

# Computational insights on the antioxidant, antinitrosant, and Xanthine Oxidase inhibitory capacities of neobavaisoflavone

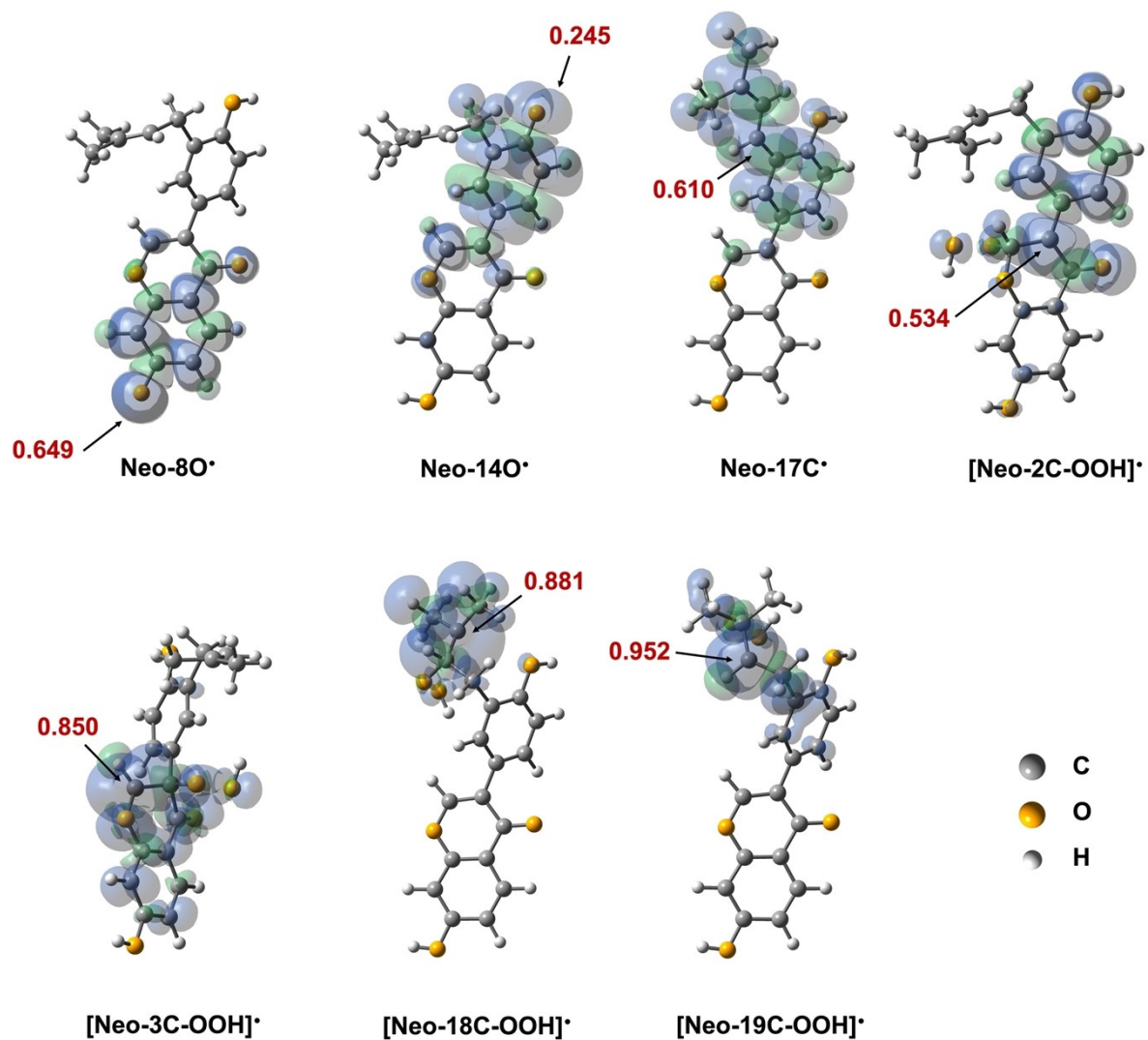
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**Figure S1.** Distribution of spin density of the radical products of Neo.

**Table S1.** Selected atom in molecule (AIM) parameters of the **Neo-17CH** and **14OH + HOO** transition states in the lipid-like environment.

Contacts	$\rho(r)$ (au)	$\nabla^2\rho(r)$ (au)	$G(r)^a$ (au)	$V(r)^b$ (au)	$G(r)/ V(r) $ (au)	$H(r)^c$	$E_{HB}^d$ (kcal/mol)
<b>Neo-14O...H...OOH</b>							
H42...O24	0.2293	-0.8554	0.0917	-0.3974	-0.2307	-0.3057	-125.2
H42...O43	0.1332	-0.0229	0.0871	-0.1667	-0.5225	-0.0796	-52.5
O44...C16	0.0155	0.0508	0.0116	-0.0105	-1.1048	0.0011	-3.3
RCP1 (C16-O24- H42-O43- O44)	0.0141	0.0665	0.0149	-0.0132	-1.1288	0.0017	-4.2
RCP1 (C16-C15- C19-H33- O43-O44)	0.0071	0.0303	0.0066	-0.0056	-1.1786	0.0010	-1.8
<b>Neo-17C...H...OOH</b>							
C8...H14	0.1772	-0.3522	0.0387	-0.1654	-0.2340	-0.1267	-52.1
H14...O42	0.1345	-0.0431	0.0841	-0.1574	-0.5343	-0.0733	-49.6
H44...O7	0.0182	0.0678	0.0155	-0.0141	-1.0993	0.0014	-4.4
RCP1 (C1-C6-C8- H14-O42- O43-H44-O7)	0.0076	0.0304	0.0065	-0.0055	-1.1818	0.0010	-1.7
(a) Electron kinetic energy density, (b) Electron potential energy density, (C) Total electron energy density, (d) Individual energies of each hydrogen bond.							

**Table S2.** The cartesian coordinates and energies of **Neo** and its radical and anionic states calculated at M06-2X/6-311++G(d,p) level in water and pentyl ethanoate.

Neo (W)				
Cartesian Coordinates				Frequency and Energy
C	-5.35297100	-0.55772800	0.66643500	Zero-point Energy Correction = 0.335739 Hartree
C	-5.42878700	0.69227400	0.02362300	Thermal Correction to Energy = 0.357072 Hartree
C	-4.29846800	1.29345500	-0.50264500	Thermal Correction to Enthalpy = 0.358016 Hartree
C	-3.08266400	0.62698600	-0.38107700	Thermal Correction to Free Energy = 0.284505
C	-2.96937300	-0.61358100	0.24639100	Hartree
C	-4.13914100	-1.19210500	0.77230500	EE + Zero-point Energy = -1073.4001 Hartree
O	-1.99387200	1.25382700	-0.91184900	EE + Thermal Energy Correction = -1073.3787
C	-0.79271000	0.65128200	-0.83573400	Hartree
C	-0.55230600	-0.54187700	-0.25233500	EE + Thermal Enthalpy Correction = -1073.3778
C	-1.66663200	-1.27128500	0.35695300	Hartree
O	-6.65577000	1.26886300	-0.05049500	EE + Thermal Free Energy Correction = -1073.4513
O	-1.52531900	-2.35167800	0.93437200	Hartree
C	0.82905600	-1.07545400	-0.21506000	
C	1.89492400	-0.24479800	0.14943400	
C	3.21175100	-0.69236800	0.15874700	
C	3.44841800	-2.02354800	-0.20820500	
C	2.40442300	-2.87041400	-0.56591100	
C	1.09788000	-2.39803500	-0.56934800	
C	4.39611600	0.18275300	0.52752800	
C	4.05580600	1.55681600	1.04443800	
C	3.66293800	2.59242600	0.29671000	
C	3.34319000	3.92976100	0.90528200	
C	3.46510000	2.51147400	-1.19152300	
O	4.75131900	-2.45027500	-0.19668500	
H	-6.25807300	-0.99695200	1.06708500	
H	-4.34680700	2.25607700	-0.99800700	
H	-4.06441800	-2.15415100	1.26446400	
H	-0.02505400	1.24853100	-1.31269500	
H	-6.60464300	2.11671000	-0.51199600	
H	1.68880500	0.77848600	0.44439600	
H	2.62387100	-3.89562100	-0.84604800	
H	0.29117900	-3.05839300	-0.86329000	
H	4.98798200	-0.34618700	1.27902700	
H	5.04258200	0.25538100	-0.35439300	
H	4.13240800	1.70146600	2.11959600	
H	3.48197100	3.92483000	1.98750200	
H	3.97973300	4.70895600	0.47401400	
H	2.30796500	4.21099500	0.68598300	
H	3.78469900	1.55843100	-1.61381500	
H	2.40459200	2.65107100	-1.43065100	
H	4.00952900	3.31751600	-1.69322900	

H	4.79350800	-3.37923900	-0.45673500	
Neo (PE)				
Cartesian Coordinates				Frequency and Energy
C	-5.38904700	-0.51542500	0.63249800	Zero-point Energy Correction = 0.336072 Hartree
C	-5.43944100	0.75606800	0.03269600	Thermal Correction to Energy = 0.35763 Hartree
C	-4.29394700	1.35090600	-0.46874800	Thermal Correction to Enthalpy = 0.358574 Hartree
C	-3.08858900	0.65842500	-0.36594200	Thermal Correction to Free Energy = 0.283881
C	-3.00473600	-0.60310300	0.21908800	Hartree
C	-4.18677100	-1.17547900	0.71917500	EE + Zero-point Energy = -1073.4004 Hartree
O	-1.99125600	1.27876500	-0.87288100	EE + Thermal Energy Correction = -1073.3788
C	-0.80045200	0.65482400	-0.80246000	Hartree
C	-0.57516200	-0.55400400	-0.24994600	EE + Thermal Enthalpy Correction = -1073.3779
C	-1.71337900	-1.30336300	0.31347800	Hartree
O	-6.65021000	1.35388400	-0.02536400	EE + Thermal Free Energy Correction = -1073.4526
O	-1.60624300	-2.40692700	0.82413600	Hartree
C	0.80167800	-1.09730400	-0.20616900	
C	1.87770600	-0.26859900	0.13633000	
C	3.19028500	-0.72519300	0.15172300	
C	3.41813300	-2.06575100	-0.18633100	
C	2.36399200	-2.91048500	-0.51780800	
C	1.06037900	-2.43035200	-0.52497500	
C	4.38164100	0.14638900	0.50618800	
C	4.04823800	1.51768200	1.03263700	
C	3.75806800	2.59124200	0.29233600	
C	3.45530000	3.92458300	0.91998000	
C	3.68129100	2.57001700	-1.20981000	
O	4.71097700	-2.49508500	-0.16917200	
H	-6.30442500	-0.94920300	1.01524800	
H	-4.31351300	2.33065700	-0.93299100	
H	-4.12416000	-2.15545800	1.17707800	
H	-0.02203200	1.25180700	-1.26179000	
H	-6.57830500	2.21580600	-0.45290700	
H	1.68507500	0.76071300	0.41951700	
H	2.56583400	-3.94686300	-0.77182400	
H	0.24630900	-3.09513900	-0.78301200	
H	4.97955800	-0.38733100	1.24989900	
H	5.02290100	0.21865100	-0.37869900	
H	4.04198400	1.62738100	2.11497200	
H	3.52538200	3.88534100	2.00818200	
H	4.15055400	4.68774400	0.55471200	
H	2.44850100	4.25930900	0.64814200	
H	3.86983000	1.58404200	-1.63463100	
H	2.68713900	2.89533600	-1.53603300	
H	4.39749600	3.27783100	-1.64057300	
H	4.74460400	-3.43218900	-0.39266800	
Neo-80* (W)				
Cartesian Coordinates				Frequency and Energy

C	-5.40715900	-0.54272700	0.65010500	Zero-point Energy Correction = 0.321874 Hartree
C	-5.51287400	0.76764400	0.02669400	Thermal Correction to Energy = 0.343183 Hartree
C	-4.31007900	1.37655700	-0.49028900	Thermal Correction to Enthalpy = 0.344127 Hartree
C	-3.11263100	0.70519400	-0.38125000	Thermal Correction to Free Energy = 0.269241
C	-3.02673100	-0.55793000	0.22049300	Hartree
C	-4.20480600	-1.16662100	0.73673300	EE + Zero-point Energy = -1072.7543 Hartree
O	-2.00648100	1.32504700	-0.88522400	EE + Thermal Energy Correction = -1072.733
C	-0.81951400	0.70170000	-0.81027200	Hartree
C	-0.59855600	-0.51017500	-0.25109700	EE + Thermal Enthalpy Correction = -1072.7321
C	-1.72359800	-1.23822600	0.32738700	Hartree
O	-6.61050100	1.35771000	-0.06304900	EE + Thermal Free Energy Correction = -1072.8069
O	-1.62196400	-2.33040800	0.88097000	Hartree
C	0.77394000	-1.06318200	-0.21258100	
C	1.85132000	-0.24790200	0.15399400	
C	3.16004800	-0.71684600	0.16958000	
C	3.37661500	-2.05282900	-0.19418300	
C	2.32105200	-2.88251900	-0.55804600	
C	1.02245300	-2.39000400	-0.56640100	
C	4.35712000	0.13873000	0.54233900	
C	4.03858300	1.52329800	1.04490100	
C	3.66560000	2.55769700	0.28537000	
C	3.36753600	3.90669400	0.87894100	
C	3.47116200	2.46456200	-1.20260400	
O	4.67101900	-2.50112900	-0.17304800	
H	-6.31602300	-0.98865900	1.03509600	
H	-4.36394400	2.35256900	-0.95693300	
H	-4.10997900	-2.14145700	1.19832700	
H	-0.03704300	1.29646400	-1.26599700	
H	1.66096800	0.77890300	0.44731200	
H	2.52513300	-3.91103500	-0.83749800	
H	0.20721900	-3.03783600	-0.86413900	
H	4.93239800	-0.39540900	1.30298900	
H	5.01221400	0.19187100	-0.33459700	
H	4.11503100	1.67751300	2.11870200	
H	3.50203100	3.91035000	1.96170200	
H	4.01983400	4.66968100	0.44228200	
H	2.33846600	4.20429700	0.65246000	
H	3.77738800	1.50244000	-1.61411800	
H	2.41370600	2.61808800	-1.44672900	
H	4.02956500	3.25698400	-1.71058800	
H	4.69956800	-3.43320700	-0.42433500	
Neo-8O* (P)				
Cartesian Coordinates				Frequency and Energy
C	-5.43730100	-0.49404000	0.62889700	Zero-point Energy Correction = 0.322429 Hartree
C	-5.52077200	0.83646400	0.04114700	Thermal Correction to Energy = 0.343814 Hartree
C	-4.30165500	1.42928000	-0.46073100	Thermal Correction to Enthalpy = 0.344759 Hartree
C	-3.11760500	0.73126000	-0.37329100	Thermal Correction to Free Energy = 0.269574

C	-3.05874500	-0.55081300	0.19408400	Hartree
C	-4.24721600	-1.14681400	0.69489600	EE + Zero-point Energy = -1072.7585 Hartree
O	-2.00215600	1.33549300	-0.86489400	EE + Thermal Energy Correction = -1072.7371
C	-0.82568300	0.69051500	-0.79438700	Hartree
C	-0.62001700	-0.53120200	-0.25682500	EE + Thermal Enthalpy Correction = -1072.7361
C	-1.76941100	-1.27140800	0.28126700	Hartree
O	-6.60108200	1.44826100	-0.03043000	EE + Thermal Free Energy Correction = -1072.8113
O	-1.69960800	-2.38446900	0.77338200	Hartree
C	0.74870200	-1.09208200	-0.20616200	
C	1.83185000	-0.27450900	0.14201700	
C	3.13828500	-0.74593500	0.16627000	
C	3.35272000	-2.08986900	-0.16959200	
C	2.29124000	-2.92276100	-0.50781200	
C	0.99330600	-2.42831100	-0.52308300	
C	4.33700300	0.11218300	0.52780400	
C	4.01637800	1.49281700	1.03773000	
C	3.74695800	2.56226200	0.28365600	
C	3.45720700	3.90624000	0.89446300	
C	3.68427000	2.52641200	-1.21886300	
O	4.63940200	-2.53312300	-0.14305200	
H	-6.35510500	-0.93044900	1.00415000	
H	-4.33695000	2.41844100	-0.90129600	
H	-4.16531100	-2.13617600	1.12825500	
H	-0.03354900	1.27998600	-1.23980400	
H	1.64988500	0.75729600	0.42298500	
H	2.48273800	-3.96130500	-0.76048900	
H	0.17457200	-3.08482600	-0.78733200	
H	4.91849400	-0.42325900	1.28324700	
H	4.98952700	0.16729300	-0.35000500	
H	4.00286700	1.61394800	2.11875200	
H	3.51506900	3.87729400	1.98369300	
H	4.16775900	4.65500900	0.52894400	
H	2.45870800	4.25338400	0.60800800	
H	3.86385400	1.53381700	-1.63203200	
H	2.69806300	2.86212800	-1.55841800	
H	4.41409300	3.22019000	-1.64951100	
H	4.66575700	-3.47022300	-0.36811700	
Neo-14O* (W)				
Cartesian Coordinates				Frequency and Energy
C	5.36371900	-0.55544600	-0.48778300	Zero-point Energy Correction = 0.322811 Hartree
C	5.38374500	0.76175400	0.00680500	Thermal Correction to Energy = 0.343938 Hartree
C	4.21471200	1.39778700	0.39216300	Thermal Correction to Enthalpy = 0.344882 Hartree
C	3.02085800	0.69587200	0.27709300	Thermal Correction to Free Energy = 0.271063
C	2.96111400	-0.60990000	-0.20702000	Hartree
C	4.16716300	-1.22260000	-0.59150500	EE + Zero-point Energy = -1072.7684 Hartree
O	1.88886800	1.35958300	0.66607900	EE + Thermal Energy Correction = -1072.7472
C	0.70845700	0.73860400	0.59307900	Hartree

C	0.51791400	-0.52886300	0.14800400	EE + Thermal Enthalpy Correction = -1072.7463
C	1.67675500	-1.30091800	-0.32119300	Hartree
O	6.59434000	1.36791800	0.08575900	EE + Thermal Free Energy Correction = -1072.8201
O	1.57939200	-2.42969800	-0.80045500	Hartree
C	-0.83613100	-1.09125100	0.14126200	
C	-1.94169300	-0.27042500	-0.18301600	
C	-3.22945500	-0.74081500	-0.16121700	
C	-3.46644200	-2.13436600	0.21456500	
C	-2.31785200	-2.95380200	0.54045500	
C	-1.05284000	-2.44978600	0.49906300	
C	-4.43924300	0.09650700	-0.48864400	
C	-4.15841500	1.49100600	-0.98421400	
C	-3.76104900	2.51708700	-0.22568300	
C	-3.49995600	3.87677300	-0.81175800	
C	-3.50291800	2.40490300	1.25109900	
O	-4.62585400	-2.60343200	0.25623200	
H	6.29746300	-1.02024800	-0.77879700	
H	4.21975800	2.41233500	0.77280200	
H	4.13487400	-2.23640900	-0.97149400	
H	-0.09069800	1.37106400	0.96093300	
H	6.50314600	2.26157600	0.44295000	
H	-1.75974700	0.75590200	-0.48179200	
H	-2.50852400	-3.98071200	0.83067200	
H	-0.20839000	-3.07092900	0.76601300	
H	-5.03031000	-0.44673700	-1.23109500	
H	-5.06552900	0.12126400	0.41144800	
H	-4.28585800	1.65867300	-2.05083900	
H	-3.67753100	3.89403200	-1.88808500	
H	-4.14117200	4.62689000	-0.33813000	
H	-2.46539600	4.18081100	-0.62194200	
H	-3.79600300	1.43967300	1.66495100	
H	-2.43521900	2.55130100	1.45119900	
H	-4.03549100	3.19383000	1.79096000	
Neo-140* (P)				
Cartesian Coordinates				Frequency and Energy
C	-5.39235300	-0.48890800	0.50519200	Zero-point Energy Correction = 0.323114 Hartree
C	-5.39507600	0.82427300	0.00106300	Thermal Correction to Energy = 0.344401 Hartree
C	-4.21752400	1.43338300	-0.40250500	Thermal Correction to Enthalpy = 0.345345 Hartree
C	-3.03279100	0.71058400	-0.29630900	Thermal Correction to Free Energy = 0.270711
C	-2.99423200	-0.59097400	0.19646500	Hartree
C	-4.20641800	-1.17686500	0.59850500	EE + Zero-point Energy = -1072.7703 Hartree
O	-1.89910800	1.34676900	-0.70583900	EE + Thermal Energy Correction = -1072.749
C	-0.72762900	0.70520000	-0.63261500	Hartree
C	-0.54550700	-0.55463600	-0.17055000	EE + Thermal Enthalpy Correction = -1072.748
C	-1.72048200	-1.31857900	0.30026000	Hartree
O	-6.59070200	1.44698400	-0.06647700	EE + Thermal Free Energy Correction = -1072.8227
O	-1.64839900	-2.44694700	0.75663900	Hartree



C	0.80641600	-1.12647600	-0.14735200	
C	1.91867700	-0.30147400	0.14760800	
C	3.20457600	-0.77700100	0.13564700	
C	3.44174900	-2.18409500	-0.20109700	
C	2.28122000	-3.00687300	-0.48707900	
C	1.01688900	-2.49748900	-0.45245200	
C	4.41723600	0.06607400	0.43941900	
C	4.13683800	1.44311000	0.97926300	
C	3.85432500	2.52810200	0.25255300	
C	3.61001300	3.86590100	0.89597000	
C	3.73733300	2.52001600	-1.24708300	
O	4.59201900	-2.65133000	-0.23852700	
H	-6.33141700	-0.93237200	0.81201400	
H	-4.19994700	2.44477100	-0.79307900	
H	-4.18106700	-2.18844900	0.98562300	
H	0.07702100	1.32013700	-1.01704900	
H	-6.48715300	2.33795100	-0.42236600	
H	1.74512300	0.73358800	0.42142700	
H	2.46574900	-4.04588400	-0.73571400	
H	0.16610200	-3.12792400	-0.67205200	
H	5.03634300	-0.48969600	1.14902100	
H	5.01966500	0.11634000	-0.47471300	
H	4.16806300	1.54679400	2.06165500	
H	3.70916700	3.81767500	1.98149500	
H	4.31875200	4.60887800	0.51556900	
H	2.60736600	4.23401100	0.65373100	
H	3.88472000	1.53246800	-1.68435800	
H	2.74676800	2.88025600	-1.54621700	
H	4.46470500	3.20800400	-1.69077000	
Neo-17C* (W)				
Cartesian Coordinates				Frequency and Energy
C	5.82344400	0.23882300	0.88350400	Zero-point Energy Correction = 0.321974 Hartree
C	5.94773100	-0.93469900	0.11614100	Thermal Correction to Energy = 0.343559 Hartree
C	4.85640000	-1.47626000	-0.54080400	Thermal Correction to Enthalpy = 0.344503 Hartree
C	3.63027300	-0.82853400	-0.42217100	Thermal Correction to Free Energy = 0.269027
C	3.46871700	0.33491200	0.32989000	Hartree
C	4.60002000	0.85529200	0.98478400	EE + Zero-point Energy = -1072.7792 Hartree
O	2.58120400	-1.39357300	-1.08615200	EE + Thermal Energy Correction = -1072.7576
C	1.37235700	-0.80628200	-1.01688800	Hartree
C	1.08596500	0.31095100	-0.31618700	EE + Thermal Enthalpy Correction = -1072.7567
C	2.15482000	0.97086500	0.43681500	Hartree
O	7.18095200	-1.49942500	0.05755300	EE + Thermal Free Energy Correction = -1072.8321
O	1.96873500	1.97833100	1.12283700	Hartree
C	-0.30033300	0.83377700	-0.30207000	
C	-1.37360600	-0.02170200	-0.09116000	
C	-2.72059700	0.40733600	-0.10606900	
C	-2.93516100	1.78779300	-0.33390800	

C	-1.86675900	2.65368700	-0.54324400	
C	-0.55851200	2.19198300	-0.53010100	
C	-3.74059000	-0.58536900	0.11881200	
C	-5.13575600	-0.44912400	0.13109900	
C	-6.00119600	-1.50082200	0.35365200	
C	-7.48179500	-1.28948400	0.34955400	
C	-5.51585600	-2.89855400	0.61064700	
O	-4.21735600	2.25828600	-0.33794300	
H	6.69941900	0.63405600	1.38266300	
H	4.94155100	-2.37954600	-1.13346600	
H	4.48832400	1.75793800	1.57309500	
H	0.64137500	-1.34571100	-1.60624400	
H	7.16276200	-2.29869900	-0.48568900	
H	-1.18189200	-1.07235500	0.10432700	
H	-2.07666600	3.70374500	-0.72145500	
H	0.25685000	2.88186000	-0.70828700	
H	-3.34358000	-1.58150900	0.29277900	
H	-5.57631300	0.52373700	-0.04394900	
H	-7.74519500	-0.24872700	0.15603700	
H	-7.95724100	-1.91981900	-0.41087200	
H	-7.91515300	-1.58914700	1.31082400	
H	-4.88859300	-2.94502500	1.50706400	
H	-6.35474000	-3.58155100	0.74962500	
H	-4.90893100	-3.27106500	-0.22105200	
H	-4.20765900	3.21535600	-0.46954600	
<b>Neo-17C* (P)</b>				
<b>Cartesian Coordinates</b>				<b>Frequency and Energy</b>
C	5.82731100	0.22630800	0.89004100	Zero-point Energy Correction = 0.322746 Hartree
C	5.94944500	-0.94675900	0.12334100	Thermal Correction to Energy = 0.344293 Hartree
C	4.85606300	-1.48059800	-0.53802500	Thermal Correction to Enthalpy = 0.345237 Hartree
C	3.62939400	-0.82860000	-0.42373600	Thermal Correction to Free Energy = 0.270398
C	3.47521400	0.33568000	0.32582700	Hartree
C	4.60593600	0.84933400	0.98324700	EE + Zero-point Energy = -1072.7794 Hartree
O	2.58420000	-1.38796300	-1.08855600	EE + Thermal Energy Correction = -1072.7579
C	1.37618600	-0.79878600	-1.01525600	Hartree
C	1.08651700	0.31615200	-0.31588000	EE + Thermal Enthalpy Correction = -1072.7569
C	2.16353100	0.99549500	0.42647200	Hartree
O	7.17509400	-1.51366500	0.06995700	EE + Thermal Free Energy Correction = -1072.8318
O	1.99211400	2.01303300	1.07854400	Hartree
C	-0.30064800	0.83434600	-0.29658800	
C	-1.37432800	-0.02546200	-0.10432000	
C	-2.72191600	0.39849400	-0.11860500	
C	-2.94010700	1.77998000	-0.33564500	
C	-1.87113800	2.65172300	-0.51438700	
C	-0.56109600	2.19594900	-0.49473500	
C	-3.74200300	-0.59473500	0.10125200	
C	-5.13557000	-0.45203900	0.13026200	

C	-6.00639900	-1.49644800	0.36125600	
C	-7.48636300	-1.27497000	0.36705100	
C	-5.53068000	-2.89967700	0.61106700	
O	-4.21975800	2.23918200	-0.35698300	
H	6.70364900	0.61571600	1.39313100	
H	4.93253900	-2.38296500	-1.13452700	
H	4.48802600	1.75378100	1.56812500	
H	0.64428700	-1.33559900	-1.60639000	
H	7.15376100	-2.30726100	-0.47836500	
H	-1.18097000	-1.07703700	0.08536800	
H	-2.07458800	3.70701100	-0.67187800	
H	0.25463600	2.89306800	-0.63487100	
H	-3.34638800	-1.59303300	0.26605400	
H	-5.56554100	0.52654300	-0.03784300	
H	-7.74403600	-0.23376700	0.16718400	
H	-7.97450600	-1.90538000	-0.38583700	
H	-7.91642400	-1.56086000	1.33438300	
H	-4.83388400	-2.94495900	1.45429300	
H	-6.36918300	-3.56202800	0.83204700	
H	-5.00565800	-3.30476000	-0.26124400	
H	-4.21500300	3.19452500	-0.48915600	
Neo-8O <sup>-</sup> (W)				
Cartesian Coordinates				Frequency and Energy
C	-5.39143100	-0.50772200	0.67684300	Zero-point Energy Correction = 0.322305 Hartree
C	-5.52217600	0.77037400	0.01915100	Thermal Correction to Energy = 0.34343 Hartree
C	-4.33059300	1.32837800	-0.51695600	Thermal Correction to Enthalpy = 0.344375 Hartree
C	-3.12913200	0.65746300	-0.39637400	Thermal Correction to Free Energy = 0.27099
C	-3.00354300	-0.58704900	0.24201000	Hartree
C	-4.18683900	-1.14638300	0.77980700	EE + Zero-point Energy = -1072.9491 Hartree
O	-2.02679400	1.27176100	-0.93987200	EE + Thermal Energy Correction = -1072.928
C	-0.82886100	0.66271700	-0.86005100	Hartree
C	-0.59663300	-0.52574500	-0.26719700	EE + Thermal Enthalpy Correction = -1072.927
C	-1.71985100	-1.24306900	0.35188300	Hartree
O	-6.65630800	1.35935200	-0.06956200	EE + Thermal Free Energy Correction = -1073.0004
O	-1.56549400	-2.32704900	0.93879100	Hartree
C	0.78154800	-1.06806300	-0.22584000	
C	1.85219100	-0.24703200	0.14682900	
C	3.16618300	-0.70436000	0.16516000	
C	3.39548700	-2.03674400	-0.20034100	
C	2.34783000	-2.87436300	-0.56866300	
C	1.04494400	-2.39181000	-0.58120600	
C	4.35440800	0.16145100	0.54420400	
C	4.02107400	1.54020700	1.05322100	
C	3.64374200	2.57632000	0.29820300	
C	3.32877700	3.91836800	0.89886400	
C	3.45895200	2.49128300	-1.19149900	
O	4.69540600	-2.47542700	-0.17688500	

H	-6.28947800	-0.95127100	1.09338600	
H	-4.36118800	2.28682500	-1.02214200	
H	-4.11626700	-2.10566500	1.28056100	
H	-0.05713900	1.25006600	-1.34329600	
H	1.65169900	0.77729300	0.44199700	
H	2.56152200	-3.90082400	-0.84893900	
H	0.23552000	-3.04565400	-0.88219800	
H	4.93362500	-0.37023600	1.30365100	
H	5.01102600	0.22591600	-0.33082400	
H	4.08834100	1.68807300	2.12858100	
H	3.45742200	3.91640300	1.98235200	
H	3.97523200	4.69107900	0.47066400	
H	2.29780600	4.20667400	0.66896800	
H	3.77760700	1.53518300	-1.60755300	
H	2.40131400	2.63503600	-1.44065300	
H	4.01178800	3.29289500	-1.69109200	
H	4.73023300	-3.40622300	-0.43151700	
Neo-14O <sup>-</sup> (W)				
Cartesian Coordinates				Frequency and Energy
C	-5.31975300	0.27470400	1.29108600	Zero-point Energy Correction = 0.322466 Hartree
C	-5.64648900	0.71382200	-0.00594300	Thermal Correction to Energy = 0.343523 Hartree
C	-4.70088500	0.72014300	-1.01562600	Thermal Correction to Enthalpy = 0.344467 Hartree
C	-3.41668400	0.27102700	-0.71793800	Thermal Correction to Free Energy = 0.270645 Hartree
C	-3.05801700	-0.17865700	0.55278300	
C	-4.04424600	-0.16098600	1.55673600	EE + Zero-point Energy = -1072.9396 Hartree
O	-2.51796600	0.28843100	-1.74026500	EE + Thermal Energy Correction = -1072.9185 Hartree
C	-1.26552600	-0.16314800	-1.51686900	
C	-0.78994100	-0.61338400	-0.33548700	EE + Thermal Enthalpy Correction = -1072.9176 Hartree
C	-1.69332500	-0.63796600	0.81853800	
O	-6.92520900	1.12485400	-0.21062500	EE + Thermal Free Energy Correction = -1072.9914 Hartree
O	-1.33850400	-1.00506000	1.94205700	
C	0.62263000	-1.03879000	-0.22523400	
C	1.65203200	-0.26004700	-0.77450700	
C	2.98449500	-0.65039800	-0.74530900	
C	3.35755100	-1.89499500	-0.14507900	
C	2.30127400	-2.66654900	0.41183000	
C	0.97911400	-2.25062600	0.37748900	
C	4.06179800	0.24505800	-1.32004700	
C	4.91305400	0.89301400	-0.24953500	
C	4.63596200	2.03178600	0.39487200	
C	5.54384900	2.56388800	1.47114400	
C	3.41032200	2.86803300	0.14576700	
O	4.59307800	-2.30111800	-0.11321100	
H	-6.08527400	0.28633400	2.05706000	
H	-4.94121100	1.05827200	-2.01686000	
H	-3.77832200	-0.50331600	2.54947000	
H	-0.67224400	-0.12013600	-2.42138400	

H	-7.05174500	1.38659900	-1.13262800
H	1.40005700	0.69247200	-1.23564100
H	2.55789200	-3.61619600	0.87185500
H	0.20920200	-2.88333900	0.80698000
H	4.71330100	-0.34857800	-1.96814200
H	3.59028100	1.00604800	-1.94565900
H	5.81501700	0.35604900	0.03617400
H	6.40119900	1.90959800	1.63726800
H	5.91086400	3.56097500	1.20665200
H	4.99797000	2.66952700	2.41462000
H	2.83791400	2.54430400	-0.72267600
H	2.75021700	2.83184400	1.01950100
H	3.69040500	3.91712800	0.00774100

**Table S3.** The cartesian coordinates and energies of the TSs of the reaction between **Neo** and **HOO\*** and **NO<sub>2</sub>** calculated at M06-2X/6-311++G(d,p) level.

Neo + HOO (RAF-W)				
Cartesian Coordinates				Frequency and Energy
C	5.22300100	-0.74220700	0.67451900	Zero-point Energy Correction = 0.351607 Hartree
C	5.35093100	0.35730800	-0.19365200	Thermal Correction to Energy = 0.375932 Hartree
C	4.24902600	0.87986700	-0.85216900	Thermal Correction to Enthalpy = 0.376876 Hartree
C	3.01178100	0.28853600	-0.63095500	Thermal Correction to Free Energy = 0.296031 Hartree
C	2.84582700	-0.80705500	0.21600000	
C	3.98600500	-1.30804500	0.86988600	EE + Zero-point Energy = -1224.2753 Hartree
O	1.95499100	0.83195500	-1.30726200	EE + Thermal Energy Correction = -1224.251 Hartree
C	0.71318600	0.39308400	-1.04671400	EE + Thermal Enthalpy Correction = -1224.2501 Hartree
C	0.43737500	-0.78545200	-0.34601200	
C	1.52590600	-1.41139900	0.40644300	EE + Thermal Free Energy Correction = -1224.3309 Hartree
O	6.59498100	0.87546800	-0.34649400	
O	1.35448300	-2.37128200	1.16204100	
C	-0.94300500	-1.26027000	-0.27724200	
C	-2.00812500	-0.34647100	-0.38931200	
C	-3.33444900	-0.74340700	-0.34956600	
C	-3.60154800	-2.11450500	-0.20809900	
C	-2.56887100	-3.04330800	-0.10724700	
C	-1.24834500	-2.62160500	-0.13177900	
C	-4.50078600	0.22552700	-0.41714100	
C	-4.12551200	1.66827300	-0.63853900	
C	-3.60929600	2.48324700	0.28662000	
C	-3.24003100	3.90595000	-0.03005500	
C	-3.30756000	2.05154500	1.69487200	
O	-4.91270000	-2.48805400	-0.17036000	
H	6.10558500	-1.12349100	1.17262500	
H	4.33685100	1.73065300	-1.51769800	
H	3.87099400	-2.15704900	1.53260000	
H	6.57810900	1.62692600	-0.95450800	
H	-1.80010400	0.71246800	-0.48281000	
H	-2.81006100	-4.09657800	-0.00890300	
H	-0.45635800	-3.35392000	-0.06274100	
H	-5.16956300	-0.10180800	-1.21757200	
H	-5.07640800	0.11577700	0.50867600	
H	-4.27307000	2.05933900	-1.64245200	
H	-3.46056200	4.15997600	-1.06800500	
H	-3.78069700	4.59796000	0.62340000	
H	-2.17230100	4.06886300	0.15145600	
H	-3.67077700	1.04888900	1.92195500	
H	-2.22423800	2.06669400	1.86024900	
H	-3.74632400	2.75386000	2.41037000	
H	-4.98081300	-3.44645600	-0.07006500	
H	0.00310300	0.81004900	-1.74677400	
O	0.18671100	1.64882700	0.39151600	

O	1.34030200	2.07632900	0.97582800	
H	1.44342100	1.52421400	1.76889600	
Neo + HOO (RAF-PE)				
Cartesian Coordinates				Frequency and Energy
C	5.25912500	-0.73728300	0.59070000	Zero-point Energy Correction = 0.352667 Hartree
C	5.35594700	0.41375800	-0.21139000	Thermal Correction to Energy = 0.376937 Hartree
C	4.23325600	0.95553000	-0.81737100	Thermal Correction to Enthalpy = 0.377881 Hartree
C	3.00553600	0.33502200	-0.61004300	Thermal Correction to Free Energy = 0.297298 Hartree
C	2.87460200	-0.81077800	0.17143500	
C	4.03312400	-1.33250200	0.77170200	EE + Zero-point Energy = -1224.2711 Hartree
O	1.93430400	0.89376000	-1.23615100	EE + Thermal Energy Correction = -1224.2468 Hartree
C	0.70326000	0.43505800	-0.96385900	EE + Thermal Enthalpy Correction = -1224.2459 Hartree
C	0.44691400	-0.78107200	-0.32339500	
C	1.56498500	-1.45861200	0.34915600	EE + Thermal Free Energy Correction = -1224.3264 Hartree
O	6.58485800	0.95587000	-0.35368400	
O	1.43673700	-2.47702900	1.01624800	
C	-0.93049000	-1.26505600	-0.24898800	
C	-2.00726400	-0.36091900	-0.34157800	
C	-3.32917500	-0.77244800	-0.31330100	
C	-3.58393100	-2.14810200	-0.18991000	
C	-2.54029500	-3.06408600	-0.09807000	
C	-1.22365500	-2.62997900	-0.11889600	
C	-4.50884000	0.18145900	-0.37011900	
C	-4.16816200	1.62057900	-0.65954800	
C	-3.66895000	2.49500100	0.21912900	
C	-3.36058800	3.91523500	-0.16851600	
C	-3.33229800	2.14097500	1.64137300	
O	-4.88561700	-2.53196800	-0.15790500	
H	6.15668800	-1.13400300	1.04839600	
H	4.28751800	1.84638300	-1.43301500	
H	3.93454800	-2.22350900	1.38021300	
H	6.54309600	1.73770200	-0.91775300	
H	-1.81299500	0.70297400	-0.40619000	
H	-2.76235200	-4.12295900	-0.00675800	
H	-0.42418300	-3.35251400	-0.04507500	
H	-5.20302500	-0.18523000	-1.13068700	
H	-5.05160700	0.09771000	0.57810300	
H	-4.34083700	1.96079200	-1.67813700	
H	-3.59633900	4.10998400	-1.21614100	
H	-3.93041700	4.61491100	0.45179000	
H	-2.30086900	4.13597200	-0.00221600	
H	-3.64878800	1.13503500	1.91832100	
H	-2.24816300	2.20394900	1.78821500	
H	-3.79057800	2.85507400	2.33305400	
H	-4.94217400	-3.49021800	-0.06429500	
H	-0.02410700	0.87730000	-1.62981500	
O	0.18907800	1.62720300	0.51724200	
O	1.34335100	2.02576100	1.12063000	
H	1.39426900	1.49120000	1.92988400	

Neo-8OH + HOO (FHT-W)				
Cartesian Coordinates				Frequency and Energy
C	4.70259400	-1.43059100	-0.41433700	Zero-point Energy Correction = 0.346097 Hartree
C	4.92591700	-0.27063900	0.38070400	Thermal Correction to Energy = 0.370475 Hartree
C	3.83390000	0.42483800	0.93435500	Thermal Correction to Enthalpy = 0.371419 Hartree
C	2.54998000	-0.04789100	0.69430400	Thermal Correction to Free Energy = 0.289083
C	2.31982500	-1.19290900	-0.06632900	Hartree
C	3.42669700	-1.87803400	-0.61797800	EE + Zero-point Energy = -1224.2663 Hartree
O	1.52528900	0.66181600	1.24427500	EE + Thermal Energy Correction = -1224.2419 Hartree
C	0.26485300	0.23860100	1.05067400	EE + Thermal Enthalpy Correction = -1224.241
C	-0.09589900	-0.84736600	0.33086800	Hartree
C	0.94362600	-1.65951300	-0.29868200	EE + Thermal Free Energy Correction = -1224.3233
O	6.15121300	0.15060800	0.60096300	Hartree
O	0.70740000	-2.65138400	-0.98631600	
C	-1.53020600	-1.18049800	0.17236000	
C	-2.45346600	-0.17964100	-0.15082400	
C	-3.81422200	-0.44046600	-0.27022500	
C	-4.24433300	-1.75656800	-0.05740900	
C	-3.34404900	-2.76937600	0.25622900	
C	-1.98964600	-2.48304500	0.36967300	
C	-4.84893300	0.62181100	-0.59345200	
C	-4.30041300	1.97528900	-0.96526500	
C	-3.80782000	2.87598900	-0.10986300	
C	-3.28071200	4.20409600	-0.57867400	
C	-3.69704000	2.63922900	1.37076500	
O	-5.58824400	-1.99991500	-0.17096600	
H	5.56130200	-1.93954000	-0.83414400	
H	3.99633000	1.30905700	1.54014900	
H	3.23565400	-2.76411700	-1.21090300	
H	-0.44599300	0.88309500	1.55428500	
H	-2.09721700	0.83063800	-0.32234900	
H	-3.71266500	-3.77746500	0.41584800	
H	-1.29643400	-3.27413400	0.62825100	
H	-5.47241800	0.25205900	-1.41162400	
H	-5.51919900	0.70433000	0.26981500	
H	-4.30370400	2.22292200	-2.02435600	
H	-3.38509600	4.32216600	-1.65855100	
H	-3.81150400	5.02365400	-0.08364800	
H	-2.22290000	4.30934100	-0.31594500	
H	-4.13729200	1.69316900	1.68722500	
H	-2.64152100	2.63955900	1.66631200	
H	-4.17889700	3.45232100	1.92301500	
H	-5.76556000	-2.93272000	0.00523400	
O	6.24515500	2.08295600	-0.73202900	
H	6.31559900	1.15005600	0.01772200	
O	4.96762000	2.03618900	-1.19151300	
H	4.45012800	2.59355600	-0.58302200	
Neo-14OH + HOO (FHT-W)				
Cartesian Coordinates				Frequency and Energy



C	-5.82441400	0.42602100	1.06238900	Zero-point Energy Correction = 0.3468 Hartree
C	-6.11366600	0.32768200	-0.31106300	Thermal Correction to Energy = 0.370926 Hartree
C	-5.11344100	0.08157300	-1.23692800	Thermal Correction to Enthalpy = 0.37187 Hartree
C	-3.81257400	-0.07121800	-0.76973300	Thermal Correction to Free Energy = 0.290591
C	-3.48841900	0.01493900	0.58397500	Hartree
C	-4.52937300	0.27174700	1.49392900	EE + Zero-point Energy = -1224.2757 Hartree
O	-2.85416800	-0.31418200	-1.71319200	EE + Thermal Energy Correction = -1224.2515 Hartree
C	-1.58248100	-0.48480500	-1.32429000	EE + Thermal Enthalpy Correction = -1224.2506
C	-1.14516700	-0.43092400	-0.04611600	Hartree
C	-2.10448900	-0.15367700	1.02698000	EE + Thermal Free Energy Correction = -1224.3319
O	-7.41071600	0.48475400	-0.67699800	Hartree
O	-1.77499700	-0.05013000	2.20922200	
C	0.28730500	-0.63920200	0.24401600	
C	1.26431900	-0.02384100	-0.54759000	
C	2.61813900	-0.22804700	-0.32189800	
C	3.00144800	-1.08633100	0.74489500	
C	2.01810600	-1.71675700	1.53563600	
C	0.68186900	-1.48527200	1.29903400	
C	3.67786600	0.45564600	-1.14620800	
C	4.40304700	1.51325000	-0.33933500	
C	3.96822100	2.75953000	-0.12730000	
C	4.74735500	3.72318800	0.72524500	
C	2.67819900	3.30638600	-0.67338500	
O	4.28852600	-1.29030200	1.01001000	
H	-6.63299100	0.61987100	1.75614400	
H	-5.32712700	0.00701400	-2.29685700	
H	-4.29049900	0.34282200	2.54819300	
H	-0.93737200	-0.69213600	-2.16940100	
H	-7.50628400	0.38168900	-1.63335400	
H	0.95976400	0.63810400	-1.35196400	
H	2.34367500	-2.37874800	2.32974100	
H	-0.07010300	-1.97334000	1.90581700	
H	4.39933600	-0.29175200	-1.48756900	
H	3.20749000	0.88835900	-2.03057500	
H	5.33408700	1.20395800	0.12865600	
H	5.65747400	3.27047000	1.12154800	
H	5.01982200	4.61224600	0.14764800	
H	4.13412300	4.06761500	1.56464800	
H	2.84011800	4.30264200	-1.09560300	
H	2.23405600	2.67271500	-1.44053100	
H	1.94891000	3.42080900	0.13630800	
H	4.70245500	-1.95435200	0.24179800	
O	4.82434500	-2.82952100	-0.71933200	
O	3.56308400	-2.86707300	-1.22052800	
H	3.10337300	-3.56568500	-0.72161800	
Neo-17CH + HOO (FHT-W)				
Cartesian Coordinates				Frequency and Energy
C	2.54697300	1.63315400	-0.18932500	Zero-point Energy Correction = 0.346595 Hartree
C	1.50939800	2.54974900	-0.33366400	Thermal Correction to Energy = 0.37023 Hartree

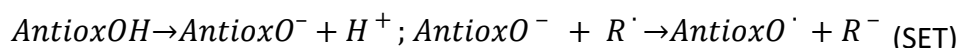
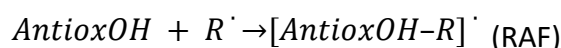
C	0.19116800	2.12821400	-0.23572300	Thermal Correction to Enthalpy = 0.371174 Hartree
C	-0.10886600	0.78513400	0.01726800	Thermal Correction to Free Energy = 0.292311
C	0.94416300	-0.12000300	0.14673700	Hartree
C	2.28003100	0.27293300	0.03282800	EE + Zero-point Energy = -1224.2763 Hartree
O	3.85822300	2.02162600	-0.21948000	EE + Thermal Energy Correction = -1224.2527 Hartree
C	3.37822200	-0.71770900	0.16746900	EE + Thermal Enthalpy Correction = -1224.2518
C	4.35864400	-0.80989200	-0.93963000	Hartree
C	5.33459200	-1.73087500	-1.02360300	EE + Thermal Free Energy Correction = -1224.3306
C	6.27324100	-1.76555800	-2.19411100	Hartree
C	5.58313800	-2.77704300	0.02318000	
H	-0.60754600	2.85294700	-0.33504700	
H	4.02750200	-0.33186400	1.13454300	
H	4.28573600	-0.06041300	-1.72353500	
H	6.20825100	-2.73275100	-2.70328100	
H	6.05505100	-0.97499800	-2.91310900	
H	7.30829200	-1.65805500	-1.85370000	
H	6.60239500	-2.67500400	0.40981800	
H	4.89273000	-2.71981200	0.86391700	
H	1.74457800	3.59475000	-0.50662000	
H	3.91897200	2.96488300	-0.42011800	
H	0.73026900	-1.17038100	0.31858100	
C	-1.51036300	0.33170900	0.17513100	
C	-2.55461800	0.73918400	-0.76776800	
C	-1.83387100	-0.49421000	1.19321400	
C	-3.88692800	0.20343900	-0.48209100	
O	-2.33426900	1.46515400	-1.73947400	
O	-3.05726000	-1.00037100	1.42714100	
H	-1.12340700	-0.83334700	1.93711700	
C	-4.08680300	-0.65496000	0.60029100	
C	-4.99702600	0.51382300	-1.28608700	
C	-5.32893200	-1.20088900	0.90020100	
C	-6.23902700	-0.00923800	-1.01214000	
H	-4.85718100	1.17926800	-2.12942500	
C	-6.40042000	-0.87264900	0.08716200	
H	-5.44845000	-1.86510300	1.74682500	
H	-7.09931900	0.23034400	-1.62749300	
O	-7.60659600	-1.41508100	0.39612000	
H	-8.27966300	-1.11685800	-0.22982900	
H	3.00552900	-1.68365900	0.51088000	
O	4.72225400	0.23718700	2.15121000	
O	3.95322900	1.28698600	2.57747900	
H	4.12046800	1.98600300	1.92070200	
H	5.51485300	-3.77583800	-0.42023200	
Neo-8OH + NO <sub>2</sub> (FHT-W)				
Cartesian Coordinates				Frequency and Energy
C	4.30997400	-0.57404300	0.15493300	Zero-point Energy Correction = 0.348828 Hartree
C	4.35253200	0.79942000	0.60823400	Thermal Correction to Energy = 0.373342 Hartree
C	3.11967600	1.46658800	0.90636600	Thermal Correction to Enthalpy = 0.374286 Hartree
C	1.92935800	0.78945800	0.74769700	Thermal Correction to Free Energy = 0.292485

C	1.90144900	-0.53995200	0.30256200	Hartree
C	3.11295000	-1.21268000	0.01032700	EE + Zero-point Energy = -1270.9883 Hartree
O	0.75000200	1.45961800	1.04356300	EE + Thermal Energy Correction = -1270.9638 Hartree
C	-0.45276400	0.80062900	0.86766100	EE + Thermal Enthalpy Correction = -1270.9628
C	-0.57724300	-0.46834200	0.41875500	Hartree
C	0.62197800	-1.25942900	0.12825500	EE + Thermal Free Energy Correction = -1271.0446
O	5.47715600	1.42582800	0.74389800	Hartree
O	0.60800300	-2.45086800	-0.24116400	
C	-1.92395800	-1.04747300	0.21913700	
C	-2.96977700	-0.22865300	-0.24266700	
C	-4.26578200	-0.70993100	-0.37721700	
C	-4.52348100	-2.05371400	-0.05803100	
C	-3.49245300	-2.88608200	0.37278500	
C	-2.19707500	-2.39048500	0.51170800	
C	-5.44087100	0.14557600	-0.83864000	
C	-5.05781800	1.53902600	-1.29153800	
C	-4.66734700	2.52523600	-0.47721200	
C	-4.28073300	3.89261800	-1.00186500	
C	-4.53050700	2.36694400	1.02260000	
O	-5.83706600	-2.47565200	-0.20698100	
H	5.25418900	-1.05774600	-0.05876500	
H	3.13401600	2.49244400	1.24769400	
H	3.04970300	-2.23923900	-0.32780300	
H	-1.28445000	1.43525500	1.14429300	
H	-2.77005600	0.80320200	-0.51189600	
H	-3.70586500	-3.92392100	0.60505600	
H	-1.40231200	-3.04340300	0.84307800	
H	-5.94656400	-0.38317300	-1.65397500	
H	-6.16039900	0.19406500	-0.00913300	
H	-5.09346200	1.72627900	-2.36255000	
H	-4.37300600	3.94379100	-2.09088900	
H	-4.92004800	4.66529000	-0.55632200	
H	-3.24455100	4.12651900	-0.72495500	
H	-5.04301900	3.18797800	1.53889200	
H	-4.93254000	1.41585600	1.38189900	
H	-3.46824300	2.41584400	1.30160500	
H	-5.93674300	-3.43537300	0.02728000	
O	7.48580700	-0.05350900	0.08030500	
H	6.67560200	0.54340100	0.34757900	
N	7.65702700	0.21878500	-1.32296000	
O	8.61108600	-0.42127100	-1.76755500	
Neo-14OH + NO <sub>2</sub> (FHT-W)				
Cartesian Coordinates				Frequency and Energy
C	-5.94904300	0.55499000	0.88996000	Zero-point Energy Correction = 0.343155 Hartree
C	-6.18622600	0.13249100	-0.43024600	Thermal Correction to Energy = 0.366935 Hartree
C	-5.14054800	-0.26923500	-1.24688100	Thermal Correction to Enthalpy = 0.367879 Hartree
C	-3.85180000	-0.24680800	-0.72344900	Thermal Correction to Free Energy = 0.287791
C	-3.58148900	0.16328100	0.57929200	Hartree
C	-4.66434800	0.56741600	1.37821600	EE + Zero-point Energy = -1278.4296 Hartree

O	-2.85468400	-0.65332900	-1.56177200	EE + Thermal Energy Correction = -1278.4058 Hartree
C	-1.59444300	-0.66017700	-1.12300900	EE + Thermal Enthalpy Correction = -1278.4049
C	-1.19433100	-0.28662400	0.11603400	Hartree
C	-2.20364300	0.17338100	1.09162200	EE + Thermal Free Energy Correction = -1278.485
O	-7.46867700	0.14057800	-0.84903300	Hartree
O	-1.92155900	0.54960100	2.21664900	
C	0.22952700	-0.36436800	0.46148300	
C	1.20897700	-0.02142600	-0.47921100	
C	2.55928100	-0.14834200	-0.20755100	
C	2.94601700	-0.69050300	1.07066100	
C	1.95447200	-0.97857300	2.04336200	
C	0.62974700	-0.81574100	1.74903900	
C	3.60776700	0.38306500	-1.14939600	
C	4.25652400	1.61642700	-0.55103300	
C	3.74120500	2.84957200	-0.56672400	
C	4.45270900	3.99762500	0.09438700	
C	2.42363800	3.20427400	-1.19817000	
O	4.20653300	-0.88283700	1.37737000	
H	-6.79052900	0.86166300	1.49886300	
H	-5.30306200	-0.59648000	-2.26788200	
H	-4.45960100	0.88849700	2.39267000	
H	-0.91505100	-1.03464900	-1.87984200	
H	-7.52927500	-0.17262800	-1.75980100	
H	0.90620400	0.39103800	-1.43602300	
H	2.28284800	-1.36024400	3.00246000	
H	-0.12512100	-1.06136700	2.48322900	
H	4.37610700	-0.36978200	-1.33496500	
H	3.13547600	0.60442600	-2.10792900	
H	5.19895800	1.45504300	-0.03548400	
H	5.37593900	3.67794900	0.57976100	
H	4.69246100	4.77383500	-0.63959100	
H	3.80558200	4.46156400	0.84637900	
H	2.50966400	4.14286300	-1.75337100	
H	2.05355600	2.43608700	-1.87673900	
H	1.66668700	3.36171000	-0.42125000	
H	4.63851600	-1.49150300	0.64958000	
O	4.71141700	-2.60469800	-0.30696700	
N	3.48441200	-2.78309500	-0.49551500	
O	3.10519500	-3.60565400	-1.28397000	

**Table S4.** The method to calculate rate constant following the conventional transition state theory.

The antiradical action of phenolic compounds is well recognized to be directed by three distinct processes; HAT, SET, and RAF <sup>1-5</sup>. A hydrogen atom is transferred from the antioxidant to the free radical in a one-step process known as HAT. The BDE of the active OH/CH bonds of the antioxidant may be used to describe this mechanism, which may occur in both polar and lipid environments <sup>6</sup>. RAF is a one-step process that leads to the product [antioxidant–free radical]• by combining free radicals with antioxidants <sup>7</sup>. The Gibbs free energy of the reaction could be used to describe this mechanism. Unlike HAT and RAF, the SET process, which involves an electron transfer, could only occur in polar environments <sup>8</sup>. In these media, the phenolic OH bonds of the antioxidant could exist in both protonated and deprotonated forms and therefore electron transfer can occur from the neutral or anionic state of the antioxidant. However, SET from an undissociated phenol is often an infeasible chemical route, thus it is only significant for deprotonated phenols. The Gibbs free energy of electron transfer may be used to describe this pathway (dominant step). The following equations describe the mentioned mechanisms.



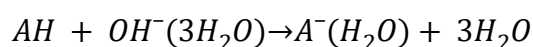
PA (proton affinity) and BDE (bond dissociation enthalpy) values were calculated as follows.

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

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

Where  $H(\text{ArOH})$ ,  $H(\text{ArO}^\cdot)$ ,  $H(\text{ArO}^-)$ ,  $H(\text{H}^\cdot)$ , and  $H(\text{H}^+)$  are enthalpies of the neutral molecule, radical, anion, hydrogen atom, and proton respectively.

The pKa values of CBDA were computed according to the literature using the following equation <sup>9</sup>:



$$\text{pK}_a = \frac{\Delta G_{sol}}{RT \ln(10)} + 14 + 3 \log_{10} [\text{H}_2\text{O}]$$

Where  $\Delta G_{sol}$  is the Gibbs free energy of the reaction in solution, R is the gas constant, and T is the temperature (298.15 K).

The kinetic calculations were carried out following the methodology of the quantum mechanics-based test for overall free radical scavenging activity (QM-ORSA)<sup>10, 11</sup>. The rate constant ( $k$ ) was calculated by using standard transition state theory (TST) and 1M standard state at 298.15 K according to the equation below:<sup>12-19</sup>

$$k = \sigma \kappa \frac{k_B T}{h} e^{-(\Delta G^\ddagger)/RT}$$

Where  $\sigma$  is the reaction symmetry number,<sup>20, 21</sup>  $\kappa$  represents tunneling corrections computed using the Eckart barrier,<sup>22</sup>  $k_B$  is the Boltzmann constant,  $h$  is the Planck constant,  $\Delta G^\ddagger$  is Gibbs free energy of activation.

The apparent rate constants ( $k_{app}$ , rate constants close to the diffusion limit) were corrected using the Collins–Kimball theory<sup>23</sup>. Branching ratios ( $\Gamma$ , %) were calculated as follows:

$$\Gamma_{path} = \frac{k}{k_{overall}} \times 100$$

Where  $k$  and  $k_{overall}$  are the rate constants of a specific reaction path and the sum of the rate constants of all reaction paths, respectively.

Marcus theory has been used to predict the Gibbs free energy of activation of the single electron transfer mechanism<sup>24</sup>:

$$\Delta G_{SET}^\ddagger = \frac{\lambda}{4} \left( 1 + \frac{\Delta G_{SET}^0}{\lambda} \right)^2$$

$$\lambda \approx \Delta E_{SET} + \Delta G_{SET}^0$$

Where  $\lambda$  is the nuclear reorganization energy,  $\Delta G_{SET}^0$  is the Gibbs free energy of reaction, and  $\Delta E_{SET}$  is the nonadiabatic energy difference between reactants and vertical products. The computational kinetic study was performed with Eyringpy software<sup>17</sup>.

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