

Supporting Information (SI)

7-O-Galloyltricetifavan: a promising natural radical scavenger

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Table S1. BDE and PA values (in Kcal/mol) of the X-H (X = O, C) bonds of the studied compounds in the gas phase at the M06-2X/6-31G+(d) levels of theory

Positions	BDE	PA
C2-H	86.6	
C3-H	101.7	
C4-H	89.0	
O5-H	84.7	334.4
O12-H	89.0	341.8
O13-H	81.7	327.6
O14-H	82.5	392.3
O3'-H	88.7	328.6
O4'-H	79.8	382.4
O5'-H	79.7	327.9

Table S2: The Cartesian coordinates and energies of TS of the reaction between compound 7OGT with HOO[•] following the FHT mechanism in studied solvents

Name				7OGT-C2-H-OOH (gas phase)
Cartesian Coordinates				Frequency and Energy
O	1.91737400	0.20382400	-0.30202300	Zero-point correction= 0.389848 (Hartree/Particle)
O	0.01708200	4.63099000	-0.64932400	Thermal correction to Energy= 0.420446
O	-2.77186500	0.83035600	-0.57994700	Thermal correction to Enthalpy= 0.421390
O	4.51804400	-3.87851700	-1.18071600	Thermal correction to Gibbs Free Energy= 0.327338
O	7.76663600	-1.00256100	0.63228100	Sum of electronic and zero-point Energies= -1751.779427
O	7.04477900	-3.40632400	-0.34259500	Sum of electronic and thermal Energies= -1751.748829
O	-2.62227200	0.00352600	1.51988900	Sum of electronic and thermal Enthalpies= -1751.747885
O	-7.21732900	-0.51404800	-2.28957200	Sum of electronic and thermal Free Energies= -1751.841936
O	-7.21909500	-2.24871100	2.08302900	
O	-8.42872600	-1.85628200	-0.28178600	
C	3.19546000	0.70090700	-0.07340700	
C	3.48766000	1.96802600	-0.85874400	
C	2.46199300	3.05135200	-0.52643400	
C	1.07192800	2.46753300	-0.52087900	
C	0.87375100	1.08713800	-0.42252800	
C	4.20430600	-0.39055500	-0.15567900	
C	-0.07142000	3.27323600	-0.58485900	
C	-0.39157100	0.50918800	-0.42926700	
C	5.50974900	-0.12575000	0.28476800	
C	3.86594600	-1.65555600	-0.63801000	
C	-1.48636600	1.35468000	-0.51654800	
C	-1.35522200	2.73177200	-0.59191700	
C	4.83675800	-2.65126300	-0.69913000	
C	6.46363900	-1.13074300	0.22653700	
C	6.13518400	-2.39126000	-0.26646700	
C	-3.24688200	0.15378800	0.49971500	
C	-4.61989500	-0.36329800	0.26367200	
C	-5.22547900	-1.05413700	1.31851200	
C	-5.27791200	-0.17476100	-0.95214400	
C	-6.56115600	-0.68523900	-1.11525300	
C	-6.50449700	-1.55594900	1.14134000	
C	-7.17293500	-1.37532300	-0.06893600	
H	3.22235100	1.06655900	1.15466700	
H	3.44564900	1.71292600	-1.92745500	
H	4.50173500	2.31103700	-0.63930100	
H	2.54124400	3.85107400	-1.27492300	
H	2.69132900	3.48414000	0.45754200	
H	-0.50281700	-0.56513900	-0.34087200	
H	5.76784300	0.84623200	0.70069300	
H	2.85897500	-1.87554100	-0.97227600	
H	-2.22442400	3.37716000	-0.64300000	
H	0.92628300	4.91749900	-0.48400800	
H	5.30642000	-4.44450000	-1.13985900	
H	7.92248700	-0.12448900	1.00700900	
H	7.89401100	-3.09691300	0.01229300	
H	-4.68655800	-1.18428500	2.25298500	
H	-4.80911800	0.35889100	-1.77044500	
H	-8.09097600	-0.93382400	-2.22591300	
H	-6.70558300	-2.34334700	2.89743900	
H	-8.73357300	-2.31174000	0.52029900	

H	1.39242100	1.48736400	2.77035400	
O	3.22018000	1.45121300	2.36109200	
O	2.04070200	2.16205600	2.49951200	
Name				7OGT-O5-H-OOH (gas phase)
Cartesian Coordinates				Frequency and Energy
O	-2.13784200	-0.09767300	-0.27266500	Zero-point correction= 0.389788 (Hartree/Particle)
O	-0.03199800	4.19950300	-0.29730800	Thermal correction to Energy= 0.419971
O	2.53415800	0.20038700	0.13666700	Thermal correction to Enthalpy= 0.420915
O	-5.52362300	-2.91408900	2.09466200	Thermal correction to Gibbs Free Energy= 0.327625
O	-7.64742400	-1.70332800	-1.92353300	Sum of electronic and zero-point Energies= -1751.784758
O	-7.57844500	-3.14601300	0.35513400	Sum of electronic and thermal Energies= -1751.754575
O	3.46352200	1.11925800	-1.71031100	Sum of electronic and thermal Enthalpies= -1751.753631
O	6.02565900	-2.67239000	2.15637800	Sum of electronic and thermal Free Energies= -1751.846921
O	8.15496500	-0.99803600	-1.68945400	
O	8.17460900	-2.51369000	0.52675600	
C	-3.37295700	0.48225200	-0.70298200	
C	-3.61046000	1.80377700	0.02611700	
C	-2.50872000	2.79919600	-0.32901800	
C	-1.16908900	2.12084300	-0.27157700	
C	-1.06037000	0.73227900	-0.22611800	
C	-4.46640300	-0.52468200	-0.45230200	
C	0.03130500	2.88587500	-0.22106900	
C	0.18605300	0.10622700	-0.11320500	
C	-5.51519500	-0.63313900	-1.36852800	
C	-4.46665800	-1.28709700	0.71402800	
C	1.34123600	0.88279100	-0.04787900	
C	1.29366600	2.26189900	-0.09362600	
C	-5.51982300	-2.16202600	0.96569500	
C	-6.56601800	-1.50512500	-1.10326100	
C	-6.57267300	-2.26877100	0.05805600	
C	3.55151000	0.39763000	-0.75010500	
C	4.75768600	-0.38721200	-0.38450400	
C	5.85752500	-0.28660000	-1.24323800	
C	4.80103600	-1.18525400	0.75943500	
C	5.96274200	-1.89280700	1.04894600	
C	7.00677800	-0.99898200	-0.94295900	
C	7.06376900	-1.79980700	0.19769700	
H	-3.29367900	0.67593200	-1.78449900	
H	-3.61435300	1.60221900	1.10467000	
H	-4.59725300	2.19378500	-0.24159400	
H	-2.51992700	3.65093900	0.35889700	
H	-2.66743900	3.21259700	-1.33437300	
H	0.24580000	-0.97631500	-0.07820300	
H	-5.51277000	-0.04702700	-2.28568500	
H	-3.64980900	-1.22356400	1.42518500	
H	2.18692400	2.87470900	-0.06762500	
H	-0.44253800	4.61452700	0.68026500	
H	-6.32407400	-3.46450000	2.09941300	
H	-7.57480000	-1.15820200	-2.71900700	
H	-8.23277400	-3.12921500	-0.36174800	
H	5.79178500	0.34428000	-2.12525800	
H	3.95069600	-1.26506700	1.42606900	
H	6.90150900	-3.09038700	2.19792500	
H	8.05634300	-0.42881900	-2.46563600	

H	8.86063300	-2.36183600	-0.14423300	
H	-0.01941500	3.27689600	2.73649800	
O	-0.77175800	4.75216800	1.88111300	
O	-0.87363700	3.45533500	2.30022600	
Name				7OGT-012-H-OOH (gas phase)
Cartesian Coordinates				Frequency and Energy
O	-2.63384100	0.35212300	0.04552800	Zero-point correction= 0.390224 (Hartree/Particle)
O	-0.71067300	4.77242400	-0.23361300	Thermal correction to Energy= 0.420361
O	2.04362500	1.02996400	0.51595400	Thermal correction to Enthalpy= 0.421306
O	-6.05108500	-2.46399800	2.38168500	Thermal correction to Gibbs Free Energy= 0.327664
O	-7.89761100	-1.70074900	-1.87616400	Sum of electronic and zero-point Energies= -1751.784413
O	-7.94121500	-2.95172300	0.51342300	Sum of electronic and thermal Energies= -1751.754276
O	2.00501200	-0.34052900	-1.28583100	Sum of electronic and thermal Enthalpies= -1751.753332
O	6.43731500	0.44647800	2.68523800	Sum of electronic and thermal Free Energies= -1751.846973
O	6.53163300	-2.67879100	-0.85595100	
O	7.71118600	-1.49446800	1.26069000	
C	-3.85986500	0.82507500	-0.50710900	
C	-4.22234800	2.16758000	0.12465300	
C	-3.15627200	3.20649900	-0.22271700	
C	-1.77378800	2.61153200	-0.08950200	
C	-1.59026100	1.23014200	0.05878100	
C	-4.91540000	-0.22376800	-0.26484700	
C	-0.62919200	3.42054100	-0.07762200	
C	-0.32760500	0.66862300	0.24674700	
C	-5.87794000	-0.46510200	-1.24765500	
C	-4.97071300	-0.89163400	0.95703200	
C	0.76419600	1.51962900	0.26505600	
C	0.64521200	2.89171400	0.10105600	
C	-5.99384900	-1.80413300	1.19818600	
C	-6.89939600	-1.37486500	-0.99366100	
C	-6.96182900	-2.04316200	0.22341600	
C	2.56705800	0.09389400	-0.31387700	
C	3.93101400	-0.32057200	0.12377600	
C	4.55869100	-1.31512800	-0.60890900	
C	4.55834500	0.27241100	1.23926300	
C	5.82895900	-0.12768800	1.61958200	
C	5.85091100	-1.73308800	-0.23220300	
C	6.47777600	-1.12435600	0.88336400	
H	-3.71726300	0.96016500	-1.59142100	
H	-4.28143100	2.02225600	1.21007600	
H	-5.21001200	2.48553700	-0.22284200	
H	-3.26828700	4.06940100	0.44847800	
H	-3.32059900	3.57322900	-1.24698300	
H	-0.22362600	-0.40471400	0.34814100	
H	-5.83008300	0.04508200	-2.20790600	
H	-4.21640200	-0.72775600	1.71957700	
H	1.51409000	3.53913300	0.11414800	
H	-1.62706300	5.04043000	-0.38818800	
H	-6.81568100	-3.06312800	2.36798900	
H	-7.77488400	-1.23582600	-2.71520400	
H	-8.52779100	-3.03893700	-0.25516000	
H	4.06479600	-1.77918200	-1.45718000	
H	4.05648400	1.04611900	1.80924300	
H	7.31977400	0.05668300	2.79772700	

H	7.00651800	-2.22297600	-1.78937500	
H	8.00765700	-2.19995600	0.65335200	
H	6.28943000	0.05827900	-2.43692900	
O	7.43560300	-1.39961200	-2.62578300	
O	7.13656900	-0.21220700	-2.03197500	
Name				7OGT-013-H-OOH (gas phase)
Cartesian Coordinates				Frequency and Energy
O	-2.73452700	0.33991400	0.04319300	Zero-point correction= 0.391140 (Hartree/Particle)
O	-0.82454400	4.77275400	-0.09127000	Thermal correction to Energy= 0.420909
O	1.94790200	1.00571900	0.45938700	Thermal correction to Enthalpy= 0.421853
O	-6.10144200	-2.59384200	2.30125000	Thermal correction to Gibbs Free Energy= 0.329412
O	-8.03974100	-1.62188600	-1.87247800	Sum of electronic and zero-point Energies= -1751.783361
O	-8.03319000	-2.98822600	0.45368100	Sum of electronic and thermal Energies= -1751.753592
O	1.90086600	-0.19590600	-1.45772100	Sum of electronic and thermal Enthalpies= -1751.752647
O	6.35264600	0.05592700	2.52138500	Sum of electronic and thermal Free Energies= -1751.845089
O	6.48224100	-2.41825000	-1.50283000	
O	7.56766100	-1.68778800	0.91123100	
C	-3.96943000	0.83188700	-0.47172400	
C	-4.32481400	2.14695300	0.21898800	
C	-3.26611700	3.20160100	-0.10256500	
C	-1.88061000	2.60519600	-0.01500400	
C	-1.69249700	1.21945800	0.07540100	
C	-5.01992000	-0.22801000	-0.25697800	
C	-0.73764800	3.41638300	0.01009500	
C	-0.42571600	0.65493000	0.22075200	
C	-6.00430100	-0.42041900	-1.22908200	
C	-5.04959300	-0.95468700	0.93167000	
C	0.66395300	1.50783200	0.25423600	
C	0.54095300	2.88457900	0.14652800	
C	-6.06903900	-1.87712200	1.15037600	
C	-7.02168900	-1.34051300	-0.99736200	
C	-7.05869900	-2.06741100	0.18673400	
C	2.46844400	0.15524700	-0.45512000	
C	3.84108900	-0.29260700	-0.07220200	
C	4.48454300	-1.15805500	-0.96833200	
C	4.45002600	0.13807100	1.10664200	
C	5.72886700	-0.31820900	1.39729000	
C	5.75472000	-1.61369200	-0.67339500	
C	6.40221700	-1.22188600	0.52727400	
H	-3.84301900	1.01106700	-1.55166500	
H	-4.36716400	1.95788000	1.29843500	
H	-5.31820400	2.47620800	-0.10051600	
H	-3.36914900	4.03643800	0.60453500	
H	-3.44684800	3.60892400	-1.10858100	
H	-0.31659500	-0.42124700	0.27930300	
H	-5.97673300	0.13625300	-2.16399600	
H	-4.27892700	-0.82808300	1.68487500	
H	1.40910200	3.53267300	0.16927400	
H	-1.74381400	5.04473700	-0.21956100	
H	-6.86884900	-3.18902200	2.27660500	
H	-7.93674700	-1.11354800	-2.68867500	
H	-8.64016700	-3.03318600	-0.30258400	
H	3.97275000	-1.44536300	-1.88273900	
H	3.94755400	0.81355900	1.78832000	

H	7.22407800	-0.38452500	2.53305700	
H	5.91304500	-2.77099300	-2.20365600	
H	8.40915900	-1.39125200	0.17391000	
H	7.81373400	-0.94284900	-1.96374200	
O	9.10652500	-0.80507000	-0.63845600	
O	8.19164600	-0.20269800	-1.44336300	
Name				7OGT-O3'-H-OOH (gas phase)
Cartesian Coordinates				Frequency and Energy
O	-1.51367900	0.32536900	-0.00107500	Zero-point correction= 0.390367 (Hartree/Particle)
O	0.42923400	4.74713900	-0.02861300	Thermal correction to Energy= 0.420469
O	3.18955700	0.95006400	0.26495700	Thermal correction to Enthalpy= 0.421413
O	-4.62502700	-2.79593600	2.25409600	Thermal correction to Gibbs Free Energy= 0.328014
O	-6.94381500	-1.44519100	-1.63541900	Sum of electronic and zero-point Energies= -1751.786415
O	-6.73735800	-3.02411900	0.55497400	Sum of electronic and thermal Energies= -1751.756313
O	3.01917800	-0.31342800	-1.60465400	Sum of electronic and thermal Enthalpies= -1751.755369
O	7.67684500	0.02415100	2.14962900	Sum of electronic and thermal Free Energies= -1751.848769
O	7.59732200	-2.65293600	-1.71809400	
O	8.85299500	-1.73801600	0.47269600	
C	-2.76036800	0.84517800	-0.44624500	
C	-3.08026000	2.13569800	0.30764900	
C	-2.02530800	3.19379800	-0.01487100	
C	-0.64256800	2.58525300	-0.00253100	
C	-0.45980900	1.19683800	0.02337000	
C	-3.80904500	-0.21700400	-0.22533000	
C	0.50759300	3.38661100	0.01236200	
C	0.80438700	0.61622500	0.09632500	
C	-4.87438100	-0.32390700	-1.10122800	
C	-3.72604200	-1.05283100	0.90946200	
C	1.90478200	1.45809100	0.12444200	
C	1.78466700	2.83951400	0.07859500	
C	-4.70761000	-1.99445800	1.16538800	
C	-5.88837500	-1.27326700	-0.85264100	
C	-5.79438700	-2.10553200	0.28690800	
C	3.65324800	0.05592000	-0.64865200	
C	5.03122100	-0.39667900	-0.32300700	
C	5.61826900	-1.30925400	-1.20588700	
C	5.71141700	0.05855600	0.80704400	
C	6.99840200	-0.40593700	1.05684900	
C	6.90060200	-1.76258600	-0.94405100	
C	7.59175500	-1.31546800	0.18157300	
H	-2.68308300	1.06272800	-1.52312300	
H	-3.08365500	1.90814200	1.38085600	
H	-4.08033100	2.48674300	0.03377400	
H	-2.09527300	4.00221100	0.72586700	
H	-2.24281100	3.63845900	-0.99738300	
H	0.90511200	-0.46203000	0.10270900	
H	-4.95138600	0.29112500	-1.99403800	
H	-2.87849200	-0.97791100	1.58322300	
H	2.65858200	3.48006500	0.09446000	
H	-0.48907600	5.03205200	-0.13233400	
H	-5.39644200	-3.38598200	2.27408700	
H	-7.72690200	-0.70369400	-1.32896100	
H	-7.40828600	-2.97705400	-0.15284000	
H	5.06124700	-1.64448400	-2.07632700	

H	5.25813800	0.76440000	1.49284300	
H	8.55077700	-0.39950900	2.16362900	
H	7.06873900	-2.92581100	-2.48113100	
H	9.14329500	-2.36401300	-0.21110800	
H	-7.06429700	0.88810700	0.46611100	
O	-8.37942900	0.15833300	-0.63617300	
O	-7.68769900	0.13930600	0.53599400	
Name				7OGT-O4'-H-OOH (gas phase)
Cartesian Coordinates				Frequency and Energy
O	-1.57705700	0.76233300	0.11085600	ero-point correction= 0.391337 (Hartree/Particle)
O	0.69975100	4.98547100	-0.38408600	Thermal correction to Energy= 0.422407
O	3.15347300	1.01823200	0.24342700	Thermal correction to Enthalpy= 0.423351
O	-4.90087000	-1.98256200	2.53403700	Thermal correction to Gibbs Free Energy= 0.326203
O	-7.26416900	-0.48409900	-1.24375500	Sum of electronic and zero-point Energies= -1751.786444
O	-7.09937100	-1.98447500	1.00828700	Sum of electronic and thermal Energies= -1751.755374
O	2.88008700	-0.24620800	-1.60393400	Sum of electronic and thermal Enthalpies= -1751.754430
O	7.49380000	-0.34007200	2.19778500	Sum of electronic and thermal Free Energies= -1751.851579
O	7.19333500	-3.02382700	-1.64976900	
O	8.50544600	-2.22847900	0.55368100	
C	-2.78770400	1.33757400	-0.36071500	
C	-2.98781900	2.71560500	0.26743700	
C	-1.86260100	3.64491500	-0.18218500	
C	-0.53263500	2.93173200	-0.12722800	
C	-0.46037700	1.54485300	0.03637600	
C	-3.91730100	0.40062700	-0.01993700	
C	0.67446700	3.63560400	-0.20835500	
C	0.75459500	0.87874600	0.15084300	
C	-5.05031600	0.39796300	-0.83927400	
C	-3.85056500	-0.38843500	1.12633100	
C	1.91507300	1.62602700	0.07924500	
C	1.90353800	2.99791400	-0.10453800	
C	-4.93143200	-1.19298000	1.44926200	
C	-6.13744200	-0.39788400	-0.51470300	
C	-6.09774900	-1.20781800	0.64518000	
C	3.53669200	0.07205500	-0.65323800	
C	4.86062100	-0.50819600	-0.30770400	
C	5.36282900	-1.48131300	-1.17361700	
C	5.56640100	-0.11779900	0.82700700	
C	6.79304200	-0.70845900	1.09966600	
C	6.58496700	-2.06177000	-0.89076500	
C	7.30118200	-1.68084200	0.24143500	
H	-2.71745400	1.44291700	-1.45274500	
H	-2.97614400	2.59005800	1.35421800	
H	-3.96455200	3.11235600	-0.01514500	
H	-1.84636300	4.52687500	0.46813400	
H	-2.06503000	3.99870100	-1.20144200	
H	0.77237000	-0.19574100	0.26709400	
H	-5.07620300	1.00608100	-1.73869500	
H	-2.96540000	-0.39536400	1.74803000	
H	2.82343700	3.56286000	-0.16542800	
H	-0.18962800	5.32192500	-0.51896300	
H	-5.75847200	-2.43018200	2.58898100	
H	-7.15685600	-0.02027300	-2.07895400	
H	-7.24937100	-2.75833800	0.24190400	

H	4.78792800	-1.76454100	-2.04816700	
H	5.17798400	0.63394100	1.50021300	
H	8.31489600	-0.84525200	2.22725200	
H	6.65781400	-3.23364700	-2.41944400	
H	8.74036800	-2.87784400	-0.11983400	
H	-5.12675300	-3.66657800	-0.93775200	
O	-6.95994300	-3.67091000	-0.63475900	
O	-5.87540200	-3.13498900	-1.24957000	
Name				7OGT-O4'-H-OOH (pentyl ethanoate)
Cartesian Coordinates				Frequency and Energy
O	-1.61303500	0.70173900	0.09894100	Zero-point correction= 0.390161 (Hartree/Particle)
O	0.75078400	4.89743300	-0.12285100	Thermal correction to Energy= 0.421220
O	3.09630900	0.83429600	0.42190500	Thermal correction to Enthalpy= 0.422164
O	-5.03543400	-1.99809300	2.45360000	Thermal correction to Gibbs Free Energy= 0.325158
O	-7.28924800	-0.41690000	-1.36442300	Sum of electronic and zero-point Energies= -1751.834764
O	-7.20876600	-1.94616500	0.87455200	Sum of electronic and thermal Energies= -1751.803705
O	3.23058300	0.38445100	-1.77807500	Sum of electronic and thermal Enthalpies= -1751.802761
O	7.11385300	-1.13938400	2.50610500	Sum of electronic and thermal Free Energies= -1751.899767
O	7.59651800	-2.32972800	-2.01497800	
O	8.48060600	-2.35861500	0.52042400	
C	-2.81417000	1.32571600	-0.35532000	
C	-2.99292000	2.67712800	0.32989100	
C	-1.84256000	3.60061900	-0.06043100	
C	-0.52725100	2.86134500	0.00304500	
C	-0.48622000	1.46681400	0.10274900	
C	-3.96132200	0.39549400	-0.05731900	
C	0.69563600	3.54496900	-0.00465200	
C	0.71595600	0.77339600	0.22926900	
C	-5.07197000	0.41697200	-0.90462800	
C	-3.93343300	-0.40854100	1.08308900	
C	1.88839200	1.50276500	0.23818800	
C	1.91117000	2.88090600	0.11557900	
C	-5.03089500	-1.20190100	1.37136300	
C	-6.17826500	-0.36546600	-0.61106900	
C	-6.17654300	-1.19078400	0.53895400	
C	3.68943500	0.29724300	-0.67173900	
C	4.95669600	-0.39829700	-0.32920900	
C	5.64497300	-1.02069400	-1.37284000	
C	5.44205700	-0.43263600	0.97644000	
C	6.63128500	-1.09756700	1.24145000	
C	6.82858500	-1.68171000	-1.09511200	
C	7.32494000	-1.72238600	0.20695000	
H	-2.73533100	1.47326400	-1.44018800	
H	-3.00597200	2.51015500	1.41135600	
H	-3.95295200	3.10863000	0.04199100	
H	-1.82947700	4.45674000	0.62296800	
H	-2.00994600	3.99405000	-1.07027600	
H	0.71971900	-0.30606600	0.30853000	
H	-5.07005000	1.03633700	-1.79679700	
H	-3.06748800	-0.42724000	1.73217600	
H	2.84312100	3.43123500	0.11414200	
H	-0.13393300	5.26341200	-0.23110100	
H	-5.89732900	-2.44009300	2.49346200	

H	-7.16905500	0.10548600	-2.16682600	
H	-7.33304700	-2.72570600	0.12923300	
H	5.25443400	-0.98240300	-2.38342300	
H	4.91329300	0.04830200	1.78849900	
H	7.94094100	-1.63830200	2.51416400	
H	7.20121400	-2.26894500	-2.89251900	
H	8.86027000	-2.75176500	-0.27668300	
H	-5.18239100	-3.67303700	-0.93735100	
O	-7.03600000	-3.66559600	-0.75269800	
O	-5.91460600	-3.15773400	-1.31866000	
Name				7OGT-O4'-H-OOH (water)
Cartesian Coordinates				Frequency and Energy
O	-1.57705700	0.76233300	0.11085600	Zero-point correction= 0.385525 (Hartree/Particle)
O	0.69975100	4.98547100	-0.38408600	Thermal correction to Energy= 0.413139
O	3.15347300	1.01823200	0.24342700	Thermal correction to Enthalpy= 0.414083
O	-4.90087000	-1.98256200	2.53403700	Thermal correction to Gibbs Free Energy= 0.326445
O	-7.26416900	-0.48409900	-1.24375500	Sum of electronic and zero-point Energies= -1751.853748
O	-7.09937100	-1.98447500	1.00828700	Sum of electronic and thermal Energies= -1751.826134
O	2.88008700	-0.24620800	-1.60393400	Sum of electronic and thermal Enthalpies= -1751.825189
O	7.49380000	-0.34007200	2.19778500	Sum of electronic and thermal Free Energies= -1751.912827
O	7.19333500	-3.02382700	-1.64976900	
O	8.50544600	-2.22847900	0.55368100	
C	-2.78770400	1.33757400	-0.36071500	
C	-2.98781900	2.71560500	0.26743700	
C	-1.86260100	3.64491500	-0.18218500	
C	-0.53263500	2.93173200	-0.12722800	
C	-0.46037700	1.54485300	0.03637600	
C	-3.91730100	0.40062700	-0.01993700	
C	0.67446700	3.63560400	-0.20835500	
C	0.75459500	0.87874600	0.15084300	
C	-5.05031600	0.39796300	-0.83927400	
C	-3.85056500	-0.38843500	1.12633100	
C	1.91507300	1.62602700	0.07924500	
C	1.90353800	2.99791400	-0.10453800	
C	-4.93143200	-1.19298000	1.44926200	
C	-6.13744200	-0.39788400	-0.51470300	
C	-6.09774900	-1.20781800	0.64518000	
C	3.53669200	0.07205500	-0.65323800	
C	4.86062100	-0.50819600	-0.30770400	
C	5.36282900	-1.48131300	-1.17361700	
C	5.56640100	-0.11779900	0.82700700	
C	6.79304200	-0.70845900	1.09966600	
C	6.58496700	-2.06177000	-0.89076500	
C	7.30118200	-1.68084200	0.24143500	
H	-2.71745400	1.44291700	-1.45274500	
H	-2.97614400	2.59005800	1.35421800	
H	-3.96455200	3.11235600	-0.01514500	
H	-1.84636300	4.52687500	0.46813400	
H	-2.06503000	3.99870100	-1.20144200	
H	0.77237000	-0.19574100	0.26709400	
H	-5.07620300	1.00608100	-1.73869500	
H	-2.96540000	-0.39536400	1.74803000	
H	2.82343700	3.56286000	-0.16542800	
H	-0.18962800	5.32192500	-0.51896300	

H	-5.75847200	-2.43018200	2.58898100	
H	-7.15685600	-0.02027300	-2.07895400	
H	-7.24937100	-2.75833800	0.24190400	
H	4.78792800	-1.76454100	-2.04816700	
H	5.17798400	0.63394100	1.50021300	
H	8.31489600	-0.84525200	2.22725200	
H	6.65781400	-3.23364700	-2.41944400	
H	8.74036800	-2.87784400	-0.11983400	
H	-5.12675300	-3.66657800	-0.93775200	
O	-6.95994300	-3.67091000	-0.63475900	
O	-5.87540200	-3.13498900	-1.24957000	

Table S3. The method to calculate rate constant following the conventional transition state theory

The rate constant (k) was calculated by using the conventional transition state theory (TST) (at 298.15 K, 1M standard state) according to the equation (1):[1-5]

$$k = \sigma \kappa \frac{k_B T}{h} e^{-(\Delta G^\ddagger)/RT} \quad (1)$$

Where: σ is the reaction symmetry number ,[6,7]

κ contains the tunneling corrections calculated using the Eckart barrier,[8]

k_B is the Boltzmann constant,

h is the Planck constant,

$\Delta G^\ddagger$ is the Gibbs free energy of activation.

The Marcus Theory was used to estimate the reaction barriers of SET reactions.[9-12] The free energy of reaction $\Delta G^\ddagger$ for the SET pathway was computed following the equations (2,3).

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

$$\lambda \approx \Delta E_{\text{SET}} - \Delta G_{\text{SET}}^0 \quad (3)$$

where ΔG_{SET} is the Gibbs energy of reaction, ΔE_{SET} is the non-adiabatic energy difference between reactants and vertical products for SET.[13,14]

For rate constants that were close to the diffusion limit a correction was applied to yield realistic results[15]. The apparent rate constants (k_{app}) were calculated following the Collins–Kimball theory in the solvents at 298.15K;[16] the steady-state Smoluchowski rate constant (k_D) for an irreversible bimolecular diffusion–controlled reaction was calculated following the literature as corroding to equations (4,5).[15,17]

$$k_{\text{app}} = \frac{k_{\text{TST}} k_D}{k_{\text{TST}} + k_D} \quad (4)$$

$$k_D = 4\pi R_{AB} D_{AB} N_A \quad (5)$$

where R_{AB} is the reaction distance, N_A is the Avogadro constant, and $D_{AB} = D_A + D_B$ (D_{AB} is the mutual diffusion coefficient of the reactants A and B), [16,18] where D_A or D_B is estimated using the Stokes–Einstein formulation (6). [19,20]

$$D_{A \text{ or } B} = \frac{k_B T}{6\pi\eta a_{A \text{ or } B}} \quad (6)$$

η is the viscosity of the solvents (i.e. $\eta(\text{H}_2\text{O}) = 8.91 \times 10^{-4} \text{ Pa s}$, $\eta(\text{pentyl ethanoate}) = 8.62 \times 10^{-4} \text{ Pa s}$) and a is the radius of the solute.

The kinetic study requires different considerations. In this study, the solvent effects of water and pentyl ethanoate were modelled by the solvation model density (SMD) method [21,22]. Water (dielectric constants, $\epsilon = 78.35$) and pentyl ethanoate ($\epsilon = 4.73$) are the *de facto* standard solvents in the literature to mimic the polar and nonpolar environments in the human body [15,23–25]. Thus, these solvents were used to model the physiological environments. The solvent cage effects were included following the corrections proposed by Okuno, [26] adjusted with the free volume theory according to the Benson correction [15,27–29] to reduce over-penalizing entropy losses in solution. For the species that have multiple conformers, all of these were investigated and the conformer with the lowest electronic energy was included in the analysis. [24,25] The hindered internal rotation treatment was also applied to the single bonds to ensure that the obtained conformer has the lowest electronic energy [25,30]. All transition states were characterized by the existence of only one single imaginary frequency. Intrinsic coordinate calculations (IRCs) were performed to ensure that each transition state is connected correctly with the pre-complex and post-complex.

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