Electronic Supporting Information (ESI†)

Light-driven (cross-)dimerization of terpenes as a route to renewable C_{15} – C_{30} crudes for fuel and lubricant oil applications

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Screening of photosensitizers

Table S1 Screening of photosensitizers. Yields of myrcene dimers when 1,1-dinaphthylmethanone **8** is used compared to other photosensitizers.

Photosensitizer	E_T (kcal mol^{-1})[a]	Dimers yield (wt%)[b]
Benzophenone	64.5	18.4
1,1-dinaphthylmethanone	**55.5**	**44.7**
Xanthone	70.1	21.6
Thioxanthone [c]	63.5	30.4

[a] Adiabatic triplet energies calculated at B3LYP/6-311+G(d,p) level.[S1, S2]

[b] Yield of myrcene dimers after 48 h of irradiation, using 0.5 mol% of photosensitizer. Samples were irradiated in quartz test tubes under 365 nm light (Rayonet photoreactor).

[c] Photosensitizer with poor solubility, therefore, the amount added was not fully solubilized.

Table S2 Optimization of photosensitizer **8** loading.

Entry	**8** (mol%)	Dimers yield (wt%)[a]
1	0.500	**77.1**
2	0.250	**35.0**
3	0.125	**35.2**
4	0.050	**29.9**
5	0.010	**12.4**

[a] Yields of α-phellandrene dimers after 12 h of irradiation. Samples were irradiated in quartz test tubes under 365 nm light (Rayonet photoreactor).

Solar irradiance

Table S3 Global horizontal yearly average solar irradiance for Stockholm and other places located in lower latitudes. Data extracted from https://energyplus.net/weather

Location	**Global horizontal yearly average solar irradiance MJ/m^2/year**
Accra, Ghana	6,825
Addis Ababa-Bole, Ethiopia	7,321
Barcelona, Spain	5,260
Beijing, China	5,025
Berlin, Germany	3,548
Cairo, Egipt	6,882
Cape Town, South Africa	6,843
Mexico City, Mexico	6,539
Miami, United States of America	6,453
Nairobi, Kenya	6,701
New Delhi, India	7,054
Paris, France	3,845
Phoenix, United Sates of America	7,621
Sao Paulo, Brazil	5,515
Stockholm, Sweden	**3,319**
Sydney, Australia	5,948
Tehran, Iran	7,703

Table S4 Monthly statistics of the global horizontal yearly average solar irradiance for Stockholm-Arlanda. Values in Wh/m^2. Data extracted from https://energyplus.net/weather

Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
260	764	1767	3743	5278	5360	5063	3810	2324	1178	447	200

Fuel and lubricant oil properties

Table S5 Computed heats of combustion.[a]

Entry	Monomer	Dimer	Heat of combustion of hydrogenated dimer kJ mol^{-1}	Heat of combustion of hydrogenated dimer MJ kg^{-1}
1	α-Phellandrene	1a	11,739.21	42.46
2	α-Phellandrene	1c	11,695.83	42.30
3	Myrcene	2a (cis)	12,142.34	43.29
4	Myrcene	2a (trans)	12,151.44	43.32
5	Myrcene	2g	12,066.60	43.02
6	Myrcene	2k	12,115.98	43.19
7	Ocimene	3h	12,089.65	43.10
8	Ocimene	3k	12,125.64	43.23

[a] Calculated according to the procedure described in the reference S4, at M06-2X/6-31+G(d,p) level.[S2-S4] The Self-Consistent Reaction Field Solvent method (SCRF) was used to model the solvent toluene, using the Solvation Model Based on Density (SMD).

Table S6 Fuel and lubricant oil properties measured for the hydrogenated dimers produced in this study.

Physical Property	HAPD	HMD	HAPID	HGOD
Molecular formula	$C_{20}H_{36}$	$C_{20}H_{40}$	$C_{20}H_{36}$ $C_{15}H_{28}$	$C_{30}H_{56}$
Hydrogen content, % mass	13.12	14.37	13.74	10.85
Gravimetric Net Heat of Combustion (NHOC), MJ/kg	43.09	43.74	43.30	-
Density at 25 °C, g/mL	0.9314	0.8606	0.9042	-
Volumetric NHOC, MJ/L at 25 °C	40.13	37.65	39.15	-
Kinematic viscosity at -20 °C, mm²/s	> 10^4	475.4	209.7	-
Kinematic viscosity at 40 °C, mm²/s	41.1	12.7	6.45	303
Kinematic viscosity at 100 °C, mm²/s	4.16	2.89	-	14.7
Viscosity Index	-	59	-	-
Pour point, °C	-21	< -45	< -45	-15

Reaction setups

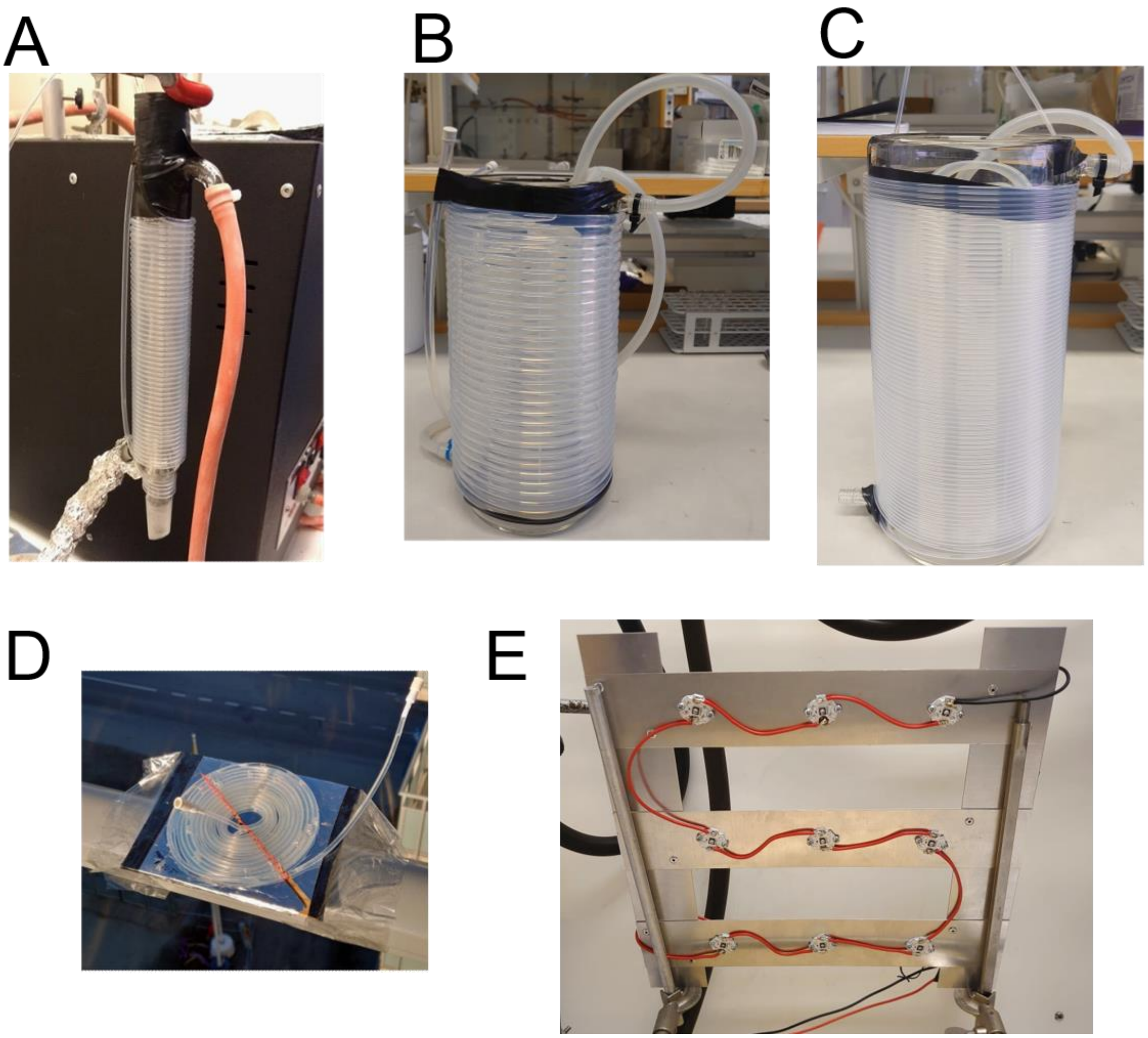


Fig. S1 Custom-made setup (CMS) with FEP tubing used in the photoreactions. **A) CMS I**, FEP tubing dimensions: O.D. × I.D. : 3.18 mm × 2.1 mm - loop volume = 20 mL. **B) CMS II**, FEP tubing dimensions: O.D. × I.D. : 7.94 mm x 6.35 mm - loop volume = 400 mL. **C) CMS III**, FEP tubing dimensions: O.D. × I.D. : 3.18 mm × 2.1 mm - loop volume = 120 mL **D) CMS IV**, flat spiral FEP tubing setup used in experiments with simulated and natural sunlight. FEP tubing dimensions: O.D. × I.D. : 3.18 mm × 2.1 mm - loop volume = 10 mL. **E)** A custom-made 30 cm x 30 cm LED panel with light intensity control used in the light intensity experiments. The panel has nine 365 nm LED lamps equally spaced from each other (LZ1-10UV0R, OSRAM Opto Semiconductors Inc.).

Screening of Photosensitizers

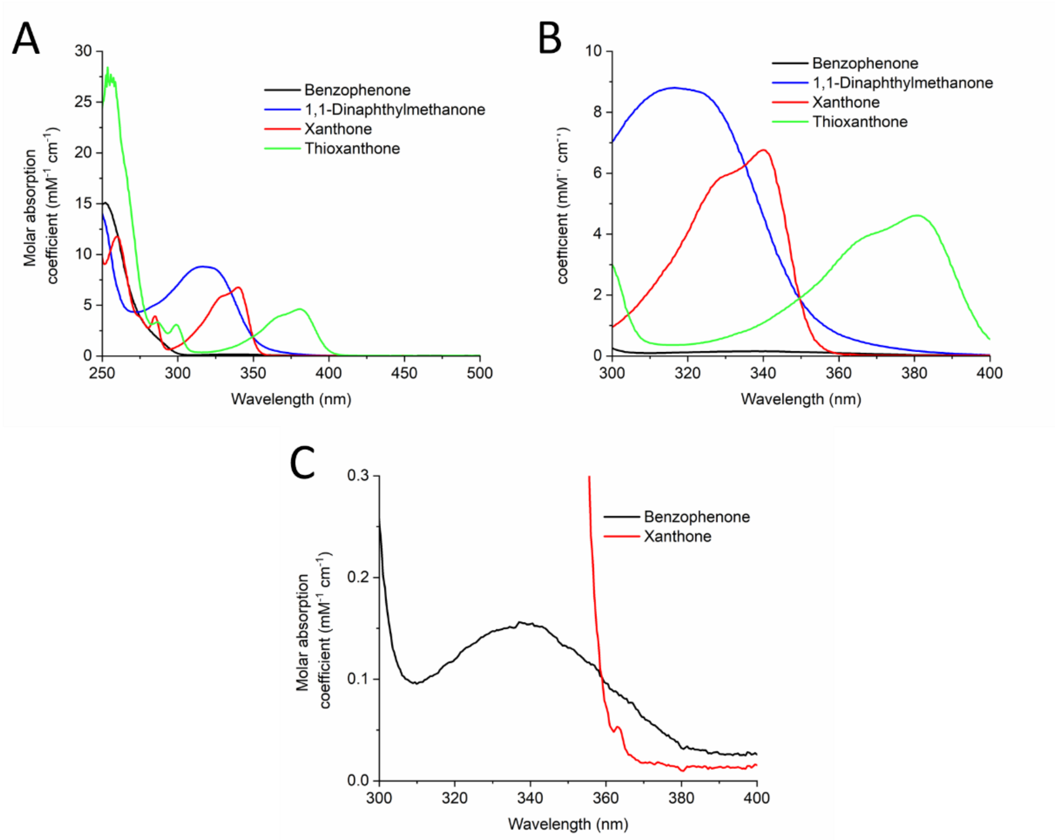


Fig. S2 A) UV-Vis absorption spectra of the photosensitizers tested. Solvent: cyclohexane. B) Near-UV region zoomed in. C) Zoomed in region showing the absorption of benzophenone and xanthone at 365 nm.

Spin density in the triplet state

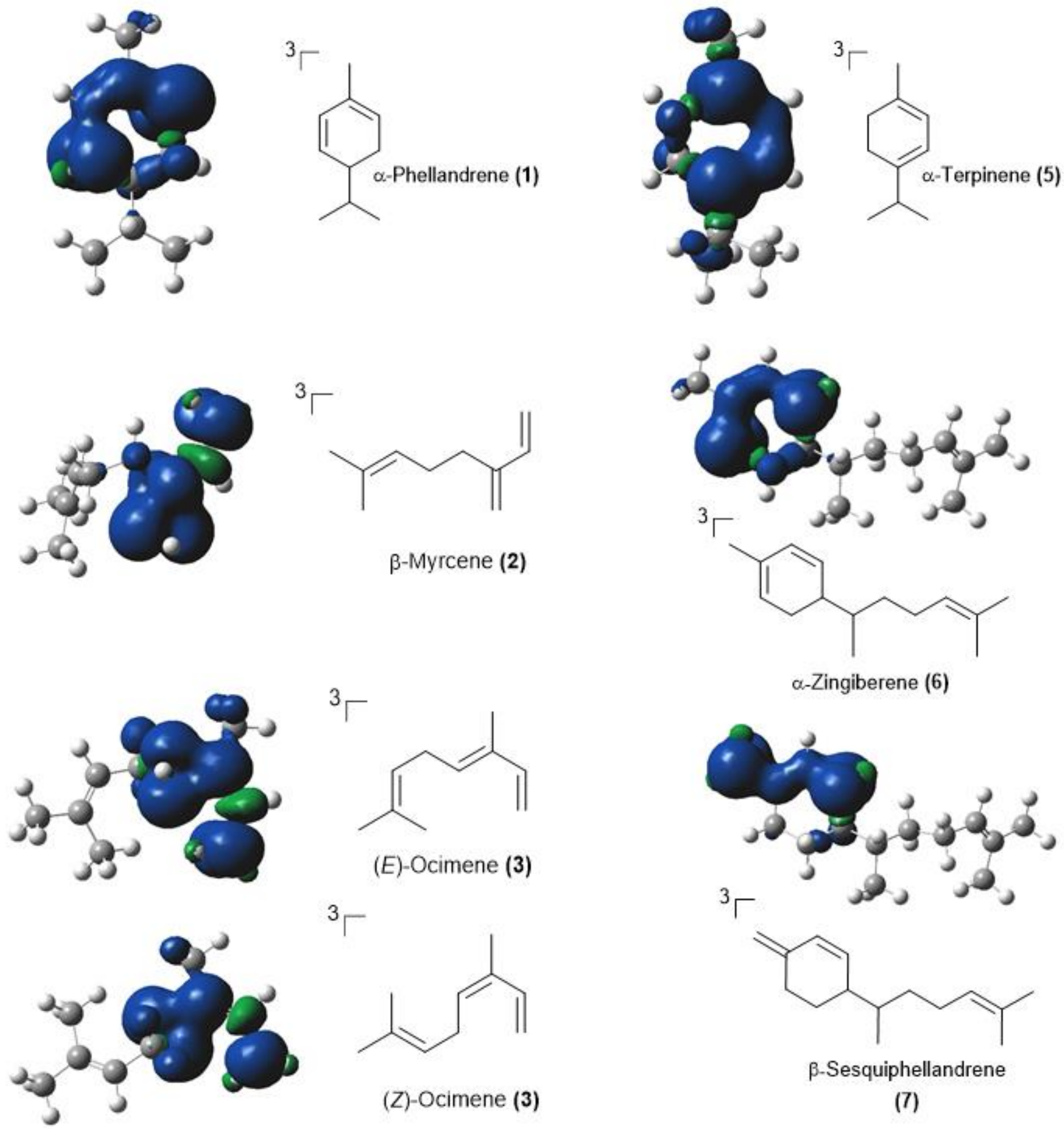


Fig. S3 Spin densities in the first triplet (T_1) state of the terpenes studied. Geometries and energies calculated at the (U)M06-2X/6-311+G(d,p) level.[S2, S3] The diene structures of **2** and **3** show twisted geometries with the allyl segment at the termini of the hydrocarbon chain. The other compounds (endocyclic dienes) do not have twisted structures in their T_1 states.

α-Terpinene dimerization

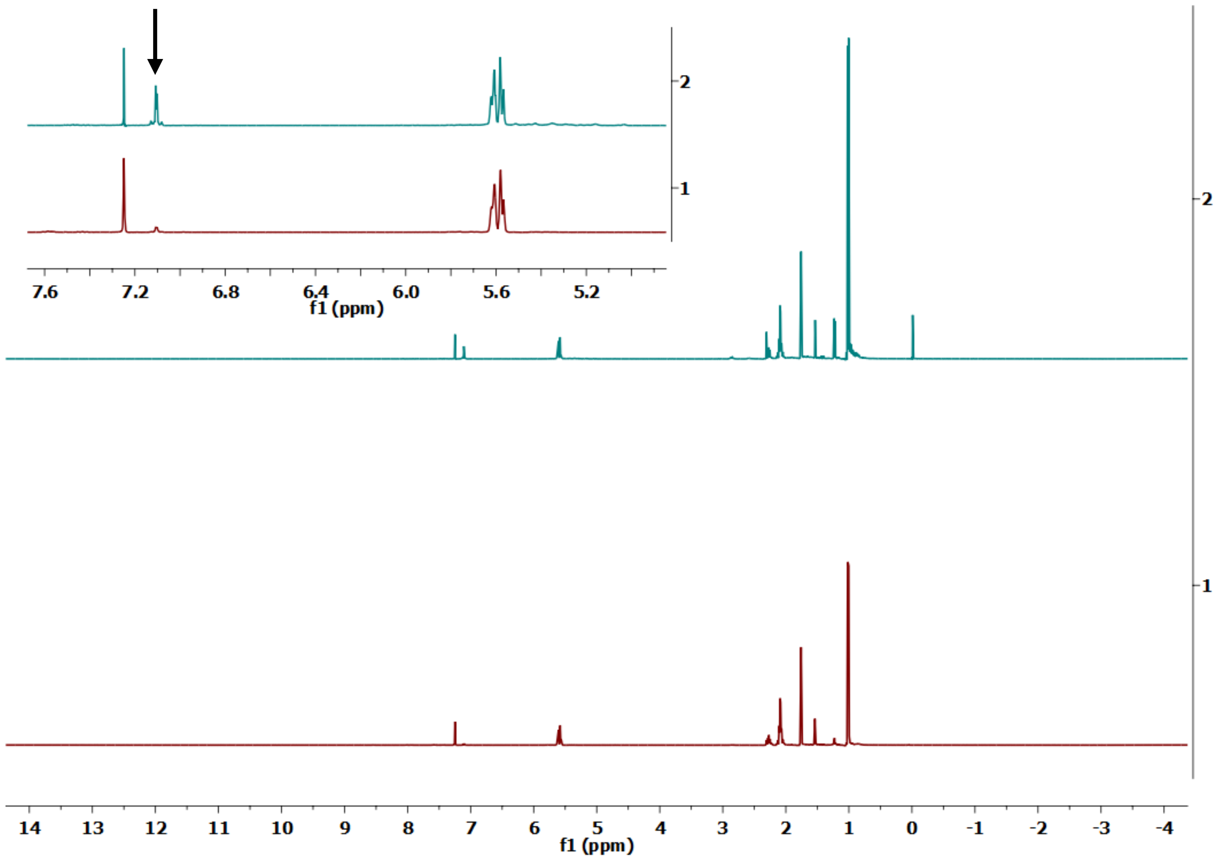
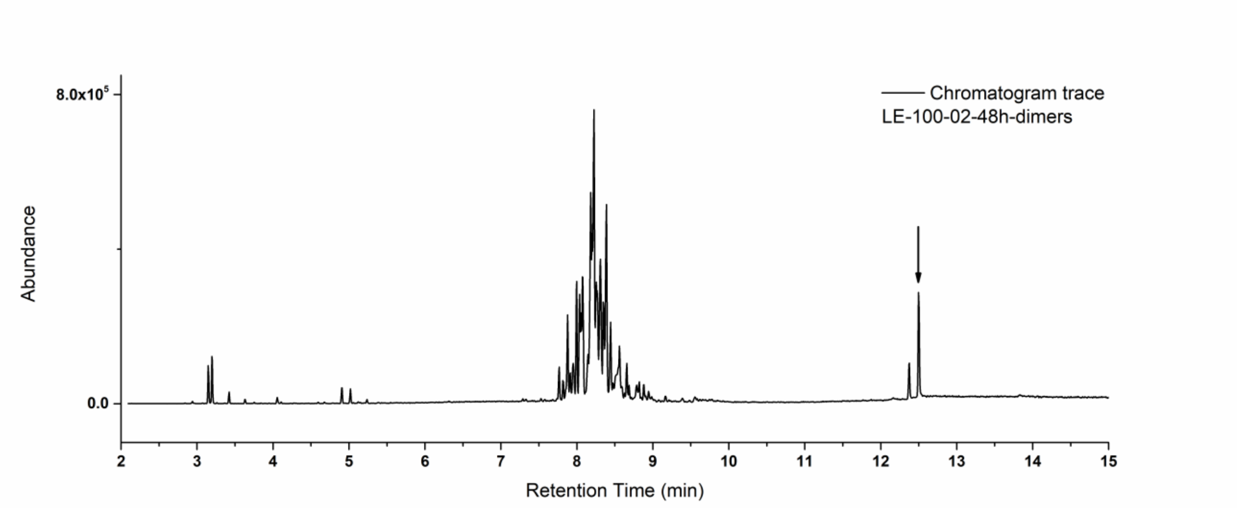


Fig. S4 ^{1}H NMR spectra of crude sample of α-terpinine **5** irradiated with **8** for 48 h (**top**) and starting material (**bottom**). The inset highlights the increase of aromatic content due to aromatization of **5** and photoreduction of **8**. The arrow indicates the aromatic product from the dehydrogenation of **5**.



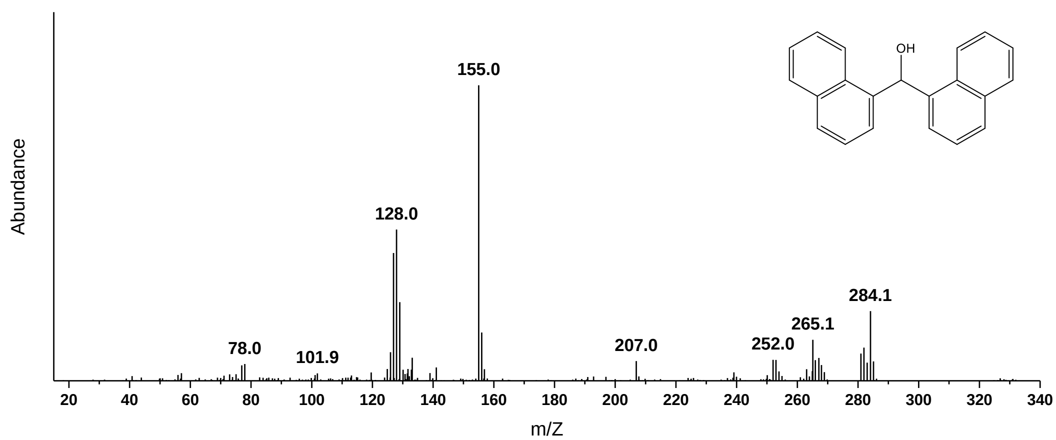


Fig. S5 Chromatogram trace of distillated sample of α-terpinine **5** irradiated with **8** for 48 h (**top**). Some C10 starting material was still present in the sample. The arrow indicates the peak of the reduced 1,1-dinaphthylmethanone **8** due to abstraction of H-atoms from **5**. The mass spectrum for that peak is also displayed (**bottom**), where it can be found the M^+ = 284.1 m/z.

α-Phellandrene dimerization

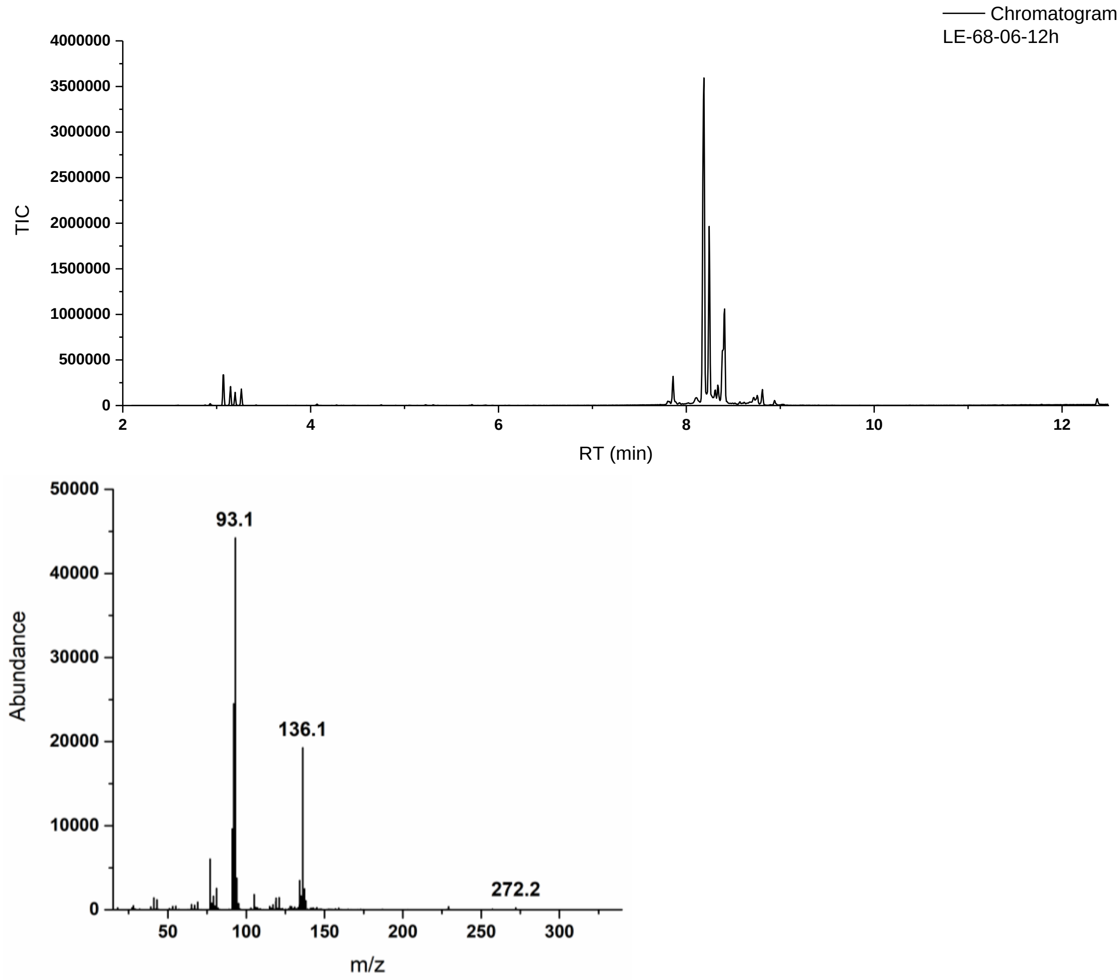


Fig. S6 Chromatogram trace for α-phellandrene **1** and 1,1-dinaphthylmethanone **8** sample irradiated for 12 h under 365 nm light (Rayonet photoreactor). The corresponding mass spectrum of the dimers is also shown (RT = 7.5 – 9.0 min).

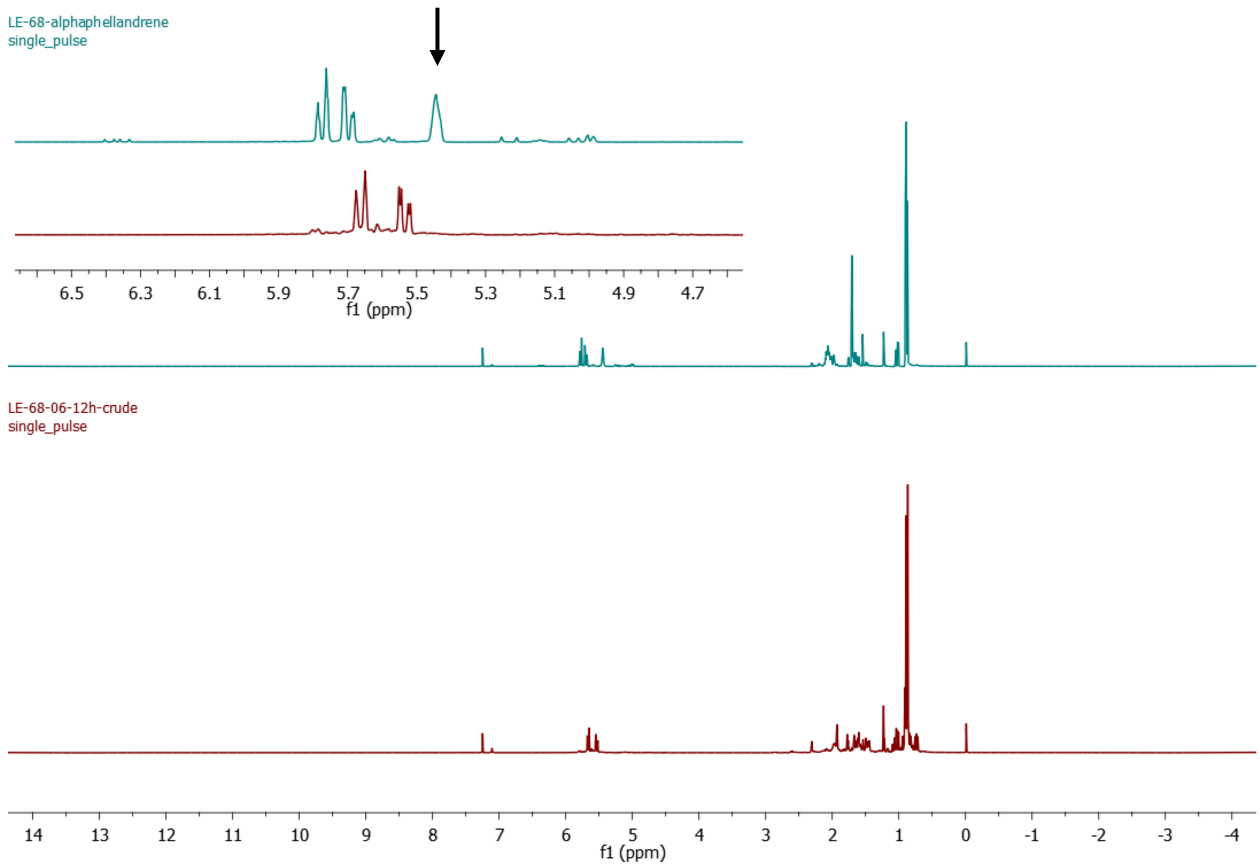


Fig. S7 [1]H NMR spectra for starting material α-phellandrene **1** (**top**, blue) compared to α-phellandrene **1** and 1,1-dinaphthylmethanone **8** sample irradiated for 12 h under 365 nm light (**bottom**, red). Inset: the black arrow indicates the multiplet at 5.44 ppm which is absent after dimerization.

Control experiments

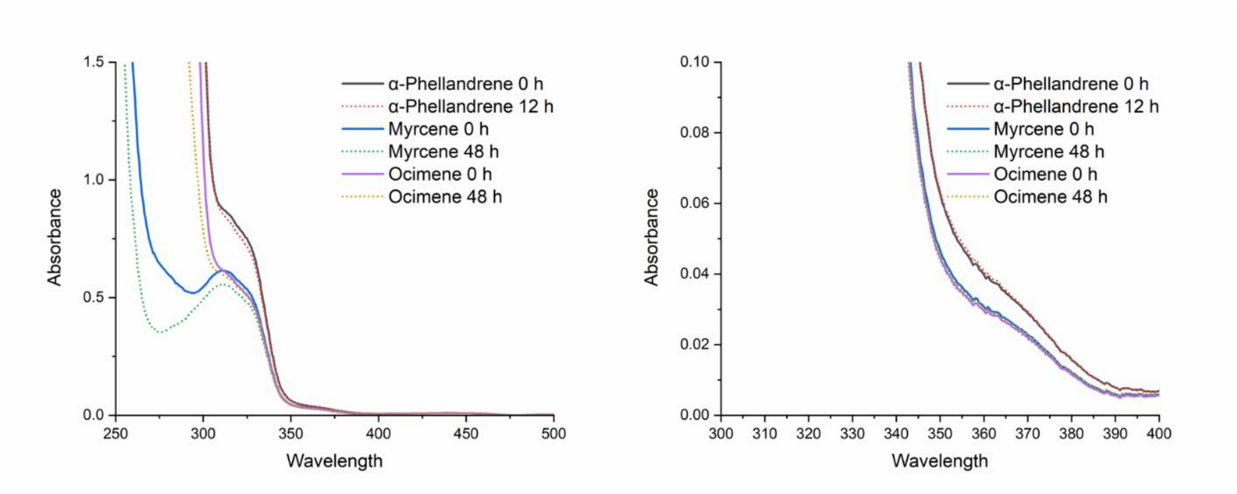


Fig. S8 UV-Vis absorption spectra of monoterpene reaction mixtures with photosensitizer **8**, measured before and after irradiation. In α-phellandrene reaction, the amount of **8** in the reaction was 0.2 mol%, while for myrcene and ocimene this amount was of 0.5 mol%. For the absorption spectra measurement the samples were diluted in cyclohexane to reach a concentration of **8** of about 100 μM.

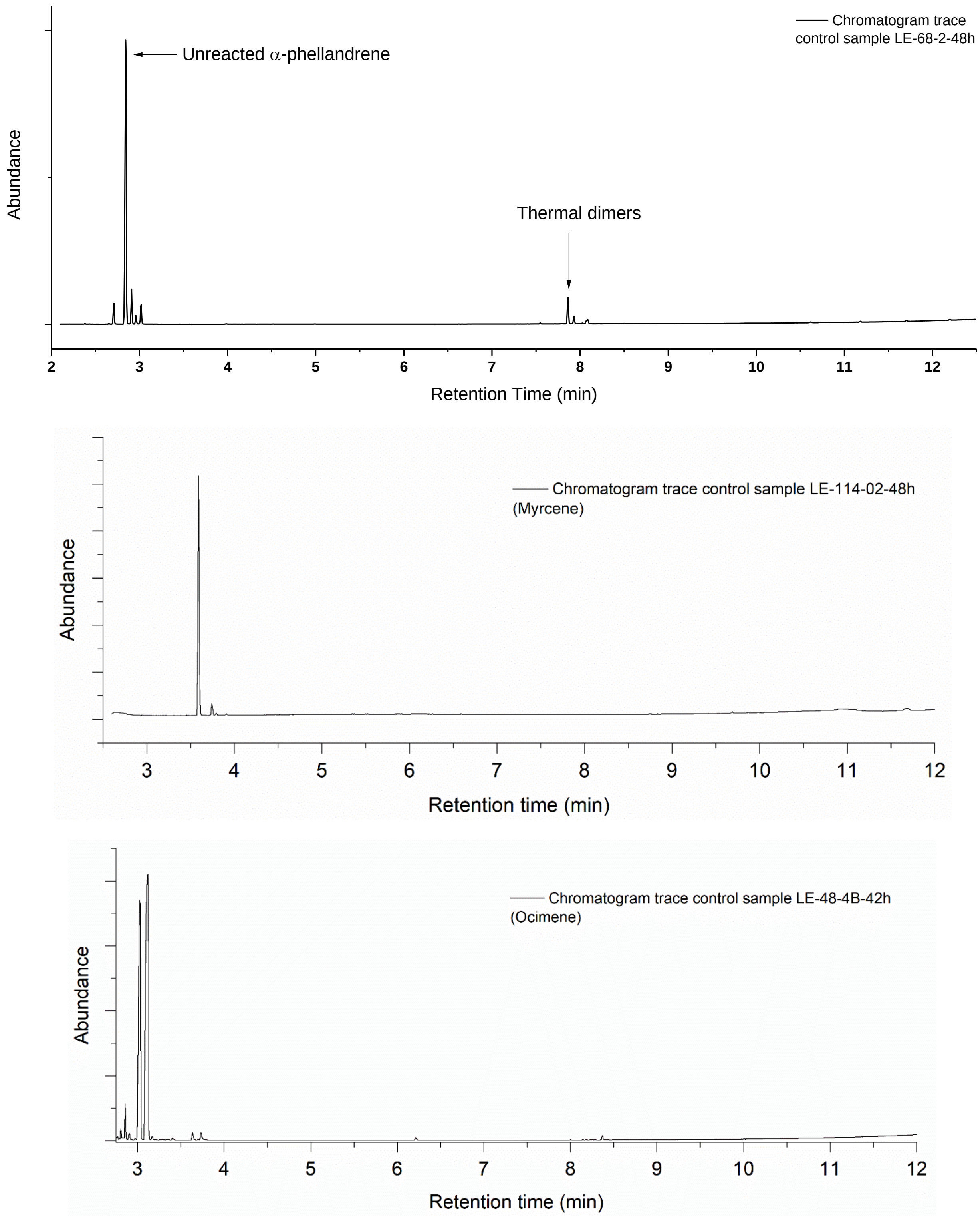


Fig. S9 GC-MS trace for α-phellandrene **1** (top), myrcene **2** (middle) and ocimene **3** (bottom) samples irradiated at 365 nm light, in quartz test tube, for 48h without photosensitizer added.

Myrcene dimerization

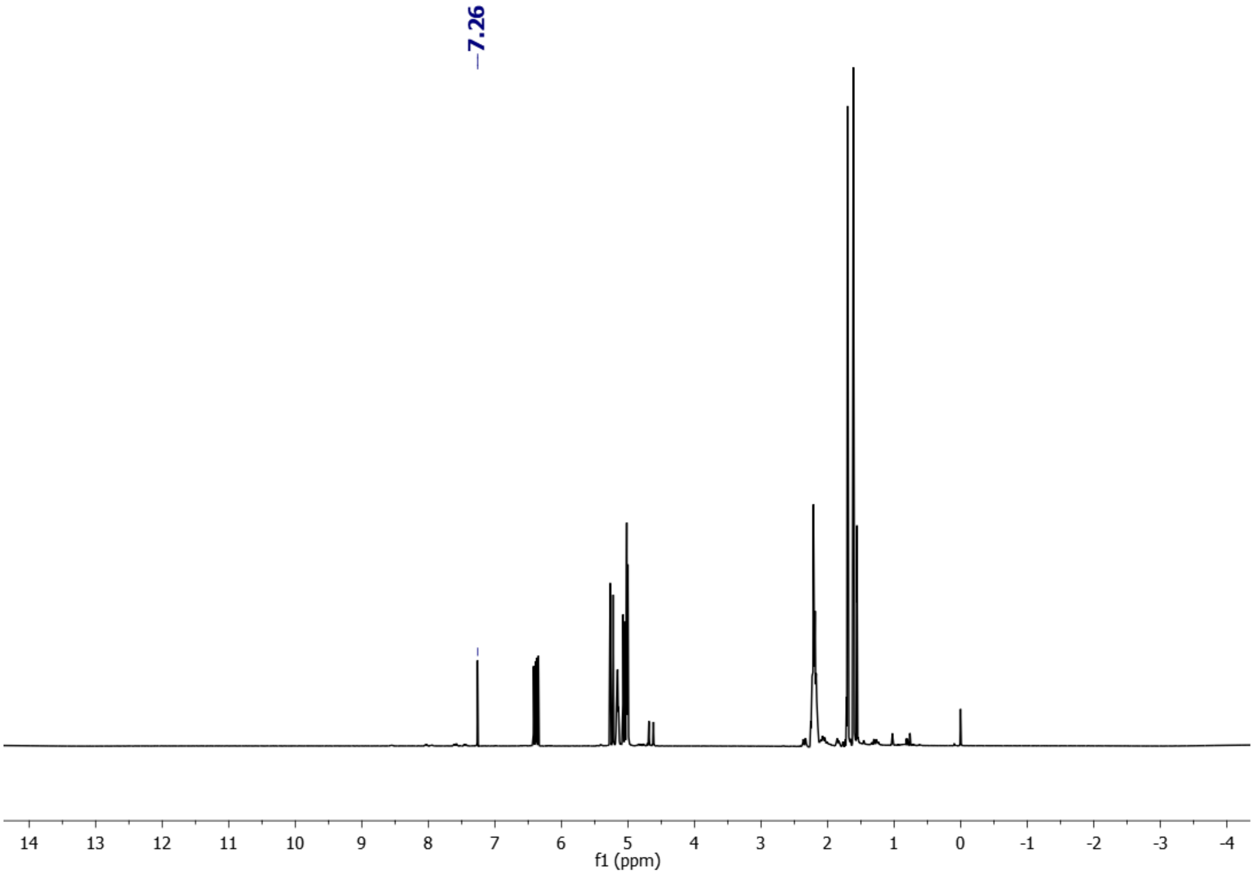
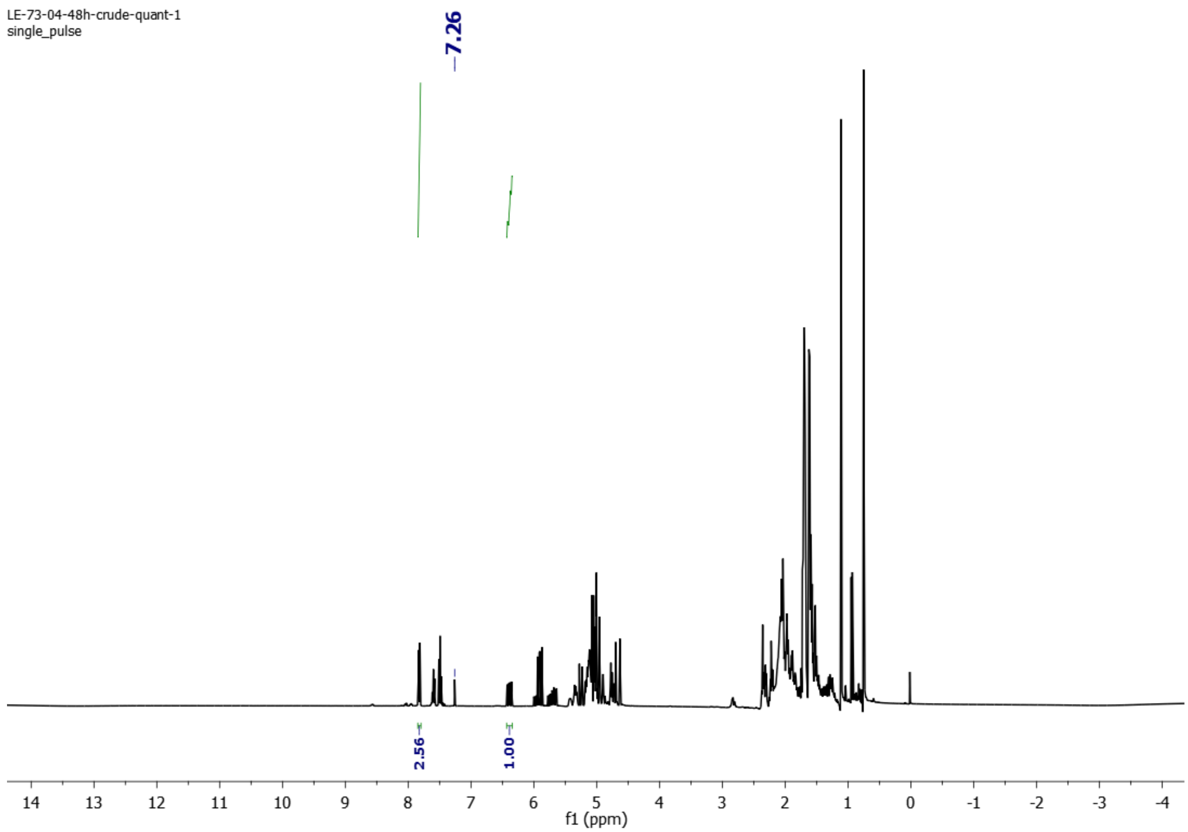


Fig. S10 Myrcene **2** and 1,1-dinaphthylmethanone **8** sample before irradiation. $CDCl_3$ was used as deuterated solvent and the spectrum was referenced to its residual peak.



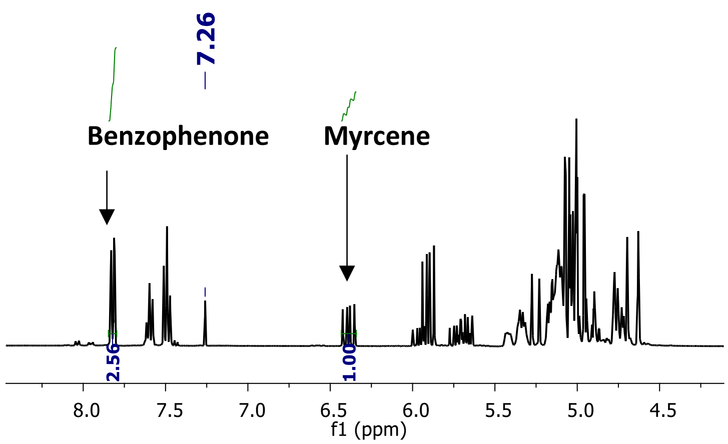


Fig. S11 ^{1}H NMR spectrum of myrcene **2** and 1,1-dinaphthylmethanone **8** crude sample after irradiation (365 nm, 48 h). Full spectrum on top, and expansion of alkene region at the bottom. ^{1}H NMR for quantification of unreacted myrcene (89.1 mg of crude sample) with benzophenone used as standard (5.6 mg). $CDCl_3$ was used as deuterated solvent and the spectrum was referenced to its residual peak. Reaction carried out in the coiled FEP setup.

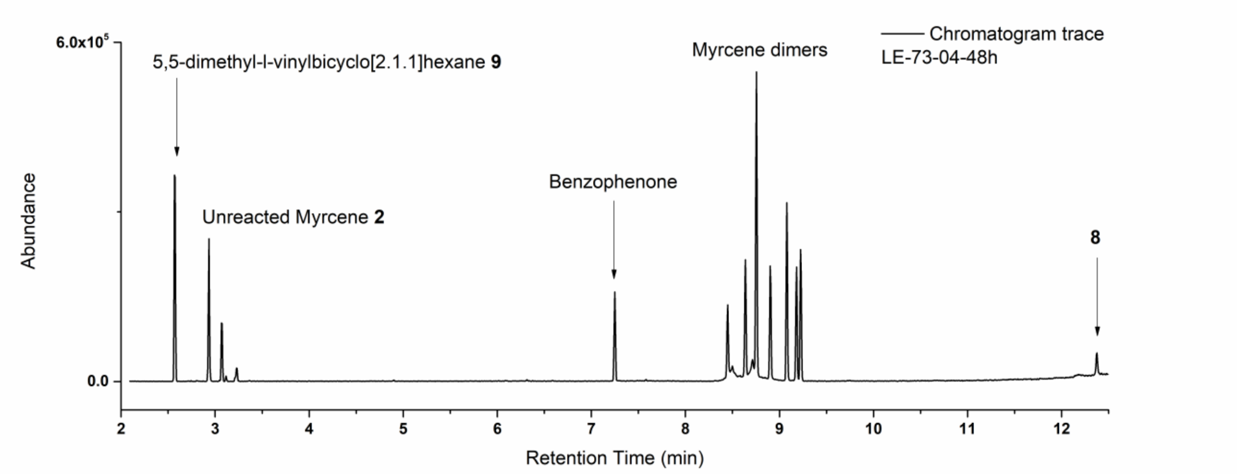


Fig. S12 Chromatogram trace for myrcene **2** and 1,1-dinaphthylmethanone **8** crude sample after irradiation (λ = 365 nm, t = 48 h) with added benzophenone used as standard on the qNMR (see Fig. S9). Byproduct **9**, as well as the unreacted myrcene are indicated.

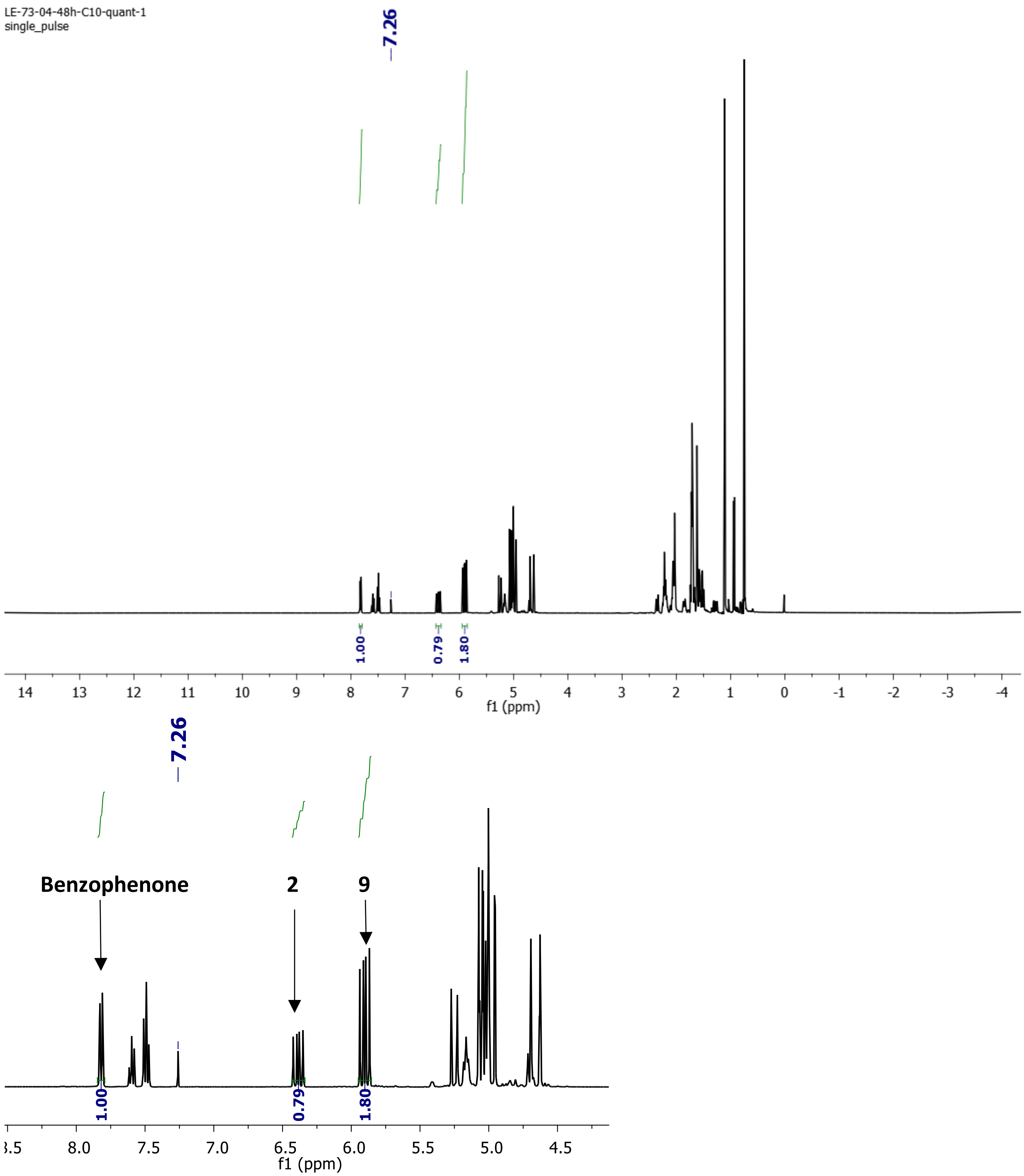
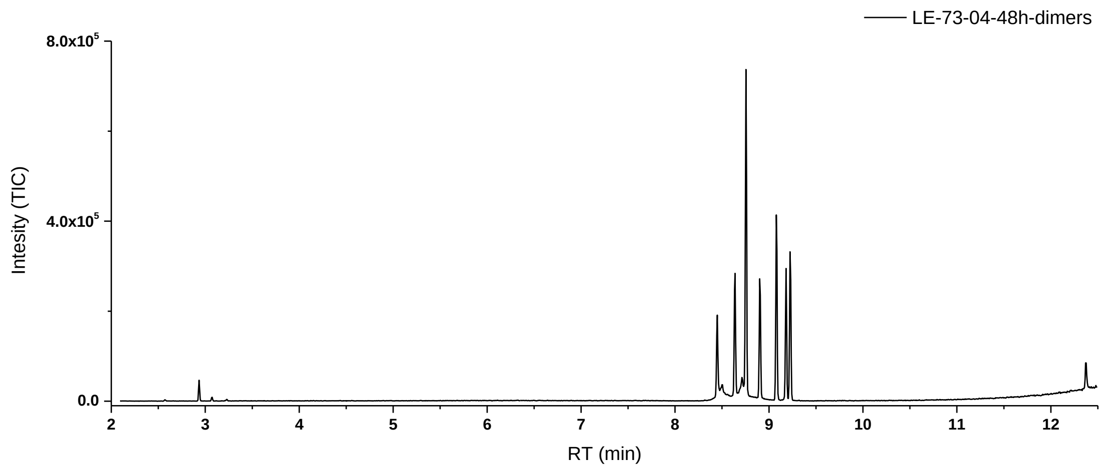


Fig. S13 C_{10} fraction recovered after distillation of crude reacted mixture of myrcene **2** and 1,1-dinaphthylmethanone **8** (365 nm, 48 h). ^{1}H NMR for quantification of recovered 5,5-dimethyl-l-vinylbicyclo[2.1.1]hexane **9** produced as byproduct during the reaction (63.3 mg of recovered C_{10} sample) with benzophenone used as standard (5.8 mg). Recovered unreacted myrcene was also verified. $CDCl_3$ was used as deuterated solvent and the spectrum was referenced to its residual peak.



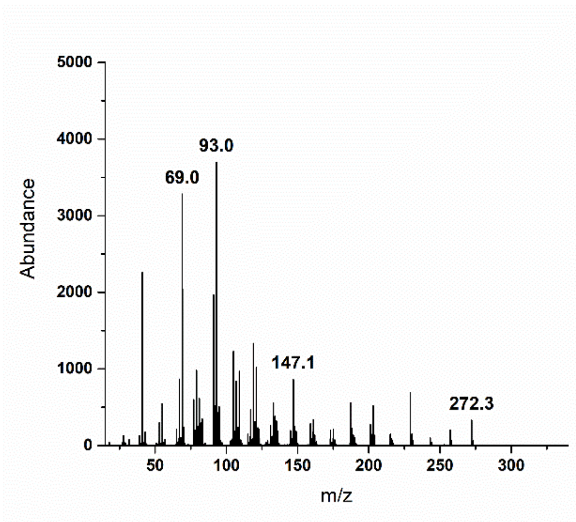


Fig. S14 GC-MS chromatogram of dimers produced through myrcene **2** dimerization (λ = 365 nm, t = 48 h). The light fraction was removed by distillation under reduced pressure. **Bottom:** Mass spectrum of dimers.

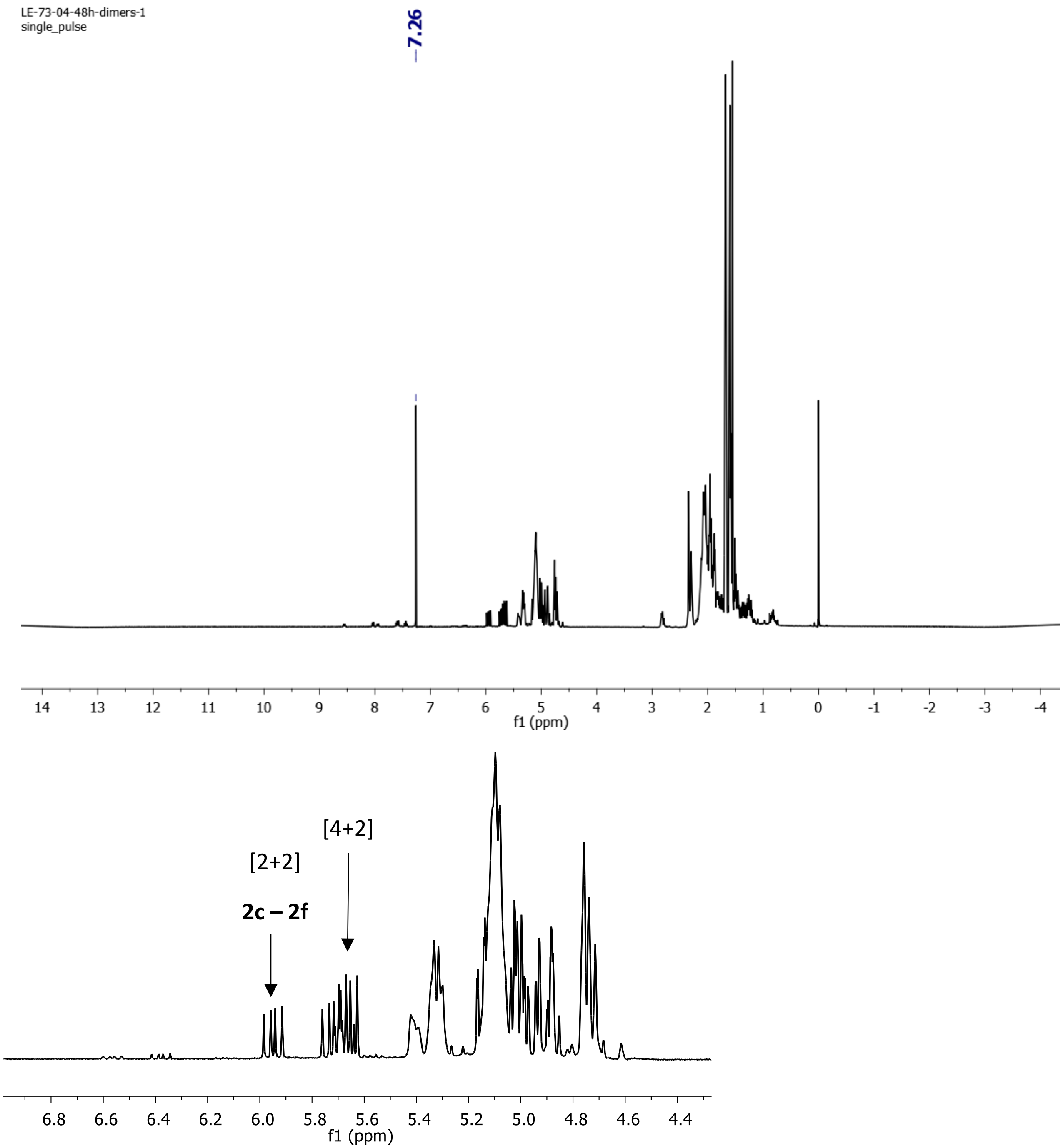


Fig. S15 ^{1}H NMR of dimers produced through myrcene **2** dimerization (λ = 365 nm, t = 48 h, top) with expansion of the alkene region (bottom). The light fraction was removed by distillation under reduced pressure. $CDCl_3$ was used as deuterated solvent and the spectrum was referenced to its residual peak. On the chromatogram it is possible to see trace amounts of unreacted myrcene that remained after the distillation.

Myrcene epoxide dimerization

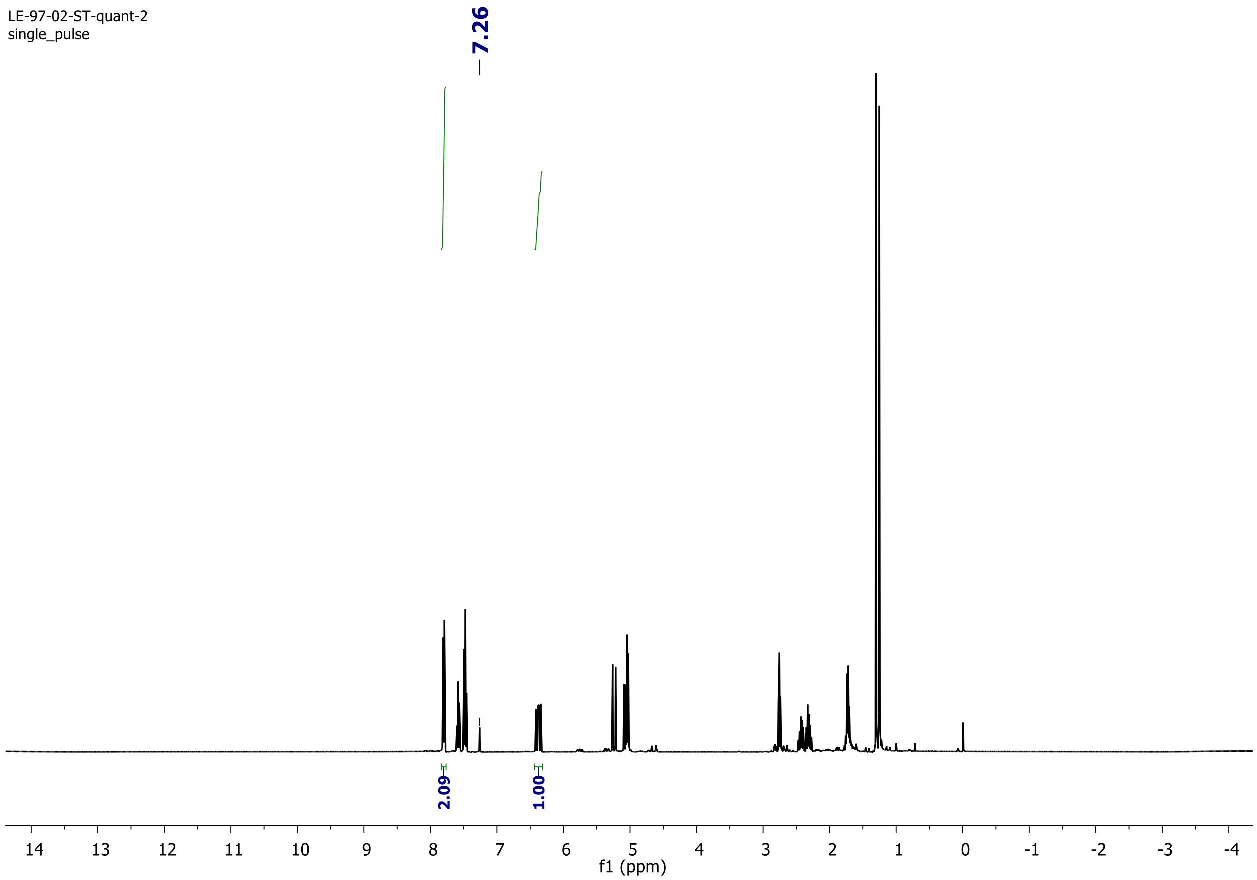


Fig. S16 ^{1}H NMR for purity quantification of myrcene epoxide **10** (11.4 mg) with benzophenone used as standard (11.3 mg). CDCl3 was used as deuterated solvent and the spectrum was referenced to its residual peak. m/m purity for myrcene epoxide was found to be of 85%.

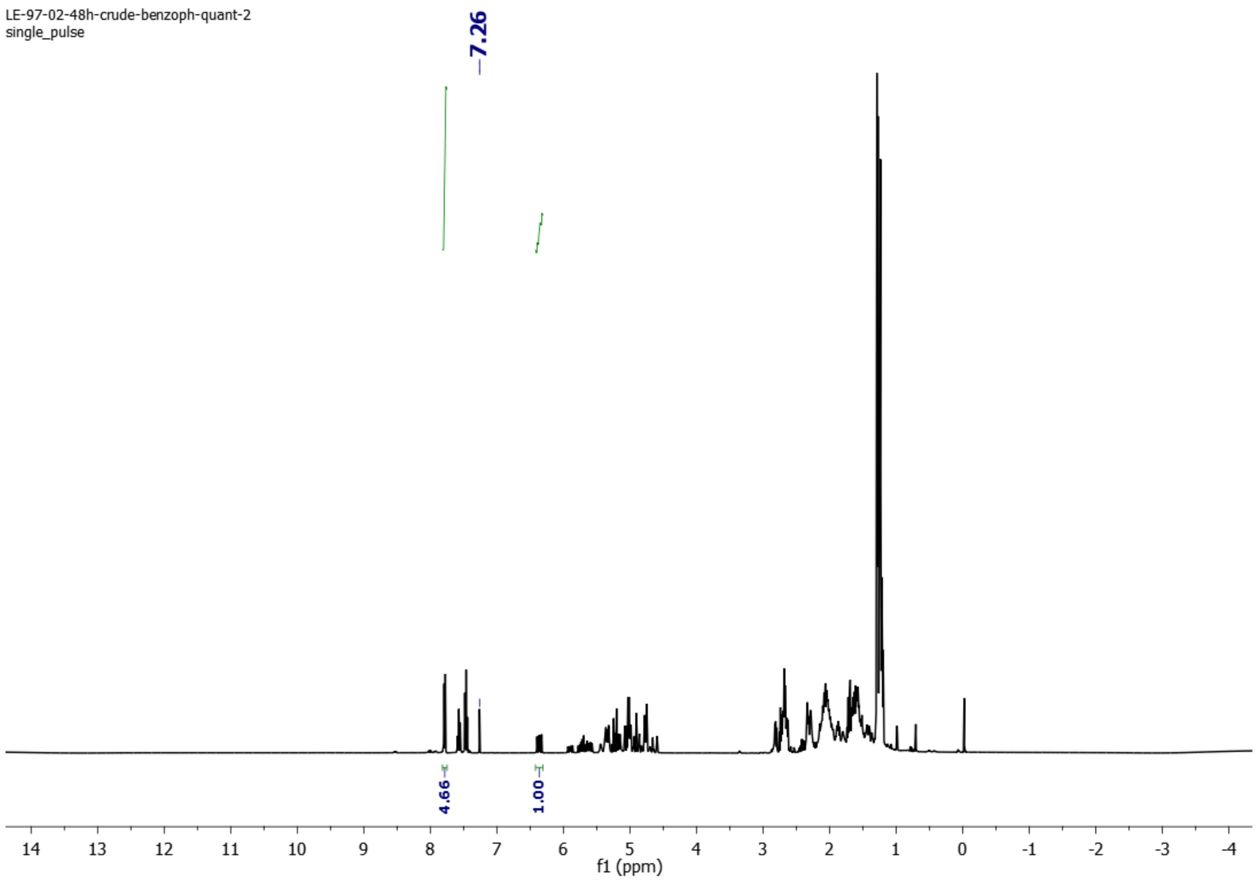


Fig. S17 [1]H NMR for quantification of unreacted myrcene epoxide **10** on the crude mixture after irradiation λ = 365 nm for 48 h (49.5 mg of crude sample) with benzophenone used as standard (4.1 mg). $CDCl_3$ was used as deuterated solvent and the spectrum was referenced to its residual peak. The unreacted myrcene epoxide **10** was found to be of 6.7 wt%.

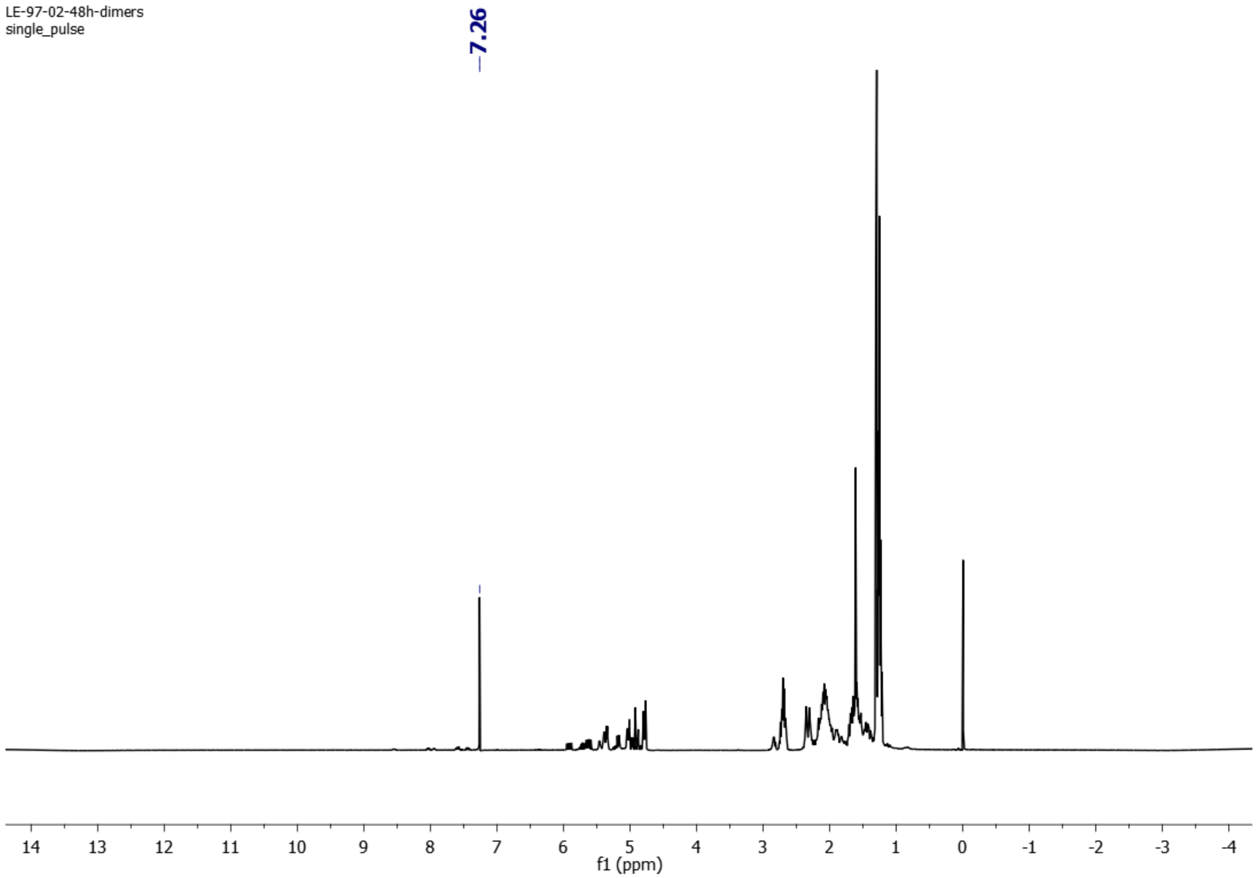


Fig. S18 ^{1}H NMR of dimers produced through myrcene epoxide **10** dimerization (λ = 365 nm, t = 48 h). The light fraction was removed by distillation under reduced pressure. $CDCl_3$ was used as deuterated solvent and the spectrum was referenced to its residual peak.

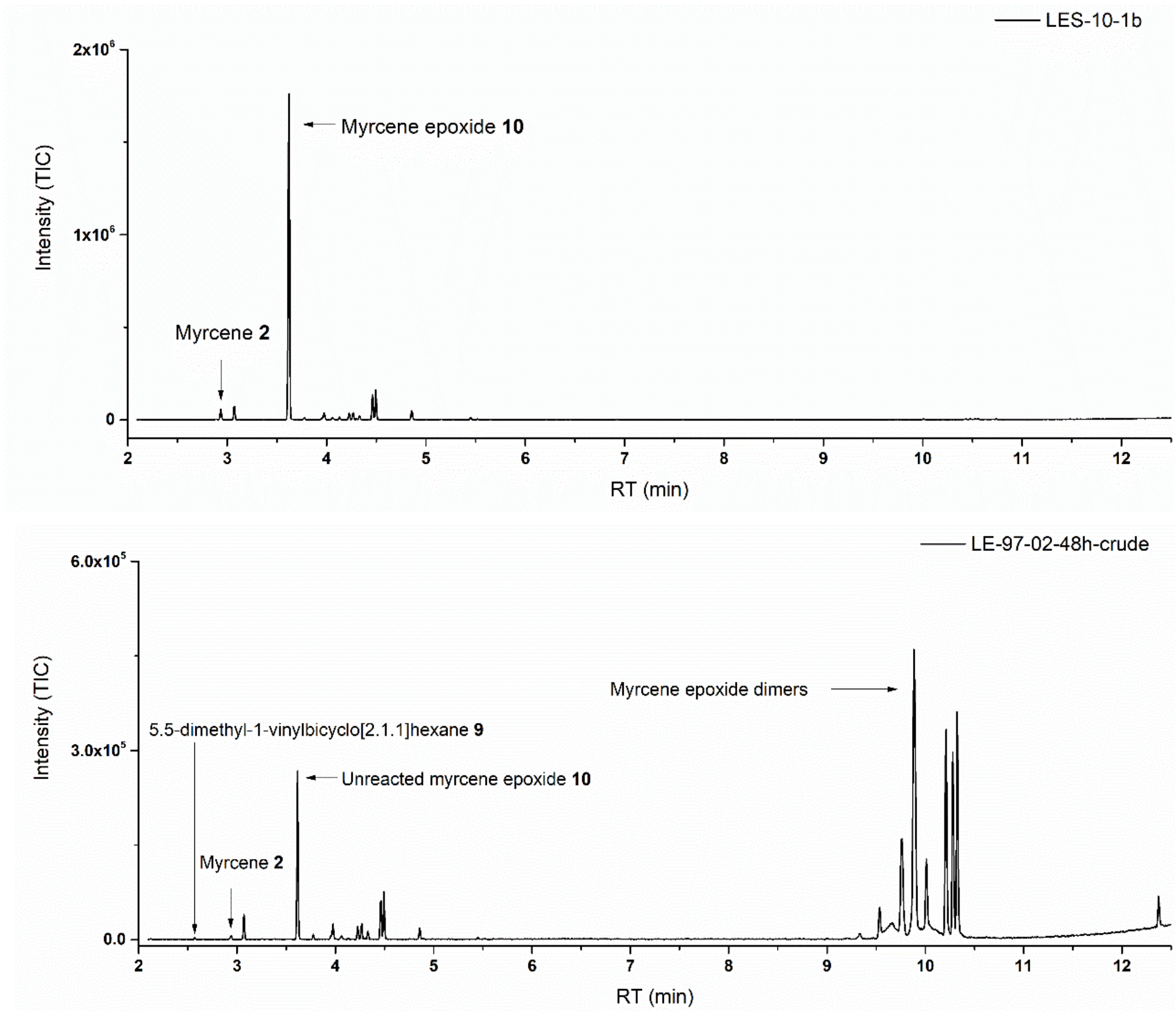
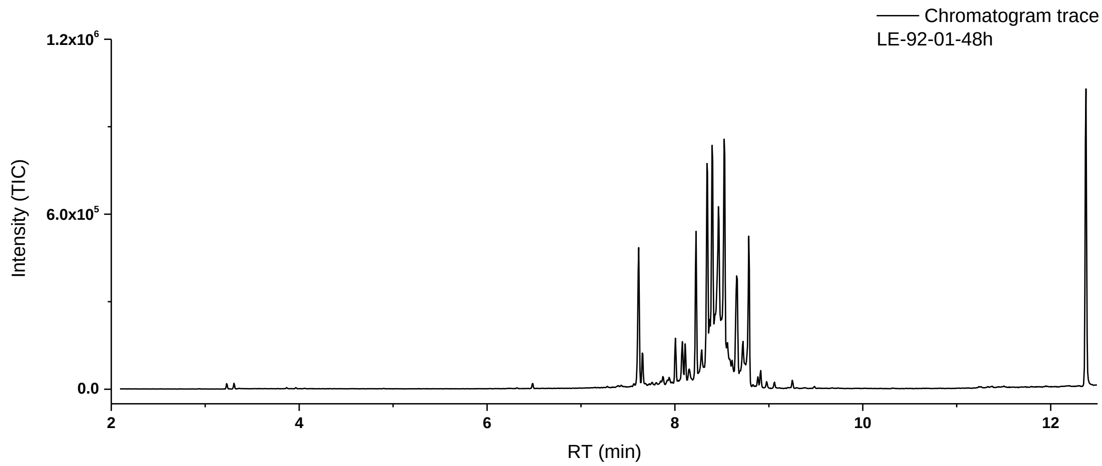


Fig. S19 Chromatogram trace for myrcene epoxide **10** starting material (**top**) and 48 h irradiated crude mixture of **10** with **8** (λ = 365 nm, t = 48 h, **bottom**). A small amount of myrcene remained after epoxidation and can be seen on the starting material chromatogram (**top**) which is partially converted to the small amount of 5,5-dimethyl-1-vinylbicyclo[2.1.1]hexane **9** on the crude reacted mixture (**bottom**). These chromatograms also show that the impurities from the epoxidation reaction remained unreacted.

Ocimene dimerization



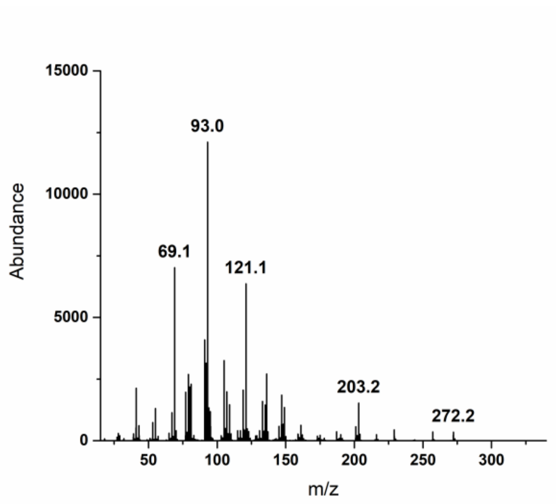


Fig. S20 Top: GC-MS chromatogram of dimers produced in the ocimene **3** dimerization (λ = 365 nm, t = 48 h). The light fraction was removed by distillation under reduced pressure. **Bottom:** Mass spectrum of dimers.

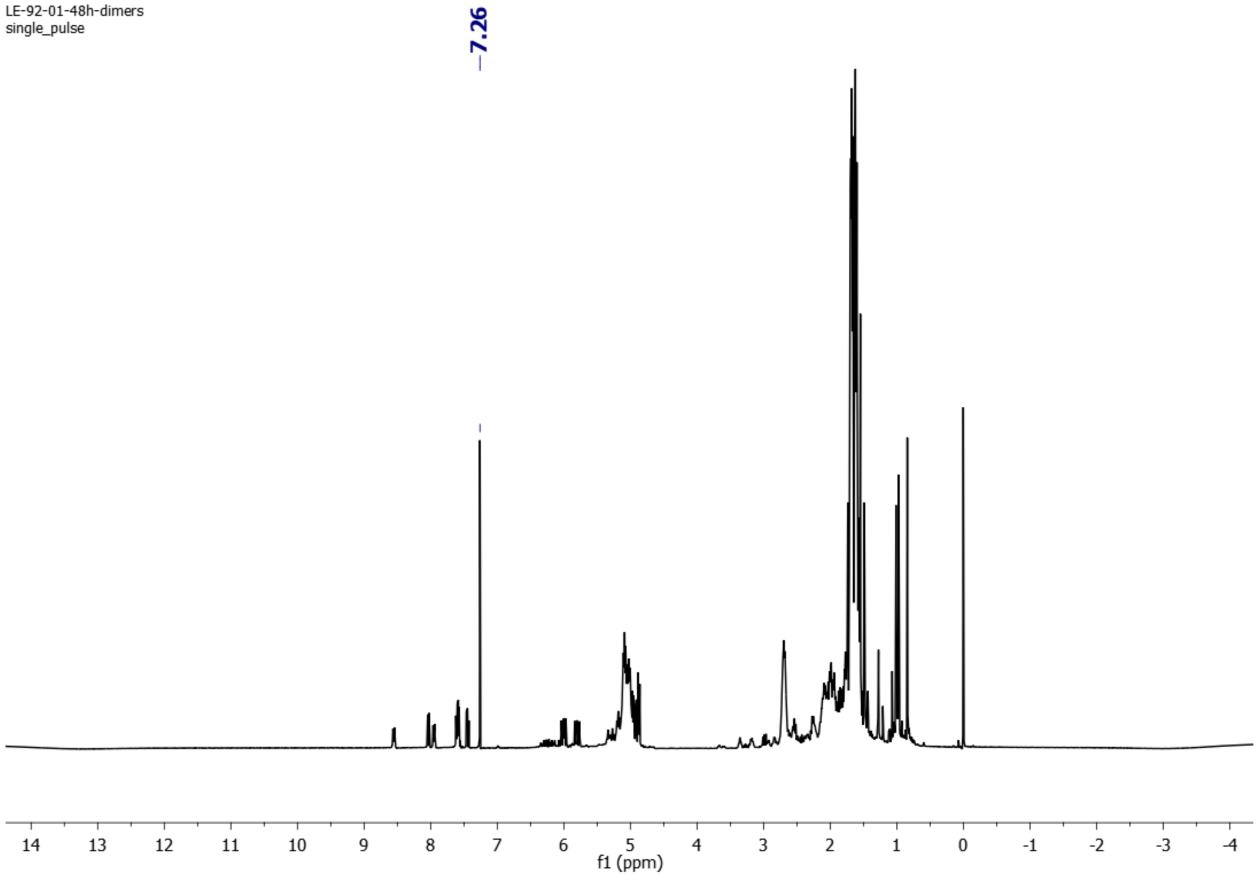


Fig. S21 [1]H NMR spectrum of dimers produced in the ocimene **3** dimerization (λ = 365 nm, t = 48 h). The light fraction was removed by distillation under reduced pressure. $CDCl_3$ was used as deuterated solvent and the spectrum was referenced to its residual peak.

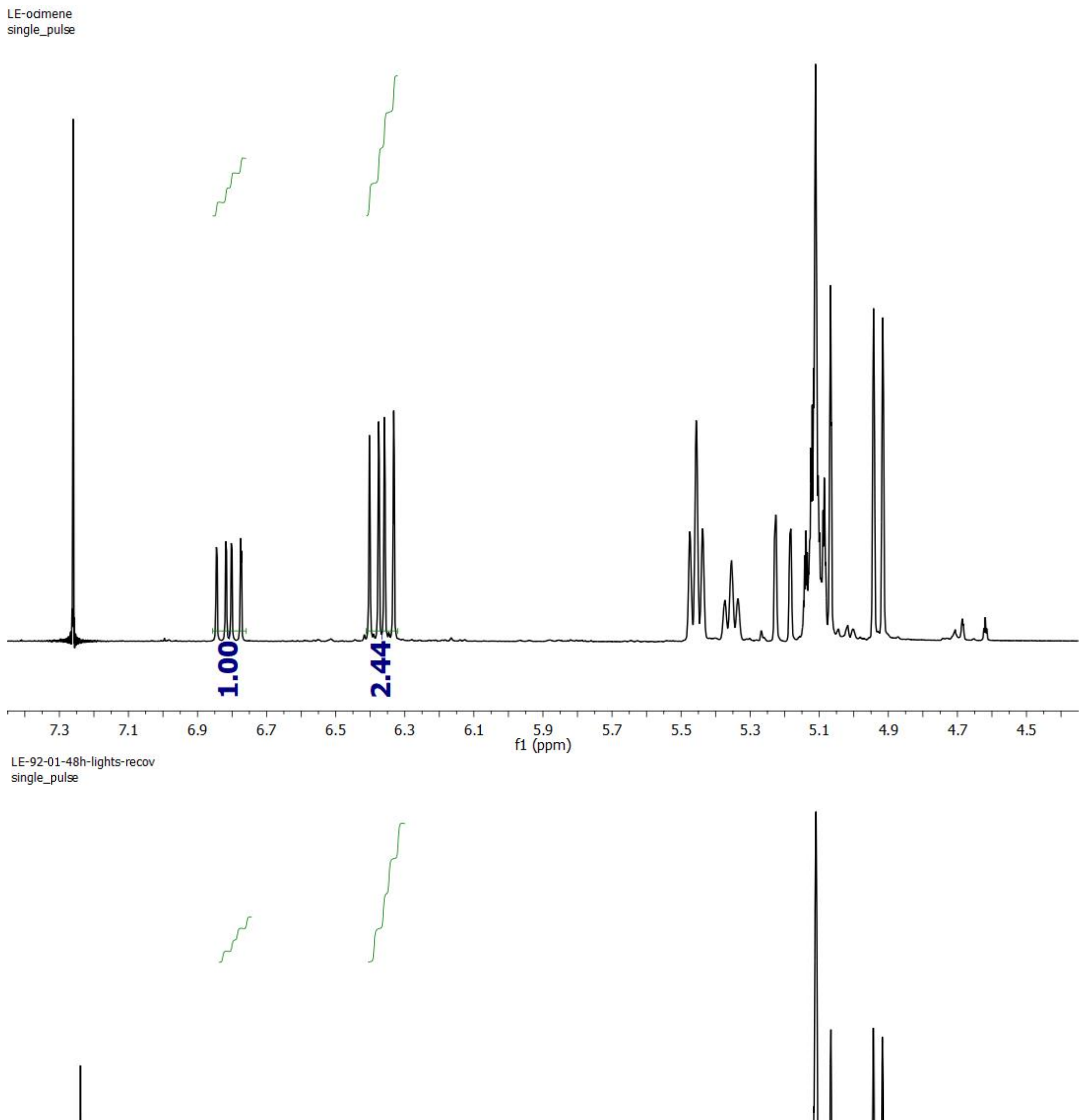


Fig. S22 ^{1}H NMR spectra of ocimene **3** before (**top**) and after irradiation (**bottom**), λ = 365 nm, t = 48 h. The *E*/*Z* ratio of ocimene was calculated based on the integrals showed on the spectra, for the proton of the conjugated diene moiety. The *E*-isomer has chemical shift at 6.35 ppm, and the *Z*-isomer has chemical shift at 6.80.

Light intensity experiments

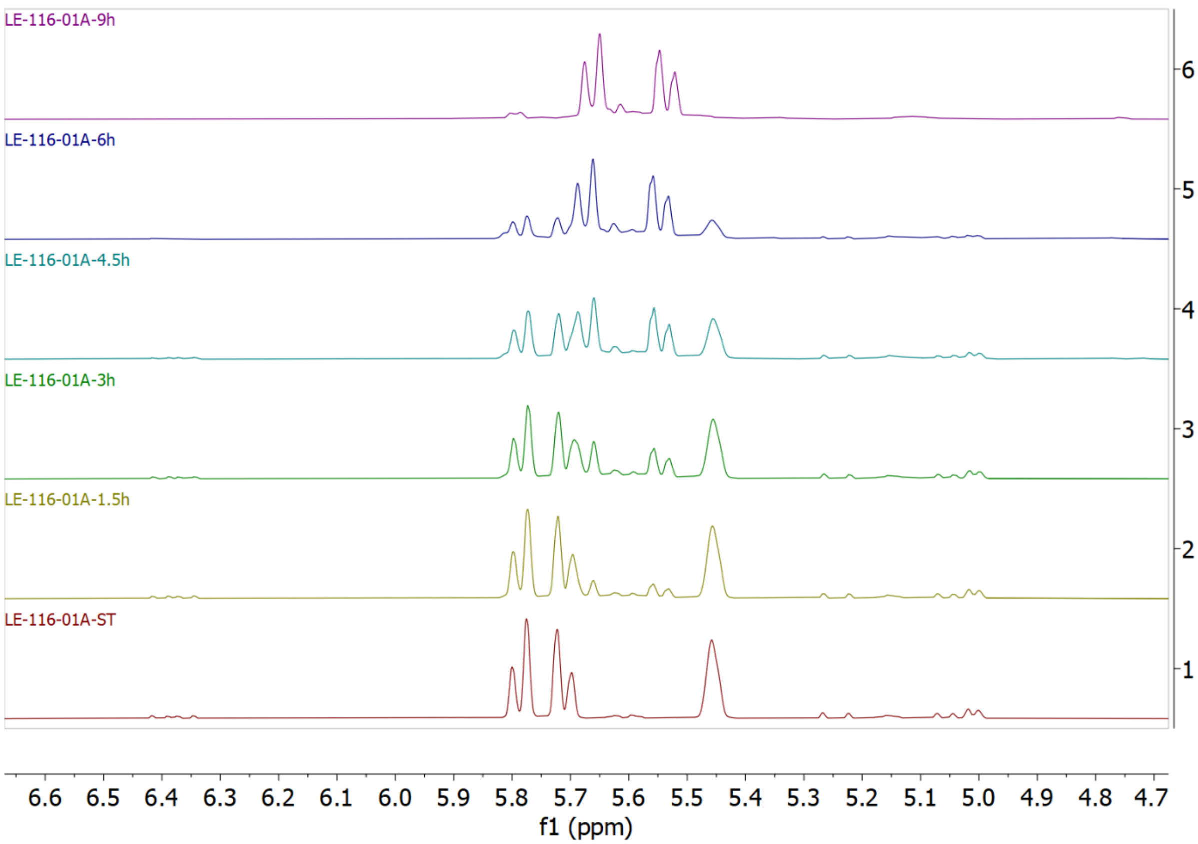


Fig. S23 ^{1}H NMR spectra of crude mixture of α-phellandrene and 0.2 mol% of **8**, in different irradiation times. Light intensity: 6.5 mW s^{-2}.

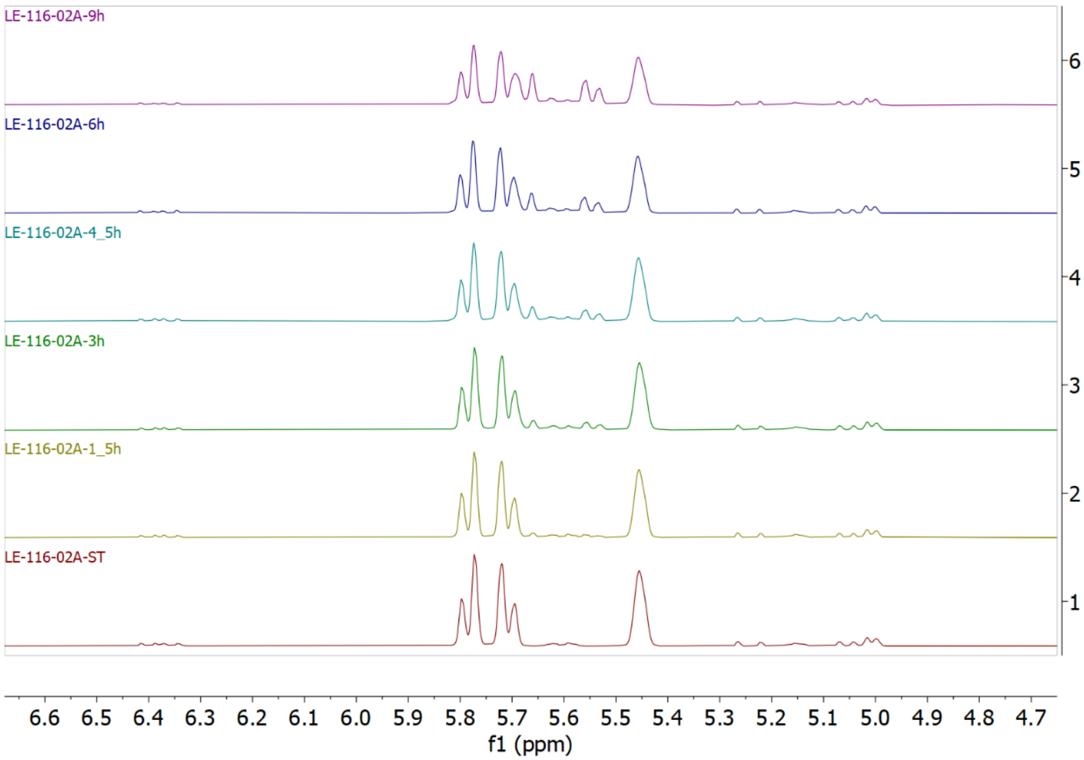


Fig. S24 ^{1}H NMR spectra of crude mixture of α-phellandrene and 0.2 mol% of **8**, in different irradiation times. Light intensity: 2.0 mW s^{-2}.

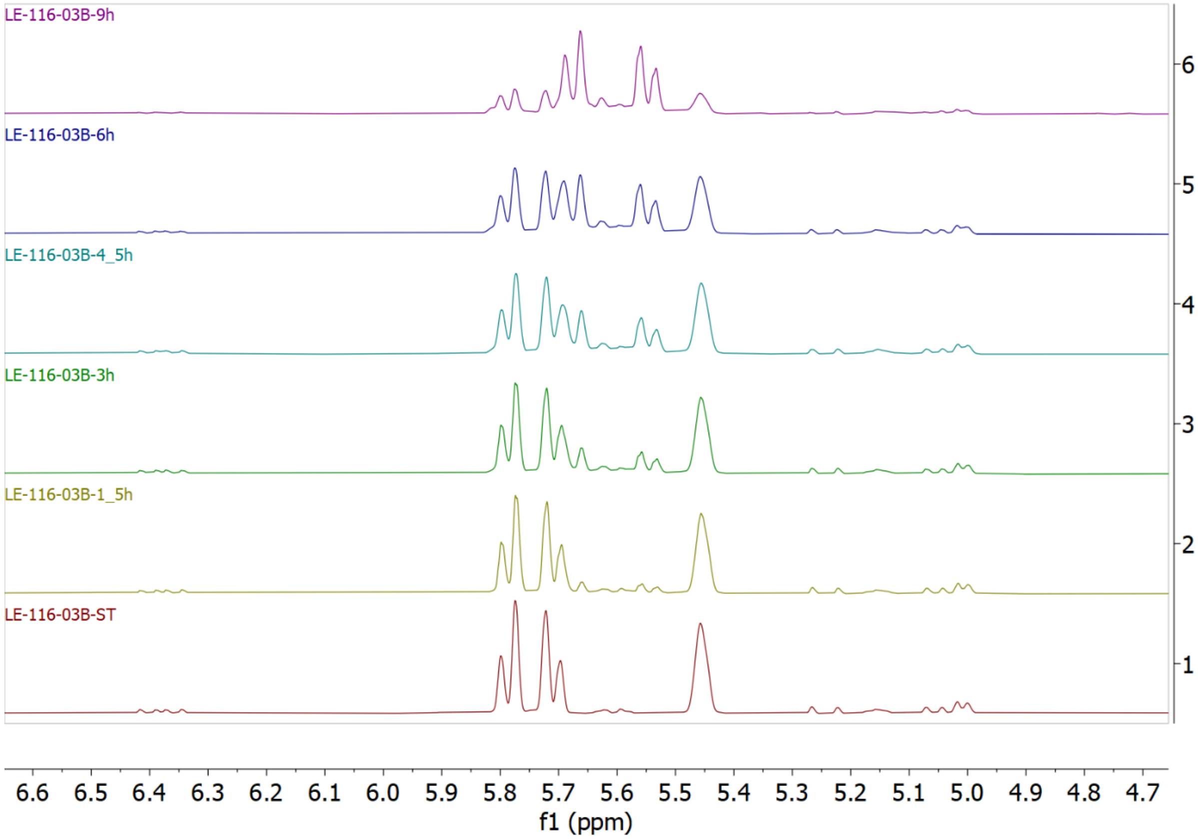


Fig. S25 ^{1}H NMR spectra of crude mixture of α-phellandrene and 0.2 mol% of **8**, in different irradiation times. Light intensity: 4.0 mW s^{-2}.

Cross-dimerization with α-phellandrene

Myrcene and α-phellandrene

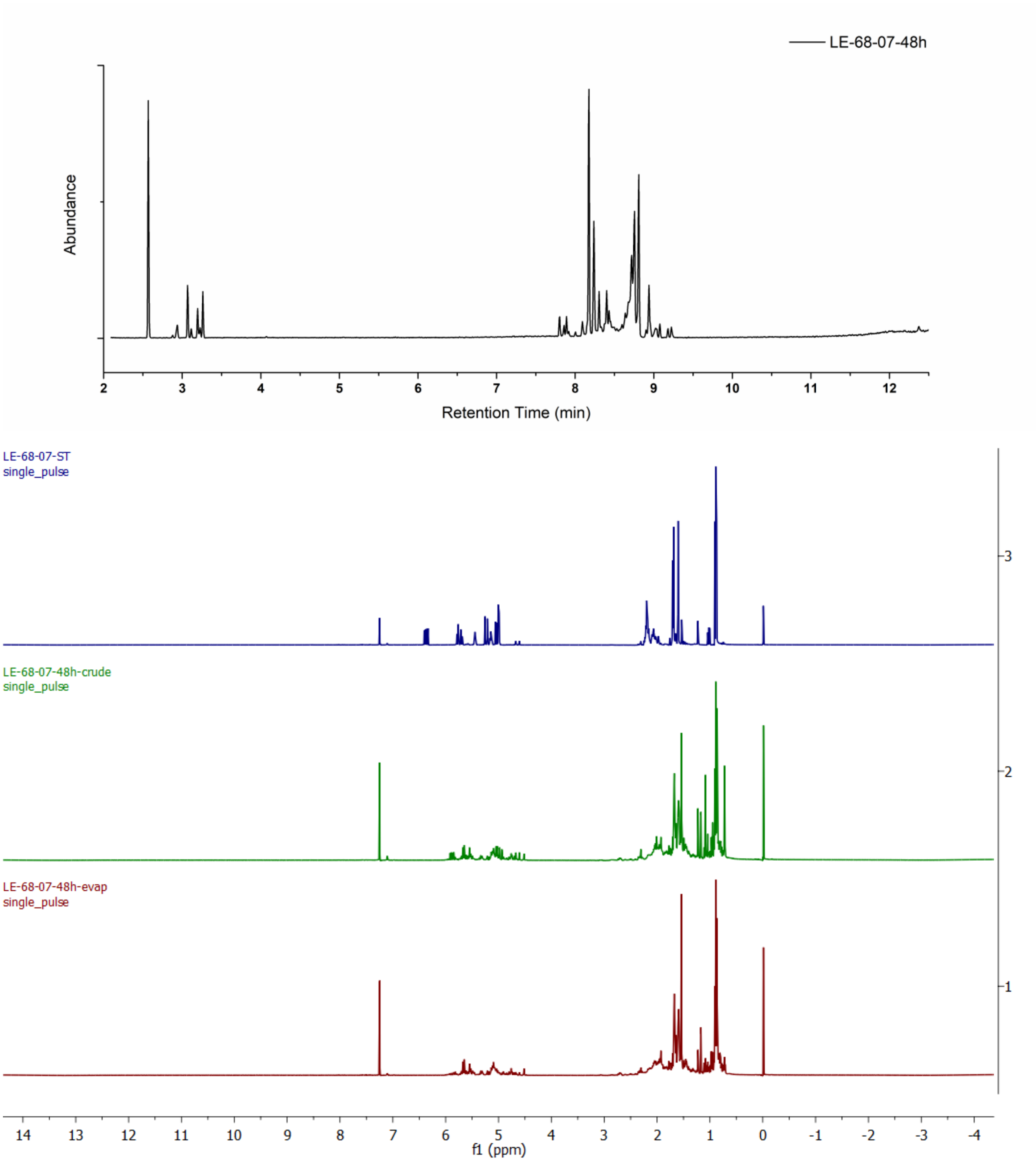


Fig. S26 Cross-dimerization between α-phellandrene **1** and myrcene **2** (coiled FEP tubing, λ = 365 nm, t = 48 h, 1:1 equivalent). **Top:** GC-MS trace of crude sample after irradiation. **Bottom:** ^{1}H NMR spectra of sample before irradiation (blue), mixture after irradiation (green) and dimers (red) after distilation of C10 fraction.

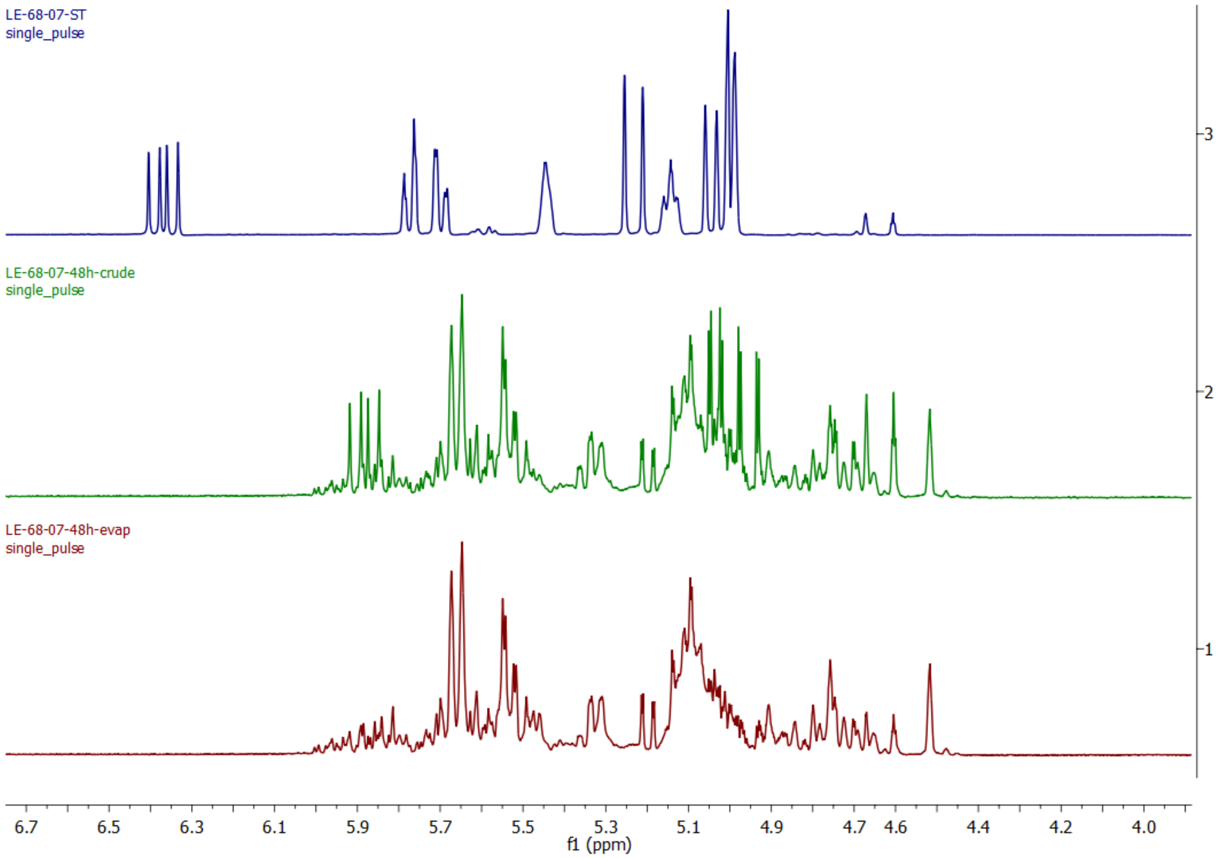
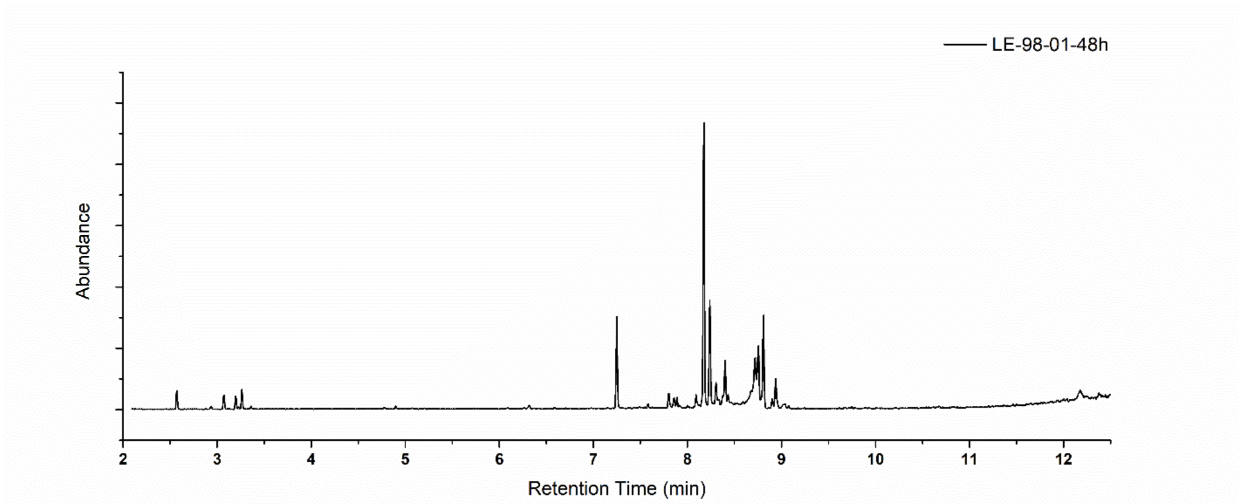


Fig. S27 Cross-dimerization between α-phellandrene **1** and myrcene **2** (coiled FEP tubing, 1:1 equivalent, $\lambda = 365$ nm, t = 48 h). Expansion of ^{1}H NMR spectra of sample before irradiation (**top**), crude mixture after irradiation (**middle**) and dimers (**bottom**) after distilation of C_{10} fraction (see Fig. S16, bottom). Green trace (**middle**) reveals that no myrcene was detected after irradiation.



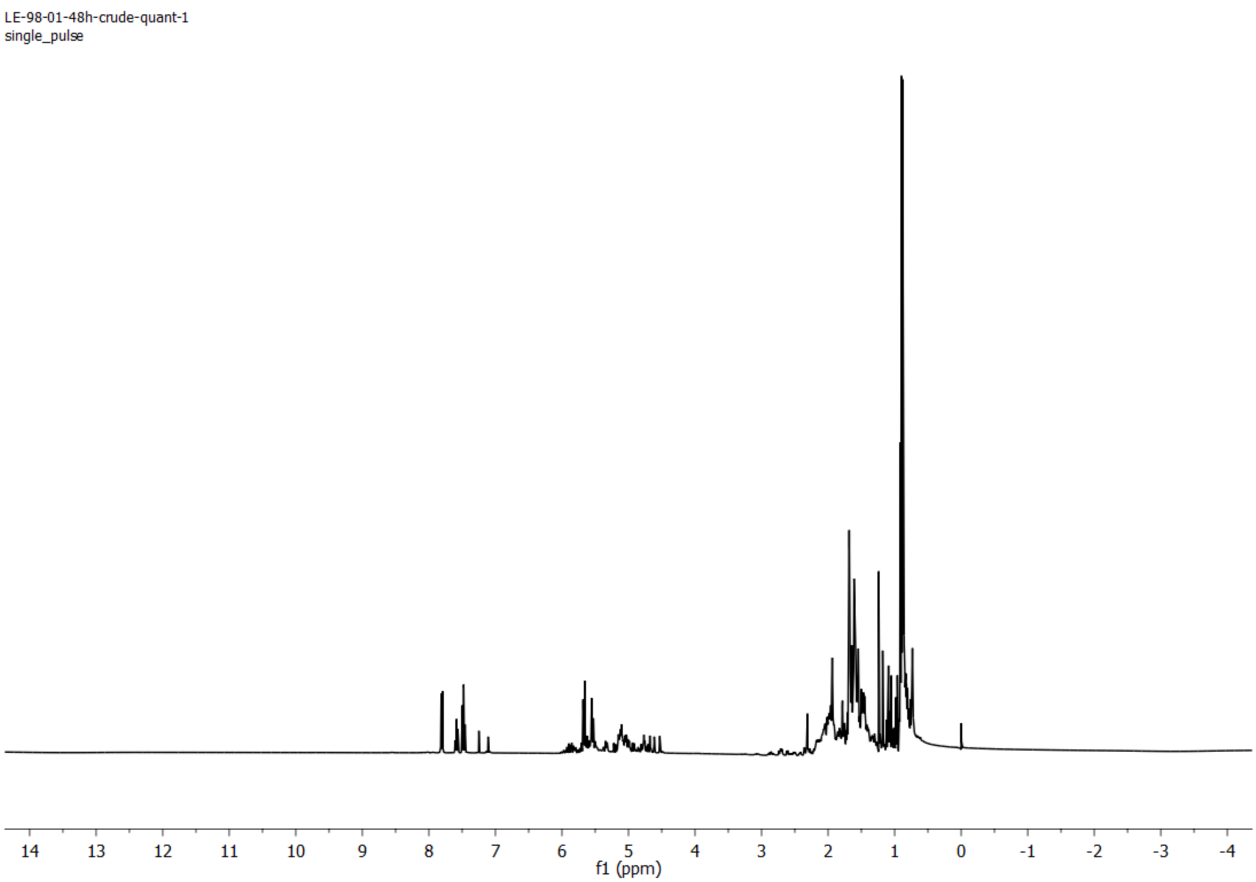


Fig. S28 Cross-dimerization between α-phellandrene **1** and myrcene **2** (coiled FEP tubing, 1:0.5 equivalent, λ = 365 nm, t = 48 h). **Top:** GC-MS trace of crude sample after irradiation. **Bottom:** ^{1}H NMR spectrum of crude sample after irradiation. Signals between 7.5 and 8.0 ppm are related to benzophenone added to the NMR sample as external standard for qNMR.

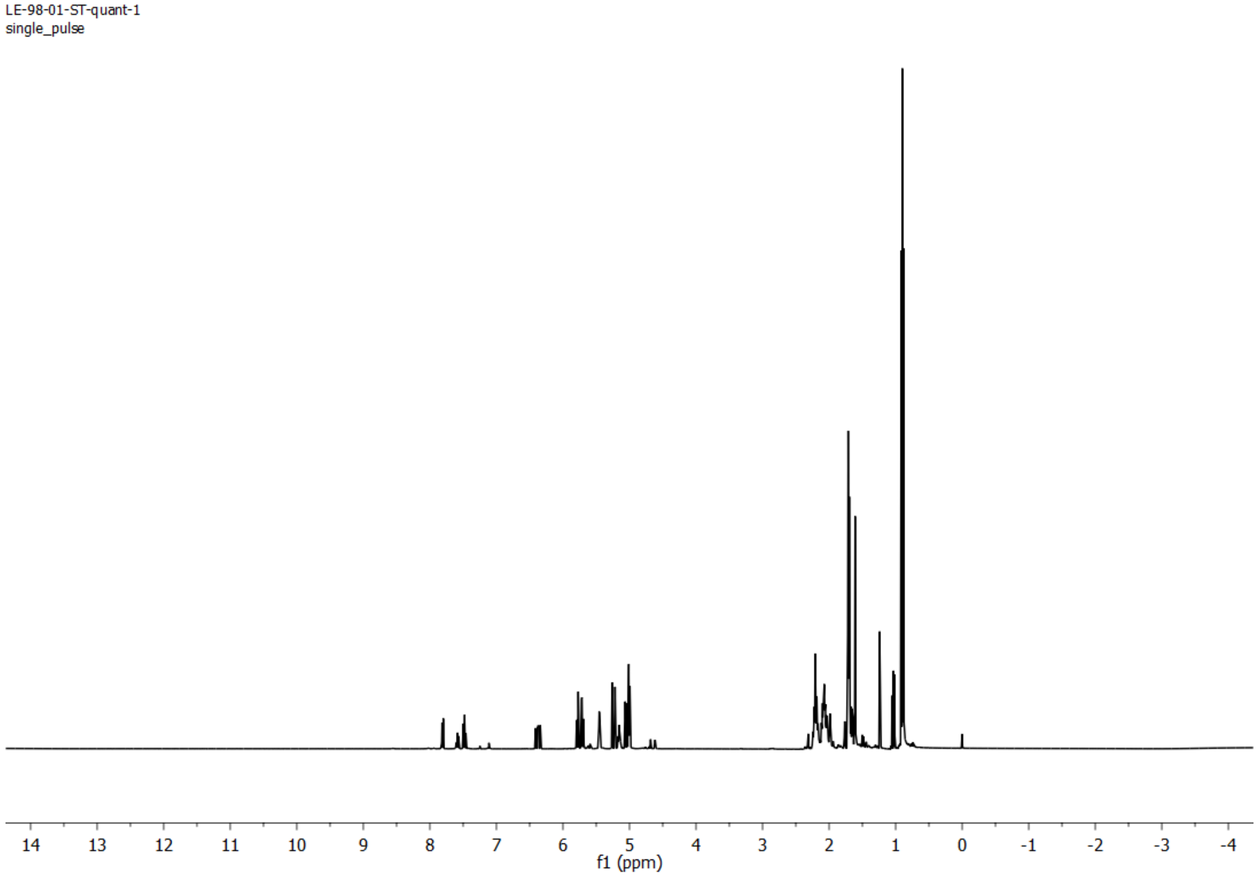


Fig. S29 Cross-dimerization between α-phellandrene **1** and myrcene **2** (coiled FEP tubing, 1:0.5 equivalent). ^{1}H NMR spectrum of sample before irradiation. Signals between 7.5 and 8.0 ppm are related to benzophenone added to the NMR sample as external standard for qNMR.

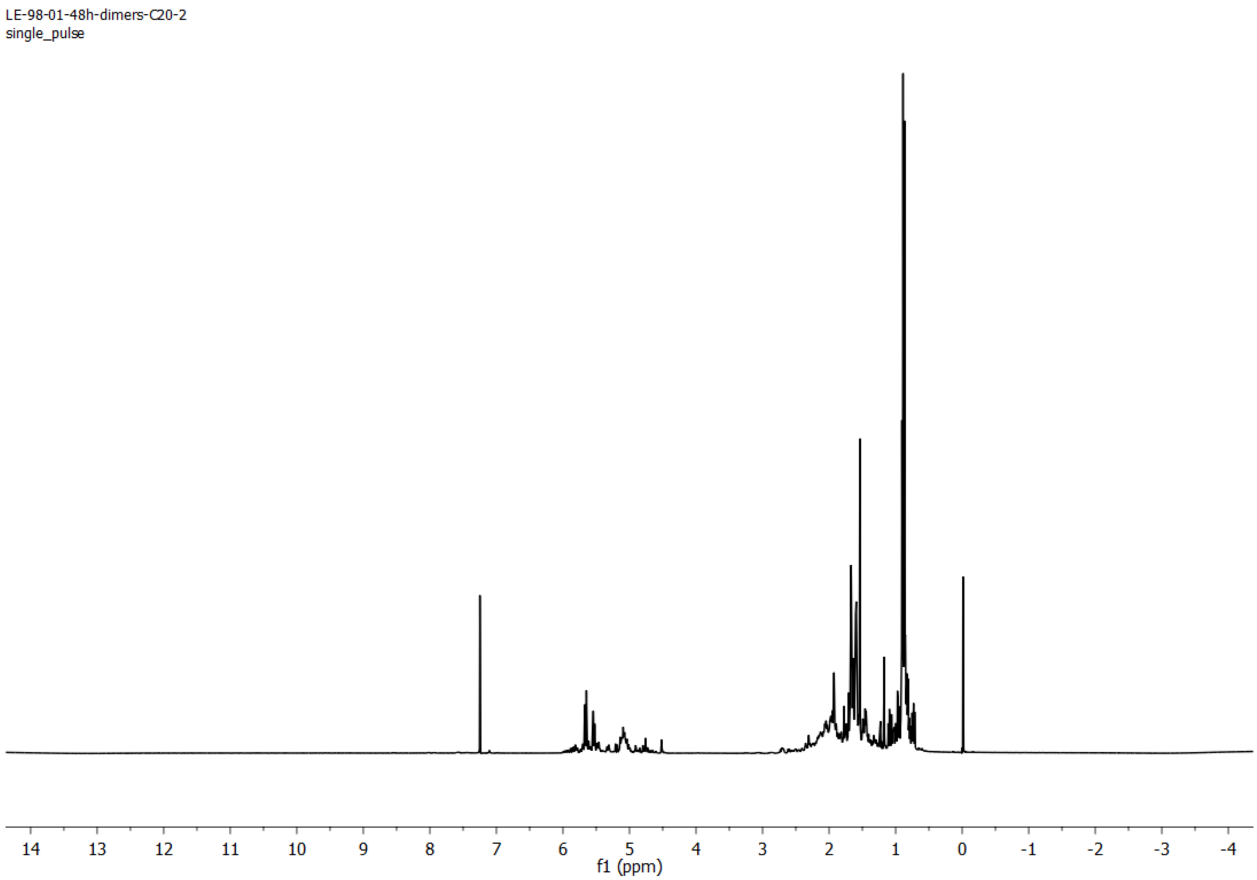


Fig. S30 Cross-dimerization between α-phellandrene **1** and myrcene **2** (coiled FEP tubing, 1:0.5 equivalent, λ = 365 nm, t = 48 h). ^{1}H NMR spectrum of dimers after C_{10} fraction evaporation.

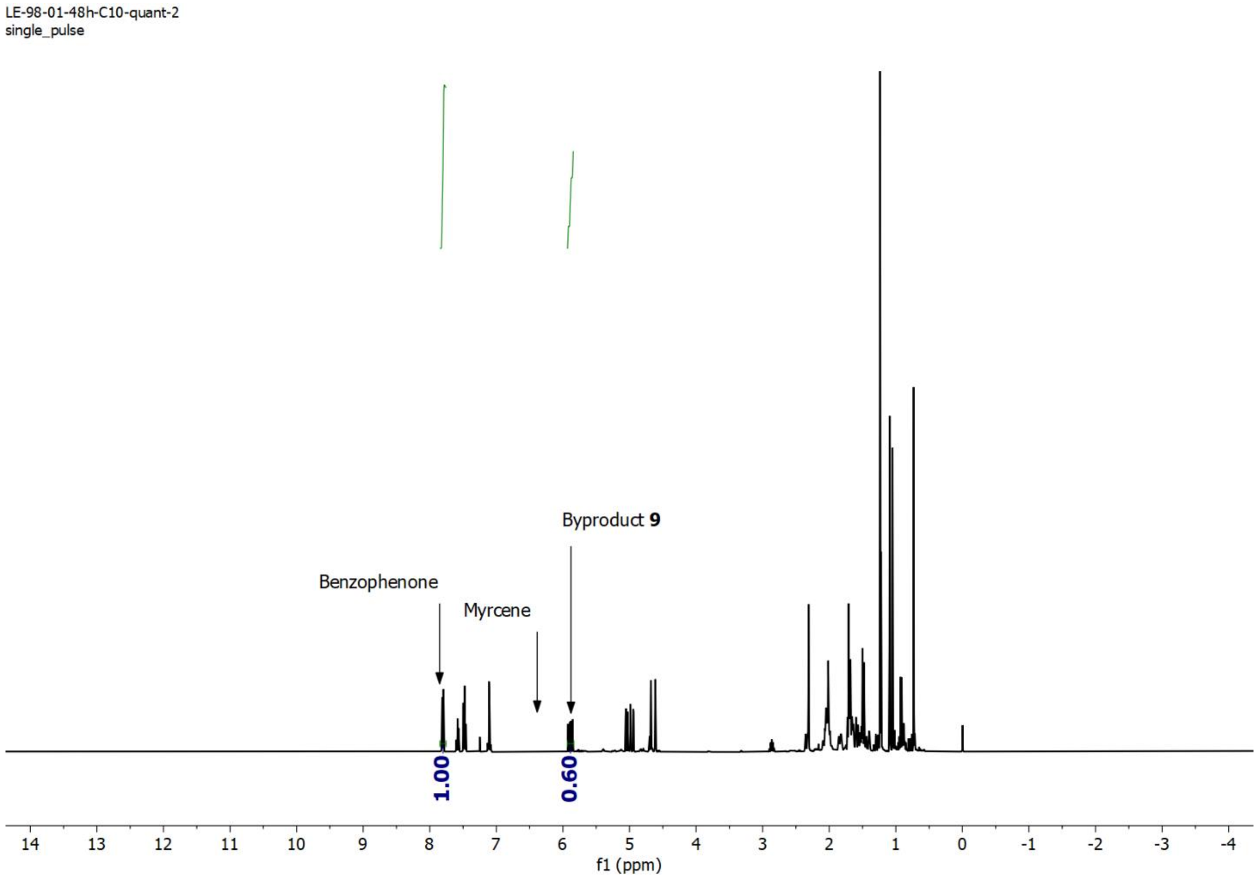
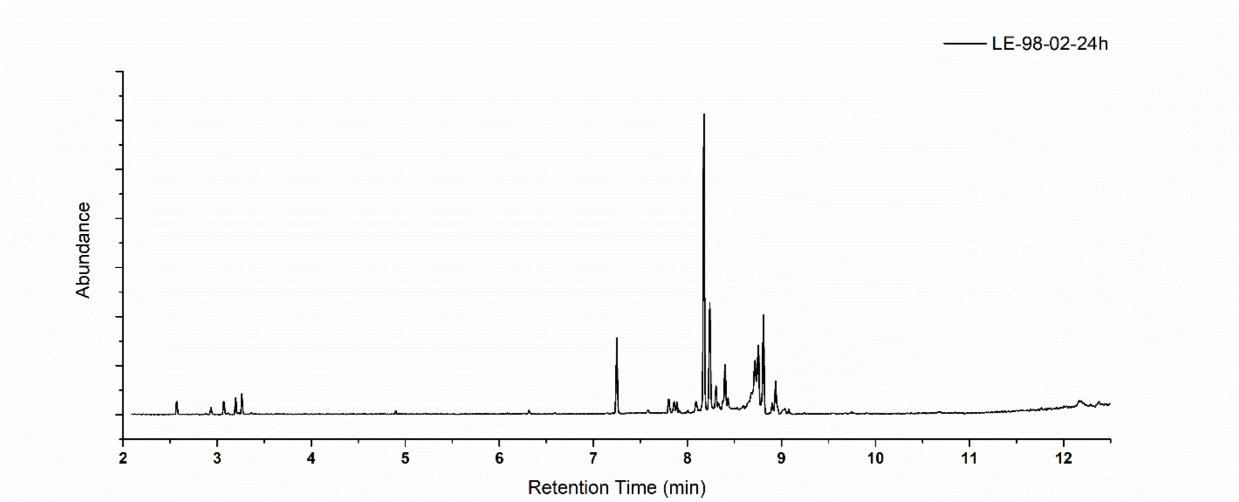


Fig. S31 Cross-dimerization between α-phellandrene **1** and myrcene **2** (coiled FEP tubing, 1:0.5, equivalent, λ = 365 nm, t = 48 h). ^{1}H NMR spectrum of recovered C_{10} fraction after irradiation. Benzophenone (8.0 mg) was added to 52.6 mg of sample as external standard for qNMR.



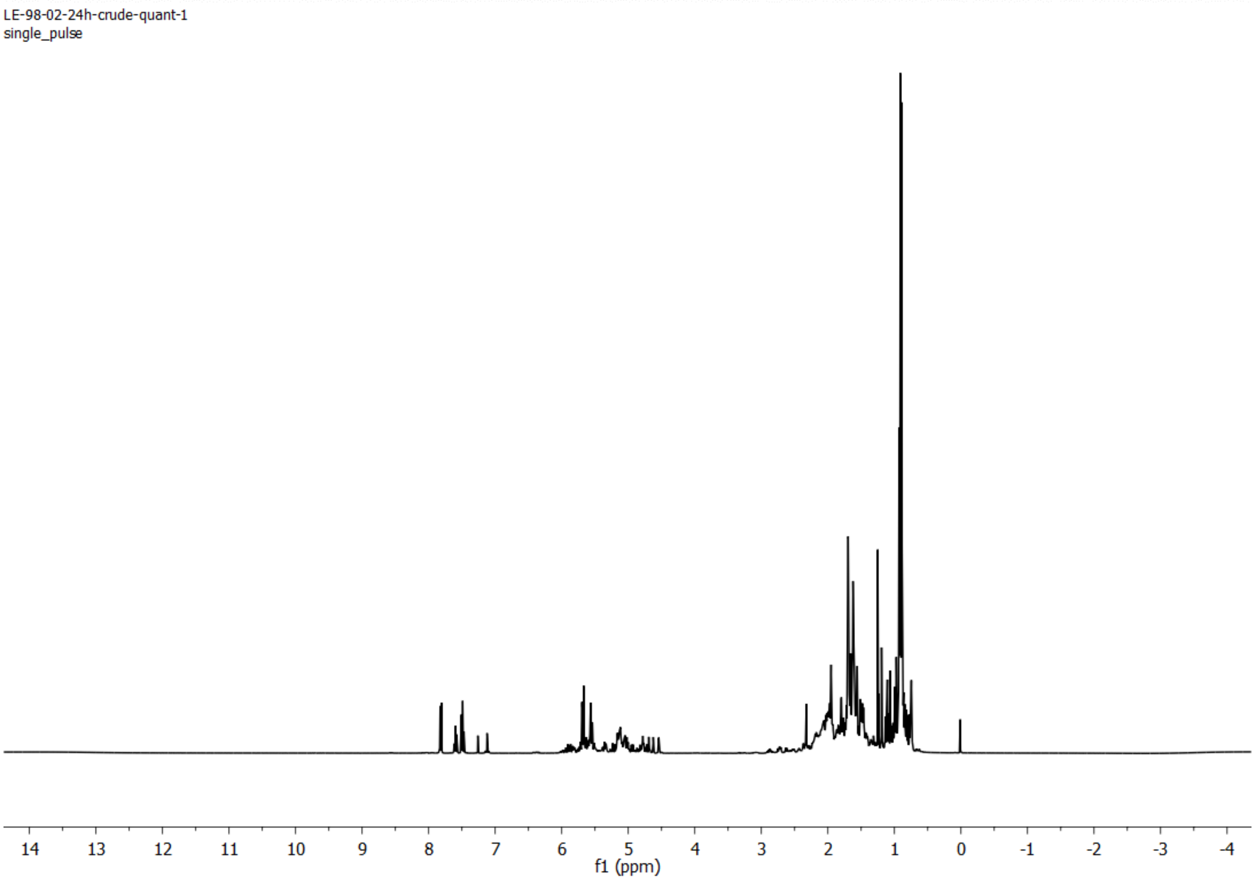


Fig. S32 Cross-dimerization between α-phellandrene **1** and myrcene **2** (coiled FEP tubing, 1:0.5, equivalent, $\lambda = 365$ nm, t = 24 h. **Top:** GC-MS trace of crude sample after irradiation. **Bottom:** ^{1}H NMR spectrum of crude sample after irradiation. Signals between 7.5 and 8.0 ppm are related to benzophenone added to the NMR as external standard for qNMR.

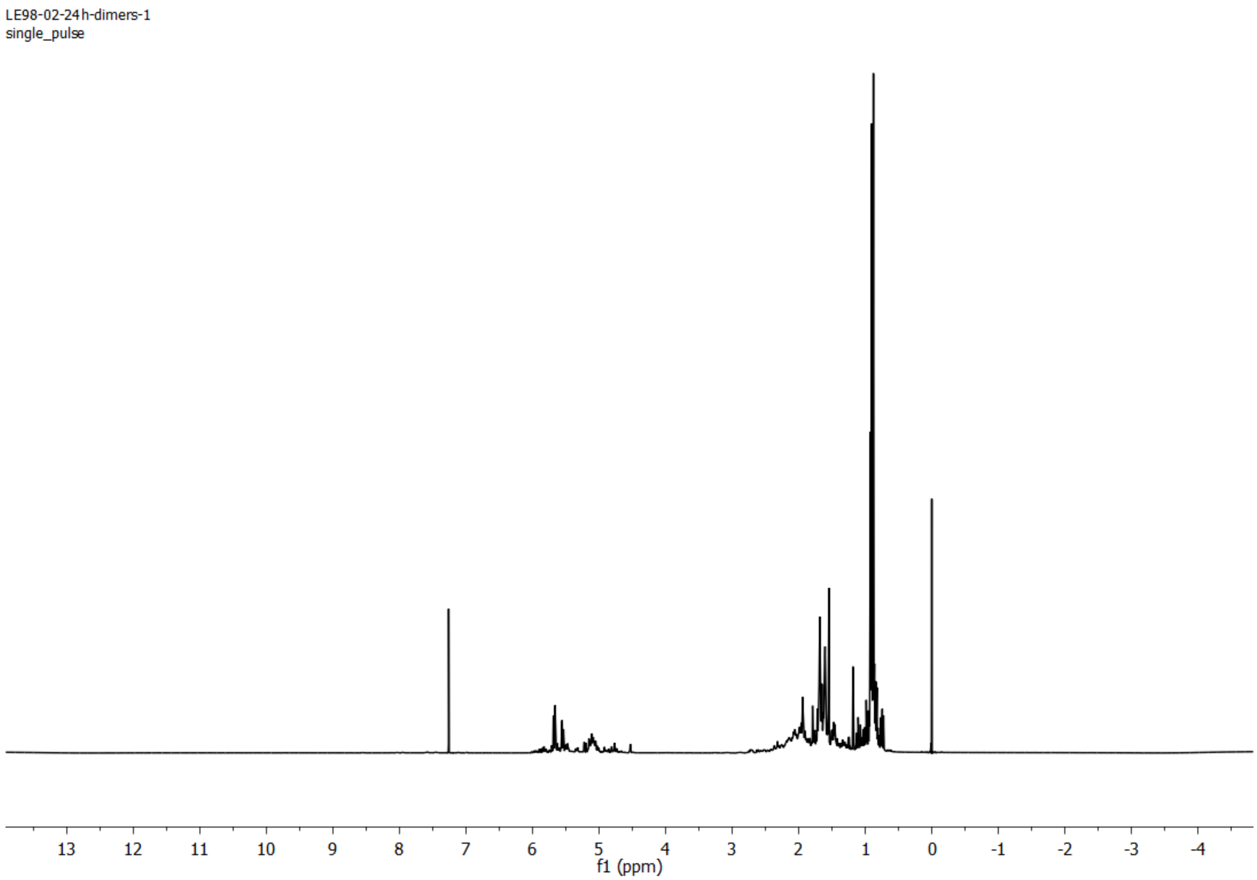


Fig. S33 Cross-dimerization between α-phellandrene **1** and myrcene **2** (coiled FEP tubing, 1:0.5, equivalent, λ = 365 nm, t = 24 h). ^{1}H NMR spectrum of dimers after C_{10} fraction evaporation.

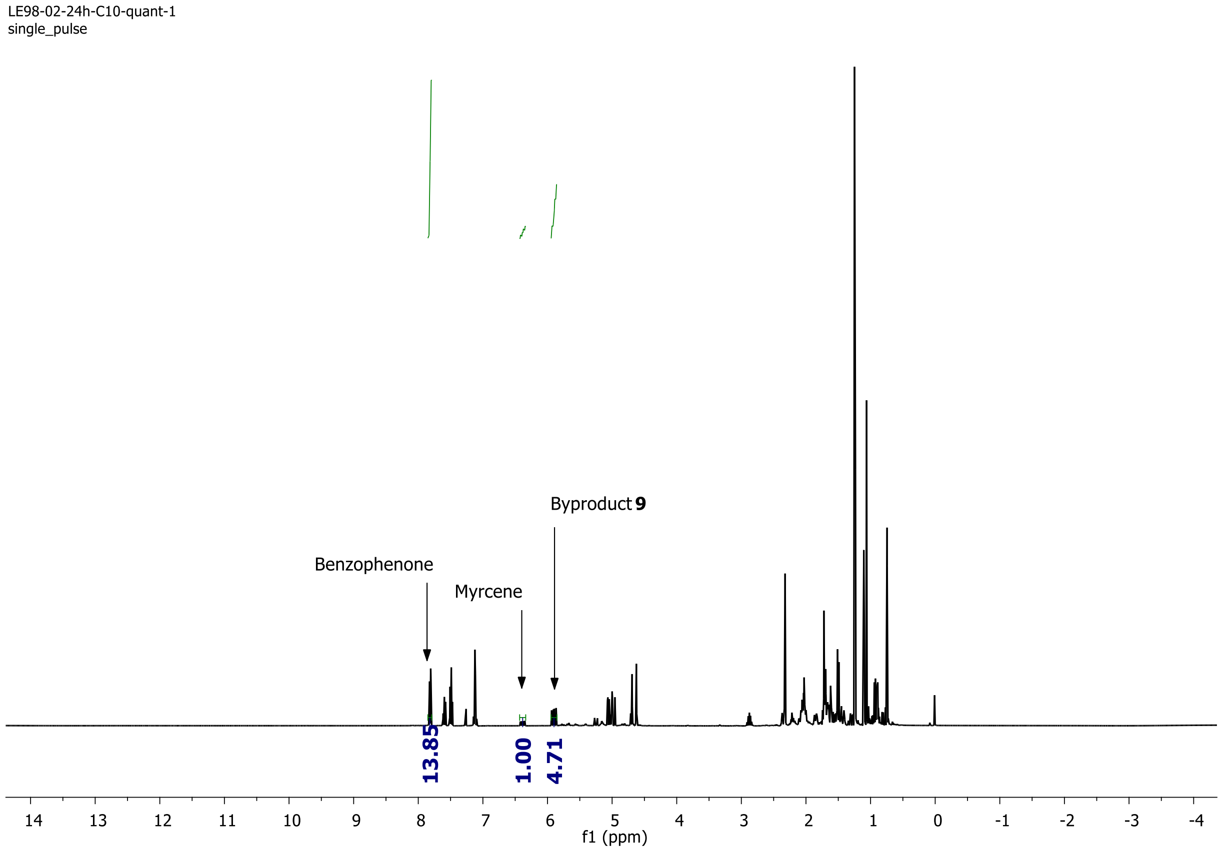


Fig. S34 Cross-dimerization between α-phellandrene **1** and myrcene **2** (coiled FEP tubing, 1:0.5, equivalent, λ = 365 nm, t = 24 h). ^{1}H NMR spectrum of recovered C_{10} fraction after irradiation. Benzophenone (7.1 mg) was added to 45.1 mg of sample as external standard for qNMR.

Ocimene and α-phellandrene

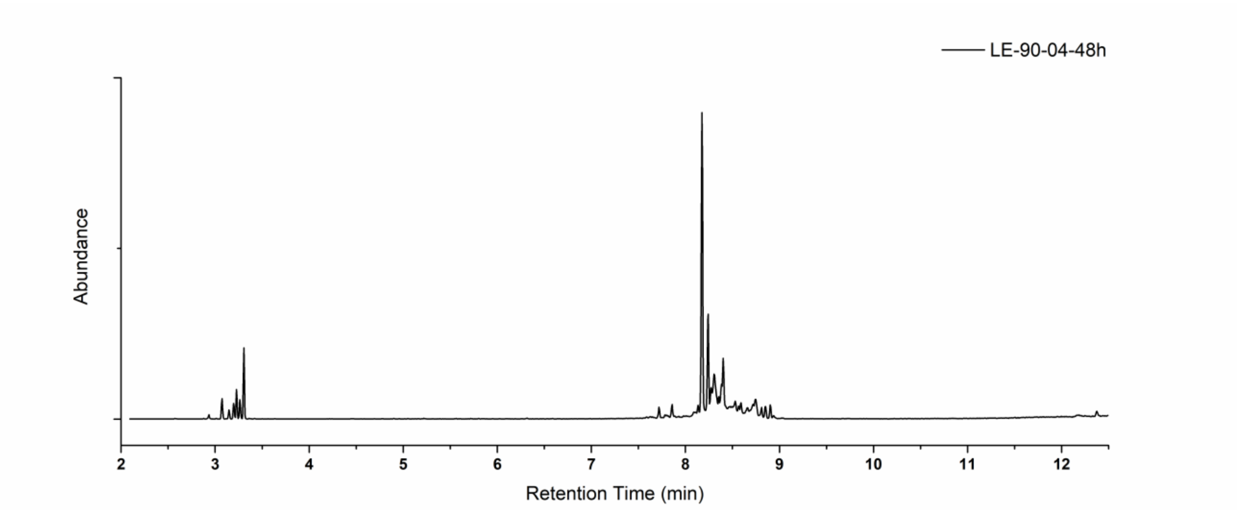


Fig. S35 Cross-dimerization between α-phellandrene **1** and ocimene **3** (coiled FEP tubing, 1:0.5, equivalent, λ = 365 nm, t = 48 h). GC-MS trace of crude sample after irradiation.

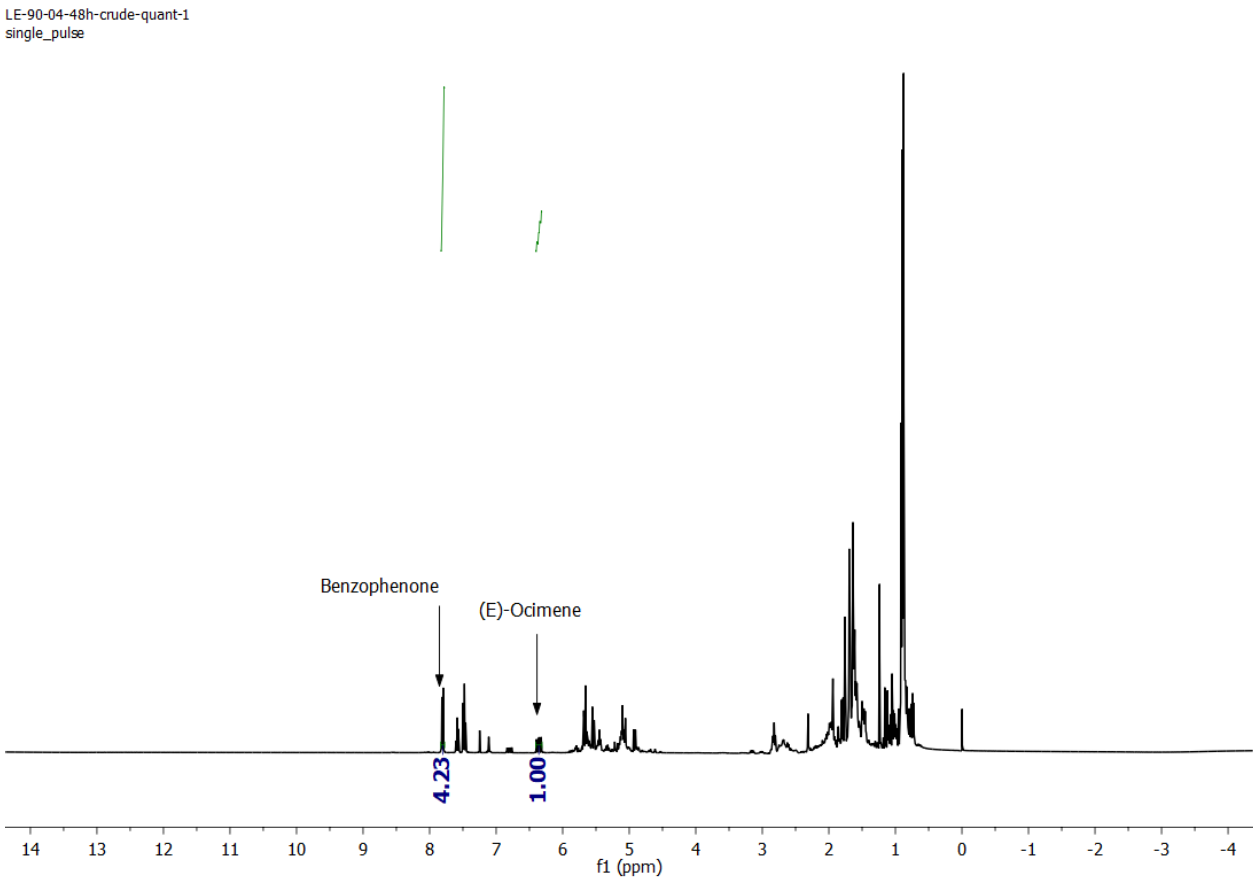


Fig. S36 Cross-dimerization between α-phellandrene **1** and ocimene **3** (coiled FEP tubing, 1:0.5 equivalent, λ = 365 nm, t = 48 h). ^{1}H NMR spectrum of crude mixture after irradiation. Benzophenone (5.6 mg) was added to 64.4 mg of sample as external standard for qNMR.

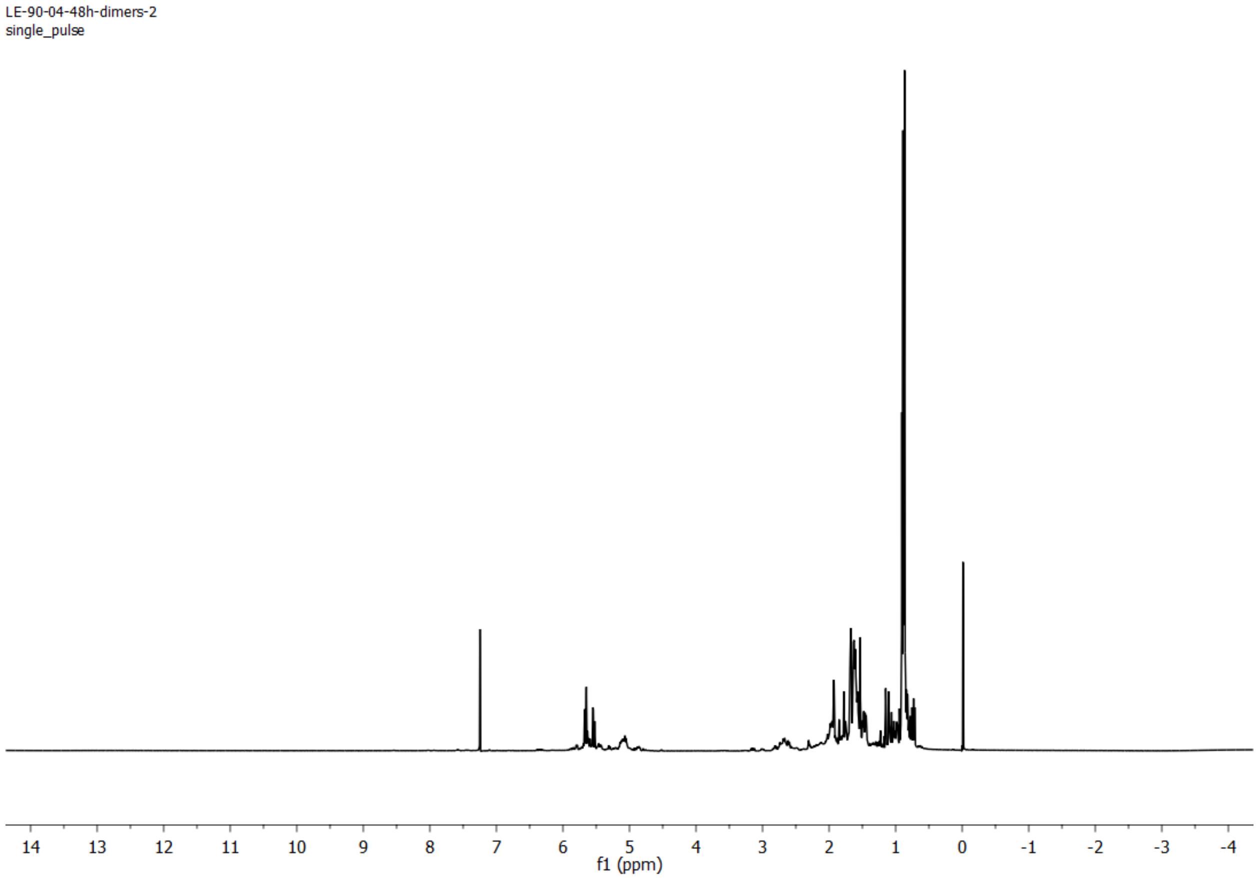


Fig. S37 Cross-dimerization between α-phellandrene and ocimene (coiled FEP tubing, 1:0.5, equivalent, λ = 365 nm, t = 48 h). ^{1}H NMR spectrum of dimers after C_{10} fraction evaporation.

Ginger oil

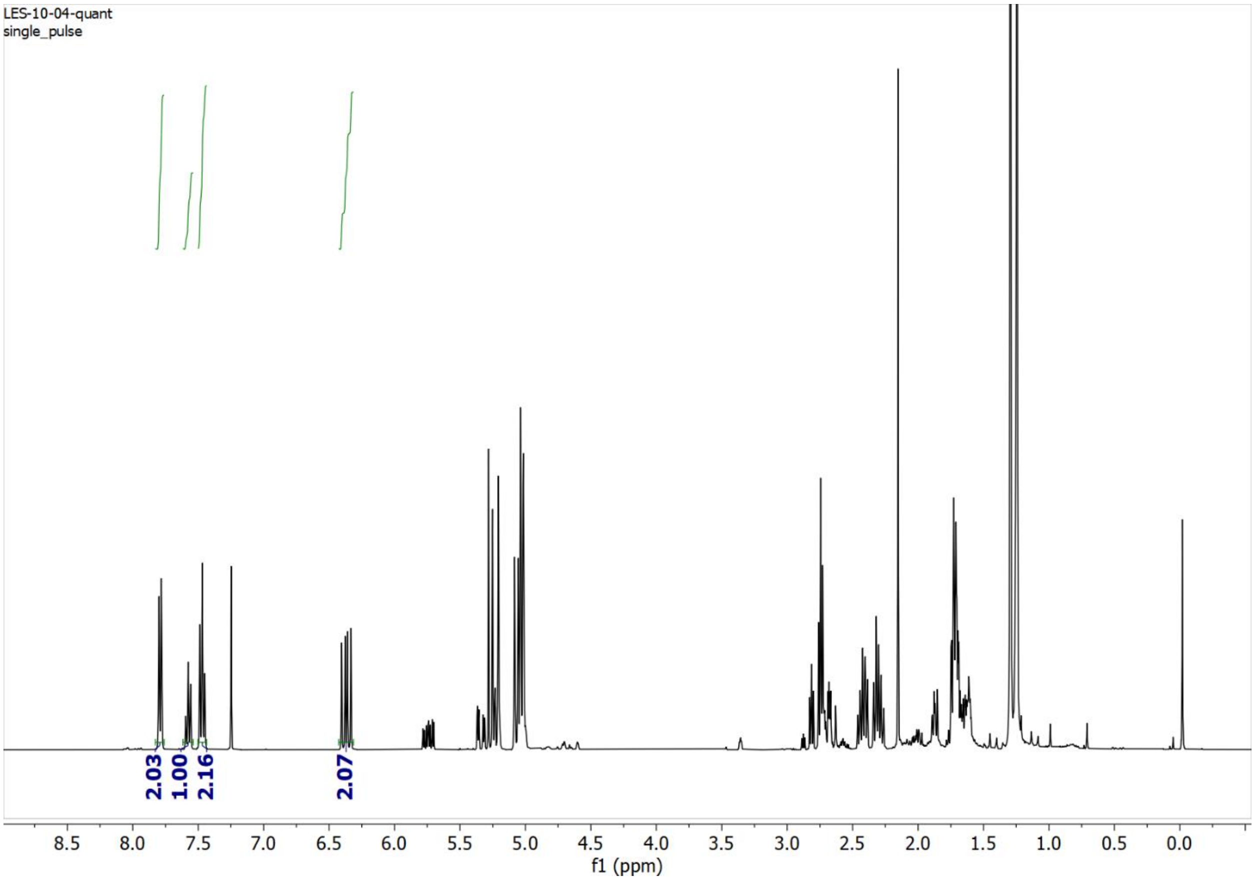


Fig. S38 ^{1}H NMR spectra of starting material of ginger oil sample (C_{15}-fraction), with internal standard for conjugated dienes quantification. Integrated peaks are for benzophenone (internal standard) and sesquiterpenens with conjugated diene moieties.

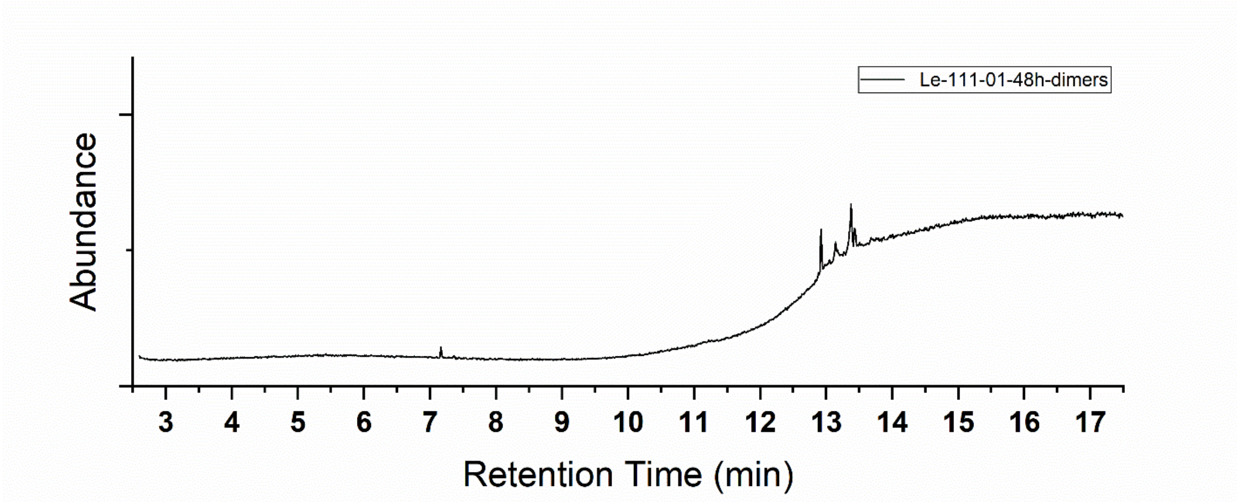


Fig. S39 Photosensitized dimerization of sesquiterpenes in ginger oil (λ = 365 nm, t = 48 h). GC-MS trace of the C_{30} dimers in the sample after irradiation and after removing the unreacted starting material and the photosensitizer.

Cartesian coordinates

M06-2X/6-311+G(d,p)

α-Phellandrene (1)
State: S_0
Absolute Gibbs Free energy at 278 K: -390.386641 a.u.

C	0.789828	-0.757748	-0.122345
C	2.321126	-0.708614	-0.173063
C	2.846279	0.700024	-0.053901
C	0.967829	1.217772	1.369586
C	0.303874	0.11424	1.014543
H	2.72859	-1.314467	0.652577
H	2.679837	-1.159488	-1.09975
H	0.411589	-0.315869	-1.060718
H	0.596936	1.85302	2.168691
H	-0.615091	-0.151678	1.526518
H	3.7871	0.947068	-0.536964
C	2.207816	1.616563	0.681896
C	2.702046	3.021379	0.877336
H	2.876973	3.223541	1.938366
H	3.633108	3.192529	0.335927
H	1.960406	3.745975	0.529123
C	0.228623	-2.190653	-0.031832
H	0.438639	-2.562569	0.979568
C	0.891846	-3.133933	-1.037863
H	1.949637	-3.291862	-0.822339
H	0.40088	-4.109784	-1.026881
H	0.807636	-2.729755	-2.052535
C	-1.286082	-2.201236	-0.253892
H	-1.689658	-3.207373	-0.119208
H	-1.817952	-1.536787	0.428984
H	-1.516332	-1.882813	-1.275636

α-Phellandrene (1)
State: T_1
Absolute Gibbs Free energy at 278 K: -390.307618 a.u.

C	0.732769	-0.751188	-0.164303
C	2.279684	-0.634744	-0.300843
C	2.733496	0.77783	-0.228202
C	0.943382	1.332025	1.309598
C	0.266533	0.110125	0.9641
H	2.71659	-1.22057	0.523349
H	2.616486	-1.095204	-1.231138
H	0.317436	-0.364491	-1.110329
H	0.496452	1.97689	2.059951
H	-0.583836	-0.19992	1.557174
H	3.495744	1.148743	-0.902737
C	2.119173	1.691214	0.735684
C	2.826548	2.975042	1.044061
H	2.267258	3.576608	1.761411
H	3.824365	2.78148	1.451078
H	2.965057	3.565071	0.131622
C	0.251009	-2.208547	-0.018942
H	0.54039	-2.548767	0.984215
C	0.897166	-3.137042	-1.049857
H	1.97323	-3.238429	-0.900906
H	0.458614	-4.135767	-0.990243
H	0.727506	-2.759338	-2.063972
C	-1.271981	-2.295524	-0.147898
H	-1.614213	-3.322564	-0.000764
H	-1.792463	-1.664618	0.574062
H	-1.580913	-1.980831	-1.149985

Myrcene (2)
State: S_0
Absolute Gibbs Free energy at 278 K: -390.359160 a.u.

C	2.650312	3.073229	-1.835955
H	1.728194	3.429569	-1.391319
H	3.062191	3.663361	-2.645189
C	3.26101	1.963661	-1.418551
H	4.184289	1.65756	-1.904381
C	2.799905	1.083453	-0.331967
C	3.523318	0.002295	-0.021522
H	3.229467	-0.690976	0.756524
H	4.437225	-0.220505	-0.561491
C	1.526653	1.469965	0.382588
H	1.668464	2.470139	0.806606
H	0.729024	1.573165	-0.363638
C	1.061333	0.513153	1.47834
H	0.22949	0.985703	2.011858

H	1.86157	0.38823	2.215658
C	0.617617	-0.826444	0.936112
H	0.562229	-0.903194	-0.148713
C	0.288948	-1.898191	1.658817
C	0.323255	-1.922721	3.163138
H	0.626976	-0.969309	3.594046
H	-0.665056	-2.176237	3.559924
H	1.012373	-2.696258	3.517546
C	-0.14966	-3.184021	1.012023
H	-1.157786	-3.457843	1.339371
H	-0.149064	-3.107067	-0.075779
H	0.512051	-4.007023	1.300872

Myrcene (2)
State: T_1
Absolute Gibbs Free energy at 278 K: -390.276146 a.u.

C	2.382087	2.120228	-2.213872
H	1.588842	2.777967	-1.884125
H	2.697948	2.21067	-3.244328
C	2.983188	1.207417	-1.38089
H	3.78439	0.603759	-1.801081
C	2.685256	0.970971	-0.033018
C	3.49118	0.00024	0.721471
H	4.373254	0.312342	1.270941
H	3.215865	-1.047575	0.756026
C	1.606876	1.73224	0.697289
H	2.052978	2.609726	1.185513
H	0.876147	2.115107	-0.020021
C	0.871341	0.892699	1.755744
H	0.1117	1.52834	2.223833
H	1.567196	0.603843	2.544508
C	0.206366	-0.305854	1.141016
H	-0.461356	-0.073854	0.31118
C	0.346997	-1.592147	1.470588
C	1.222619	-2.10905	2.581192
H	1.823048	-1.335287	3.056328
H	0.609277	-2.58789	3.351394
H	1.900394	-2.879242	2.198214
C	-0.399336	-2.668463	0.726375
H	-1.027664	-3.246916	1.411304
H	-1.034134	-2.25195	-0.056197
H	0.299868	-3.373626	0.265536

(*E*)-Ocimene (3)
State: S_0
Absolute Gibbs Free energy at 278 K: -390.359441 a.u.

C	2.370704	0.926642	-2.709903
H	1.571661	0.222341	-2.503841
H	2.428644	1.339391	-3.709851
C	3.253841	1.260788	-1.77119
H	4.074856	1.926884	-2.032767
C	3.246195	0.762593	-0.37783
C	2.093324	0.650633	0.293196
H	1.184088	0.960864	-0.217914
C	1.874079	0.107234	1.680541
H	1.322436	0.841306	2.271716
H	2.824139	-0.055478	2.192401
C	1.121916	-1.199154	1.613437
H	1.710156	-2.039154	1.248475
C	-0.16328	-1.418666	1.900547
C	-1.131235	-0.370322	2.380015
H	-0.700185	0.627857	2.429641
H	-1.997912	-0.33101	1.712773
H	-1.510684	-0.630707	3.373298
C	-0.765545	-2.791546	1.754867
H	-1.59268	-2.775445	1.038004
H	-0.029498	-3.521396	1.416538
H	-1.179215	-3.133652	2.708937
C	4.61074	0.431115	0.169824
H	4.588801	0.114343	1.21054
H	5.072322	-0.364685	-0.421776
H	5.265857	1.304339	0.094581

(*E*)-Ocimene (3) - internal twisted - most stable
State: T_1
Absolute Gibbs Free energy at 278 K: -390.283875 a.u.

C	1.529565	1.752837	-1.528221
H	0.7896	1.031291	-1.203826
H	1.190808	2.597929	-2.111785
C	2.864346	1.5875	-1.228607
H	3.565155	2.328439	-1.607128
C	3.39915	0.539772	-0.480225
C	2.539853	-0.489296	0.125293
H	2.380709	-1.432911	-0.389379
C	2.152246	-0.388296	1.574555
H	1.760132	0.618953	1.763463
H	3.05262	-0.464263	2.201694
C	1.166265	-1.446613	2.00105
H	1.582167	-2.326184	2.486707
C	-0.151223	-1.409049	1.792547
C	-0.855052	-0.270817	1.104445
H	-0.200261	0.577645	0.909422
H	-1.264833	-0.608517	0.14639
H	-1.701032	0.074452	1.706539
C	-1.04838	-2.53725	2.224725

H	-1.594776	-2.944267	1.36797
H	-0.483788	-3.345792	2.690292
H	-1.797572	-2.181595	2.939094
C	4.877644	0.426379	-0.237378
H	5.09962	0.419523	0.835561
H	5.264665	-0.515413	-0.642182
H	5.425896	1.250658	-0.696756

(*E*)-Ocimene (3)- terminal twisted - less stable
State: T_1
Absolute Gibbs Free energy at 278 K: -390.278587 a.u.

C	3.668424	-0.932917	-2.396171
H	2.82325	-1.273364	-2.984005
H	4.579957	-1.517747	-2.449681
C	3.623723	0.335497	-1.668876
H	3.918444	1.23422	-2.209564
C	3.233183	0.476326	-0.342375
C	2.843404	-0.62299	0.41761
H	2.857059	-1.602084	-0.052343
C	2.407583	-0.575728	1.85299
H	2.138354	0.446169	2.135232
H	3.25153	-0.84895	2.499165
C	1.256667	-1.517566	2.141806
H	1.483331	-2.402307	2.73117
C	0.005221	-1.352308	1.709551
C	-0.435448	-0.181471	0.873321
H	0.362227	0.54052	0.702002
H	-0.786103	-0.528447	-0.104065
H	-1.277374	0.33038	1.350092
C	-1.077126	-2.348091	2.027039
H	-1.510438	-2.751895	1.106479
H	-0.698294	-3.178557	2.623764
H	-1.892435	-1.868837	2.578171
C	3.236448	1.858711	0.272939
H	2.230561	2.159747	0.5799
H	3.873179	1.896645	1.159936
H	3.603096	2.59802	-0.439374

(*Z*)-Ocimene (3)
State: S_0
Absolute Gibbs Free energy at 278 K: -390.359421 a.u.

C	4.710119	-0.422269	1.23214
H	4.027344	-1.242692	1.424691
H	5.67438	-0.450317	1.725697
C	4.385175	0.568931	0.405122
H	5.124495	1.342072	0.199054
C	3.113535	0.692358	-0.338505
C	1.900816	0.572912	0.215098
H	1.038386	0.671028	-0.442628
C	1.560817	0.320178	1.660531
H	0.829101	1.064265	1.983155
H	2.448271	0.452029	2.282571
C	1.012944	-1.071894	1.854326
H	1.757726	-1.865299	1.820016
C	-0.262191	-1.432606	2.017011
C	-1.428494	-0.481416	2.050037
H	-1.147149	0.555093	1.873019
H	-2.16289	-0.766473	1.290192
H	-1.938266	-0.538921	3.017141
C	-0.644064	-2.880302	2.181349
H	-1.326614	-3.192225	1.384383
H	0.229351	-3.532865	2.162563
H	-1.170691	-3.034421	3.128658
C	3.279364	1.004674	-1.805242
H	2.3138	1.114292	-2.299824
H	3.843033	1.933299	-1.938834
H	3.841942	0.21289	-2.307802

(*Z*)-Ocimene (3) - internal twisted - most stable
State: T_1
Absolute Gibbs Free energy at 278 K: -390.283664 a.u.

C	5.277577	-0.615592	0.31377
H	4.786687	-1.424536	0.841925
H	6.358279	-0.619416	0.277598
C	4.548941	0.378236	-0.302041
H	5.094947	1.156951	-0.83013
C	3.15722	0.467434	-0.306377
C	2.322779	-0.506575	0.41203
H	1.941728	-1.387721	-0.094923
C	1.987127	-0.292845	1.860897
H	1.62508	0.736818	1.995689
H	2.910169	-0.340692	2.454291
C	0.982725	-1.28006	2.40277
H	1.365498	-2.052831	3.06447
C	-0.318897	-1.290706	2.108881
C	-0.971987	-0.289291	1.194293
H	-0.27596	0.46198	0.822091
H	-1.410039	-0.799131	0.330019
H	-1.792639	0.21867	1.710841
C	-1.248245	-2.32853	2.677483
H	-1.732723	-2.89388	1.875096
H	-0.720738	-3.030183	3.324495
H	-2.045933	-1.854575	3.258244
C	2.442504	1.580292	-1.017725
H	1.774386	1.179767	-1.788301

H	1.81141	2.144779	-0.321402
H	3.14035	2.273958	-1.49007

(*Z*)-Ocimene (3) - terminal twisted - less stable
State: T_1
Absolute Gibbs Free energy at 278 K: -390.278340 a.u.

C	3.122931	-0.978967	-2.338035
H	2.208435	-1.249653	-2.853976
H	3.983388	-1.623694	-2.478456
C	3.229439	0.275342	-1.592986
H	3.53867	1.162002	-2.145334
C	2.96458	0.417099	-0.235902
C	2.565315	-0.667482	0.540173
H	2.470794	-1.635896	0.057552
C	2.257052	-0.618751	2.008196
H	2.087117	0.413565	2.327239
H	3.130573	-0.964293	2.575607
C	1.069653	-1.482616	2.381169
H	1.281106	-2.393216	2.935797
C	-0.198793	-1.220341	2.060892
C	-0.623251	-0.004357	1.282744
H	0.206908	0.663024	1.054041
H	-1.07947	-0.305567	0.334179
H	-1.382753	0.555619	1.837479
C	-1.319306	-2.143562	2.455782
H	-1.856451	-2.497308	1.57001
H	-0.952282	-3.010434	3.006303
H	-2.048828	-1.619263	3.081123
C	3.116795	1.784041	0.394912
H	2.164651	2.14633	0.793387
H	3.829564	1.762018	1.222646
H	3.46993	2.510406	-0.337269

α-Terpinene (5)
State: S_0
Absolute Gibbs Free energy at 278 K: -390.392301 a.u.

C	0.864082	-0.89338	0.282909
C	2.070394	-0.6142	-0.230391
C	2.629621	0.741584	-0.174658
H	2.659856	-1.384276	-0.715089
H	3.48899	0.971894	-0.796928
C	2.131431	1.668488	0.652781
C	2.704911	3.043808	0.806843
H	3.002146	3.219329	1.846608
H	3.57775	3.188852	0.168843
H	1.9613	3.80729	0.557656
C	0.192713	-2.244937	0.225329
H	-0.086726	-2.50424	1.255913
C	1.083252	-3.358454	-0.317597
H	2.008933	-3.447312	0.254838
H	0.55933	-4.315566	-0.270445
H	1.343284	-3.172986	-1.363694
C	-1.105028	-2.156181	-0.593397
H	-1.622474	-3.118438	-0.597631
H	-1.790565	-1.40739	-0.191567
H	-0.874768	-1.885499	-1.627792
C	0.072322	0.246	0.89013
H	-0.654069	-0.137805	1.61262
H	-0.505583	0.730358	0.090037
C	0.980187	1.280485	1.551721
H	0.402524	2.164938	1.834441
H	1.399007	0.868509	2.481659

α-Terpinene (5)
State: T_1
Absolute Gibbs Free energy at 278 K: -390.313700 a.u.

C	0.760601	-0.838748	0.25536
C	1.963327	-0.484622	-0.498041
C	2.588238	0.699496	-0.288378
H	2.355314	-1.174545	-1.236621
H	3.46275	0.959764	-0.876517
C	2.131947	1.645579	0.703664
C	2.793299	2.968108	0.888383
H	3.17579	3.086563	1.910464
H	3.628838	3.102995	0.199491
H	2.084309	3.791305	0.729429
C	0.155928	-2.211321	0.243871
H	-0.204334	-2.412631	1.263108
C	1.14354	-3.316286	-0.134334
H	2.051232	-3.263855	0.470771
H	0.686798	-4.297419	0.013338
H	1.431353	-3.24479	-1.18665
C	-1.074327	-2.254755	-0.683991
H	-1.545791	-3.241055	-0.656851
H	-1.819019	-1.51163	-0.390524
H	-0.774028	-2.045869	-1.714866
C	0.016682	0.284691	0.897161
H	-0.707574	-0.100165	1.622047
H	-0.559961	0.836698	0.139549
C	0.975633	1.287144	1.578465
H	0.433688	2.193657	1.873269
H	1.33859	0.832563	2.511541

α-Zingiberene (6)
State: S_0
Absolute Gibbs Free energy at 278 K: -585.572095 a.u.

C	-6.54619	3.034734	0.397559
C	-5.543545	3.663757	-0.479271
C	-4.928378	4.795085	-0.123878
C	-5.225559	5.461015	1.20176
C	-6.695419	5.219246	1.56115
C	-7.089719	3.775998	1.369545
H	-4.186111	5.238864	-0.780136
H	-5.307559	3.177923	-1.421552
H	-4.609551	4.961125	1.969564
H	-6.885398	5.52176	2.592215
H	-7.331857	5.852825	0.922159
H	-7.865319	3.358868	2.005101
C	-6.925873	1.607345	0.12529
H	-7.688513	1.260365	0.823365
H	-7.313724	1.499524	-0.892178
H	-6.054894	0.951047	0.209224
C	-4.827464	6.950748	1.190943
H	-5.252555	7.397593	0.2812
C	-5.38505	7.700963	2.403617
H	-4.995719	8.720164	2.4492
H	-6.473825	7.76905	2.380837
H	-5.095517	7.191015	3.328832
C	-3.299279	7.099641	1.14023
H	-2.854034	6.323242	0.510225
H	-2.895999	6.933378	2.147208
C	-2.822517	8.46657	0.627984
H	-3.281799	9.267755	1.212464
H	-3.176123	8.598555	-0.399223
C	-1.321488	8.591467	0.658347
H	-0.796918	8.323043	-0.256385
C	-0.586554	8.954991	1.711802
C	-1.168433	9.321888	3.051178
H	-0.899421	0.349429	3.316658
H	-2.253767	9.230731	3.085019
H	-0.751197	8.675862	3.83028
C	0.915494	9.019326	1.64178
H	1.283849	8.750732	0.651088
H	1.270003	10.027175	1.880817
H	1.36639	8.342308	2.374351

α-Zingiberene (6)
State: T_1
Absolute Gibbs Free energy at 278 K: -585.492860 a.u.

C	-6.515839	2.982114	0.298546
C	-5.486889	3.503356	-0.416153
C	-4.841007	4.732306	-0.039084
C	-5.155355	5.417841	1.251187
C	-6.64624	5.158694	1.621261
C	-7.008117	3.727289	1.45789
H	-4.140079	5.187768	-0.727283
H	-5.139939	2.987937	-1.306477
H	-4.561235	4.961008	2.060486
H	-6.850888	5.490356	2.6405
H	-7.254212	5.786344	0.950829
H	-7.604429	3.218125	2.205379
C	-7.1811	1.684527	-0.043954
H	-8.24591	1.835448	-0.249318
H	-6.720018	1.217297	-0.914826
H	-7.116216	0.98648	0.797725
C	-4.790723	6.91599	1.207377
H	-5.227646	7.32996	0.287542
C	-5.362071	7.680703	2.405069
H	-4.995691	8.70893	2.42663
H	-6.452079	7.725043	2.384796
H	-5.058381	7.199045	3.340816
C	-3.265927	7.097466	1.150487
H	-2.808565	6.32884	0.520316
H	-2.855462	6.942347	2.15649
C	-2.819103	8.472673	0.632893
H	-3.287654	9.267255	1.218722
H	-3.18219	8.595672	-0.392112
C	-1.320376	8.624712	0.652337
H	-0.797139	8.360156	-0.26428
C	-0.585183	9.007622	1.698722
C	-1.164752	9.371676	3.039931
H	-0.914793	10.40623	3.296664
H	-2.247747	9.258749	3.082294
H	-0.728887	8.73952	3.820216
C	0.914998	9.098205	1.618466
H	1.281524	8.831665	0.626543
H	1.253203	10.113218	1.850748
H	1.382586	8.432541	2.350994

β-Sesquiphellandrene (7)
State: S_0
Absolute Gibbs Free energy at 278 K: -585.571446 a.u.

C	-6.702565	3.077769	0.203274
C	-5.511813	3.608362	-0.467904
C	-4.779968	4.606716	0.038853
C	-5.127255	5.351744	1.307289
C	-6.602737	5.117408	1.651905
H	-3.900595	4.93298	-0.508638

H	-5.230165	3.15637	-1.414457
H	-4.517759	4.943584	2.130206
H	-6.825818	5.50134	2.649257
H	-7.225639	5.670974	0.938472
C	-7.486148	2.163021	-0.374
H	-8.370366	1.7809	0.123511
H	-7.259421	1.771692	-1.359756
C	-4.754703	6.847024	1.175439
H	-5.141454	7.19545	0.207539
C	-5.388005	7.694175	2.283037
H	-5.021688	8.722237	2.247293
H	-6.475314	7.732411	2.203281
H	-5.133261	7.283622	3.266047
C	-3.229402	7.033137	1.190203
H	-2.729044	6.21358	0.665688
H	-2.879282	6.979181	2.228866
C	-2.75781	8.356618	0.570072
H	-3.271133	9.197409	1.043518
H	-3.053242	8.374213	-0.483397
C	-1.264771	8.531071	0.672441
H	-0.680246	8.197292	-0.182405
C	-0.603305	9.012712	1.727229
C	-1.273332	9.481909	2.99143
H	-1.042078	10.535502	3.178586
H	-2.356635	9.366199	2.969218
H	-0.891296	8.918652	3.848951
C	0.897998	9.1179	1.736925
H	1.331768	8.769334	0.799044
H	1.210898	10.154524	1.898319
H	1.321937	8.527466	2.555451
C	-6.954529	3.629623	1.583248
H	-6.319878	3.087046	2.295307
H	-7.992256	3.45604	1.875583

β-Sesquiphellandrene (7)

State: T_1

Absolute Gibbs Free energy at 278 K: -585.483436 a.u.

C	-6.501213	3.015859	0.252151
C	-5.535171	3.587226	-0.501848
C	-4.914032	4.852327	-0.151059
C	-5.221728	5.484556	1.169072
C	-6.699351	5.211384	1.502994
H	-4.277707	5.352996	-0.869092
H	-5.195732	3.08042	-1.400762
H	-4.621592	4.98238	1.951804
H	-6.951506	5.619337	2.483381
H	-7.3247	5.723228	0.761296
C	-7.074532	1.713476	-0.076563
H	-7.739802	1.213707	0.614
H	-6.797454	1.203997	-0.989381
C	-4.836761	6.977833	1.187955
H	-5.271854	7.437059	0.289264
C	-5.388934	7.702578	2.418568
H	-4.985748	8.714676	2.491937
H	-6.476334	7.787717	2.394166
H	-5.109756	7.165571	3.331601
C	-3.309766	7.136539	1.125305
H	-2.871483	6.380155	0.466763
H	-2.894239	6.942197	2.122444
C	-2.843906	8.519861	0.648421
H	-3.294811	9.302595	1.263568
H	-3.213254	8.682107	-0.368896
C	-1.342745	8.646736	0.659659
H	-0.831656	8.404414	-0.269868
C	-0.592422	8.982236	1.711572
C	-1.154421	9.310528	3.069397
H	-0.883536	10.330975	3.359196
H	-2.238901	9.21565	3.117261
H	-0.723865	8.64415	3.823734
C	0.908331	9.050833	1.620891
H	1.262147	8.810283	0.617769
H	1.265179	10.05227	1.882368
H	1.370982	8.354585	2.327668
C	-7.012606	3.713978	1.488199
H	-6.572116	3.232324	2.372131
H	-8.093318	3.558444	1.567862

5,5-dimethyl-1-vinylbicyclo[2,1,1]hexane (9)

State: S_0

Absolute Gibbs Free energy at 278 K: -390.354231 a.u.

Absolute total energy (S_0): -390.556967

Absolute total energy (T_1): -390.392173

C	8.021728	1.876788	3.744137
H	8.979485	2.048095	4.241631
H	7.205556	2.08363	4.429676
C	9.200679	0.562642	2.169903
H	10.049797	0.347929	2.82255
H	9.207241	-0.168465	1.360451
C	9.176737	2.042733	1.68137
H	10.019669	2.620293	2.064931
H	9.172761	2.134244	0.594546
C	7.853193	2.482052	2.328254
H	7.532427	3.513558	2.179428
C	7.874702	0.536131	2.967512
C	6.886656	1.296131	2.007059
C	7.558081	-0.737666	3.663146

H	8.175387	-0.959336	4.533609
C	6.625326	-1.610311	3.293514
H	5.995428	-1.434291	2.428516
H	6.465889	-2.532402	3.839647
C	6.757993	0.849868	0.551766
H	6.132658	-0.04386	0.477145
H	6.269482	1.637632	-0.030629
H	7.709745	0.626431	0.072575
C	5.473411	1.501381	2.557804
H	4.876168	0.595253	2.433247
H	5.440193	1.766105	3.613051
H	4.978524	2.299402	1.995919

Myrcene epoxide (10)
State: S_0
Absolute Gibbs Free energy at 278 K: -465.564660 a.u.

C	2.508862	3.151441	-1.840222
H	1.552888	3.398402	-1.392763
H	2.852542	3.793331	-2.641823
C	3.239705	2.112309	-1.434485
H	4.191399	1.917227	-1.922612
C	2.882034	1.172358	-0.359074
C	3.723006	0.176877	-0.057899
H	3.519085	-0.557619	0.711062
H	4.655355	0.07102	-0.602319
C	1.570356	1.404169	0.351353
H	1.590782	2.408128	0.789712
H	0.769976	1.427953	-0.398969
C	1.204949	0.391754	1.435418
H	0.303871	0.746841	1.946312
H	1.996468	0.336504	2.187344
C	0.946554	-0.999815	0.892046
H	0.694355	-1.038167	-0.167992
C	0.471937	-2.118746	1.725669
C	0.253215	-1.931746	3.206619
H	0.90084	-1.154246	3.609767
H	-0.787337	-1.662036	3.405227
H	0.467636	-2.864991	3.733463
C	-0.324456	-3.23157	1.091017
H	-1.396149	-3.05074	1.20368
H	-0.088428	-3.311897	0.029381
H	-0.08629	-4.18429	1.571251
O	1.829105	-2.047819	1.293118

Myrcene epoxide (10)
State: T_1
Absolute Gibbs Free energy at 278 K: -465.483303 a.u.

C	1.760759	0.383224	-1.760754
H	0.905056	1.020641	-1.580006
H	1.785263	-0.150689	-2.701191
C	2.786041	0.245462	-0.853096
H	3.599162	-0.426843	-1.11864
C	2.893059	0.869451	0.393001
C	4.029043	0.564043	1.273639
H	3.969474	-0.216855	2.024055
H	4.923244	1.177889	1.258593
C	1.869058	1.842786	0.917824
H	2.391144	2.662157	1.421334
H	1.300575	2.286998	0.096037
C	0.899687	1.191692	1.922817
H	0.278812	1.96727	2.381907
H	1.456957	0.714845	2.731554
C	-0.005438	0.195233	1.247862
H	-0.63484	0.630521	0.469339
C	0.249395	-1.251258	1.129088
C	1.464785	-1.908768	1.732987
H	1.837187	-1.35548	2.59414
H	1.202362	-2.915938	2.067837
H	2.259941	-1.989448	0.987423
C	-0.364098	-2.001312	-0.027079
H	-0.657439	-3.005835	0.289524
H	-1.250685	-1.482166	-0.394036
H	0.357257	-2.089584	-0.842981
O	-0.697764	-0.737189	2.069615

M06-2X/6-31+G(d,p)

Dimers

Dimer 1a gas-phase
Absolute energy: -783.487522296 a.u.
Absolute Gibbs Free energy at 278 K: -783.008465 a.u.

C	0.949348	3.449393	2.641819
C	2.48112	3.467336	2.94205
C	2.475912	5.009963	2.655526
C	0.923414	4.990612	2.7873
H	0.76668	3.156103	1.598647
H	0.622656	5.27516	3.805274
C	2.661781	3.109693	4.423028
H	2.088041	3.814398	5.036226
C	2.798952	5.370754	1.201446
H	2.31092	4.650283	0.53487
C	2.296011	6.782734	0.843576

H	2.209417	6.850352	-0.249402
C	2.163153	1.682441	4.728672
H	1.972453	1.609633	5.80641
C	0.106671	2.585554	3.583455
H	-0.858246	2.329908	3.127733
H	-0.119135	3.147955	4.49963
C	0.884265	1.312352	3.940354
H	1.199436	0.865185	2.984228
C	0.018512	0.244766	4.638628
H	-0.765122	-0.033918	3.918791
C	-0.685028	0.755167	5.899413
H	-1.362341	1.585595	5.680335
H	-1.2775	-0.045832	6.353099
H	0.03441	1.095565	6.652564
C	0.831976	-1.014246	4.949505
H	0.183476	-1.81916	5.30937
H	1.359976	-1.375932	4.060237
H	1.578532	-0.818849	5.727436
C	3.406851	2.613328	2.079872
H	3.202404	2.733367	1.012538
H	4.454069	2.890769	2.256044
H	3.305272	1.548987	2.314606
C	0.155123	5.835774	1.766939
H	-0.850181	6.047688	2.141903
H	0.02864	5.277686	0.82719
C	3.278506	5.891379	3.608018
H	4.348063	5.655692	3.536681
H	3.158247	6.952558	3.367365
H	2.972978	5.756274	4.649072
C	0.924588	7.13208	1.475645
H	1.101077	7.624589	2.447208
C	0.147262	8.138182	0.606334
H	-0.037983	7.657091	-0.367142
C	0.971547	9.407264	0.36512
H	1.91354	9.199806	-0.149118
H	0.411368	10.125371	-0.241687
H	1.20853	9.891344	1.32107
C	-1.203826	8.52072	1.217958
H	-1.898794	7.678733	1.259281
H	-1.068067	8.899419	2.238812
H	-1.6808	9.312036	0.631092
H	3.039078	7.533111	1.134858
H	3.875896	5.290835	1.006666
H	3.710615	3.219909	4.726351
H	2.950037	0.950968	4.512922

Dimer 1a solvent phase (toluene)

Absolute energy: -783.500802232 a.u.

C	-0.642593	0.244253	-0.581413
C	-0.771505	-1.237531	-0.106872
C	0.731975	-1.180404	0.340586
C	0.661966	0.373414	0.24314
H	-0.424983	0.283425	-1.657717
H	0.449554	0.807598	1.229952
C	-1.768535	-1.259762	1.058898
H	-1.419462	-0.578479	1.843502
C	1.717705	-1.653848	-0.733498
H	1.384095	-1.290015	-1.712231
C	3.139285	-1.118703	-0.473015
H	3.700809	-1.161694	-1.416227
C	-3.174972	-0.80851	0.614293
H	-3.731774	-0.495994	1.506341
C	-1.83726	1.143931	-0.253661
H	-1.85039	2.032506	-0.897658
H	-1.754554	1.506568	0.779931
C	-3.137543	0.346073	-0.415475
H	-3.100398	-0.104835	-1.419627
C	-4.401995	1.229011	-0.397322
H	-4.318215	1.904056	-1.261613
C	-4.520041	2.105717	0.85211
H	-3.680598	2.801467	0.944749
H	-5.43862	2.701049	0.812414
H	-4.561684	1.503664	1.767071
C	-5.668796	0.391071	-0.584726
H	-6.545262	1.03321	-0.721524
H	-5.589834	-0.261829	-1.461588
H	-5.858332	-0.242218	0.289588
C	-1.141915	-2.303405	-1.134061
H	-0.542352	-2.225304	-2.045515
H	-0.990145	-3.307587	-0.716844
H	-2.193841	-2.228659	-1.42946
C	1.88429	1.060642	-0.373414
H	1.906421	2.113801	-0.078576
H	1.818076	1.042282	-1.471532
C	1.076912	-1.809089	1.686984
H	0.90591	-2.893313	1.661723
H	2.129407	-1.649821	1.944593
H	0.47736	-1.393825	2.502076
C	3.167271	0.336579	0.05946
H	3.16125	0.30661	1.162271
C	4.463115	1.060183	-0.35439
H	4.483939	1.094164	-1.45512
C	5.698393	0.291116	0.124377
H	5.748554	-0.71887	-0.291871

H	6.617337	0.813165	-0.161984
H	5.692406	0.204229	1.21869
C	4.526528	2.496626	0.171826
H	3.766631	3.142261	-0.275837
H	4.387869	2.514669	1.260506
H	5.502893	2.942955	-0.044678
H	3.667839	-1.777661	0.22451
H	1.73185	-2.749323	-0.798937
H	-1.815972	-2.257399	1.513893
H	-3.72949	-1.655041	0.193779

Dimer 1c gas-phase

Absolute energy: -783.50809546 a.u.

Absolute Gibbs Free energy at 278 K: -783.025727 a.u.

C	-1.797698	1.806779	-0.752856
C	-0.503511	1.025554	-1.068033
C	-1.618605	-0.007677	1.00429
C	-2.27926	1.340716	0.646154
H	-2.543576	1.509474	-1.502503
H	-2.025841	2.099783	1.395322
H	-3.371158	1.254205	0.663986
C	0.431807	1.14429	0.158379
H	0.295864	2.171137	0.522329
C	-0.097454	0.21371	1.291489
H	-2.08039	-0.431526	1.905626
H	-0.013624	1.45422	-1.952722
C	-1.812366	-0.967814	-0.193761
H	-1.456655	-1.962746	0.100421
C	-0.928463	-0.425735	-1.357434
H	-0.050111	-1.061223	-1.515478
H	-1.491132	-0.436188	-2.298418
C	0.666018	-1.129915	1.34773
H	0.380676	-1.654668	2.269538
H	0.375584	-1.783892	0.522851
C	2.186111	-0.998075	1.253386
H	2.622511	-1.997375	1.343775
H	2.594579	-0.399611	2.080741
C	2.582377	-0.347425	-0.075948
H	2.177197	-0.967963	-0.893818
C	1.943665	1.045914	-0.1308
H	2.477706	1.661025	0.610572
H	2.125558	1.518757	-1.102074
C	4.111048	-0.27972	-0.272973
H	4.52272	0.311461	0.560371
C	4.755322	-1.669768	-0.235304
H	5.826667	-1.602197	-0.448218
H	4.644592	-2.157863	0.735664
H	4.305411	-2.320473	-0.995669
C	4.492042	0.416433	-1.584259
H	4.000719	-0.073942	-2.434295
H	4.211167	1.47206	-1.594862
H	5.572702	0.361984	-1.748246
C	-1.660449	3.324856	-0.843734
H	-1.367739	3.635493	-1.852116
H	-2.612715	3.810287	-0.604446
H	-0.91326	3.709897	-0.141409
C	-3.285994	-1.20079	-0.595166
H	-3.689701	-0.283916	-1.046691
C	-4.154247	-1.56836	0.612026
H	-4.239394	-0.750914	1.332854
H	-5.165775	-1.837293	0.29149
H	-3.7295	-2.434672	1.135007
C	-3.381168	-2.323258	-1.634476
H	-4.414412	-2.458525	-1.9692
H	-2.766934	-2.12899	-2.518022
H	-3.045333	-3.271157	-1.196272
C	0.087951	0.9022	2.652801
H	-0.460208	1.846718	2.71121
H	-0.261927	0.256431	3.466361
H	1.142968	1.13071	2.837269

Dimer 1c solvent phase (toluene)

Absolute energy: -783.520743914 a.u.

C	-1.797846	1.806613	-0.753557
C	-0.503122	1.025345	-1.068065
C	-1.618858	-0.007326	1.004759
C	-2.278708	1.341331	0.645883
H	-2.54376	1.507757	-1.502325
H	-2.023611	2.100532	1.394482
H	-3.370714	1.254598	0.663991
C	0.432232	1.144471	0.158824
H	0.295499	2.171044	0.523078
C	-0.097242	0.213753	1.292202
H	-2.081656	-0.429984	1.906089
H	-0.012517	1.453746	-1.952415
C	-1.812942	-0.968007	-0.193223
H	-1.457001	-1.962974	0.100208
C	-0.928493	-0.426165	-1.356557
H	-0.049796	-1.061993	-1.511985
H	-1.490505	-0.437653	-2.298009
C	0.666778	-1.12968	1.348758
H	0.382203	-1.654055	2.271239
H	0.376303	-1.783675	0.523839
C	2.187021	-0.997807	1.254585
H	2.623313	-1.997452	1.344671

H	2.594811	-0.399145	2.082232
C	2.583318	-0.347334	-0.074933
H	2.177084	-0.967732	-0.892074
C	1.944563	1.046154	-0.12967
H	2.477965	1.66127	0.612135
H	2.126907	1.518881	-1.10107
C	4.11244	-0.280564	-0.27318
H	4.525879	0.308554	0.560637
C	4.755181	-1.670892	-0.239292
H	5.827623	-1.60404	-0.449991
H	4.643985	-2.163074	0.730132
H	4.307255	-2.320637	-1.002213
C	4.493226	0.417007	-1.583245
H	4.002029	-0.070146	-2.435698
H	4.214877	1.473827	-1.592962
H	5.574346	0.362368	-1.748101
C	-1.661737	3.324215	-0.845181
H	-1.373159	3.636076	-1.855038
H	-2.614072	3.810138	-0.604169
H	-0.912893	3.71236	-0.145798
C	-3.28723	-1.200519	-0.594509
H	-3.69087	-0.282682	-1.043844
C	-4.155074	-1.570579	0.61162
H	-4.242428	-0.754761	1.334638
H	-5.167451	-1.838421	0.290631
H	-3.732751	-2.438619	1.134435
C	-3.383234	-2.320737	-1.635356
H	-4.416728	-2.454368	-1.971909
H	-2.769531	-2.12586	-2.519773
H	-3.04912	-3.271421	-1.200875
C	0.087717	0.902477	2.652846
H	-0.46141	1.84688	2.712942
H	-0.260582	0.257247	3.468165
H	1.142532	1.132878	2.838458

Dimer 2a (cis) gas-phase

Absolute energy: -785.87605671 a.u.

Absolute Gibbs Free energy at 278 K: -785.365462 a.u.

C	0.890431	-0.480346	-0.406606
C	-0.55004	-0.957462	-0.105301
C	-1.05526	0.453875	-0.48821
C	0.385028	0.975972	-0.273383
H	1.142181	-0.694628	-1.45533
H	-0.940561	-1.817803	-0.655709
H	-0.680556	-1.134431	0.971702
H	-1.30635	0.483665	-1.558344
H	0.515119	1.336246	0.756929
H	0.775364	1.728518	-0.96395
C	-3.47685	0.256882	0.141965
H	-3.270706	-0.791324	0.402692
H	-3.744366	0.264116	-0.924237
C	-4.651282	0.763335	0.983602
H	-4.273437	1.012244	1.985341
H	-5.028742	1.704401	0.564961
C	-5.912798	-1.751735	-0.906365
H	-4.997207	-1.403591	-1.391942
H	-5.651284	-2.600184	-0.265343
H	-6.582033	-2.118627	-1.69185
C	-6.93585	0.552195	-0.996087
H	-6.032747	0.973234	-1.452989
H	-7.605559	0.250269	-1.807498
H	-7.428308	1.350292	-0.429796
C	3.311232	-0.177952	0.180051
H	3.103446	0.899883	0.250699
H	3.584105	-0.370379	-0.868474
C	4.489698	-0.514713	1.095217
H	4.816843	-1.546551	0.919812
H	4.150635	-0.476852	2.13936
C	7.45319	1.477092	-0.508988
H	8.264492	1.081058	0.11378
H	7.842732	1.606014	-1.523769
H	7.184548	2.464807	-0.120353
C	6.650407	-0.845116	-1.036897
H	5.788153	-1.511316	-1.141416
H	7.120533	-0.752128	-2.021049
H	7.370207	-1.330245	-0.365598
C	-2.381174	2.540933	-0.071479
H	-2.738797	2.618717	-1.106074
H	-3.106772	3.043457	0.574289
H	-1.436128	3.089314	-0.0006
C	6.254135	0.527556	-0.490082
H	5.480608	0.949151	-1.147194
C	5.680739	0.434047	0.930719
H	6.487629	0.118784	1.608011
H	5.381778	1.441264	1.253032
C	2.21453	-2.464444	0.3645
H	2.582009	-2.718743	-0.637898
H	2.931173	-2.851322	1.094253
H	1.266662	-2.990584	0.517942
C	2.025534	-0.951536	0.49253
H	1.73551	-0.724211	1.53179
C	-6.595654	-0.640945	-0.100814
H	-7.545109	-1.059872	0.260705
C	-5.817224	-0.217327	1.161352
H	-6.531786	0.249711	1.851698
H	-5.450091	-1.121044	1.667388
C	-2.190714	1.073022	0.315346

H	-1.901652	1.028694	1.378601

Dimer 2a (cis) solvent phase (toluene)

Absolute energy: -785.891911618 a.u.

C	-0.89198	0.473745	-0.398289
C	0.547388	0.954064	-0.095857
C	1.056848	-0.455126	-0.48198
C	-0.382052	-0.981384	-0.266167
H	-1.143603	0.688458	-1.446825
H	0.935245	1.816706	-0.645075
H	0.677376	1.129131	0.981429
H	1.306449	-0.482323	-1.552401
H	-0.510296	-1.342685	0.76392
H	-0.770609	-1.734443	-0.957616
C	3.480827	-0.253619	0.143993
H	3.273222	0.793696	0.407373
H	3.746507	-0.258702	-0.922515
C	4.658785	-0.757735	0.982297
H	4.284903	-1.004965	1.986074
H	5.035886	-1.699036	0.563704
C	5.917031	1.749472	-0.9196
H	5.009713	1.393324	-1.415665
H	5.641255	2.597665	-0.283368
H	6.590567	2.123073	-1.69906
C	6.949396	-0.548169	-0.997144
H	6.049472	-0.976779	-1.453981
H	7.618485	-0.246186	-1.809902
H	7.447615	-1.342057	-0.429115
C	-3.314952	0.168326	0.184457
H	-3.106804	-0.909548	0.253835
H	-3.586213	0.363075	-0.86396
C	-4.496318	0.501211	1.097487
H	-4.820482	1.535152	0.928653
H	-4.161686	0.453553	2.142818
C	-7.469518	-1.460944	-0.526665
H	-8.280604	-1.066058	0.097812
H	-7.859234	-1.581085	-1.543062
H	-7.208307	-2.454363	-0.146002
C	-6.653467	0.859847	-1.033341
H	-5.787564	1.522372	-1.134955
H	-7.125661	0.778902	-2.018239
H	-7.369602	1.345553	-0.357931
C	2.389851	-2.539228	-0.070123
H	2.748293	-2.617577	-1.104772
H	3.115521	-3.042795	0.57559
H	1.446609	-3.091869	0.00012
C	-6.264784	-0.519596	-0.499746
H	-5.494645	-0.939256	-1.16189
C	-5.689971	-0.442616	0.921887
H	-6.495879	-0.131442	1.602475
H	-5.394117	-1.454152	1.2337
C	-2.219637	2.454589	0.375684
H	-2.588684	2.713549	-0.62533
H	-2.93465	2.84135	1.107804
H	-1.272375	2.982738	0.529876
C	-2.029491	0.941951	0.500809
H	-1.740642	0.713115	1.539858
C	6.602948	0.646363	-0.107013
H	7.549895	1.071162	0.254081
C	5.824456	0.224269	1.155781
H	6.540047	-0.241176	1.846432
H	5.457224	1.1289	1.660365
C	2.196054	-1.072741	0.319034
H	1.908882	-1.031057	1.382711

Dimer 2a (trans) gas-phase

Absolute energy: -785.87348024 a.u.

Absolute Gibbs Free energy at 278 K: -785.362101 a.u.

C	0.993785	-1.664094	-0.624285
C	-0.087483	-0.559723	-0.769799
C	-1.068364	-1.439422	0.040098
C	-0.137486	-2.646818	-0.219705
H	1.52187	-1.922268	-1.551537
H	0.147341	0.432561	-0.372497
H	-0.421683	-0.449258	-1.808038
H	-1.046316	-1.161253	1.103213
H	-0.488659	-3.241074	-1.071305
H	0.059493	-3.321855	0.619029
C	-3.202411	-0.161608	-0.303339
H	-2.608171	0.584002	-0.851178
H	-3.18068	0.140555	0.753326
C	-4.640791	-0.142319	-0.827694
H	-4.670384	-0.708495	-1.769368
H	-5.295645	-0.683468	-0.133746
C	-4.119898	2.937229	0.488047
H	-3.381599	2.262563	0.929695
H	-3.657219	3.420549	-0.378843
H	-4.338761	3.714272	1.228157
C	-6.032124	1.50719	1.300307
H	-5.343559	0.772262	1.73325
H	-6.274743	2.232623	2.083201
H	-6.954208	0.982398	1.027282
C	2.93253	-0.219105	0.094473
H	2.309298	0.656312	-0.13249

H	3.458398	-0.47084	-0.838749
C	3.945707	0.171192	1.172556
H	4.687634	-0.626163	1.298101
H	3.424822	0.256016	2.135982
C	6.112093	2.906755	-0.601258
H	6.875948	3.029894	0.176077
H	6.606865	2.9955	-1.573606
H	5.400738	3.733551	-0.505533
C	6.424421	0.413079	-0.592587
H	5.938655	-0.567823	-0.603863
H	6.998344	0.511049	-1.519544
H	7.13385	0.426979	0.244431
C	-3.26068	-2.614815	0.356926
H	-3.356297	-2.32897	1.412135
H	-4.266072	-2.785912	-0.038011
H	-2.719776	-3.56583	0.314363
C	5.414387	1.553572	-0.453709
H	4.680169	1.463239	-1.266498
C	4.662862	1.493338	0.883505
H	5.380338	1.696748	1.691599
H	3.928935	2.310987	0.908117
C	2.872582	-2.663076	0.72093
H	3.508875	-2.871045	-0.148864
H	3.52267	-2.550591	1.592779
H	2.242454	-3.54054	0.890726
C	2.034992	-1.405707	0.469348
H	1.497663	-1.15033	1.398079
C	-5.405301	2.203247	0.09054
H	-6.111561	2.975364	-0.24509
C	-5.231872	1.245468	-1.105722
H	-6.221688	1.092393	-1.555334
H	-4.623112	1.746379	-1.87129
C	-2.516903	-1.527752	-0.421404
H	-2.504494	-1.810267	-1.48753

Dimer 2a (trans) solvent phase (toluene)
Absolute energy: -785.889248281 a.u.

C	0.99461	-1.659075	-0.622754
C	-0.088348	-0.556289	-0.769569
C	-1.068997	-1.436402	0.040475
C	-0.136108	-2.64265	-0.218193
H	1.523557	-1.917367	-1.549459
H	0.145436	0.436728	-0.372969
H	-0.421947	-0.447795	-1.808323
H	-1.047698	-1.157597	1.103279
H	-0.485924	-3.237375	-1.070179
H	0.061899	-3.31716	0.620968
C	-3.207124	-0.162147	-0.304064
H	-2.614966	0.584159	-0.853315
H	-3.186461	0.141167	0.752152
C	-4.645762	-0.145549	-0.828266
H	-4.674338	-0.71075	-1.77071
H	-5.299407	-0.688424	-0.134436
C	-4.137005	2.934174	0.491695
H	-3.403149	2.263057	0.946889
H	-3.664235	3.412061	-0.373407
H	-4.361379	3.718015	1.22383
C	-6.050475	1.505278	1.295691
H	-5.364443	0.770355	1.733347
H	-6.296045	2.231847	2.077507
H	-6.973268	0.981123	1.022026
C	2.934147	-0.212594	0.095426
H	2.310334	0.662826	-0.130069
H	3.459367	-0.464544	-0.83803
C	3.94911	0.17819	1.171808
H	4.687786	-0.621771	1.300632
H	3.428356	0.270107	2.134836
C	6.136873	2.896791	-0.603185
H	6.900453	3.018347	0.175246
H	6.634601	2.982143	-1.574968
H	5.430968	3.729455	-0.511613
C	6.434411	0.40277	-0.586971
H	5.9441	-0.576268	-0.600069
H	7.013721	0.495077	-1.511876
H	7.141217	0.412413	0.252827
C	-3.260043	-2.614741	0.357173
H	-3.35872	-2.330462	1.412894
H	-4.26492	-2.790187	-0.038548
H	-2.718611	-3.566158	0.316057
C	5.430339	1.548731	-0.455645
H	4.69984	1.460202	-1.271845
C	4.672384	1.496332	0.878634
H	5.38761	1.699998	1.688876
H	3.941424	2.316911	0.896816
C	2.873672	-2.656304	0.723057
H	3.51403	-2.865048	-0.144048
H	3.520987	-2.546477	1.597915
H	2.243816	-3.535087	0.890719
C	2.036274	-1.399391	0.471117
H	1.498891	-1.1442	1.39963
C	-5.419623	2.199833	0.087789
H	-6.124565	2.971423	-0.251653
C	-5.240524	1.240745	-1.10674
H	-6.229511	1.084057	-1.55739
H	-4.632365	1.743199	-1.87194
C	-2.518048	-1.527243	-0.421544

H	-2.505025	-1.810749	-1.487192

Dimer 2g gas-phase

Absolute energy: -785.907053508 a.u.

Absolute Gibbs Free energy at 278 K: -785.393889 a.u.

C	-0.639313	1.975001	0.147891
C	0.485912	2.857325	-0.393757
C	1.849587	2.346318	0.067109
C	2.067828	0.881647	-0.322937
C	0.914038	0.010832	0.192778
C	-0.469261	0.50372	-0.259484
H	2.653763	2.965224	-0.349267
H	0.450242	2.85638	-1.492194
H	0.339362	3.894894	-0.073805
H	-0.639295	2.028818	1.247448
H	-1.606435	2.365088	-0.184458
H	2.062336	0.824132	-1.424714
H	1.064357	-1.019349	-0.141667
H	0.946171	-0.004668	1.295815
H	-0.494598	0.44789	-1.362429
H	1.917814	2.432964	1.162453
C	-1.630962	-0.368167	0.272409
H	-1.783577	-0.095639	1.329682
C	-1.322559	-1.86864	0.210337
H	-0.517222	-2.154312	0.89138
H	-2.201263	-2.460907	0.479515
H	-1.0257	-2.15624	-0.806269
C	-2.935776	-0.075979	-0.48902
H	-2.877332	-0.561335	-1.475006
H	-3.026946	0.998813	-0.685582
C	3.436278	0.39307	0.167614
H	4.188701	1.130444	-0.142445
H	3.439462	0.391153	1.268962
C	3.84796	-0.986381	-0.347204
H	3.090882	-1.727589	-0.066013
H	3.863082	-0.961658	-1.446573
C	5.209703	-1.481734	0.154297
H	5.373627	-2.483125	-0.263183
H	5.172923	-1.610866	1.245775
C	6.409598	-0.581701	-0.206724
H	6.136818	0.009826	-1.093805
C	7.635692	-1.425708	-0.564079
H	8.49905	-0.795339	-0.80091
H	7.912156	-2.069061	0.280166
H	7.437576	-2.070775	-1.425889
C	6.765853	0.384764	0.927725
H	5.909038	0.983977	1.246498
H	7.118722	-0.179234	1.799662
H	7.56618	1.068723	0.626686
C	-4.208906	-0.530826	0.226899
H	-4.242686	-0.0573	1.216553
H	-4.185468	-1.614955	0.401064
C	-5.473057	-0.184642	-0.56051
H	-5.570319	0.909701	-0.629574
H	-5.358462	-0.547796	-1.591512
C	-6.771595	-0.758802	0.018248
H	-6.672231	-1.854226	0.041109
C	-7.027124	-0.273052	1.446571
H	-6.25204	-0.610205	2.1404
H	-7.054021	0.82355	1.476452
H	-7.988989	-0.641068	1.817746
C	-7.955506	-0.405455	-0.883438
H	-7.794998	-0.756101	-1.908055
H	-8.884326	-0.850938	-0.513425
H	-8.096705	0.681582	-0.918951

Dimer 2g solvent phase (toluene)

Absolute energy: -785.923269971 a.u.

C	-0.650506	1.955789	0.117483
C	0.470158	2.836392	-0.435999
C	1.836552	2.34048	0.033674
C	2.064219	0.870024	-0.329823
C	0.913766	0.00173	0.198778
C	-0.470552	0.479541	-0.266861
H	2.636961	2.956712	-0.394287
H	0.435546	2.81993	-1.53447
H	0.317606	3.877752	-0.130415
H	-0.651776	2.026581	1.216113
H	-1.620428	2.333844	-0.221758
H	2.061195	0.793039	-1.430268
H	1.070655	-1.03358	-0.116727
H	0.942906	0.006349	1.301894
H	-0.49082	0.406838	-1.368804
H	1.903843	2.44761	1.127312
C	-1.631673	-0.388394	0.272918
H	-1.794145	-0.095758	1.323199
C	-1.317102	-1.888165	0.243496
H	-0.522969	-2.161028	0.943593
H	-2.199529	-2.47826	0.508805
H	-1.003102	-2.196109	-0.762112
C	-2.933432	-0.120897	-0.504669
H	-2.887533	-0.673408	-1.455364
H	-3.005295	0.939877	-0.773394
C	3.435177	0.398224	0.171792

H	4.184248	1.132221	-0.154027
H	3.437887	0.419647	1.272901
C	3.85374	-0.990288	-0.312612
H	3.103923	-1.729852	-0.007982
H	3.861839	-0.992274	-1.412444
C	5.222363	-1.464713	0.19098
H	5.387524	-2.476208	-0.201375
H	5.195171	-1.564679	1.285932
C	6.415521	-0.569623	-0.204439
H	6.13116	0.000375	-1.101713
C	7.640316	-1.417636	-0.554729
H	8.500433	-0.790614	-0.813892
H	7.928133	-2.043236	0.29954
H	7.437221	-2.08142	-1.401718
C	6.781085	0.423979	0.902481
H	5.925407	1.026145	1.220442
H	7.150924	-0.115832	1.783148
H	7.572081	1.10751	0.574881
C	-4.209892	-0.504503	0.246378
H	-4.248259	0.066995	1.182685
H	-4.182189	-1.565633	0.529575
C	-5.472555	-0.243566	-0.575522
H	-5.564487	0.83657	-0.767532
H	-5.35989	-0.722215	-1.558514
C	-6.775135	-0.741848	0.062934
H	-6.682702	-1.828108	0.209889
C	-7.030576	-0.096276	1.426061
H	-6.263084	-0.361783	2.159078
H	-7.046467	0.997526	1.335237
H	-7.997937	-0.41103	1.832046
C	-7.955703	-0.485678	-0.874516
H	-7.797334	-0.950348	-1.853687
H	-8.888041	-0.882759	-0.459329
H	-8.093306	0.591183	-1.033285

Dimer 2k gas-phase

Absolute energy: -785.891386784 a.u.

Absolute Gibbs Free energy at 278 K: -785.374863 a.u.

C	-1.605386	2.513473	-0.216104
C	-1.895408	1.004924	-0.29643
C	1.900225	1.393075	0.366047
C	-1.396896	0.206758	0.925919
C	1.188218	0.482972	1.388199
C	0.028828	-0.387102	0.866545
H	-2.33458	2.966895	0.470735
H	-1.393855	0.596735	-1.186799
H	-1.504625	0.821419	1.832263
H	2.487977	2.122354	0.945842
H	0.81838	1.081302	2.229553
H	-1.804747	2.948733	-1.204832
H	-2.081151	-0.638503	1.065408
H	1.946397	-0.177409	1.824125
H	0.017405	-1.29853	1.474408
H	0.234033	-0.723796	-0.159544
C	-0.195985	2.904854	0.236839
H	-0.102347	2.706619	1.309929
H	-0.086161	3.989501	0.131699
C	0.928847	2.179699	-0.525105
H	0.498267	1.483268	-1.25647
H	1.511735	2.896202	-1.115211
C	2.883641	0.60588	-0.514026
H	3.163122	1.228477	-1.375443
H	2.370414	-0.273136	-0.932606
C	-3.404583	0.799357	-0.503357
H	-3.787117	1.5803	-1.175179
H	-3.917484	0.950981	0.456865
C	4.164627	0.157875	0.190644
H	3.915913	-0.448382	1.069372
H	4.697413	1.044151	0.565301
C	5.090235	-0.635532	-0.732037
H	4.599157	-1.579571	-1.013875
H	5.229059	-0.072029	-1.665446
C	6.469881	-0.954684	-0.144131
H	6.96072	0.000245	0.095667
C	7.328837	-1.687249	-1.176186
H	8.335861	-1.878448	-0.792154
H	6.87818	-2.654415	-1.429863
H	7.421897	-1.108317	-2.100709
C	6.369604	-1.775729	1.143271
H	5.859461	-1.228849	1.941119
H	5.813841	-2.704086	0.96035
H	7.364128	-2.048621	1.510425
C	-3.775721	-0.560779	-1.101414
H	-3.294902	-1.371381	-0.535649
H	-3.346809	-0.608244	-2.109846
C	-5.290593	-0.822445	-1.168469
H	-5.536494	-1.329891	-2.109202
H	-5.826814	0.138649	-1.192923
C	-5.853031	-1.671256	-0.019753
H	-5.351726	-2.649892	-0.060172
C	-5.579779	-1.059927	1.355497
H	-4.508068	-0.966369	1.557341
H	-6.02545	-0.059862	1.426936
H	-6.014591	-1.678019	2.147684
C	-7.353408	-1.896467	-0.212187
H	-7.566925	-2.353745	-1.183741

H	-7.760791	-2.548443	0.567032
H	-7.891642	-0.942076	-0.16496

Dimer 2k solvent phase (toluene)

Absolute energy: -785.907789713 a.u.

C	-1.602648	2.507774	-0.217187
C	-1.897527	0.9998	-0.295347
C	1.904167	1.382043	0.359403
C	-1.395237	0.201162	0.925406
C	1.193284	0.469591	1.3808
C	0.029232	-0.395437	0.861243
H	-2.328924	2.964912	0.470535
H	-1.400056	0.590029	-1.187009
H	-1.498073	0.816073	1.832202
H	2.491007	2.111825	0.939339
H	0.828636	1.065372	2.226407
H	-1.801101	2.942934	-1.206314
H	-2.080215	-0.643351	1.066413
H	1.951718	-0.195828	1.809216
H	0.016941	-1.307195	1.469035
H	0.230844	-0.731577	-0.165793
C	-0.191498	2.894141	0.234199
H	-0.097688	2.692889	1.306788
H	-0.078609	3.978903	0.130439
C	0.930481	2.167454	-0.530346
H	0.497083	1.469353	-1.258544
H	1.511601	2.883353	-1.123226
C	2.888824	0.595194	-0.520448
H	3.157825	1.211452	-1.389816
H	2.380172	-0.292841	-0.925499
C	-3.40848	0.797957	-0.496142
H	-3.790792	1.579247	-1.167906
H	-3.917129	0.951471	0.466161
C	4.17819	0.166168	0.181379
H	3.9392	-0.420598	1.076069
H	4.711549	1.062672	0.530118
C	5.097958	-0.645465	-0.731519
H	4.608616	-1.598709	-0.98395
H	5.224475	-0.10442	-1.679966
C	6.486036	-0.94389	-0.151448
H	6.977756	0.018466	0.053886
C	7.333586	-1.705112	-1.171407
H	8.34765	-1.879497	-0.796428
H	6.885818	-2.682698	-1.389499
H	7.412676	-1.155574	-2.11563
C	6.404193	-1.726799	1.160211
H	5.906925	-1.156894	1.950705
H	5.845853	-2.66071	1.015138
H	7.404284	-1.989437	1.521482
C	-3.787079	-0.561412	-1.091448
H	-3.312878	-1.373131	-0.521772
H	-3.356713	-0.613645	-2.099207
C	-5.303507	-0.814386	-1.162939
H	-5.548605	-1.319488	-2.105323
H	-5.834563	0.149607	-1.187803
C	-5.87557	-1.662169	-0.017917
H	-5.379172	-2.643229	-0.05695
C	-5.606247	-1.05401	1.35891
H	-4.534921	-0.963592	1.566091
H	-6.050402	-0.053265	1.433772
H	-6.044368	-1.673613	2.148961
C	-7.375743	-1.879238	-0.217095
H	-7.588632	-2.334578	-1.190321
H	-7.790414	-2.531718	0.558649
H	-7.911868	-0.923183	-0.170306

Dimer 3h gas-phase

Absolute energy: -785.904851578 a.u.

Absolute Gibbs Free energy at 278 K: -785.387942 a.u.

C	0.092528	-0.323816	0.352162
C	-1.18855	0.473699	-0.055884
C	-1.156036	1.948801	0.39703
C	0.111934	2.644338	-0.099382
C	1.382778	1.901402	0.2971
C	1.348086	0.442296	-0.168009
H	-1.190649	0.487453	-1.161078
H	0.063886	2.711089	-1.197262
H	0.138269	3.675112	0.274952
H	2.248858	2.405333	-0.144981
H	1.524759	1.945593	1.386114
H	1.24456	0.46662	-1.26695
H	-1.147807	1.963045	1.49811
C	-2.385254	2.734797	-0.066188
H	-3.317705	2.338679	0.346573
H	-2.303855	3.782018	0.243117
H	-2.463883	2.715488	-1.16025
C	-2.491525	-0.221805	0.407345
H	-2.905932	0.328033	1.261802
H	-2.279713	-1.229884	0.785275
C	-3.541503	-0.358257	-0.698537
H	-3.750658	0.622667	-1.148184
H	-3.110682	-0.971259	-1.503604
C	-4.866826	-0.986366	-0.252031
H	-4.638617	-1.937805	0.251455

C	-5.747061	-1.286945	-1.466653
H	-6.689719	-1.756835	-1.168703
H	-5.989465	-0.359688	-1.999995
H	-5.24123	-1.955753	-2.170278
C	-5.619911	-0.089153	0.733617
H	-5.050989	0.089966	1.650178
H	-5.833381	0.883373	0.272322
H	-6.57597	-0.538996	1.019796
C	0.146677	-0.476909	1.882861
H	-0.757949	-0.954341	2.270659
H	0.994807	-1.088783	2.199402
H	0.240478	0.492012	2.379698
C	0.027798	-1.712517	-0.365669
H	-0.993914	-1.890292	-0.718301
H	0.635349	-1.652435	-1.278031
C	0.452667	-2.949186	0.431312
H	0.393362	-3.839053	-0.202466
H	1.477903	-2.877247	0.806079
H	-0.201139	-3.114374	1.293298
C	2.670759	-0.275227	0.13885
H	2.605988	-1.316386	-0.203112
H	2.822902	-0.31149	1.225177
C	3.895817	0.363357	-0.524042
H	3.638331	0.651109	-1.553972
H	4.17162	1.291028	-0.003351
C	5.128438	-0.548265	-0.562541
H	4.860348	-1.449937	-1.133201
C	6.284157	0.147497	-1.282798
H	7.155468	-0.510045	-1.364048
H	5.996115	0.45634	-2.292886
H	6.592396	1.044696	-0.732508
C	5.557884	-0.982586	0.840478
H	5.764288	-0.103626	1.464184
H	4.786406	-1.575872	1.339938
H	6.470026	-1.586497	0.800892

Dimer 3h solvent phase (toluene)

Absolute energy: -785.918646832 a.u.

C	0.092129	-0.318198	0.35179
C	-1.188559	0.480949	-0.057181
C	-1.153263	1.957345	0.392449
C	0.115673	2.649577	-0.106448
C	1.385301	1.905475	0.2915
C	1.349558	0.445077	-0.16976
H	-1.190737	0.492337	-1.162252
H	0.067359	2.71432	-1.204515
H	0.144188	3.681051	0.266448
H	2.252182	2.407639	-0.151524
H	1.526008	1.951718	1.38065
H	1.246918	0.465374	-1.26864
H	-1.144181	1.97385	1.493405
C	-2.380813	2.744302	-0.07177
H	-3.314557	2.351471	0.342059
H	-2.298693	3.792145	0.237528
H	-2.461438	2.726506	-1.165945
C	-2.492302	-0.212783	0.408167
H	-2.906514	0.339389	1.261223
H	-2.27932	-1.219917	0.787722
C	-3.543759	-0.353418	-0.69616
H	-3.760173	0.627047	-1.143452
H	-3.110651	-0.96343	-1.502258
C	-4.864677	-0.991329	-0.248428
H	-4.6289	-1.938703	0.259076
C	-5.741112	-1.304336	-1.462077
H	-6.681481	-1.779623	-1.163286
H	-5.990424	-0.382765	-2.00289
H	-5.231135	-1.975005	-2.161759
C	-5.627555	-0.097834	0.732247
H	-5.058718	0.098828	1.64584
H	-5.861479	0.867427	0.265077
H	-6.574931	-0.56124	1.027876
C	0.147502	-0.469542	1.882045
H	-0.75791	-0.943223	2.273507
H	0.993888	-1.084094	2.199452
H	0.24615	0.499428	2.378792
C	0.024265	-1.708061	-0.364147
H	-0.997001	-1.88143	-0.720637
H	0.637114	-1.652983	-1.273365
C	0.438471	-2.946231	0.434775
H	0.377252	-3.835733	-0.200634
H	1.46272	-2.882633	0.814494
H	-0.220566	-3.111168	1.293337
C	2.671415	-0.272909	0.141858
H	2.601756	-1.318151	-0.18631
H	2.826803	-0.295404	1.228138
C	3.897159	0.352387	-0.53303
H	3.639759	0.620958	-1.568152
H	4.174217	1.288969	-0.029277
C	5.129814	-0.560645	-0.556014
H	4.862301	-1.471693	-1.111685
C	6.285844	0.122968	-1.286423
H	7.156837	-0.536908	-1.359455
H	5.999108	0.417141	-2.301851
H	6.597345	1.028358	-0.75078
C	5.559616	-0.971422	0.853484
H	5.762461	-0.083455	1.466146
H	4.79155	-1.56197	1.362297

H	6.474648	-1.572662	0.824338

Dimer 3k gas-phase

Absolute energy: -785.890272275 a.u.

Absolute Gibbs Free energy at 278 K: -785.373102 a.u.

C	-1.561928	-1.965765	-0.695127
C	-2.141569	-0.871592	0.252823
C	1.675283	-0.379392	-0.258691
C	-1.10656	0.072078	0.879439
C	1.445315	-0.27308	1.26882
C	0.008486	-0.63161	1.672958
H	-2.337931	-2.102675	-1.461695
H	-2.649379	-1.39421	1.079924
H	-0.681876	0.696889	0.083239
H	1.152978	0.466265	-0.728272
H	1.621018	0.776027	1.54968
H	-1.630315	0.766259	1.543542
H	-0.105814	-0.41665	2.74198
H	-0.10349	-1.716488	1.586373
C	-0.306958	-1.58229	-1.513702
H	-0.445212	-0.576997	-1.936439
H	-0.309587	-2.261012	-2.37558
C	1.103882	-1.671291	-0.885166
H	1.149757	-2.499969	-0.166656
H	1.782995	-1.963262	-1.694817
C	3.156568	-0.206875	-0.633153
H	3.236883	-0.246897	-1.728848
H	3.72996	-1.063796	-0.256182
C	-3.216913	-0.072596	-0.506525
H	-3.961546	-0.786902	-0.878417
H	-2.756462	0.381416	-1.398316
C	3.776137	1.106702	-0.154433
H	3.847856	1.120934	0.942776
H	3.102432	1.932472	-0.426687
C	5.168096	1.395996	-0.729461
H	5.083071	1.413772	-1.826123
C	-3.92339	1.018499	0.299029
H	-3.215302	1.824771	0.52544
H	-4.247371	0.608753	1.269278
C	2.410992	-1.146711	2.077224
H	2.342143	-2.196621	1.767168
H	3.453702	-0.835303	1.969112
H	2.160373	-1.102815	3.142022
C	-1.423686	-3.348732	-0.043953
H	-2.384047	-3.668958	0.372674
H	-1.11855	-4.09138	-0.790068
H	-0.690777	-3.380897	0.765989
C	-5.606082	2.885913	0.343648
H	-4.807767	3.631958	0.409032
H	-6.465496	3.34985	-0.150728
H	-5.908136	2.627046	1.365875
C	-6.300138	0.643891	-0.5343
H	-6.030674	-0.240428	-1.117797
H	-6.622886	0.307958	0.458891
H	-7.160077	1.112687	-1.023206
C	-5.140963	1.635042	-0.404713
H	-4.82846	1.935782	-1.415897
C	5.659553	2.768012	-0.265455
H	5.771543	2.784253	0.825465
H	6.632166	3.011626	-0.704549
H	4.954336	3.558539	-0.541692
C	6.177277	0.311566	-0.345323
H	6.227348	0.209039	0.74634
H	5.912083	-0.663458	-0.763356
H	7.180102	0.565831	-0.703113

Dimer 3k solvent phase (toluene)

Absolute energy: -785.905034169 a.u.

C	1.560968	1.960384	-0.694979
C	2.141579	0.865156	0.252428
C	-1.681121	0.377687	-0.25475
C	1.104599	-0.080898	0.872425
C	-1.44685	0.265081	1.272079
C	-0.007846	0.621035	1.671479
H	2.334634	2.0969	-1.46379
H	2.644572	1.387482	1.082578
H	0.677797	-0.69755	0.071105
H	-1.161445	-0.466987	-0.728444
H	-1.624504	-0.784307	1.550395
H	1.625818	-0.781469	1.531988
H	0.110866	0.403411	2.739683
H	0.103121	1.706168	1.585605
C	0.302289	1.5797	-1.509647
H	0.43731	0.574393	-1.933415
H	0.3035	2.25984	-2.370579
C	-1.106614	1.670829	-0.876682
H	-1.146451	2.495728	-0.153329
H	-1.786638	1.968779	-1.683598
C	-3.163964	0.210533	-0.627337
H	-3.245178	0.25771	-1.722732
H	-3.735419	1.065793	-0.243492
C	3.222266	0.070835	-0.505153
H	3.962472	0.78943	-0.87777
H	2.764358	-0.387809	-1.395958
C	-3.786181	-1.105029	-0.156659

H	-3.8581	-1.12534	0.940397
H	-3.114321	-1.930435	-0.434639
C	-5.178713	-1.38981	-0.734092
H	-5.092899	-1.405385	-1.830633
C	3.937015	-1.014091	0.301958
H	3.233397	-1.821711	0.537413
H	4.266391	-0.597506	1.26744
C	-2.40739	1.137743	2.086627
H	-2.338746	2.18952	1.781823
H	-3.451738	0.828944	1.983147
H	-2.153898	1.089244	3.151211
C	1.426228	3.3421	-0.041669
H	2.390155	3.664945	0.366134
H	1.113803	4.086402	-0.783928
H	0.70091	3.373426	0.775598
C	5.632375	-2.869191	0.355826
H	4.839581	-3.620046	0.439972
H	6.489104	-3.336659	-0.141145
H	5.944442	-2.596476	1.37187
C	6.304012	-0.636331	-0.558697
H	6.026961	0.235509	-1.158094
H	6.631486	-0.278371	0.425678
H	7.165076	-1.108117	-1.044095
C	5.152483	-1.632154	-0.405185
H	4.833322	-1.948939	-1.409282
C	-5.673695	-2.761235	-0.27351
H	-5.790515	-2.780924	0.817248
H	-6.64527	-3.004052	-0.716757
H	-4.969567	-3.553859	-0.548732
C	-6.1868	-0.305364	-0.348967
H	-6.240211	-0.202852	0.742844
H	-5.921955	0.67085	-0.76574
H	-7.190048	-0.557554	-0.708949

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