Supporting Information Data for

The Liberation of Hydrogen Sulfide from Dicysteinyl Polysulfanes in Model Wine

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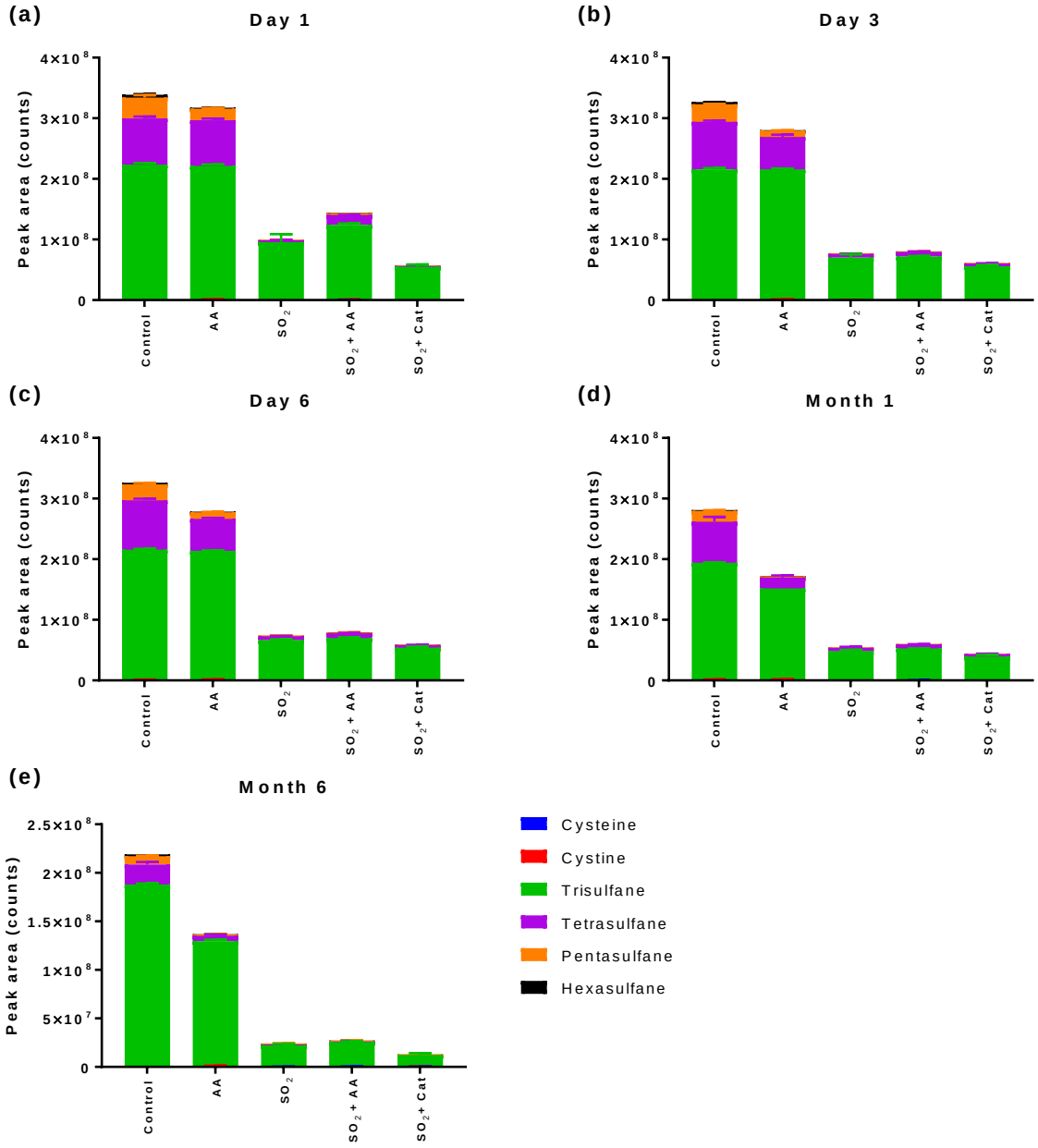

Figure S1. Stacked bar graphs displaying the total relative amounts of polysulfanes remaining in the samples as a function of time and as a function of ascorbic acid (AA), sulfur dioxide (SO_2), sulfur dioxide and ascorbic acid (SO_2 + AA), and sulfur dioxide and (+)-catechin (SO_2 + Cat) treatments.

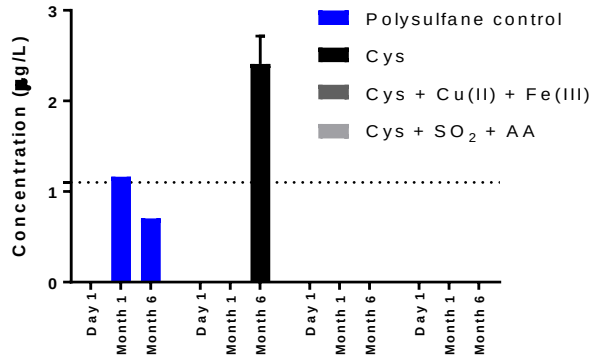

Figure S2. Hydrogen sulfide liberation in the anoxically-prepared L-cysteine control samples measured over the course of six months. The control samples were prepared in model wine and contained only cysteine (Cys), or cysteine in combination with Cu(II) and Fe(III) [Cys + Cu(II) + Fe(III)], or cysteine in combination with SO_2 and ascorbic acid (Cys + SO_2 + AA). Odor threshold of H_2S of 1.1 – 1.6 µg/L[1] indicated by dashed line parallel to the x-axis.

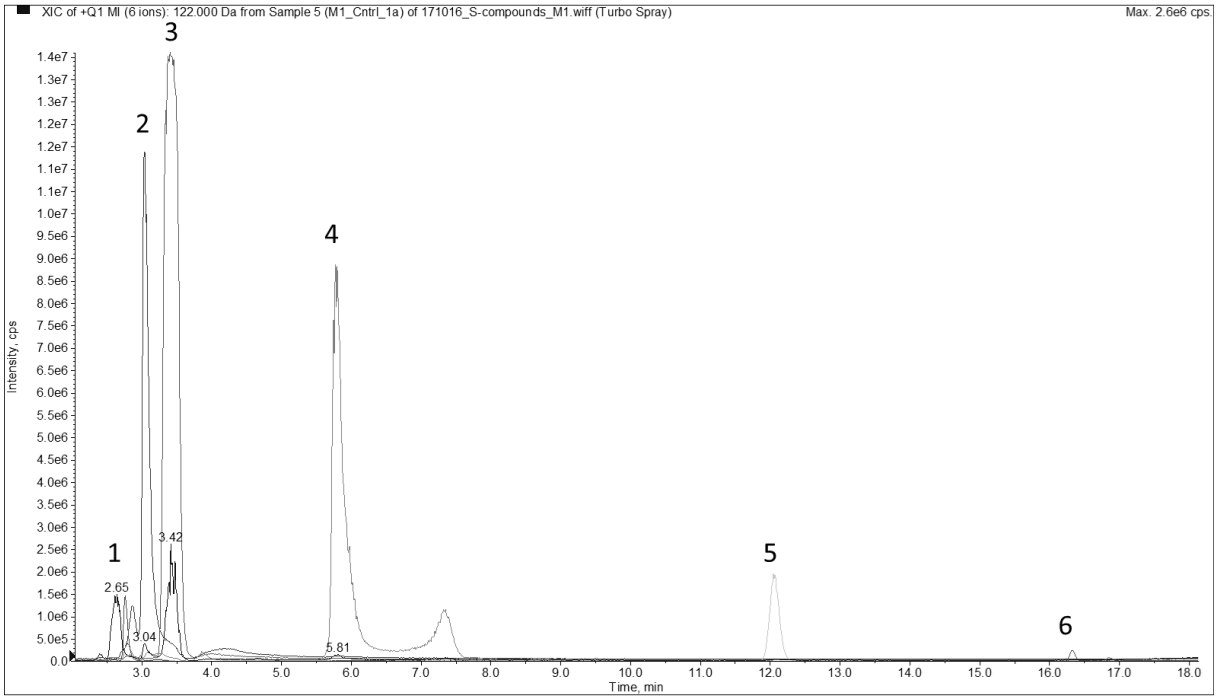

Figure S3. Representative HPLC-SIM chromatogram of the L-cysteine based polysulfanes in the control samples, showing cystine (1), cysteine (2), trisulfane (3), tetrasulfane (4), pentasulfane (5), and hexasulfane (6).

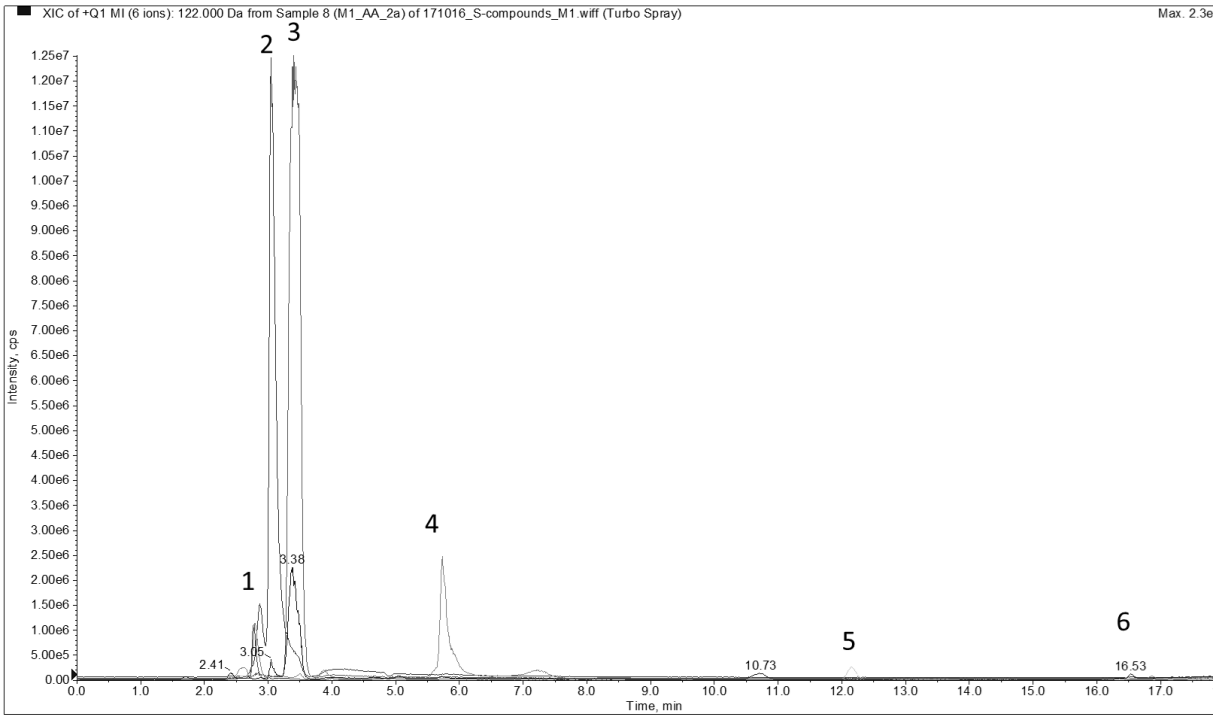

Figure S4. Representative HPLC-SIM chromatogram of the L-cysteine based polysulfanes in the ascorbic acid treated samples, showing cystine (1), cysteine (2), trisulfane (3), tetrasulfane (4), pentasulfane (5), and hexasulfane (6).

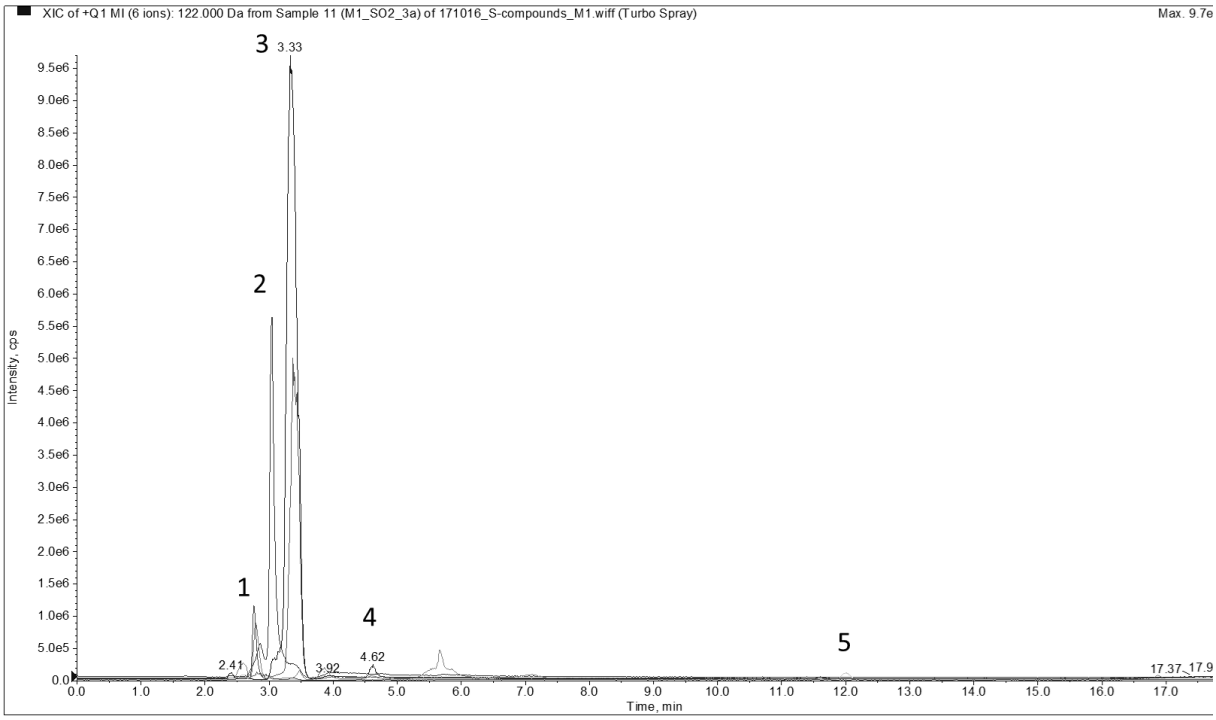

Figure S5. Representative HPLC-SIM chromatogram of the L-cysteine based polysulfanes in the sulfur dioxide treated samples, showing cystine (1), cysteine (2), trisulfane (3), tetrasulfane (4), and pentasulfane (5).

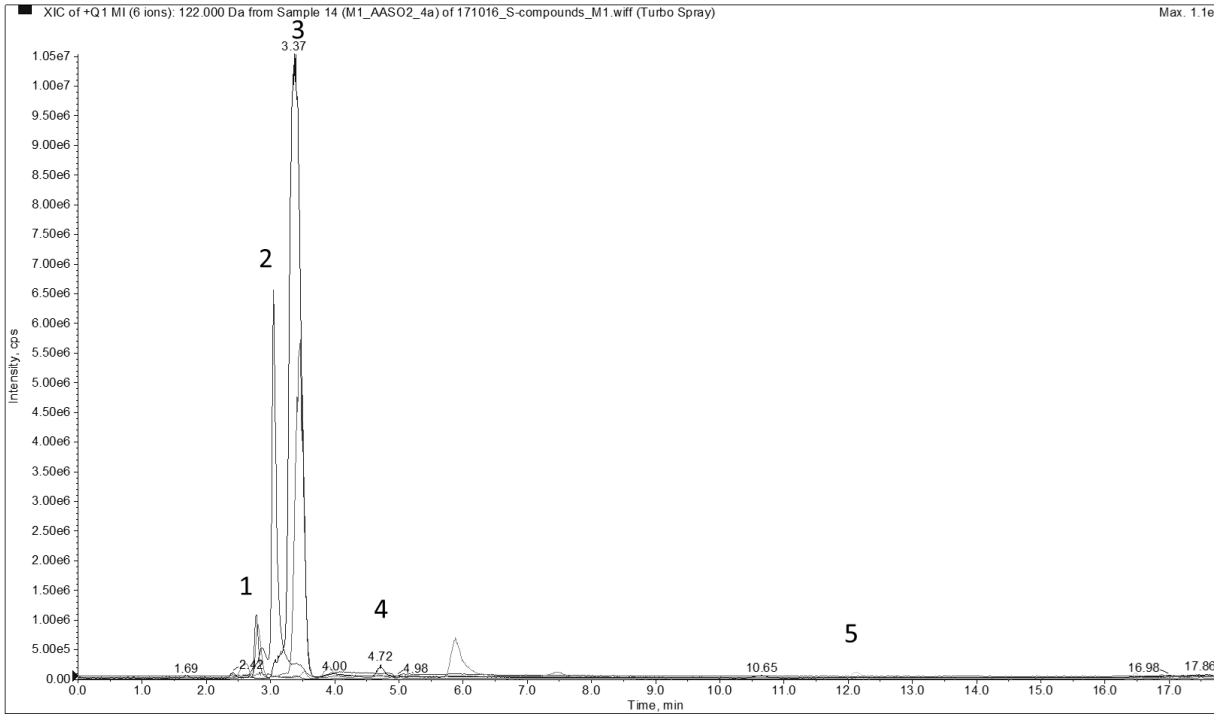

Figure S6. Representative HPLC-SIM chromatogram of the L-cysteine based polysulfanes in the sulfur dioxide and ascorbic acid treated samples, showing cystine (1), cysteine (2), trisulfane (3), tetrasulfane (4), and pentasulfane (5).

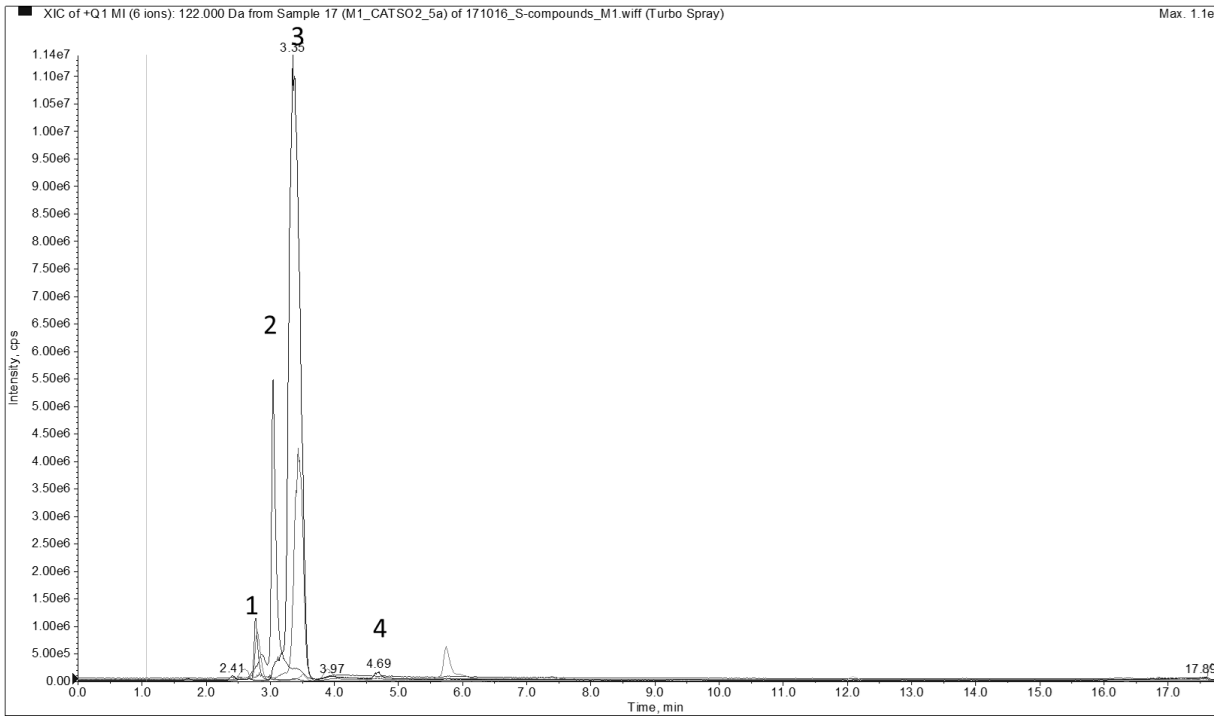

Figure S7. Representative HPLC-SIM chromatogram of the L-cysteine based polysulfanes in the sulfur dioxide and (+)-catechin treated samples, showing cystine (1), cysteine (2), trisulfane (3), and tetrasulfane (4).

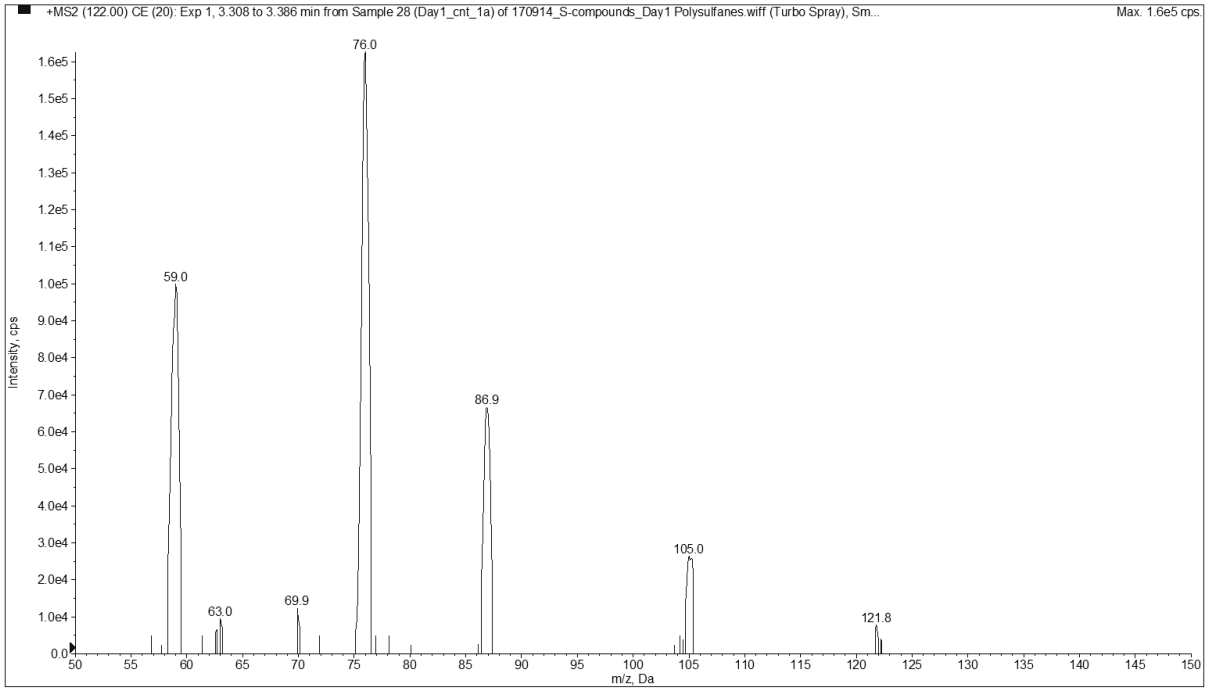

Figure S8. Representative mass spectrum of cysteine with elemental composition $C_3H_7NO_2S$ with $[M + H]^+$ ion of *m/z* 122.

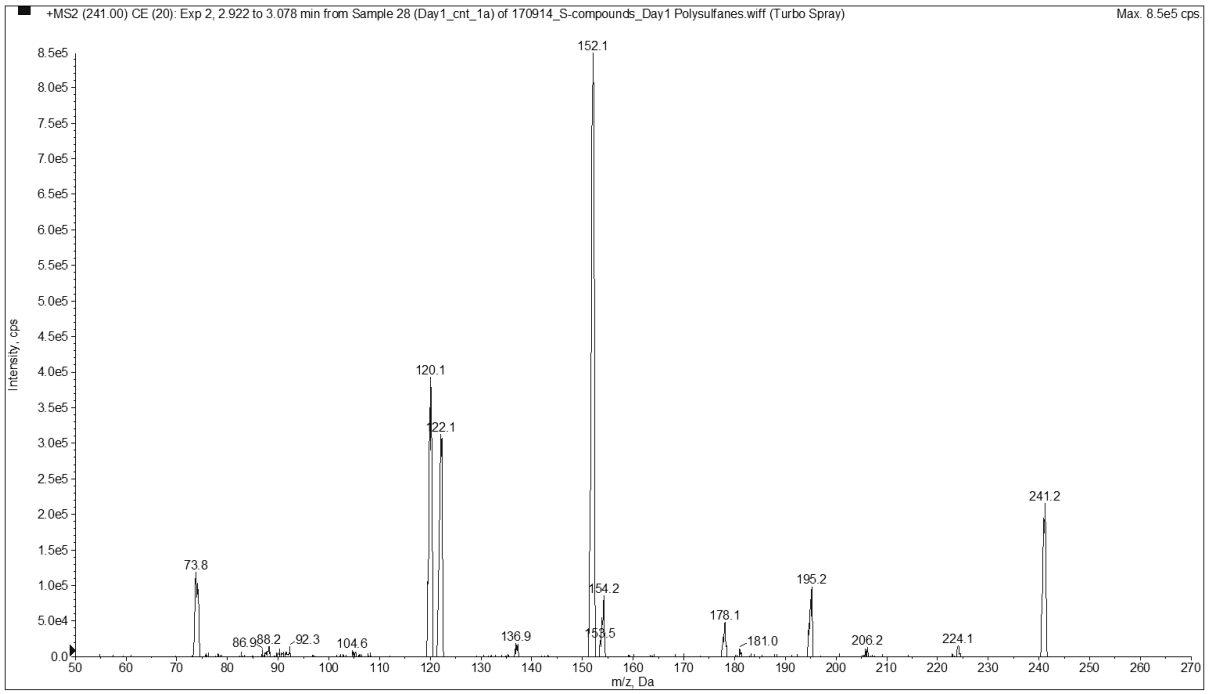

Figure S9. Representative mass spectrum of cystine with elemental composition $C_6H_{12}N_2O_4S_2$ with $[M + H]^+$ ion of *m/z* 241.

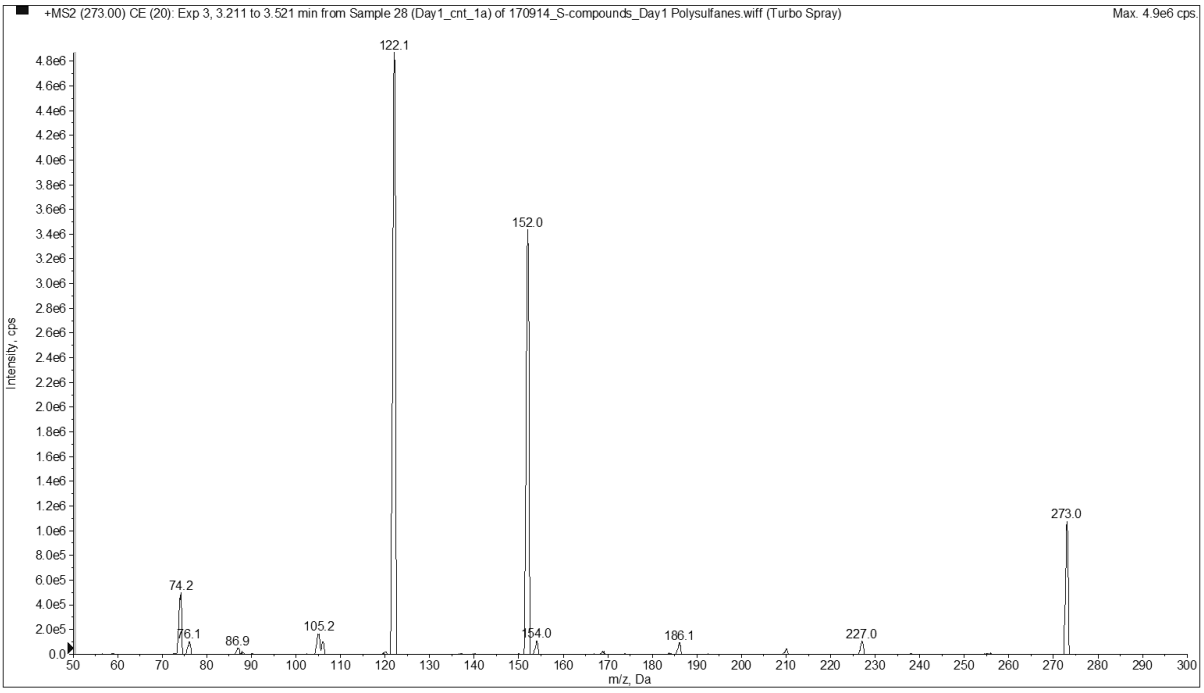

Figure S10. Representative mass spectrum of dicysteinyl trisulfane with $[M + H]^+$ ion of *m/z* 273.

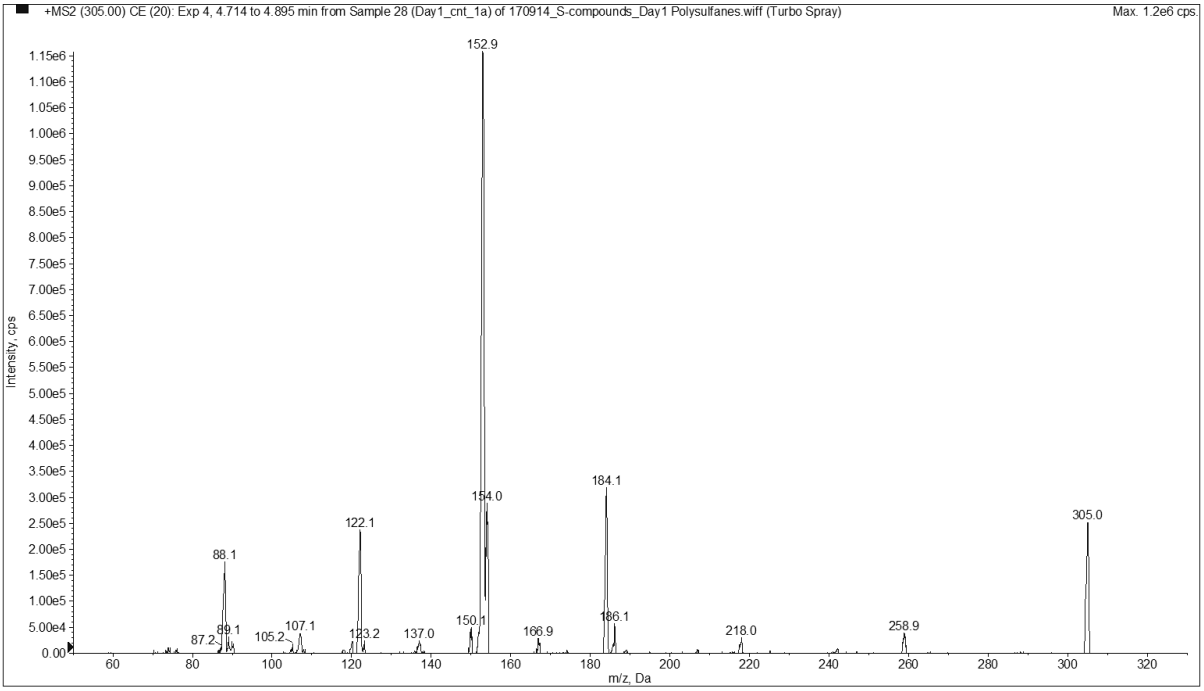

Figure S11. Representative mass spectrum of tetrasulfane with $[M + H]^+$ ion of *m/z* 305.

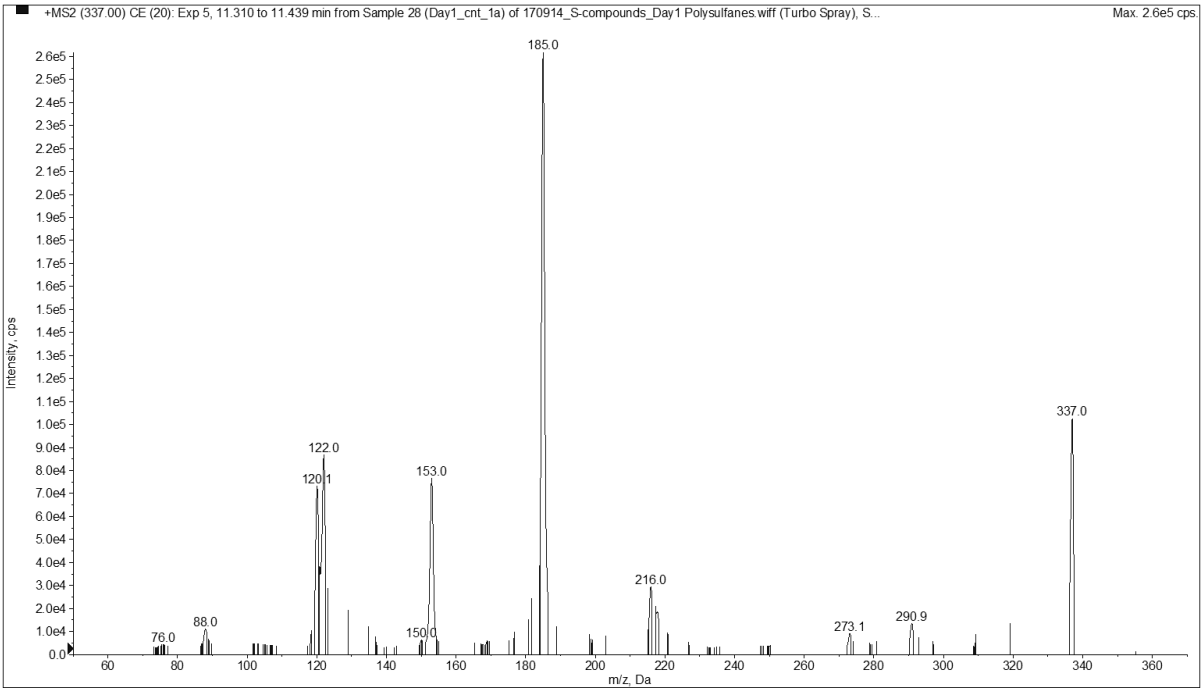

Figure S12. Representative mass spectrum of pentasulfane with $[M + H]^+$ ion of *m/z* 337.

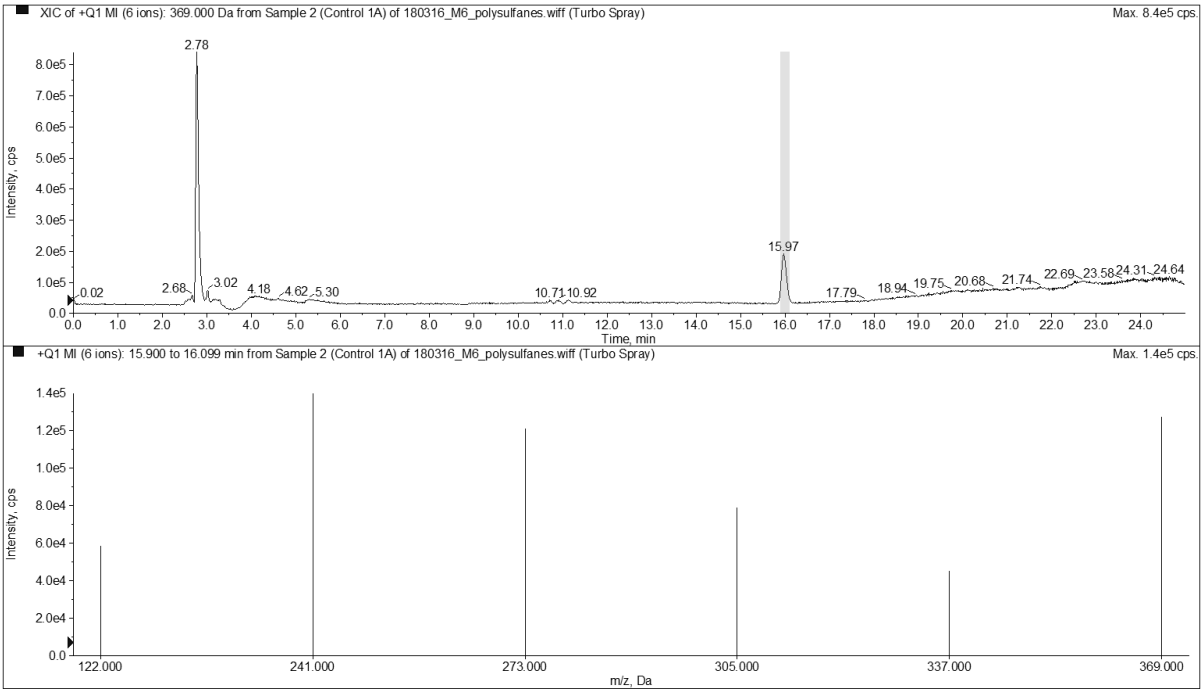

Figure S13. Representative HPLC-SIM chromatogram and extracted *m/z* 369 ion for $C_6H_{12}N_2O_4S_6$

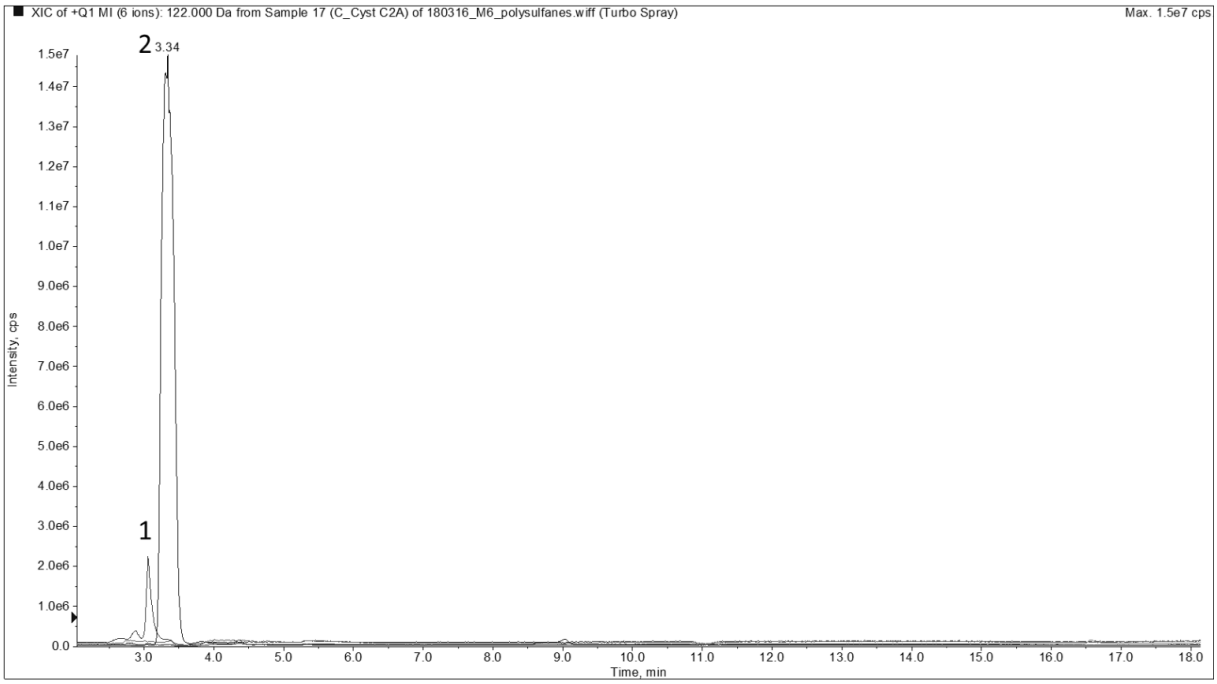

Figure S14. Representative HPLC-MSMS chromatogram of cysteine control samples showing only cystine (1) and cysteine (2).

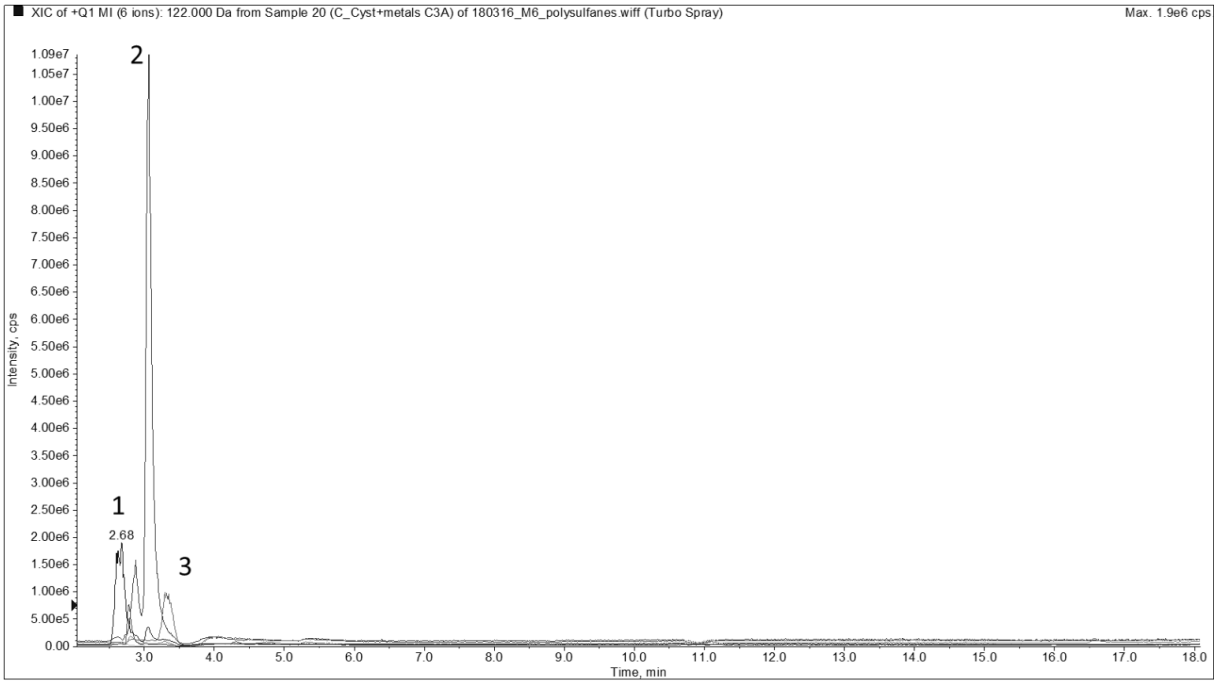

Figure S15. Representative HPLC-MSMS chromatogram of cysteine control samples containing Cu(II) and Fe(III) showing cystine (1), cysteine (2), and trisulfane (3).

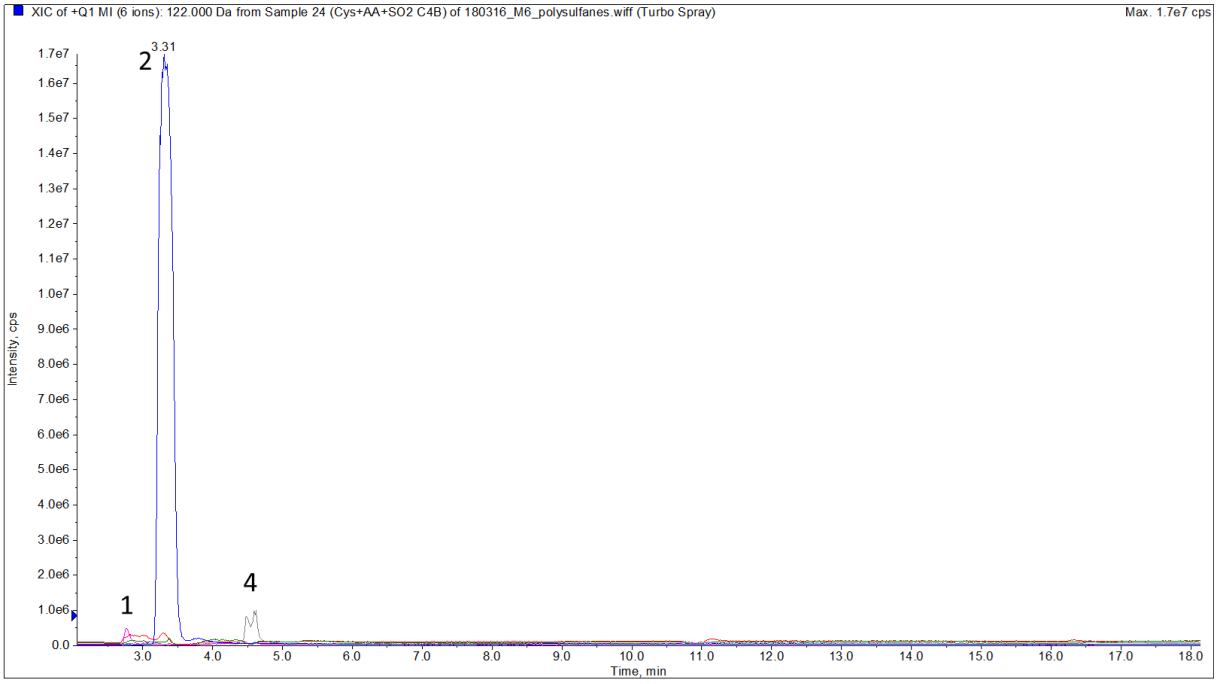

Figure S16. Representative HPLC-MSMS chromatogram of cysteine control samples containing ascorbic acid and SO_2 showing cystine (1), cysteine (2), and tetrasulfane (4).

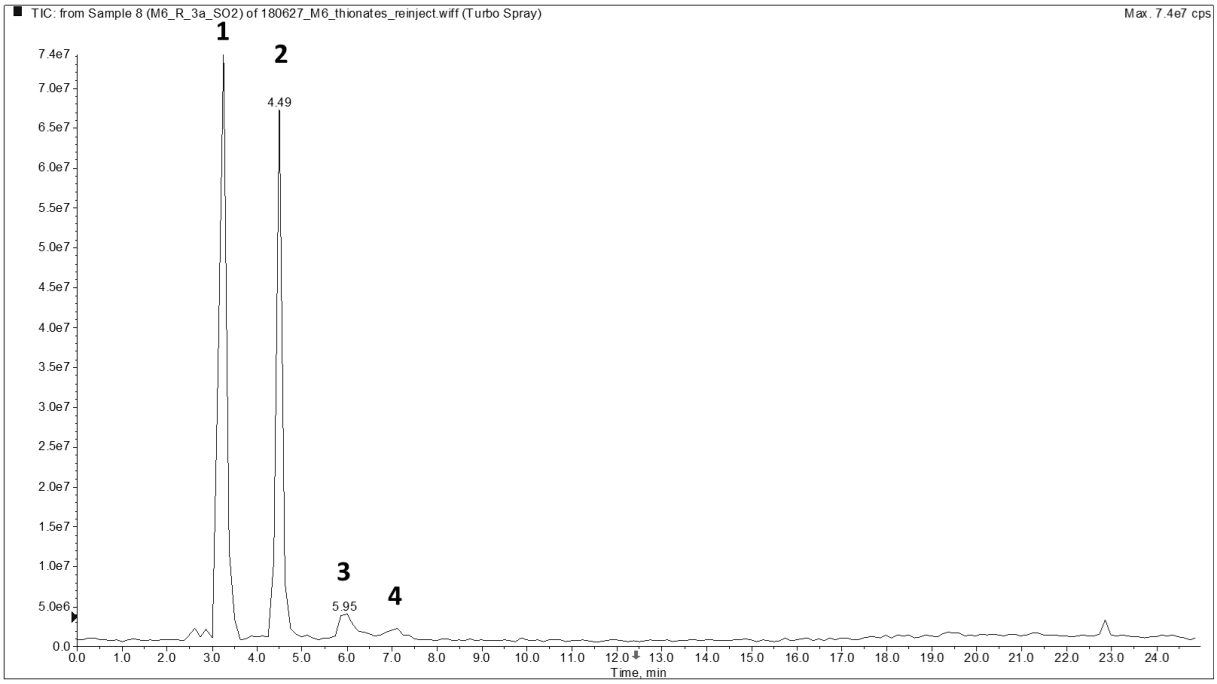

Figure S17. Representative HPLC-MSMS chromatogram of cysteine-*S*-sulfonates in sulfur dioxide treated samples, with $C_3H_7NO_5S_2$ (1), $C_3H_7NO_5S_3$ (2), and $C_3H_7NO_5S_4$ (3 and 4).

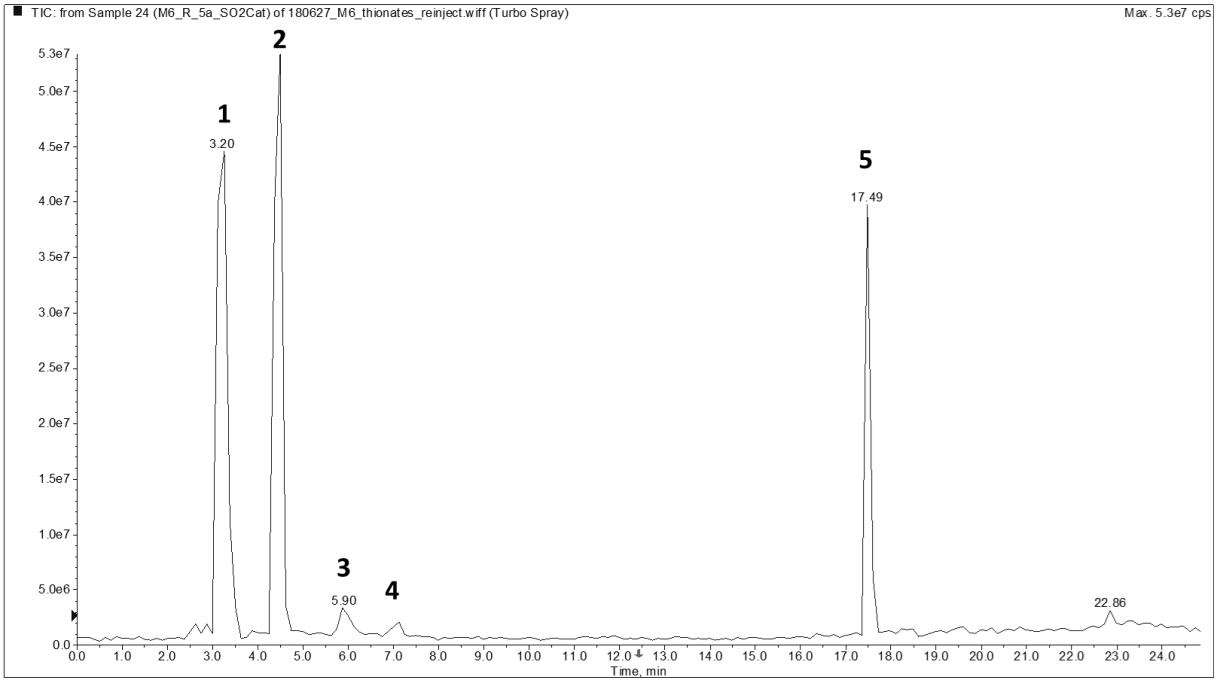

Figure S18. Representative HPLC-MSMS chromatogram of cysteine-*S*-sulfonates in sulfur dioxide and (+)-catechin treated samples, with $C_3H_7NO_5S_2$ (1), $C_3H_7NO_5S_3$ (2), $C_3H_7NO_5S_4$ (3 and 4), and an unidentified compound (5).

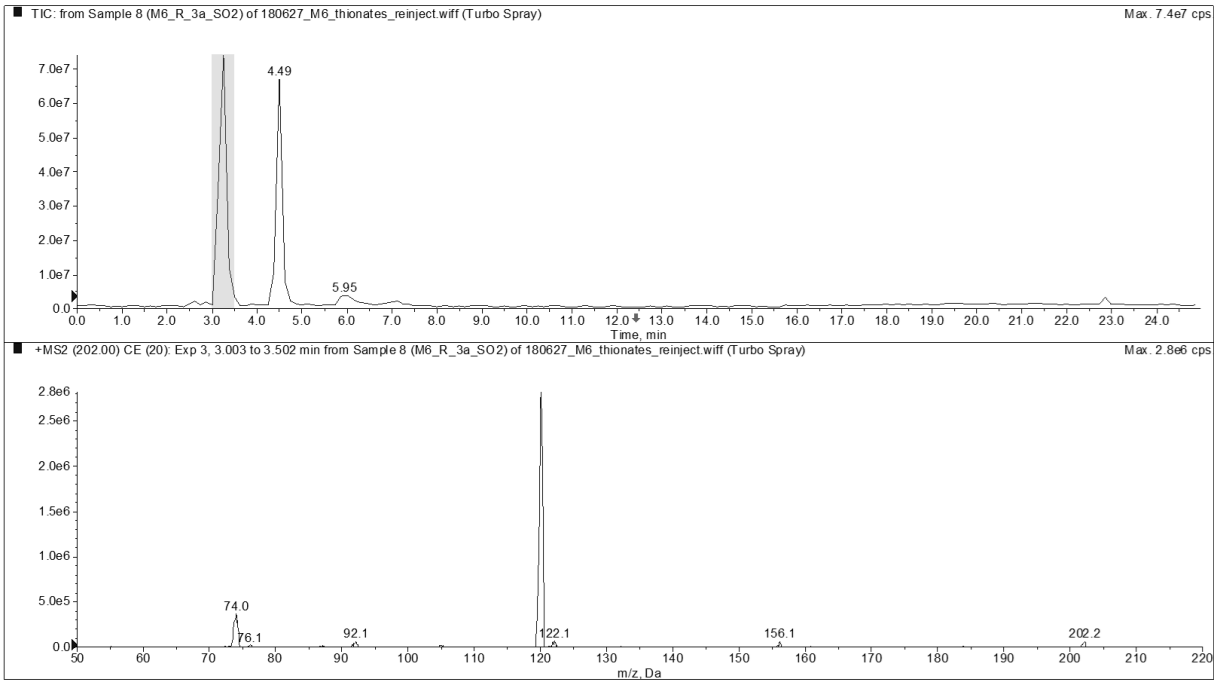

Figure S19. Representative HPLC-MSMS chromatogram and mass spectrum of $C_3H_8NO_5S_2$, retention time 3.3 min.

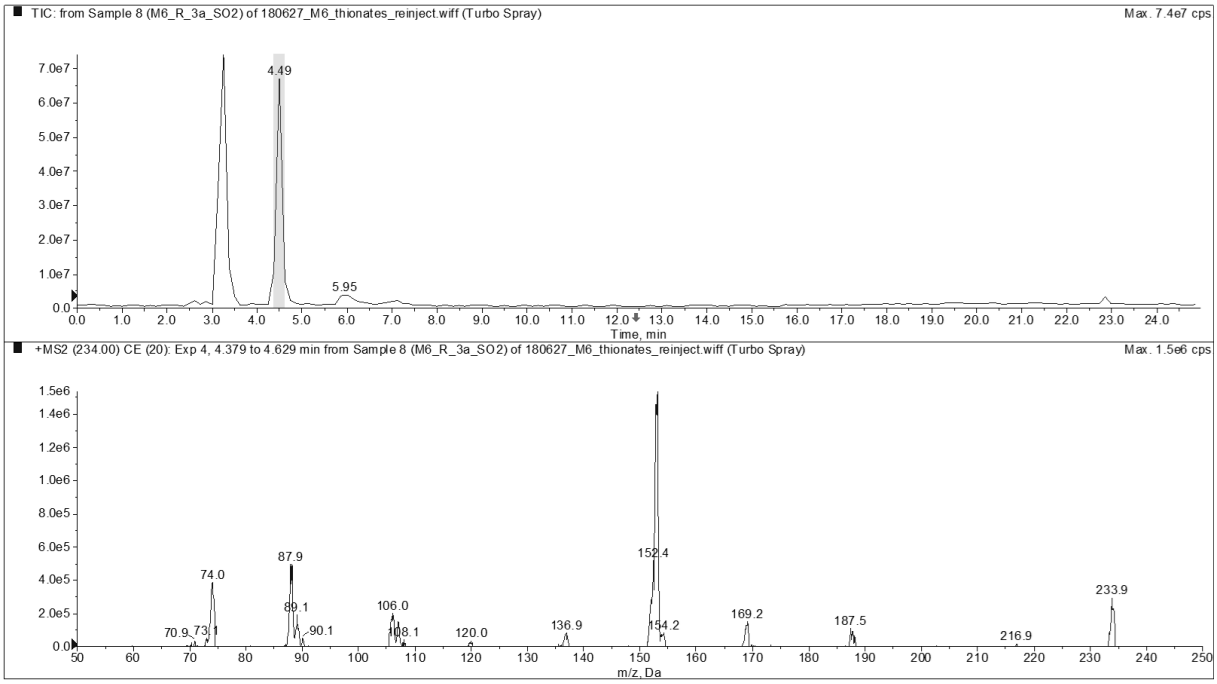

Figure S20. Representative HPLC-MSMS chromatogram and mass spectrum of $C_3H_8NO_5S_3$, retention time 4.49 min.

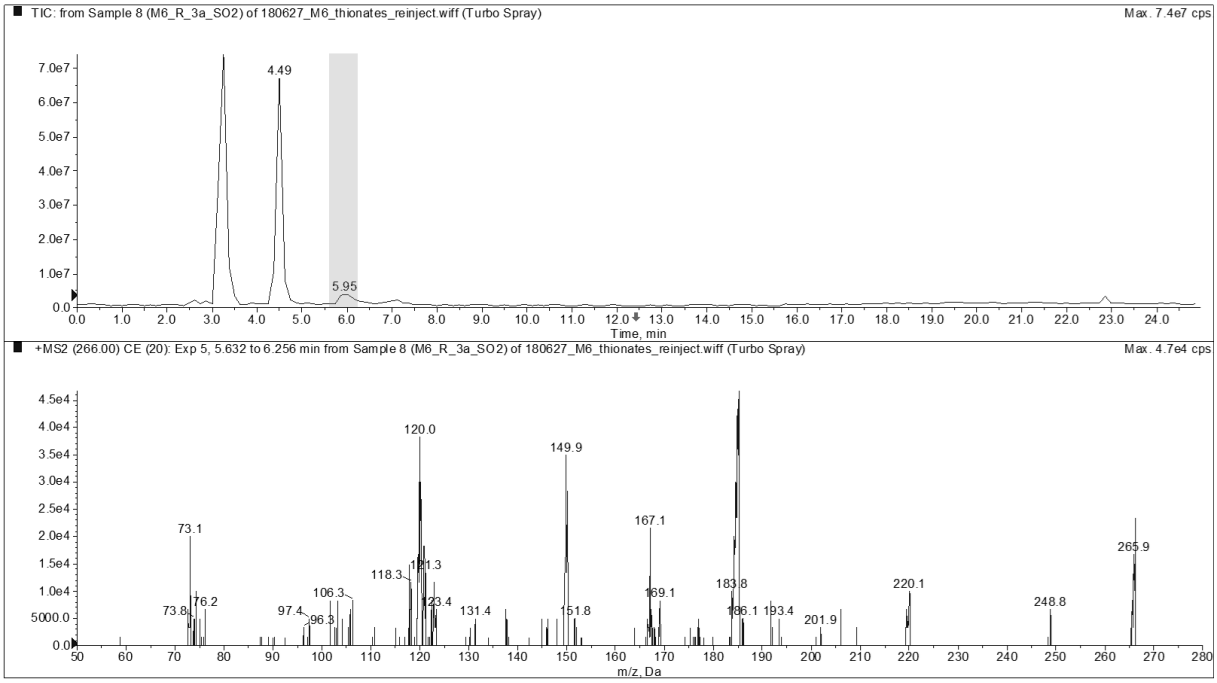

Figure S21. Representative HPLC-MSMS chromatogram and mass spectrum of $C_3H_8NO_5S_4$, retention time 6.0 min.

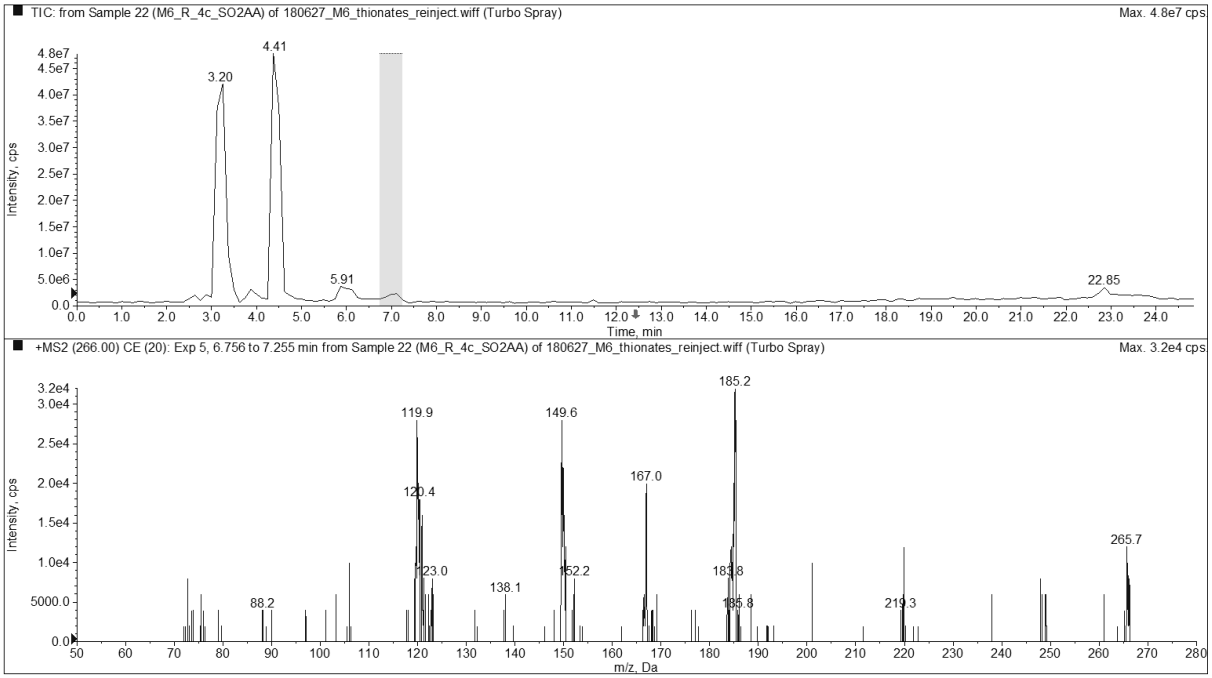

Figure S22. Representative HPLC-MSMS chromatogram and mass spectrum of $C_3H_8NO_5S_4$, retention time 7.1 min.

Table S1. Means and standard deviations of relative polysulfane concentrations (peak area) at each time point for treatments and control

	Control		AA		SO_2		SO_2 + AA		SO_2 + Catechin	
Day 1	**Mean**	**SD[a]**	**Mean**	**SD**	**Mean**	**SD**	**Mean**	**SD**	**Mean**	**SD**
Cysteine	2.19×10^{-05}	1.31×10^{-04}	2.49×10^{-05}	1.79×10^{-04}	7.05×10^{-04}	3.95×10^{-03}	2.59×10^{-05}	1.58×10^{-05}	7.31×10^{-04}	3.39×10^{-03}
Cystine	1.03×10^{-06}	2.67×10^{-04}	7.83×10^{-05}	5.56×10^{-05}	7.48×10^{-05}	4.66×10^{-04}	7.15×10^{-05}	1.19×10^{-05}	7.59×10^{-05}	8.29×10^{-04}
Trisulfane	2.20×10^{-08}	2.52×10^{-06}	2.20×10^{-08}	2.52×10^{-06}	9.50×10^{-07}	1.30×10^{-07}	1.20×10^{-08}	2.08×10^{-06}	5.40×10^{-07}	3.74×10^{-06}
Tetrasulfane	7.60×10^{-07}	2.96×10^{-06}	7.50×10^{-07}	2.80×10^{-06}	3.07×10^{-06}	3.68×10^{-05}	1.60×10^{-07}	2.00×10^{-05}	1.42×10^{-06}	2.75×10^{-05}
Pentasulfane	3.40×10^{-07}	3.87×10^{-06}	1.90×10^{-07}	7.77×10^{-05}	9.23×10^{-05}	1.24×10^{-05}	3.20×10^{-06}	2.89×10^{-04}	4.27×10^{-05}	5.29×10^{-04}
Hexasulfane	4.71×10^{-06}	1.06×10^{-06}	1.44×10^{-06}	7.37×10^{-04}	1.81×10^{-05}	2.38×10^{-04}	2.90×10^{-05}	2.36×10^{-04}	5.20×10^{-04}	1.01×10^{-04}
Day 3	**Mean**	**SD**	**Mean**	**SD**	**Mean**	**SD**	**Mean**	**SD**	**Mean**	**SD**
Cysteine	2.36×10^{-05}	1.95×10^{-04}	2.62×10^{-05}	1.88×10^{-04}	7.27×10^{-04}	7.94×10^{-03}	2.27×10^{-05}	3.58×10^{-04}	6.41×10^{-04}	2.35×10^{-02}
Cystine	9.30×10^{-05}	6.73×10^{-04}	1.06×10^{-06}	2.27×10^{-04}	3.65×10^{-05}	1.49×10^{-05}	6.30×10^{-05}	1.29×10^{-04}	4.49×10^{-05}	3.11×10^{-04}
Trisulfane	2.10×10^{-08}	2.08×10^{-06}	2.10×10^{-08}	1.15×10^{-06}	7.00×10^{-07}	5.62×10^{-06}	7.10×10^{-07}	1.07×10^{-06}	5.50×10^{-07}	1.79×10^{-06}
Tetrasulfane	7.90×10^{-07}	1.95×10^{-06}	5.30×10^{-07}	3.89×10^{-06}	6.04×10^{-06}	6.18×10^{-05}	7.32×10^{-06}	9.18×10^{-05}	4.73×10^{-06}	9.87×10^{-05}
Pentasulfane	2.90×10^{-07}	4.36×10^{-05}	1.10×10^{-07}	4.16×10^{-05}	1.24×10^{-06}	2.89×10^{-04}	1.18×10^{-06}	7.55×10^{-04}	9.26×10^{-05}	2.51×10^{-04}
Hexasulfane	3.42×10^{-06}	1.13×10^{-05}	8.66×10^{-05}	7.02×10^{-04}	9.64×10^{-04}	1.18×10^{-04}	7.34×10^{-04}	1.09×10^{-04}	5.19×10^{-04}	5.26×10^{-03}
Day 6	**Mean**	**SD**	**Mean**	**SD**	**Mean**	**SD**	**Mean**	**SD**	**Mean**	**SD**
Cysteine	1.78×10^{-05}	1.27×10^{-04}	2.24×10^{-05}	3.84×10^{-04}	6.28×10^{-04}	3.02×10^{-04}	2.71×10^{-05}	2.57×10^{-04}	7.35×10^{-04}	5.15×10^{-03}
Cystine	9.46×10^{-05}	2.41×10^{-05}	1.36×10^{-06}	1.05×10^{-05}	4.02×10^{-05}	1.35×10^{-04}	5.53×10^{-05}	2.46×10^{-04}	4.20×10^{-05}	2.13×10^{-04}
Trisulfane	2.10×10^{-08}	1.53×10^{-06}	2.10×10^{-08}	5.77×10^{-05}	6.60×10^{-07}	1.37×10^{-06}	6.90×10^{-07}	1.63×10^{-06}	5.40×10^{-07}	1.46×10^{-06}
Tetrasulfane	8.10×10^{-07}	2.58×10^{-06}	5.20×10^{-07}	1.71×10^{-06}	6.43×10^{-06}	8.50×10^{-04}	8.15×10^{-06}	4.16×10^{-05}	4.42×10^{-06}	2.36×10^{-05}
Pentasulfane	2.60×10^{-07}	2.27×10^{-06}	1.10×10^{-07}	5.29×10^{-05}	1.41×10^{-06}	5.03×10^{-04}	1.42×10^{-06}	1.05×10^{-05}	9.33×10^{-05}	6.66×10^{-04}
Hexasulfane	2.49×10^{-06}	2.71×10^{-05}	8.99×10^{-05}	8.72×10^{-04}	8.67×10^{-04}	2.54×10^{-03}	8.29×10^{-04}	1.48×10^{-04}	4.85×10^{-04}	8.80×10^{-03}
Month 1	**Mean**	**SD**	**Mean**	**SD**	**Mean**	**SD**	**Mean**	**SD**	**Mean**	**SD**
Cysteine	1.87×10^{-05}	1.57×10^{-04}	1.97×10^{-05}	2.07×10^{-04}	9.71×10^{-04}	1.31×10^{-04}	3.41×10^{-05}	5.64×10^{-04}	3.91×10^{-05}	4.67×10^{-04}
Cystine	1.43×10^{-06}	1.41×10^{-05}	1.66×10^{-06}	2.09×10^{-05}	3.02×10^{-05}	2.66×10^{-04}	4.50×10^{-05}	7.72×10^{-04}	4.60×10^{-05}	6.58×10^{-04}
Trisulfane	1.90×10^{-08}	5.77×10^{-05}	1.50×10^{-08}	$0.00 \times 10^{+00}$	4.80×10^{-07}	1.92×10^{-06}	5.20×10^{-07}	1.73×10^{-05}	3.90E+07	2.86×10^{-06}
Tetrasulfane	6.80×10^{-07}	7.77×10^{-06}	1.80×10^{-07}	3.02×10^{-06}	5.09×10^{-06}	1.78×10^{-06}	6.56×10^{-06}	6.48×10^{-05}	4.23×10^{-06}	4.63×10^{-05}
Pentasulfane	1.80×10^{-07}	8.54×10^{-05}	2.28×10^{-06}	1.61×10^{-05}	1.11×10^{-06}	7.00×10^{-04}	1.15×10^{-06}	4.62×10^{-04}	6.74×10^{-05}	6.69×10^{-04}
Hexasulfane	1.22×10^{-06}	1.15×10^{-05}	8.70×10^{-04}	2.01×10^{-04}	4.86×10^{-04}	2.14×10^{-03}	4.85×10^{-04}	4.35×10^{-03}	2.99×10^{-04}	6.53×10^{-03}
Month 6	**Mean**	**SD**	**Mean**	**SD**	**Mean**	**SD**	**Mean**	**SD**	**Mean**	**SD**
Cysteine	1.79×10^{-05}	1.09×10^{-04}	1.11×10^{-05}	7.69×10^{-04}	2.05×10^{-05}	1.62×10^{-04}	4.01×10^{-05}	3.97×10^{-04}	1.83×10^{-05}	9.36×10^{-04}

Cystine	9.06×10^{-05}	2.53×10^{-04}	8.80×10^{-05}	2.63×10^{-05}	2.42×10^{-05}	1.25×10^{-04}	2.88×10^{-05}	3.41×10^{-04}	2.65×10^{-05}	1.00×10^{-05}
Trisulfane	1.90×10^{-08}	1.00×10^{-06}	1.30×10^{-08}	1.53×10^{-06}	2.20×10^{-07}	1.39×10^{-06}	2.50×10^{-07}	5.51×10^{-05}	1.20×10^{-07}	1.80×10^{-06}
Tetrasulfane	2.10×10^{-07}	2.61×10^{-06}	5.39×10^{-06}	1.09×10^{-06}	8.08×10^{-05}	5.89×10^{-04}	3.33×10^{-05}	5.77×10^{-05}	1.61×10^{-03}	2.79×10^{-03}
Pentasulfane	8.64×10^{-06}	3.33×10^{-05}	1.47×10^{-06}	1.40×10^{-05}	1.07×10^{-06}	8.86×10^{-04}	9.75×10^{-05}	1.10×10^{-05}	8.73×10^{-05}	1.19×10^{-05}
Hexasulfane	1.78×10^{-06}	5.77×10^{-04}	1.56×10^{-05}	1.96×10^{-04}	8.40×10^{-03}	4.44×10^{-03}	5.66×10^{-04}	4.28×10^{-04}	3.45×10^{-03}	4.05×10^{-02}

[a] SD standard deviation of triplicate samples

Table S2. Significant differences in polysulfane concentrations as a function of the different treatments (refer to Materials and Methods for the treatment codes)

Polysulfanes	Day 1		Day 3		Day 6		Month 1		Month 6	
Tukey's multiple comparisons test	**Summary[a]**	**Adjusted P Value[a]**	**Summary**	**Adjusted P Value**	**Summary**	**Adjusted P Value**	**Summary**	**Adjusted P Value**	**Summary**	**Adjusted P Value**
Trisulfane										
Control vs. AA	ns	0.946	ns	>0.9999	ns	0.909	****	<0.0001	****	<0.0001
Control vs. SO_2	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Control vs. SO_2 + AA	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Control vs. SO_2 + Cat	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
AA vs. SO_2	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
AA vs. SO_2 + AA	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
AA vs. SO2 + Cat	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
SO_2 vs. SO_2 + AA	****	<0.0001	ns	0.990	ns	0.838	ns	0.628	ns	0.788
SO_2 vs. SO_2 + Cat	****	<0.0001	****	<0.0001	***	3.00×10^{-04}	**	6.60×10^{-03}	**	4.60×10^{-03}
SO_2 + AA vs. SO_2 + Cat	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	***	1.00×10^{-04}
Tetrasulfane										
Control vs. AA	ns	0.978	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Control vs. SO_2	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Control vs. SO_2 + AA	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Control vs. SO_2 + Cat	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
AA vs. SO_2	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	ns	0.113
AA vs. SO_2 + AA	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	ns	0.0634
AA vs. SO2 + Cat	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	*	0.0411
SO_2 vs. SO_2 + AA	****	<0.0001	ns	0.957	ns	0.885	ns	0.932	ns	0.999
SO_2 vs. SO_2 + Cat	ns	0.900	ns	0.953	ns	0.813	ns	0.990	ns	0.992
SO_2 + AA vs. SO_2 + Cat	****	<0.0001	ns	0.629	ns	0.275	ns	0.717	ns	1.00
Pentasulfane										
Control vs. AA	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Control vs. SO_2	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Control vs. SO_2 + AA	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Control vs. SO_2 + Cat	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
AA vs. SO_2	****	<0.0001	****	<0.0001	****	<0.0001	ns	0.555	ns	0.985

AA vs. SO_2 + AA	****	<0.0001	****	<0.0001	****	<0.0001	ns	0.590	ns	0.967
AA vs. SO2 + Cat	****	<0.0001	****	<0.0001	****	<0.0001	ns	0.243	ns	0.936
SO_2 vs. SO_2 + AA	*	0.0376	ns	>0.9999	ns	>0.9999	ns	>0.9999	ns	>0.9999
SO_2 vs. SO_2 + Cat	ns	0.967	ns	0.994	ns	0.972	ns	0.980	ns	0.999
SO_2 + AA vs. SO_2 + Cat	**	6.50×10^{-03}	ns	0.997	ns	0.969	ns	0.971	ns	>0.9999
Hexasulfane	**Day 1**		**Day 3**		**Day 6**		**Month 1**		**Month 6**	
Control vs. AA	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Control vs. SO_2	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Control vs. SO_2 + AA	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Control vs. SO_2 + Cat	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
AA vs. SO_2	****	<0.0001	***	9.00×10^{-04}	***	4.00×10^{-04}	ns	1.00	ns	0.927
AA vs. SO_2 + AA	****	<0.0001	***	6.00×10^{-04}	***	4.00×10^{-04}	ns	1.00	ns	0.982
AA vs. SO2 + Cat	****	<0.0001	***	4.00×10^{-04}	***	2.00×10^{-04}	ns	0.998	ns	0.919
SO_2 vs. SO_2 + AA	ns	0.975	ns	>0.9999	ns	>0.9999	ns	>0.9999	ns	0.999
SO_2 vs. SO_2 + Cat	ns	0.954	ns	0.999	ns	1.00	ns	>0.9999	ns	>0.9999
SO_2 + AA vs. SO_2 + Cat	ns	0.689	ns	>0.9999	ns	1.00	ns	>0.9999	ns	0.998

[a]Significance determined using repeated measures (RM) two-way ANOVA. Tukey multiple comparison test was used to correct for multiple comparisons. Significance and confidence levels were assigned for $P < 0.05$ (95% confidence interval). Significant interactions are indicated as follows: not significant (ns) for $P > 0.05$; * $P \leq 0.05$; ** $P \leq 0.01$; *** $P \leq 0.001$; **** $P \leq 0.0001$.

Table S3. Significant differences in polysulfane concentrations as a function of time (refer to Materials and Methods for the treatment codes)

	Trisulfane		Tetrasulfane		Pentasulfane		Hexasulfane	
Tukey's multiple comparisons test	**Summary[a]**	**Adjusted P value[a]**	**Summary**	**Adjusted P value**	**Summary**	**Adjusted P value**	**Summary**	**Adjusted P value**
Control								
Day 1 vs. Day 3	*	0.0345	ns	0.738	****	<0.0001	****	<0.0001
Day 1 vs. Day 6	*	0.0345	*	0.0418	****	<0.0001	****	<0.0001
Day 1 vs. Month 1	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Day 1 vs. Month 6	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Day 3 vs. Day 6	ns	>0.9999	ns	0.441	*	0.0198	***	2.00×10^{-04}
Day 3 vs. Month 1	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Day 3 vs. Month 6	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Day 6 vs. Month 1	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Day 6 vs. Month 6	****	<0.0001	****	<0.0001	****	<0.0001	**	5.10×10^{-03}
Month 1 vs. Month 6	ns	0.192	****	<0.0001	****	<0.0001	*	0.0453
Ascorbic acid								
Day 1 vs. Day 3	ns	0.192	****	<0.0001	****	<0.0001	*	0.035
Day 1 vs. Day 6	*	0.0249	****	<0.0001	****	<0.0001	ns	0.0529
Day 1 vs. Month 1	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Day 1 vs. Month 6	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Day 3 vs. Day 6	ns	0.889	ns	0.997	ns	0.968	ns	1.00
Day 3 vs. Month 1	****	<0.0001	****	<0.0001	****	<0.0001	**	2.00×10^{-03}
Day 3 vs. Month 6	****	<0.0001	****	<0.0001	****	<0.0001	**	5.50×10^{-03}
Day 6 vs. Month 1	****	<0.0001	****	<0.0001	****	<0.0001	**	1.20×10^{-03}
Day 6 vs. Month 6	****	<0.0001	****	<0.0001	****	<0.0001	**	3.40×10^{-03}
Month 1 vs. Month 6	****	<0.0001	****	<0.0001	ns	0.867	ns	0.996
SO_2								
Day 1 vs. Day 3	****	<0.0001	ns	0.426	ns	1.00	ns	0.992
Day 1 vs. Day 6	****	<0.0001	ns	0.304	ns	0.978	ns	0.988
Day 1 vs. Month 1	****	<0.0001	ns	0.764	ns	1.00	ns	0.958
Day 1 vs. Month 6	****	<0.0001	ns	0.684	ns	1.00	ns	0.896
Day 3 vs. Day 6	ns	0.623	ns	0.999	ns	1.00	ns	>0.9999
Day 3 vs. Month 1	****	<0.0001	ns	0.981	ns	1.00	ns	0.999
Day 3 vs. Month 6	****	<0.0001	*	0.0314	ns	1.00	ns	0.991
Day 6 vs. Month 1	****	<0.0001	ns	0.934	ns	1.00	ns	1.00
Day 6 vs. Month 6	****	<0.0001	*	0.0176	ns	0.994	ns	0.994
Month 1 vs. Month 6	****	<0.0001	ns	0.113	ns	>0.9999	ns	1.00
SO2 + Ascorbic acid								
Day 1 vs. Day 3	****	<0.0001	****	<0.0001	ns	0.133	ns	0.791
Day 1 vs. Day 6	****	<0.0001	***	4.00×10^{-04}	ns	0.231	ns	0.817
Day 1 vs. Month 1	****	<0.0001	****	<0.0001	ns	0.124	ns	0.718
Day 1 vs. Month 6	****	<0.0001	****	<0.0001	ns	0.0787	ns	0.743
Day 3 vs. Day 6	ns	0.926	ns	0.989	ns	0.998	ns	>0.9999
Day 3 vs. Month 1	****	<0.0001	ns	0.992	ns	>0.9999	ns	>0.9999
Day 3 vs. Month 6	****	<0.0001	**	1.90×10^{-03}	ns	0.999	ns	>0.9999

Day 6 vs. Month 1	****	<0.0001	ns	0.884	ns	0.998	ns	1.000
Day 6 vs. Month 6	****	<0.0001	***	4.00×10^{-04}	ns	0.983	ns	>0.9999
Month 1 vs. Month 6	****	<0.0001	**	6.90×10^{-03}	ns	1.00	ns	>0.9999
SO2 + catechin								
Day 1 vs. Day 3	ns	0.995	ns	0.322	ns	0.975	ns	>0.9999
Day 1 vs. Day 6	ns	0.999	ns	0.418	ns	0.973	ns	>0.9999
Day 1 vs. Month 1	****	<0.0001	ns	0.486	ns	0.998	ns	>0.9999
Day 1 vs. Month 6	****	<0.0001	ns	0.920	ns	0.983	ns	0.999
Day 3 vs. Day 6	ns	0.967	ns	1.00	ns	>0.9999	ns	>0.9999
Day 3 vs. Month 1	****	<0.0001	ns	0.998	ns	0.998	ns	>0.9999
Day 3 vs. Month 6	****	<0.0001	ns	0.0638	ns	>0.9999	ns	0.999
Day 6 vs. Month 1	****	<0.0001	ns	>0.9999	ns	0.998	ns	>0.9999
Day 6 vs. Month 6	****	<0.0001	ns	0.0946	ns	>0.9999	ns	0.999
Month 1 vs. Month 6	****	<0.0001	ns	0.121	ns	0.999	ns	>0.9999

[a]Significance determined using repeated measures (RM) two-way ANOVA. Tukey multiple comparison test was used to correct for multiple comparisons. Significance and confidence levels were assigned for $P < 0.05$ (95% confidence interval). Significant interactions are indicated as follows: not significant (ns) for $P > 0.05$; * $P \leq 0.05$; ** $P \leq 0.01$; *** $P \leq 0.001$; **** $P \leq 0.0001$.

Table S4. Significant differences in mean polysulfane concentrations as a function of the different treatments (refer to Materials and Methods for the treatment codes)

	Trisulfane		**Tetrasulfane**		**Pentasulfane**		**Hexasulfane**	
Tukey's multiple comparisons test	**Summary[a]**	**Adjusted P value[a]**	**Summary**	**Adjusted P value**	**Summary**	**Adjusted P value**	**Summary**	**Adjusted P value**
Control vs. AA	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Control vs. SO_2	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Control vs. SO_2 + AA	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001
Control vs. SO_2 + Cat	****	<0.0001	****	<0.0001	****	<0.0001	****	<0.0001

[a]Significance determined using repeated measures (RM) two-way ANOVA. Each mean was compared to the control wine sample for each time point. Tukey multiple comparison test was used to correct for multiple comparisons. Significance and confidence levels were assigned for $P < 0.05$ (95% confidence interval). Significant interactions are indicated as follows: not significant (ns) for $P > 0.05$; * $P \leq 0.05$; ** $P \leq 0.01$; *** $P \leq 0.001$; **** $P \leq 0.0001$.

Table S5. Means and standard deviations of hydrogen sulfide concentrations (µg/L) for the treatments and control (refer to Materials and Methods for the treatment codes)

	Control		**AA**		**SO_2**		**SO_2 + AA**		**SO_2 + Cat**	
	Mean	**SD[a]**	**Mean**	**SD**	**Mean**	**SD**	**Mean**	**SD**	**Mean**	**SD**
Day 1	0.00	0.00	0.00	0.00	13	1.9	2.8	0.63	5.4	0.41
Day 3	0.00	0.00	0.00	0.00	10	2.1	3.3	0.52	2.1	0.35
Day 6	0.00	0.00	0.60	0.37	114	65	15	11	4.6	0.48
Month 1	1.2	0.23	2.7	0.24	126	17	212	7.0	175	40
Month 6	0.70	0.12	5.2	0.51	58	3.2	91	1.1	66	2.2

[a] SD standard deviation

Table S6. Significant differences in hydrogen sulfide concentration as a function of ascorbic acid, sulfur dioxide, sulfur dioxide and ascorbic acid, and sulfur dioxide and (+)-catechin treatment

Hydrogen sulfide	**Day 1**		**Day 3**		**Day 6** [b]		**Month 1**		**Month 6**	
Tukey's multiple comparisons test	**Summary**[a]	**Adjusted P Value**	**Summary**	**Adjusted P Value**	**Summary**	**Adjusted P Value**	**Summary**	**Adjusted P Value**	**Summary**	**Adjusted P Value**
Control vs. AA	ns	>0.9999	ns	>0.9999	ns	1.06×10^{-01}	ns	9.26×10^{-01}	*	1.24×10^{-02}
Control vs. SO_2	****	<0.0001	****	<0.0001	***	8.00×10^{-04}	****	<0.0001	****	<0.0001
Control vs. SO_2 + AA	**	3.70×10^{-03}	**	2.10×10^{-03}	ns	1.28×10^{-01}	****	<0.0001	****	<0.0001
Control vs. SO_2 + Cat	****	<0.0001	*	2.56×10^{-02}	**	3.50×10^{-03}	****	<0.0001	****	<0.0001
AA vs. SO2	****	<0.0001	****	<0.0001	***	8.00×10^{-04}	****	<0.0001	****	<0.0001
AA vs. SO_2 + AA	**	3.70×10^{-03}	**	2.10×10^{-03}	ns	5.46×10^{-01}	****	<0.0001	****	<0.0001
AA vs. SO_2 + Cat	****	<0.0001	*	2.56×10^{-02}	ns	8.67×10^{-01}	****	<0.0001	****	<0.0001
SO_2 vs. AA + SO2	****	<0.0001	****	<0.0001	**	2.10×10^{-03}	***	4.00×10^{-04}	****	<0.0001
SO_2 vs. SO2 + Cat	****	<0.0001	****	<0.0001	**	1.00×10^{-03}	*	1.37×10^{-02}	***	6.00×10^{-04}
SO_2 + AA vs. SO_2 + Cat	**	6.50×10^{-03}	ns	1.64×10^{-01}	ns	6.60×10^{-01}	*	4.58×10^{-02}	****	<0.0001

[a]Significance determined using repeated measures (RM) two-way. Tukey multiple comparison test was used to correct for multiple comparisons. Significance and confidence levels were assigned for $P < 0.05$ (95% confidence interval). Significant interactions are indicated as follows: not significant (ns) for $P > 0.05$; * $P \leq 0.05$; ** $P \leq 0.01$; *** $P \leq 0.001$; **** $P \leq 0.0001$.

[b]The variation between the replicates of the different treatments (Table S5) impacted the two-way ANOVA evaluation of the treatment effects at Day 6.

REFERENCES

1. Siebert, T. E.; Bramley, B.; Solomon, M. R., Hydrogen Sulfide: aroma detection threshold study in white and red wine. *AWRI Technical Review* **2009,** *183,* 14-16.