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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-sulfonycatechol, 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.

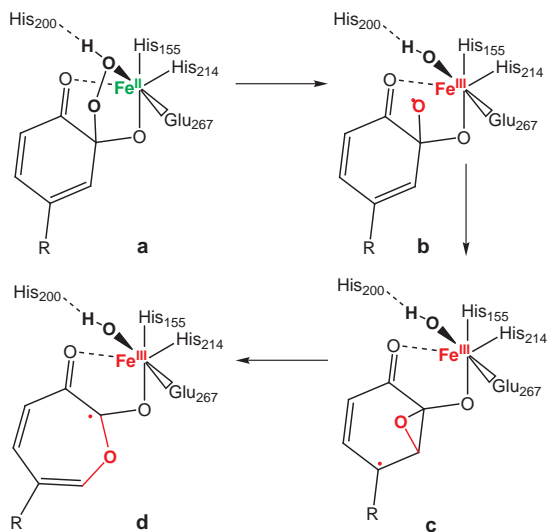


Figure 1: Reaction mechanism for O-O and C-C bond cleavage by extradiol dioxygenases as derived from previous computational studies.

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 alkoxy 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 lactone, 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

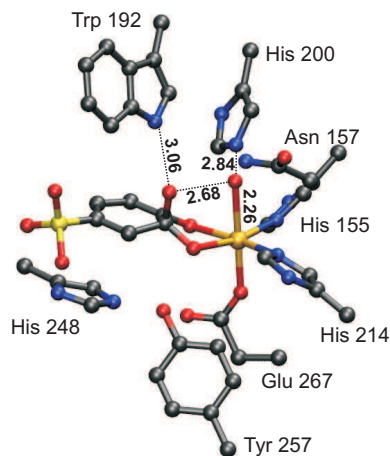


Figure 2: The active site region in the X-ray structure of the gem diol intermediate (PDB code: 3ECK, chain C).

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 alkoxy radical to an alkoxy anion. In the **radical** + e^- + H^+ variant the alkoxy 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 $r_{O-O}=2.68 \text{ \AA}$.

| redox form | homoprotocatechuate | | 4-sulfonylcatechol | |
|---------------------------------|-----------------------|----------------------------|-----------------------|----------------------------|
| | ΔE [kcal/mol] | r_{O-O} [\AA] | ΔE [kcal/mol] | r_{O-O} [\AA] |
| 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 |

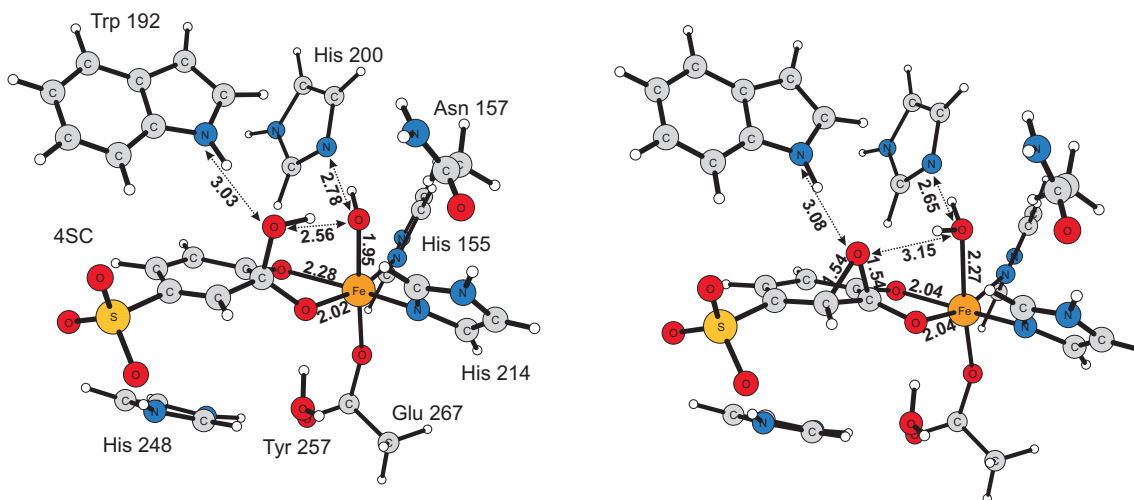


Figure 3: Optimized structures of the gem diol (left) and the epoxide (right) species for the 4-sulfonylcatechol substrate in the **radical** + e^- + H^+ form.

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 alkoxy 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 peroxy 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.”**

Tomasz Borowski, Valentin Georgiev, Per E. M. Siegbahn

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 |
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| N | 24.1154891528 | 37.8449568480 | 39.5109034133 |
| C | 22.3670598583 | 38.4397733462 | 40.7143704195 |
| C | 23.3159103252 | 38.6602699848 | 38.7550280950 |
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| H(*) | 26.2447090195 | 43.8340069987 | 33.3687670351 |
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| C | 25.0020850278 | 42.0352576406 | 32.8384542961 |
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| 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 |

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|----|---------------|---------------|---------------|
| 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 |

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|----|---------------|---------------|---------------|
| 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 |

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|----|---------------|---------------|---------------|
| 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 |

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|---|---------------|---------------|---------------|
| 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 |

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|----|---------------|---------------|---------------|
| 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 |

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|---|---------------|---------------|---------------|
| 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 |

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|---|---------------|---------------|---------------|
| 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 | 21.8688885162 | 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 |