Supplementary Information

Enantioselective sulfoxidation using *Streptomyces glaucescens* GLA.0

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Fig. S1. Multiple sequence alignment of a putative BVMO enzyme in the genome of *Streptomyces glaucescens* GLA.0 (A0A089Y245_STRGA). The Uniprot Accession number is A0A089YZ45 and Gene Bank Accession number is CP009438.1. The alignment shows sequence identity with SCO3172BVMO, a Baeyer-Villiger monooxygenase from *Streptomyces coelicolor* A3(2) (Gene Bank Accession No. CAB55657.1), PA1538BVMO, a BVMO from *Pseudomonas aeruginosa* PAO1 (Gene Bank Accession No. AAG04927.1) and BVMOAFL838, a BVMO from *Aspergillus flavus*.

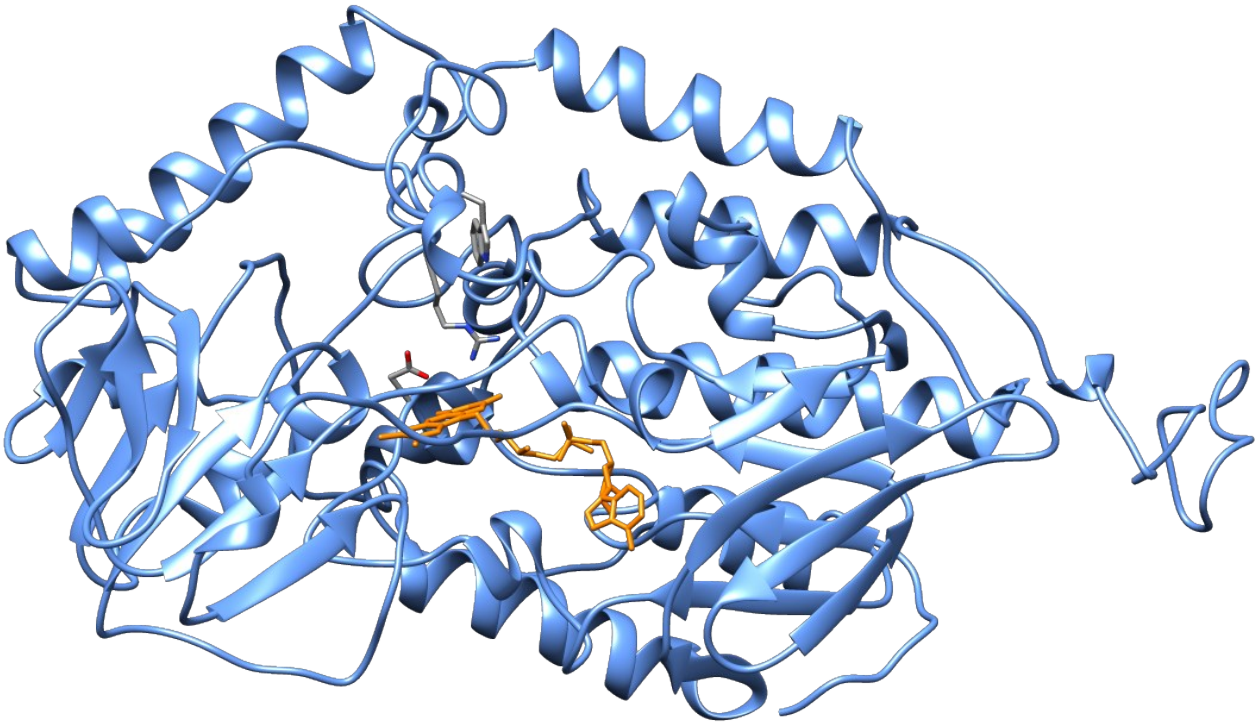

Fig. S2. A homology model of the putative BVMO identified in the genome of *S. glaucescens* GLA.0. The model was constructed using I-Tasser server.

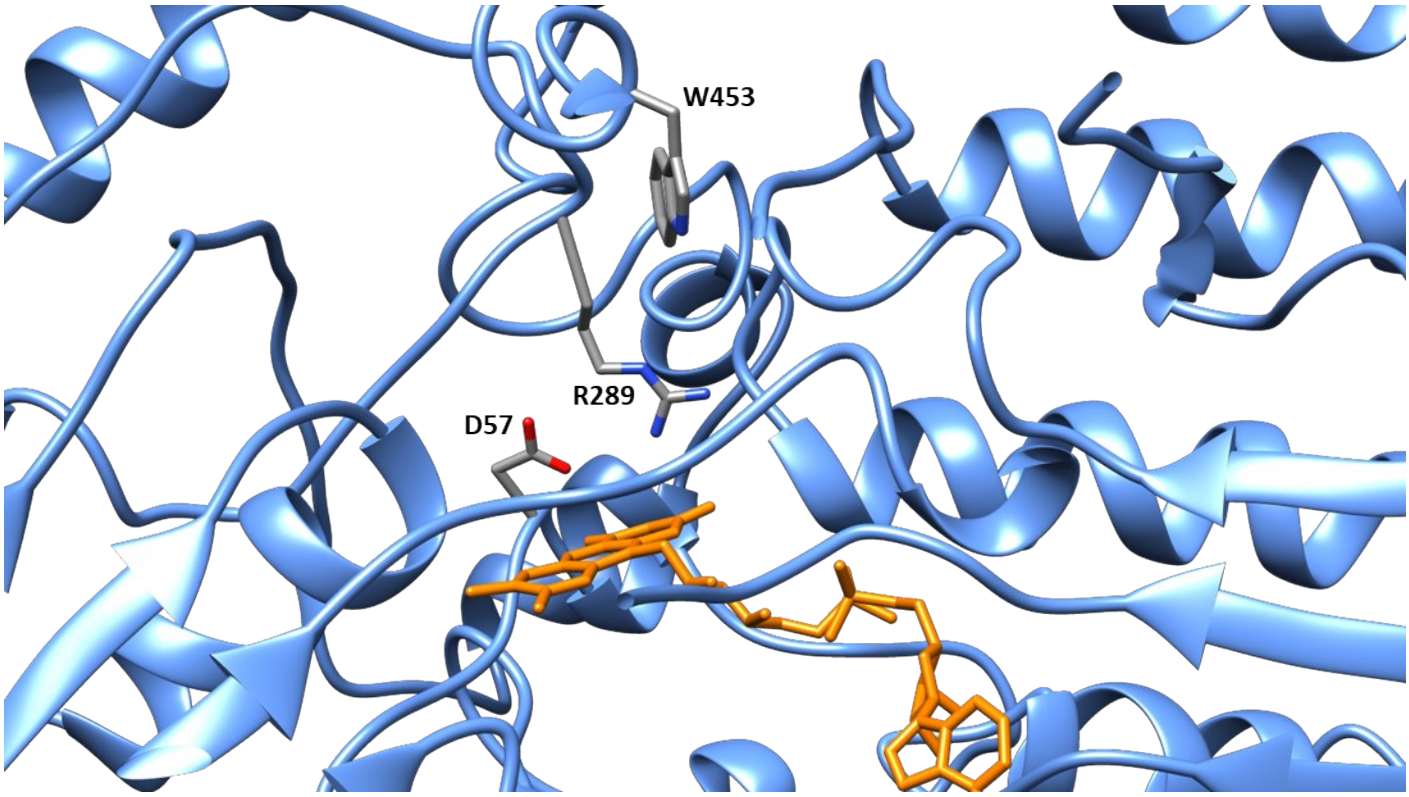

Fig. S3. Zoom-in view of the active site of the putative BVMO in *S. glaucescens* GLA.0. The residues Arg289 and Asp57 are conserved residues that contribute to substrate binding.

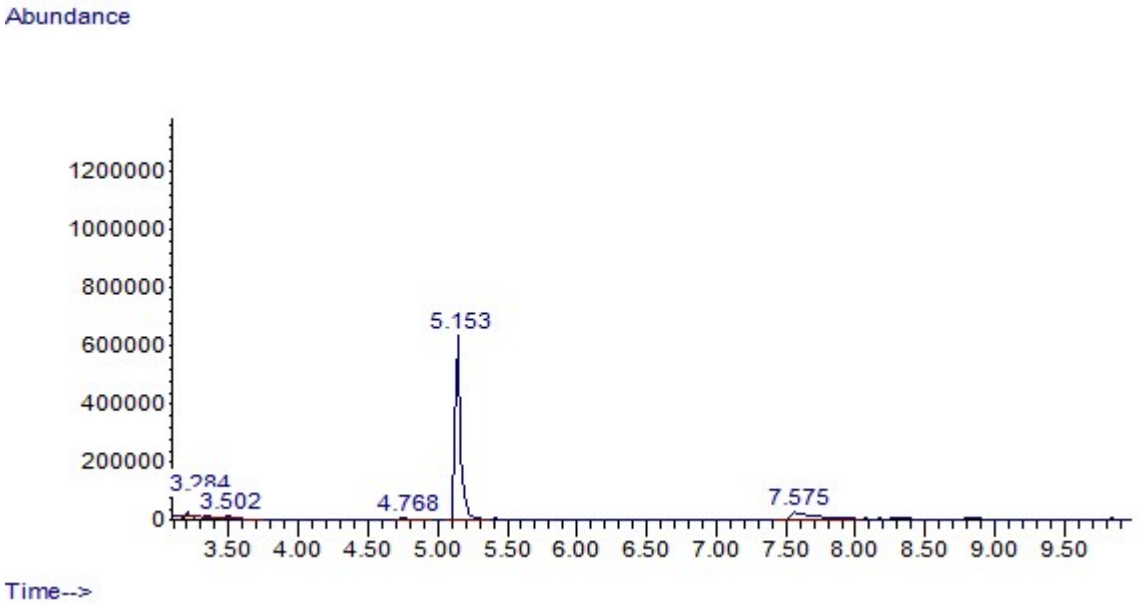

Fig. S4. GC chromatogram of phenyl methyl sulfide at the beginning of the reaction. PMS was added in an amount to form a 1 mM concentration in Medium 2. The retention time of PMS at zero time is 5.1 min.

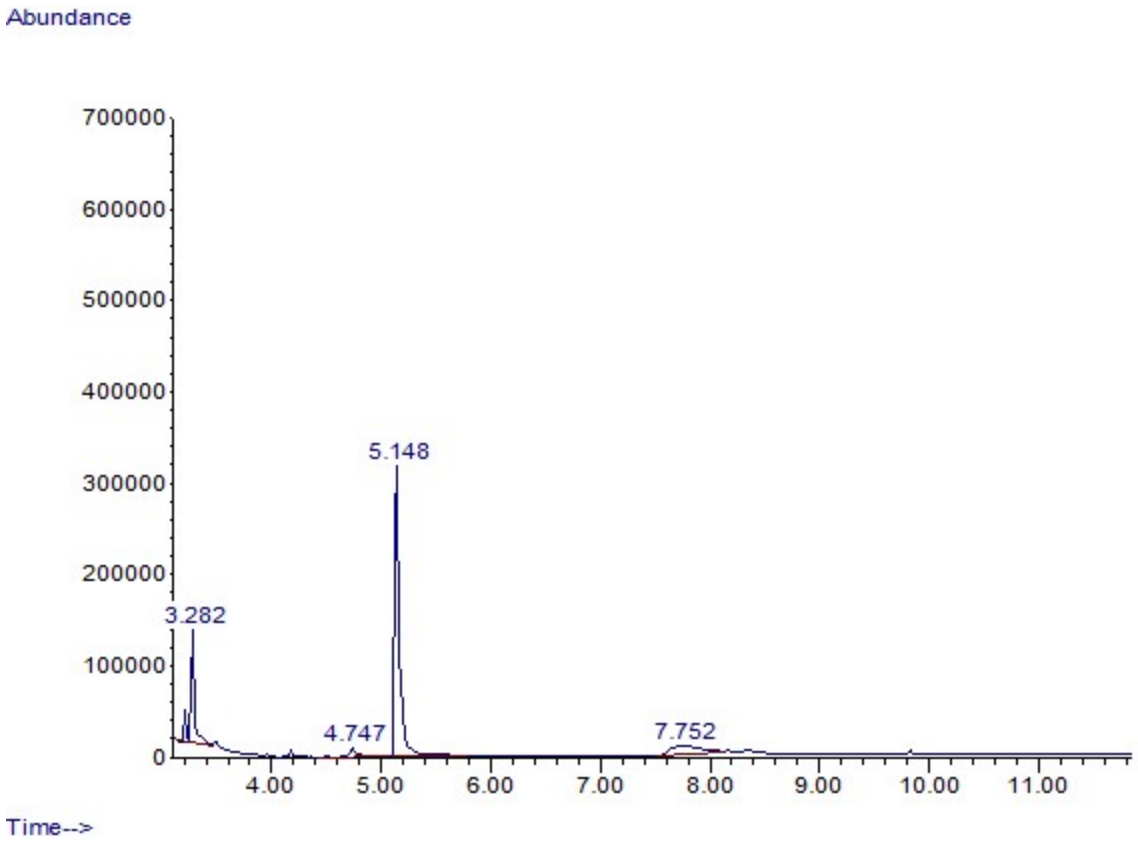

Fig. S5. GC chromatogram of phenyl methyl sulfide in a control reaction. PMS was added at an initial concentration of 1 mM to Medium 2. The reading was taken after 72 h from the beginning of the reaction and the experiment was done without the addition of bacterial culture. PMS was eluted at a retention time of 5.1 min.

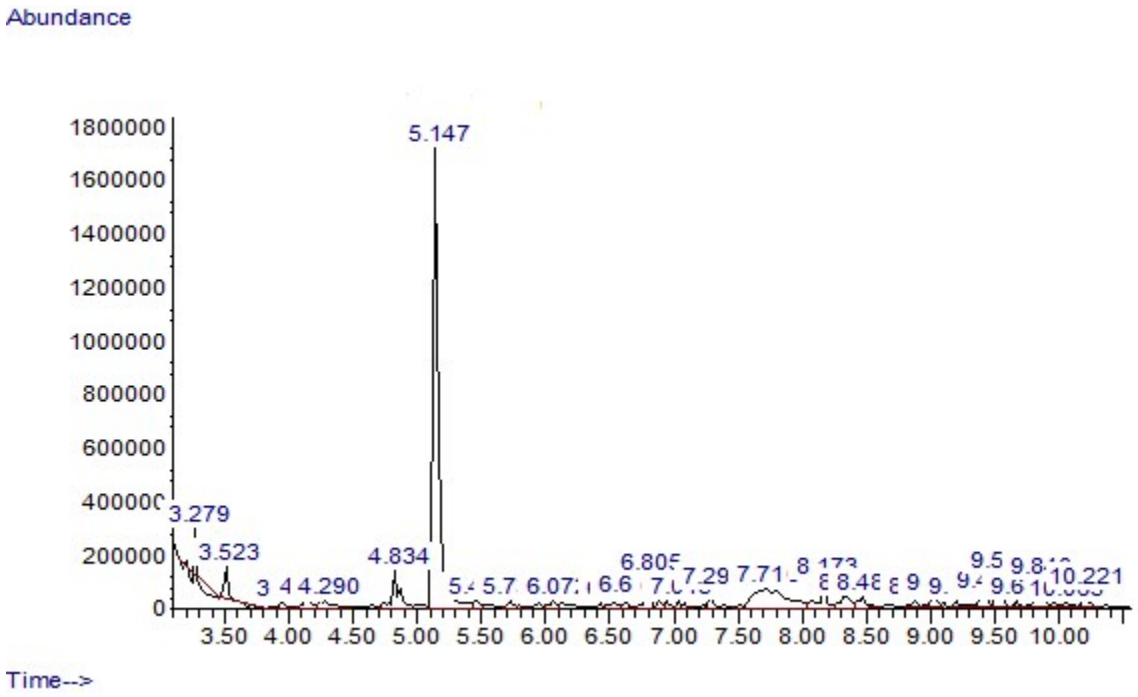

Fig. S6. Full scan GC chromatogram of phenyl methyl sulfide showing the effect of agitation on the biotransformation process. PMS was added at an initial concentration of 1 mM to Medium 3. The sample was taken after 72 h from the beginning of the reaction to give a PMS retention time of 5.1 min and a very small amount of PMSO at 7.7 min. The experiment was performed without agitation.

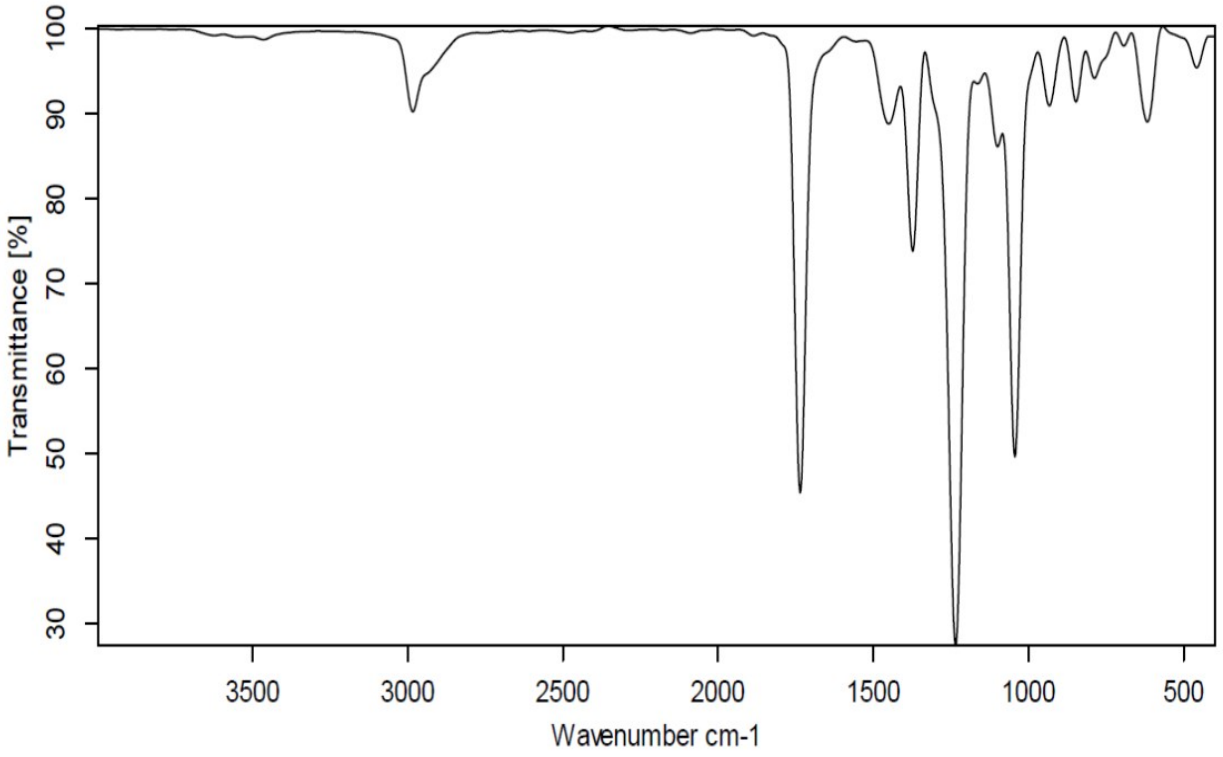

Fig. S7. IR spectrum of the chemically synthesized phenyl methyl sulfoxide.

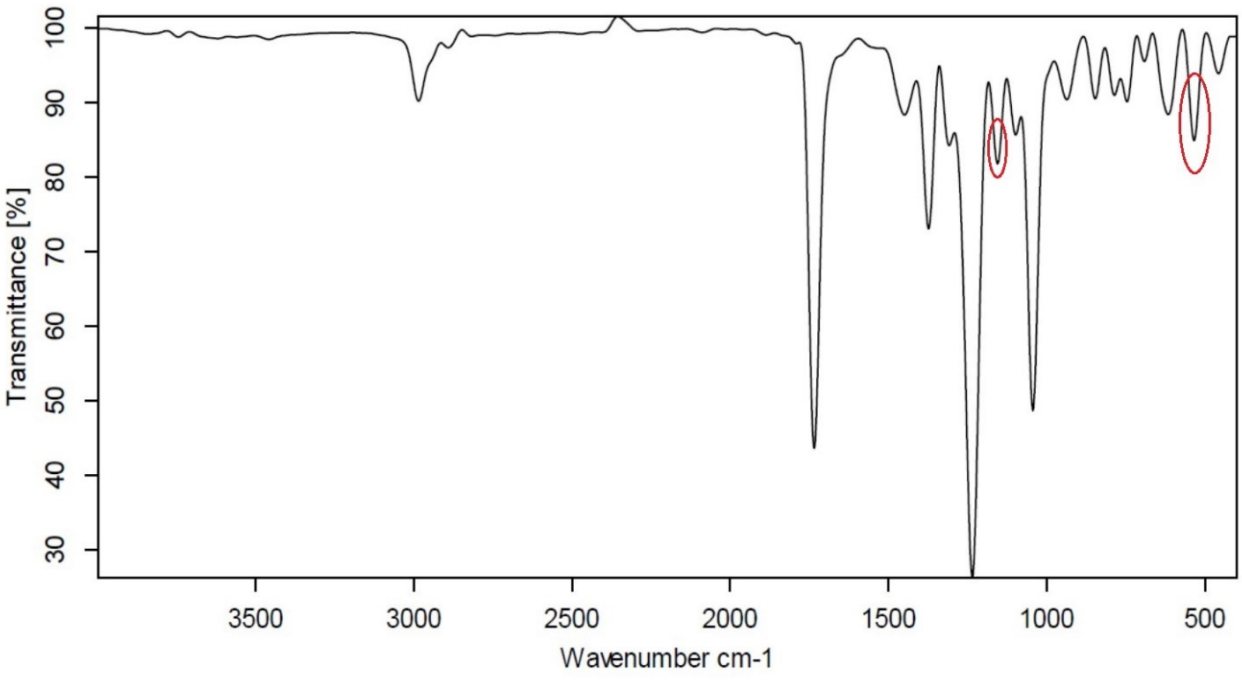

Fig. S8. IR spectrum of the chemically synthesized phenyl methyl sulfone.

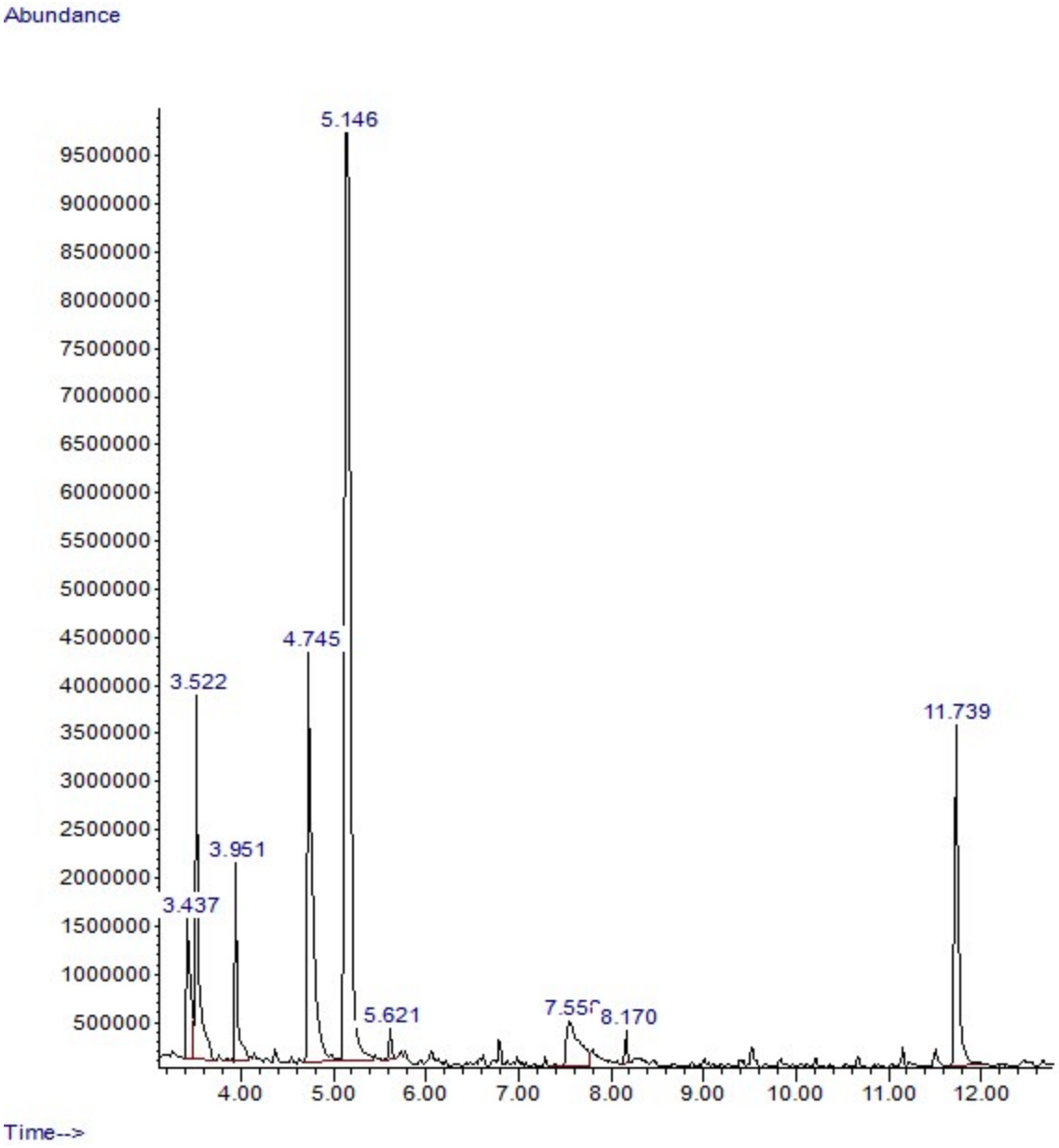

Fig. S9. Full scan GC chromatogram showing the formation of PMSO (Rt = 7.5 min) after 15 h from the beginning of the reaction. This chromatogram was taken from a sample withdrawn after 15 h from the beginning of the biotransformation of phenyl methyl sulfide (added at an initial concentration of 3 mM) by growing cells of *Streptomyces glaucescens* GLA0.

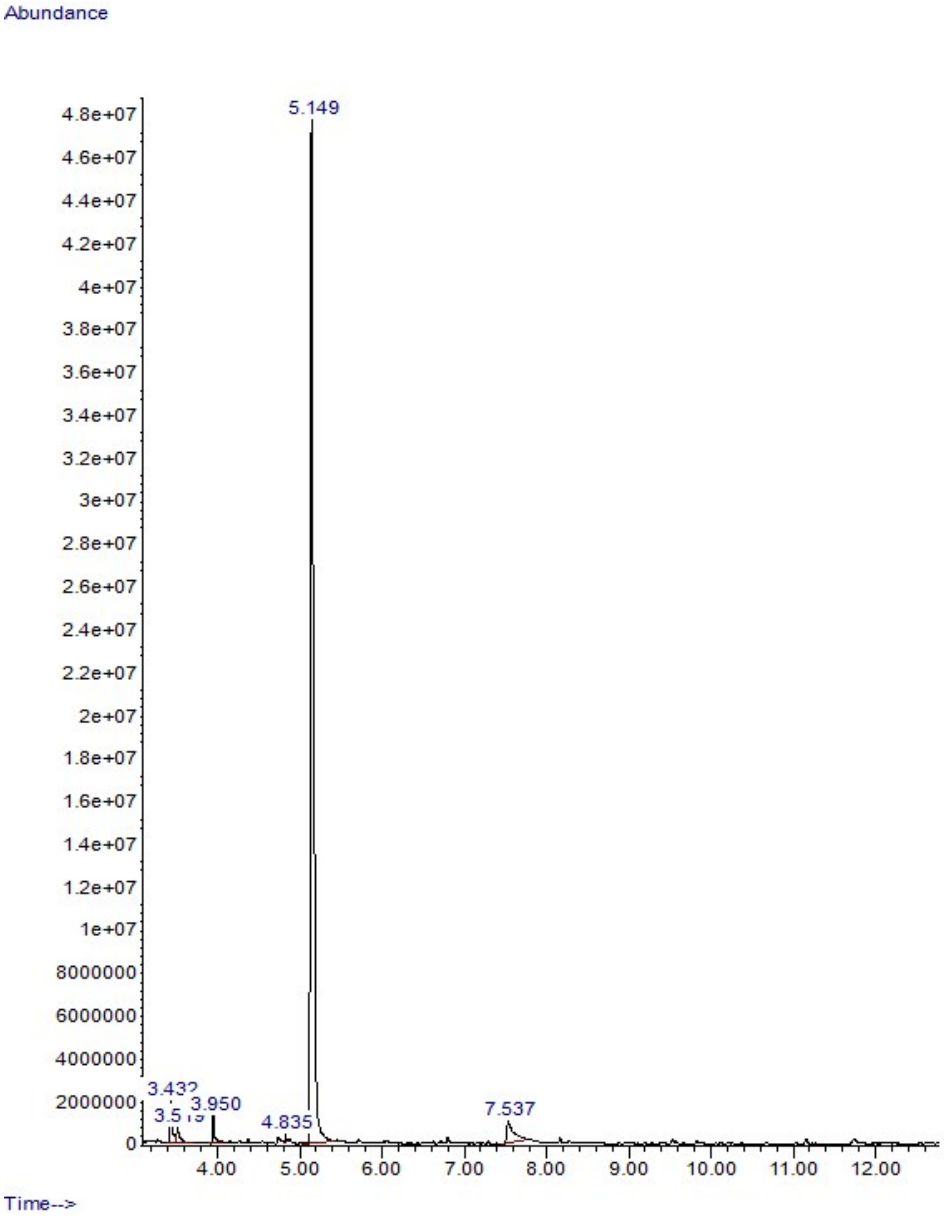

Fig. S10. Full scan GC chromatogram showing the formation of PMSO (Rt = 7.5 min) after 6 h from the beginning of the reaction. This chromatogram was taken from a sample withdrawn after 6 h from the beginning of the biotransformation of phenyl methyl sulfide (added at an initial concentration of 5 mM) by growing cells of *Streptomyces glaucescens* GLA0.

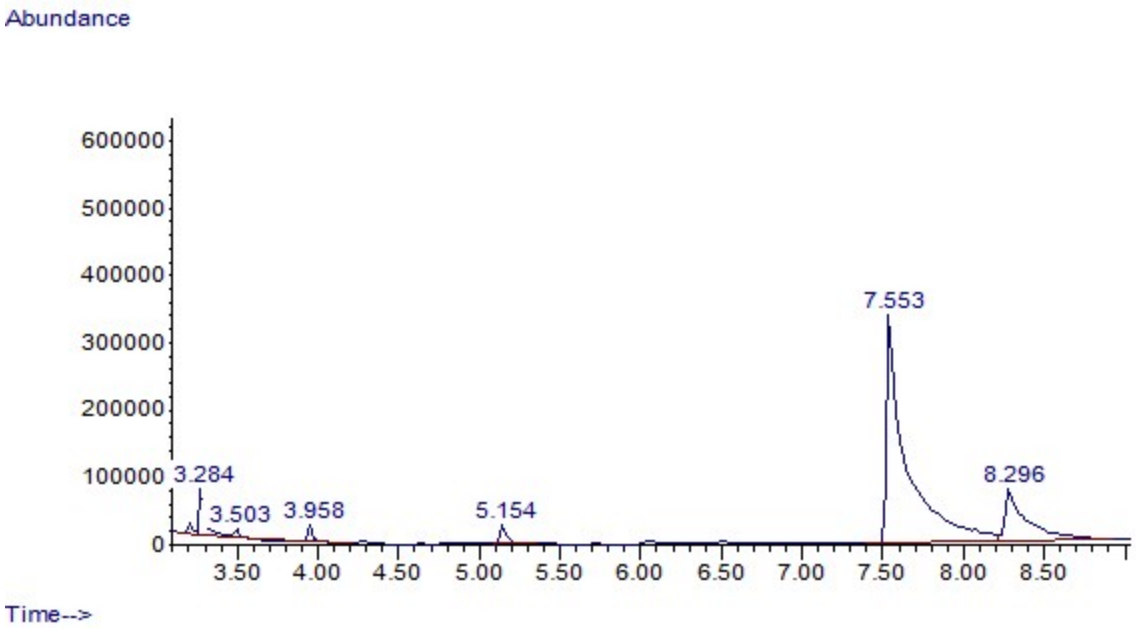

Fig. S11.A The effect of co-solvent addition on PMSO and sulfone formation. The GC chromatogram shows PMSO (Rt = 7.5 min) and phenyl methyl sulfone (Rt = 8.3 min) formed under conditions of reaction **A (**see **Table 1).** The sample was taken after 96 h from the beginning of the reaction.

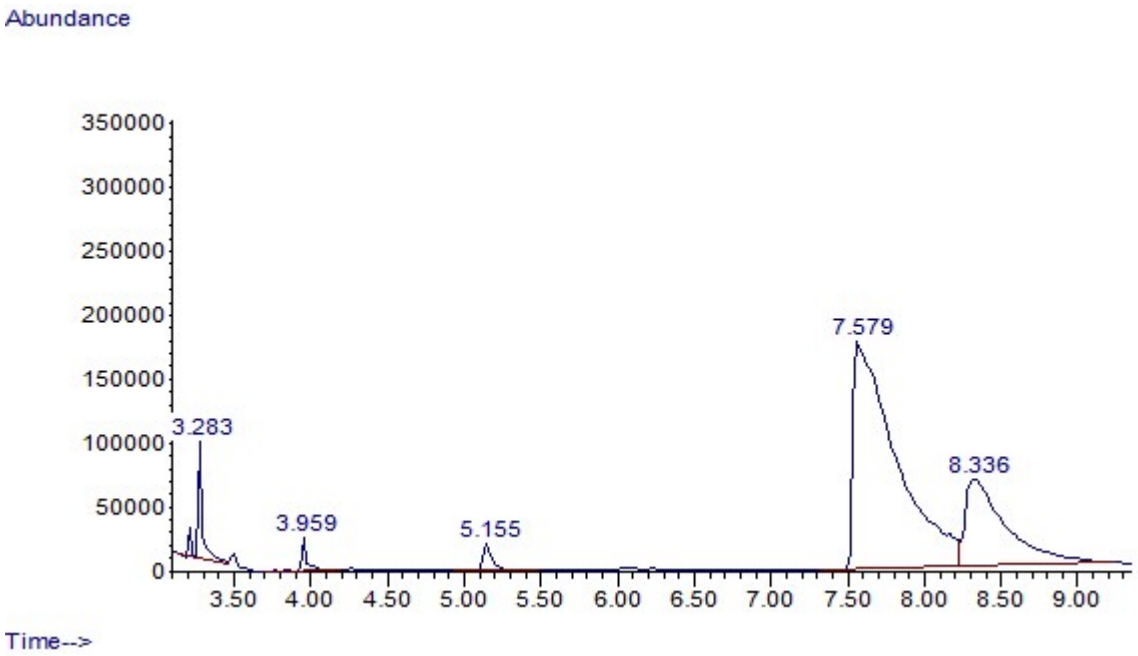

Fig. S11.B The effect of co-solvent addition on PMSO and sulfone formation. The GC chromatogram shows PMSO (Rt = 7.5 min) and phenyl methyl sulfone (Rt = 8.3 min) formed under conditions of reaction **B** (see **Table 1**). The sample was taken after 96 h from the beginning of the reaction.

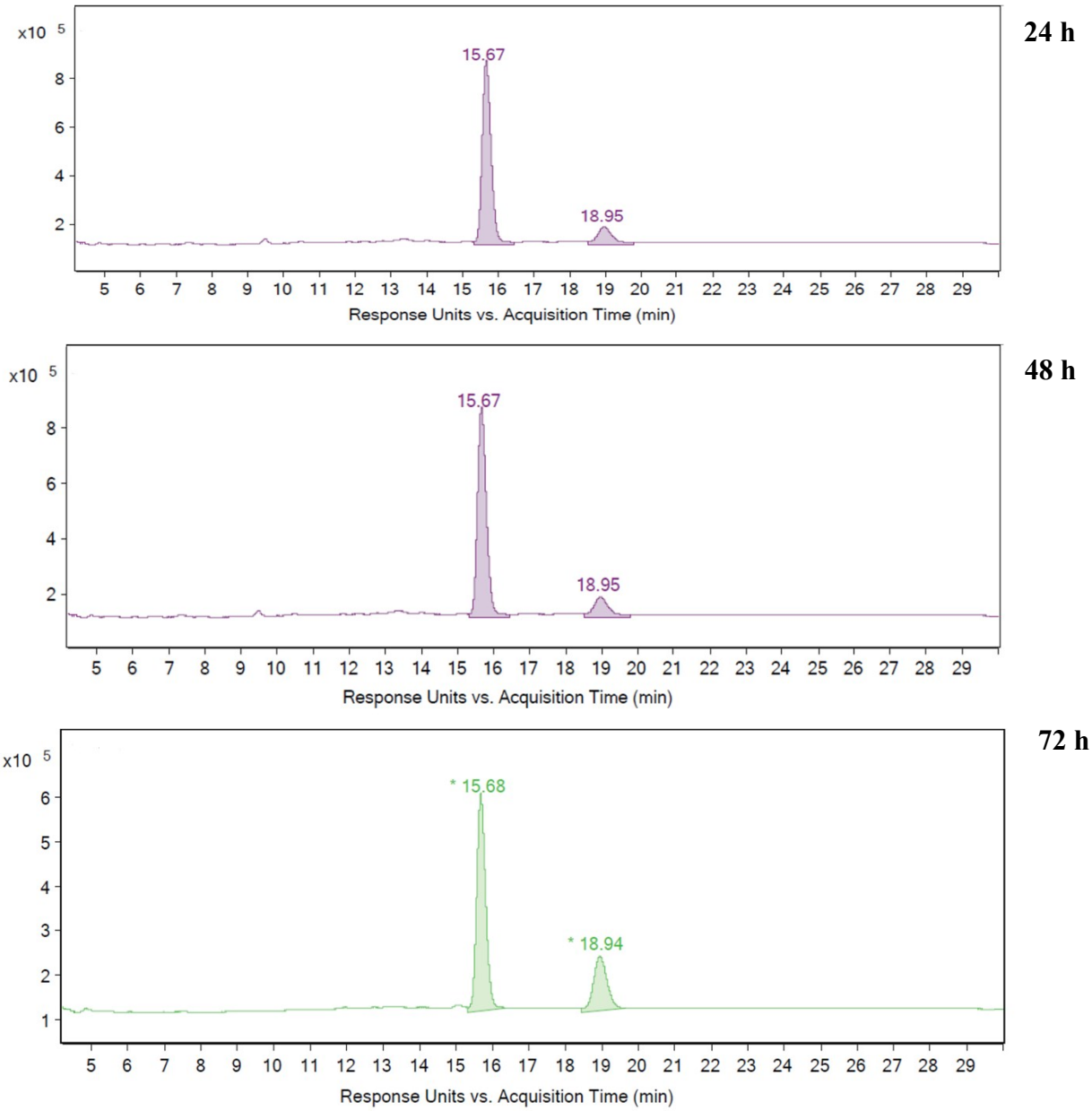

Fig. S12. Chiral GC chromatograms showing oxidized products formed from PMS biooxidation by the whole cells of *Streptomyces glaucescens* GLA.0 under conditions of reaction (**C**). Samples were taken after 24 h, 48 h, and 72 h, respectively. Retention times of *R*-PMSO and phenyl methyl sulfone were 15.6 min and 18.9 min, respectively.

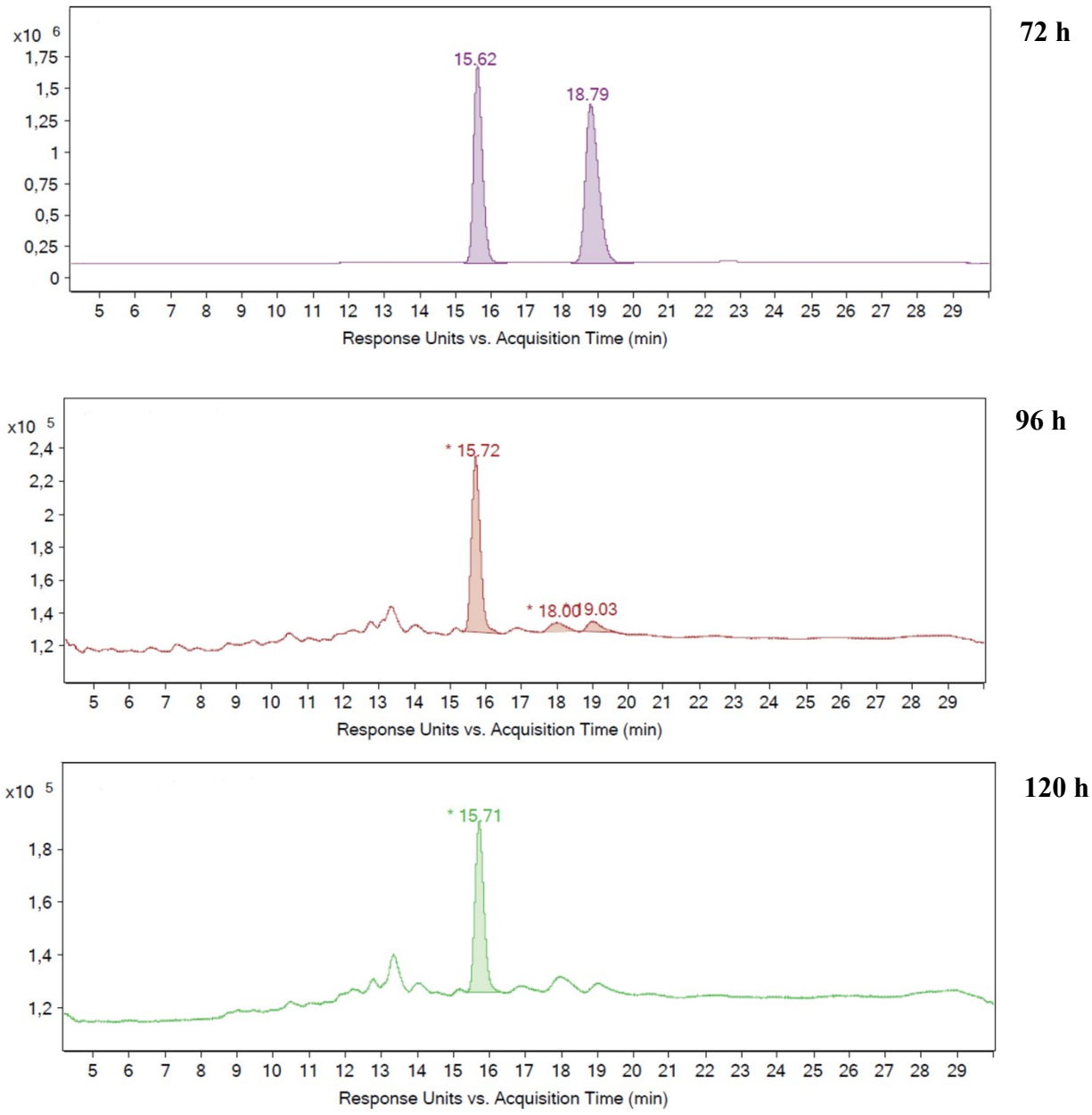

Fig. S13. Chiral GC chromatograms showing oxidized products formed from PMS biooxidation by the whole cells of *Streptomyces glaucescens* GLA.0 under conditions of reaction (**D**). Samples were taken after 72 h, 96 h and 120 h, respectively. Retention times of *R*-PMSO, *S*-PMSO and phenyl methyl sulfone were 15.6 min, 18-18.7 min and 19 min, respectively.

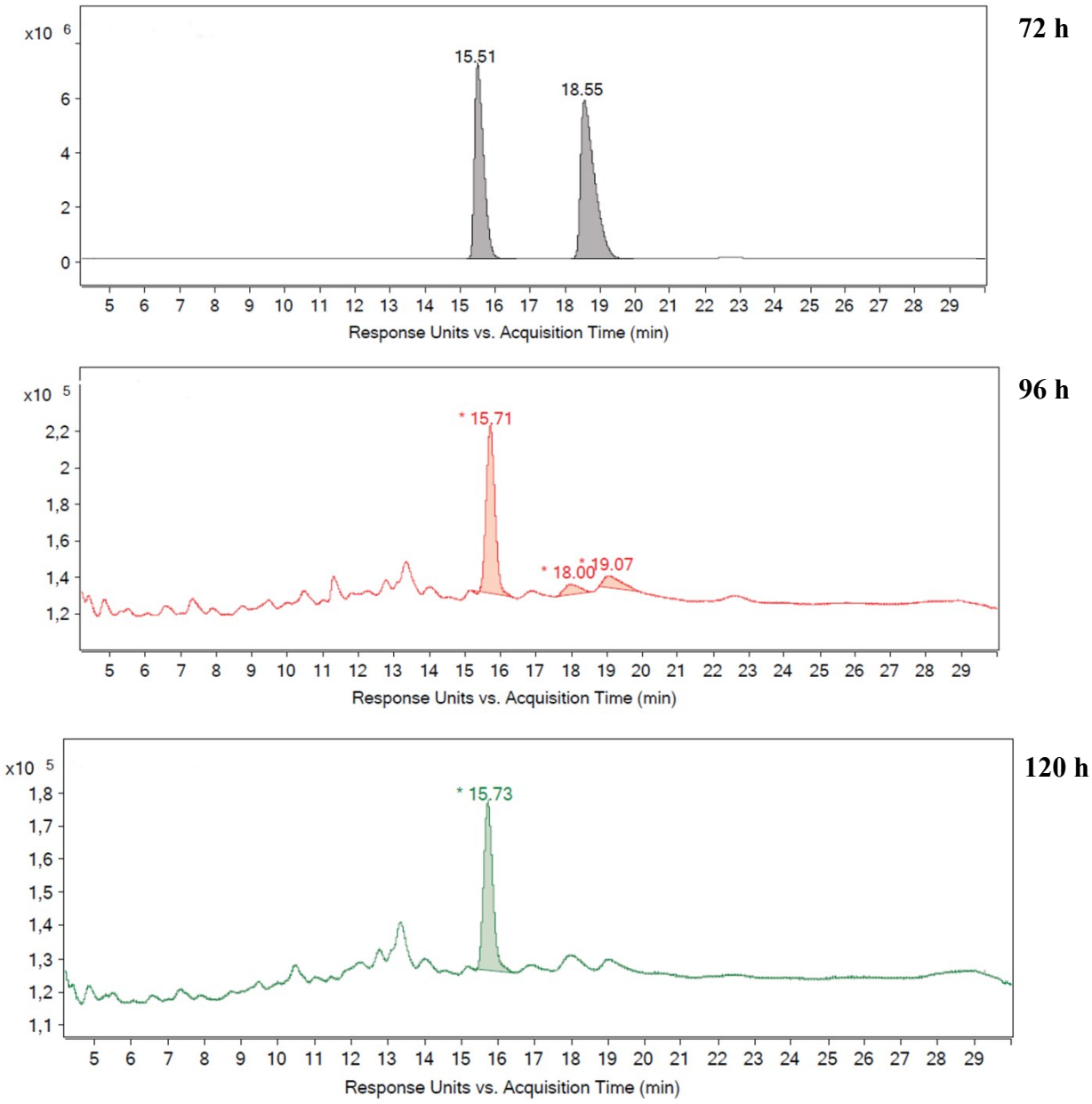

Fig. S14. Chiral GC chromatograms showing oxidized products formed from PMS biooxidation by the whole cells of *Streptomyces glaucescens* GLA.0 under conditions of reaction (**I**). Samples were taken after 72 h, 96 h and 120 h, respectively. Retention times of *R*-PMSO, *S*-PMSO and phenyl methyl sulfone were 15.5-15.7 min, 18-18.5 min and 19 min, respectively.

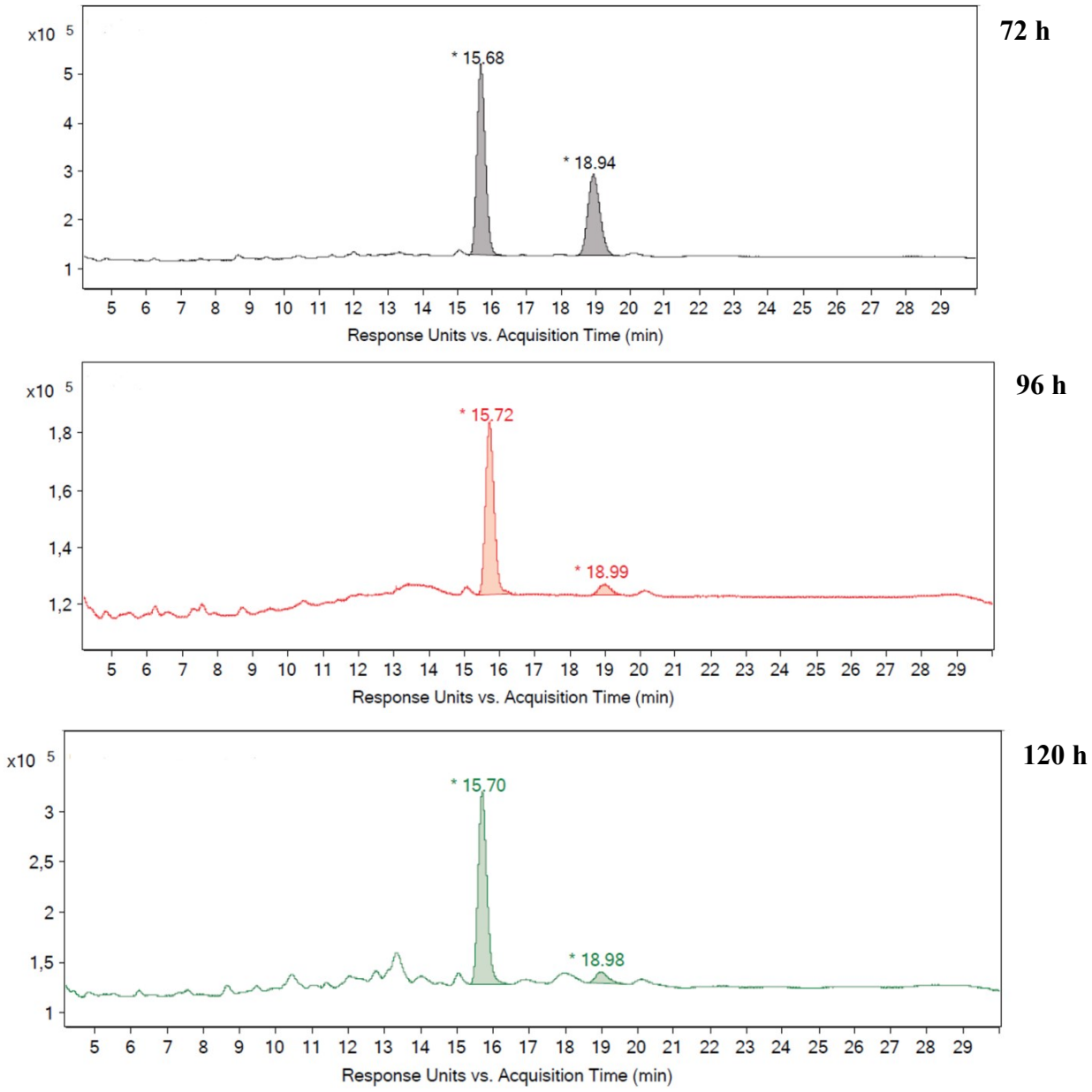

Fig. S15. Chiral GC chromatograms showing oxidized products formed from PMS biooxidation by the whole cells of *Streptomyces glaucescens* GLA.0 under conditions of reaction (**J**). Samples were taken after 72 h, 96 h and 120 h, respectively. Retention times of *R*-PMSO and phenyl methyl sulfone were 15.6-15.7 min and 18.9 min, respectively.

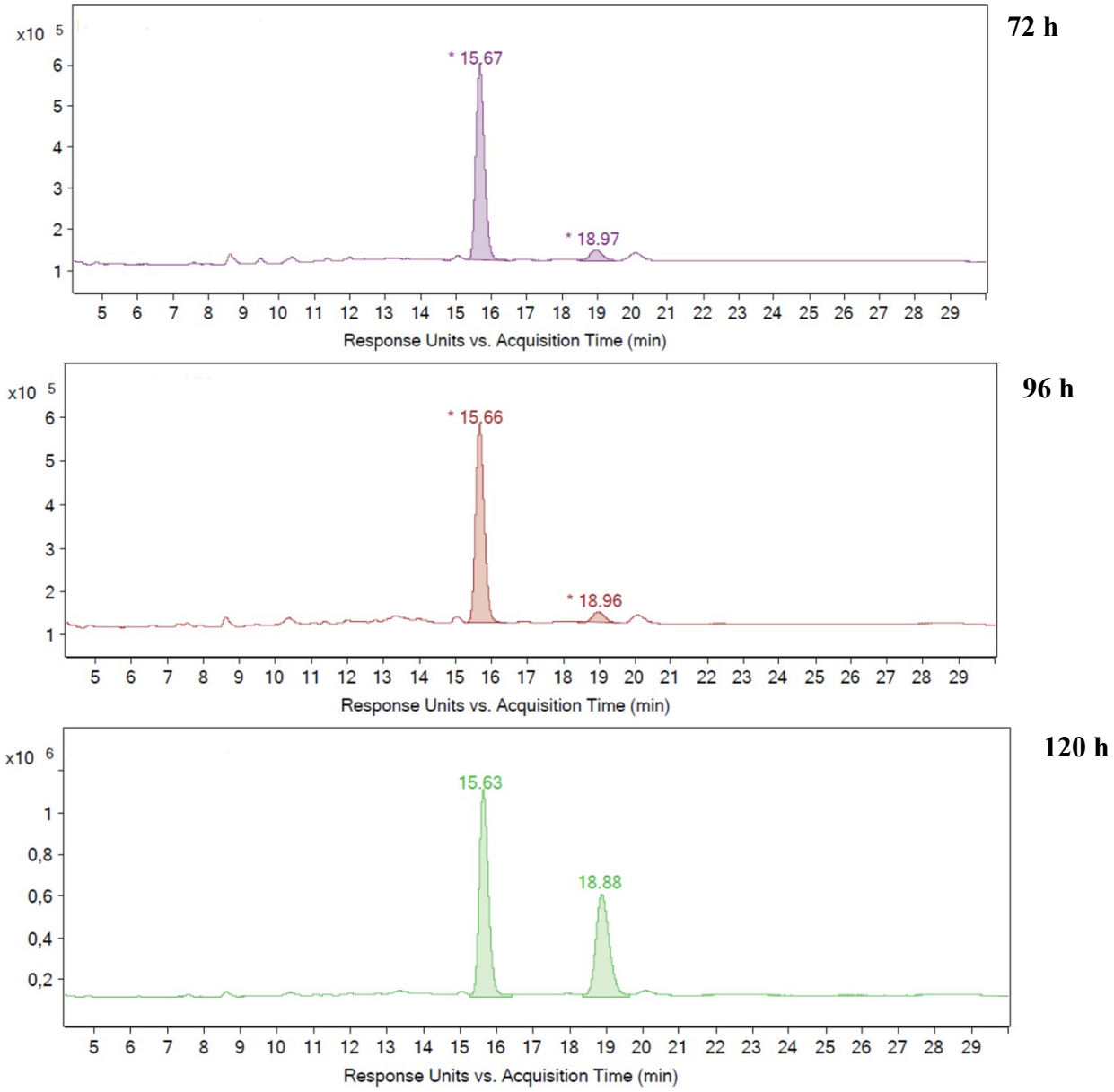

Fig. S16. Chiral GC chromatograms showing oxidized products formed from PMS biooxidation by the whole cells of *Streptomyces glaucescens* GLA.0 under conditions of reaction (**K**). Samples were taken after 72 h, 96 h and 120 h, respectively. Retention times of *R*-PMSO and phenyl methyl sulfone were 15.6 min and 18.8-18.9 min, respectively.

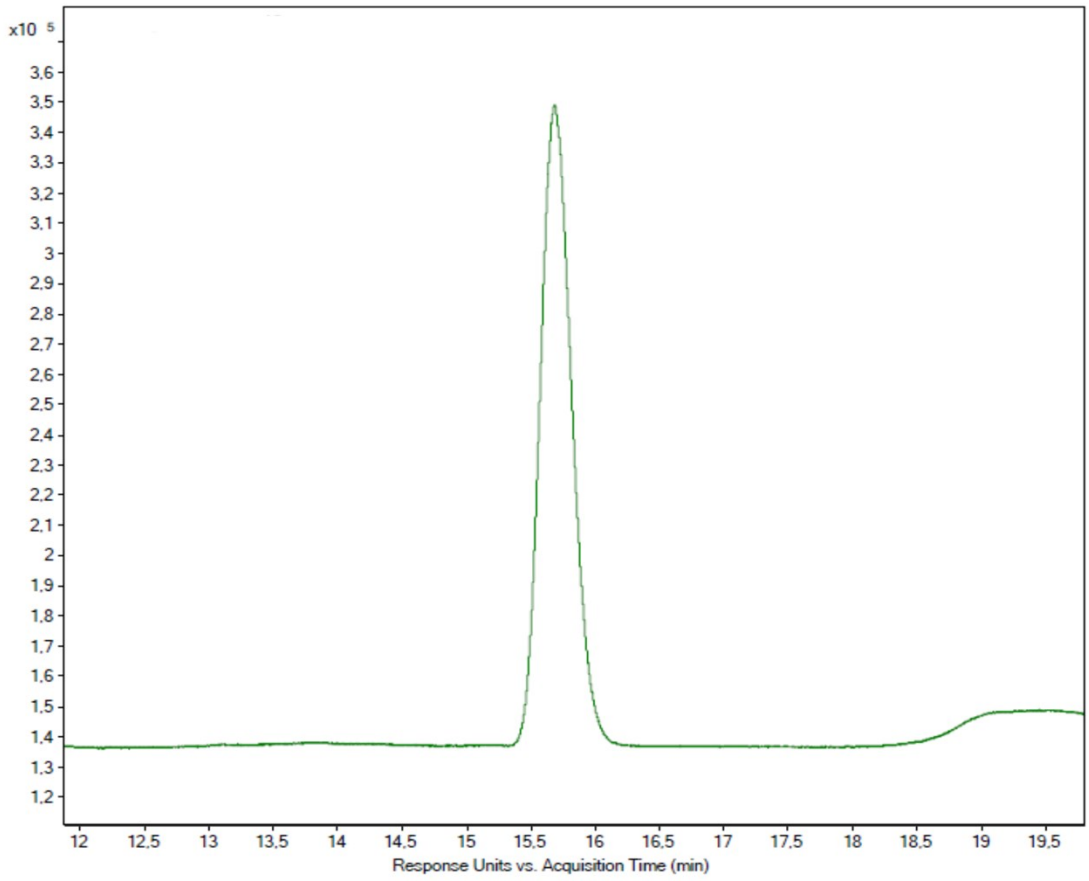

Fig. S17. Chiral GC chromatogram showing *R*-PMSO (Rt = 15.5 min) produced from enzymatic oxidation of PMS using phenyl acetone monooxygenase (PAMO).

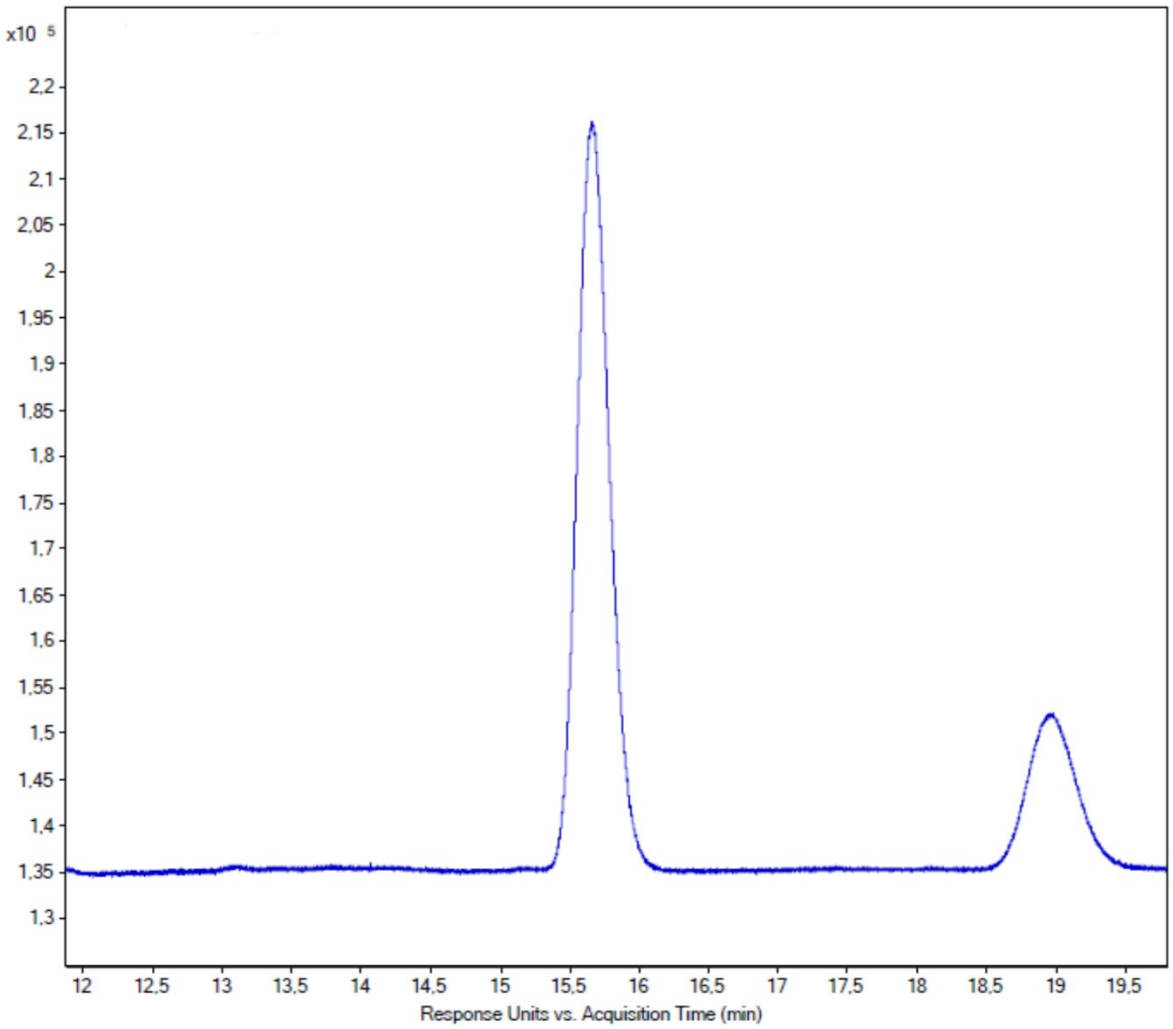

Fig. S18. Chiral GC chromatogram showing *R*-PMSO (Rt =15.5 min) produced from the enzymatic oxidation of PMS using cyclohexanone monooxygenase (CHMO).

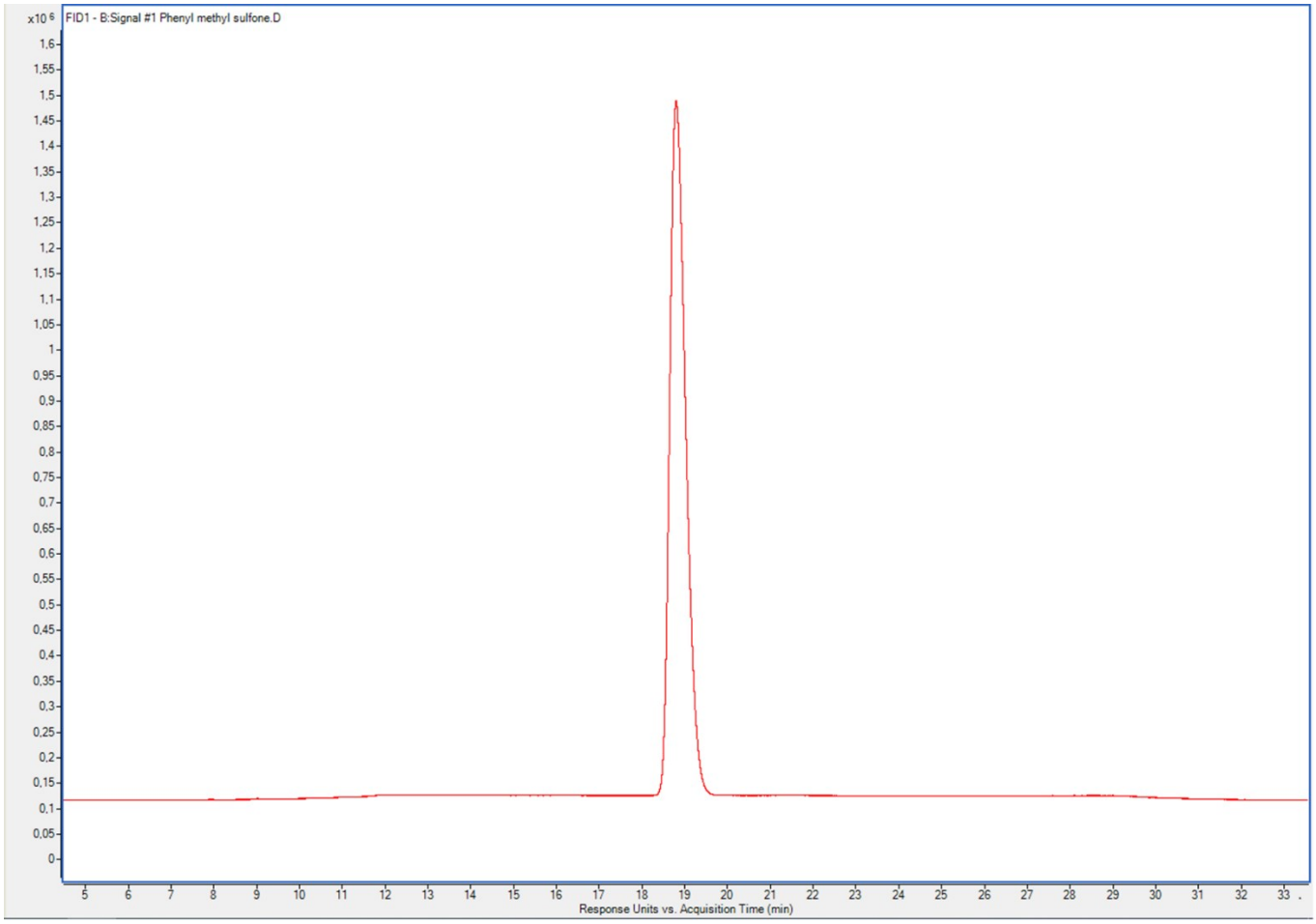

Fig. S19. Chiral GC chromatogram showing standard phenyl methyl sulfone (Rt = 18.8 min).

Table S1. Preliminary biotransformation experiments of PMS biooxidation using *S. glaucescens* GLA0 and their effects on PMS biotransformation.

Reaction	Substrate Conc.	Co solvent (%v/v)	Time of substrate addition	Reaction medium	RPM	Sampling Time [1]	PMS C% [2]	PMSO C% [2]	Sulfone C% [2]	Configuration [3]	*ee*% [3]
A	1.0 mM	IPA (0.2%)	3rd day	Medium 3	150	120	19	71	10	ND	ND
						144	7	77	16		
						168	2	78	20		
B	1.0 mM	None	3rd day	Medium 3	150	120	39	57	4	ND	ND
						144	8	74	18		
						168	1	75	24		
C	1.0 mM	None	3rd day	Medium 3	180	96	1	56	43	*R*	>99
						120	1	83	17	*R*	>99
						144	1	50	49	*R*	>99
D	1.0 mM	None	Zero	Medium 3	180	72	7	80	13	*S*	9
						96	3	82	15	*R*	83
						120	2	83	15	*R*	>99

[1] Addition of the substrate at zero time of inoculation or at the 3rd day. Sampling time was calculated from the beginning of the experiment.
[2] Relative amount of phenyl methyl sulfide, phenyl methyl sulfoxide and phenyl methyl sulfone in reaction samples as calculated by GC-MS.
[3] Configurations and (*ee* %) enantiomeric excess values were analyzed by chiral GC-FID,
ND – not determined

Table S2. Optimization of the biotransformation experiments using the whole growing cells of *S. glaucescens* GLA0.

Reaction	Substrate Conc.	IPA Conc. (% v/v)	Reaction medium	RPM	Sampling Time [1]	PMS C% [2]	PMSO C% [2]	Sulfone C% [2]	Configuration [3]	*ee*% [3]
E	1.0 mM	0.2%	Medium 2	150	72	9	79	12	ND	ND
					120	9	70	21		
					144	12	65	23		
					168	7	63	30		
F	1.0 mM	0.2%	Medium 3	150	72	45	55	0	ND	ND
					120	15	68	17		
					144	5	71	24		
					168	1	61	38		
G	5.0 mM	1%	Medium 3	150	72	10	76	14	ND	ND
					120	5	73	22		
					144	6	61	33		
					168	3	54	43		
H	5.0 mM	1%	Medium 2	150	72	4	83	13	ND	ND
					120	5	83	12		
					144	7	79	14		
					168	7	80	13		
I	1.0 mM	0.2%	Medium 3	180	72	2	43	55	*S*	11
					96	2	63	35	*R*	82
					120	0	81	19	*R*	>99
J	1.0 mM	0.2 %	Medium 2	180	72	18	71	11	*R*	>99
					96	6	90	4	*R*	>99
					120	2	90	8	*R*	>99
K	5.0 mM	1%	Medium 2	180	72	4	82	14	*R*	>99
					96	1	85	14	*R*	>99
					120	1	89	10	*R*	>99

[1] Addition of substrate at zero time of inoculation.
[2] Relative amount of phenyl methyl sulfide, phenyl methyl sulfoxide and phenyl methyl sulfone in reaction samples_ calculated by GC-MS.
[3] Configurations and (*ee* %) enantiomeric excess values were analyzed by chiral GC-FID.
ND – not determined