

Supporting Information

Regioselective DMAD-insertion reaction of silyl dienol ether of γ -pyrone under catalyst- and heating-free conditions

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DFT Calculations for the Reaction Mechanism

Density functional theory (DFT) calculations were performed using Gaussian 09 program.¹ Geometries were optimized at the B3LYP/6-31G(d) level of theory.² Thermochemical corrections were obtained from frequency calculations at the same level of theory. Calculations were carried out for the reaction between a simplified compound **S1** and DMAD. The data were summarized in Scheme S1. Calculated structures are illustrated using ChemDraw and CYLView.³

Underneath the Cartesian coordinates for the optimized geometries are listed the following gas phase energies:

B3LYP/6-31G(d) electronic energy (E)

B3LYP/6-31G(d) enthalpy at 298.15 K (H)

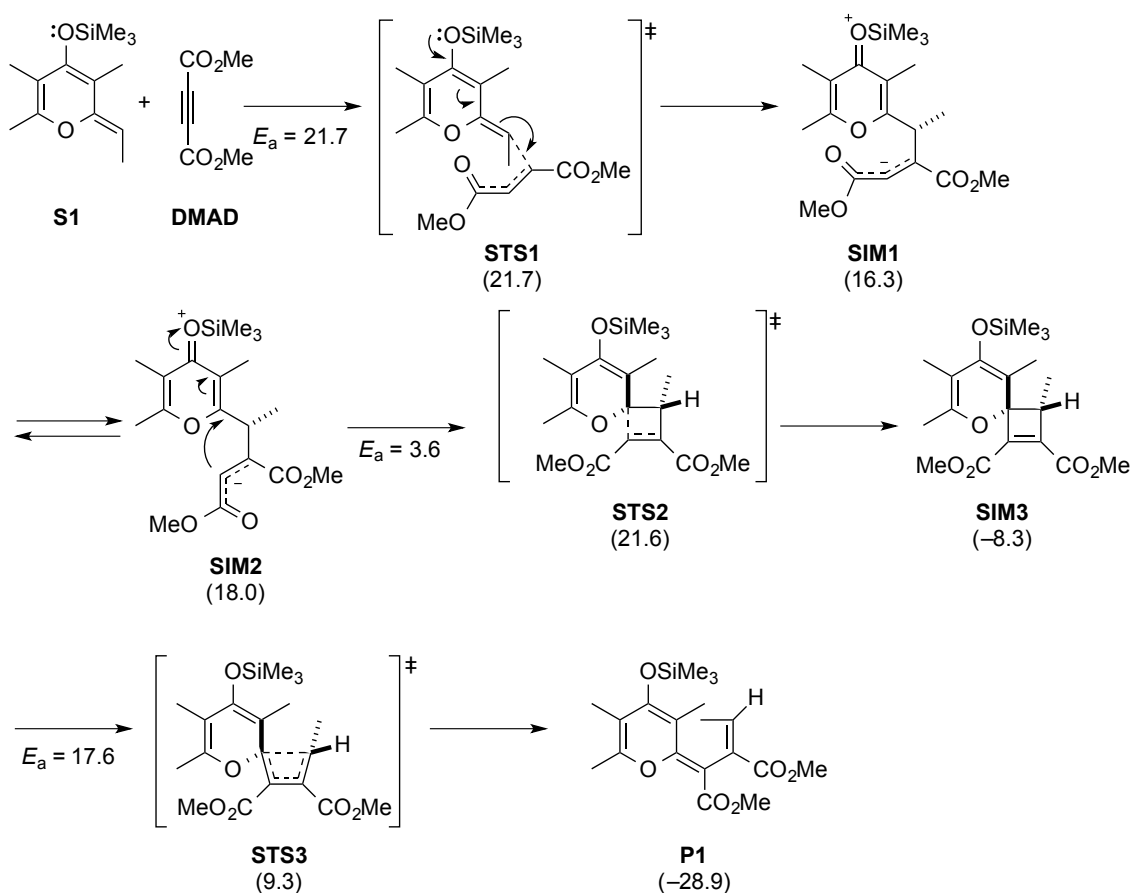
B3LYP/6-31G(d) Gibbs free energy at 298.15 K (G)

Otherwise noted, all energies are given in Hartree.

(1) *Gaussian 09, Revision E.01*, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

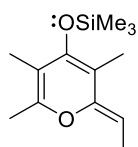
(2) (a) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648; (b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785; (c) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 1372; (d) P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch, *J. Phys. Chem.*, 1994, **98**, 11623.

(3) C. Y. Legault, CYLView, 1.0b; Université de Sherbrooke, Canada, 2009; <http://www.cylview.org>.

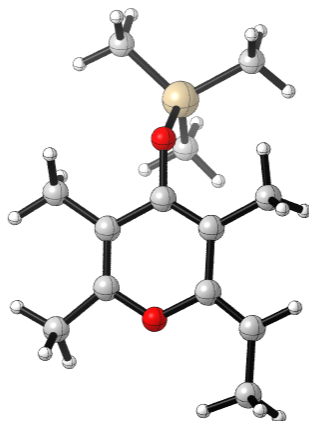


Scheme S1. A plausible mechanism with calculated energies for the reaction between **S1** and DMAD leading to **P1**. The calculations were carried out at B3LYP/6-31G(d) level of theory. In the parentheses are shown ΔG (kcal/mol). Activation energies (E_a) are also given in kcal/mol.

Computed Geometries and Energies



S1



C	-1.945366795365	1.531979966589	0.668476774231
C	-0.834460428283	2.001727559899	1.282767839752
O	0.392852937106	1.436088094647	1.095288653588
C	0.610331637115	0.382976701714	0.204798573006
C	-0.558040482030	-0.160860069852	-0.478442707758
C	-1.780382070506	0.377684797549	-0.218641393481
C	-3.315295932176	2.143092134538	0.822100955039
C	-0.707624329624	3.147740109487	2.239857891597
C	-0.347992584374	-1.277291869249	-1.462253265556
O	-2.912926438206	-0.078668406706	-0.842251644821
Si	-4.018522296487	-1.273031927157	-0.372842067736
C	-5.729451893993	-0.534538080405	-0.638778086488
C	-3.727702705638	-1.749900903866	1.427615894435
C	-3.812769546603	-2.777890400403	-1.489371968003
C	1.883160905151	-0.046863663603	0.068910417373
C	3.075791551955	0.522003564495	0.780626902200
H	-3.278900663599	3.112905492170	1.321894303354
H	-3.990716555925	1.501943653727	1.404519933761
H	-3.782864107850	2.288585338146	-0.157328082541
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H	-0.021821262361	3.903336112726	1.837081097392

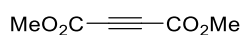
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H	0.009515657100	-2.192545466843	-0.970238163968
H	-6.513135690917	-1.274197974986	-0.433303457933
H	-5.852221069921	-0.201488191351	-1.676080117304
H	-5.905199337589	0.329901639040	0.010588303131
H	-4.430523196339	-2.535264893471	1.732299880316
H	-2.712979631247	-2.135489207692	1.579172915163
H	-3.863447725590	-0.900657671791	2.106538367834
H	-2.851489750816	-3.279502987327	-1.333518958515
H	-3.876793551623	-2.497911317289	-2.547528079810
H	-4.605635840359	-3.510996379250	-1.293528761375
H	2.056245156730	-0.878468562285	-0.605150431114
H	3.847325955396	0.850745252867	0.069682997937
H	3.552285990382	-0.224332825333	1.433275707995
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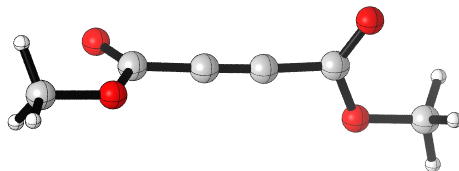
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DMAD



C	-0.400467352992	-0.457688979554	-0.358930642818
C	0.459501454552	0.394680160005	-0.362636792398
C	1.440576460299	1.460527408739	-0.431849647984
C	-1.372332759437	-1.533297808633	-0.402205183908
O	1.401497595233	2.357626396808	-1.245548598025

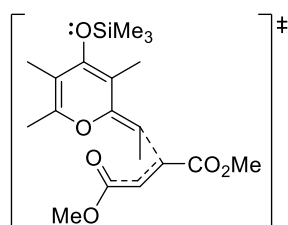
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O	-2.448332863145	-1.239511710669	0.348046976360
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H	4.066557138611	2.057672885852	1.347386845890
H	3.941508482789	2.332166665884	-0.423483788935
H	2.959283602612	3.312600758426	0.694027719433
H	-4.255352384003	-1.857651296894	1.012360371577
H	-3.854532152608	-2.425121625667	-0.644227054713
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0 imaginary frequencies

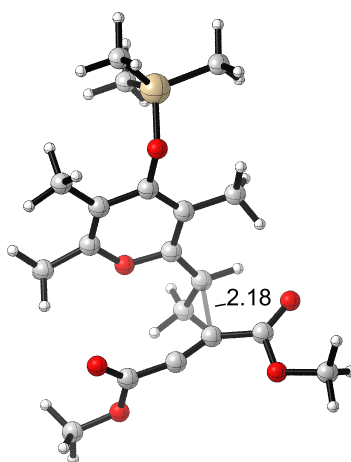
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STS1



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C	0.234640898428	-0.238179730252	1.215098138683
C	-0.911580032881	-0.731486547119	0.513520255774
C	-1.718437911213	0.182153180396	-0.125971995221
C	-2.237857434242	2.523586095470	-1.001949683878
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C	4.862965020988	3.166578096574	0.526255875309
C	3.844518144813	-4.067545384942	-1.460799804767
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O	1.935192539507	-3.351609555720	0.195597265450
O	3.712901137216	-2.704323274184	-1.030436102573
Si	-4.452207861672	-0.366489160156	-0.313488457074
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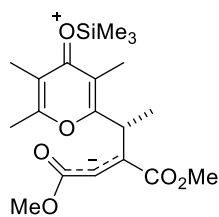
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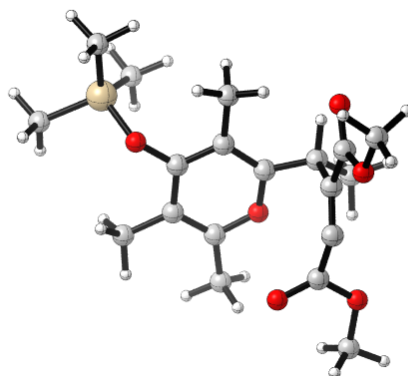
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C	-3.170611538625	-1.193379253416	-0.664791519703
C	-4.523161432827	-3.118959680824	-0.346518032337
C	-3.556637283234	4.297925089657	-1.056420872103
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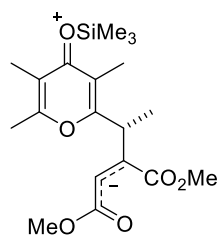
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O	-3.449646382342	2.891389175649	-0.817671114292
Si	4.445464688188	0.430599156299	-0.126429572704
H	4.176529628849	-0.999386037404	1.911831171915
H	5.435534844422	0.220192813607	2.138760607432
H	3.733107687046	0.678551239779	2.267506210328
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H	6.686190392259	-0.435324850363	-0.770835050743
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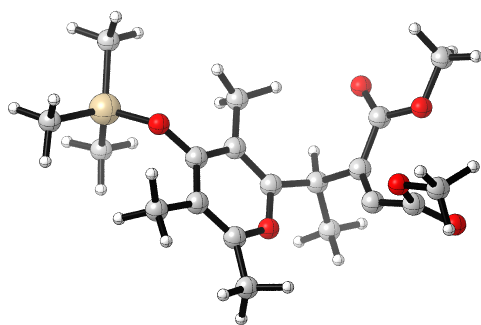
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C	-0.865790200904	-1.972711791787	1.051537935078
C	-5.770334618229	-0.687427798486	-0.973414689849
C	-4.502717079194	-0.732587836033	1.865770405141
C	-4.323822598100	-3.226781883757	-0.009604507751
C	1.316161699576	0.073808931554	1.869351202015
C	1.689729662654	1.120535989639	2.929495116996
C	2.937906785812	-1.382610395279	0.545896886399
C	2.429249567726	-0.001264088906	0.744382095702
C	2.751947810222	1.089521708782	0.060570243256
C	3.777868541769	1.381923943722	-0.885773435534
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C	4.541473594701	-2.742421062371	-0.509567145143

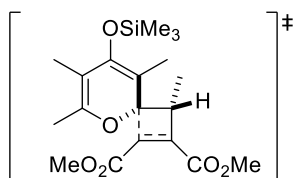
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O	3.331167691578	1.214342454789	-2.184827937386
O	2.454515373034	-2.395857706956	1.043067307101
O	4.013212538754	-1.435060754792	-0.267989119994
Si	-4.372810672368	-1.352673029741	0.094024095562
H	-4.486583971363	0.362371155820	1.916040484220
H	-5.447717303297	-1.067463955602	2.310929713479
H	-3.690016212295	-1.109749169206	2.496164871152
H	-5.856541705488	0.403044105272	-0.912070734751
H	-6.730425490354	-1.113614787364	-0.656779794554
H	-5.622974192349	-0.953140678334	-2.026562143487
H	-5.295631877730	-3.649051486709	0.274861259268
H	-4.107069720714	-3.558049550268	-1.031767366650
H	-3.566501231841	-3.660085081987	0.651627317352
H	0.883371229301	1.268527729624	3.659097714241
H	1.925874515345	2.072396945844	2.447784676497
H	2.581643057929	0.782139876756	3.465642496705
H	-2.634051505672	2.794493055241	-2.050192041439
H	-3.885361124694	1.967046909701	-1.117532007585
H	-3.034377073925	1.104123499703	-2.395569086130
H	1.233787257108	-0.913042387425	2.323742261246
H	-1.144206071249	3.989837488324	-1.246067480443
H	0.525249498754	3.629662237366	-0.713883724030
H	-0.666595246017	4.216352757374	0.449853095914
H	-1.406136154173	-2.562471800302	0.308299184254
H	-1.327806149658	-2.156673846625	2.030639591697
H	0.164811748944	-2.334619078432	1.093729808250
H	3.786962355992	1.410296663710	-4.141714303583
H	4.572168144202	2.634018358722	-3.090801840599
H	5.188801759457	0.971121189349	-3.115337991219
H	5.396051849929	-2.592639573758	-1.170662367701
H	4.859669880564	-3.212990822058	0.425326234753
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0 imaginary frequencies

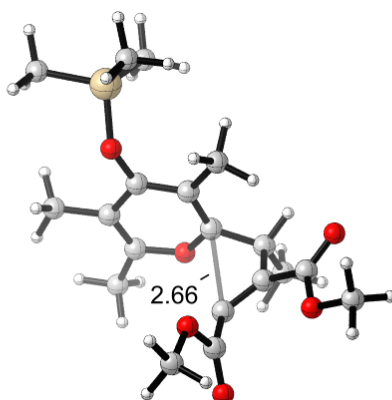
E = -1481.695761

H = -1481.221330

G = -1481.320478



STS2



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C	0.124707596916	-0.035234939226	1.451590274946
C	-0.808461885380	-0.397663706306	0.476770573924
C	-1.809948490796	0.533149714237	0.175984586159
C	-2.845596889962	2.842879590016	0.304983034535
C	-0.666856982571	3.328697913712	2.540571074868
C	-0.705552633733	-1.703042596416	-0.268994083374
C	-5.520677363870	0.482455174943	-1.382121510870
C	-4.477576575474	-1.521921878869	0.749801172583
C	-3.837033377938	-1.928647910787	-2.290916864281
C	1.319884147555	-0.829608323684	1.864093562214
C	1.885598581327	-0.457156986148	3.239961404566
C	2.989843624424	-1.766838171525	0.209655207401
C	2.315204454076	-0.545722170387	0.714709929943
C	2.375027794620	0.718868728731	0.239441488662

C	3.237382491860	1.203404941003	-0.796961501603
C	3.385981716556	1.697552892032	-3.102947677735
C	4.685547459719	-2.652173396905	-1.160296430182
O	-0.017633598745	1.125864224666	2.099320777856
O	-2.735631157634	0.278327762085	-0.752574825919
O	4.299868606070	1.795601063580	-0.646429366249
O	2.644911492282	1.090457164660	-2.048093063732
O	2.637951975751	-2.915757279093	0.467954762058
O	4.035100596785	-1.506283944468	-0.605904335137
Si	-4.137926518584	-0.697673607192	-0.907116529147
H	-4.625931586593	-0.783169341161	1.546170402703
H	-5.393414385138	-2.122490277788	0.686590828153
H	-3.667634433204	-2.191420966065	1.058955297780
H	-5.741638030498	1.202808589945	-0.586583319373
H	-6.443449719481	-0.072619790622	-1.591726438182
H	-5.264018842545	1.048195909609	-2.285067115211
H	-4.765164945670	-2.463726685488	-2.527634895695
H	-3.510453941845	-1.416665997057	-3.203402734430
H	-3.078341631526	-2.674762786025	-2.035131488067
H	1.150328476252	-0.585993418549	4.044822734643
H	2.239036632786	0.577388252622	3.238520313278
H	2.739347055550	-1.108069139144	3.451422761805
H	-2.657520099754	3.836145699109	0.713991146788
H	-3.861102984095	2.545026600962	0.591250848493
H	-2.829073723358	2.914828686529	-0.786762930671
H	1.058977429229	-1.892404082872	1.858213010867
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H	0.299638247432	3.762066840784	2.256235051317
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H	-0.880088692064	-1.534596575669	-1.335705506979
H	-1.453668416098	-2.425180592186	0.081686480823
H	0.276735005158	-2.161838021994	-0.153909472291
H	2.791624344256	1.550531164740	-4.009057955261
H	3.538394729772	2.767557516069	-2.923745617046
H	4.369667757633	1.230496147609	-3.222238628992
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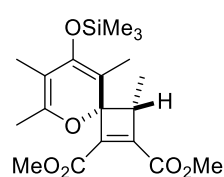
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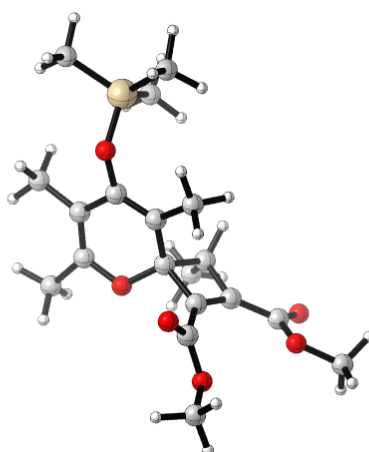
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G = -1481.314628



SIM3



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C	-0.480965422317	0.430101470633	-0.252896113549
C	0.667395972078	-0.149513786147	0.535379213291
C	1.866800650628	0.462685460924	0.419957428132
C	3.411318396258	2.318706483230	-0.443771216319
C	0.748177010597	3.753624438544	-1.263703989054
C	0.422938678739	-1.387806501039	1.350671622716
C	5.823251071510	-0.395648818768	0.882702382434
C	3.896932646863	-1.539465638270	-1.289348689239
C	3.949812010539	-2.726855628265	1.566062709449
C	-0.908581342658	-0.392307264683	-1.568584206967

C	-0.944774938345	0.367130484844	-2.891360338154
C	-3.403759354970	-1.378729945016	-1.284719536549
C	-2.233310441615	-0.586187658264	-0.853816904440
C	-1.908412942503	0.152274550503	0.226081747845
C	-2.581600426778	0.592434622313	1.469553840856
C	-4.577687776813	1.374772763264	2.431348619900
C	-5.439513996859	-2.371768984007	-0.651852999485
O	-0.345925919239	1.835722177290	-0.484448665947
O	2.991446728607	-0.016821593607	1.050661727532
O	-2.025177871427	0.655803845726	2.548155099187
O	-3.865191164839	0.940975107670	1.260611503851
O	-3.546651279361	-1.786047559189	-2.422103770468
O	-4.274555718984	-1.615610397757	-0.283430232235
Si	4.133232524914	-1.153737968228	0.542043117077
H	4.046337358229	-0.655840439165	-1.920114847764
H	4.612705719447	-2.304736258048	-1.614286635054
H	2.889219954926	-1.921982585191	-1.488322502035
H	5.996847847469	0.501206308672	0.278360921397
H	6.626210110236	-1.110038923755	0.662492274564
H	5.914764770699	-0.109123022053	1.937011110145
H	4.790168910747	-3.406910140676	1.376840868980
H	3.942657998804	-2.501790146358	2.639104989358
H	3.026500701693	-3.267344983197	1.331369628981
H	0.072419630948	0.564300511765	-3.248362098970
H	-1.461548501549	1.324912390118	-2.780208746620
H	-1.469955306653	-0.224626580784	-3.647655637459
H	3.396254604784	3.321079742387	-0.875953519910
H	4.032143472366	1.695799608479	-1.101571783627
H	3.927343563473	2.372634655135	0.520952702160
H	-0.332114621769	-1.320231992957	-1.680676240175
H	1.679876722338	4.319915430585	-1.260627668649
H	-0.002307675694	4.315855234987	-0.695083331861
H	0.382807887103	3.688451995592	-2.296694496505
H	1.319126521692	-1.667364047466	1.906129910623
H	0.122284264487	-2.247154657838	0.732927633228
H	-0.380185261065	-1.211209496527	2.075523211657

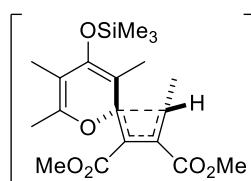
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H	-4.618550291233	0.573232737645	3.173790639817
H	-4.090240883362	2.246464654587	2.875852278381
H	-6.024264135182	-2.469568188553	0.263027442626
H	-6.011252178623	-1.844882260633	-1.420485623489
H	-5.153850573656	-3.355589363743	-1.033888964071

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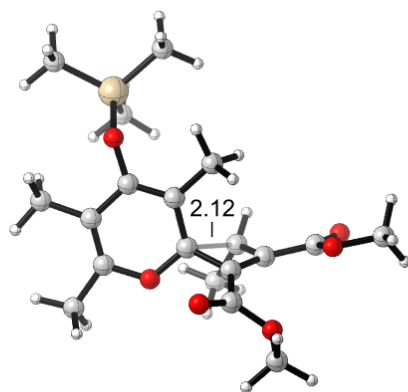
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STS3



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C	-0.904947815453	0.623890891103	-0.227543641131
C	0.302552782483	0.141963161811	0.434235433211
C	1.496935999533	0.707134630381	0.088931228488
C	2.930147222645	2.457230132886	-1.097412330488
C	0.177885007710	3.547126219794	-2.162535530826
C	0.183278950818	-0.933872742337	1.474177732274
C	5.471491719226	-0.150209339887	0.406061399213

C	3.414866117677	-1.456423757750	-1.547159305313
C	3.591300363698	-2.369946991410	1.403975619816
C	-1.632250057965	-1.063972194504	-1.290726993437
C	-1.858079433722	-0.403677396604	-2.633089849871
C	-3.312727095476	-1.999491207271	0.403268851836
C	-2.534132812925	-0.883581286315	-0.183759099740
C	-2.254763267051	0.388483222925	0.289283139978
C	-3.020833707339	1.399742013517	1.031664379912
C	-5.131999615947	2.032603048471	1.850712246027
C	-4.585083195437	-2.765759428401	2.225852268128
O	-0.788644914683	1.774261459529	-0.981666213090
O	2.669164684402	0.309403726122	0.671663403367
O	-2.527426131854	2.383100867498	1.557257103446
O	-4.347000230919	1.122002553016	1.071894236900
O	-3.463767248930	-3.072578607932	-0.152701963708
O	-3.802375869241	-1.721398056039	1.631831548580
Si	3.760519167644	-0.910907403550	0.223924273824
H	3.573015009101	-0.646465339869	-2.268264469792
H	4.079510743046	-2.283092905504	-1.827009958161
H	2.383311742889	-1.808320917431	-1.663306091715
H	5.621105907589	0.681903195070	-0.290490568477
H	6.254424132348	-0.894140819244	0.214165368864
H	5.621130834037	0.234510019278	1.421612582935
H	4.387492618856	-3.102432728037	1.219685557112
H	3.674896961342	-2.048295367440	2.448730991548
H	2.632656718259	-2.886575102202	1.287711920644
H	-0.910342781600	-0.203839008793	-3.149513883215
H	-2.404575246854	0.537994163247	-2.540114152745
H	-2.443246690537	-1.074164042227	-3.279925262688
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H	3.555232973819	1.778796551799	-1.692205000148
H	3.469909278875	2.652437397369	-0.165141509362
H	-1.122163084239	-2.029351744058	-1.374379238119
H	1.098523469407	4.078003622437	-2.404903466765
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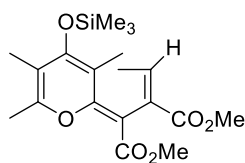
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H	-0.056519960654	-1.910153188927	1.030344500535
H	-0.626132888434	-0.700400042066	2.173920555810
H	-6.155877726842	1.660490510463	1.793360418131
H	-4.788806665862	2.052024243021	2.889279715117
H	-5.069300226876	3.045413022120	1.442265598893
H	-4.913755574231	-2.373815991235	3.189084617025
H	-5.445536053241	-3.009529096720	1.596260280201
H	-3.983440511739	-3.668674587425	2.363900789412

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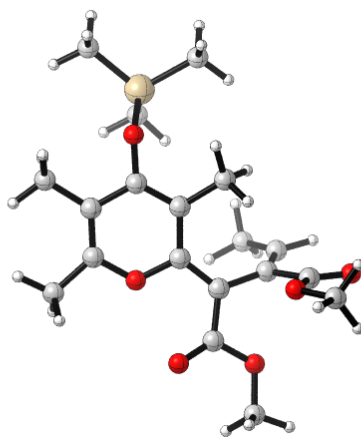
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G = -1481.334392



P1



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C	0.999236155985	2.607696133824	0.589487434239
C	-0.485245868945	0.750661634348	0.154069782478
C	0.611682217434	-0.157206891802	0.409352723635
C	1.862136604471	0.383077700122	0.612287329577

C	3.485172772703	2.316428029302	0.982977800303
C	0.891035032165	4.095641271805	0.721515121770
C	0.380735606401	-1.633443049368	0.610979940367
C	5.730827121806	-0.872433757801	0.536194452736
C	3.809227135225	-0.590418126117	-1.906372876093
C	3.674709683503	-3.080566645047	-0.057262411192
C	-1.732460447210	-1.343241438330	-1.964837336200
C	-0.799014067858	-0.662740212393	-2.915323741915
C	-3.153097018937	-1.743403686961	-0.057145396561
C	-2.171156150216	-0.870555129065	-0.780668886597
C	-1.788217839568	0.445247762030	-0.204410390448
C	-2.859505072329	1.448141441550	-0.066524446448
C	-5.149690943364	1.846032272815	-0.483185727516
C	-4.258974728685	-2.130241549375	1.984383654819
O	-0.217519731298	2.090545393681	0.305191387721
O	2.933172002848	-0.411776034528	0.877283060446
O	-2.812947211464	2.540085189790	0.473512539971
O	-4.020455795671	0.984009403697	-0.632659778385
O	-3.724214980427	-2.709166964738	-0.526165406726
O	-3.313671720972	-1.358107323374	1.233450498649
Si	4.015962202580	-1.231993804291	-0.147284177107
H	4.040867341853	0.478170802797	-1.983751673239
H	4.481676657946	-1.125134699310	-2.588379358946
H	2.785402706510	-0.735625324271	-2.269770311774
H	5.988541706166	0.189063844511	0.453780155435
H	6.494443764272	-1.445619255777	-0.003838925272
H	5.795647762183	-1.150216299776	1.594684514716
H	4.450188596841	-3.636621804610	-0.599175682278
H	3.680323569234	-3.433543209683	0.980554056596
H	2.706946359602	-3.345821024504	-0.495277658046
H	0.180173093391	-1.164427914454	-2.940110424499
H	-0.636509189547	0.385565555981	-2.652466759530
H	-1.194971061111	-0.713653991695	-3.937797327102
H	3.505444168552	3.396415036267	1.138164843059
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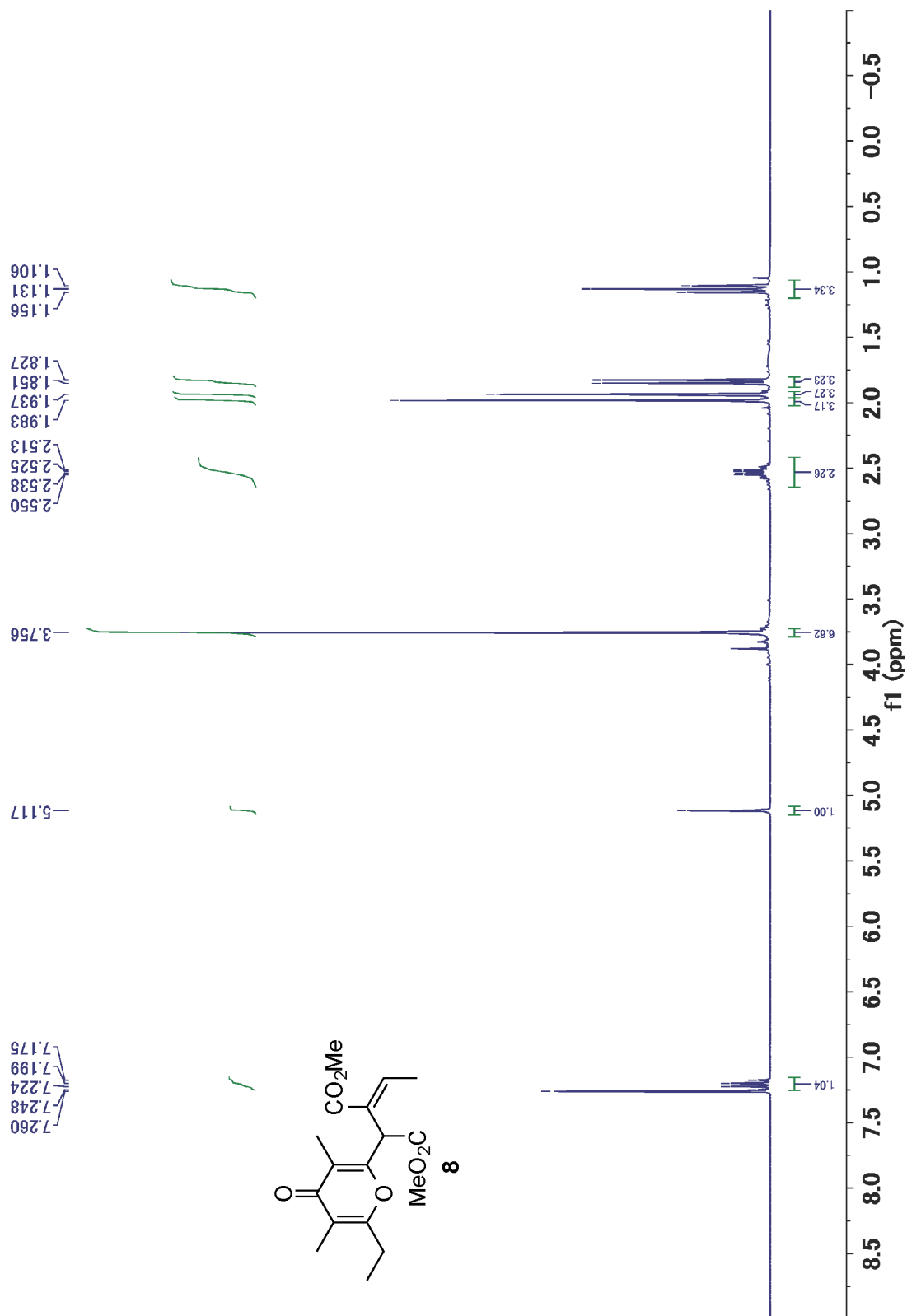
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H	0.639203889970	4.546535383390	-0.246114476995
H	1.179884568452	-2.047228392115	1.229922581442
H	0.341698496866	-2.202854759516	-0.324748676244
H	-0.571847786360	-1.795133822486	1.122624427349
H	-5.978204901076	1.332201448067	-0.974049466476
H	-5.377438446316	2.014874933844	0.573858532373
H	-4.967330528079	2.815025350491	-0.957524593011
H	-4.271208272849	-1.689082852554	2.981942146442
H	-5.250938741340	-2.073761540312	1.527349958260
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0 imaginary frequencies

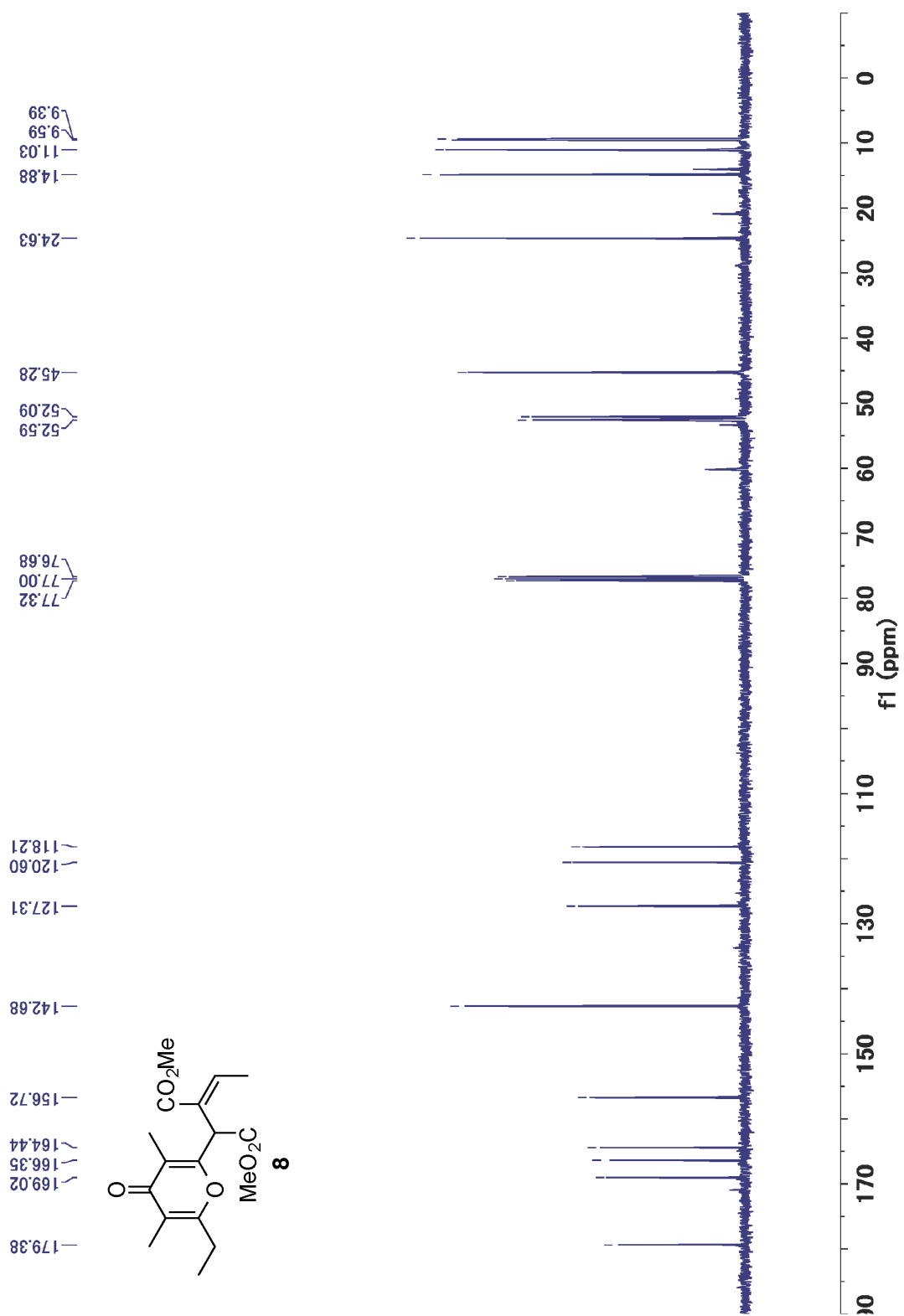
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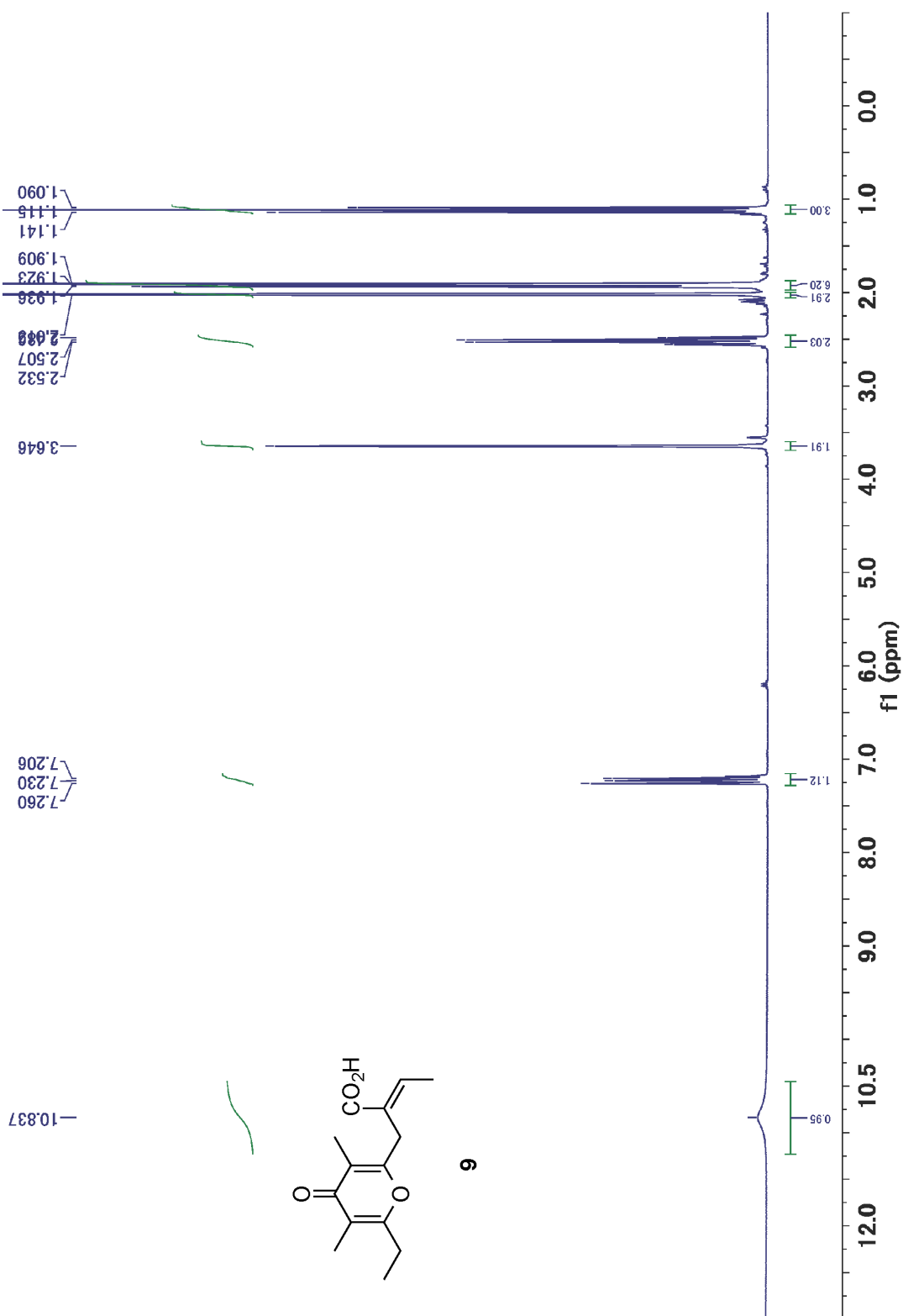
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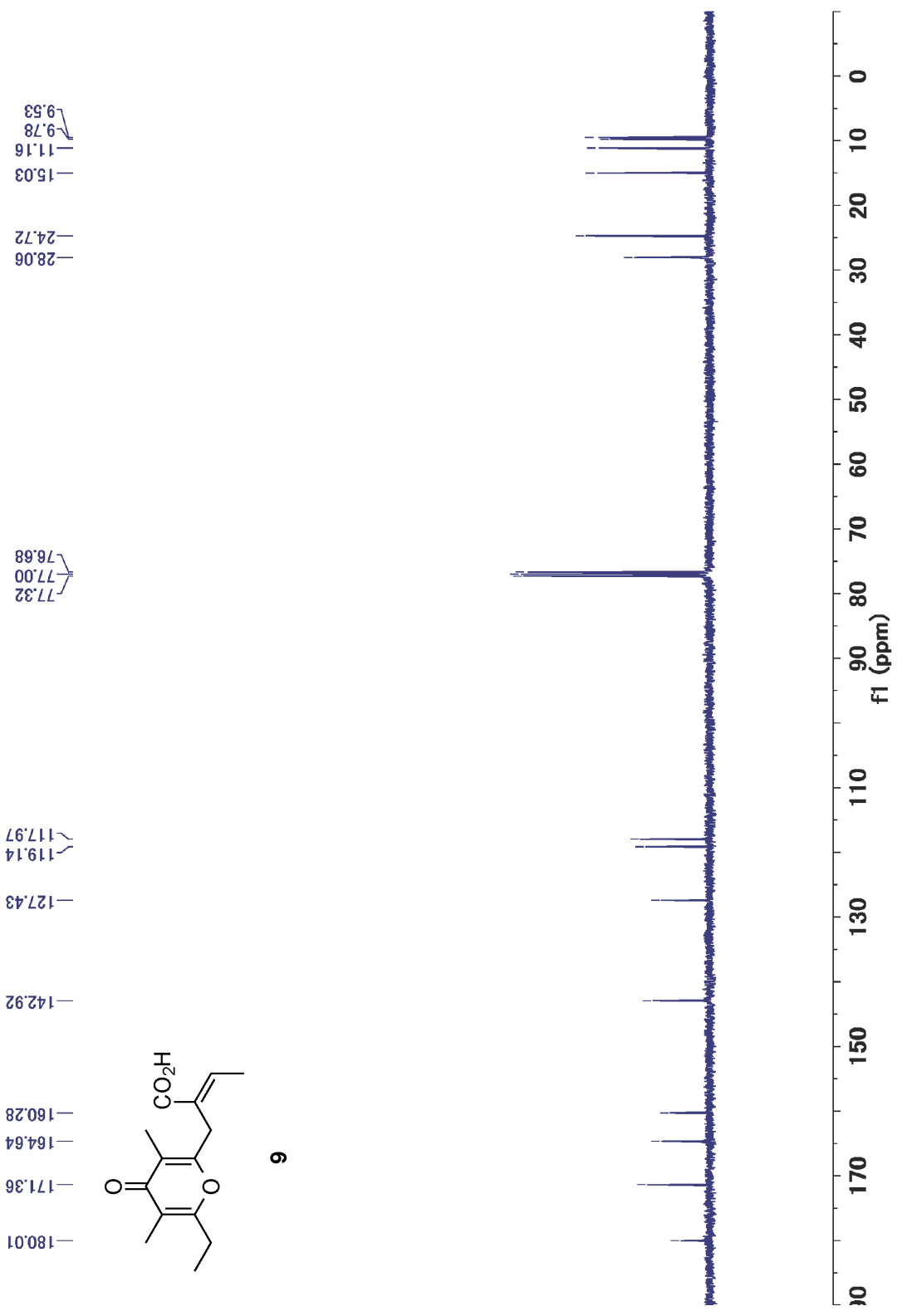
¹H NMR spectra of **8** (300 MHz, CDCl₃)



¹³C NMR spectra of **8** (150 MHz, CDCl₃)



^1H NMR spectra of **9** (300 MHz, CDCl_3)



¹³C NMR spectra of **9** (100 MHz, CDCl₃)