

# Monomer.org - A Scientific Community Platform for Sharing HELM Monomer Libraries and Translating HELM Macromolecules

Jinbo Lee, Chief Scientific Officer, Scilligence Corporation

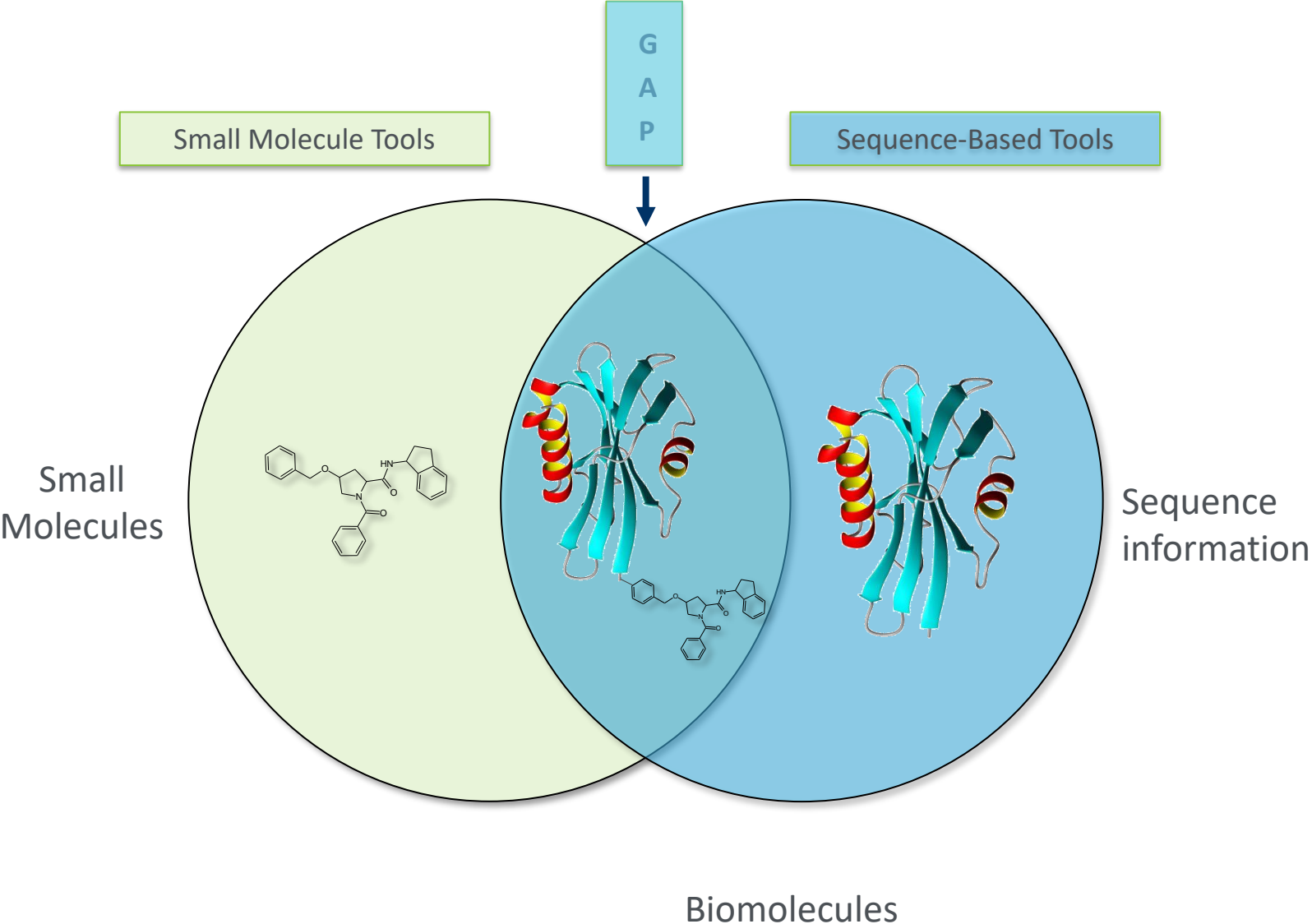


# »»» Agenda

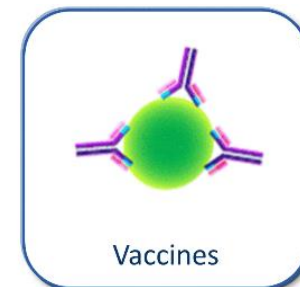
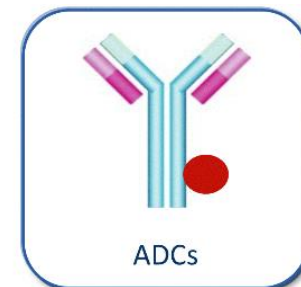
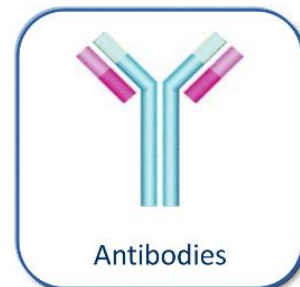
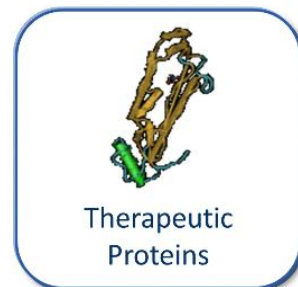
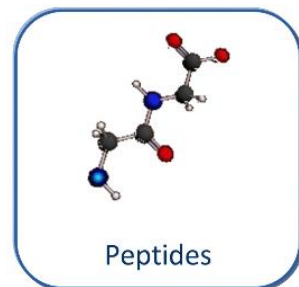
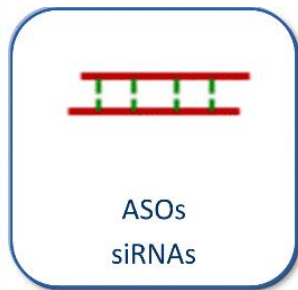
- What's HELM?
- Barriers for HELM Implementation
- History of HELM Technology Development
- Development of monomer.org



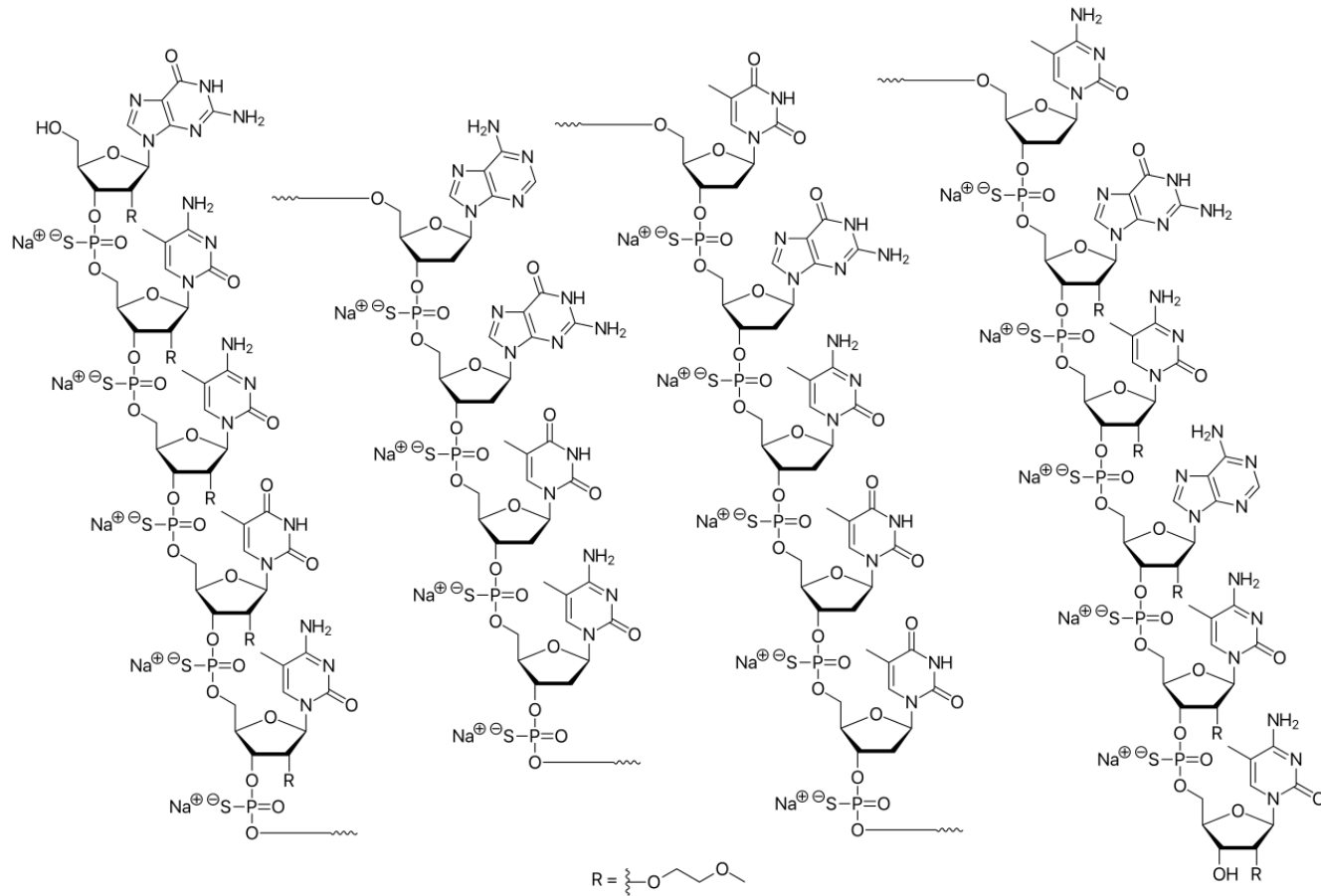
# Macromolecules – A Challenging Middle Ground



# HELM Supported Modalities

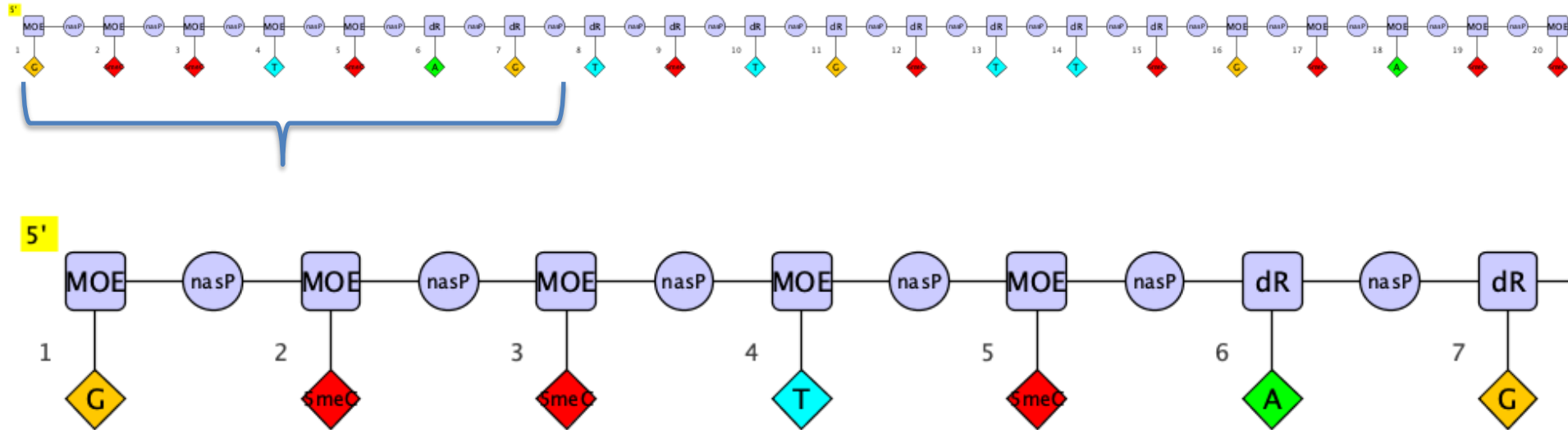


# »» Mipomersen – Atom-Bond Representation



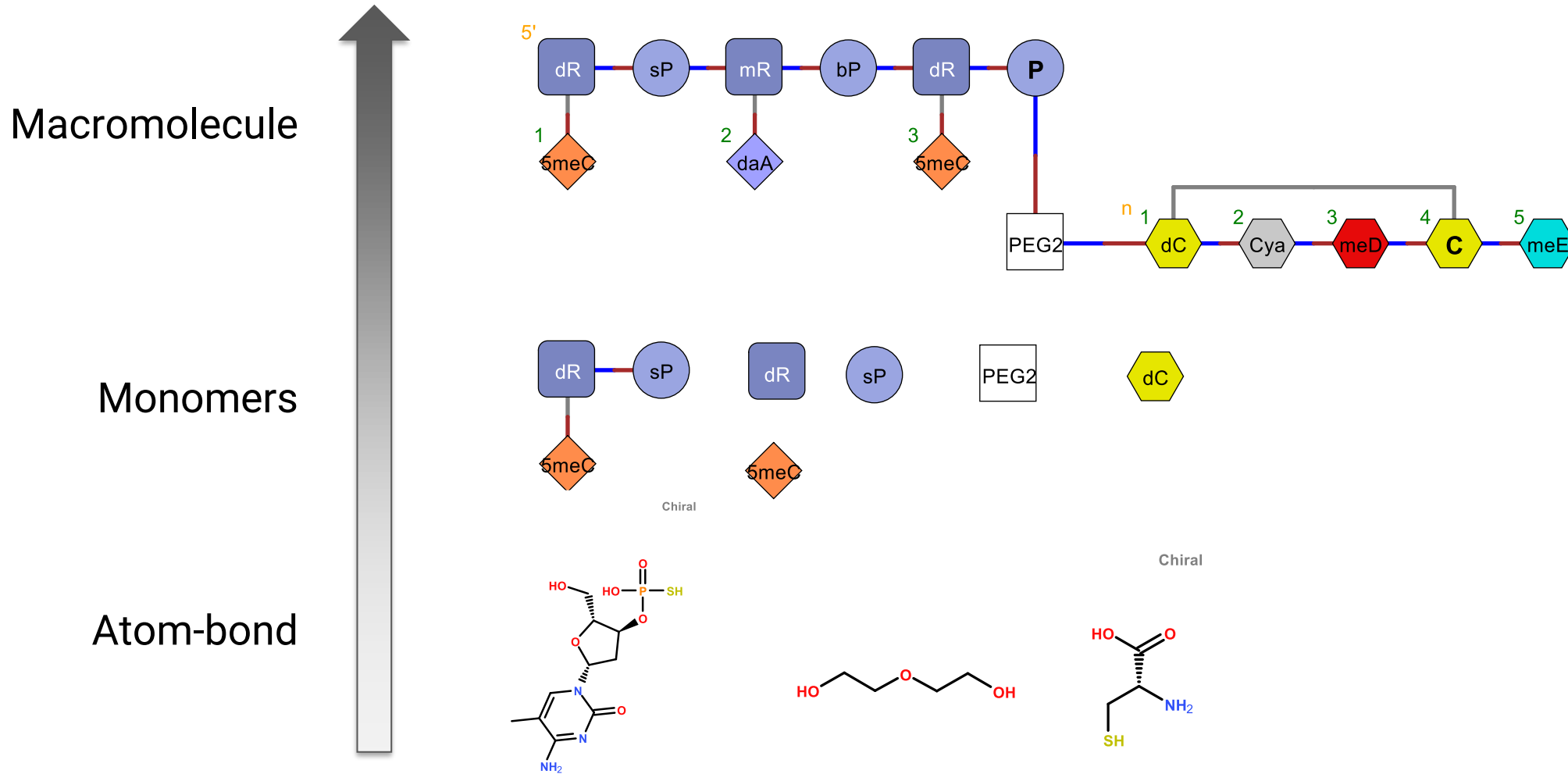
- ❑ Make chemists dizzy
- ❑ Make biologists look away

# »»» Mipomersen – HELM Representation



RNA1{[MOE](G)[nasP].[MOE]([5meC])[nasP].[MOE]([5meC])[nasP].[MOE](T)[nasP].[MOE]([5meC])[nasP].[dR](A)[nasP].  
 [dR](G)[nasP].[dR](T)[nasP].[dR]([5meC])[nasP].[dR](T)[nasP].[dR](G)[nasP].[dR]([5meC])[nasP].[dR](T)[nasP].  
 [dR](T)[nasP].[dR]([5meC])[nasP].[MOE](G)[nasP].[MOE]([5meC])[nasP].[MOE](A)[nasP].[MOE]([5meC])[nasP].  
 [MOE]([5meC]))\$\$\$\$

# »» Hierarchical Editing Language for Macromolecules







# »»» What Do You Need for HELM Implementation?

## ❑ A database system

- Manage and store monomer library
- Store HELM strings
- Interpret HELM strings

## ❑ A UI

- Input HELM
- View HELM structure, HELM string, atom-bond structure, sequence
- View calculated properties

# »» Barriers

## ❑ Set up database

- Need IT resources
- Need informatics expertise
- Cost for hardware and system software

## ❑ UI

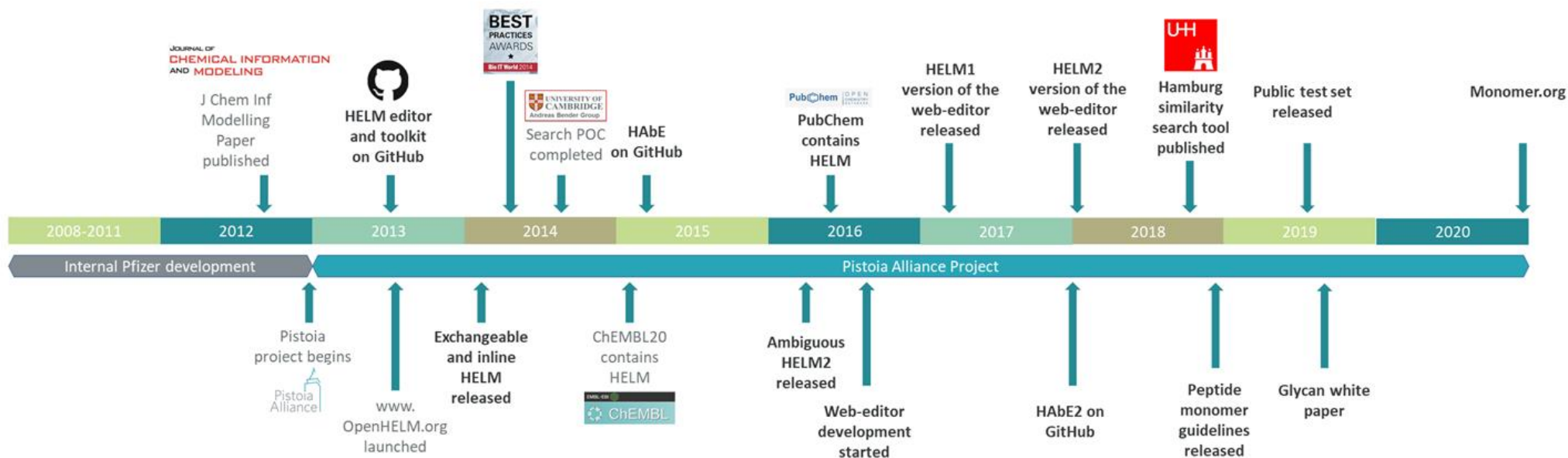
- Thick-client UI historically
- Difficult to deploy and update

## ❑ Monomer libraries

- Need well-curated monomer libraries and syntax for monomers
- Need intuitive platform for managing monomer libraries

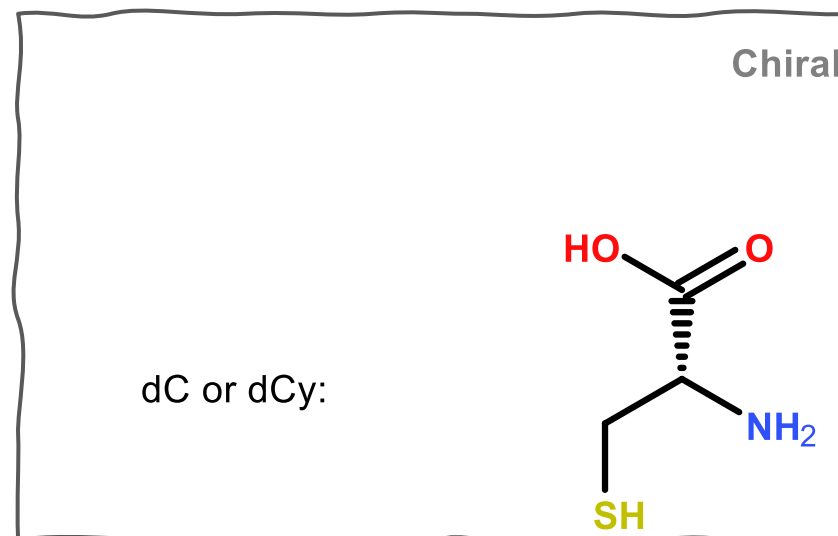


# HELM History



## »» I Can't Understand You

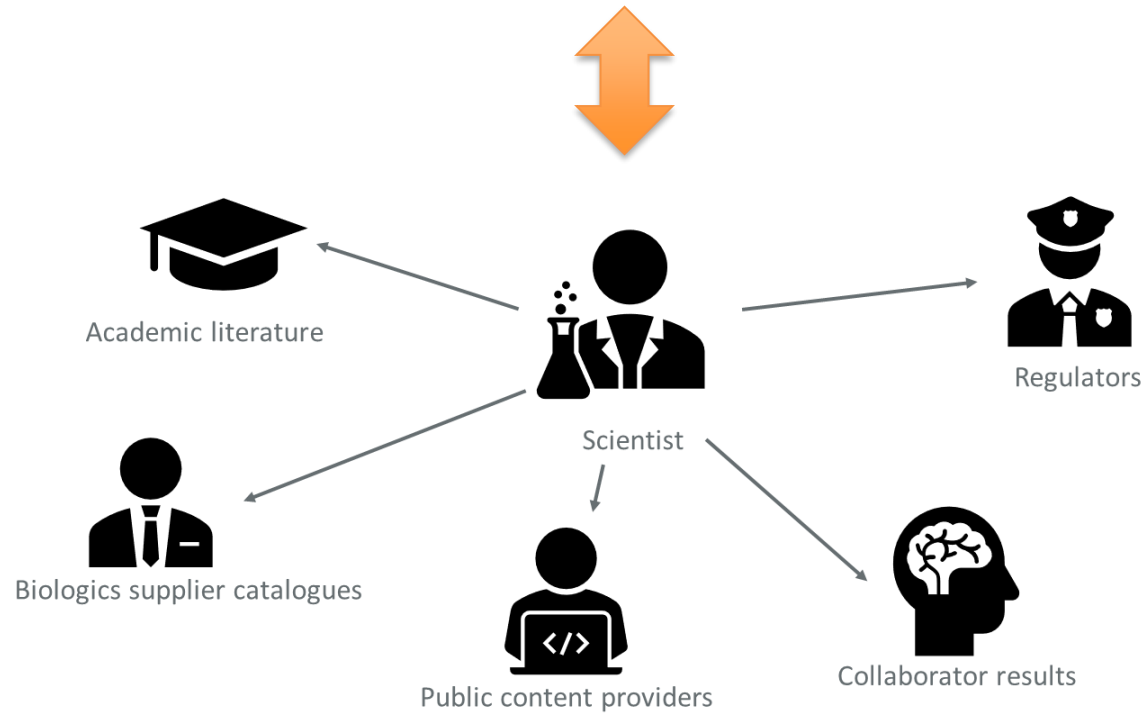
- ❑ Each company has its own system
  - Different monomer libraries
  - Different codon could mean the same monomer
  - Same codon could mean different monomers
- ❑ I can't interpret your HELM string
  - Unless I have access to your monomer library



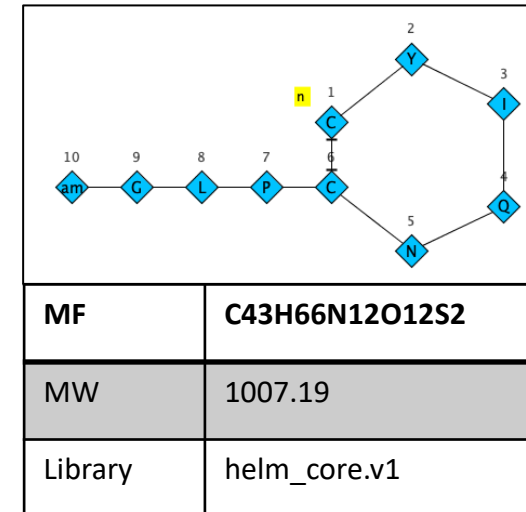


# monomer.org – A Universal Interpreter

monomer.org



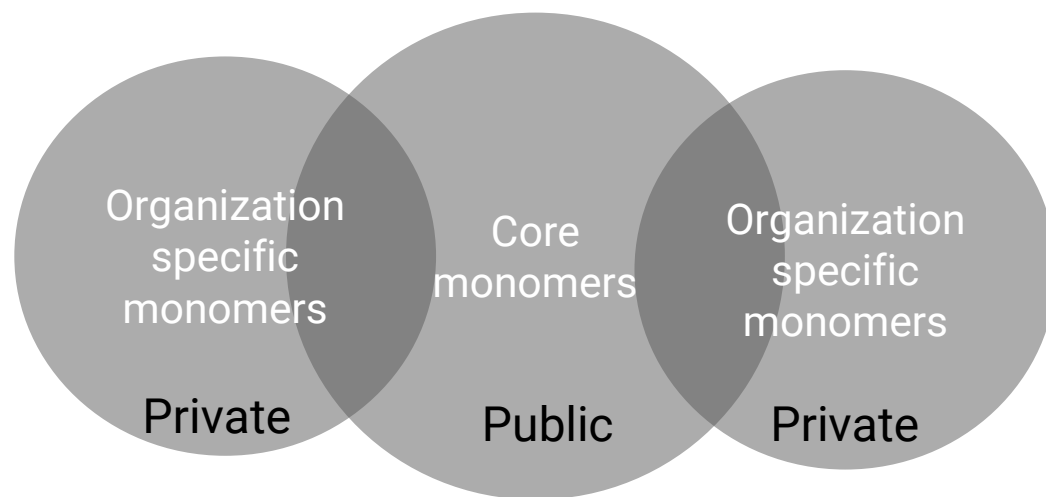
```
PEPTIDE1{C.Y.I.Q.N.C.P.L.G.[am]]}$  
PEPTIDE1,PEPTIDE1,1:R3-6:R3$$$
```



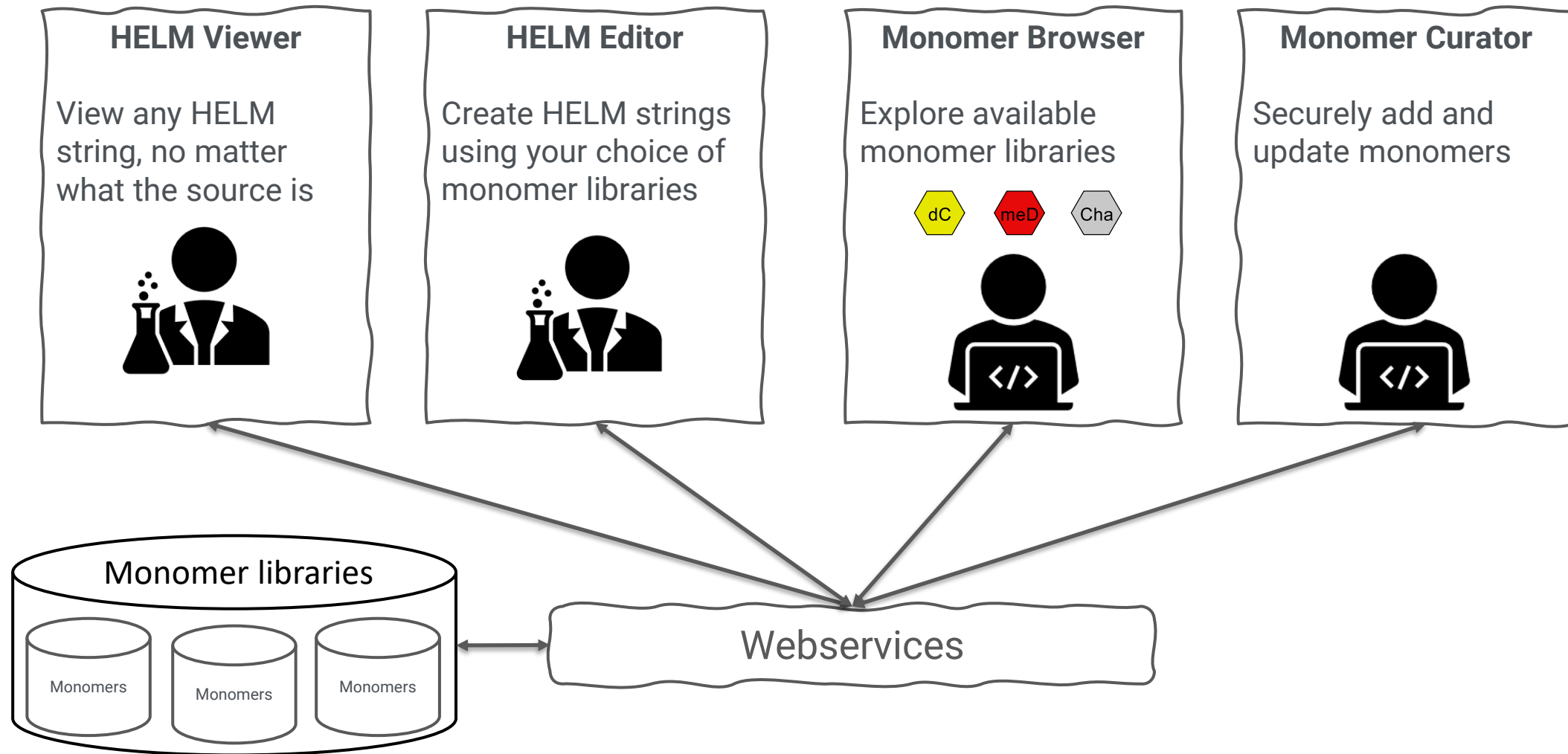


## »» Monomer.org – Dictionary of Monomer Libraries

- ❑ A standard, well-curated, core monomer set for scientific community
- ❑ A hosting service for organizations to manage their monomer libraries
- ❑ Versioning of monomer libraries for backward compatibility
- ❑ Monomer libraries can be designated as public or private



# Monomer.org – A Cloud Platform for Scientific Community



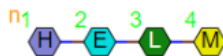
# Monomer.org

The home of HELM monomers

PEPTIDE1{H.E.L.M}\$\$\$

demokey\_1

Parse



Molecular Weight: 527.6129

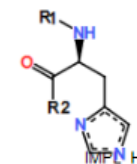
Molecular Formula C22H35N6O7S

Published Monomers												
In Version:	Symbol:	Natural Analog:	Name:	Polymer Type:	Monomer Type:	Status:	Created:	Modified:				
Library Name	Symbol	Natural Analog	Name	Polymer Type	Monomer Type	Status	R1	R2	R3	Author	Created	Modified
<input type="checkbox"/>	Demo	A	A	Alanine	PEPTIDE	Backbone	Active	H	OH		2021-Mar-28	2021-Mar-28
<input type="checkbox"/>	Demo	C	C	Cysteine	PEPTIDE	Backbone	Active	H	OH	H	2021-Mar-28	2021-Mar-28
<input type="checkbox"/>	Demo	D	D	Aspartic acid	PEPTIDE	Backbone	Active	H	OH	OH	2021-Mar-28	2021-Mar-28
<input type="checkbox"/>	Demo	E	E	Glutamic acid	PEPTIDE	Backbone	Active	H	OH	OH	2021-Mar-28	2021-Mar-28
<input type="checkbox"/>	Demo	F	F	Phenylalanine	PEPTIDE	Backbone	Active	H	OH		2021-Mar-28	2021-Mar-28
<input type="checkbox"/>	Demo	G	G	Glycine	PEPTIDE	Backbone	Active	H	OH		2021-Mar-28	2021-Mar-28
<input checked="" type="checkbox"/>	Demo	H	H	Histidine	PEPTIDE	Backbone	Active	H	OH		2021-Mar-28	2021-Mar-28
<input type="checkbox"/>	Demo	I	I	Isoleucine	PEPTIDE	Backbone	Active	H	OH		2021-Mar-28	2021-Mar-28
<input type="checkbox"/>	Demo	K	K	Lysine	PEPTIDE	Backbone	Active	H	OH	H	2021-Mar-28	2021-Mar-28
<input type="checkbox"/>	Demo	L	L	Leucine	PEPTIDE	Backbone	Active	H	OH		2021-Mar-28	2021-Mar-28

Details Log

In Version: 1  
Library Name: Demo  
Structure:\*

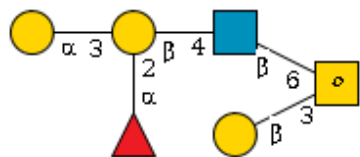
Chiral



SMILES: [H:1]N[C@@H]([Cc1cnc[nH]1])C([OH:2])=O  
Symbol: H  
Natural Analog: H  
Name: Histidine  
Polymer Type: PEPTIDE  
Monomer Type: Backbone  
Status: Active  
R1: H  
R2: OH

## »» HELM is Extendable

- Extendable to support polysaccharides



- Extendable to support chemical polymers

Presenter: Jonathan Buttrick

PAPER ID: 3556674

PAPER TITLE: "Adapting HELM technology for use with chemical polymers"

DIVISION/COMMITTEE: CINF

# »» Acknowledgement

## Pistoia HELM Team

Claire Bellamy, Pistoia  
Tianhong Zhang, Pfizer  
Sergio Rotstein , Pfizer  
Jeff Milton, Ionis

## Scilligence Team

Tony Yuan  
Elrashid Elzein  
Scotty Blechman  
Chris Ruggles