

**Supplementary Table 1:** Average and standard deviation for each interaction energy (IE) value of filtered docking poses for each P450-substrate combination. The global average IE for docking with the C15-hydroxy and C15,16-dihydroxy substrates suggests that only these two substrate species interact with the P450 active site. CPP = copalyl pyrophosphate.

Substrate	P450	Functional Group		
		C15-pyrophosphate	C15-hydroxy	C15,16-dihydroxy
8,13-CPP	CYP71Z25	-2.4±0.5	-6.5±0.5	-4.8±0.7
	CYP71Z26	-0.9±0.8	-4.6±0.8	-4.5±1.1
	CYP71Z27	-1.6±0.8	-5.8±0.8	-5.2±0.7
	CYP71Z28	-0.4±0.8	-6.1±0.4	-4.3±0.5
	CYP71Z29	-2.2±0.7	-5.5±0.4	-5.0±0.5
(+) -CPP	CYP71Z25	-1.7±0.6	-6.3±0.3	-5.6±0.5
	CYP71Z26	-0.3±1.2	-5.8±0.9	-3.8±0.8
	CYP71Z27	-1.8±0.5	-5.9±0.4	-5.8±0.5
	CYP71Z28	-0.2±0.6	-6.0±0.2	-5.5±0.4
	CYP71Z29	-1.5±0.8	-4.7±0.8	-3.9±0.8
<i>cis-trans</i> -CLPP	CYP71Z25	-1.0±1.1	-5.6±0.4	-4.7±0.6
	CYP71Z26	-0.0±0.9	-5.3±0.8	-4.8±0.8
	CYP71Z27	-1.4±0.5	-5.2±0.5	-5.9±0.9
	CYP71Z28	-0.5±1.0	-4.8±0.3	-5.6±0.2
	CYP71Z29	-1.3±0.9	-5.6±0.2	-5.4±0.4
<i>ent</i> -CPP	CYP71Z25	-1.5±0.4	-6.4±0.2	-5.6±0.2
	CYP71Z26	-0.2±0.9	-5.4±0.7	-3.6±0.6
	CYP71Z27	-1.2±0.6	-6.1±0.5	-6.2±0.4
	CYP71Z28	-0.2±0.5	-5.5±0.4	-4.2±0.5
	CYP71Z29	-0.9±1.3	-5.7±0.7	-3.6±0.8
<i>syn</i> -CPP	CYP71Z25	-1.7±0.5	-6.4±0.4	-5.9±0.6
	CYP71Z26	-0.1±1.1	-5.4±0.7	-5.1±0.7
	CYP71Z27	-0.9±0.5	-6.4±0.7	-6.2±0.5
	CYP71Z28	-0.4±0.8	-5.6±0.4	-5.5±0.4
	CYP71Z29	-1.0±0.7	-5.5±0.6	-5.3±0.4
Average		-0.9±0.9	-5.7±0.5	-5.0±0.8

**Supplementary Table 2:** Synthetic genes used in this study.

**>CYP71Z25**

ATGGCTAAAAAGACATCCTCGAAAGGGAAACTCCCCCAGGGCCTCGCATGCTGCCC  
GTAATTGGGAGCTTACACCATCTCTTGAGTTCACCTCTGCTGTTCCGTGTCTTACGGG  
GTTTAGCGAAAAAGCATGGGCCACTGATGACATTGCGCTTAGGGGAAGTGCCGGCAC  
TGGTTGCGTCAAGCATGGAAGCAGCTCAGGCGATTCTTAAAGTGCACGACACTAATT  
TTGCAGATCGGTTCACTCCTGCGACTTTTGCCACCGTTCGCTTATGGTGGCACCAATCT  
GATATTGTCTCCGTACGGTGAACGGTGGCGGCATTTGAGAAAAATCGTTGTTTCAGGA  
GATGCTTACTGCAACGCGCGTCCAGAGCTTCAAACATATTAGACAGGAGGAAGTCGG  
TCGTTTCTTACACGGAATGGCTGCGAGCGCTGCCGCAGGGACTGCGGTAAACTTCTC  
CACAGCAGTATCTAAACTGATTAACGACGCCTTTCTGCGGGAGTGTGTGCGTTCGTA  
TGTAATATCAGGATGAATTCTTGGACGCCGTTACACGCGTCCCTCTTAGCATCTG  
GGGTGACAATCGCTGATTTGTATCCCTCTAGTAGAATTATGCAGATGCTGGGAACCGC  
ACCTCGTAAAGCCCTGGCGGTAAGACGTCGTGTTGATAGAATCGTTAAACAAATTATC  
CAAGAGGCAAAAAGAAGCAATGGAGTGTGACGATAAGACTGTCGATGATTCTTTTATT  
AGTCTGCTTCTCCGGCTGCAAAAAGAAGGGAGTATGCCGATACCGCTGACGAATGAG  
ACAATAATTGCGTTAATGTTTCGATATGTTGGCTGCGGGATCCGAAACATCATCAACCAC  
CTTGAATTGGGCACTAACTGAACTGATTTCGTAGCCAGCTGCTATGGCGCGCGCCCAA  
GCAGAAGTACGTGAAGCTTTCAAAGGAAAAAGTATTATAACGGATGACGACATCGCC  
AAATCAGGCATTTCTTACCTAAACTCGTGTTCAAGGAAACACTGCGTCTGCATCCGT  
CCTCACCGTTACTGATTCCGCGCCAATGCCGAGAAACCTGTCAGGTTATGGGCTATGA  
TATCCCGAAGGGGACAGCCGTTTTTTGTTAACGTGTGGGCAATTGGGAGAGATCCGTT  
GTACTGGGAAGATCCTGAAGAATTTAAGCCGGAACGGTTTGAACGAACAACCTGG  
ATTCAGAGGAACAAACTTTGAGTTCATACCGTTCGGTGCCTGGTTCGTCGGATGTGTCC  
AGGGATTAATCTGGGTCTGGCTAACATCGAACTTGCTTTAGCTTCCCTTTTATATCATT  
TGACTGGAAATTACCGAAAGGTATGGAACCTAAAGATGTTGAAATGCGTGAGGCTGT  
AGGTATGGTAGCGAGCAAAGAAACCAGCCTGATTGTCCATCCAGTCACATTTATTCCG  
CCTGCCGTTGCGGCGTGA

**>CYP71Z26**

ATGGCGAAAAAAACCTCTAGTAAAGGTAAGTTGCCTCCGGGACCACGGATGCTGCCG  
GTTATCGGATCCTTACACCACTTGCTCAGCTACCGCTGCTGTTCCGAGTTCTGCGGG  
GCCTCGCGAAAAAGCATGGGCCCTTTGATGACCCTACGATTAGGCGAAGTACCAGCTC  
TGGTGGCTAGTTCTATGGAAGCGGCTCAGGCAATTCTCAAAGTGCACGACACGAATT  
TTGCAGATCGGTTCACTCCCGCAACGTTTGCCACGGTGGCTTACGGCGGCACAAATTT  
GATACTAAGTCCATACGGCGAGCGTTGGCGCCATCTGCGTAAGATTGTTGTTTCAGGAG  
ATGCTCACAGCCACACGTGTTTCAGAGCTTTAAACATATCCGCCAGGAGGAGGTAGGC  
AGGTTTTTACAGGGGATGGCAGCATCTGCGGCTGCGGGCACTGCCGTAAACTTTTCC  
ACCGCAGTTAGCAAACCTGATTAACGACGCTTTCTTACGAGAATGCGTAGGCTCACGTT  
GTAAGTATCAAGACGAGTTTCTGGACGCCGTTTCATACGGCCAGTCTGCTGGCAAGTG  
GGGTCACCATCGCCGATCTCTATCCATCTAGTAGGATTATGCAGATGCTGGGAACAGC  
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CAGGAAGCAAAAAGAAGCGATGGAGTGTGACGATAAAACCGTTGACGACTCTTTTATT  
TCGCTGTTACTTCGCTTACAAAAAGAAGGATCGATGCCTATCCCTTTAACCAATGAAA  
CAATTATCGCCCTGATGTTTGACATGCTGGCCGCGGGTAGTGAAACTTCCAGTACAAC  
CCTGAACTGGGCTTTGACCGAGTTAATTCGCAGTCCGGCTGCCATGGCACGCGCCCA  
GGCAGAAGTTCGTGAAGCGTTCAAGGGAAAATCCATCATTACTGATGATGATATTGCA  
AAATCGGGTATTTCTTACCTGAAATTGGTGTTCAGGAAACGCTGAGACTACACCCAT  
CATCCCCTCTGCTGATTCTCGCCAGTGTGCTGAAACCTGTCAGGTGATGGGTTACGA  
TATCCGAAGGGTACTGCTGTATTTGTAAACGCTTGGGCAATTGGTTCGCGATCCGTTG

TATTGGGAAGATCCAGAAGAGTTTAAACCTGAACGCTTTGAAACTAATAACCTCGATT  
TCCGTGGTACTAACTTCGAATTCATACCTTTTGGTGCGGGGAGACGCATGTGTCCGGG  
CATAAACCTGGGGCTGGCGAATATTGAGCTAGCGCTGGCGTCTCTACTCTACCATTTC  
GATTGGAAGTTGCCGAAAGGTATGGAGCCGAAAGATGTGGAAATGAGAGAAGCCAC  
AGGAATGGTAGCTAGCAAAGAAACGAGCCTGATCGTGCATCCCGTAACCTTTATCCCA  
CCGGCGGTGGCGTGA

**>CYP71Z27**

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GTTGCGAGCTCGATGGAGGCCGCCAGGCTATTCTTAAGGTTACGACACGAGCTTC  
GCAGATAGATATACACCTGCGACAAGTGCCACCATCGCTTATGGTGGCACTGATCTCA  
TTCTGAGCCCTTATGGTGAAGATGGCGTCACTTGCGCAAATTTGTGGTACAAGAAAT  
GCTGACTGCAACGAGAGTTCAGTCCTTTAAGTATATCCGCGAAGAGGAGGTCGCTAG  
ATTTTTGCAAGCGATGGCGGCGGCCGCTGCGACAGGGACAGCTGTCGATTTTTCCAC  
AGCAGTGGCTAAACTTGTGAACGACGCCTTTCTACGTGAATGTGTAGGTTCCCGGTG  
CAAATATCAGGACGAATACTTGGATGCAGTACATACCGTCACCCAGCTGGCCAGCGG  
GATAACCATCGCCGATCTGTATCCTTCTCTCGTATTATGCAAATGCTGGGTACAGCCC  
CACGGAAAGGTCTTGCATATCGTCAGCGTATTGACAGAATTTTGAACAGATCATCCA  
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TGAACCTGGGCGATGACCGAACTGATACGTTCTCCGGCTGCAATGGCACGGGCGCAGG  
CAGAGGTTGAGAAAGCTTTTAAAGGTAAATCGATCATTACAGATGACGATATTGCCGA  
AAGCGGCATTAGTTATCTTAAACTGGTCTTCAAAGAAACACTGCGTCTGCATCCCACG  
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TACCAAAGGAATGGCAGTTTTTTGTCAACGTTTGGGCAATTGGCCGTGATCCAAGCT  
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TTCGTGGTACAACTTTGAATTCATTCCGTTTGGAGCCGGTCGTCGCATGTGTCCAGG  
TATAAATCTTGGTCTGGCAAACATCGAACTGGCATTAGCGTCTCTGCTGTATCATTTG  
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GGTATTGTTGCATCAAAGAGACCTCGTTAATTGTACATCCGGTTACGTTTATTCCATT  
GACCGTTGCAGCATAA

**>CYP71Z28**

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TCTGGCAAAAAACATGGTCCGCTGATGACCCTGCGTTTTTGGTGAAGTTCCGGCACT  
GGTTGCAAGCAGCATGGAAGCAGCACAGGCAATTCTGAAAGTTAATGATACCCGTTT  
TGCCGATCGTTTTGCACCGGCAACCAGCGCAACCATTACCTATGGTGCAACCAATCTG  
ATTCTGAGCCCGTATGGTGAACGTTGGCGTCAGCTGCGTAAAATTGTTGTTCAAGAAA  
TGCTGACCACCACACGTGTTTCAAGGCTTTAAACATATTCGTCAAGAAGAAGTTGCC  
GTTTTCTGCAAGGTATGGCAGCAGCAGCCGCAAATGGCACCGCAGTTGATTTTTCAA  
CCGCAAGTTAGCAAACCTGGTGAATGATACCTTTCTGCGTGAATGTGTTGGTAGCCGTTG  
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CGCGTAAAGGTCTGGCATGTCTGTCAGCGTATTGATCGTATTCTGCGTCAGATTATCAA  
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AGAAGTTCGTCAGGCATTTAAAGGTAAAAGCATCATTACCGATGATGACATGGCCAAA  
TCAGGTATCAGCTATCTGAAACTGGTGTTCAAAGAAACCCTGCGTCTGCATCCGACCT  
CACCGCTGCTGATTCCGCGTCAGTGTTCGTGAAACCTGTCAGGTTATGGGTTATGATATT  
CCGAAAGGTACAGCCGTTTTTGTAAATGTTTGGGCAATTGGTCGTGATCCGAGCTATT  
GGGAAGATGCAGAAGATTTTAAACCGGAACGCTTTGAAACCAACAATCTGGATTTTC  
GTGGCACCAACTTTGAATTTATTCCGTTTGGTGCAGGTCGTCGTATGTGTCCGGGTATT  
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GAAACTGCCGAAAGGCATGGAACCGAAAGATGTGGATATGCGCGAAGTTGTTGGTAT  
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GTTGTTAA

**>CYP71Z25:MRS**

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TGTTGCGTCAAGCATGGAAGCAGCTCAGGCGATTCTTAAAGTGCACGACACTAATT  
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GATGCTTACTGCAACGCGCGTCCAGAGCTTCAAACATATTAGACAGGAGGAAGTCGG  
TCGTTTCTTACACGGAATGGCTGCGAGCGCTGCCGCAGGGACTGCGGTAAACTTCTC  
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TGACTGGAAATTACCGAAAGGTATGGAACCTAAAGATGTTGAAATGCGTGAGGCTGT  
AGGTATCGTAGCGAGCAAAGAAACCAGCCTGATTGTCCATCCAGTACATTTATTCCG  
CCTGCCGTTGCGGCGTGA

**>CYP71Z27:MRS**

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GTCATTGGAAGTCTTCATCATTAGTGTTCGTACCGTATTGTTTCGTGTACTGAGGGA  
ACTGGCTAAAAACATGGTCCTTTAATGATGTTACGCTTAGGGGAGGTTCCAGCTCTG  
GTTGCGAGCTCGATGGAGGCCGCCAGGCTATTCTTAAGGTTACGACACGAGCTTC  
GCAGATAGATTTACACCTGCGACATTTGCCACCGTCGCTTATGGTGGCACTAATCTCAT  
TCTGAGCCCTTATGGTGAAGATGGCGTCACTTGCGCAAATTTGTGGTACAAGAAAT  
GCTGACTGCAACGAGAGTTCAGTCCCTTAAAGTATATCCGCGAAGAGGAGGTCGCTAG  
ATTTTTGCAAGCGATGGCGGCGGCCGCTGCGACAGGGACAGCTGTTCGATTTTTCCAC  
AGCAGTGGCTAAACTTGTGAACGACGCCTTTCTACGTGAATGTGTAGGTTCCCGGTG  
CAAATATCAGGACGAATACTTGGATGCAGTACATACCGTCTCCCTGCTGGCCAGCGGG  
ATAACCATCGCCGATCTGTATCCTTCTTCGTATTATGCAAATGCTGGGTACAGCCCC  
ACGGAAGCTCTTGCAGTTCGTTCGTATTGACAGAATTGTGAAACAGATCATCCA

GGAAGCGAAAGAAGCTATGGAATGCGAAGACGAGACCGCTCATGAATCTTTTGTAAG  
TTTATTACTTCGGCTGCAAAAAGACGGGTCCATGCCTATCCCGCTGACGAACGAAACC  
ATAATCGCACTGATGTTTGATATGCTGGCCGCAGGAAGCGAAACCTCAAGTACCACTC  
TGA ACTGGGCGCTGACCGAACTGATACGTTCTCCGGCTGCAATGGCACGGGCGCAGG  
CAGAGGTTTCGAGAAGCTTTTAAAGGTAAATCGATCATTACAGATGACGATATTGCCGA  
AAGCGGCATTAGTTATCTTAAACTGGTCTTCAAAGAAACACTGCGTCTGCATCCCTCG  
TCTCCTTTACTCATACCACGTCAATGTCTGGGAGACATGTCAAGTTATGGGGTACGACA  
TACCAAAGGAATGGCAGTTTTTGTCAACGTTTGGGCAATTGGCCGTGATCCAAGCT  
ATTGGGATGACCCGGAAGAATTCAAACCGGAACGTTTCGAGACCAATAATCTGGACT  
TTCGTGGTACAACTTTGAATTCATTCCGTTTGGAGCCGGTCGTCGCATGTGTCCAGG  
TATAAATCTTGGTCTGGCAAACATCGAACTGGCATTAGCGTCTCTGCTGTATCATTTG  
ATTGGAACTGCCCAAAGGAATGGAACCGAAGGATGTGGATATGAGAGAAGCAGTA  
GGTATGGTTGCATCAAAGAGACCTCGTTAATTGTACATCCGGTTACGTTTATTCCATT  
GACCGTTGCAGCATAA

**Supplementary Table 3:** Oligonucleotides used in this study.

Primer name	Sequence (with mutated position underlined)
CYP71Z25-F86S-F	CGGTTCACTCCTGCGACT <u>T</u> CTGCCACCGTCGCTTAT
CYP71Z25-F86S-R	ATAAGCGACGGTGGC <u>A</u> GAAGTCGCAGGAGTGAACCG
CYP71Z27-S86F-F	AGATATACACCTGCGAC <u>A</u> TTTGCCACCATCGCTTAT
CYP71Z27-S86F-R	ATAAGCGATGGTGGC <u>A</u> AATGTCGCAGGTGTATATCT
CYP71Z25-N95D-F	GTCGCTTATGGTGGCACC <u>G</u> ATCTGATATTGTCTCCG
CYP71Z25-N95D-R	CGGAGACAATATCAG <u>A</u> TCGGTGCCACCATAAGCGAC
CYP71Z27-D95N-F	ATCGCTTATGGTGGCA <u>T</u> AATCTCATTCTGAGCCCT
CYP71Z27-D95N-R	AGGGCTCAGAATGAG <u>A</u> TAGTGCCACCATAAGCGAT
CYP71Z25-E283D-F	ATGTTGGCTGCGGGATCC <u>G</u> ATACATCATCAACCACC
CYP71Z25-E283D-R	GGTGGTTGATGATG <u>T</u> ATCGGATCCCGCAGCCAACAT
CYP71Z27-D283E-F	ATGCTGGCCGCAGGAAGC <u>G</u> AAACCTCAAGTACCATT
CYP71Z27-D283E-R	AATGGTACTTGAGGTTTCGCTTCCTGCGGCCAGCAT
CYP71Z25-T288I-F	TCCGAAACATCATCAACC <u>A</u> CTTGAATTGGGCACTA
CYP71Z25-T288I-R	TAGTGCCCAATTCAAG <u>A</u> TGGTTGATGATGTTTCGGA
CYP71Z27-I288T-F	AGCGACACCTCAAGTACC <u>A</u> CTCTGAACTGGGCGATG
CYP71Z27-I288T-R	CATCGCCAGTTCAG <u>A</u> GTGGTACTTGAGGTGTCGCT
CYP71Z25-S346T-F	ACACTGCGTCTGCATCC <u>G</u> ACCTCACCGTTACTGATT
CYP71Z25-S346T-R	AATCAGTAACGGTGAG <u>G</u> TCGGATGCAGACGCAGTGT
CYP71Z27-T346S-F	ACACTGCGTCTGCATCC <u>C</u> TCGTCTCCTTTACTCATA
CYP71Z27-T346S-R	TATGAGTAAAGGAGAC <u>G</u> AGGGATGCAGACGCAGTGT
CYP71Z25-S347T-F	CGTCTGCATCCGTCC <u>A</u> CTCCGTTACTGATTCCG
CYP71Z25-S347T-R	CGGAATCAGTAACGG <u>A</u> GTGGACGGATGCAGACG
CYP71Z27-S347T-F	CGTCTGCATCCACG <u>A</u> CTCCTTTACTCATAACCA
CYP71Z27-S347T-R	TGGTATGAGTAAAGG <u>A</u> GTTCGTGGGATGCAGACG
CYP71Z25-M463I-F	CGTGAGGCTGTAGGT <u>A</u> TTGTAGCGAGCAAAGAA
CYP71Z25-M463I-R	TTCTTTGCTCGCTACA <u>A</u> TACCTACAGCCTCACG
CYP71Z27-I463M-F	AGAGAAGCAGTAGGT <u>A</u> TGGTTGCATCAAAAGAG
CYP71Z27-I463M-R	CTCTTTTGATGCAACC <u>A</u> TACCTACTGCTTCTCT

**Supplementary Table 4:** Abbreviations and Accession numbers for proteins used for phylogenetic studies.

<b>Protein name</b>	<b>Species</b>	<b>Accession</b>
OsCYP71Z6	<i>Oryza sativa</i>	A3A871
OsCYP71Z7	<i>Oryza sativa</i>	Q6YV88
ZmCYP71Z16	<i>Zea mays</i>	Zm00001d014136
ZmCYP71Z18	<i>Zea mays</i>	Zm00001d014134
OsCYP76M6	<i>Oryza sativa</i>	XP_015625955
OsCYP76M7	<i>Oryza sativa</i>	XP_015623593
OsCYP99A3	<i>Oryza sativa</i>	XP_015634021
OsCYP701A6	<i>Oryza sativa</i>	XP_015643248
OsCYP701A8	<i>Oryza sativa</i>	XP_015640905
ZmCYP701A26	<i>Zea mays</i>	Zm00001d046342
ZmCYP701A43	<i>Zea mays</i>	Zm00001d046344
PvCYP71Z25	<i>Panicum virgatum</i>	Pavir.1KG341400 <sup>1</sup>
PvCYP71Z26	<i>Panicum virgatum</i>	Pavir.1KG382300 <sup>1</sup>
PvCYP71Z27	<i>Panicum virgatum</i>	Pavir.1KG382400 <sup>1</sup>
PvCYP71Z28	<i>Panicum virgatum</i>	Pavir.1NG304500 <sup>1</sup>
PvCYP71Z29	<i>Panicum virgatum</i>	Pavir.1NG309700 <sup>1</sup>
PhA02218	<i>Panicum hallii</i>	Pahal.1G276500 <sup>2</sup>
PhA02220	<i>Panicum hallii</i>	Pahal.1G276700 <sup>2</sup>

<sup>1</sup> Accession number for *Panicum virgatum* genome assembly v4.1 ([www.phytozome.org](http://www.phytozome.org))

<sup>2</sup> Accession number for *Panicum hallii* genome assembly v3.1 ([www.phytozome.org](http://www.phytozome.org))