SUPPLEMENTARY MATERIALS

Figure S1. Distribution diagrams with deprotonation routes of the (**a**) delphinidin; (**b**) delphinidin 3-*O*-glucoside; (**c**) peonidin; (**d**) peonidin 3-*O*-glucoside; (**e**) petunidin; (**f**) petunidin3-*O*-glucoside.

(**a**)
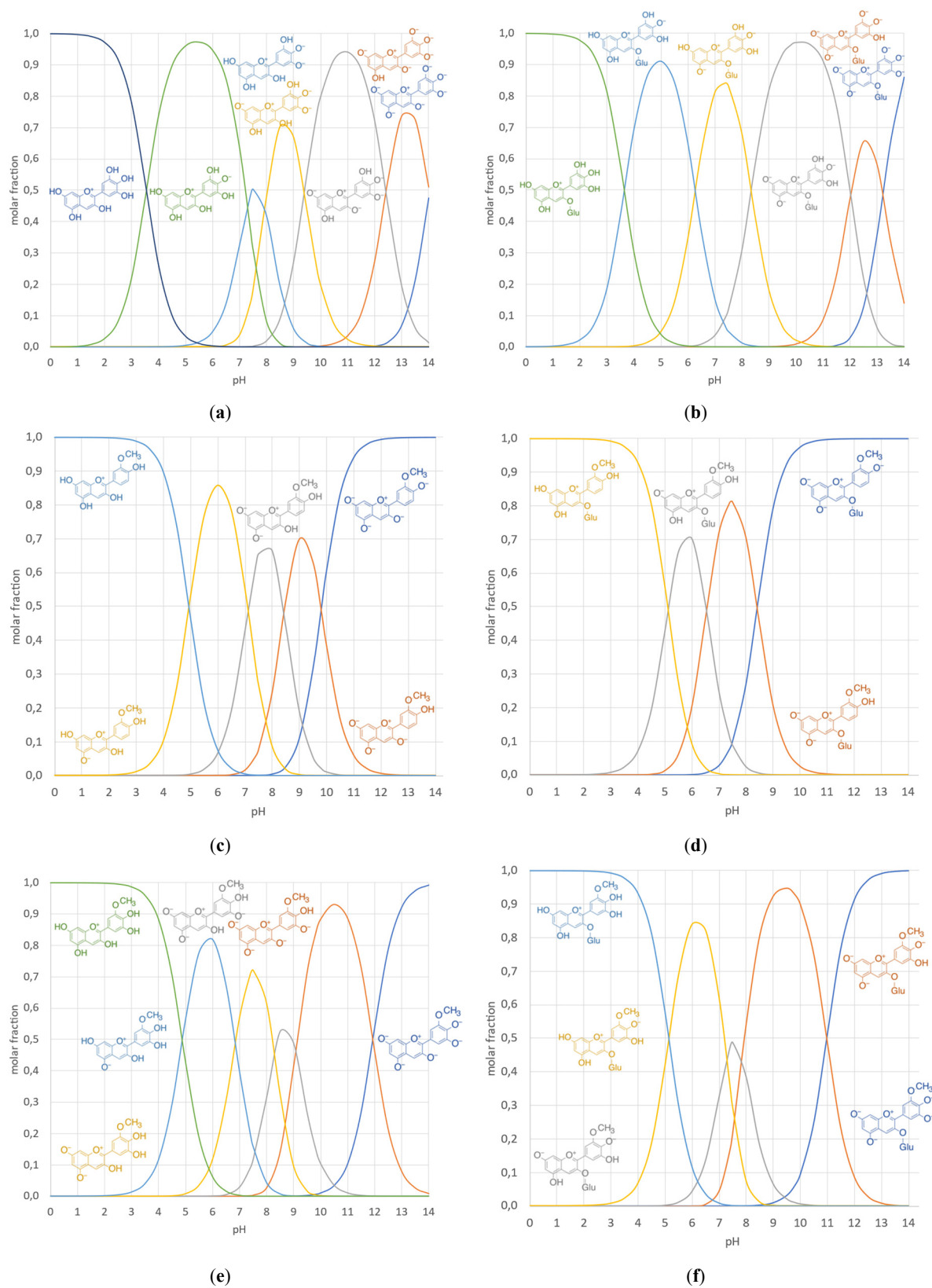
(**b**)

(**c**)

(**d**)

(**e**)

(**f**)

Table S1. Proton affinities (kcal mol^{-1}) of anthocyanidins and anthocyanins investigated along with the reaction site. The lowest values are underlined.

		1+	0	1−	2−	3−	4-
Dp	C3	25.8	**29.1**				
	C3'	26.4	37.2	39.8	45.4	**45.2**	
	C4'	**17.3**					
	C5	22.6	39.1	32.4	**35.7**		
	C5'	32.1	29.7	41.4	46.4	45.6	**50.3**
	C7	22.4	29.3	**31.2**			
Dp 3-glc	C3	-*Glu*	-*Glu*	-*Glu*	-*Glu*	-*Glu*	-*Glu*
	C3'	33.5	37.3	40.1	**44.0**		
	C4'	**17.6**					
	C5	21.4	**25.9**				
	C5'	29.2	38.0	41.4	44.6	**47.7**	
	C7	25.8	29.0	**32.4**			
Pn	C3	23.7	29.0	**32.7**			
	C4'	26.4	30.7	33.8	**37.0**		
	C5	**21.7**					
	C7	23.4	**28.5**				
Pn 3-glc	C3	-*Glu*	-*Glu*	-*Glu*	-*Glu*		
	C4'	22.8	30.1	**32.7**			
	C5	23.9	**26.7**				
	C7	**22.3**					
Pt	C3	23.2	28.7	33.3	**34.7**		
	C3'	28.8	30.3	**32.3**			
	C4'	24.2	28.3	32.6	41.3	**43.7**	
	C5	**21.5**					
	C7	22.7	**27.7**				
Pt-3-glc	C3	-*Glu*	-*Glu*	-*Glu*	-*Glu*	-*Glu*	
	C3'	29.8	35.6	37.9	**40.7**		
	C4'	**22.4**					
	C5	23.7	**29.1**	**30.9**			
	C7	23.5	**29.1**				

Table S2. Dipole momenta (μ, in D) and their corresponding vector in 3D-dimensions, obtained for the aglycones and their glycosides in pentyl ethanoate (cation form) and water (neutral form).
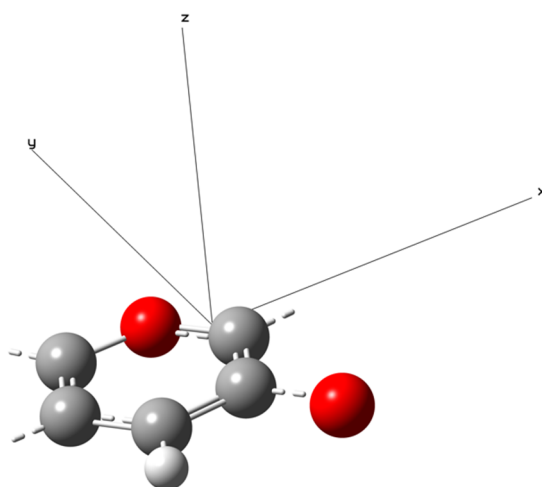
| | pentyl ethanoate | | water | |
| | + | | 0 | |
	μ [D]	vector (x,y,z)	μ [D]	(x,y,z)
Dp	10.2	(-10.1, 0.3, 1.1)	22.5 (6)	(-21.9, -5.3, 0)
Dp 3-glc	6.8	(-0.0, 5.4, -4.1)	14.1 (2)	(-11.7, 6.3, -4.9)
Pn	2.6	(1.7, 1.7, 1.1)	15.5 (4)	(-13.4, 7.7, 0.3)
Pn-3-glc	12.0	(-11.6, -2.6, 1.9)	11.2 (1)	(-9.8, -4.8, -2.6)
Pt	4.7	(-3.4, 3.2, -0.5)	15.3 (3)	(11.3, 10.3, 0.8)
Pt 3-glc	10.6	(7.6, 7.2, -2.0)	19.5 (5)	(-7.5, 17.9, -1.9)

Table S3. The reactivity of the studied anthocyanidins and their glycosides in SET and HAT mechanisms towards common radicals in water.

Delphinidin

Neutral

R-OH + OH* -> R-OH+* + OH-	[]	R-OH + OOH* -> R-OH+* + OOH-	[kcal/mol]
adiabatic	-9,2	adiabatic	14,2
vertical	-5,1	vertical	27,5
activation	1,6	activation	14,2
rate constants	8.37E+9	rate constants	2.36E+02
R-OH + OH* -> R-O* + H2O		R-OH + OOH* -> R-O* + H2O2	
C3	-45,4	**C3**	-7,7
C3'	-39,8	**C3'**	-2,2
C5	-41,1	**C5**	-3,4
C5'	-40,2	**C5'**	-2,5
C7	-41,5	**C7**	-3,9
R-OH + CH3O -> R-OH+* + CH3O-*	[kcal/mol]		
adiabatic	10,8		
vertical	17,7		
activation	11,4		
rate constants	2,96E+04		
R-OH + CH3O -> R-O* + CH3OH*			
C3	-27,2		
C3'	-21,6		
C5	-22,9		
C5'	-21,9		
C7	-23,3		
R-OH + SH -> R-OH+* + SH-*	[kcal/mol]		
adiabatic	6,4		
vertical	11,2		
activation	6,5		
rate constants	1,01E+08		
R-OH + SH -> R-O* + H2S*			
C3	-31,0		
C3'	-25,4		
C5	-26,7		
C5'	-25,7		
C7	-27,1		

Anion

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]	R-OH + OOH* -> R-OH+* + OOH-	[kcal/mol]
adiabatic	-23,1	*adiabatic*	0,2
vertical	-17,1	*vertical*	15,6
activation	12,2	*activation*	4,0
rate constants	7,27E+03	*rate constants*	3.99E+09
R-OH + OH* -> R-O* + H2O		R-OH + OOH* -> R-O* + H2O2	
C3'	-43,9	**C3'**	-6,3
C5	-51,4	**C5**	-13,7
C5'	-45,4	**C5'**	-7,8
C7	-51,9	**C7**	-14,2
R-OH + CH3O* -> R-OH+* + CH3O-	[kcal/mol]		
adiabatic	-3,1		
vertical	5,7		
activation	0,9		
rate constants	7.85E+9		
R-OH + CH3O* -> R-O* + CH3OH			
C3'	-25,7		
C5	-33,2		
C5'	-27,2		
C7	-33,7		
R-OH + SH* -> R-OH+* + SH-	[kcal/mol]		
adiabatic	-7,5		
vertical	-0,7		
activation	0,0		
rate constants	8.52E+9		
R-OH + SH* -> R-O* + H2S			
C3'	-29,5		
C5	-37,0		
C5'	-31,0		
C7	-37,5		

Dianion

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]	R-OH + OOH* -> R-OH+* + OOH-	[kcal/mol]
adiabatic	-31,6	*adiabatic*	-8,3
vertical	-25,0	*vertical*	7,7
activation	23,7	*activation*	0,9
rate constants	2,74E-05	*rate constants*	8.03E+9
R-OH + OH* -> R-O* + H2O		R-OH + OOH* -> R-O* + H2O2	
C3'	-49,2	**C3'**	-11,5
C5	-54,0	**C5**	-16,4
C5'	-48,7	**C5'**	-11,0

R-OH + CH3O* -> R-OH+* + CH3O-	[kcal/mol]
adiabatic	-11,7
vertical	-2,2
activation	0,1
rate constants	7.92E+9
R-OH + CH3O* -> R-O* + CH3OH	
C3'	-31,0
C5	-35,8
C5'	-30,5

R-OH + SH* -> R-OH+* + SH-	[kcal/mol]
adiabatic	-16,1
vertical	-8,6
activation	2,5
rate constants	7.84E+9
R-OH + SH* -> R-O* + H2S	
C3'	-34,8
C5	-39,6
C5'	-34,3

Trianion

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]
adiabatic	-38,3
vertical	-31,2
activation	34,8
rate constants	2,03E-13
R-OH + OH* -> R-O* + H2O	
C3'	-53,3
C5'	-52,6

R-OH + OOH* -> R-OH+* + OOH-	[kcal/mol]
adiabatic	-15,0
vertical	1,5
activation	0,0
rate constants	8.07E+9
R-OH + OOH* -> R-O* + H2O2	
C3'	-15,7
C5'	-15,0

R-OH + CH3O* -> R-OH+* + CH3O-	[kcal/mol]
adiabatic	-18,4
vertical	-8,4
activation	-0,7
rate constants	7.74E+9
R-OH + CH3O* -> R-O* + CH3OH	
C3'	-35,1
C5'	-34,4

R-OH + SH* -> R-OH+* + SH-	[kcal/mol]
adiabatic	-22,8
vertical	-14,8
activation	6,9
rate constants	5,96E+07
R-OH + SH* -> R-O* + H2S	
C3'	-38,9
C5'	-38,2

R-OH + OOH* -> R-OH+* + OOH-	[kcal/mol]
adiabatic	
vertical	

Delphinidin 3-*O*-glucoside

neutral

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]
adiabatic	-9,0
vertical	-4,9
activation	1,5
rate constants	8.93+09
R-OH + OH* -> R-O* + H2O	
C3'	-41,1
C5	-42,0
C5'	-41,9
C7	-40,7

R-OH + OOH* -> R-OH+* + OOH-	[kcal/mol]
adiabatic	14,3
vertical	27,8
activation	14,3
rate constants	2,00E+02
R-OH + OOH* -> R-O* + H2O2	
C3'	-3,4
C5	-4,3
C5'	-4,2
C7	-3,0

R-OH + CH3O* -> R-OH+* + CH3O-	[kcal/mol]
adiabatic	10,9
vertical	17,9
activation	11,4
rate constants	2,54E+04
R-OH + CH3O* -> R-O* + CH3OH	
C3'	-22,8
C5	-23,8
C5'	-23,7
C7	-22,4

R-OH + SH* -> R-OH+* + SH-	[kcal/mol]
adiabatic	6,6
vertical	11,5
activation	6,8
rate constants	6.97+7
R-OH + SH* -> R-O* + H2S	
C3'	-26,6
C5	-27,6
C5'	-27,5
C7	-26,2

R-OH + OOH* -> R-OH+* + OOH-	[kcal/mol]

Anion

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]
adiabatic	-16,5
vertical	-11,3
activation	6,1
rate constants	1,92E+08
R-OH + OH* -> R-O* + H2O	
C3'	-44,9
C5'	-44,5
C7	-41,0

R-OH + OOH* -> R-OH+* + OOH-	[kcal/mol]
adiabatic	6,8
vertical	21,4
activation	7,8
rate constants	1,11E+07
R-OH + OOH* -> R-O* + H2O2	
C3'	-7,3
C5'	-6,8
C7	-3,3

R-OH + CH3O* -> R-OH+* + CH3O-	[kcal/mol]
adiabatic	3,5
vertical	11,5
activation	4,1
rate constants	3.42E+09
R-OH + CH3O* -> R-O* + CH3OH	
C3'	-26,7
C5'	-26,3
C7	-22,8

R-OH + SH* -> R-OH+* + SH-	[kcal/mol]
adiabatic	-0,9
vertical	5,1
activation	1,08
rate constants	9,01E+9
R-OH + SH* -> R-O* + H2S	
C3'	-30,5
C5'	-30,1
C7	-26,6

Dianion

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]	R-OH + OOH* -> R-OH+* + OOH-	[kcal/mol]
adiabatic	-22,1	adiabatic	1,3
vertical	-16,4	vertical	16,2
activation	11,8	activation	4,4
rate constants	1,40E+04	rate constants	2.75E+09
R-OH + OH* -> R-O* + H2O		R-OH + OOH* -> R-O* + H2O2	
C3'	-47,2	**C3'**	-9,5
C5'	-47,0	**C5'**	-9,3
R-OH + CH3O* -> R-OH+* + CH3O-	[kcal/mol]		
adiabatic	-2,1		
vertical	6,4		
activation	1,20		
rate constants	8,22E+9		
R-OH + CH3O* -> R-O* + CH3OH			
C3'	-28,9		
C5'	-28,7		
R-OH + SH* -> R-OH+* + SH-	[kcal/mol]		
adiabatic	-6,5		
vertical	-0,1		
activation	0,0		
rate constants	9.12E+9		
R-OH + SH* -> R-O* + H2S			
C3'	-32,8		
C5'	-32,5		

Peonidin

Cation

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]
adiabatic	13,0
vertical	17,5
activation	17,0
rate constants	2,09E+00
R-OH + OH* -> R-O* + H2O	
C3	-37,2
C4'	-35,0
C5	-33,3
C7	-28,5

R-OH + OOH* -> R-OH+* + OOH-	[kcal/mol]
adiabatic	36,4
vertical	50,2
activation	45,7
rate constants	2,12E-21
R-OH + OOH* -> R-O* + H2O2	
C3	0,5
C4'	2,7
C5	4,4
C7	9,1

R-OH + CH3O* -> R-OH+* + CH3O-	[kcal/mol]
adiabatic	33,0
vertical	40,3
activation	55,6
rate constants	1,05E-28
R-OH + CH3O* -> R-O* + CH3OH	
C3	-19,0
C4'	-16,8
C5	-15,0
C7	-10,3

R-OH + SH* -> R-OH+* + SH-	[kcal/mol]
adiabatic	28,6
vertical	33,9
activation	54,21
rate constants	1,13E-27
R-OH + SH* -> R-O* + H2S	
C3	-22,8
C4'	-20,6
C5	-18,8
C7	-14,1

Neutral

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]	R-OH + OOH* -> R-OH+* + OOH-	[kcal/mol]
adiabatic	-3,6	*adiabatic*	19,8
vertical	-0,7	*vertical*	32,0
activation	0,0	*activation*	21,0
rate constants	8.48E+09	*rate constants*	2,57E-03
R-OH + OH* -> R-O* + H2O		R-OH + OOH* -> R-O* + H2O2	
C3	-44,2	**C3**	-6,6
C4'	-37,2	**C4'**	0,4
C7	-32,5	**C7**	5,1

R-OH + CH3O* -> R-OH+* + CH3O-	[kcal/mol]		
adiabatic	16,4		
vertical	22,1		
activation	21,4		
rate constants	1,23E-03		
R-OH + CH3O* -> R-O* + CH3OH			
C3	-26,0		
C4'	-19,0		
C7	-14,3		

R-OH + SH* -> R-OH+* + SH-	[kcal/mol]		
adiabatic	12,0		
vertical	15,7		
activation	16,65		
rate constants	3,84E+00		
R-OH + SH* -> R-O* + H2S			
C3	-29,8		
C4'	-22,8		
C7	-18,1		

Anion

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]
adiabatic	-9,6
vertical	-7,0
activation	4,7100
rate constants	1,74E+09
R-OH + OH* -> R-O* + H2O	
C3	-48,7
C4'	-39,8

R-OH + OOH* -> R-OH+* + OOH-	[kcal/mol]
adiabatic	13,7
vertical	25,6
activation	13,7700
rate constants	5,01E+02
R-OH + OOH* -> R-O* + H2O2	
C3	-11,1
C4'	-2,1

R-OH + CH3O* -> R-OH+* + CH3O-	[kcal/mol]
adiabatic	10,3
vertical	15,8
activation	11,3500
rate constants	2,98E+04
R-OH + CH3O* -> R-O* + CH3OH	
C3	-30,5
C4'	-21,5

R-OH + SH* -> R-OH+* + SH-	[kcal/mol]
adiabatic	5,9
vertical	9,3
activation	6,4
rate constants	1,35E+08
R-OH + SH* -> R-O* + H2S	
C3	-34,3
C4'	-25,3

Dianion

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]		*R-OH + OOH* -> R-OH+* + OOH-*	[kcal/mol]
adiabatic	-30,0		*adiabatic*	-6,7
vertical	-26,2		*vertical*	6,5
activation	45,16		*activation*	0,80
rate constants	4,86E-21		*rate constants*	8.04E+09
R-OH + OH* -> R-O* + H2O			*R-OH + OOH* -> R-O* + H2O2*	
C4'	-54,3		**C4'**	-16,6
R-OH + CH3O* -> R-OH+* + CH3O-	[kcal/mol]			
adiabatic	-10,0			
vertical	-3,4			
activation	0,44			
rate constants	7.91E+09			
R-OH + CH3O* -> R-O* + CH3OH				
C4'	-36,1			
R-OH + SH* -> R-OH+* + SH-	[kcal/mol]			
adiabatic	-14,4			
vertical	-9,8			
activation	5,22			
rate constants	8.35E+08			
R-OH + SH* -> R-O* + H2S				
C4'	-39,9			

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]		*R-OH + OOH* -> R-OH+* + OOH-*	[kcal/mol]
adiabatic			*adiabatic*	-6,7

Peonidin 3-*O*-glucoside

Neutral

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]	*R-OH + OOH* -> R-OH+* + OOH-*	[kcal/mol]
adiabatic	-1,9	*adiabatic*	21,4
vertical	2,9	*vertical*	35,6
activation	0,4	*activation*	22,3
rate constants	9.09E+09	*rate constants*	2,73E-04
R-OH + OH* -> R-O* + H2O		*R-OH + OOH* -> R-O* + H2O2*	
C4'	-37,6	**C4'**	0,1
C5	-31,5	**C5**	6,2
R-OH + CH3O* -> R-OH+* + CH3O-	[kcal/mol]		
adiabatic	18,1		
vertical	25,7		
activation	21,7		
rate constants	7,34E-04		
R-OH + CH3O* -> R-O* + CH3OH			
C4'	-19,3		
C5	-13,3		
R-OH + SH* -> R-OH+* + SH-	[kcal/mol]		
adiabatic	13,7		
vertical	19,3		
activation	16,63		
rate constants	4,01E+00		
R-OH + SH* -> R-O* + H2S			
C4'	-23,2		
C5	-17,1		

Anion

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]	R-OH + OOH* -> R-OH+* + OOH-	[kcal/mol]
adiabatic	-9,8	*adiabatic*	13,5
vertical	-6,1	*vertical*	26,6
activation	2,5100	*activation*	13,5000
rate constants	8,25E+9	*rate constants*	7,84E+02
R-OH + OH -> R-O* + H2O*		*R-OH + OOH* -> R-O* + H2O2*	
C4'	-39,6	**C4'**	-1,9
R-OH + CH3O* -> R-OH+* + CH3O-	[kcal/mol]		
adiabatic	10,2		
vertical	16,7		
activation	10,7300		
rate constants	8,51E+04		
R-OH + CH3O* -> R-O* + CH3OH			
C4'	-21,4		
R-OH + SH* -> R-OH+* + SH-	[kcal/mol]		
adiabatic	5,8		
vertical	10,3		
activation	5,89		
rate constants	2,87E+08		
R-OH + SH* -> R-O* + H2S			
C4'	-25,2		

Dianion

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]	R-OH + OOH* -> R-OH+* + OOH-	[kcal/mol]
adiabatic	-20,9	*adiabatic*	2,4
vertical	-16,0	*vertical*	16,7
activation	13,0600	*activation*	4,8800
rate constants	1,65E+03	*rate constants*	1,39E+09
R-OH + CH3O* -> R-OH+* + CH3O-	[kcal/mol]		
adiabatic	-0,9		
vertical	6,8		
activation	1,5000		
rate constants	8.21E+9		
R-OH + SH* -> R-OH+* + SH-	[kcal/mol]		
adiabatic	-5,3		
vertical	0,4		
activation	0,0100		
rate constants	9.08E+09		

Petunidin
Neutral

R-OH + OH -> R-OH+* + OH-*	[kcal/mol]	*R-OH + OOH* -> R-OH+* + OOH-*	[kcal/mol]
adiabatic	-2,7	*adiabatic*	20,6
vertical	-0,1	*vertical*	32,5
activation	0,0000	*activation*	22,1900
rate constants	8.45E+09	*rate constants*	3,36E-04
R-OH + OH -> R-O* + H2O*		*R-OH + OOH* -> R-O* + H2O2*	
C3	-44,0	**C3**	-6,3
C3'	-36,4	**C3'**	1,2
C4'	-38,7	**C4'**	-1,0
C7	-32,6	**C7**	5,1
R-OH + CH3O -> R-OH+* + CH3O-*	[kcal/mol]		
adiabatic	17,3		
vertical	22,6		
activation	24,0900		
rate constants	1,35E-05		
R-OH + CH3O -> R-O* + CH3OH*			
C3	-25,7		
C3'	-18,2		
C4'	-20,4		
C7	-14,4		
R-OH + SH -> R-OH+* + SH-*	[kcal/mol]		
adiabatic	12,9		
vertical	16,2		
activation	19,88		
rate constants	1,65E-02		
R-OH + SH -> R-O* + H2S*			
C3	-29,6		
C3'	-22,0		
C4'	-24,2		
C7	-18,2		

Anion

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]	R-OH + OOH* -> R-OH+* + OOH-	[kcal/mol]
adiabatic	-8,9	*adiabatic*	14,4
vertical	-7,1	*vertical*	25,6
activation	7,0000	*activation*	14,6300
rate constants	4,58E+07	*rate constants*	1,17E+02
R-OH + OH -> R-O* + H2O*		*R-OH + OOH* -> R-O* + H2O2*	
C3	-47,9	**C3**	-10,3
C3'	-37,5	**C3'**	0,2
C4'	-40,6	**C4'**	-2,9
R-OH + CH3O* -> R-OH+* + CH3O-	[kcal/mol]		
adiabatic	11,1		
vertical	15,7		
activation	13,4000		
rate constants	9,39E+02		
R-OH + CH3O -> R-O* + CH3OH*			
C3	-29,7		
C3'	-19,2		
C4'	-22,4		
R-OH + SH* -> R-OH+* + SH-	[kcal/mol]		
adiabatic	6,7		
vertical	9,3		
activation	8,32		
rate constants	4,97E+06		
R-OH + SH -> R-O* + H2S*			
C3	-33,5		
C3'	-23,0		
C4'	-26,2		

Dianion

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]	R-OH + OOH* -> R-OH+* + OOH-	[kcal/mol]
adiabatic	-18,3	*adiabatic*	5,0
vertical	-13,4	*vertical*	19,2
activation	9,1600	*activation*	6,4900
rate constants	1,19E+06	*rate constants*	1,09E+08
R-OH + OH -> R-O* + H2O*		*R-OH + OOH* -> R-O* + H2O2*	
C3	-49,3	**C3**	-11,6
C4'	-49,2	**C4'**	-11,6
R-OH + CH3O* -> R-OH+* + CH3O-	[kcal/mol]		
adiabatic	1,7		
vertical	9,4		
activation	2,8700		
rate constants	4,90E+10		
R-OH + CH3O -> R-O* + CH3OH*			
C3	-31,1		
C4'	-31,0		
R-OH + SH* -> R-OH+* + SH-	[kcal/mol]		
adiabatic	-2,7		
vertical	2,9		
activation	0,38		
rate constants	8.44E+09		
R-OH + SH -> R-O* + H2S*			
C3	-34,9		
C4'	-34,8		

Trianion

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]	*R-OH + OOH* -> R-OH+* + OOH-*	[kcal/mol]
adiabatic	-32,6	*adiabatic*	-9,3
vertical	-27,8	*vertical*	4,9
activation	40,2500	*activation*	0,4200
rate constants	1,93E-17	*rate constants*	8.04E+09
R-OH + OH* -> R-O* + H2O		*R-OH + OOH* -> R-O* + H2O2*	
C4'	-54,1	**C4'**	-16,4
R-OH + CH3O* -> R-OH+* + CH3O-	[kcal/mol]		
adiabatic	-12,6		
vertical	-5,0		
activation	0,8200		
rate constants	7.81E+09		
R-OH + CH3O* -> R-O* + CH3OH			
C4'	-35,8		
R-OH + SH* -> R-OH+* + SH-	[kcal/mol]		
adiabatic	-17,0		
vertical	-11,4		
activation	5,8		
rate constants	3,47E+08		
R-OH + SH* -> R-O* + H2S			
C4'	-39,7		

Petunidin 3-*O*-glucoside

Cation

R-OH + OH -> R-OH+* + OH-*	[kcal/mol]	*R-OH + OOH* -> R-OH+* + OOH-*	[kcal/mol]
adiabatic	10,8	*adiabatic*	34,1
vertical	15,7	*vertical*	48,3
activation	12,5800	*activation*	41,1900
rate constants	3,75E+03	*rate constants*	3,95E-18
R-OH + OH -> R-O* + H2O*		*R-OH + OOH* -> R-O* + H2O2*	
C3'	-34,9	**C3'**	2,8
C4'	-39,4	**C4'**	-1,7
C5	-31,6	**C5**	6,0
C7	-29,7	**C7**	7,9
R-OH + CH3O -> R-OH+* + CH3O-*	[kcal/mol]		
adiabatic	30,8		
vertical	38,5		
activation	48,1300		
rate constants	3,26E-23		
R-OH + CH3O -> R-O* + CH3OH*			
C3'	-16,6		
C4'	-21,1		
C5	-13,4		
C7	-11,5		
R-OH + SH -> R-OH+* + SH-*	[kcal/mol]		
adiabatic	26,4		
vertical	32,0		
activation	45,7100		
rate constants	1,91E-21		
R-OH + SH -> R-O* + H2S*			
C3'	-20,4		
C4'	-25,0		
C5	-17,2		
C7	-15,3		

Neutral

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]
adiabatic	-10,7
vertical	-5,8
activation	1,7200
rate constants	8.85E+09
R-OH + OH* -> R-O* + H2O	
C3'	-43,4
C5	-40,6
C7	-42,4

R-OH + OOH* -> R-OH+* + OOH-	[kcal/mol]
adiabatic	12,6
vertical	26,8
activation	12,6500
rate constants	3,34E+03
R-OH + OOH* -> R-O* + H2O2	
C3'	-5,7
C5	-2,9
C7	-4,7

R-OH + CH3O* -> R-OH+* + CH3O-	[kcal/mol]
adiabatic	9,2
vertical	16,9
activation	9,2700
rate constants	9,89E+05
R-OH + CH3O* -> R-O* + CH3OH	
C3'	-25,1
C5	-22,3
C7	-24,2

R-OH + SH* -> R-OH+* + SH-	[kcal/mol]
adiabatic	4,8
vertical	10,5
activation	4,84
rate constants	1,48E+09
R-OH + SH* -> R-O* + H2S	
C3'	-28,9
C5	-26,1
C7	-28,0

MonoAnion

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]	*R-OH + OOH* -> R-OH+* + OOH-*	[kcal/mol]
adiabatic	-20,2	*adiabatic*	3,1
vertical	-14,8	*vertical*	17,9
activation	10,1400	*activation*	5,4100
rate constants	2,29E+05	*rate constants*	6,23E+08
R-OH + OH* -> R-O* + H2O		*R-OH + OOH* -> R-O* + H2O2*	
C3'	-48,3	**C3'**	-10,6
C5	-44,2	**C5**	-6,6
R-OH + CH3O* -> R-OH+* + CH3O-	[kcal/mol]		
adiabatic	-0,2		
vertical	8,0		
activation	1,9500		
rate constants	7.97E+9		
R-OH + CH3O* -> R-O* + CH3OH			
C3'	-30,1		
C5	-26,0		
R-OH + SH* -> R-OH+* + SH-	[kcal/mol]		
adiabatic	-4,6		
vertical	1,6		
activation	0,1		
rate constants	9.07E+09		
R-OH + SH* -> R-O* + H2S			
C3'	-33,9		
C5	-29,8		

Dianion

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]
adiabatic	-23,8
vertical	-17,2
activation	11,2100
rate constants	3,79E+04
R-OH + OH* -> R-O* + H2O	
C3'	-50,9

R-OH + OOH* -> R-OH+* + OOH-	[kcal/mol]
adiabatic	-0,5
vertical	15,5
activation	3,7500
rate constants	4.81E+09
R-OH + OOH* -> R-O* + H2O2	
C3'	-13,2

R-OH + CH3O* -> R-OH+* + CH3O-	[kcal/mol]
adiabatic	-3,8
vertical	5,6
activation	0,8300
rate constants	8.21E+09
R-OH + CH3O* -> R-O* + CH3OH	
C3'	-32,7

R-OH + SH* -> R-OH+* + SH-	[kcal/mol]
adiabatic	-8,2
vertical	-0,8
activation	0,02
rate constants	9.07E+09
R-OH + SH* -> R-O* + H2S	
C3'	-36,5

Dianion

R-OH + OH* -> R-OH+* + OH-	[kcal/mol]
adiabatic	-23,8
vertical	-17,2
activation	11,2100
rate constants	3,79E+04

R-OH + OOH* -> R-OH+* + OOH-	[kcal/mol]
adiabatic	-0,5
vertical	15,5