

Antioxidant activity of Magnolol and Honokiol: Kinetic and Mechanistic Investigations of their Reaction with Peroxyl Radicals

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Supporting Information

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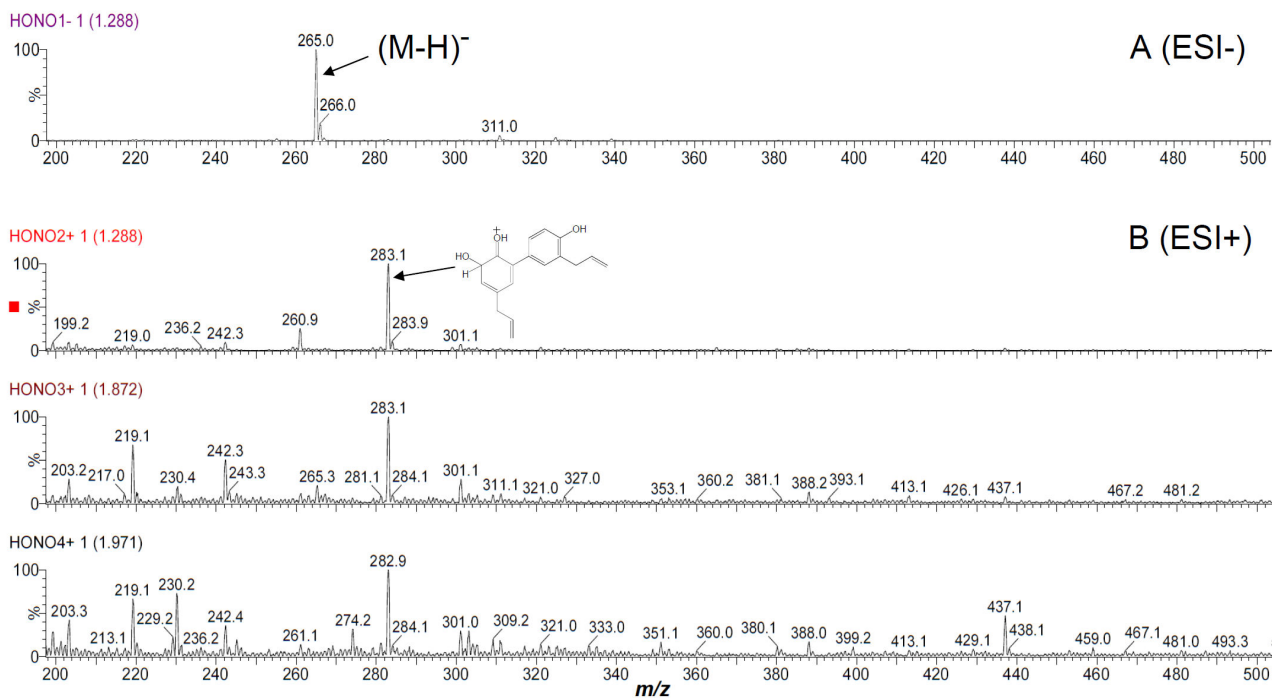
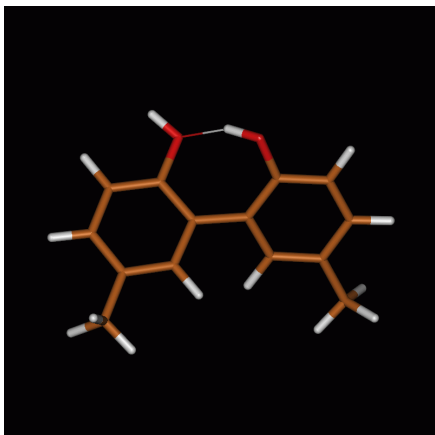


Figure S1. ESI-MS spectra of a mixture of honokiol (5 μ M) and AIBN (5 mM) in MeCN, incubated at 303K for 20 minutes. A: negative ion mode spectrum recorded immediately upon mixing the components ($t=0$ min); B: positive ion mode spectra recorded (from top to bottom) after 4 min, 8 min and 12 min of incubation.

Calculation results

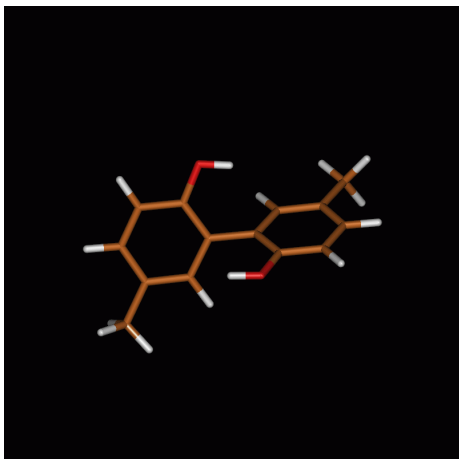
bisfaw



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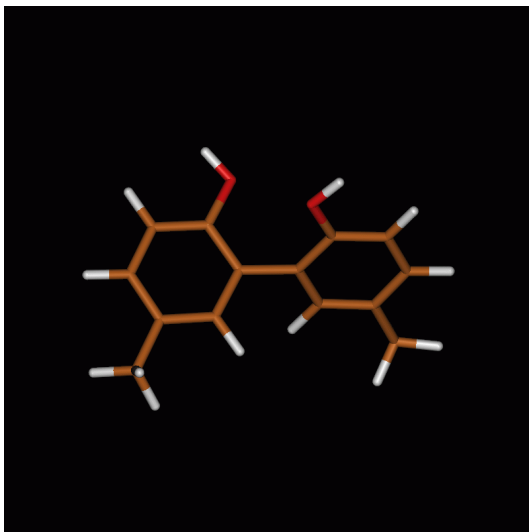
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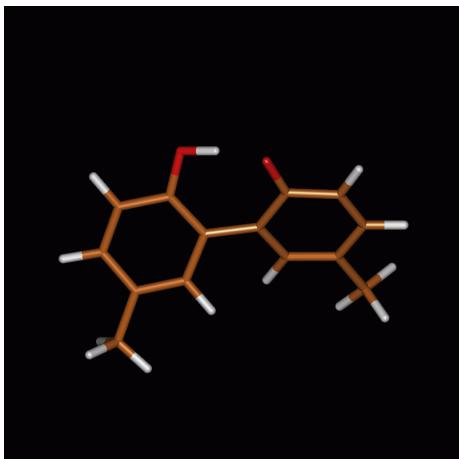
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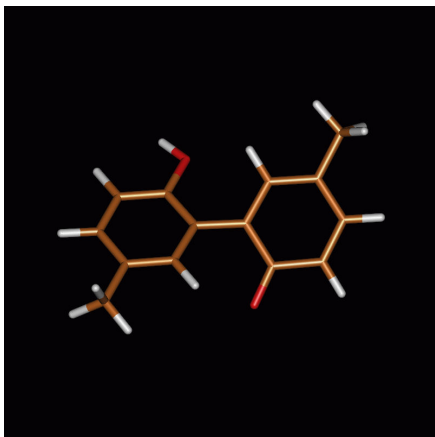
bistowrad



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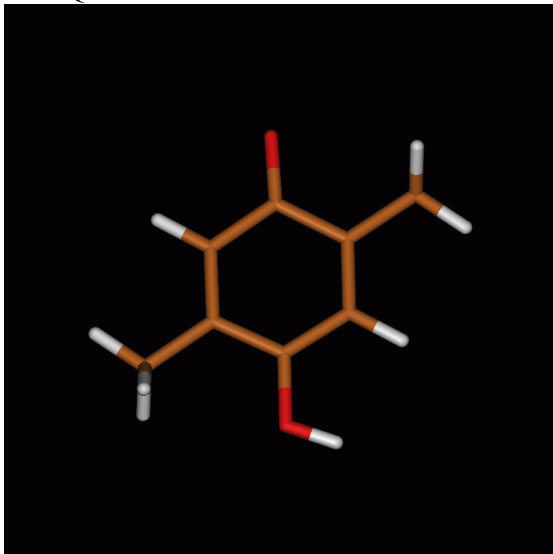
bistowradaw



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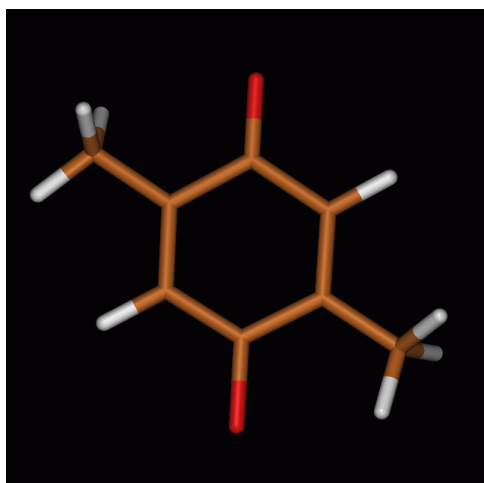
Me2QH



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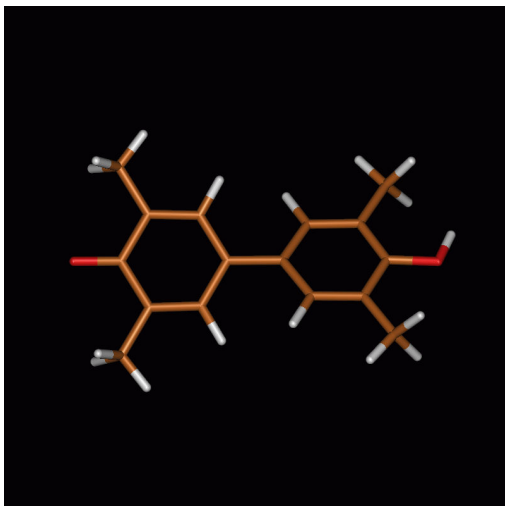
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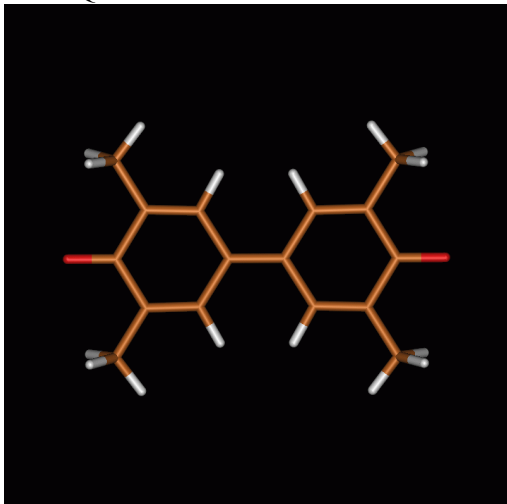
44bisfrad1



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595,-0.8277337499,1.8750381521\H,4.3625373521,0.9214233613,1.838792213  
\H,3.6473355109,0.0659398747,3.2285139393\H,-4.6668509004,1.6975914029  
,0.7832902881\H,-5.6907458707,0.5483912899,1.6683083239\H,-5.237502351  
8,2.0688590496,2.4229304253\H,-1.6679799617,-1.6735888316,5.8220824638  
\H,-2.9101453549,-0.5319962342,6.3262442697\H,-3.3640895779,-2.0662724  
745,5.5580180811\H,0.1722232801,-0.0562792082,-2.6330974884\H,1.725980  
4562,0.8164236277,-2.6323236784\H,1.7230804476,-0.9325677335,-2.591565  
0155\Version=EM64L-G09RevD.01\State=2-A\HF=-770.4419211\S2=0.77916\S2  
-1=0.\S2A=0.750664\RMSD=9.104e-09\RMSF=1.785e-05\Dipole=-1.6811332,-0.  
2748729,1.5689799\Quadrupole=-9.7584251,0.7293756,9.0290494,0.9049805,  
6.4481112,-4.1706021\PG=C01
```

No imaginary frequencies.

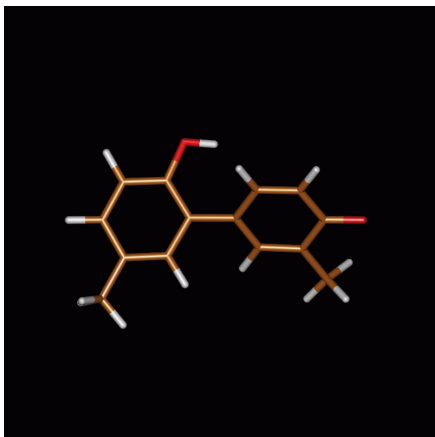
44bisQ1



```
RB3LYP/6-31+G(d,p)\C16H16O2\ROOT\10-Jul-2015\0\  
#p B3LYP/6-31+g(d,p) opt=tight freq int=ultrafine scale=0.9806\44 dii  
drossi bifenele chinone1\0,1\C,0.0132874635,-0.0000240795,0.018847109  
1\C,0.0105527223,-0.0000150905,1.4710003114\C,1.311534368,-0.000002380  
9,2.11613829\C,2.4845242923,-0.0000080855,1.4299844387\C,2.4697981805,  
-0.0000400748,-0.051302165\C,1.1505278989,-0.0000296725,-0.7250601926\  
C,-1.1846702861,-0.000009402,2.2108575\C,-2.485652447,-0.000026119,1.5  
657205082\C,-3.6586432961,-0.0000207276,2.2518737384\C,-3.6439160915,0  
.0000055706,3.7331593334\C,-2.3246444173,0.0000215395,4.406916756\C,-1  
.1874038766,0.000014,3.663010627\O,-4.695347734,0.0000078737,4.3840060  
505\C,-2.3224012895,0.0000468248,5.9074403919\C,3.8265810279,0.0000097  
441,2.101147516\O,3.5212281331,-0.0000042576,-0.7021516685\H,-0.241772  
5436,0.0000282898,4.1911580658\H,-2.536673076,-0.000045601,0.483798884  
6\C,-5.0007011756,-0.0000402525,1.5807129637\H,1.3625550985,0.00001133  
19,3.1980602946\C,1.148287531,-0.0000297582,-2.2255837903\H,-0.9323435  
564,-0.0000234779,-0.5093001061\H,4.4112394139,-0.8751247503,1.7970255  
855\H,4.4112311785,0.8751396496,1.7969962424\H,3.7260460635,0.00002771  
16,3.189724931\H,-1.3032270018,0.0000557154,6.3029044584\H,-2.85534858  
86,0.8751844694,6.2950965928\H,-2.855344972,-0.8750799077,6.2951261122  
\H,-5.5853510799,-0.8751690588,1.8848701249\H,-5.5853609788,0.87509266  
37,1.8848392489\H,-4.9001737043,-0.0000588967,0.4921360265\H,0.1291170  
67,-0.0000276947,-2.6210545186\H,1.6812396056,0.8751000646,-2.61325317  
36\H,1.6812363365,-0.8751616824,-2.6132526018\\Version=EM64L-G09RevD.0  
1\State=1-A\HF=-769.8250651\RMSD=7.847e-09\RMSF=1.027e-06\Dipole=-0.00  
00009,-0.0000129,0.000002\Quadrupole=-11.537335,5.2190056,6.3183294,0.  
0000322,17.9189873,0.0001573\PG=C01
```

No imaginary frequencies.

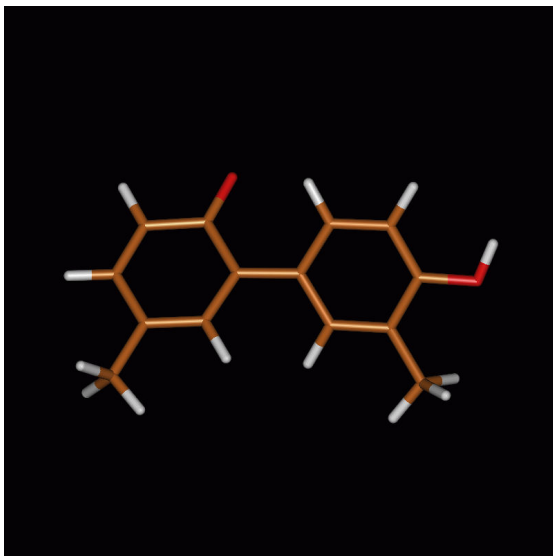
honrad2



```
UB3LYP/6-31+G(d,p)\C14H13O2(2)\ROOT\03-Jul-2015\  
0\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\honok rad2\0,2\C,0.,0.  
,0.\C,0.,0.,1.413262\C,1.2523515117,0.,2.0703430638\C,2.4367830113,0.0  
361611936,1.3263168339\C,2.3936321995,0.062182667,-0.0622661861\C,1.16  
90039762,0.0400402788,-0.7557272698\C,-1.2753233086,-0.0072475886,2.15  
23496672\C,-2.3409877893,-0.8513331268,1.7373764563\C,-3.557927403,-0.  
8924989803,2.3879159098\C,-3.7765096885,-0.0242415983,3.5507398734\C,-  
2.683970905,0.8473826729,3.9476381047\C,-1.4853920328,0.8476388986,3.2  
753456231\O,-4.8662415342,-0.0296840717,4.1741314992\C,-4.6714045181,-  
1.8036393882,1.965088482\O,1.3942737409,-0.0725832258,3.4286856469\C,1  
.1330695272,0.0768288512,-2.2663411561\H,-2.1724268216,-1.5130368334,0  
.891631318\H,-0.7078071692,1.5510138599,3.5616543832\H,-2.867117928,1.  
5117014624,4.7865334556\H,3.381278156,0.0274496478,1.86054045\H,3.3262  
574767,0.0927221098,-0.6202894807\H,-0.9593820444,0.0100368595,-0.5101  
833562\H,0.5376332896,-0.2289393864,3.851501125\H,1.7101836366,-0.7485  
484441,-2.6990620929\H,0.1087700431,0.0008667584,-2.6420841958\H,1.560  
8743824,1.0092153776,-2.6535162697\H,-4.960844503,-2.4689937242,2.7859  
227288\H,-5.5684950428,-1.2266192562,1.7143279039\H,-4.3842105604,-2.4  
082576984,1.1008430687\Version=EM64L-G09RevD.01\State=2-A\HF=-691.793  
4293\S2=0.780952\S2-1=0.\S2A=0.750714\RMSD=9.630e-09\RMSF=3.145e-06\Di  
pole=1.0305835,-0.1687785,-1.2737098\Quadrupole=-6.5113186,3.0656354,3  
.4456833,2.5910014,4.9896706,1.1517485\PG=C01
```

No imaginary frequencies.

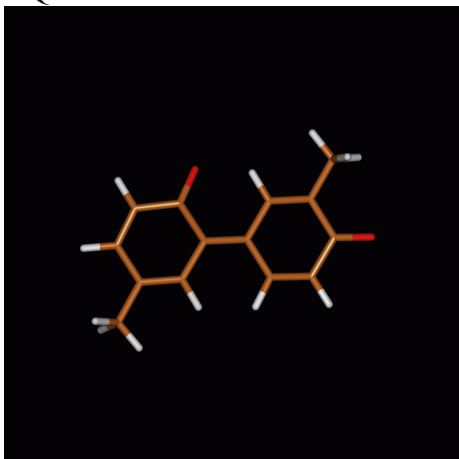
honrad3



```
UB3LYP\6-31+G(d,p)\C14H13O2(2)\ROOT\13-Jul-2015\  
0\#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\honok rad3\0,2\C,0.015  
4515637,-0.0756571922,0.0246152879\C,0.017548091,0.0038414671,1.422860  
6436\C,1.322389069,0.0676739075,2.1099349089\C,2.5155271591,0.05680918  
67,1.2773650733\C,2.4452453151,-0.0313524972,-0.086939345\C,1.18415013  
82,-0.0978939493,-0.7465415564\C,-1.2435166164,0.0158129766,2.17753393  
85\C,-2.3750764268,-0.6790385661,1.6928252182\C,-3.6031595504,-0.68520  
16955,2.3499323475\C,-3.7042865921,0.0483766544,3.5477047765\C,-2.6047  
398598,0.7453239594,4.0568665288\C,-1.3852926782,0.7249608159,3.387652  
0942\O,-4.9192441444,0.0363226954,4.1802801188\C,-4.7906663123,-1.4532  
709882,1.8271944328\O,1.4302887417,0.1060562336,3.3609840158\C,1.12641  
31464,-0.1667101417,-2.2493872459\H,-2.2847784521,-1.2697200477,0.7857  
145704\H,-0.5403577867,1.261262073,3.7978229722\H,-2.7031156189,1.3077  
374882,4.9832561744\H,-4.8701579276,0.5513482764,4.996601481\H,3.46445  
69688,0.1097365273,1.8018980172\H,3.3553403767,-0.0441422778,-0.682453  
9007\H,-0.9379600641,-0.0866899027,-0.4961676579\H,1.607490495,0.70886  
30038,-2.7031536265\H,1.6596122311,-1.0499886384,-2.6227593609\H,0.096  
7510263,-0.2135908497,-2.6131935119\H,-5.1368003446,-2.1944632496,2.55  
6162873\H,-5.6387939506,-0.7880595948,1.6297122074\H,-4.5380529403,-1.  
9741136024,0.8997015895\Version=EM64L-G09RevD.01\State=2-A\HF=-691.79  
38341\S2=0.779397\S2-1=0.\S2A=0.750648\RMSD=6.540e-09\RMSF=7.402e-06\D  
ipole=-0.5315532,0.2009139,-1.0526281\Quadrupole=-1.3957433,-4.1822944  
,5.5780377,-1.0094047,-11.1927491,4.356062\PG=C01
```

No imaginary frequencies.

HQ1

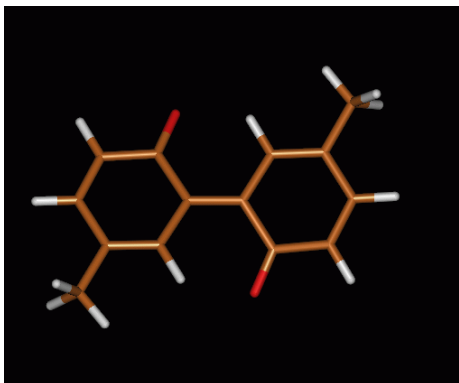


RB3LYP/6-31+G(d,p)\C14H12O2\ROOT\03-Jul-2015\0\

```
#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\\honokiol chinone 1\\0,1\C,  
-0.0098629651,-0.0971951862,0.0274852789\C,-0.0188895692,-0.0636188434  
,1.4727008271\C,1.3340834523,-0.0503264655,2.1504708426\C,2.5118494674  
,0.0609239543,1.2821355702\C,2.4125566145,0.049593486,-0.0670197222\C,  
1.1257565422,-0.0413652378,-0.7291538202\C,-1.2248432069,-0.0302573465  
,2.1946438038\C,-1.2796538861,0.2041536952,3.6280764092\C,-2.442484557  
9,0.2499488904,4.3354068023\C,-3.7368505899,0.0381090072,3.6438255559\  
C,-3.6798418191,-0.1949425729,2.192318991\C,-2.5077071278,-0.214317992  
9,1.5197598594\O,-4.8138646234,0.0617822419,4.2486079924\C,-2.48483602  
51,0.5208870004,5.8099368295\O,1.4962016729,-0.1631206933,3.3718758624  
\C,1.0878332233,-0.0494161021,-2.2340064883\H,-0.3407507478,0.35145057  
71,4.1421589368\H,-2.5308233657,-0.4111166394,0.4558687878\H,-4.628983  
9683,-0.3598626121,1.6915380885\H,3.4666478231,0.1150891004,1.79480640  
54\H,3.3088066501,0.1061111811,-0.6812374559\H,-0.9537475577,-0.128295  
6553,-0.5018270675\H,1.5436001065,0.8604881906,-2.6444401886\H,1.65654  
17088,-0.8975700274,-2.6356834388\H,0.0648097382,-0.1171547581,-2.6127  
695027\H,-3.083594044,1.4135826935,6.0231614429\H,-2.9733715157,-0.304  
7328469,6.3394294092\H,-1.4792032351,0.6591800277,6.2137511664\\Versio  
n=EM64L-G09RevD.01\State=1-A\HF=-691.1675651\RMSD=4.521e-09\RMSF=6.256  
e-06\Dipole=1.0122525,0.115927,-2.0445566\Quadrupole=-7.4943639,-0.227  
0235,7.7213874,1.1837984,0.0679449,1.522673\PG=C01
```

No imaginary frequencies.

chinoneaw

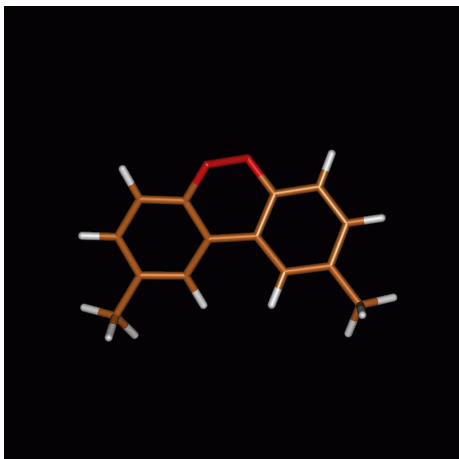


RB3LYP/6-31+G(d,p)\C14H12O2\ROOT\02-Jul-2015\0\

```
#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\4Me bifenolo chinone aw\0
,1\C,0.0201261088,-0.1715382007,0.0041132611\C,-0.0350927569,0.0400455
602,1.4293930709\C,1.2946468661,0.3181763081,2.1134616303\C,2.48235400
25,0.4285953527,1.2571924218\C,2.4243707508,0.2306562837,-0.0789315366
\C,1.169351451,-0.0786375394,-0.7344085473\C,-1.2508715933,0.006046892
5,2.1431471511\C,-1.340975696,0.4306788494,3.5182397729\C,-2.512307656
5,0.4732290637,4.2259152788\C,-3.7500733958,0.0584970924,3.596402333\C
,-3.7699434978,-0.3720388052,2.3149978961\C,-2.548785539,-0.4651480922
,1.5050106891\C,-2.5573760774,0.9606027677,5.6487101105\O,-2.630988702
3,-0.9528385787,0.3707345337\O,1.4410100417,0.416694346,3.3382070599\C
,1.1660018552,-0.2717853299,-2.2265911442\H,-0.4285068276,0.743589522,
4.0024072088\H,-4.6709526488,0.1031370303,4.1743181336\H,-4.6810297472
,-0.6915103561,1.8197115805\H,3.4083982228,0.6566248084,1.7747787901\H
,3.3256944255,0.3048247705,-0.6840028353\H,-0.9061055338,-0.400953437,
-0.5002520346\H,-3.218772024,1.8313347669,5.7456497198\H,-2.9575194479
,0.1850619015,6.3146619957\H,-1.5649516913,1.2416060945,6.0083235064\H
,0.1649411562,-0.4998832216,-2.5994732774\H,1.5289578413,0.6276810509,
-2.7406223135\H,1.8357754323,-1.0920744513,-2.5157234702\Version=EM64
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ipole=-0.0724177,0.448519,-0.1052804\Quadrupole=2.8780032,-6.0494671,3
.1714639,-1.8509966,-14.1055453,-0.2499331\PG=C01
```

No imaginary frequencies.

chinone tow



```
RB3LYP/6-31+G(d,p)\C14H12O2\ROOT\02-Jul-2015\0\  
#p B3lyp/6-31+g(d,p) opt freq scale=0.9806\\4Me bifenolo chinone tow\  
0,1\C,0.0069782952,-0.0255835237,-0.1109948122\C,-0.0863031167,-0.0020  
91132,1.2848120423\C,1.10826777,-0.0407301322,2.0249993958\C,2.3531427  
604,-0.0689780012,1.4098056529\C,2.4132505625,-0.0513821973,0.01247985  
01\C,1.2476077897,-0.0358253596,-0.7663116059\C,-1.3332443552,0.039525  
9475,2.063076066\C,-2.5828185253,0.4485747971,1.5852536968\C,-3.727743  
0257,0.4180135802,2.3958305193\C,-3.5955684688,-0.0216635171,3.7203309  
675\C,-2.3528163125,-0.3989277013,4.2399816893\C,-1.2420854921,-0.3636  
532627,3.4070638047\C,-5.062214103,0.8858635004,1.8608375414\O,-0.0355  
480686,-0.8409971205,3.889314885\O,1.0503851926,0.0466211239,3.4053759  
812\C,1.3214290959,-0.0142106621,-2.2762851475\H,-2.6705203923,0.79716  
22086,0.5594092713\H,-4.4694962197,-0.0505983425,4.3656849488\H,-2.242  
3815241,-0.7237080944,5.2691760987\H,3.2515904543,-0.1028068365,2.0168  
572637\H,3.3839758053,-0.0754278523,-0.4755940478\H,-0.9042420313,-0.0  
380067934,-0.7034094462\H,-5.8928390695,0.4207760627,2.4001468865\H,-5  
.1714167903,1.9728841144,1.9640270736\H,-5.1739357604,0.6465815451,0.7  
984741575\H,0.4853228733,-0.5590123417,-2.725921134\H,1.2865232001,1.0  
133746898,-2.6599232934\H,2.250657358,-0.4659588159,-2.6363806053\\Ver  
sion=EM64L-G09RevD.01\State=1-A\HF=-691.1252811\RMSD=6.000e-09\RMSF=1.  
975e-06\Dipole=-0.6109101,0.2390373,-0.9923925\Quadrupole=5.8788493,-6  
.6431278,0.7642785,-0.882074,-5.3736773,-0.519947\PG=C01
```

No imaginary frequencies.