

InertSearch for LC Data No. LL014-0000

## Simultaneous analysis of metabolites using LC/MS/MS (4) - compounds related to central metabolism part 1 -

The chromatograms were provided by Yudai Dempo, Takeshi Bamba, and Eiichiro Fukusaki, Department of Biotechnology, Graduate School of Engineering, Osaka University, 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan

## Conditions

Column	: InertSustain C18
	(3 $\mu$ m, 150 x 2.1 mm I.D., Metal-free hardware)
Column Cat. No	<b>.</b> : 5020-00541
Eluent	: A) 10 mM Tributylamine + 15 mM $CH_3COOH$ in $H_2O$
	B) CH <sub>3</sub> OH
Flow rate	: 0.2 mL/min
Col. Temp.	: 45 °C
Detection	: LC/MS/MS (ESI, Negative, MRM)
Injection Vol.	:3 µ L
Sample	: Standard solution (Approx. 5 $\mu$ mol/L each)

Time (min)	A (vol%)	B (vol%)
0	100	0
1	100	0
1.5	85	15
3	85	15
8	50	50
10	0	100
11	0	100
11.5	100	0
17	100	0

Analyte	Precursor ion $(m/z)$	<b>Product ion</b> $(m/z)$
Pyridoxamine 5-phosphate	247	230
Shikimic acid	173	93
Glyceric acid	105	75
Glycolic acid	75	47
Glucose 6-phosphate	259	97
Mannose 6-phosphate	259	97
Fructose 6-phosphate	259	97
Glucose 1-phosphate	259	97
Fructose 1-phosphate	259	97
Sorbitol 6-phosphate	261	97
Ribose 5-phosphate	229	79
Arabinose 5-phosphate	229	79
Ribulose 5-phosphate	229	79
Ribose 1-phosphate	229	79
Succinic semialdehyde	101	57
Lactic acid	89	43
Sedoheptulose 7-phosphate	289	199
Glycerol 3-phosphate	171	79
Glycerol 2-phosphate	171	79
Thiamine pyrophosphate	424	302
Glyceraldehyde 3-phosphate	169	97
Methylerythritol 4-phosphate	215	79
Pyruvic acid	87	43



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