



**LipidIMMS Analyzer**

# **LipidIMMS Analyzer FAQs**

Zhiwei Zhou <zhouzw@sioc.ac.cn>

Zheng-Jiang Zhu <jiangzhu@sioc.ac.cn>

June 02, 2018

**Laboratory for Mass Spectrometry and Metabolomics**

**[www.zhulab.cn](http://www.zhulab.cn)**

Interdisciplinary Research Center on Biology and Chemistry (IRCBC)

Shanghai Institute of Organic Chemistry

Chinese Academy of Sciences, Shanghai, China

**1. What is the optimal collision energy (CE) to acquire MS/MS data?**

**Answer:** In Agilent QTOF instruments, we recommend the CE value is 30 eV. In Waters QTOF instruments, we recommend the CE value of transfer cell is 30-50 eV (ramp).

**2. Why do I see the “500 Internal Privoxy Error”?**

**Answer:** The error of “500 Internal Privoxy Error” often appears when using proxy server or VPN to visit our web server. Please turn off the proxy server or VPN, and try again.

**3. Could LipidIMMS Analyzer support other IM-MS instruments (e.g. Bruker TIMS)?**

**Answer:** Currently, LipidIMMS Analyzer only supports the data generated from Agilent and Waters instruments. In fact, if users could import data with the same format as Agilent or Waters, the software could also process data from any instrument.

**4. Why do I see the error of “<html><head><title>413 Request Entity” when uploading the MS/MS data?**

**Answer:** This error would appear if **the size of data files larger than the limit** (currently, **200M** in total). In this case, we suggest reducing the number of uploaded MS/MS data files. Make sure the total size is less than 200 M.

**5. Can I use the LipidIMMS to process Q-TOF data without ion mobility?**

**Answer:** Yes, the user could simply skip the CCS match to perform lipid identification using data acquired from Q-TOF.

**6. What is the recommended LC separation condition for lipidomics?**

**Answer:** The LipidIMMS Analyzer support both reverse phase (RP) and hydrophilic liquid chromatography (HILIC) columns. For RP column, we recommend using a C18 column for the separation. For HILIC column, we recommend using the same HILIC column (Phenomenex Kinetex HILIC column, 2.1\*100mm, 1.7um), because different HILIC columns may have the significant differences of stationary chemistry.

**7. How do I determine the score weights in the “Score integration”?**

**Answer:** We recommend values for “RT score weigh”, “CCS score weight”, and “MS/MS score weight” are 0.2, 0.4 and 0.4, respectively. In general, we think MS/MS match score is more discriminative than the other two scores. Therefore, users can increase the “MS/MS score weight”, and decrease the weights for other two scores. However, the settings for score weights are completely empirical.

**8. Do I have to include all lipid species for RT calibration?**

**Answer:** No, users could select all or a portion of these lipids for the calibration according to their experiments and availability. If some lipids were not detected in your system, please remove the rows of missing lipids.