Table S1: Known terpenoid synthase structures.

Enzyme (class – family)	Organism (kingdom)	Ligand (mutation)	PDB ID	Ref.
FPP synthase (I – *trans*-IDS)	*G. gallus* (animal)	–	1FPS	11
		(F112A/F113S)	1UBV	13
		GPP, Mg^{2+} (F112A/F113S)	1UBW	13
		FPP, Mg^{2+} (F112A/F113S)	1UBX	13
		DMA, Mg^{2+} (F112A/F113S)	1UBY	13
	E. coli (bacteria)	DST, IPR, PP_i, Mg^{2+}	1RQI	14
		RIS, IPR, Mg^{2+}	1RQJ	14
	S. aureus (bacteria)	–	1RTR	14
	H. sapiens (animal)	RIS, P_i, Mg^{2+}	1YV5	15
		IPR, ZOL, Mg^{2+}	1ZW5	15
		Pi	2F7M	17
		210, Pi, Mn^{2+}	2F89	17
		ZOL, Pi, Mg^{2+}	2F8C	17
		ZOL, IPE, Mg^{2+}	2F8Z	17
		AHD, Pi, Zn^{2+}	2F92	17
		BFQ, Pi, Zn^{2+}	2F94	17
		ZOL, Pi, Zn^{2+}	2F9K	17
GGPP synthase (I – *trans*-IDS)	*S. cerevisiae* (fungi)	Mg^{2+}	2DH4	18
		IPE, Mg^{2+}	2E8U	21
		GPP, Mg^{2+}	2E8X	21
		FPP, PPi, Mg^{2+}	2E90	21
		FPS, IPE, Mg^{2+}	2E8T	21
		GRG	2E8V	21
		ZOL, Mg^{2+}	2E91	21
		MON, Mg^{2+}	2E92	21
		B29	2E93	21
		364, Mg^{2+}	2E94	21
		B75, Mg^{2+}	2E95	21
	H. sapiens (animal)	GRG, Mg^{2+}	2Q80	19
	S. alba (plant)	–	2J1O	20
		GRG	2J1P	20
GPP synthase (I – *trans*-IDS)	*M. piperita*(plant)	Mg^{2+}	3KRA	22
		IPE	3KRC	22
		DST, IPE, PPi, Mg^{2+}	3KRF	22
		DST, IPE, PPi, Mg^{2+}	3KRO	22
		GPP, PPi, Mg^{2+}	3KRP	22
Polyprenyl pyrophosphate synthase (I – *trans*-IDS)	*A. thaliana*(plant)	–	3APZ	25
		FPP, ISY, PPi, Mg^{2+}	3AQ0	25
Octaprenyl pyrophosphate synthase (I – *trans*-IDS)	*T. maritime* (bacteria)	–	1V4E	26
		– (F52A)	1V4H	26
		– (F132A)	1V4J	26
		– (V73Y)	1V4K	26
		– (S77F)	1V4I	26
		– (A76Y)	1VG2	27
		– (A76Y/S77F)	1VG3	27
		– (F132A/L128A)	1VG4	27
		– (F132A/L128A/I123A)	1VG6	27
		– (F132A/L128A/I123A/D62A)	1VG7	27
Hexaprenyl pyrophosphate synthase (I – *trans*-IDS)	*S. solfataricus* (archaea)	– (D81C)	2AZJ	28
		– (W136E)	2AZK	28
		– (F117E)	2AZL	28
	M. luteus (bacteria)	Mg^{2+}	3AQB	29
		2DE, Mg^{2+}	3AQC	29

Undecaprenyl Pyrophosphate Synthase (I – *cis*-IDS)	*M. luteus*(bacteria)	–	1F75	30
	E. coli (bacteria)	EGC	1JP3	31
		FPS, Pi, Mg^{2+}	1X06	32
		IPE, Pi, Mg^{2+}	1X07	32
		FPS, Pi, Mg^{2+} (D26A)	1X08	32
		IPE, Pi, Mg^{2+} (D26A)	1X09	32
		B29	2E98	21
		B08	2E99	21
		B28	2E9A	21
		B75	2E9C	21
		B76	2E9D	21
Z-isoprenyl pyrophosphate synthase (I – *cis*-IDS)	*M. tuberculosis* (bacteria)	–	2VFW	33
		GPP	2VG0	33
		FPP, Pi	2VG1	33
		IPE, PPi, Pi	2VG2	33
		GPP, Pi, Mg^{2+}	2VG3	33
		–	2VG4	33
Squalene synthase (I –CFP)	*H. sapiens* (animal)	IN0	1EZF	35
Pentalene synthase (I – Cyclopropyl forming prenylelongases)	*Streptomyces sp.* (bacteria)	–	1PS1	45
5-Epi-Aristolochene synthase (I – Sesquiterpene synthases)	*N. tabacum*(plant)	Mg^{2+}	5EAS	46
		FHP, Mg^{2+}	5EAT	46
		FFF, Mg^{2+}	5EAU	46
Aristolochene synthases (I – Sesquiterpene synthases)	*P. roqueforti* (fungi)	FOH	1DGP	53
		–	1DI1	53
	A. terreus (fungi)	MES	2E4O	54
		PPi, Mg^{2+}	2OA6	54
		FPP, PPi, Mg^{2+}	3BNX	55
		FPF, Mg^{2+}	3BNY	55
		FDF, PPi, Mg^{2+}	3CKE	55
Trichodiene synthase (I – Sesquiterpene synthases)	*F. sporotrichioides* (fungi)	–	1JFA	59
		PPi, Mg^{2+}	1JFG	59
		– (D100E)	1KIY	60
		PPi, Mg^{2+} (D100E)	1KIZ	60
		Mg^{2+} (R304K)	2AEK	61
		SAZ, PPi, Mg^{2+} (R304K)	2AEL	61
		PPi, Mg^{2+} (R304K)	2AET	61
		Mg^{2+} (N225D)	2PS4	62
		PPi, Mg^{2+} (N225D)	2PS5	62
		– (N225D, S229T)	2PS6	62
		Mg^{2+} (Y295F)	2PS7	62
		PPi, Mg^{2+} (Y295F)	2PS8	62
		– (Y305F)	1YJ4	63
		PPi, Mg^{2+} (Y305F)	1YYQ	63
		SAZ, PPi, Mg^{2+} (Y305F)	1YYR	63
		SAZ, PPi, Mg^{2+} (Y305F)	1YYS	63
		SAZ, PPi, Mg^{2+} (D100E)	1YYT	63
		SAZ, PPi, Mg^{2+} (D100E)	1YYU	63
(+)-D-cadinene synthase (I – Sesquiterpene synthases)	*G. arboretum* (plant)	–	3G4D	65
		FPF, Mg^{2+}	3G4F	65
Epi-isozizaene synthase (I – Sesquiterpene synthases)	*S. coelicolor* (bacteria)	BTM, PPi, Mg^{2+}	3KB9	66
		Hg^{2+}	3KBK	66
		BTM, PPi, Mg^{2+} (F198A)	3LG5	66
		– (D99N)	3LGK	66

α-Bisabolene synthase (I – Sesquiterpene synthases)	*A. grandis* (plant)	FPS, Mg^{2+}	3SAE	67
		–	3SDQ	67
		210, Mg^{2+}	3SDR	67
		AHD, Mg^{2+}	3SDT	67
		GST, Mg^{2+}	3SDU	67
		911, Mg^{2+}	3SDV	67
Limonene synthase (I – Monoterpene synthases)	*M. spicata* (plant)	FPG, Mn^{2+}	2ONG	68
		BTB, F3P, Mn^{2+}	2ONH	68
Bornyl diphosphate synthase (I – Monoterpene synthases)	*S. officinalis* (plant)	Mg^{2+}	1N1B	64
		PPi, Mg^{2+}	1N1Z	64
		3AG, Mg^{2+}	1N20	64
		3AG, Mg^{2+}	1N21	64
		7A8, PPi, Mg^{2+}	1N22	64
		2BN, PPi, Mg^{2+}	1N23	64
		BP2, Mg^{2+}	1N24	64
Cineole synthase (I – Monoterpene synthases)	*S. fruticosa* (plant)		2J5C	74
Isoprene synthase (I – Hemiterpene synthases)	*P. canescens* (plant)	– (N59D/K308R/C533W)	3N0F	5
		DST, Mg^{2+} (N59D/K308R/C533W)	3N0G	5
Taxadiene synthase (I – Diterpene synthases)	*T. brevifolia* (plant)	A3P, Mg^{2+}	3P5P	78
		FGG, Mg^{2+}	3P5R	78
Abietadiene synthase (I – Diterpene synthases/ II – diterpene cyclases)	*A. grandis* (plant)	–	3S9V	79
Squalene-hopene cyclase (II – Squalene-hopene cyclases)	*A. acidocaldarius* (bacteria)	LDA	1SQC	95
Lanosterol synthase (II – Oxido-squalene cyclases)	*H. sapiens* (animal)	BOG, C14, R71	1W6J	102
		BOG, LAN	1W6K	102
Ent-copalyl diphosphate synthase (II – diterpene cyclases)	*A. thaliana* (plant)	AG8	3PYA	105
		A3C	3PYB	105