C.X3.B04-ATC1 NR0-C.X
1.B01.H3-ATC1:NR1-C.X3.B03.H1-ATC1:NR2-C.X1.B01.H3-ATC1:NR2-C.X3.B04-A
TC1 NR0-C.X2.B02.H2-ATC1:NR1-C.X2.B02.H2-ATC1:NR1-C.X3.B03.H1-ATC1:NR2
-C.X2.B02.H2-ATC1:NR2-N.X3.B03-ATC1:NR2-O.X1.B01.H1-ATC1 NR0-C.X2.B...
```

```
FingerprintsVector;AtomTypesCount:SLogPAtomTypes:ArbitrarySize;16;NumericalValues;IDsAndValuesString;C1 C10 C11 C14 C18 C20 C21 C22 C5 CS FN11 N4 O10 O2 O9;5 1 1 1 14 4 2 1 2 2 1 1 1 1 3 1
```

```
FingerprintsVector;AtomTypesCount:SLogPAtomTypes:FixedSize;67;OrderedNumericalValues;IDsAndValuesString:C1 C2 C3 C4 C5 C6 C7 C8 C9 C10 C11 C12 C13 C14 C15 C16 C17 C18 C19 C20 C21 C22 C23 C24 C25 C26 C27 CS N1 N2 N3 N4 N5 N6 N7 N8 N9 N10 N11 N12 N13 N14 NS O1 O2 O3 O4 O5 O6 O7 O8 O9 O10 O11 O12 OS F Cl Br I Hal P S1 S2 S3 Me1 Me2;5 0 0 0 2 0 0 0 0 1 1 0 0 1 0 0 0 14 0 4 2 1 0 0 0 0 0 2 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

```
FingerprintsVector;EStateIndicies:ArbitrarySize;11;NumericalValues;IDs
AndValuesString;SaaCH SaasC SaasN SdO SdssC SsCH3 SsF SsOH SssCH2 SssN
H SsssCH;24.778 4.387 1.993 25.023 -1.435 3.975 14.006 29.759 -0.073 3
.024 -2.270
```

```
FingerprintsVector;EStateIndicies:FixedSize;87;OrderedNumericalValues;
ValuesString:0 0 0 0 0 0 0 3.975 0 -0.073 0 0 24.778 -2.270 0 0 -1.435
4.387 0 0 0 0 0 0 3.024 0 0 0 0 0 0 0 1.993 0 29.759 25.023 0 0 0 0 1
4.006 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

```
FingerprintsVector;ExtendedConnectivity:AtomicInvariantsAtomTypes:Radi
us2;60;AlphaNumericalValues;ValuesString;73555770 333564680 352413391
666191900 1001270906 1371674323 1481469939 1977749791 2006158649 21414
08799 49532520 64643108 79385615 90602769 273726379 564565671 85514103
5 906706094 988546669 1018231313 1032696425 1197507444 1331250018 1338
532734 1455473691 1607485225 1609687129 1631614296 1670251330 17303...
```

```
FingerprintsVector;ExtendedConnectivityCount;AtomicInvariantsAtomTypes
;Radius2;60;NumericalValues;IDsAndValuesString;73555770 333564680 3524
13391 666191900 1001270906 1371674323 1481469939 1977749791 2006158649
2141408799 49532520 64643108 79385615 96062769 273726379 564565671...;
3 2 1 1 1 14 1 2 10 4 3 1 1 1 1 2 1 2 1 1 1 2 1 3 3 3 8 2 2 2 6 2
1 2 1 1 2 1 1 1 2 1 2 1 2 1 1 1 1 1 1 1 1 1 1 1 2 1 1
```

```
FingerprintsBitVector;ExtendedConnectivityBits;AtomicInvariantsAtomTypes;Radius2;1024;BinaryString;Ascending;00000000000000000000000000000000  
0000000000010100000001100000110000000000001000000000000000000000000000000000
```

```
FingerprintsVector;TopologicalAtomPairs:AtomicInvariantsAtomTypes:MinDistance1:MaxDistance10;223;NumericalValues;IDsAndValuesString;C.X1.B01.H3-D1-C.X3.B03.H1 C.X2.B02.H2-D1-C.X2.B02.H2 C.X2.B02.H2-D1-C.X3.B03.H1 C.X2.B02.H2-D1-C.X3.B04 C.X2.B02.H2-D1-N.X3.B03 C.X2.B03.H1-D1-...;
```

```
2 1 4 1 1 10 8 1 2 6 1 2 2 1 2 1 2 2 1 2 1 5 1 10 12 2 2 1 2 1 9 1 3 1
1 1 2 2 1 3 6 1 6 14 2 2 2 3 1 3 1 8 2 2 1 3 2 6 1 2 2 5 1 3 1 23 1...
```

```
FingerprintsVector;TopologicalAtomPairs:FunctionalClassAtomTypes:MinDistance:MaxDistance10;144;NumericalValues;IDsAndValuesString;Ar-D1-Ar
Ar-D1-Ar.HBA Ar-D1-HBD Ar-D1-Hal Ar-D1-None Ar.HBA-D1-None HBA-D1-NI H
BA-D1-None HBA.HBD-D1-NI HBA.HBD-D1-None HBD-D1-None NI-D1-None No...;
23 2 1 1 2 1 1 1 1 2 1 1 7 28 3 1 3 2 8 2 1 1 1 5 1 5 24 3 3 4 2 13 4
1 1 4 1 5 22 4 4 3 1 19 1 1 1 1 1 2 2 3 1 1 8 25 4 5 2 3 1 26 1 4 1 ...
```

```
FingerprintsVector;TopologicalAtomTorsions:AtomicInvariantsAtomTypes;3
3;NumericalValues;IDsAndValuesString;C.X1.BO1.H3-C.X3.BO3.H1-C.X3.BO4-
C.X3.BO4 C.X1.BO1.H3-C.X3.BO3.H1-C.X3.BO4-N.X3.BO3 C.X2.BO2.H2-C.X2.BO
2.H2-C.X3.BO3.H1-C.X2.BO2.H2 C.X2.BO2.H2-C.X2.BO2.H2-C.X3.BO3.H1-O...;
2 2 1 1 2 2 1 1 3 4 4 8 4 2 2 6 2 2 1 2 1 1 2 1 1 2 6 2 4 2 1 3 1
```

```
FingerprintsVector;TopologicalAtomTorsions:EStateAtomTypes;36;Numerical
Values;IDsAndValuesString;aaCH-aaCH-aaCH-aaCH aaCH-aaCH-aaCH-aasC aaC
H-aaCH-aasC-aaCH aaCH-aaCH-aasC-aasC aaCH-aaCH-aasC-sF aaCH-aaCH-aasC-
ssNH aaCH-aasC-aasC-aasC aaCH-aasC-aasC-aasN aaCH-aasC-ssNH-dssC a...;
4 4 8 4 2 2 6 2 2 2 4 3 2 1 3 3 2 2 2 1 2 1 1 1 2 1 1 1 1 1 1 2 1 1 2
```

```
FingerprintsVector;TopologicalAtomTriplets:AtomicInvariantsAtomTypes:M
inDistance:MaxDistance10;3096;NumericalValues;IDsAndValuesString;C.X1
.BO1.H3-D1-C.X1.BO1.H3-D1-C.X3.BO3.H1-D2 C.X1.BO1.H3-D1-C.X2.BO2.H2-D1
0-C.X3.BO4-D9 C.X1.BO1.H3-D1-C.X2.BO2.H2-D3-N.X3.BO3-D4 C.X1.BO1.H3-D1
-C.X2.BO2.H2-D4-C.X2.BO2.H2-D5 C.X1.BO1.H3-D1-C.X2.BO2.H2-D6-C.X3...;
1 2 2 2 2 2 2 8 4 8 4 4 2 2 2 2 4 2 2 2 4 2 2 2 2 1 2 2 4 4 4 2 2
2 4 4 4 8 4 4 2 4 4 4 2 4 4 2 2 2 2 2 2 2 1 2 2 2 2 2 2 2 2 2 8...
```

```
FingerprintsVector;TopologicalAtomTriplets:SYBYLAtomTypes:MinDistance:MaxDistance10;2332;NumericalValues;IDsAndValuesString;C.2-D1-C.2-D9-C
.3-D10 C.2-D1-C.2-D9-C.ar-D10 C.2-D1-C.3-D1-C.3-D2 C.2-D1-C.3-D10-C.3-
D9 C.2-D1-C.3-D2-C.3-D3 C.2-D1-C.3-D2-C.ar-D3 C.2-D1-C.3-D3-C.3-D4 C.2
-D1-C.3-D3-N.ar-D4 C.2-D1-C.3-D3-O.3-D2 C.2-D1-C.3-D4-C.3-D5 C.2-D1-C.
3-D5-C.3-D6 C.2-D1-C.3-D5-O.3-D4 C.2-D1-C.3-D6-C.3-D7 C.2-D1-C.3-D7...
```

```
FingerprintsVector;TopologicalPharmacophoreAtomPairs:ArbitrarySize:MinDistance:MaxDistance10;54;NumericalValues;IDsAndValuesString;H-D1-H H
-D1-NI HBA-D1-NI HBD-D1-NI H-D2-H H-D2-HBA H-D2-HBD HBA-D2-HBA HBA-D2-
HBD H-D3-H H-D3-HBA H-D3-HBD H-D3-NI HBA-D3-NI HBD-D3-NI H-D4-H H-D4-H
BA H-D4-HBD HBA-D4-HBA HBA-D4-HBD HBD-D4-HBD H-D5-H H-D5-HBA H-D5-...;
18 1 2 1 22 12 8 1 2 18 6 3 1 1 1 22 13 6 5 7 2 28 9 5 1 1 1 36 16 10
3 4 1 37 10 8 1 35 10 9 3 3 1 28 7 7 4 18 16 12 5 1 2 1
```

```
FingerprintsVector;TopologicalPharmacophoreAtomPairs:FixedSize:MinDistance:MaxDistance10;150;OrderedNumericalValues;ValuesString;18 0 0 1 0
0 0 2 0 0 1 0 0 0 0 22 12 8 0 0 1 2 0 0 0 0 0 0 0 0 18 6 3 1 0 0 0 1
0 0 1 0 0 0 0 22 13 6 0 0 5 7 0 0 2 0 0 0 0 0 28 9 5 1 0 0 0 1 0 0 1 0
0 0 0 36 16 10 0 0 3 4 0 0 1 0 0 0 0 0 37 10 8 0 0 0 0 1 0 0 0 0 0 0
0 35 10 9 0 0 3 3 0 0 1 0 0 0 0 0 28 7 7 4 0 0 0 0 0 0 0 0 0 0 0 18...
```

```
FingerprintsVector;TopologicalPharmacophoreAtomTriplets:ArbitrarySize:MinDistance:MaxDistance10;696;NumericalValues;IDsAndValuesString;Ar1-
Ar1-Ar1 Ar1-Ar1-H1 Ar1-Ar1-HBA1 Ar1-Ar1-HBD1 Ar1-H1-H1 Ar1-H1-HBA1 Ar1
-H1-HBD1 Ar1-HBA1-HBD1 H1-H1-H1 H1-H1-HBA1 H1-H1-HBD1 H1-HBA1-HBA1 H1-
HBA1-HBD1 H1-HBA1-NI1 H1-HBD1-NI1 HBA1-HBA1-NI1 HBA1-HBD1-NI1 Ar1-...;
46 106 8 3 83 11 4 1 21 5 3 1 2 2 1 1 1 100 101 18 11 145 132 26 14 23
28 3 3 5 4 61 45 10 4 16 20 7 5 1 3 4 5 3 1 1 1 5 4 2 1 2 2 2 1 1 1
119 123 24 15 185 202 41 25 22 17 3 5 85 95 18 11 23 17 3 1 1 6 4 ...
```

```
FingerprintsVector;TopologicalPharmacophoreAtomTriplets:FixedSize:MinDistance:MaxDistance10;2692;OrderedNumericalValues;ValuesString;46 106
8 3 0 0 83 11 4 0 0 0 1 0 0 0 0 0 0 0 0 21 5 3 0 0 1 2 2 0 0 1 0 0 0
0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 100 101 18 11 0 0 145 132 26
14 0 0 23 28 3 3 0 0 5 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 61 45 10 4 0
0 16 20 7 5 1 0 3 4 5 3 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 0 0 5 ...
```

FUNCTIONS

AreFingerprintsStringValuesValid

```
$Status = AreFingerprintsStringValuesValid($FPString);
```

Returns 0 or 1 based on whether *FingerprintsString* contains valid values.

GetDefaultBitStringFormat

```
$BitStringFormat = GetDefaultBitStringFormat();
```

Returns default BitStringFormat for fingerprints bit-vector strings.

GetDefaultBitsOrder

```
$BitsOrder = GetDefaultBitsOrder();
```

Returns default BitsOrder for fingerprints bit-vector fingerprints.

GetDefaultVectorStringFormat

```
$StringFormat = GetDefaultVectorStringFormat();
```

Returns default VectorStringFormat for fingerprints vector strings.

GetFingerprintsStringDelimiter

```
$Delimiter = GetFingerprintsStringDelimiter();
```

Returns string Delimiter used to generate fingerprints bit-vector and vector strings.

GenerateFingerprintsBitVectorString

```
$FPString = GenerateFingerprintsBitVectorString($FPBitVectorObject,
[$BitStringFormat, $BitsOrder]);
```

Returns a FingerprintsString generated using *FingerprintsBitVectorObject* and optionally specified *BitStringFormat* and *BitsOrder* values.

Possible *BitStringFormat* values: *BinaryString*, *Binary*, *Bin*, *HexadecimalString*, *Hexadecimal*, or *Hex*. Default *BitStringFormat* value: *BinaryString*.

Possible *BitsOrder* values: *Ascending* or *Descending*. Default *BitsOrder* value: *Ascending*.

GenerateFingerprintsVectorString

```
$FPString = GenerateFingerprintsVectorString($FPVectorObject,
[$VectorStringFormat]);
```

Returns a FingerprintsString generated using *FingerprintsVectorObject* and optionally specified *VectorStringFormat*.

Possible *VectorStringFormat* values: *IDsAndValuesString*, *IDsAndValues*, *IDsAndValuesPairsString*, *IDsAndValuesPairs*, *ValuesAndIDsString*, *ValuesAndIDs*, *ValuesAndIDsPairsString*, *ValuesAndIDsPairs*, *ValuesString*, *Values*.

Default *VectorStringFormat* value: for *NumericalValues FPVectorType* - *IDsAndValuesString*; for all other *FPVectorTypes* - *ValuesString*.

GenerateFingerprintsString

```
$FPString = GenerateFingerprintsBitVectorString($FPBitVectorObject,
[$BitStringFormat, $BitsOrder]);
```

```
$FPString = GenerateFingerprintsVectorString($FPVectorObject,
[$VectorStringFormat]);
```

Returns a FingerprintsString generated using *FingerprintsBitVectorObject* or *FingerprintsVectorObject* and optionally specified parameters.

GetFingerprintsStringTypeAndDescription

```
($FPType, $FPDescription) = GetFingerprintsStringTypeAndDescription(
$FPString);
```

Returns FingerprintsStringType and *FingerprintsStringDescription* strings for FingerprintsString corresponding to FingerprintsBitVectorObject or FingerprintsVectorObject.

GetFingerprintsStringValues

```
@FPStringValues = GetFingerprintsStringValues($FPString);
```

Parses FingerprintsString corresponding to FingerprintsBitVectorObject or FingerprintsVectorObject and returns its individual component values as an array.

ParseFingerprintsBitVectorString

```
$FPBitVectorObject = ParseFingerprintsBitVectorString($FPBitVectorString,  
[$ValidateValues]);
```

Returns FingerprintsBitVectorObject generated by parsing *FingerprintsBitVectorString* with optional validation of its component values.

ParseFingerprintsString

```
$FPBitVectorObject = ParseFingerprintsBitVectorString($FPBitVectorString,  
[$ValidateValues]);
```

```
$FPVectorObject = ParseFingerprintsVectorString($FPVectorString,  
[$ValidateValues]);
```

Returns FingerprintsBitVectorObject or **FingerprintsVectorObject** generated by parsing *FingerprintsBitVectorString* or *FingerprintsVectorString* with optional validation of its component values.

ParseFingerprintsVectorString

```
$FPVectorObject = ParseFingerprintsVectorString($FPVectorString,  
[$ValidateValues]);
```

Returns FingerprintsVectorObject generated by parsing *FingerprintsVectorString* with optional validation of its component values.

AUTHOR

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SEE ALSO

BitVector.pm, FingerprintsBitVector.pm, FingerprintsVector.pm, Vector.pm

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