

Supporting Information

Quantification and Isotope Abundance Determination of ¹³C Labeled Intracellular Sugar Metabolites with Hydrophilic Interaction Liquid Chromatography

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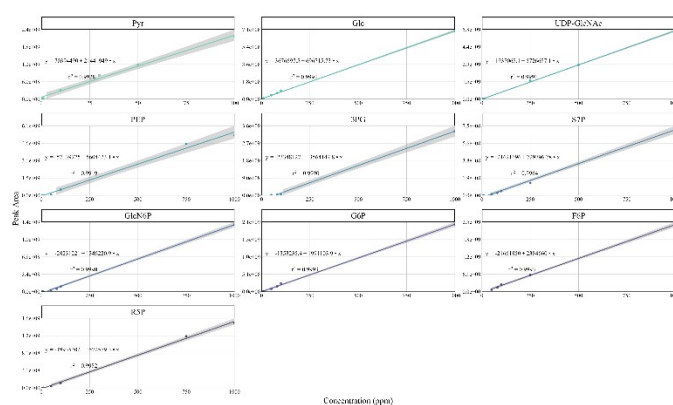


Figure S1: Peak area vs. concentration, calibration equations, and r^2 of the sugar

Table S1: Recovery, inter-day, and intra-day RSD of the standard mixture in the simulated matrix

Analyte	solution								
	Low Concentration			Mid Concentration			High Concentration		
	Recovery (%)	Intra-day Precision n RSD (%)	Inter-day Precision n RSD (%)	Recovery (%)	Intra-day Precision n RSD (%)	Inter-day Precision n RSD (%)	Recovery (%)	Intra-day Precision RSD (%)	Inter-day Precision n RSD (%)
Glc	89.32	4.61	2.28	100.06	1.59	2.10	108.81	2.68	5.25
G6P	94.43	1.36	1.82	103.26	1.58	2.22	108.21	2.02	2.17
F6P	78.15	0.45	0.59	90.61	0.70	0.90	101.40	1.11	3.80
PEP	115.18	1.41	1.85	111.07	0.85	1.11	113.75	1.03	3.75
3PG	89.45	3.88	3.65	74.52	1.50	2.03	114.68	0.61	1.71
Pyr	101.66	2.71	3.55	99.81	1.93	4.22	75.96	0.68	1.77
GlcN6P	100.6	2.20	2.33	100.60	0.73	1.88	82.40	1.45	2.00
UDP-GlcNAc	88.93	4.97	3.94	82.39	0.80	1.61	83.76	3.98	2.90
S7P	85.79	2.77	4.77	112.79	1.26	1.45	108.76	3.03	4.65
R5P	113.83	0.38	0.53	84.56	1.51	1.77	82.05	3.38	3.79

Table S2: RID and IME of the U-¹³C labeled glucose standard

Mass Isotopologue	Theoretical m/z	Measured m/z	Interfering Peak	Interfering m/z	RID/ppm	IME/ppm
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$[^{13}\text{C}_6\text{H}_{12}\text{O}_6\text{-H}]^-$	185.0762	185.07618	$[^{13}\text{C}_5\text{CH}_{12}\text{O}_6\text{-H+1}]^+$	185.0761	3.05	0.32
$[^{13}\text{C}_5\text{CH}_{12}\text{O}_6\text{-H}]^-$	184.0729	184.07281	$[^{13}\text{C}_4\text{C}_2\text{H}_{12}\text{O}_6\text{-H+1}]^+$	184.0726	1.79	0.43
$[^{13}\text{C}_4\text{C}_2\text{H}_{12}\text{O}_6\text{-H}]^-$	183.0695	/	$[^{13}\text{C}_3\text{C}_3\text{H}_{12}\text{O}_6\text{-H+1}]^+$	183.0691	2.13	/
$[^{13}\text{C}_3\text{C}_3\text{H}_{12}\text{O}_6\text{-H}]^-$	182.0662	/	$[^{13}\text{C}_2\text{C}_4\text{H}_{12}\text{O}_6\text{-H+1}]^+$	182.0658	2.36	/
$[^{13}\text{C}_2\text{C}_4\text{H}_{12}\text{O}_6\text{-H}]^-$	181.0628	/	$[^{13}\text{C}_1\text{C}_5\text{H}_{12}\text{O}_6\text{-H+1}]^+$	181.0624	2.49	/
$[^{13}\text{C}_1\text{C}_5\text{H}_{12}\text{O}_6\text{-H}]^-$	180.0595	/	$[\text{C}_6\text{H}_{12}\text{O}_6\text{-H+1}]^+$	180.0590	2.61	/
