Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Chalcogen Effects on the Primary Antioxidant Activity of Chrysin and Quercetin

Romina Castañeda-Arriaga,[1] Tiziana Marino,[2*] Nino Russo,[2] J. Raúl Alvarez-Idaboy,[3] Annia Galano.[1*]

[1]Departamento de Química. Universidad Autónoma Metropolitana-Iztapalapa. San Rafael Atlixco 186, Col. Vicentina. Iztapalapa. C. P. 09340. México D. F. México.

[2] Dipartimento di Chimica e Tecnologie Chimiche, Universitàdella Calabria, I-87036 Arcavacata di Rende, Italy

[3]Facultad de Química, Departamento de Física y Química Teórica, Universidad Nacional Autónoma de México, México DF 04510, México.

Contents:

Table S1. Gibbs free energies of reaction (kcal/mol) of OY + HOO$^\bullet$, at 298.15 K.

	H_2A (water)	HA^-	A^{2-}	H_2A (lipid)
SET	35.52	15.92	2.85	95.80
f-HAT-5a	8.13	6.44	---	15.18
f-HAT-7a	7.57	---	---	8.85
RAF-2	10.73	7.89	6.71	11.20
RAF-3	8.51	6.30	2.73	9.30
RAF-4	34.51	37.20	27.01	36.06
RAF-5	15.17	15.45	13.63	18.96
RAF-6	16.26	9.62	6.53	16.41
RAF-7	18.00	22.04	22.37	20.10
RAF-8	15.51	11.48	8.10	16.24
RAF-9	17.11	15.47	9.34	18.40
RAF-10	28.05	21.48	10.66	28.74
RAF-1´	19.81	19.68	19.18	21.12
RAF-2´	13.24	13.36	13.47	15.31
RAF-3´	16.53	16.31	16.12	18.34
RAF-4´	11.83	11.93	11.49	13.52

Table S2. Gibbs free energies of reaction (kcal/mol) of SY + HOO•, at 298.15 K.

	H_2A (water)	HA^-	A^{2-}	H_2A (lipid)
SET	35.59	17.10	-3.24	81.18
f-HAT-5a	2.87	3.55	---	6.57
f-HAT-7a	7.65	---	---	8.42
RAF-2	4.94	5.26	1.02	7.96
RAF-3	9.13	6.52	2.53	11.58
RAF-4	11.30	15.37	0.40	13.40
RAF-5	12.86	13.02	12.59	18.77
RAF-6	15.51	6.84	1.11	17.32
RAF-7	17.36	22.75	22.99	20.66
RAF-8	15.55	11.21	3.91	17.51
RAF-9	14.61	13.35	18.41	17.67
RAF-10	27.88	17.55	1.21	29.88
RAF-1′	20.29	19.98	19.49	22.89
RAF-2′	13.33	13.37	19.88	15.99
RAF-3′	16.73	16.39	16.10	19.58
RAF-4′	11.45	10.96	18.69	14.59

Table S3. Gibbs free energies of reaction (kcal/mol) of SeY + HOO$^\bullet$, at 298.15 K.

	H_2A (water)	HA^-	A^{2-}	H_2A (lipid)
SET	15.56	17.20	-4.18	64.19
f-HAT-5a	-4.73	-3.12	---	-0.19
f-HAT-7a	7.02	---	---	8.81
RAF-2	0.63	3.65	-2.06	3.01
RAF-3	10.14	7.86	3.93	11.35
RAF-4	-0.85	3.90	-1.40	1.32
RAF-5	12.60	12.38	12.70	17.25
RAF-6	15.60	5.01	-1.73	16.71
RAF-7	17.24	22.82	20.86	18.69
RAF-8	15.63	10.42	0.32	17.05
RAF-9	14.06	12.44	14.44	16.44
RAF-10	26.75	15.18	1.45	27.73
RAF-1´	20.74	20.03	19.59	22.54
RAF-2´	12.53	13.00	18.08	15.19
RAF-3´	16.68	15.83	15.52	18.97
RAF-4´	11.28	3.90	16.77	13.73

Table S4. Gibbs free energies of reaction (kcal/mol) of OQ + HOO•, RAF mechanism at 298.15 K.

	H_2A (water)	HA^-	A^{2-}	H_2A (lipid)
SET	26.82	3.19	0.72	73.52
f-HAT-3a	-4.71	-12.32	-13.73	-1.02
f-HAT-3a′	-1.37	-10.57	-11.51	2.43
f-HAT-4a′	-5.12	---	---	-5.03
f-HAT-5a	5.81	-2.85	0.61	12.05
f-HAT-7a	6.49	-6.69	---	8.27
RAF-2	-3.23	-2.02	-3.22	-1.49
RAF-3	4.37	3.74	1.14	5.71
RAF-4	18.05	3.08	7.93	37.06
RAF-5	13.57	13.48	14.81	16.90
RAF-6	16.64	16.43	10.01	16.97
RAF-7	17.57	13.78	20.44	20.55
RAF-8	14.37	14.07	11.24	16.53
RAF-9	18.96	18.24	16.95	20.59
RAF-10	29.27	27.65	19.56	30.28
RAF-1′	18.55	15.39	14.90	22.55
RAF-2′	11.89	11.70	12.84	13.27
RAF-3′	13.03	6.42	6.08	14.58
RAF-4′	8.13	9.26	8.38	8.43
RAF-5′	16.66	11.28	10.47	17.15
RAF-6′	10.39	9.64	9.36	12.58

Table S5. Gibbs free energies of reaction (kcal/mol) of SQ + HOO•, RAF mechanism at 298.15 K.

	H_2A (water)	HA^-	A^{2-}	H_2A (lipid)
SET	26.10	4.67	1.38	72.34
f-HAT-3a	-4.64	-10.73	-11.76	-1.48
f-HAT-3a´	-1.11	-9.44	-10.99	2.23
f-HAT-4a´	-5.02	---	---	-5.14
f-HAT-5a	6.50	6.47	1.48	10.40
f-HAT-7a	6.27	-6.13	---	25.04
RAF-2	-7.47	-4.79	-6.64	-5.95
RAF-3	6.93	3.94	3.34	7.56
RAF-4	15.51	2.68	6.22	18.37
RAF-5	12.46	11.91	13.23	15.23
RAF-6	14.44	14.18	6.81	15.42
RAF-7	17.18	11.51	18.52	19.00
RAF-8	14.87	14.30	10.88	15.93
RAF-9	15.64	12.10	15.81	18.04
RAF-10	28.21	26.51	18.43	28.53
RAF-1´	19.45	16.76	15.31	21.84
RAF-2´	11.46	9.31	10.85	11.76
RAF-3´	13.36	7.00	6.52	14.29
RAF-4´	7.04	9.07	8.43	7.03
RAF-5´	16.42	11.89	11.08	17.22
RAF-6´	9.49	9.63	9.38	11.08

Table S6. Gibbs free energies of reaction (kcal/mol) of SeQ + HOO•, RAF mechanism at 298.15 K.

	H_2A (water)	HA^-	A^{2-}	H_2A (lipid)
SET	20.39	5.75	1.95	69.10
f-HAT-3a	-2.93	-9.63	-11.58	-1.65
f-HAT-3a′	-0.99	-9.28	-10.62	3.90
f-HAT-4a′	-4.64	---	---	-2.92
f-HAT-5a	-1.24	-0.54	0.76	5.38
f-HAT-7a	5.55	-6.21	---	9.18
RAF-2	-8.95	-5.52	-6.92	-5.77
RAF-3	7.85	5.01	5.14	10.53
RAF-4	11.67	-1.35	3.07	17.15
RAF-5	11.68	10.97	12.53	16.26
RAF-6	14.95	15.45	5.99	17.09
RAF-7	16.63	11.01	18.22	20.27
RAF-8	14.68	13.00	11.72	17.28
RAF-9	15.66	10.58	33.50	19.52
RAF-10	27.77	25.89	16.62	30.75
RAF-1′	19.98	17.98	16.29	24.36
RAF-2′	11.64	8.61	11.10	14.24
RAF-3′	13.37	8.44	7.64	15.72
RAF-4′	7.20	10.29	9.03	8.65
RAF-5′	17.77	12.37	12.50	19.29
RAF-6′	9.40	10.31	9.71	12.85

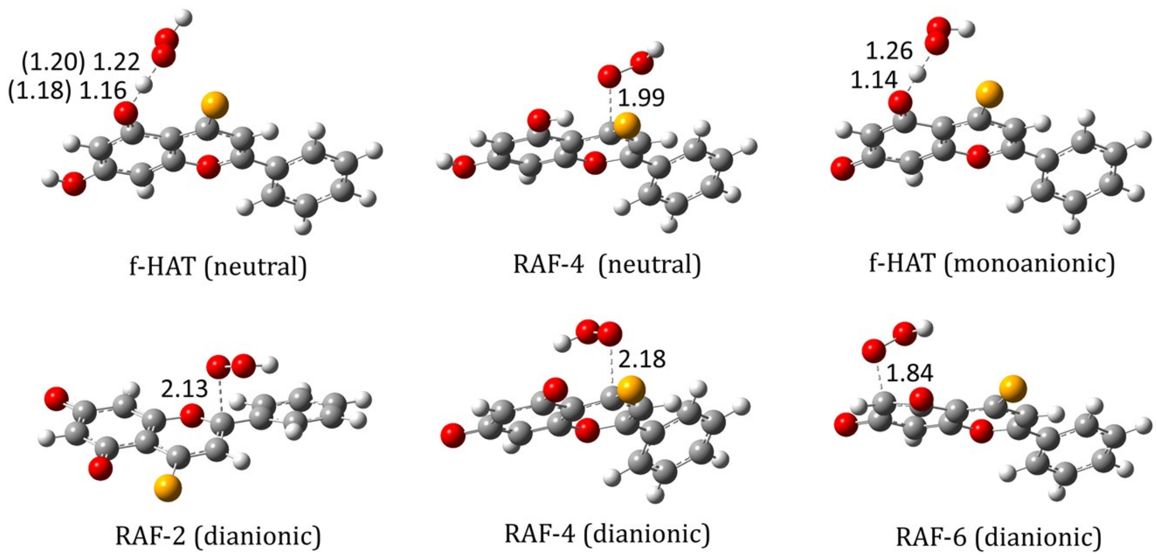

Figure S1. Optimized geometries of the transition structures for reactions between SeY + HOO$^{\bullet}$ in water (lipid). Distances are reported in Å.

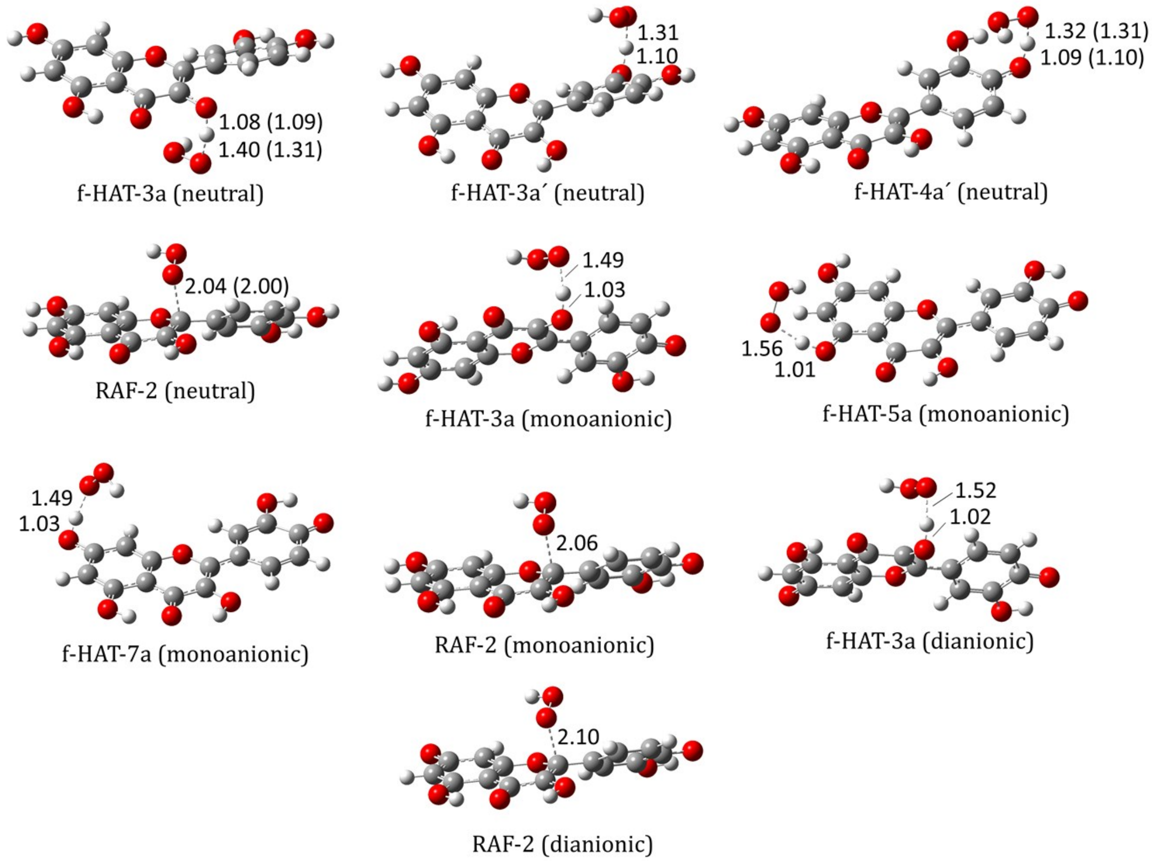

Figure S2. Optimized geometries of the transition structures for reactions between OQ + HOO$^{\bullet}$ in water (lipid). Distances are reported in Å.

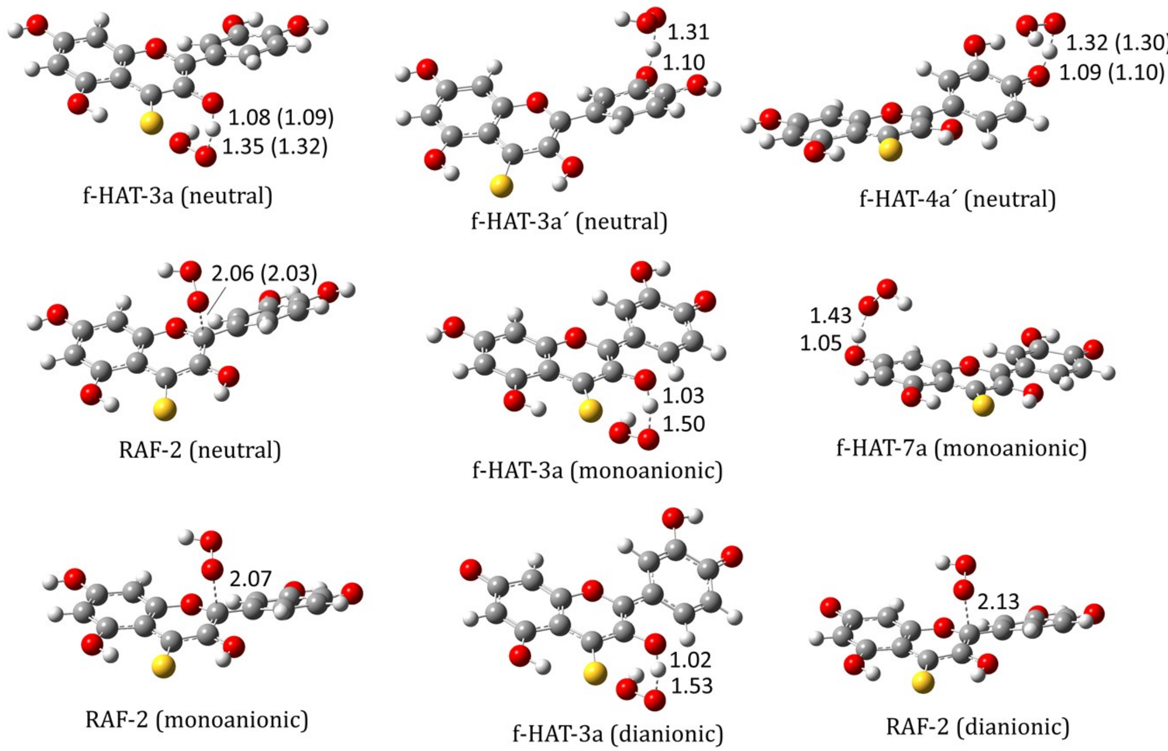

Figure S3. Optimized geometries of the transition structures for reactions between SQ + •OOH in water (lipid). Distances are reported in Å.

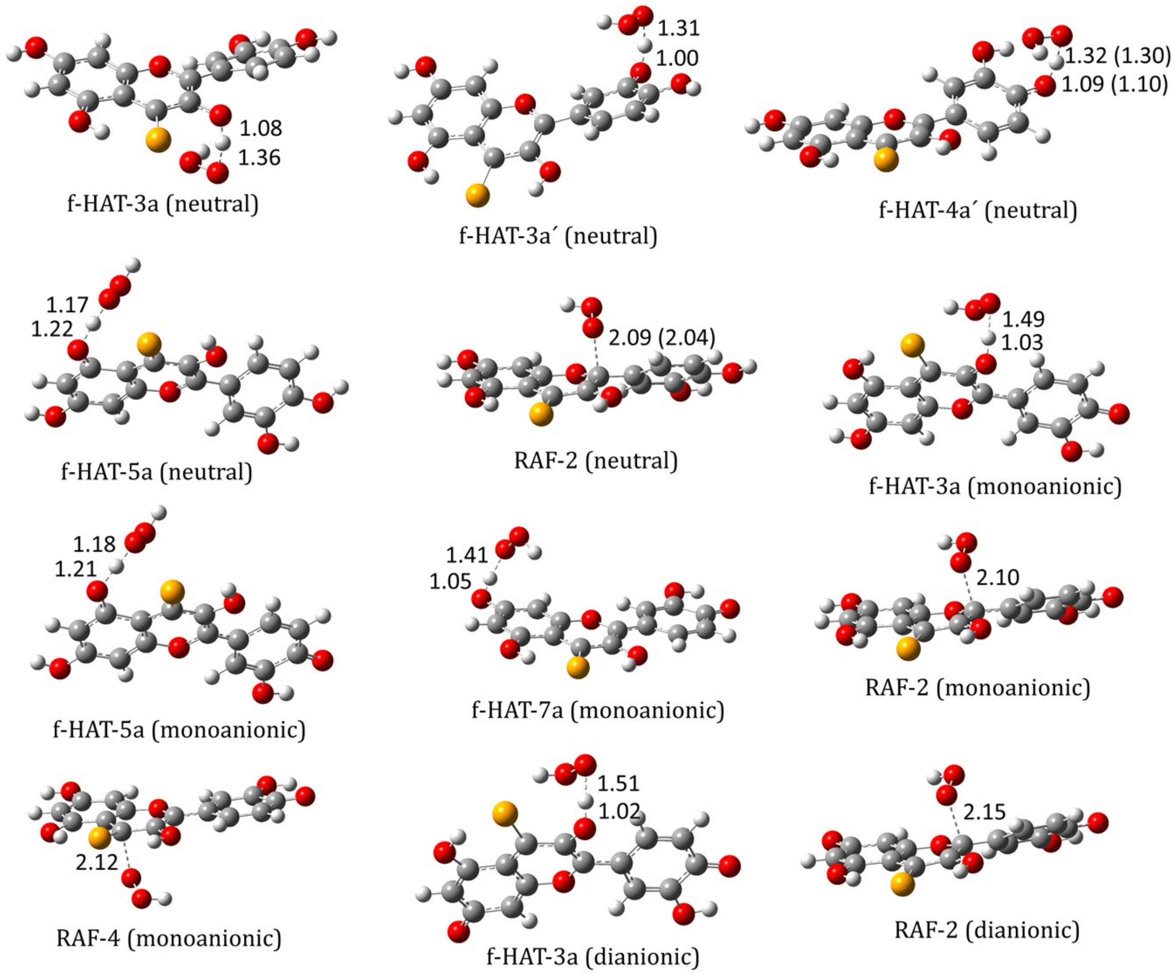

Figure S4. Optimized geometries of the transition structures for reactions between SeQ + $HOO^{\bullet}$ in water (lipid). Distances are reported in Å.

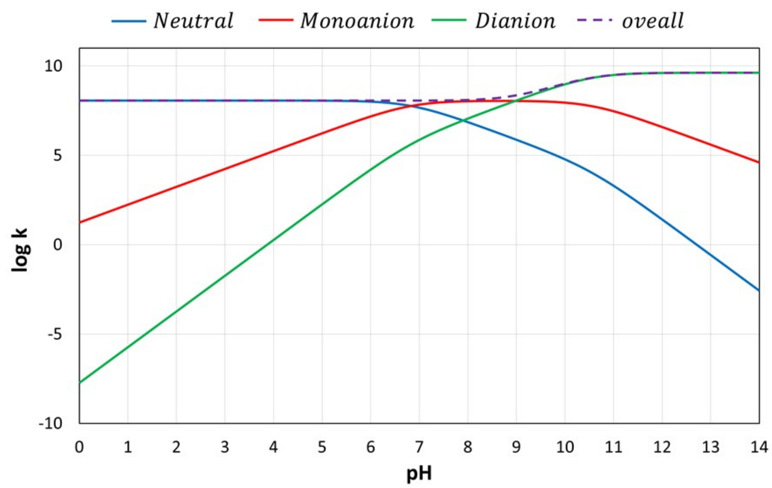

Figure S5. Variation of the overall rate constant with the *p*H, for the SeY + HOO$^{\bullet}$ reactions in aqueous solutions.

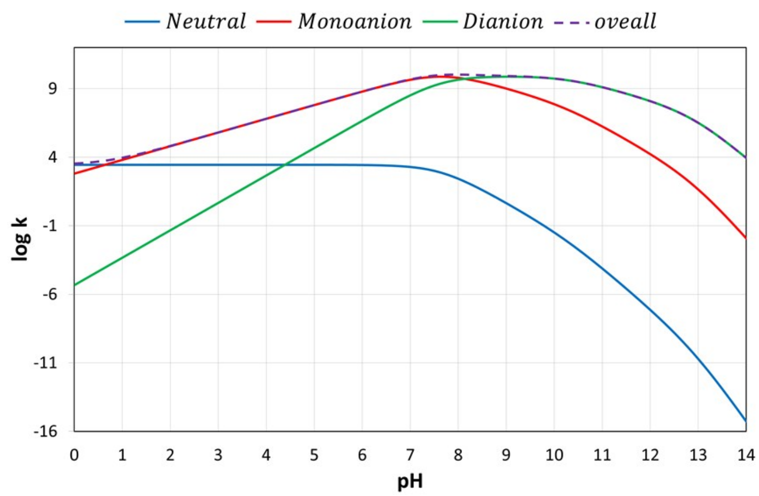

Figure S6. Variation of the overall rate constant with the *p*H, for the OQ + $HOO^{\bullet}$ reactions in aqueous solutions.

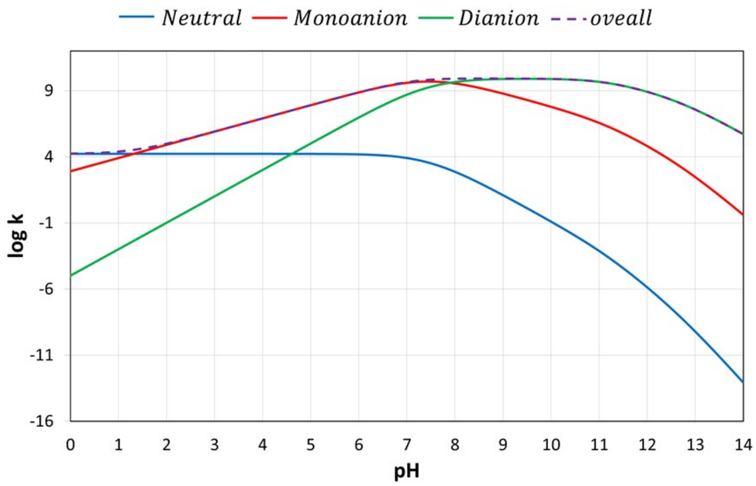

Figure S7. Variation of the overall rate constant with the *p*H, for the SQ + HOO$^•$ reactions in aqueous solutions.

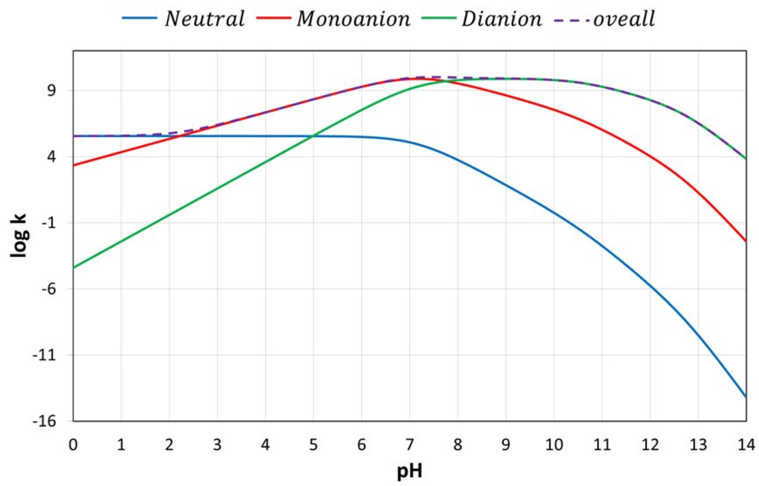

Figure S8. Variation of the overall rate constant with the *p*H, for the SeQ + HOO$^{\bullet}$ reactions in aqueous solutions.

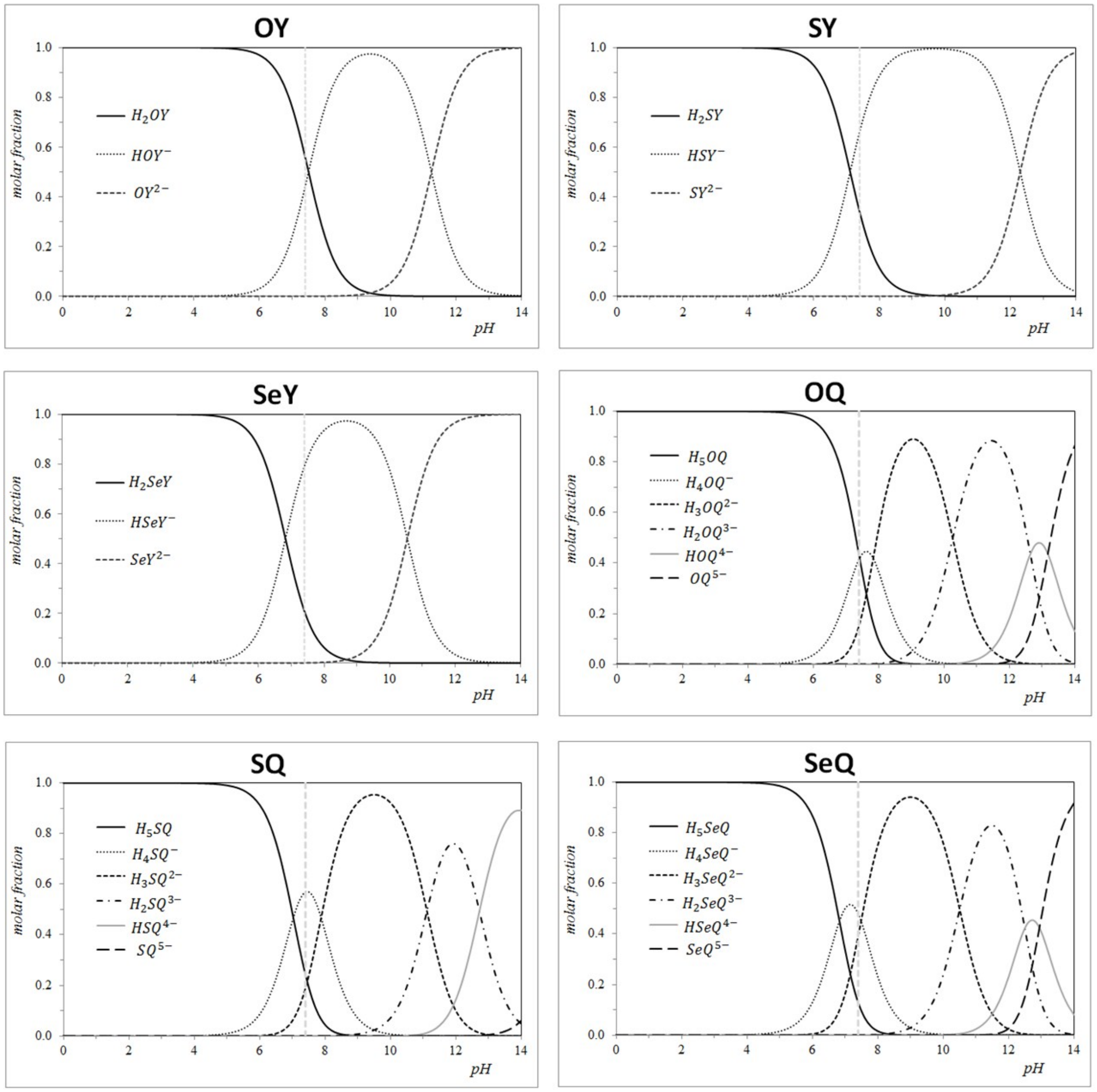

Figure S9. Distribution diagram of the acid-base species of chrysin, quercetin and their sulfur and selenium derivatives. The vertical line marks the physiological *p*H (*p*H=7.4).