JSDraw

Unified Sketcher
For Small Molecules and Macromolecules

Jinbo Lee, PhD
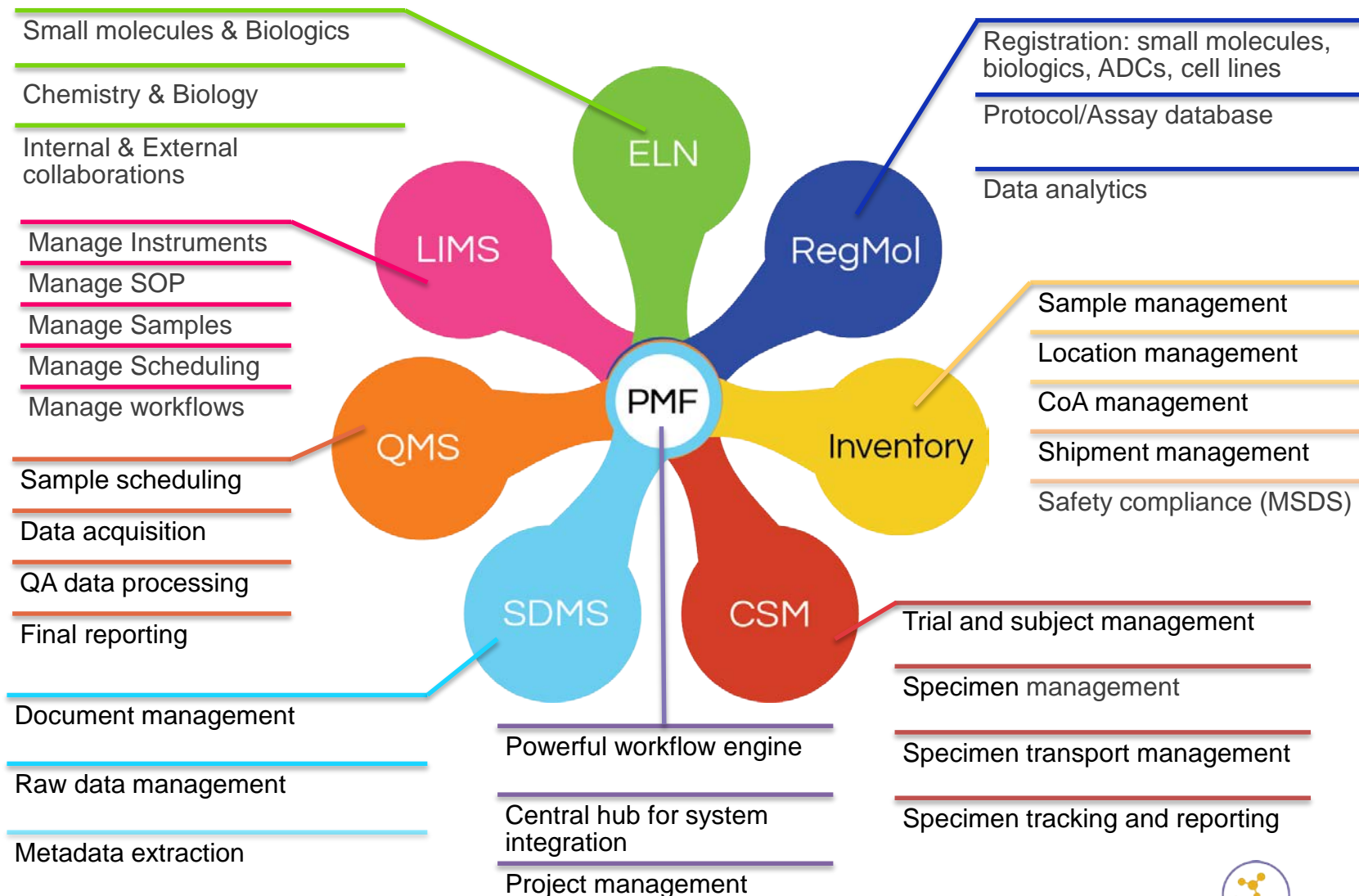Chief Scientific Office, Scilligence Corp.

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Outline

- Overview of Scilligence Informatics Solutions
- The building blocks of Scilligence Informatics Solutions
- Why do we need a new structure sketcher/editor?
- JSDraw - A unified sketcher for both small molecules & macromolecules
- What's HELM and why do we need that?
- HELM Web Editor is based on JSDraw

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Company Overview

- **Boston Based and Founded in 2010**
- **ISO9001:2015 and ISO27001:2013 certified**
- **Informatics for Data Driven Discovery**
  - Web-based and no Java-dependency
  - A single platform bridging small molecules and biologics
  - Fully supports HELM Notation
  - Collaboration, workflow, and project management
  - Powerful components for data mining and analytics
- **Broad Customer Base**
  - Pharma, Biotech, and Chemical companies
  - Government Agencies
  - Universities, Hospitals, and Institutes

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Workflow Driven Integrated Platform

Small molecules & Biologics

Chemistry & Biology

Internal & External collaborations

Registration: small molecules, biologics, ADCs, cell lines

Protocol/Assay database

Data analytics

ELN

RegMol

Manage Instruments

Manage SOP

Manage Samples

Manage Scheduling

Manage workflows

LIMS

Sample management

Location management

CoA management

Shipment management

Safety compliance (MSDS)

PMF

Inventory

Sample scheduling

Data acquisition

QA data processing

Final reporting

QMS

Document management

Raw data management

Metadata extraction

SDMS

CSM

Trial and subject management

Specimen management

Specimen transport management

Specimen tracking and reporting

Powerful workflow engine

Central hub for system integration

Project management

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Data Mining and Analytics

R-group Decomposition

SAR visualization

Gap analysis

Chrawler

SAR Analyzer

Chem4SharePoint

TouchMol4Office

Unstructured Data

Network drive

Documentum

Database

SharePoint
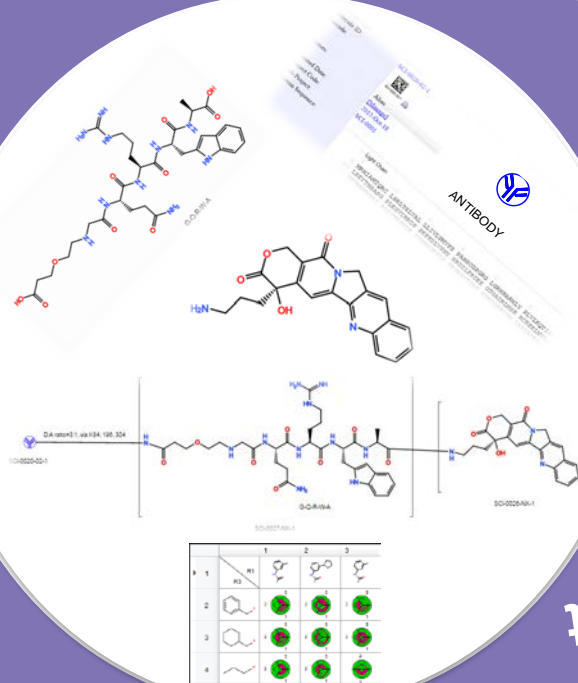
Small Molecules & Biologics

Input

View

Search

Cheminformatics inside Office

Informatics for Biologics & ADCs

Interface with databases

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Building Blocks for Scilligence Solutions

- **MolSQL (Database Tier)**
  - Unified cartridge for small molecules and macromolecules

- **MolEngine (Middle Tier)**
  - Unified .NET toolkit for cheminformatics and bioinformatics

- **JSDraw (Client)**
  - Unified sketcher for small molecules and macromolecules
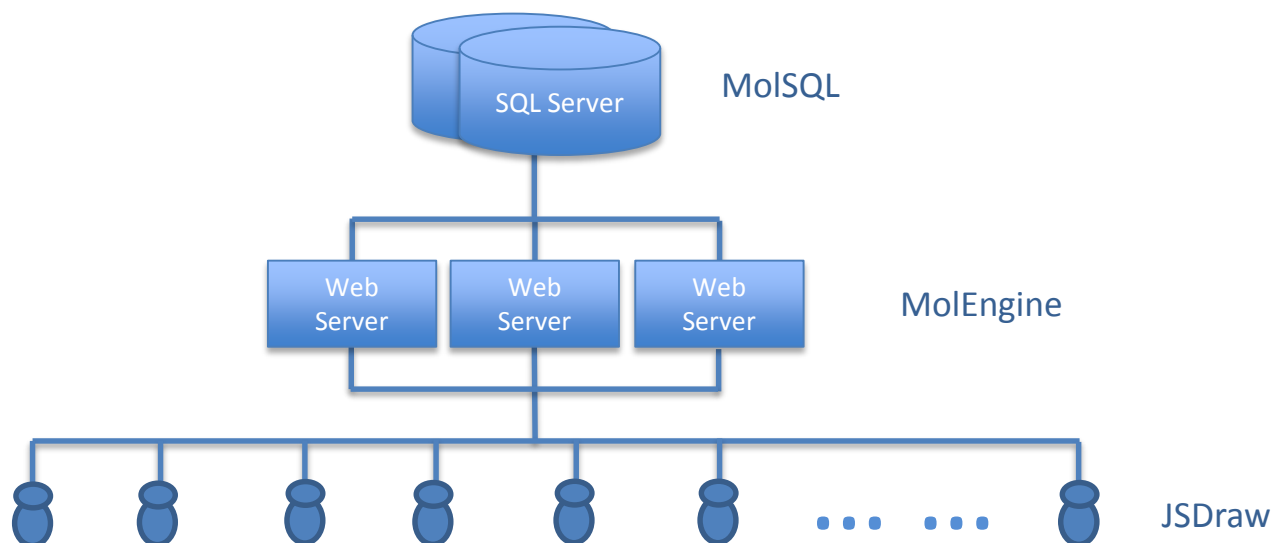
Structure Editor Landscape before 2010

- **ISIS Draw**
- **ChemDraw**
- **MarvinSketch**

  …

Not optimal for

– Web-based applications

– Java dependency

– Mobile platforms

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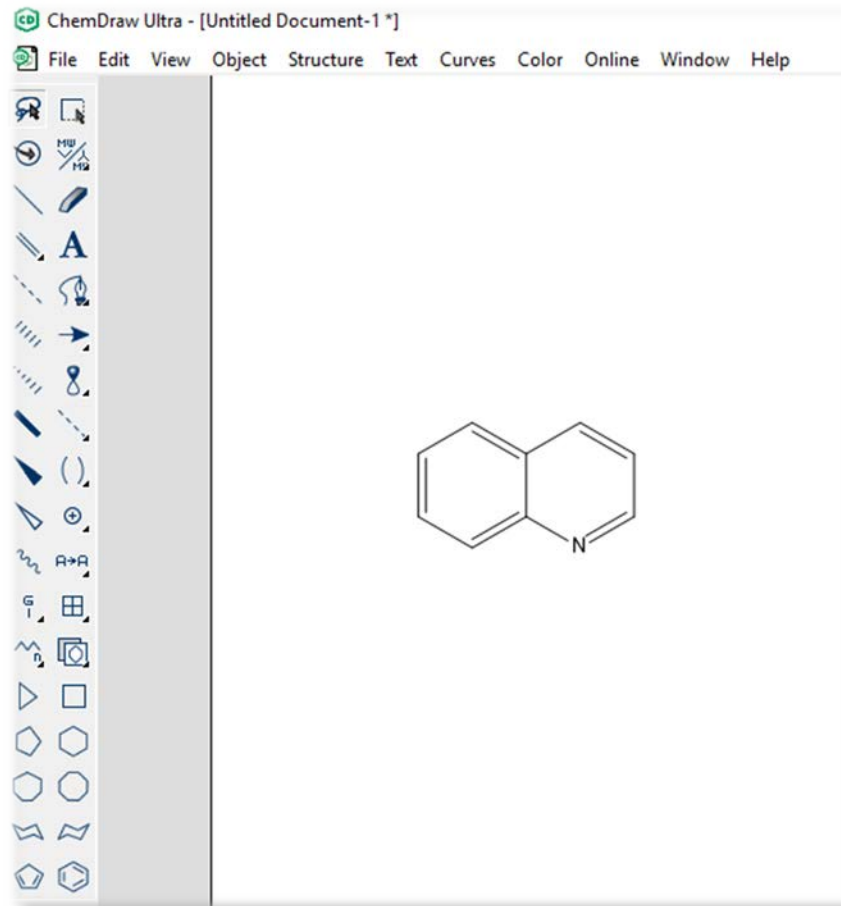
JSDraw: Designed for Web and Mobile

- – Javascript/HTML5
- – Web
- – Mobile
- – Cloud

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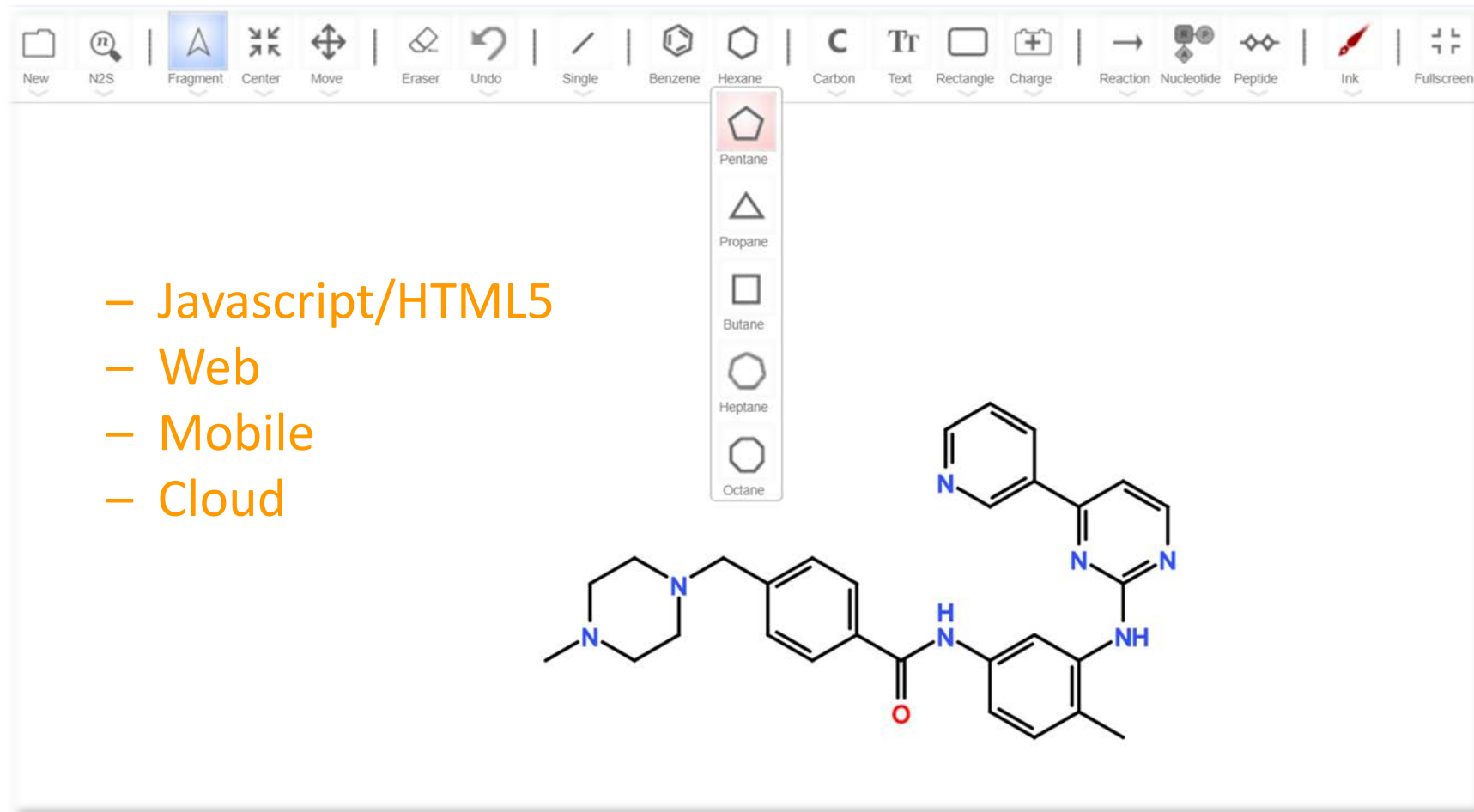
JSDraw: JavaScript Framework for Cheminformatics

- **JSDraw core Cheminformatics Javascript library**
  - Edit and display chemical structures
  - Edit and annotate biological sequences
  - Chemistry spreadsheet
- **JSDraw.Form**
  - Web Form Framework for Cheminformatics
- **JSDraw.Page**
  - Web Application Framework for Cheminformatics

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UI for Proteins and Genes

UI for Peptides

UI for Oligonucleotides/Oligonucleosides

Why HELM?

GAP

Small Molecule Tools   **Sequence-Based Tools**

Small Molecules   Biomolecules   Sequences
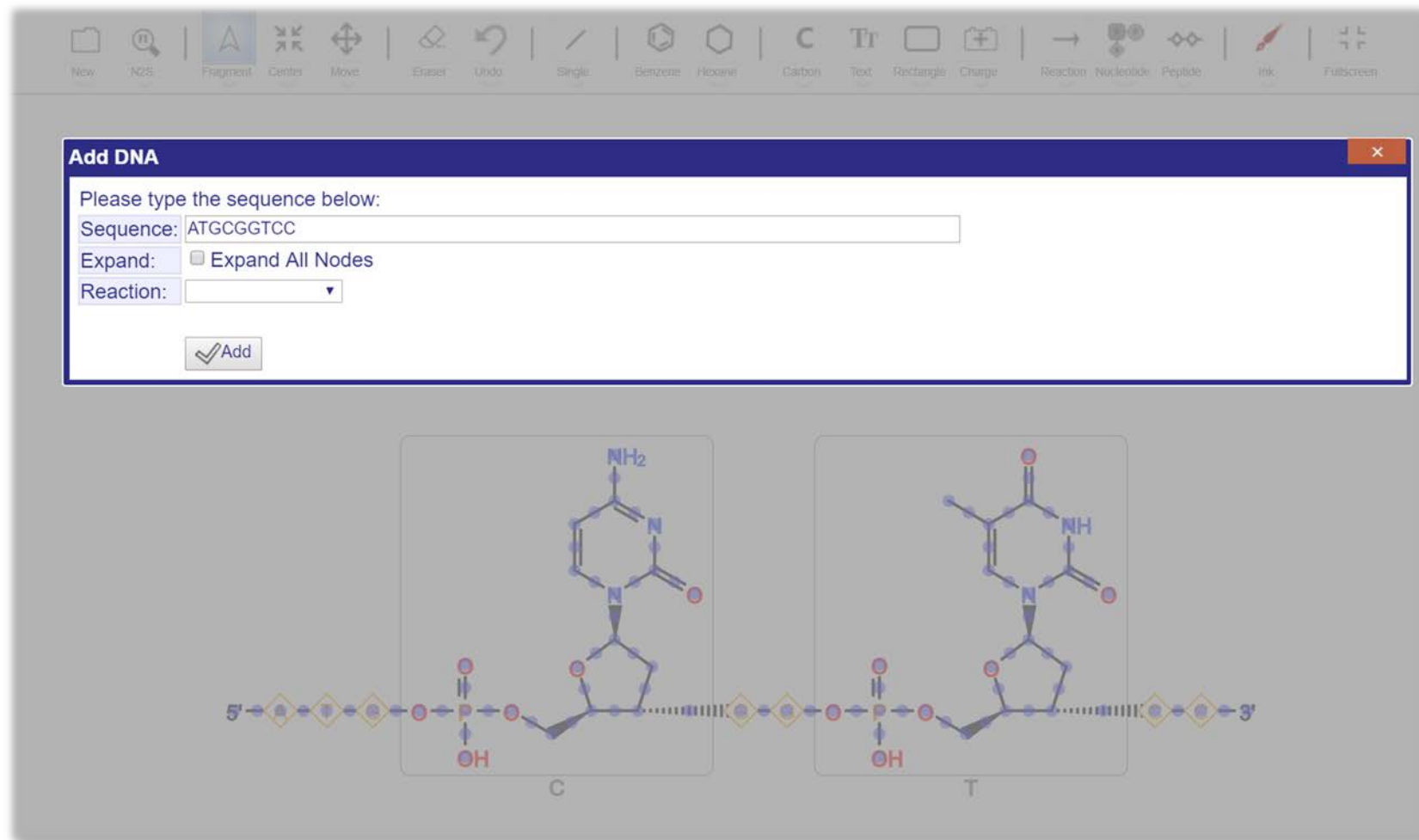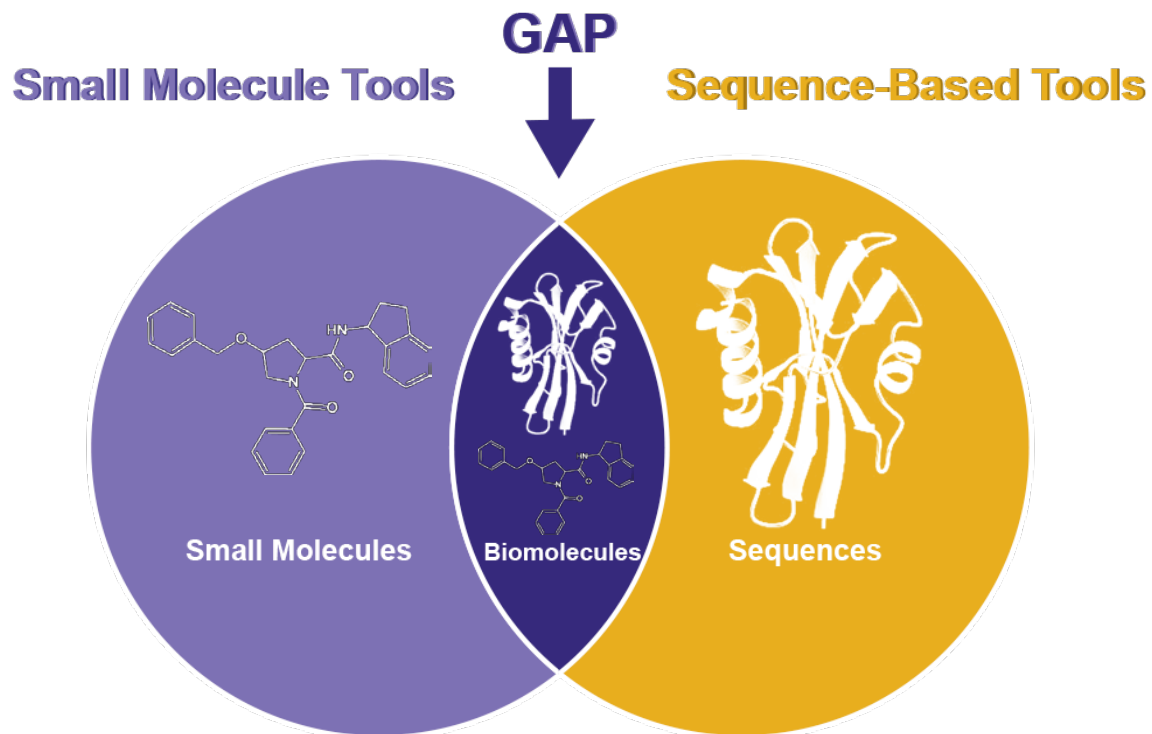
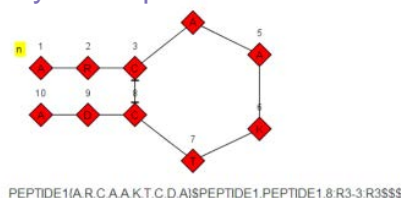**HELM:** The representation language and toolkit that remediate this gap

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What is HELM?

- **HELM stands for Hierarchical Editing Language for Macromolecules**

- **Invented by Pfizer and open-sourced by Pistoia Alliance**

- **HELM creates a standard for representing, exchanging, and manipulating macromolecules**

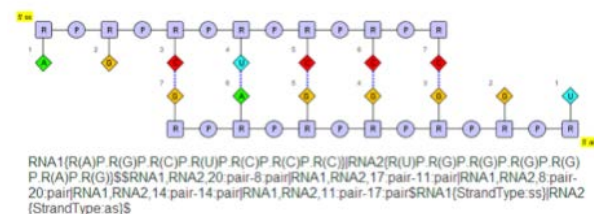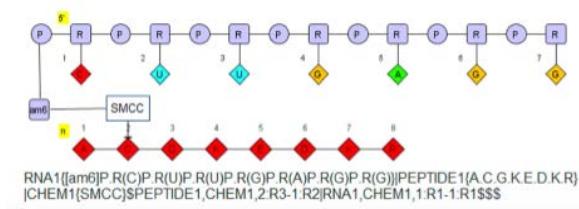- **Improves data storage and knowledge sharing in R&D**

Linear oligonucleotides

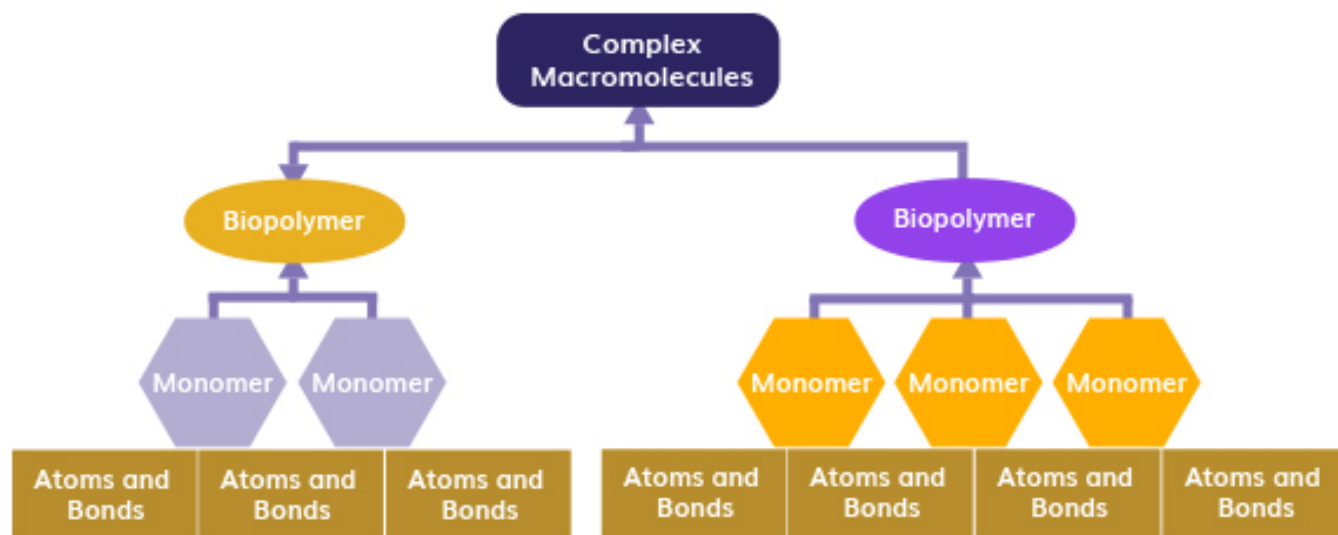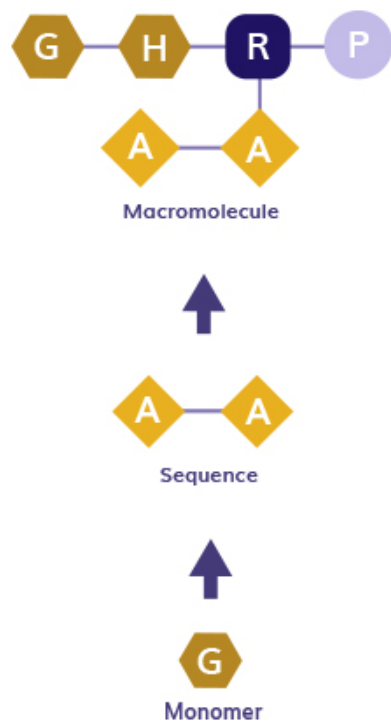RNA1{R(A)P.[mR](U)[sP].R(G)P.R([5meC])P.[dR](T)P.[dR](T)}$$$$

Cyclic Peptide

PEPTIDE1{A.R.C.A.A.K.T.C.D.A}$PEPTIDE1,PEPTIDE1,8:R3-3:R3$$$

siRNA

RNA1{R(A)P.R(G)P.R(C)P.R(U)P.R(C)P.R(C)P.R(C)}|RNA2{R(U)P.R(G)P.R(G)P.R(G)
P.R(A)P.R(G)}$$RNA1,RNA2,20:pair-8:pair|RNA1,RNA2,17:pair-11:pair|RNA1,RNA2,8:pair-
20:pair|RNA1,RNA2,14:pair-14:pair|RNA1,RNA2,11:pair-17:pair$RNA1{StrandType:ss}|RNA2
{StrandType:as}$

Oligonucleotide peptide conjugate

RNA1{[am6]P.R(C)P.R(U)P.R(U)P.R(G)P.R(A)P.R(G)P.R(G)}|PEPTIDE1{A.C.G.K.E.D.K.R}
|CHEM1{SMCC}$PEPTIDE1,CHEM1,2:R3-1:R2|RNA1,CHEM1,1:R1-1:R1$$$

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The Power of HELM's Hierarchy

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HELM Web Editor is Based On JSDraw
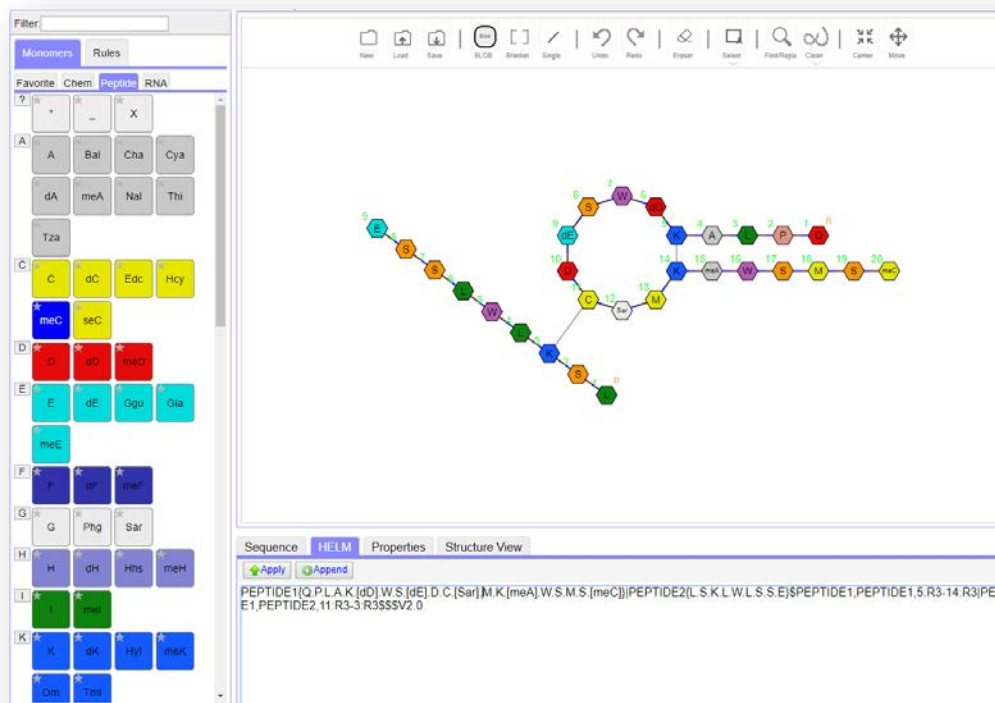
- **HELM**
  - Invented at Pfizer
  - Open sourced by Pfizer
  - Adopted by Pistoia

- **HELM Java Client**
  - Built on Java
  - Annotation is not supported
 - Ambiguity is not supported

- **HELM Web Editor**
  - Switch to JavaScript
  - Support annotation
  - Support Ambiguity

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HELM Web Editor Project

- **Scilligence was selected as the developer in 2016**
- **Three Phases**
  - Core HELM functionalities in HELM Web Editor 1.0
    - Released in February 2017
  - Ambiguity and Annotation Features
    - In Progress
  - Advance Annotation for Antibody
    - Planned
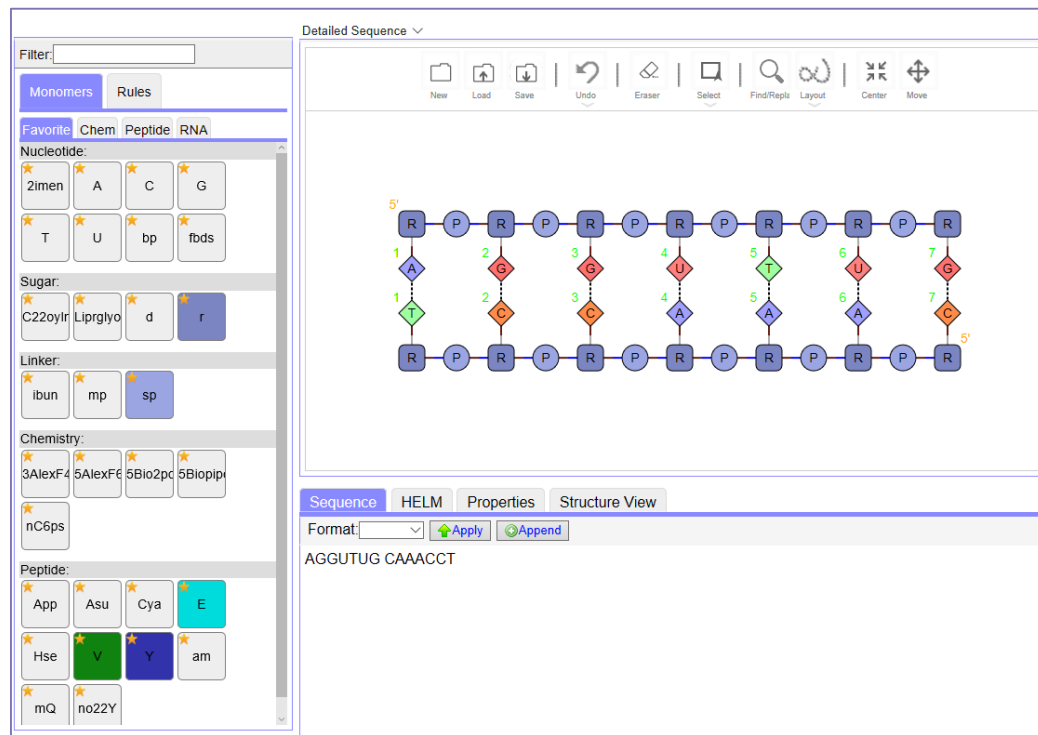
HELM Web Editor 2.0 Modules

- **HELM Editor Control**
- **HELM App**
- **HELM Monomer Manager**
- **HELM Rule Manager**

Scilligence Solutions Fully Support HELM

- **Drawing HELM molecules in**
  - Scilligence ELN
  - RegMol (Registration System)
  - Scilligence Inventory
- **HELM Molecule Registration**
  - Molecule rules
  - Uniqueness check
  - Central monomer management
- **MoISQL**
  - Chemistry Cartridge supporting HELM
- **TouchMol4Office**
  - The only Office add-on supporting HELM

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JSDraw – A Unified Sketcher/Editor

- **Web-based, Java-free**
- **Mobile compatible**
- **Cloud deployment**
- **Supports both small molecules and macromolecule**
- **Supports HELM**

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Thank You!

www.scilligence.com

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