

Sce1440

Table 1. Sesquiterpene synthase orthologs of sce1440, which were identified in the genomes of myxobacterial strains.

Myxobacterial Strain	NCBI Reference Sequence / Locus Tag	Number of Amino Acid Residues	Sequence Identity [%]	Sequence similarity [%]
<i>Sorangium cellulosum</i> So0157-2	WP_020735216	781	61.8	73.4
<i>Archangium gephyra</i> DSM 2261	WP_047855443	774	59.6	71.6
<i>Cystobacter violaceus</i> Cb vi76	WP_043389732	773	59.5	70.9
<i>Chondromyces crocatus</i>	WP_050434199	760	59.3	72.8
<i>Cystobacter fuscus</i> DSM 2262	WP_043432513	771	58.6	70.1
<i>Haliangium minutum</i> DSM 14724	WP_044199666	748	58.4	71.0
<i>Myxococcus xanthus</i> DK 1622	WP_011556189	755	57.8	70.7
<i>Myxococcus xanthus</i> DZF1	WP_011556189	755	57.8	70.7
<i>Myxococcus xanthus</i> DZ2	WP_011556189	755	57.8	70.7
<i>Myxococcus fulvus</i> HW-1	WP_013938107	755	57.3	69.9
<i>Enhygromyxa salina</i> DSM 15201	KIG18953	787	57.1	68.3
<i>Myxococcus stipitatus</i> DSM 14675	WP_015352290	750	55.9	69.7
<i>Coralloccoccus coralloides</i> DSM 2259	WP_014400162	752	55.7	71.4
<i>Haliangium ochraceum</i> DSM 14365	WP_012826426	756	55.6	68.2
<i>Chondromyces apiculatus</i> DSM 436	EYF04694	796	55.5	67.1
<i>Myxococcus virescens</i> DSM 2260	Ga0070493_11424	754	55.1	69.8
<i>Stigmatella aurantiaca</i> DW4/3-1	WP_002611863	704	53.3	65.2

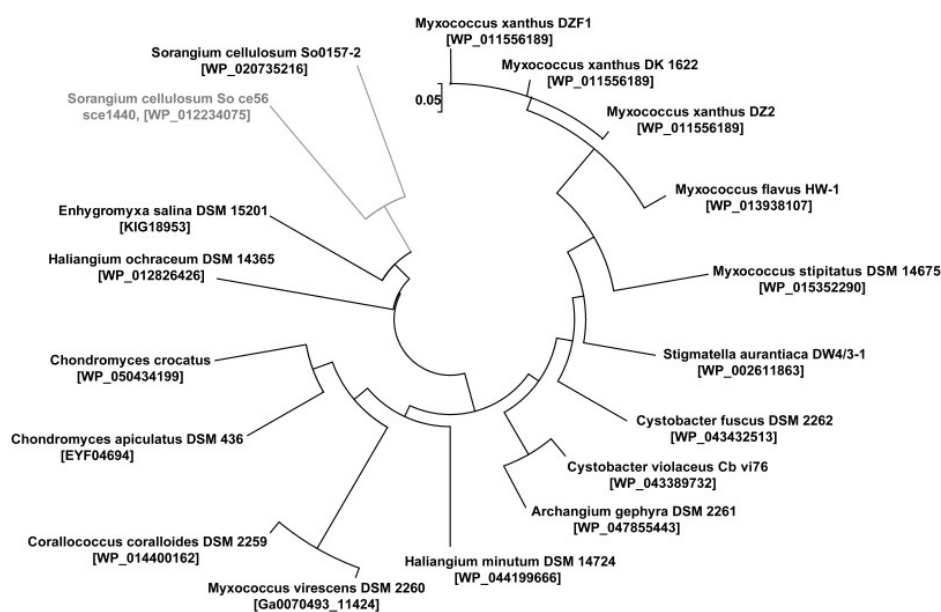


Figure 1. The radial view of an unrooted phylogenetic tree obtained by MEGA4 (version 4.0) analysis for the determination of relatedness of the sce1440 from *Sorangium cellulosum* So ce56 with other myxobacterial terpene synthases. The sce1440 gene from *S. cellulosum* So ce56 is shown in grey branches. Sce 4636 (WP_049876337)

Table 2. Sesquiterpene synthase orthologs of sce4636, which were identified in the genomes of myxobacterial strains.

Myxobacterial Strain	NCBI Reference Sequence	Number of amino acid residues	Sequence Identity [%]	Sequence similarity [%]
Cystobacter fuscus DSM 2262	WP_002627525	509	47.6	60.9
Cystobacter violaceus Cb vi76	WP_043411369	513	45.3	60.9
Archangium gephyra DSM 2261	WP_053066483	514	44.3	60.3
Chondromyces apiculatus DSM 436	WP_044234889	519	41.8	53.5
Cystobacter violaceus Cb vi76	WP_043405491	512	41.4	54.2
Archangium gephyra DSM 2261	WP_047856205	512	41.1	54.9
Cystobacter fuscus DSM 2262	EPX58993	531	40.9	53.5
Chondromyces apiculatus DSM 436	WP_052376419	542	29.9	39.6

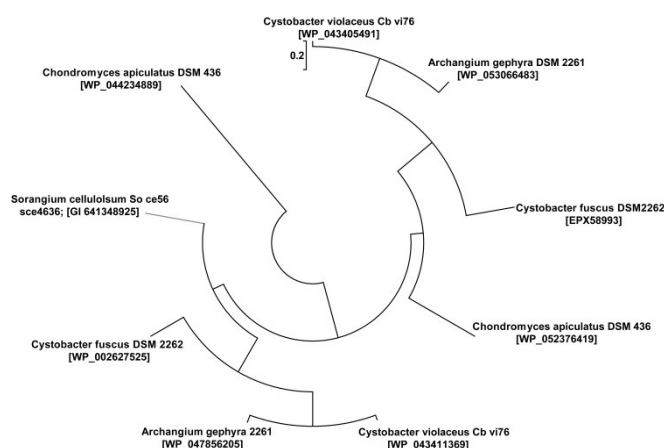


Figure 2. The radial view of an unrooted phylogenetic tree obtained by MEGA4 (version 4.0) analysis for the determination of relatedness of sce4636 from *Sorangium cellulosum* So ce56 with other myxobacterial terpene synthases. The sce4636 gene from *S. cellulosum* So ce56 is shown in grey.

Sce 6369 (CAN96536)

Table 3. Sesquiterpene synthase orthologs of sce6369, which were identified in the genomes of myxobacterial strains.

Myxobacterial Strain	NCBI Reference Sequence	Number of amino acid residues	Sequence Identity [%]	Sequence similarity [%]
<i>Chondromyces crocatus</i>	WP_050430829	313	33.2	46.7
<i>Chondromyces apiculatus</i> DSM 436	EYF00967	301	32.1	45.7
<i>Sorangium cellulosum</i> So0157-2	AGP41845	321	31.8	46.8
<i>Hyalangium minutum</i> DSM 14724	WP_044191871	293	29.5	46.2
<i>Sorangium cellulosum</i> So ce56	WP_012241161	315	28.8	44.7
<i>Myxococcus fulvus</i> 124B02	WP_046712537	331	28.4	41.8
<i>Plesiocystis pacifica</i> SIR-1	WP_006972929	364	24.1	38.1

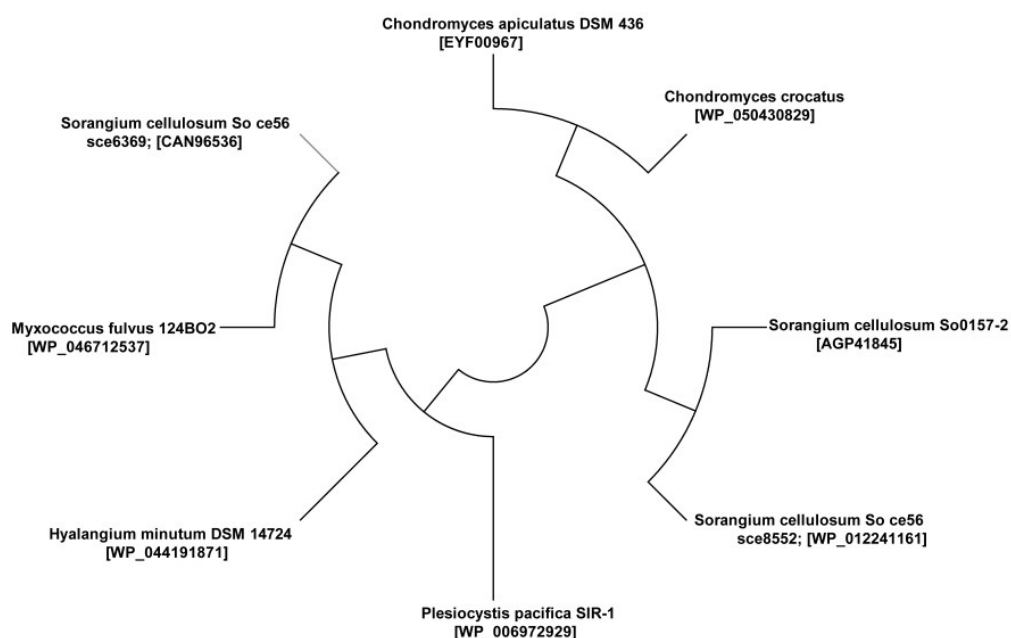


Figure 3. The radial view of an unrooted phylogenetic tree obtained by MEGA4 (version 4.0) analysis for the determination of relatedness of the sce6369 from *Sorangium cellulosum* So ce56 with other myxobacterial terpene synthases. The gene sce6369 from *S. cellulosum* So ce56 is shown in grey.

Sce 8552 (WP_012241161)

Table 4. Sesquiterpene synthase orthologs of sce8552, which were identified in the genomes of myxobacterial strains.

	NCBI Reference Sequence / Locus Tag	Number of amino acid residues	Sequence Identity [%]	Sequence similarity [%]
<i>Sorangium cellulosum</i> So0157-2	AGP41845	321	68.7	81.2
<i>Sorangium cellulosum</i> So ce56	CAN96536	315	28.8	44.7
<i>Nannocystis exedens</i> ATCC 25963	Ga0008035_06483	328	27.9	42.6
<i>Chondromyces crocatus</i>	WP_050430829	313	27.9	46.9
<i>Chondromyces apiculatus</i> DSM 436	EYF00967	301	27.7	45.5
<i>Myxococcus fulvus</i> 124B02	WP_046712537	331	27.4	46.1
<i>Hyalangium minutum</i> DSM 14724	WP_044191871	293	26.8	45.4
<i>Myxococcus stipitatus</i> DSM 14675	WP_044281543	358	25.2	37.0
<i>Cystobacter violaceus</i> Cb vi76	WP_043410615	324	25.2	39.3
<i>Plesiocystis pacifica</i> SIR-1*	WP_006972929	364	24.7	41.0
<i>Plesiocystis pacifica</i> SIR-1	EDM79289	355	24.6	42.6
<i>Archangium gephyra</i> DSM 2261	AKJ08214	343	24.5	39.8
<i>Cystobacter fuscus</i> DSM 2262	WP_002630213	365	22.1	41.4

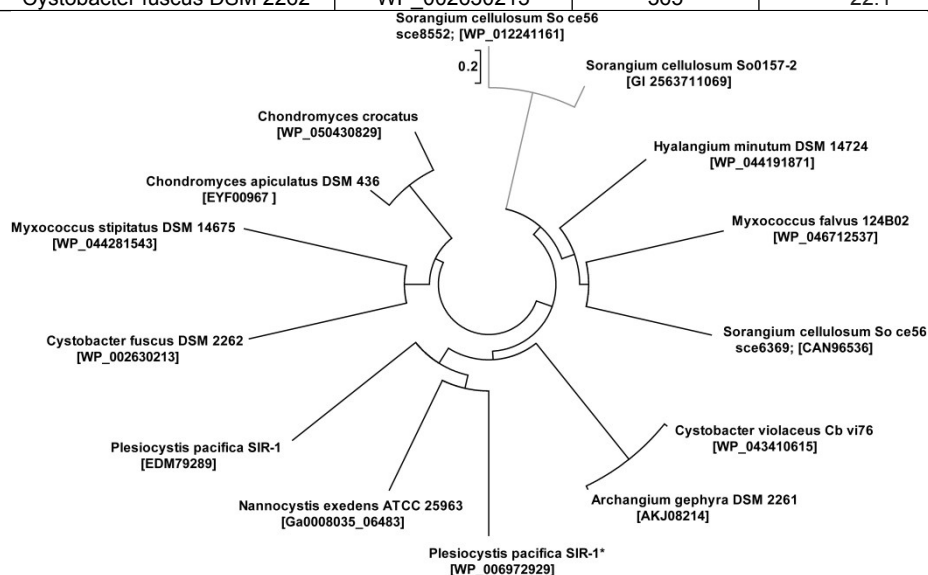
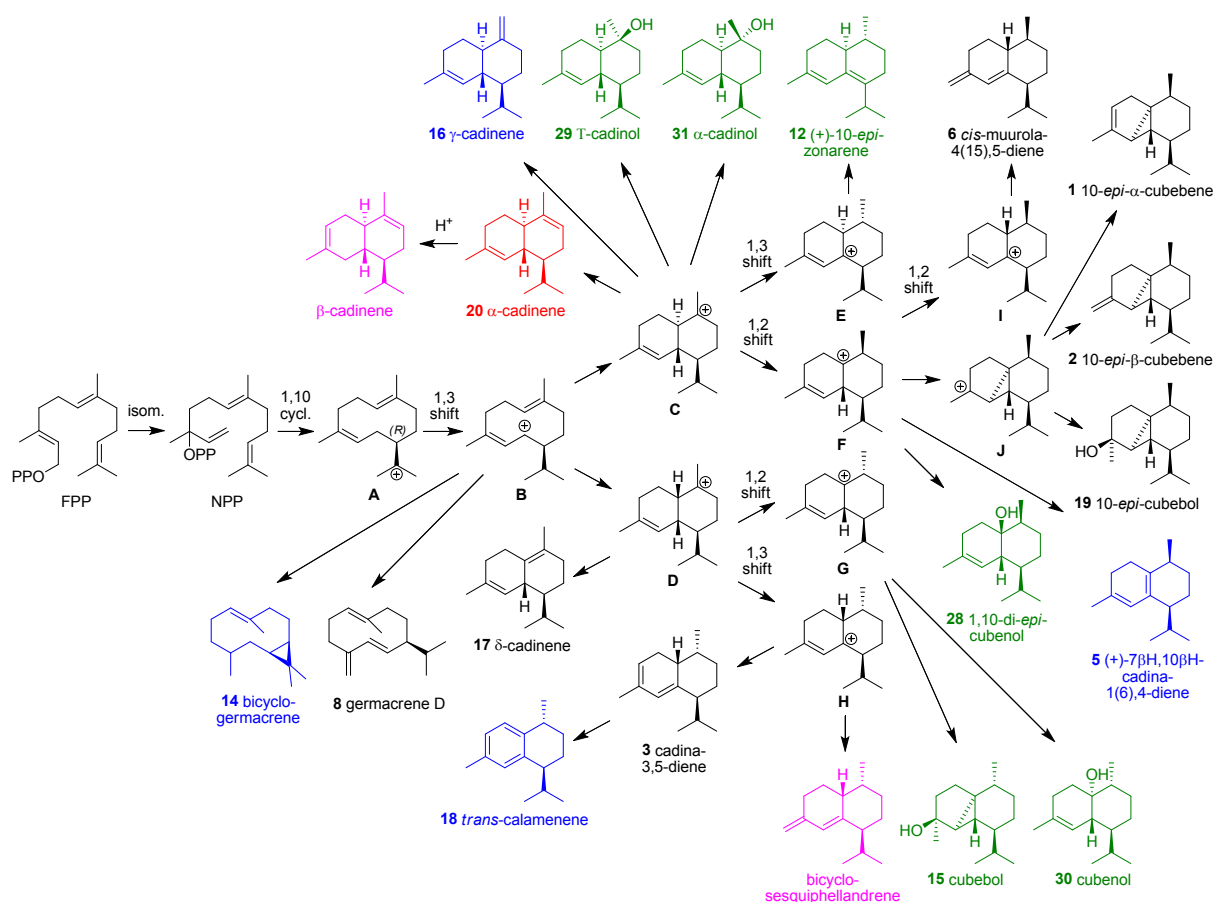
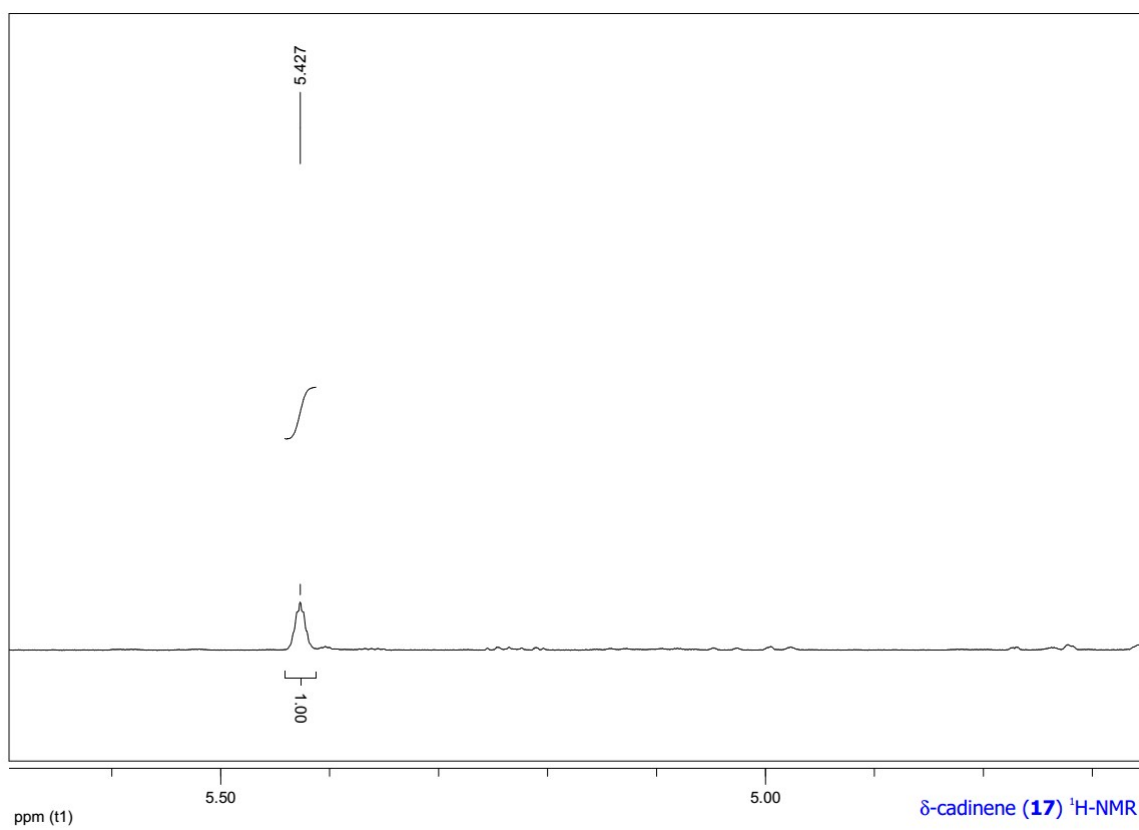


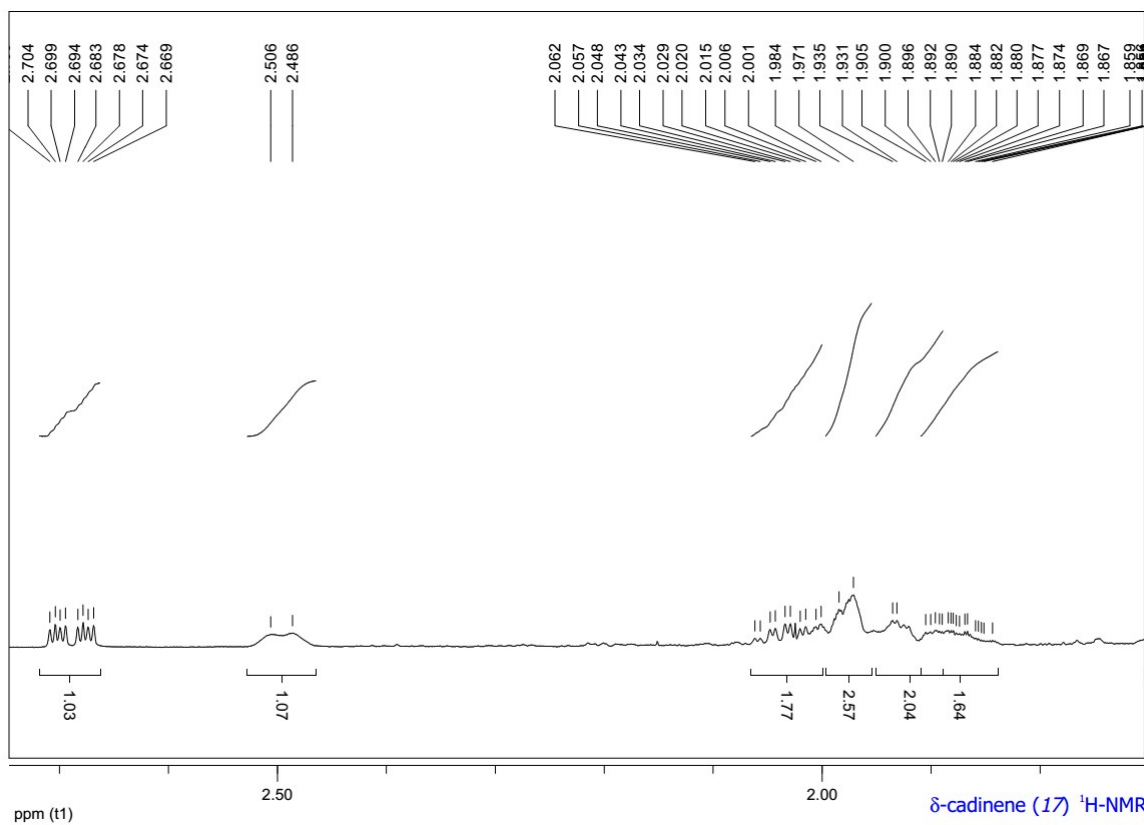
Figure 4. The radial view of an unrooted phylogenetic tree obtained by MEGA4 (version 4.0) analysis for the determination of relatedness of the sce8552 from *Sorangium cellulosum* So ce56 with other myxobacterial terpene synthases. The gene sce8552 from *S. cellulosum* is shown in grey.

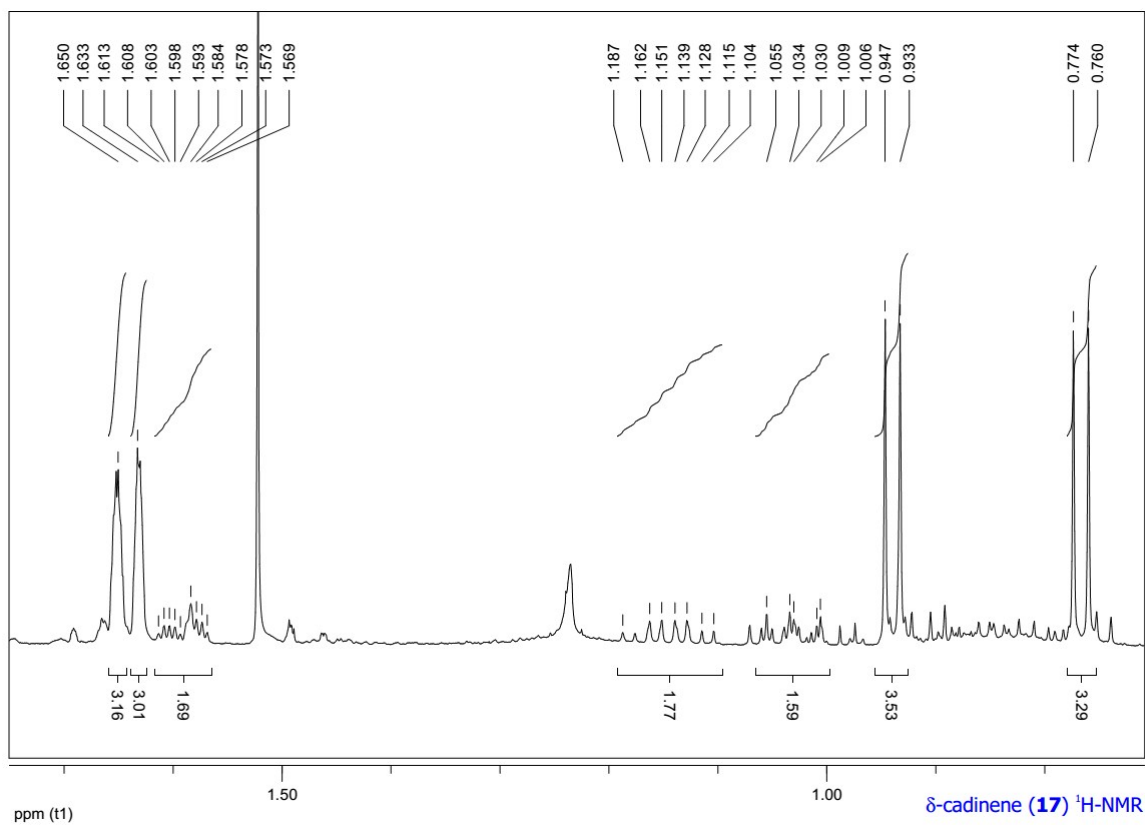


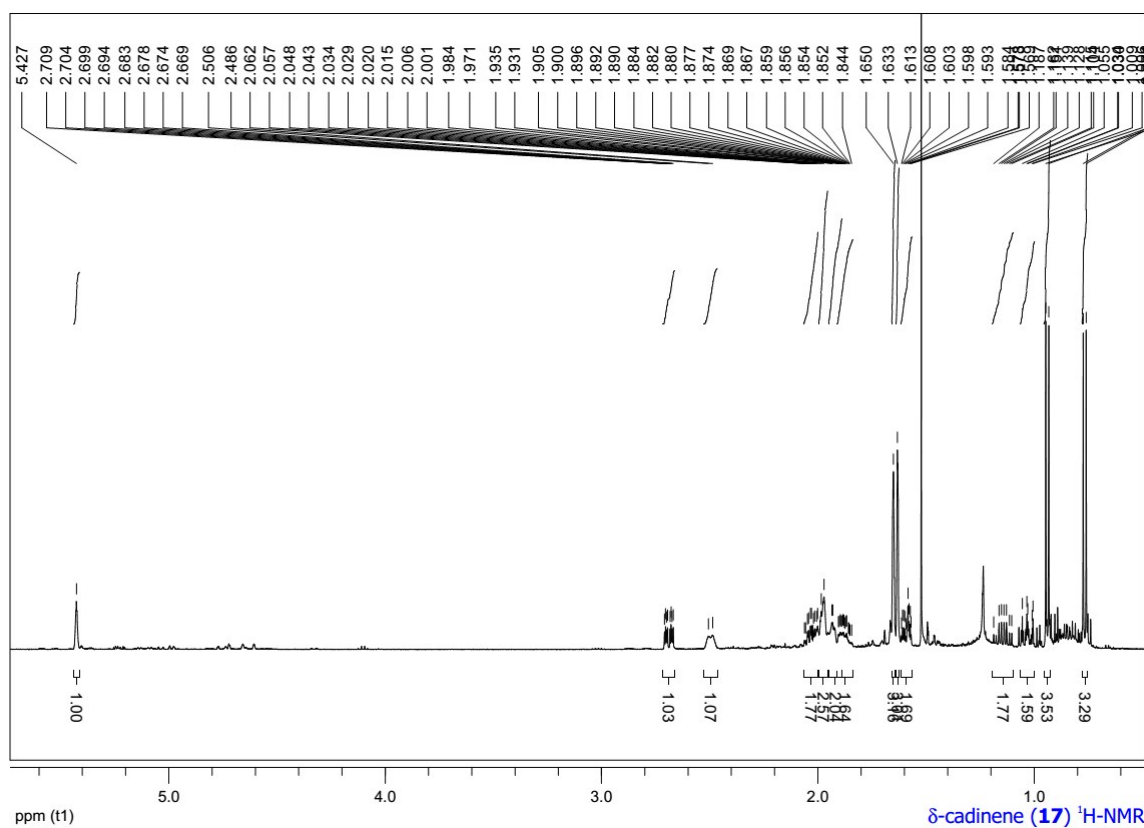
Scheme 1 Proposed alternative mechanism (involving enantiomers of all molecules) for the biosynthesis of cadalane- and cubebene-type sesquiterpenes by sce6369; sesquiterpenes observed in *S. cellulosum* and the sce6369 expressing *E. coli* strain are represented in black; sesquiterpenes observed only in *S. cellulosum* are represented in blue; sesquiterpenes observed only in the sce6369 expressing *E. coli* strain are represented in green; sesquiterpenes observed in *S. cellulosum* and the sce6369 expressing *Streptomyces avermitilis* SUKA22¹² are represented in red; sesquiterpenes observed only in the sce6369 expressing *S. avermitilis* SUKA22¹² are represented in pink; cadina-3,5-diene (3) was observed in *S. cellulosum* as well as both *E. coli* and *S. avermitilis* SUKA22 expressing sce6369¹²

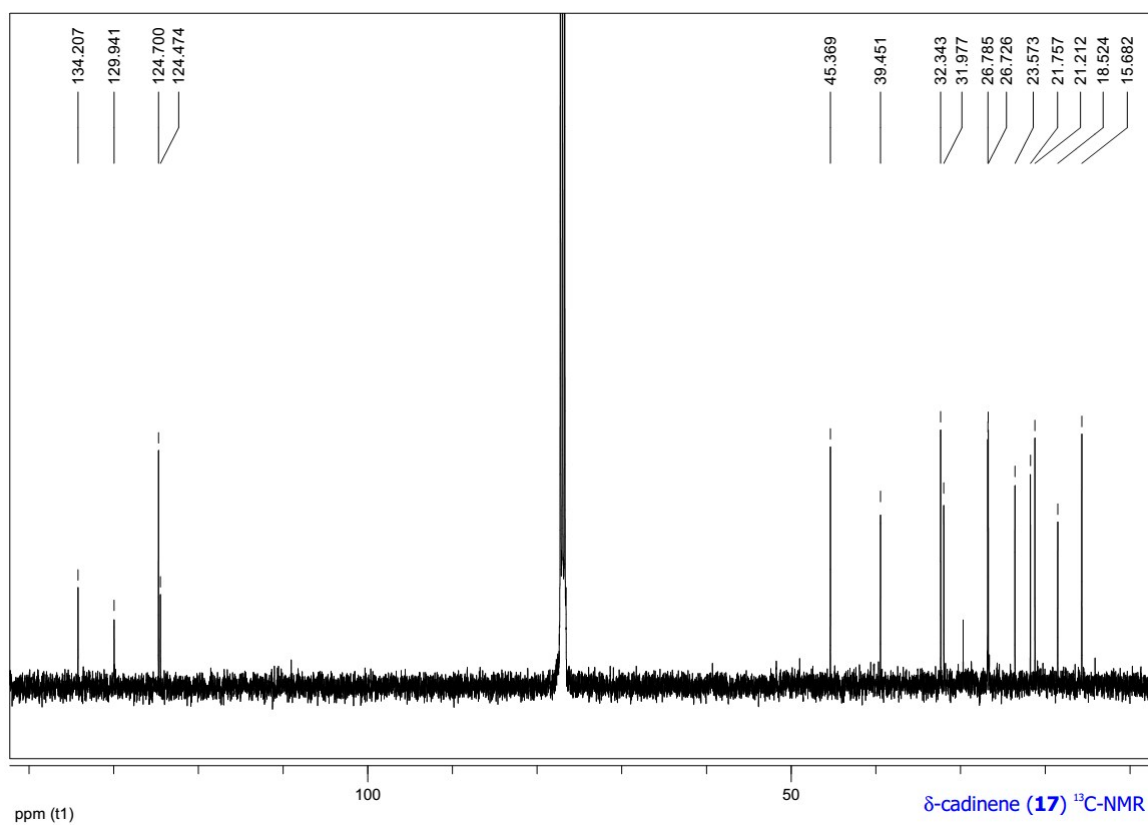
¹H- and ¹³C-NMR-Spectra

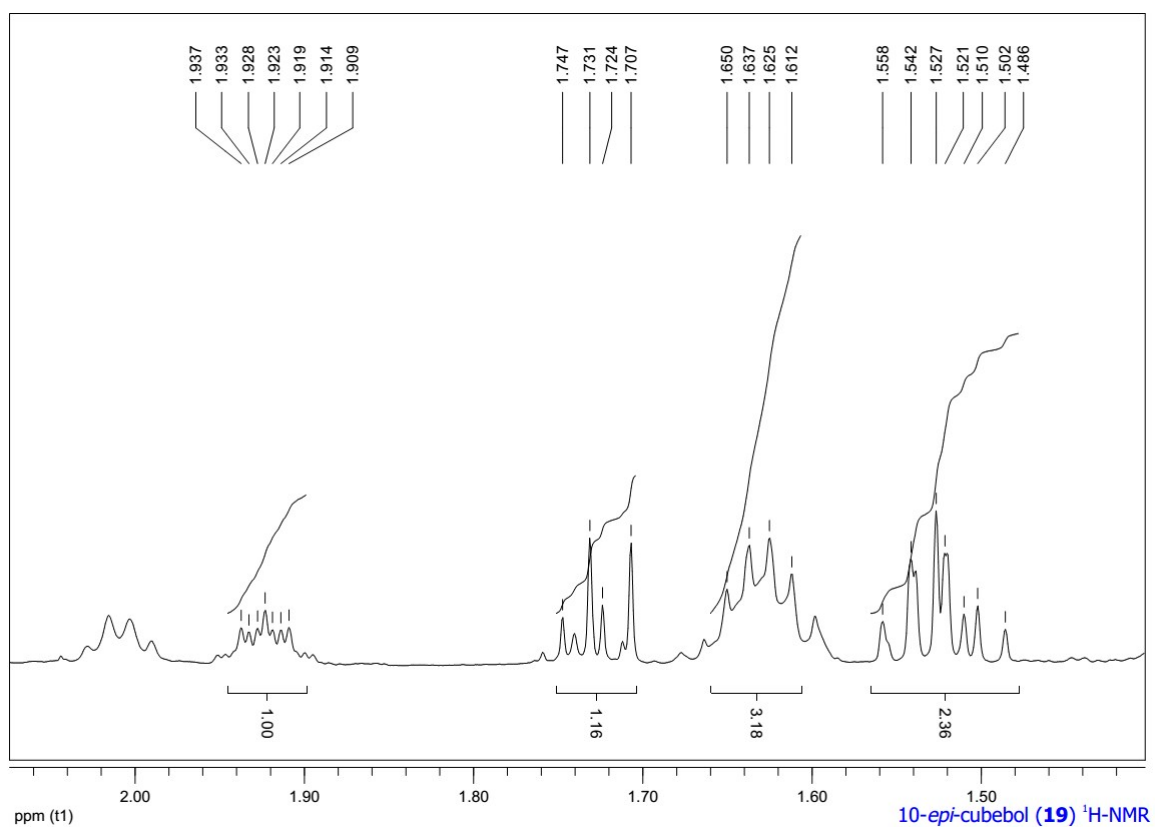


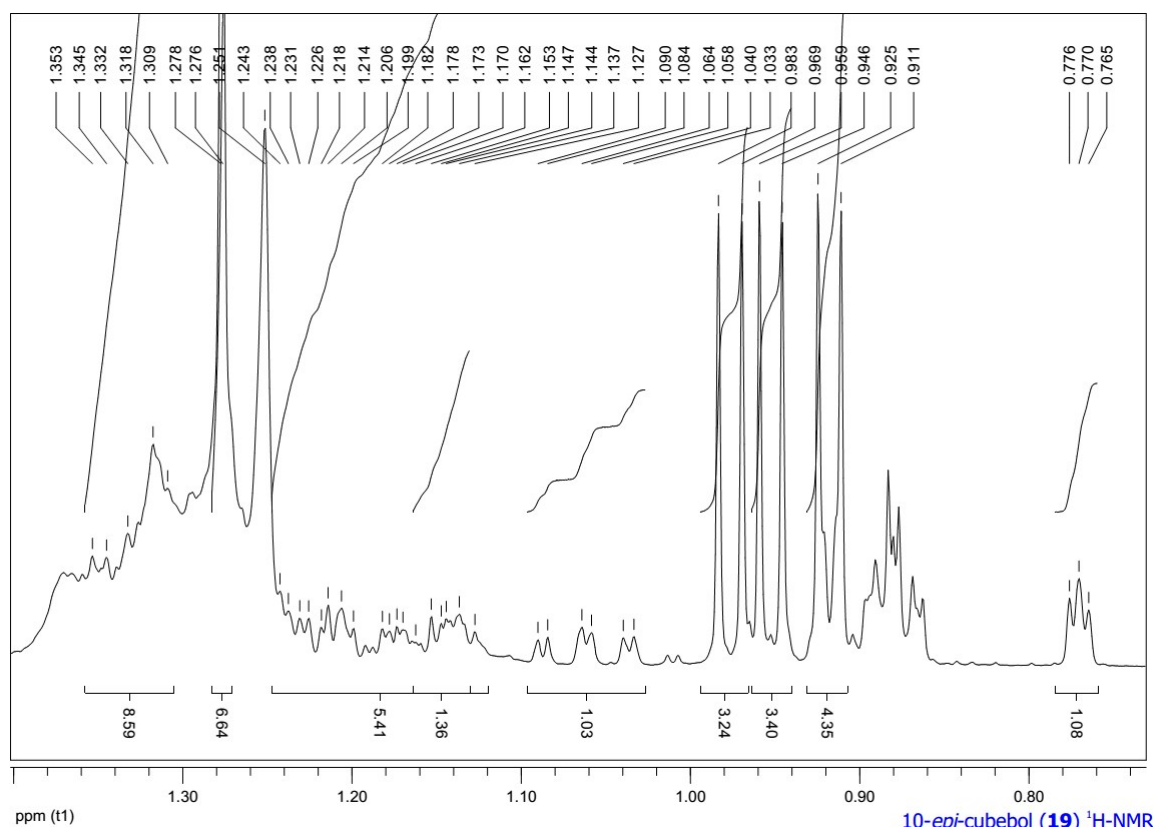




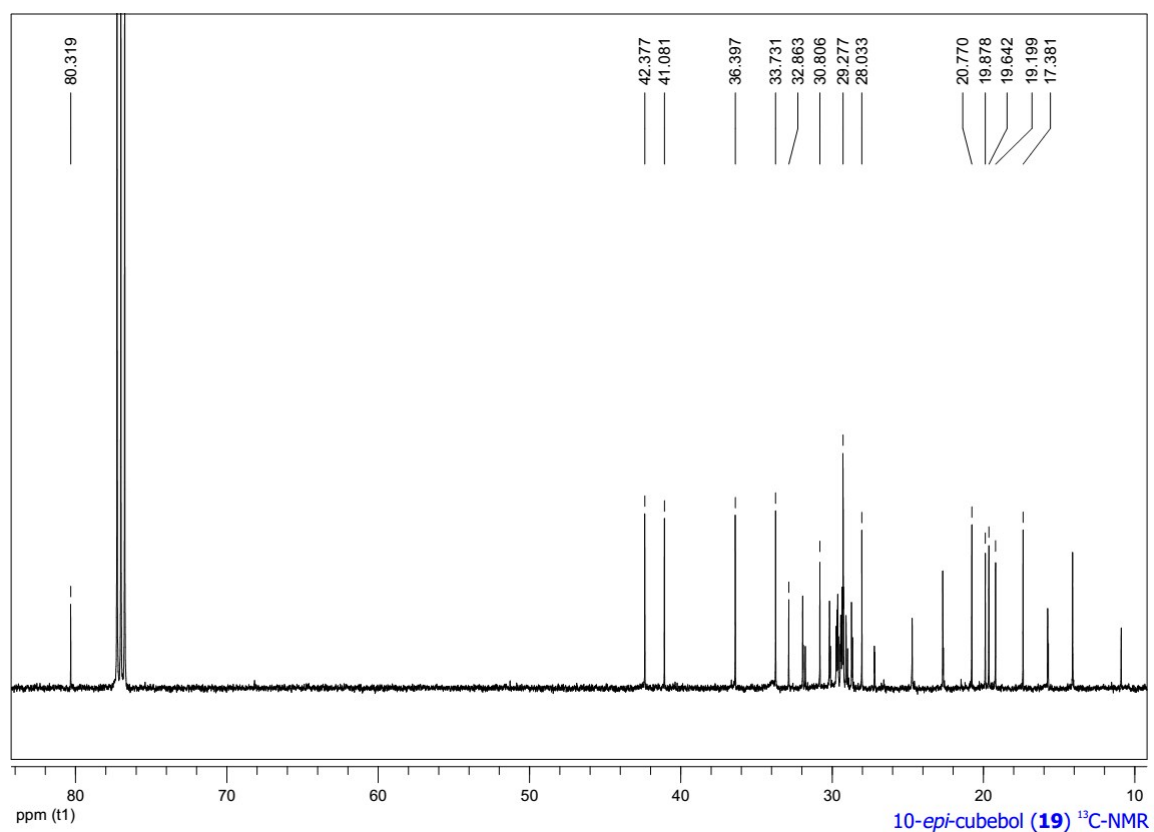




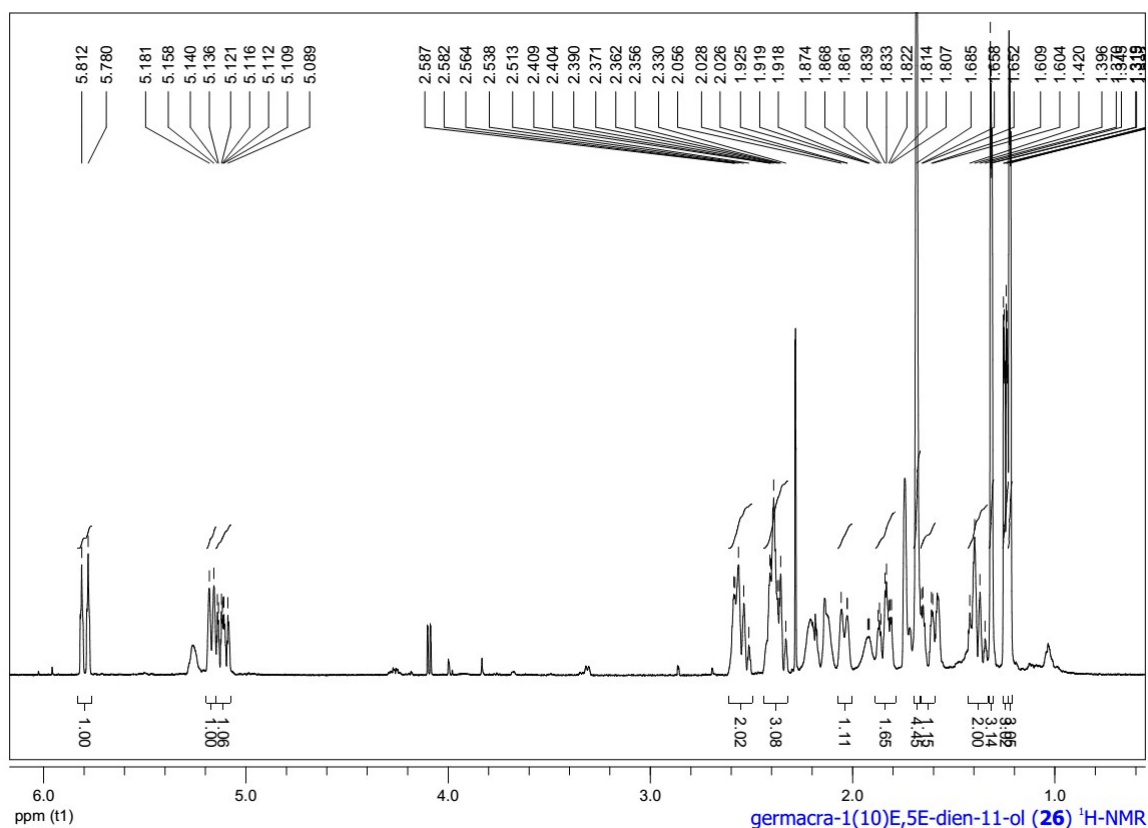




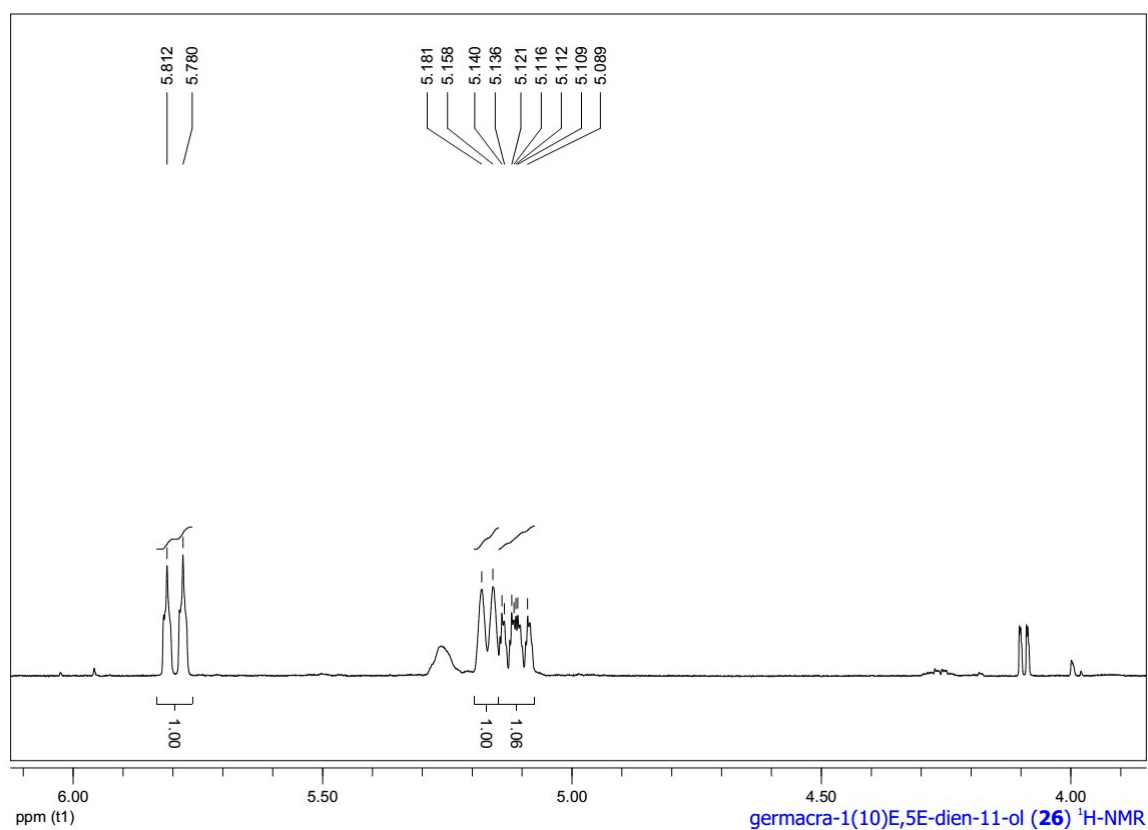
10-*epi*-cubebol (19) ¹H-NMR

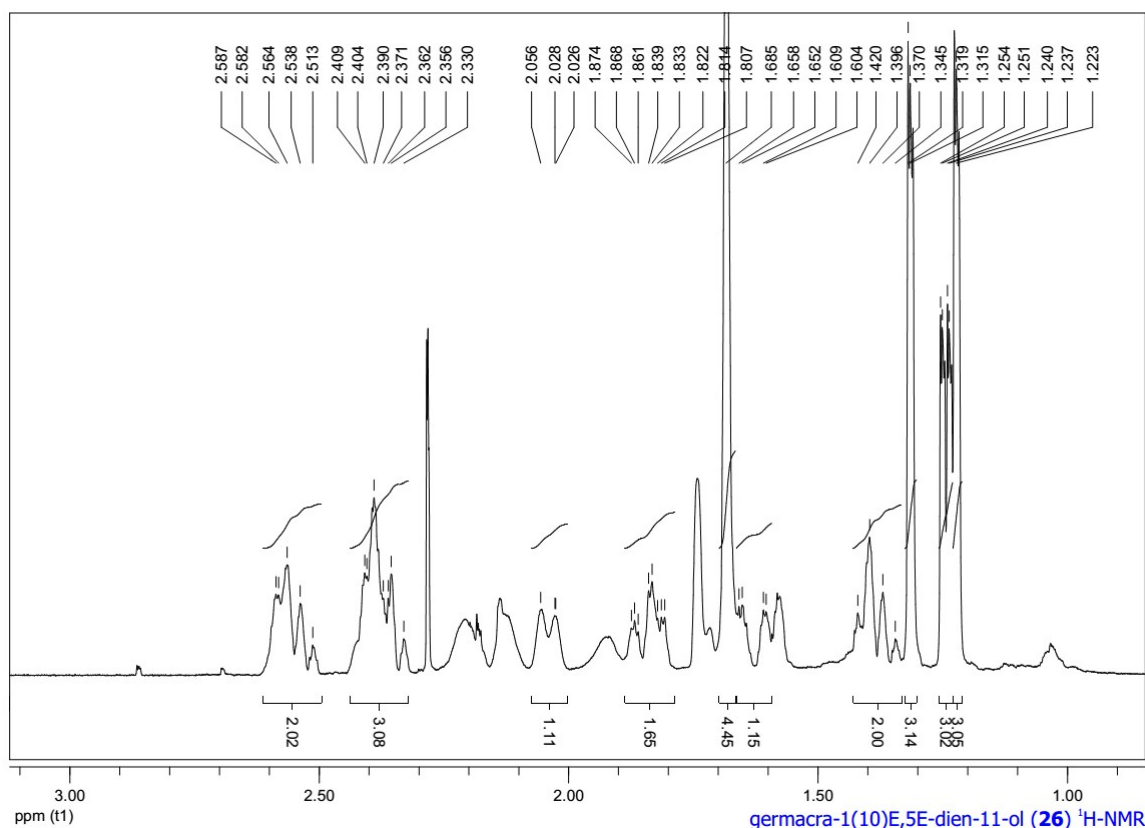


10-epi-cubebol (**19**) ¹³C-NMR

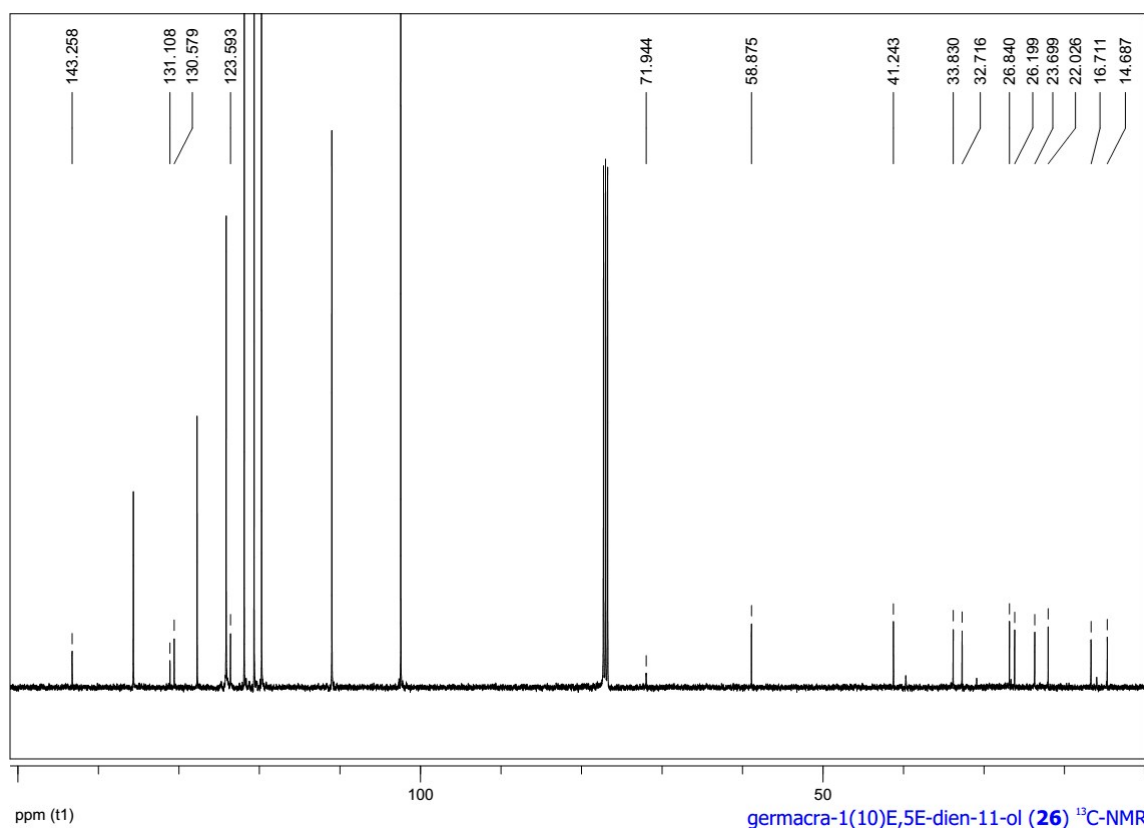


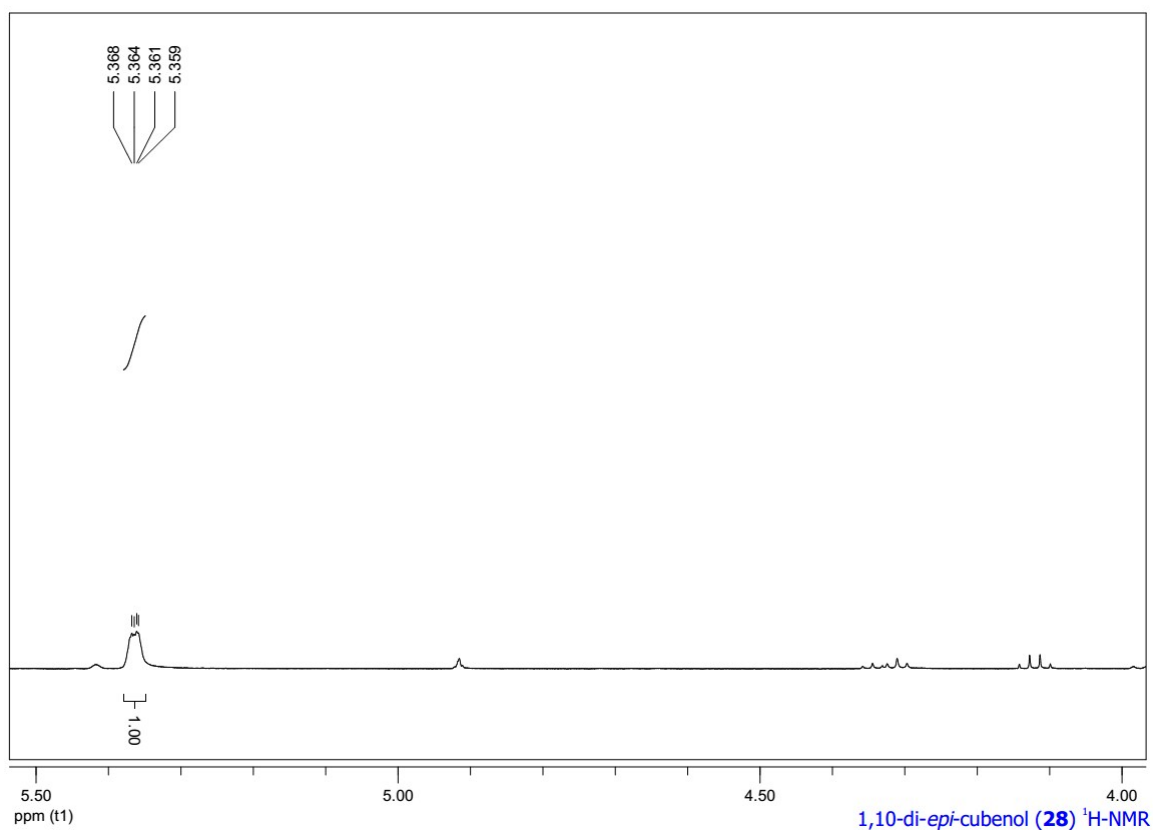
germacra-1(10)E,5E-dien-11-ol (**26**) ¹H-NMR

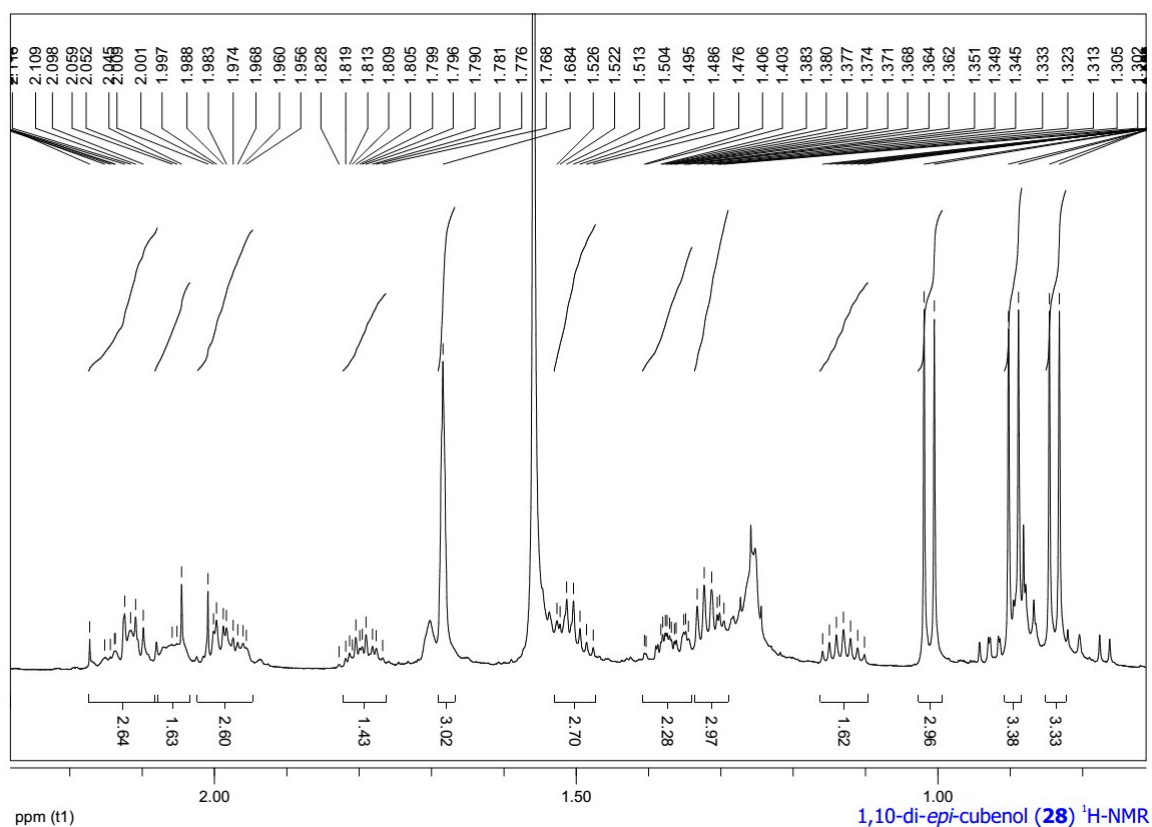




germacra-1(10)E,5E-dien-11-ol (**26**) ¹H-NMR







1,10-di-*epi*-cubenol (**28**) ¹H-NMR

