Absolute configuration through the DFT calculation of the optical rotation: importance of the quality of the input geometry. A caveat.

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Content of Supporting Information

(nineteen pages)

Computational details

All calculations have been carried out on a simple PC endowed with a single PentiumIV 3.16 GHz processor. The preliminary conformational distribution search has been performed by Spartan02 package using the MMFF94s molecular mechanics force field. A Systematic (at 5000K) search of all possible conformers has been performed using molecular mechanics method considering the degrees of freedom of system. The real minimum energy conformers found by molecular mechanics, have been further fully optimized at DFT/B3LYP/6-31G*, 6-31++G** levels as implemented in Gaussian03 package. All conformers are real minima, no imaginary vibrational frequencies have been found and the free energy values have been calculated and used for to get the Boltzmann population of conformers at 298.15 K. The ORD calculations have been carried out by means of time-dependent DFT methods using the hybrid B3LYP functional and the 6-31G* and 6-31++G** as available within Gaussian03. London orbitals (which ensures the origin independency of the results) have been used in optical rotation calculations.

Table 1 of SI: TDDFT/B3LYP/6-31G* OR values of **1** at 589.3 nm, calculated using various kind of input geometries (see Ref. 6b) versus experimental data.

Run	Input geometry	OR
1	DFT/B3LYP/ 6-31G*	+713
2	AM1	+723
3	PM3	+596
4	MM	+682
5	Exp.OR,($CHCl_3$)	+690
6	Exp.OR,(CH_3CN)	+660

Table 2 of SI. $[\alpha]_D$ (in deg [dm g/cm^3]$^{-1}$) for each conformer of (2R,3R,4R)-epoxidone in gas-phase and the corresponding averaged values. (X//Y means that the TDDFT/B3LYP/X level of calculation has been used for [α] using geometries and populations obtained at DFT/B3LYP/ Y level).

Conformers	6-31G*// 6-31G*	6-31G*// 6-31++G**	6-31++G**// 6-31++G**	6-31++G**// 6-31G*	aug-cc-pVDZ// 6-31G*(ref. 6a)	aug-cc-pVDZ// aug-cc-pVDZ(ref. 6a)
1	29	38	58	51	71	86
2	-98	-62	-75	-108	-89	-43
3	14	23	40	32	59	63
4	130	122	194	207	219	210
5	71	76	98	69	107	119
OR Average	**-20**	**13**	**28**	**-8**	**11**	**57**

Table 3 of SI. DFT/B3LYP/6-31G* populations at 298 K and TDDFT/B3LYP/6-31G* OR values (in deg [dm g/cm^3]$^{-1}$) for each conformer of trans-(4R,5S)-isocytoxazone in gas-phase and the corresponding averaged values. From ref. 11.

ORD Values (ref. 3a)	%pop	589.3 nm	546 nm	435 nm	405 nm
CONF **1**	3,8	-25	-30	-56	-69
CONF **2**	43,8	58	69	121	146
CONF **3**	36,9	16	19	26	27
CONF **4**	2,2	32	39	71	87
CONF **5**	3	32	37	71	87
CONF **6**	1,8	-43	-52	-93	-114
CONF **7**	1,8	251	298	514	618
CONF **8**	2,5	11	12	20	22
CONF **9**	3	103	122	211	255
CONF **10**	2,2	51	60	96	111
ORDs AVERAGE		**39**	**47**	**79**	**93**

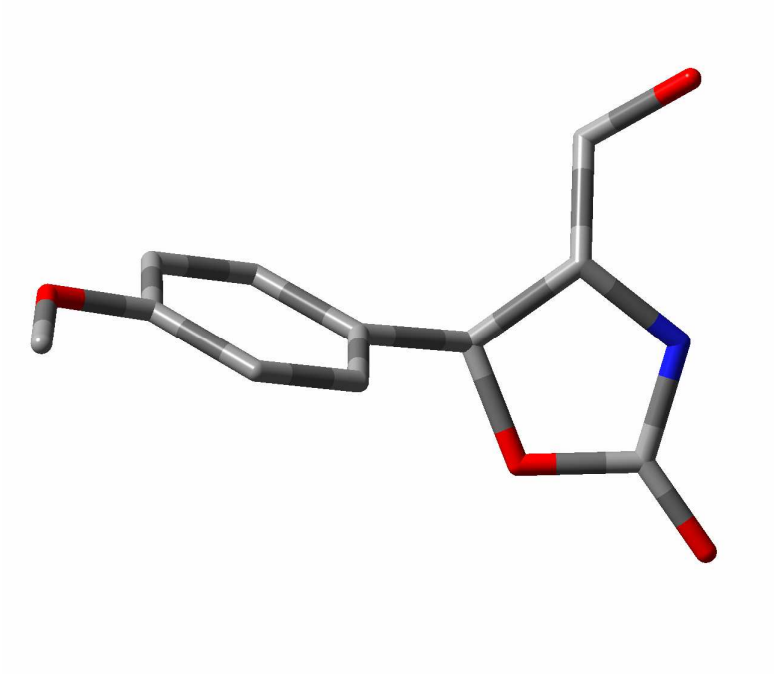
Table 4 of SI. Populations at 298 K and OR values (in deg [dm g/cm^3]$^{-1}$) for each conformer of trans-(4S,5S)- isocytoxazone in gas-phase and the corresponding averaged values. (X//Y means that the TDDFT/B3LYP/X basis set has been used for the OR using the geometries and populations obtained at DFT/B3LYP/Y basis set level).

		6-31G*//6-31++G**				6-31++G**//6-31++G**			
ORD values	**%pop**	**589.3 nm**	**546 nm**	**435 nm**	**405 nm**	**589.3 nm**	**546 nm**	**435 nm**	**405 nm**
CONF **1**	19,2	-67	-80	-142	-173	-59	-70	-123	-149
CONF **2**	17,4	-2	-2	-2,5	-2	-28	-33	-57	-69
CONF **3**	14,9	-26	-32	-62	-78	-43	-52	-95	-117
CONF **4**	5,7	28	34	64	80	0,06	0,6	5	9
CONF **5**	20,5	-21	-24	-39	-45	-21	-24	-38	-44
CONF **6**	3,4	-46	-55	-98	-120	-10	-13	-31	-42
CONF **7**	1,0	184	219	378	455	168	200	354	432
CONF **8**	8,1	-18	-22	-40	-49	-41	-50	-88	-107
CONF **9**	3,6	53	63	109	131	12	15	27	33
CONF **10**	6,2	3,4	3,1	-1,7	-6	-30	-37	-68	-84
ORDs AVERAGE		**-19**	**-23**	**-41**	**-49**	**-30**	**-36**	**-63**	**-77**

MOLECULE **5** Conformer **1**

C	-2.85118800	-1.54696900	0.04529900
O	-3.50586800	-2.55722400	-0.06594400
O	-1.61807200	-1.50763700	0.65057400
N	-3.16856000	-0.27263500	-0.36791900
H	-3.89916600	-0.15897800	-1.05626200
C	-1.14332400	-0.13815400	0.72209800
H	-1.39923700	0.24013100	1.72098600
C	-2.00335700	0.59732100	-0.33982400
H	-1.48683400	0.60413000	-1.31086400
C	-2.34270600	2.03150600	0.02759100
H	-1.41288800	2.60602000	0.14892300
H	-2.90049700	2.04490500	0.97430000
O	-3.13316200	2.55540500	-1.04056600
H	-3.42641300	3.44754400	-0.81751500
C	0.34731200	-0.06689000	0.52340200
C	3.13115800	0.13350400	0.13960800
C	0.97597000	-0.74193900	-0.52782700
C	1.13995300	0.70223200	1.38860700
C	2.51378100	0.81181600	1.20068400
C	2.35577000	-0.65185400	-0.72569400
H	0.38940700	-1.36820500	-1.19352600
H	0.67836200	1.21843000	2.22700000
H	3.12833200	1.40499400	1.86971900
H	2.80943500	-1.19709800	-1.54452100
O	4.48243100	0.29321000	0.03727700
C	5.17407800	-0.38777100	-1.00425400
H	6.22446500	-0.11954900	-0.88667300
H	4.82446500	-0.06553600	-1.99288900
H	5.06318200	-1.47517400	-0.91210400

Sum of electronic and thermal Free Energies(a.u.)= -782.508072



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C	2.97775200	-1.32308400	-0.24957300
O	3.71498400	-2.26459000	-0.42348900
O	1.76395400	-1.18257000	-0.85311900
N	3.20072800	-0.21780900	0.56223300
H	3.85808800	-0.36173400	1.31820900
C	1.15272900	0.08536300	-0.47542400
H	1.34302900	0.78882000	-1.29215200
C	1.96441700	0.53245100	0.77178300
H	1.45249700	0.22015300	1.69402600
C	2.21144500	2.04314800	0.83700200
H	2.77313400	2.27726700	1.75450600
H	1.25228300	2.56710500	0.89487700
O	2.87946200	2.54171700	-0.31010900
H	3.67752100	2.00869500	-0.44441400
C	-0.32842600	-0.06849500	-0.26360800
C	-3.10440500	-0.28362500	0.16273900
C	-0.85343300	-1.08461100	0.55481200
C	-1.21795800	0.82216100	-0.86693700
C	-2.59941800	0.73129600	-0.65780600
C	-2.22055500	-1.19630800	0.76476200
H	-0.18592400	-1.80927000	1.01226900
H	-0.83596400	1.60490500	-1.51753000
H	-3.25747000	1.44166300	-1.14342800
H	-2.63170900	-1.98501800	1.38623800
O	-4.42744600	-0.47453900	0.43486700
C	-5.37899200	0.40238000	-0.15826200
H	-6.35382300	0.06446700	0.19462400
H	-5.34696400	0.34326500	-1.25317400
H	-5.21635600	1.44014800	0.15819300

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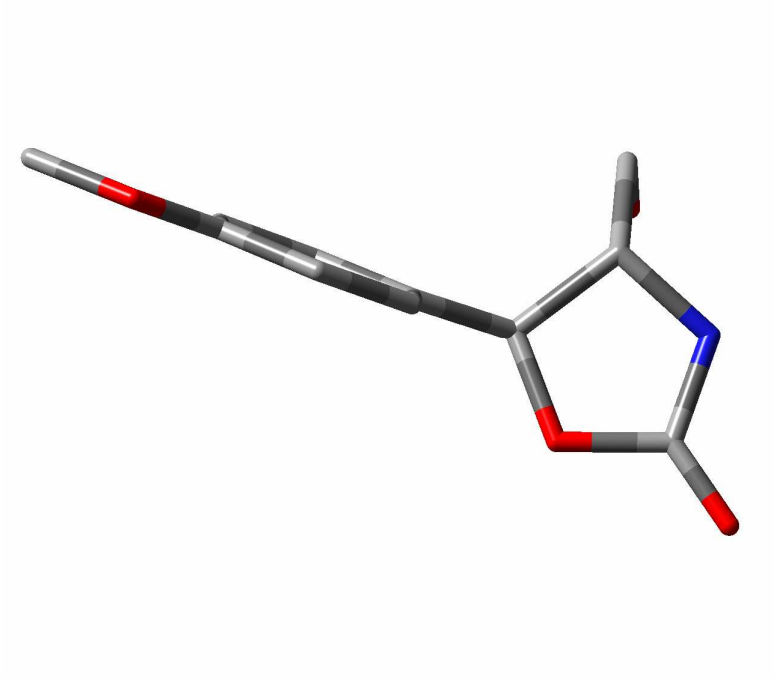

MOLECULE **5** Conformer **3**

C	2.82499300	-1.49487400	-0.19619100
O	3.46555000	-2.50810900	-0.34902400
O	1.67323600	-1.21239800	-0.86807700
N	3.11344800	-0.43579700	0.65476900
H	3.70382500	-0.66367100	1.44461800
C	1.17953600	0.10599900	-0.49761300
H	1.49643600	0.80069900	-1.28197600
C	1.95320800	0.43934900	0.80878900
H	1.35206900	0.16415400	1.68809200
C	2.35462900	1.91272000	0.93161400
H	2.88573400	2.06251400	1.88429900
H	1.45483100	2.53534200	0.95511500
O	3.13428800	2.36549800	-0.16281300
H	3.88474200	1.76121200	-0.26493700
C	-0.32075900	0.11048800	-0.37827200
C	-3.12341400	0.19170900	-0.11099900
C	-1.00671800	-0.91304600	0.28307700
C	-1.06386300	1.17364500	-0.91426800
C	-2.44717900	1.22339100	-0.77869400
C	-2.39709600	-0.88489000	0.41826100
H	-0.45679900	-1.76161100	0.67962700
H	-0.55414900	1.97080100	-1.44967700
H	-3.02416200	2.04339600	-1.19319900
H	-2.89634800	-1.70129700	0.92596400
O	-4.47975900	0.32142400	-0.03525700
C	-5.23024600	-0.70283200	0.60818900
H	-6.27320600	-0.39144900	0.54206400
H	-4.94683700	-0.80316400	1.66329000
H	-5.10534000	-1.66761300	0.10135400

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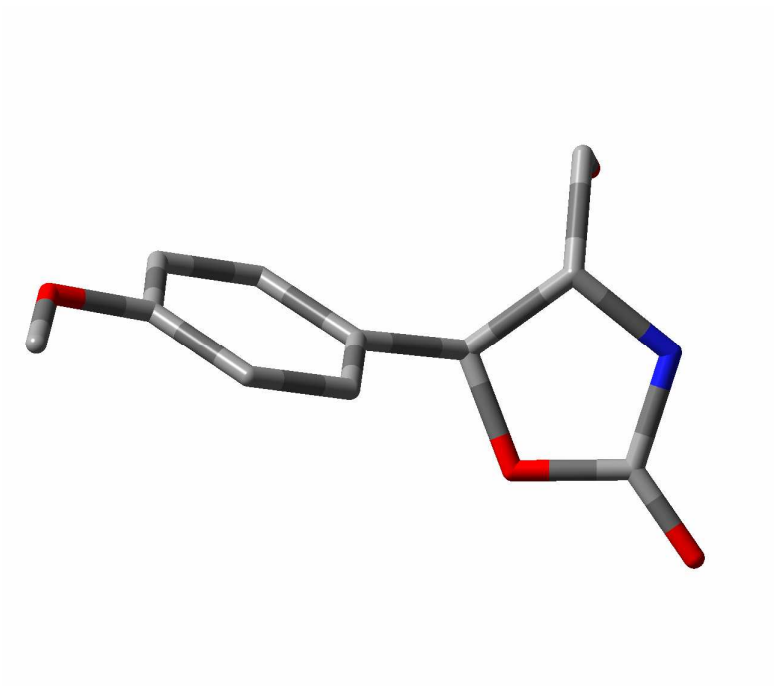
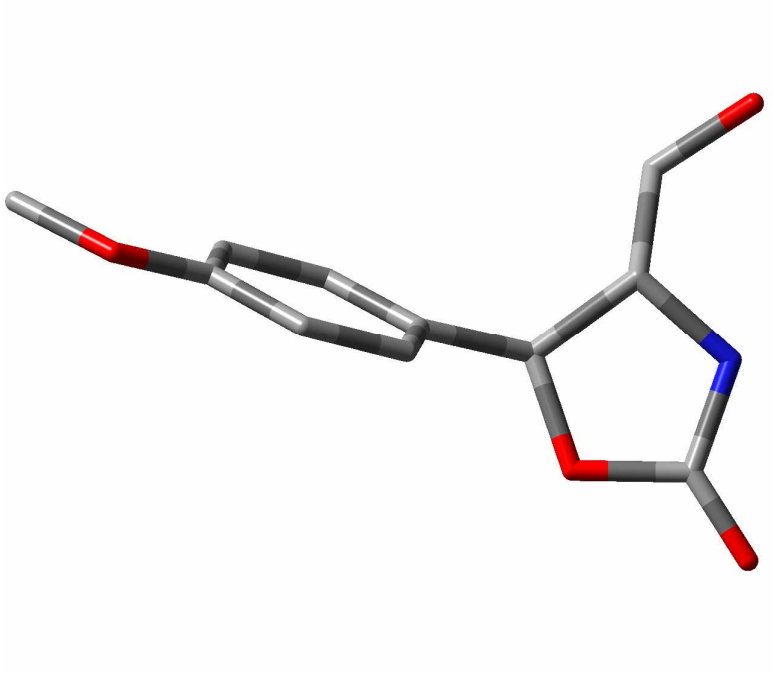


MOLECULE **5** Conformer **4**

C	-2.98687500	-1.42389200	0.10504600
O	-3.73299000	-2.37114800	0.02123800
O	-1.70167500	-1.51162600	0.58529300
N	-3.23095900	-0.11095100	-0.22677200
H	-4.03088000	0.10620200	-0.80368100
C	-1.11695500	-0.18603800	0.67662500
H	-1.25720100	0.15857900	1.71012400
C	-2.00504900	0.66708100	-0.26797900
H	-1.57113900	0.67378200	-1.28149700
C	-2.19779900	2.10808000	0.19385200
H	-1.22059900	2.60217000	0.28605100
H	-2.68652900	2.11594300	1.17255500
O	-3.06314600	2.83041700	-0.68159300
H	-2.57109600	3.09811900	-1.46880100
C	0.35169500	-0.21381200	0.34955100
C	3.09983700	-0.19764800	-0.26929100
C	0.83224800	-0.85720000	-0.80498200
C	1.27192900	0.42006200	1.18588600
C	2.63964000	0.44278800	0.88681400
C	2.18548000	-0.85331200	-1.11221000
H	0.14089200	-1.38584500	-1.45451200
H	0.92753700	0.90503900	2.09620200
H	3.32252100	0.94468300	1.56143700
H	2.56279800	-1.35718300	-1.99599200
O	4.40555000	-0.24790200	-0.66066400
C	5.38787200	0.37969500	0.15626700
H	6.34176000	0.21002200	-0.34402900
H	5.41741300	-0.06621900	1.15807300
H	5.20718900	1.45860800	0.23980000

Sum of electronic and thermal Free Energies (a.u.)= -782.506924



MOLECULE **5** Conformer **5**

C	-2.96903800	-1.43694900	0.11020900
O	-3.70255800	-2.39408000	0.02379700
O	-1.68485200	-1.50864200	0.59302400
N	-3.23225400	-0.12639700	-0.22000600
H	-4.01542000	0.06873900	-0.82739200
C	-1.11045300	-0.17673500	0.67462600
H	-1.24674200	0.16892700	1.70812100
C	-2.01186200	0.66277100	-0.26825900
H	-1.58998500	0.68453700	-1.28372800
C	-2.21462400	2.09636800	0.19160200
H	-1.23955000	2.60166400	0.24858300
H	-2.68060900	2.09928700	1.18680800
O	-3.06136800	2.72357100	-0.77260700
H	-3.26991700	3.62074700	-0.48417500
C	0.35671100	-0.19650900	0.34132400
C	3.10446400	-0.17813600	-0.27858700
C	0.83074300	-0.78987000	-0.84239700
C	1.28345800	0.38906300	1.20499300
C	2.65123500	0.41224700	0.90645200
C	2.18354600	-0.78503000	-1.15037500
H	0.13464800	-1.27897900	-1.51737500
H	0.94374200	0.83472500	2.13689200
H	3.33929200	0.87625000	1.60258500
H	2.55529700	-1.24899900	-2.05799800
O	4.40956400	-0.22226500	-0.67320600
C	5.39741700	0.36158800	0.16871300
H	6.34912400	0.20912500	-0.34121400
H	5.42662300	-0.12941000	1.14930800
H	5.22341100	1.43664600	0.30176400

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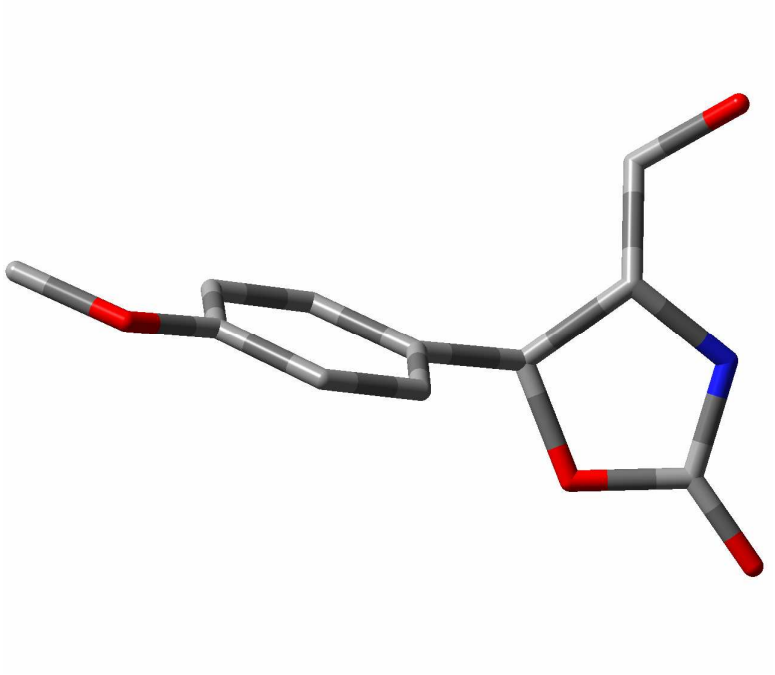
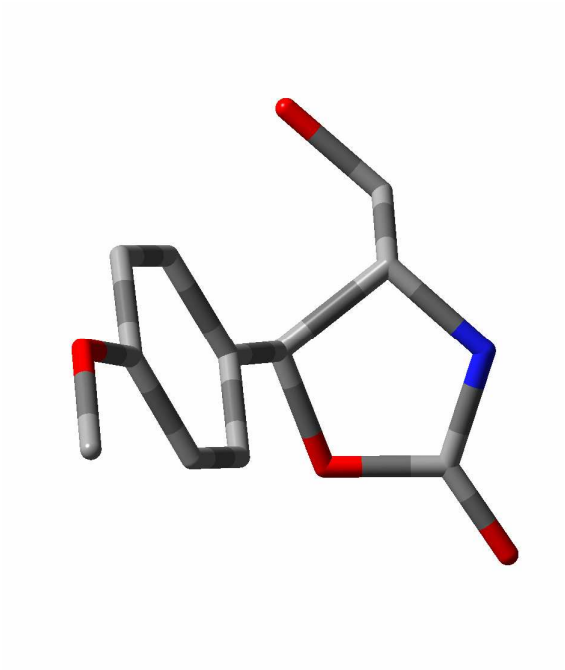


MOLECULE **5** Conformer **6**

C	2.40554600	-1.73707700	0.07190000
O	2.79945900	-2.88068300	0.09365700
O	1.71009200	-1.19221200	-0.97678400
N	2.54812800	-0.77001500	1.03456800
H	3.11282700	-0.95194800	1.84956100
C	1.25521200	0.14043800	-0.64630900
H	1.50846700	0.78210900	-1.49485200
C	2.11572700	0.54047600	0.59423000
H	1.49634600	1.03802100	1.34691100
C	3.29182300	1.45418800	0.23766100
H	3.86970200	1.00967300	-0.58516300
H	3.95380100	1.55566800	1.11016800
O	2.73764500	2.71516800	-0.13338100
H	3.43504900	3.28993100	-0.47212200
C	-0.24142500	0.17137200	-0.40613100
C	-3.01725800	0.31774400	0.04018700
C	-1.01763900	-0.98623000	-0.36778800
C	-0.87636400	1.41322000	-0.22670900
C	-2.24508500	1.49040100	-0.00443600
C	-2.39961400	-0.92356400	-0.14388500
H	-0.54920100	-1.95163100	-0.52600400
H	-0.29100500	2.32919500	-0.26355600
H	-2.74006300	2.44625200	0.13319400
H	-2.97137100	-1.84355000	-0.12159100
O	-4.35390800	0.49629900	0.26355800
C	-5.19272100	-0.65128000	0.31778700
H	-6.19910700	-0.27511000	0.50489000
H	-4.89778300	-1.32409400	1.13282100
H	-5.18008400	-1.20112000	-0.63167700

Sum of electronic and thermal Free Energies(a.u.)= -782.506446



MOLECULE **5** Conformer **7**

C	-3.10913300	-1.28232400	0.14471700
O	-3.85316900	-2.23476900	0.17204000
O	-1.92172800	-1.22554300	0.81794600
N	-3.28714400	-0.09180600	-0.53057600
H	-3.95814700	-0.08758700	-1.28563200
C	-1.26931700	0.05514400	0.61208600
H	-1.40828000	0.64175300	1.52721900
C	-2.07875300	0.71684300	-0.54807000
H	-1.53113300	0.60158800	-1.49694000
C	-2.38695700	2.20037800	-0.31363000
H	-2.93313400	2.31084400	0.62754500
H	-3.03332200	2.57633100	-1.12089700
O	-1.21158400	2.99163100	-0.18455600
H	-0.72360800	2.98751600	-1.01893300
C	0.20361500	-0.13969900	0.35178200
C	2.95407200	-0.43750900	-0.17414300
C	0.66732800	-1.17233500	-0.48104200
C	1.13871300	0.72737000	0.91918600
C	2.50797300	0.59344400	0.66136100
C	2.02335200	-1.32361400	-0.74143700
H	-0.03755600	-1.87995000	-0.90712000
H	0.80074300	1.53256800	1.56533400
H	3.20360900	1.28564900	1.12022700
H	2.38753800	-2.12633500	-1.37427000
O	4.26191300	-0.66703000	-0.49243000
C	5.25782700	0.18224300	0.06564300
H	6.21014500	-0.18471700	-0.31865500
H	5.26150500	0.12690900	1.16131400
H	5.11587000	1.22411500	-0.24788500

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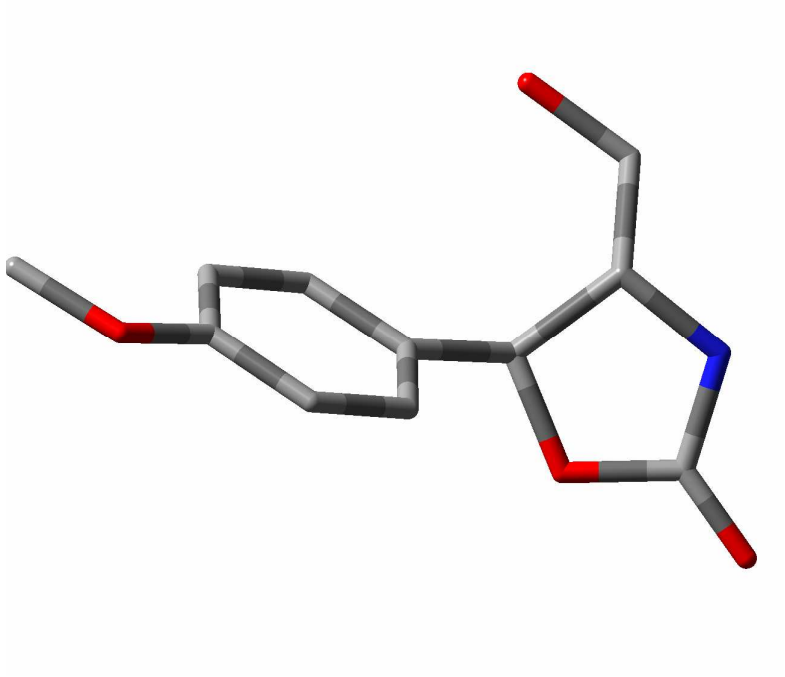
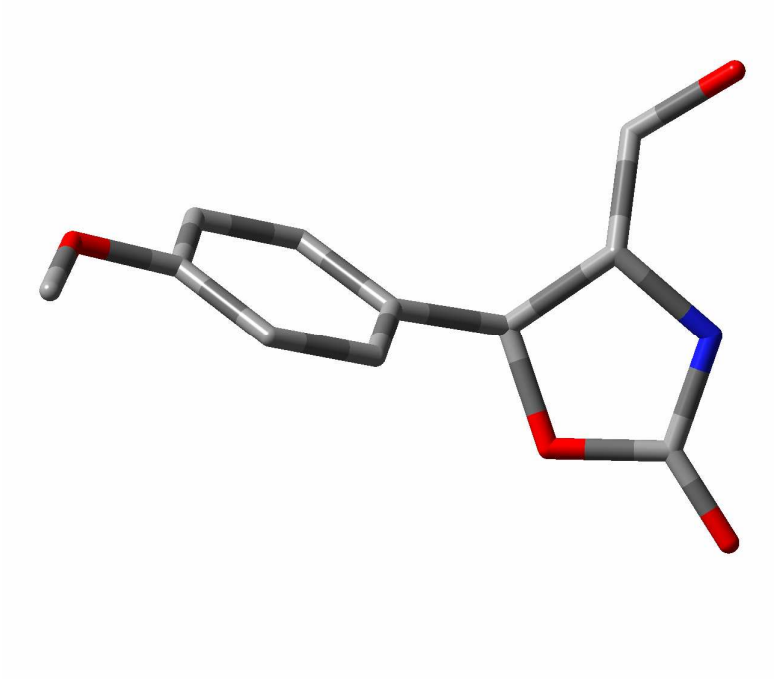


MOLECULE **5** Conformer **8**

C	-2.85734800	-1.54848500	0.04443800
O	-3.51789600	-2.55522900	-0.06148100
O	-1.62160200	-1.51370400	0.64657200
N	-3.16583500	-0.27454100	-0.37292600
H	-3.92045900	-0.14586000	-1.03163000
C	-1.14658300	-0.14599000	0.72294800
H	-1.40531900	0.23242600	1.72130600
C	-2.00306100	0.59553500	-0.33938700
H	-1.47554600	0.59290300	-1.30751200
C	-2.34714500	2.03476500	0.03074400
H	-1.42350800	2.61001400	0.18383100
H	-2.92296500	2.04527000	0.96089200
O	-3.18072900	2.64565500	-0.95367300
H	-2.63849300	2.92750500	-1.70195200
C	0.34443800	-0.07278600	0.52532000
C	3.12543600	0.14523200	0.13065400
C	0.98684300	-0.81756300	-0.46855100
C	1.12136500	0.77554600	1.32909400
C	2.49341700	0.89401000	1.13448100
C	2.36595200	-0.71919900	-0.67078500
H	0.41178900	-1.50564400	-1.08094100
H	0.64918000	1.34739500	2.12442100
H	3.09596300	1.54769900	1.75638900
H	2.83130700	-1.32078600	-1.44235900
O	4.47399100	0.31974700	0.01839700
C	5.18088600	-0.43104200	-0.96323700
H	6.22620200	-0.13663900	-0.86498300
H	4.82985000	-0.19518700	-1.97551000
H	5.08753100	-1.50920800	-0.78430700

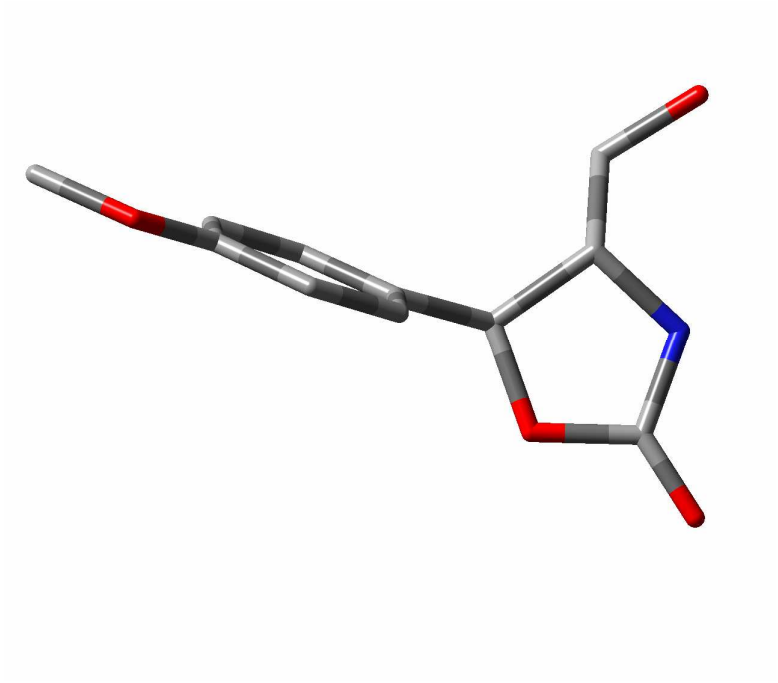
Sum of electronic and thermal Free Energies(a.u.)= -782.507256



MOLECULE **5** Conformer **9**

C	-2.93272600	-1.44831500	0.13425500
O	-3.64720100	-2.41945500	0.05385700
O	-1.67699300	-1.47268700	0.67593400
N	-3.21258200	-0.15467500	-0.27385600
H	-3.91196600	-0.06955200	-0.99929000
C	-1.10337100	-0.13765400	0.68064500
H	-1.23932200	0.26276400	1.69371700
C	-2.00018900	0.65646500	-0.30952100
H	-1.55685200	0.66148400	-1.31501000
C	-2.23911700	2.10115300	0.12628100
H	-1.29349600	2.65127400	0.08785600
H	-2.61027800	2.11874000	1.16007700
O	-3.13666100	2.78033800	-0.74862300
H	-4.04268200	2.57394000	-0.48529800
C	0.36465600	-0.17582100	0.35135500
C	3.11195700	-0.18440000	-0.26910700
C	0.84265000	-0.85250000	-0.78503200
C	1.28681000	0.47944600	1.16859500
C	2.65428200	0.49024600	0.86830300
C	2.19541800	-0.86150000	-1.09264700
H	0.15013500	-1.39466900	-1.42223000
H	0.94385800	0.99283500	2.06374500
H	3.33867400	1.01116300	1.52672700
H	2.57061600	-1.38927300	-1.96322600
O	4.41693700	-0.24900500	-0.65992000
C	5.40056000	0.40711800	0.13272700
H	6.35332900	0.22176700	-0.36411300
H	5.43337500	-0.00463600	1.14896600
H	5.21844700	1.48793900	0.17996000

Sum of electronic and thermal Free Energies (a.u.)= -782.5064810



MOLECULE **5** Conformer **10**

C	-2.80504200	-1.56682800	0.07857900
O	-3.43362100	-2.59401500	-0.02148100
O	-1.60388200	-1.47265600	0.72637800
N	-3.14425200	-0.31505200	-0.40662500
H	-3.78229100	-0.31122700	-1.19120600
C	-1.13442800	-0.09834700	0.72221000
H	-1.38882600	0.32763700	1.70156300
C	-1.99708600	0.58633900	-0.37491700
H	-1.46762300	0.58652700	-1.33791000
C	-2.38024000	2.02380500	-0.02795500
H	-1.47856800	2.64441400	-0.01158800
H	-2.84122000	2.05360900	0.96869800
O	-3.24547900	2.59471400	-1.00684200
H	-4.15410300	2.33497300	-0.80761900
C	0.35613400	-0.03271800	0.52009300
C	3.13923600	0.15726100	0.12873200
C	0.98725100	-0.75591500	-0.49699800
C	1.14545100	0.78054000	1.34714200
C	2.51892000	0.88489300	1.15489900
C	2.36688100	-0.67166400	-0.69805000
H	0.40341400	-1.41516400	-1.13274900
H	0.68134800	1.33747100	2.15754100
H	3.13090000	1.51285600	1.79379300
H	2.82281300	-1.25425100	-1.48947000
O	4.48970800	0.31560100	0.01987400
C	5.18400400	-0.40848300	-0.99051300
H	6.23318100	-0.13063300	-0.88555000
H	4.83251100	-0.13217000	-1.99226200
H	5.07793100	-1.49112500	-0.84962400

Sum of electronic and thermal Free Energies(a.u.)= -782,507005

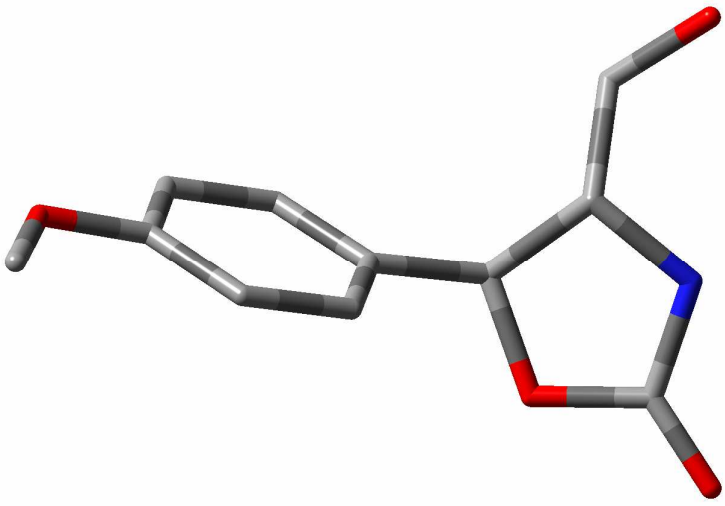
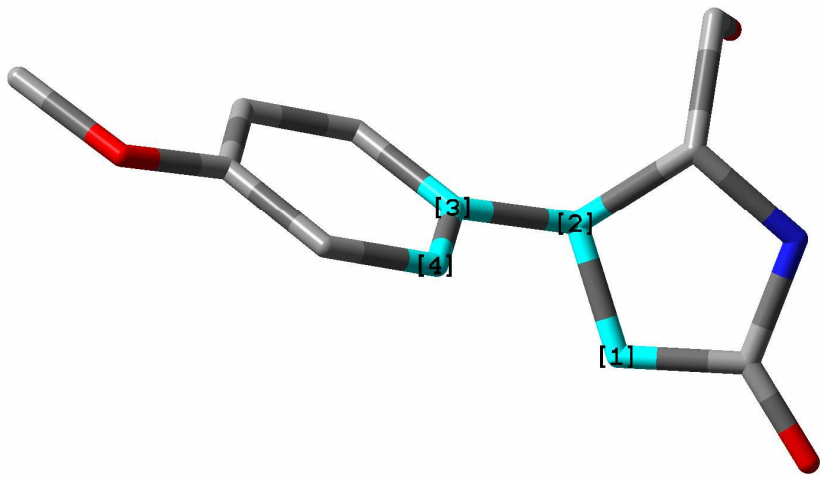


Table 5 of SI:

Epoxidone **4**			Cytoxazone **5**		
Conformers	**%pop (Emix)**	**%pop (6-31G*)**	**Conformers**	**%pop (Emix)**	**%pop (6-31G*)**
1	29.8	7.6	**1**	16.7	3.8
2	34.6	54.4	**2**	21.1	43.8
3	11.2	10.9	**3**	17.0	36.9
4	15.3	17.6	**4**	6.2	2.2
5	9.1	9.6	**5**	14.4	3.0
			6	5.1	1.8
			7	1.0	1.8
			8	6.5	2.5
			9	5.9	3.0
			10	6.1	2.2
Population used	**OR value (6-31G*)**		**Population used**	**OR value (6-31G*)**	
ΔG (6-31G*)	-20		**ΔG (6-31G*)**	+39	
E(mix)	+3		**E(mix)**	+28	

MOLECULE **5** Conformer **2**: B3LYP/6-31G* geometry and structure. Highlighted dihedral angle value is 45.1°.

C	2.99237200	-1.30667100	-0.21972200
O	3.73825000	-2.24112200	-0.36688900
O	1.77830200	-1.19145500	-0.83030600
N	3.20194000	-0.17407900	0.56539300
H	3.84697500	-0.30708100	1.33525300
C	1.15741400	0.07351100	-0.48055400
H	1.35921800	0.77429100	-1.29778800
C	1.94623800	0.54402200	0.77184700
H	1.43564900	0.22066100	1.69135800
C	2.16310400	2.06006100	0.81508300
H	2.69885900	2.32158700	1.74311100
H	1.19293200	2.56764600	0.84393900
O	2.84527300	2.53355400	-0.32885500
H	3.61486900	1.94884700	-0.44523400
C	-0.32508800	-0.08468800	-0.28268400
C	-3.09839400	-0.30155200	0.14398600
C	-0.85476100	-1.15206800	0.46147600
C	-1.20740900	0.85666800	-0.81344900
C	-2.58650500	0.76459500	-0.60292100
C	-2.22062800	-1.26376200	0.67116400
H	-0.18898800	-1.91328100	0.85823000
H	-0.81995100	1.68126000	-1.40758900
H	-3.24136400	1.51450500	-1.03119000
H	-2.63871800	-2.09096600	1.23611700
O	-4.41989400	-0.50035800	0.41092000
C	-5.35859900	0.42954000	-0.10799300
H	-6.33849400	0.08074700	0.22238100
H	-5.33396000	0.45694000	-1.20522700
H	-5.18251300	1.44051100	0.28253300



MOLECULE **5** Conformer **2**: B3LYP/6-311++G(2d,2p) geometry and structure. Highlighted dihedral angle value is 49.5°.

C	2.95953100	-1.32694500	-0.24340500
O	3.68104400	-2.27166800	-0.40660000
O	1.75969700	-1.17032800	-0.86470800
N	3.18463600	-0.22827000	0.57174100
H	3.81802800	-0.38738000	1.33913400
C	1.14869200	0.09210400	-0.47988200
H	1.33527500	0.79664300	-1.28972900
C	1.95656900	0.53481300	0.76693300
H	1.43681600	0.23334900	1.68195900
C	2.21464000	2.03902000	0.82924300
H	2.76521500	2.27213100	1.74786300
H	1.26300000	2.56832200	0.87536500
O	2.89876400	2.53035600	-0.30993400
H	3.68685500	1.98997900	-0.43777300
C	-0.32937700	-0.06341200	-0.26808200
C	-3.09430000	-0.28441000	0.15967600
C	-0.85092800	-1.08790300	0.53169600
C	-1.21658500	0.83218300	-0.85213400
C	-2.59198700	0.73809000	-0.64237500
C	-2.21135900	-1.20210400	0.74202300
H	-0.18580600	-1.81690600	0.97470300
H	-0.83800200	1.62108700	-1.48945900
H	-3.24865500	1.45251900	-1.11344200
H	-2.61810200	-1.99795500	1.34942000
O	-4.41379300	-0.47899000	0.43124100
C	-5.36087300	0.41246600	-0.14346200
H	-6.33318000	0.07581800	0.20314400
H	-5.33126600	0.37306700	-1.23441800
H	-5.19246600	1.43884200	0.18968300