

Antioxidant activity of fraxetin and its regeneration in aqueous media. A density functional theory study

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Electronic supplementary information (ESI)

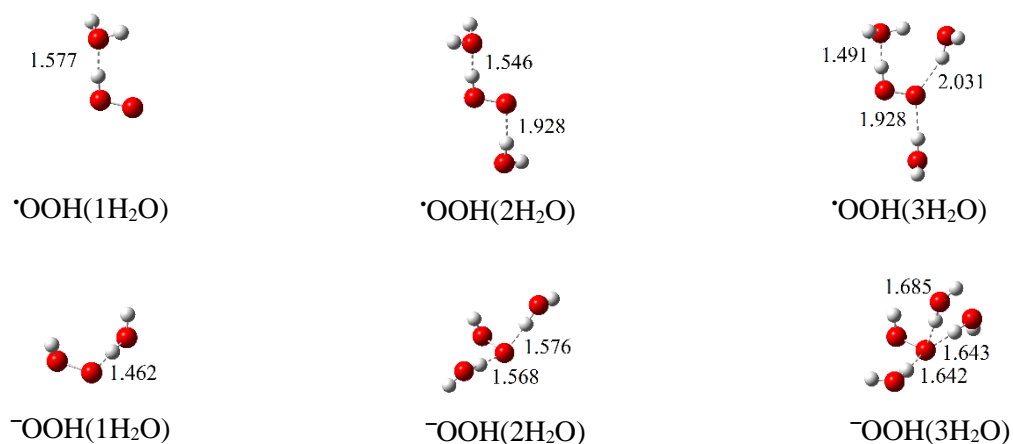


Figure A1. Geometries of complex between the $\cdot\text{OOH}$ y ^-OOH solvated with explicit water molecules.

Transition states geometries calculated in lipid				
	H	-3.24593681	0.01170280	1.91674607
	C	-2.24672557	-0.01790932	-0.01668995
TS-7(R=OOH)	C	-3.41687124	-0.09371512	-0.79521201
Freq= -2420.2275	H	-4.37169280	-0.12867167	-0.29316420
H= -912.862941	C	-3.31564124	-0.13615256	-2.16647574
G= -912.922750	O	-4.35155040	-0.26162107	-3.02647826
S2=0.773449	C	-5.67603435	-0.12658627	-2.49110441
S2A=0.75043	H	-6.34250297	-0.16628875	-3.34619457
0 2	H	-5.77720936	0.83191288	-1.98366636
	H	-5.89972204	-0.94652766	-1.80878624
	C	-2.03347035	-0.08146976	-2.79035943
O	O	-1.87427598	-0.01296454	-4.09136186
C	H	-2.27117201	-0.92980863	-4.60507119
O	C	-0.86846155	-0.03322219	-1.99609630
C	O	0.33075586	0.00933033	-2.58200591
H	H	0.18884541	-0.00962382	-3.54052274
C		-2.28407468	0.02917348	1.42132706

C -0.98771313 0.00481502 -0.61428301
O -2.59448818 -2.10724629 -4.89539599
O -2.96350384 -2.62583878 -3.69953725
H -3.80190584 -2.17683522 -3.49195510

TS-7(R=OOCH3)

Freq= -2104.6514

H= -952.141623

G= -952.204550

S2=0.774125

S2A=0.750454

0 2

O -0.11628822 -0.44136985 -0.16056564
C -0.09705431 -0.57711255 1.20253457
O 0.96066588 -0.77170765 1.73915116
C -1.38066821 -0.47251883 1.88702722
H -1.35158663 -0.57806997 2.96093672
C -2.52133217 -0.25763867 1.21051766
H -3.46715547 -0.18072511 1.73100586
C -2.50918709 -0.12292760 -0.22233325
C -3.68455280 0.10455096 -0.96312110
H -4.62292910 0.17787969 -0.43503165
C -3.61233582 0.23103381 -2.33304686
O -4.65402011 0.42697411 -3.15481125
C -5.95132921 0.49409209 -2.55982654
H -6.64616415 0.62923488 -3.38216327
H -6.01587715 1.34369080 -1.87939202
H -6.18005847 -0.43122066 -2.02914247
C -2.34798165 0.13110163 -2.98845321
O -2.21852890 0.28207462 -4.28708687
H -2.45580648 -0.69891602 -4.78564186

C -1.17909677 -0.09818185 -2.23139413
O 0.00014974 -0.19151929 -2.85089059
H -0.15610465 -0.04263006 -3.79573105
C -1.27063286 -0.22129896 -0.85207922
O -2.67675948 -1.93084037 -4.99412222
O -2.72304300 -2.39508993 -3.72795288
C -4.06332813 -2.78748809 -3.39854546
H -4.06278780 -2.96748829 -2.32639868
H -4.74950425 -1.98979872 -3.67431882
H -4.30348504 -3.70047727 -3.94151082

TS-8(OOH)

Freq= -2118.0127

H= -912.859672

G= -912.919426

S2=0.769852

S2A=0.750306

0 2

O -1.33114660 0.13160340 -0.63345646
C -0.10075139 0.12466364 -0.00822486
O -0.08490435 0.04532972 1.19020921
C 1.06207944 0.21432394 -0.87533851
H 2.02204890 0.20849747 -0.38247345
C 0.93083825 0.29653696 -2.21069962
H 1.80368055 0.36082683 -2.84811943
C -0.37210591 0.30017826 -2.81913180
C -0.56302102 0.38898234 -4.21787774
H 0.30463211 0.45669711 -4.85775240
C -1.83366117 0.39287958 -4.73872586
O -2.17319290 0.48599110 -6.04901884
C -1.10674580 0.55963239 -6.99950312

H	-1.58077387	0.64801748	-7.97129557
H	-0.50449141	-0.34830666	-6.96145811
H	-0.48974813	1.43768902	-6.80789109
C	-2.94476005	0.29845030	-3.87911249
O	-4.18833448	0.32794963	-4.37996319
H	-4.12640824	0.33970347	-5.34652479
C	-2.78893699	0.19743121	-2.48199916
O	-3.82111378	0.05321322	-1.69536060
H	-4.40100658	1.01376011	-1.64937187
C	-1.46284993	0.21753733	-1.97494924
O	-4.76884070	2.21233285	-1.74271418
O	-3.87894188	2.73206749	-2.62639342
H	-4.27165408	2.56094484	-3.49779942

TS-8(R=OOCH3)

Freq= -2233.3438

H= -952.139593

G= -952.202836

S2=0.773517

S2A=0.75042

0 2

O	-1.48239407	0.18246503	-0.69457167
C	-0.27545369	0.29671286	-0.03220667
O	-0.29115747	0.24262142	1.16778362
C	0.90111626	0.46550809	-0.86712366
H	1.84273869	0.55237144	-0.34713008
C	0.80451594	0.50683411	-2.20807517
H	1.68911449	0.63111444	-2.81989828
C	-0.47379295	0.38859646	-2.85376874
C	-0.63621800	0.43665368	-4.25771620
H	0.24008804	0.55532995	-4.87829036

C	-1.89134024	0.33045298	-4.80762829
O	-2.19936493	0.36147131	-6.13012541
C	-1.12444494	0.54874217	-7.05321591
H	-1.57446692	0.53963952	-8.04017788
H	-0.40446120	-0.26547034	-6.96858780
H	-0.63678155	1.50782034	-6.87664203
C	-3.01944782	0.17984035	-3.97825489
O	-4.23902840	0.09427371	-4.51649711
H	-4.14752625	0.14452803	-5.47905526
C	-2.89205883	0.11631581	-2.57487386
O	-3.93485982	-0.05974957	-1.81355668
H	-4.13388793	0.93165974	-1.26799884
C	-1.57834540	0.22933868	-2.03969935
O	-4.19226417	2.13919620	-1.02002804
O	-3.35292052	2.65071931	-1.95048220
C	-4.11794123	3.18295033	-3.03932646
H	-4.71863317	4.01515715	-2.67589349
H	-4.75728887	2.40301551	-3.45151612
H	-3.38965105	3.52434328	-3.77131319

Transition states geometries calculated in water

TS-7(R=OOH)

Freq=-2291.2069

H=-912.871365

G= -912.930959

S2=0.772087

S2A=0.75038

0 2

O 0.08059493 -0.11198473 -0.00043037
 C 0.11504627 -0.11473779 1.36573815
 O 1.20477775 -0.18699208 1.89287866
 C -1.15285590 -0.02755837 2.06432003
 H -1.10140997 -0.02258924 3.14232200
 C -2.31527602 0.03889226 1.39144671
 H -3.25786771 0.10098417 1.91872441
 C -2.33285952 0.02863175 -0.04683965
 C -3.52955204 0.08780089 -0.78042617
 H -4.46529778 0.13482638 -0.24500263
 C -3.47626122 0.08247257 -2.15750225
 O -4.53832411 0.10500673 -2.98273496
 C -5.83672300 0.02136462 -2.37595936
 H -6.54251257 0.00074441 -3.19873684
 H -6.01600209 0.89406953 -1.75011636
 H -5.91354103 -0.89295432 -1.78861694
 C -2.21548683 0.02304573 -2.82292688
 O -2.12635514 0.07203020 -4.14341847
 H -2.44874055 -0.88408862 -4.55416532
 C -1.02606834 -0.05314396 -2.07634150
 O 0.16778331 -0.12018235 -2.69112084
 H 0.02261533 -0.09106270 -3.64910295
 C -1.10112193 -0.04402414 -0.69305983
 O -2.76747340 -2.16368563 -4.65581416
 O -2.79304596 -2.53910365 -3.35923638
 H -3.71563167 -2.42843247 -3.07061450

TS-7(R=OOCH₃)

Freq= -2236.1250

H= -952.147664

G= -952.209857

S2=0.772473

S2A=0.750398

0 2

O -0.14708974 -0.48500165 -0.20747967
 C -0.11138703 -0.60602057 1.15253522
 O 0.96758466 -0.82165956 1.66333934
 C -1.36598980 -0.46822962 1.86633512
 H -1.31504662 -0.57144608 2.93946550
 C -2.51688042 -0.22780185 1.21308814
 H -3.44957350 -0.12673990 1.75187057
 C -2.53338684 -0.09754467 -0.21930925
 C -3.71699686 0.15589703 -0.93700167
 H -4.64268164 0.25400111 -0.39119289
 C -3.66585892 0.26969095 -2.30788274
 O -4.72029826 0.49931326 -3.11077417
 C -6.01732052 0.50346418 -2.49779723
 H -6.72266692 0.64519522 -3.30918689
 H -6.09610437 1.32502982 -1.78721479
 H -6.19877607 -0.44996072 -2.00255792
 C -2.42086229 0.12638943 -2.99045123
 O -2.34058742 0.24404654 -4.30567237
 H -2.29451256 -0.78002897 -4.73515054
 C -1.24277485 -0.12300840 -2.25849794
 O -0.06436869 -0.27656324 -2.88379687
 H -0.18946595 -0.13119583 -3.83377803
 C -1.31629981 -0.23203519 -0.87867146
 O -2.31264676 -2.07175893 -4.84228183
 O -2.61099747 -2.42920454 -3.57710532
 C -4.01370389 -2.73424662 -3.46470274
 O -0.14708974 -0.48500165 -0.20747967
 C -0.11138703 -0.60602057 1.15253522
 O 0.96758466 -0.82165956 1.66333934

TS-8(R=OOH)

Freq= -2313.5291

H= -912.869480

G= -912.929650

S2=0.768097

S2A=0.750246

0 2

O	-1.41769273	0.12948348	-0.67092646
C	-0.19733342	0.18456401	-0.03694616
O	-0.20899162	0.11912554	1.17479010
C	0.97103645	0.31406446	-0.87432946
H	1.92149678	0.35911299	-0.36579299
C	0.85894161	0.36928035	-2.21622539
H	1.73834943	0.46277755	-2.83987072
C	-0.42812516	0.30482029	-2.84672530
C	-0.60237706	0.36869665	-4.25035645
H	0.27451911	0.46347163	-4.87408649
C	-1.86263629	0.31495274	-4.79252250
O	-2.17466537	0.37564469	-6.11255081
C	-1.08945436	0.55368490	-7.03323740
H	-1.54361608	0.60734303	-8.01635776
H	-0.40845150	-0.29479810	-6.97885900
H	-0.56177498	1.48081122	-6.81244219
C	-2.98670402	0.19153189	-3.94824215
O	-4.22595815	0.15378574	-4.44802504
H	-4.18579425	0.22787165	-5.41383515
C	-2.84014469	0.11848527	-2.54992111

O -3.89396325 -0.03156978 -1.76934913

H -4.33451899 0.96665926 -1.58808671

C -1.52958239 0.18704675 -2.02455339

O -4.55232960 2.23928722 -1.59468132

O -3.51907264 2.69422350 -2.34060787

H -3.87126684 2.79657609 -3.24120313

TS-8(OOCH₃)

Freq= -2421.9348

H= -952.145822

G= -952.208584

S2=0.771176

S2A=0.750338

0 2

O	-1.51016758	0.18536763	-0.69659389
C	-0.30681207	0.33878990	-0.04504056
O	-0.33625795	0.30378255	1.16749134
C	0.86447753	0.52078168	-0.86784486
H	1.80264564	0.63482314	-0.34739429
C	0.76940742	0.54735238	-2.21232851
H	1.65060975	0.68626108	-2.82484187
C	-0.50189422	0.39598170	-2.85856943
C	-0.66658930	0.44261762	-4.26325110
H	0.20890048	0.58404888	-4.88012454
C	-1.91824610	0.31403302	-4.81665196
O	-2.21806434	0.34730186	-6.14109599
C	-1.13527704	0.57952110	-7.05240682
H	-1.57801272	0.57625842	-8.04211433
H	-0.39709882	-0.21730315	-6.96950057
H	-0.67712832	1.54658563	-6.84804342

C	-3.04305021	0.13713243	-3.98666913
O	-4.26945195	0.02424252	-4.50604190
H	-4.21603320	0.10246954	-5.47115338
C	-2.90931081	0.07867266	-2.58539178
O	-3.95867556	-0.11171123	-1.81475202
H	-4.16837611	0.86448710	-1.28915504
C	-1.60382104	0.21510039	-2.04963381
O	-4.17886235	2.10251107	-1.01342728
O	-3.29084659	2.57467622	-1.91894512
C	-3.98680765	3.16021086	-3.03297968
H	-4.51323550	4.04669368	-2.68478165
H	-4.68349927	2.43117448	-3.44305258
H	-3.21467814	3.42058884	-3.75157582

TS-8a(R=OOH)

Freq= -1877.6625

H= -912.415753

G= -912.476032

S2=0.762589

S2A=0.750124

-1 2

O	0.01685907	-0.10751741	-0.05370370
C	0.02841055	-0.09885573	1.32040466
O	1.11667734	-0.12127640	1.86002934
C	-1.25075468	-0.06492524	1.97758915
H	-1.24083730	-0.05595894	3.05587321
C	-2.40116323	-0.04838846	1.25558403
H	-3.35717453	-0.02772965	1.76392677
C	-2.38382553	-0.06093816	-0.16295102
C	-3.56146793	-0.06282348	-0.96304024
H	-4.51380303	-0.05198709	-0.45379589

C	-3.47935074	-0.08089836	-2.32548742
O	-4.54186353	-0.08302474	-3.16996867
C	-5.83429929	-0.06118947	-2.57729224
H	-5.96864479	0.84169895	-1.97946018
H	-6.54222484	-0.06553183	-3.39923571
H	-5.98820249	-0.94293794	-1.95333795
C	-2.19122587	-0.06405560	-3.01001565
O	-2.08498033	-0.04115245	-4.25561736
C	-1.02239065	-0.09279354	-2.17110074
O	0.18746523	-0.09332572	-2.75945816
H	0.17260963	-0.79509647	-3.46637731
C	-1.13811435	-0.08689627	-0.78463414
O	-0.04557192	-2.42172776	-3.82434623
O	-1.00339938	-2.70293711	-2.91694306
H	-0.53839761	-2.86663886	-2.08235736

TS-8a(OOCH₃)

Freq= -2334.6532

H= -951.697521

G= -951.760094

S2=0.763661

S2A=0.750156

-1 2

O	-0.01247666	0.08621677	0.08719168
C	0.00092244	0.11559849	1.45813003
O	1.08840556	0.11530689	1.99949806
C	-1.27870407	0.14211419	2.11888217
H	-1.26582616	0.16434232	3.19700590
C	-2.42948783	0.13497070	1.40042477
H	-3.38510764	0.14839019	1.90964821
C	-2.41322492	0.10636131	-0.02001227

C	-3.59266763	0.07213208	-0.81394190
H	-4.54406056	0.06565259	-0.30305743
C	-3.50944278	0.04337059	-2.17706078
O	-4.57073905	-0.00619903	-3.02065864
C	-5.86291137	-0.04007180	-2.42706445
H	-6.57001523	-0.08918336	-3.24824300
H	-6.04133646	0.86220930	-1.84023254
H	-5.97224781	-0.92089344	-1.79240563
C	-2.22299451	0.08733804	-2.86094544
O	-2.12819895	0.09911260	-4.11174352
C	-1.05059403	0.06745961	-2.03064862
O	0.15472831	0.04036375	-2.62073398
H	0.15520864	-0.75836486	-3.24464934
C	-1.16900710	0.08921815	-0.64366047
O	-0.12332898	-2.22878293	-3.72484528
O	-1.02452474	-2.55926741	-2.78158776
C	-2.23963689	-2.99489399	-3.39796745
H	-2.93205826	-3.18979574	-2.58319871
H	-2.60258489	-2.20013187	-4.04835329
H	-2.03845257	-3.90254664	-3.96442560