

## SUPPLEMENTARY FILES

### Evolutionary Insights into the Enzymes involved in the Biosynthesis of the Volatile Organic Compounds Isoprene and Pinene in Plants

#### SUPPLEMENTARY TABLE 1

##### List of Plants Emitting VOCs

1. *Acacia leucophloea/ Vachellia leucophloea*
2. *Adhatoda vasica*
3. *Albizia lebbeck*
4. *Atrocarpus heterophyllus*
5. *Azadirachta indica*
6. *Bombax ceiba*
7. *Butea monosperma*
8. *Casuarina equisetifolia*
9. *Citrus limon*
10. *Cocos nucifera*
11. *Dalbergia sissoo*
12. *Diospyros melanoxylon*
13. *Eucalyptus globulus*
14. *Ficus benghalensis*
15. *Ficus religiosa*
16. *Hibiscus rosasinensis*
17. *Lantana camara*
18. *Madhuca longifolia*
19. *Mangifera indica*
20. *Morus alba*
21. *Peltophorum pterocarpum*
22. *Psidium guajava*
23. *Pterocarpus marsupium*
24. *Pterospermum acerifolium*
25. *Schleichera oleosa*
26. *Syzygium jambolanum/ Syzygium cumini*
27. *Tecoma stans*
28. *Tectona grandis*

Name of Plant	Common Name	Family	Type of Plant	VOC produced	Area of growth in West Bengal	Reference
<i>Acacia leucophloea</i> / <i>Vachellia leucophloea</i>	White Bark Acacia	Mimosaceae	Deciduous	Moderate emitter – Isoprene, pinene, other VOCs	Murshidabad, Birbhum, Bankura, Purba Bardhaman, Paschim Bardhaman, Purba Medinipur, Paschim Medinipur	(1)
<i>Adhatoda vasica</i>	Malabar Nut/ Adulsa/ Vasaka	Acanthaceae	Evergreen	High emitter - Isoprene, $\alpha$ -pinene, other VOCs	Kakrajhore forest in West Medinipur, West Rarrh region, Lower Bengal	(2, 3)
<i>Albizia lebeck</i>	Shirish	Mimosaceae	Deciduous	Moderate emitter - Isoprene, $\alpha$ -pinene, other VOCs	Plains of West Bengal	(4)
<i>Atrocarpus heterophyllus</i>	Jackfruit	Moraceae	Evergreen tree	High emitter - Isoprene, monoterpenes	Throughout West Bengal	(5, 6)
<i>Azadirachta indica</i>	Neem	Meliaceae	Deciduous	Moderate emitter - Isoprene, $\alpha$ -pinene, other VOCs	Widespread	(7)
<i>Bombax ceiba</i>	Malabar silk cotton tree/ Shimul	Malvaceae	Deciduous	Moderate emitter - Isoprene, monoterpenes	Throughout plains to 800m	(8)
<i>Butea monosperma</i>	Flame of the forest tree/ Palash	Fabaceae	Deciduous	High emitter - Isoprene	Purulia, West Medinipore	(9 – 11)
<i>Casuarina equisetifolia</i>	Australian pine	Casuarinaceae	Evergreen	High emitter - Isoprene, $\alpha$ -pinene, other VOCs	Throughout West Bengal	(12)
<i>Citrus limon</i>	Lemon	Rutaceae	Deciduous	Moderate emitter - Isoprene, $\alpha$ -pinene, other VOCs	Red lateritic zone of West Bengal	(13)
<i>Cocos nucifera</i>	Coconut	Arecaceae	Evergreen	High emitter - Isoprene	Purba Bardhaman, Howrah, 24 Parganas, Midnapore	(14)

<i>Dalbergia sissoo</i>	Shisham	Papilionaceae	Deciduous	High emitter - Isoprene, $\alpha$ -pinene, other VOCs	South West Bengal	(4)
<i>Diospyros melanoxylon</i>	East Indian ebony/ Kendu	Ebenaceae	Deciduous or evergreen, , depending on habitat	Moderate emitter - Isoprene, monoterpenes	South West Bengal	(4)
<i>Eucalyptus globulus</i>	Gum tree/Striny bark	Myrtaceae	Mostly Evergreen	High emitter - Isoprene, $\alpha$ -pinene, other VOCs	Laterite soils of South and South Western Districts	(4)
<i>Ficus benghalensis</i>	Banyan	Moraceae	Evergreen	Moderate emitter – Isoprene, $\alpha$ -pinene, other VOCs	Throughout West Bengal	(15)
<i>Ficus religiosa</i>	Sacredfig	Moraceae	Deciduous tree	High emitter - Isoprene, $\alpha$ -pinene, other VOCs	From the coast up to 1200m, Bankura	(16)
<i>Hibiscus rosasinensis</i>	Hibiscus	Malvaceae	Evergreen	High emitter - Isoprene, $\alpha$ -pinene, other VOCs	Hooghly, Purba and Paschim Bardhaman, Birbhum	(17)
<i>Lantana camara</i>	Lantana	Verbenaceae	Evergreen shrub	High emitter - Isoprene, $\alpha$ -pinene, other VOCs	Howrah, purba and Paschim Bardhaman, Birbhum	(18)
<i>Madhuca longifolia</i>	Mahua	Sapotaceae	Evergreen to semi-evergreen	High emitter - Isoprene	Purulia, Bankura, West Midnapore and Jhargram.	(19)
<i>Mangifera indica</i>	Mango	Anacardiaceae	Evergreen	High emitter - Isoprene, $\alpha$ -pinene, other VOCs	Murshidabad and Malda districts	(20)
<i>Morus alba</i>	White mulberry	Moraceae	Deciduous	High emitter - Isoprene, $\alpha$ -pinene, other VOCs	Birbhum	(21)
<i>Peltophorum pterocarpum</i>	Yellow flame tree/ Radhachura	Fabaceae	Deciduous	High emitter - Isoprene	Birbhum	(22)
<i>Psidium guajava</i>	Guava	Myrtaceae	Evergreen	High emitter - Isoprene, $\alpha$ -pinene, other VOCs	North and South 24 Parganas, Nadia	(23)
<i>Pterocarpus marsupium</i>	Malabar kino/ Venkai	Fabaceae	Deciduous	High emitter - Isoprene, monoterpenes	Wild and also planted in South Bengal	(24)

<i>Pterospermum macerifolium</i>	Kanak Champa	Sterculiaceae	Deciduous	Moderate emitter - Isoprene, $\alpha$ -pinene, other VOCs	Eastern districts of Bengal	(25)
<i>Schleichera oleosa</i>	Kusum	Sapindaceae	Deciduous	Moderate emitter – Isoprene, $\alpha$ -pinene, other VOCs	Found throughout the hotter parts of south West Bengal, in red lateritic soil.	(4)
<i>Syzygium jambolanum</i> / <i>Syzygium cumini</i>	Malabar plum	Myrtaceae	Evergreen	High emitter - Isoprene, $\alpha$ -pinene, other VOCs	Throughout West Bengal	(26)
<i>Tecoma stans</i>	Yellow bells	Bignoniaceae	Semi-evergreen shrub	Moderate emitter – Isoprene, $\alpha$ -pinene, other VOCs	Purba and Paschim Bardhaman	(27)
<i>Tectona grandis</i>	Teak	Lamiaceae	Deciduous	High emitter - Isoprene	Lower Hill forests in North Bengal, Jhargram	(28)

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**SUPPLEMENTARY TABLE 2****Data for enrichment profile – MEP Pathway**

<b>Name of Enzyme</b>	<b>Number of families common to gene-specific and protein-specific trees</b>	<b>Common families</b>
Isoprene Synthase	5	Salicaceae Euphorbiaceae Fabaceae Lamiaceae Poaceae
Isopentenyl Diphosphate Isomerase	3	Brassicaceae Lamiaceae Nyssaceae
Hydroxymethylbutenyl diphosphate reductase	0	N/A
Hydroxymethylbutenyl diphosphate synthase	0	N/A
Methylerythritol 2,4-cyclodiphosphate synthase	0	N/A
CDP-ME kinase	2	Lamiaceae Solanaceae
Diphosphocytidylyl methyl erythritol synthase	2	Brassicaceae Poaceae
1-deoxyxylulose-5-phosphate reductoisomerase	0	N/A
1-deoxyxylulose 5-phosphate synthase	1	Solanaceae

**Data for enrichment profile – MVA Pathway**

<b>Name of Enzyme</b>	<b>Number of families common to gene-specific and protein-specific trees</b>	<b>Common families</b>
Pinene Synthase	2	Lamiaceae Pinaceae
Geranyl diphosphate synthase	13	Apocynaceae Asteraceae Brassicaceae Cannabaceae Fabaceae Lamiaceae Lauraceae Magnoliaceae Pinaceae Plantaginaceae Rosaceae Solanaceae Vitaceae
Mevalonate pyrophosphate decarboxylase/ Diphosphomevalonate decarboxylase	1	Brassicaceae
Phosphomevalonate kinase	1	Brassicaceae
Mevalonate 5 kinase	1	Brassicaceae
3-hydroxy-3-methylglutaryl-CoA reductase/ HMG CoA reductase	4	Solanaceae Poaceae Brassicaceae Malvaceae
3-hydroxy-3-methylglutaryl-CoA synthase/ HMG CoA synthase	0	N/A
Acetoactyl CoA thiolase	0	N/A

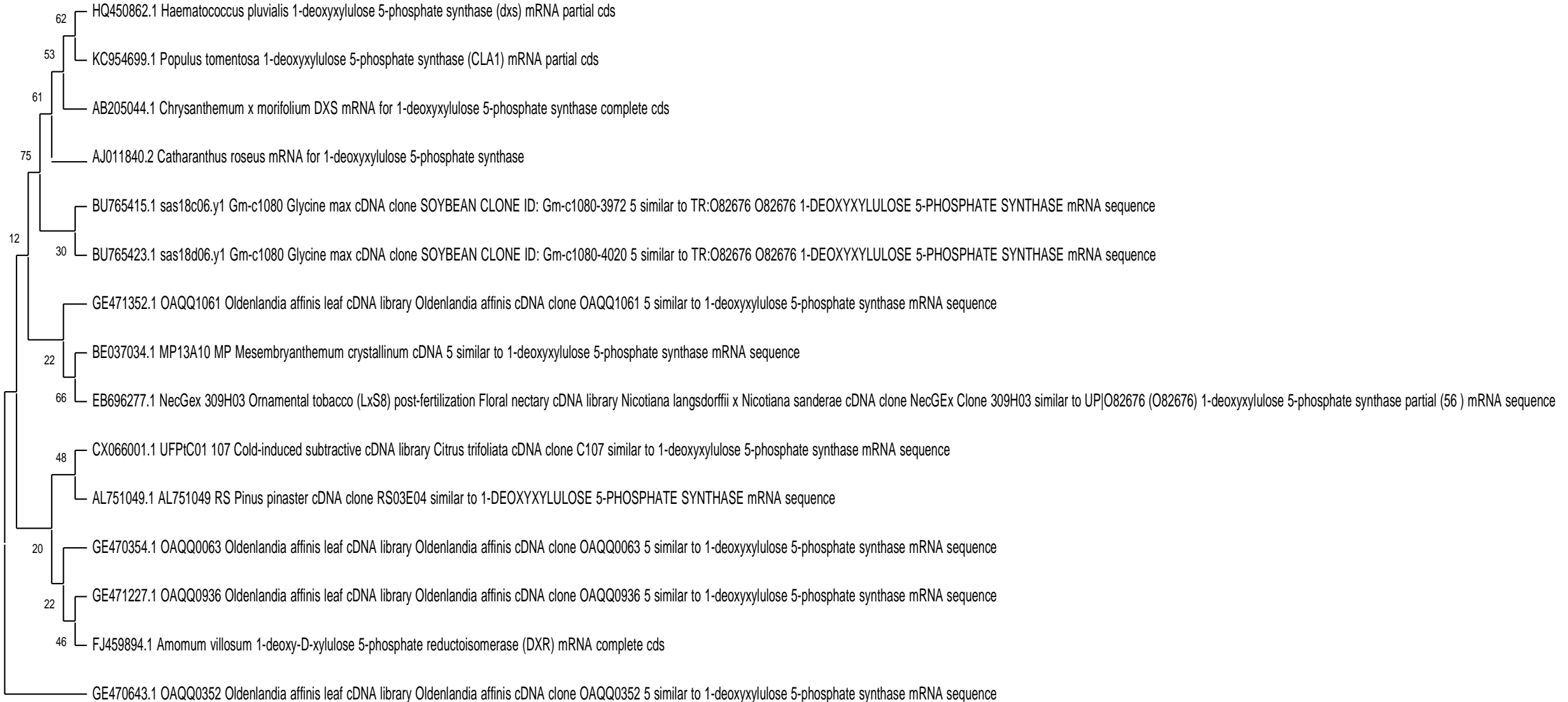
**SUPPLEMENTARY 3**  
**- PHYLOGENETIC TREES**



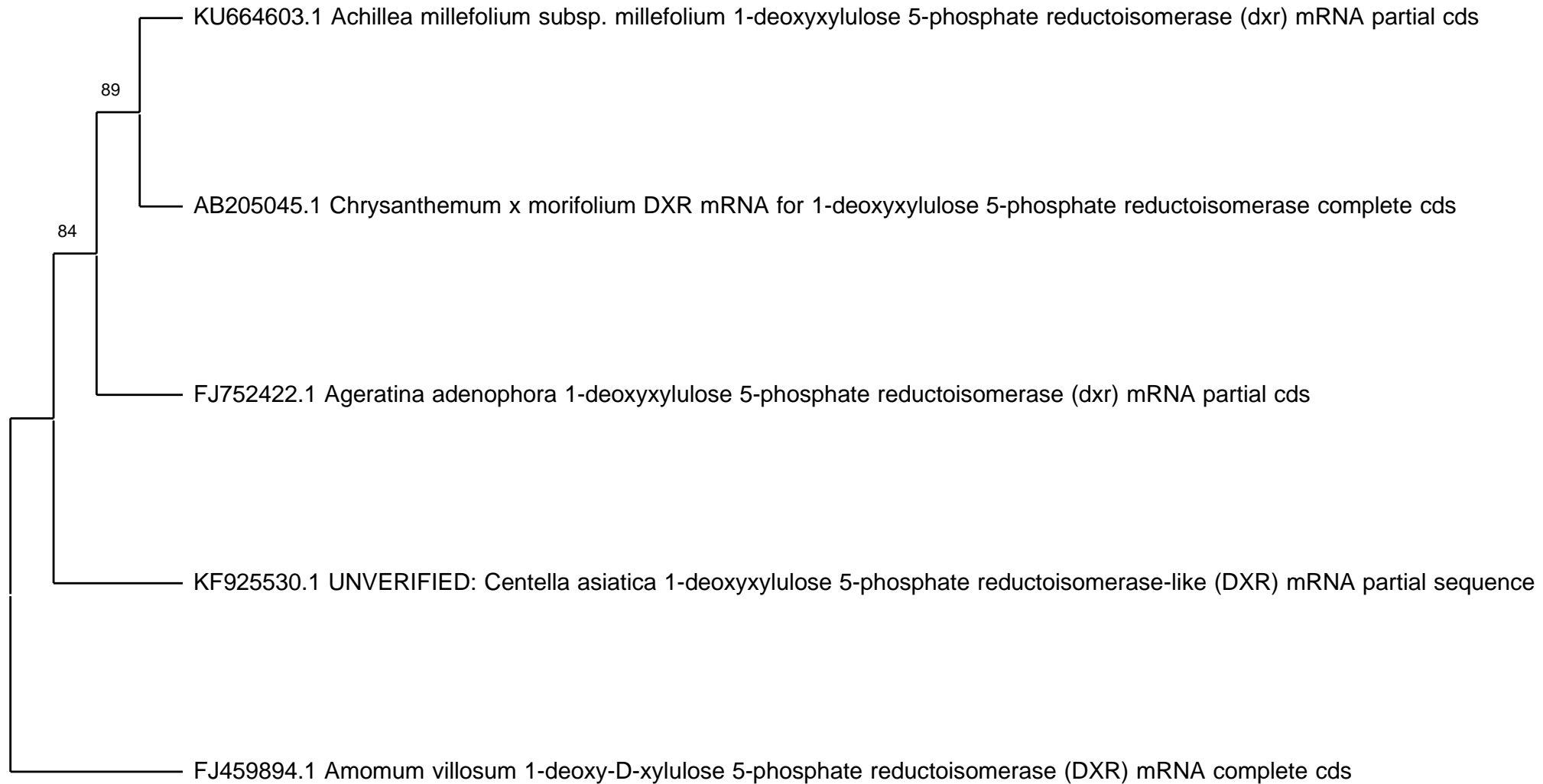
**METHYLERYTHRITOL PHOSPHATE (MEP)  
PATHWAY**

# **GENBANK PHYLOGENETIC TREES**

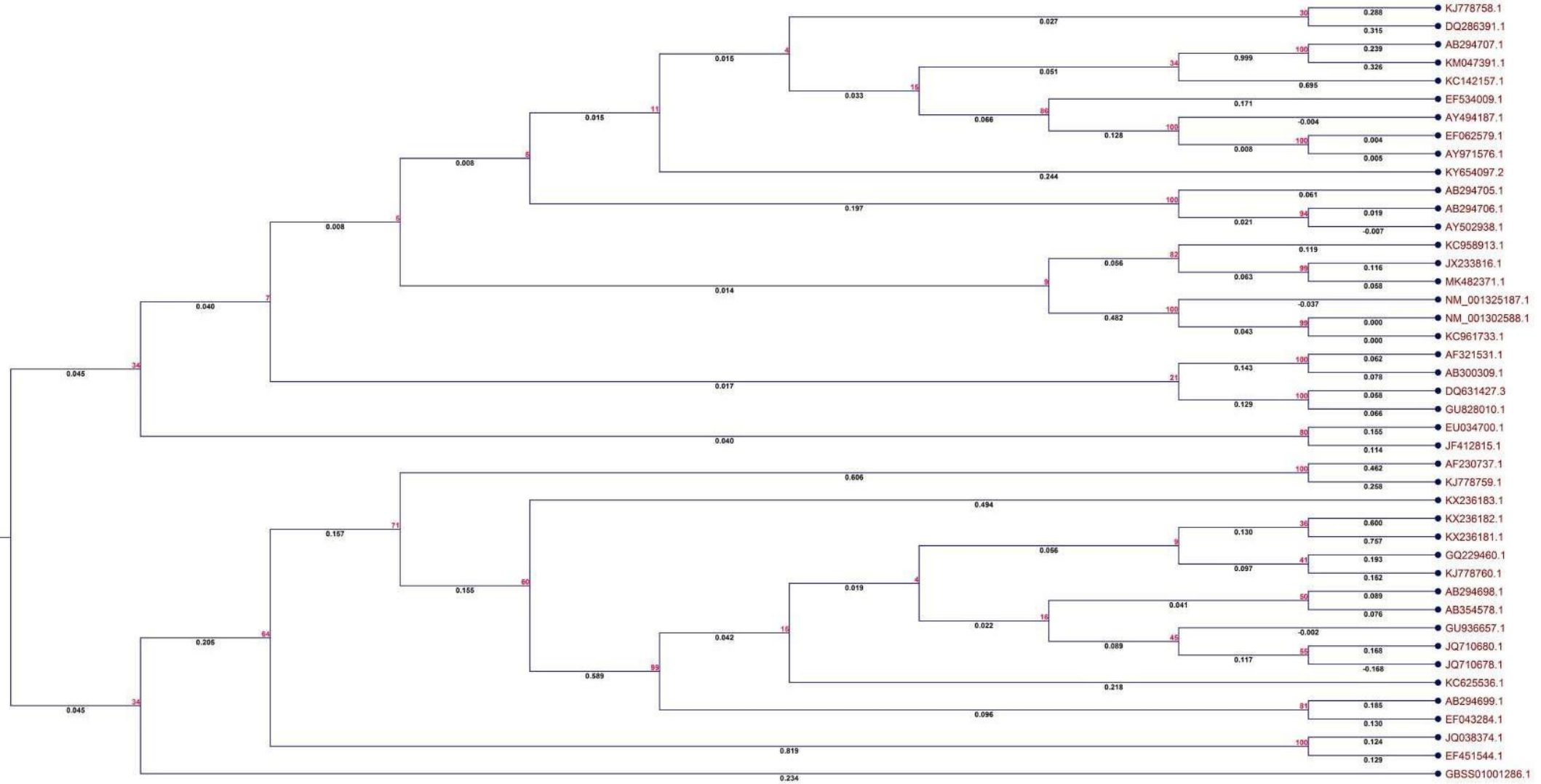
# Deoxyxylulose 5-phosphate (DXP) Synthase



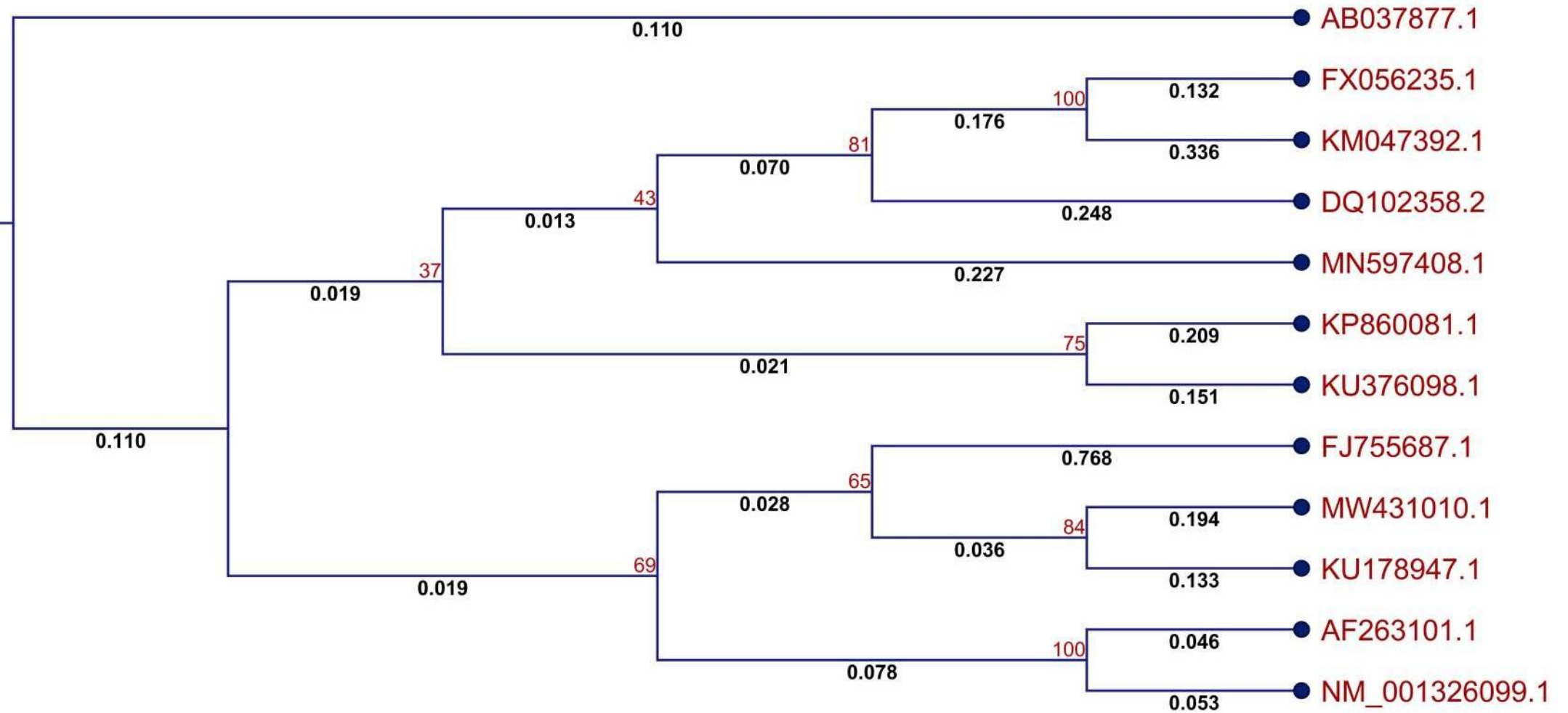
# Deoxyxylulose 5-phosphate (DXP) Reductoisomerase



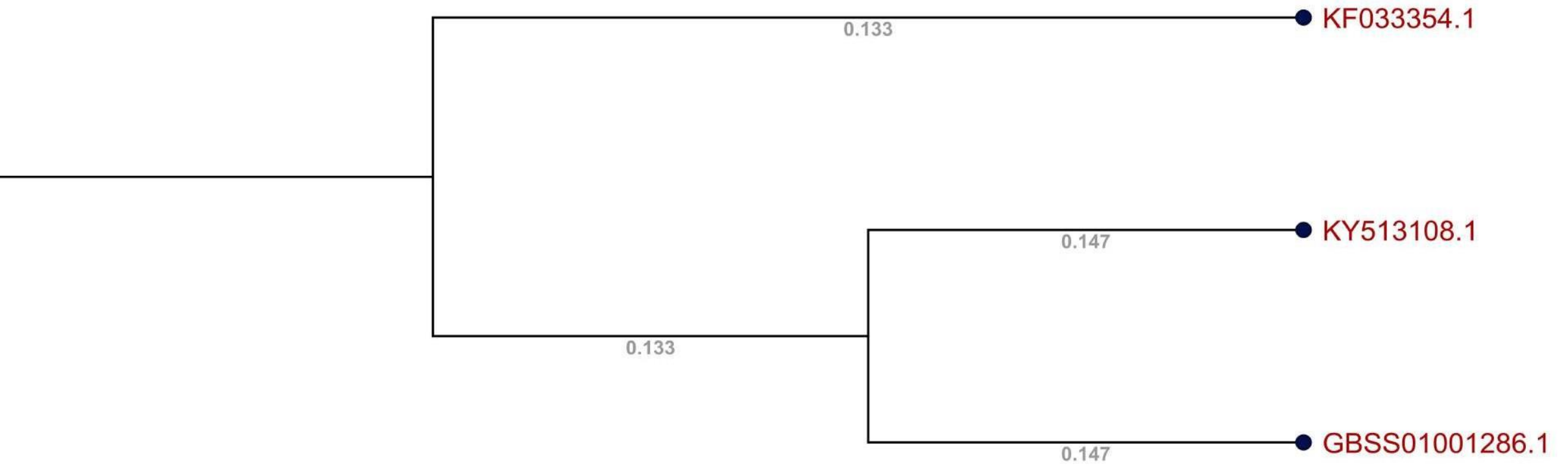
# Diphosphocytidylyl methyl erythritol (CDP-ME) Synthase



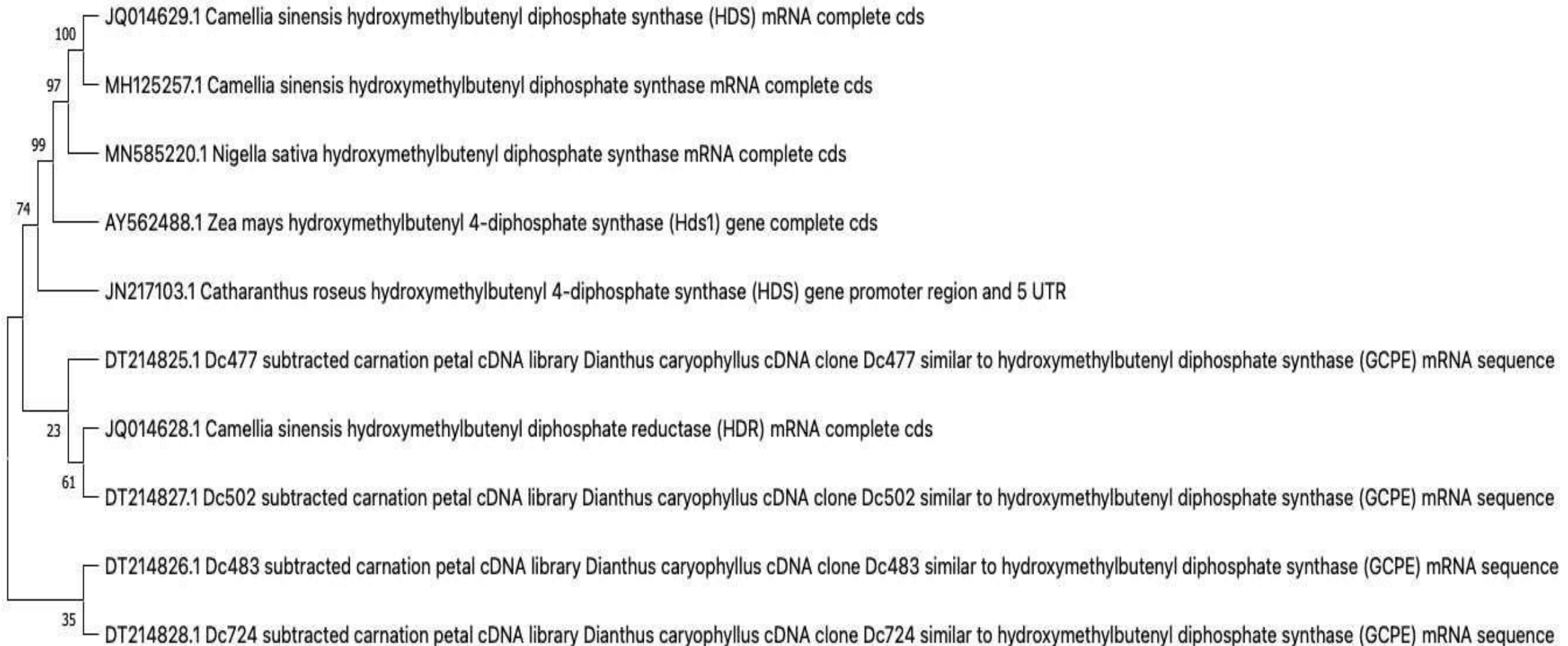
# Diphosphocytidylyl methyl erythritol (CDP-ME) Kinase



# Methylerythritol 2,4-cyclodiphosphate (ME-cPP) Synthase

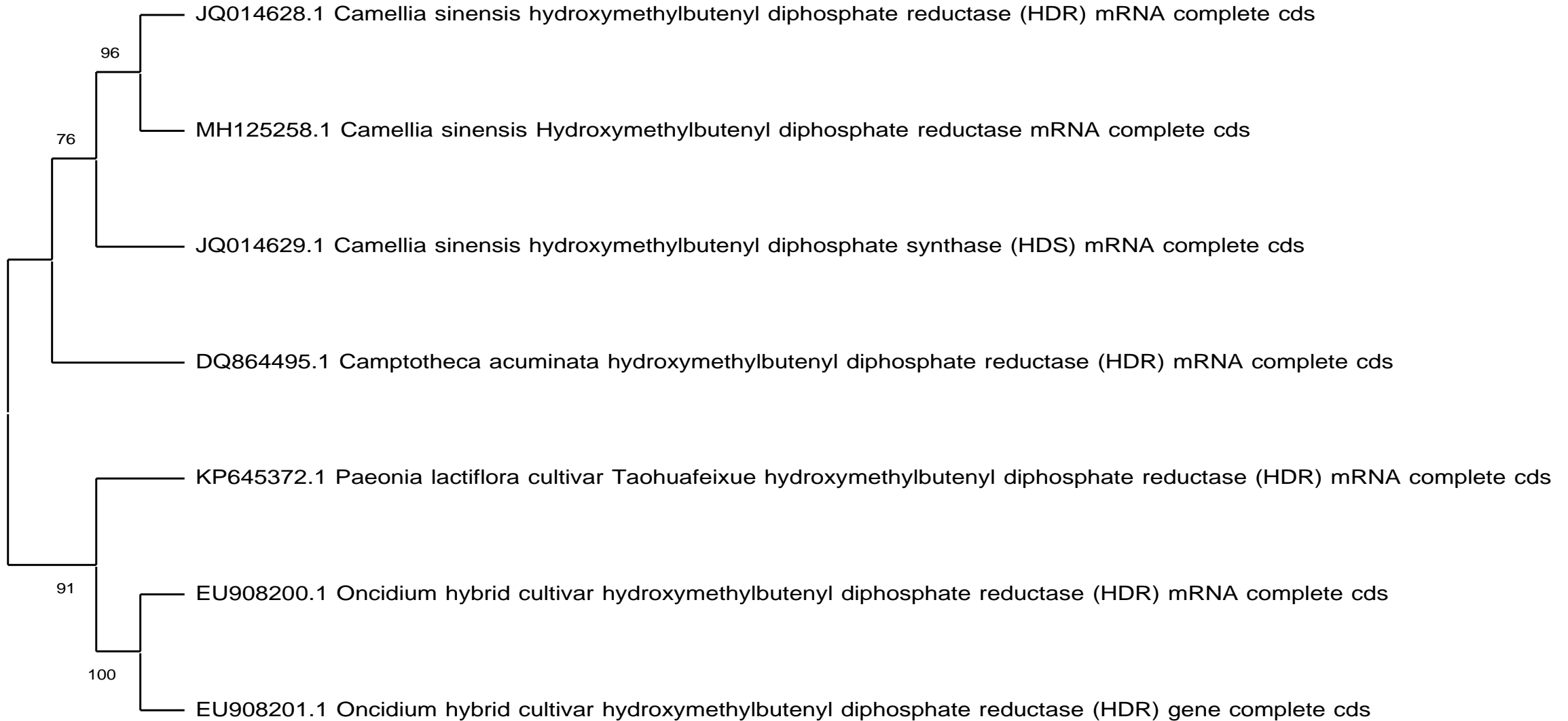


## Hydroxymethylbutenyl diphosphate (HMBPP) Synthase



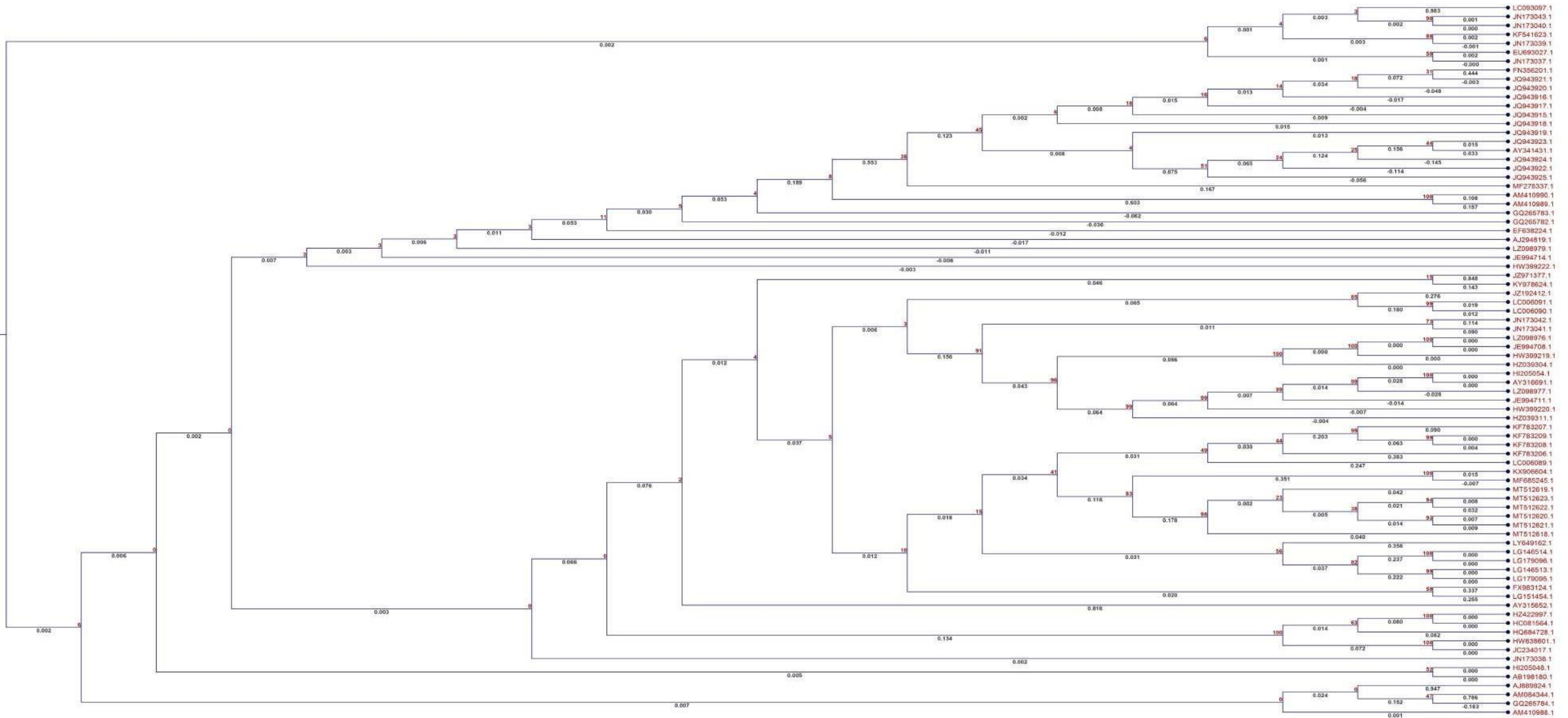


# Hydroxymethylbutenyl diphosphate (HMBPP) Reductase



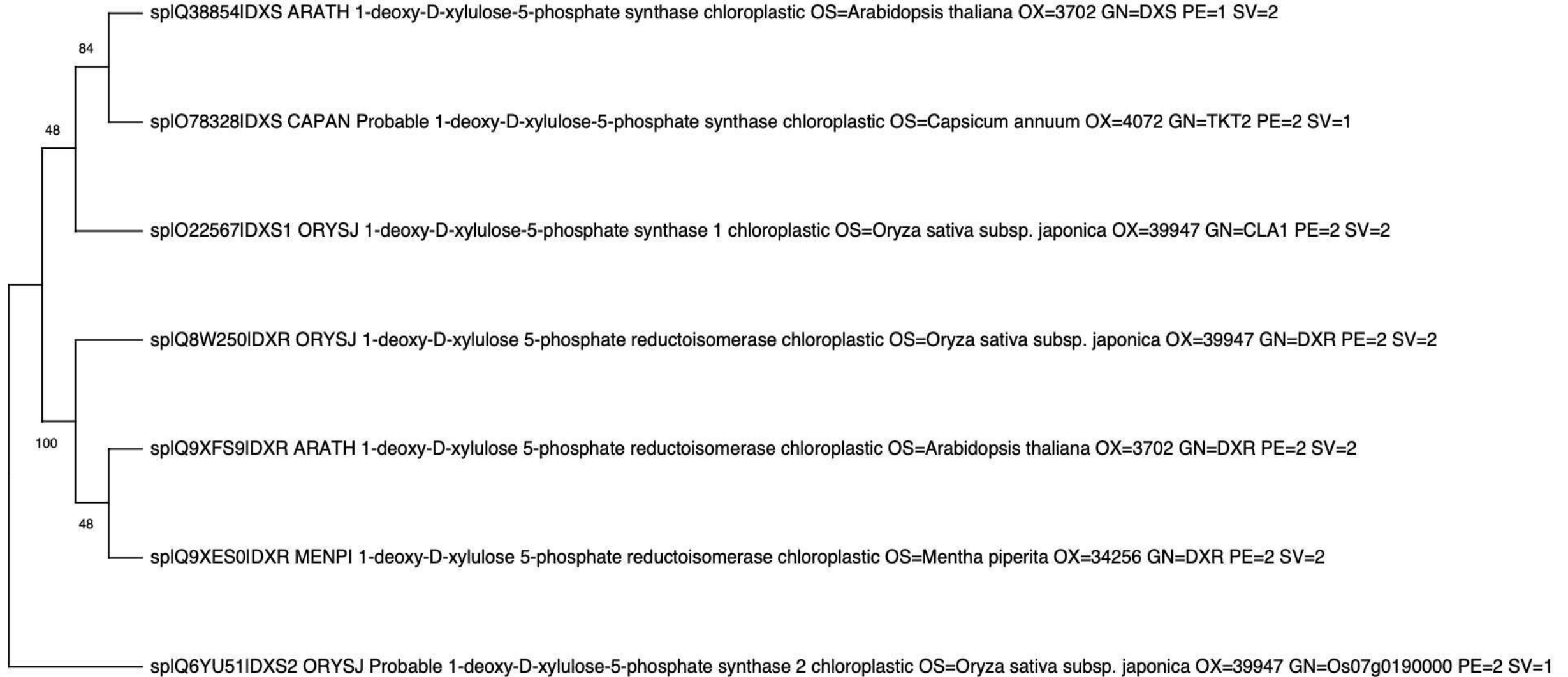


# Isoprene Synthase

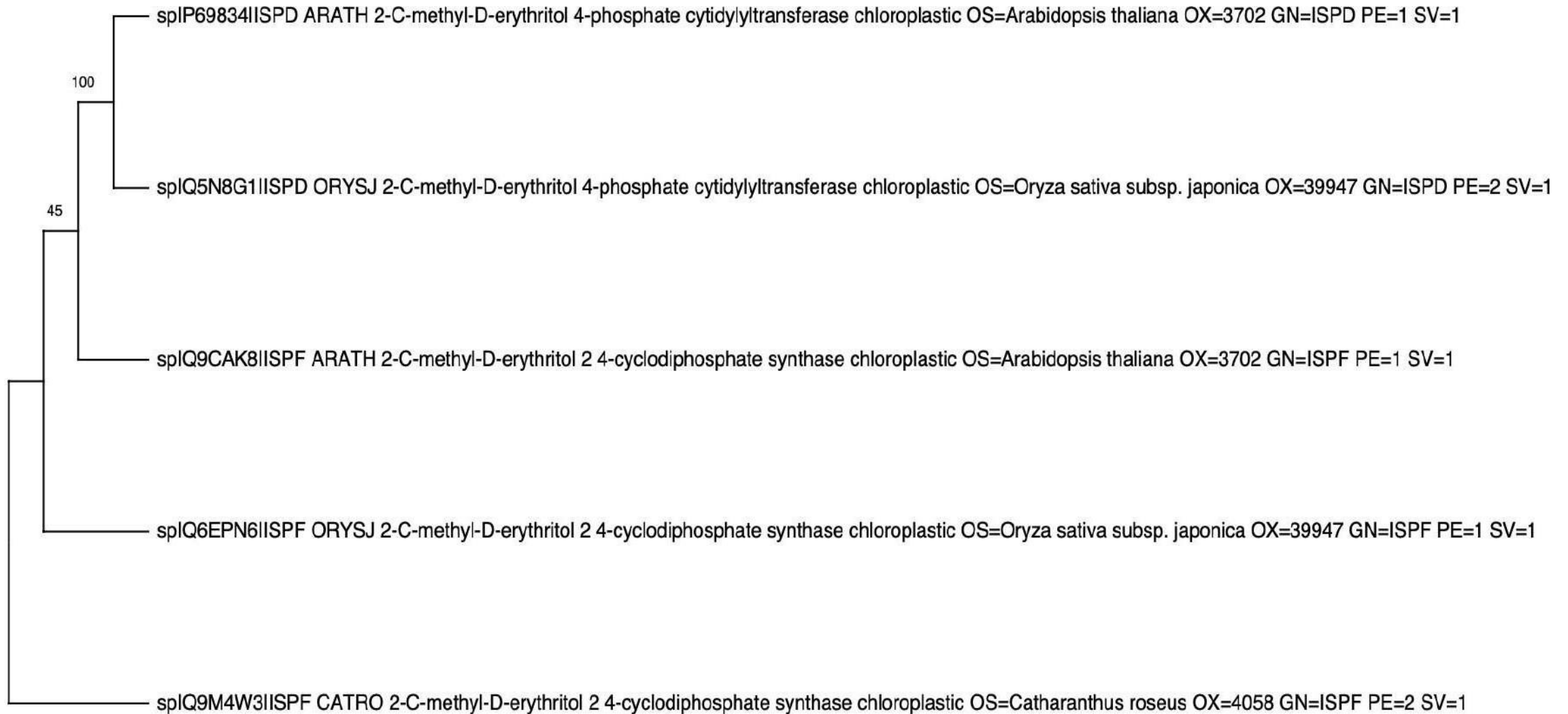


# **UNIPROT PHYLOGENETIC TREES**

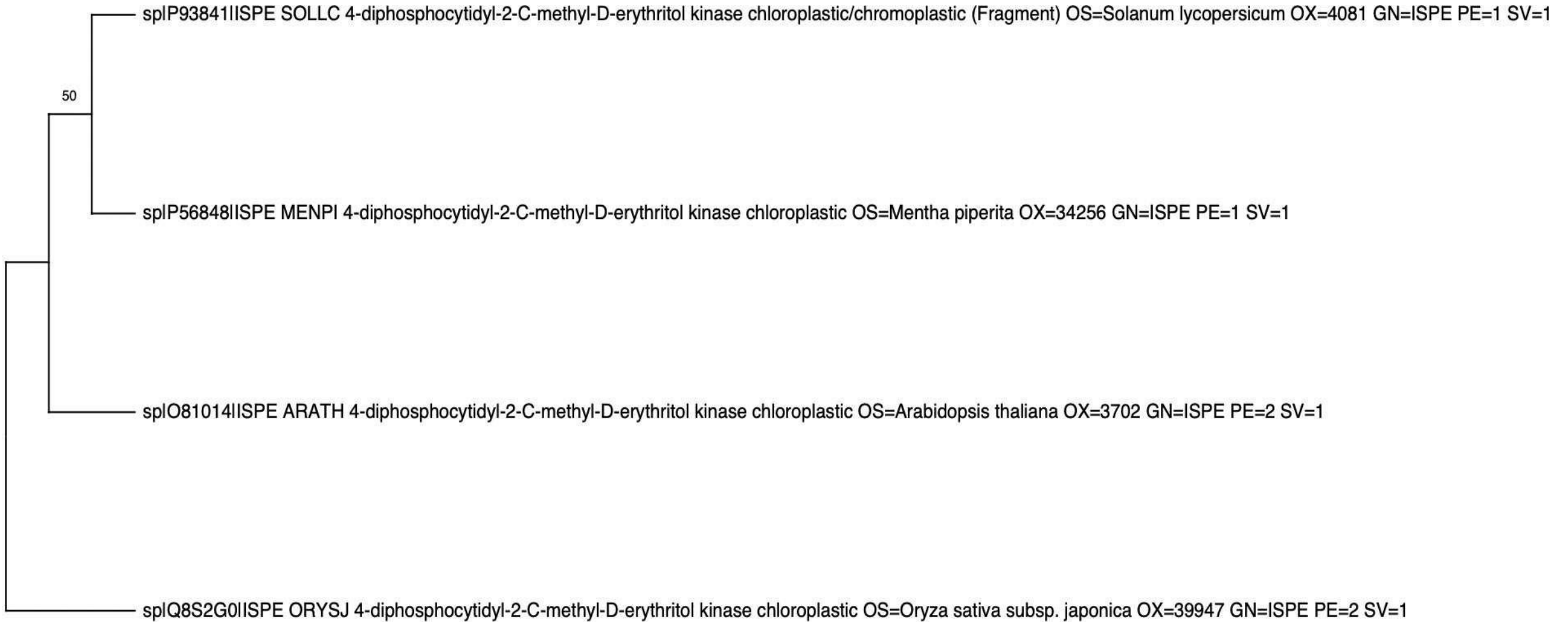
# Deoxyxylulose 5-phosphate (DXP) Synthase



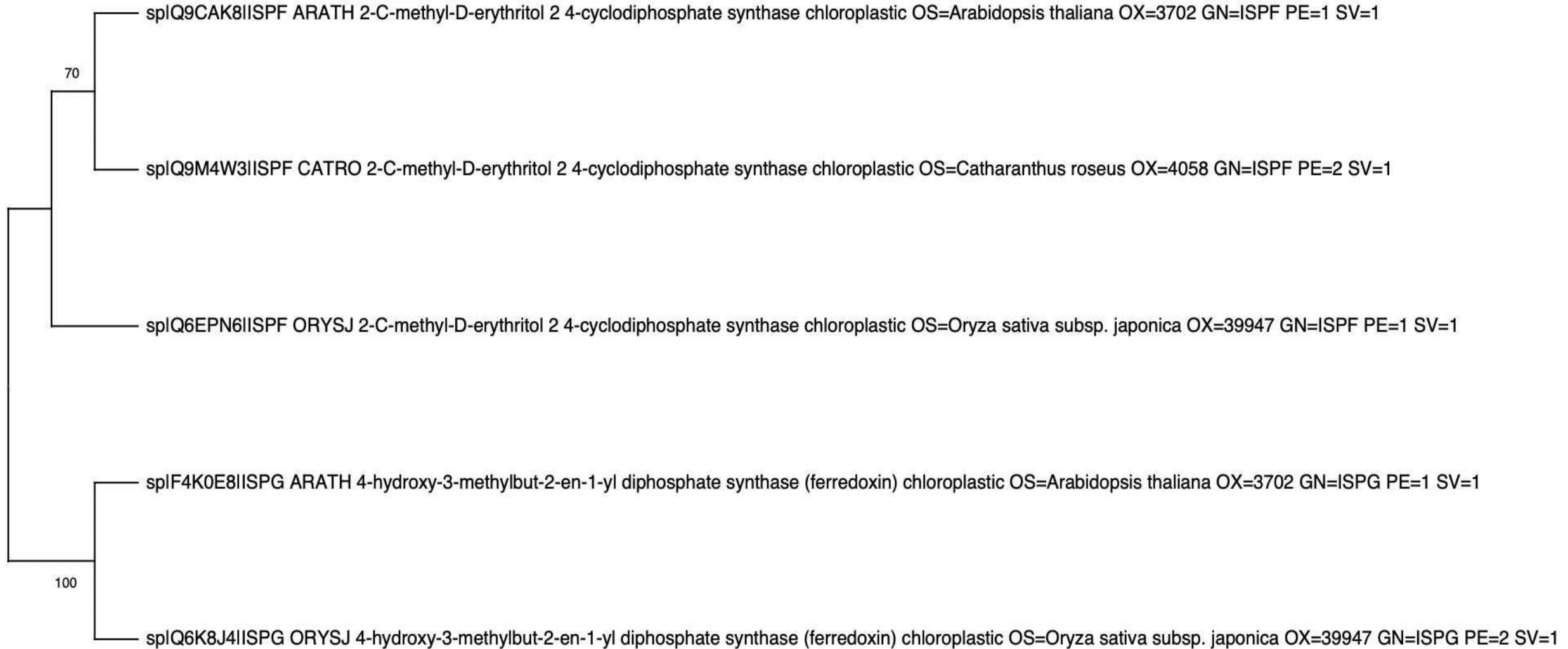
# Diphosphocytidylyl methyl erythritol (CDP-ME) Synthase



# Diphosphocytidylyl methyl erythritol (CDP-ME) Kinase

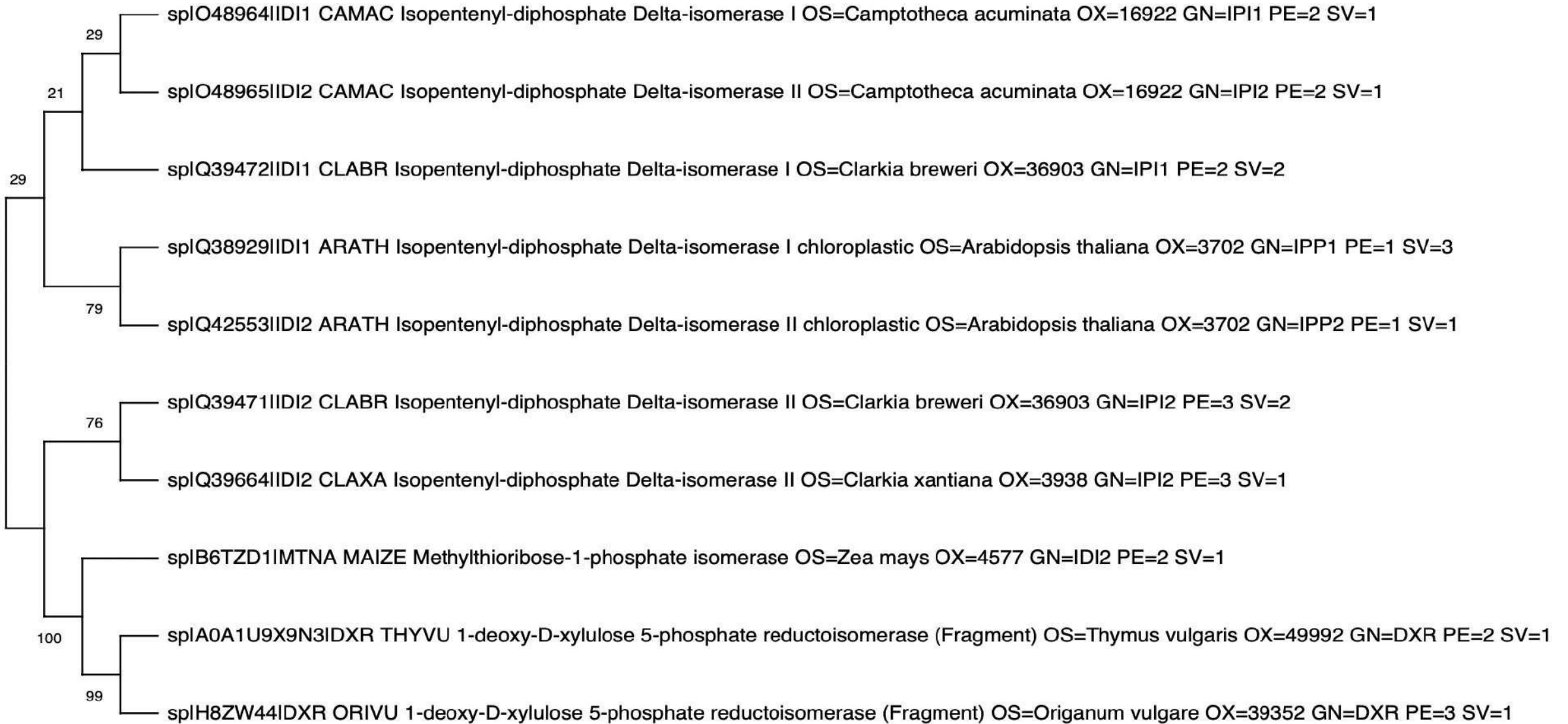


# Methylerythritol 2,4-cyclodiphosphate (ME-cPP) Synthase

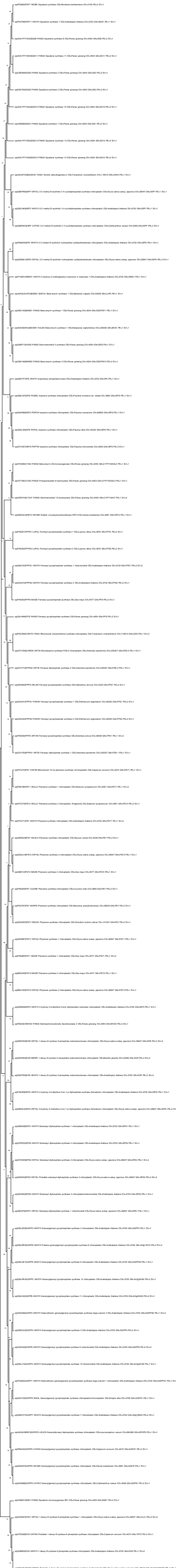




# Isopentenyl diphosphate Isomerase



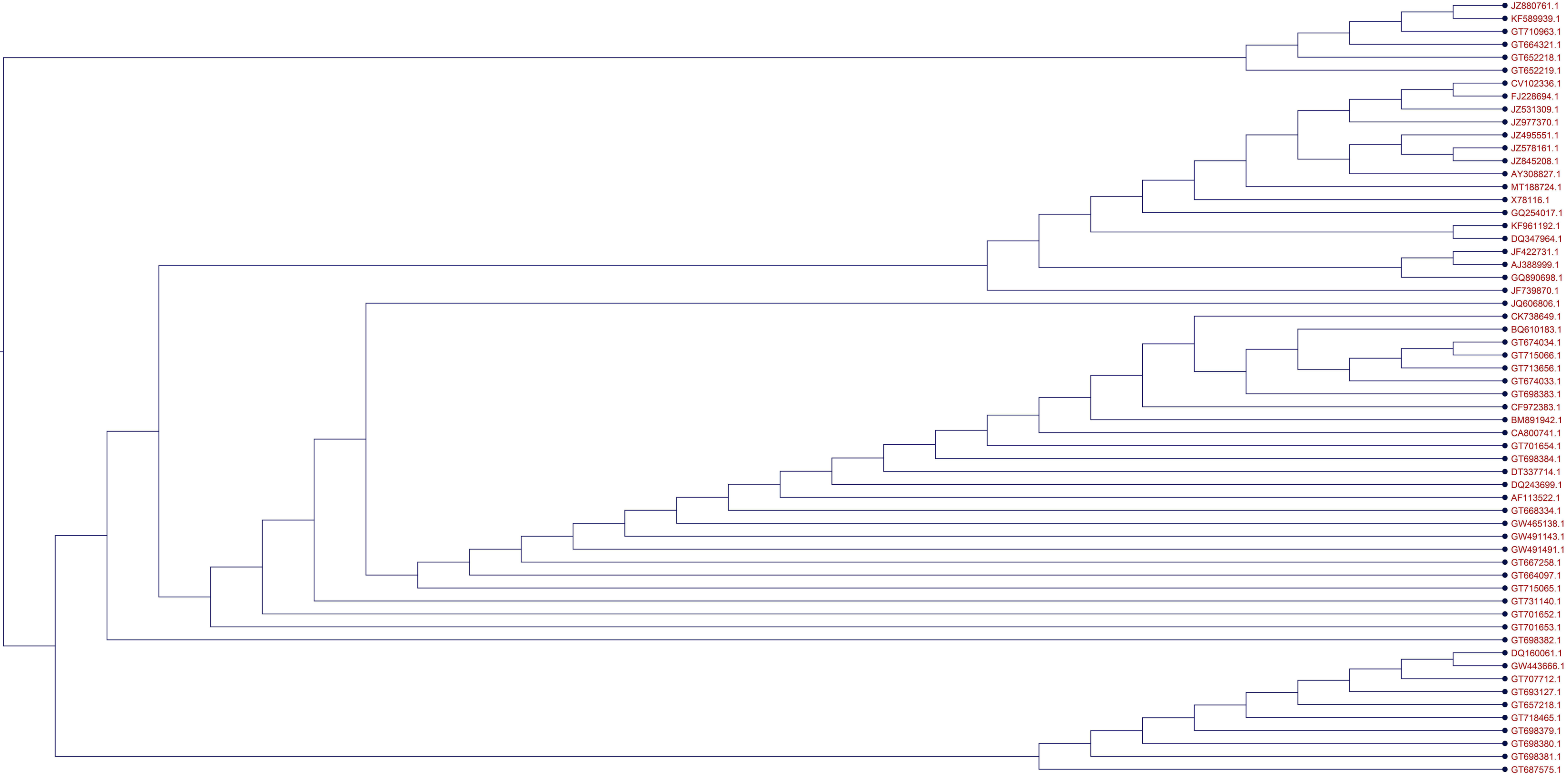
# Isoprene Synthase



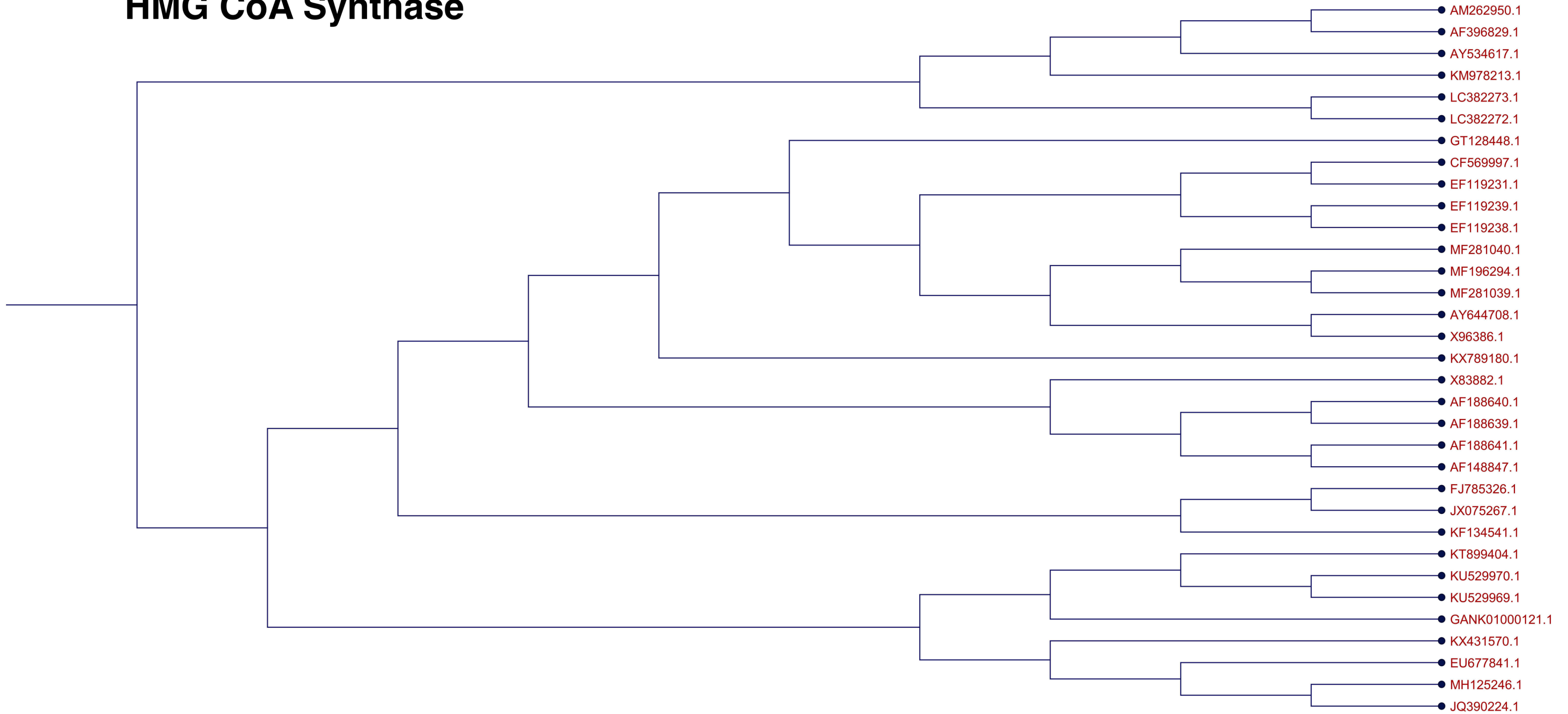
# **MEVALONIC ACID (MVA) PATHWAY**

# **GENBANK PHYLOGENETIC TREES**

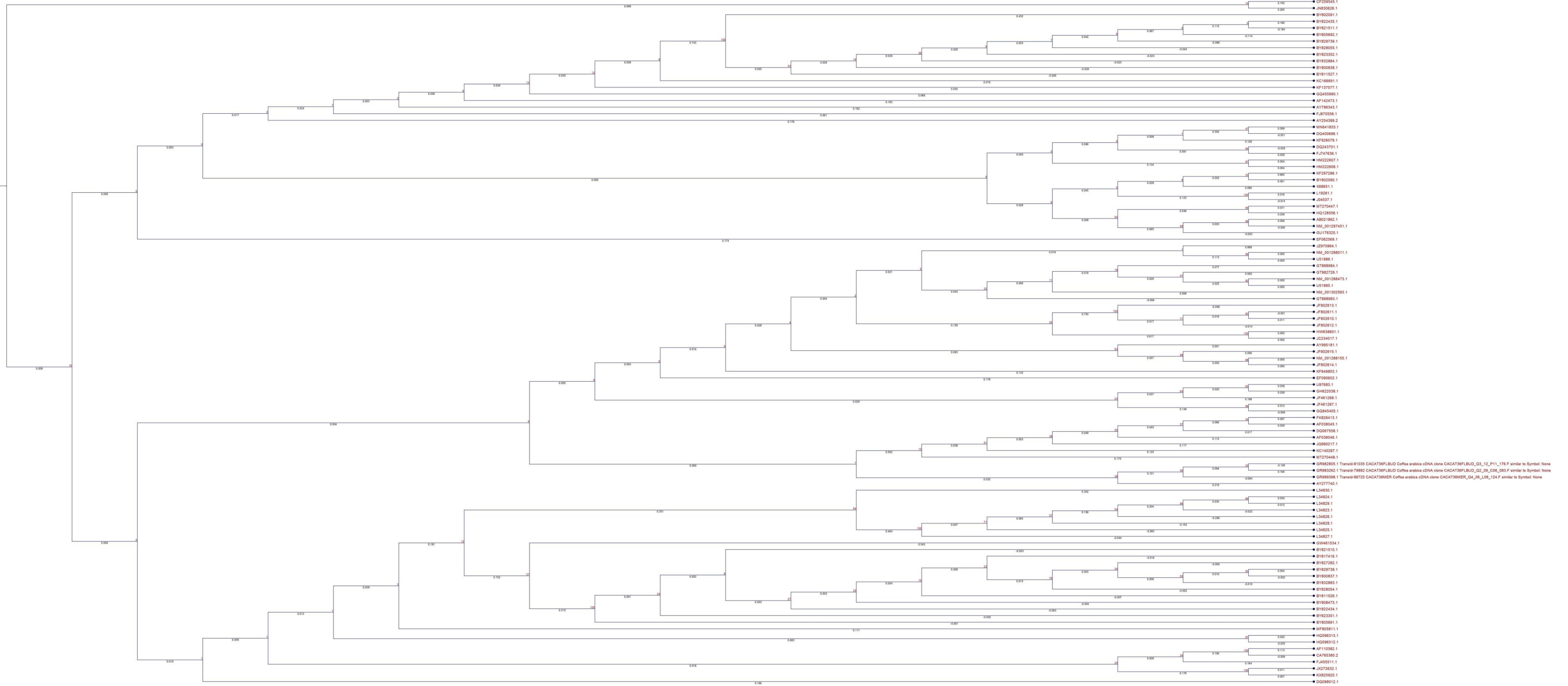
# Acetoacetyl CoA thiolase



# HMG CoA Synthase

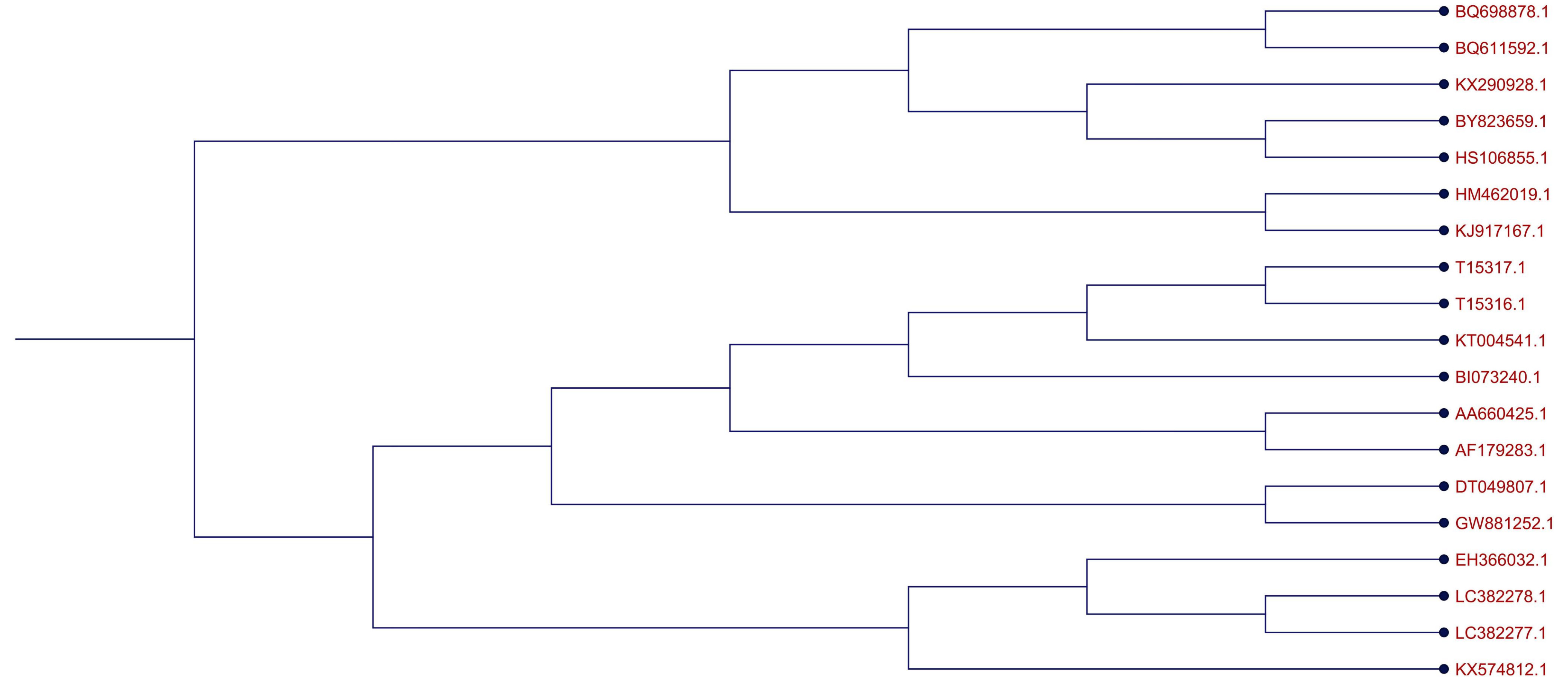


# HMG CoA reductase

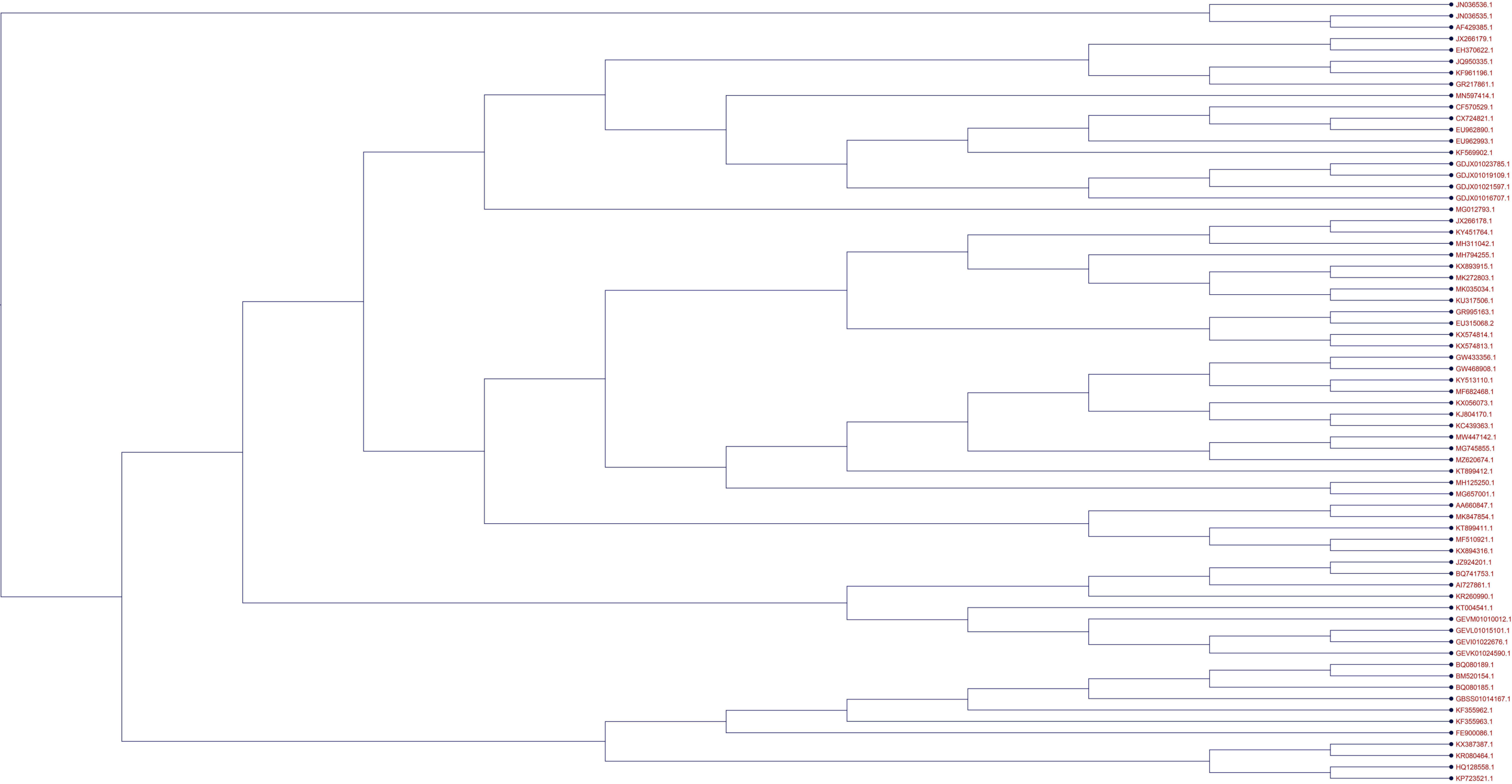




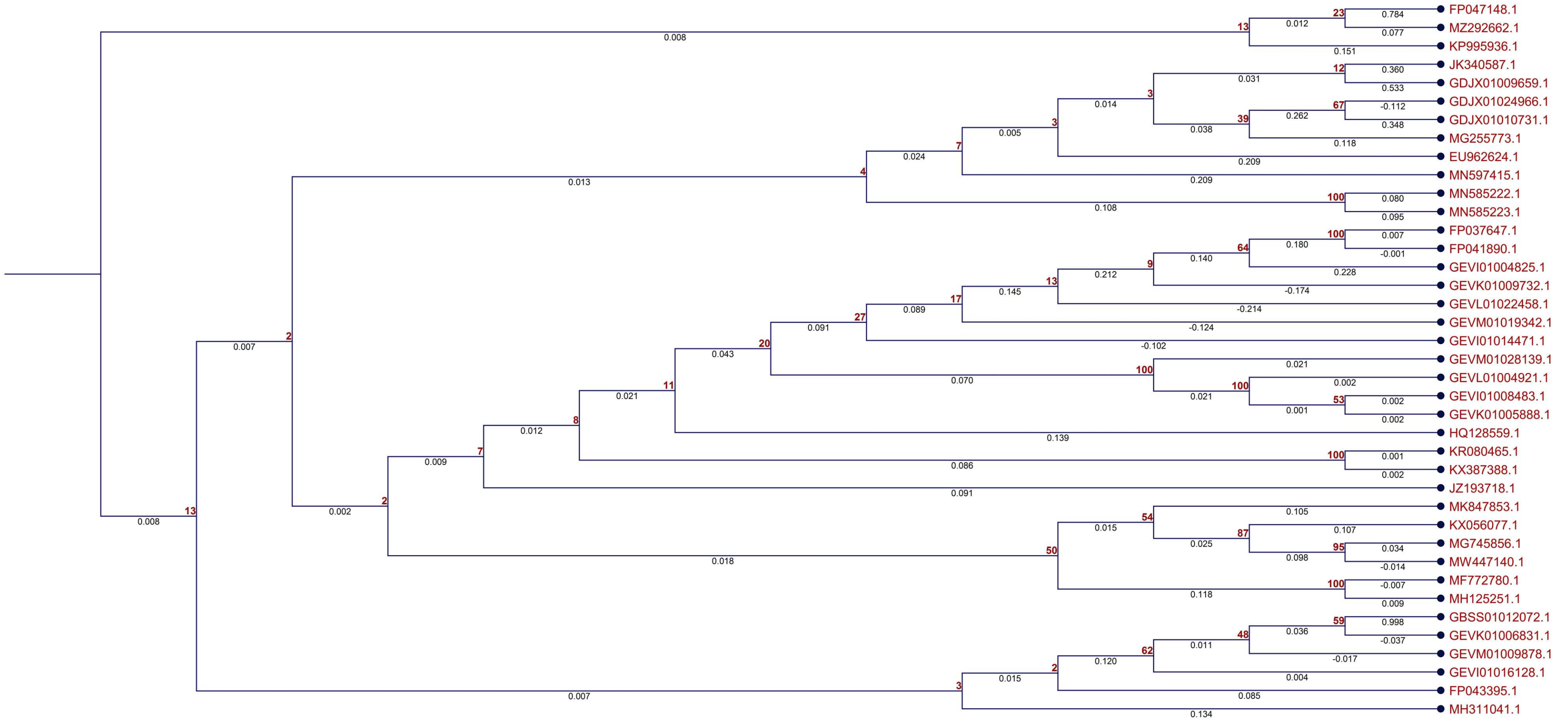
# Mevalonate 5 kinase



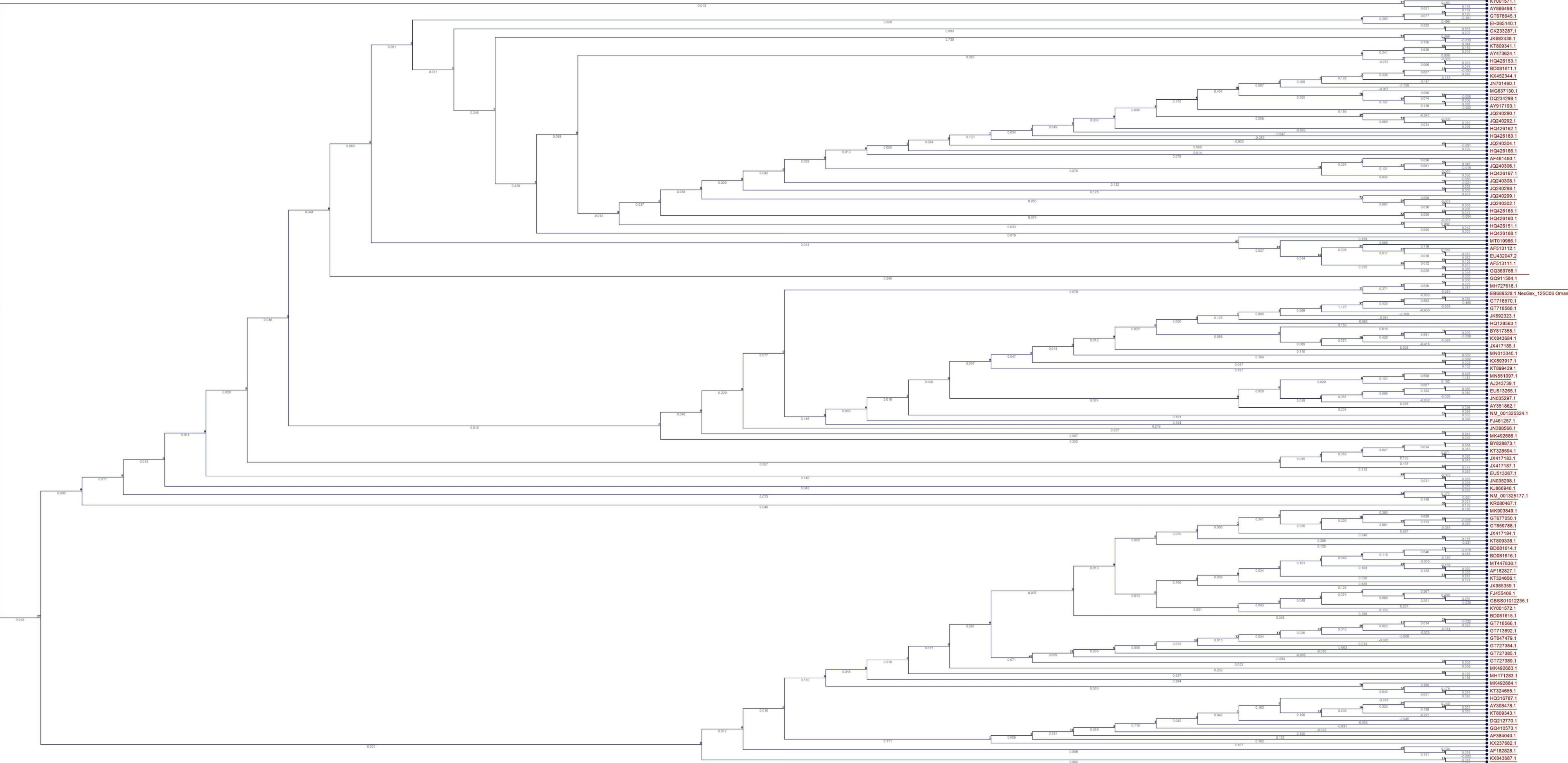
# Phosphomevalonate Kinase



# Diphosphomevalonate decarboxylase

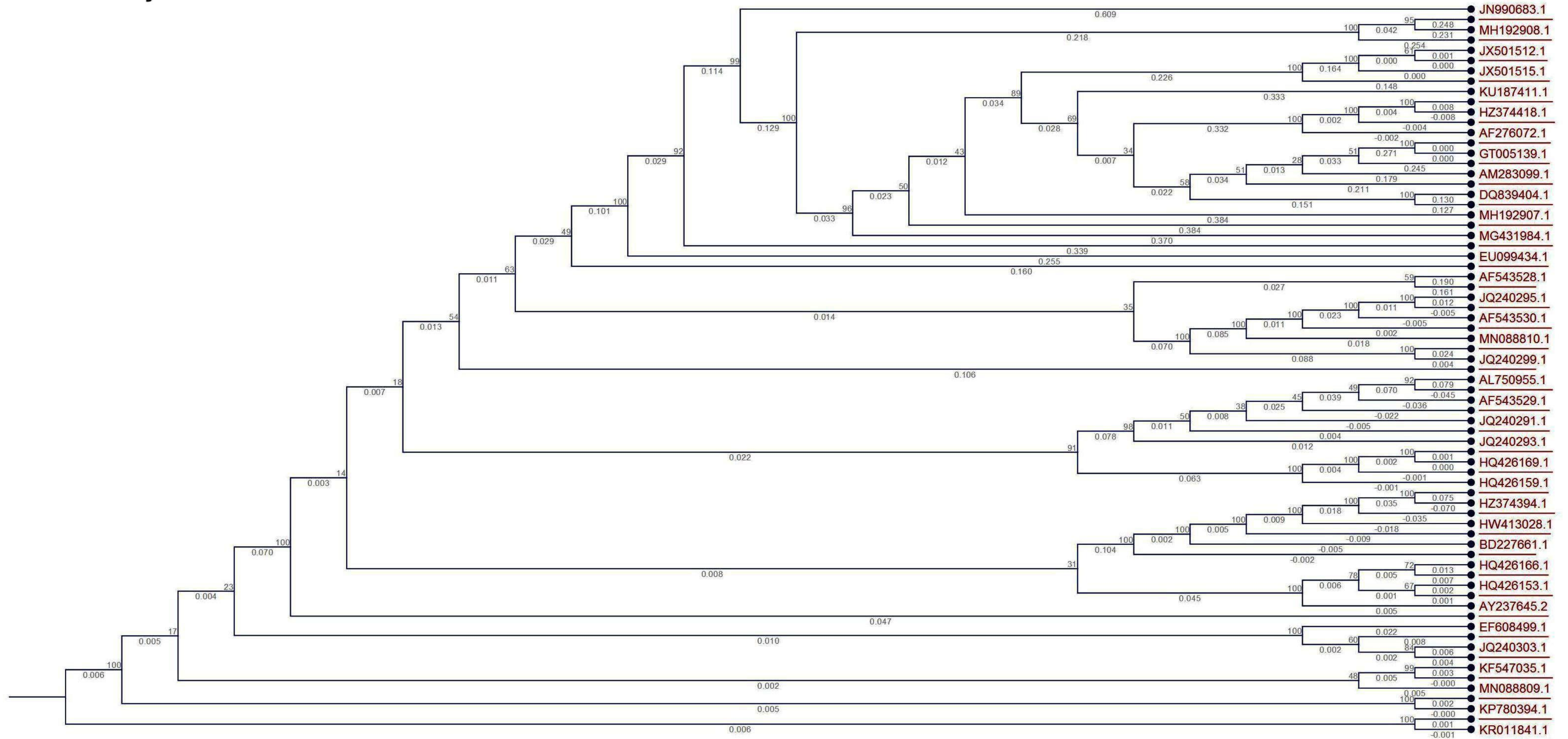


# Geranyl diphosphate synthase



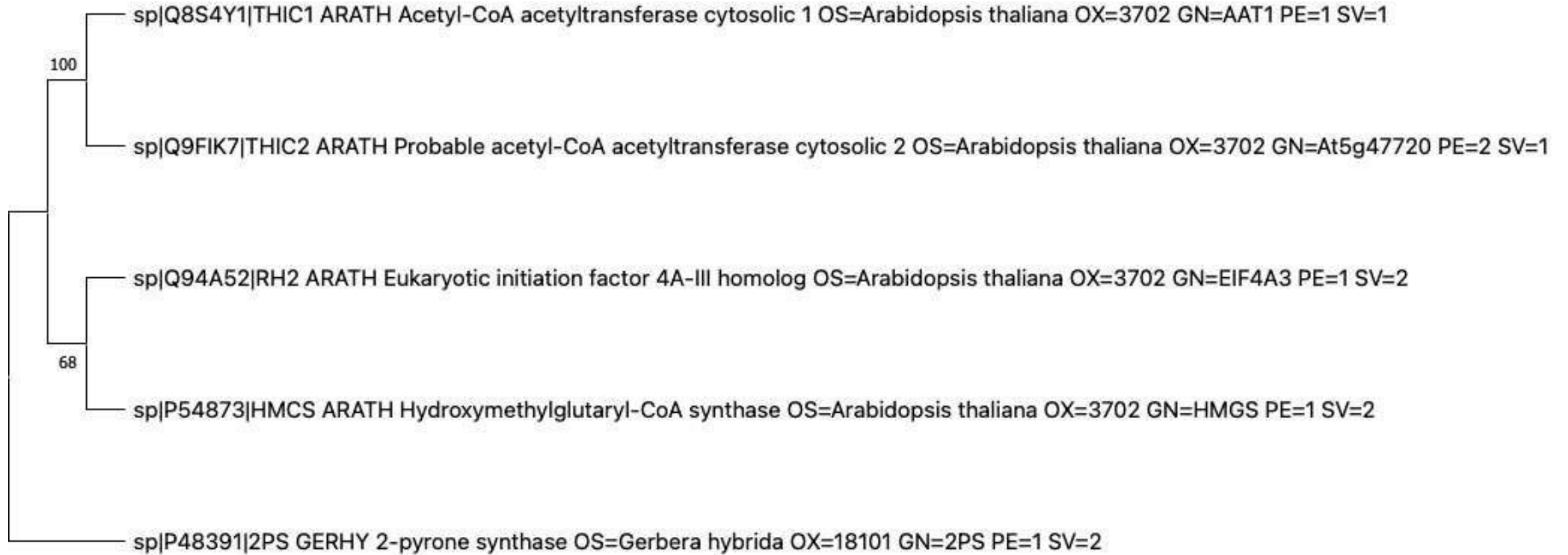


# Pinene synthase



# **UNIPROT PHYLOGENETIC TREES**

## Acetoacetyl CoA thiolase



## HMG CoA synthase

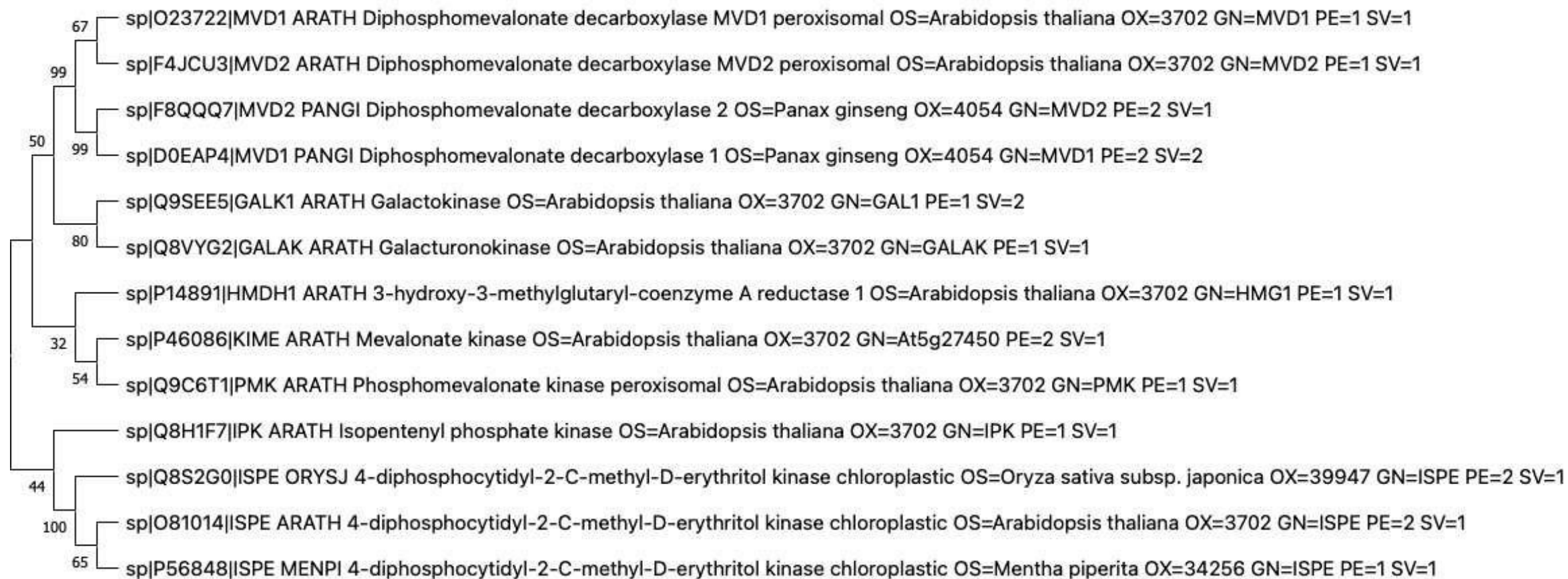
E	sp P43256 HMDH2_ARATH 0.16454
	sp P14891 HMDH1_ARATH 0.1342
	sp Q03163 HMDH_CATRO 0.15495



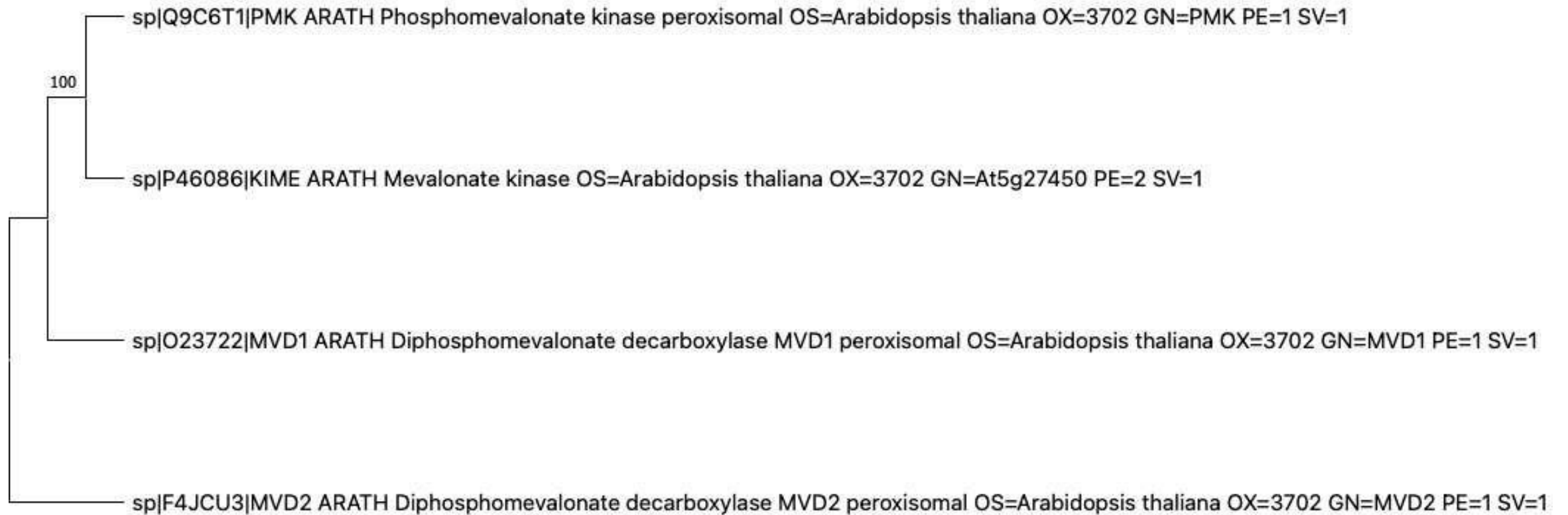
## HMG CoA reductase



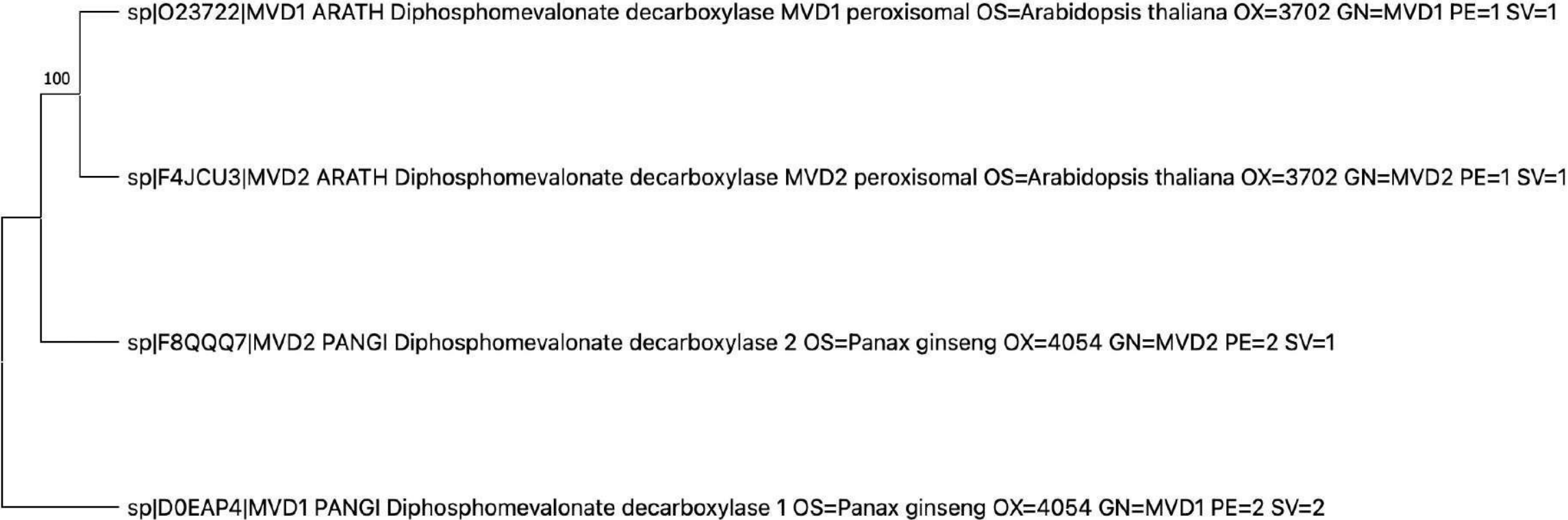
## Mevalonate 5 kinase



## Phosphomevalonate kinase



# Diphosphomevalonate decarboxylase





## Pinene synthase

