

## SUPPORTING INFORMATION

# "Cation-Stitching Cascade": an exquisite control of terpene cyclization in cyclooctatin biosynthesis

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# 1. Calculation Methods

All calculations were performed with Gaussian 09 program.<sup>[1]</sup> Geometry optimizations were performed in the gas phase at the M062X/6-31G\*\* level,<sup>[2-3]</sup> without any symmetry restrictions, and the nature of the minima was verified by frequency calculations within the harmonic approximation. IRC for all TS was performed with GRRM11<sup>[4]</sup> and/or Reaction Plus<sup>[5-7]</sup> programs based on Gaussian 09. Gibbs free energy used for discussion in this study.

## 2. Energy Profiles

	G(a.u.)
<b>INT1</b>	-780.891409
<b>TS1-2</b>	-780.883222
<b>INT2</b>	-780.899979
<b>TS2-3</b>	-780.880606
<b>INT3</b>	-780.918933
<b>TS3-4</b>	-780.909235
<b>INT4</b>	-780.919727
<b>TS4-5</b>	-780.910952
<b>INT5</b>	-780.932079
<b>TS5-6</b>	-780.920758
<b>INT6</b>	-780.934369
<b>TS6-7</b>	-780.932036
<b>INT7</b>	-780.937756
<b>TS7-8</b>	-780.935104
<b>INT8</b>	-780.941615
<b>TS8-9</b>	-780.935329
<b>INT9</b>	-780.937778
<b>TS9-10</b>	-780.935275
<b>INT10</b>	-780.937947
<b>TS10-11</b>	-780.935784
<b>INT11</b>	-780.954009
<b>TS11-12</b>	-780.943667
<b>INT12</b>	-780.960904
<b>1,3-shift-Reverse</b>	-780.924721
<b>1,3-shift-TS</b>	-780.89807
<b>1,3-shift-Forward</b>	-780.948381

# 3. Cartesian Coordinates

## INT1

C	-2.02039648	1.56258457	0.43101538
C	-2.74658985	0.89016243	1.33223888
C	-1.76921239	-1.36514886	-0.41134891
H	-2.26943497	0.61352394	2.27538171
H	-0.18736795	-2.02628163	-1.73703715
H	-0.94455861	-0.50966376	-2.21200792
C	-0.55735673	1.85381302	0.64829932
H	-0.25327258	1.56489069	1.65715936
C	0.37892627	1.26371143	-0.43476969
H	0.08761430	1.69200243	-1.40028149
H	1.38917928	1.64899258	-0.24439650
C	1.99037642	-2.21056701	0.00482020
H	1.79305361	-3.09338764	0.61852299
H	1.95850796	-2.45761578	-1.05871984
C	3.44796287	-1.68701073	0.35581792
H	4.09860198	-2.53643792	0.12729039
H	3.51261901	-1.51212755	1.43134885
H	3.94893792	-0.66799932	-1.52147665
C	-3.08071757	-1.20972833	-0.63553999
H	-1.49560264	-1.65013900	0.60293916
C	-3.99234164	-1.16916862	0.56329362
H	-4.99540954	-1.53656774	0.32678125
H	-3.59080509	-1.79613360	1.36609969
C	-4.10642025	0.30295077	1.08810532
H	-4.66680530	0.89426354	0.35893771
H	-4.69945002	0.28879611	2.00649134
C	-3.71183037	-0.91985602	-1.96642654
H	-2.98897134	-0.74313718	-2.76563190
H	-4.32807404	-1.77507097	-2.26488370
H	-4.38137879	-0.05581918	-1.90498502
C	-2.55136290	2.04111430	-0.89543692
H	-2.15987904	3.03903073	-1.12105056
H	-2.24208389	1.38378578	-1.71721557
H	-3.63945796	2.10065482	-0.91778695
C	4.08944875	0.75109950	-0.00072944
H	-0.39271576	2.93774637	0.58869375
C	4.49071494	1.84603428	-0.95253372
H	3.80895308	2.70012384	-0.86909035
H	5.48998820	2.21825731	-0.70421401
H	4.49879937	1.50589967	-1.98945369
C	4.02175744	1.18144305	1.44124516
H	3.79831634	0.37330274	2.13997034
H	4.97850390	1.61952294	1.74257476
H	3.27148306	1.97193668	1.56764031
H	1.32319641	-0.30166614	-1.52494380
C	0.81041036	-0.84691200	1.76099914
H	-0.23939578	-0.56689899	1.89684528
H	1.10328386	-1.66442592	2.41941685
H	1.38359900	0.05936193	2.02240227
C	3.84281544	-0.48660644	-0.45169541
C	0.58326819	-0.24654275	-0.71467165
C	1.09580321	-1.10464109	0.34480774
C	-0.63416728	-1.10441003	-1.34763433

## TS1-2

C	-1.92690000	1.74336700	0.47511300
C	-2.64576700	0.90254000	1.22497900
C	-1.72984300	-1.76825100	-0.14559600
H	-2.11688800	0.32149100	1.98260300
H	-0.00790800	-2.82172900	-0.94927700
H	-0.54250200	-1.47055900	-1.93030800
C	-0.41497700	1.74846300	0.55380600
H	-0.05794000	1.30081100	1.48312300
C	0.21841300	1.07169800	-0.69062600
H	-0.45035800	1.17564100	-1.55430100
H	1.11389100	1.64180900	-0.98255100
C	2.16456800	-2.27061500	-0.05800700
H	2.00005900	-3.21196700	0.47506500
H	2.22520600	-2.49210500	-1.12944400
C	3.50207600	-1.62688100	0.38719000
H	4.27935000	-2.38669700	0.25992200
H	3.46765100	-1.39865800	1.45554700
H	4.16209100	-0.63551600	-1.45804300
C	-2.86586300	-1.16441100	-0.53845400
H	-1.72719400	-2.25467100	0.82574500
C	-3.99803200	-1.02272200	0.45031000
H	-4.95863600	-1.28053500	-0.00677200
H	-3.83694100	-1.70217700	1.29224800
C	-4.05445900	0.44740600	0.98071000
H	-4.56066300	1.08273000	0.25135600
H	-4.65806100	0.46124700	1.89236200
C	-3.09171000	-0.51259600	-1.86940400
H	-2.21260800	-0.48753400	-2.51597300
H	-3.88218800	-1.05127100	-2.40313800
H	-3.44624300	0.51329700	-1.73410100
C	-2.49935900	2.70343100	-0.53635200
H	-2.24543200	3.72769700	-0.24155900
H	-2.08354700	2.55793000	-1.54043200
H	-3.58537000	2.64803500	-0.61177400
C	3.76959000	0.87044800	-0.07536400
H	-0.05284200	2.78317000	0.55503600
C	4.13840800	1.96616300	-1.04044500
H	3.32757600	2.69969100	-1.13212500
H	5.01031600	2.51848500	-0.67430900
H	4.37212100	1.57795600	-2.03353700
C	3.35515400	1.35992900	1.28702700
H	3.21799400	0.56166400	2.01778700
H	4.10938600	2.04624000	1.68488900
H	2.42195400	1.93488600	1.22166600
H	1.34579400	-0.47688100	-1.65745600
C	0.56372400	-1.25068600	1.64424800
H	-0.37285300	-0.71411100	1.76168700
H	0.46033300	-2.25829700	2.05489400
H	1.33421200	-0.73304800	2.22514000
C	3.83774700	-0.41753800	-0.43953200
C	0.78646700	-0.32377400	-0.73439800
C	1.02448400	-1.31370900	0.21669400
C	-0.47534800	-1.83843100	-0.90589400

**INT2**

C	-1.58316156	1.90599377	0.31034679
C	-2.36541413	1.12916254	1.06500346
C	-1.67337118	-1.87995274	0.11704276
H	-1.87801561	0.52818236	1.83517704
H	-0.24761424	-3.37638168	-0.36559683
H	-0.41873830	-2.17455437	-1.62880454
C	-0.08054264	1.70321947	0.35780762
H	0.18770841	1.18969798	1.28429097
C	0.28962686	0.85352888	-0.88878916
H	-0.63789466	0.40799346	-1.26739543
H	0.62964227	1.50965188	-1.69922289
C	2.14788117	-2.45447198	-0.25258058
H	2.20768888	-3.32459500	0.40605612
H	2.12099130	-2.82447824	-1.28427667
C	3.33972966	-1.50373222	-0.05827114
H	4.22351929	-1.81913693	-0.61621706
H	3.62855456	-1.46927563	0.99388435
H	3.22428951	0.10433575	-1.56972746
C	-2.72424265	-1.21898616	-0.38558758
H	-1.74051611	-2.15488058	1.16926249
C	-3.83933390	-0.78182479	0.54372964
H	-4.81905335	-1.04181309	0.12796799
H	-3.74051847	-1.31171295	1.49641998
C	-3.79612768	0.75179685	0.81935171
H	-4.20746003	1.29600708	-0.03436188
H	-4.43796489	0.96885929	1.67896832
C	-2.86814866	-0.76777431	-1.81203223
H	-2.04957617	-1.09612800	-2.45594078
H	-3.80149317	-1.15238393	-2.23584940
H	-2.92836681	0.32733535	-1.86196342
C	-2.06183646	2.84001440	-0.76882837
H	-1.69243232	3.85294132	-0.57213557
H	-1.68392001	2.55282685	-1.75783833
H	-3.14910047	2.89419874	-0.82499701
C	3.07354212	1.06561424	0.23125176
H	0.45524424	2.66144909	0.33653157
C	3.14868206	2.36410556	-0.46941787
H	2.86073401	3.20811118	0.15900703
H	4.21968975	2.48786631	-0.70658768
H	2.61703031	2.36546005	-1.42217069
C	3.25482163	1.11317836	1.69455048
H	3.47854922	0.15821832	2.16195329
H	4.02575267	1.85254947	1.93855956
H	2.32381917	1.51580481	2.12173314
H	1.28574220	-0.70748655	-1.84398173
C	0.76523328	-1.38264597	1.53161212
H	-0.09204289	-0.76110631	1.78560692
H	0.62609974	-2.34962060	2.02573195
H	1.65970364	-0.92919882	1.96438183
C	2.87567139	-0.12040981	-0.55657513
C	1.22762790	-0.34205941	-0.81245222
C	0.89699957	-1.60347208	0.02237240
C	-0.38608535	-2.30124895	-0.54070044

**TS2-3**

C	-1.76008954	1.70975164	-0.15818437
C	-2.59840918	1.57871756	0.87483447
C	1.19753871	0.00655621	-0.84150248
C	-1.75048911	-1.30276263	0.59460652
C	0.83833688	-1.10668495	0.18930135
C	-0.52614927	-1.83416019	-0.08393172
H	-2.20856677	1.76091446	1.87811871
H	-0.37676777	-2.85815488	0.28470798
H	-0.66486879	-1.92737863	-1.16831909
C	-0.32328134	2.13780122	0.04056016
H	-0.03239164	2.05029149	1.09164704
C	0.70376895	1.48231599	-0.90796106
H	0.32443312	1.62070925	-1.92382224
H	1.57942012	2.12972455	-0.87828303
C	1.95115751	-2.18388263	-0.06230082
H	2.36185759	-2.51823143	0.89619119
H	1.52629625	-3.07411417	-0.52943175
C	3.03321142	-1.59600653	-0.98624267
H	2.85619103	-1.89909261	-2.02093070
H	4.04525604	-1.92287960	-0.73576271
C	2.84967930	-0.08150460	-0.91963173
H	3.07654639	0.46040341	-1.84657197
C	-3.00705529	-1.21134786	0.14830550
H	-1.59843461	-0.99117036	1.62566549
C	-4.00616412	-0.51107704	1.03852257
H	-5.02220340	-0.88324614	0.87173693
H	-3.76011072	-0.69944422	2.08826813
C	-3.99382433	1.03067345	0.79753334
H	-4.44953573	1.24372998	-0.17292798
H	-4.63299089	1.49935504	1.55132814
C	-3.49586062	-1.64061890	-1.20634418
H	-2.69076283	-1.93794749	-1.88179704
H	-4.17688511	-2.49271402	-1.10486722
H	-4.06746176	-0.83891880	-1.68711563
C	-2.15832822	1.47883496	-1.59205218
H	-1.79334412	2.28762321	-2.23594658
H	-1.73281581	0.53925586	-1.97115060
H	-3.23742736	1.41989803	-1.72330212
C	3.56334019	0.59072018	0.14973032
H	-0.25571112	3.20827795	-0.20201650
C	3.72945247	2.05672759	0.17646993
H	2.91141758	2.43598902	0.81601841
H	4.65897520	2.34335708	0.67515868
H	3.64397430	2.53255990	-0.79887732
C	4.26732029	-0.14637004	1.21502354
H	3.87939688	-1.14291094	1.41051608
H	5.29367489	-0.25966712	0.81855124
H	4.36048934	0.44181278	2.13096278
H	0.98244851	-0.43679044	-1.82092756
C	0.89729178	-0.58255788	1.62574044
H	0.08911786	0.11969949	1.82849329
H	0.81581421	-1.40649385	2.34204885
H	1.83855023	-0.06257640	1.83831859

**INT3**

C	-1.31107134	2.02291818	0.45353973
C	-2.42554740	1.32688257	0.70618206
C	0.77876539	-0.04877880	0.21211163
C	-1.73989650	-1.84184454	0.38893731
C	0.62584853	-1.29920828	1.13217769
C	-0.31403266	-2.32174697	0.42340230
H	-2.49734369	0.84147124	1.68162272
H	-0.25250938	-3.26540481	0.97839666
H	0.05368473	-2.53630483	-0.58636739
C	-0.16989621	2.01619016	1.44766244
H	-0.49411060	1.55310688	2.38019118
C	1.09329180	1.30134739	0.89142406
H	1.53556533	1.99794169	0.16913040
H	1.83359848	1.18453810	1.69167080
C	2.05082816	-1.85672544	1.24914811
H	2.63753735	-1.20457274	1.90925229
H	2.06467799	-2.85631843	1.69158173
C	2.62209709	-1.82847793	-0.16788307
H	2.39174445	-2.75070742	-0.70586913
H	3.70947193	-1.72335761	-0.18493398
C	1.90382391	-0.67420878	-0.88866122
H	1.27309956	-1.00544716	-1.71665439
C	-2.37750829	-1.20076751	-0.59856558
H	-2.28384104	-1.96041926	1.32507801
C	-3.71172605	-0.54539950	-0.32703236
H	-4.43678901	-0.77823190	-1.11456091
H	-4.11885377	-0.92577918	0.61509038
C	-3.55886174	0.99769623	-0.22207127
H	-3.39715527	1.42258447	-1.21635172
H	-4.50132797	1.41348312	0.15010379
C	-1.81147863	-0.94532546	-1.97080120
H	-0.90855208	-1.52631560	-2.17555938
H	-2.54845250	-1.20025509	-2.73885229
H	-1.58058409	0.12194703	-2.10372798
C	-1.05535275	2.79585826	-0.81380311
H	-0.77510418	3.82783932	-0.57450258
H	-0.21933382	2.37122132	-1.38585420
H	-1.92280455	2.83289588	-1.47272810
C	2.63052383	0.49600874	-1.25200028
H	0.13334301	3.04126694	1.69351097
C	2.15688090	1.33550554	-2.36861802
H	2.24078207	2.40384257	-2.15085637
H	2.84910142	1.13649102	-3.20359800
H	1.15113357	1.07094886	-2.69828779
C	3.87110155	0.88763470	-0.55484954
H	4.01735200	1.96890839	-0.54084644
H	3.94099138	0.46317107	0.44747785
H	4.69529241	0.45576314	-1.14663659
H	-0.11448792	0.09544029	-0.39759617
C	0.08659284	-0.98884826	2.53225422
H	-0.91718840	-0.56577483	2.50399177
H	0.04041250	-1.92319930	3.10093447
H	0.74275105	-0.30487843	3.07728609

**TS3-4**

C	0.92741300	2.00584700	-0.88093700
C	1.92938100	1.09470900	-0.97143700
C	-0.64112700	-0.55466800	-0.25854700
C	1.83861500	-2.01630600	0.22837300
C	-0.65733500	-2.10484200	-0.27242400
C	0.51001500	-2.59747900	0.64380700
H	1.71947400	0.16731700	-1.49900500
H	0.53882400	-3.69273300	0.61018700
H	0.27502000	-2.32227600	1.67698700
C	-0.39039600	1.62453700	-1.37489500
H	-0.97934600	2.40100800	-1.87141000
C	-0.74295100	0.19183000	-1.61110100
H	-1.73290000	0.10505800	-2.06617500
H	-0.03173000	-0.23045500	-2.32953000
C	-2.05376300	-2.46982300	0.32550800
H	-2.53735800	-3.27967200	-0.22607700
H	-1.94057200	-2.80963200	1.36100000
C	-2.88331800	-1.17205500	0.30339100
H	-3.71872200	-1.19011800	1.00784900
H	-3.29802200	-0.99891700	-0.69716400
C	-1.81503400	-0.12501400	0.63954500
H	-1.49110900	-0.30981600	1.67398400
C	2.48994300	-0.98875500	0.79881600
H	2.26134400	-2.41968400	-0.69271500
C	3.65754200	-0.32593300	0.09188600
H	4.53735000	-0.27047400	0.74136600
H	3.93636100	-0.91349000	-0.78838100
C	3.29399800	1.12005100	-0.36304600
H	3.32758900	1.81684100	0.47930000
H	4.03769900	1.46374300	-1.09294700
C	2.07803700	-0.31713600	2.08467200
H	2.94447900	-0.20130900	2.74369100
H	1.69218600	0.69531400	1.89487500
H	1.31416200	-0.86925100	2.63272300
C	1.07792300	3.38389200	-0.28952800
H	2.12521200	3.64712300	-0.14367200
H	0.63502600	4.13409200	-0.95162100
H	0.56817200	3.45766900	0.67754900
C	-2.10353500	1.37393300	0.53328400
H	-1.21176900	1.78614700	-0.18377300
C	-1.84421600	2.14937500	1.81274600
H	-1.91854200	3.22813400	1.65859600
H	-2.60305700	1.86087400	2.54960500
H	-0.86453800	1.90509700	2.23378300
C	-3.37700900	1.77774500	-0.17886400
H	-3.46480500	1.33026700	-1.17203400
H	-4.22870900	1.42175100	0.41197700
H	-3.46034100	2.86348500	-0.26492500
H	0.28500000	-0.21908200	0.19615600
C	-0.50922600	-2.70629100	-1.67366700
H	0.43179900	-2.41903100	-2.15427600
H	-0.52550600	-3.79787900	-1.61262000
H	-1.33241100	-2.40178800	-2.32877800

**INT4**

C	1.22049311	1.98113121	-1.10500381
C	2.13713152	0.94336174	-1.17583885
C	-0.71676176	-0.37914461	-0.10645011
C	1.84607620	-1.94269390	0.22043998
C	-0.66354337	-1.95208091	-0.19375955
C	0.51230931	-2.42798187	0.71103991
H	1.83112400	0.01415783	-1.65208753
H	0.50021848	-3.52469907	0.73107553
H	0.31890347	-2.09258637	1.73465386
C	-0.12403996	1.67561910	-1.34973031
H	-0.83199412	2.50183916	-1.26179073
C	-0.68030590	0.33043780	-1.52599874
H	-1.67680870	0.36021488	-1.96708419
H	-0.03731799	-0.26522299	-2.17590679
C	-2.03782133	-2.41402800	0.38010807
H	-2.44373035	-3.26037867	-0.17933656
H	-1.91869973	-2.73908229	1.41989869
C	-2.93699413	-1.17565407	0.33883985
H	-3.80741686	-1.25719593	0.99489738
H	-3.30735375	-1.00017166	-0.68018289
C	-1.95968037	-0.07427717	0.75396471
H	-1.63478869	-0.33151827	1.77471641
C	2.61242315	-0.96495004	0.73520053
H	2.20184207	-2.41202768	-0.69786538
C	3.81554527	-0.46460514	-0.04634515
H	4.71004272	-0.40132614	0.58061279
H	4.03728083	-1.15051354	-0.86920483
C	3.51002736	0.94234689	-0.62146593
H	3.61879584	1.72701073	0.13286865
H	4.21465159	1.19091462	-1.43156332
C	2.34408090	-0.23740028	2.02615106
H	3.20099037	-0.34531928	2.69928392
H	2.21059430	0.83994092	1.86054896
H	1.46015695	-0.60391299	2.54791239
C	1.62594404	3.36000707	-0.63977173
H	2.53112283	3.70040166	-1.14620485
H	0.83375109	4.08253982	-0.84210641
H	1.81709680	3.36811381	0.43808063
C	-2.47843124	1.37501570	0.83766203
H	-1.59738745	2.03965973	0.82782304
C	-3.18411160	1.59509739	2.18072258
H	-3.55214065	2.62042329	2.26719640
H	-4.04485727	0.92480526	2.27446317
H	-2.51272963	1.40207461	3.02159170
C	-3.43090711	1.78616212	-0.29061656
H	-3.00821398	1.70054069	-1.29567049
H	-4.33497531	1.17014292	-0.26710885
H	-3.74339562	2.82528724	-0.15660806
H	0.17714565	-0.02761145	0.41314971
C	-0.50201653	-2.53042896	-1.60291918
H	0.42989833	-2.23339332	-2.09519360
H	-0.49636962	-3.62242550	-1.54553980
H	-1.33710581	-2.24250415	-2.25027186

**TS4-5**

C	1.79860600	1.61370600	-0.64455700
C	2.32754500	0.35126900	-1.03820200
C	-1.00495300	-0.10511700	-0.02161600
C	1.88615700	-1.56989500	0.34179900
C	-0.65595400	-1.64509700	-0.20619300
C	0.51864400	-2.05728100	0.71521800
H	1.68788400	-0.24323000	-1.67932900
H	0.56660200	-3.15488500	0.71245900
H	0.26663800	-1.75510900	1.73513900
C	0.45206900	1.81516300	-0.78261600
H	0.08208300	2.79488300	-0.48011500
C	-0.57868700	0.82700400	-1.21637500
H	-1.44064200	1.38321800	-1.58442000
H	-0.21711500	0.23515600	-2.05834800
C	-1.94179700	-2.36579200	0.26861100
H	-2.02939800	-3.36593200	-0.16442900
H	-1.92556000	-2.48061000	1.35964800
C	-3.07237300	-1.42041900	-0.10859700
H	-4.01583900	-1.68621300	0.37201800
H	-3.24361200	-1.41343700	-1.19353500
C	-2.53323900	-0.06780100	0.36182100
H	-2.55763200	-0.09534200	1.46234100
C	2.65130000	-0.67365800	1.03654300
H	2.35891900	-2.09058300	-0.49169500
C	4.03464200	-0.31133300	0.49816400
H	4.41364200	0.56685400	1.02306700
H	4.75654500	-1.11681400	0.65864300
C	3.79771500	0.00691200	-0.98812300
H	4.40853400	0.83955200	-1.34821700
H	3.99870700	-0.85373400	-1.62798900
C	2.18017200	0.02125400	2.27531500
H	3.02894300	0.30363400	2.90259500
H	1.65835800	0.95022900	1.99624800
H	1.48876900	-0.57772700	2.86806800
C	2.70210200	2.69008100	-0.09137500
H	3.51973300	2.91670400	-0.78113100
H	2.14114500	3.61140300	0.07183100
H	3.14644100	2.40040300	0.86510400
C	-3.37060300	1.15135900	-0.04277000
H	-3.32491500	1.27680000	-1.13339300
C	-2.86033700	2.42219800	0.63980100
H	-3.39886100	3.30526000	0.28716100
H	-3.01144800	2.34969300	1.72235200
H	-1.79247800	2.59238000	0.47421300
C	-4.84429800	0.93954700	0.31834900
H	-5.29649900	0.13192500	-0.26133700
H	-4.95065000	0.69855700	1.38211300
H	-5.41783300	1.84950200	0.12411100
H	-0.44426500	0.24208700	0.85350300
C	-0.39500100	-2.10245100	-1.64782500
H	0.51474800	-1.69824100	-2.10051600
H	-0.29112300	-3.19109200	-1.66496600
H	-1.23006300	-1.84319400	-2.30542900

**INT5**

C	1.82870196	1.59817478	-0.01625514
C	2.01565230	0.37623074	-0.88073777
C	-1.30411641	0.55108115	0.49144327
C	1.85159565	-0.91198570	-0.00586975
C	-0.72571585	-0.89389898	0.46150998
C	0.71314721	-1.04718396	1.00933404
H	1.25191398	0.37105808	-1.65702888
H	0.78727158	-2.04880154	1.45299333
H	0.87735697	-0.32559299	1.81947246
C	0.60879433	2.12707797	0.13129390
H	0.50691126	2.97320886	0.81025973
C	-0.67932155	1.60414291	-0.44632103
H	-1.37336032	2.44125666	-0.54803932
H	-0.54617867	1.20142012	-1.45561263
C	-1.69854488	-1.56874188	1.44827523
H	-1.63991053	-2.66152820	1.39994461
H	-1.43068396	-1.27116745	2.46972433
C	-3.08558081	-1.02608338	1.06856157
H	-3.73192071	-0.94322855	1.94448221
H	-3.58132707	-1.72020770	0.38957975
C	-2.85166094	0.36220995	0.39967270
H	-3.30724474	1.12676005	1.03869735
C	3.19957557	-1.26716461	0.40158787
H	1.75242200	-1.73426881	-0.76783737
C	4.20237445	-0.62164440	-0.46163389
H	4.77365467	0.03554500	0.21812968
H	4.94230713	-1.34333409	-0.83032787
C	3.40904963	0.17133227	-1.51148026
H	3.89529988	1.10886573	-1.78256040
H	3.31496631	-0.42530548	-2.42313597
C	3.53700303	-2.13159947	1.53554170
H	4.59209652	-2.39771352	1.57860623
H	3.25836241	-1.57655638	2.44627452
H	2.90185225	-3.02440495	1.54698520
C	2.99834759	2.08675414	0.79604653
H	3.88363574	2.29478716	0.18487472
H	2.74255326	3.00019705	1.33479600
H	3.29260694	1.34377719	1.55486028
C	-3.46108021	0.57977458	-1.02295192
H	-2.65804758	0.50345686	-1.76845875
C	-4.06520094	1.98684580	-1.12402535
H	-4.37918308	2.20905499	-2.14722628
H	-4.94858632	2.05681212	-0.47966061
H	-3.37146562	2.77021789	-0.80799643
C	-4.54263215	-0.42957116	-1.42133256
H	-4.15495210	-1.44098859	-1.57303297
H	-5.33174295	-0.48101613	-0.66360735
H	-5.00649719	-0.11952365	-2.36146956
H	-1.10965213	0.90241837	1.51601455
C	-0.86147605	-1.57636433	-0.90543145
H	-0.32781327	-1.05464752	-1.70709348
H	-0.48365400	-2.60536851	-0.85683438
H	-1.90791660	-1.63803138	-1.21220127

**TS5-6**

C	2.21984600	-1.65069100	-0.14927900
C	2.55084700	-0.18725600	-0.40683600
C	-0.66334500	-0.27534100	0.06078800
C	1.84953700	0.89866600	0.43844500
C	-0.28274700	0.05243300	1.54992000
C	1.17659900	0.59159400	1.75120700
H	3.61971000	-0.08705600	-0.17675600
H	1.78825000	-0.16056300	2.25641000
H	1.15076900	1.47624800	2.39613200
C	1.01592200	-2.24049800	-0.14582800
H	1.04986400	-3.32148400	-0.01250000
C	-0.39426900	-1.73153500	-0.31604200
H	-0.69010700	-1.91445000	-1.35607400
H	-1.04369500	-2.38515200	0.27615900
C	-1.33571600	1.10731400	1.94849200
H	-1.40643400	1.22355000	3.03428100
H	-1.07435800	2.08795900	1.52818200
C	-2.61522200	0.61077400	1.28265700
H	-3.40754400	1.36234300	1.27172600
H	-3.01049100	-0.26721900	1.80547000
C	-2.13784300	0.24764600	-0.13099900
H	-2.05712400	1.20644500	-0.66920600
C	1.62174400	2.03554800	-0.37011700
H	2.69667200	1.74740000	0.61772300
C	2.17257600	1.81744100	-1.75251300
H	1.48724600	2.25858200	-2.48344500
H	3.11933500	2.36326700	-1.85922000
C	2.33204400	0.29067900	-1.86264700
H	1.41359300	-0.15444900	-2.25708100
H	3.15118800	-0.00309600	-2.51951200
C	0.95425900	3.29868500	0.02763600
H	0.83209500	3.40136500	1.10606800
H	1.47094700	4.16629000	-0.38938900
H	-0.04519400	3.26764000	-0.42789100
C	3.46355200	-2.49083700	0.03206600
H	4.01788900	-2.18227000	0.92619900
H	3.22565300	-3.55049100	0.12915100
H	4.14282200	-2.37226100	-0.82024000
C	-3.08575000	-0.62108300	-0.97164200
H	-2.99146400	-1.66601300	-0.64758900
C	-2.73206000	-0.51992700	-2.46006200
H	-3.29905600	-1.24263500	-3.05204400
H	-2.98224200	0.48071400	-2.83051200
H	-1.66831100	-0.68465500	-2.65973200
C	-4.54542200	-0.20196200	-0.77745700
H	-4.88807200	-0.36030600	0.24779200
H	-4.67717600	0.85875200	-1.02064300
H	-5.19791400	-0.77672400	-1.43978800
H	-0.05490200	0.33630500	-0.61482100
C	-0.43870800	-1.15560600	2.48912100
H	0.27136900	-1.95035700	2.24949900
H	-0.25241300	-0.83788600	3.51972600
H	-1.44596500	-1.57605900	2.45046800

**INT6**

C	2.13236700	-1.49400600	-0.73899800
C	2.39999800	-0.07102400	-0.30363100
C	-0.70779500	-0.30726600	-0.01597400
C	1.71979800	0.61802300	0.79320200
C	-0.35992600	-0.60624900	1.49885000
C	1.06606100	-0.04667800	1.92146500
H	3.38776800	-0.07885200	0.23738200
H	1.69426200	-0.90207300	2.19987600
H	0.97328500	0.62783700	2.77611100
C	0.93908100	-2.03575000	-1.01579700
H	0.98531700	-3.05048500	-1.41041400
C	-0.46975500	-1.50846300	-0.92986700
H	-0.78640000	-1.26625300	-1.95108400
H	-1.11645300	-2.33942300	-0.62651400
C	-1.49201100	0.09345700	2.28115300
H	-1.60300800	-0.32312900	3.28613600
H	-1.29672300	1.16672600	2.39052000
C	-2.71087000	-0.09867200	1.38063900
H	-3.54977500	0.53372000	1.67822700
H	-3.06002500	-1.13787500	1.40153500
C	-2.16266300	0.27500500	-0.00194000
H	-2.05561800	1.37171700	0.01320700
C	1.91192200	2.08848700	0.66997100
H	2.34972200	2.43774000	1.61589600
C	2.82863600	2.27615300	-0.55864400
H	2.60007300	3.19770300	-1.09619200
H	3.87624600	2.32311900	-0.24589100
C	2.58731000	1.01157700	-1.39126800
H	1.66814800	1.07544300	-1.98504000
H	3.40635900	0.76981100	-2.06926900
C	0.55857000	2.83091800	0.51481800
H	-0.14986400	2.56511000	1.30156600
H	0.76047300	3.90097500	0.57781200
H	0.10604600	2.62169200	-0.45763300
C	3.40607900	-2.27111900	-0.97530000
H	3.95018300	-2.42964000	-0.03694400
H	3.20274500	-3.24715900	-1.41658800
H	4.07890500	-1.72927100	-1.64983100
C	-3.04799300	-0.04428500	-1.21312800
H	-3.00725000	-1.12389500	-1.40998900
C	-2.55169300	0.71544200	-2.44861100
H	-3.09273900	0.40793500	-3.34681500
H	-2.71848600	1.79015800	-2.31294000
H	-1.48205700	0.57176400	-2.63804200
C	-4.50845300	0.32507700	-0.94247100
H	-4.94259300	-0.27853800	-0.14173900
H	-4.59340400	1.38046500	-0.65887500
H	-5.11325400	0.17312800	-1.84004500
H	-0.06576600	0.49850400	-0.39798900
C	-0.39928700	-2.09838100	1.86038200
H	0.34579100	-2.68046700	1.31480200
H	-0.20451900	-2.21270000	2.93070700
H	-1.38364100	-2.52725900	1.65896200

**TS6-7**

C	-1.99644500	1.74661400	-0.25960000
C	-2.27797600	0.28631400	-0.31508300
C	0.78964600	0.24123600	0.04615500
C	-1.82710200	-0.71601000	0.57613900
C	0.43759100	0.01335800	1.56298400
C	-1.04101100	-0.45683900	1.81756400
H	-3.05209000	-0.00871500	0.61856700
H	-1.56333900	0.33340100	2.36911700
H	-1.05371400	-1.35305000	2.44425400
C	-0.76771300	2.28777800	-0.29918100
H	-0.76453500	3.37718900	-0.34203800
C	0.61372200	1.69674000	-0.38875600
H	0.93343400	1.82088600	-1.43054300
H	1.28222200	2.34871600	0.18342200
C	1.46217100	-1.04884900	2.01275200
H	1.57056400	-1.07231900	3.10119300
H	1.15000000	-2.05119000	1.69357200
C	2.73403600	-0.65905200	1.26473700
H	3.49121200	-1.44557500	1.28422400
H	3.18787000	0.23764400	1.70251500
C	2.21887000	-0.38369700	-0.15498700
H	2.05390700	-1.37497500	-0.60683700
C	-2.21947900	-2.08299500	0.06838700
H	-2.59908900	-2.69512800	0.89197600
C	-3.28518500	-1.78537700	-1.00661900
H	-3.29064100	-2.53679900	-1.79711400
H	-4.28157300	-1.77148200	-0.55262800
C	-2.93305800	-0.38039400	-1.51969400
H	-2.17306200	-0.40131400	-2.31009200
H	-3.78771400	0.17866600	-1.90143500
C	-0.97206900	-2.77270800	-0.51948700
H	-0.15626000	-2.83451300	0.20428700
H	-1.24656200	-3.78900600	-0.80786800
H	-0.60741900	-2.25435000	-1.41098600
C	-3.23980600	2.60774600	-0.28390000
H	-3.88841100	2.39738900	0.57414800
H	-2.97526200	3.66505800	-0.25108800
H	-3.83083900	2.43835600	-1.18949800
C	3.17842700	0.35560000	-1.09883000
H	3.17610100	1.42415800	-0.84330300
C	2.74045000	0.18188100	-2.55780700
H	3.33196300	0.81225400	-3.22643200
H	2.88994400	-0.85922200	-2.86497300
H	1.68388300	0.41850600	-2.72110000
C	4.61306000	-0.15592200	-0.94395300
H	5.01857500	0.04786700	0.04987800
H	4.65610300	-1.23776200	-1.11440400
H	5.26904200	0.32134300	-1.67650200
H	0.11935500	-0.35248200	-0.58278500
C	0.65815100	1.26952300	2.42335700
H	-0.02088500	2.08150300	2.14956600
H	0.47773400	1.02325700	3.47411500
H	1.68180300	1.64201900	2.34372200



**INT7**

C	-1.96898800	1.72514000	0.20801200
C	-2.19036600	0.37036400	-0.21716600
C	0.77438700	0.24009800	0.19586900
C	-1.94682500	-0.87417100	0.52153700
C	0.48129200	-0.48886500	1.54921700
C	-0.99410000	-0.94932300	1.71437900
H	-2.97009800	-0.81915200	0.99088600
H	-1.45111200	-0.34807800	2.50789100
H	-1.01876300	-1.98332200	2.07633300
C	-0.75808800	2.27080500	0.50267600
H	-0.79394900	3.33359100	0.74534900
C	0.62538700	1.75015600	0.30026600
H	0.96552600	2.24306800	-0.62266100
H	1.26972100	2.17490900	1.07750600
C	1.49593300	-1.65362700	1.55429800
H	1.66812700	-2.03178500	2.56633200
H	1.12937600	-2.49482400	0.95474500
C	2.73893200	-1.06145300	0.89450800
H	3.46350300	-1.82149200	0.59468000
H	3.25429600	-0.37385100	1.57578600
C	2.15718100	-0.30750700	-0.30968800
H	1.92231800	-1.07800600	-1.06092500
C	-2.13892300	-2.02574200	-0.50276500
H	-2.45892800	-2.92019300	0.03817600
C	-3.27511000	-1.46153300	-1.37446600
H	-3.32181700	-1.92194600	-2.36235400
H	-4.24425000	-1.61150200	-0.88804400
C	-2.96489000	0.04249700	-1.44961600
H	-2.25780300	0.26046900	-2.26902100
H	-3.81915500	0.70317500	-1.61688500
C	-0.89802600	-2.36294600	-1.32779500
H	-0.04477500	-2.61742700	-0.69601500
H	-1.11042100	-3.22611700	-1.96291500
H	-0.59613300	-1.53978900	-1.98536400
C	-3.19183100	2.63384100	0.11537100
H	-4.09321600	2.14465400	0.49208700
H	-3.02050100	3.52879700	0.71490200
H	-3.37599700	2.94772000	-0.91595100
C	3.08633500	0.69566200	-1.00663000
H	3.15067700	1.60605700	-0.39360100
C	2.54681400	1.05409000	-2.39671700
H	3.11893100	1.86892100	-2.84742000
H	2.63049800	0.18444600	-3.05779200
H	1.49159500	1.34913000	-2.38755300
C	4.50306500	0.13350900	-1.14946400
H	4.97890800	-0.03227600	-0.18021200
H	4.48468700	-0.82089400	-1.68777600
H	5.13227600	0.82343500	-1.71770800
H	0.03580500	-0.08217600	-0.55164200
C	0.79605300	0.39218900	2.77347000
H	0.13527700	1.26254800	2.83772000
H	0.64646900	-0.19541900	3.68392300
H	1.82954100	0.74822400	2.77575100

**TS7-8**

C	0.36391800	0.93823800	1.42429600
C	-1.87039800	-0.03983800	-0.48463500
C	-1.07967500	0.56456400	1.89808400
C	-1.93360400	-0.30550000	0.97021700
H	-1.62965900	1.49596000	2.06129200
H	-0.09289400	-0.24340600	-0.38070200
H	-1.03352100	0.06838000	2.87374000
H	-2.98910600	0.02985600	1.11212000
C	-0.79197000	2.04097200	-1.32388000
H	-0.94210900	2.99010700	-1.83426000
C	-1.87827500	1.28335100	-1.10682200
C	0.61751300	1.61036400	-1.07008600
H	1.67752200	0.83194200	3.18123100
H	1.19892400	-0.74511700	2.56346800
C	1.48174800	0.26914600	2.26444800
H	3.46389000	-0.47156700	1.67913200
H	3.12616800	1.18349400	1.16118200
C	2.02812500	-0.31607800	0.02506900
H	1.75764000	-1.36349500	0.22649200
C	-2.01673900	-1.84773300	1.10633900
C	4.25364100	-0.95820800	-0.97029000
H	4.14134600	-1.96388000	-0.54939200
H	4.82588700	-1.04676500	-1.89715500
H	4.84165600	-0.35991900	-0.27050600
C	2.88405800	-0.33199000	-1.24423300
H	-2.55812000	-2.09151500	2.02445100
C	-2.31910500	-1.26076000	-1.22485100
H	-3.01839500	-1.02406300	-2.03037500
H	-1.42334600	-1.66463000	-1.72230700
C	2.67744100	0.19400100	1.31761700
H	-2.71955500	-3.26935400	-0.42615500
H	-3.90307900	-2.03891800	0.02930000
C	-0.66718400	-2.55987500	1.12525500
H	-0.11575300	-2.42786700	0.18750400
H	-0.03591200	-2.21141500	1.94482200
H	-0.82168500	-3.63269800	1.26196900
C	-2.83758900	-2.22317400	-0.13994600
H	1.03887100	1.29829100	-2.03262600
H	1.21712000	2.47291600	-0.76211100
C	2.17162100	-1.11543400	-2.35267200
H	2.72567500	-1.06736500	-3.29324600
H	1.15592600	-0.75005700	-2.54824500
H	2.09369900	-2.17116700	-2.06774200
H	3.05225900	0.70155800	-1.57648700
C	0.69684100	0.49513400	-0.04246600
C	-3.25948800	1.69007800	-1.60438700
H	-3.25561600	2.76071800	-1.81276700
H	-3.52667900	1.16363800	-2.52441400
H	-4.03731300	1.49331200	-0.86078600
C	0.50681600	2.45948500	1.62889900
H	0.28601800	2.69457200	2.67372600
H	1.52344600	2.80631100	1.42387700
H	-0.18948700	3.03169400	1.00925000

**INT8**

C	0.32499600	-1.12269100	1.38854200
C	-1.44584700	0.54574500	-0.22905400
C	-1.18452200	-1.50611700	1.24750700
C	-1.97366400	-0.84223900	0.10599300
H	-1.67565300	-1.22890100	2.18396800
H	-0.21146400	0.38306000	-0.18924000
H	-1.26226400	-2.59616200	1.17337800
H	-2.97813900	-0.64354300	0.50905300
C	-0.69019800	2.02033900	1.57982600
H	-0.85959700	2.79926000	2.31694900
C	-1.67777000	1.62465000	0.77375400
C	0.70837200	1.49088500	1.41761300
H	1.53903700	-2.94285800	1.52157900
H	0.87164000	-2.65328200	-0.08287400
C	1.30583600	-2.16413100	0.79142200
H	3.17491200	-1.89081400	-0.33259800
H	3.12764200	-1.03363600	1.21327900
C	1.87478200	-0.12680200	-0.32032500
H	1.41803400	-0.51243800	-1.24734700
C	-2.22387500	-1.53355900	-1.25606500
C	4.01397400	0.52085000	-1.47523300
H	3.71963900	-0.08424800	-2.34016600
H	4.61128200	1.35839000	-1.84307300
H	4.65369200	-0.08821600	-0.83265900
C	2.78051400	1.03811300	-0.73058300
H	-3.05832500	-2.23299400	-1.14747000
C	-1.68792900	0.79979800	-1.71862500
H	-2.07104300	1.80559400	-1.90287700
H	-0.73849600	0.72201600	-2.26355800
C	2.52212200	-1.35034300	0.35489300
H	-2.58938400	-0.55277600	-3.20070800
H	-3.67217600	-0.04629900	-1.90040000
C	-1.04554800	-2.29796400	-1.84987600
H	-0.15724400	-1.66829800	-1.97402800
H	-0.77377800	-3.15692500	-1.23186300
H	-1.31174500	-2.68086500	-2.83813300
C	-2.64197400	-0.33696800	-2.13163100
H	1.32169400	2.24830400	0.92453900
H	1.16786300	1.32097400	2.39719800
C	2.01273600	2.02363600	-1.61887600
H	2.61232200	2.91199800	-1.83009600
H	1.06747900	2.36112900	-1.17568000
H	1.77796600	1.54970900	-2.57922700
H	3.13052900	1.55060200	0.17525300
C	0.72696900	0.18560100	0.65977000
C	-3.07059100	2.20010100	0.80965600
H	-3.13943700	2.97684600	1.57168400
H	-3.34305200	2.64222700	-0.15334000
H	-3.81407900	1.42978600	1.03888200
C	0.61120400	-1.00948900	2.90015600
H	0.34681400	-1.95914100	3.37205400
H	1.66867100	-0.81889300	3.10614300
H	0.00914000	-0.22609600	3.36818600

**TS8-9**

C	0.33138600	-1.26303300	0.99317800
C	-1.38407700	0.72920200	-0.29655800
C	-1.11133500	-1.09757000	1.51391500
C	-2.08973500	-0.30432900	0.61640100
H	-1.05052700	-0.59114400	2.48325300
H	-0.34393400	0.35404900	-0.49083500
H	-1.50739600	-2.09717700	1.72581900
H	-2.70134800	0.28827300	1.30858200
C	-0.11104300	2.25045400	1.16003200
H	0.01308900	3.17311200	1.71870200
C	0.99077300	0.00804100	0.57674100
C	0.56237100	-2.17048100	-0.22954800
H	0.46576600	-3.22993400	0.01870800
H	-0.17841700	-1.93822100	-0.99927300
C	1.95324100	-1.77057800	-0.72354000
H	2.13983600	-2.06038200	-1.75810900
H	2.73597800	-2.22741300	-0.11173500
C	1.96251800	-0.23171600	-0.55376600
H	1.48449100	0.19081500	-1.45421200
C	3.32643100	0.49726800	-0.43374600
C	4.39161500	-0.21376600	-1.27305500
H	4.08546900	-0.26545100	-2.32311100
H	5.32715700	0.34876500	-1.22793600
H	4.59642800	-1.22728700	-0.92307800
C	-3.12284900	-1.05147000	-0.26974400
H	-3.98504800	-1.29815100	0.35809100
C	-2.14983400	0.70377700	-1.63556900
H	-2.25628200	1.69283300	-2.08405800
H	-1.60365100	0.08665300	-2.35765300
C	-3.49342000	0.03819100	-1.29170000
H	-3.99967400	-0.36232300	-2.17350100
H	-4.16266500	0.77406400	-0.83274400
C	-2.68259200	-2.33945700	-0.96543100
H	-2.00912700	-2.15107800	-1.80709700
H	-2.19304400	-3.04082000	-0.28300500
H	-3.56128900	-2.84486700	-1.37342900
C	0.97886700	1.22049500	1.43597400
H	1.95360900	1.71142200	1.39227800
H	0.82463800	0.88275100	2.47021200
C	3.20434100	1.95313300	-0.89826800
H	3.08113500	1.97892900	-1.98644900
H	2.34864700	2.48157600	-0.46723900
H	4.10857900	2.51476500	-0.65362200
H	3.64647500	0.46567700	0.61725600
C	-1.17789600	2.05581800	0.38508500
C	-2.24743400	3.10469700	0.24120800
H	-2.06122200	3.95130600	0.90281600
H	-2.30113900	3.47934600	-0.78474600
H	-3.23024300	2.68721100	0.48643000
C	1.21645200	-1.77795400	2.18030100
H	0.90935100	-2.80693300	2.38287900
H	2.28475900	-1.78091400	1.95475800
H	1.05291700	-1.18378400	3.08058300

**INT9**

C	0.34076300	-1.33416500	0.84397900
C	-1.48593700	0.73048600	-0.37147100
C	-1.07596500	-1.17208000	1.42076600
C	-2.08566100	-0.28747100	0.64683900
H	-0.97202400	-0.77728600	2.43674600
H	-0.60288200	0.28862400	-0.84496600
H	-1.48553400	-2.18141700	1.54514600
H	-2.59060400	0.32216800	1.40671500
C	0.02410500	2.12169500	1.10339700
H	0.23078500	3.06821900	1.59474600
C	1.11357500	-0.10529600	0.64545000
C	0.54461900	-2.12071100	-0.46587000
H	0.43560100	-3.19714000	-0.31447900
H	-0.20534200	-1.81230900	-1.19876300
C	1.94496400	-1.70314300	-0.92933500
H	2.09527400	-1.82736600	-2.00189800
H	2.71971700	-2.28634100	-0.42381500
C	2.03893400	-0.21647900	-0.50730800
H	1.48792100	0.36728200	-1.27476300
C	3.42959000	0.45795000	-0.36791800
C	4.44184000	-0.18561100	-1.31909300
H	4.10730000	-0.09746500	-2.35783300
H	5.40027900	0.33181400	-1.23491800
H	4.61466200	-1.24105000	-1.10005900
C	-3.22938700	-1.01110700	-0.10056100
H	-3.95553700	-1.37559200	0.63441900
C	-2.57163100	0.86364800	-1.47901800
H	-2.78199000	1.89656500	-1.75520900
H	-2.22004100	0.36905100	-2.38854600
C	-3.81210000	0.13885000	-0.93289800
H	-4.48069400	-0.20432300	-1.72625200
H	-4.38622500	0.81130300	-0.28543800
C	-2.81807400	-2.18609200	-0.98658300
H	-2.21411900	-1.86518500	-1.84181500
H	-2.25609500	-2.94887800	-0.43826800
H	-3.70974200	-2.67131500	-1.39107700
C	1.01810300	1.04149700	1.55598100
H	2.00149700	1.50675000	1.66536500
H	0.68805800	0.69322500	2.54227800
C	3.34552300	1.96070500	-0.65622000
H	3.14624500	2.11945000	-1.72166800
H	2.55324300	2.47044100	-0.10116400
H	4.29323700	2.44902200	-0.41947800
H	3.77990700	0.29960600	0.66190300
C	-1.05244400	2.01841800	0.31699000
C	-1.93800200	3.22924400	0.16535400
H	-1.64899100	4.02196200	0.85622400
H	-1.89236400	3.63086300	-0.85111900
H	-2.98306200	2.96590500	0.36231200
C	1.24670800	-2.00122900	1.96363800
H	0.86887700	-3.02153900	2.06805700
H	2.30569300	-2.05598300	1.70349900
H	1.13981300	-1.48372000	2.91739700

**TS9-10**

C	0.32558100	-1.51170600	0.59202800
C	-1.44833400	0.73452900	-0.38383600
C	-1.11154600	-1.46260000	1.12900500
C	-2.02011800	-0.28582000	0.67245700
H	-1.07812400	-1.47215700	2.22288300
H	-0.64526300	0.27187600	-0.96757800
H	-1.55779900	-2.42135000	0.84870400
H	-2.22842800	0.31390100	1.56579800
C	0.16540100	1.95742500	1.13483500
H	0.52027400	2.88570400	1.57208700
C	1.09353200	-0.27298100	0.62226900
C	0.55353500	-2.08506700	-0.81891100
H	0.47693100	-3.17485700	-0.82619800
H	-0.21188800	-1.69897100	-1.50029500
C	1.94767000	-1.57099200	-1.20028200
H	2.09602600	-1.49039300	-2.27730900
H	2.72395800	-2.24019100	-0.81846900
C	2.05564200	-0.19148400	-0.50311900
H	1.55024100	0.55317300	-1.15323100
C	3.47108900	0.37512500	-0.20383700
C	4.45113300	-0.04058700	-1.30534000
H	4.11804300	0.33464900	-2.27868200
H	5.43304300	0.39235700	-1.10161500
H	4.57525700	-1.12251600	-1.37686600
C	-3.40404500	-0.72384100	0.12202200
H	-4.06730100	-0.97844200	0.95551300
C	-2.62942000	0.99392800	-1.35756100
H	-2.68425100	2.02277000	-1.71097600
H	-2.50653700	0.36902800	-2.24635500
C	-3.87479700	0.55085600	-0.58743500
H	-4.74102600	0.38673200	-1.23265600
H	-4.15082900	1.31013900	0.15443200
C	-3.35862000	-1.91292000	-0.84217200
H	-2.58671200	-1.79509300	-1.61095600
H	-3.17634200	-2.86091100	-0.33022300
H	-4.31824300	-2.01202800	-1.35583500
C	0.89939300	0.72451500	1.67975000
H	1.87652600	1.04996500	2.05135500
H	0.33088800	0.29434800	2.51118500
C	3.46945700	1.90228700	-0.09135500
H	3.19988200	2.34623100	-1.05579300
H	2.77209000	2.29229700	0.65238000
H	4.46811200	2.25840200	0.17095800
H	3.81233900	-0.06270200	0.74520300
C	-0.86323100	1.98508500	0.27851000
C	-1.48332300	3.32473100	-0.02587100
H	-1.04078200	4.11066700	0.58724300
H	-1.34607600	3.59568000	-1.07724500
H	-2.56109100	3.30727600	0.16511200
C	1.21820400	-2.33729200	1.61521000
H	0.77721500	-3.33788400	1.62258100
H	2.26350300	-2.42498400	1.31418900
H	1.16315900	-1.92185100	2.62246100

**INT10**

C	0.35114800	-1.61640600	0.25933700
C	-1.51659200	0.70953100	-0.51828400
C	-1.17931700	-1.69130800	0.46911200
C	-1.94330200	-0.36121900	0.54892400
H	-1.41010200	-2.28367400	1.36098300
H	-0.80690000	0.27988900	-1.24105200
H	-1.55345000	-2.27274900	-0.37943600
H	-1.77473200	0.08242800	1.53331900
C	0.15841700	1.81120900	1.03539700
H	0.61261500	2.71860700	1.42018700
C	1.08389700	-0.37951400	0.52752000
C	0.84599100	-2.06949100	-1.12748900
H	0.78068200	-3.15391200	-1.24325500
H	0.20944800	-1.61753600	-1.89676300
C	2.26924800	-1.52398600	-1.21439100
H	2.61234200	-1.37640400	-2.23840700
H	2.98039600	-2.19848800	-0.72707800
C	2.20060700	-0.18979700	-0.43557400
H	1.73182500	0.55545000	-1.11617000
C	3.54001700	0.40891100	0.06462700
C	4.64008600	0.15469800	-0.97268400
H	4.38786500	0.63227700	-1.92562700
H	5.57948100	0.58810500	-0.62324500
H	4.81372300	-0.90718500	-1.15497200
C	-3.49243200	-0.51775000	0.42959600
H	-3.91782900	-0.61731600	1.43336500
C	-2.82811800	1.04557400	-1.26219400
H	-2.84301500	2.04204900	-1.70334100
H	-2.95929500	0.33791300	-2.08583600
C	-3.91127600	0.81511300	-0.20996400
H	-4.92098500	0.78501400	-0.62653200
H	-3.88247400	1.61733400	0.53829600
C	-3.97325700	-1.71070500	-0.39983800
H	-3.56559000	-1.70753100	-1.41631000
H	-3.71196100	-2.66577700	0.06379800
H	-5.06224200	-1.68058600	-0.48370300
C	0.75562900	0.52803700	1.63436700
H	1.67662600	0.79887800	2.15945500
H	0.07456500	0.05431800	2.34472400
C	3.46790700	1.91362800	0.34164400
H	3.14765100	2.45108600	-0.55755300
H	2.79022400	2.18607400	1.15117100
H	4.45901200	2.28351800	0.61358900
H	3.81175400	-0.11922400	0.99032500
C	-0.82121500	1.91281800	0.12518100
C	-1.23724600	3.29588100	-0.30351500
H	-0.65278400	4.06117100	0.20856400
H	-1.10293300	3.42572900	-1.38247100
H	-2.29550400	3.47237800	-0.08834600
C	1.09687000	-2.47605300	1.37427000
H	0.81699000	-3.51085600	1.16033100
H	2.18718000	-2.40866700	1.34501400
H	0.74504200	-2.20733600	2.37072300

**TS10-11**

C	0.34988400	-1.55823100	0.15345500
C	-1.70549600	0.74313700	-0.51883500
C	-1.18002000	-1.66315600	0.35344800
C	-1.98643400	-0.37322400	0.53841700
H	-1.39810200	-2.33271800	1.19257800
H	-1.17718900	0.32037100	-1.38804100
H	-1.54973100	-2.17714700	-0.53980900
H	-1.78048700	0.05600300	1.52225300
C	0.19833700	1.76071700	0.87252500
H	0.80064900	2.64467400	1.05806900
C	1.10053500	-0.34945800	0.49726100
C	0.86209600	-1.94972300	-1.24387500
H	0.75917500	-3.02225100	-1.42537200
H	0.26437400	-1.42741600	-1.99972100
C	2.30701500	-1.45673700	-1.26069800
H	2.68657700	-1.27201700	-2.26579700
H	2.97453000	-2.18577600	-0.79091100
C	2.26741300	-0.15891700	-0.41926400
H	1.88607200	0.63899100	-1.08680500
C	3.61142600	0.33012900	0.17806500
C	4.74155500	0.08952000	-0.83006700
H	4.55362600	0.64270400	-1.75668900
H	5.68603500	0.44804500	-0.41552100
H	4.86942700	-0.96516300	-1.07933900
C	-3.52340900	-0.61225500	0.52943500
H	-3.85039000	-0.89258200	1.53649500
C	-3.11682600	1.19814600	-0.98828200
H	-3.18469200	2.25825000	-1.22682400
H	-3.37903900	0.65881400	-1.90213100
C	-4.05034900	0.77564700	0.14582600
H	-5.10280600	0.76502400	-0.14755900
H	-3.94548900	1.46447100	0.99294700
C	-4.00612900	-1.69027700	-0.44385100
H	-3.64030800	-1.52762100	-1.46340200
H	-3.69531200	-2.69134500	-0.13332600
H	-5.09815600	-1.68919800	-0.48246900
C	0.73074000	0.52156300	1.61333800
H	1.60697200	0.82011700	2.19118400
H	0.00338200	0.05729500	2.27770800
C	3.60568100	1.81536000	0.55518500
H	3.33756900	2.42783000	-0.31278000
H	2.92505000	2.06824900	1.36952300
H	4.60592200	2.11616700	0.87474400
H	3.81655700	-0.27119300	1.07577500
C	-0.81152100	1.87187300	-0.00979500
C	-1.03688300	3.23962300	-0.60618400
H	-0.22453100	3.92372200	-0.35848900
H	-1.12139700	3.17782900	-1.69599700
H	-1.96940700	3.67657200	-0.23679600
C	1.08327600	-2.46469700	1.24314900
H	0.82564300	-3.49081000	0.96723700
H	2.17275100	-2.38285000	1.25340500
H	0.69738100	-2.25128200	2.24036500

**INT11**

C	0.35322400	-1.44915500	-0.01891600
C	-2.10828500	0.87371800	-0.27137500
C	-1.12264000	-1.45735700	-0.44922300
C	-2.03914500	-0.52501800	0.33433600
H	-1.46471300	-2.49451300	-0.34941500
H	-2.54053100	0.76209000	-1.27864300
H	-1.19513600	-1.21691900	-1.51816000
H	-1.70107400	-0.45094600	1.37462400
C	0.40079200	1.41252400	-0.05656300
H	1.16886000	2.09757800	-0.39741100
C	1.07197600	-0.09450300	0.21711200
C	1.24068400	-2.10128500	-1.09386800
H	1.11585100	-3.18682200	-1.11753100
H	0.96353600	-1.71178100	-2.08122800
C	2.65371700	-1.65516400	-0.74322600
H	3.36182000	-1.79875600	-1.56084900
H	3.03419200	-2.21105200	0.12016900
C	2.49610700	-0.16047900	-0.39551400
H	2.46177500	0.37890600	-1.35372300
C	3.64903900	0.43401400	0.44180600
C	4.99820400	-0.08842600	-0.06727500
H	5.13879500	0.17366000	-1.12193300
H	5.81366300	0.36752400	0.49882900
H	5.09158800	-1.17118500	0.03038800
C	-3.54019300	-0.89134400	0.42201400
H	-3.67441800	-1.66336600	1.18579700
C	-3.19333200	1.58414800	0.58172200
H	-2.73923800	1.95511500	1.50653000
H	-3.64340400	2.43466400	0.06608800
C	-4.20405600	0.44154500	0.87011300
H	-5.13722400	0.60583000	0.32579100
H	-4.45297800	0.42302000	1.93292400
C	-4.12820300	-1.41682000	-0.88879900
H	-4.05103200	-0.68923800	-1.70425900
H	-3.64110400	-2.34027300	-1.21288000
H	-5.19070700	-1.63486200	-0.75619700
C	0.73783400	0.75492600	1.32850900
H	1.51036200	1.32854400	1.82971300
H	-0.11708400	0.51446800	1.94713500
C	3.69893700	1.96828900	0.41188000
H	3.79363600	2.32096800	-0.62168800
H	2.83278700	2.46510600	0.85712900
H	4.57572600	2.32438800	0.95771600
H	3.52105500	0.09398900	1.48017500
C	-0.88278800	1.66928100	-0.51181300
C	-1.07456000	2.90597200	-1.32864400
H	-0.16366300	3.21066800	-1.84563800
H	-1.89870000	2.80723700	-2.03699600
H	-1.34164200	3.71372800	-0.63191400
C	0.49294800	-2.22476000	1.30839100
H	0.24985700	-3.27752500	1.14181700
H	1.50568100	-2.17096700	1.71645100
H	-0.18810200	-1.83991200	2.07319700

**TS11-12**

C	0.37302100	-1.42744400	0.07588700
C	-2.07649300	0.85233200	-0.23948700
C	-1.10075000	-1.54964700	-0.33792400
C	-2.04913000	-0.56616500	0.34104600
H	-1.41281700	-2.57463400	-0.10065000
H	-2.42085900	0.77420500	-1.28285700
H	-1.18240000	-1.44639700	-1.42819700
H	-1.77825400	-0.47260000	1.40356000
C	0.42226700	1.05662900	-0.89786900
H	1.12711700	1.75000600	-1.35769800
C	1.02647600	-0.05927400	-0.21581900
C	1.28572600	-2.32539700	-0.78571800
H	1.15033300	-3.38273800	-0.54448500
H	1.03536600	-2.18794500	-1.84490100
C	2.69441700	-1.80804700	-0.50148000
H	3.42547400	-2.12988800	-1.24496500
H	3.04255500	-2.17280800	0.46839100
C	2.54241500	-0.27062500	-0.49152000
H	2.71927800	0.07958600	-1.51868800
C	3.52895900	0.49377400	0.41874300
C	4.93120300	-0.11985300	0.33558000
H	5.28960700	-0.11544600	-0.69962800
H	5.63330200	0.46776300	0.93173300
H	4.96354300	-1.14684100	0.70258100
C	-3.54989600	-0.93897100	0.35022800
H	-3.72185000	-1.69689800	1.12085500
C	-3.18854200	1.51685400	0.58152700
H	-2.79101500	1.80740100	1.56263700
H	-3.59166400	2.41687400	0.11260600
C	-4.25001400	0.39821200	0.72714400
H	-5.09517900	0.58192500	0.05856800
H	-4.64994100	0.37277000	1.74236500
C	-4.04934500	-1.49658600	-0.98295200
H	-3.89956400	-0.78999500	-1.80686600
H	-3.55251700	-2.43448800	-1.24614300
H	-5.12166200	-1.69813000	-0.92272300
C	0.45280500	1.17998600	0.71082300
H	1.10996200	1.94656200	1.09903100
H	-0.16819600	0.66238400	1.43152400
C	3.64128100	1.97495800	0.03400400
H	4.06246000	2.06517000	-0.97331500
H	2.69366900	2.52253200	0.03878500
H	4.31301300	2.49806000	0.71860100
H	3.17593000	0.40964700	1.45752500
C	-0.78071500	1.63163500	-0.38246700
C	-0.94691400	3.11990800	-0.58943000
H	0.00674700	3.61827400	-0.77675800
H	-1.60768400	3.29319600	-1.44363600
H	-1.41454700	3.57385200	0.28659900
C	0.56453700	-1.80340800	1.55627300
H	0.36614100	-2.87055500	1.68644800
H	1.58054300	-1.60529100	1.90500900
H	-0.11473300	-1.26877600	2.22515500

**INT12**

C	0.47140500	-1.38947000	0.19344600
C	-2.06395900	0.73839900	-0.37653700
C	-1.01458900	-1.58206500	-0.14576500
C	-2.01767200	-0.58177000	0.40381300
H	-1.26938700	-2.58886500	0.21074900
H	-2.11287700	0.49357400	-1.44528700
H	-1.11485800	-1.61320600	-1.23764100
H	-1.80366900	-0.37147300	1.46165800
C	0.60698900	1.21762200	-0.18509400
H	1.27348900	1.95811600	-0.60899900
C	1.12234800	-0.08021100	-0.15993300
C	1.31852700	-2.39211600	-0.63062400
H	1.24022100	-3.40128200	-0.21839900
H	0.93097800	-2.42317900	-1.65470600
C	2.73784300	-1.83515300	-0.61877000
H	3.32021000	-2.15588200	-1.48334600
H	3.27843300	-2.16591400	0.27418500
C	2.55685900	-0.30349400	-0.57415300
H	2.64294900	0.13431100	-1.58309800
C	3.65801000	0.38006900	0.30516500
C	5.02218300	0.04641000	-0.30927100
H	5.11024500	0.49309600	-1.30553800
H	5.82021600	0.45712800	0.31324100
H	5.19197300	-1.02794800	-0.39971800
C	-3.48929000	-1.05416700	0.36185300
H	-3.65594700	-1.80356300	1.14317400
C	-3.40892300	1.38981100	0.05514700
H	-3.23069700	2.17797400	0.79452800
H	-3.90309500	1.85992600	-0.79820800
C	-4.25258000	0.24568600	0.67072900
H	-5.27014500	0.22464000	0.27407800
H	-4.33167600	0.38394800	1.75247100
C	-3.90782900	-1.65470800	-0.98168200
H	-3.79726300	-0.93988700	-1.80434100
H	-3.33367200	-2.55138500	-1.23075100
H	-4.96131100	-1.94183000	-0.94404100
C	-0.20844500	1.80215700	1.04863800
H	0.22415800	2.74516300	1.37013900
H	-0.41725200	1.09127700	1.83788100
C	3.54384700	1.89264000	0.48814900
H	3.51743100	2.41199600	-0.47680300
H	2.67291800	2.18829400	1.07667000
H	4.42631500	2.25255900	1.02248000
H	3.59972500	-0.09147600	1.29550000
C	-0.92042500	1.71572900	-0.20540500
C	-1.03561700	2.96513800	-1.05817000
H	-0.19121500	3.64234600	-0.91077500
H	-1.09958000	2.70284400	-2.11684500
H	-1.94758900	3.50122400	-0.78300400
C	0.74400200	-1.61488100	1.70659200
H	0.44081200	-2.63716400	1.94892100
H	1.80168100	-1.50691800	1.95939900
H	0.17234800	-0.93220500	2.33765400

**1,3-shift-Forward**

C	1.32283400	2.15697100	-0.10381700
C	2.11512900	0.99980000	0.07345100
C	-1.08710100	0.08364800	0.20646300
C	1.95870500	-0.37984800	-0.48152300
C	-0.41723700	-1.31300800	0.12760200
C	1.07718500	-1.25744000	0.47439800
H	3.89559400	-0.32448600	-1.39260100
H	1.47748500	-2.27460500	0.43006000
H	1.19574500	-0.92169700	1.51238900
C	0.07018400	2.13095100	-0.68688200
H	-0.39000800	3.11256600	-0.81325500
C	-0.78310500	0.97456900	-1.04476100
H	-1.69198700	1.33904600	-1.51855300
H	-0.27243600	0.36966900	-1.80232700
C	-1.21028700	-2.07531400	1.20294100
H	-1.03493100	-3.15430100	1.17082800
H	-0.91838100	-1.71730900	2.19897200
C	-2.65747900	-1.67970900	0.90896600
H	-3.33369500	-1.89956000	1.73757700
H	-3.02504000	-2.23605200	0.04078200
C	-2.59380800	-0.16502500	0.60664600
H	-2.74777700	0.36044900	1.55874400
C	3.43635200	-0.86816800	-0.55534600
H	1.50325300	-0.36553800	-1.47381700
C	4.03321000	-0.31504600	0.74229500
H	3.72319500	-0.92877500	1.59495100
H	5.12363800	-0.28478800	0.73321200
C	3.40748500	1.07946900	0.81971200
H	3.26575000	1.49885100	1.82367900
H	4.02708200	1.82221500	0.28924100
C	3.64467500	-2.35760200	-0.79341000
H	3.03865500	-2.71807400	-1.63012900
H	4.69230000	-2.54669600	-1.03780900
H	3.40567300	-2.95506800	0.08970700
C	1.86889200	3.48313000	0.38630000
H	2.83011200	3.71938400	-0.07858200
H	1.17890700	4.29527000	0.15625000
H	2.01761400	3.47293400	1.46979000
C	-3.68468900	0.36116300	-0.34138200
H	-3.41388500	0.10173200	-1.37651100
C	-3.83274100	1.88314100	-0.20947900
H	-4.47843800	2.28957000	-0.99213500
H	-4.29156500	2.12042300	0.75614200
H	-2.87966100	2.42139300	-0.24420800
C	-5.04440600	-0.27916300	-0.04307200
H	-5.05207700	-1.35413700	-0.23312900
H	-5.32058300	-0.11675800	1.00464700
H	-5.82090000	0.17429400	-0.66455800
H	-0.62982600	0.58206600	1.06863500
C	-0.62763300	-2.00782200	-1.22885800
H	0.06077100	-1.66922300	-2.00865500
H	-0.47074900	-3.08514300	-1.12031800
H	-1.64082100	-1.85583300	-1.61047400

**1,3-shift-TS**

C	1.47051000	1.96136000	-0.23707500
C	2.04479300	0.68399600	0.26678800
C	-0.99956900	-0.07354700	0.03782100
C	1.84311200	-0.68150500	-0.40680500
C	-0.53944900	-1.55029500	-0.18546300
C	0.93595300	-1.73757800	0.20897300
H	3.23459100	0.77862000	-0.14599500
H	1.28148200	-2.72716100	-0.11572200
H	1.01890200	-1.71756700	1.30058900
C	0.27066300	2.00269500	-0.84266800
H	-0.07239700	2.99885700	-1.12051100
C	-0.67507100	0.87233700	-1.15391100
H	-1.58698500	1.31066300	-1.55722400
H	-0.25970600	0.30190000	-1.99051200
C	-1.47540500	-2.33115100	0.75316800
H	-1.46651400	-3.40745200	0.55833100
H	-1.16478700	-2.17749000	1.79552900
C	-2.83057900	-1.66806300	0.52815200
H	-3.56339400	-1.92950900	1.29444600
H	-3.25095400	-1.97509300	-0.43675900
C	-2.50115100	-0.16332900	0.53013000
H	-2.49516500	0.15414200	1.58263600
C	3.30933600	-0.64901300	-0.10858500
H	1.67715800	-0.55492300	-1.47832500
C	3.50857100	-0.67622800	1.40122100
H	3.29124900	-1.67069600	1.80025900
H	4.52192900	-0.39631200	1.69272600
C	2.45838900	0.41304600	1.72736100
H	1.61045300	0.09178100	2.33458500
H	2.90823600	1.28900900	2.19576500
C	4.36455000	-0.92178400	-1.12927700
H	4.07693300	-0.57015900	-2.12169200
H	5.33478100	-0.51454100	-0.84346500
H	4.44926700	-2.01580400	-1.17751000
C	2.27324300	3.20429100	0.05509400
H	3.26862400	3.15554900	-0.40196700
H	1.77037600	4.08810100	-0.33863900
H	2.41221600	3.35345900	1.13056700
C	-3.54189000	0.72519200	-0.16498000
H	-3.45609700	0.58950000	-1.25336400
C	-3.32844300	2.20069100	0.19251500
H	-3.96966100	2.85126800	-0.40799800
H	-3.58562300	2.36143000	1.24511000
H	-2.29306300	2.53137000	0.06285700
C	-4.96469000	0.32168200	0.23442000
H	-5.21964300	-0.68554100	-0.10250600
H	-5.08095400	0.35595500	1.32361300
H	-5.69214800	1.01301300	-0.19903300
H	-0.43036300	0.30119000	0.89889500
C	-0.75915800	-2.04027400	-1.62718600
H	0.01740700	-1.70180100	-2.32060700
H	-0.75090900	-3.13385000	-1.65129100
H	-1.71753400	-1.70304900	-2.03095500

**1,3-shift-Reverse**

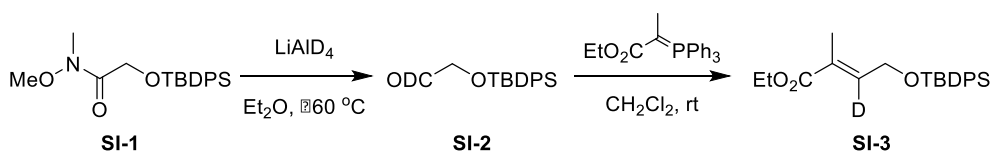
C	1.77751900	2.13330900	-0.07908000
C	2.55177000	0.88869000	-0.45807500
C	-1.11698300	0.46397800	0.46152100
C	1.80821200	-0.43891500	-0.68208500
C	-0.53465900	-0.96554500	0.41507200
C	0.99433800	-0.96247500	0.63314300
H	3.06655700	1.10559000	-1.40761100
H	1.28179200	-1.97825900	0.94731700
H	1.27464800	-0.29085400	1.44756700
C	0.46016900	2.33110300	-0.20131900
H	0.11021200	3.31164700	0.11817500
C	-0.64859100	1.41272700	-0.66340900
H	-1.47905000	2.04417000	-0.98378000
H	-0.36567600	0.85322100	-1.56068000
C	-1.22702100	-1.57959000	1.64603800
H	-1.15574200	-2.67193500	1.66433500
H	-0.75455600	-1.19992300	2.55957100
C	-2.68100400	-1.07347900	1.53231600
H	-3.11212500	-0.90650400	2.52103100
H	-3.30166100	-1.83128300	1.05327000
C	-2.64078900	0.24883000	0.70034700
H	-2.98871400	1.06116600	1.34726400
C	2.76981200	-1.48356100	-0.50481800
H	1.16436800	-0.53158900	-1.55203400
C	3.95286900	-0.97959500	0.23575000
H	4.25119600	-1.62433900	1.06849400
H	4.76887800	-1.05859700	-0.50434200
C	3.64268100	0.48673700	0.57014500
H	3.26255900	0.57338400	1.59181100
H	4.52840300	1.11823600	0.50124800
C	2.67882600	-2.84598100	-1.06032200
H	1.67622500	-3.09282900	-1.40819000
H	3.34856200	-2.84688500	-1.93394000
H	3.06161700	-3.60275600	-0.37180600
C	2.66889500	3.25429000	0.40312600
H	3.46985900	3.45489000	-0.31830800
H	2.10095400	4.17542200	0.53673700
H	3.14935300	3.01453700	1.35774100
C	-3.51824400	0.32259600	-0.58806600
H	-2.86926200	0.18213400	-1.46422500
C	-4.15807600	1.71333000	-0.69524400
H	-4.65877800	1.84573200	-1.65777500
H	-4.90837200	1.83659700	0.09355200
H	-3.43181400	2.52253700	-0.57709400
C	-4.63285600	-0.72437400	-0.66965500
H	-4.26028000	-1.74519900	-0.79496800
H	-5.25832100	-0.70229800	0.22911900
H	-5.27750700	-0.51106000	-1.52634200
H	-0.73470500	0.88767200	1.40041800
C	-0.94142800	-1.77069900	-0.82318200
H	-0.67304700	-1.29844600	-1.77309000
H	-0.49447800	-2.77104900	-0.79206200
H	-2.02372700	-1.91138900	-0.84463100

## 4. Experiment Details

### General Information

All reagents and solvents were purchased from either Aldrich Chemical Company, Inc., Kanto Kagaku Co., Inc., Merck & Co., Inc., Nacalai Tesque Company, Ltd., or Tokyo Kasei Kogyo Co., Ltd., and used without further purification unless otherwise indicated. Dichloromethane (CH<sub>2</sub>Cl<sub>2</sub>) was distilled from phosphoric pentoxide (P<sub>2</sub>O<sub>5</sub>). Tetrahydrofuran (THF), *N,N*-dimethylformamide (DMF), and diethyl ether (Et<sub>2</sub>O) of anhydrous grade were used. All reactions were performed under argon. FTIR spectra were measured on a JASCO FT/IR-6200 infrared spectrophotometer. <sup>1</sup>H NMR spectra were recorded on an either Bruker AVANCE 300 (300 MHz) or spectrometer. Chemical shifts of <sup>1</sup>H NMR were reported in parts per million (ppm, δ) relative to CHCl<sub>3</sub> (δ = 7.26) in CDCl<sub>3</sub>. <sup>13</sup>C NMR spectra were recorded on an either Bruker AVANCE 300 (75 MHz), JEOL JNM-LA 400 (100 MHz), spectrometer. Chemical shifts of <sup>13</sup>C NMR were reported in ppm (δ) relative to CHCl<sub>3</sub> (δ = 77.0) in CDCl<sub>3</sub>. Low resolution mass spectra (LRMS) and high resolution mass spectra (HRMS) were obtained on a JEOL JMS-AX500 using either fast atom bombardment ionization (FAB) or electroionizaion (EI) method. All reactions were monitored by thin layer chromatography (TLC), which was performed with precoated plates (silica gel 60 F-254, 0.25 mm thickness, manufactured by Merck). TLC visualization was accompanied using UV lamp (254 nm) or a charring solution (ethanoic phosphomolybdic acid). Daiso IR-60 1002W (40/63 mm) was used for flash column chromatography on silica gel.

### (2*E*)-Ethyl-4-[[*t*-buthyldiphenylsilyl]oxy]-3-*d*-2-methylbuta-2-enoate (**SI-3**)



To a suspension of LiAlD<sub>4</sub> (587 mg, 14.0 mmol) in Et<sub>2</sub>O (140 mL) was slowly added a solution of **SI-1**<sup>[8]</sup> (5.00 g, 14.0 mmol) in Et<sub>2</sub>O at -60 °C. The mixture was stirred for 30 min at -60 °C, quenched with 1*N* NaOH (100 mL), filtered, and extracted with Et<sub>2</sub>O (x3). The combined organic layers were washed with brine, dried over anhydrous MgSO<sub>4</sub>, and filtered. The filtrate was concentrated under reduced pressure to give the crude **SI-2**, which was subjected to the next reaction without further purification.

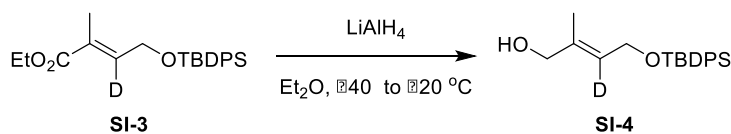
To a solution of **SI-2** (4.19 g) in CH<sub>2</sub>Cl<sub>2</sub> (140 mL) was added ethyl 2-(triphenylphosphoranylidene)propionate (6.16 g, 17 mmol) at room temperature. After stirred for 1 h, the mixture was concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to give **SI-3** (3.38 g, 63%, 2 steps from **SI-1**).

FTIR (neat) 3072, 2958, 2933, 2858, 1713, 1428, 1302, 1279, 1200, 1166, 1113, 1064 cm<sup>-1</sup>.

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.74-7.65 (m, 4 H), 7.49-7.36 (m, 6 H), 4.37 (s, 2 H), 4.21 (q, *J* = 7.1 Hz, 2 H), 1.66 (s, 3 H) 1.32 (t, *J* = 7.1 Hz, 3 H), 1.08 (s, 9 H), <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 167.6, 140.3 (t, *J* = 24.5 Hz), 135.5, 133.2, 129.7, 127.7, 127.4, 61.2, 60.5, 26.7, 19.1, 14.2, 12.5.



**(2E)-4-[[*t*-Buthyldiphenylsilyl]oxy]-3-*d*-2-methylbuta-2-en-1-ol (SI-4)**

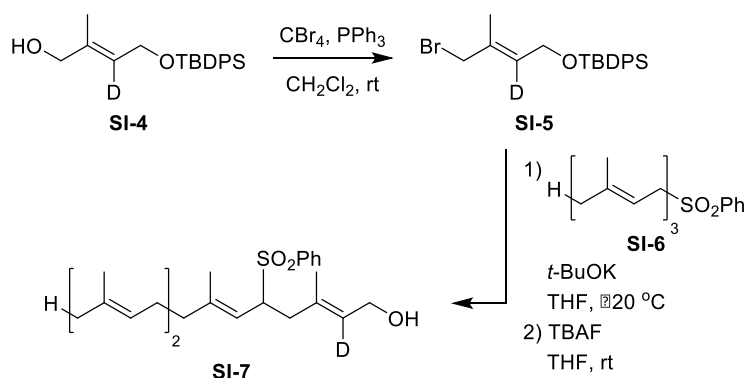


To a suspension of LiAlH<sub>4</sub> (592 mg, 15.6 mmol) in Et<sub>2</sub>O (150 mL) was slowly added a solution of **SI-3** (3.99 g, 10.4 mmol) in Et<sub>2</sub>O at -40 °C. The mixture was stirred for 1 h at -20 °C, quenched with H<sub>2</sub>O (100 mL), acidified with 1N HCl (100 mL), and extracted with Et<sub>2</sub>O (x3). The combined organic layers were washed with brine, dried over anhydrous MgSO<sub>4</sub>, and filtered. The filtrate was concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to give **SI-4** (2.91 g, 82%).

FTIR (neat) 3371, 2931, 2858, 1473, 1428, 1112, 1075, 1008 cm<sup>-1</sup>

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.84-7.65 (m, 4 H), 7.49-7.36 (m, 6 H), 4.30 (s, 2 H), 3.97 (s, 2 H), 1.50 (s, 3 H), 1.07 (s, 9 H), <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 136.5, 135.9, 134.2, 130.0, 128.0, 124.7 (t, *J* = 23.7 Hz), 68.3, 61.1, 27.2, 19.5, 14.1.

**(2E,6E,10E)-2-*d*-3,7,11,15-Tetramethyl-5-(phenylsulfonyl)hexadeca-2,6,10,14-tetraen-1-ol (SI-7)**



To a solution of **SI-4** (202 mg, 0.59 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (6 mL) was added CBr<sub>4</sub> (255 mg, 0.77 mmol) and PPh<sub>3</sub> (202 mg, 0.77 mmol) at 0 °C. The mixture was stirred at room temperature for 30 min and filtered to remove insoluble materials. The filtrate was concentrated under reduced pressure to give the crude **SI-5**, which was subjected to the next reaction without further purification.

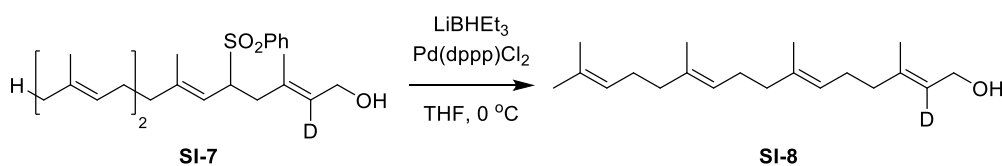
To a suspension of *t*-BuOK (269 mg, 2.4 mmol) in THF (3 mL) was added a solution of **SI-6**<sup>[9]</sup> (308 mg, 0.89 mmol) in THF (1.5 mL) at -20 °C. The mixture was stirred for 15 min. A solution of **SI-5** (239 mg) in THF (1.5 mL) was added. The mixture was stirred for 1 h, quenched with aq. NH<sub>4</sub>Cl, and extracted with AcOEt (x3). The combined organic layers were washed with brine, dried over anhydrous MgSO<sub>4</sub>, and filtered. The filtrate was concentrated under reduced pressure to give the crude product, which was subjected to the next reaction without further purification.

To a solution of the crude product (395 mg) in THF (6 mL) was added TBAF (2.4 mmol, 1.0 M THF solution) at 0 °C. After stirred for 3 h at room temperature, the mixture was concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to give **SI-7** (148 mg, 58%, 3 steps from **SI-4**).

FTIR (neat) 3439, 2966, 2918, 1659, 1447, 1382, 1304, 1146, 1085  $\text{cm}^{-1}$

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) d 7.84 (d,  $J = 7.3$  Hz, 2 H), 7.63 (t,  $J = 7.3$  Hz, 1 H), 7.51 (t,  $J = 7.3$  Hz, 2 H), 5.14-4.98 (m, 2 H), 4.93 (d,  $J = 10.4$  Hz, 1 H), 4.09 (d,  $J = 10.8$  Hz, 2 H), 3.91 (td,  $J = 10.8, 3.1$  Hz, 1 H), 2.93 (dd,  $J = 13.6, 3.0$  Hz, 1 H), 2.34 (dd,  $J = 13.6, 11.3$  Hz, 1 H), 2.11-1.87 (m, 8 H), 1.68 (s, 3 H), 1.61 (s, 3 H), 1.58 (s, 3 H), 1.48 (s, 3 H), 1.17 (s, 3 H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) d 144.8, 138.5, 137.7, 133.2, 131.6, 129.8, 129.0, 128.5, 127.3 (t,  $J = 22.8$  Hz), 123.5, 123.4, 117.0, 63.0, 58.7, 39.5, 37.0, 26.5, 26.1, 25.5, 17.5, 16.2, 16.0, 15.8.

#### (2E,6E,10E)-2-d-3,7,11,15-Tetramethylhexadeca-2,6,10,14-tetraen-1-ol (SI-8)

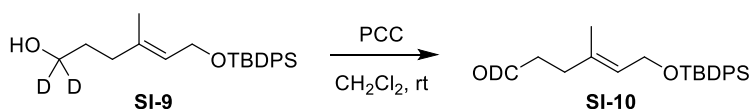


To a solution of **SI-7** (1.81 g, 4.2 mmol) and  $\text{Pd}(\text{dppp})\text{Cl}_2$  (124 mg, 0.21 mmol) in THF (85 mL) was added  $\text{LiBHET}_3$  (21 mmol, 1.0 M THF solution) at 0 °C. The mixture was stirred for 1 h at 0 °C, quenched with aq.  $\text{NH}_4\text{Cl}$ , and extracted with  $\text{AcOEt}$  (x3). The combined organic layers were washed with brine, dried over anhydrous  $\text{MgSO}_4$ , and filtered. The filtrate was concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to give **SI-8** (1.14 g, 93%).

FTIR (neat) 3342, 2966, 2925, 2857, 1653, 1438, 1376, 1107, 1006  $\text{cm}^{-1}$

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) d 5.16-5.05 (m, 3 H), 4.15 (s, 2 H), 2.17-1.92 (m, 12 H), 1.68 (s, 6 H), 1.60 (s, 9 H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) d 139.1, 135.2, 134.8, 131.0, 124.3, 124.1, 123.7, 123.0 (t,  $J = 23.4$  Hz), 59.0, 39.59, 39.56, 39.4, 26.6, 26.5, 26.2, 25.6, 25.5, 17.5, 16.1, 15.8

#### (4E)-6-[[t-Butyldiphenylsilyl]oxy]-1-d-4-methylhexa-4-enal (SI-10)

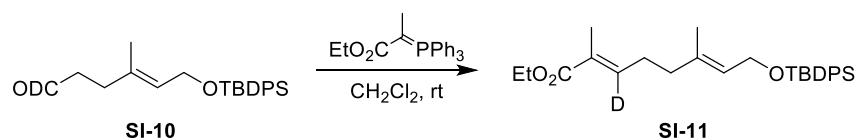


To a solution of **SI-9**<sup>[10]</sup> (7.08 g, 19.1 mmol) in  $\text{CH}_2\text{Cl}_2$  (190 mL) was added PCC (8.23 g, 38.2 mmol) at room temperature. After stirred for 3 h, the suspension was filtered through a celite pad. The filtrate was concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to give **SI-10** (5.05 g, 72%).

FTIR (neat) 3072, 2931, 2858, 2072, 1715, 1472, 1428, 1112, 1063  $\text{cm}^{-1}$

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) d 7.70-7.65 (m, 4 H), 7.46-7.34 (m, 6 H), 5.38 (t,  $J = 6.2$  Hz, 1 H), 4.21 (d,  $J = 6.2$  Hz, 2 H), 2.49 (t,  $J = 7.5$  Hz, 2 H), 2.29 (t,  $J = 7.5$  Hz, 2 H), 1.44 (s, 3 H), 1.04 (s, 9 H),  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) d 201.6 (t,  $J = 25.9$  Hz), 135.5, 134.9, 133.8, 129.5, 127.5, 124.9, 60.9, 41.5 (t,  $J = 3.6$  Hz), 31.3, 26.8, 19.1, 16.3

**(2E,6E)-Ethyl-8-[[*t*-buthyldiphenylsilyl]oxy]-3-*d*-2,6-dimethylocta-2,6-dienoate (SI-11)**

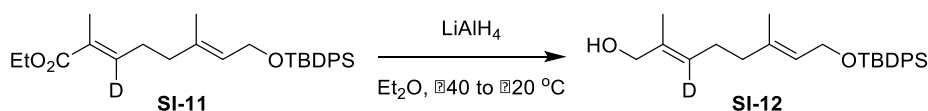


To a solution of **SI-10** (5.04 g, 13.7 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (137 mL) was added ethyl 2-(triphenylphosphoranylidene)propionate (7.43 g, 20.5 mmol) at room temperature. After stirred for 2 h, the mixture was concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to give **SI-11** (5.14 g, 83%).

FTIR (neat) 2932, 2858, 1710, 1638, 1428, 1230, 1277, 1196, 1064, 1112, 1064 cm<sup>-1</sup>

<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.71-7.63 (m, 4 H), 7.45-7.34 (m, 6 H), 5.39 (t, *J* = 6.2 Hz, 1 H), 4.25-4.13 (m, 4 H), 2.25 (t, *J* = 7.6 Hz, 2 H), 2.08 (t, *J* = 7.6 Hz, 2 H), 1.83 (s, 3 H), 1.45 (s, 3 H), 1.28 (t, *J* = 7.2 Hz, 3 H), 1.04 (s, 9 H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 168.2, 141.3 (t, *J* = 24.0 Hz), 136.0, 135.7, 134.1, 129.6, 127.7, 124.8, 61.2, 60.5, 38.0, 27.0, 26.9, 19.2, 16.4, 14.4, 12.5.

**(2E,6E)-8-[[*t*-Buthyldiphenylsilyl]oxy]-3-*d*-2,6-dimethylocta-2,6-dien-1-ol (SI-12)**



To a suspension of LiAlH<sub>4</sub> (861 mg, 22.7 mmol) in Et<sub>2</sub>O (114 mL) was slowly added a solution of **SI-11** (5.15 g, 11.4 mmol) in Et<sub>2</sub>O at -40 °C. The mixture was stirred for 1 h at -20 °C, quenched with H<sub>2</sub>O (100 mL), acidified with 1N HCl (100 mL), and extracted with Et<sub>2</sub>O (x3). The combined organic layers were washed with brine, dried over anhydrous MgSO<sub>4</sub>, and filtered. The filtrate was concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to give **SI-12** (3.27 g, 70%).

FTIR (neat) 3387, 2931, 2858, 1428, 1112, 1066, cm<sup>-1</sup>

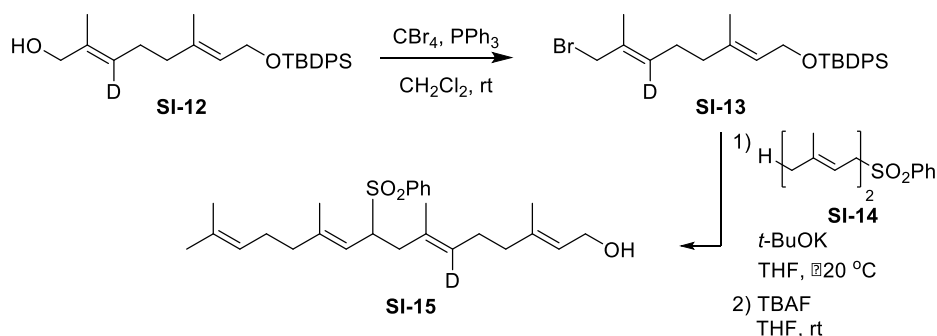
<sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) δ 7.72-7.65 (m, 4 H), 7.46-7.34 (m, 6 H), 5.38 (t, *J* = 6.2 Hz, 1 H), 4.22 (d, *J* = 6.4 Hz, 2 H), 3.99 (s, 2 H), 2.12 (t, *J* = 7.6 Hz, 2 H), 2.01 (t, *J* = 7.6 Hz, 2 H), 1.67 (s, 3 H), 1.45 (s, 3 H), 1.04 (s, 9 H); <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) δ 136.8, 135.6, 134.9, 134.1, 129.6, 127.7, 125.3 (t, *J* = 23.1 Hz), 124.3, 68.8, 61.2, 39.1, 26.9, 25.8, 19.2, 16.4, 13.7.

**(2E,6E,10E)-6-*d*-3,7,11,15-Tetramethyl-9-(phenylsulfonyl)hexadeca-2,6,10,14-tetraen-1-ol (SI-15)**

To a solution of **SI-12** (3.27 g, 7.99 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (80 mL) was added CBr<sub>4</sub> (3.45 g, 10.4 mmol) and PPh<sub>3</sub> (2.73 g, 10.4 mmol) at 0 °C. The mixture was stirred at room temperature for 30 min and filtered to remove insoluble materials. The filtrate was concentrated under reduced pressure to give the crude **SI-13**, which was subjected to the next reaction without further purification.

To a suspension of *t*-BuOK (3.59 g, 32.0 mmol) in THF (40 mL) was added a solution of **SI-14** (3.34 g, 12.0 mmol) in THF (20 mL) at -20 °C. The mixture was stirred for 15 min. A solution of **SI-13** (3.78 g) in THF (20 mL) was added. The mixture was stirred for 1 h, quenched with aq. NH<sub>4</sub>Cl, and extracted with AcOEt (x3). The combined organic

layers were washed with brine, dried over anhydrous  $\text{MgSO}_4$ , and filtered. The filtrate was concentrated under reduced pressure to give the crude product, which was subjected to the next reaction without further purification.

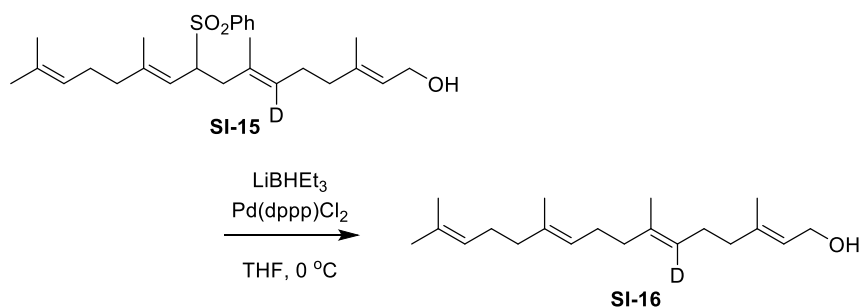


To a solution of the crude product (5.35 g) in THF (80 mL) was added TBAF (32.0 mmol, 1.0 M THF solution) at 0 °C. After stirred for 2 h at room temperature, the mixture was concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to give **SI-15** (2.17 g, 63%, 3 steps from **SI-12**).

FTIR (neat) 3437, 2970, 2919, 2856, 1447, 1304. 1145. 1085  $\text{cm}^{-1}$

$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) d 7.84 (d,  $J = 7.3$  Hz, 2 H), 7.62 (t,  $J = 7.3$  Hz, 1 H), 7.51 (t,  $J = 7.3$  Hz, 2 H), 5.37 (t,  $J = 6.7$  Hz, 1 H), 5.02 (m 1 H), 4.90 (d,  $J = 10.8$  Hz 1 H), 4.13 (d,  $J = 6.7$  Hz, 2 H), 3.88 (td,  $J = 11.0, 2.9$  Hz, 1 H), 2.88 (dd,  $J = 13.2, 2.9$  Hz, 1 H), 2.28 (dd,  $J = 13.2, 11.0$  Hz, 1 H), 2.11-1.88 (m, 8 H), 1.68 (s, 3 H), 1.64 (s, 3 H), 1.58 (s, 3 H), 1.53 (s, 3 H), 1.17 (s, 3 H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) d 144.8, 138.5, 137.7, 133.2, 131.6, 129.8, 129.0, 128.5, 127.3 (t,  $J = 22.8$  Hz), 123.5, 123.4, 117.0, 63.3, 58.9, 39.4, 38.9, 37.1, 26.04, 26.01, 25.4, 17.4, 16.1, 16.0, 15.7

#### (2E,6E,10E)-6-d-3,7,11,15-Tetramethylhexadeca-2,6,10,14-tetraen-1-ol (**SI-16**)



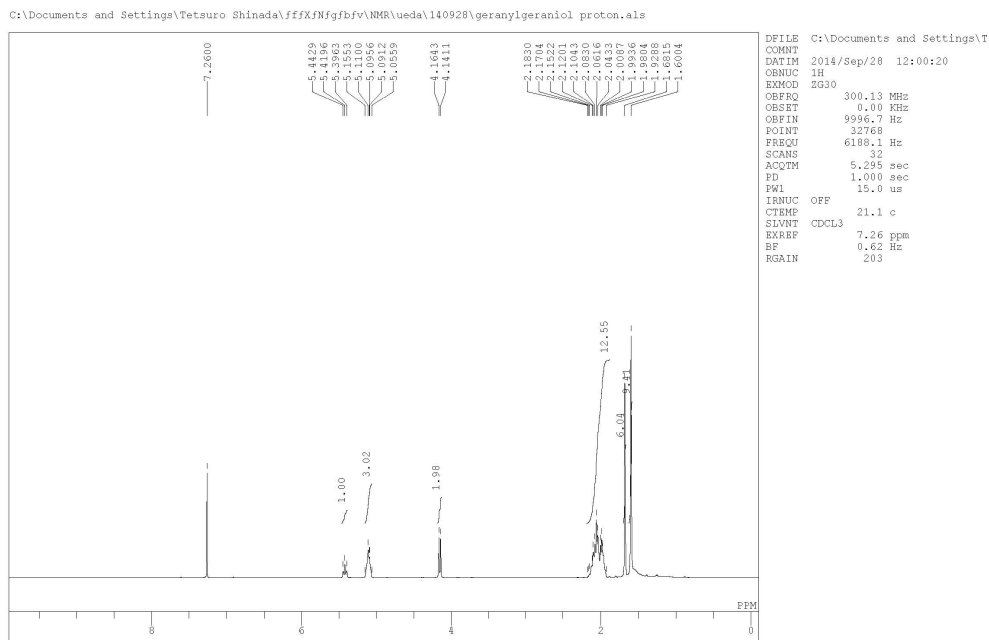
To a solution of **SI-15** (203 mg, 0.47 mmol) and  $\text{Pd(dppp)Cl}_2$  (14 mg, 24 mmol) in THF (5 mL) was added  $\text{LiBHET}_3$  (2.4 mmol, 1.0 M THF solution) at 0 °C. The mixture was stirred for 1 h at 0 °C, quenched with aq.  $\text{NH}_4\text{Cl}$ , and extracted with  $\text{AcOEt}$  (x3). The combined organic layers were washed with brine, dried over anhydrous  $\text{MgSO}_4$ , and filtered. The filtrate was concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to give **SI-16** (103 mg, 75%).

FTIR (neat) 3343, 2966, 2919, 2856, 1669, 1447, 1376, 1105, 1001  $\text{cm}^{-1}$

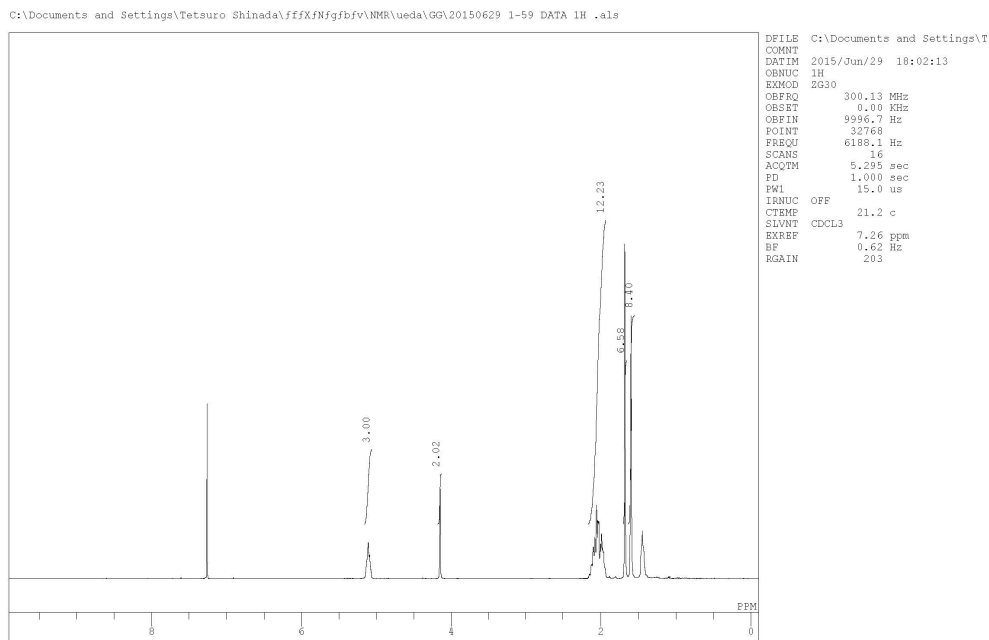
$^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) d 5.42 (t,  $J = 7.0$  Hz, 1 H), 5.15-5.06 (m, 2 H), 4.15 (d,  $J = 7.0$  Hz, 2 H), 2.16-1.93 (m, 12 H), 1.68 (s, 6 H), 1.60 (s, 9 H);  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) d 139.7, 135.2, 134.9, 131.1, 124.3, 123.80 (t,  $J = 25.7$  Hz), 123.76, 123.3, 59.2, 39.64, 39.60, 39.5, 26.7, 26.5, 26.4, 26.2, 26.0, 17.6, 16.2, 15.9

**<sup>1</sup>H-NMR data of (a) GGOH, (b) 2D-GGOH, and (c) 6D-GGOH**

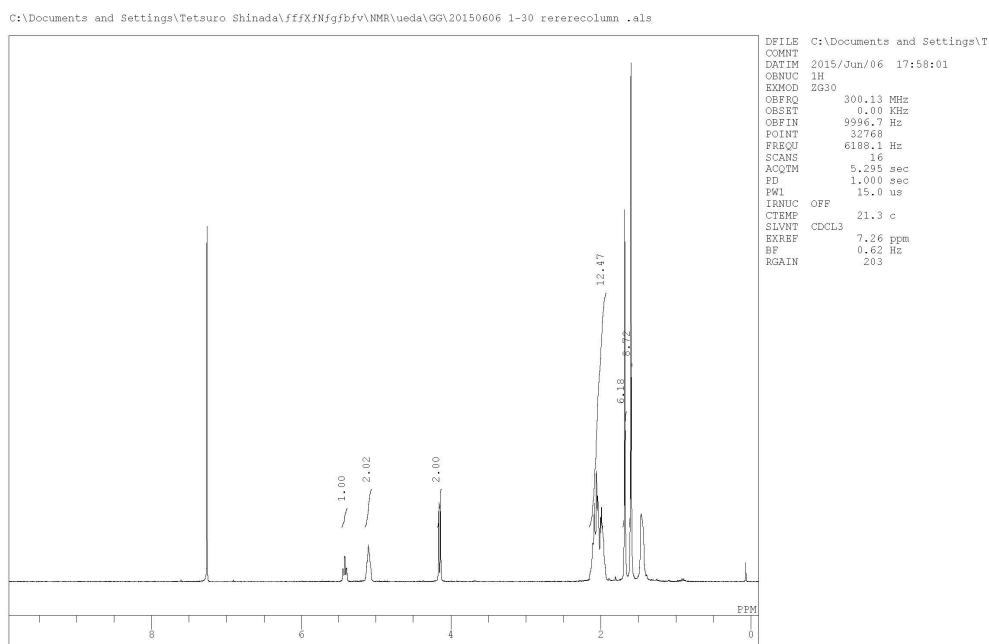
**(a) GGOH**



**(b) 2D-GGOH**



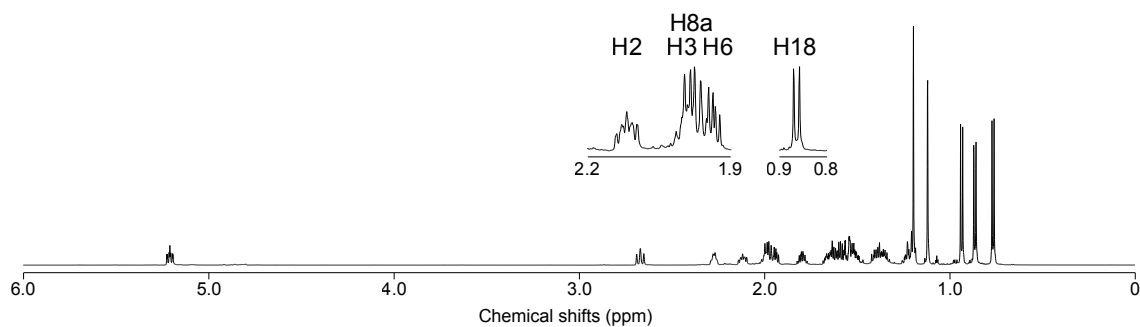
(c) 6D-GGOH



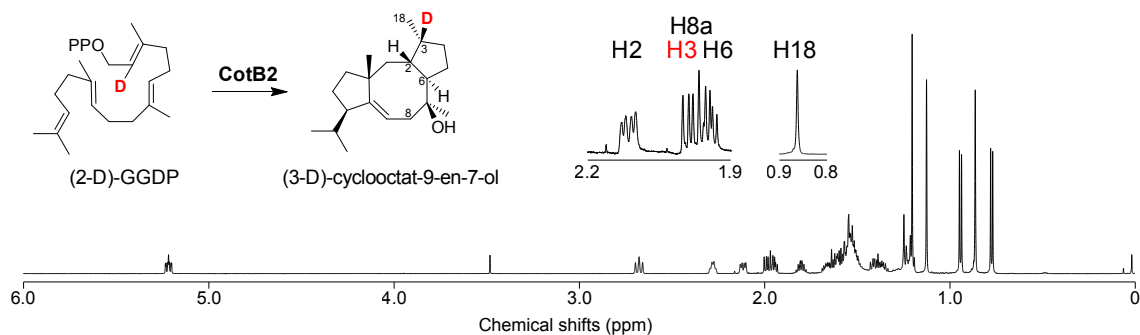
Deuterium Tracing Experiments

(a) Comparison of (3-D)-PD by <sup>1</sup>H NMR spectra with natural abundance PD.<sup>[11]</sup>

natural abundance PD

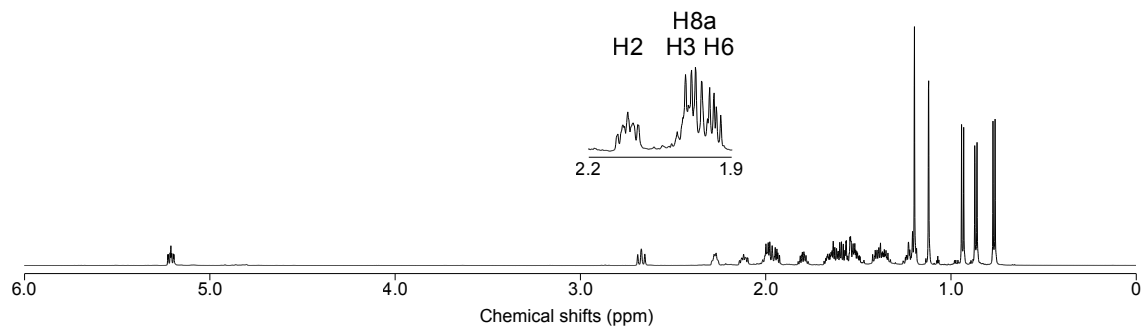


(3-D)-PD

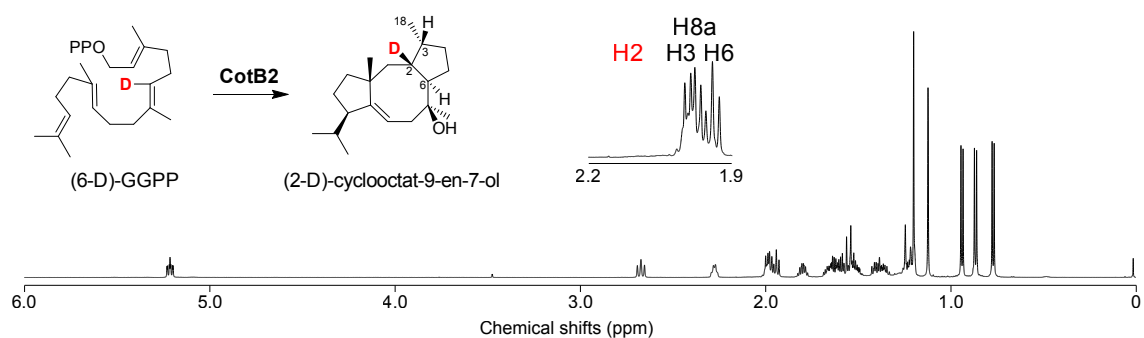


(b) Comparison of (2-D)-PD by  $^1\text{H}$  NMR spectra with natural abundance PD.<sup>[11]</sup>

natural abundance PD



(2-D)-PD



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