Supporting Information for:

The Mechanism of Radical-Trapping Antioxidant Activity of Plant-Derived Thiosulfinates

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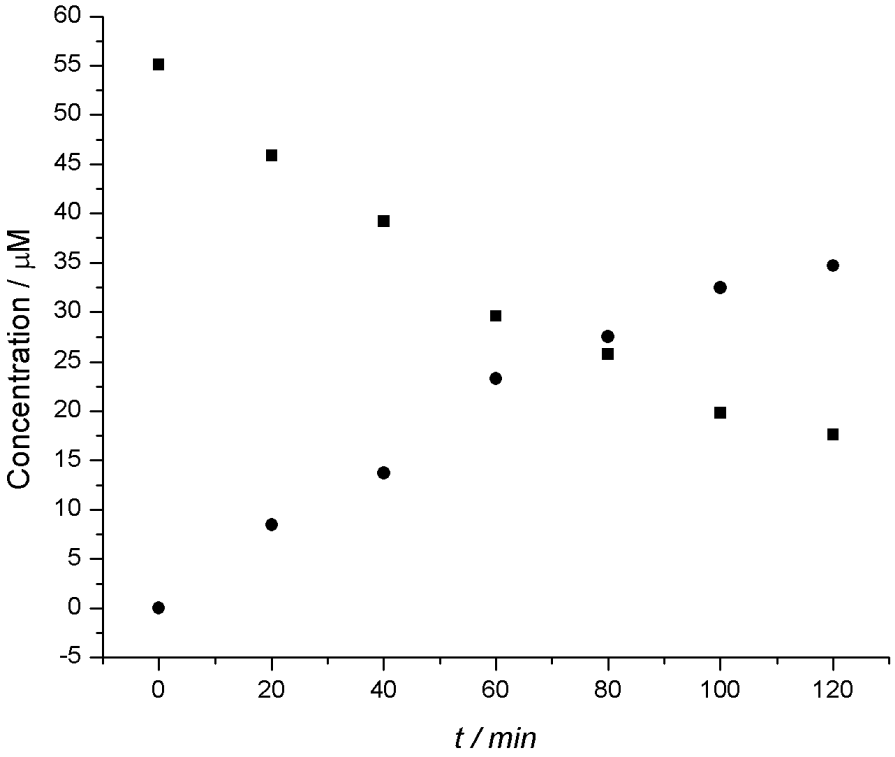

Figure S1. Decomposition of 50 μM allicin 1 (■) in the presence of 0.1 M ethyl propiolate in chlorobenzene and formation of the corresponding (*E*)-ethyl 3-(benzylsulfinyl)acrylate 4 (●).

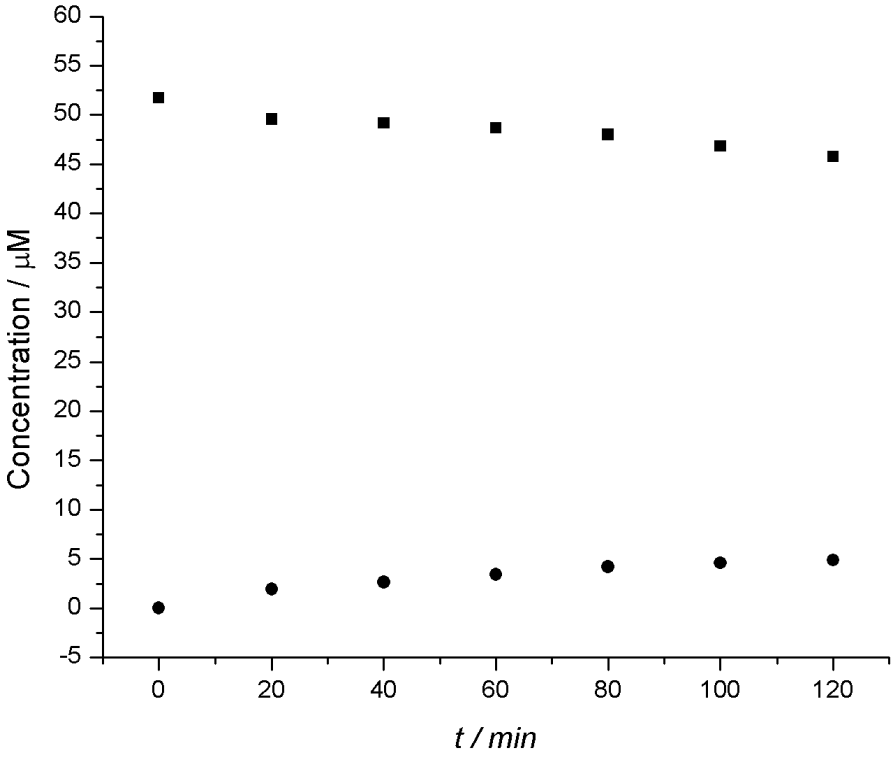

Figure S2. Decomposition of 50 μM PPT 3 (■) in the presence of 0.1 M ethyl propiolate in chlorobenzene and formation of the corresponding (*E*)-ethyl 3-(benzylsulfinyl)acrylate 6 (●).

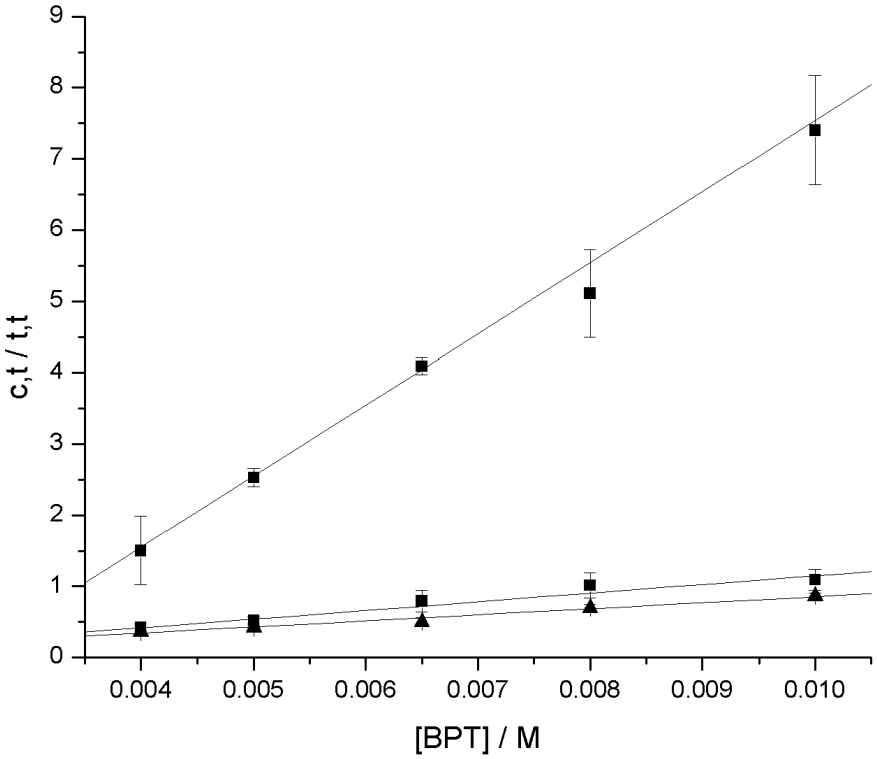

Figure S3. Product ratios in MeOAMVN-initiated autoxidations of methyl linoleate inhibited by various amounts of BPT 2 in chlorobenzene (▲), or chlorobenzene containing either HFIP (0.15 M, ●) or CH_3CN (1 M, ■).

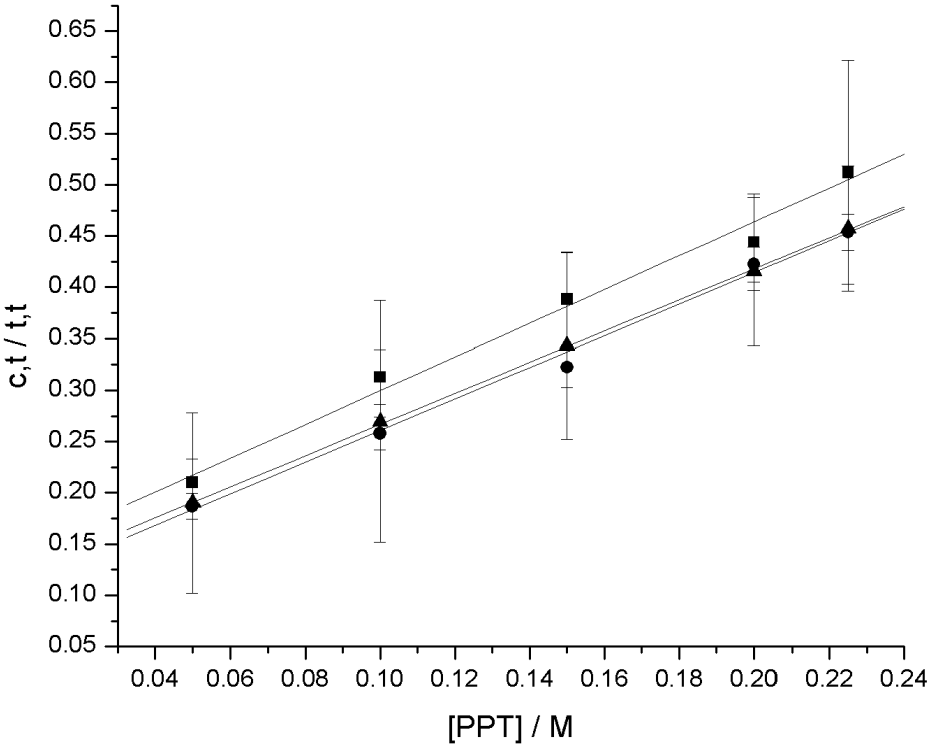

Figure S4. Product ratios in MeOAMVN-initiated autoxidations of methyl linoleate inhibited by various amounts of PPT 3 in chlorobenzene (▲), or chlorobenzene containing either HFIP (0.15 M, ●) or CH_3CN (1 M, ■).

Table S1. Relevant Enthalpies (in a.u.) for Bond Dissociation Enthalpy Calculations in Table 2.[a]

Compound	H_{298}^{o}	Compound	H_{298}^{o}
allicin	-1104.728881	allicin radical (next to divalent S)	-1104.102071
allicin	-1104.728881	allicin radical (next to tetravalent S)	-1104.093446
PPT	-1107.149627	PPT radical (next to tetravalent S)	-1106.498654
diallyldisulfide	-1029.607678	diallyldisulfide radical	-1028.978877
dipropyldisulfide	-1032.027206	dipropyldisulfide radical	-1031.378300
allylSOH	-590.513746	allylSO●	-589.906924
	-590.513723		-589.907136
	-590.513447		-589.907165
	-590.516990		
	-590.513565		
	-590.514757		
propylSOH	-591.724879	propylSO●	-591.116816
	-591.724944		-591.118024
	-591.723797		-591.116439
	-591.723812		
	-591.722524		
	-591.722686		
benzylSOH	-743.887934	benzylSO●	-743.281172
	-743.887262		-743.280304
	-743.889998		
allylSOOH	-665.662290	allylSOO●	-665.042727
	-665.662811		-665.043831
	-665.664059		-665.043630
	-665.662714		
	-665.666711		
	-665.663130		

[a] H_{298}^{o} (H-atom) = -0.497457 a.u.

Table S2. Relevant Structures for Bond Dissociation Enthalpy Calculations in Table 2.

allicin

C	3.86082300	1.41883900	0.14176800
H	4.64130200	0.66507300	0.18078200
H	4.18018300	2.44808100	0.02730900
C	2.57404600	1.09527200	0.23478600
H	1.81928900	1.87623400	0.18287700
C	2.07012200	-0.30100700	0.41467900
H	1.41553600	-0.40531000	1.29010000
H	2.88890400	-1.01323100	0.52441900
S	1.05195500	-0.90232900	-1.00327500
S	-0.90187600	-1.00447500	0.00755200
C	-1.46667200	0.75179500	-0.27473000
H	-0.70347900	1.37894100	0.19064400
H	-1.46513100	0.90269300	-1.35589000
C	-2.81562100	0.93982300	0.33862600
H	-2.85135300	0.90590200	1.42361400
C	-3.93532600	1.11565400	-0.35956900
H	-3.93378900	1.15111300	-1.44469700
H	-4.89308900	1.23982700	0.13205900
O	-0.65298200	-1.09533800	1.47587400

allicin radical (next to divalent S)

C	3.70430200	1.60203000	0.44647600
H	3.61065700	1.60193700	1.52662500
H	4.44401000	2.25999400	0.00918300
C	2.91543400	0.80115500	-0.33808600
H	3.05718100	0.83042600	-1.41564600
C	1.94269900	-0.07313400	0.16280200
H	1.72501000	-0.12585900	1.22626400
S	1.05588600	-1.17319900	-0.83382100
S	-0.93006600	-1.02751800	0.21499800
C	-1.40666200	0.65080600	-0.43949100
H	-0.57324200	1.30684600	-0.17630500
H	-1.47439200	0.54966800	-1.52474700
C	-2.69490800	1.07407400	0.18611000
H	-2.65952400	1.26722300	1.25416600
C	-3.84156700	1.20208700	-0.47819200
H	-3.90960800	1.01357600	-1.54525600
H	-4.75167500	1.51110600	0.02235500
O	-0.64966600	-0.81819400	1.66085100

allicin radical (next to tetravalent S)

C	-4.31985800	-0.48142800	0.19052100
H	-4.56742900	0.52469700	0.51416500
H	-5.09104800	-1.23514800	0.29905800
C	-3.12712400	-0.77684200	-0.31958400
H	-2.90358900	-1.79669500	-0.62234800
C	-2.02341000	0.21736200	-0.50096000
H	-2.36211200	1.23432300	-0.30498100
S	-0.64640800	-0.19210900	0.67314400
S	0.97296400	0.79861900	-0.41142800
C	2.23391200	0.15721000	0.67097400
H	2.42552900	0.81594400	1.51084900
C	3.00606400	-0.96740200	0.39705300
H	3.79156600	-1.18505100	1.11715900
C	2.86744600	-1.81882400	-0.67607100
H	2.11723300	-1.65697300	-1.44026000
H	3.51594700	-2.67728300	-0.78960600
O	0.95461600	2.26599300	-0.19141300
H	-1.61010200	0.16363100	-1.51179800

PPT

C	3.68882800	1.22838700	-0.33226400
H	3.29407900	1.15494200	-1.34937200
H	4.08421100	2.23864400	-0.19945200
C	2.60617500	0.91951800	0.70397600
H	1.79736600	1.65243700	0.62474200
C	2.02915300	-0.49413500	0.60558700
H	1.32089500	-0.70576500	1.41548000
H	2.81963200	-1.24646700	0.66134500
S	1.11013000	-0.87114000	-0.94070300
S	-0.92861300	-0.91054000	-0.10523300
C	-1.31550300	0.89408400	-0.20805700
H	-0.52615100	1.40254000	0.34748200
H	-1.23817200	1.16186200	-1.26556700
C	-2.69790600	1.19544100	0.37724300
H	-2.73180700	0.81699200	1.40313400
C	-3.86745900	0.63419100	-0.43780600
H	-3.85256900	1.01253300	-1.46455300
H	-4.82202300	0.92137300	0.00926400
O	-0.82798000	-1.19409100	1.35890000
H	-2.79076400	2.28473600	0.44827400
H	-3.84431000	-0.45776500	-0.48547200
H	3.02323600	1.02980700	1.71289100
H	4.52622100	0.52882300	-0.24649100

PPT radical (next to tetravalent S)

C	2.92684500	2.12057700	0.43142800
H	3.91357300	1.74680500	0.72132600
H	3.07268200	3.06933400	-0.09158900
C	2.18856500	1.11159200	-0.45570000
H	2.75475500	0.94058500	-1.37651000
C	1.96571500	-0.22165600	0.25942200
H	1.36306000	-0.10210300	1.16815700
S	1.13344300	-1.51264000	-0.73400500
S	-0.95583200	-1.35680100	0.25964200
C	-1.60964600	-0.06942700	-0.68017600
H	-1.82873200	-0.34230700	-1.70845000
C	-1.87862500	1.29178300	-0.14324300
H	-1.53572800	1.33411600	0.89312400
C	-3.36657500	1.68957800	-0.22769000
H	-3.72909600	1.65925200	-1.25857800
H	-3.50649500	2.70555200	0.14982900
O	-0.74210200	-0.85681000	1.64710700
H	-3.98477200	1.01615200	0.36988900
H	-1.28748000	2.02211100	-0.71352000
H	1.22187200	1.52252600	-0.76135000
H	2.36795100	2.32670300	1.34907500
H	2.91577800	-0.66787400	0.56730000

diallyldisulfide

C	3.33309000	0.21157300	-0.38867700
C	4.15512000	0.97793000	0.32412000
H	3.79996700	1.85929800	0.84940900
C	1.86563200	0.45991300	-0.53519000
H	1.58613700	1.44147100	-0.15093300
H	3.71873000	-0.67116200	-0.89262000
H	5.21276900	0.75444000	0.40274400
S	0.94993000	-0.85316100	0.41728100
S	-0.94996100	-0.85286800	-0.41739000
C	-1.86567900	0.45991500	0.53548400
H	-1.58621600	1.44158700	0.15151800
H	-1.54308200	0.36782000	1.57363200
C	-3.33310000	0.21153200	0.38872700
H	-3.71874700	-0.67132000	0.89244800
C	-4.15501100	0.97789500	-0.32421300
H	-3.79973500	1.85929500	-0.84936800
H	-5.21261400	0.75433300	-0.40322700
H	1.54297600	0.36815700	-1.57336000

diallyldisulfide radical

C	3.32174200	0.17303500	-0.07892700
C	4.22572300	1.20569700	-0.08631400
H	3.91818700	2.22757400	0.10559300
C	1.95477800	0.31968300	0.16946200
H	1.51566900	1.29902500	0.32644900
H	3.68508400	-0.83314500	-0.27531400
H	5.27377800	1.03075500	-0.29149700
S	0.90419200	-1.06175700	0.31667900
S	-0.84414200	-0.49458000	-0.71009000
C	-1.94641400	0.11232400	0.65834900
H	-1.64459000	1.12167300	0.93987400
H	-1.79680700	-0.56084500	1.50392900
C	-3.36073700	0.07686000	0.17139300
H	-3.78950700	-0.91141000	0.02592800
C	-4.08424800	1.15968800	-0.10199500
H	-3.68072500	2.16011300	0.02051200
H	-5.10694700	1.08393800	-0.45271700

dipropyldisulfide

C	3.27590200	0.07092200	0.20069900
C	4.14056500	1.32451000	0.02254900
H	4.12062700	1.67610600	-1.01310900
C	1.81148600	0.32721400	-0.16277800
H	1.38894600	1.11322800	0.46661500
H	3.34056200	-0.27506500	1.23781600
H	5.18166400	1.11995600	0.28493100
S	0.83389500	-1.21927300	0.08263200
S	-1.05210100	-0.72107900	-0.62729500
C	-1.89863700	-0.02594100	0.86394100
H	-1.37649800	0.88319600	1.17081200
H	-1.81017700	-0.76642900	1.65940000
C	-3.37074600	0.27119000	0.55864900
H	-3.85788200	-0.64293700	0.20233900
C	-3.59811000	1.41031200	-0.44070500
H	-3.12930000	2.33619600	-0.09347300
H	-4.66577200	1.60509500	-0.56969500
H	3.66763600	-0.73902800	-0.42321900
H	3.79084500	2.14227200	0.65954300
H	-3.85312600	0.52251400	1.51023100
H	-3.18155700	1.17731400	-1.42348900
H	1.71257000	0.62397700	-1.20823100

dipropyldisulfide radical

C	3.28682000	0.21646600	-0.44310500
C	4.29639400	1.06180700	0.34841200
H	3.98725800	2.11024100	0.38849100
C	1.90225700	0.27493900	0.12310600
H	1.47019100	1.23466400	0.38793500
H	3.62410200	-0.82344100	-0.49527000
H	5.28399800	1.02313500	-0.11853400
S	0.88387300	-1.10379800	0.16942100
S	-0.96822500	-0.48928000	-0.68672500
C	-1.98652700	-0.17581900	0.82282200
H	-1.57550600	0.69029300	1.34643900
H	-1.89101900	-1.05073700	1.46683400
C	-3.45396100	0.06023900	0.44997500
H	-3.82898000	-0.80474500	-0.10721900
C	-3.71257300	1.34647300	-0.34135700
H	-3.35427900	2.22333300	0.20664500
H	-4.78181000	1.48062800	-0.52349000
H	3.26280500	0.57467300	-1.48556300
H	4.38998300	0.70105900	1.37576100
H	-4.02203800	0.09127400	1.38698800
H	-3.20951600	1.33423400	-1.31127500

allylSOH – conf 1

S	1.16186200	-0.55738700	-0.32213700
O	1.82540800	0.92809400	0.16392300
H	1.57453100	1.57270600	-0.50833000
C	-0.39891900	-0.54491000	0.63635900
H	-0.11704700	-0.37497500	1.67915900
H	-0.77328600	-1.57014200	0.54760700
C	-1.40851200	0.45274900	0.16371400
H	-1.10842400	1.49554400	0.23694400
C	-2.61171000	0.14806000	-0.31324700
H	-2.95057100	-0.88058900	-0.39245500
H	-3.30340400	0.91550200	-0.64107300

allylSOH – conf 2

S	-0.92931200	-0.59090000	-0.02052100
O	-2.35075600	0.33584400	0.03235500
H	-2.59598400	0.51620300	-0.88319100
C	0.34867200	0.72962100	0.02319600
H	-0.01490000	1.46784500	0.74187800

H	0.44919300	1.19496200	-0.95953700
C	1.63698700	0.11124800	0.47293100
H	1.68861800	-0.17117800	1.52120000
C	2.66886900	-0.13523500	-0.33038400
H	2.64340400	0.12181300	-1.38491000
H	3.57754000	-0.59579800	0.03960800

allylSOH – conf 3

S	-0.91100000	-0.58350700	0.04143100
O	-2.34763300	0.28906300	-0.19727400
H	-2.67162800	0.52979300	0.67918900
C	0.34671200	0.75183700	-0.08039200
H	-0.01317900	1.59149500	0.51904700
H	0.44437700	1.06514300	-1.12056800
C	1.63112400	0.20307800	0.46246400
H	1.69350000	0.11194100	1.54376000
C	2.64616700	-0.20746200	-0.29410100
H	2.60970000	-0.14452100	-1.37724700
H	3.55027600	-0.61495600	0.14328900

allylSOH – conf 4

S	-1.31618100	-0.35615700	-0.17331400
O	-1.15911200	1.29143600	0.16460400
H	-0.64594900	1.67595900	-0.55802000
C	0.29693300	-0.95805100	0.45804900
H	0.21906400	-2.04803100	0.38288900
H	0.36910400	-0.68557000	1.51266800
C	1.43631900	-0.41712800	-0.34471300
H	1.57466600	-0.85211900	-1.33176500
C	2.21773800	0.58540500	0.05305600
H	2.09628000	1.04618100	1.02829400
H	3.01267600	0.96925500	-0.57622000

allylSOH – conf 5

S	-1.31423300	-0.40942200	-0.14797800
O	-1.24714900	1.27801600	-0.04180100
H	-1.57234800	1.51147200	0.83620000
C	0.34828000	-0.87786100	0.46287700
H	0.30960100	-1.97381600	0.41721300
H	0.45024200	-0.58952800	1.51206300
C	1.45982900	-0.33110700	-0.37391400
H	1.50023500	-0.68667300	-1.40025100

C	2.33977200	0.56853300	0.05447700
H	2.30970900	0.95549100	1.06838400
H	3.12019800	0.95228500	-0.59219600

allylSOH – conf 6

S	1.16209700	-0.56127100	-0.32131900
O	1.74749000	0.99737200	0.01256900
H	2.30181500	0.92007100	0.79875700
C	-0.40097600	-0.53215100	0.63242900
H	-0.14564800	-0.33823100	1.67913100
H	-0.77706900	-1.55872900	0.56503300
C	-1.39732900	0.45644500	0.11122700
H	-1.04323300	1.48181400	0.05237800
C	-2.63270700	0.15131600	-0.27318500
H	-3.01083300	-0.86593200	-0.23129300
H	-3.31242000	0.90871200	-0.64629100

allylSO● – conf 1

S	1.22149500	-0.40341600	-0.32608600
O	1.78922100	0.92219700	0.12690700
C	-0.36655700	-0.61336300	0.59833000
H	-0.09314000	-0.54346400	1.65553800
H	-0.70517500	-1.63067100	0.38066400
C	-1.37704500	0.41956100	0.21042100
H	-1.07640900	1.44917800	0.38324700
C	-2.56297700	0.14907000	-0.32699000
H	-2.88927200	-0.86950900	-0.51402500
H	-3.25421200	0.93993700	-0.59386900

allylSO● – conf 2

S	-1.31788400	-0.27166200	-0.15390400
O	-1.27987900	1.21890100	0.07767900
C	0.31711400	-0.92969700	0.43356500
H	0.22252800	-2.01595300	0.33554200
H	0.38179500	-0.67059800	1.49281400
C	1.45859200	-0.37370500	-0.35265100
H	1.61850600	-0.80208000	-1.33889300
C	2.22467200	0.63071300	0.06413000
H	2.07804600	1.09286100	1.03467700
H	3.02203000	1.02728900	-0.55337200

allylSO● – conf 3

S	-1.03614600	-0.49901000	0.03692100
O	-2.33293200	0.26387200	-0.09969500
C	0.32839800	0.75787400	-0.08123300
H	-0.03074400	1.61364400	0.49503300
H	0.41664600	1.04367300	-1.13170600
C	1.59402200	0.17655900	0.46046400
H	1.65767100	0.08956500	1.54232900
C	2.60009500	-0.26409900	-0.29158900
H	2.57312100	-0.19904900	-1.37502600
H	3.49000600	-0.69665700	0.15034200

propylSOH – conf 1

S	-0.93278000	-0.46985300	-0.34128800
O	-2.34641200	0.03755100	0.44968800
H	-2.81468100	0.61212500	-0.16805800
C	0.21776900	0.85606600	0.16836700
H	0.19373300	0.91357600	1.25952800
H	-0.14375300	1.80307300	-0.24034200
C	1.63854300	0.56559400	-0.33650400
H	2.23244900	1.47050700	-0.16962600
H	1.61607100	0.41655600	-1.42200400
C	2.32583000	-0.62434900	0.34238400
H	1.79941100	-1.56232800	0.15335400
H	3.35030600	-0.73637800	-0.02165700
H	2.36938400	-0.48375900	1.42642800

propylSOH – conf 2

S	-1.11639700	-0.48447000	-0.44119400
O	-1.68481900	1.02879000	0.08601200
H	-2.35346500	0.85051300	0.75861500
C	0.26627400	-0.74068700	0.71717600
H	0.63753600	-1.73841500	0.45036200
H	-0.13981200	-0.80699800	1.73032400
C	1.37700700	0.31134400	0.63377500
H	2.04004500	0.16729000	1.49531900
H	0.92131500	1.29853200	0.75432600
C	2.19340500	0.26246500	-0.65901100
H	1.55698600	0.41479900	-1.53346800
H	2.96139900	1.03997000	-0.66324800
H	2.69677700	-0.70322100	-0.77286200

propylSOH – conf 3

S	1.24455200	-0.40717700	-0.33859400
O	1.44127000	1.12344600	0.37336300
H	0.99534500	1.75833400	-0.19923100
C	-0.26595200	-0.99169100	0.49539700
H	-0.16858200	-0.68551200	1.54106300
H	-0.17344200	-2.08320200	0.46972300
C	-1.60504700	-0.55401400	-0.10565400
H	-2.40051100	-1.04038500	0.47294300
H	-1.68282000	-0.94293100	-1.12614800
C	-1.84355500	0.95844100	-0.11558300
H	-1.15990000	1.46321200	-0.80431900
H	-2.85897800	1.18895700	-0.44735300
H	-1.70677900	1.39237500	0.87895800

propylSOH – conf 4

S	-0.91148900	-0.51728700	-0.25427800
O	-2.40218100	0.18250200	0.15801400
H	-2.58243000	-0.07586700	1.06995400
C	0.21340700	0.85539000	0.18639700
H	0.22221800	0.98177700	1.27335800
H	-0.20489200	1.75605100	-0.26766300
C	1.63023800	0.59010300	-0.33775100
H	2.22174900	1.49230300	-0.14849700
H	1.59426100	0.46863400	-1.42547000
C	2.32679100	-0.61674100	0.30126500
H	1.80958100	-1.55268300	0.07523700
H	3.35319000	-0.70972800	-0.06227400
H	2.36497500	-0.51642700	1.39023000

propylSOH – conf 5

S	-1.11977300	-0.46737300	-0.45542800
O	-1.81927700	0.91263100	0.25113300
H	-1.45213300	1.67499300	-0.21132000
C	0.26668100	-0.75047900	0.68944100
H	0.62868100	-1.74805400	0.41075000
H	-0.15966700	-0.82629300	1.69247500
C	1.39586900	0.28301000	0.64272900
H	2.06419200	0.08721500	1.48962800
H	0.96902200	1.27552000	0.82357700
C	2.20189600	0.28073900	-0.65768000
H	1.56290400	0.47681900	-1.52209200

H	2.98337000	1.04439300	-0.63554900
H	2.68752900	-0.68728400	-0.81663100

propylSOH – conf 6

S	1.27440400	-0.41983200	-0.27824000
O	1.31285500	1.23130100	0.12399100
H	1.79682400	1.29955400	0.95596500
C	-0.27131200	-0.98295500	0.50380200
H	-0.25158500	-0.69314400	1.55929200
H	-0.15984700	-2.07403800	0.47216100
C	-1.57520400	-0.55798400	-0.17826400
H	-2.39051800	-1.13739400	0.27382900
H	-1.53075700	-0.85258300	-1.23161100
C	-1.89187600	0.93630600	-0.06895700
H	-1.10886500	1.54262200	-0.52617800
H	-2.84046700	1.16590000	-0.56139400
H	-1.97774600	1.24378000	0.97837000

propylSO● – conf 1

S	-1.03529100	-0.38318400	-0.29648400
O	-2.34379200	0.01986400	0.34626900
C	0.20396600	0.87017700	0.22636700
H	0.19729900	0.88417000	1.31998100
H	-0.17078100	1.83293100	-0.13063900
C	1.59271700	0.55114900	-0.33750100
H	2.23086200	1.42511400	-0.17155000
H	1.52536600	0.43171900	-1.42499700
C	2.24867900	-0.68635100	0.28469700
H	1.66168900	-1.59057300	0.10382200
H	3.24530900	-0.84999800	-0.13197700
H	2.35307400	-0.57118800	1.36756700

propylSO● – conf 2

S	1.23032200	0.14195300	-0.46527900
O	1.56566000	-0.88360700	0.59702500
C	-0.23034900	1.06263900	0.16467900
H	-0.54105700	1.70608200	-0.66628100
H	0.13332900	1.70161900	0.97447500
C	-1.35763800	0.14660100	0.64946400
H	-2.07531400	0.76143100	1.20319200
H	-0.93193500	-0.56072600	1.36698300
C	-2.07791700	-0.60851400	-0.47060600
H	-1.39686300	-1.27216500	-1.00966200

H	-2.88398800	-1.22446500	-0.06495800
H	-2.51918600	0.08148000	-1.19671300

propylSO● – conf 3

S	1.30884900	-0.27958600	-0.23303100
O	1.36409600	1.16857100	0.20627100
C	-0.22696300	-1.00254100	0.45646200
H	-0.23816400	-0.74942800	1.52078100
H	-0.07582200	-2.08356300	0.36105900
C	-1.51748300	-0.55830400	-0.24748200
H	-2.32601000	-1.20778500	0.10808700
H	-1.42282600	-0.74958900	-1.32198500
C	-1.89202300	0.90669400	-0.00487000
H	-1.11088200	1.58442900	-0.35232500
H	-2.82116200	1.15592900	-0.52364600
H	-2.04066400	1.09971200	1.06170500

benzylSOH – conf 1

S	-2.36267500	-0.45184000	-0.35776300
O	-2.36728300	1.23712500	-0.51560400
H	-3.03220700	1.56568800	0.10203900
C	-1.06627400	-0.68298300	0.91883800
H	-1.14293900	-1.75079000	1.14978100
H	-1.36782300	-0.13162500	1.81262500
C	0.32481400	-0.31839300	0.47783100
C	0.76574700	1.00745400	0.54242700
C	1.19518000	-1.29240200	-0.02161000
C	2.04651600	1.35031300	0.11776600
H	0.09613300	1.77433400	0.91375400
C	2.47735200	-0.95228200	-0.44303800
H	0.86587000	-2.32494700	-0.08138300
C	2.90703100	0.37154900	-0.37463300
H	2.37287600	2.38294000	0.17218000
H	3.14131700	-1.72058500	-0.82341200
H	3.90565100	0.63788800	-0.70202500

benzylSOH – conf 2

S	2.38664400	-0.38883900	-0.31542800
O	2.23910400	1.27970700	-0.55725200
H	1.53833400	1.40239200	-1.21065600
C	1.11207000	-0.64727400	0.97822900
H	1.39891600	-0.05479400	1.84889600
H	1.22237900	-1.70566100	1.23504500

C	-0.28392500	-0.32732700	0.52009500
C	-0.78406000	0.97411900	0.64474500
C	-1.09391000	-1.30411000	-0.07031300
C	-2.06352400	1.29043600	0.19077300
H	-0.16732000	1.73856900	1.10430900
C	-2.37285100	-0.99076500	-0.51925800
H	-0.71839500	-2.31663700	-0.17802800
C	-2.86148000	0.30921300	-0.39186400
H	-2.43778200	2.30247800	0.29847800
H	-2.99057300	-1.76124600	-0.96708700
H	-3.85859700	0.55291100	-0.74053900

benzylSOH – conf 3

S	2.36265600	-0.45187100	-0.35788000
O	2.36760900	1.23711200	-0.51517000
H	3.03276800	1.56537200	0.10238200
C	1.06621400	-0.68315200	0.91866500
H	1.36783500	-0.13188000	1.81248300
H	1.14275200	-1.75096800	1.14958500
C	-0.32485600	-0.31843600	0.47771300
C	-0.76565900	1.00747600	0.54223200
C	-1.19537100	-1.29239100	-0.02154400
C	-2.04642800	1.35041500	0.11767500
H	-0.09592300	1.77431600	0.91340000
C	-2.47756100	-0.95218400	-0.44289000
H	-0.86619400	-2.32497900	-0.08124700
C	-2.90709900	0.37168400	-0.37455400
H	-2.37270500	2.38306600	0.17204100
H	-3.14162500	-1.72046400	-0.82312200
H	-3.90572000	0.63810900	-0.70186000

benzylSOH – conf 4

S	-2.38667000	-0.38894500	-0.31532600
O	-2.23933000	1.27960700	-0.55751100
H	-1.53849100	1.40219900	-1.21085500
C	-1.11208300	-0.64690500	0.97836200
H	-1.22232300	-1.70522500	1.23548900
H	-1.39895500	-0.05422900	1.84888800
C	0.28394100	-0.32709400	0.52013600
C	0.78428900	0.97426900	0.64472500
C	1.09376900	-1.30404900	-0.07021800
C	2.06379400	1.29035900	0.19066200
H	0.16773200	1.73883400	1.10431000
C	2.37273600	-0.99093000	-0.51924400

H	0.71811000	-2.31652700	-0.17779900
C	2.86156200	0.30899600	-0.39196600
H	2.43820200	2.30234600	0.29831900
H	2.99034300	-1.76150800	-0.96704800
H	3.85868700	0.55249900	-0.74072900

benzylSO● – conf 1

S	2.16559800	0.00004100	-0.57674800
O	3.58513700	0.00006600	-0.06050400
C	1.06621400	-0.00019500	0.91968300
H	1.33507500	0.88775400	1.49502800
H	1.33496200	-0.88834500	1.49476800
C	-0.37165200	-0.00007500	0.48870700
C	-1.04805300	-1.20417600	0.26145900
C	-1.04794500	1.20411400	0.26158800
C	-2.37179800	-1.20489200	-0.16926500
H	-0.53533000	-2.14550700	0.43053700
C	-2.37169300	1.20499500	-0.16912000
H	-0.53514000	2.14538200	0.43076000
C	-3.03732200	0.00009400	-0.38525300
H	-2.88403200	-2.14605600	-0.33392700
H	-2.88384900	2.14622200	-0.33367200
H	-4.06886400	0.00016600	-0.71829000

benzylSO● – conf 2

S	-2.38080700	-0.30655400	-0.39693900
O	-2.48746300	1.19941700	-0.34228300
C	-1.09280000	-0.77898200	0.84781100
H	-1.18211500	-1.86438300	0.94635700
H	-1.41279000	-0.31305800	1.78277800
C	0.29407300	-0.36142500	0.44470500
C	0.67519600	0.98423500	0.51312000
C	1.21393700	-1.30220900	-0.02889900
C	1.95200700	1.37480700	0.12150300
H	-0.03836900	1.72264800	0.85869700
C	2.49279800	-0.91069800	-0.41734600
H	0.93037800	-2.34822000	-0.08823500
C	2.86525300	0.42924900	-0.34252600
H	2.23459600	2.41991500	0.17927600
H	3.19736300	-1.65246200	-0.77644400
H	3.86077800	0.73522900	-0.64335000

allylSOOH – conf 1

S	-1.16410800	-0.05662600	0.32317300
O	-0.73477200	1.46339500	-0.28845800
H	-1.56157400	1.89545700	-0.54174200
C	0.55754800	-0.36481200	0.92196400
H	0.45085500	-1.30315900	1.47700100
H	0.79719300	0.44052600	1.61833500
C	1.53630600	-0.48951900	-0.19895500
H	1.28140100	-1.21958000	-0.96048400
C	2.64611600	0.23439900	-0.30101800
H	2.91345200	0.98207100	0.43899300
H	3.32927400	0.10194800	-1.13200500
O	-1.39331400	-0.99735200	-0.78689300

allylSOOH – conf 2

S	-0.86545400	0.15478900	-0.45982100
O	-2.13418000	-0.66835500	0.26901200
H	-2.14336400	-0.42029400	1.20805300
C	0.50227700	-0.87634000	0.28066500
H	0.22374500	-1.91466300	0.08904100
H	0.44922700	-0.66124600	1.35131500
C	1.82157700	-0.50617500	-0.31128400
H	2.04808500	-0.92995300	-1.28660200
C	2.69048500	0.32425400	0.25988400
H	2.49506800	0.77495100	1.22717200
H	3.62633100	0.58158700	-0.22214000
O	-0.73305500	1.47367400	0.18282600

allylSOOH – conf 3

S	-1.16070900	-0.00847700	0.30777200
O	-0.63187200	1.52619600	-0.06083800
H	0.13897800	1.46040800	-0.65428300
C	0.49991400	-0.66432400	0.88409700
H	0.28247700	-1.69002700	1.19136500
H	0.77628700	-0.06612900	1.75436200
C	1.49499600	-0.59388700	-0.22028300
H	1.33480700	-1.27943300	-1.04657900
C	2.48829400	0.29518400	-0.27724000
H	2.67596600	0.99569000	0.53090000
H	3.16765500	0.32779900	-1.12131900
O	-1.45613400	-0.75551000	-0.92644300

allylSOOH – conf 4

S	0.90150100	-0.13939400	-0.44878500
O	1.05842800	1.46740400	0.01155400
H	1.43828100	1.47565500	0.90574500
C	-0.57197800	-0.54406900	0.61219300
H	-0.20529000	-0.42309300	1.63642800
H	-0.74885700	-1.60642500	0.42654100
C	-1.76070100	0.29785400	0.29146200
H	-1.68692200	1.34723400	0.56088200
C	-2.85268700	-0.15119200	-0.32286800
H	-2.95846000	-1.19192000	-0.61340800
H	-3.68350900	0.50631500	-0.55049400
O	2.00818800	-0.90403100	0.15471400

allylSOOH – conf 5

S	0.90638100	-0.14507100	-0.42767000
O	0.98764300	1.44487800	0.16824500
H	1.59004000	1.92773500	-0.41310000
C	-0.55862100	-0.49660500	0.64458800
H	-0.18754000	-0.28449800	1.65059700
H	-0.71314900	-1.57173000	0.53243900
C	-1.76069900	0.30320400	0.26754500
H	-1.71727600	1.36128400	0.50562000
C	-2.82844400	-0.19754600	-0.34947000
H	-2.90089800	-1.25048300	-0.60436900
H	-3.67354500	0.42760900	-0.61329300
O	2.01071300	-0.93776600	0.13286100

allylSOOH – conf 6

S	-0.87133100	0.19007000	-0.44530900
O	-2.01507300	-0.71656400	0.42827900
H	-2.88408200	-0.40320200	0.14378100
C	0.48004500	-0.90557900	0.20003500
H	0.19759400	-1.92125600	-0.08274700
H	0.40304600	-0.78565700	1.28243700
C	1.80596400	-0.48913000	-0.34421200
H	2.04976800	-0.83463100	-1.34593700
C	2.66335500	0.29300200	0.30625600
H	2.44854200	0.66617000	1.30186600
H	3.60780400	0.58716700	-0.13655800
O	-0.68212200	1.49913100	0.19542600

allylSOO● – conf 1

S	-0.99294300	0.09489900	-0.28330100
O	-2.13917300	-0.62378900	0.28429800
C	0.53641500	-0.93341400	0.24570600
H	0.24913800	-1.94356200	-0.04361900
H	0.51112100	-0.82454300	1.33124200
C	1.78551900	-0.44259400	-0.37952100
H	1.96020000	-0.73557000	-1.41117100
C	2.66732600	0.33601600	0.24527900
H	2.51471800	0.66005400	1.26942800
H	3.57014100	0.67578700	-0.24794300
O	-0.71755100	1.48496400	0.08646400

allylSOO● – conf 2

S	0.96955500	0.04221500	-0.30511600
O	1.05208200	1.44595300	0.11146800
C	-0.58924000	-0.67042800	0.52247000
H	-0.25160300	-0.76012900	1.55773000
H	-0.70220700	-1.65797300	0.07655000
C	-1.76285200	0.21883400	0.34697500
H	-1.71899700	1.17528300	0.85790000
C	-2.82378300	-0.09831400	-0.39355200
H	-2.89135900	-1.04417500	-0.92196300
H	-3.66628200	0.57627100	-0.48843800
O	2.04452000	-0.90411200	0.00662100

allylSOO● – conf 3

S	-1.09527900	0.06403200	0.22055000
O	-0.99245500	1.44642300	-0.25140200
C	0.60372100	-0.40877200	0.95114000
H	0.39049600	-1.34165700	1.47344100
H	0.82005700	0.39500500	1.65380100
C	1.60655000	-0.54422300	-0.13522200
H	1.52226500	-1.42973600	-0.75720100
C	2.54764300	0.36591000	-0.38134000
H	2.63560800	1.27091100	0.21073900
H	3.26294000	0.23240200	-1.18414800
O	-1.46434400	-1.02504000	-0.69021000

Table S3. Relevant Enthalpies (in a.u.) for Activation Enthalpy Calculations in Text.[a]

Transition State	H_{298}^{o}
allicin + MeOO● (HAT)	-1294.669079
PPT + MeOO● (HAT)	-1297.088647
diallyldisulfide + MeOO●	-1219.546942
dipropyldisulfide + MeOO●	-1221.965314
allylSOH + MeOO● (syn)	-780.469951 -780.470476
allylSOH + MeOO● (anti)	-780.459459 -780.459616
propylSOH + MeOO● (syn)	-781.67961 -781.679427
propylSOH + MeOO● (anti)	-781.668953 -781.668857
allicin + MeOO● (add)	-1294.671543
PPT + MeOO● (add)	-1297.094415
allylSOOH + MeOO●	-855.607244

[a] H_{298}^{o} (methylperoxyl) = -189.954741 a.u.

Table S4. Relevant Structures for Activation Enthalpy Calculations in Text.

allicin + MeOO● (HAT)

C	2.82488900	-1.49410400	-0.27917100
C	3.84525400	-2.11410200	0.33447000
H	3.77195200	-2.45146600	1.36295900
O	1.89246900	1.23311600	1.17229700
O	2.67462300	1.87628600	0.22684300
C	1.56003400	-1.16068200	0.37212700
H	1.40946300	-1.63005700	1.34543500
H	1.70273300	0.10459500	0.73749100
H	2.93897700	-1.16786600	-1.30936800
C	1.86082700	2.78042800	-0.53478100
H	1.44387800	3.54823600	0.12132200
H	2.54758300	3.22734100	-1.25560900
H	1.05046300	2.24976500	-1.03657500
H	4.78365900	-2.29082900	-0.17685500
S	0.13452000	-1.30243800	-0.70974400
S	-1.22447000	0.18274800	0.18913300
C	-2.74701400	-0.73900700	-0.37632400
H	-2.73994400	-1.70453900	0.13169200
H	-2.62341700	-0.87983800	-1.45341300
C	-3.95539800	0.07886000	-0.05330400
H	-4.03626200	1.02733500	-0.57557700
C	-4.89024900	-0.28771100	0.81975700
H	-4.83406000	-1.22859900	1.35860000
H	-5.75151700	0.33904000	1.01912200
O	-1.21888700	1.43932800	-0.60365200

PPT + MeOO● (HAT)

C	-2.68671700	-1.85598000	0.33998800
C	-3.85393400	-1.96932800	-0.64775900
H	-4.25648400	-0.98228700	-0.88154600
O	-2.72844700	1.17163600	-0.65710900
O	-2.49967900	1.94048900	0.49356100
C	-1.53768300	-1.03389400	-0.21900500
H	-1.16118300	-1.36660200	-1.18862100
H	-2.11537300	0.19359400	-0.49117900
H	-2.32067100	-2.85781800	0.60230400
C	-1.52701400	2.94600700	0.18714400
H	-1.88598200	3.57867100	-0.62888100
H	-1.43969900	3.53209000	1.10466800
H	-0.56507300	2.49928400	-0.07333500
H	-4.65674500	-2.57642600	-0.22247000

S	-0.23311000	-0.72732400	0.94777300
S	1.36441300	-0.18047300	-0.44765400
C	2.66234500	-0.31595700	0.86962200
H	2.70034000	-1.36853100	1.16226400
H	2.31020800	0.28423000	1.71113800
C	4.00483600	0.19779600	0.34564500
H	3.86380700	1.21536300	-0.02977800
C	4.64244400	-0.68596700	-0.73050800
H	4.02412400	-0.74165300	-1.63079300
H	4.79530900	-1.70670800	-0.36699600
H	4.67819600	0.27532600	1.20574800
H	5.61540600	-0.28886700	-1.02854000
H	-3.03714000	-1.40030700	1.27204100
H	-3.53685500	-2.44183300	-1.58234300
O	1.31078800	1.26052000	-0.81224600

diallyldisulfide + MeOO●

C	-2.23659600	1.69609600	-0.01555500
C	-2.82183300	2.52864500	0.85872000
H	-2.38320700	2.73550100	1.82919800
O	-1.79845200	-1.32531900	1.06607300
O	-3.12365500	-1.41468400	0.66313400
C	-1.00533400	0.95477200	0.25200400
H	-0.44532500	1.29263400	1.12474000
H	-1.38964400	-0.23916700	0.63167200
H	-2.71911700	1.51275000	-0.97291100
C	-3.19566700	-2.18382100	-0.54025500
H	-2.77072600	-3.17744600	-0.37942800
H	-4.26061600	-2.25855300	-0.76769600
H	-2.66835800	-1.68062300	-1.35542200
H	-3.76239800	3.01457800	0.62926100
S	0.02281500	0.73302500	-1.21030700
S	1.53241100	-0.55545000	-0.58607000
C	2.84656000	0.59823800	0.05415800
H	2.56349100	0.94382000	1.04872800
H	2.88355800	1.44538600	-0.63196000
C	4.14306900	-0.14768500	0.08070900
H	4.58461500	-0.37022600	-0.88736300
C	4.74543100	-0.55879600	1.19381200
H	4.32308700	-0.36484000	2.17495000
H	5.68411000	-1.09968800	1.16306500

dipropyldisulfide + MeOO●

C	2.18909200	-2.01673100	-0.16573800
C	3.09085300	-2.28839100	1.04526800
H	3.61317900	-1.37917400	1.34806000
O	2.53161000	0.99634700	0.90885500
O	2.56150400	1.88782700	-0.17538800
C	1.12182900	-0.97680200	0.13281000
H	0.47439800	-1.20040100	0.98179000
H	1.82187300	0.12207700	0.55712800
H	1.70955900	-2.95044300	-0.48890000
C	1.69830200	2.98412500	0.11744700
H	2.02649600	3.49664800	1.02587600
H	1.78403500	3.65050800	-0.74330800
H	0.66277500	2.64997100	0.23199800
H	3.83681500	-3.04952700	0.80385200
S	0.21236200	-0.46592300	-1.30825900
S	-1.45961800	0.52117400	-0.56072600
C	-2.66610200	-0.85863900	-0.30034800
H	-2.26028600	-1.53626100	0.45385300
H	-2.75427400	-1.39385700	-1.24603900
C	-4.02508500	-0.30328800	0.13941900
H	-4.37925200	0.41878100	-0.60411400
C	-4.03709600	0.32853600	1.53501300
H	-3.70009600	-0.38565000	2.29239600
H	-5.04635000	0.64900900	1.80472700
H	2.80155600	-1.67651500	-1.00787600
H	2.50868200	-2.64985700	1.89829800
H	-4.73359900	-1.13898400	0.11313700
H	-3.38508900	1.20341100	1.59190700

allylSOH + MeOO● – syn 1

S	-0.38818800	0.87528900	-0.73380500
O	0.71237900	1.80669700	-0.00344200
H	1.40281700	1.18986000	0.50559500
O	2.18431800	0.14466900	1.01770000
O	1.68277900	-0.93741100	0.35363800
C	2.58617300	-1.32273500	-0.69672100
H	2.10300600	-2.15353000	-1.21117400
H	2.74513200	-0.48227300	-1.37419300
H	3.53351300	-1.63528500	-0.25359800
C	-1.46722700	0.34440700	0.65938400
H	-2.13659300	1.16644600	0.91925400
H	-0.78441300	0.15238100	1.49021800
C	-2.20915000	-0.88863900	0.24965900

H	-1.61735400	-1.79810600	0.19068400
C	-3.50289700	-0.91606500	-0.06095200
H	-4.11833000	-0.02276800	-0.01730800
H	-3.99397400	-1.83479700	-0.35998200

allylSOH + MeOO● – syn 2

S	0.38819900	-0.87701600	-0.72556200
O	-0.70895300	-1.80572600	0.00714900
H	-1.42316700	-1.18998200	0.49884100
O	-2.25623600	-0.18413700	0.95101100
O	-1.69562200	0.91729200	0.36847500
C	-2.56179900	1.41012500	-0.66707200
H	-2.03149500	2.24824800	-1.11958400
H	-2.74639900	0.62266800	-1.39934000
H	-3.50187100	1.73878000	-0.21984700
C	1.45513100	-0.31884100	0.66610800
H	1.58703800	-1.20011100	1.29831200
H	0.91499600	0.45137000	1.21923800
C	2.75308700	0.18371400	0.11531100
H	3.43863500	-0.57056200	-0.26263900
C	3.08409400	1.47068700	0.04324700
H	2.42091100	2.24950500	0.40683700
H	4.03356500	1.78879800	-0.37147100

allylSOH + MeOO● – anti 1

S	-0.97587600	1.14739900	-0.24199300
O	0.43926500	1.39077600	0.47774800
H	1.19082600	0.75915300	-0.00241000
O	2.01574500	0.01246200	-0.69144800
O	2.63011000	-0.84808500	0.17833100
C	4.04517700	-0.63480600	0.13905900
H	4.46735700	-1.37362000	0.82111200
H	4.41597700	-0.79002300	-0.87641200
H	4.27865800	0.37852900	0.47480400
C	-1.57186900	-0.42181000	0.51629600
H	-1.86484300	-0.21712400	1.54795300
H	-0.71480400	-1.09936400	0.50972300
C	-2.70874600	-0.94929200	-0.30212000
H	-2.44430000	-1.38223400	-1.26337600
C	-3.98664100	-0.88578700	0.06354400
H	-4.28679300	-0.45235800	1.01261000
H	-4.77654800	-1.27240000	-0.56982600

allylSOH + MeOO● – anti 2

S	-0.97289900	1.19340700	-0.26932000
O	0.45783800	1.49298900	0.39592400
H	1.20770600	0.86305000	-0.09134000
O	2.03524700	0.10041100	-0.75715300
O	2.47393000	-0.86731700	0.10715700
C	3.89960700	-0.79744200	0.21599200
H	4.17858100	-1.61438500	0.88239600
H	4.35386100	-0.92949200	-0.76835200
H	4.19426000	0.16519600	0.64092600
C	-1.49398000	-0.37170600	0.55075700
H	-1.18515100	-0.26367300	1.59337900
H	-0.94603000	-1.19944700	0.09624900
C	-2.97551200	-0.53073700	0.40973400
H	-3.58809500	0.12891400	1.01908800
C	-3.55856500	-1.38948600	-0.42308000
H	-2.97683300	-2.05619100	-1.05206800
H	-4.63733100	-1.46091900	-0.49898800

propylSOH + MeOO● – syn 1

S	-0.39862100	0.69241000	-0.67087700
O	0.65193600	1.76264500	-0.06297600
H	1.42790400	1.24508100	0.42747700
O	2.36915200	0.32051100	0.91808500
O	1.94571400	-0.84188700	0.34162300
C	2.82553500	-1.19465600	-0.73898000
H	2.40099600	-2.09545500	-1.18255600
H	2.86347300	-0.38098200	-1.46507200
H	3.82208800	-1.38942100	-0.33802700
C	-1.29973200	0.14950300	0.82349400
H	-1.78456800	1.03105000	1.25158200
H	-0.53974500	-0.20768000	1.52179500
C	-2.31442100	-0.95173200	0.49876500
H	-2.69660600	-1.33202000	1.45187900
C	-3.48916800	-0.49512200	-0.37359200
H	-4.02163800	0.33967800	0.09147300
H	-4.20401400	-1.30897600	-0.51766500
H	-1.79710500	-1.79244800	0.02393600
H	-3.16054600	-0.16549200	-1.36276700

propylSOH + MeOO● – syn 2

S	0.39613800	-0.94192600	-0.76349200
O	-0.75774500	-1.85965800	-0.09595600

H	-1.41440000	-1.24438100	0.45169800
O	-2.17097600	-0.19798300	1.01604200
O	-1.62571800	0.89897200	0.41558700
C	-2.50884800	1.37661100	-0.61320100
H	-1.99448700	2.21910800	-1.07584300
H	-2.69211400	0.58292600	-1.33928500
H	-3.44789800	1.69537400	-0.15687300
C	1.49845800	-0.61871800	0.65669500
H	1.83789500	-1.59185300	1.01867300
H	0.88867400	-0.14896700	1.43298300
C	2.67904600	0.27416500	0.25769800
H	3.22169600	-0.18535900	-0.57612500
C	2.28968800	1.71378200	-0.09641100
H	1.65247200	1.75534400	-0.98305200
H	3.17843100	2.31731900	-0.29642400
H	3.37696300	0.28326100	1.10134300
H	1.74000900	2.18235900	0.72469600

propylSOH + MeOO● – anti 1

S	-0.91338500	1.04589300	-0.23630700
O	0.44807000	1.33974900	0.56750400
H	1.26709100	0.84237200	0.05097400
O	2.18815800	0.24498400	-0.67897500
O	2.69645600	-0.78689600	0.06476200
C	4.10830400	-0.61103900	0.21967500
H	4.44722600	-1.47889400	0.78661500
H	4.58861900	-0.57892100	-0.76073200
H	4.31105900	0.31177000	0.76870400
C	-1.33913700	-0.64798300	0.30390500
H	-1.38946500	-0.63645700	1.39631600
H	-0.51016200	-1.29173500	0.00067900
C	-2.66007200	-1.11515800	-0.31848500
H	-2.75972900	-2.18501300	-0.10765900
C	-3.89921900	-0.37650100	0.19921300
H	-3.98629200	-0.47111300	1.28564500
H	-4.80887500	-0.78694700	-0.24592500
H	-2.59925100	-1.02806700	-1.40901600
H	-3.86678900	0.69011200	-0.03686600

propylSOH + MeOO● – anti 2

S	-0.96505700	1.17399500	-0.30205000
O	0.50585700	1.55814600	0.22150500
H	1.21443200	0.82934700	-0.17105500
O	1.99204800	-0.06544400	-0.74229900

O	2.57058500	-0.80545400	0.25428200
C	3.99488100	-0.70868200	0.15212100
H	4.38555900	-1.34249200	0.94903800
H	4.32279100	-1.07065400	-0.82481800
H	4.30924600	0.32816400	0.29433100
C	-1.46209300	-0.15325900	0.85305600
H	-1.33823200	0.25307200	1.85972000
H	-0.76033600	-0.98190000	0.72354600
C	-2.90664300	-0.60053800	0.60170600
H	-3.57320800	0.26668100	0.66663000
C	-3.11858400	-1.32827900	-0.73053400
H	-2.89441400	-0.68592800	-1.58578000
H	-4.15405800	-1.66315200	-0.82899100
H	-3.19125900	-1.26212800	1.42658900
H	-2.47289300	-2.20836100	-0.80242000

allicin + MeOO● – add

C	-1.21385800	1.39310200	-0.71257600
H	-0.63142200	1.69809900	-1.58308500
H	-2.26739300	1.34589300	-0.98612600
S	-0.74619200	-0.36153300	-0.36271900
S	1.58232400	-0.01410700	-0.96050400
C	2.26813100	-0.49553200	0.69292300
H	1.81428300	0.19603900	1.40614100
H	1.89935800	-1.50605400	0.88650400
O	1.84636700	1.45174000	-1.12340300
O	-2.43535800	-0.58464700	0.77809200
O	-2.93393300	-1.87148100	0.65054300
C	-3.73984800	-1.96429500	-0.52614600
H	-4.13551800	-2.98113500	-0.51947200
H	-4.55680300	-1.23930000	-0.48512400
H	-3.13253800	-1.80420000	-1.42145700
C	3.76097100	-0.41859600	0.67492300
H	4.18033200	0.57522500	0.54627100
C	4.56617300	-1.47125400	0.79330600
H	4.17850800	-2.47707100	0.92287600
H	5.64416600	-1.36174400	0.77425800
C	-0.97005000	2.30686300	0.44727300
H	0.07125800	2.55197100	0.63471400
C	-1.93345000	2.81480000	1.20992700
H	-2.97855900	2.57632800	1.04130300
H	-1.70879600	3.48075500	2.03512000

PPT + MeOO● – add

C	-1.44380300	1.18343300	-1.03683200
H	-0.85160000	1.31697200	-1.94485000
H	-2.43800200	0.84491400	-1.33490500
S	-0.72606800	-0.25547100	-0.14193000
S	1.54897200	0.41337500	-0.54191000
C	2.22706800	-0.74492200	0.71689000
H	1.72033600	-0.49509600	1.65078300
H	1.92144400	-1.74795500	0.40358600
O	1.87427600	1.79245500	-0.05644200
O	-2.54310900	-0.77956700	0.63787300
O	-2.69908300	-2.15763300	0.63434300
C	-3.15719300	-2.58567300	-0.64882900
H	-3.29991000	-3.66345000	-0.55533300
H	-4.10328500	-2.09768600	-0.89726700
H	-2.40521900	-2.37092000	-1.41365600
C	3.74679200	-0.60873900	0.84555100
H	4.04820400	-1.15934100	1.74295900
C	4.53280300	-1.12406800	-0.36322800
H	4.29532100	-0.56216700	-1.27078100
H	5.60797900	-1.03146000	-0.19319100
C	-1.50942600	2.47679900	-0.21924600
H	-1.81190200	3.27736200	-0.90641900
C	-2.48094200	2.42082200	0.96177800
H	-2.22135400	1.61430800	1.65112900
H	-2.46546700	3.36179900	1.51759100
H	3.98429900	0.44228700	1.03486600
H	4.31544400	-2.17889200	-0.55751000
H	-0.50426900	2.72906000	0.12751700
H	-3.50695500	2.24585100	0.62420900

allylSOOH + MeOO●

S	-0.54300800	1.03251600	0.46883000
O	0.04913600	-0.06076100	1.40363600
H	0.85929100	-0.77577800	0.90415000
O	1.61334700	-1.39023300	0.20660500
O	2.80283400	-0.71467900	0.27535800
C	3.05977800	-0.05919900	-0.96845400
H	4.06219500	0.35728400	-0.86926500
H	3.01153000	-0.78138900	-1.78622300
H	2.31082500	0.73238700	-1.10101800
C	-1.43118700	-0.03039300	-0.80088500
H	-1.81349500	0.68267600	-1.53243400
H	-0.60594800	-0.60567400	-1.23032300

O	0.49262100	1.74358100	-0.31904700
C	-2.49056800	-0.87549600	-0.18943100
H	-2.14819900	-1.68392200	0.44941700
C	-3.79575700	-0.67979600	-0.36948300
H	-4.53266100	-1.32129300	0.09915700
H	-4.17251900	0.12148000	-0.99764700

methylperoxyl

O	-1.18649600	-0.27869000	0.00000000
C	1.09630100	-0.18319600	0.00000000
H	1.14901800	-0.80078100	-0.89700200
H	1.87508100	0.57851700	-0.00000200
H	1.14902000	-0.80077800	0.89700400
O	-0.15737000	0.54396700	0.00000000

Table S5. Relevant Enthalpies (in a.u.) for the Stationary Points in Scheme 2.

Compound	H_{298}^{o}	**Compound**	H_{298}^{o}
MeSO●	-512.667772	t-BuSO●	-630.352262
MeOO●	-189.954263	t-BuOO●	-307.648956
MeSO-OOMe	-702.611276	t-BuSO-OOt-Bu	-937.991968
MeS(O)-OOMe	-702.686387	t-BuS(O)-OOt-Bu	-938.066723
MeS(O)O●	-587.802604	t-BuS(O)O●	-705.490415
MeO●	-114.870498	t-BuO●	-232.559967
$Me(SO_2)OMe$	-702.800795	$t\text{-}Bu(SO_2)Ot\text{-}Bu$	-938.179333
MeSO-OSMe	-1025.313684	t-BuSO-OSt-Bu	-1260.687558
$[MeS(O)]_2$	-1025.368987	$[t\text{-}BuS(O)]_2$	-1260.733369
MeS(O)OSMe	-1025.370606	t-BuS(O)OSt-Bu	-1260.743201
MeS●	-437.512037	t-BuS●	-555.194064
MeS(O)O●	-587.802604	t-BuS(O)O●	-705.490415
$Me(SO_2)SMe$	-1025.405819	$t\text{-}Bu(SO_2)St\text{-}Bu$	-1260.774693
TS for isomerisation	-1025.308919	TS for isomerisation	-1260.676277

Table S6. Relevant Structures for the Stationary Points in Scheme 2.

MeSO●

O	-1.38880900	-0.04382800	0.00000000
C	1.15888200	-0.85481300	0.00000000
H	2.17331200	-0.44942300	0.00000000
H	0.99193200	-1.45730800	0.89406500
H	0.99193200	-1.45730800	-0.89406500
S	0.00000000	0.55272100	0.0000000

MeSO-OOMe

C	2.91845600	-0.29775300	0.13341900
H	3.77005700	0.13487500	0.65921700
H	2.51605100	-1.14664200	0.68856600
H	3.19940900	-0.59814800	-0.87797200
O	0.86038700	0.33821900	-0.61840600
O	-0.18662000	-0.49050500	0.50087600
C	-2.42349700	0.91604000	0.18806700
H	-1.88887500	1.72754500	-0.30551000
H	-3.43724400	0.84290800	-0.21387700
H	-2.45848600	1.07875000	1.26512800
O	1.93899200	0.75393200	0.08018400
S	-1.59829500	-0.66013600	-0.17785600

MeS(O)-OOMe

C	-1.73686000	1.27559400	0.07874300
H	-2.72652600	1.16089300	-0.36325900
H	-1.80154400	1.27762200	1.16691200
H	-1.24208000	2.17225700	-0.29328000
S	-0.78871900	-0.20187100	-0.41565000
O	-1.49745800	-1.35191500	0.15303000
O	0.47830500	0.32717200	0.64178800
O	1.63224500	-0.50891500	0.35805000
C	2.57141500	0.30011900	-0.33758500
H	2.84945600	1.17584800	0.25539500
H	3.43901300	-0.35019100	-0.46902100
H	2.18912500	0.60849000	-1.31624800

MeS(O)O●

C	1.58544100	-0.00004200	0.09434800
H	2.00944600	0.90333600	-0.33874100
H	1.67589900	-0.00028600	1.18096300

H	2.00944300	-0.90321900	-0.33916500
S	-0.21277300	0.00000300	-0.27422900
O	-0.73764600	1.28115200	0.20740500
O	-0.73773700	-1.28110500	0.20740900

$Me(SO_2)OMe$

C	2.17305000	0.12897700	-0.03469400
H	2.97899200	-0.16018400	-0.70637100
H	2.24168000	1.19859800	0.18196400
H	2.22051100	-0.44619500	0.88874300
O	-0.18348000	-0.49186200	1.43965300
C	-0.94819800	1.52638100	-0.06196000
H	-0.20762100	2.15250800	0.43413800
H	-1.04698600	1.78248000	-1.11507200
H	-1.90856600	1.60878400	0.44673600
O	-1.33300300	-0.97740900	-0.74197400
S	-0.44708100	-0.18475900	0.05736300
O	0.95725500	-0.16972800	-0.75618000

MeSO-OSMe

C	2.91352500	0.84503500	-0.05645500
H	3.88729100	0.71096000	0.42076800
H	3.03872200	1.05784600	-1.11893800
H	2.36815500	1.65621200	0.42828400
S	1.98205800	-0.70111200	0.15355900
O	0.66114700	-0.46093900	-0.59230200
O	-0.66112800	0.46083500	0.59231700
S	-1.98201500	0.70111800	-0.15355600
C	-2.91361200	-0.84495800	0.05643600
H	-3.03884900	-1.05775400	1.11891700
H	-3.88735800	-0.71081200	-0.42080800
H	-2.36829300	-1.65617900	-0.42828600

$[MeS(O)]_2$

C	0.67680000	1.91515400	0.32015100
H	0.21446400	2.76413300	0.82355800
H	1.18858500	1.25275400	1.02553500
H	1.37286800	2.25199600	-0.45089900
S	-0.67680000	1.01046400	-0.48246400
O	-1.74412900	0.81542900	0.55003900
S	0.67680000	-1.01046400	-0.48246400
O	1.74412900	-0.81542900	0.55003900
C	-0.67680000	-1.91515400	0.32015100

H	-1.18858500	-1.25275400	1.02553500
H	-1.37286800	-2.25199600	-0.45089900
H	-0.21446400	-2.76413300	0.82355800

MeS(O)OSMe

C	2.13721600	1.17919700	-0.31117200
H	3.09635800	1.15268700	0.20694800
H	2.25213400	0.89130400	-1.35608500
H	1.66725900	2.15793800	-0.21810800
S	1.08133700	-0.07510100	0.47646000
O	1.69126100	-1.37475300	0.17054700
O	-0.17217500	0.27671300	-0.68602100
C	-2.49561500	0.71732300	0.60408100
H	-2.57170100	1.65883500	0.05971100
H	-3.49956800	0.31526400	0.76891300
H	-2.00799800	0.86357100	1.56839200
S	-1.64001000	-0.52704900	-0.39292400

MeS●

S	-0.69444200	0.00001500	-0.00198600
C	1.11098200	0.00008400	-0.00888000
H	1.51114900	0.90105700	-0.47528600
H	1.42327400	-0.00423100	1.04239800
H	1.51075700	-0.89756900	-0.48205300

MeS(O)O●

C	1.58544100	-0.00004200	0.09434800
H	2.00944600	0.90333600	-0.33874100
H	1.67589900	-0.00028600	1.18096300
H	2.00944300	-0.90321900	-0.33916500
S	-0.21277300	0.00000300	-0.27422900
O	-0.73764600	1.28115200	0.20740500
O	-0.73773700	-1.28110500	0.20740900

Me(SO_2)SMe

C	-2.25283200	0.65484900	-0.10118800
H	-3.26628000	0.26545200	-0.20935600
H	-2.23344100	1.39807700	0.69524200
H	-1.92618400	1.08733500	-1.04493000
S	-1.20814500	-0.79102100	0.29553000
O	0.57770700	0.97049500	-1.24251600
C	1.25706400	0.83851700	1.28915300

H	0.56236100	1.65025800	1.49780300
H	1.29500300	0.12180900	2.10674500
H	2.25050500	1.23188800	1.06696400
O	1.55720500	-1.18701400	-0.35925200
S	0.72148000	-0.02040800	-0.19716200

TS for isomerisation

C	-1.62082000	1.46769600	0.13229000
H	-2.37157400	1.66504000	-0.63228100
H	-2.07365900	1.43207200	1.12534500
H	-0.81062500	2.19311100	0.09158900
S	-0.93753300	-0.19352600	-0.15041900
O	-2.07710800	-1.10733600	-0.08127700
O	0.06278800	-0.37818800	1.02310100
S	1.33181200	0.02437500	-0.73150200
C	2.65978100	0.05196700	0.50966400
H	2.72935000	-0.90160200	1.02821300
H	3.55800100	0.21010200	-0.10092200
H	2.54083200	0.87391000	1.21248300

t-BuSO●

O	2.04088000	0.48269800	0.00000500
C	-0.64522200	0.06014000	-0.00000100
S	1.07252200	-0.68125300	-0.00000200
C	-0.78753200	0.91589300	-1.26399400
H	-1.76060600	1.41773300	-1.26788400
H	-0.00679300	1.67838200	-1.29907800
H	-0.71470700	0.30780900	-2.16942700
C	-0.78792800	0.91491600	1.26460100
H	-1.76105400	1.41665500	1.26861400
H	-0.71526600	0.30615800	2.16959400
H	-0.00725300	1.67743600	1.30042100
C	-1.60395100	-1.13492000	-0.00060500
H	-2.63892900	-0.78001500	-0.00044200
H	-1.46746700	-1.76050400	-0.88727000
H	-1.46750800	-1.76136600	0.88546200

t-BuOO●

O	1.97220800	-0.00012300	-0.19618000
C	-0.36924300	0.00004200	0.04873000
O	0.83393800	-0.00040000	-0.85131200
C	-1.52398000	-0.00029900	-0.94520800
H	-1.48683600	-0.88688500	-1.58191800

H	-2.47587900	-0.00006300	-0.40907400
H	-1.48681000	0.88576100	-1.58265300
C	-0.31681900	1.26944700	0.89200000
H	-1.18199000	1.31105300	1.55831400
H	0.59105100	1.28254300	1.49613200
H	-0.32742300	2.15694200	0.25511900
C	-0.31699900	-1.26873500	0.89295700
H	-1.18198800	-1.30952600	1.55955900
H	-0.32810100	-2.15671400	0.25675800
H	0.59104800	-1.28166400	1.49683000

t-BuSO-OOt-Bu

C	2.92396000	0.10848400	0.05636900
O	0.73981100	-0.14431300	-0.80019300
O	-0.28359000	-0.81964200	0.49572100
C	-2.71734900	0.33870300	0.02017000
O	1.60917900	0.72468400	-0.25160800
S	-1.68069900	-1.20847200	-0.10187800
C	2.73807800	-0.99144700	1.09877000
H	2.11072900	-1.79136000	0.70632900
H	3.71136300	-1.40818100	1.37209800
H	2.26209300	-0.59345100	1.99681300
C	3.52411300	-0.42271000	-1.24394600
H	3.63607700	0.38354800	-1.97274200
H	4.50828300	-0.85882800	-1.05443100
H	2.87959700	-1.19207500	-1.67078600
C	3.70653500	1.29694700	0.60920600
H	3.22801200	1.68853900	1.50940000
H	4.72271800	0.98686800	0.86377300
H	3.76445700	2.09915100	-0.12977700
C	-2.22131000	1.36838000	-1.00350100
H	-2.83337400	2.27489800	-0.93776900
H	-1.18103900	1.63624200	-0.81659000
H	-2.29149900	0.98004300	-2.02205500
C	-2.62213100	0.88676800	1.44700000
H	-3.19388300	1.81727900	1.52615000
H	-3.02097500	0.17562800	2.17452100
H	-1.58389200	1.09894600	1.70804500
C	-4.13822900	-0.13704200	-0.31359300
H	-4.49975700	-0.87302500	0.40962100
H	-4.82200000	0.71684400	-0.29416000
H	-4.19093800	-0.57983100	-1.31261100

t-BuS(O)-OOt-Bu

C	-2.36005400	0.34415200	0.05551600
S	-0.90132200	-0.67684700	-0.58109700
O	-0.81418400	-1.86208200	0.29293800
O	0.22480600	0.51546400	-0.06285700
O	1.44534700	0.30929900	-0.84457500
C	2.57889100	0.10156400	0.05133400
C	3.72622300	0.01366400	-0.96076700
H	3.79989300	0.93431500	-1.54302500
H	4.66869800	-0.14083700	-0.43034400
H	3.57266000	-0.82238100	-1.64592200
C	2.42316700	-1.20077700	0.83555000
H	3.30304600	-1.36598500	1.46342300
H	1.54084200	-1.17064100	1.47464200
H	2.31570000	-2.04860500	0.15613900
C	2.73972700	1.31404000	0.97090700
H	1.89254100	1.39768400	1.65272900
H	3.65063800	1.21598000	1.56733400
H	2.80589800	2.23235400	0.38299400
C	-2.41539100	1.64580900	-0.74663800
H	-3.33350500	2.18770300	-0.49774800
H	-1.56275300	2.28755400	-0.52603400
H	-2.42926700	1.45204000	-1.82352000
C	-2.19983300	0.56475000	1.55997800
H	-1.38399500	1.25488700	1.77826400
H	-3.12536200	0.98361600	1.96756500
H	-2.00049500	-0.38302200	2.06430100
C	-3.57320300	-0.54877900	-0.24524200
H	-4.48403800	-0.03910300	0.08234000
H	-3.67113100	-0.75242500	-1.31586600
H	-3.50313300	-1.50156400	0.28240200

t-BuS(O)O●

C	-0.88721000	0.00000100	0.02449900
S	1.02139600	-0.00000200	-0.35891200
O	1.55138700	-1.27350000	0.14686300
O	1.55139400	1.27349600	0.14685600
C	-0.98467300	-0.00001700	1.55013200
H	-0.51427800	0.88741500	1.97639800
H	-2.04257400	-0.00001400	1.83398400
H	-0.51428800	-0.88746500	1.97637600
C	-1.44108700	1.27248600	-0.60600900
H	-1.31501900	1.27231900	-1.69149500
H	-2.51327700	1.33590000	-0.39313200

H	-0.95619000	2.16073700	-0.19999400
C	-1.44110100	-1.27246300	-0.60604500
H	-2.51330300	-1.33584200	-0.39322300
H	-1.31498000	-1.27229400	-1.69152500
H	-0.95625500	-2.16073400	-0.20001500

t-BuO●

O	0.00010200	0.26103500	1.42837500
C	-0.00001500	-0.02726500	0.08074900
C	1.27699800	-0.79258600	-0.31532700
H	1.30429200	-1.75977100	0.19265000
H	1.31429700	-0.97138400	-1.39361500
H	2.16150100	-0.22572300	-0.01841700
C	0.00054300	1.38913000	-0.57752300
H	0.00056300	1.26171600	-1.66293200
H	-0.88797000	1.94731300	-0.28040500
H	0.88944200	1.94664200	-0.28030600
C	-1.27761500	-0.79159500	-0.31533100
H	-1.30552300	-1.75888600	0.19241600
H	-2.16168200	-0.22419700	-0.01814500
H	-1.31519400	-0.97010200	-1.39365800

t-Bu(SO_2)Ot-Bu

C	-2.13187200	0.23202600	-0.02792100
O	0.55563800	-1.61930300	-1.06071600
C	1.93083400	0.45009700	-0.03031500
O	0.26548300	-1.15552000	1.36807900
S	0.46198000	-0.66464700	0.01944900
O	-0.67910100	0.42744000	-0.33358000
C	-2.36685200	0.58792100	1.43964200
H	-1.84402700	-0.10506500	2.09757200
H	-2.01670100	1.60166500	1.64670600
H	-3.43707700	0.54347700	1.65995700
C	-2.57522500	-1.19494800	-0.35204300
H	-3.65949400	-1.26372500	-0.22994300
H	-2.32335400	-1.45966400	-1.37987800
H	-2.11164600	-1.91951000	0.31838000
C	-2.79533600	1.24106200	-0.96259000
H	-2.59074700	0.99138900	-2.00532600
H	-3.87708900	1.23394200	-0.80658800
H	-2.42461600	2.24920300	-0.76594900
C	2.03665300	1.05866900	-1.43405800
H	2.08783100	0.28048600	-2.19656900

H	1.18561800	1.70455500	-1.65175800
H	2.94992800	1.65845600	-1.48989600
C	1.77339200	1.52294100	1.05224400
H	1.64655200	1.07285600	2.03769200
H	2.67531800	2.14174500	1.06952900
H	0.91818000	2.16758600	0.84798000
C	3.12774800	-0.46892400	0.26858500
H	4.04069600	0.13255400	0.26021200
H	3.03265900	-0.93716600	1.24971400
H	3.22408600	-1.25243500	-0.48453900

t-BuSO-OSt-Bu

C	-3.14725300	0.17255200	0.01529400
S	-1.81138400	-1.10819300	-0.23260600
O	-0.59244400	-0.60806500	0.55818500
O	0.59242200	0.60817800	-0.55805800
S	1.81147800	1.10828200	0.23256600
C	3.14723700	-0.17258700	-0.01531600
C	-2.73615200	1.45580600	-0.71928900
H	-3.49391400	2.23112200	-0.56026600
H	-1.77685200	1.82290300	-0.35235800
H	-2.64145500	1.28463700	-1.79419200
C	-4.40811400	-0.44791000	-0.59873800
H	-4.69840200	-1.36764200	-0.08353300
H	-5.24048600	0.25784100	-0.51923400
H	-4.26876000	-0.67675400	-1.65941900
C	-3.30420100	0.42097200	1.51877500
H	-4.03477700	1.21802100	1.69193900
H	-3.64825600	-0.47763000	2.03709500
H	-2.35181000	0.72495500	1.95686100
C	2.73629900	-1.45558400	0.71981800
H	1.77689600	-1.82278400	0.35325800
H	3.49400300	-2.23097100	0.56086300
H	2.64188400	-1.28405400	1.79468900
C	3.30374300	-0.42153500	-1.51875100
H	3.64752900	0.47691100	-2.03751800
H	4.03435600	-1.21856600	-1.69184000
H	2.35125200	-0.72579200	-1.95642600
C	4.40829700	0.44802800	0.59815400
H	5.24059400	-0.25782100	0.51873700
H	4.69852200	1.36752800	0.08250400

[t-BuS(O)]$_2$

C	-2.30655200	0.19766200	0.01895100
S	-0.82724800	-0.86157200	-0.52760700
O	-0.63296400	-1.88769000	0.54908800
S	0.82724700	0.86156700	-0.52760700
O	0.63295800	1.88768600	0.54908700
C	2.30655300	-0.19766100	0.01895200
C	-2.14317200	0.55539600	1.49652800
H	-3.06866700	1.01519200	1.85850500
H	-1.95636000	-0.34574700	2.08374200
H	-1.32118200	1.25388600	1.64935800
C	-3.50086300	-0.74698300	-0.19174300
H	-4.41428700	-0.24482200	0.14183500
H	-3.62695600	-1.01381900	-1.24476400
H	-3.38402800	-1.66441000	0.38830700
C	-2.40357100	1.41933100	-0.89844400
H	-3.37785500	1.89663300	-0.75164600
H	-1.63479000	2.15874600	-0.67297600
H	-2.33655300	1.14095500	-1.95510800
C	3.50086000	0.74699400	-0.19172800
H	3.38401400	1.66441500	0.38832900
H	4.41428500	0.24483700	0.14185200
H	3.62695800	1.01383900	-1.24474600
C	2.14316900	-0.55540800	1.49652500
H	1.32117900	-1.25390000	1.64934600
H	3.06866300	-1.01520600	1.85850100
H	1.95635400	0.34573000	2.08374500
C	2.40358300	-1.41932000	-0.89845600
H	3.37787000	-1.89661800	-0.75165800
H	1.63480600	-2.15874200	-0.67300000
H	2.33657000	-1.14093300	-1.95511600

t-BuS(O)OSt-Bu

C	2.60537300	-0.21526400	0.19134600
S	1.09670900	0.44549300	-0.72723600
O	0.87276600	1.81073400	-0.21095500
O	0.01935000	-0.64351800	0.08170200
C	-2.67681600	0.09327200	0.18313700
S	-1.45114900	-0.97364700	-0.71959600
C	3.76022000	0.64661900	-0.34041200
H	3.60761000	1.70123500	-0.10432700
H	4.69534400	0.32115400	0.12463200
H	3.87542400	0.54753900	-1.42412700
C	2.40255800	-0.00872600	1.69183800

H	1.61882600	-0.66095400	2.07822600
H	3.33489600	-0.23369500	2.21933700
H	2.12966100	1.02766200	1.90082500
C	2.78354900	-1.68515100	-0.19507300
H	2.83111400	-1.81235100	-1.28115500
H	3.72435700	-2.05931400	0.22085200
H	1.96813200	-2.29843000	0.18842300
C	-2.56041500	-0.15051700	1.69099400
H	-2.72196000	-1.20232600	1.93668000
H	-1.57352600	0.13994800	2.05421400
H	-3.30808000	0.44957800	2.22054300
C	-2.49282600	1.57647700	-0.15493400
H	-3.26075400	2.16618100	0.35833500
H	-1.51400900	1.94074900	0.15874800
H	-2.58962100	1.75014900	-1.22907700
C	-4.01917900	-0.42776800	-0.36106200
H	-4.83160000	0.15638300	0.08089800
H	-4.08672500	-0.31612200	-1.44719500
H	-4.17974900	-1.47831200	-0.10749700
C	2.60537300	-0.21526400	0.19134600
S	1.09670900	0.44549300	-0.72723600
O	0.87276600	1.81073400	-0.21095500
O	0.01935000	-0.64351800	0.08170200
C	-2.67681600	0.09327200	0.18313700
S	-1.45114900	-0.97364700	-0.71959600
C	3.76022000	0.64661900	-0.34041200
H	3.60761000	1.70123500	-0.10432700
H	4.69534400	0.32115400	0.12463200
H	3.87542400	0.54753900	-1.42412700
C	2.40255800	-0.00872600	1.69183800
H	1.61882600	-0.66095400	2.07822600
H	3.33489600	-0.23369500	2.21933700
H	2.12966100	1.02766200	1.90082500
C	2.78354900	-1.68515100	-0.19507300
H	2.83111400	-1.81235100	-1.28115500
H	3.72435700	-2.05931400	0.22085200
H	1.96813200	-2.29843000	0.18842300
C	-2.56041500	-0.15051700	1.69099400
H	-2.72196000	-1.20232600	1.93668000
H	-1.57352600	0.13994800	2.05421400
H	-3.30808000	0.44957800	2.22054300
C	-2.49282600	1.57647700	-0.15493400
H	-3.26075400	2.16618100	0.35833500
H	-1.51400900	1.94074900	0.15874800
H	-2.58962100	1.75014900	-1.22907700
C	-4.01917900	-0.42776800	-0.36106200

H	-4.83160000	0.15638300	0.08089800
H	-4.08672500	-0.31612200	-1.44719500
H	-4.17974900	-1.47831200	-0.10749700

t-BuS(O)O●

C	-0.88721000	0.00000100	0.02449900
S	1.02139600	-0.00000200	-0.35891200
O	1.55138700	-1.27350000	0.14686300
O	1.55139400	1.27349600	0.14685600
C	-0.98467300	-0.00001700	1.55013200
H	-0.51427800	0.88741500	1.97639800
H	-2.04257400	-0.00001400	1.83398400
H	-0.51428800	-0.88746500	1.97637600
C	-1.44108700	1.27248600	-0.60600900
H	-1.31501900	1.27231900	-1.69149500
H	-2.51327700	1.33590000	-0.39313200
H	-0.95619000	2.16073700	-0.19999400
C	-1.44110100	-1.27246300	-0.60604500
H	-2.51330300	-1.33584200	-0.39322300
H	-1.31498000	-1.27229400	-1.69152500
H	-0.95625500	-2.16073400	-0.20001500

t-BuS●

S	-1.53282900	0.00066300	-0.07408200
C	0.31147000	0.00010700	-0.00649100
C	0.66714300	-0.01489300	1.49486600
H	1.75782500	-0.01614900	1.59820500
H	0.27887800	0.86727800	2.00868500
H	0.27847100	-0.90693800	1.99102900
C	0.85955500	1.27200000	-0.67154100
H	1.95397100	1.28175000	-0.61430000
H	0.57863000	1.31878600	-1.72644400
H	0.47816900	2.16821900	-0.17918900
C	0.85977900	-1.25825900	-0.69664100
H	0.57873300	-1.28435500	-1.75221500
H	1.95419900	-1.26882700	-0.63968200
H	0.47870100	-2.16409400	-0.22194000

t-Bu(SO_2)St-Bu

C	2.37377200	0.17229900	0.09524000
S	0.88628500	0.11089000	-1.07101400
O	-0.34427700	-0.97037000	1.41272000
C	-2.10881100	0.53986900	0.02566100

O	-1.23579100	-1.87027700	-0.76097800
S	-0.75563200	-0.75676100	0.03359200
C	-2.45012100	0.87057000	-1.42964600
H	-3.29683600	1.56341700	-1.44226100
H	-1.61581600	1.35439800	-1.94139400
H	-2.73112400	-0.02580500	-1.98351400
C	-1.63416900	1.76719800	0.80313500
H	-0.77478200	2.23926000	0.32456400
H	-2.44748900	2.49855200	0.83320600
H	-1.36916000	1.50930900	1.82920500
C	-3.28774000	-0.14828700	0.73386200
H	-4.12443500	0.55491000	0.77491400
H	-3.60969600	-1.03869400	0.19291500
H	-3.02692300	-0.43210400	1.75463900
C	2.13028700	1.10055500	1.28767600
H	1.86792000	2.10840800	0.95848600
H	1.34067700	0.71840600	1.93310900
H	3.04989800	1.16723400	1.87962900
C	3.46056200	0.75622700	-0.82517500
H	4.39590300	0.82274400	-0.26052100
H	3.63711100	0.12087700	-1.69614700
H	3.20311700	1.75997000	-1.17177400
C	2.75849000	-1.24106900	0.54503700
H	1.98976500	-1.67710600	1.18150700
H	2.91659900	-1.89638800	-0.31370400
H	3.69174200	-1.19246000	1.11721900

TS for isomerisation

C	2.16770200	0.56442900	-0.07890300
S	0.74265800	-0.63138100	0.31470200
O	1.24956700	-1.48716400	1.39790500
O	0.60428800	-1.43404200	-1.04686100
S	-1.27061000	-0.50692500	-1.08679300
C	-2.36661600	0.29189200	0.21596200
C	3.33755600	-0.34318800	-0.46627500
H	3.06398100	-1.00032700	-1.29509200
H	4.17950400	0.27891100	-0.78577500
H	3.65421500	-0.96030300	0.37545800
C	1.74308100	1.46636100	-1.23637600
H	0.87238400	2.07489500	-0.98287800
H	2.56558300	2.14715500	-1.47898700
H	1.50842300	0.88307000	-2.12770000
C	2.44439300	1.35360900	1.20118500
H	3.30360100	2.01307100	1.04401700
H	1.59406100	1.98228100	1.48134400

H	2.67238700	0.68663100	2.03402400
C	-1.85267700	1.65026200	0.67690600
H	-2.57284900	2.11343000	1.35994300
H	-0.91143900	1.54205700	1.22014200
H	-1.69408300	2.32574800	-0.16614700
C	-2.61495700	-0.65024700	1.39275000
H	-3.34637000	-0.20832400	2.07858700
H	-2.99557600	-1.61549500	1.05384700
H	-1.69563100	-0.82709300	1.95488700
C	-3.63786300	0.44493500	-0.65128700
H	-4.00638000	-0.51750900	-1.01335600
H	-4.42070500	0.88769300	-0.02610300
H	-3.47840800	1.10832300	-1.50487200

Table S7. Relevant Enthalpies (in a.u.) for the Other Calculations Referred to in the Text.

Structure	H_{298}^{o}
allicin radical dissociation TS	-1104.09785
allylSOOMe	-704.78797
	-704.786734
	-704.786825
	-704.78581
	-704.787456
	-704.785937
propylSOOMe	-705.99729
	-705.995751
	-705.998061
	-705.994795
	-705.996248
	-705.99733
methoxyl	-114.870491
allylS(O)OMe	-704.871569
	-704.872926
	-704.871242
	-704.874218
	-704.873052
	-704.872924
propylS(O)OMe	-706.081581
	-706.082452
	-706.082700
	-706.082891
	-706.083398
	-706.082707

Table S8. Relevant Structures for the Other Calculations Referred to in the Text.

allicin radical dissociation TS

C	3.20644800	1.99600100	0.60917600
H	3.60243200	1.67889100	1.56807600
H	3.40417400	3.01654000	0.30566600
C	2.50046000	1.14736200	-0.17763000
H	2.12208300	1.49318800	-1.13579100
C	2.23697800	-0.20989300	0.16860700
H	2.62079600	-0.56655800	1.12281900
S	1.36926100	-1.28810800	-0.78267500
S	-1.05440500	-1.16817300	-0.02670500
C	-1.19744500	0.67146700	-0.18703600
H	-0.39554700	1.08141500	0.43312500
H	-1.00259200	0.89971100	-1.23708300
C	-2.55065600	1.12170900	0.26319600
H	-2.77929000	0.94531700	1.31022300
C	-3.45319100	1.69097700	-0.53174200
H	-3.25579500	1.87670200	-1.58309800
H	-4.42114000	1.99941100	-0.15442600
O	-1.17354700	-1.45373200	1.43164300

allylSOOMe – conf 1

C	1.38114800	-0.52134500	0.64446300
H	0.97109000	-0.48255400	1.65722200
H	2.20814100	-1.23872800	0.63779600
S	0.06172400	-1.30456800	-0.36824100
O	-1.28527100	-0.65731600	0.29253600
O	-1.59074600	0.70268100	-0.35748100
C	-2.87111100	1.03602100	0.13016200
H	-3.09035900	2.00721500	-0.32290100
H	-3.62506300	0.30746800	-0.18641100
H	-2.87756300	1.13507900	1.22132500
C	1.81282700	0.82379800	0.14931300
H	1.03242900	1.57816400	0.10913600
C	3.05067300	1.11528600	-0.23941300
H	3.84595600	0.37582800	-0.21873900
H	3.31469300	2.10513800	-0.59316500

allylSOOMe – conf 2

C	-1.45710400	-0.49261900	0.68138300
H	-2.15364100	-1.26948800	1.02000900
H	-1.01872300	-0.01938700	1.56130800

S	-0.14185300	-1.47400000	-0.14659600
O	0.89345400	-0.31237000	-0.64182800
O	1.81361300	0.08368600	0.51735200
C	2.59694300	1.12955400	-0.01371500
H	3.25082200	1.42484100	0.81191900
H	3.20735300	0.78883400	-0.85702100
H	1.98065800	1.98302200	-0.31626000
C	-2.11773400	0.49517600	-0.22316200
H	-2.67738100	0.08018700	-1.05768100
C	-2.02354700	1.81351900	-0.07692400
H	-1.45890900	2.25506100	0.73825200
H	-2.50840700	2.49661300	-0.76467400

allylSOOMe – conf 3

C	-1.15159600	-0.52044600	0.42922000
H	-0.53951100	-1.40896000	0.26200300
H	-1.32550100	-0.38455300	1.49719600
S	-0.15562000	0.89227500	-0.21201300
O	1.31983100	0.57788100	0.41942900
O	2.07210600	-0.40648900	-0.48730800
C	3.33185100	-0.54678000	0.13057000
H	3.24493800	-0.96182200	1.14086200
H	3.87025500	-1.25360100	-0.50741500
H	3.87526600	0.40378600	0.16023800
C	-2.43074700	-0.57528000	-0.34665000
H	-2.35169900	-0.92305300	-1.37347900
C	-3.61328200	-0.19740800	0.13308500
H	-3.72522500	0.16575400	1.15006300
H	-4.51144600	-0.24560400	-0.47157800

allylSOOMe – conf 4

C	1.39893600	-0.70520800	0.44710500
H	1.15790800	-0.90983800	1.49365600
H	2.15079900	-1.43089900	0.12121400
S	-0.12692000	-1.14792400	-0.47547000
O	-1.29825300	-0.64386500	0.59021100
O	-1.55190700	0.82936200	0.48647600
C	-2.62966000	1.00068100	-0.41528900
H	-2.80595300	2.07963400	-0.42859100
H	-2.36407500	0.66719000	-1.42509700
H	-3.52790500	0.48364500	-0.06486400
C	1.85902400	0.70268400	0.23044300
H	1.15553500	1.47467100	0.52784500
C	3.03596000	1.03090400	-0.29449400

H	3.75379800	0.27778200	-0.60636800
H	3.32633400	2.06625400	-0.43036700

allylSOOMe – conf 5

C	1.20470300	0.18092500	0.67946500
H	0.65130200	1.00685700	1.13056400
H	1.51948300	-0.52099000	1.45209100
S	0.01722500	-0.65420600	-0.45092600
O	-1.33793900	-0.74885000	0.51340300
O	-2.08020200	0.54763600	0.54977800
C	-3.04546500	0.50160300	-0.48471200
H	-3.58091100	1.45116600	-0.40172900
H	-2.57066000	0.44170800	-1.47105000
H	-3.74208400	-0.33024100	-0.34369800
C	2.35725600	0.67053100	-0.14202600
H	2.15802800	1.52648700	-0.78178500
C	3.56307900	0.10741800	-0.14900700
H	3.79178200	-0.75489100	0.46960800
H	4.36515100	0.49404600	-0.76697200

allylSOOMe – conf 6

C	-1.32313600	-0.61600300	0.75235800
H	-1.72686600	-1.52725600	1.20962700
H	-0.95357300	0.03095300	1.54943900
S	0.13612400	-1.23791100	-0.17266400
O	0.77778900	0.18239600	-0.75119000
O	1.55425800	0.89621200	0.30658800
C	2.90817000	0.51290400	0.15046300
H	3.44396300	1.08518800	0.91255600
H	3.04496100	-0.55785600	0.34113000
H	3.28500600	0.77565100	-0.84251000
C	-2.32528000	0.06871600	-0.11864300
H	-2.85503300	-0.56361400	-0.82661400
C	-2.55517300	1.37788300	-0.09329300
H	-2.02222900	2.03459500	0.58668500
H	-3.27808300	1.83904900	-0.75617200

propylSOOMe – conf 1

C	1.42053800	-0.73075700	0.68626600
H	1.11627800	-1.06855000	1.67925700
H	2.29181300	-1.32751300	0.38635000
S	0.12152200	-1.27510700	-0.47404100
O	-1.23646300	-0.71910500	0.25762900

O	-1.52069800	0.72428300	-0.17946700
C	-2.89086800	0.90747900	0.09981900
H	-3.09081100	1.94459300	-0.18478600
H	-3.51778700	0.23615000	-0.49669300
H	-3.10805600	0.77710600	1.16571400
C	1.74191700	0.76759100	0.67500700
H	2.44240400	0.95841600	1.49729900
C	2.33997800	1.27298800	-0.63900400
H	3.27069600	0.74879400	-0.88038000
H	2.56659400	2.34026600	-0.57696700
H	1.64490900	1.12701000	-1.46863100
H	0.82751200	1.32021300	0.90567200

propylSOOMe – conf 2

C	-1.36259500	-0.61789100	0.77831700
H	-1.83814300	-1.51359000	1.19390400
H	-0.79508000	-0.15042200	1.58720400
S	-0.13328100	-1.30261000	-0.38572000
O	0.90811800	-0.05426100	-0.59546400
O	1.94598700	-0.05743600	0.53415400
C	2.90028000	0.89809800	0.12877700
H	3.64176700	0.89847300	0.93297500
H	3.38284600	0.61304000	-0.81225600
H	2.46244900	1.89853600	0.03926700
C	-2.40912300	0.32585000	0.17943800
H	-3.17147200	0.50403600	0.94835800
C	-1.85144600	1.66659600	-0.30423400
H	-1.36736400	2.20887000	0.51382200
H	-2.65215600	2.29818800	-0.69772800
H	-1.10871900	1.52685900	-1.09168300
H	-2.91716200	-0.18458300	-0.64564400

propylSOOMe – conf 3

C	0.98476800	0.72982700	0.32493600
H	0.35593000	1.55847400	-0.00446900
H	1.02675300	0.72435500	1.41674700
S	0.14255600	-0.80064100	-0.23022100
O	-1.34509700	-0.59796000	0.41710800
O	-2.19088800	0.29883200	-0.50287200
C	-3.41862000	0.42441100	0.17795100
H	-4.02600900	1.06209900	-0.47104300
H	-3.91398500	-0.54494600	0.30089500
H	-3.29576300	0.90934200	1.15291000
C	2.38697700	0.83319800	-0.28540900

H	2.78390300	1.82031400	-0.02550600
C	3.36481600	-0.24810300	0.18910000
H	3.45273700	-0.24671600	1.27961700
H	4.36100500	-0.08023000	-0.22746800
H	3.04584000	-1.24906600	-0.11376500
H	2.30892600	0.81366500	-1.37773400

propylSOOMe – conf 4

C	1.44969900	-0.89499800	0.40854800
H	1.30502300	-1.44368200	1.34160600
H	2.22114000	-1.42166400	-0.16812800
S	-0.05981800	-1.14970200	-0.58181400
O	-1.24029600	-0.73934100	0.51699300
O	-1.49142400	0.73808700	0.53529300
C	-2.63347100	0.96447500	-0.26961300
H	-2.81598300	2.03965600	-0.19039300
H	-2.44417600	0.70657600	-1.31810600
H	-3.50134200	0.41467600	0.10675200
C	1.84864200	0.56138300	0.66838600
H	2.69797600	0.54718700	1.36229800
C	2.22642300	1.34504900	-0.58990100
H	3.06455900	0.87516600	-1.11516000
H	2.52333200	2.36590500	-0.33700100
H	1.38477400	1.40417600	-1.28345500
H	1.02778200	1.06181900	1.18781600

propylSOOMe – conf 5

C	-1.05401200	0.72760600	-0.41158700
H	-0.47092700	1.63006200	-0.22243100
H	-1.24003200	0.63975900	-1.48432200
S	-0.00351700	-0.68094300	0.10172600
O	1.35685200	-0.39643500	-0.81529100
O	2.21095400	0.67555900	-0.21502800
C	3.15717100	0.03062800	0.61654500
H	3.77494800	0.84266000	1.00952000
H	2.66862200	-0.48552900	1.45137000
H	3.77996300	-0.66627700	0.04751600
C	-2.36490100	0.74879600	0.38315800
H	-2.87970900	1.68308000	0.13482600
C	-3.29756500	-0.43490200	0.10188400
H	-3.53662800	-0.50164400	-0.96354400
H	-4.23689200	-0.32693600	0.64978700
H	-2.85002300	-1.38727800	0.39828000
H	-2.13964300	0.80143400	1.45393200

propylSOOMe – conf 6

C	-1.22875900	-0.76033200	0.75339200
H	-1.48132800	-1.75849800	1.12950500
H	-0.78177100	-0.20806300	1.58414700
S	0.11723400	-1.09756900	-0.42961600
O	0.82180400	0.40451100	-0.60614700
O	1.72519800	0.72132400	0.53970500
C	3.02853700	0.31725600	0.16161600
H	3.65823900	0.59802100	1.01013600
H	3.08514300	-0.76766800	0.01541600
H	3.36366300	0.84235000	-0.73785700
C	-2.46863200	-0.06178500	0.18837800
H	-3.24409800	-0.09254800	0.96421300
C	-2.23998900	1.38871900	-0.24476100
H	-1.87839300	1.99639200	0.59014900
H	-3.17108200	1.83328400	-0.60586000
H	-1.49746700	1.45452900	-1.04164600
H	-2.85160900	-0.64652500	-0.65456500

Methoxyl

O	-1.18649600	-0.27869000	0.00000000
C	1.09630100	-0.18319600	0.00000000
H	1.14901800	-0.80078100	-0.89700200
H	1.87508100	0.57851700	-0.00000200
H	1.14902000	-0.80077800	0.89700400
O	-0.15737000	0.54396700	0.00000000

allylS(O)OMe – conf 1

C	-0.89976500	-0.88669800	0.22594000
H	-0.58705000	-1.90086200	-0.02891000
H	-0.81336700	-0.72855700	1.30231000
S	0.40565300	0.23176100	-0.47536900
O	0.23180600	1.53651500	0.18439400
C	-2.24439700	-0.53076400	-0.31560700
C	-3.12980800	0.22493800	0.32870400
H	-4.08807300	0.47347000	-0.11243500
O	1.60073900	-0.66110000	0.32995100
C	2.92863100	-0.16102300	0.11328200
H	3.59735300	-0.86184700	0.61194700
H	3.17018400	-0.12532800	-0.95469200
H	3.04733400	0.83292800	0.55185800
H	-2.48009900	-0.90107300	-1.31047700
H	-2.92506300	0.62107000	1.31762500

allylS(O)OMe – conf 2

C	1.09915200	-0.56811300	-0.79214000
H	1.38309100	-1.59228200	-1.05806400
H	1.14734800	0.06141900	-1.68228000
S	-0.69188200	-0.74684400	-0.36389500
O	-0.74437300	-1.37675500	0.96962200
C	1.90633900	-0.04406500	0.34921800
C	2.70539400	1.01515600	0.27350900
H	3.27674800	1.35069600	1.13136900
O	-0.86888300	0.92447600	-0.21571300
C	-2.19236600	1.32923800	0.16575900
H	-2.17820900	2.41835400	0.17656800
H	-2.93962300	0.98176200	-0.55636600
H	-2.44059600	0.95695000	1.16261000
H	1.79670100	-0.58628600	1.28309500
H	2.81958600	1.58383600	-0.64395800

allylS(O)OMe – conf 3

C	-1.05530000	0.59601900	0.59253400
H	-0.69402300	0.61805300	1.62338600
H	-1.50428800	1.55923700	0.34101700
S	0.50727800	0.56484200	-0.40046600
O	1.31286800	1.70012400	0.08063700
C	-1.95594500	-0.55629000	0.29710800
C	-3.08497100	-0.46370400	-0.40187600
H	-3.70023300	-1.33383200	-0.59929600
O	0.99770000	-0.85423600	0.38317700
C	2.22451700	-1.40037800	-0.12514000
H	2.35583500	-2.35974400	0.37417300
H	2.16973400	-1.55899100	-1.20738000
H	3.06893600	-0.74778000	0.11071300
H	-1.62734300	-1.52025600	0.67224000
H	-3.43940700	0.48486300	-0.79366900

allylS(O)OMe – conf 4

C	0.85943400	-0.89532900	-0.65378300
H	1.00099300	-1.98290400	-0.68076600
H	0.99906400	-0.49901400	-1.66164300
S	-0.96237100	-0.76401200	-0.28336800
O	-1.07134300	-0.91407300	1.18321900
C	1.74571200	-0.26179400	0.36580000
C	2.74204400	0.57295800	0.08046300

H	3.36717200	0.99085500	0.86129800
O	-1.22852400	0.83187600	-0.70826600
C	-0.92679100	1.86312400	0.25697300
H	-1.65352400	2.65614500	0.08286400
H	-1.03703200	1.47707200	1.27192100
H	0.08695500	2.23687300	0.10752800
H	1.53646000	-0.53405900	1.39610700
H	2.97439700	0.86305200	-0.93975800

allylS(O)OMe – conf 5

C	0.85355300	-0.38218500	0.74043100
H	0.35684200	-0.01329400	1.64140200
H	1.25295300	-1.37797000	0.94695900
S	-0.52703900	-0.71393300	-0.47040900
O	-1.53348700	-1.44841900	0.32100800
C	1.88494700	0.54427800	0.19186200
C	3.09904100	0.16676700	-0.20246000
H	3.80657700	0.87733000	-0.61343400
O	-1.04218700	0.86717400	-0.69770200
C	-1.76221700	1.48840800	0.38395100
H	-2.41133300	2.23295500	-0.07493100
H	-2.36551000	0.74944100	0.91534100
H	-1.07294100	1.98055300	1.07665000
H	1.58862000	1.58416300	0.08800000
H	3.43087000	-0.86389700	-0.12259800

allylS(O)OMe – conf 6

C	-0.74338300	-0.87793300	-0.12677100
H	-0.44186000	-1.72670100	-0.74477700
H	-0.52885000	-1.07544400	0.92513800
S	0.40107200	0.52284400	-0.60455500
O	0.32667900	1.46930700	0.52424900
C	-2.16317300	-0.47352300	-0.34771200
C	-2.97578600	-0.03900400	0.61256000
H	-3.99276500	0.26678500	0.39653400
O	1.84504800	-0.33195900	-0.52477000
C	2.35606500	-0.65130700	0.78328000
H	3.43868500	-0.71093500	0.67832500
H	2.09741900	0.13474100	1.49588600
H	1.96718400	-1.61470300	1.12546900
H	-2.52194800	-0.51454100	-1.37334700
H	-2.65116300	0.02712300	1.64567900

propylS(O)OMe – conf 1

C	1.04955400	-0.58049900	-0.94967700
H	1.31094100	-1.56757600	-1.34325700
H	0.89283100	0.09847800	-1.79009900
S	-0.61518300	-0.85881200	-0.20481200
O	-0.40089800	-1.15178200	1.22697700
C	2.09779700	-0.09186600	0.05049200
H	3.08263500	-0.31039900	-0.37686300
C	2.00213900	1.39457800	0.40372900
H	2.09623700	2.02170600	-0.48815500
H	2.80042000	1.67375100	1.09640200
H	1.04524200	1.62358100	0.87262900
H	2.00796600	-0.69369200	0.95938000
O	-1.05826200	0.76883200	-0.39291900
C	-2.40053300	1.04023900	0.03826300
H	-2.49809100	0.91344600	1.11939100
H	-2.59659100	2.07863100	-0.22653600
H	-3.11912400	0.39195400	-0.47520000

propylS(O)OMe – conf 2

C	-0.94741700	0.64012200	0.75363300
H	-0.49744100	0.67350600	1.74819600
H	-1.38232300	1.61859400	0.53070400
S	0.49065300	0.53790900	-0.37957000
O	1.31724000	1.72377900	-0.08541500
C	-1.96085200	-0.49340600	0.59237800
H	-2.68729300	-0.40830200	1.40782000
C	-2.69946400	-0.48015600	-0.75086500
H	-3.24246600	0.45908100	-0.89373300
H	-3.42475300	-1.29554300	-0.80513300
H	-2.00971300	-0.59414000	-1.59129700
H	-1.44851200	-1.44824400	0.73575900
O	1.09065400	-0.80609500	0.46131000
C	2.26008400	-1.38508900	-0.13618100
H	2.46253800	-2.29851900	0.42215900
H	2.08669100	-1.63349000	-1.18881300
H	3.11555900	-0.70979600	-0.05349000

propylS(O)OMe – conf 3

C	-0.62445400	-0.98674700	-0.03667200
H	-0.30908000	-1.89957600	-0.54899100
H	-0.39429200	-1.07120100	1.02845000
S	0.45556500	0.33127800	-0.73169000

O	0.27288700	1.51366100	0.13871500
C	-2.11052200	-0.68394000	-0.27564600
H	-2.65801100	-1.62839500	-0.18874000
C	-2.71019200	0.34526900	0.68847500
H	-2.63811900	-0.00591400	1.72244000
H	-3.76732500	0.51007200	0.46517200
H	-2.18842700	1.30073400	0.62704700
H	-2.25139500	-0.35542600	-1.31282200
O	1.93966600	-0.38077400	-0.39819900
C	2.38864100	-0.36384100	0.97066600
H	3.47722300	-0.35613100	0.93136000
H	2.03194800	0.53536000	1.47744000
H	2.04718000	-1.25752000	1.50062300

propylS(O)OMe – conf 4

C	-0.78391000	-0.99933100	0.16654800
H	-0.45683300	-1.98690500	-0.16719100
H	-0.68228700	-0.93979300	1.25283500
S	0.46638500	0.15554900	-0.50687900
O	0.19053500	1.49579400	0.04786300
C	-2.19958800	-0.66376100	-0.32014700
H	-2.80783600	-1.56752600	-0.20958000
C	-2.86399600	0.49581400	0.43000200
H	-2.96271400	0.25947200	1.49385800
H	-3.86554400	0.68566100	0.03548000
H	-2.27661400	1.41053200	0.34681300
H	-2.17677900	-0.45352500	-1.39647900
O	1.67903400	-0.59796100	0.40384000
C	2.98661600	-0.04955000	0.17921800
H	3.67290900	-0.66589800	0.75881900
H	3.26109400	-0.09719900	-0.88017500
H	3.04116100	0.98469900	0.52833600

propylS(O)OMe – conf 5

C	1.04950800	-0.58042300	-0.94968900
H	1.31099400	-1.56742500	-1.34335300
H	0.89270000	0.09866500	-1.79000900
S	-0.61515000	-0.85894200	-0.20480900
O	-0.40085500	-1.15195100	1.22692600
C	2.09784700	-0.09176600	0.05043200
H	3.08262700	-0.31018200	-0.37709400
C	2.00204200	1.39461200	0.40382200
H	2.09596600	2.02186800	-0.48798800
H	2.80028500	1.67385300	1.09651900

H	1.04513100	1.62339900	0.87277300
H	2.00822200	-0.69369200	0.95928000
O	-1.05830200	0.76891100	-0.39298700
C	-2.40049200	1.04033900	0.03833100
H	-3.11923800	0.39248700	-0.47547300
H	-2.49816900	0.91294200	1.11938200
H	-2.59628000	2.07889900	-0.22597600

propylS(O)OMe – conf 6

C	0.71122800	-0.32578500	0.92393500
H	0.10811200	0.04669500	1.75547500
H	1.10410400	-1.30524900	1.21414000
S	-0.49649700	-0.72989600	-0.41149600
O	-1.56502600	-1.47358500	0.28897400
C	1.82370300	0.63537100	0.50404000
H	2.37896900	0.91984300	1.40455900
C	2.79439800	0.05069100	-0.52860500
H	3.26666300	-0.86221400	-0.15312400
H	3.58793800	0.76421300	-0.76272400
H	2.28723700	-0.19766400	-1.46426200
H	1.37472700	1.55320600	0.11370400
O	-1.02462200	0.83050800	-0.74943100
C	-1.86364300	1.47028100	0.23087400
H	-2.47179400	2.18907400	-0.31691300
H	-2.50928300	0.73663800	0.71831700
H	-1.25965400	1.99507200	0.97696300