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.DescriptorHandlerPFP51 2 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.