Supporting information

Comparison of Vitamin C and Its Derivative Antioxidant Activity: Evaluated by Using Density Functional Theory

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List of supporting information:

Table S1: BDE values of VC and its derivatives calculated in the water and gas phase at the B3LYP/6-31G* level(the lowest values are highlighted in BOLD).

Species	BDE(kJ/mol)	
	water	gas
AA-O_7	308.89	323.24
AA-O_8	**301.78**	**297.19**
AA-O_12	502.84	404.85
AA-O_10	509.69	417.28
AA2G-O_25	580.30	407.50
AA2G-O_22	420.20	418.20
AA2G-O_19	409.30	401.40
AA2G-O_30	410.10	408.10
AA2G-O_1	**309.00**	**302.80**
AA2G-O_7	423.20	402.60
AA2G-O_9	410.20	398.80
AAE-O_4	545.85	399.32
AAE-O_3	525.71	400.66
AAE-O_5	**306.15**	**300.91**
AA6P-O_7	310.87	307.02
AA6P-O_6	**309.62**	**296.91**
AA6P-O_11	424.11	412.05

Table S2: IP values of VC and its derivatives calculated in the water and gas phase at the B3LYP/6-31G* level(the lowest values are highlighted in BOLD).

Species	IP(kJ/mol)	
	water	gas
AA	**575.01**	796.79
AA2G	607.79	826.74
AAE	582.45	**762.35**
AA6P	623.08	796.74

Table S3: PDE values of VC and its derivatives calculated in the water and gas phase at the B3LYP/6-31G* level.

Species	PDE(kJ/mol)	
	water	gas
AA-O_7	1055.25	873.71
AA-O_8	1062.33	847.73
AA-O_12	1256.18	967.81
AA-O_10	1173.75	955.24
AA2G-O_25	1313.20	912.17
AA2G-O_22	1153.51	922.96
AA2G-O_19	1142.27	823.28
AA2G-O_30	1143.19	921.87
AA2G-O_1	1042.00	927.95
AA2G-O_7	1156.17	937.24
AA2G-O_9	1152.78	928.60
AAE-O_4	1297.28	968.25
AAE-O_3	1284.10	985.54
AAE-O_5	1064.55	885.78
AA6P-O_7	1029.20	902.22
AA6P-O_6	1026.33	904.52
AA6P-O_11	1140.93	1011.01

Table S4: PA values of VC and its derivatives calculated in the water and gas phase at the B3LYP/6-31G* level(the lowest values are highlighted in BOLD).

Species	PA(kJ/mol)	
	water	gas
AA-O_7	1217.20	1415.28
AA-O_8	1180.96	1361.72
AA-O_12	1688.17	**1347.80**
AA-O_10	**1178.14**	1350.33
AA2G-O_25	1257.45	1484.60
AA2G-O_22	1241.80	1449.93
AA2G-O_19	1252.78	1486.09
AA2G-O_30	1251.46	1453.69
AA2G-O_1	**1168.33**	**1285.85**
AA2G-O_7	1168.37	**1285.85**
AA2G-O_9	1290.09	1511.03
AAE-O_4	1291.10	1465.17
AAE-O_3	1289.67	1462.15
AAE-O_5	**1225.33**	**1443.71**
AA6P-O_7	1227.12	1421.62
AA6P-O_6	**1210.90**	**1376.87**
AA6P-O_11	1280.24	1513.86

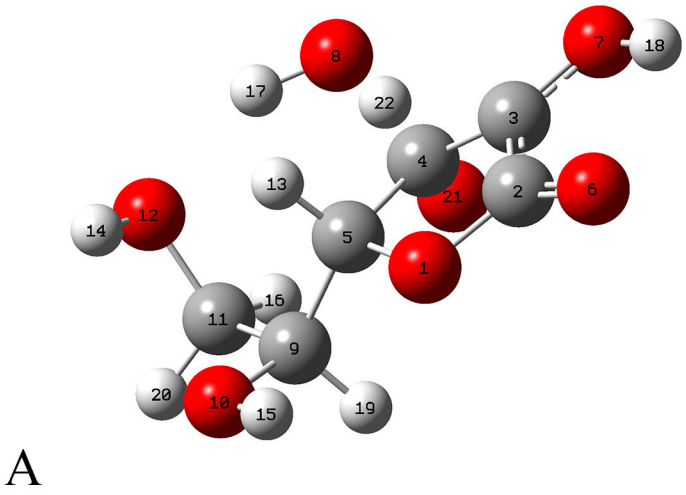
Table S5: ETE values of VC and its derivatives calculated in the water and gas phase at the B3LYP/6-31G* level(the lowest values are highlighted in BOLD).

Species	ETE(kJ/mol)	
	water	gas
AA-O_7	434.35	246.08
AA-O_8	461.57	282.66
AA-O_12	-42.07	303.24
AA-O_10	476.95	302.96
AA2G-O_25	663.50	270.08
AA2G-O_22	526.50	320.63
AA2G-O_19	497.38	262.56
AA2G-O_30	499.24	303.32
AA2G-O_1	485.98	354.52
AA2G-O_7	485.97	354.52
AA2G-O_9	460.99	234.92
AAE-O_4	474.81	280.37
AAE-O_3	466.19	273.72
AAE-O_5	421.59	204.41
AA6P-O_7	422.79	281.63
AA6P-O_6	452.72	281.23
AA6P-O_11	483.76	247.54

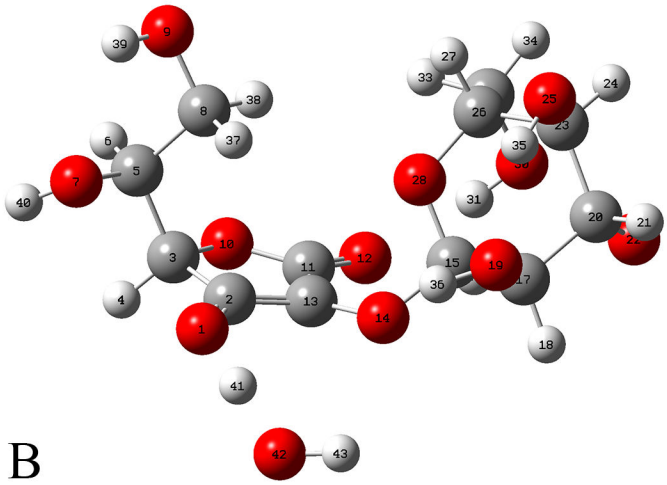
Table S6: Total energy requirements related to the HAT, SET-PT, and SPLET mechanisms of VC and its derivatives calculated in the water and gas phase.

Species	BDE(kJ/mol)		IP+PDE(kJ/mol)		PA+ETE(kJ/mol)	
	water	gas	water	gas	water	gas
AA	301.78	297.19	1630.26	1644.51	1642.53	1644.38
AA2G	309.03	302.75	1649.79	1650.02	1654.31	1640.37
AAE	306.15	300.91	1647.01	1648.13	1646.92	1648.12
AA6P	309.62	296.91	1649.41	1698.96	1649.91	1658.10

Figure S1: Optimized geometries of TS in the reaction between VC(A), AA2G(B), AAE(C), and AA6P(D) with OH•. Oxygen atoms are shown in red; gray is carbon; white is hydrogen.



A



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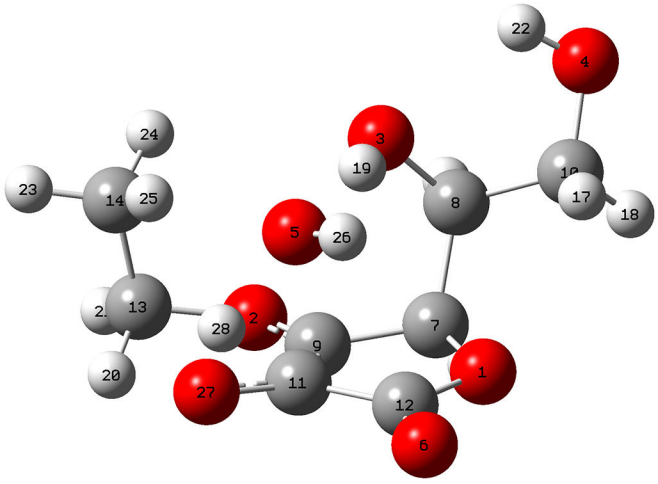

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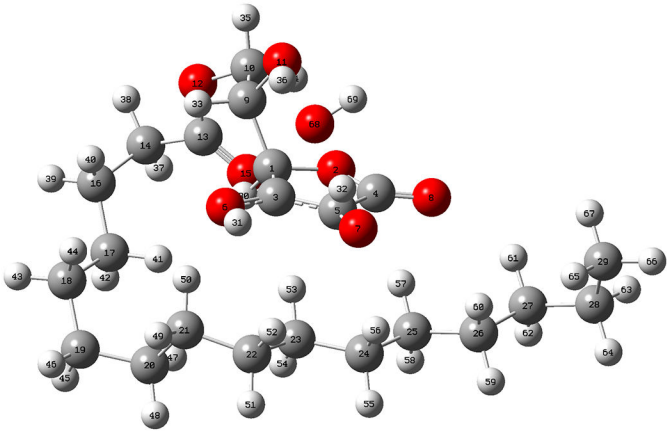

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