Supplementary Table 1. Total energy (E^{total}), zero-point energy (ZPE), and thermical contribution (G^{therm}) of **1**, their radicalar derivatives, and other species included in Equations 3 to 6, using PBE method and TZVP/6-311++G(d,p) level of theory

Estrutura	E^{total} (Hartree)	ZPE (Hartree)	G^{therm} (kcal/mol)
1	-1219.11355985	0.293612	152.961
O-5	-1218.46925865	0.280588	144.062
O-6	-1179.24304277	0.254286	129.509
O-7	-1218.46634422	0.279877	143.284
O-12	-1218.43948128	0.277857	142.124
O-13	-1218.44233222	0.278971	143.355
O-16	-1218.44509351	0.278775	143.195
C-2	-1219.65508709	0.302958	158.233
O-2	-1219.62832907	0.302789	158.189
C-2(CCl_3)	-2637.17929454	0.301270	151.438
O-2(CCl_3)	-2637.16577790	0.301027	152.329
C-2(OH)	-1294.84162117	0.308196	160.757
O-2(OH)	-1294.81673345	0.306222	159.382
C-2(CH_3)	-1258.90347732	0.329867	173.270
O-2(CH_3)	-1258.90144417	0.329315	173.893
CH_3OH	-115.619309085	0.049662	16.851
$^{\bullet}H$	-0.49981227329	0.000000	-6.685
CH_4	-40.4598513084	0.043550	14.976
$^{\bullet}CH_3$	-39.7847760607	0.029019	5.781
CCl_4	-1878.14146695	0.008926	-13.879
$^{\bullet}CCl_3$	-1418.07688775	0.006916	-14.399
$HCCl_3$	-1418.72828664	0.019194	-6.320
CH_3-CCl_3	-1458.00209039	0.045882	9.607
CH_3-CH_3	-79.7242670746	0.072560	31.010
$^{\bullet}OH$	-75.6761951287	0.008221	-5.474
H_2O	-76.3724940200	0.009833	1.532
H_2	-1.16585743700	0.009833	-1.052

Supplementary Table 2. Thermodynamic quantities (in kcal.mol^{-1}) calculated for reaction of **1** with $^{\bullet}$H using PBE/6-311++G(d,p) level of theory

Reaction	ΔE^{ele}	ΔG^{therm}	ΔG^{total}
Bergenin + $^{\bullet}$H → **O-5** + H_2	-13.65	-5.27	-18.9
Bergenin + $^{\bullet}$H → **O-6** + CH_4	-56.18	0.86	-55.3
Bergenin + $^{\bullet}$H → **O-7** + H_2	-11.82	-6.49	-18.3
Bergenin + $^{\bullet}$H → **O-12** + H_2	5.04	-8.92	-3.9
Bergenin + $^{\bullet}$H → **O-13** + H_2	3.25	-6.99	-3.7
Bergenin + $^{\bullet}$H → **O-16** + H_2	1.52	-7.27	-5.8
Bergenin + $^{\bullet}$H → **C-2**	26.18	17.82	44.0
Bergenin + $^{\bullet}$H → **O-2**	-9.39	17.67	8.3

Supplementary Table 3. Thermodynamic quantities (in kcal.mol^{-1}) calculated for reaction of **1** with $^{\bullet}$OH using PBE/6-311++G(d,p) level of theory

Reaction	ΔE^{ele}	ΔG^{therm}	ΔG^{total}
Bergenin + $^{\bullet}$OH → **O-5** + H_2O	-32.63	-2.19	-34.8
Bergenin + $^{\bullet}$OH → **O-6** + CH_3OH	-45.56	2.45	-43.1
Bergenin + $^{\bullet}$OH → **O-7** + H_2O	-30.80	-3.42	-34.2
Bergenin + $^{\bullet}$OH → **O-12** + H_2O	-13.94	-5.85	-19.8
Bergenin + $^{\bullet}$OH → **O-13** + H_2O	-15.73	-3.92	-19.7
Bergenin + $^{\bullet}$OH → **O-16** + H_2O	-17.47	-4.20	-21.7
Bergenin + $^{\bullet}$OH → **C-2(OH)**	-32.55	17.26	-15.3
Bergenin + $^{\bullet}$OH → **O-2(OH)**	-16.93	14.65	-2.3

Supplementary Table 4. Thermodynamic quantities (in kcal.mol^{-1}) calculated for reaction of **1** with $^{\bullet}CH_3$ using PBE/6-311++G(d,p) level of theory

Reaction	ΔE^{ele}	ΔG^{therm}	ΔG^{total}
Bergenin + $^{\bullet}CH_3$ → **O-5** + CH_4	-19.31	1.24	-18.1
Bergenin + $^{\bullet}CH_3$ → **O-6** + CH_3-CH_3	-43.28	4.42	-38.9
Bergenin + $^{\bullet}CH_3$ → **O-7** + CH_4	-17.48	0.02	-17.5
Bergenin + $^{\bullet}CH_3$ → **O-12** + CH_4	-0.63	-2.41	-3.0
Bergenin + $^{\bullet}CH_3$ → **O-13** + CH_4	-2.41	-0.48	-2.9
Bergenin + $^{\bullet}CH_3$ → **O-16** + CH_4	-4.15	-0.76	-4.9
Bergenin + $^{\bullet}CH_3$ → **C-2(CH_3)**	-3.23	19.07	15.8
Bergenin + $^{\bullet}CH_3$ → **O-2(CH_3)**	-1.95	19.35	17.4

Supplementary Table 5. Thermodynamic quantities (in kcal.mol^{-1}) calculated for reaction of **1** with $^{\bullet}CCl_3$ using PBE/6-311++G(d,p) level of theory

Reaction	ΔE^{ele}	ΔG^{therm}	ΔG^{total}
Bergenin + $^{\bullet}CCl_3$ → **O-5** + $CHCl_3$	-4.45	-1.29	-5.7
Bergenin + $^{\bullet}CCl_3$ → **O-6** + CH_3-CCl_3	-34.32	-0.33	-34.7
Bergenin + $^{\bullet}CCl_3$ → **O-7** + $HCCl_3$	-2.63	-2.51	-5.1
Bergenin + $^{\bullet}CCl_3$ → **O-12** + $HCCl_3$	14.23	-4.94	9.3
Bergenin + $^{\bullet}CCl_3$ → **O-13** + $HCCl_3$	12.44	-3.01	9.4
Bergenin + $^{\bullet}CCl_3$ → **O-16** + $HCCl_3$	10.71	-3.29	7.4
Bergenin + $^{\bullet}CCl_3$ → **C-2(CCl_3)**	6.99	13.34	20.3
Bergenin + $^{\bullet}CCl_3$ → **O-2(CCl_3)**	15.48	14.08	29.6