

Description of Overarching Research Objectives (OROs) for Each In-House Research Loop, associated PIs and Loop “Leads”

**Loop 1: Novel Glycomaterials**  
**Leads: Matson / Deshmukh**

**ORO 1.1** Prepare interfacially-active polysaccharide-containing copolymers. **Deshmukh, Edgar, Johnson, Matson, Moore**

**ORO 1.2** Develop new methods to synthesize, characterize, and model proteoglycan-mimetic polymers. **Deshmukh, Edgar, Johnson, Matson, Moore**

**Loop 2: Biocatalysis in Glycomaterial Creation**  
**Lead: Roman**

**ORO 2.1** Develop new enzyme-based methods to synthesize glycomaterials that are suited for automation. **Linhardt, Liu, Roman**

**ORO 2.2** Advance methods to characterize solution-, gel-, and solid-state glycomaterials at the molecular and nanostructural level. **Roman**

**ORO 2.3** Develop software for the prediction of ROA and VCD spectra for a given carbohydrate. **Crawford**

**Loop 3: Rational Glycomaterial Design**  
**Lead: Woods**

**ORO 3.1** Launch Interface Enabling Automated MD Simulation and Analysis of Engineered Glycomaterials. **Woods**

**ORO 3.2** Improve the accuracy of predicted carbohydrate interaction energies. **Woods**

**ORO 3.3** Advance the development of atomistic glycomaterial modeling. **Welborn, Woods**

**ORO 3.4** Develop high throughput methods for quantifying carbohydrate interactions. **Esker, Schulz**

**Loop 4: Machine Learning in Glycoscience**  
**Lead: Hong**

**ORO 4.1** Automated synthesis of glycans and glycomaterials. **Helm**

**ORO 4.2** Automation of glycan structure determination by NMR, LC-MS and MS<sup>n</sup>. **Azadi, Helm, Hong**

**ORO 4.3** Machine learning applied to structural analysis of glycans and glycomaterials. **Hong**

**ORO 4.4** Machine learning of automated glycan synthesis. **Kong**

**ORO 4.5** Predicting biophysical properties from molecular characterization/modeling data. **Azadi, Helm, Hong, Kong**

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