FIZ Search Service

FIZ Karlsruhe – Leibniz Institute for Information Infrastructure

Tips from FIZ Search Service

№ 2- Rethink your structure

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STNext®

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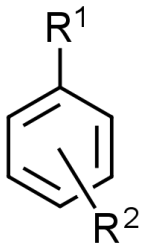
AMERICAN CHEMICAL SOCIETY

Typical structure search question

- Requested is a core structure with various substituents attached

Task: find all di-substituted benzene rings with the following formula:

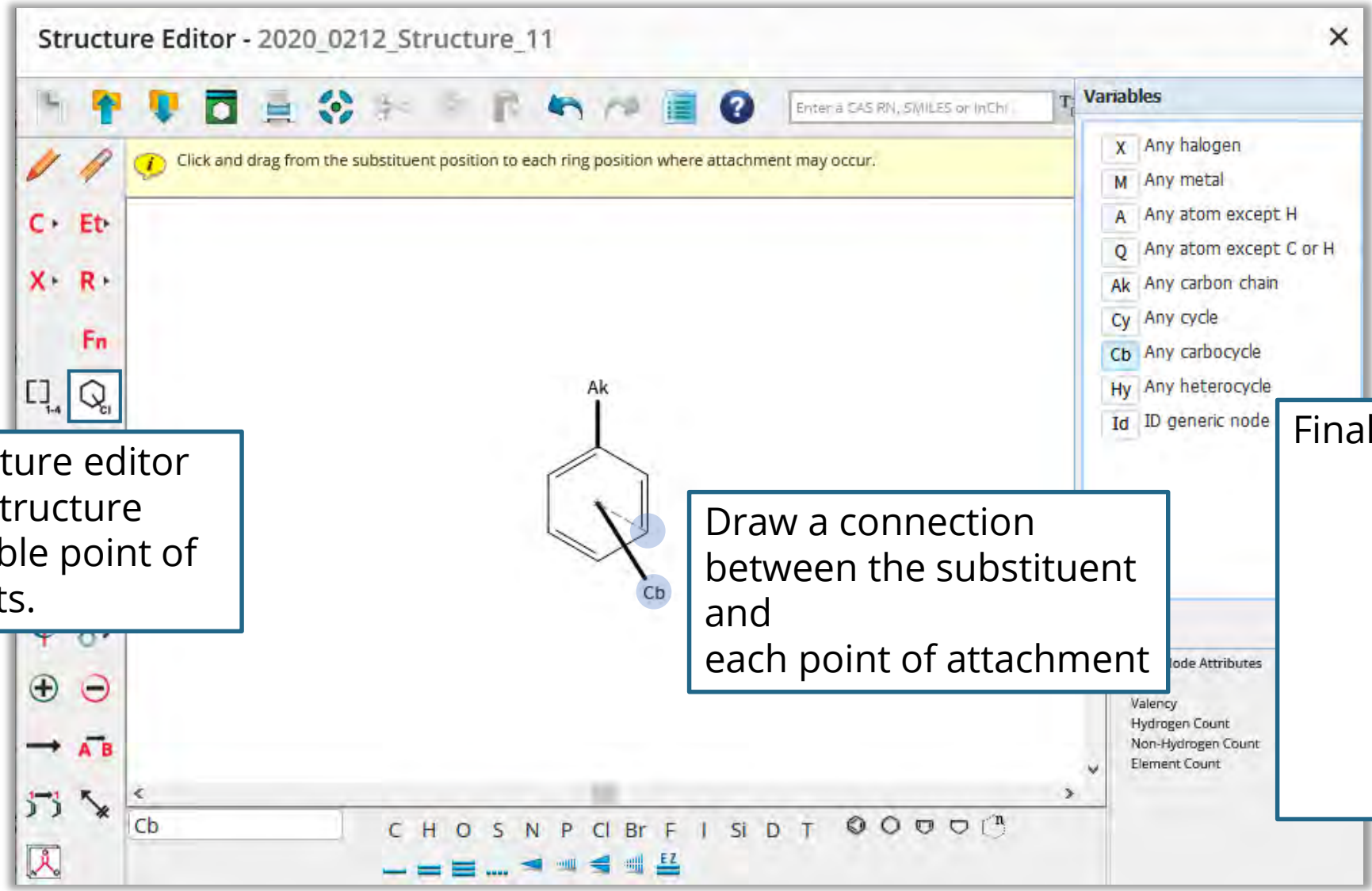


R^1 = carbon chain, opt. subst.
R^2 = $C_{3\text{-}10}$ carbocycle, opt. subst.

No further substitution at the benzene ring

- Our task is to transfer the requested structure into an STN compatible structure query
- Usually the resulting structure query looks similar to what the customer has specified
- But different approaches can be made for this request

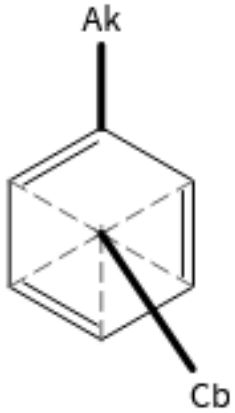
Approach 1 – variable point of attachment - SSS



Open structure editor and draw structure using variable point of attachments.

Draw a connection between the substituent and each point of attachment

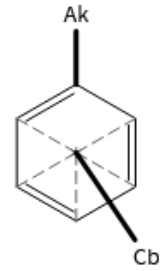
Final structure query:

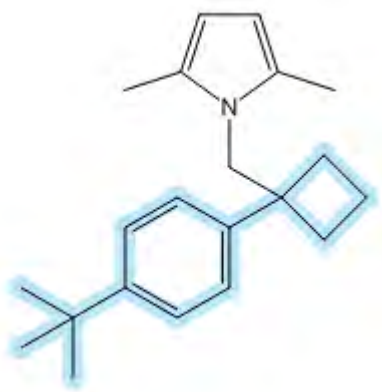


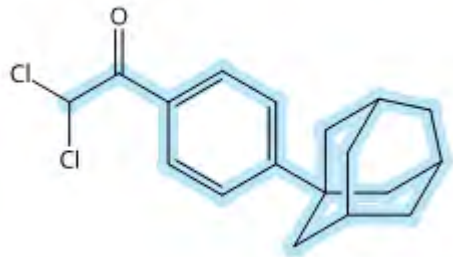
Approach 1 – variable point of attachment - SSS

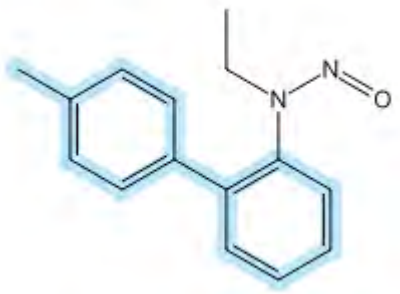
- A substructure search (SSS) will retrieve valid matches:

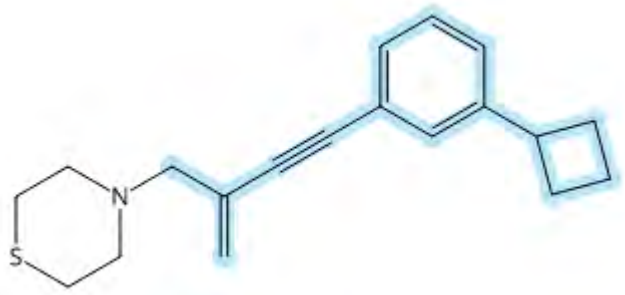
Query:
S L1 SSS FUL







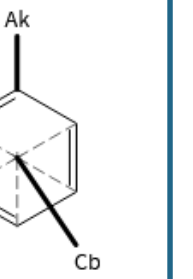


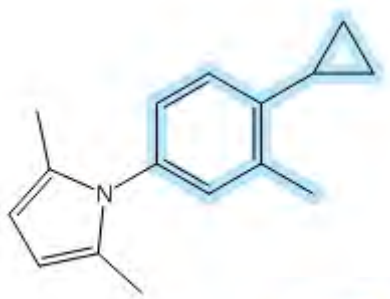


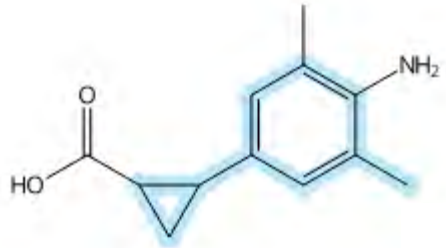
Approach 1 – variable point of attachment - SSS

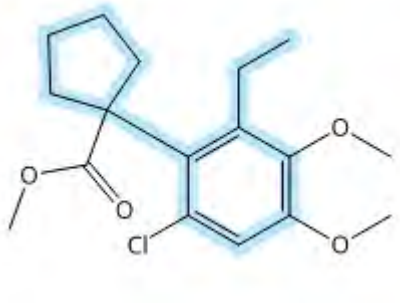
- But also unwanted hits with *more* than 2 substituents at the central benzene ring will be captured

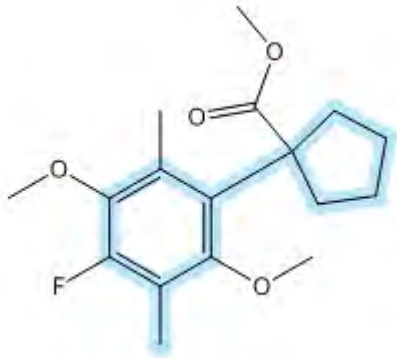
Query:
S L1 SSS FUL







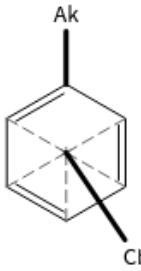


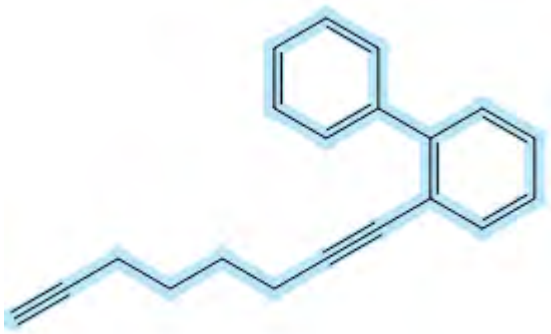


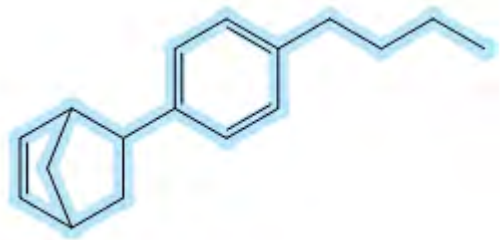
Approach 2 – variable point of attachment - CSS

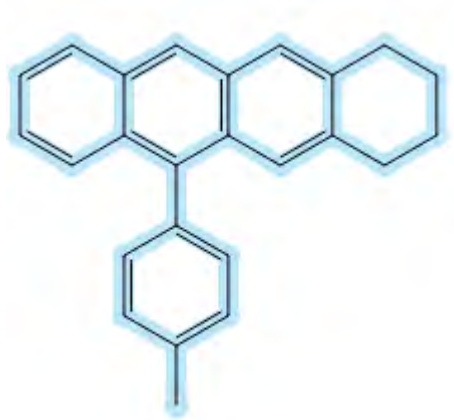
- Perform a Closed Substructure Search (CSS) using the same structure query
- Additional substitution at the benzene ring will be prevented ✓
- Also further substitution at the substituents is prevented ✗
  - „Alkyl“ will only retrieve *unsubstituted* carbon chains
  - „carbocycle“ will only retrieve *unsubstituted* rings

Query:
S L1 **CSS** FUL



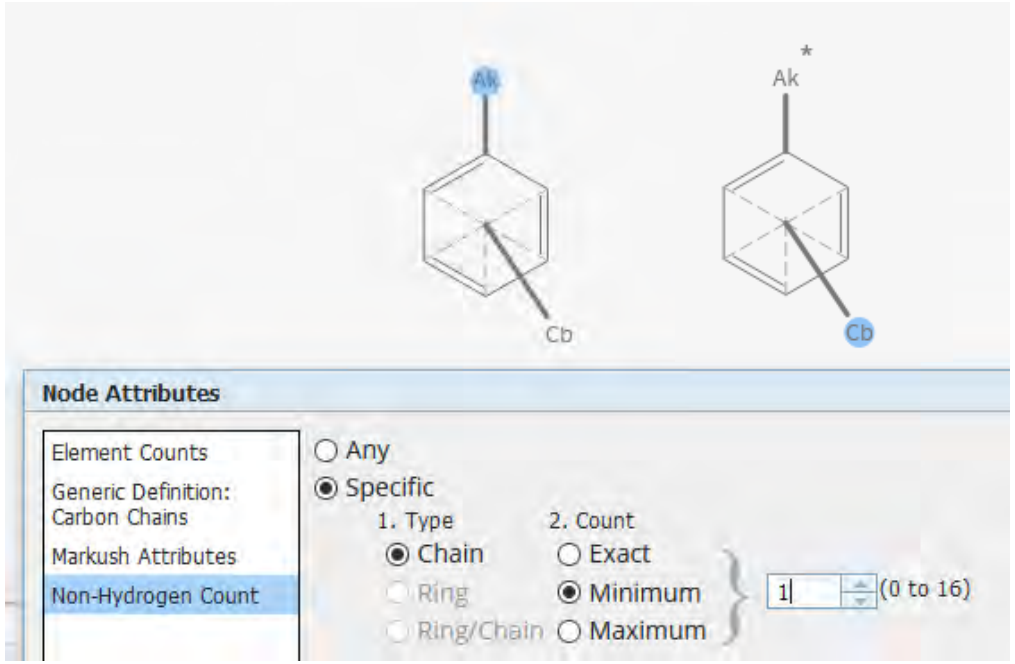


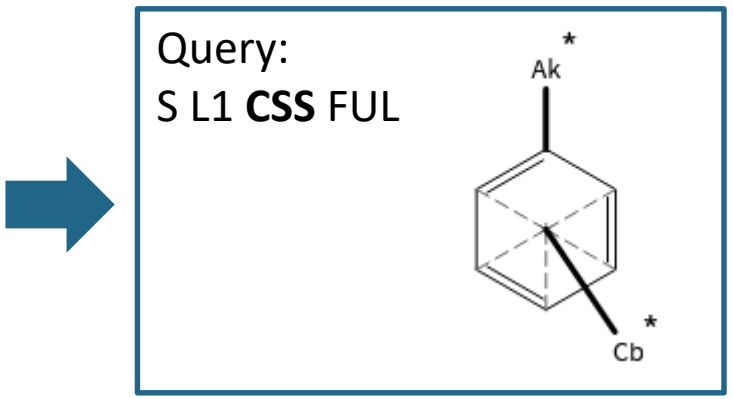


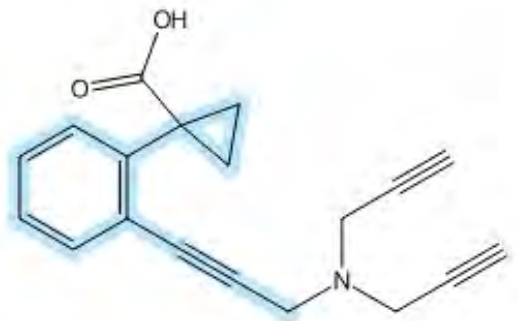


Approach 2 – variable point of attachment - CSS

- Structure query has to be adjusted
- Allow further substitution at Ak and Cb node by defining *non-H attachments*
  - Advanced structure control tool
  - In this simple example this is a good strategy
  - For larger structures it may be more effort to care for all nodes which have to be opened

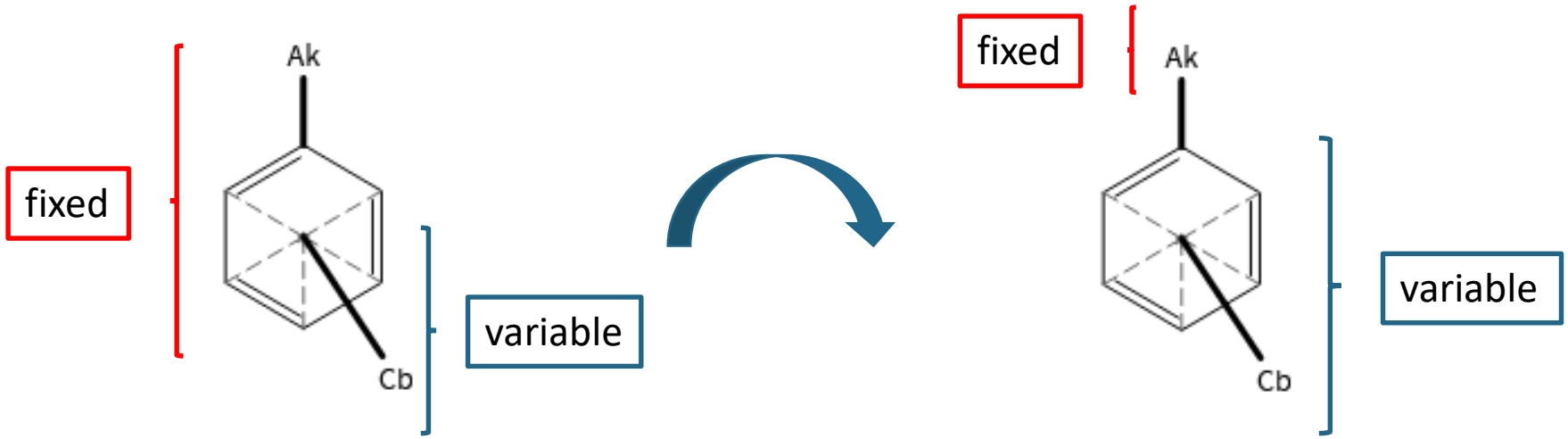






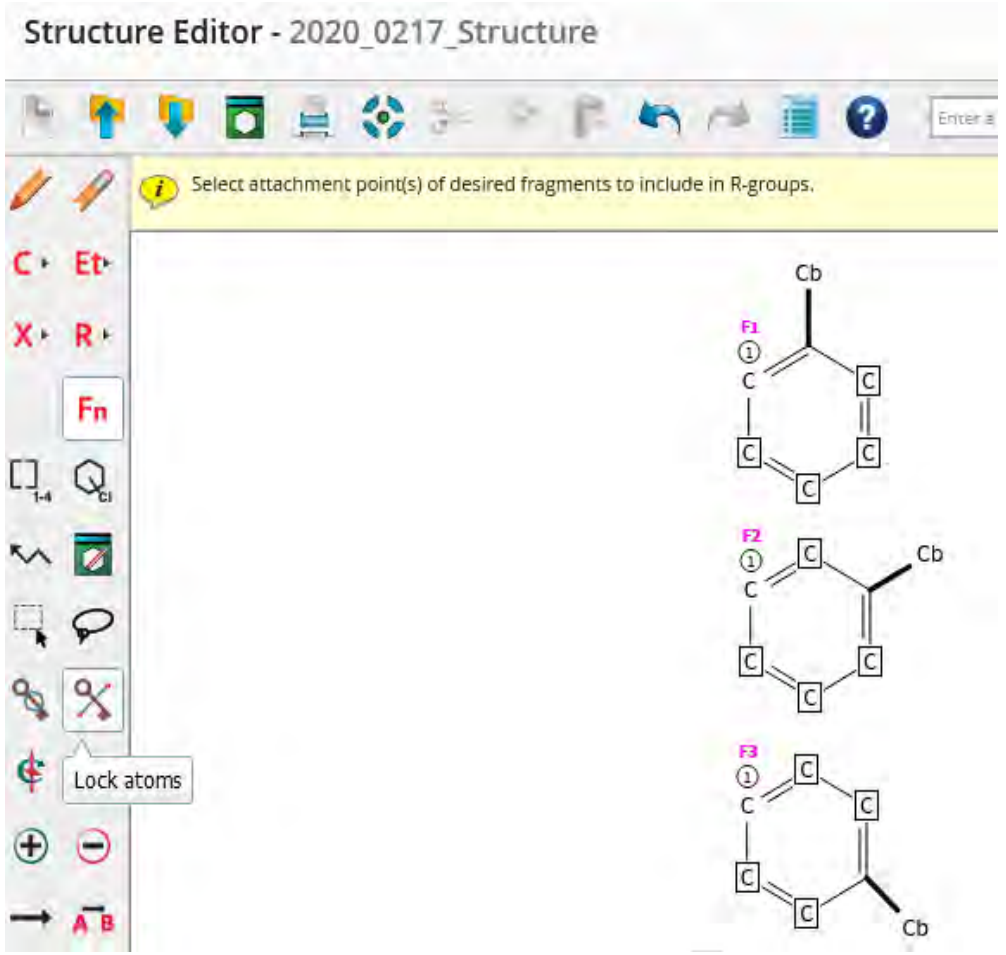
Approach 3 – change the perspective

- Find a fix node in the structure and shift the „search focus“
- Move from the central ring to the substituent



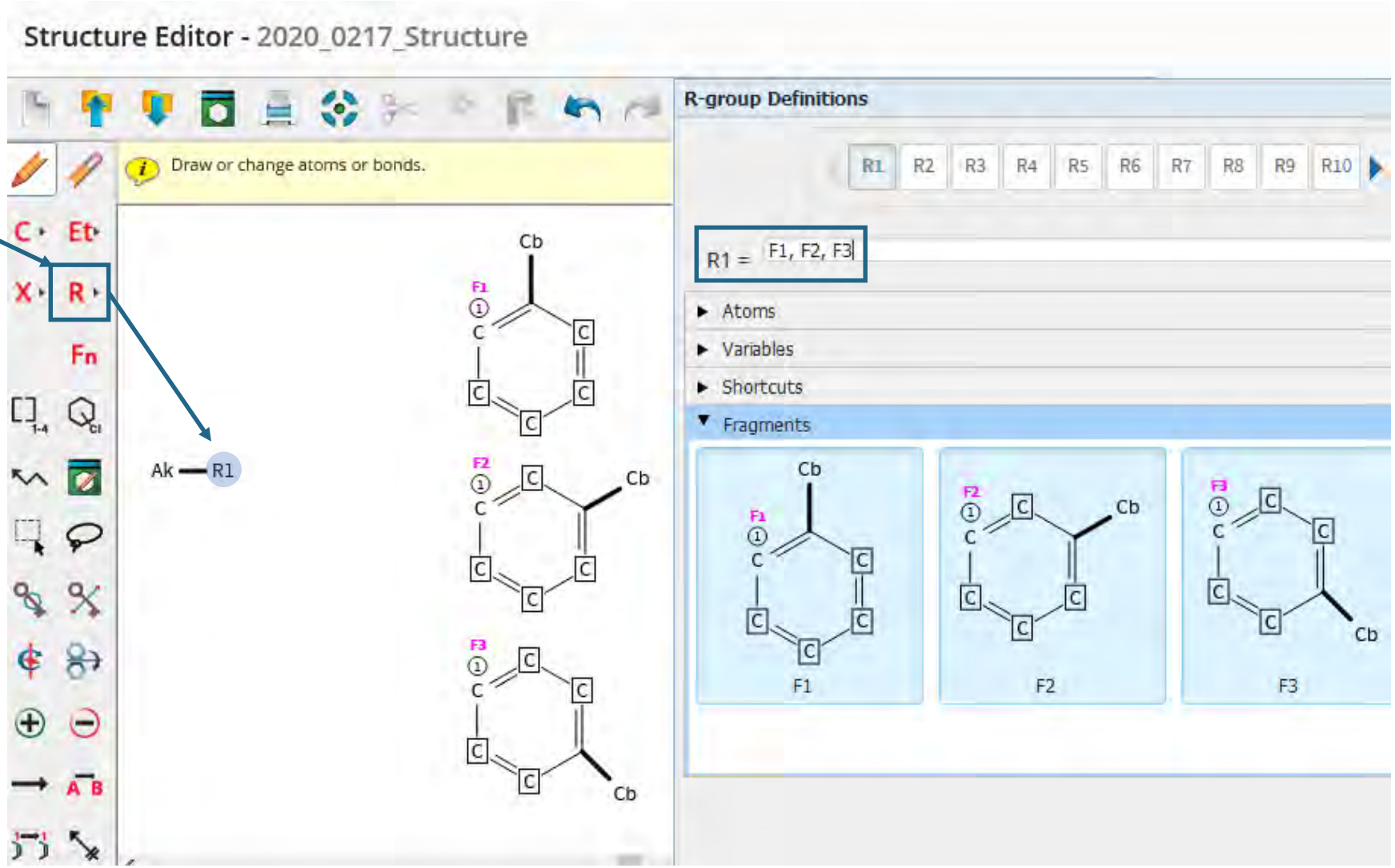
Approach 3 – change the perspective

- Use fragments for the definition of the variable part
- Define fragments Fn with the requested substitution pattern
  - Ortho, meta and para position
- Lock all other positions at the benzene ring
  - Alternative: non-H attachments on exact 2 ring/chain



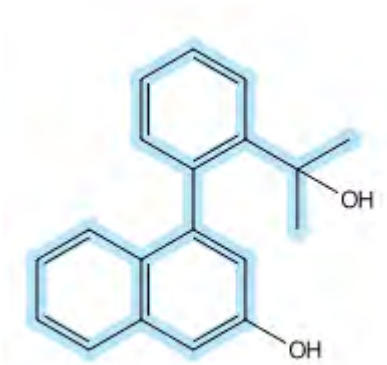
Approach 3 – change the perspective

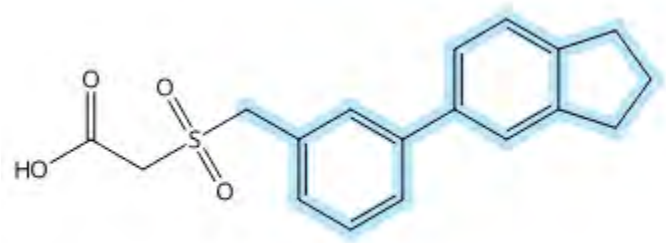
Group the fragments into an R-group



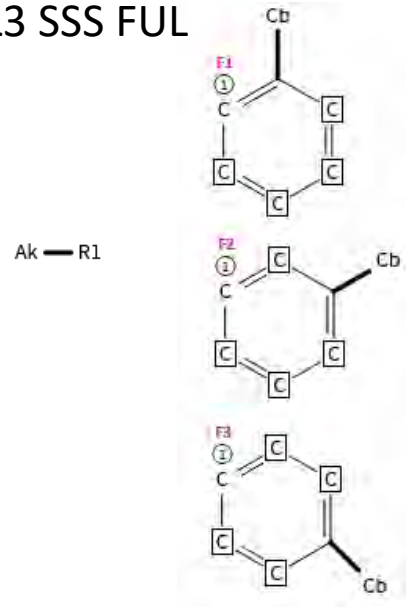
Approach 3 – change the perspective

- Only di-substituted benzene rings are retrieved
- Substitution on Ak and Cb is allowed





Query:
S L3 SSS FUL



Comparison of strategies

- Approach 1: VPA and SSS
  - Broadest strategy
  - Retrieves a lot of unwanted answers (tri- and more substituted)
- Approach 2: VPA and CSS
  - Exact matches
  - Remember to open all nodes which allow substitution
  - Be familiar with non-H attachments
- Approach 3: Fragments/R-groups and SSS
  - Exact matches
  - Change perspective
  - Be familiar with drawing fragments

Approach 2 and 3 are equivalent for the results

FIZ Search Service Team

- Scientists with several years of search experience
- We offer all kinds of patent and literature searches on STN
- Structure searches in REGISTRY/CAPLUS, MARPAT, DCR/DWPI and DWPIM/DWPI

Thank you for your attention and have a nice day!

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