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Subject: "PathFp" fingerpring bug?

Posted by [arofab](#) on Fri, 17 Mar 2017 09:30:39 GMT

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Hello,

it seems there is an error in "PathFp" descriptor calculation, where some '1' bits are outputted as '0' bits

Looking at the code (4.5.1 version), the createDescriptor() method in `com.actelion.research.chem.descriptor.DescriptorHandlerPFP512` class, there seem to be an error during the translation from `java.util.BitSet` into an `int[]` array, where `i` and `j` variables appear to be switched in line 60 of `DescriptorHandlerPFP512.java` file, where:

```
if (bitset.get(32 * i + j))
```

should be:

```
if (bitset.get(32 * j + i))
```

Greetings.

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