

## SUPPORTING INFORMATION

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# Exploring the Antioxidant Properties of Caffeoylquinic and Feruloylquinic Acids: A Computational Study on Hydroperoxyl Radical Scavenging and Xanthine Oxidase Inhibition

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**Table S1.** The cartesian coordinates and energies of the TSs of the reaction between 5-CQA and 5-FQA and HOO<sup>\*</sup> calculated at M06-2X/6-311++G(d,p) level in physiological media.

5CQA W RAF C8 dianion TS				Frequency and Energy
Cartesian Coordinates				
C	-3.53034900	-0.17879900	-0.18519900	Zero-point Energy Correction = 0.328347 Hartree
C	-4.06455300	0.90339300	-0.94672300	Thermal Correction to Energy = 0.354144 Hartree
C	-5.40184500	1.15778500	-0.94734600	Thermal Correction to Enthalpy = 0.355088 Hartree
C	-6.33897600	0.35643200	-0.18304300	Thermal Correction to Free Energy = 0.270157 Hartree
C	-5.78087300	-0.72033900	0.58105400	
C	-4.43724100	-0.97349800	0.57862100	EE + Zero-point Energy = -1447.177 Hartree
C	-2.13572400	-0.40509400	-0.19561700	EE + Thermal Energy Correction = -1447.1512 Hartree
C	-1.48416800	-1.40939300	0.49152200	EE + Thermal Enthalpy Correction = -1447.1503 Hartree
C	-0.03334000	-1.60645800	0.40012900	
O	0.62296000	-0.54590400	-0.08951000	EE + Thermal Free Energy Correction = -1447.2352 Hartree
O	0.52796500	-2.62703500	0.76372100	
C	2.06598100	-0.56423300	-0.07471400	
C	2.52411600	0.87101900	0.11930900	
C	4.05592000	0.94442000	0.16600300	
C	4.66178800	0.29434000	-1.08577700	
C	4.12513600	-1.09712500	-1.39457700	
C	2.59351800	-1.11534700	-1.39144800	
O	2.11165000	-2.42579500	-1.66519700	
O	4.52151900	0.28857100	1.34178300	
O	-7.57022400	0.64163800	-0.22535300	
O	-5.93267400	2.18651000	-1.67117800	
O	4.63652300	-2.03409500	-0.44795800	
C	4.48481300	2.43606600	0.22931100	
O	4.18037800	3.17050300	-0.73581900	
O	5.10611200	2.78456400	1.26559700	
H	-3.39689300	1.52694500	-1.53270400	
H	-6.46313400	-1.32544200	1.16783400	
H	-4.05382600	-1.79157500	1.17737200	
H	-1.53256400	0.31541900	-0.73924600	
H	2.39451700	-1.19120500	0.75652100	
H	2.15583600	1.47816700	-0.71201800	
H	2.11190400	1.26617100	1.05124800	
H	4.42715000	0.93005900	-1.94291000	
H	5.74974300	0.25411100	-0.98604000	
H	4.45710500	-1.38972200	-2.39662700	
H	2.23995800	-0.47452400	-2.20578000	
H	1.96895100	-2.88894600	-0.82843900	
H	4.93150400	0.99838200	1.86491300	
H	4.33136000	-2.91112300	-0.71057700	
H	-2.01201600	-2.26615600	0.88735800	
O	-1.16658400	-0.69107900	2.44983500	

H	-6.89123200	2.16417600	-1.51373600	
O	-1.50842700	0.66190000	2.42370200	
H	-2.47714200	0.66801900	2.41681900	
5FQA W RAF C8 dianion TS				
Cartesian Coordinates				Frequency and Energy
C	-3.32728300	-0.42771900	-0.07400000	Zero-point Energy Correction = 0.357509 Hartree
C	-3.92784000	0.77989100	-0.54644000	Thermal Correction to Energy = 0.38454 Hartree
C	-5.27629400	0.98138200	-0.46121200	Thermal Correction to Enthalpy = 0.385485 Hartree
C	-6.15810200	-0.02271800	0.12484700	Thermal Correction to Free Energy = 0.29705 Hartree
C	-5.52372600	-1.22476100	0.59422200	EE + Zero-point Energy = -1486.4316 Hartree
C	-4.17580500	-1.41928100	0.50023500	EE + Thermal Energy Correction = -1486.4046 Hartree
C	-1.92507000	-0.57525000	-0.16186700	EE + Thermal Enthalpy Correction = -1486.4036 Hartree
C	-1.21681400	-1.68736100	0.24526500	EE + Thermal Free Energy Correction = -1486.4921 Hartree
C	0.24177200	-1.78613600	0.09833000	
O	0.83654700	-0.59875600	-0.08446000	
O	0.84886000	-2.83906700	0.17280000	
C	2.26872200	-0.54881300	-0.22408200	
C	2.76035800	0.67535800	0.53223100	
C	4.27659200	0.81536900	0.37236000	
C	4.64866300	0.90007700	-1.11479400	
C	4.12171300	-0.29471000	-1.90355300	
C	2.61095700	-0.45608800	-1.70670300	
O	2.12618800	-1.58241700	-2.42013400	
O	4.90152700	-0.33496900	0.94953900	
O	-7.39936600	0.17015700	0.21343600	
O	-5.92893500	2.09520600	-0.88850400	
O	4.78768500	-1.51271600	-1.55951700	
C	4.78326800	2.08096200	1.10368700	
O	4.29639500	3.17958100	0.75745100	
O	5.66187000	1.89390900	1.98273100	
H	-3.27764400	1.53273900	-0.97582300	
H	-6.16792600	-1.97573900	1.03841800	
H	-3.74467400	-2.33802900	0.88198800	
H	-1.36631000	0.28594300	-0.51476900	
H	2.69275800	-1.46033500	0.20057500	
H	2.27266800	1.56849200	0.13334900	
H	2.50728300	0.58145200	1.59134300	
H	4.21629700	1.81194200	-1.53356000	
H	5.73582500	0.95869900	-1.21818800	
H	4.30478500	-0.14384600	-2.96963300	
H	2.10579900	0.41875600	-2.12692600	
H	2.65384000	-2.34367000	-2.14238400	
H	5.55450700	0.02240300	1.57562300	
H	4.98209700	-1.48201800	-0.61028400	
H	-1.70005300	-2.64149100	0.40434600	
O	-0.92880700	-1.50206500	2.33042000	
O	-1.42280800	-0.23751800	2.67293000	
H	-2.38571000	-0.33914700	2.64912800	
C	-5.13949900	3.12696300	-1.46903700	

H	-4.41222700	3.51011300	-0.74850700	
H	-4.62063700	2.76254700	-2.35953300	
H	-5.83362000	3.91744800	-1.74561000	
TS 5CQA 12OH PE FHT				
Cartesian Coordinates				Frequency and Energy
C	-3.42920400	-1.99580800	-0.31791900	Zero-point Energy Correction = 0.351946 Hartree
C	-2.46422800	-0.97638000	-0.14450600	Thermal Correction to Energy = 0.37776 Hartree
C	-2.85176900	0.21481700	0.45611500	Thermal Correction to Enthalpy = 0.378705 Hartree
C	-4.17198300	0.39375000	0.89074100	Thermal Correction to Free Energy = 0.292615 Hartree
C	-5.11923300	-0.65740100	0.71749800	
C	-4.73498500	-1.84980000	0.10911900	EE + Zero-point Energy = -1448.0433 Hartree
O	-4.59504600	1.50634500	1.46585000	EE + Thermal Energy Correction = -1448.0175 Hartree
O	-6.36977500	-0.48552200	1.13970200	EE + Thermal Enthalpy Correction = -1448.0166 Hartree
C	-1.09995400	-1.22616900	-0.60969900	
C	-0.02385500	-0.46622000	-0.37102900	EE + Thermal Free Energy Correction = -1448.1027 Hartree
C	1.27994000	-0.86500700	-0.92564600	
O	1.48505700	-1.85987500	-1.59153000	
H	-3.12791300	-2.92110600	-0.79717600	
H	-2.15895700	1.03671600	0.60059800	
H	-5.46648600	-2.63713700	-0.02499500	
H	-4.78658900	2.25632000	0.66806400	
H	-6.43487200	0.39448200	1.54470300	
H	-0.95715400	-2.12989400	-1.19817800	
H	-0.04678100	0.43859600	0.22377700	
O	-5.00523000	2.79385800	-0.46967500	
O	-5.11097200	1.71729600	-1.28781400	
H	-4.22264900	1.59298300	-1.66623700	
O	2.23537100	0.01737000	-0.61366400	
C	3.61700900	-0.30044300	-0.91202900	
C	4.42585500	0.49951600	0.09961400	
C	3.96556600	0.09224600	-2.34673400	
H	3.76089400	-1.37495900	-0.76783200	
C	5.93476800	0.31027200	-0.13062500	
H	4.16483200	1.55634900	0.00551600	
H	4.16522900	0.16796900	1.10741000	
C	5.47591100	0.00365500	-2.59648000	
O	3.36380100	-0.74792400	-3.31928200	
H	3.64678400	1.13140300	-2.50118100	
C	6.29380100	0.75673400	-1.55928000	
O	6.31229600	-1.02301100	0.11646900	
C	6.70708300	1.17446300	0.86582700	
O	5.88149200	-1.36448200	-2.57317500	
H	5.67188900	0.42108800	-3.58994000	
H	2.67061400	-1.27971000	-2.90241400	
H	6.09717700	1.82583900	-1.66445900	
H	7.35806000	0.58585900	-1.74232600	
H	6.25516500	-1.50338200	-0.72152400	
O	6.33897300	2.46642600	0.78526600	
O	7.54374400	0.78465400	1.62788700	

H	5.25408200	-1.85027200	-3.12500500	
H	6.86437000	2.96748900	1.42738800	
TS 5CQA 13OH PE FHT				
Cartesian Coordinates				Frequency and Energy
C	3.10178200	0.18209500	-0.40238300	Zero-point Energy Correction = 0.352706 Hartree
C	4.16914400	0.98186000	0.00571400	Thermal Correction to Energy = 0.378208 Hartree
C	5.47462500	0.60127800	-0.27719800	Thermal Correction to Enthalpy = 0.379153 Hartree
C	5.72668900	-0.60108500	-0.98848100	Thermal Correction to Free Energy = 0.294597 Hartree
C	4.63873400	-1.40014500	-1.39818400	
C	3.35050100	-1.01807500	-1.10996700	EE + Zero-point Energy = -1448.0494 Hartree
C	1.74942900	0.63715200	-0.08221300	EE + Thermal Energy Correction = -1448.0239 Hartree
C	0.60560800	0.02164600	-0.40680400	EE + Thermal Enthalpy Correction = -1448.0229 Hartree
C	-0.67872000	0.63170900	-0.01817900	
O	-1.71344100	-0.07855000	-0.47695000	EE + Thermal Free Energy Correction = -1448.1075 Hartree
O	-0.80216200	1.65271500	0.62640200	
C	-3.05670300	0.26055100	-0.05358000	
C	-3.83986300	-1.03622400	-0.20984800	
C	-5.32385100	-0.83494600	0.10241200	
C	-5.90979600	0.24654000	-0.81457500	
C	-5.14086500	1.54952400	-0.68041800	
C	-3.63463800	1.38471800	-0.91429200	
O	-3.07057100	2.65413600	-0.62547900	
O	-5.51422800	-0.52159700	1.47816500	
O	6.98479100	-0.90653600	-1.25408000	
O	6.49983300	1.36482400	0.11224300	
O	-5.36181100	2.05011700	0.63953600	
C	-6.06825100	-2.15237600	-0.15856700	
O	-6.80907900	-2.59026600	0.85454700	
O	-6.00072400	-2.73975100	-1.20318900	
H	3.99262200	1.90456500	0.54692500	
H	4.85067400	-2.31050000	-1.94823600	
H	2.52535700	-1.63970300	-1.43441100	
H	1.68119400	1.57225100	0.46877900	
H	0.55735500	-0.90913000	-0.95732500	
H	-3.01769400	0.57270300	0.99417400	
H	-3.74071800	-1.39546000	-1.23730500	
H	-3.41995200	-1.79092000	0.45906700	
H	-5.85070100	-0.10420100	-1.84743100	
H	-6.96256200	0.41619400	-0.57245200	
H	-5.51403200	2.27609200	-1.40939400	
H	-3.46978700	1.12636700	-1.96850300	
H	-2.23469800	2.53732200	-0.15141100	
H	-5.51922100	0.44438500	1.57336000	
H	7.31598000	-1.67669000	-0.54417500	
H	-4.75243500	2.79042400	0.76334200	
O	7.38638600	-2.44140500	0.50290500	
O	6.36030900	-1.98644700	1.26017700	
H	5.60356100	-2.55978700	1.04386400	
H	7.31995000	0.95151000	-0.19994300	

H	-6.69576100	-1.96192700	1.59013300	
TS 5CQA 12OH anion W FHT				
Cartesian Coordinates				Frequency and Energy
C	-3.44338700	-1.99949800	-0.28176600	Zero-point Energy Correction = 0.337551 Hartree
C	-2.45623300	-1.00908500	-0.06424200	Thermal Correction to Energy = 0.363438 Hartree
C	-2.83449100	0.19835200	0.50652500	Thermal Correction to Enthalpy = 0.364383 Hartree
C	-4.16802200	0.42412400	0.86910600	Thermal Correction to Free Energy = 0.279071 Hartree
C	-5.14290100	-0.58955000	0.63615300	
C	-4.76625600	-1.80038500	0.05937200	EE + Zero-point Energy = -1447.6225 Hartree
O	-4.56505800	1.55938700	1.43668300	EE + Thermal Energy Correction = -1447.5966 Hartree
O	-6.42307600	-0.37537900	0.96313500	EE + Thermal Enthalpy Correction = -1447.5957 Hartree
C	-1.07871800	-1.30983900	-0.45651400	
C	-0.02209100	-0.49894500	-0.32470800	EE + Thermal Free Energy Correction = -1447.681 Hartree
C	1.31075500	-0.94649400	-0.76355900	
O	1.56787900	-2.02623000	-1.25726500	
H	-3.14540800	-2.94053900	-0.73115700	
H	-2.12356100	0.99481900	0.69425000	
H	-5.51713800	-2.56173600	-0.11200500	
H	-5.01230500	2.19264000	0.65688200	
H	-6.51201500	0.50117800	1.37136100	
H	-0.92059500	-2.29226000	-0.89539700	
H	-0.08325000	0.49606600	0.09832200	
O	-5.46121600	2.63043100	-0.48629700	
O	-5.28237400	1.54812800	-1.28416400	
H	-4.39729300	1.65249000	-1.67713600	
O	2.22987000	0.00431400	-0.53786700	
C	3.60211600	-0.25693100	-0.89712000	
C	4.47504500	0.45356400	0.12271300	
C	3.86422800	0.28288900	-2.29683300	
H	3.77027900	-1.33495600	-0.87175100	
C	5.95917700	0.23375300	-0.19621200	
H	4.25292500	1.52375100	0.09900300	
H	4.25854000	0.07287800	1.12399000	
C	5.33170500	0.07021000	-2.68171900	
O	2.98906700	-0.28735300	-3.26005600	
H	3.66072800	1.35810000	-2.30070500	
C	6.26542200	0.66750700	-1.63588900	
O	6.27832700	-1.14272500	-0.01655100	
C	6.81266500	1.07340300	0.79240300	
O	5.61316000	-1.32072100	-2.84055900	
H	5.50184800	0.57642300	-3.63745000	
H	2.95392900	-1.24294200	-3.12090900	
H	6.16495600	1.75420200	-1.68965300	
H	7.29976200	0.41348700	-1.88242400	
H	6.91057600	-1.14868200	0.72203700	
O	6.67934500	2.31627900	0.76418200	
O	7.57016000	0.42050500	1.55483500	
H	5.17023800	-1.62468300	-3.64119000	
TS 5CQA 13OH anion W FHT				

Cartesian Coordinates				Frequency and Energy
C	3.05450200	0.07478400	-0.33730500	Zero-point Energy Correction = 0.337554 Hartree
C	4.13923900	0.84203900	0.08698700	Thermal Correction to Energy = 0.363494 Hartree
C	5.43764500	0.45711000	-0.22270900	Thermal Correction to Enthalpy = 0.364438 Hartree
C	5.66676900	-0.73090900	-0.96850000	Thermal Correction to Free Energy = 0.279146 Hartree
C	4.56150300	-1.50625700	-1.37446500	EE + Zero-point Energy = -1447.6214 Hartree
C	3.28087900	-1.10937800	-1.07766200	EE + Thermal Energy Correction = -1447.5955 Hartree
C	1.71260700	0.53897700	0.01121700	EE + Thermal Enthalpy Correction = -1447.5945 Hartree
C	0.56025900	-0.03287000	-0.35939700	EE + Thermal Free Energy Correction = -1447.6798 Hartree
C	-0.72185100	0.55504700	0.07310200	
O	-1.75615600	-0.13733300	-0.42240000	
O	-0.84348900	1.53003600	0.78655700	
C	-3.09496700	0.27818000	-0.07745500	
C	-3.95164300	-0.97523700	-0.03348500	
C	-5.40203500	-0.62300200	0.32430900	
C	-5.95016800	0.43537200	-0.64162000	
C	-5.05285700	1.65548800	-0.80898000	
C	-3.61527000	1.24075900	-1.13601200	
O	-2.77362900	2.37490100	-1.29102900	
O	-5.45174000	-0.14061000	1.66335600	
O	6.90421900	-1.08032800	-1.28980700	
O	6.53092800	1.14966800	0.14553600	
O	-5.08832300	2.44831000	0.37779600	
C	-6.26093300	-1.91307600	0.23054900	
O	-6.36950100	-2.45974000	-0.88871000	
O	-6.77103500	-2.31184300	1.30853900	
H	3.97717900	1.75069200	0.65817800	
H	4.75851600	-2.41316700	-1.93391300	
H	2.44520100	-1.71446200	-1.40594800	
H	1.66849100	1.43560500	0.62458800	
H	0.50384300	-0.92078100	-0.97652800	
H	-3.06574900	0.76665200	0.89846900	
H	-3.92611500	-1.45791800	-1.01421000	
H	-3.55256000	-1.67096700	0.70873100	
H	-6.05903000	-0.02839400	-1.62497900	
H	-6.94149700	0.75448500	-0.30945300	
H	-5.42406900	2.25506800	-1.64657300	
H	-3.61701100	0.72831600	-2.10320500	
H	-2.50341000	2.68359200	-0.41622300	
H	-5.95940700	-0.81699500	2.14323500	
H	7.43936000	-1.32674300	-0.38026300	
H	-4.68047200	3.29886800	0.17766300	
O	7.70049600	-1.73975700	0.85886200	
O	6.49939000	-1.56131600	1.46452300	
H	6.04420300	-2.41987000	1.40448200	
H	6.27993700	1.93014700	0.65926300	
TS 5CQA RAF C8 anion W				
Cartesian Coordinates				Frequency and Energy
C	-3.53091600	-0.16615400	-0.05188100	Zero-point Energy Correction = 0.342051 Hartree

C	-4.02946300	0.81884400	-0.92956300	Thermal Correction to Energy = 0.368028 Hartree
C	-5.38292100	1.06276700	-1.01851100	Thermal Correction to Enthalpy = 0.368972 Hartree
C	-6.27848800	0.33310700	-0.22019600	Thermal Correction to Free Energy = 0.283662 Hartree
C	-5.79923400	-0.63808700	0.65553000	
C	-4.44201500	-0.88953200	0.74147400	EE + Zero-point Energy = -1447.618 Hartree
C	-2.10964600	-0.37116800	-0.00202400	EE + Thermal Energy Correction = -1447.592 Hartree
C	-1.46436200	-1.30110800	0.78671300	EE + Thermal Enthalpy Correction = -1447.5911 Hartree
C	-0.01101200	-1.54924700	0.64079600	
O	0.64455500	-0.49523700	0.15542100	EE + Thermal Free Energy Correction = -1447.6764 Hartree
O	0.51696500	-2.59296700	0.96576700	
C	2.07761400	-0.57713700	-0.00372900	
C	2.63137300	0.81075800	0.26773200	
C	4.15549800	0.82548200	0.09488000	
C	4.54166400	0.29252900	-1.29107300	
C	3.91123000	-1.04945200	-1.64480300	
C	2.39511600	-1.01550800	-1.42649600	
O	1.79239700	-2.26134900	-1.74696600	
O	4.75235400	0.03020900	1.11411000	
O	-7.61292200	0.56304200	-0.29041900	
O	-5.95009100	1.99060300	-1.84685300	
O	4.51072300	-2.08456100	-0.86448300	
C	4.65781800	2.28672800	0.24777700	
O	4.26472400	3.12727900	-0.59060600	
O	5.42059500	2.50595000	1.22306300	
H	-3.34478700	1.39156100	-1.54764700	
H	-6.51125000	-1.18463700	1.26235300	
H	-4.08797900	-1.64488300	1.43200100	
H	-1.50291900	0.30284700	-0.59812500	
H	2.46640500	-1.30297900	0.71269800	
H	2.18038800	1.51670400	-0.43494400	
H	2.37581100	1.11831800	1.28492300	
H	4.20681500	1.01833900	-2.03605300	
H	5.62976800	0.21502600	-1.36244600	
H	4.09097200	-1.25599800	-2.70462500	
H	1.96614400	-0.28540800	-2.11966200	
H	1.96407500	-2.88506000	-1.02919800	
H	5.25623200	0.66572200	1.65044500	
H	-7.79001800	1.26199400	-0.93651500	
H	4.28169900	-2.93216900	-1.26256500	
H	-2.00005400	-2.13063900	1.23135600	
O	-1.26053900	-0.47422100	2.57488100	
H	-5.27062500	2.43820500	-2.36783000	
O	-0.85053800	0.83037100	2.47526200	
H	-1.67000300	1.34317900	2.39265700	
TS 5FQA RAF C8 anion W				
Cartesian Coordinates				Frequency and Energy
C	-3.27647900	-0.32277800	-0.08427800	Zero-point Energy Correction = 0.370855 Hartree
C	-3.83593400	0.96756600	-0.23960600	Thermal Correction to Energy = 0.398049 Hartree
C	-5.20376200	1.14140700	-0.23519800	Thermal Correction to Enthalpy = 0.398993 Hartree



C	-6.05052600	0.02629900	-0.06956900	Thermal Correction to Free Energy = 0.310996
C	-5.51235200	-1.24509100	0.08608100	Hartree
C	-4.13936800	-1.42289000	0.07960200	EE + Zero-point Energy = -1486.877 Hartree
C	-1.84639600	-0.44448500	-0.09165100	EE + Thermal Energy Correction = -1486.8498 Hartree
C	-1.15573200	-1.62525000	0.08539000	EE + Thermal Enthalpy Correction = -1486.8489
C	0.30700100	-1.70730900	-0.16342400	Hartree
O	0.92891600	-0.54132700	0.00557500	EE + Thermal Free Energy Correction = -1486.9369
O	0.86010400	-2.74550300	-0.45561700	Hartree
C	2.34498000	-0.46157900	-0.26332700	
C	2.95370700	0.47878500	0.76325600	
C	4.44916700	0.65138500	0.48649100	
C	4.66935400	1.17427800	-0.94063300	
C	4.02193200	0.27048500	-1.98566100	
C	2.53482800	0.06606600	-1.68110400	
O	1.93041200	-0.79090100	-2.63555800	
O	5.08585800	-0.62251500	0.62559500	
O	-7.39550400	0.18876900	-0.06090000	
O	-5.85791400	2.32564400	-0.37717700	
O	4.67667800	-0.99577000	-2.09311400	
C	5.08022200	1.63909700	1.49663700	
O	4.57512400	2.77962600	1.57956700	
O	6.06921900	1.20659800	2.14077300	
H	-3.17207500	1.81427600	-0.36269200	
H	-6.18815200	-2.08256400	0.21127200	
H	-3.74065700	-2.42201400	0.20250200	
H	-1.27709900	0.47476100	-0.18595600	
H	2.77240900	-1.46200400	-0.17372400	
H	2.46132400	1.45252600	0.69984500	
H	2.80673200	0.07537800	1.76808300	
H	4.22982400	2.17140100	-1.02266800	
H	5.74156500	1.25605300	-1.13945700	
H	4.09904400	0.73273900	-2.97215300	
H	2.02474600	1.03044900	-1.76392400	
H	2.45370500	-1.60361900	-2.66534200	
H	5.83199000	-0.46273400	1.22896600	
H	-7.60418900	1.12670800	-0.18426100	
H	4.97075400	-1.24860500	-1.20466500	
H	-1.65270700	-2.58126800	-0.02049700	
O	-0.94789000	-1.83186400	2.02673800	
O	-2.20739500	-1.85158900	2.57417500	
H	-2.54415400	-2.74506200	2.39934900	
C	-5.06072700	3.49818700	-0.53273000	
H	-4.42236800	3.64507200	0.34152300	
H	-4.44976400	3.42931200	-1.43577200	
H	-5.76128000	4.32480300	-0.62254100	
TS 5FQA 13OH FHT P				
Cartesian Coordinates				Frequency and Energy
C	3.09105500	0.05135700	-0.34752100	Zero-point Energy Correction = 0.381077 Hartree
C	4.18018000	0.82955600	0.06390100	Thermal Correction to Energy = 0.408055 Hartree

C	5.47952700	0.39901300	-0.16326800	Thermal Correction to Enthalpy = 0.408999 Hartree
C	5.71526400	-0.83755600	-0.84219900	Thermal Correction to Free Energy = 0.320789
C	4.60015800	-1.61598400	-1.22595400	Hartree
C	3.31864900	-1.18055100	-0.99622600	EE + Zero-point Energy = -1487.3047 Hartree
C	1.75168900	0.56482900	-0.07950900	EE + Thermal Energy Correction = -1487.2777 Hartree
C	0.59171900	-0.04438400	-0.36068600	EE + Thermal Enthalpy Correction = -1487.2767
C	-0.67517200	0.62972700	-0.02878400	Hartree
O	-1.72966500	-0.09649100	-0.41201200	EE + Thermal Free Energy Correction = -1487.3649
O	-0.77267100	1.71103800	0.51553400	Hartree
C	-3.05802300	0.30332400	0.00426400	
C	-3.86532700	-0.98767600	-0.01034400	
C	-5.33675400	-0.72920500	0.32072700	
C	-5.93118800	0.27788000	-0.67226300	
C	-5.13324700	1.57029300	-0.68217300	
C	-3.64027400	1.34748800	-0.94838900	
O	-3.03738100	2.62431400	-0.81325300	
O	-5.48264600	-0.29159700	1.66780100	
O	6.92451600	-1.21443600	-1.15669000	
O	6.58753600	1.06260900	0.22373500	
O	-5.29863900	2.19431200	0.59267500	
C	-6.11184900	-2.04903800	0.19638100	
O	-6.81896600	-2.39118500	1.26892400	
O	-6.09510000	-2.71872700	-0.79979000	
H	3.99067300	1.77319100	0.55978800	
H	4.79765000	-2.55498900	-1.72923400	
H	2.48228600	-1.78821800	-1.31896100	
H	1.70201000	1.54132500	0.39698800	
H	0.51945200	-1.01887600	-0.82676000	
H	-2.99044800	0.71418600	1.01606000	
H	-3.80009600	-1.44250600	-1.00193500	
H	-3.44031100	-1.68524100	0.71488300	
H	-5.91224900	-0.16536700	-1.67043400	
H	-6.97203900	0.49133300	-0.41376800	
H	-5.51559300	2.23607700	-1.46262800	
H	-3.51907400	0.97747300	-1.97468000	
H	-2.19755200	2.53735600	-0.33962900	
H	-5.46911000	0.67868900	1.67668700	
H	7.58857100	-1.29149700	-0.25262800	
H	-4.67332100	2.93081800	0.62772600	
O	8.07687900	-1.54309300	0.86817800	
O	7.07105400	-1.26616600	1.74087900	
H	7.01024800	-0.29469500	1.72964400	
C	6.42976500	2.37168000	0.77517500	
H	5.92022300	3.02599900	0.06425900	
H	5.87575500	2.33377000	1.71684300	
H	7.43766900	2.73784000	0.95614300	
H	-6.67111500	-1.70579100	1.94500000	
TS 5FQA 13OH FHT P				
Cartesian Coordinates				Frequency and Energy

C	3.07828200	0.11251800	-0.31392500	Zero-point Energy Correction = 0.365891 Hartree
C	4.16262600	0.86547700	0.14481700	Thermal Correction to Energy = 0.393284 Hartree
C	5.46243300	0.48398000	-0.17155700	Thermal Correction to Enthalpy = 0.394228 Hartree
C	5.68686700	-0.68957100	-0.94997100	Thermal Correction to Free Energy = 0.305769
C	4.58300900	-1.44276500	-1.38993500	Hartree
C	3.30211100	-1.04582800	-1.09080900	EE + Zero-point Energy = -1486.8769 Hartree
C	1.73579500	0.56370900	0.04995100	EE + Thermal Energy Correction = -1486.8496 Hartree
C	0.58440700	0.00093000	-0.33749000	EE + Thermal Enthalpy Correction = -1486.8486
C	-0.70009500	0.56082200	0.12345400	Hartree
O	-1.72941900	-0.12573100	-0.39035700	EE + Thermal Free Energy Correction = -1486.9371
O	-0.82807400	1.50738100	0.87316100	Hartree
C	-3.07136500	0.25203700	-0.01602600	
C	-3.90292400	-1.01912100	-0.00882900	
C	-5.35652500	-0.70858800	0.37148900	
C	-5.93314200	0.36955600	-0.55513300	
C	-5.06415200	1.61471200	-0.68214000	
C	-3.62024400	1.24321500	-1.03314700	
O	-2.80309400	2.39948900	-1.14991200	
O	-5.40418200	-0.27137800	1.72585700	
O	6.92323500	-1.04250500	-1.26748400	
O	6.57397600	1.12634200	0.21809700	
O	-5.10896100	2.36264100	0.53338900	
C	-6.19335200	-2.01023400	0.24204300	
O	-6.29005900	-2.53012800	-0.89103100	
O	-6.70095000	-2.44352100	1.30780500	
H	3.97612600	1.74951100	0.74134800	
H	4.77923500	-2.33415300	-1.97389100	
H	2.46607900	-1.63622600	-1.44387400	
H	1.69003600	1.43811200	0.69462000	
H	0.52978100	-0.86478600	-0.98542200	
H	-3.04053300	0.70466500	0.97707800	
H	-3.87639800	-1.46691500	-1.00585900	
H	-3.48394300	-1.73165800	0.70596000	
H	-6.03518100	-0.06183100	-1.55382900	
H	-6.93015500	0.65397700	-0.20872200	
H	-5.45407000	2.23653900	-1.49457900	
H	-3.61818400	0.76828800	-2.01938900	
H	-2.53516600	2.68160500	-0.26551900	
H	-5.90607400	-0.96662500	2.18447900	
H	7.46632600	-1.26915500	-0.36133400	
H	-4.72108900	3.22889900	0.36226400	
O	7.77441900	-1.66125000	0.88017200	
O	6.57530300	-1.60675500	1.51312800	
H	6.54299300	-0.72948000	1.93653300	
C	6.42495700	2.23936900	1.10395100	
H	5.87012200	3.04285100	0.61591100	
H	5.91560400	1.92847000	2.01890000	
H	7.43480600	2.56992900	1.33227200	