

# Mechanistic insights can resolve the low reactivity and selectivity issues in intermolecular Rauhut Currier (RC) reaction of $\gamma$ -hydroxyenone

## Authors

Zakir Ullah<sup>a</sup> and Renjith Thomas<sup>b,\*</sup>

## Affiliations

<sup>a</sup> Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Daejeon 34141, Republic of Korea.

<sup>b</sup> Department of Chemistry, St Berchmans College (Autonomous), Changanassery, Kerala, India

## Corresponding Author

\* Renjith Thomas: renjith@sbcollege.ac.in

## Supporting Information

**Table S1.** Computed energy components for DFT-optimized structures.

|             | E(SCF)/(eV)          | ZPE/(kcal/mol)  | S(gas)          | G(solv)/(kcal/mol) |
|-------------|----------------------|-----------------|-----------------|--------------------|
|             | cc-pVTZ(-f)/LACV3P** | 6-31G**/LACVP** | 6-31G**/LACVP** | 6-31G**/LACVP**    |
| <b>1</b>    | -12580.911           | 117.61          | 95.611          | -9.5               |
| <b>2</b>    | -12564.756           | 108.02          | 94.668          | -56.33             |
| <b>2-TS</b> | -25146.635           | 227.48          | 147.032         | -48.21             |
| <b>3</b>    | -25146.892           | 228.96          | 145.706         | -49.64             |
| <b>3-TS</b> | -25146.523           | 228.91          | 138.501         | -47.89             |
| <b>4</b>    | -25147.094           | 229.41          | 141.705         | -56.69             |
| <b>4-TS</b> | -27226.777           | 243.47          | 147.524         | -51.74             |

|                |            |        |         |        |
|----------------|------------|--------|---------|--------|
| <b>5</b>       | -25162.995 | 238.65 | 142.593 | -15.27 |
| <b>4''-TS</b>  | -25145.722 | 227.16 | 136.806 | -48.09 |
| <b>6</b>       | -25147.581 | 229.9  | 139.397 | -50.72 |
| <b>6-TS</b>    | -25146.598 | 228.15 | 140.485 | -52.42 |
| <b>6-TS</b>    | -25163.874 | 228.71 | 140.391 | -51.84 |
| <b>7</b>       | -25146.865 | 227.77 | 145.003 | -55.97 |
| <b>8</b>       | -25162.808 | 237.48 | 149.166 | -16.72 |
| <b>9</b>       | -12580.885 | 118.31 | 95.028  | -9.12  |
| <b>10</b>      | -12564.727 | 108.64 | 93.974  | -51.75 |
| <b>10-TS</b>   | -25146.561 | 228.77 | 145.785 | -48.3  |
| <b>11</b>      | -25146.825 | 230.02 | 146.090 | -54.93 |
| <b>11-TS</b>   | -25146.900 | 230.24 | 148.615 | -49.99 |
| <b>12</b>      | -25147.031 | 230.87 | 139.178 | -60.21 |
| <b>12'-TS</b>  | -27226.687 | 244.79 | 181.559 | -62.19 |
| <b>13</b>      | -25162.934 | 240.41 | 140.365 | -14.75 |
| <b>12''-TS</b> | -27226.687 | 244.79 | 189.559 | -62.19 |
| <b>14</b>      | -25147.581 | 229.9  | 149.397 | -50.72 |
| <b>14-TS</b>   | -25145.722 | 227.16 | 165.806 | -62.29 |
| <b>14'-TS</b>  | -25146.523 | 228.91 | 138.501 | -50.89 |
| <b>15</b>      | -25162.808 | 237.48 | 149.166 | -25.72 |
| <b>16</b>      | -36463.31  | 304.78 | 167.51  | -56.36 |
| <b>16-TS</b>   | -38542.61  | 319.40 | 176.88  | -55.01 |
| <b>16-TS</b>   | -36462.49  | 303.73 | 160.63  | -46.53 |
| <b>17</b>      | -36478.79  | 313.28 | 170.14  | -20.96 |
| <b>18</b>      | -36463.56  | 304.84 | 168.41  | -51.74 |
| <b>18-TS</b>   | -36462.64  | 303.36 | 168.51  | -53.33 |
| <b>18-TS</b>   | -38542.61  | 319.40 | 176.88  | -55.01 |
| <b>19</b>      | -36462.91  | 302.80 | 173.79  | -57.65 |
| <b>20</b>      | -36478.53  | 311.59 | 179.54  | -21.85 |
| <b>21</b>      | -24963.900 | 166.71 | 125.861 | -58.70 |
| <b>21-TS</b>   | -27043.276 | 181.56 | 125.963 | -55.87 |
| <b>21'-TS</b>  | -27042.503 | 180.77 | 130.815 | -64.82 |

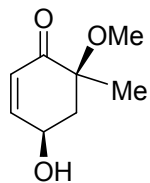
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|--------------|------------|--------|---------|--------|
| <b>22</b>    | -24979.247 | 175.3  | 127.514 | -21.64 |
| <b>23</b>    | -24964.225 | 167.24 | 123.388 | -54.71 |
| <b>23-TS</b> | -24963.243 | 165.16 | 124.261 | -55.69 |
| <b>24</b>    | -24963.087 | 164.02 | 126.579 | -58.13 |
| <b>25</b>    | -24979.196 | 174.08 | 134.165 | -21.61 |
| <b>26</b>    | -18773.064 | 136.38 | 111.766 | -12.2  |
| <b>27</b>    | -18757.307 | 128.15 | 106.726 | -51.15 |
| <b>27-TS</b> | -37531.273 | 264.36 | 170.261 | -49.81 |
| <b>28</b>    | -37531.84  | 266.67 | 171.885 | -49.78 |
| <b>28-TS</b> | -37531.447 | 267.11 | 168.151 | -48.76 |
| <b>29</b>    | -37531.97  | 267.79 | 171.169 | -55.78 |
| <b>29-TS</b> | -39611.442 | 281.63 | 177.71  | -51.95 |
| <b>29-TS</b> | -39611.267 | 281.1  | 169.63  | -56.34 |
| <b>30</b>    | -37547.402 | 276.55 | 162.911 | -19.81 |
| <b>31</b>    | -37532.374 | 267.86 | 171.286 | -52.4  |
| <b>32-TS</b> | -37531.2   | 266.16 | 164.288 | -53.96 |
| <b>32-TS</b> | -37531.2   | 266.23 | 143.652 | -53.62 |
| <b>33</b>    | -37531.649 | 265.69 | 175.342 | -54.51 |
| <b>34</b>    | -37547.365 | 275.16 | 168.368 | -19.49 |
| <b>35</b>    | -21277.626 | 82.31  | 91.689  | -10.22 |
| <b>36</b>    | -21261.716 | 72.82  | 90.792  | -53.65 |
| <b>36-TS</b> | -42540.353 | 156.18 | 139.567 | -53.65 |
| <b>37</b>    | -42540.88  | 158.49 | 138.243 | -47.71 |
| <b>37-TS</b> | -42540.374 | 158.79 | 129.156 | -45.32 |
| <b>38</b>    | -42540.629 | 158.96 | 128.067 | -53.14 |
| <b>38-TS</b> | -44620.457 | 173.72 | 139.221 | -50.63 |
| <b>38-TS</b> | -44620.306 | 172.96 | 140.176 | -52.07 |
| <b>39</b>    | -42556.572 | 168.54 | 133.078 | -15.52 |
| <b>40</b>    | -42541.415 | 159.93 | 130.643 | -49.25 |
| <b>40-TS</b> | -42540.398 | 157.84 | 131.487 | -50.25 |
| <b>41</b>    | -42540.653 | 157.45 | 136.737 | -52.7  |
| <b>42</b>    | -42556.257 | 167.02 | 140.269 | -18.4  |
| <b>43</b>    | -19747.068 | 87.65  | 93.51   | -10.47 |

|              |            |        |         |        |
|--------------|------------|--------|---------|--------|
| <b>44</b>    | -19731.108 | 78.02  | 92.527  | -54.97 |
| <b>44-TS</b> | -39478.504 | 166.62 | 137.559 | -46.08 |
| <b>45</b>    | -39479.638 | 169.12 | 144.151 | -48.81 |
| <b>45-TS</b> | -39479.135 | 169.32 | 134.549 | -47.09 |
| <b>46</b>    | -39479.889 | 170.51 | 134.953 | -53.26 |
| <b>46-TS</b> | -41559.266 | 185.07 | 145.723 | -53.02 |
| <b>46-TS</b> | -41559.101 | 183.82 | 145.905 | -54.25 |
| <b>47</b>    | -39495.536 | 179.25 | 138.047 | -14.77 |
| <b>48</b>    | -39480.149 | 170.22 | 136.987 | -50.31 |
| <b>48-TS</b> | -39479.182 | 168.49 | 136.563 | -51.14 |
| <b>49</b>    | -39479.463 | 168.05 | 141.576 | -53.99 |
| <b>50</b>    | -39495.115 | 177.47 | 139.435 | -18.38 |
| <b>51</b>    | -13558.36  | 103.09 | 94.05   | -10.84 |
| <b>52</b>    | -13542.54  | 94.26  | 90.65   | -53.81 |
| <b>52-TS</b> | -27101.94  | 198.69 | 144.98  | -48.91 |
| <b>53</b>    | -27102.45  | 201.06 | 139.62  | -47.78 |
| <b>53-TS</b> | -27102.44  | 201.60 | 131.67  | -49.77 |
| <b>54</b>    | -27102.77  | 202.17 | 132.37  | -53.43 |
| <b>54-TS</b> | -27101.44  | 198.83 | 133.36  | -48.26 |
| <b>54-TS</b> | -29181.82  | 216.27 | 141.55  | -54.86 |
| <b>54-TS</b> | -29181.95  | 214.95 | 141.70  | -53.14 |
| <b>55</b>    | -27118.10  | 210.50 | 135.90  | -16.42 |
| <b>56</b>    | -27102.841 | 201.89 | 134.66  | -48.01 |
| <b>56-TS</b> | -27101.756 | 199.72 | 132.32  | -48.82 |
| <b>57</b>    | -27102.25  | 200.09 | 140.52  | -50.94 |
| <b>58</b>    | -27117.65  | 207.57 | 132.51  | -19.55 |
| <b>59</b>    | -14626.946 | 120.42 | 102.60  | -10.49 |
| <b>60</b>    | -14611.099 | 111.31 | 99.58   | -54.27 |
| <b>60-TS</b> | -29238.908 | 233.11 | 153.31  | -49.75 |
| <b>61</b>    | -29239.252 | 235.00 | 153.40  | -51.21 |
| <b>61-TS</b> | -29238.852 | 234.64 | 152.74  | -56.35 |
| <b>62</b>    | -29239.617 | 236.09 | 149.25  | -58.1  |
| <b>62-TS</b> | -31318.693 | 249.91 | 152.53  | -55.69 |

|              |            |        |         |        |
|--------------|------------|--------|---------|--------|
| <b>62-TS</b> | -31319.08  | 249.91 | 152.53  | -54.77 |
| <b>62-TS</b> | -31319.076 | 250.79 | 159.50  | -54.88 |
| <b>63</b>    | -29255.34  | 245.09 | 150.25  | -12.87 |
| <b>64</b>    | -29240.219 | 235.87 | 153.63  | -50.26 |
| <b>64-TS</b> | -29239.347 | 234.29 | 151.25  | -50.15 |
| <b>64-TS</b> | -31319.200 | 249.3  | 157.07  | -52.37 |
| <b>65</b>    | -29239.528 | 233.97 | 157.03  | -52.92 |
| <b>66</b>    | -29255.019 | 243.53 | 157.87  | -16.87 |
| <b>67</b>    | -17742.62  | 141.68 | 114.051 | -12.57 |
| <b>68</b>    | -17726.122 | 130.92 | 105.554 | -56.64 |
| <b>68-TS</b> | -35469.789 | 273.99 | 186.988 | -53.84 |
| <b>69</b>    | -35470.634 | 276.64 | 178.717 | -52.51 |
| <b>69-TS</b> | -35469.382 | 272.87 | 158.575 | -50.45 |
| <b>70</b>    | -35471.298 | 277.63 | 175.521 | -55.05 |
| <b>70-TS</b> | -37550.191 | 290.81 | 169.583 | -55.36 |
| <b>70-TS</b> | -37550.488 | 291.9  | 176.011 | -55.02 |
| <b>71</b>    | -35486.524 | 285.07 | 173.661 | -19.33 |
| <b>72</b>    | -35471.432 | 277.57 | 177.064 | -53.12 |
| <b>72-TS</b> | -37550.713 | 299.05 | 180.76  | -55.13 |
| <b>72-TS</b> | -35470.623 | 276.14 | 179.879 | -51.54 |
| <b>73</b>    | -35471.025 | 275.97 | 174.265 | -52.92 |
| <b>74</b>    | -35486.536 | 285.28 | 184.745 | -17.55 |

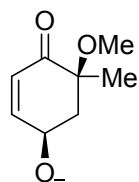
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Cartesian coordinates:

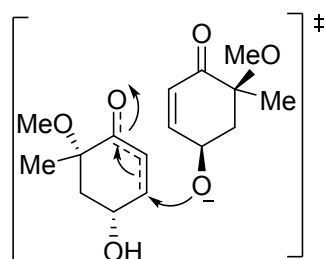


|   |              |              |              |
|---|--------------|--------------|--------------|
| O | -2.848771151 | -1.222985690 | -1.739198072 |
| C | -1.946930723 | -1.264219641 | -0.929764087 |
| C | -2.092137009 | -1.978679394 | 0.355093302  |
| C | -0.565717545 | -0.656598454 | -1.221357709 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -1.126337929 | -2.013987924 | 1.281113941  |
| C | 0.089497793  | -0.204556474 | 0.086343352  |
| C | 0.186893407  | -1.309339997 | 1.127167620  |
| H | -1.257188032 | -2.573495274 | 2.208035409  |
| H | 1.090048767  | 0.207248007  | -0.098116500 |
| O | 0.663354483  | -0.827906242 | 2.365263698  |
| H | -0.528483394 | 0.609213350  | 0.498364344  |
| H | 0.941074306  | -2.048710580 | 0.809495360  |
| H | -3.041616737 | -2.492741876 | 0.492152792  |
| H | 0.046102301  | -0.154203574 | 2.672871718  |
| C | 0.236819266  | -1.746706492 | -1.933504398 |
| H | 0.225353661  | -2.684833998 | -1.367455485 |
| H | -0.218753670 | -1.937679185 | -2.911719825 |
| H | 1.283581091  | -1.452387354 | -2.074058659 |
| O | -0.811780575 | 0.455115750  | -2.052404992 |
| C | 0.295723125  | 1.022851404  | -2.694831921 |
| H | 1.104943144  | 1.298859966  | -1.999109270 |
| H | 0.718376045  | 0.367065514  | -3.471316850 |
| H | -0.058357764 | 1.936737807  | -3.179463747 |

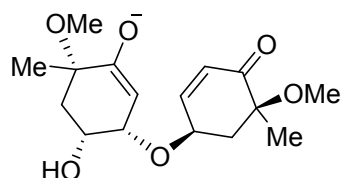


|   |              |              |              |
|---|--------------|--------------|--------------|
| O | 1.796134190  | 0.504078844  | -2.815262701 |
| C | 1.679611114  | -0.169349664 | -1.797936578 |
| C | 0.644018674  | 0.074908393  | -0.804241698 |
| C | 2.571313061  | -1.401679530 | -1.558083445 |
| C | 0.464371780  | -0.733152766 | 0.264537392  |
| C | 2.747060915  | -1.641352093 | -0.065201579 |
| C | 1.427970758  | -1.797705654 | 0.756353467  |
| H | -0.363868950 | -0.564977965 | 0.956496611  |
| H | 3.372093768  | -2.525423875 | 0.128280349  |
| O | 1.602944014  | -1.636326206 | 2.049113983  |
| H | 3.254068971  | -0.771907337 | 0.379949304  |
| H | 0.990464168  | -2.802118965 | 0.406951089  |
| H | -0.009407246 | 0.922089435  | -1.024025024 |
| C | 1.900539267  | -2.576347808 | -2.270266208 |
| H | 1.836281770  | -2.352006516 | -3.342310458 |
| H | 2.466131639  | -3.506758617 | -2.127862475 |
| H | 0.893581767  | -2.743566575 | -1.872536684 |
| O | 3.805213829  | -1.094172233 | -2.224724629 |
| C | 4.857370959  | -1.973783215 | -2.000666598 |
| H | 5.242185989  | -1.940785288 | -0.967336642 |
| H | 4.604780418  | -3.026496712 | -2.223635949 |
| H | 5.671421481  | -1.678529817 | -2.674539092 |



|   |              |              |             |
|---|--------------|--------------|-------------|
| O | 2.921850061  | -5.216260681 | 1.833669902 |
| C | 1.950172259  | -5.223935464 | 2.588394979 |
| C | 0.590062359  | -5.539317889 | 2.119650948 |
| C | 2.122488076  | -5.020990982 | 4.115346284 |
| C | -0.491094515 | -5.553428541 | 2.939867177 |
| C | 0.849820072  | -4.440298313 | 4.741661905 |
| C | -0.461663675 | -5.219721097 | 4.423532848 |
| H | -1.480334743 | -5.825486623 | 2.549262248 |
| H | 0.931926738  | -4.369949550 | 5.842880298 |
| O | -1.559211231 | -4.593714838 | 4.905757574 |
| H | 0.723636333  | -3.409378385 | 4.369701128 |
| H | -0.351054445 | -6.235400386 | 4.908165091 |
| H | 0.518834895  | -5.795473693 | 1.051908979 |
| O | -4.680771430 | -3.869131047 | 1.322879781 |
| C | -4.109878908 | -3.605133502 | 2.394697944 |
| C | -2.696050173 | -3.358067763 | 2.529842240 |
| C | -5.014435827 | -3.427845249 | 3.667438050 |
| C | -2.098450547 | -2.974697437 | 3.729547149 |
| C | -4.195708722 | -3.334591304 | 4.967526502 |
| C | -2.987733061 | -2.406197366 | 4.809282619 |
| H | -1.062396569 | -2.605776235 | 3.736530445 |
| H | -4.842763776 | -2.977987878 | 5.803895936 |
| O | -2.269998528 | -2.161901559 | 6.010765269 |
| H | -3.787083797 | -4.323863788 | 5.215714728 |
| H | -3.346462383 | -1.427527993 | 4.420096266 |
| H | -2.089302547 | -3.506931530 | 1.625099798 |
| H | -2.928840466 | -1.972625375 | 6.696873378 |
| O | 3.249109729  | -4.138899755 | 4.246507969 |
| C | 3.571710724  | -3.730130310 | 5.551925478 |
| H | 3.787734990  | -4.573241782 | 6.235805022 |
| H | 4.490031067  | -3.119284458 | 5.476207623 |
| H | 2.783259057  | -3.114288696 | 6.026647117 |
| O | -5.863476407 | -4.592726555 | 3.662433120 |
| C | -6.692799024 | -4.758590365 | 4.780963791 |
| H | -6.127548831 | -4.953019647 | 5.715060906 |
| H | -7.364503986 | -3.893553238 | 4.977778747 |
| H | -7.334942312 | -5.636542732 | 4.576045391 |
| C | 2.467429473  | -6.400157073 | 4.685395454 |
| H | 3.434860989  | -6.718804422 | 4.261890895 |

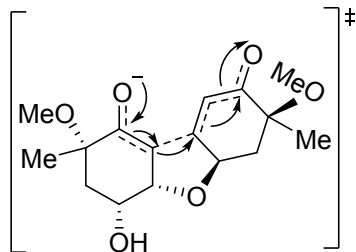
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|---|--------------|--------------|-------------|
| H | 2.533557117  | -6.375049887 | 5.788391390 |
| H | 1.696728113  | -7.144442661 | 4.415890966 |
| C | -5.875601745 | -2.183495748 | 3.432112779 |
| H | -5.238576500 | -1.291446807 | 3.284345060 |
| H | -6.458720831 | -2.353765742 | 2.508921740 |
| H | -6.565799032 | -1.972706657 | 4.277475739 |



|   |              |              |              |
|---|--------------|--------------|--------------|
| O | 1.174884659  | -4.300270453 | -0.019323485 |
| C | 0.657586452  | -4.171221636 | 1.084406567  |
| C | -0.731279095 | -4.461773876 | 1.358080105  |
| C | 1.552551670  | -3.821002353 | 2.296184493  |
| C | -1.296986870 | -4.376180802 | 2.592671413  |
| C | 0.733921185  | -3.226247375 | 3.436978959  |
| C | -0.477403103 | -4.074348822 | 3.808930709  |
| H | -2.306796963 | -4.750490598 | 2.751747194  |
| H | 1.350097854  | -3.087691140 | 4.337758898  |
| O | -1.196088302 | -3.539362259 | 4.884881149  |
| H | 0.378487725  | -2.235638094 | 3.117538525  |
| H | -0.115068977 | -5.044360863 | 4.201216466  |
| H | -1.319906924 | -4.782316978 | 0.501218508  |
| O | -4.130971851 | -2.262198547 | 1.591371197  |
| C | -3.698308255 | -2.480822581 | 2.735363249  |
| C | -2.413870141 | -2.151115485 | 3.202149308  |
| C | -4.690807604 | -3.165557633 | 3.722313374  |
| C | -1.961969616 | -2.301357255 | 4.591063434  |
| C | -4.102947534 | -3.442761996 | 5.107541334  |
| C | -3.117357521 | -2.383788922 | 5.575079748  |
| H | -1.291449554 | -1.477918495 | 4.895790514  |
| H | -4.892212524 | -3.547477797 | 5.867946415  |
| O | -2.658805341 | -2.665495237 | 6.885753276  |
| H | -3.556058088 | -4.396314086 | 5.074391101  |
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| O | 2.499283181  | -2.880922787 | 1.797901380  |
| C | 3.400692016  | -2.355225746 | 2.719972556  |
| H | 3.976828742  | -3.129227697 | 3.256401882  |
| H | 4.111814995  | -1.742139103 | 2.155040081  |
| H | 2.924095912  | -1.708282156 | 3.475818677  |
| O | -5.014036407 | -4.408603591 | 3.074658309  |
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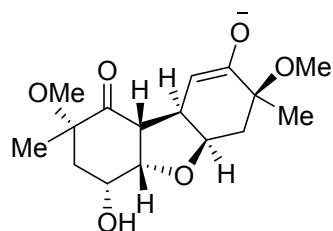


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| H | -6.054451527 | -6.126679149 | 3.115025289 |
| C | 2.256056739  | -5.119642494 | 2.691222610 |
| H | 2.896640029  | -5.428075699 | 1.857909094 |
| H | 2.862548251  | -5.005741185 | 3.599329934 |
| H | 1.526980828  | -5.917999842 | 2.874442430 |
| C | -5.915608939 | -2.264186149 | 3.800576932 |
| H | -5.628106339 | -1.286991955 | 4.209748973 |
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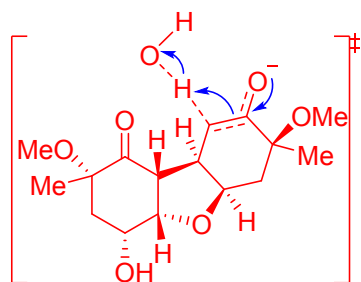
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| C | 1.658616293  | -6.043037798 | 2.142170262 |
| C | 0.332254793  | -6.533954673 | 2.175315737 |
| C | 2.008075410  | -4.860417368 | 3.087934163 |
| C | -0.705311794 | -6.024118890 | 2.989335416 |
| C | 0.768854139  | -4.099533779 | 3.544665907 |
| C | -0.356044791 | -4.998977872 | 4.031880448 |
| H | -1.462612249 | -6.744333239 | 3.313229787 |
| H | 1.006482580  | -3.376053290 | 4.340082691 |
| O | -1.497429468 | -4.238821501 | 4.376417800 |
| H | 0.401561419  | -3.524210320 | 2.681230306 |
| H | -0.060404943 | -5.503877098 | 4.967843869 |
| H | 0.146001876  | -7.429958493 | 1.586215355 |
| O | -2.742138136 | -6.406222962 | 0.517207320 |
| C | -2.886137096 | -5.790479537 | 1.570536979 |
| C | -1.938306309 | -4.827974601 | 2.067090609 |
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| H | -5.174746918 | -5.399030664 | 4.202654435 |
| O | -3.894683749 | -3.226725891 | 4.831859663 |
| H | -3.491263884 | -5.874079463 | 4.486146644 |
| H | -4.317077323 | -3.432363946 | 2.859374313 |
| H | -1.249333180 | -4.474688210 | 1.301407510 |
| H | -3.117081351 | -3.460639631 | 5.359140177 |

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| O | 2.841081685  | -3.993012974 | 2.313887688 |
| C | 3.426624215  | -2.924332668 | 2.981839239 |
| H | 4.161217563  | -3.236266036 | 3.745272889 |
| H | 3.962332015  | -2.331273841 | 2.230982952 |
| H | 2.696846941  | -2.257363450 | 3.475257080 |
| O | -3.990744538 | -7.555514420 | 2.664032495 |
| C | -4.963931234 | -8.152352282 | 3.461353823 |
| H | -4.985614454 | -7.759075414 | 4.492654472 |
| H | -5.982999141 | -8.058704008 | 3.047276527 |
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| C | 2.786030362  | -5.459160083 | 4.255477660 |
| H | 3.699457968  | -5.916221439 | 3.859172785 |
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| C | -5.351661792 | -5.860287316 | 1.586365512 |
| H | -5.408524920 | -4.791766004 | 1.342718261 |
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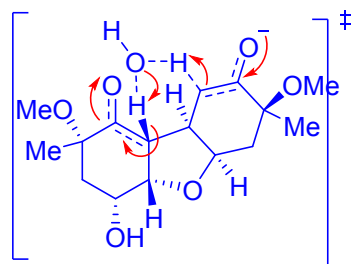
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| C | 0.951751029  | -7.308213401 | 2.808687677  |
| C | -0.227617745 | -6.884954572 | 2.196703687  |
| C | 1.368847264  | -6.600526907 | 4.136446561  |
| C | -1.107227003 | -5.801049267 | 2.660654758  |
| C | 0.662589913  | -5.262311576 | 4.344946961  |
| C | -0.826066142 | -5.335208002 | 4.078052040  |
| H | -2.170916512 | -6.088371007 | 2.599890879  |
| H | 0.822785290  | -4.867014790 | 5.361488232  |
| O | -1.431289642 | -4.045528254 | 4.216690142  |
| H | 1.115389888  | -4.542056568 | 3.645813782  |
| H | -1.320486214 | -5.987608497 | 4.812993091  |
| H | -0.543395208 | -7.446181981 | 1.317274507  |
| O | -1.494753057 | -4.600873326 | -0.432561750 |
| C | -1.902106473 | -4.392042250 | 0.695951843  |
| C | -1.012060591 | -4.377755877 | 1.883153994  |
| C | -3.430190381 | -4.212140142 | 0.913267483  |
| C | -1.354551129 | -3.355663427 | 2.969064700  |
| C | -3.743187750 | -3.685800858 | 2.315423721  |
| C | -2.705613053 | -2.671918397 | 2.776630107  |

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| H | -0.571511289 | -2.581400104 | 3.041950612  |
| H | -4.737474320 | -3.218784065 | 2.353202781  |
| O | -3.099543861 | -2.033833164 | 3.969425859  |
| H | -3.741055728 | -4.516517278 | 3.036286077  |
| H | -2.594391147 | -1.882687180 | 2.013812682  |
| H | 0.018640209  | -4.287970324 | 1.528795690  |
| H | -2.828765697 | -2.651939940 | 4.664755721  |
| O | 2.776879430  | -6.356212348 | 4.013539220  |
| C | 3.446159134  | -5.947117796 | 5.157639982  |
| H | 3.503042495  | -6.729075877 | 5.936201186  |
| H | 4.474119769  | -5.702704170 | 4.861702310  |
| H | 3.013262812  | -5.044773682 | 5.629623608  |
| O | -3.937770890 | -5.532052474 | 0.707239804  |
| C | -5.301284210 | -5.715087468 | 0.942834231  |
| H | -5.589373084 | -5.511104080 | 1.987541571  |
| H | -5.939053805 | -5.096212530 | 0.289003699  |
| H | -5.520463968 | -6.766572470 | 0.731182993  |
| C | 1.087334275  | -7.591725593 | 5.259193906  |
| H | 1.679289958  | -8.492579843 | 5.063029862  |
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| H | 0.028347981  | -7.876616353 | 5.241654763  |
| C | -3.947717225 | -3.273804071 | -0.168787630 |
| H | -3.503995021 | -2.275936815 | -0.064245087 |
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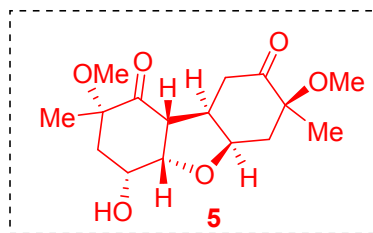
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| C | 0.086076723  | -7.103880985 | 2.995311603 |
| C | 1.662776853  | -8.997839002 | 2.319562735 |
| C | 1.281330019  | -6.221464135 | 3.375334864 |
| C | 2.404101908  | -7.796913788 | 1.733765246 |
| C | 2.623798639  | -6.729195920 | 2.797005229 |
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| H | 3.382740822  | -8.093055186 | 1.319925277 |
| O | 3.296455817  | -5.589802445 | 2.269741594 |
| H | 1.774328042  | -7.380585416 | 0.924381330 |
| H | 3.283027549  | -7.121648571 | 3.586852711 |

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| H | -0.790929497 | -6.888115112  | 3.616611674  |
| O | 0.936403816  | -3.923154264  | 5.032738757  |
| C | 1.250629842  | -3.728874846  | 3.877198057  |
| C | 1.169520262  | -4.785441179  | 2.804981848  |
| C | 1.728732952  | -2.342818022  | 3.412153940  |
| C | 2.270171346  | -4.740871499  | 1.739537382  |
| C | 3.063742493  | -2.546907856  | 2.690476828  |
| C | 2.915511249  | -3.398490474  | 1.438784782  |
| H | 1.835594394  | -5.168886154  | 0.824288339  |
| H | 3.510896186  | -1.581132283  | 2.413955047  |
| O | 4.163945285  | -3.585717417  | 0.805160880  |
| H | 3.758795353  | -3.047019831  | 3.381939588  |
| H | 2.270188683  | -2.869901472  | 0.719612252  |
| H | 0.216598598  | -4.709141810  | 2.243972233  |
| H | 4.496010955  | -4.419643937  | 1.168558381  |
| O | 1.309107007  | -9.937356747  | 1.302976048  |
| C | 2.353077085  | -10.417501852 | 0.512119134  |
| H | 3.186017361  | -10.848004681 | 1.101704427  |
| H | 1.936786181  | -11.217758624 | -0.111831576 |
| H | 2.779559413  | -9.652596061  | -0.162282286 |
| O | 1.910896971  | -1.568517662  | 4.588182169  |
| C | 2.162566300  | -0.209930322  | 4.406664028  |
| H | 3.014419109  | -0.006756476  | 3.734948678  |
| H | 1.290797434  | 0.343172565   | 4.016718496  |
| H | 2.407278983  | 0.203147553   | 5.391489802  |
| C | 2.430061959  | -9.707183933  | 3.436583197  |
| H | 1.867763799  | -10.606379226 | 3.712718958  |
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| C | 0.649756631  | -1.738921923  | 2.511801841  |
| H | 0.318783682  | -2.445535107  | 1.743597001  |
| H | -0.220181035 | -1.475567133  | 3.125514414  |
| H | 1.010339841  | -0.836051388  | 2.000735493  |
| O | -0.057034907 | -5.887393737  | 0.575791576  |
| H | -0.137090073 | -6.740534405  | 1.868415557  |
| H | -0.897463477 | -6.175660264  | -0.075132143 |



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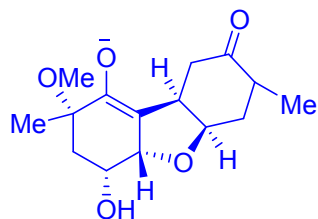
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| H | 3.300093689  | -7.082537084  | 3.686398858  |
| H | -0.785304133 | -6.907727869  | 3.495286244  |
| O | 0.991859268  | -3.930984163  | 5.049690869  |
| C | 1.297457201  | -3.751604359  | 3.887042445  |
| C | 1.210000081  | -4.801747135  | 2.830714090  |
| C | 1.739071460  | -2.363571056  | 3.387333920  |
| C | 2.294839330  | -4.776600166  | 1.763179117  |
| C | 3.068569664  | -2.554623727  | 2.650681174  |
| C | 2.922961056  | -3.435815529  | 1.419096006  |
| H | 1.875960186  | -5.223923505  | 0.846903825  |
| H | 3.492233659  | -1.587023712  | 2.345082340  |
| O | 4.165693709  | -3.624296775  | 0.775171606  |
| H | 3.783273291  | -3.024062262  | 3.343664303  |
| H | 2.262928922  | -2.934289091  | 0.694602186  |
| H | 0.248450324  | -4.724459525  | 2.245872694  |
| H | 4.528850921  | -4.426067496  | 1.178364760  |
| O | 1.445598116  | -9.957615661  | 1.273670940  |
| C | 2.557718725  | -10.496561030 | 0.629377578  |
| H | 3.283434992  | -10.962032341 | 1.323678272  |
| H | 2.187494996  | -11.280777911 | -0.041818593 |
| H | 3.108301157  | -9.761416458  | 0.013738412  |
| O | 1.923934133  | -1.561714011  | 4.544319529  |
| C | 2.137898316  | -0.201568294  | 4.331937902  |
| H | 2.974357391  | 0.009625498   | 3.643118403  |
| H | 1.246820767  | 0.321203236   | 3.943968849  |
| H | 2.386639976  | 0.237925989   | 5.304334661  |
| C | 2.324282300  | -9.728811179  | 3.524270467  |
| H | 1.704894291  | -10.600639834 | 3.762320990  |
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| H | 2.333250475  | -9.071062242  | 4.403465296  |
| C | 0.635389146  | -1.802017228  | 2.488464180  |
| H | 0.298676805  | -2.536111079  | 1.747283896  |
| H | -0.227402787 | -1.536305866  | 3.111412993  |
| H | 0.970620206  | -0.906368445  | 1.947750640  |
| O | -0.561189202 | -5.524519713  | 0.842882365  |
| H | -0.222268735 | -6.570937265  | 1.777003383  |
| H | -1.597441273 | -5.333451967  | 1.082476661  |



[3+2] Cyclized Product

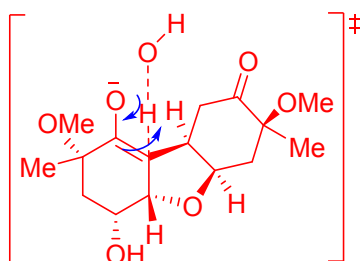
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| C | -0.303644906 | -7.275257478 | 2.589736479 |
| C | 1.402835198  | -6.747803391 | 4.463724198 |
| C | -1.226962125 | -6.184650105 | 3.118830344 |
| C | 0.553474231  | -5.514342776 | 4.800210782 |
| C | -0.937296146 | -5.693747063 | 4.536364811 |
| H | -2.264515704 | -6.543072695 | 3.076702340 |
| H | 0.695115412  | -5.225822207 | 5.850330745 |
| O | -1.612123632 | -4.448824712 | 4.616389329 |
| H | 0.937001777  | -4.680778426 | 4.193262828 |
| H | -1.386028633 | -6.348827699 | 5.296467769 |
| H | -0.640410117 | -8.255975992 | 2.956849385 |
| O | -1.618864999 | -5.220166611 | 0.022049550 |
| C | -2.050079723 | -4.951790785 | 1.120346448 |
| C | -1.136375853 | -4.860790940 | 2.317230722 |
| C | -3.574963083 | -4.791597703 | 1.341989256 |
| C | -1.499499653 | -3.784940258 | 3.354517276 |
| C | -3.890019195 | -4.129293027 | 2.690835799 |
| C | -2.834881527 | -3.103115710 | 3.083962775 |
| H | -0.712686800 | -3.017714800 | 3.421547109 |
| H | -4.866173646 | -3.628651325 | 2.666045164 |
| O | -3.225404924 | -2.341658470 | 4.194513675 |
| H | -3.937512493 | -4.894526246 | 3.478906576 |
| H | -2.690294070 | -2.392265555 | 2.252901444 |
| H | -3.093106515 | -2.908581823 | 4.966191949 |
| O | 2.773062521  | -6.438177327 | 4.546762263 |
| C | 3.312273785  | -6.247192479 | 5.825373157 |
| H | 3.354281983  | -7.176988169 | 6.413393310 |
| H | 4.336597295  | -5.892870076 | 5.681080908 |
| H | 2.771433311  | -5.490131793 | 6.415782991 |
| O | -4.008167311 | -6.150088014 | 1.313493144 |
| C | -5.397140585 | -6.353558191 | 1.359618774 |
| H | -5.869739219 | -5.852569141 | 2.219442109 |
| H | -5.900926989 | -6.018653112 | 0.441206439 |
| H | -5.554550424 | -7.430873743 | 1.460757119 |
| C | 1.039336225  | -7.954071170 | 5.330807989 |
| H | 1.728546486  | -8.779788721 | 5.118586360 |
| H | 1.108441237  | -7.704650015 | 6.396470015 |
| H | 0.018203110  | -8.303724037 | 5.147136086 |
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| H | -3.695135621 | -2.985454461 | 0.153564601 |

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| H | -5.220872401 | -3.866557784 | 0.269078826  |
| H | -0.342988347 | -7.322239755 | 1.495077817  |
| H | -0.117296661 | -4.731893237 | 1.928795631  |



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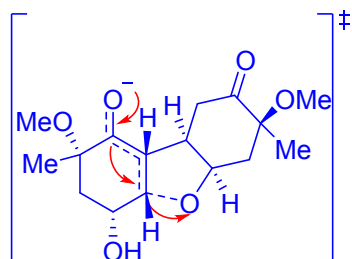
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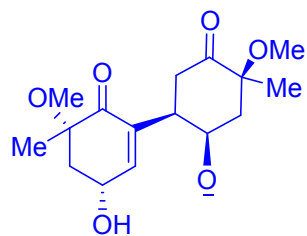


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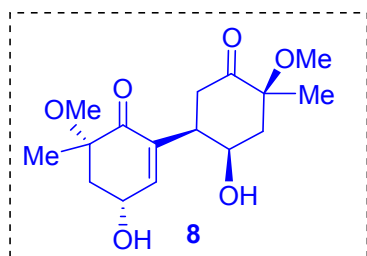
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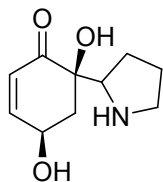
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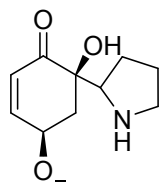
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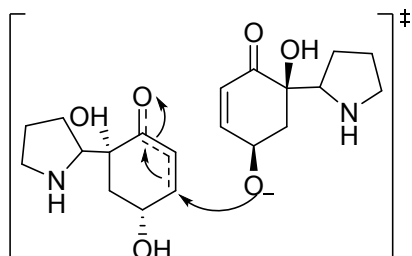
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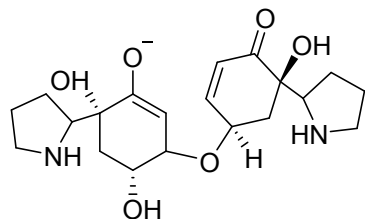
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| H | -1.731285228 | 3.005914826  | -8.662253350 |
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| H | 0.848493252  | 2.360759067  | -4.735031677 |
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| H | -0.607684128 | 1.419194327  | -4.432881234 |
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| H | -2.586009784 | 1.145386466  | -5.120896420 |



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| H | 2.032838300  | 3.584480904  | -8.970921141  |
| H | -2.024100559 | 2.123517245  | -8.986378013  |
| C | 0.010587471  | 2.776975603  | -8.734665328  |
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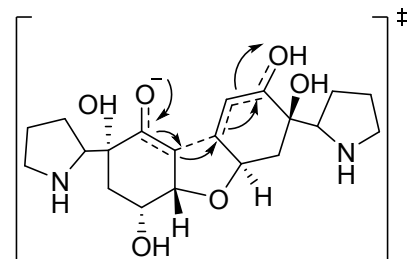
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| H | -2.350502443 | 5.253161080  | -12.108997272 |
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| C | -3.848609079 | 2.963025155 | -12.100582908 |
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| H | -4.242306254 | 1.117444301 | -11.045206540 |
| H | -4.914534909 | 3.222691838 | -12.060709775 |
| H | -1.437373682 | 1.145208431 | -12.183869043 |
| H | -3.762188274 | 0.847746921 | -12.727416551 |
| H | -3.479182399 | 3.237818313 | -13.110364349 |
| H | -1.944142282 | 0.743278726 | -10.554425489 |
| C | -0.833278164 | 4.635472684 | -9.363771696  |
| C | -0.520240211 | 5.019859679 | -8.046056058  |
| C | -1.107481263 | 3.115765489 | -9.591209385  |
| H | -0.243226894 | 6.060267821 | -7.893564691  |
| C | -0.447275150 | 4.113467700 | -6.952522649  |
| C | -1.915439794 | 2.554320464 | -8.421058713  |
| H | -0.472684771 | 4.576918593 | -5.966075056  |
| H | -2.022906283 | 1.466965679 | -8.509506086  |
| C | -1.330148795 | 2.836673963 | -7.030060935  |
| O | -0.623945469 | 1.652748966 | -6.586875183  |
| O | -0.888178866 | 5.406330888 | -10.360065671 |
| H | -2.915330046 | 2.991139045 | -8.501501293  |
| H | -1.109748112 | 3.361129050 | -11.690635150 |
| O | 0.152006496  | 2.400758029 | -9.649787542  |
| H | 0.762014400  | 2.975698764 | -10.132994038 |
| H | -2.165758092 | 2.988686775 | -6.326686250  |
| C | 5.945564867  | 2.618403127 | -2.692687493  |
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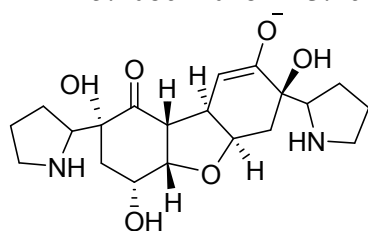


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| C | 0.488246743  | 2.082583158  | -5.817326302  |
| C | 2.449971916  | 1.541894845  | -4.424880817  |
| H | 0.120620804  | 2.563857488  | -4.896692865  |
| H | 2.096951620  | 1.361610377  | -3.404207093  |
| C | 1.378974669  | 0.942861467  | -5.372729193  |
| O | 0.649611178  | -0.067585891 | -4.666927600  |
| O | 3.331387834  | 4.258250289  | -6.600894972  |
| H | -0.173348618 | -0.163687469 | -5.168910558  |
| H | 3.405701099  | 1.028220242  | -4.554851668  |
| H | 4.160794576  | 4.572653469  | -4.219211942  |
| O | 1.754823621  | 3.731608410  | -3.698479968  |
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| H | 1.857287121  | 0.499477617  | -6.261163219  |
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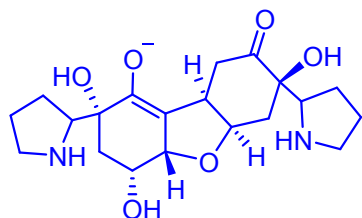
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| C | -0.520240211 | 5.019859679 | -8.046056058  |
| C | -1.107481263 | 3.115765489 | -9.591209385  |
| H | -0.243226894 | 6.060267821 | -7.893564691  |
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| C | -1.915439794 | 2.554320464 | -8.421058713  |

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| O | -0.623945469 | 1.652748966  | -6.586875183  |
| O | -0.888178866 | 5.406330888  | -10.360065671 |
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| H | -1.109748112 | 3.361129050  | -11.690635150 |
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| C | 1.378974669  | 0.942861467  | -5.372729193  |
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| H | -0.173348618 | -0.163687469 | -5.168910558  |
| H | 3.405701099  | 1.028220242  | -4.554851668  |
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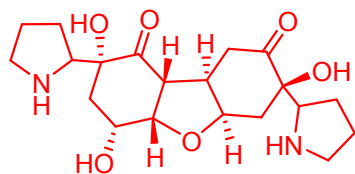
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| H | 3.482673443  | 2.344474801  | -4.754375091  |
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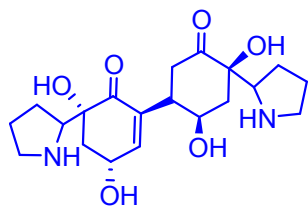
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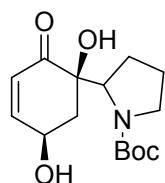
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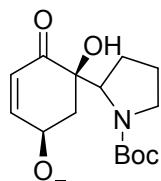
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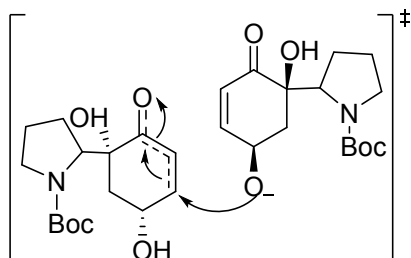
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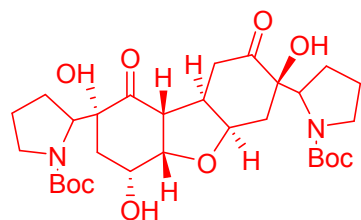


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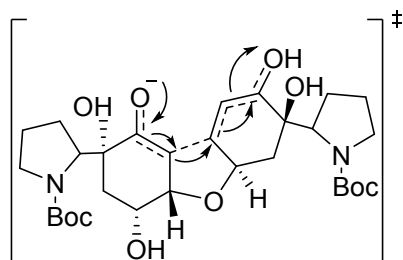
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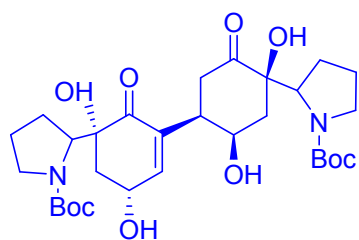
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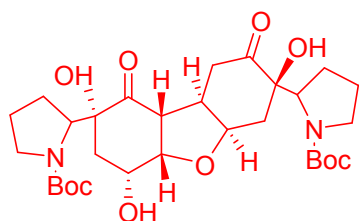
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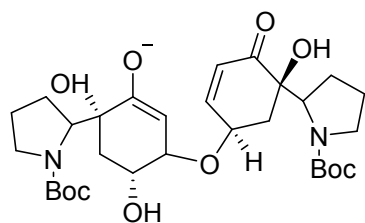


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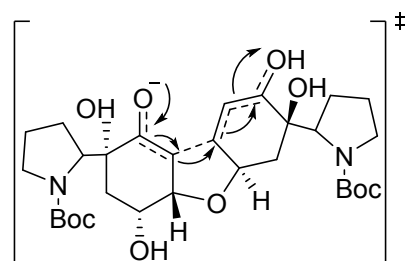
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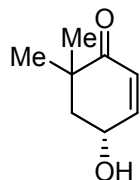
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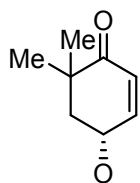
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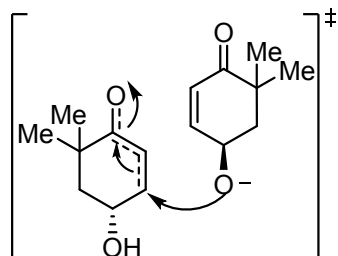


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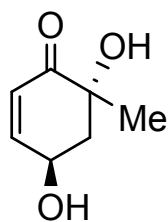


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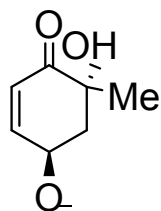


Will do this later.....

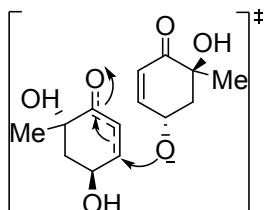


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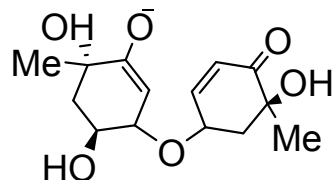
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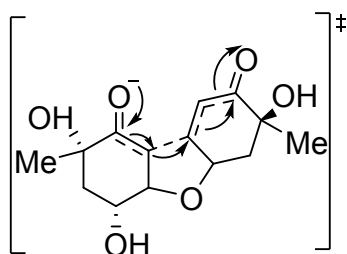


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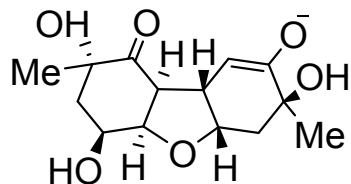
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| O | -5.769006948 | -6.126227146 | 0.706475470  |

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| O | -2.637868091 | 0.434527602  | 1.223392446  |
| H | -2.306947581 | 1.297372861  | 0.944451770  |
| C | -3.546018952 | 0.164073209  | -1.000263034 |
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| H | -3.562713796 | -0.476603584 | -1.889842762 |
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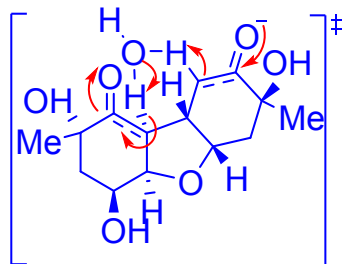
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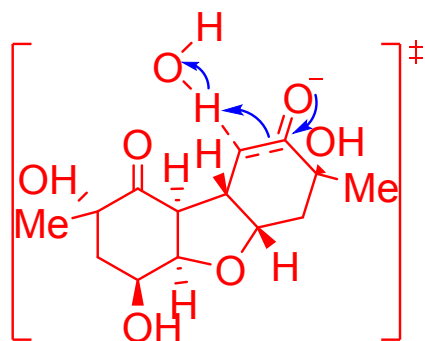
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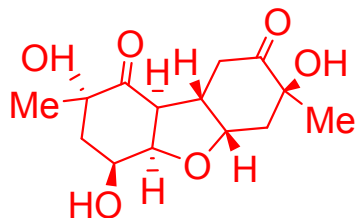
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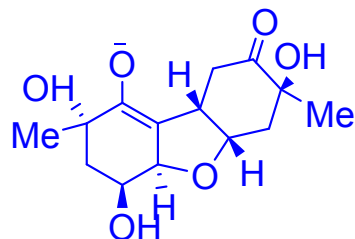
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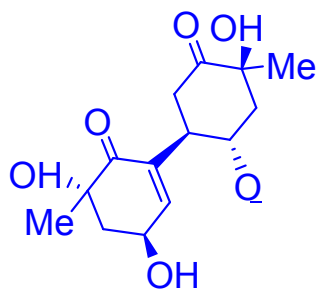
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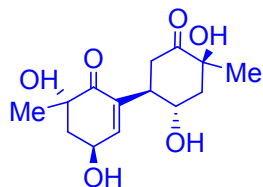
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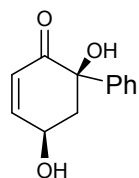


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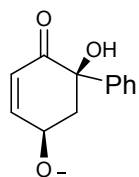
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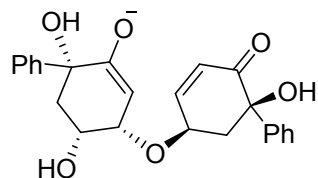


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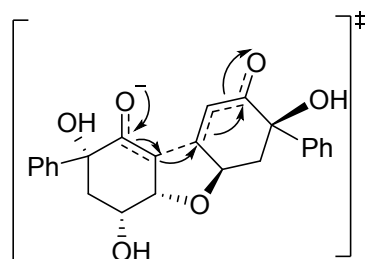
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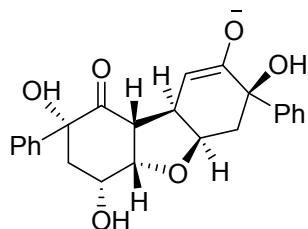
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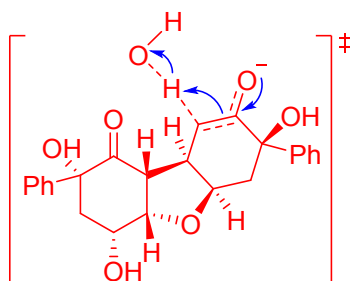
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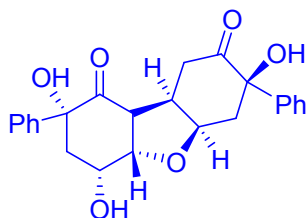


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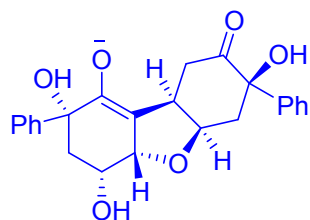
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| O | 2.319452626  | -2.601641582  | 1.036360684  |
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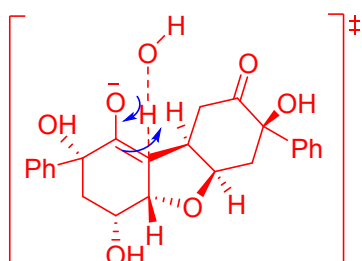
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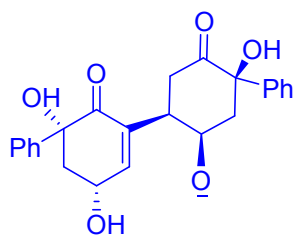
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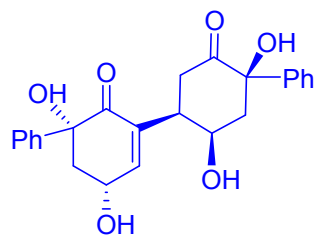
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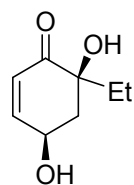
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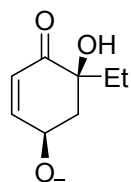
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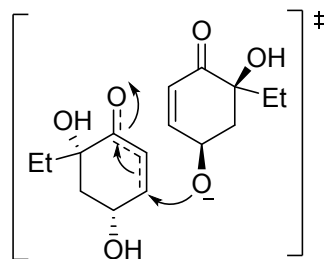
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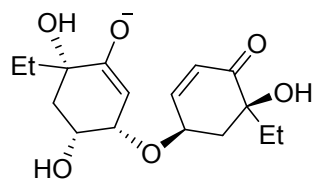


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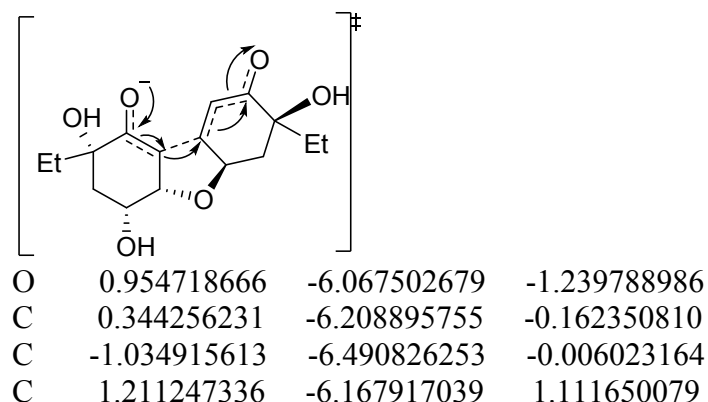
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| C | 0.636649221  | -4.421200543 | 4.015433858 |
| C | 0.208452676  | -4.966865732 | 2.629510968 |
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| H | 2.828385942  | -5.754719519 | 2.940949657  |
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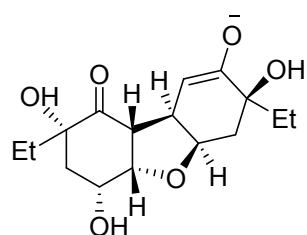


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| C | -0.514390995 | -5.995394055 | -0.214766116 |
| C | 1.596729832  | -4.603794621 | -0.407788390 |
| C | -0.820575022 | -5.371247811 | 0.960152905  |
| C | 0.885032283  | -3.606534311 | 0.498277208  |
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| H | -1.589168446 | -5.797861699 | 1.602499549  |

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| H | 1.617120947  | -2.939002504 | 0.974474170  |
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| H | 0.233970568  | -2.981696554 | -0.128471493 |
| H | 0.714366201  | -4.799167011 | 2.277333660  |
| H | -1.155647186 | -6.782956880 | -0.603482931 |
| H | 2.038121554  | -4.448056668 | -2.228978896 |
| O | -3.949786940 | -5.127899130 | -0.146429021 |
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| C | -4.282982669 | -4.442686535 | 2.082807494  |
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| H | 3.311329316  | -4.726315264 | 0.859884769  |
| H | 2.116837109  | -5.988620991 | 1.187677046  |
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| H | -6.072721464 | -4.097632218 | 1.006609255  |
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| H | -6.146510595 | -3.104012387 | 3.924528353  |
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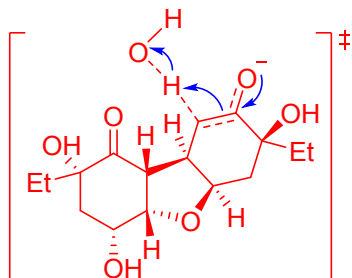


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| H | -1.744923538 | -3.925692192 | 0.931409927  |
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| H | -2.794816154 | -5.396650816 | 5.124635855  |
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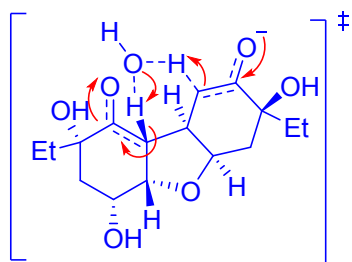
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| C | -4.311051606 | -7.541879561  | -0.942826603 |
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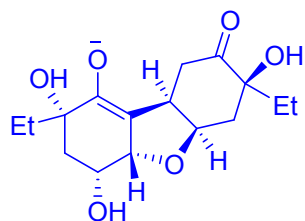
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| C | -5.567269591 | -8.681863214 | 0.955711354  |
| H | -6.490251257 | -8.163548505 | 0.674650988  |
| H | -5.066485582 | -8.066453333 | 1.712770101  |
| H | -5.831599485 | -9.643481559 | 1.411485212  |
| C | 3.066388270  | -7.252001634 | -1.686848704 |
| H | 2.457414369  | -6.337670789 | -1.697784906 |
| H | 3.380261721  | -7.403318334 | -0.643347069 |
| C | 4.288569170  | -7.084578486 | -2.573788418 |
| H | 4.011932619  | -6.795212184 | -3.595464288 |
| H | 4.847082329  | -8.025806016 | -2.627011719 |
| H | 4.956033539  | -6.308188334 | -2.183151586 |
| O | -0.702005796 | -4.717662441 | 0.480170078  |
| H | -1.270445388 | -4.362328172 | 1.325829315  |
| H | -1.432241759 | -5.780518970 | 0.221514320  |



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|---|--------------|--------------|--------------|
| O | -0.495479258 | -7.884808210 | -1.299959688 |
| C | -1.355597490 | -7.422791296 | -0.544917295 |
| C | -2.210666535 | -6.285838213 | -0.856744950 |
| C | -1.454654993 | -8.039442224 | 0.855141258  |
| C | -3.437426541 | -6.018081164 | 0.027282101  |
| C | -1.883923733 | -6.967231924 | 1.845122306  |
| C | -3.272970511 | -6.435501298 | 1.519394492  |
| O | -0.187427086 | -8.540586704 | 1.212040021  |
| H | -4.324330477 | -6.515106147 | -0.389199846 |
| H | -1.862019890 | -7.376709242 | 2.865124347  |
| O | -3.576782721 | -5.288187192 | 2.308637720  |
| H | -1.153466774 | -6.146249965 | 1.807025945  |
| H | -4.023533000 | -7.191517088 | 1.792545034  |
| H | -2.470288244 | -6.288473271 | -1.923137538 |
| H | 0.262146901  | -8.616812404 | 0.350005744  |
| O | -5.919830191 | -4.785471384 | -0.834126843 |
| C | -5.129136294 | -4.131409732 | -0.157420591 |
| C | -3.733850419 | -4.509612370 | 0.119441525  |
| C | -5.601308002 | -2.784503839 | 0.391412998  |
| C | -3.232908660 | -4.149632025 | 1.513610195  |
| C | -5.312781155 | -2.780292429 | 1.892330169  |
| C | -3.827689823 | -2.921458351 | 2.188800222  |
| O | -6.987969875 | -2.672683361 | 0.180681830  |
| H | -2.137177493 | -4.041442727 | 1.461081158  |
| H | -5.712933257 | -1.868468448 | 2.355222775  |

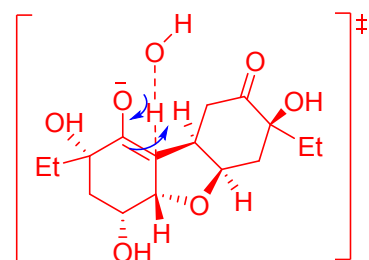


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| O | -3.579839412 | -2.964648725  | 3.579220859  |
| H | -5.848842607 | -3.629203528  | 2.343366374  |
| H | -3.292695904 | -2.041386988  | 1.799647538  |
| H | -2.997028432 | -3.967097080  | -0.573304462 |
| H | -7.184729798 | -3.431007894  | -0.399994104 |
| H | -3.639936620 | -3.901908048  | 3.810112706  |
| C | -2.472292992 | -9.200484952  | 0.810922928  |
| H | -2.645354736 | -9.518215534  | 1.851818386  |
| H | -3.437761251 | -8.836196813  | 0.430254008  |
| C | -2.009890689 | -10.385820602 | -0.019437072 |
| H | -1.076728305 | -10.791024427 | 0.385842810  |
| H | -1.819009013 | -10.094236145 | -1.058226294 |
| H | -2.760877708 | -11.184648259 | -0.018704039 |
| C | -4.879376689 | -1.671686700  | -0.390683784 |
| H | -3.789096256 | -1.816781622  | -0.370787218 |
| H | -5.185366126 | -1.798139916  | -1.440198871 |
| C | -5.255285496 | -0.279523360  | 0.087323517  |
| H | -4.852653321 | -0.069680159  | 1.086315339  |
| H | -6.345855630 | -0.180002777  | 0.135591402  |
| H | -4.868385486 | 0.491555888   | -0.588791054 |
| O | -1.337991245 | -3.727748025  | -0.795837740 |
| H | -1.165650029 | -3.601923348  | -1.734552873 |
| H | -1.562246683 | -5.278956253  | -0.786126310 |



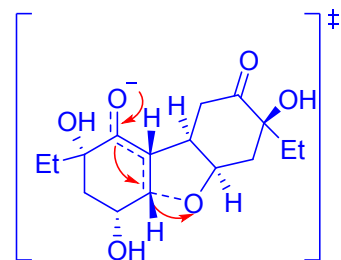
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| C | 1.239775226  | -5.232851535 | -0.048781465 |
| C | -0.136943232 | -4.624144003 | -0.137363906 |
| C | 1.857338212  | -5.377146877 | 1.340151387  |
| C | -0.957708631 | -4.717431938 | 1.141135638  |
| C | 1.330466340  | -4.243990227 | 2.219407511  |
| C | -0.172533068 | -4.325457841 | 2.412667510  |
| O | 3.248361732  | -5.242604405 | 1.228141217  |
| H | -1.322643628 | -5.749407848 | 1.244256418  |
| H | 1.856737960  | -4.265490206 | 3.181352415  |
| O | -0.665463637 | -3.038381117 | 2.787696188  |
| H | 1.576387645  | -3.283932473 | 1.744358918  |
| H | -0.420452421 | -5.039206332 | 3.215168873  |
| H | 0.051660024  | -3.562019162 | -0.369102030 |
| H | 3.461684667  | -5.480223668 | 0.311672433  |
| O | -3.606471512 | -5.019121717 | -0.243256985 |
| C | -3.429293569 | -4.494238608 | 0.840611338  |

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| C | -2.160590608 | -3.737076657 | 1.139042836  |
| C | -4.461141859 | -4.643476989 | 1.942072797  |
| C | -2.050081283 | -3.004168058 | 2.483381831  |
| C | -3.716464809 | -4.820561106 | 3.260373905  |
| C | -2.907613504 | -3.595035676 | 3.654697456  |
| O | -5.227770619 | -5.791025542 | 1.698037705  |
| H | -2.302183376 | -1.942338878 | 2.368062881  |
| H | -4.429551978 | -5.070903449 | 4.055081787  |
| O | -2.099935788 | -3.941289047 | 4.748043838  |
| H | -3.044509880 | -5.687980880 | 3.172894670  |
| H | -3.616894905 | -2.800597061 | 3.955257221  |
| H | -5.164808297 | -5.950013304 | 0.742639573  |
| H | -1.299528944 | -3.401701462 | 4.681587923  |
| C | 1.513354866  | -6.763152911 | 1.926214391  |
| H | 1.894001868  | -6.759047068 | 2.958337390  |
| H | 0.424016548  | -6.895904341 | 2.000031658  |
| C | 2.122634933  | -7.919287541 | 1.152252836  |
| H | 3.212392776  | -7.824192103 | 1.114913715  |
| H | 1.753957733  | -7.963059717 | 0.120899992  |
| H | 1.885405533  | -8.873899695 | 1.632006079  |
| C | -5.365215951 | -3.394176249 | 1.892017304  |
| H | -4.768254452 | -2.471498845 | 1.953374950  |
| H | -5.828950856 | -3.394943942 | 0.894700402  |
| C | -6.439248991 | -3.408776812 | 2.965794609  |
| H | -6.018269447 | -3.275114593 | 3.969440133  |
| H | -6.973372902 | -4.364302724 | 2.946703216  |
| H | -7.165844809 | -2.606070098 | 2.805035795  |
| H | -2.016817136 | -3.018891028 | 0.320352851  |
| H | -0.676719929 | -5.029946915 | -1.000727730 |



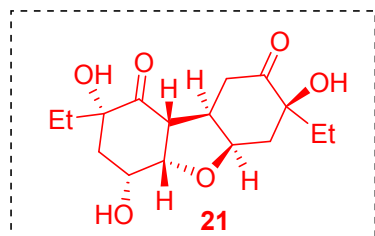
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| O | -5.189280687 | -0.429005869 | 0.679972274 |
| C | -5.058345693 | -1.588957395 | 1.041271573 |
| C | -4.029600743 | -2.527187367 | 0.484576259 |
| C | -6.063181551 | -2.160385297 | 2.050740491 |
| C | -3.747731653 | -3.736690962 | 1.375988482 |
| C | -6.314129901 | -3.620527907 | 1.689302454 |
| C | -5.047097815 | -4.480942081 | 1.777270966 |
| O | -7.266379559 | -1.431847833 | 1.933961160 |
| H | -3.193147988 | -3.415995695 | 2.269283060 |
| H | -7.124631059 | -4.012761307 | 2.323653333 |

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| O | -5.180014303 | -5.593074305 | 0.893435985  |
| H | -6.682666143 | -3.661487223 | 0.651106733  |
| H | -4.919545183 | -4.868494535 | 2.807092876  |
| H | -4.450462591 | -2.872679800 | -0.482521642 |
| H | -6.998995238 | -0.604575491 | 1.497649678  |
| O | -1.259646723 | -4.924495719 | 2.349213889  |
| C | -1.908893553 | -5.447489955 | 1.423774718  |
| C | -2.966877512 | -4.832274555 | 0.694984228  |
| C | -1.507591780 | -6.874001938 | 1.013551646  |
| C | -4.020287196 | -5.660443768 | 0.014702077  |
| C | -2.784836610 | -7.693200269 | 0.853258426  |
| C | -3.692813886 | -7.132861041 | -0.226572609 |
| O | -0.740037269 | -7.419331566 | 2.064497526  |
| H | -4.322969321 | -5.207820610 | -0.947727380 |
| H | -2.552764508 | -8.745456946 | 0.637430638  |
| O | -4.884963528 | -7.882109928 | -0.352582388 |
| H | -3.319110216 | -7.672455789 | 1.817227077  |
| H | -3.176712652 | -7.195648900 | -1.198323587 |
| H | -0.531351751 | -6.618553611 | 2.588764256  |
| H | -5.481295672 | -7.489878918 | 0.302015314  |
| C | -5.530930895 | -2.013767596 | 3.491888422  |
| H | -6.291190058 | -2.483181142 | 4.137090806  |
| H | -4.606806048 | -2.593070712 | 3.621996778  |
| C | -5.308725106 | -0.571523319 | 3.919757543  |
| H | -6.231379414 | 0.008479459  | 3.802610326  |
| H | -4.528949648 | -0.084625925 | 3.320178182  |
| H | -5.004377688 | -0.515976769 | 4.971454820  |
| C | -0.642734217 | -6.783511569 | -0.255019031 |
| H | -1.169752421 | -6.226279773 | -1.045689018 |
| H | 0.224267289  | -6.165602299 | 0.028599462  |
| C | -0.162475815 | -8.139819186 | -0.742482144 |
| H | -0.987325019 | -8.739238693 | -1.149868249 |
| H | 0.281397125  | -8.700499023 | 0.088702511  |
| H | 0.590066380  | -8.041161745 | -1.534268404 |
| H | -3.112962777 | -1.991383162 | 0.200581769  |
| O | -2.044132610 | -3.990351855 | -1.532640568 |
| H | -1.085169528 | -3.951698626 | -1.432648947 |
| H | -2.392591750 | -4.358653266 | -0.334399121 |



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| O | 2.781053628 | -5.434180058 | -0.815521269 |
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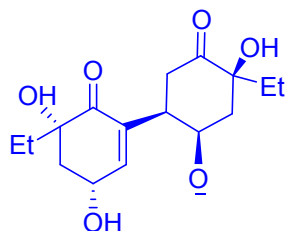
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| C | 2.156583072  | -6.659550405 | 1.148897206  |
| C | -0.325775121 | -5.155372018 | 1.245885042  |
| C | 1.802208774  | -5.996459191 | 2.485401849  |
| C | 0.296867614  | -5.658494259 | 2.609970196  |
| O | 3.486160633  | -6.975855158 | 0.788923276  |
| H | -0.961327406 | -5.923473263 | 0.778068357  |
| H | 2.134436146  | -6.634567805 | 3.319630944  |
| O | 0.104029751  | -4.697101341 | 3.596888529  |
| H | 2.377203330  | -5.058796998 | 2.576812531  |
| H | -0.254487702 | -6.588415398 | 2.880075933  |
| H | 1.161852007  | -3.708826548 | 0.528930848  |
| H | 3.631740079  | -6.435571483 | -0.041641240 |
| O | -3.033899012 | -4.259800756 | 0.301478694  |
| C | -2.331878697 | -3.678420735 | 1.247799000  |
| C | -1.081143520 | -3.931402524 | 1.618188278  |
| C | -3.151644306 | -2.620399179 | 2.027389668  |
| C | -0.392790932 | -3.249518169 | 2.639684174  |
| C | -2.642014991 | -2.572651187 | 3.466078893  |
| C | -1.154928037 | -2.274948626 | 3.502368989  |
| O | -4.487076817 | -3.070032100 | 2.027346584  |
| H | 0.639614058  | -2.912204969 | 2.452872987  |
| H | -3.202063420 | -1.816104274 | 4.045715096  |
| O | -0.610775693 | -2.255785859 | 4.806188706  |
| H | -2.811583641 | -3.556653489 | 3.929187645  |
| H | -0.992767800 | -1.280609059 | 3.028231298  |
| H | -4.452132290 | -3.681910065 | 1.252097133  |
| H | -1.197524910 | -1.691865989 | 5.331329810  |
| H | 0.269527056  | -4.516852200 | -0.763952737 |
| C | 1.287832582  | -7.894863948 | 0.831431700  |
| H | 0.220637527  | -7.641320063 | 0.765427080  |
| H | 1.601581399  | -8.240467256 | -0.166410514 |
| C | 1.512245645  | -8.998659374 | 1.856472565  |
| H | 1.102808445  | -8.723817206 | 2.838319084  |
| H | 2.587621090  | -9.187979474 | 1.974333871  |
| H | 1.025704515  | -9.931561746 | 1.545644073  |
| C | -3.088427732 | -1.242211533 | 1.339494586  |
| H | -3.559228876 | -0.500252590 | 2.009601352  |
| H | -2.036687528 | -0.936481088 | 1.217276921  |
| C | -3.780805908 | -1.225354241 | -0.014759371 |
| H | -4.852383198 | -1.424529858 | 0.111217076  |
| H | -3.379046302 | -2.016741303 | -0.660737554 |
| H | -3.662664787 | -0.252513834 | -0.512161005 |



[3+2] Cyclized Product

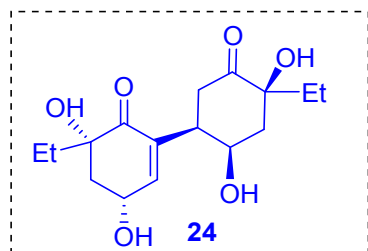
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| C | -1.976885552 | -6.899943670  | -0.113007570 |
| C | 0.058921344  | -7.694683797  | 1.220197926  |
| C | -2.729000639 | -6.534091277  | 1.199269583  |
| C | -0.444163384 | -6.861901413  | 2.398440393  |
| C | -1.967632511 | -6.802024816  | 2.532698010  |
| O | 1.464035516  | -7.664602447  | 1.171332235  |
| H | -3.651878909 | -7.135062007  | 1.178299126  |
| H | 0.009753307  | -7.245020118  | 3.323360004  |
| O | -2.305855429 | -5.735920084  | 3.407684210  |
| H | -0.058126117 | -5.840418635  | 2.264400670  |
| H | -2.325981822 | -7.727337792  | 3.009206362  |
| H | -2.242918405 | -6.188261414  | -0.901001553 |
| H | 1.657241573  | -7.206319091  | 0.333468255  |
| O | -5.201559542 | -5.403355929  | 0.211300305  |
| C | -4.442896292 | -4.759467446  | 0.996030652  |
| C | -3.151363424 | -5.100100369  | 1.353002441  |
| C | -5.070964959 | -3.511000188  | 1.654402189  |
| C | -2.466130083 | -4.562905515  | 2.557185340  |
| C | -4.708258600 | -3.544909666  | 3.139086479  |
| C | -3.207053694 | -3.481842298  | 3.353472364  |
| O | -6.467130589 | -3.626462826  | 1.505753354  |
| H | -1.435338122 | -4.188688192  | 2.369808526  |
| H | -5.196459129 | -2.729135851  | 3.692133676  |
| O | -2.854409013 | -3.548779949  | 4.723021367  |
| H | -5.090335461 | -4.490704997  | 3.551422766  |
| H | -2.845066004 | -2.504370461  | 2.993238906  |
| H | -6.508893787 | -4.365772974  | 0.853703572  |
| H | -2.718560669 | -4.491310872  | 4.892680376  |
| C | -0.402558535 | -9.154067743  | 1.306344633  |
| H | 0.012031786  | -9.557573826  | 2.242393520  |
| H | -1.496204695 | -9.198543982  | 1.404510767  |
| C | 0.062752806  | -9.988583088  | 0.125204665  |
| H | 1.148737179  | -9.904174490  | 0.014652913  |
| H | -0.393970903 | -9.649021666  | -0.813966095 |
| H | -0.192378416 | -11.046478725 | 0.252609833  |
| C | -4.605892409 | -2.241409750  | 0.926987577  |
| H | -3.507256893 | -2.191075892  | 0.910459822  |

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|---|--------------|--------------|--------------|
| H | -4.921510110 | -2.371261081 | -0.119067200 |
| C | -5.202858957 | -0.964096868 | 1.494774080  |
| H | -4.799853026 | -0.734756146 | 2.490401293  |
| H | -6.288830632 | -1.078669116 | 1.591823164  |
| H | -5.002688785 | -0.096431412 | 0.853204873  |
| H | -2.315050721 | -7.892139635 | -0.458954703 |



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| O | -2.198922557 | -8.410048246 | -1.419419970 |
| C | -1.388305481 | -8.398479705 | -0.501373303 |
| C | -1.680437434 | -8.938126034 | 0.863365568  |
| C | -0.039573558 | -7.718576386 | -0.700129894 |
| C | -1.667493263 | -7.760429251 | 1.861100286  |
| C | 0.128777080  | -6.673789801 | 0.409408484  |
| C | -0.214337460 | -7.108299838 | 1.875578434  |
| O | -0.030619597 | -7.118277496 | -1.980867570 |
| H | -1.820963016 | -8.166866098 | 2.872262935  |
| H | 1.164359859  | -6.303518731 | 0.405742836  |
| O | -0.047874124 | -6.133621933 | 2.745810282  |
| H | -0.506839983 | -5.813487185 | 0.149620986  |
| H | 0.436129223  | -8.026432712 | 2.068959490  |
| H | -2.630915434 | -9.477083155 | 0.842906889  |
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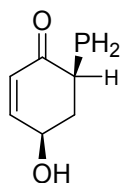
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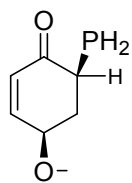
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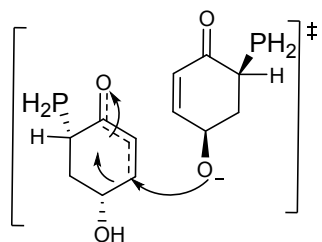
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| C | -2.079300392 | -2.243200945 | 0.536618055  |
| C | -0.984472999 | -0.715637973 | -1.177325001 |
| C | -0.975590647 | -2.188185259 | 1.291235566  |
| C | -0.195890909 | -0.198684923 | 0.026702126  |
| C | 0.207905248  | -1.328164944 | 0.961476312  |
| H | -0.890733071 | -2.779262234 | 2.203879207  |
| H | 0.694835476  | 0.356722801  | -0.290430775 |
| O | 0.844035890  | -0.855841995 | 2.127490043  |
| H | -0.827812655 | 0.506711198  | 0.593673303  |
| H | 0.964288596  | -1.955837167 | 0.460104096  |
| H | -2.933791466 | -2.860823505 | 0.806945860  |
| H | 0.219035501  | -0.288900624 | 2.593826575  |
| H | -0.346166498 | -1.433924854 | -1.721070420 |
| P | -1.329846824 | 0.678429516  | -2.384576453 |
| H | -2.316800448 | -0.009006157 | -3.139645495 |
| H | -2.293690988 | 1.330005914  | -1.558552663 |



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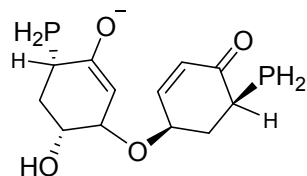


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| C | 0.455614205  | -0.749224923 | 0.287779002  |
| C | 2.839591008  | -1.202866786 | -0.168861718 |
| C | 1.662107984  | -1.533677247 | 0.788263143  |
| P | 3.916797689  | -1.197693878 | -2.769642553 |
| H | -0.330102261 | -0.670392914 | 1.042304823  |
| H | 3.682860399  | -1.875516039 | 0.044564382  |
| O | 1.878415703  | -1.192635714 | 2.037601183  |
| H | 3.161557050  | -0.182092844 | 0.091721889  |
| H | 1.435031478  | -2.640195834 | 0.560141586  |
| H | -0.427808511 | 0.666041197  | -1.074391647 |
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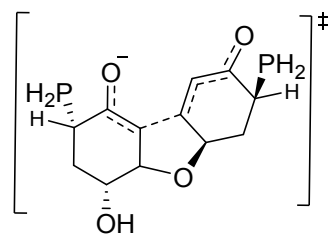
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| C | 1.761342692  | -3.319845058 | 1.680663031  |
| C | 2.116415825  | -4.003731096 | 4.085309554  |
| C | 0.651413245  | -4.084813612 | 1.643532988  |
| C | 0.604089278  | -4.193442946 | 4.114884477  |
| C | 0.120149494  | -4.870454560 | 2.821883478  |
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| H | 0.100930930  | -4.201698886 | 0.708557255  |
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| O | -1.204785935 | -5.142127483 | 2.785275879  |
| H | 0.105366033  | -3.215415313 | 4.206095354  |
| H | 0.689910359  | -5.837773698 | 2.764534060  |
| H | 2.114497133  | -2.776460569 | 0.805927911  |
| H | 4.139691175  | -3.640924611 | 5.526754075  |
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| C | -3.545382582 | -4.414948131 | 2.267370866  |
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| H | -2.291203071 | -3.437769403 | 3.775712984  |

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| H | -4.253805961 | -2.926017091 | 0.001548587  |
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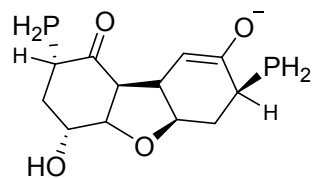


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| C | 0.961687833  | -4.620408244 | 0.360756699  |
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| P | 2.772400355  | -4.691706798 | -1.767784558 |
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| C | -4.258811509 | -4.267339552 | 2.013275443  |
| C | -1.430040495 | -3.406593745 | 1.864315077  |
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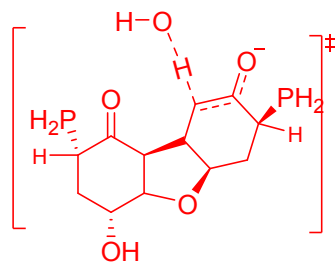
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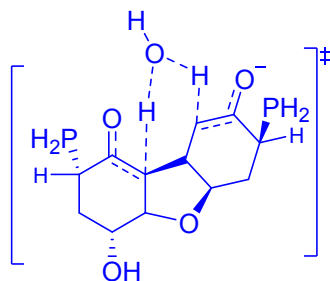
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| C | -2.173025145 | -6.494229655 | 1.347575985  |
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| H | -5.652766484 | -4.138234948 | -0.220665756 |
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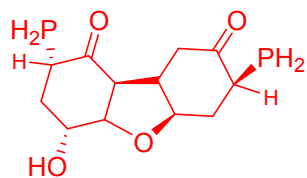
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| C | -0.512939753 | -6.880066760 | 2.129822087  |
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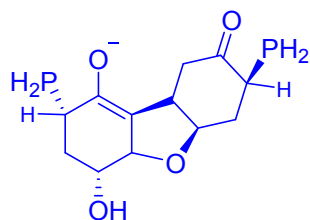
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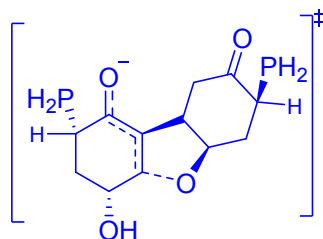


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| C | -1.057983941 | -4.458639507 | 0.958158285  |
| C | 1.203859350  | -4.750090879 | 2.118683496  |
| C | -0.302367415 | -4.654916382 | 2.289929928  |
| P | 3.388626897  | -5.977663195 | 0.785754643  |
| H | -1.609667386 | -5.383434341 | 0.723858731  |
| H | 1.667538907  | -5.091349786 | 3.052706229  |
| O | -0.619273957 | -3.536322840 | 3.104684142  |
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| H | 3.306876741  | -7.159866317 | 0.002831692  |
| O | -3.811096979 | -3.437535969 | -0.347733279 |
| C | -3.420394842 | -3.725307619 | 0.765331649  |
| C | -2.048258004 | -3.294424037 | 1.236252672  |
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| H | -1.813930425 | -1.917221600 | 2.926594152  |
| H | -4.311334683 | -5.272777633 | 3.748127373  |
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| H | -5.629407818 | -5.716884393 | -0.079659515 |
| H | -1.589334608 | -3.892560003 | 4.850090060  |
| H | -1.762433368 | -2.429513767 | 0.626743430  |
| H | -0.690801626 | -4.095304949 | -1.162271870 |
| H | -5.531914003 | -6.710734940 | 1.751754678  |
| H | -5.192352460 | -4.070543905 | 1.834787466  |
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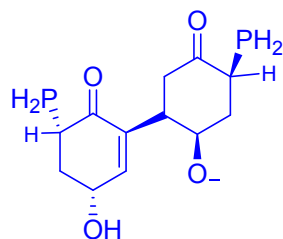


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| C | -0.476712452 | -6.888213989 | 2.361766734  |
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| C | -3.078135575 | -5.130941933 | 1.306087164  |
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| C | -3.221465354 | -3.535524440 | 3.310390213  |
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| H | -5.194631244 | -2.724228757 | 3.504014641  |
| O | -3.000407133 | -3.640988885 | 4.703061828  |
| H | -5.145299295 | -4.486137384 | 3.285591683  |
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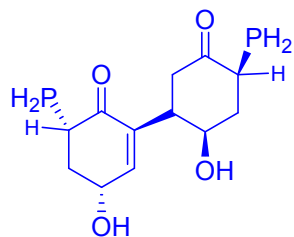




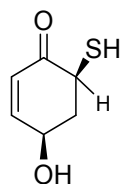
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| C | -2.899005020 | -3.341787658 | 3.808529991  |
| C | -1.577324731 | -2.619376819 | 3.786291406  |
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| H | -4.876858362 | -5.261575452 | 2.985531327  |
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| P | 3.491993602  | -7.758211619 | 1.057820562  |
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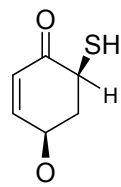
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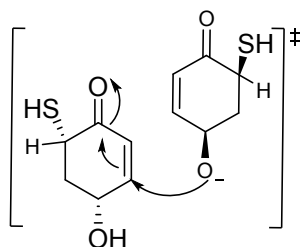
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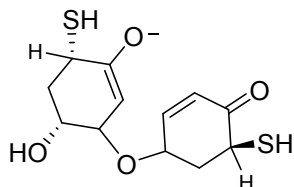
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| C | -0.754992141 | -0.610544961 | -1.109897619 |
| C | -1.095592112 | -2.261239333 | 1.192010443  |
| C | -0.048197293 | -0.240524526 | 0.189598181  |
| C | 0.173097268  | -1.473299686 | 1.054001919  |
| H | -1.137063382 | -2.943980888 | 2.041191713  |
| H | 0.909728705  | 0.253517639  | -0.008593735 |
| O | 0.722265904  | -1.153512865 | 2.310967118  |
| H | -0.674225033 | 0.479271696  | 0.741001775  |
| H | 0.925399971  | -2.119795735 | 0.570380254  |
| H | -3.051338744 | -2.715152056 | 0.487543566  |
| H | 0.110304462  | -0.556892349 | 2.757196992  |
| H | -0.163469702 | -1.391027304 | -1.618741883 |
| S | -0.894780108 | 0.830855620  | -2.221939487 |
| H | -2.124607091 | 0.473001634  | -2.656085499 |



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| C | 1.679931349  | -0.140905323 | -1.736530655 |
| C | 0.510097583  | -0.020852115 | -0.889201543 |
| C | 2.548690317  | -1.363457219 | -1.420912964 |
| C | 0.278785970  | -0.898488097 | 0.119233260  |
| C | 2.676833682  | -1.522889512 | 0.087266894  |
| C | 1.303295972  | -1.830140164 | 0.745035692  |
| H | -0.647031218 | -0.854000470 | 0.694975269  |
| H | 3.401503234  | -2.305055413 | 0.349695227  |
| O | 1.264761669  | -1.580089089 | 2.037902555  |
| H | 3.029506537  | -0.582143509 | 0.534068308  |
| H | 1.055205738  | -2.893301927 | 0.393207051  |
| H | -0.176685995 | 0.786925035  | -1.148777023 |
| S | 4.166074140  | -1.275499072 | -2.299773602 |
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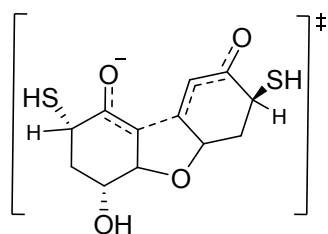


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| C | 0.510556982  | -0.485649264 | -0.967373408 |
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| C | -1.664916833 | -0.459049171 | 0.172296977  |
| C | 0.095513539  | -1.989660989 | 1.003211467  |
| C | -1.420432019 | -1.704429654 | 0.987183300  |
| S | 2.470862392  | -2.391194254 | -0.425110872 |
| H | -2.637132746 | 0.004305445  | 0.354340793  |
| H | 0.269642440  | -2.985664054 | 1.433225722  |
| O | -1.952365050 | -1.600853467 | 2.203514618  |
| H | 0.562360627  | -1.256779200 | 1.676935671  |
| H | -1.871846753 | -2.543853109 | 0.351005121  |
| H | -0.979482875 | 1.069624715  | -1.161764280 |
| H | 2.786597731  | -1.447733370 | -1.344466116 |
| O | -4.617591674 | -4.542843763 | 0.030442361  |
| C | -4.125675051 | -4.065318043 | 1.047779383  |
| C | -2.836718091 | -4.472097727 | 1.586485066  |
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| C | -2.389849911 | -3.987180497 | 2.769221340  |
| C | -4.723488244 | -3.306437883 | 3.330671011  |
| C | -3.281722425 | -3.395050322 | 3.817846806  |
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| O | -3.202653471 | -4.177725563 | 5.010005381  |
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| H | -2.891288534 | -2.407292133 | 4.077634466  |
| H | -2.208864364 | -5.075489668 | 0.933020944  |
| H | -6.344909261 | -3.431353064 | 0.220402260  |
| H | -3.480338104 | -5.067642576 | 4.762866922  |
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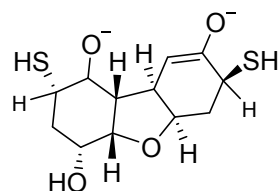
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| C | -3.064989493 | 0.038011282  | 1.559743558  |
| C | -0.756831940 | -0.611132141 | 2.334792912  |
| C | -3.294100717 | -1.240448718 | 1.216485911  |
| C | -1.378970060 | -1.973389559 | 2.616156606  |
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| H | -4.210801167 | -1.541669269 | 0.709630780  |
| H | -0.607174866 | -2.743970295 | 2.729095307  |
| O | -3.002101320 | -3.523910932 | 1.863280832  |
| H | -1.940658227 | -1.936732613 | 3.560089866  |
| H | -1.740806350 | -2.520764444 | 0.568613444  |
| H | -3.794572410 | 0.824215511  | 1.373240324  |
| O | -5.634602064 | -3.267192598 | -1.898651691 |
| C | -5.157692627 | -3.730877341 | -0.832546177 |
| C | -3.812207776 | -3.856199893 | -0.501755397 |
| C | -6.190114484 | -4.252762643 | 0.190939927  |
| C | -3.298226785 | -4.454460117 | 0.744520269  |
| C | -5.634432126 | -4.768019172 | 1.515388937  |
| C | -4.277940748 | -5.441838572 | 1.367305430  |
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| H | -5.494414922 | -3.909093687 | 2.187326522  |
| O | -4.329331847 | -6.642950246 | 0.632117296  |
| H | -6.344287739 | -5.451103029 | 2.003496969  |
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| H | -4.701484841 | -6.418063290 | -0.233807699 |
| S | -7.188219546 | -5.555236437 | -0.688991339 |
| H | -7.078791643 | -4.824807611 | -1.832557051 |
| H | -6.895021418 | -3.431521341 | 0.377422642  |
| S | 0.522644324  | -0.173598548 | 3.569010266  |
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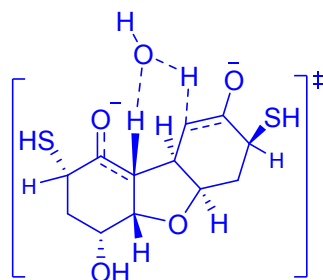
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| C | -2.010732200 | 0.036725386  | -3.076228594 |
| C | -3.295484326 | -0.525320929 | -3.358480220 |
| C | -1.481572658 | -0.097840823 | -1.620329983 |
| C | -4.040359139 | -1.192588299 | -2.403213796 |
| C | -2.578533500 | -0.383111674 | -0.596685681 |
| C | -3.328802373 | -1.580031704 | -1.140651583 |
| H | -5.114699989 | -1.029972191 | -2.358834396 |

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| H | -3.238583644 | 0.488791123  | -0.489181912 |
| H | -2.544571295 | -2.309651525 | -1.423033177 |
| H | -3.731578425 | -0.226031303 | -4.309071780 |
| O | -5.358037559 | -4.173059093 | -4.423542365 |
| C | -5.624980834 | -3.717361406 | -3.300398724 |
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| C | -6.437966301 | -2.829556626 | -0.636473798 |
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| O | -6.754019975 | -2.920105162 | 0.736029755  |
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| H | -0.789161866 | -0.955160071 | -1.621217124 |



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| O | -0.330974064 | 1.664673641  | -2.729285275 |
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| C | -2.501129475 | 0.228412134  | -0.056769880 |
| C | -2.573950401 | -1.116441425 | -0.724788930 |
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| H | -3.412418828 | 0.805243222  | -0.274821032 |
| H | -1.582992187 | -1.605011964 | -0.642132124 |
| H | -1.743396109 | -0.206470227 | -3.962527003 |
| O | -2.987442480 | -2.949164748 | -4.838305229 |
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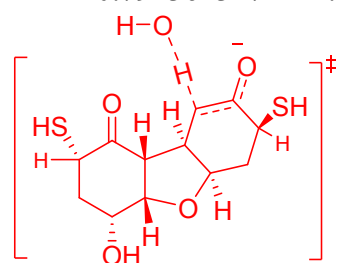
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| H | -0.525081560 | 2.885563075  | -1.357757967 |
| S | -5.841503209 | -3.156865053 | -5.603606319 |
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| H | -5.490084190 | -1.141665216 | -5.477028464 |
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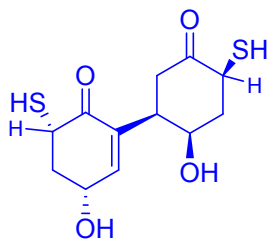


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| H | -2.497531920 | -2.693075227 | -2.741987398 |
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| H | -6.753940467 | -1.519360648 | -1.626854875 |
| H | -5.239347853 | -2.797836503 | -3.680020040 |
| S | 2.659469567  | 0.096135048  | -4.008677490 |
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| H | 0.794361317  | 1.543353866  | -4.456904319 |



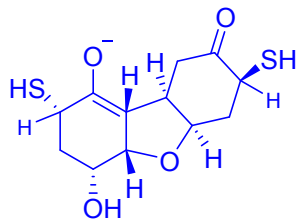
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| C | -2.827601734 | -1.774404810 | -2.401225908 |
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| C | -3.780860868 | -2.363262460 | -1.372679190 |
| C | -2.770122720 | -1.083859992 | 0.511638399  |
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| H | -2.168272905 | -3.033982080 | -0.162516920 |
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| C | -4.398735528 | -4.287888222 | -0.079774004 |
| C | -6.258974421 | -5.714514368 | -0.767002915 |
| C | -5.814281714 | -4.679793063 | 0.247979025  |
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| H | -7.203370943 | -6.174239156 | -0.448770048 |
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| H | -5.397212264 | -4.622674263 | 2.109168893  |
| O | -1.655748919 | -4.366126428 | -2.135175012 |
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| H | -7.287240724 | -4.369777167 | -2.075339806 |
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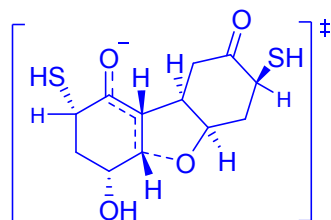


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| C | -2.134493573 | -0.931204236 | -4.859101424 |
| C | -1.491146452 | -1.246185892 | -2.039584738 |
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| C | -0.416902136 | -1.213682679 | -3.108675449 |
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| H | -0.071027576 | -0.287906505 | -5.038196883 |
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| H | -1.026718323 | 0.682173125  | -3.911566989 |
| H | -0.261974995 | -2.251213707 | -3.475688101 |
| H | -3.561217156 | -1.938403229 | -1.824164119 |
| O | -2.320723050 | -2.465013132 | 0.712636059  |
| C | -1.389652926 | -1.732712782 | 0.454363634  |
| C | -0.696030500 | -1.865602908 | -0.888140472 |
| C | -0.936578939 | -0.615924573 | 1.384151271  |
| C | 0.668598291  | -1.180238642 | -1.073938266 |
| C | 0.548195301  | -0.303913316 | 1.242190508  |
| C | 0.861525238  | 0.043110025  | -0.197382469 |
| H | 1.498272400  | -1.872660158 | -0.858520966 |
| H | 0.829045219  | 0.535181318  | 1.888809035  |
| O | 2.180700232  | 0.508963137  | -0.280395475 |
| H | 1.152065947  | -1.166561348 | 1.561669246  |
| H | 0.148477375  | 0.819863497  | -0.542937348 |
| H | -0.619002666 | -2.946525947 | -1.078395833 |
| H | 2.374664591  | 0.652389165  | -1.214568411 |
| H | -2.514785236 | -2.975530777 | -2.806987392 |
| S | -2.738296946 | 0.110103644  | -6.232161618 |

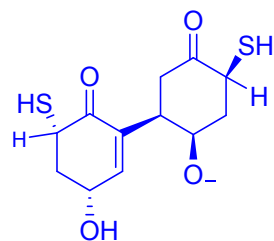
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| H | -2.433419934 | -1.711734880 | 2.819391969  |
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| H | -1.506905368 | 0.270145586  | 1.052268608  |



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| C | -2.148213109 | -0.702445661 | -4.070088154 |
| C | -2.121731001 | -1.458594282 | -2.762231270 |
| C | -0.785069968 | -0.597995040 | -4.793350214 |
| C | -0.977843657 | -0.911186179 | -1.912915152 |
| C | 0.376632941  | -0.174360543 | -3.877801148 |
| C | 0.334140156  | -1.071891650 | -2.666976896 |
| H | -1.174574526 | 0.178024532  | -1.803915886 |
| H | 1.323645374  | -0.254908398 | -4.427862800 |
| O | 1.346817005  | -0.865794273 | -1.710208068 |
| H | 0.254997697  | 0.876168500  | -3.579948137 |
| H | 0.389884430  | -2.129969981 | -3.018238814 |
| H | -3.084848447 | -1.354764470 | -2.253833036 |
| O | -2.643168293 | -1.176998998 | 0.573000698  |
| C | -1.406441597 | -1.424425800 | 0.536628122  |
| C | -0.616538614 | -1.505361098 | -0.591161794 |
| C | -0.672711504 | -1.565642809 | 1.890471084  |
| C | 0.872701573  | -1.665309699 | -0.597525776 |
| C | 0.778689457  | -2.012848912 | 1.798813580  |
| C | 1.498588508  | -1.245127351 | 0.701918070  |
| H | 1.224585753  | -2.706237129 | -0.799355477 |
| H | 1.304063892  | -1.868948070 | 2.752993764  |
| O | 2.885690194  | -1.533530376 | 0.757387087  |
| H | 0.830812796  | -3.087653311 | 1.564709884  |
| H | 1.319777147  | -0.159071934 | 0.824586198  |
| H | 3.239091190  | -1.245648732 | -0.091914372 |
| H | -1.950349731 | -2.528929266 | -2.963923111 |
| S | -0.875976094 | 0.450422742  | -6.291893799 |
| H | -2.215163736 | 0.615961471  | -6.167241536 |
| S | -1.667435287 | -2.653663249 | 3.003238131  |
| H | -2.777837023 | -2.260823011 | 2.310501823  |
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| H | -0.707719122 | -0.561317373 | 2.341209400  |

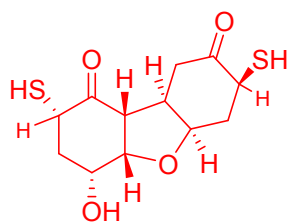


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| C | -2.131613821 | -0.152381076 | -1.700395016 |
| C | -2.921503384 | -1.378355614 | -2.093364007 |
| C | -1.639203251 | -0.148107730 | -0.250985881 |
| C | -4.007554710 | -1.655721425 | -1.056168225 |
| C | -2.727532967 | -0.540263302 | 0.755977522  |
| C | -3.383703672 | -1.870029831 | 0.359169548  |
| H | -4.649795997 | -0.756803859 | -1.014913723 |
| H | -2.284019347 | -0.629484556 | 1.756151313  |
| O | -4.259849909 | -2.355524929 | 1.241022498  |
| H | -3.492779027 | 0.248083211  | 0.810757951  |
| H | -2.496445907 | -2.567012023 | 0.163252599  |
| H | -3.330192171 | -1.217794030 | -3.097265254 |
| O | -6.288753166 | -1.687406584 | -2.851750833 |
| C | -6.121259021 | -2.633169848 | -2.071144994 |
| C | -4.951048768 | -2.801484484 | -1.267848535 |
| C | -7.230136600 | -3.691508124 | -1.915724104 |
| C | -4.833375873 | -3.821498900 | -0.352758677 |
| C | -6.742585059 | -5.010405106 | -1.342964325 |
| C | -5.973818682 | -4.738870424 | -0.062744369 |
| H | -3.863081430 | -4.142872927 | 0.018286897  |
| H | -7.580474845 | -5.690590261 | -1.137652387 |
| O | -5.564161608 | -5.973158598 | 0.492790900  |
| H | -6.077380413 | -5.511184159 | -2.060097548 |
| H | -6.642201725 | -4.204534987 | 0.642249953  |
| H | -2.231119534 | -2.237970063 | -2.130764954 |
| H | -5.020707319 | -5.753771362 | 1.257376390  |
| S | -8.124924739 | -3.937506522 | -3.502172260 |
| H | -7.749253749 | -2.701825932 | -3.922517229 |
| H | -7.947703410 | -3.248241413 | -1.205240446 |
| S | -0.811136842 | 1.430768205  | 0.194728118  |
| H | -0.880703360 | 1.905430368  | -1.071542174 |
| H | -0.873478991 | -0.941535907 | -0.226131051 |



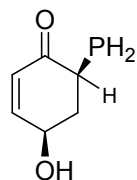
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|---|--------------|-------------|--------------|

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|---|--------------|--------------|--------------|
| C | -2.039337686 | 0.239751649  | -2.686203281 |
| C | -2.532290256 | -1.152029211 | -2.989285545 |
| C | -1.319851427 | 0.360435318  | -1.353224720 |
| C | -3.376373429 | -1.743801564 | -1.846592202 |
| C | -2.170698200 | -0.245958934 | -0.238087651 |
| C | -2.569782461 | -1.720509026 | -0.496662108 |
| H | -4.271604273 | -1.111002206 | -1.709862053 |
| H | -1.625340105 | -0.212214976 | 0.713198931  |
| O | -3.190894344 | -2.262695821 | 0.531088469  |
| H | -3.087379942 | 0.348218344  | -0.100279722 |
| H | -1.580579616 | -2.231123307 | -0.801234509 |
| H | -3.073528666 | -1.121394147 | -3.939653081 |
| O | -5.033708716 | -2.453834914 | -4.127721281 |
| C | -4.689074591 | -3.353489062 | -3.371085449 |
| C | -3.841055107 | -3.137540798 | -2.190984147 |
| C | -5.213604776 | -4.784048574 | -3.567509867 |
| C | -3.534904562 | -4.173201434 | -1.378474533 |
| C | -4.204283569 | -5.819355124 | -3.104043735 |
| C | -3.922249411 | -5.588996010 | -1.634331743 |
| H | -3.098712532 | -3.882906927 | -0.400561770 |
| H | -4.568903587 | -6.840719823 | -3.274571282 |
| O | -2.912072789 | -6.492936223 | -1.223684849 |
| H | -3.265825453 | -5.705919394 | -3.664493708 |
| H | -4.856036666 | -5.792427163 | -1.065399248 |
| H | -1.644432201 | -1.796638257 | -3.112483821 |
| H | -2.456192869 | -6.082067657 | -0.481218189 |
| S | -5.744427447 | -5.084691112 | -5.294676788 |
| H | -5.851061003 | -3.758155006 | -5.548374455 |
| S | -0.776653734 | 2.084766271  | -1.005646046 |
| H | -1.214509826 | 2.538515235  | -2.203926511 |
| H | -6.107628850 | -4.857120056 | -2.925044527 |
| H | -0.413638766 | -0.258763924 | -1.453980456 |



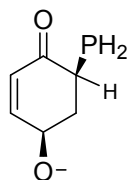
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| O | -1.833531788 | 0.927704267  | -3.854702400 |
| C | -1.856911264 | 0.135425704  | -2.940787585 |
| C | -2.312239267 | -1.295620109 | -3.118028529 |
| C | -1.419149236 | 0.469232328  | -1.519271729 |
| C | -3.368144914 | -1.722647801 | -2.082491886 |
| C | -2.511011071 | 0.040168961  | -0.538848963 |
| C | -2.861331533 | -1.436081183 | -0.676308665 |
| H | -4.262898892 | -1.098782885 | -2.236043268 |

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| H | -2.179483331 | 0.251987193  | 0.487710362  |
| O | -3.875361839 | -1.805741624 | 0.226191649  |
| H | -3.417270809 | 0.640180618  | -0.707640186 |
| H | -1.937371673 | -2.030415074 | -0.502366964 |
| H | -2.696158919 | -1.409809394 | -4.135673768 |
| O | -5.067573826 | -2.454617706 | -4.169845791 |
| C | -4.717654947 | -3.373585716 | -3.451025826 |
| C | -3.775600011 | -3.154613430 | -2.323837288 |
| C | -5.265588292 | -4.786634170 | -3.599705758 |
| C | -3.335588645 | -4.198342308 | -1.602204968 |
| C | -4.189720967 | -5.817665616 | -3.287078625 |
| C | -3.684104865 | -5.631276463 | -1.867386795 |
| H | -2.686212558 | -4.042415666 | -0.740212009 |
| H | -4.566108005 | -6.838008738 | -3.422844042 |
| O | -2.603038287 | -6.484916897 | -1.567960827 |
| H | -3.353274794 | -5.685108148 | -3.992088265 |
| H | -4.480358792 | -5.923407795 | -1.161484176 |
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| H | -1.893556891 | -6.290954406 | -2.191280664 |
| H | -3.615145192 | -1.527256726 | 1.110303231  |
| S | -5.995292428 | -5.088506171 | -5.246959205 |
| H | -6.187255287 | -3.775043393 | -5.499126565 |
| S | -0.962149341 | 2.223807300  | -1.302304466 |
| H | -1.161081723 | 2.515246836  | -2.608481649 |
| H | -6.062313986 | -4.873108648 | -2.840983754 |
| H | -0.523889082 | -0.147236560 | -1.333704150 |

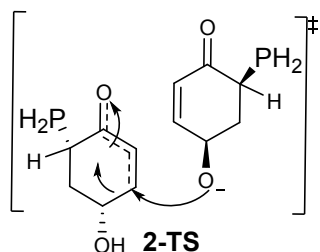


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| C | -2.030031897 | -1.372888244 | -0.782204399 |
| C | -2.025097168 | -2.169517875 | 0.460427650  |
| C | -0.739393543 | -0.644032780 | -1.110786712 |
| C | -0.998190853 | -2.142027718 | 1.318656728  |
| C | -0.069795609 | -0.139868835 | 0.166058798  |
| C | 0.218547252  | -1.285310877 | 1.127374239  |
| H | -1.007659243 | -2.750960260 | 2.223364712  |
| H | 0.858823807  | 0.398694297  | -0.055109766 |
| O | 0.729696094  | -0.832799137 | 2.361014951  |
| H | -0.743633153 | 0.576163946  | 0.666864123  |
| H | 1.019369207  | -1.914563992 | 0.702590859  |
| H | -2.912597625 | -2.774170540 | 0.636540965  |
| H | 0.064664069  | -0.261573837 | 2.762189446  |
| H | -0.076113865 | -1.393890241 | -1.576552764 |

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| P | -1.095196910 | 0.642659650 | -2.436997289 |
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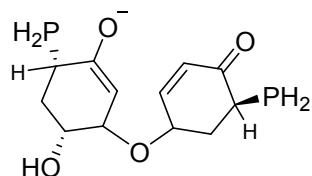


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| O | 1.855459507  | 0.671601268  | -2.605853437 |
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| C | 0.447081624  | -0.115077745 | -0.869040932 |
| C | 2.581679614  | -1.298520035 | -1.446283818 |
| C | 0.258641075  | -1.050000036 | 0.092323889  |
| C | 2.680067625  | -1.570091420 | 0.053449986  |
| C | 1.310251028  | -2.004089007 | 0.652495970  |
| H | -0.665166370 | -1.069646184 | 0.674390613  |
| H | 3.436609126  | -2.334556873 | 0.281968357  |
| O | 1.258526592  | -1.948173677 | 1.961985981  |
| H | 2.965508481  | -0.652196084 | 0.589739065  |
| H | 1.110036471  | -3.019575226 | 0.144543982  |
| H | -0.276688149 | 0.671836540  | -1.091466304 |
| P | 4.234388489  | -0.903072897 | -2.232256566 |
| H | 3.905153073  | -1.161605357 | -3.596739293 |
| H | 2.148078144  | -2.193457492 | -1.924235356 |
| H | 4.783385318  | -2.211842872 | -2.033039060 |



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| O | 0.641587443  | 1.094659368  | -1.259852850 |
| C | -0.042765057 | 0.302470477  | -0.622381571 |
| C | -1.381043213 | 0.630926480  | -0.134289853 |
| C | 0.442285487  | -1.104692537 | -0.330126996 |
| C | -2.096907649 | -0.238850856 | 0.602799876  |
| C | -0.074982504 | -1.607681797 | 1.015043131  |
| C | -1.608535841 | -1.568840338 | 1.079276741  |
| P | 2.314080585  | -1.130320020 | -0.431340826 |
| H | -3.105886104 | 0.015774504  | 0.933857121  |
| H | 0.268660165  | -2.633522977 | 1.209733553  |
| O | -2.094938769 | -1.820594028 | 2.325686646  |
| H | 0.305324983  | -0.975224681 | 1.832720915  |
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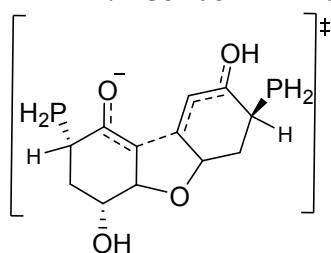
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| C | -5.062173445 | -4.028178794 | 1.478908324  |
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| C | -4.774291645 | -3.096181434 | 2.668606733  |
| C | -3.533146772 | -3.460880628 | 3.475009746  |
| P | -5.955779380 | -5.548588563 | 2.079371322  |
| H | -1.404895154 | -3.746869669 | 3.069219784  |
| H | -4.591493830 | -2.095241984 | 2.253600679  |
| O | -3.707592890 | -4.626042944 | 4.262564331  |
| H | -5.641998666 | -3.021946044 | 3.340119235  |
| H | -3.320297506 | -2.647720061 | 4.179341202  |
| H | -1.679677880 | -4.720665658 | 0.809202305  |
| H | -6.568753497 | -6.504486417 | 1.010875497  |
| H | -3.998363454 | -5.334291667 | 3.655592741  |
| H | -7.242975992 | -5.277660915 | 2.933875324  |
| H | -5.606467197 | -3.476569981 | 0.699851098  |
| H | 2.420147157  | -2.554920725 | -0.373076935 |
| H | 0.022627985  | -1.747761226 | -1.121785284 |



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| O | -1.789618935 | 1.605819106  | 2.580426743  |
| C | -1.942739918 | 0.443998750  | 2.228245966  |
| C | -3.143496480 | -0.022742460 | 1.532766362  |
| C | -0.866540558 | -0.599047175 | 2.466208161  |
| C | -3.327132690 | -1.315540617 | 1.217970231  |
| C | -1.477157277 | -1.971143716 | 2.742089656  |
| C | -2.356704436 | -2.407219063 | 1.578907497  |
| H | -4.210410311 | -1.649951608 | 0.674020537  |
| H | -0.700324441 | -2.726371838 | 2.918748252  |
| O | -3.020104140 | -3.578924205 | 1.933861054  |
| H | -2.101742595 | -1.932851017 | 3.647542284  |
| H | -1.710772867 | -2.573638821 | 0.691156518  |
| H | -3.878824859 | 0.741502298  | 1.286612356  |
| O | -5.336886246 | -3.335422886 | -1.972205271 |
| C | -4.939522182 | -3.798640583 | -0.878127075 |
| C | -3.612389641 | -4.016676687 | -0.490846253 |
| C | -6.055209332 | -4.235870871 | 0.092006739  |
| C | -3.213282051 | -4.546692033 | 0.825408893  |
| C | -5.604668144 | -4.794031543 | 1.447267090  |
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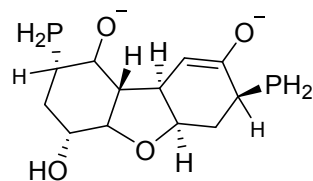


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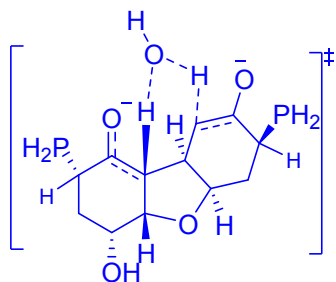
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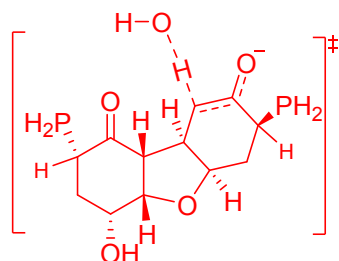
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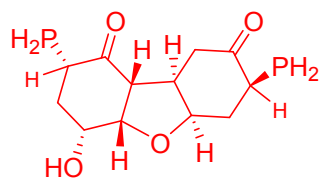


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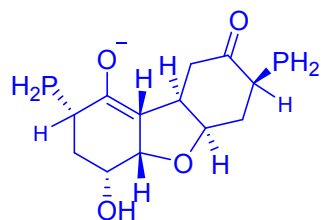
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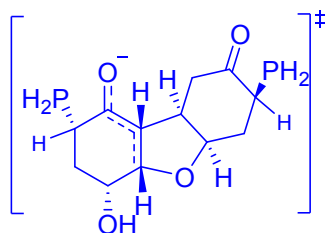
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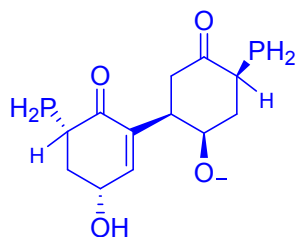
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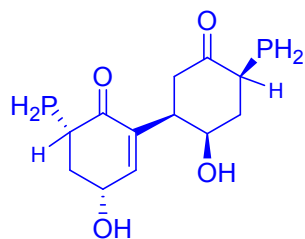


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| P | -0.969828064 | 1.571327771  | 0.129915499  |
| H | 0.258696270  | 1.464655909  | -0.585602764 |
| H | -0.857247597 | -0.876179842 | -0.203233744 |
| H | -9.070579327 | -4.833674806 | -3.123108237 |
| H | -0.376457740 | 1.173346392  | 1.370566618  |



|   |              |              |              |
|---|--------------|--------------|--------------|
| O | -2.207402791 | 1.174996473  | -3.432797181 |
| C | -2.088469513 | 0.242394033  | -2.656278740 |
| C | -2.579179403 | -1.147693219 | -2.970294686 |
| C | -1.407392976 | 0.400152298  | -1.318100404 |
| C | -3.402944027 | -1.762777369 | -1.823728014 |
| C | -2.242483617 | -0.236616376 | -0.202952944 |
| C | -2.604398697 | -1.720777016 | -0.468248433 |
| H | -4.316128276 | -1.155398413 | -1.687927277 |
| H | -1.702038621 | -0.196439928 | 0.752393495  |
| O | -3.215842423 | -2.281551623 | 0.555417028  |
| H | -3.182820132 | 0.321281545  | -0.059910568 |
| H | -1.598320089 | -2.200484916 | -0.768339093 |
| H | -3.130482777 | -1.118416192 | -3.915342391 |
| O | -5.043384169 | -2.529226729 | -4.123860606 |
| C | -4.659905365 | -3.412083569 | -3.363749681 |
| C | -3.830700194 | -3.166969413 | -2.173805152 |
| C | -5.107009523 | -4.848420277 | -3.613168023 |
| C | -3.516945107 | -4.199056156 | -1.360770878 |
| C | -4.087054486 | -5.859960733 | -3.111312822 |
| C | -3.859716766 | -5.624616697 | -1.632014757 |
| H | -3.105545008 | -3.901775087 | -0.373454323 |
| H | -4.414194280 | -6.893317927 | -3.293532542 |
| O | -2.840613250 | -6.501671966 | -1.182669419 |
| H | -3.125745039 | -5.723988200 | -3.628855946 |
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| H | -1.684627840 | -1.780552384 | -3.110777936 |
| H | -2.375219119 | -6.044160755 | -0.474234455 |
| P | -5.467022068 | -5.053034728 | -5.442435942 |
| H | -6.732080961 | -4.405417669 | -5.473080920 |
| P | -1.051305080 | 2.211845811  | -1.001657853 |
| H | 0.024358659  | 2.383395758  | -1.924119461 |
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| H | -0.463811905 | -0.166801438 | -1.386593305 |
| H | -6.041985400 | -6.357817801 | -5.305426241 |
| H | -0.173718592 | 1.968517177  | 0.102548047  |





|   |              |              |              |
|---|--------------|--------------|--------------|
| O | -1.610424840 | 0.970504509  | -4.001273752 |
| C | -1.644258960 | 0.192777588  | -3.075561984 |
| C | -1.987278599 | -1.270112860 | -3.271396927 |
| C | -1.307462442 | 0.575445408  | -1.639591954 |
| C | -3.017340392 | -1.804302840 | -2.261867628 |
| C | -2.352208932 | 0.004197375  | -0.675684432 |
| C | -2.556734982 | -1.495729937 | -0.845484185 |
| H | -3.962535747 | -1.261901150 | -2.422291971 |
| H | -2.052314229 | 0.222003486  | 0.360289671  |
| O | -3.538219033 | -1.977108839 | 0.042147614  |
| H | -3.324035659 | 0.499168018  | -0.832478577 |
| H | -1.580493540 | -1.999760228 | -0.670546025 |
| H | -2.340249325 | -1.404441964 | -4.297899644 |
| O | -4.648659448 | -2.621505708 | -4.352064848 |
| C | -4.177489259 | -3.537366158 | -3.702268754 |
| C | -3.288595901 | -3.261390604 | -2.538466343 |
| C | -4.514354291 | -4.996108504 | -3.980972719 |
| C | -2.800335678 | -4.274949198 | -1.806050235 |
| C | -3.370841702 | -5.922443998 | -3.574340709 |
| C | -3.005839240 | -5.726599110 | -2.114594029 |
| H | -2.221378658 | -4.080066623 | -0.902802985 |
| H | -3.622263718 | -6.973301325 | -3.761119668 |
| O | -1.883163573 | -6.493484278 | -1.736465066 |
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| H | -3.829680605 | -6.102627395 | -1.484279398 |
| H | -1.053982677 | -1.846968616 | -3.152622681 |
| H | -1.137646751 | -6.205671304 | -2.275767656 |
| H | -3.304942424 | -1.698778363 | 0.933748483  |
| P | -5.059088218 | -5.362759637 | -5.739874849 |
| H | -3.905234031 | -4.793039804 | -6.356359885 |
| P | -1.052728189 | 2.403833406  | -1.317460987 |
| H | -0.279600241 | 2.670366565  | -2.479321554 |
| H | -5.384765749 | -5.229305493 | -3.343322596 |
| H | -0.344451115 | 0.082645290  | -1.416433501 |
| H | -5.838682387 | -4.189413533 | -5.916609682 |
| H | -2.270352457 | 2.822186713  | -1.927250347 |