2024 ASMS
Skyline User Group Meeting

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

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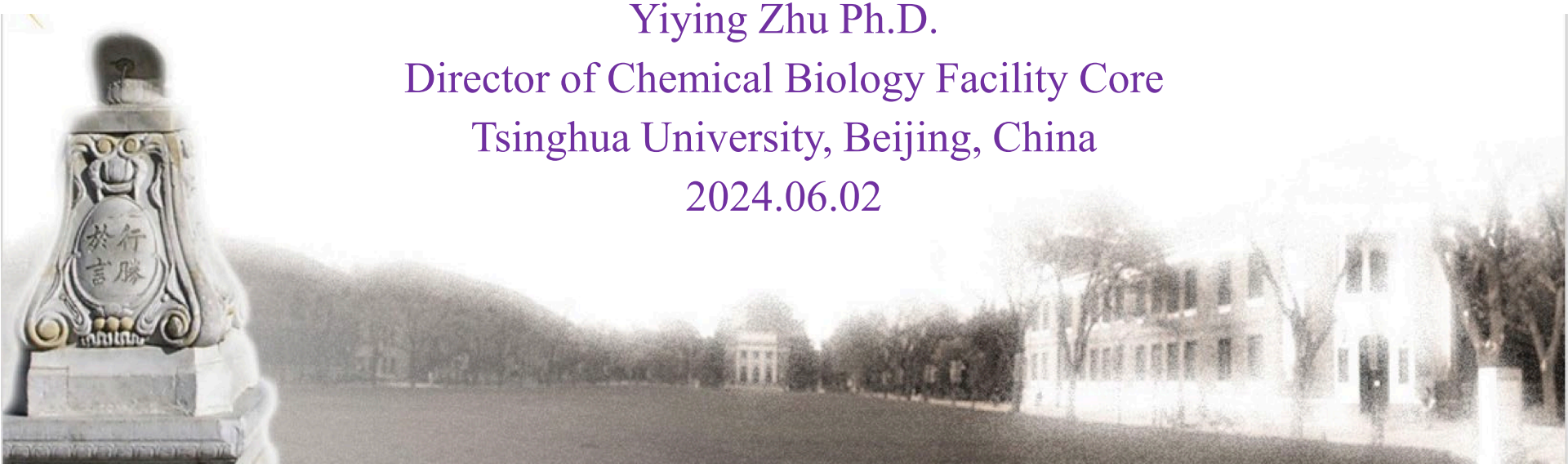
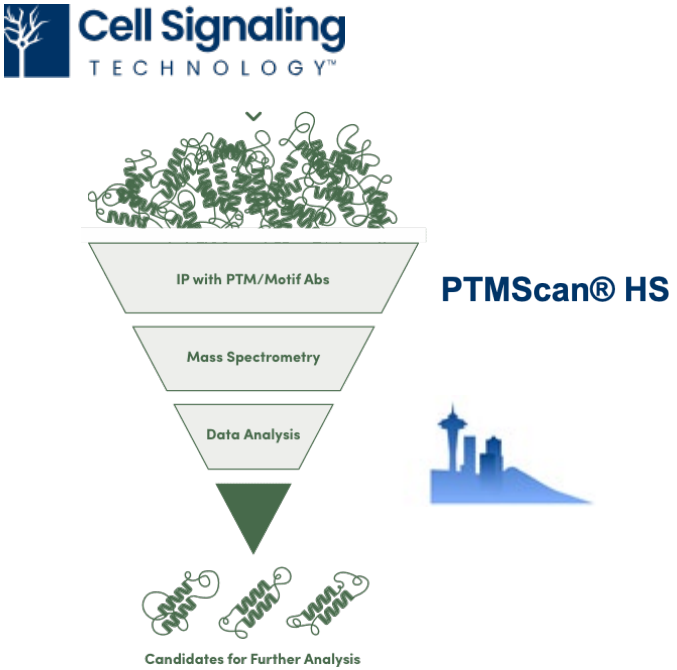
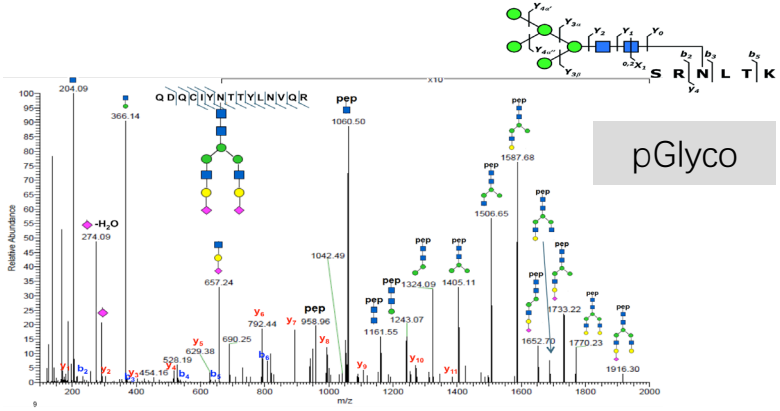


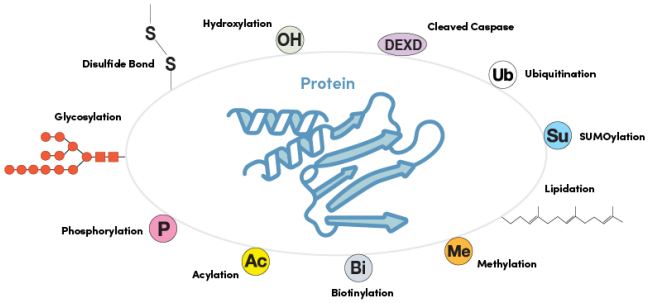
Quantitation on peptides carrying post-translational modifications

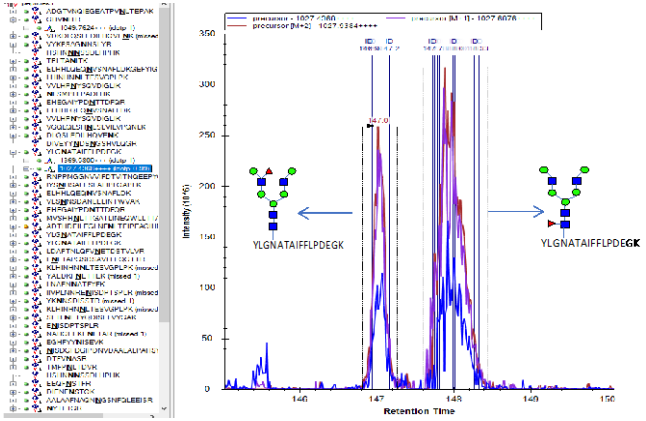


PTMScan® HS



Challenge:
Difficulty in differentiating glycan structural isomers





Differentiate glycan structural isomers by shifting masses in silico

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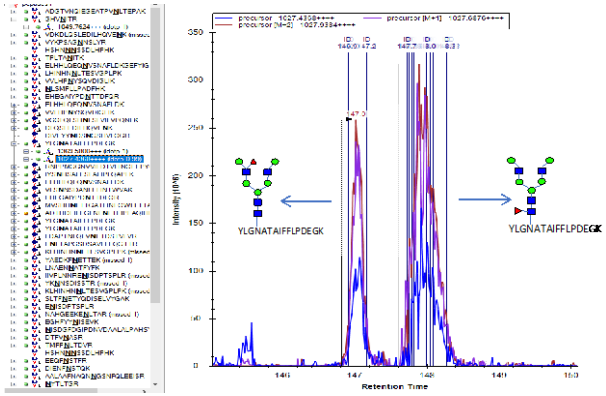
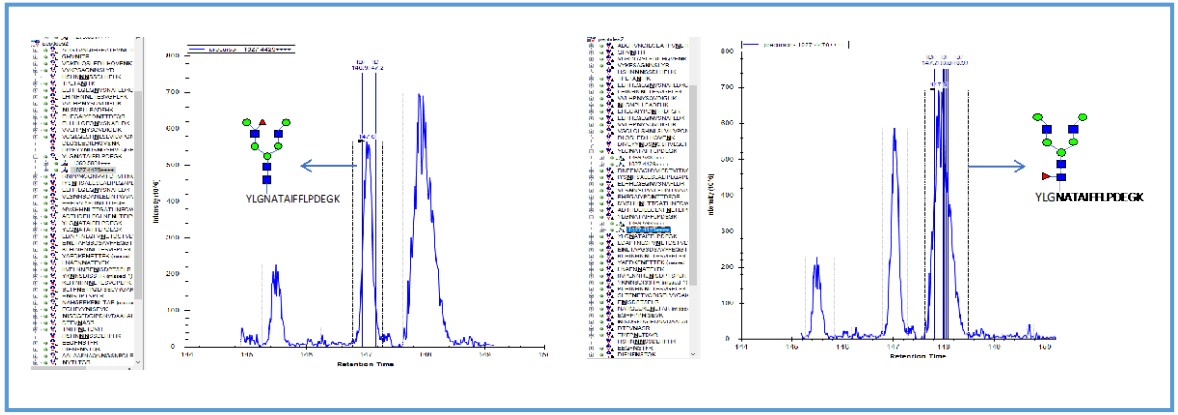
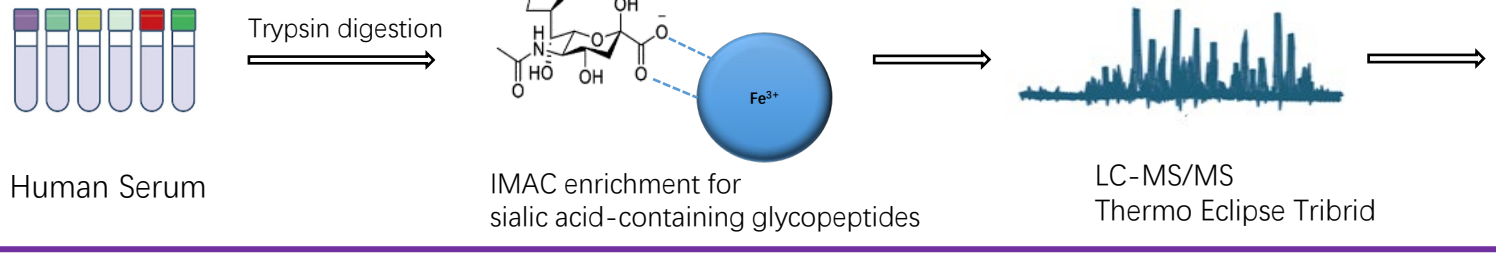
Glycan		Regular		In silico shifted	
ID	Structure	Chemical Formula	Mass (Da)	Chemical Formula	Mass (Da)
1266	(N(F)(N(H(H)(H(N(H(A)))(N(H(A)))))))	C90H146N6O65	2350.83035	C90H146N6O65	2350.83035
1267	(N(N(H(H)(H(N(H(A)))(N(F)(H(A)))))))	C90H146N6O65	2350.83035	C90H147N5O65C'1	2350.83846
1269	(N(F)(N(H(N)(H(H))(H(N(H(A(A))))))))	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(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

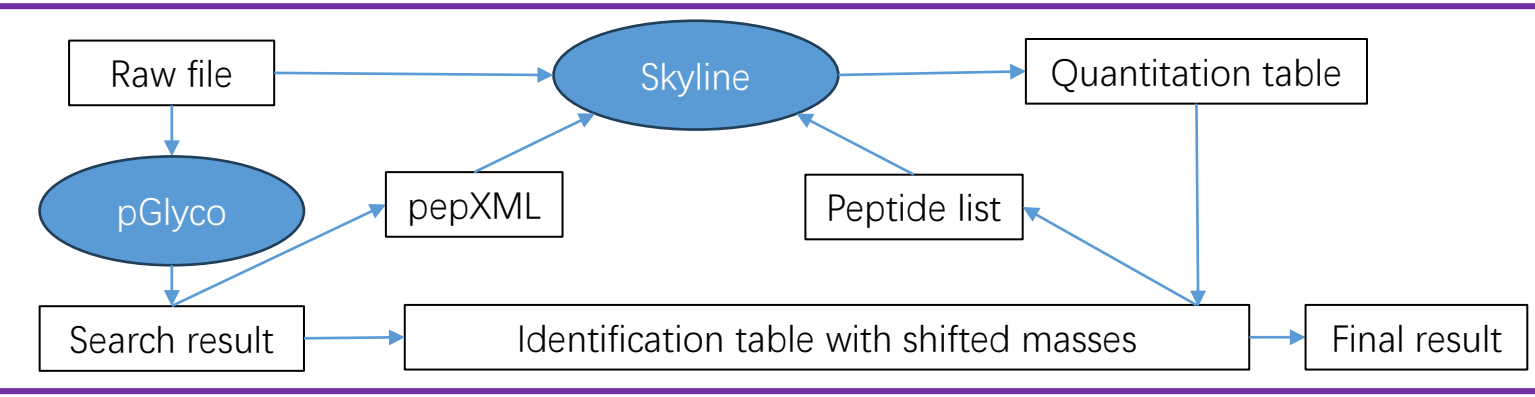




China Patent No. ZL2022 11293141.8

Application example

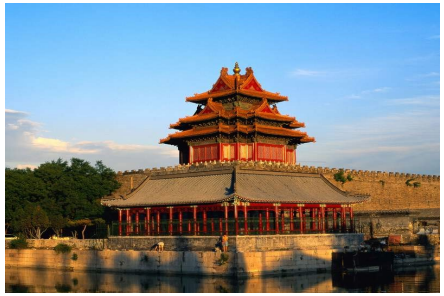


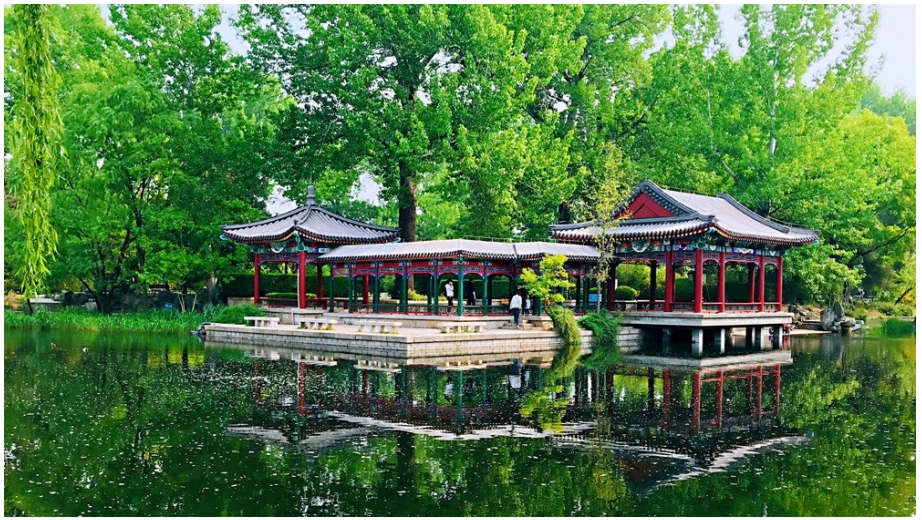


Breast cancer patient serum vs healthy control serum

	Quantified	Altered (F≥2.5, p≤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
			0.22	0.0000
	PEPTIDENPEPTIDE B		0.27	0.0002
	PEPTIDENPEPTIDE C		0.29	0.0010
	PEPTIDENPEPTIDE D		0.24	0.0002
			0.22	0.0007
			0.38	0.0001
			0.31	0.0009





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Acknowledgment

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