

Table S1. Tentative identification of the chemical constituents of Rosa by UHPLC-Q-q-Q-MS/MS under negative and positive ionization

Compound	Formula	MS/MS transition (MRM)		Fragmentor (V)	Collision energy (V)	Polarity
		Precursor ion (m/z)	Product ion (m/z)			
Epicatechin	C ₁₅ H ₁₄ O ₆	289	245	200	22	Negative
Catechin	C ₁₅ H ₁₄ O ₆	289	245	200	22	Negative
ProcyanidinB2	C ₃₀ H ₂₆ O ₁₂	577	407/125	154	25/16	Negative
Kaempferol	C ₁₅ H ₁₀ O ₆	285	185/151	171	20/25	Negative
Isorhamnetin	C ₁₆ H ₁₂ O ₇	315	300/151	180	23/31	Negative
Hyperoside	C ₂₁ H ₂₀ O ₁₂	463	300/271	200	24	Negative
Quercetin	C ₁₅ H ₁₀ O ₇	301	179/151	125	20/22	Negative
Epicatechin gallate	C ₁₅ H ₁₄ O ₇	441	169/289	130	24/23	Negative
Luteolin	C ₁₅ H ₁₀ O ₆	609	300/271	190	50	Negative
Apigenin	C ₂₁ H ₂₀ O ₁₀	269	117/151	130	23/22	Negative
Myricetin	C ₁₅ H ₁₀ O ₈	317	210	151	25	Negative
Quercetin 3-O-Glc	C ₂₁ H ₂₀ O ₁₂	463	301	200	24	Negative
kaempferol glucuronid	C ₂₁ H ₁₈ O ₁₂	461	285	210	28	Negative
Quercetin glucuronide	C ₂₁ H ₁₈ O ₁₃	477	301	200	24	Negative
Kaempferol-3-O-glucoside	C ₂₁ H ₂₀ O ₁₁	446.9	283.8	210	28	Negative
Gallic acid	C ₇ H ₆ O ₅	169	125	86	115	Negative
Syringic acid	C ₉ H ₁₀ O ₅	197	182/123	80	20	Negative
Vanillic acid	C ₈ H ₈ O ₄	167	152/108	135/80	12/16	Negative
Protocatechuic acid	C ₇ H ₆ O ₄	152.9	109	100	14	Negative
Caffeic acid	C ₉ H ₈ O ₄	297.8	268.7	160	10	Negative
4 hydroxybenzoic acid	C ₇ H ₆ O ₃	137	93/80.1	74	20285	Negative
Ferulic acid	C ₁₀ H ₁₀ O ₄	193	178/134	88	15/34	Negative
Salicylic acid	C ₇ H ₆ O ₃	137	93.03	100	15	Negative
<i>P</i> -coumaric acid	C ₉ H ₈ O ₃	162.9	119	135	12	Negative
3-hydroxybenzoic acid	C ₇ H ₆ O ₃	137	93.1	74	16/8	Negative
Chlorogenic acid	C ₁₆ H ₁₈ O ₉	353	191	110	15	Negative
Delphinidin-3-O-glucoside	C ₂₁ H ₂₁ O ₁₂ +	465	303	130	13	Positive
Delphinidin 3,5-diGlc	C ₂₇ H ₃₁ O ₁₇ +	627.2	303	130	13	Positive

Cyanidin-3-O-galactoside	C ₂₁ H ₂₁ O ₁₁ +	448.9	286.8	130	15	Positive
Cyanidin-3-O-glucoside	C ₂₁ H ₂₁ O ₁₁ +	449	287	130	15	Positive
Petunidin-3-O-glucoside	C ₂₂ H ₂₃ O ₁₂ +	479	317	140	15	Positive
Malvidin-3-O-glucoside	C ₂₃ H ₂₅ O ₁₂ +	493	316	140	14	Positive
Peonidin-3-O-glucoside	C ₂₂ H ₂₃ O ₁₁ +	463	301	130	15	Positive
Cyanidin-3-O-xyloside	C ₂₀ H ₁₉ O ₁₀ +	419	287	130	15	Positive
Peonidin-3-(5'-rutinoside)-O-glu	C ₂₁ H ₂₁ ClO ₁₁	448.9	286.8	130	15	Positive

Table S2. The relative quantification of differential metabolites in rosa and fermented rosa (n=3). Data are presented as mean \pm SD)

Compounds	R	FR	ratio
Procyanidins			
Epicatechin	101238 \pm 15.9	215847 \pm 17.8	2.1
Catechin	182217.3 \pm 6.6	626108.3 \pm 5.6	3.4
ProcyanidinB2	899731.0 \pm 5.8	632169.3 \pm 6.1	0.7
Flavonoids			
Isorhamnetin	206749 \pm 7.8	235656 \pm 7.4	1.1
Kaempferol	3534848.7 \pm 8.3	323081 \pm 9.6	0.1
Quercetin	3953086.0 \pm 31.4	2361286.7 \pm 38.6	0.6
Hyperoside	39510165.0 \pm 44.6	52466530.0 \pm 37.9	1.3
Epicatechin gallate	2220401.0 \pm 26.9	1521394.0 \pm 34.4	0.7
Luteolin	1614.3 \pm 3.2	1542.3 \pm 2.6	1.0
Apigenin	120893.7 \pm 29.4	153698.3 \pm 22.6	1.3
Myricetin	47734.0 \pm 10.2	52124.3 \pm 15.8	1.1
Quercetin 3-O-Glc	298744.7 \pm 23.9	364505.3 \pm 26.8	1.2
kaempferol glucuronid	39225.7 \pm 14.3	50182.3 \pm 16.8	1.3
Quercetin glucuronide	7690.3 \pm 12.4	9632.7 \pm 16.5	1.3
Kaempferol-3-O-glucoside	7092.0 \pm 7.6	13232.7 \pm 16.2	1.9
Phenolic acids			
Gallic acid	10670363.3 \pm 37.8	23673403.0 \pm 38.4	2.2
Protocatechuic acid	332158.7 \pm 9.1	450311.3 \pm 10.7	1.4
Chlorogenic acid	41052556 \pm 36.4	41058665.0 \pm 44.5	1.0
Syringic acid	2417968.7 \pm 21.5	7212956.7 \pm 19.5	3.0
Vanillic acid	24576156.7 \pm 36.9	30674819.7 \pm 35.6	1.2
4 hydroxybenzoic acid	27501.3 \pm 4.1	29325.7 \pm 3.2	1.1
Caffeic acid	282169.3 \pm 7.3	314311.3 \pm 6.5	1.1
Salicylic acid	1426.7 \pm 3.2	1268.7 \pm 3.6	0.9
Ferulic acid	25245.7 \pm 1.8	14575.3 \pm 1.9	0.6
<i>P</i> -coumaric acid	30667.0 \pm 15.9	28625.7 \pm 18.5	0.9
3-hydroxybenzoic acid	21177.7 \pm 5.3	20545.7 \pm 6.7	1.0
Anthocyanin			
Delphinidin-3-O-glucoside	1580369.3 \pm 26.7	1592733.3 \pm 28.8	1.0

Delphinidin 3,5-diGlc	5170716.3±35.6	5367658±38.2	1.0
Cyanidin-3-O-galactoside	425153.3±18.4	446329±14.9	1.0
Cyanidin-3-O-glucoside	70871541±32.3	43843708±33.9	0.6
Cyanidin-3-O-xyloside	306645±16.3	370780.7±15.2	1.2
Petunidin-3-O-glucoside	616645±16.5	638227.3±34.1	1.0
Malvidin-3-O-glucoside	1129±6.1	1150.7±7.6	1.0
Peonidin-3-O-glucoside	31177.3±15.2	22282±14.5	0.7
Peonidin-3-(5'-rutinoside)-O-glu	272915.7±16.7	267162±24.9	0.8

Table S3. The relative quantification of intermediate in microbial metabolite (n=3. Data are presented as mean ± SD)

Compounds	R	FR
Cyanidin	1966.7 ± 10.3	1900.0± 9.3
Penidin	766.67 ± 17.0	1733.33 ± 16.8
Eriodictyol chalcone	336.7 ± 13.0	666.7 ± 12.6
5-[(3,4-dihydroxyphenyl) methyl] oxolan-2-one	1000.0 ± 21.3	733.3±29.7
5-(3',4',5'-Trihydroxyphenyl)-gamma-valerolactone	1233.3 ± 24.0	2033.3 ± 24.2
5-(3,4-dihydroxyphenyl) pentanoic acid	1866.7 ± 19.7	2733.33 ± 13.4
Dihydrocaffeic acid	4950.2 ± 27.3	5670.1 ±20.9
3,4-Dihydroxyphenylacetic acid	8466.7 ±26.1	15533.3 ± 39.8

Table S4. Computed global chemical reactivity descriptors (eV) of the studied C3G, PB2, CATE, GA, PA (water).

Properties (eV)	C3G	PB2	CATE	GA	PA
LUMO	-2.9326	-0.0680	0.0098	-1.1851	-1.1687
HOMO	-5.9095	-5.6472	-5.7305	-5.9724	-6.0072
$\Delta E_{\text{(LUMO-HOMO)}}$	2.9769	5.5792	5.7403	4.7873	4.8385
Ionization potential	5.9095	5.6472	-0.0098	5.9724	6.0072
Electron affinity	2.9326	0.0680	5.7403	1.1851	1.1687
Chemical potential	-4.4211	-2.8576	-2.8603	-3.5787	-3.5880
Electronegativity	4.4211	2.8576	2.8603	3.5787	3.5880
Electrophilicity	6.5657	1.4637	1.4253	2.6753	2.6607
Chemical hardness	1.4885	2.7896	2.8701	2.3937	2.4192
Chemical softness	0.3359	0.1792	0.1742	0.2089	0.2067

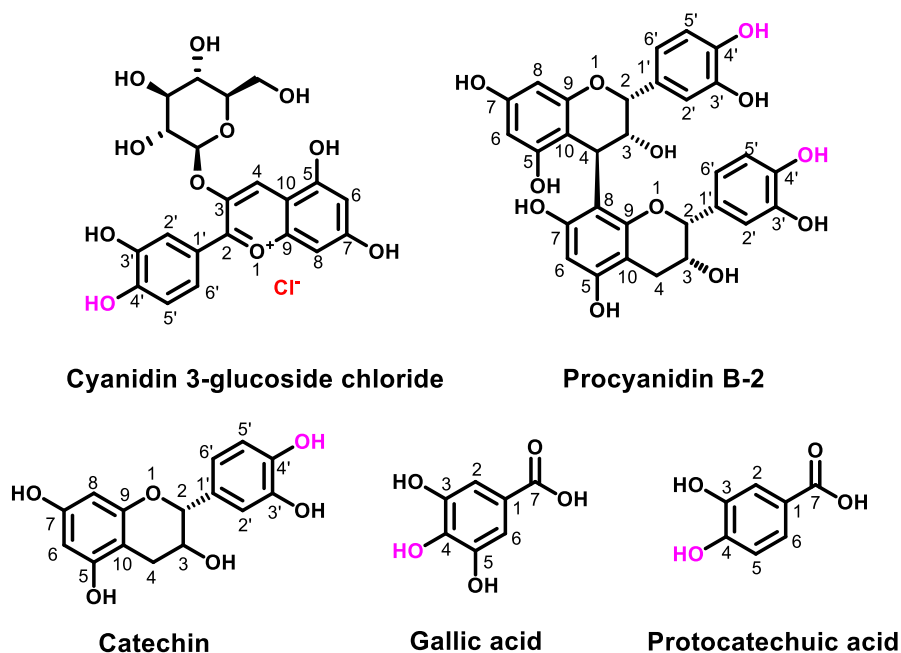


Figure. S1. Molecular structure of the main phenolic compounds

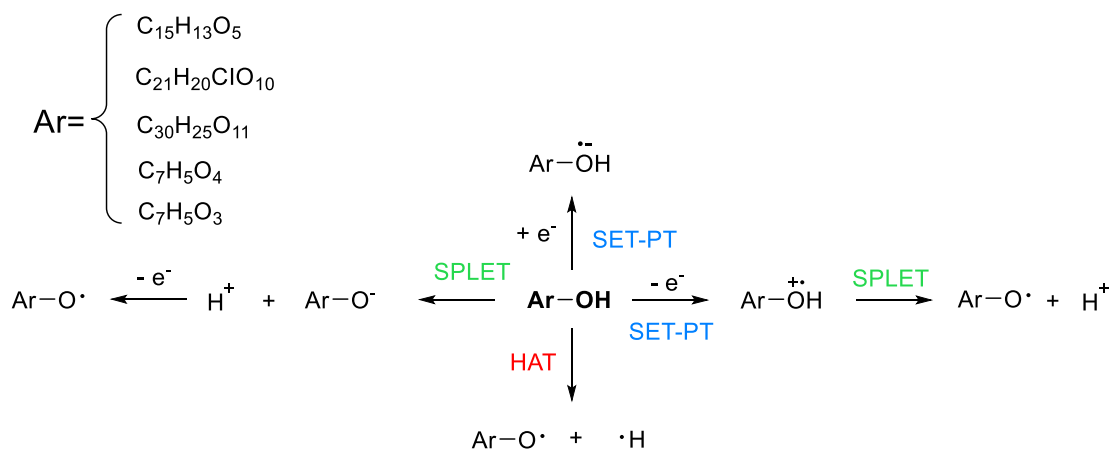
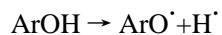


Fig. S2. Probable routes associated with different antioxidant mechanisms

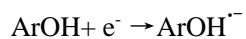
The relevant equation of the mechanisms as listed:

1. HAT:



$$\text{BDE} = H(\text{ArO}^\bullet) + H(\text{H}^\bullet) - H(\text{ArOH})$$

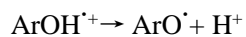
2. SET



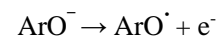
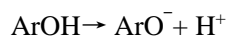
$$\text{IP} = H(\text{ArOH}^{\bullet+}) + H(\text{e}^-) - H(\text{ArOH})$$

$$\text{EA} = H(\text{ArOH}^{\bullet-}) - H(\text{e}^-) - H(\text{ArOH})$$

3. SET-PT



$$\text{PDE} = H(\text{ArOH}^\bullet) + H(\text{H}^+) - H(\text{ArOH}^{\bullet+})$$



$$\text{PA1} = H(\text{ArO}^-) + H(\text{H}^\bullet) - H(\text{ArOH})$$

$$\text{ETE} = H(\text{ArO}^\bullet) + H(\text{e}^-) - H(\text{ArO}^-)$$