

MOLECULES THAT CAN BE SUCCESSFULLY CONSTRUCTED FROM THE GIVEN FRAGMENTS

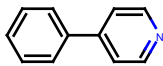
The drug molecules on the left can be successfully constructed by combining the fragments on the right. The fragments on the right are the smallest set of fragments that can achieve that from the given fragments. Therefore, instead of combining N carbons together to make a long chain of carbons, the longer alkyl chain fragments are preferred. The fragments on the right aren't the 'only' way to construct the molecule from the given fragments, just the first smallest set found (there could be other sets of fragments of equal size as well).

*** WARNING ***

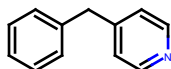
Bond orders are `_not_` taken into account because I just haven't got around to coding in the check to make sure the bond orders are the same. For example, a hydroxyl attached to a ring system is not differentiated from a double-bonded exocyclic carbonyl. Maybe it could be argued that this could be handled by tautomer enumeration instead? Thoughts?

Drug Smallest set of matching fragments

Covered

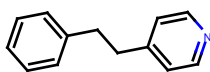


Covered



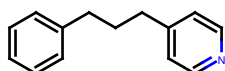
CH₄

Covered

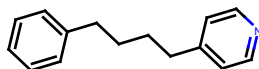


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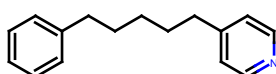
Covered



Covered

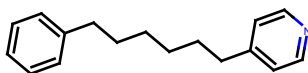


Covered



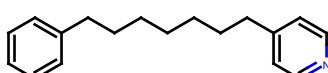
CH₄

Covered



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Covered

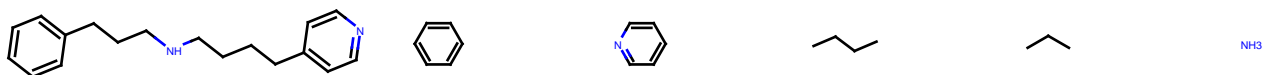


Drug Smallest set of matching fragments

Covered



Covered



Covered

