Supporting Information (SI)

The Radical Scavenging Activity of Muriolide in Physiological Environments: Mechanistic and kinetic insights into Double Processes

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Table of Contents

Table S1. **Calculated thermodynamic parameters (kcal/mol) of the MO in the studied solvents**

Positions	BDE		PA		IE	
	P	W	P	W	P	W
C2–H	89.5	91.0			136.6	109.2
C3–H	91.7	92.0				
O6–H	79.7	82.6	78.6	43.1		
O7–H	79.0	82.0	78.4	42.9		
O11–H	104.3	132.7	97.1	53.6		
C11–H	97.3	98.2				
C12–H	99.0	101.5				
P: pentyl ethanoate; W: water						

Table S2: The Cartesian coordinates and energies of TS of the reaction between MO with HOO in the studied environments at the M06-2X/6-311++G(d,p) level of theory.

Name				**TS-MO-O6-H-OOH (Gas phase)**
Cartesian Coordinates				Frequency and Energy
O	3.90414700	1.39711900	0.10297500	Zero-point correction= 0.340015 (Hartree/Particle)
C	3.33927500	1.83320300	-1.15058200	Thermal correction to Energy= 0.365063
C	1.91381100	2.24390600	-0.79342000	Thermal correction to Enthalpy= 0.366007
C	1.55228700	1.16032700	0.23418400	Thermal correction to Gibbs Free Energy= 0.282143
C	2.92878100	0.89743500	0.88840200	Sum of electronic and zero-point Energies= -1334.665694
O	1.19081200	0.03080400	-0.55836000	Sum of electronic and thermal Energies= -1334.640646
C	1.14433900	-1.22605800	0.08008000	Sum of electronic and thermal Enthalpies= -1334.639702
C	2.40856100	-2.04827200	-0.15892300	Sum of electronic and thermal Free Energies= -1334.723566
C	-0.09571200	-1.97495500	-0.41721600	
C	-1.34151600	-1.24975400	0.01611100	
O	3.38577600	-1.33545300	-0.71882700	
C	4.65498400	-1.99267000	-0.80966500	
O	2.50643500	-3.20109600	0.16032700	
O	3.13740400	0.34503500	1.92611100	
O	1.85800400	3.54700700	-0.26046900	
C	-1.81923800	-1.40636600	1.33336500	
C	-2.90577200	-0.69095100	1.80664700	
C	-3.54034200	0.21004500	0.95714900	
C	-3.08578400	0.38134700	-0.37868100	
C	-1.98474700	-0.36779800	-0.82888500	
O	-3.72236900	1.25448400	-1.13640800	
O	-4.62211000	0.89410700	1.37243300	
C	0.48054900	1.52856700	1.23676100	
H	3.35607600	0.99402600	-1.84701700	
H	3.93916100	2.66398200	-1.51656700	
H	1.23166200	2.21110700	-1.64143200	
H	1.08251200	-1.11402500	1.16899100	
H	-0.04813600	-2.03998200	-1.50680600	
H	-0.06571100	-2.98891500	-0.01390600	
H	5.33226700	-1.26160900	-1.24276900	
H	4.99043800	-2.28389300	0.18544300	
H	4.57592400	-2.87639800	-1.44222600	
H	2.57616000	3.67021600	0.36949300	
H	-1.31757300	-2.10610100	1.99474900	
H	-3.27248000	-0.81265800	2.81816400	
H	-1.64675400	-0.21246700	-1.84688200	
H	-4.70256700	0.80708700	-1.45045400	
H	-4.84485100	1.54376000	0.68820900	
H	0.35545200	0.73773300	1.97816500	
H	0.74771500	2.44500600	1.76258900	
H	-0.46458300	1.68371400	0.71220700	
H	-5.72701400	-0.98246400	0.04769400	
O	-5.76547000	0.12058200	-1.44647900	
O	-5.37194700	-1.03585700	-0.85500500	

Name				**TS-MO-O6-H-OOH (Pentyl ethanoate)**
Cartesian Coordinates				Frequency and Energy
O	3.98603000	1.28150200	-0.00210100	Zero-point correction= 0.339348 (Hartree/Particle)
C	3.37701800	1.78017200	-1.21609800	Thermal correction to Energy= 0.364412
C	1.98388100	2.22906700	-0.78789100	Thermal correction to Enthalpy= 0.365356
C	1.63844100	1.16615500	0.26890200	Thermal correction to Gibbs Free Energy= 0.282037

C	3.03818300	0.83207400	0.83342300	Sum of electronic and zero-point Energies= -1334.699943
O	1.16556000	0.05498400	-0.48958500	Sum of electronic and thermal Energies= -1334.674879
C	1.10321600	-1.19683300	0.15654500	Sum of electronic and thermal Enthalpies= -1334.673935
C	2.35614400	-2.03781000	-0.07382200	Sum of electronic and thermal Free Energies= -1334.757254
C	-0.14155400	-1.93106200	-0.35385600	
C	-1.38351800	-1.18798100	0.06133300	
O	3.25306600	-1.42804600	-0.84167600	
C	4.51475600	-2.09489000	-0.98568800	
O	2.50224100	-3.13015700	0.40937200	
O	3.28740800	0.26194900	1.85721100	
O	1.97577800	3.54327800	-0.27707900	
C	-1.85685300	-1.30455500	1.38577000	
C	-2.94663000	-0.58192500	1.83880400	
C	-3.59009400	0.28735300	0.96201100	
C	-3.14122500	0.41335900	-0.37954200	
C	-2.03390500	-0.33711900	-0.80988800	
O	-3.79219300	1.25566100	-1.16908400	
O	-4.66626500	0.98605400	1.36328100	
C	0.65456400	1.59318600	1.33550400	
H	3.33740600	0.96465400	-1.93865100	
H	3.99159800	2.59844200	-1.58642000	
H	1.26427000	2.19928500	-1.60451100	
H	1.02636700	-1.08366300	1.24332200	
H	-0.08344700	-2.00561600	-1.44239800	
H	-0.13822400	-2.94081400	0.06163300	
H	5.11632700	-1.45277900	-1.62432100	
H	4.98730200	-2.21001400	-0.00966000	
H	4.37628300	-3.07187300	-1.44864600	
H	2.69606000	3.65419400	0.35553400	
H	-1.34938500	-1.97967100	2.06808800	
H	-3.30708700	-0.67601500	2.85611700	
H	-1.70234200	-0.21892900	-1.83549200	
H	-4.72972500	0.78047300	-1.48711200	
H	-4.89460200	1.62147400	0.66685100	
H	0.49175600	0.79280900	2.05931000	
H	1.02532900	2.46311300	1.87905600	
H	-0.29710500	1.85059200	0.86443500	
H	-5.76298800	-1.03285400	0.00709700	
O	-5.78437700	0.01543400	-1.53413900	
O	-5.36254200	-1.09415300	-0.87836100	

Name				**TS-MO-O6-H-OOH (Water)**
Cartesian Coordinates				Frequency and Energy
O	3.97648900	1.28018500	-0.03145200	Zero-point correction= 0.339615 (Hartree/Particle)
C	3.37199000	1.82491600	-1.23338000	Thermal correction to Energy= 0.364436
C	1.95666300	2.21975200	-0.82198300	Thermal correction to Enthalpy= 0.365381
C	1.63130700	1.16578100	0.25294000	Thermal correction to Gibbs Free Energy= 0.283248
C	3.03340000	0.83764000	0.80372600	Sum of electronic and zero-point Energies= -1334.711578
O	1.15824700	0.03727600	-0.48633100	Sum of electronic and thermal Energies= -1334.686756
C	1.09854300	-1.20562200	0.18630000	Sum of electronic and thermal Enthalpies= -1334.685812
C	2.35581900	-2.03578600	-0.03632400	Sum of electronic and thermal Free Energies= -1334.767944
C	-0.14653100	-1.95203500	-0.30356300	
C	-1.37780400	-1.18203400	0.09317600	
O	3.22493400	-1.45771000	-0.84771500	
C	4.49415600	-2.11552600	-1.00591800	

O	2.53069200	-3.10688300	0.49960300
O	3.29632200	0.25898300	1.82719300
O	1.87331500	3.54926700	-0.35131900
C	-1.80184400	-1.19167800	1.44013600
C	-2.87247700	-0.43137400	1.87188900
C	-3.54999500	0.36954400	0.95434100
C	-3.14817500	0.38739800	-0.40642200
C	-2.05829400	-0.39924400	-0.81704500
O	-3.81604800	1.17521500	-1.25115700
O	-4.60107400	1.11170300	1.35366200
C	0.66033100	1.59778500	1.32806700
H	3.37623500	1.04387900	-1.99352900
H	3.97206600	2.67534700	-1.54745700
H	1.25419000	2.13484600	-1.64917700
H	1.02444200	-1.07198900	1.26996500
H	-0.09038500	-2.06186900	-1.38878800
H	-0.14860800	-2.94541400	0.14955400
H	5.06762800	-1.48160800	-1.67644400
H	4.98676000	-2.19514600	-0.03687500
H	4.35006400	-3.10393900	-1.44051000
H	2.53525700	3.70378700	0.33545500
H	-1.26675200	-1.80917400	2.15470000
H	-3.19599100	-0.44236800	2.90552400
H	-1.76292100	-0.36205300	-1.86003500
H	-4.75495700	0.69389700	-1.49857300
H	-4.91203000	1.64686100	0.60605300
H	0.51604600	0.80450600	2.06367200
H	1.03997200	2.47751800	1.84929000
H	-0.30063000	1.84001200	0.86691500
H	-5.74629600	-1.03663000	0.09062000
O	-5.77936900	-0.15312900	-1.55721200
O	-5.34183700	-1.17585200	-0.78477100

Name			**TS-MO-O7-H-OOH (Gas phase)**
Cartesian Coordinates			Frequency and Energy
O	3.97925400	1.27588700	0.31394900
C	3.53747900	1.76148000	-0.97031700
C	2.10655000	2.22881300	-0.72034900
C	1.61638700	1.14517900	0.25248100
C	2.92272000	0.80649700	1.00752600
O	1.27004300	0.04706000	-0.59067700
C	1.11462300	-1.21620200	0.01592300
C	2.35618600	-2.09332800	-0.13297000
C	-0.10876200	-1.90178400	-0.60168800
C	-1.35376800	-1.13256100	-0.25383200
O	3.40741800	-1.41876100	-0.59658900
C	4.65000900	-2.13131500	-0.59014600
O	2.37359800	-3.25412200	0.17151900
O	3.02214600	0.22403800	2.04495300
O	2.06237500	3.52415000	-0.16847700
C	-1.94456000	-1.30504300	1.01548900
C	-3.03172600	-0.54650700	1.39420300
C	-3.56910200	0.40728700	0.50862400
C	-2.97586600	0.56928100	-0.77236700
C	-1.87116900	-0.19556900	-1.13687600

Zero-point correction= 0.339858 (Hartree/Particle)
Thermal correction to Energy= 0.365031
Thermal correction to Enthalpy= 0.365975
Thermal correction to Gibbs Free Energy= 0.281448
Sum of electronic and zero-point Energies= -1334.666368
Sum of electronic and thermal Energies= -1334.641195
Sum of electronic and thermal Enthalpies= -1334.640251
Sum of electronic and thermal Free Energies= -1334.724778

O	-3.47913800	1.47283000	-1.61679100
O	-4.60943800	1.16683800	0.80586800
C	0.48556000	1.54395400	1.17517600
H	3.57452300	0.93628200	-1.68245200
H	4.20046000	2.57134800	-1.26782900
H	1.49511700	2.23982900	-1.62122500
H	0.96410400	-1.12013000	1.09751700
H	0.02904800	-1.94663000	-1.68452500
H	-0.15408700	-2.92259000	-0.21761400
H	5.39293900	-1.42625300	-0.95289200
H	4.88618500	-2.44854700	0.42531100
H	4.58638100	-3.00311600	-1.24068000
H	2.72954300	3.60579900	0.52143300
H	-1.52863200	-2.03825900	1.69866000
H	-3.49451200	-0.65460400	2.36858100
H	-1.42397800	-0.03933300	-2.11125600
H	-4.22247500	1.90767300	-1.17191600
H	-5.53122900	0.57320300	0.63563300
H	0.26717600	0.74704600	1.88783400
H	0.75041000	2.43771300	1.73977000
H	-0.40717700	1.75215400	0.58197700
H	-5.18323900	-1.79516200	-0.04976400
O	-6.32181700	-0.34564400	0.22196200
O	-5.52168200	-1.06946500	-0.59844300

Name			**TS-MO-O7-H-OOH (Pentyl ethanoate)**
Cartesian Coordinates			Frequency and Energy
O	4.06039600	1.16872000	0.25808800
C	3.58696500	1.72995400	-0.98872800
C	2.17979000	2.22575300	-0.67371800
C	1.69521300	1.14480100	0.30765000
C	3.02179200	0.73394600	0.98680500
O	1.25429200	0.07868900	-0.53144900
C	1.08148400	-1.18880800	0.06118300
C	2.31660200	-2.07596900	-0.07763700
C	-0.13341900	-1.85600000	-0.59465000
C	-1.38013300	-1.08106200	-0.26455000
O	3.30730600	-1.48187100	-0.73361200
C	4.54982500	-2.19765000	-0.77767500
O	2.37026000	-3.18807700	0.37867300
O	3.15127700	0.12154100	2.00831700
O	2.17824800	3.52124100	-0.11716600
C	-1.97403900	-1.23420600	1.00634900
C	-3.07086800	-0.48118300	1.36536400
C	-3.61452900	0.44688100	0.45696100
C	-3.01721000	0.59245200	-0.82278200
C	-1.90294700	-0.16646300	-1.16859800
O	-3.52720100	1.47421900	-1.69011500
O	-4.66264500	1.20926000	0.73937700
C	0.63169300	1.57615000	1.29252000
H	3.58033700	0.93918900	-1.73935600
H	4.26600200	2.53106100	-1.27364400
H	1.53894800	2.25509600	-1.55370500
H	0.90287600	-1.10708800	1.13864000
H	0.02680700	-1.89270800	-1.67480300

Zero-point correction= 0.339358 (Hartree/Particle)
Thermal correction to Energy= 0.364480
Thermal correction to Enthalpy= 0.365425
Thermal correction to Gibbs Free Energy= 0.281612
Sum of electronic and zero-point Energies= -1334.701276
Sum of electronic and thermal Energies= -1334.676154
Sum of electronic and thermal Enthalpies= -1334.675210
Sum of electronic and thermal Free Energies= -1334.759023

H	-0.20530600	-2.87827700	-0.21786200
H	5.23525300	-1.56426600	-1.33525700
H	4.92052500	-2.35924200	0.23510400
H	4.41750700	-3.15464400	-1.28232900
H	2.84316700	3.58060900	0.57970600
H	-1.55365300	-1.94975500	1.70541700
H	-3.53560000	-0.58075200	2.34030200
H	-1.45379100	-0.02955900	-2.14554900
H	-4.27374000	1.91928700	-1.25936000
H	-5.56539800	0.60577100	0.62446800
H	0.37630700	0.76153300	1.97238500
H	0.97947400	2.41626300	1.89491500
H	-0.26319800	1.88129200	0.74491200
H	-5.22011500	-1.79544900	0.08709800
O	-6.38757400	-0.34857900	0.26432000
O	-5.59907500	-1.12888600	-0.51294100

Name			**TS-MO-O7-H-OOH (Water)**
Cartesian Coordinates			Frequency and Energy
O	4.02216900	1.24759800	0.18999100
C	3.51102400	1.84547700	-1.02985800
C	2.07131300	2.23638300	-0.70879500
C	1.66176100	1.14809800	0.30082400
C	3.01785300	0.78213500	0.93660600
O	1.22995300	0.05419700	-0.51270900
C	1.10385500	-1.21214000	0.10416000
C	2.36384100	-2.05341600	-0.05479300
C	-0.10743600	-1.92047000	-0.51183400
C	-1.35301400	-1.14166600	-0.18640200
O	3.30206200	-1.45569900	-0.76883800
C	4.57287500	-2.12479700	-0.84879400
O	2.48118800	-3.14834000	0.44710300
O	3.20146400	0.15999700	1.95176800
O	1.96207500	3.54877600	-0.19750900
C	-1.86259100	-1.17044000	1.12982600
C	-2.95113500	-0.40313600	1.47749800
C	-3.56346900	0.42436400	0.51880900
C	-3.05703800	0.43906900	-0.80615000
C	-1.95347800	-0.33900300	-1.14546900
O	-3.64486900	1.20726200	-1.74262900
O	-4.60297700	1.20913200	0.81282800
C	0.62261800	1.55202200	1.32174900
H	3.56708000	1.09535400	-1.81861400
H	4.13752900	2.70244200	-1.26442000
H	1.43109100	2.18760000	-1.58773200
H	0.94853400	-1.12049700	1.18370000
H	0.03512400	-1.99471900	-1.59185300
H	-0.16278100	-2.92700500	-0.09216500
H	5.20585800	-1.47426000	-1.44582500
H	4.98368700	-2.24718900	0.15334000
H	4.45391600	-3.09406000	-1.33137600
H	2.57048700	3.66801400	0.54337800
H	-1.38153200	-1.80124600	1.86972100
H	-3.35665100	-0.41071100	2.48258400
H	-1.57445200	-0.30291300	-2.16058100

Zero-point correction= 0.339493 (Hartree/Particle)
Thermal correction to Energy= 0.364455
Thermal correction to Enthalpy= 0.365399
Thermal correction to Gibbs Free Energy= 0.282065
Sum of electronic and zero-point Energies= -1334.712414
Sum of electronic and thermal Energies= -1334.687453
Sum of electronic and thermal Enthalpies= -1334.686509
Sum of electronic and thermal Free Energies= -1334.769843

H	-4.37705100	1.69760900	-1.33657900
H	-5.50874600	0.69444900	0.52784200
H	0.42653900	0.73655000	2.02004600
H	0.97088300	2.41172600	1.89566700
H	-0.30420900	1.81581100	0.80573000
H	-5.32075400	-1.77706900	0.21900600
O	-6.35506200	-0.22551600	0.04765300
O	-5.49680500	-1.12675100	-0.48467300

Name	**TS-MO-O7-RAD-O6-OOH (Pentyl ethanoate)**

Cartesian Coordinates				Frequency and Energy
O	3.75636600	1.17891400	-0.60773000	Zero-point correction= 0.325593 (Hartree/Particle)
C	2.97678500	1.35397200	-1.81429500	Thermal correction to Energy= 0.350718
C	1.65214300	1.93313600	-1.32956800	Thermal correction to Enthalpy= 0.351662
C	1.47243700	1.19124900	0.00554200	Thermal correction to Gibbs Free Energy= 0.266577
C	2.94159200	0.98359700	0.43870200	Sum of electronic and zero-point Energies= -1334.052264
O	0.91488700	-0.07199800	-0.36040100	Sum of electronic and thermal Energies= -1334.027139
C	0.96671900	-1.10744500	0.59515600	Sum of electronic and thermal Enthalpies= -1334.026195
C	2.18996900	-2.00661300	0.43044500	Sum of electronic and thermal Free Energies= -1334.111279
C	-0.32118500	-1.93342700	0.46170600	
C	-1.50045800	-1.05584000	0.75594400	
O	2.96492400	-1.63931800	-0.58260300	
C	4.20943200	-2.34354000	-0.70920700	
O	2.41076500	-2.93607700	1.16135400	
O	3.33740700	0.69233500	1.53109100	
O	1.70094000	3.33353100	-1.17884300	
C	-1.95649300	-0.87727500	2.05661200	
C	-2.97654000	0.02473300	2.33436300	
C	-3.63858600	0.78883600	1.30344800	
C	-3.14598900	0.58966200	-0.07254200	
C	-2.09763900	-0.30393800	-0.30071700	
O	-3.71869600	1.21498300	-1.05605100	
O	-4.56828800	1.56742000	1.56026200	
C	0.63569100	1.90227000	1.04535800	
H	2.84729400	0.37796100	-2.28269800	
H	3.52251900	2.03019300	-2.46926600	
H	0.82508300	1.71189200	-2.00289800	
H	1.02698300	-0.71170200	1.61455200	
H	-0.38069000	-2.33314100	-0.55400300	
H	-0.27143400	-2.76381500	1.16770800	
H	4.70784200	-1.90742400	-1.57119400	
H	4.80876600	-2.19917400	0.19029100	
H	4.02791600	-3.40625800	-0.86924000	
H	2.50708000	3.58677000	-0.71255100	
H	-1.49617900	-1.43604600	2.86482300	
H	-3.31524600	0.18529500	3.35191700	
H	-1.70743800	-0.40371800	-1.30650700	
H	-4.06400200	0.43139400	-1.87096300	
H	0.56860000	1.31405900	1.96233900	
H	1.07274200	2.86820600	1.30075200	
H	-0.36875400	2.06714000	0.64739100	
H	-4.55041100	-1.99422400	-1.31362900	
O	-4.49632300	-0.51329800	-2.44559200	
O	-3.86530000	-1.57715900	-1.86464500	

Name	**TS-MO-O6-RAD-O7-OOH (Pentyl ethanoate)**

Cartesian Coordinates				Frequency and Energy
O	4.00803900	1.14347300	0.43895500	Zero-point correction= 0.325437 (Hartree/Particle)
C	3.58799000	1.76040200	-0.80096700	Thermal correction to Energy= 0.350612
C	2.16473700	2.23422300	-0.52706800	Thermal correction to Enthalpy= 0.351556
C	1.64397800	1.10623900	0.38008700	Thermal correction to Gibbs Free Energy= 0.266205
C	2.94134100	0.66495200	1.09494000	Sum of electronic and zero-point Energies= -1334.050668
O	1.24150000	0.07872700	-0.52629400	Sum of electronic and thermal Energies= -1334.025493
C	1.05791500	-1.21809900	-0.00436000	Sum of electronic and thermal Enthalpies= -1334.024549
C	2.30771700	-2.08716100	-0.12486800	Sum of electronic and thermal Free Energies= -1334.109900
C	-0.11550500	-1.86250400	-0.75355400	
C	-1.36781500	-1.07154300	-0.49124300	
O	3.32012800	-1.45456200	-0.70589900	
C	4.57315600	-2.15407100	-0.72295500	
O	2.34960200	-3.21883400	0.28112200	
O	3.02732700	-0.00233400	2.08609900	
O	2.12886300	3.50121400	0.08944000	
C	-2.14841700	-1.32768300	0.62451200	
C	-3.26826800	-0.51615500	0.94301600	
C	-3.64325700	0.56023700	0.13698600	
C	-2.85348300	0.85106400	-1.07361100	
C	-1.70885800	0.00862100	-1.31652400	
O	-3.15104500	1.77719400	-1.84431200	
O	-4.68559800	1.28503900	0.40936400	
C	0.53775700	1.49050600	1.33722900	
H	3.62097600	1.00544000	-1.58703500	
H	4.27403900	2.57682500	-1.01736000	
H	1.56284800	2.30171900	-1.43234200	
H	0.82047300	-1.19096100	1.06458000	
H	0.11396300	-1.87696500	-1.82208200	
H	-0.22627700	-2.89043300	-0.40532500	
H	5.27673200	-1.48588400	-1.21319000	
H	4.89477400	-2.36194900	0.29803200	
H	4.47859000	-3.08576900	-1.28063400	
H	2.76429000	3.53261100	0.81509700	
H	-1.89214400	-2.14796200	1.28664600	
H	-3.83017500	-0.70988700	1.84829000	
H	-1.10360700	0.24886600	-2.18418900	
H	-5.63181000	0.59982200	0.54514300	
H	0.24276300	0.64050300	1.95520800	
H	0.86330700	2.28956600	2.00439000	
H	-0.32622800	1.84135200	0.76734400	
H	-5.86025000	-1.71845500	-0.49831200	
O	-6.48164800	-0.22700200	0.43108800	
O	-5.79419300	-1.40824000	0.42119200	
Name				**TS-MO-O7-RAD-O6-OOH (Water)**
Cartesian Coordinates				Frequency and Energy
O	3.83739400	1.16144100	-0.43351300	Zero-point correction= 0.325965 (Hartree/Particle)
C	3.08901100	1.66799600	-1.56878700	Thermal correction to Energy= 0.350155
C	1.74752700	2.13423200	-1.00432300	Thermal correction to Enthalpy= 0.351099
C	1.56737100	1.22026400	0.22292000	Thermal correction to Gibbs Free Energy= 0.268936
C	3.02225200	0.86489500	0.57857300	Sum of electronic and zero-point Energies= -1334.065255
O	0.92924100	0.05178300	-0.30219800	Sum of electronic and thermal Energies= -1334.041066
C	0.92067700	-1.11432400	0.49669700	Sum of electronic and thermal Enthalpies= -1334.040122
C	2.15056300	-1.98649400	0.27528000	Sum of electronic and thermal Free Energies= -1334.122285

C	-0.35155200	-1.89338900	0.13480400
C	-1.54367200	-1.06934600	0.51592300
O	2.84656400	-1.63237400	-0.79127100
C	4.09167400	-2.32255300	-1.00232300
O	2.43996200	-2.90115700	1.01146700
O	3.41627300	0.36670500	1.60262200
O	1.73388000	3.51177000	-0.69516600
C	-1.94236700	-0.96675800	1.84769200
C	-2.98176700	-0.12945300	2.21409100
C	-3.71532300	0.64842800	1.24602400
C	-3.28468000	0.53813200	-0.15159300
C	-2.22027500	-0.30279700	-0.47828200
O	-3.94363100	1.18095700	-1.07902800
O	-4.67233200	1.38132000	1.57273800
C	0.80575600	1.81319900	1.38587700
H	2.97936000	0.85593700	-2.28690400
H	3.66286400	2.48658900	-1.99678700
H	0.93433100	1.96081100	-1.70669700
H	0.90404500	-0.87592700	1.56403900
H	-0.34706700	-2.09577800	-0.93803800
H	-0.34926500	-2.83903500	0.68084800
H	4.53360300	-1.86097400	-1.88076400
H	4.73424200	-2.18781200	-0.13218900
H	3.90498900	-3.38154600	-1.17626000
H	2.48033000	3.72557000	-0.12023800
H	-1.41734500	-1.53953900	2.60439400
H	-3.28148000	-0.03326800	3.25154800
H	-1.87656900	-0.33499200	-1.50523200
H	-4.37445300	0.37382700	-1.83990300
H	0.78286200	1.11994100	2.22833000
H	1.28103100	2.73562000	1.72143900
H	-0.21709400	2.03132500	1.06924400
H	-4.55748300	-2.03339000	-1.16928600
O	-4.80401800	-0.60478100	-2.35381200
O	-4.02184400	-1.60560800	-1.86221200