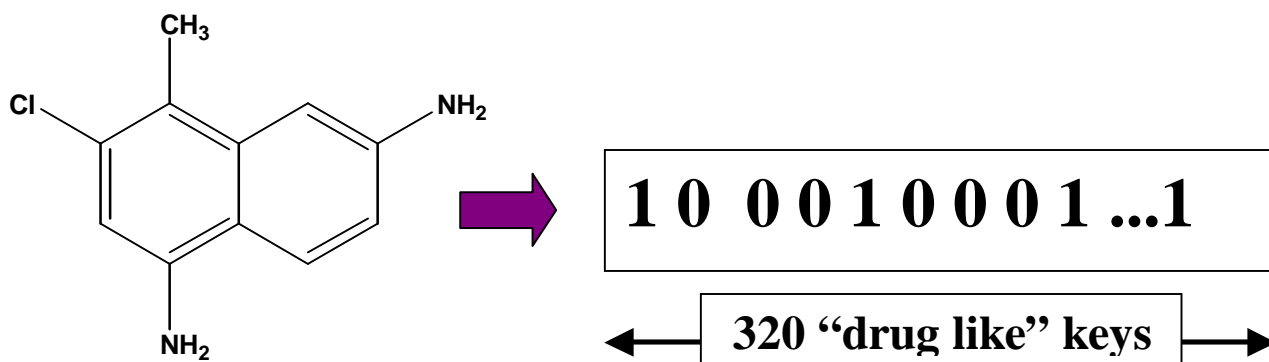


Fingerprint Module



The **Fingerprint Module** reads SMILES strings and creates 320 bit (or 164 of the 166 keys) structural Molecular Design Limited MACCS key representations. The 320 “drug like” keys have been published in “Reoptimization of MDL Keys for use in Drug Discovery”, JCICS, 42(6), 2002, 1273-1280. (Separate bit string analysis tool programs such as the Measures and ChemTattoo programs from the **Grouping Module** can be bundled with the Fingerprint Module. All programs are available as standalone programs or C++ library functions.

System Architecture: Linux Red Hat 7.x, Irix 6.5, Windows 2000

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