# Dispiro-1,2,4-trioxane Analogs of a Prototype Dispiro-1,2,4-trioxolane: Mechanistic Comparators for Artemisinin in the Context of Reaction Pathways with Iron (II).

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## SUPPORTING INFORMATION

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**General.** The melting points are uncorrected. $^{1}H$ and $^{13}C$ NMR spectra were recorded on a 500 MHz spectrometer using $CDCl_3$ as solvent. All chemical shifts are reported in parts per million (ppm) and are relative to internal $(CH_3)_4Si$ (0 ppm) for $^{1}H$ and $CDCl_3$ (77.0 ppm) for $^{13}C$ NMR.

**Adamantane-2-spiro-3'-1',2',4'-trioxaspiro[5.5]undecane (5):** 10-Camphorsulfonic acid (23 mg, 0.1 mmol) was added to a mixture of (1-triethylsilylperoxycyclohexyl)methanol (260 mg, 1 mmol), 2-adamantanone (150 mg, 1 mmol) and $CH_2Cl_2$ (10 ml). The reaction mixture was stirred at room temperature overnight, washed with saturated $NaHCO_3$ (15 ml), water (15 ml) and brine (15 ml), dried over $MgSO_4$, filtered and concentrated. The crude product was purified by flash chromatography using gradient elution (sg, 2-4% ether in hexane) to afford **5** as a colorless solid (215 mg, 77%).

**7,8,15-Trioxadispiro[5.2.5.2]hexadecane (7):** *p*-Toluenesulfonic acid monohydrate (40 mg, 0.2 mmol) was added to a mixture of **10**[1] (420 mg, 2.87 mmol), cyclohexanone (338 mg, 3.45 mmol) and $CH_2Cl_2$ (30 ml). The reaction mixture was stirred at room temperature overnight, washed with saturated $NaHCO_3$ (20 ml), water (20 ml) and brine (20 ml), dried over $MgSO_4$, filtered and concentrated. The crude product was purified by flash chromatography (sg, 4% ether in hexane) to afford **7**[2,3] as a colorless solid (450 mg, 69%). mp 40-41 °C (90% aq. ethanol) lit.[4] mp 34-35 °C; $^{1}H$ NMR $\delta$ 1.22–1.78 (m, 17H), 1.91 (brs, 1H), 2.19 (brs, 1H), 2.39 (brs, 1H), 3.50 (brs, 1H), 3.72 (brs, 1H); $^{13}C$ NMR $\delta$ 21.3, 22.3, 25.6, 25.9, 28.3, 30.1, 32.2, 34.7, 65.9, 77.5, 101.1.

**Spiro Epoxide Synthesis.** Spiro epoxides **8** and **9** were prepared according to published procedures[5-7] and characterized by $^1$H NMR.

**1-Hydroperoxy-1-hydroxymethylcyclohexane (10):** Anhydrous $MgSO_4$ (10 g) was added to a mixture of 50% $H_2O_2$ (10.0 g, 114 mmol) and ether (150 ml) at 0 °C and stirred for 20 min. After filtration, the filtrate was added to a mixture of methylenecyclohexane oxide **8** (1.57 g, 14 mmol), molybdenyl acetylacetonate (228 mg, 0.7 mmol) and ether (10 ml) and stirred overnight at room temperature. The reaction mixture was washed with water (100 ml), brine (100 ml) and dried over $MgSO_4$, filtered and concentrated. The crude product was purified by flash chromatography (sg, 25% EtOAc in hexane) to afford **10**[1] as a colorless oil (1.2 g, 59%) and 1-hydroxy-1-hydroxymethylcyclohexane (**12**)[8] as a colorless oil (0.2 g, 10%).

**2-Hydroperoxy-2-hydroxymethyladamantane (11):** Anhydrous $MgSO_4$ (24 g) was added to a mixture of 50% $H_2O_2$ (23.8 g, 350 mmol) and THF (300 ml) at 0 °C and stirred for 20 min. After filtration, the filtrate was added to a mixture of 2-methyleneadamantane oxide **9** (5.81 g, 35 mmol), molybdenyl acetylacetonate (570 mg, 1.7 mmol) and THF (10 ml) and stirred overnight at room temperature. The reaction mixture was concentrated and the crude product was dissolved in chloroform (250 ml), washed with water (200 ml) and brine (200 ml), and dried over $MgSO_4$, filtered and concentrated. The crude product was purified by flash chromatography using gradient elution (sg, 10-25% EtOAc in hexane) to afford **11** as colorless solid (2.0 g, 29%). mp 104-107 °C (ether) and 2-hydroxy-2-hydroxymethyladamantane (**13**)[9] as a colorless solid (1.27 g, 20%). mp 210-211 °C (lit.[9] mp 212-213 °C; For **11**: $^1$H NMR $\delta$ 1.54 (d, J = 12.7 Hz, 2H), 1.71 (brs, 2H), 1.74-1.82 (m, 4H), 1.84-1.96 (m, 2H), 2.08 (brs, 2H), 2.12 (d, J = 12.4 Hz, 2H),

2.60 (brs, 1H), 3.94 (s, 2H), 7.55 (s, 1H); $^{13}$C NMR □27.3, 27.4, 30.5, 32.4, 34.2, 37.9, 63.1, 86.8. Anal. Calcd for $C_{11}H_{18}O_3$: C, 66.64; H, 9.15. Found: C, 66.80; H, 9.23.

A mixture of **4** (528 mg, 2.0 mmol), $FeBr_2$ (430 mg, 2.0 mmol) and THF (20 ml) was stirred at ambient temperature under a $N_2$ atmosphere for 16 h and concentrated. The crude product was dissolved in $CH_2Cl_2$ (20 ml) and acetic acid (3 ml). The resulting mixture was washed with water and brine, dried over $MgSO_4$, filtered and concentrated. The crude product was purified by flash chromatography using gradient elution (sg, 10-50% EtOAc in hexane) to give 2-adamantanone (10 mg, 3%), lactone **14** (212 mg, 64%), bicyclo[3.3.1]non-6-ene-3-carboxylic acid (**16**, 21 mg, 6%),[10] 6-bromohexanoic acid (**17**, 12 mg, 3%),[11] and 7-bromobicyclo[3.3.1]nonane-3-carboxylic acid (**15**, 8 mg, 2%). For **7-bromobicyclo[3.3.1]nonane-3-carboxylic acid (15)**: $^1$H NMR □ 1.24-1.32 (m, 1H), 1.52-1.60 (m, 1H), 1.84-1.94 (m, 2H), 2.06-2.16 (m, 2H), 2.20-2.28 (m, 2H), 2.30-2.38 (m, 2H), 2.39-2.46 (m, 2H), 2.72 (tt, J = 7.3, 5.7 Hz, 1H), 4.35 (tt, J = 9.6, 6.3 Hz, 1H); $^{13}$C NMR □ 26.36, 26.42, 31.0, 34.7, 38.2, 47.2, 180.3. HRMS-EI for $C_{10}H_{15}BrO_2$, $[M+H]^+$: calc 246.0255; found 246.0255.

A mixture of **5** (278 mg, 1.0 mmol), $FeBr_2$ (215 mg, 1.0 mmol) and THF (15 ml) was stirred at ambient temperature under a $N_2$ atmosphere for 16 h and concentrated. The crude product was dissolved in EtOAc, washed with water and brine, dried over $MgSO_4$, filtered and concentrated. The crude product was purified by flash chromatography using gradient elution (sg, 10-25% EtOAc in hexane) to give 2-adamantanone (30 mg, 20%), (1-hydroxycyclohexyl)methylbicyclo[3.3.1]non-6-ene-3-carboxylate (**20**, 3 mg, 1%), and two

additional fractions. For **20**: $^{1}$H NMR δ 1.28–1.80 (m, 15H), 2.08 (brs, 1H, OH), 2.10-2.40 (m, 4H), 2.45 (d, J = 14.2 Hz, 1H), 2.60 (t, J = 6.8 Hz, 1H), 3.84 (d, J = 11.2 Hz, 1H), 3.91 (d, J = 11.2 Hz, 1H), 5.56-5.64 (m, 2H); $^{13}$C NMR δ 22.0, 26.0, 25.7, 26.6, 28.7, 30.2, 31.78, 31.81, 32.3, 34.7, 34.8, 36.2, 70.8, 71.6, 129.3, 130.8, 175.9. HRMS-FAB for $C_{17}H_{27}O_3$, $[M+H]^+$: calc 279.1960; found 279.1971. The less polar fraction (140 mg, 39%) was a mixture of 4 isomers of (1-hydroxycyclohexyl)methyl 7-bromobicyclo[3.3.1]nonane-3-carboxylate (**18**) which were purified by preparative C18 RP-HPLC (75% methanol). **Isomer 1** (**18a**): colorless oil (10 mg, 2.8%); $^{1}$H NMR δ 1.28–1.36 (m, 2H), 1.44-1.72 (m, 10H), 1.78 (brs, 1H, OH), 1.85-1.93 (m, 2H), 2.04-2.12 (m, 2H), 2.20-2.26 (m, 2H), 2.26-2.27 (m, 2H), 2.42-2.48 (m, 2H), 2.68-2.75 (m, 1H), 4.04 (s, 2H), 4.34-4.41 (m, 1H); $^{13}$C NMR δ 21.6, 25.7, 26.2, 26.5, 30.9, 34.4, 35.3, 38.3, 47.3, 70.7, 71.7, 176.3. HRMS-FAB for $C_{17}H_{28}O_3Br$ $[M+H]^+$: calc 359.1222; found 359.1218. **Isomer 2** (**18b**): colorless oil (12 mg, 3.3%); $^{1}$H NMR δ 1.26–1.34 (m, 2H), 1.40-1.76 (m, 14H), 1.79-1.84 (m, 2H), 2.25-2.31 (m, 2H), 2.51-2.59 (m, 2H), 2.88-2.96 (m, 1H), 4.00 (s, 2H), 4.21-4.30 (m, 1H); $^{13}$C NMR δ 21.9, 25.9, 26.6, 28.1, 34.54, 34.58, 36.0, 38.2, 47.6, 70.9, 71.8, 176.5. HRMS-FAB for $C_{17}H_{28}O_3Br$ $[M+H]^+$: calc 359.1222; found 359.1227. **Isomer 3** (**18c**): colorless oil (6 mg, 1.7%); $^{1}$H NMR δ 1.24–1.34 (m, 2H), 1.40-1.72 (m, 14H), 1.85-1.93 (m, 2H), 2.12-2.24 (m, 4H), 2.53-2.62 (m, 1H), 3.99 (s, 2H), 4.43-4.51 (m, 1H); $^{13}$C NMR δ 21.6, 25.6, 27.8, 28.1, 28.8, 34.3, 35.5, 44.9, 46.4, 70.7, 71.5, 176.2. HRMS-FAB for $C_{17}H_{28}O_3Br$ $[M+H]^+$: calc 359.1222; found 359.1238. **Isomer 4** (**18d**): colorless oil (17 mg, 4.7%); $^{1}$H NMR δ 1.26–1.34 (m, 1H), 1.40-1.70 (m, 11H), 1.76 (s, 1H, OH), 1.78-1.87 (m, 2H), 1.93-2.00 (m, 2H), 2.10-2.23 (m, 4H), 2.35-2.41 (m, 2H), 2.82-2.91 (m, 1H), 3.98 (s, 2H), 4.68-4.76 (m, 1H); $^{13}$C NMR δ 21.6, 25.6, 30.9, 32.8, 33.2, 34.3, 39.7, 43.5, 49.2, 70.7, 71.5, 175.8. HRMS-FAB for $C_{17}H_{28}O_3Br$ $[M+H]^+$: calc 359.1222; found 359.1209. The more polar fraction (40 mg) was purified by RP-

HPLC (75% methanol) to afford (1-hydroxycyclohexyl)methyl 6-bromohexanoate (**19**, 12 mg, 3.9%) as colorless oil. $^{1}$H NMR $\delta$1.25–1.35 (m, 1H), 1.40-1.72 (m, 13H), 1.77 (s, 1H, OH), 1.95-1.92 (m, 2H), 2.39 (t, J = 7.3 Hz, 2H), 3.41 (t, J = 6.8 Hz, 2H), 4.00 (s, 2H); $^{13}$C NMR $\delta$ 21.6, 24.1, 25.6, 27.6, 32.3, 33.4, 34.0, 34.3, 70.6, 71.4, 173.5. HRMS-FAB for $C_{13}H_{24}O_3Br$ $[M+H]^+$: calc 307.0909; found 307.0911.

A mixture of **6** (278 mg, 1.0 mmol), $FeBr_2$ (215 mg, 1.0 mmol) and THF (15 ml) was stirred at ambient temperature under a $N_2$ atmosphere for 16 h and concentrated. The crude product was dissolved in EtOAc, washed with water and brine, dried over $MgSO_4$, filtered and concentrated. The crude product was purified by flash chromatography using gradient elution (sg, 10-25% EtOAc in hexane) to give 2-adamantanone (80 mg, 53%) and (2-hydroxy-2-adamantyl)methyl 6-bromohexanoate (**21**, 80 mg, 22%) as colorless oil. $^{1}$H NMR $\delta$1.45-1.58 (m, 4H), 1.62-1.80 (m, 14H), 2.07 (s, 1H, OH), 2.39 (t, J = 7.3 Hz, 2H), 3.41 (t, J = 6.8 Hz, 2H), 4.29 (s, 2H); $^{13}$C NMR: $\delta$24.1, 27.0, 27.4, 27.6, 32.3, 32.4, 33.4, 34.0, 34.4, 34.6, 38.1, 69.0, 74.0, 173.6. HRMS-FAB for $C_{17}H_{28}O_3Br$ $[M+H]^+$: calc 359.1222; found 359.1223.

A mixture of **7** (113 mg, 0.5 mmol), $FeBr_2$ (108 mg, 0.5 mmol) and THF (10 ml) was stirred at ambient temperature under a $N_2$ atmosphere for 16 h and concentrated. The crude product was dissolved in EtOAc, washed with water and brine, dried over $MgSO_4$, filtered and concentrated. The crude product was purified by flash chromatography using gradient elution (sg, 10-20% EtOAc in hexane) to give cyclohexanone (10 mg, 14%) and **19** (80 mg, 52%).

A mixture of **4** (132 mg, 0.5 mmol), $FeBr_2$ (162 mg, 0.75 mmol), 4-oxo-TEMPO (170 mg, 1.0 mmol) and THF (10 ml) was stirred at ambient temperature under a $N_2$ atmosphere for 16 h and concentrated. The crude product was dissolved in $CH_2Cl_2$ (20 ml) and acetic acid (3 ml), washed with water and brine, dried over $MgSO_4$, filtered and concentrated. $^1$H NMR of the crude product showed the presence of **14** (70%), **15** (8%), **16** (3%), **17** (6%), and **22** (7%).

***O*-Benzyl Oximes of 2-Adamantanone, Cyclohexanone, and Formaldehyde.** To monitor and quantitate 2-adamantanone, cyclohexanone, and formaldehyde formed in the reactions of **4**-**7** with $FeBr_2$, reactions were quenched with *O*-benzylhydroxylamine hydrochloride in the presence of pyridine to form the corresponding oxime ethers. 2-adamantanone, cyclohexanone, and formaldehyde *O*-benzyl oximes[12,13] were independently prepared to identify diagnostic signals in their $^1$H NMR spectra appropriate for quantitation: □3.57 (s), 2.20 (t), and 7.08 (d), respectively.

A mixture of the peroxide (1.0 mmol), $FeBr_2$ (215 mg, 1.0 mmol) and THF (10 ml) was stirred at ambient temperature under a $N_2$ atmosphere for 16 h. Pyridine (400 mg, 5.1 mmol) and *O*-benzylhydroxylamine hydrochloride (480 mg, 3.0 mmol) were added. The resulting mixture was stirred at ambient temperature for 48 h before concentration. The residue was dissolved in $CH_2Cl_2$ (20 ml) and acetic acid (3 ml), washed with water and brine, dried over $MgSO_4$, filtered and concentrated. For **4**, the $^1$H NMR of the crude product showed that the ratio of 2-adamantanone and cyclohexanone *O*-benzyl oximes was 1:22. For **5**, $^1$H-NMR of the crude product showed that the ratio (**18** + **20**):2-adamantanone *O*-benzyl oxime:cyclohexanone *O*-benzyl oxime:formaldehyde *O*-benzyl oxime was 2:1:1:0.43. For **6**, $^1$H-NMR of the crude product showed that the ratio **21**:2-adamantanone *O*-benzyl oxime:cyclohexanone *O*-benzyl

oxime:formaldehyde *O*-benzyl oxime was 1:3.1:3.3:1.5. For **7**, $^1$H-NMR of the crude product showed that the ratio **19**:cyclohexanone *O*-benzyl oxime:formaldehyde *O*-benzyl oxime was 1:1.4:0.35. For **5**-**7**, $^1$H-NMR also revealed the presence (d 8.14) of benzaldehyde *O*-benzyl oxime.[12]

**Antimalarial Screens.** In vitro and in vivo antimalarial data was obtained as previously described.[14-16]

**Computational Chemistry.** The LUMO calculations were performed with PM3[17,18] using SPARTAN.[19] The latter was also used for the conformational analyses with MMFF94 and the Monte Carlo method. The *ab initio* geometry optimizations via HF/6-31G* were carried out with the Gaussian 98 program.[20]

**Cartesian Coordinates and Total Energies for the Optimized Structures of 1 and 4-6.**

**4**_eq_peroxide_linkage MMFF94 E=39.246 kcal/mol

Final Energy Calculation

| | ---- Energy ---- | \|Gmax\| --- | <\|Gi\|> --- |
|---|---|---|---|
| Totals | 39.24638233 | 271.4264e-6 | 150.1516e-6 |

| | | FF Atom Type | | Cartesian Coordinates (Angstroms) | | | |
|---|---|---|---|---|---|---|---|
| | Atom Label | Symbol | # | chrg | X | Y | Z | Charge |
| 1 | H1 | HC | 5 | | -0.6590 | -2.1368 | 0.5670 | 0.000 |
| 2 | C1 | CHR3 | 1 | | -1.2417 | -1.2405 | 0.3236 | 0.000 |
| 3 | C2 | CHR3 | 1 | | -3.3847 | 0.0020 | 0.8061 | 0.000 |
| 4 | C3 | CHR3 | 1 | | -1.2687 | 1.2778 | 0.2929 | 0.000 |
| 5 | C4 | CH2R | 1 | | -2.5717 | 1.2718 | 1.1173 | 0.000 |
| 6 | C5 | CR | 1 | | -0.4241 | 0.0336 | 0.6442 | 0.560 |
| 7 | C6 | CH2R | 1 | | -2.5444 | -1.2418 | 1.1484 | 0.000 |
| 8 | C7 | CH2R | 1 | | -3.7281 | -0.0204 | -0.6940 | 0.000 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 9 | C8 | CH2R | 1 | -1.6306 | 1.2541 | -1.2060 | 0.000 |
| 10 | H2 | HC | 5 | -2.3474 | 1.3210 | 2.1895 | 0.000 |
| 11 | O1 | OR | 6 | -0.0733 | 0.0603 | 2.0270 | -0.280 |
| 12 | H3 | HC | 5 | -2.3185 | -1.2592 | 2.2212 | 0.000 |
| 13 | C9 | CH2R | 1 | -1.6026 | -1.2603 | -1.1754 | 0.000 |
| 14 | H4 | HC | 5 | -4.3077 | -0.0007 | 1.3964 | 0.000 |
| 15 | H5 | HC | 5 | -0.7025 | 2.1902 | 0.5152 | 0.000 |
| 16 | H6 | HC | 5 | -3.1665 | 2.1627 | 0.8801 | 0.000 |
| 17 | O2 | OR | 6 | 0.7825 | 0.0464 | -0.1172 | -0.560 |
| 18 | H7 | HC | 5 | -3.1200 | -2.1509 | 0.9339 | 0.000 |
| 19 | H8 | HC | 5 | -0.6937 | -1.2916 | -1.7880 | 0.000 |
| 20 | H9 | HC | 5 | -4.3241 | -0.9110 | -0.9286 | 0.000 |
| 21 | C11 | CH2R | 1 | 3.4546 | 1.3885 | -0.2654 | 0.000 |
| 22 | H11 | HC | 5 | -2.2185 | 2.1445 | -1.4612 | 0.000 |
| 23 | H12 | HC | 5 | -2.6884 | -0.0321 | -2.5980 | 0.000 |
| 24 | H13 | HC | 5 | -4.3436 | 0.8506 | -0.9503 | 0.000 |
| 25 | C10 | CHR3 | 1 | -2.4370 | -0.0164 | -1.5317 | 0.000 |
| 26 | H14 | HC | 5 | -2.1702 | -2.1694 | -1.4097 | 0.000 |
| 27 | H21 | HC | 5 | -0.7232 | 1.2911 | -1.8205 | 0.000 |
| 28 | C14 | CR | 1 | 1.8235 | -0.2236 | 0.8196 | 0.560 |
| 29 | O4 | OR | 6 | 1.2348 | -0.5813 | 2.0666 | -0.280 |
| 30 | C13 | CH2R | 1 | 3.4351 | -1.0427 | -0.9589 | 0.000 |
| 31 | H20 | HC | 5 | 3.3805 | 0.8846 | 1.8352 | 0.000 |
| 32 | H17 | HC | 5 | 2.0472 | 1.8835 | 1.2826 | 0.000 |
| 33 | C12 | CH2R | 1 | 2.6609 | -1.3972 | 0.3093 | 0.000 |
| 34 | H18 | HC | 5 | 2.0118 | -2.2571 | 0.1018 | 0.000 |
| 35 | C15 | CH2R | 1 | 2.6808 | 1.0327 | 1.0027 | 0.000 |
| 36 | H15 | HC | 5 | 3.3593 | -1.7220 | 1.0912 | 0.000 |
| 37 | H10 | HC | 5 | 4.1106 | 2.2437 | -0.0676 | 0.000 |
| 38 | H16 | HC | 5 | 2.7544 | 1.7005 | -1.0500 | 0.000 |
| 39 | C16 | CH2R | 1 | 4.2860 | 0.2096 | -0.7645 | 0.000 |
| 40 | H25 | HC | 5 | 4.7720 | 0.4754 | -1.7100 | 0.000 |
| 41 | H23 | HC | 5 | 2.7342 | -0.8836 | -1.7875 | 0.000 |
| 42 | H24 | HC | 5 | 4.0775 | -1.8834 | -1.2442 | 0.000 |
| 43 | H19 | HC | 5 | 5.0850 | -0.0025 | -0.0434 | 0.000 |

**4**_eq_peroxide_linkage Gaussian Std HF/6-31G* E(HF) = -844.403718 a.u.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -0.666783 | -0.392357 | -2.084203 |
| 2 | 6 | 0 | -1.268049 | -0.136643 | -1.218895 |
| 3 | 6 | 0 | -3.369978 | -0.651821 | 0.063431 |

| | | | | | |
|---|---|---|---|---|---|
| 4 | 6 | 0 | -1.254822 | -0.071051 | 1.292837 |
| 5 | 6 | 0 | -2.528713 | -0.933796 | 1.318300 |
| 6 | 6 | 0 | -0.440241 | -0.403313 | 0.043533 |
| 7 | 6 | 0 | -2.540656 | -0.999652 | -1.182532 |
| 8 | 6 | 0 | -3.754472 | 0.835639 | 0.025593 |
| 9 | 6 | 0 | -1.641303 | 1.417123 | 1.249025 |
| 10 | 1 | 0 | -2.270783 | -1.986783 | 1.370898 |
| 11 | 8 | 0 | -0.015543 | -1.744971 | 0.123947 |
| 12 | 1 | 0 | -2.278180 | -2.052237 | -1.179427 |
| 13 | 6 | 0 | -1.655262 | 1.351483 | -1.253228 |
| 14 | 1 | 0 | -4.268413 | -1.262665 | 0.085059 |
| 15 | 1 | 0 | -0.636952 | -0.276708 | 2.160317 |
| 16 | 1 | 0 | -3.098148 | -0.700862 | 2.214671 |
| 17 | 8 | 0 | 0.770038 | 0.308264 | 0.017569 |
| 18 | 1 | 0 | -3.122153 | -0.818542 | -2.083207 |
| 19 | 1 | 0 | -0.764569 | 1.969445 | -1.297550 |
| 20 | 1 | 0 | -4.366074 | 1.040346 | -0.850428 |
| 21 | 6 | 0 | 3.418653 | 0.400498 | 1.434410 |
| 22 | 1 | 0 | -2.205615 | 1.664681 | 2.144716 |
| 23 | 1 | 0 | -2.754871 | 2.750887 | -0.030595 |
| 24 | 1 | 0 | -4.356276 | 1.088546 | 0.895947 |
| 25 | 6 | 0 | -2.483364 | 1.698912 | -0.005613 |
| 26 | 1 | 0 | -2.230057 | 1.553270 | -2.153768 |
| 27 | 1 | 0 | -0.749159 | 2.034453 | 1.252048 |
| 28 | 6 | 0 | 1.814289 | -0.596793 | -0.236429 |
| 29 | 8 | 0 | 1.138694 | -1.757654 | -0.655787 |
| 30 | 6 | 0 | 3.482718 | 1.134974 | -0.983538 |
| 31 | 1 | 0 | 3.310327 | -1.668554 | 0.825797 |
| 32 | 1 | 0 | 1.962818 | -1.166329 | 1.820929 |
| 33 | 6 | 0 | 2.683343 | -0.109431 | -1.384744 |
| 34 | 1 | 0 | 2.047422 | 0.093134 | -2.238357 |
| 35 | 6 | 0 | 2.628401 | -0.846930 | 1.028310 |
| 36 | 1 | 0 | 3.359643 | -0.913828 | -1.661343 |
| 37 | 1 | 0 | 4.023949 | 0.179496 | 2.308554 |
| 38 | 1 | 0 | 2.725315 | 1.186247 | 1.721182 |
| 39 | 6 | 0 | 4.304660 | 0.892793 | 0.286086 |
| 40 | 1 | 0 | 4.818929 | 1.805060 | 0.574487 |
| 41 | 1 | 0 | 2.795187 | 1.959746 | -0.818657 |
| 42 | 1 | 0 | 4.132337 | 1.425324 | -1.803807 |
| 43 | 1 | 0 | 5.075364 | 0.151169 | 0.081625 |

**5**_eq_peroxide_linkage MMFF94 E=70.970 kcal/mol

Final Energy Calculation

| | ---- Energy ---- | \|Gmax\| --- | <\|Gi\|> --- |
|---|---|---|---|
| Totals | 70.97012908 | 124.8443e-6 | 70.1875e-6 |

| | | FF Atom Type | | Cartesian Coordinates (Angstroms) | | | |
|---|---|---|---|---|---|---|---|
| Atom | Label | Symbol | # | chrg | X | Y | Z | Charge |
| 1 | H1 | HC | 5 | | 1.5632 | 2.1824 | 0.0380 | 0.000 |
| 2 | C1 | CHR3 | 1 | | 1.1451 | 1.7375 | -0.8734 | 0.000 |
| 3 | C2 | CHR3 | 1 | | 1.7339 | 0.6354 | -3.0649 | 0.000 |
| 4 | C3 | CHR3 | 1 | | -0.3527 | -0.0463 | -1.8194 | 0.000 |
| 5 | C4 | CH2R | 1 | | 0.8042 | -0.5385 | -2.7118 | 0.000 |
| 6 | C5 | CR | 1 | | 0.2169 | 0.5476 | -0.4983 | 0.560 |
| 7 | C6 | CH2R | 1 | | 2.2996 | 1.2460 | -1.7713 | 0.000 |
| 8 | C7 | CH2R | 1 | | 0.9270 | 1.7089 | -3.8163 | 0.000 |
| 9 | C8 | CH2R | 1 | | -1.1471 | 1.0338 | -2.5820 | 0.000 |
| 10 | H2 | HC | 5 | | 1.3706 | -1.3281 | -2.2041 | 0.000 |
| 11 | O1 | OR | 6 | | 1.0255 | -0.3912 | 0.2352 | -0.560 |
| 12 | H3 | HC | 5 | | 2.9117 | 0.5060 | -1.2423 | 0.000 |
| 13 | C9 | CH2R | 1 | | 0.3500 | 2.8136 | -1.6409 | 0.000 |
| 14 | H4 | HC | 5 | | 2.5552 | 0.2807 | -3.6975 | 0.000 |
| 15 | H5 | HC | 5 | | -1.0240 | -0.8871 | -1.6146 | 0.000 |
| 16 | H6 | HC | 5 | | 0.4015 | -0.9827 | -3.6306 | 0.000 |
| 17 | O2 | OR | 6 | | -0.8240 | 1.0719 | 0.3453 | -0.280 |
| 18 | H7 | HC | 5 | | 2.9645 | 2.0842 | -2.0144 | 0.000 |
| 19 | H8 | HC | 5 | | -0.4581 | 3.2138 | -1.0173 | 0.000 |
| 20 | H9 | HC | 5 | | 1.5816 | 2.5448 | -4.0921 | 0.000 |
| 21 | H10 | HC | 5 | | -2.1381 | -2.6222 | 1.2837 | 0.000 |
| 22 | H11 | HC | 5 | | -1.5695 | 0.6051 | -3.4994 | 0.000 |
| 23 | H12 | HC | 5 | | -0.7973 | 2.9798 | -3.4746 | 0.000 |
| 24 | H13 | HC | 5 | | 0.5305 | 1.2938 | -4.7511 | 0.000 |
| 25 | C10 | CHR3 | 1 | | -0.2281 | 2.2152 | -2.9344 | 0.000 |
| 26 | H14 | HC | 5 | | 1.0059 | 3.6593 | -1.8823 | 0.000 |
| 27 | C15 | CH2R | 1 | | 0.1127 | -0.8582 | 4.0070 | 0.000 |
| 28 | H23 | HC | 5 | | -1.9948 | 1.3820 | -1.9801 | 0.000 |
| 29 | C11 | CH2R | 1 | | 0.2509 | -1.4258 | 0.8458 | 0.280 |
| 30 | H15 | HC | 5 | | -1.3352 | 0.5509 | 3.2574 | 0.000 |
| 31 | H16 | HC | 5 | | -2.8077 | -1.5408 | 2.4759 | 0.000 |
| 32 | O3 | OR | 6 | | -1.6860 | -0.0448 | 0.7466 | -0.280 |
| 33 | C12 | CH2R | 1 | | -0.4736 | -0.0143 | 2.8769 | 0.000 |
| 34 | H24 | HC | 5 | | 0.2620 | 0.7435 | 2.5822 | 0.000 |
| 35 | C16 | CH2R | 1 | | -1.2707 | -2.8322 | 3.2513 | 0.000 |
| 36 | H21 | HC | 5 | | -0.1085 | -2.0929 | 0.0540 | 0.000 |
| 37 | C13 | CR | 1 | | -0.9227 | -0.8551 | 1.6632 | 0.280 |
| 38 | H22 | HC | 5 | | 0.9305 | -2.0151 | 1.4683 | 0.000 |
| 39 | C14 | CH2R | 1 | | -1.8621 | -1.9816 | 2.1310 | 0.000 |
| 40 | H27 | HC | 5 | | -1.7233 | -1.5320 | 4.9066 | 0.000 |
| 41 | H18 | HC | 5 | | 0.3293 | -0.2147 | 4.8676 | 0.000 |
| 42 | H19 | HC | 5 | | 1.0693 | -1.2907 | 3.6919 | 0.000 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 43 | H20 | HC | 5 | -2.0145 | -3.5644 | 3.5859 | 0.000 |
| 44 | C17 | CH2R | 1 | -0.8368 | -1.9725 | 4.4337 | 0.000 |
| 45 | H26 | HC | 5 | -0.4140 | -3.4039 | 2.8761 | 0.000 |
| 46 | H25 | HC | 5 | -0.3528 | -2.6011 | 5.1896 | 0.000 |

**5**_eq_peroxide_linkage Gaussian Std HF/6-31G* E(HF) = -883.422018 a.u.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 1.204357 | 2.268997 | -0.318818 |
| 2 | 6 | 0 | 1.741555 | 1.338190 | -0.171749 |
| 3 | 6 | 0 | 3.300909 | 0.063591 | 1.332312 |
| 4 | 6 | 0 | 1.414675 | -1.127975 | 0.168541 |
| 5 | 6 | 0 | 2.255060 | -1.055473 | 1.455274 |
| 6 | 6 | 0 | 0.700830 | 0.220930 | -0.037042 |
| 7 | 6 | 0 | 2.578938 | 1.402736 | 1.116682 |
| 8 | 6 | 0 | 4.219837 | -0.223820 | 0.134411 |
| 9 | 6 | 0 | 2.336644 | -1.403456 | -1.031873 |
| 10 | 1 | 0 | 1.617657 | -0.878669 | 2.315471 |
| 11 | 8 | 0 | -0.144816 | 0.558794 | 1.022978 |
| 12 | 1 | 0 | 1.945354 | 1.633046 | 1.965292 |
| 13 | 6 | 0 | 2.666217 | 1.052901 | -1.367321 |
| 14 | 1 | 0 | 3.890932 | 0.111459 | 2.243898 |
| 15 | 1 | 0 | 0.684400 | -1.923089 | 0.245538 |
| 16 | 1 | 0 | 2.747386 | -2.012021 | 1.614158 |
| 17 | 8 | 0 | -0.050893 | 0.248954 | -1.223003 |
| 18 | 1 | 0 | 3.302970 | 2.209073 | 1.027549 |
| 19 | 1 | 0 | 2.098589 | 1.034603 | -2.290732 |
| 20 | 1 | 0 | 4.977659 | 0.552347 | 0.050864 |
| 21 | 1 | 0 | -2.668471 | -2.301042 | 0.109167 |
| 22 | 1 | 0 | 2.827190 | -2.363462 | -0.888754 |
| 23 | 1 | 0 | 4.034766 | -0.490548 | -2.002068 |
| 24 | 1 | 0 | 4.746876 | -1.163660 | 0.285212 |
| 25 | 6 | 0 | 3.385313 | -0.287731 | -1.154529 |
| 26 | 1 | 0 | 3.391206 | 1.858795 | -1.453482 |
| 27 | 6 | 0 | -3.931864 | 1.430495 | 0.127706 |
| 28 | 1 | 0 | 1.752795 | -1.476334 | -1.942568 |
| 29 | 6 | 0 | -1.325691 | -0.192538 | 1.131856 |
| 30 | 1 | 0 | -2.889176 | 0.993988 | -1.707737 |
| 31 | 1 | 0 | -3.374269 | -1.532909 | -1.286742 |
| 32 | 8 | 0 | -1.071194 | -0.696469 | -1.153142 |
| 33 | 6 | 0 | -2.657914 | 1.075888 | -0.649242 |
| 34 | 1 | 0 | -1.924538 | 1.864351 | -0.546054 |

| | | | | | |
|---|---|---|---|---|---|
| 35 | 6 | 0 | -4.362427 | -1.018190 | 0.554085 |
| 36 | 1 | 0 | -1.103796 | -1.198486 | 1.474722 |
| 37 | 6 | 0 | -2.050823 | -0.263890 | -0.213795 |
| 38 | 1 | 0 | -1.919640 | 0.295660 | 1.890428 |
| 39 | 6 | 0 | -3.104874 | -1.372859 | -0.246627 |
| 40 | 1 | 0 | -5.320786 | 0.186165 | -0.945617 |
| 41 | 1 | 0 | -4.352738 | 2.343993 | -0.281776 |
| 42 | 1 | 0 | -3.688716 | 1.650012 | 1.165116 |
| 43 | 1 | 0 | -5.086023 | -1.821676 | 0.455072 |
| 44 | 6 | 0 | -4.966349 | 0.304196 | 0.076744 |
| 45 | 1 | 0 | -4.126560 | -0.949675 | 1.614363 |
| 46 | 1 | 0 | -5.832417 | 0.560875 | 0.680242 |

**6**_eq_peroxide_linkage MMFF94 E=71.777 kcal/mol

Final Energy Calculation

| | ---- Energy ---- | \|Gmax\| --- | <\|Gi\|> --- |
|---|---|---|---|
| Totals | 71.77654195 | 245.1267e-6 | 110.9049e-6 |

| Atom | Label | FF Atom Type Symbol | # | chrg | Cartesian Coordinates (Angstroms) X | Y | Z | Charge |
|---|---|---|---|---|---|---|---|---|
| 1 | H1 | HC | 5 | | 1.4478 | 2.3298 | -0.5835 | 0.000 |
| 2 | C1 | CHR3 | 1 | | 1.8509 | 1.3399 | -0.3368 | 0.000 |
| 3 | C2 | CHR3 | 1 | | 3.3071 | 0.0441 | 1.2674 | 0.000 |
| 4 | C3 | CHR3 | 1 | | 1.3175 | -1.0675 | 0.1758 | 0.000 |
| 5 | C4 | CH2R | 1 | | 2.1763 | -0.9818 | 1.4542 | 0.000 |
| 6 | C5 | CR | 1 | | 0.6889 | 0.3201 | -0.1577 | 0.280 |
| 7 | C6 | CH2R | 1 | | 2.7079 | 1.4233 | 0.9417 | 0.000 |
| 8 | C7 | CH2R | 1 | | 4.1992 | -0.4042 | 0.0968 | 0.000 |
| 9 | C8 | CH2R | 1 | | 2.2307 | -1.5132 | -0.9888 | 0.000 |
| 10 | H2 | HC | 5 | | 1.5611 | -0.7143 | 2.3198 | 0.000 |
| 11 | C11 | CH2R | 1 | | -0.3388 | 0.8145 | 0.8812 | 0.280 |
| 12 | H3 | HC | 5 | | 2.1138 | 1.7868 | 1.7870 | 0.000 |
| 13 | C9 | CH2R | 1 | | 2.7651 | 0.8880 | -1.4991 | 0.000 |
| 14 | H4 | HC | 5 | | 3.9056 | 0.1069 | 2.1829 | 0.000 |
| 15 | H5 | HC | 5 | | 0.5413 | -1.8284 | 0.3152 | 0.000 |
| 16 | H6 | HC | 5 | | 2.6051 | -1.9672 | 1.6773 | 0.000 |
| 17 | O2 | OR | 6 | | -0.0421 | 0.2806 | -1.4038 | -0.280 |
| 18 | H7 | HC | 5 | | 3.5153 | 2.1528 | 0.7990 | 0.000 |
| 19 | H8 | HC | 5 | | 2.2040 | 0.8537 | -2.4405 | 0.000 |
| 20 | H9 | HC | 5 | | 5.0249 | 0.3052 | -0.0389 | 0.000 |
| 21 | H10 | HC | 5 | | -2.5211 | -2.3174 | 0.3111 | 0.000 |
| 22 | H11 | HC | 5 | | 2.6538 | -2.5019 | -0.7709 | 0.000 |
| 23 | H12 | HC | 5 | | 4.0049 | -0.8133 | -2.0235 | 0.000 |
| 24 | H13 | HC | 5 | | 4.6510 | -1.3785 | 0.3207 | 0.000 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 25 | C10 | CHR3 | 1 | 3.3656 | -0.4945 | -1.1927 | 0.000 |
| 26 | H14 | HC | 5 | 3.5698 | 1.6197 | -1.6443 | 0.000 |
| 27 | C15 | CH2R | 1 | -3.9996 | 1.3112 | -0.0491 | 0.000 |
| 28 | H23 | HC | 5 | 1.6512 | -1.6199 | -1.9132 | 0.000 |
| 29 | O4 | OR | 6 | -1.4839 | -0.0394 | 0.9454 | -0.560 |
| 30 | H15 | HC | 5 | -3.1601 | 0.6740 | -1.9359 | 0.000 |
| 31 | H16 | HC | 5 | -3.3889 | -1.8260 | -1.1325 | 0.000 |
| 32 | O3 | OR | 6 | -1.0583 | -0.7683 | -1.2720 | -0.280 |
| 33 | C12 | CH2R | 1 | -2.8120 | 0.9092 | -0.9214 | 0.000 |
| 34 | H24 | HC | 5 | -2.1500 | 1.7748 | -1.0323 | 0.000 |
| 35 | C16 | CH2R | 1 | -4.2379 | -1.0862 | 0.7117 | 0.000 |
| 36 | H26 | HC | 5 | -3.9056 | -0.8877 | 1.7378 | 0.000 |
| 37 | C13 | CR | 1 | -2.0543 | -0.3028 | -0.3480 | 0.560 |
| 38 | H25 | HC | 5 | -5.7573 | 0.4396 | 0.8498 | 0.000 |
| 39 | C14 | CH2R | 1 | -3.0388 | -1.4691 | -0.1550 | 0.000 |
| 40 | H27 | HC | 5 | -5.4342 | -0.1132 | -0.7912 | 0.000 |
| 41 | H18 | HC | 5 | -4.5361 | 2.1426 | -0.5202 | 0.000 |
| 42 | H19 | HC | 5 | -3.6406 | 1.6739 | 0.9217 | 0.000 |
| 43 | H20 | HC | 5 | -4.9371 | -1.9285 | 0.7635 | 0.000 |
| 44 | C17 | CH2R | 1 | -4.9569 | 0.1422 | 0.1630 | 0.000 |
| 45 | H17 | HC | 5 | 0.0758 | 0.8636 | 1.8906 | 0.000 |
| 46 | H21 | HC | 5 | -0.6811 | 1.8268 | 0.6375 | 0.000 |

**6**_eq_peroxide_linkage Gaussian Std HF/6-31G* E(HF) = -883.420927 a.u.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 1.343814 | 2.293332 | -0.487011 |
| 2 | 6 | 0 | 1.807613 | 1.337667 | -0.258782 |
| 3 | 6 | 0 | 3.353889 | 0.114665 | 1.307929 |
| 4 | 6 | 0 | 1.355840 | -1.061353 | 0.318114 |
| 5 | 6 | 0 | 2.257513 | -0.930363 | 1.560310 |
| 6 | 6 | 0 | 0.699831 | 0.297526 | -0.006778 |
| 7 | 6 | 0 | 2.696536 | 1.467641 | 0.992171 |
| 8 | 6 | 0 | 4.211658 | -0.331448 | 0.113848 |
| 9 | 6 | 0 | 2.221691 | -1.504622 | -0.874136 |
| 10 | 1 | 0 | 1.680262 | -0.668031 | 2.441934 |
| 11 | 6 | 0 | -0.326901 | 0.768059 | 1.027280 |
| 12 | 1 | 0 | 2.123486 | 1.816741 | 1.847426 |
| 13 | 6 | 0 | 2.681231 | 0.892437 | -1.445709 |
| 14 | 1 | 0 | 3.977775 | 0.212441 | 2.192569 |
| 15 | 1 | 0 | 0.583375 | -1.795581 | 0.505227 |
| 16 | 1 | 0 | 2.707055 | -1.897428 | 1.770617 |

| | | | | | |
|---|---|---|---|---|---|
| 17 | 8 | 0 | -0.028933 | 0.240594 | -1.232226 |
| 18 | 1 | 0 | 3.457950 | 2.220803 | 0.806846 |
| 19 | 1 | 0 | 2.087445 | 0.832125 | -2.349441 |
| 20 | 1 | 0 | 5.005850 | 0.389877 | -0.066831 |
| 21 | 1 | 0 | -2.479874 | -2.259067 | 0.306338 |
| 22 | 1 | 0 | 2.666027 | -2.472257 | -0.652037 |
| 23 | 1 | 0 | 3.930902 | -0.782852 | -1.979441 |
| 24 | 1 | 0 | 4.693131 | -1.280787 | 0.337849 |
| 25 | 6 | 0 | 3.325529 | -0.466642 | -1.134021 |
| 26 | 1 | 0 | 3.451543 | 1.640956 | -1.617676 |
| 27 | 6 | 0 | -3.946018 | 1.371992 | 0.019259 |
| 28 | 1 | 0 | 1.606591 | -1.631944 | -1.756898 |
| 29 | 8 | 0 | -1.478361 | -0.036202 | 0.990622 |
| 30 | 1 | 0 | -3.053396 | 0.738437 | -1.843053 |
| 31 | 1 | 0 | -3.329300 | -1.714964 | -1.126086 |
| 32 | 8 | 0 | -1.030595 | -0.721594 | -1.134190 |
| 33 | 6 | 0 | -2.735135 | 0.980277 | -0.833165 |
| 34 | 1 | 0 | -2.040881 | 1.805314 | -0.918447 |
| 35 | 6 | 0 | -4.225898 | -1.038715 | 0.720609 |
| 36 | 1 | 0 | -3.902852 | -0.853429 | 1.740221 |
| 37 | 6 | 0 | -2.036150 | -0.259907 | -0.270769 |
| 38 | 1 | 0 | -5.749559 | 0.489465 | 0.818963 |
| 39 | 6 | 0 | -3.011437 | -1.421561 | -0.129963 |
| 40 | 1 | 0 | -5.361275 | -0.025041 | -0.802536 |
| 41 | 1 | 0 | -4.444103 | 2.225061 | -0.432630 |
| 42 | 1 | 0 | -3.608906 | 1.689143 | 1.002351 |
| 43 | 1 | 0 | -4.917289 | -1.875701 | 0.754779 |
| 44 | 6 | 0 | -4.926619 | 0.205687 | 0.168945 |
| 45 | 1 | 0 | 0.037299 | 0.708973 | 2.039951 |
| 46 | 1 | 0 | -0.580996 | 1.803993 | 0.822509 |

**1** MFF94 E=64.687 kcal/mol
Final Energy Calculation

| | ---- Energy ---- | \|Gmax\| --- | <\|Gi\|> --- |
|---|---|---|---|
| Totals | 64.68726090 | 438.6221e-9 | 190.7309e-9 |

| Atom Label | FF Atom Type Symbol | # | chrg | Cartesian Coordinates (Angstroms) X | Y | Z | Charge |
|---|---|---|---|---|---|---|---|
| 1 C1 | CHR3 | 1 | | 0.1416 | -1.0127 | 2.0055 | 0.000 |
| 2 C2 | CR | 1 | | -0.2452 | 0.2654 | -0.2053 | 0.280 |
| 3 C3 | CH2R | 1 | | 1.1641 | 1.2881 | 1.6530 | 0.000 |
| 4 C4 | CHR3 | 1 | | 0.1982 | 1.5626 | 0.4929 | 0.000 |
| 5 C5 | CH2R | 1 | | 0.5547 | 0.3142 | 2.6551 | 0.000 |
| 6 C6 | CHR3 | 1 | | -0.8107 | -0.7768 | 0.8012 | 0.000 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 7 | H1 | HC | 5 | 2.1182 | 0.8928 | 1.2862 | 0.000 |
| 8 | H2 | HC | 5 | -0.6953 | 2.0425 | 0.9206 | 0.000 |
| 9 | H3 | HC | 5 | -0.3176 | 0.7835 | 3.1285 | 0.000 |
| 10 | H4 | HC | 5 | -1.7487 | -0.3576 | 1.1973 | 0.000 |
| 11 | H5 | HC | 5 | 1.0523 | -1.5100 | 1.6469 | 0.000 |
| 12 | H6 | HC | 5 | 1.3942 | 2.2180 | 2.1848 | 0.000 |
| 13 | H7 | HC | 5 | 1.2821 | 0.1265 | 3.4544 | 0.000 |
| 14 | C7 | CH3R | 1 | -0.4807 | -1.9204 | 3.0732 | 0.000 |
| 15 | H8 | HC | 5 | -0.6545 | -2.9300 | 2.6890 | 0.000 |
| 16 | H9 | HC | 5 | -1.4365 | -1.5192 | 3.4266 | 0.000 |
| 17 | H10 | HC | 5 | 0.1856 | -2.0162 | 3.9375 | 0.000 |
| 18 | C8 | CHR3 | 1 | 0.7514 | 2.5361 | -0.5642 | 0.061 |
| 19 | H11 | HC | 5 | -0.0573 | 2.7936 | -1.2621 | 0.000 |
| 20 | C9 | CH3R | 1 | 1.2272 | 3.8578 | 0.0441 | 0.000 |
| 21 | H12 | HC | 5 | 2.1512 | 3.7352 | 0.6188 | 0.000 |
| 22 | H13 | HC | 5 | 0.4619 | 4.2872 | 0.6988 | 0.000 |
| 23 | H14 | HC | 5 | 1.4370 | 4.5891 | -0.7449 | 0.000 |
| 24 | C10 | COO | 3 | 1.8377 | 1.9120 | -1.4215 | 0.659 |
| 25 | O1 | O=C | 7 | 2.8459 | 2.5169 | -1.7689 | -0.570 |
| 26 | C11 | CHR3 | 1 | 0.9269 | -0.2942 | -1.0549 | 0.560 |
| 27 | O2 | OR | 6 | 0.5302 | -1.4107 | -1.8622 | -0.560 |
| 28 | C12 | CR | 1 | -0.8301 | -1.2725 | -2.2757 | 0.560 |
| 29 | H15 | HC | 5 | 1.7164 | -0.6813 | -0.4028 | 0.000 |
| 30 | O3 | OC=x | 6 | 1.5757 | 0.6745 | -1.8951 | -0.430 |
| 31 | C13 | CH2R | 1 | -1.2004 | -2.1186 | 0.1322 | 0.000 |
| 32 | H16 | HC | 5 | -0.3284 | -2.7863 | 0.1220 | 0.000 |
| 33 | H17 | HC | 5 | -1.9512 | -2.6235 | 0.7532 | 0.000 |
| 34 | C14 | CH2R | 1 | -1.7515 | -2.0349 | -1.2995 | 0.000 |
| 35 | H18 | HC | 5 | -1.8734 | -3.0710 | -1.6412 | 0.000 |
| 36 | H19 | HC | 5 | -2.7537 | -1.5895 | -1.2905 | 0.000 |
| 37 | C15 | CH3R | 1 | -0.9469 | -1.8505 | -3.6828 | 0.000 |
| 38 | H20 | HC | 5 | -0.6313 | -2.8988 | -3.7136 | 0.000 |
| 39 | H21 | HC | 5 | -0.3006 | -1.3000 | -4.3767 | 0.000 |
| 40 | H22 | HC | 5 | -1.9713 | -1.7707 | -4.0618 | 0.000 |
| 41 | O4 | OR | 6 | -1.1902 | 0.1113 | -2.3740 | -0.280 |
| 42 | O5 | OR | 6 | -1.3841 | 0.6323 | -1.0240 | -0.280 |

**1** Gaussian Std HF/6-31G* E(HF) = -955.0688063 a.u.

Cartesian Coordinates (Angstroms)

| Atom | Label | X | Y | Z |
|---|---|---|---|---|
| C | C1 | 0.1364063 | -1.0150308 | 2.0444567 |
| C | C2 | -0.2159794 | 0.2495666 | -0.1749529 |
| C | C3 | 1.1868790 | 1.2811776 | 1.6614819 |

| | | | | |
|---|---|---|---|---|
| C | C4 | 0.2208527 | 1.5525471 | 0.5024681 |
| C | C5 | 0.5639637 | 0.3174088 | 2.6712345 |
| C | C6 | -0.7840744 | -0.7848055 | 0.8245976 |
| H | H1 | 2.1314510 | 0.8798544 | 1.2974110 |
| H | H2 | -0.6791968 | 1.9916109 | 0.9251473 |
| H | H3 | -0.3041032 | 0.7929991 | 3.1254688 |
| H | H4 | -1.6981364 | -0.3201339 | 1.1883888 |
| H | H5 | 1.0362999 | -1.5262633 | 1.7046099 |
| H | H6 | 1.4277947 | 2.2144015 | 2.1568695 |
| H | H7 | 1.2670265 | 0.1267452 | 3.4770201 |
| C | C7 | -0.5224671 | -1.9068838 | 3.1029526 |
| H | H8 | -0.7116412 | -2.9090993 | 2.7370290 |
| H | H9 | -1.4686421 | -1.4855351 | 3.4327716 |
| H | H10 | 0.1198589 | -1.9956797 | 3.9734729 |
| C | C8 | 0.7346935 | 2.5271667 | -0.5703063 |
| H | H11 | -0.1035898 | 2.7121294 | -1.2359267 |
| C | C9 | 1.2102486 | 3.8736973 | -0.0254117 |
| H | H12 | 2.1273140 | 3.7820447 | 0.5436769 |
| H | H13 | 0.4480843 | 4.3053860 | 0.6162443 |
| H | H14 | 1.4012943 | 4.5604759 | -0.8384072 |
| C | C10 | 1.7824923 | 1.9033579 | -1.4703935 |
| O | O1 | 2.6587672 | 2.5160271 | -1.9776992 |
| C | C11 | 0.9322630 | -0.3384457 | -1.0003218 |
| O | O2 | 0.5067466 | -1.3313022 | -1.8535460 |
| C | C12 | -0.8341593 | -1.2321403 | -2.2713523 |
| H | H15 | 1.6499609 | -0.7958995 | -0.3386434 |
| O | O3 | 1.6453178 | 0.6048846 | -1.7645522 |
| C | C13 | -1.1670021 | -2.1089601 | 0.1296945 |
| H | H16 | -0.2961046 | -2.7549172 | 0.0906413 |
| H | H17 | -1.9007135 | -2.6228408 | 0.7403558 |
| C | C14 | -1.7376230 | -1.9976662 | -1.2910258 |
| H | H18 | -1.8679996 | -3.0063749 | -1.6690037 |
| H | H19 | -2.7141033 | -1.5282342 | -1.2926446 |
| C | C15 | -0.9147171 | -1.7243376 | -3.7000492 |
| H | H20 | -0.5087841 | -2.7264538 | -3.7577318 |
| H | H21 | -0.3338896 | -1.0737835 | -4.3405663 |
| H | H22 | -1.9447802 | -1.7356742 | -4.0357690 |
| O | O4 | -1.1689666 | 0.1224077 | -2.3164362 |
| O | O5 | -1.3110420 | 0.6065734 | -1.0212532 |

**4**_ax_peroxide_linkage MMFF94 E=39.522 kcal/mol
Final Energy Calculation

| | ---- Energy ---- | \|Gmax\| --- | <\|Gi\|> --- |
|---|---|---|---|
| Totals | 39.52192824 | 390.8067e-6 | 163.7540e-6 |

FF Atom Type Cartesian Coordinates (Angstroms)

| Atom Label | Symbol | # | chrg | X | Y | Z | Charge |
|---|---|---|---|---|---|---|---|
| 1 H1 | HC | 5 | 0.5674 | -1.6329 | -1.2676 | 0.000 | |
| 2 C1 | CHR3 | 1 | 1.2493 | -0.9450 | -0.7539 | 0.000 | |
| 3 C2 | CHR3 | 1 | 3.3061 | 0.4901 | -1.0358 | 0.000 | |
| 4 C3 | CHR3 | 1 | 1.4528 | 1.2222 | 0.5129 | 0.000 | |
| 5 C4 | CH2R | 1 | 2.5316 | 1.6992 | -0.4803 | 0.000 | |
| 6 C5 | CR | 1 | 0.4682 | 0.2726 | -0.2037 | 0.560 | |
| 7 C6 | CH2R | 1 | 2.3280 | -0.4640 | -1.7452 | 0.000 | |
| 8 C7 | CH2R | 1 | 3.9786 | -0.2554 | 0.1306 | 0.000 | |
| 9 C8 | CH2R | 1 | 2.1430 | 0.4772 | 1.6734 | 0.000 | |
| 10 H2 | HC | 5 | 2.0741 | 2.2622 | -1.3025 | 0.000 | |
| 11 O1 | OR | 6 | -0.1818 | 0.9636 | -1.2695 | -0.280 | |
| 12 H3 | HC | 5 | 1.8641 | 0.0411 | -2.6007 | 0.000 | |
| 13 C9 | CH2R | 1 | 1.9388 | -1.6867 | 0.4089 | 0.000 | |
| 14 H4 | HC | 5 | 4.0687 | 0.8324 | -1.7441 | 0.000 | |
| 15 H5 | HC | 5 | 0.9141 | 2.0915 | 0.9088 | 0.000 | |
| 16 H6 | HC | 5 | 3.2237 | 2.3859 | 0.0229 | 0.000 | |
| 17 O2 | OR | 6 | -0.5333 | -0.1607 | 0.7164 | -0.560 | |
| 18 H7 | HC | 5 | 2.8743 | -1.3259 | -2.1480 | 0.000 | |
| 19 H8 | HC | 5 | 1.1926 | -2.0686 | 1.1158 | 0.000 | |
| 20 H9 | HC | 5 | 4.5506 | -1.1101 | -0.2511 | 0.000 | |
| 21 H10 | HC | 5 | -2.6283 | 0.9502 | 1.7832 | 0.000 | |
| 22 H11 | HC | 5 | 2.8324 | 1.1543 | 2.1929 | 0.000 | |
| 23 H12 | HC | 5 | 3.3997 | -1.2693 | 1.9590 | 0.000 | |
| 24 H13 | HC | 5 | 4.6938 | 0.4059 | 0.6351 | 0.000 | |
| 25 C10 | CHR3 | 1 | 2.9145 | -0.7400 | 1.1314 | 0.000 | |
| 26 H14 | HC | 5 | 2.4818 | -2.5589 | 0.0243 | 0.000 | |
| 27 H23 | HC | 5 | -4.9214 | -0.3261 | 1.2164 | 0.000 | |
| 28 H15 | HC | 5 | -3.9113 | 1.6171 | -0.9165 | 0.000 | |
| 29 O4 | OR | 6 | -1.5034 | 0.3524 | -1.3246 | -0.280 | |
| 30 C11 | CH2R | 1 | -4.7289 | -0.0559 | 0.1708 | 0.000 | |
| 31 H16 | HC | 5 | -4.4868 | -2.1261 | -0.3859 | 0.000 | |
| 32 H17 | HC | 5 | -2.0390 | 2.0886 | 0.5850 | 0.000 | |
| 33 C12 | CH2R | 1 | -2.5414 | -1.3136 | 0.0738 | 0.000 | |
| 34 H18 | HC | 5 | -1.9954 | -2.0809 | -0.4892 | 0.000 | |
| 35 C13 | CH2R | 1 | -3.9725 | 1.2690 | 0.1218 | 0.000 | |
| 36 H19 | HC | 5 | -3.8866 | -0.9840 | -1.5837 | 0.000 | |
| 37 C14 | CR | 1 | -1.7724 | 0.0079 | 0.0332 | 0.560 | |
| 38 H20 | HC | 5 | -4.5287 | 2.0309 | 0.6795 | 0.000 | |
| 39 C15 | CH2R | 1 | -2.5664 | 1.1338 | 0.7029 | 0.000 | |
| 40 H21 | HC | 5 | 1.4034 | 0.1533 | 2.4153 | 0.000 | |
| 41 C16 | CH2R | 1 | -3.9481 | -1.1794 | -0.5062 | 0.000 | |
| 42 H22 | HC | 5 | -2.6006 | -1.6764 | 1.1080 | 0.000 | |
| 43 H24 | HC | 5 | -5.7049 | 0.0587 | -0.3140 | 0.000 | |

**4**_ax_peroxide_linkage Gaussian Std HF/6-31G* E(HF) = -844.404030 a.u.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -0.573291 | 1.661069 | -1.171462 |
| 2 | 6 | 0 | -1.272567 | 1.000374 | -0.671209 |
| 3 | 6 | 0 | -3.278625 | -0.489434 | -0.960404 |
| 4 | 6 | 0 | -1.438401 | -1.147777 | 0.621613 |
| 5 | 6 | 0 | -2.478582 | -1.668959 | -0.385412 |
| 6 | 6 | 0 | -0.489770 | -0.178396 | -0.081928 |
| 7 | 6 | 0 | -2.312164 | 0.469616 | -1.672727 |
| 8 | 6 | 0 | -3.991386 | 0.253482 | 0.180615 |
| 9 | 6 | 0 | -2.152830 | -0.399466 | 1.759852 |
| 10 | 1 | 0 | -1.989530 | -2.218030 | -1.183876 |
| 11 | 8 | 0 | 0.227413 | -0.884146 | -1.070296 |
| 12 | 1 | 0 | -1.815584 | -0.036228 | -2.494001 |
| 13 | 6 | 0 | -1.988228 | 1.740431 | 0.471543 |
| 14 | 1 | 0 | -4.012067 | -0.861352 | -1.670731 |
| 15 | 1 | 0 | -0.847317 | -1.965934 | 1.018758 |
| 16 | 1 | 0 | -3.143454 | -2.366012 | 0.118629 |
| 17 | 8 | 0 | 0.522005 | 0.265824 | 0.783854 |
| 18 | 1 | 0 | -2.859771 | 1.306995 | -2.098283 |
| 19 | 1 | 0 | -1.262117 | 2.134774 | 1.174567 |
| 20 | 1 | 0 | -4.575281 | 1.079339 | -0.219921 |
| 21 | 1 | 0 | 2.599741 | -0.917665 | 1.815579 |
| 22 | 1 | 0 | -2.816128 | -1.088291 | 2.277132 |
| 23 | 1 | 0 | -3.457351 | 1.303636 | 1.992389 |
| 24 | 1 | 0 | -4.690616 | -0.412939 | 0.681232 |
| 25 | 6 | 0 | -2.953514 | 0.779735 | 1.184517 |
| 26 | 1 | 0 | -2.534091 | 2.588346 | 0.065105 |
| 27 | 1 | 0 | 4.925760 | 0.262697 | 1.250414 |
| 28 | 1 | 0 | 3.787065 | -1.543962 | -0.922565 |
| 29 | 8 | 0 | 1.402304 | -0.147174 | -1.192859 |
| 30 | 6 | 0 | 4.716274 | 0.035464 | 0.206139 |
| 31 | 1 | 0 | 4.525381 | 2.127970 | -0.311497 |
| 32 | 1 | 0 | 1.915901 | -1.983566 | 0.609776 |
| 33 | 6 | 0 | 2.573451 | 1.380638 | 0.198304 |
| 34 | 1 | 0 | 2.011507 | 2.163108 | -0.298280 |
| 35 | 6 | 0 | 3.899337 | -1.256541 | 0.119162 |
| 36 | 1 | 0 | 3.856749 | 1.036415 | -1.495525 |
| 37 | 6 | 0 | 1.760225 | 0.096551 | 0.150788 |
| 38 | 1 | 0 | 4.424454 | -2.068419 | 0.613716 |
| 39 | 6 | 0 | 2.511885 | -1.089103 | 0.746103 |

| | | | | | |
|---|---|---|---|---|---|
| 40 | 1 | 0 | -1.428264 | -0.046396 | 2.485901 |
| 41 | 6 | 0 | 3.961340 | 1.207256 | -0.427409 |
| 42 | 1 | 0 | 2.668853 | 1.661357 | 1.243213 |
| 43 | 1 | 0 | 5.677010 | -0.096161 | -0.283149 |

**5**_ax_peroxide_linkage MMFF94 E=70.135 kcal/mol

Final Energy Calculation

| | ---- Energy ---- | \|Gmax\| --- | <\|Gi\|> --- |
|---|---|---|---|
| Totals | 70.13470713 | 107.8593e-6 | 63.4456e-6 |

| Atom | Label | FF Atom Type Symbol | # | chrg | Cartesian Coordinates (Angstroms) X | Y | Z | Charge |
|---|---|---|---|---|---|---|---|---|
| 1 | H1 | HC | 5 | | -1.9239 | 1.9098 | 0.0967 | 0.000 |
| 2 | C1 | CHR3 | 1 | | -1.4547 | 1.5160 | -0.8135 | 0.000 |
| 3 | C2 | CHR3 | 1 | | -0.2832 | 2.1624 | -2.9520 | 0.000 |
| 4 | C3 | CHR3 | 1 | | 0.3459 | 0.0335 | -1.7514 | 0.000 |
| 5 | C4 | CH2R | 1 | | 0.8729 | 1.2130 | -2.5929 | 0.000 |
| 6 | C5 | CR | 1 | | -0.2834 | 0.5672 | -0.4317 | 0.560 |
| 7 | C6 | CH2R | 1 | | -0.9282 | 2.6933 | -1.6604 | 0.000 |
| 8 | C7 | CH2R | 1 | | -1.3394 | 1.3874 | -3.7595 | 0.000 |
| 9 | C8 | CH2R | 1 | | -0.7164 | -0.7286 | -2.5699 | 0.000 |
| 10 | H2 | HC | 5 | | 1.6510 | 1.7574 | -2.0447 | 0.000 |
| 11 | O1 | OR | 6 | | 0.6384 | 1.3453 | 0.3549 | -0.560 |
| 12 | H3 | HC | 5 | | -0.2001 | 3.2830 | -1.0911 | 0.000 |
| 13 | C9 | CH2R | 1 | | -2.5129 | 0.7534 | -1.6368 | 0.000 |
| 14 | H4 | HC | 5 | | 0.0962 | 2.9997 | -3.5483 | 0.000 |
| 15 | H5 | HC | 5 | | 1.1754 | -0.6505 | -1.5424 | 0.000 |
| 16 | H6 | HC | 5 | | 1.3417 | 0.8349 | -3.5100 | 0.000 |
| 17 | O2 | OR | 6 | | -0.8407 | -0.4948 | 0.3630 | -0.280 |
| 18 | H7 | HC | 5 | | -1.7540 | 3.3721 | -1.9079 | 0.000 |
| 19 | H8 | HC | 5 | | -2.9375 | -0.0700 | -1.0505 | 0.000 |
| 20 | H9 | HC | 5 | | -2.1619 | 2.0569 | -4.0399 | 0.000 |
| 21 | H10 | HC | 5 | | 2.7268 | -1.9804 | 1.3123 | 0.000 |
| 22 | H11 | HC | 5 | | -0.2635 | -1.1263 | -3.4867 | 0.000 |
| 23 | H12 | HC | 5 | | -2.6322 | -0.3362 | -3.5089 | 0.000 |
| 24 | H13 | HC | 5 | | -0.8992 | 1.0164 | -4.6932 | 0.000 |
| 25 | C10 | CHR3 | 1 | | -1.8802 | 0.2102 | -2.9290 | 0.000 |
| 26 | H14 | HC | 5 | | -3.3463 | 1.4232 | -1.8830 | 0.000 |
| 27 | H25 | HC | 5 | | 0.8290 | 0.4037 | 3.6072 | 0.000 |
| 28 | C15 | CH2R | 1 | | -0.3243 | -1.4096 | 3.7282 | 0.000 |
| 29 | C11 | CH2R | 1 | | 1.6504 | 0.5434 | 0.9661 | 0.280 |
| 30 | C17 | CH2R | 1 | | 0.8008 | -2.3426 | 4.1634 | 0.000 |
| 31 | C16 | CH2R | 1 | | 1.6538 | -2.7873 | 2.9803 | 0.000 |
| 32 | O3 | OR | 6 | | 0.2552 | -1.3804 | 0.7699 | -0.280 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 33 | C12 | CH2R | 1 | 0.2126 | -0.2138 | 2.9410 | 0.000 |
| 34 | H19 | HC | 5 | 2.4966 | -3.3882 | 3.3406 | 0.000 |
| 35 | H26 | HC | 5 | 2.9018 | -1.0402 | 2.7988 | 0.000 |
| 36 | H21 | HC | 5 | 2.3429 | 0.2123 | 0.1839 | 0.000 |
| 37 | C13 | CR | 1 | 1.0525 | -0.6526 | 1.7233 | 0.280 |
| 38 | H22 | HC | 5 | 2.2199 | 1.1885 | 1.6439 | 0.000 |
| 39 | C14 | CH2R | 1 | 2.1818 | -1.5934 | 2.1825 | 0.000 |
| 40 | H23 | HC | 5 | -1.0886 | -1.5915 | -2.0050 | 0.000 |
| 41 | H16 | HC | 5 | 1.0602 | -3.4366 | 2.3252 | 0.000 |
| 42 | H24 | HC | 5 | -0.6382 | 0.4070 | 2.6383 | 0.000 |
| 43 | H28 | HC | 5 | 1.4354 | -1.8300 | 4.8968 | 0.000 |
| 44 | H18 | HC | 5 | -1.0457 | -1.9634 | 3.1154 | 0.000 |
| 45 | H20 | HC | 5 | -0.8660 | -1.0529 | 4.6116 | 0.000 |
| 46 | H17 | HC | 5 | 0.3792 | -3.2207 | 4.6655 | 0.000 |

**5**_ax_peroxide_linkage Gaussian Std HF/6-31G* E(HF) = -883.424320 a.u.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 1.206386 | -1.114642 | -2.010105 |
| 2 | 6 | 0 | 1.719145 | -0.706517 | -1.145754 |
| 3 | 6 | 0 | 3.494612 | 0.887153 | -0.354320 |
| 4 | 6 | 0 | 1.356848 | 0.630990 | 0.948240 |
| 5 | 6 | 0 | 2.446433 | 1.619551 | 0.497800 |
| 6 | 6 | 0 | 0.678583 | 0.035452 | -0.299368 |
| 7 | 6 | 0 | 2.805723 | 0.287278 | -1.589877 |
| 8 | 6 | 0 | 4.133405 | -0.237902 | 0.475241 |
| 9 | 6 | 0 | 1.998671 | -0.501650 | 1.768085 |
| 10 | 1 | 0 | 2.008482 | 2.435414 | -0.067869 |
| 11 | 8 | 0 | 0.086233 | 1.003837 | -1.114316 |
| 12 | 1 | 0 | 2.371404 | 1.070670 | -2.199944 |
| 13 | 6 | 0 | 2.364253 | -1.831310 | -0.318418 |
| 14 | 1 | 0 | 4.261036 | 1.589824 | -0.670870 |
| 15 | 1 | 0 | 0.622521 | 1.140084 | 1.559055 |
| 16 | 1 | 0 | 2.916621 | 2.056246 | 1.375749 |
| 17 | 8 | 0 | -0.299010 | -0.918450 | 0.032497 |
| 18 | 1 | 0 | 3.531966 | -0.235966 | -2.207206 |
| 19 | 1 | 0 | 1.618883 | -2.560524 | -0.021870 |
| 20 | 1 | 0 | 4.892477 | -0.749880 | -0.112432 |
| 21 | 1 | 0 | -2.674672 | 1.650274 | 1.616287 |
| 22 | 1 | 0 | 2.463796 | -0.077230 | 2.654774 |
| 23 | 1 | 0 | 3.500825 | -2.029027 | 1.505620 |
| 24 | 1 | 0 | 4.636672 | 0.179129 | 1.345067 |

| | | | | | |
|---|---|---|---|---|---|
| 25 | 6 | 0 | 3.049585 | -1.232902 | 0.919278 |
| 26 | 1 | 0 | 3.092183 | -2.351481 | -0.936472 |
| 27 | 1 | 0 | -3.209976 | 0.456644 | -1.914805 |
| 28 | 6 | 0 | -3.693331 | -1.298595 | -0.767833 |
| 29 | 6 | 0 | -1.079965 | 1.600764 | -0.609875 |
| 30 | 6 | 0 | -4.780507 | -0.659032 | 0.098970 |
| 31 | 6 | 0 | -4.168764 | 0.128192 | 1.260181 |
| 32 | 8 | 0 | -1.324163 | -0.308571 | 0.750493 |
| 33 | 6 | 0 | -2.695536 | -0.252225 | -1.268540 |
| 34 | 1 | 0 | -4.947033 | 0.635714 | 1.823236 |
| 35 | 1 | 0 | -3.651979 | 1.932880 | 0.194559 |
| 36 | 1 | 0 | -0.837081 | 2.277287 | 0.204077 |
| 37 | 6 | 0 | -2.066188 | 0.543312 | -0.119904 |
| 38 | 1 | 0 | -1.498416 | 2.183416 | -1.419473 |
| 39 | 6 | 0 | -3.146622 | 1.159782 | 0.770519 |
| 40 | 1 | 0 | 1.237459 | -1.194816 | 2.108216 |
| 41 | 1 | 0 | -3.681170 | -0.558044 | 1.945270 |
| 42 | 1 | 0 | -1.919576 | -0.714936 | -1.862709 |
| 43 | 1 | 0 | -5.383512 | 0.009797 | -0.514188 |
| 44 | 1 | 0 | -3.164240 | -2.053232 | -0.193995 |
| 45 | 1 | 0 | -4.141671 | -1.805479 | -1.617794 |
| 46 | 1 | 0 | -5.453929 | -1.420684 | 0.481896 |

**6**_ax_peroxide_linkage MMFF94 E=71.706 kcal/mol

Final Energy Calculation

| | ---- Energy ---- | \|Gmax\| --- | <\|Gi\|> --- |
|---|---|---|---|
| Totals | 71.70550714 | 135.7808e-6 | 54.1900e-6 |

| Atom Label | FF Atom Type Symbol | # | chrg | Cartesian Coordinates (Angstroms) X | Y | Z | Charge |
|---|---|---|---|---|---|---|---|
| 1 H1 | HC | 5 | | 1.4745 | -0.3298 | -2.3907 | 0.000 |
| 2 C1 | CHR3 | 1 | | 1.8491 | -0.2280 | -1.3647 | 0.000 |
| 3 C2 | CHR3 | 1 | | 3.5119 | 0.9583 | 0.1187 | 0.000 |
| 4 C3 | CHR3 | 1 | | 1.2649 | 0.2557 | 1.0369 | 0.000 |
| 5 C4 | CH2R | 1 | | 2.3749 | 1.3255 | 1.0875 | 0.000 |
| 6 C5 | CR | 1 | | 0.6807 | 0.1385 | -0.4041 | 0.280 |
| 7 C6 | CH2R | 1 | | 2.9575 | 0.8419 | -1.3118 | 0.000 |
| 8 C7 | CH2R | 1 | | 4.1065 | -0.3974 | 0.5380 | 0.000 |
| 9 C8 | CH2R | 1 | | 1.8815 | -1.0984 | 1.4550 | 0.000 |
| 10 H2 | HC | 5 | | 1.9738 | 2.3149 | 0.8434 | 0.000 |
| 11 C11 | CH2R | 1 | | -0.0710 | 1.3966 | -0.8861 | 0.280 |
| 12 H3 | HC | 5 | | 2.5801 | 1.8123 | -1.6514 | 0.000 |
| 13 C9 | CH2R | 1 | | 2.4666 | -1.5805 | -0.9402 | 0.000 |
| 14 H4 | HC | 5 | | 4.2909 | 1.7280 | 0.1527 | 0.000 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 15 | H5 | HC | 5 | 0.4827 | 0.5153 | 1.7592 | 0.000 |
| 16 | H6 | HC | 5 | 2.7697 | 1.3995 | 2.1088 | 0.000 |
| 17 | O2 | OR | 6 | -0.2943 | -0.9246 | -0.4911 | -0.280 |
| 18 | H7 | HC | 5 | 3.7671 | 0.5703 | -2.0012 | 0.000 |
| 19 | H8 | HC | 5 | 1.7208 | -2.3817 | -1.0022 | 0.000 |
| 20 | H9 | HC | 5 | 4.9340 | -0.6668 | -0.1298 | 0.000 |
| 21 | H10 | HC | 5 | -2.5405 | 1.0000 | 2.1068 | 0.000 |
| 22 | H11 | HC | 5 | 2.2695 | -1.0289 | 2.4790 | 0.000 |
| 23 | H12 | HC | 5 | 3.4462 | -2.4470 | 0.7908 | 0.000 |
| 24 | H13 | HC | 5 | 4.5246 | -0.3273 | 1.5497 | 0.000 |
| 25 | C10 | CHR3 | 1 | 3.0183 | -1.4835 | 0.4924 | 0.000 |
| 26 | H14 | HC | 5 | 3.2733 | -1.8536 | -1.6321 | 0.000 |
| 27 | H25 | HC | 5 | -3.3169 | 1.1153 | -1.6275 | 0.000 |
| 28 | C15 | CH2R | 1 | -3.9044 | -0.8880 | -1.0617 | 0.000 |
| 29 | O4 | OR | 6 | -1.2312 | 1.6585 | -0.0920 | -0.560 |
| 30 | C17 | CH2R | 1 | -4.8743 | -0.5334 | 0.0604 | 0.000 |
| 31 | C16 | CH2R | 1 | -4.1406 | -0.2252 | 1.3610 | 0.000 |
| 32 | O3 | OR | 6 | -1.3342 | -0.6365 | 0.5015 | -0.280 |
| 33 | C12 | CH2R | 1 | -2.8455 | 0.1968 | -1.2547 | 0.000 |
| 34 | H19 | HC | 5 | -4.8598 | 0.1039 | 2.1196 | 0.000 |
| 35 | H26 | HC | 5 | -3.5650 | 1.8124 | 0.9367 | 0.000 |
| 36 | H20 | HC | 5 | -4.4602 | -1.0276 | -1.9958 | 0.000 |
| 37 | C13 | CR | 1 | -2.0784 | 0.5052 | 0.0451 | 0.560 |
| 38 | H17 | HC | 5 | -5.5752 | -1.3606 | 0.2184 | 0.000 |
| 39 | C14 | CH2R | 1 | -3.0783 | 0.8541 | 1.1611 | 0.000 |
| 40 | H23 | HC | 5 | 1.1159 | -1.8831 | 1.4653 | 0.000 |
| 41 | H16 | HC | 5 | -3.6729 | -1.1402 | 1.7442 | 0.000 |
| 42 | H24 | HC | 5 | -2.1627 | -0.1335 | -2.0455 | 0.000 |
| 43 | H28 | HC | 5 | -5.4708 | 0.3382 | -0.2363 | 0.000 |
| 44 | H18 | HC | 5 | -3.4167 | -1.8443 | -0.8368 | 0.000 |
| 45 | H15 | HC | 5 | 0.5481 | 2.2958 | -0.8478 | 0.000 |
| 46 | H21 | HC | 5 | -0.3903 | 1.2826 | -1.9286 | 0.000 |

**6**_ax_peroxide_linkage Gaussian Std HF/6-31G* E(HF) = -883.421158 a.u.

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 1.369710 | -0.312276 | -2.327655 |
| 2 | 6 | 0 | 1.805787 | -0.233998 | -1.335583 |
| 3 | 6 | 0 | 3.563175 | 0.904506 | 0.063316 |
| 4 | 6 | 0 | 1.326061 | 0.314817 | 1.064547 |
| 5 | 6 | 0 | 2.477423 | 1.338364 | 1.058646 |
| 6 | 6 | 0 | 0.709231 | 0.202422 | -0.345848 |

| | | | | | |
|---|---|---|---|---|---|
| 7 | 6 | 0 | 2.946510 | 0.800763 | -1.340714 |
| 8 | 6 | 0 | 4.116218 | -0.465625 | 0.484574 |
| 9 | 6 | 0 | 1.887663 | -1.055083 | 1.483650 |
| 10 | 1 | 0 | 2.119244 | 2.334765 | 0.817717 |
| 11 | 6 | 0 | -0.040824 | 1.454249 | -0.810273 |
| 12 | 1 | 0 | 2.592721 | 1.774540 | -1.669649 |
| 13 | 6 | 0 | 2.375987 | -1.600504 | -0.913887 |
| 14 | 1 | 0 | 4.365578 | 1.637587 | 0.053519 |
| 15 | 1 | 0 | 0.563135 | 0.630074 | 1.764094 |
| 16 | 1 | 0 | 2.895126 | 1.401675 | 2.060164 |
| 17 | 8 | 0 | -0.264671 | -0.839902 | -0.402121 |
| 18 | 1 | 0 | 3.700278 | 0.490805 | -2.059822 |
| 19 | 1 | 0 | 1.601623 | -2.357233 | -0.941049 |
| 20 | 1 | 0 | 4.900771 | -0.779543 | -0.200712 |
| 21 | 1 | 0 | -2.497597 | 0.979489 | 2.062905 |
| 22 | 1 | 0 | 2.302871 | -0.978918 | 2.486081 |
| 23 | 1 | 0 | 3.368212 | -2.467971 | 0.793819 |
| 24 | 1 | 0 | 4.569152 | -0.394836 | 1.471010 |
| 25 | 6 | 0 | 2.978607 | -1.498272 | 0.495302 |
| 26 | 1 | 0 | 3.141052 | -1.899294 | -1.627057 |
| 27 | 1 | 0 | -3.248518 | 1.083638 | -1.620992 |
| 28 | 6 | 0 | -3.792091 | -0.942589 | -1.099638 |
| 29 | 8 | 0 | -1.225565 | 1.630881 | -0.075835 |
| 30 | 6 | 0 | -4.801415 | -0.610051 | 0.001529 |
| 31 | 6 | 0 | -4.091418 | -0.298249 | 1.320979 |
| 32 | 8 | 0 | -1.285850 | -0.569499 | 0.503751 |
| 33 | 6 | 0 | -2.759998 | 0.175338 | -1.278514 |
| 34 | 1 | 0 | -4.812488 | 0.002035 | 2.075838 |
| 35 | 1 | 0 | -3.539984 | 1.747418 | 0.889622 |
| 36 | 1 | 0 | -4.305922 | -1.109173 | -2.042165 |
| 37 | 6 | 0 | -2.052589 | 0.513905 | 0.036033 |
| 38 | 1 | 0 | -5.493947 | -1.436174 | 0.136263 |
| 39 | 6 | 0 | -3.052066 | 0.812119 | 1.146666 |
| 40 | 1 | 0 | 1.092408 | -1.789831 | 1.523639 |
| 41 | 1 | 0 | -3.603717 | -1.195042 | 1.691164 |
| 42 | 1 | 0 | -2.038429 | -0.107773 | -2.032695 |
| 43 | 1 | 0 | -5.396508 | 0.250378 | -0.301454 |
| 44 | 1 | 0 | -3.277529 | -1.866944 | -0.854310 |
| 45 | 1 | 0 | 0.526170 | 2.360075 | -0.670254 |
| 46 | 1 | 0 | -0.262297 | 1.358018 | -1.869097 |

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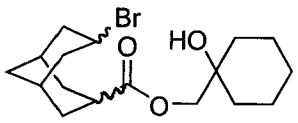
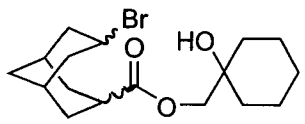
Apr 20 2004 : /export/home/jvenners/TANG/ST01_FeBr2_HPLC_1_13C_040420.fid

| INDEX | FREQUENCY | PPM | HEIGHT |
|---|---|---|---|
| 1 | 22142.124 | 176.265 | 16.3 |
| 2 | 9703.812 | 77.248 | 276.2 |
| 3 | 9671.662 | 76.992 | 286.2 |
| 4 | 9639.513 | 76.736 | 278.4 |
| 5 | 9008.049 | 71.710 | 19.7 |
| 6 | 8878.973 | 70.682 | 23.4 |
| 7 | 5944.775 | 47.324 | 37.3 |
| 8 | 4806.604 | 38.264 | 110.5 |
| 9 | 4438.090 | 35.330 | 56.7 |
| 10 | 4324.848 | 34.428 | 107.0 |
| 11 | 3885.319 | 30.930 | 118.8 |
| 12 | 3328.709 | 26.499 | 61.4 |
| 13 | 3291.281 | 26.201 | 125.3 |
| 14 | 3224.584 | 25.670 | 58.2 |
| 15 | 2717.877 | 21.636 | 77.2 |



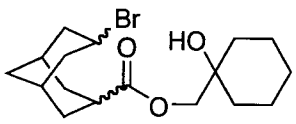

**18a**

| INDEX | FREQUENCY | PPM | HEIGHT |
|---|---|---|---|
| 1 | 22167.134 | 176.464 | 16.9 |
| 2 | 9738.418 | 77.524 | 288.3 |
| 3 | 9706.269 | 77.268 | 298.4 |
| 4 | 9674.600 | 77.016 | 287.7 |
| 5 | 9015.785 | 71.771 | 20.2 |
| 6 | 8911.661 | 70.942 | 23.2 |
| 7 | 5974.104 | 47.558 | 36.6 |
| 8 | 5669.888 | 45.136 | 17.5 |
| 9 | 4797.066 | 38.188 | 106.4 |
| 10 | 4518.281 | 35.968 | 105.5 |
| 11 | 4344.101 | 34.582 | 98.5 |
| 12 | 4339.302 | 34.544 | 42.5 |
| 13 | 3654.576 | 29.093 | 15.5 |
| 14 | 3534.137 | 28.134 | 116.9 |
| 15 | 3526.460 | 28.073 | 15.5 |
| 16 | 3335.485 | 26.553 | 53.6 |
| 17 | 3257.752 | 25.934 | 57.6 |
| 18 | 2747.206 | 21.869 | 85.6 |



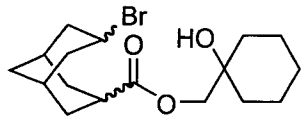

**18b**

| INDEX | FREQUENCY | PPM | HEIGHT |
|---|---|---|---|
| 1 | 22137.805 | 176.230 | 17.3 |
| 2 | 9703.812 | 77.248 | 288.8 |
| 3 | 9671.662 | 76.992 | 305.2 |
| 4 | 9639.513 | 76.736 | 300.4 |
| 5 | 8977.340 | 71.465 | 17.8 |
| 6 | 8875.614 | 70.655 | 16.4 |
| 7 | 5826.256 | 46.381 | 32.6 |
| 8 | 5635.281 | 44.860 | 78.0 |
| 9 | 4761.979 | 37.908 | 13.9 |
| 10 | 4461.122 | 35.513 | 35.4 |
| 11 | 4309.974 | 34.310 | 73.7 |
| 12 | 4306.615 | 34.283 | 23.1 |
| 13 | 3616.610 | 28.790 | 76.6 |
| 14 | 3534.079 | 28.133 | 39.7 |
| 15 | 3500.010 | 27.862 | 13.6 |
| 16 | 3492.333 | 27.801 | 100.1 |
| 17 | 3221.705 | 25.647 | 50.0 |
| 18 | 2710.200 | 21.575 | 67.8 |



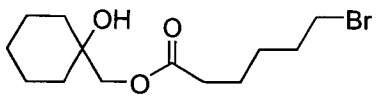

**18c**

| INDEX | FREQUENCY | PPM | HEIGHT |
|---|---|---|---|
| 1 | 22084.544 | 175.806 | 23.7 |
| 2 | 9704.291 | 77.252 | 108.9 |
| 3 | 9672.622 | 77.000 | 115.6 |
| 4 | 9640.473 | 76.744 | 111.9 |
| 5 | 8980.699 | 71.492 | 21.2 |
| 6 | 8875.614 | 70.655 | 32.6 |
| 7 | 6184.214 | 49.230 | 36.8 |
| 8 | 5464.459 | 43.500 | 121.4 |
| 9 | 4987.502 | 39.704 | 46.2 |
| 10 | 4305.175 | 34.272 | 99.5 |
| 11 | 4168.422 | 33.183 | 65.1 |
| 12 | 4121.398 | 32.809 | 127.2 |
| 13 | 3884.359 | 30.922 | 127.4 |
| 14 | 3221.225 | 25.643 | 64.0 |
| 15 | 2707.801 | 21.556 | 86.0 |




**18d**

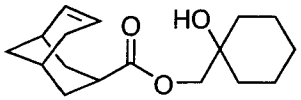
| INDEX | FREQUENCY | PPM | HEIGHT |
|---|---|---|---|
| 1 | 21796.642 | 173.515 | 20.4 |
| 2 | 9704.291 | 77.252 | 220.0 |
| 3 | 9672.622 | 77.000 | 224.8 |
| 4 | 9640.473 | 76.744 | 224.8 |
| 5 | 8972.541 | 71.427 | 23.3 |
| 6 | 8863.139 | 70.556 | 34.3 |
| 7 | 4307.095 | 34.287 | 118.7 |
| 8 | 4266.788 | 33.966 | 70.3 |
| 9 | 4200.571 | 33.439 | 52.0 |
| 10 | 4062.858 | 32.343 | 61.6 |
| 11 | 3470.260 | 27.625 | 73.7 |
| 12 | 3222.665 | 25.654 | 74.2 |
| 13 | 3025.452 | 24.084 | 64.2 |
| 14 | 2711.160 | 21.582 | 95.4 |




**19**

May 4 2004 : /export/home/jvenners/TANG/ST01_FeCl2_F5_13C_040504

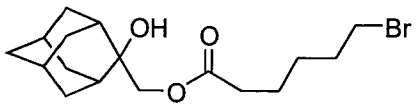
| INDEX | FREQUENCY | PPM | HEIGHT |
|---|---|---|---|
| 1 | 22094.199 | 175.883 | 18.1 |
| 2 | 16430.213 | 130.795 | 51.6 |
| 3 | 16242.597 | 129.301 | 52.4 |
| 4 | 9736.979 | 77.512 | 499.2 |
| 5 | 9705.309 | 77.260 | 515.5 |
| 6 | 9673.160 | 77.004 | 514.8 |
| 7 | 8993.233 | 71.592 | 17.5 |
| 8 | 8892.947 | 70.793 | 22.9 |
| 9 | 4619.046 | 36.770 | 12.0 |
| 10 | 4551.390 | 36.232 | 46.9 |
| 11 | 4373.370 | 34.815 | 49.2 |
| 12 | 4358.495 | 34.696 | 45.7 |
| 13 | 4050.920 | 32.248 | 60.7 |
| 14 | 3996.215 | 31.812 | 58.3 |
| 15 | 3991.901 | 31.778 | 51.9 |
| 16 | 3928.562 | 31.274 | 14.0 |
| 17 | 3798.527 | 30.239 | 53.0 |
| 18 | 3601.794 | 28.672 | 52.8 |
| 19 | 3337.884 | 26.572 | 51.5 |
| 20 | 3261.590 | 25.964 | 49.7 |
| 21 | 2758.722 | 21.961 | 67.2 |
| 22 | 29.894 | 0.238 | 11.6 |




**20**

Feb 13 2004 : /export/home/jvenners/TANG/TR002-FeBr2-f8~13C-040213

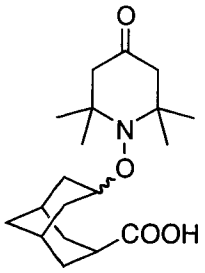
| INDEX | FREQUENCY | PPM | HEIGHT |
|---|---|---|---|
| 1 | 21803.360 | 173.568 | 13.9 |
| 2 | 9704.291 | 77.252 | 220.3 |
| 3 | 9672.622 | 77.000 | 218.7 |
| 4 | 9640.473 | 76.744 | 221.4 |
| 5 | 9299.310 | 74.028 | 22.0 |
| 6 | 8667.845 | 69.001 | 39.2 |
| 7 | 4779.733 | 38.050 | 40.0 |
| 8 | 4348.840 | 34.619 | 62.1 |
| 9 | 4319.570 | 34.386 | 76.4 |
| 10 | 4270.147 | 33.993 | 43.0 |
| 11 | 4200.091 | 33.435 | 37.2 |
| 12 | 4075.334 | 32.442 | 72.8 |
| 13 | 4062.858 | 32.343 | 39.8 |
| 14 | 3469.781 | 27.622 | 41.7 |
| 15 | 3440.031 | 27.385 | 34.6 |
| 16 | 3397.805 | 27.049 | 34.5 |
| 17 | 3030.251 | 24.123 | 38.0 |




**21**

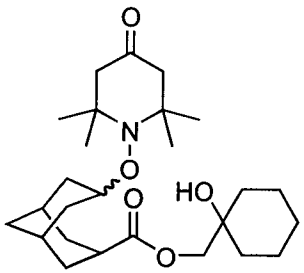
Sep 1 2004 : /export/home/jvenners/TANG/OZ03_FeOAc2_OXO_TMPO_fr13_13C_040901

| INDEX | FREQUENCY | PPM | HEIGHT |
|---|---|---|---|
| 1 | 26207.310 | 208.626 | 25.8 |
| 2 | 22828.733 | 181.731 | 19.0 |
| 3 | 9704.686 | 77.255 | 348.1 |
| 4 | 9672.623 | 77.000 | 363.0 |
| 5 | 9640.559 | 76.745 | 358.8 |
| 6 | 9560.400 | 76.107 | 42.6 |
| 7 | 7887.602 | 62.790 | 91.7 |
| 8 | 6718.200 | 53.481 | 115.6 |
| 9 | 4960.205 | 39.486 | 91.1 |
| 10 | 4442.150 | 35.362 | 43.4 |
| 11 | 4240.150 | 33.754 | 17.4 |
| 12 | 3667.588 | 29.196 | 92.4 |
| 13 | 3602.545 | 28.678 | 40.9 |
| 14 | 3261.297 | 25.962 | 122.5 |
| 15 | 2849.969 | 22.687 | 17.7 |




**22**

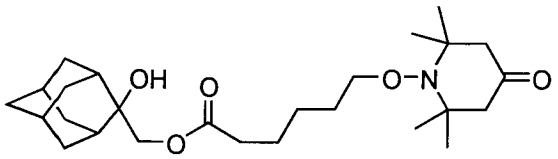
| INDEX | FREQUENCY | PPM | HEIGHT |
|---|---|---|---|
| 1 | 26205.857 | 208.615 | 23.3 |
| 2 | 22167.556 | 176.467 | 32.8 |
| 3 | 9704.772 | 77.256 | 155.7 |
| 4 | 9672.623 | 77.000 | 159.6 |
| 5 | 9640.954 | 76.748 | 156.5 |
| 6 | 9558.422 | 76.091 | 60.5 |
| 7 | 8959.586 | 71.324 | 24.0 |
| 8 | 8862.659 | 70.552 | 44.4 |
| 9 | 7869.399 | 62.645 | 96.4 |
| 10 | 6724.509 | 53.531 | 129.3 |
| 11 | 4964.950 | 39.524 | 119.8 |
| 12 | 4473.598 | 35.613 | 72.0 |
| 13 | 4304.216 | 34.264 | 123.9 |
| 14 | 4263.430 | 33.940 | 19.7 |
| 15 | 3698.183 | 29.440 | 127.5 |
| 16 | 3585.421 | 28.542 | 52.4 |
| 17 | 3257.214 | 25.929 | 167.6 |
| 18 | 3218.827 | 25.624 | 68.1 |
| 19 | 2836.397 | 22.579 | 23.3 |
| 20 | 2704.442 | 21.529 | 102.6 |




**23**

Jun 1 2004 : /export/home/jvenners/TANG/ST02_FeBr2-TMPO_Fr12_8_13C_040601

| INDEX | FREQUENCY | PPM | HEIGHT |
|---|---|---|---|
| 1 | 26167.949 | 208.313 | 10.9 |
| 2 | 21827.831 | 173.763 | 16.8 |
| 3 | 9704.771 | 77.256 | 309.3 |
| 4 | 9672.622 | 77.000 | 314.1 |
| 5 | 9640.953 | 76.748 | 309.6 |
| 6 | 9296.911 | 74.009 | 23.5 |
| 7 | 8658.249 | 68.925 | 37.0 |
| 8 | 7901.067 | 62.897 | 52.9 |
| 9 | 6722.110 | 53.512 | 21.7 |
| 10 | 6689.961 | 53.256 | 72.7 |
| 11 | 4777.334 | 38.031 | 31.1 |
| 12 | 4347.401 | 34.608 | 72.2 |
| 13 | 4316.212 | 34.360 | 70.2 |
| 14 | 4288.381 | 34.138 | 33.4 |
| 15 | 4082.531 | 32.499 | 22.5 |
| 16 | 4073.415 | 32.427 | 69.5 |
| 17 | 3551.833 | 28.275 | 34.0 |
| 18 | 3437.152 | 27.362 | 39.7 |
| 19 | 3394.446 | 27.022 | 30.7 |
| 20 | 3266.810 | 26.006 | 31.4 |
| 21 | 3145.891 | 25.043 | 31.4 |
| 22 | 2821.042 | 22.457 | 22.7 |




**24**