1. Isotopologue Peaks

In [91]:
```
cd /Users/dippercheng/Documents/groningen/Visualization_UMCG
```

```
/Users/dippercheng/Documents/groningen/Visualization_UMCG
```

In [92]:
```
%run ms_graph.py
eic_path = "./MatlabEIVVisualisation"
text_path = "./MatlabEIVVisualisation/inputTIC_10MelindaSerumAscii.
txt.txt"
spectra = ExtractedIonChrome(eic_path, text_path)
```

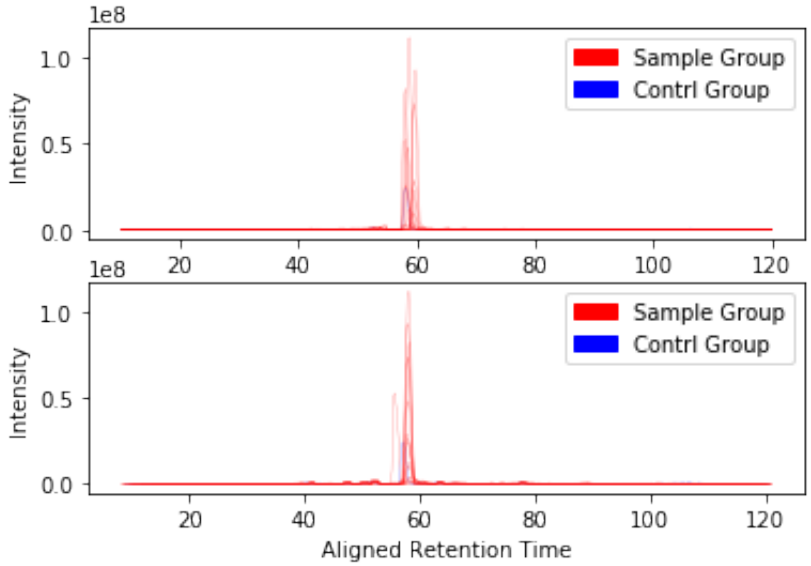
The analytical samples are divided into 2 groups: **contrl group** and **sample group**.

In [93]:
```
spectra.contrl_group_list
```

Out[93]:
```
['150210_1_01',
 '150210_1_01_150210_1_01',
 '150210_1_01_150210_5_01',
 '150210_1_01_150210_9_01',
 '150210_1_01_150210_2_01',
 '150210_1_01_150210_3_01',
 '150210_1_01_150210_4_01',
 '150210_1_01_150210_6_01',
 '150210_1_01_150210_8_01',
 '150210_1_01_150210_7_01']
```

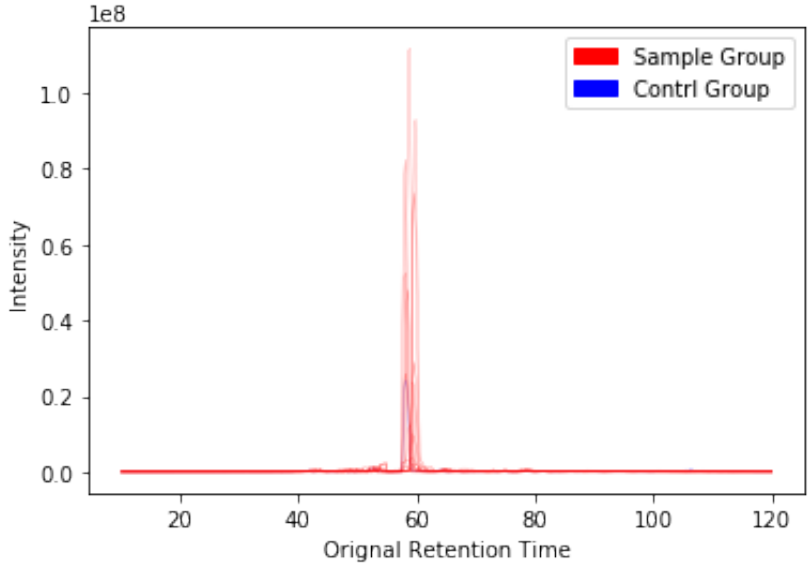
1.1. Raw LC-MS data in form of extracted ion chromatograms before and after retention time alignment

In [94]:
```
mlist = spectra.mass_list
spectra.rt_int_plot(mlist[20], after_alignment=1, before_alignment=
1)
```



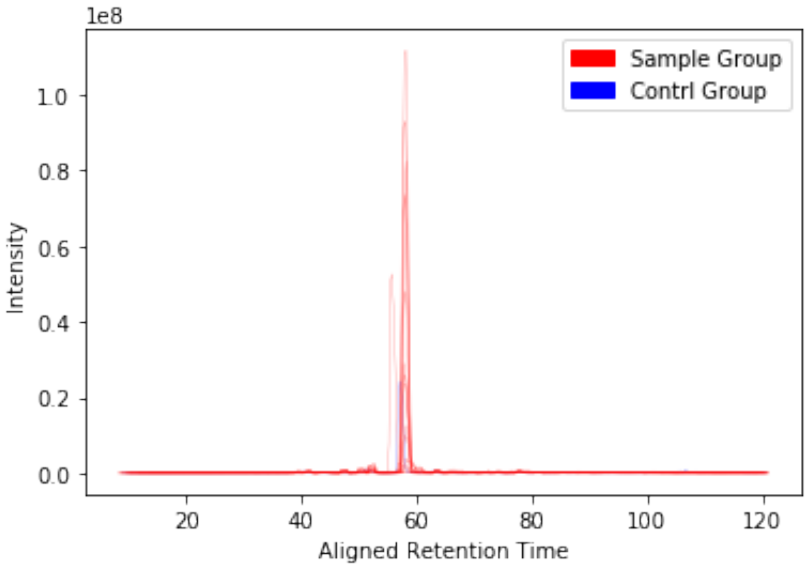
1.2 Raw LC-MS data in form of extracted ion chromatograms before retention time alignment

In [95]:
```
spectra.rt_int_plot(mlist[20], after_alignment=0, before_alignment=
1)
```



1.3 Raw LC-MS data in form of extracted ion chromatogramsafter retention time alignment

In [97]:
```
spectra.rt_int_plot(mlist[20], after_alignment=1, before_alignment=
0)
```



2. Volcano plots

In [100]:
```
cd /Users/dippercheng/Documents/groningen/Visualization_UMCG
```

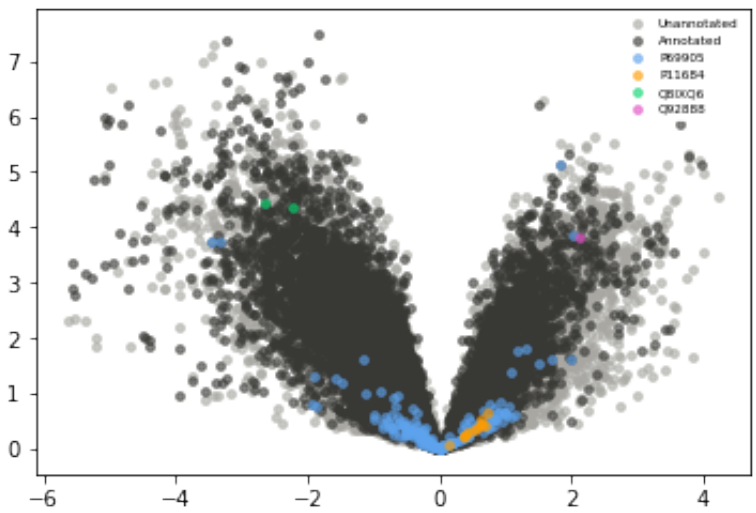
```
/Users/dippercheng/Documents/groningen/Visualization_UMCG
```

In [105]:
```
%run volcanoPlot.py
```

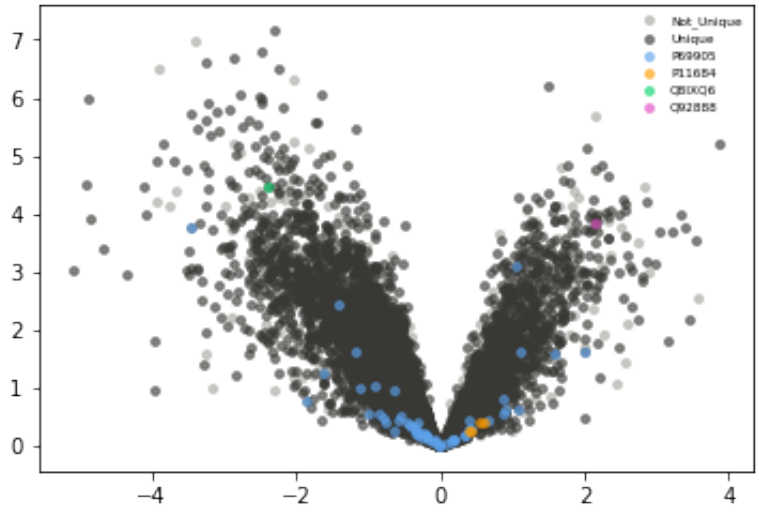
In [110]:
```
ms_tables, peptide_tables, protein_tables, dicts, meta_data = data_
parsing()
# about 5-10 minutes
```

In [111]:
```
selections = 'P69905;P11684;Q8IXQ6;Q92888'
```

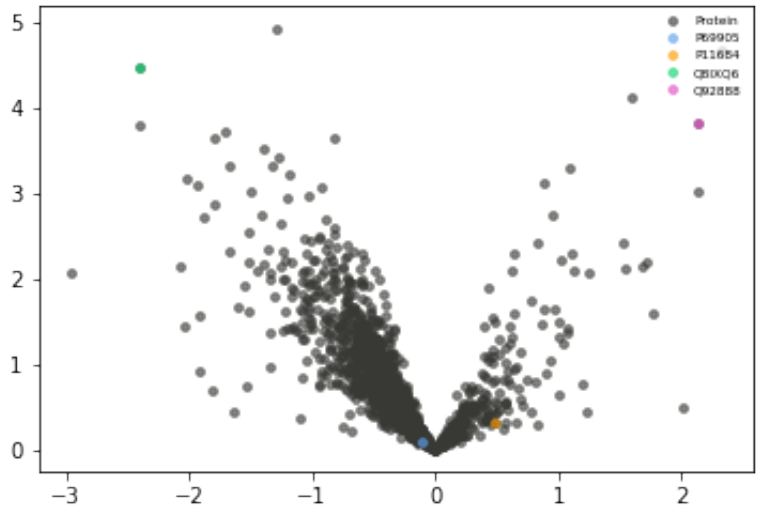
In [112]:
```
ms_data_graph(ms_tables[0], ms_tables[1], win_id=1, selected=select
ions)
```



In [113]:
```
ms_data_graph(peptide_tables[0], peptide_tables[1], win_id=2, selected=selections)
```



In [114]:
```
ms_data_graph(protein_tables[0], protein_tables[1], win_id=3, selected=selections)
```



Interactive Actions

Double click: Recover

Left click: Annotation

Right click: Detail infomation

Other actions like Zoom, box selecting, highlight Outlier

3. boxplots of peptides and isotopologue peaks

In [115]:
```
protein_fasta_id = 'P11684'
box_plot(protein_fasta_id, dicts, meta_data)
```