Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Kinetic study of the reaction of thiophene-tocopherols with peroxyl radicals enlightens the role of O•---S noncovalent interactions on H-atom transfer

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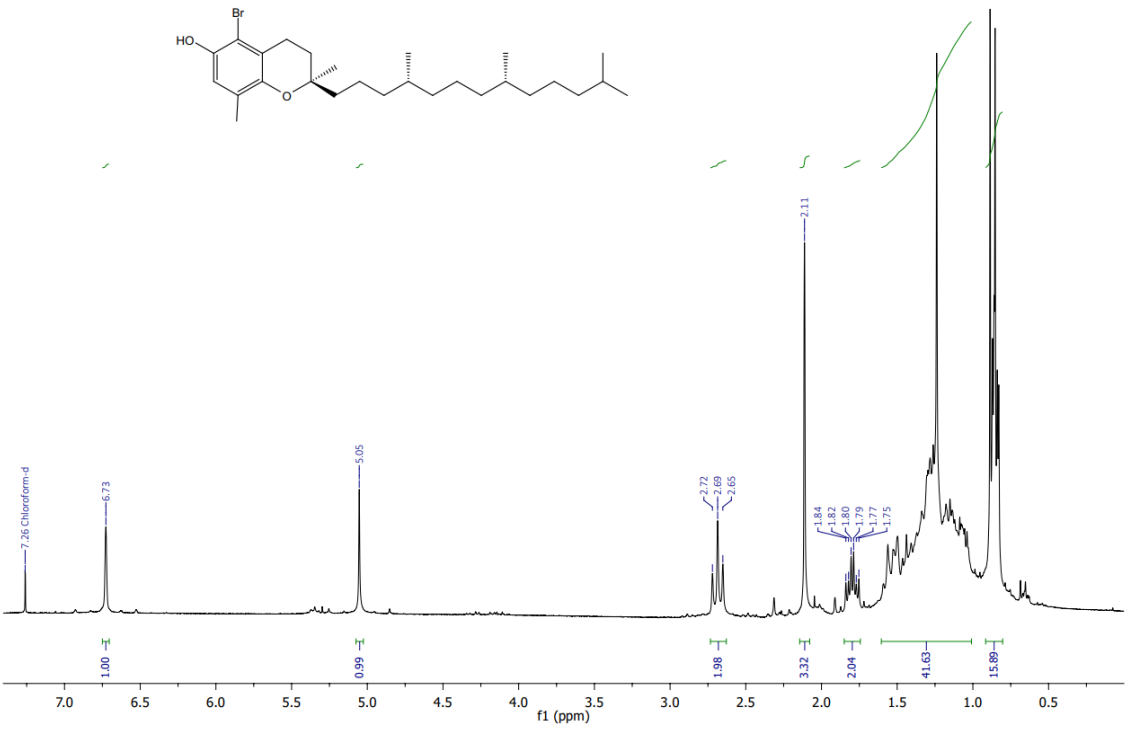


Figure S1. ^{1}H NMR spectrum of intermediate **11** in $CDCl_3$.

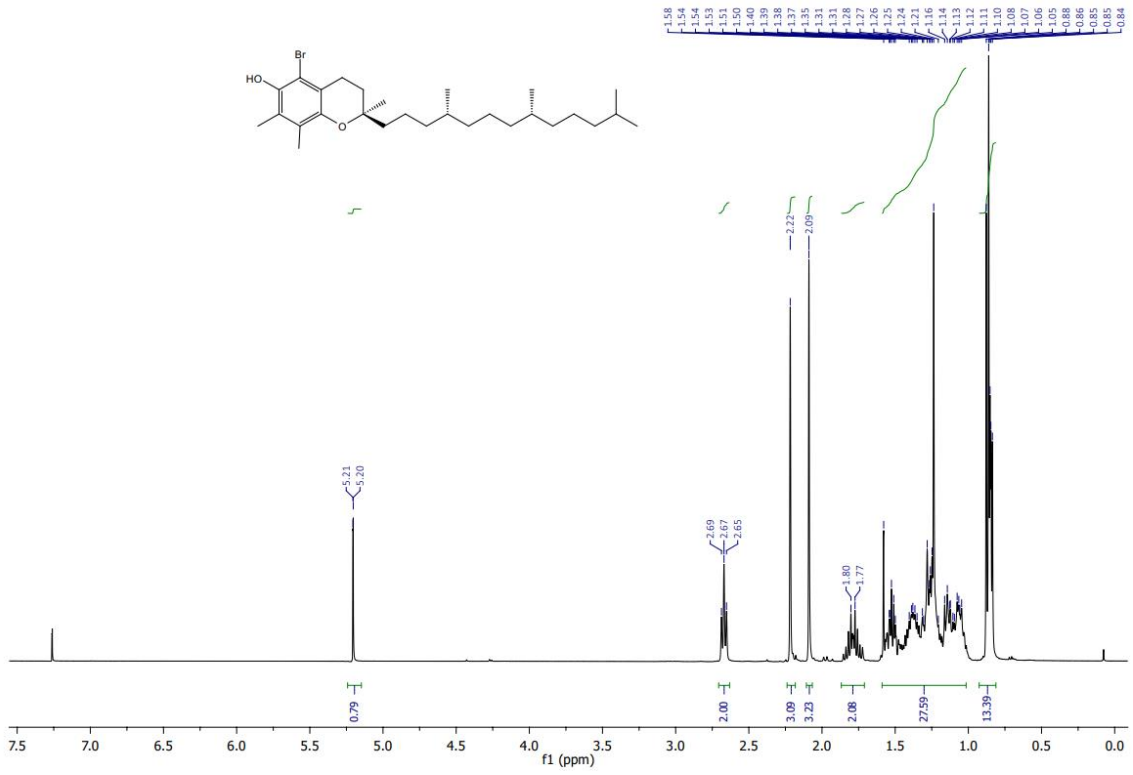


Figure S2. ^{1}H NMR spectrum of intermediate **12** in $CDCl_3$.

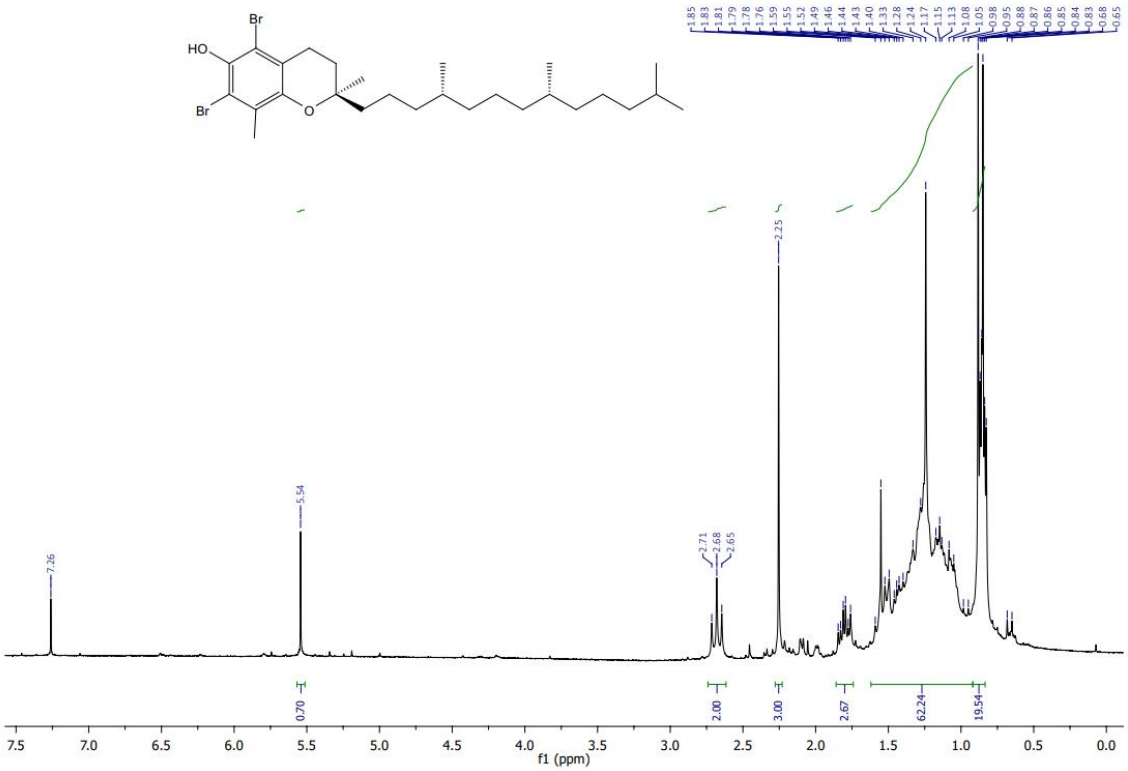


Figure S3. ^{1}H NMR spectrum of intermediate **13** in $CDCl_3$.

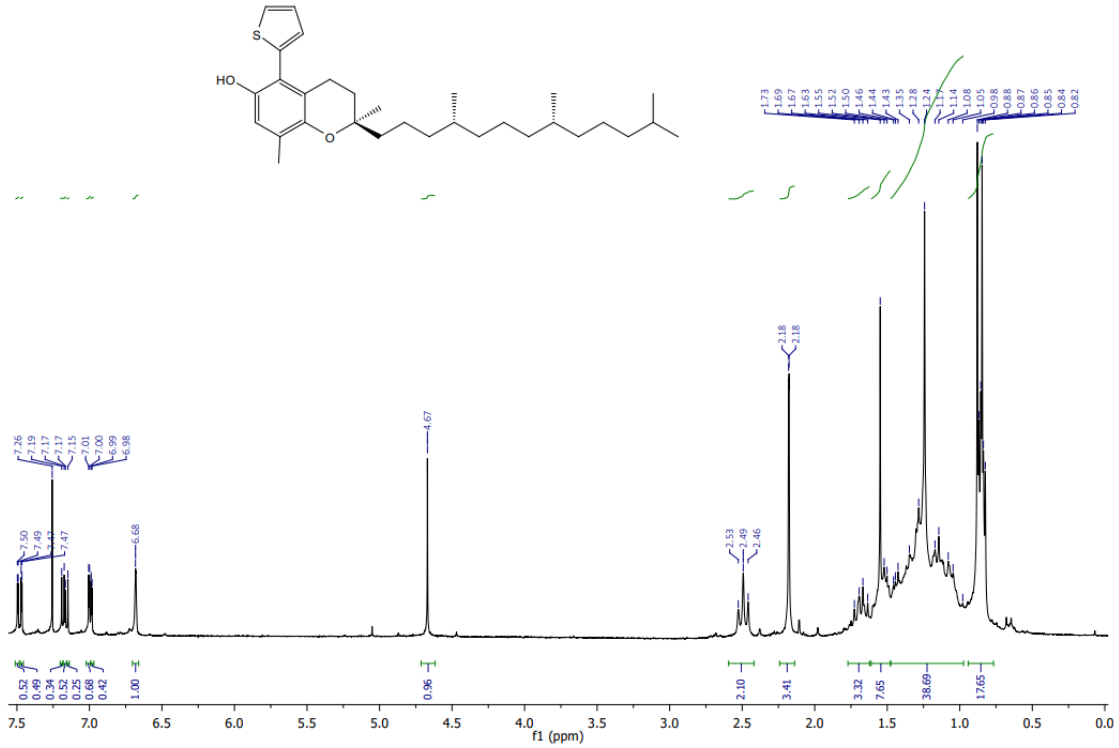


Figure S4. ^{1}H NMR spectrum of antioxidant **8** in $CDCl_3$.

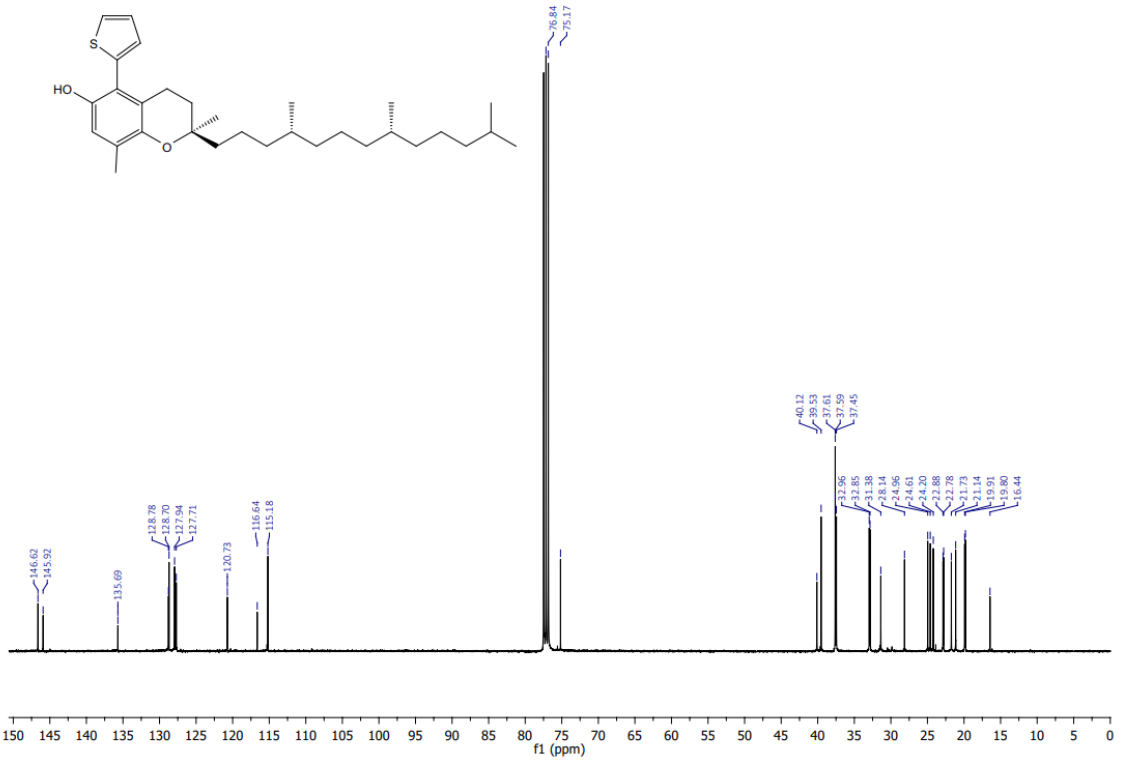


Figure S5. ^{13}C {^{1}H} NMR spectrum of antioxidant **8** in $CDCl_3$.

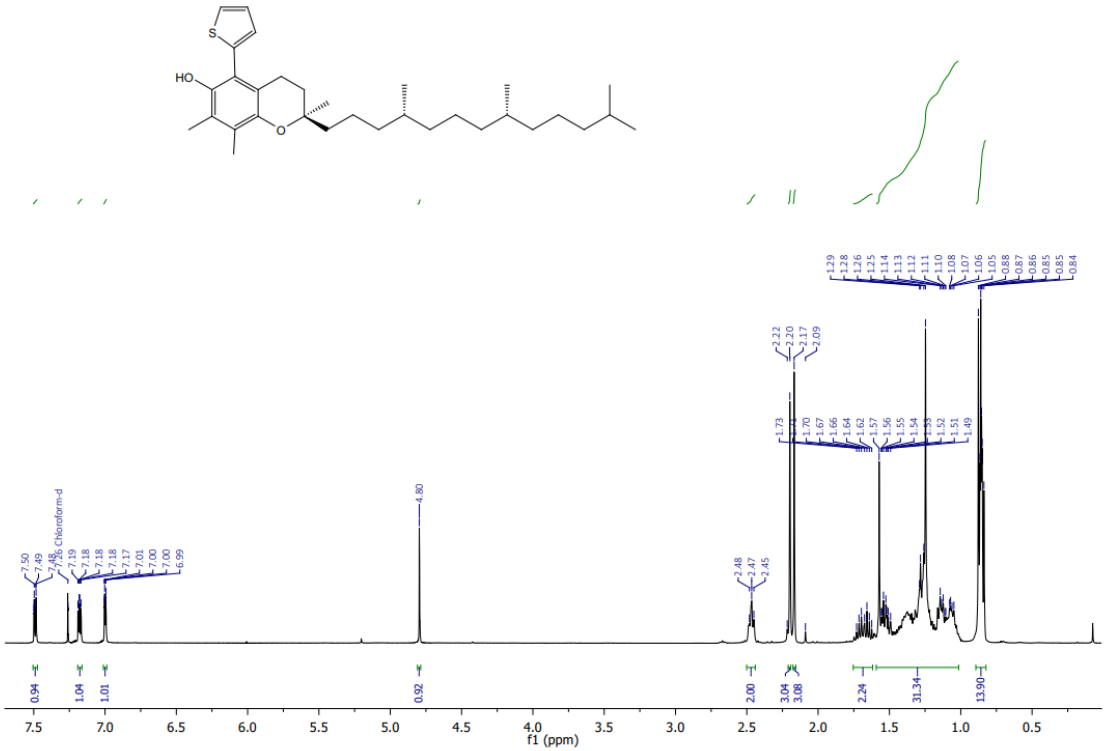


Figure S6. ^{1}H NMR spectrum of antioxidant **9** in $CDCl_3$.

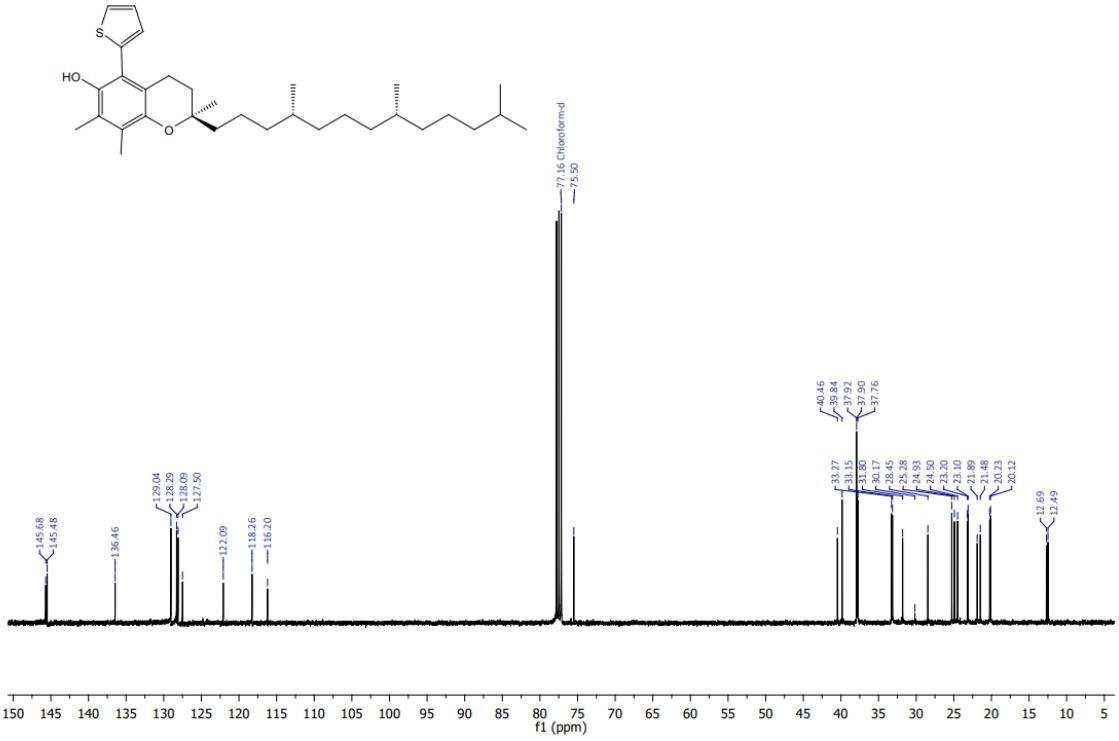


Figure S7. ^{13}C $\{^{1}H\}$ NMR spectrum of antioxidant **9** in $CDCl_3$.

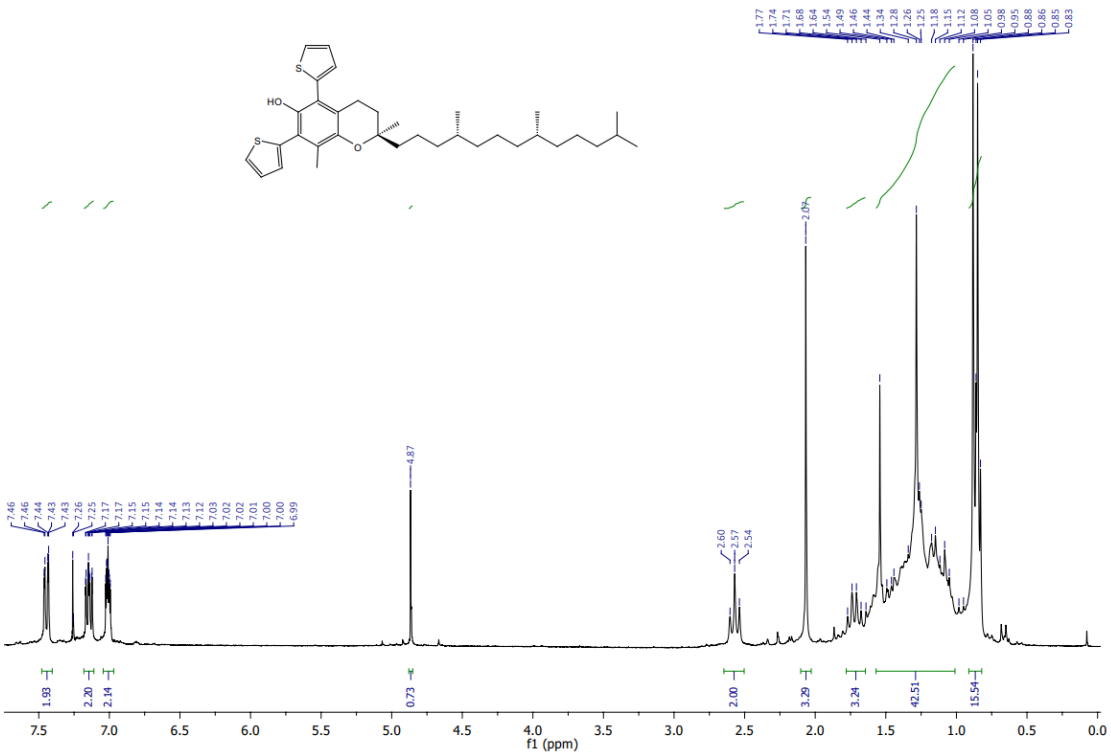


Figure S8. ^{1}H NMR spectrum of antioxidant **10** in $CDCl_3$.

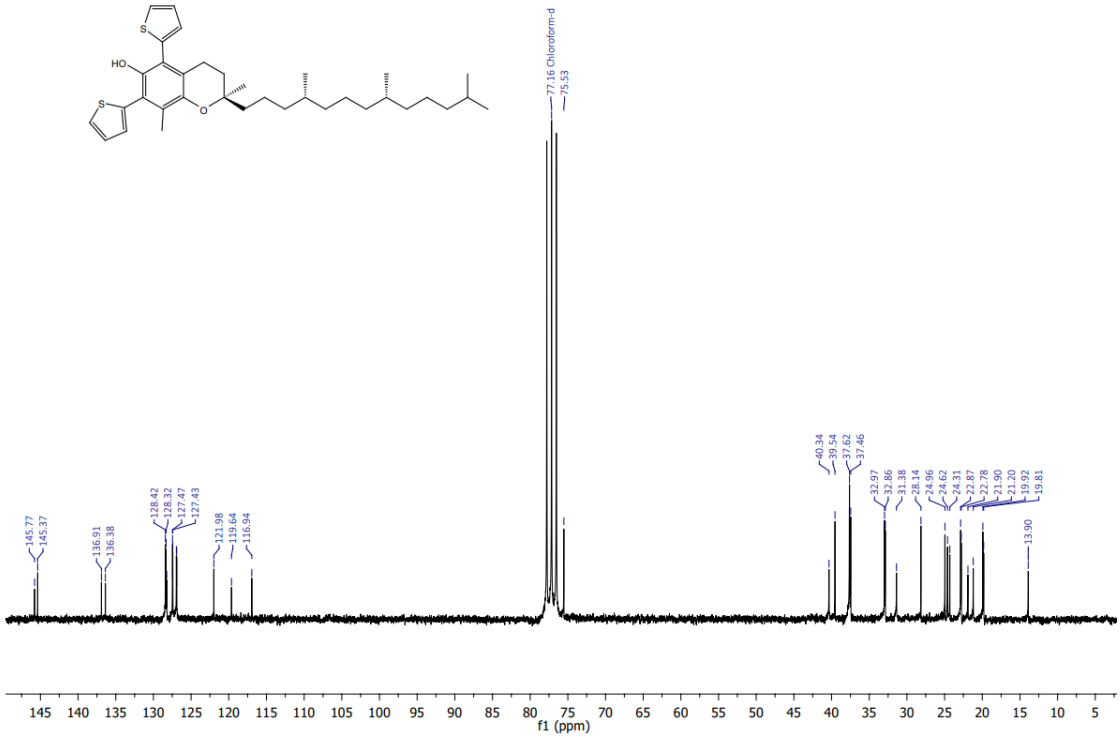
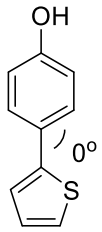


Figure S9. ^{13}C $\{^{1}H\}$ NMR spectrum of antioxidant **10** in $CDCl_3$.

CBS-QB3 optimized structures and energies in gas phase



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0 1

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C	0.75670300	-0.96844200	0.00000000
C	2.12037000	-1.15894200	0.00000000
C	2.51292500	-2.52452700	0.00000000
C	0.00000000	0.29012700	0.00000000
C	0.66007800	1.52886800	0.00000000
C	-0.04301900	2.72673500	0.00000000
C	-1.43915800	2.72274000	0.00000000
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C	-1.40557500	0.31395600	0.00000000
H	0.49753000	3.66904000	0.00000000
H	-3.20094100	1.50627400	0.00000000
H	-1.96064200	-0.61733800	0.00000000
H	1.44919800	-4.45924600	0.00000000
H	3.54368900	-2.85401000	0.00000000
H	2.83175800	-0.34422000	0.00000000
H	1.74233100	1.56646300	0.00000000
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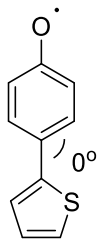
H	-1.59933500	4.62875300	0.00000000



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C	0.65597300	-0.95119100	0.00000000
C	2.01683200	-1.23318700	0.00000000
C	2.31526000	-2.61215400	0.00000000
C	0.00000000	0.33203600	0.00000000
C	0.76324600	1.53952700	0.00000000
C	0.16162200	2.76355000	0.00000000
C	-1.28903400	2.90371200	0.00000000
C	-2.04513000	1.65828300	0.00000000
C	-1.42183200	0.44423800	0.00000000
H	0.73982400	3.68017800	0.00000000
H	-3.12551500	1.74232500	0.00000000
H	-2.02260400	-0.45902400	0.00000000
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H	3.32032500	-3.01203400	0.00000000
H	2.77831300	-0.46614300	0.00000000
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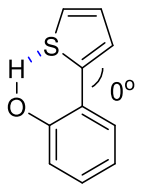

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C	0.29099600	3.12076600	0.00000000
C	0.81059900	1.83914400	0.00000000
C	0.00000000	0.68236600	0.00000000
H	-3.00049800	2.29266400	0.00000000
H	0.95886700	3.97377800	0.00000000
H	1.88570700	1.72041700	0.00000000
C	0.66746800	-0.63280200	0.00000000

O	-2.35480900	-0.08105500	0.00000000
H	-1.98478700	-0.96924500	0.00000000
C	2.02370400	-0.89083700	0.00000000
S	-0.18248900	-2.16372300	0.00000000
H	-1.52204500	4.29566900	0.00000000
C	1.27023500	-3.09058400	0.00000000
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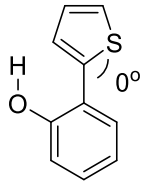

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C	1.06449000	-1.79417100	0.00000000
C	0.64906400	-3.15375500	0.00000000
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C	1.03686000	2.81657300	0.00000000
C	-0.20326700	3.43140600	0.00000000
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H	1.95471700	3.39189600	0.00000000
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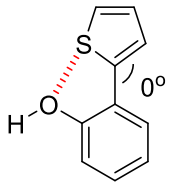

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C	-1.38291900	-3.01352900	0.00000000
C	0.00000000	0.69203500	0.00000000
C	1.40510600	0.82093600	0.00000000
C	2.01912400	2.07369500	0.00000000
C	1.25880900	3.23564500	0.00000000
C	-0.13097800	3.14012400	0.00000000
C	-0.73647900	1.89159600	0.00000000
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H	3.10425700	2.12814900	0.00000000
H	-0.74215900	4.03471900	0.00000000
H	-1.81727900	1.84141700	0.00000000
H	1.74805800	4.20252100	0.00000000
H	-3.48458500	-2.49407600	0.00000000
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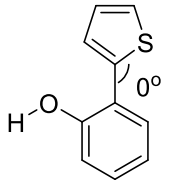

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C	1.21473700	2.71752800	0.00000000

C	0.02512900	3.43488600	0.00000000
C	-1.18461300	2.74646200	0.00000000
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S	-1.60503300	-1.69358300	0.00000000
C	-0.86323400	-3.24950500	0.00000000
C	0.49799300	-3.15278200	0.00000000
C	0.95834200	-1.80842700	0.00000000
O	2.39570900	0.63300700	0.00000000
H	2.16694800	3.24137000	0.00000000
H	-2.12487800	3.28443900	0.00000000
H	-2.13486300	0.84126200	0.00000000
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H	-1.47845000	-4.13603400	0.00000000
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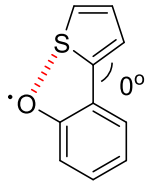

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H	3.21874600	1.98123200	0.00000000
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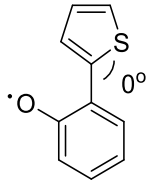

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C	-1.17924000	1.35168500	0.00000000
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H	2.20179500	3.26893600	0.00000000
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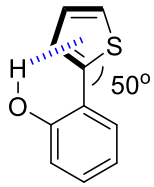

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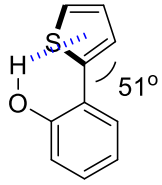
C	-1.43927200	0.95456800	-0.20705000
C	-2.82714800	0.81136000	-0.24357300
C	-3.41200800	-0.41229700	0.05512200
C	-2.61846300	-1.51082300	0.38674200
C	0.84404900	0.01251900	0.18090500
O	-0.93009100	2.17579900	-0.52826800
H	-3.42408200	1.67278500	-0.51742000
H	-3.07219400	-2.46645500	0.61993500
H	-0.61290700	-2.20990100	0.70241800
H	-4.49140100	-0.50911500	0.02495200
S	1.88931400	-1.10648400	-0.65437700
C	1.59861400	0.97795200	0.81135800
C	3.00118300	0.80968300	0.63642900
C	3.30952300	-0.27936500	-0.12777400
H	1.15944400	1.75406300	1.42592000
H	3.74529200	1.46345100	1.07184600
H	4.28391300	-0.64526500	-0.41268700
H	0.03345000	2.10679400	-0.57637800



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C	-1.61699700	-1.20302500	0.79602700
C	-0.83620400	-0.32111400	0.09061500
S	-1.85842700	0.79126900	-0.79982100
C	-3.29912200	0.06059300	-0.18855400
C	0.63527500	-0.28236300	0.00138300
C	1.34747300	-1.44456500	-0.33249200
C	2.73495200	-1.45389700	-0.39274000
C	3.43934500	-0.28050600	-0.12167200
C	2.76023300	0.88303200	0.21376700
C	1.36569200	0.89090200	0.28002200
O	0.77398700	2.06640100	0.63298000
H	3.28774400	1.80203100	0.43851600
H	3.26125800	-2.36294000	-0.65783500

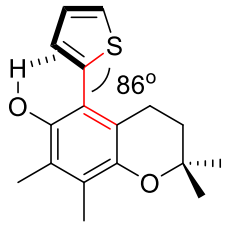
H	0.78611000	-2.34317400	-0.56131300
H	4.52235800	-0.27082600	-0.17057400
H	-4.26337100	0.44965000	-0.47703400
H	-3.77490100	-1.58661200	1.12242800
H	-0.17965700	1.93640500	0.71849100
H	-1.19174200	-1.97303100	1.42654100

B3LYP/6-31+g(d,p) optimized structures and energies in gas phase

$H^{\bullet}$ Sum of electronic and thermal Enthalpies: -0.497921

0 2

H	-0.92984050	2.58277519	0.41701857



Sum of electronic and thermal Enthalpies: -1208.204694

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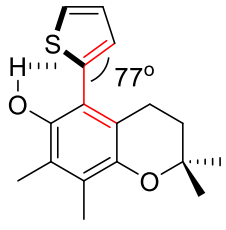
C	-0.33670500	-0.32667600	-0.03658900
C	-0.36749700	-1.84114500	-0.05737100
C	-1.71225800	-2.36968000	-0.56443400
C	-1.53423800	1.81450500	-0.10741200
C	-0.32105900	2.51192600	0.00734500
C	0.87490300	1.78259800	0.11366000
C	0.88066400	0.37871100	0.08799100

C	2.17924600	-0.33336200	0.19290800
S	3.06783400	-0.83838200	-1.23895000
C	4.34325100	-1.52073800	-0.28387800
C	4.10888600	-1.36427900	1.05663500
C	2.87894300	-0.68720500	1.32462700
C	-2.83655200	2.57176200	-0.21957400
C	-0.29292700	4.02262700	0.02267600
O	2.04385600	2.49561100	0.24141400
C	-4.21697300	-2.03174800	-0.57460000
C	-2.95143100	-1.76864500	1.58954300
H	2.51071700	-0.47146400	2.32204400
H	4.78547600	-1.71672200	1.82693800
H	2.77805600	1.87112400	0.34263100
H	-3.68965000	1.89672700	-0.16371400
H	-2.92994700	3.31899000	0.57658100
H	-2.89746000	3.11408000	-1.17209100
H	-5.03877200	-1.42699600	-0.17890200
H	-4.18182900	-1.89647500	-1.65979600
H	-4.42703800	-3.08465100	-0.35955300
H	-0.80432300	4.43786400	-0.85349300
H	-0.80335100	4.42236500	0.90823600
H	0.73116500	4.39542400	0.02921200
H	5.19077200	-1.99098100	-0.76432000
H	-3.04257700	-2.82541900	1.86416200
H	-2.05697800	-1.36562400	2.07210100
H	-3.81872600	-1.23228400	1.98617200
H	0.44079200	-2.22675300	-0.68659600
H	-0.16428200	-2.22787800	0.95080500
H	-1.80678100	-3.44121400	-0.35518900
H	-1.77262500	-2.24479800	-1.65247800

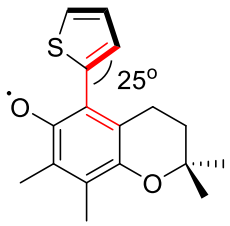


Sum of electronic and thermal Enthalpies: -1208.205087

0 1

C	-2.86046600	-1.62619900	-0.01533000

O	-2.76678500	-0.18961900	-0.19817300
C	-1.53019500	0.41916900	-0.11824800
C	-0.33076000	-0.29966400	-0.19638000
C	-0.35488500	-1.80547900	-0.36133700
C	-1.73290400	-2.29564700	-0.81422000
C	-1.54306900	1.82500300	0.00341000
C	-0.32904300	2.52885300	0.04270300
C	0.87678100	1.81045400	-0.02058400
C	0.88899000	0.41077800	-0.13861800
C	2.19577700	-0.28820000	-0.20527600
S	2.84905800	-1.15414000	1.17708400
C	4.27946500	-1.59826200	0.30477000
C	4.26622200	-1.10134600	-0.97168400
C	3.08193700	-0.35457300	-1.25867700
C	-2.85590500	2.56883300	0.07613000
C	-0.30823700	4.03528100	0.16069000
O	2.04671900	2.53038400	0.04331400
C	-4.23174700	-1.99674500	-0.57996000
C	-2.79024500	-1.94100200	1.48706200
H	2.87438200	0.10720900	-2.21833700
H	5.06679300	-1.26266100	-1.68468200
H	2.79236300	1.91681500	-0.04202500
H	-3.68957900	1.88094800	0.21290000
H	-2.85749900	3.28897700	0.90158300
H	-3.03975400	3.13899900	-0.84407900
H	-5.02073700	-1.44707800	-0.05747300
H	-4.28855700	-1.75108900	-1.64469000
H	-4.41727700	-3.06891300	-0.45744100
H	-0.94097800	4.50208000	-0.60266500
H	-0.68914100	4.36463800	1.13605000
H	0.70462900	4.42245900	0.05049400
H	5.04474200	-2.19507300	0.78261500
H	-2.84871800	-3.02202100	1.65586200
H	-1.86262000	-1.57450100	1.93467100
H	-3.62625100	-1.46417600	2.00754100
H	0.40775800	-2.11113100	-1.08573700
H	-0.07628700	-2.29273300	0.58252900
H	-1.80495200	-3.38452300	-0.71435000
H	-1.88302700	-2.05562000	-1.87394500

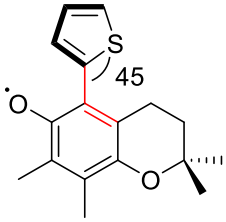


Sum of electronic and thermal Enthalpies: -1207.585839

0 2

C	2.33928300	-1.88074100	0.58689900
C	2.15368700	-0.58728700	0.10425900
S	3.70217500	0.04794800	-0.45704900
C	4.50843600	-1.43449200	-0.09247500
C	3.66924800	-2.35826600	0.48255500
C	0.92447600	0.19592400	0.04574300
C	-0.35689600	-0.38496000	-0.02900600
C	-1.48596300	0.46416500	0.00321700
C	-1.40561600	1.89264900	0.08833000
C	-0.16585600	2.49021700	0.09843400
C	1.04391200	1.66660100	0.03614300
C	-0.59144400	-1.87054500	-0.21847700
C	-1.96302900	-2.14851800	-0.83634300
C	-3.07446400	-1.41706900	-0.08153900
O	-2.76389500	0.01060800	-0.07377500
C	-4.41257100	-1.51465300	-0.81325000
C	-3.21679000	-1.87225200	1.37743700
C	-2.69672800	2.67364700	0.13437100
C	0.02511100	3.98516500	0.15152900
O	2.17308500	2.20954700	-0.03104000
H	1.55191500	-2.46133700	1.04519100
H	3.98672200	-3.33687400	0.82440300
H	-3.32330900	2.34625000	0.97091500
H	-2.51418600	3.74294100	0.23859100
H	-3.28642200	2.51188000	-0.77512100
H	-5.17104900	-0.90924500	-0.30808300
H	-4.31685000	-1.16023200	-1.84377500
H	-4.75614000	-2.55394300	-0.83259900
H	-0.43624900	4.48147800	-0.71046300
H	-0.42513500	4.41474100	1.05418700
H	1.09010000	4.21801300	0.15123000

H	5.56914200	-1.53220700	-0.28470000
H	-3.45538000	-2.94040500	1.42001600
H	-2.29999700	-1.70162500	1.94765200
H	-4.02469200	-1.31883300	1.86474500
H	0.19509500	-2.28466300	-0.85651900
H	-0.51507400	-2.40335500	0.73773300
H	-2.16970800	-3.22432300	-0.83812400
H	-1.97588300	-1.81416900	-1.88094700

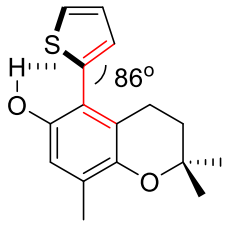


Sum of electronic and thermal Enthalpies: -1207.584565

0 2

C	3.38877400	0.21659600	-0.81272400
C	2.25947000	-0.22476600	-0.14813900
S	2.65630000	-1.66946100	0.78278500
C	4.29884400	-1.64930600	0.24048400
C	4.53685900	-0.59671800	-0.60577900
C	0.94423900	0.42008600	-0.09398300
C	-0.26351500	-0.28785100	-0.14351300
C	-1.47708500	0.43183100	-0.03729500
C	-1.54041700	1.85614800	0.08285300
C	-0.36731400	2.58012800	0.09193500
C	0.92744300	1.89357300	0.00569400
C	-0.33000600	-1.78546400	-0.37950300
C	-1.69906100	-2.20820400	-0.91686400
C	-2.83724700	-1.61629400	-0.08222300
O	-2.69767200	-0.16084300	-0.07924100
C	-4.19922700	-1.86780400	-0.72751700
C	-2.82768600	-2.09203800	1.37693500
C	-2.90458400	2.49651700	0.17994800
C	-0.33763900	4.08411100	0.19899700
O	1.99302800	2.55509900	0.02414400
H	3.38406400	1.11157200	-1.41937600
H	5.50180600	-0.40337700	-1.06041200
H	-3.46421600	2.09768500	1.03297900

H	-2.83326400	3.57814200	0.29129600
H	-3.50439100	2.28011200	-0.71128000
H	-4.98908400	-1.35860200	-0.16728100
H	-4.21340600	-1.49982500	-1.75766700
H	-4.41850300	-2.94029200	-0.73745800
H	-0.88733300	4.55714400	-0.62318800
H	-0.79232500	4.42917000	1.13539200
H	0.69534300	4.43125600	0.17107000
H	4.98765500	-2.41291800	0.57569600
H	-2.93482200	-3.18114600	1.42087800
H	-1.90110400	-1.81779800	1.88773900
H	-3.66111500	-1.64098800	1.92322800
H	0.45198900	-2.07743300	-1.08669100
H	-0.11544700	-2.33464900	0.54490200
H	-1.78402500	-3.30025600	-0.92774900
H	-1.81655300	-1.86374000	-1.95170500

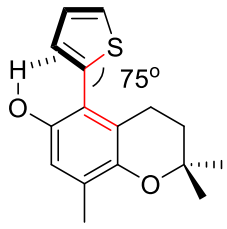


Sum of electronic and thermal Enthalpies: -1168.916789

0 1

C	2.94022200	-1.32667100	0.05919500
O	2.78161500	0.08630900	-0.23666900
C	1.53332300	0.65785700	-0.11016500
C	0.35171200	-0.08820600	-0.02762300
C	0.41588400	-1.60126700	-0.04931500
C	1.76910300	-2.09603600	-0.56958500
C	1.51697700	2.06929700	-0.10138000
C	0.29149200	2.71866100	0.01298800
C	-0.90056400	1.99554600	0.11492700
C	-0.88554500	0.59259000	0.09147000
C	-2.17120000	-0.14137900	0.19395000
S	-3.04360800	-0.67138200	-1.23850000
C	-4.31531700	-1.36263900	-0.28495700
C	-4.09183700	-1.19009400	1.05546800
C	-2.87316800	-0.49352800	1.32476300
C	2.80721000	2.84058500	-0.21180500

O	-2.06056800	2.71697100	0.23376800
C	3.01374700	-1.50477800	1.58360900
C	4.26764300	-1.71108000	-0.59355200
H	0.24337200	3.80311200	0.02907800
H	-2.51453100	-0.26286300	2.32232900
H	-4.76850300	-1.54466100	1.82471500
H	-5.15295900	-1.84943100	-0.76622800
H	-2.80420600	2.10317800	0.33366600
H	3.32911200	2.60690700	-1.14653500
H	2.61973600	3.91707200	-0.17852400
H	3.49463700	2.58043500	0.60067400
H	3.87382200	-0.95847800	1.98222800
H	2.11544100	-1.12594800	2.07856700
H	3.12651800	-2.56371000	1.84132000
H	4.50099700	-2.76190300	-0.39287300
H	4.22081400	-1.56381700	-1.67674500
H	5.07984400	-1.09396200	-0.19732200
H	-0.38838900	-2.00456200	-0.67244900
H	0.23014300	-1.99332800	0.96008600
H	1.88591000	-3.16792000	-0.37420900
H	1.81950400	-1.95740600	-1.65649600

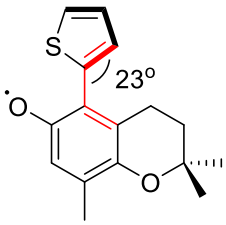


Sum of electronic and thermal Enthalpies: -1168.917234

0 1

C	-2.91197300	-1.33418500	0.03676800
O	-2.78571100	0.10711400	0.16357300
C	-1.53362900	0.67809500	0.08519200
C	-0.34586400	-0.05648900	0.17948200
C	-0.40550300	-1.55702200	0.37826300
C	-1.79322900	-1.99974600	0.85199900
C	-1.52334200	2.08247200	-0.05799900
C	-0.29561500	2.73495900	-0.11290800
C	0.90479900	2.02271300	-0.03456400
C	0.89452600	0.62637900	0.11138600

C	2.18738000	-0.09402900	0.19583000
S	2.81239700	-1.03051800	-1.15302300
C	4.24664700	-1.45506500	-0.27727700
C	4.25568800	-0.89996000	0.97499100
C	3.08546500	-0.12392600	1.24088400
C	-2.82177100	2.84326600	-0.14067500
O	2.06576000	2.74818700	-0.11279700
C	-2.85769000	-1.70291000	-1.45382000
C	-4.28717800	-1.65425100	0.62193500
H	-0.25125800	3.81394100	-0.22450200
H	2.89563400	0.38365400	2.18087500
H	5.06235500	-1.04029100	1.68553700
H	4.99730600	-2.08479100	-0.73563700
H	2.81988100	2.14420300	-0.03106000
H	-3.42692900	2.69284200	0.76041300
H	-2.63699200	3.91408400	-0.26020300
H	-3.42984400	2.49754900	-0.98392600
H	-3.68644900	-1.22677400	-1.98626100
H	-1.92505400	-1.37220100	-1.91867500
H	-2.94010500	-2.78765800	-1.58424600
H	-4.49898400	-2.72496400	0.53434700
H	-4.33074500	-1.37428400	1.67879500
H	-5.06628600	-1.10215600	0.08745900
H	0.35393700	-1.86465200	1.10518500
H	-0.14569200	-2.07282800	-0.55558700
H	-1.89027100	-3.08933800	0.78853600
H	-1.93151400	-1.72226500	1.90418200

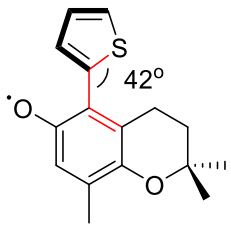


Sum of electronic and thermal Enthalpies: -1168.295870

0 2

C	-2.34562800	-1.67728000	0.53507000
C	-2.15703000	-0.36688000	0.09825000
S	-3.70960300	0.29959100	-0.41799200
C	-4.52001300	-1.18983000	-0.09632100
C	-3.67971800	-2.14085700	0.43168000
C	-0.93064800	0.41714500	0.05520100

C	0.35954000	-0.15555100	-0.02753900
C	1.49306000	0.68753100	0.01828000
C	1.40617200	2.11736100	0.11647800
C	0.16085200	2.67760700	0.13588300
C	-1.05144600	1.89007000	0.07381900
C	0.59629200	-1.63837900	-0.23779700
C	1.97185200	-1.90926300	-0.85089700
C	3.08129200	-1.18977200	-0.08162200
O	2.77141700	0.23854900	-0.05778800
C	3.21505900	-1.66230900	1.37248000
C	4.42267900	-1.27979600	-0.80791600
C	2.66495500	2.94320200	0.17013200
O	-2.16898400	2.45774000	0.03087900
H	0.02685300	3.75396500	0.18321000
H	-1.55728800	-2.28066100	0.96058100
H	-3.99972000	-3.12959200	0.74025700
H	-5.58367400	-1.27394200	-0.27846400
H	3.28086000	2.78780300	-0.72229400
H	2.41925600	4.00530000	0.24372000
H	3.28446300	2.66741000	1.03042400
H	4.02033900	-1.11524700	1.87111300
H	2.29504800	-1.49837200	1.93949300
H	3.45302600	-2.73097600	1.40324400
H	4.76526400	-2.31911000	-0.83813600
H	4.33254200	-0.91280300	-1.83452200
H	5.17921400	-0.68146200	-0.29156100
H	-0.18496200	-2.04249400	-0.88860000
H	0.51189700	-2.18455400	0.71018600
H	2.17685900	-2.98523500	-0.86551900
H	1.99060300	-1.56179500	-1.89108600

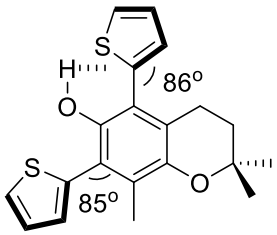


Sum of electronic and thermal Enthalpies: -1168.294717

0 2

C	-3.39795800	0.42930500	-0.74275500

C	-2.24505900	-0.03653900	-0.13394800
S	-2.60018800	-1.54633000	0.70893500
C	-4.25525900	-1.51384900	0.20918500
C	-4.52852900	-0.41253100	-0.56152800
C	-0.94594700	0.63301900	-0.06841700
C	0.28632400	-0.04237500	-0.12970900
C	1.48885800	0.69447000	-0.01144700
C	1.51733900	2.12073200	0.13034200
C	0.32125200	2.78284400	0.15108100
C	-0.95824100	2.10773400	0.06007900
C	0.38809200	-1.53439400	-0.39037000
C	1.76620300	-1.91915200	-0.93403600
C	2.89338900	-1.32008300	-0.08976700
O	2.72211300	0.13221100	-0.05993800
C	2.89517800	-1.82160600	1.36062900
C	4.25945100	-1.53078100	-0.74070700
C	2.83900200	2.83639600	0.23786000
O	-2.02036100	2.77309200	0.10102300
H	0.27972200	3.86356900	0.24825400
H	-3.41999100	1.36095100	-1.29049800
H	-5.50676300	-0.20528900	-0.98005700
H	-4.92533700	-2.30780100	0.51022400
H	3.46292600	2.65373600	-0.64378900
H	2.68130900	3.91308700	0.33648700
H	3.41060300	2.48642100	1.10433900
H	3.71855700	-1.36190800	1.91483900
H	1.96293300	-1.57760200	1.87647500
H	3.02683200	-2.90861000	1.38474300
H	4.50140100	-2.59799100	-0.77013200
H	4.26476400	-1.14410100	-1.76405100
H	5.03893300	-1.01523400	-0.17183400
H	-0.38542900	-1.83311800	-1.10382100
H	0.18523500	-2.10289800	0.52505400
H	1.87261700	-3.00890900	-0.96407300
H	1.87611000	-1.55457900	-1.96275500

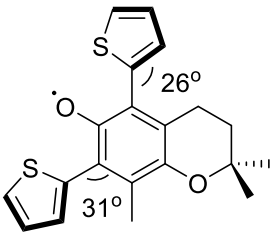


Sum of electronic and thermal Enthalpies: -1720.678979

0 1

S	-3.95851300	0.26186000	-1.20463800
C	-2.99156600	-0.10465300	0.20873800
C	-3.79614700	-0.23233000	1.31398700
C	-5.18507800	-0.04212900	1.03681500
C	-5.42716400	0.23078600	-0.28349600
C	-1.51510700	-0.22739300	0.12252000
C	-0.88455600	-1.47401000	-0.03077200
C	0.52473900	-1.52680500	-0.08362900
C	1.31291800	-0.37334800	-0.01599300
C	0.67282200	0.87767500	0.13768000
C	-0.72703700	0.93902900	0.20951900
O	1.05437800	-2.78975700	-0.24143100
C	2.47059800	-2.99608000	0.00649700
C	3.25622100	-1.84532700	-0.63884600
C	2.82110100	-0.48241300	-0.09209000
C	1.45014600	2.13913900	0.22691400
C	1.87958200	2.80783000	1.35113300
C	2.60737600	4.00496300	1.06883700
C	2.72688700	4.24474700	-0.27452800
S	1.94736700	3.01532500	-1.21503000
C	-1.65676700	-2.76453900	-0.14354200
O	-1.38503000	2.12770300	0.36881600
C	2.78951500	-4.32960200	-0.66869900
C	2.69622800	-3.08861700	1.52354000
H	1.68118600	2.44107400	2.35267800
H	3.02046200	4.65554500	1.83130100
H	3.22072300	5.07296700	-0.76484000
H	-0.73033800	2.83895700	0.44271200
H	-1.38126000	-3.45253700	0.66358600
H	-2.73209200	-2.59126600	-0.10358100
H	-1.41479500	-3.27787700	-1.08061600
H	2.16032300	-5.12493100	-0.25765500

H	2.60725800	-4.26896000	-1.74583100
H	3.83848000	-4.59794300	-0.50562200
H	-6.37672700	0.41604500	-0.76716500
H	-5.96569200	-0.10505700	1.78675700
H	-3.39877600	-0.45113300	2.29907000
H	3.75884700	-3.23748700	1.74504800
H	2.36322700	-2.18313600	2.03805900
H	2.13590100	-3.93425400	1.93329400
H	3.22517400	0.31541900	-0.72290900
H	3.25300800	-0.31626300	0.90429000
H	3.08073500	-1.88216600	-1.72092100
H	4.32962200	-1.99705400	-0.47955300



Sum of electronic and thermal Enthalpies: -1720.059783

0 2

S	-4.01981500	0.28387700	-0.53299500
C	-2.83719500	-0.82759600	0.14485200
C	-3.49292200	-1.84801400	0.82056100
C	-4.90832300	-1.75923100	0.77151800
C	-5.33582000	-0.67232200	0.04834900
C	-1.39296200	-0.63621400	0.00665600
C	-0.49149400	-1.69339300	-0.07619500
C	0.90819400	-1.39974000	-0.07652000
C	1.44746100	-0.09007400	-0.01659400
C	0.56197300	0.99747300	0.03702200
C	-0.88528500	0.74436200	-0.06834800
O	1.68616400	-2.50979600	-0.16782800
C	3.14368400	-2.44908400	-0.09102100
C	3.61003900	-1.15137500	-0.75131700
C	2.95171600	0.06846900	-0.10569100
C	1.00182800	2.38419500	0.15599300
C	2.15641900	2.87492600	0.75961700
C	2.29280600	4.28426200	0.69780500
C	1.24636600	4.87803600	0.03434000
S	0.05558900	3.73432300	-0.47097700

C	-0.89809600	-3.14061100	-0.22868200
O	-1.67941100	1.69570800	-0.23483900
C	3.61952500	-3.67858800	-0.86420800
C	3.53680200	-2.55160700	1.38928200
H	2.86847200	2.24604500	1.27482700
H	3.12356400	4.82908600	1.13169000
H	1.09271300	5.93310900	-0.15195700
H	-0.86337300	-3.68090100	0.72595800
H	-1.91127600	-3.22040900	-0.62339000
H	-0.21098100	-3.65598400	-0.90265200
H	3.20120600	-4.59113800	-0.42922300
H	3.31010200	-3.62073700	-1.91189200
H	4.71151100	-3.74690300	-0.82675500
H	-6.35439400	-0.36025300	-0.14220600
H	-5.57477200	-2.46338400	1.25654300
H	-2.96896700	-2.62097500	1.36751600
H	4.62650500	-2.52079200	1.49510900
H	3.11062700	-1.73731400	1.98093800
H	3.17611800	-3.49592900	1.80700900
H	3.18764800	0.96844300	-0.68119700
H	3.38557000	0.22636900	0.88981600
H	3.35420600	-1.19252200	-1.81713000
H	4.70081700	-1.07756300	-0.68262700