Biomolecule Uniqueness Check Using HELM and Hashcode

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Scilligence

Scilligence's Uniqueness Check

- **Scilligence's cartridge supports both small molecules and biomolecules**
- **Uniqueness check uses a proprietary Hashcode approach**
  - Similar to InChIKey
  - For both small and biomolecules
- **Leading support in HELM for biomolecules**

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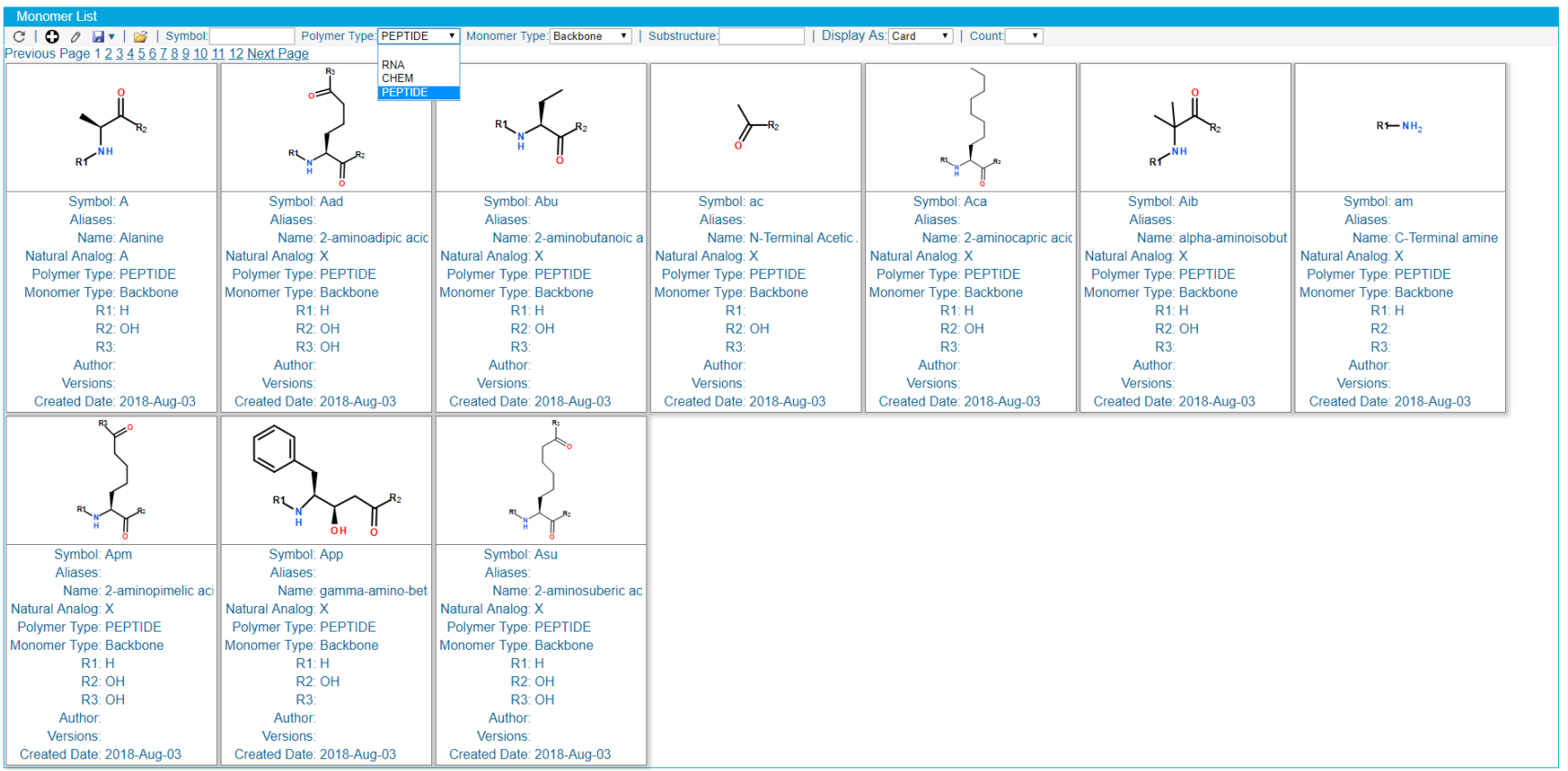
HELM Monomer Library Management



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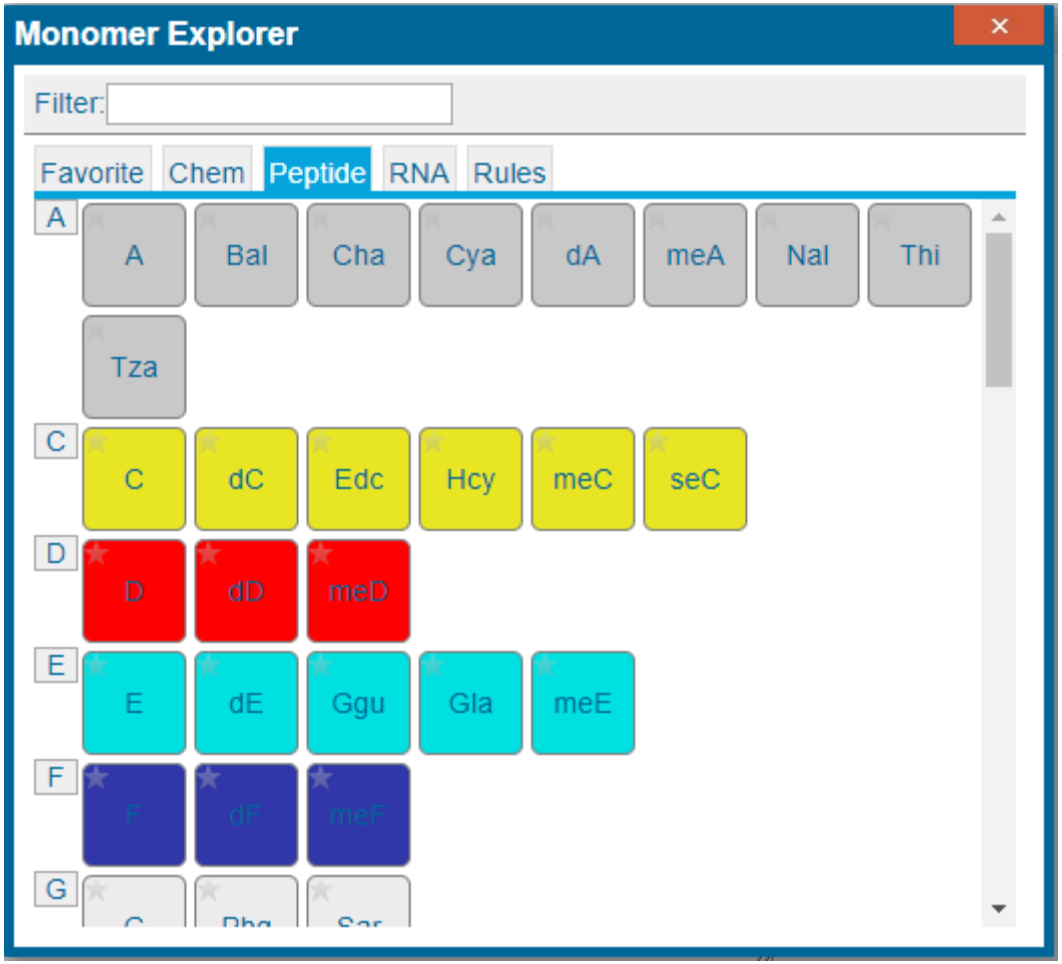
HELM Sketcher: Monomer Selection



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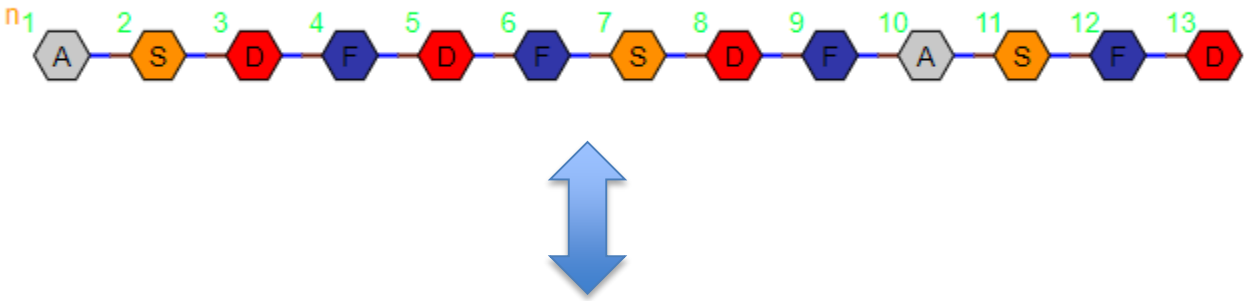
HELM Sketcher: HELM Structure/String Conversion



PEPTIDE1{A.S.D.F.D.F.S.D.F.A.S.F.D}$$$$V2.0

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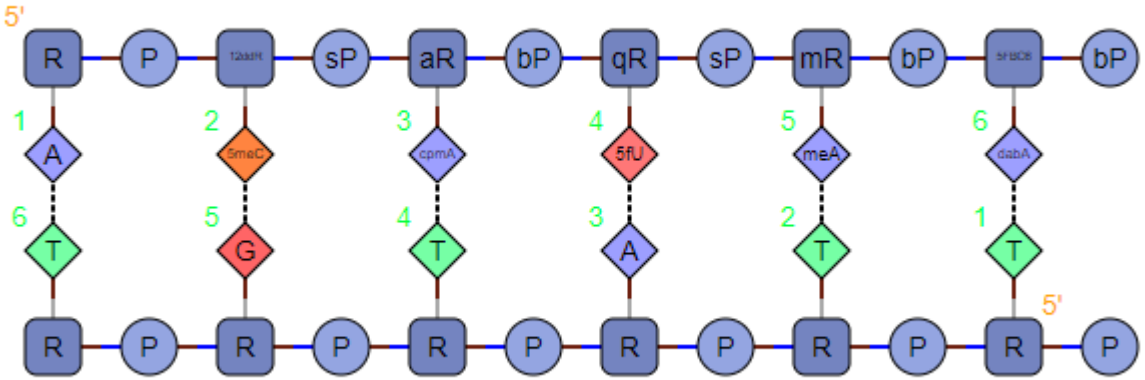
HELM Sketcher: RNA Complementary Strand



RNA1{R(A)P.[12ddR]([5meC])[sP].[aR]([cpmA])[bP].[qR]([5fU])[sP].[mR]([meA])[bP].[5FBC6]([dabA])[bP]}$$$$V2.0

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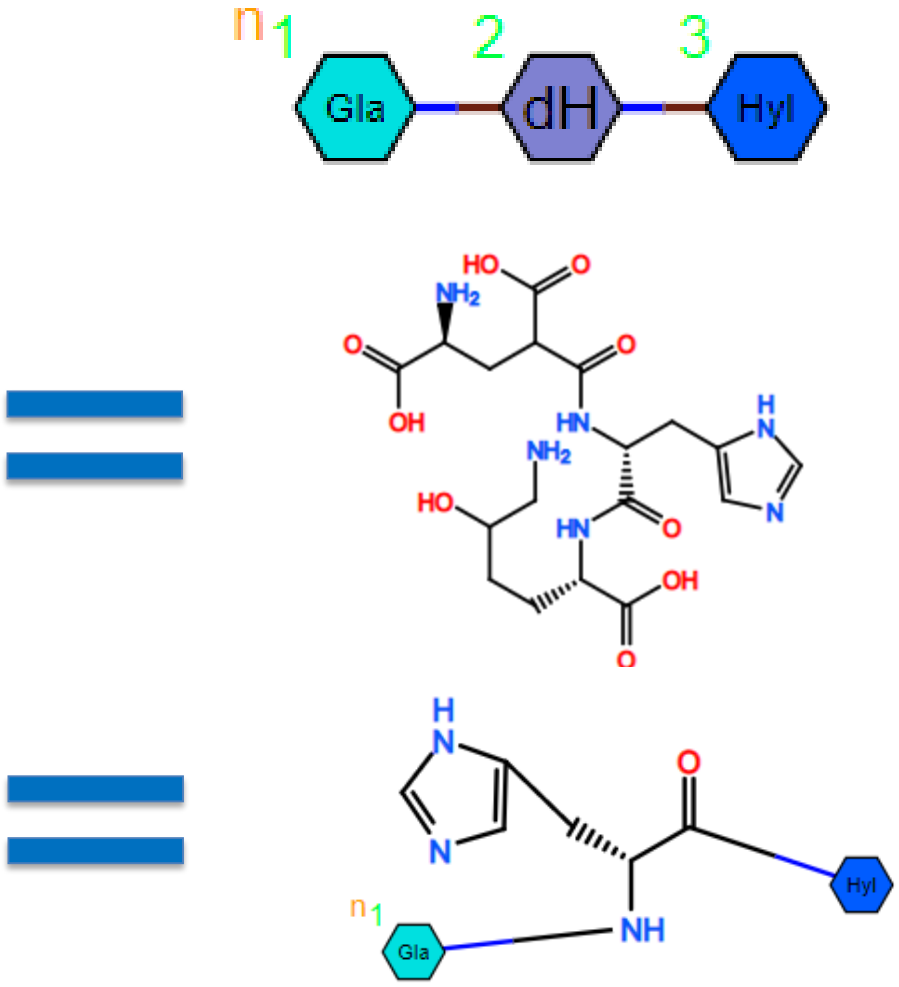
Backend: Scilligence's Uniqueness Check



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However ….

Expanding is not always practical

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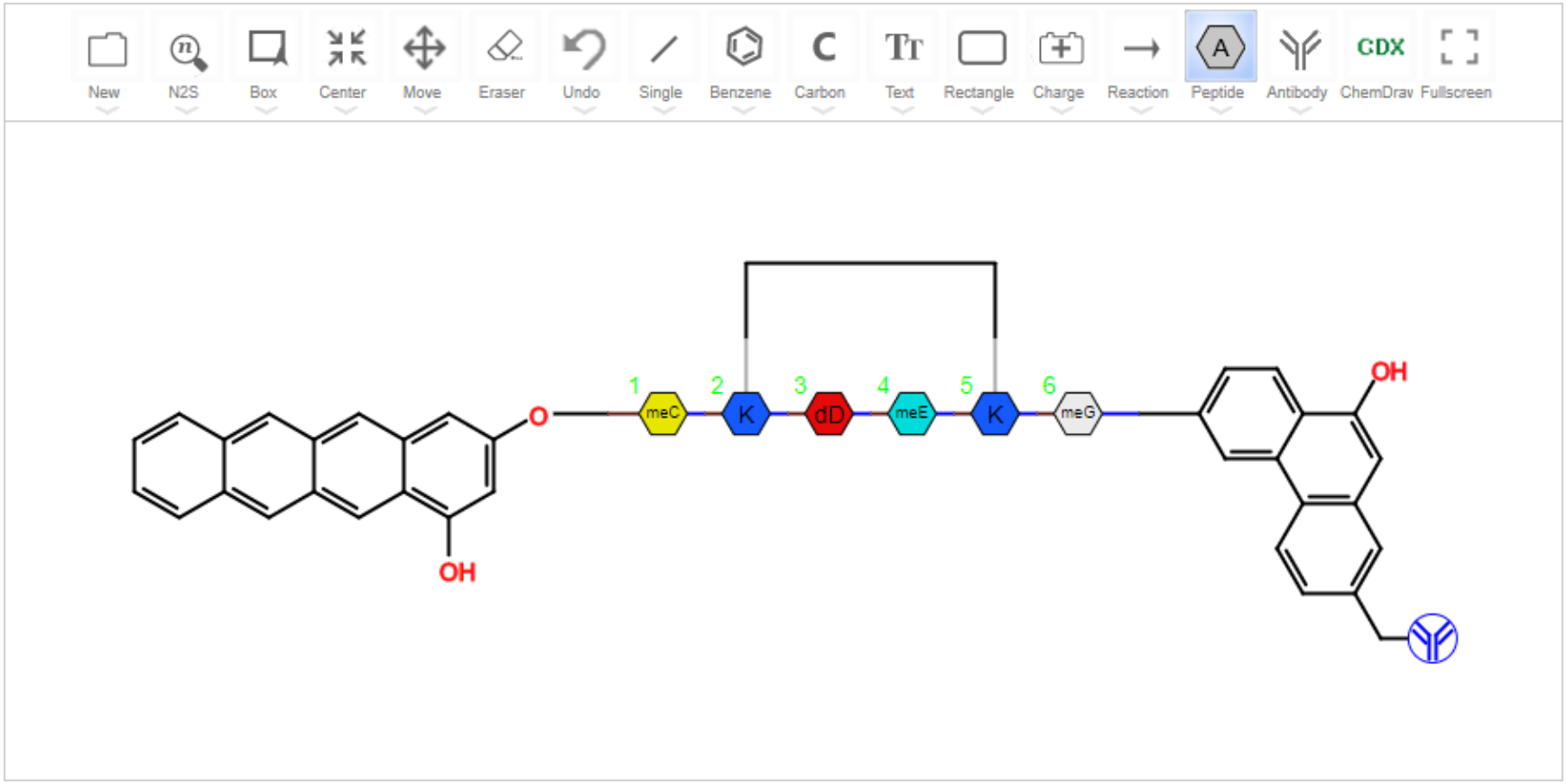
HELM Sketcher: Hybrid of Entities (Mixed Mode)



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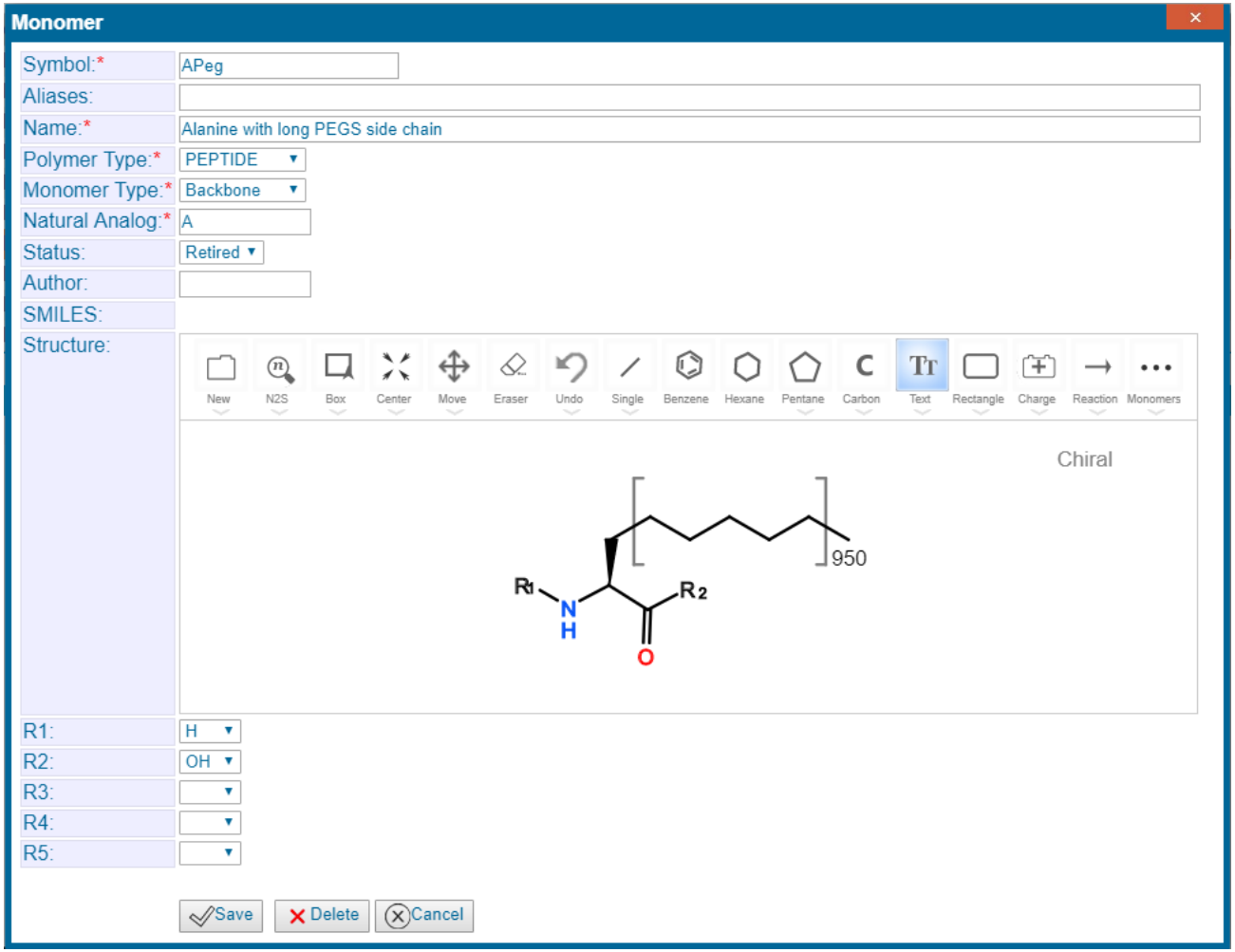
PEGS Monomer



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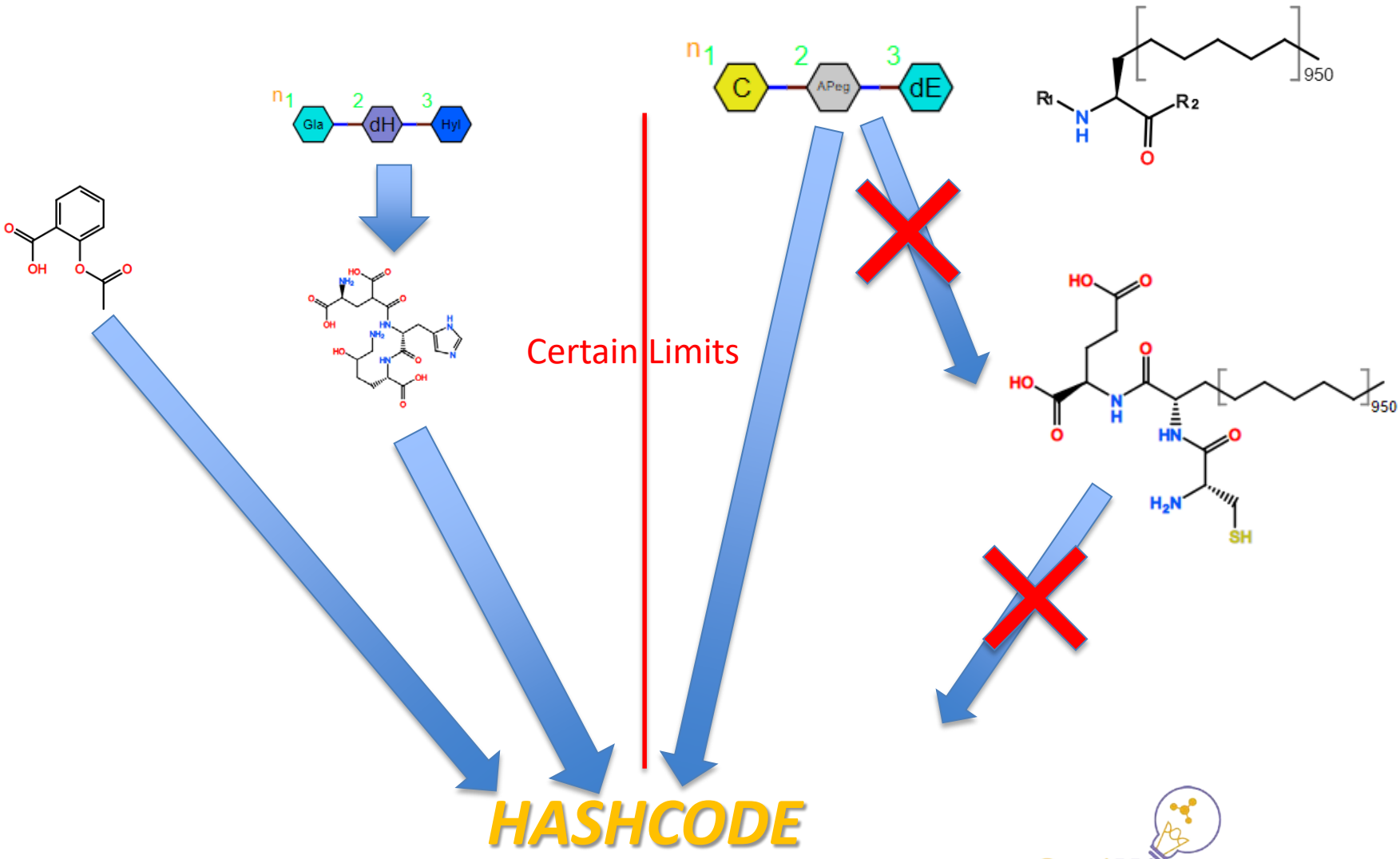
When to Hash??



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Pros vs. Cons

- **Pros**
  - Works for most common biopolymers
  - Balance between accuracy and performances
  - “Limit” configurable

- **Cons**
  - Monomer library dependent
  - Modifying monomer structures will change the HashCode

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Thank You!

www.scilligence.com

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