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Abstract: Catalytic cycle intermediates of a representative extradiol dioxygenase - homoprotocatechuate 2,3-dioxygenase (HPCD) have recently been characterized in crystallo by Kovaleva and Lipscomb. Structures of the identified species indicate that the process of oxygen insertion into the catechol ring is stepwise, and involves an Fe(II)-alkylperoxo intermediate and its O-O cleavage product - a gem diol species. In general, these findings corroborate the results of our previous computational studies, yet, the fact that the gem diol species is stable enough to be observed in the crystal form seems to be at odds with the computational mechanistic data, which suggests that this intermediate very readily and spontaneously should convert to the epoxide species. The key question then becomes what is actually observed in the X-ray experiments. Here we report additional computational studies undertaken with the hope to clarify this issue. The results obtained for active site models, hosting both native and the alternative substrate - 4-sulfonylecatechol, indicate that the stability of the gem diol species is substantially increased if an electron and a proton are added. If this occurs somehow, the life-time of the intermediate should be sufficient for observation.

Response to Reviewers: In the revised version of the manuscript we have followed the suggestions of the Referees and:

- 1) moved Computational Details from Supporting Information to the manuscript
- 2) included the results of additional calculations with a larger (15) dielectric constant, the results are in Table 1
- 3) performed Solvent Accessible Surface Area to support the choice of a small dielectric constant

On the observation of a gem diol intermediate after O-O bond cleavage by extradiol dioxygenases. A Hybrid DFT Study.

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Abstract

Catalytic cycle intermediates of a representative extradiol dioxygenase - homoprotocatechuate 2,3-dioxygenase (HPCD) have recently been characterized *in crystallo* by Kovaleva and Lipscomb. Structures of the identified species indicate that the process of oxygen insertion into the catechol ring is stepwise, and involves an Fe(II)-alkylperoxo intermediate and its O-O cleavage product - a gem diol species. In general, these findings corroborate the results of our previous computational studies, yet, the fact that the gem diol species is stable enough to be observed in the crystal form seems to be at odds with the computational mechanistic data, which suggests that this intermediate very readily and spontaneously should convert to the epoxide species. The key question then becomes what is actually observed in the X-ray experiments. Here we report additional computational studies undertaken with the hope to clarify this issue. The results obtained for active site models, hosting both native and the alternative substrate - 4-sulfonylcatechol, indicate that the stability of the gem diol species is substantially increased if an electron and a proton are added. If this occurs somehow, the life-time of the intermediate should be sufficient for observation.

Keywords: homoprotocatechuate 2,3-dioxygenase, extradiol, ring cleavage, density functional calculations.

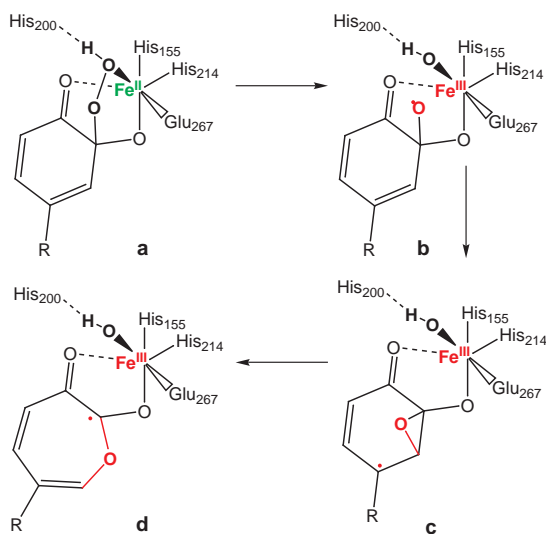


Figure 1: Reaction mechanism for O-O and C-C bond cleavage by extradiol dioxygenases as derived from previous computational studies.

Extradiol dioxygenases are mononuclear metalloenzymes hosting a single Fe(II) or Mn(II) ion in their active site. The inorganic cofactor is coordinated by three protein ligands forming the 2-His-1-carboxylate facial triad motif, whereas the three remaining coordination sites are used by the catecholic and O₂ substrates. The catalytic reaction involves oxidative cleavage of the C-C bond adjacent to the diol group of the catecholic substrate, and leads to 2-hydroxymuconaldehyde acids.

Our previous computational studies on Fe- and Mn-dependent extradiol dioxygenases [1–3], and a related homogentisate dioxygenase [4], suggest that the catalytic reaction proceeds through a bidentate coordination of catecholic substrate to the metal ion and subsequent trapping of dioxygen, which leads to a species with a peroxide bridge between the metal ion and the catecholic ring (**a** in Fig. 1). In the subsequent step the O-O bond is cleaved homolytically yielding an alkoxyl radical species (**b**). This is predicted to be a short-lived intermediate that easily and spontaneously converts to the epoxide species (**c**). The exothermicity of this step (**b** → **c**) exceeds 10 kcal/mol. Expansion of the oxirane ring, via C-C bond cleavage (**c** → **d**), followed by hydrolysis of the cyclic lacton, finish the chemical steps of the catalytic reaction.

Recently, Kovaleva and Lipscomb have characterized crystal structures of several oxygenated intermediates of homoprotocatechuate 2,3-dioxygenase (HPCD) [5, 6]. In the first

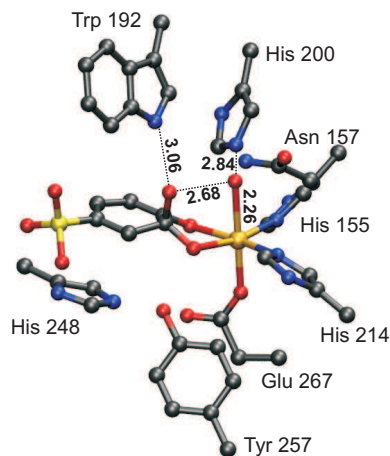


Figure 2: The active site region in the X-ray structure of the gem diol intermediate (PDB code: 3ECK, chain C).

study, a slow alternative substrate - 4-nitrocatechol has been used and this has allowed for trapping three intermediates, including the alkylperoxo species with a peroxo bridge between the substrate molecule and iron (**a** in Fig. 1) [5]. With the use of another alternative substrate, 4-sulfonylcatechol (4SC), and by introducing a single point mutation that alters the crystal packing (Glu323Leu), the next intermediate was trapped and characterized [6]. This species has the O-O bond cleaved and a structure of a gem diol (Fig. 2). Based on computational studies it was previously proposed that such an intermediate participates in the catalytic cycle. This intermediate was found to have radical character on an oxygen on the ring, see Fig. 1b. However, its stability, allowing for a successful X-ray structure determination, seems to be in conflict with the energetic data derived from the computations. More specifically, in the previous work devoted to the mechanism of extradiol dioxygenases, the calculated barriers and exothermicity for the conversion of the gem diol intermediate into the epoxide species (**b** \rightarrow **c** in Fig. 1) are around 0 and 13 kcal/mol, respectively [1,3,4]. Thus, this particular step of the catalytic cycle should proceed efficiently and practically irreversibly, which in turn, would make it impossible to observe the gem diol intermediate.

Kovaleva and Lipscomb proposed three plausible origins of this apparent discrepancy [6]: (1) at the stage of the gem diol intermediate the active site provides a somewhat

different environment than in the enzyme-substrate complex, whose structure was used as a starting point in the previous calculations; (2) 4SC has a different reactivity than homoprotocatechuate (HPCA), which was the substrate in the previous calculations; and (3) crystal packing forces, which were not accounted for in the computations, are important for stabilizing this gem diol intermediate. To these three suggestions can, of course, be added that the method or model used in the previous calculations could have a very much larger error than usual. These possibilities, and others, will be discussed below.

The active site models used in this study are based on the crystal structure of the enzyme - gem diol intermediate complex (PDB code: 3ECK), and thus the first plausible source of differences (point 1 above) is eliminated. Moreover, the computations were performed for both native (HPCA) and alternative (4SC) substrates, and by comparing the results it is possible to estimate to what extent 4SC differs in reactivity from HPCA (see point 2 above).

The first question addressed is if it could be possible that another, similar, species is observed in the experiments, rather than the radical intermediate obtained in the previous calculations. Computations were therefore first made for that radical and for the subsequent epoxide species, and the results were compared to the ones obtained by adding either one electron, or one electron and one proton, or two electrons and one proton to the radical. The **radical** gem diol and epoxide species are the ones encountered in the native catalytic cycle. In the **radical** + e^- form, one additional electron has reduced the alkoxyl radical to an alkoxyl anion. In the **radical** + e^- + H^+ variant the alkoxyl anion was protonated to form a charge neutral hydroxyl group, whereas the **radical** + $2e^-$ + H^+ species features an OH group and a high spin Fe(II), as opposed to other forms where iron is present as the high spin Fe(III) ion.

The results reported here have been obtained with the hybrid B3LYP functional [7,8] using the Jaguar [9] and Gaussian 03 [10] programs. The models and methods employed in this study are described in full length in Computational Details.

The calculated energy difference between the epoxide and the gem diol species and the distance between the two atoms derived from dioxygen are reported in Table 1, both for the native and the alternative (4-sulfonylcatechol) substrates. The optimized structures of the **radical** + e^- + H^+ forms of the gem diol and epoxide species for the 4-sulfonylcatechol

Table 1: Computed energy difference and interatomic distance for various redox forms of the gem diol and epoxide species. ΔE is the energy difference between the epoxide and gem diol species including the solvent effect calculated with the dielectric constant of 4, in parentheses the values calculated with the dielectric constant of 15; r_{O-O} is the distance between the two oxygen atoms derived from dioxygen in the gem diol; in the X-ray structure $r_{O-O}=2.68$ Å.

redox form	homoprotocatechuate		4-sulfonylcatechol	
	ΔE [kcal/mol]	r_{O-O} [Å]	ΔE [kcal/mol]	r_{O-O} [Å]
radical	-17.7 (-17.2)	2.80	-15.4 (-14.5)	2.97
radical + e^-	-10.8 (-11.1)	3.04	-12.8 (-12.8)	3.16
radical + e^- + H^+	+5.7 (+6.8)	2.52	+5.6 (+4.9)	2.56
radical + $2e^-$ + H^+	+5.0 (+4.7)	2.51	+0.1 (-1.2)	2.52

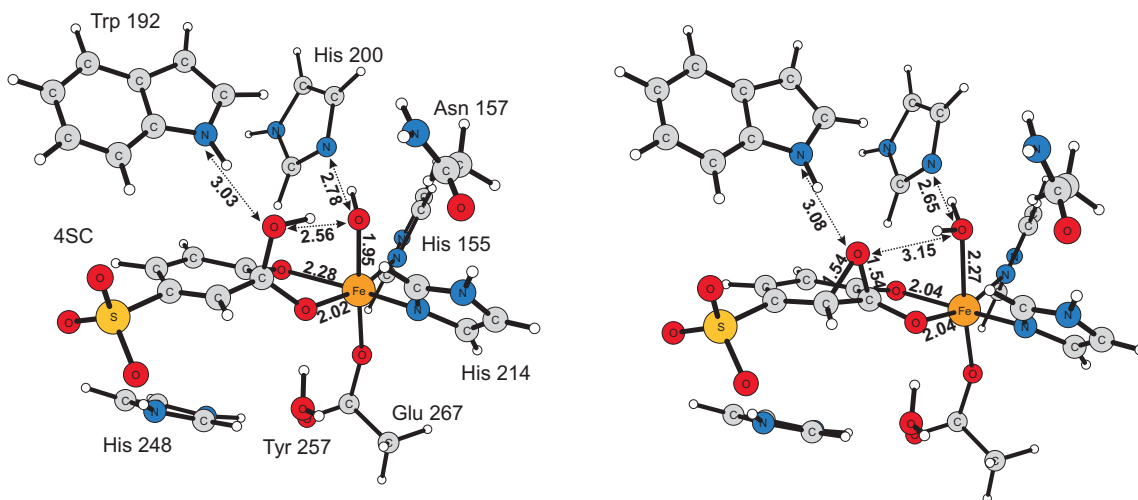


Figure 3: Optimized structures of the gem diol (left) and the epoxide (right) species for the 4-sulfonylcatechol substrate in the **radical** + e^- + H^+ form.

substrate are presented in Fig. 3.

The results presented in Table 1 show that there are no big differences between active sites hosting 4SC or HPCA concerning the relative stabilities of the epoxide and gem diol species. For both substrates, in the **radical** and **radical** + e^- forms, it is the epoxide intermediate which is more stable, whereas for the **radical** + e^- + H^+ and **radical** + $2e^-$ + H^+ variants, the gem diol species has a lower energy than the epoxide. This means that one of the suggestions in the experimental paper for why the gem diol species is observed for 4SC only, is not supported by the calculations.

In the crystal structure of the gem diol the distance between the two atoms derived

from dioxygen is 2.68 Å, which might suggest that a hydrogen bond is present between these two oxygens. In the models for the gem diol in the **radical** + e^- + H^+ and **radical** + 2e^- + H^+ forms, there is indeed such a hydrogen bond present, and the O—O distance ranges from 2.51 to 2.56 Å, somewhat shorter than the X-ray value, a typical discrepancy using the present basis set.

Concerning the relative energies, the data gathered in Table 1 show that for the “native” and reduced forms obtained without protonating the alkoxyl oxygen, i.e. **radical** and **radical** + e^- , the gem diol species is markedly less stable than the epoxide intermediate. The energy difference is larger than 10 kcal/mol, which is in line with the results obtained previously for the **radical** forms produced during the catalytic cycle [1,3,4]. Importantly, for the reduced forms that feature a neutral hydroxyl group, i.e. **radical** + e^- + H^+ , the transformation of the gem diol into the epoxide species is an endothermic reaction. This is also true for the **radical** + 2e^- + H^+ species for the natural substrate, but not for the 4-sulfonylcatechol substrate, which makes this double reduction less likely. As can be noticed in Fig. 3, closure of the epoxide ring requires in this case that a proton of the gem diolate hydroxide is shuttled to the hydroxide ligand bound to iron. In the case of the **radical** + e^- + H^+ form the gem diol species are more than 5 kcal/mol more stable than the epoxide. This energy difference is sufficient to make gem diol the prevalent species observed in the X-ray structure.

To test if the method employed is not biased towards the epoxide or the gem diol species, a benchmark computation was performed for a small monoprotonated model derived from catechol only. In the case of the standard DFT method the computed energy difference is -0.5 kcal/mol, whereas the very accurate G2 scheme [11] yields +0.2 kcal/mol. This good numerical agreement shows that for the present case a big error of the DFT method is quite unlikely.

These computational results suggest that the first two possibilities given in the experimental paper, to rationalize the discrepancy between theory and experiments are both unlikely. A simple structural argument can be brought against the third suggestion: the transformation of the gem diol into the epoxide intermediate requires only a rather small geometry change of the substrate molecule and the active site residues hardly interfere with this process. Moreover, in the present calculations the backbone atoms were frozen from

the X-ray structure where the intermediate was observed, and any strain effect from crystal packing should therefore be included in the computed results. It could be added that a large strain effect on the relative energies of the quite similar species as the gem diol and the epoxide, of more than 10 kcal/mol is required to yield enough stability for the gem diol. Such a large effect on a case like this has never been observed in model calculations.

The above calculations have thus answered the main questions raised in the present study, and the most likely answer is that somehow a reduction and protonation has occurred. The question of how this has occurred is probably best answered by expert experimentalists. X-ray reduction is a common phenomenon in X-ray structural studies [14]. Another tentative suggestion is that the gem diol species in the **radical** + e^- + H^+ form is obtained, by first forming a hydrogen peroxide that binds to iron. Such a reduced and protonated peroxo species is calculated to be markedly less stable than the gem diol, for 4SC and HPCA. It lies 37.6 and 34.2 kcal/mol, respectively, higher in energy. Thus, for the **radical** + e^- + H^+ redox form, the gem diol is more stable than both the preceding and subsequent intermediate, which could lead to its observation in the X-ray experiment.

Another possibility could be that the reduced species is formed by first oxidizing the diol substrate to an orthoquinone, and the hydrating one of the carbonyls. This is a process commonly observed for biomimetic species [15]. One problem with this explanation is that it is difficult to see why this happens only for the 4SC substrate and not for the native HPCD one.

In summary, based on the computed energy difference between the gem diol and epoxide species, that has been calculated for various redox forms, we propose that the experimentally observed gem diol intermediate is obtained by reduction and protonation of some intermediate of the “native” catalytic cycle. The observed species should therefore not be an intermediate of that cycle itself, at least according to any mechanism suggested so far.

Computational Details

The models of the homoprotocatechuate 2,3-dioxygenase active site are based on the crystal structure solved for the (mutated) enzyme complexed with 4-sulfonylcatechol (PDB code: 3ECK, chain C). Two models were used: one with 4-sulfonylcatechol, and the other with the native substrate - homoprotocatechuate. Besides the substrate, the models in-

cluded four histidine side chains (His155, His200, His214 and His248) modeled with imidazoles, Glu267 and Asn157 represented by acetate and acetamide, respectively, and Tyr257 and Trp192 truncated to water and indol.

Restrained optimizations were performed with several terminal atoms (marked with asterisk in the first coordinate listing in Supporting Information) constrained to their positions in the crystal structure. In this way, the rigidity of the protein backbone was taken into account in the model.

Calculations were performed with two programs, Gaussian03 [10] and Jaguar [9], employing hybrid DFT with the B3LYP exchange-correlation functional [7,8], whereas in the benchmark computations for a small model also the G2 extrapolation scheme was used [11]. Geometry optimizations were done with a valence double-zeta basis set coupled with an effective core potential describing the innermost electrons on iron. This particular basis set is labeled lacvp in Jaguar. For the optimized structures the electronic energy was computed with a bigger basis set of triple-zeta quality with polarization functions on all atoms except iron (lacv3p+ for iron and cc-pVTZ(-f) for other atoms). The solvent corrections were calculated with the self-consistent reaction field method implemented in Jaguar [12,13]. Two dielectric constant of 4 and 15 together with a probe radius of 1.4 Å were used to model the protein surrounding of the active site. The smaller value would correspond to a buried and hydrophobic surroundings of the active site, whereas the larger to a more solvent exposed site. Visual inspection of the protein structure reveals that the active site is buried with none of the amino acid side chains depicted in Fig. 2 exposed to solvent. This observation is corroborated by the results of solvent accessible surface area calculations performed with the program Surface Racer 5 [16]. For seven residues the calculated solvent accessible surface area is zero, and only for one, namely His248, it is 0.5 Å² (Richards van der Waals radii together with a probe radius of 1.4 Å were used in this calculation). Thus, the results obtained with a low dielectric constant should be reliable.

The electronic state for the **radical** form is a spin quintet with the high spin Fe(III) antiferromagnetically coupled with the organic radical. In the **radical** + e⁻ form, the high spin configuration on Fe(III) results in the sextet ground state; the spin quartet lies around 15 kcal/mol higher in energy. Similarly, for the **radical** + e⁻ + H⁺ form, spin sextet is the ground state with the quartet at least 7 kcal/mol less stable. Finally, for the **radical**

+ $2e^-$ + H^+ form the ground state is a spin quintet with high spin Fe(II).

Acknowledgments

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Supporting Information Available:

Cartesian coordinates and calculated energies for all structures. This material is available free of charge via the Internet at <http://xxx>

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Supporting Information for the Manuscript:

**“On the observation of a gem diol intermediate after
O-O bond cleavage by extradiol dioxygenases. A
Hybrid DFT Study.”**

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1 Cartesian coordinates and energies for optimized structures

4-sulfonylcatechol : radical : gem diol

E lacvp = -3061.787511

H(*)	20.5454729912	35.5478670798	38.8164249805
C	20.4528646772	36.2676780249	38.0146124885
N	20.9554710177	36.0528738262	36.7270563189
C	19.9641058014	37.5484165270	38.0065545728
C	20.7647431944	37.1920357708	35.9930715664
N	20.1745778516	38.1203452234	36.7486737663
H	17.3449127422	40.6461153295	41.2136191622
C(*)	17.2520009320	40.8040010011	40.1320000637
C	17.5672240569	42.2536450632	39.8052929354
O	16.6632962723	43.1311003633	39.7363319238
N	18.8831941548	42.5206764991	39.5962184168
H(*)	25.2808687232	40.9541400991	42.6521445573
C	24.9819596957	41.7066710929	41.9301579328
C	23.8459547562	41.6631580189	41.1477083876
C	25.6734196905	42.9306369384	41.5988410165
N	23.7874231065	42.7870590516	40.3397791155
C	24.8951868569	43.5896230594	40.5939904946
C	26.8618236809	43.5421950232	42.0421102525
C	25.2746992948	44.8163001908	40.0333038754
C	27.2442573345	44.7648819848	41.4873241128
C	26.4620798734	45.3925112364	40.4939911354
H(*)	23.9726830293	37.1214329846	41.5313610379
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C	22.3670598583	38.4397733462	40.7143704195
C	23.3159103252	38.6602699848	38.7550280950
N	22.2504412335	39.0386439705	39.4604132755
H(*)	14.9011790388	40.6201100244	36.0719110301
C	15.9449782263	40.8496653005	36.1775713055
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C	17.7605683299	42.0352720379	36.7119390234
N	18.1909219448	40.8908195794	36.1770424653
H(*)	26.2447090195	43.8340069987	33.3687670351
C	25.3143070812	43.3450849306	33.1100143318
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C	25.0020850278	42.0352576406	32.8384542961
C	23.0887392437	43.1929851112	32.8882979991
N	23.6144438873	41.9643860409	32.7108111374
H(*)	19.4852371287	43.7230800479	33.5937001696
O	20.2818719873	43.1673061649	33.6108036016
H	18.4607370592	39.3881706026	32.6602184958
C(*)	19.2579991075	40.0299989870	32.2789990720
C	20.4986837331	39.9523418157	33.1620173528
O	20.2759435457	39.7509022440	34.4485578165
O	21.6481966387	40.0803049680	32.6578742284
Fe	20.2059285994	40.3229753765	36.3473171704
O	22.4778674851	40.3522840850	36.5246826097
C	22.9107976488	41.5289002364	36.6999936732
C	21.8637842930	42.6633640371	36.7594918629
O	21.6394905280	42.9619545232	38.1408584716
O	20.7386714795	42.2763694970	36.0487752253
C	22.4601460519	44.0241995269	36.3921789126
C	24.3079606357	41.8411593306	36.8669145693
C	24.7318426008	43.1310321902	36.7197636700
C	23.7998735832	44.1891269526	36.4175323085
S	24.5895387676	45.8384262496	35.8838125673
O	26.1055102510	45.3429814515	35.4469214417

O	24.4914388316	46.8780132647	37.1467725865
O	23.6354910205	46.2457731442	34.5655469257
O	20.2548747149	40.4720507736	38.2255980781
H	21.3784019836	35.2028382665	36.3903430664
H	21.0629365139	37.3301933315	34.9689107282
H	19.5271410769	38.1228510328	38.8007242200
H	16.2226445650	40.5807996178	39.8441105726
H	17.9437729057	40.1261497148	39.6233676983
H	19.5320718644	41.7858123986	39.2828443394
H	19.1645910497	43.4786644838	39.4391050570
H	23.0716106170	40.9179872831	41.0971581302
H	23.0613041044	42.9652558535	39.6521655459
H	24.6821589350	45.3215624003	39.2767746510
H	26.7808846768	46.3405190725	40.0743320443
H	28.1580138703	45.2444197904	41.8245575646
H	27.4716635856	43.0702819664	42.8071990517
H	24.9989639788	37.4524036415	39.2283955669
H	23.5074016367	38.9395932426	37.7341698669
H	20.9758054605	39.9958951481	38.7432670322
H	21.6276466462	38.5885437948	41.4826787425
H	15.8533769691	42.7315910921	37.2355841410
H	18.3948773000	42.8089851758	37.0991749488
H	17.1604920011	39.1790605669	35.3578442426
H	23.9727009581	45.0261113230	33.4782180658
H	22.0193218891	43.4069038032	32.9358537360
H	23.0105240800	41.1262019943	32.6141811339
H	25.6308544613	41.1688166513	32.7388873673
H	20.4386607826	42.8231987293	34.5419328965
H	18.9142840342	41.0710944336	32.3007191255
H	19.5097652647	39.7654342140	31.2501720945
H	21.7630861393	44.8239556496	36.1740565449
H	25.7827538775	43.3983964905	36.7503388531
H	25.0114771609	41.0266997348	36.9922195131

4-sulfonylcatechol : radical : epoxide

E_{lacvp} = -3061.799130

H	20.5454729999	35.5478669999	38.8164250000
C	20.4545753540	36.2629425419	38.0116027361
N	20.9568072461	36.0439037591	36.7247140040
C	19.9657131632	37.5430896288	38.0007824430
C	20.7673982653	37.1808869627	35.9877687333
N	20.1777027019	38.1110112211	36.7417435834
H	17.3618710875	40.6629889151	41.2142365674
C	17.2520009999	40.8040009999	40.1320000000
C	17.5693619659	42.2466739075	39.7752922357
O	16.6667689881	43.1216870893	39.6727816136
N	18.8889641453	42.5120987462	39.5771446448
H	25.2808690000	40.9541400000	42.6521449999
C	25.0400711147	41.7127436347	41.9139560306
C	23.9239099013	41.7309024100	41.1033339588
C	25.8117923206	42.8911719476	41.5927442900
N	23.9556709963	42.8509719750	40.2841103334
C	25.0990869777	43.5909441991	40.5680235708
C	27.0234880341	43.4304832784	42.0623541517
C	25.5560420337	44.7985945765	40.0237360997
C	27.4895923125	44.6284739729	41.5167354657
C	26.7648667102	45.3032526388	40.5109212220
H	23.9726830000	37.1214330001	41.5313609999
C	23.5169483844	37.7195700371	40.7742128857
N	24.0963757046	37.8859472145	39.5233704199
C	22.3578151148	38.4540728331	40.7542303624
C	23.2869312054	38.7103680059	38.7883880566
N	22.2263229751	39.0715602431	39.5106485065
H	14.9011790001	40.6201100001	36.0719110000
C	15.9486687296	40.8445446667	36.1696975071

N	16.4111560577	42.0414399318	36.7158409157
C	17.0693974598	40.1313619780	35.8200788044
C	17.7707439883	42.0295676451	36.6854543301
N	18.1973596255	40.8786131628	36.1608046080
H	26.2447089999	43.8340070000	33.3687670000
C	25.3150514416	43.3341903859	33.1306703320
N	24.0987004269	44.0109495872	33.1916726609
C	25.0160424664	42.0257375347	32.8367948144
C	23.0883496437	43.1525114145	32.9609348465
N	23.6270236441	41.9363856658	32.7418057871
H	19.4852370001	43.7230799999	33.5937000001
O	20.2544192955	43.1315133789	33.6287524263
H	18.4654746111	39.3808847801	32.6583628784
C	19.2579990000	40.0299990000	32.2789990000
C	20.5055405426	39.9464027172	33.1514216268
O	20.3016837771	39.7382571744	34.4400615535
O	21.6485864656	40.0761915885	32.6311445892
Fe	20.2171891781	40.2947713086	36.3521057066
O	22.4779920106	40.3294671836	36.4576768358
C	22.9330330225	41.5188634974	36.6286943274
C	21.9234287897	42.6340985154	36.6142558324
O	21.9681853509	43.4160720252	37.9188560876
O	20.7337697950	42.2884630132	36.0839487133
C	22.4808664612	44.0446677897	36.6255266857
C	24.3193355555	41.8104130884	36.7821286461
C	24.7952107924	43.1274150119	36.6958567066
C	23.9232810021	44.1873195608	36.5241773533
S	24.6340698236	45.8366522213	35.9708195525
O	26.1653175601	45.4540974376	35.4898944985
O	24.4799396120	46.8789477387	37.2279907599
O	23.6054451809	46.1615409102	34.6778978078
O	20.2406911516	40.4502669376	38.2215517266
H	21.3803198283	35.1930404165	36.3908036025
H	21.0669743997	37.3183194179	34.9639432366
H	19.5284948081	38.1198977397	38.7929852402
H	16.2181357761	40.5811043097	39.8615572035
H	17.9343889872	40.1158700360	39.6241897166
H	19.5338965314	41.7676764800	39.2772310430
H	19.1679556007	43.4688491021	39.4046510395
H	23.1092287146	41.0306500286	41.0329866064
H	23.2537553169	43.0868729914	39.5890476706
H	25.0018111450	45.3425583093	39.2649671350
H	27.1456970223	46.2344125904	40.1055400711
H	28.4230003553	45.0526945388	41.8736852060
H	27.5867190585	42.9241115532	42.8409620640
H	24.9792383432	37.5028746295	39.2262931476
H	23.4634461097	39.0047555339	37.7681696682
H	20.9526824914	39.9851558378	38.7625837969
H	21.6264211618	38.5891054423	41.5326026242
H	15.8695539068	42.7338833293	37.2155545861
H	18.4072866910	42.8061873857	37.0631985694
H	17.1566938327	39.1622942082	35.3617395682
H	23.9580904137	44.9869343669	33.5717312783
H	22.0168755526	43.3542828358	33.0180286760
H	23.0282095705	41.0949952625	32.6338634437
H	25.6553995062	41.1722319635	32.6996708234
H	20.3878180348	42.8048096672	34.5667602553
H	18.9104127966	41.0692825270	32.3157940919
H	19.5036210870	39.7779694521	31.2456999507
H	21.8559365701	44.8508546997	36.2622093333
H	25.8607351551	43.3312540931	36.6670861986
H	25.0139930946	40.9811166979	36.8446646060

4-sulfonylcatechol : radical + e⁻ : gem diol
E lacvp = -3061.913979

H	20.5454729879	35.5478670680	38.8164249939
C	20.5012112800	36.2146546815	37.9643841425
N	21.3175233893	36.0761025209	36.8352456114
C	19.8295119914	37.3967145659	37.7837906888
C	21.1171324712	37.1697451113	36.0273430149
N	20.2286227145	37.9904051581	36.5831702719
H	17.4763609315	40.6817446483	41.1988713156
C	17.2520009217	40.8040009982	40.1320000711
C	17.5584689362	42.2332909526	39.7046888949
O	16.6403607057	43.1001058547	39.5797701634
N	18.8662596592	42.4840269287	39.4699871411
H	25.2808688286	40.9541400485	42.6521447279
C	24.9118649062	41.6465976088	41.8984798687
C	23.7662115109	41.5037987106	41.1364818476
C	25.5238920900	42.8900814489	41.4969155446
N	23.6242499457	42.5820895900	40.2767527694
C	24.6863539229	43.4512365096	40.4766822846
C	26.6856653270	43.5905606532	41.8804020023
C	24.9873610851	44.6713278888	39.8523522597
C	26.9876505736	44.7997725735	41.2560763875
C	26.1468087838	45.3338030095	40.2508938599
H	23.9726830375	37.1214329802	41.5313610469
C	23.4024082846	37.6777404425	40.8230050814
N	23.9389731019	38.0508857435	39.5984664377
C	22.1226448326	38.1765087536	40.8408287052
C	22.9857003222	38.7642345446	38.9199220327
N	21.8729193585	38.8563231107	39.6482979229
H	14.9011789954	40.6201100261	36.0719110274
C	15.9494551287	40.8558387942	36.1115323809
N	16.4425920325	42.0241516896	36.6956773016
C	17.0460721324	40.1814268223	35.6314192093
C	17.7978044622	42.0267979528	36.5533465160
N	18.1914239350	40.9188751577	35.9236911849
H	26.2447090493	43.8340070329	33.3687670053
C	25.3200641828	43.3386315421	33.0942058038
N	24.1089816181	44.0285971324	33.1021581011
C	25.0160166786	42.0245127699	32.8306413612
C	23.0985687728	43.1690467030	32.8801146746
N	23.6293092530	41.9414472426	32.7041604826
H	19.4852370600	43.7230800844	33.5937000222
O	20.2770452612	43.1589288937	33.6271867976
H	18.5170069642	39.3420125393	32.6942510725
C	19.2579990898	40.0299989843	32.2789990517
C	20.5727125984	39.9564064561	33.0554558426
O	20.4834287878	39.7512711039	34.3447752044
O	21.6657984575	40.0973351475	32.4239303754
Fe	20.2368212833	40.3474435859	36.2661508498
O	22.3854853127	40.3393396543	36.5886209537
C	22.8748548004	41.5258502304	36.6791764485
C	21.8768964716	42.6776150580	36.8478028680
O	21.6404938085	42.8753818289	38.2039870949
O	20.7087485751	42.2830811889	36.0834490538
C	22.4701777185	44.0057978191	36.4178587954
C	24.2797807568	41.7770786155	36.6902952680
C	24.7275424061	43.0583367467	36.4862690545
C	23.8147580785	44.1465321494	36.3072715831
S	24.6170024214	45.7944548532	35.8331715187
O	26.1588441726	45.3430693241	35.4200375148
O	24.4899480641	46.8819957797	37.0542318469
O	23.7283871321	46.2382987167	34.4663117227
O	19.8929266750	40.2412983165	38.1247205100
H	21.9569611240	35.3201280438	36.6542732046
H	21.6230922002	37.3535795068	35.0955590047
H	19.1533267291	37.9119797122	38.4388983611
H	16.1917708679	40.5966099827	39.9718935175

H	17.8742054512	40.1040204242	39.5651585441
H	19.4976065972	41.7267677787	39.1729680967
H	19.1752771775	43.4170042044	39.2322228851
H	23.0323131973	40.7148591456	41.1369389204
H	22.8856560103	42.6904050658	39.5601136846
H	24.3505784311	45.0988286493	39.0858280784
H	26.4024377802	46.2711521711	39.7675829463
H	27.8841348825	45.3439500056	41.5425311043
H	27.3385872099	43.1910504113	42.6533022507
H	24.8894893020	37.9073980559	39.2999626497
H	23.1078488058	39.1807573592	37.9326468368
H	20.5581913232	39.8079623211	38.7253444745
H	21.3779877666	38.1065617119	41.6153012091
H	15.9558725916	42.6563267137	37.3206467300
H	18.4713544731	42.7720764635	36.9326908553
H	17.1040901641	39.2403637022	35.1131945859
H	23.9720502831	45.0218859624	33.4868649438
H	22.0279659540	43.3742532568	32.9406732976
H	23.0210468222	41.0989171821	32.6009739747
H	25.6494381781	41.1594444624	32.7482598617
H	20.4394774742	42.8361688173	34.5753334361
H	18.8846934782	41.0553732102	32.3859449869
H	19.4313973293	39.8215358967	31.2212759365
H	21.7825748696	44.8393377802	36.3321802260
H	25.7849770069	43.2926710805	36.4228511450
H	24.9687976393	40.9433013775	36.7717923592

4-sulfonylcatechol : radical + e⁻ : epoxide

E_{lacvp} = -3061.9243928781

H	20.5454729979	35.5478669427	38.8164250060
C	20.4749553543	36.2380355286	37.9908041738
N	21.1551690480	36.0651326366	36.7793367172
C	19.8722703183	37.4650465727	37.9020055761
C	20.9493100752	37.1821542086	36.0111479852
N	20.1825109519	38.0472004018	36.6728011703
H	17.4710008932	40.6776805830	41.1997047043
C	17.2520010452	40.8040010033	40.1319999551
C	17.5059142688	42.2498371922	39.7297551968
O	16.5707772438	43.1010313109	39.6685095061
N	18.8017541832	42.5337205832	39.4500616655
H	25.2808690464	40.9541399411	42.6521450607
C	25.0294289019	41.7161475540	41.9203182672
C	23.9670885929	41.6851562642	41.0398478170
C	25.7427221247	42.9466663689	41.6744741415
N	23.9737832313	42.8277054367	40.2517789295
C	25.0530059963	43.6232434322	40.6153240257
C	26.8892219572	43.5490382196	42.2305579055
C	25.4834051182	44.8599713111	40.1095333261
C	27.3188143577	44.7773550805	41.7315992490
C	26.6232690262	45.4231944668	40.6815783867
H	23.9726828789	37.1214331328	41.5313607453
C	23.4060624571	37.7260041061	40.8517894633
N	23.8829811892	38.0532490683	39.5863056527
C	22.1728476486	38.3244025000	40.9485454408
C	22.9431863549	38.8351772668	38.9616035574
N	21.8939955161	39.0151737498	39.7674786394
H	14.9011788931	40.6201099688	36.0719108986
C	15.9550738977	40.8390942128	36.1148095937
N	16.4512009838	42.0281516274	36.6528291792
C	17.0553277455	40.1317421769	35.6881755218
C	17.8101668375	42.0088214641	36.5384711068
N	18.2044189882	40.8695823023	35.9709898874
H	26.2447089247	43.8340069529	33.3687669678
C	25.3159111341	43.3311284666	33.1244268462
N	24.0987681667	44.0028073302	33.2079751292

C	25.0199248370	42.0233972480	32.8213215566
C	23.0929431581	43.1380374593	32.9868510803
N	23.6305486686	41.9255927003	32.7408461884
H	19.4852369575	43.7230800430	33.5936999566
O	20.2289411318	43.0993467101	33.6178006935
H	18.4772109402	39.3559978436	32.6533565336
C	19.2579992670	40.0299990689	32.2789995557
C	20.5367089673	39.9036252071	33.0808529829
O	20.3793037598	39.6389844398	34.3528157973
O	21.6546840186	40.0526655114	32.4979503125
Fe	20.2760238498	40.2697683721	36.2973062977
O	22.3120266002	40.2342104757	36.4883766449
C	22.8932390933	41.4353299899	36.5917183822
C	21.9386019012	42.5876107197	36.6008794457
O	21.9666843786	43.3910668853	37.8992652015
O	20.7122327619	42.2676370323	36.0772512616
C	22.5226150371	43.9754496243	36.5886816629
C	24.2502599647	41.6564942556	36.6476802930
C	24.7794259964	42.9879390509	36.5721866204
C	23.9682248696	44.0759133807	36.4839493015
S	24.7076443511	45.7137246918	35.9947763619
O	26.2476452589	45.3599838473	35.5031988674
O	24.5710644374	46.7944212534	37.2245049532
O	23.7166618744	46.1271618496	34.6788750621
O	19.9550368179	40.3690641378	38.1896547265
H	21.7152211375	35.2696511720	36.5203244624
H	21.3681258245	37.3615132634	35.0363268481
H	19.3011329575	38.0103371873	38.6284769657
H	16.2016726390	40.5569419182	39.9615969529
H	17.9060597417	40.1358073820	39.5632442685
H	19.4304673651	41.7780105488	39.1179241257
H	19.0645336951	43.4870106166	39.2376621909
H	23.1987440402	40.9411204818	40.9066323352
H	23.3231360249	43.0103319481	39.4891576235
H	24.9671527566	45.3665606500	39.2986533942
H	26.9837272025	46.3747608885	40.3029247385
H	28.2040722907	45.2487993702	42.1509643148
H	27.4306296503	43.0598569765	43.0373945204
H	24.7919603574	37.8270381783	39.2178044865
H	23.0123674572	39.2319995601	37.9537387577
H	20.6073225674	39.9421224701	38.8095448690
H	21.4798908987	38.3192629248	41.7726305164
H	15.9494989128	42.6947242220	37.2252770558
H	18.4799272409	42.7688944730	36.8931615057
H	17.1143042232	39.1686912576	35.2123117590
H	23.9634675860	44.9767290002	33.6539002904
H	22.0219748410	43.3294439106	33.0597836582
H	23.0310412750	41.0799093083	32.6348177168
H	25.6608107981	41.1714488986	32.6825294988
H	20.3805908472	42.7807487444	34.5628394525
H	18.9120691424	41.0590217470	32.3832610925
H	19.4559524586	39.8434306308	31.2268369501
H	21.9152983791	44.7914883141	36.2134447062
H	25.8514971461	43.1387612570	36.4956138442
H	24.9310273376	40.8126086556	36.6468268809

4-sulfonylcatechol : radical + e⁻ + H⁺ : gem diol

E lacvp = -3062.462934

H	20.5454730022	35.5478670020	38.8164249978
C	20.4846103970	36.2716364790	38.0139654373
N	21.1367642866	36.1037321254	36.7886317664
C	19.9271572414	37.5240760442	37.9606288103
C	20.9649886469	37.2393524620	36.0464137007
N	20.2444799073	38.1242121051	36.7390765041
H	17.4107807036	40.3223306674	41.1027554521

C	17.2520009934	40.8040010014	40.1319990038
C	16.8963997116	42.2678940019	40.2906138947
O	16.1050276516	42.8706015893	39.5125793270
N	17.5095291165	42.9326297093	41.3044109218
H	25.2808680010	40.9541399994	42.6521440002
C	24.9574765685	41.6773926382	41.9098837295
C	23.7982714578	41.6152134795	41.1665607740
C	25.6493675456	42.8803724527	41.5085159811
N	23.7197698322	42.7133483272	40.3175821086
C	24.8425723163	43.5097742354	40.5064445253
C	26.8628749820	43.4907422270	41.8826443034
C	25.2192592750	44.7120710894	39.8878397825
C	27.2429401390	44.6805253869	41.2642729704
C	26.4299567727	45.2838450721	40.2768048307
H	23.9726820022	37.1214329962	41.5313620021
C	23.4590757829	37.7032543647	40.8008820294
N	24.0286799277	37.9820489183	39.5676755124
C	22.2303178438	38.3152372035	40.7968738793
C	23.1470435823	38.7517209786	38.8592024348
N	22.0459895065	38.9718897633	39.5796722097
H	14.9011790015	40.6201099989	36.0719099985
C	15.9531365336	40.8157467378	36.1853991859
N	16.4285285115	41.8307205538	37.0096483575
C	17.0644330901	40.2151516608	35.6389634003
C	17.7830080992	41.8245378625	36.9543108115
N	18.2016110934	40.8502243940	36.1387326569
H	26.2447090009	43.8340060008	33.3687669993
C	25.3245431721	43.3354625843	33.0883220389
N	24.1086943816	44.0181712592	33.0893702209
C	25.0311969408	42.0230477535	32.8080441236
C	23.1040427144	43.1594090451	32.8424464903
N	23.6457456795	41.9366208937	32.6648469426
H	19.4852370005	43.7230790006	33.5936989990
O	20.2583979646	43.1338607294	33.5771849659
H	18.4936073737	39.3313396698	32.6272197667
C	19.2579979992	40.0299990005	32.2789979984
C	20.5250735890	39.9166759224	33.1089615533
O	20.3410367706	39.6801839184	34.4010782944
O	21.6598465804	40.0435083627	32.5803076346
Fe	20.2304841329	40.2979062242	36.2527365513
O	22.4996624303	40.3087173456	36.4660213771
C	22.9484586564	41.4878349364	36.6323028640
C	21.9063566729	42.6226200875	36.7378629318
O	21.5872463654	42.7061649542	38.1657812316
O	20.7795434066	42.2249539595	35.9954848649
C	22.4743313558	43.9726641207	36.3616845413
C	24.3459135655	41.7903811525	36.7767776378
C	24.7528909556	43.0856191538	36.6494701063
C	23.8047175439	44.1465003441	36.3657253341
S	24.5855293977	45.7989221490	35.8436373419
O	26.1055874148	45.3125496940	35.4009637435
O	24.4929218947	46.8580678187	37.0882081198
O	23.6307029125	46.1997798301	34.5185476618
O	20.2142585098	40.5410852167	38.1885659605
H	21.6414169742	35.2829929032	36.4946151834
H	21.3617082503	37.4068973343	35.0606907940
H	19.3726157275	38.0598123896	38.7074236481
H	16.4452457971	40.2889053098	39.6087029554
H	18.1757386714	40.7028895917	39.5413773377
H	18.1816205410	42.4876318299	41.9089409616
H	17.3495921867	43.9246300764	41.4039387510
H	23.0185517591	40.8720164601	41.1650213951
H	22.9859166860	42.8635496515	39.6276881536
H	24.6022185552	45.2025601474	39.1417110482
H	26.7456557990	46.2092141468	39.8068472705

H	28.1780516503	45.1566492480	41.5442333095
H	27.4938491618	43.0391002894	42.6434069614
H	24.9540891282	37.7169704137	39.2715222592
H	23.3079554676	39.1028448242	37.8545526237
H	20.7698823910	39.9316399765	38.7603111725
H	21.4825064571	38.3367071861	41.5709773644
H	15.9281866336	42.3573924812	37.7326898984
H	18.4278183702	42.4794124598	37.5106614476
H	17.1386169282	39.3950972393	34.9470896554
H	23.9604684753	45.0028865263	33.4595995397
H	22.0336401221	43.3643837373	32.8799282718
H	23.0571813411	41.0930503396	32.5589052922
H	25.6705476006	41.1636765616	32.7146513126
H	20.4485501762	42.8044850140	34.5066212898
H	18.8856621830	41.0541323736	32.4005848154
H	19.4812454402	39.8594047510	31.2242551171
H	21.7775244179	44.7705747984	36.1320288510
H	25.8003280986	43.3661340664	36.6821308303
H	25.0537956496	40.9797429334	36.9032779369
H	20.9598872629	41.8968650648	38.3361681376

4-sulfonylcatechol : radical + e⁻ + H⁺ : epoxide

E lacvp = -3062.445964

H	20.5454729995	35.5478669791	38.8164250108
C	20.4712671975	36.2856234919	38.0367956062
N	21.0405614225	36.1044393304	36.7749066705
C	19.9569594137	37.5569929484	38.0323658465
C	20.8684254153	37.2512366721	36.0551855223
N	20.2242192068	38.1535441312	36.8005028758
H	17.3721381840	40.2684494598	41.0797064368
C	17.2520009990	40.8040009988	40.1320000006
C	16.7754066997	42.2269551978	40.3501076111
O	16.0949232564	42.8613504238	39.4992568798
N	17.1476970098	42.8202830123	41.5156343706
H	25.2808690459	40.9541399513	42.6521451129
C	25.0476684278	41.7316531507	41.9329988003
C	23.9886527574	41.7304220132	41.0507947486
C	25.7791019442	42.9564022172	41.7107168059
N	24.0118648961	42.8876184294	40.2819165481
C	25.1020379063	43.6617226857	40.6652710541
C	26.9343902479	43.5299035676	42.2786909921
C	25.5475614133	44.9022898306	40.1846414242
C	27.3811113971	44.7607154691	41.8038283894
C	26.6950409159	45.4374635227	40.7677904660
H	23.9726830004	37.1214329990	41.5313610000
C	23.4713040918	37.7365545182	40.8116206916
N	24.0019079683	37.9663799644	39.5473484702
C	22.2898274366	38.4351028007	40.8549703941
C	23.1501620183	38.7884242217	38.8661123549
N	22.1014687179	39.0904581081	39.6365660012
H	14.9011789990	40.6201099985	36.0719110003
C	15.9627160382	40.7821289985	36.2052449947
N	16.4486120647	41.8312674520	36.9799449283
C	17.0751444451	40.1308792544	35.7149506823
C	17.8056801540	41.7958122183	36.9435318961
N	18.2240013424	40.7699680886	36.1935163848
H	26.2447090057	43.8340069999	33.3687670297
C	25.3166689521	43.3266531691	33.1397071492
N	24.0907900224	43.9809370154	33.2394911422
C	25.0380432211	42.0213290348	32.8148458961
C	23.0940040820	43.1109534330	32.9994960570
N	23.6502266437	41.9105842187	32.7343444281
H	19.4852370087	43.7230799857	33.5937000624
O	20.2184888004	43.0933401604	33.6935890375
H	18.4924163316	39.3133543835	32.5858073494

C	19.2579980046	40.0299990065	32.2789989940
C	20.5186732919	39.8597938069	33.0947002516
O	20.3110723756	39.5407556574	34.3641415754
O	21.6579183612	40.0169200792	32.5842838341
Fe	20.3176255890	40.2318605164	36.1982996550
O	22.3475174668	40.2341049102	36.3918913588
C	22.9014331448	41.4262866828	36.5678082208
C	21.9275723582	42.5550657713	36.6450719053
O	21.9785782734	43.2770710122	38.0026088374
O	20.6867381835	42.2402595204	36.1740274659
C	22.4799134635	43.9515305420	36.7080871220
C	24.2632278257	41.6676899924	36.6435151856
C	24.7646603766	43.0058907757	36.6246845042
C	23.9224288409	44.0789040026	36.5746523607
S	24.6235304165	45.7400770486	36.0662348890
O	26.1621871156	45.3932926292	35.5812545677
O	24.4451234922	46.7927851016	37.3110293437
O	23.6019859145	46.0743327422	34.7603238689
O	20.3170025605	40.6320546183	38.4345322415
H	21.4897136926	35.2661133331	36.4425443740
H	21.2076395581	37.4218956593	35.0488186550
H	19.4588596557	38.0981982169	38.8149660714
H	16.5278249441	40.2703004244	39.5134974054
H	18.2172412249	40.7962181980	39.6073509756
H	17.7078196853	42.3499759819	42.2080392569
H	16.8927912604	43.7848165652	41.6733408975
H	23.2147886927	40.9960606015	40.9047504252
H	23.3655449973	43.1004795664	39.5270715798
H	25.0334412207	45.4334334902	39.3883756318
H	27.0687831924	46.3924010679	40.4129116077
H	28.2717599769	45.2113564271	42.2323417727
H	27.4693378531	43.0178316507	43.0741336695
H	24.8910806054	37.6326748394	39.2111752560
H	23.2762072366	39.1185595403	37.8467081976
H	20.9690381852	40.0390502533	38.9744851394
H	21.5818503660	38.5206709136	41.6612344110
H	15.9501367554	42.3910698232	37.6757937858
H	18.4466099911	42.4970061470	37.4444493027
H	17.1444350347	39.2763568489	35.0652450680
H	23.9375457062	44.9448146838	33.6752905423
H	22.0212660490	43.2914474800	33.0767381074
H	23.0720181076	41.0643080933	32.6056284095
H	25.6902521144	41.1830767775	32.6479113131
H	20.3193625567	42.8217519336	34.6512251026
H	18.8868835185	41.0447099511	32.4690650566
H	19.4708609917	39.9304873835	31.2121988852
H	21.8521081717	44.7790287097	36.4016335123
H	25.8314213561	43.1868939000	36.5419255763
H	24.9558996195	40.8343099526	36.6114635333
H	20.5528905667	41.5788169683	38.5329624387

4-sulfonylcatechol : radical + 2e⁻ + H⁺ : gem diol

E lacvp =	-3062.574184		
H	20.5454730000	35.5478670000	38.8164250000
C	20.4613912227	36.2728575318	38.0154546602
N	21.1344580815	36.1383637241	36.7969240397
C	19.8498141851	37.5026709818	37.9562915083
C	20.9173898263	37.2769709984	36.0591798464
N	20.1500744574	38.1262627840	36.7416646410
H	17.4887492770	40.7609886706	41.2021341099
C	17.2520010000	40.8040009999	40.1319990000
C	17.3108892325	42.2452718087	39.6533378616
O	16.2743832487	42.9641023457	39.5437154916
N	18.5598112488	42.6765368261	39.3625859068
H	25.2808679999	40.9541400001	42.6521439997

C	25.0002374215	41.6839711715	41.8994400468
C	23.8828468233	41.6281390890	41.0906635426
C	25.7133653645	42.8876464670	41.5448538903
N	23.8531620433	42.7269209148	40.2448084987
C	24.9626901936	43.5201932147	40.4991620071
C	26.9022263996	43.4997908243	41.9900609979
C	25.3754709183	44.7236876801	39.9065340387
C	27.3143285497	44.6937362881	41.4006939566
C	26.5587893376	45.2978894669	40.3683831826
H	23.9726820001	37.1214330000	41.5313620001
C	23.3532069463	37.7146242084	40.8957742705
N	23.7660228109	38.0901758363	39.6244994242
C	22.1043904251	38.2638629080	41.0610132562
C	22.7732278654	38.8515948229	39.0645972328
N	21.7509185907	38.9739130681	39.9131796611
H	14.9011790000	40.6201100000	36.0719100000
C	15.9538910440	40.8439145375	36.0808326367
N	16.4584262421	42.0520061984	36.5641939385
C	17.0434304171	40.1275755541	35.6452319561
C	17.8168761980	42.0302915681	36.4038671424
N	18.2016336614	40.8740649477	35.8632692124
H	26.2447090000	43.8340060000	33.3687670001
C	25.3211449884	43.3583321757	33.0584686174
N	24.1256838672	44.0758679384	33.0551664229
C	24.9898365877	42.0575036645	32.7639178519
C	23.0990496422	43.2449284241	32.7930705434
N	23.6045699139	42.0092314384	32.6073659353
H	19.4852370001	43.7230789999	33.5936990002
O	20.3598338351	43.3015070466	33.5961740128
H	18.5593217868	39.3261523567	32.7381709574
C	19.2579980000	40.0299990000	32.2789980000
C	20.6226885267	39.9832408681	32.9742069032
O	20.6378955109	39.7233724440	34.2502743216
O	21.6598397454	40.2073954250	32.2649852262
Fe	20.3131807241	40.3886881937	36.2013406224
O	22.6190805270	40.3712480461	36.4968344447
C	23.0784076004	41.5532215347	36.5721765227
C	22.0797287095	42.7255938515	36.6894646846
O	21.8342830764	42.7524390597	38.1500331455
O	20.9124170654	42.4542653093	35.9872928123
C	22.7068025010	44.0647579407	36.3562454902
C	24.4996811559	41.8152931313	36.6387041792
C	24.9582386347	43.0878623902	36.4976476791
C	24.0414856458	44.1914102135	36.2928814886
S	24.8557703572	45.8296832521	35.7828350942
O	26.3639544204	45.3396449545	35.2973945621
O	24.8211633262	46.8834024652	37.0398679556
O	23.8991160080	46.3086098536	34.4841761324
O	20.2410311829	40.7975040765	38.2532946286
H	21.6887562682	35.3491138741	36.5091466605
H	21.3255505818	37.4812732420	35.0839711575
H	19.2684140872	38.0071256558	38.7053613246
H	16.2449042348	40.4097779865	39.9812852362
H	17.9849912263	40.1941192053	39.5952722350
H	19.2930060526	41.9899579643	39.0856479505
H	18.6878155228	43.6449095979	39.1019108360
H	23.0967465560	40.8920524827	41.0473242728
H	23.1489210550	42.8750215558	39.5132608426
H	24.8092855037	45.2066945845	39.1166252271
H	26.9009927427	46.2232482213	39.9164418804
H	28.2315915258	45.1707139238	41.7362394314
H	27.4907929287	43.0450908685	42.7831769852
H	24.6643484761	37.9008792984	39.2115254698
H	22.8251578898	39.2723144888	38.0722055130
H	20.5579172898	40.1141710715	38.8914452018

H	21.4475675536	38.2084537406	41.9124649216
H	15.9687459173	42.7134543382	37.1548104994
H	18.4955919353	42.8068612979	36.7049946257
H	17.0895488641	39.1477658590	35.2029267974
H	24.0225212711	45.0598283679	33.4396136412
H	22.0320582140	43.4759245812	32.8387517713
H	22.9715690882	41.1758291701	32.4801359423
H	25.6036842306	41.1786750207	32.6792225295
H	20.5906215108	42.9811367306	34.5357286243
H	18.8660033211	41.0458572358	32.4097445741
H	19.3691397803	39.8295261627	31.2109836274
H	22.0290249219	44.8926853414	36.1816619000
H	26.0168703599	43.3228288611	36.4766753145
H	25.1751484413	40.9713931995	36.7303522989
H	21.1743494265	41.9313961612	38.2997665201

4-sulfonylcatechol : radical + 2e⁻ + H⁺ : epoxide

E lacvp = -3062.565213

H	20.5454729980	35.5478670013	38.8164249987
C	20.4946218191	36.2730375390	38.0162320212
N	21.1245885968	36.0740981920	36.7855420312
C	19.9354342162	37.5273629242	37.9420101722
C	20.9395954065	37.1961615632	36.0209071135
N	20.2239741509	38.0945635763	36.6975839662
H	17.2701763965	40.5617574728	41.2016936285
C	17.2520010043	40.8040009961	40.1319999993
C	17.0722649116	42.3010729128	39.9433722903
O	15.9830321332	42.7981042433	39.5119666389
N	18.1543657275	43.0454528066	40.2433716687
H	25.2808689926	40.9541400051	42.6521449871
C	25.0961441662	41.7601597503	41.9511746976
C	24.0483710881	41.8234130463	41.0570185677
C	25.8904374379	42.9484835760	41.7519719286
N	24.1416907079	42.9809953693	40.3008548359
C	25.2638134793	43.6944132900	40.7000597751
C	27.0584915490	43.4675593558	42.3458125393
C	25.7774775329	44.9133718105	40.2326726025
C	27.5680662928	44.6819408399	41.8904313246
C	26.9353156219	45.3935831788	40.8436512106
H	23.9726829931	37.1214330037	41.5313609964
C	23.3185079133	37.7957798520	41.0153611012
N	23.5342303773	38.1310659460	39.6835974015
C	22.2012761862	38.4999900243	41.3965814389
C	22.5659523684	39.0164665589	39.2966706022
N	21.7377417701	39.2611021108	40.3183116840
H	14.9011790076	40.6201100007	36.0719110017
C	15.9727403808	40.7481801896	36.1624415531
N	16.5265633880	41.7738305435	36.9223864590
C	17.0405702246	40.0654381901	35.6192647883
C	17.8861848830	41.6941303057	36.8193718690
N	18.2344357769	40.6632209634	36.0381142923
H	26.2447089931	43.8340069985	33.3687670022
C	25.3163511125	43.3380849555	33.1093728098
N	24.0891183734	43.9695228671	33.2961820238
C	25.0384188464	42.0639321901	32.6752269124
C	23.0947032167	43.1116547601	33.0092645748
N	23.6501804483	41.9448377714	32.6196563161
H	19.4852370106	43.7230799950	33.5937000125
O	20.2088731537	43.0903624680	33.7480672318
H	18.6010233153	39.2541645907	32.6808185552
C	19.2579980007	40.0299989996	32.2789990022
C	20.6695339586	39.8709139856	32.8056384552
O	20.7568664324	39.4758104305	34.0550596681
O	21.6635034981	40.1347781200	32.0681321707
Fe	20.3756420974	40.1719706452	35.8705206979

O	22.3138674645	40.1424005002	36.6336453412
C	22.9047722373	41.3349211179	36.6957412504
C	21.9540477443	42.4931947336	36.7017136379
O	22.0233510045	43.2499089298	38.0771147206
O	20.7131048032	42.2129882442	36.2245630199
C	22.5426931458	43.8719400841	36.7521444607
C	24.2647930547	41.5544115405	36.7401701884
C	24.7959436664	42.8827254060	36.6618763281
C	23.9861283062	43.9782128186	36.6194683636
S	24.7102339017	45.6190305825	36.1333399696
O	26.2410318163	45.2805600694	35.6033999160
O	24.5928005676	46.6949522116	37.3704833960
O	23.6921635402	46.0372729258	34.8388015819
O	20.4289067921	41.7036737579	39.8358189835
H	21.6346338148	35.2524847443	36.5064914489
H	21.3344737709	37.3576497748	35.0319188083
H	19.3954987619	38.0748595472	38.6935909613
H	16.4191091840	40.2765320703	39.6643846141
H	18.2053725804	40.4813416831	39.7032733627
H	19.0898464513	42.5908428229	40.3107802664
H	18.0884381879	44.0476016067	40.1283506509
H	23.2281405555	41.1430474614	40.9065581870
H	23.5186791086	43.2090098047	39.5289616918
H	25.3050136540	45.4628551637	39.4220781489
H	27.3602871468	46.3321254730	40.5011737453
H	28.4684783432	45.0908397932	42.3421194615
H	27.5539343401	42.9271430972	43.1489914965
H	24.3053989516	37.8324216635	39.1098788060
H	22.4939214198	39.4231586770	38.2899814387
H	20.8438249231	40.8333926718	40.0843055007
H	21.7100867209	38.5261321069	42.3543113653
H	16.0475726825	42.3436650057	37.6249043399
H	18.5898962424	42.3524652993	37.2985112681
H	17.0450421349	39.2092838853	34.9673242543
H	23.9441581712	44.9139610998	33.8075239759
H	22.0239938597	43.2759564937	33.1348714747
H	23.0682046207	41.1109241242	32.4017188020
H	25.6915752687	41.2468238571	32.4264169430
H	20.3134392496	42.8590378910	34.7242131500
H	18.8969182339	41.0080418689	32.6196168094
H	19.2459349391	40.0125892865	31.1864750903
H	21.9304020594	44.7077126186	36.4341775533
H	25.8663904719	43.0315993462	36.5586968624
H	24.9404348717	40.7060904783	36.7410390475
H	20.9849175824	42.2344547077	39.2221786091

homoprotocatechuate : radical : gem diol

E lacvp = -2666.023849

H	20.5454730000	35.5478670000	38.8164250000
C	20.4936187707	36.3076547998	38.0425095990
N	21.0340035832	36.1361430298	36.7629401287
C	20.0161108392	37.5945504844	38.0633184116
C	20.8732734154	37.3031266117	36.0640126540
N	20.2671869973	38.2106182641	36.8319299249
H	17.3750691569	40.5781662642	41.1987627736
C	17.2520010000	40.8040010000	40.1320010000
C	17.4711350181	42.2863609921	39.8995978616
O	16.5167680599	43.1090635284	39.8349603211
N	18.7738539065	42.6409192162	39.7604591717
H	25.2808679999	40.9541400001	42.6521449999
C	24.9088461337	41.7357731401	41.9987542937
C	23.7262085921	41.7009776210	41.2936315129
C	25.5393651668	42.9999607420	41.7001434120
N	23.5774223877	42.8713555537	40.5589175838
C	24.6721966089	43.6913395737	40.7934086645

C	26.7359291694	43.6252365809	42.1011278169
C	24.9742004873	44.9692474843	40.3024263884
C	27.0403402361	44.8930199368	41.6085250341
C	26.1670393795	45.5598499521	40.7186868472
H	23.9726820000	37.1214330000	41.5313610000
C	23.5139022596	37.7721952654	40.8161458416
N	24.1470403941	38.1449250552	39.6360387052
C	22.2929561329	38.3997293755	40.8003329858
C	23.3060860839	38.9825466112	38.9497040440
N	22.1758989660	39.1541549226	39.6333249867
H	14.9011790000	40.6201100000	36.0719110000
C	15.9274954728	40.8570396326	36.2237387258
N	16.3388005496	42.0421316738	36.8258550990
C	17.0682932375	40.1754850651	35.8898184640
C	17.6966406249	42.0593869581	36.8407395266
N	18.1602788750	40.9352848093	36.2919814073
H	26.2447089999	43.8340060000	33.3687680000
C	25.2929302907	43.3475231630	33.2143272547
N	24.1171139888	44.0861175134	33.1790631153
C	24.9394183203	42.0268502234	33.0759658617
C	23.0701878760	43.2542687735	33.0434761090
N	23.5509623717	41.9934570557	32.9759182548
H	19.4852370001	43.7230810000	33.5937010001
O	20.2330136974	43.1126454214	33.7013676777
H	18.4460123971	39.4090717436	32.6651682507
C	19.2579990000	40.0299990000	32.2789990000
C	20.4661715092	40.0233552496	33.2269485692
O	20.2327410644	39.9083009542	34.5214242867
O	21.6278917281	40.1237824108	32.7342479039
Fe	20.1755225338	40.4555272735	36.4664095273
O	22.4167231691	40.8321836099	36.6487740802
C	22.6824922095	42.0662545269	36.7989358479
C	21.4905075847	43.0009543020	36.9832351338
O	21.3115639221	43.0940120132	38.4247687475
O	20.4126775649	42.4882590898	36.2770297056
C	21.7901071890	44.4631633938	36.7690037328
C	24.0107239228	42.6236015573	36.8334911025
C	24.1790242662	43.9825384808	36.7925145999
C	23.0774788483	44.9392849589	36.7545067590
C	23.3480568165	46.3939509334	36.5171603043
H	24.3784560888	46.6604874069	36.7605632208
H	22.6529788166	47.0249515129	37.0740323646
C	23.1117093489	46.6512030565	34.9695062636
O	20.1771325860	40.5347494880	38.3448478555
H	21.4619483595	35.2958017111	36.4087650355
H	21.1978226469	37.4695780296	35.0518179852
H	19.5521386315	38.1432879871	38.8603729850
H	16.2339445766	40.5349642696	39.8429940799
H	17.9788706008	40.2120496268	39.5681811282
H	19.4697425114	41.9545871838	39.4536795087
H	19.0078327395	43.6144178975	39.6308476606
H	22.9720726605	40.9349691154	41.2471811687
H	22.8106916231	43.0587836043	39.9187951107
H	24.2947771743	45.4892596205	39.6344032308
H	26.4259545219	46.5514889991	40.3605423320
H	27.9592624863	45.3830241543	41.9158369493
H	27.4114238995	43.1272012404	42.7908495690
H	25.0790363658	37.8835900442	39.3577119313
H	23.5203015190	39.4276670563	37.9926297203
H	20.8858431063	40.0746268264	38.8889671743
H	21.5059360710	38.3705588062	41.5343704941
H	15.7630717813	42.7097317740	37.3200029155
H	18.3117309047	42.8372493707	37.2465413140
H	17.1911483354	39.2264823957	35.3992192090
H	24.0727293693	45.1365432746	33.4238130268

H	22.0071398430	43.4947451179	33.0838847065
H	22.9189660880	41.1640232083	32.9095627762
H	25.5380266583	41.1340522669	33.0419842349
H	20.3033269688	42.8626751627	34.6698891450
H	18.9092797578	41.0672993825	32.2169008351
H	19.5662333811	39.6970232380	31.2867960805
H	20.9350533198	45.1258586096	36.7191570715
H	25.1841885044	44.3913512408	36.7649945573
H	24.8598883649	41.9508399391	36.7996240224
O	24.1476307578	46.3855763787	34.2374583631
O	21.9474303624	46.9650786231	34.6177619901

homoprotocatechuate : radical : epoxide

E lacvp = -2666.043448

H	20.5454730000	35.5478670005	38.8164249997
C	20.4879537511	36.2821691963	38.0237826660
N	21.0037878881	36.0737453822	36.7398052901
C	20.0251306842	37.5724002393	38.0266316566
C	20.8454874523	37.2264281907	36.0186157671
N	20.2640762376	38.1561899887	36.7790699145
H	17.3633909485	40.6152225341	41.2062379682
C	17.2520010001	40.8040010000	40.1320010001
C	17.5660568362	42.2609060014	39.8393440125
O	16.6601477579	43.1359835363	39.7646968705
N	18.8856026160	42.5332211763	39.6639167624
H	25.2808679992	40.9541400005	42.6521449993
C	24.9222290451	41.7740776138	42.0394263281
C	23.8086269955	41.7554058025	41.2282926645
C	25.5094745831	43.0882113825	41.9190846466
N	23.6624886357	42.9872505895	40.5989625885
C	24.6921130004	43.8248653480	41.0032604811
C	26.6320060325	43.7242419942	42.4848321122
C	24.9737380133	45.1527148001	40.6550361932
C	26.9135893455	45.0448737164	42.1383495197
C	26.0917639482	45.7523035914	41.2319098423
H	23.9726819996	37.1214330004	41.5313609996
C	23.5278704500	37.7611568639	40.7996724147
N	24.1528506639	38.0648292402	39.5953722833
C	22.3315783292	38.4323700406	40.7818607541
C	23.3313865306	38.9067225880	38.8914265993
N	22.2213220395	39.1444283243	39.5887701592
H	14.9011790001	40.6201100004	36.0719109999
C	15.9409997625	40.8378774494	36.2066099483
N	16.3828363106	42.0249443094	36.7867986645
C	17.0707312257	40.1339628830	35.8723136526
C	17.7422110317	42.0180053023	36.7887126438
N	18.1858208332	40.8801441686	36.2485983932
H	26.2447089963	43.8340060001	33.3687679998
C	25.2880396798	43.3564100036	33.2280283286
N	24.1128173573	44.0970468083	33.2683918866
C	24.9274292157	42.0464495621	33.0263226430
C	23.0606521479	43.2742068918	33.1119049776
N	23.5375164169	42.0205156575	32.9625552657
H	19.4852370050	43.7230809978	33.5937010022
O	20.2292196331	43.1062161443	33.6868114170
H	18.4674838078	39.3834688383	32.6684389456
C	19.2579989997	40.0299990005	32.2789989993
C	20.4913347746	40.0077680779	33.1841338390
O	20.2869957696	39.8458345634	34.4757361007
O	21.6386839217	40.1462722016	32.6672792024
Fe	20.2276979638	40.3725538800	36.4192313234
O	22.4815065846	40.6886040850	36.5662056247
C	22.7708047956	41.9268498118	36.7864735159
C	21.6142870652	42.8751100027	36.8360411930
O	21.5021470539	43.4976402878	38.2389610033

O	20.5026697707	42.4113367384	36.2291903547
C	21.9136912310	44.3272957531	37.0179131363
C	24.0856459549	42.4388545981	36.9407701642
C	24.3313918001	43.8178371858	37.0127596002
C	23.3159687302	44.7833332770	36.9915022014
C	23.5725952372	46.2224870491	36.7709007158
H	24.6243710154	46.4897040956	36.8916577671
H	22.9342543238	46.8593660536	37.3880857289
C	23.1421552036	46.5267800397	35.2390642317
O	20.2218694945	40.4654881600	38.2914109230
H	21.4168885128	35.2208039618	36.3985328146
H	21.1565858195	37.3685753169	34.9986116856
H	19.5837998243	38.1455047571	38.8191701059
H	16.2180273928	40.5921429448	39.8534347438
H	17.9355017366	40.1407792488	39.5938907146
H	19.5306914884	41.7961432149	39.3520861560
H	19.1770449919	43.4864467932	39.5006051380
H	23.1012454096	40.9653538173	41.0411810116
H	22.9433011902	43.2149973337	39.9212656145
H	24.3379546470	45.6995174737	39.9667599202
H	26.3328372064	46.7817619774	40.9847525387
H	27.7747308113	45.5442228715	42.5720620150
H	27.2689913551	43.1923595701	43.1850026508
H	25.0677529619	37.7554890160	39.3102881893
H	23.5386610545	39.3075703024	37.9125419283
H	20.9416992686	40.0204546955	38.8357379682
H	21.5584567250	38.4617850542	41.5306093308
H	15.8258720679	42.7099717954	37.2789284814
H	18.3708868005	42.7919064247	37.1826840613
H	17.1718819916	39.1744368567	35.3971969771
H	24.0665999541	45.1194047697	33.5401032215
H	21.9976329203	43.5169653854	33.1693393685
H	22.9029860752	41.1930879948	32.8698976001
H	25.5225864687	41.1566706192	32.9261112576
H	20.3018695137	42.8287833152	34.6471505048
H	18.8926928597	41.0636058360	32.2649276173
H	19.5358969845	39.7380806766	31.2650132881
H	21.1593752925	45.0451877004	36.7157061655
H	25.3614530407	44.1577233564	37.0567106396
H	24.9131349940	41.7391301087	36.9324292266
O	24.1047026845	46.4212518694	34.3926111246
O	21.9171834304	46.7174231130	35.0556750150

homoprotocatechuate : radical + e⁻ : gem diol

E lacvp =	-2666.138169		
H	20.5454730000	35.5478670000	38.8164250000
C	20.5488233216	36.2299151198	37.9746175438
N	21.4370412400	36.1186901239	36.8977895216
C	19.8719495479	37.4050049294	37.7667083009
C	21.2686873868	37.2216056295	36.0923928678
N	20.3350620554	38.0220527004	36.6007843162
H	17.5044292008	40.6424301094	41.1874286280
C	17.2520010000	40.8040010000	40.1320010000
C	17.4650276441	42.2630270878	39.7684125785
O	16.4909420927	43.0632672709	39.6141933726
N	18.7560125855	42.6314563280	39.6123773196
H	25.2808680000	40.9541400000	42.6521450000
C	24.7870297472	41.6846737437	42.0169536839
C	23.6962663621	41.4539450366	41.1987864416
C	25.1389932547	43.0728877665	41.8537429813
N	23.3450490689	42.6103899891	40.5226746727
C	24.2092525962	43.6212640477	40.9077396110
C	26.1274972016	43.9170342766	42.3986792576
C	24.2539471640	44.9675039102	40.5180383357
C	26.1734485339	45.2539778117	42.0074297695

C	25.2439018990	45.7749436701	41.0759204413
H	23.9726820000	37.1214330000	41.5313610000
C	23.3976595275	37.6904074420	40.8289617472
N	23.9348625973	38.1526007556	39.6317342279
C	22.0995039675	38.1416516823	40.8513347748
C	22.9623319242	38.8695638756	38.9777911704
N	21.8389635194	38.8787436377	39.6960900277
H	14.9011790000	40.6201100000	36.0719110000
C	15.9395729166	40.8666821752	36.1337755502
N	16.4008948646	42.0163592939	36.7729894272
C	17.0511208238	40.2290213471	35.6409865305
C	17.7564119110	42.0459526370	36.6511326523
N	18.1763904506	40.9723877319	35.9810928467
H	26.2447090000	43.8340060000	33.3687680000
C	25.3001703029	43.3352119914	33.2253744992
N	24.1208552292	44.0254616385	33.4624731602
C	24.9611833583	42.0543802468	32.8588734677
C	23.0842177939	43.2011349905	33.2539223592
N	23.5707779577	41.9930047844	32.8836876062
H	19.4852370000	43.7230810000	33.5937010000
O	20.2593058698	43.1689720904	33.7821021010
H	18.5290503622	39.3222055609	32.6836796230
C	19.2579990000	40.0299990000	32.2789990000
C	20.5532028764	40.0171111718	33.1005477144
O	20.4418359965	39.8936572249	34.3970728443
O	21.6575933020	40.1258561791	32.4801496408
Fe	20.2253404577	40.4486632886	36.3405070890
O	22.4354558008	40.6741149493	36.6622692273
C	22.7542149380	41.9171337366	36.8042250727
C	21.6170043297	42.8797544979	37.1232751794
O	21.3802508759	42.8106065017	38.5024229212
O	20.5072663688	42.4248029645	36.2982507307
C	21.9679097871	44.3245506998	36.8942080892
C	24.0906273941	42.4148004898	36.7264506698
C	24.3041391913	43.7750690579	36.6821489368
C	23.2523789869	44.7708289309	36.7690058851
C	23.6084689222	46.2415470465	36.8302765985
H	24.3844948653	46.3983911118	37.5958151965
H	22.7402089485	46.8195869375	37.1645383077
C	24.1430486309	46.9451745830	35.5467722860
O	19.8196293488	40.2202959609	38.1614368053
H	22.0978740697	35.3745124122	36.7475157612
H	21.8257904968	37.4173538755	35.1924829850
H	19.1485965642	37.9041305285	38.3828396413
H	16.2035688951	40.5417105842	39.9765302540
H	17.9083768194	40.1749657805	39.5198418139
H	19.4911540721	41.9663918492	39.3594619574
H	18.9837857639	43.5922343799	39.3996014406
H	23.1268443320	40.5531074476	41.0532110150
H	22.6076690987	42.6853128288	39.7894263442
H	23.5368043636	45.3600517560	39.8055920130
H	25.3028797185	46.8213513341	40.7908721471
H	26.9330285181	45.9111025343	42.4227857340
H	26.8452642979	43.5300285023	43.1181562597
H	24.8916976840	38.0556908346	39.3342254414
H	23.0904587138	39.3690593278	38.0277879059
H	20.4899357484	39.8409245701	38.7885221926
H	21.3477321037	38.0026972069	41.6095281526
H	15.8970666427	42.6125534593	37.4204973015
H	18.4185131615	42.7811698424	37.0667938242
H	17.1312741154	39.3120088513	35.0840728666
H	24.1610732585	45.0363622536	33.9562148910
H	22.0204199419	43.4090196447	33.3851300031
H	22.9462003289	41.1680838574	32.7358937929
H	25.5674798355	41.2056855333	32.5958460188

H	20.3115553025	42.9173836155	34.7642323038
H	18.8396430646	41.0403805112	32.3547006962
H	19.4767392654	39.8060566952	31.2334263077
H	21.1407152193	45.0168621550	37.0228622745
H	25.3210630559	44.1439327838	36.5779794919
H	24.9119122759	41.7126856852	36.6272785952
O	24.5550330410	46.1972661214	34.5563667081
O	24.1991367794	48.2008519492	35.5797930494

homoprotocatechuate : radical + e⁻ : epoxide

E lacvp = -2666.145179

H	20.5454730026	35.5478669661	38.8164250050
C	20.5058419572	36.2474852855	37.9939485281
N	21.2397542937	36.0925031527	36.8112004007
C	19.9001164741	37.4726353950	37.8899194813
C	21.0587234148	37.2175823403	36.0455587949
N	20.2397027203	38.0708872702	36.6813019360
H	17.4757577244	40.6462051087	41.1946723170
C	17.2520010051	40.8040010033	40.1319999920
C	17.5252543381	42.2555089873	39.7644662499
O	16.5998138396	43.1186351179	39.7083698149
N	18.8270670780	42.5220994129	39.5035700565
H	25.2808689570	40.9541400077	42.6521450075
C	24.8866569802	41.7623080205	42.0432490947
C	23.8981395597	41.6576415327	41.0850182190
C	25.2955101453	43.1450366869	42.0725566986
N	23.6637849099	42.8962288667	40.5068146450
C	24.5064983015	43.8293035073	41.0902067765
C	26.2372499391	43.8819457735	42.8178011991
C	24.6474126262	45.2028392308	40.8495733298
C	26.3760709758	45.2481524223	42.5797880683
C	25.5885612490	45.9023094747	41.6034197158
H	23.9726829874	37.1214330011	41.5313609869
C	23.4149258358	37.7247493603	40.8463429907
N	23.9070347293	38.0773102679	39.5928674673
C	22.1727441904	38.3040658150	40.9350870006
C	22.9634356736	38.8544683592	38.9676114137
N	21.9019451581	39.0076932437	39.7623532880
H	14.9011789480	40.6201099874	36.0719109746
C	15.9538506882	40.8425987262	36.1319504407
N	16.4368948219	42.0213547178	36.7035062620
C	17.0641018218	40.1549197697	35.6993750852
C	17.7974897680	42.0138357836	36.6013381617
N	18.2065683687	40.8922871955	36.0099473480
H	26.2447089728	43.8340069968	33.3687670302
C	25.3020644130	43.3186177039	33.2586455610
N	24.1064406916	43.9609854815	33.5490065130
C	24.9982759997	42.0386747629	32.8561565570
C	23.0971779346	43.1072280242	33.3251558922
N	23.6124040798	41.9282969695	32.9037077357
H	19.4852369488	43.7230800272	33.5936999895
O	20.1752762646	43.0488072283	33.7044553405
H	18.4940023100	39.3381569045	32.6443372536
C	19.2579990419	40.0299989970	32.2789990498
C	20.5379534652	39.9181038538	33.1046424403
O	20.3836035484	39.7006724179	34.3870398523
O	21.6575342311	40.0394662863	32.5193188765
Fe	20.3047093341	40.3191681003	36.3325429024
O	22.3204908434	40.3912312044	36.5506882114
C	22.8334339568	41.6255870542	36.7323207373
C	21.8116327247	42.7129341859	36.7909919880
O	21.7229940643	43.4055933277	38.1619624363
O	20.6243820444	42.3581568713	36.2021591932
C	22.3000596480	44.1229698242	36.9089504778
C	24.1615248386	41.9433312574	36.8285358453

C	24.5945627810	43.3189861606	36.9359874022
C	23.7495979773	44.3940716649	36.9259572034
C	24.2289057006	45.8220896740	36.9905084656
H	25.3152212835	45.8287590228	37.1612483291
H	23.7817323298	46.3500507000	37.8423683605
C	23.9716798851	46.7484504228	35.7598049531
O	19.9230616284	40.3454679521	38.2249836758
H	21.8132533952	35.3022500478	36.5671102668
H	21.5128792763	37.4040479075	35.0879792418
H	19.2953523883	38.0105770759	38.5947027107
H	16.1969086662	40.5774502444	39.9623386048
H	17.8933155407	40.1425158167	39.5412924114
H	19.4375208960	41.7567143127	39.1590734969
H	19.1140328524	43.4688219821	39.2938885590
H	23.3249911812	40.8025236280	40.7713607334
H	23.0220739666	43.0681803655	39.7292819749
H	24.0476337438	45.7027492301	40.0969355453
H	25.7204518220	46.9669996594	41.4355129619
H	27.1005871317	45.8234444765	43.1500188625
H	26.8483589908	43.3895852962	43.5702390020
H	24.8197010759	37.8579334620	39.2293357665
H	23.0425781516	39.2781699642	37.9718660366
H	20.5891804255	39.9238969378	38.8302933283
H	21.4691975286	38.2768690150	41.7496982845
H	15.9263896404	42.6774824237	37.2797297360
H	18.4594360750	42.7703579195	36.9763958493
H	17.1351061117	39.2055133110	35.1982190806
H	24.0165998632	44.9933662391	34.0617042921
H	22.0310749599	43.2920820240	33.4431906121
H	23.0102383938	41.0953478854	32.7452966969
H	25.6286990041	41.2213228110	32.5532048661
H	20.2827835695	42.8032938088	34.6775538305
H	18.8927475497	41.0558557932	32.4053398910
H	19.4693079055	39.8512888556	31.2223965650
H	21.6347276838	44.9184113921	36.5868662614
H	25.6657049188	43.4990401060	36.9987371407
H	24.9068016689	41.1561420809	36.7757580328
O	23.9279029152	46.2106576875	34.5676528234
O	23.8843954241	47.9811850287	35.9888219409

homoprotocatechuate : radical + e⁻ + H⁺ : gem diol

E lacvp =	-2666.697148		
H	20.5454730000	35.5478670000	38.8164250000
C	20.5266277247	36.2807814192	38.0149235172
N	21.3220306327	36.1772226487	36.8692864910
C	19.9001425705	37.4980772446	37.9101231988
C	21.1599524597	37.3152663606	36.1239364969
N	20.3123848360	38.1427043022	36.7382070769
H	17.3844989765	40.4445055928	41.1597519264
C	17.2520010000	40.8039999999	40.1320020000
C	17.0684282306	42.3069020245	40.1147946179
O	16.0631561094	42.8682073479	39.5959259499
N	18.0727534487	43.0400426509	40.6665138559
H	25.2808679997	40.9541400001	42.6521449994
C	24.7804381010	41.7011202899	42.0451131318
C	23.6271031675	41.5137842352	41.3138849247
C	25.1891461774	43.0699841189	41.8404066836
N	23.2851150206	42.6886441382	40.6539623493
C	24.2261077589	43.6614671940	40.9608980100
C	26.2603491579	43.8594224197	42.3028045860
C	24.3155617857	44.9992644662	40.5509386479
C	26.3526843487	45.1875162162	41.8921103220
C	25.3886721133	45.7524144829	41.0250477549
H	23.9726830000	37.1214330000	41.5313600000
C	23.4800758708	37.7210388353	40.7955173903

N	24.1289921947	38.2052819194	39.6656214499
C	22.1894079302	38.1806482045	40.7127527963
C	23.2274075761	38.9419318534	38.9411809605
N	22.0440357893	38.9427956261	39.5548950720
H	14.9011790002	40.6201100000	36.0719120000
C	15.9392098792	40.8173102381	36.2115436791
N	16.3778870843	41.8516672801	37.0265598253
C	17.0651248458	40.2123822651	35.7084915798
C	17.7332545709	41.8577347890	37.0067250459
N	18.1774452291	40.8699233532	36.2233437291
H	26.2447079998	43.8340069999	33.3687680001
C	25.2993269579	43.3460038117	33.2084582598
N	24.1195772348	44.0538741421	33.3797672106
C	24.9592823176	42.0575267401	32.8773941353
C	23.0781398897	43.2327453669	33.1747725184
N	23.5681359769	42.0102072090	32.8636440682
H	19.4852360002	43.7230810000	33.5937020004
O	20.2309364613	43.1304116066	33.7807523257
H	18.5076287680	39.3241343703	32.6448977795
C	19.2579990001	40.0300000000	32.2790000001
C	20.5119347908	40.0051574094	33.1508086202
O	20.3329904532	39.8912761442	34.4585647979
O	21.6496942594	40.0878761533	32.6153914155
Fe	20.2110086761	40.4004325736	36.3477182272
O	22.4323595650	40.8294617431	36.6422828796
C	22.6557351025	42.0735424707	36.8623003704
C	21.4211669701	42.9357399921	37.1615900179
O	21.1070063112	42.7059776587	38.5815129038
O	20.3870306363	42.4293814091	36.3375504872
C	21.6371184080	44.4122238407	37.0396190938
C	23.9444294587	42.6885430999	36.8581269654
C	24.0350166387	44.0586260073	36.8907903052
C	22.8738404095	44.9546956832	36.9650570001
C	23.1091751974	46.4433085411	36.8691354514
H	23.9408449427	46.7398591496	37.5235828510
H	22.2229067595	47.0074276985	37.1685841912
C	23.4832397156	46.8277528896	35.4133599588
O	20.1048073231	40.4121875931	38.2965724008
H	21.9104494497	35.3967383822	36.6259751330
H	21.6514663244	37.5160351505	35.1877588900
H	19.2322917784	37.9871886605	38.5940624390
H	16.3679066909	40.3303767659	39.7044305132
H	18.1425761163	40.5239001561	39.5497280687
H	18.9441422251	42.6254903861	40.9589665746
H	18.0124386323	44.0473050777	40.6351117079
H	23.0127342875	40.6358543609	41.2113876450
H	22.5161381886	42.7857526415	39.9879707956
H	23.5704345431	45.4342614474	39.8930024554
H	25.4849569410	46.7917514182	40.7263703817
H	27.1749927684	45.8035768471	42.2431388326
H	27.0043686789	43.4381759427	42.9730249120
H	25.1057037565	38.0887247599	39.4488489066
H	23.4407674009	39.4497207361	38.0144487695
H	20.7268471159	39.8021635391	38.7976371179
H	21.3703506683	38.0248198792	41.3936740694
H	15.8386878431	42.3904485458	37.7047619312
H	18.3652653261	42.5352050260	37.5477081880
H	17.1637555604	39.3795642221	35.0352882005
H	24.1262293523	45.0417340279	33.8637050847
H	22.0146896497	43.4457590778	33.2902482981
H	22.9554285847	41.1842110214	32.7314572649
H	25.5656892225	41.1970783362	32.6574694724
H	20.2576435903	42.9038657061	34.7577462925
H	18.8420974437	41.0423885987	32.3365930576
H	19.5234484127	39.8074847511	31.2448355028

H	20.7436602317	45.0241993506	37.1042027241
H	25.0070910464	44.5326154731	36.8370192202
H	24.8267594022	42.0672423953	36.7560588475
O	24.3723423408	46.0138842021	34.8876440291
O	22.9455338191	47.8146707821	34.8661151956
H	20.6404746647	41.7694705666	38.5979273913

homoprotocatechuate : radical + e⁻ + H⁺ : epoxide

E lacvp = -2666.686490

H	20.5454730000	35.5478669983	38.8164250004
C	20.5254675687	36.3146185563	38.0541249041
N	21.1406195612	36.1550436354	36.8105328698
C	20.0275598087	37.5954961629	38.0530352492
C	21.0060200547	37.3249029109	36.1095999935
N	20.3450223249	38.2201281055	36.8445517622
H	17.3432297457	40.3268844623	41.1148443160
C	17.2520009999	40.8040010011	40.1320040000
C	16.9695769286	42.2866486222	40.2701118307
O	16.1206335334	42.8971656215	39.5666571977
N	17.7219130218	42.9552261724	41.1884105373
H	25.2808689991	40.9541400006	42.6521449987
C	24.9000837730	41.8124056792	42.1119385565
C	23.8627092540	41.7974834000	41.2057004580
C	25.3740239556	43.1731751939	42.1857395387
N	23.6539434410	43.0738267501	40.7009989809
C	24.5685970901	43.9405595086	41.2827028551
C	26.3890455975	43.8263476019	42.9121834214
C	24.7631672738	45.3171021776	41.1005921087
C	26.5828891163	45.1940262895	42.7308466543
C	25.7774244343	45.9325009077	41.8326680146
H	23.9726829983	37.1214330011	41.5313609986
C	23.4960562790	37.7713288280	40.8254654349
N	24.0598633075	38.0715828899	39.5894175568
C	22.3124336708	38.4642334736	40.8739554692
C	23.2202025774	38.9289099886	38.9308927793
N	22.1525960117	39.1844128658	39.6902067918
H	14.9011790007	40.6201099993	36.0719110005
C	15.9465841705	40.8027511474	36.2233376279
N	16.3995788673	41.8647947509	36.9947109715
C	17.0719093796	40.1636802393	35.7541649757
C	17.7606333318	41.8472479093	36.9743507209
N	18.2009599623	40.8230133202	36.2381576739
H	26.2447069990	43.8340069994	33.3687669993
C	25.2894396122	43.3584513498	33.2356355024
N	24.1116767604	44.0538814021	33.4719406595
C	24.9357800200	42.0857930753	32.8610821187
C	23.0636062112	43.2390453316	33.2557277589
N	23.5461039707	42.0354783035	32.8835648863
H	19.4852350008	43.7230799986	33.5937000024
O	20.2735691212	43.2341874405	33.8706824969
H	18.5659855138	39.2623994062	32.6357431710
C	19.2579990022	40.0299990014	32.2789990002
C	20.5624615052	39.9990504021	33.0678090047
O	20.4736711671	39.7444476641	34.3500214845
O	21.6508742154	40.2165504685	32.4529111924
Fe	20.3143195011	40.3633929981	36.2704993534
O	22.5446070308	40.7153559184	36.5912784898
C	22.8277197758	41.9571031814	36.8132202544
C	21.6681300985	42.8961217256	36.9267554761
O	21.6277423609	43.3535807688	38.5332685117
O	20.5237399505	42.4950090225	36.3962670383
C	21.9410660752	44.2843336078	37.3623954481
C	24.1375418832	42.4881628895	36.9134791130
C	24.3610693759	43.8620198589	37.1025693424
C	23.3310917278	44.7915953352	37.2862422273

C	23.5577224029	46.2456433082	37.2418574013
H	24.5709649298	46.5162320664	37.5548092727
H	22.8199732414	46.8120221793	37.8114668986
C	23.4424461179	46.7661070763	35.6984874250
O	20.2951462847	40.7202881290	38.5288388245
H	21.5878006235	35.3178107397	36.4741297125
H	21.3766608663	37.5057951163	35.1154928366
H	19.4998973118	38.1253702836	38.8241925001
H	16.4392581791	40.3304095422	39.5809094652
H	18.1921748925	40.6507874818	39.5836735977
H	18.4341012354	42.5007791851	41.7370292406
H	17.6096144111	43.9546433638	41.2744079910
H	23.2481745444	40.9792796801	40.8732669477
H	22.9778964362	43.2925487408	39.9686397711
H	24.1443719380	45.8854589294	40.4135852661
H	25.9520698734	46.9972689995	41.7124470110
H	27.3633101625	45.7054202373	43.2861788854
H	27.0133781664	43.2696461716	43.6053980639
H	24.9504927742	37.7448225937	39.2510501599
H	23.3839162667	39.3386073271	37.9451305816
H	20.9617271296	40.1401509022	39.0366292379
H	21.5824759381	38.5042717633	41.6639568422
H	15.8767317042	42.4234462065	37.6670406610
H	18.3889097185	42.5614107690	37.4717043060
H	17.1585076497	39.3024611466	35.1151778480
H	24.0822459118	45.0196842792	33.9150030852
H	22.0006384074	43.4528644378	33.3945748161
H	22.9126065643	41.2143977750	32.7146401787
H	25.5366590132	41.2369945026	32.5877156271
H	20.2369774381	42.9962806769	34.8403031825
H	18.7950407001	41.0109922847	32.4406663760
H	19.4562534839	39.9039019814	31.2133773635
H	21.1529801234	45.0150640912	37.2023410628
H	25.3817194732	44.2291504796	37.0831112296
H	24.9744405579	41.8090217685	36.7939052804
O	24.2692060186	46.1879680918	34.9027509289
O	22.5842712976	47.6504687882	35.4836246068
H	20.4935630017	41.6725633759	38.6721452176

homoprotocatechuate : radical + 2e⁻ + H⁺ : gem diol

E_{lacvp} = -2666.800792

H	20.5454729998	35.5478670000	38.8164249997
C	20.4930232457	36.2766163955	38.0135269135
N	21.2268839493	36.1526342767	36.8288880969
C	19.8722959146	37.5004050809	37.9252523967
C	21.0274049926	37.2903149006	36.0812835809
N	20.2160426208	38.1284140258	36.7241014655
H	17.5008287407	40.7192939714	41.1970739341
C	17.2520009998	40.8039999995	40.1320020001
C	17.3381129170	42.2586824351	39.6993784920
O	16.3191459908	43.0037595943	39.6020765068
N	18.6002017838	42.6619130115	39.4342619100
H	25.2808679997	40.9541400002	42.6521449992
C	24.8671745100	41.7238547103	42.0089302407
C	23.7689146560	41.5892194091	41.1825547230
C	25.3544680949	43.0697954684	41.8379696692
N	23.5388771906	42.7709442931	40.4958612119
C	24.4915828946	43.6998204846	40.8804083115
C	26.4178012472	43.8148970803	42.3853448783
C	24.6744274089	45.0309265301	40.4797206640
C	26.6003510126	45.1371497021	41.9847383990
C	25.7355308295	45.7398431367	41.0409816490
H	23.9726830005	37.1214330001	41.5313600007
C	23.4103058236	37.7210961667	40.8465218419
N	23.9362606013	38.1940741189	39.6485714325

C	22.1225376120	38.1946892422	40.8995389008
C	22.9673757870	38.9437590544	39.0250901884
N	21.8571731122	38.9559506652	39.7639659219
H	14.9011789999	40.6201100002	36.0719120000
C	15.9503476799	40.8478027609	36.0948416473
N	16.4452221340	42.0488719712	36.6058413974
C	17.0453511037	40.1449603778	35.6528874427
C	17.8039466367	42.0390628647	36.4516235539
N	18.1959755349	40.8955372314	35.8892319974
H	26.2447079989	43.8340069999	33.3687680001
C	25.2977542201	43.3693912413	33.1609224783
N	24.1301569463	44.0958339435	33.3332573111
C	24.9336864728	42.1005101626	32.7830625055
C	23.0740399690	43.3031924639	33.0871626784
N	23.5422264989	42.0814753475	32.7476709743
H	19.4852360013	43.7230809997	33.5937020003
O	20.3462757144	43.3094303118	33.7515815385
H	18.5913431816	39.2937956383	32.7363959110
C	19.2579990001	40.0300000003	32.2789999998
C	20.6212891657	40.0533501535	32.9861108513
O	20.6484185995	39.8663366151	34.2742583618
O	21.6517031807	40.2625378246	32.2615458548
Fe	20.3161723968	40.4741026083	36.2300444145
O	22.8069101741	40.8407866291	36.5827848915
C	22.9999067645	42.0947093226	36.6794154982
C	21.7909563168	43.0074168864	36.9514586791
O	21.5632504705	42.7856196809	38.4058636139
O	20.6801512965	42.5895432127	36.2107091261
C	22.0788583953	44.4774662665	36.8324491146
C	24.3141442399	42.6953159186	36.6175318139
C	24.4537308933	44.0532880315	36.6248481038
C	23.3269814420	44.9885484647	36.7262603010
C	23.6121953465	46.4704424636	36.7300853924
H	24.3431880076	46.7042758971	37.5210431154
H	22.7071563077	47.0368299294	36.9777591546
C	24.1995852826	47.0750537338	35.4168706116
O	20.2010442144	40.6867453731	38.2802646850
H	21.8080918669	35.3728550757	36.5694608327
H	21.4756122737	37.4923306302	35.1232172205
H	19.2500512545	38.0012340027	38.6434481620
H	16.2343689176	40.4365310172	39.9823541677
H	17.9656012125	40.1995808628	39.5633706428
H	19.3075621383	41.9549468379	39.1690731187
H	18.7774557425	43.6236145517	39.1818129781
H	23.1184250077	40.7449400335	41.0313491832
H	22.8198431142	42.8915991172	39.7656232704
H	24.0099068282	45.4906859026	39.7557233708
H	25.9018662186	46.7721690654	40.7474843602
H	27.4186720553	45.7183137171	42.4013562720
H	27.0875171422	43.3635037760	43.1133005486
H	24.8822587595	38.0738646316	39.3255019097
H	23.1006360023	39.4617521923	38.0852082030
H	20.5932241613	39.9858217131	38.8551725796
H	21.3805085746	38.0524489936	41.6665452185
H	15.9503982175	42.7018932977	37.2010108194
H	18.4866110571	42.8097566718	36.7627853604
H	17.0982728949	39.1729645248	35.1938252108
H	24.1735288269	45.0764531698	33.7939837641
H	22.0110264053	43.5363165051	33.2004164476
H	22.8976445301	41.2643325699	32.5732426506
H	25.5240883133	41.2300656753	32.5581849106
H	20.4604804296	43.0546807530	34.7356712642
H	18.8107228336	41.0233832847	32.4040034280
H	19.3912666901	39.8281911090	31.2145104507
H	21.2070126754	45.1191327771	36.9192039650

H	25.4418152145	44.4929843616	36.5332544036
H	25.1701890487	42.0368070766	36.5122465007
O	24.6845228542	46.2337444366	34.5453011586
O	24.2088667480	48.3300825472	35.3277754348
H	21.0399117522	41.8619323272	38.4365651224

homoprotocatechuate : radical + 2e⁻ + H⁺ : epoxide

E_{lacvp} = -2666.783705

H	20.5454729712	35.5478674011	38.8164246436
C	20.4888931905	36.2919516750	38.0322978564
N	21.0539276405	36.0917928919	36.7702048284
C	19.9790116253	37.5696810759	38.0046389989
C	20.8792864935	37.2353619190	36.0339886309
N	20.2337466813	38.1495875355	36.7581017954
H	17.2148653472	40.5006682805	41.1858678117
C	17.2520011460	40.8040009751	40.1320038723
C	17.0420191909	42.3034768330	40.0236850498
O	15.9596700326	42.8044806987	39.5798554594
N	18.0971336196	43.0469122741	40.4138665653
H	25.2808693206	40.9541398611	42.6521446249
C	24.9326834870	41.8068113276	42.0802728461
C	24.0578503399	41.7479762283	41.0165861448
C	25.2615017352	43.1979191746	42.2718627367
N	23.8130042572	43.0182763241	40.5259575929
C	24.5368942659	43.9325754189	41.2732514994
C	26.0845828192	43.9079328870	43.1679328004
C	24.6222387785	45.3276451768	41.1693529896
C	26.1703140556	45.2952511983	43.0628643656
C	25.4449943043	45.9989089416	42.0729219240
H	23.9726828200	37.1214331356	41.5313607676
C	23.3279347525	37.7923601971	40.9962617666
N	23.5467462696	38.1073662627	39.6580660099
C	22.2245842190	38.5229893614	41.3689442315
C	22.5915381750	39.0067193412	39.2597818883
N	21.7714607623	39.2771535677	40.2830634157
H	14.9011786221	40.6201099689	36.0719109730
C	15.9681691107	40.7612711388	36.1878386052
N	16.4915715607	41.7635116150	36.9988620110
C	17.0565079294	40.1149837910	35.6399701310
C	17.8537135672	41.7031429464	36.9225316272
N	18.2327525539	40.7103653009	36.1078393109
H	26.2447068423	43.8340066654	33.3687666350
C	25.3034102266	43.3224231922	33.2260071985
N	24.1042865878	43.9156029529	33.5979929473
C	25.0127594227	42.0807039520	32.7086929693
C	23.1059814965	43.0660801858	33.3159390263
N	23.6309359042	41.9408343675	32.7723573602
H	19.4852346674	43.7230807513	33.5936992818
O	20.1336382505	43.0354080117	33.8270726869
H	18.5966783667	39.2371947603	32.6401182482
C	19.2580002760	40.0299992103	32.2790009719
C	20.6498774151	39.8796160612	32.8584813804
O	20.6947837178	39.5072102141	34.1177825477
O	21.6661462405	40.1253469983	32.1462786580
Fe	20.3881263022	40.2519706981	35.9351979941
O	22.3258785132	40.2859489904	36.6686428151
C	22.8678703750	41.5108739004	36.7790352637
C	21.868885162	42.6184223106	36.8323613469
O	21.8751760791	43.3027037577	38.3156774215
O	20.6469532528	42.3112356953	36.3415883081
C	22.3686653485	44.0065324867	37.0221935766
C	24.2034970433	41.8153369826	36.8344862413
C	24.6545549961	43.1852992269	36.9229206926
C	23.8216561409	44.2682598276	36.9691153612
C	24.3163242798	45.6899405852	37.0468974932

H	25.4119163313	45.6842127920	37.1451634976
H	23.9329795016	46.1966048557	37.9423351961
C	23.9832444388	46.6432563722	35.8616846501
O	20.3296185369	41.6725265275	39.9043049046
H	21.5141232371	35.2551735728	36.4521555151
H	21.2304598614	37.3998909460	35.0290937922
H	19.4992422224	38.1259217999	38.7896351366
H	16.4621892282	40.2821556771	39.5898032688
H	18.2385992872	40.5366550511	39.7435757659
H	19.0317572994	42.5915517281	40.4751613067
H	18.0237083787	44.0525091714	40.3458116102
H	23.5719623215	40.8992311867	40.5734561738
H	23.2100305145	43.2104498583	39.7193256921
H	24.0700360060	45.8656454479	40.4057009458
H	25.5328153899	47.0797038319	42.0128979257
H	26.8049799729	45.8488544466	43.7498054980
H	26.6480561875	43.3788909304	43.9325647770
H	24.3021679457	37.7754659163	39.0814903879
H	22.5406435858	39.4333131035	38.2546760773
H	20.8136160095	40.8325037294	40.1278675578
H	21.7398527940	38.5755313423	42.3289685651
H	15.9955233437	42.3101524738	37.7086960769
H	18.5375331616	42.3522870263	37.4405994788
H	17.0867498074	39.2871362748	34.9529308762
H	23.9995266477	44.9498069096	34.1685595798
H	22.0416661505	43.2165996826	33.4819167110
H	23.0416782855	41.1237103600	32.5211406223
H	25.6496730345	41.3072305196	32.3169755835
H	20.2084075195	42.8922636838	34.8204812623
H	18.8705303760	40.9947751754	32.6278558379
H	19.2891974303	40.0334502415	31.1869071621
H	21.7004368209	44.8212193050	36.7552454703
H	25.7296393994	43.3553441194	36.9345958498
H	24.9353316012	41.0158889480	36.7772782057
O	23.8769156807	46.1315154877	34.6572268298
O	23.8906998157	47.8694045684	36.1163048551
H	20.8417705877	42.2482971536	39.2871944582

small model : gem diol

E lacvp = -457.155029

H	20.4493678898	41.5300245266	36.1236579028
O	22.3968343152	40.2777795066	36.7218429083
C	22.8535505260	41.4570777848	36.7163495538
C	21.8945518633	42.6511520874	36.8575567183
O	21.4912499139	42.7699284909	38.1529207647
O	20.7896803119	42.4187089062	35.8736227198
C	22.5224630077	43.9727386461	36.5167694731
C	24.2859948386	41.7245542683	36.6618006533
C	24.7500870720	42.9992811122	36.4928877565
C	23.8702968747	44.1446335182	36.4230437670
H	24.3109269721	45.1358863580	36.3360606285
H	21.8286455256	44.8081949200	36.5134849442
H	25.8245062722	43.1740772857	36.4268879653
H	24.9571776069	40.8704607723	36.7140257769

small model : epoxide

E lacvp = -457.152588

H	20.8088313722	41.2816060596	36.1572947179
O	22.3799893523	40.3168336152	36.5287726377
C	22.9460361817	41.4801103682	36.6627049343
C	21.9862639687	42.6554868865	36.6733328632
O	21.9283059695	43.4662410412	37.9115499243
O	20.7479372070	42.2810951576	36.1280821955
C	22.5232507652	44.0368607692	36.5547697588
C	24.3106395288	41.7756801991	36.7318840164

C	24.7786867429	43.1188481586	36.6276283051
C	23.9635481041	44.2215531690	36.4859994625
H	24.3743932776	45.2205384894	36.3674289722
H	21.8553338324	44.8040094390	36.1721641078
H	25.8600384370	43.2705304269	36.6252574635
H	25.0185170241	40.9527015407	36.7612444583