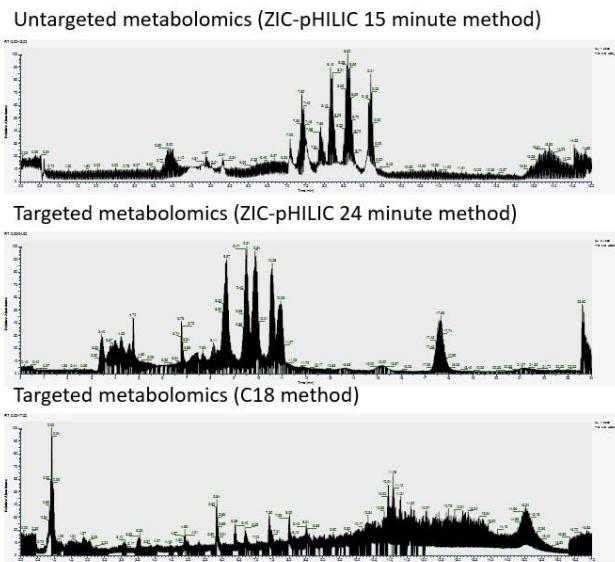


Chromatograms for the paper submitted to MDPI cancers

**Characterisation of aberrant metabolic pathways in hepatoblastoma using liquid chromatography and tandem mass spectrometry (LC-MS/MS)**

Alison Whitby\*, Pardeep Pabla\*, Bhoomi Shastri, Laudina Amugi, Álvaro Del Río-Álvarez, Dong-Hyun Kim, Laura Royo, Carolina Armengol, and Madhumita Dandapani.

## Total Ion Chromatograms (posneg)



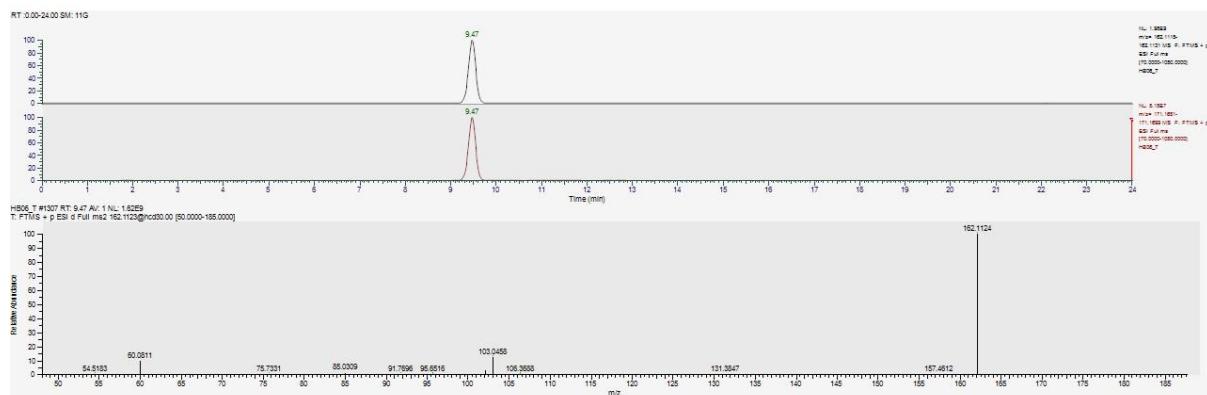
Targeted metabolomics chromatograms of statistically significant metabolites

## HILIC

### Carnitine

Top: Metabolite in sample HB06\_T  
Bottom: Internal standard (IS) in HB06\_T

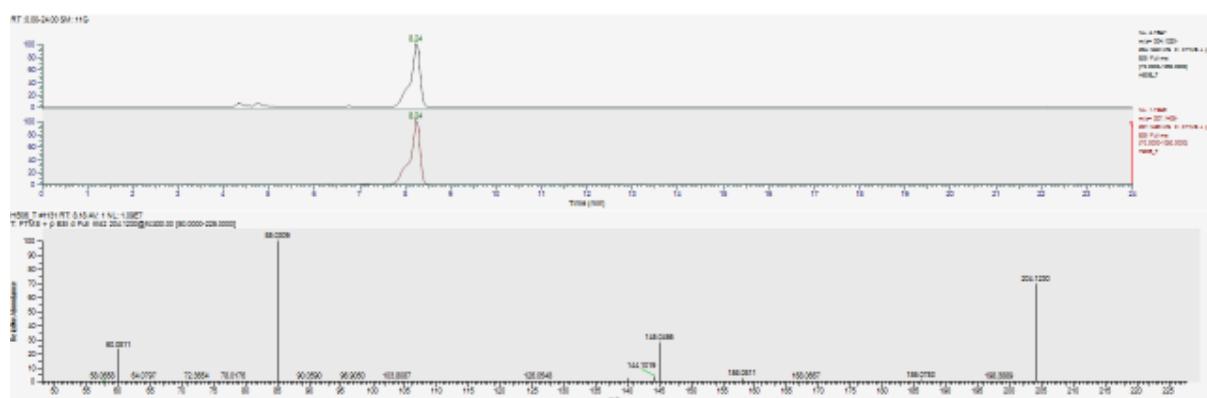
#### MS/MS of metabolite in HB06\_T



### Acetylcarnitine

Top: Metabolite in sample HB06\_T  
Bottom: Internal standard (IS) in HB06\_T

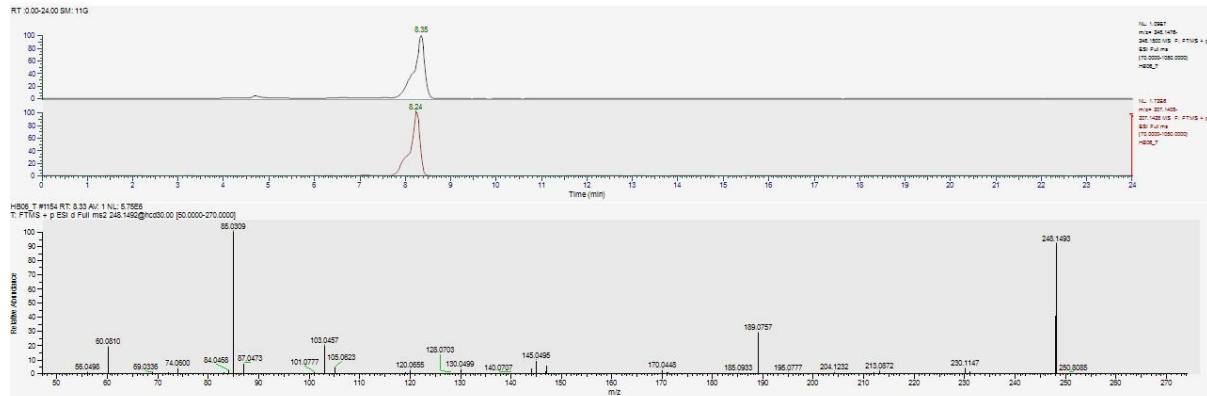
#### MS/MS of metabolite in HB06\_T



**Hydroxybutyrylcarnitine  
(using the acetylcarnitine IS for quantification)**

**Top:** Metabolite in sample HB06\_T  
**Bottom:** Internal standard (IS) of acetylcarnitine in HB06\_T

**MS/MS of metabolite in HB06\_T**

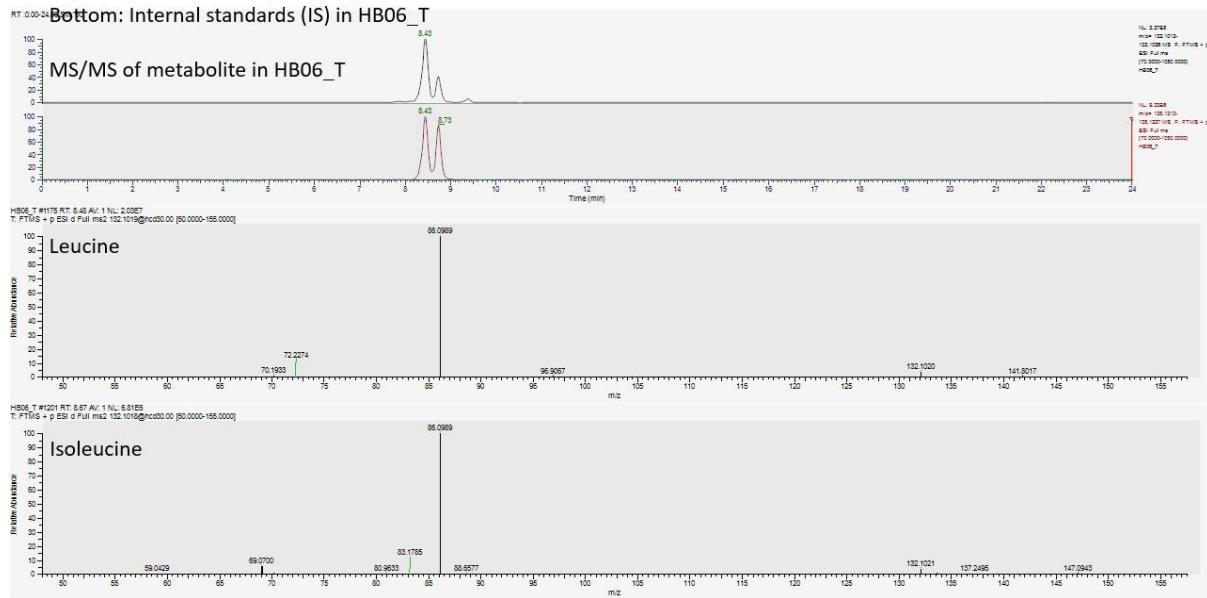


**Leucine at 8.43 min, isoleucine at 8.73 min**

**Top:** Metabolites in sample HB06\_T

**Bottom:** Internal standards (IS) in HB06\_T

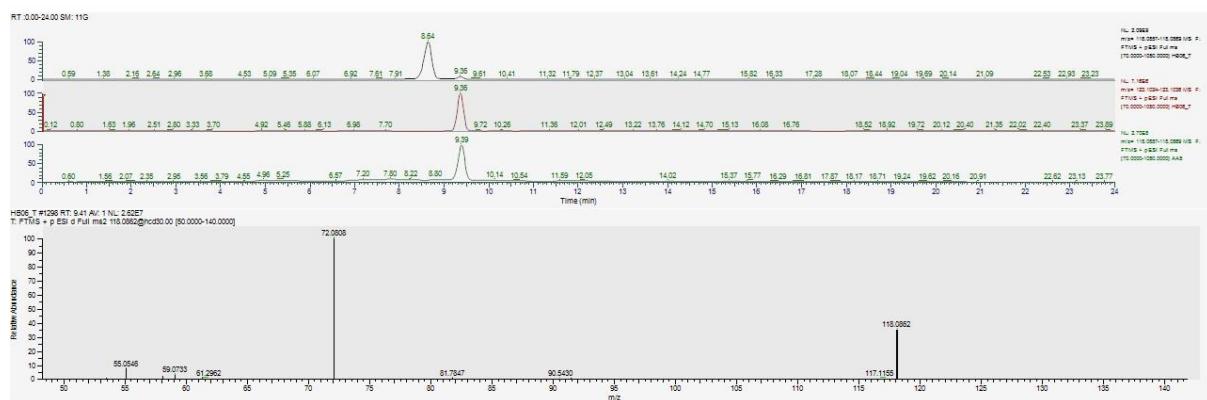
**MS/MS of metabolite in HB06\_T**



## Valine

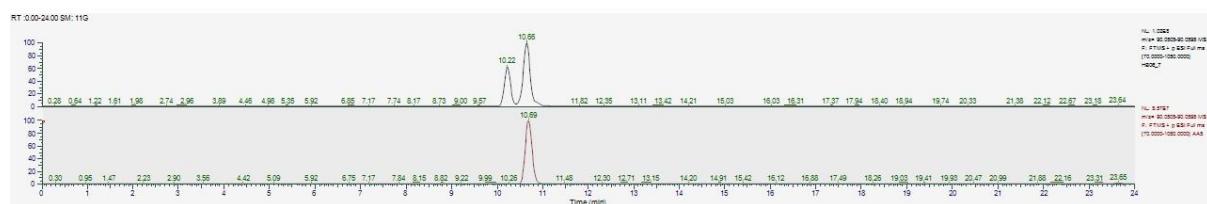
Top: Metabolite in sample HB06\_T  
Middle: Internal standard (IS) in HB06\_T  
Bottom: Standard of valine in calibration curve level 5

MS/MS of metabolite in HB06\_T



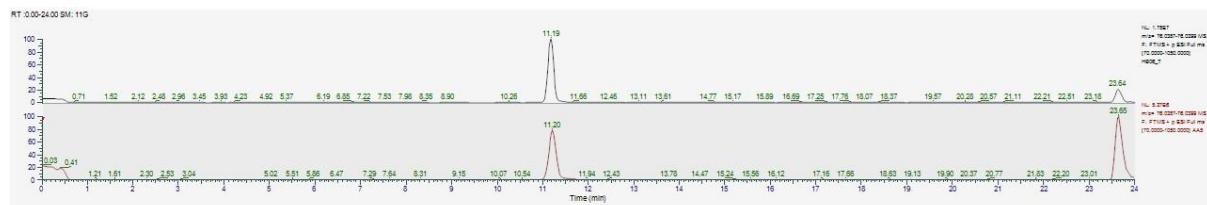
## Alanine

Top: Metabolite in sample HB06\_T  
Bottom: Standard of alanine in calibration curve level 5  
(Valine IS was used)



## Glycine

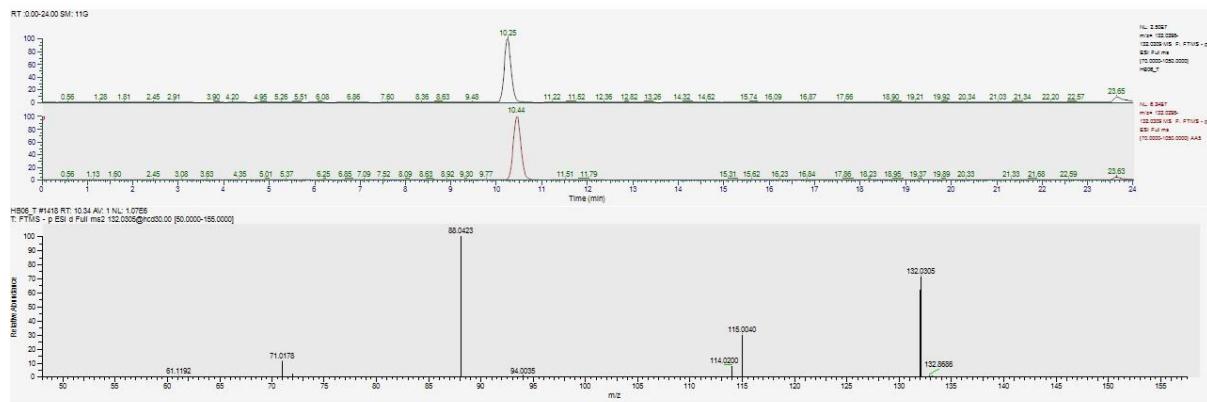
Top: Metabolite in sample HB06\_T  
Bottom: Standard of glycine in calibration curve level 5  
(Valine IS was used)



## Aspartate

Top: Metabolite in sample HB06\_T  
Bottom: Standard of aspartate in calibration curve level 5  
(Valine IS was used)

MS/MS of metabolite in HB06\_T



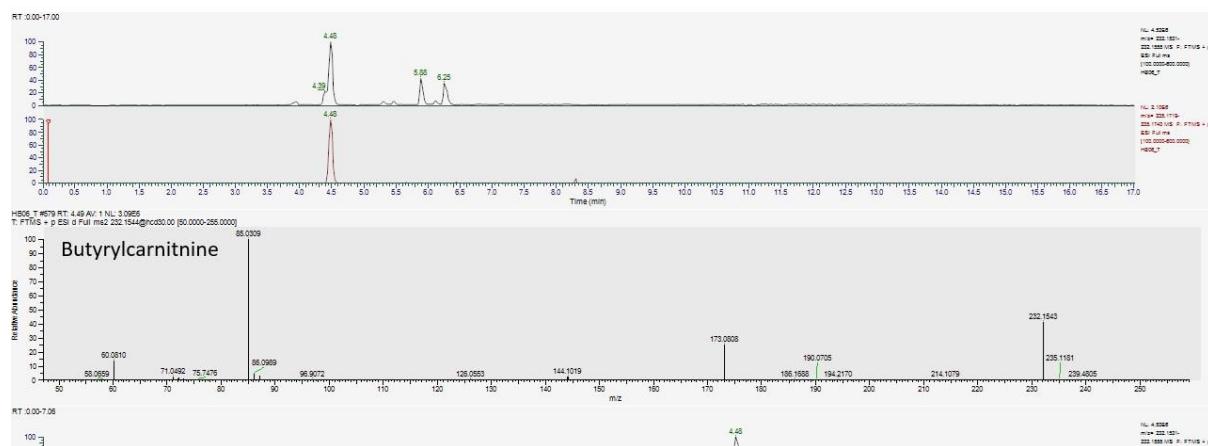
C18

Isobutyrylcarnitine at 4.39 min, butyrylcarnitine (O-butanoylcarnitine) at 4.48 min

### Top: Metabolites in sample HB06 T

Bottom: Internal standard (IS) of D3-butyrylcarnitine in HB06 T

## MS/MS of butyrylcarnitine metabolite in HB06\_T



### Propionylcarnitine

Top: Metabolite in sample HB06\_T  
Bottom: Internal standard (IS) in HB06\_T

MS/MS of metabolite in HB06\_T

RT: 0.00-17.00 min; 11.15

Relative Abundance (%)

m/z

Time (min)

Mass Spectrum (m/z)

Relative Abundance (%)

m/z

2-Methylbutyroylcarnitine at 5.27 min, Isovalerylcarnitine at 5.47 min

Top: Total of isovalerylcarnitine and 2-methylbutyroylcarnitine metabolites as entire smoothed peak in sample HB06\_T

Middle: Metabolites in sample HB06\_T

Bottom: Internal standard (IS) of D9-C5-Isovalerylcarnitine in HB06\_T

