Plants accumulate human beneficial metabolites such as amino acids, flavonoids and sulfur-containing metabolites (S-metabolites) with a wide range of biological activities related to antioxidation, platelet aggregation inhibition, and anti-inflammatory benefit. Profiling methods of S-metabolites with high accuracy and throughput are being required for efficient phytochemical functional genomics and crop breeding. Here, we describe the S-metabolite-targeted analysis using liquid chromatography (LC)-fourier transform ion cyclotron resonance mass spectrometry (FT-ICR-MS) with U-13C-labeled onion bulb. Natural abundance of $^{32}$S ($32.065073$ Da) and its isotope $^{34}$S ($33.067868$ Da) is $95.02\%$ and $4.21\%$, respectively. These facts are obviously reflected on molecular ion peaks of S-metabolites. Thus, the isotope $^{15}$N-substituted C13H21N3O6S2 isotope $^{13}$C-labeled onion bulb was purchased from parents of higher-yielding hybrids and JP-US, JST Research Program (SICORP) for JP-NZ Japan Advanced Plant Science Network.

**Summary**

- **Health-promoting crops**
  - Genomics
  - Transcriptomics
  - Next-generation sequencing etc.
  - AGRc

- **Phytochemical genomics**
  - Crop breeding
  - Diverse population of plants/chromosomes
  - GS/GM

- **Metabolomics**
  - LC-MS etc
  - Sulfur-containing metabolite-targeted analysis using liquid chromatography-mass spectrometry highly accurate analysis
  - MS/MS
  - Hexapol ion transfer

**Peak picking of S-metabolite**

FT-ICR-MS (Solarix 7.0 T)

**Profiling of S-metabolites using LC-FT-MS in non-labeled and 13C-labeled onion bulb**

**Conclusion**

- Onion bulb includes quite rare S-metabolites which have strong anti-inflammatory activity.
- Strategy of biomarker screening will be changed by this method with approaches of natural products chemistry

**Acknowledgements**

Strategic International Collaborative Research Program (SICORP) for JP-NZ and JP-US, JST

Japan Advanced Plant Science Network

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**Table of S-metabolites**

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<td>C13H21N3O6S2</td>
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- C13H21N3O6S2
- Comparison of peak pattern
- Determination of elemental composition
- MS/MS analysis

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**Image of picking S-metabolite peaks**

FT-ICR-MS (Solarix 7.0 T)

**EICs of 6 representative S-metabolites**

- S-propylmercapto glutathione
- S-propylmercapto glutathione (S-proglutathione)
- 13C-labeled S-propylmercapto glutathione
- C13H21N3O6S2
- 1 elemental composition
- S-peak picking
- C,H,N,O,S < 1 mDa
- S-peak picking
- C13H21N3O6S2
- C13H21N3O6S2
- S-metabolite peaks

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**Image of picking S-metabolite peaks**

FT-ICR-MS (Solarix 7.0 T)

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