Supplementary Materials

Tissue-Specific Accumulation of Sulfur Compounds and Saponins in Different Parts of Garlic Cloves from Purple and White Ecotypes

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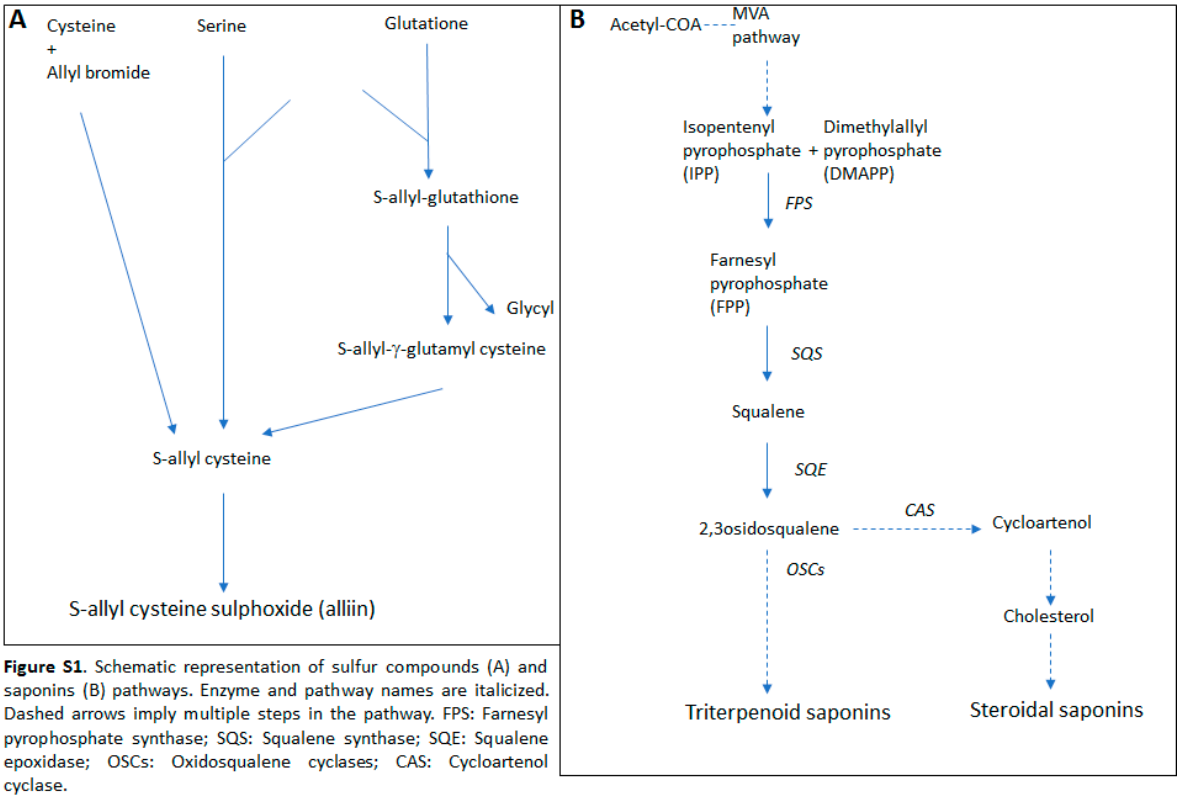

Figure S1. Schematic representation of sulfur compounds (A) and saponins (B) pathways. Enzyme and pathway names are italicized. Dashed arrows imply multiple steps in the pathway. FPS: Farnesyl pyrophosphate synthase; SQS: Squalene synthase; SQE: Squalene epoxidase; OSCs: Oxidosqualene cyclases; CAS: Cycloartenol cyclase.

Table S1. LC-HRMS analyses of sulfur compounds in three tissues (SS, ES and IS) of white and purple garlic ecotypes. Data are expressed as AVG+ST.DEV. AVGs, which represent, for each metabolite, the fold over the internal standard (IS) have been obtained by using, at least, 3 independent biological replicates. Asterisks indicate significance of the fold change in an ANOVA plus Tukey's t-test (*: $p \leq 0.05$;**: $p \leq 0.01$; ***: $p \leq 0.001$).

	WHITE-SS	PURPLE-SS	WHITE-ES	PURPLE-ES	WHITE-IS	PURPLE-IS
2-vinyl-2,4-dihydro-1,3-dithiin	0.0028±0.0001	1.8123±0.0003***	0.0082±0.0015	0.0118±0.0007	0.0005±0.0001	0.0008±0.0001*
ajoene	0.0756±0.0020	2.7861±0.0048***	0.1318±0.0065	0.1815±0.0103*	0.0075±0.0004	0.0088±0.0010
allicin	0.5215±0.0001	3.3462±0.0006***	2.2306±0.1522	3.7611±0.2797**	0.4038±0.0054	nd
alliin	5.9797±0.0943***	0.2654±0.0597	7.5575±0.2785**	5.8623±0.0399	0.8561±0.0105	0.7598±0.0469
allitridin	0.0002±0.0001	nd	0.4448±0.0002***	0.0039±0.0005	0.0001±0.0001	0.0001±0.0001
diallyl disulfide	0.0029±0.0004	2.2207±0.2014***	0.0036±0.0001*	0.0015±0.0002	nd	nd
diallyl sulfide	nd	nd	0.0007±0.0001	0.0005±0.0001	nd	nd
methyl allyl disulfide	nd	nd	0.0002±0.0001	0.0001±0.0001	0.0001±0.0001	nd
s-allyl-L-cysteine (SAC) (S-1-Propenyl-l-cysteine)	0.5209±0.0295*	0.3271±0.0171	0.2822±0.0153***	0.0022±0.0004	nd	nd
s-methyl-L-cysteine (SMC)	0.0122±0.0013*	0.0069±0.0003	0.0508±0.0027***	0.0004±0.0001	nd	nd
s-methyl mercapto-L-cysteine	0.0001±0.0001	0.0006±0.0001**	0.0006±0.0001	0.0005±0.0001	0.0003±0.0001	0.0008±0.0001**
s-methyl-L-cysteine sulfoxide	0.0341±0.0036	0.0582±0.0054*	0.0527±0.0094	0.0679±0.0033	0.0139±0.0016	0.0188±0.0009*
TOTAL	7.1500±0.1211	10.8235±0.0768**	10.7637±0.4622	9.8937±0.4106	1.2823±0.0149**	0.7891±0.08102

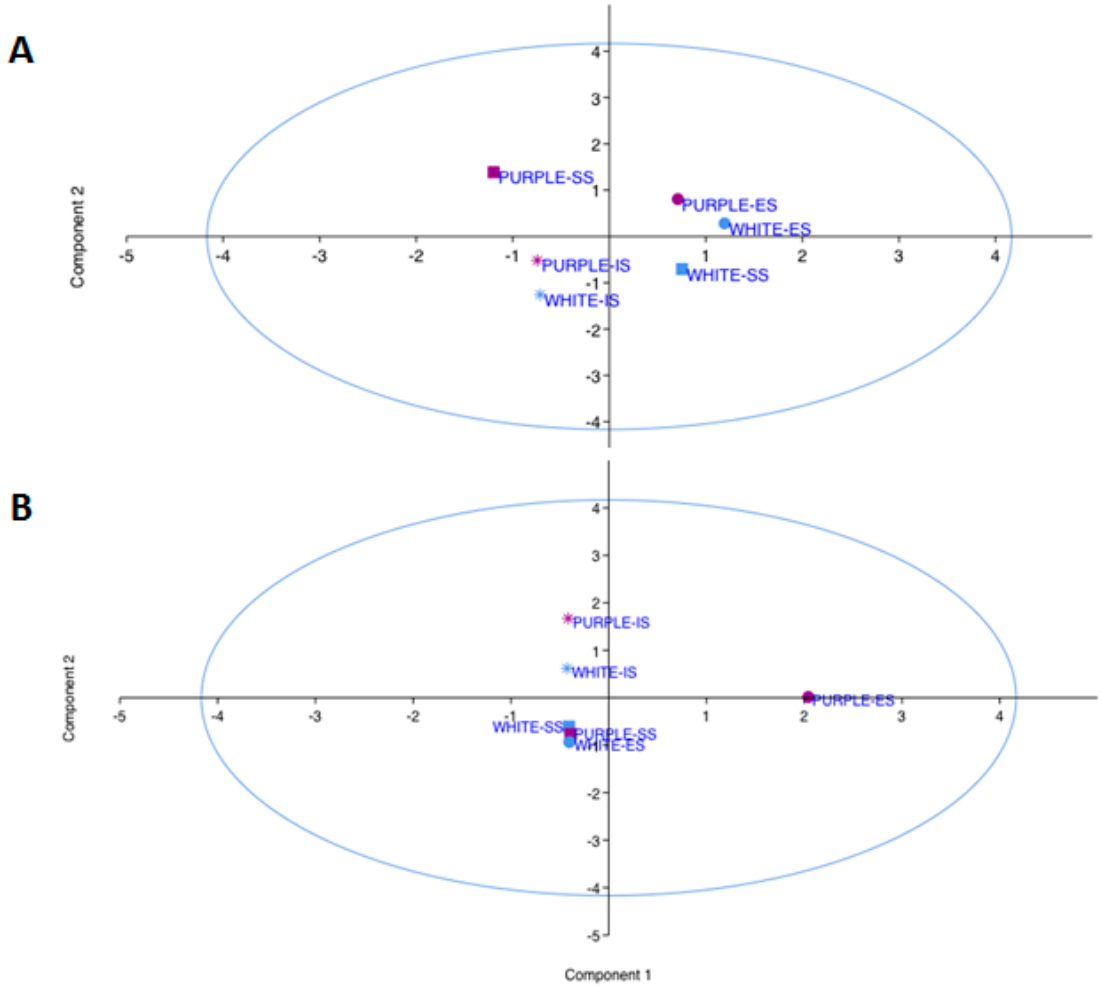

Figure S2. Principal component analysis (PCA), according the tissues/ecotypes, of sulfur compounds (A) and saponins (B) detected in three tissues (SS, ES and IS) of the white and purple ecotypes of garlic. Data represent, for each metabolite, the fold over the internal standard (IS) intensity.

Table S2. LC-HRMS analyses of saponin compounds in three tissues (SS, ES and IS) of white and purple garlic ecotypes. Data are expressed as AVG+ST.DEV. AVGs, which represent, for each metabolite, the fold over the internal standard (IS) have been obtained by using, at least, 3 independent biological replicates. Asterisks indicate significance of the fold change in an ANOVA plus Tukey's t-test (*: $p \leq 0.05$;**: $p \leq 0.01$; ***: $p \leq 0.001$).

	WHITE-SS	PURPLE-SS	WHITE-ES	PURPLE-ES	WHITE-IS	PURPLE-IS
agapanthagenin	nd	0.0010±0.0003	0.0009±0.0002	0.2928±0.0209***	nd	nd
b-chlorogenin	0.0536±0.0123	0.0841±0.0092*	0.0654±0.0153	5.0366±0.5253***	0.0011±0.0003	0.0010±0.0002
desgalactotigonin	0.0005±0.0001	0.0025±0.0006**	0.0011±0.0002	0.1043±0.0112***	nd	0.0009±0.0002
desgalactotigonin-rhamnose	nd	nd	nd	0.0018±0.0001	nd	nd
diosgenin	0.0086±0.0020	0.0111±0.0009	0.0088±0.0019	0.8386±0.0506***	nd	nd
eruboside B	0.0461±0.0062	0.0349±0.0058	0.0140±0.0040	0.8999±0.1672***	0.0002±0.0001	nd
eruboside B-rhamnose	0.0076±0.0010	0.0654±0.0071***	0.0171±0.0026	0.6389±0.1680***	0.0002±0.0001	nd
gitogenin	0.0536±0.0123	0.0806±0.0088	0.0652±0.0153	5.0270±0.5245***	0.0011±0.0003	0.0010±0.0002
proto-desgalactotigonin	nd	nd	nd	0.0004±0.0001	nd	nd
proto-desgalactotigonin-rhamnose	nd	0.0003±0.0001	nd	nd	nd	nd
proto-eruboside B	0.0004±0.0001	0.0024±0.0006***	0.0002±0.0001	0.0446±0.0107***	0.001±0.0001	0.0005±0.0002*
sativoside B1-rhamnose	nd	nd	nd	0.0026±0.0002	nd	nd
sativoside R1	nd	nd	nd	0.0014±0.0004	nd	nd
sativoside R2	0.0064±0.0002	0.0296±0.0031***	0.0134±0.0020	0.8516±0.2098***	0.0001±0.0001	0.0001±0.0001
sativoside R2-rhamnose	0.0001±0.0001	0.0063±0.0003***	0.0003±0.0001	0.0274±0.0076***	nd	nd
voghieroside D1	0.0001±0.0001	0.0003±0.0001**	nd	0.0046±0.0007	nd	nd
voghieroside E1	nd	0.0005±0.0001	0.0001±0.0001	0.0074±0.0021***	0.0016±0.0001***	0.0003±0.0001
TOTAL	0.1768±0.0342	0.3192±0.0368***	0.1865±0.0416	13.7800±1.6995***	0.0054±0.0007	0.0038±0.0008

Figure S3. White (A) and purple (B) garlic ecotypes under study.