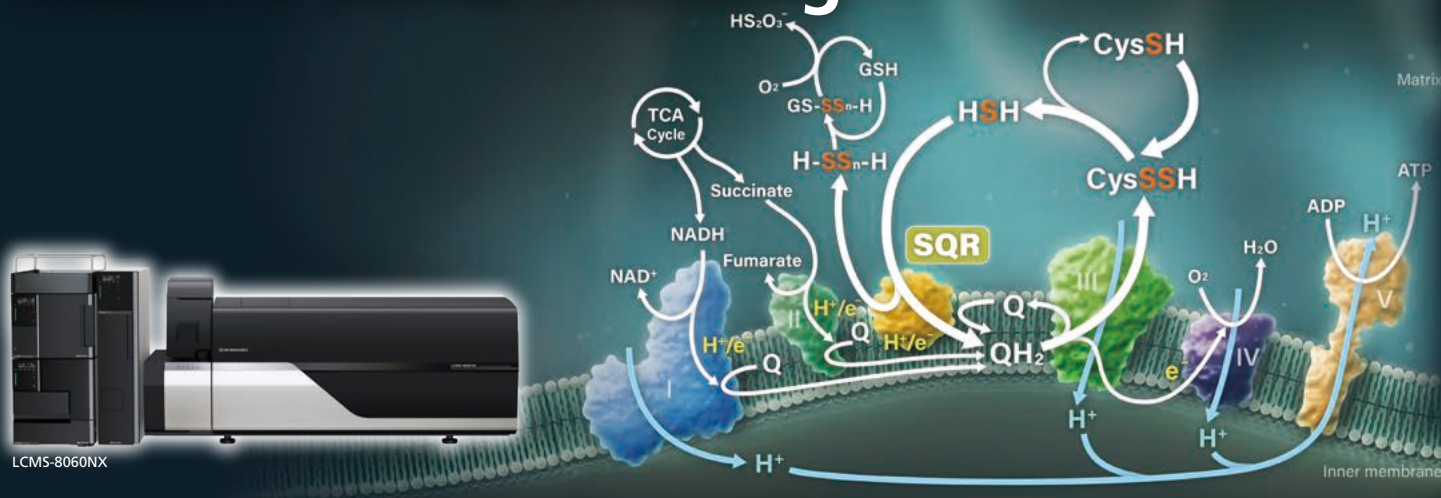


For LabSolutions™ LCMS

# LC/MS/MS Method Package for Reactive Sulfur Profiling



## Sample Pretreatment Protocols and Analytical Methods for 17 Sulfur-Containing Metabolites, Including Reactive Sulfur Species

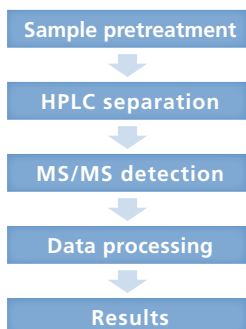
Oxidative stress and the subsequent degradation of biological molecules related to various reactive oxygen species is an important field of clinical research. Recently, an expansive sulfur metabolome investigation conducted by Professor Takaaki Akaike et al. of Tohoku University Graduate School of Medicine has shown that cysteine persulfide and other reactive sulfur species play an important role in biological defense and antioxidant response systems. Reactive sulfur species are found in every organ of the body, including the brain, heart, and liver, and are even found in the blood in healthy people. Researchers are investigating the role of these compounds in relation to aging and conditions associated with oxidative stress such as respiratory disease, heart disease, and cancer.

This LC/MS/MS Method Package for Reactive Sulfur Profiling offers analytical methods for LC/MS/MS that target all 17 sulfur-containing metabolites, including reactive sulfur species, with separation conditions and MS parameters that are optimized for each compound. It also comes with example pretreatment protocols, including derivatization steps, for biological samples containing cells and blood plasma. The method package allows the user to analyze sulfur-containing metabolites without time-consuming investigation into sample preparation and analytical conditions. The Shimadzu Multi-omics Analysis Package also offers a tool to visualize quantitative results obtained with this method package. The tool helps users interpret results by providing easy-to-understand graphical displays of the relationships and ratios between metabolic components in different sample sets.

### LC/MS/MS Method Package for Reactive Sulfur Profiling

- Chromatographic parameters optimized for the analysis of 17 sulfur-containing metabolites
- Individually optimized MS/MS parameters allowing determination of relative quantities
- Example pretreatment protocols for cell and blood plasma samples
- Use with Multi-omics Analysis Package to visualize quantitative results

Total support from sample pretreatment to analysis of results



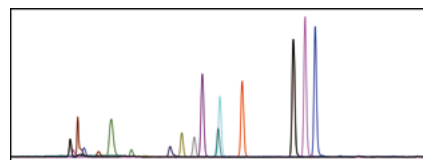
### Registered Compounds

Compound Name	Name in Method Package
Cysteine	CysSH
Cysteine hydrodisulfide	CysSSH
Cysteine hydrotrisulfide	CysSSSH
Cystine	CysSSCys
Cystine trisulfide	CysSSSCys
Cystine tetrasulfide	CysSSSSCys
Glutathione	GSH
Glutathione hydrodisulfide	GSSH
Glutathione hydrotrisulfide	GSSSH
Glutathione disulfide	GSSG
Glutathione trisulfide	GSSSG
Glutathione tetrasulfide	GSSSSG
Sulfite	HSO3-
Thiosulfite	HS2O3-
Reaction By-product_1	Bis-S-HPE-AM
Reaction By-product_2	Bis-SS-HPE-AM
Reaction By-product_3	Bis-SSS-HPE-AM

# LC/MS/MS Method Package for Reactive Sulfur Profiling

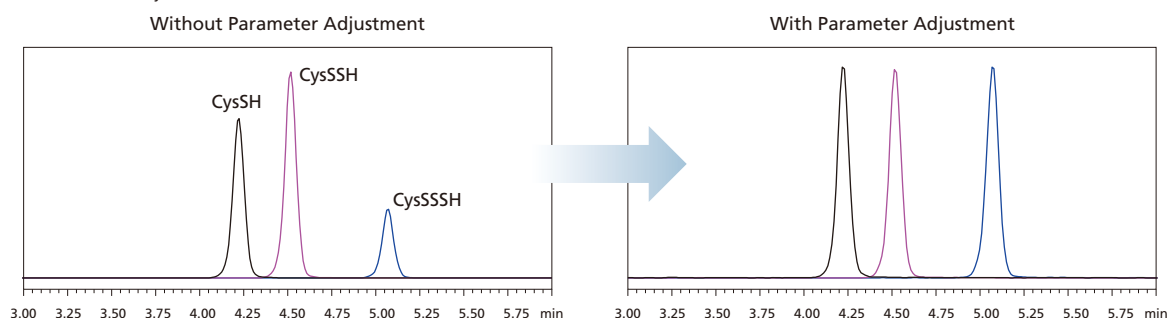
## LC Parameters Optimized for Analysis of 17 Sulfur-Containing Metabolites

Conventional analytical methods have trouble with the simultaneous analysis of reduced and oxidized glutathione, and cysteine and cystine, due to their different polarities and compounds with different numbers of sulfur atoms. When this method package is combined with a PFPP column and optimized LC parameters, matrix effects are reduced while analysis is completed in around 17 minutes.



## MS/MS Parameters Allowing Determination of Relative Quantities

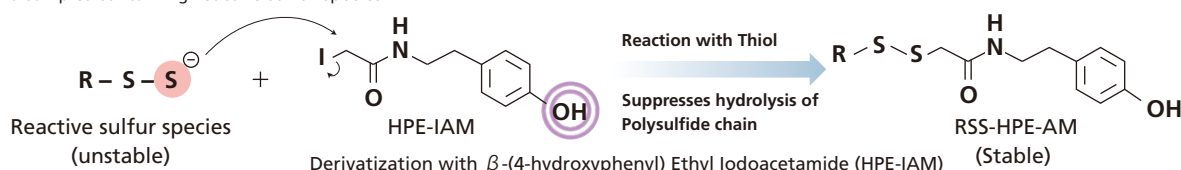
Reactive sulfur species pose a significant challenge for quantitative analysis due to their instability and the difficulty of obtaining reference standards. The methods included in this method package adjust MS parameters so the intensities of each component within a group are roughly equivalent for a given concentration. This allows the relative quantities of components within each group to be determined accurately across a wide dynamic range. Furthermore, an external standard method is adopted with readily available standards, such as cysteine and glutathione, to allow the estimation of absolute amounts for components without readily available standards.



\* The scaling of the peak intensities changes depending on if you use parameter adjustment or not.

## Example Pretreatment Protocols for Cell and Blood Plasma Samples: Stabilization of Reactive Sulfur Species

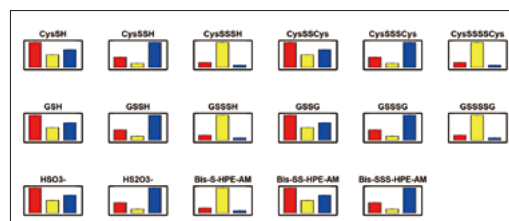
Among sulfur-containing metabolites, reduced reactive sulfur species are extremely unstable and samples containing them require proper pretreatment protocols that include derivatization steps. The instruction manual for this method package includes example pretreatment protocols for cell and blood plasma samples containing reactive sulfur species.



## Visualization of Quantitative Results

The method package includes a blank map compatible with the Shimadzu Multi-omics Analysis Package for visualizing quantitative results. This blank map helps to interpret quantitative results by providing an easy-to-understand visual representation of the metabolic relationships and ratios between each component in sulfur-containing metabolites, as well as the differences between groups of samples.

\* Multi-omics Analysis Package sold separately.



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### Notes

1. LabSolutions™ LCMS version 5.114 or later is required.
2. This method package is for research purposes.



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