Supplementary materials

Table S1. Concentration levels of each internal standard in stock solution, mixed stock solution, and final sample solution.

Internal standards	SIM ion	Stock solution (g/L)	Mixed stock solution (mg/L)	Sample solution (μg/L)
For esters and volatile phenols				
ethyl butyrate-4,4,4 d_3	74	1	50	25
ethyl-d_5 hexanoate	110	1	125	62.5
ethyl-octanoate d_{15}	142	2.5	125	62.5
ethyl trans cinnamate d_5	181	2.5	0.75	37.5
For higher alcohols				
2-octanol	55	0.1	10	50
For terpenes				
geraniol d_6	75	0.1	10	50
linalool d_5	98	0.1	10	50
2-octanol	55	0.1	10	50
ethyl trans cinnamate d_5	181	2.5	0.75	3.75
For norisoprenoids				
ethyl trans cinnamate d_5	181	2.5	0.75	3.75

Table S2: List of quantified compounds in GJM medium, including SIM ions, assigned internal standards, calibration ranges and curve parameters, R^2, recovery, RSD, inter-day precision, LOD, and LOQ.

Compound	Assessed ion (*m*/*z*)	Calibration range (µg/L)	Calibration curve (y = kx + n)	R^2	Recovery	RSD	Inter-day precision	LOD (µg/L)	LOQ (µg/L)
Esters									
ethyl propanoate[1]	102	1 - 250	0.0000770x - 0.0002	0.995	98.2	9.2	9.8	0.2	0.5
ethyl isobutyrate[1]	116	1 - 250	0.000149 x - 0.0003	0.996	94.1	10.2	10.3	0.2	0.5
propyl acetate[1]	61	1 - 250	0.000260 x - 0.0003	0.996	103.0	8.6	8.9	0.2	0.5
isobutyl acetate[1]	56	1 - 250	0.000400 x - 0.0007	0.997	107.4	5.7	5.8	0.2	0.5
ethyl butyrate[1]	88	1 - 250	0.000620 x - 0.0009	0.996	100.0	7.7	7.6	0.2	0.5
ethyl 2-methylbutyrate[1]	102	1 - 250	0.00130x - 0.002	0.997	98.8	8.2	8.7	0.2	0.5
ethyl isovalerate[1]	88	1 - 250	0.00146x - 0.006	0.998	100.5	11.2	12.1	0.2	0.5
phenylethyl acetate[7]	104	1 - 250	0.227x - 0.03	0.994	118.9	9.5	9.9	0.2	0.5

butyl acetate[1]	56	1 - 250	0.000820 x + 0.0005	0.991	109.9	7.2	8.0	0.2	0.5
isoamyl acetate[1]	70	25 - 5000	0.00197x - 0.064	0.993	92.5	5.1	5.8	0.2	0.5
ethyl hexanoate[2]	88	10 - 2500	0.000890 x - 0.005	0.98	104.5	7.7	8.1	0.3	1
ethyl octanoate[3]	88	10 - 2500	0.00145x - 0.002	0.98	109.1	8.2	8.3	0.3	1
hexyl acetate[2]	56	2.5 - 500	0.000910 x - 0.003	0.994	92.7	10.4	11.1	0.3	1
ethyl decanoate[3]	88	2.5 - 500	0.00212x - 0.006	0.997	105.9	11.4	11.2	0.3	1
ethyl leucate[2]	87	2.5 - 500	0.00009x	0.999	112.0	8.8	9.2	0.3	1
ethyl valerate[1]	88	0.25 - 50	0.00270x - 0.001	0.997	93.5	7.2	7.5	0.03	0.1
Z-3-hexenyl acetate[2]	82	0.25 - 50	0.000910 x - 0.0001	0.996	112.0	9.7	10.2	0.03	0.1
E-2-hexenyl acetate[2]	82	0.25 - 50	0.000629 x	0.997	94.0	9.2	9.6	0.03	0.1
octyl acetate[3]	70	0.25 - 50	0.000672 x - 0.0002	0.992	92.1	7.2	7.9	0.03	0.1
ethyl dodecanoate[3]	88	0.25 - 50	0.000580 x - 0.002	0.993	113.3	9.6	9.8	0.03	0.1
ethyl phenyl acetate[7]	91	0.25 - 50	0.395x - 0.092	0.994	103.4	6.9	7.0	0.03	0.1

ethyl cinnamate[7]	176	0.025 – 5	0.0536x - 0.007	0.997	139.1	12.6	13.2	0,005	0,01
ethyl dihydro cinnamate[7]	178	0.025 – 5	0.122x - 0.003	0.9995	121.1	11.7	12.0	0,005	0,01
Higher alcohols									
Hexanol[6]	56	100 - 20000	0.000106 x + 0.009	0.98	119.9	10.5	10.4	0.3	1
Z-3-hexenol[6]	82	2.5 - 500	0.000025 x	0.996	119.2	8.2	8.7	0.3	1
E-2-hexenol[6]	82	2.5 - 500	0.000016 x + 0.0003	0.995	135.6	7.9	8.0	0.3	1
E-3-hexenol[6]	82	2.5 - 500	0.000028 x	0.995	120.2	9.3	10.1	0.3	1
Volatile phenols									
4-ethyl phenol[7]	107	5 - 1000	0.0432x - 0.195	0.998	113.2	6.6	6.7	0.1	0.3
4-ethyl guaiacol[7]	137	2.5 - 500	0.0773x - 0.020	0.9997	119.5	8.5	8.6	0.1	0.3
methyl salicilate[7]	120	0.5 - 100	0.105x - 0.049	0.998	122.9	11.2	11.9	0.1	0.3
4-vinyl guaiacol[7]	150	5 - 1000	0.00340x - 0.058	0.996	106.6	7.9	8.4	0.1	0.3
4-vinyl phenol[7]	120	25 - 5000	0.000580 x - 0.0610	0.995	118.8	8.4	8.3	0.1	0.3
Guaiacol[7]	124	1 - 250	0.0133x - 0.0066	0.9993	105.6	9.1	9.4	0.1	0.3
Terpenes									

3-carene[6]	93	0.01 - 2	0.00492x	0.998	77.2	12.2	12.9	0.002	0.005
α-terpinene[6]	136	0.01 - 2	0.00241x	0.998	88.1	8.7	9.0	0.001	0.004
1,4-cineole[6]	111	0.01 - 2	0.00382x	0.998	105.1	9.3	9.2	0.002	0.005
limonene[6]	136	0.01 - 2	0.00449x - 0.0001	0.998	85.7	5.7	6.0	0.001	0.004
eucalyptol[6]	108	0.01 - 2	0.00147x	0.997	110.6	6.1	6.5	0.002	0.005
γ-terpinene[6]	136	0.01 - 2	0.00128x	0.998	84.5	8.1	8.9	0.002	0.005
p-cymene[6]	119	0.01 - 2	0.0194x - 0.0001	0.9999	85.2	8.6	8.7	0.002	0.005
α-terpinolene[6]	136	0.01 - 2	0.00512x - 0.0001	0.997	86.2	5.3	5.8	0.001	0.004
cis-rose oxide[6]	139	0.05 - 10	0.00800x - 0.0009	0.9999	88.3	7.7	8.1	0.002	0.005
trans-rose oxide[6]	139	0.05 - 10	0.00290x - 0.0001	0.9998	84.3	9.2	10.0	0.003	0.008
trans-linalool oxide[5]	94	0.5 - 100	0.000631x - 0.0007	0.994	92.6	10.1	10.5	0.003	0.009
cis-linalool oxide[5]	94	0.5 - 100	0.000383x - 0.0005	0.994	90.6	11.2	12.0	0.003	0.009
vitispirane 1[7]	192	0.5 - 100	0.0360x - 0.015	0.996	95.3	9.9	9.8	0.002	0.006
vitispirane 2[7]	192	0.5 - 100	0.0622x - 0.031	0.995	91.8	10.6	10.7	0.002	0.006
Linalool[5]	93	0.5 - 100	0.00550x - 0.010	0.993	86.0	6.7	6.8	0.003	0.008

4-terpineol[5]	111	0.05 - 10	0.00572x - 0.001	0.996	85.3	6.3	6.9	0.002	0.005
Hotrienol[5]	71	0.5 - 100	0.0128x - 0.010	0.9991	87.3	9.6	10.5	0.003	0.009
α - terpineol[5]	93	0.5 - 100	0.00319x - 0.002	0.998	90.6	5.4	6.1	0.002	0.006
TDN[7]	157	0.05 - 10	0.772x - 0.030	0.9992	77.6	8.3	8.9	0.002	0.006
cis-geraniol (nerol)[4]	93	0.5 - 100	0.00180x - 0.003	0.9998	82.1	9.4	9.3	0.003	0.01
trans- β - damascenone[7]	190	0.05 - 10	0.0862x - 0.037	0.998	83.8	10.7	11.2	0.002	0.006
trans geraniol[4]	136	0.5 - 100	0.000117 x + 0.0001	0.9991	96.1	9.5	10.0	0.003	0.01
α - ionone[7]	121	0.01 - 2	0.318x - 0.0006	0.996	74.6	8.5	8.5	0.003	0.01
β - ionone[7]	177	0.01 - 2	0.476x + 0.0003	0.9995	92.3	7.9	8.0	0.003	0.01
trans-nerolidol[4]	93	0.05 - 10	0.00110x - 0.0002	0.999	77.6	11.4	11.6	0.003	0.009
E-nerolidol[4]	93	0.05- 10	0.00147x - 0.0002	0.9993	78.0	10.2	11.1	0.003	0.009
citronellol [4]	95	0.5 - 100	0.00210x + 0.0009	0.9992	97.7	6.8	7.0	0.002	0.006

[1] ethyl butyrate-4,4,4 d_3

[2]ethyl-d_5 hexanoate

[3]ethyl-octanoate d_{15}

[4]geraniol d_6

[5]linalool d_5

[6]2-octanol

[7]ethyl trans cinnamate d_5

Table S3: List of quantified compounds with SIM ions, corresponding internal standards, calibration curves, R^2 values, and recoveries measured in SCM medium.

[a]Compound	Calibration curve (y = kx +n)	R^2	Recovery
Esters			
ethyl propanoate[1]	0.000078x + 0.000084	0.9998	105.3
ethyl isobutyrate[1]	0.000158x - 0.000182	0.9991	91.4
propyl acetate[1]	0.00026x + 0.00032	0.9997	108.7
isobutyl acetate[1]	0.00045x - 0.00014	0.9997	101.3
ethyl butyrate[1]	0.00065x + 0.00023	0.9998	103.9
ethyl 2-methylbutyrate[1]	0.0014x - 0.0014	0.9994	95.5
ethyl isovalerate[1]	0.001612x - 0.002495	0.9997	95.2
phenylethyl acetate[7]	0.2447x + 0.0019	0.9998	123.7
butyl acetate[1]	0.000921x - 0.000241	0.999	103.6
isoamyl acetate[1]	0.00158x + 0.096932	0.998	123.6
ethyl hexanoate[2]	0.00094x + 0.0082	0.997	102.2
ethyl octanoate[3]	0.001413x + 0.024421	0.995	107.7
hexyl acetate[2]	0.00085x + 0.00082	0.9997	103.6
ethyl decanoate[3]	0.00233x - 0.01626	0.997	98.8
ethyl leucate[2]	0.00009x + 0.0004	0.994	116.9
ethyl valerate[1]	0.0027x - 0.0005	0.9998	98.2
Z-3-hexenyl acetate[2]	0.00102x + 0.00012	0.9994	105.7
E-2-hexenyl acetate[2]	0.000543x + 0.000266	0.998	109.3
octyl acetate[2]	0.00065x - 0.000058	0.9993	93.4
ethyl dodecanoate[3]	0.00027x - 0.00077	0.997	122.4
ethylphenyl acetate[7]	0.3953x + 0.0176	0.9999	116.2
ethyl cinnamate[7]	0.0523x - 0.0084	0.9992	146.1
ethyl dihydrocinnamate[7]	0.11995x - 0.00339	0.998	135.1
Higher alcohols			
hexanol [6]	0.000117x + 0.016524	0.98	116.3

Z-3-hexenol[6]	0.000026x + 0.000072	0.997	117.4
E-2-hexenol[6]	0.000016x + 0.000214	0.9998	128.2
E-3-hexenol[6]	0.000027x + 0.000105	0.998	129.9
Volatile phenols			
4-ethyl phenol[7]	0.0444x + 0.0075	0.9998	120.2
4-ethyl guaiacol[7]	0.0823x - 0.0735	0.9999	120.5
methyl salicilate[7]	0.114096x - 0.0821	0.99993	122.9
4-vinyl guaiacol[7]	0.0012x - 0.0281	0.998	116.5
4-vinyl phenol[7]	0.00048x - 0.06697	0.998	115.5
Guaiacol[7]	0.0135x - 0.0089	0.9998	112.4
Terpenes			
3-carene[6]	0.0035x - 0.00003	0.998	80.5
α -terpinene[6]	0.001646x + 0.0000007	0.99991	94.7
1,4-cineole[6]	0.003933x - 0.00006	0.998	99.3
limonene [6]	0.003353x - 0.000002	0.99997	95.0
eucalyptol [6]	0.00144x + 0.00001	0.999	102.9
γ -terpinene[6]	0.000909x + 0.000005	0.9995	90.1
p-cymene[6]	0.0162x - 0.00004	0.996	85.9
α -terpinolene[6]	0.003554x - 0.000014	0.99994	93.3
cis-rose oxide[6]	0.0076x - 0.0005	0.9996	86.9
trans-rose oxide[6]	0.0027x - 0.0002	0.9997	86.3
trans-linalool oxide[5]	0.000528x + 0	0.996	102.0
cis-linalool oxide[5]	0.000312x + 0	0.994	101.8
vitispirane 1[7]	0.097148x - 0.598	0.996	55.9
vitispirane 2[7]	0.1019x - 0.2958	0.998	59.2
linalool[5]	0.0044x - 0.0037	0.98	102.5
4-terpineol[5]	0.00486x - 0.00006	0.994	101.0
hotrienol[5]	0.0102x - 0.0037	0.998	86.8
α -terpineol[5]	0.00255x + 0.00146	0.994	113.5
TDN[7]	0.8277x - 0.0724	0.998	77.3
cis-geraniol (nerol)[4]	0.00097x - 0.00039	0.9998	81.0
trans-β-damascenone[7]	0.0849x + 0.0199	0.992	88.9
trans geraniol[4]	0.000102x + 0.000149	0.9994	106.5
α -ionone[7]	0.2847x - 0.0076	0.998	81.1
β-ionone[7]	0.4626x - 0.0033	0.999	90.9
trans-nerolidol[4]	0.00097x - 0.00034	0.995	71.5
E-nerolidol[4]	0.00122x - 0.00042	0.997	77.1

citronellol[4]	0.00202x - 0.00028	0.99998	90.5

[a]Assessed ions, Calibration ranges, RSDs, LODs and LOQs are already presented in Table S2.

[1]ethyl butyrate-4,4,4 d_3

[2]ethyl-d_5 hexanoate

[3]ethyl-octanoate d_{15}

[4]geraniol d_6

[5]linalool d_5

[6]2-octanol

[7]ethyl trans cinnamate d_5

.

Table S5. Effective concentrations (EC_{50}, µL/L airspace) of synthetic volatile organic compounds (VOCs) required to inhibit 50% of *Botrytis cinerea* F61 mycelial growth. Values were estimated using four-parameter log-logistic (LL.4) or constant relative slope (CRS.4c) models, depending on best model fit.

Compound	Model[1] tested	EC_{50} (mean ± SE[2]) (µL/L)	95% CI[3] (lower-upper)	Hill slope ± SE[2]	AIC[4]	Summary of model fit assessment
citronellol	LL.4	6.7 ± 0.1	6.5–6.9	3.99 ± 0.34	94	Best model: CRS.4c (lower AIC)
	CRS.4c	6.3 ± 0.1	6.0–6.7	5.72 ± 1.91	89	
geraniol	LL.4	15.8 ± 0.5	14.7–16.9	3.39 ± 0.47	112	Best model: CRS.4c (lower AIC); EC_{50} unstable (wide CI)
	CRS.4c	13.2 ± 3.8	5.3–21.2	8.93 ± 27.86	97	
nerol	LL.4	14.7 ± 0.8	13.1–16.4	2.63 ± 0.34	129	Best model: CRS.4c (lower AIC); EC_{50} unstable (wide CI)
	CRS.4c	8.4 ± 3.1	1.9–14.9	5.20 ± 1.91	116	
α-terpineol	LL.4	31.2 ± 1.0	29.2–33.3	3.65 ± 0.41	109	Best model: CRS.4c (lower AIC)
	CRS.4c	30.4 ± 1.7	26.7–34.1	5.42 ± 1.87	104	
linalool	LL.4	36.3 ± 0.9	34.3–38.3	3.44 ± 0.41	107	Best model: CRS.4c (lower AIC)
	CRS.4c	33.9 ± 1.3	31.1–36.8	4.10 ± 0.52	104	
4-vinyl phenol	LL.4	50.1 ± 2.3	45.3–55.0	3.41 ± 0.40	131	Models equivalent; LL.4 selected (more stable)
	CRS.4c	48.4 ± 3.5	41.0–55.8	3.55 ± 0.41	131	
isoamyl acetate	LL.4	63.6 ± 7.3	48.1–79.1	3.36 ± 1.78	176	Models equivalent; CRS.4c selected (more stable).
	CRS.4c	60.0 ± 7.0	45.2–74.8	4.65 ± 5.11	176	
vitispirane[5]	LL.4	165.7 ± 106.5	-59.0–390.3	2.07 ± 1.92	109	LL.4: EC_{50} not reached within tested range; no model convergence; CRS.4c: no model convergence, EC_{50} not estimable
	CRS.4c	> max tested conc.	-	-	-	
isobutyl acetate[5]	LL.4	196.9 ± 53.2	84.6–309.2	4.56 ± 4.18	119	Best model: CRS.4c (lower AIC); LL.4 unstable
	CRS.4c	162.6 ± 39.9	78.4–246.9	12.09 ± 29.50	114	
eucalyptol	LL.4	169.0 ± 12.6	142.4–195.6	1.57 ± 0.15	100	Best model: LL.4 (lower AIC)
	CRS.4c	131.8 ± 8.8	113.3–150.3	2.15 ± 0.23	108	
ethyl butyrate	LL.4	234.3 ± 31.3	168.2–300.4	1.66 ± 0.23	114	Best model: LL.4 (lower AIC)
	CRS.4c	162.7 ± 11.6	138.2–187.2	2.72 ± 0.45	117	
ethyl propionate[5]	LL.4				123	
		466.3 ± 1028.2	-1702.9–2635.6	2.39 ± 3.01		Best model: CRS.4c; LL.4 EC_{50} unstable
	CRS.4c	663.7 ± 47.7	563.0–764.4	2.10 ± 0.60	123	
4-vinyl guaiacol[5]	LL.4	703.6 ± 2225.0	-3990.8–5398.0	-1.48 ± 3.60	113	LL.4: EC_{50} not reached within tested dose range; CRS.4c: no model convergence, EC_{50} not estimable
	CRS.4c	> max tested conc.	-	-	-	

[1] Open source package "drc" in R. LL.4 is four-parameter log-logistic model, and CRS.4c is the constant relative slope 4-parameter logistic model from the drc package.

[2] SE = standard error.

[3] CI = 95% confidence interval for EC_{50}

[4]AIC = Akaike Information Criterion

[5] For these compounds, 50% inhibition of *B. cinerea* growth was not achieved within the tested concentration range (max tested: 735 µL/L). EC_{50} values are therefore extrapolated by the model or expressed as "> max tested concentration."