

2024 ASMS
Skyline User Group Meeting



清華大學
Tsinghua University

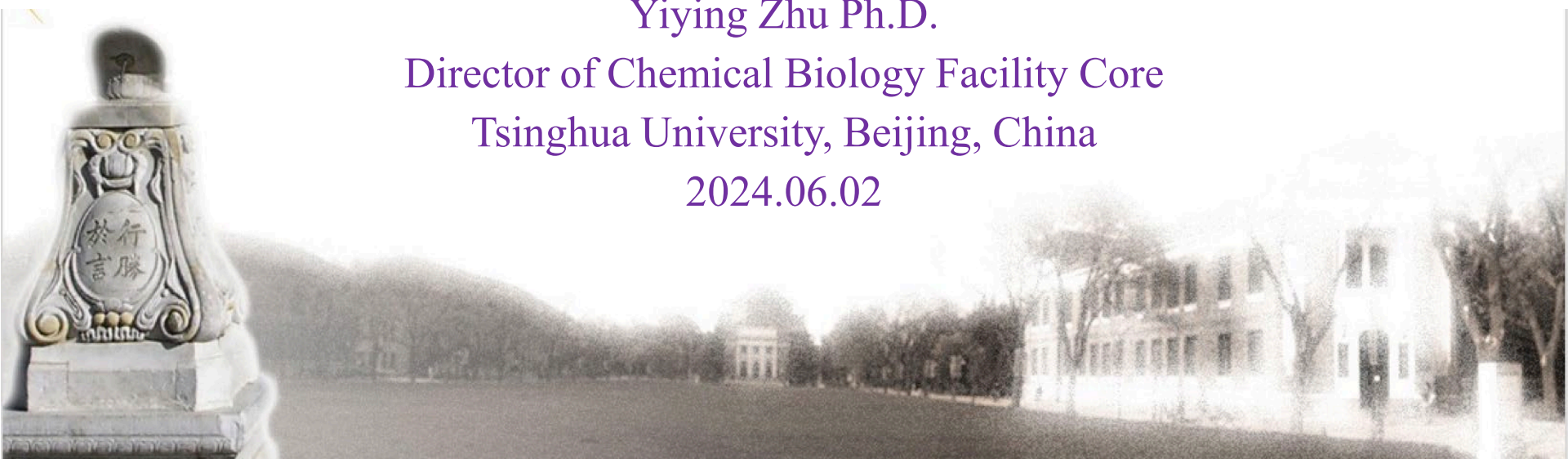
An in-silico method for distinguishing the glycan structural isomers by the isotope substitution

Yiying Zhu Ph.D.

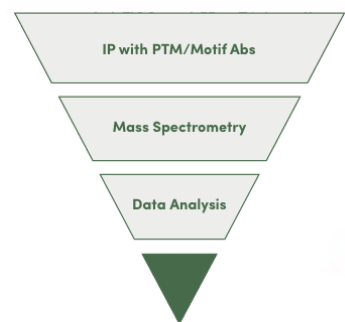
Director of Chemical Biology Facility Core

Tsinghua University, Beijing, China

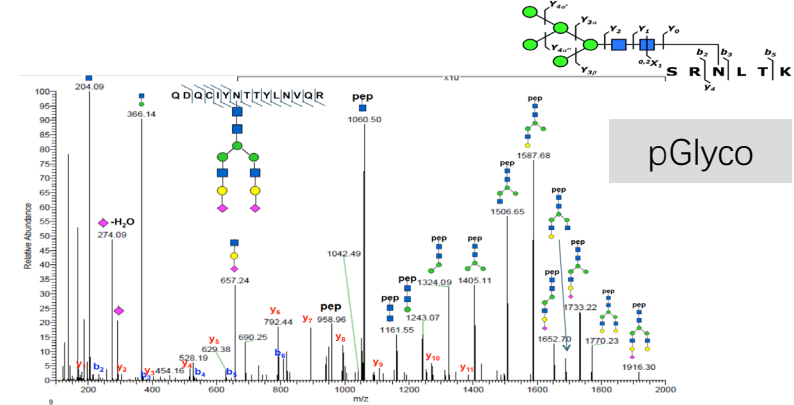
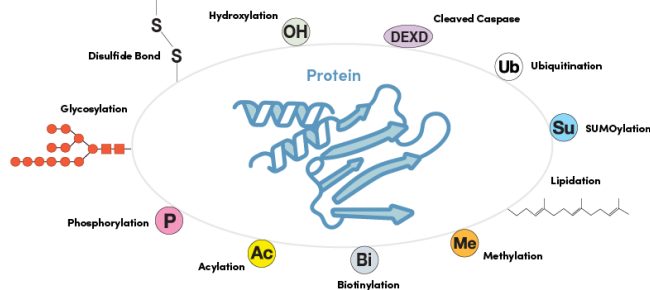
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Quantitation on peptides carrying post-translational modifications

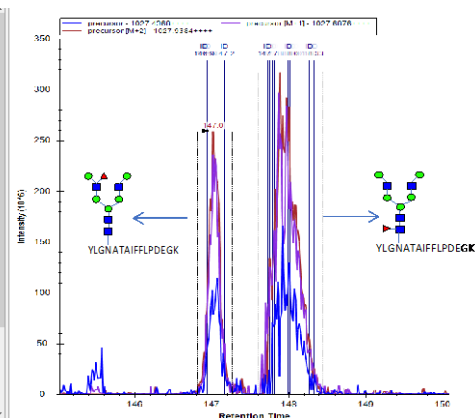


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Challenge:
Difficulty in differentiating glycan structural isomers

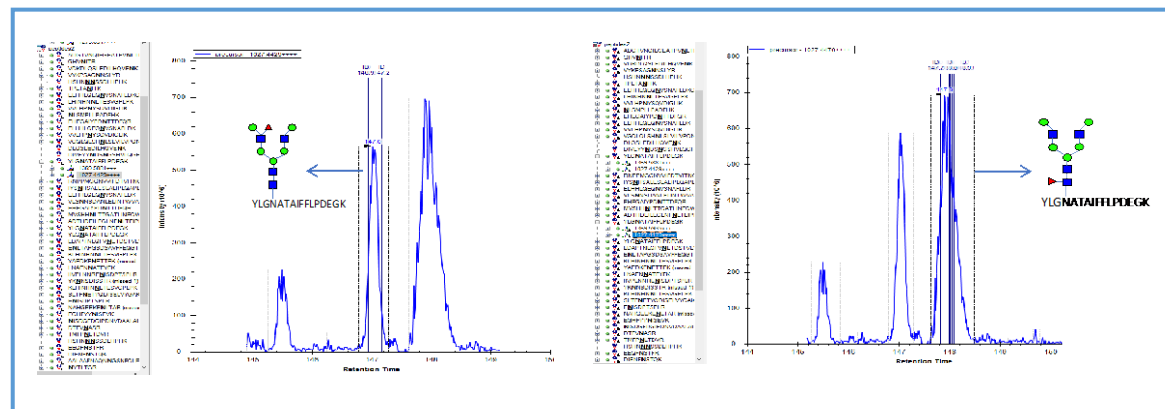
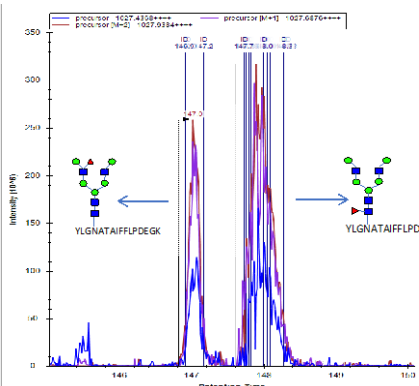
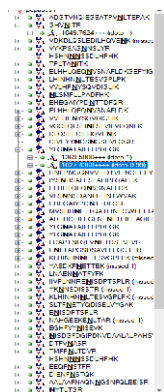
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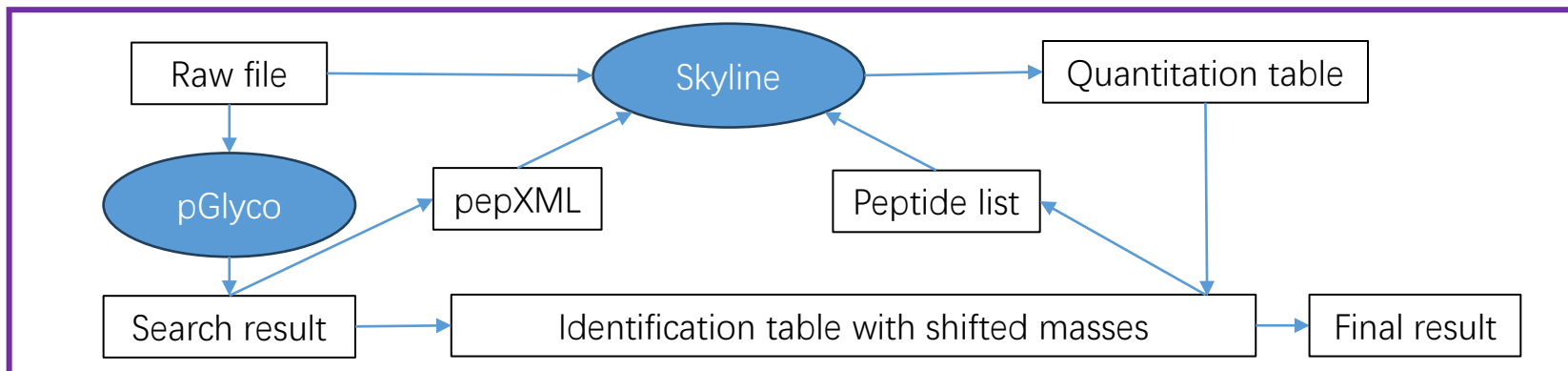
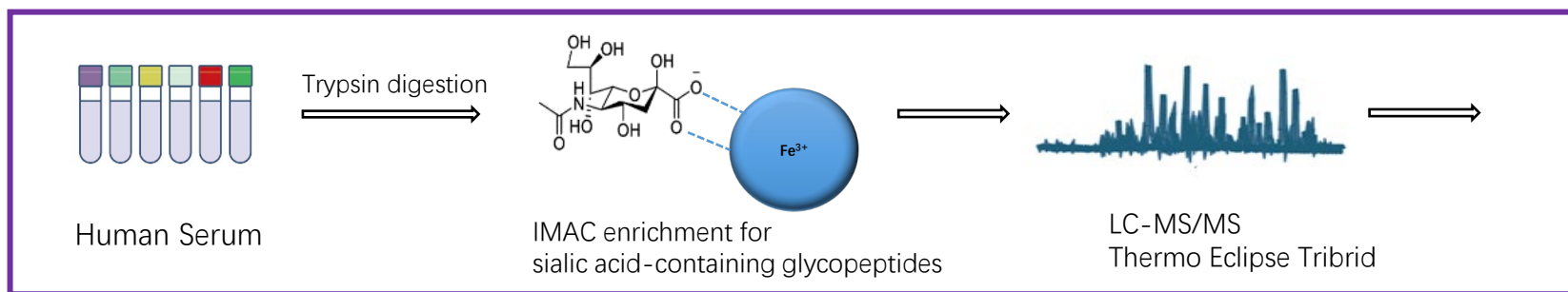
Differentiate glycan structural isomers by shifting masses in silico



Glycan		Regular		In silico shifted	
ID	Structure	Chemical Formula	Mass (Da)	Chemical Formula	Mass (Da)
1266	(N(F)(N(H(H)(H(N(H(A))))(N(H(A))))))	C90H146N6O65	2350.83035	C90H146N6O65	2350.83035
1267	(N(N(H(H)(H(N(H(A))))(N(F)(H(A))))))	C90H146N6O65	2350.83035	C90H147N5O65C'1	2350.83846
1269	(N(F)(N(H(N)(H(H)(H(N(H(A))))))	C90H146N6O65	2350.83035	C90H148N4O65C'2	2350.84656
1270	(N(F)(N(H(H(N(H(A))))(H(N(H(A))))))	C90H146N6O65	2350.83035	C90H149N3O65C'3	2350.85467
1272	(N(N(H(N)(H(H)(H(N(F)(H(A))))))	C90H146N6O65	2350.83035	C90H150N2O65C'4	2350.86277
1273	(N(N(H(H(N(H(A))))(H(N(F)(H(A))))))	C90H146N6O65	2350.83035	C90H151N1O65C'5	2350.87088



Application example

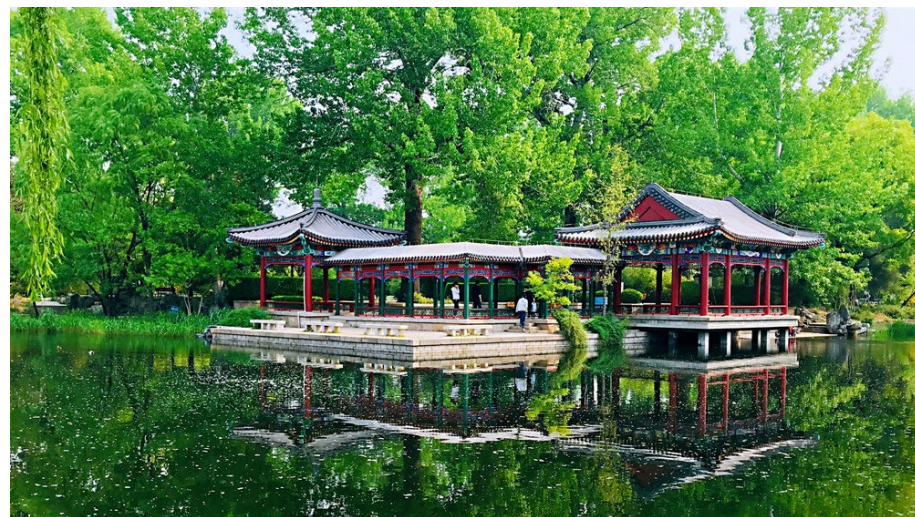


Breast cancer patient serum vs healthy control serum

	Quantified	Altered ($F \geq 2.5, p \leq 0.01$)
Glycoproteins	~ 150	~ 50
Glycopeptides	~ 1500	~ 100

Protein	Peptide Sequence	Glycan structure	Fold change (Patient vs Normal)	Anova p value
xxx	PEPTIDENPEPTIDE A		0.35	0.0010
	PEPTIDENPEPTIDE B		0.22	0.0000
	PEPTIDENPEPTIDE C		0.27	0.0002
	PEPTIDENPEPTIDE D		0.29	0.0010
			0.24	0.0002
			0.22	0.0007
			0.38	0.0001
			0.31	0.0009

北京 BEIJING



化学生物学平台



平台主管 朱奕颖



李海芳



韩强



石文武



吴海铭



杜翼

Acknowledgment



景杰生物
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