

Electronic Supplementary Information (ESI) for the article

Resveratrol-Based Benzoselenophenes with Enhanced Antioxidant and Chain Breaking Capacity

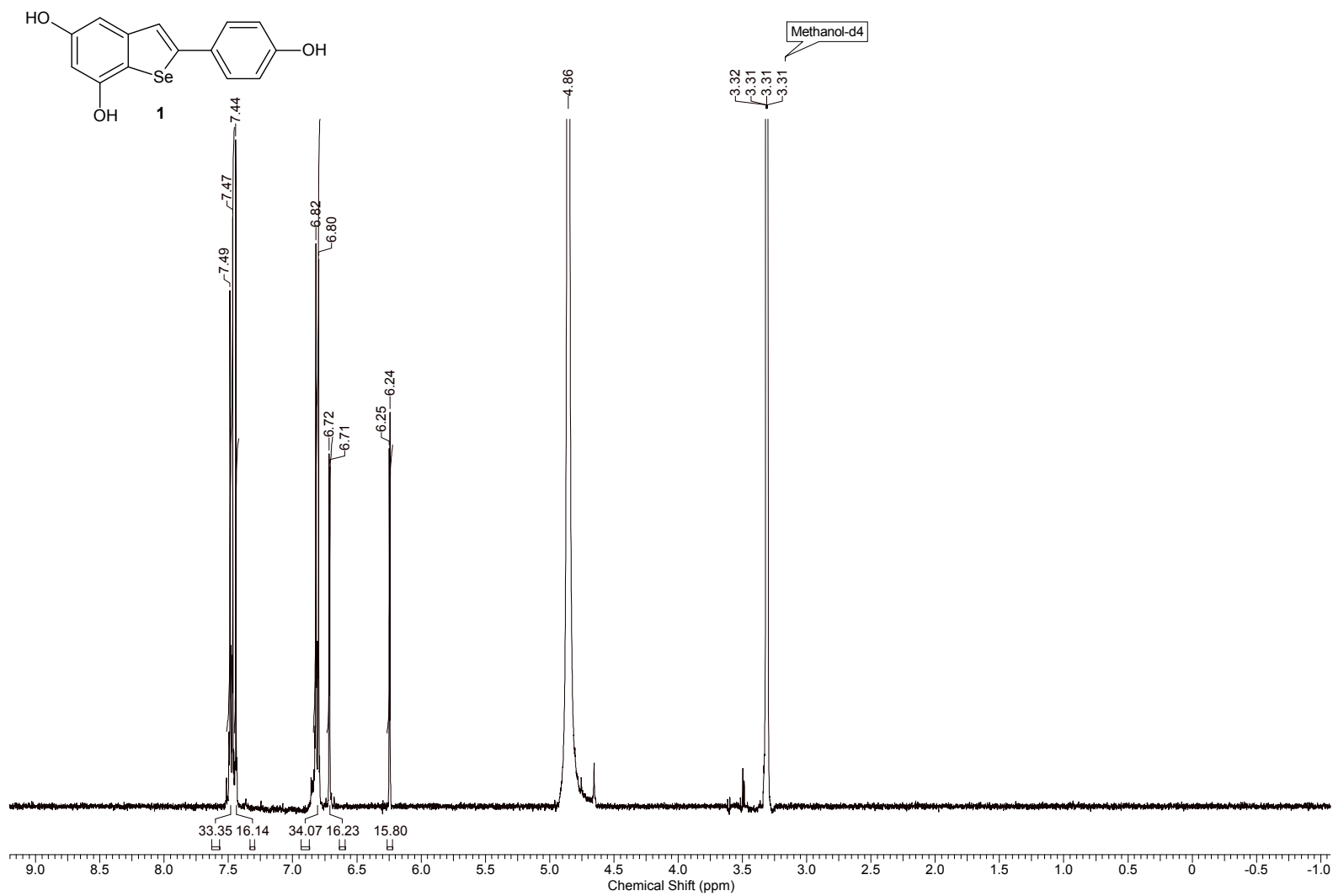
Damiano Tanini, Lucia Panzella,* Riccardo Amorati, Antonella Capperucci,* Elio Pizzo,

Alessandra Napolitano, Stefano Menichetti and Marco d'Ischia

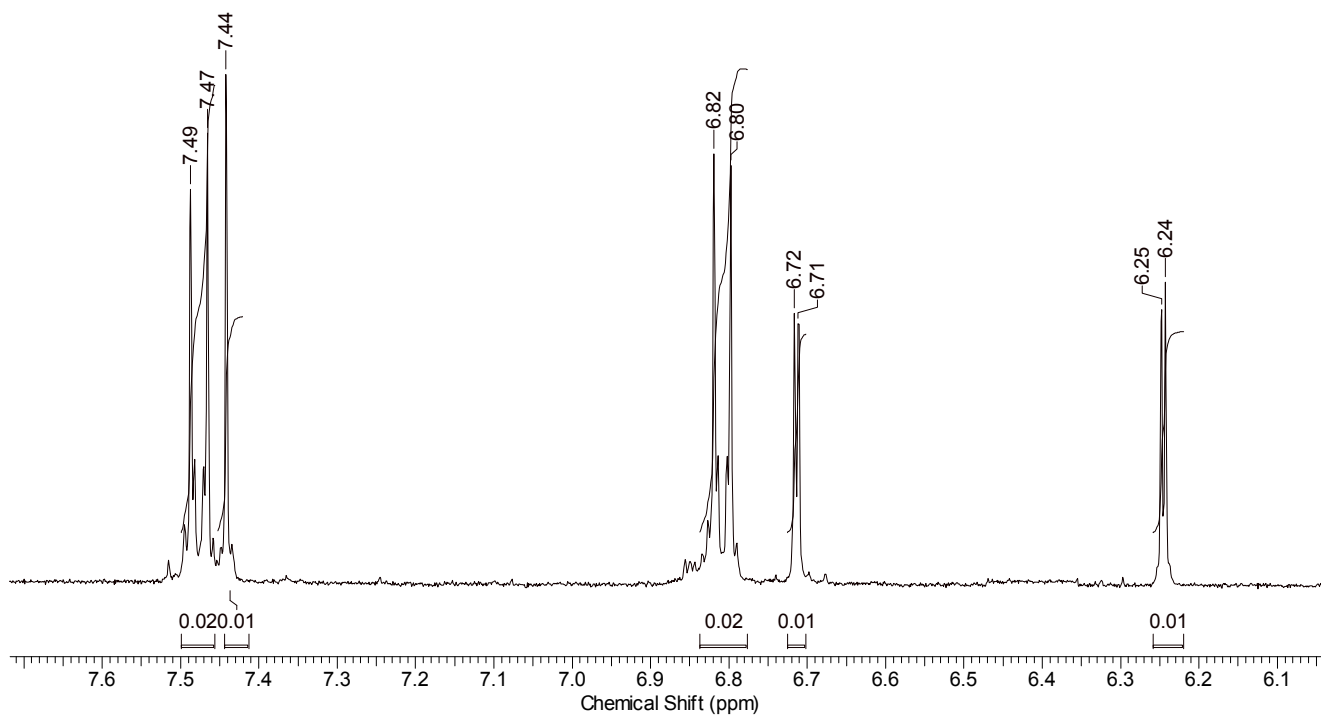
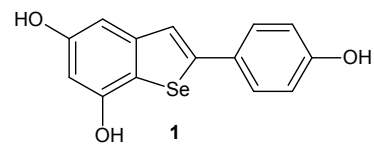
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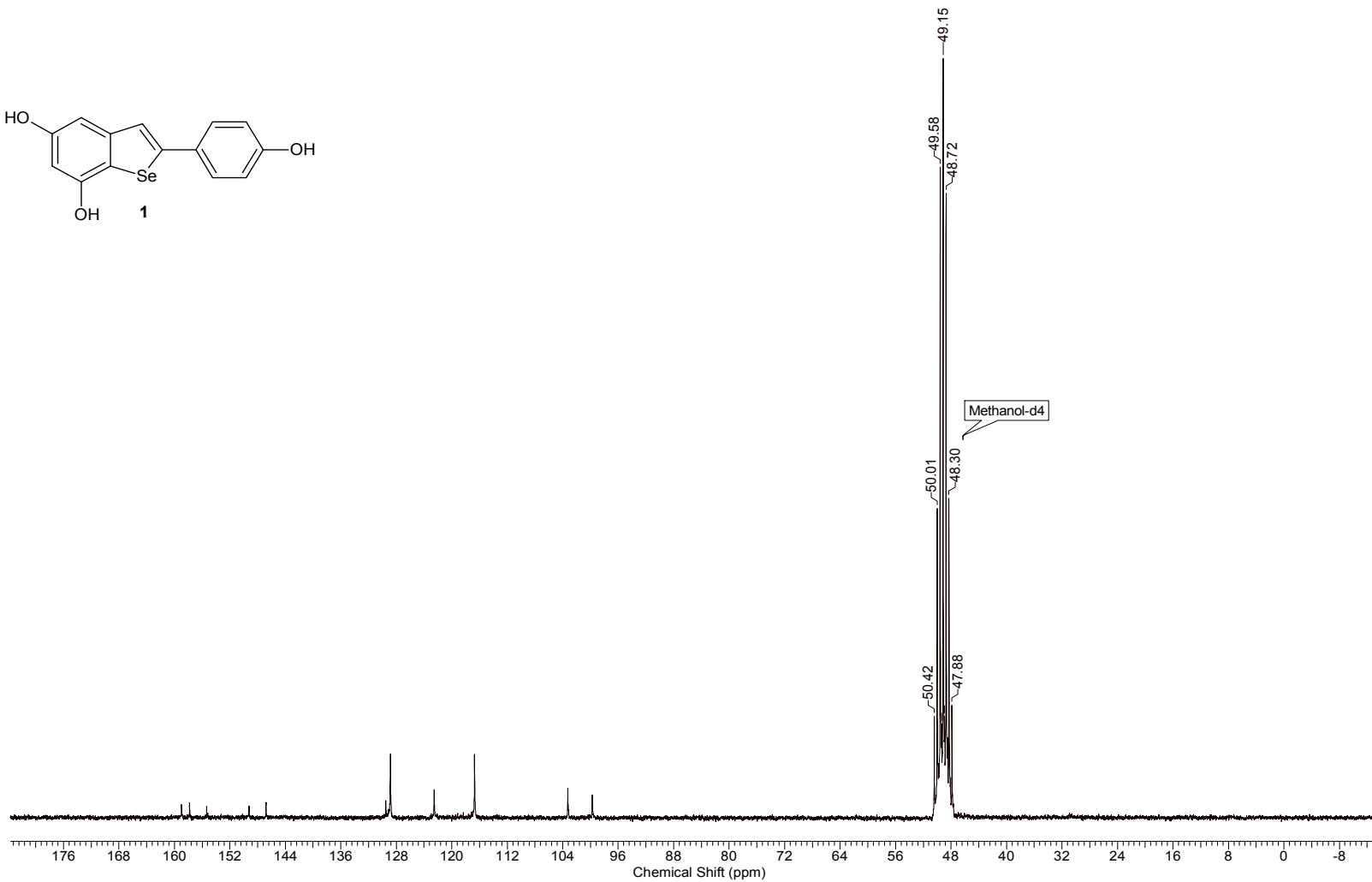
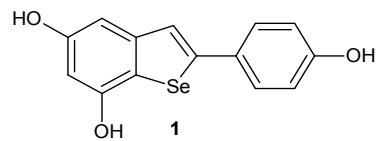
Compound 1, ^1H NMR, 400MHz, CD_3OD



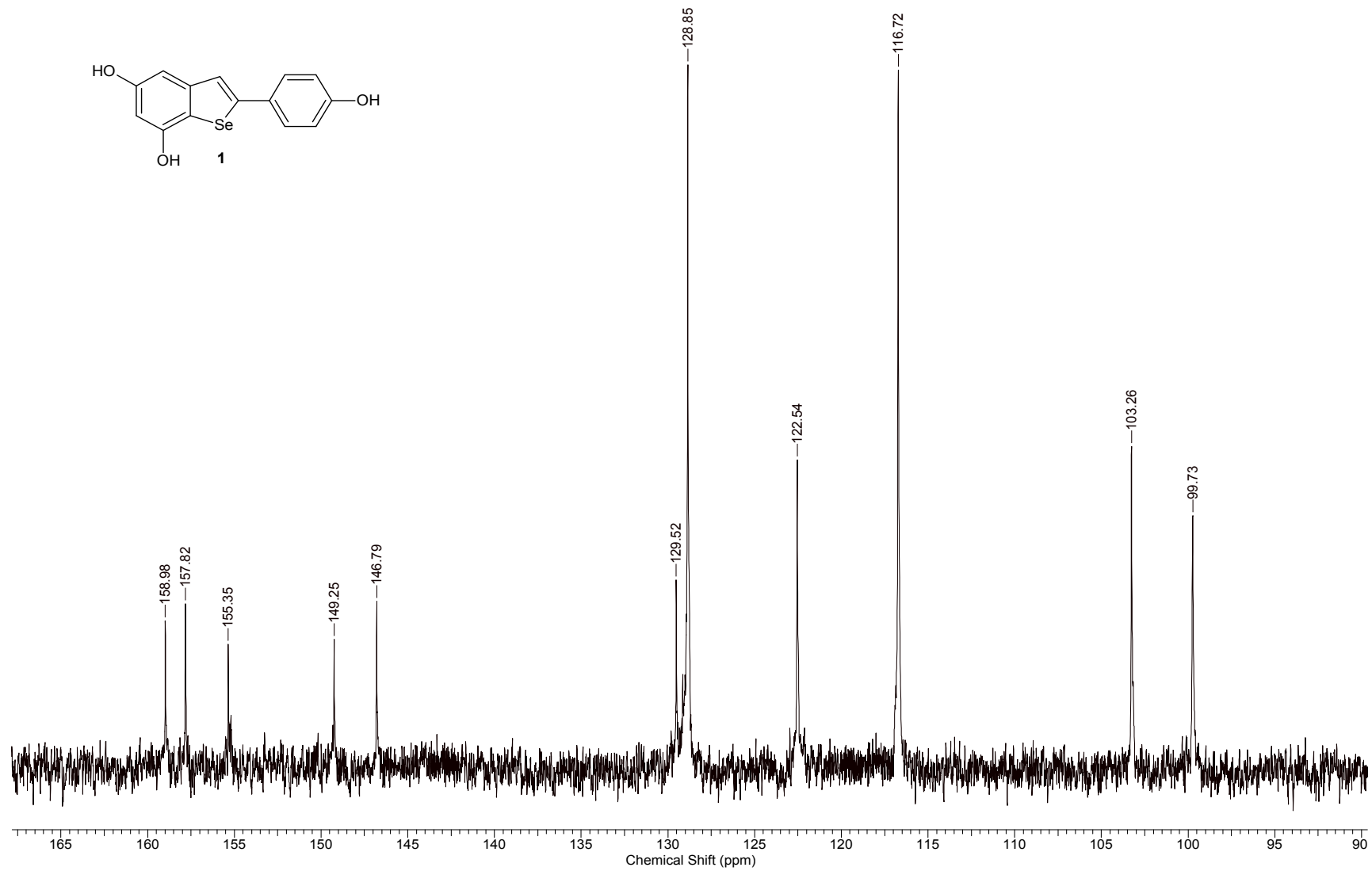
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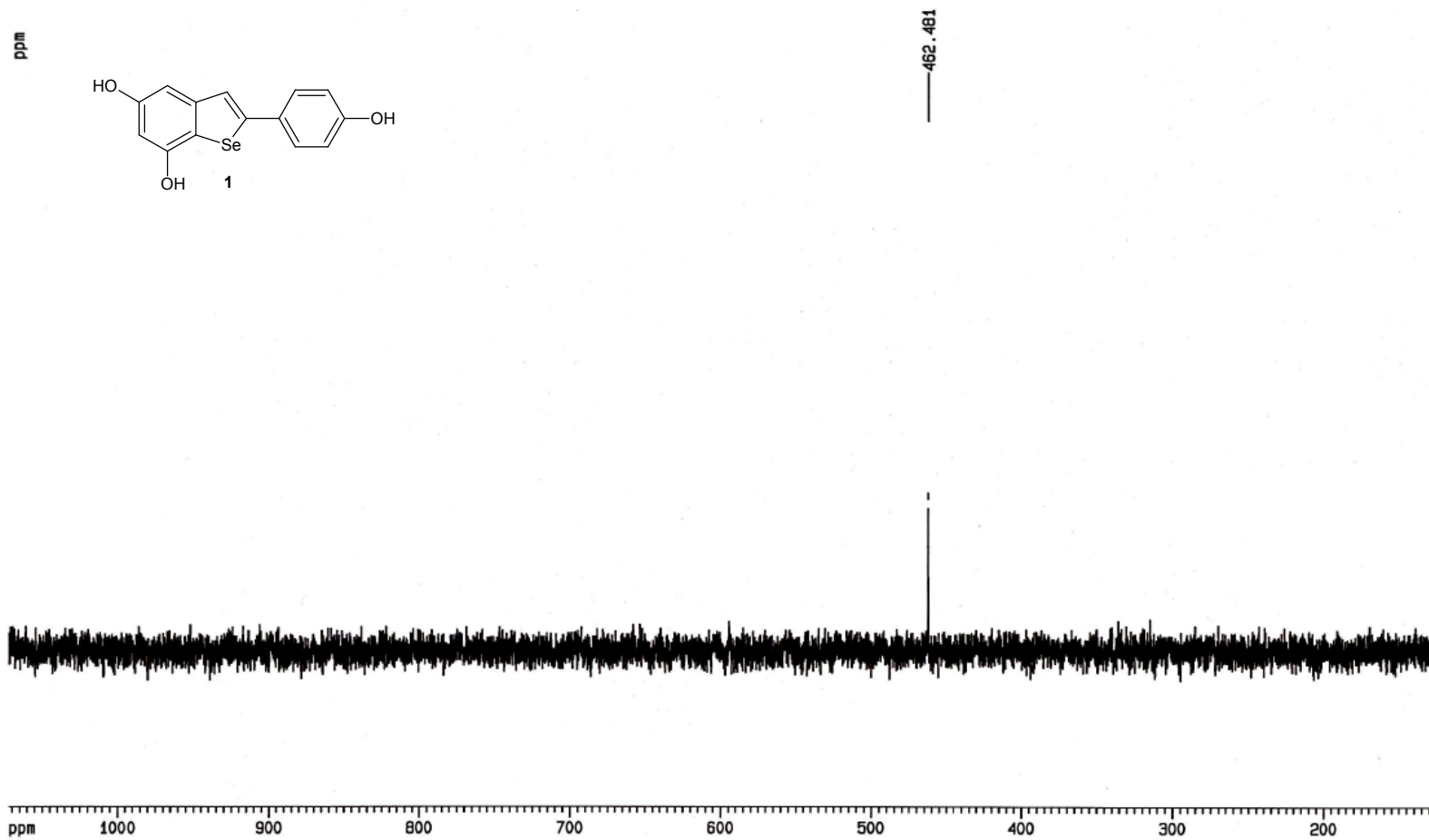
Compound **1**, ^{13}C NMR, 50 MHz, CD_3OD



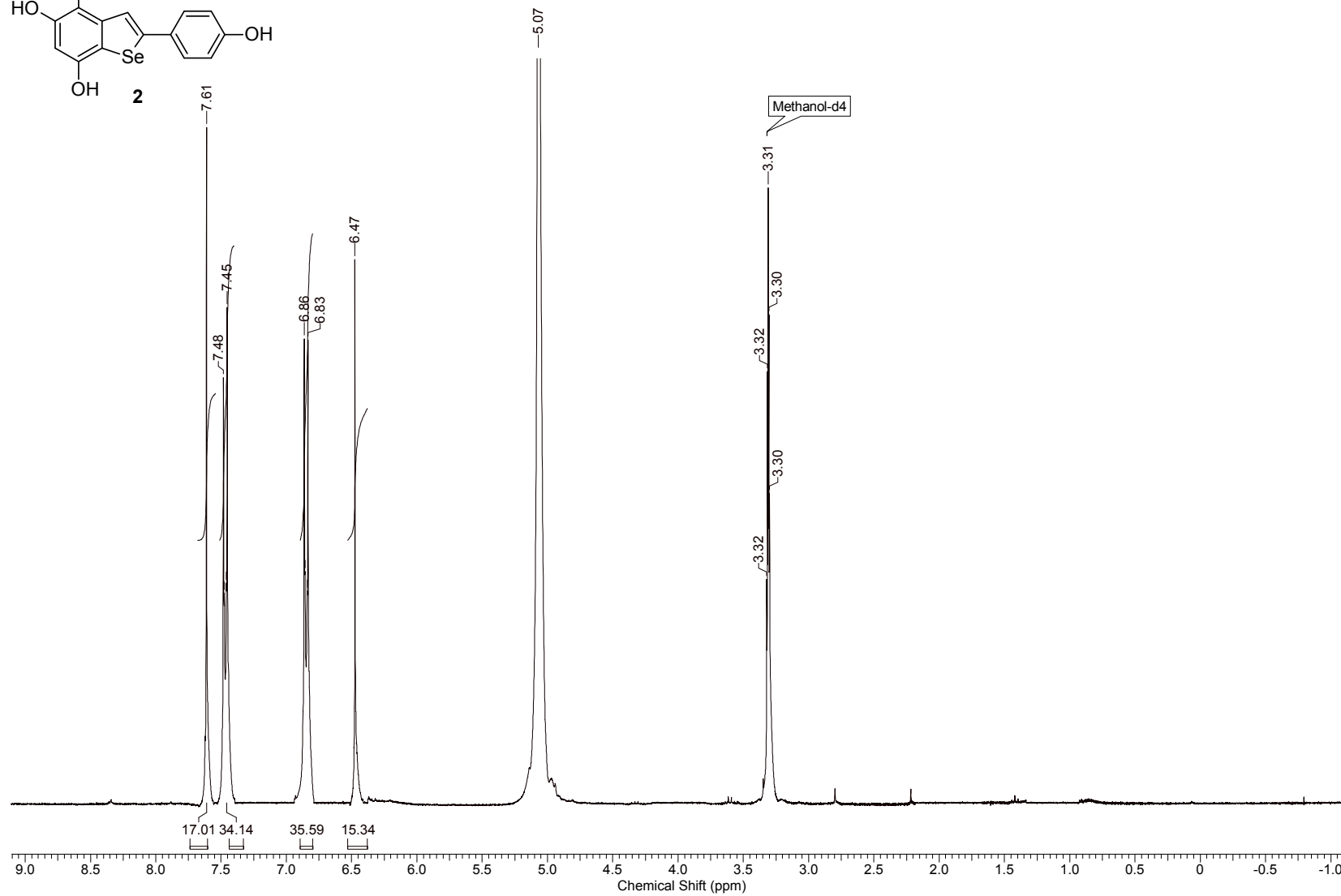
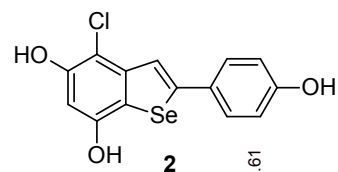
Compound **1**, ^{13}C NMR (expansion), 50 MHz, CD_3OD



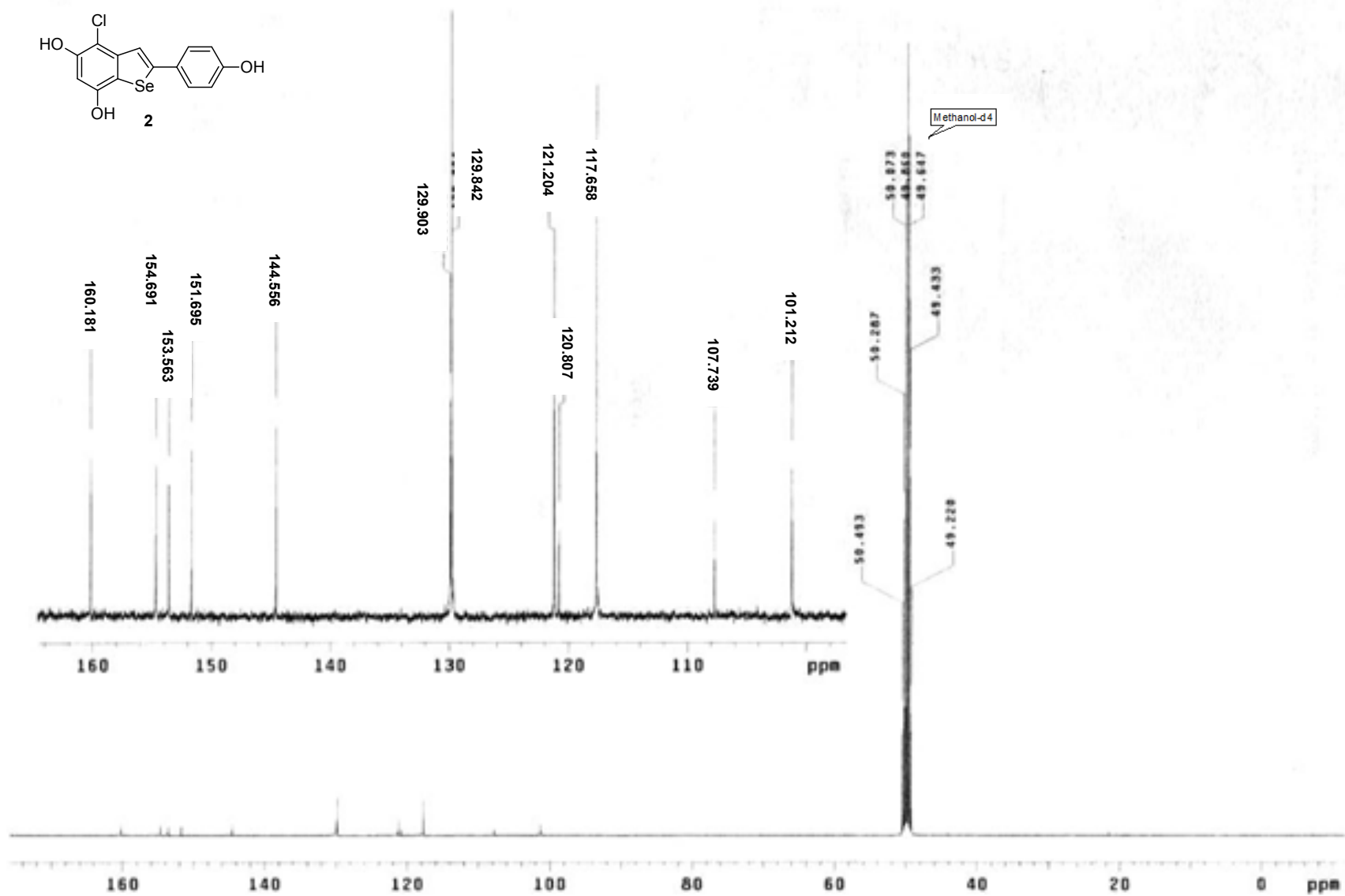
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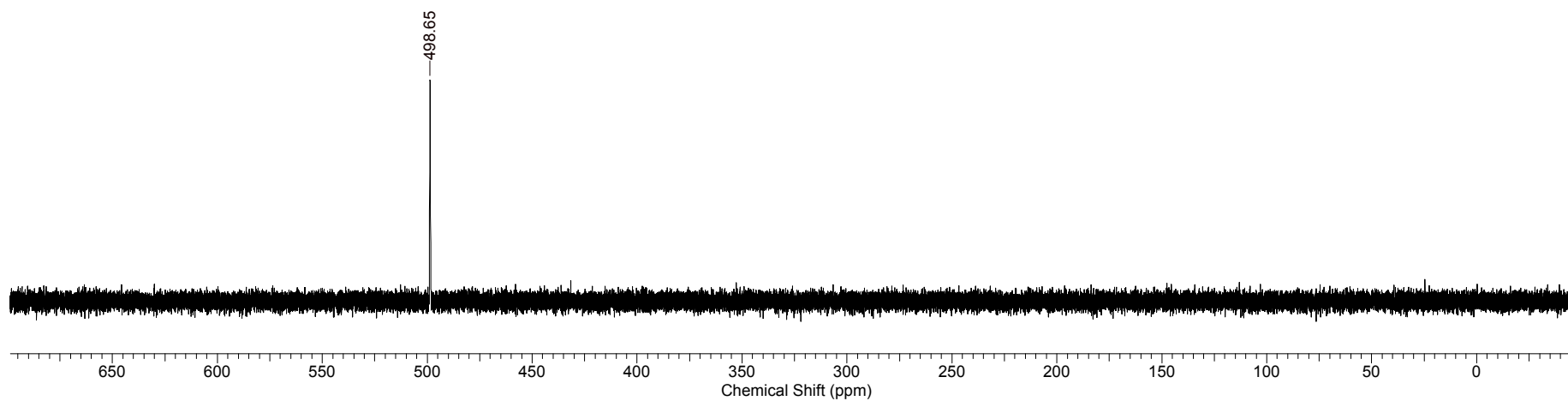
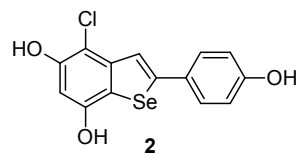
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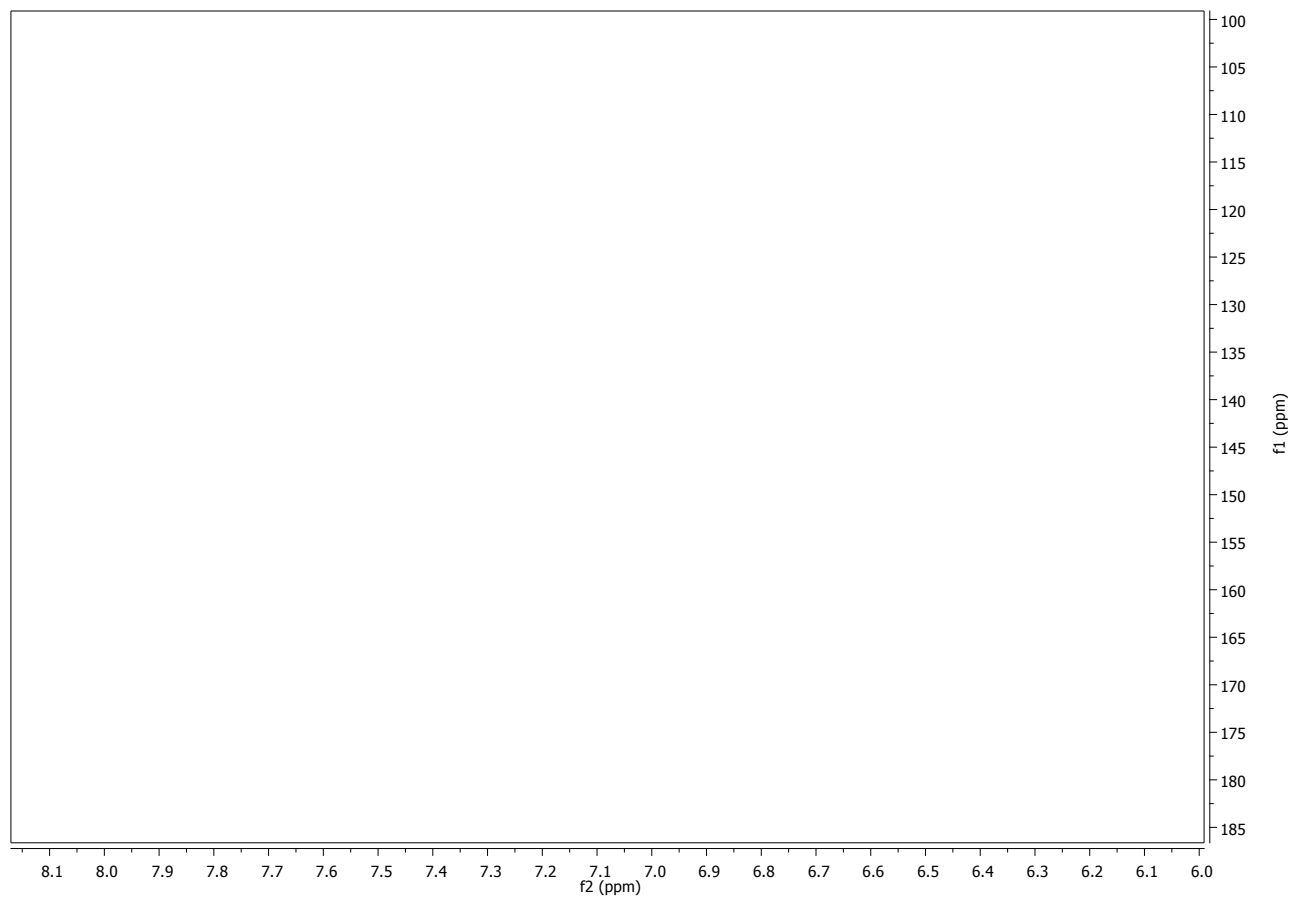
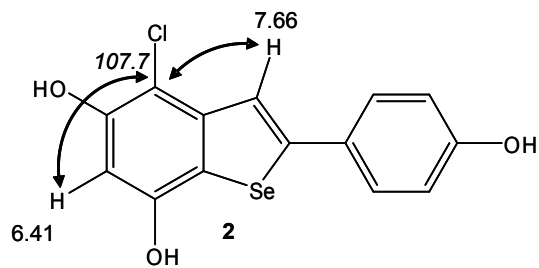
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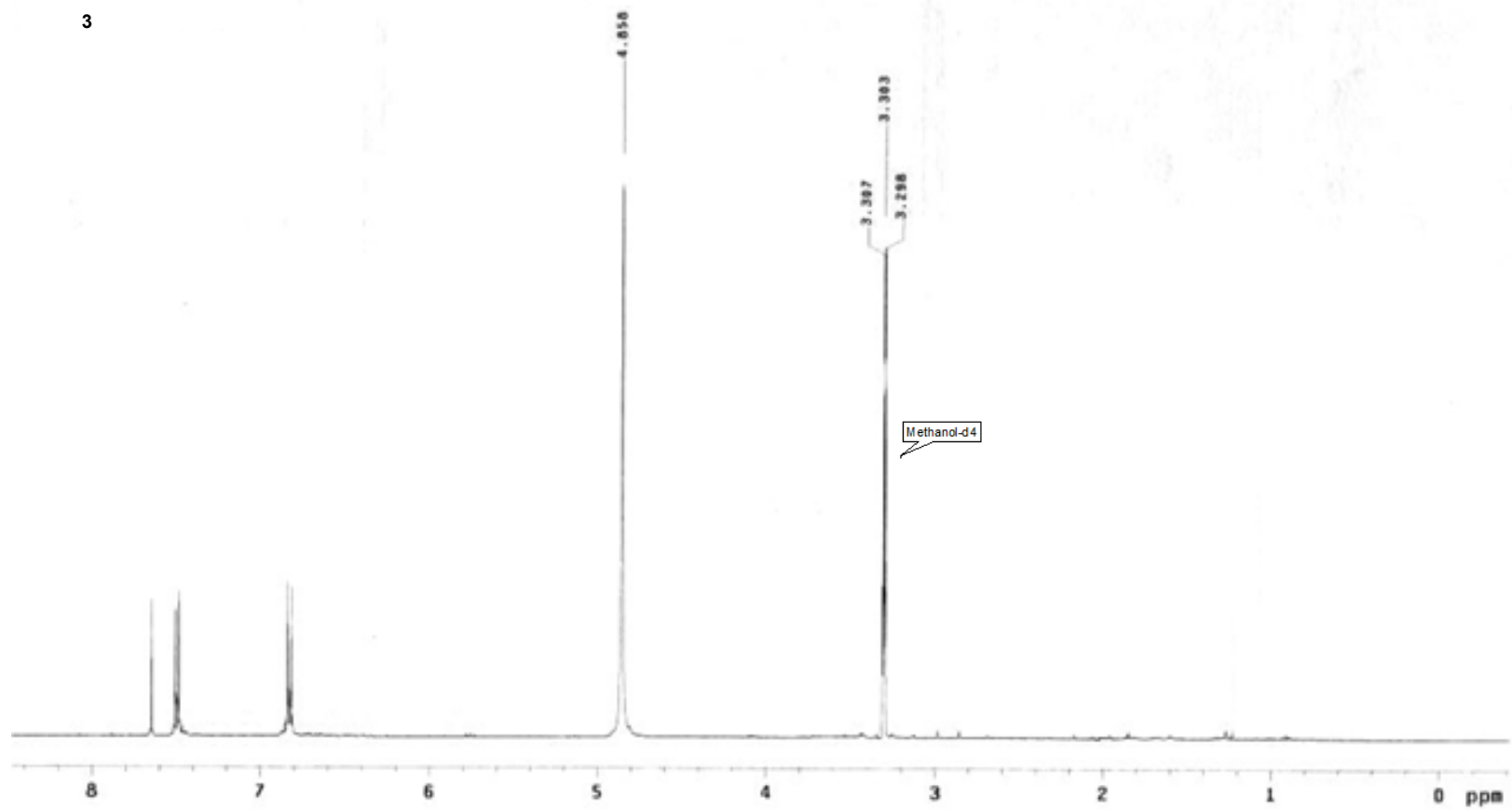
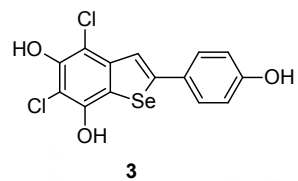
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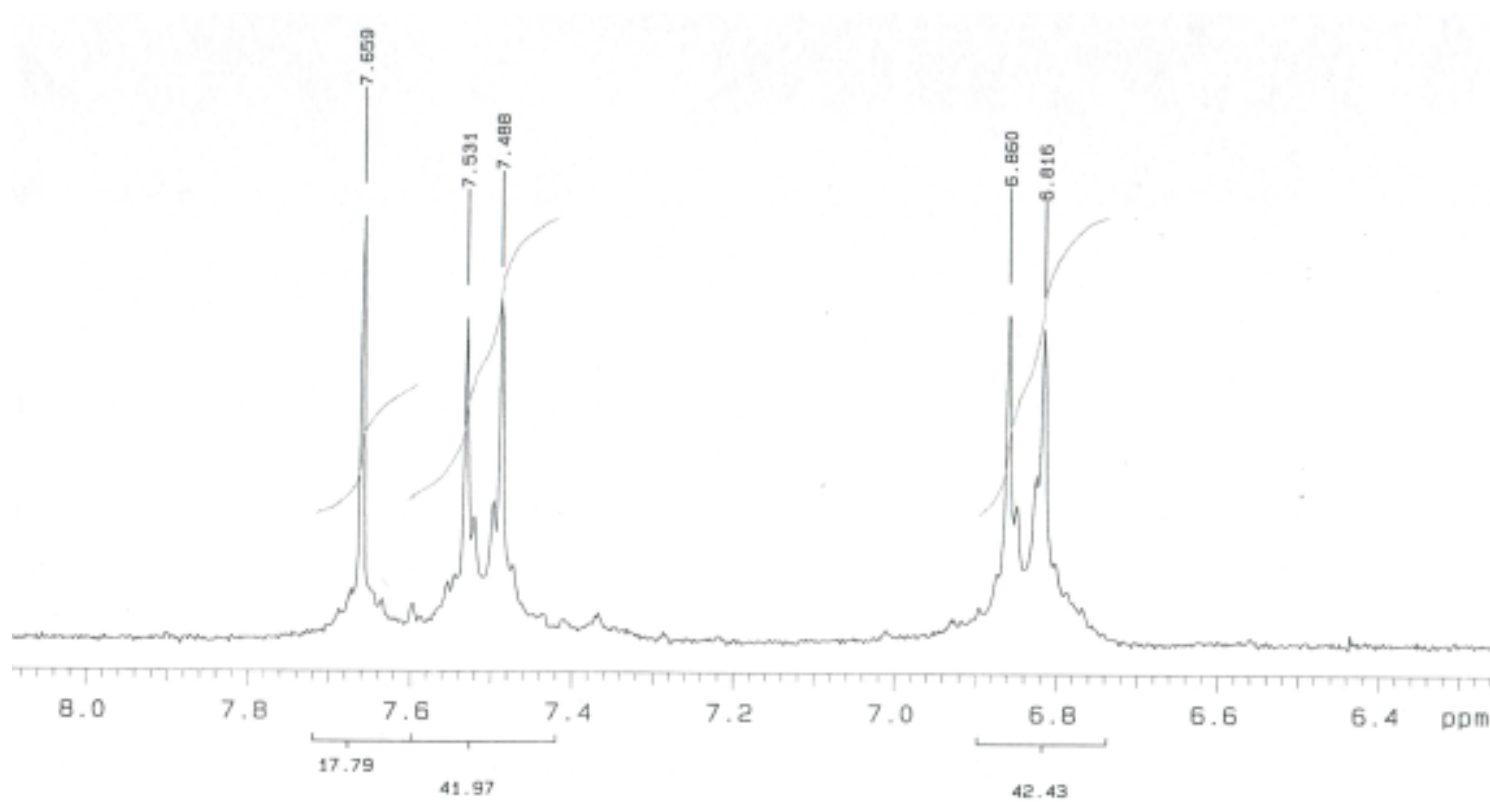
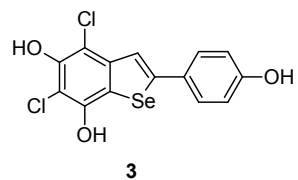
Compound **2**, region of the ^1H , ^{13}C HMBC spectrum, 400 MHz, CD_3OD (arrows indicate diagnostic long-range couplings)



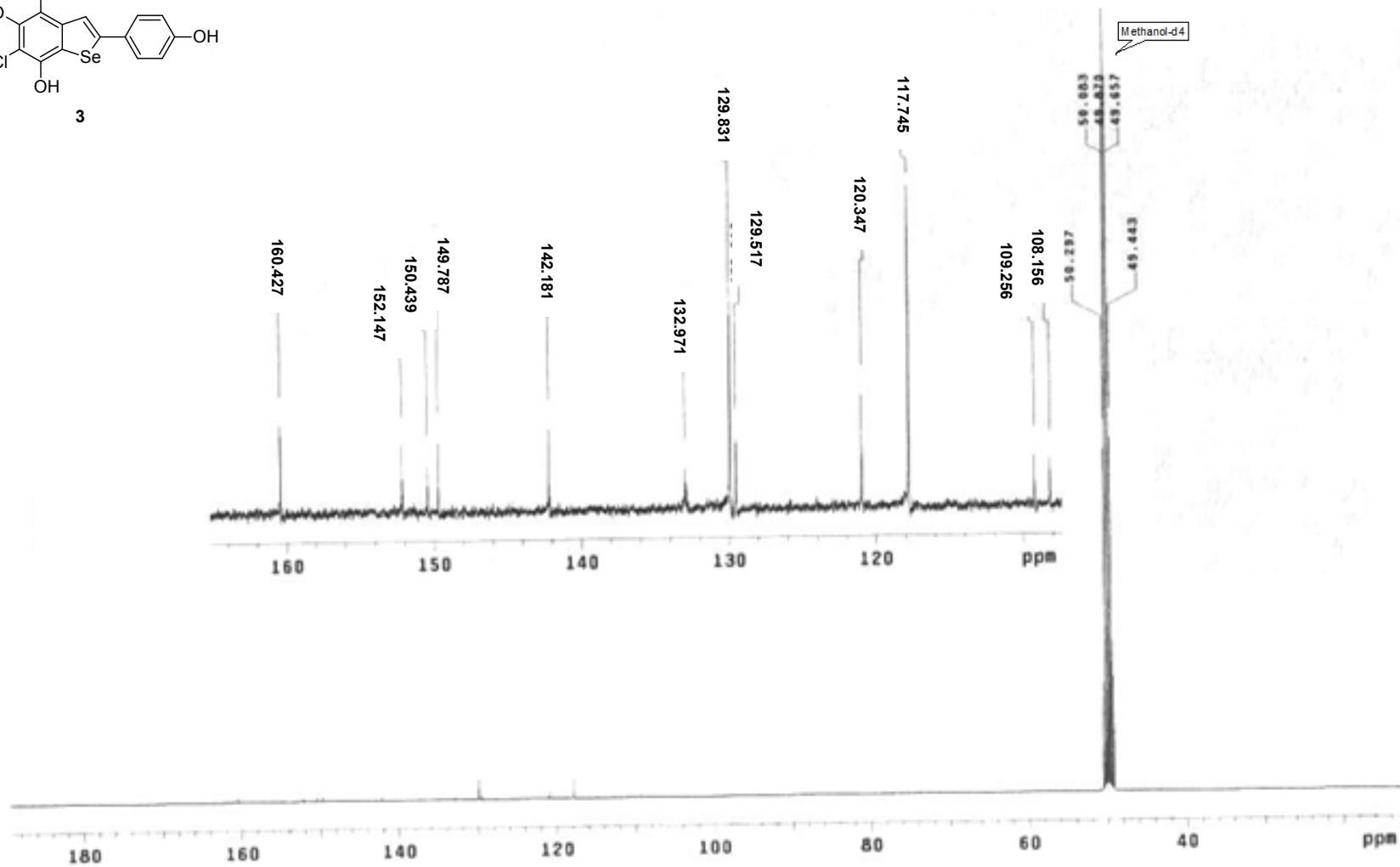
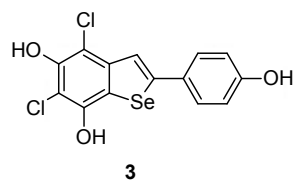
Compound **3**, ^1H NMR, 200 MHz, CD_3OD



Compound **3**, ^1H NMR (expansion), 200 MHz, CD_3OD



Compound **3**, ^{13}C NMR, 100 MHz, CD_3OD



Compound **3**, ^{77}Se NMR, 38 MHz, CD_3OD

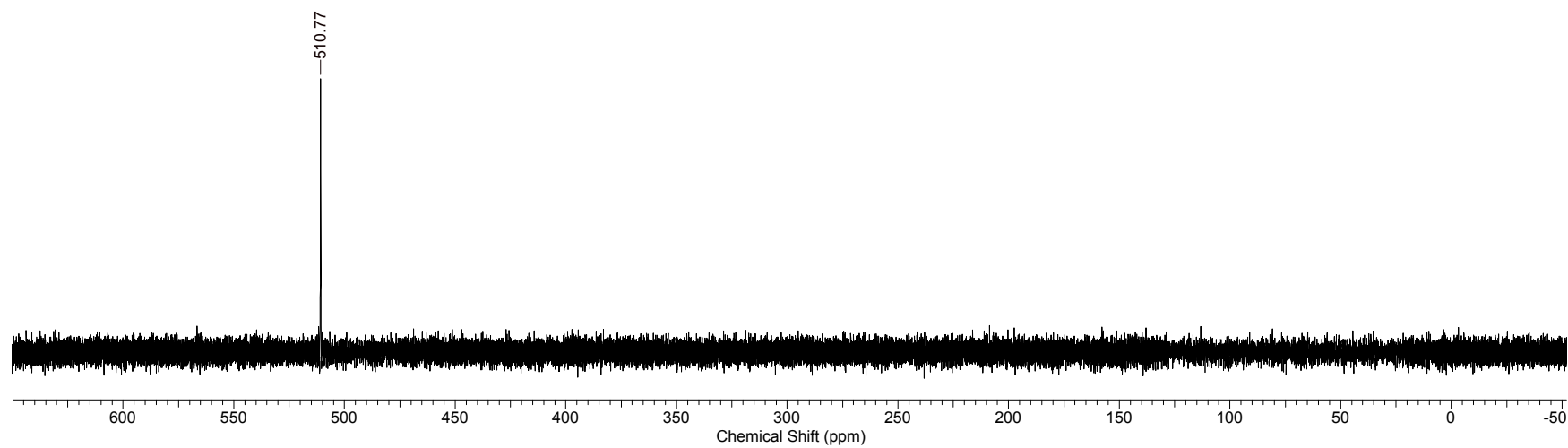
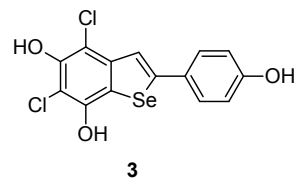


Table S1 Optimized stoichiometry ratios for the isolation of **1**, **2** and **3**.

Entry	Se(0) equiv	SO ₂ Cl ₂ equiv	Resveratrol equiv	Products	Yield (%) ^a
1	1.0	0.8	0.4	1:2 = 70:30	48
2	1.0	1.0	0.4	2:3 = 85:15	71
3	1.0	2.0	0.4	3	82

^aIsolated yield of major product

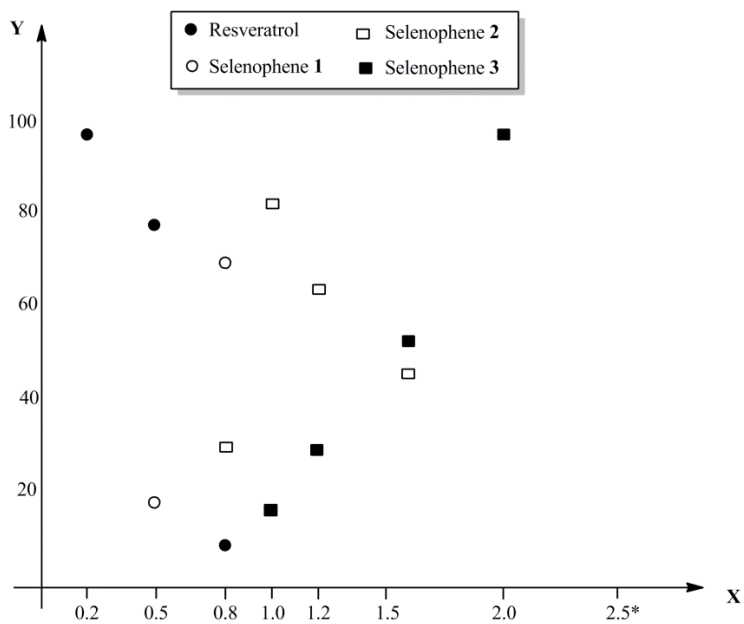


Fig. S1 Relative percentage of resveratrol and selenophenes **1-3** vs SO₂Cl₂ equiv in the reaction of resveratrol (0.4 equiv) with Se (0) (1.0 equiv) as determined by ¹H NMR analysis of the ethyl acetate extractable fraction from crude reaction mixtures after 24 h (SD ≤ 4%). With 2.5 equiv of SO₂Cl₂ or more a complex mixture was obtained with no trace of any selenophene.

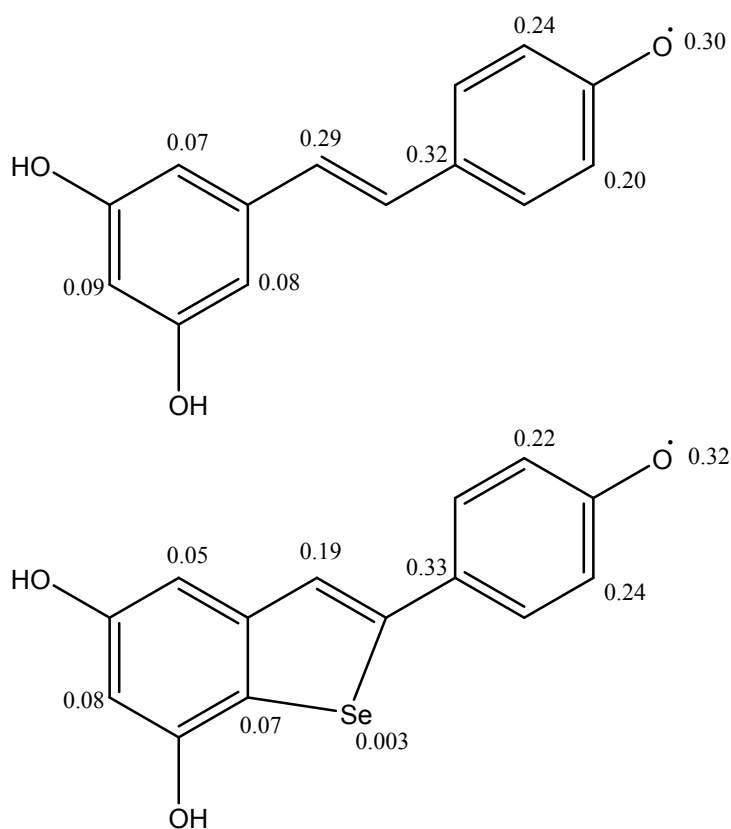
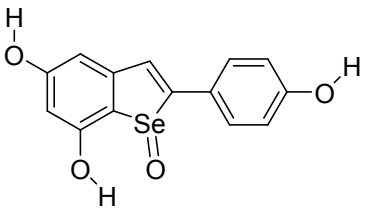


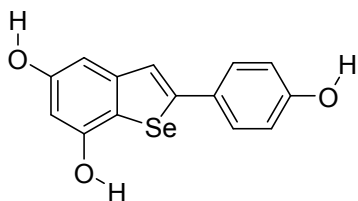
Fig. S2 Spin densities calculated at the B3LYP/LANL2DZdp level for the 4'-OH radicals of resveratrol (upper) and **1** (lower).

Table S2 Calculated BDE(OH) in the gas-phase at the B3LYP/LANL2DZdp level for the Se-oxide of 1

compd	BDE (O-H) (kcal/mol)		
	4'-OH	3-OH	5-OH
	85.1	90.7	87.3

Computational data

resvse1



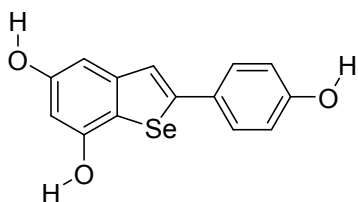
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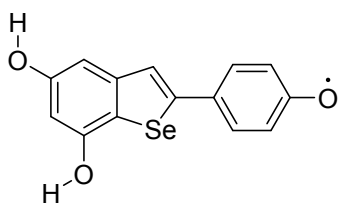
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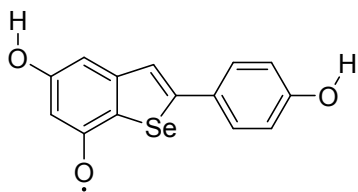
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no imaginary frequencies

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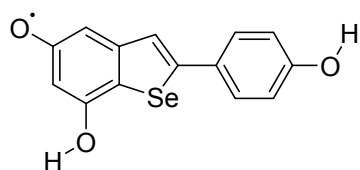
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32810627\H,-6.1796266937,0.0040088268,3.7016607707\H,-4.0682787173,0.0
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no imaginary frequencies

Sum of electronic and thermal Enthalpies= -766.253731

resveratrol radical 4'

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\C,1.2348750821,-0.0022472877,2.0973118539\C,2.4285301248,-0.002105691
3,1.3730894611\C,2.4252436247,-0.0001350916,-0.0347966617\C,1.19557986
47,0.0017267501,-0.7123487501\C,-1.2906732737,-0.0004206207,2.09830413
18\C,-1.4892226189,-0.0026061165,3.4558352398\C,-2.7568382639,-0.00261
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05387\C,-3.9376878952,-0.0054684939,6.2877955805\C,-2.7665473209,-0.00
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02\State=2-A\HF=-765.8563596\S2=0.799397\S2-1=0.\S2A=0.751818\RMSD=5.4
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no imaginary frequencies

Sum of electronic and thermal Enthalpies= -765.631194

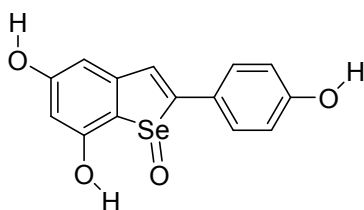
resveratrol radical 3

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,1.2160116334,-0.0013651901,2.048413812\C,2.4442264466,-0.0012605913,1
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02836579\C,-4.0418597732,0.0010023115,3.5018663964\C,-5.2264507599,0.0
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.9432705656,-0.0068458649,6.3001771279\C,-2.7619083028,-0.0064893389,5
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0.0025450864,2.1168692377\O,1.2107544415,0.0027683931,-2.0499537977\H,
1.2651405173,-0.0023133741,3.1351140811\H,3.3998008938,0.0002512786,-0
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, -1.8036131739,-0.0093017367,6.0725452804\H,-3.9038754302,-0.009882817
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77,0.0042189676,2.4144656964\H,-6.2165104963,-0.0062176337,7.263031433
6\H,4.356026276,-0.0022809934,1.5447310235\\Version=AM64L-G03RevD.02\S
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09\RMSF=2.077e-05\Thermal=0.\Dipole=0.041446,-0.0031249,2.0275574\PG=C
01 [X(C14H11O3)]\@

no imaginary frequencies

Sum of electronic and thermal Enthalpies= -765.624323

resvseox1



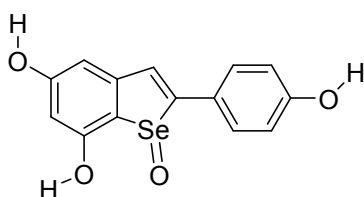
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0343539,1.3693777247\C,2.4231546672,-0.0191400084,-0.0370590834\C,1.19
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605334658\Se,-2.8596442274,0.9338356305,1.4415431892\O,-3.5410824306,0
.1924101652,0.1076664587\O,3.5654326154,-0.0266398856,-0.7914617945\C,
-1.5212368942,-0.4579908187,3.4205377382\C,-2.9013432647,-0.3502507085
,3.9054407634\C,-3.3969839687,-0.8029443369,5.1352141587\C,-4.78298447
01,-0.69981366,5.3795119219\C,-5.6688736795,-0.1912228268,4.4172293872
\C,-5.163427578,0.2627165368,3.1865736124\C,-3.7821021369,0.2290273363
,2.9714851806\H,-2.7347511235,-1.2443064473,5.8816945105\O,-6.04107967
93,0.7090991744,2.2426967386\O,-5.3383646398,-1.1234800118,6.557733193
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7013,4.0411198611\H,-5.6248111292,0.6490644675,1.3623838972\H,-4.64354
13087,-1.4777610776,7.1319060776\H,1.2745450525,0.0613733102,3.1717937

73\H,3.3990924404,0.0243318971,1.8996103582\H,1.1940275142,-0.04677383
 14,-1.8082470471\H,-0.9465822272,-0.0492691715,-0.537712138\H,4.338829
 518,-0.0216251562,-0.2081661433\\Version=AM64L-G03RevD.02\State=1-A\HF
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no imaginary frequencies

Sum of electronic and thermal Enthalpies= -849.488920

resvseox2



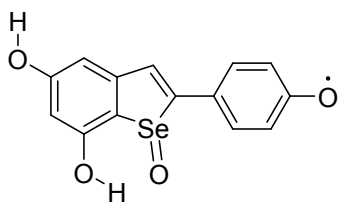
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 ,0.0955462466,1.4021357938\C,2.4300331331,0.0245683633,-0.0021381476\C
 ,1.2223061971,-0.0585878871,-0.7147951712\C,-1.3084786517,-0.048749537
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 65,-0.1816120117,0.0160773324\O,3.5929991728,0.0400351497,-0.726509366
 3\C,-1.5662728482,-0.5380582261,3.347042138\C,-2.9458909767,-0.4403648
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 081\C,-5.1835355199,0.3335188432,3.2495058279\C,-3.8370752799,0.157660

5779,2.9182432534\H,-2.7212610372,-1.3434887222,5.7982211251\O,-5.9939
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 15673\H,-6.7075874406,-0.0210551939,4.7690631622\H,-0.8018958703,-1.02
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no imaginary frequencies

Sum of electronic and thermal Enthalpies= -849.486175

resvseoxrad1



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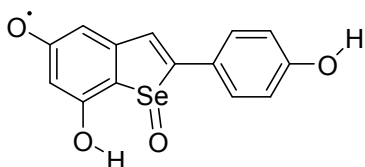
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 C,1.1978237457,0.3398957813,-0.6941777896\C,-1.2709230162,0.0209270303

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82,-0.1552481097,0.0764241798\O,3.5498891962,-0.002420625,-0.670331224
1\C,-1.5078665573,-0.3042531751,3.4438762323\C,-2.8860245082,-0.260343
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6588922,2.9147944174\H,-2.6629054765,-0.9281441131,5.9670259128\O,-6.0
871648159,0.3797797755,2.1478145208\O,-5.2789327023,-0.936480168,6.624
7011754\H,-6.7272705867,-0.3115784781,4.5921961398\H,-0.7128808664,-0.
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5702670819,-1.1764836566,7.2399534051\H,1.1896862882,-0.6084543475,3.1
121033625\H,3.3323247943,-0.6171592847,1.8665828146\H,1.2336450268,0.5
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no imaginary frequencies

Sum of electronic and thermal Enthalpies= -848.861990

resvseoxrad2

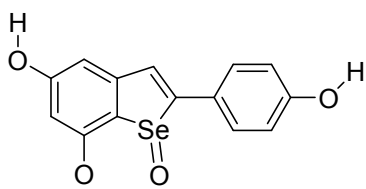


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,1.1685135696,0.0177551445,-0.7182512065\C,-1.2556939184,-0.002634936,
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no imaginary frequencies

Sum of electronic and thermal Enthalpies= -848.855729

resvseoxrad3



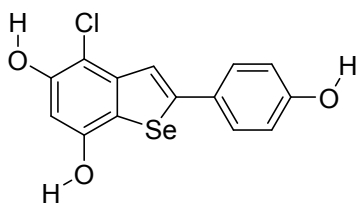
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,0.0604995615,1.3989960033\\C,2.4382383642,0.0130555537,-0.0069255184\\C
,1.228159505,-0.0376166074,-0.7194456227\\C,-1.2964075905,-0.0340397849
,2.1068838532\\Se,-2.9229147689,0.8041078611,1.3102561784\\O,-3.36700854
14,-0.1242351611,0.0084554214\\O,3.598380827,0.0214165396,-0.7323984215
\\C,-1.557866512,-0.5189285612,3.3470395916\\C,-2.9426350434,-0.41007942
44,3.8179171498\\C,-3.4224466902,-0.8588748476,5.0725790542\\C,-4.795979
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375\\C,-5.2242388122,0.403852249,3.2394278749\\C,-3.826235756,0.18244530
79,2.9173012221\\H,-2.7385575851,-1.3259139765,5.7844952509\\O,-6.001313
9566,1.0172448567,2.4611467413\\O,-5.2852739136,-1.1529488186,6.6053042
068\\H,-6.732543972,0.0179991571,4.7850054903\\H,-0.7997167464,-1.005111
8739,3.9639511125\\H,-4.5765480808,-1.5657421218,7.120444333\\H,1.206355
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\\H,1.255860332,-0.0775568869,-1.8073889296\\H,-0.9179295221,-0.11134778
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no imaginary frequencies

Sum of electronic and thermal Enthalpies= -848.849883

resvsecl3



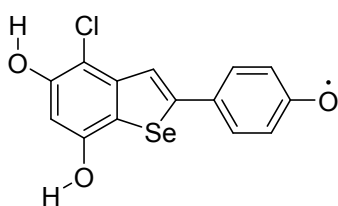
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883\C,1.1976644999,0.0023376889,-0.7311390754\C,-1.1497645243,-0.01308
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42269979\H,-5.0392651774,0.9904246027,5.4478652634\H,-3.3814861147,1.0
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9Cl1O3Se1)]\@

no imaginary frequencies

Sum of electronic and thermal Enthalpies= -788.682197

resvseclrad4 (4')



B3lyp/gen pseudo=read opt freq scale=0.9806\\Se Cl resv rad\\0,2\

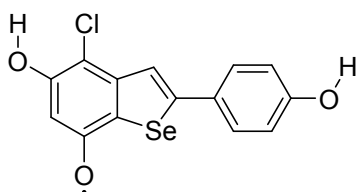
C,-0.0068372268,-0.0804709045,-0.0201569167\C,-0.0125973106,-0.0333016
804,1.3970643597\C,1.2318871451,0.0381303241,2.0788236744\C,2.44500821
85,0.0618705543,1.3706034245\C,2.4280299785,0.014604305,-0.0233431282\
C,1.2010477477,-0.0568062978,-0.7244432547\C,-1.1467792923,-0.04843276
02,2.2716302355\C,-0.8705141547,0.0077120309,3.6304974826\Se,1.0149668

811,0.0923192567,3.952137971\O,3.5978784649,0.131555879,2.1054832116\O
,1.2732552188,-0.0994059092,-2.0832069381\Cl,-1.5075755065,-0.16948963
82,-0.927336225\C,-1.8320114084,0.0061889246,4.7125399916\C,-3.2426047
751,-0.057359484,4.444630768\C,-4.1659600657,-0.0595684014,5.460443524
2\C,-3.758095862,0.0026938039,6.865252901\C,-2.3175645323,0.0668383656
,7.1162541212\C,-1.4128093142,0.0677212167,6.0816372765\O,-4.593590981
6,0.0011673786,7.7991494691\H,3.3516271027,0.0313850197,-0.6022635965\
H,-2.1591029799,-0.1011114483,1.8807901741\H,4.3641328207,0.1415632203
,1.5129432585\H,0.3714847728,-0.1467985818,-2.4445928164\H,-0.34686193
13,0.1165618778,6.3095268067\H,-1.9970650291,0.113643184,8.1566905574\
H,-5.2358450481,-0.1077021652,5.2584374057\H,-3.5856133984,-0.10473722
91,3.4127427993\\Version=AM64L-G03RevD.02\State=2-A\HF=-788.2539994\S2
=0.792045\S2-1=0.\S2A=0.751376\RMSD=8.680e-10\RMSF=5.333e-06\Thermal=0
.\Dipole=1.6976226,0.0070983,-1.7735127\PG=C01 [X(C14H8Cl1O3Se1)]\@

no imaginary frequencies

Sum of electronic and thermal Enthalpies= -788.056680

resvseclrad2 (3)



#p B3lyp/gen pseudo=read opt freq scale=0.9806\\Se Cl resv rad 3\\0,

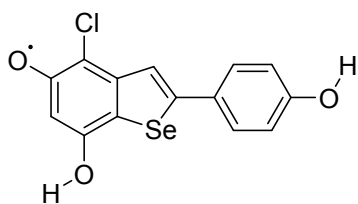
2\C,0.0050999248,-0.2151766463,0.0142677233\C,-0.0028727635,0.00101424

01,1.4103226484\C,1.238418286,0.2105206098,2.0516004675\C,2.4374336772
,0.214369864,1.3380274945\C,2.4214269912,0.0090164454,-0.0515833684\C,
1.1984037512,-0.2059228203,-0.7112458942\C,-1.2723566963,0.0091131084,
2.1507431362\C,-2.5240251431,0.3030411757,1.6833483182\C,-3.6075210712
,0.2052261077,2.6350527788\C,-3.1927891659,-0.1806460378,3.9440302715\
C,-4.1223141018,-0.3123092799,5.0231089359\C,-5.4579448742,-0.07383632
12,4.7979867883\C,-5.965168025,0.3176633909,3.4886261434\C,-4.97118363
92,0.4529264284,2.4067848701\Se,-1.3355698349,-0.4750593869,4.00557505
51\O,-3.7279476282,-0.6783895736,6.2820620472\O,-7.1819020035,0.531946
3682,3.2920091457\Cl,-5.5359249259,0.9228749657,0.8445518439\O,3.62310
00038,0.0223714731,-0.7060161678\H,-6.1812799097,-0.1706818093,5.60519
09392\H,-2.7002785884,0.6224902671,0.658943941\H,-2.7637468703,-0.7467
569202,6.3372639844\H,1.2688891863,0.397107404,3.1258462226\H,3.390149
6023,0.3815866368,1.8382561956\H,1.1833283378,-0.3802169593,-1.7889731
742\H,-0.9307723218,-0.4121738318,-0.5064661888\H,3.4788792713,-0.1252
994302,-1.652557242\\Version=AM64L-G03RevD.02\State=2-A\HF=-788.245854
4\S2=0.783949\S2-1=0.\S2A=0.750794\RMSD=5.899e-09\RMSF=9.083e-06\Therm
al=0.\Dipole=2.8359914,-0.4117739,-0.7226098\PG=C01 [X(C14H8Cl1O3Se1)]
\@

no imaginary frequencies

Sum of electronic and thermal Enthalpies= -788.048761

resvseclrad5 (5)

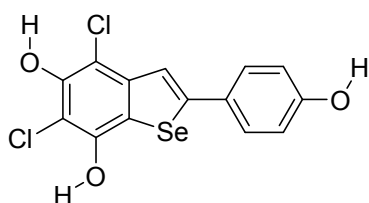


```
#p B3lyp/gen pseudo=read opt freq scale=0.9806\\Se Cl resv rad\\0,2\
C,-0.0060870922,-0.0024060236,-0.0207132959\C,-0.0121482528,-0.0002777
12,1.3857559734\C,1.2359171394,-0.0034481923,2.0689950368\C,2.48023298
36,-0.0051250166,1.3687897687\C,2.4921661888,-0.0041543448,-0.00507026
37\C,1.2568377634,-0.0028859571,-0.7858331995\C,-1.154500705,-0.007372
6766,2.2711656286\C,-0.8756871214,-0.0093577063,3.612776145\Se,1.01566
58487,0.0017734322,3.9255689821\O,3.6007955454,-0.0067375914,2.1541498
092\O,1.270345262,-0.0018632962,-2.0353221826\Cl,-1.4851231857,-0.0011
026235,-0.9110719709\C,-1.833092219,0.0064059611,4.7290929904\C,-3.125
2668904,0.5500882168,4.5552404867\C,-4.0535060255,0.5572901956,5.59895
81162\C,-3.7054482683,0.0269205466,6.8536328339\C,-2.4223137416,-0.508
7694027,7.0522220482\C,-1.5055284579,-0.5165502218,6.0001370608\O,-4.5
690424197,0.0112364324,7.9160163333\H,3.4235018277,-0.0032435146,-0.57
223767\H,-2.1703116442,-0.0391882713,1.8846587596\H,4.389406408,-0.008
2021648,1.5905160411\H,-0.5227351707,-0.9591314007,6.1668634087\H,-2.1
638389969,-0.9185109183,8.0275362884\H,-5.0451601016,0.9876126049,5.44
4989981\H,-3.4004677397,0.9908746345,3.5982278596\H,-5.4150254675,0.40
17599485,7.65098895\\Version=AM64L-G03RevD.02\State=2-A\HF=-788.251252
3\S2=0.780063\S2-1=0.\S2A=0.750619\RMSD=7.359e-09\RMSF=6.915e-06\Therm
al=0.\Dipole=-0.4100777,0.2306501,1.9871703\PG=C01 [X(C14H8Cl1O3Se1)]\
\@
```

no imaginary frequencies

Sum of electronic and thermal Enthalpies= -788.053890

resvSeCl22



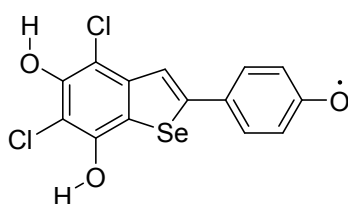
```
p B3lyp/gen pseudo=read opt freq scale=0.9806\\resveratrolo Se Cl2\\0,  
1\C,-0.0055111595,0.0001090668,-0.0212883652\C,-0.0130955666,-0.001896  
4788,1.3925084324\C,1.2332787376,-0.0058496076,2.0688794013\C,2.450204  
3255,-0.0028587318,1.37158715\C,2.4207419768,0.0028674657,-0.030709650  
7\C,1.1958296614,0.0041720065,-0.7425869953\C,-1.1515352772,-0.0149119  
117,2.2758257852\C,-0.8678744481,-0.023546468,3.6198449391\Se,1.012721  
78,-0.0074908119,3.9456560124\O,3.6068315347,-0.0050144383,2.087373059  
2\O,1.2493532815,0.0089290376,-2.099226631\Cl,-1.5100293703,0.00078711  
41,-0.9315206517\C,-1.8342414382,-0.0184703242,4.7299367073\C,-3.11977  
98076,0.5411925332,4.5596290187\C,-4.0532173746,0.5422653242,5.5994686  
712\C,-3.7165051606,-0.010881421,6.8469240232\C,-2.4405074263,-0.56402  
06333,7.0421851592\C,-1.5188451327,-0.565220354,5.9941243789\O,-4.5858  
142319,-0.0333682246,7.9061361394\Cl,3.9349937266,0.011054277,-0.90327  
77181\H,-2.1699167939,-0.0482926934,1.8954746616\H,4.3585403602,-0.002  
2575955,1.4691712493\H,0.3387817673,0.0082431735,-2.4416275784\H,-0.54  
14992936,-1.0210237398,6.1560739183\H,-2.1908131355,-0.9922122924,8.01
```

19212924\H,-5.0395115285,0.9858223155,5.4480302272\H,-3.3852076787,1.0
 007238311,3.6086142506\H,-5.4246230101,0.3734260505,7.6431255668\\Vers
 ion=AM64L-G03RevD.02\State=1-A\HF=-803.2477078\RMSD=8.179e-09\RMSF=1.5
 51e-06\Thermal=0.\Dipole=-1.054992,0.2302738,0.3493258\PG=C01 [X(C14H8
 Cl2O3Se1)]\@

no imaginary frequencies

Sum of electronic and thermal Enthalpies= -803.045152

resvSeCl2rad6 (4')



B3lyp/gen pseudo=read opt freq scale=0.9806\\Se Cl2 resv rad\\0,2

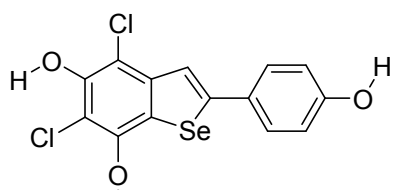
\C,-0.018833558,-0.0001541409,0.001403757\C,-0.007024819,-0.0002302682
 ,1.4345184751\C,1.2689380835,0.0000437452,2.0960914938\C,2.4437452033,
 0.0000464854,1.38605873\C,2.4530433506,-0.0008579917,-0.0781675069\C,1
 .1434719706,-0.0001480741,-0.7319289449\C,-1.2380769284,-0.0001791912,
 2.1956395011\Se,-2.9522308132,-0.0001237698,1.3415566409\C,-3.69832723

31,-0.0000712684,3.0743702571\C,-2.7026535188,-0.0000762828,4.08672982
 \C,-3.1186769298,-0.0000360599,5.4412373452\C,-4.4763588306,0.00000984
 02,5.7791687496\C,-5.4429108875,0.0000145399,4.7387451673\C,-5.0657419
 76,-0.0000250798,3.3880229143\Cl,-1.9436100556,-0.0000406749,6.7446606
 807\C,-1.3642218249,-0.0001240181,3.5775658464\O,-5.9610735473,-0.0000
 222519,2.3663412595\Cl,-7.1408666346,0.0000740164,5.1346943154\O,-4.92
 72508739,0.0000528003,7.0573860626\O,3.5203620013,0.0004766436,-0.7342
 627841\H,-0.5067602225,-0.0001356898,4.2445460195\H,-6.8627269557,0.00
 00117225,2.7330931291\H,-4.1610469108,0.0000452993,7.6570556688\H,-0.9
 759706175,-0.0000393641,-0.5225431977\H,1.1328141909,0.0000846319,-1.8
 21534121\H,3.4122353806,0.0004346899,1.8858302961\H,1.3044215693,0.000
 3286936,3.1840089589\\Version=AM64L-G03RevD.02\State=2-A\HF=-802.60861
 97\S2=0.79263\S2-1=0.\S2A=0.751416\RMSD=1.429e-09\RMSF=6.469e-05\Therm
 al=0.\Dipole=-1.4613753,-0.00041,1.1134844\PG=C01 [X(C14H7Cl2O3Se1)]\
 @

no imaginary frequencies

Sum of electronic and thermal Enthalpies= -802.419116

resvSeCl2rad3 (3)



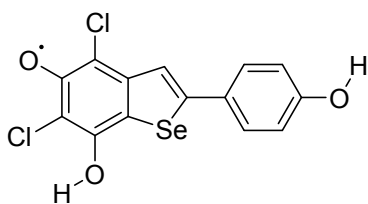
B3lyp/gen pseudo=read opt freq scale=0.9806\\Se Cl2 resv rad\\0,2

\C,0.019525546,-0.0039012869,-0.0043524153\C,0.0038211453,-0.004578073
1,1.4192971447\C,1.2351707501,-0.0033465255,2.1005716249\C,2.534673618
6,0.0021559106,1.4418821355\C,2.4577159862,0.0063168157,-0.0254179015\
C,1.2531824592,0.0033502559,-0.7261622325\C,-1.1475789248,-0.019512668
,2.2842065105\C,-0.8725938373,-0.0248384992,3.6324889124\Se,1.00740672
76,-0.0024300064,3.9522904442\O,3.6123860154,0.0034186777,2.0665076222
\O,1.186940347,0.0073706047,-2.0788123905\Cl,-1.4583930449,-0.00879596
79,-0.9000210008\C,-1.8433217415,-0.0191713019,4.7383941076\C,-3.12590
85315,0.5452763481,4.5624770713\C,-4.0639839269,0.5473119894,5.5979125
27\C,-3.7348823294,-0.0102873044,6.8456135804\C,-2.4615069807,-0.56876
37499,7.0456619916\C,-1.5351704017,-0.5709011578,6.0021839349\O,-4.607
9226132,-0.0328429027,7.9001528114\Cl,3.942762848,0.0170161502,-0.9254
527367\H,-2.16177853,-0.0562021527,1.893520266\H,2.0962306595,0.012779
4029,-2.4280449111\H,-0.5605349744,-1.0310557284,6.1684690915\H,-2.218
2726606,-1.0006100772,8.0153414267\H,-5.0478924968,0.9946609,5.4429290
543\H,-3.3854509674,1.0080473306,3.6113546512\H,-5.4450628911,0.376937
4915,7.6361538804\\Version=AM64L-G03RevD.02\State=2-A\HF=-802.610326\S
2=0.779736\S2-1=0.\S2A=0.750619\RMSD=9.657e-09\RMSF=7.140e-06\Thermal=
0.\Dipole=-1.9815787,0.2327447,0.2547834\PG=C01 [X(C14H7Cl2O3Se1)]\@

no imaginary frequencies

Sum of electronic and thermal Enthalpies= -802.420726

resvSeCl2rad5 (5)



```

B3lyp/gen pseudo=read opt freq scale=0.9806\\Se Cl2 resv rad\\0,2
\\C,-0.0320351556,0.0097816845,-0.0349134522\\C,-0.0355785152,-0.0005494
519,1.3691975032\\C,1.2143684137,-0.0143810993,2.0500085278\\C,2.4609697
781,-0.012545344,1.3605815099\\C,2.458784989,0.0008120433,-0.0203357615
\\C,1.2218303796,0.0132254103,-0.8156750171\\C,-1.1758976666,-0.01218977
08,2.257576521\\C,-0.8934459605,-0.0277456959,3.5979761685\\Se,0.9999782
047,-0.0255197157,3.9067718219\\O,3.5845861435,-0.0237758679,2.12249491
34\\O,1.228880242,0.026040013,-2.0587620474\\Cl,-1.5096770692,0.02309922
43,-0.9250511576\\C,-1.8444850718,-0.0184277018,4.7191621257\\C,-3.13665
55917,0.5289066007,4.5564728236\\C,-4.0582986392,0.5311600167,5.6058618
308\\C,-3.7033730664,-0.008126893,6.8549674398\\C,-2.4202055759,-0.54832
09673,7.042018918\\C,-1.5099528112,-0.550772704,5.9845664688\\O,-4.55925
25191,-0.0287560452,7.9226860297\\Cl,3.9803724212,0.0063822843,-0.86325
56907\\H,-2.1928784064,-0.0367407705,1.8737587786\\H,4.3595188006,-0.021
3658142,1.5317576198\\H,-0.5272452548,-0.9967460038,6.1426219266\\H,-2.1
567736346,-0.9651848297,8.0129484763\\H,-5.0499072229,0.9644869024,5.46
08499442\\H,-3.4168123615,0.9767065796,3.6041447782\\H,-5.4059019305,0.3
670601042,7.6676411741\\Version=AM64L-G03RevD.02\\State=2-A\\HF=-802.608
1586\\S2=0.778937\\S2-1=0.\\S2A=0.750575\\RMSD=8.078e-10\\RMSF=1.095e-05\\Th
ermal=0.\\Dipole=-1.0203013,0.2143929,2.2638998\\PG=C01 [X(C14H7Cl2O3Se1)]\\@

```

no imaginary frequencies

Sum of electronic and thermal Enthalpies= -802.418493