

Supplementary material

Powering the antioxidant properties of tyrosol by selenylation: tyrosol selenide and diselenide as potent reactive oxygen species scavengers and glutathione peroxidase mimics

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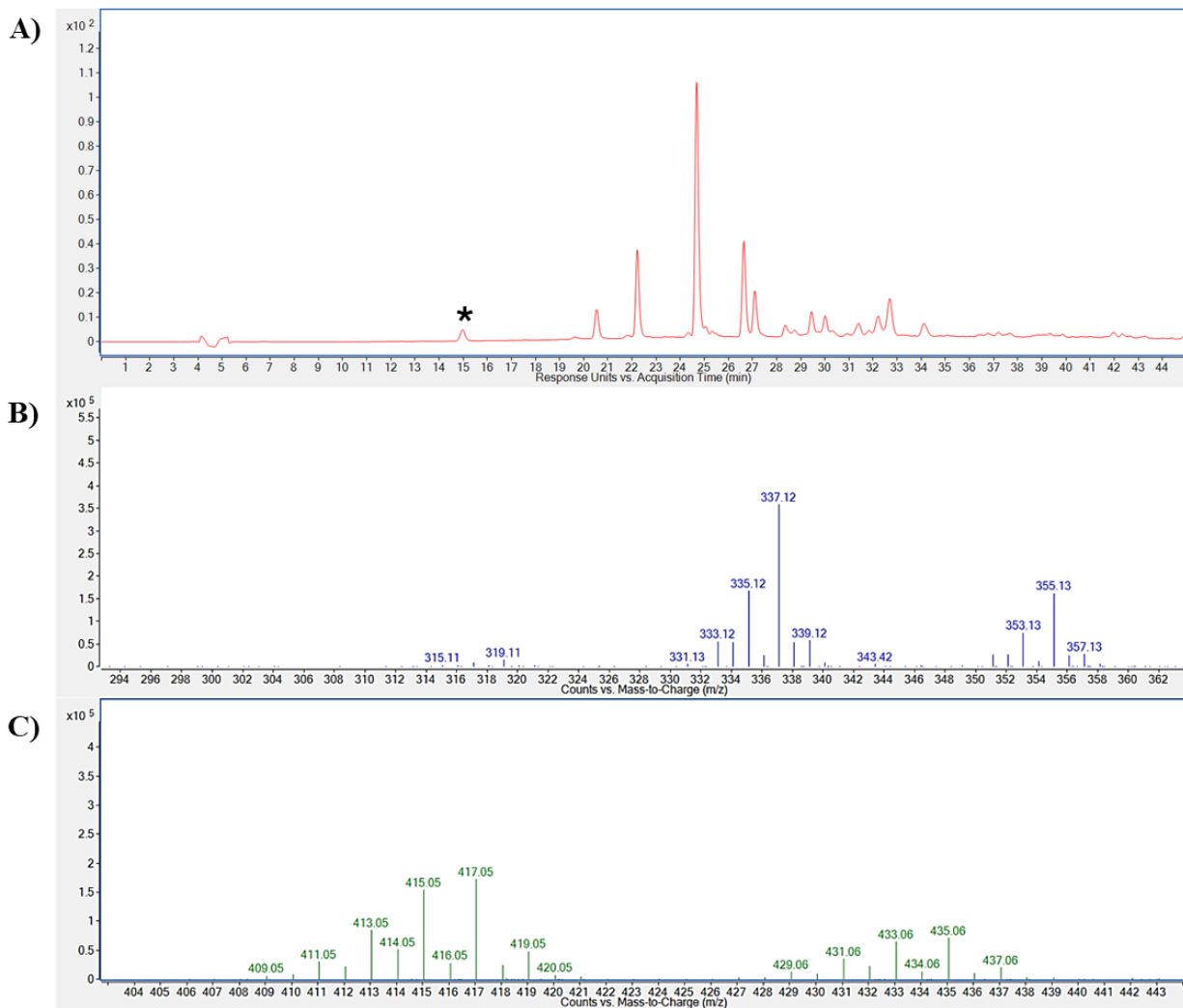


Figure S1. LC-UV-MS analysis of the reaction mixture of Tyr in the presence of 1 molar eq. of SeCl₄ after 24 h. A) UV-detection profile (254 nm). Asterisk indicates residual Tyr. B) and C) Mass spectra of the compounds eluted at 22.4 and 24.8 min, respectively.

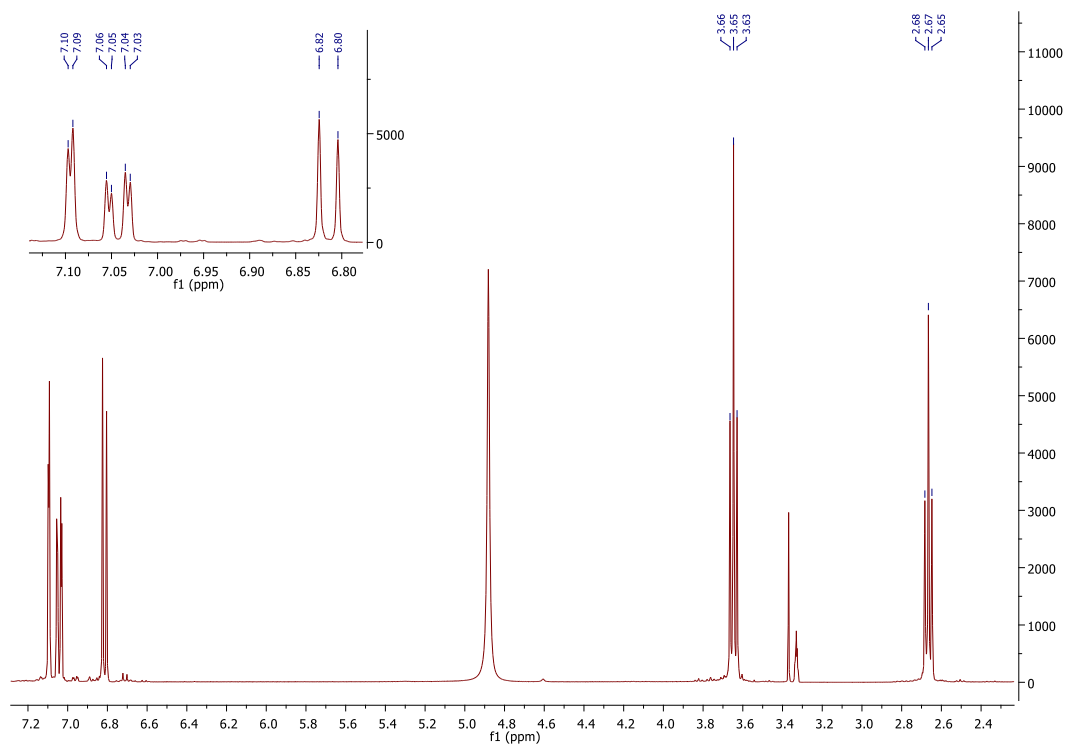


Figure S2. ^1H NMR spectrum of **1** in methanol- d_4 .

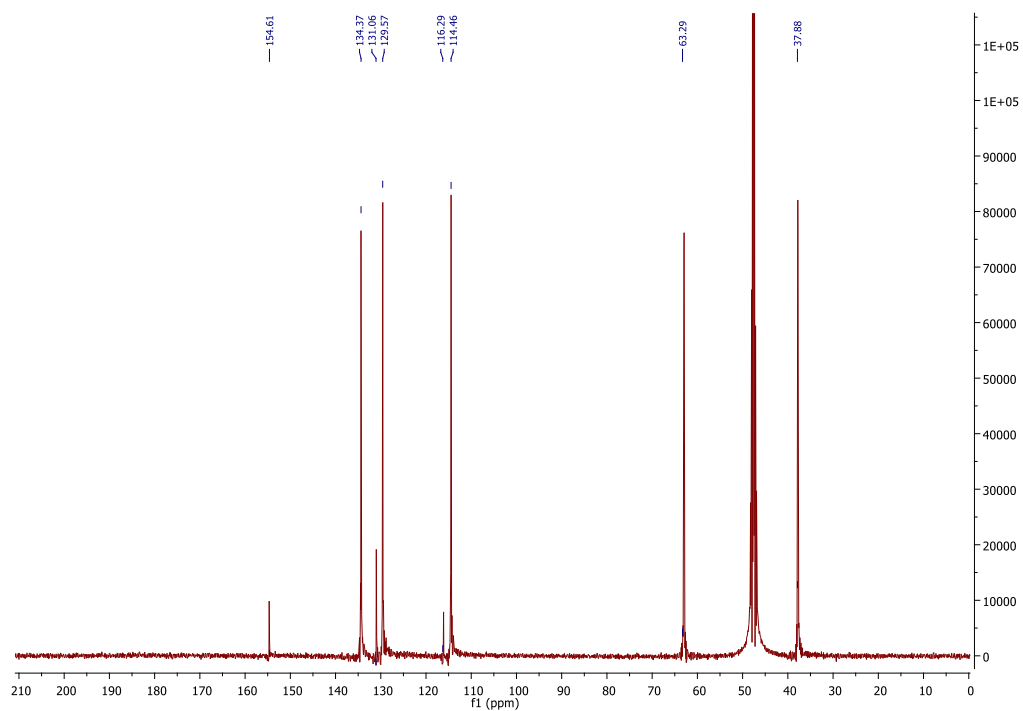


Figure S3. ^{13}C NMR spectrum of **1** in methanol- d_4 .

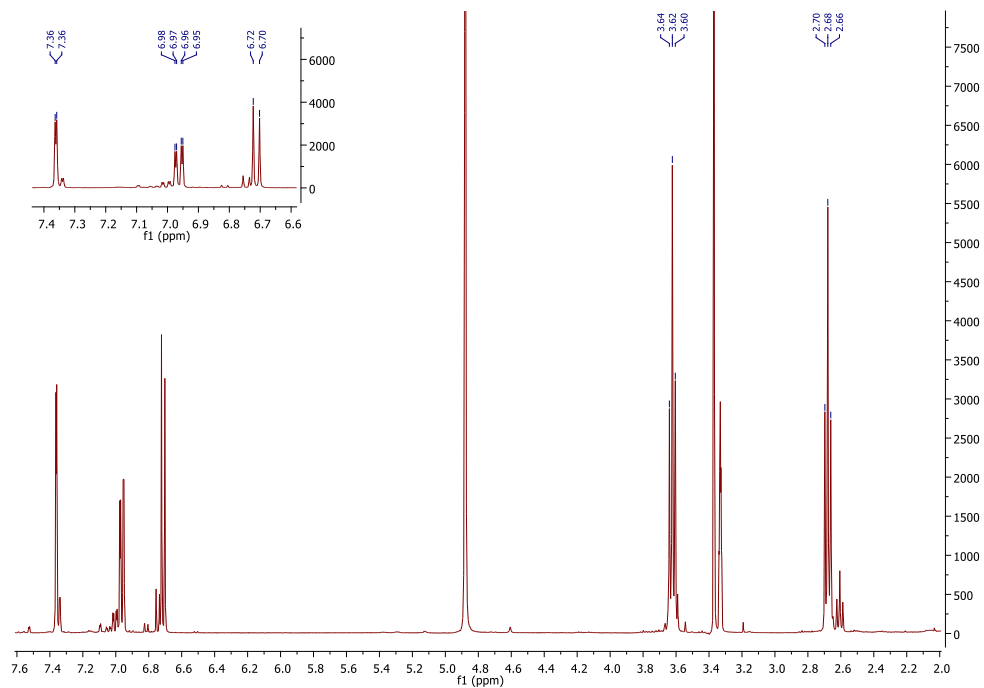


Figure S4. ^1H NMR spectrum of **2** in methanol- d_4 .

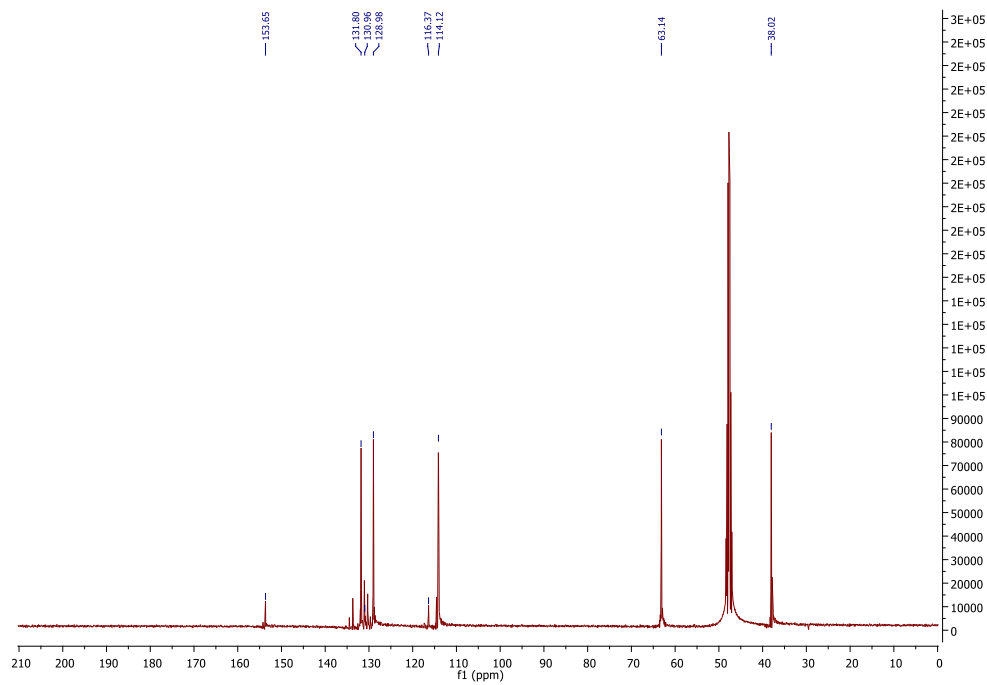


Figure S5. ^{13}C NMR spectrum of **2** in methanol- d_4 .

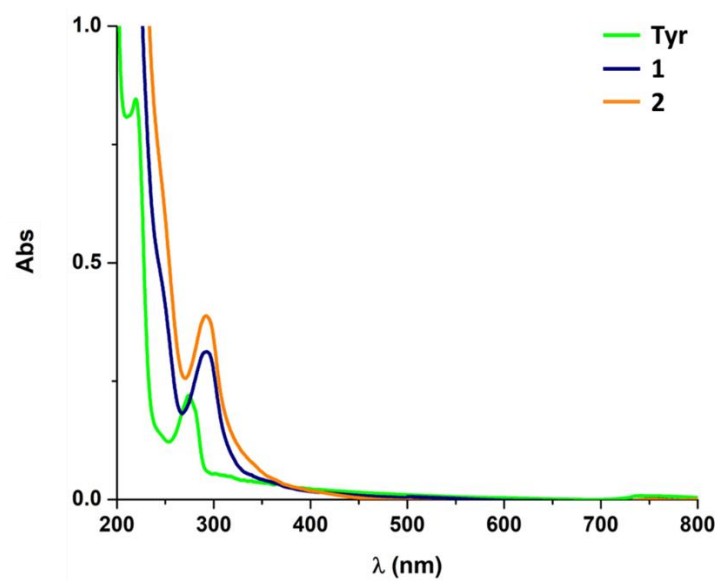


Figure S6. UV-Vis absorption spectra of Tyr (100 μM), **1** and **2** (50 μM) in methanol.

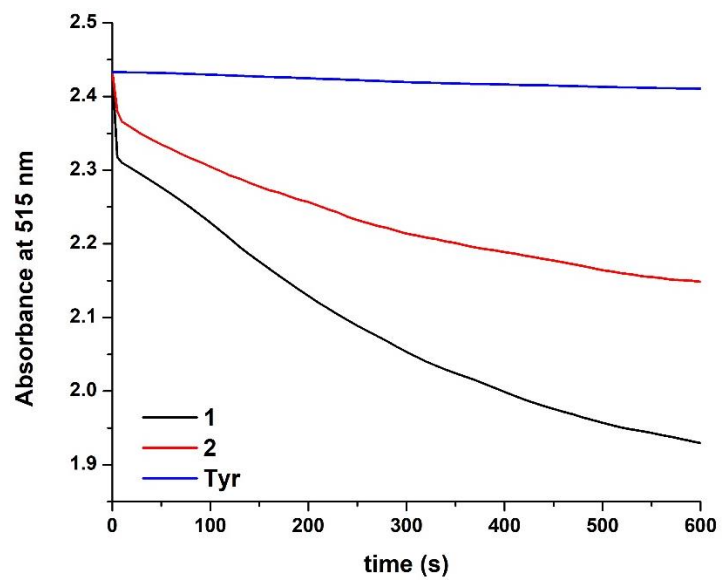
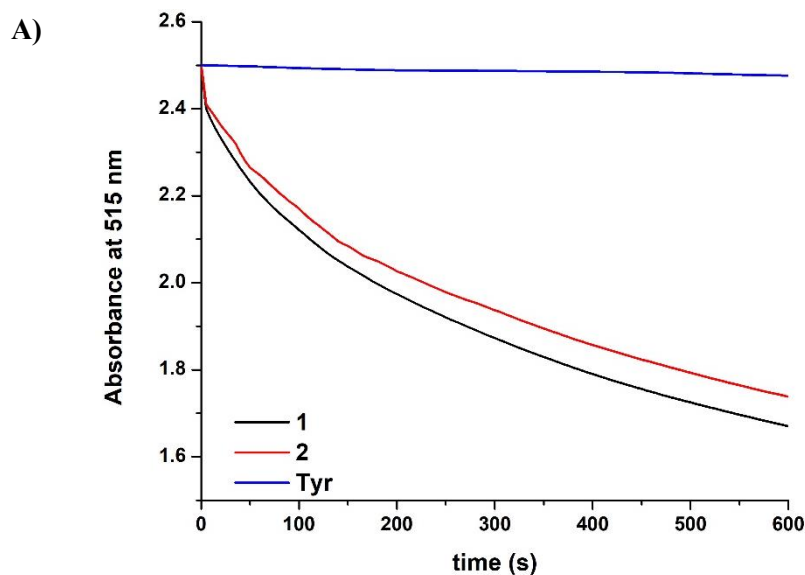


Figure S7. Decrease in the absorbance at 515 nm of a 200 μM DPPH solution in methanol in the presence of 50 μM **1** or **2** or 2.2 mM Tyr.



B)

DPPH assay				
Compound	DPPH reduced (%) ^{a,b}	$K^{a,c}$ ($M^{-1}s^{-1}$)	$n^{a,d}$	$n_{tot}^{a,e}$
1	33.2 ± 0.1	339 ± 2	0.22 ± 0.02	1.48 ± 0.02
2	30.5 ± 0.2	332 ± 4	0.19 ± 0.03	1.35 ± 0.05
Tyr	1.0 ± 0.2	0.5 ± 0.1	< 0.01	0.04 ± 0.01

^a1 and 2 50 μ M, Tyr 2.2 mM. ^bCalculated after 10 min of reaction. ^cRate constant for the fast step. ^dNumber of H atoms transferred in the fast step. ^eNumber of H-atoms transferred after 10 min.

Figure S8. A) Decrease in the absorbance (515 nm) of a 200 μ M DPPH solution in acetonitrile in the presence of 50 μ M 1 or 2 or 2.2 mM Tyr. B) Results from the DPPH assays run on Tyr and on its selenoderivatives 1 and 2 in acetonitrile. Values are means \pm SD ($n = 3$).

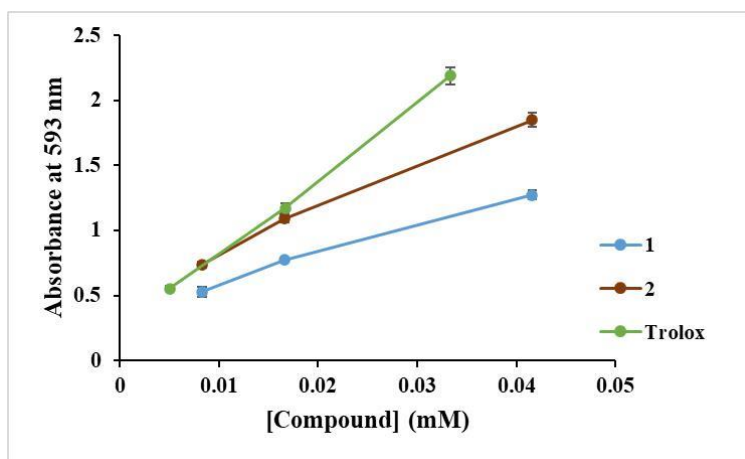


Figure S9. Reduction of Fe^{3+} by the selenoderivatives **1** and **2** and Trolox. Data for Tyr are not reported since a very different range of concentrations was tested due to its lower activity. Reported are the values \pm SD ($n = 3$).

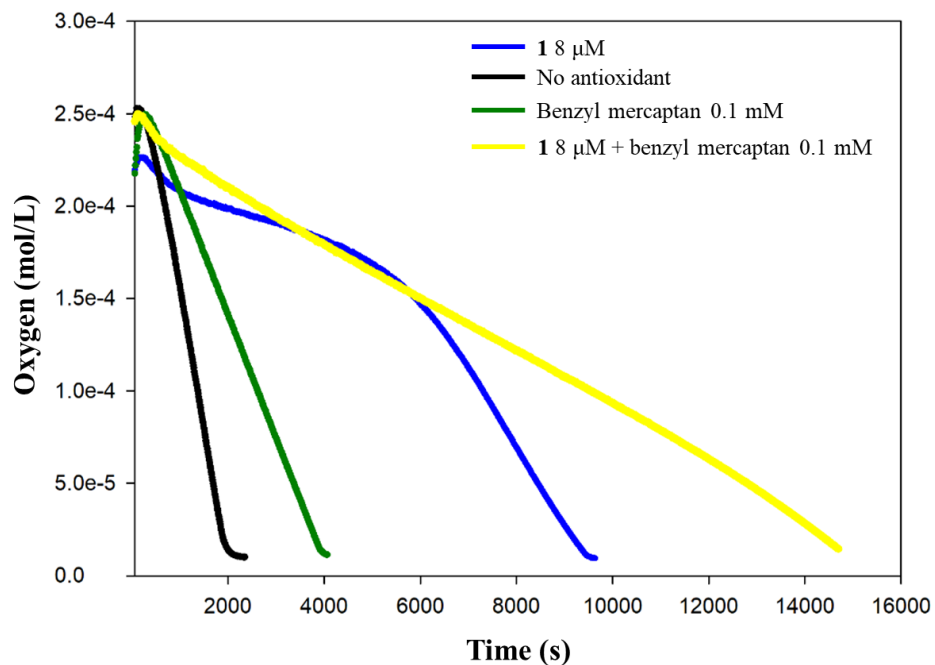


Figure S10. Oxygen consumption plots recorded during the autoxidation of aqueous micelles of 2.74 mM MeLin and 8 mM Triton X-100 initiated by 2.5 mM AAPH at 37°C (pH 7.4) and inhibited by compound **1** alone or in combination as reported in the legend.

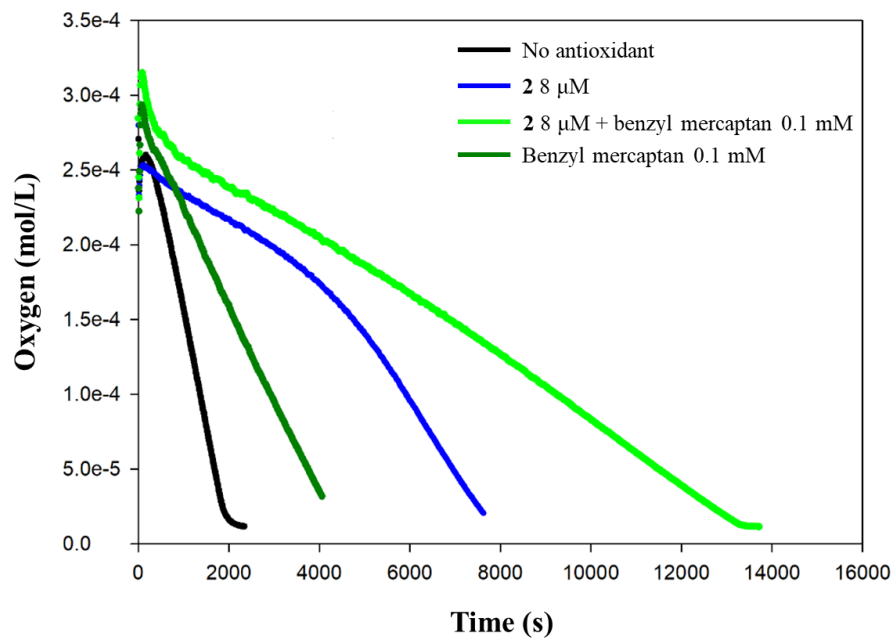


Figure S11. Oxygen consumption plots recorded during the autoxidation of aqueous micelles of 2.74 mM MeLin and 8 mM Triton X-100 initiated by 2.5 mM AAPH at 37°C (pH 7.4) and inhibited by compound **2** alone or in combination as reported in the legend.

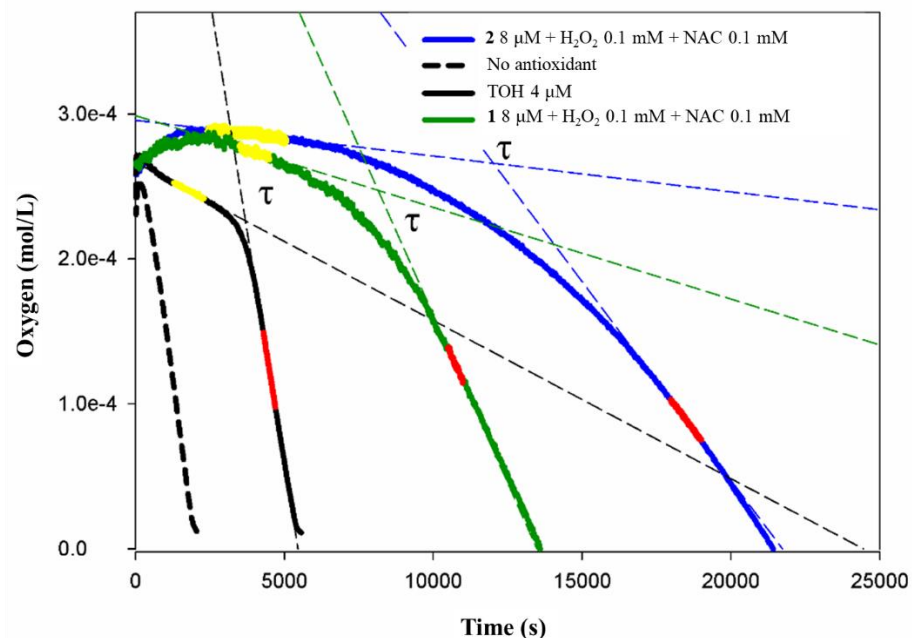


Figure S12. Oxygen consumption plots recorded during the autoxidation of aqueous micelles of 2.74 mM MeLin and 8 mM Triton X-100 initiated by 2.5 mM AAPH at 37°C (pH 7.4) and inhibited compound **1** or **2** in combination with NAC and H₂O₂ as reported in the legend. Inhibition by TOH is reported for comparison. Regression lines and endpoint of the nominal inhibited period τ are reported.

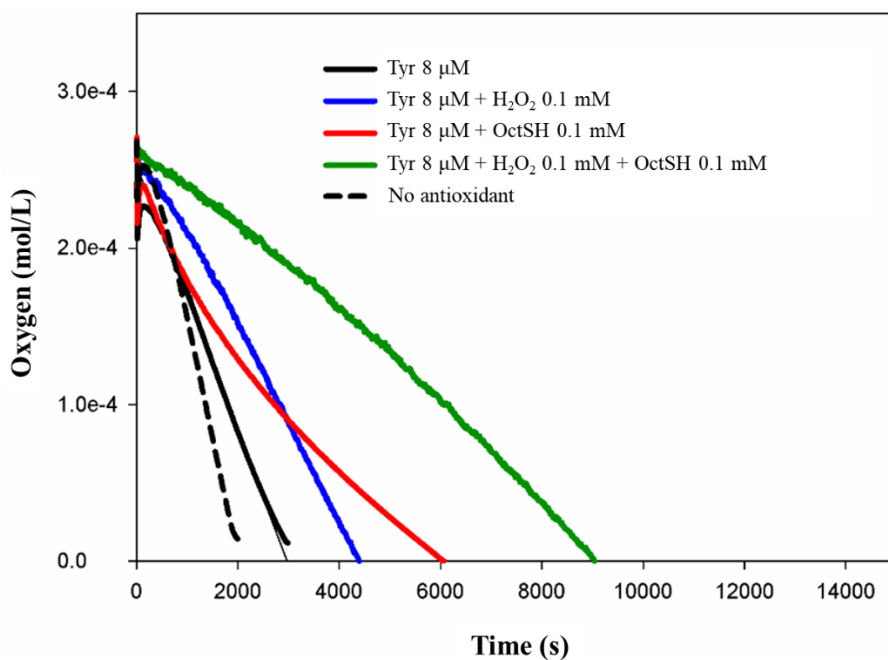


Figure S13. Oxygen consumption plots recorded during the autoxidation of aqueous micelles of 2.74 mM MeLin and 8 mM Triton X-100 initiated by 2.5 mM AAPH at 37°C (pH 7.4) and inhibited by Tyr alone or in combination as reported in the legend.

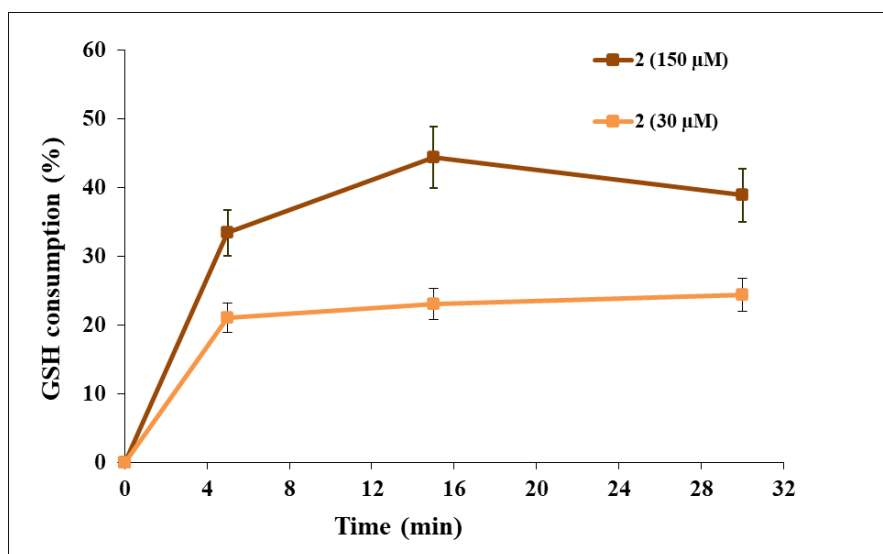


Figure S14. GSH consumption over time (percentage with respect to control run in the absence of **2**) in the presence of different concentrations of **2**. Mean \pm SD values from three separate experiments are reported.

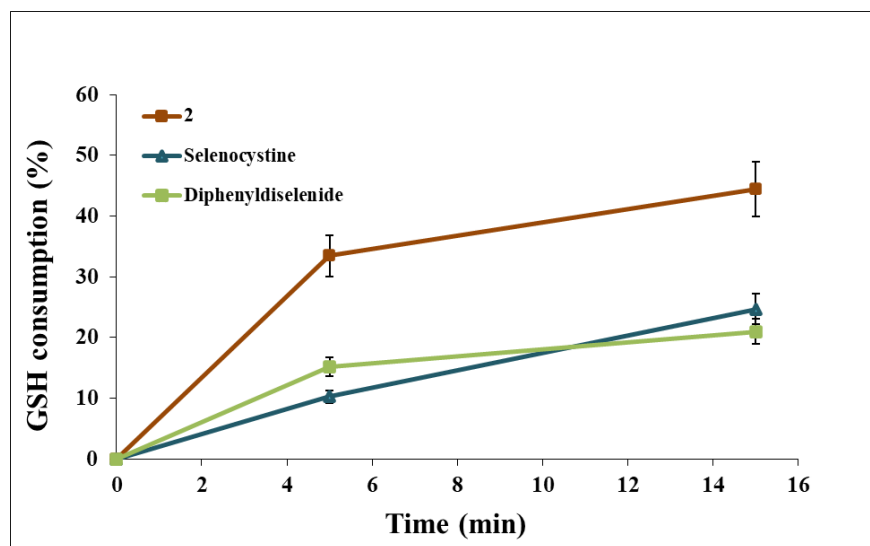


Figure S15. GSH consumption over time (percentage with respect to control run in the absence of **2**) in the presence of 150 μM **2**, selenocystine or diphenyldiselenide. Mean \pm SD values from three separate experiments are reported.

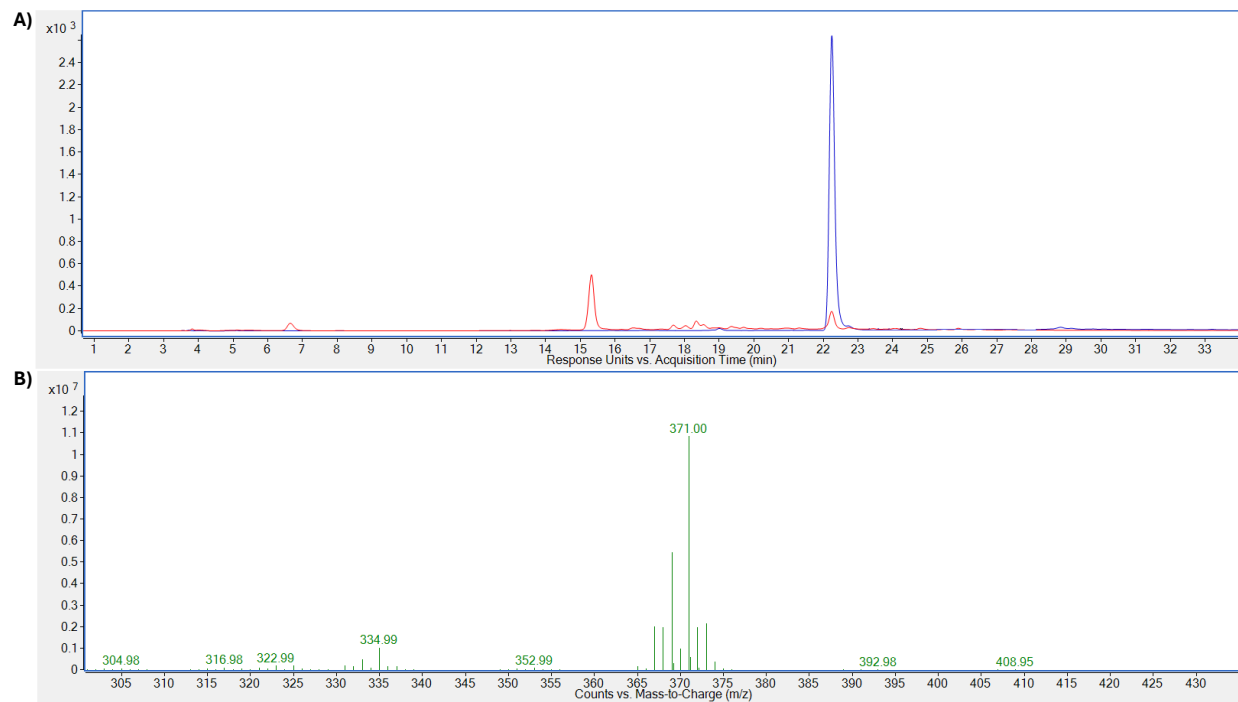


Figure S16. A) LC-UV-MS profile (UV detection at 254 nm) of the reaction mixture of **1** with H_2O_2 (blue trace: time zero; red trace: 1 h); B) Mass spectrum of the product eluted at 15 min.

Conformational analysis

The search of the preferred conformations of the selenoderivatives of Tyr was performed at the M052X/6-311++G(d,p) level of theory by keeping in mind the known conformational preferences of *ortho*-alkylseleno phenols reported in Fig. S17A already discussed in previous works and recently reviewed in Alfieri et al. *Biomolecules* **2022**, *12*, 90, <https://doi.org/10.3390/biom12010090>. The CH₂CH₂OH chains were set in an extended conformation.

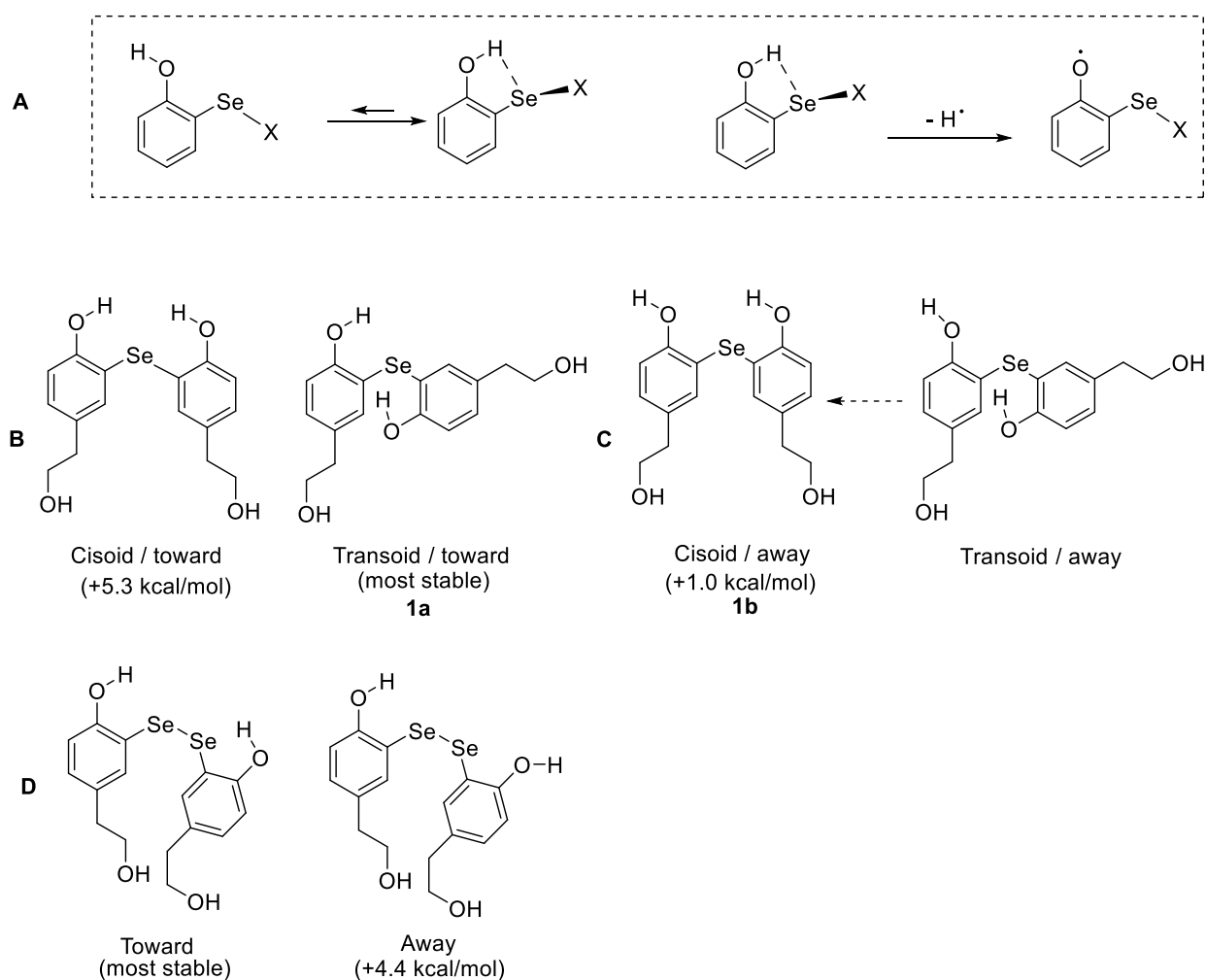


Figure S17. Conformational analysis.

The conformational search started from the limit structures reported in Fig. S17B, which were built considering a cisoid or transoid relative arrangement of the aromatic rings, and a “toward” or “away” conformation of one of the OH groups. The conformation with two “away” OH groups was high in energy and was not considered further. Two toward conformers were found, with a relatively high energy difference (see Fig. S17B). Instead, only one “away” conformer was found (see Fig- S17C) as both structures converged to **1b** during optimization.

A similar approach was used in case of the diselenoderivative **2**, however in this case we found only one transoid/toward conformation, whereas the away ones were much higher in energy and were not considered further (Fig. S17D). This is because the Se-Se-R substituent can better accept two H-bonds from the OH groups at the same time, whereas the Se-R substituent is somewhat a less good acceptor for the second H-bond, this providing some convenience for the away conformation.

The search of the transition states (TS) was done by starting from the most stable conformation of the parent phenols, and by stepwise increasing the O–H bond length of the hydroxyl group in H-bond contact with the CH₃OO• (MeOO•) until an energy maximum was reached. This structure (and the relative frequency) served as a starting geometry for subsequent optimization to the TS. In this way we ensured that the TS is relative to a specific conformer, and at the same time we could keep trace of the geometrical changes occurring during the optimization steps. The conformation of the phenoxyl radicals (**1-H•** and **2-H•**) was obtained by relaxing the geometry of the radical found in the TS.

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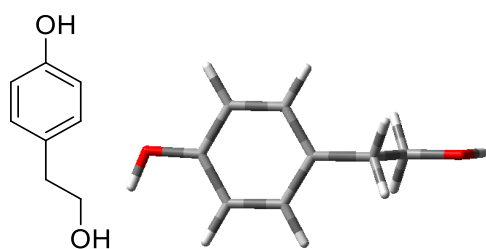
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ROOH

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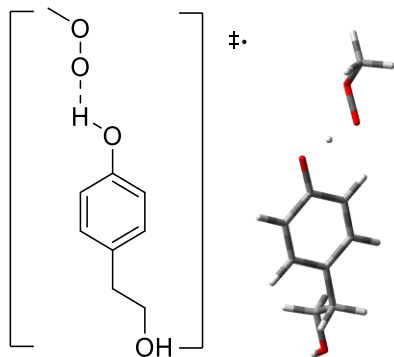
Tyrosol transition state



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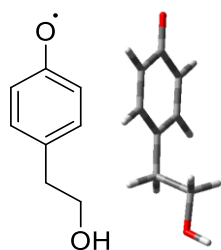
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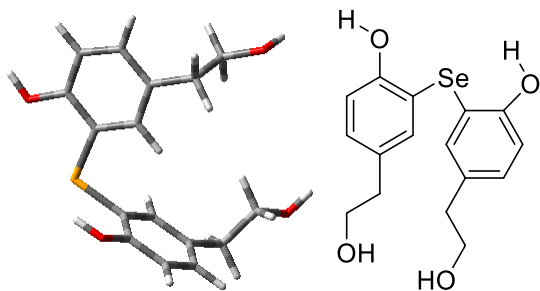
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1st transition state of single selenium



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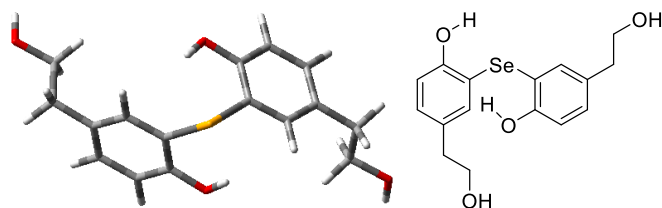
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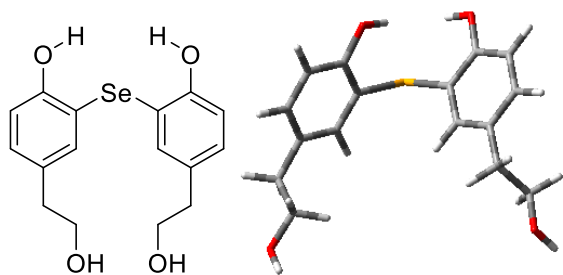
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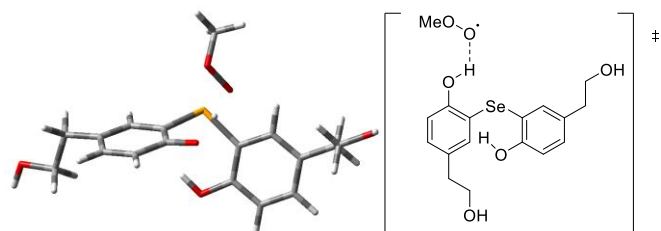
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H -3.09209700 3.16608000 -1.29327100
H -4.57866000 2.97895400 -0.33416800
H -4.01312600 5.23469700 -0.65729300
H 0.02703900 -2.94887400 0.89845200
H -1.91206600 -3.28824600 -0.62665500

```



Sum of electronic and thermal Enthalpies= -3512.883370

Sum of electronic and thermal Free Energies= -3512.965633

```

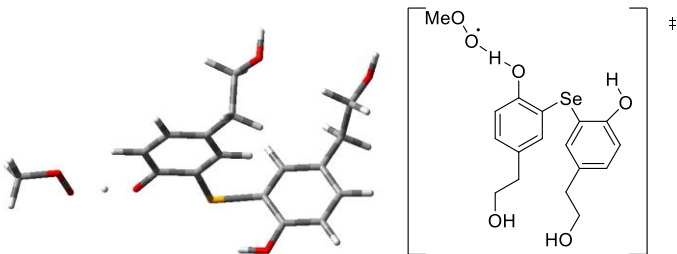
0 2
C -2.79090700 0.23064100 -0.52062200
C -1.45452700 0.31887800 -0.08689100
C -1.13996600 0.62778100 1.28237700

```

```

C -2.24516700 0.72440600 2.17967300
C -3.54427700 0.59556400 1.73551800
C -3.85159800 0.36241100 0.36959000
Se -0.08781200 0.22418500 -1.40646700
C 1.23707900 -0.93343900 -0.61900100
C 2.57492300 -0.53403300 -0.71116500
C 3.61260800 -1.35599500 -0.26364500
C 3.26795000 -2.60531300 0.27630400
C 1.94152400 -3.01706400 0.36913700
C 0.90714900 -2.18949900 -0.08023800
O -0.36264900 -2.66662500 0.03718400
C 5.04757200 -0.87872600 -0.30377400
C 5.40109700 -0.02684100 0.91787700
O 6.76624900 0.37814600 0.78524300
O 0.06930000 0.83200600 1.70114100
C -5.28437800 0.21132400 -0.08546400
C -5.82375100 -1.20520900 0.13381000
O -7.17822300 -1.22515500 -0.31894000
O 1.37389300 2.19370300 0.20059200
O 0.64979700 3.39785300 0.28136800
C 0.89847700 4.12991400 -0.91245200
H 4.05223000 -3.26836200 0.63278200
H -2.99629400 0.03198800 -1.57008500
H -2.01948300 0.93285800 3.22044400
H -4.36075400 0.69657500 2.44718100
H -5.37606500 0.45162300 -1.15027100
H -5.93150100 0.91038800 0.45736000
H -5.21184600 -1.92643600 -0.42784500
H -5.76343800 -1.46834200 1.20013200
H -7.54609200 -2.10764400 -0.18502200
H 0.78699800 1.51129100 0.95482100
H -1.00393800 -1.98033900 -0.20367600
H 2.80229700 0.44719500 -1.11717000
H 1.68077700 -3.98430600 0.78655700
H 5.73359600 -1.73217200 -0.34313800
H 5.22970600 -0.27992700 -1.20348000
H 4.73585900 0.84687000 0.96605600
H 5.25515500 -0.61388800 1.83653900
H 7.00599800 0.93161300 1.53895500
H 0.36255500 5.07367600 -0.78428600
H 1.97089700 4.31448300 -1.03496600
H 0.50915300 3.58234900 -1.77992300

```



Sum of electronic and thermal Enthalpies= -3512.883486
Sum of electronic and thermal Free Energies= -3512.965028

```

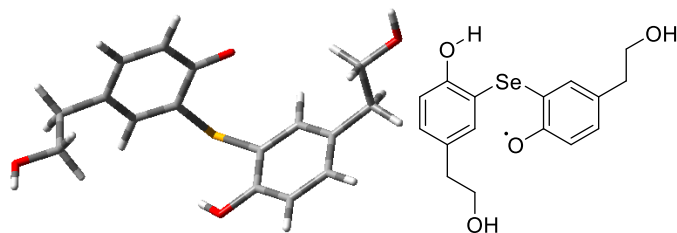
0 2
C -0.34870500 0.93178800 0.57188300
C -1.04472000 -0.19100000 0.13900500
C -2.45436700 -0.12292100 -0.09478100
C -3.11931300 1.11124500 0.14242900
C -2.40461800 2.21056800 0.58285700
C -1.00958600 2.14591400 0.80653900
Se -0.26680800 -1.90598900 -0.21222700
C 1.56086200 -1.56403200 0.29420800
C 1.96216600 -1.78789400 1.62299800
C 3.31142700 -1.62561800 1.96274500
C 4.23704400 -1.26195500 0.98916300
C 3.85967500 -1.04883000 -0.34829100
C 2.50880900 -1.20715900 -0.67244300
O 1.10166000 -2.15445300 2.60875300
C 4.87400300 -0.64472100 -1.39642100
C 5.09805800 0.86815100 -1.44427400
O 6.06968000 1.13108700 -2.45846100
O -3.05739700 -1.20677500 -0.51181900

```

```

C -0.24505600 3.36720700 1.25858200
C 0.09043100 4.31076900 0.09864300
O 0.80270300 5.42297500 0.64286900
O -5.39944400 -1.38480900 -0.95587100
O -6.02405000 -0.16509900 -0.71071100
C -7.42121400 -0.32566400 -0.95523000
H -2.92736700 3.14521300 0.77034100
H 2.18074700 -1.06085500 -1.69806900
H 3.61534200 -1.80222600 2.98941800
H 5.28213800 -1.15725200 1.27088500
H 4.54893600 -0.97527400 -2.38908000
H 5.83823600 -1.12749100 -1.20028200
H 4.14913300 1.37745200 -1.66977200
H 5.44896000 1.22514500 -0.46465600
H 6.24493000 2.07971400 -2.49400700
H 0.22112300 -2.29970600 2.21595700
H 0.72098600 0.86610500 0.74552300
H -4.18961200 1.16495700 -0.02454100
H -0.82912900 3.93126900 1.99536500
H 0.69106300 3.07431800 1.74540300
H 0.70029100 3.78118900 -0.64787000
H -0.83571100 4.64228700 -0.39314300
H 1.01036800 6.04545000 -0.06523200
H -4.19017500 -1.19787500 -0.70292000
H -7.86324500 0.65258800 -0.75148900
H -7.58687400 -0.61564800 -1.99763900
H -7.83327500 -1.08422700 -0.28223900

```



Sum of electronic and thermal Enthalpies= -3322.077489
Sum of electronic and thermal Free Energies= -3322.155032

```

0 2
C -2.50106900 0.03789500 -0.72880200
C -1.16842300 0.28012900 -0.94026800
C -0.59159200 1.58357300 -0.61444400
C -1.48715300 2.54526200 0.00200900
C -2.80765200 2.26436000 0.20542300
C -3.34545200 1.01277800 -0.16108400
Se -0.05802100 -1.05954200 -1.74424200
C 1.27446200 -1.17134500 -0.35653700
C 2.47481800 -0.48240900 -0.47875700
C 3.44225400 -0.55141200 0.51593000
C 3.17674400 -1.33904200 1.63686000
C 1.98964900 -2.04078100 1.76598500
C 1.02321100 -1.96231200 0.76725900
O -0.12808900 -2.65715500 0.93835700
O 0.58397400 1.87484000 -0.86511300
C -4.77675000 0.68364300 0.13225100
C -4.90763900 0.03929100 1.50965000
O -6.28520900 -0.23672500 1.70578000
H 3.91788800 -1.40544500 2.42381200
H -2.91976600 -0.92758900 -0.98641700
H -1.05412400 3.50013000 0.26493600
H -3.46186000 3.00377800 0.64997400
H -5.17323900 -0.01057400 -0.60900100
H -5.39007800 1.58463200 0.11524200
H -4.31232200 -0.87754300 1.54432100
H -4.53063100 0.72555900 2.27339200
H -6.40518400 -0.66224600 2.55551600
H -0.65280200 -2.56817000 0.13137400
H 2.63139000 0.13875900 -1.35003300
H 1.78811700 -2.65768100 2.63026300

```

```

C 4.69589300 0.27601000 0.41033400
H 5.47465700 -0.11955900 1.06293000
H 5.08162900 0.26446400 -0.60973600
C 4.41331200 1.71871200 0.80036900
H 3.63669800 2.12801600 0.14807100
H 4.04938400 1.75312000 1.83181200
O 5.62981700 2.44624400 0.66854000
H 5.46134000 3.37102600 0.85019000

```

Delta G:

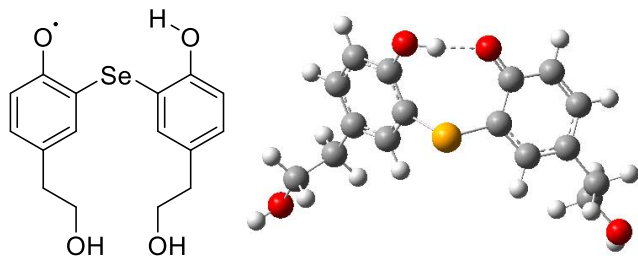
Phase 1: = -3512.965633-(-3322.792675-190.216370) = 0.043412*627.509474= 27.24 kcal/mol

Phase 2: = (-3322.155032-190.845075)+ 3512.965633= -0.034474*627.509474= -21.63 kcal/mol

Delta H:

Phase 1: = -3512.883370 +(3322.715477+190.186372)= 0.018479*627.509474=11.59 kcal/mol

Phase 2: =(-3322.077200-190.815049)+3512.883370 = -0.008878*627.509474= -5.57 kcal/mol



Sum of electronic and thermal Enthalpies= -3322.080710

Sum of electronic and thermal Free Energies= -3322.151398

```

0 2
C 2.48836900 0.13222400 -0.71329200
C 1.52248900 -0.81968600 -0.41909000
C 1.74031100 -1.76045700 0.68047100
C 2.94250600 -1.57497100 1.47359700
C 3.86453200 -0.61016500 1.15634700
C 3.66487100 0.26199400 0.05007900
Se -0.01358300 -0.97472400 -1.55262100
C -1.48299900 -0.78609400 -0.30154400
C -2.01638100 0.49678300 -0.11725800
C -3.17155900 0.70935800 0.64017000
C -3.78928200 -0.41582500 1.21211800
C -3.26124500 -1.69260300 1.05575500
C -2.09396700 -1.90059200 0.30367700
C -3.75888400 2.09503200 0.79967300
C -4.83937300 2.39695900 -0.24059600
O -5.31613600 3.72364100 -0.00052700
O -1.62063400 -3.16296500 0.20186800
O 0.96353100 -2.71935700 0.92338700
C 4.66385300 1.34668400 -0.25808100
C 4.39758500 2.62917700 0.54288600
O 5.40805100 3.56746600 0.18028700
H 3.08524900 -2.25572000 2.30670900
H 2.32461500 0.81470200 -1.54310800
H 4.76936000 -0.50759300 1.75034700
H -1.52164600 1.34203300 -0.58784700
H -3.72478100 -2.55450200 1.52485500
H -4.68879300 -0.28521100 1.80954400
H -0.63743300 -3.13266900 0.20226600
H 4.64004500 1.59919400 -1.32339700
H 5.67892800 1.00625300 -0.02430000
H 3.39602300 3.01529300 0.30437000
H 4.43053900 2.41153500 1.62042500
H 5.26403500 4.39380200 0.65856900

```

```

H -2.97527700 2.85571100 0.71048400
H -4.20155400 2.20993100 1.79599400
H -4.41671300 2.31066500 -1.25247700
H -5.65693700 1.66647700 -0.15195900
H -6.00727900 3.93352500 -0.64093200

```

Delta G:

Phase 1: = -3512.965028-(-3322.791095-190.216370) = 0.042437*627.509474= 26.62 kcal/mol

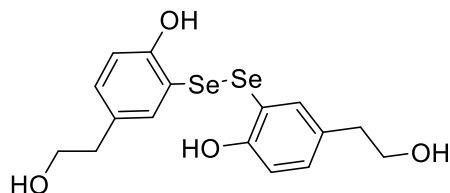
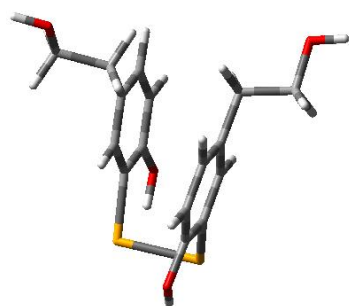
Phase 2: = (-3322.151398-190.845075)+ 3512.965028= -0.031445*627.509474= -19.73 kcal/mol

Delta H:

Phase 1: = -3512.883486+(3322.713094+190.186372)= 0.01598*627.509474=10.02 kcal/mol

Phase 2: =(-3322.080710-190.815049)+ 3512.883486= -0.012272*627.509474= -7.70 kcal/mol

Two selenium:



Sum of electronic and thermal Enthalpies= -5724.204751

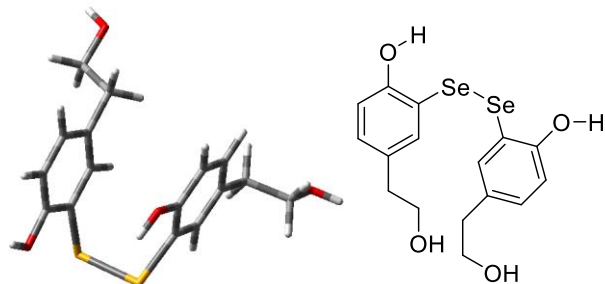
Sum of electronic and thermal Free Energies= -5724.285217

```

0 1
C -0.31874700 1.49110400 -0.48615200
C 0.83721700 1.65128100 0.27596900
C 0.75563600 2.13522500 1.58698500
C -0.49347700 2.45955000 2.10801500
C -1.63252800 2.29651000 1.33514800
C -1.56937900 1.80949000 0.02896100
Se 2.52069200 1.10756500 -0.45057200
Se 2.52102400 -1.10664500 0.45062800
C 0.83783200 -1.65102900 -0.27600400
C -0.31825800 -1.49101400 0.48595000
C -1.56872600 -1.81001900 -0.02918700
C -1.63154600 -2.29759800 -1.33517400
C -0.49235400 -2.46047100 -2.10788600
C 0.75657300 -2.13542700 -1.58687800
O 1.83643800 -2.28761100 -2.38259400
O 1.83533900 2.28747700 2.38289200
H -2.59673800 -2.54334200 -1.76128300
H -2.59786200 2.54170700 1.76125600
H -0.23293800 1.07953900 -1.48465800
H 2.62269700 2.02251500 1.88894200
H -0.23272300 -1.07902300 1.48430700
H -0.54609500 -2.82980700 -3.12219400
H -0.54746400 2.82850000 3.12245200
C -2.80802800 1.64537400 -0.81128700

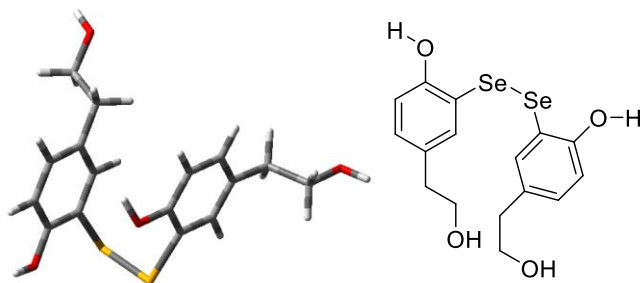
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H	-3.68143000	1.48953000	-0.17688100
H	-2.71087200	0.77321200	-1.45994000
C	-3.05113400	2.87042900	-1.67812100
H	-3.17089800	3.75213900	-1.04136700
H	-2.18931000	3.03235800	-2.33244600
C	-2.80746900	-1.64604600	0.81094400
H	-3.68087300	-1.49066600	0.17642500
H	-2.71064000	-0.77364700	1.45934500
C	-3.05029200	-2.87089900	1.67813900
H	-3.16992000	-3.75282700	1.04166700
H	-2.18839300	-3.03249000	2.33245600
O	-4.22733800	-2.62937000	2.43850400
H	-4.40509100	-3.38888500	2.99386900
O	-4.22814600	2.62889100	-2.43851000
H	-4.40570900	3.38826400	-2.99412800
H	2.62363800	-2.02221700	-1.88862700



Sum of electronic and thermal Enthalpies= -5724.196383
 Sum of electronic and thermal Free Energies= -5724.278264

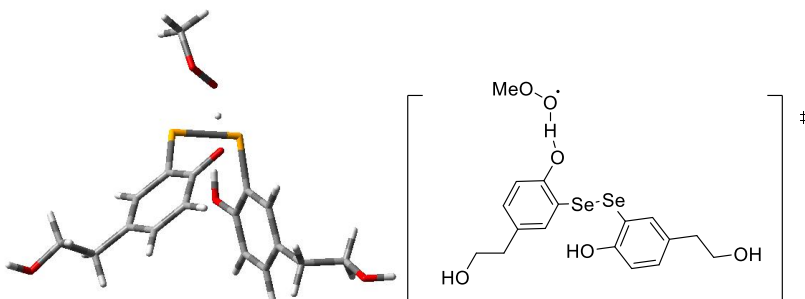
0	1		
C	-3.21409400	-0.26491000	0.19570300
C	-2.02184200	-0.16116400	-0.52695100
C	-1.30573200	1.03223300	-0.50912600
C	-1.74695400	2.13638600	0.21528800
C	-2.93985000	2.01712300	0.92073200
C	-3.66961400	0.83579100	0.91240200
Se	-1.30687800	-1.65037200	-1.49324500
Se	-0.06913300	-2.59250000	0.29559300
C	1.03450300	-1.06861300	0.66856500
C	0.66076900	-0.19715900	1.69721700
C	1.43558500	0.93810900	1.93612500
C	2.54714100	1.19686800	1.15570700
C	2.92850700	0.34095600	0.11709000
C	2.15840700	-0.79093200	-0.10847800
O	-0.42408000	-0.39059500	2.47807600
C	4.17108400	0.60878700	-0.69056000
C	5.39697000	0.01258800	-0.01658400
O	6.52354000	0.31947600	-0.82831500
C	-0.96156400	3.42059200	0.20341600
C	-1.29819200	4.25854200	-1.01973800
O	-0.51856600	5.44609400	-0.95252000
O	-3.87982300	-1.44832000	0.19003700
H	-0.37115300	1.08299300	-1.05493200
H	-4.59123800	0.76211000	1.47761700
H	-3.30352300	2.85764100	1.49858300
H	0.10833500	3.20788400	0.19683200
H	-1.17720700	4.00753000	1.09687900
H	-1.06843300	3.69090700	-1.92636000
H	-2.36704000	4.49286800	-1.02128600
H	-0.69824900	5.98466400	-1.72356900
H	-4.66703900	-1.37677800	0.73394700
H	3.13112200	2.08948500	1.34567600
H	2.41599100	-1.47077200	-0.91112500
H	-0.91274200	-1.15434000	2.14007400
H	1.13053900	1.60910400	2.72698100
H	4.32853200	1.68178500	-0.80672700
H	4.08068900	0.17884400	-1.68839500
H	5.26872900	-1.06935700	0.08263500
H	5.50885600	0.43969000	0.98464100
H	7.30890500	-0.06105000	-0.43437500



Sum of electronic and thermal Enthalpies= -5724.188845
 Sum of electronic and thermal Free Energies= -5724.270232

```

0 1
C -3.07514000 -0.72496900 0.26991900
C -1.97428200 -0.41337800 -0.53444200
C -1.48212500 0.88600600 -0.55352800
C -2.05543800 1.89827700 0.21672900
C -3.15053900 1.56957800 1.01095600
C -3.66103300 0.27614500 1.03651100
Se -1.03080900 -1.77246200 -1.50181100
Se 0.24551400 -2.54642000 0.33009300
C 1.17070200 -0.89733400 0.66117800
C 0.64570500 0.02650700 1.56776200
C 1.27375200 1.26187400 1.72003900
C 2.40231700 1.57024200 0.97806200
C 2.94600600 0.65543400 0.07576600
C 2.31417600 -0.57465500 -0.06570700
O -0.46132500 -0.29780500 2.28702300
C 4.20824600 0.96811000 -0.68365600
C 5.43440400 0.50946300 0.09019400
O 6.57950900 0.84863400 -0.68170500
C -1.51977600 3.30426800 0.15176100
C -2.10234500 4.05939100 -1.03259900
O -1.55162300 5.37018000 -1.01387300
O -3.52349400 -2.00223600 0.28892000
H -0.60766700 1.09852900 -1.15708500
H -4.51337900 0.04106000 1.66297000
H -3.61793500 2.33488700 1.61900000
H -0.43315200 3.29161400 0.05397800
H -1.76565000 3.85148000 1.06306400
H -1.84476000 3.53924800 -1.95977000
H -3.19255500 4.09216600 -0.94621600
H -1.88363700 5.86256800 -1.76504100
H -4.21021800 -2.09493900 0.95237400
H 2.87050500 2.53932100 1.10092900
H 2.69468400 -1.29809600 -0.77608900
H -0.95575000 0.50106500 2.49191300
H 0.86403500 1.98014600 2.42008300
H 4.29271500 2.04064700 -0.86177500
H 4.20536300 0.47131400 -1.65422000
H 5.37907800 -0.57064400 0.25494300
H 5.45923500 1.00604300 1.06495200
H 7.36680100 0.55565100 -0.22220800
  
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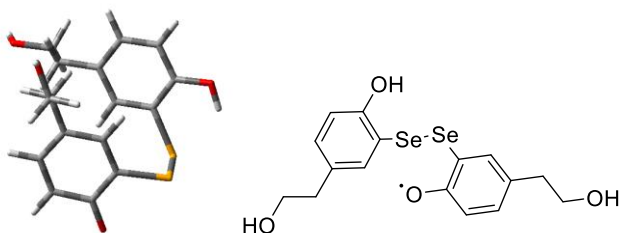
Sum of electronic and thermal Enthalpies= -5914.365165
 Sum of electronic and thermal Free Energies= -5914.451955

0 2

```

C -2.15204400 1.05840800 0.52002100
C -1.39056300 0.01730100 -0.05336900
C -0.87750100 0.12979100 -1.39393300
C -1.09706400 1.37935800 -2.05003800
C -1.81725900 2.38915000 -1.45184300
C -2.37934400 2.24817200 -0.15440000
Se -1.30572100 -1.59509800 0.88067100
Se 1.08001900 -2.10795400 0.92134600
C 1.80561600 -0.35389300 1.01737000
C 2.36016900 0.22741400 -0.13242500
C 3.01562300 1.45893000 -0.07980700
C 3.10134900 2.10068400 1.16861100
C 2.57182500 1.53489700 2.32501300
C 1.92746500 0.29496600 2.26260200
O 1.43975800 -0.22761200 3.41671000
O -0.25946900 -0.82491700 -2.00880400
H 3.59535200 3.06710700 1.23614800
H -1.96411100 3.32421000 -1.98836100
H -2.53808200 0.93285300 1.52829400
H -0.54748800 -2.03939600 -1.72663000
H 2.24232700 -0.28881800 -1.08057500
H 2.65157900 2.03463100 3.28477900
H -0.68466600 1.49191600 -3.04758800
C -3.18949900 3.36550400 0.46058000
H -2.70802200 4.33321600 0.27347600
H -3.24507300 3.24335900 1.54748000
C -4.61541700 3.43586600 -0.09176500
H -4.58852500 3.56495500 -1.18385900
H -5.14579500 2.49695600 0.12501000
C 3.63281600 2.06866900 -1.31926200
H 3.61275200 3.16259900 -1.25569400
H 3.05825700 1.78859500 -2.20862500
C 5.08403100 1.62825100 -1.52313200
H 5.68443300 1.90056500 -0.64211800
H 5.12792700 0.53518300 -1.63789800
O 5.57669700 2.28398800 -2.69334600
H 6.48084900 1.99262500 -2.86477100
O -5.26513800 4.54461400 0.53339800
H -6.17157700 4.60793600 0.20745700
H 1.10856100 -1.12578500 3.22993100
O -0.84622700 -3.10250300 -1.44591100
O -1.97104400 -3.32581100 -2.26969300
C -2.56546300 -4.54536200 -1.84657700
H -2.92517500 -4.45664700 -0.81404100
H -3.40443500 -4.70195400 -2.52929600
H -1.85028400 -5.37104900 -1.92641400

```



Sum of electronic and thermal Enthalpies= -5723.562454
Sum of electronic and thermal Free Energies= -5723.644438

```

0 2
C -0.45180000 1.45340100 -0.49328400
C 0.71445500 1.67306200 0.23812800
C 0.63751800 2.15556300 1.54984100
C -0.61432300 2.41177300 2.10313800
C -1.76283100 2.18744200 1.36032400
C -1.70556900 1.70571700 0.05158900
Se 2.40452500 1.20804600 -0.53448300
Se 2.61279800 -0.93210600 0.47397300
C 0.99631000 -1.61941900 -0.27308300
C -0.16200500 -1.54085500 0.45216900
C -1.40496400 -1.94009100 -0.09173500
C -1.45119700 -2.43319600 -1.40925600

```

```

C -0.31342100 -2.52772700 -2.16396400
C 0.98336300 -2.12516200 -1.64623100
O 1.99863400 -2.20159300 -2.34386400
O 1.72589700 2.37002600 2.31691000
H -2.40654600 -2.72920100 -1.82414700
H -2.72875900 2.38260400 1.81048300
H -0.36859200 1.05527500 -1.49777900
H 2.51355700 2.14222900 1.80478700
H -0.13823000 -1.12145700 1.45095900
H -0.32668100 -2.89805900 -3.17943900
H -0.66188300 2.77934600 3.11844300
C -2.95445900 1.48540800 -0.76094400
H -3.79969700 1.25777000 -0.10987200
H -2.82259800 0.64038900 -1.43935500
C -3.29961500 2.71418200 -1.58724800
H -3.45901800 3.56883200 -0.92312700
H -2.46826800 2.94888000 -2.25848700
C -2.64082200 -1.83968600 0.74733800
H -3.53321000 -1.83276700 0.12176700
H -2.62328400 -0.91393400 1.32588400
C -2.73838600 -3.00916200 1.72167800
H -2.78281200 -3.94947700 1.16482000
H -1.85364600 -3.02787700 2.36444500
O -3.91850700 -2.81178700 2.48451000
H -4.01630200 -3.53177600 3.10861400
O -4.47866100 2.41391600 -2.32289900
H -4.72545200 3.17527300 -2.84867200

```

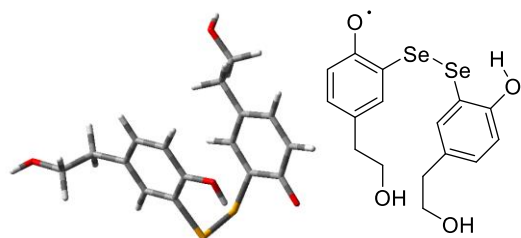
Phase 1: = -5914.451955-(-5724.285217-190.216370) = 0.049631*627.509474= 31.14 kcal/mol

Phase 2: = (-5723.644438-190.845075)+ 5914.451955= -0.037558*627.509474= -23.56 kcal/mol

Delta H:

Phase 1: = -5914.365165+(5724.204751+190.186372)= 0.025958*627.509474=16.28 kcal/mol

Phase 2: =(-5723.562454-190.815049)+ 5914.365165= -0.012337*627.509474= -7.74 kcal/mol



Sum of electronic and thermal Enthalpies= -5723.562198

Sum of electronic and thermal Free Energies= -5723.644444

```

0 2
C -0.56671900 -0.27798500 1.68053000
C -0.96072100 -1.12294300 0.63642400
C -2.09647900 -0.82211600 -0.11430700
C -2.85874200 0.30634600 0.15307900
C -2.45712900 1.13465300 1.20662100
C -1.33313800 0.85363800 1.96162100
Se 0.14333300 -2.62961200 0.20942800
Se 1.36929300 -1.60892000 -1.54788700
C 1.98912200 -0.12406600 -0.52127300
C 1.28105900 1.04731000 -0.54918900
C 1.66252600 2.16042700 0.23530600
C 2.80182100 2.06572500 1.05487400
C 3.53076900 0.90970200 1.11345600
C 3.16049300 -0.26595900 0.34485200
O 3.79523500 -1.32009200 0.44671700
H 3.08723900 2.92026500 1.65519800
H -3.03739000 2.02175400 1.43099800
H 0.38861200 1.11640400 -1.15976200

```

H 4.39944300 0.80915000 1.74875800
C 0.86351000 3.42425400 0.15837400
H 1.01819300 4.03193300 1.04978300
H -0.19992900 3.19080600 0.08583300
C 1.25818100 4.24812500 -1.06314100
H 2.31834200 4.51046200 -1.00328700
H 1.09687500 3.66036100 -1.97133300
O 0.44420100 5.41070200 -1.05665400
H 0.65566700 5.94957600 -1.81975100
H -2.36962600 -1.48052600 -0.92958100
O 0.53532100 -0.48969500 2.43158500
H 0.98444600 -1.28608500 2.11196800
H -1.01650400 1.49984300 2.76860800
C -4.11417800 0.59834300 -0.62570600
H -4.27206300 1.67433700 -0.70870900
H -4.04130600 0.19681600 -1.63670900
C -5.33032200 -0.01504300 0.05102600
H -5.20353100 -1.09974700 0.11597800
H -5.42462400 0.38242900 1.06617400
O -6.46784000 0.31911600 -0.73323200
H -7.24878500 -0.07041400 -0.33917300