

**Conditions**

**Column:** ACE Excel 2 C18-PFP  
**Dimensions:** 100 x 2.1 mm  
**Part Number:** EXL-1010-1002U  
**Mobile Phase:** A: 0.1% formic acid in H<sub>2</sub>O  
 B: 0.1% formic acid in MeCN

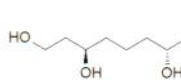
Gradient:	Time (mins)	%B
	0	0
	1	0
	11	65
	13	65
	18	95
	20	95

**Flow Rate:** 0.35 mL/min  
**Injection:** 5 µL  
**Temperature:** 35 °C  
**Detection:** Thermo Scientific Q Exactive Orbitrap MS  
 Heated electrospray ionisation in positive mode  
 Spray Voltage: 3.3 kV  
 Capillary Temperature: 300 °C  
 Heater Temperature: 350 °C  
 Mass Scan Range: *m/z* 70-1000  
 Resolution: 70,000

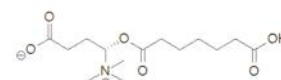
TIC overlay for Jurkat T-lymphocyte cells rinsed with either 0.3% ammonium formate (darker line) or 0.3% ammonium acetate.

**Analytes**

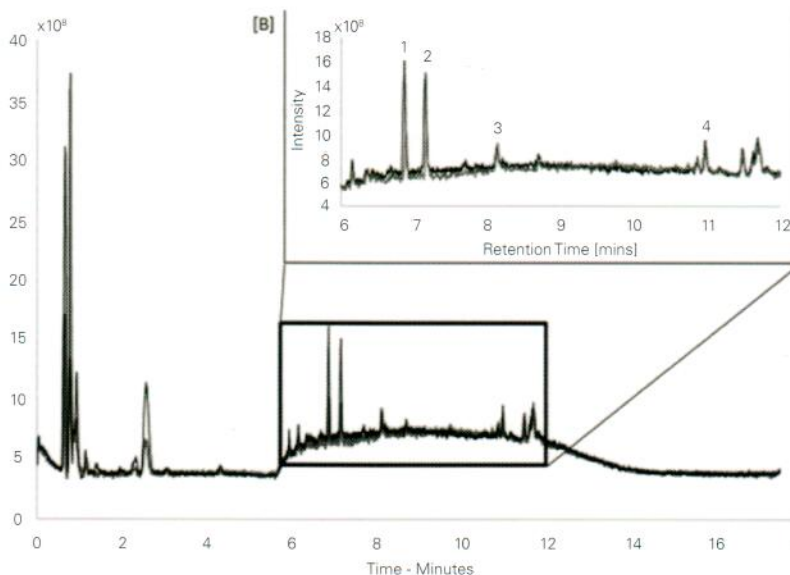
1. Caffeine-d3 (IS)
2. Tryptophan-d3 (IS)
3. 1,3,7-Octanetriol
4. Pimelylcarnitine



1,3,7-Octanetriol



Pimelylcarnitine



Ulmer CZ, Yost RA, Chen J, Mathews CE, Garrett TJ. Liquid-Chromatography-Mass Spectrometry Metabolic and Lipidomic Sample Preparation Workflow for Suspension-Cultured Mammalian Cells using Jurkat T Lymphocyte Cells, *J. Proteomics Bioinform.* (2015), 8(6), 126-132. doi:10.4172/jpb.1000360

Metabolomic Biomarkers in Ethylmalonic Encephalopathy

**Conditions**

**Column:** ACE 3 C18-PFP  
**Dimensions:** 150 x 2.1 mm  
**Part Number:** ACE-1110-1502  
**Mobile Phase:** A: 0.1% formic acid in H<sub>2</sub>O  
 B: 0.1% formic acid in MeCN

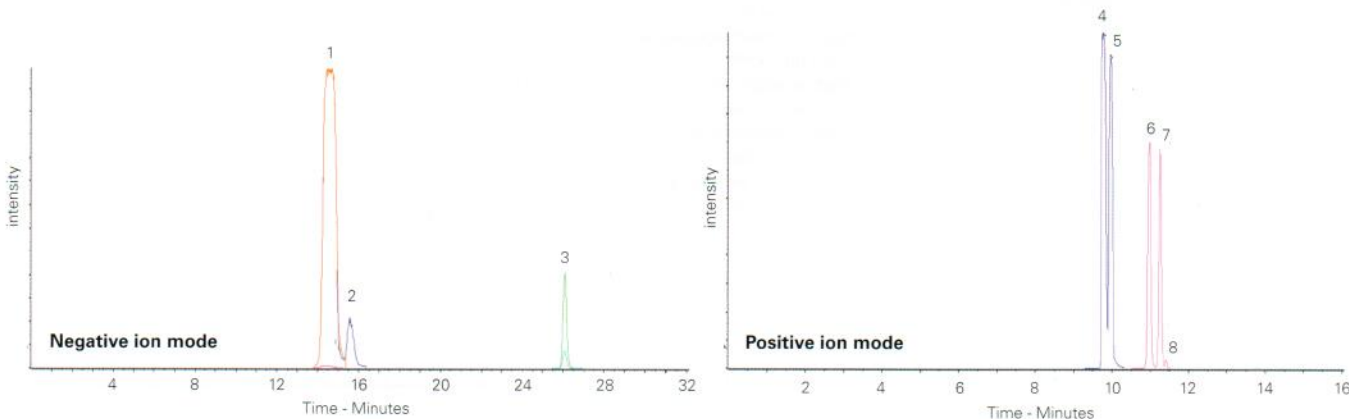
**Detection:** Sciex API 4000 triple quad MS  
 ESI in negative ion mode

**Sample:** Urine sample from patient with ethylmalonic encephalopathy is filtered and extracted with ice-cold methanol, evaporated to dryness and reconstituted in 0.1% formic acid in water

**Analytes**

- |                                                  |                                                       |                                                  |
|--------------------------------------------------|-------------------------------------------------------|--------------------------------------------------|
| 1. Ethylmalonic acid<br>( <i>m/z</i> 131 → 87)   | 4. Isobutyrylcarnitine<br>( <i>m/z</i> 232 → 85)      | 7. Isovalerylcarnitine<br>( <i>m/z</i> 246 → 85) |
| 2. Methylsuccinic acid<br>( <i>m/z</i> 131 → 87) | 5. Butyrylcarnitine<br>( <i>m/z</i> 232 → 85)         | 8. Valerylcarnitine<br>( <i>m/z</i> 246 → 85)    |
| 3. Adipic acid<br>( <i>m/z</i> 145 → 83)         | 6. 2-Methylbutyrylcarnitine<br>( <i>m/z</i> 246 → 85) |                                                  |

Please contact info@ace-hplc.com for additional information on the chromatographic conditions used for this analysis.



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