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Trapped Ion Mobility Spectrometry Enables Selective Analysis of Sugar Phosphates and Acyl-CoA Metabolites

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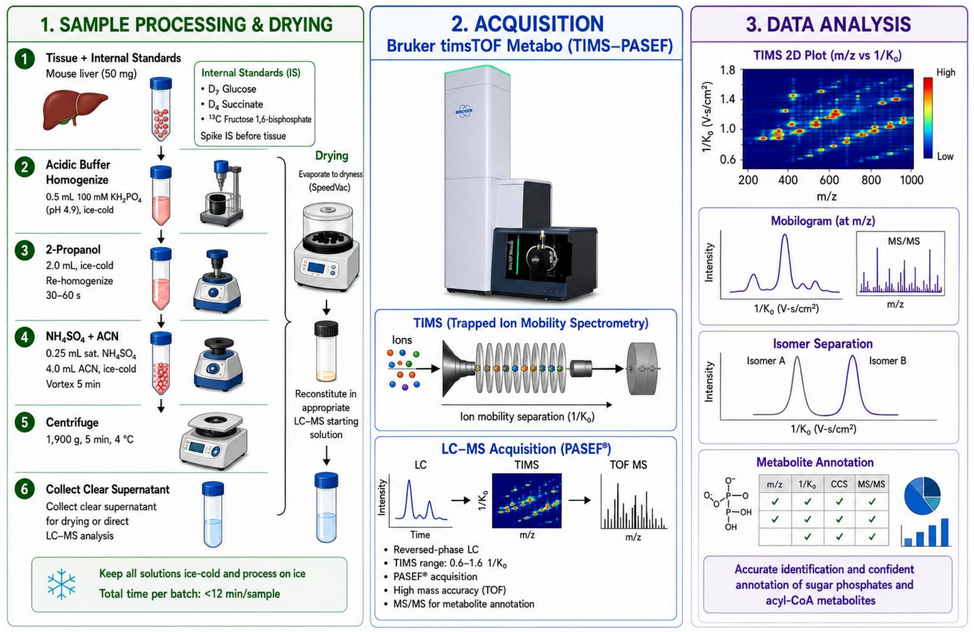
Introduction

- Sugar phosphates and acyl-CoA metabolites are central intermediates in cellular energy metabolism, and lipid metabolism.
- Accurate quantification and annotation of these metabolites remains analytically challenging due to their high polarity, structural similarity, low abundance, and the presence of isomeric species.
- Conventional LC–MS workflows often suffer from limited chromatographic resolution, ion suppression, and co-eluting interferences when analyzing phosphorylated and CoA-containing metabolites.
- Trapped Ion Mobility Spectrometry (TIMS) with high-resolution mass spectrometry enables enhanced separation of isomeric and isobaric metabolites while increasing analytical specificity in complex biological matrices.
- This study demonstrates the application of TIMS-enabled metabolomics for the selective analysis of sugar phosphates and acyl-CoA metabolites, highlighting its potential for advancing targeted and untargeted metabolic profiling.

Methods



- Sugar phosphate and Acyl-CoA metabolite standards were used for initial method development.
- Mouse liver tissues (50 mg) were rapidly homogenized in ice-cold acidic KH_2PO_4 buffer containing isotope-labeled internal standards.
- A rapid 3 min reversed phase UPLC method with Bruker Bio-AQ column. Data was acquired in PASEF mode in both positive and negative ion modes.

Results

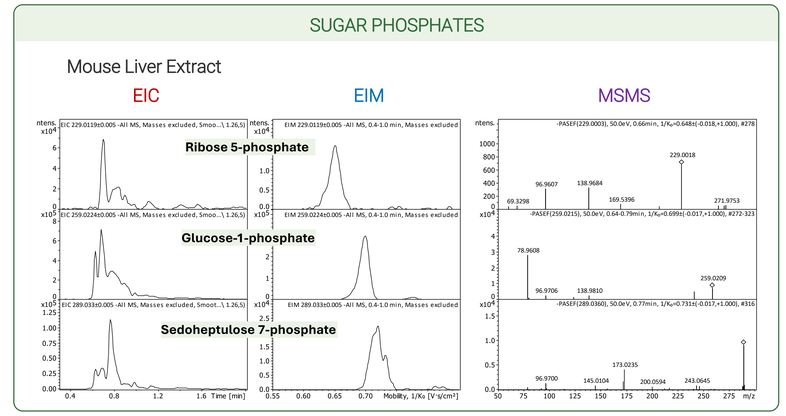
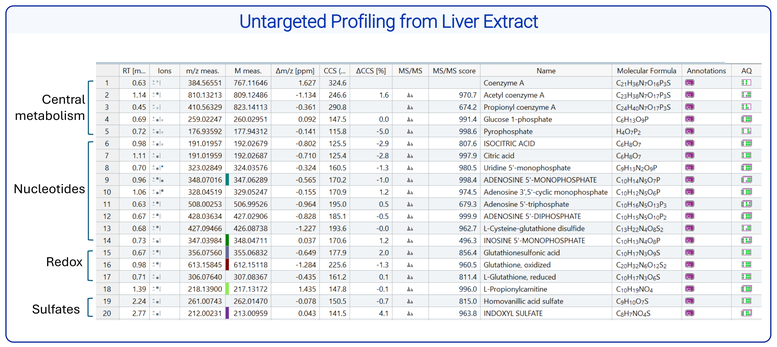


Figure 3. Sugar phosphates (R5P, G1P, and S7P) directly detected from liver extract samples. EICs are smoothed using Savitzky Golay algorithm.



	RT [m...	Ions	m/z meas.	M meas.	Δm/z [ppm]	CCS [...	ΔCCS [%]	MS/MS	MS/MS score	Name	Molecular Formula	Annotations	AQ
1	0.63		384.56551	767.11646	1.627	324.6				Coenzyme A	$C_{21}H_{36}N_7O_{16}P_3S$		
2	1.14		810.13213	809.12486	-1.134	246.6	1.6		970.7	Acetyl coenzyme A	$C_{23}H_{38}N_7O_{17}P_3S$		
3	0.45		410.56329	823.14113	-0.361	290.8			674.2	Propionyl coenzyme A	$C_{24}H_{40}N_7O_{17}P_3S$		
4	0.69		259.02247	260.02951	0.092	147.5	0.0		991.4	Glucose 1-phosphate	$C_6H_{13}O_9P$		
5	0.72		176.93592	177.94312	-0.141	115.8	-5.0		998.6	Pyrophosphate	$H_4O_7P_2$		
6	0.98		191.01957	192.02679	-0.802	125.5	-2.9		807.6	ISOCITRIC ACID	$C_6H_8O_7$		
7	1.11		191.01959	192.02687	-0.710	125.4	-2.8		997.9	Citric acid	$C_6H_8O_7$		
8	0.70		323.02849	324.03576	-0.324	160.5	-1.3		980.5	Uridine 5'-monophosphate	$C_9H_{13}N_2O_9P$		
9	0.96		348.07016	347.06289	-0.565	170.2	-1.0		998.4	ADENOSINE 5'-MONOPHOSPHATE	$C_{10}H_{14}N_5O_7P$		
10	1.06		328.04519	329.05247	-0.155	170.9	1.2		974.5	Adenosine 3',5'-cyclic monophosphate	$C_{10}H_{12}N_5O_6P$		
11	0.63		508.00253	506.99526	-0.964	195.0	0.5		679.3	Adenosine 5'-triphosphate	$C_{10}H_{16}N_5O_{13}P_3$		
12	0.67		428.03634	427.02906	-0.828	185.1	-0.5		999.9	ADENOSINE 5'-DIPHOSPHATE	$C_{10}H_{15}N_5O_{10}P_2$		
13	0.68		427.09466	426.08738	-1.227	193.6	-0.0		962.7	L-Cysteine-glutathione disulfide	$C_{13}H_{22}N_4O_8S_2$		
14	0.73		347.03984	348.04711	0.037	170.6	1.2		496.3	INOSINE 5'-MONOPHOSPHATE	$C_{10}H_{13}N_4O_8P$		
15	0.67		356.07560	355.06832	-0.649	177.9	2.0		856.4	Glutathionesulfonic acid	$C_{10}H_{17}N_3O_9S$		
16	0.98		613.15845	612.15118	-1.284	225.6	-1.3		960.5	Glutathione, oxidized	$C_{20}H_{32}N_6O_{12}S_2$		
17	0.71		306.07640	307.08367	-0.435	161.2	0.1		811.4	L-Glutathione, reduced	$C_{10}H_{17}N_3O_6S$		
18	1.39		218.13900	217.13172	1.435	147.8	-0.1		996.0	L-Propionylcarnitine	$C_{10}H_{19}NO_4$		
19	2.24		261.00743	262.01470	-0.078	150.5	-0.7		815.0	Homovanillic acid sulfate	$C_9H_{10}O_7S$		
20	2.77		212.00231	213.00959	0.043	141.5	4.1		963.8	INDOXYL SULFATE	$C_8H_7NO_4S$		

Figure 4. ~1600 unique features were annotated by MetaboScape 2026 (~1200 from positive, ~500 from negative). Some representative compound categories are displayed.

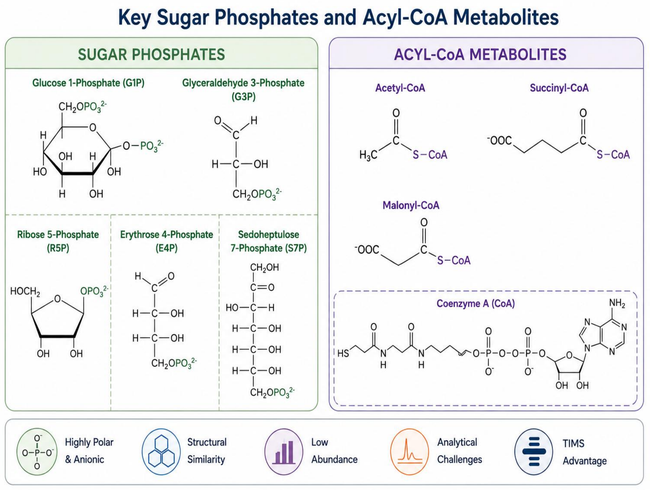


Figure 1. Representative sugar phosphate and acyl-CoA metabolites analyzed in this study.

Results

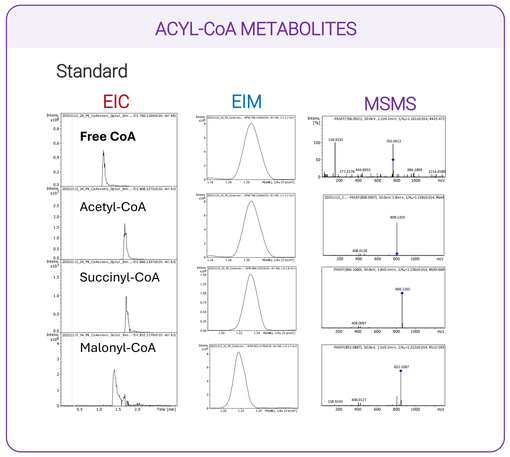


Figure 2. CoA metabolites analyzed from chemical standards.

Conclusion

- A fast UPLC-TIMS-MSMS method is developed to analyze sugar phosphates and acyl-CoA metabolites
- Acyl-CoA standards analysis demonstrated good LC separation, CCS measurement, and MSMS (Fig. 2).
- Sugar phosphates, e.g. R5P, G1P, and S7P, can be detected from mouse liver extract. RT, CCS, and MSMS all matched well with chemical standard (Fig. 3).
- Central metabolism energy metabolites, nucleotides, amino acids & di/tripeptides, glutathione & redox, sulfates, etc. were annotated with high confidence in untargeted manner

Summary

- Fast 3-min RPLC-TIMS-MSMS method developed to profile sugar phosphate and acyl-CoA metabolites
- Compounds detected from liver extract was compared with chemical standard
- High confidence annotation is achieved using MetaboScape

timsMetabo

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